Appendix A

Protocols for the HET-CAM Test Method

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Appendix A1

INVITTOX Protocol 47. The HET-CAM Test – Method of Spielmann and Liebsch

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HET-CAM TEST

The potential irritancy of compounds may be detected by observing adverse changes which occur in the chorionallantoic membrane of the egg after exposure to test chemicals.

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Rationale

Chemicals are placed directly onto the chorionallantoic membrane of the hen's egg. The occurrence of vascular injury or coagulation in response to a compound is the basis for employing this technique as an indication of the potential of a chemical to damage mucous membranes (in particular the eye) *in vivo*.

Basic Procedure

Hen's eggs are rotated in an incubator for 9 days after which time any defective eggs are discarded. The shell around the air cell is removed and the inner membranes are extracted to reveal the chorionallantoic membrane. Test chemicals are added to the membrane and left in contact for 5 minutes. The membrane is examined for vascular damage and the time taken for injury to occur is recorded. Irritancy is scored according to the severity and speed at which damage occurs.

Critical Assessment

The test has several advantages including its simplicity, rapidity, sensitivity, ease of performance and its relative cheapness.

A factor to consider is the fertility and the ability of the eggs to hatch. The survival of chickens is dependent on a complex interrelationship of ecological factors (e.g. the genetic background and the age of the mated birds, the nutritional status and general management of the flock, and in part seasonal variations). Eggs should, therefore, be obtained from reliable local contractors. (The authors have produced some empirical data on the fertility of the particular flocks they use. The fertility of middle-aged flock is approximately 90% with 10-15% defective eggs. On average there are 20% lesions produced during preparation.)

The major disadvantage of the procedure is the subjective nature of the evaluation of the results. This is overcome to a certain extent by the inclusion of positive standards and by using a comprehensive scheme for scoring the irritant effects of the chemicals.

The exposure period of 5 minutes to the test chemical has been found to be sufficient to reveal irritant/toxic effects (longer exposure does not appear to yield any additional information).
A factor for consideration is whether the Hen's egg test may be considered as an animal experiment. At present the test is often looked upon as being borderline, although it has potential to be used in a manner likely to reduce the number of mammals used in conventional testing and also to contribute towards a reduction in the associated suffering.

Test Status

This test, along with several other *in vitro* systems, is presently undergoing validation as an alternative test to replace the Draize Rabbit Eye Test, in a national interlaboratory study started in June 1988, by the Federal Health Office (BGA) of the Federal Republic of Germany (FRG).

The aim of this collaborative study is to validate the classification of chemicals, with regard to their irritation potential, using the Neutral Red/ Kenacid Blue (NR/KB) cytotoxicity assay and the Hen's Egg Test Chorioallantoic Membrane (HET-CAM) assay according to Lupke. The FRG Public Health Office (BGA) is coordinating the scheme which includes, 12 toxicology laboratories in the chemical industry, universities, the BGA and other research institutions who will study 44 substances with a variety of chemical, biochemical, and toxicological characteristics. The validation test is intended to provide comparative data for the development of an alternative routine test scheme, and which is performed under routine laboratory conditions.

The validation project of alternatives for the Draize test consists of three parts: a preliminary phase, an interlaboratory assessment, and, finally, the development of a database of results. During the preliminary phase the cytotoxicity test and the HET-CAM assay have been established in the different laboratories. The participants have agreed on standard and mandatory protocols and on the choice of chemicals. Two preliminary trials have been performed with 4 test substances.

During the interlaboratory assessment 35 chemical substances of a variety of chemical structure groups have been tested with both alternative techniques in 12 laboratories under conditions that will be defined in the preliminary phase of the study. The main purpose of the validation phase is the comparative and statistical evaluation of all data at the BGA followed by a final scientific validation which could prove of interest to regulatory authorities. This assessment determines both the reproducibility of the results within a given laboratory and of a given test between laboratories.

Preliminary findings indicate that data from the HET-CAM test appears to correlate better than the two cytotoxicity tests when compared to *in vivo* Draize scores. The cytotoxicity tests give a greater number of false positives and negatives compared to the HET-CAM test. The cytotoxicity tests have, however, given better reproducibility of test data, within and between laboratories, than the HET-CAM. This is most probably due to the automated determination of NR and KB values and to the highly subjective determination of the toxicological endpoints in the HET-CAM test which are difficult to standardize. In conclusion, both the cytotoxicity tests and the HET-CAM test can provide reproducible results if carried out under routine conditions with well trained operators.

The third phase of the validation project, database development, commenced on June 1st, 1990. Seven laboratories are testing a total of 200 chemicals which again include a variety of chemical classes.

Chemicals Tested

Acetone Acetonitrile Acrylamide Aniline Ascorbic acid Benzalkonium chloride (0.5%) Benzoic acid 2-Butoxyethanol Copper(*II*) sulphate Cyclohexanol DEHP (100%) Dimethylsulphoxide EDTA-Na salt Ethanol	Lactic acid (5%) *n*-Hexane Nicotinamide Nitrobenzene Phenol Propanediole 2-Propane-1-ol Pyridine SDS (1%) Sodium chloride Tetrachloroethane Thiourea Toluene

References

Lüpke, N.P. (1986)
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Kalweit, S., Besolke, R., Gerner, I. & Spielmann, H. (1990)
A national validation project of alternative methods for the Draize rabbit eye test.
Toxic. in Vitro, **4**, 702-706.

Spielmann, H., Gerner, I., Kalweit, S., Moog, R., Wirnsberger, T., Krauser, K., Kreiling, R., Kreuzer,H., Lupke, N.P. Miltenburger, H.G. Muller, N. Murmann, P. Pape, W. Siegmund, B. Spengler, J. Steiling, W. & Wiebel, F.J. (1991)
Interlaboratory assessment of alternatives to the Draize eye irritation test in Germany.
Toxic. in Vitro, **5 No.5/6**, 539-542.

Procedure Details

Note: The herewith included details on the procedure have been sent to the person responsible for the method to update or confirm it. As soon as new information will become available this version will be updated.

Animal
White Leghorn chicken eggs (Shaver Starcross 288A)
The White Leghorn chicken has been selected for several reasons;
The ability to hatch the eggs of this breed is very consistent and reproducible. There does not appear to be any hereditary defects in this

breed.

Equipment

Incubator with an automatic rotating device, e.g. Ehret GmbH, 220 V, 50 Hz, 360 watt
Optimum temperature: 37.5^{0}C (± 0.5^{0}C)
Relative humidity 62.5% (± 7.5%)

Candling light
Dentist's rotating sawblade
Computer with appropriate software (HET-CAM evaluation program) - not commercially available (authors will give assistance to interested scientists)
Cold-light lamp
pH-meter
Thermometers
Tapered forceps
Pipettes (300µl application)
Stopclock

Materials

NaCl
SDS
0.1 N NaOH

Make up the following solutions:
0.9% NaCl solution in distilled water
1% SDS solution in distilled water

Test chemicals
Make up the chemicals in 0.9% NaCl solution or olive oil.

Method

N.B. Avoid any shaking, unnecessary tilting, knocking, and all other mechanical irritation of the eggs when preparing them for the assay.

Incubation of eggs
Select fresh fertile 50-60g eggs. Candle the eggs and discard any which are defective.

Place the eggs flat onto incubator trays in a 37.5^{0}C incubator and rotate for 8 days to prevent the attachment of the embryo to one side of the egg.
Check the temperature and humidity at the same time each day.
Candle the eggs on the 9th day and discard any non-viable eggs.
Replace in the incubator with the large end upwards but do not rotate, thus ensuring accessibility to the chorionallantoic membrane.
On day 10 prepare the eggs for assaying.

Assay preparation
Candle each egg to ensure that all are viable. Use cold lamp to ensure an optimal illumination of the chorioallantoic membrane.

Carry out in a fume cupboard with safety goggles to prevent inhalation and contact with the fine egg shell powder. Mark the air cell using a rotating dentist-sawblade and pare the section of the shell off.

Carefully moisten the membrane with 0.9% NaCl solution at 37^0C.

Replace eggs in incubator until ready for assaying (maximum of 30 minutes between opening the eggs and starting the assay).

Freshly prepare standards and test solution (in the appropriate solvent) before each assay at room temperature. Measure and record ph.

Assay procedure
Take the opened egg out of the incubator, pour off the 0.9% NaCl solution, carefully remove the egg membrane without injuring any underlying blood vessels using tapered forceps.

Add 0.3ml of the standard, or test chemical solution to the CAM.

Observe the reactions on the CAM over a period of 5 minutes. Monitor the appearance of:

haemorrhage (Bleedings)
vascular lysis (Blood vessel disintegration)
coagulation (protein denaturation intra- and extra vascular)

Record in seconds, the time for each reaction to occur and calculate an **irritation score (IS)**.

$$IS = \frac{301 - sec\ H}{300} \cdot 5 + \frac{301 - sec\ L}{300} \cdot 7 + \frac{301 - sec\ C}{300} \cdot 9$$

H : Haemorrhage
L : Vessel lysis
C : Coagulation
sec : Start Second

When determining the threshold the degree of severity of each reaction after treatment time has to be recorded according to the following scheme:
0 = no reaction
1 = slight reaction
2 = moderate reaction
3 = severe reaction

The threshold is then defined to be the highest concentration, at which slight reactions occur. To determine the threshold apply 0.3ml of the starting concentration (a good choice is 5% if no further information is given) to three eggs each. Graduate the severity of the main reaction after 5 minutes. If the observed reaction is slight , double the concentration. If the reaction is moderate or severe, divide the concentration by two or ten to get the next test concentration. Proceed further until the threshold concentration is found.

Test Scheme
For a given chemical the procedure consists of four steps:
1) Determine the irritation score (IS) for the two standards with two eggs

each.

N.B. 1% SDS should give an IS of 10±2 and 0.1 NaOH an IS of 15±3.

2) Determine the threshold concentration of the test chemical as described above.

3) Determine the IS for a 10% solution for three eggs. For insoluble substances take the supernatant of a standard solution.

4) Determine the IS for the pure substance (100%). If the test chemical is an insoluble solid substance, proceed as follows: Instead of determining the IS, put some grains of the substance onto the CAM to cover approximately half of its surface. After 5 minutes carefully rinse off the test material with NaCl solution and record the severity of each of the three reactions (haemorrhage, lysis, coagulation) according to:
0 = no
1 = slight
2 = moderate
3 = severe

If any reaction of degree 3 has been observed, repeat the procedure with three new eggs, rinsing after one minute.

At the end of the assay kill the embryos as quickly as possible (e.g. by placing the eggs into a freezer at -20^{0}C).

Calculations and Classifications
Calculate the mean value of the IS for the three eggs for each of the two runs and both concentrations as well as the mean over both runs of the IS and threshold concentration.

A classification of the irritating potential can be carried out according to the following (preliminary) classification scheme.

Threshold (TH) concentration	Irritation score (10%)	Severity	Classification
TH < 1%			severe/corr
1.0 < TH < 2.5	> 16		severe/corr.
2.5 < TH < 10.0	< 16	severe reaction after 1 min.	severe/corr.
1.0 < TH < 2.5	< 16		irritant
2.5 < TH < 10.0	> 16		irritant
2.5 < TH < 10.0	< 16	severe reaction after 5 min	irritant
2.5 < TH < 10.0	< 16	weak or no reaction	moderate
10.0 < TH	> 16		moderate
10.0 < TH	< 16	severe reaction	moderate
10.0 < TH	< 10		no/slight

Experimental Data

Preliminary results of the interlaboratory study are published in:
Spielmann, H. *et al.* (1991): Interlaboratory assessment of alternatives to the Draize eye irritation test in Germany. *Toxic. in Vitro*, **5 No. 5/6** , 539-542.

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Appendix A2

Table of HET-CAM Protocols from the Reviewed Literature

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	Luepke 1985	Luepke and Kemper (1986)	Kalweit et al. (1987)	Reinhardt et al. (1987)	Kalweit et al. (1990)
Hen Strain	White Leghorn (Shaver Starcross 288A, Lohmann Selected Leghorn LSL)	Lohmann Selected Leghorn, LSL	White Leghorn	Not Noted	White Leghorn
Egg Criteria for Use	Prior to use, eggs are candled to remove defective eggs. Eggs weighing < 50 g or > 60 g are rejected	Not Noted	Not Noted	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.5 $\pm$ 0.5	Not Noted	38	Not Noted	38
Relative Humidity (%)	62.5 $\pm$ 7.5	Not Noted	60	Not Noted	60
Egg Rotation?	Yes	Not Noted	Yes	Not Noted	Yes
Checking Egg Viability	Eggs candled on Day 5 and every day thereafter; non-viable embryos removed	Not Noted	Eggs candled on Day 9 and non-viable embryos removed	Not Noted	Eggs candled on Day 9 and non-viable embryos removed
Incubation Period	10 Days	10 Days	9 Days	10 Days	9 Days
Procedure for Opening Egg	Eggshell is scratched around the air cell by a dentist's rotary saw and then pared off. After removal of the inner egg membranes, the CAM is exposed.	Eggshell is scratched around the air cell by a dentist's rotary saw and then pared off. After removal of the inner egg membranes, the CAM is exposed.	Eggshell is scratched around the air cell and opened. After removal of shell, the CAM is exposed.	Not Noted	Eggshell is scratched around the air cell and opened. After removal of shell, the CAM is exposed.
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Vehicles, antimicrobial agents, oxidation dyes, shampoos, pyrithones, phenols, and isothiazolinones	Substances and formulations	Chemicals from various chemical classes	Surfactants	Chemicals from various chemical classes
Total Test Substances Evaluated	37	190	44	12	5
Test Substance Quantity or Volume	0.2 mL or 0.1 g	0.2-0.3 mL or 0.1 g	0.3 mL	Not Noted	0.3 mL
Test Substance Concentrations Tested	0.1%-100%	Tested concentrations not noted	Various concentrations tested. Solutions of 0.05 to 100% (w/v) tested.	300 mM or 10% mixtures	1% and 10% solution

	Luepke 1985	Luepke and Kemper (1986)	Kalweit et al. (1987)	Reinhardt et al. (1987)	Kalweit et al. (1990)
Application of Solids to CAM	Placed directly on CAM	Placed directly on CAM	All tested substances appear to be solubilized	All tested substances appear to be solubilized	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	Yes, 20 seconds after test substance applied rinsed with 5 mL warm water	Yes, 20 seconds after test substance applied rinsed with 5 mL warm water	Not Noted	Not Noted	Not Noted
Evaluation Period	At 0.5, 2, and 5 minutes after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	Between 0.5 and 5 minutes after test substance applied	Up to 300 seconds after test substance applied
Controls and Test Standards	Vehicle	Not Noted	Not Noted	SDS	Not Noted
Number of Control Eggs	2 eggs	Not Noted	Not Noted	Not Noted	Not Noted
Replicate Eggs	4 eggs	4 eggs	Not Noted	6 eggs	6 eggs per concentration
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	Not Noted	4
Endpoints Assessed	Hyperemia, hemorrhage, coagulation	Injection, hemorrhage, coagulation	Hemorrhage, vessel lysis, coagulation	Not Noted	Hemorrhage, lysis, coagulation
Endpoint Evaluation	Numerical time-dependent scores for each of the three endpoints. Scoring scheme is noted below.	Numerical time-dependent scores for each of the three endpoints. Scoring scheme is same as Luepke (1985).	The starting second that each of the three endpoints is observed is recorded.	Not Noted	The starting second that each of the three endpoints is observed is recorded.
Analysis Method	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Irritation Index is calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second	Not Noted	Irritation Index is calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second

	Luepke 1985	**Luepke and Kemper (1986)**	**Kalweit et al. (1987)**	**Reinhardt et al. (1987)**	**Kalweit et al. (1990)**
Classification Scheme	**Non Irritation**: <0.5; **Slight Irritant**: 0.5-3.4; **Moderate Irritant**: 3.5-4.9; **Severe Irritant**: ≥5	**Non Irritation**: <0.5; **Slight Irritant**: 0.5-3.4; **Moderate Irritant**: 3.5-4.9; **Severe Irritant**: ≥5	**Non Irritation**: <0.5; **Slight Irritant**: 0.5-3.4; **Moderate Irritant**: 3.5-4.9; **Severe Irritant**: ≥5	**Non Irritation**: <0.5; **Slight Irritant**: 0.5-3.4; **Moderate Irritant**: 3.5-4.9; **Severe Irritant**: ≥5	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes			Cites Luepke (1985) as basis for protocol	Cites Luepke (1985) as basis for protocol and analysis method	

	Lawrence et al. (1990)	Sterzel et al. (1990)	van Erp et al. (1990)	Blein et al. (1991)	CEC (1991)	Hagino et al. (1991)	Gettings et al. (1991)
Hen Strain	Not Noted	Not Noted	Not Noted	White Leghorn	Lohmann Selected Leghorn	White Leghorn	Lohmann's Selected White Leghorn LSL
Egg Criteria for Use	Not Noted	Not Noted	Not Noted	Not Noted	Weight range of eggs between 50 g and 60 g	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	Not Noted	Not Noted	Not Noted	37.5 $\pm$ 0.5	37.5 $\pm$ 0.5	37.6	Not Noted
Relative Humidity (%)	Not Noted	Not Noted	Not Noted	62.5 $\pm$ 7.5	62.5 $\pm$ 7.5	about 70	Not Noted
Egg Rotation?	Yes	Not Noted	Yes, once each hour	Not Noted	Yes	Yes, once per hour	Not Noted
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted	Eggs candled on Day 5 and every day thereafter; non-viable embryos removed	Not Noted	Not Noted
Incubation Period	10 Days	9 Days	10 Days	10 Days	10 Days	10 Days	10 Days
Procedure for Opening Egg	Eggshell over the air space was removed with a small rotary cutter on Day 10. Small drop of water placed and spread over the shell membrane to aid in removal of the membrane without damaging the CAM.	Egg shell was scratched above the air chamber with a dentist's rotary saw blade and piece of the shell removed.	Shell with the attached membrane was removed up to the margin of the air chamber. The inner egg membrane was the eliminated to expose the CAM.	Eggshell pierced in the region of the air chamber to expose CAM.	Egg shell was scratched around the air chamber with a rotating dentist saw blade and then pared off. The inner shell was removed and the CAM was layed open.	Eggshell above air space was removed. Drop of water was placed on shell membrane to avoid capillary bleeding. CAM was exposed using forceps.	Not Noted
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Commercial and industrial products	Fatty acid derivatives	Chemicals from various chemical classes	Chemicals from various chemical classes	Chemicals from various chemical classes	Surfactants (cationic, anionic, non ionic,) and amphoteric agents	Hydro-alcoholic formulations
Total Test Substances Evaluated	34	10	147	40	21	12	10
Test Substance Quantity or Volume	0.2 mL or 0.1 g	0.3 mL	0.2 mL	Not Noted	0.3 mL or 0.1 g	0.2 mL	Not Noted
Test Substance Concentrations Tested	Tested concentrations not noted	Not Noted. Data presented for tested concentrations of 0.5% and 1%	Not Noted	Undiluted or 10% solution	0.1% to 100%	10% solution	Not Noted

	Lawrence et al. (1990)	Sterzel et al. (1990)	van Erp et al. (1990)	Blein et al. (1991)	CEC (1991)	Hagino et al. (1991)	Gettings et al. (1991)
Application of Solids to CAM	Not Noted	All tested substances appear to be solubilized	Not Noted	All tested substances appear to be solubilized	Placed directly on CAM	All tested substances appear to be solubilized	Not Noted
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	20 seconds after application of test substance, rinsed with 5 mL distilled water	Not Noted	Not Noted	Not Noted	Yes, for solids. 20 seconds after application of test substance, rinsed with 5 mL warm water or saline solution	Yes, 20 seconds after test substance applied rinsed with water	Not Noted
Evaluation Period	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Not Noted
Controls and Test Standards	Not Noted	Laureth-8-sulfate	Negative: blank, Reference Substances: toluene and acetone	Yes, but test substances used are not noted	Not Noted	Not Noted	Not Noted
Number of Control Eggs	Not Noted	Not Noted	3 eggs per control or reference substance	2 eggs	Not Noted	Not Noted	Not Noted
Replicate Eggs	6 eggs per test substance	6 eggs	Not Noted	6 eggs	Minimum 6 eggs	4 eggs per sample	Not Noted
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Injection, hemorrhage, coagulation	Blood vessels and albumin examined for such effects as hemorrhage, lysis, and coagulation	Injection, hemorrhage, coagulation	Hyperemia, hemorrhage, coagulation (in terms of opacity and thrombosis)	Hemorrhage, lysis, and coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, vascular lysis, coagulation
Endpoint Evaluation	Numerical time-dependent scores for three endpoints.	The starting second that each of the three endpoints is observed is recorded.	Numerical time-dependent scores for three endpoints.	Scored according to Luepke and Kemper (1986) scale	The starting second that each of the three endpoints is observed is recorded.	Numerical time-dependent scores for three endpoints.	The starting second that each of the three endpoints is observed is recorded.
Analysis Method	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Reaction Time score is calculated for each egg. Then a ratio of the mean Reaction Time score (for all 6 tested eggs) to the Reaction Time score observed for the reference was calculated.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Not Noted	Irritation Index is calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second	Not Noted	Two different analyses were used. Both calculated an irritation index using time (seconds) of appearance of hemorrhage vascular lysis, or coagulation. The differences between the two methods was in the particular calculations used.

	Lawrence et al. (1990)	Sterzel et al. (1990)	van Erp et al. (1990)	Blein et al. (1991)	CEC (1991)	Hagino et al. (1991)	Gettings et al. (1991)
Classification Scheme	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21	Not Noted	**Non Irritation**: <0.5; **Slight Irritant**: 0.5-3.4; **Moderate Irritant**: 3.5-4.9; **Severe Irritant**: ≥5	Not Noted	Not Noted	Not Noted	Not Noted
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes	Cites Luepke (1985) as basis for protocol, scoring scheme, and analysis method	Cites Luepke (1985) as basis for protocol	Cites Luepke 1985 as basis for protocol	Cites Luepke and Kemper (1986) as basis for protocol and analysis method		Cites Luepke (1985) as basis for scoring scheme and analysis method	Cites Luepke (1985) as basis for protocol used

	Spielmann et al. (1991)	Bagley et al. (1992)	Rougier et al. (1992)	de Silva et al. (1992)	InVittox Protocol (Spielmann and Liebsh 1992)	Hagino et al. (1993)	Spielmann et al. (1993)
Hen Strain	Not Noted	White Leghorn	White Leghorn	White Leghorn	White Leghorn (Shaver Starcross 288A)	White Leghorn	Not Noted
Egg Criteria for Use	Not Noted	Weight range of eggs between 50 g and 60 g	Weight range of eggs between 50 g and 60 g	Weighing between 50 g and 60 g	Not Noted	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{o}C)	Not Noted	37.5 $\pm$ 0.5	37.5 $\pm$ 0.5	38 $\pm$ 0.5	37.5 $\pm$ 0.5	37.6	Not Noted
Relative Humidity (%)	Not Noted	62.5 $\pm$ 7.5	62.5 $\pm$ 7.5	60 $\pm$ 5	62.5 $\pm$ 7.5	about 70	Not Noted
Egg Rotation?	Not Noted	Yes	Yes	Yes	Yes	Yes, once per hour	Not Noted
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted	Eggs candled on Day 9 and non-viable embryos removed	Not Noted	Not Noted
Incubation Period	Not Noted	10 Days	10 Days	10 Days	Eggs incubated for 8 days with rotation. After checking for viability on Day 9, viable eggs are placed in incubator with the large end up and incubated without rotation until the next day. Eggs used on Day 10.	10 Days	Not Noted
Procedure for Opening Egg	Not Noted	Egg shell around the air pocket was removed with a dental rotary saw	Egg shell around the air pocket was removed with a dental rotary saw. Inner membrane is removed to expose CAM.	Egg shell around the air pocket was removed using a rotary saw. Inner membrane is removed to expose CAM.	The air cell is marked with a rotating dentist-saw blade and the section is pared off.	Egg shell around the air pocket was removed. Drop of water is placed on the shell membrane to avoid capillary bleeding. Then the CAM is exposed.	Not Noted
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Membrane is moistened with 0.9% NaCl solution at 37. Eggs placed back into the incubator until ready for use (max. of 30 minutes). When ready for use, the NaCl solution is poured off. Then the egg membrane is removed to expose the CAM.	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Chemicals from various chemical classes, commercial products, and personal care products	Surfactants (non ionic, amphoteric, anionic, cationic) and surfactant-based cosmetic preparations	Surfactants, unidentified chemicals, and cosmetic formulations	Chemicals from various chemical classes	Chemicals from various chemical classes	Chemicals from various chemical classes
Total Test Substances Evaluated	32	32	41	101	27	12	136
Test Substance Quantity or Volume	0.3 mL	0.3 mL or 0.1 g	0.3 mL	0.3 mL	0.3 mL	0.2 mL or 0.2 g	Not Noted
Test Substance Concentrations Tested	1-100% solutions tested	Tested solutions at concentrations that were 10% of those tested *in vivo*	Not Noted	Tested solutions at concentrations that were 10% of those tested *in vivo*	Not Noted	Undiluted or as noted in manuscript	10% solution and threshold concentration (lowest concentration to produce a slight reaction)

	Spielmann et al. (1991)	Bagley et al. (1992)	Rougier et al. (1992)	de Silva et al. (1992)	InVittox Protocol (Spielmann and Liebsh 1992)	Hagino et al. (1993)	Spielmann et al. (1993)
Application of Solids to CAM	All tested substances appear to be solubilized	All tested substances appear to be solubilized	Not Noted	Placed directly on CAM	All tested substances appear to be solubilized	Placed directly on CAM	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	0.9% NaCl or olive oil	Not Noted	Not Noted
Rinse after Test Substance Application?	Not Noted	20 seconds after test substance applied rinsed with 5 mL warm water	Not Noted	For opaque, colored, or solid substances: after 20 seconds test substance rinsed with 5 mL warm saline	Not Noted	Yes, after 20 seconds	Insoluble substances: Yes, after 5 minutes
Evaluation Period	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Not Noted
Controls and Test Standards	Not Noted	Vehicle	Not Noted	Not Noted	1% SDS and 0.1 N NaOH	Not Noted	Not Noted
Number of Control Eggs	Not Noted	2 eggs	Not Noted	Not Noted	2 eggs for each control substance	Not Noted	Not Noted
Replicate Eggs	3 eggs per concentration	4 eggs	4 eggs	4 eggs	3 eggs	4 eggs	3 eggs
Number of Replicate Experiments	2	Not Noted	Not Noted	Not Noted	2	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, coagulation, lysis	Hyperemia, hemorrhage, coagulation	Hyperemia, hemorrhage, coagulation	Hyperemia, hemorrhage, coagulation (opacity and/or thrombosis)	Hemorrhage, vessel lysis, coagulation	Hyperemia, hemorrhage, coagulation	Not Noted
Endpoint Evaluation	The starting second that each of the endpoints is observed is recorded	Numerical time-dependent scores for three endpoints.	Numerical time-dependent scores for three endpoints.	Numerical time-dependent scores for three endpoints.	The starting second that one of the endpoints is observed is recorded. The degree of severity of each endpoint after the 5 minutes is noted. Severity is ranked from 0 (no reaction) to 3 (severe reaction).	Numerical time-dependent scores for three endpoints.	Not Noted
Analysis Method	Irritation Score calculated. Mean Irritation Score is calculated from individual assays.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Irritation Score (IS; determined at 10% concentration) and Irritation Threshold Concentration (ITC; highest concentration producing a slight reaction during observation period) calculated. Mean IS of 3 eggs calculated for each experiment. Mean value over both experiments calculated for IS and ITC.	Not Noted	Irritation Score (IS; determined at 10% concentration) and Irritation Threshold Concentration (ITC; lowest concentration producing a slight reaction during observation period) calculated

	Spielmann et al. (1991)	Bagley et al. (1992)	Rougier et al. (1992)	de Silva et al. (1992)	InVittox Protocol (Spielmann and Liebsh 1992)	Hagino et al. (1993)	Spielmann et al. (1993)
Classification Scheme	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-9.9; **Strong Irritation**: 10-21	Not Noted	Not Noted	Not Noted	**Non/Slight:** ITC > 10 and IS <10; Moderate: (1) ITC between 2.5 and 10 and IS <16 and weak or no reaction noted or (2) ITC > 10 and IS > 16 or (3) ITC > 10 and IS < 16 and severe reaction is noted; **Irritant:** (1) ITC between 1 and 2.5 and IS < 16 or (2) ITC between 2.5 and 10 and IS >16 or (3) ITC between 2.5 and 10 and IS >16 and severe reaction noted after 5 minutes; **Severe:** (1) ITC < 1% or (2) ITC between 1 and 2.5% and IS > 16 or (3) ITC between 2.5 and 10 and IS < 16 and severe reaction noted after 1 minute	Not Noted	**Non/Slight:** ITC > 10 and IS <16; **Moderate:** ITC <10 and IS <16 or ITC >10 and IS 16; **Irritant:** ITC <2.5 and IS <16 or ITC <10 and IS >16; **Severe**: ITC < 1% or ITC <2.5% and IS > 16
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes	Cites Luepke (1985) as modified by Kalweit (1990) as basis for protocol and analysis method	Cites Luepke and Kemper (1986) as basis for protocol	Cites Luepke (1985) as basis for scoring scheme	Cites Luepke (1981) as basis for protocol and scoring scheme	Not Noted	Cites Luepke (1985) as basis for scoring scheme	Cites Luepke (1985) as modified by Kalweit (1990) and Spielmann (1991) as basis for protocol

	Gettings et al. (1994)	Vinardell and Macián (1994)	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)
Hen Strain	White Leghorn	Leghorn SA31	Not Noted	Not Noted	Not Noted
Egg Criteria for Use	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	38	Not Noted	Not Noted	Not Noted	37.6
Relative Humidity (%)	60	Not Noted	Not Noted	Not Noted	about 70
Egg Rotation?	Yes	Not Noted	Not Noted	Not Noted	Yes, once per hour
Checking Egg Viability	Candled on Day 9 and non-viable embryos removed	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Period	9 Days	10 Days	9 Days	9 Days	10 Days
Procedure for Opening Egg	Eggshell was scratched around the air cells and a small aperture was opened.	Egg shell was scratched around the air cell by a dentist's rotary saw and then pared off. After removal of the inner membrane, the CAM was exposed.	Not Noted	Not Noted	A portion of the egg shell was removed and a drop of water was placed onto the shell membrane to avoid bleeding. Then the CAM was exposed with forceps.
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Oil/water -based personal care formulations	Commercial disinfectants	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Surfactants, solvents, formaldehyde
Total Test Substances Evaluated	18	6	59	59	24
Test Substance Quantity or Volume	0.3 mL	0.3 mL	Not Noted	Not Noted	0.2 mL
Test Substance Concentrations Tested	3 concentrations tested: threshold concentration, 10% solution, undiluted	Diluted or undiluted	Not Noted	Not Noted	10% solution

	Gettings et al. (1994)	Vinardell and Macián (1994)	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)
Application of Solids to CAM	All tested substances appear to be solubilized	All tested substances appear to be solubilized	Not Noted	Not Noted	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Distilled water	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	Not Noted	Not Noted	After 3 minute exposure	Not Noted	Yes, after 20 seconds test substance was rinsed with water
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Within 30 seconds of rinsing	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed
Controls and Test Standards	Not Noted	0.1 M NaOH, 1% SDS, 0.9% NaCl, distilled water	5% Texapon AV (internal reference standard)	5% Texapon AV (internal reference standard)	Not Noted
Number of Control Eggs	Not Noted	2 eggs per substance	Not Noted	Not Noted	Not Noted
Replicate Eggs	3 eggs per concentration tested	6 eggs	6 eggs	6 eggs	4 eggs
Number of Replicate Experiments	2	Not Noted	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, coagulation, lysis	Hemorrhage, vasoconstriction, coagulation	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation	Hyperemia, hemorrhage, coagulation
Endpoint Evaluation	Seconds for the three endpoints recorded (see Kalweit, 1990)	The starting second that each of the endpoints is observed is recorded	Endpoints scored from 0 (no reaction) to 3 (strong reaction)	The starting second that each of the endpoints is observed is recorded	Not Noted
Analysis Method	Calculation of an Irritation Score for each egg. Mean value of individual Irritation Scores calculated.	Irritancy Potential calculated using the formula: (301-sec H)/300*5+(301-sec v)/300*7=(301-sec C)*9; where H=Hemorrhage, V=vasoconstriction; C=Coagulation of protein or blood; sec=starting second	Calculation of "S Score". "S Score" is calculated using the most sensitive endpoint (endpoint can change from chemical to chemical). The scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18)	Computer program calculates an Irritation Index. Irritation Index Is used to calculate a "Q Score". "Q Score" is a comparison of the Irritation Index of a test chemical with that of the reference chemical. If the effect of test chemical is identical to reference, Q is 1.0. If effect of test chemical is less irritating, Q is lower. If effect of test chemical is more irritating, Q is higher.	Score was calculated based on the time of onset for each endpoint. Mean value of 4 eggs calculated.

	Gettings et al. (1994)	Vinardell and Macián (1994)	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)
Classification Scheme	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-9.9; **Strong Irritation**: 10-21	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9 21	**Non Irritation**: S < 6 ; **Moderately Irritating**: 6<= S <15; **Severely Irritating**: S ≥15	**Non Irritating**: Q < 1.5; **Moderately Irritating:** 1.5 < Q <2.0; **Severely Irritating**: Q < 2.0	Not Noted
GLP Compliance?	Not Noted	Not Noted	Yes	Yes	Not Noted
Notes	Cites Luepke (1985) as basis for scoring scheme	Cites Ergatt/Frame Data Bank (1990) as basis for protocol and analysis method			Cites Luepke (1985) and Luepke and Wallat (1985) as basis for scoring scheme and analysis method.
	To study the effects of slow acting materials, CAM scored 15 and 30 minutes after application on range from 0 (no reactions) to 3 (strong reactions)				

	Spielmann (1995)	Macian et al. (1996)	Gilleron et al. (1996)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Hen Strain	White Leghorn (Shaver Starcross 288A)	Leghorn SA31	White Essex	Lohmann's Selected White Leghorn	White Leghorn
Egg Criteria for Use	Weighing 50-60 g. Eggs are candled and non-viable eggs removed	Not Noted	Eggs were 7 days old prior to start of incubation and weighed 60 ± 5 g	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.5 ± 0.5	Not Noted	37.0 ± 0.5	Not Noted	38 ± 0.5
Relative Humidity (%)	62.5 ± 7.5	Not Noted	62.5 ± 1.5	Not Noted	60 ± 5
Egg Rotation?	Yes, for 8 days	Not Noted	Yes, with large ends upward for 9 days	Not Noted	Yes
Checking Egg Viability	Eggs candled on Day 9 and non-viable eggs removed. Eggs replaced in incubator with large ends up but were not rotated	Not Noted	Not Noted	Not Noted	Candled on Day 9 and returned to incubator in vertical position
Incubation Period	10 Days	10 Days	10 Days	10 Days	10 Days
Procedure for Opening Egg	Air cell is marked using a rotating dentist-saw blade. The egg shell is then pared off.	Egg shell was scratched around the air cell by a dentist's rotary saw and pared off. After removal of inner egg membrane, the CAM was exposed.	Eggs were candled and non-viable eggs were discarded. The airspace delimited by the inner membrane at the large end of the egg was marked. The eggshell was removed using a dentist's rotating saw blade. The inner membrane was moistened with 1.5-2.0 mL of 0.9% NaCl and the egg was returned to the incubator (at 37) for a maximum of 20 mins. After incubation, the NaCl solution was removed, using a vacuum pump, and the inner membrane was removed with forceps.	Not Noted	Shell and inner shell membrane were removed around the area defined by the air cell
Manipulation of CAM	Membrane is moistened with 0.9% NaCl solution at 37. Eggs are then placed back in to the incubator until ready for use (maximum of 30 minutes). When ready for use the NaCl solution is poured off and the membrane is removed with tapered forceps.	Not Noted	A test substance applicator (TSA), which is comprised of a perlon mesh (pore diameter = 63 micron) locked between two Teflon rings, was placed on the CAM	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Not Applicable	Polyoxyethylene non ionic surfactants	Chemicals from various chemical classes	Surfactant-based personal care formulations	Surfactant-based personal care formulations
Total Test Substances Evaluated	Not Applicable	9	46	25	25
Test Substance Quantity or Volume	0.3 mL (for insoluble solids: put some grains onto CAM to cover approximately half the surface)	0.3 mL	0.3 mL or 0.3 g of test substance placed inside the TSA	0.3 mL	0.1 mL
Test Substance Concentrations Tested	10% solution and several additional concentrations as determined by investigator	Different concentrations	Undiluted	3 concentrations tested: threshold concentration, 10% solution, undiluted	10% solution

	Spielmann (1995)	Macian et al. (1996)	Gilleron et al. (1996)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Application of Solids to CAM	All tested substances appear to be solubilized	All tested substances appear to be solubilized	Placed inside TSA	All test substances appear to be in liquid form	All test substances appear to be in liquid form
Preferred Solvent	0.9% NaCl or olive oil	Soluble Substances: 0.9% NaCl; Insoluble Substances: carboxymethylcellulose	0.9% NaCl	Not Noted	Not Noted
Rinse after Test Substance Application?	For insoluble test chemical: after 5 minutes rinse off with NaCl	Not Noted	TSA (which contains the test substance) is removed after 20 seconds	Not Noted	After 20 seconds, with a saline rinse
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed
Controls and Test Standards	1% SDS and 0.1 N NaOH	1% SDS and 0.1 N NaOH	Positive Controls: benzalkonium chloride, dimethylformamide, imidazole	Not Noted	Not Noted
Number of Control Eggs	2 eggs per standard	2 eggs per standard	Not Noted	Not Noted	Not Noted
Replicate Eggs	3 eggs	6 eggs	3	3 eggs per concentration tested	Not Noted
Number of Replicate Experiments	2	Not Noted	3	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, vascular lysis, coagulation	Hemorrhage, vasoconstriction, coagulation	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation	Dilation, hemorrhage, coagulation
Endpoint Evaluation	The starting second that each of the endpoints is observed is recorded. Additionally, the severity of the reaction is graded (between 0 and 3) after 5 minutes of exposure to test substance.	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded (see Kalweit 1990)	Numerical time-dependent scores for three endpoints.
Analysis Method	Irritation Score (IS; determined at 10% concentration) and Irritation Threshold Concentration (ITC; lowest concentration producing a slight reaction during observation period) calculated. Mean IS of 3 eggs calculated for each experiment. Mean value over both experiments calculated for IS and ITC.	Irritancy Potential calculated using the formula: (301-sec H)/300*5+(301-sec v)/300*7=(301-sec C)*9; where H=Hemorrhage, V=vasoconstriction; C=Coagulation of protein or blood; sec=starting second. Mean value and SEM of 6 separate experiments are calculated.	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean of 3 assays were calculated. Reproducibility also was assessed.	Mean Irritation Score (IS; determined at 10% concentration) of 3 eggs is calculated. The Irritation Threshold Concentration (ITC; lowest concentration producing a slight reaction during observation period) is calculated.	Time-dependent scores were used to calculate a single value (maximum of 21).

	Spielmann (1995)	Macian et al. (1996)	Gilleron et al. (1996)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Classification Scheme	**Non/Slight: I**TC > 10 and IS <10; Moderate: (1) ITC between 2.5 and 10 and IS <16 and weak or no reaction noted or (2) ITC > 10 and IS > 16 or (3) ITC > 10 and IS < 16 and severe reaction is noted; **Irritant:** (1) ITC between 1 and 2.5 and IS < 16 or (2) ITC between 2.5 and 10 and IS >16 or (3) ITC between 2.5 and 10 and IS >16 and severe reaction noted after 5 minutes; **Severe:** (1) ITC < 1% or (2) ITC between 1 and 2.5% and IS > 16 or (3) ITC between 2.5 and 10 and IS < 16 and severe reaction noted after 1 minute	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	**Irritant (According to FHSA)**: IS ≥ 5.1 or IS/ITC ≥ 3.0	**Irritant (According to FHSA)**: Score ≥ 4.83
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes					

	Spielmann et al. (1996)	Brantom et al. (1997)	Budai et al. (1997)	Gilleron et al. (1997)	Spielmann et al. (1997) (HETCAM-1)	Spielmann et al. (1997) (HETCAM-1, Laboratory A)
Hen Strain	Not Noted	Not Noted	White Leghorn (Shaver Starcross 288)	White Essex	White Leghorn	White Leghorn
Egg Criteria for Use	Not Noted	Not Noted	Eggs were candled and non viable eggs were discarded	Eggs were 7 days old	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{o}C)	Not Noted	Not Noted	37	37 $\pm$ 0.5	38	38
Relative Humidity (%)	Not Noted	Not Noted	60-70	52.5 $\pm$ 2.5	60	60
Egg Rotation?	Not Noted	Not Noted	Yes, for 8 days	Not Noted	Yes	Yes
Checking Egg Viability	Not Noted	Not Noted	Eggs were candled on the 9th day and non viable eggs were discarded.	Not Noted	Not Noted	Not Noted
Incubation Period	Not Noted	9 Days	9 Days, then eggs were candled and non-viable eggs were discarded. Eggs were placed in incubator (but not rotated) until Day 10	10 Days	9 Days	9 Days
Procedure for Opening Egg	Not Noted	Not Noted	The air cell of eggs were marked and the section of shell was removed with scissors. The membrane was moistened with 0.9% NaCl and eggs were placed in incubator until ready for use.	Not Noted	Egg shells were opened at the air cell	Egg shells were opened at the air cell
Manipulation of CAM	Not Noted	Not Noted	Not Noted	A test substance applicator (TSA) was placed on the CAM	Not Noted	Not Noted
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Substances representative of cosmetic ingredients and finished personal product formulations	Pesticides	Chemicals from various chemical classes	Inorganic chemicals, aliphatic organics, aromatics, heterocyclics	See Gettings et al. lists
Total Test Substances Evaluated	200	55	4	60	133	53
Test Substance Quantity or Volume	Not Noted	Not Noted	0.3 mL	0.3 mL or 0.3 g of test substance placed inside the TSA	0.3 mL	0.3 mL
Test Substance Concentrations Tested	1-100% solutions tested	Not Noted	1, 10, and 100%	Not Noted	Undiluted and 10% concentration	Undiluted and 10% concentration

	Spielmann et al. (1996)	Brantom et al. (1997)	Budai et al. (1997)	Gilleron et al. (1997)	Spielmann et al. (1997) (HETCAM-1)	Spielmann et al. (1997) (HETCAM-1, Laboratory A)
Application of Solids to CAM	All tested substances appear to be solubilized	All test substances appear to be in liquid form	All tested substances appear to be solubilized	Placed inside TSA	All tested substances appear to be solubilized	Not Noted
Preferred Solvent	0.9% NaCl or olive oil	Not Noted	Not Noted	Not Noted	0.9% NaCl or olive oil	Not Noted
Rinse after Test Substance Application?	Yes, after 5 minutes (for substances that were insoluble in eater or oil and were colored).	Non-trasnparent substances were rinsed off of the CAM after 30 seconds	Not Noted	TSA (which contains the test substance) is removed after 20 seconds	Not Noted	Not Noted
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds for transparent test susbtances	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied
Controls and Test Standards	Not Noted	5% solution of Texapon ASV	Standards: 1% SDS and 0.1M NaOH; Control: 0.9% NaCl	Not Noted	0.1 N NaOH, 0.1% SDS, 0.9% NaCl	0.1 N NaOH, 0.1% SDS, 0.9% NaCl
Number of Control Eggs	Not Noted	Not Noted	2 eggs per control and standard	Not Noted	Not Noted	Not Noted
Replicate Eggs	Not Noted	6 eggs	6 eggs for each concentration	Not Noted	3 eggs	3 eggs
Number of Replicate Experiments	Not Noted	Not Noted	4	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, coagulation, lysis	Hemorrhage, coagulation, lysis	Hemorrhage, vascular lysis, coagulation	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation
Endpoint Evaluation	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded for transparent substances and quality of the effects is determined for the nontransparent substances	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	Not Noted
Analysis Method	Irritation Score calculated ((301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second) for 10% solution calculated (IS10). Irritation Threshold (ITC; lowest concentration of a test substance to induce an irritant reaction on the CAM) calculated.	Computer program calculates an Irritation Index. Irritation Index Is used to calculate a "Q Score". "Q Score" is a comparison of the Irritation Index of a test chemical with that of the reference chemical. If the effect of test chemical is identical to reference, Q is 1.0. If effect of test chemical is less irritating, Q is lower. If effect of test chemical is more irritating, Q is higher. Calculation of "S Score". "S Score" is calculated using the most sensitive endpoint (endpoint can change from chemical to chemical). The scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18)	Not Noted	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean value and SEM of are calculated.	Irritation Score calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second.	Not Noted

	Spielmann et al. (1996)	Brantom et al. (1997)	Budai et al. (1997)	Gilleron et al. (1997)	Spielmann et al. (1997) (HETCAM-1)	Spielmann et al. (1997) (HETCAM-1, Laboratory A)
Classification Scheme	**BGA Classification Model: Non/Slight**: ITC > 10 and IS10 <16; **Moderate**: (1) ITC > 16 and IS10 > 16 or (2) ITC < 10 and IS10 < 16; **Irritant (R36)**: (1) ITC < 10 and IS10 > 16 or (2) ITC < 2.5 and IS10 < 16; **Severe (R41)**: (1) ITC ≤ 1% or (2) ITC between 1 and 2.5% and IS10 ≥ 16. **Proposed model using mtc10 (see notes below): R41**: mtc10 < 50 seconds.	**Q-SCORE: Slightly Irritating:** Q <= 0.8; **Moderately Irritating:** 0.8 < Q <1.2; **Irritating:** 1.2 <=Q<2.0; **Severely Irritating:** Q <= 2.0; **S-SCORE: Slightly Irritating** S < 6 ; **Moderately Irritating**: 6<= S <12; **Irritating**: 12 <= S ≥16; **Severely Irritating** S>=16	**No Irritation**: 0-0.9; **Weak Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Severe Irritation**: 9-21	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	Not Noted	Not Noted
GLP Compliance?	Yes	Yes	Not Noted	Not Noted	Not Noted	Not Noted
Notes	Cites Luepke (1985) as basis for protocol. Cites Kalweit (1990) and Spielmann (1991) as publishing the protocol used. Cites the standard protocol for the test method as InVittox Protocol.			Cites Gilleron 1996 as basis for protocol and analysis method		
	Nine additional endpoints were conducted using the raw data and the IS and IT scores in this analysis. Of these the endpoints evaluated, that best correlated with in vivo classification was mtc10 (mean detection time for appearance of coagulation when using a 10% solution).					

	Spielmann et al. (1997) (HETCAM-II)	Spielmann et al. (1997) (HETCAM-III)	Vives et al. (1997)	Doucet et al. (1999)	Hagino et al. (1999)	Lönnroth et al. (1999)
Hen Strain	White Leghorn	White Leghorn	Leghorn SA31	White Leghorn	White Leghorn	Not Noted
Egg Criteria for Use	Not Noted	Not Noted	Not Noted	Eggs weighed between 50-60 g	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.8	37.5 $\pm$ 1	Not Noted	37.5 $\pm$ 1	37.6	38
Relative Humidity (%)	55%	40-60	Not Noted	60 $\pm$ 5	about 70	Not Noted
Egg Rotation?	Not Noted	Not Noted	Not Noted	Yes, eggs were placed on their long axis	Yes, once an hour	Not Noted
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not noted	Not Noted	Not Noted
Incubation Period	9 Days	10 Days	10 Days	10 Days	10 Days	9 Days
Procedure for Opening Egg	Not Noted	Not Noted	Egg shell was scratched around the air cell by a dentist's rotary saw and pared off. After removal of inner egg membrane, the CAM was exposed.	Eggshell around the airspace was removed. 5 mL of 0.9% NaCl was placed on the inner membrane and then the CAM was exposed	Portion of the egg shell above the air space was removed.	Egg shell above the air cell was opened using a dental drill saw blade and forceps. The shell membrane was moistened with 0.9% NaCl solution at 37 degrees Celsius. The NaCl was aspirated, the shell membrane removed, and CAM exposed.
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not noted	Drop of water is placed on the membrane (to avoid capillary bleeding). A silicone rubber ring is placed on the CAM.	Eggs were examined using a microscope. Photo-micrographs were taken 2 minutes after application of each material.
Investigator Defined Test Substance Classes	Surfactants and formulations	Inorganics, aliphatics, alicyclics, heterocyclic, alkyl derivatives, polymers	Surfactants derived from lysine	Skin-care products, sunscreen products, surfactant-based products, and alcoholic products	Surfactant, polyols, color additives, organic salts, PABA derivative, esters, inorganic chemicals, alcohols, amines, alkanolamines, carboxylic acids	Dental polymer products
Total Test Substances Evaluated	42	97	6	40	39	8
Test Substance Quantity or Volume	0.3 mL	0.3 mL	0.3 mL	0.3 mL	0.2 mL (placed inside the rubber ring on the CAM). Solids (0.2 g) are reduced to a fine powder with a No. 200 sieve and placed inside a rubber ring on the CAM.	0.1-0.2 mL
Test Substance Concentrations Tested	Not Noted	Solids and liquids were generally tested undiluted; turbid materials were diluted to concentrations that allowed observation of the CAM	Different concentrations	Surfactant products: 3% concentration; Alcoholic products: 10% alcohol concentration; Emulsion type products: undiluted	0.1, 1, 10, and 100%	Not Noted

	Spielmann et al. (1997) (HETCAM-II)	Spielmann et al. (1997) (HETCAM-III)	Vives et al. (1997)	Doucet et al. (1999)	Hagino et al. (1999)	Lönnroth et al. (1999)
Application of Solids to CAM	All tested substances appear to be solubilized	Not Noted	All tested substances appear to be solubilized	Not Noted	Placed inside rubber ring	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Water or solvents	Distilled water	Sterilized water	Not Noted	Cell culture media (MEM, 2 mM L-glutamine, 100 IU/mL penicillin, 100 mg/ml Streptomycin, 5% FBS). Solutions were incubated for 24 hrs in a water bath at 37 degrees. The suspensions were centrifuged and the supernatants applied
Rinse after Test Substance Application?	Not Noted	Not Noted	Not Noted	Yes, 20 seconds after test substance application it was rinsed with 5 mL of warm saline by irrigation of the tilted egg	Yes, after 20 seconds with distilled water	Not Noted
Evaluation Period	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	At 0.5, 2, and 5 minutes after test substance applied	Up to 240 seconds after test substance applied
Controls and Test Standards	Water, other additional controls depend upon the class of chemicals being evaluated	Not Noted	1% SDS and 0.1 N NaOH	Positive control: 0.3% SDS; Negative control: saline solution	Not Noted	Positive: 0.1N NaOH; Negative: 0.9% NaCl
Number of Control Eggs	1 egg per control	Not Noted	2 eggs per standard	2 eggs per control	Not Noted	Not Noted
Replicate Eggs	4 eggs	6 eggs	6 eggs	4 eggs for each test sample	4 eggs	3 eggs
Number of Replicate Experiments	1 assay with 4 eggs or 2 assays with 2 eggs	Not Noted	Not Noted	1	Not Noted	2
Endpoints Assessed	Hyperemia, hemorrhage, coagulation	Hemorrhage, lysis, coagulation	Hemorrhage, vasoconstriction, coagulation	Hyperemia, hemorrhage, coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, lysis, coagulation
Endpoint Evaluation	Numerical time-dependent scores for three endpoints.	The starting second that each endpoint is observed is recorded. Additionally, the endpoint score "S" is determined at 0.5, 1, 3, or 5 mins.	The starting second that each of the endpoints is observed is recorded	Numerical time-dependent scores for three endpoints.	Numerical time-dependent scores for three endpoints.	The starting second that each of the endpoints is observed is recorded
Analysis Method	Time-dependent scores were used to calculate a single value (maximum of 21).	"S Score" is calculated using scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18); "Q Score" is a comparison of the Irritation Score of a test chemical with that of the reference chemical.	Irritancy Potential calculated using the formula: (301-sec H)/300*5+(301-sec v)/300*7=(301-sec C)*9; where H=Hemorrhage, V=vasoconstriction; C=Coagulation of protein or blood; sec=starting second. Mean value and SEM of 6 separate experiments are calculated.	Mean of the calculated scores were determined for each test substance.	Not Noted	Irritation Score calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second

	Spielmann et al. (1997) (HETCAM-II)	Spielmann et al. (1997) (HETCAM-III)	Vives et al. (1997)	Doucet et al. (1999)	Hagino et al. (1999)	Lönnroth et al. (1999)
Classification Scheme	Not Noted	Not Noted	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21	Not noted	Not Noted	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9 21
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not noted	Not Noted	Not Noted
Notes			Cites Ergatt/Frame Data Bank (1990) as basis for protocol	Cites Luepke (1985) as basis for protocol, scoring scheme, and analysis method	Cites Luepke 1985 as basis for scoring method	Cites Kalweit (1990) as basis of protocol

	Schlage et al. (1999)	Steiling et al. (1999)	Budai and Várnagy (2000)	Djabari et al. (2002)
Hen Strain	White Leghorn	White Leghorn (Shaver Starcross 288)	White Leghorn Shaver 288	White Leghorn
Egg Criteria for Use	Not Noted	Less than 1 week after laying (approximate weight about 50 g)	Eggs were candled and all defective ones were discarded	Eggs weighing between 50-65 g
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.5	37.5 $\pm$ 0.5	37	37.8
Relative Humidity (%)	Not Noted	55 $\pm$ 7	60-70	Not Noted
Egg Rotation?	Not Noted	Yes	Yes for first 8 days	Not Noted
Checking Egg Viability	Not Noted	On day 10 the eggs are candled and non-viable eggs removed	On day 9 the eggs are candled and non-viable eggs removed	Not Noted
Incubation Period	9 or 10 Days	10 Days	9 Days, then eggs were candled and non-viable eggs were discarded. Eggs were placed in incubator (but not rotated) until Day 10	10 Days
Procedure for Opening Egg	Egg shell was opened at the airspace with a dentist's saw and the apical parts of the shell were removed.	Egg shell was opened with an electric drill and the white egg membrane was removed	Airspace is marked and section of shell removed with scissors.	Not Noted
Manipulation of CAM	Not Noted	Not Noted	Membrane is moistened with 0.9% NaCl after CAM is exposed. Egg is placed back in incubator until ready for use.	Not Noted
Investigator Defined Test Substance Classes	Cigarette smoke	Substances representing a range of chemicals used in the cosmetics industry	Pesticides	Substances with vegetal, marine, biotechnological, or chemical synthetic origin
Total Test Substances Evaluated	2	100	6	20
Test Substance Quantity or Volume	0.2 mL	0.3 mL	0.3 mL	Not Noted
Test Substance Concentrations Tested	Not Noted	Undiluted	Not Noted	Undiluted and 10%

	Schlage et al. (1999)	Steiling et al. (1999)	Budai and Várnagy (2000)	Djabari et al. (2002)
Application of Solids to CAM	Not Applicable	Amount sufficient to cover at least 25% of the CAM was applied	All tested substances appear to be solubilized	All tested substances appear to be solubilized
Preferred Solvent	Not Applicable	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	Not Noted	For non-transparent substances, rinsed off after 30 seconds	Not Noted	Not Noted
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds for transparent substances and	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied
Controls and Test Standards	PBS	Texapon ASV	0.9% NaCl; solution of 1% SDS and 0.1 M NaOH	Not Noted
Number of Control Eggs	Not Noted	6 eggs	2 eggs for each substance	Not Noted
Replicate Eggs	3 to 4 eggs for each dose	6 eggs	6 eggs	Not Noted
Number of Replicate Experiments	Not Noted	Not Noted	4	Not Noted
Endpoints Assessed	Injection, hemorrhage, coagulation (IHC) or hemorrhage, vessel lysis, coagulation (HVC)	Hemorrhage, lysis, coagulation	Hemorrhage, vessel lysis, coagulation	Hyperemia, hemorrhage, coagulation
Endpoint Evaluation	Numerical time-dependent scores for three endpoints and the starting second that each of the endpoints is observed is recorded.	The starting second that each of the endpoints is observed is recorded for transparent substances and quality of the effects is determined for the nontransparent substances	The starting second that each of the endpoints is observed is recorded	Numerical time-dependent scores for three endpoints.
Analysis Method	A cumulative discontinuous irritation score (maximum value of 21) calculated for IHC and HVC. Additionally, a continuous Irritation Score calculated using the formulation: (301-sec I)/300*5+(301-sec H)/300*7=(301-sec C)*9; where I=Injection, H=Hemorrhage, C=Coagulation, sec=starting second or (301 sec H)/300*5+(301-sec V)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis, C=Coagulation, sec=starting second	Computer program calculates an Irritation Index. Irritation Index Is used to calculate a "Q Score". "Q Score" is a comparison of the Irritation Index of a test chemical with that of the reference chemical. If the effect of test chemical is identical to reference, Q is 1.0. If effect of test chemical is less irritating, Q is lower. If effect of test chemical is more irritating, Q is higher. Calculation of "S Score". "S Score" is calculated using the most sensitive endpoint (endpoint can change from chemical to chemical). The scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18)	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second	Not Noted

	Schlage et al. (1999)	Steiling et al. (1999)	Budai and Várnagy (2000)	Djabari et al. (2002)
Classification Scheme		**Q-SCORE: Slightly Irritating:** Q <= 0.8; **Moderately Irritating:** 0.8 < Q <1.2; **Irritating:** 1.2 <=Q<2.0; **Severely Irritating:** Q <= 2.0; **S-SCORE: Slightly Irritating** S < 6 ; **Moderately Irritating**: 6<= S <12; **Irritating**: 12 <= S ≥16; **Severely Irritating** S>=16	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9-21
GLP Compliance?		Yes	Not Noted	Not Noted
Notes				Cites Luepke 1985 and Luepke and Kemper 1986 as basis for protocol and scoring scheme

Abbreviations: CAM = Chorioallantoic membrane, ECETOC = European Centre for Ecotoxicology and Toxicology of Chemicals, FHSA = Federal Hazardous Substances Act (1964), IS = Irritation score, IT = Irritation threshold concentration, NaCl = Sodium chloride, NaOH = Sodium hydroxide, PBS = Phosphate buffered saline, SDS = Sodium dodecyl sulfate, Sec = seconds, TSA = Test substance applicator.

Appendix B

Chemical and Product Class Information for the Substances Tested in the HET-CAM Test Method

B1 Table of Chemical and Product Class Information..... B-3

B2 Table of Formulation Components in Gettings et al. (1991)..... B-19

B3 Table of Formulation Components in Gettings et al. (1994)..... B-25

B4 Table of Formulation Components in Gettings et al. (1996)..... B-35

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Appendix B1

Table of Chemical and Product Class Information

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Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Acetic acid	64-19-7	-	Carboxylic acid	-
Acetoacetic acid glycolester	5459-04-1	-	Acetate	-
Acetone	67-64-1	-	Ketone	Solvent; Antiseptic; Chemical intermediate; Raw material
Acetonitrile	75-05-8	-	Nitrile	-
7-Acetoxyheptanal	-	-	-	-
n-Acetyl-Methionine	1115-47-5	N-acetyl-DL-methionine	Amino acid	-
Acetylsalicylic acid	50-78-2	-	Carboxylic acid	Analgesic
Acrylamide	79-06-1	-	Amide, Hydrocarbon	Laboratory reagent
Allyl alcohol	107-18-6	-	Alcohol	-
Aluminium hydroxide	21645-51-2	-	Alkali	-
Ambuphylline	5634-34-4	-	Heterocyclic	-
4-Amino-azobenzene-4-sulfonic acid	-	-	Acid	-
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	4-Amino-5-methoxy-o-toluenesulfonic acid	Hydrocarbon, Sulfur containing	-
Ammonium nitrate	6484-52-2	-	Inorganic	Fertilizer; Chemical intermediate; Industrial explosive
Ammonium persulfate	7727-54-0	-	Inorganic	-
Aniline	62-53-3	-	Amine	-
p-Anisidine	104-94-9	-	Amine	-
Anisole	100-66-3	Anisole D	Ether; Phenol	-
9,10-Anthracenedione	84-65-1	-	Quinone	-
Arcopal	-	-	-	-
Ascorbic acid	50-81-7	-	Acid	Metabolite
Aspartic acid	56-84-8	-	Amino acid	Neurotransmitter

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
L-Aspartic acid	70-47-3	-	Acid	Organic intermediate; Ingredient of Aspartame; Fungicides; Germicides
Azelaic acid	123-99-9	-	Carboxylic acid	-
B 25	-	-	-	-
Behydima	-	-	-	-
Benzalkonium chloride	8001-54-5	-	Surfactant, Cationic	Bactericide; Fungicide; Cationic surface active agent; Preservative
Benzoic acid	65-85-0	-	Carboxylic acid	Preservative
Benzoyl-L-tartaric acid	2743-38-6	-	Acid	-
Bis-(3-triethoxisilylpropyl)-tetrasulfide	-	-	-	-
n-Butanal	123-72-8	-	Aldehyde	-
Butanol	71-36-3	-	Alcohol	-
n-Butanol	71-36-3	-	Alcohol	-
Butyl acetate	123-86-4	-	Acetate	Solvent; Synthetic flavor ingredient
Butyl carbamate	592-35-8	-	Carboxylic acid	
gamma-Butyrolactone	96-48-0	-	Lactone	Synthetic intermediate; Solvent
Caffeine sodium benzoate	8000-95-1	-	Heterocyclic	-
Caffeine sodium salicylate	8002-85-5	-	Heterocyclic	-
Camphen	79-92-5	Camphene	Hydrocarbon	-
Captan 90 concentrate	133-06-2	Captan	Sulfur containing; Heterocyclic	Pesticide
Carbon black	1333-86-4	-	Inorganic	-
4-Carboxybenzaldehyde	619-66-9	-	Aldehyde	-
Cerium-2-ethylhexanoate	24593-34-8	Cerium ethyl hexonate	Carboxylic acid	-
Cetylpyridinium bromide	140-72-7	-	Surfactant, Cationic	Germicide; Laboratory reagent

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Cetyltrimethylammonium bromide	57-09-0	-	Amine; surfactant, Anionic	-
Chlorhexidine	55-56-1	-	Amidine	Disinfectant; Mouthwash; Anti-infective agent
Chlorhexidine gluconate Solution (20% Solution)	18472-51-0	-	Gluconate	-
Chlorhexidine hydrochloride	3697-42-5	-	Hydrocarbon	Disinfectant; Mouthwash; Anti-infective agent
1-Chloroctane-8-ol	-	-	Alcohol	-
4-Chloro-methanilic acid	98-36-2	-	Hydrocarbon, Sulfur containing	-
4-Chloro-4-Nitrodiphenylether	1836-74-4	-	Ether	-
Cupric sulfate	7758-98-7	-	Inorganic	-
Cyclohexanol	108-93-0	-	Alcohol	Solvent; Chemical intermediate
3-Cyclohexene-1-methanol	1679-51-2	-	Alcohol	-
DC 8	-	-	-	-
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	-	Ester; Surfactant, Anionic	-
Dibenzyl phosphate	1623-08-1	-	Organophosphate	-
1,4-Dibutoxy-benzene	104-36-9	-	Hydrocarbon	-
2,6-Dichlorobenzoyl chloride	4659-45-4	-	Acyl halide	-
Diepoxid 126	2386-87-0	Epoxy cyclohexane carboxylate	Ester; Epoxide	-
Diethylhexyl phthalate	117-81-7	-	Carboxylic acid	-
3-5-Dihydroxy-acetophenone	35086-59-0	-	Ketone	-
Diisopropanolamine	110-97-4	-	Alcohol; Amine	-
N,N-Dimethylacetamide	127-19-5	-	Amide	-
2,2-Dimethylbutanoic acid	595-37-9	-	Acid	Pharmaceutical metabolite
2,5-Dimethylhexanediol	110-03-2	-	Diol	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
2,5-Dimethylhexanediol	110-03-2	-	Diol	-
3,6-Dimethyloctanol	-	-	Alcohol	-
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	-	Nitrile	-
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	-	Ketone	-
m-Dinitrobenzene	99-65-0	-	Cyclocarbon	-
Diphocars	-	-		-
1,2-Dodecanediol	1119-87-5	-	Alcohol	-
Domiphen bromide	538-71-6	-	Amine; Surfactant, Cationic	-
DTPA Pentasodium salt	140-01-2	Pentasodium pentetate	Amine; Carboxylic acid	-
E4	-	-	-	-
Ede 140	-	-	-	-
EDTA	60-00-4	-	Amine; Carboxylic acid	Pharmaceutical intermediate, Food additive
EDTA-4-Na salt	13235-36-4	-	Amine; Carboxylic acid	-
1,2-Epoxycyclooctane	286-62-4	-	Hydrocarbon	-
1,2-Epoxycyclopentane	285-67-6	-	Hydrocarbon	-
1,2-Epoxydodecane	2855-19-8	-	Hydrocarbon	-
Ethanol	64-17-5	-	Alcohol	Solvent; Beverages; Antifreeze agent
Ethiosan	-	-	-	-
Ethyl acetate	141-78-6	-	Carboxylic acid	Solvent; Synthetic flavoring
Ethylacrolein	922-63-4	-	Aldehyde	-
Ethyl butanal	97-96-1	-	Aldehyde	-
2-Ethyl-1-hexanol	104-76-7	-	Alcohol	Solvent; Plasticizer
Ethyl-2-methylacetoacetate	609-14-3	-	Acetate	-
Ethyl trimethyl acetate	3938-95-2	-	Acetate	Solvent
Fomesafen	72128-02-0	-	Amide	Pesticide
Gadopentetic acid dimeglumine salt	86050-77-3	Gadolinium complex N-methyl glucamine salt	Amine; Carboxylic acid	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Genagen	68139-91-3	-	-	-
Genomoll	115-96-8	Chlorophophate ethanol	Organophosphate	-
C12/C14-Glucoside	-	-	-	-
Glutamic acid	56-86-0	-	Amino acid	Neurotransmitter
L-Glutamic acid hydrochloride	138-15-8	-	Amino acid	Neurotransmitter
Glycediol	-	-	Alcohol	-
Glycerin	56-81-5	-	Alcohol	-
Glycerol	56-81-5	-	Alcohol	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle
Glycolic acid	79-14-1	-	Carboxylic acid	-
Granuform	30525-89-4	Para-formaldehyde	Aldehyde	-
Hexachlorocyclopentadiene	77-47-4	-	Hydrocarbon	-
Hexahydrofarnesyl- acetone	502-69-2	-	Hydrocarbon	-
Hexamethylenetetramine	100-97-0	-	Amine	Antibacterial agent
2,5-Hexandion	110-13-4	-	Ketone	-
n-Hexane	110-54-3	-	Hydrocarbon	-
1,2,6-Hexanetriol	106-69-4	-	Alcohol	-
n-Hexanol	111-27-3	-	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient
Hnol	-	-	-	-
Hoe MBF	-	-	-	-
Hoe T 3761	-	-	-	-
Hydo 98	-	-	-	-
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)	-	-	Formulation	Fragrances
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)	-	-	Formulation	Cosmetics

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)	-	-	Formulation	Cosmetics
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)	-	-	Formulation	Cosmetics
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)	-	-	Formulation	Lotions
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)	-	-	Formulation	Cosmetics
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)	-	-	Formulation	Sunscreens
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)	-	-	Formulation	Cosmetics
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)	-	-	Formulation	Fragrances
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)	-	-	Formulation	Cosmetics
2-Hydroxyethyliminodi-sodiumacetate	135-37-5	-	Carboxylic acid	-
2-Hydroxyisobutyric acid	594-61-6	-	Carboxylic acid; Fatty acid	-
2-Hydroxyisobutyric acid ethylester	80-55-7	-	Ester	-
Hypo 20	-	-	-	-
Hypo 36	-	-	-	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Hypo 45	-	-	-	-
Hypo 54	-	-	-	-
Hyton	-	-	-	-
Imidazole	288-32-4	-	Heterocyclic	Laboratory reagent
Iminodiacetic acid	142-73-4	Acetocacetic acid isopropyl ester	Carboxylic acid; Imine	-
Isobornyl acetate	125-12-2		Hydrocarbon	-
Isobutanal	78-84-2	Isobutyraldehyde	Aldehyde	-
Isobutanol	78-83-1	-	Alcohol	Solvent; Chemical intermediate; Flavor ingredient
Isodecylglucoside	-	-	-	-
Isononylaldehyde	35127-50-5	Isononanal	Aldehyde	-
Isopropanol	67-63-0	-	Alcohol	Solvent; Aerosol formulations (ingredient)
Isopropyl acetoacetate	542-08-5	-	Carboxylic acid	-
Isotridecanal	61497-46-9	-	-	-
Kerobit TP	-	-	-	-
alpha-Ketoglutaric acid	328-50-7	-	Carboxylic acid	-
Kuppler 43	-	-		-
Lactic acid	50-21-5	-	Carboxylic acid	-
alpha-Lactid	4511-42-6	Dimethyl dioxane dione	Heterocyclic	-
Lial-111-Glucoside	-	-	-	-
L-Lysine Monohydrate	39665-12-8	-	Amino acid	-
Maneb	12427-38-2	-	Carboxylic acid; Organometallic compound	Pesticide
Mecre	-	-	-	-
3-Mercapto-1,2,4-triazole	3179-31-5	-	Heterocyclic, Sulfur containing	-
m-Methoxybenzaldehyde	591-31-1	-	Aldehyde	-
Methyl acetate	79-20-9	-	Carboxylic acid	Solvent; Chemical intermediate; Synthetic flavor ingredient

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Methyl acetate	79-20-9	-	Carboxylic acid	-
Methyl cyanoacetate	105-34-0	-	Acetate	-
Methylcyclopentane	96-37-7	-	Hydrocarbon	-
Methyl ethyl ketone	78-93-3	-	Ketone	-
Methyl isobutyl ketone	108-10-1	-	Ketone	-
5-Methyl-1,3,4-thiadiazol-2-amine	108-33-8	-	Amine	-
Methylpentynol	77-75-8	-	Alcohol	-
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	o-Tolyl biguanidine	Amide	-
Methylphosphonic acid bis (oxianylmethyl) ester	77275-34-9	-	Ester	-
2-Methyl-1-propanol	78-83-1	Isobutyl alcohol	Alcohol	-
Methyltetraglycol	9004-74-4	-	Alcohol	-
Methyltriglycol	112-35-6	-	Alcohol	-
Monoethanolamine	141-43-5	-	Alcohol; Amine	Surfactant, Laboratory reagent
1-Naphthalene acetic acid	86-87-3	-	Carboxylic acid	Pesticide
1-Naphthalene acetic acid, Na salt	61-31-4	-	Carboxylic acid	Pesticide
Napt	-	-	-	-
Nicotinamide	98-92-0	-	Amide	-
Nitroaniline	88-74-4	-	Amine	-
Nitrobenzene	98-95-3	-	Hydrocarbon	-
p-Nitrobenzoic acid	62-23-7	-	Carboxylic acid	-
Nitro-bis-octylamide	-	-	-	-
Nitropropane	108-03-2	-	Hydrocarbon	-
n-Octanol	111-87-5	-	Alcohol	-
Oil/Water Emulsion-HZA	-	-	Formulation	Conditioners, Hair
Oil/Water Emulsion-HZC	-	-	Formulation	Emollients
Oil/Water Emulsion-HZE	-	-	Formulation	Lotions
Oil/Water Emulsion-HZF	-	-	Formulation	Sunscreens
Oil/Water Emulsion-HZH	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZI	-	-	Formulation	Conditioners, Hair

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Oil/Water Emulsion-HZJ	-	-	Formulation	Cream
Oil/Water Emulsion-HZL	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZM	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZN	-	-	Formulation	Lotions
Oil/Water Emulsion-HZO	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZR	-	-	Formulation	Cleaners
Oil/Water Emulsion-HZS	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZT	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZU	-	-	Formulation	Sunscreens
Oil/Water Emulsion-HZV	-	-	Formulation	Cosmetics
Oil/Water Emulsion-HZW	-	-	Formulation	Roll-on Antiperspirant
Oil/Water Emulsion-HZY	-	-	Formulation	Shampoos, Hair
Olak	-	-	-	-
Ölesulf	-	-	-	-
Oxoöl 9N	-	-	-	-
P 32	-	-	-	-
Parafluoraniline	371-40-4	-	Aromatic	-
Phenol	108-95-2	-	Alcohol	Antiseptic, Disinfectant
o-Phenylenediamine	95-54-5	-	Amine	-
(-)Phenylephrine	59-42-7	-	Alcohol; Amine	-
(+)Phenylephrine	614-03-9	-	Alcohol; Amine	-
Phenylephrine hydrochloride	61-76-7	-	Alcohol; Amine	-
Phenylthiourea	103-85-5	-	Sulfur containg; Urea	-
Phosphonat A	-	-	-	-
Phthalic anhydride	85-44-9	-	Carboxylic acid	-
Piperazine	18833-13-1	Acefyllin piperazinate	Heterocyclic	-
PO 2	-	-	-	-
Polyethylene glycol 400	25322-68-3	-	Surfactant, nonionic	Polymer

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Polyethylene glycol butyl ether	9004-77-7	-	Alcohol	-
Polyethylene glycol dimethyl ether	24991-55-7	Dimethoxy polyethylene glycol	Ether	-
Polyethylene glycol	25322-68-3	-	Alcohol	-
Polyhexamethylene guanidine	-	-	-	Biocide
Polysolvan	7397-62-8	Butyl hydroxy acetate	Alcohol	-
Potassium cyanate	590-28-3	-	Inorganic	-
Potassium hexacyanoferrate II	14459-95-1	-	Inorganic	-
Potassium hexacyanoferrate III	13756-66-2	-	Inorganic	-
Potassium laurate	10124-65-9	-	Carboxylic acid; Surfactant, Cationic	-
Potato starch	56780-58-6	-	Hydrocarbon	-
Promethazine HCl	58-33-3	Phenergan, Promethergan	Sulfur containg; Heterocyclic	Pharmaceutical agent (antihistamine)
2-Propanol	67-63-0	-	Alcohol	Solvent, Disinfectant
Propylene glycol	57-55-6	-	Alcohol	
2-Pseudojonon	-	-	-	-
Pyridine	110-86-1	-	Heterocyclic	-
Quinacrine	69-05-6	Mepacrine	Heterocyclic; Hydrocarbon	Pharmaceutical agent (antiprotozoal)
Remolgan	-	-	-	-
beta-Resorcylic acid	89-86-1	-	Carboxylic acid	
Rigly	-	-	-	-
RK Blau	-	-	-	-
Rubinrot Y	-	-	-	-
Sacyclo	-	-	-	-
Salicylic acid	69-72-7	-	Carboxylic acid	
Sept	-	-	-	-
Silan 103	1067-25-0	Trimethoxyprop yl silane	Hydrocarbon; Ether	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Silan 108	3069-40-7	Trimethoxyoctyl silane	Hydrocarbon; Ether	-
Silan 165	29055-11-6	Bis(3-trimethoxysilylpropyl)sulfide	Hydrocarbon; Ether; Sulfur containing	-
Silan 167	41453-78-5	3,3,14,14-Tetramethoxy-2,15-dioxa-7,8,9,10-tetrathia-3,14-disilahexadecane	-	-
Silan 253	18784-74-2	-	-	-
Silver nitrate	7761-88-8	-	Inorganic	-
Sodium bisulfite	7631-90-5	-	Inorganic	-
Sodium sulfite	7757-83-7	-	Inorganic	-
Sodium chloride	7647-14-5	-	Inorganic	-
Sodium cyanate	917-61-3	-	Cyanate	-
Sodium disilicate	13870-28-5	Silane 69	Inorganic	-
Sodium hydrogen sulfate	7681-38-1	Sodium bisulfate	Inorganic	-
Sodium hydroxide	1310-73-2	-	Alkali	-
Sodium lauryl ether sulfate	3088-31-1	Diethylene glycol monolauryl ether sodium sulfate	-	-
Sodium lauryl sulfate	151-21-3	-	Surfactant, Anionic	Detergent
Sodium monochloroacetate	3926-62-3	Sodium chloroacetate	Carboxylic acid	-
Sodium oxalate	62-76-0	-	Inorganic	-
Sodium perborate	10486-00-7	-	Inorganic	-
Sodiumpyrosulfite	7681-57-4	Sodium metabisufite	Inorganic	-
Stearyltrimethylammonium chloride	15461-40-2	-	Surfactant, Cationic	-
Styrene	100-42-5	-	Hydrocarbon	-
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	2-Sulfanyl ethanol hydrogen sulfate	Amide	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Surfactant Based Formulation 1-HZA	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 2-HZB	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 3-HZC	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 4-HZD	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 5-HZE	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 6-HZF	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 7-HZG	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 8-HZH	-	-	Formulation	Cosmetics
Surfactant Based Formulation 9-HZI	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 10-HZJ	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 11-HZK	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 12-HZL	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 13-HZM	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 14-HZN	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 15-HZP	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 16-HZQ	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 17-HZR	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 18-HZS	-	-	Formulation	Soaps and Surfactants

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Surfactant Based Formulation 19-HZT	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 20-HZU	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 21-HZV	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 22-HZW	-	-	Formulation	Soaps and Surfactants
Surfactant Based Formulation 23-HZX	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 24-HZY	-	-	Formulation	Shampoos, Hair
Surfactant Based Formulation 25-HZZ	-	-	Formulation	Soaps and Surfactants
TA 01946 Alkylsilan	-	-	-	-
Tetraaminopyrimidine sulfate	5392-28-9	-	Heterocyclic	-
Tetrachloroethylene	127-18-4	-	Hydrocarbon	-
1,6,7,12-Tetrachloro-3,4,9,10-tetracarbonic acid anhydride	-	-	-	-
Tetrahydrofurfuryl alcohol	97-99-4	-	Alcohol	-
Theobromine	83-67-0	-	Heterocyclic	-
Theophylline sodium	3485-82-3	-	Heterocyclic	-
Theophylline sodium acetate	8002-89-9	-	Carboxylic acid	-
Thiourea	62-56-6	-	Sulfur containg	-
Tin-II-chloride	7772-99-8	-	Inorganic	-
Tocla	-	-	-	-
Toluene	108-88-3	-	Aromatic	-
Tributylamine	102-82-9	-	Amine	-
Trichloroacetic acid	76-03-9	-	Acid	-
Trichloroethane	71-55-6	-	Hydrocarbon	-
Triethanolamine	102-71-6	-	Alcohol; Amine	-
Triisooctylamine	25549-16-0	-	Amine	-
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	-	Aldehyde	-

Substances Used In HET-CAM Accuracy Analysis (Chemical and Product Classes)

Substance	CASRN	Synonyms	Chemical Class	Product Class
Trioxane	110-88-3	-	Heterocyclic	-
Triton X-100	9002-93-1	-	Surfactant, Nonionic	Detergent
Tween 20	9005-64-5	-	Surfactant, Nonionic	Detergent
Wessalith Slurry	-	-	-	-
Xanthinol nicotinate	437-74-1	-	Heterocyclic	-

Abbreviation: CASRN = Chemical Abstract Service Registry Number, EDTA = ethylenediaminetetraacetic acid.

Appendix B2

Table of Formulation Components in Gettings et al. (1991)

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Components of Formulations in Gettings et al. (1991)

Formulation	Formulation Components	% (w/w)
5% Alcohol-Cologne	PPG-5 Ceteth-20	6.00
	SD Alcohol 40	5.00
	Methylchloroiosthiazolinone/ Methylisothiazolinone	0.03
	Fragrance	1.00
	Water	87.97
10% Alcohol-Mouthwash	Sorbitol	20.000
	Cinnamon Oil	0.050
	Peppermint Oil	0.100
	Citric Acid	0.100
	FD&C Red No. 2	0.001
	Polysorbate 60	0.300
	SD Alcohol 40	10.000
	Water	69.349
15% Alcohol-Freshener	SD Alcohol 40	15.0
	Glycerin	2.0
	Allantoin	0.2
	Sodium Lactate	0.2
	Lactic Acid	0.2
	Imidizolidinyl Urea	0.1
	FD&C Color(s)	<0.01
	Fragrance	<0.01
	Water	Q.S.
20% Alcohol-Aftershave	SD Alcohol	21.10
	Methylparaben	0.20
	FD&C Blue No. 1*	0.10
	Water	78.60
	*(0.1% w/w solution)	
33% Alcohol-Perfumed Skin Lotion	Water	56.67
	SD Alcohol 40	33.00
	Isopropyl Palmitate	5.00
	Cetyl Alcohol	1.50
	PEG-40 Sterate	1.25
	Steareth-2	0.75
	Fragrance	0.50
	Oleth-10	0.50

Components of Formulations in Gettings et al. (1991)

Formulation	Formulation Components	% (w/w)
	Triethanolamine	0.38
	Carbomer	0.30
	Disodium EDTA	0.10
	Benzophernone-4	0.05
40% Alcohol-Deodorant	Water	56.5
	SD Alcohol 40	40.0
	Benzethonium chloride	0.5
	Urea	2.0
	Aluminum Chloride	1.0
55% Alcohol-Sunblock	SD Alcohol 40	55.00
	Water	20.75
	Methyl Gluceth-20	10.00
	Glycerin	10.00
	Ethyl Dihydroxypropyl PABA	3.00
	Hydroxypropylcellulose	1.25
65% Alcohol-Hair Styling Lotion	SD Alcohol 40	60.0
	PVP/VA Copolymer*	10.0
	Dimethicone Copolyol	0.2
	Fragrance	0.1
	Water	29.8
	*PVP/VA Copolymer is 50% alcohol; (i.e., contributes 5% alcohol to total)	
83% Alcohol-Cologne	SD Alcohol 40	82.35
	Fragrance	4.625
	Fragrance	5.375
	Water	7.5
	Benzophenone-2	0.1
	BHA	0.05
	FD&C Blue No. 1*	0.01 Q.S.
	D&C Orange No. 4*	0.01 Q.S.
	* (0.1% w/w solution)	
	* (2.0% w/w solution)	

Components of Formulations in Gettings et al. (1991)

Formulation	Formulation Components	% (w/w)
90% Alcohol-Pump Hair Spray	SD Alcohol 40	90.43
	Ethyl ester PVM/MA Copolymer	9.00
	Aminomethyl Propanol	0.45
	Fragrance	0.10
	Dimethicone Copolyol	0.02

Abbreviations: BHA = Butylated hydroxyanisole; D&C = Drug and Cosmetic; EDTA = ethylenediaminetetraacetic acid; FD&C = Food, Drug, and Cosmetic; PABA = *p*-Aminobenzoic acid; PEG = Polyethylene glycol; PPG = Polypropylene glycol; SD = Specially denatured.

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Appendix B3

Table of Formulation Components in Gettings et al. (1994)

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Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
HZA-Hair Masque	Deionized water	80.163
	Emulsifying wax	6.000
	Glyceryl stearate	5.000
	Stearalkonium chloride	2.350
	Dye: Green Base HJI-01-180C	2.187
	Protein CPI	2.000
	Cocamidopropyl betaine	0.500
	Hydrochloric acid (10 w/w)	0.400
	Peach pit meal (30/100)	0.300
	Lanogel 21	0.250
	Glydant	0.150
	Methylparaben	0.150
	Extrapone #3	0.100
	Extrapone #5	0.100
	Extrapone Alpine Herbs Special	0.100
HZC-Emollient Cream	Emulsifying wax NP	5.00
	PPG-2 myristyl ether proprionate	2.50
	Oleth-10	1.00
	Mineral Oil	0.50
	Squalane	3.00
	Beeswax	1.00
	Dimethicone	1.00
	Glycerin	5.00
	Imidazolidinyl urea	0.50
	Methylparaben	0.30
	Sodium borate	0.10
	Water	80.10

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
HZE-Hand and Body Lotion	Deionized water	84.10
	Glycerin, USP	5.00
	Mineral oil, 70 SUS	3.00
	Stearic acid	2.50
	Glycol stearate	1.50
	Triethanolamine 85-89%	1.00
	Acetulan	1.00
	Glyceryl monostearate C	0.70
	Cetyl alcohol	0.30
	Silicone oil 200 cSt[1]	0.20
	Veegum	0.20
	Methylparaben, USP	0.15
	Propylene glycol, USP	0.15
	Propylparaben, USP	0.10
	Carbopol 934	0.05
	Disodium sequestrene	0.05
HZF-Sunscreen SPF 15	Octyl methoxycinnamate	7.50
	Coconut oil	0.50
	Dimethicone	0.10
	Caprylic-capric triglyceride	0.50
	Squalane	0.50
	Tocopherol	0.10
	Stearic acid	2.50
	Glyceryl stearate	3.0
	Shea butter	0.25
	Butylparaben	0.10
	Propylparaben	0.15
	Octyl salicylate	0.50
	Benzphenone-3	6.00
	Propylene glycol	6.00
	Deionized water	60.96
	Methylparaben	0.30
	Triethanolamine (99%)	1.33
	Trisodium EDTA	0.10
	Allantoin	0.10
	Imidazolidinyl urea	0.30
	Ethylparaben	0.10

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
	Carbomer 934 (2% Aq)	9.00
	Polyacrylamide	0.01
	Fragrance	0.10
HZH-Cuticle Remover Cream	Carbopol 940	1.0
	Dewaxed lanolin	1.0
	Multi sterol base	1.0
	PDE (20M) sorbitan monolaurate	2.0
	Glycerin	10.0
	Potassium hydroxide 85%	1.4
	Deionized water	83.6
HZI-Hair Conditioner	Water	79.6
	Stearamidopropyl cetearyl dimonium tosylate (and) propylene glycol	3.5
	Cetearyl alcohol/ceteareth-20	3.5
	Methyl gluceth-20	3.0
	PPG-10 lanolin ether	3.0
	C12-15 alcohols benzoate	1.5
	Cetyl alcohol	1.5
	Myristyl lactate	1.0
	Hydrolyzed animal protein	1.0
	Polyquaternium-10	0.75
	Citric acid	0.7
	DL-Panthenol	0.5
	Methylparaben	0.25
	Quanternium-15	0.2
HZJ-Foot Care Cream	Deionized water	70.5
	Veegum	2.0
	Triethanolamine 99%	1.25
	Pumice #1	1.0
	Methylparaben	0.30
	Stearic acid	4.0
	Paraffin wax	15.0
	Dimethyl polysiloxane	1.0
	Glyceryl monostearate	2.0
	Cetyl alcohol	1.0
	POE (40M) stearate	1.0

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
	POB (2M) stearyl alcohol	0.75
	Germall	0.2
HZL-Hydrophilic Ointment (5% SLS)	Methyl paraben	0.025
	Propyl paraben	0.015
	Sodium lauryl sulfate	5.0
	Propylene glycol	12.0
	Stearyl alcohol	25.0
	White petrolatum	25.0
	Purified water	33.0
HZM-Hydrophilic Ointment (10% SLS)	Methyl paraben	0.025
	Propyl paraben	0.015
	Sodium lauryl sulfate	10.0
	Propylene glycol	12.0
	Stearyl alcohol	25.0
	White petrolatum	25.0
	Purified water	28.0
HZN-Moisturizing Cream	Water	84.1
	Cetearyl alcohol	6.0
	Octyldodecanol	4.0
	PEG-7 glyceryl cocoate	3.5
	Sodium lauryl sulfate	2.0
	Quaternium-15	0.2
	Methylparaben	0.2
HZO-Cleansing Cream (1)	Deionized water	70-75
	Mineral oil	15-20
	Glycerine	1-5
	Octyl palmitate	1-5
	Cetearyl alcohol	1-5
	PEG stearate	1-5
	Steareth-2	1-5
	Carbopol	<1
	Preservatives	<1
	Triethanolamine	<1
	Botanical extract	<1

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
HZR-Hand Cleanser	Deionized water	50-95
	Mineral spirits	24-40
	Tall oil fatty acid	<4
	Nonoxynol-6	<4
	Nonoxynol-9	<4
	Carbomer-940	<1
	Sodium hydroxide	<1
	Lanolin	<0.5
	Methylparaben	<0.5
	Propylparaben	<0.5
HZS-Cleansing Cream	Water	52
	Paraffin	20
	Ceresin	8.0
	Stearic acid	9.0
	Triethanolamine	5.5
	Methyl, ethyl, and propyl parabens	0.4
	Imidazolidinyl urea	0.3
	Propylene glycol	3.0
HZT-Benzoyl Peroxide Cream (2.5%)	Deionized water	86.60
	Benzoyl peroxide (70%)	3.60
	Laureth-4	5.00
	Carbomer 940	1.00
	Butylene glycol	3.00
	Triethanolamine (99%)	0.50
	Trisodium EDTA	0.10
	Methylparaben	0.20
HZU-Sunscreen Lotion	Propylene glycol	5.0
	Lanolin	5.0
	Perfecta	2.5
	Methyl paraben	0.1
	Triethanolamine (99%)	1.0
	Hystrene 5016	4.0
	Water	74.3
	Sequestrene Na_2	0.05
	Propyl paraben	0.05
	Homosalate	8.0

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
HZV-Hand and Nail Lotion	Deionized water	76.95
	2% Carbopol 934	9.0
	Hexyl laurate	2.50
	Stearic acid	2.00
	Sorbitol	1.50
	Cetyl alcohol	1.50
	Mineral oil 70 SUS	1.50
	Silicone 200/50 cSt[1]	1.00
	TEA 85-89%	0.95
	Cyclomethicone & dimethicone copolyol	0.75
	PEG-100 stearate	0.50
	Glycol stearate	0.50
	Glyceryl stearate	0.40
	Glydant	0.25
	Veegum, regular	0.20
	Methylparaben	0.15
	Propylparaben	0.10
	0.5% Yellow #10	0.10
	0.5% Red #4	0.10
	Disodium EDTA	0.05
HZW-Roll-on Antiperspirant	Water	50-75
	Aluminum zirconium tetrachlorohydrex GLY	20-35
	Magnesium aluminum silicate	1-5
	Modified starch	<4
	Glycine	<4
	Laureth-4	<4
	Laureth-23	<4
	Isopropyl myristate	<4
	Cetyl alcohol	<4
	Glyceryl stearate	<1
	Methylparaben	<1
	Propylparaben	<1
	Trisodium HEDTA	<1
	Triclosan	<0.5

Components of Formulations in Gettings et al. (1994)

Formulation	Formulation Components	% (w/w)
HZY-Cleansing Cream (II)	Deionized water	84.5
	Carbomer 934	0.3
	Propylene glycol	5.0
	Methylparaben	0.3
	Sodium lauryl sulfate*	1.0
	Sodium hydroxide	0.2
	Stearic acid	2.0
	Glyceryl stearate	2.0
	Mineral oil	3.0
	Isopropyl palmitate	1.5
	Propylparaben	0.2
	Methylchloroisothiazolinone (and) methylisothiazolinone	0.1
	* Anhydrous base	

Abbreviations: cSt = Centistrokes; PEG = Polyethylene glycol; POB = polyoxybenzylene; POE = Polyoxyethylene; PPG = Polypropylene glycol; SUS = Saybolt Universal Seconds; TEA = Triethanolamine; USP = U.S. Pharmacopoeia; w/w = weight to weight ratio.

[1]In Gettings et al. (1994), Cts is noted. However, it is proposed that the correct abbreviation is cSt.

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Appendix B4

Table of Formulation Components in Gettings et al. (1996)

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Formulation	Formulation Components	% (w/w)
HZA-Shampoo No. 7	Water	53.86
	Sodium lauryl sulfate (30%)	25.00
	Disodium laureth sulfocuccinate (40%)	15.00
	Lauramide DEA	0.50
	Butylene glucol	5.00
	Methyl and propylparabens	0.25
	Carageenan	0.35
	Methyl and methylchloroisothiazolinone	0.04
HZB-Liquid Soap No. 1	Water and volatiles	65-85
	Ammonium lauryl sulfate	1-10
	Sodium laureth sulfate	1-10
	Lauramide DEA	1-10
	Glycerine	1-10
	Isostearamidopropyl morpholine lactate	0.1-1.0
	Disodium ricinoleamido MEA-sulfosuccinate	0.1-1.0
	DMDM hydantoin	0.1-1.0
	Citric acid	0.1-1.0
	Triclosan	0.1-1.0
	Tetrasodium EDTA	<0.1
	FD&C Yellow No. 5	<0.1
	FD&C Red No. 4	<0.1
HZC-Shampoo No. 1	Water	14.037
	Laurylamidopropyl betaine (30%)	60.000
	Cetrimonium chloride	16.000
	PEG-3 cocamide	4.500
	Citric acid	3.500
	Sodium chloride	1.000
	Ditallowdimonium chloride (73%)	0.700
	Lauryl alcohol	0.250
	Methyl and chloroisothiazolinone (1.5%)	0.033

Formulation	Formulation Components	% (w/w)
HZD-Shampoo No. 5	Water	54.120
	Sodium laureth sulfate (26%)	38.00
	Cocamide DEA	3.000
	Cocamide propyl betaine (37%)	1.750
	Disodium EDTA	0.050
	Methylparaben	0.150
	Propylparaben	0.100
	Citric acid	0.250
	FD&C Yellow No. 5 (1%)	0.050
	D&C Red No. 33 (0.5%)	0.015
	DMDM hydantoin (54%)	0.300
	BHT	0.050
	Sodium glutamate	2.000
	Sodium choride	0.170
HZE-Gel Cleanser	Water	59.974
	Acylglutamate CT-12 (30%)	15.000
	Cocoamphodiacetate (50%)	15.000
	Sodium nonoxynol-6 phosphate (88.5%)	6.000
	Quaternium-26 (58%)	1.500
	PEG-120-methyl glucose dioleate	1.500
	Citric acid	0.100
	Sodium citrate	0.500
	Disodium EDTA	0.050
	Methylparaben	0.150
	DMDM hydentoin (55%)	0.200
	FD&C Yellow No. 10 (1%)	0.001
	D&C Blue No. 1 (0.746%)	0.025
HZF-Baby Shampoo No. 2	Water	57.653
	Sodium laureth (2EO) sulfate (28%)	21.430
	Disodium laureth-3-sulfosuccinate (40%)	9.090
	Cocamidopropyl betaine (30%)	10.000
	Lauramide DEA	1.500
	Kathon CG (1.5%)	0.067
	Tetrasodium EDTA (30%)	0.260

Formulation	Formulation Components	% (w/w)
HZG-Shampoo No. 8	Water	48.43
	Sodium laureth sulfate (28%)	20.00
	Sodium lauryl sulfate (30%)	25.00
	Lauramide-DEA	5.00
	Hydroxyethyl tallow glycinate	1.00
	Citric acid	0.20
	PEG-45M	0.20
	Methyl and propylparabens	0.13
	Methyl and chloromethyl-isothiazolinone	0.04
HZH-Eye Make-Up Remover	Water	96.242
	Sodium laureth sulfate (21%)	0.900
	Cocoamphocarboxyglycinate (40%)	1.100
	Hexylene glycol	1.000
	Dipotassium phosphate	0.394
	Potassium phosphate	0.102
	Allantoin	0.050
	Methyl paraben	0.150
	EDTA	0.150
	Rose water	0.008
	Thimerosal	0.003
HZI-Skin Cleanser	Water	44.0
	Sodium laureth sulfate (30%)	50.0
	Cocamide MEA	5.0
	Sodium chloride	0.4
	Disodium EDTA	0.2
	Imidizolidinyl urea	0.2
	Methylparaben	0.2
	Benzoic acid	0.1

Formulation	Formulation Components	% (w/w)
HZJ-Mild Shampoo	Water	52.09
	Tween 20	12.63
	Cocoamphodiacetate (24%)	21.25
	PEG 6000	2.60
	Cedepal TD403 (75%)	6.53
	Hydrochloric acid (15%)	1.68
	Arlacel 20	0.92
	Benzyl alcohol	0.10
	Dowicil 200	0.10
	D&C Yellow No. 10 (0.2%)	1.70
	D&C Orange No. 4 (0.2%)	0.20
HZK-Bubble Bath	Water	68.75
	Sodium laureth sulfate (60%)	25.00
	Lauramide DEA	4.50
	SD Alcohol 3-A	3.75
	Sodium chloride	0.80
	Triethanolamine	0.40
	Phosphoric acid (86.5%)	0.35
	Sorbic acid	0.20
HZL-Foam Bath	Water	47.760
	Sodium laureth sulfate (26%)	46.000
	Cocamido propyl betaine (30%)	2.500
	Sodium chloride	2.400
	Glycol monostearate	0.400
	Color solution	0.300
	DMDM hydantoin (54%)	0.250
	Methylparaben	0.200
	Propylparaben	0.100
	BHT	0.050
	Aloe vera gel	0.015
	Citric acid	0.016
	Tetrasodium EDTA	0.010

Formulation	Formulation Components	% (w/w)
HZM-Shampoo No. 3	Water	80-90
	Ammonium lauryl sulfate	5-10
	Lauramide DEA	1-5
	Cocamidopropyl sultaine	1-5
	Citric acid	<1.0
	Ammonium chloride	<1.0
	DMDM Hydantoin	<1.0
	Tetrasodium EDTA	<1.0
	Methylparaben	<1.0
	FD&C Yellow No. 5	<0.1
	D&C Yellow No. 10	<0.1
	FD&C Red No. 4	<0.1
	PPG-9	q.s.
HZN-Shampoo No. 6	Water	44.381
	Sodium laureth (2EO) sulfate (28%)	43.634
	cocamidopropyl betaine (30%)	11.760
	Tetrasodium EDTA	0.125
	Formalin	0.100
HZP-Baby Shampoo No. 1	Water	49.54
	PEG-80 sorbitan laurate (50%)	23.60
	Sodium trideceth sulfate (50%)	17.40
	Lauroamphocarboxyglycinate (50%)	5.40
	PEG-150 distearate (50%)	5.00
	Cocamidoroyl hydroxysultane (50%)	4.00
	Sodium laureth-13 carboxylate (50%)	1.00
	Quaternium 15	0.03
	Benzyl alcohol	0.05
	FD&C Yellow No. 5 (1.0%)	0.25
	FD&C Yellow No. 6 (1.0%)	0.05
	Citric acid	0.08

Formulation	Formulation Components	% (w/w)
HZQ-Cleansing Gel	Water	68.93
	Lauramphocarboxyglycinate (25%)	10.40
	Sodium trideceth sulfate (16%)	10.60
	TEA-lauryl sulfate (40%)	3.50
	Lauramide DEA	0.50
	PEG-150 distearate	2.80
	Propylene glycol	1.40
	Hexylene glycol	1.05
	Citric acid	0.28
	Diazolidinyl urea	0.20
	Methylparaben	0.20
	Sodium citrate	0.14
HZR-Facial Cleansing Foam	Water	32.97
	Sodium cocoyl isethionate	20.00
	Sodium lauroyl sarcosinate (30%)	25.00
	PPG-5-ceteth-10 phosphate	4.00
	Linoleamide DEA	2.00
	Sorbitol (70%)	2.75
	Glycol stearate	5.50
	Glycerin	2.00
	Diglycerol	2.00
	Cetearyl alcohol	2.75
	Mineral oil	0.50
	Methylparaben	0.15
	Propylparaben	0.10
	Trisodium EDTA	0.10
	Beeswax	0.10
	Ceresin	0.06
	Sodium borate	0.02

Formulation	Formulation Components	% (w/w)
HZS-Shower Gel	Water	27.567
	Sodium lauroyl sarcosinate (30%)	25.000
	Laurimidopropyl betaine (30%)	25.000
	Cocamidopropyl hydroxysultaine (50%)	15.000
	Linoleamide DEA	4.500
	Glycol stearate	1.000
	Polyquaternium-2	1.000
	Phosphoric acid (86.5%)	0.600
	Tetrasodium EDTA	0.200
	BHT	0.050
	PPG-12-buteth-16	0.050
	Methyl and chlorosothiazolinone (1.5%)	0.033
HZT-Polishing Scrub	Water	33.85
	Mineral oil	10.00
	Lauroamphocarboxyglycinate (25%)	8.80
	Sodium trideceth sulfate (16%)	9.40
	Petrolatum	6.60
	Isopropyl palmitate	6.60
	Propylene glycol	5.00
	Cetyl palmitate	4.40
	Glyceryl stearate and PEG-100 stearate	4.40
	Aluminum silicate	3.00
	Cetyl alcohol	2.50
	Polypropylene	2.50
	Magnesium aluminum silicate	1.00
	Titanium dioxide	0.50
	Hexylene glycol	0.40
	Imidazolidinyl urea	0.30
	Methylparaben	0.30
	Lactic acid	0.25
	Propylparaben	0.20

Formulation	Formulation Components	% (w/w)
HZU-Hand Soap	Water	37.95
	Sodium C14-16 olefin sulfonate (36%)	20.25
	Sodium lauroyl sarcosinate	20.00
	Cocamidopropyl hydroxysultaine	8.00
	Propylene glycol	3.00
	Glycerol stearate	3.00
	PPG-12-PEG-50 lanolin	3.00
	Polyquaternium-7	2.00
	Citric acid	1.00
	Hydrolysed animal protein	1.00
	Polyquaternium-10	0.50
	Quaternium-15	0.20
	Aloe vera gel	0.10
HZV-Shampoo No. 4	Water	80-90
	Ammonium lauryl sulfate	5-10
	Lauramide DEA	1-5
	Cocamidopropyl sultaine	<1.0
	Ammonium chloride USP	<1.0
	Citric acid	<1.0
	DMDM hydantoin	<1.0
	Tetrasodium EDTA	<1.0
	Methylparaben	<1.0
	FD&C Yellow No. 5	<1.0
	D&C Yellow No. 10	<1.0
	FD&C Red No. 4	<1.0
	PPG-9	q.s.
HZW-Liquid Soap No. 2	Water and volatiles	60-80
	TEA-lauryl sulfate	1-10
	Sodium laureth sulfate	1-10
	Sodium lauroyl sarcosinate	1-10
	Lauramide DEA	1-10
	Glycol distearate	1-10
	Isostearamideopropyl morpholine lactate	0.1-1.0
	Disodium ricinoleamido MEA-sulfosuccinate	0.1-1.0
	DMDM hydantoin	0.1-1.0
	Citric acid	0.1-1.0
	Tetrasodium EDTA	<0.1

Formulation	Formulation Components	% (w/w)
HZX-Shampoo No. 2	Water	69.1895
	Ammonium lauryl sulfate (25%)	25.0000
	Cocamide DEA	3.0000
	Hydroxypropyl methylcellulose	1.4500
	EDTA	0.6000
	Formaldehyde	0.2000
	Benzyl alcohol	0.2000
	Benzophenone-4 sodium hydroxide	0.0400
	Citric acid	0.0100
	Ammonium chloride	0.0100
	FD&C Blue No. 1	0.0005
HZY-Anti-Dandruff Shampoo	Water	27.13
	Sodium lauroyl sarcosinate (30%)	15.00
	Lauramide DEA	4.50
	TEA-lauryl sulfate (40%)	45.00
	Glycol distearate	3.00
	Zinc pyrithione	2.10
	Sodium chloride	1.20
	Citric acid	0.90
	Imidazolidinyl urea	0.50
	Methylparaben	0.30
	Propylparaben	0.10
	Xanthan gum	0.27

Formulation	Formulation Components	% (w/w)
HZZ-Facial Cleanser	Water	32.55
	Mineral oil	40.00
	Beeswax	2.30
	PEG-16 soya sterol	5.00
	PEG-8 dilaurate	2.00
	Cetearyl alcohol (70%)	0.80
	Ceteareth 20 (30%)	0.80
	Beheme acid	0.80
	Sodium borate	0.75
	Ceresin	0.50
	Carbopol dispersion (25%)	15.00
	Methylparaben	0.15
	Propylparaben	0.10
	Disodium EDTA	0.05

Abbreviations: 2EO = diethoxylated; BHT = Butylated hydroxytoluene; D&C = Drug and Cosmetic; DEA = Diethanolamide; EDTA = ethylenediaminetetraacetic acid; FD&C = Food, Drug, and Cosmetic; MEA = Monoethanolamide; PEG = Polyethylene glycol; PPG = Polypropylene glycol; TEA = Triethanolamine; USP = U.S. Pharmacopoeia; w/w = weight to weight ratio.

Appendix C

In Vitro Data for Substances Tested in the HET-CAM Test Method

C1 Test Method Protocols used to Generate *In Vitro* Data C-3

C2 Data Sorted by Reference C-15

C3 Data Sorted by Substance for IS(A) Analysis Method.....C-53

C4 Data Sorted by Substance for IS(A)-10 Analysis Method.....C-63

C5 Data Sorted by Substance for IS(A)-100 Analysis Method.....C-69

C6 Data Sorted by Substance for IS(B) Analysis Method C-75

C7 Data Sorted by Substance for IS(A)-10 Analysis Method.....C-89

C8 Data Sorted by Substance for IS(A)-100 Analysis Method.....C-111

C9 Data Sorted by Substance for Q-Score Analysis Method C-139

C10 Data Sorted by Substance for S-Score Analysis Method C-149

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Appendix C1

Test Method Protocols used to Generate *In Vitro* Data

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	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Hen Strain	Lohmann Selected Leghorn	Lohmann's Selected White Leghorn LSL	White Leghorn	White Leghorn	Leghorn SA31
Egg Criteria for Use	Weight range of eggs between 50 g and 60 g	Not Noted	Weight range of eggs between 50 g and 60 g	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.5 $\pm$ 0.5	Not Noted	37.5 $\pm$ 0.5	38	Not Noted
Relative Humidity (%)	62.5 $\pm$ 7.5	Not Noted	62.5 $\pm$ 7.5	60	Not Noted
Egg Rotation?	Yes	Not Noted	Yes	Yes	Not Noted
Checking Egg Viability	Eggs candled on Day 5 and every day thereafter; non-viable embryos removed	Not Noted	Not Noted	Candled on Day 9 and non-viable embryos removed	Not Noted
Incubation Period	10 Days	10 Days	10 Days	9 Days	10 Days
Procedure for Opening Egg	Egg shell was scratched around the air chamber with a rotating dentist saw blade and then pared off. The inner shell was removed and the CAM was layed open.	Not Noted	Egg shell around the air pocket was removed with a dental rotary saw	Eggshell was scratched around the air cells and a small aperture was opened.	Egg shell was scratched around the air cell by a dentist's rotary saw and then pared off. After removal of the inner membrane, the CAM was exposed.
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted

	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Hydro-alcoholic formulations	Chemicals from various chemical classes, commercial products, and personal care products	Oil/water -based personal care formulations	Commercial disinfectants
Total Test Substances Evaluated	21	10	32	18	6
Test Substance Quantity or Volume	0.3 mL or 0.1 g	Not Noted	0.3 mL or 0.1 g	0.3 mL	0.3 mL
Test Substance Concentrations Tested	0.1% to 100%	Not Noted	Tested solutions at concentrations that were 10% of those tested *in vivo*	3 concentrations tested: threshold concentration, 10% solution, undiluted	Diluted or undiluted
Application of Solids to CAM	Placed directly on CAM	Not Noted	All tested substances appear to be solubilized	All tested substances appear to be solubilized	All tested substances appear to be solubilized
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Distilled water
Rinse after Test Substance Application?	Yes, for solids. 20 seconds after application of test substance, rinsed with 5 mL warm water or saline solution	Not Noted	20 seconds after test substance applied rinsed with 5 mL warm water	Not Noted	Not Noted
Evaluation Period	Up to 300 seconds after test substance applied	Not Noted	At 0.5, 2, and 5 minutes after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied
Controls and Test Standards	Not Noted	Not Noted	Vehicle	Not Noted	0.1 M NaOH, 1% SDS, 0.9% NaCl, distilled water
Number of Control Eggs	Not Noted	Not Noted	2 eggs	Not Noted	2 eggs per substance
Replicate Eggs	Minimum 6 eggs	Not Noted	4 eggs	3 eggs per concentration tested	6 eggs
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	2	Not Noted
Endpoints Assessed	Hemorrhage, lysis, and coagulation	Hemorrhage, vascular lysis, coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, coagulation, lysis	Hemorrhage, vasoconstriction, coagulation
Endpoint Evaluation	The starting second that each of the three endpoints is observed is recorded.	The starting second that each of the three endpoints is observed is recorded.	Numerical time-dependent scores for three endpoints.	Seconds for the three endpoints recorded (see Kalweit, 1990)	The starting second that each of the endpoints is observed is recorded

	CEC (1991)	Gettings et al. (1991)	Bagley et al. (1992)	Gettings et al. (1994)	Vinardell and Macián (1994)
Analysis Method	Irritation Index is calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second	Two different analyses were used. Both calculated an irritation index using time (seconds) of appearance of hemorrhage vascular lysis, or coagulation. The differences between the two methods was in the particular calculations used.	Scores are totaled to give a single value (maximum of 21). Mean value of 4 eggs calculated for final value.	Calculation of an Irritation Score for each egg. Mean value of individual Irritation Scores calculated.	Irritancy Potential calculated using the formula: (301-sec H)/300*5+(301-sec v)/300*7=(301-sec C)*9; where H=Hemorrhage, V=vasoconstriction; C=Coagulation of protein or blood; sec=starting second
Classification Scheme	Not Noted	Not Noted	Not Noted	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-9.9; **Strong Irritation**: 10-21	**Practically None**: 0-0.9; **Slight Irritation**: 1-4.9; **Moderate Irritation**: 5-8.9; **Strong Irritation**: 9 21
GLP Compliance?	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Notes		Cites Luepke (1985) as basis for protocol used	Cites Luepke and Kemper (1986) as basis for protocol	Cites Luepke (1985) as basis for scoring scheme	Cites Ergatt/Frame Data Bank (1990) as basis for protocol and analysis method
				To study the effects of slow acting materials, CAM scored 15 and 30 minutes after application on range from 0 (no reactions) to 3 (strong reactions)	

	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Hen Strain	Not Noted	Not Noted	Not Noted	Lohmann's Selected White Leghorn	White Leghorn
Egg Criteria for Use	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	Not Noted	Not Noted	37.6	Not Noted	38 $\pm$ 0.5
Relative Humidity (%)	Not Noted	Not Noted	about 70	Not Noted	60 $\pm$ 5
Egg Rotation?	Not Noted	Not Noted	Yes, once per hour	Not Noted	Yes
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted	Candled on Day 9 and returned to incubator in vertical position
Incubation Period	9 Days	9 Days	10 Days	10 Days	10 Days
Procedure for Opening Egg	Not Noted	Not Noted	A portion of the egg shell was removed and a drop of water was placed onto the shell membrane to avoid bleeding. Then the CAM was exposed with forceps.	Not Noted	Shell and inner shell membrane were removed around the area defined by the air cell
Manipulation of CAM	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted

	Balls et al. (1995) (Non-Transparent Substances)	Balls et al. (1995) (Transparent Substances)	Kojima et al. (1995)	Gettings et al. (1996) (HET-CAM I, II)	Gettings et al. (1996) (HET-CAM III)
Investigator Defined Test Substance Classes	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Chemicals selected from the ECETOC database (acids, acyl halides, alcohols, aldehye, alkalis, esters, hetercyclics, hydrocarbons, inorganic chemicals, ketones, organophosphates, pesticides, surfactants, misc.)	Surfactants, solvents, formaldehyde	Surfactant-based personal care formulations	Surfactant-based personal care formulations
Total Test Substances Evaluated	59	59	24	25	25
Test Substance Quantity or Volume	Not Noted	Not Noted	0.2 mL	0.3 mL	0.1 mL
Test Substance Concentrations Tested	Not Noted	Not Noted	10% solution	3 concentrations tested: threshold concentration, 10% solution, undiluted	10% solution
Application of Solids to CAM	Not Noted	Not Noted	All tested substances appear to be solubilized	All test substances appear to be in liquid form	All test substances appear to be in liquid form
Preferred Solvent	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Rinse after Test Substance Application?	After 3 minute exposure	Not Noted	Yes, after 20 seconds test substance was rinsed with water	Not Noted	After 20 seconds, with a saline rinse
Evaluation Period	Within 30 seconds of rinsing	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance rinsed
Controls and Test Standards	5% Texapon AV (internal reference standard)	5% Texapon AV (internal reference standard)	Not Noted	Not Noted	Not Noted
Number of Control Eggs	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Replicate Eggs	6 eggs	6 eggs	4 eggs	3 eggs per concentration tested	Not Noted
Number of Replicate Experiments	Not Noted	Not Noted	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, lysis, coagulation	Hemorrhage, lysis, coagulation	Hyperemia, hemorrhage, coagulation	Hemorrhage, lysis, coagulation	Dilation, hemorrhage, coagulation
Endpoint Evaluation	Endpoints scored from 0 (no reaction) to 3 (strong reaction)	The starting second that each of the endpoints is observed is recorded	Not Noted	The starting second that each of the endpoints is observed is recorded (see Kalweit 1990)	Numerical time-dependent scores for three endpoints.

	Balls et al. (1995) (Non-Transparent Substances)	**Balls et al. (1995) (Transparent Substances)**	**Kojima et al. (1995)**	**Gettings et al. (1996) (HET-CAM I, II)**	**Gettings et al. (1996) (HET-CAM III)**
Analysis Method	Calculation of "S Score". "S Score" is calculated using the most sensitive endpoint (endpoint can change from chemical to chemical). The scores recorded for the most sensitive endpoint are summarized for the 6 eggs. (Maximum for 6 eggs is 18)	Computer program calculates an Irritation Index. Irritation Index Is used to calculate a "Q Score". "Q Score" is a comparison of the Irritation Index of a test chemical with that of the reference chemical. If the effect of test chemical is identical to reference, Q is 1.0. If effect of test chemical is less irritating, Q is lower. If effect of test chemical is more irritating, Q is higher.	Score was calculated based on the time of onset for each endpoint. Mean value of 4 eggs calculated.	Mean Irritation Score (IS; determined at 10% concentration) of 3 eggs is calculated. The Irritation Threshold Concentration (ITC; lowest concentration producing a slight reaction during observation period) is calculated.	Time-dependent scores were used to calculate a single value (maximum of 21).
Classification Scheme	**Non Irritation**: S < 6 ; **Moderately Irritating**: 6<= S <15; **Severely Irritating**: S ≥15	**Non Irritating**: Q < 1.5; **Moderately Irritating:** 1.5 < Q <2.0; **Severely Irritating**: Q < 2.0	Not Noted	**Irritant (According to FHSA)**: IS ≥ 5.1 or IS/ITC ≥ 3.0	**Irritant (According to FHSA)**: Score ≥ 4.83
GLP Compliance?	Yes	Yes	Not Noted	Not Noted	Not Noted
Notes			Cites Luepke (1985) and Luepke and Wallat (1985) as basis for scoring scheme and analysis method.		

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Hen Strain	White Essex	Not Noted	White Essex	White Leghorn
Egg Criteria for Use	Eggs were 7 days old prior to start of incubation and weighed 60 ± 5 g	Not Noted	Eggs were 7 days old	Not Noted
Egg Storage (Prior to use)	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Temperature (^{0}C)	37.0 ± 0.5	Not Noted	37 ± 0.5	37.6
Relative Humidity (%)	62.5 ± 1.5	Not Noted	52.5 ± 2.5	about 70
Egg Rotation?	Yes, with large ends upward for 9 days	Not Noted	Not Noted	Yes, once an hour
Checking Egg Viability	Not Noted	Not Noted	Not Noted	Not Noted
Incubation Period	10 Days	Not Noted	10 Days	10 Days
Procedure for Opening Egg	Eggs were candled and non-viable eggs were discarded. The airspace delimited by the inner membrane at the large end of the egg was marked. The eggshell was removed using a dentist's rotating saw blade. The inner membrane was moistened with 1.5-2.0 mL of 0.9% NaCl and the egg was returned to the incubator (at 37) for a maximum of 20 mins. After incubation, the NaCl solution was removed, using a vacuum pump, and the inner membrane was removed with forceps.	Not Noted	Not Noted	Portion of the egg shell above the air space was removed.
Manipulation of CAM	A test substance applicator (TSA), which is comprised of a perlon mesh (pore diameter = 63 micron) locked between two Teflon rings, was placed on the CAM	Not Noted	A test substance applicator (TSA) was placed on the CAM	Drop of water is placed on the membrane (to avoid capillary bleeding). A silicone rubber ring is placed on the CAM.

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Investigator Defined Test Substance Classes	Chemicals from various chemical classes	Chemicals from various chemical classes	Chemicals from various chemical classes	Surfactant, polyols, color additives, organic salts, PABA derivative, esters, inorganic chemicals, alcohols, amines, alkanolamines, carboxylic acids
Total Test Substances Evaluated	46	200	60	39
Test Substance Quantity or Volume	0.3 mL or 0.3 g of test substance placed inside the TSA	Not Noted	0.3 mL or 0.3 g of test substance placed inside the TSA	0.2 mL (placed inside the rubber ring on the CAM). Solids (0.2 g) are reduced to a fine powder with a No. 200 sieve and placed inside a rubber ring on the CAM.
Test Substance Concentrations Tested	Undiluted	1-100% solutions tested	Not Noted	0.1, 1, 10, and 100%
Application of Solids to CAM	Placed inside TSA	All tested substances appear to be solubilized	Placed inside TSA	Placed inside rubber ring
Preferred Solvent	0.9% NaCl	0.9% NaCl or olive oil	Not Noted	Not Noted
Rinse after Test Substance Application?	TSA (which contains the test substance) is removed after 20 seconds	Yes, after 5 minutes (for substances that were insoluble in eater or oil and were colored).	TSA (which contains the test substance) is removed after 20 seconds	Yes, after 20 seconds with distilled water
Evaluation Period	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	Up to 300 seconds after test substance applied	At 0.5, 2, and 5 minutes after test substance applied
Controls and Test Standards	Positive Controls: benzalkonium chloride, dimethylformamide, imidazole	Not Noted	Not Noted	Not Noted
Number of Control Eggs	Not Noted	Not Noted	Not Noted	Not Noted
Replicate Eggs	3	Not Noted	Not Noted	4 eggs
Number of Replicate Experiments	3	Not Noted	Not Noted	Not Noted
Endpoints Assessed	Hemorrhage, lysis, coagulation	Hemorrhage, coagulation, lysis	Hemorrhage, lysis, coagulation	Hyperemia, hemorrhage, coagulation
Endpoint Evaluation	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	The starting second that each of the endpoints is observed is recorded	Numerical time-dependent scores for three endpoints.

	Gilleron et al. (1996)	Spielmann et al. (1996)	Gilleron et al. (1997)	Hagino et al. (1999)
Analysis Method	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean of 3 assays were calculated. Reproducibility also was assessed.	Irritation Score calculated ((301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Lysis; C=Coagulation; sec=starting second) for 10% solution calculated (IS10). Irritation Threshold (ITC; lowest concentration of a test substance to induce an irritant reaction on the CAM) calculated.	Irritation Index calculated using the formula: (301-sec H)/300*5+(301-sec L)/300*7=(301-sec C)*9; where H=Hemorrhage, L=Vessel Lysis; C=Coagulation; sec=starting second. Mean value and SEM of are calculated.	Not Noted
Classification Scheme	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	**BGA Classification Model: Non/Slight**: ITC > 10 and IS10 <16; **Moderate**: (1) ITC > 16 and IS10 > 16 or (2) ITC < 10 and IS10 < 16; **Irritant (R36)**: (1) ITC < 10 and IS10 > 16 or (2) ITC < 2.5 and IS10 < 16; **Severe (R41)**: (1) ITC $\leq$ 1% or (2) ITC between 1 and 2.5% and IS10 $\geq$ 16. **Proposed model using mtc10 (see notes below): R41**: mtc10 < 50 seconds.	**Non Irritant**: 0-4.9; **Irritant**: 5.0-21	Not Noted
GLP Compliance?	Not Noted	Yes	Not Noted	Not Noted
Notes		Cites Luepke (1985) as basis for protocol. Cites Kalweit (1990) and Spielmann (1991) as publishing the protocol used. Cites the standard protocol for the test method as InVitox Protocol.	Cites Gilleron 1996 as basis for protocol and analysis method	Cites Luepke 1985 as basis for scoring method
		Nine additional endpoints were conducted using the raw data and the IS and IT scores in this analysis. Of these the endpoints evaluated, that best correlated with in vivo classification was mtc10 (mean detection time for appearance of coagulation when using a 10% solution).		

Abbreviations: CAM = Chorioallantoic membrane, ECETOC = European Centre for Ecotoxicology and Toxicology of Chemicals, FHSA = Federal Hazardous Substances Act (1964), IS = Irritation score, IT = Irritation threshold concentration, NaCl = Sodium chloride, NaOH = Sodium hydroxide, SDS = Sodium dodecyl sulfate, Sec = seconds.

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Appendix C2

Data Sorted by Reference

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Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6		10%	Solution	n.p.			10.75		Severe	Severe																	Bagley et al. (1992)
Triton X-100	9002-93-1		1%	Solution	n.p.			9		Severe	Severe																	Bagley et al. (1992)
Acetone	67-64-1	1	100%	Liquid	>99	water soluble													18.36	Severe								Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble													13.53	Severe								Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble													0.80	Nonirritant	Severe							Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble													10.31	Severe								Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble													1.80	Moderate								Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble													1.30	Nonirritant	Moderate							Balls et al. (1995)
Ammonium nitrate	6484-52-2	2	100%	Solid	>99.9	water soluble										18.00	Severe											Balls et al. (1995)
Ammonium nitrate	6484-52-2	4	100%	Solid	>99.9	water soluble										12.00	Moderate	Severe										Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble													0.00	Nonirritant	Nonirritant							Balls et al. (1995)
L-Aspartic acid	70-47-3	2	100%	Solid	95	water soluble										1.00	Nonirritant											Balls et al. (1995)
L-Aspartic acid	70-47-3	3	100%	Solid	95	water soluble										2.00	Nonirritant	Moderate										Balls et al. (1995)
L-Aspartic acid	70-47-3	4	100%	Solid	95	water soluble										6.00	Moderate											Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant													3.41	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant													5.00	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant													3.90	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant													4.39	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant													6.93	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant													4.43	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant													1.20	Nonirritant	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant													6.49	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant													6.09	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant													7.03	Severe								Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant													3.10	Severe	Severe							Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant													6.14	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Benzoyl-L-tartaric acid	2743-38-6	1	100%	Solid	n.p.	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	3	100%	Solid	n.p.	water soluble										4.00	Nonirritant											Balls et al. (1995)
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble													1.55	Moderate	Moderate							Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble													1.23	Nonirritant								Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble													1.80	Moderate								Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble													1.93	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble													22.04	Severe	Severe							Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble													6.64	Severe								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble													1.97	Moderate								Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble													4.02	Severe								Balls et al. (1995)
Captan 90 concentrate	133-06-2	1	100%	Solid	90	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Captan 90 concentrate	133-06-2	3	100%	Solid	90	water soluble										0.00	Nonirritant											Balls et al. (1995)
Captan 90 concentrate	133-06-2	4	100%	Solid	90	water soluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	1	100%	Solid	95	water insoluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	2	100%	Solid	95	water insoluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	3	100%	Solid	95	water insoluble										6.00	Moderate											Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	4	100%	Solid	95	water insoluble										4.00	Nonirritant											Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant													2.43	Severe	Nonirritant							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant													0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant													1.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant													0.00	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant													2.34	Severe	Severe							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant													2.42	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant													1.30	Nonirritant								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant													3.11	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant													2.71	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant													2.73	Severe								Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant													1.80	Moderate	Severe							Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant													4.67	Severe								Balls et al. (1995)
Chlorhexidine	55-56-1	1	100%	Solid	99.5	water insoluble										3.00	Nonirritant											Balls et al. (1995)
Chlorhexidine	55-56-1	3	100%	Solid	99.5	water insoluble										6.00	Moderate	Moderate										Balls et al. (1995)
Chlorhexidine	55-56-1	4	100%	Solid	99.5	water insoluble										11.00	Moderate											Balls et al. (1995)
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble													3.28	Severe								Balls et al. (1995)
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble													4.48	Severe								Balls et al. (1995)
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble													5.20	Severe	Severe							Balls et al. (1995)
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble													6.69	Severe								Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	1	100%	Solid	99.5	water insoluble										0.00	Nonirritant											Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	2	100%	Solid	99.5	water insoluble										18.00	Severe											Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	3	100%	Solid	99.5	water insoluble										0.00	Nonirritant	Severe										Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	4	100%	Solid	99.5	water insoluble										15.00	Severe											Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble													10.14	Severe								Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble													8.81	Severe								Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble													1.90	Moderate	Severe							Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble													2.53	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble													14.05	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble													10.64	Severe								Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble													11.70	Severe	Severe							Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble													14.73	Severe								Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble													2.07	Severe								Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble													0.80	Nonirritant	Severe							Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	2	100%	Solid	99.5	water insoluble										18.00	Severe											Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	4	100%	Solid	99.5	water insoluble										18.00	Severe	Severe										Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Ethanol	64-17-5	1	100%	Liquid	n.p.	water soluble													6.45	Severe	Severe							Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid	n.p.	water soluble													10.63	Severe								Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid	n.p.	water soluble													1.47	Nonirritant								Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid	n.p.	water soluble													5.95	Severe								Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble													3.94	Severe	Severe							Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble													1.87	Moderate								Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble													0.90	Nonirritant								Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble													3.37	Severe								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble													1.24	Nonirritant	Nonirritant							Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble													0.61	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble													1.00	Nonirritant								Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble													3.12	Severe								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	1	100%	Liquid	ca. 97	water insoluble													2.40	Severe	Severe							Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	2	100%	Liquid	ca. 97	water insoluble													2.51	Severe								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	3	100%	Liquid	ca. 97	water insoluble													1.10	Nonirritant								Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	4	100%	Liquid	ca. 97	water insoluble													2.35	Severe								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble													0.10	Nonirritant	Nonirritant							Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble													0.19	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble													0.30	Nonirritant								Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble													1.01	Nonirritant								Balls et al. (1995)
Fomesafen	72128-02-0	1	100%	Solid	97.5	water soluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
Fomesafen	72128-02-0	2	100%	Solid	97.5	water soluble										9.00	Moderate											Balls et al. (1995)
Fomesafen	72128-02-0	3	100%	Solid	97.5	water soluble										6.00	Moderate											Balls et al. (1995)
Fomesafen	72128-02-0	4	100%	Solid	97.5	water soluble										6.00	Moderate											Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Glycerol	56-81-5	1	100%	Liquid	99.5	water soluble													0.08	Nonirritant	Nonirritant							Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	99.5	water soluble													1.24	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	99.5	water soluble													0.60	Nonirritant								Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	99.5	water soluble													1.22	Nonirritant								Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble													5.01	Severe	Severe							Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble													3.98	Severe								Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble													1.80	Moderate								Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble													4.71	Severe								Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble													11.19	Severe	Severe							Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble													3.50	Severe								Balls et al. (1995)
Imidazole	288-32-4	2	100%	Solid	99	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Imidazole	288-32-4	4	100%	Solid	99	water soluble										18.00	Severe											Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble													4.59	Severe	Severe							Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble													3.58	Severe								Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble													1.20	Nonirritant								Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble													5.89	Severe								Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble													11.90	Severe	Severe							Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble													5.79	Severe								Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble													1.80	Moderate								Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble													4.36	Severe								Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble													0.00	Nonirritant	Nonirritant							Balls et al. (1995)
Maneb	12427-38-2	3	100%	Solid	90	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble													1.88	Moderate	Severe							Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble													5.39	Severe								Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble													1.70	Moderate								Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble													3.15	Severe								Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble													1.51	Moderate	Moderate							Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble													1.21	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble													1.00	Nonirritant								Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble													1.78	Moderate								Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble													0.18	Nonirritant	Nonirritant							Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble													1.22	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble													0.20	Nonirritant								Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble													8.09	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble													5.83	Severe	Severe							Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble													3.89	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble													2.50	Severe								Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble													6.17	Severe								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble													2.29	Severe	Moderate							Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble													1.04	Nonirritant								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble													1.50	Moderate								Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble													1.86	Moderate								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble													3.84	Severe	Severe							Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble													4.90	Severe								Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	2	100%	Solid	95	water soluble										18.00	Severe	Severe										Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	4	100%	Solid	95	water soluble										18.00	Severe											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	1	100%	Solid	99	water soluble										6.00	Moderate	Moderate										Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	2	100%	Solid	99	water soluble										13.00	Moderate											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	3	100%	Solid	99	water soluble										0.00	Nonirritant											Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	4	100%	Solid	99	water soluble										4.00	Nonirritant											Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Octanol	111-87-5	1	100%	Liquid	>99	water insoluble													2.10	Severe								Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble													1.00	Nonirritant								Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble													1.80	Moderate	Moderate							Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble													1.78	Moderate								Balls et al. (1995)
Parafluoraniline	371-40-4	1	100%	Liquid	99	water insoluble													5.25	Severe								Balls et al. (1995)
Parafluoraniline	371-40-4	2	100%	Liquid	99	water insoluble													4.46	Severe								Balls et al. (1995)
Parafluoraniline	371-40-4	3	100%	Liquid	99	water insoluble													1.90	Moderate	Severe							Balls et al. (1995)
Parafluoraniline	371-40-4	4	100%	Liquid	99	water insoluble													2.57	Severe								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid	n.p.	surfactant													1.59	Moderate								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid	n.p.	surfactant													0.72	Nonirritant								Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid	n.p.	surfactant													0.60	Nonirritant	Nonirritant							Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid	n.p.	surfactant													1.22	Nonirritant								Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble													2.17	Severe								Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble													2.50	Severe	Severe							Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble													6.07	Severe								Balls et al. (1995)
Potassium cyanate	590-28-3	2	100%	Solid	97	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	98	water soluble													3.20	Severe								Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	98	water soluble													3.00	Severe	Severe							Balls et al. (1995)
Promethazine HCl	58-33-3	2	100%	Solid	98	water soluble										18.00	Severe											Balls et al. (1995)
Promethazine HCl	58-33-3	4	100%	Solid	98	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Pyridine	110-86-1	1	100%	Liquid	>99	water soluble													3.84	Severe								Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99	water soluble													7.76	Severe								Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99	water soluble													12.90	Severe	Severe							Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99	water soluble													10.44	Severe								Balls et al. (1995)
Quinacrine	69-05-6	1	100%	Solid	n.p.	water soluble										0.00	Nonirritant											Balls et al. (1995)
Quinacrine	69-05-6	3	100%	Solid	n.p.	water soluble										4.00	Nonirritant	Nonirritant										Balls et al. (1995)
Quinacrine	69-05-6	4	100%	Solid	n.p.	water soluble										3.00	Nonirritant											Balls et al. (1995)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium hydroxide	1310-73-2	1	1%	Solution	n.p.	water soluble													6.34	Severe	Severe							Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	1%	Solution	n.p.	water soluble													6.17	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	1%	Solution	n.p.	water soluble													4.80	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	1%	Solution	n.p.	water soluble													4.36	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	10%	Solution	n.p.	water soluble													13.13	Severe	Severe							Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	10%	Solution	n.p.	water soluble													7.82	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	10%	Solution	n.p.	water soluble													23.00	Severe								Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	10%	Solution	n.p.	water soluble													9.82	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant													2.68	Severe	Severe							Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant													1.62	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant													1.70	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant													2.46	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant													2.86	Severe	Severe							Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant													2.34	Severe								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant													1.80	Moderate								Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant													4.37	Severe								Balls et al. (1995)
Sodium oxalate	62-76-0	1	100%	Solid	>99	water soluble										0.00	Nonirritant	Moderate										Balls et al. (1995)
Sodium oxalate	62-76-0	2	100%	Solid	>99	water soluble										12.00	Moderate											Balls et al. (1995)
Sodium oxalate	62-76-0	3	100%	Solid	>99	water soluble										11.00	Moderate											Balls et al. (1995)
Sodium oxalate	62-76-0	4	100%	Solid	>99	water soluble										9.00	Moderate											Balls et al. (1995)
Sodium perborate	10486-00-7	1	100%	Solid	98.6	water soluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Sodium perborate	10486-00-7	3	100%	Solid	98.6	water soluble										0.00	Nonirritant											Balls et al. (1995)
Sodium perborate	10486-00-7	4	100%	Solid	98.6	water soluble										7.00	Moderate											Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	1	100%	Solid	97	water insoluble										0.00	Nonirritant	Nonirritant										Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	3	100%	Solid	97	water insoluble										0.00	Nonirritant											Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	4	100%	Solid	97	water insoluble										6.00	Moderate											Balls et al. (1995)

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Thiourea	62-56-6	1	100%	Solid	>99	water soluble													1.31	Nonirritant	Nonirritant							Balls et al. (1995)
Thiourea	62-56-6	3	100%	Solid	>99	water soluble													0.50	Nonirritant								Balls et al. (1995)
Thiourea	62-56-6	2	100%	Solid	>99	water soluble										18.00	Severe	Severe										Balls et al. (1995)
Thiourea	62-56-6	4	100%	Solid	>99	water soluble										13.00	Moderate											Balls et al. (1995)
Toluene	108-88-3	1	100%	Liquid	99	water soluble													3.18	Severe	Severe							Balls et al. (1995)
Toluene	108-88-3	2	100%	Liquid	99	water soluble													5.84	Severe								Balls et al. (1995)
Toluene	108-88-3	3	100%	Liquid	99	water soluble													2.90	Severe								Balls et al. (1995)
Toluene	108-88-3	4	100%	Liquid	99	water soluble													2.98	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	3%	Solution	n.p.	water soluble													18.76	Severe	Severe							Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	3%	Solution	n.p.	water soluble													9.15	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	3%	Solution	n.p.	water soluble													9.90	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	3%	Solution	n.p.	water soluble													5.33	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	30%	Solution	n.p.	water soluble													14.39	Severe	Severe							Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	30%	Solution	n.p.	water soluble													9.96	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	30%	Solution	n.p.	water soluble													13.10	Severe								Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	30%	Solution	n.p.	water soluble													11.81	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant													2.66	Severe	Severe							Balls et al. (1995)
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant													2.72	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant													1.40	Nonirritant								Balls et al. (1995)
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant													2.20	Severe								Balls et al. (1995)
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant													3.45	Severe	Severe							Balls et al. (1995)
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant													1.71	Moderate								Balls et al. (1995)
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant													1.70	Moderate								Balls et al. (1995)
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant													2.40	Severe								Balls et al. (1995)

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Tween 20	9005-64-5	1	100%	Liquid	98	surfactant													0.39	Nonirritant	Nonirritant							Balls et al. (1995)
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant													0.38	Nonirritant								Balls et al. (1995)
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant													0.60	Nonirritant								Balls et al. (1995)
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant													0.95	Nonirritant								Balls et al. (1995)
Acetic acid	64-19-7	2	100%	Liquid	>99							14.8		Severe	Severe													CEC (1991)
Acetic acid	64-19-7	3	100%	Liquid	>99							13.7		Severe														CEC (1991)
Acetic acid	64-19-7	4	100%	Liquid	>99							9.3		Severe														CEC (1991)
Acetic acid	64-19-7	2	10%	Solution	>99							20.2		Severe	Severe													CEC (1991)
Acetic acid	64-19-7	3	10%	Solution	>99							13.6		Severe														CEC (1991)
Acetic acid	64-19-7	4	10%	Solution	>99							10.2		Severe														CEC (1991)
Benzalkonium chloride	8001-54-5	2	100%	Unknown	n.p.							14.5		Severe	Severe													CEC (1991)
Benzalkonium chloride	8001-54-5	3	100%	Unknown	n.p.							13.1		Severe														CEC (1991)
Benzalkonium chloride	8001-54-5	5	100%	Unknown	n.p.							5.8		Moderate														CEC (1991)
Benzalkonium chloride	8001-54-5	6	100%	Unknown	n.p.							6.9		Moderate														CEC (1991)
Benzalkonium chloride	8001-54-5	7	100%	Unknown	n.p.							13.3		Severe														CEC (1991)
Brij 35	9002-92-0	1	100%	Solid	>99							2.3		Slight	Slight													CEC (1991)
Brij 35	9002-92-0	2	100%	Solid	>99							4.3		Slight														CEC (1991)
Brij 35	9002-92-0	3	100%	Solid	>99							12.9		Severe														CEC (1991)
Brij 35	9002-92-0	4	100%	Solid	>99							4.4		Slight														CEC (1991)
Brij 35	9002-92-0	5	100%	Solid	>99							3.8		Slight														CEC (1991)
Brij 35	9002-92-0	6	100%	Solid	>99							2.6		Slight														CEC (1991)
Brij 35	9002-92-0	7	100%	Solid	>99							4		Slight														CEC (1991)
Butanol	71-36-3	1	100%	Liquid	99							11.7		Severe	Severe													CEC (1991)
Butanol	71-36-3	2	100%	Liquid	99							11.8		Severe														CEC (1991)
Butanol	71-36-3	3	100%	Liquid	99							12.6		Severe														CEC (1991)
Butanol	71-36-3	4	100%	Liquid	99							11.2		Severe														CEC (1991)
Butanol	71-36-3	5	100%	Liquid	99							3.9		Slight														CEC (1991)
Butanol	71-36-3	6	100%	Liquid	99							10.7		Severe														CEC (1991)
Butanol	71-36-3	7	100%	Liquid	99							9.9		Severe														CEC (1991)
Butanol	71-36-3	2	10%	Solution	99							14.2		Severe														CEC (1991)

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Butanol	71-36-3	3	10%	Solution	99							4.8		Slight	Severe													CEC (1991)
Butanol	71-36-3	4	10%	Solution	99							12.5		Severe														CEC (1991)
2-Butoxyethyl acetate	112-07-2	1	100%	Liquid	99							4.6		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	100%	Liquid	99							5.3		Moderate														CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	100%	Liquid	99							4.7		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	100%	Liquid	99							4.7		Slight	Slight													CEC (1991)
2-Butoxyethyl acetate	112-07-2	5	100%	Liquid	99							4		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	6	100%	Liquid	99							3.9		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	7	100%	Liquid	99							4.5		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	10%	Solution	99							4.1		Slight														CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	10%	Solution	99							0		Nonirritant	Slight													CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	10%	Solution	99							3.2		Slight														CEC (1991)
Dibutyltin chloride	683-18-1	1	100%	Solid	97							11.6		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	2	100%	Solid	97							10.8		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	4	100%	Solid	97							12.6		Severe														CEC (1991)
Dibutyltin chloride	683-18-1	5	100%	Solid	97							5.1		Moderate	Severe													CEC (1991)
Dibutyltin chloride	683-18-1	6	100%	Solid	97							5		Moderate														CEC (1991)
Dibutyltin chloride	683-18-1	7	100%	Solid	97							13		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	1	100%	Liquid	99.9							11.7		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	2	100%	Liquid	99.9							10.9		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	3	100%	Liquid	99.9							11.3		Severe														CEC (1991)
Dimethyl sulfoxide	67-68-5	4	100%	Liquid	99.9							4.1		Slight	Severe													CEC (1991)
Dimethyl sulfoxide	67-68-5	5	100%	Liquid	99.9							4.9		Slight														CEC (1991)
Dimethyl sulfoxide	67-68-5	6	100%	Liquid	99.9							7.3		Moderate														CEC (1991)
Dimethyl sulfoxide	67-68-5	7	100%	Liquid	99.9							11.4		Severe														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Dimethyl sulfoxide	67-68-5	2	10%	Solution	99.9							4.4		Slight														CEC (1991)
Dimethyl sulfoxide	67-68-5	3	10%	Solution	99.9							4.1		Slight	Slight													CEC (1991)
Dimethyl sulfoxide	67-68-5	4	10%	Solution	99.9							4.1		Slight														CEC (1991)
Glycerol	56-81-5	1	100%	Liquid	>99							10.8		Severe														CEC (1991)
Glycerol	56-81-5	2	100%	Liquid	>99							11.3		Severe														CEC (1991)
Glycerol	56-81-5	3	100%	Liquid	>99							10.3		Severe														CEC (1991)
Glycerol	56-81-5	4	100%	Liquid	>99							4.8		Slight	Severe													CEC (1991)
Glycerol	56-81-5	5	100%	Liquid	>99							0		Nonirritant														CEC (1991)
Glycerol	56-81-5	6	100%	Liquid	>99							0		Nonirritant														CEC (1991)
Glycerol	56-81-5	7	100%	Liquid	>99							9.4		Severe														CEC (1991)
Glycerol	56-81-5	2	10%	Solution	>99							8.7		Moderate														CEC (1991)
Glycerol	56-81-5	3	10%	Solution	>99							4.4		Slight	Slight													CEC (1991)
Glycerol	56-81-5	4	10%	Solution	>99							3.6		Slight														CEC (1991)
n-Hexane	110-54-3	1	100%	Liquid	99							2.9		Slight														CEC (1991)
n-Hexane	110-54-3	2	100%	Liquid	99							5.4		Moderate														CEC (1991)
n-Hexane	110-54-3	3	100%	Liquid	99							4.2		Slight														CEC (1991)
n-Hexane	110-54-3	4	100%	Liquid	99							10.3		Severe	Slight													CEC (1991)
n-Hexane	110-54-3	5	100%	Liquid	99							2.3		Slight														CEC (1991)
n-Hexane	110-54-3	6	100%	Liquid	99							8.1		Moderate														CEC (1991)
n-Hexane	110-54-3	7	100%	Liquid	99							2.4		Slight														CEC (1991)
n-Hexane	110-54-3	2	10%	Solution	99							3.7		Slight														CEC (1991)
n-Hexane	110-54-3	3	10%	Solution	99							0		Nonirritant	Severe													CEC (1991)
n-Hexane	110-54-3	4	10%	Solution	99							10.1		Severe														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
2-Methoxyethanol	109-86-4	1	100%	Liquid	99							9.7		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	2	100%	Liquid	99							12.2		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	3	100%	Liquid	99							12.1		Severe														CEC (1991)
2-Methoxyethanol	109-86-4	4	100%	Liquid	99							8.6		Moderate	Severe													CEC (1991)
2-Methoxyethanol	109-86-4	5	100%	Liquid	99							4.5		Slight														CEC (1991)
2-Methoxyethanol	109-86-4	6	100%	Liquid	99							0.8		Nonirritant														CEC (1991)
2-Methoxyethanol	109-86-4	7	100%	Liquid	99							3.1		Slight														CEC (1991)
2-Methoxyethanol	109-86-4	2	10%	Solution	99							7		Moderate														CEC (1991)
2-Methoxyethanol	109-86-4	3	10%	Solution	99							0		Nonirritant	Moderate													CEC (1991)
2-Methoxyethanol	109-86-4	4	10%	Solution	99							3.1		Slight														CEC (1991)
Sodium lauryl sulfate	151-21-3	1	100%	Solid	98							11.4		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	2	100%	Solid	98							10.3		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	3	100%	Solid	98							13.9		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	4	100%	Solid	98							4.8		Slight	Severe													CEC (1991)
Sodium lauryl sulfate	151-21-3	6	100%	Solid	98							11.1		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	7	100%	Solid	98							9.7		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	2	10%	Solution	98							18.4		Severe														CEC (1991)
Sodium lauryl sulfate	151-21-3	3	10%	Solution	98							14.1		Severe	Severe													CEC (1991)
Sodium lauryl sulfate	151-21-3	4	10%	Solution	98							5.1		Moderate														CEC (1991)
Toluene	108-88-3	1	100%	Liquid	99.9							8.8		Moderate														CEC (1991)
Toluene	108-88-3	2	100%	Liquid	99.9							14.8		Severe														CEC (1991)
Toluene	108-88-3	3	100%	Liquid	99.9							15.2		Severe														CEC (1991)
Toluene	108-88-3	4	100%	Liquid	99.9							11.5		Severe	Severe													CEC (1991)
Toluene	108-88-3	5	100%	Liquid	99.9							4.6		Slight														CEC (1991)
Toluene	108-88-3	6	100%	Liquid	99.9							3.1		Slight														CEC (1991)
Toluene	108-88-3	7	100%	Liquid	99.9							4.9		Slight														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triacetin	102-76-1	1	100%	Liquid	99							3.6		Slight														CEC (1991)
Triacetin	102-76-1	2	100%	Liquid	99							4.3		Slight														CEC (1991)
Triacetin	102-76-1	3	100%	Liquid	99							5.5		Moderate														CEC (1991)
Triacetin	102-76-1	4	100%	Liquid	99							4.4		Slight	Slight													CEC (1991)
Triacetin	102-76-1	5	100%	Liquid	99							3.3		Slight														CEC (1991)
Triacetin	102-76-1	6	100%	Liquid	99							4.3		Slight														CEC (1991)
Triacetin	102-76-1	7	100%	Liquid	99							3.1		Slight														CEC (1991)
Triacetin	102-76-1	2	10%	Solution	99							13.6		Severe														CEC (1991)
Triacetin	102-76-1	3	10%	Solution	99							2		Slight	Slight													CEC (1991)
Triacetin	102-76-1	4	10%	Solution	99							3.3		Slight														CEC (1991)
Tributyltin chloride	1461-22-9	1	100%	Solid	96							6.7		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	2	100%	Solid	96							8.9		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	3	100%	Solid	96							13.7		Severe														CEC (1991)
Tributyltin chloride	1461-22-9	4	100%	Solid	96							8.8		Moderate	Moderate													CEC (1991)
Tributyltin chloride	1461-22-9	5	100%	Solid	96							7.4		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	6	100%	Solid	96							7.9		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	7	100%	Solid	96							6.6		Moderate														CEC (1991)
Tributyltin chloride	1461-22-9	2	10%	Solution	96							15.6		Severe														CEC (1991)
Tributyltin chloride	1461-22-9	3	10%	Solution	96							9.6		Severe	Severe													CEC (1991)
Tributyltin chloride	1461-22-9	4	10%	Solution	96							11.2		Severe														CEC (1991)
Triethanolamine	102-71-6	1	100%	Liquid	97							8.6		Moderate														CEC (1991)
Triethanolamine	102-71-6	2	100%	Liquid	97							10.4		Severe														CEC (1991)
Triethanolamine	102-71-6	3	100%	Liquid	97							11.9		Severe														CEC (1991)
Triethanolamine	102-71-6	4	100%	Liquid	97							4.2		Slight	Severe													CEC (1991)
Triethanolamine	102-71-6	5	100%	Liquid	97							0		Nonirritant														CEC (1991)
Triethanolamine	102-71-6	6	100%	Liquid	97							3.7		Slight														CEC (1991)
Triethanolamine	102-71-6	7	100%	Liquid	97							7.5		Moderate														CEC (1991)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Triethanolamine	102-71-6	2	10%	Solution	97							11.3		Severe														CEC (1991)
Triethanolamine	102-71-6	3	10%	Solution	97							2.8		Slight	Slight													CEC (1991)
Triethanolamine	102-71-6	4	10%	Solution	97							1.1		Slight														CEC (1991)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)			100%	Solution	n.a.							4.6		Slight														Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)			100%	Solution	n.a.							5		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)			100%	Solution	n.a.							8.5		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)			100%	Solution	n.a.							5.3		Moderate														Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)			100%	Solution	n.a.																							Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)			100%	Solution	n.a.							11.9		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)			100%	Solution	n.a.							12.8		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)			100%	Solution	n.a.							12.7		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)			100%	Solution	n.a.							13.8		Severe														Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)			100%	Solution	n.a.							13.6		Severe														Gettings et al. (1991)
Oil/Water Emulsion-HZA			100%	Solution	n.a.			0		Nonirritant	Nonirritant	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution	n.a.			0.283		Nonirritant	Nonirritant	3		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution	n.a.			0.533		Nonirritant	Nonirritant	3.67		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution	n.a.			7.33		Moderate	Moderate	3.67		Slight														Gettings et al. (1994)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Oil/Water Emulsion-HZH[a]			100%	Solution	n.a.			17.8		Severe	Severe	23		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution	n.a.			1.97		Slight	Slight	0.333		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution	n.a.			0.917		Nonirritant	Nonirritant	3		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution	n.a.			4.83		Slight	Slight	10.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution	n.a.			8.33		Moderate	Moderate	14.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution	n.a.			3.33		Slight	Slight	3.67		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution	n.a.			0.5		Nonirritant	Nonirritant	0		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution	n.a.			10.6		Severe	Severe	16.3		Severe														Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution	n.a.			11.6		Severe	Severe	8.33		Moderate														Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution	n.a.			4.1		Slight	Slight	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution	n.a.			0		Nonirritant	Nonirritant	1		Slight														Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution	n.a.			0.6		Nonirritant	Nonirritant	0		Nonirritant														Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution	n.a.			0.167		Nonirritant	Nonirritant	5		Moderate														Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution	n.a.			17		Severe	Severe	9.67		Severe														Gettings et al. (1994)
Surfactant Based Formulation 1-HZA			10%	Solution	n.a.			7.8		Moderate	Moderate	9.6		Severe														Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution	n.a.			4.8		Slight	Slight	7.3		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution	n.a.			9.5		Severe	Severe	15.3		Severe														Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution	n.a.			5.2		Moderate	Moderate	8.7		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution	n.a.			3.8		Slight	Slight	11.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution	n.a.			8.3		Moderate	Moderate	10.9		Severe														Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution	n.a.			6.3		Moderate	Moderate	7.1		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution	n.a.			1.3		Slight	Slight	3.5		Slight														Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution	n.a.			9.3		Severe	Severe	15.2		Severe														Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution	n.a.			2.2		Slight	Slight	6.2		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution	n.a.			8.8		Moderate	Moderate	9.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution	n.a.			9.6		Severe	Severe	12.4		Severe														Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution	n.a.			4.1		Slight	Slight	2.7		Slight														Gettings et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Surfactant Based Formulation 14-HZN			10%	Solution	n.a.			6.1		Moderate	Moderate	8		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution	n.a.			4.7		Slight	Slight	4.4		Slight														Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution	n.a.			4.9		Slight	Slight	4.2		Slight														Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution	n.a.			7.7		Moderate	Moderate	5.3		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution	n.a.			8.8		Moderate	Moderate	12.2		Severe														Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution	n.a.			0.2		Nonirritant	Nonirritant	3.5		Slight														Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution	n.a.			3.7		Slight	Slight	6.2		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution	n.a.			7.7		Moderate	Moderate	8.7		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution	n.a.			7.8		Moderate	Moderate	5.1		Moderate														Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution	n.a.			9		Severe	Severe	11.3		Severe														Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution	n.a.			8.7		Moderate	Moderate	11.7		Severe														Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution	n.a.			0.7		Nonirritant	Nonirritant	1.1		Slight														Gettings et al. (1996)
Allyl alcohol	107-18-6		100%	Liquid	n.p.							12.4	2.3	Severe														Gilleron et al. (1996)
2-Aminophemol	95-55-6		100%	Solid	n.p.							0.8	0.7	Nonirritant														Gilleron et al. (1996)
Anthracene	120-12-7		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
Benzethonium chloride	121-54-0		100%	Solid	n.p.							15.4	3.1	Severe														Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%	Liquid	n.p.							13.9	1.8	Severe														Gilleron et al. (1996)
Cyclohexanone	108-94-1		100%	Liquid	n.p.							14.5	3.8	Severe														Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%	Solid	n.p.							9.7	5.8	Severe														Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%	Liquid	n.p.							15.1	2.7	Severe														Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.							4.2	2.5	Slight														Gilleron et al. (1996)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%	Solid	n.p.							3.8	2.2	Slight														Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9		100%	Solid	n.p.							8.4	2.2	Moderate														Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5		100%	Liquid	n.p.							11.3	3.7	Severe														Gilleron et al. (1996)
EDTA dipotassium	25105-12-9		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid	n.p.							11.3	2.8	Severe														Gilleron et al. (1996)
2-Ethoxyethanol	110-80-5		100%	Liquid	n.p.							10.5	2.7	Severe														Gilleron et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Ethylacetoacetate	141-97-9		100%	Liquid	n.p.							10	3.2	Severe														Gilleron et al. (1996)
Furan	110-00-9		100%	Liquid	n.p.							5.5	1	Moderate														Gilleron et al. (1996)
Gluconolactone	90-80-2		100%	Solid	n.p.							4.6	3.2	Slight														Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7		100%	Solid	n.p.							0.7	1.2	Nonirritant														Gilleron et al. (1996)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%	Liquid	n.p.							4.3	1	Slight														Gilleron et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%	Liquid	n.p.							10.8	4.8	Severe														Gilleron et al. (1996)
Hexane	110-54-3		100%	Liquid	n.p.							3.1	2.7	Slight														Gilleron et al. (1996)
Imidazole	288-32-4		100%	Solid	n.p.							18.7	0.9	Severe														Gilleron et al. (1996)
Iminodibenzyl	94-19-9		100%	Solid	n.p.							0	0	Nonirritant														Gilleron et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%	Solid	n.p.							12.7	4.3	Severe														Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%	Unknown	n.p.							8.3	1.2	Moderate														Gilleron et al. (1996)
Magnesium carbonate	56378-72-4		100%	Solid	n.p.							1.4	1.9	Slight														Gilleron et al. (1996)
Methanol	67-56-1		100%	Liquid	n.p.							12.2	3.3	Severe														Gilleron et al. (1996)
2-Methoxyethanol	109-86-4		100%	Liquid	n.p.							14.5	0.7	Severe														Gilleron et al. (1996)
Methyl isobutyl ketone	108-10-1		100%	Liquid	n.p.							10.5	1.5	Severe														Gilleron et al. (1996)
MYRJ 45			100%	Unknown	n.p.							0.00	0.00	Nonirritant														Gilleron et al. (1996)
1-Nitropropane	108-03-2		100%	Liquid	n.p.							2.8	2.7	Slight														Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid	n.p.							9.8	1.7	Severe														Gilleron et al. (1996)
2,4-Pentadione	123-54-6		100%	Liquid	n.p.							8.8	3	Moderate														Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%	Solid	n.p.							0.5	0.4	Nonirritant														Gilleron et al. (1996)
Polyoxyethylene 23 lauryl ether			100%	Solid	n.p.							1.5	2.6	Slight														Gilleron et al. (1996)
Promethazine HCl	58-33-3		100%	Solid	n.p.							13.9	2.1	Severe														Gilleron et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3		100%	Solid	n.p.							1.9	1	Slight														Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid	n.p.							15.8	3.6	Severe														Gilleron et al. (1996)
Quinacrine	69-05-6		100%	Solid	n.p.							6.5	2.2	Moderate														Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	n.p.							0.5	0.9	Nonirritant														Gilleron et al. (1996)
Thiourea	62-56-6		100%	Solid	n.p.							13.7	4.4	Severe														Gilleron et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
1,2,3-Trichloropropane	96-18-4		100%	Liquid	n.p.							7.9	1.7	Moderate														Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%	Liquid	n.p.							4.5	2.9	Slight														Gilleron et al. (1996)
Triethanolamine	102-71-6		100%	Liquid	n.p.							9.6	3.5	Severe														Gilleron et al. (1996)
Triton X-155	9010-44-0		100%	Surfactant	n.p.							3.9	2.3	Slight														Gilleron et al. (1996)
Acetone	67-64-1		100%	Liquid	>99	water soluble						15.32	0.33	Severe														Gilleron et al. (1997)
Ammonium nitrate	6484-52-2		100%	Solid	>99.9	water soluble						15.34	1.24	Severe														Gilleron et al. (1997)
L-Aspartic acid	70-47-3		100%	Solid	95	water soluble						1.06	1.2	Slight														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						14.8	0.53	Severe														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						15.05	0.27	Severe														Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Unknown	98	surfactant						15.14	0.25	Severe														Gilleron et al. (1997)
Benzoyl-L-tartaric acid	2743-38-6		100%	Solid	n.p.	water soluble						13.34	4.24	Severe														Gilleron et al. (1997)
Butyl acetate	123-86-4		100%	Liquid	99	water insoluble						17.21	1.84	Severe														Gilleron et al. (1997)
Gamma-butyrolactone	96-48-0		100%	Liquid	>99	water soluble						19.39	0.83	Severe														Gilleron et al. (1997)
Captan 90 concentrate	133-06-2		100%	Solid	90	water soluble						15.07	0.27	Severe														Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%	Solid	95	water insoluble						3.95	4.69	Slight														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						12.68	1.52	Severe														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						13.53	2.42	Severe														Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Solid	98	surfactant						14.6	0.43	Severe														Gilleron et al. (1997)
Chlorhexidine	55-56-1		100%	Solid	99.5	water insoluble						14.87	3.78	Severe														Gilleron et al. (1997)
Cyclohexanol	108-93-0		100%	Liquid	97	water soluble						18.96	0.1	Severe														Gilleron et al. (1997)
Dibenzyl phosphate	1623-08-1		100%	Solid	99.5	water insoluble						15.16	0.47	Severe														Gilleron et al. (1997)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%	Liquid	99	water insoluble						10.74	1.74	Severe														Gilleron et al. (1997)
2,2-Dimethylbutanoic acid	595-37-9		100%	Liquid	>99	water insoluble						15.31	0.24	Severe														Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2		100%	Solid	99.5	water insoluble						15.33	0.38	Severe														Gilleron et al. (1997)
Ethanol	64-17-5		100%	Liquid	n.p.	water soluble						14.97	0.04	Severe														Gilleron et al. (1997)
Ethyl acetate	141-78-6		100%	Liquid	99	water soluble						19.32	0.06	Severe														Gilleron et al. (1997)
2-Ethyl-1-hexanol	104-76-7		100%	Liquid	99	water soluble						12.71	2.96	Severe														Gilleron et al. (1997)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Ethyl-2-methylacetoacetate	609-14-3		100%	Liquid	ca. 97	water insoluble						12.94	2.94	Severe														Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%	Liquid	99	water insoluble						13.82	2.73	Severe														Gilleron et al. (1997)
Fomesafen	72128-02-0		100%	Solid	97.5	water soluble						1.21	1.29	Slight														Gilleron et al. (1997)
Glycerol	56-81-5		100%	Liquid	99.5	water soluble						14.78	0.75	Severe														Gilleron et al. (1997)
Hexanol	111-27-3		100%	Liquid	98	water insoluble						17.56	0.4	Severe														Gilleron et al. (1997)
Imidazole	288-32-4		100%	Solid	99	water soluble						19.43	0.49	Severe														Gilleron et al. (1997)
Isobutanol	78-83-1		100%	Liquid	99.9	water insoluble						19.41	0.08	Severe														Gilleron et al. (1997)
Isopropanol	67-63-0		100%	Liquid	99.9	water soluble						14.8	0.21	Severe														Gilleron et al. (1997)
Maneb	12427-38-2		100%	Solid	90	water soluble						0.16	0.24	Nonirritant														Gilleron et al. (1997)
Methyl acetate	79-20-9		100%	Liquid	98	water soluble						18.98	0.75	Severe														Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%	Liquid	99	water soluble						16.31	1.23	Severe														Gilleron et al. (1997)
Methylcyclopentane	96-37-7		100%	Liquid	>99	water insoluble						17.14	1.63	Severe														Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%	Liquid	99	water soluble						18.35	2.52	Severe														Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid	98	water insoluble						17.75	2.2	Severe														Gilleron et al. (1997)
1-Naphthalene acetic acid	86-87-3		100%	Solid	99	water soluble						7.46	2.37	Moderate														Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%	Solid	95	water soluble						15.16	0.49	Severe														Gilleron et al. (1997)
Octanol	111-87-5		100%	Liquid	>99	water insoluble						16.7	0.81	Severe														Gilleron et al. (1997)
Parafluoraniline	371-40-4		100%	Liquid	99	water insoluble						15.49	1.63	Severe														Gilleron et al. (1997)
Polyethylene glycol 400	25322-68-3		100%	Liquid	n.p.	surfactant						14.68	0.55	Severe														Gilleron et al. (1997)
Potassium cyanate	590-28-3		100%	Solid	97	water soluble						14.27	1.15	Severe														Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid	98	water soluble						6.27	1.41	Moderate														Gilleron et al. (1997)
Pyridine	110-86-1		100%	Liquid	>99	water soluble						17.79	2.44	Severe														Gilleron et al. (1997)
Quinacrine	69-05-6		100%	Solid	n.p.	water soluble						7.29	0.6	Moderate														Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble						19.01	0.13	Severe														Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Solid	n.p.	water soluble						20.56	0.08	Severe														Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant						12.38	1.82	Severe														Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Solid	98	surfactant						15.05	0.29	Severe														Gilleron et al. (1997)

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Sodium oxalate	62-76-0		100%	Solid	>99	water soluble						14.2	0.71	Severe														Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%	Solid	98.6	water soluble						13.19	1.78	Severe														Gilleron et al. (1997)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	97	water insoluble						4.33	0.23	Slight														Gilleron et al. (1997)
Thiourea	62-56-6		100%	Solid	>99	water soluble						17.89	1.53	Severe														Gilleron et al. (1997)
Toluene	108-88-3		100%	Liquid	99	water soluble						16.09	1.62	Severe														Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble						15.7	0.11	Severe														Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid	n.p.	water soluble						15.72	0.15	Severe														Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant						10.94	0.8	Severe														Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant						13.73	0.48	Severe														Gilleron et al. (1997)
Tween 20	9005-64-5		100%	Liquid	98	surfactant						14.47	0.36	Severe														Gilleron et al. (1997)
Acetic acid	64-19-7	1	10%	Solution	n.p.		2.4	16.5	2.89	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	2	10%	Solution	n.p.		2.4	16	3.92	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	3	10%	Solution	n.p.		2.4	17.25	6.24	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	4	10%	Solution	n.p.		2.4	19.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	5	10%	Solution	n.p.		2.4	17.5	4.04	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	1	10%	Suspension	n.p.		7.31	8.25	2.87	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	2	10%	Suspension	n.p.		7.31	10.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	3	10%	Suspension	n.p.		7.31	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	4	10%	Suspension	n.p.		7.31	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	5	10%	Suspension	n.p.		7.31	5.75	1.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data

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Cetyltrimethylammonium bromide	57-09-0	1	10%	Solution	n.p.		5.89	19	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	2	10%	Solution	n.p.		5.89	13.25	2.22	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	3	10%	Solution	n.p.		5.89	18.5	1.91	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	4	10%	Solution	n.p.		5.89	11	2.45	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	5	10%	Solution	n.p.		5.89	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	1	10%	Solution	n.p.		6.56	19	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	2	10%	Solution	n.p.		6.56	13.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	3	10%	Solution	n.p.		6.56	16	2.45	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	4	10%	Solution	n.p.		6.56	11.75	4.86	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	5	10%	Solution	n.p.		6.56	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	1	10%	Suspension	n.p.		6.54	10	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	2	10%	Suspension	n.p.		6.54	10	1.63	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	3	10%	Suspension	n.p.		6.54	10.25	3.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	4	10%	Suspension	n.p.		6.54	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	5	10%	Suspension	n.p.		6.54	5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	1	10%	Solution	n.p.		11.89	8.25	2.36	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	2	10%	Solution	n.p.		11.89	8.5	4.04	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	3	10%	Solution	n.p.		11.89	9	1.15	Severe	Moderate																	Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	4	10%	Solution	n.p.		11.89	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	5	10%	Solution	n.p.		11.89	5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Domiphen bromide	538-71-6	1	10%	Solution	n.p.		6.22	19	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	2	10%	Solution	n.p.		6.22	15.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	3	10%	Solution	n.p.		6.22	14.75	1.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	4	10%	Solution	n.p.		6.22	12.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	5	10%	Solution	n.p.		6.22	9	1.22	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	10%	Solution	n.p.		5.9	0	0.00	Nonirritant																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	10%	Solution	n.p.		5.9	1.25	2.50	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	10%	Solution	n.p.		5.9	10.5	1.91	Severe	Slight																	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	10%	Solution	n.p.		5.9	1.5	1.73	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	10%	Solution	n.p.		5.9	1.25	2.50	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	100%	Liquid	n.p.			18.75	3.30	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid	n.p.			16	2.45	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid	n.p.			11.5	1.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid	n.p.			17	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid	n.p.			10.5	1.73	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	1	10%	Solution	n.p.		1.76	19.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	2	10%	Solution	n.p.		1.76	20	1.15	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	3	10%	Solution	n.p.		1.76	17.75	3.95	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	4	10%	Solution	n.p.		1.76	12.25	2.36	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	5	10%	Solution	n.p.		1.76	12.75	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Lactic acid	50-21-5	1	10%	Solution	n.p.		1.94	20.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	10%	Solution	n.p.		1.94	14.25	2.06	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	10%	Solution	n.p.		1.94	19.5	1.91	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	10%	Solution	n.p.		1.94	18.5	1.91	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	10%	Solution	n.p.		1.94	10.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid	n.p.			21	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid	n.p.			6.25	2.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid	n.p.			16	1.15	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid	n.p.			15.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid	n.p.			11.5	2.89	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	1	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	2	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	3	10%	Solution	n.p.		12.58	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	4	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	5	10%	Solution	n.p.		12.58	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	1	10%	Solution	n.p.		10.49	20	1.15	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	2	10%	Solution	n.p.		10.49	13.25	2.50	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	3	10%	Solution	n.p.		10.49	12	0.00	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	4	10%	Solution	n.p.		10.49	12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	5	10%	Solution	n.p.		10.49	19.33	0.82	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Stearyltrimethylammonium chloride	15461-40-2	1	10%	Solution	n.p.		4.24	16.75	2.06	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	2	10%	Solution	n.p.		4.24	13	2.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	3	10%	Solution	n.p.		4.24	15.75	3.50	Severe	Severe																	Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	4	10%	Solution	n.p.		4.24	13.5	1.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	5	10%	Solution	n.p.		4.24	9	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	1	10%	Solution	n.p.		11.26	1.5	2.38	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	10%	Solution	n.p.		11.26	3.75	4.79	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	10%	Solution	n.p.		11.26	11	1.15	Severe	Slight																	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	10%	Solution	n.p.		11.26	6	1.63	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	10%	Solution	n.p.		11.26	2.5	2.89	Slight																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	1	100%	Liquid	n.p.			5	0.00	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid	n.p.			6.75	3.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid	n.p.			11.5	1.00	Severe	Moderate																	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid	n.p.			12	0.00	Severe																		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid	n.p.			6.75	3.50	Moderate																		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5		10%	Solution	n.p.		7.2	4		Slight	Slight																	Kojima et al. (1995)
Potassium laurate	10124-65-9		10%	Solution	98		9.4	14.3		Severe	Severe																	Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3		10%	Solution	98		5.4	7.5		Moderate	Moderate																	Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2		10%	Solution	65		5.5	19.3		Severe	Severe																	Kojima et al. (1995)
Triton X-100	9002-93-1		10%	Solution	n.p.		5.75	5		Moderate	Moderate																	Kojima et al. (1995)
7-Acetoxyheptanal[7]		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.1	Slight	Slight	4.9	Slight	Severe	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		17	Severe		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	100%, 10%, and ITC	-	n.p.	83	2.2															13.6	Severe	Severe	n.p.		Severe	Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
n-Acetyl-Methionine	1115-47-5	WA	100%, 10%, and ITC	-	n.p.	83	2.2															6.1	Moderate	Severe	10.6	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	BG	100%, 10%, and ITC	-	n.p.	600	9															10.7	Severe	Severe	12.8	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	100%, 10%, and ITC	-	n.p.	600	9															15.8	Severe		16.9	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	100%, 10%, and ITC	-	n.p.	3	1.5															14.8	Severe	Moderate	14.4	Severe	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	100%, 10%, and ITC	-	n.p.	3	1.5															7	Moderate		13.6	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	100%, 10%, and ITC	-	n.p.	3	1.5															7.6	Moderate		8.5	Moderate		Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	HO	100%, 10%, and ITC	-	n.p.	560	1.5															4.4	Slight	Slight	n.p.			Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	100%, 10%, and ITC	-	n.p.	560	1.5															n.p.			n.p.			Spielmann et al. (1996)
Anisole	100-66-3	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															7.3	Moderate	Moderate	19.1	Severe	Severe	Spielmann et al. (1996)
Anisole	100-66-3	HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		18.5	Severe		Spielmann et al. (1996)
B 25		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
n-Butanal	123-72-8	HK	100%, 10%, and ITC	-	n.p.	71	<7															1.2	Slight	Moderate	20.3	Severe	Severe	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	100%, 10%, and ITC	-	n.p.	71	<7															6.7	Moderate		18.1	Severe		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	100%, 10%, and ITC	-	n.p.	79	7															9.6	Severe	Severe	13	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	100%, 10%, and ITC	-	n.p.	79	7															18.3	Severe		20.2	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BD	100%, 10%, and ITC	-	n.p.	1	n.s.															0	Nonirritant	Severe	11.5	Severe	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	100%, 10%, and ITC	-	n.p.	1	n.s.															10.9	Severe		11.6	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	100%, 10%, and ITC	-	n.p.	1	n.s.															9.5	Severe		14.9	Severe		Spielmann et al. (1996)

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Caffeine sodium benzoate	8000-95-1	BD	100%, 10%, and ITC	-	n.p.	500	7															4.6	Slight	Moderate	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	100%, 10%, and ITC	-	n.p.	500	7															7.9	Moderate		17.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	100%, 10%, and ITC	-	n.p.	500	7															6.6	Moderate		14	Severe		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	100%, 10%, and ITC	-	n.p.	400	7															7.4	Moderate	Severe	16	Severe	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	100%, 10%, and ITC	-	n.p.	400	7															9.8	Severe		18.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	7															2	Severe	Severe	4	Slight	Slight	Spielmann et al. (1996)
Camphen	79-92-5	HK	100%, 10%, and ITC	-	n.p.	insoluble	7															10	Severe		n.p.			Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	BG	100%, 10%, and ITC	-	n.p.		3															6.9	Moderate	Moderate	15.1	Severe	Severe	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	100%, 10%, and ITC	-	n.p.		3															7.9	Moderate		19.25	Severe		Spielmann et al. (1996)
1-Chloroctane-8-ol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															6.8	Moderate	Moderate	18.7	Severe	Severe	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.3	Slight		14.3	Severe		Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															10.1	Severe	Severe	18.9	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															11.8	Severe		19	Severe		Spielmann et al. (1996)
DC 8		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Nonirritant	0	Nonirritant	Moderate	Spielmann et al. (1996)
DC 8		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		5	Moderate		Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	HO	100%, 10%, and ITC	-	n.p.	0.2	7															4.2	Slight	Slight	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	100%, 10%, and ITC	-	n.p.	0.2	7															0	Nonirritant		n.p.			Spielmann et al. (1996)
Diepoxid 126	2386-87-0	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															6	Moderate	Moderate	10	Severe	Severe	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															8.6	Moderate		15.6	Severe		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.9	Slight		6	Moderate		Spielmann et al. (1996)

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2,5-Dimethylhexanediol	110-03-2	HK	100%, 10%, and ITC	-	n.p.		n.s.															9.2	Severe	Severe	16.6	Severe	Severe	Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	100%, 10%, and ITC	-	n.p.		n.s.															4.1	Slight		11.1	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	100%, 10%, and ITC	-	n.p.		n.s.																					Spielmann et al. (1996)
3,6-Dimethyloctanol		BG	100%, 10%, and ITC	-	n.p.	poorly soluble	7															0.3	Nonirritant	Nonirritant	4.3	Slight	Slight	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	100%, 10%, and ITC	-	n.p.	poorly soluble	7															0	Nonirritant		4.3	Slight		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	100%, 10%, and ITC	-	n.p.	0.6	n.s.															4.3	Slight	Moderate	6.7	Moderate	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	100%, 10%, and ITC	-	n.p.	0.6	n.s.															5.6	Moderate		5.7	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	100%, 10%, and ITC	-	n.p.	insoluble	5															18.9	Severe	Severe	19.3	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	100%, 10%, and ITC	-	n.p.	insoluble	5															2.6	Slight		12	Severe		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	100%, 10%, and ITC	-	n.p.	insoluble	5															0.75	Nonirritant		4.1	Slight		Spielmann et al. (1996)
Diphocars		HK	100%, 10%, and ITC	-	n.p.	soluble	n.s.															18.3	Severe	Severe	17.9	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	100%, 10%, and ITC	-	n.p.	soluble	n.s.															11.1	Severe		12.3	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															12.1	Severe	Slight	2.3	Slight	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.8	Slight		4.1	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															2.54	Slight			Nonirritant		Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	BG	100%, 10%, and ITC	-	n.p.	readily soluble	11.5															15.66	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	100%, 10%, and ITC	-	n.p.	readily soluble	11.5															15.5	Severe		19.9	Severe		Spielmann et al. (1996)
Ede 140		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.4	Slight		4.6	Slight		Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	100%, 10%, and ITC	-	n.p.	<2.5	4.5															n.p.		Severe	n.p.		Moderate	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	100%, 10%, and ITC	-	n.p.	<2.5	4.5															3.1	Slight		7	Moderate		Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	1.4	Slight	Moderate	Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
1,2-Epoxydodecane	2855-19-8	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.1	Slight	Slight	8.5	Moderate	Moderate	Spielmann et al. (1996)
Ethiosan		AP	100%, 10%, and ITC	-	n.p.	5	8.5															3.8	Slight	Slight	n.p.			Spielmann et al. (1996)
Ethiosan		WA	100%, 10%, and ITC	-	n.p.	5	8.5															0	Nonirritant		n.p.			Spielmann et al. (1996)
Ethyl butanal	97-96-1	HO	100%, 10%, and ITC	-	n.p.	10	<7															3.6	Slight	Slight	17.4	Severe	Severe	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	100%, 10%, and ITC	-	n.p.	10	<7															0	Nonirritant		18.7	Severe		Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	WA	100%, 10%, and ITC	-	n.p.	soluble	n.s.															6.4	Severe	Severe	8.2	Moderate	Moderate	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	100%, 10%, and ITC	-	n.p.	soluble	n.s.															3	Severe		3.2	Slight		Spielmann et al. (1996)
Genomoll	115-96-8	HO	100%, 10%, and ITC	-	n.p.	5	6															9.2	Severe	Severe	11.6	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	100%, 10%, and ITC	-	n.p.	5	6															9.4	Severe		9.9	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BD	100%, 10%, and ITC	-	n.p.	readily soluble	9															8.4	Moderate	Severe	16.7	Severe	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	100%, 10%, and ITC	-	n.p.	readily soluble	9															10.1	Severe		16.3	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	100%, 10%, and ITC	-	n.p.	readily soluble	9															10.2	Severe		16.5	Severe		Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	HO	100%, 10%, and ITC	-	n.p.	490	0.9															14.2	Severe	Severe	11.7	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	100%, 10%, and ITC	-	n.p.	490	0.9															11.7	Severe		15.2	Severe		Spielmann et al. (1996)
Glycediol		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant	Slight	0.58	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.8	Slight		3.5	Slight		Spielmann et al. (1996)
Granuform	30525-89-4	BD	100%, 10%, and ITC	-	n.p.	250	4															2.9	Slight	Slight	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Granuform	30525-89-4	HO	100%, 10%, and ITC	-	n.p.	250	4															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															2.3	Slight	Slight	8	Moderate	Moderate	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															1.2	Slight		4.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	100%, 10%, and ITC	-	n.p.	874	8.5															5.8	Moderate	Moderate	11.1	Severe	Severe	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	100%, 10%, and ITC	-	n.p.	874	8.5															4.3	Slight		11.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
1,2,6-Hexanetriol	106-69-4	HK	100%, 10%, and ITC	-	n.p.		4.5															11.5	Severe	Severe	18.8	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	100%, 10%, and ITC	-	n.p.		4.5															4.3	Slight		15.3	Severe		Spielmann et al. (1996)
Hnol		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0.8	Nonirritant	Nonirritant	2.1	Slight	Moderate	Spielmann et al. (1996)
Hnol		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		6	Moderate		Spielmann et al. (1996)
Hoe MBF		BD	100%, 10%, and ITC	-	n.p.	100	4.3															0	Nonirritant	Nonirritant	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	100%, 10%, and ITC	-	n.p.	100	4.3															0	Nonirritant		0.35	Nonirritant		Spielmann et al. (1996)
Hydo 98		BD	100%, 10%, and ITC	-	n.p.	soluble	6.5															10.4	Severe	Severe	11.2	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	100%, 10%, and ITC	-	n.p.	soluble	6.5															12.9	Severe		n.p.			Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	100%, 10%, and ITC	-	n.p.		10.6															13.4	Severe	Severe	15.5	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	100%, 10%, and ITC	-	n.p.		10.6															8.9	Moderate		11	Severe		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	100%, 10%, and ITC	-	n.p.	1900	1															10.8	Severe	Severe	11.3	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	100%, 10%, and ITC	-	n.p.	1900	1															14.9	Severe		15.6	Severe		Spielmann et al. (1996)
Hypo 20		BG	100%, 10%, and ITC	-	n.p.	readily soluble	6.5															7.2	Moderate	Moderate	8.9	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	100%, 10%, and ITC	-	n.p.	readily soluble	6.5															0	Nonirritant		4.12	Slight		Spielmann et al. (1996)
Hypo 36		AP	100%, 10%, and ITC	-	n.p.	readily soluble	7															4	Severe	Severe	15.9	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.2	Severe		10	Severe		Spielmann et al. (1996)
Hypo 45		BD	100%, 10%, and ITC	-	n.p.	readily soluble	7															11.1	Severe	Slight	4.4	Slight	Severe	Spielmann et al. (1996)
Hypo 45		WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															2.5	Slight		8.7	Moderate		Spielmann et al. (1996)
Hypo 45		BG	100%, 10%, and ITC	-	n.p.	readily soluble	7															1.9	Slight		11.9	Severe		Spielmann et al. (1996)
Hypo 54		BG	100%, 10%, and ITC	-	n.p.	soluble	6.5															4.3	Slight	Slight	4.1	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	100%, 10%, and ITC	-	n.p.	soluble	6.5															4	Slight		4.2	Slight		Spielmann et al. (1996)
Hyton		AP	100%, 10%, and ITC	-	n.p.	soluble	8.5															17	Severe	Severe	18.6	Severe	Severe	Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Hyton		BG	100%, 10%, and ITC	-	n.p.	soluble	8.5															13.5	Severe	Severe	18.2	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	AP	100%, 10%, and ITC	-	n.p.	42	2.3															15.6	Severe	Severe	12.8	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	100%, 10%, and ITC	-	n.p.	42	2.3															0.75	Nonirritant		0.85	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	100%, 10%, and ITC	-	n.p.	42	2.3															8.4	Moderate		6.9	Moderate		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	HO	100%, 10%, and ITC	-	n.p.	< 1	n.s.															4.1	Slight	Slight	4.6	Slight	Moderate	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	100%, 10%, and ITC	-	n.p.	< 1	n.s.															1.7	Slight		8.1	Moderate		Spielmann et al. (1996)
Isobutanal	78-84-2	WA	100%, 10%, and ITC	-	n.p.	67	<7															2.1	Slight	Slight	19.4	Severe	Severe	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	100%, 10%, and ITC	-	n.p.	67	<7															0	Nonirritant		20	Severe		Spielmann et al. (1996)
Isodecylglucoside		AP	100%, 10%, and ITC	-	n.p.	readily soluble	9															17.2	Severe	Severe	18	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	100%, 10%, and ITC	-	n.p.	readily soluble	9															9.9	Severe		10.7	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	100%, 10%, and ITC	-	n.p.	0.1	<7															0	Nonirritant	Nonirritant	4.5	Slight	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	100%, 10%, and ITC	-	n.p.	0.1	<7															0	Nonirritant		10	Severe		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	AP	100%, 10%, and ITC	-	n.p.	1000	1.75															19.1	Severe	Severe	19.8	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	100%, 10%, and ITC	-	n.p.	1000	1.75															18.8	Severe		19.7	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	100%, 10%, and ITC	-	n.p.	readily soluble	2															17.6	Severe	Severe	19.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	100%, 10%, and ITC	-	n.p.	soluble	3															13.5	Severe	Severe	4	Slight	Slight	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3															1.8	Slight		1.1	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%, 10%, and ITC	-	n.p.	soluble	3															10.5	Severe		6.6	Moderate		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	100%, 10%, and ITC	-	n.p.	1500	10															10	Severe	Severe	10.4	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	100%, 10%, and ITC	-	n.p.	1500	10															8.25	Moderate		16.9	Severe		Spielmann et al. (1996)
Mecre		HK	100%, 10%, and ITC	-	n.p.	mixable	7															n.p.			n.p.			Spielmann et al. (1996)
Mecre		MD	100%, 10%, and ITC	-	n.p.	mixable	7															n.p.			n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	100%, 10%, and ITC	-	n.p.	85	4															18.3	Severe	Severe	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	100%, 10%, and ITC	-	n.p.	85	4															4.3	Slight		n.p.			Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															4.1	Slight	Slight	13.7	Severe	Severe	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															2.2	Slight		11.6	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Methyl acetate	79-20-9	BD	100%, 10%, and ITC	-	n.p.	250	7															4.4	Slight	Slight	19.8	Severe	Severe	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	100%, 10%, and ITC	-	n.p.	250	7															4.3	Slight		16.1	Severe		Spielmann et al. (1996)
Methylpentynol	77-75-8	AP	100%, 10%, and ITC	-	n.p.	soluble	n.s.															15.4	Severe	Severe	20.1	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	100%, 10%, and ITC	-	n.p.	soluble	n.s.															12.3	Severe		12.9	Severe		Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	100%, 10%, and ITC	-	n.p.	40	11.5															17.1	Severe	Severe	4.7	Slight	Slight	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	100%, 10%, and ITC	-	n.p.	40	11.5															17.7	Severe		n.p.			Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	100%, 10%, and ITC	-	n.p.	15	3															17.7	Severe	Severe	20.4	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	100%, 10%, and ITC	-	n.p.	15	3															17.9	Severe		19.2	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.9	Slight	Severe	12.5	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.1	Severe		17	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	AP	100%, 10%, and ITC	-	n.p.	readily soluble	7															11	Severe	Severe	20.4	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															3	Severe		12.8	Severe		Spielmann et al. (1996)
Napt		HO	100%, 10%, and ITC	-	n.p.	1000	n.s.															4.3	Slight	Slight	10.3	Severe	Severe	Spielmann et al. (1996)
Napt		WA	100%, 10%, and ITC	-	n.p.	1000	n.s.															1.9	Slight		5.7	Moderate		Spielmann et al. (1996)
Nitro-bis-octylamide		BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															1.7	Slight	Slight	6.5	Moderate	Moderate	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		1.6	Slight		Spielmann et al. (1996)
Olak		HK	100%, 10%, and ITC	-	n.p.	soluble	8.3															18.9	Severe	Severe	19.5	Severe	Severe	Spielmann et al. (1996)
Olak		MD	100%, 10%, and ITC	-	n.p.	soluble	8.3															16.1	Severe		17	Severe		Spielmann et al. (1996)
Ölesulf		BD	100%, 10%, and ITC	-	n.p.	soluble	8															16.9	Severe	Severe	18.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	100%, 10%, and ITC	-	n.p.	soluble	8															16.8	Severe		19.6	Severe		Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	100%, 10%, and ITC	-	n.p.	1000	7															8.6	Moderate	Severe	18.3	Severe	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	100%, 10%, and ITC	-	n.p.	1000	7															11.1	Severe		19.9	Severe		Spielmann et al. (1996)

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Phenylthiourea	103-85-5	AP	100%, 10%, and ITC	-	n.p.	1	5.5															4	Slight	Slight	3.1	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	100%, 10%, and ITC	-	n.p.	1	5.5															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Phosphonat A		AP	100%, 10%, and ITC	-	n.p.	3.6	2.1															6.8	Moderate	Moderate	3.5	Slight	Severe	Spielmann et al. (1996)
Phosphonat A		BG	100%, 10%, and ITC	-	n.p.	3.6	2.1															6.6	Moderate		10.1	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	HK	100%, 10%, and ITC	-	n.p.	625	5															18.5	Severe	Severe	15.3	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	100%, 10%, and ITC	-	n.p.	625	5															0	Nonirritant		14.6	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	100%, 10%, and ITC	-	n.p.	625	5															2.9	Slight		9	Severe		Spielmann et al. (1996)
PO 2		AP	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															4.3	Slight	Slight	0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
PO 2		WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	100%, 10%, and ITC	-	n.p.	1000	6															10.9	Severe	Severe	19.3	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	100%, 10%, and ITC	-	n.p.	1000	6															15.7	Severe		19.2	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	100%, 10%, and ITC	-	n.p.	readily soluble	7															4.1	Slight	Slight	7.6	Moderate	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	100%, 10%, and ITC	-	n.p.	readily soluble	7															0	Nonirritant		19.8	Severe		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	100%, 10%, and ITC	-	n.p.	750	n.s.															1	Slight	Slight	6.6	Moderate	Moderate	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	100%, 10%, and ITC	-	n.p.	750	n.s.															0	Nonirritant		7.7	Moderate		Spielmann et al. (1996)
Polyhexamethylene guanidine		BD	100%, 10%, and ITC	-	n.p.	soluble	7.1															9.2	Severe	Severe	15.5	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	100%, 10%, and ITC	-	n.p.	soluble	7.1															11	Severe		14.6	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	100%, 10%, and ITC	-	n.p.	80	7															16.5	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	100%, 10%, and ITC	-	n.p.	80	7															15.8	Severe		15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3	AP	100%, 10%, and ITC	-	n.p.	750	10															18.8	Severe	Severe	19.4	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	100%, 10%, and ITC	-	n.p.	750	10															15.8	Severe		15.9	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HK	100%, 10%, and ITC	-	n.p.	250	9.5															17.8	Severe	Severe	17.2	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	100%, 10%, and ITC	-	n.p.	250	9.5															15.2	Severe		6.3	Moderate		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	100%, 10%, and ITC	-	n.p.	310	8															4.2	Slight	Moderate	5.7	Moderate	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	100%, 10%, and ITC	-	n.p.	310	8															6.25	Moderate		6.45	Moderate		Spielmann et al. (1996)
2-Pseudojonon		HK	100%, 10%, and ITC	-	n.p.	0.1	n.s.															8.7	Moderate	Moderate	7.3	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	100%, 10%, and ITC	-	n.p.	0.1	n.s.															2.8	Slight		4.1	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
RK Blau		HK	100%, 10%, and ITC	-	n.p.	100	2.6															4	Slight	Slight	n.p.			Spielmann et al. (1996)
RK Blau		MD	100%, 10%, and ITC	-	n.p.	100	2.6															0	Nonirritant		n.p.			Spielmann et al. (1996)
Rubinrot Y		AP	100%, 10%, and ITC	-	n.p.	172																n.p.		Slight	5.3	Moderate	Moderate	Spielmann et al. (1996)
Rubinrot Y		HO	100%, 10%, and ITC	-	n.p.	172																4	Slight		n.p.			Spielmann et al. (1996)
Sacyclo		HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															3.4	Slight	Slight	4.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		3.3	Slight		Spielmann et al. (1996)
Sept		BD	100%, 10%, and ITC	-	n.p.	soluble	3															4	Severe	Severe	15.9	Severe	Severe	Spielmann et al. (1996)
Sept		HK	100%, 10%, and ITC	-	n.p.	soluble	3															10	Severe		19.8	Severe		Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															3.7	Slight	Slight	4.5	Slight	Severe	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	100%, 10%, and ITC	-	n.p.	poorly soluble	n.s.															3.9	Slight		13.7	Severe		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															7.9	Moderate	Moderate	8.4	Moderate	Severe	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															2.1	Slight		10	Severe		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0.7	Nonirritant	Nonirritant	4.1	Slight	Moderate	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	100%, 10%, and ITC	-	n.p.	insoluble	n.s.															0	Nonirritant		7.2	Moderate		Spielmann et al. (1996)
Silan 167	41453-78-5	WA	100%, 10%, and ITC	-	n.p.	soluble	n.s.															2.7	Slight	Slight	4.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	100%, 10%, and ITC	-	n.p.	soluble	n.s.															0.1	Nonirritant		2.3	Slight		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	100%, 10%, and ITC	-	n.p.	insoluble	<7															3	Severe	Severe	9.9	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	100%, 10%, and ITC	-	n.p.	insoluble	<7															3	Severe		14.7	Severe		Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	AP	100%, 10%, and ITC	-	n.p.	readily soluble	4.5															12.7	Severe	Severe	20	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	100%, 10%, and ITC	-	n.p.	readily soluble	4.5															13.9	Severe		16.8	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	100%, 10%, and ITC	-	n.p.	250	10															13.2	Severe	Severe	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	100%, 10%, and ITC	-	n.p.	250	10															11.3	Severe		12.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	100%, 10%, and ITC	-	n.p.	110	10.4															14.8	Severe	Severe	8.2	Moderate	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	100%, 10%, and ITC	-	n.p.	110	10.4															10.5	Severe		10.7	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	100%, 10%, and ITC	-	n.p.	3.5	11.4															19.7	Severe	Severe	18.2	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	100%, 10%, and ITC	-	n.p.	3.5	11.4															20.7	Severe		16.6	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[a]	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[6]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium hydrogen sulfate	7681-38-1	HK	100%, 10%, and ITC	-	n.p.	1080	1.1															18.8	Severe	Severe	19.2	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	100%, 10%, and ITC	-	n.p.	1080	1.1															16.7	Severe		18.1	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	100%, 10%, and ITC	-	n.p.	soluble	8															10.5	Severe	Severe	17.9	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	100%, 10%, and ITC	-	n.p.	soluble	8															17.7	Severe		19	Severe		Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	HO	100%, 10%, and ITC	-	n.p.	440	4.5															7.5	Moderate	Moderate	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	100%, 10%, and ITC	-	n.p.	440	4.5															0	Nonirritant		10.8	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	AP	100%, 10%, and ITC	-	n.p.	650	4.6															17.4	Severe	Severe	17.7	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	100%, 10%, and ITC	-	n.p.	650	4.6															12.6	Severe		11.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BG	100%, 10%, and ITC	-	n.p.	650	4.6															14.6	Severe		14.5	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	100%, 10%, and ITC	-	n.p.	soluble	7															18	Severe	Severe	10.4	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	100%, 10%, and ITC	-	n.p.	soluble	7															20.1	Severe		n.p.	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	100%, 10%, and ITC	-	n.p.	0.014	n.s.															7.6	Moderate	Severe	16.2	Severe	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	100%, 10%, and ITC	-	n.p.	0.014	n.s.															10	Severe		10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	100%, 10%, and ITC	-	n.p.	50	11															13.4	Severe	Severe	6.9	Moderate	Moderate	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	100%, 10%, and ITC	-	n.p.	50	11															5.4	Moderate		n.p.	Severe		Spielmann et al. (1996)
Tocla		BD	100%, 10%, and ITC	-	n.p.	40	6															12.9	Severe	Severe	13.5	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	100%, 10%, and ITC	-	n.p.	40	6															19.7	Severe		20.4	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	100%, 10%, and ITC	-	n.p.	0.5	7															0.8	Nonirritant	Nonirritant	14.1	Severe	Severe	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	100%, 10%, and ITC	-	n.p.	0.5	7															0	Nonirritant		4	Slight		Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	100%, 10%, and ITC	-	n.p.	< 2.5	2.3															2.9	Slight	Slight	9.7	Severe	Severe	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	100%, 10%, and ITC	-	n.p.	< 2.5	2.3															2.3	Slight		14.7	Severe		Spielmann et al. (1996)
Trioxane	110-88-3	HK	100%, 10%, and ITC	-	n.p.	172	n.s.															9.25	Severe	Severe	18	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	100%, 10%, and ITC	-	n.p.	172	n.s.															13.4	Severe		17.8	Severe		Spielmann et al. (1996)
Wessalith Slurry		BG	100%, 10%, and ITC	-	n.p.	readily soluble	11															3.13	Slight	Severe	4.1	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	100%, 10%, and ITC	-	n.p.	readily soluble	11															10	Severe		15.7	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	100%, 10%, and ITC	-	n.p.	250	6															4	Slight	Severe	9	Severe	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	100%, 10%, and ITC	-	n.p.	250	6															11.3	Severe		17.4	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility*	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	IS(B)[2]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	S-Score[3]	S-Score Classification	Overall S-Score Classification	Q-Score[4]	Q-Score Classification	Overall Q-Score Classification	IS(B)-10[5]	IS(B)-10 Class.	Overall IS(B)-10 Class.	IS(B)-100[5]	IS(B)-100 Class.	Overall IS(B)-100 Class.	Reference
Sodium lauryl sulfate	151-21-3		1%	Solution	n.p.		3.3					14.22		Severe														Vinardell and Macián (1994)
Tween 20	9005-64-5		100%	Liquid	n.p.		7.21					3.22		Slight														Vinardell and Macián (1994)

Abbreviations: CASRN = Chemical Abstract Service Registry Number, n.a. = not applicable, n.p. = not provided, Conc. = Concentration, IS = Irritation Score, ITC = Irritation Threshold Concentration, SD = standard deviation.

* Solubility = obtained from literature references; where available, expressed as g/mL

[1] IS(A) represents irritation scores that were calculated using the method described in Leupke (1985)

[2] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990)

[3] S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

[4] Q-Score represents irritation scores that were calcualted using the method described in Balls et al. (1995)

[5] IS(B)-10 and IS(B)-100 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990) where the *in vitro* score was obtained using a 10% or 100% concentration, respectively.

[6] The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8), the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.

[7] No information on the *in vitro* physical form of substances tested by Spielmann et al. (1996) were added since the tested form depended on the concentration being evaluated (10% or 100%). For information on the tested form *in vivo* see **Appendix D**.

Appendix C3

Data Sorted by Substance for IS(A) Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Acetic acid	64-19-7	1	10%	Solution			2.4	16.5	2.89	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	2	10%	Solution			2.4	16	3.92	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	3	10%	Solution			2.4	17.25	6.24	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	4	10%	Solution			2.4	19.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Acetic acid	64-19-7	5	10%	Solution			2.4	17.5	4.04	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	1	10%	Suspension			7.31	8.25	2.87	Moderate	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	2	10%	Suspension			7.31	10.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	3	10%	Suspension			7.31	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	4	10%	Suspension			7.31	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	5	10%	Suspension			7.31	5.75	1.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	1	10%	Solution			5.89	19	1.63	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	2	10%	Solution			5.89	13.25	2.22	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	3	10%	Solution			5.89	18.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	4	10%	Solution			5.89	11	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	5	10%	Solution			5.89	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Chlorhexidine gluconate solution (20% solution)	18472-51-0	1	10%	Solution			6.56	19	1.63	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	2	10%	Solution			6.56	13.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	3	10%	Solution			6.56	16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	4	10%	Solution			6.56	11.75	4.86	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate solution (20% solution)	18472-51-0	5	10%	Solution			6.56	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	1	10%	Suspension			6.54	10	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	2	10%	Suspension			6.54	10	1.63	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	3	10%	Suspension			6.54	10.25	3.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	4	10%	Suspension			6.54	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	5	10%	Suspension			6.54	5	0.00	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	1	10%	Solution			11.89	8.25	2.36	Moderate	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	2	10%	Solution			11.89	8.5	4.04	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	3	10%	Solution			11.89	9	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	4	10%	Solution			11.89	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	5	10%	Solution			11.89	5	0.00	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Domiphen bromide	538-71-6	1	10%	Solution			6.22	19	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	2	10%	Solution			6.22	15.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	3	10%	Solution			6.22	14.75	1.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	4	10%	Solution			6.22	12.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	5	10%	Solution			6.22	9	1.22	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	1	10%	Solution			5.9	0	0.00	Nonirritant	Slight	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	10%	Solution			5.9	1.25	2.50	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	10%	Solution			5.9	10.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	10%	Solution			5.9	1.5	1.73	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	10%	Solution			5.9	1.25	2.50	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5		10%	Solution			7.2	4		Slight		Kojima et al. (1995)
Ethanol	64-17-5	1	100%	Liquid				18.75	3.30	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid				16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid				17	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid				10.5	1.73	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Glycolic acid	79-14-1	1	10%	Solution			1.76	19.5	1.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	2	10%	Solution			1.76	20	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	3	10%	Solution			1.76	17.75	3.95	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	4	10%	Solution			1.76	12.25	2.36	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	5	10%	Solution			1.76	12.75	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	10%	Solution			1.94	20.5	1.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	10%	Solution			1.94	14.25	2.06	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	10%	Solution			1.94	19.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	10%	Solution			1.94	18.5	1.91	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	10%	Solution			1.94	10.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid				21	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid				6.25	2.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid				16	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid				15.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid				11.5	2.89	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Monoethanolamine	141-43-5	1	10%	Solution			12.58	12	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	2	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	3	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	4	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	5	10%	Solution			12.58	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				0.283		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				0.533		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution				7.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				17.8		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				1.97		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				0.917		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				4.83		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				8.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.33		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0.5		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				10.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				11.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution				4.1		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution				0.6		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				0.167		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				17		Severe	Severe	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Potassium laurate	10124-65-9	1	10%	Solution			10.49	20	1.15	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	2	10%	Solution			10.49	13.25	2.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	3	10%	Solution			10.49	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	4	10%	Solution			10.49	12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	5	10%	Solution			10.49	19.33	0.82	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9		10%	Solution	98%		9.4	14.3		Severe		Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3		10%	Solution	98%		5.4	7.5		Moderate	Severe	Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2	1	10%	Solution			4.24	16.75	2.06	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	2	10%	Solution			4.24	13	2.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	3	10%	Solution			4.24	15.75	3.50	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	4	10%	Solution			4.24	13.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	5	10%	Solution			4.24	9	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2		10%	Solution			5.5	19.3		Severe		Kojima et al. (1995)
Surfactant Based Formulation 1-HZA			10%	Solution				7.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution				4.8		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution				9.5		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution				5.2		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution				3.8		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution				8.3		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution				6.3		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution				1.3		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution				9.3		Severe	Severe	Gettings et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Surfactant Based Formulation 10-HZJ			10%	Solution				2.2		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution				8.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution				9.6		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution				4.1		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution				6.1		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution				4.7		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution				4.9		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution				7.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution				8.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution				0.2		Nonirritant	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution				3.7		Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution				7.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution				7.8		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution				9		Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution				8.7		Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution				0.7		Nonirritant	Nonirritant	Gettings et al. (1996)
Triethanolamine	102-71-6		10%	Solution				10.75		Severe	Slight	Bagley et al. (1992)
Triethanolamine	102-71-6	1	10%	Solution			11.26	1.5	2.38	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	10%	Solution			11.26	3.75	4.79	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	10%	Solution			11.26	11	1.15	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	10%	Solution			11.26	6	1.63	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	10%	Solution			11.26	2.5	2.89	Slight		Hagino et al. (1999)/Submitted Y. Ohno Data

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)[1]	IS(A) SD	IS(A) Classification	Overall IS(A) Classification	Reference
Triethanolamine	102-71-6	1	100%	Liquid				5	0.00	Moderate	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid				6.75	3.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid				12	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid				6.75	3.50	Moderate		Hagino et al. (1999)/Submitted Y. Ohno Data
Triton X-100	9002-93-1		1%	Solution				9		Severe	Severe	Bagley et al. (1992)
Triton X-100	9002-93-1		10%	Solution			5.75	5		Moderate	Moderate	Kojima et al. (1995)

Abbreviations: CASRN = Chemical Abstract Service Registry Number, SD = Standard Deviation.

[1] IS(A) represents irritation scores that were calculated using the method described in Leupke (1985).

Appendix C4

Data Sorted by Substance for IS(A)-10 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 1-HZA		10%	Solution				7.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Solution				4.8	Slight	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Solution				9.5	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Solution				5.2	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Solution				3.8	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Solution				8.3	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Solution				6.3	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 8-HZH		10%	Solution				1.3	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Solution				9.3	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Solution				2.2	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Solution				8.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Solution				9.6	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Solution				4.1	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Solution				6.1	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 15-HZP		10%	Solution				4.7	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Solution				4.9	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Solution				7.7	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Solution				8.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Solution				0.2	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Solution				3.7	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Solution				7.7	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-10[1]	IS(A)-10 Classification	Reference
Surfactant Based Formulation 22-HZW		10%	Solution				7.8	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Solution				9	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Solution				8.7	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Solution				0.7	Nonirritant	Gettings et al. (1996)

Abbreviation: CASRN: Chemical Abstracts Service Registy Number.

[1] IS(A)-10 represents irritation scores that were calculated using a method similar to the one described in Luepke (1985) where the *in vitro* score was obtained using a 10% concentration and where *in vivo* data were obtained at 100% concentration.

Appendix C5

Data Sorted by Substance for IS(A)-100 Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Ethanol	64-17-5	1	100%	Liquid				18.75	3.30	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	2	100%	Liquid				16	2.45	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	3	100%	Liquid				11.5	1.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	4	100%	Liquid				17	0.00	Severe		Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	5	100%	Liquid				10.5	1.73	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	1	100%	Liquid				21	0.00	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	2	100%	Liquid				6.25	2.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	3	100%	Liquid				16	1.15	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	4	100%	Liquid				15.25	2.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	5	100%	Liquid				11.5	2.89	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				0.283		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				0.533		Nonirritant	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Oil/Water Emulsion-HZF			100%	Solution				7.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				17.8		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				1.97		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				0.917		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				4.83		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				8.33		Moderate	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.33		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0.5		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				10.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				11.6		Severe	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT			100%	Solution				4.1		Slight	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	*In Vitro* Conc. Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(A)-100[1]	IS(A)-100 SD	IS(A)-100 Classification	Overall IS(A)-100 Classification	Reference
Oil/Water Emulsion-HZV			100%	Solution				0.6		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				0.167		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				17		Severe	Severe	Gettings et al. (1994)
Triethanolamine	102-71-6	1	100%	Liquid				5	0.00	Severe	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	2	100%	Liquid				6.75	3.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	3	100%	Liquid				11.5	1.00	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	4	100%	Liquid				12	0.00	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	5	100%	Liquid				6.75	3.50	Nonirritant		Hagino et al. (1999)/Submitted Y. Ohno Data

Abbreviation: CASRN: Chemical Abstracts Service Registy Number, Conc.: concentration, SD: standard deviation.

[1] IS(A)-10 represents irritation scores that were calculated using a method similar to the one described in Luepke (1985) where the *in vitro* score was obtained using a 100% concentration and where *in vivo* results were obtained at 100% concentration.

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Appendix C6

Data Sorted by Substance for IS(B) Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Acetic acid	64-19-7	2	100%	Liquid	>99			14.8		Severe	Severe	CEC (1991)
Acetic acid	64-19-7	3	100%	Liquid	>99			13.7		Severe		CEC (1991)
Acetic acid	64-19-7	4	100%	Liquid	>99			9.3		Severe		CEC (1991)
Acetic acid	64-19-7	2	10%	Solution	>99			20.2		Severe	Severe	CEC (1991)
Acetic acid	64-19-7	3	10%	Solution	>99			13.6		Severe		CEC (1991)
Acetic acid	64-19-7	4	10%	Solution	>99			10.2		Severe		CEC (1991)
Acetone	67-64-1		100%	Liquid	>99	water soluble		15.32	0.33	Severe	Severe	Gilleron et al. (1997)
Allyl alcohol	107-18-6		100%	Liquid				12.4	2.3	Severe	Severe	Gilleron et al. (1996)
2-Aminophemol	95-55-6		100%	Solid				0.8	0.7	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2		100%	Solid	>99.9	water soluble		15.34	1.24	Severe	Severe	Gilleron et al. (1997)
Anthracene	120-12-7		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3		100%	Solid	95	water soluble		1.06	1.2	Slight	Slight	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		14.8	0.53	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		15.05	0.27	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5		100%	Liquid	98	surfactant		15.14	0.25	Severe	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	2	100%	Unknown	n.p.			14.5		Severe	Severe	CEC (1991)
Benzalkonium chloride	8001-54-5	3	100%	Unknown	n.p.			13.1		Severe		CEC (1991)
Benzalkonium chloride	8001-54-5	5	100%	Unknown	n.p.			5.8		Moderate		CEC (1991)
Benzalkonium chloride	8001-54-5	6	100%	Unknown	n.p.			6.9		Moderate		CEC (1991)
Benzalkonium chloride	8001-54-5	7	100%	Unknown	n.p.			13.3		Severe		CEC (1991)
Benzethonium chloride	121-54-0		100%	Solid	n.p.			15.4	3.1	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Brij 35	9002-92-0	1	100%	Solid	>99			2.3		Slight	Slight	CEC (1991)
Brij 35	9002-92-0	2	100%	Solid	>99			4.3		Slight		CEC (1991)
Brij 35	9002-92-0	3	100%	Solid	>99			12.9		Severe		CEC (1991)
Brij 35	9002-92-0	4	100%	Solid	>99			4.4		Slight		CEC (1991)
Brij 35	9002-92-0	5	100%	Solid	>99			3.8		Slight		CEC (1991)
Brij 35	9002-92-0	6	100%	Solid	>99			2.6		Slight		CEC (1991)
Brij 35	9002-92-0	7	100%	Solid	>99			4		Slight		CEC (1991)
Butanol	71-36-3	1	100%	Liquid	99			11.7		Severe	Severe	CEC (1991)
Butanol	71-36-3	2	100%	Liquid	99			11.8		Severe		CEC (1991)
Butanol	71-36-3	3	100%	Liquid	99			12.6		Severe		CEC (1991)
Butanol	71-36-3	4	100%	Liquid	99			11.2		Severe		CEC (1991)
Butanol	71-36-3	5	100%	Liquid	99			3.9		Slight		CEC (1991)
Butanol	71-36-3	6	100%	Liquid	99			10.7		Severe		CEC (1991)
Butanol	71-36-3	7	100%	Liquid	99			9.9		Severe		CEC (1991)
Butanol	71-36-3	2	10%	Solution	99			14.2		Severe	Severe	CEC (1991)
Butanol	71-36-3	3	10%	Solution	99			4.8		Slight		CEC (1991)
Butanol	71-36-3	4	10%	Solution	99			12.5		Severe		CEC (1991)
2-Butoxyethyl acetate	112-07-2	1	100%	Liquid	99			4.6		Slight	Slight	CEC (1991)
2-Butoxyethyl acetate	112-07-2	2	100%	Liquid	99			5.3		Moderate		CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	100%	Liquid	99			4.7		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	100%	Liquid	99			4.7		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	5	100%	Liquid	99			4		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	6	100%	Liquid	99			3.9		Slight		CEC (1991)
2-Butoxyethyl acetate	112-07-2	7	100%	Liquid	99			4.5		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2-Butoxyethyl acetate	112-07-2	2	10%	Solution	99			4.1		Slight	Slight	CEC (1991)
2-Butoxyethyl acetate	112-07-2	3	10%	Solution	99			0		Nonirritant		CEC (1991)
2-Butoxyethyl acetate	112-07-2	4	10%	Solution	99			3.2		Slight		CEC (1991)
Butyl acetate	123-86-4		100%	Liquid	99	water insoluble		17.21	1.84	Severe	Severe	Gilleron et al. (1997)
Gamma-butyrolactone	96-48-0		100%	Liquid				13.9	1.8	Severe	Severe	Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%	Liquid	>99	water soluble		19.39	0.83	Severe		Gilleron et al. (1997)
Captan 90 concentrate	133-06-2		100%	Solid	90	water soluble		15.07	0.27	Severe	Severe	Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%	Solid	95	water insoluble		3.95	4.69	Slight	Slight	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		12.68	1.52	Severe	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		13.53	2.42	Severe	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7		100%	Liquid	98	surfactant		14.6	0.43	Severe	Severe	Gilleron et al. (1997)
Chlorhexidine	55-56-1		100%	Solid	99.5	water insoluble		14.87	3.78	Severe	Severe	Gilleron et al. (1997)
Cyclohexanol	108-93-0		100%	Liquid	97	water soluble		18.96	0.1	Severe	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1		100%	Liquid				14.5	3.8	Severe	Severe	Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%	Solid				9.7	5.8	Severe	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%	Liquid				15.1	2.7	Severe	Severe	Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid	np	water soluble		13.34	4.24	Severe	Severe	Gilleron et al. (1997)
Dibenzoyl-L-tartaric acid	2743-38-6		100%	Solid				4.2	2.5	Slight		Gilleron et al. (1996)
Dibenzyl phosphate	1623-08-1		100%	Solid	99.5	water insoluble		15.16	0.47	Severe	Severe	Gilleron et al. (1997)
Dibutyltin chloride	683-18-1	1	100%	Solid	97			11.6		Severe	Severe	CEC (1991)
Dibutyltin chloride	683-18-1	2	100%	Solid	97			10.8		Severe		CEC (1991)
Dibutyltin chloride	683-18-1	4	100%	Solid	97			12.6		Severe		CEC (1991)
Dibutyltin chloride	683-18-1	5	100%	Solid	97			5.1		Moderate		CEC (1991)
Dibutyltin chloride	683-18-1	6	100%	Solid	97			5		Moderate		CEC (1991)
Dibutyltin chloride	683-18-1	7	100%	Solid	97			13		Severe		CEC (1991)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%	Liquid	99	water insoluble		10.74	1.74	Severe	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%	Solid				3.8	2.2	Slight	Slight	Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9		100%	Solid				8.4	2.2	Moderate	Moderate	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2,2-Dimethylbutanoic acid	595-37-9		100%	Liquid	>99	water insoluble		15.31	0.24	Severe	Severe	Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2		100%	Solid	99.5	water insoluble		15.33	0.38	Severe	Severe	Gilleron et al. (1997)
Dimethyl sulfoxide	67-68-5		100%	Liquid				11.3	3.7	Severe	Severe	Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5	1	100%	Liquid	99.9			11.7		Severe	Severe	CEC (1991)
Dimethyl sulfoxide	67-68-5	2	100%	Liquid	99.9			10.9		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	3	100%	Liquid	99.9			11.3		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	4	100%	Liquid	99.9			4.1		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	5	100%	Liquid	99.9			4.9		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	6	100%	Liquid	99.9			7.3		Moderate		CEC (1991)
Dimethyl sulfoxide	67-68-5	7	100%	Liquid	99.9			11.4		Severe		CEC (1991)
Dimethyl sulfoxide	67-68-5	2	10%	Solution	99.9			4.4		Slight	Slight	CEC (1991)
Dimethyl sulfoxide	67-68-5	3	10%	Solution	99.9			4.1		Slight		CEC (1991)
Dimethyl sulfoxide	67-68-5	4	10%	Solution	99.9			4.1		Slight		CEC (1991)
EDTA dipotassium	25105-12-9		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid				11.3	2.8	Severe	Severe	Gilleron et al. (1996)
Ethanol	64-17-5		100%	Liquid		water soluble		14.97	0.04	Severe		Gilleron et al. (1997)
2-Ethoxyethanol	110-80-5		100%	Liquid				10.5	2.7	Severe	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6		100%	Liquid	99	water soluble		19.32	0.06	Severe	Severe	Gilleron et al. (1997)
2-Ethyl-1-hexanol	104-76-7		100%	Liquid	99	water soluble		12.71	2.96	Severe	Severe	Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3		100%	Liquid	ca. 97	water insoluble		12.94	2.94	Severe	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%	Liquid	99	water insoluble		13.82	2.73	Severe	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9		100%	Liquid				10	3.2	Severe	Severe	Gilleron et al. (1996)
Fomesafen	72128-02-0		100%	Solid	97.5	water soluble		1.21	1.29	Slight	Slight	Gilleron et al. (1997)
Furan	110-00-9		100%	Liquid				5.5	1	Moderate	Moderate	Gilleron et al. (1996)
Gluconolactone	90-80-2		100%	Solid				4.6	3.2	Slight	Slight	Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7		100%	Solid				0.7	1.2	Nonirritant	Nonirritant	Gilleron et al. (1996)
Glycerol	56-81-5		100%	Liquid	99.5	water soluble		14.78	0.75	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Glycerol	56-81-5	1	100%	Liquid	>99			10.8		Severe	Severe	CEC (1991)
Glycerol	56-81-5	2	100%	Liquid	>99			11.3		Severe		CEC (1991)
Glycerol	56-81-5	3	100%	Liquid	>99			10.3		Severe		CEC (1991)
Glycerol	56-81-5	4	100%	Liquid	>99			4.8		Slight		CEC (1991)
Glycerol	56-81-5	5	100%	Liquid	>99			0		Nonirritant		CEC (1991)
Glycerol	56-81-5	6	100%	Liquid	>99			0		Nonirritant		CEC (1991)
Glycerol	56-81-5	7	100%	Liquid	>99			9.4		Severe		CEC (1991)
Glycerol	56-81-5	2	10%	Solution	>99			8.7		Moderate	Slight	CEC (1991)
Glycerol	56-81-5	3	10%	Solution	>99			4.4		Slight		CEC (1991)
Glycerol	56-81-5	4	10%	Solution	>99			3.6		Slight		CEC (1991)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%	Liquid				4.3	1	Slight	Slight	Gilleron et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%	Liquid				10.8	4.8	Severe	Severe	Gilleron et al. (1996)
Hexane	110-54-3		100%	Liquid				3.1	2.7	Slight	Slight	Gilleron et al. (1996)
n-Hexane	110-54-3	1	100%	Liquid	99			2.9		Slight	Slight	CEC (1991)
n-Hexane	110-54-3	2	100%	Liquid	99			5.4		Moderate		CEC (1991)
n-Hexane	110-54-3	3	100%	Liquid	99			4.2		Slight		CEC (1991)
n-Hexane	110-54-3	4	100%	Liquid	99			10.3		Severe		CEC (1991)
n-Hexane	110-54-3	5	100%	Liquid	99			2.3		Slight		CEC (1991)
n-Hexane	110-54-3	6	100%	Liquid	99			8.1		Moderate		CEC (1991)
n-Hexane	110-54-3	7	100%	Liquid	99			2.4		Slight		CEC (1991)
n-Hexane	110-54-3	2	10%	Solution	99			3.7		Slight	Severe	CEC (1991)
n-Hexane	110-54-3	3	10%	Solution	99			0		Nonirritant		CEC (1991)
n-Hexane	110-54-3	4	10%	Solution	99			10.1		Severe		CEC (1991)
Hexanol	111-27-3		100%	Liquid	98	water insoluble		17.56	0.4	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Hydroalcoholic Formulation 1-5% Alcohol Containing			Undiluted	Solution				4.6		Slight	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing			Undiluted	Solution				5		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing			Undiluted	Solution				8.5		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing			Undiluted	Solution				5.3		Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing			Undiluted	Solution				11.9		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing			Undiluted	Solution				12.8		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing			Undiluted	Solution				12.7		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing			Undiluted	Solution				13.8		Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing			Undiluted	Solution				13.6		Severe	Severe	Gettings et al. (1991)
Imidazole	288-32-4		100%	Solid				18.7	0.9	Severe	Severe	Gilleron et al. (1996)
Imidazole	288-32-4		100%	Solid	99	water soluble		19.43	0.49	Severe		Gilleron et al. (1997)
Iminodibenzyl	94-19-9		100%	Solid				0	0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobutanol	78-83-1		100%	Liquid	99.9	water insoluble		19.41	0.08	Severe	Severe	Gilleron et al. (1997)
Isopropanol	67-63-0		100%	Liquid	99.9	water soluble		14.8	0.21	Severe	Severe	Gilleron et al. (1997)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%	Solid				12.7	4.3	Severe	Severe	Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%	Uknown				8.3	1.2	Moderate	Moderate	Gilleron et al. (1996)
Magnesium carbonate	56378-72-4		100%	Solid				1.4	1.9	Slight	Slight	Gilleron et al. (1996)
Maneb	12427-38-2		100%	Solid	90	water soluble		0.16	0.24	Nonirritant	Nonirritant	Gilleron et al. (1997)
Methanol	67-56-1		100%	Liquid				12.2	3.3	Severe	Severe	Gilleron et al. (1996)
2-Methoxyethanol	109-86-4		100%	Liquid				14.5	0.7	Severe	Severe	Gilleron et al. (1996)
2-Methoxyethanol	109-86-4	1	100%	Liquid	99			9.7		Severe	Severe	CEC (1991)
2-Methoxyethanol	109-86-4	2	100%	Liquid	99			12.2		Severe		CEC (1991)
2-Methoxyethanol	109-86-4	3	100%	Liquid	99			12.1		Severe		CEC (1991)
2-Methoxyethanol	109-86-4	4	100%	Liquid	99			8.6		Moderate		CEC (1991)
2-Methoxyethanol	109-86-4	5	100%	Liquid	99			4.5		Slight		CEC (1991)
2-Methoxyethanol	109-86-4	6	100%	Liquid	99			0.8		Nonirritant		CEC (1991)
2-Methoxyethanol	109-86-4	7	100%	Liquid	99			3.1		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
2-Methoxyethanol	109-86-4	2	10%	Solution	99			7		Moderate	Moderate	CEC (1991)
2-Methoxyethanol	109-86-4	3	10%	Solution	99			0		Nonirritant		CEC (1991)
2-Methoxyethanol	109-86-4	4	10%	Solution	99			3.1		Slight		CEC (1991)
Methyl acetate	79-20-9		100%	Liquid	98	water soluble		18.98	0.75	Severe	Severe	Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%	Liquid	99	water soluble		16.31	1.23	Severe	Severe	Gilleron et al. (1997)
Methyl cyclopentane	96-37-7		100%	Liquid	>99	water insoluble		17.14	1.63	Severe	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%	Liquid	99	water soluble		18.35	2.52	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid	98	water insoluble		17.75	2.2	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%	Liquid				10.5	1.5	Severe		Gilleron et al. (1996)
MYRJ 45			100%	Unknown				0.00	0.00	Nonirritant	Nonirritant	Gilleron et al. (1996)
1-Naphthalene acetic acid	86-87-3		100%	Solid	99	water soluble		7.46	2.37	Moderate	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%	Solid	95	water soluble		15.16	0.49	Severe	Severe	Gilleron et al. (1997)
1-Nitropropane	108-03-2		100%	Liquid				2.8	2.7	Slight	Slight	Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid				9.8	1.7	Severe	Severe	Gilleron et al. (1996)
Octanol	111-87-5		100%	Liquid	>99	water insoluble		16.7	0.81	Severe		Gilleron et al. (1997)
Oil/Water Emulsion-HZA			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC			Undiluted	Solution				3		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZH[2]			Undiluted	Solution				23		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZI			Undiluted	Solution				0.333		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			Undiluted	Solution				3		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL			Undiluted	Solution				10.3		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZM			Undiluted	Solution				14.3		Severe	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZN			Undiluted	Solution				3.67		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZO			Undiluted	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			Undiluted	Solution				16.3		Severe	Nonirritant	Gettings et al. (1994)

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Oil/Water Emulsion-HZS			Undiluted	Solution				8.33		Moderate	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZT			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZU			Undiluted	Solution				1		Slight	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV			Undiluted	Solution				0		Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			Undiluted	Solution				5		Moderate	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY			Undiluted	Solution				9.67		Severe	Nonirritant	Gettings et al. (1994)
Parafluoraniline	371-40-4		100%	Liquid	99	water insoluble		15.49	1.63	Severe	Severe	Gilleron et al. (1997)
2,4-Pentadione	123-54-6		100%	Liquid				8.8	3	Moderate	Moderate	Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%	Solid				0.5	0.4	Nonirritant	Nonirritant	Gilleron et al. (1996)
Polyethylene glycol 400	25322-68-3		100%	Liquid		surfactant		14.68	0.55	Severe	Severe	Gilleron et al. (1997)
Polyoxyethylene 23 lauryl ether			100%	Solid				1.5	2.6	Slight	Slight	Gilleron et al. (1996)
Potassium cyanate	590-28-3		100%	Solid	97	water soluble		14.27	1.15	Severe	Severe	Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid	98	water soluble		6.27	1.41	Moderate	Severe	Gilleron et al. (1997)
Promethazine HCl	58-33-3		100%	Solid				13.9	2.1	Severe		Gilleron et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3		100%	Solid				1.9	1	Slight	Slight	Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid				15.8	3.6	Severe	Severe	Gilleron et al. (1996)
Pyridine	110-86-1		100%	Liquid	>99	water soluble		17.79	2.44	Severe		Gilleron et al. (1997)
Quinacrine	69-05-6		100%	Solid				6.5	2.2	Moderate	Moderate	Gilleron et al. (1996)
Quinacrine	69-05-6		100%	Solid		water soluble		7.29	0.6	Moderate		Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	1	100%	Solid	98			11.4		Severe	Severe	CEC (1991)
Sodium lauryl sulfate	151-21-3	2	100%	Solid	98			10.3		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	3	100%	Solid	98			13.9		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	4	100%	Solid	98			4.8		Slight		CEC (1991)
Sodium lauryl sulfate	151-21-3	6	100%	Solid	98			11.1		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	7	100%	Solid	98			9.7		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	2	10%	Solution	98			18.4		Severe	Severe	CEC (1991)
Sodium lauryl sulfate	151-21-3	3	10%	Solution	98			14.1		Severe		CEC (1991)
Sodium lauryl sulfate	151-21-3	4	10%	Solution	98			5.1		Moderate		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Sodium lauryl sulfate	151-21-3		1%	Solution			3.3	14.22		Severe	Nonirritant	Vinardell and Macián (1994)
Sodium lauryl sulfate	151-21-3		100%	Liquid	98	surfactant		12.38	1.82	Severe	Severe	Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3		100%	Liquid	98	surfactant		15.05	0.29	Severe	Severe	Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Liquid		water soluble		19.01	0.13	Severe	Severe	Gilleron et al. (1997)
Sodium hydroxide	1310-73-2		100%	Liquid		water soluble		20.56	0.08	Severe	Severe	Gilleron et al. (1997)
Sodium oxalate	62-76-0		100%	Solid	>99	water soluble		14.2	0.71	Severe	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%	Solid	98.6	water soluble		13.19	1.78	Severe	Severe	Gilleron et al. (1997)
Surfactant Based Formulation 1-HZA			10%	Solution				9.6		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution				7.3		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution				15.3		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution				8.7		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution				11.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution				10.9		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution				7.1		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution				3.5		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution				15.2		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution				6.2		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution				9.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution				12.4		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution				2.7		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution				8		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution				4.4		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution				4.2		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR			10%	Solution				5.3		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution				12.2		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution				3.5		Slight	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution				6.2		Moderate	Nonirritant	Gettings et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Surfactant Based Formulation 21-HZV			10%	Solution				8.7		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution				5.1		Moderate	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution				11.3		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution				11.7		Severe	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution				1.1		Slight	Nonirritant	Gettings et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid				0.5	0.9	Nonirritant	Slight	Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%	Solid	97	water insoluble		4.33	0.23	Slight		Gilleron et al. (1997)
Thiourea	62-56-6		100%	Solid				13.7	4.4	Severe	Severe	Gilleron et al. (1996)
Thiourea	62-56-6		100%	Solid	>99	water soluble		17.89	1.53	Severe		Gilleron et al. (1997)
Toluene	108-88-3		100%	Liquid	99	water soluble		16.09	1.62	Severe	Severe	Gilleron et al. (1997)
Toluene	108-88-3	1	100%	Liquid	99.9			8.8		Moderate	Severe	CEC (1991)
Toluene	108-88-3	2	100%	Liquid	99.9			14.8		Severe		CEC (1991)
Toluene	108-88-3	3	100%	Liquid	99.9			15.2		Severe		CEC (1991)
Toluene	108-88-3	4	100%	Liquid	99.9			11.5		Severe		CEC (1991)
Toluene	108-88-3	5	100%	Liquid	99.9			4.6		Slight		CEC (1991)
Toluene	108-88-3	6	100%	Liquid	99.9			3.1		Slight		CEC (1991)
Toluene	108-88-3	7	100%	Liquid	99.9			4.9		Slight		CEC (1991)
Triacetin	102-76-1	1	100%	Liquid	99			3.6		Slight	Slight	CEC (1991)
Triacetin	102-76-1	2	100%	Liquid	99			4.3		Slight		CEC (1991)
Triacetin	102-76-1	3	100%	Liquid	99			5.5		Moderate		CEC (1991)
Triacetin	102-76-1	4	100%	Liquid	99			4.4		Slight		CEC (1991)
Triacetin	102-76-1	5	100%	Liquid	99			3.3		Slight		CEC (1991)
Triacetin	102-76-1	6	100%	Liquid	99			4.3		Slight		CEC (1991)
Triacetin	102-76-1	7	100%	Liquid	99			3.1		Slight		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Triacetin	102-76-1	2	10%	Solution	99			13.6		Severe	Slight	CEC (1991)
Triacetin	102-76-1	3	10%	Solution	99			2		Slight		CEC (1991)
Triacetin	102-76-1	4	10%	Solution	99			3.3		Slight		CEC (1991)
Tributyltin chloride	1461-22-9	1	100%	Solid	96			6.7		Moderate	Moderate	CEC (1991)
Tributyltin chloride	1461-22-9	2	100%	Solid	96			8.9		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	3	100%	Solid	96			13.7		Severe		CEC (1991)
Tributyltin chloride	1461-22-9	4	100%	Solid	96			8.8		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	5	100%	Solid	96			7.4		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	6	100%	Solid	96			7.9		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	7	100%	Solid	96			6.6		Moderate		CEC (1991)
Tributyltin chloride	1461-22-9	2	10%	Solution	96			15.6		Severe	Severe	CEC (1991)
Tributyltin chloride	1461-22-9	3	10%	Solution	96			9.6		Severe		CEC (1991)
Tributyltin chloride	1461-22-9	4	10%	Solution	96			11.2		Severe		CEC (1991)
Trichloroacetic acid	76-03-9		100%	Liquid		water soluble		15.7	0.11	Severe	Severe	Gilleron et al. (1997)
Trichloroacetic acid	76-03-9		100%	Liquid		water soluble		15.72	0.15	Severe	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4		100%	Liquid				7.9	1.7	Moderate	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%	Liquid				4.5	2.9	Slight	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6		100%	Liquid				9.6	3.5	Severe	Severe	Gilleron et al. (1996)
Triethanolamine	102-71-6	1	100%	Liquid	97			8.6		Moderate	Severe	CEC (1991)
Triethanolamine	102-71-6	2	100%	Liquid	97			10.4		Severe		CEC (1991)
Triethanolamine	102-71-6	3	100%	Liquid	97			11.9		Severe		CEC (1991)
Triethanolamine	102-71-6	4	100%	Liquid	97			4.2		Slight		CEC (1991)
Triethanolamine	102-71-6	5	100%	Liquid	97			0		Nonirritant		CEC (1991)
Triethanolamine	102-71-6	6	100%	Liquid	97			3.7		Slight		CEC (1991)
Triethanolamine	102-71-6	7	100%	Liquid	97			7.5		Moderate		CEC (1991)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility	pH	IS(B)[1]	IS(B) SD	IS(B) Classification	Overall IS(B) Classification	Reference
Triethanolamine	102-71-6	2	10%	Solution	97			11.3		Severe	Slight	CEC (1991)
Triethanolamine	102-71-6	3	10%	Solution	97			2.8		Slight		CEC (1991)
Triethanolamine	102-71-6	4	10%	Solution	97			1.1		Slight		CEC (1991)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant		10.94	0.8	Severe	Severe	Gilleron et al. (1997)
Triton X-100	9002-93-1		100%	Liquid	98	surfactant		13.73	0.48	Severe	Severe	Gilleron et al. (1997)
Triton X-155	9010-44-0		100%	Surfactant				3.9	2.3	Slight	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5		100%	Liquid	98	surfactant		14.47	0.36	Severe	Severe	Gilleron et al. (1997)
Tween 20	9005-64-5		100%	Liquid			7.21	3.22		Slight		Vinardell and Macián (1994)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, SD = standard deviation.

[1] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990).

[2] The IS(B) analysis method does not yield an IS value greater than 21 and the calculated result of 23 for this substance is not possible. Based on results with the IS(A) analysis method (IS(A) = 17.8) in the same report, the formulation would be classified as a severe irritant and was classified as such for the IS(B) analysis method.

Appendix C7

Data Sorted by Substance for IS(B)-10 Analysis Method

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Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
7-Acetoxyheptanal		MD	10%	Unknown		insoluble	n.s.	3.1	Slight	Slight	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	10%	Solid		83	2.2	13.6	Severe	Severe	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	WA	10%	Solid		83	2.2	6.1	Moderate		Spielmann et al. (1996)
Ambuphylline	5634-34-4	BG	10%	Solid		600	9	10.7	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	10%	Solid		600	9	15.8	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	10%	Unknown		3	1.5	14.8	Severe	Moderate	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	10%	Unknown		3	1.5	7	Moderate		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	10%	Unknown		3	1.5	7.6	Moderate		Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	HO	10%	Solid		560	1.5	4.4	Slight	Slight	Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	10%	Solid		560	1.5	n.p.			Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Anisole	100-66-3	AP	10%	Liquid		insoluble	n.s.	7.3	Moderate	Moderate	Spielmann et al. (1996)
Anisole	100-66-3	HK	10%	Liquid		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
B 25		BG	10%	Unknown		insoluble	n.s.	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
n-Butanal	123-72-8	HK	10%	Liquid		71	<7	1.2	Slight	Moderate	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	10%	Liquid		71	<7	6.7	Moderate		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	10%	Liquid		79	7	9.6	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	10%	Liquid		79	7	18.3	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BD	10%	Solid		1	n.s.	0	Nonirritant	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	10%	Solid		1	n.s.	10.9	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	10%	Solid		1	n.s.	9.5	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Caffeine sodium benzoate	8000-95-1	BD	10%	Solid		500	7	4.6	Slight	Moderate	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	10%	Solid		500	7	7.9	Moderate		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	10%	Solid		500	7	6.6	Moderate		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	10%	Solid		400	7	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	10%	Solid		400	7	9.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	10%	Solid		insoluble	7	2	Severe	Severe	Spielmann et al. (1996)
Camphen	79-92-5	HK	10%	Solid		insoluble	7	10	Severe		Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	BG	10%	Unknown		n.s.	3	6.9	Moderate	Moderate	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	10%	Unknown		n.s.	3	7.9	Moderate		Spielmann et al. (1996)
1-Chloroctane-8-ol		AP	10%	Unknown		insoluble	n.s.	6.8	Moderate	Moderate	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	10%	Unknown		insoluble	n.s.	4.3	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
3-Cyclohexene-1-methanol	1679-51-2	BG	10%	Unknown		insoluble	n.s.	10.1	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	10%	Unknown		insoluble	n.s.	11.8	Severe		Spielmann et al. (1996)
DC 8		BG	10%	Unknown		insoluble	n.s.	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
DC 8		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	HO	10%	Unknown		0.2	7	4.2	Slight	Slight	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	10%	Unknown		0.2	7	0	Nonirritant		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	AP	10%	Liquid		insoluble	n.s.	6	Moderate	Moderate	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	10%	Liquid		insoluble	n.s.	8.6	Moderate		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	10%	Liquid		insoluble	n.s.	1.9	Slight		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HK	10%	Solid		n.s.	n.s.	9.2	Severe	Severe	Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	10%	Solid		n.s.	n.s.	4.1	Slight		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	10%	Solid		n.s.	n.s.				Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
3,6-Dimethyloctanol		BG	10%	Unknown		poorly soluble	7	0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	10%	Unknown		poorly soluble	7	0	Nonirritant		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	10%	Solid		0.6	n.s.	4.3	Slight	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	10%	Solid		0.6	n.s.	5.6	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	10%	Liquid		insoluble	5	18.9	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	10%	Liquid		insoluble	5	2.6	Slight		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	10%	Liquid		insoluble	5	0.75	Nonirritant		Spielmann et al. (1996)
Diphocars		HK	10%	Unknown		soluble	n.s.	18.3	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	10%	Unknown		soluble	n.s.	11.1	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	10%	Solid		insoluble	n.s.	12.1	Severe	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	10%	Solid		insoluble	n.s.	1.8	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	10%	Solid		insoluble	n.s.	2.54	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
DTPA Pentasodium salt	140-01-2	BG	10%	Unknown		readily soluble	11.5	15.66	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	10%	Unknown		readily soluble	11.5	15.5	Severe		Spielmann et al. (1996)
Ede 140		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	10%	Unknown		insoluble	n.s.	3.4	Slight		Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	10%	Solid		<2.5	4.5	np		Severe	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	10%	Solid		<2.5	4.5	3.1	Slight		Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	MD	10%	Solid		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	HO	10%	Solid		insoluble	n.s.	4.1	Slight		Spielmann et al. (1996)
Ethiosan		AP	10%	Unknown		5	8.5	3.8	Slight	Slight	Spielmann et al. (1996)
Ethiosan		WA	10%	Unknown		5	8.5	0	Nonirritant		Spielmann et al. (1996)
Ethyl butanal	97-96-1	HO	10%	Liquid		10	<7	3.6	Slight	Slight	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	10%	Liquid		10	<7	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Gadopentetic acid dimeglumine salt	86050-77-3	WA	10%	Unknown		soluble	n.s.	6.4	Severe	Severe	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	10%	Unknown		soluble	n.s.	3	Severe		Spielmann et al. (1996)
Genomoll	115-96-8	HO	10%	Solid		5	6	9.2	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	10%	Solid		5	6	9.4	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BD	10%	Unknown		readily soluble	9	8.4	Moderate	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	10%	Unknown		readily soluble	9	10.1	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	10%	Unknown		readily soluble	9	10.2	Severe		Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	HO	10%	Unknown		490	0.9	14.2	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	10%	Unknown		490	0.9	11.7	Severe		Spielmann et al. (1996)
Glycediol		MD	10%	Unknown		insoluble	n.s.	0	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	10%	Unknown		insoluble	n.s.	1.8	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Granuform	30525-89-4	BD	10%	Solid		250	4	2.9	Slight	Slight	Spielmann et al. (1996)
Granuform	30525-89-4	HO	10%	Solid		250	4	0	Nonirritant		Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	10%	Unknown		poorly soluble	n.s.	2.3	Slight	Slight	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	10%	Unknown		poorly soluble	n.s.	1.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	10%	Unknown		874	8.5	5.8	Moderate	Moderate	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	10%	Unknown		874	8.5	4.3	Slight		Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HK	10%	Solid		n.s.	4.5	11.5	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	10%	Solid		n.s.	4.5	4.3	Slight		Spielmann et al. (1996)
Hnol		AP	10%	Unknown		insoluble	n.s.	0.8	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hnol		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Hoe MBF		BD	10%	Unknown		100	4.3	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	10%	Unknown		100	4.3	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Hydo 98		BD	10%	Unknown		soluble	6.5	10.4	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	10%	Unknown		soluble	6.5	12.9	Severe		Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	10%	Unknown		n.s.	10.6	13.4	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	10%	Unknown		n.s.	10.6	8.9	Moderate		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	10%	Solid		1900	1	10.8	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	10%	Solid		1900	1	14.9	Severe		Spielmann et al. (1996)
Hypo 20		BG	10%	Unknown		readily soluble	6.5	7.2	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	10%	Unknown		readily soluble	6.5	0	Nonirritant		Spielmann et al. (1996)
Hypo 36		AP	10%	Unknown		readily soluble	7	4	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	10%	Unknown		readily soluble	7	4.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Hypo 45		BD	10%	Unknown		readily soluble	7	11.1	Severe	Slight	Spielmann et al. (1996)
Hypo 45		WA	10%	Unknown		readily soluble	7	2.5	Slight		Spielmann et al. (1996)
Hypo 45		BG	10%	Unknown		readily soluble	7	1.9	Slight		Spielmann et al. (1996)
Hypo 54		BG	10%	Unknown		soluble	6.5	4.3	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	10%	Unknown		soluble	6.5	4	Slight		Spielmann et al. (1996)
Hyton		AP	10%	Unknown		soluble	8.5	17	Severe	Severe	Spielmann et al. (1996)
Hyton		BG	10%	Unknown		soluble	8.5	13.5	Severe		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	AP	10%	Solid		42	2.3	15.6	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	10%	Solid		42	2.3	0.75	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	10%	Solid		42	2.3	8.4	Moderate		Spielmann et al. (1996)
Isobornyl acetate	125-12-2	HO	10%	Solid		< 1	n.s.	4.1	Slight	Slight	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	10%	Solid		< 1	n.s.	1.7	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Isobutanal	78-84-2	WA	10%	Liquid		67	<7	2.1	Slight	Slight	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	10%	Liquid		67	<7	0	Nonirritant		Spielmann et al. (1996)
Isodecylglucoside		AP	10%	Unknown		readily soluble	9	17.2	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	10%	Unknown		readily soluble	9	9.9	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	10%	Liquid		0.1	<7	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	10%	Liquid		0.1	<7	0	Nonirritant		Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	AP	10%	Solid		1000	1.75	19.1	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	10%	Solid		1000	1.75	18.8	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	10%	Unknown		readily soluble	2	17.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	10%	Solid		soluble	3	13.5	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	10%	Solid		soluble	3	1.8	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	10%	Solid		soluble	3	10.5	Severe		Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	10%	Solid		1500	10	10	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	10%	Solid		1500	10	8.25	Moderate		Spielmann et al. (1996)

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Mecre		HK	10%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
Mecre		MD	10%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	10%	Solid		85	4	18.3	Severe	Severe	Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	10%	Solid		85	4	4.3	Slight		Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	10%	Solid		poorly soluble	n.s.	4.1	Slight	Slight	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	10%	Solid		poorly soluble	n.s.	2.2	Slight		Spielmann et al. (1996)
Methyl acetate	79-20-9	BD	10%	Liquid		250	7	4.4	Slight	Slight	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	10%	Liquid		250	7	4.3	Slight		Spielmann et al. (1996)
Methylpentynol	77-75-8	AP	10%	Liquid		soluble	n.s.	15.4	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	10%	Liquid		soluble	n.s.	12.3	Severe		Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	10%	Solid		40	11.5	17.1	Severe	Severe	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	10%	Solid		40	11.5	17.7	Severe		Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	10%	Liquid		15	3	17.7	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	10%	Liquid		15	3	17.9	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	10%	Liquid		readily soluble	7	4.9	Slight	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	10%	Liquid		readily soluble	7	4.1	Severe		Spielmann et al. (1996)

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Methyltriglycol	112-35-6	AP	10%	Liquid		readily soluble	7	11	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	10%	Liquid		readily soluble	7	3	Severe		Spielmann et al. (1996)
Napt		HO	10%	Unknown		1000	n.s.	4.3	Slight	Slight	Spielmann et al. (1996)
Napt		WA	10%	Unknown		1000	n.s.	1.9	Slight		Spielmann et al. (1996)
Nitro-bis-octylamide		BG	10%	Unknown		insoluble	n.s.	1.7	Slight	Slight	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Olak		HK	10%	Unknown		soluble	8.3	18.9	Severe	Severe	Spielmann et al. (1996)
Olak		MD	10%	Unknown		soluble	8.3	16.1	Severe		Spielmann et al. (1996)
Ölesulf		BD	10%	Unknown		soluble	8	16.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	10%	Unknown		soluble	8	16.8	Severe		Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	10%	Solid		1000	7	8.6	Moderate	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	10%	Solid		1000	7	11.1	Severe		Spielmann et al. (1996)
Phenylthiourea	103-85-5	AP	10%	Solid		1	5.5	4	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	10%	Solid		1	5.5	0	Nonirritant		Spielmann et al. (1996)
Phosphonat A		AP	10%	Unknown		3.6	2.1	6.8	Moderate	Moderate	Spielmann et al. (1996)
Phosphonat A		BG	10%	Unknown		3.6	2.1	6.6	Moderate		Spielmann et al. (1996)

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Acefyllin piperazinate	18833-13-1	HK	10%	Solid		625	5	18.5	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	10%	Solid		625	5	0	Nonirritant		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	10%	Solid		625	5	2.9	Slight		Spielmann et al. (1996)
PO 2		AP	10%	Unknown		insoluble	n.s.	4.3	Slight	Slight	Spielmann et al. (1996)
PO 2		WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	10%	Liquid		1000	6	10.9	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	10%	Liquid		1000	6	15.7	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	10%	Unknown		readily soluble	7	4.1	Slight	Slight	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	10%	Unknown		readily soluble	7	0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	10%	Unknown		750	n.s.	1	Slight	Slight	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	10%	Unknown		750	n.s.	0	Nonirritant		Spielmann et al. (1996)
Polyhexamethylene guanidine		BD	10%	Unknown		soluble	7.1	9.2	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	10%	Unknown		soluble	7.1	11	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	10%	Liquid		80	7	16.5	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	10%	Liquid		80	7	15.8	Severe		Spielmann et al. (1996)

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Potassium cyanate	590-28-3	AP	10%	Solid		750	10	18.8	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	10%	Solid		750	10	15.8	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HK	10%	Solid		250	9.5	17.8	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	10%	Solid		250	9.5	15.2	Severe		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	10%	Solid		310	8	4.2	Slight	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	10%	Solid		310	8	6.25	Moderate		Spielmann et al. (1996)
2-Pseudojonon		HK	10%	Unknown		0.1	n.s.	8.7	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	10%	Unknown		0.1	n.s.	2.8	Slight		Spielmann et al. (1996)
RK Blau		HK	10%	Unknown		100	2.6	4	Slight	Slight	Spielmann et al. (1996)
RK Blau		MD	10%	Unknown		100	2.6	0	Nonirritant		Spielmann et al. (1996)
Rubinrot Y		AP	10%	Unknown		172		n.p.		Slight	Spielmann et al. (1996)
Rubinrot Y		HO	10%	Unknown		172		4	Slight		Spielmann et al. (1996)
Sacyclo		HO	10%	Unknown		insoluble	n.s.	3.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)
Sept		BD	10%	Unknown		soluble	3	4	Severe	Severe	Spielmann et al. (1996)
Sept		HK	10%	Unknown		soluble	3	10	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Surfactant Based Formulation 1-HZA			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ			10%	Solution					Slight	Slight	Gettings et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Surfactant Based Formulation 17-HZR			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT			10%	Solution					Slight	Slight	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW			10%	Solution					Moderate	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY			10%	Solution					Severe	Severe	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ			10%	Solution					Slight	Slight	Gettings et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	10%	Liquid		poorly soluble	n.s.	3.7	Slight	Slight	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	10%	Liquid		poorly soluble	n.s.	3.9	Slight		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	10%	Liquid		insoluble	n.s.	7.9	Moderate	Moderate	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	10%	Liquid		insoluble	n.s.	2.1	Slight		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	10%	Unknown		insoluble	n.s.	0.7	Nonirritant	Nonirritant	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	10%	Unknown		insoluble	n.s.	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Silan 167	41453-78-5	WA	10%	Unknown		soluble	n.s.	2.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	10%	Unknown		soluble	n.s.	0.1	Nonirritant		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	10%	Unknown		insoluble	<7	3	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	10%	Unknown		insoluble	<7	3	Severe		Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	AP	10%	Solid		readily soluble	4.5	12.7	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	10%	Solid		readily soluble	4.5	13.9	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	10%	Solid		250	10	13.2	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	10%	Solid		250	10	11.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	10%	Solid		110	10.4	14.8	Severe	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	10%	Solid		110	10.4	10.5	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	10%	Solid		3.5	11.4	19.7	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	10%	Solid		3.5	11.4	20.7	Severe		Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	HK	10%	Solid		1080	1.1	18.8	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	10%	Solid		1080	1.1	16.7	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	10%	Unknown		soluble	8	10.5	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	10%	Unknown		soluble	8	17.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
Sodium monochloroacetate	3926-62-3	HO	10%	Solid		440	4.5	7.5	Moderate	Moderate	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	10%	Solid		440	4.5	0	Nonirritant		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	AP	10%	Solid		650	4.6	17.4	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	10%	Solid		650	4.6	12.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	bg	10%	Solid		650	4.6	14.6	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	10%	Unknown		soluble	7	18	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	10%	Unknown		soluble	7	20.1	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	10%	Unknown		0.014	n.s.	7.6	Moderate	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	10%	Unknown		0.014	n.s.	10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	10%	Unknown		50	11	13.4	Severe	Severe	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	10%	Unknown		50	11	5.4	Moderate		Spielmann et al. (1996)
Tocla		BD	10%	Unknown		40	6	12.9	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	10%	Unknown		40	6	19.7	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	10%	Solid		0.5	7	0.8	Nonirritant	Nonirritant	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	10%	Solid		0.5	7	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-10[2]	IS(B)-10 Classification	Overall IS(B)-10 Classification	Reference
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	10%	Solid		< 2.5	2.3	2.9	Slight	Slight	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	10%	Solid		< 2.5	2.3	2.3	Slight		Spielmann et al. (1996)
Trioxane	110-88-3	HK	10%	Solid		172	n.s.	9.25	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	10%	Solid		172	n.s.	13.4	Severe		Spielmann et al. (1996)
Wessalith Slurry		BG	10%	Unknown		readily soluble	11	3.13	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	10%	Unknown		readily soluble	11	10	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	10%	Solid		250	6	4	Slight	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	10%	Solid		250	6	11.3	Severe		Spielmann et al. (1996)

Abbreviation: CASRN: Chemical Abstracts Service Registy Number.

[1] Solubility = obtained from literature references; where available, expressed as g/mL

[2] IS(B)-10 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987) where the *in vitro* score was obtained using a 10% concentration and where *in vivo* results were obtained at 100% concentration.

Appendix C8

Data Sorted by Substance for IS(B)-100 Analysis Method

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Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Acetone	67-64-1		100%					15.32	Severe	Severe	Gilleron et al. (1997)
7-Acetoxyheptanal		MD	100%	Unknown		insoluble		4.9	Slight	Severe	Spielmann et al. (1996)
7-Acetoxyheptanal		WA	100%	Unknown		insoluble		17	Severe		Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	MD	100%	Solid		83	2.2	n.p.		Severe	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	WA	100%	Solid		83	2.2	10.6	Severe		Spielmann et al. (1996)
Allyl alcohol	107-18-6		100%					12.4	Severe	Severe	Gilleron et al. (1996)
Ambuphylline	5634-34-4	BG	100%	Solid		600	9	12.8	Severe	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4	MD	100%	Solid		600	9	16.9	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	AP	100%	Unknown		3	1.5	14.4	Severe	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	WA	100%	Unknown		3	1.5	13.6	Severe		Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	BG	100%	Unknown		3	1.5	8.5	Moderate		Spielmann et al. (1996)
2-Aminophemol	95-55-6		100%					0.8	Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2		100%					15.34	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Ammonium persulfate	7727-54-0	HO	100%	Solid		560	1.5	n.p.			Spielmann et al. (1996)
Ammonium persulfate	7727-54-0	WA	100%	Solid		560	1.5	n.p.			Spielmann et al. (1996)
Anisole	100-66-3	AP	100%	Liquid		insoluble		19.1	Severe	Severe	Spielmann et al. (1996)
Anisole	100-66-3	HK	100%	Liquid		insoluble		18.5	Severe		Spielmann et al. (1996)
Anthracene	120-12-7		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3		100%					1.06	Slight	Slight	Gilleron et al. (1997)
B 25		BG	100%	Unknown		insoluble		0	Nonirritant	Nonirritant	Spielmann et al. (1996)
B 25		WA	100%	Unknown		insoluble		0	Nonirritant		Spielmann et al. (1996)
Benzethonium chloride	121-54-0		100%					15.4	Severe	Severe	Gilleron et al. (1996)
n-Butanal	123-72-8	HK	100%	Liquid		71	<7	20.3	Severe	Severe	Spielmann et al. (1996)
n-Butanal	123-72-8	HO	100%	Liquid		71	<7	18.1	Severe		Spielmann et al. (1996)
n-Butanol	71-36-3	BD	100%	Liquid		79	7	13	Severe	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	HK	100%	Liquid		79	7	20.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Butyl acetate	123-86-4		100%					17.21	Severe	Severe	Gilleron et al. (1997)
Butyl carbamate	592-35-8	BD	100%	Solid		1		11.5	Severe	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8	MD	100%	Solid		1		11.6	Severe		Spielmann et al. (1996)
Butyl carbamate	592-35-8	BG	100%	Solid		1		14.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BD	100%	Solid		500	7	7.4	Moderate	Severe	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	WA	100%	Solid		500	7	17.9	Severe		Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	BG	100%	Solid		500	7	14	Severe		Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	BG	100%	Solid		400	7	16	Severe	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	WA	100%	Solid		400	7	18.8	Severe		Spielmann et al. (1996)
Camphen	79-92-5	BG	100%	Solid		insoluble	7	4	Slight	Slight	Spielmann et al. (1996)
Camphen	79-92-5	HK	100%	Solid		insoluble	7	n.p.			Spielmann et al. (1996)
Captan 90 concentrate	133-06-2		100%					15.07	Severe	Severe	Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9		100%					3.95	Slight	Slight	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Cerium-2-ethylhexanoate	24593-34-8	BG	100%	Unknown		n.s.	3	15.1	Severe	Severe	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	WA	100%	Unknown		n.s.	3	19.25	Severe		Spielmann et al. (1996)
Chlorhexidine	55-56-1		100%					14.87	Severe	Severe	Gilleron et al. (1997)
1-Chloroctane-8-ol		AP	100%	Unknown		insoluble		18.7	Severe	Severe	Spielmann et al. (1996)
1-Chloroctane-8-ol		MD	100%	Unknown		insoluble		14.3	Severe		Spielmann et al. (1996)
Cyclohexanol	108-93-0		100%					18.96	Severe	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1		100%					14.5	Severe	Severe	Gilleron et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	BG	100%	Unknown		insoluble		18.9	Severe	Severe	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	HO	100%	Unknown		insoluble		19	Severe		Spielmann et al. (1996)
DC 8		BG	100%	Unknown		insoluble		0	Nonirritant	Moderate	Spielmann et al. (1996)
DC 8		WA	100%	Unknown		insoluble		5	Moderate		Spielmann et al. (1996)
Deoxycholic acid, sodium salt	302-95-4		100%					9.7	Severe	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2		100%					15.1	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Dibenzoyl-L-tartaric acid	2743-38-6		100%					13.34	Severe	Severe	Gilleron et al. (1997)
Dibenzoyl-L-tartaric acid	2743-38-6		100%					4.2	Slight		Gilleron et al. (1996)
Dibenzyl phosphate	1623-08-1		100%					15.16	Severe	Severe	Gilleron et al. (1997)
1,4-Dibutoxy-benzene	104-36-9	HO	100%	Unknown		0.2	7	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	WA	100%	Unknown		0.2	7	n.p.			Spielmann et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4		100%					10.74	Severe	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4		100%					3.8	Slight	Slight	Gilleron et al. (1996)
Diepoxid 126	2386-87-0	AP	100%	Liquid		insoluble		10	Severe	Severe	Spielmann et al. (1996)
Diepoxid 126	2386-87-0	MD	100%	Liquid		insoluble		15.6	Severe		Spielmann et al. (1996)
Diepoxid 126	2386-87-0	BG	100%	Liquid		insoluble		6	Moderate		Spielmann et al. (1996)
Dimethyl biguanidine	657-24-9		100%					8.4	Moderate	Moderate	Gilleron et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9		100%					15.31	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
2,5-Dimethylhexanediol	110-03-2		100%					15.33	Severe	Severe	Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2	HK	100%	Solid		n.s.		16.6	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	HO	100%	Solid		n.s.		11.1	Severe		Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	BG	100%	Solid		n.s.					Spielmann et al. (1996)
3,6-Dimethyloctanol		BG	100%	Unknown		poorly soluble	7	4.3	Slight	Slight	Spielmann et al. (1996)
3,6-Dimethyloctanol		BD	100%	Unknown		poorly soluble	7	4.3	Slight		Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	AP	100%	Solid		0.6		6.7	Moderate	Moderate	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	WA	100%	Solid		0.6		5.7	Moderate		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	HK	100%	Liquid		insoluble	5	19.3	Severe	Severe	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	WA	100%	Liquid		insoluble	5	12	Severe		Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	BG	100%	Liquid		insoluble	5	4.1	Slight		Spielmann et al. (1996)
Dimethyl sulfoxide	67-68-5		100%					11.3	Severe	Severe	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Diphocars		HK	100%	Unknown		soluble		17.9	Severe	Severe	Spielmann et al. (1996)
Diphocars		HO	100%	Unknown		soluble		12.3	Severe		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	AP	100%	Solid		insoluble		2.3	Slight	Slight	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%	Solid		insoluble		4.1	Slight		Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	BG	100%	Solid		insoluble			Nonirritant		Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	BG	100%	Unknown		readily soluble	11.5	19.4	Severe	Severe	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	WA	100%	Unknown		readily soluble	11.5	19.9	Severe		Spielmann et al. (1996)
Ede 140		WA	100%	Unknown		insoluble		0	Nonirritant	Slight	Spielmann et al. (1996)
Ede 140		BD	100%	Unknown		insoluble		4.6	Slight		Spielmann et al. (1996)
EDTA dipotassium	25105-12-9		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
1,2-Epoxycyclooctane	286-62-4	MD	100%	Solid		<2.5	4.5	n.p.		Moderate	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	AP	100%	Solid		<2.5	4.5	7	Moderate		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
1,2-Epoxydodecane	2855-19-8	MD	100%	Solid		insoluble		1.4	Slight	Moderate	Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	HO	100%	Solid		insoluble		8.5	Moderate		Spielmann et al. (1996)
Ethanol	64-17-5		100%					11.3	Severe	Severe	Gilleron et al. (1996)
Ethanol	64-17-5		100%					14.97	Severe		Gilleron et al. (1997)
Ethiosan		AP	100%	Unknown		5	8.5	n.p.			Spielmann et al. (1996)
Ethiosan		WA	100%	Unknown		5	8.5	n.p.			Spielmann et al. (1996)
2-Ethoxyethanol	110-80-5		100%					10.5	Severe	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6		100%					19.32	Severe	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9		100%					10	Severe	Severe	Gilleron et al. (1996)
Ethyl butanal	97-96-1	HO	100%	Liquid		10	<7	17.4	Severe	Severe	Spielmann et al. (1996)
Ethyl butanal	97-96-1	WA	100%	Liquid		10	<7	18.7	Severe		Spielmann et al. (1996)
2-Ethyl-1-hexanol	104-76-7		100%					12.71	Severe	Severe	Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3		100%					12.94	Severe	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2		100%					13.82	Severe	Severe	Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Fomesafen	72128-02-0		100%					1.21	Slight	Slight	Gilleron et al. (1997)
Furan	110-00-9		100%					5.5	Moderate	Moderate	Gilleron et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	WA	100%	Unknown		soluble		8.2	Moderate	Moderate	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	BG	100%	Unknown		soluble		3.2	Slight		Spielmann et al. (1996)
Gamma-butyrolactone	96-48-0		100%					13.9	Severe	Severe	Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0		100%					19.39	Severe		Gilleron et al. (1997)
Genomoll	115-96-8	HO	100%	Solid		5	6	11.6	Severe	Severe	Spielmann et al. (1996)
Genomoll	115-96-8	WA	100%	Solid		5	6	9.9	Severe		Spielmann et al. (1996)
Gluconolactone	90-80-2		100%					4.6	Slight	Slight	Gilleron et al. (1996)
C12/C14-Glucoside		BD	100%	Unknown		readily soluble	9	16.7	Severe	Severe	Spielmann et al. (1996)
C12/C14-Glucoside		HK	100%	Unknown		readily soluble	9	16.3	Severe		Spielmann et al. (1996)
C12/C14-Glucoside		BG	100%	Unknown		readily soluble	9	16.5	Severe		Spielmann et al. (1996)
DL-Glutamic acid	19285-83-7		100%					0.7	Nonirritant	Nonirritant	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
L-Glutamic acid hydrochloride	138-15-8	HO	100%	Unknown		490	0.9	11.7	Severe	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	MD	100%	Unknown		490	0.9	15.2	Severe		Spielmann et al. (1996)
Glycediol		MD	100%	Unknown		insoluble		0.58	Nonirritant	Slight	Spielmann et al. (1996)
Glycediol		HO	100%	Unknown		insoluble		3.5	Slight		Spielmann et al. (1996)
Glycerol	56-81-5		100%					14.78	Severe	Severe	Gilleron et al. (1997)
3-Glycidopropyltrimethoxysilane	2530-83-8		100%					4.3	Slight	Slight	Gilleron et al. (1996)
Granuform	30525-89-4	BD	100%	Solid		250	4	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Granuform	30525-89-4	HO	100%	Solid		250	4	0	Nonirritant		Spielmann et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0		100%					10.8	Severe	Severe	Gilleron et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BG	100%	Unknown		poorly soluble		8	Moderate	Moderate	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	BD	100%	Unknown		poorly soluble		4.2	Slight		Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	WA	100%	Unknown		874	8.5	11.1	Severe	Severe	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	MD	100%	Unknown		874	8.5	11.2	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hexane	110-54-3		100%					3.1	Slight	Slight	Gilleron et al. (1996)
1,2,6-Hexanetriol	106-69-4	HK	100%	Solid		n.s.	4.5	18.8	Severe	Severe	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	HO	100%	Solid		n.s.	4.5	15.3	Severe		Spielmann et al. (1996)
Hexanol	111-27-3		100%					17.56	Severe	Severe	Gilleron et al. (1997)
Hnol		AP	100%	Unknown		insoluble		2.1	Slight	Moderate	Spielmann et al. (1996)
Hnol		WA	100%	Unknown		insoluble		6	Moderate		Spielmann et al. (1996)
Hoe MBF		BD	100%	Unknown		100	4.3	0	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF		MD	100%	Unknown		100	4.3	0.35	Nonirritant		Spielmann et al. (1996)
Hydo 98		BD	100%	Unknown		soluble	6.5	11.2	Severe	Severe	Spielmann et al. (1996)
Hydo 98		MD	100%	Unknown		soluble	6.5	n.p.			Spielmann et al. (1996)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation			100%	Solution				4.6	Slight	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing			100%	Solution				5	Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing			100%	Solution				8.5	Moderate	Moderate	Gettings et al. (1991)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hydroalcoholic Formulation 4-20% Alcohol Containing			100%	Solution				5.3	Moderate	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)			100%	Solution				n.p.	No Data	No Data	Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing			100%	Solution				11.9	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing			100%	Solution				12.8	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing			100%	Solution				12.7	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing			100%	Solution				13.8	Severe	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing			100%	Solution				13.6	Severe	Severe	Gettings et al. (1991)
2-Hydroxyethyl imino disodium acetate	135-37-5	AP	100%	Unknown		n.s.	10.6	15.5	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyethyl imino disodium acetate	135-37-5	HO	100%	Unknown		n.s.	10.6	11	Severe		Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	BD	100%	Solid		1900	1	11.3	Severe	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	WA	100%	Solid		1900	1	15.6	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Hypo 20		BG	100%	Unknown		readily soluble	6.5	8.9	Moderate	Moderate	Spielmann et al. (1996)
Hypo 20		HO	100%	Unknown		readily soluble	6.5	4.12	Slight		Spielmann et al. (1996)
Hypo 36		AP	100%	Unknown		readily soluble	7	15.9	Severe	Severe	Spielmann et al. (1996)
Hypo 36		WA	100%	Unknown		readily soluble	7	10	Severe		Spielmann et al. (1996)
Hypo 45		BD	100%	Unknown		readily soluble	7	4.4	Slight	Severe	Spielmann et al. (1996)
Hypo 45		WA	100%	Unknown		readily soluble	7	8.7	Moderate		Spielmann et al. (1996)
Hypo 45		BG	100%	Unknown		readily soluble	7	11.9	Severe		Spielmann et al. (1996)
Hypo 54		BG	100%	Unknown		soluble	6.5	4.1	Slight	Slight	Spielmann et al. (1996)
Hypo 54		HO	100%	Unknown		soluble	6.5	4.2	Slight		Spielmann et al. (1996)
Hyton		AP	100%	Unknown		soluble	8.5	18.6	Severe	Severe	Spielmann et al. (1996)
Hyton		BG	100%	Unknown		soluble	8.5	18.2	Severe		Spielmann et al. (1996)
Imidazole	288-32-4		100%					18.7	Severe	Severe	Gilleron et al. (1996)
Imidazole	288-32-4		100%					19.43	Severe		Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Iminodiacetic acid	142-73-4	AP	100%	Solid		42	2.3	12.8	Severe	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BD	100%	Solid		42	2.3	0.85	Nonirritant		Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	BG	100%	Solid		42	2.3	6.9	Moderate		Spielmann et al. (1996)
Iminodibenzyl	494-19-9		100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobornyl acetate	125-12-2	HO	100%	Solid		< 1		4.6	Slight	Moderate	Spielmann et al. (1996)
Isobornyl acetate	125-12-2	BD	100%	Solid		< 1		8.1	Moderate		Spielmann et al. (1996)
Isobutanal	78-84-2	WA	100%	Liquid		67	<7	19.4	Severe	Severe	Spielmann et al. (1996)
Isobutanal	78-84-2	HK	100%	Liquid		67	<7	20	Severe		Spielmann et al. (1996)
Isobutanol	78-83-1		100%					19.41	Severe	Severe	Gilleron et al. (1997)
Isodecylglucoside		AP	100%	Unknown		readily soluble	9	18	Severe	Severe	Spielmann et al. (1996)
Isodecylglucoside		HO	100%	Unknown		readily soluble	9	10.7	Severe		Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	BG	100%	Liquid		0.1	<7	4.5	Slight	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	WA	100%	Liquid		0.1	<7	10	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Isopropanol	67-63-0		100%					14.8	Severe	Severe	Gilleron et al. (1997)
alpha-Ketoglutaric acid	328-50-7	AP	100%	Solid		1000	1.75	19.8	Severe	Severe	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	BG	100%	Solid		1000	1.75	19.7	Severe		Spielmann et al. (1996)
Lactic acid	79-33-4	PhI	100%	Unknown		readily soluble	2	19.6	Severe	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	AP	100%	Solid		soluble	3	4	Slight	Slight	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%	Solid		soluble	3	1.1	Slight		Spielmann et al. (1996)
alpha-Lactid	4511-42-6	BG	100%	Solid		soluble	3	6.6	Moderate		Spielmann et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3		100%					12.7	Severe	Severe	Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5		100%					8.3	Moderate	Moderate	Gilleron et al. (1996)
L-Lysine Monohydrate	39665-12-8	BD	100%	Solid		1500	10	10.4	Severe	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	HO	100%	Solid		1500	10	16.9	Severe		Spielmann et al. (1996)
Magnesium carbonate	56378-72-4		100%					1.4	Slight	Slight	Gilleron et al. (1996)
Maneb	12427-38-2		100%					0.16	Nonirritant	Nonirritant	Gilleron et al. (1997)
Mecre		HK	100%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
Mecre		MD	100%	Unknown		mixable	7	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	HK	100%	Solid		85	4	n.p.			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	MD	100%	Solid		85	4	n.p.			Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Methanol	67-56-1		100%					12.2	Severe	Severe	Gilleron et al. (1996)
m-Methoxybenzaldehyde	591-31-1	MD	100%	Solid		poorly soluble		13.7	Severe	Severe	Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	BD	100%	Solid		poorly soluble		11.6	Severe		Spielmann et al. (1996)
2-Methoxyethanol	109-86-4		100%					14.5	Severe	Severe	Gilleron et al. (1996)
Methyl acetate	79-20-9	BD	100%	Liquid		250	7	19.8	Severe	Severe	Spielmann et al. (1996)
Methyl acetate	79-20-9	HO	100%	Liquid		250	7	16.1	Severe		Spielmann et al. (1996)
Methyl acetate	79-20-9		100%					18.98	Severe		Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0		100%					16.31	Severe	Severe	Gilleron et al. (1997)
Methylcyclopentane	96-37-7		100%					17.17	Severe	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3		100%					18.35	Severe	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1		100%					10.5	Severe	Severe	Gilleron et al. (1996)
Methyl isobutyl ketone	108-10-1		100%					17.75	Severe		Gilleron et al. (1997)
Methylpentynol	77-75-8	AP	100%	Liquid		soluble		20.1	Severe	Severe	Spielmann et al. (1996)
Methylpentynol	77-75-8	BD	100%	Liquid		soluble		12.9	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	AP	100%	Solid		40	11.5	4.7	Slight	Slight	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	MD	100%	Solid		40	11.5	n.p.			Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	HK	100%	Liquid		15	3	20.4	Severe	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	MD	100%	Liquid		15	3	19.2	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	BD	100%	Liquid		readily soluble	7	12.5	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%	Liquid		readily soluble	7	17	Severe		Spielmann et al. (1996)
Methyltriglycol	112-35-6	AP	100%	Liquid		readily soluble	7	20.4	Severe	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6	HO	100%	Liquid		readily soluble	7	12.8	Severe		Spielmann et al. (1996)
MYRJ 45			100%					0	Nonirritant	Nonirritant	Gilleron et al. (1996)
Napt		HO	100%	Unknown		1000		10.3	Severe	Severe	Spielmann et al. (1996)
Napt		WA	100%	Unknown		1000		5.7	Moderate		Spielmann et al. (1996)
1-Naphthalene acetic acid	86-87-3		100%					7.46	Moderate	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4		100%					15.16	Severe	Severe	Gilleron et al. (1997)
Nitro-bis-octylamide		BG	100%	Unknown		insoluble		6.5	Moderate	Moderate	Spielmann et al. (1996)
Nitro-bis-octylamide		HK	100%	Unknown		insoluble		1.6	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
1-Nitropropane	108-03-2		100%					2.8	Slight	Slight	Gilleron et al. (1996)
Octanol	111-87-5		100%					9.8	Severe	Severe	Gilleron et al. (1996)
Octanol	111-87-5		100%					16.7	Severe		Gilleron et al. (1997)
Oil/Water Emulsion-HZA			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZC			100%	Solution				3	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZE			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZF			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZH			100%	Solution				23	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI			100%	Solution				0.333	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZJ			100%	Solution				3	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZL			100%	Solution				10.3	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZM			100%	Solution				14.3	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZN			100%	Solution				3.67	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO			100%	Solution				0	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR			100%	Solution				16.3	Category 1	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS			100%	Solution				8.33	Nonirritant	Moderate	Gettings et al. (1994)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Oil/Water Emulsion-HZT			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU			100%	Solution				1	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZV			100%	Solution				0	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW			100%	Solution				5	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZY			100%	Solution				9.67	Nonirritant	Severe	Gettings et al. (1994)
Olak		HK	100%	Unknown		soluble	8.3	19.5	Severe	Severe	Spielmann et al. (1996)
Olak		MD	100%	Unknown		soluble	8.3	17	Severe		Spielmann et al. (1996)
Ölesulf		BD	100%	Unknown		soluble	8	18.9	Severe	Severe	Spielmann et al. (1996)
Ölesulf		HK	100%	Unknown		soluble	8	19.6	Severe		Spielmann et al. (1996)
Parafluoraniline	371-40-4		100%					15.49	Severe	Severe	Gilleron et al. (1997)
2,4-Pentadione	123-54-6		100%					8.8	Moderate	Moderate	Gilleron et al. (1996)
Phenylephrine hydrochloride	61-76-7	AP	100%	Solid		1000	7	18.3	Severe	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	HK	100%	Solid		1000	7	19.9	Severe		Spielmann et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3		100%					0.5	Nonirritant	Nonirritant	Gilleron et al. (1996)
Phenylthiourea	103-85-5	AP	100%	Solid		1	5.5	3.1	Slight	Slight	Spielmann et al. (1996)
Phenylthiourea	103-85-5	BD	100%	Solid		1	5.5	0	Nonirritant		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Phosphonat A		AP	100%	Unknown		3.6	2.1	3.5	Slight	Severe	Spielmann et al. (1996)
Phosphonat A		BG	100%	Unknown		3.6	2.1	10.1	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	HK	100%	Solid		625	5	15.3	Severe	Severe	Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	WA	100%	Solid		625	5	14.6	Severe		Spielmann et al. (1996)
Acefyllin piperazinate	18833-13-1	BG	100%	Solid		625	5	9	Severe		Spielmann et al. (1996)
PO 2		AP	100%	Unknown		insoluble		0.3	Nonirritant	Nonirritant	Spielmann et al. (1996)
PO 2		WA	100%	Unknown		insoluble		0	Nonirritant		Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	AP	100%	Liquid		1000	6	19.3	Severe	Severe	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	WA	100%	Liquid		1000	6	19.2	Severe		Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	HO	100%	Unknown		readily soluble	7	7.6	Moderate	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	WA	100%	Unknown		readily soluble	7	19.8	Severe		Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	MD	100%	Unknown		750		6.6	Moderate	Moderate	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	WA	100%	Unknown		750		7.7	Moderate		Spielmann et al. (1996)
Polyethylene glycol 400	25322-68-3		100%	Liquid				14.68	Severe		Gilleron et al. (1997)
Polyoxyethylene 23 lauryl ether	9002-92-0		100%					1.5	Slight	Slight	Gilleron et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Polyhexamethylene guanidine		BD	100%	Unknown		soluble	7.1	15.5	Severe	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		BG	100%	Unknown		soluble	7.1	14.6	Severe		Spielmann et al. (1996)
Polysolvan	7397-62-8	AP	100%	Liquid		80	7	19.4	Severe	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8	HO	100%	Liquid		80	7	15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3	AP	100%	Solid		750	10	19.4	Severe	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	MD	100%	Solid		750	10	15.9	Severe		Spielmann et al. (1996)
Potassium cyanate	590-28-3		100%					14.27	Severe		Gilleron et al. (1997)
Potassium hexacyanoferrate II	14459-95-1	HK	100%	Solid		250	9.5	17.2	Severe	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	HO	100%	Solid		250	9.5	6.3	Moderate		Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	BD	100%	Solid		310	8	5.7	Moderate	Moderate	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	MD	100%	Solid		310	8	6.45	Moderate		Spielmann et al. (1996)
Promethazine HCl	58-33-3		100%					11.9	Severe	Severe	Gilleron et al. (1996)
Promethazine HCl	58-33-3		100%					6.27	Moderate		Gilleron et al. (1997)
Propyl-4-hydroxybenzoate	94-13-3		100%					1.9	Slight	Slight	Gilleron et al. (1996)
2-Pseudojonon		HK	100%	Unknown		0.1		7.3	Moderate	Moderate	Spielmann et al. (1996)
2-Pseudojonon		BG	100%	Unknown		0.1		4.1	Slight		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Pyridine	110-86-1		100%					15.8	Severe	Severe	Gilleron et al. (1996)
Pyridine	110-86-1		100%					17.79	Severe		Gilleron et al. (1997)
Quinacrine	69-05-6		100%					6.5	Moderate	Moderate	Gilleron et al. (1996)
Quinacrine	69-05-6		100%					7.29	Moderate		Gilleron et al. (1997)
RK Blau		HK	100%	Unknown		100	2.6	n.p.			Spielmann et al. (1996)
RK Blau		MD	100%	Unknown		100	2.6	n.p.			Spielmann et al. (1996)
Rubinrot Y		AP	100%	Unknown		172		5.3	Moderate	Moderate	Spielmann et al. (1996)
Rubinrot Y		HO	100%	Unknown		172		n.p.			Spielmann et al. (1996)
Sacyclo		HO	100%	Unknown		insoluble		4.4	Slight	Slight	Spielmann et al. (1996)
Sacyclo		MD	100%	Unknown		insoluble		3.3	Slight		Spielmann et al. (1996)
Sept		BD	100%	Unknown		soluble	3	15.9	Severe	Severe	Spielmann et al. (1996)
Sept		HK	100%	Unknown		soluble	3	19.8	Severe		Spielmann et al. (1996)
Sodium oxalate	62-76-0		100%					14.2	Severe	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7		100%					13.19	Severe	Severe	Gilleron et al. (1997)
Tetraaminopyrimidine sulfate	5392-28-9		100%					0.5	Nonirritant	Slight	Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9		100%					4.33	Slight		Gilleron et al. (1997)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Thiourea	62-56-6		100%					13.7	Severe	Severe	Gilleron et al. (1996)
Thiourea	62-56-6		100%					17.89	Severe		Gilleron et al. (1997)
Toluene	108-88-3		100%					16.09	Severe	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4		100%					7.9	Moderate	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6		100%					4.5	Slight	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6		100%					9.6	Severe	Severe	Gilleron et al. (1996)
Trimethoxypropylsilane	1067-25-0	BD	100%	Liquid		poorly soluble		4.5	Slight	Severe	Spielmann et al. (1996)
Trimethoxypropylsilane	1067-25-0	AP	100%	Liquid		poorly soluble		13.7	Severe		Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	HO	100%	Liquid		insoluble		8.4	Moderate	Severe	Spielmann et al. (1996)
Trimethoxyoctylsilane	3069-40-7	BG	100%	Liquid		insoluble		10	Severe		Spielmann et al. (1996)
Silan 165	29055-11-6	HO	100%	Unknown		insoluble		4.1	Slight	Moderate	Spielmann et al. (1996)
Silan 165	29055-11-6	WA	100%	Unknown		insoluble		7.2	Moderate		Spielmann et al. (1996)
Silan 167	41453-78-5	WA	100%	Unknown		soluble		4.7	Slight	Slight	Spielmann et al. (1996)
Silan 167	41453-78-5	HO	100%	Unknown		soluble		2.3	Slight		Spielmann et al. (1996)
Silan 253	18784-74-2	BD	100%	Unknown		insoluble	<7	9.9	Severe	Severe	Spielmann et al. (1996)
Silan 253	18784-74-2	MD	100%	Unknown		insoluble	<7	14.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Sodium bisulfite	7631-90-5	AP	100%	Solid		readily soluble	4.5	20	Severe	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	MD	100%	Solid		readily soluble	4.5	16.8	Severe		Spielmann et al. (1996)
Sodium sulfite	7757-83-7	AP	100%	Solid		250	10	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	BG	100%	Solid		250	10	12.3	Severe		Spielmann et al. (1996)
Sodium cyanate	917-61-3	MD	100%	Solid		110	10.4	8.2	Moderate	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	WA	100%	Solid		110	10.4	10.7	Severe		Spielmann et al. (1996)
Sodium disilicate	13870-28-5	BG	100%	Solid		3.5	11.4	18.2	Severe	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	HK	100%	Solid		3.5	11.4	16.6	Severe		Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	HK	100%	Solid		1080	1.1	19.2	Severe	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	WA	100%	Solid		1080	1.1	18.1	Severe		Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	BG	100%	Unknown		soluble	8	17.9	Severe	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	MD	100%	Unknown		soluble	8	19	Severe		Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	HO	100%	Solid		440	4.5	16.1	Severe	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	BD	100%	Solid		440	4.5	10.8	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Sodiumpyrosulfite	7681-57-4	AP	100%	Solid		650	4.6	17.7	Severe	Severe	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	BD	100%	Solid		650	4.6	11.6	Severe		Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	bg	100%	Solid		650	4.6	14.5	Severe		Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	AP	100%	Unknown		soluble	7	10.4	Severe	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	HK	100%	Unknown		soluble	7	n.p.	Severe		Spielmann et al. (1996)
TA 01946 Alkylsilan		AP	100%	Unknown		0.014		16.2	Severe	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		HK	100%	Unknown		0.014		10	Severe		Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	AP	100%	Unknown		50	11	6.9	Moderate	Moderate	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	HO	100%	Unknown		50	11	n.p.	Severe		Spielmann et al. (1996)
Tocla		BD	100%	Unknown		40	6	13.5	Severe	Severe	Spielmann et al. (1996)
Tocla		HK	100%	Unknown		40	6	20.4	Severe		Spielmann et al. (1996)
Triisooctylamine	25549-16-0	BG	100%	Solid		0.5	7	14.1	Severe	Severe	Spielmann et al. (1996)
Triisooctylamine	25549-16-0	MD	100%	Solid		0.5	7	4	Slight		Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	BG	100%	Solid		< 2.5	2.3	9.7	Severe	Severe	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclo-pentene-1-acetaldehyde	4501-58-0	AP	100%	Solid		< 2.5	2.3	14.7	Severe		Spielmann et al. (1996)

Substance Name	CASRN	Test Lab	Concentration Tested	Physical Form Tested	Purity (%)	Solubility[1]	pH	IS(B)-100[2]	IS(B)-100 Classification	Overall IS(B)-100 Classification	Reference
Trioxane	110-88-3	HK	100%	Solid		172		18	Severe	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	WA	100%	Solid		172		17.8	Severe		Spielmann et al. (1996)
Triton X-155	9010-44-0		100%					3.9	Slight	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5		100%					14.47	Severe	Severe	Gilleron et al. (1997)
Tween 20	9005-64-5		100%					3.22	Slight		Vinardell and Macián (1994)
Wessalith Slurry		BG	100%	Unknown		readily soluble	11	4.1	Slight	Severe	Spielmann et al. (1996)
Wessalith Slurry		WA	100%	Unknown		readily soluble	11	15.7	Severe		Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	WA	100%	Solid		250	6	9	Severe	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	HK	100%	Solid		250	6	17.4	Severe		Spielmann et al. (1996)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number.

[1] Solubility = obtained from literature references, where available, expressed as g/mL

[2] IS(B)-100 represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987) where the *in vitro* scores was obtained using a 100% concentration and where the *in vivo* results were obtained at 100% concentration.

Appendix C9

Data Sorted by Substance for Q-Score Analysis Method

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Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Acetone	67-64-1	1	100%	Liquid	>99	water soluble		18.36	Severe	Severe	Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble		13.53	Severe		Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble		0.80	Nonirritant		Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble		10.31	Severe		Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble		1.80	Moderate	Moderate	Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble		1.30	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant		3.41	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant		5.00	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant		3.90	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant		4.39	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant		6.93	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant		4.43	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant		1.20	Nonirritant		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant		6.49	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant		6.09	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant		7.03	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant		3.10	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant		6.14	Severe		Balls et al. (1995)
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble		1.55	Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble		1.23	Nonirritant		Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble		1.80	Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble		1.93	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble		22.04	Severe	Severe	Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble		6.64	Severe		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble		1.97	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble		4.02	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant		2.43	Severe	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant		1.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant		2.34	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant		2.42	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant		1.30	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant		3.11	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant		2.71	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant		2.73	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant		4.67	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble		3.28	Severe	Severe	Balls et al. (1995)
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble		4.48	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble		5.20	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble		6.69	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble		10.14	Severe	Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble		8.81	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble		2.53	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble		14.05	Severe	Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble		10.64	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble		11.70	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble		14.73	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble		2.07	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble		0.80	Nonirritant		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Ethanol	64-17-5	1	100%	Liquid		water soluble		6.45	Severe	Severe	Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid		water soluble		10.63	Severe		Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid		water soluble		1.47	Nonirritant		Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid		water soluble		5.95	Severe		Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble		3.94	Severe	Severe	Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble		1.87	Moderate		Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble		0.90	Nonirritant		Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble		3.37	Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble		1.24	Nonirritant	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble		0.61	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble		3.12	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	1	100%	Liquid	ca. 97	water soluble		2.40	Severe	Severe	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	2	100%	Liquid	ca. 97	water soluble		2.51	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	3	100%	Liquid	ca. 97	water soluble		1.10	Nonirritant		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	4	100%	Liquid	ca. 97	water soluble		2.35	Severe		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble		0.10	Nonirritant	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble		0.19	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble		0.30	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble		1.01	Nonirritant		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Glycerol	56-81-5	1	100%	Liquid	>99.5	water soluble		0.08	Nonirritant	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	>99.5	water soluble		1.24	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	>99.5	water soluble		0.60	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	>99.5	water soluble		1.22	Nonirritant		Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble		5.01	Severe	Severe	Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble		3.98	Severe		Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble		1.80	Moderate		Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble		4.71	Severe		Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble		11.19	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble		3.50	Severe		Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble		4.59	Severe	Severe	Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble		3.58	Severe		Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble		1.20	Nonirritant		Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble		5.89	Severe		Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble		11.90	Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble		5.79	Severe		Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble		1.80	Moderate		Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble		4.36	Severe		Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble		1.88	Moderate	Severe	Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble		5.39	Severe		Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble		1.70	Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble		3.15	Severe		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble		1.51	Moderate	Moderate	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble		1.21	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble		1.78	Moderate		Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble		0.18	Nonirritant	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble		1.22	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble		0.20	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble		8.09	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble		5.83	Severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble		3.89	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble		2.50	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble		6.17	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble		2.29	Severe	Moderate	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble		1.04	Nonirritant		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble		1.50	Moderate		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble		1.86	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble		3.84	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble		4.90	Severe		Balls et al. (1995)
Octanol	111-87-5	1	100%	Liquid	>99	water insoluble		2.10	Severe	Moderate	Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble		1.00	Nonirritant		Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble		1.80	Moderate		Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble		1.78	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	1	100%	Liquid	99	water insoluble		5.25	Severe	Severe	Balls et al. (1995)
Parafluoraniline	371-40-4	2	100%	Liquid	99	water insoluble		4.46	Severe		Balls et al. (1995)
Parafluoraniline	371-40-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	4	100%	Liquid	99	water insoluble		2.57	Severe		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid		surfactant		1.59	Moderate	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid		surfactant		0.72	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid		surfactant		0.60	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid		surfactant		1.22	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble		2.17	Severe	Severe	Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble		2.50	Severe		Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble		6.07	Severe		Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	100	water soluble		3.20	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	100	water soluble		3.00	Severe		Balls et al. (1995)

Substance Name	CASRN	Lab Number	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	Q-Score[2]	Q-Score Classification	Overall Q-Score Classification	Reference
Pyridine	110-86-1	1	100%	Liquid	>99.9	water soluble		3.84	Severe	Severe	Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99.9	water soluble		7.76	Severe		Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99.9	water soluble		12.90	Severe		Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99.9	water soluble		10.44	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	1%	Solution		water soluble		6.34	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	1%	Solution		water soluble		6.17	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	1%	Solution		water soluble		4.80	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	1%	Solution		water soluble		4.36	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	10%	Solution		water soluble		13.13	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	10%	Solution		water soluble		7.82	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	10%	Solution		water soluble		23.00	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	10%	Solution		water soluble		9.82	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant		2.68	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant		1.62	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant		2.46	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant		2.86	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant		2.34	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant		4.37	Severe		Balls et al. (1995)
Thiourea	62-56-6	1	100%	Solid	>99	water soluble		1.31	Nonirritant	Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	3	100%	Solid	>99	water soluble		0.50	Nonirritant		Balls et al. (1995)
Toluene	108-88-3	1	100%	Liquid	99	water insoluble		3.18	Severe	Severe	Balls et al. (1995)
Toluene	108-88-3	2	100%	Liquid	99	water insoluble		5.84	Severe		Balls et al. (1995)
Toluene	108-88-3	3	100%	Liquid	99	water insoluble		2.90	Severe		Balls et al. (1995)
Toluene	108-88-3	4	100%	Liquid	99	water insoluble		2.98	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	3%	Solution		water soluble		18.76	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	3%	Solution		water soluble		9.15	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	3%	Solution		water soluble		9.90	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	3%	Solution		water soluble		5.33	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	30%	Solution		water soluble		14.39	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	30%	Solution		water soluble		9.96	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	30%	Solution		water soluble		13.10	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	30%	Solution		water soluble		11.81	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant		2.66	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant		2.72	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant		1.40	Nonirritant		Balls et al. (1995)
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant		2.20	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant		3.45	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant		1.71	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant		2.40	Severe		Balls et al. (1995)
Tween 20	9005-64-5	1	100%	Liquid	98	surfactant		0.39	Nonirritant	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant		0.38	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant		0.60	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant		0.95	Nonirritant		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

[1] Solubility obtained from literature references, where availble, expressed as g/mL

[2] Q-Score represents irritation scores that were calcualted using the method described in Balls et al. (1995)

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Appendix C10

Data Sorted by Substance for S-Score Analysis Method

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	S-Score[2]	S-Score Classification	Overall S-Score Classification	Reference
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	Solid	>99.9	water soluble		12.00	Moderate		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		1.00	Nonirritant	Nonirritant	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		2.00	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	Solid	100	water soluble		6.00	Moderate		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	Solid	98	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		0.00	Nonirritant		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	Solid	90	water soluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		6.00	Moderate		Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	Solid	95	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		3.00	Nonirritant	Moderate	Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		6.00	Moderate		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	Solid		water insoluble		11.00	Moderate		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant	Severe	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	Solid	99.5	water insoluble		15.00	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	Solid	99.5	water insoluble		18.00	Severe		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		9.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Fomesafen	72128-02-0	100%	Solid	97.5	water soluble		6.00	Moderate		Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
Maneb	12427-38-2	100%	Solid	ca. 90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vitro* Physical Form Tested	Purity (%)	Solubility[1]	pH	S-Score[2]	S-Score Classification	Overall S-Score Classification	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	Solid	99	water soluble		18.00	Severe		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		6.00	Moderate	Moderate	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		13.00	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		0.00	Nonirritant		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	Solid	96	water insoluble		4.00	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	100%	Solid	97	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	Solid	98	water soluble		18.00	Severe		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		4.00	Nonirritant		Balls et al. (1995)
Quinacrine	69-05-6	100%	Solid		water soluble		3.00	Nonirritant		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		0.00	Nonirritant	Moderate	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		12.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		11.00	Moderate		Balls et al. (1995)
Sodium oxalate	62-76-0	100%	Solid	>99	water soluble		9.00	Moderate		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		0.00	Nonirritant		Balls et al. (1995)
Sodium perborate	10486-00-7	100%	Solid	98.6	water soluble		7.00	Moderate		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		0.00	Nonirritant		Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	Solid	97	water insoluble		6.00	Moderate		Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		18.00	Severe	Severe	Balls et al. (1995)
Thiourea	62-56-6	100%	Solid	>99	water soluble		13.00	Moderate		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

[1] Solubility obtained from literature sources, where available expressed as g/mL

[2] S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

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Appendix D

In Vivo and In Vitro Comparison of Ocular Irritancy Classification

D1 Data Sorted by Reference D-3

D2 Data Sorted by Substance for IS(A) Analysis Method D-17

D3 Data Sorted by Substance for IS(A)-10 Analysis Method D-23

D4 Data Sorted by Substance for IS(A)-100 Analysis Method D-27

D5 Data Sorted by Substance for IS(B) Analysis Method D-31

D6 Data Sorted by Substance for IS(B)-10 Analysis Method D-45

D7 Data Sorted by Substance for IS(B)-100 Analysis Method D-57

D8 Data Sorted by Substance for Q-Score Analysis Method D-75

D9 Data Sorted by Substance for S-Score Analysis Method D-81

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Appendix D1

Data Sorted by Reference

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Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vivo* Concentration Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[2]	GHS Category 1 Subclass[3]	*In Vivo* (EPA) Classification[4]	*In Vivo* (EU) Classification[5]	*In Vitro* Classification (IS(A))[6]	*In Vitro* Classification (IS(B))[7]	*In Vitro* Classification (IS(B)-10)[8]	*In Vitro* Classification (IS(B)-100)[9]	*In Vitro* Classification (Q-Score)[10]	11*In Vitro* Classification (S-Score)[11]	Reference
Triethanolamine	102-71-6	10%	10%	Amine, Alcohol	Solution			Nonirritant		Category IV	Nonirritant	Severe						Bagley et al. (1992)
Triton X-100	9002-93-1	1%	1%	Ether	Solution			Nonirritant		Category III	Nonirritant	Severe						Bagley et al. (1992)
Acetone	67-64-1	100%	100%	Ketone	Liquid			Category 2A		Category II	R36					Severe		Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36					Moderate	Severe	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM					Nonirritant	Nonirritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1%	1%	Onium	Solution			Category 1/Category 2A	1	Category I	R36/R41					Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	5%	5%	Onium	Solution			Category 1	2	Category I	R41					Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	10%	10%	Onium	Solution			Category 1	4	Category I	R41					Severe		Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid			Category 1	2	SCNM	R41						Nonirritant	Balls et al. (1995)
Butyl acetate	123-86-4	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant					Moderate		Balls et al. (1995)
gamma-Butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid			Category 2A		Category II	R36					Severe		Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	100%	Imide, Organic sulfur compound	Solid			Category 1	4	Category I	R41						Nonirritant	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	100%	Carboxylic acid, Aldehyde	Solid			Category 2A		Category II	R36						Moderate	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	0.1%	0.1%	Heterocyclic compounds, Onium	Solution			Nonirritant		Category III	Nonirritant					Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	6%	6%	Heterocyclic compounds, Onium	Solution			Category 1	2	SCNM	R41					Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	10%	10%	Heterocyclic compounds, Onium	Solution			Category 1	4	Category I	R41					Severe		Balls et al. (1995)
Chlorhexidine	55-56-1	100%	100%	Amidine	Solid			Category 1	4	SCNM	SCNM						Moderate	Balls et al. (1995)
Cyclohexanol	108-93-0	100%	100%	Alcohol	Liquid			Category 1	2	Category I	R41					Severe		Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	100%	Ester	Solid			Category 2A		Category II	R36						Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	100%	Acyl halide	Liquid			Category 2A		Category II	SCNM					Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	100%	100%	Carboxylic acid	Liquid			SCNM		Category I	SCNM					Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	100%	Alcohol	Solid			Category 1	1	Category I	R41					Severe	Severe	Balls et al. (1995)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			Category 2A		Category III	Nonirritant					Severe		Balls et al. (1995)
Ethyl acetate	141-78-6	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant					Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36					Nonirritant		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	100%	100%	Ketone, Ester	Liquid			Category 2B		Category III	Nonirritant					Severe		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant					Nonirritant		Balls et al. (1995)
Fomesafen	72128-02-0	100%	100%	Imide, Ether, Nitro compound	Solid			Nonirritant		Category III	Nonirritant						Moderate	Balls et al. (1995)
Glycerol	56-81-5	100%	100%	Alcohol	Liquid			Nonirritant		Category IV	Nonirritant					Nonirritant		Balls et al. (1995)
n-Hexanol	111-27-3	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36					Severe		Balls et al. (1995)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41					Severe	Severe	Balls et al. (1995)
Isobutanol	78-83-1	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36					Severe		Balls et al. (1995)
Isopropanol	67-63-0	100%	100%	Alcohol	Liquid			Category 2A		Category III	SCNM					Severe		Balls et al. (1995)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM					Nonirritant	Nonirritant	Balls et al. (1995)
Methyl acetate	79-20-9	100%	100%	Ester	Liquid			Category 2A		Category II	R36					Severe		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	100%	100%	Ester, Nitrile	Liquid			Category 2A		Category II	R36					Moderate		Balls et al. (1995)
Methylcyclopentane	96-37-7	100%	100%	Cyclic hydrocarbon	Liquid			Nonirritant		Category III	Nonirritant					Nonirritant		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	100%	100%	Ketone	Liquid			Category 2A		Category III	R36					Severe		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid			Nonirritant		Category III	Nonirritant					Moderate		Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	100%	Carboxylic acid, Polycyclic compound	Solid			Category 1	NC	Category I	SCNM						Moderate	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41					Severe	Severe	Balls et al. (1995)
n-Octanol	111-87-5	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36					Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	100%	100%	Amine	Liquid			SCNM		SCNM	SCNM					Severe		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	100%	100%	Alcohol, Ether	Liquid			Nonirritant		Category IV	Nonirritant					Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM					Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid			Category 1	1	Category I	R41					Severe	Severe	Balls et al. (1995)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid			Category 1	4	Category I	R41					Severe		Balls et al. (1995)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid			Category 1	3	Category I	R41						Nonirritant	Balls et al. (1995)
Sodium hydroxide	1310-73-2	1%	1%	Alkali	Solution			Category 2B		Category III	R36					Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	10%	10%	Alkali	Solution			Category 1	4	Category I	R41					Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3%	3%	Organic salt, Carboxylic acid salt	Solution			Nonirritant		Category III	Nonirritant					Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	15%	15%	Organic salt, Carboxylic acid salt	Solution			Category 1	NC	Category I	SCNM					Severe		Balls et al. (1995)

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Sodium oxalate	62-76-0	100%	100%	Organic salt, Carboxylic acid salt	Solid			Category 1	4	Category I	R41						Moderate	Balls et al. (1995)
Sodium perborate	10486-00-7	100%	100%	Inorganic salt, Boron containing compound	Solid			Category 1	4	Category I	R41						Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid			Nonirritant		Category III	Nonirritant						Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid											Nonirritant	Severe	Balls et al. (1995)
Toluene	108-88-3	100%	100%	Polycyclic compound	Liquid			Nonirritant		Category III	Nonirritant					Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3%	3%	Carboxylic acid	Solution			Nonirritant		Category III	Nonirritant					Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	30%	30%	Carboxylic acid	Solution			Category 1	4	Category I	R41					Severe		Balls et al. (1995)
Triton X-100	9002-93-1	5%	5%	Ether	Solution			Categorry 2A/Category 2B		Category III	Nonirritant/R36					Severe		Balls et al. (1995)
Triton X-100	9002-93-1	10%	10%	Ether	Solution			Category 1	4	Category II	SCNM					Severe		Balls et al. (1995)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid			Nonirritant		Category III	Nonirritant					Nonirritant		Balls et al. (1995)
Acetic acid	64-19-7	100%	n.a.	Carboxylic acid	Liquid						R41		Severe					CEC (1991)
Acetic acid	64-19-7	10%	n.a.	Carboxylic acid	Solution						R41		Severe					CEC (1991)
Benzalkonium chloride	8001-54-5	100%	n.a.	Onium	Unknown		Cationic Surfactant				R41		Severe					CEC (1991)
Brij 35	9002-92-0	100%	n.a.	Alcohol	Solid		Nonionic Surfactant				Nonirritant		Slight					CEC (1991)
Butanol	71-36-3	100%	n.a.	Alcohol	Liquid						R36		Severe					CEC (1991)
Butanol	71-36-3	10%	n.a.	Alcohol	Solution						R36		Severe					CEC (1991)
Dimethyl sulfoxide	67-68-5	100%	n.a.	Organic sulfur compound	Liquid						Nonirritant		Severe					CEC (1991)
Dimethyl sulfoxide	67-68-5	10%	n.a.	Organic sulfur compound	Solution						Nonirritant		Slight					CEC (1991)
Glycerol	56-81-5	100%	n.a.	Alcohol	Liquid						Nonirritant		Severe					CEC (1991)
Glycerol	56-81-5	10%	n.a.	Alcohol	Solution						Nonirritant		Slight					CEC (1991)
n-Hexane	110-54-3	100%	n.a.	Acyclic hydrocarbon	Liquid						Nonirritant		Slight					CEC (1991)
n-Hexane	110-54-3	10%	n.a.	Acyclic hydrocarbon	Solution						Nonirritant		Severe					CEC (1991)
2-Methoxyethanol	109-86-4	100%	n.a.	Alcohol	Liquid						Nonirritant		Severe					CEC (1991)
2-Methoxyethanol	109-86-4	10%	n.a.	Alcohol	Solution						Nonirritant		Moderate					CEC (1991)
Sodium dodecyl sulfate	151-21-3	100%	n.a.	Organic salt, Carboxylic acid salt	Solid		Anionic Surfactant				R41		Severe					CEC (1991)
Sodium dodecyl sulfate	151-21-3	10%	n.a.	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant				R36		Severe					CEC (1991)
Toluene	108-88-3	100%	n.a.	Polycyclic compound	Liquid						Nonirritant		Severe					CEC (1991)
Triethanolamine	102-71-6	100%	n.a.	Amine, Alcohol	Liquid						Nonirritant		Severe					CEC (1991)
Triethanolamine	102-71-6	10%	n.a.	Amine, Alcohol	Solution						Nonirritant		Slight					CEC (1991)
Triacetin	102-76-1	100%	n.a.	Ester	Liquid						Nonirritant		Slight					CEC (1991)
Triacetin	102-76-1	10%	n.a.	Ester	Solution						Nonirritant		Slight					CEC (1991)
Tributyltin chloride	1461-22-9	100%	n.a.	Organometallic compound	Solid						R41		Moderate					CEC (1991)
Tributyltin chloride	1461-22-9	10%	n.a.	Organometallic compound	Solution						R41		Severe					CEC (1991)
2-Butoxyethyl acetate	112-07-2	100%	n.a.	Ester	Liquid						Nonirritant		Slight					CEC (1991)
2-Butoxyethyl acetate	112-07-2	10%	n.a.	Ester	Solution						Nonirritant		Slight					CEC (1991)
Dibutyltin chloride	683-18-1	100%	n.a.	Organic salt	Solid						R41		Severe					CEC (1991)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant		Slight					Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant		Moderate					Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant		Moderate					Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant		Moderate					Gettings et al. (1991)

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Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant		No Data					Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41		Severe					Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41		Severe					Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)		Undiluted	Undiluted	Formulation	Solution			Category 2B		Category II	Nonirritant		Severe					Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)		Undiluted	Undiluted	Formulation	Solution			Category 2A		Category II	SCNM		Severe					Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41		Severe					Gettings et al. (1991)
Oil/Water Emulsion-HZA		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZC		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZE		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZF		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZH		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Severe					Gettings et al. (1994)
Oil/Water Emulsion-HZI		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Nonirritant					Gettings et al. (1994)
Oil/Water Emulsion-HZJ		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZL		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Severe					Gettings et al. (1994)
Oil/Water Emulsion-HZM		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Severe					Gettings et al. (1994)
Oil/Water Emulsion-HZN		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZO		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Nonirritant					Gettings et al. (1994)
Oil/Water Emulsion-HZR		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Severe					Gettings et al. (1994)
Oil/Water Emulsion-HZS		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Moderate					Gettings et al. (1994)
Oil/Water Emulsion-HZT		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZU		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Slight					Gettings et al. (1994)
Oil/Water Emulsion-HZV		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Nonirritant					Gettings et al. (1994)
Oil/Water Emulsion-HZW		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Moderate					Gettings et al. (1994)
Oil/Water Emulsion-HZY		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Severe					Gettings et al. (1994)
Surfactant Based Formulation 1-HZA		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Severe					Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Severe					Gettings et al. (1996)

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Surfactant Based Formulation 4-HZD		10%	Undiluted	Formulation	Solution			Category 2B		Category III	Nonirritant	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Undiluted	Formulation	Solution			SCNM		Category I	SCNM	Slight	Severe					Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Severe					Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 8-HZH		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Slight					Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Severe					Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Severe					Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Severe					Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Slight					Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 15-HZP		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Slight					Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Slight					Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Severe					Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Slight					Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Undiluted	Formulation	Solution			Category 2B		Category III	R36	Slight	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 22-HZW		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Moderate					Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Severe					Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Severe					Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Slight					Gettings et al. (1996)
2-Methoxyethanol	109-86-4	100%	100%	Alcohol, Ether	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Triton X-155	9010-44-0	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant				Nonirritant		Slight					Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7	100%	100%	Amino acid	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Allyl alcohol	107-18-6	100%	100%	Alcohol	Liquid						R36		Severe					Gilleron et al. (1996)
1-Nitropropane	108-03-2	100%	100%	Acyclic hydrocarbon, Nitro compound	Liquid						Nonirritant		Slight					Gilleron et al. (1996)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Cyclohexanone	108-94-1	100%	100%	Ketone, Cyclic hydrocarbon	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6	100%	100%	Cyclic hydrocarbon	Liquid						Nonirritant		Slight					Gilleron et al. (1996)
Furan	110-00-9	100%	100%	Heterocycle	Liquid						Nonirritant		Moderate					Gilleron et al. (1996)
Hexane	110-54-3	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant		Slight					Gilleron et al. (1996)
2-Ethoxyethanol	110-80-5	100%	100%	Alcohol	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid						R36		Severe					Gilleron et al. (1996)
Octanol	111-87-5	100%	100%	Alcohol	Liquid						R36		Severe					Gilleron et al. (1996)
Anthracene	120-12-7	100%	100%	Polycyclic compound	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Benzethonium chloride	121-54-0	100%	100%	Amine, Onium	Solid		Cationic Surfactant				R41		Severe					Gilleron et al. (1996)
Diacetone alcohol	123-42-2	100%	100%	Ketone	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
2,4-Pentadione	123-54-6	100%	100%	Ketone	Liquid						Nonirritant		Moderate					Gilleron et al. (1996)
Ethylacetoacetate	141-97-9	100%	100%	Carboxylic acid, Ketone	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5	100%	100%	Amine, Onium	Unknown		Zwitterionic Surfactant				R36		Moderate					Gilleron et al. (1996)
3-Glycidopropyltrimethoxysilane	2530-83-8	100%	100%	Ether, Organosilicon compound	Liquid						Nonirritant		Slight					Gilleron et al. (1996)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vivo* Concentration Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[2]	GHS Category 1 Subclass[3]	*In Vivo* (EPA) Classification[4]	*In Vivo* (EU) Classification[5]	*In Vitro* Classification (IS(A))[6]	*In Vitro* Classification (IS(B))[7]	*In Vitro* Classification (IS(B)-10)[8]	*In Vitro* Classification (IS(B)-100)[9]	*In Vitro* Classification (Q-Score)[10]	*11n Vitro* Classification (S-Score)[11]	Reference
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4	100%	100%	Amide, Organic sulfur compound	Solid						Nonirritant		Slight					Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid						R41		Slight					Gilleron et al. (1996)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid						R36		Severe					Gilleron et al. (1996)
Iminodibenzyl	494-19-9	100%	100%	Heterocycle	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Magnesium carbonate	56378-72-4	100%	100%	Alcohol	Solid						Nonirritant		Slight					Gilleron et al. (1996)
Hexadecyltrimethylam monium bromide	57-09-0	100%	100%	Organic salt, Onium	Liquid		Cationic Surfactant				R36		Severe					Gilleron et al. (1996)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid						R41		Severe					Gilleron et al. (1996)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid						R36		Severe					Gilleron et al. (1996)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Dimethyl biguanidine	657-24-9	100%	100%	Amidine	Solid						Nonirritant		Moderate					Gilleron et al. (1996)
Methanol	67-56-1	100%	100%	Alcohol	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Dimethyl sulfoxide	67-68-5	100%	100%	Organic sulfur compound	Liquid						Nonirritant		Severe					Gilleron et al. (1996)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid						R36		Moderate					Gilleron et al. (1996)
Gluconolactone	90-80-2	100%	100%	Carboxylic acid, Lactone, Carbohydrate	Solid						Nonirritant		Slight					Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3	100%	100%	Heterocycle	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Propyl-4-hydroxybenzoate	94-13-3	100%	100%	Carboxylic acid, Phenol	Solid						Nonirritant		Slight					Gilleron et al. (1996)
1,2,3-Trichloropropane	96-18-4	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant		Moderate					Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid						R36		Severe					Gilleron et al. (1996)
Polyoxyethylene 23 lauryl ether	9002-92-0	100%	100%	Alcohol	Solid		Nonionic Surfactant				Nonirritant		Slight					Gilleron et al. (1996)
EDTA dipotassium	25105-12-9	100%	100%	Amine, Carboxylic acid, Organic salt	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4	100%	100%	Alcohol, Carboxylic acid, Organic salt	Solid		Nonionic Surfactant				R36		Severe					Gilleron et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3	100%	100%	Aminde, Amine Salt	Solid		Anionic Surfactant				Nonirritant		Severe					Gilleron et al. (1996)
2-Aminophemol	95-55-6	100%	100%	Amine, Phenol	Solid						Nonirritant		Nonirritant					Gilleron et al. (1996)
MYRJ 45		100%	100%	Unknown	Solid		Nonionic Surfactant				Nonirritant		Nonirritant					Gilleron et al. (1996)
1-Naphthalene acetic acid	86-87-3	100%	100%	Carboxylic acid, Polycyclic compound	Solid			Category 1	NC	Category I	SCNM		Moderate					Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41		Severe					Gilleron et al. (1997)
2,2-Dimethylbutanoic acid	595-37-9	100%	100%	Carboxylic acid	Liquid			SCNM		Category I	SCNM		Severe					Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2	100%	100%	Alcohol	Solid			Category 1	1	Category I	R41		Severe					Gilleron et al. (1997)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	100%	Acyl halide	Liquid			Category 2A		Category II	SCNM		Severe					Gilleron et al. (1997)
2-Ethyl-1-hexanol	104-76-7	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9	100%	100%	Carboxylic acid, Aldehyde	Solid			Category 2A		Category II	R36		Slight					Gilleron et al. (1997)
Acetone	67-64-1	100%	100%	Ketone	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36		Severe					Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	5%	Onium	Solution		Cationic Surfactant	Category 1/Category 2A	2	Category I	R36/R41		Severe					Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	10%	Onium	Solution		Cationic Surfactant	Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	1%	Onium	Solution		Cationic Surfactant	Category 1	1	Category I	R41		Severe					Gilleron et al. (1997)
Benzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid			Category 1	2	SCNM	R41		Severe					Gilleron et al. (1997)
Butyl acetate	123-86-4	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Captan 90 concentrate	133-06-2	100%	100%	Imide, Organic sulfur compound	Solid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7	100%	0.10%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7	100%	10%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Category 1	4	SCNM	R41		Severe					Gilleron et al. (1997)

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Cetylpyridinium bromide	140-72-7	100%	6%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Category 1	2	Category I	R41		Severe					Gilleron et al. (1997)
Chlorhexidine	55-56-1	100%	100%	Amidine	Solid			Category 1	4	SCNM	SCNM		Severe					Gilleron et al. (1997)
Cyclohexanol	108-93-0	100%	100%	Alcohol	Liquid			Category 1	2	Category I	R41		Severe					Gilleron et al. (1997)
Dibenzyl phosphate	1623-08-1	100%	100%	Ester	Solid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			Category 2A		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Ethyl acetate	141-78-6	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3	100%	100%	Ketone, Ester	Liquid			Category 2B		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Fomesafen	72128-02-0	100%	100%	Imide, Ether, Nitro compound	Solid			Nonirritant		Category III	Nonirritant		Slight					Gilleron et al. (1997)
Gamma-butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Glycerol	56-81-5	100%	100%	Alcohol	Liquid			Nonirritant		Category IV	Nonirritant		Severe					Gilleron et al. (1997)
Hexanol	111-27-3	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Isobutanol	78-83-1	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Isopropanol	67-63-0	100%	100%	Alcohol	Liquid			Category 2A		Category III	SCNM		Severe					Gilleron et al. (1997)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM		Slight					Gilleron et al. (1997)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM		Nonirritant					Gilleron et al. (1997)
Methyl acetate	79-20-9	100%	100%	Ester	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0	100%	100%	Ester, Nitrile	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3	100%	100%	Ketone	Liquid			Category 2A		Category III	R36		Severe					Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Methylcyclopentane	96-37-7	100%	100%	Cyclic hydrocarbon	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Octanol	111-87-5	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36		Severe					Gilleron et al. (1997)
Parafluoraniline	371-40-4	100%	100%	Amine	Liquid			SCNM		SCNM	SCNM		Severe					Gilleron et al. (1997)
Polyethylene glycol 400	25322-68-3	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category IV	Nonirritant		Severe					Gilleron et al. (1997)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM		Severe					Gilleron et al. (1997)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid			Category 1	1	Category I	R41		Moderate					Gilleron et al. (1997)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid			Category 1	3	Category I	R41		Moderate					Gilleron et al. (1997)
Sodium hydroxide	1310-73-2	100%	1%	Alkali	Solution			Category 2B		Category III	R36		Severe					Gilleron et al. (1997)
Sodium hydroxide	1310-73-2	100%	10%	Alkali	Solution			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	100%	3%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	100%	15%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Category 1	NC	Category I	SCNM		Severe					Gilleron et al. (1997)
Sodium oxalate	62-76-0	100%	100%	Organic salt, Carboxylic acid salt	Solid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Sodium perborate	10486-00-7	100%	100%	Inorganic salt, Boron containing compound	Solid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Tetraaminopyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid			Nonirritant		Category III	Nonirritant		Slight					Gilleron et al. (1997)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid								Severe					Gilleron et al. (1997)
Toluene	108-88-3	100%	100%	Polycyclic compound	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Trichloroacetic acid	76-03-9	100%	30%	Carboxylic acid	Liquid			Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Trichloroacetic acid	76-03-9	100%	3%	Carboxylic acid	Liquid			Category 1	4	Category I	R41		Severe					Gilleron et al. (1997)
Triton X-100	9002-93-1	Undiluted	5%	Ether	Liquid		Nonionic Surfactant	Categorry 2A/Category 2B		Category III	Nonirritant/R36		Severe					Gilleron et al. (1997)
Triton X-100	9002-93-1	Undiluted	10%	Ether	Liquid		Nonionic Surfactant	Category 1	4	Category II	SCNM		Severe					Gilleron et al. (1997)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category III	Nonirritant		Severe					Gilleron et al. (1997)
Acetic acid	64-19-7	10%	10%	Carboxylic acid	Solution			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	10%	10%	Alcohol	Solution			Category 1	4	SCNM	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	10%	10%	Organic salt, Onium	Solution			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate Solution (20% Solution)	18472-51-0	10%	10%	Amidine, Ester	Solution			Category 2B		Category II	Nonirritant	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data

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Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	10%	10%	Organic salt, Sulfur containing compound, Ester	Solution			Category 1	4	Category I	R36	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	10%	10%	Amine, Alcohol	Solution			Nonirritant		Category III	Nonirritant	Moderate						Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	10%	10%	Organic salt, Onium, Ether	Solution			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	10%	10%	Alcohol	Solution			Nonirritant		Category IV	Nonirritant	Slight						Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			SCNM		SCNM	SCNM	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Glycolic acid	79-14-1	10%	10%	Carboxylic acid, Alcohol	Solution			Category 2B		Category III	Nonirritant	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	10%	10%	Carboxylic acid, Alcohol	Solution			SCNM		Category III	SCNM	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	100%	100%	Carboxylic acid, Alcohol	Liquid			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Potassium laurate	10124-65-9	10%	10%	Organic salt, Carboxylic acid salt	Solution			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Stearyltrimethylammonium chloride	15461-40-2	10%	10%	Organic salt, Onium	Solution			Category 1	4	Category I	R41	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	10%	10%	Amine, Alcohol	Solution			Nonirritant		Category IV	Nonirritant	Slight						Hagino et al. (1999)/Submitted Y.
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid			Nonirritant		Category III	Nonirritant	Moderate						Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	10%	10%	Amine, Alcohol	Solution			Category 2B		Category III	Nonirritant	Severe						Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	10%		Alcohol	Unknown			Nonirritant		Category IV	Nonirritant	Slight						Kojima et al. (1995)
Potassium laurate	10124-65-9	10%		Organic salt, Carboxylic acid salt	Unknown			Category 1	4	Category I	R41	Severe						Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3	10%		Organic salt, Carboxylic acid salt	Unknown			Category 1/Category 2A	4	Category I/Category II	R41/Nonirritant	Moderate						Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2	10%		Organic salt, Onium	Unknown			Category 1	4	Category I	R41	Severe						Kojima et al. (1995)
Triton X-100	9002-93-1	10%		Ether	Unknown			Category 1		Category II	SCNM	Moderate						Kojima et al. (1995)
C12/C14-Glucoside		100%, 10%, and ITC		Alcohol, Ether	Unknown	9		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Isodecylglucoside		100%, 10%, and ITC		Alcohol, Ether	Unknown	9		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Nitro-bis-octylamide		100%, 10%, and ITC		Alcohol, Ether	Unknown	ns		Nonirritant		Category III	Nonirritant			Slight	Moderate			Spielmann et al. (1996)
7-Acetoxyheptanal		100%, 10%, and ITC		Aldehyde, Ester	Unknown	ns		Category 1	1	Category I	R41			Slight	Severe			Spielmann et al. (1996)
Sodium disilicate	13870-28-5	100%, 10%, and ITC		Inorganic salt	Solid	11.4		Category 1	4	SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	100%, 10%, and ITC		Inorganic salt	Solid	1.1		Category 1	4	SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	100%, 10%, and ITC		Amide, Amino acid	Solid	2.2		Category 1	4	SCNM	R41			Severe	Severe			Spielmann et al. (1996)
Ambuphylline	5634-34-4	100%, 10%, and ITC		Amine, Heterocycle, Alcohol	Solid	9		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	100%, 10%, and ITC		Amine, Ether, Organic sulfur compound	Unknown	1.5		Category 1	4	SCNM	SCNM			Moderate	Severe			Spielmann et al. (1996)
Ammoniumpersulfate	7727-54-0	100%, 10%, and ITC		Inorganic salt	Solid	1.5		SCNM		SCNM	SCNM			Slight	Severe			Spielmann et al. (1996)
Anisole	100-66-3	100%, 10%, and ITC		Ether	Liquid	ns		SCNM		SCNM	SCNM			Moderate	Severe			Spielmann et al. (1996)
B 25		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Nonirritant	Nonirritant			Spielmann et al. (1996)
n-Butanal	123-72-8	100%, 10%, and ITC		Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant			Moderate	Severe			Spielmann et al. (1996)

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n-Butanol	71-36-3	100%, 10%, and ITC		Alcohol	Liquid	ns		Category 1	4	SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Butyl carbamate	592-35-8	100%, 10%, and ITC		Ester	Solid	ns		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1	100%, 10%, and ITC		Heterocycle, Organic salt, Carboxylic acid salt	Solid	7		Nonirritant		Category IV	Nonirritant			Moderate	Severe			Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	100%, 10%, and ITC		Heterocycle, Phenol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Camphen	79-92-5	100%, 10%, and ITC		Cyclic hydrocarbon	Solid	7		Category 2B		Category III	R36			Severe	Slight			Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8	100%, 10%, and ITC		Organic salt, Carboxylic acid salt	Unknown	3		Nonirritant		Category III	Nonirritant			Moderate	Severe			Spielmann et al. (1996)
1-Chloroctane-8-ol		100%, 10%, and ITC		Alcohol	Unknown	ns		Category 1	1	Category I	R41			Moderate	Severe			Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	100%, 10%, and ITC		Alcohol	Unknown	ns		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
DC 8		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Nonirritant	Moderate			Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9	100%, 10%, and ITC		Ether	Unknown	7		Category 2B		Category III	R36			Slight	Nonirritant			Spielmann et al. (1996)
Diepoxid 126	2386-87-0	100%, 10%, and ITC		Heterocycle, Ester, Ether	Liquid	ns		SCNM		SCNM	SCNM			Moderate	Severe			Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2	100%, 10%, and ITC		Alcohol	Solid	ns		Category 1	1	Category I	R36			Severe	Severe			Spielmann et al. (1996)
3,6-Dimethyloctanol		100%, 10%, and ITC		Alcohol	Unknown	7		Category 1	1	Category I	R41			Nonirritant	Slight			Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	100%, 10%, and ITC		Ketone, Nitrile	Solid	ns		Nonirritant		Category IV	Nonirritant			Moderate	Moderate			Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	100%, 10%, and ITC		Alcohol, Ether	Liquid	5		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Diphocars		100%, 10%, and ITC		Unknown	Unknown	ns		Category 1	4	Category I	R41			Severe	Severe			Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	100%, 10%, and ITC		Alcohol	Solid	ns		SCNM		SCNM	SCNM			Slight	Slight			Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2	100%, 10%, and ITC		Organic salt, Carboxylic acid salt, Amino acid	Unknown	11.5		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Ede 140		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Slight	Slight			Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4	100%, 10%, and ITC		Ether	Solid	4.5		Nonirritant		Category III	Nonirritant			Severe	Moderate			Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	100%, 10%, and ITC		Ether	Solid	ns		SCNM		SCNM	SCNM			Slight	Moderate			Spielmann et al. (1996)
Ethiosan		100%, 10%, and ITC		Unknown	Unknown	8.5		SCNM		Category III	SCNM			Slight	-			Spielmann et al. (1996)
Ethyl butanal	97-96-1	100%, 10%, and ITC		Aldehyde	Liquid	<7		SCNM		SCNM	SCNM			Nonirritant	Severe			Spielmann et al. (1996)
Genomoll	115-96-8	100%, 10%, and ITC		Ester, Organophophorous compound	Solid	6		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	100%, 10%, and ITC		Organic salt, Carboxylic acid salt, Amino acid	Unknown	0.9		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Glycediol		100%, 10%, and ITC		Ether	Unknown	ns		Nonirritant		Category IV	Nonirritant			Slight	Slight			Spielmann et al. (1996)
Granuform	30525-89-4	100%, 10%, and ITC		Ether	Solid	4		Category 1	4	SCNM	SCNM			Slight	Nonirritant			Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2	100%, 10%, and ITC		Ketone	Unknown	ns		Nonirritant		Category III	Nonirritant			Slight	Moderate			Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	100%, 10%, and ITC		Amine	Solid	8.5		Nonirritant		Category IV	Nonirritant			Moderate	Severe			Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4	100%, 10%, and ITC		Alcohol	Solid	4.5		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Hnol		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Nonirritant	Moderate			Spielmann et al. (1996)
Hoe MBF		100%, 10%, and ITC		Unknown	Unknown	4.3		Nonirritant		Category III	Nonirritant			Nonirritant	Nonirritant			Spielmann et al. (1996)
Hydo 98		100%, 10%, and ITC		Unknown	Unknown	6.5		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vivo* Concentration Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[2]	GHS Category 1 Subclass[3]	*In Vivo* (EPA) Classification[4]	*In Vivo* (EU) Classification[5]	*In Vitro* Classification (IS(A))[6]	*In Vitro* Classification (IS(B))[7]	*In Vitro* Classification (IS(B)-10)[8]	*In Vitro* Classification (IS(B)-100)[9]	*In Vitro* Classification (Q-Score)[10]	11*In Vitro* Classification (S-Score)[11]	Reference
2-Hydroxyethyliminodiso diumacetate	135-37-5	100%, 10%, and ITC		Amine, Alcohol, Organic salt	Unknown	10.6		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	100%, 10%, and ITC		Carboxylic acid	Solid	1		Category 1	4	SCNM	R41			Severe	Severe			Spielmann et al. (1996)
Hypo 20		100%, 10%, and ITC		Unknown	Unknown	6.5		Nonirritant		Category IV	Nonirritant			Moderate	Moderate			Spielmann et al. (1996)
Hypo 36		100%, 10%, and ITC		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Hypo 45		100%, 10%, and ITC		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant			Slight	Severe			Spielmann et al. (1996)
Hypo 54		100%, 10%, and ITC		Unknown	Unknown	6.5		SCNM		SCNM	SCNM			Slight	Slight			Spielmann et al. (1996)
Hyton		100%, 10%, and ITC		Unknown	Unknown	8.5		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Iminodiacetic acid	142-73-4	100%, 10%, and ITC		Amine, Carboxylic acid	Solid	2.3		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Isobornyl acetate	125-12-2	100%, 10%, and ITC		Ester	Solid	ns		Nonirritant		Category IV	Nonirritant			Slight	Moderate			Spielmann et al. (1996)
Isobutanal	78-84-2	100%, 10%, and ITC		Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant			Slight	Severe			Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	100%, 10%, and ITC		Aldehyde	Liquid	<7		Nonirritant		Category III	Nonirritant			Nonirritant	Severe			Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7	100%, 10%, and ITC		Carboxylic acid	Solid	1.75		Category 1	4	SCNM	R41			Severe	Severe			Spielmann et al. (1996)
Lactic acid	79-33-4	100%, 10%, and ITC		Carboxylic acid, Alcohol	Unknown	2		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
alpha-Lactid	4511-42-6	100%, 10%, and ITC		Heterocycle, Lactone	Solid	3		SCNM		Category III	SCNM			Severe	Slight			Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8	100%, 10%, and ITC		Amino acid	Solid	10		SCNM		Category III	SCNM			Severe	Severe			Spielmann et al. (1996)
Mecre		100%, 10%, and ITC		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant			Severe	-			Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	100%, 10%, and ITC		Heterocycle, Organic sulfur compound, Alcohol	Solid	4		SCNM		SCNM	SCNM			Severe	-			Spielmann et al. (1996)
m-Methoxybenzaldehyde	591-31-1	100%, 10%, and ITC		Aldehyde, Ether	Solid	ns		Nonirritant		Category IV	Nonirritant			Slight	Severe			Spielmann et al. (1996)
Methyl acetate	79-20-9	100%, 10%, and ITC		Ester	Liquid	7		Category 2B		Category III	R36			Slight	Severe			Spielmann et al. (1996)
Methylpentynol	77-75-8	100%, 10%, and ITC		Alcohol	Liquid	ns		Category 1	4	Category I	R41			Severe	Severe			Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	100%, 10%, and ITC		Amidine	Solid	11.5		Category 1	4	SCNM	SCNM			Severe	Slight			Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	100%, 10%, and ITC		Alcohol	Liquid	3		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Methyltriglycol	112-35-6	100%, 10%, and ITC		Alcohol, Ether	Liquid	7		Nonirritant		Category III	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Methyltriglycol	112-35-6	100%, 10%, and ITC		Alcohol, Ether	Liquid	7		Nonirritant		Category III	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Napt		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Slight	Severe			Spielmann et al. (1996)
Olak		100%, 10%, and ITC		Unknown	Unknown	8.3		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Ölesulf		100%, 10%, and ITC		Unknown	Unknown	8		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7	100%, 10%, and ITC		Phenol, Alcohol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Phenylthiourea	103-85-5	100%, 10%, and ITC		Organic sulfur compound, Urea	Solid	5.5		Nonirritant		Category IV	Nonirritant			Slight	Slight			Spielmann et al. (1996)
Phosphonat A		100%, 10%, and ITC		Unknown	Unknown	2.1		Nonirritant		Category III	Nonirritant			Moderate	Severe			Spielmann et al. (1996)
Piperazine	18833-13-1	100%, 10%, and ITC		Heterocycle	Solid	5		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
PO 2		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Slight	Nonirritant			Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7	100%, 10%, and ITC		Ether	Liquid	6		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	100%, 10%, and ITC		Ether	Unknown	7		Nonirritant		Category IV	Nonirritant			Slight	Severe			Spielmann et al. (1996)
Polyethylene glycol	25322-68-3	100%, 10%, and ITC		Alcohol, Ether	Unknown	ns		SCNM		SCNM	SCNM			Slight	Moderate			Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vivo* Concentration Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[2]	GHS Category 1 Subclass[3]	*In Vivo* (EPA) Classification[4]	*In Vivo* (EU) Classification[5]	*In Vitro* Classification (IS(A))[6]	*In Vitro* Classification (IS(B))[7]	*In Vitro* Classification (IS(B)-10)[8]	*In Vitro* Classification (IS(B)-100)[9]	*In Vitro* Classification (Q-Score)[10]	11*In Vitro* Classification (S-Score)[11]	Reference
Polysolvan	7397-62-8	100%, 10%, and ITC		Alcohol, Ester	Liquid	7		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Potassium cyanate	590-28-3	100%, 10%, and ITC		Inorganic salt	Solid	10		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1	100%, 10%, and ITC		Carboxylic acid	Solid	9.5		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	100%, 10%, and ITC		Carboxylic acid	Solid	8		SCNM		SCNM	SCNM			Moderate	Moderate			Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3	100%, 10%, and ITC		Amine, Carboxylic acid, Organic salt	Unknown	ns		SCNM		SCNM	SCNM			Severe	Moderate			Spielmann et al. (1996)
RK Blau		100%, 10%, and ITC		Unknown	Unknown	2.6		Nonirritant		Category IV	Nonirritant			Slight	-			Spielmann et al. (1996)
Rubinrot Y		100%, 10%, and ITC		Unknown	Unknown			SCNM		Category IV	SCNM			Slight	Moderate			Spielmann et al. (1996)
Sacyclo		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Slight	Slight			Spielmann et al. (1996)
Sept		100%, 10%, and ITC		Unknown	Unknown	3		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Silan 103	1067-25-0	100%, 10%, and ITC		Organosilicon compound	Liquid	ns		SCNM		SCNM	SCNM			Slight	Severe			Spielmann et al. (1996)
Silan 108	3069-40-7	100%, 10%, and ITC		Organosilicon compound	Liquid	ns		Nonirritant		Category III	Nonirritant			Moderate	Severe			Spielmann et al. (1996)
Silan 165	29055-11-6	100%, 10%, and ITC		Organosilicon compound	Unknown	ns		Nonirritant		Category IV	Nonirritant			Nonirritant	Moderate			Spielmann et al. (1996)
Silan 167	41453-78-5	100%, 10%, and ITC		Organosilicon compound, Organic sulfur compound	Unknown	ns		SCNM		SCNM	SCNM			Slight	Slight			Spielmann et al. (1996)
Silan 253	18784-74-2	100%, 10%, and ITC		Organosilicon compound	Unknown	<7		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	100%, 10%, and ITC		Inorganic acid, Inorganic salt	Solid	4.5		Nonirritant		Category III	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Sodium sulfite	7757-83-7	100%, 10%, and ITC		Inorganic salt	Solid	10		SCNM		Category III	SCNM			Severe	Severe			Spielmann et al. (1996)
Sodium cyanate	917-61-3	100%, 10%, and ITC		Inorganic salt	Solid	10		SCNM		Category III	SCNM			Severe	Severe			Spielmann et al. (1996)
Polyhexamethylene guanidine		100%, 10%, and ITC		Amidine	Unknown	7.1		Category 1	4	Category I	R41			Severe	Severe			Spielmann et al. (1996)
2-Pseudojonon		100%, 10%, and ITC		Unknown	Unknown	ns		Category 2B		Category III	Nonirritant			Moderate	Moderate			Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	100%, 10%, and ITC		Organic salt, Ester, Ether	Unknown	8		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	100%, 10%, and ITC		Organic salt, Carboxylic acid salt	Solid	4.5		Category 2B		Category III	R36			Moderate	Severe			Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4	100%, 10%, and ITC		Inorganic salt	Solid	4.6		SCNM		SCNM	SCNM			Severe	Severe			Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	100%, 10%, and ITC		Amine, Organic sulfur compound, Ether	Unknown	7		Category 1	4	SCNM	R41			Severe	Severe			Spielmann et al. (1996)
TA 01946 Alkylsilan		100%, 10%, and ITC		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9	100%, 10%, and ITC		Heterocycle, Organic salt, Carboxylic acid salt	Unknown	11		Nonirritant		Category IV	Nonirritant			Severe	Moderate			Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Concentration Tested	*In Vivo* Concentration Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[2]	GHS Category 1 Subclass[3]	*In Vivo* (EPA) Classification[4]	*In Vivo* (EU) Classification[5]	*In Vitro* Classification (IS(A))[6]	*In Vitro* Classification (IS(B))[7]	*In Vitro* Classification (IS(B)-10)[8]	*In Vitro* Classification (IS(B)-100)[9]	*In Vitro* Classification (Q-Score)[10]	*1In Vitro* Classification (S-Score)[11]	Reference
Tocla		100%, 10%, and ITC		Unknown	Unknown	6		Category 1	1	Category I	R41			Severe	Severe			Spielmann et al. (1996)
Triisooctylamine	25549-16-0	100%, 10%, and ITC		Amine	Solid	7		Nonirritant		Category IV	Nonirritant			Nonirritant	Severe			Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclopentene-1-acetaldehyde	4501-58-0	100%, 10%, and ITC		Aldehyde	Solid	2.3		SCNM		SCNM	SCNM			Slight	Severe			Spielmann et al. (1996)
Trioxane	110-88-3	100%, 10%, and ITC		Heterocycle, Ether	Solid	ns		Nonirritant		Category III	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Wessalith Slurry		100%, 10%, and ITC		Unknown	Unknown	11		Category 2A		Category II	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	100%, 10%, and ITC		Amine, Heterocycle, Alcohol	Solid	6		Nonirritant		Category IV	Nonirritant			Severe	Severe			Spielmann et al. (1996)
Sodium lauryl sulfate	151-21-3	1%	1%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Nonirritant		Category IV	Nonirritant		Severe					Vinardell and Macián (1994)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category III	Nonirritant		Slight					Vinardell and Macián (1994)

Abbreviations: CASRN = Chemical Abstract Service Registry Number, EPA = United States Environmental Protection Agency, EU = European Union, GHS = Globally Harmonized System, ITC = irritatation threshold concentration, n.a. = not applicable, SCNM = study criteria not met.

[2]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[3]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[4]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[5]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[6]IS(A) represents irritation scores that were calculated using the method described in Leupke (1985)

[7]IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990)

[8]IS(B)-10 represents irritation scores that were calculated using the method described in Luepke (1985) when substances were tested at a 10% concentration in Spielmann et al. (1996)

[9]IS(B)-100 represents irritation scores that were calculated using the method described in Luepke (1985) when substances were tested at a 100% concentration in Spielmann et al. (1996)

[10]Q-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

[11]S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)

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Appendix D2

Data Sorted by Substance for IS(A) Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A))[5]	Reference
Acetic acid	64-19-7	10%	10%	Carboxylic acid	Solution			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Butanol	71-36-3	10%	10%	Alcohol	Solution			Category 1	4	SCNM	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Cetyltrimethylammonium bromide	57-09-0	10%	10%	Organic salt, Onium	Solution			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Chlorhexidine gluconate Solution (20% Solution)	18472-51-0	10%	10%	Amidine, Ester	Solution			Category 2B		Category II	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Di(2-ethylhexyl) sodium sulfosuccinate	577-11-7	10%	10%	Organic salt, Sulfur containing compound, Ester	Solution			Category 1	4	Category I	R36	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Diisopropanolamine	110-97-4	10%	10%	Amine, Alcohol	Solution			Nonirritant		Category III	Nonirritant	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Domiphen bromide	538-71-6	10%	10%	Organic salt, Onium, Ether	Solution			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			SCNM		SCNM	SCNM	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Ethanol	64-17-5	10%	10%	Alcohol	Solution			Nonirritant		Category IV	Nonirritant	Slight	Hagino et al. (1999)/Submitted Y. Ohno Data/ Kojima et al. (1995)
Glycolic acid	79-14-1	10%	10%	Carboxylic acid, Alcohol	Solution			Category 2B		Category III	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	10%	10%	Carboxylic acid, Alcohol	Solution			SCNM		Category III	SCNM	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	100%	100%	Carboxylic acid, Alcohol	Liquid			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Monoethanolamine	141-43-5	10%	10%	Amine, Alcohol	Solution			Category 2B		Category III	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A))[5]	Reference
Oil/Water Emulsion-HZE		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Potassium laurate	10124-65-9	10%	10%	Organic salt, Carboxylic acid salt	Solution			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data/ Kojima et al. (1995)
Sodium lauryl sulfate	151-21-3	10%		Organic salt, Carboxylic acid salt	Unknown			Category 1/Category 2A	4	Category I/Category II	R41/Nonirritant	Moderate	Kojima et al. (1995)
Stearyltrimethylammonium chloride	15461-40-2	10%	10%	Organic salt, Onium	Solution			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data/ Kojima et al. (1995)
Surfactant Based Formulation 1-HZA		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A))[5]	Reference
Surfactant Based Formulation 3-HZC		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Undiluted	Formulation	Solution			Category 2B		Category III	Nonirritant	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Undiluted	Formulation	Solution			SCNM		Category I	SCNM	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Undiluted	Formulation	Solution			Category 2B		Category III	R36	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A))[5]	Reference
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid			Nonirritant		Category III	Nonirritant	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data
Triethanolamine	102-71-6	10%	10%	Amine, Alcohol	Solution			Nonirritant		Category IV	Nonirritant	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data/ Bagley et al. (1992)
Triton X-100	9002-93-1	1%	1%	Ether	Solution			Nonirritant		Category III	Nonirritant	Severe	Bagley et al. (1992)
Triton X-100	9002-93-1	10%		Ether	Unknown			Category 1	NC	Category II	SCNM	Moderate	Kojima et al. (1995)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirrita

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(A) represents irritation scores that were calculated using the method described in Leupke (1985); classification scheme used as described in Leupke (1985).

Appendix D3

Data Sorted by Substance for IS(A)-10 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A)-10)[5]	Reference
Surfactant Based Formulation 1-HZA		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Undiluted	Formulation	Solution			Category 2B		Category III	Nonirritant	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Undiluted	Formulation	Solution			SCNM		Category I	SCNM	Slight	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A)-10)[5]	Reference
Surfactant Based Formulation 16-HZQ		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Undiluted	Formulation	Solution			Category 2B		Category III	R36	Slight	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1996)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eve irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(A)-10 represents irritation scores that were calculated using the method described in Leupke (1985) where the *in vitro* evaluation was conducted with a 10% concentration of the test substance and the *in vivo* evaluation was conducted with a 100% concentration of the test susbtances; classification scheme used as described in Leupke (1985).

Appendix D4

Data Sorted by Substance for IS(A)-100 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A)-100)[5]	Reference
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			SCNM		SCNM	SCNM	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Lactic acid	50-21-5	100%	100%	Carboxylic acid, Alcohol	Liquid			Category 1	4	Category I	R41	Severe	Hagino et al. (1999)/Submitted Y. Ohno Data
Oil/Water Emulsion-HZA		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZC		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZE		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZF		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZH		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZJ		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZL		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZM		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZN		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZT		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(A)-100)[5]	Reference
Oil/Water Emulsion-HZU		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZV		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZY		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid			Nonirritant		Category III	Nonirritant	Moderate	Hagino et al. (1999)/Submitted Y. Ohno Data

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(A)-100 represents irritation scores that were calculated using the method described in Leupke (1985) where the *in vitro* evaluation was conducted with a 100% concentration of the test substance and the *in vivo* evaluation was conducted with a 100% concentration of the test susbtances; classification scheme used as described in Leupke (1985).

Appendix D5

Data Sorted by Substance for IS(B) Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B))[5]	Reference
Acetic acid	64-19-7	10%	n.a.	Carboxylic acid	Solution						R41	Severe	CEC (1991)
Acetic acid	64-19-7	100%	n.a.	Carboxylic acid	Liquid						R41	Severe	CEC (1991)
Acetone	67-64-1	100%	100%	Ketone	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Allyl alcohol	107-18-6	100%	100%	Alcohol	Liquid						R36	Severe	Gilleron et al. (1996)
2-Aminophemol	95-55-6	100%	100%	Amine, Phenol	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36	Severe	Gilleron et al. (1997)
Anthracene	120-12-7	100%	100%	Polycyclic compound	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM	Slight	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	n.a.	Onium	Unknown		Cationic Surfactant				R41	Severe	CEC (1991)
Benzalkonium chloride	8001-54-5	100%	5%	Onium	Solution		Cationic Surfactant	Category 1/Category 2A	2	Category I	R41/R36	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	10%	Onium	Solution		Cationic Surfactant	Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Benzalkonium chloride	8001-54-5	100%	1%	Onium	Solution		Cationic Surfactant	Category 1	1	Category I	R41	Severe	Gilleron et al. (1997)
Benzethonium chloride	121-54-0	100%	100%	Amine, Onium	Solid		Cationic Surfactant				R41	Severe	Gilleron et al. (1996)
Brij 35	9002-92-0	100%	n.a.	Alcohol	Solid		Nonionic Surfactant				Nonirritant	Slight	CEC (1991)
Butanol	71-36-3	10%	n.a.	Alcohol	Solution						R36	Severe	CEC (1991)
Butanol	71-36-3	100%	n.a.	Alcohol	Liquid						R36	Severe	CEC (1991)
2-Butoxyethyl acetate	112-07-2	10%	n.a.	Ester	Solution						Nonirritant	Slight	CEC (1991)
2-Butoxyethyl acetate	112-07-2	100%	n.a.	Ester	Liquid						Nonirritant	Slight	CEC (1991)
Butyl acetate	123-86-4	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B))[5]	Reference
Captan 90 concentrate	133-06-2	100%	100%	Imide, Organic sulfur compound	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
4-Carboxy-benzaldehyde	619-66-9	100%	100%	Carboxylic acid, Aldehyde	Solid			Category 2A		Category II	R36	Slight	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7	100%	0.10%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7	100%	10%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Category 1	4	SCNM	R41	Severe	Gilleron et al. (1997)
Cetylpyridinium bromide	140-72-7	100%	6%	Heterocyclic compounds, Onium	Solution		Cationic Surfactant	Category 1	2	Category I	R41	Severe	Gilleron et al. (1997)
Chlorhexidine	55-56-1	100%	100%	Amidine	Solid			Category 1	4	SCNM	SCNM	Severe	Gilleron et al. (1997)
Cyclohexanol	108-93-0	100%	100%	Alcohol	Liquid			Category 1	2	Category I	R41	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1	100%	100%	Ketone, Cyclic hydrocarbon	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Deoxycholic acid, sodium salt	302-95-4	100%	100%	Alcohol, Carboxylic acid, Organic salt	Solid		Nonionic Surfactant				R36	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2	100%	100%	Ketone	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid			Category 1	2	SCNM	R41	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Dibenzyl phosphate	1623-08-1	100%	100%	Ester	Solid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Dibutyltin chloride	683-18-1	100%	n.a.	Organic salt	Solid						R41	Severe	CEC (1991)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	100%	Acyl halide	Liquid			Category 2A		Category II	SCNM	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4	100%	100%	Amide, Organic sulfur compound	Solid						Nonirritant	Slight	Gilleron et al. (1996)

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Dimethyl biguanidine	657-24-9	100%	100%	Amidine	Solid						Nonirritant	Moderate	Gilleron et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	100%	100%	Carboxylic acid	Liquid			SCNM		Category I	SCNM	Severe	Gilleron et al. (1997)
2,5-Dimethyl-hexanediol	110-03-2	100%	100%	Alcohol	Solid			Category 1	1	Category I	R41	Severe	Gilleron et al. (1997)
Dimethyl sulfoxide	67-68-5	10%	n.a.	Organic sulfur compound	Solution						Nonirritant	Slight	CEC (1991)
Dimethyl sulfoxide	67-68-5	100%	n.a.	Organic sulfur compound	Liquid						Nonirritant	Severe	CEC (1991)
Dimethyl sulfoxide	67-68-5	100%	100%	Organic sulfur compound	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
EDTA dipotassium	25105-12-9	100%	100%	Amine, Carboxylic acid, Organic salt	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			Category 2A		Category III	Nonirritant	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
2-Ethoxyethanol	110-80-5	100%	100%	Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9	100%	100%	Carboxylic acid, Ketone	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
2-Ethyl-1-hexanol	104-76-7	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Ethyl-2-methyl-acetoacetate	609-14-3	100%	100%	Ketone, Ester	Liquid			Category 2B		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Fomesafen	72128-02-0	100%	100%	Imide, Ether, Nitro compound	Solid			Nonirritant		Category III	Nonirritant	Slight	Gilleron et al. (1997)
Furan	110-00-9	100%	100%	Heterocycle	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)
Gamma-butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)

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Gluconolactone	90-80-2	100%	100%	Carboxylic acid, Lactone, Carbohydrate	Solid						Nonirritant	Slight	Gilleron et al. (1996)
DL-Glutamic acid	19285-83-7	100%	100%	Amino acid	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Glycerol	56-81-5	10%	n.a.	Alcohol	Solution						Nonirritant	Slight	CEC (1991)
Glycerol	56-81-5	100%	n.a.	Alcohol	Liquid						Nonirritant	Severe	CEC (1991)
Glycerol	56-81-5	100%	100%	Alcohol	Liquid			Nonirritant		Category IV	Nonirritant	Severe	Gilleron et al. (1997)
3-Glycidopropyltrimethoxysilane	2530-83-8	100%	100%	Ether, Organosilicon compound	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0	100%	100%	Organic salt, Onium	Liquid		Cationic Surfactant				R36	Severe	Gilleron et al. (1996)
Hexane	110-54-3	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
n-Hexane	110-54-3	10%	n.a.	Acyclic hydrocarbon	Solution						Nonirritant	Severe	CEC (1991)
n-Hexane	110-54-3	100%	n.a.	Acyclic hydrocarbon	Liquid						Nonirritant	Slight	CEC (1991)
Hexanol	111-27-3	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)

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Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	No Data	Gettings et al. (1991)
Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)		Undiluted	Undiluted	Formulation	Solution			Category 2B		Category II	Nonirritant	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)		Undiluted	Undiluted	Formulation	Solution			Category 2A		Category II	SCNM	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)

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Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41/R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Iminodibenzyl	494-19-9	100%	100%	Heterocycle	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobutanol	78-83-1	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Isopropanol	67-63-0	100%	100%	Alcohol	Liquid			Category 2A		Category III	SCNM	Severe	Gilleron et al. (1997)
N-Lauroylsarcosine, sodium salt	7631-98-3	100%	100%	Aminde, Amine Salt	Solid		Anionic Surfactant				Nonirritant	Severe	Gilleron et al. (1996)
Laurylsulfo betaine	14933-08-5	100%	100%	Amine, Onium	Unknown		Zwitterionic Surfactant				R36	Moderate	Gilleron et al. (1996)
Magnesium carbonate	56378-72-4	100%	100%	Alcohol	Solid						Nonirritant	Slight	Gilleron et al. (1996)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM	Nonirritant	Gilleron et al. (1997)
Methanol	67-56-1	100%	100%	Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
2-Methoxyethanol	109-86-4	10%	n.a.	Alcohol	Solution						Nonirritant	Moderate	CEC (1991)
2-Methoxyethanol	109-86-4	100%	n.a.	Alcohol	Liquid						Nonirritant	Severe	CEC (1991)
2-Methoxyethanol	109-86-4	100%	100%	Alcohol, Ether	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Methyl acetate	79-20-9	100%	100%	Ester	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0	100%	100%	Ester, Nitrile	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Methylcyclopentane	96-37-7	100%	100%	Cyclic hydrocarbon	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3	100%	100%	Ketone	Liquid			Category 2A		Category III	R36	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
MYRJ 45		100%	100%	Unknown	Solid		Nonionic Surfactant				Nonirritant	Nonirritant	Gilleron et al. (1996)

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1-Naphthalene acetic acid	86-87-3	100%	100%	Carboxylic acid, Polycyclic compound	Solid			Category 1	NC	Category I	SCNM	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41	Severe	Gilleron et al. (1997)
1-Nitropropane	108-03-2	100%	100%	Acyclic hydrocarbon, Nitro compound	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Octanol	111-87-5	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Oil/Water Emulsion-HZA		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZC		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZE		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZF		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZH		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZJ		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZL		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZM		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZN		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR		Undiluted	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1994)

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Oil/Water Emulsion-HZT		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZV		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZY		Undiluted	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Parafluoraniline	371-40-4	100%	100%	Amine	Liquid			SCNM		SCNM	SCNM	Severe	Gilleron et al. (1997)
2,4-Pentadione	123-54-6	100%	100%	Ketone	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3	100%	100%	Heterocycle	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Polyethylene glycol 400	25322-68-3	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category IV	Nonirritant	Severe	Gilleron et al. (1997)
Polyoxyethylene 23 lauryl ether	9002-92-0	100%	100%	Alcohol	Solid		Nonionic Surfactant				Nonirritant	Slight	Gilleron et al. (1996)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM	Severe	Gilleron et al. (1997)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid			Category 1	1	Category I	R41	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Propyl-4-hydroxybenzoate	94-13-3	100%	100%	Carboxylic acid, Phenol	Solid						Nonirritant	Slight	Gilleron et al. (1996)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid			Category 1	4	Category I	R41/R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid			Category 1	3	Category I	R41/R36	Moderate	Gilleron et al. (1996); Gilleron et al. (1997)
Sodium dodecyl sulfate	151-21-3	10%	n.a.	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant				R36	Severe	CEC (1991)

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Sodium dodecyl sulfate	151-21-3	100%	n.a.	Organic salt, Carboxylic acid salt	Solid		Anionic Surfactant				R41	Severe	CEC (1991)
Sodium hydroxide	1310-73-2	100%	1%	Alkali	Solution			Category 2B		Category III	R36	Severe	Gilleron et al. (1997)
Sodium hydroxide	1310-73-2	100%	10%	Alkali	Solution			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	100%	3%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	100%	15%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Category 1	NC	Category I	SCNM	Severe	Gilleron et al. (1997)
Sodium lauryl sulfate	151-21-3	1%	1%	Organic salt, Carboxylic acid salt	Solution		Anionic Surfactant	Nonirritant		Category IV	Nonirritant	Severe	Vinardell and Macián (1994)
Sodium oxalate	62-76-0	100%	100%	Organic salt, Carboxylic acid salt	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7	100%	100%	Inorganic salt, Boron containing compound	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Surfactant Based Formulation 1-HZA		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Undiluted	Formulation	Solution			Category 2B		Category III	Nonirritant	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Undiluted	Formulation	Solution			SCNM		Category I	SCNM	Severe	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)

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Surfactant Based Formulation 7-HZG		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 11-HZK		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Undiluted	Formulation	Solution			Category 2B		Category III	R36	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B))[5]	Reference
Surfactant Based Formulation 21-HZV		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 25-HZZ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Tetraamino pyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid			Nonirritant		Category III	Nonirritant	Slight	Gilleron et al. (1996); Gilleron et al. (1997)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid						R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Toluene	108-88-3	100%	n.a.	Polycyclic compound	Liquid						Nonirritant	Severe	CEC (1991)
Toluene	108-88-3	100%	100%	Polycyclic compound	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Triacetin	102-76-1	10%	n.a.	Ester	Solution						Nonirritant	Slight	CEC (1991)
Triacetin	102-76-1	100%	n.a.	Ester	Liquid						Nonirritant	Slight	CEC (1991)
Tributyltin chloride	1461-22-9	10%	n.a.	Organometallic compound	Solution						R41	Severe	CEC (1991)
Tributyltin chloride	1461-22-9	100%	n.a.	Organometallic compound	Solid						R41	Moderate	CEC (1991)
Trichloroacetic acid	76-03-9	100%	30%	Carboxylic acid	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Trichloroacetic acid	76-03-9	100%	3%	Carboxylic acid	Liquid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6	100%	100%	Cyclic hydrocarbon	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6	10%	n.a.	Amine, Alcohol	Solution						Nonirritant	Slight	CEC (1991)
Triethanolamine	102-71-6	100%	n.a.	Amine, Alcohol	Liquid						Nonirritant	Severe	CEC (1991)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B))[5]	Reference
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Triton X-100	9002-93-1	Undiluted	5%	Ether	Liquid		Nonionic Surfactant	Categorry 2A/Category 2B		Category III	Nonirritant/R36	Severe	Gilleron et al. (1997)
Triton X-100	9002-93-1	Undiluted	10%	Ether	Liquid		Nonionic Surfactant	Category 1	4	Category II	SCNM	Severe	Gilleron et al. (1997)
Triton X-155	9010-44-0	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant				Nonirritant	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category III	Nonirritant	Severe	Vinardell and Macián (1994); Gilleron et al. (1997)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; n.a. = not applicable, SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(B) represents irritation scores that were calculated using the method described in Kalweit et al. (1987).

Appendix D6

Data Sorted by Substance for IS(B)-10 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
7-Acetoxyheptanal			100%, 10%, and ITC	Aldehyde, Ester	Unknown	n.s.		Category 1	1	Category I	R41	Slight	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5		100%, 10%, and ITC	Amide, Amino acid	Solid	2.2		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Ambuphylline	5634-34-4		100%, 10%, and ITC	Amine, Heterocycle, Alcohol	Solid	9		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzene sulfonic acid	6471-78-9		100%, 10%, and ITC	Amine, Ether, Organic sulfur compound	Unknown	1.5		Category 1	4	SCNM	SCNM	Moderate	Spielmann et al. (1996)
Ammonium persulfate	7727-54-0		100%, 10%, and ITC	Inorganic salt	Solid	1.5		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Anisole	100-66-3		100%, 10%, and ITC	Ether	Liquid	n.s.		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)
B 25			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
n-Butanal	123-72-8		100%, 10%, and ITC	Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
n-Butanol	71-36-3		100%, 10%, and ITC	Alcohol	Liquid	n.s.		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
Butyl carbamate	592-35-8		100%, 10%, and ITC	Ester	Solid	n.s.		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Caffeine sodium benzoate	8000-95-1		100%, 10%, and ITC	Heterocycle, Organic salt, Carboxylic acid salt	Solid	7		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5		100%, 10%, and ITC	Heteroycle, Phenol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Camphen	79-92-5		100%, 10%, and ITC	Cyclic hydrocarbon	Solid	7		Category 2B		Category III	R36	Severe	Spielmann et al. (1996)
Cerium-2-ethylhexanoate	24593-34-8		100%, 10%, and ITC	Organic salt, Carboxylic acid salt	Unknown	3		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
1-Chloroctane-8-ol			100%, 10%, and ITC	Alcohol	Unknown	n.s.		Category 1	1	Category I	R41	Moderate	Spielmann et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2		100%, 10%, and ITC	Alcohol	Unknown	n.s.		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
DC 8			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
1,4-Dibutoxy-benzene	104-36-9		100%, 10%, and ITC	Ether	Unknown	7		Category 2B		Category III	R36	Slight	Spielmann et al. (1996)
Diepoxid 126	2386-87-0		100%, 10%, and ITC	Heterocycle, Ester, Ether	Liquid	n.s.		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)
2,5-Dimethylhexanediol	110-03-2		100%, 10%, and ITC	Alcohol	Solid	n.s.		Category 1	1	Category I	R36	Severe	Spielmann et al. (1996)
3,6-Dimethyloctanol			100%, 10%, and ITC	Alcohol	Unknown	7		Category 1	1	Category I	R41	Nonirritant	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2		100%, 10%, and ITC	Ketone, Nitrile	Solid	n.s.		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2		100%, 10%, and ITC	Alcohol, Ether	Liquid	5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Diphocars			100%, 10%, and ITC	Unknown	Unknown	n.s.		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5		100%, 10%, and ITC	Alcohol	Solid	n.s.		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
DTPA Pentasodium salt	140-01-2		100%, 10%, and ITC	Organic salt, Carboxylic acid salt, Amino acid	Unknown	11.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Ede 140			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
1,2-Epoxycyclooctane	286-62-4		100%, 10%, and ITC	Ether	Solid	4.5		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
1,2-Epoxydodecane	2855-19-8		100%, 10%, and ITC	Ether	Solid	n.s.		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Ethiosan			100%, 10%, and ITC	Unknown	Unknown	8.5		SCNM		Category III	SCNM	Slight	Spielmann et al. (1996)
Ethyl butanal	97-96-1		100%, 10%, and ITC	Aldehyde	Liquid	<7		SCNM		SCNM	SCNM	Nonirritant	Spielmann et al. (1996)
Gadopentetic acid dimeglumine salt	86050-77-3		100%, 10%, and ITC	Amine, Carboxylic acid, Organic salt	Unknown	n.s.		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Genomoll	115-96-8		100%, 10%, and ITC	Ester, Organophophorous compound	Solid	6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
C12/C14-Glucoside			100%, 10%, and ITC	Alcohol, Ether	Unknown	9		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
L-Glutamic acid hydrochloride	138-15-8		100%, 10%, and ITC	Organic salt, Carboxylic acid salt, Amino acid	Unknown	0.9		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Glycediol			100%, 10%, and ITC	Ether	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Granuform	30525-89-4		100%, 10%, and ITC	Ether	Solid	4		Category 1	4	SCNM	SCNM	Slight	Spielmann et al. (1996)
Hexahydrofarnesylacetone	502-69-2		100%, 10%, and ITC	Ketone	Unknown	n.s.		Nonirritant		Category III	Nonirritant	Slight	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0		100%, 10%, and ITC	Amine	Solid	8.5		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
1,2,6-Hexanetriol	106-69-4		100%, 10%, and ITC	Alcohol	Solid	4.5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Hnol			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hoe MBF			100%, 10%, and ITC	Unknown	Unknown	4.3		Nonirritant		Category III	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hydo 98			100%, 10%, and ITC	Unknown	Unknown	6.5		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
2-Hydroxyethylimino disodiumacetate	135-37-5		100%, 10%, and ITC	Amine, Alcohol, Organic salt	Unknown	10.6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6		100%, 10%, and ITC	Carboxylic acid	Solid	1		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Hypo 20			100%, 10%, and ITC	Unknown	Unknown	6.5		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Hypo 36			100%, 10%, and ITC	Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Hypo 45			100%, 10%, and ITC	Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Hypo 54			100%, 10%, and ITC	Unknown	Unknown	6.5		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Hyton			100%, 10%, and ITC	Unknown	Unknown	8.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Iminodiacetic acid	142-73-4		100%, 10%, and ITC	Amine, Carboxylic acid	Solid	2.3		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Isobornyl acetate	125-12-2		100%, 10%, and ITC	Ester	Solid	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Isobutanal	78-84-2		100%, 10%, and ITC	Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant	Slight	Spielmann et al. (1996)
Isodecylglucoside			100%, 10%, and ITC	Alcohol, Ether	Unknown	9		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5		100%, 10%, and ITC	Aldehyde	Liquid	<7		Nonirritant		Category III	Nonirritant	Nonirritant	Spielmann et al. (1996)
alpha-Ketoglutaric acid	328-50-7		100%, 10%, and ITC	Carboxylic acid	Solid	1.75		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Lactic acid	79-33-4		100%, 10%, and ITC	Carboxylic acid, Alcohol	Unknown	2		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
alpha-Lactid	4511-42-6		100%, 10%, and ITC	Heterocycle, Lactone	Solid	3		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
L-Lysine Monohydrate	39665-12-8		100%, 10%, and ITC	Amino acid	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
Mecre			100%, 10%, and ITC	Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5		100%, 10%, and ITC	Heterocycle, Organic sulfur compound, Alcohol	Solid	4		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
m-Methoxybenz aldehyde	591-31-1		100%, 10%, and ITC	Aldehyde, Ether	Solid	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Methyl acetate	79-20-9		100%, 10%, and ITC	Ester	Liquid	7		Category 2B		Category III	R36	Slight	Spielmann et al. (1996)
Methylpentynol	77-75-8		100%, 10%, and ITC	Alcohol	Liquid	n.s.		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6		100%, 10%, and ITC	Amidine	Solid	11.5		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1		100%, 10%, and ITC	Alcohol	Liquid	3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6		100%, 10%, and ITC	Alcohol, Ether	Liquid	7		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Methyltriglycol	112-35-6		100%, 10%, and ITC	Alcohol, Ether	Liquid	7		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Napt			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Nitro-bis-octylamide			100%, 10%, and ITC	Alcohol, Ether	Unknown	n.s.		Nonirritant		Category III	Nonirritant	Slight	Spielmann et al. (1996)
Olak			100%, 10%, and ITC	Unknown	Unknown	8.3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
Ölesulf			100%, 10%, and ITC	Unknown	Unknown	8		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Phenylephrine hydrochloride	61-76-7		100%, 10%, and ITC	Phenol, Alcohol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Phenylthiourea	103-85-5		100%, 10%, and ITC	Organic sulfur compound, Urea	Solid	5.5		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Phosphonat A			100%, 10%, and ITC	Unknown	Unknown	2.1		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
Piperazine	18833-13-1		100%, 10%, and ITC	Heterocycle	Solid	5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
PO 2			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Polyethylene glycol butyl ether	9004-77-7		100%, 10%, and ITC	Ether	Liquid	6		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7		100%, 10%, and ITC	Ether	Unknown	7		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Polyethylene glycol	25322-68-3		100%, 10%, and ITC	Alcohol, Ether	Unknown	n.s.		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Polyhexamethylene guanidine			100%, 10%, and ITC	Amidine	Unknown	7.1		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
Polysolvan	7397-62-8		100%, 10%, and ITC	Alcohol, Ester	Liquid	7		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3		100%, 10%, and ITC	Inorganic salt	Solid	10		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate II	14459-95-1		100%, 10%, and ITC	Carboxylic acid	Solid	9.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2		100%, 10%, and ITC	Carboxylic acid	Solid	8		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
2-Pseudojonon			100%, 10%, and ITC	Unknown	Unknown	n.s.		Category 2B		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
RK Blau			100%, 10%, and ITC	Unknown	Unknown	2.6		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Rubinrot Y			100%, 10%, and ITC	Unknown	Unknown			SCNM		Category IV	SCNM	Slight	Spielmann et al. (1996)
Sacyclo			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Sept			100%, 10%, and ITC	Unknown	Unknown	3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Silan 103	1067-25-0		100%, 10%, and ITC	Organosilicon compound	Liquid	n.s.		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Silan 108	3069-40-7		100%, 10%, and ITC	Organosilicon compound	Liquid	n.s.		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
Silan 165	29055-11-6		100%, 10%, and ITC	Organosilicon compound	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
Silan 167	41453-78-5		100%, 10%, and ITC	Organosilicon compound, Organic sulfur compound	Unknown	n.s.		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Silan 253	18784-74-2		100%, 10%, and ITC	Organosilicon compound	Unknown	<7		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5		100%, 10%, and ITC	Inorganic acid, Inorganic salt	Solid	4.5		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7		100%, 10%, and ITC	Inorganic salt	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3		100%, 10%, and ITC	Inorganic salt	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5		100%, 10%, and ITC	Inorganic salt	Solid	11.4		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
Sodium hydrogen sulfate	7681-38-1		100%, 10%, and ITC	Inorganic salt	Solid	1.1		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1		100%, 10%, and ITC	Organic salt, Ester, Ether	Unknown	8		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3		100%, 10%, and ITC	Organic salt, Carboxylic acid salt	Solid	4.5		Category 2B		Category III	R36	Moderate	Spielmann et al. (1996)
Sodiumpyrosulfite	7681-57-4		100%, 10%, and ITC	Inorganic salt	Solid	4.6		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5		100%, 10%, and ITC	Amine, Organic sulfur compound, Ether	Unknown	7		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Surfactant Based Formulation 1-HZA		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 2-HZB		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 3-HZC		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 4-HZD		10%	Undiluted	Formulation	Solution			Category 2B		Category III	Nonirritant	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 5-HZE		10%	Undiluted	Formulation	Solution			SCNM		Category I	SCNM	Severe	Gettings et al. (1996)
Surfactant Based Formulation 6-HZF		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 7-HZG		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 8-HZH		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 9-HZI		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 10-HZJ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
Surfactant Based Formulation 11-HZK		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 12-HZL		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 13-HZM		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Slight	Gettings et al. (1996)
Surfactant Based Formulation 14-HZN		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 15-HZP		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 16-HZQ		10%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 17-HZR		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 18-HZS		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 19-HZT		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
Surfactant Based Formulation 20-HZU		10%	Undiluted	Formulation	Solution			Category 2B		Category III	R36	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 21-HZV		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 22-HZW		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Moderate	Gettings et al. (1996)
Surfactant Based Formulation 23-HZX		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)
Surfactant Based Formulation 24-HZY		10%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-10)[5]	Reference
Surfactant Based Formulation 25-HZZ		10%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1996)
TA 01946 Alkylsilan			100%, 10%, and ITC	Unknown	Unknown	n.s.		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Theophylline sodium acetate	8002-89-9		100%, 10%, and ITC	Heterocycle, Organic salt, Carboxylic acid salt	Unknown	11		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Tocla			100%, 10%, and ITC	Unknown	Unknown	6		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Triisooctylamine	25549-16-0		100%, 10%, and ITC	Amine	Solid	7		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclopentene-1-acetaldehyde	4501-58-0		100%, 10%, and ITC	Aldehyde	Solid	2.3		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Trioxane	110-88-3		100%, 10%, and ITC	Heterocycle, Ether	Solid	n.s.		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Wessalith Slurry			100%, 10%, and ITC	Unknown	Unknown	11		Category 2A		Category II	Nonirritant	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1		100%, 10%, and ITC	Amine, Heterocycle, Alcohol	Solid	6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; n.s. = not specified, SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(B)-10 represents irritation scores that were calculated using the method described in Kalweit et al. (1987) where the *in vitro* evaluation was conducted with a 10% concentration of the test substance and the *in vivo* evaluation was conducted with a 100% concentration of the test susbtances; classification scheme used as described in Leupke (1985).

Appendix D7

Data Sorted by Substance for IS(B)-100 Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Acetone	67-64-1	100%	100%	Ketone	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
7-Acetoxyheptanal		100%		Aldehyde, Ester	Unknown	ns		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
n-Acetyl-Methionine	1115-47-5	100%		Amide, Amino acid	Solid	2.2		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Allyl alcohol	107-18-6	100%	100%	Alcohol	Liquid						R36	Severe	Gilleron et al. (1996)
Ambuphylline	5634-34-4	100%		Amine, Heterocycle, Alcohol	Solid	9		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
4-Amino-5-methoxy-2-methylbenzenesulfonic acid	6471-78-9	100%		Amine, Ether, Organic sulfur compound	Unknown	1.5		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
2-Aminophemol	95-55-6	100%	100%	Amine, Phenol	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36	Severe	Gilleron et al. (1997)
Ammoniumpersulfate	7727-54-0	100%		Inorganic salt	Solid	1.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Anisole	100-66-3	100%		Ether	Liquid	ns		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Anthracene	120-12-7	100%	100%	Polycyclic compound	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM	Slight	Gilleron et al. (1997)
B 25		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
Benzethonium chloride	121-54-0	100%	100%	Amine, Onium	Solid		Cationic Surfactant				R41	Severe	Gilleron et al. (1996)
n-Butanal	123-72-8	100%		Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant	Severe	Spielmann et al. (1996)
n-Butanol	71-36-3	100%		Alcohol	Liquid	ns		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
Butyl acetate	123-86-4	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Butyl carbamate	592-35-8	100%		Ester	Solid	ns		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Caffeine sodium benzoate	8000-95-1	100%		Heterocycle, Organic salt, Carboxylic acid salt	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Caffeine sodium salicylate	8002-85-5	100%		Heteroycle, Phenol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Camphen	79-92-5	100%		Cyclic hydrocarbon	Solid	7		Category 2B		Category III	R36	Slight	Spielmann et al. (1996)
Captan 90 concentrate	133-06-2	100%	100%	Imide, Organic sulfur compound	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
4-Carboxybenzaldehyde	619-66-9	100%	100%	Carboxylic acid, Aldehyde	Solid			Category 2A		Category II	R36	Slight	Gilleron et al. (1997)
Cerium-2-ethylhexanoate	24593-34-8	100%		Organic salt, Carboxylic acid salt	Unknown	3		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Chlorhexidine	55-56-1	100%	100%	Amidine	Solid			Category 1	4	SCNM	SCNM	Severe	Gilleron et al. (1997)
1-Chloroctane-8-ol		100%		Alcohol	Unknown	ns		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Cyclohexanol	108-93-0	100%	100%	Alcohol	Liquid			Category 1	2	Category I	R41	Severe	Gilleron et al. (1997)
Cyclohexanone	108-94-1	100%	100%	Ketone, Cyclic hydrocarbon	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
3-Cyclohexene-1-methanol	1679-51-2	100%		Alcohol	Unknown	ns		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
DC 8		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Deoxycholic acid, sodium salt	302-95-4	100%	100%	Alcohol, Carboxylic acid, Organic salt	Solid		Nonionic Surfactant				R36	Severe	Gilleron et al. (1996)
Diacetone alcohol	123-42-2	100%	100%	Ketone	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Dibenzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid			Category 1	2	SCNM	R41	Severe	Gilleron et al. (1996); Gilleron et al. (1997)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Dibenzyl phosphate	1623-08-1	100%	100%	Ester	Solid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
1,4-Dibutoxy-benzene	104-36-9	100%		Ether	Unknown	7		Category 2B		Category III	R36	Nonirritant	Spielmann et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	100%	Acyl halide	Liquid			Category 2A		Category II	SCNM	Severe	Gilleron et al. (1997)
2,4-Dicholor-5-sulfamolyl-benzoic acid	2736-23-4	100%	100%	Amide, Organic sulfur compound	Solid						Nonirritant	Slight	Gilleron et al. (1996)
Diepoxid 126	2386-87-0	100%		Heterocycle, Ester, Ether	Liquid	ns		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Dimethyl biguanidine	657-24-9	100%	100%	Amidine	Solid						Nonirritant	Moderate	Gilleron et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	100%	100%	Carboxylic acid	Liquid			SCNM		Category I	SCNM	Severe	Gilleron et al. (1997)
2,5-Dimethylhexanediol	110-03-2	100%	100%	Alcohol	Solid	ns		Category 1	1	Category I	R41/R36	Severe	Spielmann et al. (1996); Gilleron et al. (1997)
3,6-Dimethyloctanol		100%		Alcohol	Unknown	7		Category 1	1	Category I	R41	Slight	Spielmann et al. (1996)
4,4-Dimethyl-3-oxo-pentanenitrile	59997-51-2	100%		Ketone, Nitrile	Solid	ns		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
1-(2,6-dimethylphenoxy)-2-propanone	53012-41-2	100%		Alcohol, Ether	Liquid	5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Dimethyl sulfoxide	67-68-5	100%	100%	Organic sulfur compound	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Diphocars		100%		Unknown	Unknown	ns		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
1,2-Dodecanediol	1119-87-5	100%		Alcohol	Solid	ns		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
DTPA Pentasodium salt	140-01-2	100%		Organic salt, Carboxylic acid salt, Amino acid	Unknown	11.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Ede 140		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
EDTA dipotassium	25105-12-9	100%	100%	Amine, Carboxylic acid, Organic salt	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
1,2-Epoxycyclooctane	286-62-4	100%		Ether	Solid	4.5		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
1,2-Epoxydodecane	2855-19-8	100%		Ether	Solid	ns		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			Category 2A		Category III	Nonirritant	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Ethiosan		100%		Unknown	Unknown	8.5		SCNM		Category III	SCNM	-	Spielmann et al. (1996)
2-Ethoxyethanol	110-80-5	100%	100%	Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Ethyl acetate	141-78-6	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Ethylacetoacetate	141-97-9	100%	100%	Carboxylic acid, Ketone	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Ethyl butanal	97-96-1	100%		Aldehyde	Liquid	<7		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
2-Ethyl-1-hexanol	104-76-7	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Ethyl-2-methylacetoacetate	609-14-3	100%	100%	Ketone, Ester	Liquid			Category 2B		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Ethyl trimethyl acetate	3938-95-2	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Fomesafen	72128-02-0	100%	100%	Imide, Ether, Nitro compound	Solid			Nonirritant		Category III	Nonirritant	Slight	Gilleron et al. (1997)
Furan	110-00-9	100%	100%	Heterocycle	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Gadopentetic acid dimeglumine salt	86050-77-3	100%		Amine, Carboxylic acid, Organic salt	Unknown	ns		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)
Gamma-butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Genomoll	115-96-8	100%		Ester, Organophophorous compound	Solid	6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Gluconolactone	90-80-2	100%	100%	Carboxylic acid, Lactone, Carbohydrate	Solid						Nonirritant	Slight	Gilleron et al. (1996)
C12/C14-Glucoside		100%		Alcohol, Ether	Unknown	9		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
DL-Glutamic acid	19285-83-7	100%	100%	Amino acid	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
L-Glutamic acid hydrochloride	138-15-8	100%		Organic salt, Carboxylic acid salt, Amino acid	Unknown	0.9		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Glycediol		100%		Ether	Unknown	ns		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Glycerol	56-81-5	100%	100%	Alcohol	Liquid			Nonirritant		Category IV	Nonirritant	Severe	Gilleron et al. (1997)
3-Glycidopropyltrimethoxysilane	2530-83-8	100%	100%	Ether, Organosilicon compound	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Granuform	30525-89-4	100%		Ether	Solid	4		Category 1	4	SCNM	SCNM	Nonirritant	Spielmann et al. (1996)
Hexadecyltrimethylammonium bromide	57-09-0	100%	100%	Organic salt, Onium	Liquid		Cationic Surfactant				R36	Severe	Gilleron et al. (1996)
Hexahydrofarnesylacetone	502-69-2	100%		Ketone	Unknown	ns		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
Hexamethylenetetramine	100-97-0	100%		Amine	Solid	8.5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)

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Hexane	110-54-3	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
1,2,6-Hexanetriol	106-69-4	100%		Alcohol	Solid	4.5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Hexanol	111-27-3	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Hnol		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Hoe MBF		100%		Unknown	Unknown	4.3		Nonirritant		Category III	Nonirritant	Nonirritant	Spielmann et al. (1996)
Hydo 98		100%		Unknown	Unknown	6.5		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Hydroalcoholic Formulation 1-5% Alcohol Containing Formulation (PROD-00187)		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1991)
Hydroalcoholic Formulation 2-10% Alcohol Containing Formulation (PROD-00183)		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 3-15% Alcohol Containing Formulation (PROD-00186)		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 4-20% Alcohol Containing Formulation (PROD-00185)		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1991)
Hydroalcoholic Formulation 5-33% Alcohol Containing Formulation (PROD-00184)		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	No Data	Gettings et al. (1991)

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Hydroalcoholic Formulation 6-40% Alcohol Containing Formulation (PROD-00189)		100%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 7-55% Alcohol Containing Formulation (PROD-00188)		100%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 8-65% Alcohol Containing Formulation (PROD-00180)		100%	Undiluted	Formulation	Solution			Category 2B		Category II	Nonirritant	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 9-83% Alcohol Containing Formulation (PROD-00181)		100%	Undiluted	Formulation	Solution			Category 2A		Category II	SCNM	Severe	Gettings et al. (1991)
Hydroalcoholic Formulation 10-90% Alcohol Containing Formulation (PROD-00182)		100%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1991)
2-Hydroxyethyliminodisodiumacetate	135-37-5	100%		Amine, Alcohol, Organic salt	Unknown	10.6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
2-Hydroxyisobutyric acid	594-61-6	100%		Carboxylic acid	Solid	1		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Hypo 20		100%		Unknown	Unknown	6.5		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Hypo 36		100%		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Hypo 45		100%		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)

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Hypo 54		100%		Unknown	Unknown	6.5		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)
Hyton		100%		Unknown	Unknown	8.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41/R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Iminodiacetic acid	142-73-4	100%		Amine, Carboxylic acid	Solid	2.3		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Iminodibenzyl	494-19-9	100%	100%	Heterocycle	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Isobornyl acetate	125-12-2	100%		Ester	Solid	ns		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Isobutanal	78-84-2	100%		Aldehyde	Liquid	<7		Category 2B		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Isobutanol	78-83-1	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Isodecylglucoside		100%		Alcohol, Ether	Unknown	9		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Isononylaldehyde	35127-50-5	100%		Aldehyde	Liquid	<7		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Isopropanol	67-63-0	100%	100%	Alcohol	Liquid			Category 2A		Category III	SCNM	Severe	Gilleron et al. (1997)
alpha-Ketoglutaric acid	328-50-7	100%		Carboxylic acid	Solid	1.75		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
Lactic acid	79-33-4	100%		Carboxylic acid, Alcohol	Unknown	2		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
alpha-Lactid	4511-42-6	100%		Heterocycle, Lactone	Solid	3		SCNM		Category III	SCNM	Slight	Spielmann et al. (1996)
N-Lauroylsarcosine, sodium salt	7631-98-3	100%	100%	Aminde, Amine Salt	Solid		Anionic Surfactant				Nonirritant	Severe	Gilleron et al. (1996)
Laurylsulfobetaine	14933-08-5	100%	100%	Amine, Onium	Unknown		Zwitterionic Surfactant				R36	Moderate	Gilleron et al. (1996)
L-Lysine Monohydrate	39665-12-8	100%		Amino acid	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)

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Magnesium carbonate	56378-72-4	100%	100%	Alcohol	Solid						Nonirritant	Slight	Gilleron et al. (1996)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM	Nonirritant	Gilleron et al. (1997)
Mecre		100%		Unknown	Unknown	7		Nonirritant		Category IV	Nonirritant	-	Spielmann et al. (1996)
3-Mercapto-1,2,4-triazole	3179-31-5	100%		Heterocycle, Organic sulfur compound, Alcohol	Solid	4		SCNM		SCNM	SCNM	-	Spielmann et al. (1996)
Methanol	67-56-1	100%	100%	Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
m-Methoxybenzaldehyde	591-31-1	100%		Aldehyde, Ether	Solid	ns		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
2-Methoxyethanol	109-86-4	100%	100%	Alcohol, Ether	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Methyl acetate	79-20-9	100%	100%	Ester	Liquid	7	Category 2A/Category 2B			Category III	R36	Severe	Spielmann et al. (1996); Gilleron et al. (1997)
Methyl cyanoacetate	105-34-0	100%	100%	Ester, Nitrile	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1997)
Methylcyclopentane	96-37-7	100%	100%	Cyclic hydrocarbon	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
Methyl ethyl ketone	78-93-3	100%	100%	Ketone	Liquid			Category 2A		Category III	R36	Severe	Gilleron et al. (1997)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Methylpentynol	77-75-8	100%		Alcohol	Liquid	ns		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
N-(2-methylphenyl)-Imidodi-carbonimidic diamide	93-69-6	100%		Amidine	Solid	11.5		Category 1	4	SCNM	SCNM	Slight	Spielmann et al. (1996)
2-Methyl-1-propanol	78-83-1	100%		Alcohol	Liquid	3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)

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Methyltriglycol	112-35-6	100%		Alcohol, Ether	Liquid	7		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
MYRJ 45		100%	100%	Unknown	Solid		Nonionic Surfactant				Nonirritant	Nonirritant	Gilleron et al. (1996)
1-Naphthalene acetic acid	86-87-3	100%	100%	Carboxylic acid, Polycyclic compound	Solid			Category 1	NC	Category I	SCNM	Moderate	Gilleron et al. (1997)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41	Severe	Gilleron et al. (1997)
Napt		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Nitro-bis-octylamide		100%		Alcohol, Ether	Unknown	ns		Nonirritant		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
1-Nitropropane	108-03-2	100%	100%	Acyclic hydrocarbon, Nitro compound	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Octanol	111-87-5	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Oil/Water Emulsion-HZA		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZC		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZE		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZF		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZH		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZI		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)

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Oil/Water Emulsion-HZJ		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZL		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZM		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZN		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZO		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZR		100%	Undiluted	Formulation	Solution			Category 1	1	Category I	R41	Severe	Gettings et al. (1994)
Oil/Water Emulsion-HZS		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZT		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZU		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Slight	Gettings et al. (1994)
Oil/Water Emulsion-HZV		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Gettings et al. (1994)
Oil/Water Emulsion-HZW		100%	Undiluted	Formulation	Solution			Nonirritant		Category III	Nonirritant	Moderate	Gettings et al. (1994)
Oil/Water Emulsion-HZY		100%	Undiluted	Formulation	Solution			Nonirritant		Category IV	Nonirritant	Severe	Gettings et al. (1994)
Olak		100%		Unknown	Unknown	8.3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Ölesulf		100%		Unknown	Unknown	8		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Parafluoraniline	371-40-4	100%	100%	Amine	Liquid			SCNM		SCNM	SCNM	Severe	Gilleron et al. (1997)

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2,4-Pentadione	123-54-6	100%	100%	Ketone	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)
Phenylephrine hydrochloride	61-76-7	100%		Phenol, Alcohol, Organic salt	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
1-Phenyl-3-pyrazolidine	92-43-3	100%	100%	Heterocycle	Solid						Nonirritant	Nonirritant	Gilleron et al. (1996)
Phenylthiourea	103-85-5	100%		Organic sulfur compound, Urea	Solid	5.5		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Phosphonat A		100%		Unknown	Unknown	2.1		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Piperazine	18833-13-1	100%		Heterocycle	Solid	5		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
PO 2		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Nonirritant	Spielmann et al. (1996)
Polyethylene glycol 400	25322-68-3	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996); Gilleron et al. (1997)
Polyethylene glycol butyl ether	9004-77-7	100%		Ether	Liquid	6		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Polyethylene glycol dimethyl ether	24991-55-7	100%		Ether	Unknown	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Polyhexamethylene guanidine		100%		Amidine	Unknown	7.1		Category 1	4	Category I	R41	Severe	Spielmann et al. (1996)
Polyoxyethylene 23 lauryl ether	9002-92-0	100%	100%	Alcohol	Solid		Nonionic Surfactant				Nonirritant	Slight	Gilleron et al. (1996)
Polysolvan	7397-62-8	100%		Alcohol, Ester	Liquid	7		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996); Gilleron et al. (1997)

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Potassium hexacyanoferrate II	14459-95-1	100%		Carboxylic acid	Solid	9.5		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Potassium hexacyanoferrate III	13756-66-2	100%		Carboxylic acid	Solid	8		SCNM		SCNM	SCNM	Moderate	Spielmann et al. (1996)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid						R41	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Propyl-4-hydroxybenzoate	94-13-3	100%	100%	Carboxylic acid, Phenol	Solid						Nonirritant	Slight	Gilleron et al. (1996)
2-Pseudojonon		100%		Unknown	Unknown	ns		Category 2B		Category III	Nonirritant	Moderate	Spielmann et al. (1996)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid			Category 1	4	Category I	R41/R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid			Category 1	3	Category I	R41/R36	Moderate	Gilleron et al. (1996); Gilleron et al. (1997)
RK Blau		100%		Unknown	Unknown	2.6		Nonirritant		Category IV	Nonirritant	-	Spielmann et al. (1996)
Rubinrot Y		100%		Unknown	Unknown			SCNM		Category IV	SCNM	Moderate	Spielmann et al. (1996)
Sacyclo		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Slight	Spielmann et al. (1996)
Sept		100%		Unknown	Unknown	3		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Silan 103	1067-25-0	100%		Organosilicon compound	Liquid	ns		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Silan 108	3069-40-7	100%		Organosilicon compound	Liquid	ns		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Silan 165	29055-11-6	100%		Organosilicon compound	Unknown	ns		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Silan 167	41453-78-5	100%		Organosilicon compound, Organic sulfur compound	Unknown	ns		SCNM		SCNM	SCNM	Slight	Spielmann et al. (1996)

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Silan 253	18784-74-2	100%		Organosilicon compound	Unknown	<7		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium bisulfite	7631-90-5	100%		Inorganic acid, Inorganic salt	Solid	4.5		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)
Sodium sulfite	7757-83-7	100%		Inorganic salt	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
Sodium cyanate	917-61-3	100%		Inorganic salt	Solid	10		SCNM		Category III	SCNM	Severe	Spielmann et al. (1996)
Sodium disilicate	13870-28-5	100%		Inorganic salt	Solid	11.4		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium hydrogen sulfate	7681-38-1	100%		Inorganic salt	Solid	1.1		Category 1	4	SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium lauryl ether sulfate	3088-31-1	100%		Organic salt, Ester, Ether	Unknown	8		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Sodium monochloroacetate	3926-62-3	100%		Organic salt, Carboxylic acid salt	Solid	4.5		Category 2B		Category III	R36	Severe	Spielmann et al. (1996)
Sodium oxalate	62-76-0	100%	100%	Organic salt, Carboxylic acid salt	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Sodium perborate	10486-00-7	100%	100%	Inorganic salt, Boron containing compound	Solid			Category 1	4	Category I	R41	Severe	Gilleron et al. (1997)
Sodiumpyrosulfite	7681-57-4	100%		Inorganic salt	Solid	4.6		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
4-((2-sulfatoethyl)sulfonyl)-aniline	2494-89-5	100%		Amine, Organic sulfur compound, Ether	Unknown	7		Category 1	4	SCNM	R41	Severe	Spielmann et al. (1996)
TA 01946 Alkylsilan		100%		Unknown	Unknown	ns		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
Tetraaminopyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid			Nonirritant		Category III	Nonirritant	Slight	Gilleron et al. (1996); Gilleron et al. (1997)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Theophylline sodium acetate	8002-89-9	100%		Heterocycle, Organic salt, Carboxylic acid salt	Unknown	11		Nonirritant		Category IV	Nonirritant	Moderate	Spielmann et al. (1996)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid						R36	Severe	Gilleron et al. (1996); Gilleron et al. (1997)
Tocla		100%		Unknown	Unknown	6		Category 1	1	Category I	R41	Severe	Spielmann et al. (1996)
Toluene	108-88-3	100%	100%	Polycyclic compound	Liquid			Nonirritant		Category III	Nonirritant	Severe	Gilleron et al. (1997)
1,2,3-Trichloropropane	96-18-4	100%	100%	Acyclic hydrocarbon	Liquid						Nonirritant	Moderate	Gilleron et al. (1996)
1,2,4-Trichloropropane	95-63-6	100%	100%	Cyclic hydrocarbon	Liquid						Nonirritant	Slight	Gilleron et al. (1996)
Triethanolamine	102-71-6	100%	100%	Amine, Alcohol	Liquid						Nonirritant	Severe	Gilleron et al. (1996)
Triisooctylamine	25549-16-0	100%		Amine	Solid	7		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)
2,2,3-Trimethyl-3-Cyclopentene-1-acetaldehyde	4501-58-0	100%		Aldehyde	Solid	2.3		SCNM		SCNM	SCNM	Severe	Spielmann et al. (1996)
Trioxane	110-88-3	100%		Heterocycle, Ether	Solid	ns		Nonirritant		Category III	Nonirritant	Severe	Spielmann et al. (1996)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (IS(B)-100)[5]	Reference
Triton X-155	9010-44-0	100%	100%	Alcohol, Ether	Liquid		Nonionic Surfactant				Nonirritant	Slight	Gilleron et al. (1996)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid		Nonionic Surfactant	Nonirritant		Category III	Nonirritant	Severe	Vinardell and Macián (1994); Gilleron et al. (1997)
Wessalith Slurry		100%		Unknown	Unknown	11		Category 2A		Category II	Nonirritant	Severe	Spielmann et al. (1996)
Xanthinol nicotinate	437-74-1	100%		Amine, Heterocycle, Alcohol	Solid	6		Nonirritant		Category IV	Nonirritant	Severe	Spielmann et al. (1996)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; n.s. = not specified, SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]IS(B)-100 represents irritation scores that were calculated using the method described in Kalweit et al. (1987) where the *in vitro* evaluation was conducted with a 100% concentration of the test substance and the *in vivo* evaluation was conducted with a 100% concentration of the test susbtances; classification scheme used as described in Leupke (1985).

Appendix D8

Data Sorted by Substance for Q-Score Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (Q-Score)[5]	Reference
Acetone	67-64-1	100%	100%	Ketone	Liquid			Category 2A		Category II	R36	Severe	Balls et al. (1995)
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36	Moderate	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM	Nonirritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1%	1%	Onium	Solution			Category 1/Category 2A	1	Category I	R36/R41	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	5%	5%	Onium	Solution			Category 1	2	Category I	R41	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	10%	10%	Onium	Solution			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Butyl acetate	123-86-4	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Moderate	Balls et al. (1995)
gamma-Butyrolactone	96-48-0	100%	100%	Heterocycle, Lactone	Liquid			Category 2A		Category II	R36	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	0.1%	0.1%	Heterocyclic compounds, Onium	Solution			Nonirritant		Category III	Nonirritant	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	6%	6%	Heterocyclic compounds, Onium	Solution			Category 1	2	SCNM	R41	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	10%	10%	Heterocyclic compounds, Onium	Solution			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Cyclohexanol	108-93-0	100%	100%	Alcohol	Liquid			Category 1	2	Category I	R41	Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	100%	100%	Acyl halide	Liquid			Category 2A		Category II	SCNM	Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	100%	100%	Carboxylic acid	Liquid			SCNM		Category I	SCNM	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	100%	Alcohol	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
Ethanol	64-17-5	100%	100%	Alcohol	Liquid			Category 2A		Category III	Nonirritant	Severe	Balls et al. (1995)
Ethyl acetate	141-78-6	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Severe	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Nonirritant	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	100%	100%	Ketone, Ester	Liquid			Category 2B		Category III	Nonirritant	Severe	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	100%	100%	Ester	Liquid			Nonirritant		Category III	Nonirritant	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	100%	100%	Alcohol	Liquid			Nonirritant		Category IV	Nonirritant	Nonirritant	Balls et al. (1995)
n-Hexanol	111-27-3	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Balls et al. (1995)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Isobutanol	78-83-1	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Severe	Balls et al. (1995)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (Q-Score)[5]	Reference
Isopropanol	67-63-0	100%	100%	Alcohol	Liquid			Category 2A		Category III	SCNM	Severe	Balls et al. (1995)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM	Nonirritant	Balls et al. (1995)
Methyl acetate	79-20-9	100%	100%	Ester	Liquid			Category 2A		Category II	R36	Severe	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	100%	100%	Ester, Nitrile	Liquid			Category 2A		Category II	R36	Moderate	Balls et al. (1995)
Methylcyclopentane	96-37-7	100%	100%	Cyclic hydrocarbon	Liquid			Nonirritant		Category III	Nonirritant	Nonirritant	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	100%	100%	Ketone	Liquid			Category 2A		Category III	R36	Severe	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	100%	100%	Ketone	Liquid			Nonirritant		Category III	Nonirritant	Moderate	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
n-Octanol	111-87-5	100%	100%	Alcohol	Liquid			Category 2A		Category II	R36	Moderate	Balls et al. (1995)
Parafluoraniline	371-40-4	100%	100%	Amine	Liquid			SCNM		SCNM	SCNM	Severe	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	100%	100%	Alcohol, Ether	Liquid			Nonirritant		Category IV	Nonirritant	Nonirritant	Balls et al. (1995)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
Pyridine	110-86-1	100%	100%	Heterocycle	Liquid			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	1%	1%	Alkali	Solution			Category 2B		Category III	R36	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	10%	10%	Alkali	Solution			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3%	3%	Organic salt, Carboxylic acid salt	Solution			Nonirritant		Category III	Nonirritant	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	15%	15%	Organic salt, Carboxylic acid salt	Solution			Category 1	NC	Category I	SCNM	Severe	Balls et al. (1995)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid							Nonirritant	Balls et al. (1995)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (Q-Score)[5]	Reference
Toluene	108-88-3	100%	100%	Polycyclic compound	Liquid			Nonirritant		Category III	Nonirritant	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	3%	3%	Carboxylic acid	Solution			Nonirritant		Category III	Nonirritant	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	30%	30%	Carboxylic acid	Solution			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	5%	5%	Ether	Solution			Categorry 2A/Category 2B		Category III	Nonirritant/R36	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	10%	10%	Ether	Solution			Category 1	4	Category II	SCNM	Severe	Balls et al. (1995)
Tween 20	9005-64-5	100%	100%	Ester, Ether	Liquid			Nonirritant		Category III	Nonirritant	Nonirritant	Balls et al. (1995)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]Q-Score represents irritation scores that were calculated using the method described in Balls et al. (1995).

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Appendix D9

Data Sorted by Substance for S-Score Analysis Method

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Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (S-Score)[5]	Reference
Ammonium nitrate	6484-52-2	100%	100%	Inorganic salt, Onium	Solid			Category 2B		Category III	R36	Severe	Balls et al. (1995)
L-Aspartic acid	70-47-3	100%	100%	Amino acid	Solid			SCNM		SCNM	SCNM	Nonirritant	Balls et al. (1995)
Benzoyl-L-tartaric acid	2743-38-6	100%	100%	Carboxylic acid, Ester	Solid			Category 1	2	SCNM	R41	Nonirritant	Balls et al. (1995)
Captan 90 concentrate	133-06-2	100%	100%	Imide, Organic sulfur compound	Solid			Category 1	4	Category I	R41	Nonirritant	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	100%	100%	Carboxylic acid, Aldehyde	Solid			Category 2A		Category II	R36	Moderate	Balls et al. (1995)
Chlorhexidine	55-56-1	100%	100%	Amidine	Solid			Category 1	4	SCNM	SCNM	Moderate	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	100%	100%	Ester	Solid			Category 2A		Category II	R36	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	100%	100%	Alcohol	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
Fomesafen	72128-02-0	100%	100%	Imide, Ether, Nitro compound	Solid			Nonirritant		Category III	Nonirritant	Moderate	Balls et al. (1995)
Imidazole	288-32-4	100%	100%	Heterocycle	Solid			Category 1	4	Category I	R41	Severe	Balls et al. (1995)
Maneb	12427-38-2	100%	100%	Amine, Organic salt, Urea	Solid			SCNM		Category III	SCNM	Nonirritant	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	100%	100%	Carboxylic acid, Polycyclic compound	Solid			Category 1	NC	Category I	SCNM	Moderate	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	100%	100%	Organic salt, Carboxylic acid salt, Polycyclic compound	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
Potassium cyanate	590-28-3	100%	100%	Inorganic salt	Solid			SCNM		SCNM	SCNM	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	100%	100%	Amine, Heterocycle, Organic sulfur compound	Solid			Category 1	1	Category I	R41	Severe	Balls et al. (1995)
Quinacrine	69-05-6	100%	100%	Amine, Heterocycle, Polycyclic compound	Solid			Category 1	3	Category I	R41	Nonirritant	Balls et al. (1995)
Sodium oxalate	62-76-0	100%	100%	Organic salt, Carboxylic acid salt	Solid			Category 1	4	Category I	R41	Moderate	Balls et al. (1995)

Substance Name	CASRN	*In Vitro* Conc. Tested	*In Vivo* Conc. Tested	Chemical Class	*In Vivo* Physical Form Tested	pH	Property of Interest	*In Vivo* (GHS) Classification[1]	GHS Category 1 Subclass[2]	*In Vivo* (EPA) Classification[3]	*In Vivo* (EU) Classification[4]	*In Vitro* Classification (S-Score)[5]	Reference
Sodium perborate	10486-00-7	100%	100%	Inorganic salt, Boron containing compound	Solid			Category 1	4	Category I	R41	Nonirritant	Balls et al. (1995)
Tetraamino-pyrimidine sulfate	5392-28-9	100%	100%	Amine, Heterocycle	Solid			Nonirritant		Category III	Nonirritant	Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	100%	100%	Organic sulfur compound	Solid							Severe	Balls et al. (1995)

Abbreviations: CASRN = Chemical Abstracts Service Registry Number; Conc. = Concentration; EPA = U.S. Environmental Protection Agency; EU = European Union; GHS = Globally Harmonized System; SCNM - Study Criteria Not Met.

[1]Eye Irritant Category 1 = irreversible effects on the eye/serious damage to the eye; Category 2A = reversible effects on the eye/irritating to the eyes; Category 2B = reversible effects on the eye/mildly irritating to the eyes; Nonirritant = not an eye irritant

[2]NICEATM-defined subgroups assigned based on the lesions that drove classification of a GHS Category 1 substance. 1: based on lesions that are persistent; 2: based on lesions that are severe (not including corneal opacity score equal to 4); 3: based on lesions that are severe (not including corneal opacity score equal to 4) and persistent; 4: corneal opacity score equal to 4 at any time; NC: No subclassification could be made based on the data.

[3]Toxicity Category I for the Primary Eye Irritation Study = Corrosive, or corneal involvement or irritation not reversible within 21 days; Category II = Corneal involvement or irritation clearing in 8-21 days; Category III = Corneal involvement or irritation clearing in 7 days or less; Category IV = Minimal effects clearing within 24 hr.

[4]Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.

[5]S-Score represents irritation scores that were calculated using the method described in Balls et al. (1995).

Appendix E

Intralaboratory Repeatability and Intralaboratory Reproducibility Data and Results for Gilleron et al. (1996, 1997)

E1 Individual Egg HET-CAM Scores (Endpoints Evaluated and Overall Irritancy) for Data of Gilleron et al. (1996) E-3

E2 Individual Egg HET-CAM Scores (Endpoints Evaluated and Overall Irritancy) for Data of Gilleron et al. (1997) E-11

E3 Intralaboratory Repeatability Results (Expressed as %CV) for Data of Gilleron et al. (1996) E-21

E4 Intralaboratory Repeatability Results (Expressed as %CV) for Data of Gilleron et al. (1997) E-29

E5 Intralaboratory Reproducibility Results (Expressed as %CV) for Data of Gilleron et al. (1996) E-37

E6 Intralaboratory Reproducibility Results (Expressed as %CV) for Data of Gilleron et al. (1997) E-41

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Appendix E1

Individual Egg HET-CAM Scores (Endpoints Evaluated and Overall Irritancy) for Data of Gilleron et al. (1996)

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Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
2-Ethoxyethanol	86	0.00	2.55	0.00	0.00	1.26	0.00	8.76	8.22	8.88	8.76	12.03	8.88
	95	1.00	4.47	0.00	0.00	0.00	0.00	6.21	6.00	6.45	7.21	10.47	6.45
	99	0.00	0.00	0.00	5.30	5.76	5.83	8.25	7.47	7.71	13.55	13.23	13.54
Quinacrine	90	4.62	4.62	4.68	0.00	0.00	0.00	0.00	0.00	3.15	4.62	4.62	7.83
	93	4.85	4.85	4.77	0.00	0.00	0.00	0.00	0.00	0.00	4.85	4.85	4.77
	103	0.00	0.20	0.00	5.06	3.45	2.64	7.02	4.83	3.72	12.08	8.48	6.36
Anthracene	91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	95	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hexadecyltrimethyammonium bromide	90	4.70	4.37	4.70	5.37	4.29	2.99	7.53	7.20	8.01	17.60	15.86	15.70
	97	0.00	4.33	4.10	5.53	3.57	5.46	0.00	0.00	0.00	5.53	7.90	9.56
	103	0.00	0.00	0.00	6.44	6.11	6.42	3.81	2.64	0.00	10.25	8.75	6.42
Allyl Alcohol	86	0.00	0.00	0.00	5.79	5.95	0.00	8.73	8.88	8.85	14.52	14.83	8.85
	95	1.85	0.00	0.00	4.13	0.00	0.00	8.10	7.83	8.16	14.08	7.83	8.16
	99	0.00	0.00	0.00	6.28	6.53	5.93	8.31	8.34	8.16	14.59	14.87	14.09
Thiourea	90	3.88	3.97	3.80	6.84	6.88	6.74	8.04	6.99	7.41	18.76	17.84	17.95
	103	3.80	3.78	3.90	6.63	6.63	6.58	0.00	0.00	0.00	10.43	10.41	10.48
	107	4.15	3.90	4.02	6.72	6.74	6.63	0.00	0.00	0.00	10.87	10.64	10.65
EDTA dipotassium	91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	94	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dimethyl biguanidine	92	0.00	0.00	0.00	0.00	0.00	0.00	8.25	8.49	7.47	8.25	8.49	7.47
	93	0.00	0.00	0.00	4.60	5.55	1.91	8.37	4.77	7.14	12.97	10.32	9.05
	103	0.00	0.00	0.00	6.35	6.58	6.44	0.00	0.00	0.00	6.35	6.58	6.44
Hexane	86	0.57	1.05	2.10	0.00	0.00	0.00	4.77	4.41	4.68	5.34	5.46	6.78
	93	0.00	0.00	0.00	0.00	0.00	0.00	1.71	0.00	0.00	1.71	0.00	0.00
	105	0.00	0.00	0.00	4.67	3.80	0.00	0.00	0.00	0.00	4.67	3.80	0.00

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Triton X-155	92	0.00	0.00	0.75	0.00	0.00	0.00	0.30	2.79	0.00	0.30	2.79	0.75
	98	1.40	2.97	3.95	0.00	4.27	4.67	0.00	0.00	0.00	1.40	7.24	8.62
	104	0.00	0.00	0.00	4.74	4.90	4.57	0.00	0.00	0.00	4.74	4.90	4.57
2,4-Pentanedione	86	4.52	4.67	4.03	0.00	0.00	0.00	3.72	7.59	6.27	8.24	12.26	10.30
	87	4.50	4.47	4.15	0.00	0.00	0.00	6.39	7.29	5.49	10.89	11.76	9.64
	93	4.12	4.43	3.97	0.00	0.00	0.00	3.60	0.00	0.00	7.72	4.43	3.97
1,2,3-Tricholorpropane	89	0.00	1.48	0.10	0.00	0.00	0.00	7.08	6.72	2.70	7.08	8.20	2.80
	98	3.10	3.82	4.17	0.00	0.56	1.87	5.67	4.56	4.74	8.77	8.94	10.78
	104	3.12	2.80	3.88	4.13	4.11	3.29	1.05	1.17	0.51	8.30	8.08	7.68
1-Nitropropane	86	0.00	0.00	1.27	0.00	0.00	0.00	3.54	0.00	4.38	3.54	0.00	5.65
	87	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	95	1.53	0.35	2.07	4.64	0.00	0.00	0.00	4.80	2.73	6.17	5.15	4.80
Cyclohexanone	89	3.90	4.73	4.38	0.00	0.00	0.00	8.40	7.74	7.62	12.30	12.47	12.00
	98	4.88	4.95	4.10	6.42	6.65	6.77	8.04	7.92	6.81	19.34	19.52	17.68
	104	4.83	4.62	4.45	6.46	6.77	3.15	4.14	1.77	0.69	15.43	13.16	8.29
3-Glycidopropyltrimethoxysilane	99	4.02	3.10	3.77	0.00	0.00	0.00	0.00	0.00	0.00	4.02	3.10	3.77
	100	3.45	3.75	3.68	0.00	0.00	0.00	2.37	2.13	0.87	5.82	5.88	4.55
	105	4.02	3.80	3.87	0.00	0.00	0.00	0.00	0.00	0.00	4.02	3.80	3.87
Diacetone alcohol	89	3.60	4.85	2.92	0.00	0.00	0.00	8.91	7.05	8.43	12.51	11.90	11.35
	98	4.87	4.90	4.93	5.37	5.90	5.44	5.58	6.75	7.26	15.82	17.55	17.63
	104	4.87	4.78	4.87	6.28	5.95	6.07	6.90	5.58	3.36	18.05	16.31	14.30
1,2,4-Trimethylbenzene	88	1.00	0.10	0.00	0.00	0.00	0.00	6.27	4.56	1.44	7.27	4.66	1.44
	95	1.85	0.00	0.00	0.00	0.00	0.00	2.64	0.00	0.00	4.49	0.00	0.00
	100	0.00	0.00	0.00	5.48	3.69	5.53	3.39	3.24	0.63	8.87	6.93	6.16
Pyridine	89	0.00	4.87	4.05	0.00	0.00	0.00	8.94	8.58	8.52	8.94	13.45	12.57
	98	4.30	4.77	4.87	6.93	6.86	6.88	7.53	7.65	2.04	18.76	19.28	13.79
	104	4.72	4.95	3.35	6.42	6.88	6.93	7.59	6.72	7.62	18.73	18.55	17.90
DL-Glutamic acid	91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	95	2.77	3.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.77	3.33	0.00
	100	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Iminodibenzyl	92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	96	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.27	0.00	0.00	0.27	0.00
	102	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Butyrolactone	88	4.98	4.97	4.98	0.00	0.00	0.00	8.25	8.07	7.35	13.23	13.04	12.33
	95	4.95	4.98	4.90	0.00	0.00	0.00	7.65	7.77	8.10	12.60	12.75	13.00
	100	4.90	4.33	4.93	4.76	3.97	4.92	7.44	6.69	5.88	17.10	14.99	15.73
Octanol	88	3.23	2.80	0.00	0.00	0.00	4.53	2.73	4.65	6.03	5.96	7.45	10.56
	102	4.00	3.67	3.00	3.76	3.97	3.78	2.76	3.09	2.85	10.52	10.73	9.63
	106	3.27	3.30	3.55	5.86	5.20	6.14	0.60	3.60	2.22	9.73	12.10	11.91
24-dicholor-5-sulfamolyl-benzoic acid	91	0.00	4.82	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.82	0.00
	93	4.85	4.82	4.78	0.00	0.00	0.00	2.25	0.00	1.38	7.10	4.82	6.16
	100	4.17	2.53	4.32	0.00	0.00	0.00	0.00	0.00	0.00	4.17	2.53	4.32
Methyl isobutyl ketone	88	0.00	2.75	3.52	0.00	0.00	0.00	6.96	6.81	7.71	6.96	9.56	11.23
	96	2.90	4.25	4.23	1.87	2.59	2.71	7.56	4.08	6.30	12.33	10.92	13.24
	105	3.85	3.55	2.98	6.74	6.39	6.67	0.00	0.00	0.00	10.59	9.94	9.65
furan	88	0.00	0.00	0.00	0.00	1.28	0.00	5.97	0.60	5.67	5.97	1.88	5.67
	95	0.00	2.77	0.00	2.22	0.00	2.99	1.59	6.33	3.72	3.81	9.10	6.71
	100	0.00	0.00	0.00	5.58	4.64	4.95	0.27	1.05	0.00	5.85	5.69	4.95
Dibenzoyl-L-tartaric acid	90	4.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.15	0.00	0.00
	93	4.85	4.85	4.80	0.00	0.00	0.00	0.00	0.00	0.00	4.85	4.85	4.80
	102	4.83	4.70	4.62	3.43	0.00	1.33	0.00	0.00	0.00	8.26	4.70	5.95
1-phenyl-3-pyrazolidone	91	0.00	0.00	0.00	0.00	0.00	0.00	1.80	0.00	0.00	1.80	0.00	0.00
	96	0.00	0.00	0.00	0.00	0.00	0.00	0.39	1.98	0.00	0.39	1.98	0.00
	101	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethanol	89	0.00	0.00	0.00	0.00	0.00	0.00	8.19	8.49	8.61	8.19	8.49	8.61
	97	0.00	0.00	0.00	5.88	5.74	5.74	6.03	5.34	5.67	11.91	11.08	11.41
	102	0.00	0.00	0.00	6.44	6.60	5.76	7.47	7.92	8.01	13.91	14.52	13.77
2-Aminophenol	91	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.43	1.83	0.00	2.43	1.83
	96	0.00	0.00	0.00	0.00	0.00	0.00	0.21	3.06	0.00	0.21	3.06	0.00
	101	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Deooxycholic acid, sodium salt	89	3.93	1.95	0.00	6.56	5.69	6.02	8.73	8.16	8.13	19.22	15.80	14.15
	97	2.63	0.00	1.18	4.95	6.09	5.62	0.00	0.00	0.00	7.58	6.09	6.80
	102	0.00	0.00	0.00	5.93	5.34	6.39	0.00	0.00	0.00	5.93	5.34	6.39
Gluconolactone	91	0.00	0.00	0.00	0.00	0.00	0.00	7.71	8.13	8.67	7.71	8.13	8.67
	93	0.00	0.00	0.00	0.00	0.00	6.25	0.00	0.00	0.00	0.00	0.00	6.25
	101	0.00	0.00	0.00	5.27	1.14	3.80	0.00	0.00	0.00	5.27	1.14	3.80
MYRJ 45	92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	102	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dimethylsulfoxide	88	0.00	0.00	0.00	6.14	6.35	6.65	8.73	8.31	8.43	14.87	14.66	15.08
	93	0.00	1.18	0.00	0.00	0.00	0.00	7.29	7.11	6.60	7.29	8.29	6.60
	101	0.00	0.00	0.00	6.44	6.28	5.72	4.65	5.67	5.76	11.09	11.95	11.48
Polyoxythethylene 23 lauryl ether	92	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	97	4.43	4.57	4.55	0.00	0.00	0.00	0.00	0.00	0.00	4.43	4.57	4.55
	103	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Magnesium carobonate	92	0.00	0.00	0.00	0.00	0.00	0.00	4.50	4.08	2.01	4.50	4.08	2.01
	101	0.00	0.00	0.00	0.00	0.00	0.00	2.28	0.00	0.00	2.28	0.00	0.00
	106	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Tetraaminopyrimidine sulfate	92	4.77	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.77	0.00	0.00
	93	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	103	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propyl-4-hydroxybenzoate	92	0.00	0.00	3.33	0.00	0.00	0.00	0.00	0.00	1.14	0.00	0.00	4.47
	96	2.25	2.82	3.40	0.00	0.00	0.00	0.00	0.75	0.00	2.25	3.57	3.40
	101	0.28	0.93	2.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28	0.93	2.00
Imidazole	96	4.53	4.03	4.67	4.85	3.31	4.78	8.91	8.91	8.91	18.29	16.25	18.36
	100	4.83	4.80	4.85	5.51	6.56	6.60	4.35	5.82	6.24	14.69	17.18	17.69
	105	4.92	4.92	4.87	6.91	6.91	6.86	6.72	7.38	7.77	18.55	19.21	19.50
	118	4.43	4.77	4.85	6.91	6.79	6.86	6.90	7.26	6.93	18.24	18.82	18.64
	115	4.87	4.90	4.92	6.28	6.67	6.74	8.82	8.46	8.16	19.97	20.03	19.82
	116	4.75	4.82	4.82	6.49	6.79	6.84	7.83	7.47	7.80	19.07	19.08	19.46

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
2-Methoxyethanol	88	0.00	0.00	0.00	4.62	6.60	6.60	8.64	8.31	8.22	13.26	14.91	14.82
	89	0.00	0.00	0.00	3.94	4.95	6.37	8.64	8.10	8.61	12.58	13.05	14.98
	96	0.00	0.00	0.00	5.67	5.04	5.46	7.95	8.01	7.92	13.62	13.05	13.38
	101	0.00	0.00	0.00	5.69	6.25	6.11	6.63	5.55	4.80	12.32	11.80	10.91
Methanol	89	0.00	0.00	0.00	6.32	4.76	0.00	8.70	8.49	8.52	15.02	13.25	8.52
	93	0.00	0.00	0.00	0.00	0.00	0.00	8.01	8.07	7.83	8.01	8.07	7.83
	102	0.00	0.00	0.00	6.70	6.79	6.88	8.34	8.28	8.52	15.04	15.07	15.40
	105	0.00	0.00	0.00	6.79	6.84	6.88	7.38	5.85	4.20	14.17	12.69	11.08
Promethazine hydrochloride	85	0.00	0.00	0.00	6.60	6.65	6.81	7.56	8.67	8.88	14.16	15.32	15.69
	90	2.35	3.43	1.97	0.00	0.00	0.00	8.43	8.61	8.67	10.78	12.04	10.64
	102	0.00	0.00	0.00	6.79	6.67	6.67	8.49	8.52	8.52	15.28	15.19	15.19
	97	0.00	0.00	0.00	6.88	6.70	6.53	8.34	8.19	8.34	15.22	14.89	14.87
N-Lauroylsarcosine, sodium salt	92	0.00	3.50	4.53	6.42	6.58	5.69	8.76	8.73	8.64	15.18	18.81	18.86
	94	0.00	4.50	4.22	6.07	6.49	6.46	2.49	0.90	0.00	8.56	11.89	10.68
	106	0.00	0.00	0.00	6.93	6.88	6.91	3.96	3.90	4.32	10.89	10.78	11.23
	103	0.00	0.00	4.38	6.65	6.63	6.60	0.72	0.00	0.00	7.37	6.63	10.98
Benzethonium chloride	90	4.88	4.72	4.52	0.00	0.00	0.00	8.25	7.47	7.41	13.13	12.19	11.93
	98	4.10	4.23	4.85	5.88	5.30	6.35	8.49	7.47	7.41	18.47	17.00	18.61
	104	0.00	0.00	0.00	6.49	6.60	6.51	0.72	0.06	0.33	7.21	6.66	6.84
	107	0.00	0.00	0.00	6.74	6.81	6.74	6.33	6.12	5.79	13.07	12.93	12.53
Laurylsulfobetaine	92	0.00	0.00	0.00	6.09	6.02	6.32	2.07	2.97	3.72	8.16	8.99	10.04
	94	0.67	0.00	0.00	4.06	6.56	6.51	0.18	5.13	5.94	4.91	11.69	12.45
	104	0.00	0.00	0.00	6.84	6.81	6.84	0.00	0.00	0.00	6.84	6.81	6.84
Triethanolamine	89	0.00	0.00	0.00	3.80	3.03	2.85	8.37	7.62	6.78	12.17	10.65	9.63
	104	0.00	0.00	0.00	6.88	6.70	6.53	6.30	4.71	6.15	13.18	11.41	12.68
	107	0.00	0.00	0.00	6.46	5.97	6.65	5.76	7.47	7.02	12.22	13.44	13.67
Ethylacetoacetate	89	3.93	3.83	4.15	0.00	0.00	0.00	2.88	3.66	4.02	6.81	7.49	8.17
	97	3.53	3.48	2.48	0.68	0.00	3.66	0.00	0.00	0.00	4.21	3.48	6.14
	102	3.58	3.93	4.47	4.25	4.83	4.64	5.76	4.44	4.92	13.59	13.20	14.03

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Appendix E2

Individual Egg HET-CAM Scores (Endpoints Evaluated and Overall Irritancy) for Data of Gilleron et al. (1997)

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Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Sodium hydroxide (10%)	127	5.00	4.98	4.98	6.91	6.91	6.91	8.43	8.70	8.64	20.34	20.59	20.53
	132	5.00	4.98	4.98	7.00	7.00	7.00	8.55	8.67	8.73	20.55	20.65	20.71
	140	4.80	4.93	4.93	6.98	6.95	7.00	8.94	8.64	8.46	20.72	20.52	20.39
Promethazine	206	0.00	0.00	0.00	0.00	0.00	0.00	4.11	5.58	4.92	4.11	5.58	4.92
	214	0.00	0.00	0.00	0.93	3.43	2.61	4.26	3.45	4.05	5.19	6.88	6.66
	220	0.00	0.00	0.00	0.00	2.15	1.66	6.69	6.81	5.76	6.69	8.96	7.42
Sodium hydroxide (1%)	127	4.90	4.95	4.97	6.84	6.91	6.93	7.47	7.41	7.08	19.21	19.27	18.98
	132	4.93	4.95	4.95	6.93	6.95	6.95	7.29	7.38	6.63	19.15	19.28	18.53
	141	4.90	4.88	4.87	6.98	6.93	6.93	7.50	6.69	7.02	19.38	18.50	18.82
Sodium oxalate	116	4.15	3.72	3.75	6.58	6.37	6.39	3.72	3.66	1.83	14.45	13.75	11.97
	120	0.00	0.00	0.00	6.65	6.84	6.84	8.22	8.19	7.38	14.87	15.03	14.22
	125	0.00	0.00	0.00	6.77	6.74	6.81	8.10	7.74	7.38	14.87	14.48	14.19
Trichloroacetic acid (30%)	127	0.00	0.00	0.00	6.91	6.86	6.88	8.64	8.73	8.76	15.55	15.59	15.64
	133	0.00	0.00	0.00	6.86	6.95	6.93	8.82	8.91	8.94	15.68	15.86	15.87
	141	0.00	0.00	0.00	6.91	6.91	6.91	8.85	8.79	8.79	15.76	15.70	15.70
Thiourea	149	4.35	4.38	4.47	6.93	6.79	6.79	5.46	5.67	3.63	16.74	16.84	14.89
	121	3.95	3.98	4.07	6.91	6.88	6.91	7.98	7.32	7.38	18.84	18.18	18.36
	125	4.08	4.27	4.10	6.88	6.93	6.93	7.74	8.16	8.10	18.70	19.36	19.13
2,2-Dimethylbutanoic acid	127	0.00	0.00	0.00	6.60	6.74	6.79	8.13	8.49	8.40	14.73	15.23	15.19
	133	0.00	0.00	0.00	6.98	6.93	6.95	8.46	8.49	8.22	15.44	15.42	15.17
	141	0.00	0.00	0.00	6.95	6.88	6.91	8.61	8.61	8.64	15.56	15.49	15.55
Imidazole	116	4.82	4.78	4.78	6.81	6.88	6.88	7.44	7.62	7.11	19.07	19.28	18.77
	121	4.52	4.68	4.72	6.88	6.93	6.91	7.68	7.83	7.68	19.08	19.44	19.31
	125	4.85	4.88	4.87	6.93	6.93	6.93	8.52	8.16	7.86	20.30	19.97	19.66
Trichloroacetic acid (3%)	209	0.00	0.00	0.00	6.93	6.91	6.88	8.58	8.73	8.70	15.51	15.64	15.58
	216	0.00	0.00	0.00	6.95	7.00	6.98	8.82	8.94	8.91	15.77	15.94	15.89
	217	0.00	0.00	0.00	6.91	6.95	6.95	8.73	8.79	8.82	15.64	15.74	15.77

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Sodium perborate, $4H_2O$	117	0.00	0.00	0.00	6.53	6.67	6.67	4.50	5.31	4.17	11.03	11.98	10.84
	121	0.00	0.00	0.00	6.67	6.81	6.79	7.05	6.63	6.45	13.72	13.44	13.24
	125	0.00	0.00	0.00	6.72	6.74	6.81	7.83	8.13	8.19	14.55	14.87	15.00
n-Hexanol	127	4.85	3.37	3.30	6.67	6.49	6.53	7.77	7.29	7.83	19.29	17.15	17.66
	133	4.38	4.45	4.33	6.95	6.91	6.91	6.27	6.15	5.58	17.60	17.51	16.82
	141	4.37	4.00	4.00	6.67	6.72	6.77	6.99	6.66	5.88	18.03	17.38	16.65
Potassium cyanate	117	0.00	0.00	0.00	6.74	6.84	6.72	6.45	5.91	6.21	13.19	12.75	12.93
	122	0.00	0.00	0.00	6.84	6.88	6.86	8.34	8.10	8.22	15.18	14.98	15.08
	150	0.00	0.00	0.00	6.65	6.58	6.74	7.83	8.28	8.25	14.48	14.86	14.99
Isobutanol	127	4.52	4.30	4.43	6.70	6.79	6.79	8.37	7.98	8.10	19.59	19.07	19.32
	133	4.65	4.75	4.62	6.91	6.81	6.95	8.04	7.95	7.80	19.60	19.51	19.37
	141	4.85	4.65	4.68	6.98	6.91	6.88	7.89	7.38	7.98	19.72	18.94	19.54
Ammonium nitrate	117	1.47	0.00	1.65	6.72	6.77	6.79	5.88	7.53	5.43	14.07	14.30	13.87
	122	0.50	0.53	0.12	6.81	6.88	6.91	7.98	8.22	8.19	15.29	15.63	15.22
	126	1.77	1.87	1.38	6.86	6.84	6.88	7.98	8.10	7.98	16.61	16.81	16.24
n-Octanol	205	4.77	4.75	4.52	5.53	5.25	4.99	8.07	7.62	7.38	18.37	17.62	16.89
	209	4.75	4.67	4.62	4.11	4.53	4.36	7.74	7.20	6.90	16.60	16.40	15.88
	213		3.78	4.25		5.90	5.37		6.48	6.57		16.16	16.19
2,5-Dimethylhexandiol	150	4.35	4.58	4.25	6.91	6.81	6.72	4.53	4.83	4.32	15.79	16.22	15.29
	122	4.18	4.33	3.72	6.32	6.11	6.39	5.61	4.89	3.54	16.11	15.33	13.65
	126	4.00	4.13	4.07	4.18	4.43	5.13	6.51	6.42	6.72	14.69	14.98	15.92
2,6-Dichlorobenzoyl chloride	128	0.00	0.00	0.00	4.22	5.62	5.18	5.10	5.07	4.65	9.32	10.69	9.83
	133	0.00	0.00	0.00	6.58	6.63	6.60	6.06	5.61	6.72	12.64	12.24	13.32
	141	0.00	0.00	0.00	6.35	6.51	6.04	8.04	0.72	0.93	14.39	7.23	6.97
Fomesafen	117	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	123	0.00	0.00	0.00	0.00	0.00	0.00	0.57	0.87	1.77	0.57	0.87	1.77
	150	0.00	0.00	0.00	0.00	0.00	0.00	3.24	1.92	2.52	3.24	1.92	2.52
Methyl cyanoacetate	128	4.35	4.40	4.65	3.59	4.83	5.20	6.60	7.02	7.50	14.54	16.25	17.35
	142	4.85	4.87	4.75	6.65	6.58	6.49	4.68	2.73	4.08	16.18	14.18	15.32
	161	4.43	4.77	4.80	6.09	6.44	6.32	5.91	7.26	6.93	16.43	18.47	18.05

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
L-Aspartic Acid	206	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	214	0.00	0.00	0.00	3.87	0.00	0.00	3.21	0.00	0.00	7.08	0.00	0.00
	220	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.43	0.00	0.00	2.43
Ethyl-2-methylacetoacetate	128	4.40	4.47	4.43	0.00	0.00	0.00	6.78	6.54	6.99	11.18	11.01	11.42
	134	4.65	4.43	4.37	6.72	6.51	6.23	5.49	4.44	6.15	16.86	15.38	16.75
	142	4.42	4.77	4.50	6.86	6.58	6.74	0.00	0.00	0.00	11.28	11.35	11.24
Dibenzoyl-L-tartaric acid	206	4.27	4.10	4.27	0.00	0.00	0.00	4.17	4.53	4.47	8.44	8.63	8.74
	214	4.72	4.42	4.80	4.74	5.13	4.99	4.68	5.58	4.95	14.14	15.13	14.74
	220	4.73	4.82	4.73	5.09	5.09	5.11	6.96	6.87	6.87	16.78	16.78	16.71
n-Butyl acetate	207	4.70	4.73	4.78	0.00	3.03	4.71	7.53	7.95	7.83	12.23	15.71	17.32
	211	4.83	4.72	4.82	6.35	5.76	5.95	7.53	7.14	7.38	18.71	17.62	18.15
	217	4.28	4.33	4.12	6.32	6.35	6.11	7.98	7.92	7.71	18.58	18.60	17.94
Captan 90 concentrate	115	0.00	0.00	0.00	6.81	6.88	6.88	8.28	8.37	7.89	15.09	15.25	14.77
	118	0.00	0.00	0.00	6.91	6.81	6.81	7.71	8.04	8.19	14.62	14.85	15.00
	124	0.00	0.00	0.00	6.74	6.79	6.88	8.49	8.55	8.64	15.23	15.34	15.52
Methyl isobutyl ketone	207	4.83	4.75	4.80	3.45	2.38	5.11	6.63	6.42	7.68	14.91	13.55	17.59
	211	4.82	4.85	4.90	6.42	6.25	6.37	8.46	8.49	8.49	19.70	19.59	19.76
	217	4.28	3.52	3.85	6.09	5.90	5.81	8.46	8.46	8.28	18.83	17.88	17.94
Chlorhexidine	115	4.52	4.62	4.35	6.28	5.97	5.90	0.00	0.00	0.00	10.80	10.59	10.25
	118	4.68	4.55	4.63	5.72	5.55	5.74	7.50	7.50	6.90	17.90	17.60	17.27
	124	4.08	4.60	4.27	5.37	5.97	5.79	5.49	7.26	6.54	14.94	17.83	16.60
Methyl cyclopentane	128	3.85	2.75	4.18	6.88	6.86	6.77	8.25	8.34	7.89	18.98	17.95	18.84
	134	0.00	3.57	3.62	6.93	6.81	6.88	8.13	8.19	8.19	15.06	18.57	18.69
	151	4.35	0.00	0.00	6.81	6.51	6.79	7.62	6.96	7.11	18.78	13.47	13.90
4-Carboxybenzaldehyde	206	3.88	3.71	3.77	0.00	0.00	0.00	5.79	5.07	5.16	9.67	8.78	8.93
	214	4.12	4.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.12	4.02	0.00
	220	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethytrimethyl acetate	207	0.13	0.40	0.00	2.92	3.59	3.87	6.72	7.38	7.44	9.77	11.37	11.31
	211	2.77	2.97	3.43	3.55	3.64	4.64	7.92	6.99	7.62	14.24	13.60	15.69
	217	4.33	4.08	3.97	5.32	3.69	5.39	7.14	7.08	7.41	16.79	14.85	16.77

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Quinacrine	206	1.03	0.45	2.75	0.00	0.00	0.00	6.87	3.30	5.49	7.90	3.75	8.24
	214	1.62	1.20	1.57	0.00	0.00	0.00	6.12	5.85	5.91	7.74	7.05	7.48
	220	0.00	0.00	0.00	1.61	2.17	2.12	5.79	5.82	5.91	7.40	7.99	8.03
Toluene	207	0.00	0.00	0.00	6.70	6.74	6.67	8.52	8.43	8.43	15.22	15.17	15.10
	211	0.00	0.00	0.00	6.91	6.86	6.72	8.40	8.37	8.16	15.31	15.23	14.88
	217	4.50	4.22	3.30	6.84	6.91	6.86	6.84	6.93	7.47	18.18	18.06	17.63
Dibenzyl phosphate	116	0.00	0.00	0.00	6.95	6.98	6.98	8.67	8.67	8.79	15.62	15.65	15.77
	119	0.00	0.00	0.00	6.91	6.86	6.91	8.73	8.10	7.62	15.64	14.96	14.53
	124	0.00	0.00	0.00	6.77	6.81	6.86	7.65	8.04	8.19	14.42	14.85	15.05
Acetone	131	0.00	0.00	0.00	6.91	6.95	6.95	8.67	8.79	8.76	15.58	15.74	15.71
	137	0.00	0.00	0.00	6.98	6.98	6.98	7.95	8.13	8.13	14.93	15.11	15.11
	144	0.00	0.00	0.00	6.81	6.91	6.95	8.40	7.92	8.67	15.21	14.83	15.62
Tetraaminopyrimidine sulfate	116	4.72	4.75	3.72	0.00	0.00	0.00	0.00	0.00	0.00	4.72	4.75	3.72
	120	4.47	3.62	4.12	0.00	0.00	0.00	0.00	0.00	0.00	4.47	3.62	4.12
	125	4.62	4.40	4.55	0.00	0.00	0.00	0.00	0.00	0.00	4.62	4.40	4.55
Cyclohexanol	131	4.10	4.27	4.20	6.81	6.88	6.77	7.68	8.13	7.74	18.59	19.28	18.71
	137	4.00	4.00	4.17	6.86	6.88	6.88	8.07	8.40	7.92	18.93	19.28	18.97
	144	4.75	4.58	4.57	6.93	6.79	6.88	7.62	6.69	8.07	19.30	18.06	19.52
Benzalkonium chloride (10%)	129	0.00	0.00	0.00	6.93	6.91	6.93	8.25	8.34	8.04	15.18	15.25	14.97
	134	0.00	0.00	0.00	6.77	6.95	6.95	8.07	8.49	8.58	14.84	15.44	15.53
	143	0.00	0.00	0.00	6.91	6.91	6.91	7.80	7.80	7.89	14.71	14.71	14.80
Parafluoroaniline	131	0.00	3.15	3.30	6.86	6.84	6.84	8.49	8.25	7.89	15.35	18.24	18.03
	137	0.00	0.00	0.00	6.93	6.91	6.93	8.46	8.37	8.37	15.39	15.28	15.30
	145	0.00	0.00	0.00	6.91	6.93	6.93	6.42	6.99	7.71	13.33	13.92	14.64
Cetylperidinium bromide (6%)	129	0.00	0.00	0.00	6.79	6.84	6.81	7.59	7.47	7.98	14.38	14.31	14.79
	135	0.00	0.00	0.00	6.86	6.88	6.91	8.07	8.34	8.19	14.93	15.22	15.10
	143	0.00	0.00	0.00	6.84	6.72	6.91	7.56	7.41	7.29	14.40	14.13	14.20
Methyl acetate	131	4.73	4.68	4.63	6.88	6.88	6.81	7.65	8.04	8.07	19.26	19.60	19.51
	137	4.33	4.10	4.47	7.00	6.98	6.93	8.04	7.77	8.49	19.37	18.85	19.89
	146	3.58	3.35	3.92	6.93	6.88	6.93	7.65	7.53	7.59	18.16	17.76	18.44

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Cetylperidinium bromide (10%)	129	0.00	0.00	0.00	6.86	6.91	6.93	7.56	7.95	7.77	14.42	14.86	14.70
	135	0.00	0.00	0.00	6.84	6.93	6.91	7.92	8.49	8.46	14.76	15.42	15.37
	143	0.00	0.00	0.00	6.86	6.86	6.93	3.54	3.33	4.74	10.40	10.19	11.67
Gamma-butyrolactone	131	4.93	4.93	4.95	6.93	6.93	6.95	7.86	7.50	7.68	19.72	19.36	19.58
	137	4.93	4.95	4.88	6.98	6.98	6.91	8.28	8.43	8.04	20.19	20.36	19.83
	145	4.90	4.93	4.93	6.93	6.98	6.93	7.02	6.03	6.81	18.85	17.94	18.67
Benzalkonium chloride (5%)	129	0.00	0.00	0.00	6.91	6.91	6.93	7.83	8.07	8.34	14.74	14.98	15.27
	135	0.00	0.00	0.00	6.88	6.98	6.95	8.37	8.10	8.34	15.25	15.08	15.29
	143	0.00	0.00	0.00	6.95	6.91	6.93	7.68	6.63	7.53	14.63	13.54	14.46
2-Ethyl-1-hexanol	131	3.97	4.18	4.40	0.00	0.00	0.00	6.93	5.82	6.33	10.90	10.00	10.73
	137	4.17	4.03	3.92	6.21	6.16	6.07	6.42	5.46	5.82	16.80	15.65	15.81
	145	4.00	3.83	3.95	5.76	6.04	6.28	2.58	1.20	0.84	12.34	11.07	11.07
Triton X-100 (10%)	129	4.60	4.57	4.47	6.77	6.79	6.79	2.49	0.81	2.64	13.86	12.17	13.90
	135	4.20	3.80	3.12	6.91	6.91	6.88	2.76	4.95	3.24	13.87	15.66	13.24
	143	3.73	4.28	4.20	6.65	6.72	6.86	4.56	1.71	2.13	14.94	12.71	13.19
Methyl ethyl ketone	205	4.95	4.95	4.97	6.63	6.65	6.77	8.55	8.61	8.58	20.13	20.21	20.32
	209	3.90	3.85	3.85	6.86	6.84	6.81	8.67	8.64	8.61	19.43	19.33	19.27
	213	0.00	0.00	0.00	6.88	6.81	6.86	8.70	8.55	8.67	15.58	15.36	15.53
Sodium lauryl sulfate (15%)	205	0.00	0.00	0.00	6.91	6.91	6.93	8.49	8.55	8.37	15.40	15.46	15.30
	210	0.00	0.00	0.00	6.91	6.88	6.84	7.89	8.37	7.77	14.80	15.25	14.61
	213	0.00	0.00	0.00	6.95	6.88	6.86	8.10	7.92	7.89	15.05	14.80	14.75
Isopropanol	132	0.00	0.00	0.00	6.86	6.93	6.93	7.38	8.13	8.10	14.24	15.06	15.03
	137	0.00	0.00	0.00	6.98	6.98	6.95	7.98	8.04	8.13	14.96	15.02	15.08
	152	0.00	0.00	0.00	6.86	6.91	6.88	7.53	7.92	7.74	14.39	14.83	14.62
Triton X-100 (5%)	130	4.30	3.70	3.97	6.32	6.44	6.42	0.00	0.00	0.00	10.62	10.14	10.39
	143	4.35	4.35	4.12	6.60	6.70	6.72	0.00	1.50	1.23	10.95	12.55	12.07
	152	3.57	3.80	4.18	6.72	6.72	6.79	0.00	0.00	0.00	10.29	10.52	10.97
Ethanol	132	0.00	0.00	0.00	6.91	6.93	6.93	8.01	7.98	8.04	14.92	14.91	14.97
	140	0.00	0.00	0.00	6.72	6.93	6.91	8.19	7.98	7.86	14.91	14.91	14.77
	145	0.00	0.00	0.00	6.86	6.91	6.88	8.13	8.31	7.59	14.99	15.22	14.47

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Sodium lauryl sulfate (3%)	130	0.00	0.00	0.00	6.84	6.79	6.51	6.30	4.83	6.18	13.14	11.62	12.69
	136	0.00	0.00	0.00	6.86	6.86	6.81	6.78	7.32	7.83	13.64	14.18	14.64
	143	0.00	0.00	0.00	6.91	6.81	6.70	4.80	3.63	2.67	11.71	10.44	9.37
Pyridine	132	4.93	0.00	4.93	6.95	6.93	6.95	8.52	8.64	8.52	20.40	15.57	20.40
	140	0.00	0.00	0.00	6.93	6.93	6.86	8.01	8.16	8.13	14.94	15.09	14.99
	145	4.80	4.57	4.72	6.86	6.91	6.88	8.16	7.89	7.86	19.82	19.37	19.46
PEG 400	210	0.00	0.00	0.00	6.70	5.27	6.70	8.49	6.57	8.43	15.19	11.84	15.13
	216	0.00	0.00	0.00	6.65	6.77	6.67	8.25	8.37	8.28	14.90	15.14	14.95
	219	0.00	0.00	0.00	6.65	6.49	6.09	8.73	8.55	8.46	15.38	15.04	14.55
Glycerol	209	0.00	0.00	0.00	5.27	5.46	5.58	8.67	8.58	8.58	13.94	14.04	14.16
	216	0.00	0.00	0.00	6.77	6.74	6.81	8.76	8.76	8.82	15.53	15.50	15.63
	220	0.00	0.00	0.00	6.14	6.25	6.28	8.61	8.61	8.67	14.75	14.86	14.95
Benzalkonium chloride (1%)	130	0.00	0.00	0.00	6.86	6.88	6.88	8.55	8.49	8.46	15.41	15.37	15.34
	136	0.00	0.00	0.00	6.88	6.98	6.95	8.25	8.25	8.19	15.13	15.23	15.14
	144	0.00	0.00	0.00	6.88	6.91	6.95	7.92	8.13	7.95	14.80	15.04	14.90
Ethyl acetate	205	4.90	4.88	4.92	6.58	6.60	6.58	7.86	8.01	7.77	19.34	19.49	19.27
	209	4.00	3.92	4.12	6.88	6.77	6.81	8.58	8.40	8.58	19.46	19.09	19.51
	213	3.83	4.37	4.05	6.60	6.58	6.51	8.70	8.64	8.46	19.13	19.59	19.02
Cetylperidinium bromide (0.1%)	210	0.00	0.00	0.00	5.90	6.04	5.93	7.11	7.35	7.32	13.01	13.39	13.25
	216	0.00	0.00	0.00	6.35	6.30	6.33	7.62	7.41	7.52	13.97	13.71	13.85
	219	0.00	0.00	0.00	5.83	5.86	5.90	5.10	6.36	3.84	10.93	12.22	9.74
Maneb	117	0.00	0.00	0.00	5.06	5.39	4.81	0.00	0.00	0.00	5.06	5.39	4.81
	123	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	126	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	150	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1-Napthalene acetic acid, sodium salt	115	0.00	0.00	0.00	6.67	6.70	6.81	7.71	7.17	8.07	14.38	13.87	14.88
	124	0.00	0.00	0.00	6.91	6.91	6.95	8.55	8.28	8.49	15.46	15.19	15.44
	149	0.00	2.27	0.00	6.84	6.86	6.81	8.28	7.98	7.53	15.12	17.11	14.34

Substance	Sequence Number	Hemorrhage Score			Lysis Score			Coagulation Score			*In Vitro* Score		
		Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
Tween 20	130	0.00	0.00	0.00	6.49	6.23	6.53	7.86	6.09	7.20	14.35	12.32	13.73
	136	0.00	0.00	0.00	5.51	6.21	6.74	5.49	6.99	7.77	11.00	13.20	14.51
	144	0.00	0.00	0.00	6.91	6.88	6.84	8.94	8.91	8.82	15.85	15.79	15.66
	210	0.00	0.00	0.00	6.88	6.21	6.44	8.16	7.71	7.62	15.04	13.92	14.06
	219	1.90	1.68	2.33	6.35	6.28	5.23	8.40	8.40	8.19	16.65	16.36	15.75
1-Napthalene acetic acid	115	0.38	3.00	2.17	0.00	0.00	0.00	0.00	2.40	0.36	0.38	5.40	2.53
	118	1.92	2.62	2.03	4.50	3.83	3.66	4.95	3.87	2.88	11.37	10.32	8.57
	124	0.00	2.00	0.00	1.91	3.34	4.11	3.27	3.36	4.44	5.18	8.70	8.55
	149	2.42	3.52	2.57	0.00	0.00	0.00	0.00	0.00	0.00	2.42	3.52	2.57

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Appendix E3

Intralaboratory Repeatability Results (Expressed as %CV) for Data of Gilleron et al. (1996)

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Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
Allyl Alcohol	86	0.00	0.00		3.91	3.39	**86.63**	8.82	0.08	**0.90**	12.73	3.37	**26.44**
	95	0.62	1.07	**173.21**	1.38	2.38	**173.21**	8.03	0.18	**2.19**	10.02	3.52	**35.09**
	99	0.00	0.00		6.25	0.30	**4.82**	8.27	0.10	**1.17**	14.52	0.40	**2.72**
2-Aminophenol	91	0.00	0.00		0.00	0.00		1.42	1.27	**89.14**	1.42	1.27	**89.14**
	96	0.00	0.00		0.00	0.00		1.09	1.71	**156.82**	1.09	1.71	**156.82**
	101	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Anthracene	91	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	95	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	99	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Butyrolactone	88	4.98	0.01	**0.12**	0.00	0.00		7.89	0.48	**6.04**	12.87	0.47	**3.69**
	95	4.94	0.04	**0.82**	0.00	0.00		7.84	0.23	**2.97**	12.78	0.20	**1.58**
	100	4.72	0.34	**7.16**	4.55	0.51	**11.18**	6.67	0.78	**11.70**	15.94	1.07	**6.72**
Cyclohexanone	89	4.34	0.42	**9.61**	0.00	0.00		7.92	0.42	**5.30**	12.26	0.24	**1.94**
	98	4.64	0.47	**10.16**	6.61	0.18	**2.69**	7.59	0.68	**8.93**	18.85	1.01	**5.38**
	104	4.63	0.19	**4.11**	5.46	2.01	**36.75**	2.20	1.76	**80.22**	12.29	3.65	**29.67**
Deoxycholic acid, sodium salt	89	1.96	1.97	**100.26**	6.09	0.44	**7.21**	8.34	0.34	**4.05**	16.39	2.59	**15.78**
	97	1.27	1.32	**103.73**	5.55	0.57	**10.32**	0.00	0.00		6.82	0.75	**10.92**
	102	0.00	0.00		5.89	0.53	**8.94**	0.00	0.00		5.89	0.53	**8.94**
Diacetone alcohol	89	3.79	0.98	**25.83**	0.00	0.00		8.13	0.97	**11.88**	11.92	0.58	**4.87**
	98	4.90	0.03	**0.61**	5.57	0.29	**5.17**	6.53	0.86	**13.19**	17.00	1.02	**6.02**
	104	4.84	0.05	**1.07**	6.10	0.17	**2.74**	5.28	1.79	**33.88**	16.22	1.88	**11.57**
Dibenzoyl-L-tartaric acid	90	1.38	2.40	**173.21**	0.00	0.00		0.00	0.00		1.38	2.40	**173.21**
	93	4.83	0.03	**0.60**	0.00	0.00		0.00	0.00		4.83	0.03	**0.60**
	102	4.72	0.11	**2.25**	1.59	1.73	**108.99**	0.00	0.00		6.30	1.81	**28.65**
2,4-Dichloro-5-sulfamoyl-	91	1.61	2.78	**173.21**	0.00	0.00		0.00	0.00		1.61	2.78	**173.21**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
benzoic acid	93	4.82	0.04	**0.73**	0.00	0.00		1.21	1.13	**93.77**	6.03	1.15	**19.01**
	100	3.67	0.99	**27.03**	0.00	0.00		0.00	0.00		3.67	0.99	**27.03**
Dimethyl biguanidine	92	0.00	0.00		0.00	0.00		8.07	0.53	**6.61**	8.07	0.53	**6.61**
	93	0.00	0.00		4.02	1.89	**46.97**	6.76	1.83	**27.07**	10.78	2.00	**18.55**
	103	0.00	0.00		6.46	0.12	**1.80**	0.00	0.00		6.46	0.12	**1.80**
Dimethyl sulfoxide	88	0.00	0.00		6.38	0.26	**4.02**	8.49	0.22	**2.55**	14.87	0.21	**1.41**
	93	0.39	0.68	**173.21**	0.00	0.00		7.00	0.36	**5.11**	7.39	0.85	**11.49**
	101	0.00	0.00		6.15	0.38	**6.15**	5.36	0.62	**11.50**	11.51	0.43	**3.74**
Ethanol	89	0.00	0.00		0.00	0.00		8.43	0.22	**2.57**	8.43	0.22	**2.57**
	97	0.00	0.00		5.79	0.08	**1.40**	5.68	0.35	**6.08**	11.47	0.42	**3.64**
	102	0.00	0.00		6.27	0.45	**7.12**	7.80	0.29	**3.71**	14.07	0.40	**2.83**
2-Ethoxyethanol	86	0.85	1.47	**173.21**	0.42	0.73	**173.21**	8.62	0.35	**4.08**	9.89	1.85	**18.75**
	95	1.82	2.35	**128.66**	0.00	0.00		6.22	0.23	**3.62**	8.04	2.14	**26.55**
	99	0.00	0.00		5.63	0.29	**5.11**	7.81	0.40	**5.12**	13.44	0.18	**1.35**
Ethylenediaminetetra-acetic acid, dipotassium	91	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	94	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	99	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Furan	88	0.00	0.00		0.43	0.74	**173.21**	4.08	3.02	**73.96**	4.51	2.28	**50.59**
	95	0.92	1.60	**173.21**	1.74	1.55	**89.39**	3.88	2.37	**61.19**	6.54	2.65	**40.51**
	100	0.00	0.00		5.06	0.48	**9.47**	0.44	0.55	**123.92**	5.50	0.48	**8.74**
Gluconolactone	91	0.00	0.00		0.00	0.00		8.17	0.48	**5.89**	8.17	0.48	**5.89**
	93	0.00	0.00		2.08	3.61	**173.21**	0.00	0.00		2.08	3.61	**173.21**
	101	0.00	0.00		3.40	2.09	**61.51**	0.00	0.00		3.40	2.09	**61.51**
DL-Glutamic acid	91	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	95	2.03	1.78	**87.69**	0.00	0.00		0.00	0.00		2.03	1.78	**87.69**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
	100	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
3-Glycidopropyl-trimethoxysilane	99	3.63	0.48	**13.10**	0.00	0.00		0.00	0.00		3.63	0.48	**13.10**
	100	3.63	0.16	**4.33**	0.00	0.00		1.79	0.81	**45.01**	5.42	0.75	**13.87**
	105	3.90	0.11	**2.88**	0.00	0.00		0.00	0.00		3.90	0.11	**2.88**
Hexadecyltrimethyl-ammonium bromide	90	4.59	0.19	**4.15**	4.22	1.19	**28.26**	7.58	0.41	**5.37**	16.39	1.05	**6.43**
	97	2.81	2.44	**86.70**	4.85	1.11	**22.91**	0.00	0.00		7.66	2.03	**26.43**
	103	0.00	0.00		6.32	0.19	**2.93**	2.15	1.95	**90.78**	8.47	1.93	**22.78**
Hexane	86	1.24	0.78	**63.10**	0.00	0.00		4.62	0.19	**4.06**	5.86	0.80	**13.63**
	93	0.00	0.00		0.00	0.00		0.57	0.99	**173.21**	0.57	0.99	**173.21**
	105	0.00	0.00		2.82	2.48	**87.96**	0.00	0.00		2.82	2.48	**87.96**
Iminodibenzyl	92	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	96	0.00	0.00		0.00	0.00		0.09	0.16	**173.21**	0.09	0.16	**173.21**
	102	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Magnesium carbonate	92	0.00	0.00		0.00	0.00		3.53	1.33	**37.76**	3.53	1.33	**37.76**
	101	0.00	0.00		0.00	0.00		0.76	1.32	**173.21**	0.76	1.32	**173.21**
	106	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Methyl isobutyl ketone	88	2.09	1.85	**88.54**	0.00	0.00		7.16	0.48	**6.73**	9.25	2.15	**23.26**
	96	3.79	0.77	**20.40**	2.39	0.45	**19.01**	5.98	1.76	**29.46**	12.16	1.17	**9.61**
	105	3.46	0.44	**12.77**	6.60	0.19	**2.81**	0.00	0.00		10.06	0.48	**4.78**
MYRJ 45	92	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	97	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	102	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
1-Nitropropane	86	0.42	0.73	**173.21**	0.00	0.00		2.64	2.32	**88.05**	3.06	2.86	**93.20**
	87	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	95	1.32	0.88	**66.81**	1.55	2.68	**173.21**	2.51	2.41	**95.92**	5.37	0.71	**13.25**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
Octanol	88	2.01	1.75	**87.26**	1.51	2.62	**173.21**	4.47	1.66	**37.08**	7.99	2.35	**29.37**
	102	3.56	0.51	**14.33**	3.84	0.12	**3.02**	2.90	0.17	**5.88**	10.29	0.58	**5.67**
	106	3.37	0.15	**4.56**	5.73	0.48	**8.42**	2.14	1.50	**70.17**	11.25	1.32	**11.71**
2,4-Pentanedione	86	4.41	0.33	**7.60**	0.00	0.00		5.86	1.97	**33.57**	10.27	2.01	**19.58**
	87	4.37	0.19	**4.44**	0.00	0.00		6.39	0.90	**14.08**	10.76	1.07	**9.90**
	93	4.17	0.23	**5.62**	0.00	0.00		1.20	2.08	**173.21**	5.37	2.05	**38.06**
1-Phenyl-3-pyrazolidone	91	0.00	0.00		0.00	0.00		0.60	1.04	**173.21**	0.60	1.04	**173.21**
	96	0.00	0.00		0.00	0.00		0.79	1.05	**132.77**	0.79	1.05	**132.77**
	101	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Polyoxythethylene 23 lauryl ether	92	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	97	4.52	0.08	**1.68**	0.00	0.00		0.00	0.00		4.52	0.08	**1.68**
	103	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Propyl-4-hydroxy-benzoate	92	1.11	1.92	**173.21**	0.00	0.00		0.38	0.66	**173.21**	1.49	2.58	**173.21**
	96	2.82	0.58	**20.37**	0.00	0.00		0.25	0.43	**173.21**	3.07	0.72	**23.36**
	101	1.07	0.87	**81.17**	0.00	0.00		0.00	0.00		1.07	0.87	**81.17**
Pyridine	89	2.97	2.61	**87.69**	0.00	0.00		8.68	0.23	**2.62**	11.65	2.39	**20.51**
	98	4.65	0.30	**6.55**	6.89	0.04	**0.52**	5.74	3.20	**55.83**	17.28	3.03	**17.54**
	104	4.34	0.87	**19.93**	6.74	0.28	**4.17**	7.31	0.51	**6.99**	18.39	0.44	**2.37**
Quinacrine	90	4.64	0.03	**0.75**	0.00	0.00		1.05	1.82	**173.21**	5.69	1.85	**32.57**
	93	4.82	0.05	**0.96**	0.00	0.00		0.00	0.00		4.82	0.05	**0.96**
	103	0.07	0.12	**173.21**	3.72	1.23	**33.14**	5.19	1.68	**32.35**	8.97	2.89	**32.23**
Tetraaminopyrimidine sulfate	92	1.59	2.75	**173.21**	0.00	0.00		0.00	0.00		1.59	2.75	**173.21**
	93	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	103	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Thiourea	90	3.88	0.09	**2.19**	6.82	0.07	**1.06**	7.48	0.53	**7.07**	18.18	0.50	**2.76**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
	103	3.83	0.06	**1.68**	6.61	0.03	**0.44**	0.00	0.00		10.44	0.04	**0.35**
	107	4.02	0.13	**3.11**	6.70	0.06	**0.87**	0.00	0.00		10.72	0.13	**1.21**
1,2,3-Tricholoropropane	89	0.53	0.83	**157.05**	0.00	0.00		5.50	2.43	**44.21**	6.03	2.85	**47.29**
	98	3.70	0.55	**14.76**	0.81	0.96	**118.49**	4.99	0.60	**11.94**	9.50	1.11	**11.74**
	104	3.27	0.55	**16.98**	3.84	0.48	**12.47**	0.91	0.35	**38.63**	8.02	0.31	**3.92**
1,2,4-Trimethylbenzene	88	0.37	0.55	**150.21**	0.00	0.00		4.09	2.45	**59.88**	4.46	2.92	**65.53**
	95	0.62	1.07	**173.21**	0.00	0.00		0.88	1.52	**173.21**	1.50	2.59	**173.21**
	100	0.00	0.00		4.90	1.05	**21.39**	2.42	1.55	**64.13**	7.32	1.40	**19.08**
Triton X-155	92	0.25	0.43	**173.21**	0.00	0.00		1.03	1.53	**148.70**	1.28	1.33	**103.67**
	98	2.77	1.29	**46.38**	2.98	2.59	**86.86**	0.00	0.00		5.75	3.83	**66.62**
	104	0.00	0.00		4.74	0.17	**3.48**	0.00	0.00		4.74	0.17	**3.48**
Benzethonium chloride[1]	90	4.71	0.18	**3.83**	0.00	0.00		7.71	0.47	**6.08**	12.42	0.63	**5.08**
	98	4.39	0.40	**9.12**	5.84	0.53	**9.00**	7.79	0.61	**7.79**	18.03	0.89	**4.95**
	104	0.00	0.00		6.53	0.06	**0.90**	0.37	0.33	**89.68**	6.90	0.28	**4.06**
	107	0.00	0.00		6.76	0.04	**0.60**	6.08	0.27	**4.48**	12.84	0.28	**2.18**
Ethylacetoacetate[1]	89	3.97	0.16	**4.12**	0.00	0.00		3.52	0.58	**16.56**	7.49	0.68	**9.08**
	97	3.16	0.59	**18.72**	1.45	1.95	**134.57**	0.00	0.00		4.61	1.37	**29.81**
	102	3.99	0.45	**11.23**	4.57	0.30	**6.47**	5.04	0.67	**13.26**	13.61	0.42	**3.05**
Imidazole[1]	96	4.41	0.34	**7.63**	4.31	0.87	**20.16**	8.91	0.00	**0.00**	17.63	1.20	**6.80**
	100	4.83	0.03	**0.52**	6.22	0.62	**9.93**	5.47	0.99	**18.14**	16.52	1.61	**9.72**
	105	4.90	0.03	**0.59**	6.89	0.03	**0.42**	7.29	0.53	**7.28**	19.09	0.49	**2.55**
	118	4.68	0.22	**4.76**	6.85	0.06	**0.88**	7.03	0.20	**2.84**	18.57	0.30	**1.60**
	115	4.90	0.03	**0.51**	6.56	0.25	**3.78**	8.48	0.33	**3.90**	19.94	0.11	**0.54**
	116	4.80	0.04	**0.84**	6.71	0.19	**2.82**	7.70	0.20	**2.59**	19.20	0.22	**1.16**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Substance	Test Number	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
N-Laurylsarcosine, sodium salt[1]	92	2.68	2.37	**88.71**	6.23	0.47	**7.62**	8.71	0.06	**0.72**	17.62	2.11	**11.98**
	94	2.91	2.52	**86.74**	6.34	0.23	**3.70**	1.13	1.26	**111.58**	10.38	1.69	**16.24**
	106	0.00	0.00		6.91	0.03	**0.36**	4.06	0.23	**5.59**	10.97	0.23	**2.14**
	103	1.46	2.53	**173.21**	6.63	0.03	**0.38**	0.24	0.42	**173.21**	8.33	2.33	**27.95**
Laurylsulfobetaine[1]	92	0.00	0.00		6.14	0.16	**2.55**	2.92	0.83	**28.29**	9.06	0.94	**10.40**
	94	0.22	0.39	**173.21**	5.71	1.43	**25.03**	3.75	3.12	**83.15**	9.68	4.15	**42.87**
	104	0.00	0.00		6.83	0.02	**0.25**	0.00	0.00		6.83	0.02	**0.25**
Methanol[1]	89	0.00	0.00		3.69	3.29	**89.14**	8.57	0.11	**1.33**	12.26	3.36	**27.40**
	93	0.00	0.00		0.00	0.00		7.97	0.12	**1.57**	7.97	0.12	**1.57**
	102	0.00	0.00		6.79	0.09	**1.33**	8.38	0.12	**1.49**	15.17	0.20	**1.32**
	105	0.00	0.00		6.84	0.05	**0.66**	5.81	1.59	**27.37**	12.65	1.55	**12.22**
2-Methoxyethanol[1]	88	0.00	0.00		5.94	1.14	**19.25**	8.39	0.22	**2.64**	14.33	0.93	**6.47**
	89	0.00	0.00		5.09	1.22	**24.00**	8.45	0.30	**3.59**	13.54	1.27	**9.40**
	96	0.00	0.00		5.39	0.32	**5.95**	7.96	0.05	**0.58**	13.35	0.29	**2.14**
	101	0.00	0.00		6.02	0.29	**4.84**	5.66	0.92	**16.25**	11.68	0.71	**6.11**
Promethazine hydrochloride[1]	85	0.00	0.00		6.69	0.11	**1.64**	8.37	0.71	**8.47**	15.06	0.80	**5.30**
	90	2.58	0.76	**29.32**	0.00	0.00		8.57	0.12	**1.46**	11.15	0.77	**6.91**
	102	0.00	0.00		6.71	0.07	**1.03**	8.51	0.02	**0.20**	15.22	0.05	**0.34**
	97	0.00	0.00		6.70	0.18	**2.61**	8.29	0.09	**1.04**	14.99	0.20	**1.31**
Triethanolamine[1]	89	0.00	0.00		3.23	0.50	**15.64**	7.59	0.80	**10.48**	10.82	1.28	**11.82**
	104	0.00	0.00		6.70	0.18	**2.61**	5.72	0.88	**15.35**	12.42	0.91	**7.34**
	107	0.00	0.00		6.36	0.35	**5.52**	6.75	0.89	**13.13**	13.11	0.78	**5.94**

Abbreviations: %CV = percent coefficient of variation; SD = standard deviation
[1]Data not originally presented in Gilleron et al. (1996).

Appendix E4

Intralaboratory Repeatability Results (Expressed as %CV) for Data of Gilleron et al. (1997)

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Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
Acetone	131	0.00	0.00		6.94	0.02	**0.33**	8.74	0.06	**0.71**	15.68	0.09	**0.54**
	137	0.00	0.00		6.98	0.00	**0.00**	8.07	0.10	**1.29**	15.05	0.10	**0.69**
	144	0.00	0.00		6.89	0.07	**1.05**	8.33	0.38	**4.56**	15.22	0.40	**2.60**
Ammonium nitrate	117	1.04	0.91	**87.03**	6.76	0.04	**0.53**	6.28	1.11	**17.61**	14.08	0.22	**1.53**
	122	0.38	0.23	**59.62**	6.87	0.05	**0.75**	8.13	0.13	**1.61**	15.38	0.22	**1.43**
	126	1.67	0.26	**15.47**	6.86	0.02	**0.29**	8.02	0.07	**0.86**	16.55	0.29	**1.75**
L-Aspartic Acid	206	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	214	0.00	0.00		1.29	2.23	**173.21**	1.07	1.85	**173.21**	2.36	4.09	**173.21**
	220	0.00	0.00		0.00	0.00		0.81	1.40	**173.21**	0.81	1.40	**173.21**
Benzalkonium chloride (1%)	130	0.00	0.00		6.87	0.01	**0.17**	8.50	0.05	**0.54**	15.37	0.04	**0.23**
	136	0.00	0.00		6.94	0.05	**0.74**	8.23	0.03	**0.42**	15.17	0.06	**0.36**
	144	0.00	0.00		6.91	0.04	**0.51**	8.00	0.11	**1.42**	14.91	0.12	**0.81**
Benzalkonium chloride (10%)	129	0.00	0.00		6.92	0.01	**0.17**	8.21	0.15	**1.88**	15.13	0.15	**0.96**
	134	0.00	0.00		6.89	0.10	**1.51**	8.38	0.27	**3.25**	15.27	0.38	**2.46**
	143	0.00	0.00		6.91	0.00	**0.00**	7.83	0.05	**0.66**	14.74	0.05	**0.35**
Benzalkonium chloride (5%)	129	0.00	0.00		6.92	0.01	**0.17**	8.08	0.26	**3.16**	15.00	0.27	**1.77**
	135	0.00	0.00		6.94	0.05	**0.74**	8.27	0.15	**1.79**	15.21	0.11	**0.73**
	143	0.00	0.00		6.93	0.02	**0.29**	7.28	0.57	**7.80**	14.21	0.59	**4.13**
n-Butyl acetate	207	4.74	0.04	**0.85**	2.58	2.39	**92.52**	7.77	0.22	**2.78**	15.09	2.60	**17.24**
	211	4.79	0.06	**1.27**	6.02	0.30	**5.00**	7.35	0.20	**2.68**	18.16	0.55	**3.00**
	217	4.24	0.11	**2.59**	6.26	0.13	**2.09**	7.87	0.14	**1.80**	18.37	0.38	**2.04**
Gamma-butyrolactone	131	4.94	0.01	**0.23**	6.94	0.01	**0.17**	7.68	0.18	**2.34**	19.55	0.18	**0.93**
	137	4.92	0.04	**0.73**	6.96	0.04	**0.58**	8.25	0.20	**2.38**	20.13	0.27	**1.34**
	145	4.92	0.02	**0.35**	6.95	0.03	**0.42**	6.62	0.52	**7.88**	18.49	0.48	**2.61**
Captan 90 concentrate	115	0.00	0.00		6.86	0.04	**0.59**	8.18	0.26	**3.12**	15.04	0.24	**1.63**
	118	0.00	0.00		6.84	0.06	**0.84**	7.98	0.25	**3.08**	14.82	0.19	**1.29**
	124	0.00	0.00		6.80	0.07	**1.04**	8.56	0.08	**0.88**	15.36	0.15	**0.95**
4-Carboxybenzalde-hyde	206	3.79	0.09	**2.28**	0.00	0.00		5.34	0.39	**7.35**	9.13	0.48	**5.22**
	214	2.71	2.35	**86.62**	0.00	0.00		0.00	0.00		2.71	2.35	**86.62**
	220	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Cetylpyridinium-	210	0.00	0.00		5.96	0.07	**1.24**	7.26	0.13	**1.80**	13.22	0.19	**1.45**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
bromide (0.1%)	216	0.00	0.00		6.33	0.03	**0.40**	7.52	0.11	**1.40**	13.84	0.13	**0.94**
	219	0.00	0.00		5.86	0.04	**0.60**	5.10	1.26	**24.71**	10.96	1.24	**11.31**
Cetylpyridinium-bromide (6%)	129	0.00	0.00		6.81	0.03	**0.37**	7.68	0.27	**3.47**	14.49	0.26	**1.79**
	135	0.00	0.00		6.88	0.03	**0.37**	8.20	0.14	**1.65**	15.08	0.15	**0.97**
	143	0.00	0.00		6.82	0.10	**1.41**	7.42	0.14	**1.82**	14.24	0.14	**0.98**
Cetylpyridinium bromide (10%)	129	0.00	0.00		6.90	0.04	**0.52**	7.76	0.20	**2.52**	14.66	0.22	**1.52**
	135	0.00	0.00		6.89	0.05	**0.69**	8.29	0.32	**3.87**	15.18	0.37	**2.42**
	143	0.00	0.00		6.88	0.04	**0.59**	3.87	0.76	**19.66**	10.75	0.80	**7.45**
Chlorhexidine	115	4.50	0.14	**3.04**	6.05	0.20	**3.34**	0.00	0.00		10.55	0.28	**2.63**
	118	4.62	0.07	**1.42**	5.67	0.10	**1.84**	7.30	0.35	**4.75**	17.59	0.32	**1.79**
	124	4.32	0.26	**6.10**	5.71	0.31	**5.39**	6.43	0.89	**13.84**	16.46	1.45	**8.81**
Cyclohexanol	131	4.19	0.09	**2.04**	6.82	0.06	**0.82**	7.85	0.24	**3.11**	18.86	0.37	**1.95**
	137	4.06	0.10	**2.42**	6.87	0.01	**0.17**	8.13	0.25	**3.02**	19.06	0.19	**1.01**
	144	4.63	0.10	**2.18**	6.87	0.07	**1.03**	7.46	0.70	**9.43**	18.96	0.79	**4.15**
Dibenzoyl-L-tartaric acid	206	4.21	0.10	**2.33**	0.00	0.00		4.39	0.19	**4.39**	8.60	0.15	**1.76**
	214	4.65	0.20	**4.31**	4.95	0.20	**3.99**	5.07	0.46	**9.11**	14.67	0.50	**3.40**
	220	4.76	0.05	**1.09**	5.10	0.01	**0.23**	6.90	0.05	**0.75**	16.76	0.04	**0.24**
Dibenzyl phosphate	116	0.00	0.00		6.97	0.02	**0.25**	8.71	0.07	**0.80**	15.68	0.08	**0.51**
	119	0.00	0.00		6.89	0.03	**0.42**	8.15	0.56	**6.83**	15.04	0.56	**3.72**
	124	0.00	0.00		6.81	0.05	**0.66**	7.96	0.28	**3.50**	14.77	0.32	**2.18**
2,6-Dichlorobenzoyl chloride	128	0.00	0.00		5.01	0.72	**14.30**	4.94	0.25	**5.09**	9.95	0.69	**6.96**
	133	0.00	0.00		6.60	0.03	**0.38**	6.13	0.56	**9.11**	12.73	0.55	**4.29**
	141	0.00	0.00		6.30	0.24	**3.79**	3.23	4.17	**129.01**	9.53	4.21	**44.19**
2,2-Dimethylbutanoic acid	127	0.00	0.00		6.71	0.10	**1.47**	8.34	0.19	**2.25**	15.05	0.28	**1.85**
	133	0.00	0.00		6.95	0.03	**0.36**	8.39	0.15	**1.76**	15.34	0.15	**0.98**
	141	0.00	0.00		6.91	0.04	**0.51**	8.62	0.02	**0.20**	15.53	0.04	**0.24**
2,5-Dimethyl-hexandiol	150	4.39	0.17	**3.85**	6.81	0.10	**1.39**	4.56	0.26	**5.62**	15.77	0.47	**2.95**
	122	4.08	0.32	**7.80**	6.27	0.15	**2.32**	4.68	1.05	**22.45**	15.03	1.26	**8.36**
	126	4.07	0.07	**1.60**	4.58	0.49	**10.75**	6.55	0.15	**2.35**	15.20	0.64	**4.23**
Ethanol	132	0.00	0.00		6.92	0.01	**0.17**	8.01	0.03	**0.37**	14.93	0.03	**0.22**
	140	0.00	0.00		6.85	0.12	**1.69**	8.01	0.17	**2.09**	14.86	0.08	**0.54**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
	145	0.00	0.00		6.88	0.03	**0.37**	8.01	0.37	**4.68**	14.89	0.38	**2.58**
Ethyl acetate	205	4.90	0.02	**0.41**	6.59	0.01	**0.18**	7.88	0.12	**1.54**	19.37	0.11	**0.58**
	209	4.01	0.10	**2.51**	6.82	0.06	**0.82**	8.52	0.10	**1.22**	19.35	0.23	**1.19**
	213	4.08	0.27	**6.65**	6.56	0.05	**0.72**	8.60	0.12	**1.45**	19.25	0.30	**1.57**
2-Ethyl-1-hexanol	131	4.18	0.22	**5.14**	0.00	0.00		6.36	0.56	**8.74**	10.54	0.48	**4.54**
	137	4.04	0.13	**3.10**	6.15	0.07	**1.15**	5.90	0.48	**8.22**	16.09	0.62	**3.87**
	145	3.93	0.09	**2.23**	6.03	0.26	**4.32**	1.54	0.92	**59.64**	11.49	0.73	**6.38**
Ethyl-2-methyl-acetoacetate	128	4.43	0.04	**0.79**	0.00	0.00		6.77	0.23	**3.33**	11.20	0.21	**1.84**
	134	4.48	0.15	**3.29**	6.49	0.25	**3.79**	5.36	0.86	**16.09**	16.33	0.82	**5.05**
	142	4.56	0.18	**4.02**	6.73	0.14	**2.09**	0.00	0.00		11.29	0.06	**0.49**
Ethyltrimethyl acetate	207	0.18	0.20	**115.50**	3.46	0.49	**14.11**	7.18	0.40	**5.56**	10.82	0.91	**8.38**
	211	3.06	0.34	**11.07**	3.94	0.61	**15.34**	7.51	0.47	**6.32**	14.51	1.07	**7.38**
	217	4.13	0.18	**4.47**	4.80	0.96	**20.04**	7.21	0.18	**2.44**	16.14	1.11	**6.91**
Fomesafen	117	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	123	0.00	0.00		0.00	0.00		1.07	0.62	**58.36**	1.07	0.62	**58.36**
	150	0.00	0.00		0.00	0.00		2.56	0.66	**25.82**	2.56	0.66	**25.82**
Glycerol	209	0.00	0.00		5.44	0.16	**2.88**	8.61	0.05	**0.60**	14.05	0.11	**0.78**
	216	0.00	0.00		6.77	0.04	**0.52**	8.78	0.03	**0.39**	15.55	0.07	**0.44**
	220	0.00	0.00		6.22	0.07	**1.18**	8.63	0.03	**0.40**	14.85	0.10	**0.67**
n-Hexanol	127	3.84	0.88	**22.80**	6.56	0.09	**1.44**	7.63	0.30	**3.88**	18.03	1.12	**6.20**
	133	4.39	0.06	**1.37**	6.92	0.02	**0.33**	6.00	0.37	**6.14**	17.31	0.43	**2.47**
	141	4.12	0.21	**5.18**	6.72	0.05	**0.74**	6.51	0.57	**8.76**	17.35	0.69	**3.98**
Imidazole	116	4.79	0.02	**0.48**	6.86	0.04	**0.59**	7.39	0.26	**3.50**	19.04	0.26	**1.35**
	121	4.64	0.11	**2.28**	6.91	0.03	**0.36**	7.73	0.09	**1.12**	19.28	0.18	**0.95**
	125	4.87	0.02	**0.31**	6.93	0.00	**0.00**	8.18	0.33	**4.04**	19.98	0.32	**1.60**
Isobutanol	127	4.42	0.11	**2.50**	6.76	0.05	**0.77**	8.15	0.20	**2.45**	19.33	0.26	**1.35**
	133	4.67	0.07	**1.46**	6.89	0.07	**1.05**	7.93	0.12	**1.53**	19.49	0.12	**0.59**
	141	4.73	0.11	**2.28**	6.92	0.05	**0.74**	7.75	0.32	**4.18**	19.40	0.41	**2.11**
Isopropanol	132	0.00	0.00		6.91	0.04	**0.59**	7.87	0.42	**5.40**	14.78	0.47	**3.15**
	137	0.00	0.00		6.97	0.02	**0.25**	8.05	0.08	**0.94**	15.02	0.06	**0.40**
	152	0.00	0.00		6.88	0.03	**0.37**	7.73	0.20	**2.53**	14.61	0.22	**1.51**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
Methyl acetate	131	4.68	0.05	**1.07**	6.86	0.04	**0.59**	7.92	0.23	**2.96**	19.46	0.18	**0.91**
	137	4.30	0.19	**4.34**	6.97	0.04	**0.52**	8.10	0.36	**4.49**	19.37	0.52	**2.68**
	146	3.62	0.29	**7.93**	6.91	0.03	**0.42**	7.59	0.06	**0.79**	18.12	0.34	**1.89**
Methyl cyanoacetate	128	4.47	0.16	**3.60**	4.54	0.84	**18.57**	7.04	0.45	**6.40**	16.05	1.42	**8.82**
	142	4.82	0.06	**1.33**	6.57	0.08	**1.22**	3.83	1.00	**26.08**	15.23	1.00	**6.59**
	161	4.67	0.21	**4.40**	6.28	0.18	**2.83**	6.70	0.70	**10.50**	17.65	1.08	**6.10**
Methyl cyclopentane	128	3.59	0.75	**20.84**	6.84	0.06	**0.86**	8.16	0.24	**2.92**	18.59	0.56	**3.01**
	134	2.40	2.08	**86.61**	6.87	0.06	**0.88**	8.17	0.03	**0.42**	17.44	2.06	**11.82**
	151	1.45	2.51	**173.21**	6.70	0.17	**2.50**	7.23	0.35	**4.79**	15.38	2.95	**19.17**
Methyl ethyl ketone	205	4.96	0.01	**0.23**	6.68	0.08	**1.13**	8.58	0.03	**0.35**	20.22	0.10	**0.47**
	209	3.87	0.03	**0.75**	6.84	0.03	**0.37**	8.64	0.03	**0.35**	19.34	0.08	**0.42**
	213	0.00	0.00		6.85	0.04	**0.53**	8.64	0.08	**0.92**	15.49	0.12	**0.74**
Methyl isobutyl ketone	207	4.79	0.04	**0.84**	3.65	1.38	**37.72**	6.91	0.68	**9.77**	15.35	2.06	**13.39**
	211	4.86	0.04	**0.83**	6.35	0.09	**1.38**	8.48	0.02	**0.20**	19.68	0.09	**0.44**
	217	3.88	0.38	**9.81**	5.93	0.14	**2.41**	8.40	0.10	**1.24**	18.22	0.53	**2.92**
n-Octanol	205	4.68	0.14	**2.97**	5.26	0.27	**5.14**	7.69	0.35	**4.56**	17.63	0.74	**4.20**
	209	4.68	0.07	**1.40**	4.33	0.21	**4.88**	7.28	0.43	**5.85**	16.29	0.37	**2.28**
	213	4.02	0.33	**8.28**	5.64	0.37	**6.65**	6.53	0.06	**0.98**	16.18	0.02	**0.13**
Parafluoroaniline	131	2.15	1.86	**86.67**	6.85	0.01	**0.17**	8.21	0.30	**3.68**	17.21	1.61	**9.36**
	137	0.00	0.00		6.92	0.01	**0.17**	8.40	0.05	**0.62**	15.32	0.06	**0.38**
	145	0.00	0.00		6.92	0.01	**0.17**	7.04	0.65	**9.18**	13.96	0.66	**4.70**
PEG 400	210	0.00	0.00		6.22	0.83	**13.27**	7.83	1.09	**13.94**	14.05	1.92	**13.64**
	216	0.00	0.00		6.70	0.06	**0.96**	8.30	0.06	**0.75**	15.00	0.13	**0.84**
	219	0.00	0.00		6.41	0.29	**4.50**	8.58	0.14	**1.60**	14.99	0.42	**2.78**
Potassium cyanate	117	0.00	0.00		6.77	0.06	**0.95**	6.19	0.27	**4.37**	12.96	0.22	**1.71**
	122	0.00	0.00		6.86	0.02	**0.29**	8.22	0.12	**1.46**	15.08	0.10	**0.66**
	150	0.00	0.00		6.66	0.08	**1.20**	8.12	0.25	**3.10**	14.78	0.27	**1.79**
Pyridine	132	3.29	2.85	**86.60**	6.94	0.01	**0.17**	8.56	0.07	**0.81**	18.79	2.79	**14.84**
	140	0.00	0.00		6.91	0.04	**0.59**	8.10	0.08	**0.98**	15.01	0.08	**0.51**
	145	4.70	0.12	**2.49**	6.88	0.03	**0.37**	7.97	0.17	**2.07**	19.55	0.24	**1.22**
Promethazine	206	0.00	0.00		0.00	0.00		4.87	0.74	**15.12**	4.87	0.74	**15.12**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
	214	0.00	0.00		2.32	1.27	**54.85**	3.92	0.42	**10.72**	6.24	0.92	**14.72**
	220	0.00	0.00		1.27	1.13	**88.73**	6.42	0.57	**8.95**	7.69	1.16	**15.07**
Quinacrine	206	1.41	1.20	**84.83**	0.00	0.00		5.22	1.80	**34.49**	6.63	2.50	**37.71**
	214	1.46	0.23	**15.68**	0.00	0.00		5.96	0.14	**2.38**	7.42	0.35	**4.69**
	220	0.00	0.00		1.97	0.31	**15.76**	5.84	0.06	**1.07**	7.81	0.35	**4.52**
Sodium hydroxide (1%)	127	4.94	0.04	**0.73**	6.89	0.05	**0.69**	7.32	0.21	**2.87**	19.15	0.15	**0.80**
	132	4.94	0.01	**0.23**	6.94	0.01	**0.17**	7.10	0.41	**5.77**	18.99	0.40	**2.11**
	141	4.88	0.02	**0.31**	6.95	0.03	**0.42**	7.07	0.41	**5.76**	18.90	0.45	**2.36**
Sodium hydroxide (10%)	127	4.99	0.01	**0.23**	6.91	0.00	**0.00**	8.59	0.14	**1.65**	20.49	0.13	**0.64**
	132	4.99	0.01	**0.23**	7.00	0.00	**0.00**	8.65	0.09	**1.06**	20.64	0.08	**0.39**
	140	4.89	0.08	**1.54**	6.98	0.03	**0.36**	8.68	0.24	**2.79**	20.54	0.17	**0.81**
Sodium lauryl sulfate (3%)	130	0.00	0.00		6.71	0.18	**2.65**	5.77	0.82	**14.15**	12.48	0.78	**6.25**
	136	0.00	0.00		6.84	0.03	**0.42**	7.31	0.53	**7.18**	14.15	0.50	**3.54**
	143	0.00	0.00		6.81	0.11	**1.54**	3.70	1.07	**28.83**	10.51	1.17	**11.15**
Sodium lauryl sulfate (15%)	205	0.00	0.00		6.92	0.01	**0.17**	8.47	0.09	**1.08**	15.39	0.08	**0.53**
	210	0.00	0.00		6.88	0.04	**0.51**	8.01	0.32	**3.96**	14.89	0.33	**2.21**
	213	0.00	0.00		6.90	0.05	**0.69**	7.97	0.11	**1.43**	14.87	0.16	**1.08**
Sodium oxalate	116	3.87	0.24	**6.20**	6.45	0.12	**1.80**	3.07	1.07	**34.99**	13.39	1.28	**9.55**
	120	0.00	0.00		6.78	0.11	**1.62**	7.93	0.48	**6.01**	14.71	0.43	**2.92**
	125	0.00	0.00		6.77	0.04	**0.52**	7.74	0.36	**4.65**	14.51	0.34	**2.35**
Sodium perborate, $4H_2O$	117	0.00	0.00		6.62	0.08	**1.22**	4.66	0.59	**12.59**	11.28	0.61	**5.41**
	121	0.00	0.00		6.76	0.08	**1.12**	6.71	0.31	**4.59**	13.47	0.24	**1.79**
	125	0.00	0.00		6.76	0.05	**0.70**	8.05	0.19	**2.40**	14.81	0.23	**1.56**
tetra-Aminopyrimidine sulfate	116	4.40	0.59	**13.33**	0.00	0.00		0.00	0.00		4.40	0.59	**13.33**
	120	4.07	0.43	**10.50**	0.00	0.00		0.00	0.00		4.07	0.43	**10.50**
	125	4.52	0.11	**2.48**	0.00	0.00		0.00	0.00		4.52	0.11	**2.48**
Thiourea	149	4.40	0.06	**1.42**	6.84	0.08	**1.18**	4.92	1.12	**22.81**	16.16	1.10	**6.80**
	121	4.00	0.06	**1.56**	6.90	0.02	**0.25**	7.56	0.36	**4.83**	18.46	0.34	**1.85**
	125	4.15	0.10	**2.52**	6.91	0.03	**0.42**	8.00	0.23	**2.84**	19.06	0.34	**1.76**
Toluene	207	0.00	0.00		6.70	0.04	**0.52**	8.46	0.05	**0.61**	15.16	0.06	**0.40**
	211	0.00	0.00		6.83	0.10	**1.44**	8.31	0.13	**1.57**	15.14	0.23	**1.51**

Intralaboratory Repeatability Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Substance	Test #	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
		Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs	Mean for 3 Eggs	SD for 3 Eggs	%CV for 3 Eggs
	217	4.01	0.63	**15.67**	6.87	0.04	**0.52**	7.08	0.34	**4.81**	17.96	0.29	**1.61**
Trichloroacetic acid (3%)	209	0.00	0.00		6.91	0.03	**0.36**	8.67	0.08	**0.92**	15.58	0.07	**0.42**
	216	0.00	0.00		6.98	0.03	**0.36**	8.89	0.06	**0.70**	15.87	0.09	**0.55**
	217	0.00	0.00		6.94	0.02	**0.33**	8.78	0.05	**0.52**	15.72	0.07	**0.43**
Trichloroacetic acid (30%)	127	0.00	0.00		6.88	0.03	**0.37**	8.71	0.06	**0.72**	15.59	0.05	**0.29**
	133	0.00	0.00		6.91	0.05	**0.68**	8.89	0.06	**0.70**	15.80	0.11	**0.68**
	141	0.00	0.00		6.91	0.00	**0.00**	8.81	0.03	**0.39**	15.72	0.03	**0.22**
Triton X-100 (10%)	129	4.55	0.07	**1.50**	6.78	0.01	**0.17**	1.98	1.02	**51.31**	13.31	0.99	**7.42**
	135	3.71	0.55	**14.73**	6.90	0.02	**0.25**	3.65	1.15	**31.54**	14.26	1.26	**8.81**
	143	4.07	0.30	**7.30**	6.74	0.11	**1.59**	2.80	1.54	**54.95**	13.61	1.17	**8.62**
Triton X-100 (5%)	130	3.99	0.30	**7.53**	6.39	0.06	**1.01**	0.00	0.00		10.38	0.24	**2.31**
	143	4.27	0.13	**3.11**	6.67	0.06	**0.96**	0.91	0.80	**87.86**	11.86	0.82	**6.92**
	152	3.85	0.31	**8.00**	6.74	0.04	**0.60**	0.00	0.00		10.59	0.35	**3.27**
Maneb[1]	117	0.00	0.00		5.09	0.29	**5.72**	0.00	0.00		5.09	0.29	**5.72**
	123	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	126	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
	150	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
1-Napthalene acetic acid[1]	115	1.85	1.34	**72.38**	0.00	0.00		0.92	1.29	**140.68**	2.77	2.52	**90.92**
	118	2.19	0.38	**17.19**	4.00	0.44	**11.11**	3.90	1.04	**26.55**	10.09	1.41	**14.02**
	124	0.67	1.15	**173.21**	3.12	1.12	**35.78**	3.69	0.65	**17.64**	7.48	1.99	**26.62**
	149	2.84	0.60	**21.03**	0.00	0.00		0.00	0.00		2.84	0.60	**21.03**
1-Napthalene acetic acid, sodium salt[1]	115	0.00	0.00		6.73	0.07	**1.10**	7.65	0.45	**5.92**	14.38	0.51	**3.51**
	124	0.00	0.00		6.92	0.02	**0.33**	8.44	0.14	**1.68**	15.36	0.15	**0.98**
	149	0.76	1.31	**173.21**	6.84	0.03	**0.37**	7.93	0.38	**4.76**	15.52	1.43	**9.20**
Tween 20[1]	130	0.00	0.00		6.42	0.16	**2.54**	7.05	0.89	**12.69**	13.47	1.04	**7.73**
	136	0.00	0.00		6.15	0.62	**10.03**	6.75	1.16	**17.17**	12.90	1.77	**13.75**
	144	0.00	0.00		6.88	0.04	**0.51**	8.89	0.06	**0.70**	15.77	0.10	**0.62**
	210	0.00	0.00		6.51	0.34	**5.23**	7.83	0.29	**3.69**	14.34	0.61	**4.26**
	219	1.97	0.33	**16.78**	5.95	0.63	**10.54**	8.33	0.12	**1.46**	16.25	0.46	**2.83**

Abbreviations: %CV = percent coefficient of variation; SD = standard deviation.
[1]Data not originally presented in Gilleron et al. (1997).

Appendix E5

Intralaboratory Reproducibility Results (Expressed as %CV) for Data of Gilleron et al. (1996)

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Intralaboratory Reproducibility Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Chemical	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.
1,2,3-Tricholorpropane	2.50	1.72	68.87	1.55	2.03	130.62	3.80	2.52	66.20	7.85	1.74	22.19
1,2,4-Trimethylbenzene	0.33	0.31	94.63	1.63	2.83	173.21	2.46	1.61	65.17	4.42	2.91	65.81
1-Nitropropane	0.58	0.67	115.89	0.52	0.89	173.21	1.72	1.49	86.69	2.81	2.70	95.85
1-Phenyl-3-pyrazolidone	0.00	0.00		0.00	0.00		0.46	0.41	89.00	0.46	0.41	89.00
2,4-Dicholor-5-sulfamolyl-benzoic acid	3.37	1.63	48.34	0.00	0.00		0.40	0.70	173.21	3.77	2.21	58.68
2,4-Pentanedione	4.32	0.13	2.92	0.00	0.00		4.48	2.86	63.70	8.80	2.98	33.85
2-Aminophenol	0.00	0.00		0.00	0.00		0.84	0.74	88.82	0.84	0.74	88.82
2-Ethoxyethanol	0.89	0.91	102.38	2.02	3.14	155.52	7.55	1.22	16.17	10.46	2.74	26.23
3-Glycidopropyl trimethoxysilane	3.72	0.15	4.17	0.00	0.00		0.60	1.03	173.21	4.31	0.96	22.34
Allyl alcohol	0.21	0.36	173.21	3.85	2.44	63.34	8.37	0.41	4.84	12.42	2.26	18.21
Anthracene	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Butyrolactone	4.88	0.14	2.86	1.52	2.63	173.21	7.47	0.69	9.25	13.86	1.80	12.98
Cyclohexanone	4.54	0.17	3.84	4.02	3.53	87.78	5.90	3.21	54.40	14.47	3.79	26.23
Deooxycholic acid, sodium salt	1.08	0.99	92.34	5.84	0.27	4.64	2.78	4.82	173.21	9.70	5.81	59.92
Diacetone alcohol	4.51	0.62	13.84	3.89	3.38	86.87	6.65	1.43	21.49	15.05	2.74	18.18
Dibenzoyl-L-tartaric acid	3.64	1.96	53.75	0.53	0.92	173.21	0.00	0.00		4.17	2.53	60.52
Dimethyl biguanidine	0.00	0.00		3.49	3.26	93.37	4.94	4.33	87.61	8.44	2.18	25.90
Dimethyl sulfoxide	0.13	0.23	173.21	4.18	3.62	86.65	6.95	1.57	22.53	11.26	3.74	33.27
DL-Glutamic acid	0.68	1.17	173.21	0.00	0.00		0.00	0.00		0.68	1.17	173.21
Ethanol	0.00	0.00		4.02	3.49	86.81	7.30	1.44	19.73	11.32	2.82	24.92
Ethylenediaminetetraacetic acid dipotassium	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Furan	0.31	0.53	173.21	2.41	2.39	99.17	2.80	2.05	73.08	5.51	1.02	18.44
Gluconolactone	0.00	0.00		1.83	1.72	93.82	2.72	4.72	173.21	4.55	3.20	70.34
Hexadecyltrimethylammonium bromide	2.47	2.31	93.82	5.13	1.08	21.06	3.24	3.91	120.45	10.84	4.82	44.46
Hexane	0.41	0.72	173.21	0.94	1.63	173.21	1.73	2.52	145.61	3.08	2.65	86.07

Intralaboratory Reproducibility Results for HET-CAM IS(B) Data of Gilleron et al. (1996)

Chemical	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.
Iminodibenzyl	0.00	0.00		0.00	0.00		0.03	0.05	173.21	0.03	0.05	173.21
Magnesium carobonate	0.00	0.00		0.00	0.00		1.43	1.86	129.93	1.43	1.86	129.93
Methyl isobutyl ketone	3.11	0.90	28.98	3.00	3.34	111.51	4.38	3.84	87.64	10.49	1.50	14.33
MYRJ 45	0.00	0.00		0.00	0.00		0.00	0.00		0.00	0.00	
Octanol	2.98	0.85	28.36	3.69	2.12	57.27	3.17	1.19	37.48	9.84	1.67	17.01
Polyoxythethylene 23 lauryl ether	1.51	2.61	173.21	0.00	0.00		0.00	0.00		1.51	2.61	173.21
Propyl-4-hydroxybenzoate	1.67	1.00	60.02	0.00	0.00		0.21	0.19	91.97	1.88	1.06	56.26
Pyridine	3.99	0.89	22.35	4.54	3.94	86.62	7.24	1.47	20.31	15.77	3.61	22.90
Quinacrine	3.18	2.69	84.83	1.24	2.15	173.21	2.08	2.74	131.92	6.50	2.19	33.70
Tetraaminopyrimidine sulfate	0.53	0.92	173.21	0.00	0.00		0.00	0.00		0.53	0.92	173.21
Thiourea	3.91	0.10	2.59	6.71	0.10	1.55	2.49	4.32	173.21	13.11	4.39	33.49
Triton X-155	1.01	1.53	152.23	2.57	2.39	93.09	0.34	0.59	173.21	3.92	2.34	59.77
2-Methoxyethanol[1]	0.00	0.00		5.61	0.45	7.95	7.62	1.32	17.35	13.22	1.12	8.43
Benzethonium chloride[1]	2.28	2.63	115.61	4.79	3.21	67.17	5.49	3.50	63.81	12.55	4.55	36.23
Ethylacetoacetate[1]	3.71	0.47	12.74	2.01	2.34	116.49	2.85	2.59	90.61	8.57	4.59	53.62
Imidazole[1]	4.75	0.19	3.91	6.26	0.98	15.71	7.48	1.21	16.23	18.49	1.23	6.66
Laurylsulfobetaine[1]	0.07	0.13	173.21	6.23	0.56	9.07	2.22	1.97	88.59	8.53	1.50	17.60
Methanol[1]	0.00	0.00		4.33	3.24	74.82	7.68	1.27	16.57	12.01	2.99	24.87
N-Laurylsarcosine, sodium salt[1]	1.76	1.33	75.79	6.53	0.30	4.66	3.54	3.82	107.96	11.82	4.03	34.05
Promethazine hydrochloride[1]	0.65	1.29	200.00	5.03	3.35	66.67	8.44	0.13	1.52	14.11	1.97	13.97
Triethanolamine[1]	0.00	0.00		5.43	1.92	35.28	6.69	0.94	14.01	12.12	1.18	9.71

Abbreviations: %CV = percent coefficient of variation; Exp. = experiment; SD = standard deviation.
[1]Data not originally presented in Gilleron et al. (1996).

Appendix E6

Intralaboratory Reproducibility Results (Expressed as %CV) for Data of Gilleron et al. (1997)

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Intralaboratory Reproducibility Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Chemical	GHS Cat. 1	EPA Cat. I	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
			Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.
2,2-Dimethy-butanoic acid		X	0.00	0.00		6.86	0.13	1.90	8.45	0.15	1.77	15.31	0.24	1.59
2,5-Dimethyl-hexandiol	X	X	4.18	0.19	4.45	5.89	1.17	19.79	5.26	1.12	21.20	15.33	0.39	2.52
2,6-Dichloro-benzoyl chloride			0.00	0.00		5.97	0.85	14.20	4.77	1.46	30.58	10.74	1.74	16.22
2-Ethyl-1-hexanol			4.05	0.13	3.18	4.06	3.51	86.62	4.60	2.66	57.83	12.71	2.96	23.33
4-Carboxybenz-aldehyde			2.17	1.95	90.08	0.00	0.00		1.78	3.08	173.21	3.95	4.69	118.75
Acetone			0.00	0.00		6.94	0.05	0.65	8.38	0.34	4.03	15.32	0.32	2.12
Ammonium nitrate			1.03	0.65	62.49	6.83	0.06	0.87	7.48	1.04	13.88	15.34	1.24	8.07
Benzalkonium chloride (1%)	X	X	0.00	0.00		6.91	0.03	0.46	8.24	0.25	3.04	15.15	0.23	1.52
Benzalkonium chloride (10%)	X	X	0.00	0.00		6.91	0.02	0.24	8.14	0.28	3.46	15.05	0.28	1.83
Benzalkonium chloride (5%)	X	X	0.00	0.00		6.93	0.01	0.15	7.88	0.53	6.67	14.80	0.53	3.55
Captan 90 concentrate	X	X	0.00	0.00		6.83	0.03	0.41	8.24	0.29	3.58	15.07	0.27	1.80
Cetylpyridinium bromide (0.1%)			0.00	0.00		6.05	0.25	4.05	6.63	1.33	20.03	12.67	1.51	11.95
Cetylpyridinium bromide (10%)	X	X	0.00	0.00		6.89	0.01	0.12	6.64	2.41	36.35	13.53	2.42	17.89
Cetylpyridinium bromide (6%)	X		0.00	0.00		6.84	0.04	0.55	7.77	0.40	5.11	14.61	0.43	2.95
Chlorhexidine	X		4.48	0.15	3.41	5.81	0.21	3.59	4.58	3.99	87.12	14.86	3.78	25.44
Cyclohexanol	X	X	4.29	0.30	7.03	6.85	0.03	0.42	7.81	0.34	4.31	18.96	0.10	0.53
Dibenzoyl-L-tartaric acid	X		4.54	0.29	6.36	3.35	2.90	86.63	5.45	1.30	23.80	13.34	4.24	31.74
Dibenzyl phosphate			0.00	0.00		6.89	0.08	1.14	8.27	0.39	4.71	15.17	0.47	3.07
Ethanol			0.00	0.00		6.89	0.04	0.51	8.01	0.00	0.00	14.90	0.04	0.24

Intralaboratory Reproducibility Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Chemical	GHS Cat. 1	EPA Cat. I	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
			Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.
Ethyl acetate			4.33	0.49	11.38	6.66	0.14	2.13	8.33	0.39	4.74	19.32	0.07	0.34
Ethyl-2-methyl-acetoacetate			4.49	0.07	1.46	4.40	3.82	86.65	4.04	3.57	88.34	12.94	2.94	22.68
Ethytrimethyl acetate			2.45	2.04	83.27	4.07	0.68	16.68	7.30	0.18	2.50	13.82	2.73	19.72
Fomesafen			0.00	0.00		0.00	0.00		1.21	1.29	106.26	1.21	1.29	106.26
Gamma-butyro-lactone			4.93	0.01	0.20	6.95	0.01	0.14	7.52	0.83	11.00	19.39	0.83	4.29
Glycerol			0.00	0.00		6.14	0.67	10.93	8.67	0.09	1.07	14.82	0.75	5.09
Imidazole			4.77	0.12	2.43	6.90	0.04	0.54	7.77	0.40	5.10	19.43	0.49	2.51
Isobutanol	X	X	4.61	0.17	3.60	6.86	0.09	1.26	7.94	0.20	2.52	19.41	0.08	0.43
Isopropanol			0.00	0.00		6.92	0.04	0.65	7.88	0.16	2.03	14.80	0.20	1.38
L-Aspartic Acid			0.00	0.00		0.43	0.74	173.21	0.63	0.56	89.05	1.06	1.20	113.49
Methyl acetate			4.20	0.54	12.83	6.91	0.06	0.82	7.87	0.26	3.29	18.98	0.75	3.94
Methyl cyanoacetate			4.65	0.18	3.84	5.80	1.10	18.97	5.86	1.76	30.11	16.31	1.23	7.56
Methyl cyclopentane			2.48	1.07	43.31	6.80	0.09	1.31	7.85	0.54	6.87	17.14	1.62	9.48
Methyl ethyl ketone			2.94	2.60	88.56	6.79	0.09	1.36	8.62	0.03	0.40	18.35	2.52	13.71
Methyl isobutyl ketone			4.51	0.54	12.07	5.31	1.45	27.39	7.93	0.88	11.15	17.75	2.20	12.42
n-Butyl acetate			4.59	0.30	6.57	4.95	2.06	41.57	7.66	0.28	3.60	17.21	1.84	10.69
n-Hexanol			4.12	0.27	6.64	6.74	0.18	2.68	6.71	0.83	12.42	17.57	0.41	2.31
n-Octanol			4.46	0.38	8.61	5.08	0.67	13.19	7.17	0.59	8.25	16.70	0.81	4.83
Parafluoroaniline			0.72	1.24	173.21	6.90	0.04	0.64	7.88	0.74	9.34	15.50	1.63	10.51
PEG 400			0.00	0.00		6.44	0.24	3.70	8.24	0.38	4.60	14.68	0.54	3.70
Potassium cyanate			0.00	0.00		6.76	0.10	1.51	7.51	1.14	15.24	14.27	1.15	8.05
Promethazine	X	X	0.00	0.00		1.20	1.16	97.13	5.07	1.26	24.89	6.27	1.41	22.50
Pyridine	X	X	2.66	2.41	90.56	6.91	0.03	0.44	8.21	0.31	3.78	17.78	2.43	13.69
Quinacrine	X	X	0.96	0.83	86.65	0.66	1.14	173.21	5.67	0.40	7.00	7.29	0.60	8.24
Sodium hydroxide (1%)			4.92	0.03	0.69	6.93	0.03	0.43	7.16	0.14	1.91	19.01	0.13	0.68

Intralaboratory Reproducibility Results for HET-CAM IS(B) Data of Gilleron et al. (1997)

Chemical	GHS Cat. 1	EPA Cat. I	Hemorrhage			Lysis			Coagulation			Overall *In Vitro* Score		
			Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.	Mean of Exp.	SD of Exp.	%CV of Exp.
Sodium hydroxide (10%)	X	X	4.95	0.06	1.17	6.96	0.05	0.67	8.64	0.05	0.53	20.56	0.08	0.37
Sodium lauryl sulfate (15%)	X	X	0.00	0.00		6.90	0.02	0.29	8.15	0.28	3.41	15.05	0.29	1.96
Sodium lauryl sulfate (3%)			0.00	0.00		6.79	0.07	0.99	5.59	1.81	32.39	12.38	1.83	14.74
Sodium oxalate	X	X	1.29	2.24	173.21	6.67	0.19	2.84	6.25	2.75	44.07	14.20	0.71	5.01
Sodium perborate, $4H_2O$	X	X	0.00	0.00		6.71	0.08	1.15	6.47	1.71	26.38	13.19	1.78	13.49
Tetraamino-pyrimidine sulfate			4.33	0.23	5.40	0.00	0.00		0.00	0.00		4.33	0.23	5.40
Thiourea			4.18	0.20	4.83	6.88	0.04	0.60	6.83	1.67	24.40	17.89	1.53	8.57
Toluene			1.34	2.31	173.21	6.80	0.09	1.28	7.95	0.76	9.52	16.09	1.62	10.07
Trichloroacetic acid (3%)			0.00	0.00		6.94	0.04	0.51	8.78	0.11	1.25	15.72	0.15	0.92
Trichloroacetic acid (30%)	X	X	0.00	0.00		6.90	0.02	0.24	8.80	0.09	1.02	15.71	0.11	0.67
Triton X-100 (10%)	X		4.11	0.42	10.26	6.81	0.08	1.20	2.81	0.84	29.72	13.73	0.48	3.52
Triton X-100 (5%)			4.04	0.22	5.34	6.60	0.19	2.80	0.30	0.53	173.21	10.94	0.80	7.28
1-Napthalene acetic acid[1]	X	X	1.89	0.91	48.25	1.78	2.09	117.21	2.13	1.96	92.30	5.79	3.61	62.36
1-Napthalene acetic acid, sodium salt[1]	X	X	0.25	0.44	173.21	6.83	0.10	1.44	8.01	0.40	5.00	15.09	0.62	4.12
Maneb[1]			0.00	0.00		1.27	2.54	200.00	0.00	0.00		1.27	2.54	200.00
Tween 20[1]			0.39	0.88	223.61	6.38	0.35	5.53	7.77	0.88	11.39	14.55	1.44	9.91

Abbreviations: Cat. = category; %CV = percent coefficient of variation; EPA = U.S. Environmental Protection Agency; Exp. = experiment; GHS = Globally Harmonized System; SD = standard deviation.

[1]Data not originally presented in Gilleron et al. (1997).

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Appendix F

Interlaboratory Reproducibility Data

F1 Individual HET-CAM Test Laboratory Data for CEC (1991) ..F-3

F2 Average HET-CAM Scores and Coefficient of Variations for Substances Evaluated in Hagino et al. (1999) and Ohno et al. (1999) F-13

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Appendix F1

Individual HET-CAM Test Laboratory Data for CEC (1991)

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In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
Acetic acid	64-19-7	2	10%	20.2
Acetic acid	64-19-7	3	10%	13.6
Acetic acid	64-19-7	4	10%	10.2
Brij 35	9002-92-0	1	100%	2.3
Brij 35	9002-92-0	2	100%	4.3
Brij 35	9002-92-0	3	100%	12.9
Brij 35	9002-92-0	4	100%	4.4
Brij 35	9002-92-0	7	100%	4
Butanol	71-36-3	1	100%	11.7
Butanol	71-36-3	2	100%	11.8
Butanol	71-36-3	3	100%	12.6
Butanol	71-36-3	4	100%	11.2
Butanol	71-36-3	7	100%	9.9
Butanol	71-36-3	2	10%	14.2
Butanol	71-36-3	3	10%	4.8
Butanol	71-36-3	4	10%	12.5

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
2-Butoxyethyl acetate	112-07-2	1	100%	4.6
2-Butoxyethyl acetate	112-07-2	2	100%	5.3
2-Butoxyethyl acetate	112-07-2	3	100%	4.7
2-Butoxyethyl acetate	112-07-2	4	100%	4.7
2-Butoxyethyl acetate	112-07-2	7	100%	4.5
2-Butoxyethyl acetate	112-07-2	2	10%	4.1
2-Butoxyethyl acetate	112-07-2	3	10%	0
2-Butoxyethyl acetate	112-07-2	4	10%	3.2
Chloroform	67-66-3	1	100%	12.9
Chloroform	67-66-3	2	100%	15.4
Chloroform	67-66-3	3	100%	15
Chloroform	67-66-3	4	100%	10.4
Chloroform	67-66-3	7	100%	10.3
Chloroform	67-66-3	2	10%	12.8
Chloroform	67-66-3	3	10%	4.4
Chloroform	67-66-3	4	10%	4.4

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
Dimethyl sulfoxide	67-68-5	1	100%	11.7
Dimethyl sulfoxide	67-68-5	2	100%	10.9
Dimethyl sulfoxide	67-68-5	3	100%	11.3
Dimethyl sulfoxide	67-68-5	4	100%	4.1
Dimethyl sulfoxide	67-68-5	7	100%	11.4
Dimethyl sulfoxide	67-68-5	2	10%	4.4
Dimethyl sulfoxide	67-68-5	3	10%	4.1
Dimethyl sulfoxide	67-68-5	4	10%	4.1
Glycerol	56-81-5	1	100%	10.8
Glycerol	56-81-5	2	100%	11.3
Glycerol	56-81-5	3	100%	10.3
Glycerol	56-81-5	4	100%	4.8
Glycerol	56-81-5	7	100%	9.4
Glycerol	56-81-5	2	10%	8.7
Glycerol	56-81-5	3	10%	4.4
Glycerol	56-81-5	4	10%	3.6

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
n-Hexane	110-54-3	1	100%	2.9
n-Hexane	110-54-3	2	100%	5.4
n-Hexane	110-54-3	3	100%	4.2
n-Hexane	110-54-3	4	100%	10.3
n-Hexane	110-54-3	7	100%	2.4
n-Hexane	110-54-3	2	10%	3.7
n-Hexane	110-54-3	3	10%	0
n-Hexane	110-54-3	4	10%	10.1
Mercuric chloride	7546-30-7	1	100%	9.9
Mercuric chloride	7546-30-7	2	100%	13.8
Mercuric chloride	7546-30-7	3	100%	13.1
Mercuric chloride	7546-30-7	4	100%	13
Mercuric chloride	7546-30-7	7	100%	2.8
2-Methoxyethanol	109-86-4	1	100%	9.7
2-Methoxyethanol	109-86-4	2	100%	12.2
2-Methoxyethanol	109-86-4	3	100%	12.1
2-Methoxyethanol	109-86-4	4	100%	8.6

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
2-Methoxyethanol	109-86-4	7	100%	3.1
2-Methoxyethanol	109-86-4	2	10%	7
2-Methoxyethanol	109-86-4	3	10%	0
2-Methoxyethanol	109-86-4	4	10%	3.1
Sodium dodecyl sulfate	151-21-3	1	100%	11.4
Sodium dodecyl sulfate	151-21-3	2	100%	10.3
Sodium dodecyl sulfate	151-21-3	3	100%	13.9
Sodium dodecyl sulfate	151-21-3	4	100%	4.8
Sodium dodecyl sulfate	151-21-3	7	100%	9.7
Sodium dodecyl sulfate	151-21-3	2	10%	18.4
Sodium dodecyl sulfate	151-21-3	3	10%	14.1
Sodium dodecyl sulfate	151-21-3	4	10%	5.1
Toluene	108-88-3	1	100%	8.8
Toluene	108-88-3	2	100%	14.8
Toluene	108-88-3	3	100%	15.2
Toluene	108-88-3	4	100%	11.5
Toluene	108-88-3	7	100%	4.9

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
Triacetin	102-76-1	1	100%	3.6
Triacetin	102-76-1	2	100%	4.3
Triacetin	102-76-1	3	100%	5.5
Triacetin	102-76-1	4	100%	4.4
Triacetin	102-76-1	7	100%	3.1
Triacetin	102-76-1	2	10%	13.6
Triacetin	102-76-1	3	10%	2
Triacetin	102-76-1	4	10%	3.3
Tributyltin chloride	1461-22-9	1	100%	6.7
Tributyltin chloride	1461-22-9	2	100%	8.9
Tributyltin chloride	1461-22-9	3	100%	13.7
Tributyltin chloride	1461-22-9	4	100%	8.8
Tributyltin chloride	1461-22-9	7	100%	6.6
Tributyltin chloride	1461-22-9	2	10%	15.6
Tributyltin chloride	1461-22-9	3	10%	9.6
Tributyltin chloride	1461-22-9	4	10%	11.2

In Vitro Data for Substances in CEC (1991) for %CV Analysis

Substance Name	CASRN	Lab Number[1]	Conc. Tested	IS(B)[2]
Triethanolamine	102-71-6	1	100%	8.6
Triethanolamine	102-71-6	2	100%	10.4
Triethanolamine	102-71-6	3	100%	11.9
Triethanolamine	102-71-6	4	100%	4.2
Triethanolamine	102-71-6	7	100%	7.5
Triethanolamine	102-71-6	2	10%	11.3
Triethanolamine	102-71-6	3	10%	2.8
Triethanolamine	102-71-6	4	10%	1.1

Abbreviations: CASRN = Chemical Abstract Service Registry Number, Conc. = Concentration.

[1] Lab Number Legend: 1 = Instituut voor Hygiene en Epidemiologie, 2 = University of Osnabrueck, 3 = L'Oreal, 4 = Centre International de Toxicologie, 7 = TNO/CIVO Institutes.

[2] IS(B) represents irritation scores that were calculated using a method similar to the one described in Kalweit et al. (1987, 1990)

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Appendix F2

Average HET-CAM Scores and Coefficient of Variations for Substances Evaluated in Hagino et al. (1999) and Ohno et al. (1999)

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Results of HET-CAM Test in Five Laboratories (Hagino et al. 1999 and Ohno et al. 1999)

Substance	Conc. (%)	Laboratory HET-CAM test score (mean IS ± SD)					Mean ± SD	Coefficient of Variation (%)
		A	B	C	D	E		
S1-1	100	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00[1]	1.75 ± 1.50	0.00 ± 0.00	0.35 ± 0.78	224
				(6.50 ± 1.00)				
S1-2	10	0.75 ± 1.50	1.25 ± 2.50	2.75 ± 3.10[1]	2.50 ± 1.00	0.00 ± 0.00	1.45 ± 1.16	80
				(9.25 ± 5.50)				
S1-3	10	1.00 ± 1.41	5.50 ± 4.93	3.00 ± 2.16[1]	9.50 ± 1.91	7.50 ± 2.89	5.30 ± 3.40	64
				(11.00 ± 1.15)				
S1-4	10	4.75 ± 2.36	6.75 ± 2.75	2.25 ± 2.50[1]	10.00 ± 2.83	11.00 ± 1.15	6.95 ± 3.63	52
				(15.75 ± 2.50)				
S1-5	10	11.50 ± 1.00	9.50 ± 1.91	9.50 ± 1.00[1]	12.00 ± 0.00	9.00 ± 2.00	10.30 ± 1.35	13
				(17.25 ± 3.86)				
S1-6	10	11.00 ± 1.15	7.00 ± 2.45	7.50 ± 3.00[1]	12.00 ± 0.00	10.50 ± 1.00	9.60 ± 2.22	23
				(11.75 ± 2.36)				
S1-7	10	12.00 ± 0.00	11.00 ± 1.15	10.50 ± 1.91[1]	11.00 ± 1.15	10.60 ± 3.50	11.02 ± 0.59	5
				(17.00 ± 0.00)				
S1-8	10	10.00 ± 1.63	9.00 ± 2.00	6.25 ± 3.30[1]	6.75 ± 2.99	8.75 ± 2.99	8.15 ± 1.59	19
				(14.00 ± 3.56)				
S1-9	10	12.00 ± 0.00	11.00 ± 2.00	10.50 ± 1.00[1]	10.50 ± 1.00	9.50 ± 1.00	10.70 ± 0.91	8
				(15.75 ± 4.79)				
S1-10	10	14.75 ± 1.50	11.50 ± 2.52	13.25 ± 1.50[1]	15.75 ± 1.50	14.00 ± 1.63	13.85 ± 1.61	12
				(15.50 ± 1.00)				
S2-1	100	3.00 ± 0.00	0.00 ± 0.00	10.50 ± 0.87	5.00 ± 3.46	3.75 ± 2.50	4.45 ± 3.85	87
	10	0.00 ± 0.00	1.50 ± 2.38	9.50 ± 1.66	12.00 ± 0.00	0.00 ± 0.00	4.60 ± 5.72	124
	1	0.00 ± 0.00	1.25 ± 2.50	6.25 ± 1.09	10.00 ± 2.83	0.00 ± 0.00	3.50 ± 4.45	127
	0.1	0.00 ± 0.00	0.00 ± 0.00	3.00 ± 1.41	4.75 ± 1.50	0.00 ± 0.00	1.55 ± 2.21	143
S2-2	100	1.25 ± 2.50	1.25 ± 2.50	6.75 ± 3.42	1.50 ± 1.73	12.00 ± 0.00	4.55 ± 4.78	105
	10	0.00 ± 0.00	0.00 ± 0.00	3.75 ± 2.17	0.00 ± 0.00	1.25 ± 2.50	1.00 ± 1.63	163
	1	0.00 ± 0.00	0.00 ± 0.00	4.25 ± 4.92	0.00 ± 0.00	0.00 ± 0.00	0.85 ± 1.90	224
	0.1	0.00 ± 0.00	0.00 ± 0.00	0.25 ± 0.43	0.00 ± 0.00	0.00 ± 0.00	0.05 ± 0.11	224

Results of HET-CAM Test in Five Laboratories (Hagino et al. 1999 and Ohno et al. 1999)

Substance	Conc. (%)	Laboratory HET-CAM test score (mean IS ± SD)					Mean ± SD	Coefficient of Variation (%)
		A	B	C	D	E		
S2-3	100	1	*	*	*	*	*	-
	10	*	*	*	*	*	*	-
	1	*	*	*	*	*	*	-
	0.1	0.00 ± 0.00	0.00 ± 0.00	8.50 ± 0.87	4.50 ± 1.73	0.00 ± 0.00	2.60 ± 3.83	147
S2-4	100	3.00 ± 1.00	2.50 ± 2.89	2.50 ± 2.50	3.50 ± 2.52	5.75 ± 1.50	3.45 ± 1.35	39
	10	0.00 ± 0.00	0.75 ± 1.50	0.00 ± 0.00	0.00 ± 0.00	3.25 ± 2.36	0.80 ± 1.41	176
	1	0.00 ± 0.00	1.50 ± 1.73	2.75 ± 1.79	2.75 ± 3.77	0.00 ± 0.00	1.40 ± 1.38	98
	0.1	0.00 ± 0.00	0.25 ± 0.50	2.50 ± 2.50	0.00 ± 0.00	0.00 ± 0.00	0.55 ± 1.10	199
S2-5	100	21.00 ± 0.00	12.00 ± 0.00	10.75 ± 2.17	21.00 ± 0.00	12.00 ± 0.00	15.35 ± 5.18	34
	10	12.00 ± 0.00	12.00 ± 0.00	5.50 ± 5.55	21.00 ± 0.00	12.00 ± 0.00	12.50 ± 5.52	44
	1	0.50 ± 0.58	0.00 ± 0.00	1.50 ± 0.87	12.00 ± 0.00	2.50 ± 2.89	3.30 ± 4.96	150
	0.1	0.00 ± 0.00	1.50 ± 3.00	0.00 ± 0.00	3.50 ± 1.00	0.00 ± 0.00	1.00 ± 1.54	154
S2-6	100	11.50 ± 1.00	2.50 ± 2.89	11.00 ± 1.73	8.00 ± 1.63	8.50 ± 4.04	8.30 ± 3.58	43
	10	NT	NT	NT	NT	NT	NT	-
	1	NT	NT	NT	NT	NT	NT	-
	0.1	NT	NT	NT	NT	NT	NT	-
S2-7	100	0.00 ± 0.00	0.00 ± 0.00	2.25 ± 1.92	0.00 ± 0.00	1.25 ± 2.50	0.70 ± 1.02	146
	10	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.00 ± 1.41	1.25 ± 2.50	0.45 ± 0.62	138
	1	0.00 ± 0.00	0.00 ± 0.00	0.25 ± 0.43	0.50 ± 0.58	0.00 ± 0.00	0.15 ± 0.22	149
	0.1	0.00 ± 0.00	0.25 ± 0.50	1.00 ± 1.73	0.00 ± 0.00	0.00 ± 0.00	0.25 ± 0.43	173
S2-8	100	18.00 ± 1.15	14.00 ± 0.00	14.00 ± 0.00	19.50 ± 1.91	10.25 ± 2.50	15.15 ± 3.66	24
	10	14.25 ± 2.06	12.50 ± 1.00	14.00 ± 0.00	20.00 ± 1.15	9.00 ± 0.00	13.95 ± 3.98	29
	1	12.00 ± 0.00	7.75 ± 1.26	13.50 ± 0.87	15.75 ± 3.77	7.00 ± 0.00	11.20 ± 3.75	33
	0.1	2.00 ± 1.15	0.25 ± 0.50	10.50 ± 0.87	8.00 ± 2.83	0.00 ± 0.00	4.15 ± 4.80	116
S2-9	100	5.50 ± 2.89	0.00 ± 0.00	8.25 ± 2.05	10.00 ± 2.31	9.75 ± 2.06	6.70 ± 4.15	62
	10	NT	NT	NT	NT	NT	NT	-
	1	NT	NT	NT	NT	NT	NT	-
	0.1	NT	NT	NT	NT	NT	NT	-

Results of HET-CAM Test in Five Laboratories (Hagino et al. 1999 and Ohno et al. 1999)

Substance	Conc. (%)	Laboratory HET-CAM test score (mean IS ± SD)					Mean ± SD	Coefficient of Variation (%)
		A	B	C	D	E		
S2-10	100	0.00 ± 0.00	1.75 ± 2.22	2.50 ± 2.50	5.75 ± 2.06	3.75 ± 2.50	2.75 ± 2.16	78
	10	0.00 ± 0.00	0.00 ± 0.00	8.25 ± 2.49	9.50 ± 1.91	1.25 ± 2.50	3.80 ± 4.68	123
	1	0.00 ± 0.00	0.00 ± 0.00	7.00 ± 4.12	5.25 ± 3.30	0.00 ± 0.00	2.45 ± 3.41	139
	0.1	0.00 ± 0.00	0.00 ± 0.00	5.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	1.00 ± 2.24	224
S2-11	100	0.50 ± 0.58	2.00 ± 4.00	0.75 ± 1.30	7.75 ± 2.06	6.75 ± 3.50	3.55 ± 3.44	97
	10	0.00 ± 0.00	1.25 ± 2.50	4.50 ± 3.50	11.00 ± 1.15	1.75 ± 3.50	3.70 ± 4.40	119
	1	0.00 ± 0.00	0.25 ± 0.50	4.50 ± 0.87	0.75 ± 1.50	0.00 ± 0.00	1.10 ± 1.93	175
	0.1	0.00 ± 0.00	1.25 ± 1.89	1.25 ± 2.17	0.00 ± 0.00	1.25 ± 2.50	0.75 ± 0.68	91
S2-12	100	2.00 ± 2.00	3.00 ± 2.16	1.50 ± 2.06	1.50 ± 1.73	0.00 ± 0.00	1.60 ± 1.08	68
	10	NT	NT	NT	NT	NT	NT	-
	1	NT	NT	NT	NT	NT	NT	-
	0.1	NT	NT	NT	NT	NT	NT	-
S2-13	100	19.00 ± 0.00	9.75 ± 3.30	10.00 ± 2.00	21.00 ± 0.00	10.50 ± 1.00	14.05 ± 5.48	39
	10	10.00 ± 0.00	9.25 ± 3.40	10.00 ± 1.41	16.50 ± 5.20	10.25 ± 1.00	11.20 ± 2.99	27
	1	0.00 ± 0.00	2.00 ± 2.45	8.50 ± 0.87	9.50 ± 1.00	3.75 ± 4.79	4.75 ± 4.12	87
	0.1	0.00 ± 0.00	0.00 ± 0.00	7.25 ± 1.30	9.00 ± 1.15	0.00 ± 0.00	3.25 ± 4.49	138
S2-14	100	21.00 ± 0.00	9.50 ± 1.00	11.50 ± 0.87	21.00 ± 0.00	11.50 ± 1.00	14.90 ± 5.63	38
	10	5.00 ± 0.00	2.50 ± 2.89	11.50 ± 0.87	12.00 ± 0.00	0.75 ± 1.50	6.35 ± 5.16	81
	1	0.00 ± 0.00	1.25 ± 2.50	6.25 ± 2.17	6.50 ± 4.04	0.00 ± 0.00	2.80 ± 3.30	118
	0.1	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00	0.25 ± 0.50	0.00 ± 0.00	0.05 ± 0.11	224
S2-15[2]	100	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	-
	10	5.00 ± 0.00	5.00 ± 0.00	11.00 ± 1.00	12.00 ± 0.00	5.75 ± 2.99	7.75 ± 3.46	-
	1	0.00 ± 0.00	0.00 ± 0.00	4.75 ± 2.49	9.00 ± 1.15	0.00 ± 0.00	2.75 ± 4.05	-
	0.1	0.00 ± 0.00	0.00 ± 0.00	0.25 ± 0.43	4.25 ± 2.50	0.00 ± 0.00	0.90 ± 1.88	-
S3-1	100	18.75 ± 3.30	16.00 ± 2.45	11.50 ± 1.00	17.00 ± 0.00	10.50 ± 1.73	14.75 ± 3.58	24
	10	0.00 ± 0.00	1.25 ± 2.50	10.50 ± 1.91	1.50 ± 1.73	1.25 ± 2.50	2.90 ± 4.29	148
	1	0.00 ± 0.00	1.50 ± 2.38	10.50 ± 1.91	2.50 ± 1.00	2.50 ± 2.89	3.40 ± 4.10	121
S3-2	100	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	0
	10	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	0
	1	10.50 ± 1.00	11.00 ± 1.15	12.00 ± 0.00	12.00 ± 0.00	5.00 ± 0.00	10.10 ± 2.92	29

Results of HET-CAM Test in Five Laboratories (Hagino et al. 1999 and Ohno et al. 1999)

Substance	Conc. (%)	Laboratory HET-CAM test score (mean IS ± SD)					Mean ± SD	Coefficient of Variation (%)
		A	B	C	D	E		
S3-3	100	5.00 ± 0.00	6.75 ± 3.50	11.50 ± 1.00	12.00 ± 0.00	6.75 ± 3.50	8.40 ± 3.15	37
	10	1.50 ± 2.38	3.75 ± 4.79	11.00 ± 1.15	6.00 ± 1.63	2.50 ± 2.89	4.95 ± 3.78	76
	1	0.00 ± 0.00	2.50 ± 2.89	9.75 ± 3.30	3.50 ± 2.08	1.25 ± 2.50	3.40 ± 3.79	111
S3-4	100	15.75 ± 3.50	14.00 ± 0.00	16.50 ± 3.32	13.50 ± 1.00	12.17 ± 5.15	14.38 ± 1.74	12
	10	16.75 ± 2.06	13.00 ± 2.00	15.75 ± 3.50	13.50 ± 1.00	9.00 ± 0.00	13.60 ± 3.00	22
	1	13.00 ± 1.15	3.25 ± 2.36	15.00 ± 4.69	9.00 ± 0.00	7.25 ± 2.06	9.50 ± 4.66	49
S3-5	100	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	0
	10	8.25 ± 2.36	8.50 ± 4.04	9.00 ± 1.15	12.00 ± 0.00	5.00 ± 0.00	8.55 ± 2.49	29
	1	2.75 ± 2.06	1.25 ± 2.50	11.00 ± 1.15	2.25 ± 2.22	3.75 ± 2.50	4.20 ± 3.91	93
S3-6	100	21.00 ± 0.00	20.00 ± 1.15	20.00 ± 1.15	18.75 ± 4.50	15.00 ± 1.15	18.95 ± 2.35	12
	10	20.00 ± 1.15	13.25 ± 2.50	12.00 ± 0.00	12.00 ± 0.00	19.33 ± 0.82	15.32 ± 4.01	26
	1	10.50 ± 1.00	10.50 ± 1.00	12.00 ± 0.00	6.75 ± 2.99	15.75 ± 2.22	11.10 ± 3.24	29
S3-7	100	19.00 ± 1.63	16.25 ± 1.50	19.50 ± 1.91	10.25 ± 2.50	9.00 ± 0.00	14.80 ± 4.90	33
	10	19.00 ± 1.63	13.25 ± 2.22	18.50 ± 1.91	11.00 ± 2.45	9.00 ± 0.00	14.15 ± 4.46	32
	1	14.00 ± 0.00	13.50 ± 1.00	16.50 ± 1.00	9.75 ± 1.50	9.00 ± 0.00	12.55 ± 3.12	25
S3-8	100	16.50 ± 2.89	15.00 ± 1.41	14.00 ± 4.97	14.00 ± 0.00	10.75 ± 3.50	14.05 ± 2.11	15
	10	16.50 ± 2.89	16.00 ± 3.92	17.25 ± 6.24	19.50 ± 1.91	17.50 ± 4.04	17.35 ± 1.34	8
	1	10.50 ± 4.93	18.75 ± 3.30	10.50 ± 1.91	14.50 ± 0.58	12.75 ± 2.50	13.40 ± 3.43	26
S3-9	100	12.00 ± 0.00	20.00 ± 1.15	12.00 ± 0.00	12.00 ± 0.00	8.75 ± 2.50	12.95 ± 4.18	32
	10	8.25 ± 2.87	10.50 ± 1.91	12.00 ± 0.00	12.00 ± 0.00	5.75 ± 1.50	9.70 ± 2.69	28
	1	0.75 ± 1.50	2.00 ± 2.45	12.00 ± 0.00	6.00 ± 2.31	0.00 ± 0.00	4.15 ± 4.96	120
S3-10	100	19.50 ± 1.00	14.00 ± 0.00	15.50 ± 1.73	9.75 ± 1.50	9.00 ± 0.00	13.55 ± 4.32	32
	10	19.00 ± 1.63	13.50 ± 1.00	16.00 ± 2.45	11.75 ± 4.86	9.00 ± 0.00	13.85 ± 3.85	28
	1	6.25 ± 3.95	2.50 ± 2.89	10.50 ± 1.00	3.00 ± 0.00	1.25 ± 2.50	4.70 ± 3.73	79
S3-11	100	19.00 ± 1.63	17.25 ± 2.36	17.00 ± 3.56	16.50 ± 2.89	12.33 ± 2.58	16.42 ± 2.47	15
	10	19.00 ± 0.00	15.25 ± 2.36	14.75 ± 1.50	12.25 ± 2.36	9.00 ± 0.00	14.05 ± 3.71	26
	1	15.00 ± 2.45	19.00 ± 1.63	16.50 ± 3.42	11.75 ± 2.63	8.50 ± 1.22	14.15 ± 4.11	29
S3-12	100	21.00 ± 0.00	6.25 ± 2.50	16.00 ± 1.15	15.25 ± 2.50	11.50 ± 2.89	14.00 ± 5.50	39
	10	20.50 ± 1.00	14.25 ± 2.06	19.50 ± 1.91	18.50 ± 1.91	10.25 ± 2.50	16.60 ± 4.27	26
	1	4.50 ± 1.00	2.50 ± 5.00	9.00 ± 1.15	5.00 ± 4.24	9.00 ± 0.00	6.00 ± 2.89	48

Results of HET-CAM Test in Five Laboratories (Hagino et al. 1999 and Ohno et al. 1999)

Substance	Conc. (%)	Laboratory HET-CAM test score (mean IS ± SD)					Mean ± SD	Coefficient of Variation (%)
		A	B	C	D	E		
S3-13	100	21.00 ± 0.00	16.75 ± 3.69	12.00 ± 0.00	17.00 ± 3.56	14.67 ± 4.59	16.28 ± 3.31	20
	10	19.50 ± 1.00	20.00 ± 1.15	17.75 ± 3.95	12.25 ± 2.36	12.75 ± 2.50	16.45 ± 3.71	23
	1	12.75 ± 2.50	2.00 ± 2.45	18.50 ± 1.00	3.50 ± 1.00	10.25 ± 2.50	9.40 ± 6.79	72
S3-14	100	12.00 ± 0.00	9.25 ± 3.40	12.00 ± 0.00	12.00 ± 0.00	12.00 ± 0.00	11.45 ± 1.23	11
	10	10.00 ± 0.00	10.00 ± 1.63	10.25 ± 3.50	12.00 ± 0.00	5.00 ± 0.00	9.45 ± 2.62	28
	1	8.25 ± 2.36	7.75 ± 2.06	6.75 ± 3.50	12.00 ± 0.00	5.00 ± 0.00	7.95 ± 2.58	32
Correlation coefficient		0.963	0.928	0.839	0.864	0.882		
Rank correlation coefficient		0.95	0.916	0.856	0.879	0.863		

Abbreviations: Conc. = Concentration, IS = Irritation Score, NT = Not Tested, SD = standard deviation.

NT: Test was not performed, because chemicals could not be dissolved or suspended at 10% concentration.

*: test was not performed because observation was disturbed by stain of CAM after application of chemicals.

[1]: results of laboratory C were of retest after breaking sample codes, because of higher scores indicated in parenthesis. They were previously reported by Hagino et al. (1995) in detail.

[2]Data were removed due to lack of chemical stability

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Appendix G

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

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Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	BCOPP9	60	a	1.000				
A	BCOPP10	60	b	0.777	1.000			
A	BCOPP11	60	c	0.886	0.862	1.000		
A	BCOPP12	60	d	0.797	0.683	0.859	1.000	
A	BCOPP13	60	e	0.856	0.788	0.906	0.892	1.000
A	BCOPO9	60	a	1.000				
A	BCOPO10	60	b	0.924	1.000			
A	BCOPO11	60	c	0.934	0.898	1.000		
A	BCOPO12	60	d	0.946	0.905	0.978	1.000	
A	BCOPO13	60	e	0.970	0.936	0.953	0.955	1.000
A	BCOPI9	60	a	1.000				
A	BCOPI10	60	b	0.894	1.000			
A	BCOPI11	60	c	0.922	0.896	1.000		
A	BCOPI12	60	d	0.924	0.867	0.957	1.000	
A	BCOPI13	60	e	0.955	0.901	0.947	0.958	1.000
A	BCOPI9b	60	a	1.000				
A	BCOPI10b	60	b	0.898	1.000			
A	BCOPI11b	60	c	0.913	0.913	1.000		
A	BCOPI12b	60	d	0.908	0.848	0.916	1.000	
A	BCOPP13b	60	e	0.939	0.885	0.938	0.938	1.000
A	HETQ14	49	a	1.000				
A	HETQ15	40	b	0.790	1.000			
A	HETQ16	47	c	0.473	0.521	1.000		
A	HETQ17	41	d	0.550	0.734	0.664	1.000	
A	HETS14	11	a	1.000				
A	HETS15	13	b	0.174	1.000			
A	HETS16	13	c	-0.171	-0.171	1.000		
A	HETS17	17	d	-0.103	0.808	0.031	1.000	
A	HETQ14b	49	a	1.000				
A	HETQ15b	40	b	0.627	1.000			
A	HETQ16b	47	c	0.709	0.638	1.000		
A	HETQ17b	41	d	0.449	0.814	0.528	1.000	
A	HETS14b	11	a	1.000				
A	HETS15b	13	b	*	1.000			
A	HETS16b	13	c	-0.043	-0.316	1.000		
A	HETS17b	41	d	*	*	*	*	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
A	ICES 22	60	a	1.000				
A	ICES 27	60	b	0.721	1.000			
A	ICES 24	59	c	0.750	0.715	1.000		
A	ICES 25	58	d	0.627	0.668	0.734	1.000	
A	ICEO 22	60	a	1.000				
A	ICEO 27	60	b	0.700	1.000			
A	ICEO 24	60	c	0.759	0.716	1.000		
A	ICEO 25	60	d	0.752	0.679	0.732	1.000	
A	ICEF 22	60	a	1.000				
A	ICEF 27	60	b	0.693	1.000			
A	ICEF 24	59	c	0.768	0.525	1.000		
A	ICEF 25	60	d	0.719	0.654	0.690	1.000	
A	ICEC 22	60	a	1.000				
A	ICEC 27	60	b	0.829	1.000			
A	ICEC 24	60	c	0.849	0.759	1.000		
A	ICEC 25	60	d	0.844	0.801	0.853	1.000	
A	IREA 26	60	a	1.000				
A	IREA 23	60	b	0.441	1.000			
A	IREA 28	60	c	0.585	0.695	1.000		
A	IREA 29	60	d	0.619	0.587	0.677	1.000	
A	IREB 26	60	a	1.000				
A	IREB 23	60	b	0.728	1.000			
A	IREB 28	60	c	0.714	0.688	1.000		
A	IREB 29	60	d	0.688	0.617	0.808	1.000	
A	IREC 26	58	a	1.000				
A	IREC 23	60	b	0.524	1.000			
A	IREC 28	58	c	0.485	0.414	1.000		
A	IREC 29	60	d	0.625	0.681	0.819	1.000	
A	IRED 26	58	a	1.000				
A	IRED 23	60	b	0.623	1.000			
A	IRED 28	58	c	0.707	0.618	1.000		
A	IRED 29	60	d	0.813	0.698	0.882	1.000	
A	IRESUM 26	60	a	1.000				
A	IRESUM 23	59	b	0.502	1.000			
A	IRESUM 28	60	c	0.574	0.834	1.000		
A	IRESUM 29	54	d	0.689	0.709	0.798	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	BCOPP9	30	a	1.000				
B	BCOPP10	30	b	0.733	1.000			
B	BCOPP11	30	c	0.864	0.818	1.000		
B	BCOPP12	30	d	0.760	0.521	0.807	1.000	
B	BCOPP13	30	e	0.880	0.666	0.870	0.840	1.000
B	BCOPO9	30	a	1.000				
B	BCOPO10	30	b	0.945	1.000			
B	BCOPO11	30	c	0.971	0.932	1.000		
B	BCOPO12	30	d	0.962	0.927	0.964	1.000	
B	BCOPO13	30	e	0.959	0.938	0.946	0.928	1.000
B	BCOPI9	30	a	1.000				
B	BCOPI10	30	b	0.906	1.000			
B	BCOPI11	30	c	0.952	0.936	1.000		
B	BCOPI12	30	d	0.929	0.855	0.944	1.000	
B	BCOPI13	30	e	0.950	0.864	0.949	0.948	1.000
B	BCOPI9b	30	a	1.000				
B	BCOPI10b	30	b	0.888	1.000			
B	BCOPI11b	30	c	0.936	0.938	1.000		
B	BCOPI12b	30	d	0.892	0.823	0.916	1.000	
B	BCOPP13b	30	e	0.930	0.850	0.952	0.926	1.000
B	HETQ14	25	a	1.000				
B	HETQ15	17	b	0.711	1.000			
B	HETQ16	23	c	0.355	0.387	1.000		
B	HETQ17	18	d	0.456	0.760	0.679	1.000	
B	HETS14	5	a	*				
B	HETSd15	9	b	*	1.000			
B	HETS16	7	c	*	0.949	1.000		
B	HETS17	11	d	*	0.831	0.420	1.000	
B	HETQ14b	25	a	1.000				
B	HETQ15b	17	b	0.727	1.000			
B	HETQ16b	23	c	0.645	0.594	1.000		
B	HETQ17b	18	d	0.927	0.470	0.535	1.000	
B	ICES 22	30	a	1.000				
B	ICES 27	30	b	0.808	1.000			
B	ICES 24	29	c	0.722	0.789	1.000		
B	ICES 25	29	d	0.691	0.795	0.789	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
B	ICEO 22	30	a	1.000				
B	ICEO 27	30	b	0.775	1.000			
B	ICEO 24	30	c	0.775	0.821	1.000		
B	ICEO 25	30	d	0.847	0.812	0.771	1.000	
B	ICEF 22	30	a	1.000				
B	ICEF 27	30	b	0.803	1.000			
B	ICEF 24	29	c	0.846	0.692	1.000		
B	ICEF 25	30	d	0.676	0.727	0.704	1.000	
B	ICEC 22	30	a	1.000				
B	ICEC 27	30	b	0.892	1.000			
B	ICEC 24	30	c	0.881	0.860	1.000		
B	ICEC 25	30	d	0.881	0.896	0.858	1.000	
B	IREA 26	30	a	1.000				
B	IREA 23	30	b	0.503	1.000			
B	IREA 28	30	c	0.624	0.814	1.000		
B	IREA 29	30	d	0.608	0.706	0.701	1.000	
B	IREB 26	30	a	1.000				
B	IREB 23	30	b	0.754	1.000			
B	IREB 28	30	c	0.699	0.746	1.000		
B	IREB 29	30	d	0.690	0.674	0.912	1.000	
B	IREC 26	29	a	1.000				
B	IREC 23	30	b	0.606	1.000			
B	IREC 28	28	c	0.655	0.439	1.000		
B	IREC 29	30	d	0.777	0.733	0.855	1.000	
B	IRED 26	29	a	1.000				
B	IRED 23	30	b	0.663	1.000			
B	IRED 28	28	c	0.799	0.598	1.000		
B	IRED 29	30	d	0.855	0.747	0.939	1.000	
B	IRESUM 26	30	a	1.000				
B	IRESUM 23	29	b	0.568	1.000			
B	IRESUM 28	30	c	0.595	0.955	1.000		
B	IRESUM 29	25	d	0.835	0.749	0.799	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	BCOPP9	18	a	1.000				
C	BCOPP10	18	b	0.915	1.000			
C	BCOPP11	18	c	0.932	0.893	1.000		
C	BCOPP12	18	d	0.785	0.688	0.894	1.000	
C	BCOPP13	18	e	0.901	0.889	0.963	0.922	1.000
C	BCOPO9	18	a	1.000				
C	BCOPO10	18	b	0.959	1.000			
C	BCOPO11	18	c	0.913	0.896	1.000		
C	BCOPO12	18	d	0.942	0.928	0.991	1.000	
C	BCOPO13	18	e	0.982	0.972	0.961	0.978	1.000
C	BCOPI9	18	a	1.000				
C	BCOPI10	18	b	0.946	1.000			
C	BCOPI11	18	c	0.898	0.879	1.000		
C	BCOPI12	18	d	0.937	0.915	0.980	1.000	
C	BCOPI13	18	e	0.981	0.964	0.947	0.978	1.000
C	BCOPI9b	18	a	1.000				
C	BCOPI10b	18	b	0.943	1.000			
C	BCOPI11b	18	c	0.864	0.877	1.000		
C	BCOPI12b	18	d	0.949	0.916	0.923	1.000	
C	BCOPP13b	18	e	0.971	0.954	0.905	0.968	1.000
C	HETQ14	12	a	1.000				
C	HETQ15	11	b	0.944	1.000			
C	HETQ16	12	c	0.809	0.745	1.000		
C	HETQ17	11	d	0.621	0.580	0.782	1.000	
C	HETS14	6	a	1.000				
C	HETS15	4	b	0.096	1.000			
C	HETS16	6	c	-0.159	-0.910	1.000		
C	HETS17	4	d	-0.288	0.852	-0.094	1.000	
C	HETQ14b	12	a	1.000				
C	HETQ15b	11	b	0.692	1.000			
C	HETQ16b	12	c	0.816	0.642	1.000		
C	HETQ17b	11	d	0.626	0.830	0.562	1.000	
C	ICES 22	18	a	1.000				
C	ICES 27	18	b	0.671	1.000			
C	ICES 24	18	c	0.757	0.599	1.000		
C	ICES 25	17	d	0.514	0.210	0.732	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
C	ICEO 22	18	a	1.000				
C	ICEO 27	18	b	0.498	1.000			
C	ICEO 24	18	c	0.704	0.414	1.000		
C	ICEO 25	18	d	0.786	0.442	0.851	1.000	
C	ICEF 22	18	a	1.000				
C	ICEF 27	18	b	0.433	1.000			
C	ICEF 24	18	c	0.847	0.371	1.000		
C	ICEF 25	18	d	0.745	0.517	0.763	1.000	
C	ICEC 22	18	a	1.000				
C	ICEC 27	18	b	0.705	1.000			
C	ICEC 24	18	c	0.844	0.569	1.000		
C	ICEC 25	18	d	0.763	0.595	0.905	1.000	
C	IREA 26	18	a	1.000				
C	IREA 23	18	b	0.413	1.000			
C	IREA 28	18	c	0.599	0.722	1.000		
C	IREA 29	18	d	0.656	0.480	0.634	1.000	
C	IREB 26	18	a	1.000				
C	IREB 23	18	b	0.629	1.000			
C	IREB 28	18	c	0.683	0.552	1.000		
C	IREB 29	18	d	0.607	0.409	0.575	1.000	
C	IREC 26	17	a	1.000				
C	IREC 23	18	b	0.169	1.000			
C	IREC 28	18	c	0.276	0.456	1.000		
C	IREC 29	18	d	0.210	0.392	0.748	1.000	
C	IRED 26	17	a	1.000				
C	IRED 23	18	b	0.490	1.000			
C	IRED 28	18	c	0.704	0.689	1.000		
C	IRED 29	18	d	0.790	0.615	0.874	1.000	
C	IRESUM 26	18	a	1.000				
C	IRESUM 23	18	b	0.481	1.000			
C	IRESUM 28	18	c	0.555	0.861	1.000		
C	IRESUM 29	18	d	0.628	0.964	0.896	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
D	BCOPP9	12	a	1.000				
D	BCOPP10	12	b	0.835	1.000			
D	BCOPP11	12	c	0.932	0.912	1.000		
D	BCOPP12	12	d	0.843	0.966	0.922	1.000	
D	BCOPP13	12	e	0.766	0.924	0.921	0.958	1.000
D	BCOPO9	12	a	1.000				
D	BCOPO10	12	b	0.957	1.000			
D	BCOPO11	12	c	0.971	0.981	1.000		
D	BCOPO12	12	d	0.947	0.972	0.957	1.000	
D	BCOPO13	12	e	0.967	0.995	0.985	0.973	1.000
D	BCOPI9	12	a	1.000				
D	BCOPI10	12	b	0.914	1.000			
D	BCOPI11	12	c	0.951	0.952	1.000		
D	BCOPI12	12	d	0.915	0.989	0.936	1.000	
D	BCOPI13	12	e	0.915	0.959	0.947	0.966	1.000
D	BCOPI9b	12	a	1.000				
D	BCOPI10b	12	b	0.914	1.000			
D	BCOPI11b	12	c	0.951	0.952	1.000		
D	BCOPI12b	12	d	0.915	0.989	0.936	1.000	
D	BCOPP13b	12	e	0.915	0.959	0.947	0.966	1.000
D	HETQ14	12	a	1.000				
D	HETQ15	12	b	0.793	1.000			
D	HETQ16	12	c	0.438	0.779	1.000		
D	HETQ17	12	d	0.816	0.876	0.579	1.000	
D	HETQ14b	12	a	1.000				
D	HETQ15b	12	b	0.721	1.000			
D	HETQ16b	12	c	0.670	0.768	1.000		
D	HETQ17b	12	d	0.420	0.966	0.721	1.000	
D	ICES 22	12	a	1.000				
D	ICES 27	12	b	0.741	1.000			
D	ICES 24	12	c	0.920	0.696	1.000		
D	ICES 25	12	d	0.641	0.392	0.543	1.000	
D	ICEO 22	12	a	1.000				
D	ICEO 27	12	b	0.618	1.000			
D	ICEO 24	12	c	0.719	0.759	1.000		
D	ICEO 25	12	d	0.438	0.834	0.483	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
D	ICEF 22	12	a	1.000				
D	ICEF 27	12	b	0.663	1.000			
D	ICEF 24	12	c	0.636	0.546	1.000		
D	ICEF 25	12	d	0.950	0.748	0.664	1.000	
D	ICEC 22	12	a	1.000				
D	ICEC 27	12	b	0.827	1.000			
D	ICEC 24	12	c	0.854	0.805	1.000		
D	ICEC 25	12	d	0.870	0.759	0.724	1.000	
D	IREA 26	12	a	1.000				
D	IREA 23	12	b	0.433	1.000			
D	IREA 28	12	c	0.317	0.567	1.000		
D	IREA 29	12	d	0.678	0.462	0.480	1.000	
D	IREB 26	12	a	1.000				
D	IREB 23	12	b	0.786	1.000			
D	IREB 28	12	c	0.894	0.789	I.000		
D	IREB 29	12	d	0.814	0.736	0.845	1.000	
D	IREC 26	12	a	1.000				
D	IREC 23	12	b	0.091	1.000			
D	IREC 28	12	c	-0.148	0.269	1.000		
D	IREC 29	12	d	-0.010	0.527	0.835	1.000	
D	IRED 26	12	a	1.000				
D	IRED 23	12	b	0.647	1.000			
D	IRED 28	12	c	0.405	0.635	1.000		
D	IRED 29	12	d	0.686	0.589	0.758	1.000	
D	IRESUM 26	12	a	1.000				
D	IRESUM 23	12	b	0.363	1.000			
D	IRESUM 28	12	c	0.769	0.498	1.000		
D	IRESUM 29	11	d	0.665	0.614	0.872	1.000	
E	BCOPP9	20	a	1.000				
E	BCOPP10	20	b	0.773	1.000			
E	BCOPP11	20	c	0.926	0.843	1.000		
E	BCOPP12	20	d	0.878	0.563	0.889	1.000	
E	BCOPP13	20	e	0.932	0.670	0.934	0.886	1.000

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
E	BCOPO9	20	a	1.000				
E	BCOPO10	20	b	0.941	1.000			
E	BCOPO11	20	c	0.908	0.887	1.000		
E	BCOPO12	20	d	0.912	0.903	0.977	1.000	
E	BCOPO13	20	e	0.966	0.930	0.952	0.942	1.000
E	BCOPI9	20	a	1.000				
E	BCOPI10	20	b	0.902	1.000			
E	BCOPI11	20	c	0.897	0.872	1.000		
E	BCOPI12	20	d	0.880	0.852	0.960	1.000	
E	BCOPI13	20	e	0.945	0.884	0.943	0.942	1.000
E	BCOPI9b	20	a	1.000				
E	BCOPI10b	20	b	0.881	1.000			
E	BCOPI11b	20	c	0.887	0.869	1.000		
E	BCOPI12b	20	d	0.870	0.776	0.889	1.000	
E	BCOPP13b	20	e	0.921	0.824	0.925	0.930	1.000
E	HETQ14	9	a	1.000				
E	HETQ15	0	b	*	*			
E	HETQ16	7	c	0.500	*	1.000		
E	HETQ17	1	d	*	*	*	*	
E	HETS14	11	a	1.000				
E	HETS15	13	b	0.174	1.000			
E	HETS16	13	c	-0.171	-0.171	1.000		
E	HETS17	17	d	-0.103	0.808	0.031	1.000	
E	HETQ14b	9	a	1.000				
E	HETQ15b	0	b	*	*			
E	HETQ16b	7	c	0.985	*	1.000		
E	HETQ17b	1	d	*	*	*	*	
E	ICES 22	20	a	1.000				
E	ICES 27	20	b	0.869	1.000			
E	ICES 24	20	c	0.847	0.734	1.000		
E	ICES 25	19	d	0.778	0.722	0.811	1.000	
E	ICEO 22	20	a	1.000				
E	ICEO 27	20	b	0.595	1.000			
E	ICEO 24	20	c	0.752	0.602	1.000		
E	ICEO 25	20	d	0.868	0.649	0.752	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
E	ICEF 22	20	a	1.000				
E	ICEF 27	20	b	0.729	1.000			
E	ICEF 24	20	c	0.864	0.678	1.000		
E	ICEF 25	20	d	0.739	0.869	0.674	1.000	
E	ICEC 22	20	a	1.000				
E	ICEC 27	20	b	0.806	1.000			
E	ICEC 24	20	c	0.874	0.752	1.000		
E	ICEC 25	20	d	0.883	0.816	0.880	1.000	
E	IREA 26	20	a	1.000				
E	IREA 23	20	b	0.195	1.000			
E	IREA 28	20	c	0.394	0.908	1.000		
E	IREA 29	20	d	0.405	0.543	0.468	1.000	
E	IREB 26	20	a	1.000				
E	IREB 23	20	b	0.782	1.000			
E	IREB 28	20	c	0.629	0.649	1.000		
E	IREB 29	20	d	0.569	0.524	0.672	1.000	
E	IREC 26	19	a	1.000				
E	IREC 23	20	b	0.335	1.000			
E	IREC 28	20	c	0.670	0.404	1.000		
E	IREC 29	20	d	0.559	0.628	0.829	1.000	
E	IRED 26	19	a	1.000				
E	IRED 23	20	b	0.540	1.000			
E	IRED 28	20	c	0.791	0.685	1.000		
E	IRED 29	20	d	0.798	0.689	0.949	1.000	
E	IRESUM 26	20	a	1.000				
E	IRESUM 23	19	b	0.199	1.000			
E	IRESUM 28	20	c	0.191	0.991	1.000		
E	IRESUM 29	15	d	0.432	0.606	0.635	1.000	
F	BCOPP9	14	a	1.000				
F	BCOPP10	14	b	0.731	1.000			
F	BCOPP11	14	c	0.901	0.864	1.000		
F	BCOPP12	14	d	0.795	0.903	0.896	1.000	
F	BCOPP13	14	e	0.699	0.846	0.875	0.933	1.000

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
F	BCOPO9	14	a	1.000				
F	BCOPO10	14	b	0.984	1.000			
F	BCOPO11	14	c	0.985	0.959	1.000		
F	BCOPO12	14	d	0.989	0.968	0.987	1.000	
F	BCOPO13	14	e	0.984	0.988	0.955	0.976	1.000
F	BCOPI9	14	a	1.000				
F	BCOPI10	14	b	0.917	1.000			
F	BCOPI11	14	c	0.975	0.920	1.000		
F	BCOPI12	14	d	0.974	0.914	0.974	1.000	
F	BCOPI13	14	e	0.969	0.926	0.954	0.980	1.000
F	BCOPI9b	14	a	1.000				
F	BCOPI10b	14	b	0.899	1.000			
F	BCOPI11b	14	c	0.970	0.928	1.000		
F	BCOPI12b	14	d	0.955	0.921	0.962	1.000	
F	BCOPP13b	14	e	0.946	0.918	0.976	0.972	1.000
F	HETQ14	14	a	1.000				
F	HETQ15	14	b	0.880	1.000			
F	HETQ16	14	c	0.776	0.730	1.000		
F	HETQ17	14	d	0.712	0.842	0.765	1.000	
F	HETQ14b	14	a	*				
F	HETQ15b	14	b	*	1.000			
F	HETQ16b	14	c	*	0.591	1.000		
F	HETQ17b	14	d	*	0.974	0.590	1.000	
F	ICES 22	14	a	1.000				
F	ICES 27	14	b	0.617	1.000			
F	ICES 24	13	c	0.757	0.856	1.000		
F	ICES 25	13	d	0.539	0.889	0.821	1.000	
F	ICEO 22	14	a	1.000				
F	ICEO 27	14	b	0.797	1.000			
F	ICEO 24	14	c	0.796	0.907	1.000		
F	ICEO 25	14	d	0.794	0.868	0.717	1.000	
F	ICEF 22	14	a	1.000				
F	ICEF 27	14	b	0.781	1.000			
F	ICEF 24	13	c	0.604	0.543	1.000		
F	ICEF 25	14	d	0.901	0.689	0.772	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
F	ICEC 22	14	a	1.000				
F	ICEC 27	14	b	0.873	1.000			
F	ICEC 24	14	c	0.877	0.905	1.000		
F	ICEC 25	14	d	0.907	0.913	0.868	1.000	
F	IREA 26	14	a	1.000				
F	IREA 23	14	b	0.648	1.000			
F	IREA 28	14	c	0.733	0.712	1.000		
F	IREA 29	14	d	0.789	0.596	0.817	1.000	
F	IREB 26	14	a	1.000				
F	IREB 23	14	b	0.808	1.000			
F	IREB 28	14	c	0.862	0.812	1.000		
F	IREB 29	14	d	0.789	0.746	0.906	1.000	
F	IREC 26	13	a	1.000				
F	IREC 23	14	b	0.914	1.000			
F	IREC 28	12	c	0.464	0.682	1.000		
F	IREC 29	14	d	0.805	0.815	0.845	1.000	
F	IRED 26	13	a	1.000				
F	IRED 23	14	b	0.776	1.000			
F	IRED 28	12	c	0.613	0.575	1.000		
F	IRED 29	14	d	0.868	0.696	0.781	1.000	
F	IRESUM 26	14	a	1.000				
F	IRESUM 23	14	b	0.770	1.000			
F	IRESUM 28	14	c	0.863	0.811	1.000		
F	IRESUM 29	14	d	0.884	0.800	0.957	1.000	
G	BCOPP9	26	a	1.000				
G	BCOPP10	26	b	0.733	1.000			
G	BCOPP11	26	c	0.801	0.856	1.000		
G	BCOPP12	26	d	0.781	0.612	0.801	1.000	
G	BCOPP13	26	e	0.893	0.794	0.858	0.845	1.000
G	BCOPO9	26	a	1.000				
G	BCOPO10	26	b	0.961	1.000			
G	BCOPO11	26	c	0.935	0.955	1.000		
G	BCOPO12	26	d	0.949	0.961	0.967	1.000	
G	BCOPO13	26	e	0.961	0.964	0.913	0.940	1.000

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	BCOPI9	26	a	1.000				
G	BCOPI10	26	b	0.873	1.000			
G	BCOPI11	26	c	0.875	0.939	1.000		
G	BCOPI12	26	d	0.897	0.851	0.902	1.000	
G	BCOPI13	26	e	0.953	0.891	0.898	0.956	1.000
G	BCOPI9b	26	a	1.000				
G	BCOPI10b	26	b	0.873	1.000			
G	BCOPI11b	26	c	0.875	0.939	1.000		
G	BCOPI12b	26	d	0.897	0.851	0.902	1.000	
G	BCOPP13b	26	e	0.953	0.891	0.898	0.956	1.000
G	HETQ14	26	a	1.000				
G	HETQ15	26	b	0.755	1.000			
G	HETQ16	26	c	0.221	0.450	1.000		
G	HETQ17	26	d	0.492	0.692	0.704	1.000	
G	HETQ14b	26	a	1.000				
G	HETQ15b	26	b	0.721	1.000			
G	HETQ16b	26	c	0.771	0.638	1.000		
G	HETQ17b	26	d	0.675	0.765	0.591	1.000	
G	ICES 22	26	a	1.000				
G	ICES 27	26	b	0.779	1.000			
G	ICES 24	26	c	0.690	0.736	1.000		
G	ICES 25	26	d	0.626	0.461	0.560	1.000	
G	ICEO 22	26	a	1.000				
G	ICEO 27	26	b	0.757	1.000			
G	ICEO 24	26	c	0.770	0.695	1.000		
G	ICEO 25	26	d	0.719	0.692	0.764	1.000	
G	ICEF 22	26	a	1.000				
G	ICEF 27	26	b	0.607	1.000			
G	ICEF 24	26	c	0.748	0.394	1.000		
G	ICEF 25	26	d	0.594	0.494	0.654	1.000	
G	ICEC 22	26	a	1.000				
G	ICEC 27	26	b	0.856	1.000			
G	ICEC 24	26	c	0.830	0.745	1.000		
G	ICEC 25	26	d	0.778	0.751	0.803	1.000	

Interlaboratory Correlation Coefficients from the EC/HO Validation Study (Balls et al., 1995)

Chemical Category[1]	*In Vitro* Endpoint	No. samples tested *In Vitro*	Interlaboratory correlation of *in vitro* data					
			Lab	Lab a	Lab b	Lab c	Lab d	Lab e
G	IREA 26	26	a	1.000				
G	IREA 23	26	b	0.496	1.000			
G	IREA 28	26	c	0.685	0.518	1.000		
G	IREA 29	26	d	0.709	0.625	0.704	1.000	
G	IREB 26	26	a	1.000				
G	IREB 23	26	b	0.525	1.000			
G	IREB 28	26	c	0.628	0.526	1.000		
G	IREB 29	26	d	0.664	0.470	0.824	1.000	
G	IREC 26	26	a	1.000				
G	IREC 23	26	b	0.137	1.000			
G	IREC 28	26	c	0.245	0.214	1.000		
G	IREC 29	26	d	0.342	0.101	0.808	1.000	
G	IRED 26	26	a	1.000				
G	IRED 23	26	b	0.539	1.000			
G	IRED 28	26	c	0.712	0.507	1.000		
G	IRED 29	26	d	0.790	0.613	0.906	1.000	
G	IRESUM 26	26	a	1.000				
G	IRESUM 23	26	b	0.527	1.000			
G	IRESUM 28	26	c	0.693	0.793	1.000		
G	IRESUM 29	25	d	0.626	0.696	0.716	1.000	

Abbreviations: BCOPI = Index; BCOPIb = Index, cut-off at 200; BCOPO = Opacity; BCOPP = Permeability; ICEC = Irritation Index; ICEF = Fluorescein retention; ICEO = Opacity; ICES = Swelling; IREA = Opacity (1 hr); IREB = Opacity (4 hr); IREC = Swelling (1 hr); IRED = Swelling (4 hr); IRESUM = Summary score; HETQ = Q Score; HETQB = Q Score, cutoff at 2; HETS = S Score; HETSB = S Score, cutoff at 2.

[1]A = Full set of chemicals, B = Water soluble, C = Water insoluble, D = Surfactants, E = Solids, F = Solutions, G = Liquids.
The numbers 1-38 against each endpoint in the Table refer to the laboratories which conducted each particular test. Laboratory 36 left the study without submitting any results.
* = No data

Appendix H

Positive Control Data

H1 Individual HET-CAM Egg Data for Dimethylformamide (provided by Drs. Vanparys and van Goethem) H-3

H2 Individual HET-CAM Egg Data for Imidazole (provided by Drs. Vanparys and van Goethem) H-7

H3 Individual HET-CAM Egg Data for Sodium Dodecyl Sulfate and Sodium Hydroxide (provided by Drs. Spielmann and Liebsch) H-11

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Appendix H1

Individual HET-CAM Egg Data for Dimethylformamide (provided by Drs. Vanparys and van Goethem)

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HET-CAM Test Scores for Dimethylformanide

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
183	0.00	0.00	0.00	6.74	6.86	6.88	8.79	8.85	8.85	15.53	15.71	15.73
185	0.00	0.00	0.00	6.91	6.86	6.84	8.61	8.58	8.64	15.52	15.44	15.48
186	0.00	0.00	0.00	6.93	6.74	6.88	8.67	8.52	8.37	15.60	15.26	15.25
188	0.00	0.00	0.00	6.95	6.88	6.88	8.49	8.25	8.34	15.44	15.13	15.22
189	0.00	0.00	0.00	6.86	6.84	6.93	8.55	8.58	8.73	15.41	15.42	15.66
190	0.00	0.00	0.00	6.93	6.91	6.91	8.79	8.79	8.76	15.72	15.70	15.67
191	0.00	0.00	0.00	6.98	6.91	6.91	8.82	8.82	8.82	15.80	15.73	15.73
192	0.00	0.00	0.00	6.93	6.98	6.95	8.76	8.85	8.76	15.69	15.83	15.71
193	0.00	0.00	0.00	6.86	6.95	6.93	8.88	8.94	8.91	15.74	15.89	15.84
194	0.00	0.00	0.00	6.77	6.84	6.84	8.88	8.94	8.88	15.65	15.78	15.72
196	0.00	0.00	0.00	6.95	6.93	6.91	8.79	8.67	8.76	15.74	15.60	15.67
198	0.00	0.00	0.00	6.91	6.88	6.93	8.76	8.67	8.73	15.67	15.55	15.66
201	0.00	0.00	0.00	6.86	6.95	6.93	8.58	8.70	8.67	15.44	15.65	15.60
202	0.00	0.00	0.00	6.98	6.93	6.93	8.85	8.79	8.73	15.83	15.72	15.66
203	0.00	0.00	0.00	6.93	6.91	6.93	8.76	8.76	8.79	15.69	15.67	15.72
205	0.00	0.00	0.00	6.93	6.95	6.98	8.85	8.88	8.88	15.78	15.83	15.86
207	0.00	0.00	0.00	6.91	6.95	6.95	8.76	8.85	8.88	15.67	15.80	15.83
208	4.27	0.00	0.00	6.91	6.91	6.93	8.61	8.67	8.76	19.78	15.58	15.69
209	0.00	0.00	0.00	6.95	6.93	6.95	8.82	8.76	8.79	15.77	15.69	15.74
211	0.00	0.00	0.00	6.93	6.95	6.95	8.79	8.88	8.85	15.72	15.83	15.80
212	0.00	0.00	0.00	6.93	6.98	6.93	8.85	8.85	8.85	15.78	15.83	15.78
213	0.00	0.00	0.00	6.91	6.93	6.93	8.79	8.73	8.82	15.70	15.66	15.75
215	0.00	0.00	0.00	6.88	6.81	6.79	8.76	8.70	8.67	15.64	15.51	15.46
217	0.00	0.00	0.00	6.88	6.91	6.95	8.79	8.79	8.82	15.67	15.70	15.77
230	0.00	0.00	0.00	6.91	6.88	6.93	8.91	8.91	8.94	15.82	15.79	15.87
231	0.00	0.00	0.00	6.98	6.98	6.98	8.85	8.88	8.88	15.83	15.86	15.86
232	0.00	0.00	0.00	6.95	6.98	6.95	8.85	8.88	8.85	15.80	15.86	15.80
233	0.00	0.00	0.00	6.98	6.98	6.93	8.88	8.82	8.82	15.86	15.80	15.75
234	0.00	0.00	0.00	6.95	6.93	6.95	8.82	8.85	8.85	15.77	15.78	15.80
235	0.00	0.00	0.00	6.98	6.95	6.95	8.88	8.85	8.85	15.86	15.80	15.80
236	0.00	0.00	0.00	6.95	6.98	6.98	8.88	8.88	8.91	15.83	15.86	15.89
237	0.00	0.00	0.00	6.98	6.98	6.95	8.67	8.79	8.85	15.65	15.77	15.80
238	0.00	0.00	0.00	6.95	6.95	6.93	8.85	8.88	8.85	15.80	15.83	15.78
240	0.00	0.00	0.00	6.98	6.98	6.95	8.88	8.88	8.85	15.86	15.86	15.80
241	0.00	0.00	0.00	6.98	6.95	6.98	8.91	8.85	8.91	15.89	15.80	15.89
242	0.00	0.00	0.00	6.93	6.95	6.95	8.85	8.88	8.88	15.78	15.83	15.83
243	0.00	0.00	0.00	6.98	6.95	6.95	8.91	8.91	8.88	15.89	15.86	15.83
244	0.00	0.00	0.00	6.98	6.95	6.93	8.94	8.88	8.88	15.92	15.83	15.81
245	0.00	0.00	0.00	6.98	6.95	6.95	8.91	8.88	8.88	15.89	15.83	15.83
251	0.00	0.00	0.00	6.98	6.95	6.86	8.85	8.85	8.73	15.83	15.80	15.59
252	0.00	0.00	0.00	6.95	6.95	6.93	8.88	8.85	8.85	15.83	15.80	15.78
253	0.00	0.00	0.00	6.95	6.98	6.93	8.91	8.85	8.76	15.86	15.83	15.69

HET-CAM Test Scores for Dimethylformanide

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
254	0.00	0.00	0.00	6.95	6.88	6.91	8.88	8.73	8.82	15.83	15.61	15.73
255	0.00	0.00	0.00	6.93	6.93	6.93	8.82	8.76	8.85	15.75	15.69	15.78
256	0.00	0.00	0.00	6.95	6.95	6.93	8.88	8.85	8.85	15.83	15.80	15.78
257	0.00	0.00	0.00	6.91	6.93	6.95	8.82	8.85	8.85	15.73	15.78	15.80
258	0.00	0.00	0.00	6.98	6.95	6.95	8.88	8.82	8.85	15.86	15.77	15.80
259	0.00	0.00	0.00	6.95	6.88	6.95	8.88	8.76	8.91	15.83	15.64	15.86
260	0.00	0.00	0.00	6.95	6.95	6.93	8.88	8.85	8.82	15.83	15.80	15.75
261	0.00	0.00	0.00	6.98	6.95	6.93	8.91	8.85	8.82	15.89	15.80	15.75
262	0.00	0.00	0.00	6.95	6.95	6.93	8.88	8.85	8.88	15.83	15.80	15.81
263	0.00	0.00	0.00	6.95	6.91	6.95	8.88	8.85	8.85	15.83	15.76	15.80
264	0.00	0.00	0.00	6.95	6.98	6.98	8.88	8.85	8.88	15.83	15.83	15.86
265	0.00	0.00	0.00	6.98	6.95	6.95	8.91	8.85	8.88	15.89	15.80	15.83
266	0.00	0.00	0.00	6.95	6.93	6.79	8.85	8.82	8.61	15.80	15.75	15.40
267	0.00	0.00	0.00	6.95	6.95	6.93	8.82	8.85	8.85	15.77	15.80	15.78
268	0.00	0.00	0.00	6.95	6.95	6.95	8.88	8.91	8.88	15.83	15.86	15.83
269	0.00	0.00	0.00	6.95	6.95	6.95	8.91	8.88	8.88	15.86	15.83	15.83
270	0.00	0.00	0.00	6.93	6.95	6.95	8.85	8.88	8.91	15.78	15.83	15.86
271	0.00	0.00	0.00	6.95	6.93	6.93	8.82	8.85	8.85	15.77	15.78	15.78
272	0.00	0.00	0.00	6.91	6.98	6.95	8.73	8.85	8.85	15.64	15.83	15.80
273	0.00	0.00	0.00	6.93	6.98	6.93	8.82	8.88	8.85	15.75	15.86	15.78
274	0.00	0.00	0.00	6.95	6.91	6.95	8.88	8.79	8.91	15.83	15.70	15.86
275	0.00	0.00	0.00	6.95	6.98	6.95	8.91	8.88	8.88	15.86	15.86	15.83
277	0.00	0.00	0.00	6.86	6.91	6.93	8.73	8.82	8.85	15.59	15.73	15.78
278	0.00	0.00	0.00	6.95	6.91	6.95	8.82	8.79	8.85	15.77	15.70	15.80
279	0.00	0.00	0.00	6.93	6.93	6.93	8.85	8.79	8.85	15.78	15.72	15.78
280	0.00	0.00	0.00	6.93	6.95	6.81	8.85	8.88	8.70	15.78	15.83	15.51
282	0.00	0.00	0.00	6.95	6.91	6.91	8.88	8.82	8.85	15.83	15.73	15.76
1A[1]	3.48	3.63	3.38	6.81	6.74	6.79	8.82	8.82	8.85	19.11	19.19	19.02
1B	3.35	3.15	4.02	6.65	6.74	6.67	8.88	8.91	8.85	18.88	18.80	19.54
2A	2.98	2.72	3.18	5.72	6.23	6.39	8.67	8.70	8.70	17.37	17.65	18.27
2B	3.77	3.98	3.98	6.56	6.58	6.72	8.79	8.82	8.88	19.12	19.38	19.58
3A	2.93	3.18	3.18	6.42	6.51	6.60	8.88	8.79	8.76	18.23	18.48	18.54
4A	3.20	3.33	3.38	6.46	6.49	6.63	8.76	8.82	8.82	18.42	18.64	18.83
4B	3.62	3.47	3.58	6.56	6.70	6.67	8.73	8.79	8.82	18.91	18.96	19.07
6A	2.02	2.58	3.97	6.70	4.90	5.86	8.76	8.82	8.88	17.48	16.30	18.71
8A-10A	3.97	2.60	3.02	6.65	6.88	6.91	8.76	8.82	8.88	19.38	18.30	18.81
11A	3.38	3.92	3.82	6.84	6.93	6.91	8.73	8.85	8.82	18.95	19.70	19.55
133	4.20	3.97	4.00	6.79	6.86	6.88	8.70	8.79	8.88	19.69	19.62	19.76
16-17-18	4.07	3.95	3.80	6.84	6.88	6.77	8.73	8.79	8.67	19.64	19.62	19.24

[1] Test Method Data 183 to 282 represent studies where a Test Substance Applicator was used and the hemorrhage endpoint was evaluated inside of the Test Substance Applicator.

[2] Test Method Data 1A to 11A represent studies where a Test Substance Applicator was used and the hemorrhage endpoint was evaluated outside of the Test Substance Applicator.

[3] Test Method Data 133 to 16-17-18 represent studies where a Test Substance Applicator was not used.

Appendix H2

Individual HET-CAM Egg Data for Imidazole (provided by Drs. Vanparys and van Goethem)

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HET-CAM Test Scores for Imidazole

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
186	3.40	4.83	4.83	6.84	6.84	6.79	8.31	8.43	8.46	18.55	20.10	20.08
190	4.92	4.92	4.88	6.93	6.93	6.88	8.73	8.79	8.70	20.58	20.64	20.46
194	4.03	4.45	4.32	6.70	6.81	6.84	8.85	8.85	8.88	19.58	20.11	20.04
214	4.03	3.88	3.95	6.88	6.88	6.91	8.76	8.73	8.79	19.67	19.49	19.65
220	4.30	4.48	4.25	6.95	6.79	6.88	8.79	8.58	8.76	20.04	19.85	19.89
269	4.03	4.02	3.47	6.95	6.91	6.91	8.73	8.70	8.76	19.71	19.63	19.14
270	4.13	3.88	4.00	6.67	6.72	6.81	8.25	8.22	8.46	19.05	18.82	19.27
274	4.18	4.20	4.37	6.77	6.86	6.86	8.52	8.52	8.58	19.47	19.58	19.81
278	4.67	4.68	4.45	6.88	6.93	6.93	8.76	8.79	8.82	20.31	20.40	20.20
281	4.57	4.57	4.55	6.93	6.91	6.93	8.76	8.73	8.76	20.26	20.21	20.24
5A	4.85	4.88	4.90	6.58	6.65	6.74	8.85	8.88	8.91	20.28	20.41	20.55
7A-9A	4.93	4.95	4.95	6.84	6.88	6.88	8.55	8.43	8.49	20.32	20.26	20.32
12A	4.92	4.93	4.93	6.81	6.84	6.79	8.61	8.55	8.46	20.34	20.32	20.18
13	4.92	4.95	4.92	6.84	6.91	6.81	8.40	8.76	8.55	20.16	20.62	20.28
14	4.78	4.77	4.73	6.88	6.84	6.88	8.85	8.73	8.85	20.51	20.34	20.46

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Appendix H3

Individual HET-CAM Egg Data for Sodium Dodecyl Sulfate and Sodium Hydroxide (provided by Drs. Spielmann and Liebsch)

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German HET-CAM Validation Study: Retrospective Analysis of Positive Controls (1% SLS and 0.1n NaOH), concurrently tested with coded test chemicals

Elke Genschow, Manfred Liebsch, Elisabeth Schmidt, Dieter Traue and Horst Spielmann

ZEBET at the BfR, Berlin

DATA SET USED FOR ANLAYSIS

In the German Validation Study, 1% SLS and 0.1 NaOH served as Positive Controls (PC). They were concurrently tested with the test chemicals and used as acceptance criteria for the results. For the purpose of the present assessment of intra- and interlaboratory variability of the HET-CAM, PC data of 105 coded test chemicals were analysed. This amounts to about 2/3 of the total of 150 chemicals that were tested in phase II (data base development) of the German validation study.

Since each test chemical was tested on two independent runs (run 1 and run 2) and in two different laboratories (lab 1 and lab 2), in theory, four sets of SLS data and four sets of NaOH data were generated together with each coded test chemical. In practice, however, one PC sometimes served for more then one test chemical, and is therefore only listed in the files of one of the coded chemicals.

Since each coded test chemical was randomly assigned (by a computer) to be tested in two of the 12 participating laboratories, in the present analysis, "lab1" is representing the total of all 12 participating labs, and "lab2" as well. Using these randomly generated "virtual laboratories 1 and 2" for the interlaboratory analysis, is a compromise, due to the fact that data had to be extracted from coded test chemical files in our archieves from paper hardcopies. Decoding all info and assigning the data to the 12 individual laboratories would have been too much work. However, from a biostatistical standpoint, the random generation of assignments of the 12 laboratories allows application of the procedures described below.

BIOSTATISTICAL PROCEDURES

The GLM (General Linear Model) Multivariate procedure was used for analysis of inter- and intra- laboratory variances. The advantage of this procedure is, that it provides the analysis of variance for multiple dependent variables by one or more factors.

Each level of a factor can have a different linear effect on the value of the dependent variables. The GLM Multivariate procedure assumes that all the model factors are fixed; that is, they are generally thought of as variables whose values of interest are all represented in the data file, usually by design.

In the HET-CAM the dependent variables are *haemorrhage*, *coagulation*, *vessel lysis* and the factors are "*laboratories*" (interlaboratory reproducibility) and "*runs*" (intralaboratory repeatability over time). Per each of the two positive control chemicals SLS and NaOH, values obtained for *haemorrhage*, *coagulation*, and *vessel lysis* were used for determination of the

statistical variability between "laboratories" and “runs”. Intralaboratory and interlaboratory differences are regarded significant if the error probability values $p < 0.05$.

RESULTS

Table 1 shows the means ± standard deviation for the parameters *haemorrhage*, *coagulation*, and *vessel lysis* as observed for the two PC's, 1% SLS and 0.1n NaOH. From these data it is already obvious that differences between labs are not likely. *Note*: Coagulation does not occur upon exposure with 0.1% SLS. It was, however, in one single case, observed. Since non existing values were calculated with the arbitrary value "0", the mean ± SD marked yellow are meaningless.

Table 2 shows, for each of the three parameters *haemorrhage*, *coagulation*, and *vessel lysis* the means and lower / upper boundaries of the 95% confidence intervals. Confidence intervals are sufficiently narrow, and do not show obvious differences between the laboratories 1 and 2.

Figure 1 and **Figure 2** are visualisations of the content of **Table 1** showing, separately for the two PC's 0.1n NaOH and 1% SLS the variability measures (SD) obtained in lab 1 and lab 2 for the three parameters *haemorrhage*, *coagulation*, and *vessel lysis.*

The results of the GLM Multivariate procedure is given in **Table 3 and 4**. Each multivariate statistic is transformed into a test statistic with an approximate or exact F distribution, given as F. The variances can be divided up and can be computed as the sum of squared deviations (Sums of squares) from the overall mean. Although there are n levels of each factor, one degree of freedom is lost because of the deviations are subject to one constraint. Therefore, the degrees of freedom are n-1.

In summary, no significant differences between runs in the two laboratories were determined indicating a very good intra-laboratory performance of the assay. The differences between laboratories were very low and not significant for the three endpoint values haemorrage and coagulation and vessel lysis. Therefore we conclude that the assay proved sufficient reliability.

Table 1: **Mean and standard deviation (SD) for the endpoint values haemorrage, coagulation and vessel lysis (detection time in [sec])**

Endpoint	CHEMICAL	LAB	Mean	Std. Deviation	n
haemorrage	0.1n NaOH	1	9.16	6.491	176
		2	8.74	2.294	160
		Total	8.96	4.955	336
	1% SLS	1	15.16	5.812	206
		2	14.12	4.711	171
		Total	14.69	5.359	377
coagulation	0.1n NaOH	1	51.02	35.907	176
		2	44.76	32.816	160
		Total	48.04	34.561	336
	1% SLS	1	.00	.000	206
		2	.35	4.588	171
		Total	.16	3.090	377
vessel lysis	0.1n NaOH	1	37.99	24.433	176
		2	32.98	24.816	160
		Total	35.60	24.707	336
	1% SLS	1	36.50	17.060	206
		2	33.60	17.179	171
		Total	35.18	17.152	377

Table 2: **Mean, standard error and 95% Confidence Interval for the endpoint values *haemorrhage*, *coagulation* and *vessel lysis* (detection time in [sec])**

Endpoint	CHEMICAL				95% Confidence Interval	
		LAB	Mean	std. error	Lower Bound	Upper Bound
haemorrage	0.1n NaOH	1	**9.165**	.389	**8.401**	**9.929**
		2	**8.738**	.408	**7.936**	**9.539**
	1% SLS	1	**15.155**	.360	**14.449**	**15.862**
		2	**14.123**	.395	**13.347**	**14.898**
coagulation	0.1n NaOH	1	**51.023**	1.791	**47.506**	**54.540**
		2	**44.763**	1.879	**41.074**	**48.451**
	1% SLS	1	**.000**	1.656	**-3.251**	**3.251**
		2	**.351**	1.817	**-3.217**	**3.919**
vessel lysis	0.1n NaOH	1	**37.994**	1.582	**34.889**	**41.100**
		2	**32.975**	1.659	**29.718**	**36.232**
	1% SLS	1	**36.495**	1.462	**33.625**	**39.366**
		2	**33.602**	1.605	**30.452**	**36.753**

Figure 1: **Error bars of the endpoint values haemorrage, coagulation and vessel lysis (detection time in [sec]) ± standard deviation for 0.1n NaOH**

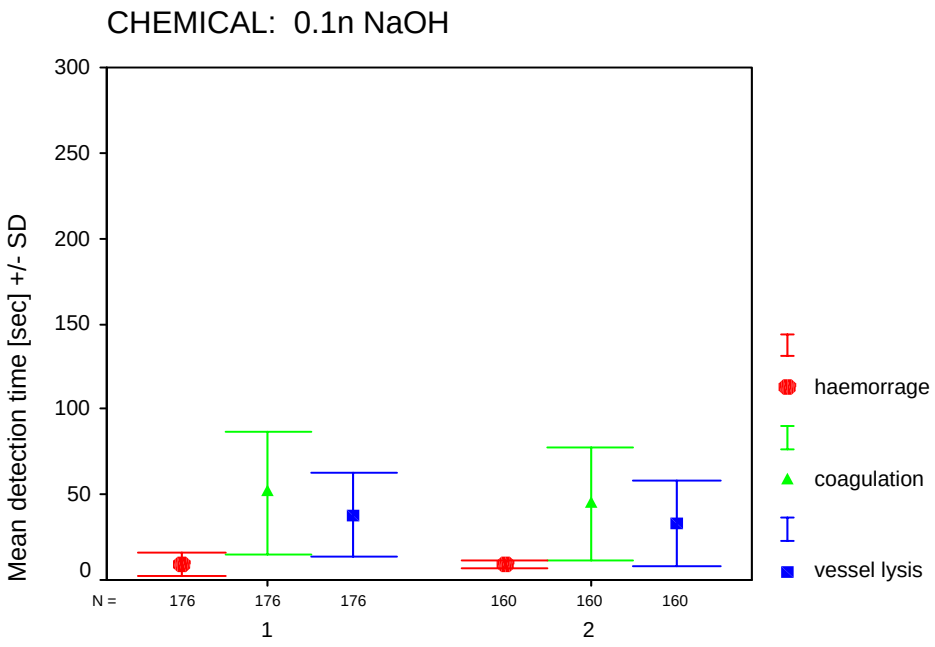

Figure 2: **Error bars of the endpoint values haemorrage, coagulation and vessel lysis (detection time in [sec] +/- Standard deviation (SD) for 1% SLS**

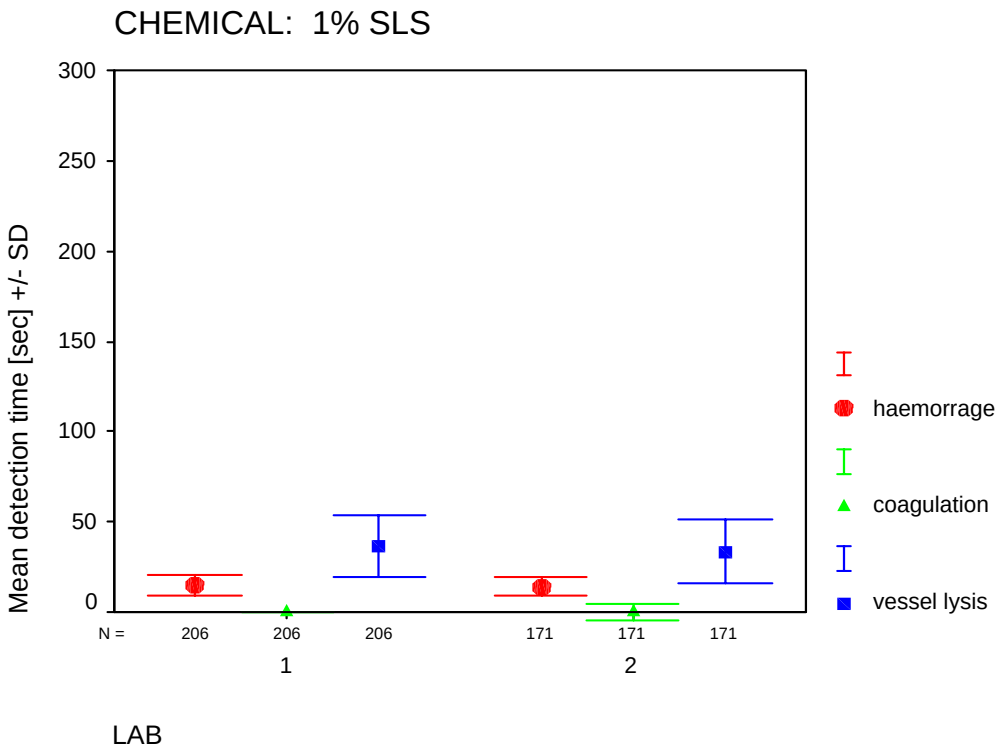

Table 3: **Results of the GLM (General Linear Model) Multivariate procedure for analysis of inter- and intra- laboratory variances for <u>Positive Control 0.1n NaOH</u>**
Sig. = significance = p value

Source	Dependent Variable	Type III Sum of Squares	df	Mean Square	F	Sig.
LAB	haemorrage	15,326	1	15,326	,622	,431
	coagulation	3284,037	1	3284,037	2,756	,098
	vessel lysis	2113,058	1	2113,058	3,481	,063
RUN	haemorrage	8,489	1	8,489	,345	,558
	coagulation	14,236	1	14,236	,012	,913
	vessel lysis	235,342	1	235,342	,388	,534
Error	haemorrage	8200,708	333	24,627		
	coagulation	396836,648	333	1191,702		
	vessel lysis	202147,552	333	607,050		
Total	haemorrage	35207,000	336			
	coagulation	1175624,00	336			
	vessel lysis	630427,000	336			

No significant differences between laboratories (Interlaboratory) and independent runs (intralaboratory) within a laboratory

Table 4: **Results of the GLM (General Linear Model) Multivariate procedure for analysis of inter- and intra- laboratory variances for <u>Positive Control 1% SDS</u>**

Source	Dependent Variable	Type III Sum of Squares	df	Mean Square	F	Sig.
LAB	haemorrage	99,599	1	99,599	3,482	,063
	coagulation	11,484	1	11,484	1,203	,273
	vessel lysis	781,086	1	781,086	2,666	,103
RUN	haemorrage	,861	1	,861	,030	,862
	coagulation	9,890	1	9,890	1,036	,309
	vessel lysis	253,701	1	253,701	,866	,353
Error	haemorrage	10696,589	374	28,601		
	coagulation	3569,057	374	9,543		
	vessel lysis	109576,753	374	292,986		
Total	haemorrage	92119,000	377			
	coagulation	3600,000	377			
	vessel lysis	577280,000	377			

Sig. = significance = p value
No significant differences between laboratories (Interlaboratory) and independent runs (intralaboratory) within a laboratory

Test	1% SLS												0.1n NaOH											
Chem	Laboratory 1						Laboratory 2						Laboratory 1						Laboratory 2					
Code	run1			run2			run1			run2			run1			run2			run1			run2		
	H	C	L	H	C	L	H	C	L	H	C	L	H	C	L	H	C	L	H	C	L	H	C	L
51	9	-	14	14	-	21	18	-	55	16	-	34	8	42	10	11	44	13	14	24	36	10	15	27
53	22	-	47	13	-	24	15	-	22	14	-	22	6	38	-	9	25	-	8	21	14	8	22	13
54	18	-	55	16	-	34	13	-	22	15	-	24	14	24	36	10	15	27	9	23	13	9	19	13
59	17	-	28	18	-	33	13	-	18	10	-	17	11	17	28	12	16	30	8	47	12	7	34	13
60	15	-	22	14	-	22	19	-	78	9	-	65	8	21	14	8	22	13	9	44	61	8	14	88
64	13	-	56	11	-	34	11	-	17	9	-	14	9	38	53	7	53	54	7	41	14	7	46	14
65	10	-	81	9	-	65	10	-	17	13	-	19	5	49	72	8	14	88	9	52	17	6	42	9
66	13	-	35	13	-	22	9	-	65	10	-	76	11	110	20	8	118	41	4	39	74	8	20	87
67	19	-	28	13	-	30	10	-	76	12	-	70	9	82	20	9	92	18	8	20	87	7	15	93
68	25	-	34	13	-	24	21	-	45	15	-	34	11	44	-	9	25	-	12	19	44	12	19	31
72	11	-	86	10	-	76	10	-	15	9	-	14	5	37	104	8	20	87	8	48	12	7	36	13
73	16	-	37	15	-	36	15	-	22	14	-	22	16	24	44	9	15	30	8	21	14	8	22	13
74	26	-	46	21	-	25	12	-	23	17	-	25	10	31	-	10	29	-	8	161	19	7	168	22
75	13	-	58	11	-	34	26	-	46	16	-	34	9	49	66	7	53	54	10	31	-	9	41	-
76	21	-	39	19	-	29	13	-	18	14	-	21	9	33	-	9	45	-	7	28	11	7	31	13
79	15	-	51	18	-	38	17	-	28	18	-	33	10	58	65	10	44	73	11	17	28	12	16	30
80	10	-	76	12	-	70	13	-	18	14	-	21	8	20	87	7	15	93	7	28	11	7	31	13
81	13	-	18	14	-	21				15	-	28	7	28	11	7	31	13				11	76	25
83	16	-	34	17	-	34	14	-	24	17	-	56	12	18	29	10	17	31	7	131	20	10	99	25
84	21	-	39	21	-	25	13	-	18	14	-	21	9	33	-	10	29	-	7	28	11	7	31	13
85	9	-	55	12	-	71							5	17	73	5	21	78						
89	15	-	21	13	-	17	12	-	25	13	-	26	9	39	13	11	52	13	10	163	34	11	104	24
90	12	-	25	12	-	22	14	-	49	11	-	64	9	109	31	10	162	40	10	75	48	8	61	70
91	18	-	34	21	-	31							10	17	33	13	18	30						

96	9	-	36	10	-	25	18	-	36	19	-	36	10	97	25	6	131	18	7	19	29	13	23	34
98	16	-	33	18	-	30	16	-	23	13	-	22	9	13	27	13	18	34	8	15	11	9	21	15
101	16	-	23	13	-	22	17	-	20	13	-	17	8	15	11	9	2	15	8	56	17	10	49	12
102	9	-	55	13	-	54	18	-	34	19	-	36	5	17	73	5	21	64	10	17	33	13	23	34
105	13	-	51	11	-	49	16	-	23	13	-	22	9	48	68	7	54	70	8	15	11	9	21	15
105	11	-	29	13	-	26	16	-	21	14	-	19	9	79	25	7	91	38	12	74	15	10	68	14
107	20	-	41	20	-	39							10	20	33	16	20	39						
108	17	-	44	7	-	41	13	-	19	14	-	18	11	49	56	7	51	58	12	41	15	11	50	16
109	9	-	55	13	-	54	16	-	23	13	-	22	5	17	73	5	21	64	8	15	11	9	21	15
110	20	-	59	14	-	51	11	-	24	13	-	60	7	27	77	5	80	82	7	40	51	7	45	61
111	12	-	31	13	-	27	13	-	35				11	104	24	9	181	22	9	110	23			
113	10	-	25	13	-	29	17	-	41	20	-	37	6	150	18	7	95	48	15	27	47	10	10	31
114	23	-	38	20	-	37							9	18	30	10	20	31						
116	13	-	76	17	-	69							8	23	104	4	17	75						
117	20	-	59	9	-	55	13	-	74	11	-	49	7	27	77	5	17	73	8	57	47	7	54	70
118	10	-	36	22	-	41	14	-	68	12	-	54	16	24	33	15	21	36	8	39	81	5	21	64
119	12	-	52	10	-	55	13	-	35	9	-	36	7	45	75	7	51	61	9	107	23	10	97	25
122	16	-	32	13	-	22							8	15	11	9	21	15						
123	14	-	25	16	-	30							10	120	128	10	104	30						
125	11	-	32	11	-	52	18	-	66	14	-	34	7	41	53	7	57	72	11	17	42	9	21	36
126	22	-	27	12	-	24	19	-	44	30	60	90	7	71	17	10	85	12	9	18	-	8	48	-
127	19	-	44	16	-	30							9	18	-	10	31	-						
128	13	-	59				16	-	18	15	-	21	5	35	73				12	57	16	10	35	16
130	7	-	16	11	-	25	10	-	17	14	-	17	8	107	16	9	76	19	8	23	12	10	29	17
131	19	-	44	16	-	30	16	-	32	16	-	37	9	18	-	10	31	-	9	19	33	10	22	31
132	19	-	44	30	-	75	16	-	18	15	-	21	9	18	-	8	48	-	12	57	16	10	35	16
133	19	-	44	30	-	75	10	-	78	11	-	68	9	18	-	8	48	-	4	21	91	8	38	77
135	16	-	18	15	-	21	11	-	17	9	-	17	12	57	16	10	35	16	11	47	14	7	50	10

136	18	-	66	18	-	38	10	-	21	10	-	45	11	17	42	10	17	36	9	72	19	8	95	20
140	12	-	18	11	-	17							9	44	13	8	27	13						
143	9	-	21	11	-	23	7	-	21	11	-	31	7	104	15	8	103	33	6	52	53	9	41	70
145	10	-	21	13	-	28	9	-	17	14	-	20	9	72	19	8	99	24	7	50	10	9	47	14
146	18	-	38	13	-	36							10	17	36	13	22	38						
147	12	-	25	9	-	26	12	-	72				7	43	53	5	40	55	8	37	88			
148	14	-	57	12	-	46	19	-	44	28	-	54	7	57	68	8	31	58	9	18	-	9	47	-
149	11	-	20	13	-	23	12	-	30	16	-	39	11	48	17	11	48	18	12	22	35	16	22	36
150	14	-	73				19	-	51	14	-	60	5	24	73				7	56	47	11	53	59
151	18	-	65	6	-	27	15	-	22	12	-	19	7	54	54	8	54	62	10	43	18	11	44	15
154	11	-	23	7	-	19	14	-	37	16	-	36	8	103	33	7	117	19	8	15	29	10	19	23
156	11	-	43	13	-	39	12	-	31	14	-	32	9	42	62	7	44	67	7	14	27	10	17	33
159	16	-	23	9	-	21							8	88	20	9	121	35						
160	10	-	32	9	-	26	14	-	19	17	-	20	9	43	54	7	44	61	10	60	13	10	58	12
161	18	-	22	15	-	23							7	22	12	7	21	22						
163	14	-	31	14	-	30	18	-	22	15	-	23	9	13	29	9	15	33	7	22	12	7	21	12
164	23	-	36	22	-	40	9	-	37	9	-	26	15	37	-	13	36	-	10	43	64	7	44	61
165	9	-	52				13	-	18	13	-	18	4	17	84				10	59	14	10	57	13
168	10	-	31	15	-	15	15	-	20	13	-	19	6	67	20	9	141	24	12	62	15	10	57	12
171	10	-	31	15	-	25	18	-	22	15	-	23	6	67	20	9	143	24	7	22	12	7	21	12
172	12	-	30	12	-	64	11	-	22	10	-	24	6	58	55	7	59	69	8	90	26	8	114	26
173	30	-	50	41	-	71	10	-	51				9	34	-	25	49	-	4	22	89			
174	9	-	27	13	-	48	8	-	52	9	-	71	7	43	50	6	35	47	4	18	76	4	21	77
175	10	-	15	13	-	23	6	-	53				7	42	10	7	47	12	4	26	94			
177	30	-	50	41	-	71	14	-	34	15	-	30	9	34	-	25	49	-	13	20	32	8	15	30
178	15	-	34	15	-	39	7	-	33	9	-	23	13	20	32	9	17	31	6	27	49	6	29	43
180	12	-	16	12	-	16	15	-	21	14	-	18	8	31	11	8	21	11	9	54	13	11	52	15
182	30	-	50	41	-	71	12	-	30	13	-	3	9	34	-	25	49	-	10	21	34	10	17	29

184	19	-	53	22	-	61	12	-	62	13	-	48	9	98	29	10	85	35	7	48	46	6	35	47
187	18	-	100	18	-	79	12	-	16	12	-	16	10	143	94	10	16	52	8	31	11	8	21	11
188	15	-	21	15	-	19	33	-	48	33	-	48	12	43	15	8	31	11	11	32	-	11	32	-
189	10	-	37	10	-	42	29	-	51	29	-	51	4	32	49	6	29	46	11	26	-	11	26	-
190	15	-	19	16	-	21	10	-	56	12	-	53	89	31	11	8	37	10	5	29	98	4	23	85
192	11	-	21	12	-	20	15	-	19	14	-	20	14	117	24	12	90	28	8	31	11	9	35	11
193	33	-	48	33	-	52	12	-	33	8	-	22	11	32	-	9	28	-	6	43	54	7	45	61
195	15	-	21	14	-	20	10	-	51				12	43	15	9	35	11	6	21	75			
196	13	-	30	14	-	38							10	19	32	11	18	31						
198	11	-	28	11	-	33	17	-	31	15	-	22	6	35	44	9	35	52	13	74	16	9	58	16
199	15	-	21	14	-	20							12	43	15	9	35	11						
201	12	-	25	13	-	24	29	-	51	29	-	51	7	79	19	9	121	32	11	26	-	11	26	-
202	17	-	50				17	-	21	15	-	22	11	22	58				13	74	16	9	58	16
203	16	-	21	14	-	19	12	-	25	15	-	27	12	74	15	10	68	14	7	79	19	15	88	44
204	9	-	28	13	-	47	13	-	30	10	-	29	6	31	43	8	34	50	10	19	32	9	17	30
206	13	-	24	11	-	27	7	-	54	5	-	68	9	101	32	10	94	24	6	21	109	5	21	117
207	15	-	19	14	-	20	11	-	32	11	-	23	8	31	11	9	32	11	9	79	23	10	97	20
210	13	-	47	8	-	22	14	-	36	16	-	38	8	34	50	8	28	38	8	16	30	8	17	33
211	14	-	36	16	-	38							8	16	30	8	17	33						
212	18	-	40	18	-	40	14	-	38	13	-	28	8	18	-	8	18	-	11	18	31	12	22	36
214	17	-	22	15	-	19	9		27	12	-	25	12	68	16	11	73	14	6	111	35	10	151	26
215	29	-	14	14	-	19	13	-	24	10	-	27	9	70	15	10	63	13	9	118	29	10	117	35
216	14	-	21	13	-	21							10	65	17	10	66	17						
219	17	-	28	11	-	30	13	-	22	13	-	21	7	85	21	12	83	29	9	21	15	6	17	11
223	14	-	18	13	-	17	11	-	24	13	-	29	10	50	14	10	49	12	8	101	24	11	98	46

H = haemorrage; C = coagulation; L = vessel lysis;
detection time of endpoints [sec];
Positive Controls for 105 of 150 coded phase II chemicals were randomly extracted

Appendix I

Individual HET-CAM Scores for Eggs Treated with 0.9% Sodium Chloride

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HET-CAM Test Scores for 0.9% Sodium Chloride

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
183	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
185	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
186	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
188	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
189	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
190	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
191	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
192	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
193	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
194	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
196	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
201	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
202	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
203	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
205	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
207	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
208	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
209	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
210	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
211	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
212	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
213	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
214	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
216	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
217	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
219	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
220	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
222	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
223	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
225	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
230	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
231	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
232	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
233	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
234	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
235	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
236	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
240	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
241	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
242	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
243	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
244	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

HET-CAM Test Scores for 0.9% Sodium Chloride

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
245	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
251	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
252	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
253	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
254	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
255	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
256	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
257	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
258	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
259	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
260	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
261	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
262	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
263	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
264	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
265	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
266	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
267	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
268	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
269	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
270	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
271	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
272	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
273	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
274	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
275	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
276	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
277	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
278	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
279	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
280	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
281	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
282	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1B	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2B	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4B	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
6A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

HET-CAM Test Scores for 0.9% Sodium Chloride

Sequence Number	Hemorrhage Endpoint Score			Lysis Endpoint Score			Coagulation Endpoint Score			*In vitro* score		
	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3	Egg 1	Egg 2	Egg 3
7,8,9,10A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12A	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
16-17-18[1]	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

[1] Studies where a Test Substance Applicator was not used.

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