

## **APPENDIX III-A**

### **SUBSTANCES USED IN THE BCOP TEST METHOD REANALYSIS**

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## **Substances Used in BCOP Test Method Reanalysis**

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Call <sup>5</sup>	In Vitro Consensus Call <sup>6</sup>	In Vivo GHS <sup>15</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>16</sup>	In Vivo Et <sup>17,18</sup>	Reference
gamma-Butyrolactone	96-48-0	Heterocyclic, Lactone	Synthetic intermediate; Solvent	liquid	water soluble	100%	>99	5	Severe	Severe	Category 2A	4	Category II	R36	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water soluble	20%	90	1	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water soluble	20%	90	2	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water soluble	20%	90	3	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water soluble	20%	90	4	Very severe	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water soluble	20%	90	5	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Captan 90 concentrate	133-06-2	Imide, Organic sulfur compound	Pesticide	solid	water insoluble*	20%	95	1	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Not classified	solid	water insoluble*	20%	95	2	Very severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Not classified	solid	water insoluble*	20%	95	3	Severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Not classified	solid	water insoluble*	20%	95	4	Severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
4-Carboxybenzaldehyde	619-66-9	Carboxylic acid, Aldehyde	Not classified	solid	water insoluble*	20%	95	5	Severe	Severe	Category 2A		Category II	R36	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	6%	98	1	Severe	Severe	Category 1	2	SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	6%	98	2	Very severe	Severe	Category 1		SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	6%	98	3	Severe	Severe	Category 1		SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	6%	98	4	Severe	Severe	Category 1		SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	6%	98	5	Severe	Severe	Category 1		SCNM	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	10%	98	1	Moderate	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	10%	98	2	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	10%	98	3	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	10%	98	4	Severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	10%	98	5	Severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	0.10%	98	1	Mild	Mild	Nonirritant	4	Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	0.10%	98	2	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	0.10%	98	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	0.10%	98	4	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic), Germicide, Laboratory reagent	liquid	surfactant	0.10%	98	5	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Chlorhexidine	55-56-1	Amine/Amine	Disinfectant, Mouthwash; Antiseptic	solid	water insoluble*	20%	n.p. <sup>12</sup>	1	Very severe	Very Severe	Category 1	4	SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	Amine/Amine	Disinfectant, Mouthwash; Anti-infective agent	solid	water insoluble*	20%	n.p.	2	Very severe	Very Severe	Category 1		SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	Amine/Amine	Disinfectant, Mouthwash; Anti-infective agent	solid	water insoluble*	20%	n.p.	3	Very severe	Very Severe	Category 1		SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	Amine/Amine	Disinfectant, Mouthwash; Anti-infective agent	solid	water insoluble*	20%	n.p.	4	Very severe	Very Severe	Category 1		SCNM	SCNM	Balls et al. (1995)
Chlorhexidine	55-56-1	Amine/Amine	Disinfectant, Mouthwash; Anti-infective agent	solid	water insoluble*	20%	n.p.	5	Very severe	Very Severe	Category 1		SCNM	SCNM	Balls et al. (1995)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	97	1	Very severe	Moderate	Category 1	2	Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	97	2	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	97	3	Severe	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	97	4	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	97	5	Moderate	Moderate	Category 1		Category I	R41	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	water insoluble*	20%	99	1	Very severe	Very Severe	Category 2A	4	Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	water insoluble*	20%	99	2	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	water insoluble*	20%	99	3	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	water insoluble*	20%	99	4	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Dibenzyl phosphate	1623-08-1	Ester, Organophosphorus compound	Not classified	solid	water insoluble*	20%	99	5	Very severe	Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
2,6-Dichlorobenzyl chloride	4659-45-4	Acyl halide	Anti-infective, Anti-fungal, Preservative	liquid	water insoluble*	100%	99	1	Mild	Mild	Category 2A	4	Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzyl chloride	4659-45-4	Acyl halide	Anti-infective, Anti-fungal, Preservative	liquid	water insoluble*	100%	99	2	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzyl chloride	4659-45-4	Acyl halide	Anti-infective, Anti-fungal, Preservative	liquid	water insoluble*	100%	99	3	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzyl chloride	4659-45-4	Acyl halide	Anti-infective, Anti-fungal, Preservative	liquid	water insoluble*	100%	99	4	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,6-Dichlorobenzyl chloride	4659-45-4	Acyl halide	Anti-infective, Anti-fungal, Preservative	liquid	water insoluble*	100%	99	5	Mild	Mild	Category 2A		Category II	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	96	1	Very severe	Very Severe	SCNM	4	Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	96	2	Very severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	96	3	Very severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	96	4	Very severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	96	5	Severe	Very Severe	SCNM		Category I	SCNM	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes	solid	water insoluble	20%	99.5	1	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Call <sup>5</sup>	In Vitro Consensus Call <sup>5</sup>	In Vivo GHS <sup>6</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>7a</sup>	In Vivo Et <sup>7a,b</sup>	Reference
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes	solid	water insoluble	20%	99.5	2	Moderate	Mild	Category 1	1	Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes	solid	water insoluble	20%	99.5	3	Mild	Mild	Category 1		Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes	solid	water insoluble	20%	99.5	4	Moderate	Mild	Category 1		Category I	R41	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	Alcohol	Intermediate for pharmaceuticals, pesticides, perfumes	solid	water insoluble	20%	99.5	5	Mild	Mild	Category 1		Category I	R41	Balls et al. (1995)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1	Severe	Severe	Category 2A	1	Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2	Moderate	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3	Severe	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	4	Very severe	Severe	Category 2A		Category III	Nonirritant	Balls et al. (1995)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	5	Severe	Severe	Category 2A	1	Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	water soluble	100%	99	1	Mild	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	water soluble	100%	99	2	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	water soluble	100%	99	3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	water soluble	100%	99	4	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Ethyl acetate	141-78-6	Ester	Solvent; Synthetic flavoring	liquid	water soluble	100%	99	5	Mild	Moderate	Nonirritant	1	Category III	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	water soluble	100%	99	1	Severe	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	water soluble	100%	99	2	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	water soluble	100%	99	3	Moderate	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	water soluble	100%	99	4	Severe	Nonsevere	Category 2A		Category II	R36	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	Alcohol	Solvent; Plasticizer	liquid	water soluble	100%	99	5	Mild	Nonsevere	Category 2A	1	Category II	R36	Balls et al. (1995)
Ethyl 2-methylacetocetate	609-14-3	Ketone; Ester	Not classified	liquid	water soluble*	100%	97	1	Moderate	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl 2-methylacetocetate	609-14-3	Ketone; Ester	Not classified	liquid	water soluble*	100%	97	2	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl 2-methylacetocetate	609-14-3	Ketone; Ester	Not classified	liquid	water soluble*	100%	97	3	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl 2-methylacetocetate	609-14-3	Ketone; Ester	Not classified	liquid	water soluble*	100%	97	4	Mild	Mild	Category 2B		Category III	Nonirritant	Balls et al. (1995)
Ethyl 2-methylacetocetate	609-14-3	Ketone; Ester	Not classified	liquid	water soluble*	100%	97	5	Mild	Mild	Category 2B	1	Category III	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	water insoluble*	100%	99	1	Moderate	Mild	Nonirritant		Category II	R36	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	water insoluble*	100%	99	2	Moderate	Mild	Nonirritant		Category II	R36	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	water insoluble*	100%	99	3	Mild	Mild	Nonirritant		Category II	R36	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	water insoluble*	100%	99	4	Mild	Mild	Nonirritant		Category II	R36	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	Ester	Solvent	liquid	water insoluble*	100%	99	5	Mild	Mild	Nonirritant	1	Category II	R36	Balls et al. (1995)
Fomesafen	72128-02-0	Imide; Ether; Nitro compound	Pesticide	solid	water soluble	20%	97.5	1	Moderate	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	Imide; Ether; Nitro compound	Pesticide	solid	water soluble	20%	97.5	2	Very severe	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	Imide; Ether; Nitro compound	Pesticide	solid	water soluble	20%	97.5	3	Severe	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Fomesafen	72128-02-0	Imide; Ether; Nitro compound	Pesticide	solid	water soluble	20%	97.5	4	Mild	Nonsevere	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	Alcohol	Solvent; Plasticizer; Lubricant; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	1	Mild	Mild	Nonirritant	1	Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	Alcohol	Lubricant; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	Alcohol	Lubricant; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	3	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	Alcohol	Lubricant; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	4	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	Alcohol	Lubricant; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	5	Mild	Mild	Nonirritant	1	Category IV	Nonirritant	Balls et al. (1995)
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water insoluble*	100%	98	1	Severe	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water insoluble*	100%	98	2	Very severe	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water insoluble*	100%	98	3	Severe	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water insoluble*	100%	98	4	Moderate	Severe/Very Severe	Category 2A	1	Category II	R36	Balls et al. (1995)
n-Hexanol	111-27-3	Alcohol	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water insoluble*	100%	98	5	Moderate	Severe/Very Severe	Category 2A		Category II	R36	Balls et al. (1995)
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	99	1	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	99	2	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	99	3	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	99	4	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	99	5	Very severe	Very Severe	Category 1	1	Category I	R41	Balls et al. (1995)
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	99.9	1	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	99.9	2	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	99.9	3	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	99.9	4	Moderate	Moderate	Category 2A	1	Category II	R36	Balls et al. (1995)
Isobutanol	78-83-1	Alcohol	Solvent; Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	99.9	5	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro/Test Cat <sup>5</sup>	In Vitro/Consensus Cat <sup>5</sup>	In Vivo GHS <sup>6</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>7a</sup>	In Vivo Et <sup>7a,b</sup>	Reference
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulation (ingredient)	liquid	water soluble	100%	99.9	1	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)	liquid	water soluble	100%	99.9	2	Severe	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulation (ingredient)	liquid	water soluble	100%	99.9	3	Severe	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)	liquid	water soluble	100%	99.9	4	Severe	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Isopropanol	67-63-0	Alcohol	Solvent; Aerosol formulations (ingredient)	liquid	water soluble	100%	99.9	5	Moderate	Severe	Category 2A		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	Amine/Aminine, Organic salt, Urea compound	Pesticide	solid	water soluble	20%	90	1	Severe	None severe	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	Amine/Aminine, Organic salt, Urea compound	Pesticide	solid	water soluble	20%	90	2	Mild	None severe	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	Amine/Aminine, Organic salt, Urea compound	Pesticide	solid	water soluble	20%	90	3	Mild	None severe	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	Amine/Aminine, Organic salt, Urea compound	Pesticide	solid	water soluble	20%	90	4	Severe	None severe	SCNM		Category III	SCNM	Balls et al. (1995)
Maneb	12427-38-2	Amine/Aminine, Organic salt, Urea compound	Pesticide	solid	water soluble	20%	90	5	Moderate	None severe	SCNM		Category III	SCNM	Balls et al. (1995)
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	98	1	Severe	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	98	2	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	98	3	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	98	4	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	98	5	Moderate	Moderate	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	water soluble*	100%	99	1	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	water soluble*	100%	99	2	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	water soluble*	100%	99	3	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	water soluble*	100%	99	4	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methyl cyanacetate	105-34-0	Ester, Nitrile compound	Adhesive; Pharmaceutical intermediate	liquid	water soluble*	100%	99	5	Mild	Mild	Category 2A		Category II	R36	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	2	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	4	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	5	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water insoluble*	100%	>99	6	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	1	Very severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	2	Severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	3	Moderate	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	4	Severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	5	Severe	Severe	Category 2A		Category III	R36	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Dye/coloring	liquid	water insoluble*	100%	98	1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Dye/coloring	liquid	water insoluble*	100%	98	2	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Dye/coloring	liquid	water insoluble*	100%	98	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Dye/coloring	liquid	water insoluble*	100%	98	4	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Dye/coloring	liquid	water insoluble*	100%	98	5	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	water insoluble*	20%	96	1	Very severe	Very Severe	Category 1		Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	water insoluble*	20%	96	2	Severe	Very Severe	Category 1		Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	water insoluble*	20%	96	3	Moderate	Very Severe	Category 1		Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	water insoluble*	20%	96	4	Mild	Mild	Nonirritant		Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid	86-87-3	Carboxylic acid, Polycyclic compound	Pesticide	solid	water insoluble*	20%	96	5	Mild	Mild	Nonirritant		Category I	SCNM	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	water soluble*	20%	95	1	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	water soluble*	20%	95	2	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	water soluble*	20%	95	3	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic compound	Pesticide	solid	water soluble*	20%	95	4	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Cat <sup>5</sup>	In Vitro Consensus Cat <sup>6</sup>	In Vivo GHS <sup>12</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>13</sup>	In Vivo Et <sup>14</sup>	Reference
1-Naphthalene acetic acid, Na salt	61-31-4	Carboxylic acid (salt), Polycyclic aromatic	Pesticide	solid	water soluble*	20%	95	5	Very severe	Very Severe	Category 1	Category I	R41	SCNM	Balls et al. (1995)
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	water insoluble*	100%	>99	1	Moderate	Moderate	Category 2B	Category II	R36	SCNM	Balls et al. (1995)
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	water insoluble*	100%	>99	2	Moderate	Moderate	Category 2B	Category II	R36	SCNM	Balls et al. (1995)
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	water insoluble*	100%	>99	3	Moderate	Moderate	Category 2B	Category II	R36	SCNM	Balls et al. (1995)
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	water insoluble*	100%	>99	4	Mild	Moderate	Category 2B	Category II	R36	SCNM	Balls et al. (1995)
n-Octanol	111-87-5	Alcohol	Solvent; Fragrance	liquid	water insoluble*	100%	>99	5	Moderate	Moderate	Category 2B	Category II	R36	SCNM	Balls et al. (1995)
Parahuaniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	1	Moderate	Moderate	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Parahuaniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	2	Moderate	Moderate	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Parahuaniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3	Moderate	Moderate	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Parahuaniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	4	Moderate	Moderate	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Parahuaniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	5	Moderate	Moderate	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	surfactant	100%	n.p.	1	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	surfactant	100%	n.p.	2	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	surfactant	100%	n.p.	3	Nonirritant	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	surfactant	100%	n.p.	4	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant (nonionic), Lubricant, Plasticizer, Solvent	liquid	surfactant	100%	n.p.	5	Mild	Mild	Nonirritant		Category IV	Nonirritant	Balls et al. (1995)
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	water soluble	20%	97	1	Mild	Mild	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	water soluble	20%	97	2	Mild	Mild	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	water soluble	20%	97	3	Mild	Mild	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	water soluble	20%	97	4	Mild	Mild	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Potassium cyanate	590-28-3	Inorganic salt	Herbicide; Pharmaceutical intermediate	solid	water soluble	20%	97	5	Mild	Mild	SCNM	SCNM	SCNM	SCNM	Balls et al. (1995)
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	water soluble*	20%	98	1	Very severe	Very Severe	Category 1				3
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	water soluble*	20%	98	2	Very severe	Very Severe	Category 1				
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	water soluble*	20%	98	3	Very severe	Very Severe	Category 1				
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	water soluble*	20%	98	4	Very severe	Very Severe	Category 1				
Promethazine hydrochloride	58-33-3	Amine/Amidine, Heterocyclic Organic sulfur compound	Antihistamine; Anti-nausea drug	solid	water soluble*	20%	98	5	Very severe	Very Severe	Category 1				
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	water soluble	100%	>99.9	1	Very severe	Very Severe	Category 1				4
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	water soluble	100%	>99.9	2	Very severe	Very Severe	Category 1				
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	water soluble	100%	>99.9	3	Very severe	Very Severe	Category 1				
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	water soluble	100%	>99.9	4	Very severe	Very Severe	Category 1				
Pyridine	110-86-1	Heterocyclic	Solvent; Intermediate for pharmaceuticals, dyes, pesticides	liquid	water soluble	100%	>99.9	5	Very severe	Very Severe	Category 1				
Oximecarme	69-05-6	Heterocyclic	Drug/Therapeutic agent	solid	water soluble*	20%	n.p.	1	Mild	Mild	Category 1				1
Oximecarme	69-05-6	Heterocyclic	Drug/Therapeutic agent	solid	water soluble*	20%	n.p.	2	Mild	Mild	Category 1				
Oximecarme	69-05-6	Heterocyclic	Drug/Therapeutic agent	solid	water soluble*	20%	n.p.	3	Mild	Mild	Category 1				
Oximecarme	69-05-6	Heterocyclic	Drug/Therapeutic agent	solid	water soluble*	20%	n.p.	4	Mild	Mild	Category 1				
Oximecarme	69-05-6	Heterocyclic	Drug/Therapeutic agent	solid	water soluble*	20%	n.p.	5	Mild	Mild	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	reagent grade	1	Very severe	Very Severe	Category 1				4
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	reagent grade	2	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	reagent grade	3	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	reagent grade	4	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	reagent grade	5	Very severe	Very Severe	Category 1				
Sodium hydroxide (1%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	1%	reagent grade	1	Very severe	Very Severe	Category 2B				NC
Sodium hydroxide (1%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	1%	reagent grade	2	Very severe	Very Severe	Category 2B				
Sodium hydroxide (1%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	1%	reagent grade	3	Very severe	Very Severe	Category 2B				
Sodium hydroxide (1%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	1%	reagent grade	4	Very severe	Very Severe	Category 2B				
Sodium hydroxide (1%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	1%	reagent grade	5	Very severe	Very Severe	Category 2B				
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	3%	98	1	Moderate	Moderate	Nonirritant	Category III	Nonirritant	Balls et al. (1995)	
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	3%	98	2	Moderate	Moderate	Nonirritant	Category III	Nonirritant	Balls et al. (1995)	
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	3%	98	3	Moderate	Moderate	Nonirritant	Category III	Nonirritant	Balls et al. (1995)	
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	3%	98	4	Moderate	Moderate	Nonirritant	Category III	Nonirritant	Balls et al. (1995)	
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	3%	98	5	Mild	Moderate	Nonirritant	Category III	Nonirritant	Balls et al. (1995)	
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	15%	98	1	Moderate	Severe	Category 1				NC
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	15%	98	2	Very severe	Severe	Category 1				
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	15%	98	3	Severe	Severe	Category 1				
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	15%	98	4	Severe	Severe	Category 1				
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic), Detergent	liquid	surfactant	15%	98	5	Moderate	Severe	Category 1				
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing, Pyrotechnic, Industrial byproduct	solid	water soluble	20%	>99	1	Mild	Mild	Category 1				

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Cat <sup>5</sup>	In Vitro Consensus Cat <sup>5</sup>	In Vivo GHS <sup>6</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>7a</sup>	In Vivo Et <sup>7a,b</sup>	Reference
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial hydrex product	solid	water soluble	20%	>99	2	Mild	Mild	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial hydrex product	solid	water soluble	20%	>99	3	Mild	Mild	Category 1		Category I	R41	Balls et al. (1995)
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial hydrex product	solid	water soluble	20%	>99	4	Moderate	Mild	Category 1		Category I	R41	Balls et al. (1995)
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial hydrex product	solid	water soluble	20%	>99	5	Mild	Mild	Category 1		Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	Inorganic salt; Boron compound	Household cleaner; Detergent	solid	water soluble	20%	98.6	1	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	Inorganic salt; Boron compound	Household cleaner; Detergent	solid	water soluble	20%	98.6	2	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	Inorganic salt; Boron compound	Household cleaner; Detergent	solid	water soluble	20%	98.6	3	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	Inorganic salt; Boron compound	Household cleaner; Detergent	solid	water soluble	20%	98.6	4	Severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Sodium perborate	10486-00-7	Inorganic salt; Boron compound	Household cleaner; Detergent	solid	water soluble	20%	98.6	5	Severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified	solid	water insoluble <sup>8</sup>	20%	97	1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified	solid	water insoluble <sup>8</sup>	20%	97	2	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified	solid	water insoluble <sup>8</sup>	20%	97	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified	solid	water insoluble <sup>8</sup>	20%	97	4	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Tetraaminopyrimidine sulfate	5392-28-9	Amine, Heterocycle, Inorganic salt	Not classified	solid	water insoluble <sup>8</sup>	20%	97	5	Mild	Mild	Nonirritant	4	Category III	Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent	solid	water soluble	20%	>99	1	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent	solid	water soluble	20%	>99	2	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent	solid	water soluble	20%	>99	3	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent	solid	water soluble	20%	>99	4	Very severe	Very Severe	Animal died		Animal died	Animal died	Balls et al. (1995)
Thiourea	62-56-6	Organic sulfur compound	Photographic agent; Flame-retardant; Chelation reagent and catalyst; Chemical intermediate; Pesticide; Drug/Therapeutic agent	solid	water soluble	20%	>99	5	Very severe	Very Severe	Animal died	4	Animal died	Animal died	Balls et al. (1995)
Toluene	108-88-3	Hydrocarbon (cycle)	Solvent	liquid	water insoluble <sup>8</sup>	100%	99	1	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	Hydrocarbon (cycle)	Solvent	liquid	water insoluble <sup>8</sup>	100%	99	2	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	Hydrocarbon (cycle)	Solvent	liquid	water insoluble <sup>8</sup>	100%	99	3	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	Hydrocarbon (cycle)	Solvent	liquid	water insoluble <sup>8</sup>	100%	99	4	Moderate	Moderate	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Toluene	108-88-3	Hydrocarbon (cycle)	Solvent	liquid	water insoluble <sup>8</sup>	100%	99	5	Moderate	Moderate	Nonirritant	4	Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	30%	reagent grade	1	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	30%	reagent grade	2	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	30%	reagent grade	3	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	30%	reagent grade	4	Very severe	Very Severe	Category 1		Category I	R41	Balls et al. (1995)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	30%	reagent grade	5	Very severe	Very Severe	Category 1	4	Category I	R41	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	3%	reagent grade	1	Very severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	3%	reagent grade	2	Moderate	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	3%	reagent grade	3	Severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	3%	reagent grade	4	Very severe	Severe/Very Severe	Nonirritant	4	Category III	Nonirritant	Balls et al. (1995)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Caustic agent; Fixative; Herbicide	liquid	water soluble	3%	reagent grade	5	Severe	Severe/Very Severe	Nonirritant		Category III	Nonirritant	Balls et al. (1995)
Triton X-100 (5 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	5%	98	1	Severe	Very Severe	Category 2A	Category III	Nonirritant	Balls et al. (1995)		
Triton X-100 (5 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	5%	98	2	Very severe	Very Severe	Category 2A	Category III	Nonirritant	Balls et al. (1995)		
Triton X-100 (5 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	5%	98	3	Very severe	Very Severe	Category 2A	Category III	Nonirritant	Balls et al. (1995)		
Triton X-100 (5 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	5%	98	4	Very severe	Very Severe	Category 2A	Category III	Nonirritant	Balls et al. (1995)		
Triton X-100 (5 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	5%	98	5	Moderate	Very Severe	Category 2A	NC	Category III	Nonirritant	Balls et al. (1995)	
Triton X-100 (10 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	10%	98	1	Very severe	Severe/Very Severe	Category 1		Category II	R41	Balls et al. (1995)	
Triton X-100 (10 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	10%	98	2	Severe	Severe/Very Severe	Category 1		Category II	R41	Balls et al. (1995)	
Triton X-100 (10 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	10%	98	3	Very severe	Severe/Very Severe	Category 1		Category II	R41	Balls et al. (1995)	
Triton X-100 (10 %)	9002-93-1	Ether	Surfactant (nonionic); Detergent; Emulsifier	surfactant	10%	98	4	Severe	Severe/Very Severe	Category 1	NC	Category II	R41	Balls et al. (1995)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic); Detergent	surfactant	n.p.	98	1	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic); Detergent	surfactant	n.p.	98	2	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic); Detergent	surfactant	n.p.	98	3	Mild	Mild	Nonirritant		Category III	Nonirritant	Balls et al. (1995)	





















Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Cat <sup>5</sup>	In Vitro Consensus Cat <sup>5</sup>	In Vivo GHS <sup>6</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>7a</sup>	In Vivo Et <sup>7a,b</sup>	Reference
Benzalkonium chloride (100%)	8001-54-5	Onium compound	Surfactant (cationic); Bactericide; Fungicide; Preservative	liquid	surfactant	10%	n.p.	3 (7)	Very severe	Very Severe	Category 1		SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	Onium compound	Surfactant (cationic); Bactericide; Fungicide; Preservative	liquid	surfactant	10%	n.p.	3 (8)	Very severe	Very Severe	Category 1		SCNM	R41	Southee (1998)
Benzalkonium chloride (100%)	8001-54-5	Onium compound	Bactericide; Fungicide; Preservative	liquid	surfactant	10%	n.p.	3 (9)	Very severe	Very Severe	Category 1		SCNM	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	1 (1)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	1 (2)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	2 (1)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	2 (2)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	3 (1)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
Butyl cellulose	111-76-2	Alcohol/Ester	Solvent	liquid	n.n.	100%	n.p.	3 (2)	Very severe	Very Severe	Category 1		Category II	R41	Southee (1998)
4-Carboxycbenzaldehyde	619-66-9	Carboxylic acid; Aldehyde	Not classified	solid	water insoluble*	20%	95	1 (1)	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)
4-Carboxycbenzaldehyde	619-66-9	Carboxylic acid; Aldehyde	Not classified	solid	water insoluble*	20%	95	1 (2)	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)
4-Carboxycbenzaldehyde	619-66-9	Carboxylic acid; Aldehyde	Not classified	solid	water insoluble*	20%	95	2 (1)	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)
4-Carboxycbenzaldehyde	619-66-9	Carboxylic acid; Aldehyde	Not classified	solid	water insoluble*	20%	95	3 (1)	Moderate	Moderate	Category 2A		Category II	R36	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (1)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (2)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (3)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (4)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (5)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (6)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	1 (7)	Severe	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (1)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (2)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (3)	Severe	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (4)	Severe	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (5)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (6)	Severe	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (7)	Severe	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	2 (8)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (1)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (2)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (3)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (4)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (5)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (6)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Ethanol	64-17-5	Alcohol	Solvent; Beverages; Antifreeze agent	liquid	water soluble	100%	n.p.	3 (7)	Moderate	Moderate	Category 2A		Category III	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	1 (1)	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	1 (2)	Mild	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	2 (1)	Nonirritant	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	2 (2)	Nonirritant	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	3 (1)	Nonirritant	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Glycerol	56-81-5	Alcohol	Lubricant; Plasticizer; Emollient; Drug vehicle	liquid	water soluble	100%	>99.5	3 (2)	Nonirritant	Nonirritant	Nonirritant		Category IV	Nonirritant	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	1 (1)	Mild	Moderate	Category 1		Category I	R41	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	1 (2)	Mild	Moderate	Category 1		Category I	R41	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	2 (1)	Moderate	Moderate	Category 1		Category I	R41	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	2 (2)	Moderate	Moderate	Category 1		Category I	R41	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	3 (1)	Moderate	Moderate	Category 1		Category I	R41	Southee (1998)
Hexadecytrimethylammonium bromide	57-09-0	Organic salt; Onium compound	Agricultural chemical; Germicide; Drug/Therapeutic agent	surfactant	n.p.	10%	n.p.	3 (2)	Moderate	Moderate	Category 1		Category I	R41	Southee (1998)
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (1)	Very severe	Very Severe	Category 1		Category I	R41	Southee (1998)
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (2)	Very severe	Very Severe	Category 1		Category I	R41	Southee (1998)
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (3)	Very severe	Very Severe	Category 1		Category I	R41	Southee (1998)
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (4)	Very severe	Very Severe	Category 1		Category I	R41	Southee (1998)
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (5)	Very severe	Very Severe	Category 1		Category I	R41	Southee (1998)

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro/Test Cat <sup>5</sup>	In Vitro Consensus Cat <sup>6</sup>	In Vivo GHS <sup>15</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>16</sup>	In Vivo Et <sup>17,18</sup>	Reference
Imidazole	288-32-4	Heterocycle	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (6)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	1 (7)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (1)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (2)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (3)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (4)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (5)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (6)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	2 (7)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (1)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (2)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (3)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (4)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (5)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (6)	Very severe	Very Severe	Category 1				
Imidazole	288-32-4	Heterocyclic	Anti-fungal; Enzyme inhibitor	solid	water soluble	20%	n.p.	3 (7)	Very severe	Very Severe	Category 1				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	1 (1)	Severe	Severe	Category 2B				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	1 (2)	Severe	Severe	Category 2B				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	2 (1)	Very severe	Severe	Category 2B				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	2 (2)	Very severe	Severe	Category 2B				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	3 (1)	Severe	Severe	Category 2B				
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	99	3 (2)	Severe	Severe	Category 2B				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	1 (1)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	1 (2)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	2 (1)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	2 (2)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (1)	Mild	Mild	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (2)	Mild	Mild	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (3)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (4)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (5)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (6)	Moderate	Moderate	SCNM				
Parafluoraniline	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	99	3 (7)	Moderate	Moderate	SCNM				
Benzyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	1 (1)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	1 (2)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	2 (1)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	2 (2)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (1)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (2)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (3)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (4)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (5)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (6)	Mild	Mild	Nonirritant	Category III			
Pronyl 4-hydroxybenzoate	94-13-3	Carboxylic acid; Phenol	Antimicrobial	solid	n.n.	20%	100	3 (7)	Mild	Mild	Nonirritant	Category III			
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	1 (1)	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	1 (2)	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	2 (1)	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	2 (2)	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	3 (1)	Very severe	Very Severe	Category 1				
Sodium hydroxide (10%)	1310-73-2	Alkali	Carcinogen agent	liquid	water soluble	10%	n.p.	3 (2)	Very severe	Very Severe	Category 1				
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	1 (1)	Mild	Mild	Category 1	SCNM			
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	1 (2)	Mild	Mild	Category 1	SCNM			
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	2 (1)	Mild	Mild	Category 1	SCNM			
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	2 (2)	Mild	Mild	Category 1	SCNM			
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	3 (1)	Mild	Mild	Category 1	SCNM			
Sodium lauryl sulfate (15%)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	10%	98	3 (2)	Mild	Mild	Category 1	SCNM			
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	1 (1)	Mild	Mild	Nonirritant	Category 1			
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	1 (2)	Mild	Mild	Nonirritant	Category 1			
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	2 (1)	Nonirritant	Nonirritant	Category 1				
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	2 (2)	Nonirritant	Nonirritant	Category 1				
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	3 (1)	Nonirritant	Nonirritant	Category 1				
Sodium oxalate	62-76-0	Carboxylic acid (salt)	Textile finishing; Pyrotechnic; Industrial byproduct	solid	water soluble	20%	99	3 (2)	Mild	Mild	Nonirritant	Category 1			
Triton X-100 (5%)	9002-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	1 (1)	Mild	Mild	Category 2B				
Triton X-100 (5%)	9002-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	1 (2)	Mild	Mild	Category 2B				

Substance	CASRN <sup>1</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro/Test Cat <sup>2</sup>	In Vitro Consensus Cat <sup>2</sup>	In Vivo GHS <sup>3</sup>	GHS Category 1 SubClass <sup>4</sup>	In Vivo EPA <sup>5</sup>	In Vivo Et <sup>6</sup>	Reference	
Triton X-00 (5%)	9005-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	2(1)	Mild	Category 2B	Category IV	Category II	R36	SCNM	Southee (1998)	
Triton X-00 (5%)	-	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	-	Mild	Category 2B	Category IV	Category II	R34	SCNM	Southee (1998)	
Triton X-00 (5%)	9005-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	3(1)	Nonirritant	Category 2B	Category IV	Category III	R36	SCNM	Southee (1998)	
Triton X-100 (5%)	9005-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	98	3(2)	Nonirritant	Category 2B	Category IV	Category III	R36	SCNM	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	1(1)	Mild	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	1(2)	Mild	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	2(1)	Mild	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	2(2)	Nonirritant	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	3(1)	Nonirritant	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic), Detergent	liquid	surfactant	100%	98	3(2)	Nonirritant	Nonirritant	Nonirritant	Category III	Nonirritant	Nonirritant	Southee (1998)	
Adult-Danduff Shampoo (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category I	1	Category I	R41	SCNM	Gettins et al. (1996)	
Baby Shampoo No. 1 (HZP) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category III	Category III	R41	SCNM	Gettins et al. (1996)	
Baby Shampoo No. 2 (HZP) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category I	1	Category I	R41	SCNM	Gettins et al. (1996)	
Bubble Bath (HZK) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Cleaning Gel (HZQ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category IV	Category IV	R36	SCNM	Gettins et al. (1996)	
Deodorant (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category IV	Category IV	R36	SCNM	Gettins et al. (1996)	
Facial Cleaning Foam (HZZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category I	1	Category IV	R36	SCNM	Gettins et al. (1996)	
Facial Cleanser (HZZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category IV	Category IV	Category IV	R41	SCNM	Gettins et al. (1996)	
From Bath (HZL) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Gel (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category IV	Category IV	R36	SCNM	Gettins et al. (1996)	
Hand Soap (HZU) 25%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category III	Category III	R41	SCNM	Gettins et al. (1996)	
Liquid Soap No. 2 (HZW) 25%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category III	Category III	R41	SCNM	Gettins et al. (1996)	
Liquid Soap No. 1 (HZW) 25%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category III	Category III	Category III	R41	SCNM	Gettins et al. (1996)	
Mild Shampoo (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category IV	Category IV	Category IV	R36	SCNM	Gettins et al. (1996)	
Shampoo Scrub (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Nonirritant	Category IV	Category IV	Category IV	R36	SCNM	Gettins et al. (1996)	
Shampoo No. 1 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 2 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 3 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 4 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 5 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 6 (HZ) 25%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo No. 7 (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shampoo Gel (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Shower Gel (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Skin Cleanser (HZ) 100%	-	-	-	-	-	10%	n.p.	-	Severe	Category 1	1	Category I	R41	SCNM	Gettins et al. (1996)	
Anti-Dandruff Shampoo (HZY)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Baby Shampoo No. H (HZP)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category III	Category III	Nonirritant	Category IV	Nonirritant	Casteron et al. (1996)
Bubble Bath (HZ)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Bubble Bath (HZK)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category III	Category III	Nonirritant	Category IV	Nonirritant	Casteron et al. (1996)
Cleaning Gel (HZO)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category III	Category III	Nonirritant	Category IV	Nonirritant	Casteron et al. (1996)
Fax Make-Up Remover (HZU)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Hand Cream (HZ)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Hand Soap (HZ)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
From Bath (HZL)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Gel Cleanser (HZE)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Mild Shampoo (HZ)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category IV	Category IV	Nonirritant	Category V	Nonirritant	Casteron et al. (1996)
Polishing Scrub (HZ)	-	-	-	-	-	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Shampoo No. 2 (HZ)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Shampoo No. 7 (HZ)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Shower Gel (HZ)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Skin Cleanser (HZI)	-	-	-	-	-	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Acetone	67-64-1	Ketone	Solvent, Antiseptic, Chemical intermediate, Raw material	liquid	water soluble	100%	n.p.	-	Severe	Severe	Category 2A	1	Category II	R36	SCNM	Casteron et al. (1996)
Benzalkonium chloride (1%)	8001-54-5	Inorganic salt, Ozone compound	Surfactant (cationic); Bactericide; Fungicide; Preservative	liquid	surfactant	1%	n.p.	-	Severe	Severe	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Benzalkonium chloride (10%)	8001-54-5	Inorganic salt, Ozone compound	Surfactant (cationic); Bactericide; Fungicide; Preservative	liquid	surfactant	10%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	SCNM	Casteron et al. (1996)
Benzalkonium chloride (5%)	8001-54-5	Inorganic salt, Ozone compound	Surfactant (cationic); Bactericide; Fungicide; Preservative	liquid	surfactant	5%	n.p.	-	Severe	Severe	Category 1	2	Category I	R41	SCNM	Casteron et al. (1996)
4-Bromobenzenoate	-	-	Not classified	n.p.	n.p.	100%	n.p.	-	Mild	Mild	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
β-Butyryl ester	71-36-2	Alcohol	Ingredient of spray paint, nail polish	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
2-Butoxyethanol	111-76-2	Ether	Solvent	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
2-Chlorobutylbenzaldehyde	519-66-9	Carboxylic acid, Aldehyde	Not classified	solid	water insoluble*	100%	n.p.	-	Mild	Mild	Category 2A	1	Category II	R36	SCNM	Casteron et al. (1996)
Cetylpyridinium bromide (0.1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic); Germicide, Laboratory reagent	liquid	surfactant	0%	n.p.	-	Mild	Mild	Nonirritant	Category III	Nonirritant	Category IV	Nonirritant	Casteron et al. (1996)
Cetylpyridinium bromide (1%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic); Germicide, Laboratory reagent	liquid	surfactant	1%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	SCNM	Casteron et al. (1996)
Cetylpyridinium bromide (10%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic); Germicide, Laboratory reagent	liquid	surfactant	10%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	SCNM	Casteron et al. (1996)
Cetylpyridinium bromide (6%)	140-72-7	Heterocyclic, Omin compound	Surfactant (cationic); Germicide, Laboratory reagent	liquid	surfactant	6%	n.p.	-	Severe	Severe	Category 1	2	Category I	R41	SCNM	Casteron et al. (1996)
Cyclohexanol	108-93-0	Alcohol	Solvent, Chemical intermediate	liquid	water soluble	100%	n.p.	-	Severe	Severe	Category 1	2	Category I	R41	SCNM	Casteron et al. (1996)
2,6-Dichlorobenzoyl chloride	4659-45-4	Acyl Halide	Anti-Fungal, Anti-Infective	liquid	water insoluble*	100%	n.p.	-	Mild	Mild	Category 2A	1	Category II	R36	SCNM	Casteron et al. (1996)
2,4-Difluorotriobenzene	446-35-5	Hydrocarbon (halogenated)	Pesticide, Pharmaceutical Intermediate	liquid	n.p.	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
1,3-Diisopropylbenzene	99-62-7	Hydrocarbon (cyclic)	Chloroform, Intermediate, Solvent	liquid	n.p.	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
2,2-Dimethylbutanoic acid	595-37-9	Carboxylic acid	Pharmaceutical metabolite	liquid	water insoluble	100%	n.p.	-	Severe	Severe	SCNM	Category I	SCNM	Casteron et al. (1996)		
Dodecane	112-40-7	Hydrocarbon, cyclic	Indole chemical	liquid	n.p.	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
2-Ethylhexanol	104-76-7	Alcohol	Solvent	liquid	water soluble	100%	n.p.	-	Moderate	Moderate	Category 2A	1	Category II	R36	SCNM	Casteron et al. (1996)
3-Ethyltoluene	620-14-9	Hydrocarbon (cyclic)	Industrial Chemical, Laboratory Chemical	liquid	n.p.	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
Ethyl trimethyl acetate	3938-95-2	Ester	Chemical intermediate	liquid	water insoluble*	100%	n.p.	-	Moderate	Moderate	Nonirritant	Category III	Nonirritant	Category IV	Nonirritant	Casteron et al. (1996)
Glycerol	56-81-5	Alcohol	Lubricant, Emollient, Drug vehicle	liquid	water soluble	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
1,5-Hexadiene	592-42-7	Hydrocarbon (acyclic)	Chemical Intermediate, Industrial Chemical	liquid	n.p.	100%	n.p.	-	Mild	Mild	Mild	Mild	Mild	Mild	Mild	Casteron et al. (1996)
Isobutanol	78-83-1	Alcohol	Solvent, Chemical intermediate; Flavor ingredient	liquid	water insoluble*	100%	n.p.	-	Severe	Severe	Category 2A	1	Category II	R36	SCNM	Casteron et al. (1996)
Isopropanol	67-63-0	Alcohol	Solvent, Alcohol, formulations (ingredient)	liquid	water soluble	100%	n.p.	-	Moderate	Moderate	Category 2A	1	Category III	SCNM	Casteron et al. (1996)	

Substance	CASRN <sup>4</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Call <sup>5</sup>	In Vitro Consensus Call <sup>5</sup>	In Vivo GHS <sup>6</sup>	GHS Category 1 SubClass <sup>6</sup>	In Vivo EPA <sup>7a</sup>	In Vivo Et <sup>7a,b</sup>	Reference
Methyl acetate	79-20-9	Ester	Solvent; Chemical intermediate; Synthetic flavor ingredient	liquid	water soluble	100%	n.p.	-	Moderate	Moderate	Category 2A		Category II	R36	Casteron et al. (1996)
Methyl ethyl ketone	78-93-3	Ketone	Solvent; Manufacture of lacquers, varnishes, cosmetics, pharmaceuticals	liquid	water soluble	100%	n.p.	-	Moderate	Moderate	Category 2A		Category III	R36	Casteron et al. (1996)
Methyl isobutyl ketone	108-10-1	Ketone	Solvent; Synthetic flavor; Solvent cleaning	liquid	water insoluble <sup>8</sup>	100%	n.p.	-	Moderate	Moderate	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
1-Methylpropylbenzene	135-98-8	Hydrocarbon (cyclic)	Solvent	liquid	n.p.	100%	n.p.	-	Mild	Mild					Casteron et al. (1996)
Parahexamethylene diamine	371-40-4	Amine/Amidine	Intermediate for herbicides	liquid	water insoluble	100%	n.p.	-	Moderate	Moderate	SCNM		SCNM	SCNM	Casteron et al. (1996)
Polyethylene glycol 400	25322-68-3	Alcohol, Polyether	Surfactant; Lubricant; Plasticizer; Solvent	liquid	surfactant	100%	n.p.	-	Mild	Mild	Nonirritant		Category IV	Nomirrant	Casteron et al. (1996)
Polyethylene glycol 600	-	Alcohol, Polyether	Surfactant (nonionic); Lubricant; Plasticizer; Solvent	liquid	surfactant	100%	n.p.	-	Mild	Mild					Casteron et al. (1996)
Propylene glycol	57-55-6	Alcohol	Solvent	liquid	n.p.	100%	n.p.	-	Mild	Mild					Casteron et al. (1996)
Sodium hydroxide (1%)	1310-73-2	Alkali	Cause agent	liquid	water soluble	1%	n.p.	-	Severe	Severe	Category 2B		Category III	R36	Casteron et al. (1996)
Sodium hydroxide (10%)	1310-73-2	Alkali	Cause agent	liquid	water soluble	10%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Casteron et al. (1996)
Sodium lauryl sulfate (15 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	15%	n.p.	-	Moderate	Moderate	Category 1	NC	Category I	R36	Casteron et al. (1996)
Sodium lauryl sulfate (3 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	3%	n.p.	-	Mild	Mild	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
Sodium lauryl sulfate (30 %)	151-21-3	Carboxylic acid (salt)	Surfactant (anionic); Detergent	liquid	surfactant	30%	n.p.	-	Moderate	Moderate					Casteron et al. (1996)
Toluene	108-88-3	Hydrocarbon (cyclic)	Cause agent; Irritative; Herbicide	liquid	water insoluble <sup>8</sup>	100%	n.p.	-	Severe	Severe	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
Trichloroacetic acid (3%)	76-03-9	Carboxylic acid	Cause agent; Irritative; Herbicide	liquid	water soluble	3%	n.p.	-	Mild	Mild	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
Trichloroacetic acid (30%)	76-03-9	Carboxylic acid	Cause agent; Irritative; Herbicide	liquid	water soluble	30%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Casteron et al. (1996)
Triton X-100 (5%)	9002-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	5%	n.p.	-	Moderate	Moderate	Category 2A		Category III	Nomirrant	Casteron et al. (1996)
Triton X-100 (1%)	9002-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	1%	n.p.	-	Mild	Mild					Casteron et al. (1996)
Triton X-100 (10%)	9002-93-1	Ether	Surfactant (nonionic)	liquid	surfactant	10%	n.p.	-	Severe	Severe	Category 1	NC	Category II	R41	Casteron et al. (1996)
Tween 20	9005-64-5	Ester, Polyester	Surfactant (nonionic); Detergent	liquid	surfactant	100%	n.p.	-	Mild	Mild	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
Xylene	1130-20-7	Hydrocarbon (cyclic)	Industrial Chemical; Laboratory Chemical; Pharmaceutical; Intermediate; Solvent	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Nonirritant		Category II	Nomirrant	Casteron et al. (1996)
Amway all fabric bleach	-	Formulation	Bleach (laundry)	n.p.	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Casteron et al. (1996)
Amway automatic dishwashing compound for soft water	-	Formulation	Detergent	n.p.	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Casteron et al. (1996)
Amway automatic dishwashing compound, standard formula	-	Formulation	Detergent	n.p.	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category I	R41	Casteron et al. (1996)
Amway concrete floor cleaner	-	Formulation	Cleaner	n.p.	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	SCNM	R41	Casteron et al. (1996)
Amway fresh Down's dishwashing liquid	-	Formulation	Detergent	n.p.	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category I	R41	Casteron et al. (1996)
Amway all purpose bleach	-	Formulation	Detergent	n.p.	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category II	R41	Casteron et al. (1996)
Amway fabric softener	-	Formulation	Fabric softener	n.p.	n.p.	100%	n.p.	-	Mild	Mild	Nonirritant		Category III	Nomirrant	Casteron et al. (1996)
Amway Kool Wash delicate fabric detergent	-	Formulation	Detergent	n.p.	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category I	R36	Casteron et al. (1996)
Amway 1-OC all purpose cleaner	-	Formulation	Cleaner	n.p.	n.p.	100%	n.p.	-	Mild	Mild	SCNM		SCNM	Nomirrant	Casteron et al. (1996)
Amway prewash liquid	-	Formulation	Detergent	liquid	n.p.	100%	n.p.	-	Mild	Mild	SCNM		SCNM	Casteron et al. (1996)	
Amway Purpose disinfectant cleaner	-	Formulation	Cleaner	n.p.	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Casteron et al. (1996)
Amway Red's dye stain remover	-	Formulation	Stain remover	n.p.	n.p.	100%	n.p.	-	Mild	Mild	Category 2A		Category II	Nomirrant	Casteron et al. (1996)
Amway SAS laundry liquid	-	Formulation	Detergent	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	1	Category I	R41	Casteron et al. (1996)
Amway SAS limited phos laundry powder	-	Formulation	Detergent	sold	n.p.	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category I	R41	Casteron et al. (1996)
Toilet Bowl Cleaner (#1)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Mild	Mild	Nonirritant		Category IV	Nomirrant	Swanson et al. (1995)
Floor Cleaner (#2)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Nonirritant	Nonirritant					Swanson et al. 1995
Meat Room Degreaser (#3)	-	Formulation	Degreaser	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. 1995
Toilet Bowl Cleaner (#4)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Mild	Mild	Nonirritant		SCNM	Nomirrant	Swanson et al. (1995)
All Purpose Cleaner (#5)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Bathroom Cleaner (#6)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe	SCNM		Category III	Nomirrant	Swanson et al. (1995)
All Purpose Cleaner (#7)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Pot and Pan Cleaner (#8)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Nonirritant	Nonirritant					Swanson et al. (1995)
Heavy Duty Cleaner/Degreaser (#9)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Floor Cleaner (#10)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
General Cleaner (#11)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
General Cleaner (#12)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Cleaner/Degreaser (#13)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Floor Stripper (#14)	-	Formulation	Floor stripper	liquid	n.p.	100%	n.p.	-	Severe	Severe					Swanson et al. (1995)
Heavy Duty Cleaner (#15)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)
Degreaser (#16)	-	Formulation	Degreaser	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Floor Stripper (#17)	-	Formulation	Floor stripper	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	NC	Category I	R41	Swanson et al. (1995)
Floor Stripper (#18)	-	Formulation	Floor stripper	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Glass Cleaner (#19)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
Metal Cleaner (#20)	-	Formulation	Cleaner	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	4	Category I	R41	Swanson et al. (1995)
1-1 (#1)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)
1-2 (#2)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Mild	Mild	Category 2A		Category II	R36	Swanson and Harbell (2000)
1-3 (#3)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Category 2A		Category II	R36	Swanson and Harbell (2000)
2-4 (#4)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Mild	Mild	Nonirrant		Category IV	Nonirrant	Swanson and Harbell (2000)
2-7 (#7)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Nonirrant		Category IV	Nonirrant	Swanson and Harbell (2000)
2-8 (#8)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Nonirrant		Category III	Nonirrant	Swanson and Harbell (2000)
Benchmark-Group 1 (#12)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 2A		Category I	R36	Swanson and Harbell (2000)

Substance	CASRN <sup>1</sup>	Chemical Class	Product Class	Form Tested	Solubility	Concentration Tested	Purity (%)	Lab No.	In Vitro Test Call <sup>2</sup>	In Vitro Consensus Call <sup>3</sup>	In Vivo GHS <sup>4</sup>	GHS Category 1 SubClass <sup>5</sup>	In Vivo EPA <sup>6</sup>	In Vivo EU <sup>7,8</sup>	Reference
Benchmark-Group 2 (#13)	-	Formulation	Insect repellent	liquid	n.p.	100%	n.p.	-	Severe	Severe	Category 1	1	Category I	R41	Swanson and Harbell (2000)
Ethanol (#14)	64-17-5	Alcohol	Solvent; Beverages; Antifreeze/antifrost	liquid	n.p.	100%	n.p.	-	Moderate	Moderate	Category 2A	-	Category I	R36	Swanson and Harbell (2000)
Alkyl phosphoric acid ester/amine salt	-	Formulation, petrochemical	Lubricant additive; petrochemical product	liquid	moderate	100%	n.p.	-	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
Aromatic hydrocarbon #1	-	Aromatic hydrocarbon	Solvent/industrial chemical; Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Aromatic hydrocarbon #2	-	Aromatic hydrocarbon	Solvent/industrial chemical; Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Aryl phosphonates	-	Formulation, petrochemical	Lubricant additive; petrochemical product	liquid	moderate	100%	n.p.	-	Moderate	Moderate	Category 2B	-	SCNM	SCNM	Bailey et al. (2004)
Carboxylic acid amides	-	Formulation, petrochemical	Lubricant additive; petrochemical product	solid	moderate	100%	n.p.	-	Moderate	Moderate	Category 1	4	Category I	R41	Bailey et al. (2004)
2-Chloro-2,4,4-trimethylpentane	-	Chlorinated hydrocarbon	Solvent/industrial chemical; Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Clarified slurry oil	-	Oil	Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #1	-	-	Petrochemical product	liquid	emulsifies	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Cutting fluid (conc.) #2	-	-	Cutting fluid; Petrochemical product	liquid	emulsifies	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category III	Nonirritant	Bailey et al. (2004)
Ethyhexyl acid phosphate ester	-	Formulation, petrochemical	Lubricant additive; petrochemical product	liquid	moderate	100%	n.p.	-	Severe	Severe	Category 1	4	SCNM	R41	Bailey et al. (2004)
5-Ethylidene-2-norbornene	16219-75-3	Terpene	Solvent/industrial chemical; Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Methyl cyclopentadiene dimer	-	Cyclic hydrocarbon	Solvent/industrial chemical; Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Petroleum wax	-	Wax	Petrochemical product	solid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Polyalkylene succinate ester/amine salt	-	Formulation, petrochemical	Lubricant additive; petrochemical product	liquid	moderate	100%	n.p.	-	Mild	Mild	SCNM	-	Category III	SCNM	Bailey et al. (2004)
Process oil	-	Oil	Petrochemical product	liquid	negligible	100%	n.p.	-	Mild	Mild	Nonirritant	-	Category IV	Nonirritant	Bailey et al. (2004)
Thiadiazole alkyl derivative	-	Formulation, petrochemical	Lubricant additive; petrochemical product	liquid	negligible	100%	n.p.	-	Moderate	Moderate	SCNM	-	Category III	SCNM	Bailey et al. (2004)

<sup>1</sup>CASRN=Chemical Abstract Services Registry Number<sup>2</sup>In Vitro Test Call represents the BCOP ocular irritancy classification assigned for each chemical in the study for each test for a specific substance<sup>3</sup>Concensus call represents the overall BCOP ocular irritancy classification assigned for each chemical in the study based on the majority of ocular irritancy classification calls<sup>4</sup>GHS=Globally Harmonized System (UN [2003])<sup>5</sup>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<sup>6</sup>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.<sup>7</sup>EPA=U.S. Environmental Protection Agency (EPA [1996]).<sup>8</sup>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.<sup>9</sup>EU=European Union (EU [2001]).<sup>10</sup>Risk phrase R41 = risk of serious damage to the eyes; R36 = irritating to the eyes; nonirritant = not an eye irritant.<sup>11</sup>SCNM=Study Criteria Not Met<sup>12</sup>n n =not provided<sup>13</sup>n a =not applicable

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