

RC Chemicals with Rat LD50 Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
29	Mercury II chloride	7487-94-7	Neg	4.07	1	184	Hypothetical: Changes membrane potentials & blocks enzyme reactions in cells by targeting the sulfhydryl part of active sites of some enzymes.	
143	Triethylene melamine	51-18-3	Neg	0.16	1	38	Genotoxic; binds with DNA; alkylating agent; alkylates proteins	
177	Busulphan	55-98-1	Neg	11.33	2	272	Hypothetical: Alkylation of sulfhydryl groups; Anti-neoplastic	
13	Cycloheximide	66-81-9	Neg	0.17	2	47	Inhibition of protein synthesis?; metabolic inhibitor; liver toxicity	requires metabolic activation
51	Disulfoton	298-04-4	Neg	30.19	2	443	Assumed to be same as malathion: Inhibition of acetylcholinesterase resulting in acetylcholine accumulation in CNS & effector organs; irreversible cholinesterase inhibitor	
49	Parathion	56-38-2	Neg	27.09	2	437	Assume to be same as malathion: Inhibition of acetylcholinesterase resulting in acetylcholine accumulation in CNS & effector organs; irreversible cholinesterase inhibitor	
234	Phenylthiourea	103-85-5	Neg	82.20	3	491	Destroys cytochrome p450; interferes with pulmonary, thyroid functions.	
37	Aflatoxin B1	1162-65-8	Neg	10.62	5	303	Hepatotoxicity	requires metabolic activation
137	Triethyltin chloride	994-31-0	Neg	0.11	5	36	Neurotoxic	
2	Actinomycin D	50-76-0		0.01	7	32	Bone marrow depression; binds with double helical DNA; blocks transcription of DNA by RNA polymerase	
252	Potassium cyanide	151-50-8	Neg	72.93	10	288	General enzyme inhibition. Interferes with ATP synthesis. High affinity for Fe ⁺⁺⁺ . Inhibits cell respiration by inhibition of cytochrome oxidase.	
148	Nitrogen mustard * HCl	55-86-7	Neg	0.50	10	61	Alkylating agent	
60	Indomethacin	53-86-1	Neg	57.25	12	680	Nephrotoxicity	

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14	Mitomycin C	50-07-7		0.28	14	65	Carcinogenic; bone marrow depression; suppresses normal defense mechanisms	
153	Arsenic III trioxide	1327-53-3		0.83	20	77	Cellular poison. Multisystem failure due to uncoupling oxidative phosphorylation & inhibition of pyruvate and succinate oxidative pathways; Apoptosis induction; angiogenesis inhibition; cellular growth inhibition	
192	1,3-Bis(2-chloroethyl)-1-nitrosourea	154-93-8	Neg	16.70	20	298	Alkylating agent	requires metabolic activation
150	Cis-platinum	15663-27-1		0.84	26	98	Causes kidney failure; myelosuppression; causes apoptosis in proximal tubule cells	
68	2,4-Dinitrophenol	51-28-5	Neg	38.67	29	394	Interferes with ATP synthesis	requires metabolic activation
43	Aldrin	309-00-2	Neg	24.45	40	475	Neuronal	
185	Heptachlor	76-44-8	Neg	22.02	41	460	Neuronal	
132	Triphenyltin hydroxide	76-87-9		0.02	44	21	Affects immune system; causes lymphopenia; clastogenic	
241	Sodium azide	26628-22-8	Neg	46.16	45	236	Interferes with ATP synthesis (like potassium cyanide)	
207	Dieldrin	60-57-1	Neg	68.56	46	762	Neuronal	
179	Acrolein	107-02-8		2.64	46	63	Cytotoxic; inhibits nucleic acid synthesis; affects respiratory functions; reacts w/ protein and nonprotein sulfhydryl groups	
144	Sodium bichromate VI	10588-01-9		0.24	50	53	Inhibition of respiratory chain activity; carcinogenic	
103	Nicotine	54-11-5	Neg	290.45	50	881	CNS nicotinic receptor; cholinergic block causing polarization of CNS and PNS synapses.	
173	Pentachlorophenol	87-86-5	Neg	9.59	51	264	Uncouples oxidative phosphorylation	
262	Amphetamine sulfate	60-13-9	Neg	726.02	55	2087	Neurotoxic	
8	Digitoxin	71-63-6		0.08	56	61	Cardiotoxic; neurotoxic; causes hyperkalemia	

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235	Paraquat	4685-14-7	Neg	100.58	58	601	Multisystem failure due to depletion of superoxide dismutase, with formation of free radicals & lipid peroxidation. Lung fibrosis due to accumulation; interferes with ATP synthesis.	
157	Hexachlorophene	70-30-4		3.21	61	209	Hypothetical: Uncoupling of oxidative phosphorylation. Binding to proteins in cytoplasmic membrane & cell organelles.	
292	Allylalcohol	107-18-6	Neg	403.14	64	569	Hepatatoxin; aldehyde; acrolein	requires metabolic activation
10	Emetine	483-18-1		0.08	67	45	Myotoxin; inhibits protein synthesis; disrupts mitochondrial oxidative phosphorylation; affects cardiovascular system; muscle necrosis	
223	Lindane	58-89-9	Neg	119.24	76	832	CNS depression through inhibition of GABA receptor linked chloride channel at the picrotoxin binding site, leading to blockade of chloride influx into neurons?	
255	Sodium monochloroacetate	3926-62-3	Neg	168.90	76	577	Herbicide	
190	Chlorambucil	305-03-3	Neg	23.12	76	418	Alkylating agent	
149	Chromium VI trioxide	1333-82-0		0.27	80	32	Affects respiratory functions; causes nephritis; corrosive	
180	p-Phenylenediamine	106-50-3		5.41	80	124	Affects kidney functions; breaks down muscle fibers	
62	Cobalt II chloride	7646-79-9		20.77	80	247	Cardiotoxic; hematotoxic	
110	Acrylonitrile	107-13-1		128.43	82	329	Carcinogenic; affects respiratory functions	
237	Beryllium II sulfate	13510-49-1		64.09	82	357	Carcinogenic; causes liver necrosis; inhibits ATP	
220	m-Dinitrobenzene	99-65-0	Neg	65.57	82	471	Interferes with ATP synthesis	
229	Dextropropoxyphene * HCl	1639-60-7	Neg	184.23	83	1163	CNS, respiratory depressor	

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20	Cadmium II chloride	10108-64-2		1.17	88	86	Alters calcium translocation; affects membrane ATP and mitochondrial respiration	
219	Hydralazine	86-54-4 304-20-1		52.87	90	417	Cardiotoxic; arteriolar vasodilator; clastogenic effect in liver	
160	N-Methyl-N'-nitro-N-nitroso- guanidine	70-25-7		1.77	90	91	Alkylating agent; teratogen; affects liver	
283	Milrinone	78415-72-2	Neg	1007.61	91	1758	Cardiac-positive ionotropic action	
116	Cyclophosphamide * H ₂ O	6055-19-2 50-18-0	Neg	870.89	95	1931	Alkylating agent	requires metabolic activation
217	Amrinone	60719-84-8		52.42	101	454	Cardiac drug; calcium channel blocker	
194	p-Toluylendiamine	95-70-5		11.49	101	184	Hair dye; skin sensitizer	
74	Nickel II chloride	7718-54-9		34.99	105	309	affects ATP activity in the brain; affects enzymes	
281	1,2-Dibromomethane	106-93-4 74-95-3	Neg	730.17	108	1369	Covalent binding to macromolecules	requires metabolic activation
196	VerapamilHCl	152-11-4	Neg	49.11	108	761	Inhibition of transmembrane Ca++ flux in excitatory tissues. Cardiac-Ca++ channel blocker. Also alpha-adrenergic blockade.	
198	loxynil	1689-83-4	Neg	40.80	111	599	Herbicide	
151	Hexachlorocyclopentadiene	77-47-4		0.85	112	93	Affects respiratory functions; toxicity a consequence of reactivity in Diels-Alder reactions where a conjugated diene combines with a substituted or unsubstituted alkene (a dienophile) in a cycloaddition reaction	
167	p,p'-DDD	72-54-8		7.68	112	266	Carcinogenic; neurotoxic	
61	p,p'-DDT	50-29-3	Neg	56.72	113	674	Inhibits ADP phosphorolation	
138	Tributyltin chloride	1461-22-9		0.18	120	52	Neurotoxic	
232	o-Cresol	95-48-7		56.24	121	343	Affects respiratory, circulatory, and cardiac systems; protoplasmic poison	
347	Thiourea	62-56-6	Neg	6547.18	125	2229	Inhibits thyroperoxidase	

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69	Secobarbital sodium	309-43-3		54.66	125	557	Affects respiratory functions; CNS depression; Enhancement of inhibition occurs primarily at synapses where neurotransmission is mediated by GABA acting at GABAa receptors	
134	Rotenone	83-79-4		0.05	130	34	Inhibitor of the mitochondrial oxidative phosphorylation-electron transport system; mitochondrial poison; blocks NADH oxidation	
9	Amethopterin	59-05-2		0.06	136	40	Folic acid antagonist; inhibits RNA and protein synthesis	
199	Cupric chloride	7447-39-4 1344-67-8		14.79	140	217	Affects enzymes; affects respiratory, liver and kidney functions	
27	Chlorpromazine	50-53-3		4.46	140	210	Alpha-adrenergic antagonistic activity; CNS depression	
96	Cygon	60-51-5	Neg	284.29	151	1062	Inhibits cholinesterase - mustard agent?	
227	Sodium oxalate	62-76-0		58.96	155	395	Hypothetical: Ca ⁺⁺ -complexing action, depressing the level of ionized Ca ⁺⁺ in body fluids, but doesn't explain action on GI, vasculature, & kidney. Corrosivity not due to acidity	
118	Phenobarbital	50-06-6	Neg	884.91	163	1753	Neurotoxic; CNS depression through inhibition of GABA synapses? Inhibits hepatic NADH cytochrome oxidoreductase;	
225	Ammonium sulfide	12135-76-1 12124-99-1		21.47	168	148	Irritant	
16	Azaserine	115-02-6		0.35	170	49	Amino acid antagonist;	
102	Acrylamide	79-06-1		114.45	170	369	Acute administration of acrylamide inhibits the oxidative enzyme complex nicotinamide adenine dinucleotide (reduced form)-tetrazolium reductase and slows retrograde axoplasmic transport; carcinogenic	
64	Bendiocarb	22781-23-3		40.19	179	447	Cholinesterase inhibitor	

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106	Sodium I fluoride	7681-49-4		77.68	180	231	Hypothetical: Protoplasmic poison interfering with many enzymes. May lower sarcoplasmic Ca ⁺⁺ & induce K ⁺ efflux from cells	
112	Caffeine	58-08-2	Neg	512.74	192	1249	Hypothetical: Inhibition of phosphodiesterase leading to AMP accumulation. Translocation of intracellular Ca ⁺⁺ ? Adenosine receptor antagonism?; neurotoxic	
253	Isoxepac	55453-87-7	Neg	356.81	199	1281	Interferes with kidney and heart functions	
318	Trifluoroacetic acid	76-05-1	Neg	2337.62	200	1789	Metabolic poison?	
87	Pentobarbital sodium	57-33-0		176.29	201	902	Affects respiratory functions	
212	p-Cresol	106-44-5		23.79	207	236	Affects respiratory, circulatory, and cardiac systems; protoplasmic poison	
17	5-Fluorouracil	51-21-8	Pos	0.34	230	41	Antimetabolite; pyrimidine analog	
206	Diquat dibromide	85-00-7		55.05	231	654	Hypothetical: Multisystem failure due to depletion of superoxide dismutase, formation of free radicals & lipid peroxidation. Lung fibrosis due to accumulation.	
239	m-Cresol	108-39-4		71.38	242	381	affects respiratory, circulatory, and cardiac systems; protoplasmic poison	
269	Potassium I fluoride	7789-23-3		181.85	245	402	fluoride inhibits acetylcholinesterase	
73	Carbaryl	63-25-2		52.32	250	472	inhibition of acetylcholinesterase; carcinogenic	
35	Flufenamic acid	530-78-9		8.16	273	254	affects respiratory functions	
260	Coumarin	91-64-5		249.92	292	778	inhibit glucose-6-phosphatase in liver; induces hepatotoxicity; CNS depressant; rodenticide	requires metabolic activation
228	2,4,5-Trichlorophenoxyacetic acid	93-76-5		112.41	299	754	carcinogenic; hepatotoxin	
81	Cupric sulfate * 5 H ₂ O	7758-99-8		82.40	300	650	Hypothetical: Copper is reduced by thiol groups in cell membranes. superoxide is formed by reoxidation of copper, inducing lipid peroxidation	
245	Resorcinol	108-46-3		88.10	301	421	may cause methemoglobinemia	

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279	Thioacetamide	62-55-5		313.33	301	590	decreases the synthesis of cytochrome p450b; carcinogenic; hepatotoxin	requires metabolic activation
38	Imipramine * HCl	113-52-0		17.11	304	375	antidepressant; affects parasympathetic nervous system, CNS and cardiovascular system	
205	Versalide	88-29-9		38.77	315	477	polycyclic musk; used in fragrances; neurotoxic	
261	Ferrous sulfate	7720-78-7		281.03	319	837	hepatotoxin; causes coagulopathy	
183	Amitriptyline	50-48-6		15.54	319	334	Hypothetical: Blocks norepinephrine, 5-hydroxytryptamine, and dopamine presynaptic uptake; prevents reuptake of heart norepinephrine.	
86	Warfarin	81-81-2		206.59	324	1092	anticoagulant rodenticide; Depresses formation of prothrombin & increases capillary fragility, leading to hemorrhages; decreases H thymidine and C leucine incorporation	
176	Papaverine	58-74-2		15.27	326	371	inhibitor of cyclic nucleotide phosphodiesterase; inhibitor of cellular respiration and a weak calcium-channel blocking agent	
249	3-Cyano-2-morpholino-5-(pyrid-4-yl)-pyridine (Chemical 122)			255.66	346	1103	??	
282	(-)Phenylephrine	59-42-7		744.17	350	1350	CNS stimulant; alpha-receptor stimulant	
55	Zinc II chloride	7646-85-7		17.72	350	237	corrosive; affects respiratory functions	
278	Phenylephrine * HCl	61-76-7		847.35	350	1597	CNS stimulant; alpha-receptor stimulant	
210	p-Nitrophenol	100-02-7		27.82	351	291	may cause methemoglobinemia; uncouple the metabolic process of oxidative phosphorylation; CNS depressant	
246	Barium II nitrate	10022-31-8		211.70	355	1006	causes hypokalemia	
90	Iproniazid	54-92-2		141.61	366	682	monoamine oxidase (MAO) inhibitors; antidepressant; hepatotoxin	metabolizes to isopropylhydrazine

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254	Buflomedil	55837-25-7		415.03	366	1477	phosphodiesterase enzyme inhibitor	
89	2,4-Dichlorophenoxy-acetic acid	94-75-7		170.20	369	832	causes metabolic acidosis	
79	Phenylbutazone	50-33-9		98.69	376	792	Inhibits biosynthesis of prostaglandins, uncouples oxidative phosphorylation, & inhibits ATP-dependent biosynthesis of mucopolysaccharide sulfates in cartilage	
172	Nabam	142-59-6		8.97	395	251	inhibits enzyme activity by complexing with metal-containing enzymes	
155	Benzalkonium chloride	8001-54-5		1.90	402	156	causes metabolic acidosis; corrosive	
159	Hexadecyltrimethylammoniumbromide	57-09-0		3.24	408	197	cationic surfactant	
115	Phenol	108-95-2		283.30	414	641	General protoplasmic poison that denatures proteins; depresses vasomotor center	
230	Orphenadrine * HCl	341-69-5		149.88	425	946	cardiotoxic; affects respiratory functions	
291	Aniline	62-53-3		642.67	440	910	induces DNA damage in vivo in the liver and kidneys of rat; induces methemoglobinemia	
75	Trichlorfon	52-68-6		69.51	451	614	carcinogenic; inhibits cholinesterase (its entire anticholinesterase action is the result of its nonenzymatic conversion to form dichlorvos)	
339	1-Nitropropane	79-46-9 108-03-2		5159.47	455	2196	induces methemoglobinemia; hepatotoxin	
53	Quinidine sulfate	50-54-4		50.70	456	708	myocardial depressant; anticholinergic properties	
40	Chlordan	57-74-9		24.59	459	508	alters enzymatic properties of nerve cell membranes; affects kinetics of Na ⁺ and K ⁺ ion flow through membrane. Disturbances of Ca transport of Ca ²⁺ -ATPase activity may be involved; carcinogenic; hepatotoxin	

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163	Cetyltrimethylammonium chloride	112-02-7 13287-79-1		7.61	474	284	irritant; cationic surfactant	
264	Chloral hydrate	302-17-0		438.31	480	1066	Proposed: potentiation of GABA _A receptor activity, inhibition of N-methyl-D-aspartate activity, & modulation of 5-hydroxytryptamine ₃ receptor-mediated depolarization of the vagus nerve; CNS Depressant	
204	Azathioprine	446-86-6		38.82	535	497	inhibits purine synthesis; inhibits cell proliferation; immunosuppressive drug	
310	Tributylamine	102-82-9		2855.16	540	2569	solvent; ??	
187	4-Hexylresorcinol	136-77-6		12.44	550	248	anti-infective; antinematodal; antiseptic; antihelminthic	
26	Kelthane	115-32-2		4.45	574	228	inhibits the ATPase associated with oxidative phosphorylation & cation transport in plasma membranes.	
39	2,4-Dichlorophenol	120-83-2		8.97	580	195	inhibits oxidative phosphorylation in rat liver mitochondria and rat brain homogenates; induces methemoglobinemia	
280	Theophylline sodium acetate	8002-89-9		1098.74	582	2062	smooth muscle relaxant; CNS stimulant	
147	Mitoxantrone	65271-80-9		1.07	587	136	cardiotoxic	
101	Glutethimide	77-21-4		338.97	600	1112	CNS depression; anticholinergic activity	
45	Quinine * HCl	130-89-2		27.07	621	493	interfers with plasmoidal DNA;	
70	Atropine sulfate	55-48-1		148.92	623	1477	Antimuscarinic, anticholinergic action. Competitive antagonism of anticholinesterase at cardiac & CNS receptor sites	
302	Nitrobenzene	98-95-3		1502.06	640	1541	induces methemoglobinemia; hepatotoxin; solvent	
123	Isoniazid	54-85-3		1027.33	650	1389	hepatotoxin; metabolic acidosis; affects CNS	requires metabolic activation
256	Tin II chloride	7772-99-8		286.28	700	956	damages DNA; affects liver and kidney functions	

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63	Diazepam	439-14-5		45.56	709	541	causes potentiation of the neural inhibition that is mediated by GABA; CNS depressant	
168	Dicoumarol	66-76-2		9.08	710	295	hepatic synthesis of vitamin K1-dependent clotting factors; anticoagulant; inhibits liver enzymes;	
311	1-Hexanol	111-27-3		1573.88	719	1416	solvent	
174	Ambazone	539-21-9		9.02	750	241	membrane active antitumor drug; increases the cAMP level in leukemia cells and macrophages	
242	1,2,4-Trichlorobenzene	120-82-1		128.82	757	659	solvent; affects CNS, liver and kidneys	
333	Lithium I chloride	7447-41-8		1636.25	759	876	Unknown: Partial substitution for normal cations of cells may disturb energy processes?	
114	Natulan * HCl	366-70-1		706.37	784	1685	alkylating agent; inhibits DNA, RNA, and protein synthesis; antineoplastic agent	
48	Mefenamic acid	61-68-7		20.99	789	352	inhibits prostaglandin synthesis	
338	1-Butanol	71-36-3		3892.35	793	1751	solvent	
202	Formaldehyde	50-00-0	Pos	3.60	799	50	formate metabolite toxicity	
188	t-Butyl hydroquinone	1948-33-0		11.47	800	219	neurotoxic	
354	1,3,5-Trioxane	110-88-3		19189.17	800	3913	?? Same internal toxicity as formaldehyde; affects proteins	
58	Dihydralazine sulfate	7327-87-9		40.36	819	517	relaxes arteriolar smooth muscle.	
213	Ammonium persulfate	7727-54-0		52.49	819	508	decomposes under in vivo conditions to form hydrogen peroxide which can alter cellular function by altering intracellular redox status	
71	Diphenhydramine * HCl	147-24-0		70.04	855	662	anticholinergic activity; H1 antagonist; CNS depressant	
285	Caffeine sodium benzoate	8000-95-1		1918.33	859	3035	CNS stimulant; Hypothetical: Inhibition of phosphodiesterase leading to AMP accumulation. Translocation of intracellular Ca++? Adenosine receptor antagonism?	
197	p,p'-DDE	72-55-9		31.80	881	493	carcinogenic; CNS stimulant; hepatotoxin	

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67	Malathion	121-75-5		66.08	885	692	cholinesterase inhibitor	
259	Methyl salicylate	119-36-8		258.67	887	808	local analgesic; similar toxic effects as aspirin; affects CNS; metabolic acidosis	
184	Butylated hydroxytoluene	128-37-0		12.34	890	265	affects liver functions	
272	Salicylic acid	69-72-7		466.88	891	989	induces uncoupling of oxidative phosphorylation; metabolic acidosis; CNS stimulant	
337	Pyridine	110-86-1		3710.26	894	1779	solvent; hepatotoxin; carcinogenic	
308	Chloroform	67-66-3		1599.56	908	1557	solvent; hepatotoxin; carcinogenic	
44	Hydroxyzine * HCl	1244-76-4		27.56	950	535	anticholinergic acitivity; CNS depressant	
31	Chloroquine diphosphate	50-63-5		8.77	970	370	cardiotoxic; neurotoxic; causes hypokalemia	
214	Thymol	89-83-8		34.56	980	334	pesticide; resembles phenol in systemic actions but is less toxic	
65	Oxyphenbutazone	129-20-4		61.64	999	664	inhibits biosynthesis of prostaglandins, uncouples oxidative phosphorylation, & inhibits atp-dependent biosynthesis of mucopolysaccharide sulfates in cartilage.	
121	Aminophenazole	58-15-1		1246.87	999	2030	bone marrow toxicity; causes agranulocytosis and angioneurotic edema	
80	2-Thiouracil	141-90-2		41.01	1000	329	hepatotoxin; inhibit formation of thyroid hormone	
304	Calcium II chloride	10043-52-4		1376.15	1000	1399	provokes arrhythmia	
107	Acetylsalicylic acid	50-78-2		408.99	1000	1085	General cell poison, works by uncoupling oxidation phosphorylation and inhibition of Kreb's cycle dehydrogenases	
233	Ibuprofen	15687-27-1		107.28	1009	655	cyclooxygenase inhibitor; has inhibitory effect on platelet function	
47	Naftipramide	1505-95-9		25.07	1030	429	??	
218	o-Phenylenediamine	95-54-5		33.53	1070	274	induces methemoglobinemia; hepatotoxin	

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41	Chloroquine sulfate	132-73-0		25.08	1087	518	cardiotoxic; neurotoxic; causes hypokalemia	
296	Homatropine methylbromide	80-49-9		3332.97	1200	4061	affects CNS; antitussive;	
152	8-Hydroxyquinoline	148-24-3	Pos	0.48	1201	51	fungitoxin by steric mechanism; cytotoxic	
287	Benzylalcohol	100-51-6		628.35	1233	980	solvent; CNS depression	
111	Clofibrate acid	882-09-7		560.26	1249	1374	plant growth regulator (antiauxin); antilipemic agent	metabolite of clofibrate
226	Dodecylbenzene sodiumsulfonate	25155-30-0		146.38	1262	1008	anionic surfactant	
251	Scopolamine * HBr	6533-68-2 <u>114-49-8</u>		415.05	1268	1676	CNS depressant; antagonization of acetylcholine at the muscarinic receptor; belladonna alkaloid	
76	Sodium dodecyl sulfate	151-21-3		78.15	1288	691	anionic surfactant	
191	Dimenhydrinate	523-87-5		35.72	1321	646	anticholinergic acitivity; CNS depressant	
99	Nalidixic acid	389-08-2		348.39	1349	1168	metabolic acidosis; inhibits DNA sysnthesis	
243	p-Anisidine	104-94-9		89.91	1404	453	induces methemoglobinemia; cardiovascular toxicant	
270	Propionaldehyde	123-38-6		188.79	1412	409	exerts cardioinhibitory effects; dermatotoxin; affects liver functions	
164	Oxatomide	60607-34-3		8.11	1412	321	enzyme inhibitor; histamine H1 receptor antagonist	
275	Nitrilotriacetic acid	139-13-9		690.09	1470	1409	chelating agent; affects kidney functions; carcinogenic	
324	2-Butoxyethanol	111-76-2		3073.20	1478	2057	hematotoxin; solvent; hepatotoxin; affects lungs, liver, CNS, and kidneys	
56	Manganese IIchloride *4 H ₂ O	13446-34-9		25.73	1484	344	affects liver functions and CNS	
136	Diethyldithiocarbamate sodium* 3H ₂ O	20624-25-3	Pos	0.09	1501	31	fungicide; cytotoxic	
328	Dichloromethane	75-09-2		2964.06	1597	1680	binds to hemoglobin; affects CNS and liver; solvent	
119	Sodium salicylate	54-21-7		693.28	1599	1277	induces uncoupling of oxidative phosphorylation; CNS stimulant	

RC Chemicals with Rat LD₅₀ Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
166	Triisooctylamine	2757-28-0	Pos	8.14	1620	289		
284	Ammonium chloride	12125-02-9		295.32	1648	474	inhibits lysosomal function; metabolic acidosis	
97	Phenacetin	62-44-2		227.63	1651	839	induces methemoglobinemia; affects kidney functions	requires metabolic activation
42	p-Aminophenol	23-30-8 123-30-8	Pos	6.77	1659	137	p450 or PHS; metabolism to cytotoxic agent; hepatotoxic; nephrotoxic	
248	m-Aminophenol	591-27-5		93.86	1659	431	affects CNS; induces methemoglobinemia	
78	6-Methylcoumarin	92-48-8		49.66	1682	406	photoallergenicity and phototoxicity; induces hepatitis	
200	Dimethylaminoethyl methacrylate (polymer)	2867-47-2	Pos	17.30	1745	254	cytotoxic	
57	L-Dopa	59-92-7	Pos	25.64	1781	342	CNS; dopamine	
182	Triton X-100	9002-93-1		35.59	1799	773	nionic surfactant	
300	Antipyrine	60-80-0		2183.70	1800	2306	causes agranulocytosis; anti-inflammatory	
95	Salicylamide	65-45-2		148.12	1893	598	CNS depressant; anti-inflammatory	
342	Piperazine	110-85-0		5789.95	1904	2266	Antinematodal; may have a presynaptic site of action at central cholinergic nerve terminals; affects respiratory functions	
263	Acetaldehyde	75-07-0	Pos	107.95	1930	274	genotoxic; chemically reactive	
139	Retinol	68-26-8	Pos	0.15	2000	46	retinoic acid; involved in cell maintenance	metabolism to retioic acid
52	all-trans-Retinoic acid	302-79-4		33.05	2001	485	antineoplastic; derivative of vitamin A; may affect pancreas	
325	Cyclohexanol	108-93-0		2634.73	2064	1752	CNS depressant; solvent; dermatotoxin; neurotoxin	
330	Sulfuric acid	7664-93-9		3530.88	2138	1966	affects respiratory functions; carcinogenic; dermatotoxin; corrosive	
72	Butylated hydroxyanisole	8003-24-5 25013-16-5	Pos	43.26	2199	409	anti-oxidant	
165	Isoproterenol * HCl	51-30-9	Pos	5.45	2220	199	B-adrenergic	
331	Strontium II chloride	10476-85-4		5770.13	2251	3193	irritant; can lower WBC	
113	Acetaminophen	103-90-2		409.70	2404	984	Covalent NAPQI binding and lipid peroxidation	requires metabolic activation

RC Chemicals with Rat LD50 Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
356	2-Methoxyethanol	109-86-4		19103.61	2458	3551	solvent; neurotoxin; hepatotoxin; nephrotoxin	
334	Isobutanol	78-83-1		2973.01	2461	1557	solvent; CNS depression	
305	n-Butanal	123-72-8		923.14	2488	922	aldehyde; CNS depressant	
350	Tetrahydrofurfuryl alcohol	97-99-4		11338.65	2503	3342	irritant; solvent	
208	Undecylenic acid	112-38-9	Pos	33.18	2507	369	anti-bacterial, fungal; cell membrane disruption	
312	Benzoic acid	65-85-0		1917.44	2528	1706	irritant; affects CNS and respiratory functions	
238	Imidazolidinyl urea	39236-46-9 78491-02-8		100.17	2599	752	preservative; skin sensitizer	
109	Frusemide	54-31-9		770.67	2600	2015	diuretic; affects kidney function; metabolic acidosis; can cause hyperkalemia	requires metabolic activation
346	Potassium I chloride	7447-40-7		6113.10	2602	2138	Essential cellular electrolyte maintains normal transmembrane potential, necessary for heart conduction	
158	Dichlorophene	97-23-4	Pos	2.23	2691	141	membrane disruption	
273	Bromobenzene	108-86-1		543.29	2701	1136	hepatotoxin	requires metabolic activation
295	2,5-Hexanedione	110-13-4		964.65	2706	1218	neurotoxic	metabolite of 2-hexanone
125	Carbon tetrachloride	56-23-5		1308.92	2799	1646	solvent; Hypothetical: Covalent binding of toxic intracellular metabolites. Free radicals inducing lipid peroxidation?	requires metabolic activation
351	Dimethylformamide	68-12-2		8334.54	2800	2420	solvent; affects CNS; hepatotoxin; dermatotoxin	
309	Isobutanal	78-84-2		973.62	2813	944	CNS depressant; caused depressed protein synthesis in liver & hepatoma & caused a shifting of cytosolic oxidation-reduction state & a diminution of atp in the liver	
298	Dichloroacetic acid	79-43-6		1482.81	2824	1573	carcinogen	

RC Chemicals with Rat LD₅₀ Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
344	Sodium chloride	7647-14-5		4435.60	2998	1620	Acute dehydration of brain cells caused by osmotic shift of water to the outside of the blood:brain barrier.	
322	1-Pentanol	71-41-0		2195.43	3033	1505	amylalcohol; food additive	
221	2-Nitro-p-phenylene-diamine	5307-14-2	Pos	59.73	3079	429	hair dye; positive in AMES	
216	Reportan bis(4-chlorophenoxy)acetic acid	29815-94-9		78.28	3162	722		
94	Menthol	89-78-1		148.49	3173	645	antipruritic	
257	Isononylaldehyde	5435-64-3 35127-50-5		216.25	3244	720	component of fragrances	
288	1-Heptanol	111-70-6		726.44	3254	1088	natural product	
321	Acetic acid	64-19-7		1459.46	3309	1015	natural product	
91	Chloramphenicol	56-75-7		255.29	3393	1230	Hypothetical: Binds to mitochondrial ribosomes & inhibits enzyme syntheses (, e.g., those necessary for oxidative phosphorylation)	
349	Ethyl methyl ketone	78-93-3		7500.48	3397	2293	solvent; irritant	
345	Sodium I bromide	7647-15-6		8120.81	3504	2934	sedative; hypnotic	
336	Nicotinamide	98-92-0		5423.02	3505	2682	vitamin; NAD	
306	Anisole	100-66-3		1427.58	3699	1401	irritant	
341	Lactic acid	598-82-3 50-21-5		5945.94	3730	2351	Disturbance of metabolism (lactic acidosis).	
358	Acetonitrile	75-05-8		15110.08	3798	2262	Assumed to be same as cyanide: General enzyme inhibition. High affinity for Fe ⁺⁺⁺ . Inhibits cell respiration by inhibition of cytochrome oxidase; solvent	
211	Catechol	120-80-9	Pos	22.02	3887	231	topical anesthetic	benzene metabolite
307	2-Ethylbutanal	97-96-1		1322.38	3977	1298		
315	Isobenzoic furano dione	85-44-9		2518.04	4014	2142	irritant	
332	1,4-Dioxane	123-91-1		3357.37	4203	1810	carcinogen	

RC Chemicals with Rat LD₅₀ Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
301	Xylene	1330-20-7		1274.16	4300	1320	Unknown: Heart failure caused by sensitization of heart to catecholamines?; solvent	
154	Maneb	12427-38-2	Pos	1.12	4501	104	fungicide; cytotoxic	
294	Trichloroacetic acid	76-03-9		1338.08	4999	1720	corrosive; possible carcinogen	
271	Styrene	100-42-5	Pos	343.73	5000	738	styrene oxide; binds to DNA	
316	Toluene	108-88-3		1575.77	5004	1336	solvent	metabolized to benzoic acid
320	N,N-Dimethylacetamide	127-19-5		2108.79	5089	1470	solvent; affects liver and kidneys	
224	n-Butyl benzoate	136-60-7	Pos	73.08	5134	510	inhibit cell growth in culture	
186	Zineb	12122-67-7	Pos	16.27	5211	339	fungicide; cytotoxic	
348	1-Propanol	71-23-8		5800.62	5398	1850	solvent	metabolized to propionic acid
326	Halothane	151-67-7		6138.83	5685	3713	anesthetic	
128	2-Propanol	67-63-0		10038.37	5843	2349	solvent	metabolized to acetone
50	Trypan blue	72-57-1		91.66	6204	1461	carcinogen; microsomal enzyme induction	
108	Gibberellic acid	77-06-5		796.74	6305	2099	plant growth regulator	
335	Potassium hexacyano-ferrate II	13943-58-3		15582.05	6410	7920		
59	Tetracycline * HCl	64-75-5	Pos	67.33	6445	862	antibacterial	
127	Dimethyl phthalate	131-11-3		4544.28	6894	3227	miticide; irritant; CNS depressant	
286	Benzylpenicillin sodium	69-57-8		2042.17	6914	3212	anti-microbial	
126	Triethyl citrate	77-93-0		4061.90	6991	3751	citrate metabolite can bind Ca++	
85	Metamizol	68-89-3	Pos	193.94	7189	1113	non-steroidal anti-inflammatory drug; reduces platelet aggregation; causes agranulocytosis and aplastic anemia	
343	Magnesium II chloride * 6 H ₂ O	7791-18-6		14314.43	8093	5456	affects cardiac functions	

RC Chemicals with Rat LD50 Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
360	Ethylene glycol	107-21-1		34454.40	8567	4090	Hypothetical: Metabolites inhibit mitochondria to produce metabolic acidosis. Oxalate decreases sarcoplasmic Ca++; affects kidney function; oxalic acid is toxic metabolite	
122	Diethyl phthalate	84-66-2		1226.88	8601	1971	CNS depressant; hepatotoxin	
289	Tetrachloroethylene	127-18-4	Pos	1084.46	8855	1583	TCA is metabolite; solvent; hepatotoxin; neurotoxin; nephrotoxin	
117	Di(2-ethylhexyl)adipate	103-23-1		1167.52	9118	2575	peroxisome proliferator; carcinogen	
162	Chlorhexidine	55-56-1	Pos	7.58	9200	343	antiseptic; disinfectant	
359	Acetone	67-64-1		25791.96	9759	3473	solvent; natural product	
18	Captan	133-06-2	Pos	1.17	10010	114	fungicide; cytotoxic	
297	1,1,1-Trichloroethane	71-55-6	Pos	1374.02	10298	1551	solvent	
353	Ethyl acetate	141-78-6		11279.36	11015	3067	solvent; sensory irritant	
100	L-Ascorbic acid	50-81-7	Pos	267.73	11907	891	anti-oxidant	
88	Dibutyl phthalate	84-74-2	Pos	211.57	11998	1042	peroxisome proliferator; hepatotoxin	
131	Glycerol	56-81-5		57476.64	12619	6386	Cellular dehydration; osmotic effect	
361	Methanol	67-56-1		29806.50	13012	2643	Hypothetical: Accumulation of formic acid leads to metabolic acidosis. Lactate inhibits mitochondrial respiration; formaldehyde metabolite	
130	Ethanol	64-17-5	Pos	17464.32	14008	2572	Hypothetical: Interferes with cell membrane fluidity, perturbing proteins such as ion channels. Depression of postsynaptic potentials in CNS; solvent	
313	Xanthinol nicotinate	437-74-1		6865.26	14122	6087	form of vitamin B3; affects brain ATP levels	
258	Diethyl sebacate	110-40-7	Pos	421.19	14470	1348	peroxisome proliferator	
340	Diethylene glycol	111-46-6	Pos	6591.29	14753	2697	Nephrotoxic; CNS depressant	
329	Sodium cyclamate	139-05-9		7123.90	15254	4004	sweetner	
352	1,2,6-Hexanetriol	106-69-4		16506.60	15970	4591	contact dermatitis	
129	Dimethyl sulfoxide	75-18-3 67-68-5	Pos	19691.28	19691	3652	solvent	

RC Chemicals with Rat LD50 Values

RC No	Chemical	CASRN	Outlier Status ¹	IC ₅₀ ug/mL ²	LD ₅₀ mg/kg ³	Predicted LD ₅₀ mg/kg ⁴	Toxicity Mechanism ⁵	Metabolic Activation/ Inactivation ⁶
357	Propylene glycol	57-55-6		26029.62	20017	4062	metabolized to lactate	
355	D-Glucose	50-99-7		40720.68	25766	8031		
92	Di(2-ethylhexyl)phthalate	117-81-7	Pos	328.12	31015	1527	peroxisome proliferator	

Chemicals for which the primary mechanism of toxicity is expected to require specialized cells; includes alkylating agents, cholinesterase inhibitors, neurotoxins, energy pathway inhibitors, and cardiotoxic compounds.

¹Chemicals that fall outside of the + log 5 acceptance interval; outlier determination: if log of observed LD50 value (in mmol/kg) minus log of predicted LD50 value (see **Appendix J**) > 0.699 (or log 5), then positive (Pos) outlier; if < -0.699 (or -log 5) then negative (Neg) outlier

²IC50 value from the RC; converted from mmol/L to ug/mL

³LD50 value from the RC; collected from 83/84 RTECS

⁴calculated from the RC regression: log (LD50) = 0.435 x log (IC50x) + 0.625; converted from mmol/kg to mg/kg

⁵Information obtained from databases (Hazardous Substance Database [HSDB]; Haz-Map; Pesticide Action Network [PAN] Pesticides Database; IPCS INTOX Database) and Casaretti & Doull's Toxicology (2001)

⁶Identification made by RC author (Halle 2003)