NHK NRU Predictions: RC Millimole Regression

RC Millimole Regression: Log LD_{50} (mmol/kg) = 0.435 log IC_{50} (mM) + 0.625

Chemical	Log Observed LD_{50} (mmol/kg)[1]	NHK Log IC_{50} (mM)[2]	Log Predicted LD_{50} (mmol/kg)[3]	Log Observed LD_{50} - Log Predicted LD_{50} (mmol/kg)	Statistical Outlier[4]	Observed LD_{50} (mg/kg)[5]	NHK IC_{50} (ug/mL)[3]	Predicted LD_{50} (mg/kg)[6]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[7] (mg/kg)	Predicted Toxicity Category[7] (mg/kg)
Acetaminophen	1.20	0.535	0.858	0.344		2404	518	1089	1315	2000-5000	300-2000
Acetonitrile	1.97	2.37	1.65	0.312		3798	9528	1851	1947	2000-5000	300-2000
Acetylsalicylic acid	0.744	0.526	0.854	-0.110		1000	605	1287	-287	300-2000	300-2000
Aminopterin	-2.17	0.182	0.704	-2.87	Negative	3.00	669	2228	-2225	< 5	2000-5000
5-Aminosalicylic acid	1.70	-0.516	0.401	1.30	Positive	7749	46.7	385	7364	> 5000	300-2000
Arsenic II trioxide	-1.00	-1.58	-0.060	-0.940	Negative	19.8	5.26	172	-152	5-50	50-300
Boric acid	1.63	0.833	0.988	0.646		2660	421	601	2059	2000-5000	300-2000
Busulfan	-2.09	0.024	0.635	-2.73	Negative	2.00	260	1064	-1062	< 5	300-2000
Cadmium II chloride	-0.319	-2.00	-0.244	-0.075		88.0	1.84	105	-16.5	50-300	50-300
Chloramphenicol	1.02	0.033	0.639	0.382		3393	348	1408	1985	2000-5000	300-2000
Citric acid	1.19	0.318	0.763	0.430		3000	400	1114	1886	2000-5000	300-2000
Cupric sulfate pentahydrate	0.080	-0.104	0.580	-0.500		300	197	949	-649	50-300	300-2000
Cycloheximide	-2.15	-3.58	-0.934	-1.21	Negative	2.00	0.073	32.8	-30.8	< 5	5-50
Dibutyl phthalate	1.63	-0.987	0.196	1.44	Positive	11998	28.7	437	11561	> 5000	300-2000
Diethyl phthalate	1.59	-0.266	0.509	1.08	Positive	8602	120	718	7884	> 5000	300-2000
Digoxin	-1.64	-5.89	-1.94	0.299		18.0	0.001	9.04	8.96	5-50	5-50
Dimethylformamide	1.58	2.03	1.51	0.077		2800	7760	2345	455	2000-5000	2000-5000
Diquat dibromide monohydrate	-0.173	-1.91	-0.205	0.032		243	4.48	226	17.2	50-300	50-300
Ethanol	2.48	2.34	1.64	0.841	Positive	14008	10018	2019	11989	> 5000	2000-5000
Ethylene glycol	2.14	2.83	1.86	0.284		8567	41852	4451	4116	> 5000	2000-5000
Gibberellic acid	1.26	0.916	1.02	0.237		6305	2856	3657	2648	> 5000	2000-5000
Glycerol	2.14	2.43	1.96	0.175		12691	24730	8481	4211	> 5000	> 5000
Hexachlorophene	-0.824	-4.15	-1.18	0.356		61.0	0.029	26.9	34.1	50-300	5-50
Lactic acid	1.62	1.16	1.13	0.487		3730	1304	1215	2515	2000-5000	300-2000
Lithium II carbonate	1.21	0.801	0.974	0.232		1187	468	695	492	300-2000	300-2000
Meprobamate	0.561	0.213	0.718	-0.157		794	357	1140	-346	300-2000	300-2000
Mercury II chloride	-2.43	-1.67	-0.102	-2.33	Negative	1.00	5.80	215	-214	<5	50-300
Methanol	2.61	1.68	1.36	1.25	Positive	13012	1529	726	12286	> 5000	300-2000
Phenol	0.643	-0.098	0.582	0.061		414	75.0	360	54	300-2000	300-2000
Phenylthiourea	-1.71	0.344	0.775	-2.48	Negative	3.00	336	906	-903	< 5	300-2000
Potassium I chloride	1.54	1.48	1.27	0.275		2602	2237	1381	1221	2000-5000	300-2000

NHK NRU Predictions: RC Millimole Regression

Chemical	Log Observed LD_{50} (mmol/kg)[1]	NHK Log IC_{50} (mM)[2]	Log Predicted LD_{50} (mmol/kg)[3]	Log Observed LD_{50} - Log Predicted LD_{50} (mmol/kg)	Statistical Outlier[4]	Observed LD_{50} (mg/kg)[5]	NHK IC_{50} (ug/mL)[3]	Predicted LD_{50} (mg/kg)[6]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[7] (mg/kg)	Predicted Toxicity Category[7] (mg/kg)
2-Propanol	1.99	1.95	1.47	0.514		5843	5364	1788	4055	> 5000	300-2000
Propranolol HCl	0.201	-0.923	0.224	-0.023		470	35.3	495	-25.0	300-2000	300-2000
Sodium arsenite	-0.501	-2.44	-0.434	-0.066		41.0	0.477	47.8	-6.78	5-50	5-50
Sodium chloride	1.71	1.53	1.29	0.418		2998	1997	1145	1853	2000-5000	300-2000
Sodium dichromate dihydrate	-0.719	-2.62	-0.513	-0.206		56.9	0.721	91.4	-34.6	50-300	50-300
Sodium I fluoride	0.632	0.074	0.657	-0.025		180	49.8	191	-10.6	50-300	50-300
Sodium hypochlorite	2.08	1.30	1.19	0.885	Positive	8910	1502	1160	7750	> 5000	300-2000
Sodium oxalate	0.063	0.400	0.799	-0.736	Negative	155	337	844	-689	50-300	300-2000
Sodium selenate	-2.07	-1.27	0.074	-2.15	Negative	1.60	10.2	224	-222	< 5	50-300
Thallium I sulfate	-1.24	-3.52	-0.907	-0.333		29.0	0.152	62.5	-33.5	5-50	50-300
Trichloroacetic acid	1.49	0.403	0.800	0.685		4999	413	1032	3967	2000-5000	300-2000
1,1,1-Trichloroethane	1.89	1.78	1.40	0.486		10298	8122	3361	6938	> 5000	2000-5000
Triethylenemelamine	-2.31	-2.04	-0.263	-2.05	Negative	1.00	1.85	111	-110	<5	50-300
Triphenyltin hydroxide	-0.921	-4.56	-1.36	0.438		44.0	0.010	16.0	28.0	5-50	5-50
Valproic acid	1.01	0.550	0.864	0.144		1471	512	1055	416	300-2000	300-2000
Xylene	1.61	0.642	0.904	0.703	Positive	4300	466	852	3448	2000-5000	300-2000

[a]Three chemicals were excluded because no rat LD_{50} was identified: epinephrine bitartrate, colchicine, and propylparaben. Carbon tetrachloride and methanol were excluded because IC_{50} values could not be determined. Twenty-one chemicals were excluded based on their mechanisms of action: amitriptyline HCl, atropine sulfate, caffeine, carbamazepine, chloral hydrate, dichlorvos , disulfoton, endosulfan, fenpropathrin, glutethimide, haloperidol, lindane, nicotine, paraquat, parathion, phenobarbital, physostigmine, potassium cyanide, procainamide HCl, strychnine, and verapamil HCl (see **Section 6**, **Table 6-3**).

[1]original RC LD_{50} values came largely from the 1983/84 RTECS®. Values for nonRC chemicals came from current RTECS® and Hazardous Substances Data Bank.

[2]combined NHK IC_{50} values from three laboratories

[3]LD_{50} determined using RC regression: Log LD_{50} (mmol/kg) = 0.435 log IC_{50} (mM) + 0.625

[4]a difference > 0.699 (or log 5) identifies a chemical as discordant (i.e., an "outlier")

[5]converted from mmol/kg to mg/kg

[6]LD_{50} in mg/kg converted from results of RC regression

[7]Globally Harmonized System (GHS) hazard classification:

Category	Oral LD_{50} Limits
1	$LD_{50} \leq 5$ mg/kg
2	$5 < LD_{50} \leq 50$ mg/kg
3	$50 < LD_{50} \leq 300$ mg/kg
4	$300 < LD_{50} \leq 2000$ mg/kg
5	$2000 < LD_{50} \leq 5000$ mg/kg
Unclassified	$LD_{50} > 5000$ mg/kg