NHK NRU Predictions: RC Rat-Only Weight Regression

RC Rat-Only Weight Regression: log LD50 (mg/kg) =0.372 log IC50 (ug/mL) + 2.024

Chemical[a]	Log Reference LD_{50} (mg/kg)[1]	NHK Log IC_{50} (ug/mL)[2]	Log Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} (mg/kg)[1]	NHK IC_{50} (ug/mL)[2]	Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[4] (mg/kg)	Predicted Toxicity Category[4] (mg/kg)
Acetaminophen	3.33	2.71	3.03	2162	518	1081	1081	2000-5000	300-2000
Acetonitrile	3.56	3.98	3.50	3595	9528	3193	402	2000-5000	2000-5000
Acetylsalicylic acid	3.18	2.78	3.06	1506	605	1145	361	300-2000	300-2000
Aminopterin	0.845	2.83	3.08	7.00	669	1189	-1182	5-50	300-2000
5-Aminosalicylic acid	3.54	1.67	2.64	3428	46.7	442	2986	2000-5000	300-2000
Arsenic III trioxide	1.40	0.721	2.29	25.1	5.26	196	-171	5-50	50-300
Boric acid	3.53	2.62	3.00	3426	421	1001	2425	2000-5000	300-2000
Busulfan	1.08	2.42	2.92	12.1	260	836	-824	5-50	300-2000
Cadmium II chloride	2.13	0.266	2.12	135	1.84	133	2.52	50-300	50-300
Chloramphenicol	3.54	2.54	2.97	3490	348	932	2558	2000-5000	300-2000
Citric acid	3.77	2.60	2.99	5929	400	981	4948	> 5000	300-2000
Cupric sulfate pentahydrate	2.68	2.29	2.88	475	197	754	-279	300-2000	300-2000
Cycloheximide	0.301	-1.13	1.60	2.00	0.073	40.0	-38.0	< 5	5-50
Dibutyl phthalate	3.95	1.46	2.57	8892	29	368	8524	> 5000	300-2000
Diethyl phthalate	3.97	2.08	2.80	9311	120	628	8683	> 5000	300-2000
Digoxin	1.45	-3.00	0.909	28.3	0.001	8.12	20.2	5-50	5-50
Dimethylformamide	3.72	3.89	3.47	5305	7760	2958	2347	> 5000	2000-5000
Diquat dibromide monohydrate	2.20	0.651	2.27	160	4.48	185	-24.6	50-300	50-300
Ethanol	4.05	4.00	3.51	11324	10018	3253	8071	> 5000	2000-5000
Ethylene glycol	3.85	4.62	3.74	7161	41852	5537	1624	> 5000	>5000
Gibberellic acid	3.78	3.46	3.31	6039	2856	2040	4000	> 5000	2000-5000
Glycerol	4.30	4.39	3.66	19770	24730	4553	15217	> 5000	2000-5000
Hexachlorophene	1.91	-1.54	1.45	82.0	0.03	28.3	53.7	50-300	5-50
Lactic acid	3.56	3.12	3.18	3635	1304	1524	2111	2000-5000	300-2000
Lithium I carbonate	2.77	2.67	3.02	590	468	1040	-450	300-2000	300-2000
Meprobamate	3.14	2.55	2.97	1387	357	941	446	300-2000	300-2000
Mercury II chloride	1.60	0.763	2.31	40.2	5.80	203	-163	5-50	50-300
Methanol	3.94	3.18	3.21	8710	1529	1616	7093	> 5000	300-2000
Phenol	2.74	1.88	2.72	548	75.0	527	21.0	300-2000	300-2000
Phenylthiourea	0.477	2.53	2.96	3.00	336	920	-917	< 5	300-2000
Potassium I chloride	3.45	3.35	3.27	2802	2237	1862	940	2000-5000	300-2000

NHK NRU Predictions: RC Rat-Only Weight Regression

Chemical[a]	Log Reference LD_{50} (mg/kg)[1]	NHK Log IC_{50} (ug/mL)[2]	Log Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} (mg/kg)[1]	NHK IC_{50} (ug/mL)[2]	Predicted LD_{50} (mg/kg)[3]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Observed Toxicity Category[4] (mg/kg)	Predicted Toxicity Category[4] (mg/kg)
2-Propanol	3.71	3.73	3.41	5105	5364	2579	2526	> 5000	2000-5000
Propranolol HCl	2.67	1.55	2.60	466	35.3	398	67.9	300-2000	300-2000
Sodium arsenite	1.64	-0.322	1.90	43.6	0.477	80.2	-36.6	5-50	50-300
Sodium chloride	3.61	3.30	3.25	4050	1997	1786	2264	2000-5000	300-2000
Sodium dichromate dihydrate	1.70	-0.142	1.97	50.5	0.72	93.6	-43.1	50-300	50-300
Sodium hypochlorite	4.01	3.18	3.21	10328	1502	1606	8722	> 5000	300-2000
Sodium I fluoride	2.10	1.70	2.66	127	49.8	452	-325	50-300	300-2000
Sodium oxalate	2.80	2.53	2.96	633	337	921	-288	300-2000	300-2000
Sodium selenate	0.477	1.01	2.40	3.00	10.2	251	-248	< 5	50-300
Thallium I sulfate	1.40	-0.819	1.72	25.0	0.152	52.4	-27.4	5-50	50-300
Trichloroacetic acid	3.72	2.62	3.00	5229	413	994	4235	> 5000	300-2000
1,1,1-Trichloroethane	4.08	3.91	3.48	12078	8122	3009	9069	> 5000	2000-5000
Triethylenemelamine	0.602	0.268	2.12	4.00	1.85	133	-129	< 5	50-300
Triphenyltin Hydroxide	2.52	-2.00	1.28	329	0.01	19.1	310	300-2000	5-50
Valproic acid	3.00	2.71	3.03	996	512	1076	-80.1	300-2000	300-2000
Xylene	3.67	2.67	3.02	4665	466	1039	3626	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 an IC_{50} value 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] reference LD_{50} values that were collected from the literature

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

[3] LD_{50} determined regression: log LD_{50} (mg/kg) = 0.372 log IC_{50} (ug/mL) + 2.024

[4]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