NHK NRU Predictions: NHK Combined-Laboratory Regression

NHK Combined-Laboratory Regression: Log LD_{50} (mmol/kg) = 0.510 log IC_{50} (mM) + 0.452

Chemical[a]	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	1.16	0.535	0.725	0.431		2162	518	802	1360	2000-5000	300-2000
Acetonitrile	1.94	2.37	1.66	0.284		3595	9528	1870	1725	2000-5000	300-2000
Acetylsalicylic acid	0.922	0.526	0.720	0.202		1506	605	947	559	300-2000	300-2000
Aminopterin	-1.80	0.182	0.545	-2.34	Negative	7.00	669	1543	-1536	5-50	300-2000
5-Aminosalicylic acid	1.35	-0.516	0.189	1.16		3428	46.7	237	3191	2000-5000	50-300
Amitriptyline HCl	0.046	-1.54	-0.336	0.382		349	8.96	145	204	300-2000	50-300
Arsenic II trioxide	-0.897	-1.58	-0.351	-0.545		25.1	5.26	88.1	-63.0	5-50	50-300
Atropine sulfate	0.071	-0.929	-0.022	0.093		819	81.8	661	158	300-2000	300-2000
Boric acid	1.74	0.833	0.877	0.867		3426	421	466	2960	2000-5000	300-2000
Busulfan	-1.31	0.024	0.464	-1.77	Negative	12.1	260	717	-705	5-50	300-2000
Cadmium II chloride	-0.132	-2.00	-0.567	0.435		135	1.84	49.7	85.5	50-300	50-300
Caffeine	0.203	0.516	0.715	-0.512		310	638	1008	-698	300-2000	300-2000
Carbamazepine	1.07	-0.453	0.221	0.854		2807	83.2	393	2414	2000-5000	300-2000
Chloral hydrate	0.586	-0.094	0.404	0.182		638	133	419	219	300-2000	300-2000
Chloramphenicol	1.03	0.033	0.469	0.565		3490	348	951	2539	2000-5000	300-2000
Citric acid	1.49	0.318	0.614	0.875		5929	400	790	5139	> 5000	300-2000
Colchicine	-1.43	-4.78	-1.99	0.560		15.0	0.01	4.13	10.9	5-50	< 5
Cupric sulfate pentahydrate	0.279	-0.104	0.399	-0.120		475	197	626	-151	300-2000	300-2000
Cycloheximide	-2.15	-3.58	-1.38	-0.773		2.00	0.073	11.9	-9.85	< 5	5-50
Dibutyl phthalate	1.50	-0.987	-0.051	1.56		8892	28.7	247	8645	> 5000	50-300
Dichlorvos	-0.576	-1.32	-0.219	-0.357		58.7	10.7	134	-74.8	50-300	50-300
Diethyl phthalate	1.62	-0.266	0.316	1.31		9311	120	460	8851	> 5000	300-2000
Digoxin	-1.44	-5.89	-2.55	1.11		28.3	0.001	2.19	26.1	5-50	< 5
Dimethylformamide	1.86	2.03	1.49	0.376		5305	7760	2234	3071	> 5000	2000-5000
Diquat dibromide monohydrate	-0.355	-1.91	-0.521	0.166		160	4.48	109	50.9	50-300	50-300
Disulfoton	-1.74	-0.007	0.448	-2.19	Negative	5.00	270	770	-765	< 5	300-2000
Endosulfan	-1.17	-2.28	-0.712	-0.454		27.8	2.13	79.0	-51.2	5-50	50-300
Epinephrine bitartrate	-1.92	-0.581	0.156	-2.08	Negative	4.00	87.4	477	-473	< 5	300-2000
Ethanol	2.39	2.34	1.64	0.747		11324	10018	2030	9294	> 5000	2000-5000
Ethylene glycol	2.06	2.83	1.89	0.167		7161	41852	4871	2290	> 5000	2000-5000
Fenpropathrin	-0.664	-2.16	-0.649	-0.016		75.7	2.43	78.5	-2.75	50-300	50-300
Gibberellic acid	1.24	0.916	0.919	0.322		6039	2856	2876	3163	> 5000	2000-5000

NHK NRU Predictions: NHK Combined-Laboratory Regression

Chemical[a]	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)
Glutethimide	0.441	-0.098	0.402	0.039		600	174	549	51.4	300-2000	300-2000
Glycerol	2.33	2.43	1.69	0.641		19770	24730	4519	15251	> 5000	2000-5000
Haloperidol	-0.057	-2.05	-0.593	0.536		330	3.36	95.9	234	300-2000	50-300
Hexachlorophene	-0.696	-4.15	-1.66	0.968		82.0	0.029	8.82	73.2	50-300	5-50
Lactic acid	1.61	1.16	1.04	0.562		3635	1304	997	2638	2000-5000	300-2000
Lindane	-0.464	-1.19	-0.155	-0.308		100	18.7	203	-103	50-300	50-300
Lithium I carbonate	0.902	0.801	0.861	0.042		590	468	536	53.9	300-2000	300-2000
Meprobamate	0.803	0.213	0.561	0.242		1387	357	794	593	300-2000	300-2000
Mercury II chloride	-0.830	-1.67	-0.400	-0.430		40.2	5.80	108	-67.9	5-50	50-300
Methanol	2.43	1.68	1.31	1.13		8710	1529	651	8058	> 5000	300-2000
Nicotine	-0.367	-0.182	0.359	-0.726		69.7	107	371	-301	50-300	300-2000
Paraquat	-0.443	-0.621	0.135	-0.579		92.7	61.6	351	-259	50-300	300-2000
Parathion	-1.68	-0.983	-0.050	-1.63		6.10	30.3	260	-254	5-50	50-300
Phenobarbital	-0.016	0.285	0.597	-0.613		224	448	919	-695	50-300	300-2000
Phenol	0.908	-0.098	0.402	0.507		762	75.0	237	525	300-2000	50-300
Phenylthiourea	-1.71	0.344	0.628	-2.33	Negative	3.00	336	646	-643	< 5	300-2000
Physostigmine	-1.74	-0.493	0.201	-1.94	Negative	5.00	88.5	437	-432	< 5	300-2000
Potassium I chloride	1.58	1.48	1.21	0.370		2802	2237	1196	1606	2000-5000	300-2000
Potassium cyanide	-0.956	-0.352	0.272	-1.23		7.20	29.0	122	-115	5-50	50-300
Procainamide HCl	0.856	0.807	0.863	-0.008		1950	1741	1984	-34.4	300-2000	300-2000
2-Propanol	1.93	1.95	1.45	0.482		5105	5364	1682	3423	> 5000	300-2000
Propranolol HCl	0.197	-0.923	-0.019	0.216		466	35.3	283	183	300-2000	50-300
Propylparaben	1.55	-1.04	-0.076	1.62		6332	16.6	151	6181	> 5000	50-300
Sodium arsenite	-0.474	-2.44	-0.790	0.316		43.6	0.477	21.1	22.5	5-50	5-50
Sodium chloride	1.84	1.53	1.23	0.607		4050	1997	1002	3048	2000-5000	300-2000
Sodium dichromate dihydrate	-0.771	-2.62	-0.882	0.111		50.5	0.721	39.1	11.4	50-300	5-50
Sodium I fluoride	0.480	0.074	0.490	-0.010		127	49.8	130	-2.91	50-300	50-300
Sodium hypochlorite	2.14	1.30	1.12	1.02		10328	1502	976	9352	> 5000	300-2000
Sodium oxalate	0.674	0.400	0.656	0.018		633	337	607	25.8	300-2000	300-2000
Sodium selenate	-1.80	-1.27	-0.194	-1.61		3.00	10.2	121	-118	< 5	50-300
Strychnine	-1.72	-0.729	0.080	-1.81	Negative	6.30	62.5	402	-396	5-50	300-2000
Thallium I sulfate	-1.31	-3.52	-1.34	0.039		25.0	0.152	22.8	2.16	5-50	5-50
Trichloroacetic acid	1.28	0.403	0.658	0.624		3127	413	743	2384	2000-5000	300-2000

NHK NRU Predictions: NHK Combined-Laboratory Regression

Chemical[a]	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)
1,1,1-Trichloroethane	1.96	1.78	1.36	0.595		12078	8122	3071	9007	> 5000	2000-5000
Triethylenemelamine	-1.71	-2.04	-0.590	-1.12		4.00	1.85	52.5	-48.5	< 5	50-300
Triphenyltin hydroxide	-0.047	-4.56	-1.87	1.83	Positive	329	0.010	4.90	324	300-2000	< 5
Valproic acid	0.839	0.550	0.733	0.107		996	512	779	217	300-2000	300-2000
Verapamil HCl	-0.646	-0.869	0.009	-0.655		111	66.5	501	-390	50-300	300-2000
Xylene	1.64	0.642	0.779	0.863		4665	466	639	4026	2000-5000	300-2000

[a]carbon tetrachloride was excluded because IC_{50} values could not be determined.

[1]reference LD_{50} values that were collected from the literature

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

[3]LD_{50} determined using regression: Log LD_{50} (mmol/kg) = 0.510 log IC_{50} (mM) + 0.452

[4]outlier range = 1.639 - 1.701 (90% prediction interval)

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

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