3T3 NRU Predictions: 3T3 Combined-Laboratory Regression

3T3 Combined-Laboratory Regression: Log LD_{50} (mmol/kg) = 0.589 log IC_{50} (mM) + 0.425

Chemical[a]	Log Observed LD_{50} (mmol/kg)[1]	3T3 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]	3T3 IC_{50} (ug/mL)[3]	Predicted LD_{50} (mg/kg)[6]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Reference Toxicity Category[7] (mg/kg)	Predicted Toxicity Category[7] (mg/kg)
Acetaminophen	1.16	-0.501	0.130	1.03		2162	47.7	204	1958	2000-5000	50-300
Acetonitrile	1.94	2.29	1.77	0.170		3595	7951	2429	1166	2000-5000	2000-5000
Acetylsalicylic acid	0.922	0.574	0.763	0.159		1506	676	1045	461	300-2000	300-2000
Aminopterin	-1.80	-4.85	-2.43	0.632		7.00	0.006	1.63	5.37	5-50	< 5
5-Aminosalicylic acid	1.35	1.04	1.04	0.314		3428	1667	1662	1766	2000-5000	300-2000
Amitriptyline HCl	0.046	-1.65	-0.546	0.592		349	7.05	89.3	260	300-2000	50-300
Arsenic II trioxide	-0.897	-2.00	-0.755	-0.142		25.1	1.96	34.8	-9.68	5-50	5-50
Atropine sulfate	0.071	-0.961	-0.141	0.212		819	76.0	502	317	300-2000	300-2000
Boric acid	1.74	1.48	1.29	0.449		3426	1850	1218	2208	2000-5000	300-2000
Busulfan	-1.31	-0.501	0.130	-1.44		12.1	77.7	332	-320	5-50	300-2000
Cadmium II chloride	-0.132	-2.55	-1.08	0.944		135	0.518	15.4	120	50-300	5-50
Caffeine	0.203	-0.105	0.363	-0.160		310	153	448	-138	300-2000	300-2000
Carbamazepine	1.07	-0.360	0.213	0.862		2807	103	386	2421	2000-5000	300-2000
Chloral hydrate	0.586	0.044	0.451	0.135		638	183	467	171	300-2000	300-2000
Chloramphenicol	1.03	-0.402	0.189	0.845		3490	128	499	2991	2000-5000	300-2000
Citric acid	1.49	0.617	0.789	0.701		5929	796	1181	4748	> 5000	300-2000
Colchicine	-1.43	-4.07	-1.97	0.544		15.0	0.034	4.28	10.7	5-50	< 5
Cupric sulfate pentahydrate	0.279	-0.773	-0.030	0.310		475	42.1	233	242	300-2000	50-300
Cycloheximide	-2.15	-3.18	-1.45	-0.702		2.00	0.187	10.1	-8.08	< 5	5-50
Dibutyl phthalate	1.50	-0.748	-0.016	1.52	Positive	8892	49.7	268	8624	> 5000	50-300
Dichlorvos	-0.576	-1.10	-0.220	-0.356		58.7	17.7	133	-74.4	50-300	50-300
Diethyl phthalate	1.62	-0.316	0.239	1.38		9311	107	385	8926	> 5000	300-2000
Digoxin	-1.44	-0.225	0.293	-1.73	Negative	28.3	466	1532	-1504	5-50	300-2000
Dimethylformamide	1.86	1.85	1.52	0.344		5305	5224	2404	2901	> 5000	2000-5000
Diquat dibromide monohydrate	-0.355	-1.65	-0.549	0.194		160	8.04	102	57.7	50-300	50-300
Disulfoton	-1.74	-0.314	0.240	-1.98	Negative	5.00	133	477	-472	< 5	300-2000
Endosulfan	-1.17	-1.81	-0.639	-0.526		27.8	6.35	93.4	-65.6	5-50	50-300
Epinephrine bitartrate	-1.92	-0.752	-0.018	-1.90	Negative	4.00	59.0	320	-316	< 5	300-2000
Ethanol	2.39	2.15	1.69	0.699		11324	6523	2267	9057	> 5000	2000-5000
Ethylene glycol	2.06	2.59	1.95	0.110		7161	24317	5562	1599	> 5000	> 5000
Fenpropathrin	-0.664	-1.16	-0.258	-0.407		75.7	24.2	193	-117	50-300	50-300
Gibberellic acid	1.24	1.35	1.22	0.019		6039	7810	5775	265	> 5000	> 5000

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Chemical[a]	Log Observed LD_{50} (mmol/kg)[1]	3T3 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]	3T3 IC_{50} (ug/mL)[3]	Predicted LD_{50} (mg/kg)[6]	Observed LD_{50} - Predicted LD_{50} (mg/kg)	Reference Toxicity Category[7] (mg/kg)	Predicted Toxicity Category[7] (mg/kg)
Glutethimide	0.441	-0.095	0.369	0.072		600	174	508	92.0	300-2000	300-2000
Glycerol	2.33	2.43	1.85	0.477		19770	24655	6594	13176	> 5000	> 5000
Haloperidol	-0.057	-1.79	-0.628	0.572		330	6.13	88.5	241	300-2000	50-300
Hexachlorophene	-0.696	-1.99	-0.745	0.050		82.0	4.19	73.2	8.84	50-300	50-300
Lactic acid	1.61	1.53	1.33	0.280		3635	3044	1906	1729	2000-5000	300-2000
Lindane	-0.464	-0.432	0.171	-0.634		100	108	431	-331	50-300	300-2000
Lithium I carbonate	0.902	0.881	0.944	-0.042		590	562	649	-59.2	300-2000	300-2000
Meprobamate	0.803	0.376	0.646	0.156		1387	519	967	420	300-2000	300-2000
Mercury II chloride	-0.830	-1.82	-0.646	-0.183		40.2	4.12	61.3	-21.1	5-50	50-300
Nicotine	-0.367	0.347	0.630	-1.00		69.7	361	691	-622	50-300	300-2000
Paraquat	-0.443	-1.11	-0.227	-0.217		92.7	20.1	153	-59.9	50-300	50-300
Parathion	-1.68	-0.891	-0.100	-1.58	Negative	6.10	37.4	231	-225	5-50	50-300
Phenobarbital	-0.016	0.392	0.656	-0.672		224	573	1052	-828	50-300	300-2000
Phenol	0.908	-0.152	0.335	0.573		762	66.3	204	558	300-2000	50-300
Phenylthiourea	-1.71	-0.285	0.257	-1.96	Negative	3.00	79.0	275	-272	< 5	50-300
Physostigmine	-1.74	-1.03	-0.181	-1.56	Negative	5.00	25.8	182	-177	< 5	50-300
Potassium I chloride	1.58	1.68	1.41	0.162		2802	3551	1931	871	2000-5000	300-2000
Potassium cyanide	-0.956	-0.274	0.264	-1.22		7.20	34.6	119	-112	5-50	50-300
Procainamide HCl	0.856	0.210	0.549	0.307		1950	441	961	989	300-2000	300-2000
2-Propanol	1.93	1.78	1.47	0.456		5105	3618	1787	3318	> 5000	300-2000
Propranolol HCl	0.197	-1.33	-0.358	0.555		466	13.9	130	336	300-2000	50-300
Propylparaben	1.55	-0.84	-0.069	1.62	Positive	6332	26.1	154	6178	> 5000	50-300
Sodium arsenite	-0.474	-2.23	-0.891	0.416		43.6	0.759	16.7	26.9	5-50	5-50
Sodium chloride	1.84	1.91	1.55	0.292		4050	4730	2068	1982	2000-5000	2000-5000
Sodium dichromate dihydrate	-0.771	-2.71	-1.17	0.398		50.5	0.587	20.2	30.3	50-300	5-50
Sodium I fluoride	0.480	0.269	0.583	-0.104		127	78.0	161	-34.1	50-300	50-300
Sodium hypochlorite	2.14	1.17	1.11	1.03		10328	1103	969	9359	> 5000	300-2000
Sodium oxalate	0.674	-0.550	0.101	0.573		633	37.7	169	464	300-2000	50-300
Sodium selenate	-1.80	-0.814	-0.054	-1.74	Negative	3.00	29.0	167	-164	< 5	50-300
Strychnine	-1.72	-0.326	0.233	-1.96	Negative	6.30	158	572	-566	5-50	300-2000
Thallium I sulfate	-1.31	-1.94	-0.720	-0.585		25.0	5.74	96.2	-71.2	5-50	50-300
Trichloroacetic acid	1.28	0.742	0.862	0.420		3127	902	1189	1938	2000-5000	300-2000
1,1,1-Trichloroethane	1.96	2.11	1.67	0.288		12078	17248	6222	5857	> 5000	> 5000

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Triethylenemelamine	-1.71	-2.88	-1.27	-0.440		4.00	0.272	11.0	-7.01	< 5	5-50
Triphenyltin hydroxide	-0.047	-4.33	-2.12	2.08	Positive	329	0.017	2.75	326	300-2000	< 5
Valproic acid	0.839	0.803	0.898	-0.059		996	916	1140	-144	300-2000	300-2000
Verapamil HCl	-0.646	-1.15	-0.251	-0.395		111	34.9	275	-164	50-300	50-300
Xylene	1.64	0.832	0.915	0.728		4665	721	873	3792	2000-5000	300-2000

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

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

[2]combined 3T3 IC_{50} values from three laboratories

[3]LD_{50} determined using regression: Log LD_{50} (mmol/kg) = 0.589 log IC_{50} (mM) + 0.425

[4]outlier range = 1.510 - 1.573 (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