

Integrating Drug's Mode of Action into Quantitative Structure-Activity Relationships for Improved Prediction of Drug-Induced Liver Injury

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Tox21_111 591	5402	terbinafine	Most DILI- concern	NA	-0.868	NA	-0.832
Tox21_111 821	15250	ibufenac	Most DILI- concern	-0.960	0.963	-0.692	-0.846
Tox21_112 629	9887054	oxaliplatin	Most DILI- concern	NA	-0.875	-0.749	NA
Tox21_113 319	71467	phenoxypropazine	Most DILI- concern	-0.790	-0.814	0.036	-0.683
Tox21_113 285	6179	mebanazine	Most DILI- concern	-0.899	-0.767	0.088	-0.937
Tox21_110 623	3869	labetalol	Most DILI- concern	-0.982	-0.988	NA	-0.952
Tox21_111 038	2478	busulfan	Most DILI- concern	-0.858	-0.765	-0.457	-0.617
Tox21_111 437	3034010	orlistat	Most DILI- concern	NA	-0.994	-0.994	-0.994
Tox21_111 311	12560	erythromycin	Most DILI- concern	-0.994	-0.657	-0.327	-0.838
Tox21_111 258	4528	nomifensine	Most DILI- concern	-0.640	-0.805	-0.764	-0.652
Tox21_112 198	60953	capecitabine	Most DILI- concern	-0.428	-0.691	-0.723	-0.859
Tox21_113 167	9904	nandrolone	Most DILI- concern	-0.688	-0.988	-0.982	-0.976
Tox21_110 066	2081	alaproclate	Most DILI- concern	NA	-0.947	-0.930	-0.777
Tox21_200 071	9902	oxymetholone	Most DILI- concern	-0.664	NA	-0.901	-0.969
Tox21_112 007	5360515	naltrexone	Most DILI- concern	-0.975	-0.963	NA	-0.919
Tox21_110 168	3657	hydroxyurea	Most DILI- concern	-0.718	-0.894	-0.582	-0.924
Tox21_110 194	4260	moxisylyte	Most DILI- concern	NA	-0.976	-0.994	-0.964
Tox21_113 313	34869	amineptine	Most DILI- concern	-0.917	-0.941	-1.000	-0.864
Tox21_111 597	441184	acarbose	Most DILI- concern	-0.982	-0.982	-0.895	-0.988
Tox21_111	3121	valproic acid	Most DILI-	-1.000	-0.988	-0.932	-0.994

091			concern				
Tox21_110 494	3279	ethambutol	Most DILI- concern	-1.000	-1.000	-1.000	-1.000
Tox21_110 148	3373	flumazenil	no DILI- concern	0.965	0.900	0.859	0.894
Tox21_111 639	19988	sulisobenzone	no DILI- concern	0.969	0.701	0.894	0.981
Tox21_112 433	5394	temozolomide	no DILI- concern	0.850	0.908	0.734	0.890
Tox21_110 835	4421	nalidixic acid	no DILI- concern	0.590	0.627	0.645	0.843
Tox21_110 472	2391	bisacodyl	no DILI- concern	0.778	0.516	0.328	0.897
Tox21_113 419	30751	fludarabine	no DILI- concern	NA	0.853	0.988	0.760
Tox21_110 736	1130	thiamine	no DILI- concern	0.598	0.441	0.622	0.640
Tox21_110 829	4756	phenazopyridine	no DILI- concern	NA	0.925	-0.874	0.981
Tox21_112 613	4192	midazolam	no DILI- concern	NA	0.916	NA	0.987
Tox21_112 714	3011155	nelarabine	no DILI- concern	NA	0.768	0.417	0.364
Tox21_400 061	298	chloramphenicol	no DILI- concern	0.578	0.506	0.266	0.435
Tox21_110 821	10531	dihydroergotamine	no DILI- concern	NA	NA	NA	0.815
Tox21_110 537	3354	flavoxate	no DILI- concern	0.027	0.416	-0.362	0.793
Tox21_110 150	3385	fluorouracil	no DILI- concern	0.819	0.405	0.466	0.110
Tox21_110 505	441141	vancomycin	no DILI- concern	0.589	0.450	NA	0.698
Tox21_110 331	5342	sulfinpyrazone	no DILI- concern	0.286	0.205	-0.205	0.621
Tox21_201 834	4993	pyrimethamine	no DILI- concern	0.860	NA	-0.398	0.912
Tox21_201 633	6759	riboflavin	no DILI- concern	0.684	0.386	0.082	0.581

Tox21_113 621	6918456	prasugrel hydrochloride	no DILI- concern	0.331	-0.058	-0.270	0.627
Tox21_301 943	5920	liothyronine	no DILI- concern	0.526	0.045	0.378	NA
Tox21_113 395	2140	diatrizoate	no DILI- concern	-0.171	0.190	0.241	0.589
Tox21_111 493	5746	mitomycin	no DILI- concern	NA	NA	NA	0.768
Tox21_110 601	4189	miconazole	no DILI- concern	NA	0.253	NA	0.499
Tox21_112 184	5281081	entacapone	no DILI- concern	NA	0.284	0.836	-0.044
Tox21_111 999	4046	mefloquine	no DILI- concern	NA	0.959	NA	0.431
Tox21_111 253	441350	metyrosine	no DILI- concern	0.263	0.106	0.233	0.323
Tox21_111 478	60700	topotecan	no DILI- concern	0.865	NA	0.944	-0.129
Tox21_113 050	171548	biotin	no DILI- concern	0.248	-0.025	0.466	0.447
Tox21_110 461	3168	droperidol	no DILI- concern	0.205	-0.066	-0.155	0.344
Tox21_111 498	13342	vinblastine	no DILI- concern	0.871	NA	0.964	-0.635
Tox21_110 185	3957	loratadine	no DILI- concern	NA	-0.102	0.467	NA
Tox21_110 323	4174	metyrapone	no DILI- concern	-0.152	-0.012	0.661	-0.121
Tox21_110 103	4211	mitotane	no DILI- concern	NA	-0.340	0.531	NA
Tox21_111 559	6037	folic acid	no DILI- concern	0.245	-0.331	0.303	0.222
Tox21_201 159	30323	daunorubicin	no DILI- concern	NA	0.966	NA	NA
Tox21_112 178	71329	dofetilide	no DILI- concern	0.103	-0.172	-0.379	0.361
Tox21_110 325	9552079	chlorhexidine	no DILI- concern	NA	-0.535	0.679	NA
Tox21_110	2141	amifostine	no DILI-	-0.278	0.061	0.419	-0.201

077			concern				
Tox21_400006	1923	oxyquinoline	no DILI-concern	NA	0.962	-0.630	-0.103
Tox21_110255	5035	raloxifene	no DILI-concern	NA	NA	-0.216	0.813
Tox21_110790	47319	atracurium	no DILI-concern	-0.744	NA	NA	0.506
Tox21_202117	2244	aspirin	no DILI-concern	0.125	-0.364	0.052	0.242
Tox21_110180	3955	loperamide	no DILI-concern	NA	NA	-0.375	NA
Tox21_110244	4976	protriptyline	no DILI-concern	NA	-0.246	-0.713	0.587
Tox21_112339	439302	oxytocin	no DILI-concern	NA	-0.335	NA	-0.006
Tox21_301293	4875	potassium iodide	no DILI-concern	-0.063	-0.236	0.385	-0.701
Tox21_113125	3348	fexofenadine	no DILI-concern	-0.283	-0.173	NA	-0.399
Tox21_302427	6230	norethindrone	no DILI-concern	0.369	-0.351	-0.093	-0.447
Tox21_110482	149351	alprostadil	no DILI-concern	-0.970	NA	NA	NA
Tox21_111025	30322	digoxin	no DILI-concern	-0.623	NA	NA	-0.532
Tox21_112446	129211	tamsulosin	no DILI-concern	-0.301	-0.673	NA	0.072
Tox21_113437	988	pantothenic acid	no DILI-concern	-0.956	-0.943	NA	0.689
Tox21_112593	13505	diphenoxylate	no DILI-concern	NA	NA	-0.422	-0.404
Tox21_303658	13109	levonorgestrel	no DILI-concern	NA	-0.747	-0.338	-0.638
Tox21_110837	3404	fluvoxamine	no DILI-concern	NA	NA	NA	-0.568
Tox21_113347	708857	pyrantel	no DILI-concern	0.044	-0.213	-0.944	-0.119
Tox21_112640	64147	valganciclovir	no DILI-concern	NA	-0.455	NA	-0.560

Tox21_110 950	3083544	arformoterol	no DILI- concern	-0.411	-0.571	NA	-0.417
Tox21_110 364	5775	phentolamine	no DILI- concern	NA	-0.468	NA	-0.582
Tox21_110 760	54575	leucovorin	no DILI- concern	-0.246	-0.478	NA	-0.442
Tox21_110 098	2754	cilostazol	no DILI- concern	-0.274	-0.274	-0.495	NA
Tox21_111 129	5147	salicylamide	no DILI- concern	0.123	-0.368	-0.245	-0.523
Tox21_111 339_1	10917	levocarnitine	no DILI- concern	NA	NA	-0.941	NA
Tox21_111 578	6221	cholecalciferol	no DILI- concern	NA	NA	-0.933	-0.994
Tox21_110 641	37464	penbutolol	no DILI- concern	NA	NA	NA	-0.983
Tox21_111 663	6137	l-methionine	no DILI- concern	-0.578	-0.470	NA	-0.476
Tox21_201 078	12035	acetylcysteine	no DILI- concern	-0.392	-0.494	NA	-0.483
Tox21_110 044	5904	penicillin g	no DILI- concern	-0.444	-0.296	-0.550	-0.314
Tox21_111 566	5284569	hydrocodone	no DILI- concern	-0.775	-0.594	NA	NA
Tox21_110 350	4908	primaquine	no DILI- concern	NA	-0.601	NA	NA
Tox21_112 087	2367383 7	docusate sodium	no DILI- concern	NA	-0.824	0.392	-0.805
Tox21_111 703	3821	ketamine	no DILI- concern	-0.512	-0.657	NA	-0.395
Tox21_110 529	4195	midodrine	no DILI- concern	-0.618	-0.353	-0.471	-0.182
Tox21_110 193	4201	minoxidil	no DILI- concern	-0.307	-0.360	-0.147	-0.540
Tox21_110 766	5360696	dextromethorphan	no DILI- concern	NA	-0.726	NA	-0.762
Tox21_202 176	6869	penicillin v	no DILI- concern	-0.462	-0.376	-0.474	-0.602
Tox21_300	679	dimethyl sulfoxide	no DILI-	-0.659	-0.426	-0.735	-0.426

957			concern				
Tox21_113 609	115237	paliperidone	no DILI- concern	-0.370	-0.215	-0.754	-0.467
Tox21_111 266	4991	pyridostigmine	no DILI- concern	-0.712	-0.147	-0.353	-0.526
Tox21_110 238	4909	primidone	no DILI- concern	-0.469	-0.592	0.126	-0.625
Tox21_113 006	60753	ibutilide	no DILI- concern	NA	-0.830	NA	-0.903
Tox21_111 102	3610	hexylresorcinol	no DILI- concern	NA	NA	-0.955	-0.872
Tox21_110 497	4034	meclizine	no DILI- concern	NA	-0.667	-0.798	-0.583
Tox21_111 196	5280360	dinoprostone	no DILI- concern	NA	-0.903	-0.897	NA
Tox21_111 655	4812	phytonadione	no DILI- concern	-0.840	-0.412	-0.591	-0.395
Tox21_112 404	5280793	ergocalciferol	no DILI- concern	NA	NA	-0.870	-0.981
Tox21_112 861	5288826	morphine	no DILI- concern	-0.353	-0.694	-0.741	-0.582
Tox21_110 674	5401	terazosin	no DILI- concern	-0.652	-0.372	-0.756	-0.604
Tox21_112 700	31378	fludrocortisone	no DILI- concern	-0.942	-0.955	NA	-0.909
Tox21_110 574	26987	clemastine	no DILI- concern	NA	-0.952	NA	-0.928
Tox21_112 606	5826	dextroamphetamine	no DILI- concern	-0.698	-0.741	NA	-0.722
Tox21_110 711	3724	iodixanol	no DILI- concern	-0.867	-0.759	-0.203	-0.127
Tox21_110 507	4634	oxybutynin	no DILI- concern	NA	-0.983	NA	-0.943
Tox21_110 441	4173	metronidazole	no DILI- concern	-0.267	-0.393	-0.411	-0.688
Tox21_110 511	2710	chlorcyclizine	no DILI- concern	NA	-1.000	NA	-0.970
Tox21_110 909	2562	carbetapentane	no DILI- concern	NA	-0.981	-0.968	NA

Tox21_110 500	5526	tranexamic acid	no DILI- concern	-0.861	-0.715	NA	-0.695
Tox21_110 028	6832	benztropine	no DILI- concern	NA	-0.993	NA	-1.000
Tox21_111 583	19649	streptomycin	no DILI- concern	-0.663	-0.713	NA	-0.838
Tox21_110 668	65492	iopamidol	no DILI- concern	-0.844	-0.820	-0.550	NA
Tox21_110 809	8226	methylergonovine	no DILI- concern	-0.655	-0.749	-0.944	-0.655
Tox21_110 818	445354	vitamin a	no DILI- concern	0.448	-0.935	-0.976	NA
Tox21_112 033	27350	pancuronium	no DILI- concern	-0.994	-0.795	NA	-0.795
Tox21_111 014	5865	prednisone	no DILI- concern	-0.896	-0.859	-0.963	-0.037
Tox21_111 614	2707	chloral hydrate	no DILI- concern	-0.630	-0.721	-0.497	-0.733
Tox21_112 336	2564	carbinoxamine	no DILI- concern	NA	-0.858	NA	-0.878
Tox21_113 592	5493444	aliskiren	no DILI- concern	-0.931	-0.688	0.156	-0.644
Tox21_112 884	5284371	codeine	no DILI- concern	-0.814	-0.758	-0.441	-0.720
Tox21_113 128	60714	gadoteridol	no DILI- concern	-0.901	-0.895	NA	-0.839
Tox21_112 965	338	salicylic acid	no DILI- concern	-0.318	-0.747	-0.553	-0.765
Tox21_112 611	3345	fentanyl	no DILI- concern	-0.885	-0.931	NA	-0.862
Tox21_110 741	2973	deferoxamine	no DILI- concern	-0.945	-0.855	0.752	-0.836
Tox21_110 167	681	dopamine	no DILI- concern	NA	-0.919	-0.919	NA
Tox21_110 895	9681	methysergide	no DILI- concern	-0.737	-0.773	-0.970	-0.666
Tox21_110 398	7699	benzonatate	no DILI- concern	-0.970	-0.922	NA	NA
Tox21_112	441290	rocuronium	no DILI-	-0.988	-0.862	NA	-0.925

437			concern				
Tox21_113 569	3658	hydroxyzine	no DILI- concern	NA	-0.994	-0.880	-0.982
Tox21_111 475	5486971	pregabalin	no DILI- concern	-0.943	-0.943	NA	-0.943
Tox21_112 856	10836	methamphetamine	no DILI- concern	-0.954	-0.928	NA	-0.961
Tox21_112 349	165580	paromomycin	no DILI- concern	-1.000	-0.917	NA	-0.935
Tox21_113 570	33036	dexchlorpheniramin e maleate	no DILI- concern	NA	NA	-0.894	-0.963
Tox21_113 619	4454	neomycin	no DILI- concern	-0.988	-0.909	NA	-0.964
Tox21_110 099	2519	caffeine	no DILI- concern	-0.837	-0.717	NA	-0.861
Tox21_200 122	9782	betamethasone	no DILI- concern	-0.870	-0.893	-0.910	-0.921
Tox21_110 827	2153	theophylline	no DILI- concern	-0.663	-0.729	-0.428	-0.837
Tox21_200 417	3305	etidronic acid	no DILI- concern	-0.881	-0.660	-0.767	-0.742
Tox21_110 592	15541	spectinomycin	no DILI- concern	-0.872	-0.789	-0.623	-0.636
Tox21_110 126	36811	dobutamine	no DILI- concern	-0.659	-0.908	-0.974	-0.836
Tox21_110 498	4091	metformin	no DILI- concern	-0.878	-0.841	-0.474	-0.872
Tox21_110 431	26934	phenylpropanolamin e	no DILI- concern	-0.858	-0.871	-0.378	-0.877
Tox21_111 201	37768	amikacin	no DILI- concern	-0.958	-0.940	-0.367	-0.922
Tox21_110 389	3516	guaifenesin	no DILI- concern	-0.563	-0.925	-0.594	-0.719
Tox21_111 318	11333	lactulose	no DILI- concern	-0.636	-0.877	-0.754	-0.894
Tox21_112 000	16960	dexbrompheniramin e	no DILI- concern	NA	-0.976	-0.845	-0.875
Tox21_110 883	5754	hydrocortisone	no DILI- concern	-0.967	-0.987	-0.980	-0.802

Tox21_110 087	4768	phenoxybenzamine	no DILI- concern	-0.889	-0.981	-0.957	NA
Tox21_113 496	59768	esmolol	no DILI- concern	-0.975	-0.919	-0.938	-0.869
Tox21_112 876	441278	pentazocine	no DILI- concern	0.099	-0.956	-0.994	-0.978
Tox21_200 323	441281	dimenhydrinate	no DILI- concern	NA	-1.000	-0.963	-0.956
Tox21_111 640	439260	norepinephrine	no DILI- concern	NA	-0.950	-0.932	-0.981
Tox21_111 268	5314	succinylcholine	no DILI- concern	NA	-0.976	-0.934	-0.964
Tox21_110 127	3100	diphenhydramine	no DILI- concern	NA	-0.993	-0.987	-0.974
Tox21_110 290	5411	tetracaine	no DILI- concern	NA	-0.993	-0.939	-0.980
Tox21_111 373	247	betaine	no DILI- concern	-0.977	-0.884	-0.555	-0.948
Tox21_111 737	60774	tolterodine	no DILI- concern	NA	-0.994	-0.974	-1.000
Tox21_110 919	5282443	triprolidine	no DILI- concern	NA	-0.988	-0.982	-0.977
Tox21_110 230	4992	pyrilamine maleate	no DILI- concern	NA	-0.989	-0.994	-0.994
Tox21_110 340	3518	guanethidine	no DILI- concern	-0.912	-0.893	-0.697	-0.874
Tox21_110 035	5184	scopolamine	no DILI- concern	-0.845	-0.840	-0.971	-0.817
Tox21_113 571	3042	dicyclomine	no DILI- concern	NA	-1.000	-0.994	-1.000
Tox21_111 274	5572	trihexyphenidyl	no DILI- concern	-1.000	-1.000	-1.000	NA
Tox21_112 785	2381	biperiden	no DILI- concern	NA	-1.000	-1.000	-1.000
Tox21_110 717	57363	finasteride	no DILI- concern	-0.994	-0.983	-0.357	-0.911
Tox21_112 104	5467850 1	vitamin c	no DILI- concern	-0.634	-0.891	-0.886	-0.869
Tox21_111	2088	alendronate	no DILI-	-0.968	-0.801	-0.808	-0.910

553			concern				
Tox21_111 310	9294	ephedrine	no DILI- concern	-0.981	-0.968	-0.672	-0.974
Tox21_110 612	6032	kanamycin	no DILI- concern	-0.988	-0.959	-0.710	-0.976
Tox21_111 086	6433328	ethanolamine	no DILI- concern	-0.964	-0.843	-0.928	-0.916
Tox21_110 122	2576	carisoprodol	no DILI- concern	-0.983	-0.936	-0.878	-0.883
Tox21_110 183	3676	lidocaine	no DILI- concern	-0.988	-0.929	-0.924	-0.924
Tox21_110 572	26757	selegiline	no DILI- concern	-0.982	-0.994	-0.752	-0.970
Tox21_111 491	14985	vitamin e	no DILI- concern	-0.994	-0.914	-0.914	-0.957
Tox21_301 002	24705	dimethicone	no DILI- concern	-0.982	-0.951	-0.951	-0.951
Tox21_110 579	23897	molindone	no DILI- concern	-1.000	-0.917	-0.900	-0.933
Tox21_110 433	6726	cyclizine	no DILI- concern	-0.819	-1.000	-0.934	-0.988
Tox21_111 562	5816	epinephrine	no DILI- concern	-0.867	-0.982	-0.970	-0.970
Tox21_302 861	3162	doxylamine	no DILI- concern	-0.945	-0.956	-0.972	-0.961
Tox21_112 028	2370	bethanechol	no DILI- concern	-0.988	-0.977	-0.930	-0.971
Tox21_113 644	1054	pyridoxine	no DILI- concern	-0.958	-0.940	-0.964	-0.988
Tox21_110 138	3202	edrophonium	no DILI- concern	-0.994	-0.972	-0.923	-0.983
Tox21_110 816	174174	atropine	no DILI- concern	-0.968	-0.981	-0.981	-0.948
Tox21_111 563	4678	dexpanthenol	no DILI- concern	-0.994	-0.988	-0.988	-0.946
Tox21_111 643	82170	sorbitol	no DILI- concern	-1.000	-0.988	-0.988	-1.000
Tox21_110 266	2083	albuterol	no DILI- concern	-0.982	-0.976	-0.994	-1.000

Tox21_111 706	2474	bupivacaine	no DILI- concern	-1.000	-1.000	-0.983	-0.965
Tox21_110 551	4086	metaproterenol	no DILI- concern	-0.988	-0.994	-0.988	-1.000
Tox21_110 172	3779	isoproterenol	no DILI- concern	-1.000	-1.000	-0.988	-1.000
Tox21_110 508	4919	procyclidine	no DILI- concern	-1.000	-1.000	-1.000	-1.000