

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

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Table S1. Tox21 Assay information of 333 DILI annotated drugs. Y = Active; N = Inactive; NA = not_used

			Assay ID	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17		
Tox21_ID	PubChem_ID	SMILES	DILI_label	AHR	AR-bla-agonist	AR-bla-antagonist	ARE-bla	AR-mda-kb2-luc-agonist	AR-mda-kb2-luc-antagonist	aromatase	ER-bla-antagonist	ER-luc-bg1-4e2-agonist	ER-luc-bg1-4e2-antagonist	gh3-tre-antagonist	GR-hela-bla-antagonist	HSE-bla	Mitotox	p53	PPARG-bla-agonist	PPARG-bla-antagonist		
Tox21_111373	247	<chem>C[N+](C)(C)CC(=O)[O-]</chem>	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_400061	298	<chem>C1=CC(=CC=C1C(C(=O)NC(=O)C(C1)O)[N+](=O)[O-]</chem>	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_112965	338	<chem>C1=CC=C(C(=C1)C(=O)O)O</chem>	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_300957	679	<chem>CS(=O)C</chem>	no DILI-concern	N	N	N	Y	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_110167	681	<chem>C1=CC(=C(C=C1)C(C)O)O</chem>	no DILI-concern	N	N	N	Y	N	N	N	N	Y	NA	NA	N	N	N	N	N	N	N	
Tox21_110337	938	<chem>C1=CC(=CN=C1)C(=O)O</chem>	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_113437	988	<chem>CC(C)(CO)C(C(=O)NCCC(=O)O)O</chem>	no DILI-concern	N	Y	N	NA	Y	Y	Y	NA	N	Y	N	Y	NA	N	N	N	NA	NA	
Tox21_113644	1054	<chem>CC1=NC=C(C(=C1)O)CO</chem>	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_110736	1130	<chem>CC1=C(SC=[N+]1C(C2=CN=C(N=C2N)C)CCO</chem>	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_400006	1923	<chem>C1=CC2=C(C(=C1)O)N=CC=C2</chem>	no DILI-concern	N	N	NA	Y	N	NA	NA	N	N	N	NA	N	Y	N	Y	Y	Y	N	
Tox21_110073	1935	<chem>C1CCC2=NC3=CC=CC=C3C(=C2)C1N</chem>	Most DILI-concern	Y	N	NA	N	N	NA	N	NA	NA	Y	Y	N	N	N	NA	N	N	N	
Tox21_110397	1983	<chem>CC(=O)NC1=CC=C(C=C1)O</chem>	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_110078	1986	<chem>CC(=O)NC1=NN=C(S1)S(=O)(=O)N</chem>	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_202482	2019	<chem>CC1C(C(=O)NC(C(=O)N2CCCC2C(=O)N(CC(=O)N(C(C(=O)O)1)C(C)C)C(C)C(C)C)NC(=O)C3=C4C(=C(C=C3)C)OC5=C(C(=O)C(=C(C5=N4)C(=O)NC6C(O</chem>	Most DILI-concern	N	Y	Y	Y	N	Y	Y	Y	Y	Y	Y	NA	NA	N	Y	Y	Y	Y	Y

		C(=O)C(N(C(=O)C N(C(=O)C7CCCN7 C(=O)C(NC6=O)C(C)C)C)C(C)C)C N)C																		
Tox21_11 0066	2081	CC(C(=O)OC(C)C) CC1=CC=C(C=C1) C)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	Y	N	N	N
Tox21_11 0266	2083	CC(C)C)NCC(C1= CC(=C(C=C1)O)CO)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1553	2088	C(CC(O)(P(=O)(O) O)P(=O)(O)O)CN	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3395	2140	CC(=O)NC1=C(C(= C(C(=C1)C(=O)O)I)NC(=O)C)I	no DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N
Tox21_11 0077	2141	C(CN)CNCCSP(=O) (O)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N
Tox21_11 0406	2145	CCC1(CCC(=O)NC 1=O)C2=CC=C(C=C 2)N	Most DILI- concern	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N	N	N
Tox21_11 0827	2153	CN1C2=C(C(=O)N(C1=O)C)NC=N2	no DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N
Tox21_11 0083	2157	CCCCC1=C(C2=CC =CC=C2O1)C(=O)C 3=CC(=C(C(=C3)I) OCCN(CC)CC)I	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	NA	NA	Y	N	NA	NA
Tox21_20 2117	2244	CC(=O)OC1=CC=C C=C1C(=O)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2465	2313	C1=CC=C(C=C1)C N2C3=CC=CC=C3 C(=N2)OCC(=O)O	Most DILI- concern	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0041	2333	CCC1=C(C2=CC=C C=C2O1)C(=O)C3= CC(=C(C(=C3)Br)O)Br	Most DILI- concern	N	N	N	NA	N	N	N	Y	N	N	NA	NA	Y	Y	Y	Y	Y
Tox21_11 2028	2370	CC(C[N+](C)C)C) OC(=O)N	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2785	2381	C1CCN(CC1)CCC(C2CC3CC2C=C3)(C4=CC=CC=C4)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	NA
Tox21_11 0472	2391	CC(=O)OC1=CC=C (C=C1)C(C2=CC=C (C=C2)OC(=O)C)C 3=CC=CC=N3	no DILI- concern	N	N	N	N	N	NA	Y	Y	Y	Y	N	N	N	Y	Y	N	N
Tox21_11 1706	2474	CCCCN1CCCCC1C (=O)NC2=C(C=CC= C2)C	no DILI- concern	N	N	N	N	N	NA	N	N	N	N	N	N	N	NA	N	N	N
Tox21_11	2478	CS(=O)(=O)OCCCC	Most DILI-	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N

1038		OS(=O)(=O)C	concern																	
Tox21_11 0099	2519	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	no DILI-concern	N	N	N	NA	N	N	N	N	NA	N	N	N	N	N	N	N	N
Tox21_11 0300	2520	CC(C)C(CCCN(C)C CC1=CC(=C(C=C1) OC)OC)(C#N)C2=C C(=C(C=C2)OC)OC	Most DILI-concern	N	N	Y	N	N	NA	N	NA	Y	NA	NA	N	N	Y	N	NA	NA
Tox21_11 0104	2554	C1=CC=C2C(=C1)C =CC3=CC=CC=C3 N2C(=O)N	Most DILI-concern	N	NA	N	N	NA	NA	NA	N	N	N	N	NA	N	N	N	N	N
Tox21_11 0909	2562	CCN(CC)CCOCCO C(=O)C1(CCCC1)C 2=CC=CC=C2	no DILI-concern	N	N	Y	N	N	NA	N	NA	N	NA	NA	N	N	Y	N	N	N
Tox21_11 2336	2564	CN(C)CCOC(C1=C C=C(C=C1)C1)C2= CC=CC=N2	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0122	2576	CCCC(C)COC(=O) N)COC(=O)NC(C)C	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_20 1964	2662	CC1=CC=C(C=C1) C2=CC(=NN2C3=C C=C(C=C3)S(=O)(=O)N)C(F)F	Most DILI-concern	N	N	NA	Y	N	N	NA	NA	Y	N	NA	Y	N	NA	N	N	N
Tox21_11 1614	2707	C(C(Cl)(Cl)Cl)(O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0511	2710	CN1CCN(CC1)C(C 2=CC=CC=C2)C3= CC=C(C=C3)Cl	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	Y	N	N	NA
Tox21_11 0093	2717	CN1C(S(=O)(=O)C CC1=O)C2=CC=C(C C=C2)Cl	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0105	2733	C1=CC2=C(C=C1Cl)NC(=O)O2	Most DILI-concern	N	N	N	N	N	N	N	NA	N	N	N	N	N	NA	N	N	N
Tox21_11 0098	2754	C1CCC(CC1)N2C(=NN=N2)CCCCOC3=CC4=C(C=C3)NC(=O)CC4	no DILI-concern	N	N	N	Y	N	N	N	N	N	NA	N	N	N	N	N	N	N
Tox21_11 0712	2764	C1CC1N2C=C(C(=O)C3=CC(=C(C=C3)2)N4CCNCC4)F(C(=O)O	Most DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0117	2801	CN(C)CCCN1C2=C C=CC=C2CCC3=C1 C=C(C=C3)Cl	Most DILI-concern	N	N	N	N	N	NA	NA	Y	N	NA	NA	N	N	Y	N	Y	NA
Tox21_11 2259	2898	CC(=O)OC1=CC=C (C=C1)C(=C2CCCC C2)C3=CC=C(C=C3))OC(=O)C	Most DILI-concern	N	N	N	Y	N	N	N	N	N	N	N	N	NA	N	N	Y	NA
Tox21_11 2013	2952	C1C(=O)NC(=O)N1 N=CC2=CC=C(O2)	Most DILI-concern	Y	N	N	N	N	N	N	NA	N	N	NA	N	N	Y	N	N	N

		C3=CC=C(C=C3)[N+](=O)[O-]																			
Tox21_11 0741	2973	CC(=O)N(CCCCCN C(=O)CCC(=O)N(C CCCCNC(=O)CCC(=O)N(CCCCCN)O) O)O	no DILI- concern	N	N	N	Y	N	NA	N	N	N	N	N	N	N	N	N	N	N	NA
Tox21_11 0770	3033	C1=CC=C(C=C1)C C(=O)NC2=C(C=CC=C2C)Cl	Most DILI- concern	N	N	NA	NA	N	N	N	N	NA	N	NA	N	N	N	NA	N	Y	
Tox21_11 3571	3042	CCN(CC)CCOC(=O) C1(CCCCC1)C2CC CCC2	no DILI- concern	N	N	NA	N	N	N	NA	N	N	N	NA	N	N	NA	N	N	N	
Tox21_11 0598	3059	C1=CC(=C(C=C1)C2 =C(C=C(C=C2)F)F) C(=O)O)O	Most DILI- concern	N	NA	N	NA	N	N	N	N	N	N	N	NA	N	NA	N	NA	Y	
Tox21_11 0127	3100	CN(C)CCOC(C1=C C=CC=C1)C2=CC=CC=C2	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	NA	N	N	N	
Tox21_11 0133	3108	C1CCN(CC1)C2=N C(=NC3=C2N=C(N=C3N4CCCC4)N(C CCO)CCO)N(CCO) CCO	Most DILI- concern	N	NA	NA	NA	N	N	NA	NA	Y	NA	Y	NA	NA	NA	Y	N	NA	
Tox21_40 0072	3117	CCN(CC)C(=S)SSC (=S)N(CC)CC	Most DILI- concern	Y	NA	NA	NA	N	NA	NA	Y	Y	Y	NA	NA	Y	Y	NA	Y	N	
Tox21_11 1091	3121	CCCC(CCC)C(=O) O	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_30 2861	3162	CC(C1=CC=CC=C1)C2=CC=CC=N2)O CCN(C)C	no DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N	
Tox21_11 0461	3168	C1CN(CC=C1N2C3 =CC=CC=C3NC2=O)CCCC(=O)C4=C C=C(C=C4)F	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_11 0138	3202	CC[N+](C)(C)C1=C C(=CC=C1)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	
Tox21_11 0494	3279	CCC(CO)NCCNC(C C)CO	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_20 0417	3305	CC(O)(P(=O)(O)O) P(=O)(O)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_11 0644	3308	CCC1=CC=CC2=C1 NC3=C2CCOC3(CC)CC(=O)O	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_11 0145	3331	C1=CC=C(C=C1)C COC(=O)N)COC(=O)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	
Tox21_11 0785_1	3342	CC(C1=CC(=CC=C 1)OC2=CC=CC=C2	Most DILI- concern	NA	NA	NA	N	NA	NA	NA	NA	NA	NA	NA	NA	N	NA	NA	NA	N	

)C(=O)O																		
Tox21_11 2611	3345	CCC(=O)N(C1CCN (CC1)CCC2=CC=C C=C2)C3=CC=CC= C3	no DILI- concern	N	Y	N	NA	Y	N	N	N	N	N	N	NA	NA	N	N	N	NA
Tox21_11 3125	3348	CC(C)(C1=CC=C(C =C1)C(CCCN2CCC (CC2)C(C3=CC=CC =C3)(C4=CC=CC= C4)O)O)C(=O)O	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1394	3351	C1CN(CCN1CC2=C C3=C(C=C2)OCO3) C(=O)COC4=CC=C (C=C4)Cl	Most DILI- concern	N	N	N	Y	N	N	NA	N	Y	Y	N	N	N	N	N	N	N
Tox21_11 0537	3354	CC1=C(OC2=C(C1 =O)C=CC=C2C(=O) OCCN3CCCC3)C 4=CC=CC=C4	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1419	3365	C1=CC(=C(C=C1F) F)C(CN2C=NC=N2) (CN3C=NC=N3)O	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0148	3373	CCOC(=O)C1=C2C N(C(=O)C3=C(N2C =N1)C=CC(=C3)F) C	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0150	3385	C1=C(C(=O)NC(=O)N1)F	no DILI- concern	N	N	N	N	N	N	N	NA	N	N	Y	N	N	N	Y	N	N
Tox21_11 0154	3397	CC(C)C(=O)NC1=C C(=C(C=C1)[N+](=O) [O-])C(F)(F)F	Most DILI- concern	N	N	Y	Y	N	Y	NA	NA	Y	Y	Y	NA	N	Y	N	N	N
Tox21_11 0837	3404	COC(C)C(=O)N(C N)C1=CC=C(C=C1) C(F)(F)F	no DILI- concern	N	N	N	NA	N	NA	NA	N	N	N	NA	N	N	Y	N	NA	N
Tox21_11 0678	3474	C1=CC=C(C(=C1)C (=O)OCC(CO)O)NC 2=C3C=CC(=CC3= NC=C2)Cl	Most DILI- concern	NA	N	N	Y	N	N	Y	NA	N	N	N	N	Y	NA	N	N	N
Tox21_11 0389	3516	COC1=CC=CC=C1 OCC(CO)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0340	3518	C1CCCN(CCC1)CC N=C(N)N	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1102	3610	CCCCC1=C(C=C C(C=C1)O)O	no DILI- concern	N	N	N	Y	N	Y	N	NA	Y	N	NA	NA	N	Y	N	NA	Y
Tox21_11 0168	3657	C(=O)(N)NO	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3569	3658	C1CN(CCN1CCOC CO)C(C2=CC=CC= C2)C3=CC=C(C=C3)Cl	no DILI- concern	N	N	N	N	N	N	N	NA	N	N	NA	N	N	Y	N	N	NA

Tox21_11 0183	3676	CCN(CC)CC(=O)N C1=C(C=CC=C1C) C	no DILI- concern	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0711	3724	CC(=O)N(CC(CN(C 1=C(C(=C(C(=C1) C(=O)NCC(CO)O)I C(=O)NCC(CO)O)I C(=O)C)O)C2=C(C =C(C(=C2)C(=O)N CC(CO)O)I)C(=O)N CC(CO)O)I	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1341	3748	CC(C)NNC(=O)C1= CC=NC=C1	Most DILI- concern	NA	N	N	N	N	N	N	N	Y	N	NA	N	N	N	N	N	N	N
Tox21_11 0336	3759	CC1=CC(=NO1)C(= O)NNCC2=CC=CC =C2	Most DILI- concern	NA	N	N	NA	N	N	NA	N	Y	Y	N	N	NA	N	N	N	N	NA
Tox21_11 3640	3767	C1=CN=CC=C1C(= O)NN	Most DILI- concern	Y	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0172	3779	CC(C)NCC(C1=CC(=C(C=C1)O)O)O	no DILI- concern	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1703	3821	CNC1(CCCCC1=O) C2=CC=CC=C2C1	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	N	NA
Tox21_11 0594	3825	CC(C1=CC=CC(=C 1)C(=O)C2=CC=CC =C2)C(=O)O	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0623	3869	CC(CCC1=CC=CC= C1)NCC(C2=CC(=C (C=C2)O)C(=O)N)O	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	N	N
Tox21_11 0182	3899	CC1=C(C=NO1)C(= O)NC2=CC=C(C=C 2)C(F)(F)F	Most DILI- concern	Y	NA	NA	Y	N	Y	Y	N	N	Y	NA	N	NA	Y	N	N	N	N
Tox21_11 0719	3902	C1=CC(=CC=C1C# N)C(C2=CC=C(C=C 2)C#N)N3C=NC= N3	Most DILI- concern	N	N	NA	N	N	N	Y	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0180	3955	CN(C)C(=O)C(CCN 1CCC(CC1)(C2=CC =C(C=C2)C1)O)(C3 =CC=CC=C3)C4=C C=CC=C4	no DILI- concern	N	N	NA	N	N	NA	NA	NA	Y	NA	NA	NA	N	N	N	N	NA	N
Tox21_11 0185	3957	CCOC(=O)N1CCC(=C2C3=C(CCC4=C 2N=CC=C4)C=C(C =C3)C1)CC1	no DILI- concern	N	N	NA	Y	N	Y	N	Y	Y	NA	NA	NA	NA	NA	Y	N	Y	Y
Tox21_11 0497	4034	CC1=CC(=CC=C1) CN2CCN(CC2)C(C 3=CC=CC=C3)C4= CC=C(C=C4)Cl	no DILI- concern	N	N	N	Y	N	N	N	N	N	N	NA	NA	N	N	N	N	N	N
Tox21_11 1999	4046	C1CCNC(C1)C(C2= CC(=NC3=C2C=CC	no DILI- concern	NA	NA	NA	NA	N	NA	NA	NA	Y	N	NA	NA	N	Y	NA	Y	NA	NA

		=C3C(F)(F)F)C(F)(F)F)O																			
Tox21_11 0551	4086	CC(C)NCC(C1=CC(=CC(=C1)O)O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0498	4091	CN(C)C(=N)N=C(N)N	no DILI-concern	N	N	N	N	NA	NA	Y	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0441	4173	CC1=NC=C(N1CCO)[N+](=O)[O-]	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0323	4174	CC(C)(C1=CN=CC=C1)C(=O)C2=CN=CC=C2	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0601	4189	C1=CC(=C(C=C1C1)C1)COC(CN2C=CN=C2)C3=C(C=C(C=C3)C1)C1	no DILI-concern	Y	N	N	NA	N	N	Y	N	N	N	NA	N	NA	N	NA	N	NA	NA
Tox21_11 2613	4192	CC1=NC=C2N1C3=C(C=C(C=C3)C1)C(=NC2)C4=CC=CC=C4F	no DILI-concern	NA	N	NA	NA	N	N	Y	NA	Y	Y	NA	Y	N	NA	N	N	N	N
Tox21_11 0529	4195	COC1=CC(=C(C=C1)OC)C(CNC(=O)CN)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0193	4201	C1CCN(CC1)C2=NC(=N)N(C(=C2)N)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0103	4211	C1=CC=C(C(=C1)C(C2=CC=C(C=C2)C1)C(C1)C1)C1	no DILI-concern	N	N	N	N	N	N	N	NA	Y	N	NA	Y	N	Y	NA	N	N	N
Tox21_11 0194	4260	CC1=CC(=C(C=C1)OC(=O)C(C)C)OCCN(C)C	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N
Tox21_11 0835	4421	CCN1C=C(C(=O)C2=C1N=C(C=C2)C)C(=O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3574	4449	CCC1=NN(C(=O)N1CCOC2=CC=CC=C2)CCCN3CCN(CC3)C4=CC(=CC=C4)Cl	Most DILI-concern	NA	N	NA	NA	N	NA	NA	NA	Y	Y	NA	NA	N	Y	N	NA	NA	NA
Tox21_11 3619	4454	C1C(C(C(C(C1N)O)C2C(C(C(C(O2)CN)O)O)N)OC3C(C(C(O3)CO)OC4C(C(C(C(O4)CN)O)O)N)O)N	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	N	NA
Tox21_11 0982	4463	CC1=C2C(=NC=C1)N(C3=C(C=CC=N3)C(=O)N2)C4CC4	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0208	4472	C1=CC=C(C=C1)CNC(=O)CCNNC(=O)	Most DILI-concern	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N

)C2=CC=NC=C2																		
Tox21_30 1589	4493	CC1(C(=O)N(C(=O)N1)C2=CC(=C(C=C2)[N+](=O)[O-])C(F)(F)FC	Most DILI-concern	N	N	Y	Y	N	Y	N	N	Y	Y	Y	N	N	N	N	N	N
Tox21_11 0207	4495	CS(=O)(=O)NC1=C(C=C(C=C1)[N+](=O)[O-])OC2=CC=CC=C2	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	Y	N	N	Y
Tox21_11 1258	4528	CN1CC(C2=C(C1)C(=CC=C2)N)C3=CC=CC=C3	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N
Tox21_11 0682	4539	CCN1C=C(C(=O)C2=CC(=C(C=C21)N3CCNCC3)F)C(=O)O	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0048	4543	CNCCC=C1C2=CC=CC=C2CCC3=CC=CC=C31	Most DILI-concern	N	N	NA	NA	N	NA	NA	NA	N	N	NA	N	NA	Y	N	NA	NA
Tox21_11 0507	4634	CCN(CC)CC#CCOC(=O)C(C1CCCC1)(C2=CC=CC=C2)O	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	NA	N	N	NA
Tox21_11 1563	4678	CC(C)(CO)C(C(=O)NCCCO)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0226	4680	COC1=C(C=C(C=C1)CC2=NC=CC3=C(C=C(C=C32)OC)OC	Most DILI-concern	NA	N	N	Y	N	NA	N	N	Y	Y	NA	N	N	NA	N	N	N
Tox21_11 2509_1	4723	C1=CC=C(C=C1)C2C(=O)N=C(O2)N	Most DILI-concern	NA	NA	NA	N	NA	NA	NA	NA	NA	NA	NA	NA	N	NA	NA	NA	N
Tox21_11 1395	4746	C1CCC(CC1)C(CC2CCCCN2)C3CCCCC3	Most DILI-concern	NA	NA	NA	NA	N	NA	NA	NA	NA	NA	NA	NA	NA	Y	NA	NA	NA
Tox21_11 0829	4756	C1=CC=C(C=C1)N=NC2=C(N=C(C=C2)N)N	no DILI-concern	Y	N	Y	Y	N	Y	Y	Y	Y	Y	NA	Y	N	Y	NA	N	NA
Tox21_11 0087	4768	CC(COC1=CC=CC=C1)N(CCC1)CC2=CC=CC=C2	no DILI-concern	N	N	N	Y	N	N	N	N	NA	NA	N	Y	Y	NA	NA	N	NA
Tox21_11 1655	4812	CC1=C(C(=O)C2=C(C=CC2C1=O)CC=C(C)CCCC(C)CC(C)CCCC(C)C	no DILI-concern	Y	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N
Tox21_30 1293	4875	[K+].[I-]	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0350	4908	CC(CCCN)NC1=C2C(=CC(=C1)OC)C=CC=N2	no DILI-concern	NA	N	N	NA	N	N	N	N	NA	NA	NA	NA	N	N	N	N	N

Tox21_11 0238	4909	CCC1(C(=O)NCNC 1=O)C2=CC=CC=C 2	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0508	4919	C1CCC(CC1)C(CC N2CCCC2)(C3=CC =CC=C3)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N
Tox21_11 0244	4976	CNCCCC1C2=CC= CC=C2C=CC3=CC =CC=C13	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	NA	N	N	NA
Tox21_11 1266	4991	C[N+](=O)C(=O)C 1)OC(=O)N(C)C	no DILI- concern	N	N	N	N	Y	NA	N	N	Y	N	N	N	N	N	N	N	N
Tox21_11 0230	4992	CN(C)CCN(CC1=C C=C(C=C1)OC)C2= CC=CC=N2	no DILI- concern	N	N	N	N	N	NA	N	N	N	N	NA	N	N	NA	N	N	N
Tox21_20 1834	4993	CCC1=C(C(=NC(=N 1)N)N)C2=CC=C(C =C2)Cl	no DILI- concern	N	NA	NA	Y	NA	Y	N	N	Y	Y	Y	NA	N	N	Y	NA	N
Tox21_11 0255	5035	C1CCN(CC1)CCOC 2=CC=C(C=C2)C(=O) C3=C(SC4=C3C=CC =C4)O)C5=CC=C(C =C5)O	no DILI- concern	N	Y	NA	N	N	NA	Y	Y	Y	Y	NA	NA	NA	Y	Y	NA	NA
Tox21_11 0252	5070	C1=CC2=C(C=C1O C(F)(F)F)SC(=N2)N	Most DILI- concern	Y	N	Y	N	N	NA	Y	N	Y	Y	Y	Y	N	N	Y	N	N
Tox21_11 1129	5147	C1=CC=C(C(=C1)C =O)N)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0035	5184	CN1C2CC(CC1C3C 2O3)OC(=O)C(CO) C4=CC=CC=C4	no DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N
Tox21_11 1684	5291	CC1=C(C=C(C=C1) NC(=O)C2=CC=C(C =C2)CN3CCN(CC 3)C)NC4=NC=CC(=N 4)C5=CN=CC=C5	Most DILI- concern	Y	N	NA	NA	N	NA	NA	NA	N	NA	NA	NA	N	Y	N	N	NA
Tox21_11 1268	5314	C[N+](C)(C)CCOC(=O) CCC(=O)OCC[N+](C)(C)C	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0480	5329	CC1=CC(=NO1)NS(=O) (=O)C2=CC=C(C=C2)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0363	5340	C1=CC(=CC=C1N) S(=O)(=O)NC2=NC=CS2	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N
Tox21_11 0331	5342	C1=CC=C(C=C1)N 2C(=O)C(C(=O)N2 C3=CC=CC=C3)CC S(=O)C4=CC=CC=C4	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11	5352	CC1=C(C2=C(C1=C	Most DILI-	Y	N	N	NA	N	N	N	N	N	N	N	N	N	NA	N	N	N

0270		C3=CC=C(C=C3)S(=O)C)C=CC(=C2)F)CC(=O)O	concern																	
Tox21_11 0858	5354	CCCCCCCNC(C)C(C1=CC=C(C=C1)SC(C)C)O	Most DILI-concern	N	NA	NA	NA	N	N	NA	NA	Y	NA	NA	NA	Y	NA	NA	N	NA
Tox21_11 2433	5394	CN1C(=O)N2C=NC(=C2N=N1)C(=O)N	no DILI-concern	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0674	5401	COC1=C(C=C2C(=C1)C(=NC(=N2)N3CCN(CC3)C(=O)C4CCCO4)N)OC	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N
Tox21_11 1591	5402	CC(C)(C)C#CC=CCN(C)CC1=CC=CC2=CC=CC=C21	Most DILI-concern	N	N	N	NA	N	N	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0290	5411	CCCCNC1=CC=C(C=C1)C(=O)OCCN(C)C	no DILI-concern	NA	N	N	N	N	N	NA	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0658	5472	C1CN(CC2=C1SC=C2)CC3=CC=CC=C3C1	Most DILI-concern	N	N	N	N	N	N	N	N	Y	N	NA	N	N	NA	N	N	N
Tox21_11 0792	5509	CC1=CC=C(C=C1)C(=O)C2=CC=C(N2C)CC(=O)O	Most DILI-concern	N	NA	NA	N	N	N	N	NA	N	N	N	N	N	N	N	N	N
Tox21_11 0500	5526	C1CC(CCC1CN)C(=O)O	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 1274	5572	C1CCCC(CC1)C(CC2CCCCC2)(C3=C C=CC=C3)O	no DILI-concern	N	N	N	N	N	N	N	N	N	NA	N	N	N	NA	N	N	N
Tox21_11 2119	5591	CC1=C(C(=C2CCC(OC2=C1C)(C)COC3=CC=C(C=C3)CC4C(=O)NC(=O)S4)C)O	Most DILI-concern	N	N	NA	Y	N	NA	NA	NA	Y	Y	NA	NA	NA	Y	Y	Y	NA
Tox21_11 2176	5717	CC1=CC=CC=C1S(=O)(=O)NC(=O)C2=CC(=C(C=C2)CC3=CN(C4=C3C=C(C=C4)NC(=O)OC5C CCC5)C)OC	Most DILI-concern	Y	N	NA	Y	N	N	N	NA	N	N	NA	NA	N	Y	NA	Y	NA
Tox21_11 1569	5734	C1=CC=C2C(=C1)C(=NO2)CS(=O)(=O)N	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1493	5746	CC1=C(C(=O)C2=C(C1=O)N3C[C@H]4[C@@H]([C@@]3([C@@H]2COC(=O)N)OC)N4)N	no DILI-concern	N	N	N	NA	N	Y	NA	Y	Y	Y	NA	NA	N	N	Y	NA	Y
Tox21_11 0883	5754	C[C@]12CCC(=O)C=C1CC[C@@H]3[C	no DILI-concern	N	Y	N	N	Y	Y	Y	NA	NA	Y	N	Y	N	N	N	N	N

		@H]2[C@@]1(CCC C2=CC=C3C[C@H] (CCC3=C)O)C																		
Tox21_30 2427	6230	C[C@]12CC[C@H] 3[C@H]([C@@H]1 CC[C@]2(C#C)O)C CC4=CC(=O)CC[C@ H]34	no DILI- concern	N	Y	Y	Y	Y	N	N	NA	Y	N	Y	Y	N	N	N	N	N
Tox21_11 1793	6237	CCC1=C(C2=CC=C C=C2O1)C(=O)C3= CC(=C(C(=C3))O)I	Most DILI- concern	N	N	N	NA	N	Y	NA	NA	Y	NA	NA	NA	Y	Y	Y	Y	NA
Tox21_11 1203	6253	C1=CN(C(=O)N=C1 N)[C@H]2[C@H]([C@@H]([C@H](O2)CO)O)O	Most DILI- concern	N	N	Y	N	N	N	N	NA	NA	N	NA	NA	N	N	Y	N	N
Tox21_11 0433	6726	CN1CCN(CC1)C(C 2=CC=CC=C2)C3= CC=CC=C3	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_20 1633	6759	CC1=CC2=C(C=C1 C)N(C3=NC(=O)NC (=O)C3=N2)C[C@H]([C@H]([C@H](C O)O)O)O	no DILI- concern	NA	N	NA	N	N	N	N	N	N	N	N	N	N	Y	N	N	N
Tox21_11 0028	6832	CN1[C@@H]2CC[C@H]1CC(C2)O C(C3=CC=CC=C3) C4=CC=CC=C4	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	NA	N	N	NA
Tox21_20 2176	6869	CC1([C@@H](N2[C@H](S1)[C@@H] (C2=O)NC(=O)COC 3=CC=CC=C3)C(= O)O)C	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	Y	N	N	N	N	N
Tox21_11 0398	7699	CCCCNC1=CC=C(C=C1)C(=O)OCCO CCOCCOCCOCCO CCOCCOCCOCCO C	no DILI- concern	N	N	N	NA	N	Y	N	N	N	NA	N	N	N	Y	N	N	N
Tox21_11 0809	8226	CC[C@@H](CO)N C(=O)[C@H]1CN([C@@H]2CC3=CNC 4=CC=CC(=C34)C2 =C1)C	no DILI- concern	NA	N	Y	N	N	N	N	Y	N	N	N	N	N	N	N	N	N
Tox21_40 0022	8593	C1=CC=C(C=C1)C2 =NC3=CC=CC=C3 C(=C2)C(=O)O	Most DILI- concern	N	NA	N	N	N	N	Y	N	N	N	N	N	N	N	N	Y	N
Tox21_11 1310	9294	C[C@@H]([C@@H]](C1=CC=CC=C1)O)NC	no DILI- concern	N	N	N	N	N	N	N	N	Y	N	N	N	N	N	N	N	N
Tox21_11 0895	9681	CC[C@@H](CO)N C(=O)[C@H]1CN([no DILI- concern	Y	N	NA	N	N	NA	N	NA	N	N	N	N	N	N	N	N	N

		C@[H]2CC3=CN(C4=CC=CC(=C34)C2=C1)C																		
Tox21_20 0122	9782	C[C@H]1C[C@H]2[C@H]3CCC4=C(C=O)C=C[C@@]4([C@]3([C@H](C[C@@]2([C@]1(C(=O)CO)C)O)F)C	no DILI-concern	NA	Y	N	N	Y	Y	Y	N	N	Y	N	Y	N	N	N	N	N
Tox21_20 0071	9902	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@]2(C)O)CC[C@H]4[C@@]3(CC(=CO)C(=O)C4)C	Most DILI-concern	N	Y	Y	Y	Y	NA	Y	N	Y	N	Y	N	Y	Y	NA	NA	NA
Tox21_11 3167	9904	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@H]2O)CC4=CC(=O)CC[C@H]34	Most DILI-concern	N	Y	NA	Y	Y	Y	N	Y	Y	N	Y	Y	N	N	N	N	N
Tox21_11 0821	10531	C[C@@]1(C(=O)N2[C@H](C(=O)N3CC[C@H]3[C@@]2(O)O)CC4=CC=CC=C4)NC(=O)[C@@H]5C[C@H]6[C@@H](CC7=CNC8=CC=CC6=C78)N(C5)C	no DILI-concern	N	N	Y	NA	N	N	N	N	NA	N	NA	N	N	NA	N	NA	N
Tox21_11 2856	10836	C[C@@H](CC1=CC=CC1)NC	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 1339_1	10917	C[N+](C)(C)C[C@@H](CC(=O)[O-])O	no DILI-concern	NA	NA	NA	N	NA	NA	NA	NA	NA	NA	NA	NA	N	NA	NA	NA	N
Tox21_11 2170	11033	C1=CC(=CC=C1N)S(=O)(=O)NC(=O)N	Most DILI-concern	N	Y	N	N	Y	N	NA	N	NA	N	N	NA	N	NA	N	N	N
Tox21_11 1318	11333	C([C@@H]1[C@@H]([C@@H]([C@@H](O)O)C[C@@H]2[C@H](O)[C@@]([C@H]2O)(CO)O)O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_20 1078	12035	CC(=O)N[C@@H](CS)C(=O)O	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1311	12560	CC[C@@H]1[C@@]([C@@H]([C@H](C=O)[C@@H](C[C@@]([C@@H]([C@H]([C@H](C(=O)O1)C)O[C@@H]2[C@@]([C@H]([C@@H](O2)	Most DILI-concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N

		C)O)(C)OC)O[C@H]3[C@@H]([C@H](C[C@H](O3)C)N(C)C)O)(C)C)O)(C)O																		
Tox21_30 3658	13109	CC[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@]2(C#C)O)CCC4=CC(=O)CC[C@H]34	no DILI-concern	N	Y	Y	Y	Y	N	NA	Y	Y	N	NA	Y	N	N	N	N	N
Tox21_11 1498	13342	CC[C@]1(C[C@H]2C[C@@](C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)[C@]78CCN9[C@H]7[C@@](C=CC9)([C@H]([C@@]([C@@H]8N6C)(C(=O)OC)O)OC(=O)C)CC)OC(=O)OC)O	no DILI-concern	N	NA	Y	Y	N	Y	NA	Y	Y	Y	Y	Y	NA	Y	Y	NA	Y
Tox21_11 2593	13505	CCOC(=O)C1(CCN(CC1)CCC(C#N)(C2=CC=CC=C2)C3=CC=CC=C3)C4=CC=CC=C4	no DILI-concern	N	Y	Y	Y	N	Y	N	Y	Y	N	NA	NA	N	Y	Y	NA	Y
Tox21_11 1491	14985	CC1=C(C(=C2CC[C@@](OC2=C1C)(C)CCC[C@H](C)CCC[C@H](C)CCCC(C)C)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1821	15250	CC(C)CC1=CC=C(C=C1)CC(=O)O	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	Y	N
Tox21_11 0592	15541	C[C@@H]1CC(=O)[C@]2([C@@H](O1)O[C@@H]3[C@H]([C@@H]([C@@H]([C@H]3O2)NC)O)NC)O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0080	16231	C1(=C(N=C(C(=N1)C)N)N)C(=O)N=C(N)N	Most DILI-concern	Y	N	NA	Y	N	N	N	N	N	N	Y	NA	N	N	NA	N	N
Tox21_11 2000	16960	CN(C)CC[C@H](C1=CC=C(C=C1)Br)C2=CC=CC=N2	no DILI-concern	N	N	N	N	N	NA	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 0886	18283	CC1=CN(C(=O)NC1=O)[C@H]2C=C[C@H](O2)CO	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1583	19649	C[C@H]1[C@@]([C@H]([C@@H](O1	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA

)O[C@@H]2[C@H]([C@@H]([C@H]([C@@H]([C@H]2O)N=C(N)N)O)N=C(N)N)O[C@H]3[C@H]([C@@H]([C@H]([C@H]([C@@H]([C@H](O3)C)O)O)NC)(C=O)O																		
Tox21_11 1639	19988	COC1=C(C=C(C=C1)O)C(=O)C2=CC=CC=C2S(=O)(=O)O	no DILI-concern	N	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0579	23897	CCC1=C(NC2=C1C(=O)C(CC2)CN3CCOCC3)C	no DILI-concern	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3491	24066	C1C[C@@H]([C@H]([C@@H]1CO)N2C=C(C=NC2=O)N	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_30 1002	24705	C[Si](C)(C)O[Si](C)(C)O[Si](C)(C)C	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N
Tox21_11 0572	26757	C[C@H](CC1=CC=CC=C1)N(C)CC#C	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0431	26934	C[C@H]([C@H](C1=CC=CC=C1)O)N	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0574	26987	C[C@@](C1=CC=C(C=C1)(C2=CC=C(C=C2)Cl)OCC[C@H]3CCCN3C	no DILI-concern	N	N	NA	NA	N	N	N	N	N	N	NA	N	N	Y	N	N	NA
Tox21_11 2033	27350	CC(=O)O[C@H]1C[C@@H]2CC[C@@H]3[C@H]([C@H]2(C[C@H]1[N+])4(CCCCC4)C)CC[C@H]5([C@H]3C[C@@H]([C@H]5OC(=O)C)[N+])6(CCCC6)C.[Br-].[Br-]	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 2114	28417	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@]2(C#C)O)C(C4=CC5=C(C[C@]34)C=NO5	Most DILI-concern	N	Y	Y	NA	Y	N	Y	Y	Y	NA	NA	Y	NA	N	N	N	NA
Tox21_11 1819	28858	C1=CC(=CC=C1C2=NC(=CS2)CC(=O)O)Cl	Most DILI-concern	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_30 2974	29327	CN(C(=O)N[C@@H]1[C@H]([C@@H]([C@H]([C@H]1O)CO)O)N=O	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N

Tox21_11 1025	30322	C[C@@H]1[C@H]([C@H](C[C@@H](O1)O[C@@H]2[C @H](O[C@H](C[C @@H]2O)O[C@@ H]3[C@H](O[C@H)(C[C@@H]3O)O[C @H]4CC[C@]5([C @@H](C4)CC[C@ @H]6[C@@H]5C[C @H]([C@]7([C@@]6(CCC7C8=CC(=O)OC8)O)C)O)C)C)O)O	no DILI- concern	N	Y	NA	NA	NA	Y	Y	NA	Y	Y	N	Y	N	Y	NA	NA	NA
Tox21_20 1159	30323	C[C@H]1[C@H]([C @H](C[C@@H](O1)O[C@H]2C[C@@] (CC3=C(C4=C(C(= C23)O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)C)O)N)O	no DILI- concern	NA	Y	NA	NA	N	Y	Y	Y	Y	NA	NA	Y	N	Y	Y	Y	Y
Tox21_11 3419	30751	C1=NC2=C(N1[C@ H]3[C@H]([C@@H])([C@H](O3)COP(= O)(O)O)O)N=C(N=C2N)F	no DILI- concern	N	N	N	Y	N	N	N	NA	N	N	NA	N	N	N	Y	N	N
Tox21_11 1726	30951	C=CCOC1=C(C=C(C=C1)CC(=O)O)Cl	Most DILI- concern	N	N	N	NA	Y	NA	N	NA	Y	N	N	N	NA	N	N	Y	NA
Tox21_11 2700	31378	C[C@]12CCC(=O)C =C1CC[C@@H]3[C @@]2([C@H](C[C @]4([C@H]3CC[C @]4(C(=O)CO)O) C)O)F	no DILI- concern	N	Y	N	NA	Y	Y	Y	NA	Y	Y	N	Y	NA	N	N	N	NA
Tox21_11 3570	33036	CN(C)CC[C@@H](C1=CC=C(C=C1)Cl)C2=CC=CC=N2	no DILI- concern	N	N	N	N	NA	N	NA	N	N	N	NA	N	N	N	N	NA	N
Tox21_11 3309	33176	CC1=C(C2=C(N1C C(=O)O)C=C(C=C2)OC)C(=O)C3=CC= C(C=C3)Cl	Most DILI- concern	Y	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0910	34359	C[C@](C1=CC(=C (C=C1)O)O)(C(=O) O)NN	Most DILI- concern	NA	N	N	NA	N	N	N	N	NA	N	N	N	NA	N	N	N	NA
Tox21_11 3313	34869	C1CC2=CC=CC=C2 C(C3=CC=CC=C31 [NH2+])CCCCCCC(=O)O.[Cl-]	Most DILI- concern	Y	N	N	N	N	N	Y	N	N	N	N	N	N	N	N	N	N
Tox21_11 0062	35370	CC1=CN(C(=O)NC 1=O)[C@H]2C[C@	Most DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N

		@H]([C@H](O2)C O)N=[N+]=[N-]																		
Tox21_11 0126	36811	CC(CCC1=CC=C(C =C1)O)NCCC2=CC (=C(C=C2)O)O	no DILI- concern	NA	N	NA	N	N	N	NA	NA	N	N	N	N	N	NA	N	N	N
Tox21_11 0641	37464	CC(C)(C)NC[C@@ H](COC1=CC=CC= C1C2CCCC2)O	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	Y	N	NA	NA
Tox21_11 1201	37768	C1[C@@H]([C@H] ([C@@H]([C@H]([C@@H]1NC(=O)[C @H](CCN)O)O[C@ @H]2[C@@H]([C @H]([C@@H]([C@ H](O2)CO)O)N)O O)O[C@@H]3[C@ @H]([C@H]([C@@ H]([C@H](O3)CN) O)O)O)N	no DILI- concern	N	N	N	N	N	N	N	N	Y	N	N	N	N	N	N	N	N
Tox21_11 1681	38409	C1=CSC(=C1)C(=O)C2=C(C(=C(C=C2) OCC(=O)O)C)C1	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 0917	38853	C[C@](CC1=CC(=C (C=C1)O)O)(C(=O) O)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0898	39186	CC(=O)O[C@@H]1 [C@@H](SC2=CC= CC=C2N(C1=O)CC N(C)C)C3=CC=C(C =C3)OC	Most DILI- concern	N	N	N	N	N	N	N	NA	N	NA	NA	NA	N	N	NA	N	N
Tox21_20 1450	40399	C1=CC(=C(C(=C1C (=O)C2=CC(=C(C(= C2)O)O)O)O)O	Most DILI- concern	Y	N	Y	NA	N	N	N	N	N	N	NA	N	N	Y	Y	NA	NA
Tox21_11 2061	41867	C[C@H]1[C@@H]([C@H](C[C@@H]([O1)O[C@H]2[C@ @](CC3=C(C4=C(C =C23)O)C(=O)C5= C(C4=O)C=CC=C5 OC)O)(C(=O)CO)O N)O	Most DILI- concern	N	NA	NA	Y	N	NA	NA	NA	NA	N	N	NA	N	NA	NA	NA	Y
Tox21_11 0790	47319	C[N+]1(CCC2=CC(=C(C=C2C1CC3=C C(=C(C=C3)OC)OC)OC)OC)CCC(=O)O CCCCOC(=O)CC[N+]4(CCC5=CC(=C (C=C5C4CC6=CC(= C(C=C6)OC)OC)O C)OC)C	no DILI- concern	N	N	N	NA	Y	Y	Y	NA	NA	Y	N	Y	NA	N	N	NA	NA

Tox21_11 0676	47576	CC(=O)N1CCN(CC 1)C2=CC=C(C=C2) OC[C@@H]3CO[C @@](O3)(CN4C=C N=C4)C5=C(C=C(C =C5)C)C1	Most DILI- concern	Y	N	N	Y	N	N	N	N	Y	Y	NA	N	Y	NA	N	N	NA
Tox21_11 1732	50599	C1C[C@@H](O)[C @@H]1CO)N2C=N C3=C2NC=NC3=O	Most DILI- concern	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N	N	N
Tox21_11 3316	53359	CN(CC(=O)O)C(=S) C1=CC=CC2=C1C= CC(=C2C(F)(F)F)O C	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N
Tox21_11 0760	54575	C1C(N(C2=C(N1)N C(=NC2=O)N)C=O) CNC3=CC=C(C=C3)C(=O)N[C@H](CC C(=O)O)C(=O)O	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 0292	54841	CC1=CC=CC=C1O[C@H](CCNC)C2=C C=CC=C2	Most DILI- concern	N	N	N	NA	N	NA	N	N	N	N	NA	N	N	N	N	NA	N
Tox21_11 3593	54897	CCCN(CCC)C(=O) CC1=C(N=C2N1C= C(C=C2)C1)C3=CC =C(C=C3)C1	Most DILI- concern	NA	N	N	NA	N	N	N	NA	N	N	Y	N	N	Y	N	N	Y
Tox21_11 0854	55283	CCC(C)N1C(=O)N(C=N1)C2=CC=C(C =C2)N3CCN(CC3)C 4=CC=C(C=C4)OC[C@H]5CO[C@](O5)CN6C=NC=N6)C7 =C(C=C(C=C7)C)C 1	Most DILI- concern	NA	N	N	Y	N	N	N	NA	Y	Y	NA	NA	N	N	N	N	N
Tox21_11 2488	56069	C[C@](CS(=O)(=O) C1=CC=C(C=C1)F) (C(=O)NC2=CC(=C (C=C2)C#N)C(F)(F) F)O	Most DILI- concern	N	N	Y	Y	N	Y	N	NA	N	Y	NA	N	N	Y	N	NA	N
Tox21_11 0717	57363	C[C@]12CC[C@H] 3[C@H]([C@@H]1 CC[C@@H]2C(=O) NC(C)(C)C)CC[C@ @H]4[C@@]3(C=C C(=O)N4)C	no DILI- concern	N	N	NA	Y	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3496	59768	CC(C)NCC(COC1= CC=C(C=C1)CCC(= O)OC)O	no DILI- concern	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N	N
Tox21_11 1882	60172	C1=NC2=C(C(=N1) N)N=CN2CCOCP(= O)(O)O	Most DILI- concern	NA	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA

Tox21_11 1499	60198	C[C@]12CC[C@H] 3[C@H]([C@@H]1 CCC=O)CC(=C)C4 =CC(=O)C=C[C@]3 4C	Most DILI- concern	N	Y	Y	Y	Y	NA	Y	Y	Y	Y	NA	NA	N	N	N	N	N
Tox21_11 1680	60490	CC(C1=CC2=CC=C C=C2S1)N(C(=O)N) O	Most DILI- concern	NA	N	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N
Tox21_11 1478	60700	CC[C@]1(C2=C(COC1=O)C(=O)N3 CC4=C(C3=C2)N= C5C=CC(=C(C5=C4)CN(C)C)O)O	no DILI- concern	N	NA	Y	Y	N	Y	Y	Y	Y	Y	Y	NA	NA	N	Y	NA	NA
Tox21_11 3128	60714	CC(CN1CCN(CCN(CCN(CC1)CC(=O)[O-])CC(=O)[O-)])CC(=O)[O-)O.[Gd+3]	no DILI- concern	N	N	N	NA	N	N	N	N	Y	N	N	N	NA	N	N	N	NA
Tox21_11 2181	60726	C1=CC(=C(C(=C1) CC(=O)O)N)C(=O) C2=CC=C(C=C2)Br	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	Y	NA
Tox21_11 3006	60753	CCCCCCN(CC)C CCC(C1=CC=C(C= C1)NS(=O)(=O)C)O	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	NA	NA	N	NA
Tox21_11 1737	60774	CC1=CC(=C(C=C1) O)[C@@H](CCN(C (C)C(C)C)C2=CC =CC=C2	no DILI- concern	N	NA	N	N	N	N	N	N	N	N	NA	N	N	Y	N	N	N
Tox21_11 1685	60823	CC(C)C1=C(C(=C(N1CC[C@H])(C[C@ H](CC(=O)O)O)O)C 2=CC=C(C=C2)F)C 3=CC=CC=C3)C(= O)NC4=CC=CC=C4	Most DILI- concern	N	N	Y	NA	N	N	Y	N	NA	N	N	Y	N	NA	N	N	NA
Tox21_11 1585	60825	C1[C@H](O)[C@H](S1)CO)N2C=CC(=N C2=O)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2188	60835	CNCC[C@]1(C1 =CC=CS1)OC2=CC =CC3=CC=CC=C32	Most DILI- concern	NA	N	NA	NA	N	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
Tox21_11 2193	60877	C1[C@H](O)[C@H](S1)CO)N2C=C(C(= NC2=O)N)F	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 2198	60953	CCCCOC(=O)NC 1=NC(=O)N(C=C1F)C@H]2[C@@H]([C@@H])([C@H](O2)C)O)O	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0980	62959	C1[C@@]2[C@@ H](C2N)CN1C3=C(Most DILI- concern	N	Y	Y	Y	N	Y	Y	NA	NA	Y	NA	N	N	Y	Y	Y	Y

		C=C4C(=O)C(=CN(C4=N3)C5=C(C=C(C=C5)F)F)C(=O)O)F																		
Tox21_11 1582	64139	C1CC1C#C[C@]2(C3=C(C=CC(=C3)C1)NC(=O)O2)C(F)(F)F	Most DILI-concern	N	N	NA	Y	N	Y	NA	NA	Y	Y	NA	NA	Y	Y	NA	N	NA
Tox21_11 2640	64147	CC(C)[C@@H](C(=O)OCC(CO)OCN1C=NC2=C1NC(=NC2=O)N)N	no DILI-concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	N	N	N	NA
Tox21_11 2962	65027	CCC[C@]1(CC(=O)C(=C(O1)O)[C@H](CC)C2=CC(=CC=C2)NS(=O)(=O)C3=NC=C(C=C3)C(F)(F)F)CCC4=CC=CC=C4	Most DILI-concern	N	N	N	NA	N	N	N	NA	N	N	Y	Y	NA	Y	N	NA	NA
Tox21_11 2189	65140	C1CC1NC2=NC(=NC3=C2N=CN3C4C[C@H](C=C4)CO)N	Most DILI-concern	Y	N	N	NA	N	Y	Y	N	Y	Y	N	N	NA	N	N	N	NA
Tox21_11 0668	65492	C[C@@H](C(=O)NC1=C(C(=C(C=C1)C(=O)NC(CO)CO)I)C(=O)NC(CO)CO)I)O	no DILI-concern	N	N	N	N	Y	Y	Y	N	N	NA	N	NA	N	N	N	N	N
Tox21_11 2178	71329	CN(CCC1=CC=C(C=C1)NS(=O)(=O)C)COC2=CC=C(C=C2)NS(=O)(=O)C	no DILI-concern	N	N	N	N	Y	Y	Y	NA	N	N	N	Y	N	NA	N	N	N
Tox21_11 3319	71467	CC(COC1=CC=CC=C1)NN	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 3308	71900	CC1=NC(=CN1C2=CC=C(C=C2)[N+](=O)[O-])[N+](=O)[O-]	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1434	77999	CN(CCOC1=CC=C(C=C1)CC2C(=O)NC(=O)S2)C3=CC=C(C=N3)	Most DILI-concern	N	NA	NA	NA	N	N	N	N	N	N	Y	Y	N	Y	N	Y	N
Tox21_11 2666	82146	CC1=CC2=C(C=C1)C(=C)C3=CC=C(C=C3)C(=O)O)C(CCC2(C)C)C)C	Most DILI-concern	N	N	Y	NA	N	N	N	Y	NA	Y	NA	NA	Y	Y	NA	Y	NA
Tox21_11 1643	82170	C([C@H])([C@@H])([C@H])([C@H](CO)O)O)O	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2630	93860	B([C@@H](CC(C)C)NC(=O)[C@@H]	Most DILI-concern	N	N	Y	Y	N	Y	Y	Y	Y	Y	NA	Y	Y	N	Y	NA	NA

		(CC1=CC=CC=C1)NC(=O)C2=NC=CN=C2(O)O																		
Tox21_11 2444	104865	CC(C)(C)C1=CC=C(C=C1)S(=O)(=O)N C2=C(C(=NC(=N2)C3=NC=CC=N3)OC CO)OC4=CC=CC=C4OC	Most DILI-concern	N	NA	NA	NA	N	N	N	N	N	N	N	N	N	N	N	NA	N
Tox21_11 3609	115237	CC1=C(C(=O)N2C CCC(C2=N1)O)CC N3CCC(CC3)C4=N OC5=C4C=CC(=C5)F	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0944	126941	CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)N[C@@H](CCC(=O)O)C(=O)O	Most DILI-concern	N	N	N	NA	N	N	N	NA	N	NA	NA	N	N	N	Y	NA	NA
Tox21_11 2446	129211	CCOC1=CC=CC=C1OCCN[C@H](C)C C2=CC(=C(C=C2)O)C)S(=O)(=O)N	no DILI-concern	N	Y	N	NA	Y	N	N	N	N	N	Y	N	Y	N	N	N	N
Tox21_11 2781	148124	CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@]4[C@]([C@@H]3[C@@]4)[C@@]([C@@]([C@@]([C@@]1OC(=O)[C@@]([C@H](C5=CC=CC=C5)NC(=O)OC(C)(C)O)O)C(=O)C6=CC=CC=C6)(CO4)OC(=O)C)O)C)O	Most DILI-concern	N	NA	Y	N	N	N	N	N	NA	Y	Y	N	Y	Y	NA	NA	
Tox21_11 0703	149096	C[C@H]1COC2=C3N1C=C(C(=O)C3=C(C(=C2N4CCN(CC4)C)F)C(=O)O	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0482	149351	CCCC[C@@H](C=C[C@H]1[C@@H](CC(=O)[C@@H]1CCCCCCC(=O)O)O	no DILI-concern	N	NA	NA	NA	N	Y	N	Y	N	NA	N	NA	NA	N	N	NA	NA
Tox21_11 3566	151166	CC1=CC(=C(C=C1)NC2=C(C=CC=C2C1)F)CC(=O)O	Most DILI-concern	NA	N	NA	NA	N	N	N	N	N	N	N	N	NA	N	Y	Y	
Tox21_11 3616	152946	COC1=C2C(=CC(=C1N3C[C@@H]4CCN[C@@H]4C3)F	Most DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N

)C(=O)C(=CN2C5C C5)C(=O)O																		
Tox21_11 2192	153941	C=C1[C@H](C[C@ @H]([C@H]1CO)O)N2C=NC3=C2NC(=NC3=O)N	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 1560	159269	CC1=CN(C(=O)NC 1=O)[C@@H]2C[C @H]([C@@H](O2) CO)O	Most DILI- concern	NA	N	N	NA	NA	N	N	N	N	N	N	NA	NA	N	N	N	NA
Tox21_11 2349	165580	C1[C@H]([C@@H] ([C@H]([C@@H]([C@H]1N)O)[C@@H]2[C@@H]([C@H] [C@@H]([C@H](O 2)CO)O)N)O)[C@ H]3[C@@H]([C@ @H]([C@H](O3)C O)O)[C@@H]4[C@ @H]([C@H]([C@@ H]([C@@H](O4)C N)O)O)N)O)N	no DILI- concern	N	N	N	NA	N	N	N	N	Y	N	N	N	NA	N	N	N	NA
Tox21_11 3050	171548	C1[C@H]2[C@@H] ([C@@H](S1)CCC CC(=O)O)NC(=O)N 2	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	NA
Tox21_11 0816	174174	CN1[C@@H]2CC[C@H]1CC(C2)OC(=O)C(CO)C3=CC= CC=C3	no DILI- concern	N	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1967	197712	CC1=CC(=NC(=N1) OC(C(=O)O)C(C2= CC=CC=C2)(C3=C C=CC=C3)OC)C	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2505	208908	CS(=O)(=O)CCNCC 1=CC=C(O1)C2=C C3=C(C=C2)N=CN =C3NC4=CC(=C(C =C4)OCC5=CC(=C C=C5)F)Cl	Most DILI- concern	N	NA	N	Y	N	N	N	N	NA	N	N	N	Y	N	N	NA	NA
Tox21_11 2634	213039	CC(C)CN(C[C@H] [C@H](CC1=CC=C C=C1)NC(=O)O[C @H]2CO[C@@H]3 [C@H]2CCO3)O)S(=O)(=O)C4=CC=C(C=C4)N	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	NA	N	N	N	N	NA
Tox21_11 3431	392622	CC(C)C1=NC(=CS1)CN(C)C(=O)N[C@ @H](C(C)C)C(=O)	Most DILI- concern	N	N	N	NA	N	N	NA	NA	NA	N	NA	NA	N	N	N	NA	Y

		N[C@@H](CC=C C=CC=C2)C[C@@ H]([C@H](CC3=CC =CC=C3)NC(=O)O CC4=CN=CS4)O																			
Tox21_11 1640	439260	C1=CC(=C(C=C1)[C @H](CN)O)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	
Tox21_11 2339	439302	CC[C@H](C)[C@H]]C(=O)N[C@H](C(=O)N[C@H](C(=O) N[C@@H](CSSC[C @H](C(=O)N[C@ H](C(=O)N1)CC2= CC=C(C=C2)O)N)C (=O)N3CCC[C@H] 3C(=O)N[C@@H](CC(C)C(=O)NCC (=O)N)CC(=O)N)C CC(=O)N	no DILI- concern	N	N	N	NA	N	N	N	N	Y	N	NA	N	NA	N	N	N	NA	
Tox21_11 0505	441141	C[C@H]1[C@H]([C @@H](C[C@@H](O 1)O)[C@@H]2[C@ H]([C@@H]([C@H][O][C@H]2OC3=C4 C=C5C=C3OC6=C(C=C(C=C6)[C@H](C(C(=O)N[C@H](C (=O)N[C@H]5C(=O)N[C@@H]7C8=CC (=C(C=C8)O)C9=C(C=C(C=C9)[C@@H] (NC(=O)[C@H]([C @@H](C1=CC(=C(O4)C=C1)C)O)NC7 =O)C(=O)O)O)C C(=O)N)NC(=O)[C @@H](CC(C)C)NC)O)C)O)O)(C) N)O	no DILI- concern	N	N	N	NA	NA	NA	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 1597	441184	C[C@@H]1[C@H]([C@@H]([C@H]([C @H](O1)O)[C@@H] 2[C@H](O[C@@H] ([C@@H]([C@H]2 O)O)O)[C@@H]3[C @H](O[C@H]([C@ @H]([C@H]3O)O) O)CO)CO)O)N[C @H]4C=C([C@@H]][C@@H]([C@H]4	Most DILI- concern	N	N	N	N	N	N	N	N	Y	N	N	N	N	N	N	N	N	

		O)O)O)CO																		
Tox21_11 2876	441278	C[C@H]1[C@H]2C C3=C([C@@]1(CC N2CC=C(C)C)C)= C(C=C3)O	no DILI- concern	N	N	N	N	N	N	N	N	NA	N	Y	N	N	N	N	N	N
Tox21_20 0323	441281	CN1C(=C2C(=NC(=N2)C1)N(C1=O)C)[O-].C[NH+](C)CCOC(C1=CC=CC=C1)C2 =CC=CC=C2	no DILI- concern	N	N	NA	N	N	N	N	N	N	N	NA	N	N	NA	N	N	NA
Tox21_11 2437	441290	CC(=O)O[C@H]1[C @H](C[C@H]2[C @@]1(CC[C@H]3[C@H]2CC[C@H] 4[C@@]3(C[C@@ H)([C@H](C4)O)N5 CCOCC5)C)C][N+] 6(CCCC6)CC=C	no DILI- concern	N	Y	N	NA	Y	N	NA	N	Y	N	N	NA	NA	N	N	N	NA
Tox21_11 1253	441350	C[C@](CC1=CC=C(C=C1)O)(C(=O)O)N	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0818	445354	CC1=C(C(CCC1)(C)C=C/C(=C/C=C/ C(=C/CO)/C)/C	no DILI- concern	N	N	N	Y	N	NA	Y	N	NA	NA	Y	NA	Y	NA	N	N	Y
Tox21_11 2532	464205	C[C@H](CN1C=NC 2=C1N=CN=C2N)O CP(=O)(O)O	Most DILI- concern	NA	N	N	NA	N	N	N	N	N	N	NA	N	NA	N	N	N	NA
Tox21_11 0882	657298	CCCC1=CC(=O)NC (=S)N1	Most DILI- concern	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N	N	N
Tox21_11 1158	667490	C1=NC2=C(N1)C(= S)N=CN2	Most DILI- concern	Y	N	NA	Y	N	Y	Y	NA	N	Y	N	NA	N	N	Y	NA	NA
Tox21_11 3347	708857	CN1CCCN=C1/C=C/ /C2=CC=CS2	no DILI- concern	N	N	N	Y	N	N	N	N	Y	N	N	N	N	N	N	N	N
Tox21_11 0278	941651	CN1CCN(CC1)CC/ C=C\2/C3=CC=CC= C3SC4=C2C=C(C=C C4)S(=O)(=O)N(C) C	Most DILI- concern	N	N	NA	NA	N	NA	NA	N	N	N	NA	N	NA	NA	NA	NA	NA
Tox21_11 0341	134990 7	CN1C=CNC1=S	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N
Tox21_11 0938	273352 6	CC/C(=C(\C1=CC= CC=C1)/C2=CC=C(C=C2)OCCN(C)C)/ C3=CC=CC=C3	Most DILI- concern	N	N	N	NA	N	N	Y	Y	Y	Y	NA	NA	NA	NA	NA	N	NA
Tox21_30 0211	300132 2	CCCCN1C(=O)[C@ H](NC(=O)C12CCN (CC2)CC3=CC=C(C =C3)OC4=CC=C(C =C4)C(=O)O)[C@	Most DILI- concern	N	NA	Y	Y	N	NA	N	N	NA	NA	NA	NA	N	Y	Y	NA	NA

		@H](C5CCCC5)O																		
Tox21_11 3369	300297 7	CC1=NN=C(N1C2C [C@H]3CC[C@@H (C2)N3CC[C@@H (C4=CC=CC=C4)N C(=O)C5CCC(CC5) (F)C(C)C	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 2714	301115 5	COC1=NC(=NC2=C 1N=CN2[C@H]3[C @H]([C@@H]([C@ H](O3)CO)O)O)N	no DILI- concern	NA	N	N	N	N	N	NA	N	N	N	NA	N	N	NA	N	N	N
Tox21_11 1437	303401 0	CCCCCCCCC[C @@H](C[C@H]1[C @@H](C(=O)O1)C CCCC)OC(=O)[C @H](CC(C)C)NC= O	Most DILI- concern	N	N	N	N	N	NA	N	NA	N	N	NA	Y	N	NA	N	N	NA
Tox21_11 0950	308354 4	C[C@H](CC1=CC= C(C=C1)OC)NC[C @@H](C2=CC(=C(C=C2)O)NC=O)O	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	NA	N	N	N	NA
Tox21_11 2963	465956 9	CC1=CC=C(C=C1) C(=O)C2=CC(=C(C =C2)O)O)[N+](=O) [O-]	Most DILI- concern	NA	NA	N	NA	N	N	N	NA	NA	NA	NA	Y	N	Y	N	NA	NA
Tox21_11 1196	528036 0	CCCC[C@@H](/C =C/[C@H]1[C@@H (CC(=O)[C@@H]1 C/C=C\CCCC(=O)O)O)O	no DILI- concern	N	NA	Y	N	N	Y	N	NA	Y	NA	NA	Y	N	N	N	N	N
Tox21_11 2404	528079 3	C[C@H](/C=C/[C@ H](C)C(C)C)[C@H] 1CC[C@@H]2[C@ @]1(CCC/C2=C\C=C C/3[C@H](CCC3 =C)O)C	no DILI- concern	N	N	N	Y	N	NA	N	NA	NA	N	NA	Y	Y	N	NA	NA	NA
Tox21_11 2184	528108 1	CCN(CC)C(=O)/C(= C/C1=CC(=C(C(=C 1)O)O)[N+](=O)[O-)]/C#N	no DILI- concern	N	NA	N	Y	N	N	N	N	N	N	NA	N	Y	NA	Y	N	N
Tox21_11 0919	528244 3	CC1=CC=C(C=C1)/ C(=CN2CCCC2)/ C3=CC=CC=N3	no DILI- concern	N	N	N	N	N	N	N	N	N	N	NA	N	N	N	N	N	N
Tox21_11 2884	528437 1	CN1CC[C@]23[C@ @H]4[C@H]1CC5= C2C(=C(C=C5)OC) O[C@H]3[C@H](C =C4)O	no DILI- concern	N	N	N	Y	NA	N	N	N	N	N	N	N	NA	N	N	N	NA

Tox21_11 1566	528456 9	CN1CC[C@]23[C@ @H]4[C@H]1CC5= C2C(=C(C=C5)OC) O[C@H]3C(=O)CC 4	no DILI- concern	N	N	N	NA	N	N	N	N	N	NA	N	N	NA	N	N	N	NA
Tox21_11 2861	528882 6	CN1CC[C@]23[C@ @H]4[C@H]1CC5= C2C(=C(C=C5)O)O [C@H]3[C@H](C= C4)O	no DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2249	532910 2	CCN(CC)CCNC(=O))C1=C(NC(=C1C)/C =C\2/C3=C(C=CC(= C3)F)NC2=O)C	Most DILI- concern	NA	NA	N	NA	N	Y	NA	Y	N	N	NA	NA	N	Y	NA	NA	NA
Tox21_11 1171	535116 6	CN(C)N/N=C\1/C(= NC=N1)C(=O)N	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_20 1924	535383 0	C1C(=O)NC(=O)N1 /N=C\VC2=CC=C(O2)[N+](=O)[O-]	Most DILI- concern	N	NA	NA	Y	N	Y	NA	Y	NA	N	N	N	N	Y	N	Y	N
Tox21_11 1037	535398 0	C1=CC=NC(=C1)N S(=O)(=O)C2=CC= C(C=C2)N/N=C/3VC =CC(=O)C(=C3)C(= O)O	Most DILI- concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 2007	536051 5	C1CC1CN2CC[C@]]34[C@ @H]5C(=O) CC[C@]3([C@H]2 CC6=C4C(=C(C=C6)O)O5)O	Most DILI- concern	N	N	N	NA	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 0766	536069 6	CN1CC[C@ @]23C CCC[C@ @H]2[C@ @H]1CC4=C3C=C(C=C4)OC	no DILI- concern	N	N	N	NA	N	N	N	N	N	N	NA	N	NA	N	N	N	NA
Tox21_11 1441	536212 4	CCOC(=O)[C@H](CCC1=CC=CC=C1) N[C@H]2CCC3=C C=CC=C3N(C2=O) CC(=O)O	Most DILI- concern	N	Y	NA	NA	N	Y	NA	N	Y	N	NA	NA	Y	Y	Y	NA	N
Tox21_30 2415	536244 0	CC(C)(C)NC(=O)[C @H]1CN(CCN1C [C@H](C[C@ @H](CC2=CC=CC=C2)C (=O)N[C@ @H]3[C @ @H](CC4=CC=C C=C34)O)O)CC5=C N=CC=C5	Most DILI- concern	N	N	N	N	N	N	NA	NA	N	N	N	NA	N	N	N	N	N
Tox21_11 1329	538122 6	C[C@H]1/C=C/C=C (\C(=O)NC2=C(C3 =C(C(=C4C(=C3C(=O))/C2=C/NN5CC	Most DILI- concern	N	N	Y	N	N	N	N	N	N	N	N	Y	N	Y	N	N	N

		N(CC5)C)C(=O)[C@](O4)(O/C=C/[C@@H]([C@H]([C@H]([C@H]([C@H]([C@H]([C@H]1O)C)O)C)OC(=O)C)C)OC)C)O)/C																			
Tox21_11 2203	546251 6	CC[C@H]1[C@@]2([C@@H]([C@H](C(=O)[C@@H](C[C@]([C@@H]([C@H](C(=O)[C@H](C(=O)O1)C)C)O[C@H]3[C@@H]([C@H](C[C@H](O3C)N(C)C)O)(C)OC)C)N(C(=O)O2)CCC CN4C=C(N=C4)C5=CN=CC=C5)C	Most DILI-concern	NA	N	Y	NA	N	NA	NA	N	Y	NA	NA	NA	NA	N	N	N	NA	
Tox21_11 1475	548697 1	CC(C)C[C@@H](C(=O)O)CN	no DILI-concern	N	N	N	NA	N	N	N	N	Y	N	N	N	NA	N	N	N	NA	
Tox21_11 2926	549338 1	C1=C/C(=C/2\N/C=C3/C=CC=CC3=O)/N(N2)C4=CC=C(C=C4)C(=O)O)/C(=O)C=C1	Most DILI-concern	N	N	Y	NA	N	N	NA	Y	NA	NA	NA	Y	N	NA	N	NA	NA	
Tox21_11 3592	549344 4	CC(C)[C@@H](CC1=CC(=C(C=C1)OC)OCCOC)C[C@@H]([C@H](C[C@@H](C(C)C)C(=O)NC(C)(C)C(=O)N)O)N	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tox21_11 1086	643332 8	CCCCCCC/C=C/C CCCCCC(=O)O.C(CO)N	no DILI-concern	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	Y
Tox21_11 2012	643784 1	CC1=CC(=C(C=C1)/C=C/C(=C/C=C/C(=C\C(=O)O)/C)/C)C)C)OC	Most DILI-concern	NA	N	NA	NA	N	NA	Y	Y	NA	Y	NA	NA	NA	N	Y	NA	NA	
Tox21_11 3621	691845 6	CC(=O)OC1=CC2=C(S1)CCN(C2)C(C3=CC=CC=C3F)C(=O)C4CC4	no DILI-concern	N	N	N	N	N	N	N	N	N	N	Y	N	N	N	N	N	N	
Tox21_11 1996	691850 8	CN1CCCC(C1)NC2=NC=C3C(=N2)C(=NC=N3)NC4=CC(=C(C=C4)F)C1	Most DILI-concern	Y	Y	NA	Y	N	N	NA	NA	N	N	NA	Y	Y	Y	Y	Y	Y	

Tox21_11 0325	955207 9	C1=CC(=CC=C1N/C(=N/C(=NCCCCCN=C(N=C(NC2=CC=C(C=C2)Cl)N)N)N)/N)Cl	no DILI-concern	N	NA	Y	Y	NA	N	NA	Y	Y	NA	NA	NA	N	NA	NA	N	N
Tox21_11 3633	957410 1	CCOC(=O)CN[C@H](C1CCCC1)C(=O)N2CC[C@H]2C(=O)NCC3=CC=C(C=C3)/C(=N/O)N	Most DILI-concern	N	N	N	NA	N	N	N	NA	N	N	N	N	NA	N	N	N	NA
Tox21_11 2629	988705 4	C1CC[C@H]([C@@H](C1)N)N.C(=O)(C(=O)[O-])[O-].[Pt+2]	Most DILI-concern	N	N	N	N	N	N	N	N	N	NA	NA	N	N	N	NA	N	N
Tox21_11 3965	991592 6	CC1=C(C=C(C=C1)N2C(=O)C(=C(N2)C)N/N=C/3\C=CC=C(C3=O)C4=CC(=CC=C4)C(=O)O)C.C(CO)N.C(CO)N	Most DILI-concern	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	Y	NA	NA	NA	NA
Tox21_11 3174	101139 78	CC1=C(C=C(C=C1)NC2=NC=CC(=N2)N(C)C3=CC4=NN(C=C4C=C3)C)C)S(=O)(=O)N	Most DILI-concern	Y	N	Y	NA	N	NA	NA	Y	Y	NA	Y	NA	N	NA	Y	NA	Y
Tox21_11 2087	236738 37	CCCCC(CC)COC(=O)CC(C(=O)OCC(C)CCCC)S(=O)(=O)[O-].[Na+]	no DILI-concern	N	Y	N	Y	N	N	N	Y	NA	N	NA	N	NA	N	NA	N	Y
Tox21_11 2104	546785 01	C([C@@H](C1C(=C(C(=O)O1)O)O)O)O	no DILI-concern	N	N	NA	N	N	N	N	N	NA	N	N	N	N	N	N	N	N

Table 2. Frequency of assays used in 1000 MAQs-DILI models

MOA ID	Assay Name	Active Drugs	Inactive Drugs	Frequency in
				MAQs-DILI models
MOA-11	GH3-tre-antagonist	20	202	382
MOA-16	PPARG-bla-agonist	21	260	343
MOA-4	ARE-bla	53	180	313
MOA-10	ER-luc-bg1-4e2-antagonist	38	256	311
MOA-8	ER-bla-antagonist	30	239	266
MOA-6	AR-mda-kb2-luc-antagonist	36	250	232
MOA-3	AR-bla-antagonist	33	247	203
MOA-1	AHR	23	271	199
MOA-7	aromatase	34	248	198
MOA-13	HSE-bla	20	246	169
MOA-17	PPARG-bla-antagonist	22	213	161
MOA-12	GR-hela-bla-antagonist	36	238	151
MOA-15	p53	31	267	146
MOA-5	AR-mda-kb2-luc-agonist	20	298	134
MOA-9	ER-luc-bg1-4e2-agonist	65	224	117
MOA-14	mitotox	57	224	116
MOA-2	AR-bla-agonist	24	276	115

Table S3. Detailed DILI prediction of the top 4 assay specific QSAR-MOA models

Tox21_ID	PubChem_ID	Drug name	DILI_label	tox21-GH3-tre-antagonist	tox21-PPARG-bla-agonist	tox21-ARE-bla	tox21-ER-luc-bg1-4e2-antagonist
Tox21_111569	5734	zonisamide	Most DILI-concern	0.982	0.952	0.994	0.970
Tox21_110363	5340	sulfathiazole	Most DILI-concern	0.961	0.928	0.980	0.980
Tox21_110480	5329	sulfamethoxazole	Most DILI-concern	0.925	0.950	0.931	0.969
Tox21_110252	5070	riluzole	Most DILI-concern	0.733	0.976	0.879	0.958
Tox21_111732	50599	didanosine	Most DILI-concern	0.988	0.956	0.925	0.931
Tox21_112465	2313	bendazac	Most DILI-concern	0.963	0.804	0.840	0.945
Tox21_110062	35370	zidovudine	Most DILI-concern	0.933	0.927	0.866	0.903
Tox21_111585	60825	lamivudine	Most DILI-concern	0.921	0.921	0.805	0.982
Tox21_400022	8593	cinchophen	Most DILI-concern	0.918	0.899	0.918	0.848
Tox21_110886	18283	stavudine	Most DILI-concern	0.981	0.894	0.826	0.938
Tox21_111819	28858	fenclozic acid	Most DILI-concern	0.903	0.641	0.931	0.966
Tox21_110207	4495	nimesulide	Most DILI-concern	0.898	0.705	0.705	0.940
Tox21_301589	4493	nilutamide	Most DILI-concern	0.833	0.649	0.988	0.953
Tox21_113566	151166	lumiracoxib	Most DILI-concern	0.994	0.939	NA	0.976
Tox21_110182	3899	leflunomide	Most DILI-concern	NA	0.988	0.916	0.964
Tox21_113491	24066	zalcitabine	Most DILI-concern	0.914	0.834	0.827	0.807
Tox21_112181	60726	bromfenac	Most DILI-concern	0.780	0.973	0.399	0.839

Tox21_110 078	1986	acetazolamide	Most DILI- concern	0.495	0.805	0.670	0.865
Tox21_201 924	5353830	nitrofurantoin	Most DILI- concern	0.970	0.629	0.743	0.976
Tox21_110 154	3397	flutamide	Most DILI- concern	0.805	0.831	0.901	0.988
Tox21_113 308	71900	nitrefazole	Most DILI- concern	0.442	0.818	0.509	0.733
Tox21_110 598	3059	diflunisal	Most DILI- concern	0.986	NA	NA	0.980
Tox21_110 594	3825	ketoprofen	Most DILI- concern	0.761	0.033	0.749	0.803
Tox21_112 193	60877	emtricitabine	Most DILI- concern	0.987	0.962	NA	0.994
Tox21_110 270	5352	sulindac	Most DILI- concern	0.634	0.451	NA	0.987
Tox21_110 712	2764	ciprofloxacin	Most DILI- concern	0.822	0.778	NA	0.676
Tox21_111 680	60490	zileuton	Most DILI- concern	0.766	NA	0.766	0.844
Tox21_111 037	5353980	sulfasalazine	Most DILI- concern	0.851	0.399	-0.268	0.935
Tox21_112 013	2952	dantrolene	Most DILI- concern	NA	0.830	0.830	0.937
Tox21_113 309	33176	clometacin	Most DILI- concern	0.644	0.417	-0.178	0.920
Tox21_110 678	3474	glafenine	Most DILI- concern	0.834	0.252	0.595	0.933
Tox21_112 176	5717	zafirlukast	Most DILI- concern	NA	0.961	0.666	0.958
Tox21_110 770	3033	diclofenac	Most DILI- concern	NA	0.589	NA	0.975
Tox21_111 419	3365	fluconazole	Most DILI- concern	0.715	0.766	0.570	0.165
Tox21_112 170	11033	sulfacarbamide	Most DILI- concern	0.574	0.724	0.386	0.618
Tox21_112 505	208908	lapatinib	Most DILI- concern	0.634	NA	0.994	0.935
Tox21_111	6253	cytarabine	Most DILI-	NA	0.921	0.660	0.927

203			concern				
Tox21_111 560	159269	telbivudine	Most DILI- concern	0.811	0.726	NA	0.883
Tox21_110 682	4539	norfloxacin	Most DILI- concern	0.767	0.627	-0.125	0.545
Tox21_110 105	2733	chlorzoxazone	Most DILI- concern	0.837	0.251	0.722	0.438
Tox21_111 882	60172	adefovir	Most DILI- concern	0.523	0.807	NA	0.807
Tox21_111 681	38409	ticrynafen	Most DILI- concern	0.791	0.296	NA	0.881
Tox21_113 316	53359	tolrestat	Most DILI- concern	0.445	NA	0.097	0.711
Tox21_110 093	2717	chlormezanone	Most DILI- concern	0.190	0.280	0.303	0.717
Tox21_400 072	3117	disulfiram	Most DILI- concern	NA	0.971	NA	0.982
Tox21_110 041	2333	benzbromarone	Most DILI- concern	NA	0.965	NA	0.803
Tox21_110 854	55283	itraconazole	Most DILI- concern	NA	0.616	0.935	0.427
Tox21_201 964	2662	celecoxib	Most DILI- concern	NA	0.839	0.994	0.881
Tox21_110 676	47576	ketoconazole	Most DILI- concern	NA	0.607	0.914	0.742
Tox21_110 980	62959	trovafloxacin	Most DILI- concern	NA	0.586	0.975	0.159
Tox21_112 444	104865	bosentan	Most DILI- concern	0.218	NA	NA	0.885
Tox21_111 685	60823	atorvastatin	Most DILI- concern	0.469	0.723	NA	0.794
Tox21_113 616	152946	moxifloxacin	Most DILI- concern	0.543	0.707	-0.384	0.601
Tox21_110 719	3902	letrozole	Most DILI- concern	0.558	0.277	0.502	0.196
Tox21_111 582	64139	efavirenz	Most DILI- concern	NA	0.693	0.955	0.894
Tox21_112 666	82146	bexarotene	Most DILI- concern	NA	0.977	NA	0.485

Tox21_110 104	2554	carbamazepine	Most DILI- concern	0.259	0.153	0.533	0.520
Tox21_112 119	5591	trogliatzone	Most DILI- concern	NA	0.958	0.626	0.088
Tox21_112 192	153941	entecavir	Most DILI- concern	0.953	0.289	NA	0.481
Tox21_201 450	40399	exifone	Most DILI- concern	NA	NA	NA	0.602
Tox21_110 703	149096	levofloxacin	Most DILI- concern	0.401	0.346	-0.199	0.428
Tox21_111 329	5381226	rifampin	Most DILI- concern	-0.339	0.415	0.439	0.333
Tox21_112 488	56069	bicalutamide	Most DILI- concern	NA	NA	0.981	0.956
Tox21_111 996	6918508	falnidamol	Most DILI- concern	NA	0.964	0.488	0.434
Tox21_112 532	464205	tenofovir	Most DILI- concern	NA	0.536	NA	0.583
Tox21_111 726	30951	alclofenac	Most DILI- concern	0.340	0.936	NA	0.564
Tox21_110 910	34359	carbidopa	Most DILI- concern	0.486	0.371	NA	0.492
Tox21_110 792	5509	tolmetin	Most DILI- concern	0.495	0.093	0.399	0.315
Tox21_110 080	16231	amiloride	Most DILI- concern	0.725	0.419	-0.593	0.527
Tox21_111 793	6237	benziodarone	Most DILI- concern	NA	0.958	NA	NA
Tox21_110 336	3759	isocarboxazid	Most DILI- concern	0.409	0.023	NA	0.813
Tox21_113 640	3767	isoniazid	Most DILI- concern	0.131	0.266	0.615	-0.034
Tox21_110 982	4463	nevirapine	Most DILI- concern	0.406	0.321	0.242	0.121
Tox21_113 593	54897	alpidem	Most DILI- concern	0.649	-0.297	NA	0.741
Tox21_112 962	65027	tipranavir	Most DILI- concern	0.764	NA	NA	0.665
Tox21_112	41867	epirubicin	Most DILI-	0.091	NA	0.776	0.515

061			concern				
Tox21_112 012	6437841	acitretin	Most DILI- concern	NA	NA	NA	0.718
Tox21_110 785_1	3342	fenoprofen	Most DILI- concern	NA	NA	0.614	NA
Tox21_113 174	1011397 8	pazopanib	Most DILI- concern	0.632	NA	NA	NA
Tox21_111 158	667490	mercaptopurine	Most DILI- concern	0.628	NA	-0.841	0.847
Tox21_112 509_1	4723	pemoline	Most DILI- concern	NA	NA	0.743	NA
Tox21_112 963	4659569	tolcapone	Most DILI- concern	NA	NA	NA	NA
Tox21_110 117	2801	clomipramine	Most DILI- concern	NA	0.951	-0.957	NA
Tox21_110 944	126941	methotrexate	Most DILI- concern	NA	NA	NA	NA
Tox21_112 781	148124	docetaxel	Most DILI- concern	-0.053	NA	0.358	NA
Tox21_111 434	77999	rosiglitazone	Most DILI- concern	0.526	0.966	NA	-0.329
Tox21_110 278	941651	thiothixene	Most DILI- concern	NA	NA	NA	0.639
Tox21_111 684	5291	imatinib	Most DILI- concern	NA	0.194	NA	NA
Tox21_112 926	5493381	deferasirox	Most DILI- concern	NA	NA	NA	NA
Tox21_110 226	4680	papaverine	Most DILI- concern	NA	-0.438	-0.021	0.317
Tox21_113 574	4449	nefazodone	Most DILI- concern	NA	NA	NA	0.868
Tox21_111 394	3351	fipexide	Most DILI- concern	-0.535	-0.559	0.459	0.894
Tox21_112 203	5462516	telithromycin	Most DILI- concern	NA	0.303	NA	NA
Tox21_110 938	2733526	tamoxifen	Most DILI- concern	NA	-0.828	NA	0.695
Tox21_110 133	3108	dipyridamole	Most DILI- concern	0.613	-0.613	NA	NA

Tox21_111 395	4746	perhexiline	Most DILI- concern	NA	NA	NA	NA
Tox21_112 188	60835	duloxetine	Most DILI- concern	NA	NA	NA	NA
Tox21_113 965	9915926	eltrombopag	Most DILI- concern	NA	NA	NA	NA
Tox21_111 842	6075	mepazine	Most DILI- concern	NA	NA	NA	-0.744
Tox21_110 073	1935	tacrine	Most DILI- concern	-0.475	-0.199	0.099	0.635
Tox21_202 482	2019	dactinomycin	Most DILI- concern	NA	0.976	0.594	-0.725
Tox21_113 431	392622	ritonavir	Most DILI- concern	NA	NA	NA	-0.208
Tox21_110 145	3331	felbamate	Most DILI- concern	-0.333	-0.195	0.044	0.025
Tox21_110 048	4543	nortriptyline	Most DILI- concern	NA	NA	NA	-0.406
Tox21_111 441	5362124	benazepril	Most DILI- concern	NA	NA	NA	-0.085
Tox21_110 083	2157	amiodarone	Most DILI- concern	NA	NA	-0.910	0.652
Tox21_112 634	213039	darunavir	Most DILI- concern	-0.264	-0.145	NA	0.098
Tox21_112 630	93860	bortezomib	Most DILI- concern	NA	NA	-0.494	0.578
Tox21_112 249	5329102	sunitinib	Most DILI- concern	NA	NA	NA	0.214
Tox21_112 259	2898	cyclofenil	Most DILI- concern	-0.887	0.963	-0.681	0.050
Tox21_110 898	39186	diltiazem	Most DILI- concern	NA	-0.321	-0.679	NA
Tox21_300 211	3001322	aplaviroc	Most DILI- concern	NA	NA	-0.052	NA
Tox21_112 189	65140	abacavir	Most DILI- concern	-0.180	-0.148	NA	0.249
Tox21_110 858	5354	suloctidil	Most DILI- concern	NA	-0.987	NA	NA
Tox21_111	197712	ambrisentan	Most DILI-	-0.366	-0.124	-0.640	-0.199

967			concern				
Tox21_110 337	938	niacin	Most DILI- concern	0.018	-0.399	0.327	-0.631
Tox21_110 882	657298	propylthiouracil	Most DILI- concern	-0.345	-0.424	0.509	-0.200
Tox21_111 499	60198	exemestane	Most DILI- concern	NA	-0.817	-0.896	-0.297
Tox21_110 397	1983	acetaminophen	Most DILI- concern	-0.277	-0.645	0.213	-0.213
Tox21_110 644	3308	etodolac	Most DILI- concern	-0.635	-0.485	NA	-0.120
Tox21_110 208	4472	nialamide	Most DILI- concern	-0.169	-0.270	-0.335	-0.157
Tox21_110 658	5472	ticlopidine	Most DILI- concern	NA	-0.655	0.197	-0.260
Tox21_110 300	2520	verapamil	Most DILI- concern	NA	NA	-0.925	NA
Tox21_110 917	38853	methyldopa	Most DILI- concern	-0.132	-0.305	-0.700	0.011
Tox21_112 114	28417	danazol	Most DILI- concern	NA	-0.893	NA	NA
Tox21_110 341	1349907	methimazole	Most DILI- concern	-0.461	-0.549	-0.009	-0.737
Tox21_111 171	5351166	dacarbazine	Most DILI- concern	-0.528	-0.178	-0.436	-0.448
Tox21_111 341	3748	iproniazid	Most DILI- concern	NA	-0.505	-0.051	-0.637
Tox21_113 369	3002977	maraviroc	Most DILI- concern	-0.876	-0.392	NA	-0.673
Tox21_113 633	9574101	ximelagatran	Most DILI- concern	-0.893	-0.875	NA	-0.850
Tox21_302 415	5362440	indinavir	Most DILI- concern	-0.568	-0.276	-0.854	-0.587
Tox21_110 406	2145	aminoglutethimide	Most DILI- concern	-0.504	-0.510	-0.263	-0.221
Tox21_302 974	29327	streptozocin	Most DILI- concern	-0.244	-0.545	-0.609	-0.449
Tox21_110 292	54841	atomoxetine	Most DILI- concern	NA	NA	NA	-0.982

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