

Drug Metabolism and Disposition

A PREDICTIVE LIGAND-BASED BAYESIAN MODEL FOR HUMAN DRUG INDUCED LIVER INJURY

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Supplemental Table 2. Subset of compounds of most interest. False =DILI negative (0), True = DILI Positive (1).

Compound Name	DILI Bayesian Prediction	Human	DILI	DILI	DILI Bayesian Closest Sample	True Positive	True Negative	False Positive	False Negative
		DILI Bin (1=positive; 0=negative)	DILI Bayesian score	DILI Bayesian Closest Similarity					
Alpidem	TRUE	1	2.69	0.31	Sample 249	1			
Benoxaprofen	TRUE	1	4.55	0.57	Sample 126	1			
Bromfenac	TRUE	1	2.50	0.48	Sample 295	1			
Candesartan	FALSE	0	-6.75	0.37	Sample 270		1		
Ciglitizone	FALSE	1	-8.23	0.48	Sample 27				1
Dilevalol	TRUE	1	2.74	1.00	Sample 157				
Entacapone	TRUE	0	3.84	0.32	Sample 204			1	
Flunoxaprofen	TRUE	0	2.11	0.57	Sample 126			1	
Ibuprofen	FALSE	1	-3.01	0.43	Sample 53				1

Ibuprofen	FALSE	0	-0.81	0.50	Sample 126		1	
Irbesartan	FALSE	0	-5.62	0.24	Sample 227		1	
Ketoprofen	TRUE	0	7.35	0.55	Sample 126			1
Losartan	FALSE	1	-8.59	0.29	Sample 270			1
Lumiracoxib	TRUE	1	5.33	0.55	Sample 173	1		
Pemoline	TRUE	1	0.29	0.41	Sample 115	1		
Pirprofen	TRUE	1	3.65	0.54	Sample 126	1		
Tasosartan	FALSE	1	-2.87	0.24	Sample 197			1
Tolcapone	TRUE	1	7.71	0.35	Sample 162	1		
Troleandomycin	FALSE	1	-14.09	0.46	Sample 106			1
Ximelagatran	FALSE	1	-1.55	0.35	Sample 165			1
Zolpidem	TRUE	0	1.19	0.28	Sample 281			1
Azithromycin	FALSE	0	-16.25	0.80	Sample 105		1	
Buspirone	FALSE	0	-3.12	0.29	Sample 258		1	
Diclofenac	TRUE	1	5.69	0.56	Sample 173	1		

Nefazodone	TRUE	1	3.73	0.67	Sample 283	1			
Pioglitazone	FALSE	0	-5.14	0.40	Sample 27		1		
Propranolol	FALSE	0	-9.58	0.64	Sample 232		1		
Rosiglitazone	FALSE	0	-1.96	0.35	Sample 27		1		
Telithromycin	FALSE	1	-6.25	0.39	Sample 105				1
Troglitazone	FALSE	1	-2.52	0.37	Sample 27				1
Valsartan	FALSE	0	-2.26	0.32	Sample 250		1		
Sudoxicam	TRUE	1	2.33	0.35	Sample 45	1			
Meloxicam	TRUE	0	10.07	0.64	Sample 233			1	
Olmesartan	FALSE	0	-12.75	0.32	Sample 270		1		
Celecoxib	TRUE	1	6.15	0.31	Sample 160	1			
Lapatinib	TRUE	1	5.78	0.31	Sample 138	1			
Gefitinib	TRUE	1	5.51	0.37	Sample 18	1			
Sum						13	10	5	8