

Drug Metabolism and Disposition

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

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Supplemental Table 3. Compounds greater than 70% similar to training set. False =DILI negative (0), True = DILI Positive (1).

Compound Name	Human DILI Bin		DILI Bayesian score	DILI Bayesian Closest Similarity	DILI Bayesian Closest Sample	True Positive	True Negative	False Positive	False Negative
	DILI Prediction	(1=positive; 0=negative)							
Streptomycin	FALSE	0	-45.49	0.97	Sample 264		1		
Quinine Sulfate	TRUE	1	30.57	0.96	Sample 251	1			
Clarithromycin	FALSE	1	-13.31	0.91	Sample 105				1
Tobramycin	FALSE	1	-38.58	0.91	Sample 154				1
Glutethimide	FALSE	1	-6.73	0.81	Sample 16				1
Azithromycin	FALSE	0	-16.25	0.80	Sample 105		1		

Nafcillin Sodium	TRUE	0	8.21	0.80	Sample 182		1	
Tolazamide	FALSE	1	-2.78	0.80	Sample 139			1
Ampicillin								
Sodium	TRUE	0	2.95	0.79	Sample 220		1	
Ifosfamide	TRUE	1	3.09	0.79	Sample 78	1		
Terbutaline								
Sulfate	TRUE	1	1.20	0.79	Sample 180	1		
Adriamycin	FALSE	0	-25.50	0.78	Sample 146		1	
Doxorubicin HCl	FALSE	1	-25.50	0.78	Sample 146			1
Calcifediol	FALSE	1	-18.49	0.78	Sample 103			1
Econazole Nitrate	FALSE	0	-13.38	0.78	Sample 191		1	
Sulconazole								
Nitrate	FALSE	0	-9.79	0.78	Sample 191		1	
Fexofenadine	FALSE	0	-30.23	0.78	Sample 272		1	
Methyldopa	FALSE	1	-8.21	0.78	Sample 162			1

Acenocoumarol	FALSE	1	-7.29	0.77	Sample 290				1
Epirubicin	FALSE	0	-25.70	0.76	Sample 146			1	
Fialuridine	TRUE	1	3.44	0.76	Sample 120		1		
Grepafloxacin	TRUE	1	3.23	0.74	Sample 64		1		
Lactose	FALSE	0	-14.06	0.73	Sample 90			1	
Ethinyl estradiol	TRUE	1	7.39	0.72	Sample 108		1		
Prochlorperazine									
Maleate	TRUE	1	6.07	0.72	Sample 58		1		
Atomoxetine	FALSE	1	-9.79	0.71	Sample 125				1
Iproniazid	TRUE	1	3.58	0.71	Sample 150		1		
Minocycline HCl	TRUE	1	12.49	0.70	Sample 86		1		
sum						9	8	2	9