

Table IIIa. List of 40 chemically closest compound pairs and their hepatotoxicities. Twenty pairs (50%) have opposite toxicities despite their chemical similarity (0=dissimilar, 1=identical)^a.

No.	Compounds	Chemical similarity	Observed hepatotoxicity
74,118	mefenamic acid, phenylanthranilic acid	0.97	0, 0
40,53	methyltestosterone, ethinylestradiol	0.90	1, 1
63,64	imipramine, amitriptyline	0.89	0, 0
20,110	benzbromarone, benziodarone	0.88	1, 1
83,84	theophylline, caffeine	0.87	1, 0
72,127	erythromycin ethylsuccinate, doxorubicin	0.87	0, 0
5,14	valproic acid, aspirin	0.86	0, 1
24,94	methapyrilene, promethazine	0.86	1, 1
11,25	phenylbutazone, phenytoin	0.86	0, 0
16,115	thioacetamide, ethanol	0.85	1, 0
116,117	phenacetin, buccetin	0.85	1, 1
30,66	gemfibrozil, ibuprofen	0.85	1, 0
52,67	tamoxifen, quinidine	0.85	0, 0
44,105	perhexiline, terbinafine	0.85	0, 1
17,49	carbamazepine, pemoline	0.84	0, 0
19,62	nitrofurantoin, nitrofurazone	0.84	0, 0
10,112	allyl alcohol, bromoethanamine	0.84	1, 0
8,46	rifampicin, tetracycline	0.84	0, 0
85,95	papaverine, colchicine	0.83	0, 1
77,103	chlorpheniramine, clomipramine	0.83	0, 1
99,111	simvastatin, etoposide	0.83	1, 0
38,122	adapin, acetamidofluorene	0.83	0, 1
2,60	isoniazid, iproniazid	0.83	0, 0
39,82	labetalol, enalapril	0.82	0, 0
104,123	trimethadione, nitrosodiethylamine	0.80	1, 1
58,90	tacrine, mexiletine	0.80	0, 1
9,113	naphthyl isothiocyanate, ethionamide	0.80	1, 1
56,78	monocrotaline, nifedipine	0.79	1, 0
69,107	fenofibrate, chlormadinone	0.79	1, 0
1,54	acetaminophen, methyl dopa	0.79	1, 0
70,96	chlorpropamide, tolbutamide	0.79	1, 0
31,55	bromobenzene, methimazole	0.79	1, 0
33,97	sulfasalazine, sulpiride	0.77	1, 0
15,124	chlorpromazine, ticlopidine	0.77	0, 1
81,91	captopril, tiopronin	0.77	0, 0
22,47	diazepam, lomustine	0.77	1, 1
7,121	methotrexate, puromycin aminonucleoside	0.77	0, 1
6,18	clofibrate, diclofenac	0.76	0, 0
35,65	haloperidol, hydroxyzine	0.73	0, 0
76,79	ranitidine, diltiazem	0.72	0, 1

^a Similarity = 1 - normalized pairwise Euclidean distance.

Identical pairs have a similarity of 1; completely different pairs have zero similarity.