

Compounds	C _{max}	C _{max} (μM)	100X C _{max} (μM)	DILI concern (*)	Concentrations used for exposure	TC ₅₀ (μM)	TC ₅₀ (μM)	TC ₅₀ (μM)	TC ₅₀ (μM)
						3D_HepaRG_24h	3D_HepaRG_repeated	2D_HepaRG_24h	PHH 24h
Aspirin	5.5 μM	5.5	550	non-DILI	2 mM to 1 μM	Undetermined	Undetermined	Undetermined	Undetermined
Gemfibrozil	184 μM	184	18400	non-DILI	2 mM to 1 μM	Undetermined	Undetermined	Undetermined	Undetermined
Trovafloxacin	4.078 μM	4.078	407.8	DILI (WD)	316 μM to 0.1 μM	Approximate value above the dose level tested	53.01	Approximate value above the dose level tested	Undetermined
Troglitazone	6.3 μM	6.3	630	DILI (WD)	316 μM to 0.1 μM	173.6	46.52	131.5	142.6
Rosiglitazone	1 μM	1	100	non-DILI	316 μM to 0.1 μM	Undetermined	17358	Approximate value above the dose level tested	5006
Levofloxacin	15 μM	15	1500	non-DILI	316 μM to 0.1 μM	Undetermined	Undetermined	Undetermined	Undetermined
Acetaminophen	139 μM	139	13900	DILI (NA)	50 mM to 50 μM	6113	2879	28831	5759
Diclofenac	8.03 μM	8.03	803	DILI (7)	2 mM to 1 μM	820.2	261.8	1823	1005
Isoniazid	76.6 μM	76.6	7660	DILI (8)	50 mM to 50 μM	146685	13080	Approximate value above the dose level tested	15944
Cyclosporine A	0.7 μM	0.7	70	DILI (2)	100 μM to 0.0316 μM	Approximate value above the dose level tested	1.909	Approximate value above the dose level tested	Approximate value above the dose level tested

Supplementary S5: List of compounds used for cytotoxicity assays (Human therapeutic C_{max} values were as described in earlier publications (Khetani, et al., 2013; Xu, et al., 2008). TC₅₀ values in various cell culture and exposure conditions.

(*) -DILI score 1 to 8: 1 is lowest and 8 is highest as described in Chen, M., Vijay, V., Shi, Q., Liu, Z., Fang, H., and Tong, W. (2011). FDA-approved drug labeling for the study of drug-induced liver injury. Drug Discov Today 16(15-16), 697-703, 10.1016/j.drudis.2011.05.007.