

Table 3. Comparison of metabolomics and transcriptomics data. Includes median, first quartile (Q1), and lowest consistent response dose (LCRD) benchmark concentrations (in μM) as well as the number of features changed.

Chemical	Metabolomics				Transcriptomics							
	# of Features Changed	Median	Q1	LCRD	# of Features Changed	Median	Q1	LCRD	Therapeutic/Normal Blood Levels ¹	Toxic Blood Levels ¹	T-test of all BMC values (p-value)	T-test of BMC values in CRGB (p-value)
Chlorpromazine	150	12.63	5.57	0.65	970	11.07	5.71	0.70	0.20	4.69	0.6	0.4
KCl	185	127.30	45.74	3.78	11	159.38	33.84	159.38	4400.00	6000.00	0.7	0.004
Rifampicin	464	80.13	18.39	1.23	293	79.68	43.06	8.56	6.14	247.89	0.9	0.5
Ritonavir	184	12.73	1.80	0.20	544	13.80	7.28	0.32	11.10	110.97	0.07	0.002
Sucrose	91	149.37	61.99	20.02	13	187.88	72.74	72.74	-----	-----	0.6	0.09
Tamoxifen	137	10.89	2.72	0.54	67	7.33	3.29	1.20	0.74	7.40	0.06	0.07

1. For Chlorpromazine, Rifampicin, Ritonavir and Tamoxifen therapeutic dose levels were derived from (Schulz et al. 2012) Normal and toxic levels of potassium were derived from standard clinical guidance. Toxic levels of Chlorpromazine and Rifampicin were taken from (Schulz et al. 2012). Toxic dose levels of Ritonavir and Tamoxifen not identified by search the literature and were therefore estimated by multiplying the therapeutic dose level by 10. Therapeutic/Normal and toxic dose levels of sucrose were not found when searching the literature.