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Table SI2 1. 67 Metabolites that were Altered Significantly in *P. putida* on Exposure to Pharmaceuticals.

Metabolites are listed together with the p-value and fold difference in median GC-MS peak response. In order to view alterations which are common to exposure to the different pharmaceuticals, the 67 metabolites are ordered firstly by significance (p-value) for exposure to propranolol, followed significance for exposure to diclofenac, ibuprofen, acetaminophen etc.

			Exposure to Propranolol		Exposure to Diclofenac		Exposure to Ibuprofen		Exposure to Acetaminophen		Exposure to Atenolol		Exposure to Mefenamic acid	
Metabolite ID	Metabolite Name	Definitive ID	p-value	Fold Difference exposed / control*	p-value	Fold Difference exposed / control	p-value	Fold Difference exposed / control	p-value	Fold Difference exposed / control	p-value	Fold Difference exposed / control	p-value	Fold Difference exposed / control
129			8.90E-06	0.00	2.19E-03	0.74	1.06E-01	0.89	7.35E-02	0.8847	3.26E-01	0.9571	5.96E-05	0.3480
139			8.90E-06	Inf										
142			8.90E-06	Inf										
145			8.90E-06	Inf										
150	Propranolol	*	8.90E-06	Inf										
13	glutamic acid	*	2.80E-05	0.02	9.54E-01	0.68	2.25E-01	0.79	1.52E-02	0.3128	1.00E+00	0.8133	1.00E+00	0.7686
37	myo-inositol	*	3.23E-05	0.66	3.89E-03	0.86	9.08E-01	0.94	9.41E-02	0.8846	5.58E-03	0.8838	6.44E-01	1.0357
46	glycerol-2-phosphate		3.23E-05	2.03	3.89E-03	0.88	1.19E-01	1.29	1.84E-01	1.1955	1.82E-03	1.2809	6.03E-01	0.8168
68	2-chlorotriethanolamine		3.23E-05	0.84	4.76E-04	0.89	9.08E-01	0.99	1.49E-01	0.9335	4.53E-01	0.9673	3.77E-02	0.7701
113			3.23E-05	0.81	1.19E-01	1.04	1.66E-01	1.03	7.73E-01	1.0045	3.86E-01	1.0555	9.37E-03	1.2101
125	sugar phosphate		6.78E-05	2.13	8.62E-01	0.74	2.25E-01	1.21	4.96E-02	1.4344	2.25E-01	1.2519	4.88E-01	0.8603
52	2-monopalmitin		9.08E-05	0.00	9.38E-02	0.81	1.24E-02	0.16	4.36E-03	0.1522	1.12E-03	0.1557	9.16E-02	0.4651
45	heptadecanoic acid		1.10E-04	0.49	3.86E-01	1.02	5.67E-02	1.06	2.82E-02	1.0682	4.88E-01	0.9672	9.54E-01	0.9734
111	2-aminoethyldihydrogenphosphate		1.39E-04	0.83	1.00E+00	0.99	1.11E-02	0.87	3.56E-01	1.1104	2.73E-01	1.1762	6.03E-01	0.9609
44	sugar phosphate		2.17E-04	1.31	7.49E-01	0.92	9.06E-01	0.52	2.72E-04	1.3325	6.44E-02	1.1129	1.38E-01	1.2641
47			2.76E-04	0.58	3.86E-01	0.98	3.23E-03	0.65	3.23E-05	0.6517	1.22E-03	0.7118	5.25E-01	0.9069
130			3.38E-04	0.00										
134			3.38E-04	Inf										
135			3.38E-04	Inf										
97	glutamic acid	*	4.24E-04	0.21	6.44E-01	0.72	2.25E-01	0.78	8.33E-02	0.4998	1.00E+00	0.8133	1.00E+00	0.7686
89	alanine	*	5.26E-04	0.46	3.75E-02	0.74	3.26E-01	1.01	2.98E-01	0.6288	1.33E-01	0.7220	4.17E-02	0.3188
88	phosphate	*	1.22E-03	0.82	2.85E-01	0.97	2.82E-02	0.85	1.53E-02	0.8176	4.53E-01	0.9565	2.48E-01	1.0666

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			Exposure to Propranolol		Exposure to Diclofenac		Exposure to Ibuprofen		Exposure to Acetaminophen		Exposure to Atenolol		Exposure to Mefenamic acid	
Metabolite ID	**Metabolite Name**	**Definitive ID**	**p-value**	**Fold Difference exposed / control***	**p-value**	**Fold Difference exposed / control**	**p-value**	**Fold Difference exposed / control**	**p-value**	**Fold Difference exposed / control**	**p-value**	**Fold Difference exposed / control**	**p-value**	**Fold Difference exposed / control**
20	phenylalanine	*	1.50E-03	0.73	3.26E-01	1.08	1.30E-02	1.27	2.80E-05	0.28	7.29E-01	1.00	9.38E-02	0.77
131			1.67E-03	Inf										
126			1.82E-03	1.89	2.73E-01	1.09	6.86E-01	1.08	2.98E-01	0.92	2.99E-01	1.07	8.62E-01	1.03
140	trehalose	*	1.82E-03	0.51	7.29E-01	1.02	2.76E-04	0.41	2.76E-04	0.41	5.58E-03	0.45	3.77E-02	0.61
149	succinic acid	*	1.82E-03	2.91	1.49E-01	0.39	1.53E-02	2.22	3.27E-02	2.10	4.96E-02	1.52	2.98E-01	0.53
12	glutamic acid	*	2.68E-03	0.73	1.00E+00	1.14	2.48E-01	0.98	2.68E-03	0.73	2.99E-01	0.75	7.86E-03	0.60
25			2.68E-03	0.79	8.62E-01	0.99	3.27E-02	0.87	3.26E-01	0.93	4.53E-01	0.99	9.41E-02	0.88
146	glycine	*	2.68E-03	0.57	6.47E-02	0.67	8.62E-01	0.98	6.03E-01	0.79	6.03E-01	1.13	1.66E-01	0.69
48	octadecanoic acid	*	4.67E-03	8.04	1.53E-02	8.44	1.66E-01	1.18	2.82E-02	7.51	7.35E-02	3.57	7.73E-01	1.05
147			4.67E-03	0.78	8.17E-01	0.90	4.96E-02	0.77	9.31E-03	0.52	9.08E-01	0.94	6.03E-01	0.87
137	cellobiose	*	5.58E-03	0.76	9.08E-01	0.90	1.12E-03	0.33	1.71E-02	0.30	3.75E-02	0.60	1.33E-01	0.92
120			6.25E-03	3.62	1.05E-02	3.23			9.06E-01	1.71	9.02E-01	1.03	1.00E+00	0.65
114			9.37E-03	0.87	3.56E-01	1.02	1.49E-01	1.05	8.62E-01	1.01	6.03E-01	0.95	1.82E-03	1.13
128			9.37E-03	0.79	6.66E-03	1.23	3.26E-01	1.08	2.09E-02	1.18	2.25E-01	1.20	2.43E-02	1.24
144	monostearin		9.37E-03	0.84	4.19E-01	0.95	3.86E-01	0.89	2.09E-02	0.82	3.77E-02	0.84	3.56E-01	0.89
143					1.96E-05	Inf								
10	xylitol	*	2.09E-02	1.36	2.76E-04	0.65	9.54E-01	0.99	1.06E-01	1.24	1.00E+00	0.98	3.86E-01	1.03
73	9-octadecenoic acid methyl ester		8.84E-01	0.97	3.38E-04	0.00	4.06E-01	0.30	2.26E-03	0.00	4.12E-03	0.00	6.69E-02	0.65
98	putrescine	*			3.38E-04	0.00								
82	impurity				2.26E-03	Inf								
3	aspartic acid	*	1.19E-01	0.72	2.68E-03	0.62	6.86E-01	0.97	4.88E-01	1.03	1.00E+00	1.00	8.30E-02	0.76
108			6.69E-02	0.69	3.38E-03	0.00	2.82E-02	0.23	2.26E-03	0.00	2.26E-03	0.00	3.38E-04	0.00
95			1.19E-01	1.45	7.91E-03	0.47	3.89E-03	2.70	1.82E-03	2.50	5.67E-02	1.69	2.48E-01	0.87
35			3.77E-02	0.65	9.37E-03	0.61	9.89E-04	0.29	1.66E-01	0.41	1.53E-02	0.50	3.56E-01	0.39
81	ethanolamine		3.86E-01	1.04	9.37E-03	1.68	7.73E-01	1.12	3.56E-01	0.92	1.19E-01	1.28	3.86E-01	1.29
14	putrescine	*	7.32E-02	1.32	8.17E-01	0.92	1.81E-03	1.85	1.19E-01	1.52	1.91E-01	1.31	4.32E-01	0.85
36	pentadecanoic acid		3.27E-02	1.15	7.29E-01	1.04	3.23E-03	1.14	5.58E-03	1.13	2.73E-01	1.10	7.73E-01	1.09
91	beta-alanine		1.30E-02	0.66	1.79E-02	0.72	3.89E-03	1.40	2.99E-01	0.97	2.99E-01	1.35	6.03E-01	0.75
75	sugar or sugar alcohol		2.04E-01	1.26	5.25E-01	1.06	3.89E-03	0.80	2.68E-03	0.67	2.99E-01	0.81	4.53E-01	0.89
42	sugar or sugar alcohol		3.86E-01	0.87	9.08E-01	1.05	6.25E-03	0.05	3.25E-02	0.18	3.75E-02	0.16	3.63E-03	0.09
100	tropic acid		3.77E-02	0.61	4.33E-02	1.43	6.66E-03	0.46	4.96E-02	0.60	9.08E-01	0.99	1.84E-01	0.83
39	hexadecenoic acid	*	5.25E-01	1.00	3.86E-01	0.97	7.91E-03	0.90	1.33E-01	0.98	3.26E-01	0.97	4.96E-02	0.93

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90	glycerol	*	6.03E-01	0.92	5.64E-01	0.84	7.91E-03	1.38	1.00E+00	0.87	2.09E-02	1.26	5.64E-01	0.92
34	2-deoxycytidine-5-monophosphate		6.86E-01	0.91	8.17E-01	1.08	7.91E-03	0.86	9.08E-01	1.02	3.86E-01	1.04	7.29E-01	1.11
56	maltose	*	1.53E-02	1.38	1.19E-01	1.24	9.37E-03	0.69	2.04E-01	0.83	4.53E-01	0.95	6.03E-01	1.12
124	sugar or sugar alcohol		3.56E-01	0.93	5.67E-02	0.86	1.30E-02	0.75	1.75E-04	0.62	3.77E-02	0.81	4.19E-01	0.96
112			4.19E-01	0.92	2.73E-01	1.03	2.25E-01	0.94	8.04E-04	0.76	1.49E-01	0.93	9.41E-02	1.09
79			6.03E-01	0.98	2.73E-01	0.85	2.99E-01	1.02	1.82E-03	1.87	8.33E-02	1.20	4.19E-01	1.61
29	citric acid	*									3.38E-04	Inf		
63			6.35E-01	1.88	3.24E-01	0.78	8.53E-01	0.92	8.55E-02	2.28	1.12E-03	2.57	7.52E-02	2.76
19	impurity		1.46E-01	1.73	5.03E-02	3.32	5.37E-01	1.49	2.82E-02	4.44	1.68E-03	3.50	1.23E-01	3.39
65	glycerol-2-phosphate		1.06E-01	0.78	6.21E-01	0.87	9.54E-01	0.95	4.88E-01	0.98	3.21E-03	1.30	9.30E-01	1.03
109			9.54E-01	1.01	8.33E-02	1.09	5.67E-02	1.16	1.33E-01	1.07	3.86E-01	1.05	8.12E-04	1.23
122	N-acetylglucosamine	*	3.86E-01	0.98	1.84E-01	1.36	8.33E-02	1.07	3.77E-02	1.19	4.19E-01	1.27	4.67E-03	1.29
72	sugar or sugar alcohol		1.00E+00	1.60	7.11E-01	0.94	4.17E-02	2.33	1.81E-01	2.18	8.12E-01	1.86	7.45E-03	2.75

* fold difference is the fold difference in GC-MS peak response. Inf(inity) implies an increase in exposed cells from zero in control cells, while zero implies a fall to zero in exposed cells from some value in control cells. Statistically significant alterations are highlighted in yellow.