

## SUPPLEMENTARY DATA

Supplementary Table 1. Experimental, calculated activities and residuals from CoMFA studies

Compounds	Experimental pK <sub>i</sub>			Calculated pK <sub>i</sub>			Residual		
	Oat1	Oat6	Selective	Oat1	Oat6	Selective	Oat1	Oat6	Selective
<b>Training set</b>									
Acetylsalicylate	3.16	3.99	0.83	3.20	4.13	0.59	-0.04	-0.14	0.24
Adipate	6.39	2.8	-3.58	5.89	2.57	-2.86	0.50	0.23	-0.73
Benzoate	3.6	4.86	1.26	3.49	4.42	1.22	0.12	0.44	0.04
Butyrate	2.46	4.09	1.63	2.34	4.18	1.81	0.12	-0.09	-0.18
Carbenicillin	2.89	2.87	-0.02	2.81	3.02	0.22	0.08	-0.15	-0.24
Eosiny	7.05	5.36	-1.69	6.88	5.53	-2.15	0.17	-0.17	0.46
Estradioldisulfate	3.66	2.14	-1.52	3.61	2.46	-1.43	0.05	-0.32	-0.09
Estrone-3-sulfate	3.69	4.24	0.55	3.55	4.15	0.25	0.14	0.09	0.30
Fluorescein	5.53	4	-1.53	5.42	4.47	-1.25	0.11	-0.47	-0.28
Glutarate	5.17	2.27	-2.91	5.32	2.64	-2.73	-0.15	-0.37	-0.18
Heptanoate	4.78	5.09	0.31	5.00	4.90	-0.12	-0.22	0.19	0.43
Hexanoate	4.43	5.04	0.62	4.84	4.70	-0.23	-0.41	0.34	0.85
Hippurate	4.25	3.51	-0.75	4.54	3.62	-0.57	-0.29	-0.11	-0.18
Ibuprofen	5.33	5.95	0.62	5.23	5.44	0.36	0.10	0.51	0.26
3-methylbutyrate	2.63	4.49	1.86	2.60	4.29	1.63	0.03	0.20	0.23
4-Hydroxy-phenyl-pyruvate	4.14	4.18	0.04	4.13	4.16	0.26	0.01	0.02	-0.22
Methotrexate	3.05	3.22	0.18	3.14	2.79	-0.35	-0.09	0.43	0.53
Ochratoxin A	5.2	4.31	-0.89	5.16	4.42	-1.26	0.04	-0.11	0.37
Penicillin G	3.48	3.34	-0.14	3.53	3.70	0.33	-0.05	-0.36	-0.47
Phenylpyruvate	4.1	4.54	0.44	4.19	4.67	0.62	-0.09	-0.13	-0.18
Probenicid	5.2	5.07	-0.12	5.55	5.08	-0.59	-0.35	-0.01	0.47
Propionate	2.09	3.55	1.47	1.88	3.23	2.00	0.21	0.32	-0.53
Prostaglandin-E2	5.47	4.74	-0.73	5.61	5.16	-1.03	-0.14	-0.42	0.30
Pyruvate	1.92	3.57	1.64	2.48	3.30	1.26	-0.56	0.28	0.38
P-amino-hippurate	5.03	3.35	-1.68	4.81	3.79	-0.67	0.23	-0.44	-1.02
Salicylate	3.84	4.36	0.52	3.66	4.44	1.07	0.19	-0.07	-0.55
Suberate	4.47	2.95	-1.52	4.45	2.77	-1.65	0.02	0.18	0.13
Ticarcillin	3.28	3.27	-0.01	3.01	3.15	0.14	0.27	0.13	-0.15
<b>Test set</b>									
(S)-2-Hydroxy-3-methyl-butyrate	1.85	3.5	1.65	2.50	3.27	1.30	-0.65	0.23	0.35
(R)-2-Hydroxy-3-methyl-butyrate	1.85	3.5	1.65	2.96	4.36	1.33	-1.11	-0.86	0.32
(S)-2-Methyl butyrate	3.04	4.39	1.35	3.94	4.40	0.34	-0.90	-0.01	1.01
(R)-2-Methyl butyrate	3.04	4.39	1.35	3.44	4.28	0.84	-0.40	0.11	0.51
(S)-3-Hydroxy butyrate	2.49	3.72	1.23	2.92	3.35	0.88	-0.43	0.37	0.35
(R)-3-Hydroxy butyrate	2.49	3.72	1.23	2.84	3.35	1.02	-0.35	0.37	0.21
(S)-2-Ethyl hexanoate	4.25	5.18	0.93	5.29	4.62	-0.66	-1.04	0.56	1.59
(R)-2-Ethyl hexanoate	4.25	5.18	0.93	5.28	4.67	-0.63	-1.03	0.51	1.56
(S)-4-Hydroxy phenyl lactate	3.65	3.74	0.09	3.88	4.62	0.80	-0.23	-0.88	-0.71
(S)-N-acetyl aspartate	3.08	1.56	-1.52	2.80	2.38	0.00	0.28	-0.82	-1.52
Fumarate	3.21	1.5	-1.71	1.61	2.33	1.17	1.60	-0.83	-2.88