Table 7. Experimental and 2D-QSAR predicted pIC_{50} values for UPPS enzyme inhibition

	Experimental	Predicted		Cross-validated†	
Cpd ID*	UPPS pIC_{50}, M	Predicted pIC_{50}, M	Residual	Predicted pIC_{50}, M	Residual
BPH-629	6.23	5.76	0.47	5.71	0.53
BPH-608	6.16	5.9	0.26	5.86	0.3
BPH-628	6.04	5.83	0.21	5.81	0.23
BPH-625	5.99	5.87	0.12	5.85	0.14
BPH-675	5.95	6.34	-0.39	6.92	-0.98
BPH-676	5.89	5.44	0.45	5.41	0.48
BPH-640	5.75	5.61	0.14	5.6	0.16
BPH-626	5.7	5.88	-0.18	5.91	-0.21
BPH-621	5.51	5.5	0.01	5.5	0.01
BPH-622	5.26	5.26	0	5.27	0
BPH-294	5.17	4.99	0.18	4.96	0.21
BPH-228	5.11	5.02	0.09	5.01	0.1
BPH-364	5	4.78	0.22	4.76	0.24
BPH-618	4.99	5.37	-0.38	5.42	-0.43
BPH-646	4.92	5.3	-0.38	5.35	-0.43
BPH-642	4.87	4.54	0.33	4.5	0.37
BPH-633	4.67	4.63	0.03	4.63	0.04
BPH-632	4.56	4.58	-0.02	4.58	-0.02
BPH-641	4.47	4.54	-0.08	4.55	-0.09
BPH-620	4.45	4.6	-0.14	4.61	-0.16
BPH-300	4.32	3.84	0.48	3.77	0.55
BPH-614	4.17	4.59	-0.41	4.64	-0.46
BPH-674	4.16	4.12	0.03	4.11	0.05
BPH-663	4.06	3.6	0.46	3.27	0.79
BPH-601	4.05	3.94	0.11	3.82	0.23
BPH-619	3.91	4.62	-0.72	4.71	-0.8
BPH-11	3.7	4.02	-0.33	4.13	-0.43
BPH-461	3.31	3.13	0.17	3.07	0.24
BPH-2	3.18	3.93	-0.75	4.19	-1.01

*Structures are shown in SI Fig. 9.

†Cross validated predictions obtained using a leave-one-out validation scheme as implemented in the QuaSAR validation module of MOE 2006.08 (Chemical Computing Group Inc., Montreal, Canada).