



## Supporting Information

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# Probing Binding and Cellular Activity of Pyrrolidinone and Piperidinone Small Molecules Targeting the Urokinase Receptor

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**Supporting information Table S1.** Performance of PLS-based regression (QSAR) with various hypotheses.

Hypothesis	Factors	R <sup>2</sup>	Stability	Q <sup>2</sup>	P(Pearson
<b>HS1133</b>	1	0.77	0.64	0.08	0.42
	2	0.96	0.31	0.33	0.62
	3	0.99	0.32	0.26	0.57
<b>HS1135</b>	1	0.78	0.65	0.14	0.46
	2	0.95	0.37	0.38	0.66
	3	0.98	0.36	0.29	0.61
<b>HS1119</b>	1	0.80	0.54	0.25	0.53
	2	0.93	0.40	0.39	0.64
	3	0.99	0.38	0.35	0.62
<b>HS1040</b>	1	0.70	0.63	0.29	0.54
	2	0.95	0.16	0.38	0.67
	3	0.99	0.16	0.37	0.66
<b>HS1047</b>	1	0.86	0.36	0.29	0.57
	2	0.96	0.28	0.31	0.62
	3	0.99	0.17	0.35	0.64
<b>HS1143</b>	1	0.77	0.55	0.18	0.49
	2	0.97	0.18	0.20	0.55
	3	0.99	0.17	0.20	0.54