

## SUPPLEMENTARY MATERIAL

### **Solvent-guided quantitative structure-activity relationship (SG-QSAR): In silico SG-QSAR-based improvement of the human uridine phosphorylase-2 inhibitor binding affinity with potential applications in reducing the toxicity of chemotherapy**

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**Contents:** Table S1. Details of all the analogs that were analyzed in this study.

Analogue	B. A. (Kcal/mol)	No.of Rot. bonds	No.of H-bonds	Mol. Wt. (Da)	Log-P value
AG01001	-8.4	7	8	276.29	0.72+/-0.38
AG01002	-7.3	7	9	278.26066	1.10+/-0.75
AG01003	-7.9	8	9	373.40302	0.69+/-0.62
AG01004	-7.5	9	8	375.4189	0.91+/-0.60
AG01005	-7.8	9	8	306.31382	0.58+/-0.48
AG01006	-7.5	9	9	370.3786514	N/A
AG01007	-7.6	9	8	371.38714	1.49+/-0.62
AG01008	-6.1	26	12	811.91582	3.60+/-0.65
AG01009	-5.2	26	14	812.90058	4.07+/-0.78
AG01010	-8.5	25	3	860.94338	5.75+/-0.83
AG01011	-16.5	25	5	858.97716	1.75+/-0.79
AG01012	-15.9	22	4	814.9246	3.06+/-0.67
AG01013	-4.4	21	4	748.86652	3.28+/-0.62
AG01014	-15.6	23	0	825.95	3.89+/-0.70
AG01015	-5.1	23	3	763.881	2.75+/-0.71
AG01016	-11.1	24	4	846.966	2.29+/-0.89
AG01017	-9	20	4	734.839	2.34+/-0.59
AG01018	-8.4	20	4	736.855	1.95+/-0.65
AG01019	-5	9	4	368.3832	2.41+/-0.45
AG01020	-9.2	8	6	351.39904	2.58+/-0.53
AG01021	-8	9	3	367.398	1.75+/-0.54
AG01022	-6.8	8	8	351.399	2.58+/-0.53
AG01023	-6.7	9	12	367.398	1.75+/-0.54
AG01024	-6.6	9	10	367.39	1.63+/-0.54
AG01025	-6.1	10	11	383.39	0.70+/-0.55
AG01026	-6.8	8	2	367.398	0.97+/-0.42
AG01027	-6.7	8	2	383.39	1.04+/-0.53
AG01028	-5.9	8	14	383.39	1.04+/-0.53
AG01029	-7.2	7	5	318.32	0.40+/-0.61
AG01030	-5.5	6	10	331.36	1.96+/-0.60
AG01031	-6.5	7	2	344.4	0.88+/-0.45
AG01032	-6.4	7	1	344.408	0.65+/-0.44
AG01033	-6.7	7	2	343.42	1.85+/-0.39
AG01034	-9.3	9	10	367.398	2.20+/-0.58
AG01035	-5.8	10	12	451.51	2.67+/-0.61
AG01036	-6.4	10	12	447.48	2.32+/-0.64
AG01037	-6.6	10	0	451.51	2.67+/-0.61
AG01038	-6.6	10	10	447.48	2.32+/-0.64
AG01039	-8.3	10	12	447.483	2.32+/-0.64
AG01040	-7.3	11	7	461.5	2.35+/-0.85

Analog	B. A. (Kcal/mol)	No.of Rot. bonds	No.of H-bonds	Mol. Wt. (Da)	Log-P value
AG01041	-8.6	10	11	451.51	2.67+/-0.61
AG01042	-8.5	10	11	493.551	2.10+/-0.65
AG01043	-6.7	10	5	535.588	1.53+/-0.68
AG01044	-9.2	9	8	367.39	2.20+/-0.58
AG01045	-8.9	11	13	397.42	2.59+/-0.85
AG01046	-9.1	10	13	383.39	2.52+/-0.72
AG01047	-8.8	11	7	397.42	2.59+/-0.85
AG01048	-8.7	13	9	427.45	3.15+/-0.83
AG01049	-6.4	12	6	425.43	3.25+/-0.69
AG01050	-7.8	14	4	513.53	3.77+/-0.86
AG01051	-8.5	11	7	396.43	2.25+/-0.50
AG01052	-9	10	9	382.41	3.11+/-0.72
AG01053	-6.6	10	8	409.43	2.50+/-0.59
AG01054	-9.1	7	7	381.42832	3.03+/-0.72
AG01055	-7.5	11	5	395.45	2.40+/-0.58
AG01056	-9.7	7	8	408.45	2.56+/-0.59
AG01057	-6.5	8	2	409.48	2.75+/-0.58
AG01058	-7.1	7	4	422.48	2.91+/-0.59
AG01059	-6.9	7	5	426.49	3.22+/-0.64
AG01060	-5	8	4	506.57	3.42+/-0.60

**Table S1.** Details of analogs in this study including the parent, BAU.