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Supplementary material:

Table 1: Docking results of 1-(substituted phenyl)-3-(naphtha[1,2-*d*]thiazol-2-yl)urea/thiourea derivatives with $AA_{2A}R$. Data of % reduction in catalepsy were taken from reference **[10]**. Compound number is same as given in the literature. [a)]Binding free energy (kcal/mol); [b)]Inhibition constant estimated by docking (in nM); [c)]Root mean square deviation (in Å); [d)]Amino acid; [e)]Bond distance (in Å); [f)]No H-bond or pi-interaction.

Comp.	R	X	% Reduction in catalepsy	ΔG_b[a]	K_i[b]	RMSD[c]	Hydrogen bonds		π-Interactions	
							AA[d]	Dist[e]	AA[d]	Dist[e]
3	H	O	44.44	-8.27	863.78	4.29	[f]	-	Phe-168	4.14
									Phe-168	5.25
									Phe-168	6.43
4	4-OCH_3	O	58.51	-8.81	346.16	3.99	Glu-169	2.16	Phe-168	4.53
							Tyr-271	1.95	Phe-168	5.26
5	2-OCH_3	O	76.9	-9.00	250.84	4.21	Phe-168	1.97	Phe-168	4.52
							Tyr-271	1.94	Phe-168	5.24
6	2,4-OCH_3	O	75	-9.25	164.57	4.03	Phe-168	2.15	Phe-168	4.43
							Glu-169	2.38	Phe-168	5.14
							Tyr-271	1.96		
7	3,4,5-OCH_3	O	70.29	-9.07	224.23	3.93	His-278	1.87	Phe-168	4.44
									Phe-168	5.65
8	4-Phenoxy	O	55.56	-9.53	102.63	2.52	[f]	-	Phe-168	5.19
9	2-F	O	29.12	-8.16	1040	4.85	Phe-168	2.02	[f]	-
							Tyr-271	2.08		
10	4-F	O	30.3	-8.14	1080	4.83	Phe-168	2.07	[f]	-
							Tyr-271	2.05		
11	2-Br	O	38.74	-8.72	405.86	4.15	Tyr-271	2.18	Phe-168	4.55
									Phe-168	5.26
12	4-Br	O	37.76	-8.55	542.28	4.36	Tyr-271	2.11	Phe-168	4.61
									Phe-168	5.19
13	2-Cl	O	37.37	-8.54	546.60	4.09	Tyr-271	2.22	Phe-168	4.54
									Phe-168	5.28
14	4-Cl	O	38.61	-8.38	721.26	4.34	Tyr-271	2.09	Phe-168	4.60
									Phe-168	5.19
15	2-Cl, 5-CF_3	O	51.37	-8.94	281.80	4.1	Tyr-271	2.13	[f]	-
16	2-NO_2	O	72.05	-9.87	58.72	4.69	Glu-169	2.1	[f]	-
							Glu-169	2.1		
17	4-NO_2	O	31.28	-8.61	484.40	3.93	Val-84	2.04	Phe-168	5.11
18	2-CH_3	O	47.64	-8.46	626.58	4.01	Phe-168	1.74	Phe-168	4.13
							Tyr-271	1.89	Phe-168	4.57
									Phe-168	6.03
19	4-CH_3	O	48.56	-8.65	455.03	4.03	[f]	-	Phe-168	4.38
									Phe-168	5.45
								-	Phe-168	6.38
20	H	S	44.63	-8.45	636.96	3.95	Ala-81	2.17	f	-
21	4-OCH_3	S	58.05	-9.26	162.54	5.02	Glu-169	2.09	Phe-168	4.27
							Tyr-271	1.88	Phe-168	3.76
									Phe-168	3.95
22	2-OCH_3	S	75.46	-9.06	229.22	2.72	Glu-169	1.95	Phe-168	4.01
							Asn-253	2.39	Phe-168	5.26
							Glu-169	1.98		
							Glu-169	3.19		
							Asn-253	3.02		
23	2-F	S	38.35	-8.18	1010	1.39	[f]	-	Phe-168	3.99
									Phe-168	4.69
									Phe-168	5.91
24	4-F	S	34.95	-8.11	1130	4.24	[f]	-	Phe-168	3.91
									Phe-168	3.81
									Phe-168	4.45
25	2-Br	S	30.96	-8.53	562.85	4.05	[f]	-	Phe-168	3.68
									Phe-168	3.79
									Phe-168	4.49
26	4-Br	S	35.27	-8.75	388.83	4.22	[f]	-	-	-
27	2-Cl	S	39.14	-8.55	544.16	3.1	[f]	-	Phe-168	4.06
									Phe-168	4.80

									Phe-168	3.88
28	4-Cl	S	27.88	-8.68	432.38	4.05	Tyr-271	2.22	Phe-168	4.92
									Phe-168	4.1
									Phe-168	3.81
29	2-NO_2	S	72.97	-9.61	90.07	2.63	Phe-168	2.15	-	-
							Phe-168	1.99		
							Ile-66	3.19		
30	4-NO_2	S	32.13	-8.72	405.62	4.45	His-278	2.05	Phe-168	3.95
									Phe-168	3.99
									Phe-168	4.33
31	2-CH_3	S	49.87	-8.66	448.49	4.77	[f]	-	Phe-168	4.12
									Phe-168	4.81
									Phe-168	6.27
32	4-CH_3	S	47.97	-8.56	529.05	4.30	[f]	-	Phe-168	4.18
									Phe-168	5.00
									Phe-168	6.26