Supplementary material

Table S1. Binding modes and docking scores for compounds **10**–**24**

Table S1. Binding modes and docking scores for compounds **10**–**24**

	Lowest energy conformation		**Binding mode for the top nine low energy conformations**					
Code	**Bind**	**Score**	**Bind A (A2)[1]**	**Bind B**	**Bind C**	**Max. Score[2]**	**Min. Score[3]**	**Mean Score[4]**
10	B	-5.8	1	6	2	-5.8	-4.9	-5.3
11	B	-6.3	1	6	2	-6.3	-5.6	-5.9
12	A2	-6.9	4 (3)	0	5	-6.9	-6.2	-6.5
13	B	-5.9	2 (2)	2	5	-5.9	-5.7	-5.8
14	B	-6.0	1	4	4	-6.0	-5.1	-5.6
15	A	-6.8	3	0	6	-6.8	-5.7	-6.1
16	A2	-6.3	4 (2)	0	5	-6.3	-5.9	-6.1
17	A2	-7.4	5 (3)	0	4	-7.4	-6.5	-6.8
18	A2	-7.4	5 (3)	0	4	-7.4	-6.5	-7
19	A2	-8.0	1 (1)	0	8	-8.0	-6.9	-7.4
20	C	-7.8	0	1	8	-7.8	-6.7	-7.1
21	B	-5.9	1	3	5	-6.9	-6.4	-5.5
22	C	-6.9	2	2	5	-6.9	-6.4	-6.6
23	C	-5.8	0	2	7	-5.8	-5.1	-5.4
24	A, B	-6.3	2	1	6	-6.3	-5.8	-6.0

[1] Represents the population from the top nine conformations with binding mode A.
[2] Maximum score found in the top nine conformations.
[3] Minimum score found in the top nine conformations.
[4] Mean score found in the top nine conformations.