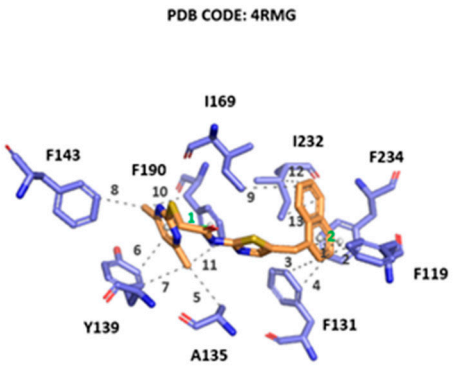


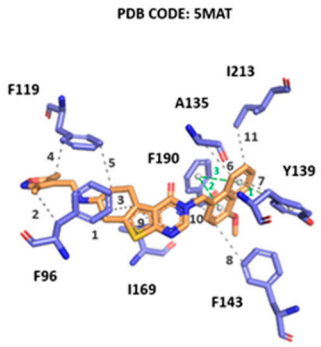
Hydrophobic interactions

Index	Residue number	Residue	Distance	Ligand Atom
1	119A	PHE	3.51	2357
2	119A	PHE	3.45	2378
3	131A	PHE	3.82	2378
4	131A	PHE	3.64	2379
5	135A	ALA	3.91	2373
6	139A	TYR	3.60	2374
7	139A	TYR	3.79	2373
8	143A	PHE	3.74	2376
9	169A	ILE	3.77	2362
10	190A	PHE	3.54	2376
11	190A	PHE	3.45	2373
12	232A	ILE	3.85	2364
13	232A	ILE	3.45	2365

π-Stacking

Index	Residue number	Residue	Distance	Ligand atom
1	190A	PHE	4.05	2363, 2370, 2371, 2372, 2374, 2375
2	234A	PHE	4.86	2357, 2358, 2378, 2379, 2380, 2381

Figure S1. Scheme of the most relevant interactions involving the SIRT2 inhibitor SirReal2 (3TE) and the biological target (*PDB code = 4RMG*) [22]. Distance values are reported in Å. Hydrophobic interactions are represented as grey dotted lines, and indexed with dark grey numbers. π-Stacking are represented as dark green long-dash dotted lines, and indexed with green numbers. Hydrogen bonds are represented as blue solid lines, indexes with red numbers. Water bridges are indicated with light blue solid lines, indexes with blue numbers. The white spheres indicate the center of an aromatic ring (involved in pi-stacking).



Hydrophobic interactions

Index	Residue number	Residue	Distance	Ligand Atom
1	96A	PHE	3.36	9626
2	96A	PHE	3.80	9635
3	96A	PHE	3.75	9624
4	119A	PHE	3.77	9631
5	119A	PHE	3.85	9628
6	135A	ALA	3.95	9611
7	139A	TYR	3.98	9611
8	143A	PHE	3.91	9616
9	169A	ILE	3.58	9624
10	190A	PHE	3.99	9616
11	213A	ILE	3.88	9610

π-Stacking

Index	Residue number	Residue	Distance	Ligand atom
1	139A	TYR	4.66	9608, 9609, 9610, 9611, 9612, 9613
2	190A	PHE	3.80	9612, 9613, 9614, 9615, 9616, 9617
3	190A	PHE	4.04	9608, 9609, 9610, 9611, 9612, 9613

Figure S2. Scheme of the most relevant interactions involving the selective thienopyrimidinone based SIRT2 inhibitor (7KJ) and the biological target (*PDB code = 5MAT*) [25]. Distance values are reported in Å. Hydrophobic interactions are represented as grey dotted lines, and indexed with dark grey numbers. π-Stacking are represented as dark green long-dash dotted lines, and indexed with green numbers. Hydrogen bonds are represented as blue solid lines, indexes with red numbers. Water bridges are indicated with light blue solid lines, indexes with blue numbers. The white spheres indicate the center of an aromatic ring (involved in pi-stacking).

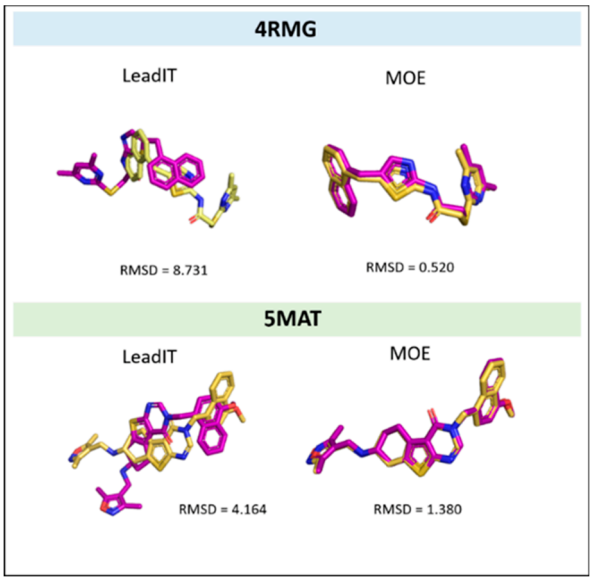


Figure S3. Comparison of the best scored 4RMG and 5MAT ligand docking poses (purple ligand) with respect to the same crystallized compounds at the corresponding 4RMG and 5MAT PDB codes (yellow ligand) as obtained by LeadIT and MOE molecular docking. RMSD values (Å) have been evaluated by Pymol [The PyMOL Molecular Graphics System, Version 1.2r3pre, Schrödinger, LLC].

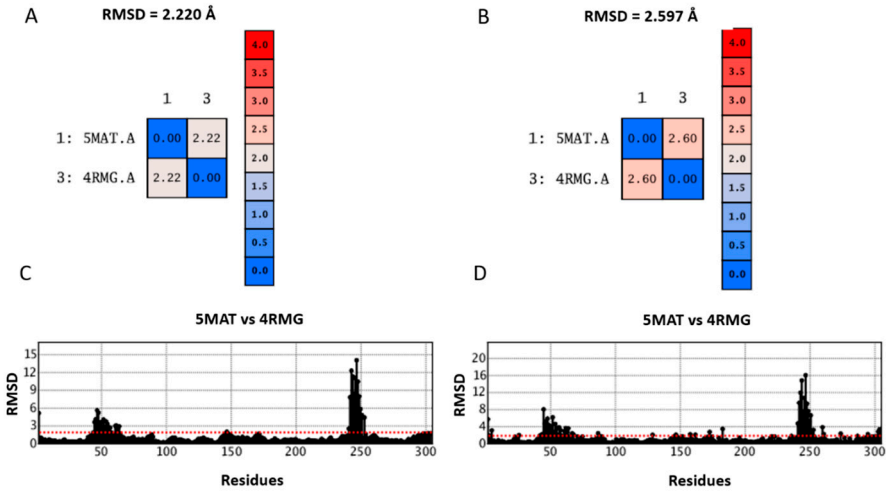


Figure S4. RMSD values (Å) as obtained by superimposition of 4RMG and 5MAT are shown based on the carbon atom alignment (A) and at the whole structure (B). The corresponding overall RMSD variation trend is also reported (C,D).

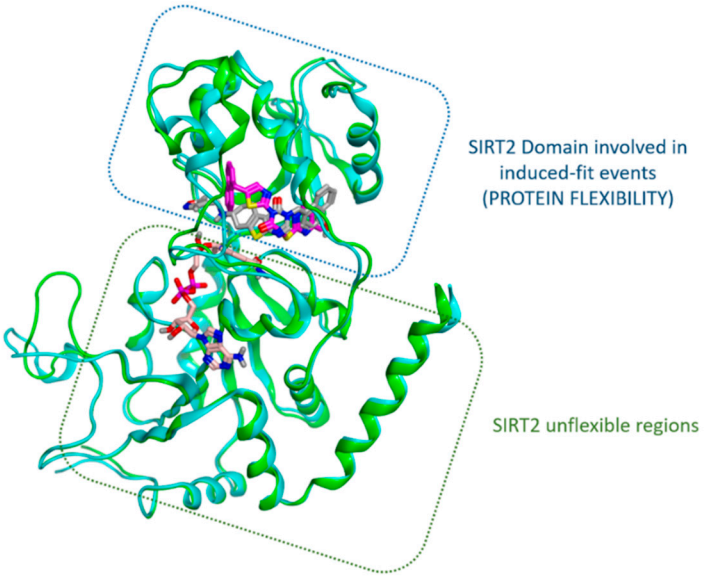


Figure S5. Superimposition of the 4RMG (in cyan) and 5MAT (in green) PDB codes in presence of the co-crystallized ligands is also depicted. Most flexible areas due to the inhibitor structure are also highlighted.

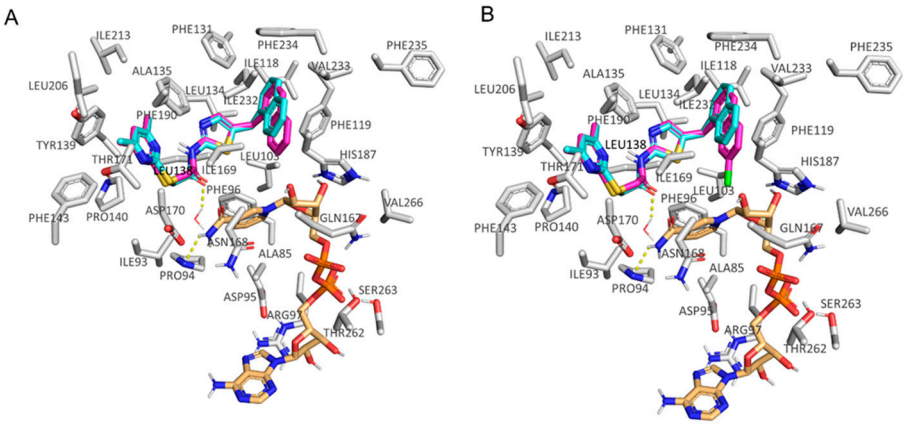


Figure S6 Docking positioning of SirReal2 (C atom, magenta) (A) and of the analogue **11** (C atom; magenta) (B) at the 4RMG binding site. The co-crystallized SirReal2 (C atom; cyan) and NAD^+ (C atom; light orange) structures are also reported.

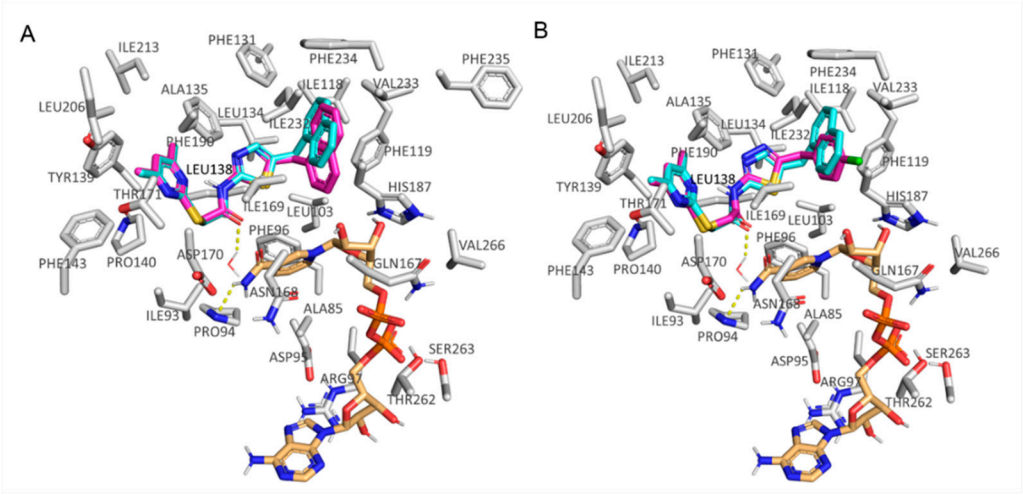


Figure S7 Docking positioning of compound **25** (C atom, magenta) (A) and of **23** (C atom; magenta) (B) at the 4RMG binding site. The co-crystallized SirReal2 (C atom; cyan) and NAD^+ (C atom; light orange) structures are also reported.

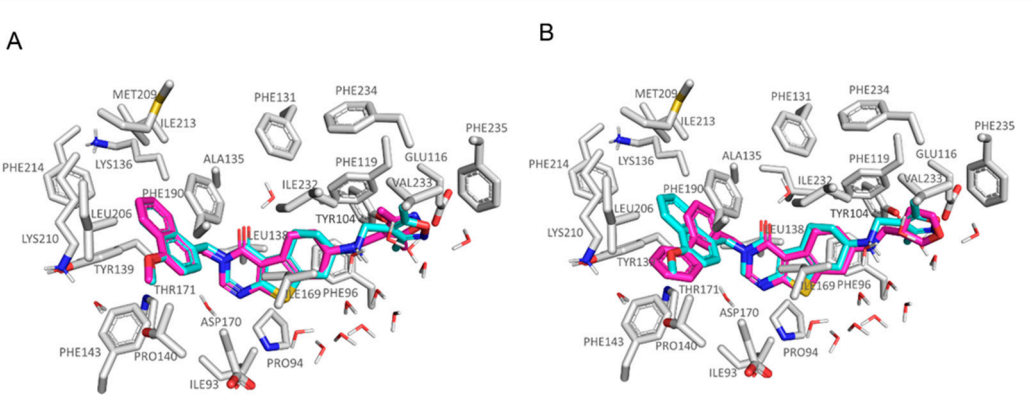


Figure S8. Docking positioning of compound **36** (C atom, magenta) (A) and of **94** (C atom; magenta) (B) at the 5MAT binding site. The co-crystallized thienopyrimidinone inhibitor **36** (C atom; cyan) structure is also reported.

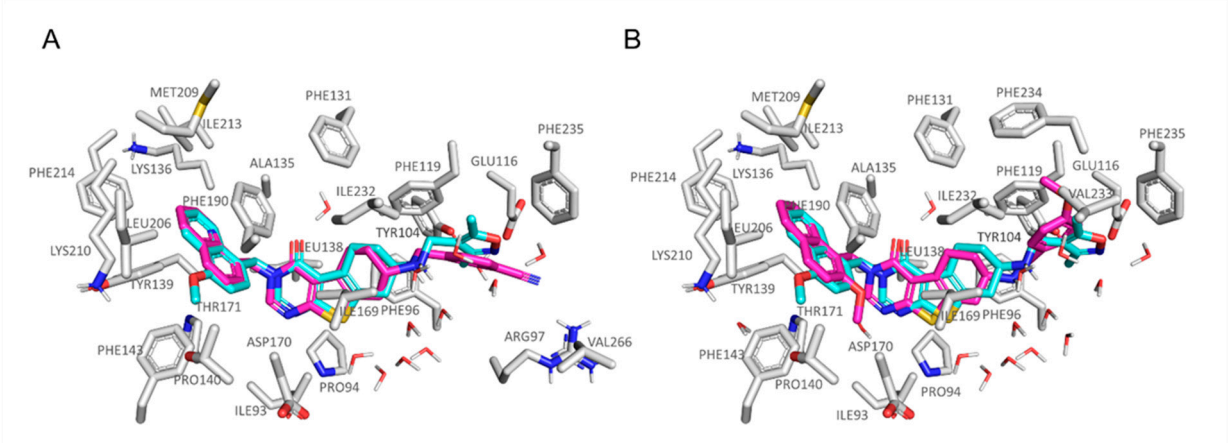


Figure S9. Docking positioning of compound **49** (C atom, magenta) (A) and of **56** (C atom; magenta) (B) at the 5MAT binding site. The co-crystallized thienopyrimidinone inhibitor **36** (C atom; cyan) structure is also reported.

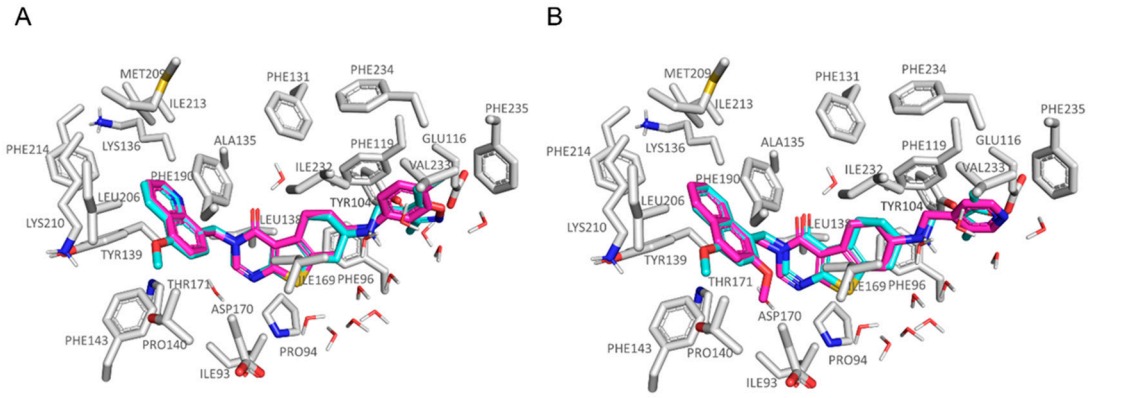


Figure S10. Docking positioning of compound **62** (C atom, magenta) (A) and of **66** (C atom; magenta) (B) at the 5MAT binding site. The co-crystallized thienopyrimidinone inhibitor **36** (C atom; cyan) structure is also reported.

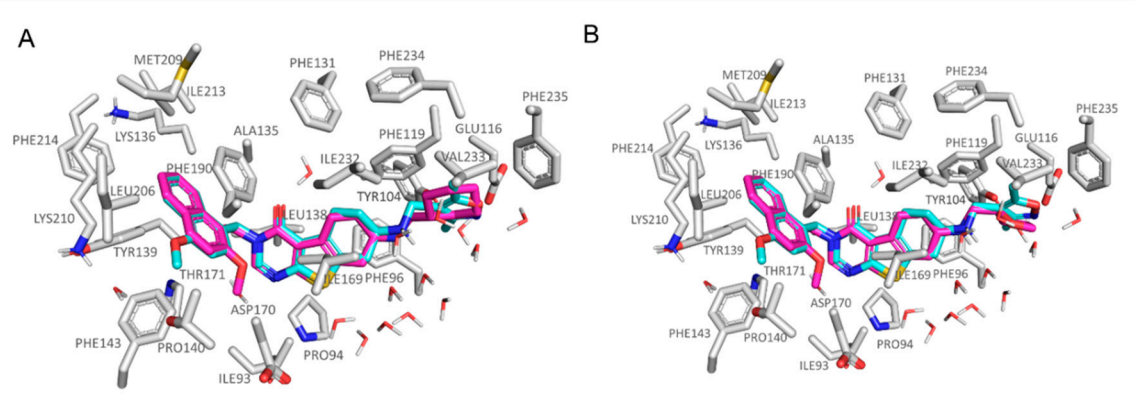


Figure S11. Docking positioning of compound **86** (C atom, magenta) (A) and of **90** (C atom; magenta) (B) at the 5MAT binding site. The co-crystallized thienopyrimidinone inhibitor **36** (C atom; cyan) structure is also reported.

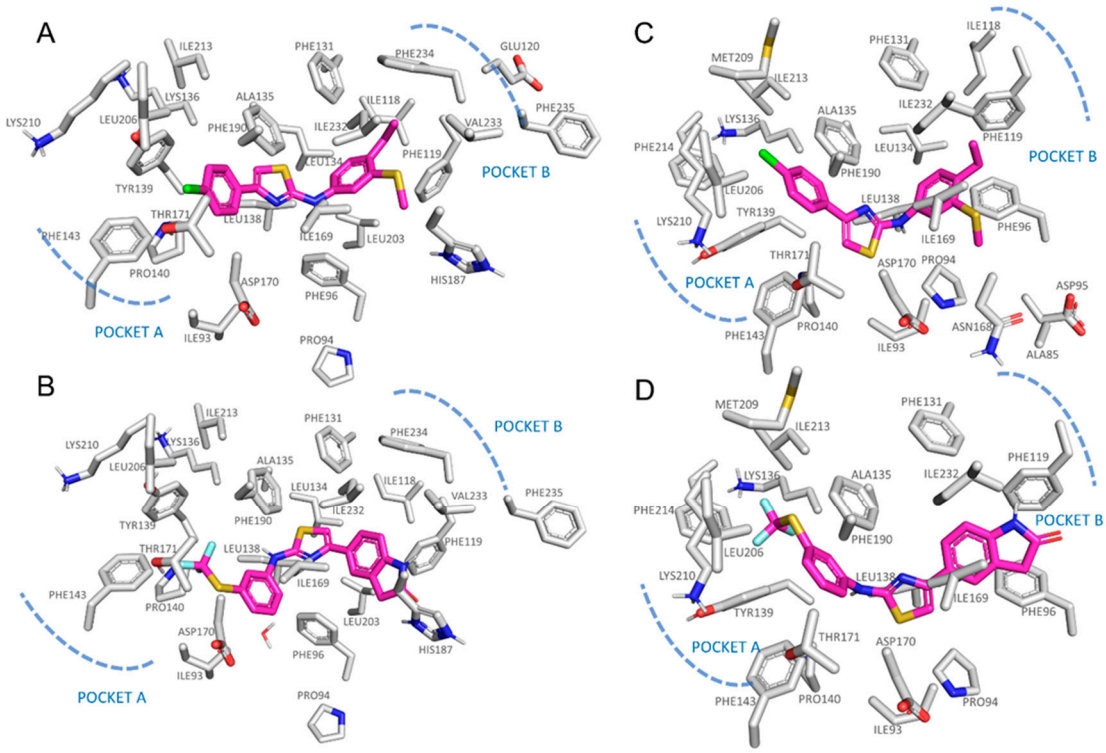


Figure S12. Docking positioning of compound **2a** (C atom, magenta) at the 4RMG (A) and at the 5MAT PDB code (C) binding site. The docking mode of the analogue **6a** (taken as representative of the most related analogues of YM-08 herein described) at the 4RMG (B) and at the 5MAT PDB code (D) binding site is also reported.

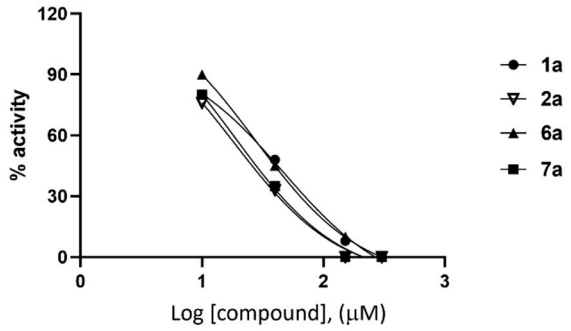


Figure S13. Concentration-response plots of the putative SIRT2 inhibitors, tested on SIRT2 recombinant protein. Data are plotted as % activity vs. inhibitor logarithmic micromolar concentration.

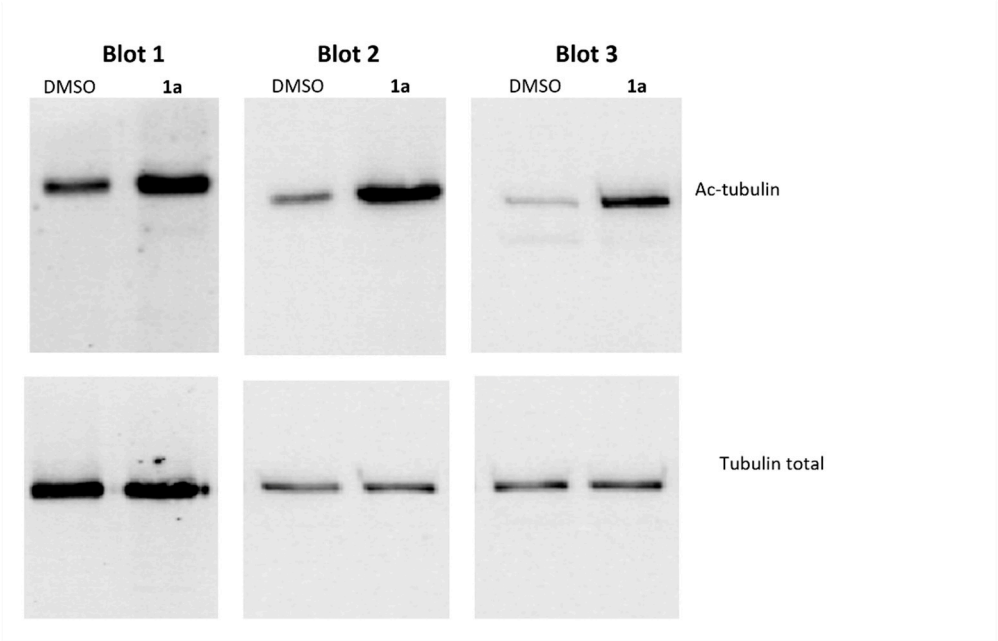
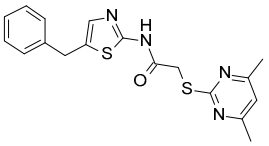
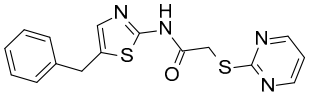
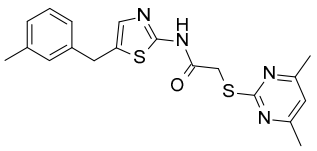
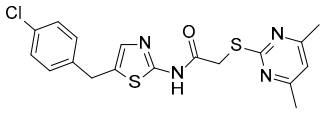
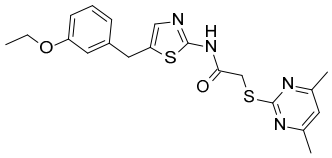
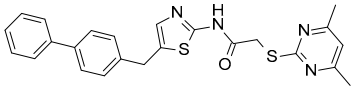
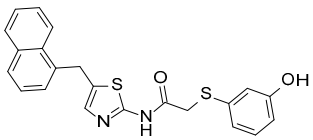
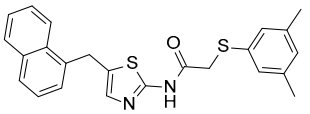
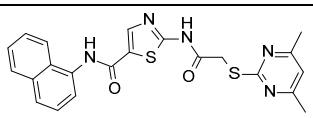
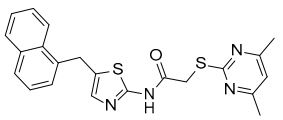
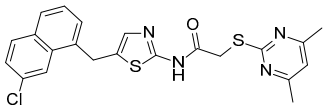
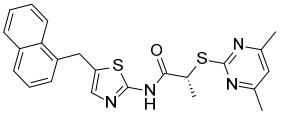
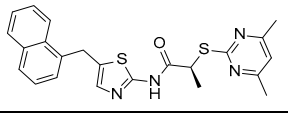


Figure S14. Compound **1a** increase α-tubulin acetylation in cultured cells. Cells were incubated with 10 μM compound **1a**, or the respective amount of vehicle DMSO, and used for protein lysate generation, and total and acetylated α-tubulin levels were detected by Immunoblotting. The three performed Western blot analysis are shown.

Table S1. Chemical structure and SIRT2 inhibitory ability featured by compounds **1**-**26** (as SirReal2 analogues) [24].

Compound	Chemical Structure	IC_{50} (μM)
1		3.75
2		16.8
3		1.64
4		3.40
5		1.33
6		164.5
7		143
8		207
9		33
10 (SirReal2)		0.44
11		0.18
12		9.77
13		0.26

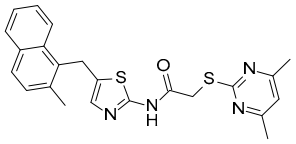
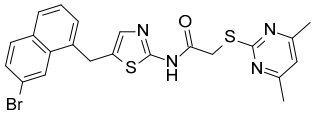
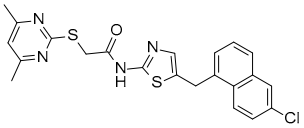
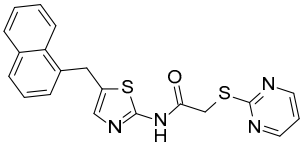
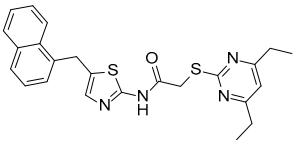
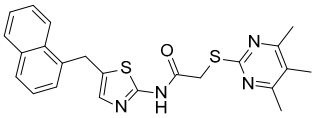
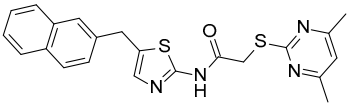
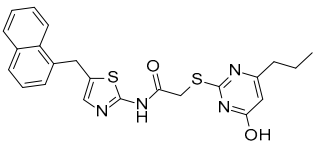
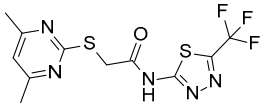
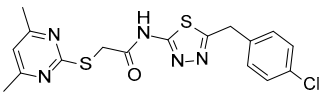
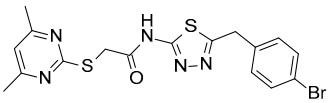
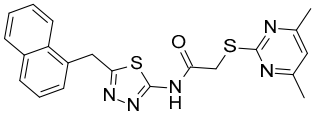
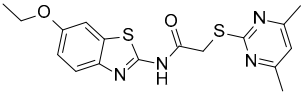
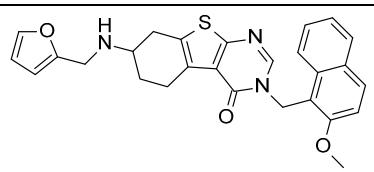
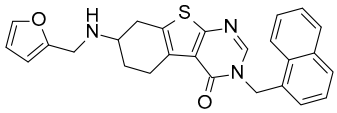
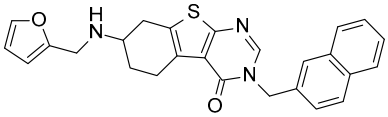
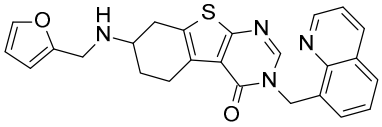
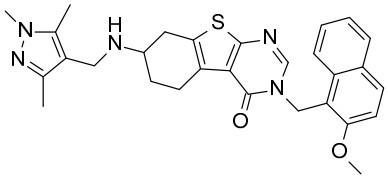
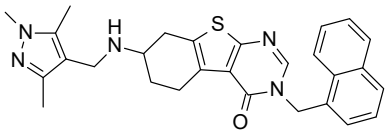
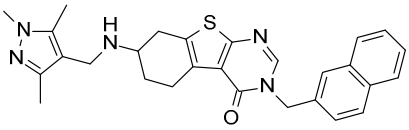
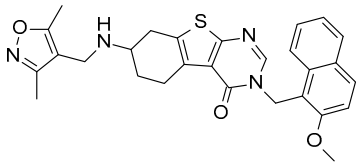
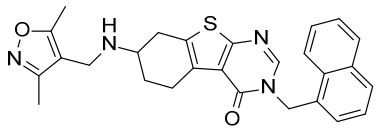
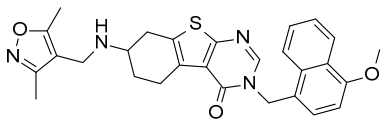
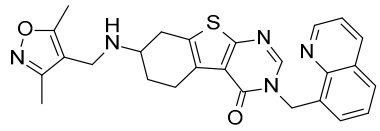
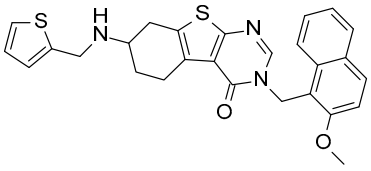
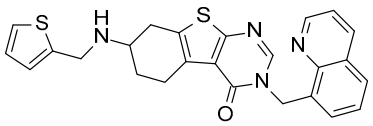
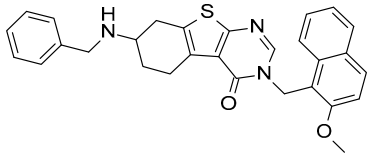
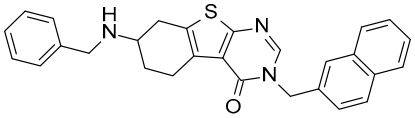
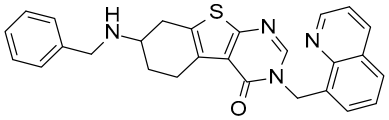
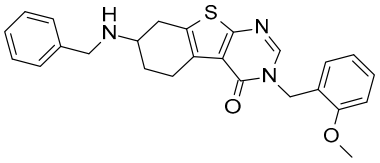
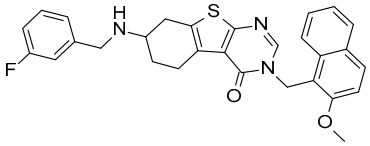
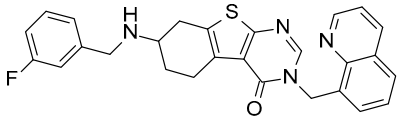
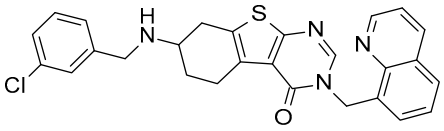
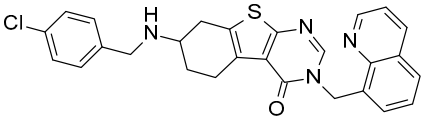
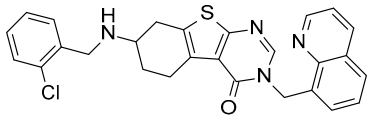
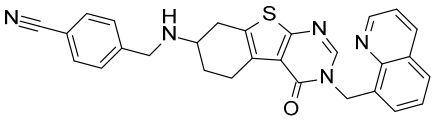
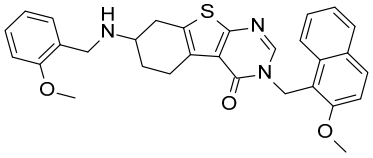
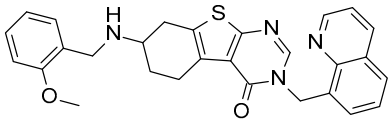
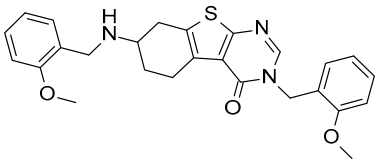
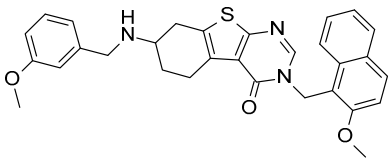
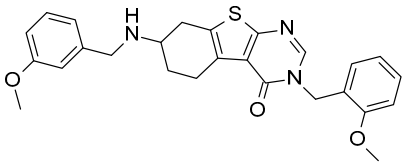
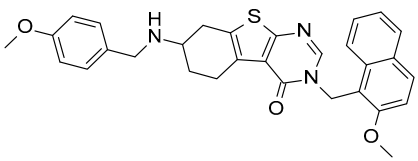
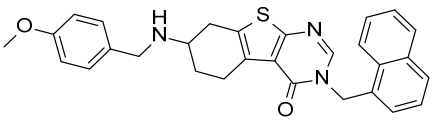
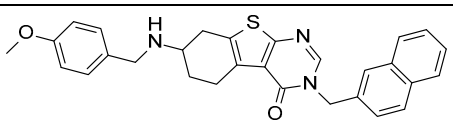
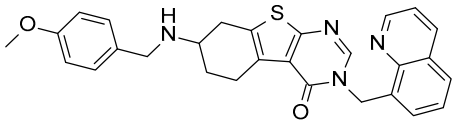
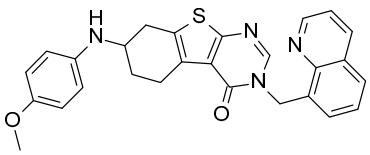
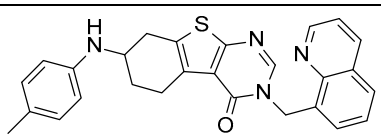
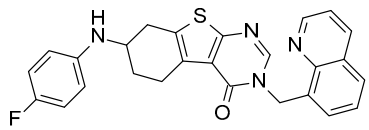
14		0.31
15		0.21
16		0.48
17		2.34
18		45.6
19		15.0
20		65
21		127.2
22		502.8
23		30.9
24		167.7
25		1.89
26		207

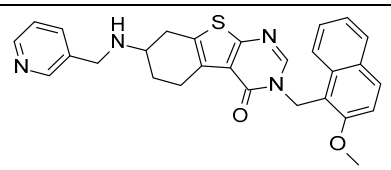
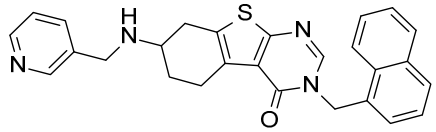
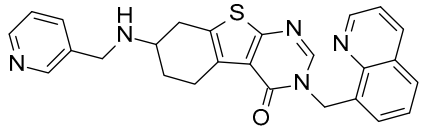
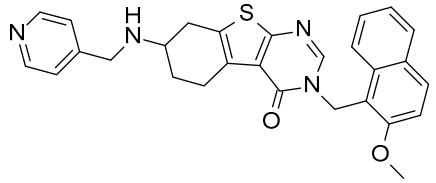
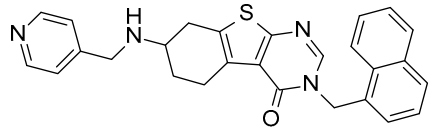
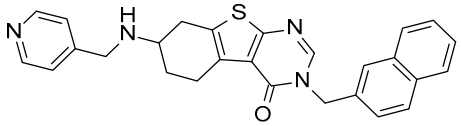
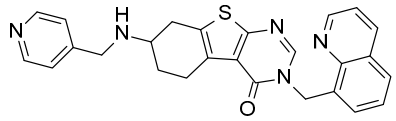
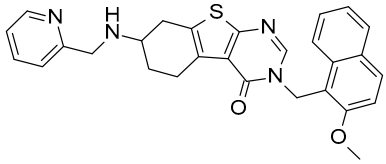
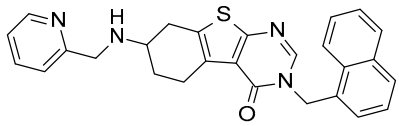
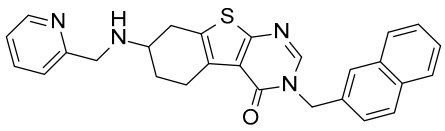
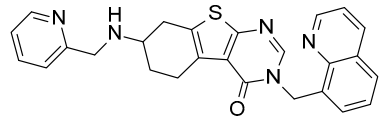
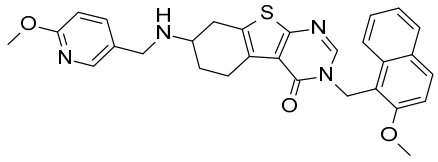
Table S2. Chemical structure and SIRT2 inhibitory ability featured by compounds **27-111** [25].

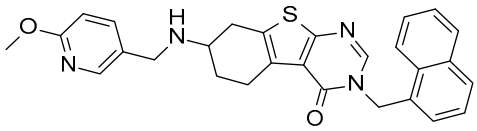
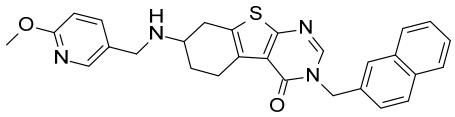
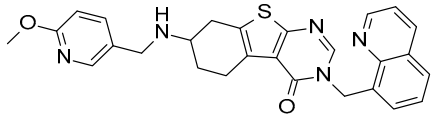
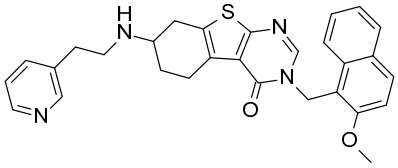
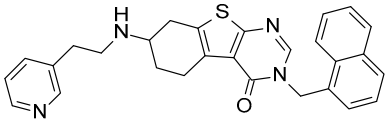
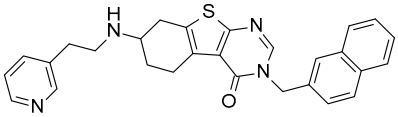
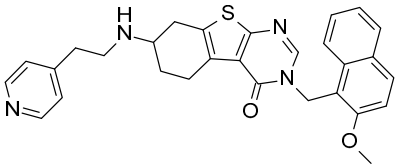
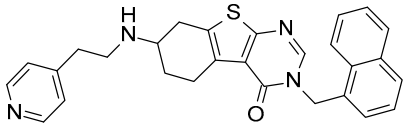
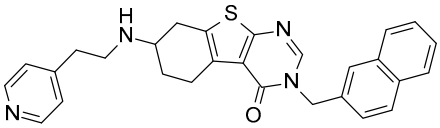
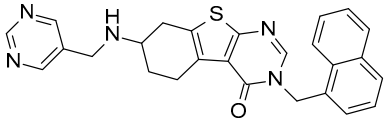
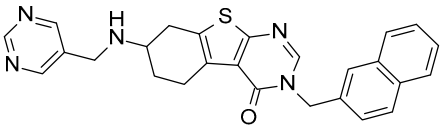
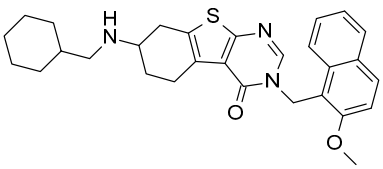
Compound	Chemical Structure	IC_{50} (μM)

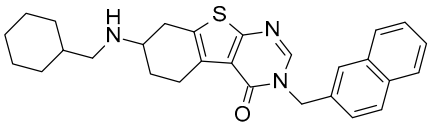
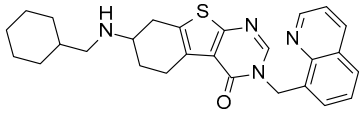
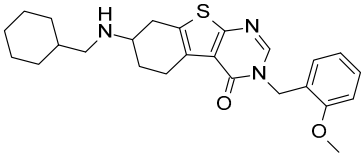
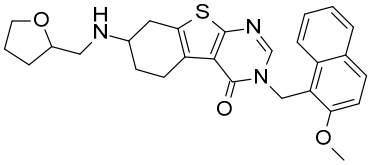
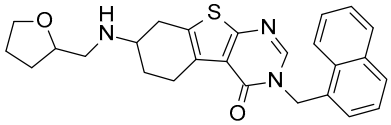
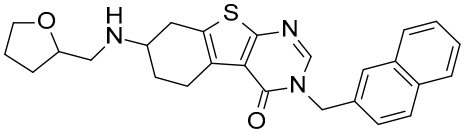
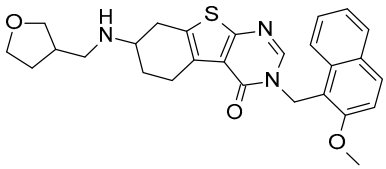
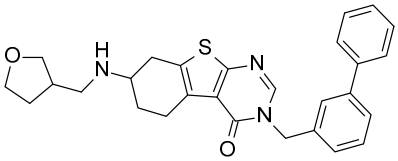
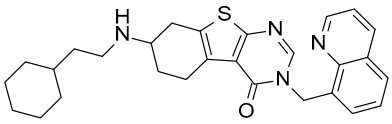
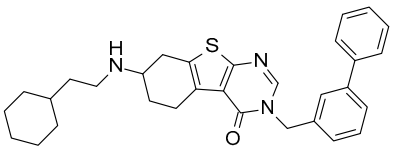
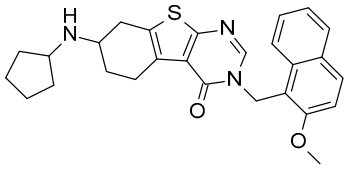
27		5.24
28		7.61
29		11.68
30		4.16
31		5.11
32		4.20
33		7.43
34		4.00
35		1.85
36		0.58
37		6.94
38		6.03

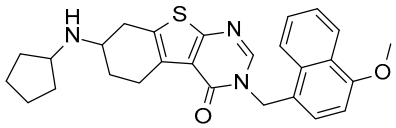
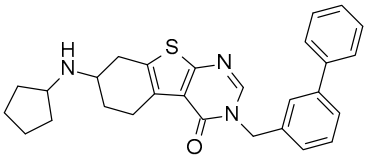
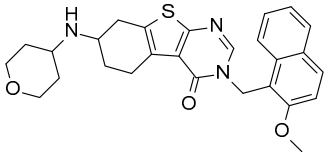
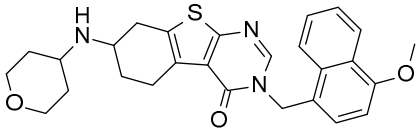
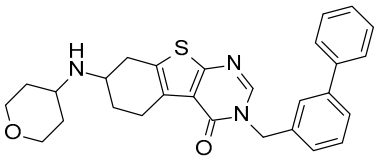
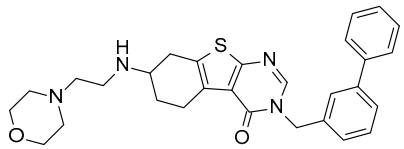
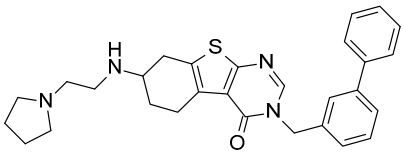
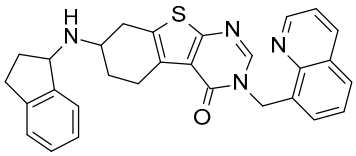
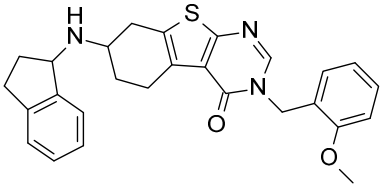
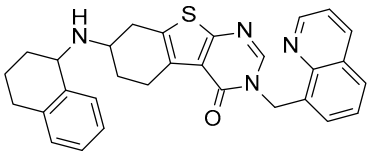
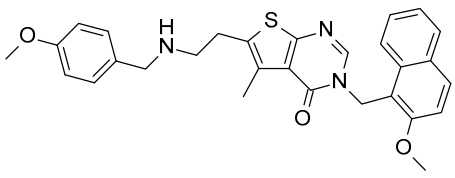
39		2.56
40		21.10
41		5.45
42		2.50
43		10.42
44		4.07
45		1.72
46		2.84
47		1.27
48		3.80
49		0.39
50		2.24

51		4.22
52		5.61
53		9.59
54		1.90
55		13.40
56		0.65
57		3.2
58		3.82
59		1.83
60		2.48
61		4.25
62		0.97

63		1.45
64		2.99
65		2.92
66		1.20
67		3.58
68		3.14
69		3.68
70		3.12
71		7.68
72		8.67
73		2.61
74		1.9

75		7.59
76		10.17
77		2.65
78		10.31
79		9.57
80		8.68
81		2.75
82		5.79
83		9.60
84		6.45
85		5.30
86		1.65

87		5.53
88		2.43
89		9.18
90		1.90
91		12.48
92		13.14
93		6.03
94		2.58
95		5.85
96		3.74
97		1.18

98		0.73
99		1.52
100		1.11
101		5.06
102		1.74
103		3.14
104		3.78
105		3.09
106		16.32
107		5.49
108		3.36

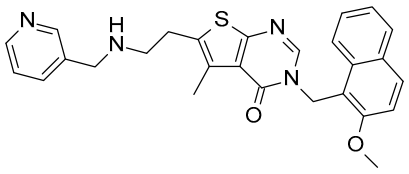
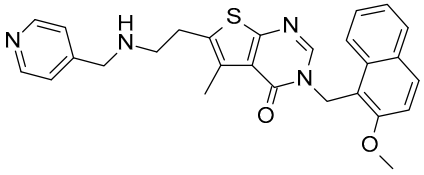
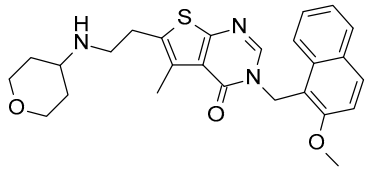
109		2.15
110		2.93
111		8.15

Table S3. Chemical structure and SIRT2 inhibitory ability featured by compounds **112-116** ([26].

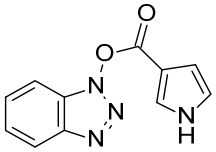
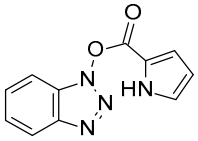
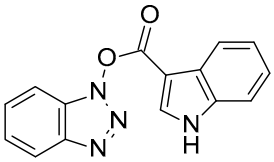
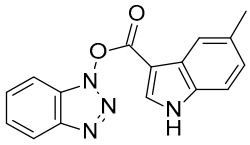
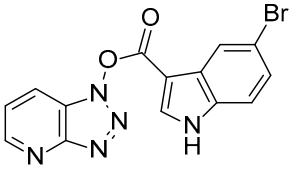
Compound	Chemical Structure	IC_{50} (μM)
112		56.6
113		42.7
114		14.3
115		74.0
116		77.1

Table S4. Five top scored re-docking positioning of the 4RMG and 5MAT co-crystallized ligands at the corresponding experimental data, based on the LeadIT and MOE software (see material and method section for details). The predicted ΔG value of each protein-ligand complex has been reported.

	LeadIT re-docking	**MOE re-docking**

SIRT2 co-crystallized inhibitor	**4RMG** Binding Affinity Energy **(**kJ/mol)	**5MAT** Binding Affinity Energy (kJ/mol)	**4RMG** Binding Affinity Energy (kcal/mol)	**5MAT** Binding Affinity Energy (kcal/mol)
4RMG ligand pose 1	-25.9191	-	-10,3013	-
4RMG ligand pose 2	-25.7311	-	-9,94133	-
4RMG ligand pose 3	-24.9027	-	-9,62434	-
4RMG ligand pose 4	-24.8213	-	-9,55069	-
4RMG ligand pose 5	-24.2870	-	-9,52854	-
5MAT ligand pose 1	-	-26.1502	-	-13,602593
5MAT ligand pose 2	-	-24.6139	-	-13,588899
5MAT ligand pose 3	-	-22.7001	-	-13,042794
5MAT ligand pose 4	-	-21.7195	-	-12,688121
5MAT ligand pose 5	-	-21.6132	-	-12,586191

Table S5. Ten top scored docking positioning of SirReal2 (**10**) and of the related analogues (**1**-**26**) at the 4RMG PDB code (MOE software). The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	**S**	**E_conf**	**E_place**	**E_score1**	**E_refine**	**E_score2**
1	-9.6736	-33.1359	-22.7067	-8.4093	-8.3120	-9.6736
1	-9.0728	-47.8155	-23.2848	-9.8777	-26.1328	-9.0728
1	-8.9807	-44.9250	-33.6730	-10.8258	-23.7357	-8.9807
1	-8.9344	-41.2470	-28.1481	-7.9972	-23.2107	-8.9344
1	-8.6167	-48.5433	-27.4762	-7.8290	-29.6131	-8.6167
1	-7.9467	-42.3455	-25.6510	-9.6144	-5.7398	-7.9467
1	-7.8165	-48.3387	-18.7807	-9.1360	-19.5343	-7.8165
1	-7.7813	-39.4436	-18.4346	-8.5048	-13.8324	-7.7813
1	-7.3651	-49.1032	-20.0311	-8.1013	-15.2034	-7.3651
1	-7.2839	-47.3109	-21.0416	-8.2842	-16.6757	-7.2839
2	-8.1144	-50.7917	-25.3729	-9.3513	-26.1691	-8.1144
2	-8.0771	-39.1846	-19.6832	-9.5829	-7.5630	-8.0771
2	-7.4749	-51.0584	-17.8084	-8.7937	-29.0829	-7.4749
2	-7.4748	-51.0620	-32.6211	-8.6946	-29.0796	-7.4748
2	-7.3055	-47.1204	-18.6753	-8.4466	-17.7960	-7.3055
2	-7.1458	-43.6664	-22.3148	-8.8797	-13.1793	-7.1458
2	-7.0571	-50.5811	-21.4530	-8.5875	-17.2021	-7.0571

2	-6.9682	-48.3567	-33.7238	-11.2191	-12.2058	-6.9682
2	-6.9432	-45.4379	-22.9673	-9.5667	-3.6194	-6.9432
2	-6.9389	-45.7644	-21.3027	-9.6643	-14.8018	-6.9389
3	-10.5878	-18.9457	-31.4863	-10.1438	7.0218	-10.5878
3	-9.5626	-42.2045	-20.2995	-8.6613	-19.2315	-9.5626
3	-9.3506	-38.9212	-17.5137	-8.2308	-24.7261	-9.3506
3	-9.3231	-42.5655	-26.5405	-9.0895	-25.1933	-9.3231
3	-9.0031	-45.2524	-38.7712	-11.1381	-28.2734	-9.0031
3	-8.8932	-38.5696	-30.9905	-9.4520	-11.4654	-8.8932
3	-8.4852	-32.0124	-21.0520	-7.9074	-2.9656	-8.4852
3	-7.9748	-49.6609	-24.3158	-8.8533	-20.5586	-7.9748
3	-7.7630	-45.5956	-24.9819	-9.4224	-17.9371	-7.7630
3	-7.6503	-29.1979	-25.3221	-8.5440	-3.4975	-7.6503
4	-9.6325	-39.6040	-30.8450	-9.4190	-18.6845	-9.6325
4	-8.8963	-38.9960	-29.0621	-8.7822	-22.9874	-8.8963
4	-8.2922	-33.7673	-22.1036	-9.7895	13.6997	-8.2922
4	-8.2484	-45.4510	-24.6903	-8.9422	-12.4736	-8.2484
4	-8.2292	-53.1790	-24.0905	-9.8634	-17.0082	-8.2292
4	-8.2195	-37.3738	-19.3905	-8.6728	-17.8328	-8.2195
4	-8.1213	-45.5405	-27.4410	-9.0916	-8.7742	-8.1213
4	-8.0147	-51.0825	-24.6135	-9.6065	-13.9583	-8.0147
4	-8.0053	-42.8437	-23.6788	-9.1258	-4.9787	-8.0053
4	-7.8601	-44.9619	-29.9113	-9.6261	-14.8783	-7.8601
5	-8.9024	6.7965	-21.2115	-8.9830	6.9895	-8.9024
5	-8.6758	-36.1406	-31.6933	-8.8887	-15.4207	-8.6758
5	-7.7182	-35.3433	-21.9398	-8.5505	-14.9504	-7.7182
5	-7.7043	-43.6640	-24.9165	-8.8838	-18.8552	-7.7043
5	-7.6287	-40.6700	-19.4641	-7.9739	-13.8240	-7.6287
5	-7.5847	-38.9270	-25.1764	-8.7668	-25.6075	-7.5847
5	-7.1810	-38.1658	-25.1428	-8.2855	-25.1012	-7.1810
5	-7.1136	-38.9045	-25.9766	-9.9756	-16.3470	-7.1136
5	-7.1081	-47.6091	-25.5370	-8.9308	-15.3825	-7.1081
5	-6.8486	-43.6880	-15.8370	-8.5546	-22.7091	-6.8486
6	-10.2206	-18.3512	-20.8563	-8.0137	-29.2764	-10.2206
6	-10.1788	-14.6657	-19.3076	-8.8039	-25.0414	-10.1788
6	-10.1258	-27.5984	-19.4824	-8.3457	-20.2695	-10.1258
6	-10.1151	-20.2532	-23.2904	-7.7866	-27.3793	-10.1151
6	-9.9975	-7.3810	-16.8774	-9.4954	51.6183	-9.9975
6	-9.5889	-17.8983	-20.4954	-7.9549	-20.1281	-9.5889
6	-9.4249	-19.6337	-23.0076	-8.3819	-19.3121	-9.4249
6	-9.3384	-2.3643	-24.5323	-9.1810	-11.1050	-9.3384
6	-9.2658	-17.5509	-23.8552	-11.6104	-14.9267	-9.2658
6	-9.1761	-14.7681	-24.0717	-7.6903	-17.0571	-9.1761
7	-10.6856	17.3195	-27.4333	-8.9435	-18.4120	-10.6856
7	-10.6822	34.8136	-23.6160	-8.6588	10.1869	-10.6822
7	-10.5591	21.4632	-36.2113	-8.8634	-14.0017	-10.5591

7	-10.3860	28.1219	-22.6676	-8.7134	9.1169	-10.3860
7	-10.2416	14.3181	-32.8900	-9.6292	-4.3309	-10.2416
7	-10.1546	24.4966	-36.0244	-11.1829	-13.7041	-10.1546
7	-10.0031	17.4580	-33.5266	-8.8884	8.2728	-10.0031
7	-9.9702	16.7595	-28.3186	-9.1978	-14.5834	-9.9702
7	-9.6948	9.7073	-19.7065	-9.4492	-16.3879	-9.6948
7	-9.3994	20.0443	-27.0758	-9.0775	-23.4827	-9.3994
8	-11.7580	40.0966	-29.1720	-7.8238	-1.2025	-11.7580
8	-11.6980	42.5667	-31.3180	-7.8524	-13.9896	-11.6980
8	-11.5612	41.7446	-28.0426	-9.0847	-6.9450	-11.5612
8	-10.9653	38.1951	-32.7198	-8.4754	-14.6462	-10.9653
8	-10.4682	41.3565	-26.8452	-8.1665	-15.6221	-10.4682
8	-10.3436	41.5951	-28.2643	-9.8387	3.7742	-10.3436
8	-10.2528	37.3372	-27.3794	-9.1686	-8.8902	-10.2528
8	-10.0720	59.8457	-28.9742	-7.6376	17.5465	-10.0720
8	-9.9405	42.9009	-14.2820	-8.5186	-21.5935	-9.9405
8	-9.5348	49.6718	-24.1953	-8.9034	13.8869	-9.5348
9	-8.2959	-51.1083	-17.5034	-7.6183	-21.9051	-8.2959
9	-8.2330	-44.7898	-15.3641	-7.4359	-3.5915	-8.2330
9	-8.2169	-39.4007	-20.7057	-10.2535	-6.6024	-8.2169
9	-8.1991	-57.5728	-13.9010	-9.7210	-15.5623	-8.1991
9	-8.1117	-52.1246	-21.2162	-7.5788	-25.9125	-8.1117
9	-7.8609	-54.2362	-17.8920	-9.9149	-24.2803	-7.8609
9	-7.8525	-47.1343	-23.1347	-7.8417	-21.8377	-7.8525
9	-7.8255	-54.9607	-28.4475	-10.5584	-28.8390	-7.8255
9	-7.7479	-53.5500	-18.6650	-9.8284	7.0213	-7.7479
9	-7.4265	-50.0922	-20.2700	-7.4052	-22.1531	-7.4265
10	-10.3013	-24.7614	-34.0070	-9.0498	-25.9820	-10.3013
10	-9.9413	-30.5955	-27.3615	-9.0646	-9.6791	-9.9413
10	-9.6243	-32.5099	-23.1356	-9.6876	-24.2546	-9.6243
10	-9.5507	-24.9688	-35.1714	-8.2626	-8.1118	-9.5507
10	-9.5285	-28.3704	-27.7602	-9.4189	-24.8285	-9.5285
10	-9.3648	-18.8765	-25.0676	-7.7735	-7.3949	-9.3648
10	-9.1062	-26.4878	-20.6396	-7.5317	-17.7843	-9.1062
10	-8.8971	-33.5893	-31.8139	-8.7369	-3.9934	-8.8971
10	-8.7971	-27.0707	-30.9790	-8.4944	-8.3836	-8.7971
10	-8.6063	-28.5688	-22.6237	-9.0123	-2.4891	-8.6063
11	-10.6562	-28.6143	-30.2226	-10.0730	-27.0208	-10.6562
11	-10.4639	-32.6675	-34.6832	-8.2885	-25.0037	-10.4639
11	-10.3029	-21.6914	-16.9705	-7.7928	-17.4857	-10.3029
11	-10.1306	-33.2248	-24.6398	-7.9922	-25.0305	-10.1306
11	-9.6599	-36.0355	-24.0793	-8.0476	-12.0786	-9.6599
11	-9.6021	-26.2137	-28.9337	-10.1389	-10.5818	-9.6021
11	-9.3068	-29.2502	-28.9363	-8.0988	22.9821	-9.3068
11	-9.2230	-10.1949	-22.7890	-8.5630	34.6320	-9.2230
11	-8.8541	-23.0532	-33.5683	-8.6387	10.6831	-8.8541

11	-8.6680	-4.6168	-18.9917	-7.9516	46.3885	-8.6680
12	-10.4594	-20.3199	-29.2042	-7.5386	-16.1867	-10.4594
12	-10.2066	-23.6985	-18.6446	-7.4939	-23.7270	-10.2066
12	-10.1864	-14.3867	-33.4577	-8.2143	-15.5228	-10.1864
12	-10.1074	5.0938	-30.5640	-8.6197	-16.7069	-10.1074
12	-9.9647	-20.5903	-42.4968	-10.2617	-15.0006	-9.9647
12	-9.6585	-8.4244	-38.5863	-7.5063	7.8775	-9.6585
12	-9.5658	6.0184	-25.9751	-9.1940	4.5910	-9.5658
12	-9.2844	-2.6998	-25.6502	-7.7236	10.8821	-9.2844
12	-9.2085	-14.7410	-29.3802	-9.5225	8.3429	-9.2085
12	-9.1918	-7.4412	-38.2670	-9.2751	-0.6775	-9.1918
13	-10.2202	-4.9189	-30.9119	-7.5871	-7.2494	-10.2202
13	-9.3077	-6.8987	-23.2635	-7.0652	13.2543	-9.3077
13	-9.2865	-15.4676	-22.0314	-7.0299	-8.6863	-9.2865
13	-9.1559	-6.8228	-27.6958	-7.1761	13.0956	-9.1559
13	-9.1208	-10.8410	-30.6928	-8.3212	-23.0170	-9.1208
13	-9.0966	-12.1160	-27.5214	-6.8693	6.5325	-9.0966
13	-8.7387	-20.5482	-18.4107	-7.0563	-17.3811	-8.7387
13	-8.6515	-9.4790	-38.0645	-8.9112	-5.0422	-8.6515
13	-8.5797	-1.5751	-22.5957	-8.9429	11.9075	-8.5797
13	-8.4716	-12.0293	-12.9102	-6.8801	70.4553	-8.4716
14	-10.9063	-26.4287	-23.8714	-8.2233	-28.9128	-10.9063
14	-10.7691	-17.6250	-31.2709	-10.0769	-24.6988	-10.7691
14	-10.6037	-15.7013	-34.5166	-10.0945	-25.2533	-10.6037
14	-10.5381	-13.1540	-36.5153	-11.1021	-18.3544	-10.5381
14	-10.3331	-19.0223	-45.5135	-8.8616	-10.1119	-10.3331
14	-10.0489	-23.5580	-31.9473	-10.9461	-7.1689	-10.0489
14	-9.8798	-13.3115	-30.7720	-9.6762	-11.8429	-9.8798
14	-9.6127	-18.0083	-34.3563	-7.8220	-12.8450	-9.6127
14	-9.5808	-15.6977	-27.5591	-9.4734	-18.5116	-9.5808
14	-9.5779	-18.1302	-29.9098	-7.2881	-16.4635	-9.5779
15	-10.9934	-31.4326	-35.4511	-8.8395	-23.6716	-10.9934
15	-10.6488	-27.4007	-32.7834	-8.0095	-27.4353	-10.6488
15	-10.0166	-26.9978	-25.3344	-9.0240	26.9721	-10.0166
15	-9.9849	-27.5636	-28.3650	-12.2052	-16.1783	-9.9849
15	-9.9638	-16.6293	-30.1041	-7.5196	-19.0977	-9.9638
15	-9.7594	-29.4214	-22.8583	-7.2011	-17.4539	-9.7594
15	-9.4975	-23.1519	-28.0405	-10.2808	-3.8178	-9.4975
15	-9.3298	-28.7265	-31.8064	-7.0323	0.0171	-9.3298
15	-9.0968	-16.9413	-32.0815	-8.8226	12.2085	-9.0968
15	-9.0501	-13.6634	-25.6612	-8.1658	40.9827	-9.0501
16	-10.6166	-25.9804	-37.6326	-9.0688	-12.3348	-10.6166
16	-10.1895	-33.9157	-38.8749	-9.7439	-33.1806	-10.1895
16	-9.9181	-24.0170	-30.0355	-8.0552	-18.1332	-9.9181
16	-9.4597	-27.6432	-26.4770	-7.9959	-22.0286	-9.4597
16	-9.4071	-21.7246	-23.3507	-8.5213	6.5402	-9.4071

16	-9.3512	-15.3919	-16.8763	-8.4363	-13.6957	-9.3512
16	-9.2732	-20.0033	-22.0248	-8.1488	-13.4452	-9.2732
16	-9.0266	-32.3940	-20.4978	-8.0440	-19.4790	-9.0266
16	-8.8986	-29.4664	-20.0783	-8.3610	-20.4193	-8.8986
16	-8.8841	-17.0353	-29.4641	-8.4029	13.5789	-8.8841
17	-9.1257	-34.3286	-25.1491	-8.5305	-11.0866	-9.1257
17	-9.0535	-32.0351	-38.1564	-11.2084	-25.2556	-9.0535
17	-8.9872	-35.3704	-26.4558	-10.7152	-21.7535	-8.9872
17	-8.8453	-35.0594	-34.8193	-9.1521	-31.2273	-8.8453
17	-8.8197	-25.2356	-35.4336	-9.2441	-20.6142	-8.8197
17	-8.7712	-29.3959	-29.5622	-9.3473	-14.1821	-8.7712
17	-8.7319	-15.5646	-29.5904	-10.1696	-0.7843	-8.7319
17	-8.6685	-28.9091	-39.3241	-10.0620	16.0342	-8.6685
17	-8.4218	-35.4225	-27.6388	-9.1644	-14.6738	-8.4218
17	-8.3903	-29.5489	-23.4110	-9.1690	-25.7979	-8.3903
18	-10.9132	-28.8382	-29.2158	-9.0911	-23.4994	-10.9132
18	-10.7645	18.6252	-29.5605	-9.5664	40.6146	-10.7645
18	-10.7488	-15.5522	-36.4968	-8.7999	4.2133	-10.7488
18	-10.3054	-31.6483	-16.6813	-7.0013	-9.1165	-10.3054
18	-10.2512	-31.4450	-31.6273	-8.0424	-10.4274	-10.2512
18	-10.0207	-29.2022	-21.0523	-7.8890	-17.7643	-10.0207
18	-9.7634	-25.7046	-20.5480	-8.4192	-18.0784	-9.7634
18	-9.6922	-24.0033	-20.8684	-8.0622	-4.4832	-9.6922
18	-9.6305	-20.5643	-27.1845	-8.6961	-8.8487	-9.6305
18	-9.5857	-28.5568	-23.2858	-7.4273	-7.0697	-9.5857
19	-10.5465	-21.4047	-19.6544	-7.3632	-24.8632	-10.5465
19	-10.3235	-15.3884	-24.6740	-9.1857	-11.7835	-10.3235
19	-10.3089	-19.0376	-38.2177	-7.2021	-8.0437	-10.3089
19	-10.0874	-26.4603	-24.7009	-9.7398	-24.5458	-10.0874
19	-10.0660	-22.2702	-31.1315	-7.5225	-16.6384	-10.0660
19	-9.5875	-18.0126	-28.1411	-12.1383	-9.5315	-9.5875
19	-9.4035	-11.7819	-24.8886	-7.6191	18.9914	-9.4035
19	-9.1588	-10.3560	-33.1363	-7.5553	-2.3734	-9.1588
19	-8.9529	-12.5664	-22.2521	-9.1346	-6.0371	-8.9529
19	-8.7488	-17.6764	-25.6652	-7.4175	-19.3158	-8.7488
20	-9.8997	-23.2073	-38.4303	-10.1196	-22.4494	-9.8997
20	-9.8335	-31.9465	-21.3469	-8.9687	-20.5395	-9.8335
20	-9.7847	-35.4399	-25.3276	-8.2725	-8.5359	-9.7847
20	-9.7056	-35.4825	-24.4275	-9.2452	-15.0068	-9.7056
20	-9.6922	-36.1153	-25.5113	-9.4894	3.0631	-9.6922
20	-9.5823	-33.9328	-29.4496	-8.2530	-29.6905	-9.5823
20	-9.1916	-2.2633	-26.7092	-8.6151	-8.2384	-9.1916
20	-9.0225	-7.9301	-28.2626	-9.9367	11.8937	-9.0225
20	-9.0159	5.6404	-31.1558	-8.9310	7.7178	-9.0159
20	-8.9593	-27.5656	-29.4755	-8.6201	-9.2410	-8.9593
21	-10.3466	-74.5313	-26.5733	-7.8552	1.1872	-10.3466

21	-10.1784	-65.6338	-29.5907	-7.8150	-9.4752	-10.1784
21	-10.1400	-73.8693	-17.7255	-7.2412	-13.5851	-10.1400
21	-9.8201	-71.4550	-26.7174	-10.4892	-16.9526	-9.8201
21	-9.6702	-75.3307	-28.0195	-8.3123	-13.0244	-9.6702
21	-9.6097	-74.1524	-22.4535	-9.4349	-25.2809	-9.6097
21	-9.2538	-59.2648	-20.9093	-7.6330	-1.7428	-9.2538
21	-9.0444	-76.8688	-21.0809	-10.5278	-12.8067	-9.0444
21	-8.8755	-70.9223	-34.8721	-9.2474	11.8864	-8.8755
21	-8.8673	-74.1085	-22.1266	-7.0535	-15.2793	-8.8673
22	-6.5829	-45.2019	-24.1186	-11.0163	-21.3166	-6.5829
22	-6.2949	-39.1498	-29.4145	-9.8431	-18.5776	-6.2949
22	-6.2614	-41.2986	-24.1521	-10.3302	-22.6898	-6.2614
22	-6.1403	-39.8166	-14.3284	-9.6674	-8.9823	-6.1403
22	-6.0049	-35.6872	-23.6061	-11.1338	-15.8810	-6.0049
22	-5.8925	-36.0508	-22.5130	-9.6932	-9.9161	-5.8925
22	-5.7120	-38.8513	-17.1319	-9.4724	-16.8881	-5.7120
22	-5.6929	-39.0247	-21.8272	-9.2551	-5.0394	-5.6929
22	-5.5749	-28.8211	-19.6026	-10.2740	7.1840	-5.5749
22	-5.4436	-36.3360	-15.2979	-9.1857	5.5821	-5.4436
23	-7.9453	-32.5525	-29.2791	-10.1585	-21.6102	-7.9453
23	-7.8743	-38.8735	-21.0039	-9.1751	-6.9734	-7.8743
23	-7.8520	-47.6927	-25.3313	-10.1763	-19.4091	-7.8520
23	-7.7916	-44.5202	-19.7182	-10.0078	-6.8589	-7.7916
23	-7.6041	-38.2136	-18.8017	-9.3837	-10.6959	-7.6041
23	-7.1665	-25.0813	-32.5311	-10.5645	-7.9834	-7.1665
23	-6.8596	-41.3360	-21.4407	-8.9792	-20.0473	-6.8596
23	-6.8152	-31.4049	-30.8381	-10.5613	-17.1668	-6.8152
23	-6.5691	-36.5193	-24.6843	-9.2312	-15.9135	-6.5691
23	-6.5479	-37.8798	-20.8198	-9.5899	-3.9509	-6.5479
24	-8.2257	-37.3468	-21.3838	-8.9584	-10.4321	-8.2257
24	-7.9658	-46.7672	-25.2297	-10.1278	-16.4499	-7.9658
24	-7.9354	-37.1187	-21.0829	-9.4778	-3.1675	-7.9354
24	-7.8835	-31.9361	-29.3573	-10.4310	-21.6342	-7.8835
24	-7.8481	-43.8213	-19.4112	-10.0983	-3.4339	-7.8481
24	-7.6514	-43.1165	-25.8889	-9.1070	-14.5444	-7.6514
24	-7.1150	-40.0278	-20.7802	-8.9239	-18.7713	-7.1150
24	-7.1086	-23.9030	-27.9680	-9.5643	-8.3010	-7.1086
24	-6.9847	-40.2804	-19.9925	-10.2596	-19.3855	-6.9847
24	-6.8436	-30.8219	-30.7609	-10.6322	-17.2149	-6.8436
25	-9.8010	-0.2864	-25.3180	-8.9122	1.6786	-9.8010
25	-9.5036	48.0792	-27.6488	-8.3412	13.2863	-9.5036
25	-9.4333	-23.8532	-21.7237	-8.0486	-27.9726	-9.4333
25	-9.2903	-22.9323	-34.9015	-9.2897	-25.1079	-9.2903
25	-9.1747	-15.1628	-25.4830	-9.4153	-19.4816	-9.1747
25	-8.8014	-24.9057	-27.7189	-8.5957	-25.2209	-8.8014
25	-8.6933	-22.0933	-23.5723	-8.6786	-20.8280	-8.6933

25	-8.6250	-22.1995	-28.8001	-9.0128	-18.5694	-8.6250
25	-8.4322	-20.3900	-31.6146	-8.4239	-7.7097	-8.4322
25	-8.2039	-26.0399	-30.1917	-10.8389	-15.9871	-8.2039
26	-8.4188	-48.4585	-32.6319	-9.2593	-12.0207	-8.4188
26	-8.3322	-51.8575	-29.8560	-9.2534	-10.6359	-8.3322
26	-8.1416	-38.1972	-28.0455	-9.3176	-6.3073	-8.1416
26	-7.5334	-48.7150	-27.7979	-9.0693	-18.6052	-7.5334
26	-7.5296	-45.4954	-26.8853	-8.7970	-6.1994	-7.5296
26	-7.4183	-29.0929	-23.5025	-9.0357	14.3720	-7.4183
26	-7.1307	-45.2895	-18.2753	-9.5477	-11.6866	-7.1307
26	-6.8220	-52.5688	-20.7508	-8.6127	-26.3605	-6.8220
26	-6.8126	-52.7980	-23.9842	-8.9408	-24.1386	-6.8126
26	-6.7481	-48.3484	-24.7800	-8.7916	-21.9452	-6.7481

Table S6. Ten top scored docking positioning of the 5MAT co-crystallized ligand (**36**) and of the related analogues (**27**-**111**) at the 5MAT PDB code (MOE software). The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
27	-13.8512	19.8990	-43.1961	-11.7123	-33.0118	-13.8512
27	-13.2111	14.3341	-47.6496	-13.2845	-49.7220	-13.2111
27	-13.0939	22.3950	-38.0595	-10.6986	-45.1665	-13.0939
27	-13.0310	23.0860	-40.7726	-9.5778	-36.0707	-13.0310
27	-12.8640	26.9085	-32.5700	-9.9519	-39.0048	-12.8640
27	-12.8452	22.9183	-40.1373	-12.6830	-11.0974	-12.8452
27	-12.7959	23.2919	-30.5397	-9.4822	-12.0560	-12.7959
27	-12.4992	15.0494	-41.6590	-12.4822	-46.9961	-12.4992
27	-12.4291	20.3228	-25.6230	-10.3228	-12.7027	-12.4291
27	-12.2688	47.6150	-35.3863	-9.5620	-19.7380	-12.2688
28	-13.7933	20.5136	-36.3695	-11.9576	-33.1795	-13.7933
28	-13.5993	23.7646	-34.3127	-10.2732	-31.9539	-13.5993
28	-13.2294	21.3097	-38.4485	-11.0205	-43.3686	-13.2294
28	-12.7786	16.0013	-41.6782	-10.2130	-50.6158	-12.7786
28	-12.6065	43.0109	-34.7978	-10.5834	-34.3015	-12.6065
28	-12.5922	27.5169	-36.9508	-10.9090	-22.2423	-12.5922
28	-12.4279	20.9377	-38.9122	-9.9867	-41.8661	-12.4279
28	-11.8322	21.6933	-34.8426	-12.5748	-38.1605	-11.8322
28	-11.1703	28.1473	-39.7805	-10.1053	-36.8209	-11.1703
28	-11.1669	28.1785	-39.2714	-10.0919	-36.8644	-11.1669
29	-13.5610	28.9188	-35.3942	-9.8132	-25.6281	-13.5610
29	-13.2728	21.7737	-37.3687	-9.8373	-33.9999	-13.2728
29	-13.1734	25.6240	-40.6709	-10.1765	-26.8896	-13.1734
29	-12.9733	15.2370	-47.3552	-12.5202	-37.1424	-12.9733
29	-12.8407	22.0143	-37.1096	-16.8381	-39.3378	-12.8407
29	-12.8074	17.1666	-36.4757	-10.9632	-20.0087	-12.8074
29	-12.7987	24.3451	-35.8327	-12.9319	-26.8087	-12.7987

29	-12.6550	20.4753	-50.8925	-13.1994	-26.8969	-12.6550
29	-12.5750	27.1464	-40.3263	-10.8245	-23.8529	-12.5750
29	-12.4757	22.0879	-38.8985	-10.7238	-26.6940	-12.4757
30	-12.8481	18.7634	-30.4731	-10.3969	-34.6136	-12.8481
30	-12.7308	30.2546	-42.4051	-10.7245	-29.0960	-12.7308
30	-12.7022	19.0084	-40.0123	-13.0794	-33.2987	-12.7022
30	-12.2533	12.1384	-34.0683	-10.2952	-49.3284	-12.2533
30	-11.4523	32.6988	-33.5936	-10.9802	-26.9011	-11.4523
30	-11.4246	14.3461	-45.0312	-10.6579	-43.0877	-11.4246
30	-11.3941	14.6740	-40.7159	-11.1659	-44.4056	-11.3941
30	-11.3395	37.7396	-29.8846	-10.4495	-26.8998	-11.3395
30	-11.2993	36.7691	-41.1554	-12.3046	-26.6708	-11.2993
30	-10.5868	44.5546	-33.7568	-10.1709	4.2797	-10.5868
31	-13.7665	-34.2014	-44.8527	-8.5284	-29.5514	-13.7665
31	-13.7433	-33.5328	-38.7338	-9.0976	-35.9491	-13.7433
31	-13.6748	-30.6335	-38.1154	-10.0175	-35.7954	-13.6748
31	-13.6614	-36.6577	-44.6026	-8.9577	-32.5031	-13.6614
31	-13.5418	-38.6822	-44.8596	-7.7302	-41.2775	-13.5418
31	-13.4707	-17.3477	-42.9367	-8.0465	-15.7683	-13.4707
31	-13.4185	-2.0717	-33.6429	-9.6503	-11.8363	-13.4185
31	-13.1154	-35.0731	-38.6715	-9.5445	-14.7303	-13.1154
31	-12.4509	-29.4201	-44.5714	-10.5895	-32.7545	-12.4509
31	-11.9655	-29.8461	-43.1771	-10.4825	-7.6319	-11.9655
32	-14.0006	-44.5943	-35.9708	-7.3518	-52.2306	-14.0006
32	-13.6284	-36.2096	-36.5015	-8.9155	-43.4281	-13.6284
32	-13.4924	-39.8865	-33.2457	-6.8563	-45.5756	-13.4924
32	-12.9146	-13.4036	-35.5605	-8.9820	-25.9612	-12.9146
32	-12.5734	-23.2643	-36.1002	-11.5443	-14.4709	-12.5734
32	-12.4554	-25.4020	-32.1846	-6.7077	-30.1256	-12.4554
32	-12.3419	-19.4887	-44.4752	-10.6278	-38.6995	-12.3419
32	-12.3198	-21.7785	-46.9182	-9.1131	-24.7787	-12.3198
32	-12.2493	-32.8255	-38.4893	-7.6205	-45.2202	-12.2493
32	-12.0440	20.5016	-26.4206	-6.7671	34.0724	-12.0440
33	-14.0138	-40.8196	-34.4410	-10.6657	-39.5058	-14.0138
33	-13.7676	-38.6884	-44.9758	-12.5074	-32.7214	-13.7676
33	-13.6296	-41.4731	-36.6718	-9.5051	-40.5945	-13.6296
33	-13.3244	-5.1951	-48.3929	-14.1228	-18.7416	-13.3244
33	-13.0774	-28.4142	-40.9996	-12.7552	-23.4711	-13.0774
33	-13.0024	-31.3044	-45.4761	-10.8068	-29.5890	-13.0024
33	-12.9963	-22.3188	-34.6624	-7.7080	-8.4716	-12.9963
33	-12.9222	-32.3423	-49.9409	-9.0198	-38.5617	-12.9222
33	-12.7077	-33.7822	-33.3698	-7.8915	-9.5056	-12.7077
33	-12.5227	-32.4870	-46.5041	-8.9804	-24.6842	-12.5227
34	-13.7640	-17.6397	-50.3886	-11.3216	-37.9434	-13.7640
34	-13.6336	-17.4945	-40.2624	-9.0534	-40.7014	-13.6336
34	-13.4175	-26.1063	-46.5903	-13.5878	-48.8494	-13.4175

34	-13.3141	-14.5793	-44.2070	-8.5712	-15.7644	-13.3141
34	-12.9640	-21.1294	-42.4607	-9.3006	-15.5032	-12.9640
34	-12.3468	-7.6987	-45.6512	-9.1846	-33.8373	-12.3468
34	-12.3335	4.0365	-38.9412	-7.7351	-14.6884	-12.3335
34	-12.1722	-24.7566	-46.6333	-7.4150	-47.6785	-12.1722
34	-11.9837	2.5043	-38.5293	-12.6012	-20.6687	-11.9837
34	-11.7222	3.0986	-36.0657	-10.2526	13.6257	-11.7222
35	-13.9123	-30.6940	-52.1551	-9.0691	-52.0915	-13.9123
35	-13.6736	-30.8008	-41.9155	-9.8979	-52.2860	-13.6736
35	-13.6055	-29.9868	-47.2390	-11.4017	-52.8482	-13.6055
35	-13.5708	-6.0863	-48.9925	-12.9954	-34.4562	-13.5708
35	-13.3191	-23.6444	-50.0908	-11.9080	-46.4736	-13.3191
35	-12.8048	-14.8350	-41.4670	-10.5112	-26.0041	-12.8048
35	-12.7660	3.8861	-35.3415	-8.8830	-30.8438	-12.7660
35	-12.6380	2.7028	-42.2043	-9.9033	-35.4931	-12.6380
35	-12.4982	-22.0239	-54.2046	-8.9687	-47.0820	-12.4982
35	-12.3641	-1.9847	-48.3263	-11.5155	-14.0503	-12.3641
36	-13.6026	-20.6210	-53.7004	-15.1157	-51.4327	-13.6026
36	-13.5889	-10.2977	-35.2132	-7.9602	-46.4230	-13.5889
36	-13.0428	-14.6524	-37.4798	-7.1726	-44.4309	-13.0428
36	-12.6881	-1.1768	-42.7482	-8.0616	-32.6498	-12.6881
36	-12.5862	-8.4642	-34.2406	-9.7077	-45.9022	-12.5862
36	-12.4366	16.4665	-45.3031	-9.1396	-8.9867	-12.4366
36	-12.1411	-19.3406	-55.5793	-12.9646	-48.8317	-12.1411
36	-11.9847	-4.0796	-37.5540	-9.6170	-14.5390	-11.9847
36	-11.7261	1.3808	-43.5532	-12.5893	-29.4314	-11.7261
36	-11.5957	-11.7872	-40.2544	-7.2610	-42.6412	-11.5957
37	-13.3214	-33.5584	-38.1982	-10.1945	-53.8128	-13.3214
37	-13.1623	-32.9282	-44.0711	-10.3494	-54.4239	-13.1623
37	-12.9758	-33.1496	-51.1265	-11.4095	-53.0920	-12.9758
37	-12.5409	-11.0960	-39.6599	-9.8869	-37.7167	-12.5409
37	-12.4724	-28.6984	-44.1670	-11.8351	-49.5563	-12.4724
37	-12.3752	-4.2760	-39.9129	-9.8124	-28.6775	-12.3752
37	-12.0415	-0.1026	-37.2286	-9.3720	-44.1187	-12.0415
37	-11.9801	-29.9448	-41.7596	-12.2597	-53.7466	-11.9801
37	-11.9653	-7.7805	-35.1027	-8.8405	-21.4743	-11.9653
37	-11.7270	-13.1977	-39.6514	-10.7935	-23.8043	-11.7270
38	-13.3981	4.9575	-40.9022	-10.5418	-42.4481	-13.3981
38	-13.1662	-3.0783	-38.3598	-11.5197	-50.6553	-13.1662
38	-12.6364	49.0696	-36.0929	-10.5468	-17.3932	-12.6364
38	-12.4161	-0.8939	-45.8682	-15.5214	-28.3246	-12.4161
38	-12.3289	0.6280	-42.2444	-7.6989	-49.0106	-12.3289
38	-11.9959	-1.4598	-38.1605	-6.7193	-39.7205	-11.9959
38	-11.5525	-3.1377	-35.3100	-10.3129	-30.2601	-11.5525
38	-11.3778	30.8752	-40.2948	-7.0241	-15.6522	-11.3778
38	-11.1596	16.1104	-34.7962	-9.0941	-29.0040	-11.1596

38	-10.8567	27.7468	-32.3571	-7.3581	11.8447	-10.8567
39	-12.5896	1.2284	-40.8510	-10.4871	-43.7443	-12.5896
39	-12.3767	-1.0193	-22.7414	-8.2605	-36.5567	-12.3767
39	-12.2847	10.6079	-27.8917	-10.7867	-30.6461	-12.2847
39	-12.0136	-6.5238	-46.5636	-9.7272	-50.5142	-12.0136
39	-11.9907	1.6301	-32.0365	-9.6012	-39.8792	-11.9907
39	-11.7289	0.1328	-47.9350	-13.1341	-44.3061	-11.7289
39	-11.3853	-4.1783	-47.0634	-12.6566	-42.2848	-11.3853
39	-11.3514	7.3164	-28.8458	-8.7414	-40.5488	-11.3514
39	-11.2344	18.2430	-29.3209	-10.1047	-16.5838	-11.2344
39	-11.2288	-4.3136	-40.0282	-9.3302	-50.0569	-11.2288
40	-14.0032	-0.7707	-44.3738	-9.0391	-23.8177	-14.0032
40	-13.7801	-10.6646	-43.5544	-8.6926	-37.1141	-13.7801
40	-13.4991	-10.0892	-28.7787	-10.8442	-34.0532	-13.4991
40	-13.2724	-12.3719	-54.1408	-10.1707	-41.0531	-13.2724
40	-12.9570	-20.3420	-49.5140	-10.9151	-52.6283	-12.9570
40	-12.7464	36.5059	-39.6774	-11.0504	-8.2966	-12.7464
40	-12.6200	-11.5706	-38.5458	-9.1477	-9.6088	-12.6200
40	-12.5950	-14.9929	-41.2096	-11.9880	-12.1407	-12.5950
40	-12.2539	-16.4771	-31.9248	-8.7512	-30.8365	-12.2539
40	-12.0013	52.5555	-39.3035	-9.7990	16.3370	-12.0013
41	-13.5511	-13.2100	-31.4676	-9.9335	-33.4003	-13.5511
41	-13.4789	-9.6950	-29.7862	-9.7098	-20.8234	-13.4789
41	-13.3264	-3.9835	-32.6615	-11.5881	-24.4862	-13.3264
41	-12.9364	-18.8923	-36.7402	-12.0232	-20.1154	-12.9364
41	-12.8886	-11.5050	-40.0701	-12.3425	-24.4412	-12.8886
41	-12.7519	-12.1727	-37.1982	-11.6345	-34.0868	-12.7519
41	-12.4783	-18.4015	-37.1894	-11.1595	-45.7812	-12.4783
41	-12.2522	-16.9492	-40.5469	-13.8644	-38.2157	-12.2522
41	-12.1766	-11.4505	-38.4546	-9.9999	-24.1538	-12.1766
41	-12.0101	-15.5218	-41.4840	-9.8669	-42.8378	-12.0101
42	-12.7192	-17.2847	-30.2507	-10.7294	-35.1065	-12.7192
42	-12.5080	-4.1715	-27.4738	-11.2150	-28.7673	-12.5080
42	-12.4262	-21.7582	-46.0773	-11.0130	-42.1385	-12.4262
42	-12.2180	-15.7704	-26.7758	-10.6742	-43.9343	-12.2180
42	-12.1684	-11.4512	-34.4844	-9.0041	-37.4335	-12.1684
42	-11.7978	-19.1810	-35.3161	-10.5006	-41.8872	-11.7978
42	-11.5818	-12.6694	-33.7600	-8.7547	-36.6595	-11.5818
42	-10.9494	6.0429	-33.1513	-10.2307	-20.5989	-10.9494
42	-10.0181	45.4687	-25.7773	-8.5781	14.4853	-10.0181
42	-9.9754	12.2522	-31.5069	-8.5314	20.5793	-9.9754
43	-11.4166	-26.6021	-36.2197	-10.0276	-32.7049	-11.4166
43	-11.4124	-14.3273	-28.5823	-11.1820	-38.9501	-11.4124
43	-10.9305	-30.3217	-17.2587	-9.2917	-47.8341	-10.9305
43	-10.8638	-15.0178	-38.7550	-9.4134	-40.0438	-10.8638
43	-10.4175	-13.7642	-34.0909	-11.2312	-2.7356	-10.4175

43	-10.3609	-18.7102	-29.5760	-10.2758	-36.1569	-10.3609
43	-10.2125	0.0244	-40.3844	-11.4903	-12.3740	-10.2125
43	-9.5179	54.7409	-40.8698	-9.6923	38.5640	-9.5179
43	-9.1669	10.3397	-24.2023	-9.1047	7.8721	-9.1669
43	-8.8457	-6.9708	-34.6096	-9.3115	-22.1128	-8.8457
44	-14.0347	-10.3253	-48.3179	-9.6834	-39.1517	-14.0347
44	-13.7515	-7.8029	-38.7942	-7.4995	-41.2130	-13.7515
44	-13.6749	-16.2315	-43.2363	-7.7794	-35.4194	-13.6749
44	-13.6075	-11.5926	-28.4547	-7.6838	-42.5105	-13.6075
44	-13.3390	-19.8514	-40.8796	-7.4622	-53.5541	-13.3390
44	-13.3031	-18.9304	-37.4423	-11.4599	-46.0426	-13.3031
44	-13.2797	-10.7259	-34.9186	-8.3613	-34.7792	-13.2797
44	-13.1579	1.2545	-39.5438	-8.9292	-32.3028	-13.1579
44	-13.0512	-12.9617	-39.7622	-8.2985	-45.6125	-13.0512
44	-12.9888	13.6495	-50.4482	-13.0184	-17.1723	-12.9888
45	-13.5419	-22.1804	-46.8147	-13.1392	-46.6126	-13.5419
45	-13.2754	-23.9385	-58.3942	-14.0385	-50.3643	-13.2754
45	-12.7223	-19.3172	-47.5019	-13.0683	-45.1110	-12.7223
45	-12.4114	-17.5152	-55.0891	-13.6121	-38.1268	-12.4114
45	-12.2561	-11.7990	-33.6952	-10.4369	-23.3546	-12.2561
45	-12.1918	3.1134	-36.4149	-11.6763	-25.4335	-12.1918
45	-11.7655	-16.1135	-48.2648	-12.0478	-49.9158	-11.7655
45	-11.6072	-8.6433	-37.3349	-11.9411	-36.5438	-11.6072
45	-11.5378	-13.1703	-43.0023	-13.3392	-32.3785	-11.5378
45	-10.5546	23.7107	-35.9571	-11.2383	-10.6790	-10.5546
46	-13.2975	-21.8807	-53.9858	-13.4737	-41.6838	-13.2975
46	-13.1141	-26.1278	-38.8115	-9.6114	-49.0905	-13.1141
46	-12.5069	-21.4024	-44.1080	-9.3995	-44.1746	-12.5069
46	-12.3053	-15.6082	-42.5636	-12.6769	-27.3567	-12.3053
46	-11.7313	2.9387	-44.5826	-10.2653	-33.1775	-11.7313
46	-11.6241	-19.7851	-51.7702	-9.5639	-48.4754	-11.6241
46	-11.5807	-20.7137	-32.8293	-8.9874	-44.5154	-11.5807
46	-11.3473	3.0037	-39.7755	-10.7785	-24.1779	-11.3473
46	-11.3098	-8.5977	-48.0245	-10.3266	-37.5450	-11.3098
46	-11.0659	-13.0864	-43.3921	-9.1659	-44.6833	-11.0659
47	-13.3821	-26.1688	-43.8762	-11.0187	-52.1650	-13.3821
47	-13.1587	15.8179	-37.3004	-10.8657	-23.6752	-13.1587
47	-12.9265	-20.5126	-40.7651	-10.1491	-44.4801	-12.9265
47	-12.3689	11.1423	-44.0544	-11.7004	-26.6998	-12.3689
47	-12.1380	-13.2793	-50.9958	-11.6710	-24.3165	-12.1380
47	-12.0682	-8.7567	-36.4372	-11.7053	-41.2941	-12.0682
47	-12.0459	3.9665	-43.3981	-11.1840	-29.4694	-12.0459
47	-11.8545	2.1064	-36.1844	-10.5664	-35.8327	-11.8545
47	-11.8284	-3.4644	-36.8583	-8.6710	-29.7918	-11.8284
47	-11.6973	-24.1103	-43.5626	-12.6398	-45.7107	-11.6973
48	-13.1556	-25.1576	-40.2821	-9.8775	-50.5338	-13.1556

48	-12.9981	-22.8460	-37.1197	-10.5051	-42.4775	-12.9981
48	-12.6963	-20.0537	-46.8380	-11.4574	-46.6118	-12.6963
48	-12.2934	7.9757	-33.5355	-9.4604	-32.5550	-12.2934
48	-12.2479	-12.6121	-45.4599	-11.3318	-23.8446	-12.2479
48	-12.0097	0.3862	-44.2684	-8.7827	-27.2750	-12.0097
48	-11.6771	-17.4411	-51.7076	-10.7034	-47.2686	-11.6771
48	-11.5257	8.5557	-36.5825	-8.9421	-24.3018	-11.5257
48	-11.1817	16.6081	-26.0066	-9.5603	-6.4803	-11.1817
48	-10.9613	5.1344	-41.0108	-12.3577	-14.0886	-10.9613
49	-12.7933	-9.7074	-21.9221	-8.0964	-40.3094	-12.7933
49	-12.7521	-3.6040	-26.8038	-6.6101	-45.3566	-12.7521
49	-12.7319	1.5786	-34.3900	-6.2885	-35.0355	-12.7319
49	-12.1493	1.4253	-32.3483	-9.5886	-40.9433	-12.1493
49	-11.6715	0.8774	-39.0125	-11.3212	-43.5050	-11.6715
49	-11.6030	-2.6652	-32.2241	-7.3582	-43.4429	-11.6030
49	-11.3078	-8.2726	-39.3298	-10.8798	-49.7030	-11.3078
49	-10.8580	61.9777	-34.3435	-7.1691	-4.2323	-10.8580
49	-10.5481	32.7679	-37.9815	-10.4339	-2.6278	-10.5481
49	-10.3671	13.2774	-22.6225	-8.9539	-30.0671	-10.3671
50	-13.8392	-18.1751	-30.4046	-8.6235	-45.7203	-13.8392
50	-13.6661	-27.0785	-49.3611	-13.1180	-49.3480	-13.6661
50	-13.0172	28.3814	-38.5343	-10.0422	-14.8785	-13.0172
50	-12.9278	12.8394	-44.8245	-12.7765	-26.7866	-12.9278
50	-12.4505	-5.9417	-36.7734	-13.6128	-39.4881	-12.4505
50	-11.8804	11.3783	-37.1219	-9.1164	20.4044	-11.8804
50	-11.8518	-13.2095	-48.1415	-9.4808	-38.0760	-11.8518
50	-11.7239	5.5817	-34.6484	-9.1148	-29.0115	-11.7239
50	-11.7075	-10.2921	-37.2823	-13.3676	-0.5119	-11.7075
50	-11.5107	31.9435	-29.3437	-9.4338	29.9620	-11.5107
51	-13.7883	7.6509	-46.8929	-10.1293	-27.7185	-13.7883
51	-13.2380	-26.6568	-58.3904	-18.9680	-41.9473	-13.2380
51	-13.2136	9.9830	-36.0956	-9.5590	-3.3990	-13.2136
51	-13.1540	-26.7450	-54.9873	-13.0011	-43.2851	-13.1540
51	-13.1158	-26.7594	-47.2821	-9.5956	-37.9855	-13.1158
51	-13.0159	4.1678	-33.2303	-10.3080	-9.3978	-13.0159
51	-12.9518	-2.9867	-33.9749	-14.2296	-29.9339	-12.9518
51	-12.7569	-13.5937	-34.7216	-9.5843	-30.9802	-12.7569
51	-12.7455	-24.3533	-51.5597	-12.3108	-42.6786	-12.7455
51	-12.6641	-9.4377	-31.6432	-9.6153	-28.9647	-12.6641
52	-12.9806	-28.9372	-52.8971	-11.4308	-52.9894	-12.9806
52	-12.4618	4.3009	-44.4114	-12.1447	-37.9971	-12.4618
52	-12.3771	-23.6996	-45.6748	-13.0755	-47.3868	-12.3771
52	-12.3157	-8.4034	-37.3597	-11.2706	-25.9177	-12.3157
52	-11.8850	-11.4651	-31.8572	-8.6076	-32.3071	-11.8850
52	-11.8782	-6.7971	-55.1378	-13.0544	-44.9926	-11.8782
52	-11.8701	2.5317	-26.9295	-11.0123	-31.3625	-11.8701

52	-11.7362	-21.1704	-49.8952	-10.0522	-49.6559	-11.7362
52	-11.4888	0.1870	-32.7496	-11.6447	-29.6304	-11.4888
52	-11.4493	-10.6219	-29.3432	-13.2205	-41.0117	-11.4493
53	-12.1244	-16.3808	-33.7633	-9.7718	-45.8756	-12.1244
53	-11.7586	-24.9152	-37.9334	-13.3320	-37.7661	-11.7586
53	-11.6973	-36.7841	-50.3262	-15.1446	-45.0810	-11.6973
53	-11.6679	-15.0802	-31.6507	-10.7842	-30.4491	-11.6679
53	-11.5853	-29.8594	-27.4664	-9.5643	-40.5194	-11.5853
53	-11.5847	-6.3379	-28.5108	-10.5223	-22.9851	-11.5847
53	-11.5283	-14.6597	-37.9745	-9.5021	-38.4061	-11.5283
53	-11.1510	-5.1789	-34.4352	-12.8692	-31.8544	-11.1510
53	-10.8981	-13.4692	-41.4048	-10.2757	-18.1005	-10.8981
53	-10.6784	-22.2780	-44.1126	-10.4752	-45.7846	-10.6784
54	-14.6185	-26.0278	-34.5468	-8.7438	-49.7642	-14.6185
54	-14.2622	-27.0783	-53.4028	-14.8399	-50.4705	-14.2622
54	-13.6954	-21.1861	-34.2916	-8.4222	-46.1712	-13.6954
54	-13.6003	-28.7744	-50.8359	-11.7983	-50.4383	-13.6003
54	-13.5535	-15.6099	-36.1169	-13.3530	-43.7820	-13.5535
54	-13.4837	-11.6425	-38.2003	-10.0242	-16.9913	-13.4837
54	-13.4012	-23.8097	-50.3499	-10.3969	-56.0773	-13.4012
54	-13.2315	-12.9052	-43.5539	-8.7183	-18.7741	-13.2315
54	-13.1380	25.0088	-37.3259	-9.2597	-20.4772	-13.1380
54	-13.0218	11.7680	-46.9775	-9.7545	-29.4251	-13.0218
55	-12.5108	-38.6145	-34.1747	-10.2303	-48.8318	-12.5108
55	-12.0345	-30.7563	-40.6124	-10.7600	-34.9088	-12.0345
55	-11.5653	-39.5727	-56.9283	-13.5959	-49.2778	-11.5653
55	-11.5252	-35.8523	-40.4632	-10.6461	-44.6601	-11.5252
55	-11.2118	-9.8840	-40.5530	-10.7072	-34.5762	-11.2118
55	-11.2021	-16.6496	-29.5262	-10.5766	-27.9855	-11.2021
55	-11.1291	-20.9423	-46.9576	-11.2346	-28.8825	-11.1291
55	-10.8769	-25.1403	-46.7387	-12.1593	-42.4818	-10.8769
55	-10.5114	-35.6424	-44.2518	-12.7907	-44.8490	-10.5114
55	-10.4169	-21.7600	-35.5243	-11.7051	-12.1192	-10.4169
56	-14.1830	-8.8564	-31.8562	-5.7408	-20.9343	-14.1830
56	-13.7064	1.0132	-34.2297	-6.0833	-12.6849	-13.7064
56	-13.6645	-25.1134	-57.5025	-15.7181	-44.3644	-13.6645
56	-13.5320	-23.6290	-62.6683	-15.0014	-48.6397	-13.5320
56	-12.8553	12.3955	-51.4116	-10.1350	-16.4720	-12.8553
56	-12.7569	-12.3379	-44.3988	-7.9754	-40.5060	-12.7569
56	-12.7087	16.5573	-41.9856	-6.8657	-23.4981	-12.7087
56	-12.6397	-12.0491	-50.2470	-7.2176	-42.0270	-12.6397
56	-12.4116	-8.2579	-33.9495	-6.3058	-42.9889	-12.4116
56	-12.1113	-18.5716	-34.9932	-7.2034	-51.1063	-12.1113
57	-13.6550	-26.9699	-40.6004	-6.9055	-51.6924	-13.6550
57	-13.4206	-20.1427	-41.7333	-9.9497	-42.8487	-13.4206
57	-12.7985	0.4067	-31.3176	-7.6495	-21.1334	-12.7985

57	-12.6458	-7.7168	-39.1107	-7.9225	-36.7553	-12.6458
57	-12.5077	-4.9713	-40.4629	-7.3566	-23.8941	-12.5077
57	-12.1400	-22.4970	-35.3129	-7.2954	-51.5332	-12.1400
57	-12.1142	2.5505	-37.3789	-7.8197	-14.2406	-12.1142
57	-12.0795	-16.9935	-33.2184	-6.5594	-44.7513	-12.0795
57	-11.9635	-18.1802	-47.0230	-8.4971	-47.5477	-11.9635
57	-11.8314	-4.4014	-38.9400	-8.5301	-21.5823	-11.8314
58	-14.3016	-0.3993	-27.4885	-7.7850	-28.3905	-14.3016
58	-13.4936	-27.0620	-42.3317	-12.9667	-41.4724	-13.4936
58	-13.2147	-27.4859	-28.0230	-7.0678	-39.7205	-13.2147
58	-13.1740	-22.8668	-27.4706	-9.0573	-39.3521	-13.1740
58	-13.1523	-18.1139	-52.1759	-11.9675	-29.9761	-13.1523
58	-12.9894	156.3997	-25.8789	-8.0220	-24.5266	-12.9894
58	-12.7916	-11.4853	-30.7798	-10.9079	-30.0139	-12.7916
58	-12.6407	-25.9884	-40.7841	-11.3975	-39.0247	-12.6407
58	-12.1244	-13.3346	-34.9376	-9.6400	-27.7983	-12.1244
58	-12.0252	-14.2841	-36.6422	-9.9344	-40.2411	-12.0252
59	-13.2718	-20.2551	-39.2537	-9.4082	-40.0476	-13.2718
59	-13.0911	-28.4623	-40.8507	-9.1953	-50.1638	-13.0911
59	-12.2647	-27.3340	-31.1926	-8.5219	-46.9763	-12.2647
59	-11.9778	-17.2239	-32.3321	-8.0337	-24.7821	-11.9778
59	-11.9341	-10.3280	-40.7646	-10.9912	-27.2495	-11.9341
59	-11.9087	-16.1516	-32.4795	-13.6776	-21.4284	-11.9087
59	-11.7667	-11.6529	-32.7501	-8.8027	-39.3952	-11.7667
59	-11.6463	-0.6526	-34.8905	-10.6542	-34.6521	-11.6463
59	-11.4428	-20.8476	-49.0451	-12.3816	-48.8932	-11.4428
59	-11.3742	-20.4922	-45.3874	-11.5512	-50.4936	-11.3742
60	-13.2075	-48.4054	-40.1493	-10.8937	-49.1921	-13.2075
60	-12.7155	-35.5933	-34.3425	-10.8909	-34.8162	-12.7155
60	-12.6208	-43.9062	-35.6014	-8.3528	-43.7297	-12.6208
60	-12.4807	-39.5102	-33.1673	-8.2524	-26.5661	-12.4807
60	-12.3872	-49.0280	-55.8362	-11.7723	-52.6159	-12.3872
60	-12.0067	-44.7143	-44.5592	-11.8999	-47.4870	-12.0067
60	-11.9919	-61.8779	-43.8852	-8.1424	-56.4139	-11.9919
60	-11.9806	-34.5630	-36.6362	-9.5903	-38.8203	-11.9806
60	-11.9268	-38.1599	-35.1911	-9.4343	-26.4134	-11.9268
60	-11.4305	-53.1167	-31.8499	-8.6353	-53.4131	-11.4305
61	-12.5530	-49.8130	-51.9517	-9.8812	-51.0399	-12.5530
61	-12.2047	-61.3790	-46.0253	-6.9513	-53.7175	-12.2047
61	-12.0921	-54.1304	-31.6421	-6.4168	-38.5454	-12.0921
61	-11.9229	-51.1252	-29.0060	-7.6181	-37.7394	-11.9229
61	-11.9068	-26.2420	-29.1773	-6.7668	-34.8186	-11.9068
61	-11.7751	-51.9403	-36.6503	-7.0082	-42.8068	-11.7751
61	-11.6799	-28.9007	-38.1284	-6.3571	-31.8758	-11.6799
61	-11.5330	-56.7927	-38.2355	-8.3208	-47.8067	-11.5330
61	-11.3320	-33.9165	-33.1656	-10.0188	-28.0285	-11.3320

61	-10.9573	-24.1948	-33.2862	-7.3768	0.9153	-10.9573
62	-12.8540	-42.3809	-39.9832	-10.4330	-53.1147	-12.8540
62	-12.4902	-30.3087	-46.0509	-11.1391	-35.2665	-12.4902
62	-12.3279	-53.2756	-55.4473	-12.8699	-54.9192	-12.3279
62	-12.3272	-37.8065	-33.9747	-7.4054	-47.4412	-12.3272
62	-11.8563	-43.6080	-35.1313	-10.3697	-44.3985	-11.8563
62	-11.6217	-48.5963	-48.5129	-11.9105	-49.1575	-11.6217
62	-11.5146	-22.4542	-41.2770	-8.9547	-32.1601	-11.5146
62	-11.4508	-26.6763	-37.6921	-7.6513	-28.6058	-11.4508
62	-11.3525	-37.8352	-42.4645	-11.8782	-31.9592	-11.3525
62	-10.3463	-35.8754	-33.8431	-10.5629	-23.4638	-10.3463
63	-13.2525	-6.2756	-42.5933	-8.9734	-26.0298	-13.2525
63	-12.9550	-16.7276	-34.1030	-8.7086	-35.7748	-12.9550
63	-12.9088	29.5713	-39.5973	-8.1115	-16.8710	-12.9088
63	-12.7972	-21.3276	-39.8552	-9.5525	-35.7076	-12.7972
63	-12.5679	-24.0458	-42.6747	-9.4972	-49.8591	-12.5679
63	-12.5286	5.3555	-42.2068	-9.1755	-27.5184	-12.5286
63	-12.5125	-23.3497	-36.7474	-7.6593	-46.8865	-12.5125
63	-12.1636	-0.6526	-43.1836	-8.9224	-26.4689	-12.1636
63	-12.0483	-11.6229	-31.8981	-7.1367	-38.4928	-12.0483
63	-11.8618	-17.9441	-43.2079	-13.1748	-13.4143	-11.8618
64	-13.8097	-7.3049	-38.3513	-12.8912	-29.0650	-13.8097
64	-13.2814	-17.2722	-32.7194	-10.3465	-35.1301	-13.2814
64	-12.6986	-8.5669	-38.6921	-8.8118	-31.4763	-12.6986
64	-12.4663	0.8389	-43.2471	-11.4945	-14.0134	-12.4663
64	-12.4062	-23.5899	-39.3265	-10.2675	-46.5382	-12.4062
64	-12.3469	-23.5615	-42.8033	-9.0918	-46.6341	-12.3469
64	-12.1303	-11.5912	-46.0056	-8.6503	-38.6653	-12.1303
64	-12.0466	-8.8167	-38.4024	-8.9616	-17.4070	-12.0466
64	-11.5609	-16.4439	-42.0832	-10.2160	-40.0849	-11.5609
64	-11.5365	-22.3071	-41.7942	-8.5068	-43.2138	-11.5365
65	-12.9602	-21.1204	-37.6510	-12.2081	-34.8482	-12.9602
65	-12.3153	-20.7404	-41.5716	-11.1575	-36.4752	-12.3153
65	-11.9880	-8.1979	-31.4857	-9.0963	-35.2679	-11.9880
65	-11.9637	-26.5573	-43.3226	-9.6534	-45.3685	-11.9637
65	-11.8193	-10.5129	-40.4252	-11.6558	-31.7654	-11.8193
65	-11.7695	-26.2150	-36.8579	-9.8613	-47.6667	-11.7695
65	-11.6979	-26.2258	-23.6157	-8.2318	-47.6878	-11.6979
65	-11.6623	-19.9120	-35.4432	-8.4619	-39.8155	-11.6623
65	-11.4905	-19.9490	-41.6359	-9.0957	-43.1325	-11.4905
65	-11.2418	-21.1449	-46.6909	-11.4705	-43.5161	-11.2418
66	-13.6990	-26.1916	-45.1097	-8.6150	-43.8589	-13.6990
66	-13.3732	-20.1699	-42.8221	-12.1253	-31.0348	-13.3732
66	-13.2886	-17.6663	-49.9053	-12.7866	-40.6390	-13.2886
66	-13.0796	-9.1628	-37.1722	-9.0928	-25.3483	-13.0796
66	-13.0780	-19.4362	-38.7221	-9.4091	-11.8869	-13.0780

66	-12.8610	-23.8370	-49.1472	-11.9056	-36.0190	-12.8610
66	-12.8095	-19.1408	-47.6619	-10.9694	-42.8989	-12.8095
66	-12.1663	-25.0890	-30.4856	-8.1567	-30.2497	-12.1663
66	-12.1067	5.8700	-37.8185	-9.4969	-18.8537	-12.1067
66	-12.0772	-21.6829	-45.7581	-13.7578	-13.5120	-12.0772
67	-13.9796	-20.6041	-43.0267	-10.7297	-34.4042	-13.9796
67	-13.4776	-25.7803	-39.5777	-10.3523	-40.7110	-13.4776
67	-13.0869	-20.8451	-34.4727	-9.0522	-34.8810	-13.0869
67	-12.7911	-24.7405	-39.2548	-8.7914	-47.0249	-12.7911
67	-12.5278	-20.3770	-39.3209	-10.2211	-43.9894	-12.5278
67	-12.5162	-11.4448	-42.1218	-8.9182	-16.9667	-12.5162
67	-12.3918	-25.9171	-49.7430	-10.3040	-46.3417	-12.3918
67	-12.1342	-18.9841	-44.7963	-8.9992	-40.4572	-12.1342
67	-12.0536	-16.1618	-40.0572	-9.5105	-37.3238	-12.0536
67	-11.9251	14.2625	-37.3588	-9.3029	-24.1452	-11.9251
68	-14.0554	-18.1182	-37.9432	-11.7738	-33.8052	-14.0554
68	-13.9820	-17.5183	-50.4422	-12.3431	-23.0904	-13.9820
68	-13.6401	-17.5452	-46.8268	-11.9360	-26.7259	-13.6401
68	-13.4916	-14.3456	-37.4747	-10.7835	-28.3440	-13.4916
68	-13.1126	-18.3998	-37.6185	-13.0567	-34.7212	-13.1126
68	-13.0386	-24.3894	-39.0903	-12.1890	-18.4818	-13.0386
68	-12.9899	-25.7458	-39.8891	-11.8399	-30.8272	-12.9899
68	-12.9545	-16.1429	-32.9921	-10.8480	-27.9704	-12.9545
68	-12.7784	-25.3711	-45.4381	-13.5095	-32.5497	-12.7784
68	-12.6078	-25.7272	-50.4269	-12.3277	-37.7286	-12.6078
69	-12.9563	-23.8870	-40.8116	-11.9337	-36.5296	-12.9563
69	-12.3779	-22.3282	-39.4844	-11.8521	-43.2589	-12.3779
69	-11.8656	-25.0779	-39.2201	-10.2093	-37.8377	-11.8656
69	-11.7229	-28.6378	-42.2671	-11.7101	-48.2044	-11.7229
69	-11.5304	-16.2834	-31.1486	-9.6968	-18.6652	-11.5304
69	-10.8914	-18.4420	-36.4562	-9.0827	-38.3225	-10.8914
69	-10.8306	-21.4203	-40.4016	-9.4648	-36.4363	-10.8306
69	-10.5235	37.0160	-30.8162	-9.0301	13.1881	-10.5235
69	-10.4766	-25.2370	-45.2662	-9.5556	-39.9727	-10.4766
69	-9.7537	1.3724	-35.7753	-9.8240	-7.9178	-9.7537
70	-13.5819	10.0278	-42.4961	-10.1223	-40.8663	-13.5819
70	-13.3155	0.5682	-39.9373	-9.6047	-33.6458	-13.3155
70	-13.1174	5.3806	-48.4417	-9.3742	-41.6500	-13.1174
70	-13.0864	5.5582	-29.0141	-8.5717	-35.6014	-13.0864
70	-12.9534	0.9420	-32.6021	-8.0287	-46.4601	-12.9534
70	-12.8138	4.2039	-42.0227	-9.0392	-42.7179	-12.8138
70	-12.6226	-0.3812	-41.6789	-8.1908	-44.8631	-12.6226
70	-12.5749	-1.1950	-42.8061	-8.9154	-52.2435	-12.5749
70	-12.5177	21.5870	-42.2501	-10.9006	-17.8454	-12.5177
70	-12.1809	3.3880	-42.1251	-12.0814	-12.7195	-12.1809
71	-13.1870	2.8624	-27.5499	-8.8430	-34.3427	-13.1870

71	-12.9428	3.1183	-43.6675	-13.1180	-41.9389	-12.9428
71	-12.5911	5.8723	-46.0598	-10.6032	-30.0194	-12.5911
71	-12.4529	-1.7383	-41.6535	-9.2859	-45.1535	-12.4529
71	-12.2625	-0.5289	-42.1070	-10.0975	-40.7761	-12.2625
71	-12.0157	21.8958	-34.8732	-9.2158	-44.8307	-12.0157
71	-12.0082	12.1940	-40.1841	-10.0431	-37.3950	-12.0082
71	-11.9563	0.0098	-39.1102	-9.5417	-42.3112	-11.9563
71	-11.8663	22.5822	-41.6244	-9.1570	-14.8974	-11.8663
71	-11.8458	21.3186	-37.8986	-11.2390	-24.7929	-11.8458
72	-13.0397	9.2150	-40.0832	-9.2682	-27.8820	-13.0397
72	-12.8774	0.7065	-45.2566	-11.2030	-40.8816	-12.8774
72	-12.8314	5.6678	-33.5344	-9.5180	-22.8113	-12.8314
72	-12.5340	-0.3338	-30.7183	-10.6726	-21.1406	-12.5340
72	-12.3659	-0.0542	-38.7093	-12.1875	-19.0222	-12.3659
72	-12.3029	2.3869	-37.9407	-11.7040	-17.4233	-12.3029
72	-12.1687	7.7400	-48.0398	-12.5223	-24.5363	-12.1687
72	-12.0770	-0.9942	-33.5715	-9.2360	-42.9842	-12.0770
72	-11.9319	-0.5503	-42.4828	-9.8406	-37.1244	-11.9319
72	-11.7902	6.7056	-40.9639	-10.5717	-22.2223	-11.7902
73	-12.1242	11.0783	-44.0825	-10.9884	-30.8833	-12.1242
73	-12.0210	-4.3143	-42.0468	-9.7059	-49.1064	-12.0210
73	-11.9897	1.5939	-47.1845	-11.5558	-35.3343	-11.9897
73	-11.8780	0.4270	-40.2111	-9.5763	-34.9995	-11.8780
73	-11.7647	-1.3834	-36.7558	-11.7671	-51.0333	-11.7647
73	-11.6986	-5.0755	-45.2331	-8.8916	-48.0791	-11.6986
73	-11.3383	11.7065	-45.1391	-11.6144	-34.6996	-11.3383
73	-11.1974	44.0495	-36.1861	-10.3426	5.6609	-11.1974
73	-10.9940	2.4898	-40.9806	-12.2828	-37.2986	-10.9940
73	-10.9881	6.1537	-35.0667	-8.8060	-40.7933	-10.9881
74	-13.8489	-32.5307	-48.8934	-10.0055	-46.4677	-13.8489
74	-13.7663	0.4675	-43.6974	-12.7331	-28.3803	-13.7663
74	-13.6627	-38.9106	-47.2444	-8.2327	-52.8485	-13.6627
74	-13.5468	-40.5021	-59.6758	-11.9006	-52.4207	-13.5468
74	-13.3689	-41.0621	-47.6604	-9.5703	-49.9103	-13.3689
74	-12.8775	8.2213	-43.6956	-10.7965	-23.6472	-12.8775
74	-12.7754	-27.1977	-36.3298	-7.7630	-44.8754	-12.7754
74	-12.7703	-17.1736	-32.1398	-7.9922	-2.1970	-12.7703
74	-12.7087	-20.3114	-33.7432	-7.3479	-40.3846	-12.7087
74	-12.5402	-19.8285	-32.1602	-10.4698	-38.4415	-12.5402
75	-14.0655	-33.8764	-60.1582	-12.0739	-44.1596	-14.0655
75	-13.6964	-38.0821	-43.9529	-8.0344	-52.5235	-13.6964
75	-13.5125	-37.6699	-42.7299	-8.4829	-50.9122	-13.5125
75	-13.4173	-34.2776	-37.9330	-7.9206	-42.9651	-13.4173
75	-13.4130	-17.6552	-43.2731	-15.6438	-22.6807	-13.4130
75	-13.3757	-31.0101	-45.5880	-10.3648	-46.5985	-13.3757
75	-13.1609	-32.9860	-45.7972	-8.8278	-45.5647	-13.1609

75	-12.9492	-12.1716	-44.4738	-9.2814	-27.7082	-12.9492
75	-12.8156	-0.4991	-37.4895	-8.7986	-26.4949	-12.8156
75	-12.7967	-26.6143	-52.9189	-12.3132	-25.1914	-12.7967
76	-13.9292	-39.2634	-46.8367	-7.1933	-44.9765	-13.9292
76	-13.6377	-40.0015	-44.2593	-7.1998	-44.0657	-13.6377
76	-13.2951	-39.3029	-43.2114	-8.6893	-48.7937	-13.2951
76	-13.1568	-5.9274	-37.0760	-8.4328	-27.8270	-13.1568
76	-13.0170	-30.1591	-36.7141	-9.7943	-31.9130	-13.0170
76	-12.9779	-36.4143	-49.2342	-12.0558	-42.7715	-12.9779
76	-12.9476	-40.7417	-41.7939	-9.1464	-42.2070	-12.9476
76	-12.7055	-20.2260	-30.4988	-9.6003	-29.8102	-12.7055
76	-12.7024	-24.1763	-31.6757	-9.2527	-28.8197	-12.7024
76	-12.6973	-22.3260	-40.1837	-11.7373	-24.8877	-12.6973
77	-13.1494	-40.9720	-44.4650	-7.7308	-53.6862	-13.1494
77	-12.5211	-19.7384	-27.6489	-7.9245	-18.9267	-12.5211
77	-12.2440	-24.5346	-37.6091	-8.0572	-22.6872	-12.2440
77	-12.0505	-23.4653	-45.2955	-11.8167	-29.4346	-12.0505
77	-12.0385	-37.3485	-34.3170	-9.0752	-56.5688	-12.0385
77	-11.9113	-23.5212	-35.7438	-10.3223	-43.5955	-11.9113
77	-11.8806	-29.2447	-28.5172	-7.3497	-23.6369	-11.8806
77	-11.8451	-10.1206	-35.8086	-7.5769	-30.9538	-11.8451
77	-11.7148	-31.6879	-39.8384	-10.2185	-28.9841	-11.7148
77	-11.6427	-14.1719	-33.7296	-7.2354	-36.9870	-11.6427
78	-13.7127	-11.9609	-38.9126	-9.2917	-47.6524	-13.7127
78	-13.7080	-15.6706	-51.4639	-8.9759	-39.7048	-13.7080
78	-12.6542	-17.4139	-48.4204	-11.3897	-46.6990	-12.6542
78	-12.5349	0.2403	-41.5929	-11.5606	-21.2611	-12.5349
78	-12.3488	18.2204	-40.8288	-10.3538	-10.6153	-12.3488
78	-12.3158	24.4893	-35.8284	-9.3144	-13.5906	-12.3158
78	-12.2359	-10.4053	-47.4087	-12.8263	-40.3314	-12.2359
78	-12.0949	-8.6991	-44.0252	-10.8340	-39.1762	-12.0949
78	-12.0448	-11.0023	-56.2595	-14.1227	-38.8541	-12.0448
78	-11.9904	-14.2157	-50.3168	-12.2318	-35.4613	-11.9904
79	-13.5783	-9.6244	-28.5713	-8.1905	-32.1612	-13.5783
79	-13.5338	1.6005	-32.8018	-7.9744	-28.6620	-13.5338
79	-13.3020	-15.3187	-39.8662	-8.5615	-44.3143	-13.3020
79	-13.0831	-9.9464	-50.4527	-13.0995	-15.7197	-13.0831
79	-13.0581	-8.9146	-32.2325	-8.1431	-41.1142	-13.0581
79	-13.0538	-13.4696	-42.1817	-11.2506	-34.2131	-13.0538
79	-12.7238	-12.9127	-38.9388	-8.4341	-43.9016	-12.7238
79	-12.6669	7.3694	-33.2255	-7.9134	-25.0437	-12.6669
79	-12.3578	-10.0294	-39.3106	-8.8944	-40.4550	-12.3578
79	-11.8933	7.1920	-37.1769	-12.7055	-29.6640	-11.8933
80	-13.5807	-2.9438	-25.1830	-7.7461	-35.7039	-13.5807
80	-12.8395	-8.2114	-37.1248	-11.3045	-42.8457	-12.8395
80	-12.6798	-16.3280	-38.2686	-10.4726	-41.1080	-12.6798

80	-12.3440	-6.4297	-38.7004	-10.3908	-18.9840	-12.3440
80	-12.2792	-16.9464	-46.8010	-10.1235	-37.4462	-12.2792
80	-12.1758	-6.1300	-38.3413	-7.8417	-16.8723	-12.1758
80	-12.1220	54.1123	-37.2876	-7.8236	3.5829	-12.1220
80	-12.1200	0.6304	-42.1236	-8.7064	-26.9395	-12.1200
80	-12.0274	-8.2192	-32.0882	-9.6428	-37.5808	-12.0274
80	-12.0254	-12.6888	-48.2743	-12.7981	-37.0943	-12.0254
81	-13.8635	-0.9588	-25.7723	-8.4823	-21.8148	-13.8635
81	-13.3440	-19.4423	-38.7022	-8.3717	-51.1949	-13.3440
81	-13.2104	-9.4154	-36.7844	-9.8440	-31.7950	-13.2104
81	-12.9909	-14.5574	-36.3770	-7.3751	-33.1154	-12.9909
81	-12.9057	-20.0879	-46.3741	-12.7324	-50.0250	-12.9057
81	-12.6703	5.7517	-37.6269	-9.9348	-40.4023	-12.6703
81	-12.4983	-8.4826	-28.3721	-6.8995	-13.9851	-12.4983
81	-12.3620	-13.3281	-44.1061	-10.5991	-37.8319	-12.3620
81	-12.2562	13.0142	-36.2380	-7.2822	1.1568	-12.2562
81	-12.1909	1.5850	-48.5786	-9.2893	-19.2153	-12.1909
82	-13.3763	-11.2995	-27.8871	-7.0627	-31.7551	-13.3763
82	-12.9238	-11.9657	-30.7983	-6.4638	-41.2247	-12.9238
82	-12.7450	-11.6619	-27.9851	-7.9038	-43.7151	-12.7450
82	-12.6822	-19.3048	-31.9379	-8.8644	-47.4579	-12.6822
82	-12.0889	-13.4276	-38.0894	-8.9778	-41.3184	-12.0889
82	-12.0323	89.3799	-30.4810	-7.1199	27.9690	-12.0323
82	-11.6772	-4.4790	-32.3876	-9.2907	-42.1362	-11.6772
82	-11.6658	-9.6134	-33.7373	-7.7566	-39.9283	-11.6658
82	-11.5773	8.0243	-44.5695	-7.9707	-12.5444	-11.5773
82	-11.2818	-21.0810	-27.9960	-7.6907	-40.3111	-11.2818
83	-13.5041	1.8909	-29.2747	-8.8026	-10.2890	-13.5041
83	-13.3887	-5.3410	-48.4571	-9.9986	-28.2679	-13.3887
83	-13.2746	-2.6635	-42.9937	-10.2999	-31.7051	-13.2746
83	-13.2689	-3.2716	-41.2662	-12.3487	-28.8410	-13.2689
83	-13.1639	-15.4407	-27.1616	-11.2763	-36.2101	-13.1639
83	-12.9995	-12.4921	-36.6920	-9.4923	-29.4996	-12.9995
83	-12.5798	-20.9689	-40.9530	-9.9993	-23.7916	-12.5798
83	-12.3839	-18.7045	-49.1671	-13.8296	-39.0576	-12.3839
83	-12.3249	-5.0651	-41.6906	-12.0144	-26.8852	-12.3249
83	-12.1410	-9.6615	-37.0586	-10.4422	-19.9166	-12.1410
84	-13.7292	-43.5559	-36.4758	-10.7279	-35.9567	-13.7292
84	-12.4794	-42.7991	-50.0231	-12.2554	-44.2433	-12.4794
84	-12.2209	-46.8118	-42.0033	-9.0031	-43.5279	-12.2209
84	-11.9696	-40.1553	-38.3872	-9.2466	-42.2933	-11.9696
84	-11.9297	-49.3002	-48.8397	-8.9035	-48.0797	-11.9297
84	-11.8177	-42.7888	-46.1511	-11.0035	-28.1249	-11.8177
84	-11.7754	-35.2531	-26.8742	-10.6422	-18.3834	-11.7754
84	-11.6475	-36.0332	-37.4634	-8.5906	-40.7431	-11.6475
84	-11.3862	-30.1285	-35.6603	-9.5415	-24.7191	-11.3862

84	-11.3612	-25.1234	-44.7449	-10.8499	-25.9267	-11.3612
85	-13.9937	-37.1017	-38.9227	-9.2007	-26.8317	-13.9937
85	-13.6675	-47.0856	-28.4074	-9.7649	-19.4134	-13.6675
85	-12.8726	-39.8817	-33.2359	-9.2673	-12.6688	-12.8726
85	-12.6802	-48.6437	-39.3814	-11.9011	-21.6797	-12.6802
85	-12.1771	-24.3002	-31.4457	-10.0486	-22.8425	-12.1771
85	-12.0712	-48.3243	-33.3138	-7.8322	-21.6805	-12.0712
85	-12.0576	-49.5344	-44.1639	-11.8245	-39.1487	-12.0576
85	-12.0073	-42.6267	-32.3827	-9.2204	-27.7584	-12.0073
85	-11.8975	-45.9039	-31.2898	-8.6356	-30.4558	-11.8975
85	-11.8289	-37.0484	-34.4369	-10.3849	-38.0292	-11.8289
86	-13.4674	12.9371	-39.9251	-9.9919	-20.1446	-13.4674
86	-13.0039	-6.6287	-43.8492	-11.0712	-34.8960	-13.0039
86	-12.8396	-6.2100	-51.1604	-10.2534	-41.6212	-12.8396
86	-12.6036	0.6042	-45.1440	-13.0242	-8.8051	-12.6036
86	-12.5198	7.2407	-43.5730	-11.3119	-34.5468	-12.5198
86	-12.4805	11.1198	-35.9104	-11.1566	-20.5348	-12.4805
86	-12.4163	10.2412	-43.1777	-9.5461	-10.6918	-12.4163
86	-12.3050	6.9629	-33.0746	-9.6911	-36.3442	-12.3050
86	-12.1339	-0.3357	-41.5631	-8.6176	-4.2349	-12.1339
86	-12.1212	23.1674	-46.3229	-9.8474	-10.7022	-12.1212
87	-12.9954	-4.0605	-49.2907	-11.5911	-21.4262	-12.9954
87	-12.9733	-2.2964	-40.8098	-10.1865	-16.1659	-12.9733
87	-12.7482	-8.7386	-51.3103	-12.5613	-34.5428	-12.7482
87	-12.7213	-11.8251	-48.2523	-11.3425	-31.6242	-12.7213
87	-12.6088	-5.0393	-37.0931	-9.6164	-27.2284	-12.6088
87	-12.5390	7.0597	-36.7786	-8.5678	-12.8320	-12.5390
87	-12.5003	21.2080	-39.4921	-9.5336	-27.3395	-12.5003
87	-12.2936	-1.8823	-43.7573	-8.8381	-23.6493	-12.2936
87	-12.2008	-8.4143	-42.1121	-11.8940	-35.4405	-12.2008
87	-12.1806	-3.5948	-39.3524	-10.5868	-22.9031	-12.1806
88	-12.7342	5.8495	-40.1297	-9.6141	-22.5045	-12.7342
88	-12.5622	68.0577	-36.1308	-8.6487	-31.1004	-12.5622
88	-12.1604	-14.7695	-35.9630	-10.3657	-43.6620	-12.1604
88	-12.0852	7.8119	-36.9324	-9.7443	-39.6953	-12.0852
88	-11.9696	-8.6191	-28.4365	-10.5247	-37.8635	-11.9696
88	-11.9201	-7.7737	-45.7793	-9.2854	-37.5770	-11.9201
88	-11.5748	19.8798	-43.5620	-8.9382	-30.0991	-11.5748
88	-11.1686	-14.1114	-37.9269	-8.6622	-42.6069	-11.1686
88	-11.1375	15.9338	-31.9512	-11.0535	-6.9461	-11.1375
88	-10.1629	33.4688	-31.2268	-8.6143	0.9080	-10.1629
89	-11.2663	-19.5650	-25.4088	-11.1716	-31.0858	-11.2663
89	-11.2613	-23.5647	-42.9328	-12.8033	-43.1894	-11.2613
89	-11.2119	-9.4170	-48.1790	-12.1475	-27.8597	-11.2119
89	-10.7179	-7.5765	-36.9239	-13.3674	-41.9690	-10.7179
89	-10.6897	-22.5527	-30.8005	-12.2071	-40.8529	-10.6897

89	-10.6641	-16.2914	-42.0831	-13.1148	-45.9563	-10.6641
89	-10.5300	6.7861	-37.9527	-11.8838	-12.9789	-10.5300
89	-10.2582	0.4689	-39.4858	-11.5951	-16.6348	-10.2582
89	-10.0778	-11.2147	-44.0639	-14.5549	-34.7081	-10.0778
89	-9.9028	-2.4405	-35.4604	-12.0495	-0.3214	-9.9028
90	-13.8590	13.1680	-38.0706	-10.2550	-27.9050	-13.8590
90	-13.1791	8.9931	-37.2911	-14.0228	-41.0536	-13.1791
90	-13.1683	80.5309	-49.5756	-13.9895	-36.4972	-13.1683
90	-13.1632	-0.5836	-39.6205	-9.5786	-49.5375	-13.1632
90	-13.1429	8.5313	-37.6738	-10.2067	-33.4056	-13.1429
90	-12.8594	47.4779	-38.4251	-12.0024	7.5140	-12.8594
90	-12.6800	3.2718	-34.7189	-9.7617	-40.6281	-12.6800
90	-12.6717	1.0736	-64.0310	-16.4241	-44.2712	-12.6717
90	-12.5353	6.0032	-44.2606	-13.0404	-49.4581	-12.5353
90	-12.3582	1.1166	-49.6893	-12.3235	-49.7518	-12.3582
91	-13.3454	9.9835	-30.9117	-10.1492	-29.3657	-13.3454
91	-13.1630	6.7998	-48.2559	-14.4090	-33.1569	-13.1630
91	-12.9596	1.3747	-27.2621	-11.7099	-42.8474	-12.9596
91	-12.7923	14.5641	-44.7034	-12.1732	-32.7024	-12.7923
91	-12.7810	0.1678	-43.2299	-11.6169	-46.2483	-12.7810
91	-12.5531	1.3355	-37.7158	-10.4195	-44.0535	-12.5531
91	-12.4248	8.7583	-35.7176	-10.8665	-31.8071	-12.4248
91	-12.3177	6.0665	-28.2569	-11.9020	-39.8519	-12.3177
91	-11.9176	13.7163	-39.0770	-13.0110	-39.9833	-11.9176
91	-11.7936	19.8411	-21.1634	-11.9447	-14.2891	-11.7936
92	-13.0542	13.4183	-36.3850	-12.4458	-17.5246	-13.0542
92	-13.0233	12.2847	-37.9384	-12.1429	-26.6823	-13.0233
92	-12.6971	20.8813	-34.0421	-11.0487	-28.3829	-12.6971
92	-12.5321	0.4878	-42.7410	-12.7845	-36.2890	-12.5321
92	-12.3533	4.8483	-37.0533	-11.5794	-33.6788	-12.3533
92	-12.3520	3.3256	-31.9319	-11.0824	-39.4432	-12.3520
92	-12.2147	2.7955	-50.3960	-13.1704	-34.1562	-12.2147
92	-12.1991	9.8715	-37.9514	-14.9525	-15.9127	-12.1991
92	-12.1954	21.5887	-34.3911	-12.3635	-22.7578	-12.1954
92	-12.1244	12.8165	-30.1254	-15.3613	-36.1771	-12.1244
93	-13.2111	4.8886	-43.3855	-11.2262	-20.5617	-13.2111
93	-13.1524	-8.2416	-41.0684	-14.4546	-23.9217	-13.1524
93	-12.8903	-15.9776	-42.4820	-8.4368	-40.4906	-12.8903
93	-12.8487	-11.1363	-26.3779	-9.3881	-31.9574	-12.8487
93	-12.8018	-7.3385	-57.2448	-15.1656	-36.3498	-12.8018
93	-12.6979	-16.9454	-29.0977	-8.3558	-49.7025	-12.6979
93	-12.6234	11.1479	-34.8955	-8.3154	-27.8868	-12.6234
93	-12.4812	-0.4833	-46.2384	-11.1240	-33.2299	-12.4812
93	-12.4605	2.1008	-35.7131	-8.9620	-21.5447	-12.4605
93	-12.4348	-14.7429	-37.8944	-11.4776	-42.6508	-12.4348
94	-14.7354	-1.0279	-32.3593	-14.5450	-33.8984	-14.7354

94	-14.0562	-5.2422	-42.2528	-12.7699	-38.1726	-14.0562
94	-13.2998	6.8338	-43.0476	-11.0767	-30.9423	-13.2998
94	-13.2900	50.3850	-25.6118	-10.4848	-5.6198	-13.2900
94	-13.2433	-1.2567	-41.7737	-14.3898	-39.5145	-13.2433
94	-13.1513	16.5591	-40.5401	-9.5555	-4.3337	-13.1513
94	-12.9513	10.0144	-29.1608	-9.4250	-33.8971	-12.9513
94	-12.7658	-0.9663	-37.9641	-10.2871	-44.1351	-12.7658
94	-12.1620	0.4050	-25.9777	-8.6356	-18.4207	-12.1620
94	-12.0182	-2.4422	-45.8407	-11.0095	-29.6805	-12.0182
95	-12.3766	-12.1972	-51.2275	-17.6383	-34.0699	-12.3766
95	-11.8799	-9.9223	-27.5891	-7.7444	-49.4120	-11.8799
95	-11.8656	-14.4250	-35.3432	-9.1372	-33.3051	-11.8656
95	-11.8068	-10.0160	-40.7283	-10.3029	-39.7951	-11.8068
95	-11.6522	-9.1207	-52.8089	-12.1215	-30.0574	-11.6522
95	-11.5235	-15.4745	-38.7375	-10.3189	-47.0297	-11.5235
95	-11.4101	-11.8624	-41.8945	-9.0792	-37.4561	-11.4101
95	-11.1561	-5.8247	-34.9782	-9.8621	-23.7122	-11.1561
95	-11.1332	2.0815	-34.5314	-8.7344	-16.2902	-11.1332
95	-10.9658	-12.6013	-23.0802	-7.6482	-30.4575	-10.9658
96	-14.6195	-0.8405	-37.3090	-6.3603	-22.8470	-14.6195
96	-14.0935	4.1846	-41.0414	-8.6213	-34.7579	-14.0935
96	-13.3558	4.4736	-37.5415	-9.2392	-46.7056	-13.3558
96	-13.2010	2.0624	-33.4244	-6.5634	-40.1751	-13.2010
96	-13.0038	1.9770	-39.0518	-7.6848	-31.0678	-13.0038
96	-12.9538	15.9759	-42.9145	-9.0495	-20.3619	-12.9538
96	-12.9372	10.8657	-40.3189	-9.7336	-16.1621	-12.9372
96	-12.8614	-7.4547	-41.0380	-10.7541	-33.5752	-12.8614
96	-12.8274	23.7866	-48.8104	-11.1061	0.7036	-12.8274
96	-12.6846	84.7454	-44.0955	-10.3136	-23.7683	-12.6846
97	-13.3304	-24.5703	-49.0163	-11.0230	-30.8610	-13.3304
97	-13.1635	-20.0867	-37.7952	-9.8732	-28.3674	-13.1635
97	-12.8602	-25.4620	-38.7572	-9.8146	-39.0184	-12.8602
97	-12.7921	-17.9071	-41.4749	-12.1254	-31.8300	-12.7921
97	-12.7398	-25.4656	-43.9066	-12.2088	-29.7967	-12.7398
97	-12.6935	-21.8543	-40.8358	-10.1121	-39.5953	-12.6935
97	-12.4111	-22.7470	-45.4096	-11.0269	-6.1895	-12.4111
97	-12.3330	-27.4712	-47.0457	-9.9912	-46.6368	-12.3330
97	-12.2227	-18.9319	-49.1407	-13.3323	-34.1142	-12.2227
97	-12.1864	-16.1442	-41.2943	-9.1904	-34.5707	-12.1864
98	-13.4227	-17.5114	-40.4191	-9.3156	-36.4300	-13.4227
98	-13.2230	-19.9317	-33.6085	-9.8399	-35.2011	-13.2230
98	-12.8312	-20.1104	-46.0131	-11.0959	-40.9733	-12.8312
98	-12.5762	-14.6197	-46.8107	-11.8351	-33.8089	-12.5762
98	-12.5660	-7.9760	-56.1773	-13.5254	-37.1161	-12.5660
98	-12.5300	-24.2390	-37.9830	-12.2539	-48.1097	-12.5300
98	-11.9017	-21.3340	-32.4216	-9.5874	-46.0007	-11.9017

98	-10.9865	5.9273	-42.1137	-9.9681	-13.9880	-10.9865
98	-10.8688	-16.8738	-34.3212	-9.9346	-38.2974	-10.8688
98	-10.7222	-19.2029	-40.2702	-10.3189	-39.6409	-10.7222
99	-14.1808	-15.6865	-51.9739	-14.5404	-37.5294	-14.1808
99	-13.3362	-11.9272	-48.8634	-14.3463	-1.9061	-13.3362
99	-13.2625	-13.6035	-37.0675	-11.5392	-38.7433	-13.2625
99	-12.5848	4.9486	-41.5335	-12.8515	0.8082	-12.5848
99	-12.4844	-16.9982	-41.8407	-11.9458	-19.3008	-12.4844
99	-12.2211	-12.8482	-31.5898	-9.8695	-28.4952	-12.2211
99	-12.0000	-11.6801	-42.8295	-9.9208	-27.0926	-12.0000
99	-11.7579	-15.8025	-28.3239	-8.6243	-6.8642	-11.7579
99	-11.6953	-20.3853	-45.8889	-8.6606	-27.7201	-11.6953
99	-11.4940	-9.8924	-37.9150	-9.3780	-9.9677	-11.4940
100	-13.7395	-23.0151	-34.7119	-12.0881	-22.1072	-13.7395
100	-13.1641	-28.4244	-39.2442	-10.2343	-21.8913	-13.1641
100	-13.1256	-39.4389	-34.6059	-9.8571	-34.8704	-13.1256
100	-12.5709	-36.8977	-48.2958	-13.7595	-38.6504	-12.5709
100	-12.5023	-46.5177	-44.8318	-10.6950	-40.1470	-12.5023
100	-12.2203	-52.8602	-31.1938	-9.9321	-47.2122	-12.2203
100	-12.0710	-41.2436	-34.0261	-9.5133	-35.8714	-12.0710
100	-12.0382	-43.7804	-35.6730	-11.4595	-13.6700	-12.0382
100	-11.9937	-39.9087	-32.4278	-12.3799	-39.4459	-11.9937
100	-11.2824	-39.9517	-40.4745	-9.6173	-11.6118	-11.2824
101	-13.3825	-37.2189	-31.0806	-14.5262	-38.6110	-13.3825
101	-13.2907	-38.7707	-29.4022	-9.5721	-38.1629	-13.2907
101	-13.1736	-34.6124	-40.0989	-11.9855	-37.9284	-13.1736
101	-12.9531	-30.0726	-37.8847	-8.5912	-34.8291	-12.9531
101	-12.3782	-35.1537	-44.1844	-11.3348	-38.6330	-12.3782
101	-12.3331	-39.9221	-46.1734	-9.4938	-47.9343	-12.3331
101	-11.9863	-5.9200	-32.2947	-10.3757	-21.5055	-11.9863
101	-11.9631	-15.9066	-38.6443	-11.6264	-38.1876	-11.9631
101	-11.8252	-35.3674	-30.3239	-9.3134	-28.7323	-11.8252
101	-11.7870	-32.8359	-42.1618	-10.4219	-44.3118	-11.7870
102	-13.9996	-36.7640	-30.5189	-8.8516	-40.3827	-13.9996
102	-13.0901	-28.8061	-41.7748	-9.6394	-42.1042	-13.0901
102	-13.0091	-34.6618	-31.2806	-12.9475	-40.4160	-13.0091
102	-12.8506	-29.6797	-32.4309	-10.1556	-42.0117	-12.8506
102	-12.3459	-37.1109	-47.9727	-14.3032	-20.5489	-12.3459
102	-12.1038	-27.7561	-32.8162	-8.8914	-14.9359	-12.1038
102	-12.0589	-25.3789	-37.0422	-9.9461	-24.7876	-12.0589
102	-12.0402	-21.8883	-40.9404	-9.3810	-14.4076	-12.0402
102	-12.0375	-35.2435	-37.3068	-9.0291	-33.1743	-12.0375
102	-11.6383	-39.9270	-46.4264	-10.6671	-20.1731	-11.6383
103	-13.9227	61.9473	-36.7259	-14.0740	-34.3617	-13.9227
103	-13.4717	71.4960	-41.5629	-10.5234	-33.6952	-13.4717
103	-13.1443	84.3240	-36.3993	-11.4807	-41.3370	-13.1443

103	-13.1089	69.3533	-41.2107	-10.1049	-29.3865	-13.1089
103	-13.0656	94.8442	-39.1437	-10.5228	4.4025	-13.0656
103	-13.0345	68.6549	-47.7202	-11.6415	-25.8877	-13.0345
103	-13.0237	70.8886	-50.9413	-15.2267	-15.9869	-13.0237
103	-13.0026	65.7438	-53.9544	-13.7864	-15.9103	-13.0026
103	-12.8744	59.6733	-24.4681	-10.1935	-49.8896	-12.8744
103	-12.6055	71.7170	-44.2729	-9.9470	-6.9944	-12.6055
104	-13.2724	19.5220	-39.9818	-6.5987	-49.4039	-13.2724
104	-13.1122	21.5552	-39.1112	-5.6352	-28.1167	-13.1122
104	-13.1041	22.8839	-37.1550	-9.4690	-29.9720	-13.1041
104	-13.0803	33.8209	-38.4192	-8.9328	-12.2988	-13.0803
104	-12.9031	20.4442	-46.5151	-13.8524	-25.7183	-12.9031
104	-12.8882	31.8225	-31.9359	-5.8592	-7.2517	-12.8882
104	-12.4466	19.6747	-38.3936	-8.4242	-25.6282	-12.4466
104	-12.1980	32.7334	-30.4606	-5.9682	-22.8145	-12.1980
104	-12.1112	25.1185	-31.6749	-6.2887	-28.6773	-12.1112
104	-11.8779	28.2488	-33.3980	-6.0777	-21.9809	-11.8779
105	-13.2919	-26.3136	-29.3754	-10.0072	-34.1212	-13.2919
105	-13.1857	-24.1791	-31.7074	-8.1089	-40.4823	-13.1857
105	-12.7027	-18.4323	-41.9287	-11.5208	-36.6389	-12.7027
105	-12.2611	-9.3337	-34.3203	-8.9552	-22.6323	-12.2611
105	-11.9169	-29.0456	-43.3516	-8.5363	-42.9096	-11.9169
105	-11.9161	-19.0928	-41.7480	-11.8161	-32.5323	-11.9161
105	-11.8276	0.4808	-38.1390	-12.8112	-1.2999	-11.8276
105	-11.6509	-19.1721	-42.9286	-13.0212	-15.4250	-11.6509
105	-11.5686	-4.1587	-31.7187	-8.0392	-26.6310	-11.5686
105	-11.5016	-5.3967	-45.9726	-8.7194	5.8071	-11.5016
106	-12.8380	-31.3624	-39.3547	-8.3808	-36.8283	-12.8380
106	-12.6549	-32.0140	-43.9789	-8.6597	-34.1170	-12.6549
106	-12.0849	-35.5942	-36.1921	-9.2492	-31.7051	-12.0849
106	-11.8003	-32.0328	-31.7923	-8.9200	-37.4884	-11.8003
106	-11.5836	-25.4816	-42.5848	-8.6374	-34.3041	-11.5836
106	-10.8650	-24.8079	-34.0322	-8.5941	-3.0885	-10.8650
106	-10.7710	1.0294	-27.8828	-10.1598	-14.1422	-10.7710
106	-10.7505	-15.8679	-46.1101	-12.4416	-24.9690	-10.7505
106	-10.5953	-27.4131	-39.3755	-11.4717	-12.4948	-10.5953
106	-10.4992	-12.8825	-37.0383	-7.9968	-15.4262	-10.4992
107	-13.6560	-19.8593	-39.0524	-8.5377	-34.9460	-13.6560
107	-13.3772	-11.7068	-36.4815	-9.6916	-36.2841	-13.3772
107	-13.0635	-16.9323	-35.6122	-7.2690	-43.3134	-13.0635
107	-12.7387	-3.1966	-44.0839	-10.4600	-21.2817	-12.7387
107	-12.4258	-17.2141	-39.7807	-6.3906	-43.2329	-12.4258
107	-12.3761	5.3447	-38.1959	-7.9616	-19.7997	-12.3761
107	-11.8839	-8.8793	-30.7997	-6.3548	-33.6431	-11.8839
107	-11.8830	-20.4228	-48.6990	-9.8811	-39.5900	-11.8830
107	-11.7609	19.4223	-32.0701	-7.3757	-35.5953	-11.7609

107	-11.2813	5.4342	-38.0325	-8.4482	13.9282	-11.2813
108	-14.2532	-6.5554	-32.7844	-7.7837	-39.5474	-14.2532
108	-13.2128	-2.3095	-38.0058	-6.9601	-35.0498	-13.2128
108	-13.1052	-18.0063	-41.1221	-8.8349	-54.4797	-13.1052
108	-13.1012	-14.8590	-40.1797	-5.8418	-45.1053	-13.1012
108	-12.8433	-19.2143	-36.5176	-6.6693	-45.3297	-12.8433
108	-12.8241	-11.5783	-51.4954	-11.5156	-48.2989	-12.8241
108	-12.5439	-17.6870	-31.0016	-7.1412	-32.5006	-12.5439
108	-12.4551	9.6269	-44.3344	-8.7019	-21.2275	-12.4551
108	-11.9461	-8.4717	-28.0856	-7.4854	-51.6835	-11.9461
108	-11.7638	37.1281	-21.3482	-7.0689	15.1441	-11.7638
109	-13.6486	-15.8015	-38.3429	-9.7004	-34.1549	-13.6486
109	-13.1803	-19.3264	-38.0090	-9.6534	-47.5871	-13.1803
109	-12.4202	-16.3452	-37.0547	-10.1882	-32.0035	-12.4202
109	-12.3547	-17.4839	-50.4476	-12.6722	-46.0893	-12.3547
109	-12.3148	-16.4322	-37.3541	-9.2936	-47.6331	-12.3148
109	-12.1717	-8.2175	-50.9096	-14.4905	-35.8276	-12.1717
109	-12.1344	-16.2296	-34.7105	-8.7344	-25.2731	-12.1344
109	-12.0240	-15.7676	-42.4748	-11.6449	-25.7179	-12.0240
109	-11.9406	-8.4269	-33.4581	-8.8052	-44.3456	-11.9406
109	-11.9282	-9.9562	-32.8257	-9.6981	-39.7703	-11.9282
110	-13.6251	-16.5257	-36.8799	-7.2498	-49.8227	-13.6251
110	-13.3715	-14.1777	-39.9236	-12.9280	-42.3020	-13.3715
110	-13.3419	-21.0900	-33.0154	-10.6558	-46.0461	-13.3419
110	-13.3095	-20.5705	-30.2201	-7.0429	-45.6255	-13.3095
110	-13.1535	-5.9211	-39.0711	-6.8718	-43.0037	-13.1535
110	-13.0845	-19.8865	-41.2342	-8.1642	-36.3238	-13.0845
110	-13.0420	-10.1343	-40.8746	-7.9904	-24.1019	-13.0420
110	-12.8191	-18.8791	-43.5433	-10.3859	-34.9438	-12.8191
110	-12.5993	-5.3241	-25.3167	-9.5287	-28.4308	-12.5993
110	-12.3990	-18.5326	-26.1022	-9.0165	-32.8311	-12.3990
111	-13.8409	-43.1323	-46.8640	-15.1132	-32.6597	-13.8409
111	-12.9402	-45.9776	-42.0135	-9.7253	-32.8162	-12.9402
111	-12.7890	-45.1864	-39.3825	-8.4628	-50.8492	-12.7890
111	-12.7423	-48.2903	-38.4855	-7.9859	-51.1652	-12.7423
111	-12.0338	-36.0260	-26.8280	-8.1676	-48.6688	-12.0338
111	-11.7969	-37.9090	-31.3148	-11.8390	-36.4672	-11.7969
111	-11.6041	-26.7128	-32.9927	-8.8547	-29.5818	-11.6041
111	-11.4976	-42.4848	-50.0180	-12.4750	-33.0035	-11.4976
111	-11.2706	-35.8504	-49.9056	-12.2222	-37.2042	-11.2706
111	-10.8648	-42.8687	-35.6526	-8.2007	-41.5713	-10.8648

Table S7. Ten top scored docking positioning of the SIRT2 inhibitors **112**-**116** at the 4RMG PDB code (MOE software). The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
112	-5.3404	59.8378	-16.3372	-8.6437	-26.4935	-5.3404
112	-5.3265	61.6343	-18.8272	-8.2548	-28.2900	-5.3265
112	-5.3083	60.0833	-20.3968	-8.6529	-29.6896	-5.3083
112	-5.2745	63.1445	-21.8302	-8.2616	-27.0410	-5.2745
112	-5.2461	61.5283	-23.3147	-8.4870	-28.8639	-5.2461
112	-5.2074	62.8579	-20.4852	-8.3638	-28.0144	-5.2074
112	-5.1784	56.8209	-18.8881	-8.7044	-25.9658	-5.1784
112	-5.0579	57.1992	-18.6478	-8.3481	-26.9594	-5.0579
112	-4.9180	61.9024	-19.2827	-8.4992	-29.0794	-4.9180
112	-4.7806	60.1270	-19.1407	-8.4167	-24.3645	-4.7806
113	-6.3165	44.2262	-15.2498	-8.5265	-31.4510	-6.3165
113	-5.4965	38.3458	-16.9127	-7.9596	-28.8435	-5.4965
113	-5.2981	39.7475	-16.5890	-8.1990	-27.5821	-5.2981
113	-5.1898	42.3413	-15.6630	-8.0201	-25.2773	-5.1898
113	-5.1765	40.3803	-16.6091	-8.3596	-28.0338	-5.1765
113	-5.1283	36.8748	-18.1882	-8.3079	-26.4272	-5.1283
113	-5.1130	39.1993	-18.4080	-8.6236	-29.9559	-5.1130
113	-5.1074	40.9832	-19.3570	-8.2924	-28.2961	-5.1074
113	-5.0882	39.4675	-17.5327	-8.1827	-27.2754	-5.0882
113	-4.8356	39.0311	-17.2206	-7.9864	-28.2777	-4.8356
114	-7.6047	56.1428	-19.8853	-8.4233	-32.8524	-7.6047
114	-7.5091	53.3907	-24.5982	-8.2436	-35.7618	-7.5091
114	-7.2908	48.8385	-19.2412	-8.2456	-33.5995	-7.2908
114	-7.2465	60.1492	-19.9816	-8.9000	-35.4482	-7.2465
114	-7.0725	54.4772	-22.4791	-9.8409	-32.5215	-7.0725
114	-7.0702	52.3370	-26.0485	-9.5573	-28.7765	-7.0702
114	-7.0329	58.9761	-24.8942	-8.3054	-1.6790	-7.0329
114	-6.7586	52.4518	-29.2516	-8.3379	-27.2222	-6.7586
114	-6.7520	49.1823	-17.1326	-8.4774	-25.2842	-6.7520
114	-6.7231	50.2336	-24.7436	-8.4636	-32.5501	-6.7231
115	-8.1909	56.1645	-24.7630	-8.9699	-32.9392	-8.1909
115	-8.0161	47.2657	-24.2299	-9.4777	-36.1067	-8.0161
115	-7.9050	49.7090	-20.4748	-10.7569	-34.0771	-7.9050
115	-7.8454	46.6672	-21.5455	-8.8880	-32.5392	-7.8454
115	-7.7931	42.1018	-22.5821	-8.7167	-34.2423	-7.7931
115	-7.6376	45.2911	-28.3659	-9.0910	-34.4934	-7.6376
115	-7.5658	43.7207	-26.5945	-9.5005	-35.2860	-7.5658
115	-7.3632	48.1657	-22.4882	-8.8172	-30.9688	-7.3632
115	-7.3009	43.1822	-27.0364	-10.0190	-30.9944	-7.3009
115	-7.2491	48.6016	-22.4063	-9.5644	-25.4465	-7.2491
116	-7.2539	46.7363	-19.6167	-9.5343	-36.4286	-7.2539
116	-7.1088	42.0126	-29.5901	-9.4017	-32.8432	-7.1088
116	-6.7788	43.3001	-17.9842	-9.1838	-25.6907	-6.7788
116	-6.7039	37.7617	-20.8041	-9.9379	-33.4346	-6.7039
116	-6.6723	41.8600	-18.2389	-9.2197	-31.6015	-6.6723

116	-6.6704	40.0015	-23.4932	-10.2214	-35.0815	-6.6704
116	-6.6428	37.6876	-21.8879	-9.4988	-35.0622	-6.6428
116	-6.4847	40.2980	-24.3624	-10.4979	-28.6348	-6.4847
116	-6.4783	39.2429	-26.3302	-9.7845	-33.8369	-6.4783
116	-6.4019	41.5733	-23.6571	-9.9247	-29.7559	-6.4019

Table S8. Ten top scored docking positioning of the SIRT2 inhibitors **112**-**116** at the 5MAT PDB code (MOE software). The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
112	-5.4023	58.0304	-24.6803	-9.0243	-31.3765	-5.4023
112	-5.3284	58.0911	-29.9347	-8.9925	-28.4771	-5.3284
112	-5.2932	57.3992	-21.7561	-9.7625	-30.7691	-5.2932
112	-5.0898	60.5048	-21.2533	-9.1751	-20.4286	-5.0898
112	-5.0898	56.9218	-24.3986	-10.3952	-22.9202	-5.0898
112	-5.0698	58.6302	-21.6301	-9.1057	-27.5706	-5.0698
112	-4.9684	58.6663	-26.4878	-9.4748	-27.9082	-4.9684
112	-4.7547	61.2353	-21.2899	-8.9922	-23.9356	-4.7547
112	-4.7182	57.3022	-24.1629	-10.3518	-23.2956	-4.7182
112	-4.7069	57.8997	-23.2594	-9.5909	-24.2361	-4.7069
113	-5.9011	42.4399	-21.5776	-9.2598	-28.3076	-5.9011
113	-5.6987	39.7731	-20.0498	-9.5829	-25.0967	-5.6987
113	-5.5278	44.2905	-19.7953	-9.1534	-32.5271	-5.5278
113	-5.3895	37.7410	-20.5915	-9.9990	-24.5152	-5.3895
113	-5.3248	36.2321	-27.8934	-9.1819	-31.0722	-5.3248
113	-5.3060	39.8297	-18.1193	-10.0368	-14.2443	-5.3060
113	-5.1056	36.2650	-28.8735	-9.1303	-30.1118	-5.1056
113	-5.0768	35.2090	-25.7017	-9.7220	-24.0103	-5.0768
113	-5.0683	37.6896	-20.6784	-10.5521	-24.9659	-5.0683
113	-5.0535	37.3638	-18.6594	-9.2848	-30.8609	-5.0535
114	-7.5841	54.1520	-35.8740	-10.0868	-36.3495	-7.5841
114	-7.4988	49.1339	-23.6264	-10.5368	-34.0066	-7.4988
114	-7.2571	56.0720	-27.0842	-9.4126	-26.3210	-7.2571
114	-6.9616	49.7687	-27.4455	-10.4168	-22.8566	-6.9616
114	-6.9084	48.9685	-25.7429	-9.7629	-26.6270	-6.9084
114	-6.8979	49.6057	-28.9360	-13.0813	-28.1924	-6.8979
114	-6.8454	49.5683	-29.4569	-9.7046	-36.0863	-6.8454
114	-6.8243	50.9265	-31.4947	-9.6330	-34.2884	-6.8243
114	-6.7689	52.3632	-31.4140	-9.4984	-31.5505	-6.7689
114	-6.7566	58.4894	-25.4328	-9.3952	-21.7167	-6.7566
115	-8.9498	50.2785	-34.2241	-9.7881	-24.0972	-8.9498
115	-8.7633	43.5833	-34.4952	-10.8327	-26.8257	-8.7633
115	-8.4265	56.7462	-25.5619	-10.7349	-9.5371	-8.4265

115	-7.9018	48.0603	-34.2411	-9.4160	-28.8188	-7.9018
115	-7.7322	60.0283	-29.8330	-10.0257	-13.0355	-7.7322
115	-7.7089	44.9534	-35.7338	-9.3509	-31.4795	-7.7089
115	-7.6974	47.9193	-38.3521	-9.2723	-36.8062	-7.6974
115	-7.3669	43.7385	-23.4590	-9.8761	-29.2321	-7.3669
115	-7.2136	45.6139	-28.2125	-9.5690	-28.4975	-7.2136
115	-7.1958	44.1212	-40.2594	-9.4507	-37.3636	-7.1958
116	-7.8486	44.7246	-30.2459	-11.5293	-23.6337	-7.8486
116	-7.8246	40.9332	-33.7298	-11.7900	-27.2326	-7.8246
116	-7.5013	50.5289	-28.8678	-10.3889	-8.3230	-7.5013
116	-7.3001	40.2446	-28.6276	-10.7942	-26.2434	-7.3001
116	-7.0524	39.7383	-32.6974	-10.2507	-22.8952	-7.0524
116	-7.0260	43.3439	-33.3518	-10.2843	-29.9638	-7.0260
116	-6.9430	43.6470	-30.9061	-10.1495	-38.6868	-6.9430
116	-6.8599	44.5372	-28.3784	-11.2958	-30.0644	-6.8599
116	-6.7727	39.4847	-27.2874	-10.8823	-24.1711	-6.7727
116	-6.6726	46.7541	-28.0513	-10.6129	-23.5490	-6.6726

Table S9. Rigid protein Virtual screening. Ten top scored docking positioning of the novel identified SIRT2 inhibitors **1a**-**7a** at the 4RMG PDB code (MOE software). The SIRT2 inhibitor AGK2 has been also considered as reference compound. The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
1a	-9.4004	34.2832	-26.4484	-8.8771	-7.4778	-9.4004
1a	-9.0980	39.6262	-23.6360	-10.5270	-14.8229	-9.0980
1a	-8.9235	37.4397	-19.8001	-8.5350	-16.4555	-8.9235
1a	-8.7738	46.7376	-25.1603	-8.8724	0.3711	-8.7738
1a	-8.2850	38.8720	-20.8246	-8.6022	-21.8182	-8.2850
1a	-8.0325	28.0057	-21.1364	-9.2539	-25.5420	-8.0325
1a	-8.0218	26.5764	-26.4965	-9.4738	-26.9227	-8.0218
1a	-7.9091	28.2035	-19.0495	-8.5543	-26.2193	-7.9091
1a	-7.8140	27.2928	-23.5073	-8.8179	-19.9696	-7.8140
1a	-7.7192	44.5577	-26.3606	-8.3942	-15.0075	-7.7192
2a	-10.0158	33.7044	-28.5256	-8.9755	-4.1568	-10.0158
2a	-10.0043	47.1255	-26.2476	-8.9433	2.5064	-10.0043
2a	-9.9162	69.4167	-17.9713	-8.7402	23.6811	-9.9162
2a	-9.7029	31.5735	-21.8140	-8.1540	-15.1579	-9.7029
2a	-9.2695	31.8094	-23.5908	-8.3551	-3.6524	-9.2695
2a	-8.9896	22.3920	-23.9999	-9.0055	-21.4666	-8.9896
2a	-8.8657	34.1510	-17.8360	-7.9587	-9.5086	-8.8657
2a	-8.7431	27.0064	-16.2796	-8.1977	-23.0232	-8.7431
2a	-8.6515	31.1323	-14.2086	-8.8127	-13.8846	-8.6515
2a	-8.5009	37.6623	-19.3668	-8.1114	-11.6729	-8.5009

3a	-9.4095	13.5647	-26.2863	-10.8934	-4.9516	-9.4095
3a	-9.3214	11.9038	-20.8187	-8.5315	-8.9750	-9.3214
3a	-9.2346	12.7771	-21.7444	-8.5093	-12.6848	-9.2346
3a	-9.1770	16.1019	-18.6855	-9.4505	-10.3090	-9.1770
3a	-9.0238	18.5116	-26.9030	-10.0900	0.3880	-9.0238
3a	-8.9911	16.6799	-19.2242	-8.7453	-22.7360	-8.9911
3a	-8.9487	20.5321	-17.3321	-8.6670	14.3788	-8.9487
3a	-8.8221	27.8127	-20.2365	-9.8340	16.7268	-8.8221
3a	-8.3943	22.0333	-21.6604	-8.8903	-6.6167	-8.3943
3a	-8.2425	7.9952	-23.9063	-8.6930	-25.1096	-8.2425
4a	-8.9714	1.8032	-20.7065	-7.9314	-7.7120	-8.9714
4a	-8.8710	11.6294	-21.3511	-9.6427	-11.4867	-8.8710
4a	-8.7651	11.6405	-29.4715	-9.8587	-15.2393	-8.7651
4a	-8.3924	48.8920	-15.6768	-8.5757	39.5095	-8.3924
4a	-8.2901	7.0567	-20.5867	-8.0299	-11.5678	-8.2901
4a	-8.1999	20.3162	-25.8684	-11.0583	53.5885	-8.1999
4a	-8.1857	0.5710	-22.8665	-9.3643	-26.9827	-8.1857
4a	-7.8969	12.1843	-26.1390	-9.0207	-13.4661	-7.8969
4a	-7.8297	17.5383	-28.9195	-8.2356	-9.4861	-7.8297
4a	-7.7045	27.0419	-13.6158	-8.4785	0.8708	-7.7045
5a	-9.0509	-5.3699	-19.7405	-9.5322	-14.4267	-9.0509
5a	-8.7092	-11.3884	-14.5392	-10.3442	-11.5082	-8.7092
5a	-8.5754	-3.5155	-22.0600	-8.7457	-4.9687	-8.5754
5a	-8.3696	-10.0206	-32.3261	-8.8055	-23.6363	-8.3696
5a	-8.2574	-4.8716	-25.9557	-10.7752	-9.6070	-8.2574
5a	-8.0120	-23.1228	-25.9350	-8.3756	-23.5931	-8.0120
5a	-7.8355	10.0989	-24.5592	-10.1955	17.2742	-7.8355
5a	-7.8120	2.1871	-24.3836	-8.5911	7.2494	-7.8120
5a	-7.7134	-11.9154	-19.3414	-10.2077	-17.1831	-7.7134
5a	-7.6351	30.3790	-22.1878	-8.4060	42.9440	-7.6351
6a	-10.2478	7.8728	-21.8975	-10.1859	3.6999	-10.2478
6a	-9.8349	7.8143	-30.6188	-9.4173	4.1768	-9.8349
6a	-9.8206	0.2044	-25.9691	-10.3372	-24.0262	-9.8206
6a	-9.8161	13.4661	-28.7141	-11.9312	-10.1151	-9.8161
6a	-9.7389	10.8004	-22.6697	-10.0088	-11.3049	-9.7389
6a	-9.7264	11.0218	-26.8641	-8.5777	-14.7350	-9.7264
6a	-9.5483	17.2348	-17.3659	-8.6805	7.1432	-9.5483
6a	-9.4567	8.2724	-26.6179	-9.3536	-19.4069	-9.4567
6a	-9.2866	-1.4136	-22.5072	-9.9414	-20.6150	-9.2866
6a	-9.1944	9.2750	-17.4803	-8.3166	-8.3928	-9.1944
7a	-10.7072	61.5467	-23.1041	-8.5819	-8.9134	-10.7072
7a	-10.6169	75.2277	-20.0870	-8.6678	5.8752	-10.6169
7a	-10.6089	58.8829	-20.4931	-9.5911	-4.9472	-10.6089
7a	-10.5852	43.2278	-22.9289	-8.6362	-3.6911	-10.5852
7a	-10.5111	55.2774	-18.9151	-9.5828	0.5999	-10.5111
7a	-10.4843	44.5222	-21.0537	-8.8491	-3.4183	-10.4843

7a	-10.3800	44.4986	-21.2328	-8.9472	-3.9157	-10.3800
7a	-10.3766	53.8000	-20.9551	-8.8092	8.2720	-10.3766
7a	-10.3617	58.3304	-27.6435	-9.3668	4.5437	-10.3617
7a	-10.1839	43.9191	-26.2669	-9.1892	-7.1624	-10.1839
AGK2	-12.3545	43.1796	-27.9120	-7.9005	-1.2242	-12.3545

Table S10. Rigid protein Virtual screening. Ten top scored docking positioning of the novel identified SIRT2 inhibitors **1a**-**7a** at the 5MAT PDB code (MOE software). The SIRT2 inhibitor AGK2 has been also considered as reference compound. The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
1a	-8.5706	39.7190	-31.6267	-9.1109	-17.4603	-8.5706
1a	-8.2475	29.7915	-27.8109	-8.2177	-12.4591	-8.2475
1a	-8.0268	42.9923	-29.6301	-8.1718	-0.9737	-8.0268
1a	-7.9812	34.1350	-35.0882	-10.5088	4.1888	-7.9812
1a	-7.9694	29.8000	-26.6836	-8.2964	1.4244	-7.9694
1a	-7.7901	30.0656	-20.3196	-9.3502	-10.5859	-7.7901
1a	-7.6679	38.4283	-18.6014	-8.0613	-1.0470	-7.6679
1a	-7.6545	34.4443	-20.4333	-9.0135	-12.1696	-7.6545
1a	-7.6514	32.4146	-26.3872	-9.4187	5.6106	-7.6514
1a	-7.6252	35.6247	-28.3564	-12.4230	-5.9837	-7.6252
2a	-9.4364	35.2733	-35.3793	-8.6924	3.9134	-9.4364
2a	-9.4276	27.6578	-35.4135	-8.1682	-12.1070	-9.4276
2a	-9.2711	31.7483	-25.4143	-8.1453	-20.1741	-9.2711
2a	-9.2337	48.8123	-26.4006	-9.0498	11.0988	-9.2337
2a	-9.0424	36.7183	-36.0633	-10.4274	-5.8903	-9.0424
2a	-8.9952	46.9316	-35.4645	-9.2158	-2.0447	-8.9952
2a	-8.9628	43.4355	-26.3714	-8.1427	14.3257	-8.9628
2a	-8.9233	33.1059	-35.0816	-9.2701	1.3757	-8.9233
2a	-8.6349	42.3913	-32.4158	-8.5784	-4.2029	-8.6349
2a	-8.5070	54.7463	-33.5414	-8.4096	32.2391	-8.5070
3a	-8.8986	14.2885	-21.5164	-9.8610	4.9477	-8.8986
3a	-8.8334	17.8821	-29.8018	-9.9412	29.0717	-8.8334
3a	-8.4582	23.4765	-33.4347	-9.2954	15.3096	-8.4582
3a	-8.4518	9.6196	-29.1194	-9.4483	-6.3696	-8.4518
3a	-8.3834	13.0392	-30.4483	-9.8047	-3.0555	-8.3834
3a	-8.3659	15.7303	-34.8093	-9.8573	-3.2631	-8.3659
3a	-8.3309	14.0364	-32.2264	-9.7231	-14.8324	-8.3309
3a	-8.3302	18.8577	-32.4724	-10.4734	-18.3485	-8.3302
3a	-8.0978	19.3630	-35.6233	-9.8700	-17.9022	-8.0978
3a	-7.9813	20.6845	-36.2188	-9.7647	-7.8962	-7.9813
4a	-9.7765	8.9145	-28.6109	-10.2765	-18.7757	-9.7765
4a	-9.7092	13.1769	-33.3017	-9.6286	-12.7891	-9.7092
4a	-9.4539	17.1454	-36.0267	-11.4404	27.1018	-9.4539
4a	-9.1791	4.3688	-31.1896	-10.4415	-16.5454	-9.1791

4a	-9.1107	11.1215	-40.8968	-9.9579	-17.2215	-9.1107
4a	-9.0711	12.7261	-30.8175	-10.3442	-14.2492	-9.0711
4a	-8.9619	21.3356	-29.3996	-9.7596	17.6367	-8.9619
4a	-8.9590	5.4430	-33.1400	-10.6194	-3.1835	-8.9590
4a	-8.7561	5.7262	-28.7116	-10.8634	-14.9002	-8.7561
4a	-8.5978	5.0440	-25.7699	-9.8994	-8.2443	-8.5978
5a	-9.9680	-13.4394	-26.9203	-9.0680	-20.1495	-9.9680
5a	-9.8936	-9.2862	-34.5184	-8.7033	-10.2397	-9.8936
5a	-9.4852	-11.6869	-33.0015	-10.6444	-19.3875	-9.4852
5a	-9.3342	-11.0063	-25.1340	-9.4906	-16.7457	-9.3342
5a	-9.2818	-6.4384	-30.3503	-8.8831	-12.4089	-9.2818
5a	-9.2224	-10.6289	-27.7229	-11.8456	-10.7057	-9.2224
5a	-9.0125	-8.9704	-27.9633	-9.2092	1.7897	-9.0125
5a	-8.9629	-3.1532	-29.7299	-9.6717	17.6341	-8.9629
5a	-8.8553	-17.9331	-24.4935	-10.0497	-13.4442	-8.8553
5a	-8.5990	17.7923	-27.9206	-11.3114	66.8918	-8.5990
6a	-10.9884	10.8527	-39.5053	-10.7373	-16.0098	-10.9884
6a	-10.8360	3.7936	-30.9982	-10.7509	-14.6279	-10.8360
6a	-10.7763	24.2042	-32.5021	-9.7274	27.5252	-10.7763
6a	-10.6794	8.1983	-27.2891	-10.0424	-5.1963	-10.6794
6a	-10.5061	10.6062	-29.3086	-11.2600	-11.8971	-10.5061
6a	-10.4118	13.6811	-35.3761	-11.0359	-11.4316	-10.4118
6a	-9.7078	9.6792	-30.7673	-9.6506	2.2642	-9.7078
6a	-9.5490	19.0121	-33.4839	-9.7753	44.5090	-9.5490
6a	-9.5220	28.8933	-35.4535	-10.1640	6.9597	-9.5220
6a	-9.2936	23.3174	-25.7204	-9.6846	12.8830	-9.2936
7a	-9.9227	54.2778	-34.6917	-10.7258	3.1148	-9.9227
7a	-9.5259	55.9304	-25.8540	-8.9765	11.5004	-9.5259
7a	-9.4850	53.3920	-37.1103	-8.7369	4.6319	-9.4850
7a	-9.4821	66.4844	-29.7207	-9.1317	25.4970	-9.4821
7a	-9.3514	71.9428	-31.3255	-8.4030	2.5715	-9.3514
7a	-9.1916	54.6667	-27.3826	-9.1572	12.3761	-9.1916
7a	-9.1491	64.0590	-32.5278	-8.3140	1.9188	-9.1491
7a	-9.1452	69.7133	-27.9359	-10.4305	61.2354	-9.1452
7a	-9.0220	72.5005	-33.1113	-8.4135	2.6576	-9.0220
7a	-8.6434	67.3448	-22.7825	-8.3873	27.7506	-8.6434
AGK2	-11.7728	62.7179	-28.1687	-7.6774	40.1252	-11.7728

Table S11. Flexible protein Virtual screening. Five top scored docking positioning of the novel identified SIRT2 inhibitors **1a**-**7a** at the 4RMG PDB code (MOE software). The SIRT2 inhibitor AGK2 has been also considered as reference compound. The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

Compound	S	E_conf	E_place	E_score1	E_refine	E_score2
1a	-9.5617	30.1341	-24.8953	-10.5752	-19.1446	-9.5617
1a	-9.5488	29.3902	-27.6763	-9.1281	-19.0177	-9.5488
1a	-9.4884	30.6250	-23.8048	-8.3081	-19.0965	-9.4884
1a	-8.6303	35.2950	-27.9394	-8.3756	-18.3631	-8.6303
1a	-8.4510	36.3321	-26.9235	-8.5330	-23.6778	-8.4510
2a	-10.5439	25.8577	-24.2694	-8.2227	-3.8073	-10.5439
2a	-10.3583	38.9237	-25.5446	-8.0893	-2.8473	-10.3583
2a	-10.3562	38.3786	-28.0415	-8.5344	-17.9208	-10.3562
2a	-10.3326	44.1909	-18.3727	-8.3089	-0.7735	-10.3326
2a	-10.1423	31.8108	-28.2591	-10.5753	15.9216	-10.1423
3a	-9.5571	8.7658	-26.6166	-9.8003	-13.9148	-9.5571
3a	-9.4864	14.3085	-26.5698	-9.8797	-13.9755	-9.4864
3a	-9.4290	8.0651	-22.8752	-8.8471	-19.1138	-9.4290
3a	-9.2953	17.4309	-25.9498	-8.8664	-21.3621	-9.2953
3a	-9.2666	13.5796	-16.8761	-8.8021	-24.3819	-9.2666
4a	-9.4795	12.7061	-25.8140	-9.0960	-13.9820	-9.4795
4a	-9.3082	9.7623	-21.8115	-8.9848	-13.0469	-9.3082
4a	-9.2204	9.5686	-13.0012	-10.4389	-5.5669	-9.2204
4a	-9.0953	19.4831	-24.8256	-8.7022	-18.3639	-9.0953
4a	-8.9591	8.0038	-24.6987	-8.6367	-12.7982	-8.9591
5a	-9.8703	-14.6966	-24.8607	-9.8611	-1.1262	-9.8703
5a	-9.1115	-9.5073	-24.4054	-10.5811	-20.8337	-9.1115
5a	-8.9825	-11.2181	-18.8741	-9.7312	-21.6268	-8.9825
5a	-8.4246	-20.7734	-24.6435	-8.7084	-7.7907	-8.4246
5a	-8.2710	-8.8776	-26.1773	-9.3543	-13.5277	-8.2710
6a	-10.3828	13.7101	-26.5277	-9.7503	-20.0673	-10.3828
6a	-10.3184	15.6072	-28.9513	-10.3406	-3.2860	-10.3184
6a	-10.2685	11.6418	-20.3297	-8.6215	-22.0868	-10.2685
6a	-10.0371	10.4418	-30.7654	-9.9595	-23.8399	-10.0371
6a	-9.8793	8.3028	-27.7035	-8.8663	-19.4066	-9.8793
7a	-10.9785	56.5435	-17.8592	-8.8760	-8.7181	-10.9785
7a	-10.6662	57.6456	-22.3537	-10.9067	-20.4469	-10.6662
7a	-10.6378	52.9520	-31.1625	-10.4170	-17.9076	-10.6378
7a	-10.5375	47.8347	-20.8423	-9.3579	-11.9879	-10.5375
7a	-10.2985	53.1118	-26.2195	-10.1949	-6.5685	-10.2985
AGK2	-11,5559	43.7486	-25.3648	-8.7591	12.0598	-11.5559

Table S12. Flexible protein Virtual screening. Five top scored docking positioning of the novel identified SIRT2 inhibitors **1a**-**7a** at the 5MAT PDB code (MOE software). The SIRT2 inhibitor AGK2 has been also considered as reference compound. The predicted ΔG value of each protein-ligand complex has been reported, as calculated in terms of final scoring function (S, as Kcal/mol).

mseq	S	E_conf	E_place	E_score1	E_refine	E_score2
1a	-8.5504	35.8090	-27.4786	-9.3227	-23.9326	-8.5504
1a	-8.0335	41.8086	-25.0820	-9.1672	10.4411	-8.0335
1a	-8.0008	38.8853	-35.6432	-10.6364	-16.4839	-8.0008
1a	-7.4592	33.5926	-25.0119	-9.2003	-23.2686	-7.4592
1a	-7.4078	26.0521	-28.1108	-11.1153	-15.4990	-7.4078
2a	-9.2688	34.1839	-31.3363	-9.5055	-13.4631	-9.2688
2a	-9.2660	33.1133	-37.1513	-9.7663	-17.8508	-9.2660
2a	-9.1151	44.0130	-37.4914	-9.8515	-12.3586	-9.1151
2a	-9.0434	30.5912	-36.5789	-11.0853	-28.2654	-9.0434
2a	-8.9878	25.2055	-33.9332	-10.2823	-12.3852	-8.9878
3a	-8.7362	9.0098	-29.7506	-9.6353	-20.9744	-8.7362
3a	-8.5721	11.6969	-32.7220	-10.0383	-21.4420	-8.5721
3a	-8.3286	18.8645	-34.1676	-10.0219	-7.1967	-8.3286
3a	-8.2745	16.7642	-21.2420	-10.0014	10.4518	-8.2745
3a	-7.9579	15.2782	-30.4212	-9.3204	-23.0374	-7.9579
4a	-11.4785	11.4543	-34.4188	-11.2323	-17.4558	-11.4785
4a	-9.2090	6.0519	-44.9981	-12.8925	-25.0428	-9.2090
4a	-9.1721	2.5929	-28.8207	-10.7807	-17.6604	-9.1721
4a	-8.9668	6.5661	-26.4576	-10.5660	-19.8077	-8.9668
4a	-8.6980	4.8363	-36.4894	-10.3089	-23.3939	-8.6980
5a	-9.3488	-16.3453	-36.5596	-10.9406	-26.6234	-9.3488
5a	-8.3594	-9.6579	-30.5816	-10.6039	-14.0273	-8.3594
5a	-8.3582	-17.5326	-31.7400	-12.9923	-23.3486	-8.3582
5a	-7.7948	-18.6275	-21.7908	-10.0312	-14.3554	-7.7948
5a	-7.7711	-19.1781	-25.8513	-10.2661	-16.3643	-7.7711
6a	-10.3401	6.2178	-40.5129	-10.4845	-21.7718	-10.3401
6a	-9.4694	9.7539	-29.7817	-11.2655	-8.4563	-9.4694
6a	-9.2092	10.4676	-30.5862	-10.1482	2.5850	-9.2092
6a	-9.0809	3.4790	-25.3108	-9.6256	-16.1220	-9.0809
6a	-8.8716	3.3537	-34.1313	-11.6179	-14.0789	-8.8716
7a	-10.3930	71.2262	-34.2017	-10.5311	14.9904	-10.3930
7a	-10.0579	47.7010	-35.7014	-10.1342	-17.5108	-10.0579
7a	-9.9081	50.9382	-35.1110	-9.0981	-8.4001	-9.9081
7a	-9.8345	70.1906	-30.3143	-9.7857	12.3281	-9.8345
7a	-9.8066	49.0991	-31.0803	-9.2944	-12.4422	-9.8066
AGK2	-11.3868	38.5745	-23.2340	-8.2233	-3.2912	-11.3868

Table S13. Calculated propertied based on the Lipinski's and Veber's rules as referred to the novel SIRT2 inhibitors **1a**-**7a** and to the reference compounds AGK2, SirReal2. Reliability index values for a number of descriptors are shown as R.I. (values higher than 0.30 are ranked as reliable by the software).

Comp.	MW[a]	N. H-bond acceptor [b]	N. H-bond donor [c]	N. rotable bonds [d]	cLogP GALAS [e] (R.I. ≥ 0.46)	TPSA [f]	HIA (%) [g]	Vd (l/kg) [h]	%PPB [i] (R.I. ≥ 0.34)	LogKa l HAS (R.I. ≥ 0.34)	%F (oral) [m] 50mg
1a	355.50	3	1	4	4.99	119.59	100	4.3	99.59	4.91	83.9
2a	360.93	2	1	5	5.88	78.65	100	4.8	99.69	5.07	64.3
3a	332.87	2	1	4	5.40	78.46	100	3.8	99.69	5.05	67.1
4a	353.46	4	2	4	4.06	107.56	100	2.3	99.13	4.42	96.5
5a	371.50	4	2	4	4.17	132.86	100	0.69	99.55	4.60	90.0
6a	407.43	4	2	5	4.32	107.65	100	2.7	99.71	4.77	81.4
7a (YM08)	367.49	4	0	2	3.14	87.04	100	2.2	98.07	4.73	98.5
AGK2	434.27	5	1	5	4.85	78.92	100	3.1	99.93	5.15	13.9
SirReal 2	420.55	5	1	6	4.99	121.31	100	2.5	98.71	4.69	21.9

a Molecular weight; b Number of H-bond acceptors; c Number of H-bond donors; d Number of rotatable bonds; e Logarithmic ratio of the octanol–water partitioning coefficient; f Topological polar surface area; g HIA represents the human intestinal absorption, expressed as percentage of the molecule able to pass through the intestinal membrane; h prediction of Volume of Distribution (Vd) of the compound in the body; i percentage of plasmatic protein bound drug; l Ligand affinity toward human serum albumin (HSA); m Percentage oral bioavailability.

Table S14. Calculated ADMET descriptors concerning the novel SIRT2 inhibitors **1a**-**7a** and the reference compounds AGK2, SirReal2 (n.d.; not determined). Reliability index values for a number of descriptors are shown as R.I. (values higher than 0.30 are ranked as reliable by the software).

Comp.	**CYP3A4**[a]		**LD_{50} (mg/kg)**[b] Mouse oral (R.I. ≥ 0.3)	**PAINS** (Pan Assay Interference structures)
	Inhibitor (IC_{50} < 10mM) (R.I. ≥ 0.3)	**Substrate** (R.I. ≥ 0.3)		
1a	0.06	0.84	800	0 ALERT
2a	0.08	0.86	730	0 ALERT
3a	0.08	0.87	n.d.	0 ALERT
4a	0.07	0.88	n.d.	0 ALERT
5a	0.03	0.87	n.d.	0 ALERT
6a	0.10	0.90	n.d.	0 ALERT
7a (YM-08)	0.16	0.93	360	0 ALERT
AGK2	0.45	0.95	900	0 ALERT
SirReal2	0.89	0.97	1100	0 ALERT

a Prediction of the ligand inhibitor/substrate behavior towards cytochrome CYP3A4; b Acute toxicity (LD_{50}) for mouse after oral administration