Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Table S1. Physicochemical properties of the twenty-seven hit compounds.

Compound	SPECS ID	AlogP	MW[a]	N_A[b]	N_D[c]	N_RB[d]	PSA[e]
1	**AE-848/32734039**	2.76	314.3	5	1	5	101.22
2	**AG-205/37106132**	1.00	277.3	5	2	5	139.52
3	**AG-205/37007270**	0.50	399.5	7	1	4	121.95
4	**AG-205/36590056**	4.17	238.2	4	2	8	124.63
5	**AG-690/11240073**	0.63	284.2	6	1	2	115.96
6	**AO-081/41934562**	1.62	338.4	4	2	5	107.29
7	**AO-008/13599001**	4.17	470.1	8	4	7	198.83
8	**AN-329/43449414**	1.49	338.4	4	2	3	123.12
9	**AO-854/43450565**	3.87	331.3	5	1	5	76.06
10	**AO-080/43441552**	4.35	211.2	4	1	4	116.04
11	**AK-968/15606187**	3.54	335.3	4	1	3	116.04
12	**AF-399/15539023**	4.51	297.3	5	2	5	105.48
13	**AN-465/15280004**	1.89	219.2	3	2	3	64.68
14	**AP-906/41641275**	4.89	359.4	5	1	3	78.27
15	**AH-979/40711131**	0.94	286.3	2	3	3	70.22
16	**AP-685/41280834**	0.99	394.2	5	2	9	76.82
17	**AN-465/42889348**	0.12	315.8	5	2	10	82.81
18	**AG-205/40650398**	5.39	327.4	4	1	5	68.9
19	**AK-968/12268011**	-1.88	375.3	5	2	5	81.78
20	**AP-906/42708958**	3.32	408.5	4	0	4	45.4
21	**AP-906/42712578**	4.92	367.4	3	1	5	63.78
22	**AG-690/10769052**	1.73	347.4	5	2	3	106.84
23	**AM-807/14146364**	3.76	359.8	5	1	4	78.35
24	**AP-970/42897159**	2.08	387.9	7	1	10	80.75
25	**AP-853/41701196**	2.44	398.9	8	3	7	160.1
26	**AK-778/43420882**	1.44	449.89	5	2	6	134
27	**AN-465/43411003**	3.05	282.34	4	3	9	89.37

[a] MW, Molecular Weight.

[b] N_A, Number of H-bond Acceptors.

[c] N_D, Number of H-bond Donors.

[d] N_RB, Number of Rotatable Bonds.

[e] PSA, Molecular_Polar Surface Area.

Table S2. Pharmacophore mapping fit values and docked binding affinities of the twenty-seven hit compounds.

Compounds	Fit Value		Relative Energy		Predicted average -log (Kd)[a]	Predicted binding energy (kcal/mol)[b]
	Pharm1	Pharm2	Pharm1	Pharm2		
1	2.68074	2.69667	7.8603	8.72842	6.04	-8.24
2	2.92045	2.50669	3.64374	2.76788	5.10	-6.96
3	2.59787	2.4223	6.84827	5.35376	5.06	-6.91
4	3.10679	3.13729	8.20731	1.27786	6.55	-8.94
5	2.60017	1.96304	1.59365	0.756621	5.48	-7.47
6	3.31914	2.8848	6.80285	11.3397	6.05	-8.26
7	2.56844	1.99965	17.3547	4.07524	5.07	-6.91
8	2.84084	2.8166	7.77097	5.30931	5.52	-7.53
9	3.48288	2.91874	17.4011	17.9902	6.49	-8.86
10	3.34258	2.89784	11.7986	8.62182	6.12	-8.34
11	3.23238	2.86055	5.87323	8.51512	5.86	-7.99
12	2.8446	2.96117	4.91806	6.06724	6.05	-8.25
13	2.92843	2.89537	9.50878	6.0475	6.16	-8.41
14	2.92465	3.1769	9.34371	6.11616	6.29	-8.58
15	2.4861	2.70236	18.9617	3.5329	5.37	-7.33
16	2.97101	2.72914	7.42589	8.41023	4.68	-6.39
17	2.95171	2.83277	11.5225	8.08934	4.70	-6.41
18	2.77815	2.9218	9.90153	7.35985	6.14	-8.38
19	2.91782	2.30294	4.98644	10.0942	4.72	-6.44
20	2.44603	2.15889	8.4663	0.0181385	5.93	-8.09
21	2.95468	2.83561	3.61977	6.05434	5.66	-7.72
22	2.80343	2.85461	8.95141	8.73511	5.43	-7.40
23	2.72763	2.9831	4.96761	3.15217	6.39	-8.71
24	2.86334	2.92987	9.69933	6.68367	5.66	-7.71
25	3.47708	3.02276	4.19222	3.97714	5.92	-8.07
26	3.47071	2.95574	8.00741	7.48183	5.95	-8.12
27	2.96498	2.86494	10.2645	9.34114	6.24	-8.51

[a] The predicted activity values by XSCORE function.

[b] The predicted activity values by GlideScore function scores in Schrödinger suite.