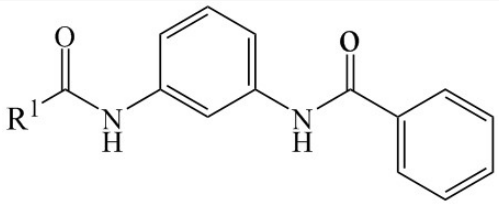
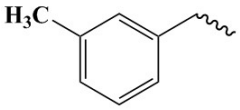
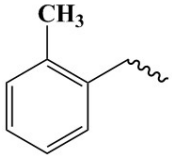
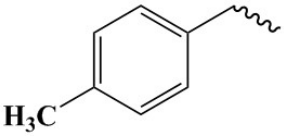
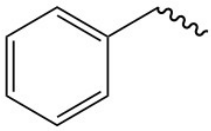
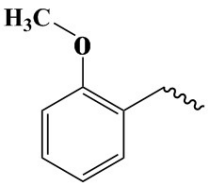
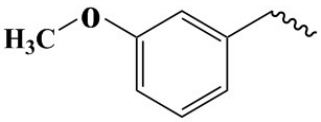
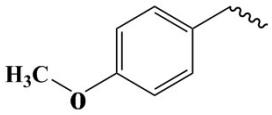
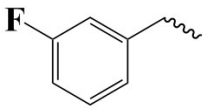
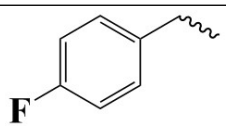
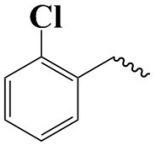
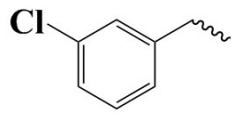
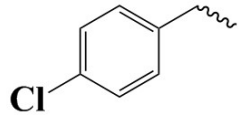
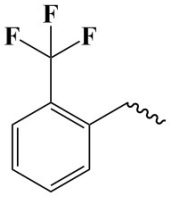
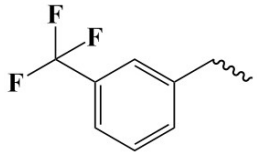
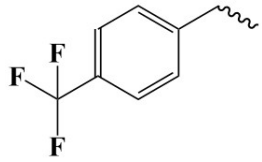
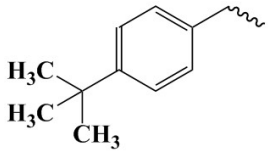
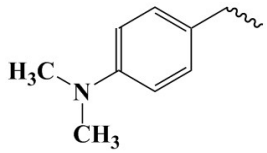
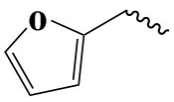
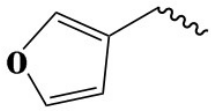
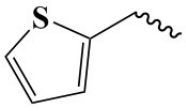
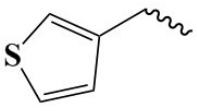
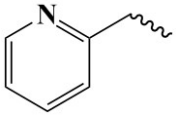
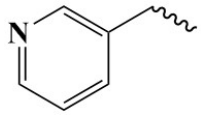
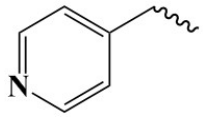
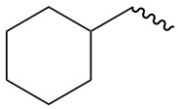
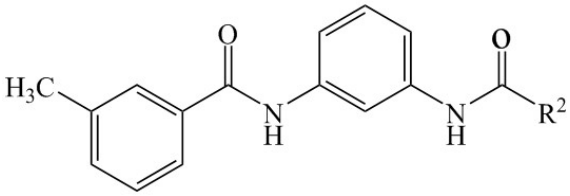
Figure S1 Activity values of bis-amide derivatives against TASK-1 and TASK-3.

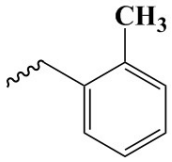
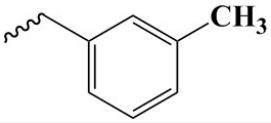
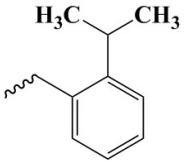
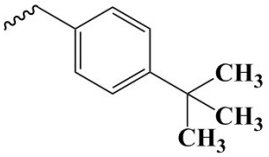
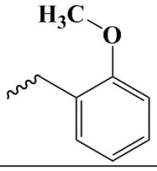
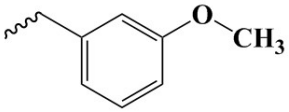
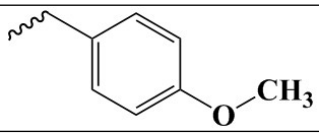


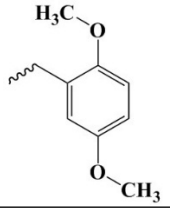
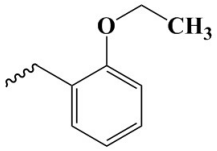
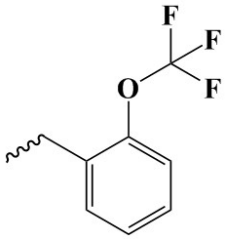
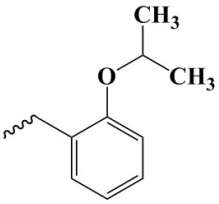
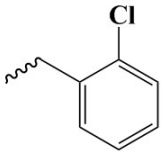
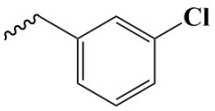
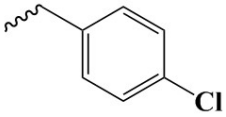
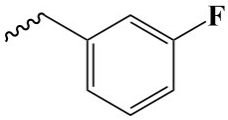
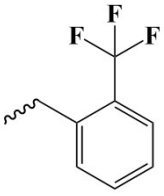
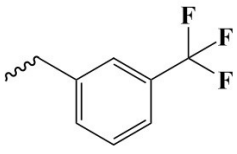
No.	Chemical Structures	Inhibitory Activity (IC_{50}(μM))	
	R^1	TASK-1	TASK-3
1		0.027	0.50
2		0.10	6.5
3		>3	>30
4		0.021	23
5		0.22	1.5
6		0.33	4.3
7		>3	2.1
8		0.045	>30
9		0.31	20
10		0.50	7.1

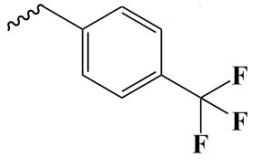
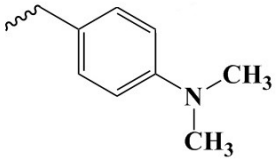
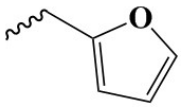
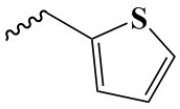
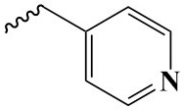
11		0.052	2.4
12		>3	>30
13		0.13	2.5
14		0.16	>30
15		>3	>30
16		>3	3.2
17		0.26	>30
18		0.037	5.9
19		0.80	25
20		0.029	0.97
21		0.16	5.6
22		0.086	2.5

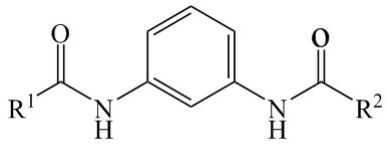
23		1.29	>30
24		0.25	>30
25		0.079	5.48

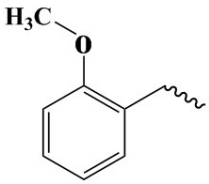
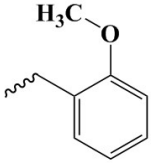
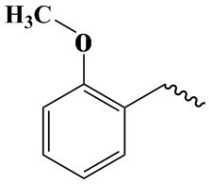
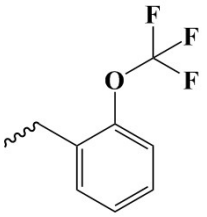
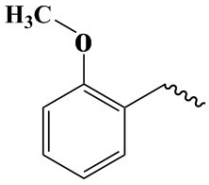
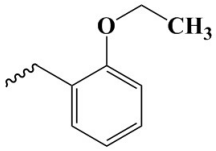


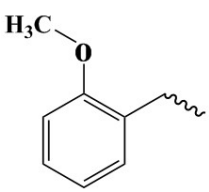
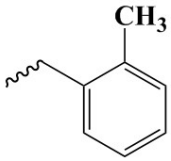
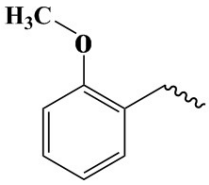
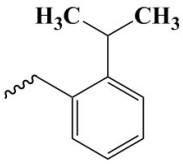
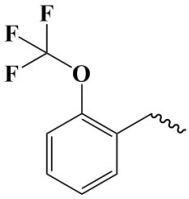
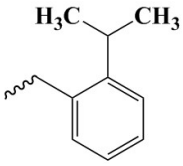
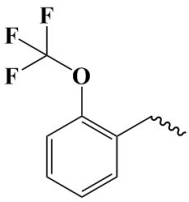
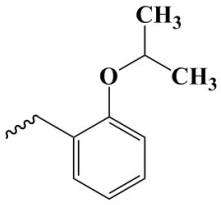
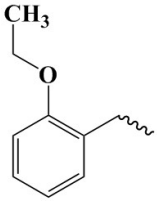
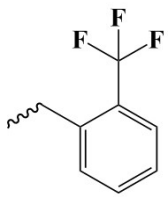
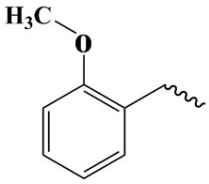
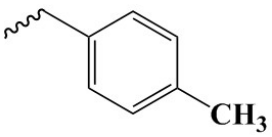
No.	Chemical Structures	Inhibitory Activity (IC_{50}(μM))	
	R^2	TASK-1	TASK-3
26		0.091	0.96
27		0.030	0.15
28		0.33	1.7
29		0.19	>30
30		0.004	0.39
31		0.031	2.2
32		1.3	>30

33		0.15	2.3
34		0.009	0.41
35		0.029	0.75
36		0.21	2.7
37		0.023	1.34
38		0.003	0.48
39		0.15	>30
40		0.025	0.60
41		0.014	1.4
42		0.010	5.5

43		>3	>30
44		0.15	>30
45		0.14	2.7
46		0.005	0.33
47		0.095	>30



No.	Chemical Structures		Inhibitory Activity (IC_{50}(μM))	
	R^1	R^2	TASK-1	TASK-3
48			0.010	1.88
49			0.004	0.41
50			0.002	0.066

51			0.073	2.2
52			0.007	1.0
53			0.011	0.73
54			0.001	0.11
55			0.002	0.31
56			0.18	2.43

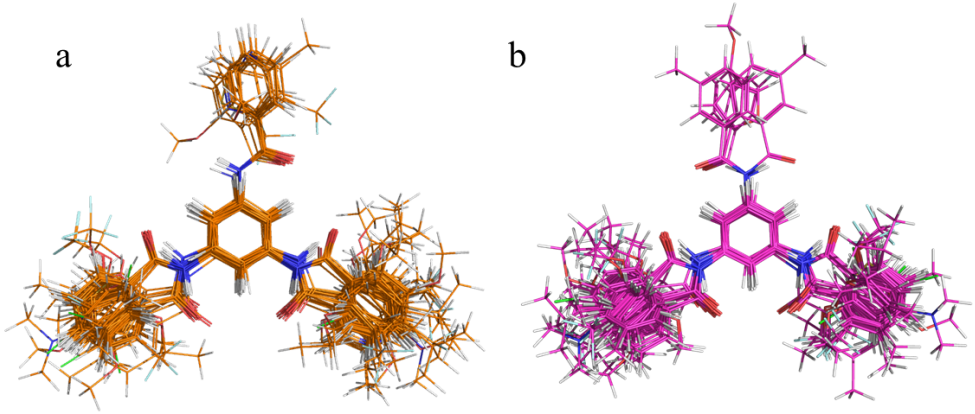


Figure S1. a, b are the molecular superimposition diagrams of models TASK-1 (orange) and TASK-3 (magenta), respectively

Figure S2. Prediction of molecular activity values.

No.	Compound	TASK-1		TASK-3	
		Affinity (kcal/mol)	pIC_{50} (prediction)	Affinity (kcal/mol)	pIC_{50} (prediction)
1	Molecule 47	-10.1	7.6296	-10.2	6.0816
2	Molecule 146	-10.1	7.452	-10.1	4.2919
3	Molecule 170	-10.2	7.4103	-9.7	5.5788
4	Molecule 223	-10.2	6.729	-10.3	5.244
5	Molecule 248	-10.2	7.5322	-10.6	6.4324
6	Molecule 296	-11.5	7.3151	-11.4	5.3488
7	Molecule 307	-10.1	7.3376	-10.3	5.1009
8	Molecule 351	-10.0	6.2521	-10.2	5.7156
9	Molecule 359	-10.0	7.2641	-9.7	5.3939
10	Molecule 398	-10.1	7.6574	-10.1	5.5559
11	Molecule 456	-10.4	6.5356	-10.6	5.4896
12	Molecule 472	-10.2	7.6376	-10.5	5.0062
13	Molecule 551	-10.3	7.3672	-10.6	5.3357
14	Molecule 563	-10.0	7.404	-10.0	5.7323
15	Molecule 613	-120.	7.2252	-11.7	5.3428
16	Molecule 635	-10.2	9.1984	-10.4	5.144
17	Molecule 641	-100.	10.3563	-9.6	10.3994
18	Molecule 706	-10.1	7.3484	-10.1	5.5682
19	Molecule 718	-10.1	10.1	-9.6	6.004
20	Molecule 1045	-100.	5.8396	-10.1	4.3985
21	Molecule 1144	-10.2	7.5191	-10.2	5.4218
22	Molecule 1307	-10.1	7.1311	-10.2	5.6322
23	Molecule 1492	-10.5	7.8535	-10.5	5.2136
24	Molecule 1699	-10.3	7.2066	-10.3	5.3646
25	Molecule 1741	-10.1	8.4732	-10.5	6.0471
26	Molecule 1774	-10.1	8.4087	-9.9	8.8457
27	Molecule 1850	-10.0	7.4103	-10.0	5.6763
28	Molecule 1882	-10.1	7.9807	-10.3	5.4146
29	Molecule 1962	-10.2	6.402	-10.2	5.0007
30	Molecule 1993	-10.0	7.8189	-10.0	5.8829
31	Molecule 2041	-10.3	8.1984	-10.0	5.8669
32	Molecule 2056	-11.4	8.097	-11.5	6.2311
33	Molecule 2123	-10.1	6.429	-10.3	4.6542
34	Molecule 2155	-10.0	6.938	-10	5.9778
35	Molecule 2445	-10.5	6.9522	-10.7	5.9317
36	Molecule 2502	-11.1	7.4807	-11.2	5.8633
37	Molecule 2726	-10.2	6.5302	-10.9	5.4972
38	Molecule 2757	-10.0	7.0276	-10	7.0984
39	Molecule 2795	-11.0	8.0444	-11.7	6.0793

40	Molecule 2924	-10.0	7.1043	-9.9	5.6967
41	Molecule 3049	-10.1	6.4071	-10.0	5.2882
42	Molecule 3132	-10.3	7.7894	-10.4	5.9773
43	Molecule 3281	-10.2	6.508	-10.0	5.7875
44	Molecule 3295	-10.6	8.8363	-11.1	6.0218
45	Molecule 3348	-10.1	7.7608	-10.0	6.065
46	Molecule 3444	-10.0	8.7177	-9.4	4.6901
47	Molecule 3591	-10.1	6.1478	-10.1	6.061
48	Molecule 3620	-10.1	7.6907	-10.4	5.9181
49	Molecule 3693	-10.0	6.9968	-10.2	5.8291
50	Molecule 3967	-10.0	7.2818	-9.9	5.0991
51	Molecule 3999	-10.0	7.1002	-9.8	5.2439
52	Molecule 4080	-10.0	7.1539	-10.4	5.8426
53	Molecule 4139	-10.0	7.165	-9.6	4.0781
54	Molecule 4226	-10.2	7.7764	-9.9	5.0197
55	Molecule 4797	-10.1	7.0397	-10.7	6.1401
56	Molecule 4979	-10.5	7.8132	10.2	6.2463
57	Molecule 5168	-10.1	7.0995	-10.4	5.7246
58	Molecule 5217	-10.1	6.9763	-10.0.	6.1365
59	Molecule 5373	-10.3	7.2192	-10.2	6.0313
60	Molecule 5561	-10.2	6.6403	-10.3	5.4534
61	Molecule 5805	-10.2	7.1412	-10.2	5.5468
62	Molecule 5839	-10.0	6.5462	-9.9	6.4024
63	Molecule 5945	-10.2	7.933	-10.0	6.6689
64	Molecule 6031	-10.2	7.928	-10.3	5.9059
65	Molecule 6194	-12.7	8.2459	-11.4	6.0753
66	Molecule 6220	-10.0	7.547	-10.3	5.9833
67	Molecule 6239	-10.0	7.63	10.1	6.1133
68	Molecule 6240	-10.0	6.9929	-10.1	6.4038