

Supplementary Material

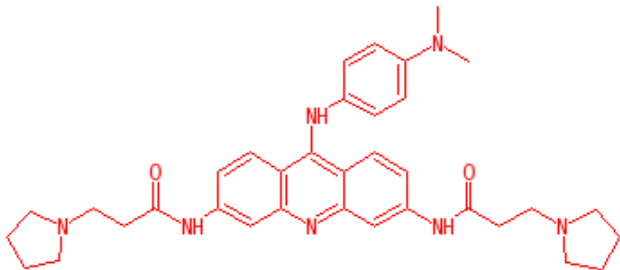
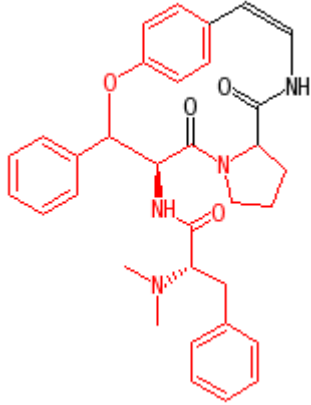
Prediction of Hit-to-Lead Ligand Molecule Interaction with G-Quadruplex DNA from c-Myc Oncogene Promoter Region

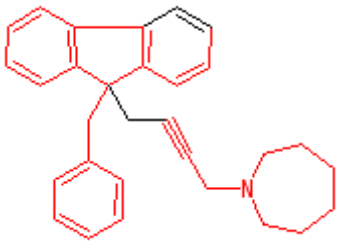
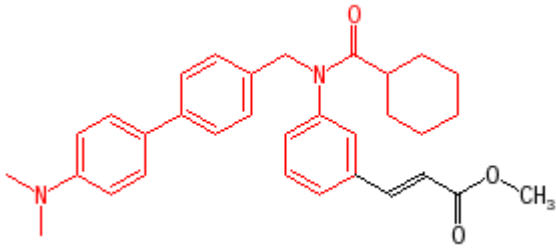
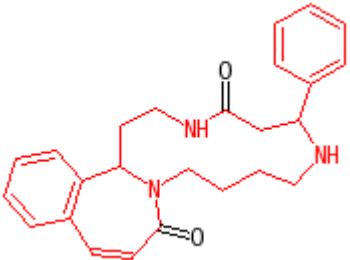
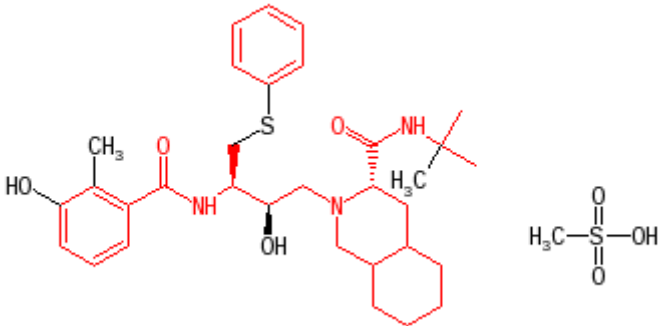
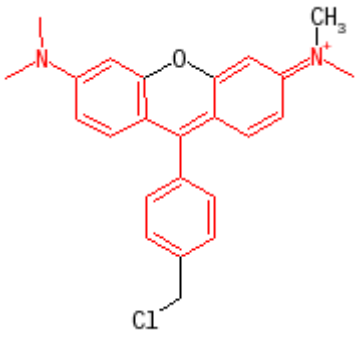
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Results of the high-throughput virtual screening for hits against G-quadruplex DNA (PDB ID: 2A5P). Hits were obtained by the BRACO-19 pharmacophore-based search of the Kyoto Encyclopedia of Genes and Genomes (KEGG) databases COMPOUND (Table S1) and DRUG (Table S2).

Table S1. Hits obtained by the BRACO-19 pharmacophore-based search of the KEGG-COMPOUND database

No Entry	Structure	Name	ΔG (kcal/mol)	K_d (μM)	$\Delta G_{intermolecular}$ (kcal/mol)
1 C20202	 Similarity-Score : 1.00	BRACO-19 9-[4-(N,N-Dimethylamino)phenylamino]- 3,6-bis(3-pyrrolodino-propionamido)acridine	-6.77	12.02	-9.99
2 C10000	 Similarity-Score : 0.50	Canthiumine	-8.45	0.64	-8.75

7 C13788	 Similarity-Score : 0.45	UCL 1608	-6.41	19.95	-7.61
8 C15649	 Similarity-Score : 0.44	Fexaramine	-7.62	2.58	-8.82
9 C10612	 Similarity-Score : 0.42	Pleurostyline	-9.27	0.16	-9.27
10 C08091	 Similarity-Score : 0.42	Nelfinavir mesylate Nelfinavir mesilate	-6.57	15.17	-8.36
11 C11622		Tetramethylrosamine	-5.57	82.13	-6.47

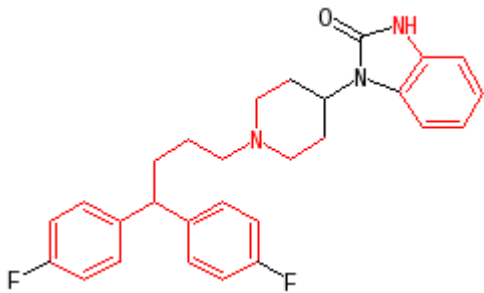
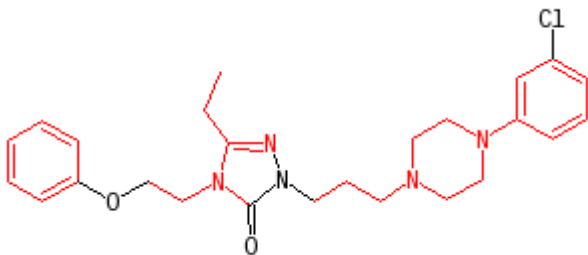
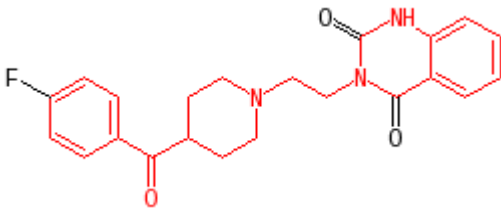
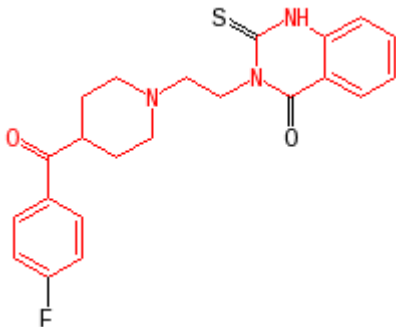
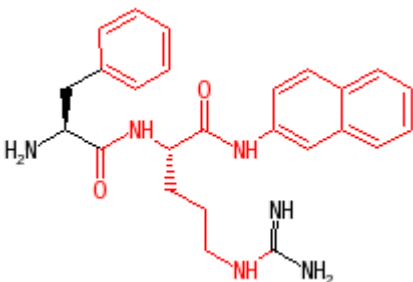
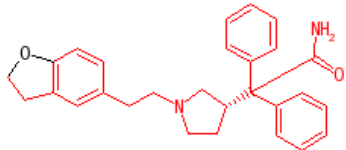
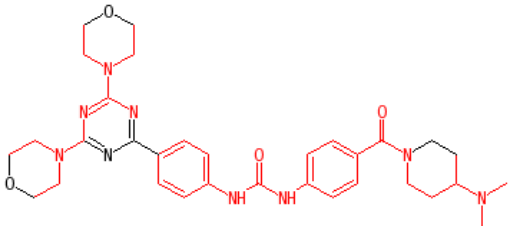
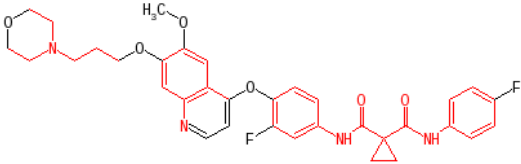
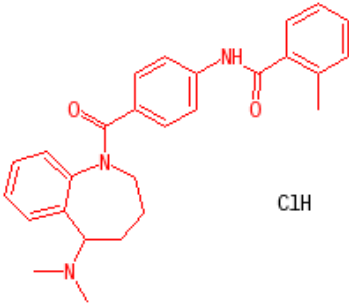
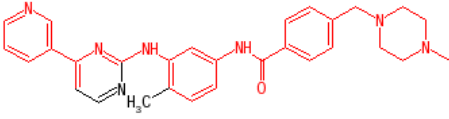
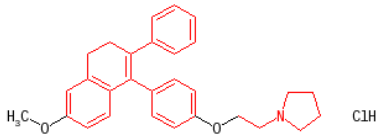
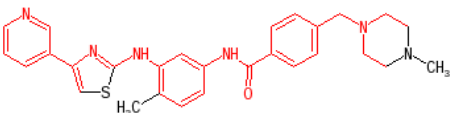
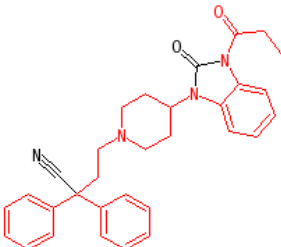
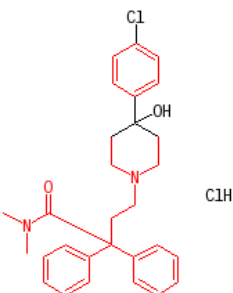
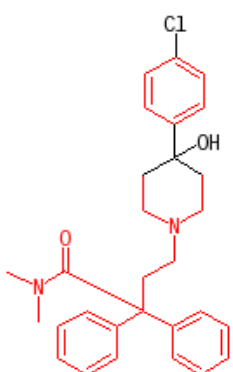
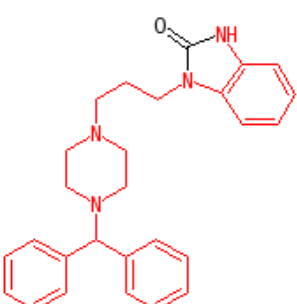
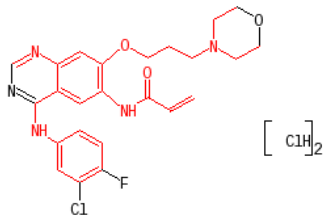
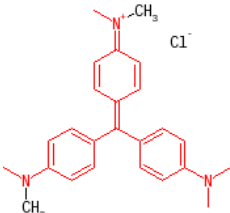
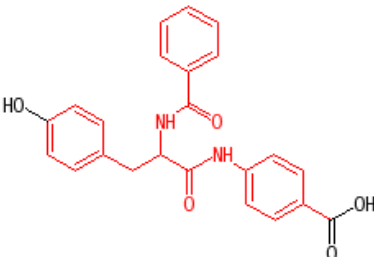
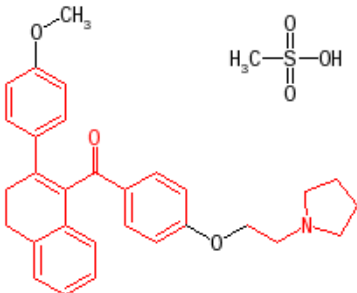
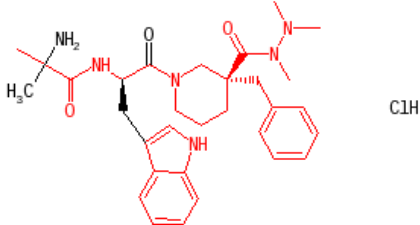
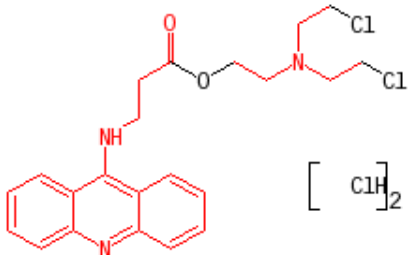
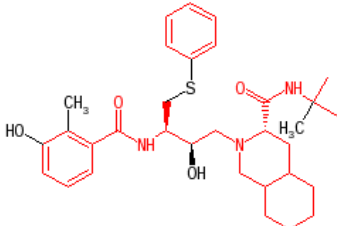
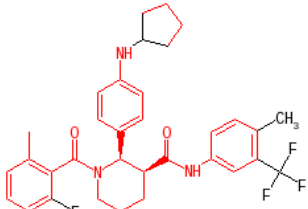
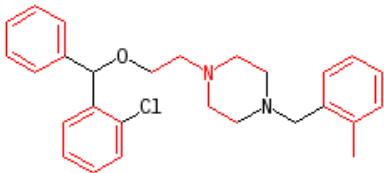
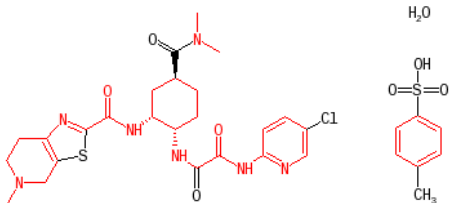
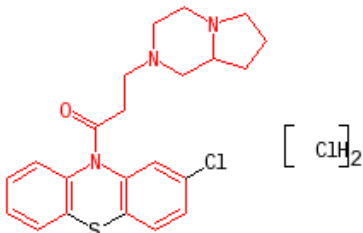
	Similarity-Score : 0.42				
12 C07566	 Similarity-Score : 0.41	Pimozide	-5.55	85.55	-6.44
13 C07256	 Similarity-Score : 0.41	Nefazodone	-6.18	29.44	-8.27
14 C07464	 Similarity-Score : 0.41	Ketanserin	-6.63	13.73	-7.53
15 C11734	 Similarity-Score : 0.41	Altanserin	-7.37	3.99	-8.26
16 C11602		MC-207,110	-6.36	21.72	-8.15

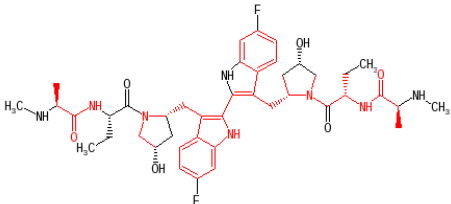
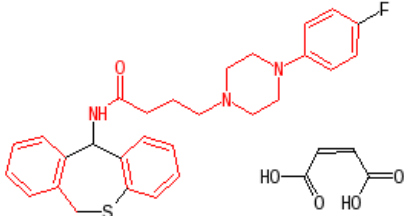
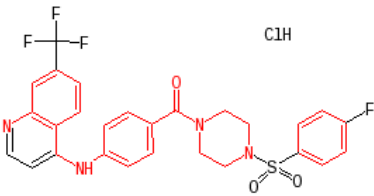
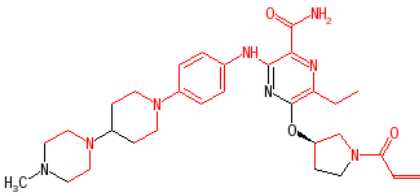
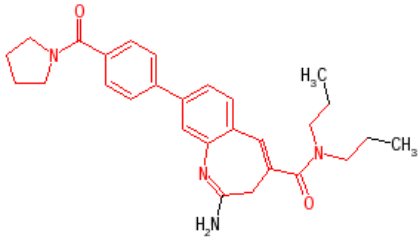
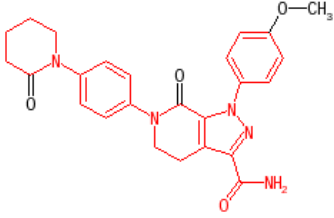
Table S2. Hits obtained by the BRACO-19 pharmacophore-based search of the KEGG-DRUG database

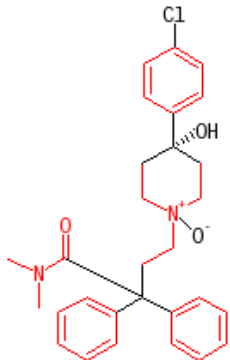
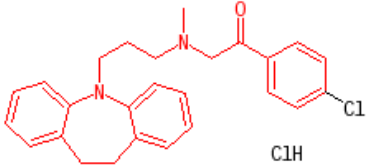
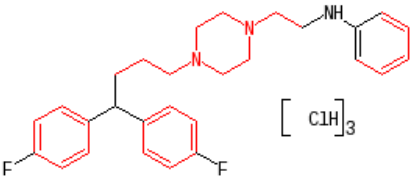
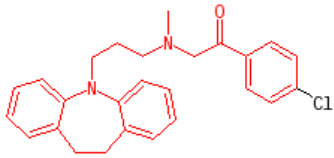
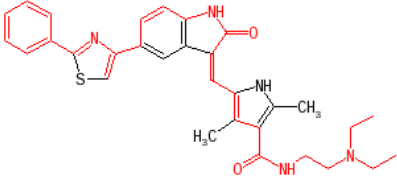
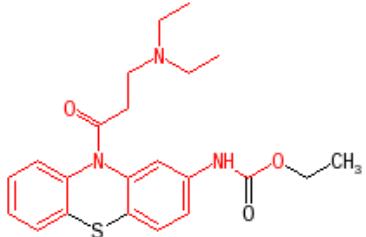
No Entry	Structure	Name	ΔG (kcal/mol)	K_d (μM)	$\Delta G_{\text{intermolecular}}$ (kcal/mol)
1 D03654	 Similarity-Score : 0.50	Darifenacin (USAN/INN) [DG:DG00482 DG00482]	-6.82	9.96	-8.61
2 D10635	 Similarity-Score : 0.50	Gedatolisib (USAN/INN)	-10.50	0.02	-11.69
3 D09618	 Similarity-Score : 0.49	Foretinib (USAN/INN)	-6.15	30.56	-8.84
4 D01855	 Similarity-Score : 0.49	Mozavaptane hydrochloride (JAN)	-6.48	17.93	-7.67
5 D08066	 Similarity-Score : 0.49	Imatinib (INN) Glamox (TN) [DG:DG00710 DG00710]	-10.36	0.025	-11.56
6 D05106	 Similarity-Score : 0.48	Nafoxidine hydrochloride (USAN)	-6.95	8.06	-8.14

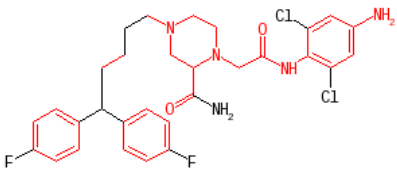
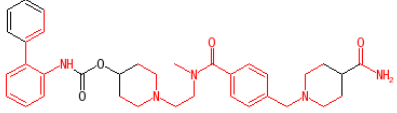
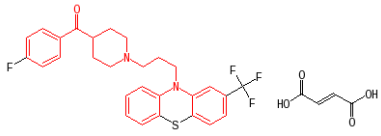
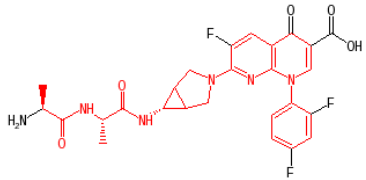
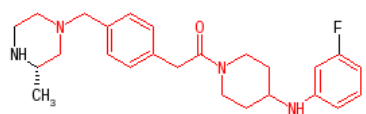
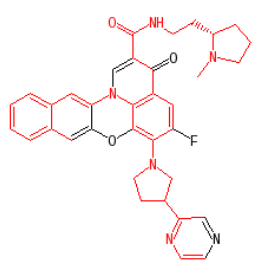
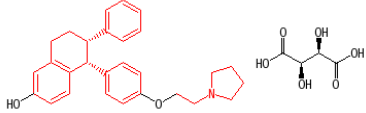
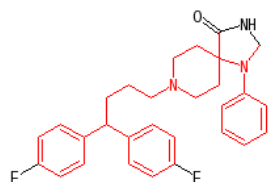
7 D10229	 Similarity-Score : 0.47	Masitinib (INN)	-11.85	0.0021	-13.04
8 D07289	 Similarity-Score : 0.47	Bezitramide (INN) Burgodin (TN)	-6.77	10.82	-8.27
9 D00729	 Similarity-Score : 0.47	Loperamide hydrochloride (JAN/USP) Imodium (TN) [DG:DG00092 DG00092]	-7.59	2.74	-8.48
10 D08144	 Similarity-Score : 0.47	Loperamide (INN) Diamide (TN) [DG:DG00092 DG00092]	-8.68	0.43	-9.57
11 D01773	 Similarity-Score : 0.47	Oxatamide (JAN/USAN/INN) Celtect (TN)	-5.25	142.16	-7.34

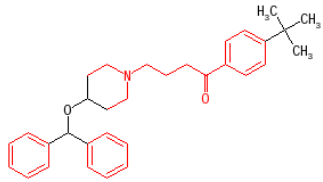
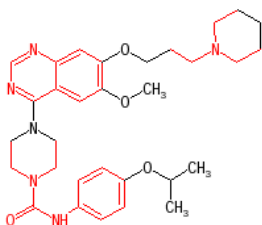
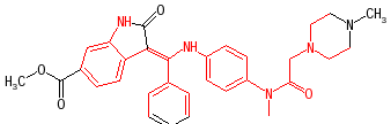
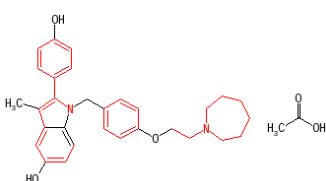
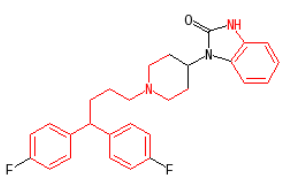
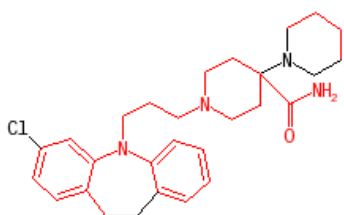
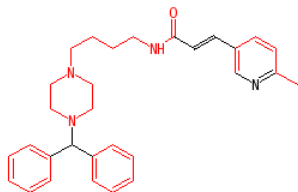
12 D03350	 Similarity-Score : 0.46	Canertinib dihydrochloride (USAN)	-6.84	9.77	-7.43
13 D01046	 Similarity-Score : 0.46	Gentian violet (USP) Methylrosanilinium chloride (JP17/INN) Methylrosaniline chloride Crystal violet Genapax (TN)	-4.13	936.00	-5.92
14 D01346	 Similarity-Score : 0.46	Bentiromide (JAN/USAN/INN) PFD (TN)	-7.07	6.52	-8.27
15 D06245	 Similarity-Score : 0.45	Trioxifene mesylate (USAN)	-7.37	3.96	-8.56
16 D08856	 Similarity-Score : 0.45	Anamorelin hydrochloride (JAN/USAN)	-8.32	0.80	-9.21

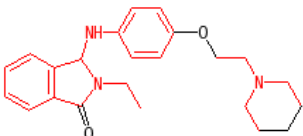
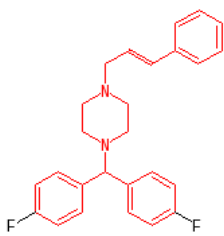
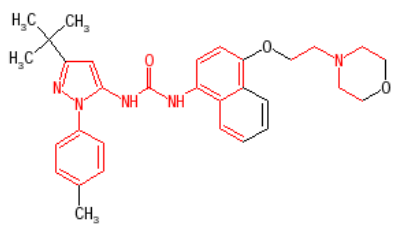
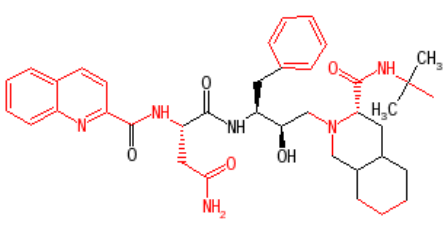
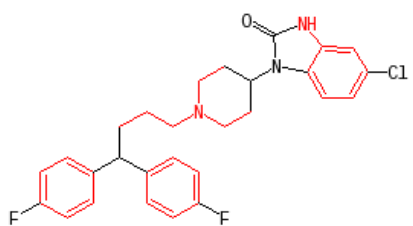
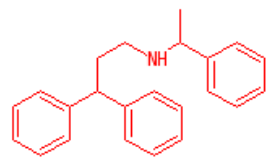
17 D03209	 Similarity-Score : 0.45	Amustaline dihydrochloride (USAN)	-5.80	56.39	-7.88
18 D08259	 Similarity-Score : 0.45	Nelfinavir (INN) Viracept (TN) [DG:DG00655 DG00655]	-7.62	2.60	-9.41
19 D11093	 Similarity-Score : 0.45	Avacopan (JAN/USAN/INN)	-6.80	10.34	-8.29
20 D07093	 Similarity-Score : 0.44	Chlorbenzoxamine (INN)	-6.46	18.44	-7.65
21 D09546	 Similarity-Score : 0.44	Edoxaban tosylate hydrate (JAN) Edoxaban tosylate Lixiana (TN) [DG:DG01398 DG01398]	-6.71	12.06	-8.20
22 D03022	 Similarity-Score : 0.44	Azaclozine hydrochloride (USAN)	-7.81	1.90	-8.40

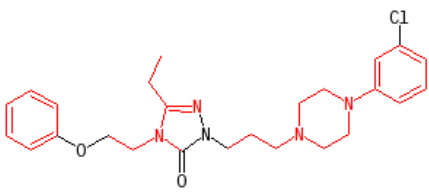
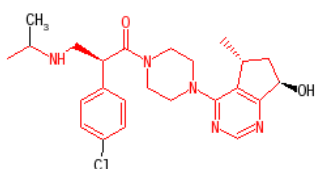
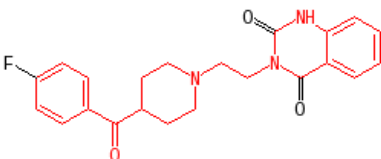
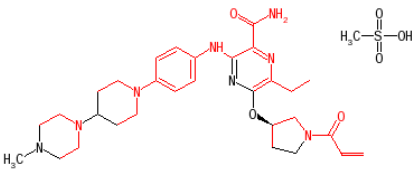
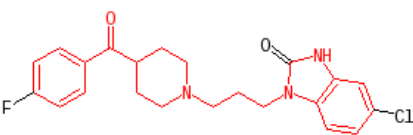
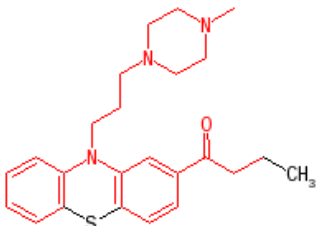
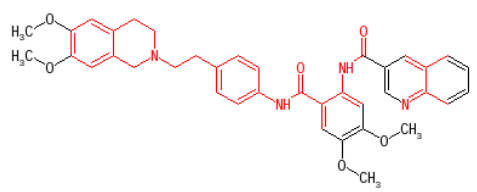
23 D10417	 Similarity-Score : 0.44	Birinapant (USAN/INN)	-9.17	0.19	-10.66
24 D01171	 Similarity-Score : 0.44	Monatepil maleate (JAN/USAN)	-8.14	1.08	-9.03
25 D04784	 Similarity-Score : 0.43	Losulazine hydrochloride (USAN)	-6.90	8.72	-7.80
26 D10958	 Similarity-Score : 0.43	Naquotinib (USAN/INN)	-8.2	0.97	-9.99
27 D10716	 Similarity-Score : 0.43	Motolimod (USAN/INN)	-6.98	7.60	-9.07
28 D03213	 Similarity-Score : 0.43	Apixaban (JAN/USAN/INN) Eliquis (TN)	-6.02	38.84	-7.51

29 D07113	 Similarity-Score : 0.43	Loperamide oxide (INN) [DG:DG00092 DG00092]	-8.45	0.64	-9.05
30 D01285	 Similarity-Score : 0.43	Lofepramine hydrochloride (JAN/USAN) Amplit (TN) [DG:DG00932 DG00932]	-7.07	6.59	-7.96
31 D03811	 Similarity-Score : 0.43	Difluanine hydrochloride (USAN)	-5.63	74.64	-7.12
32 D08140	 Similarity-Score : 0.43	Lofepramine (INN) [DG:DG00932 DG00932]	-8.29	0.84	-9.18
33 D10903	 Similarity-Score : 0.43	Amcasertib (USAN/INN)	-6.37	21.28	-8.76
34 D10503	 Similarity-Score : 0.43	Ethacizine	-5.48	96.94	-7.56

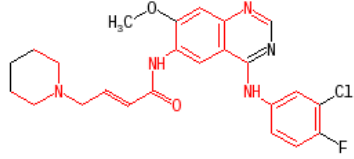
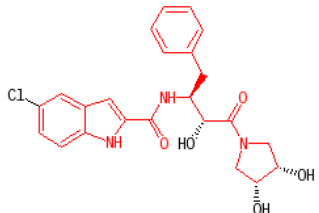
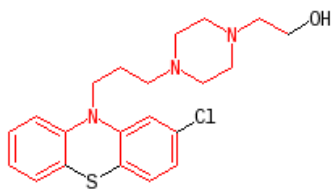
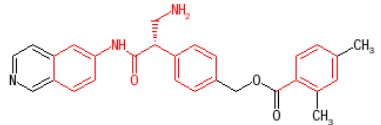
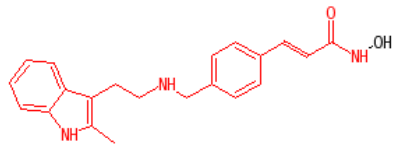
35 D03906	 Similarity-Score : 0.42	Draflazine (USAN/INN)	-9.18	0.19	-9.77
36 D10978	 Similarity-Score : 0.42	Revefenacin (USAN/INN)	-6.88	9.13	-8.97
37 D03921	 Similarity-Score : 0.42	Duoperone fumarate (USAN)	-6.89	8.98	-7.78
38 D07562	 Similarity-Score : 0.42	Alatrofloxacin (INN) [DG:DG01214]	-5.65	71.82	-7.44
39 D10330	 Similarity-Score : 0.42	Camicinal (USAN/INN)	-6.03	38.14	-7.52
40 D08981	 Similarity-Score : 0.42	Quarfloxin (USAN)	-7.99	1.39	-8.89
41 D04672	 Similarity-Score : 0.42	Lasofoxifene tartrate (JAN/USAN)	-8.14	1.08	-9.03
42 D02629	 Similarity-Score : 0.42	Fluspirilene (USAN/INN) Imap (TN)	-6.51	17.04	-7.10

43 D01478	 Similarity-Score : 0.42	Ebastine (JP17/USAN/INN) Kestine (TN)	-9.48	0.11	-10.97
44 D06005	 Similarity-Score : 0.42	Tandutinib (USAN/INN)	-8.52	0.57	-10.01
45 D10481	 Similarity-Score : 0.42	Nintedanib (USAN/INN) Ofev (TN) [DG:DG01374 DG01374]	-6.62	14.13	-8.11
46 D03062	 Similarity-Score : 0.42	Bazedoxifene acetate (JAN/USAN) Viviant (TN)	-6.79	10.49	-8.28
47 D00560	 Similarity-Score : 0.41	Pimozide (JP17/USP/INN) Orap (TN)	-6.86	9.38	-7.75
48 D07718	 Similarity-Score : 0.41	Clocapramine (INN) [DG:DG01313 DG01313]	-8.21	0.95	-8.21
49 D09838	 Similarity-Score : 0.41	Broizine (JAN) Tagorizine	-4.86	273.62	-7.55

50 D01359	 Similarity-Score : 0.41	Etomidolone (JAN/INN) Smedolin (TN)	-7.20	5.28	-8.09
51 D07971	 Similarity-Score : 0.41	Flunarizine (INN) Sibelium (TN) [DG:DG01006]	-5.52	90.07	-7.61
52 D03736	 Similarity-Score : 0.41	Doramapimod (USAN/INN)	-6.15	31.11	-8.24
53 D00429	 Similarity-Score : 0.41	Saquinavir (JAN/USP/INN) Fortovase (TN) [DG:DG00653 DG00653]	-9.45	0.12	-10.35
54 D02649	 Similarity-Score : 0.41	Clopimozide (USAN/INN)	-7.23	4.93	-8.13
55 D07185	 Similarity-Score : 0.41	Fendiline (INN) [DG:DG00332]	-6.36	21.80	-6.86

56 D08257	 Similarity-Score : 0.41	Nefazodone (INN) [DG:DG00953 DG00953]	-5.76	59.53	-7.35
57 D10641	 Similarity-Score : 0.41	Ipatasertib (USAN/INN) [DG:DG02851]	-5.94	44.15	-7.13
58 D02363	 Similarity-Score : 0.41	Ketanserin (USAN/INN) [DG:DG00265]	-7.42	3.66	-8.31
59 D10886	 Similarity-Score : 0.41	Naquotinib mesilate (JAN) Naquotinib mesylate (USAN)	-5.61	77.79	-7.40
60 D02628	 Similarity-Score : 0.41	Milenperone (USAN/INN)	-6.45	18.71	-8.24
61 D02642	 Similarity-Score : 0.41	Butaperazine (USAN) [DG:DG00880]	-5.88	48.62	-7.67
62 D06008	 Similarity-Score : 0.40	Tariquidar (USAN/INN)	-9.38	0.132	-10.87

63 D08873	Similarity-Score : 0.40	Betrixaban (USAN)	-8.84	0.332	-9.73
64 D10396	Similarity-Score : 0.40	Nintedanib esylate (USAN) Nintedanib ethanesulfonate (JAN) Ofev (TN) [DG:DG01374 DG01374]	-6.73	11.76	-8.22
65 D05780	Similarity-Score : 0.40	Sabeluzole (USAN/INN)	-6.49	17.42	-8.58
66 D01295	Similarity-Score : 0.40	Cinnarizine (JAN/USAN/INN) [DG:DG01005]	-3.18	1210	-6.07
67 D01548	Similarity-Score : 0.40	Mosapramine hydrochloride (JAN) Cremin (TN) [DG:DG00905 DG00905]	-8.23	0.92	-8.53
68 D10576	Similarity-Score : 0.40	Ombitasvir (USAN) [DG:DG01819]	-9.82	0.064	-11.90
69 D01001	Similarity-Score : 0.40	Ambenonium chloride (JP17/INN) Mytelase (TN) [DG:DG00990 DG00990]	-9.88	0.06	-11.07

70 D09883	 Similarity-Score : 0.40	Dacomitinib (USAN/INN) [DG:DG01793]	-4.71	355.22	-6.50
71 D04537	 Similarity-Score : 0.40	Inglistat (USAN/INN)	-7.16	5.69	-8.35
72 D00503	 Similarity-Score : 0.40	Perphenazine (JP17/USP/INN) Trilafon (TN) [DG:DG00875 DG00875]	-6.87	9.23	-7.17
73 D11030	 Similarity-Score : 0.40	Netarsudil (USAN/INN) [DG:DG02692 DG02692]	-6.65	13.35	-8.74
74 D10319	 Similarity-Score : 0.40	Panobinostat (USAN/INN) Farydak (TN) [DG:DG01403 DG01403]	-7.38	3.89	-9.47