BIOINFORMATION

open access

Supplementary material:

Table 1: Comparison of various parameters of ligand molecules obtained by Pharmacophore based similarity searching using ZINC database.

ZINC ID	M. Wt. (dalton)	Total Energy(KJ/mol)	H. Bonding Energy(KJ/mol)	xLogP (KJ/mol)	B. affinity(KJ/mol)
ID -[00]ZINC1025445	372.421	-151.029	-0.0206	3.61	-116.398
ID-[01]ZINC1025451	371.421	-158.326	-0.339	3.61	-120.465
ID-[02]ZINC5553120	292.296	-117.324	-8.003	0.01	-101.15
ID-[03]ZINC636503	355.349	-132.789	-2.232	4.50	-113.391
ID-[04]ZINC753995	355.349	-134.974	-1.350	4.15	-108.543
ID-[05]ZINC856324	415.401	-153.856	-1.170	4.21	-126.366
ID-[06]ZINC856325	415.405	-152.931	-3.062	4.16	-122.806
ID- [07]ZINC856326	443.455	-175.99	-2.17	4.96	-33.027
ID-[08]ZINC2478323	387.347	-148.81	-5.322	3.14	-24.577
ID-[09]ZINC4217469	450.69	-63.444	-0.2227	4.08	-88.974
ID-[010]ZINC24890	322.409	-32.576	-1.086	3.42	-100.85
ID- [011]ZINC1542199	351.471	-41.799	-2.670	4.05	-11.568

Table 2(a) and 2(b): Previously known ligands and their docking energy (KJ/mol) values used to develop analogues **[2].**

Ligands	AMN082	PTEB	CPPHA	Fenobam	Ro01-6128	Ro67-7476	Ro67-4853	CPCCOEt
Energy value	-145.879	-142.98	-139.9	-133.78	-129.165	-129.091	-126.491	-126.052

Table 2(b)

Ligands	SIB-1757	SIB-1893	MTEP	5MPEP	MPEP	MPEP-gamma	PHCCC
Energy value	-103.186	-102.282	-102.314	-101.01	-99.897	-96.861	-105.279

Table 3: Comparison of various parameters of the drug analogues obtained by de novo method and their IUPAC names (by Marvin sketch).

ID of molecules	IUPAC name of molecules	M. Wt. (Dalton)	Total Energy(KJ/mol)	H. Bonding Energy(KJ/mol)	xLogP	B.affinity (KJ/mol)
ID-result_001	(4S,6S,8E,12E,14E)-8-(1-carbamoyleth-1-en-1-yl)-4-[ethane-1,2-bis(ylium)-1-yl]-6-hydroxy-14-(prop-2-en-1-ylidene)heptadeca-8,11,12- triene-1,2,3,9,17-pentakis(ylium)	387.6	159.827	-5.1906	4.75	-57.807
ID- result_002	(4S,6S,8E,12E,14E)-8-(1-carbamoyleth-1-en-1-yl)-4-[ethane-1,2-bis(ylium)-1-yl]-6-hydroxy-14-(prop-3-en-1-ylidene)heptadeca-8,11,12-triene-1,2,3,9,17-pentakis(ylium)	387.5	-164.761	-5.26	4.76	-71.44
ID- result_003	(6R)-1-(ethan-2-ylium-1-yl)-2-[(1E,5E,8S)-8-hydroxy-6-[1-(methylcarbamoyl)eth-1-en-1-yl]dodeca-1,2,5-triene-5,11,12-tris(ylium)-1-yl]-4-methylidene-6-methyliumylcyclohex-2-en-1-ide	399.6	-169.566	-6.456	4.41	-40.10
ID- result_004	(5S,7E,11E,13E)-5-hydroxy-7-[1-(methylcarbamoyl)eth-1-en-1-yl]-13-(prop-2-en-1-ylidene)hexadeca-7,10,11-triene-1,2,8,16-tetrakis(ylium)	359.5	-156.661	-2.32	4.73	-121.532
ID- result_005	(4E,5E)-9-[(1E,2S,5R)-2-[(1Z)-buta-1,3-dien-1-ylium-1-yl]-5-[2-(carbamoylamino)-2-oxoethyl]cyclohexan-4-ylium-1-ylidene]-4-(prop-2-en-1-ylidene)nona-5,6-diene-1,9-bis(ylium)	396.6	-158.947	-0.557	4.70	-14.94
ID- result_006	(3E,7E,9E)-3-[(2R,4R)-2,4-dihydroxyhexyl]-9-(prop-2-en-1-ylidene)dodeca-1,3,6,7-tetraene-1,4,12-tris(ylium)	318.5	-156.896	-7.59	4.50	-107.004
ID- result_007	(5S,7E,11E,13E)-7-(1-carbamoyleth-1-en-1-yl)-5-hydroxy-13-(prop-2-en-1-ylidene)hexadeca-7,10,11-triene-1,2,8,16-tetrakis(ylium)	445.5	-153.66	-0.73	4.33	-54.69
ID- result_008	[(3E,5E,9E,14R,15E)-14-(2-oxoethyl)-4-(propan-3-ylium-1-yl)heptadeca-3,5,6,9,15-pentaene-9,10,12,15,16,17-exakis(ylium)-1-yl]urea	374.6	-165.401	-3.66	4.23	-130.615
ID- result_009	[(3E,5E,9E,14R,15E)-14-(2-oxoethyl)-4-(propan-3-ylium-1-yl)heptadeca-3,5,6,9,14-pentaene-9,10,12,15,16,17-hexakis(ylium)-1-yl]urea	374.6	-170.744	-4.833	4.32	-140.22
ID- result_010	(4E,6E,10E,12R,17R)-12-ethenyl-17,19-dihydroxy-6-methyl-13-oxo-5-(propan-3-ylium-1-yl)nonadeca-4,6,7,10-tetraene-1,10-bis(ylium)	392.6	-156.275	-9.49	4.56	-104.845
ID- result_016	(4E,5E,9E,11S)-12-[(4R)-4-hydroxycyclohex-1-en-2-ylium-1-yl]-11-(2-hydroxyethyl)-4-(3-oxopropylidene)trideca-5,6,9,12-tetraene-1,9,10-tris(ylium)	372.5	-186.026	-5.73	4.98	-110.593
ID- result_025	[(3E,5E,9E,14R,15E)-14-(2-oxoethyl)-4-(propan-3-ylium-1-yl)heptadeca-3,5,6,9,15-pentaene-9,10,12,15,17-pentakis(ylium)-1-yl]urea	374.6	-162.96	-3.348	4.32	-85.30
ID- result_056	(4E,6E,9E)-10-[(3S)-3-[(1S)-1,2-dicarboxyethyl]cyclopent-1-ene-2,4-bis(ylium)-1-yl]-5-(propan-3-ylium-1-yl)deca-1,4,6,8,9-pentaene-1,2,7-tris(ylium)	358.5	-165.279	-7.744	4.32	-104.75
ID- result_078	(4E,6E,9E)-10-[(3S)-3-[(1R)-1-carboxy-2-hydroxyethyl]cyclopent-1-ene-2,4-bis(ylium)-1-yl]-5-(propan-3-ylium-1-yl)deca-1,4,6,8,9-pentaene-1,2,7-tris(ylium)	330.5	-161.192	-5.190	5.01	-108.786
ID- result_101	[(3R,4E,6S,10E,12E)-11-methyl-6-(2-methylprop-2-en-1-yl)-12-(3-oxopropylidene)pentadeca-4,9,10-triene-1,7,15-tris(ylium)-3-yl]urea	388.6	-162.623	-2.74	4.05	-85.424
ID- result_089	(4E,6E,9E)-10-[(3S)-3-[(1R)-1-carboxy-2-hydroxyethyl]cyclopent-1-ene-2,4-bis(ylium)-1-yl]-5-(propan-3-ylium-1-yl)deca-1,4,6,8,9-pentaene-1,2,7-tris(ylium)	320.5	-159.478	-4.24	4.95	-93.99