

ChemistrySelect

Supporting Information

An Extensive Computational Investigation of *Mycobacterium tuberculosis* Pantothenate Synthetase Inhibitors from Diverse-Lib Compounds Library

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S.no	Compound	Energy
1	26535897_Intermediate	-11.3
2	24357538_Intermediate	-11.3
3	4264938_Intermediate	-11.2
4	99495293_Intermediate	-11.2
5	125001301_Accepted	-11.1
6	17514560_Intermediate	-11
7	124948823_Accepted	-11
8	26616245_Intermediate	-10.8
9	24344872_Intermediate	-10.8
10	26726479_Accepted	-10.8
11	49733540_Intermediate	-10.8
12	24337900_Intermediate	-10.8
13	14744067_Intermediate	-10.8
14	46493464_Accepted	-10.7
15	24352301_Intermediate	-10.7
16	57256966_Intermediate	-10.7
17	17450998_Accepted	-10.7
18	121285583_Intermediate	-10.7
19	103060682_Accepted	-10.7
20	26649447_Intermediate	-10.7
21	124948790_Intermediate	-10.7
22	49675052_Intermediate	-10.7
23	4248241_Intermediate	-10.7
24	49826940_Intermediate	-10.7
25	24779390_Intermediate	-10.7
26	24410630_Intermediate	-10.7
27	17450594_Accepted	-10.6
28	124754843_Intermediate	-10.6
29	24328053_Accepted	-10.6
30	24292058_Intermediate	-10.6
31	17437878_Intermediate	-10.6
32	842308_Accepted	-10.6
33	49677660_Accepted	-10.6
34	26614187_Accepted	-10.6
35	14732732_Intermediate	-10.6
36	17386179_Intermediate	-10.5
37	17447688_Accepted	-10.5
38	24782939_Intermediate	-10.5
39	56322754_Accepted	-10.5
40	26730849_Intermediate	-10.5
41	24831806_Intermediate	-10.5
42	17516687_Intermediate	-10.5
43	3714834_Intermediate	-10.4
44	26725965_Intermediate	-10.4
45	4242551_Accepted	-10.4

46	124948997_Accepted	-10.4
47	103163258_Accepted	-10.4
48	24323741_Intermediate	-10.4
49	124951241_Intermediate	-10.4
50	24369777_Intermediate	-10.4
51	124948103_Accepted	-10.4
52	24825808_Intermediate	-10.4
53	124949182_Accepted	-10.4
54	26636558_Intermediate	-10.4
55	24321313_Intermediate	-10.4
56	26629614_Intermediate	-10.4
57	11537903_Intermediate	-10.4
58	124949254_Intermediate	-10.4
59	24317932_Intermediate	-10.4
60	4260101_Intermediate	-10.4
61	24792453_Intermediate	-10.4
62	24365989_Intermediate	-10.4
63	24294253_Intermediate	-10.4
64	852045_Intermediate	-10.3
65	24404246_Intermediate	-10.3
66	26535843_Intermediate	-10.3
67	49646407_Intermediate	-10.3
68	17438811_Intermediate	-10.3
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70	24366769_Intermediate	-10.3
71	26538970_Intermediate	-10.3
72	49820496_Intermediate	-10.3
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84	24315340_Intermediate	-10.3
85	137275991_Intermediate	-10.3
86	861653_Intermediate	-10.3
87	49670548_Intermediate	-10.3
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91	49736867_Intermediate	-10.2

92	17409942_Intermediate	-10.2
93	24796179_Intermediate	-10.2
94	24322316_Intermediate	-10.2
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96	4242752_Intermediate	-10.2
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101	26641954_Accepted	-10.2
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117	56422086_Intermediate	-10.2
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119	99359897_Intermediate	-10.1
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123	24394898_Intermediate	-10.1
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125	24321333_Intermediate	-10.1
126	17461582_Intermediate	-10.1
127	24409237_Intermediate	-10.1
128	144097173_Intermediate	-10.1
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130	124948197_Accepted	-10.1
131	851996_Intermediate	-10.1
132	85268789_Intermediate	-10.1
133	49721304_Accepted	-10.1
134	24358949_Accepted	-10.1
135	85303730_Intermediate	-10.1
136	87345664_Intermediate	-10.1
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139	848200_Intermediate	-10.1
140	26537871_Accepted	-10.1
141	26617108_Accepted	-10.1
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158	4251241_Accepted	-10
159	24327576_Accepted	-10
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161	124755588_Accepted	-10
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163	860033_Intermediate	-10
164	136889484_Intermediate	-10
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166	49728809_Intermediate	-10
167	124948315_Intermediate	-10
168	24406151_Intermediate	-10
169	57267915_Intermediate	-10
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172	17510383_Intermediate	-10
173	103051125_Intermediate	-10
174	24799186_Intermediate	-10
175	124949457_Intermediate	-10
176	24783630_Intermediate	-10
177	104223052_Intermediate	-10
178	24831842_Accepted	-10
179	26661608_Intermediate	-10
180	16953518_Intermediate	-10
181	24387390_Intermediate	-10
182	103050604_Intermediate	-10
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186	24811431_Accepted	-10
187	24279941_Intermediate	-10
188	26646508_Accepted	-10
189	161004441_Intermediate	-10
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196	7999387_Intermediate	-10
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210	26663782_Accepted	-10
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1056	26636835_Intermediate	-9.2
1057	17410015_Intermediate	-9.2

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1059	24838719_Accepted	-9.2
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1062	49732549_Intermediate	-9.2
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1067	26647804_Intermediate	-9.2
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1070	49721753_Intermediate	-9.2
1071	24354071_Intermediate	-9.2
1072	24797731_Intermediate	-9.2
1073	26618396_Accepted	-9.2
1074	26539574_Accepted	-9.2
1075	26532576_Intermediate	-9.2
1076	57266553_Accepted	-9.2
1077	14723781_Intermediate	-9.2
1078	3711570_Intermediate	-9.2
1079	26650023_Intermediate	-9.2
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1086	4256987_Intermediate	-9.2
1087	26536890_Accepted	-9.2
1088	17509286_Accepted	-9.2
1089	47196399_Intermediate	-9.2
1090	24818429_Accepted	-9.2
1091	4258564_Intermediate	-9.2
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1095	24837479_Accepted	-9.2
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1098	57263773_Intermediate	-9.2
1099	49719190_Accepted	-9.2
1100	56423661_Intermediate	-9.2
1101	24825759_Accepted	-9.2
1102	125001350_Intermediate	-9.2
1103	24412810_Intermediate	-9.2

1104	24302230_Intermediate	-9.2
1105	49719684_Intermediate	-9.2
1106	51086909_Accepted	-9.2
1107	92764682_Intermediate	-9.2
1108	24837738_Accepted	-9.2
1109	17443089_Intermediate	-9.2
1110	49675322_Intermediate	-9.2
1111	124949476_Intermediate	-9.2
1112	48409975_Intermediate	-9.2
1113	49728601_Accepted	-9.2
1114	26648235_Intermediate	-9.2
1115	26651444_Intermediate	-9.2
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1140	99360905_Accepted	-9.2
1141	843683_Accepted	-9.2
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1179	17514679_Intermediate	-9.2
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1203	24353556_Intermediate	-9.2
1204	26617784_Accepted	-9.2
1205	862744_Accepted	-9.2
1206	24809224_Intermediate	-9.2
1207	24406675_Intermediate	-9.2
1208	853538_Intermediate	-9.2
1209	858089_Intermediate	-9.2
1210	56319324_Intermediate	-9.2
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1212	17470377_Intermediate	-9.2
1213	26653285_Intermediate	-9.2
1214	57259764_Intermediate	-9.2
1215	7969123_Intermediate	-9.2
1216	24792133_Accepted	-9.2
1217	3717707_Intermediate	-9.2
1218	22408661_Intermediate	-9.2
1219	26534494_Accepted	-9.2
1220	14718970_Intermediate	-9.2
1221	24839631_Intermediate	-9.2
1222	14744602_Intermediate	-9.2
1223	24708097_Intermediate	-9.2
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1226	24781151_Intermediate	-9.2
1227	49678950_Intermediate	-9.2
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1232	144205205_Intermediate	-9.2
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1236	3716089_Accepted	-9.1
1237	17410440_Intermediate	-9.1
1238	24345989_Intermediate	-9.1
1239	864678_Intermediate	-9.1
1240	861905_Intermediate	-9.1
1241	844796_Intermediate	-9.1

1242	24834152_Intermediate	-9.1
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1244	17449937_Accepted	-9.1
1245	24409762_Intermediate	-9.1
1246	24785142_Intermediate	-9.1
1247	49644723_Intermediate	-9.1
1248	845028_Intermediate	-9.1
1249	24312309_Intermediate	-9.1
1250	26617763_Intermediate	-9.1
1251	103061849_Accepted	-9.1
1252	144091837_Intermediate	-9.1
1253	24799789_Accepted	-9.1
1254	26614591_Intermediate	-9.1
1255	24823152_Intermediate	-9.1
1256	49679425_Accepted	-9.1
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1259	99454299_Intermediate	-9.1
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1262	26647157_Accepted	-9.1
1263	24839636_Intermediate	-9.1
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1271	49823381_Intermediate	-9.1
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1273	14741574_Accepted	-9.1
1274	24833093_Intermediate	-9.1
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1276	56317618_Accepted	-9.1
1277	49723394_Intermediate	-9.1
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1293	49672645_Intermediate	-9.1
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1298	24798942_Accepted	-9.1
1299	863711_Intermediate	-9.1
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1302	24798666_Intermediate	-9.1
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1304	4256510_Accepted	-9.1
1305	7969193_Intermediate	-9.1
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1308	89852803_Intermediate	-9.1
1309	24785220_Accepted	-9.1
1310	4243000_Intermediate	-9.1
1311	17461139_Accepted	-9.1
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1313	103076188_Intermediate	-9.1
1314	845751_Accepted	-9.1
1315	24839762_Intermediate	-9.1
1316	26620940_Intermediate	-9.1
1317	49643309_Accepted	-9.1
1318	124949845_Intermediate	-9.1
1319	7969088_Intermediate	-9.1
1320	17407647_Intermediate	-9.1
1321	24402123_Intermediate	-9.1
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1323	17515744_Intermediate	-9.1
1324	57261219_Intermediate	-9.1
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1326	24268620_Intermediate	-9.1
1327	103073401_Intermediate	-9.1
1328	24302224_Intermediate	-9.1
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1342	56318700_Accepted	-9.1
1343	26540691_Accepted	-9.1
1344	51089643_Intermediate	-9.1
1345	85270336_Accepted	-9.1
1346	24792876_Intermediate	-9.1
1347	49822873_Intermediate	-9.1
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1349	24385973_Intermediate	-9.1
1350	24404998_Intermediate	-9.1
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1356	4246925_Intermediate	-9.1
1357	57268550_Intermediate	-9.1
1358	26731959_Intermediate	-9.1
1359	24800578_Accepted	-9.1
1360	24390845_Intermediate	-9.1
1361	14741364_Intermediate	-9.1
1362	4263550_Intermediate	-9.1
1363	24377820_Intermediate	-9.1
1364	26665252_Accepted	-9.1
1365	51089580_Intermediate	-9.1
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1367	49720353_Accepted	-9.1
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1370	26618088_Intermediate	-9.1
1371	57256439_Intermediate	-9.1
1372	26648090_Intermediate	-9.1
1373	850145_Accepted	-9.1
1374	17464376_Intermediate	-9.1
1375	49732330_Intermediate	-9.1
1376	160646433_Intermediate	-9.1
1377	17403222_Intermediate	-9.1
1378	24283635_Intermediate	-9.1
1379	17474573_Intermediate	-9.1

1380	104222904_Intermediate	-9.1
1381	85270624_Intermediate	-9.1
1382	57259466_Accepted	-9.1
1383	14735188_Intermediate	-9.1
1384	49718573_Intermediate	-9.1
1385	24834374_Intermediate	-9.1
1386	14739637_Intermediate	-9.1
1387	17388200_Intermediate	-9.1
1388	49725521_Accepted	-9.1
1389	85271222_Intermediate	-9.1
1390	24395037_Accepted	-9.1
1391	3712187_Intermediate	-9.1
1392	24782635_Accepted	-9.1
1393	24808503_Accepted	-9.1
1394	24292803_Accepted	-9.1
1395	87348736_Intermediate	-9.1
1396	56324685_Intermediate	-9.1
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1398	4244694_Intermediate	-9.1
1399	49826552_Accepted	-9.1
1400	7977086_Accepted	-9.1
1401	14747102_Intermediate	-9.1
1402	24428667_Accepted	-9.1
1403	24404863_Accepted	-9.1
1404	26649713_Accepted	-9.1
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1406	51090442_Intermediate	-9.1
1407	49666921_Intermediate	-9.1
1408	136947502_Intermediate	-9.1
1409	24840176_Intermediate	-9.1
1410	26642293_Accepted	-9.1
1411	848691_Intermediate	-9.1
1412	865480_Intermediate	-9.1
1413	49730197_Intermediate	-9.1
1414	57263522_Intermediate	-9.1
1415	103073498_Accepted	-9.1
1416	85268797_Intermediate	-9.1
1417	4240985_Accepted	-9.1
1418	17433527_Intermediate	-9.1
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1425	26611623_Intermediate	-9.1

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1437	104224688_Intermediate	-9.1
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1440	57256935_Accepted	-9.1
1441	24787533_Accepted	-9.1
1442	56317238_Intermediate	-9.1
1443	49732995_Accepted	-9.1
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1446	49731006_Intermediate	-9.1
1447	853565_Intermediate	-9.1
1448	17466065_Intermediate	-9.1
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1450	24346118_Intermediate	-9.1
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1452	49675384_Accepted	-9.1
1453	24369160_Intermediate	-9.1
1454	124350134_Intermediate	-9.1
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1456	49674830_Intermediate	-9.1
1457	14719126_Intermediate	-9.1
1458	14735128_Intermediate	-9.1
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1460	24802616_Intermediate	-9.1
1461	57266358_Intermediate	-9.1
1462	17441979_Intermediate	-9
1463	47202635_Intermediate	-9
1464	3714376_Intermediate	-9
1465	14730133_Intermediate	-9
1466	24793824_Accepted	-9
1467	49718529_Intermediate	-9
1468	852886_Intermediate	-9
1469	3714831_Accepted	-9
1470	99454528_Intermediate	-9
1471	24396661_Intermediate	-9

1472	14740362_Intermediate	-9
1473	124756617_Intermediate	-9
1474	24395342_Accepted	-9
1475	26665721_Intermediate	-9
1476	24386985_Intermediate	-9
1477	87346119_Intermediate	-9
1478	26614300_Accepted	-9
1479	864329_Intermediate	-9
1480	24782017_Intermediate	-9
1481	26543574_Intermediate	-9
1482	3713483_Accepted	-9
1483	24271238_Intermediate	-9
1484	104222939_Intermediate	-9
1485	57265768_Intermediate	-9
1486	49644179_Intermediate	-9
1487	17473633_Accepted	-9
1488	26646711_Intermediate	-9
1489	57258490_Intermediate	-9
1490	4246955_Intermediate	-9
1491	24799063_Intermediate	-9
1492	103163187_Intermediate	-9
1493	49721379_Intermediate	-9
1494	4244815_Intermediate	-9
1495	26659792_Intermediate	-9
1496	99431120_Accepted	-9
1497	24336245_Intermediate	-9
1498	49649231_Intermediate	-9
1499	49719186_Intermediate	-9
1500	17452112_Accepted	-9

Table S1 – List of 1500 selected compounds after the screening on the basis of their binding energy

Compound	CID2813602	CID24357538	CID753354	CID 4798023	Control
smiles	<chem>CC1=CC2=C(C=C1)OC(=O)N2CCC3=NOC(=N3)C4=C(N=C(C=C4)C(F)(F)F)C</chem>	<chem>CN1C(=CC2=C1C1=CC=CC=C1OC2=O)C(=O)NC1=CC=CC(=C1)C(F)(F)F</chem>	<chem>O=C(CC(=O))/C=C/c1ccc(cc1)O)/C=C/c1c cc(cc1)O.COc1cc /C=C/C/C(=O)CC(=O)/C=C/c2ccc(c(c2)OC)O)ccc 1O.COc1cc(/C=C /C(=O)CC(=O)/C=C /c2 ccc(cc2)O)ccc1O</chem>	<chem>C1CN(CCN1C(=O)CC2=CNC3=CC=CC=C32)S(=O)(=O)C4=CC=C(C=C4)F</chem>	<chem>CC(C)(CO)[C@H](C(=O)O[P@](=O)(O)OC[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2ncnc3N)O)O)O</chem>
LogS	-4.405	-7.133	-4.107	-3.762	-1.719
LogD	3.634	3.954	2.531	2.802	-0.738
LogP	3.603	4.577	5.67	2.676	-2.198
Pgp-inh	0.089	0.886	0.024	0.97	0.002
Pgp-sub	0.004	0.794	0	0.99	0.984
HIA	0.004	0.005	0.98	0.006	0.969
F(20%)	0.001	0.011	0.923	0.001	0.952
F(30%)	0.003	0.955	0.991	0.005	0.973
Caco-2	-4.651	-5.1	-5.551	-4.758	-6.155
MDCK	2.02E-05	1.56E-05	1.03E-05	1.96E-05	1.21E-05
BBB	0.664	0.322	0.008	0.829	0.391
PPB	97.86%	98.05%	100.44%	96.70%	21.69%
VDss	1.217	0.662	-0.209	0.986	0.524
Fu	1.73%	0.85%	0.02%	2.17%	78.58%
CYP1A2-inh	0.416	0.898	0.277	0.206	0.005
CYP1A2-sub	0.927	0.77	0.005	0.342	0.019
CYP2C19-inh	0.86	0.925	0.163	0.861	0.016
CYP2C19-sub	0.066	0.125	0.021	0.547	0.046
CYP2C9-inh	0.863	0.878	0.648	0.901	0.002
CYP2C9-sub	0.107	0.84	1	0.92	0.501
CYP2D6-inh	0.892	0.495	0	0.508	0.03
CYP2D6-sub	0.548	0.761	0.908	0.856	0.106
CYP3A4-inh	0.733	0.643	0.965	0.907	0.024
CYP3A4-sub	0.519	0.106	0.229	0.853	0.022
CL	4.938	3.172	8.827	9.611	1.571
T12	0.149	0.043	0.968	0.084	0.766
hERG	0.082	0.057	0.121	0.595	0.016
H-HT	0.956	0.933	0.001	0.983	0.469

DILI	0.984	0.958	0.979	0.984	0.989
Ames	0.3	0.219	0.142	0.02	0.383
ROA	0.044	0.674	0.026	0.539	0.023
FDAMDD	0.805	0.878	0.07	0.647	0.944
SkinSen	0.063	0.115	0.983	0.039	0.365
Carcinogenicity	0.886	0.512	0.716	0.259	0.061
EC	0.003	0.003	0.004	0.003	0.003
EI	0.012	0.491	0.944	0.011	0.025
Respiratory	0.936	0.753	0.014	0.224	0.821
BCF	1.704	1.467	0.798	0.611	0.182
IGC50	3.779	4.774	7.064	3.077	1.646
LC50	4.567	5.534	4.631	3.973	4.501
LC50DM	5.055	6.567	5.743	5.593	4.665
NR-AR	0.165	0.126	0.17	0.379	0.076
NR-AR-LBD	0.136	0.008	1	0.015	0.003
NR-AhR	0.92	0.935	0.507	0.563	0.038
NR-Aromatase	0.086	0.604	0.773	0.538	0.133
NR-ER	0.905	0.465	0.994	0.175	0.068
NR-ER-LBD	0.019	0.009	0.995	0.008	0.035
NR-PPAR-gamma	0.311	0.787	0.998	0.013	0.011
SR-ARE	0.909	0.521	0.993	0.718	0.258
SR-ATAD5	0.904	0.01	1	0.006	0.036
SR-HSE	0.004	0.036	0.956	0.017	0.008
SR-MMP	0.216	0.885	0.98	0.365	0.165
SR-p53	0.757	0.862	1	0.007	0.286
MW	404.11	386.09	1014.35	401.12	477.13
Vol	367.787	360.453	1064.849	383.096	409.154
Dense	1.099	1.071	0.953	1.047	1.166
nHA	7	5	15	6	15
nHD	0	1	6	1	7
TPSA	86.95	64.24	251.49	73.48	232.6
nRot	5	4	21	5	9
nRing	4	4	6	4	3
MaxRing	9	13	6	9	9
nHet	10	8	15	8	16
fChar	0	0	0	0	0
nRig	22	23	48	25	17
Flex	0.227	0.174	0.438	0.2	0.529
nStereo	0	0	0	0	6
NonGenotoxic_Carcinogenicity	0	1	1	1	0
LD50_oral	0	0	0	0	0

Genotoxic_Carcinogenicity_Mutagenicity	0	5	1	0	5
SureChEMBL	0	0	0	0	0
NonBiodegradable	2	1	1	1	1
Skin_Sensitization	0	4	8	0	2
Acute_Aquatic_Toxicity	2	2	2	1	0
Toxicophores	1	3	3	2	1
QED	0.512	0.514	0.029	0.73	0.227
Synth	2.747	2.315	3.578	2.035	4.5
Fsp3	0.263	0.1	0.1	0.25	0.625
MCE-18	25	25	33	53.36	82.692
Natural Product-likeness	-1.956	-1.192	0.31	-1.656	1.186
Alarm_NMR	1	1	3	1	0
BMS	0	0	1	0	0
Chelating	0	0	2	0	1
PAINS	0	0	0	0	0
Lipinski	Accepted	Accepted	Rejected	Accepted	Rejected
Pfizer	Accepted	Rejected	Accepted	Accepted	Accepted
GSK	Rejected	Rejected	Rejected	Rejected	Rejected
GoldenTriangle	Accepted	Accepted	Rejected	Accepted	Accepted

Table S2 – ADMET analysis of selected compounds