

**Exploiting Butyrylcholinesterase inhibitors through a combined 3-D pharmacophore modeling, QSAR, molecular docking, and molecular dynamics investigation**

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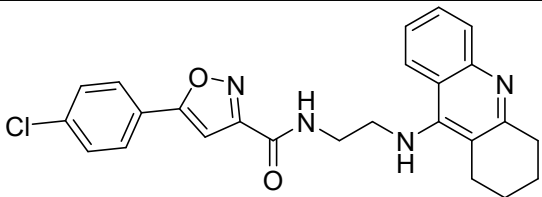
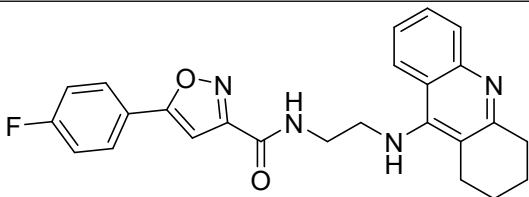
\*Corresponding Authors:

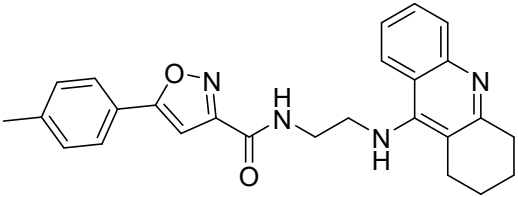
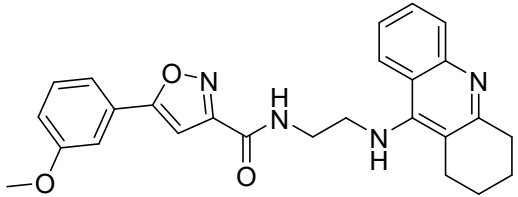
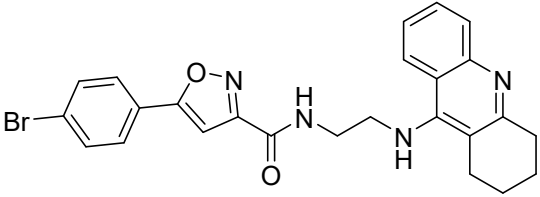
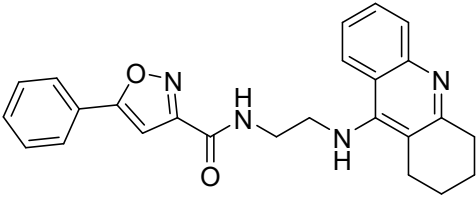
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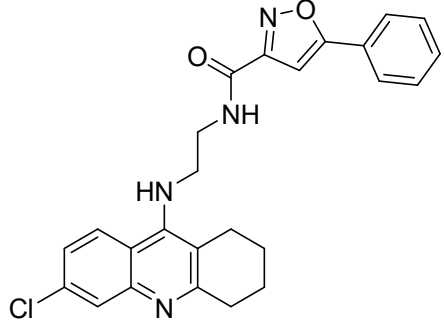
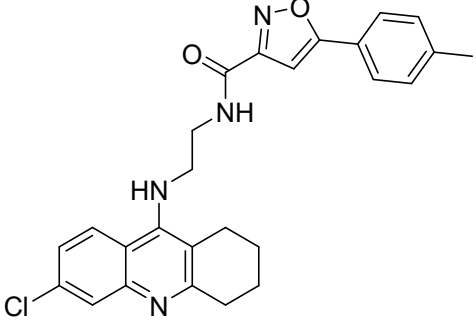
T. P. Aneesh ([aneeshtp@aims.amrita.edu](mailto:aneeshtp@aims.amrita.edu))

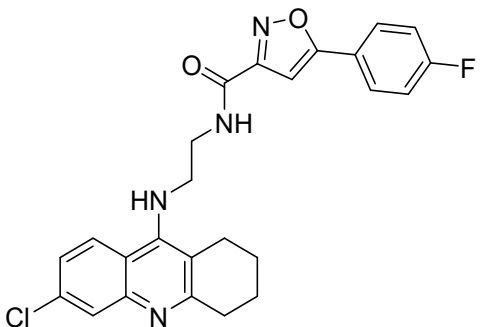
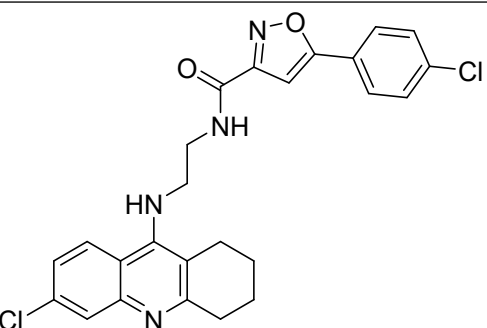


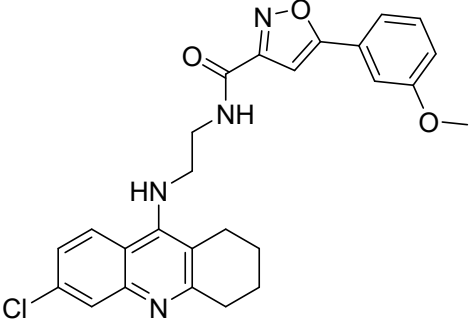
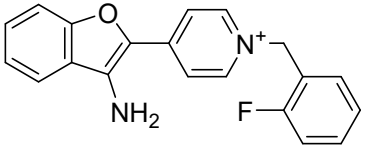
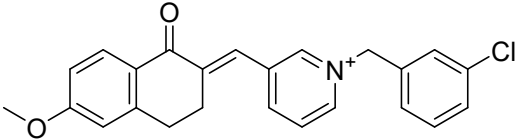
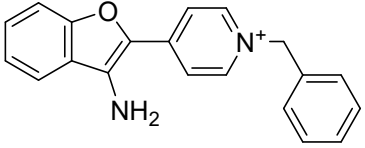
**Table S1.** BuChE for QSAR predicted and Actual activity

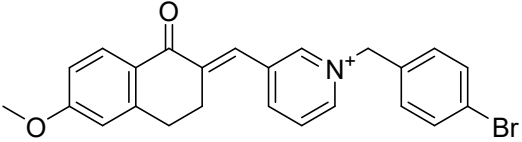
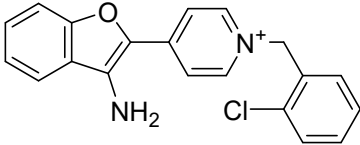
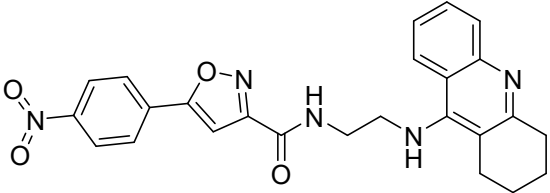
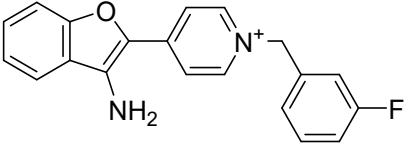
Ligand Name	QSAR Set	Actual Activity (pIC <sub>50</sub> )	Field-based QSAR for Predicted Activity (PLS 5)	QSAR Set	Atom based QSAR for Predicted Activity (PLS 3)
 Compound 1	training	7.409	7.01747	training	7.1583
 Compound 2	training	7.328	6.92972	training	7.13788

 <p>Compound 3</p>	Test	7.292	6.95671	training	7.16023
 <p>Compound 4</p>	training	7.125	6.80468	training	7.09444
 <p>Compound 5</p>	training	7.06	7.03326	test	7.16062
	training	7.056	6.91335	training	7.10718

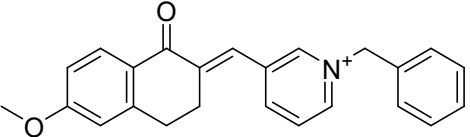
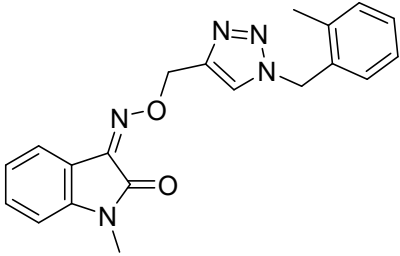
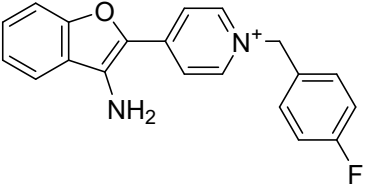
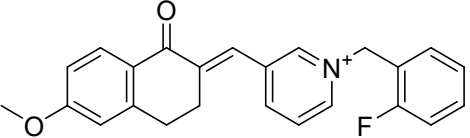
Compound 6					
 <p data-bbox="449 639 617 672">Compound 7</p>	training	7.056	6.86385	training	7.05836
 <p data-bbox="449 1083 617 1115">Compound 8</p>	Test	6.983	6.90626	test	7.11863

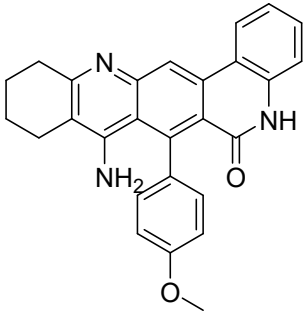
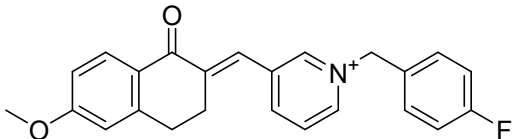
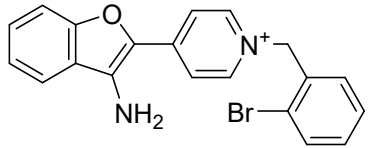
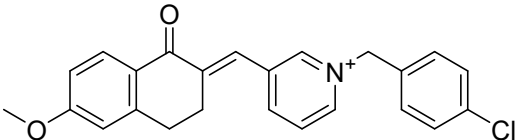
 <p>Compound 9</p>	training	6.695	6.88183	training	7.08906
 <p>Compound 10</p>	Test	6.429	6.96956	training	7.10948

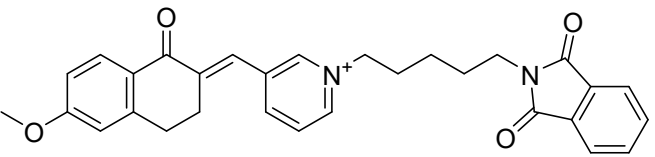
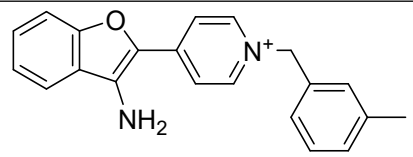
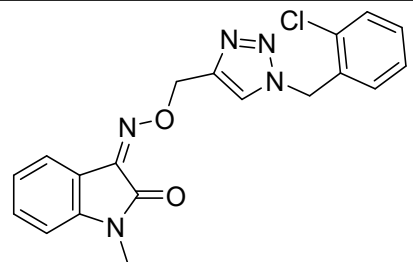
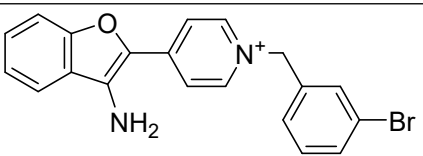
 <p>Compound 11</p>	training	6.384	6.7491	test	7.04661
 <p>Compound 12</p>	training	6.26	5.08415	training	4.96704
 <p>Compound 13</p>	training	6.145	5.63036	training	5.37106
 <p>Compound 14</p>	training	6.086	5.06577	test	4.9599

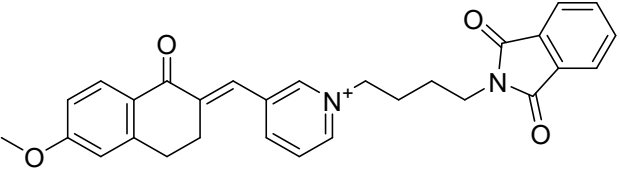
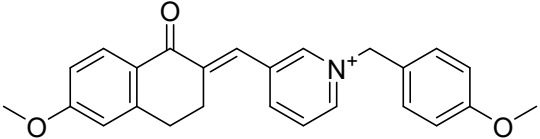
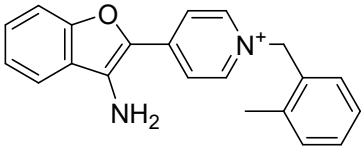
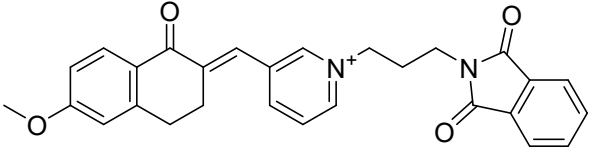
 <p>Compound 15</p>	Test	6.054	5.49175	training	5.39839
 <p>Compound 16</p>	training	6.004	5.13524	training	4.96745
 <p>Compound 17</p>	training	5.973	6.8144	test	7.09513
 <p>Compound 18</p>	Test	5.539	5.04063	training	4.96209

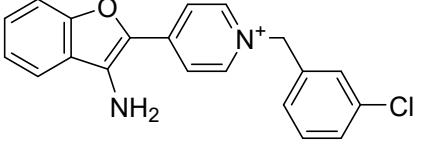
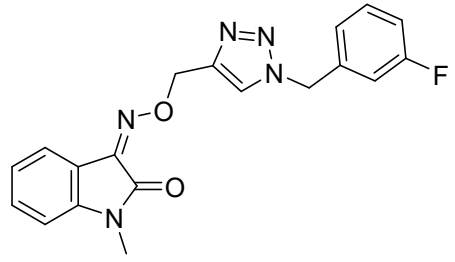
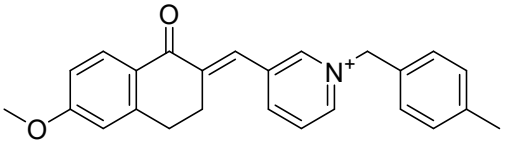
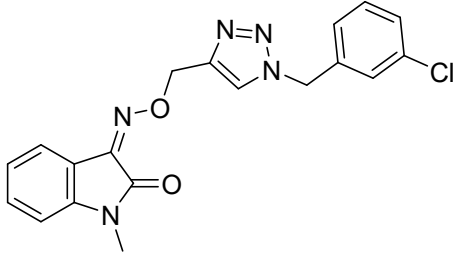


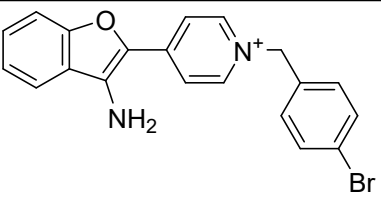
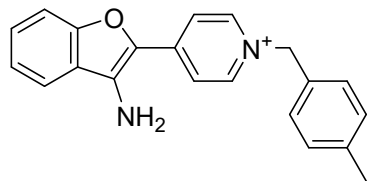
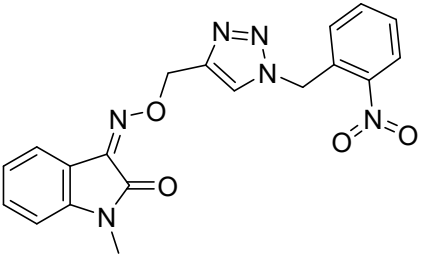
 <p>Compound 19</p>	training	5.531	5.08863	training	4.9037
 <p>Compound 20</p>	training	5.321	4.72085	training	4.66346
 <p>Compound 21</p>	Test	5.297	5.02728	training	4.95009
 <p>Compound 22</p>	training	5.247	5.57774	test	5.35398

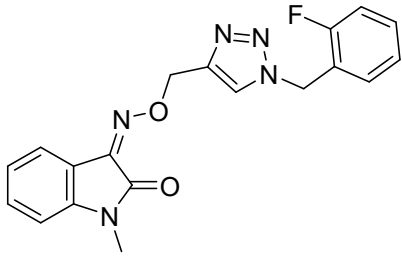
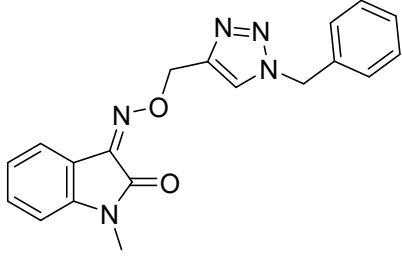
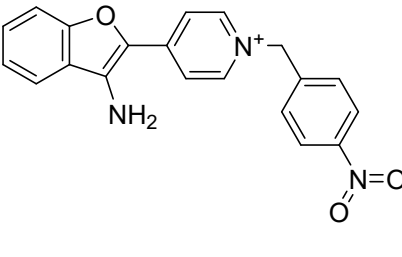
 <p>Compound 23</p>	Test	5.246	4.16236	training	4.38751
 <p>Compound 24</p>	training	5.202	5.50657	test	5.39353
 <p>Compound 25</p>	training	4.977	5.14092	training	4.96781
 <p>Compound 26</p>	training	4.928	5.5032	training	5.39352

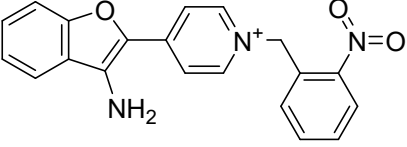
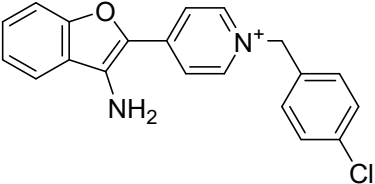
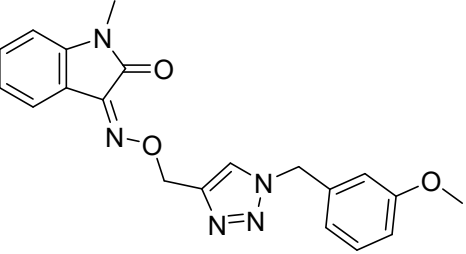
 <p>Compound 27</p>	training	4.893	4.78543	training	4.96557
 <p>Compound 28</p>	Test	4.89	5.09527	test	4.94496
 <p>Compound 29</p>	training	4.862	4.52889	training	4.56369
 <p>Compound 30</p>	training	4.855	5.04828	training	4.94011

 <p>Compound 31</p>	Test	4.799	4.75247	test	4.95427
 <p>Compound 32</p>	training	4.795	4.96831	training	4.90528
 <p>Compound 33</p>	Test	4.761	5.07329	training	4.96823
 <p>Compound 34</p>	training	4.735	4.52077	training	4.9408

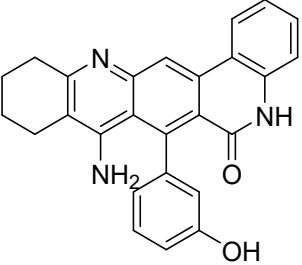
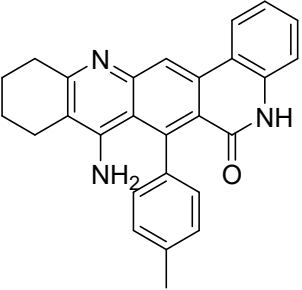
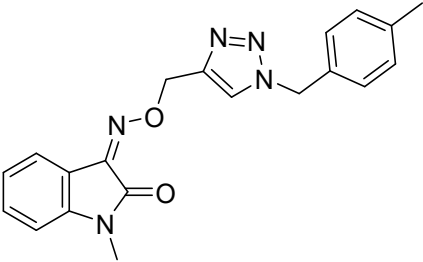
 <p>Compound 35</p>	training	4.727	5.05447	test	4.94493
 <p>Compound 36</p>	training	4.694	4.51215	training	4.55197
 <p>Compound 37</p>	Test	4.686	5.06602	test	4.88908
	training	4.661	4.50473	training	4.53675

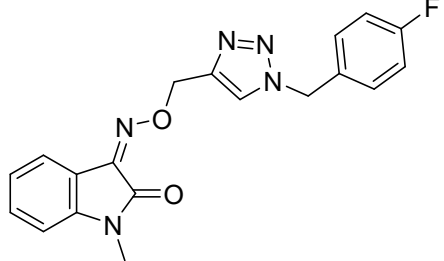
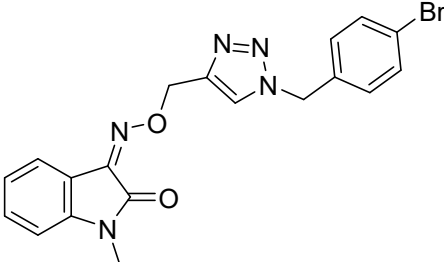
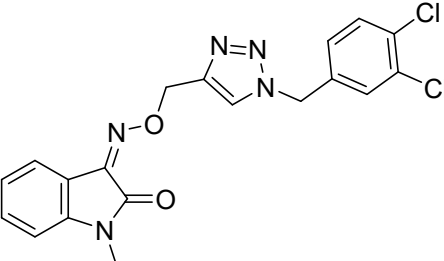
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	training	4.647	5.02471	training	4.93686
Compound 39					
	training	4.596	5.04273	training	4.94246
Compound 40					
	training	4.581	4.54142	training	4.56224
Compound 41					

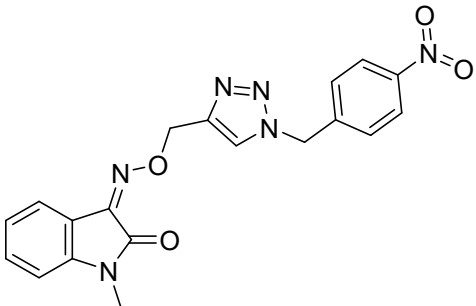
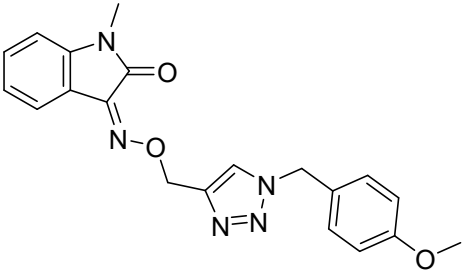
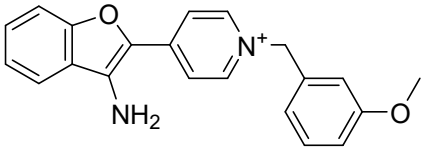
 <p>Compound 42</p>	Test	4.567	4.52572	training	4.5539
 <p>Compound 43</p>	Test	4.56	4.61829	test	4.61094
 <p>Compound 44</p>	training	4.549	4.92555	test	4.95284

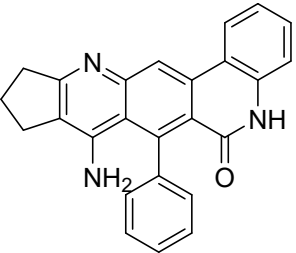
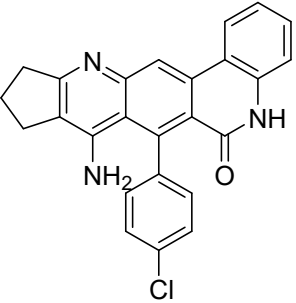
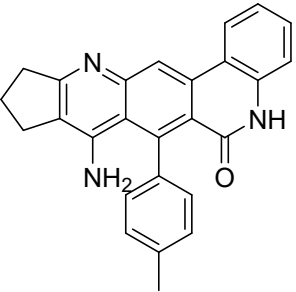
 <p>Compound 45</p>	training	4.543	4.91151	training	4.8981
 <p>Compound 46</p>	training	4.506	5.03493	training	4.9398
 <p>Compound 47</p>	training	4.403	4.44188	training	4.54792

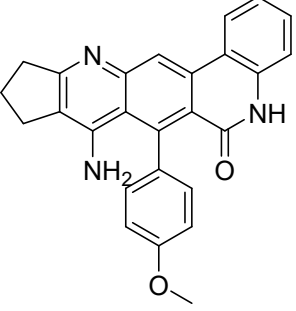
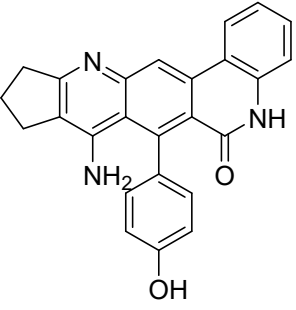
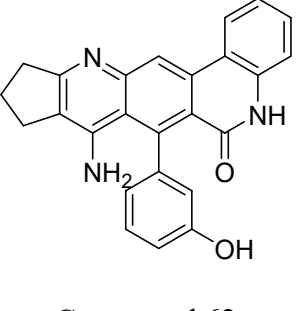


 <p>Compound 48</p>	Test	4.378	4.19165	training	4.37168
 <p>Compound 49</p>	training	4.244	4.13395	training	4.3722
 <p>Compound 50</p>	Test	4.208	4.53433	test	4.53704

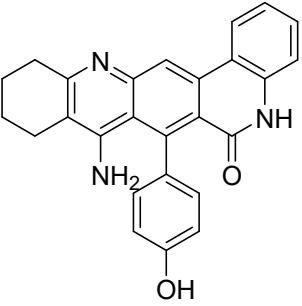
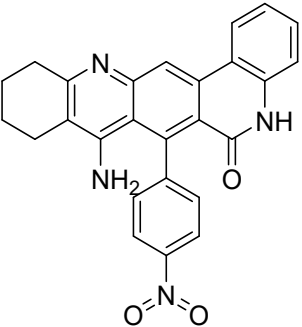
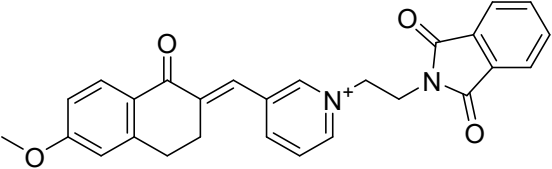
 <p>Compound 51</p>	training	4	4.4863	test	4.54588
 <p>Compound 52</p>	Test	4	4.48513	training	4.5214
 <p>Compound 53</p>	training	4	4.4672	training	4.51285

 <p>Compound 54</p>	training	4	4.42237	test	4.55175
 <p>Compound 55</p>	training	4	4.4656	training	4.51797
 <p>Compound 56</p>	Test	4	4.96642	training	4.88115

 <p>Compound 57</p>	Test	4	3.79702	training	4.0359
 <p>Compound 58</p>	training	4	3.78282	test	4.04397
 <p>Compound 59</p>	training	4	3.78324	test	4.04822

 <p>Compound 60</p>	Test	4	3.83309	training	4.02512
 <p>Compound 61</p>	training	4	3.83536	training	4.02444
 <p>Compound 62</p>	training	4	3.82083	training	4.04059

<p>Compound 63</p>	training	4	3.78918	training	4.02303
<p>Compound 64</p>	training	4	4.17606	training	4.38877
<p>Compound 65</p>	training	4	4.15722	test	4.3764

 <p>Compound 66</p>	Test	4	4.18808	test	4.38807
 <p>Compound 67</p>	training	4	4.15993	training	4.31344
 <p>Compound 68</p>	training	4	4.29067	training	4.78356

**Table S2.** Hit compounds with the associated smiles and docking scores.

Title	Smiles	Docking score (XP mode)	Predicted activity 5 by Field based QSAR (pIC <sub>50</sub> )	Estimate by 3D Pharmacophore Modeling (nM)	Fit Value for 3D pharmacophore model
Molecule5093	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc(cc1)ccc1Cl)C2=O</chem>	-9.9396	4.779075529	484.354	6.32114
Molecule1076	<chem>Cc1ccc(CNCC2=Cc(c(C)ccc3C)c3NC2=O)cc1</chem>	-9.85266	5.031473031	483.841	6.3216
Molecule4412	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc(cc1)cc3c1OCO3)C2=O</chem>	-9.72215	4.703024498	463.151	6.34058
Molecule1053	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc1cc(OC)c cc1)C2=O</chem>	-9.57104	4.888115675	485.046	6.32052
Molecule3344	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc(cc1)ccc1OC)C2=O</chem>	-9.07798	4.918060849	492.702	6.31372
Molecule1695	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc1cccc(F)c1)C2=O</chem>	-8.8853	4.716451827	483.084	6.32228
Molecule4651	<chem>OC1(CCN(Cc2c(C(F)(F)F)[nH]c3c2ccc n3)CC1)c(ccc1)c1F</chem>	-8.84899	4.749806312	1001.64	6.00559
Molecule3440	<chem>Cc1ccc([C@H](c2cnccc2)NCc(cc2OC) cc3c2OCCO3)cc1</chem>	-8.83569	5.065871666	864.521	6.06952
Molecule4313	<chem>CCC(N[C@H](CN(Cc1cccc1)C1)[C@ @H]1c1c(C2CC2)[nH]c2c1cccn2)=O</chem>	-8.67985	4.544218884	415.368	6.38787
Molecule1723	<chem>Cc1ccc(CNCC2=Cc(cc(C)cc3C)c3NC2=O)cc1</chem>	-8.51909	4.86938829	943.076	6.03175
Molecule4046	<chem>CC(C)c([nH]1)c(CN(CC2)CCC2(c2ccc cc2)NC(C)=O)c2c1ncc(C)c2</chem>	-8.38236	5.20825585	970.178	6.01945
Molecule5921	<chem>Cc1cccc(C=C2CN(C3CCCC3)C(c3cccs 3)=O)c1NC2=O</chem>	-8.26656	4.693281721	270.079	6.57481
Molecule4676	<chem>CCCOc(c(CN(CCC1)C[C@H]1c([nH]1 )cc2c1nccc2)ccc1)c1OC</chem>	-8.15113	4.705824876	528.527	6.28323



Molecule6046	<chem>CC1(C)OCC[C@](CCNCc(cc2)cc3c2O CO3)(Cc2ccccc2)C1</chem>	-8.13833	4.748465488	489.826	6.31626
Molecule2163	<chem>C[C@@H](c1nc(N2CCC(C)CC2)nc(O) c1)NCc(cc1)cc(N2C)c1N(C)C2=O</chem>	-8.12944	4.571676446	965.18	6.02169
Molecule5712	<chem>COc(cc1)c([C@H](CN(CCC2)[C@H]2 c(cc2)cc(OC)c2OC)O)cc1F</chem>	-8.04025	4.752099537	332.473	6.48454
Molecule4717	<chem>CC(C)n1nc(C)c(CN(CCC2)C[C@H]2c 2cc3ccnc3[nH]2)c1C</chem>	-7.8545	5.030468784	793.148	6.10695
Molecule5470	<chem>Cc(cc1C)cc(C=C2CNc(cc3)cc4c3OC O4)c1NC2=O</chem>	-7.76977	4.700456031	945.072	6.03084
Molecule4043	<chem>Cc1cc([C@@H](CN(CC2)CCC2(c2cc( C(F)(F)F)ccc2)O)O)c(C)s1</chem>	-7.71816	4.894167236	637.958	6.20151
Molecule3841	<chem>Cc1ccc([C@@H]([C@@H](CCC2)NC c3cc(OC)ccc3)N2C(C2CC2)=O)s1</chem>	-7.68353	4.608620101	408.293	6.39533
Molecule3943	<chem>CN(CC1)CCN1c1cc(CCNS(c(ccc2)c2 OC)(=O)=O)nc(C2CC2)n1</chem>	-7.63122	4.32593379	332.581	6.4844
Molecule2553	<chem>CNc1c(CN(C)CC2)c2nc([C@@H](CC C2)CN2C(CCc2c[nH]c3c2ccccc3)=O)n1</chem>	-7.56795	4.583408926	140.624	6.85824
Molecule2825	<chem>Cc1nc(CC(N(CC2)CCC2(Nc2c3ccccc2) NC3=O)=O)c(-c2ccccc2)s1</chem>	-7.50992	4.612387659	217.51	6.66882
Molecule6047	<chem>CC(C)(C1)OCC[C@H]1[C@@H](CCN Cc(cc1)cc2c1OCO2)c1ccc(C)cc1</chem>	-7.4206	5.049996878	466.418	6.33752
Molecule3264	<chem>CN(C)Cc1cc([C@H](CCC2)N2C(CCC c2c[nH]c3c2ccccc3)=O)nn1C</chem>	-7.3493	4.894776192	356.861	6.4538
Molecule5679	<chem>Cc1nn(CC=C)cc1CN(CCC1)CC[C@]1( c(cc1)ccc1F)O</chem>	-7.33668	5.283088576	329.256	6.48877
Molecule5409	<chem>COC(Cn1c(ccc2)c2c(CN(CC2)CCC2(c (cc2)ccc2F)O)c1)=O</chem>	-7.27092	5.208353134	914.499	6.04512
Molecule3976	<chem>CN(CC1)CCN1c1cc(CCNS(c(cc2)ccc2 OC)(=O)=O)nc(C2CC2)n1</chem>	-7.24062	4.487505846	609.71	6.22118
Molecule4415	<chem>Cc1nc(O)cc([C@H]2CN(Cc(cc(CCCC3 )c3c3)c3OC)CC2)n1</chem>	-7.16979	4.947756836	973.244	6.01808
Molecule4407	<chem>Cc(c(C)c1)cc2c1OC1(CCN(C[C@H](c( C1)O)C)C)C1</chem>	-7.11615	4.724985896	108.023	6.97278

	<chem>cc3)cc4c3OCCO4)O)CC1)C=C2</chem>				
Molecule4454	<chem>COc(ccc([C@H](C1)c(ccc2ccccc22)c2NC1=O)c1)c1OC</chem>	-7.11384	4.629830094	395.572	6.40907
Molecule1623	<chem>Cc1ccc(C)c(N2)c1C=C(CNc1ccccc1)C2=O</chem>	-7.03559	4.737497223	682.246	6.17236
Molecule4227	<chem>Cc1ccc(C2(CCN(Cc(c(C)c3)cc(OC)c3OC)CC2)O)cc1</chem>	-6.9741	4.818348073	362.272	6.44727
Molecule5570	<chem>CCOc(cc(CN(CC1)CCC1c([nH]1)cc2c1nccc2)c(C)c1)c1OC</chem>	-6.9619	4.613083754	910.706	6.04692
Molecule5077	<chem>Cc1ccc(C)c(N2)c1C=C(CNCc(cccc1)c1Cl)C2=O</chem>	-6.91658	4.769590782	483.04	6.32232
Molecule2903	<chem>CCc1noc(C)c1C(N(C[C@H]1c2cccc(F)c2)[C@H]2[C@H]1NCCCCC2)=O</chem>	-6.91614	5.137455039	588.439	6.2366
Molecule853	<chem>COc(cc1)c(C=C(CNc2ccccc2)C(N2)=O)c2c1OC</chem>	-6.89497	4.737307427	507.673	6.30072
Molecule5898	<chem>Cc1nn2c(N)cc([C@@H]3CN(Cc(cc(cc4)OC)c4OC)CCC3)nc2c1</chem>	-6.81438	4.757576926	96.9679	7.01967
Molecule5415	<chem>C[C@@H](CCN(CCC1)C[C@H]1c1nc2cc(C)nn2c(N)c1)c1ccc(C)o1</chem>	-6.62465	4.726507908	670.846	6.17968
Molecule4534	<chem>Cc1noc(C)c1S(NCCc1nc(C2CC2)nc(N2CCN(C)CC2)c1)(=O)=O</chem>	-6.61864	4.329782793	501.09	6.30638
Molecule4990	<chem>Cc(cc1)cc(CN([C@H](CC2)C3)[C@@H]2C[C@]3(c2cccc(F)c2)O)c1OC</chem>	-6.61405	4.983256889	743.704	6.1349
Molecule2254	<chem>Cc1enc(CCNS(c2cc([C@H](CC3)NC(C4CCCC4)=O)c3cc2)(=O)=O)s1</chem>	-6.60758	4.609783239	149.195	6.83255
Molecule4446	<chem>Cc1c(CN(CC2)CCC2(c(Enc(OC)n2)c2OC)O)c(cccc2)c2o1</chem>	-6.44109	4.425278461	310.776	6.51385
Molecule5403	<chem>COc1ccc(C2(CCCC2)NCc2c[nH]c3c2ccc(OC)c3)cc1</chem>	-6.39607	4.927540192	375.268	6.43196
Molecule5703	<chem>Cc1nn2c(N)cc([C@@H]3CN(Cc(cccc4)c4OCC=C)CCC3)nc2c1</chem>	-6.37246	4.611953029	234.88	6.63545
Molecule4930	<chem>Cc1c(C)sc([C@@H](Cc2csc2)NC(c2n[nH]cc2)=O)n1</chem>	-6.36825	4.54137217	857.82	6.0729

Molecule5390	<chem>CC(C)(C)c1csc(CCNC(c2c3nc(C4CC4)cc(C(F)F)n3nc2)=O)n1</chem>	-6.24483	4.531604094	556.932	6.2605
Molecule316	<chem>Cc1nn(CC=C)cc1CN(CC1)CCC1(c1c(C)cccc1)O</chem>	-6.1694	4.787468789	612.985	6.21885
Molecule3792	<chem>Cc1ccc([C@@H]([C@@H](CCC2)NCc3cccc3)N2C(C2CC2)=O)s1</chem>	-6.01437	4.54331046	643.445	6.19779
Molecule1436	<chem>CCOc(ccc(CNCc1cccc1)c1)c1OCC</chem>	-6.0086	4.79675048	372.339	6.43536
Molecule5037	<chem>Cc1nn(CC=C)cc1CN([C@H](CC1)C2)[C@@H]1C[C@@]2(c1cccc(F)c1)O</chem>	-5.83013	5.198136557	529.136	6.28273
Molecule3749	<chem>C[C@@H](Cc(cc1)cc2c1OCO2)CN(Cc1nc2cc(-c3noc(C)c3)nn2)Cc1c2O</chem>	-5.77804	4.925416841	309.642	6.51544
Molecule4435	<chem>Cc(c(CN([C@H](CC1)C2)[C@@H]1C[C@@]2(c(cc1)ccc1OC)O)c1)cc(OC)c1OC</chem>	-5.66664	4.827255188	454.746	6.34853
Molecule2699	<chem>Cc(c(C)c1)cc2c1OC1(CCN(CC(c(cc3)cc3)NC(C3CC3)=O)O)CC1)C=C2</chem>	-5.64837	5.103055779	66.6952	7.18221
Molecule5182	<chem>Cc1cc(CN(CCCc2nc(-c3ccncc3)n3)Cc2c3O)c(C)s1</chem>	-5.62624	4.663043631	932.383	6.03671
Molecule223	<chem>CCOc(ccc(CNCc1cccc1)c1)c1OC</chem>	-5.60263	4.874840205	609.791	6.22112
Molecule5589	<chem>COc1cc(OC)c(CN(CC2)CCc3c2c(O)nc(N2CCCC2)n3)cc1</chem>	-5.52662	4.750573521	329.59	6.48833
Molecule5752	<chem>COc(ccc([C@@H]([C@H]1[C@H]2CC1)[C@H]2NCc1ncccc1)c1)c1OC</chem>	-5.40279	4.92627287	942.07	6.03222
Molecule4400	<chem>CC(C)Oc(ccc(CN([C@H](CC1)C2)[C@@H]1C[C@@]2(c(cc1)ccc1F)O)c1)c1OC</chem>	-5.30529	5.038125981	816.756	6.09421
Molecule434	<chem>CCOc(ccc(CNCc1cccc1)c1)c1OCC</chem>	-5.2572	4.831791571	95.3676	7.0269
Molecule2913	<chem>CCOc(cc(CNCc1ncccc1)cc1)c1OC</chem>	-5.1791	4.834743702	91.2055	7.04628
Molecule4635	<chem>COc(cc1)cc(CN2CCc3nc(N4CCOCC4)nc(O)c3CC2)c1OC</chem>	-5.14847	5.011585408	342.832	6.47122
Molecule2688	<chem>Cc1ccc([C@@H]([C@@H](CCC2)NCc(ccc(OC)c3)c3OC)N2C(C2CC2)=O)s1</chem>	-5.09101	4.945599123	792.002	6.10757
Molecule4487	<chem>CC(COc1cc(CN([C@H](CC2)C3)[C@</chem>	-5.01601	4.730340726	704.08	6.15868

	<chem>@H]2C[C@]3(c2nccn2C)O)ccc1)=C</chem>				
Molecule82	<chem>CCc(cc(cc1)S(Nc2cnccc2)(=O)=O)c1O</chem> <chem>CC</chem>	-4.95451	4.610287339	721.283	6.14819
Molecule5636	<chem>CCc(cccc1)c1NC(N[C@H]1C[C@H](C</chem> <chem>CC2)N(Cc3cccs3)[C@H]2C1)=O</chem>	-4.94066	4.518330864	507.812	6.3006
Molecule5152	<chem>Cc1cc(CN(CC2)Cc3c2nc(-</chem> <chem>c2ncccc2)nc3O)cc(C)c1O</chem>	-4.93352	5.210810478	723.383	6.14693
Molecule5134	<chem>Cc(cc1)cc(CN([C@H](CC2)C3)[C@@</chem> <chem>H]2C[C@]3(c(cccc2)c2F)O)c1OC</chem>	-4.93034	5.053211128	835.102	6.08456
Molecule2712	<chem>Cc1ccc([C@@H]([C@@H](CCC2)NC</chem> <chem>c(c(OC)ccc3)c3OC)N2C(C2CC2)=O)s1</chem>	-4.56306	4.788040287	196.749	6.71239
Molecule4424	<chem>Cc1nn2c(O)c(CCN(Cc3cn(CC=C)nc3C)</chem> <chem>CC3)c3nc2c1</chem>	-4.46739	5.127688103	393.691	6.41114
Molecule1150	<chem>CN(c(ccc(CNCc1ccc1)c1)c1N1C)C1=</chem> <chem>O</chem>	-4.41713	4.763926812	460.353	6.34321
Molecule3654	<chem>CCCOc(c(C)c1)cc(C)c1S(Nc1cnccc1)(=</chem> <chem>O)=O</chem>	-3.9087	4.841660235	1000.87	6.00592
Molecule2099	<chem>Cc1cccc(C)c1OCC(N1Cc2c(NC)nc([C</chem> <chem>@@H]3CN(C)CCC3)nc2CC1)=O</chem>	-3.52271	4.269645322	607.706	6.22261
Molecule3838	<chem>Cc1ccc([C@@H]([C@@H](CCC2)NC</chem> <chem>c(cc3)ccc3OC)N2C(C2CC2)=O)s1</chem>	-3.44294	4.567924802	99.569	7.00818
Molecule4058	<chem>CC(C)Oc(cc(CN1[C@H]2Cc3nc4cc(C)</chem> <chem>nn4c(O)c3C[C@@H]1CC2)cc1)c1OC</chem>	-2.83909	4.718920826	925.558	6.0399
Molecule2091	<chem>CC(C)n1nc(C)c(CN2C[C@H](c3c(C(N</chem> <chem>C)=O)sc4ncccc34)OCC2)c1C</chem>	-1.941	4.988493157	453.31	6.3499
Molecule5943	<chem>CCc(cccc1)c1NC(NC1C[C@H](CCC2)</chem> <chem>N(Cc3ccccc3)[C@@H]2C1)=O</chem>	-1.86596	4.878245943	754.657	6.12855
Tacrine		-6.215			

Training: 48

Prediction: 20

Variables: 740

Excluded: 0

Missing: 0

Unknown: 0

Table S3: Correlation matrix for QSARINS model\_1\_best scored.

QI View correlation matrix

	RDF15Se	SpMax2_TheMAXDP2	ETA_Beta_m	ETA_Extap_B	bcutp13
RDF15Se	1.0000				
SpMax2_TheMAXDP2	0.1940	1.0000			
MAXDP2	0.3653	0.1820	1.0000		
ETA_Beta_m	0.2155	0.2326	0.3429	1.0000	
ETA_Extap_B	0.0396	-0.1944	0.0187	1.0000	
bcutp13	0.4328	0.3499	0.7188	0.3063	1.0000

Table S4: Modelling results for all QSARINS models with Var. 1 to 6 along with their statistical validations.

QI View and select models

St.	No.	ID	Size	Variables	R2	R2adj	R2R2adj	Q2	Kkx	Delta K	RMSE tr	MAE tr	RSS tr	ICCC tr	ls	Q2boot	R2-Q2boot	RMSE cv	MAE cv	PRESS cv	CCC cv	Q2 LMO	R2 Yscr	RMSE AV Yscr	Q2 Yscr	ln. ext. OK	RMSE ext	MAE ext	PRESS ext	R2 ext
U	1	198	4	SpMax2_TheMAXDP2	0.8949	0.8134	0.1909	0.3471	0.0728	0.3277	2.599	1.1553	0.5220	0.3546	67.7200	0.8729	0.0355	0.3859	0.3065	7.1494	0.9338	0.8634	0.1289	1.0095	-0.2023	3	0.4908	0.3937	4.8169	0.74
U	2	197	6	AATSC8_SpMax2_TheMAXDP2	0.8945	0.8135	0.1918	0.4028	0.0725	0.3284	2.469	1.1773	0.5518	0.3554	67.4010	0.8724	0.0355	0.3866	0.2905	7.1246	0.9337	0.8634	0.1289	1.0095	-0.2023	3	0.5050	0.4005	5.0997	
U	3	195	6	SpMax2_TheMAXDP2	0.8940	0.8135	0.1927	0.4310	0.0401	0.3292	2.432	1.2025	0.5515	0.3562	67.0440	0.8723	0.0352	0.3868	0.2854	7.1809	0.9335	0.8634	0.1289	1.0095	-0.2023	3	0.4694	0.3636	4.4072	
U	4	199	6	AATSC8_SpMax2_TheMAXDP2	0.8937	0.8136	0.1931	0.4340	0.0685	0.3296	2.444	1.2135	0.5514	0.3566	66.8880	0.8735	0.0338	0.3851	0.2855	7.1170	0.9339	0.8634	0.1289	1.0095	-0.2023	3	0.5408	0.4405	5.8487	
U	5	196	6	AATSC8_SpMax2_TheMAXDP2	0.8930	0.8137	0.1945	0.3773	0.0509	0.3308	2.621	1.2516	0.5510	0.3579	66.3520	0.8724	0.0342	0.3867	0.3067	7.1768	0.9334	0.8634	0.1289	1.0095	-0.2023	3	0.5018	0.3887	5.0369	
U	6	193	6	AATSC8_MATS2s_SpMax2_TheMAXDP2	0.8929	0.8137	0.1947	0.4586	0.0639	0.3309	2.474	1.2568	0.5510	0.3581	66.2800	0.8710	0.0356	0.3889	0.2903	7.2581	0.9328	0.8634	0.1289	1.0095	-0.2023	3	0.5656	0.4742	6.3990	
U	7	194	6	LODMIN_SpMax2_TheMAXDP2	0.8922	0.8138	0.1959	0.3908	0.0552	0.3320	2.598	1.2899	0.5507	0.3592	65.8220	0.8711	0.0348	0.3886	0.3043	7.2492	0.9327	0.8634	0.1289	1.0095	-0.2023	3	0.5122	0.3950	5.2471	
U	8	192	6	AATSC8_SpMax2_TheMAXDP2	0.8921	0.8138	0.1961	0.4800	0.0580	0.3321	2.482	1.2949	0.5506	0.3594	65.7540	0.8708	0.0351	0.3891	0.2907	7.2882	0.9324	0.8634	0.1289	1.0095	-0.2023	3	0.5477	0.4191	5.9997	
U	9	191	6	LODMIN_SpMax2_TheMAXDP2	0.8918	0.8141	0.2003	0.3947	0.0711	0.3357	2.492	1.4084	0.9495	0.3632	64.2310	0.8703	0.0335	0.3899	0.2924	7.2952	0.9321	0.8634	0.1289	1.0095	-0.2023	3	0.5018	0.4000	5.0356	
U	10	190	5	SpMax2_TheMAXDP2	0.8888	0.8118	0.1858	0.3066	0.1468	0.3412	2.780	1.5896	0.9477	0.3648	76.1250	0.8661	0.0345	0.3961	0.3219	7.5293	0.9294	0.8634	0.1289	1.0095	-0.2023	3	1.0218	0.5124	20.8795	
U	11	189	5	SpMax2_TheMAXDP2	0.8882	0.8119	0.1868	0.4438	0.0728	0.3422	2.737	1.6209	0.9474	0.3658	75.6540	0.8650	0.0351	0.3977	0.3160	7.5925	0.9290	0.8634	0.1289	1.0095	-0.2023	3	0.4669	0.3726	4.3597	
U	12	187	5	SpMax2_TheMAXDP2	0.8880	0.8121	0.1904	0.4433	0.0793	0.3455	2.666	1.7283	0.9463	0.3693	74.0790	0.8634	0.0348	0.4001	0.3076	7.6829	0.9285	0.8634	0.1289	1.0095	-0.2023	3	0.4920	0.4119	4.8411	
U	13	188	5	SpMax2_TheMAXDP2	0.8871	0.8122	0.1923	0.3750	0.0799	0.3472	2.691	1.7859	0.9458	0.3712	73.2570	0.8635	0.0336	0.3999	0.3092	7.6781	0.9283	0.8634	0.1289	1.0095	-0.2023	3	0.5013	0.4089	5.0260	
U	14	186	5	MATS2s_SpMax2_TheMAXDP2	0.8842	0.8123	0.1934	0.4068	0.0508	0.3482	2.744	1.8189	0.9455	0.3722	72.7950	0.8632	0.0333	0.4004	0.3143	7.6935	0.9282	0.8634	0.1289	1.0095	-0.2023	3	0.5709	0.4599	6.5189	
U	15	183	5	SpMax2_TheMAXDP2	0.8841	0.8123	0.1936	0.4822	0.0750	0.3483	2.673	1.8234	0.9454	0.3724	72.7210	0.8623	0.0342	0.4017	0.3085	7.7449	0.9277	0.8634	0.1289	1.0095	-0.2023	3	0.4919	0.4157	4.8393	
U	16	185	5	GATS3_SpMax2_TheMAXDP2	0.8840	0.8123	0.1938	0.4429	0.0355	0.3486	2.709	1.8316	0.9453	0.3728	72.6160	0.8621	0.0332	0.4025	0.3098	7.6992	0.9280	0.8634	0.1289	1.0095	-0.2023	3	0.5273	0.4439	5.3608	
U	17	184	5	SpMax2_TheMAXDP2	0.8827	0.8125	0.1959	0.4235	0.0835	0.3504	2.714	1.8933	0.9447	0.3746	71.7700	0.8623	0.0339	0.4017	0.3121	7.7443	0.9276	0.8634	0.1289	1.0095	-0.2023	3	0.5101	0.4141	5.2041	
U	18	181	5	SpMax2_TheMAXDP2	0.8825	0.8125	0.1963	0.4770	0.0659	0.3507	2.681	1.9041	0.9446	0.3749	71.6260	0.8622	0.0338	0.4018	0.3078	7.7508	0.9275	0.8634	0.1289	1.0095	-0.2023	3	0.4962	0.3981	4.9250	
U	19	182	5	SpMax2_TheMAXDP2	0.8825	0.8125	0.1963	0.4638	0.0792	0.3508	2.711	1.9053	0.9446	0.3749	71.6060	0.8622	0.0338	0.4018	0.3114	7.7473	0.9274	0.8634	0.1289	1.0095	-0.2023	3	0.4949	0.3981	4.8982	
U	20	180	4	SpMax2_TheMAXDP2	0.8833	0.8125	0.1968	0.3841	0.1239	0.3697	2.709	1.9615	0.9381	0.3906	81.4000	0.8622	0.0312	0.4162	0.3051	8.1353	0.9215	0.8634	0.1289	1.0095	-0.2023	3	0.4928	0.3954	4.8562	0.66
U	21	179	4	SpMax2_TheMAXDP2	0.8833	0.8125	0.1968	0.4496	0.0920	0.3786	2.836	2.0797	0.9349	0.4000	77.1370	0.8479	0.0298	0.4222	0.3187	8.5570	0.9191	0.8291	0.0851	1.0349	-0.1422	1	0.5320	0.4109	5.6599	0.65
U	22	178	4	MATS1s_SpMax2_TheMAXDP2	0.8862	0.8114	0.2066	0.4129	0.0416	0.3788	2.997	2.0860	0.9348	0.4002	77.0570	0.8469	0.0306	0.4235	0.3354	8.6090	0.9186	0.8230	0.0851	1.0349	-0.1454	2	0.4604	0.3554	4.6565	0.68
U	23	177	4	SpMax2_TheMAXDP2	0.8854	0.8115	0.2078	0.5693	0.0282	0.3798	2.945	2.1252	0.9344	0.4011	76.5610	0.8453	0.0316	0.4258	0.3295	8.7030	0.9180	0.8225	0.0843	1.0354	-0.1451	0	0.5321	0.4203	5.6337	0.22
U	24	172	4	GATS1s_SpMax2_TheMAXDP2	0.8850	0.8115	0.2084	0.4305	0.0967	0.3805	3.008	2.1479	0.9342	0.4020	76.2710	0.8453	0.0312	0.4258	0.3269	8.7013	0.9176	0.8192	0.0845	1.0352	-0.1422	1	0.5346	0.4304	5.7170	0.66
U	25	175	4	SpMax2_TheMAXDP2	0.8818	0.8118	0.2133	0.3338	0.1073	0.3849	2.920	2.1100	0.9325	0.4066	74.2910	0.8393	0.0343	0.4339	0.3286	9.0379	0.9141	0.8221	0.0870	1.0338	-0.1396	1	0.4569	0.3268	4.1746	0.62
U	26	176	4	SpMax2_TheMAXDP2	0.8817	0.8118	0.2135	0.4085	0.1247	0.3851	3.069	2.1183	0.9324	0.4069	74.1920	0.8416	0.0319	0.4308	0.3435	9.1020	0.9155	0.8223	0.0836	1.0358	-0.1442	2	0.5040	0.4069	5.0798	0.70
U	27	174	4	SpMax2_TheMAXDP2	0.8815	0.8118	0.2139	0.3808	0.0865	0.3854	3.063	2.1284	0.9323	0.4072	74.0590	0.8390	0.0342	0.4343	0.3447	9.0554	0.9141	0.8191	0.0853	1.0348	-0.1421	3	0.4532	0.3531	4.1087	0.72
U	28	171	4	MATS3s_SpMax2_TheMAXDP2	0.8828	0.8119	0.2152	0.3921	0.0555	0.3866	2.848	2.1736	0.9319	0.4084	73.5360	0.8406	0.0318	0.4321	0.3196	8.9630	0.9149	0.8340	0.0851	1.0349	-0.1427	1	0.5669	0.4487	6.4283	0.63
U	29	173	4	SpMax2_TheMAXDP2	0.8890	0.8120	0.2177	0.4155	0.1154	0.3899	3.226	2.2579	0.9310	0.4108	72.5570	0.8388	0.0322	0.4346	0.3622	9.0670	0.9139	0.8175	0.0862	1.0342	-0.1403	1	0.5229	0.3875	5.4689	0.60
U	30	182	3	SpMax2_TheMAXDP2	0.8846	0.8142	0.2078	0.2866	0.1761	0.4255	3.322	2.7217	0.9158	0.4457	79.7980	0.8165	0.0283	0.4638	0.3629	10.3234	0.9005	0.8091	0.0635	1.0472	-0.1167	1	0.5751	0.4284	6.4154	0.61
U	31	161	3	SpMax2_TheMAXDP2	0.8307	0.8108	0.2426	0.2684	0.1445	0.4310	3.455	3.9166	0.9139	0.4502	77.8500	0.8109	0.0306	0.4708	0.3782	10.6374	0.8981	0.8035	0.0602	1.0491	-0.1222	1	0.5576	0.4361	6.2178	0.64
U	32	159	3	SpMax2_TheMAXDP2	0.8204	0.8115	0.2573	0.2653	0.0436	0.4439	3.949	4.5470	0.9082	0.4636	7															