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Quantitative Structure-Activity Relationship (QSAR) Studies and Molecular docking Simulation of Norepinephrine Transporter (NET) Inhibitors as Anti-psychotic Therapeutic Agents

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Supplementary Table S1: Molecule ID, Chemical Names, RMSD values (PDB: 4M48 and PDB: 2A65) with Predicted pKi, Experimental pKi and Binding Affinity values of the studied molecules

S/N	CHEM ID	NAME	Experimental pKi	Predicted pKi	Residual	Binding Affinity (kcal/mol) PDB: 4M48	RMSD (PDB: 4M48)	Binding Affinity (kcal/mol) PDB: 2A65	RMSD (PDB: 2A65)
1.	CHEMBL32540	(Z)-5-((Z)-2-(7a-methyl-1-(6-methylheptan-2-yl)hexahydro-1H-inden-4(2H)-ylidene)ethylidene)-	6.000	6.072	-0.073	-7.2	±1.889	-8.6	±1.853

		4-methylenecyclohexane-1,3-diol							
2.	CHEMBL781	5-(4-chlorophenyl)-3,5-dihydro-2H-imidazo[2,1-a]isoindol-5-ol	8.899	7.945	0.954	-6.9	±1.789	-7.2	±1.966
3.	CHEMBL808	1-(2-((4-chlorobenzyl) oxy)-2-(2,4-dichlorophenyl)ethyl)-1H-imidazole	5.617	5.817	-0.200	-6.15	±1.204	-7.5	±1.617
4.	CHEMBL822	(E)-N,6,6-trimethyl-N-(naphthalen-1-ylmethyl)hept-2-en-4-yn-1-amine	5.388	5.404	-0.016	-6.7	±1.237	-8.0	±0.146
5.	CHEMBL828	10H-phenothiazine	6.340	6.496	-0.156	-5.7	±1.943	-7.1	±0.504
6.	CHEMBL42553	methyl 3-(3,4-dichlorophenyl)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate	8.301	8.531	-0.230	-6.15	±0.349	-6.9	±1.851
7.	CHEMBL926	N-(3,4-dihydroxyphenethyl)-4-(4-	6.420	6.482	-0.062	-6.8	±0.535	-6.5	±0.575

		hydroxyphenyl)butan-2-aminium							
8.	CHEMBL482903	2-(3-(5-fluoro-1H-indol-3-yl)propyl)-6-methoxy-1,2,3,4-tetrahydroisoquinolin-2-ium	5.775	6.095	0.010	-7.4	±0.743	-8.0	±0.835
9.	CHEMBL63703	4-((2-(benzhydryloxy)ethyl)ammonio)-1-benzylpiperidin-1-ium	6.745	6.735	0.447	-7.1	±1.207	-9.2	±1.072
10.	CHEMBL67024	1-(2-(benzhydryloxy)ethyl)-4-((4-fluorophenethyl)ammonio)piperidin-1-ium	7.102	6.655	0.316	-7.0	±1.527	-8.9	±1.112
11.	CHEMBL165	(E)-5-(4-hydroxystyryl)benzene-1,3-diol	5.639	5.323	-0.252	-6.25	±0.655	-7.1	±0.963
12.	CHEMBL67078	1-(2-(benzhydryloxy)ethyl)-3-(((3-phenylpropyl)ammonio)methyl)piperidin-1-ium	7.387	7.639	-0.214	-7.35	±1.365	-9.3	±1.379

13.	CHEMBL99653	1-(1-hydroxycyclohexyl)-N,N-dimethyl-1-(3-(trifluoromethyl)phenyl)methanaminium	7.678	7.891	0.047	-6.5	±1.723	-6.7	±1.707
14.	CHEMBL81	1-(2-(4-(6-hydroxy-2-(4-hydroxyphenyl)benzo[b]thiophene-3-carbonyl)phenoxy)ethyl)piperidin-1-ium	6.553	6.506	0.159	-8.0	±0.140	-8.5	±1.453
15.	CHEMBL109571	N,N-dimethyl-1-(3-(naphthalen-2-yl)bicyclo[2.2.1]heptan-2-yl)methanaminium	6.955	6.796	-0.854	-7.0	±0.111	-8.3	±1.623
16.	CHEMBL121027	N1-(2-(benzhydryloxy)ethyl)-N2-(4-fluorophenethyl)-N1,N2-dimethylethane-1,2-diaminium	6.432	6.751	-0.319	-6.0	±0.672	-7.9	±1.795
17.	CHEMBL12161	N1-(2-(bis(4-fluorophenyl)metho	7.086	7.939	0.239	-6.5	±1.232	-8.9	±1.589

	1	xy)ethyl)-N3-phenethylpropane-1,3-diaminium							
18.	CHEMBL123252	N1-(2-(benzhydryloxy)ethyl)-N1,N3-dimethyl-N3-(3-phenylpropyl)propane-1,3-diaminium	7.523	6.696	0.826	-5.9	±1.444	-8.2	±0.395
19.	CHEMBL121460	N1,N2-bis(2-(bis(4-fluorophenyl)methoxy)ethyl)-N1,N2-dimethylethane-1,2-diaminium	6.583	6.328	-0.336	-5.85	±0.121	-6.5	±0.186
20.	CHEMBL1231	3-(2-cyclohexyl-2-hydroxy-2-phenylacetoxy)-N-isopropylprop-2-yn-1-aminium	5.589	5.350	0.510	-6.4	±1.329	-7.2	±1.50
21.	CHEMBL139245	3-(4-chlorophenyl)-N-methyl-3-(naphthalen-1-yloxy) propan-1-aminium	7.108	7.349	0.053	-7.25	±1.043	-7.6	±1.307
22.	CHEMBL139277	N-methyl-3-(naphthalen-1-yloxy)-3-(m-	7.398	7.734	-0.326	-6.8	±1.803	-8.3	±1.823

		tolyl)propan-1-aminium							
23.	CHEMBL141114	N-methyl-3-(naphthalen-1-yloxy)-3-(p-tolyl)propan-1-aminium	7.444	7.357	0.086	-6.7	±0.884	-6.7	±0.873
24.	CHEMBL142028	N-methyl-3-(naphthalen-1-yloxy)-3-(thiophen-3-yl)propan-1-aminium	7.678	7.168	0.186	-6.25	±1.432	-7.4	±1.271
25.	CHEMBL141681	N-methyl-3-(naphthalen-1-yloxy)-3-phenylpropan-1-aminium	7.699	7.645	-0.383	-6.55	±1.754	-6.5	±1.087
26.	CHEMBL141974	N-methyl-3-(naphthalen-1-yloxy)-3-(3-(trifluoromethyl)phenyl)propan-1-aminium	7.155	7.074	0.081	-7.35	±1.076	-8.0	±0.870
27.	CHEMBL1289	1,2,4-trichloro-5-((3-iodoprop-2-yn-1-yl)oxy)benzene	5.561	5.887	-0.174	-4.4	±0.555	-5.0	±0.510
28.	CHEMB	4-nonylphenol	5.905	6.110	0.250	-5.45	±1.111	-5.9	±1.813

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29.	CHEMBL179249	2-(phenyl(o-tolylthio)methyl)morpholin-4-ium	9.523	9.337	-0.355	-6.75	±1.332	-7.1	±2.640
30.	CHEMBL188248	1-(2-((2-aminophenyl)thio)phenyl)-N-methylmethanaminium	7.426	7.809	0.492	-5.4	±1.266	-6.5	±1.209
31.	CHEMBL189374	1-(2-((2-amino-4-methylphenyl)thio)phenyl)-N-methylmethanaminium	6.719	8.035	-1.316	-5.85	±1.543	-7.1	±1.733
32.	CHEMBL190700	1-(2-((2-aminophenyl)thio)phenyl)-N,N-dimethylmethanaminium	8.305	8.399	-0.094	-5.25	±1.355	-6.5	±1.066
33.	CHEMBL194205	N-methyl-3-(3-methyl-2-oxo-1-phenyl-1,2,3,4-tetrahydroquinolin-3-yl)propan-1-aminium	7.357	7.636	-0.279	-5.9	±0.923	-7.4	±0.315

34.	CHEMBL194781	3-(6-fluoro-2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	8.301	8.082	-0.039	6.6	±1.541	-7.9	±1.901
35.	CHEMBL196751	3-(3-ethyl-2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	7.769	7.942	-0.072	-6.3	±1.894	-6.7	±1.897
36.	CHEMBL196110	3-(3-butyl-2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	8.097	7.846	0.010	-5.75	±0.123	-6.9	±0.428
37.	CHEMBL196368	3-(1-(3-fluorophenyl)-2-oxo-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	7.745	8.429	-0.684	-6.95	±1.325	-7.4	±1.021
38.	CHEMBL19738	8-(2-(1H-indol-3-yl)ethyl)-3-((bis(4-	5.084	5.438	-0.319	-7.5	±1.721	-10.3	±1.817

	4	fluorophenyl)methyl)ammonio)-8-azabicyclo[3.2.1]octan-8-ium							
39.	CHEMBL198033	N-methyl-3-(2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)propan-1-aminium	8.523	8.031	0.826	-6.6	±1.974	-7.5	±1.481
40.	CHEMBL198215	3-(6-chloro-3-methyl-2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	7.367	7.403	0.086	-6.4	±1.024	-6.8	±1.140
41.	CHEMBL197643	3-(1-(4-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinolin-3-yl)-N-methylpropan-1-aminium	7.678	8.177	-0.499	-6.7	±1.437	-6.8	±1.531
42.	CHEMBL197707	3-((bis(4-fluorophenyl)methyl)ammonio)-8-(4-phenylbutyl)-8-	5.788	5.449	-1.316	-7.0	±1.543	-7.9	±1.697

		azabicyclo[3.2.1]octan-8-ium							
43.	CHEMBL1988807	3-(((4-chlorophenyl)(phenyl)methyl)ammonio)-8-methyl-8-azabicyclo[3.2.1]octan-8-ium	5.499	5.504	-0.094	-7.35	±0.822	-7.2	±0.744
44.	CHEMBL2003110	3-((bis(4-fluorophenyl)methyl)ammonio)-8-(3-oxo-3-(phenylamino)propyl)-8-azabicyclo[3.2.1]octan-8-ium	5.607	4.500	1.107	-8.45	±1.237	-9.9	±0.281
45.	CHEMBL1989960	N-methyl-3-(2-oxo-1-phenyl-4-propyl-1,2,3,4-tetrahydroquinolin-4-yl)propan-1-aminium	8.155	8.936	-0.781	-6.25	±1.398	-7.3	±2.716
46.	CHEMBL1988842	3-(3,4-dichlorophenyl)-8-(2-(4-(9-(dimethyliminio)-11,11-dimethyl-	6.511	6.550	-0.499	-7.5	±2.124	-8.4	±1.570

		3,4-dihydronaphtho[2,3-g]quinolin-1(2H,9H,11H)-yl)butanamido)ethyl)-2-(methoxycarbonyl)-8-azabicyclo[3.2.1]octan-8-ium							
47.	CHEMBL199116	N-methyl-3-(2-oxo-3-propyl-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)propan-1-aminium	7.959	8.031	1.107	-6.15	±2.332	-6.6	±1.422
48.	CHEMBL198176	N-methyl-3-(3-methyl-2-oxo-1-(p-tolyl)-1,2,3,4-tetrahydroquinolin-3-yl)propan-1-aminium	8.046	7.760	-0.781	-6.4	±0.978	-7.6	±1.792
49.	CHEMBL202410	1-(1-oxo-1-(p-tolyl)pent-4-en-2-yl)pyrrolidin-1-ium	5.854	7.285	0.286	-5.75	±1.521	-6.9	±1.471
50.	CHEMB	1-(1-(4-(furan-2-	7.022	7.012	-1.431	-6.3	±1.379	-7.1	±1.285

	L201976	yl)phenyl)-1-oxopentan-2-yl)pyrrolidin-1-ium							