Supplementary Information

Identifying Potential Machine Learning Algorithms for the Simulation of Binding Affinities to Molecularly Imprinted Polymers

Joseph W. Lowdon [1]*, Hikaru Ishikura [2], Malene K. Kvernenes [2], Manlio Caldara [1], Thomas J. Cleij [1] and Bart van Grinsven [1], Kasper Eersels [1], Hanne Diliën [1]

[1] Sensor Engineering Department, Faculty of Science and Engineering, Maastricht University, PO Box 616, 6200 MD Maastricht, the Netherlands

[2] Maastricht Science Programme, Faculty of Science and Engineering, Maastricht University, PO Box 616, 6200 MD Maastricht, the Netherlands

* Correspondence: Joseph Lowdon: joe.lowdon@maastrichtuniversity.nl

Supplementary Table S1. MIP training data set

Molecule	SMILE	C_i/ mM	C_f / mM	S_b /µmol g^{-1}
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3 0.1	0.1	5.89	24.25494
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C 0.1	0.1	102.63	-0.65789
paracetamol	CC(=O)NC1=CC=C(C=C1)O 0.1	0.1	67.83	8.04315
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O 0.1	0.1	51.58	12.10526
aspirin	CC(=O)Oc1ccccc1C(=O)O 0.1	0.1	52.63	11.84211
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.1	0	2.5
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.1	0	2.5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.1	8.99	0.02533
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.1	7.87E-01	0.05315
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3 0.1	0.1	70.88	7.28047
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.1	385.83	28.542
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.1	370.65	32.3367
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.1	220.36	69.9111
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3 0.2	0.2	0.0107	46.85651
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C 0.1	0.2	0.18684	3.2569
paracetamol	CC(=O)NC1=CC=C(C=C1)O 0.1	0.2	0.15915	10.11039
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O 0.1	0.2	0.11579	20.84419
aspirin	CC(=O)Oc1ccccc1C(=O)O 0.1	0.2	0.09474	26.05524
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.2	1.09E-04	0.47279
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.2	0	5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.2	0.0018	0.04935
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.2	0.00169	0.07677
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3 0.1	0.2	0.15945	10.13785
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.2	0.17309	6.7266
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.2	0.12073	19.81764
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.2	0.0712	32.2
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.3	0.01815	69.42034
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.3	0.27368	6.48172
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.3	0.25262	11.6707
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.3	0.15263	36.29764
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.3	0.16684	32.79751
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.3	1.14E-04	0.72138
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.3	0	7.5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.3	0.0026	0.0995
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.3	0.00274	0.06524
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.3	0.17443	31.39314
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.3	0.25845	10.38778
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.3	0.1981	25.47605
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.3	0.11573	46.06667
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.4	0.02699	95.1557
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.4	0.36895	7.92159
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.4	0.34608	13.75513

Molecule	SMILE			
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.4	0.26263	35.04296
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.4	0.26053	35.58002
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.4	1.22E-04	0.96951
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.4	2.95E-04	12.42634
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.4	0.00348	0.13005
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.4	0.00371	0.0734
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.4	0.2096	47.60122
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.4	0.29354	26.61395
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.4	0.30059	24.8528
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.4	0.17084	57.28889
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.5	0.03571	115.4961
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.5	0.46895	7.72454
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.5	0.44008	14.90624
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.5	0.32105	44.51427
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.5	0.33211	41.76486
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.5	1.56E-04	1.21106
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.5	0.00787	18.03348
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.5	0.00439	0.15146
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.5	0.00467	0.08296
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.5	0.25768	60.58016
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.5	0.38583	28.54203
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.5	0.37065	32.33665
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.5	0.22036	69.91111

Supplementary Table S2. NIP training data set

Molecule	SMILE	Ci$_i$/ mM	C$_f$ / mM	S$_b$/ µmol g^{-1}
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.1	0.01178	21.20633
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.1	0.19684	0.78947
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.1	0.0753	6.17389
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.1	0.04737	13.15789
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.1	0.05789	10.52632
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.1	8.44E-05	0.22889
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.1	0	2.5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.1	7.00E-04	0.07496
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.1	7.71E-04	0.05737
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.1	0.01631	20.92351
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.1	0.12101	19.7479
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.1	0.06646	58.38509
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.1	0.00522	23.69506
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.2	0.02416	42.47235
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.2	0.28947	2.63158
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.2	0.15915	10.21149
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.2	0.10526	23.68421
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.2	0.1	25
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.2	1.11E-04	0.47232
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.2	0	5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.2	0.0013	0.17605
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.2	0.0017	0.07396
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.2	0.07264	31.84109
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.2	0.09076	52.31092
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.2	0.14472	63.81988
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.2	0.06264	34.34075
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.3	0.03859	67.72254
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.3	0.38421	3.88903
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.3	0.25742	10.64409
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.3	0.15789	35.52632
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.3	0.16842	32.89474
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.3	1.16E-04	0.72092
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.3	0	7.5
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.3	0.00224	0.19093
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.3	0.00271	0.07227
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.3	0.08449	53.87637
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.3	0.22185	44.53782
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.3	0.24845	62.8882
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.3	0.09082	52.29408
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.4	0.05476	85.0343
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.4	0.47684	5.78947
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.4	0.34875	12.62309
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.4	0.26316	33.70495
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.4	0.25789	35.0013
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.4	1.18E-04	0.97045

Molecule	SMILE			
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.4	1.07E-04	12.47321
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.4	0.00319	0.20189
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.4	0.00364	0.08886
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.4	0.15565	61.08805
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.4	0.25882	60.29412
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.4	0.46522	33.03495
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.4	0.21192	47.01952
2-methoxphenidine	COc1ccccc1C(Cc2ccccc2)N3CCCCC3	0.5	0.0877	98.63604
caffeine	CN1C=NC2=C1C(=O)N(C(=O)N2C)C	0.5	0.55632	10.70691
paracetamol	CC(=O)NC1=CC=C(C=C1)O	0.5	0.44115	14.71374
sucrose	OCC2OC(OC1(CO)OC(CO)C(O)C1O)C(O)C(O)C2O	0.5	0.33158	42.10526
aspirin	CC(=O)Oc1ccccc1C(=O)O	0.5	0.33684	40.78947
crystal violet	CN(C)c3ccc(C(c1ccc(N(C)C)cc1)=c2ccc(=[N+](C)C)cc2)cc3	0.5	1.58E-04	1.2106
basic blue	CCNc3ccc(C(c1ccc(N(CC)CC)cc1)=c2ccc(=[N+](CC)CC)cc2)c4ccccc34	0.5	0.00135	19.66295
methyl orange	CN(C)c2ccc(/N=N/c1ccc(S(=O)(=O)[O-])cc1)cc2	0.5	0.00409	0.22853
phenol red	O=S(=O)([O-])c3ccc(C(c1ccc(O)cc1)=c2ccc(=[OH+])cc2)cc3	0.5	0.00457	0.10686
4-methoxphenidine	COc3ccc(C(Cc1ccccc1)N2CCCCC2)cc3	0.5	0.28313	54.21731
ephenidine	CCNC(Cc1ccccc1)c2ccccc2	0.5	0.39328	50.66733
2-methoxephenidine	CCNC(Cc1ccccc1)c2ccccc2OC	0.5	0.3559	86.02484
4-methoxephenidine	CCNC(Cc1ccccc1)c2ccc(OC)cc2	0.5	0.24115	64.71187

Supplementary Table S3. MIP testing data set

Molecule	SMILE	C_{i_i}/ mM	C_f / mM	S_b /µmol g^{-1}
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.1	35.75	16.06232
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.1	77.83	5.54237
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.1	331.93	15.5798
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.2	0.06604	33.48929
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.2	0.16827	7.9322
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.2	0.07211	31.97227
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.3	0.10893	47.76708
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.3	0.21559	21.10169
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.3	0.12196	44.50876
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.4	0.1577	60.57525
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.4	0.23607	40.98305
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.4	0.26118	34.70545
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.5	0.2157	71.07402
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.5	0.31878	45.30508
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.5	0.33193	42.01771
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.1	35.75	16.06232
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.1	77.83	5.54237
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.1	331.93	15.5798
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.2	0.06604	33.48929
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.2	0.16827	7.9322
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.2	0.07211	31.97227
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.3	0.10893	47.76708
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.3	0.21559	21.10169
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.3	0.12196	44.50876
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.4	0.1577	60.57525
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.4	0.23607	40.98305
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.4	0.26118	34.70545
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.5	0.2157	71.07402
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.5	0.31878	45.30508
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.5	0.33193	42.01771

Supplementary Table S4. NIP testing data set

Molecule	SMILE	C_{i_i}/ mM	C_f / mM	S_b /µmol g^{-1}
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.1	0.05416	11.45973
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.1	0.09503	1.24327
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.1	0.05592	11.01974
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.2	0.09667	25.83134
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.2	0.11086	22.28381
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.2	0.08355	2.91E+01
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.3	0.11007	47.48267
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.3	0.18055	29.86221
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.3	0.14539	38.65132
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.4	0.14385	64.0382

Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.4	0.31992	20.01901
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.4	0.20461	48.84868
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.5	0.26032	59.91934
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.5	0.19639	75.90276
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.5	0.29671	50.82237
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.1	0.05416	11.45973
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.1	0.09503	1.24327
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.1	0.05592	11.01974
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3 0.1	0.2	0.09667	25.83134
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3 0.1	0.2	0.11086	22.28381
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.2	0.08355	2.91E+01
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.3	0.11007	47.48267
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.3	0.18055	29.86221
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.3	0.14539	38.65132
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.4	0.14385	64.0382
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.4	0.31992	20.01901
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.4	0.20461	48.84868
3-MXP	COc3cccc(C(Cc1ccccc1)N2CCCCC2)c3	0.5	0.26032	59.91934
Diphenidine	c3ccc(CC(c1ccccc1)N2CCCCC2)cc3	0.5	0.19639	75.90276
3-MEPE	CCNC(Cc1ccccc1)c2cccc(OC)c2	0.5	0.29671	50.82237