

ChemOracle® (/)

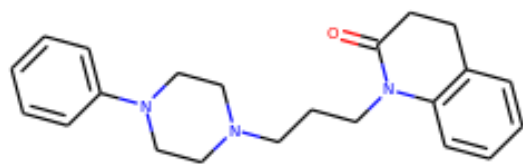
An integrated web-based platform for target prediction: your compounds our solutions!

[HOME \(/\)](#)

[PREDICTION \(/PREDICTION/\)](#)

[ABOUT US \(/ABOUT_US/\)](#)

Your molecule

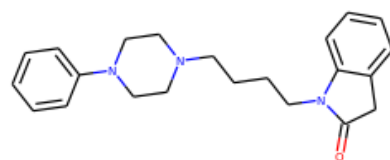


has 35 possible target(s) !

Dopamine D2 receptor: ki = N.A.00 nM Score = 10.3125

Best Fingerprints Similarity

ECFP2



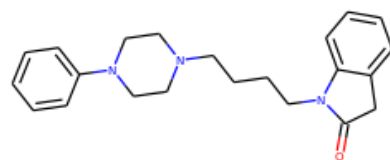
CHEMBL395933

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933>)

ki = 162.0 nM

simil = 0.904761904762

FCFP2



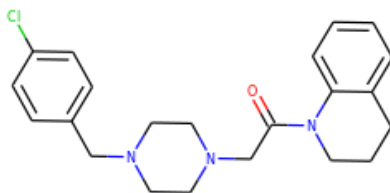
CHEMBL395933

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933>)

ki = 162.0 nM

simil = 1.0

DAY



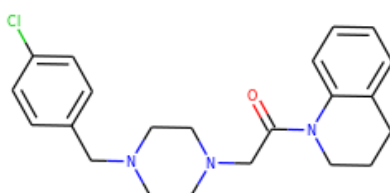
CHEMBL323537

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL323537>)

ki = 2629.0 nM

simil = 0.706329113924

PAT



CHEMBL323537

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL323537>)

ki = 2629.0 nM

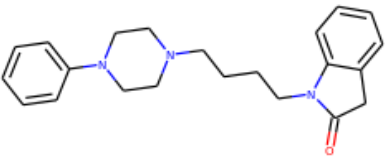
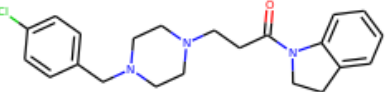
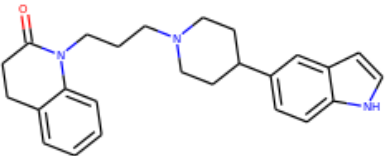
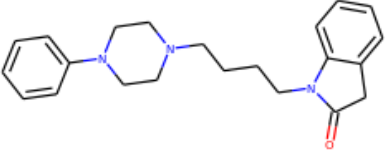
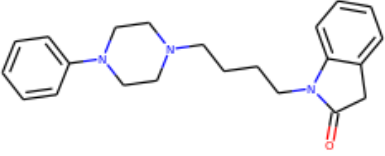
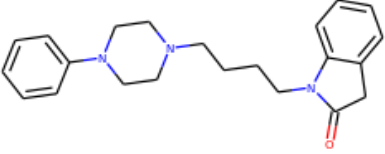
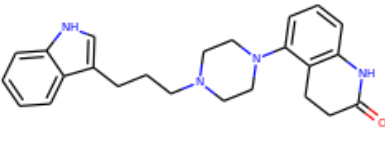
simil = 0.917553191489

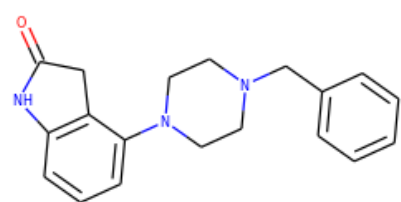
Latest News

Website alpha-v
Launched

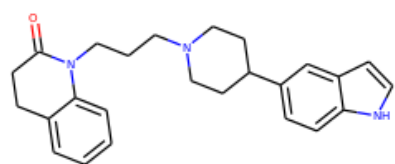
October 10th, 201

Work in progress.

PAIR		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 162.0 nM simil = 0.709401709402</p>
TORS		<p><u>CHEMBL104498</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL104498) ki = 5847.0 nM simil = 0.78125</p>
FP2		<p><u>CHEMBL2059305</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2059305) ki = 42.0 nM simil = 0.733944954128</p>
PUB		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 162.0 nM simil = 0.906779661017</p>
MACCS		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 162.0 nM simil = 0.934782608696</p>
KR		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 162.0 nM simil = 0.760563380282</p>
GRAPH		<p><u>CHEMBL383396</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL383396) ki = 11.4 nM simil = 0.924050632911</p>
SUB		<p><u>CHEMBL314952</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL314952) ki = 8.0 nM simil = 1.0</p>



HYB



CHEMBL2059305

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2059305>)

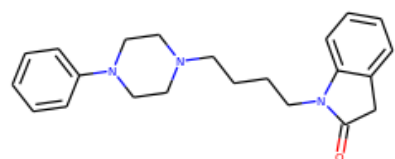
ki = 42.0 nM

simil = 0.739473684211

Serotonin 1a (5-HT1a) receptor: ki = N.A.00 nM Score = 9.4165

Best Fingerprints Similarity

ECFP2



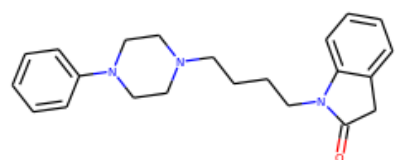
CHEMBL395933

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933>)

ki = 124.0 nM

simil = 0.904761904762

FCFP2



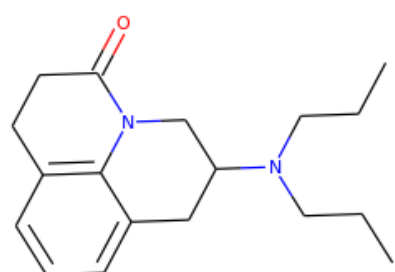
CHEMBL395933

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933>)

ki = 124.0 nM

simil = 1.0

DAY



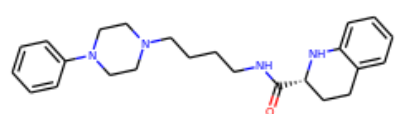
CHEMBL11577

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11577>)

ki = 2.4 nM

simil = 0.690366972477

PAT



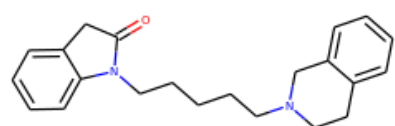
CHEMBL3358505

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358505>)

ki = 9.9 nM

simil = 0.886243386243

PAIR

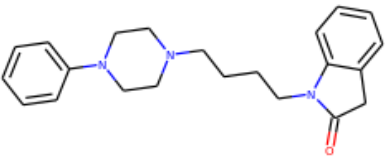
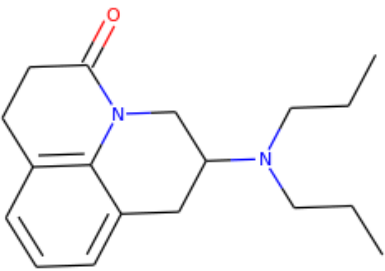
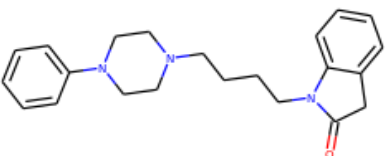
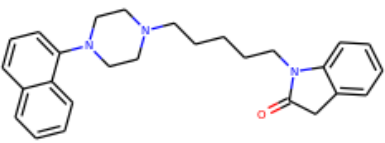
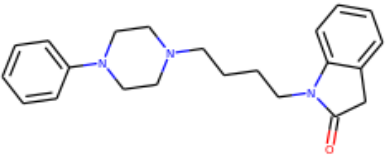
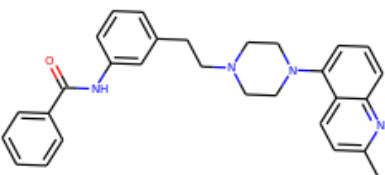
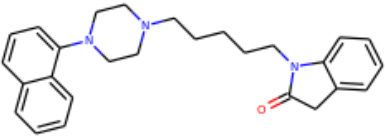


CHEMBL3321777

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3321777>)

ki = 523.0 nM

simil = 0.719298245614

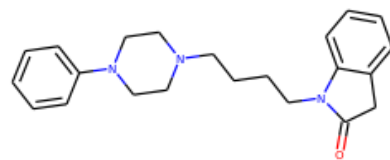
TORS		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933 ki = 124.0 nM simil = 0.6875</p>
FP2		<p><u>CHEMBL11577</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11577 ki = 2.4 nM simil = 0.768518518519</p>
PUB		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933 ki = 124.0 nM simil = 0.906779661017</p>
MACCS		<p><u>CHEMBL506875</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL506875 ki = 16.0 nM simil = 0.934782608696</p>
KR		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933 ki = 124.0 nM simil = 0.760563380282</p>
GRAPH		<p><u>CHEMBL1632210</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210 ki = 1.0 nM simil = 0.848101265823</p>
SUB		<p><u>CHEMBL506875</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL506875 ki = 16.0 nM simil = 1.0</p>

HYB

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933))

ki = 124.0 nM

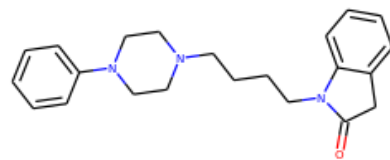
simil = 0.611979166667



Dopamine D3 receptor: ki = N.A.00 nM Score = 9.4092

Best Fingerprints Similarity

ECFP2



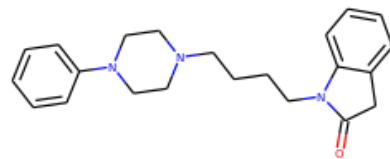
CHEMBL395933

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933))

ki = 80.0 nM

simil = 0.904761904762

FCFP2



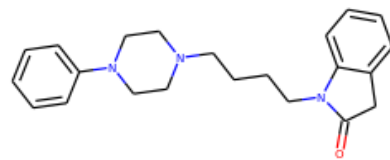
CHEMBL395933

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933))

ki = 80.0 nM

simil = 1.0

DAY



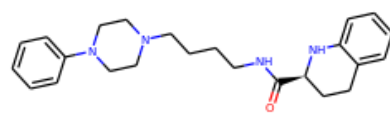
CHEMBL395933

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933))

ki = 80.0 nM

simil = 0.636246786632

PAT



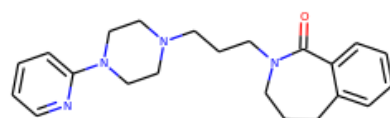
CHEMBL3358507

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507))

ki = 45.0 nM

simil = 0.886243386243

PAIR



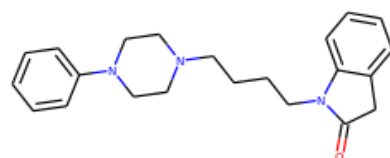
CHEMBL476841

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL476841](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL476841))

ki = 4168.69 nM

simil = 0.711111111111

TORS

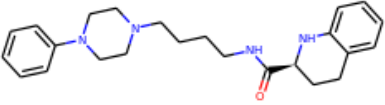
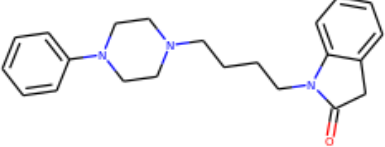
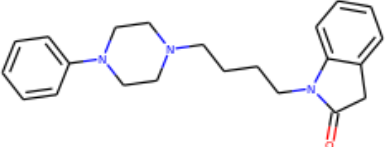
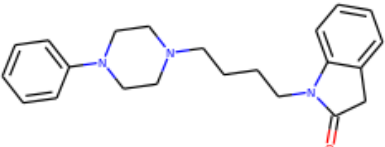
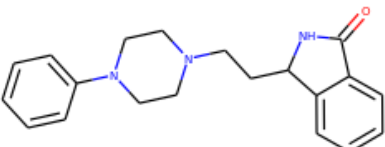
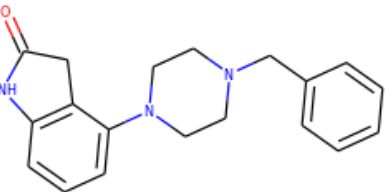
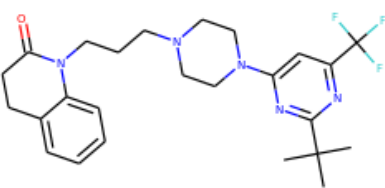


CHEMBL395933

[.https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933))

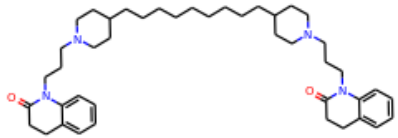
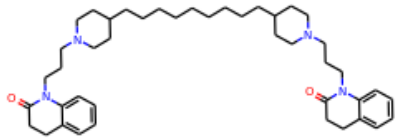
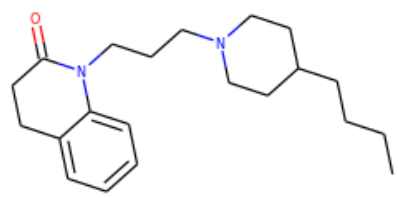
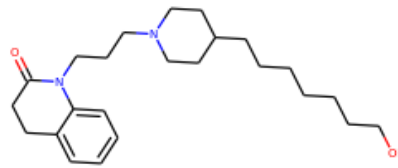
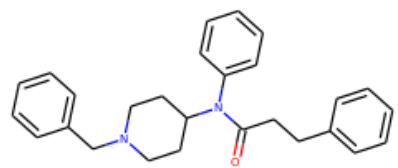
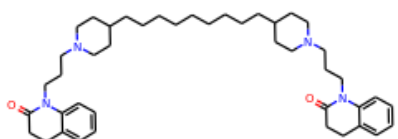
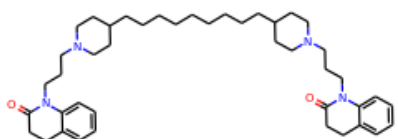
ki = 80.0 nM

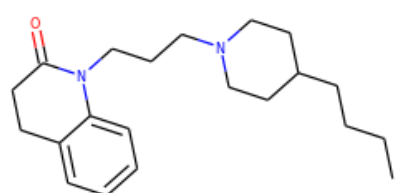
simil = 0.6875

FP2		<u>CHEMBL3358507</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507) ki = 45.0 nM simil = 0.694444444444
PUB		<u>CHEMBL395933</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 80.0 nM simil = 0.906779661017
MACCS		<u>CHEMBL395933</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 80.0 nM simil = 0.934782608696
KR		<u>CHEMBL395933</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 80.0 nM simil = 0.760563380282
GRAPH		<u>CHEMBL34239</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL34239) ki = 2682.0 nM simil = 0.910256410256
SUB		<u>CHEMBL314952</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL314952) ki = 5.4 nM simil = 1.0
HYB		<u>CHEMBL201742</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL201742) ki = 93.8 nM simil = 0.707259953162

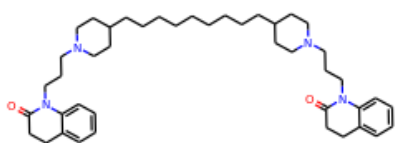
Muscarinic acetylcholine receptor M2: ki = 257.8084 nM Score = 9.0038

Best Fingerprints Similarity

ECFP2		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 79.43 nM simil = 0.75</p>
FCFP2		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 79.43 nM simil = 0.8125</p>
DAY		<p><u>CHEMBL3354065</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065) ki = 204.17 nM simil = 0.847507331378</p>
PAT		<p><u>CHEMBL3354074</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074) ki = 208.93 nM simil = 0.89010989011</p>
PAIR		<p><u>CHEMBL85950</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL85950) ki = 794.33 nM simil = 0.624060150376</p>
TORS		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 79.43 nM simil = 0.806451612903</p>
FP2		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 79.43 nM simil = 0.824742268041</p>
PUB		<p><u>CHEMBL3354065</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065) ki = 204.17 nM simil = 0.905982905983</p>



MACCS



CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 79.43 nM

simil = 0.891304347826

CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 79.43 nM

simil = 0.602409638554

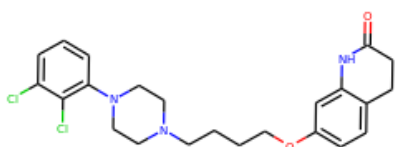
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 79.43 nM

simil = 0.864864864865

SUB

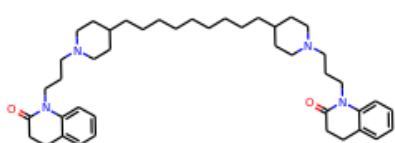


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)

ki = 1000.0 nM

simil = 0.857142857143

HYB



CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

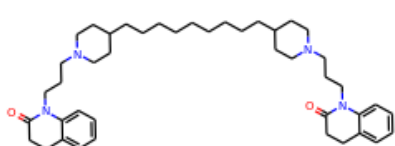
ki = 79.43 nM

simil = 0.786350148368

Muscarinic acetylcholine receptor M3: ki = N.A.00 nM Score = 9.0038

Best Fingerprints Similarity

ECFP2

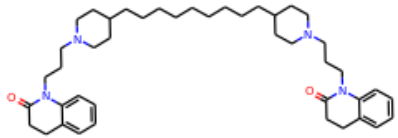
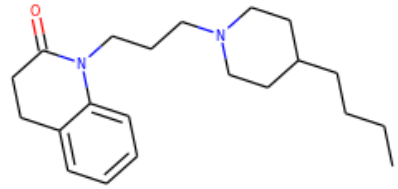
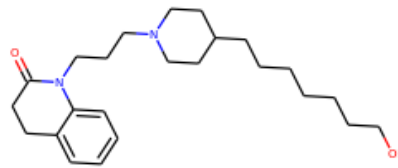
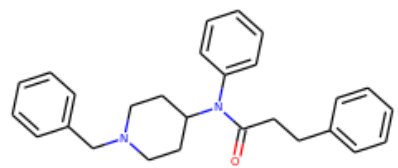
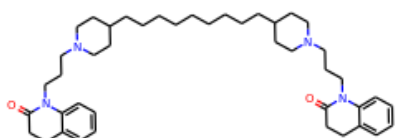
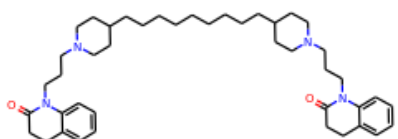
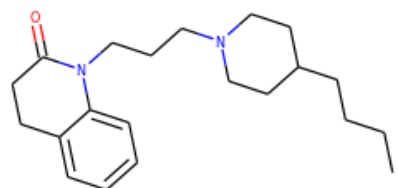


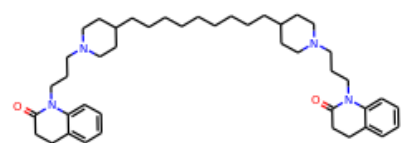
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

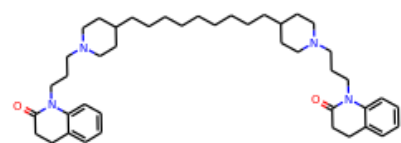
ki = 57.54 nM

simil = 0.75

FCFP2		<u>CHEMBL3354078</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 57.54 nM simil = 0.8125
DAY		<u>CHEMBL3354065</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065) ki = 1202.26 nM simil = 0.847507331378
PAT		<u>CHEMBL3354074</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074) ki = 630.96 nM simil = 0.89010989011
PAIR		<u>CHEMBL85950</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL85950) ki = 79.43 nM simil = 0.624060150376
TORS		<u>CHEMBL3354078</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 57.54 nM simil = 0.806451612903
FP2		<u>CHEMBL3354078</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 57.54 nM simil = 0.824742268041
PUB		<u>CHEMBL3354065</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065) ki = 1202.26 nM simil = 0.905982905983
MACCS		<u>CHEMBL3354078</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 57.54 nM simil = 0.891304347826



KR



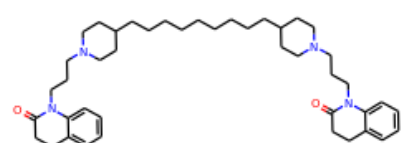
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 57.54 nM

simil = 0.602409638554

GRAPH



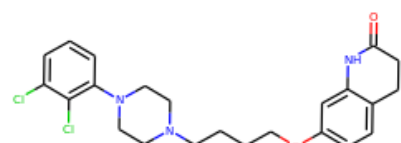
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 57.54 nM

simil = 0.864864864865

SUB

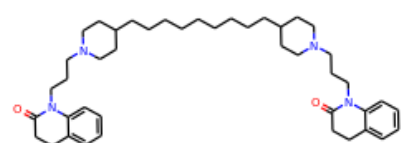


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)

ki = 1000.0 nM

simil = 0.857142857143

HYB



CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

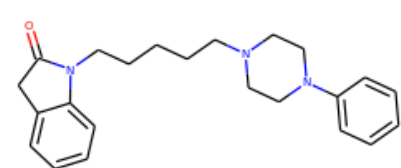
ki = 57.54 nM

simil = 0.786350148368

Serotonin 7 (5-HT7) receptor: ki = 64.5988 nM Score = 8.644

Best Fingerprints Similarity

ECFP2



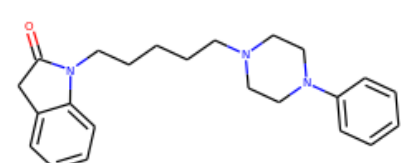
CHEMBL489029

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489029>)

ki = 63.0 nM

simil = 0.904761904762

FCFP2

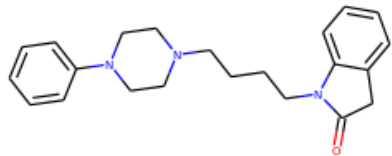
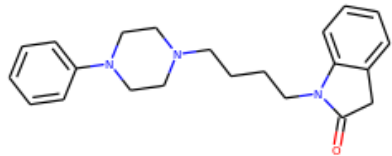
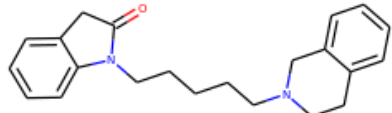
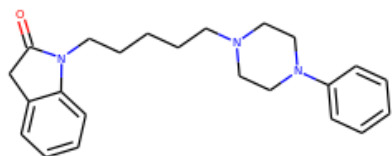
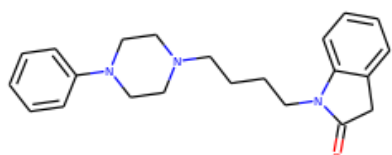
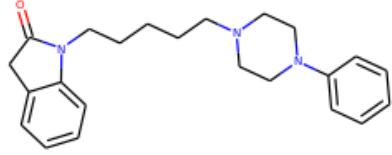
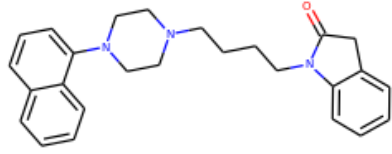


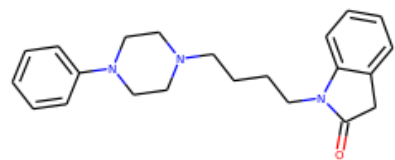
CHEMBL489029

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489029>)

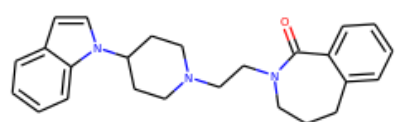
ki = 63.0 nM

simil = 1.0

DAY		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 74.0 nM simil = 0.636246786632</p>
PAT		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 74.0 nM simil = 0.880319148936</p>
PAIR		<p><u>CHEMBL3321777</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3321777) ki = 28.0 nM simil = 0.719298245614</p>
TORS		<p><u>CHEMBL489029</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489029) ki = 63.0 nM simil = 0.6875</p>
FP2		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 74.0 nM simil = 0.67619047619</p>
PUB		<p><u>CHEMBL489029</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489029) ki = 63.0 nM simil = 0.906779661017</p>
MACCS		<p><u>CHEMBL489028</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489028) ki = 22.0 nM simil = 0.934782608696</p>
KR		<p><u>CHEMBL395933</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933) ki = 74.0 nM simil = 0.760563380282</p>



GRAPH

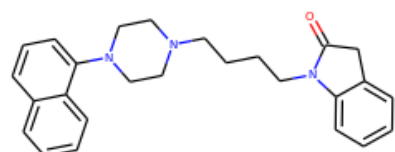


CHEMBL9952 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL9952>)

ki = 2.754 nM

simil = 0.85

SUB



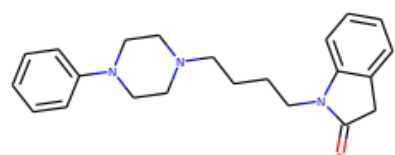
CHEMBL489028

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL489028>)

ki = 22.0 nM

simil = 1.0

HYB



CHEMBL395933

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933>)

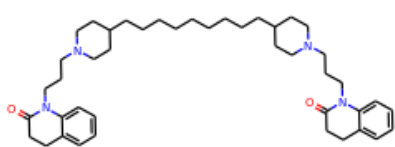
ki = 74.0 nM

simil = 0.611979166667

Muscarinic acetylcholine receptor M1: ki = 214.5401 nM Score = 8.3798

Best Fingerprints Similarity

ECFP2



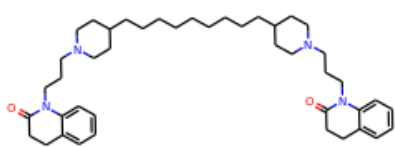
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 29.51 nM

simil = 0.75

FCFP2



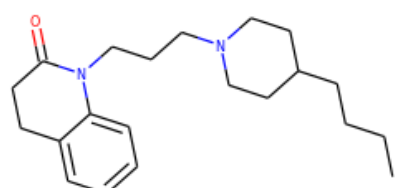
CHEMBL3354078

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)

ki = 29.51 nM

simil = 0.8125

DAY



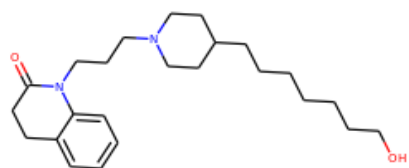
CHEMBL3354065

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)

ki = 316.23 nM

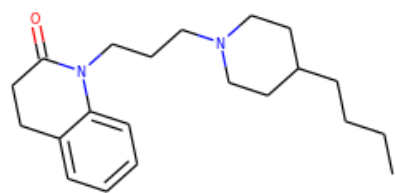
simil = 0.847507331378

PAT



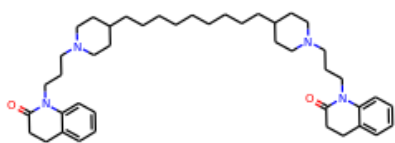
CHEMBL3354074
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074>)
ki = 354.81 nM
simil = 0.89010989011

PAIR



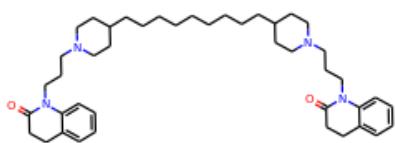
CHEMBL3354065
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)
ki = 316.23 nM
simil = 0.52380952381

TORS



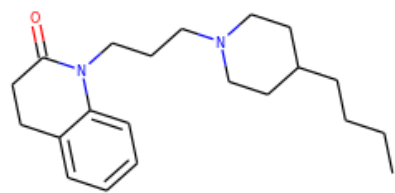
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.806451612903

FP2



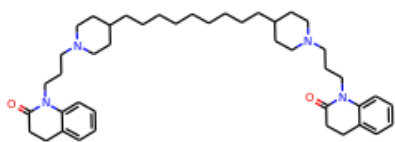
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.824742268041

PUB

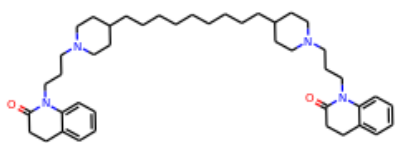


CHEMBL3354065
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)
ki = 316.23 nM
simil = 0.905982905983

MACCS



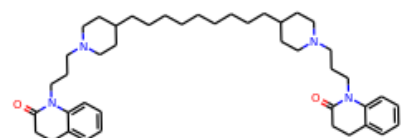
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.891304347826



KR

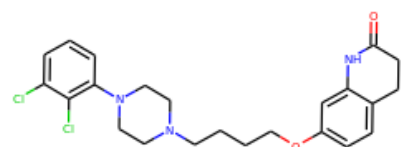
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.602409638554

GRAPH



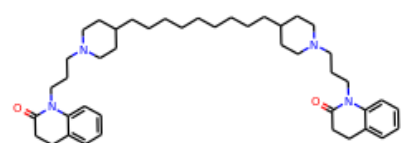
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.864864864865

SUB



CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 1000.0 nM
simil = 0.857142857143

HYB

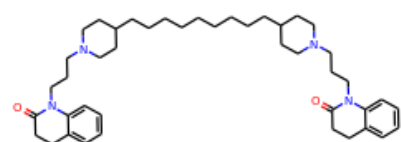


CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 29.51 nM
simil = 0.786350148368

Muscarinic acetylcholine receptor M5: ki = 2496.1638 nM Score = 8.3798

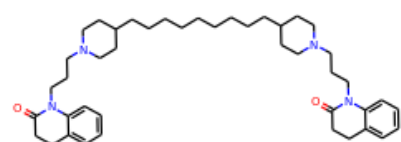
Best Fingerprints Similarity

ECFP2



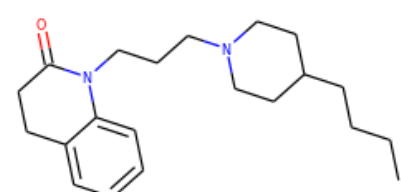
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.75

FCFP2



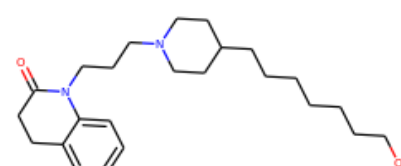
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.8125

DAY



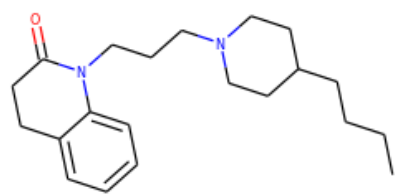
CHEMBL3354065
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)
ki = 5370.32 nM
simil = 0.847507331378

PAT



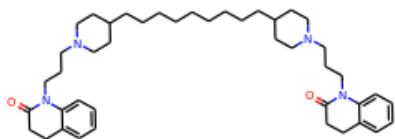
CHEMBL3354074
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074>)
ki = 3090.3 nM
simil = 0.89010989011

PAIR



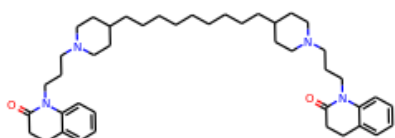
CHEMBL3354065
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)
ki = 5370.32 nM
simil = 0.52380952381

TORS



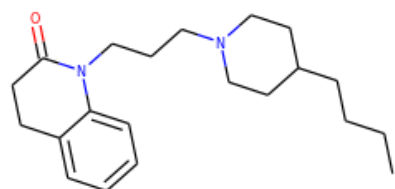
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.806451612903

FP2



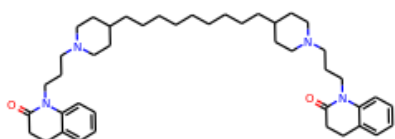
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.824742268041

PUB



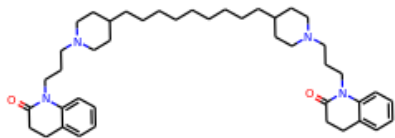
CHEMBL3354065
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065>)
ki = 5370.32 nM
simil = 0.905982905983

MACCS



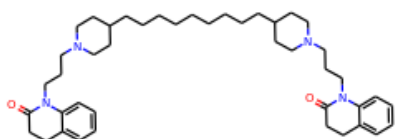
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.891304347826

KR

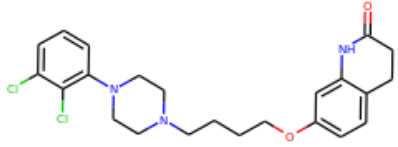


CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.602409638554

GRAPH



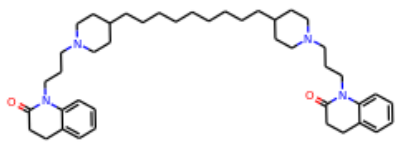
CHEMBL3354078
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078>)
ki = 48.98 nM
simil = 0.864864864865

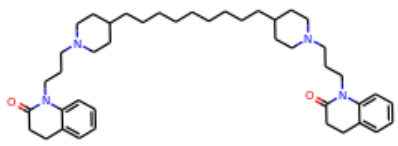
SUB  [CHEMBL1112 \(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112)
ki = 1000.0 nM
simil = 0.857142857143

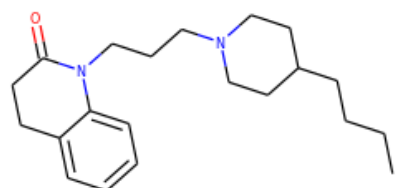
HYB  [CHEMBL3354078
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078)
ki = 48.98 nM
simil = 0.786350148368

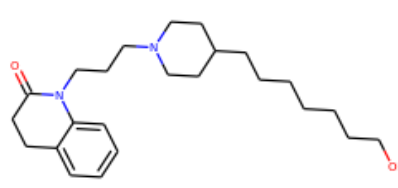
Muscarinic acetylcholine receptor M4: ki = 150.2055 nM Score = 8.3798

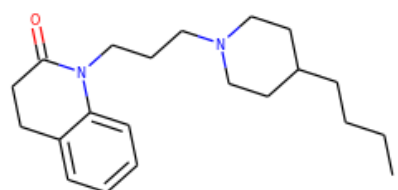
Best Fingerprints Similarity

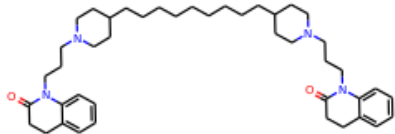
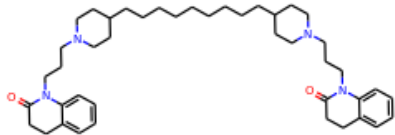
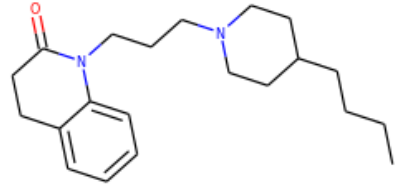
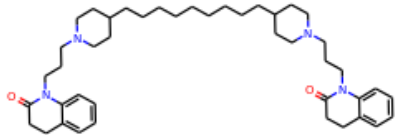
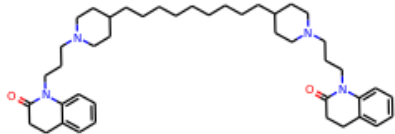
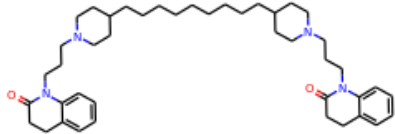
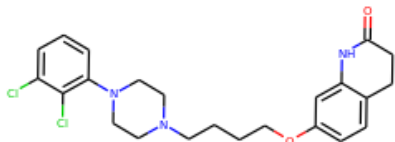
ECFP2  [CHEMBL3354078
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078)
ki = 32.36 nM
simil = 0.75

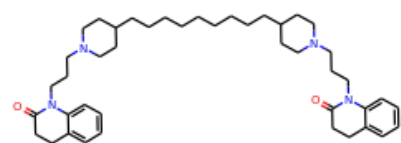
FCFP2  [CHEMBL3354078
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078)
ki = 32.36 nM
simil = 0.8125

DAY  [CHEMBL3354065
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065)
ki = 208.93 nM
simil = 0.847507331378

PAT  [CHEMBL3354074
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354074)
ki = 389.05 nM
simil = 0.89010989011

PAIR  [CHEMBL3354065
\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065)
ki = 208.93 nM
simil = 0.52380952381

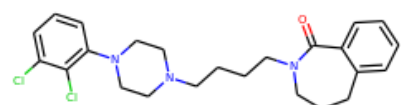
TORS		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.806451612903</p>
FP2		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.824742268041</p>
PUB		<p><u>CHEMBL3354065</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354065) ki = 208.93 nM simil = 0.905982905983</p>
MACCS		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.891304347826</p>
KR		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.602409638554</p>
GRAPH		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.864864864865</p>
SUB		<p><u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) ki = 1000.0 nM simil = 0.857142857143</p>
HYB		<p><u>CHEMBL3354078</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3354078) ki = 32.36 nM simil = 0.786350148368</p>



Serotonin 2a (5-HT2a) receptor: k_i = N.A.00 nM Score = 7.8079

Best Fingerprints Similarity

ECFP2



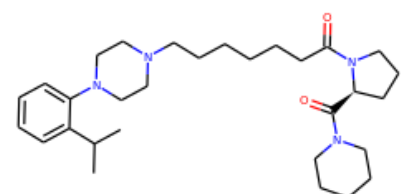
CHEMBL476394

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL476394>)

k_i = 10.0 nM

simil = 0.607142857143

FCFP2



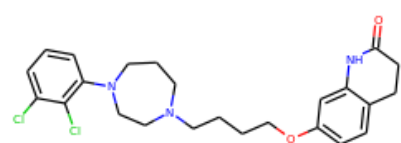
CHEMBL3409037

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3409037>)

k_i = 2148.0 nM

simil = 0.823529411765

DAY



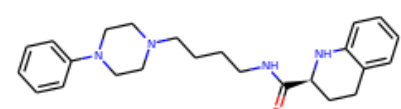
CHEMBL2165126

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2165126>)

k_i = 0.6 nM

simil = 0.575824175824

PAT



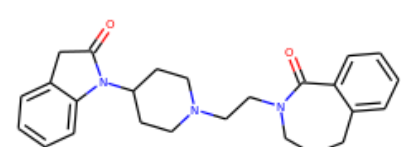
CHEMBL3358507

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507>)

k_i = 22.0 nM

simil = 0.886243386243

PAIR



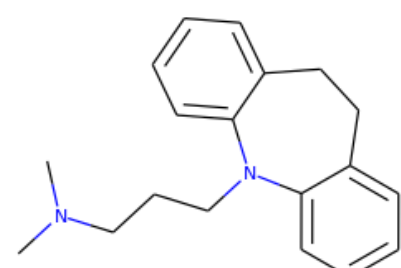
CHEMBL275258

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL275258>)

k_i = 223.87 nM

simil = 0.633333333333

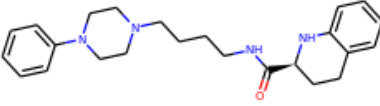
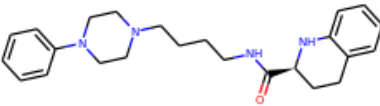
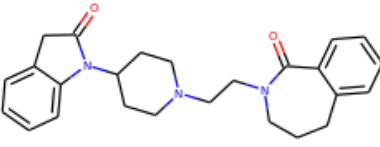
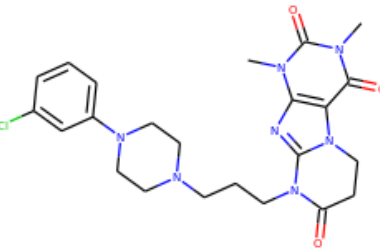
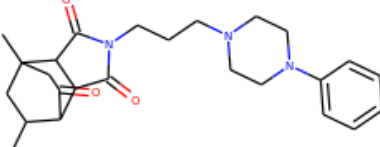
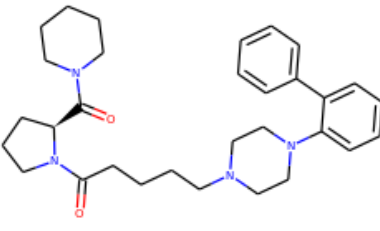
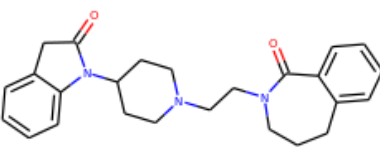
TORS



CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)

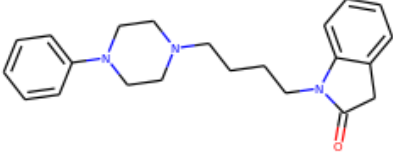
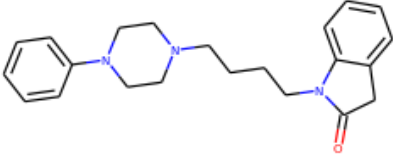
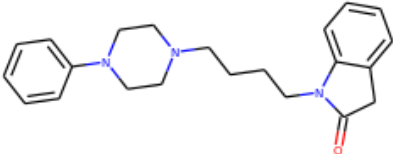
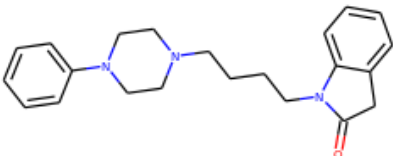
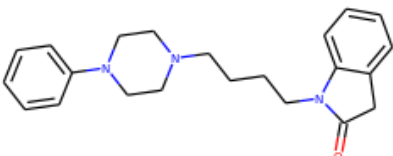
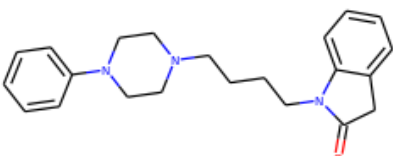
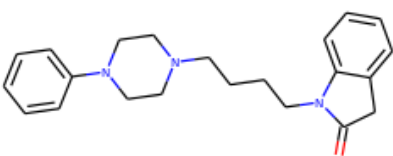
k_i = 94.0 nM

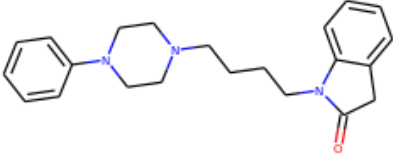
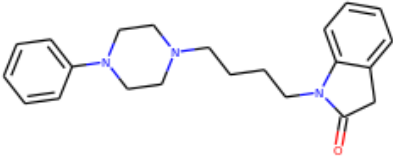
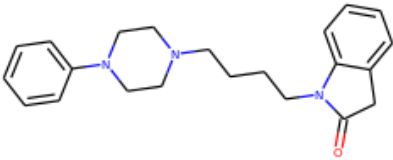
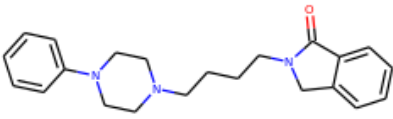
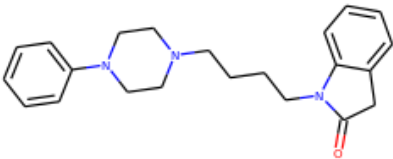
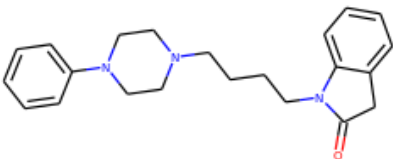
simil = 0.642857142857

FP2		<p><u>CHEMBL3358507</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507) ki = 22.0 nM simil = 0.694444444444</p>
PUB		<p><u>CHEMBL3358507</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358507) ki = 22.0 nM simil = 0.870967741935</p>
MACCS		<p><u>CHEMBL275258</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL275258) ki = 223.87 nM simil = 0.897959183673</p>
KR		<p><u>CHEMBL2237162</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2237162) ki = 181.97 nM simil = 0.662337662338</p>
GRAPH		<p><u>CHEMBL473981</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL473981) ki = 292.0 nM simil = 0.860465116279</p>
SUB		<p><u>CHEMBL3409039</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3409039) ki = 1684.0 nM simil = 0.923076923077</p>
HYB		<p><u>CHEMBL275258</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL275258) ki = 223.87 nM simil = 0.541474654378</p>

Dopamine D5 receptor: ki = 259.0052 nM Score = 7.7841

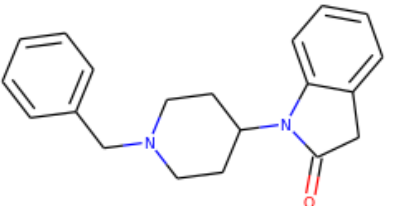
Best Fingerprints Similarity

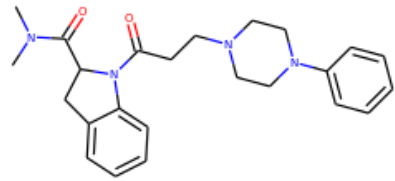
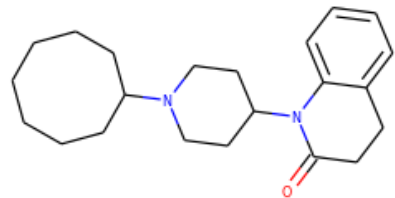
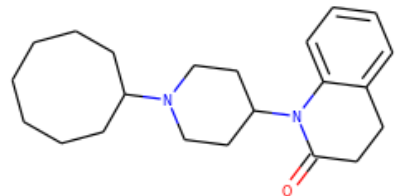
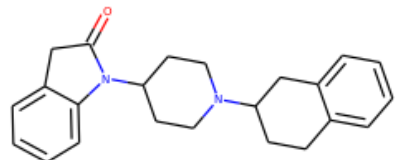
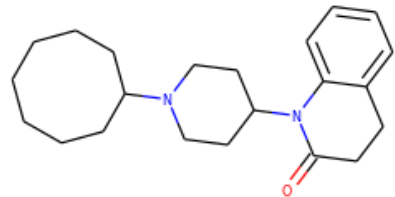
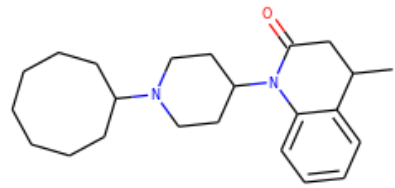
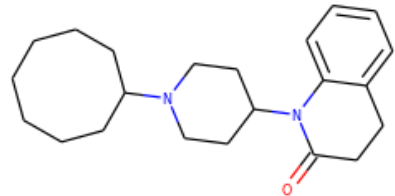
ECFP2		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.904761904762
FCFP2		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 1.0
DAY		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.636246786632
PAT		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.880319148936
PAIR		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.709401709402
TORS		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.6875
FP2		CHEMBL395933 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.67619047619

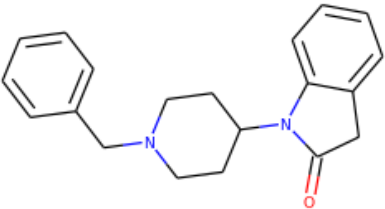
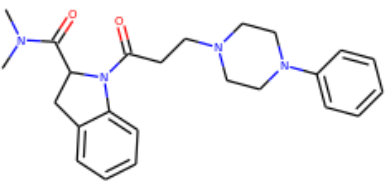
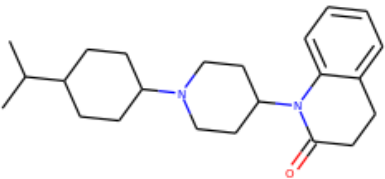
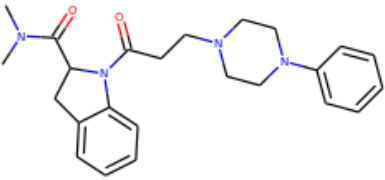
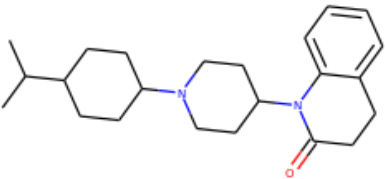
PUB		. (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.906779661017
MACCS		CHEMBL395933 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.934782608696
KR		CHEMBL395933 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.760563380282
GRAPH		CHEMBL240774 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL240774). ki = 80.0 nM simil = 0.662790697674
SUB		CHEMBL395933 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 1.0
HYB		CHEMBL395933 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL395933). ki = 313.0 nM simil = 0.611979166667

Mu opioid receptor: ki = N.A.00 nM Score = 7.6159

Best Fingerprints Similarity

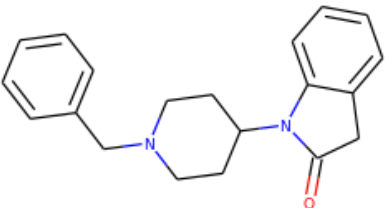
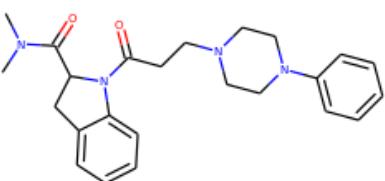
ECFP2		CHEMBL320874 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874). ki = 91.1 nM simil = 0.518518518519
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FCFP2		<u>CHEMBL2064133</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133) ki = 397.0 nM simil = 0.882352941176
DAY		<u>CHEMBL2387199</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 46.97 nM simil = 0.743918053777
PAT		<u>CHEMBL2387199</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 46.97 nM simil = 0.901069518717
PAIR		<u>CHEMBL101676</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL101676) ki = 38.9 nM simil = 0.593984962406
TORS		<u>CHEMBL2387199</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 46.97 nM simil = 0.487179487179
FP2		<u>CHEMBL2387200</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387200) ki = 23.27 nM simil = 0.824742268041
PUB		<u>CHEMBL2387199</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 46.97 nM simil = 0.898305084746

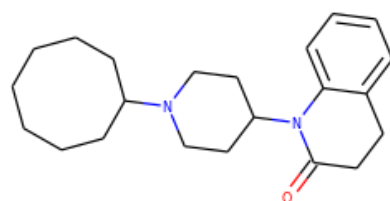
MACCS		<u>CHEMBL320874</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874) ki = 91.1 nM simil = 0.934782608696
KR		<u>CHEMBL2064133</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133) ki = 397.0 nM simil = 0.644444444444
GRAPH		<u>CHEMBL2387198</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387198) ki = 7.62 nM simil = 0.864864864865
SUB		<u>CHEMBL2064133</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133) ki = 397.0 nM simil = 0.923076923077
HYB		<u>CHEMBL2387198</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387198) ki = 7.62 nM simil = 0.792792792793

Nociceptin receptor: ki = 24.4983 nM Score = 7.6159

Best Fingerprints Similarity

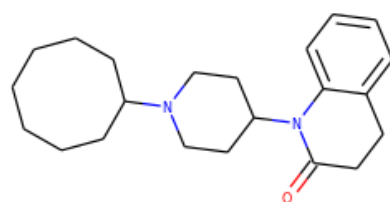
ECFP2		<u>CHEMBL320874</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874) ki = 201.0 nM simil = 0.518518518519
FCFP2		<u>CHEMBL2064133</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133) ki = 250.0 nM simil = 0.882352941176

DAY



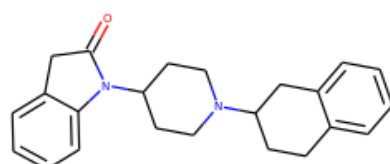
CHEMBL2387199
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)
ki = 18.66 nM
simil = 0.743918053777

PAT



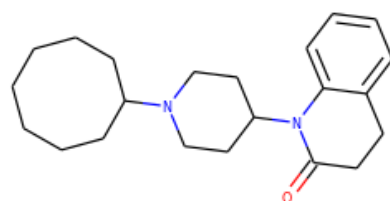
CHEMBL2387199
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)
ki = 18.66 nM
simil = 0.901069518717

PAIR



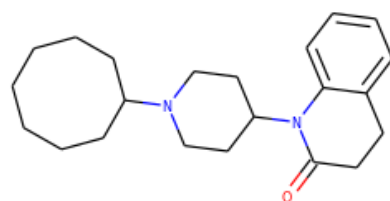
CHEMBL101676
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL101676>)
ki = 29.3 nM
simil = 0.593984962406

TORS



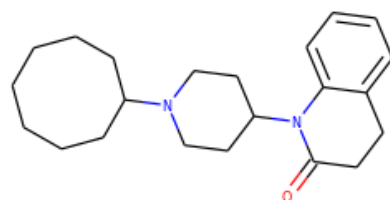
CHEMBL2387199
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)
ki = 18.66 nM
simil = 0.487179487179

FP2



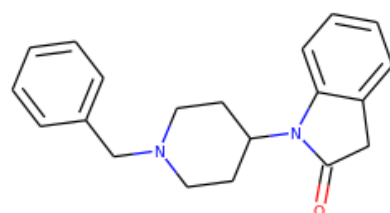
CHEMBL2387199
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)
ki = 18.66 nM
simil = 0.824742268041

PUB



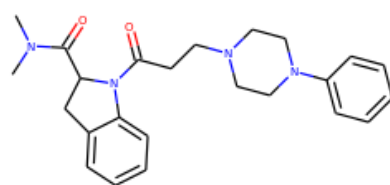
CHEMBL2387199
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)
ki = 18.66 nM
simil = 0.898305084746

MACCS



CHEMBL320874
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874>)
ki = 201.0 nM
simil = 0.934782608696

KR



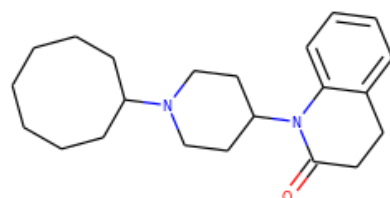
CHEMBL2064133

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133>)

ki = 250.0 nM

simil = 0.644444444444

GRAPH



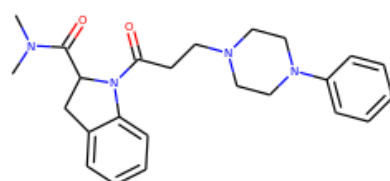
CHEMBL2387199

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)

ki = 18.66 nM

simil = 0.864864864865

SUB



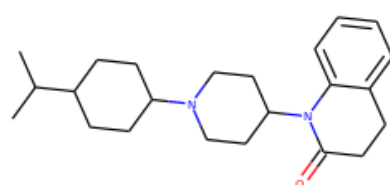
CHEMBL2064133

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2064133>)

ki = 250.0 nM

simil = 0.923076923077

HYB



CHEMBL2387198

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387198>)

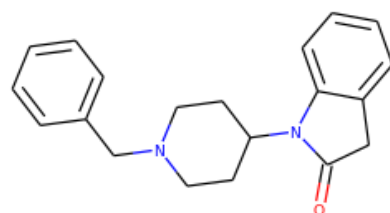
ki = 20.4 nM

simil = 0.792792792793

Kappa opioid receptor: ki = 78.5391 nM Score = 7.5397

Best Fingerprints Similarity

ECFP2



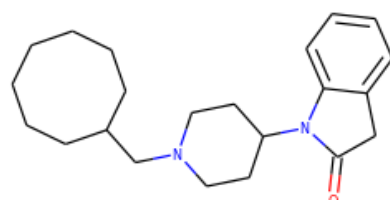
CHEMBL320874

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874>)

ki = 84.5 nM

simil = 0.518518518519

FCFP2



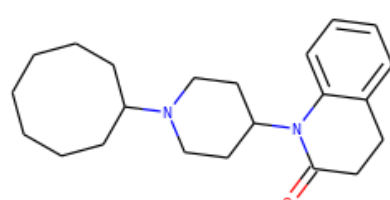
CHEMBL317152

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL317152>)

ki = 229.0 nM

simil = 0.8125

DAY

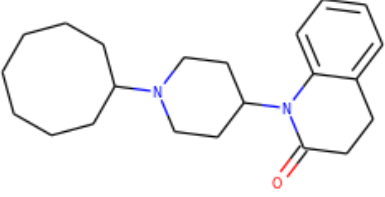
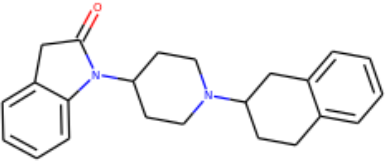
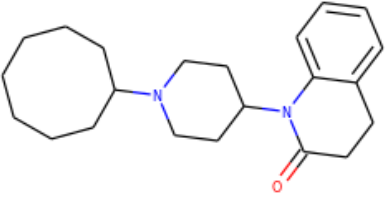
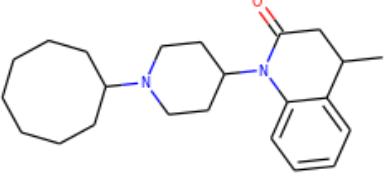
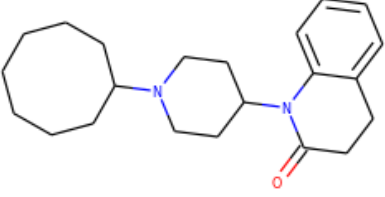
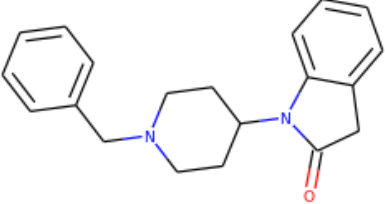
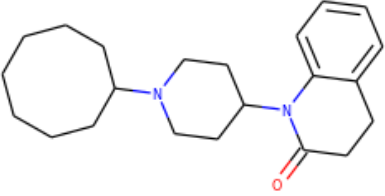


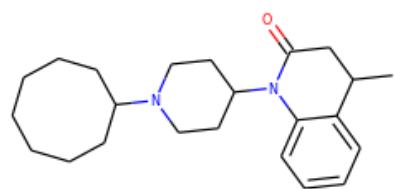
CHEMBL2387199

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199>)

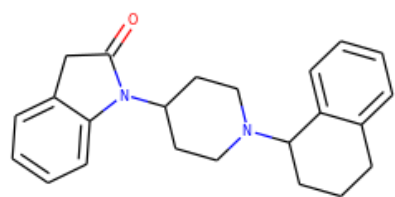
ki = 37.92 nM

simil = 0.743918053777

PAT		<p><u>CHEMBL2387199</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 37.92 nM simil = 0.901069518717</p>
PAIR		<p><u>CHEMBL101676</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL101676) ki = 55.1 nM simil = 0.593984962406</p>
TORS		<p><u>CHEMBL2387199</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 37.92 nM simil = 0.487179487179</p>
FP2		<p><u>CHEMBL2387200</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387200) ki = 27.69 nM simil = 0.824742268041</p>
PUB		<p><u>CHEMBL2387199</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 37.92 nM simil = 0.898305084746</p>
MACCS		<p><u>CHEMBL320874</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL320874) ki = 84.5 nM simil = 0.934782608696</p>
KR		<p><u>CHEMBL2387199</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387199) ki = 37.92 nM simil = 0.546511627907</p>
GRAPH		<p><u>CHEMBL2387200</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387200) ki = 27.69 nM simil = 0.864864864865</p>



SUB



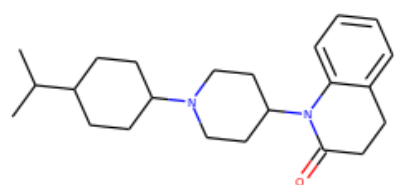
CHEMBL101118

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL101118>)

ki = 21.5 nM

simil = 0.916666666667

HYB



CHEMBL2387198

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387198>)

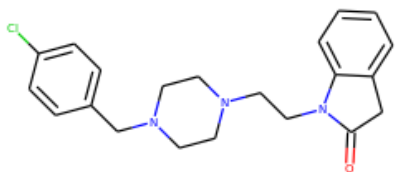
ki = 70.04 nM

simil = 0.792792792793

Dopamine D4 receptor: ki = N.A.00 nM Score = 7.3618

Best Fingerprints Similarity

ECFP2



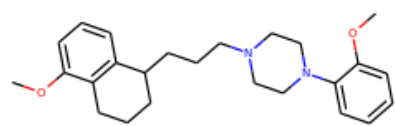
CHEMBL322326

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL322326>)

ki = 8.0 nM

simil = 0.615384615385

FCFP2



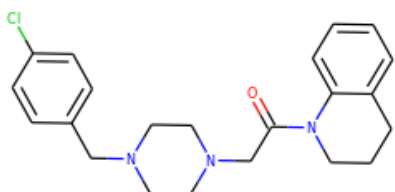
CHEMBL26929

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL26929>)

ki = 37.0 nM

simil = 0.764705882353

DAY



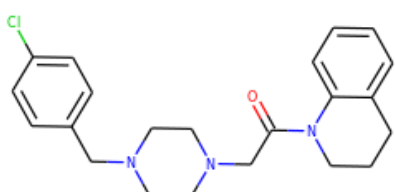
CHEMBL323537

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL323537>)

ki = 47.0 nM

simil = 0.706329113924

PAT

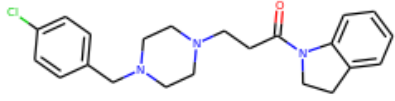
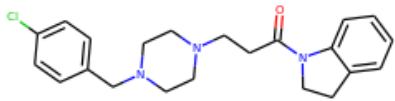
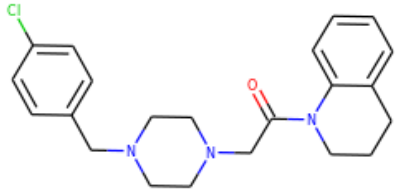
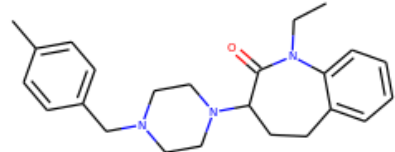
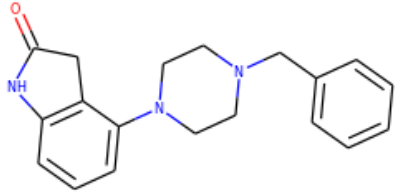
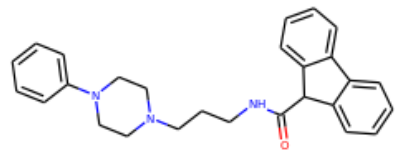
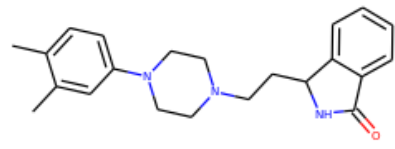


CHEMBL323537

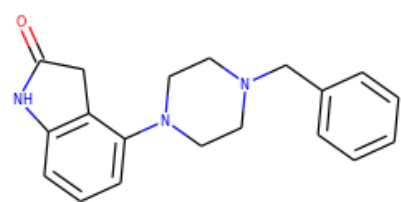
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL323537>)

ki = 47.0 nM

simil = 0.917553191489

PAIR		CHEMBL104498 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL104498) ki = 726.0 nM simil = 0.618055555556
TORS		CHEMBL104498 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL104498) ki = 726.0 nM simil = 0.78125
FP2		CHEMBL323537 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL323537) ki = 47.0 nM simil = 0.678260869565
PUB		CHEMBL302340 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL302340) ki = 2960.0 nM simil = 0.877049180328
MACCS		CHEMBL314952 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL314952) ki = 3.0 nM simil = 0.877551020408
KR		CHEMBL302796 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL302796) ki = 2170.0 nM simil = 0.6375
GRAPH		CHEMBL38262 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL38262) ki = 8.8 nM simil = 0.910256410256

SUB



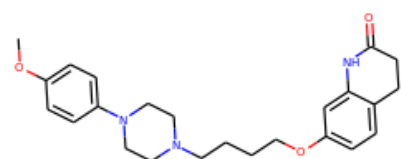
CHEMBL314952

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL314952>)

ki = 3.0 nM

simil = 1.0

HYB



CHEMBL1813585

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1813585>)

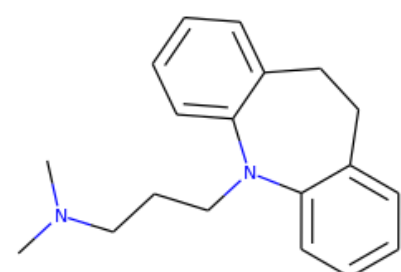
ki = 359.0 nM

simil = 0.556354916067

Serotonin transporter: ki = N.A.00 nM Score = 6.369

Best Fingerprints Similarity

ECFP2

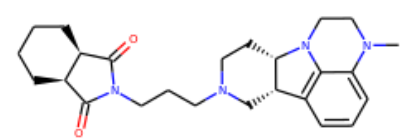


CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)

ki = 0.52 nM

simil = 0.52

FCFP2



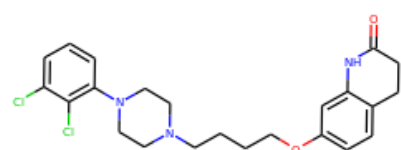
CHEMBL3233418

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3233418>)

ki = 1000.0 nM

simil = 0.777777777778

DAY

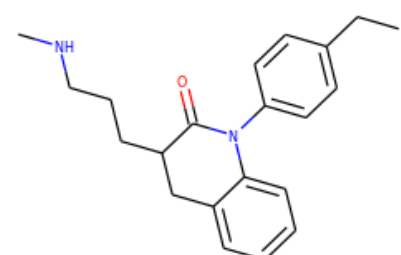


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)

ki = 31.62 nM

simil = 0.56

PAT



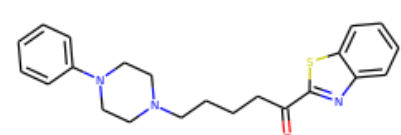
CHEMBL198038

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL198038>)

ki = 100.0 nM

simil = 0.870026525199

PAIR

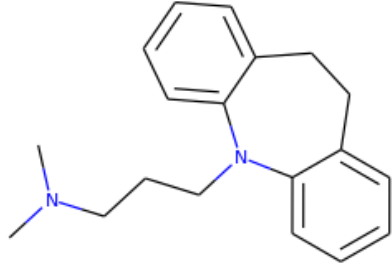
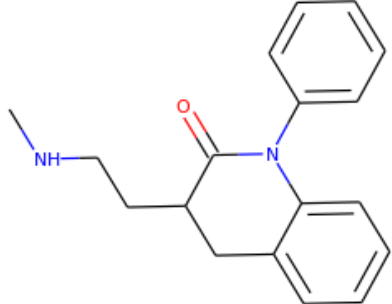
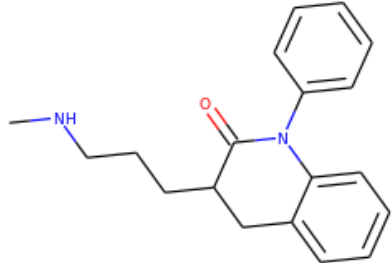
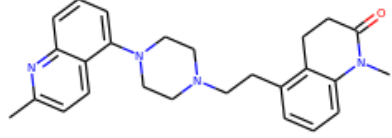
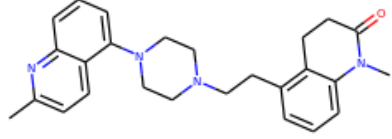
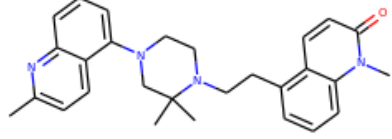
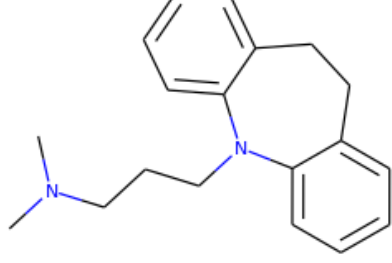


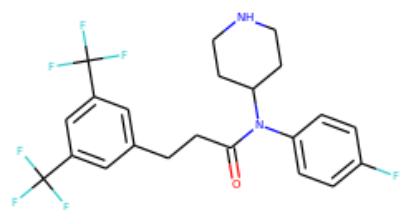
CHEMBL2037530

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2037530>)

ki = 298.0 nM

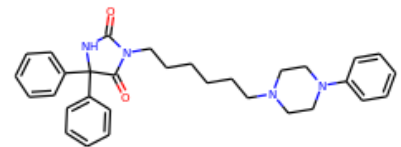
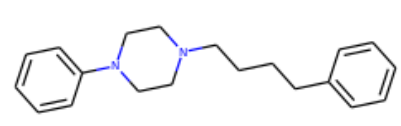
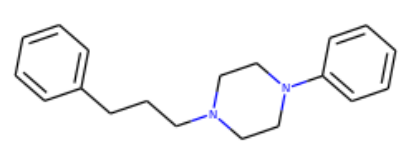
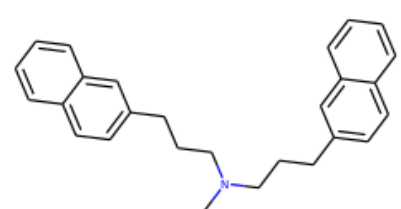
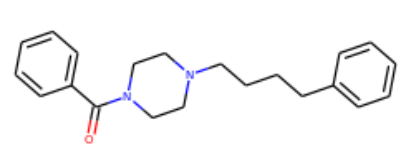
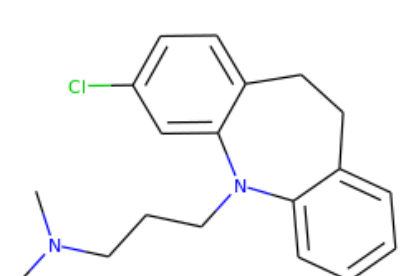
simil = 0.55033557047

TORS		<u>CHEMBL11</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11) ki = 0.52 nM simil = 0.642857142857
FP2		<u>CHEMBL194310</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL194310) ki = 100.0 nM simil = 0.62037037037
PUB		<u>CHEMBL196365</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL196365) ki = 100.0 nM simil = 0.868852459016
MACCS		<u>CHEMBL1290487</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1290487) ki = 12.59 nM simil = 0.88
KR		<u>CHEMBL1290487</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1290487) ki = 12.59 nM simil = 0.64
GRAPH		<u>CHEMBL1289618</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1289618) ki = 0.2512 nM simil = 0.8625
SUB		<u>CHEMBL11</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11) ki = 0.52 nM simil = 0.916666666667
HYB		<u>CHEMBL89245</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL89245) ki = 251.19 nM simil = 0.654596100279

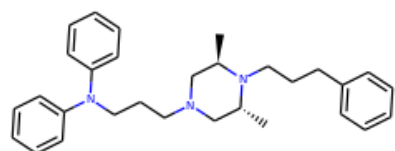


Sigma opioid receptor: k_i = N.A.00 nM Score = 6.175

Best Fingerprints Similarity

ECFP2		<p><u>CHEMBL71104</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL71104) k_i = 11.0 nM simil = 0.615384615385</p>
FCFP2		<p><u>CHEMBL85879</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL85879) k_i = 2.6 nM simil = 0.8</p>
DAY		<p><u>CHEMBL111896</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL111896) k_i = 6.7 nM simil = 0.48188976378</p>
PAT		<p><u>CHEMBL19985</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL19985) k_i = 30.0 nM simil = 0.804347826087</p>
PAIR		<p><u>CHEMBL19351</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL19351) k_i = 125.0 nM simil = 0.706422018349</p>
TORS		<p><u>CHEMBL415</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415) k_i = 572.0 nM simil = 0.558823529412</p>

FP2



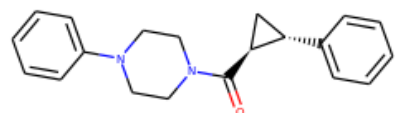
CHEMBL316244

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL316244>)

ki = 97.2 nM

simil = 0.648936170213

PUB



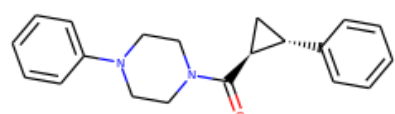
CHEMBL3218990

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3218990>)

ki = 1258.93 nM

simil = 0.889830508475

MACCS



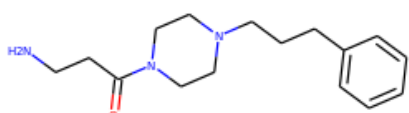
CHEMBL3218990

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3218990>)

ki = 1258.93 nM

simil = 0.863636363636

KR



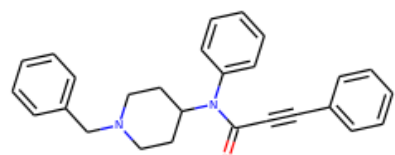
CHEMBL356738

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL356738>)

ki = 148.0 nM

simil = 0.64

GRAPH

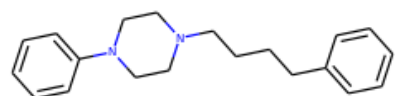


CHEMBL112170

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL112170>)

ki = 6.0 nM

simil = 0.824324324324



SUB

CHEMBL85879

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL85879>)

ki = 2.6 nM

simil = 0.916666666667

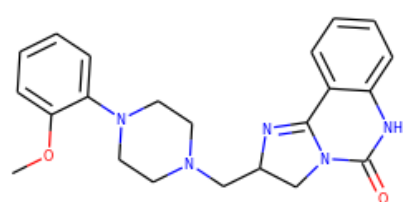
HYB

CHEMBL302021

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL302021>)

ki = 4000.0 nM

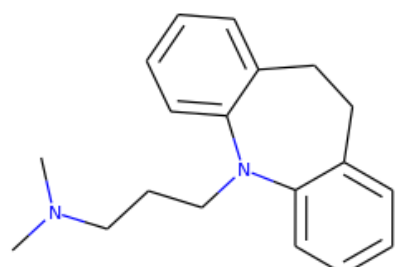
simil = 0.447311827957



Serotonin 2c (5-HT2c) receptor: k_i = N.A.00 nM Score = 5.5387

Best Fingerprints Similarity

ECFP2

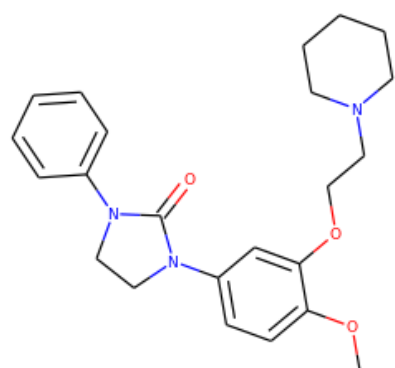


CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)

k_i = 160.0 nM

simil = 0.52

FCFP2



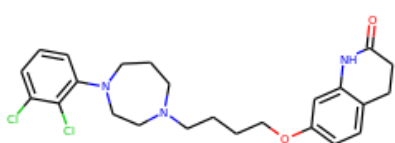
CHEMBL383800

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL383800>)

k_i = 1.259 nM

simil = 0.823529411765

DAY



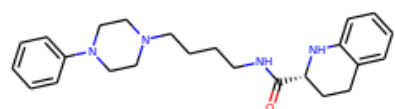
CHEMBL2165126

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2165126>)

k_i = 0.6 nM

simil = 0.575824175824

PAT



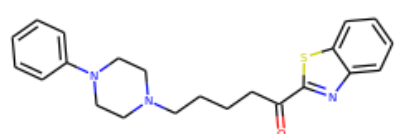
CHEMBL3358505

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358505>)

k_i = 1000.0 nM

simil = 0.886243386243

PAIR



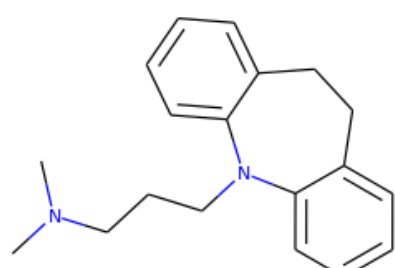
CHEMBL2037530

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2037530>)

k_i = 2140.0 nM

simil = 0.55033557047

TORS

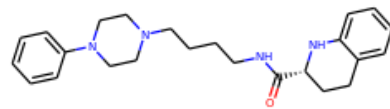


CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)

k_i = 160.0 nM

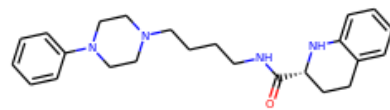
simil = 0.642857142857

FP2



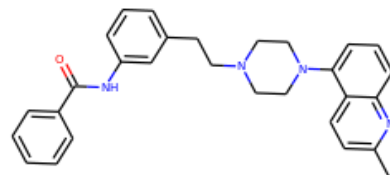
CHEMBL3358505
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358505>)
ki = 1000.0 nM
simil = 0.694444444444

PUB



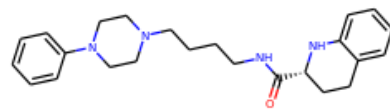
CHEMBL3358505
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358505>)
ki = 1000.0 nM
simil = 0.870967741935

MACCS



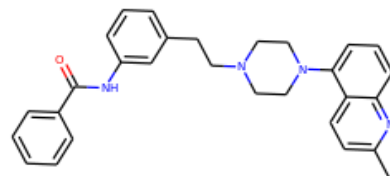
CHEMBL1632210
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210>)
ki = 794.33 nM
simil = 0.8125

KR



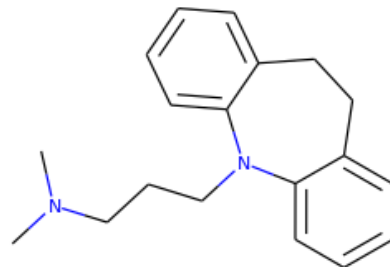
CHEMBL3358505
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3358505>)
ki = 1000.0 nM
simil = 0.612903225806

GRAPH



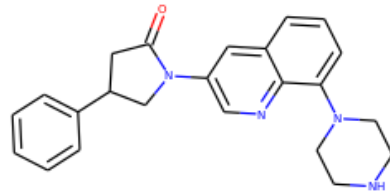
CHEMBL1632210
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210>)
ki = 794.33 nM
simil = 0.848101265823

SUB



CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)
ki = 160.0 nM
simil = 0.916666666667

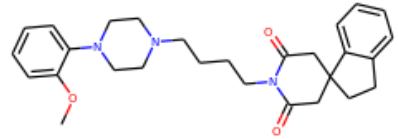
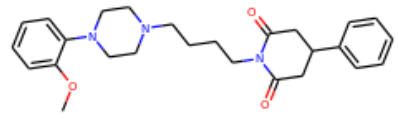
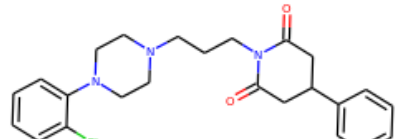
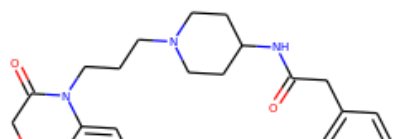
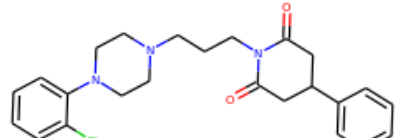
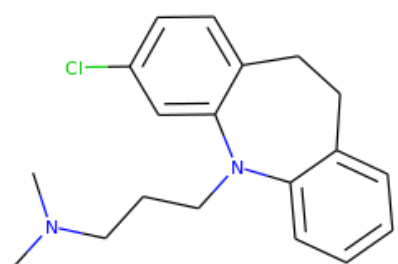
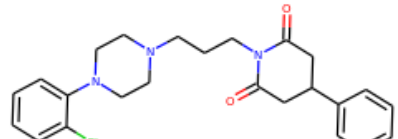
HYB



CHEMBL3260795
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260795>)
ki = 30000.0 nM
simil = 0.524945770065

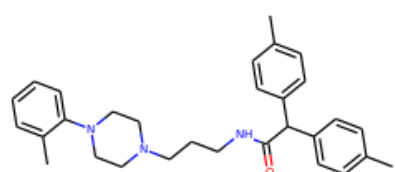
Alpha-1d adrenergic receptor: ki = N.A.00 nM Score = 5.1392

Best Fingerprints Similarity

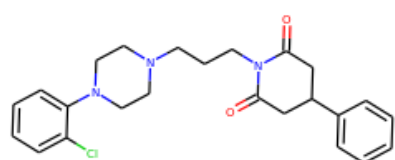
ECFP2		<u>CHEMBL1796050</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796050) ki = 16.22 nM simil = 0.633333333333
FCFP2		<u>CHEMBL1796033</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796033) ki = 15.85 nM simil = 0.777777777778
DAY		<u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031) ki = 43.65 nM simil = 0.503052503053
PAT		<u>CHEMBL1242923</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923) ki = 1000.0 nM simil = 0.780952380952
PAIR		<u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031) ki = 43.65 nM simil = 0.5625
TORS		<u>CHEMBL415</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415) ki = 88.0 nM simil = 0.558823529412
FP2		<u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031) ki = 43.65 nM simil = 0.654545454545

PUB

ki = 36.0 nM
simil = 0.858267716535

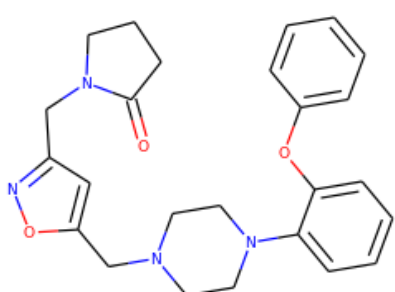


MACCS



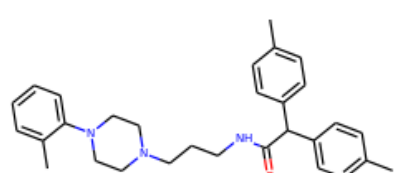
CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>).
ki = 43.65 nM
simil = 0.843137254902

KR



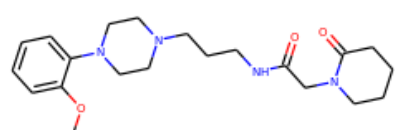
CHEMBL80109
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL80109>).
ki = 34.5 nM
simil = 0.6125

GRAPH



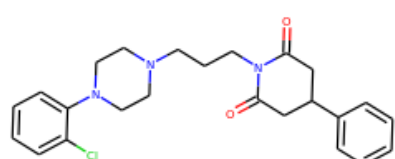
CHEMBL415887
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415887>).
ki = 36.0 nM
simil = 0.905405405405

SUB



CHEMBL12501
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL12501>).
ki = 10000.0 nM
simil = 0.857142857143

HYB

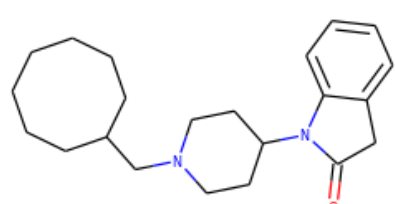


CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>).
ki = 43.65 nM
simil = 0.607242339833

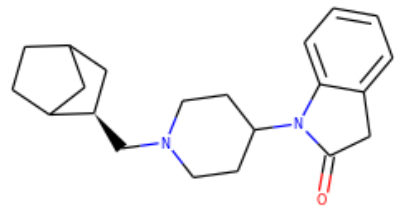
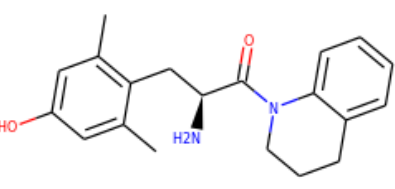
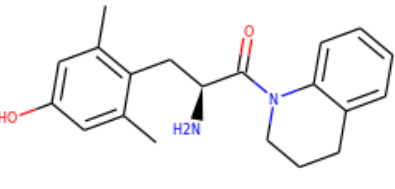
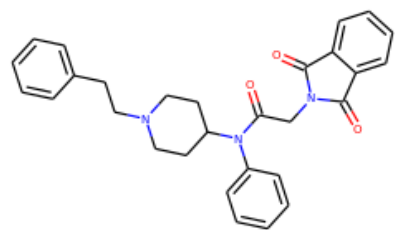
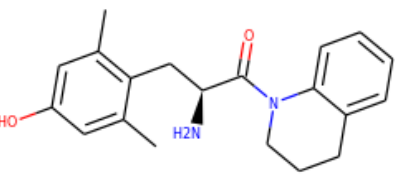
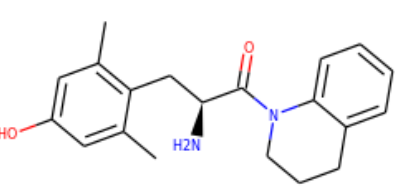
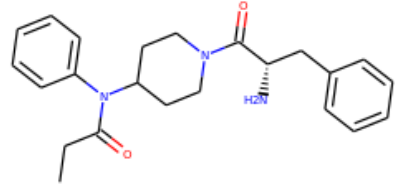
Delta opioid receptor: ki = 10342.6454 nM Score = 4.8099

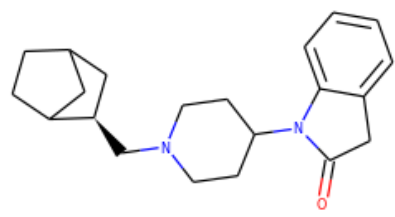
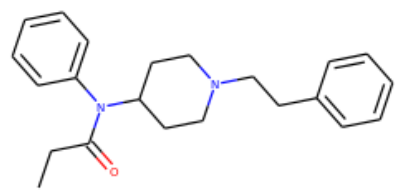
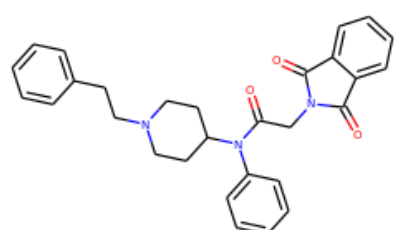
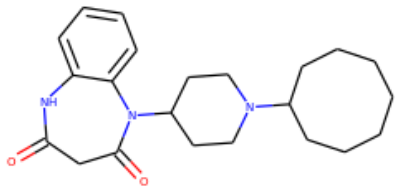
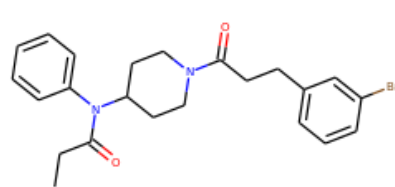
Best Fingerprints Similarity

ECFP2



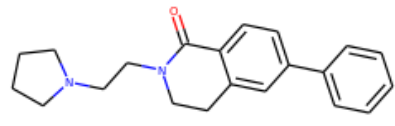
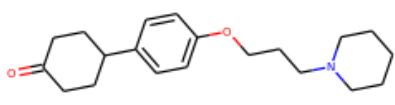
CHEMBL317152
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL317152>).
ki = 10000.0 nM
simil = 0.5

FCFP2		<u>CHEMBL2111608</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2111608) ki = 10000.0 nM simil = 0.8125
DAY		<u>CHEMBL3104104</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3104104) ki = 33.0 nM simil = 0.654929577465
PAT		<u>CHEMBL3104104</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3104104) ki = 33.0 nM simil = 0.825
PAIR		<u>CHEMBL2387334</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387334) ki = 13000.0 nM simil = 0.564417177914
TORS		<u>CHEMBL3104104</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3104104) ki = 33.0 nM simil = 0.431818181818
FP2		<u>CHEMBL3104104</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3104104) ki = 33.0 nM simil = 0.727272727273
PUB		<u>CHEMBL231352</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL231352) ki = 6900.0 nM simil = 0.876033057851

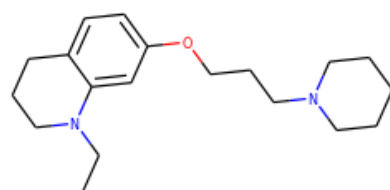
MACCS		<u>CHEMBL2111608</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2111608) ki = 10000.0 nM simil = 0.913043478261
KR		<u>CHEMBL596</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL596) ki = 570.0 nM simil = 0.517647058824
GRAPH		<u>CHEMBL2387334</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2387334) ki = 13000.0 nM simil = 0.795454545455
SUB		<u>CHEMBL3665425</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3665425) ki = 16200.0 nM simil = 0.916666666667
HYB		<u>CHEMBL389109</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL389109) ki = 12000.0 nM simil = 0.606060606061

Histamine H3 receptor: ki = N.A.00 nM Score = 4.7234

Best Fingerprints Similarity

ECFP2		<u>CHEMBL2031742</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031742) ki = 11.4 nM simil = 0.538461538462
FCFP2		<u>CHEMBL1824229</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1824229) ki = 1.7 nM simil = 0.875

DAY



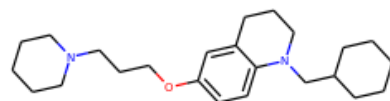
CHEMBL210761

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL210761>)

ki = 156.0 nM

simil = 0.526381909548

PAT



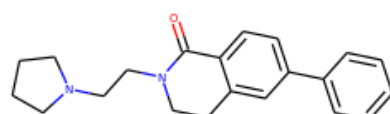
CHEMBL210252

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL210252>)

ki = 31.0 nM

simil = 0.851063829787

PAIR



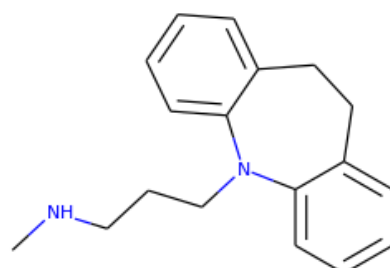
CHEMBL2031742

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031742>)

ki = 11.4 nM

simil = 0.55737704918

TORS

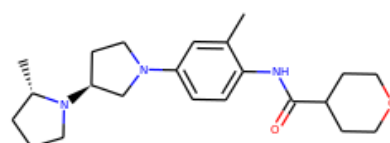


CHEMBL72 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL72>)

ki = 5000.0 nM

simil = 0.620689655172

FP2



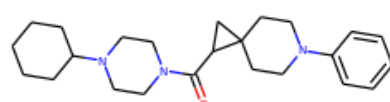
CHEMBL2441636

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2441636>)

ki = 1.0 nM

simil = 0.591304347826

PUB

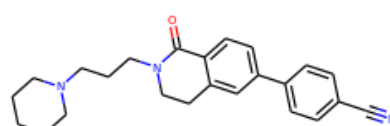


CHEMBL3127668

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3127668>)

ki = 1670.0 nM

simil = 0.827868852459



CHEMBL2031756

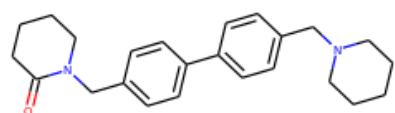
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031756>)

ki = 18.0 nM

simil = 0.888888888889

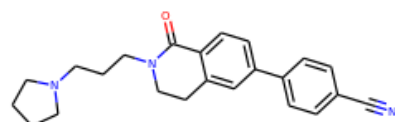
MACCS

KR



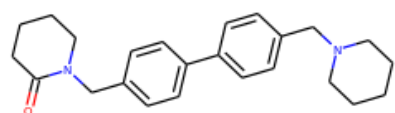
CHEMBL211370
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL211370>)
ki = 46.77 nM
simil = 0.470588235294

GRAPH



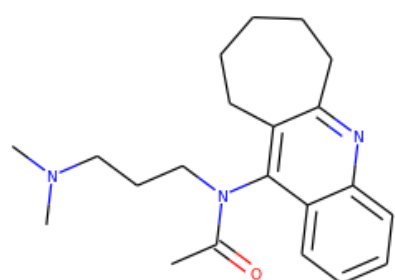
CHEMBL2031755
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031755>)
ki = 6.9 nM
simil = 0.864864864865

SUB



CHEMBL211370
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL211370>)
ki = 46.77 nM
simil = 0.916666666667

HYB

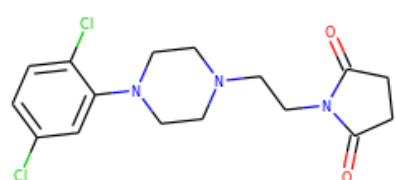


CHEMBL67518
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL67518>)
ki = 1000.0 nM
simil = 0.483801295896

Alpha-1b adrenergic receptor: ki = N.A.00 nM Score = 4.6328

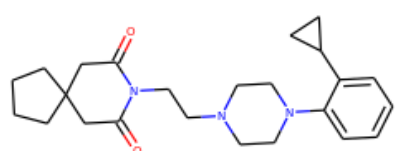
Best Fingerprints Similarity

ECFP2



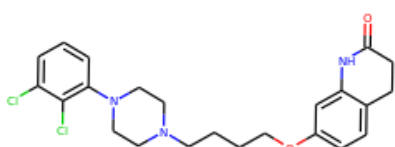
CHEMBL294646
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL294646>)
ki = 86.38 nM
simil = 0.64

FCFP2

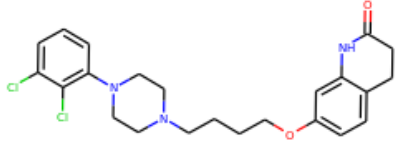
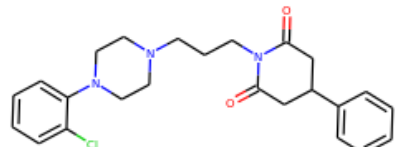
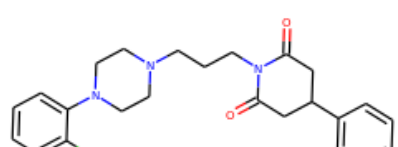
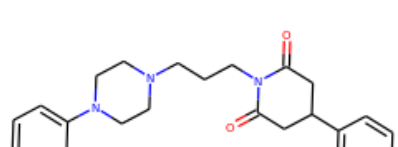
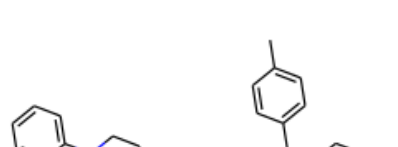
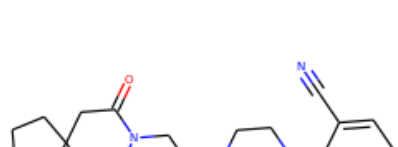
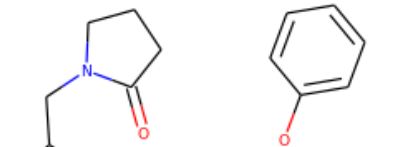


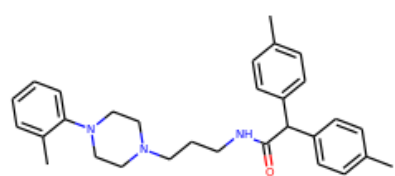
CHEMBL56804
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL56804>)
ki = 35.56 nM
simil = 0.823529411765

DAY

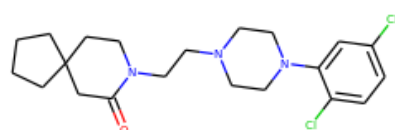


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 100.0 nM
simil = 0.56

PAT		<p><u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112).</p> <p>ki = 100.0 nM simil = 0.82380952381</p>
PAIR		<p><u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031).</p> <p>ki = 112.2 nM simil = 0.5625</p>
TORS		<p><u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031).</p> <p>ki = 112.2 nM simil = 0.472222222222</p>
FP2		<p><u>CHEMBL1796031</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031).</p> <p>ki = 112.2 nM simil = 0.654545454545</p>
PUB		<p><u>CHEMBL415887</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415887).</p> <p>ki = 6.6 nM simil = 0.858267716535</p>
MACCS		<p><u>CHEMBL299022</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL299022).</p> <p>ki = 46.18 nM simil = 0.843137254902</p>
KR		<p><u>CHEMBL80109</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL80109).</p> <p>ki = 5000.0 nM simil = 0.6125</p>
GRAPH		<p><u>CHEMBL415887</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415887).</p> <p>ki = 6.6 nM simil = 0.905405405405</p>

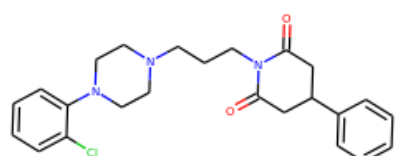


SUB



CHEMBL301224
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL301224>)
ki = 7.95 nM
simil = 0.857142857143

HYB

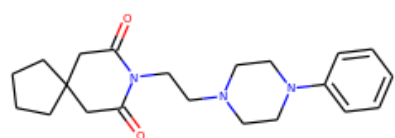


CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 112.2 nM
simil = 0.607242339833

Alpha-1a adrenergic receptor: ki = N.A.00 nM Score = 4.587

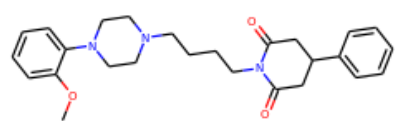
Best Fingerprints Similarity

ECFP2



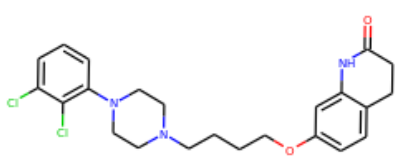
CHEMBL293968
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL293968>)
ki = 2684.0 nM
simil = 0.64

FCFP2



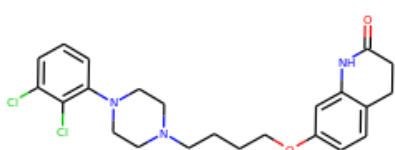
CHEMBL1796033
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796033>)
ki = 1.82 nM
simil = 0.777777777778

DAY



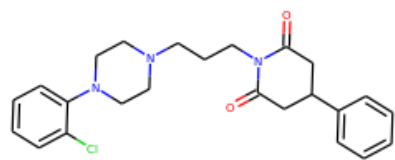
CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 26.0 nM
simil = 0.56

PAT



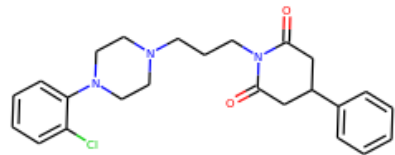
CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 26.0 nM
simil = 0.82380952381

PAIR



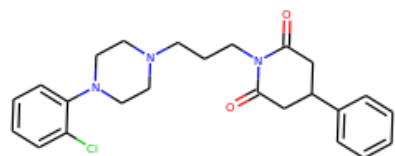
CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 47.86 nM
simil = 0.5625

TORS



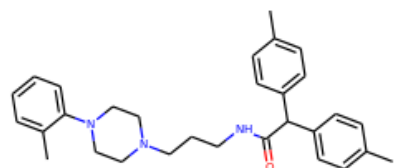
CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 47.86 nM
simil = 0.4722222222

FP2



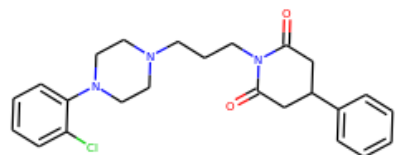
CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 47.86 nM
simil = 0.6545454545

PUB



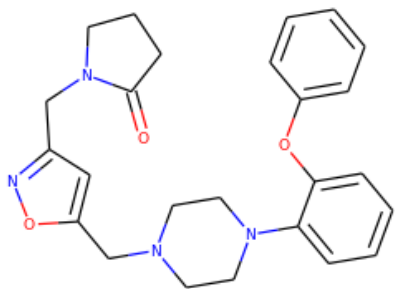
CHEMBL415887
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415887>)
ki = 1.1 nM
simil = 0.858267716535

MACCS



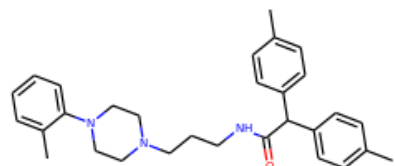
CHEMBL1796031
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 47.86 nM
simil = 0.843137254902

KR

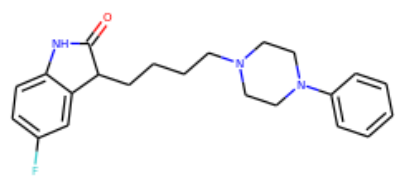


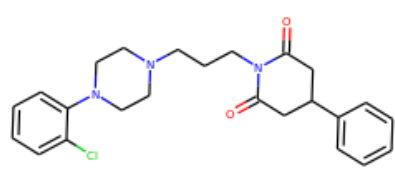
CHEMBL80109
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL80109>)
ki = 28.0 nM
simil = 0.6125

GRAPH



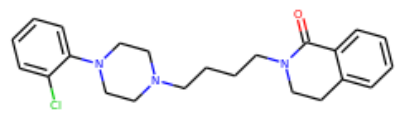
CHEMBL415887
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415887>)
ki = 1.1 nM
simil = 0.905405405405

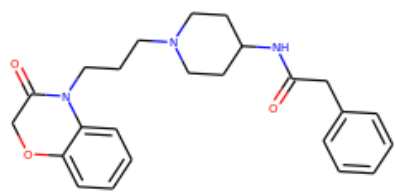
SUB  [CHEMBL411663](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL411663)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL411663>)
ki = 20.0 nM
simil = 0.857142857143

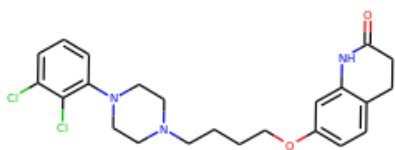
HYB  [CHEMBL1796031](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1796031>)
ki = 47.86 nM
simil = 0.607242339833

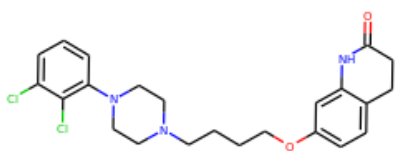
Dopamine D1 receptor: ki = 1980.4512 nM Score = 4.4591

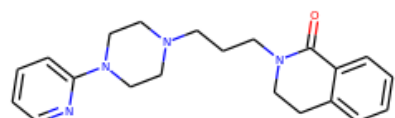
Best Fingerprints Similarity

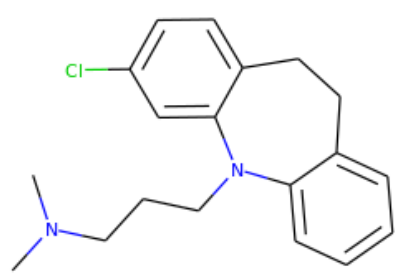
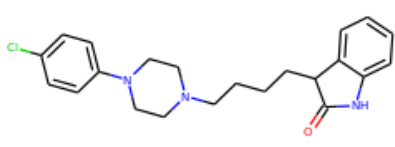
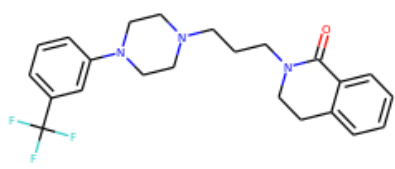
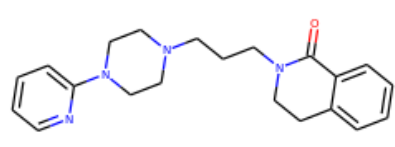
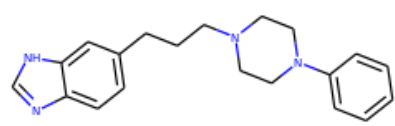
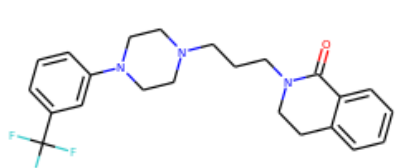
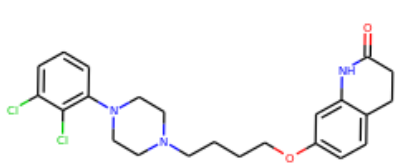
ECFP2  [CHEMBL514382](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL514382)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL514382>)
ki = 346.74 nM
simil = 0.653846153846

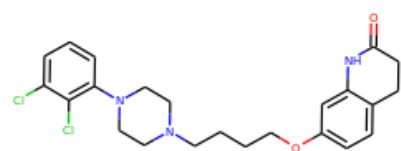
FCFP2  [CHEMBL1242923](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923>)
ki = 1000.0 nM
simil = 0.75

DAY  [CHEMBL1112](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 310.0 nM
simil = 0.56

PAT  [CHEMBL1112](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 310.0 nM
simil = 0.82380952381

PAIR  [CHEMBL477961](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL477961)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL477961>)
ki = 1698.24 nM
simil = 0.679104477612

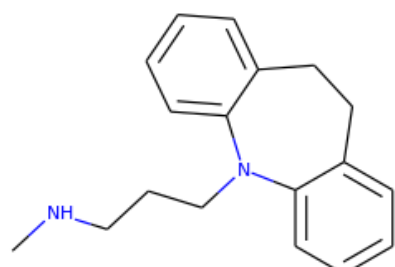
TORS		<u>CHEMBL415</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415) ki = 557.0 nM simil = 0.558823529412
FP2		<u>CHEMBL260994</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL260994) ki = 2400.0 nM simil = 0.6
PUB		<u>CHEMBL516270</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL516270) ki = 1737.8 nM simil = 0.830769230769
MACCS		<u>CHEMBL477961</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL477961) ki = 1698.24 nM simil = 0.914893617021
KR		<u>CHEMBL2298813</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2298813) ki = 1000.0 nM simil = 0.573529411765
GRAPH		<u>CHEMBL516270</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL516270) ki = 1737.8 nM simil = 0.90243902439
SUB		<u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) ki = 310.0 nM simil = 0.857142857143
HYB		<u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) ki = 310.0 nM simil = 0.520454545455



Norepinephrine transporter: k_i = N.A.00 nM Score = 4.0484

Best Fingerprints Similarity

ECFP2

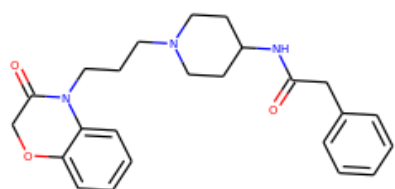


CHEMBL72 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL72>)

k_i = 0.6 nM

simil = 0.52

FCFP2



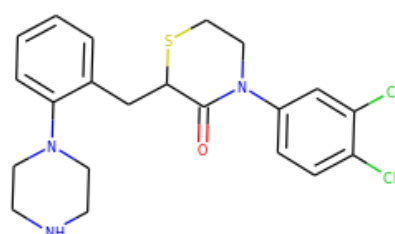
CHEMBL1242923

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923>)

k_i = 1000.0 nM

simil = 0.75

DAY



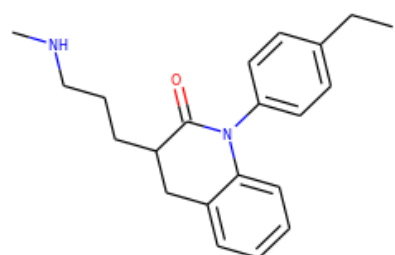
CHEMBL574126

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL574126>)

k_i = 5.0 nM

simil = 0.556468172485

PAT



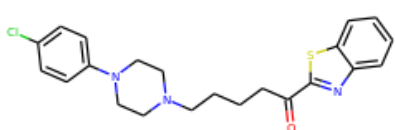
CHEMBL198038

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL198038>)

k_i = 150.0 nM

simil = 0.870026525199

PAIR



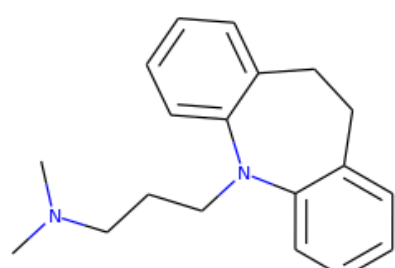
CHEMBL2037528

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2037528>)

k_i = 10000.0 nM

simil = 0.462427745665

TORS

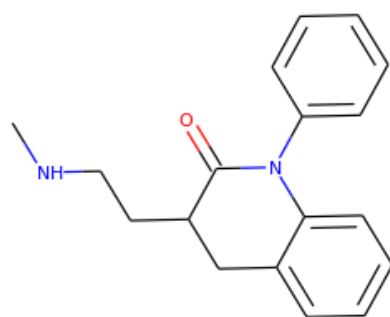


CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)

k_i = 16.0 nM

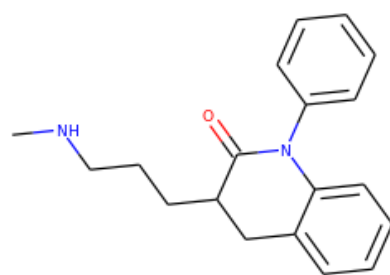
simil = 0.642857142857

FP2



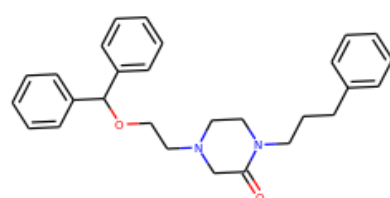
CHEMBL194310
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL194310>)
ki = 38.0 nM
simil = 0.62037037037

PUB



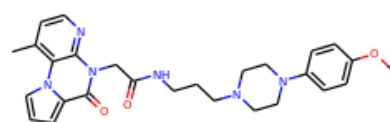
CHEMBL196365
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL196365>)
ki = 8.0 nM
simil = 0.868852459016

MACCS



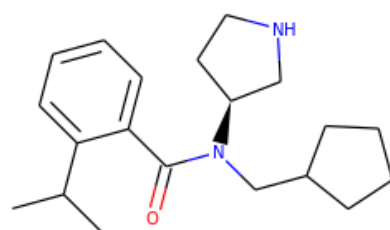
CHEMBL124222
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL124222>)
ki = 5850.0 nM
simil = 0.76

KR



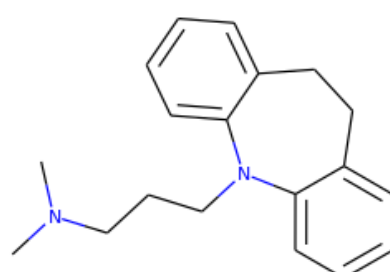
CHEMBL1729417
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1729417>)
ki = 1000.0 nM
simil = 0.5

GRAPH



CHEMBL550402
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL550402>)
ki = 18.0 nM
simil = 0.76404494382

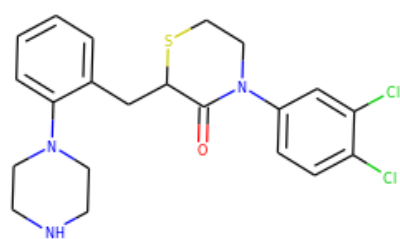
SUB



CHEMBL11 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL11>)
ki = 16.0 nM
simil = 0.916666666667

HYB

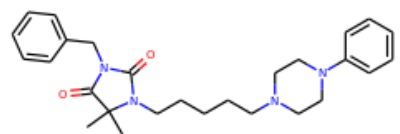
CHEMBL574126
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL574126>)
ki = 5.0 nM
simil = 0.503080082136



Serotonin 6 (5-HT6) receptor: k_i = 2047.3227 nM Score = 4.0272

Best Fingerprints Similarity

ECFP2



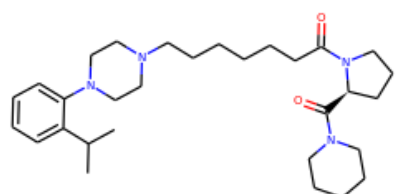
CHEMBL3233668

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3233668>)

k_i = 4368.0 nM

simil = 0.551724137931

FCFP2



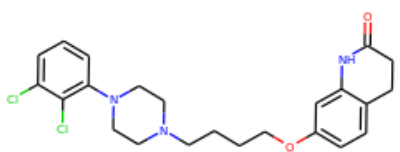
CHEMBL3409037

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3409037>)

k_i = 603.0 nM

simil = 0.823529411765

DAY

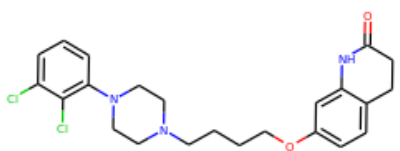


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)

k_i = 90.0 nM

simil = 0.56

PAT

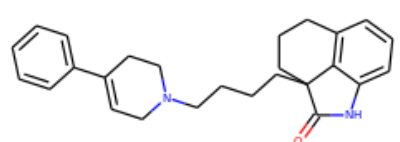


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)

k_i = 90.0 nM

simil = 0.82380952381

PAIR



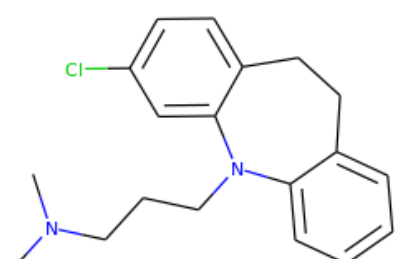
CHEMBL69257

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL69257>)

k_i = 524.81 nM

simil = 0.472392638037

TORS

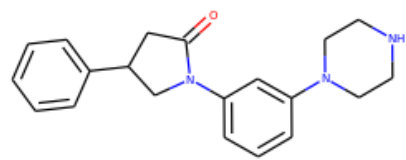


CHEMBL415 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415>)

k_i = 112.0 nM

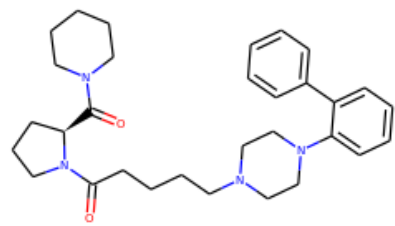
simil = 0.558823529412

FP2



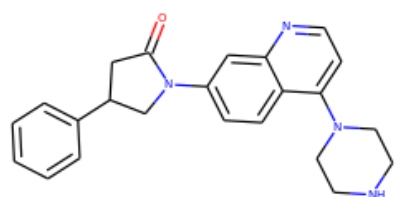
CHEMBL3260791
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260791>)
ki = 84.0 nM
simil = 0.660377358491

PUB



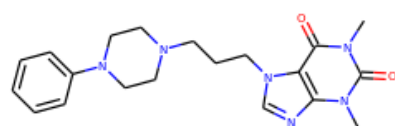
CHEMBL3409039
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3409039>)
ki = 376.0 nM
simil = 0.856

MACCS



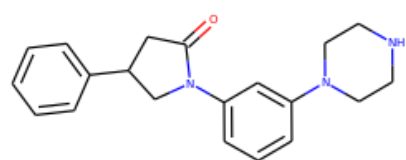
CHEMBL3260796
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260796>)
ki = 55.0 nM
simil = 0.823529411765

KR



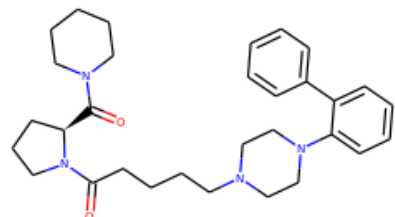
CHEMBL3360991
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3360991>)
ki = 20080.0 nM
simil = 0.597222222222

GRAPH



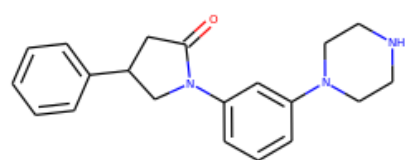
CHEMBL3260791
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260791>)
ki = 84.0 nM
simil = 0.865853658537

SUB



CHEMBL3409039
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3409039>)
ki = 376.0 nM
simil = 0.923076923077

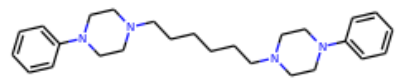
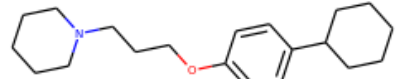
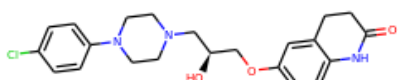
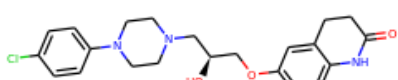
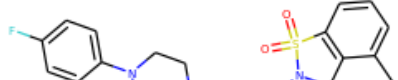
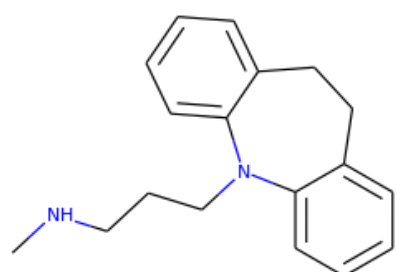
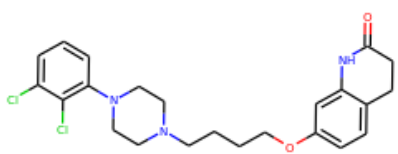
HYB



CHEMBL3260791
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260791>)
ki = 84.0 nM
simil = 0.595419847328

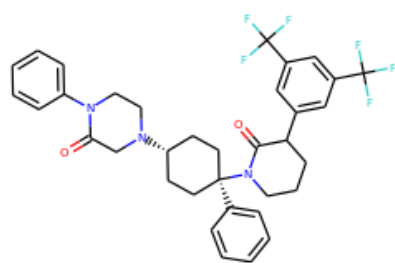
HERG: ki = N.A.00 nM Score = 3.7854

Best Fingerprints Similarity

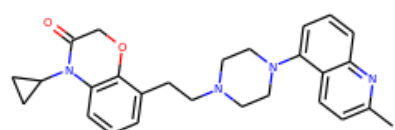
ECFP2		<p><u>CHEMBL1172205</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1172205) ki = 8000.0 nM simil = 0.65</p>
FCFP2		<p><u>CHEMBL1822854</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1822854) ki = 13.0 nM simil = 0.75</p>
DAY		<p><u>CHEMBL3688396</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3688396) ki = 5000.0 nM simil = 0.582456140351</p>
PAT		<p><u>CHEMBL3688396</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3688396) ki = 5000.0 nM simil = 0.840294840295</p>
PAIR		<p><u>CHEMBL83894</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL83894) ki = 200.0 nM simil = 0.518987341772</p>
TORS		<p><u>CHEMBL72</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL72) ki = 22816.6 nM simil = 0.620689655172</p>
FP2		<p><u>CHEMBL1112</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) ki = 598.0 nM simil = 0.569343065693</p>

PUB

ki = 6529.0 nM
simil = 0.775362318841

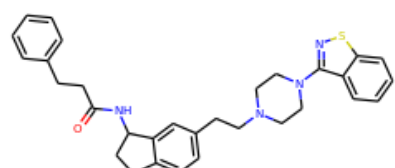


MACCS



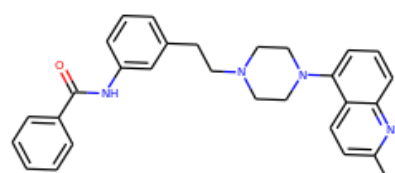
CHEMBL469568
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL469568>)
ki = 1584.89 nM
simil = 0.814814814815

KR



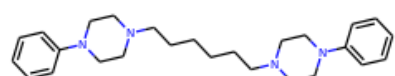
CHEMBL252201
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL252201>)
ki = 511.0 nM
simil = 0.58024691358

GRAPH



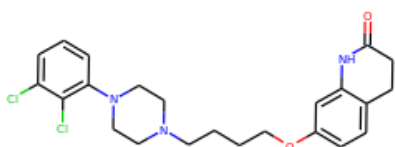
CHEMBL1632210
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210>)
ki = 50.12 nM
simil = 0.848101265823

SUB



CHEMBL1172205
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1172205>)
ki = 8000.0 nM
simil = 0.916666666667

HYB

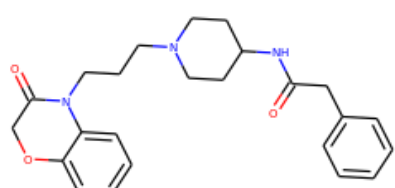


CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 598.0 nM
simil = 0.520454545455

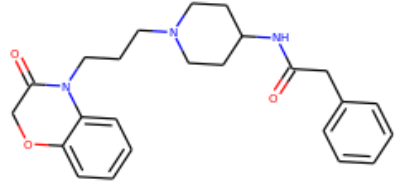
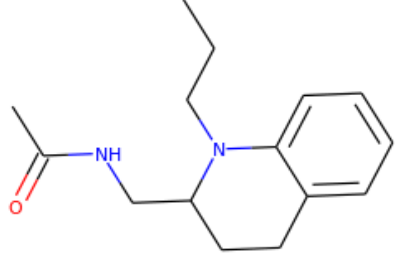
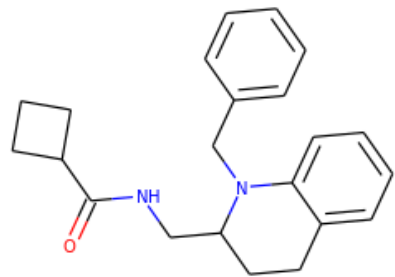
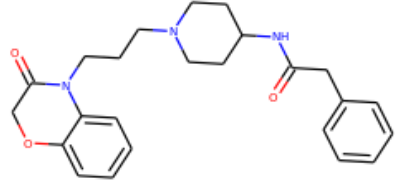
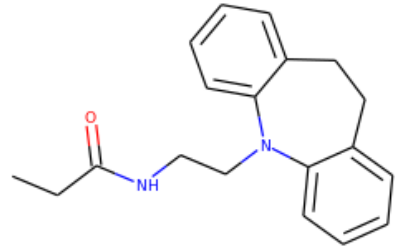
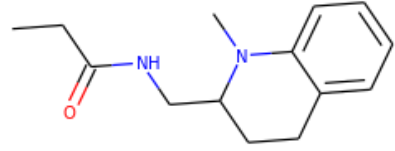
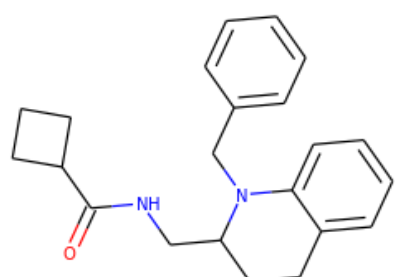
Melatonin receptor 1A: ki = N.A.00 nM Score = 3.2366

Best Fingerprints Similarity

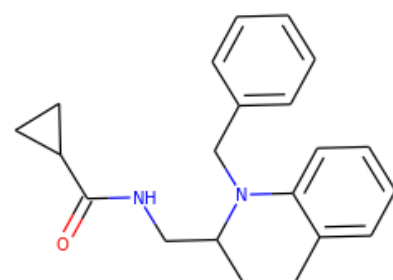
ECFP2



CHEMBL1242923
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923>)
ki = 1000.0 nM
simil = 0.470588235294

FCFP2		<p><u>CHEMBL1242923</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923 ki = 1000.0 nM simil = 0.75</p>
DAY		<p><u>CHEMBL3612606</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612606 ki = 5.8 nM simil = 0.584158415842</p>
PAT		<p><u>CHEMBL3612602</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612602 ki = 633.0 nM simil = 0.893333333333</p>
PAIR		<p><u>CHEMBL1242923</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923 ki = 1000.0 nM simil = 0.426395939086</p>
TORS		<p><u>CHEMBL360600</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL360600 ki = 549.54 nM simil = 0.515151515152</p>
FP2		<p><u>CHEMBL3612604</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612604 ki = 0.7 nM simil = 0.732673267327</p>
PUB		<p><u>CHEMBL3612602</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612602 ki = 633.0 nM simil = 0.860655737705</p>

MACCS



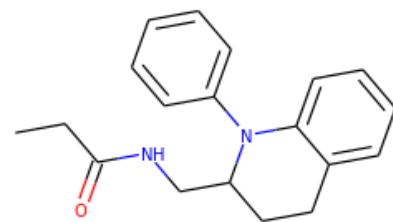
CHEMBL3612471

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612471>)

ki = 291.0 nM

simil = 0.75

KR



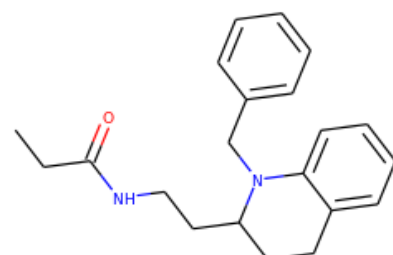
CHEMBL3612608

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612608>)

ki = 1.6 nM

simil = 0.457831325301

GRAPH



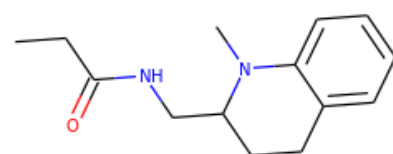
CHEMBL3612610

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612610>)

ki = 326.0 nM

simil = 0.746666666667

SUB



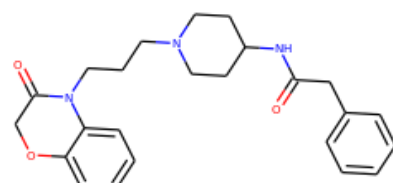
CHEMBL3612604

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3612604>)

ki = 0.7 nM

simil = 0.785714285714

HYB



CHEMBL1242923

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923>)

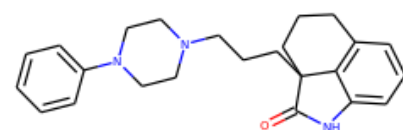
ki = 1000.0 nM

simil = 0.454138702461

Serotonin 2 (5-HT2) receptor: ki = N.A.00 nM Score = 3.1664

Best Fingerprints Similarity

ECFP2



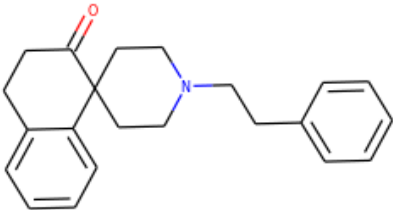
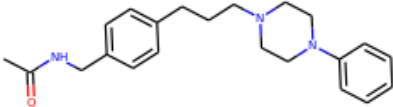
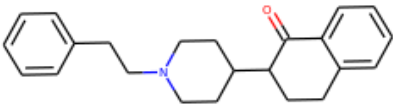
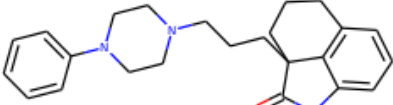
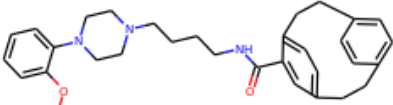
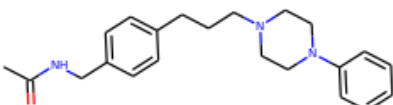
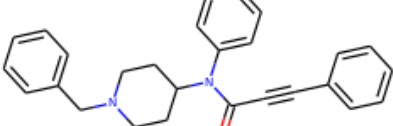
CHEMBL13052

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL13052>)

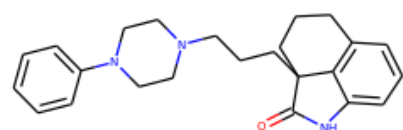
ki = 16.0 nM

simil = 0.586206896552

CHEMBL331172

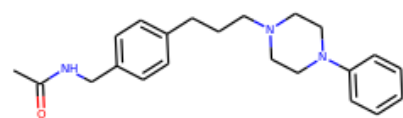
FCFP2		.(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL331172). ki = 183.0 nM simil = 0.75
DAY		CHEMBL352617 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL352617). ki = 160.0 nM simil = 0.46875
PAT		CHEMBL539288 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL539288). ki = 7.3 nM simil = 0.794270833333
PAIR		CHEMBL13052 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL13052). ki = 16.0 nM simil = 0.669064748201
TORS		CHEMBL210567 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL210567). ki = 1600.0 nM simil = 0.382978723404
FP2		CHEMBL352617 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL352617). ki = 160.0 nM simil = 0.586538461538
PUB		CHEMBL112170 .(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL112170). ki = 3100.0 nM simil = 0.831932773109

MACCS



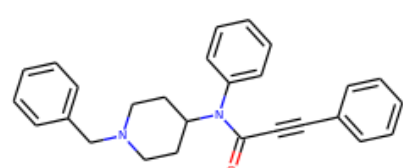
CHEMBL13052
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL13052>)
ki = 16.0 nM
simil = 0.823529411765

KR



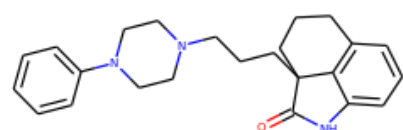
CHEMBL352617
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL352617>)
ki = 160.0 nM
simil = 0.626666666667

GRAPH



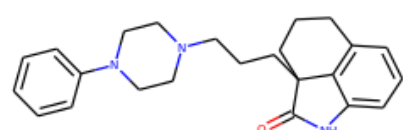
CHEMBL112170
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL112170>)
ki = 3100.0 nM
simil = 0.824324324324

SUB



CHEMBL13052
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL13052>)
ki = 16.0 nM
simil = 0.923076923077

HYB

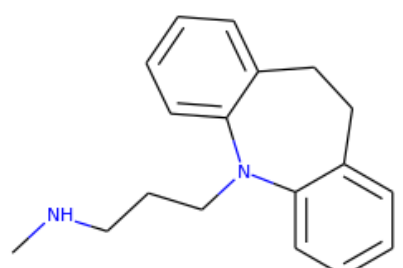


CHEMBL13052
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL13052>)
ki = 16.0 nM
simil = 0.460698689956

Dopamine transporter: ki = 478.0114 nM Score = 3.1095

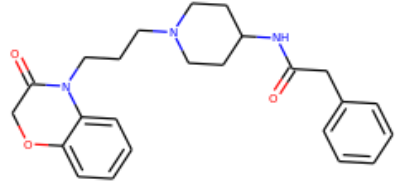
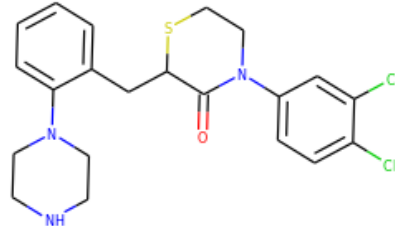
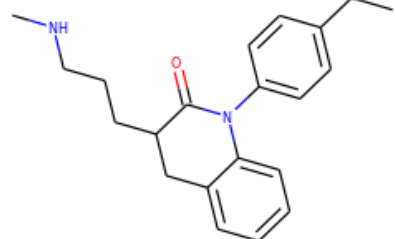
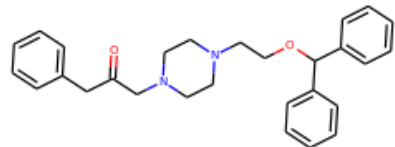
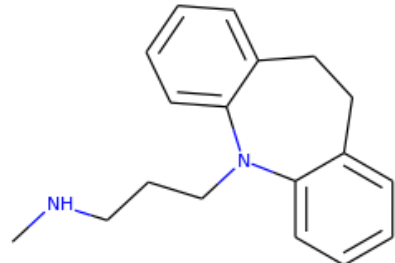
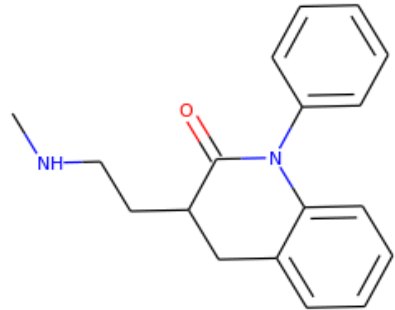
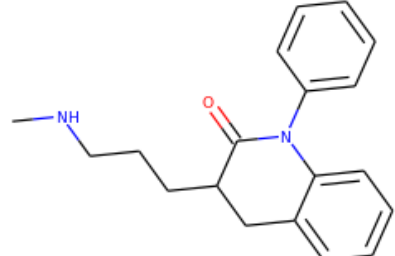
Best Fingerprints Similarity

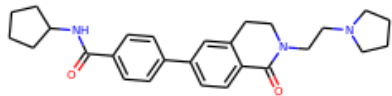
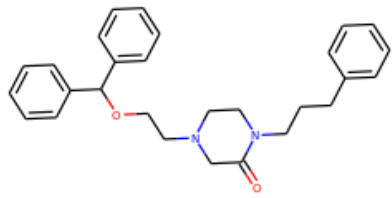
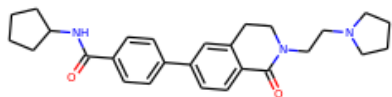
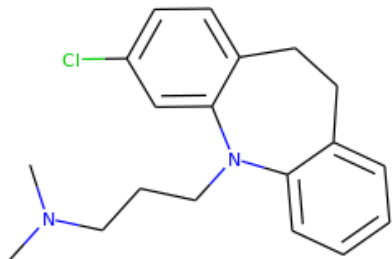
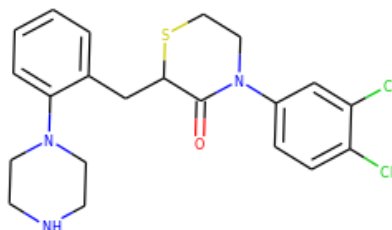
ECFP2



CHEMBL72 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL72>)
ki = 0.49 nM
simil = 0.52

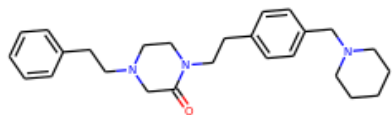
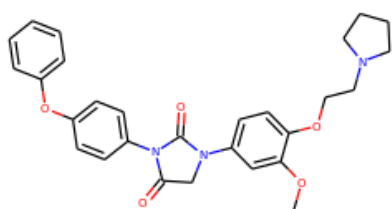
CHEMBL1242923

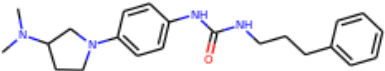
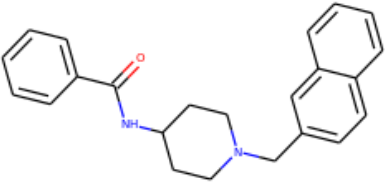
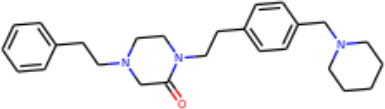
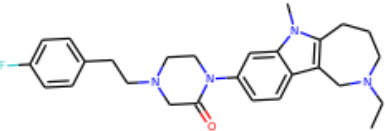
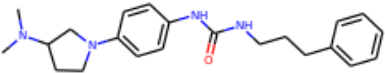
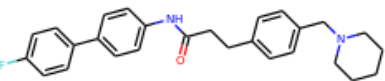
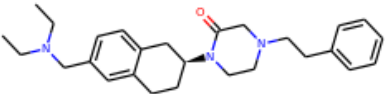
FCFP2		. (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923) ki = 1000.0 nM simil = 0.75
DAY		CHEMBL574126 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL574126) ki = 87.0 nM simil = 0.556468172485
PAT		CHEMBL198038 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL198038) ki = 200.0 nM simil = 0.870026525199
PAIR		CHEMBL466750 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL466750) ki = 10.0 nM simil = 0.483870967742
TORS		CHEMBL72 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL72) ki = 0.49 nM simil = 0.620689655172
FP2		CHEMBL194310 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL194310) ki = 200.0 nM simil = 0.62037037037
PUB		CHEMBL196365 (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL196365) ki = 200.0 nM simil = 0.868852459016

MACCS		. (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031873) ki = 10000.0 nM simil = 0.788461538462
		
KR		CHEMBL124222 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL124222) ki = 8200.0 nM simil = 0.457446808511
GRAPH		CHEMBL2031873 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2031873) ki = 10000.0 nM simil = 0.782051282051
SUB		CHEMBL415 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415) ki = 2182.0 nM simil = 0.846153846154
HYB		CHEMBL574126 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL574126) ki = 87.0 nM simil = 0.503080082136

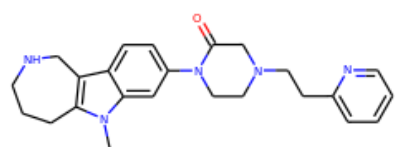
Melanin-concentrating hormone receptor 1: ki = N.A.00 nM Score = 2.5579

Best Fingerprints Similarity

ECFP2		CHEMBL217637 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL217637) ki = 11.0 nM simil = 0.5
FCFP2		CHEMBL246794 . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246794) ki = 164.0 nM simil = 0.777777777778

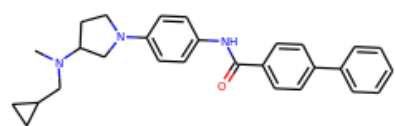
DAY		<p><u>CHEMBL178772</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL178772) ki = 43.0 nM simil = 0.482260183968</p>
PAT		<p><u>CHEMBL215388</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL215388) ki = 347.0 nM simil = 0.795698924731</p>
PAIR		<p><u>CHEMBL217637</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL217637) ki = 11.0 nM simil = 0.5</p>
TORS		<p><u>CHEMBL3665381</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3665381) ki = 9.8 nM simil = 0.333333333333</p>
FP2		<p><u>CHEMBL178772</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL178772) ki = 43.0 nM simil = 0.638095238095</p>
PUB		<p><u>CHEMBL388181</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL388181) ki = 25.0 nM simil = 0.8046875</p>
MACCS		<p><u>CHEMBL229739</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL229739) ki = 16.0 nM simil = 0.857142857143</p>

KR



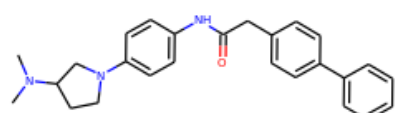
CHEMBL3665364
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3665364>)
ki = 44.0 nM
simil = 0.506024096386

GRAPH



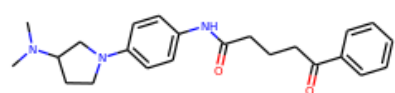
CHEMBL179346
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL179346>)
ki = 5.5 nM
simil = 0.817073170732

SUB



CHEMBL361423
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL361423>)
ki = 4300.0 nM
simil = 0.923076923077

HYB

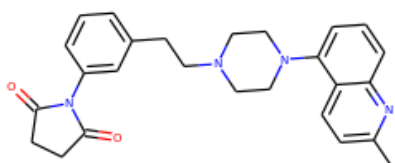


CHEMBL360567
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL360567>)
ki = 250.0 nM
simil = 0.471544715447

Serotonin 1b (5-HT1b) receptor: ki = N.A.00 nM Score = 2.4412

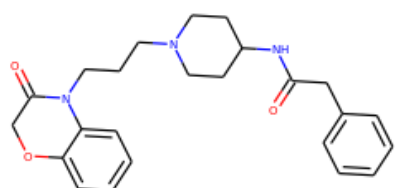
Best Fingerprints Similarity

ECFP2



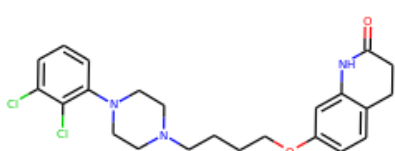
CHEMBL1631544
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1631544>)
ki = 39.81 nM
simil = 0.548387096774

FCFP2

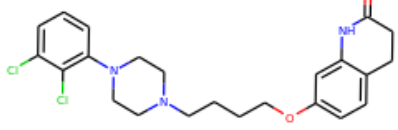
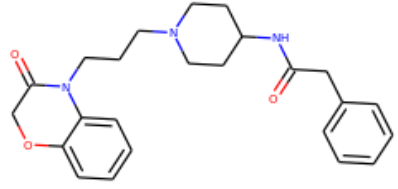
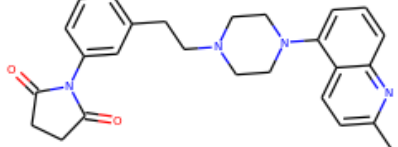
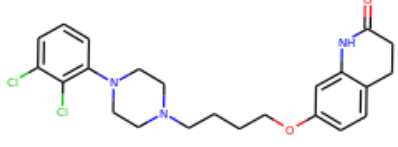
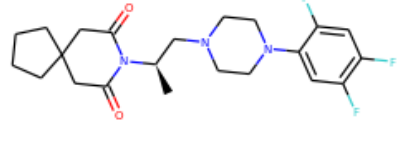
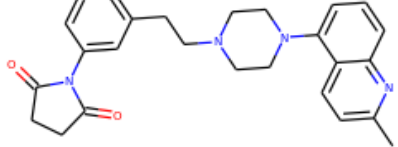
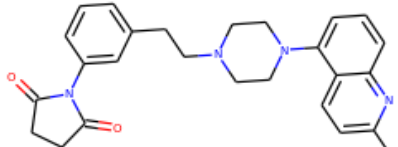


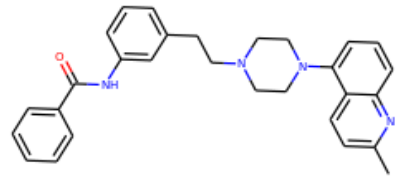
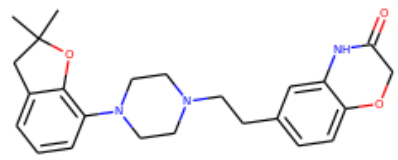
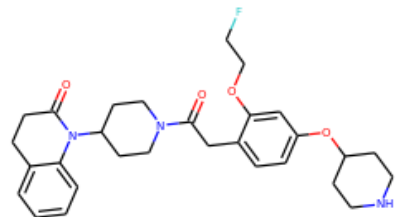
CHEMBL1242923
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923>)
ki = 1000.0 nM
simil = 0.75

DAY



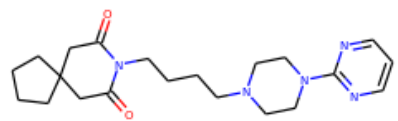
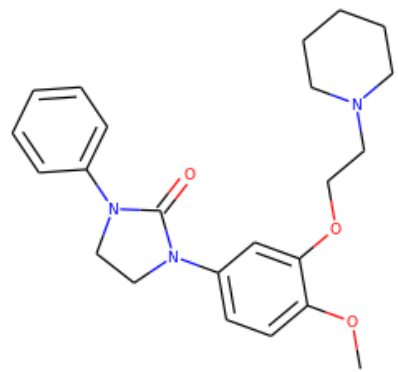
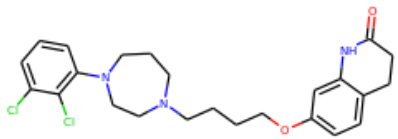
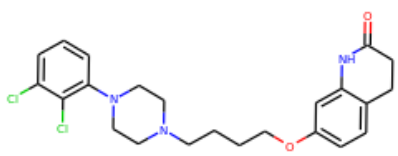
CHEMBL1112 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112>)
ki = 1000.0 nM
simil = 0.56

PAT		<u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112). ki = 1000.0 nM simil = 0.82380952381
PAIR		<u>CHEMBL1242923</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1242923). ki = 1000.0 nM simil = 0.426395939086
TORS		<u>CHEMBL1631544</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1631544). ki = 39.81 nM simil = 0.463414634146
FP2		<u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112). ki = 1000.0 nM simil = 0.569343065693
PUB		<u>CHEMBL98241</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL98241). ki = 7700.0 nM simil = 0.7734375
MACCS		<u>CHEMBL1631544</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1631544). ki = 39.81 nM simil = 0.843137254902
KR		<u>CHEMBL1631544</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1631544). ki = 39.81 nM simil = 0.566265060241

GRAPH		<u>CHEMBL1632210</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210) ki = 2.512 nM simil = 0.848101265823
SUB		<u>CHEMBL491839</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL491839) ki = 0.631 nM simil = 0.857142857143
HYB		<u>CHEMBL2424668</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2424668) ki = 700.0 nM simil = 0.580508474576

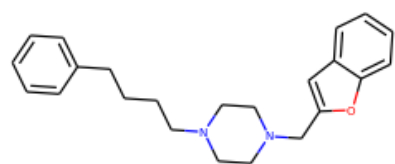
Serotonin 2b (5-HT2b) receptor: ki = N.A.00 nM Score = 2.2304

Best Fingerprints Similarity

ECFP2		<u>CHEMBL49</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL49) ki = 477.0 nM simil = 0.51724137931
FCFP2		<u>CHEMBL383800</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL383800) ki = 1258.93 nM simil = 0.823529411765
DAY		<u>CHEMBL2165126</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2165126) ki = 0.6 nM simil = 0.575824175824
PAT		<u>CHEMBL1112</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112) ki = 0.36 nM

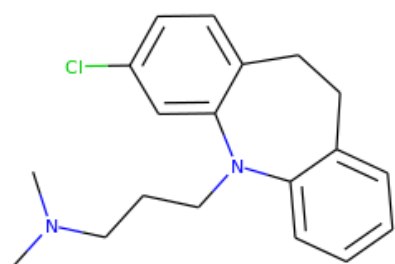
simil = 0.82380952381

PAIR



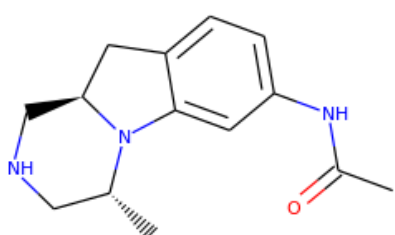
CHEMBL1834258
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1834258>)
ki = 275.0 nM
simil = 0.5234375

TORS



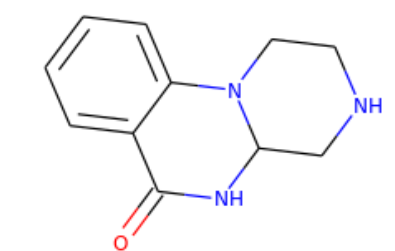
CHEMBL415 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL415>)
ki = 152.0 nM
simil = 0.558823529412

FP2



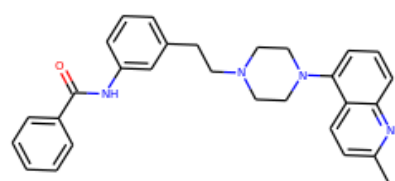
CHEMBL187787
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL187787>)
ki = 960.0 nM
simil = 0.691588785047

PUB



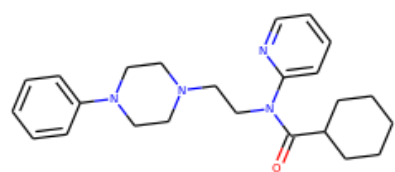
CHEMBL590077
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL590077>)
ki = 137.0 nM
simil = 0.77037037037

MACCS



CHEMBL1632210
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210>)
ki = 125.89 nM
simil = 0.8125

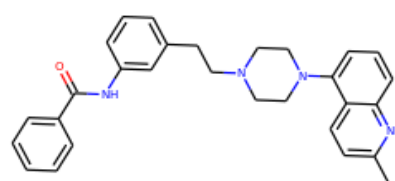
KR



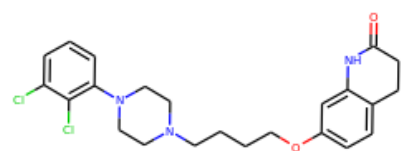
CHEMBL2164350
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2164350>)
ki = 327.0 nM
simil = 0.536082474227

GRAPH

CHEMBL1632210
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1632210>)
ki = 125.89 nM
simil = 0.848101265823



SUB

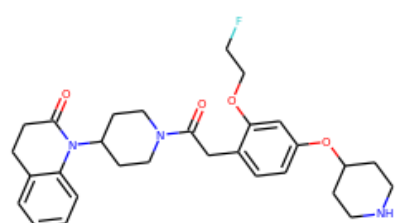


[CHEMBL1112 \(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1112)

ki = 0.36 nM

simil = 0.857142857143

HYB



[CHEMBL2424668](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2424668)

[\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2424668\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2424668)

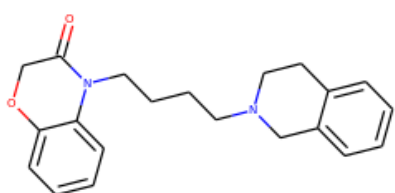
ki = 500.0 nM

simil = 0.580508474576

Neuronal acetylcholine receptor protein alpha-7 subunit: ki = N.A.00 nM Score = 2.2068

Best Fingerprints Similarity

ECFP2



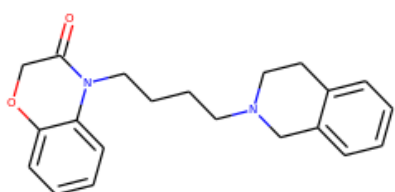
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

[\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

ki = 4.5 nM

simil = 0.72

FCFP2



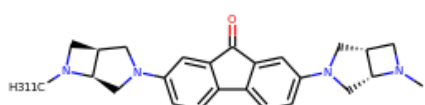
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

[\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

ki = 4.5 nM

simil = 0.882352941176

DAY



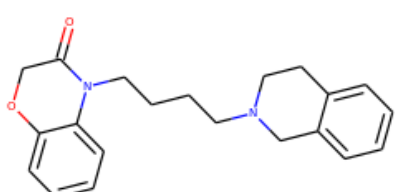
[CHEMBL3235498](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3235498)

[\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3235498\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3235498)

ki = 0.092 nM

simil = 0.384756657484

PAT



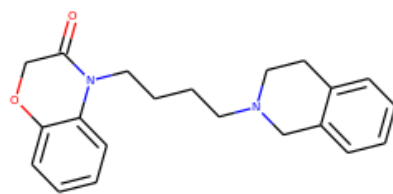
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

[\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)

ki = 4.5 nM

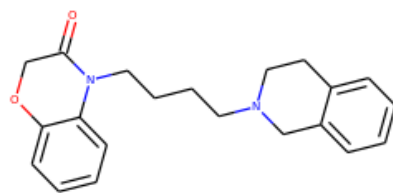
simil = 0.780193236715

PAIR



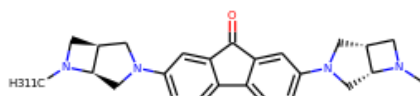
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844>)
ki = 4.5 nM
simil = 0.60447761194

TORS



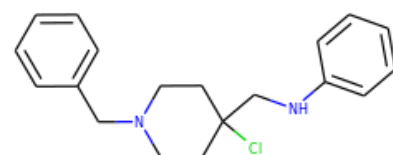
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844>)
ki = 4.5 nM
simil = 0.512195121951

FP2



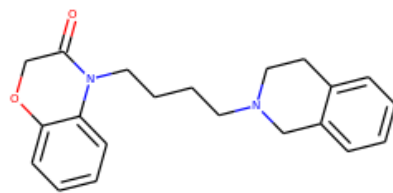
[CHEMBL3235498](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3235498)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3235498>)
ki = 0.092 nM
simil = 0.449612403101

PUB



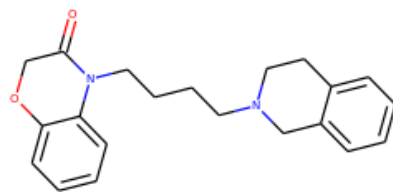
[CHEMBL1740345](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1740345)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1740345>)
ki = 4.5 nM
simil = 0.715447154472

MACCS



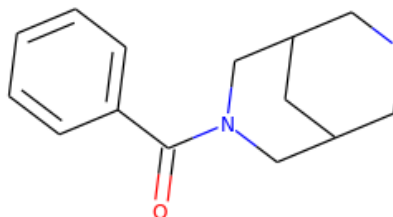
[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844>)
ki = 4.5 nM
simil = 0.769230769231

KR



[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844>)
ki = 4.5 nM
simil = 0.443181818182

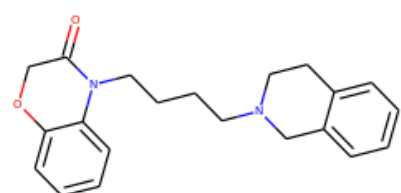
GRAPH



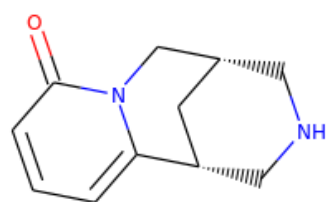
[CHEMBL2179522](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2179522)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2179522>)
ki = 34000.0 nM
simil = 0.717948717949

SUB

[CHEMBL1828844](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844)
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1828844>)
ki = 4.5 nM
simil = 0.846153846154



HYB

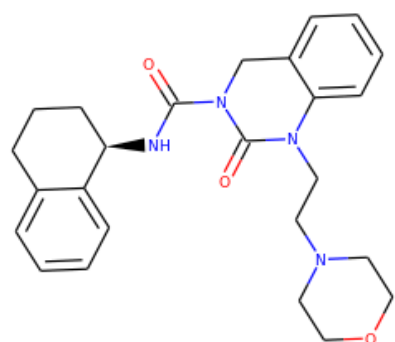


CHEMBL497939
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL497939>)
ki = 1420.0 nM
simil = 0.412997903564

Cannabinoid CB2 receptor: ki = N.A.00 nM Score = 2.1196

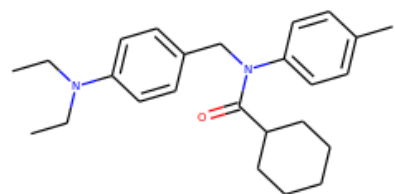
Best Fingerprints Similarity

ECFP2



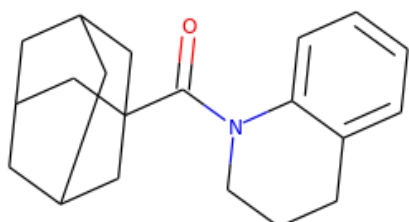
CHEMBL521668
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL521668>)
ki = 9.0 nM
simil = 0.444444444444

FCFP2



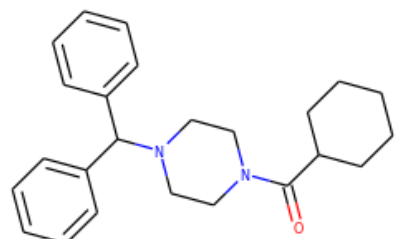
CHEMBL2326303
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2326303>)
ki = 221.82 nM
simil = 0.722222222222

DAY



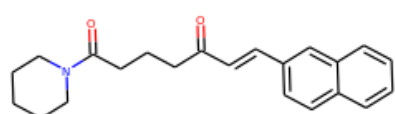
CHEMBL246952
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246952>)
ki = 790.0 nM
simil = 0.665399239544

PAT

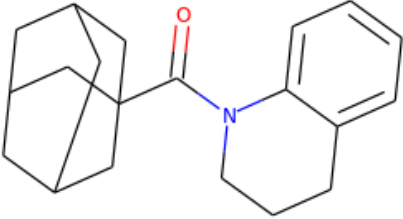
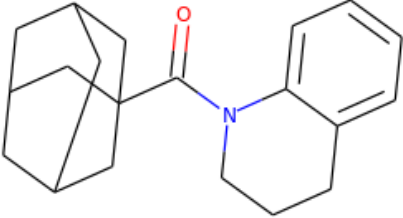
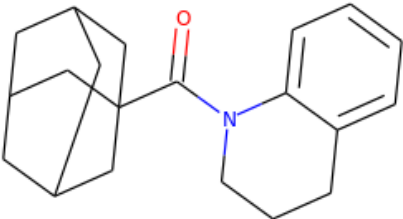
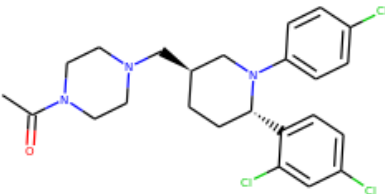
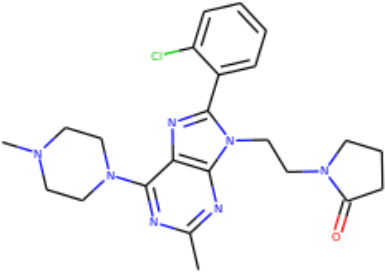
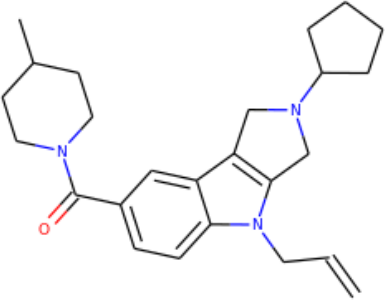
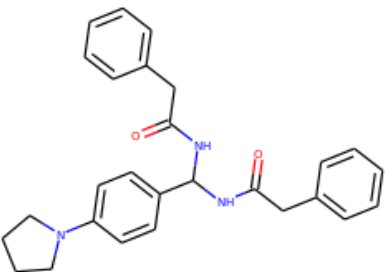


CHEMBL1088730
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1088730>)
ki = 3050.0 nM
simil = 0.797843665768

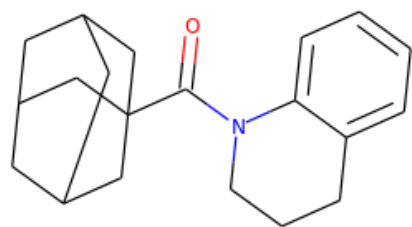
PAIR



CHEMBL1288181
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1288181>)
ki = 10000.0 nM
simil = 0.540145985401

TORS		<p><u>CHEMBL246952</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246952) ki = 790.0 nM simil = 0.527777777778</p>
FP2		<p><u>CHEMBL246952</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246952) ki = 790.0 nM simil = 0.72</p>
PUB		<p><u>CHEMBL246952</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246952) ki = 790.0 nM simil = 0.859504132231</p>
MACCS		<p><u>CHEMBL590551</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL590551) ki = 1846.0 nM simil = 0.78431372549</p>
KR		<p><u>CHEMBL3092895</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3092895) ki = 459.0 nM simil = 0.517647058824</p>
GRAPH		<p><u>CHEMBL250026</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL250026) ki = 23.3 nM simil = 0.784090909091</p>
SUB		<p><u>CHEMBL2179754</u> .https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2179754) ki = 71.0 nM simil = 0.846153846154</p>

HYB



CHEMBL246952

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL246952>)

ki = 790.0 nM

simil = 0.534391534392