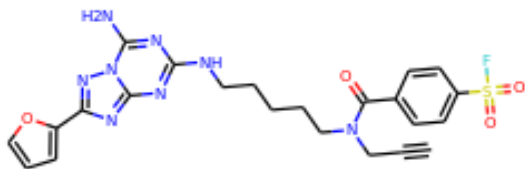


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Your molecule

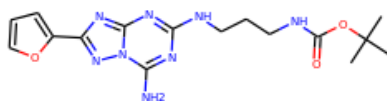


has 3 possible target(s) !

Adenosine A2a receptor: ki = N.A.00 nM Score = 4.6646

Best Fingerprints Similarity

ECFP2



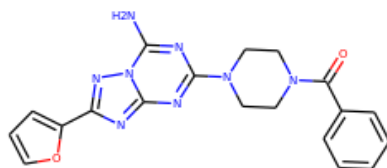
CHEMBL1927428

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927428>)

ki = 38.6 nM

simil = 0.54

FCFP2



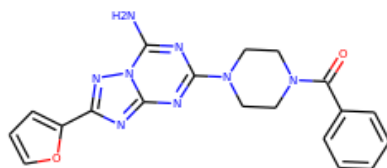
CHEMBL1927440

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927440>)

ki = 348.0 nM

simil = 0.666666666667

DAY



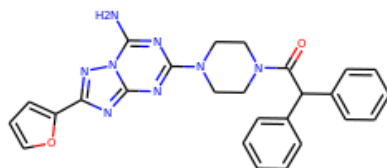
CHEMBL1927440

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927440>)

ki = 348.0 nM

simil = 0.783945345858

PAT



CHEMBL1927447

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927447>)

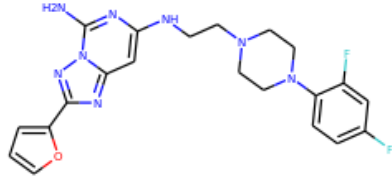
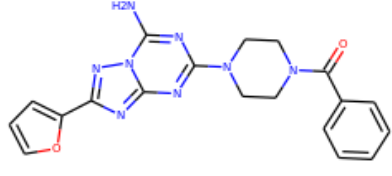
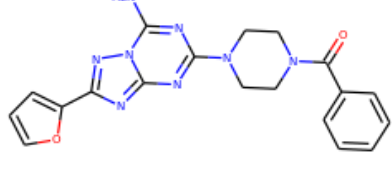
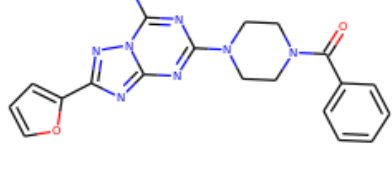
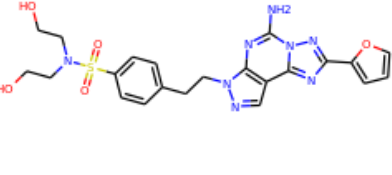
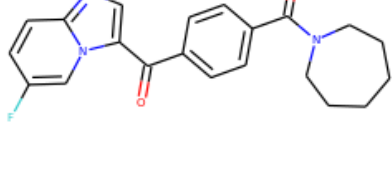
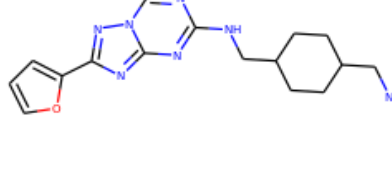
ki = 92.9 nM

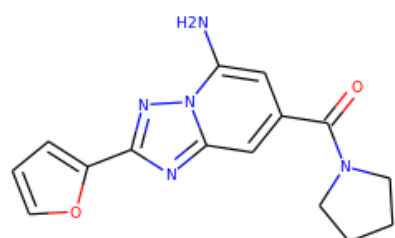
simil = 0.86308492201

Latest News

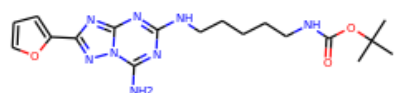
Website alpha-v
Launched
October 10th, 201

Work in progress.

PAIR		<p><u>CHEMBL361687</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL361687) ki = 1.5 nM simil = 0.420454545455</p>
TORS		<p><u>CHEMBL1927440</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927440) ki = 348.0 nM simil = 0.613636363636</p>
FP2		<p><u>CHEMBL1927440</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927440) ki = 348.0 nM simil = 0.71186440678</p>
PUB		<p><u>CHEMBL1927440</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927440) ki = 348.0 nM simil = 0.876777251185</p>
MACCS		<p><u>CHEMBL22717</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL22717) ki = 0.12 nM simil = 0.802197802198</p>
KR		<p><u>CHEMBL3260729</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3260729) ki = 12.0 nM simil = 0.536585365854</p>
GRAPH		<p><u>CHEMBL1927444</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927444) ki = 16.9 nM simil = 0.760233918129</p>
SUB		<p><u>CHEMBL109499</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL109499) ki = 11.0 nM simil = 0.809523809524</p>



HYB

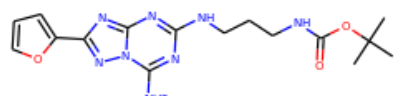


CHEMBL1927429
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927429>)
ki = 44.7 nM
simil = 0.815384615385

Adenosine A1 receptor: ki = 2358.7828 nM Score = 3.1608

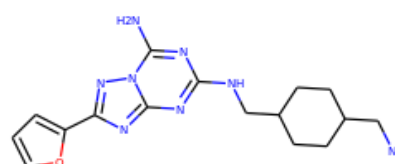
Best Fingerprints Similarity

ECFP2



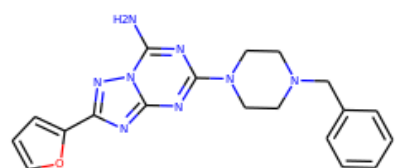
CHEMBL1927428
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927428>)
ki = 344.0 nM
simil = 0.54

FCFP2



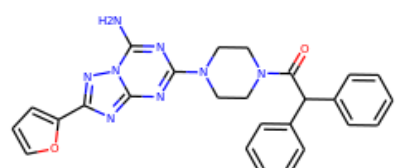
CHEMBL1927444
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927444>)
ki = 1350.0 nM
simil = 0.655172413793

DAY



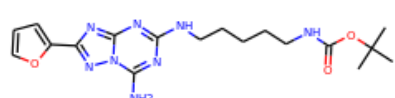
CHEMBL188897
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL188897>)
ki = 978.0 nM
simil = 0.74632034632

PAT

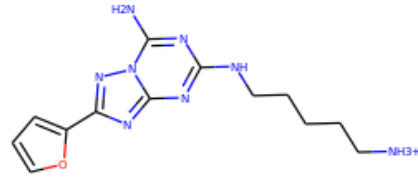
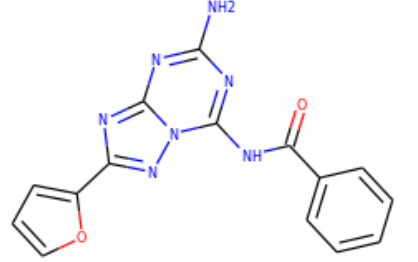
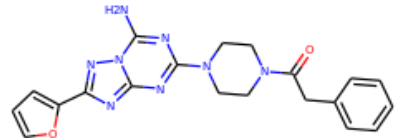
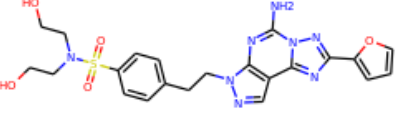
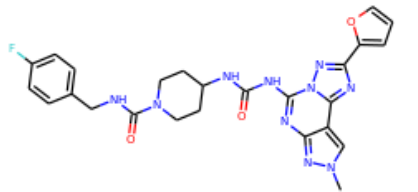
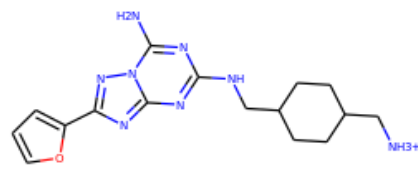
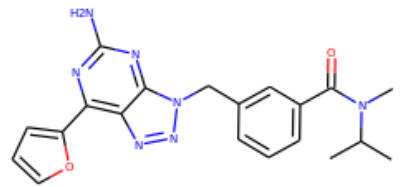


CHEMBL1927447
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927447>)
ki = 7470.0 nM
simil = 0.86308492201

PAIR



CHEMBL1927429
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927429>)
ki = 963.0 nM
simil = 0.334831460674

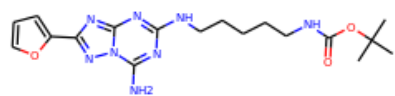
TORS		<u>CHEMBL1927446</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927446) ki = 2950.0 nM simil = 0.609756097561
FP2		<u>CHEMBL1927634</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927634) ki = 1800.0 nM simil = 0.698863636364
PUB		<u>CHEMBL1927436</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927436) ki = 3510.0 nM simil = 0.872641509434
MACCS		<u>CHEMBL22717</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL22717) ki = 2495.0 nM simil = 0.802197802198
KR		<u>CHEMBL2071046</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2071046) ki = 408.0 nM simil = 0.43137254902
GRAPH		<u>CHEMBL1927444</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927444) ki = 1350.0 nM simil = 0.760233918129
SUB		<u>CHEMBL460805</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL460805) ki = 1133.0 nM simil = 0.727272727273

HYB

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1927429>).

ki = 963.0 nM

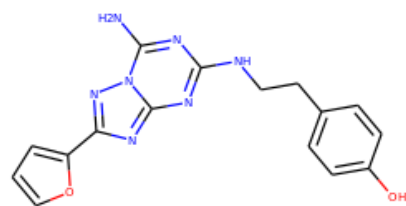
simil = 0.815384615385



Adenosine A3 receptor: ki = N.A.00 nM Score = 3.0506

Best Fingerprints Similarity

ECFP2



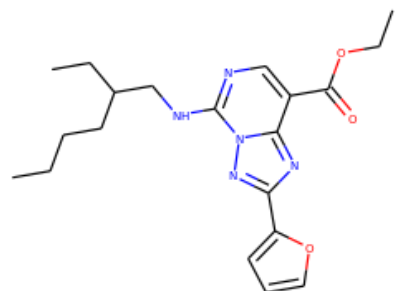
CHEMBL113142

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL113142>).

ki = 300.0 nM

simil = 0.521739130435

FCFP2



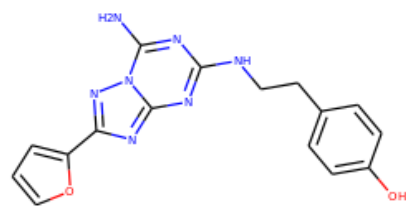
CHEMBL3314891

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3314891>).

ki = 39.3 nM

simil = 0.59375

DAY



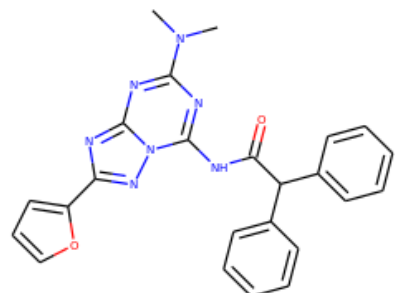
CHEMBL113142

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL113142>).

ki = 300.0 nM

simil = 0.702464788732

PAT



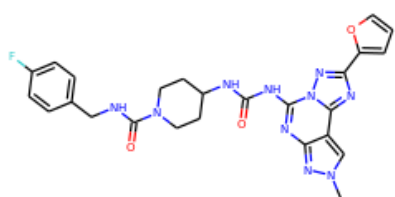
CHEMBL1089112

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1089112>).

ki = 473.0 nM

simil = 0.873394495413

PAIR



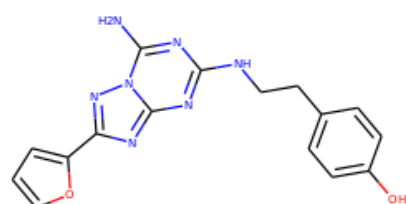
CHEMBL2071046

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL2071046>).

ki = 4.9 nM

simil = 0.3125

TORS



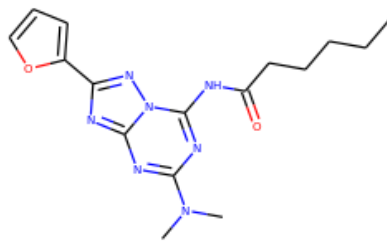
CHEMBL113142

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL113142>).

ki = 300.0 nM

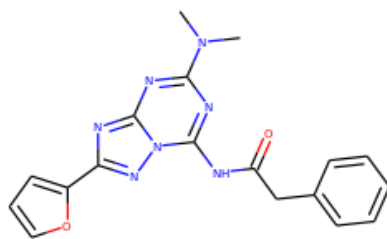
simil = 0.568181818182

FP2



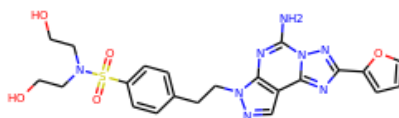
CHEMBL1089798
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1089798>)
ki = 2200.0 nM
simil = 0.664804469274

PUB



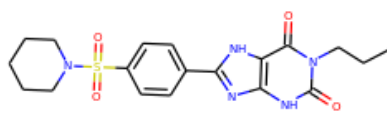
CHEMBL1089113
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL1089113>)
ki = 1050.0 nM
simil = 0.870813397129

MACCS



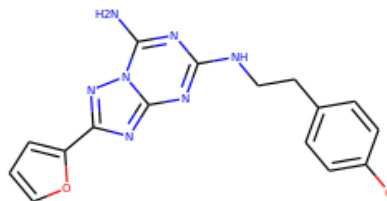
CHEMBL22717
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL22717>)
ki = 10000.0 nM
simil = 0.802197802198

KR



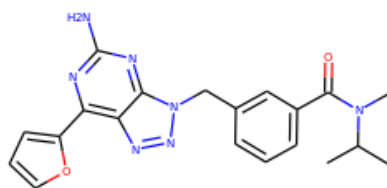
CHEMBL486281
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL486281>)
ki = 140.0 nM
simil = 0.442105263158

GRAPH



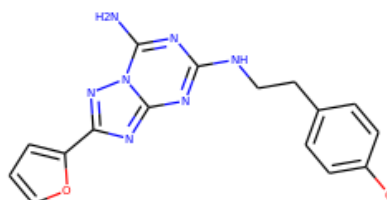
CHEMBL113142
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL113142>)
ki = 300.0 nM
simil = 0.757225433526

SUB



CHEMBL460805
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL460805>)
ki = 2467.0 nM
simil = 0.727272727273

HYB



CHEMBL113142
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL113142>)
ki = 300.0 nM
simil = 0.738229755179