

ChemOracle[®] (/)

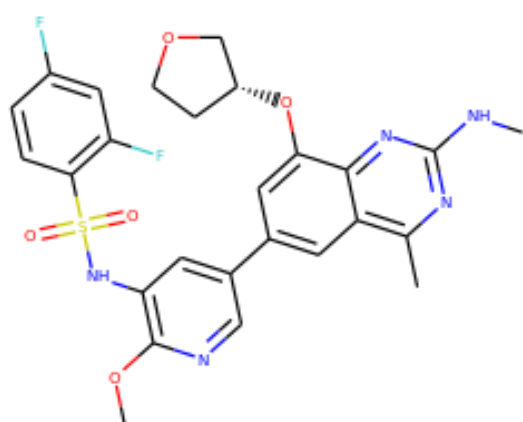
An integrated web-based platform for target prediction: your compounds our solutions!

[HOME \(/\)](#)

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

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

Your molecule

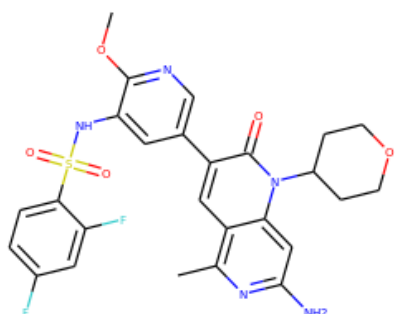


has 4 possible target(s) !

PI3-kinase p110-alpha subunit: ic50 = N.A. nM Score = 7.5725

Best Fingerprints Similarity

ECFP2



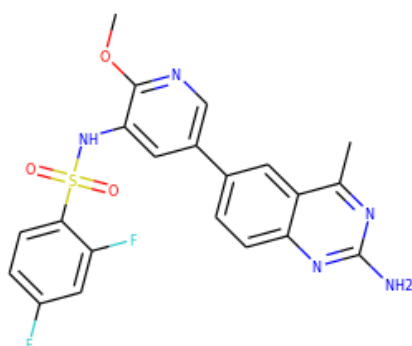
CHEMBL3112713

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112713>)

ic50 = 8.6 nM

simil = 0.660377358491

FCFP2



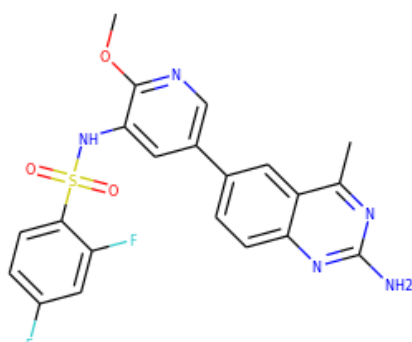
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 3.43 nM

simil = 0.764705882353

DAY



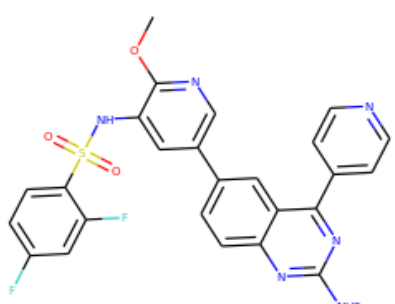
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 3.43 nM

simil = 0.822142857143

PAT



CHEMBL3577914

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3577914>)

ic50 = 0.07 nM

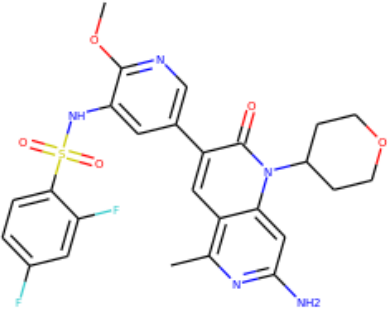
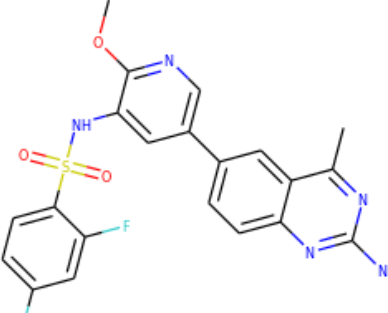
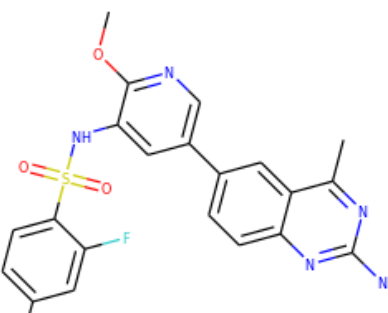
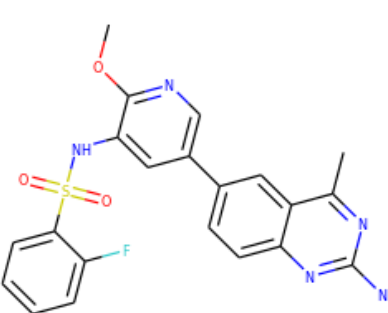
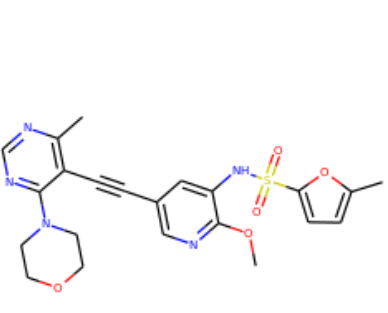
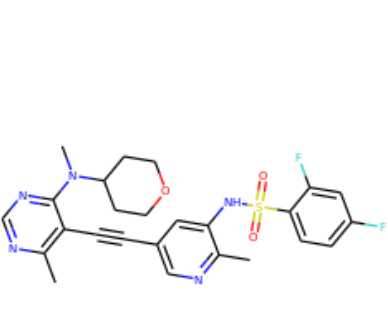
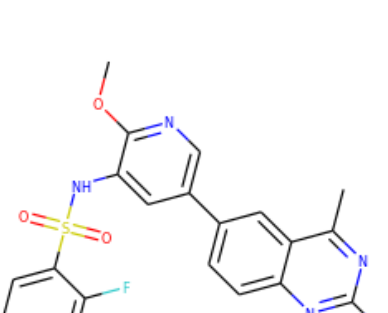
simil = 0.888888888889

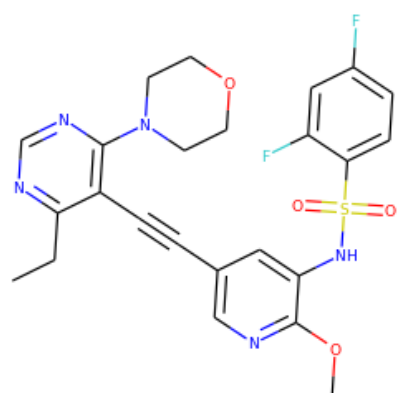
Latest News

Website alpha-v
Launched

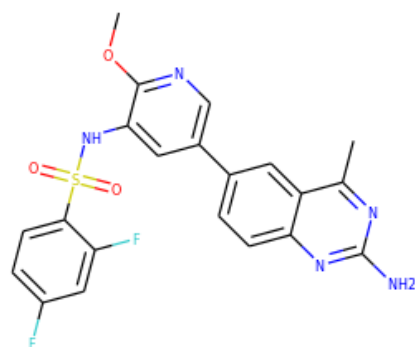
October 10th, 201

Work in progress.

PAIR		<u>CHEMBL3112713</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112713) ic50 = 8.6 nM simil = 0.560810810811
TORS		<u>CHEMBL3112720</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720) ic50 = 3.43 nM simil = 0.672413793103
FP2		<u>CHEMBL3112720</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720) ic50 = 3.43 nM simil = 0.778301886792
PUB		<u>CHEMBL3112720</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720) ic50 = 3.43 nM simil = 0.891774891775
MACCS		<u>CHEMBL3660132</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3660132) ic50 = 0.53 nM simil = 0.827956989247
KR		<u>CHEMBL3655870</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3655870) ic50 = 0.86 nM simil = 0.578947368421
GRAPH		<u>CHEMBL3112720</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720) ic50 = 3.43 nM simil = 0.72972972973
SUB		<u>CHEMBL3655879</u> (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3655879) ic50 = 0.63 nM simil = 0.842105263158



HYB

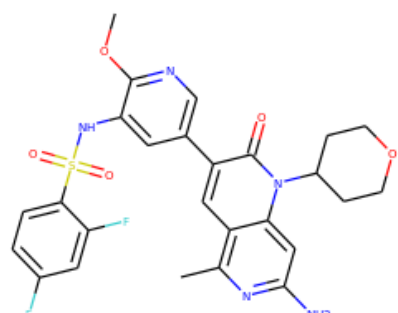


CHEMBL3112720
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)
 ic50 = 3.43 nM
 simil = 0.705179282869

Serine/threonine-protein kinase mTOR: ic50 = N.A. nM Score = 7.5487

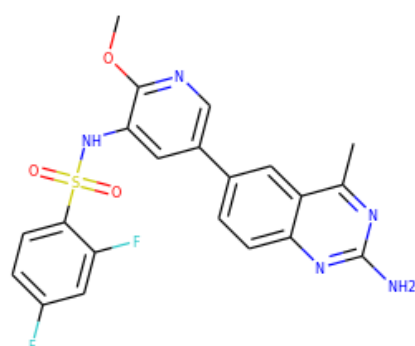
Best Fingerprints Similarity

ECFP2



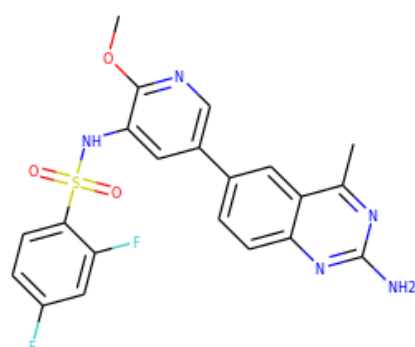
CHEMBL3112713
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112713>)
 ic50 = 13.36 nM
 simil = 0.660377358491

FCFP2



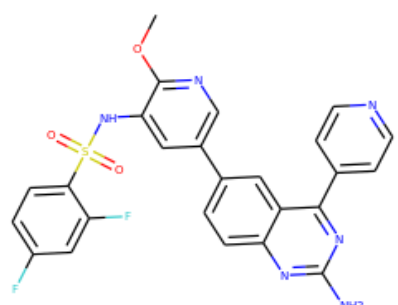
CHEMBL3112720
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)
 ic50 = 2.32 nM
 simil = 0.764705882353

DAY



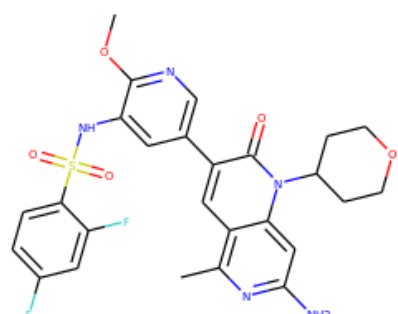
CHEMBL3112720
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)
 ic50 = 2.32 nM
 simil = 0.822142857143

PAT



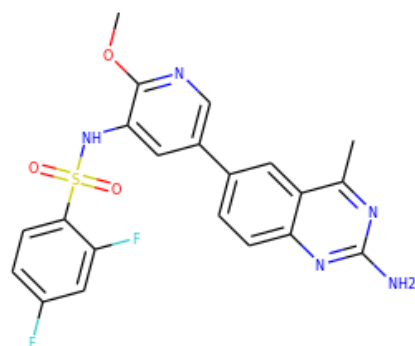
CHEMBL3577914
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3577914>)
 ic50 = 0.29 nM
 simil = 0.888888888889

PAIR



CHEMBL3112713
 (<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112713>)
 ic50 = 13.36 nM
 simil = 0.560810810811

TORS



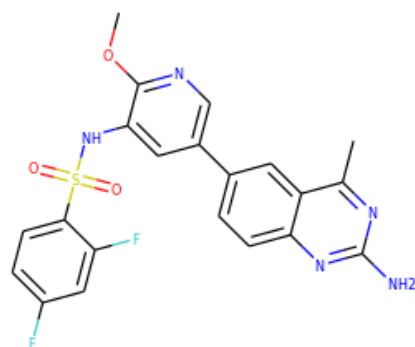
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 2.32 nM

simil = 0.672413793103

FP2



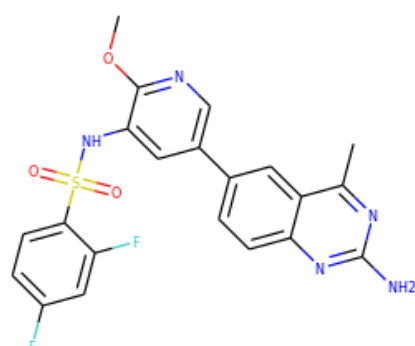
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 2.32 nM

simil = 0.778301886792

PUB



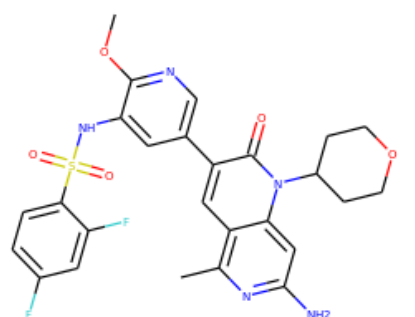
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 2.32 nM

simil = 0.891774891775

MACCS



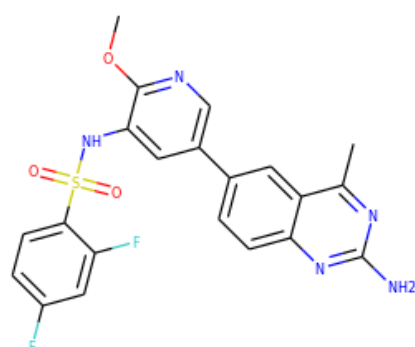
CHEMBL3112713

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112713>)

ic50 = 13.36 nM

simil = 0.80412371134

KR



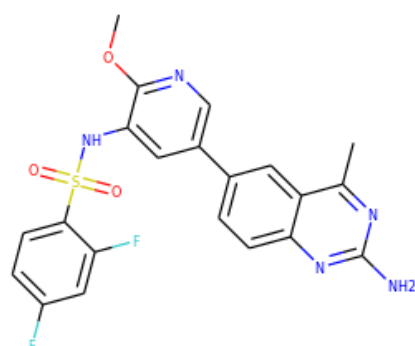
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 2.32 nM

simil = 0.551724137931

GRAPH



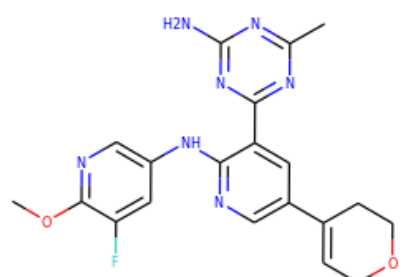
CHEMBL3112720

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720>)

ic50 = 2.32 nM

simil = 0.72972972973

SUB



CHEMBL3646622

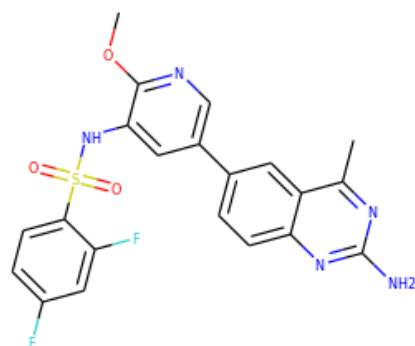
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3646622>)

ic50 = 10000.0 nM

simil = 0.789473684211

CHEMBL3112720

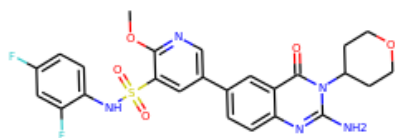
HYB [.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3112720)
ic50 = 2.32 nM
simil = 0.705179282869



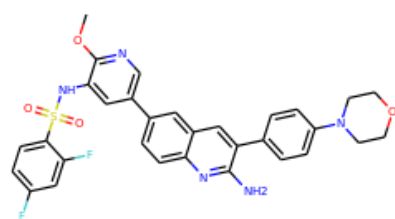
PI4-kinase alpha subunit: ic50 = N.A. nM Score = 7.134

Best Fingerprints Similarity

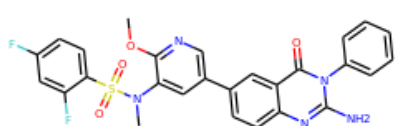
ECFP2 [CHEMBL3121326](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121326)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121326\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121326)
ic50 = 10.0 nM
simil = 0.634615384615



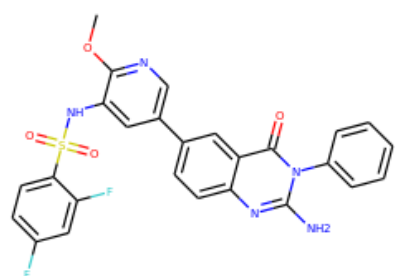
FCFP2 [CHEMBL3121328](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121328)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121328\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121328)
ic50 = 39.81 nM
simil = 0.722222222222



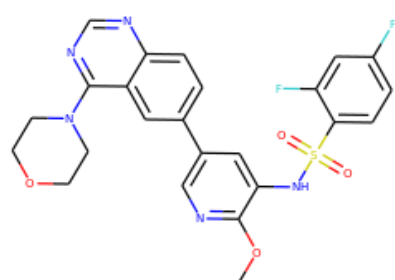
DAY [CHEMBL3121315](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315)
ic50 = 3981.07 nM
simil = 0.734582829504



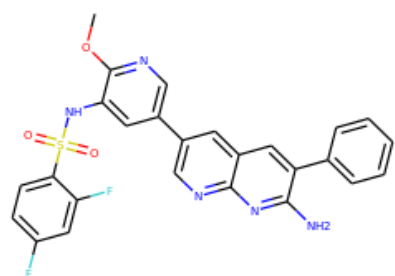
PAT [CHEMBL3121334](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121334)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121334\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121334)
ic50 = 1.585 nM
simil = 0.859675036928



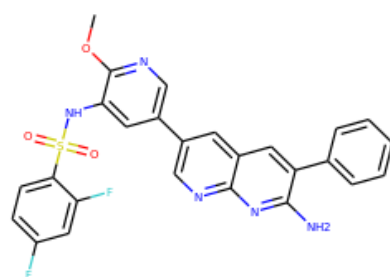
PAIR [CHEMBL3121327](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327)
ic50 = 1.585 nM
simil = 0.537688442211



TORS [CHEMBL3121330](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330)
[.\(https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330\)](https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330)
ic50 = 630.96 nM
simil = 0.590163934426



FP2



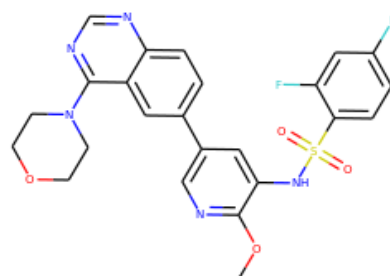
CHEMBL3121330

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330>)

ic50 = 630.96 nM

simil = 0.685840707965

PUB



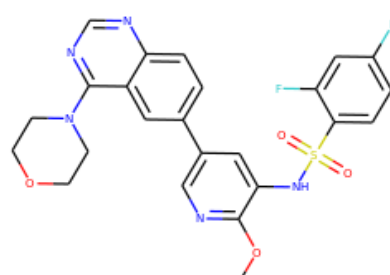
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 1.585 nM

simil = 0.886075949367

MACCS



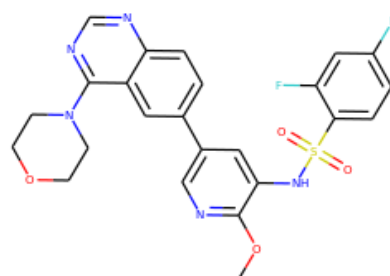
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 1.585 nM

simil = 0.826086956522

KR



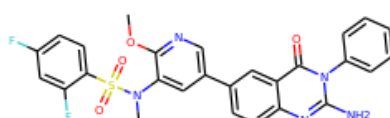
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 1.585 nM

simil = 0.565217391304

GRAPH



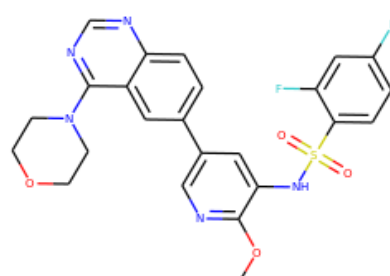
CHEMBL3121315

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315>)

ic50 = 3981.07 nM

simil = 0.70036101083

SUB



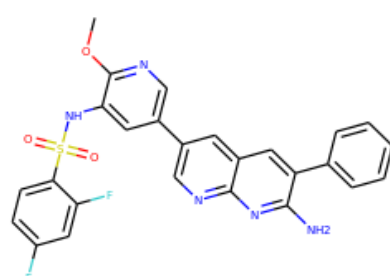
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 1.585 nM

simil = 0.823529411765

HYB



CHEMBL3121330

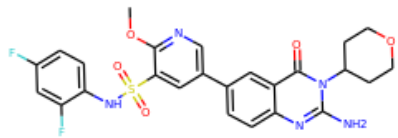
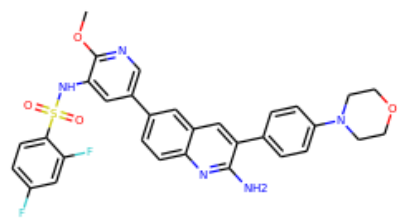
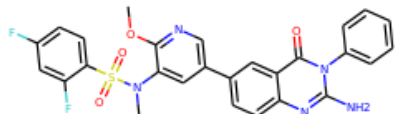
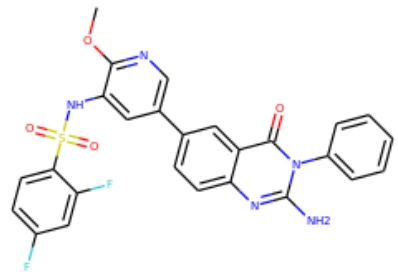
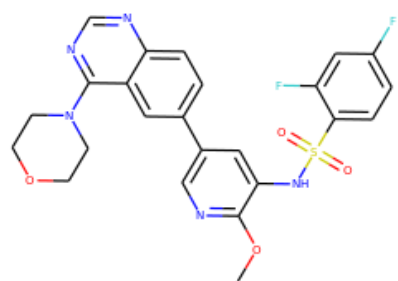
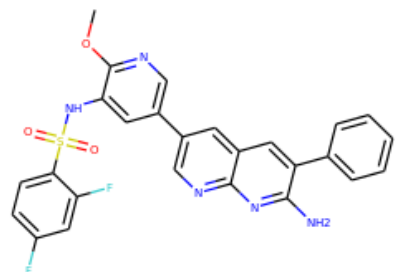
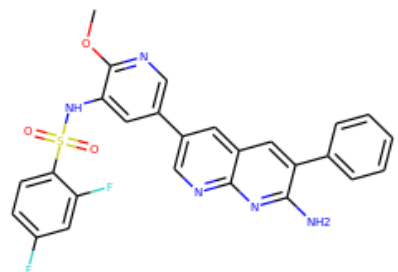
(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330>)

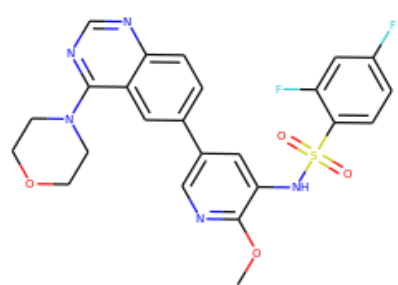
ic50 = 630.96 nM

simil = 0.657088122605

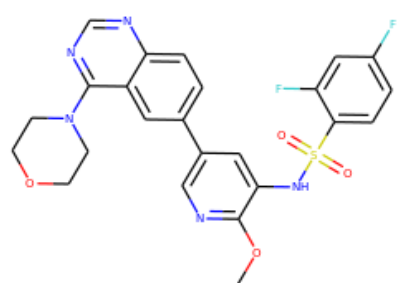
PI3-kinase p110-gamma subunit: ic50 = N.A. nM Score = 7.134

Best Fingerprints Similarity

ECFP2		<p><u>CHEMBL3121326</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121326) ic50 = 501.19 nM simil = 0.634615384615</p>
FCFP2		<p><u>CHEMBL3121328</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121328) ic50 = 630.96 nM simil = 0.722222222222</p>
DAY		<p><u>CHEMBL3121315</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315) ic50 = 3981.07 nM simil = 0.734582829504</p>
PAT		<p><u>CHEMBL3121334</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121334) ic50 = 3.981 nM simil = 0.859675036928</p>
PAIR		<p><u>CHEMBL3121327</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327) ic50 = 2.512 nM simil = 0.537688442211</p>
TORS		<p><u>CHEMBL3121330</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330) ic50 = 6309.57 nM simil = 0.590163934426</p>
FP2		<p><u>CHEMBL3121330</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330) ic50 = 6309.57 nM simil = 0.685840707965</p>
PUB		<p><u>CHEMBL3121327</u> . (https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327) ic50 = 2.512 nM simil = 0.886075949367</p>



MACCS



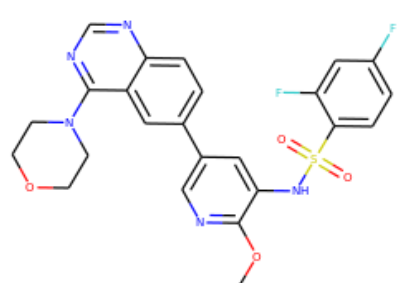
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 2.512 nM

simil = 0.826086956522

KR



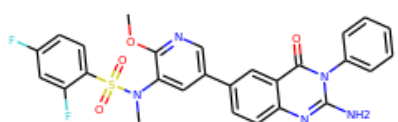
CHEMBL3121327

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121327>)

ic50 = 2.512 nM

simil = 0.565217391304

GRAPH



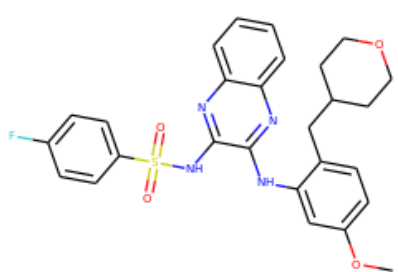
CHEMBL3121315

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121315>)

ic50 = 3981.07 nM

simil = 0.70036101083

SUB



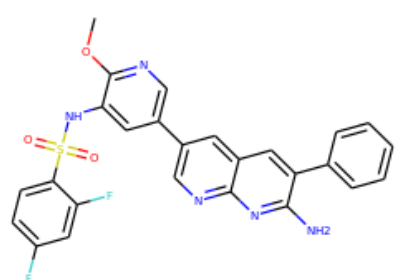
CHEMBL3652126

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3652126>)

ic50 = 150.0 nM

simil = 0.833333333333

HYB



CHEMBL3121330

(<https://pubchem.ncbi.nlm.nih.gov/compound/CHEMBL3121330>)

ic50 = 6309.57 nM

simil = 0.657088122605