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Recommended Citation

Worah, Pratik; Tornng, Wen; and Feng, JW, "Predicted Binders for MNK2 but not MNK1 Protein Targets from Machine Learning", Technical Disclosure Commons, (August 22, 2022)
https://www.tdcommons.org/dpubs_series/5323



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Predicted Binders for MNK2 but not MNK1 Protein Targets from Machine Learning

Anonymous

August 2022

Abstract

We used datasets from affinity screening to train machine learning models. The models were then used to rank compounds from commercially available compound collections to generate the following lists of predicted binders for MNK2 but non-binders for MNK1.

Predicted molecules that are hits for MNK2 but non-hits for MNK1

Hits for: <https://www.uniprot.org/uniprotkb/Q9HBH9/entry>

But non-hits for: <https://www.uniprot.org/uniprotkb/Q9BUB5/entry>

```
index,smiles,example_id
0,0=C(c1cccc(C(=O)N2CCC=C(c3ccccc3)C2)n1)N1CCC=C(c2ccccc2)C1,MCULE-9443234838
1,0=C(c1nn2cccnc2c1C1)N1CCC=C(c2ccccc2)C1,MCULE-9055908765
2,FC(F)(F)c1cc(N2CCC(Oc3cncn3)CC2)nc(-c2cccnc2)n1,MCULE-8972621019
3,CNC(=O)C1CCCN1C(=O)CNC(=O)c1cc(C1)c[nH]1,MCULE-3412481267
4,0=C(C1C01)N1CCC=C(c2ccccc2)C1,MCULE-6688898145
5,CNC(=O)c1ccc(CCNC(=O)[C@@H](N)CC2CCCC2)cc1,MCULE-2765522073
6,CC(=O)N1CCCC(O)(C(=O)N2CCC=C(c3ccccc3)C2)C1,MCULE-9851125279
7,C=CC(=O)N1CC(C(=O)N2CCC=C(c3ccccc3)C2)C1,MCULE-2314228129
8,0=C(CN1CCCC(O)C1=O)N1CCC=C(c2ccccc2)C1,MCULE-9548378769
9,0=C(c1ccc(Oc2cccnc2)cc1)N1CCC(Oc2cncc(C1)n2)CC1,MCULE-7962378858
10,0=C(c1cncc(C(=O)N2CCC=C(c3ccccc3)C2)c1)N1CCC=C(c2ccccc2)C1,MCULE-6274706587
11,0=C(c1cccc(Oc2cncn2)c1)N1CCC(Oc2cncc(C1)n2)CC1,MCULE-2930987240
12,0=C(CC1)N1CCC=C(c2ccccc2)C1,MCULE-8414446141
13,C0c1ccc(-c2cncc(C(=O)N3CCC=C(c4ccnnc4)C3)c2)cc1,MCULE-9450442284
14,Cn1cnc1[C@@H]1OCC[C@H]1C(=O)N1CCC=C(c2ccccc2)C1,MCULE-8447709606
15,Cc1cc(Oc2ccccc2)nc(N2CCC=C(c3ccnnc3)C2)n1,MCULE-6551453906
16,CN1CCCC1CNC(=O)N1CCC=C(c2ccccc2)C1,MCULE-8949989403
17,0=C(C1C0CC1c1ccccc1)N1CCC=C(c2cccc(O)c2)C1,MCULE-4740663125
18,0=C(O)C1CCC(C(=O)N2CCC=C(c3ccccc3)C2)N1C1CC1,MCULE-8591033399
```