

MuSSEL Prediction k_i:

1 rank

Canalicular multispecific organic anion transporter 1 : Rattus norvegicus
score: 4.145 on ChEMBL2073676 based on 5 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|---------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL1743143 | 0.619048 | 1620.0 | |
| MFP1 | CHEMBL1743143 | 0.507463 | 1620.0 | |
| RDKit7 | CHEMBL1743143 | 0.899092 | 1620.0 | * |
| Pattern | CHEMBL1743143 | 0.925813 | 1620.0 | * |
| AP_bits | CHEMBL1743143 | 0.518750 | 1620.0 | |
| TT_bits | CHEMBL2074578 | 0.423729 | 18300.0 | |
| FP2 | CHEMBL1743143 | 0.709779 | 1620.0 | * |
| hybridization | CHEMBL1743143 | 0.765333 | 1620.0 | * |
| substructure | CHEMBL2074700 | 0.666667 | 56900.0 | |
| graph | CHEMBL2074712 | 0.609442 | 96600.0 | |
| pubchem | CHEMBL2074712 | 0.824786 | 96600.0 | |
| cdk_maccs | CHEMBL2074712 | 0.845238 | 96600.0 | * |
| klekota_roth | CHEMBL1743143 | 0.536313 | 1620.0 | |

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 11046.981

["Pattern", "RDKit7", "hybridization", "cdk_maccs", "FP2"]

MuSsel Prediction IC₅₀:

1 rank

DNA topoisomerase I : Homo sapiens

score: 9.090 on ChEMBL1781 based on 12 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL72627 | | 0.684211 | 1118.0 | * |
| MFP1 | ChEMBL545250 | | 0.586207 | 430.0 | * |
| RDKit7 | ChEMBL545250 | | 0.920808 | 430.0 | * |
| Pattern | ChEMBL159322 | | 0.896690 | 340.0 | * |
| AP_bits | ChEMBL312690 | | 0.574635 | 4597.0 | * |
| TT_bits | ChEMBL539032 | | 0.638095 | 5500.0 | * |
| FP2 | ChEMBL543849 | | 0.791667 | 1100.0 | * |
| hybridization | ChEMBL545250 | | 0.843165 | 430.0 | * |
| substructure | ChEMBL170532 | | 0.724138 | 2100.0 | |
| graph | ChEMBL539032 | | 0.775862 | 5500.0 | * |
| pubchem | ChEMBL88605 | | 0.840517 | 21000.0 | * |
| cdk_maccs | ChEMBL275538 | | 0.878049 | 1494.0 | * |
| klekota_roth | ChEMBL539032 | | 0.660256 | 5500.0 | * |

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 5875.206

["TT_bits", "cdk_maccs", "Pattern", "FP2", "MFP1", "klekota_roth",
"pubchem", "graph", "AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

2 rank

DNA topoisomerase I : Mus musculus

score: 7.201 on ChEMBL2814 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL445883 | | 0.564103 | 12000.0 | |
| MFP1 | ChEMBL44044 | | 0.533333 | 41000.0 | * |
| RDKit7 | ChEMBL84 | | 0.911797 | 20000.0 | * |
| Pattern | ChEMBL289665 | | 0.852329 | 5000.0 | * |
| AP_bits | ChEMBL289665 | | 0.478326 | 5000.0 | * |
| TT_bits | ChEMBL44044 | | 0.539823 | 41000.0 | * |
| FP2 | ChEMBL84 | | 0.784722 | 20000.0 | * |
| hybridization | ChEMBL837 | | 0.775510 | 4000.0 | * |
| substructure | ChEMBL65 | | 0.586207 | 12000.0 | |
| graph | ChEMBL289665 | | 0.720339 | 5000.0 | |
| pubchem | ChEMBL289665 | | 0.842553 | 5000.0 | * |
| cdk_maccs | ChEMBL289665 | | 0.886076 | 5000.0 | * |
| klekota_roth | ChEMBL44044 | | 0.596273 | 41000.0 | * |

*** ic50 ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 22518.935

["TT_bits", "cdk_maccs", "Pattern", "AP_bits", "MFP1", "klekota_roth",
"pubchem", "FP2", "RDKit7", "hybridization"]

3 rank

Nuclear receptor coactivator 3 : Homo sapiens

score: 7.184 on ChEMBL1615382 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL1566908 | | 0.675676 | 3860.0 | |
| MFP1 | ChEMBL1445386 | | 0.532258 | 1049.0 | * |
| RDKit7 | ChEMBL1200512 | | 0.897051 | 1315.0 | * |
| Pattern | ChEMBL1200512 | | 0.901508 | 1315.0 | * |
| AP_bits | ChEMBL1200512 | | 0.520408 | 1315.0 | * |
| TT_bits | ChEMBL1445386 | | 0.517857 | 1049.0 | * |
| FP2 | ChEMBL1200512 | | 0.762215 | 1315.0 | * |
| hybridization | ChEMBL1200512 | | 0.760274 | 1315.0 | * |
| substructure | ChEMBL1566908 | | 0.714286 | 3860.0 | |
| graph | ChEMBL1200512 | | 0.742489 | 1315.0 | |
| pubchem | ChEMBL1200512 | | 0.841202 | 1315.0 | * |
| cdk_maccs | ChEMBL1200512 | | 0.857143 | 1315.0 | * |

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    klekota_roth CHEMBL1445386          0.593750    1049.0      *
    *** ic50 ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 1183.069
    ["TT_bits", "cdk_maccs", "Pattern", "AP_bits", "MFP1", "klekota_roth",
    "pubchem", "FP2", "RDKit7", "hybridization"]

```

4 rank

Cytochrome P450 3A4 : Homo sapiens

score: 6.051 on ChEMBL340 based on 8 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL2048199 | | 0.575000 | 4000.0 | |
| MFP1 | CHEMBL84 | | 0.500000 | 1521.1 | |
| RDKit7 | CHEMBL84 | | 0.911797 | 1521.1 | * |
| Pattern | CHEMBL84 | | 0.847893 | 1521.1 | * |
| AP_bits | CHEMBL3634394 | | 0.528283 | 10000.0 | * |
| TT_bits | CHEMBL84 | | 0.517857 | 1521.1 | * |
| FP2 | CHEMBL84 | | 0.784722 | 1521.1 | * |
| hybridization | CHEMBL84 | | 0.774052 | 1521.1 | * |
| substructure | CHEMBL1778481 | | 0.785714 | 8900.0 | |
| graph | CHEMBL84 | | 0.673913 | 1521.1 | |
| pubchem | CHEMBL84 | | 0.834061 | 1521.1 | * |
| cdk_maccs | CHEMBL84 | | 0.851852 | 1521.1 | * |
| klekota_roth | CHEMBL84 | | 0.586420 | 1521.1 | |

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    *** ic50 ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 8007.669
    ["TT_bits", "cdk_maccs", "Pattern", "AP_bits", "pubchem", "FP2",
    "RDKit7", "hybridization"]

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5 rank

ATP-binding cassette sub-family G member 2 : Homo sapiens

score: 6.008 on ChEMBL5393 based on 8 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL837 | | 0.500000 | 176.0 | |
| MFP1 | CHEMBL84 | | 0.500000 | 170.0 | |
| RDKit7 | CHEMBL84 | | 0.911797 | 170.0 | * |
| Pattern | CHEMBL84 | | 0.847893 | 170.0 | * |
| AP_bits | CHEMBL2013174 | | 0.484689 | 1400.0 | * |
| TT_bits | CHEMBL84 | | 0.517857 | 170.0 | * |
| FP2 | CHEMBL84 | | 0.784722 | 170.0 | * |
| hybridization | CHEMBL837 | | 0.775510 | 176.0 | * |
| substructure | CHEMBL551696 | | 0.633333 | 9100.0 | |
| graph | CHEMBL84 | | 0.673913 | 170.0 | |
| pubchem | CHEMBL84 | | 0.834061 | 170.0 | * |
| cdk_maccs | CHEMBL84 | | 0.851852 | 170.0 | * |
| klekota_roth | CHEMBL84 | | 0.586420 | 170.0 | |

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    *** ic50 ACTIVITY *** value prediction
    based on 8 locally validated fgps ---> 272.749
    ["TT_bits", "cdk_maccs", "Pattern", "AP_bits", "pubchem", "FP2",
    "RDKit7", "hybridization"]

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6 rank

Alpha trans-inducing protein (VP16) : Herpes simplex virus (type 1 / strain 17)

score: 5.540 on ChEMBL4218 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL1566908 | | 0.675676 | 18440.0 | |
| MFP1 | CHEMBL1200512 | | 0.470588 | 41996.0 | |
| RDKit7 | CHEMBL1200512 | | 0.897051 | 41996.0 | * |
| Pattern | CHEMBL1200512 | | 0.901508 | 41996.0 | * |
| AP_bits | CHEMBL1200512 | | 0.520408 | 41996.0 | * |

| | | | | |
|---------------|---------------|----------|---------|---|
| TT_bits | CHEMBL1200512 | 0.404255 | 41996.0 | |
| FP2 | CHEMBL1200512 | 0.762215 | 41996.0 | * |
| hybridization | CHEMBL1200512 | 0.760274 | 41996.0 | * |
| substructure | CHEMBL1566908 | 0.714286 | 18440.0 | |
| graph | CHEMBL1200512 | 0.742489 | 41996.0 | |
| pubchem | CHEMBL1200512 | 0.841202 | 41996.0 | * |
| cdk_maccs | CHEMBL1200512 | 0.857143 | 41996.0 | * |
| klekota_roth | CHEMBL1200512 | 0.540541 | 41996.0 | |

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 37322.814
 ["cdk_maccs", "Pattern", "AP_bits", "pubchem", "FP2", "RDKit7",
 "hybridization"]

7 rank

Solute carrier family 22 member 2 : Homo sapiens

score: 5.522 on ChEMBL1743122 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|-----------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL84 | 0.465116 | 61000.0 | |
| MFP1 | CHEMBL84 | 0.500000 | 61000.0 | |
| RDKit7 | CHEMBL84 | 0.911797 | 61000.0 | * |
| Pattern | CHEMBL84 | 0.847893 | 61000.0 | * |
| AP_bits | CHEMBL603 | 0.467254 | 9700.0 | |
| TT_bits | CHEMBL84 | 0.517857 | 61000.0 | * |
| FP2 | CHEMBL84 | 0.784722 | 61000.0 | * |
| hybridization | CHEMBL84 | 0.774052 | 61000.0 | * |
| substructure | CHEMBL85 | 0.545455 | 11000.0 | |
| graph | CHEMBL84 | 0.673913 | 61000.0 | |
| pubchem | CHEMBL84 | 0.834061 | 61000.0 | * |
| cdk_maccs | CHEMBL84 | 0.851852 | 61000.0 | * |
| klekota_roth | CHEMBL84 | 0.586420 | 61000.0 | |

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 60280.389
 ["TT_bits", "cdk_maccs", "Pattern", "pubchem", "FP2", "RDKit7",
 "hybridization"]

8 rank

Multidrug and toxin extrusion protein 1 : Homo sapiens

score: 5.522 on ChEMBL1743126 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL84 | 0.465116 | 1300.0 | |
| MFP1 | CHEMBL84 | 0.500000 | 1300.0 | |
| RDKit7 | CHEMBL84 | 0.911797 | 1300.0 | * |
| Pattern | CHEMBL84 | 0.847893 | 1300.0 | * |
| AP_bits | CHEMBL603 | 0.467254 | 1300.0 | |
| TT_bits | CHEMBL84 | 0.517857 | 1300.0 | * |
| FP2 | CHEMBL84 | 0.784722 | 1300.0 | * |
| hybridization | CHEMBL84 | 0.774052 | 1300.0 | * |
| substructure | CHEMBL1017 | 0.642857 | 17900.0 | |
| graph | CHEMBL84 | 0.673913 | 1300.0 | |
| pubchem | CHEMBL84 | 0.834061 | 1300.0 | * |
| cdk_maccs | CHEMBL84 | 0.851852 | 1300.0 | * |
| klekota_roth | CHEMBL84 | 0.586420 | 1300.0 | |

*** ic50 ACTIVITY *** value prediction
 based on 7 locally validated fgps ---> 1397.245
 ["TT_bits", "cdk_maccs", "Pattern", "pubchem", "FP2", "RDKit7",
 "hybridization"]

9 rank

Multidrug and toxin extrusion protein 2 : Homo sapiens

score: 5.522 on ChEMBL1743127 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid | fg |
|------------------|-----------|----------|------------|----------|-------|----|
| FeatMFP1 | CHEMBL84 | | 0.465116 | 8600.0 | | |
| MFP1 | CHEMBL84 | | 0.500000 | 8600.0 | | |
| RDKit7 | CHEMBL84 | | 0.911797 | 8600.0 | * | |
| Pattern | CHEMBL84 | | 0.847893 | 8600.0 | * | |
| AP_bits | CHEMBL603 | | 0.467254 | 7600.0 | | |
| TT_bits | CHEMBL84 | | 0.517857 | 8600.0 | * | |
| FP2 | CHEMBL84 | | 0.784722 | 8600.0 | * | |
| hybridization | CHEMBL84 | | 0.774052 | 8600.0 | * | |
| substructure | CHEMBL46 | | 0.533333 | 160.0 | | |
| graph | CHEMBL84 | | 0.673913 | 8600.0 | | |
| pubchem | CHEMBL84 | | 0.834061 | 8600.0 | * | |
| cdk_maccs | CHEMBL84 | | 0.851852 | 8600.0 | * | |
| klekota_roth | CHEMBL84 | | 0.586420 | 8600.0 | | |

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 8859.319

["TT_bits", "cdk_maccs", "Pattern", "pubchem", "FP2", "RDKit7",
"hybridization"]

10 rank

Hypoxia-inducible factor 1 alpha : Homo sapiens

score: 5.522 on ChEMBL4261 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid | fg |
|------------------|--------------|----------|------------|----------|-------|----|
| FeatMFP1 | CHEMBL84 | | 0.465116 | 60.0 | | |
| MFP1 | CHEMBL84 | | 0.500000 | 60.0 | | |
| RDKit7 | CHEMBL84 | | 0.911797 | 60.0 | * | |
| Pattern | CHEMBL84 | | 0.847893 | 60.0 | * | |
| AP_bits | CHEMBL383824 | | 0.455711 | 57.0 | | |
| TT_bits | CHEMBL84 | | 0.517857 | 60.0 | * | |
| FP2 | CHEMBL84 | | 0.784722 | 60.0 | * | |
| hybridization | CHEMBL84 | | 0.774052 | 60.0 | * | |
| substructure | CHEMBL430393 | | 0.655172 | 800.0 | | |
| graph | CHEMBL84 | | 0.673913 | 60.0 | | |
| pubchem | CHEMBL84 | | 0.834061 | 60.0 | * | |
| cdk_maccs | CHEMBL84 | | 0.851852 | 60.0 | * | |
| klekota_roth | CHEMBL84 | | 0.586420 | 60.0 | | |

*** ic50 ACTIVITY *** value prediction

based on 7 locally validated fgps ---> 105.797

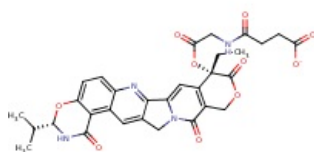
["TT_bits", "cdk_maccs", "Pattern", "pubchem", "FP2", "RDKit7",
"hybridization"]

SwissTargetPrediction report:

Reference:

Gfeller D., Michielin O. & Zoete V.
Shaping the interaction landscape of
bioactive molecules, *Bioinformatics*
(2013) 29:3073-3079.

Query Molecule



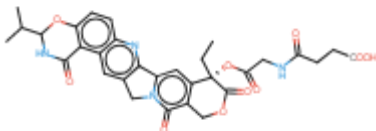
Frequency of Target Class

| Target | Uniprot ID | Gene code | ChEMBL ID | Probability | # sim. cmpds (3D / 2D) | Target Class |
|---|---------------|-------------|---------------|------------------------|------------------------|-------------------|
| 22 kDa interstitial collagenase | P03956 | MMP1 | CHEMBL332 | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Stromelysin-1 (<i>by homology</i>) | P08254 | MMP3 | CHEMBL283 | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Collagenase 3 | P45452 | MMP13 | CHEMBL280 | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Stromelysin-2 (<i>by homology</i>) | P09238 | MMP10 | CHEMBL4270 | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Macrophage metalloelastase (<i>by homology</i>) | P39900 | MMP12 | CHEMBL4393 | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Matrix metalloproteinase-27 (<i>by homology</i>) | Q9H306 | MMP27 | | <div><div></div></div> | 34 / 1 | Metallo Protease |
| Neutrophil collagenase | P22894 | MMP8 | CHEMBL4588 | <div><div></div></div> | 5 / 1 | Metallo Protease |
| Complex | P06756/P05106 | ITGAV/ITGB3 | CHEMBL1907598 | <div><div></div></div> | 44 / 3 | Membrane receptor |
| Complex | P06756/P18084 | ITGAV/ITGB5 | CHEMBL2096675 | <div><div></div></div> | 6 / 3 | Membrane receptor |
| Muscleblind-like protein 1 | Q9NR56 | MBNL1 | CHEMBL1293317 | <div><div></div></div> | 5 / 3 | Unclassified |
| Muscleblind-like protein 2 (<i>by homology</i>) | Q5VZF2 | MBNL2 | | <div><div></div></div> | 5 / 3 | Unclassified |
| Muscleblind-like protein 3 (<i>by homology</i>) | Q9NUK0 | MBNL3 | | <div><div></div></div> | 5 / 3 | Unclassified |
| DNA topoisomerase 1 | P11387 | TOP1 | CHEMBL1781 | <div><div></div></div> | 0 / 160 | Enzyme |
| DNA topoisomerase I, mitochondrial (<i>by homology</i>) | Q969P6 | TOP1MT | | <div><div></div></div> | 0 / 160 | Enzyme |
| Cytochrome P450 3A4 | P08684 | CYP3A4 | CHEMBL340 | <div><div></div></div> | 0 / 1 | Enzyme |

Polypharmacology Browser 2 Prediction:

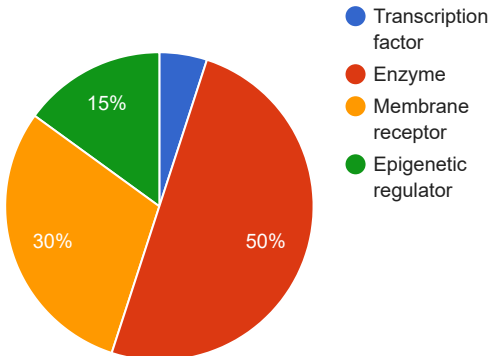
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



| Rank | ChEMBL ID | Common name | Nearest neighbours |
|------|--|--|--------------------|
| 1 | CHEMBL1781 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1781) | DNA topoisomerase I | Show NN |
| 2 | CHEMBL325 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325) | Histone deacetylase 1 | Show NN |
| 3 | CHEMBL1865 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1865) | Histone deacetylase 6 | Show NN |
| 4 | CHEMBL3192 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3192) | Histone deacetylase 8 | Show NN |
| 5 | CHEMBL1945 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1945) | Melatonin receptor 1A | Show NN |
| 6 | CHEMBL2334 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2334) | Caspase-3 | Show NN |
| 7 | CHEMBL1946 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1946) | Melatonin receptor 1B | Show NN |
| 8 | CHEMBL1835 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1835) | Thromboxane-A synthase | Show NN |
| 9 | CHEMBL217 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL217) | Dopamine D2 receptor | Show NN |
| 10 | CHEMBL2069 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2069) | Thromboxane A2 receptor | Show NN |
| 11 | CHEMBL4829 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4829) | Acetyl-CoA carboxylase 2 | Show NN |
| 12 | CHEMBL3892 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3892) | Sphingosine 1-phosphate receptor Edg-3 | Show NN |
| 13 | CHEMBL220 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL220) | Acetylcholinesterase | Show NN |
| 14 | CHEMBL204 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL204) | Thrombin | Show NN |
| 15 | CHEMBL3105 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3105) | Poly [ADP-ribose] polymerase-1 | Show NN |
| 16 | CHEMBL244 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL244) | Coagulation factor X | Show NN |
| 17 | CHEMBL259 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL259) | Melanocortin receptor 4 | Show NN |
| 18 | CHEMBL4801 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4801) | Caspase-1 | Show NN |

| | | | |
|----|---|--|---------|
| 19 | CHEMBL248 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL248) | Leukocyte elastase | Show NN |
| 20 | CHEMBL235 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL235) | Peroxisome proliferator-activated receptor gamma | Show NN |