

MuSSEL Prediction k_i:

1 rank

Thrombin : Homo sapiens

score: 7.800 on ChEMBL204 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | ChEMBL179210 | 0.766667 | 1.10 | * |
| MFP1 | ChEMBL164138 | 0.666667 | 12300.00 | * |
| RDKit7 | ChEMBL366882 | 0.824427 | 3.10 | * |
| Pattern | ChEMBL366882 | 0.921348 | 3.10 | * |
| AP_bits | ChEMBL366882 | 0.620787 | 3.10 | * |
| TT_bits | ChEMBL366882 | 0.594059 | 3.10 | * |
| FP2 | ChEMBL366882 | 0.826667 | 3.10 | * |
| hybridization | ChEMBL403735 | 0.773616 | 1.10 | * |
| substructure | ChEMBL164138 | 0.913043 | 12300.00 | * |
| graph | ChEMBL319615 | 0.762658 | 5300.00 | |
| pubchem | ChEMBL366882 | 0.892523 | 3.10 | * |
| cdk_maccs | ChEMBL322307 | 0.813333 | 50.00 | |
| klekota_roth | ChEMBL282830 | 0.596639 | 0.65 | |

*** ki ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 1850.557

["TT_bits", "substructure", "Pattern", "FP2", "MFP1", "pubchem",
"AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

2 rank

Trypsin I : Bos taurus

score: 7.782 on ChEMBL3769 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | ChEMBL179210 | 0.766667 | 22.0 | * |
| MFP1 | ChEMBL360684 | 0.666667 | 30.0 | * |
| RDKit7 | ChEMBL366882 | 0.824427 | 2.0 | * |
| Pattern | ChEMBL366882 | 0.921348 | 2.0 | * |
| AP_bits | ChEMBL366882 | 0.620787 | 2.0 | * |
| TT_bits | ChEMBL366882 | 0.594059 | 2.0 | * |
| FP2 | ChEMBL366882 | 0.826667 | 2.0 | * |
| hybridization | ChEMBL366882 | 0.756058 | 2.0 | * |
| substructure | ChEMBL360684 | 0.913043 | 30.0 | * |
| graph | ChEMBL257898 | 0.760714 | 16.0 | |
| pubchem | ChEMBL366882 | 0.892523 | 2.0 | * |
| cdk_maccs | ChEMBL368894 | 0.805556 | 22.0 | |
| klekota_roth | ChEMBL180219 | 0.636364 | 250.0 | |

*** ki ACTIVITY *** value prediction

based on 10 locally validated fgps ---> 75.164

["TT_bits", "substructure", "Pattern", "FP2", "MFP1", "pubchem",
"AP_bits", "FeatMFP1", "RDKit7", "hybridization"]

3 rank

Serine protease hepsin : Homo sapiens

score: 3.655 on ChEMBL2079849 based on 5 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|---------------|---------------------|----------|----------|
| FeatMFP1 | ChEMBL3746517 | 0.700000 | 2.91 | |
| MFP1 | ChEMBL3746517 | 0.652174 | 2.91 | * |
| RDKit7 | ChEMBL3746517 | 0.727202 | 2.91 | |
| Pattern | ChEMBL3402437 | 0.709635 | 3500.00 | |
| AP_bits | ChEMBL3402438 | 0.538776 | 2600.00 | * |
| TT_bits | ChEMBL3746517 | 0.537500 | 2.91 | |
| FP2 | ChEMBL3746517 | 0.740385 | 2.91 | * |
| hybridization | ChEMBL3746517 | 0.807207 | 2.91 | * |
| substructure | ChEMBL3747468 | 0.916667 | 2.88 | * |
| graph | ChEMBL3746517 | 0.773438 | 2.91 | |
| pubchem | ChEMBL3746517 | 0.805000 | 2.91 | |
| cdk_maccs | ChEMBL3746517 | 0.746479 | 2.91 | |

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klekota_roth CHEMBL3746517          0.605042      2.91
*** ki ACTIVITY *** value prediction
based on 5 locally validated fgps ---> 522.183
["AP_bits", "hybridization", "MFP1", "substructure", "FP2"]

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4 rank

Trypsin I : Homo sapiens

score: 3.610 on ChEMBL209 based on 5 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL164138 | | 0.724138 | 30.0 | |
| MFP1 | CHEMBL164138 | | 0.666667 | 30.0 | * |
| RDKit7 | CHEMBL341148 | | 0.716385 | 160.0 | |
| Pattern | CHEMBL332716 | | 0.808140 | 4000.0 | |
| AP_bits | CHEMBL311198 | | 0.568460 | 13.5 | * |
| TT_bits | CHEMBL164138 | | 0.481481 | 30.0 | |
| FP2 | CHEMBL341148 | | 0.710407 | 160.0 | * |
| hybridization | CHEMBL164138 | | 0.751351 | 30.0 | * |
| substructure | CHEMBL164138 | | 0.913043 | 30.0 | * |
| graph | CHEMBL339703 | | 0.778210 | 53.0 | |
| pubchem | CHEMBL341148 | | 0.831683 | 160.0 | |
| cdk_maccs | CHEMBL340098 | | 0.808824 | 260.0 | |
| klekota_roth | CHEMBL164138 | | 0.572650 | 30.0 | |

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 52.604

["AP_bits", "hybridization", "MFP1", "substructure", "FP2"]

5 rank

Matriptase : Homo sapiens

score: 3.560 on ChEMBL3018 based on 5 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL2089124 | | 0.700000 | 1.4 | |
| MFP1 | CHEMBL2089124 | | 0.666667 | 1.4 | * |
| RDKit7 | CHEMBL2089124 | | 0.699449 | 1.4 | |
| Pattern | CHEMBL2089121 | | 0.765926 | 6124.0 | |
| AP_bits | CHEMBL3402438 | | 0.538776 | 6700.0 | * |
| TT_bits | CHEMBL2089124 | | 0.487179 | 1.4 | |
| FP2 | CHEMBL2089124 | | 0.725962 | 1.4 | * |
| hybridization | CHEMBL2089124 | | 0.777982 | 1.4 | * |
| substructure | CHEMBL2089124 | | 0.740741 | 1.4 | |
| graph | CHEMBL2089121 | | 0.750929 | 6124.0 | |
| pubchem | CHEMBL2089124 | | 0.785000 | 1.4 | |
| cdk_maccs | CHEMBL2089121 | | 0.850746 | 6124.0 | * |
| klekota_roth | CHEMBL2089124 | | 0.620370 | 1.4 | |

*** ki ACTIVITY *** value prediction

based on 5 locally validated fgps ---> 1947.147

["AP_bits", "hybridization", "MFP1", "cdk_maccs", "FP2"]

6 rank

Tryptase beta-1 : Homo sapiens

score: 3.021 on ChEMBL2617 based on 4 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL340547 | | 0.724138 | 88.0 | |
| MFP1 | CHEMBL340547 | | 0.666667 | 88.0 | * |
| RDKit7 | CHEMBL341148 | | 0.716385 | 250.0 | |
| Pattern | CHEMBL311936 | | 0.742029 | 6900.0 | |
| AP_bits | CHEMBL211638 | | 0.502558 | 11.0 | |
| TT_bits | CHEMBL340547 | | 0.481481 | 88.0 | |
| FP2 | CHEMBL341148 | | 0.710407 | 250.0 | * |
| hybridization | CHEMBL421643 | | 0.730634 | 41.0 | * |
| substructure | CHEMBL340547 | | 0.913043 | 88.0 | * |

| | | | |
|--------------|--------------|----------|-------|
| graph | CHEMBL339703 | 0.778210 | 20.0 |
| pubchem | CHEMBL341148 | 0.831683 | 250.0 |
| cdk_maccs | CHEMBL340098 | 0.808824 | 470.0 |
| klekota_roth | CHEMBL340547 | 0.572650 | 88.0 |

*** ki ACTIVITY *** value prediction

based on 4 locally validated fgps ---> 156.257

["hybridization", "MFp1", "substructure", "FP2"]

MuSSEL Prediction IC₅₀:

1 rank

Metacaspase : Trypanosoma brucei

score: 9.500 on ChEMBL1075193 based on 12 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL1077318 | | 0.793103 | 600.0 | * |
| MFP1 | ChEMBL1077318 | | 0.761905 | 600.0 | * |
| RDKit7 | ChEMBL1082043 | | 0.770912 | 1100.0 | * |
| Pattern | ChEMBL1082042 | | 0.750000 | 1400.0 | |
| AP_bits | ChEMBL1082042 | | 0.655864 | 1400.0 | * |
| TT_bits | ChEMBL1082042 | | 0.558140 | 1400.0 | * |
| FP2 | ChEMBL1082043 | | 0.792627 | 1100.0 | * |
| hybridization | ChEMBL1082043 | | 0.831858 | 1100.0 | * |
| substructure | ChEMBL1082042 | | 0.916667 | 1400.0 | * |
| graph | ChEMBL1082042 | | 0.928571 | 1400.0 | * |
| pubchem | ChEMBL1082042 | | 0.879227 | 1400.0 | * |
| cdk_maccs | ChEMBL1082043 | | 0.897059 | 1100.0 | * |
| klekota_roth | ChEMBL1082042 | | 0.714286 | 1400.0 | * |

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 1425.881

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

2 rank

Thrombin : Homo sapiens

score: 9.227 on ChEMBL204 based on 12 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL179210 | | 0.766667 | 11.0 | * |
| MFP1 | ChEMBL360684 | | 0.666667 | 82000.0 | * |
| RDKit7 | ChEMBL366882 | | 0.824427 | 95.0 | * |
| Pattern | ChEMBL366882 | | 0.921348 | 95.0 | * |
| AP_bits | ChEMBL407142 | | 0.652231 | 11200.0 | * |
| TT_bits | ChEMBL366882 | | 0.594059 | 95.0 | * |
| FP2 | ChEMBL366882 | | 0.826667 | 95.0 | * |
| hybridization | ChEMBL366882 | | 0.756058 | 95.0 | * |
| substructure | ChEMBL360684 | | 0.913043 | 82000.0 | * |
| graph | ChEMBL257898 | | 0.760714 | 56.0 | |
| pubchem | ChEMBL366882 | | 0.892523 | 95.0 | * |
| cdk_maccs | ChEMBL368894 | | 0.805556 | 29.0 | * |
| klekota_roth | ChEMBL289477 | | 0.607692 | 42000.0 | * |

*** ic50 ACTIVITY *** value prediction

based on 12 locally validated fgps ---> 11129.924

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

3 rank

Coagulation factor VII : Homo sapiens

score: 7.307 on ChEMBL3991 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|---------------|----------|------------|----------|----------|
| FeatMFP1 | ChEMBL282830 | | 0.718750 | 270.0 | * |
| MFP1 | ChEMBL1797527 | | 0.555556 | 16000.0 | * |
| RDKit7 | ChEMBL27852 | | 0.705432 | 200.0 | * |
| Pattern | ChEMBL27852 | | 0.847059 | 200.0 | * |
| AP_bits | ChEMBL407142 | | 0.652231 | 17800.0 | * |
| TT_bits | ChEMBL27852 | | 0.386792 | 200.0 | |
| FP2 | ChEMBL27852 | | 0.729730 | 200.0 | * |
| hybridization | ChEMBL27852 | | 0.736089 | 200.0 | * |
| substructure | ChEMBL339956 | | 0.875000 | 3300.0 | * |
| graph | ChEMBL27852 | | 0.727941 | 200.0 | |

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        pubchem    CHEMBL282830          0.830918      270.0      *
        cdk_maccs  CHEMBL1797527        0.746269     16000.0
        klekota_roth CHEMBL1797527      0.655738     16000.0      *
*** ic50 ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 3142.794
["substructure", "Pattern", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"FP2", "FeatMFP1", "RDKit7", "hybridization"]

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4 rank

Coagulation factor X : Homo sapiens

score: 7.273 on CHEMBL244 based on 10 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL282830 | | 0.718750 | 270.0 | * |
| MFP1 | CHEMBL27852 | | 0.545455 | 19.3 | * |
| RDKit7 | CHEMBL27852 | | 0.705432 | 19.3 | * |
| Pattern | CHEMBL27852 | | 0.847059 | 19.3 | * |
| AP_bits | CHEMBL407142 | | 0.652231 | 3140.0 | * |
| TT_bits | CHEMBL27852 | | 0.386792 | 19.3 | |
| FP2 | CHEMBL27852 | | 0.729730 | 19.3 | * |
| hybridization | CHEMBL27852 | | 0.736089 | 19.3 | * |
| substructure | CHEMBL339956 | | 0.875000 | 2700.0 | * |
| graph | CHEMBL27852 | | 0.727941 | 19.3 | |
| pubchem | CHEMBL282830 | | 0.830918 | 270.0 | * |
| cdk_maccs | CHEMBL191264 | | 0.792208 | 14300.0 | |
| klekota_roth | CHEMBL41722 | | 0.632812 | 11000.0 | * |

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*** ic50 ACTIVITY *** value prediction
    based on 10 locally validated fgps ---> 1156.327
["substructure", "Pattern", "AP_bits", "MFP1", "klekota_roth", "pubchem",
"FP2", "FeatMFP1", "RDKit7", "hybridization"]

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5 rank

Trypsin I : Homo sapiens

score: 6.579 on CHEMBL209 based on 9 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL352928 | | 0.709677 | 1.0 | * |
| MFP1 | CHEMBL352928 | | 0.545455 | 1.0 | * |
| RDKit7 | CHEMBL352928 | | 0.724138 | 1.0 | * |
| Pattern | CHEMBL352928 | | 0.870398 | 1.0 | * |
| AP_bits | CHEMBL79245 | | 0.581098 | 11000.0 | * |
| TT_bits | CHEMBL352928 | | 0.362832 | 1.0 | |
| FP2 | CHEMBL352928 | | 0.735160 | 1.0 | * |
| hybridization | CHEMBL83001 | | 0.701183 | 3700.0 | * |
| substructure | CHEMBL116297 | | 0.875000 | 31600.0 | * |
| graph | CHEMBL352928 | | 0.709790 | 1.0 | |
| pubchem | CHEMBL83001 | | 0.836538 | 3700.0 | * |
| cdk_maccs | CHEMBL169291 | | 0.760000 | 2.0 | |
| klekota_roth | CHEMBL163543 | | 0.583942 | 115.0 | |

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*** ic50 ACTIVITY *** value prediction
    based on 9 locally validated fgps ---> 3323.134
["substructure", "Pattern", "AP_bits", "MFP1", "pubchem", "FP2",
"FeatMFP1", "RDKit7", "hybridization"]

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6 rank

Tissue-type plasminogen activator : Homo sapiens

score: 6.267 on CHEMBL1873 based on 9 fingerprints

| Fingerprint type | Ligand | Tanimoto | Similarity | activity | Valid fg |
|------------------|--------------|----------|------------|----------|----------|
| FeatMFP1 | CHEMBL282830 | | 0.718750 | 495.0 | * |
| MFP1 | CHEMBL27852 | | 0.545455 | 93.0 | * |
| RDKit7 | CHEMBL27852 | | 0.705432 | 93.0 | * |
| Pattern | CHEMBL27852 | | 0.847059 | 93.0 | * |

| | | | | |
|---------------|--------------|----------|--------|---|
| AP_bits | CHEMBL27852 | 0.556497 | 93.0 | * |
| TT_bits | CHEMBL27852 | 0.386792 | 93.0 | |
| FP2 | CHEMBL27852 | 0.729730 | 93.0 | * |
| hybridization | CHEMBL27852 | 0.736089 | 93.0 | * |
| substructure | CHEMBL162461 | 0.833333 | 4010.0 | |
| graph | CHEMBL27852 | 0.727941 | 93.0 | |
| pubchem | CHEMBL282830 | 0.830918 | 495.0 | * |
| cdk_maccs | CHEMBL27852 | 0.716216 | 93.0 | |
| klekota_roth | CHEMBL282830 | 0.596639 | 495.0 | * |

*** ic50 ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 317.917
 ["Pattern", "AP_bits", "MFP1", "klekota_roth", "pubchem", "FP2",
 "FeatMFP1", "RDKit7", "hybridization"]

7 rank

Plasminogen : Rattus norvegicus

score: 6.267 on ChEMBL3204 based on 9 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL282830 | 0.718750 | 415.0 | * |
| MFP1 | CHEMBL27852 | 0.545455 | 251.0 | * |
| RDKit7 | CHEMBL27852 | 0.705432 | 251.0 | * |
| Pattern | CHEMBL27852 | 0.847059 | 251.0 | * |
| AP_bits | CHEMBL436851 | 0.556978 | 1320.0 | * |
| TT_bits | CHEMBL27852 | 0.386792 | 251.0 | |
| FP2 | CHEMBL27852 | 0.729730 | 251.0 | * |
| hybridization | CHEMBL27852 | 0.736089 | 251.0 | * |
| substructure | CHEMBL27852 | 0.740741 | 251.0 | |
| graph | CHEMBL27852 | 0.727941 | 251.0 | |
| pubchem | CHEMBL282830 | 0.830918 | 415.0 | * |
| cdk_maccs | CHEMBL27852 | 0.716216 | 251.0 | |
| klekota_roth | CHEMBL282830 | 0.596639 | 415.0 | * |

*** ic50 ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 400.797
 ["Pattern", "AP_bits", "MFP1", "klekota_roth", "pubchem", "FP2",
 "FeatMFP1", "RDKit7", "hybridization"]

8 rank

Urokinase-type plasminogen activator : Homo sapiens

score: 6.267 on ChEMBL3286 based on 9 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL282830 | 0.718750 | 600.0 | * |
| MFP1 | CHEMBL27852 | 0.545455 | 335.0 | * |
| RDKit7 | CHEMBL27852 | 0.705432 | 335.0 | * |
| Pattern | CHEMBL27852 | 0.847059 | 335.0 | * |
| AP_bits | CHEMBL27852 | 0.556497 | 335.0 | * |
| TT_bits | CHEMBL27852 | 0.386792 | 335.0 | |
| FP2 | CHEMBL27852 | 0.729730 | 335.0 | * |
| hybridization | CHEMBL27852 | 0.736089 | 335.0 | * |
| substructure | CHEMBL27852 | 0.740741 | 335.0 | |
| graph | CHEMBL27852 | 0.727941 | 335.0 | |
| pubchem | CHEMBL282830 | 0.830918 | 600.0 | * |
| cdk_maccs | CHEMBL27852 | 0.716216 | 335.0 | |
| klekota_roth | CHEMBL282830 | 0.596639 | 600.0 | * |

*** ic50 ACTIVITY *** value prediction
 based on 9 locally validated fgps ---> 495.620
 ["Pattern", "AP_bits", "MFP1", "klekota_roth", "pubchem", "FP2",
 "FeatMFP1", "RDKit7", "hybridization"]

9 rank

Trypsin I : Bos taurus

score: 5.746 on ChEMBL3769 based on 8 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL176329 | 0.709677 | 5.8 | * |
| MFP1 | CHEMBL176329 | 0.545455 | 5.8 | * |
| RDKit7 | CHEMBL176329 | 0.730906 | 5.8 | * |
| Pattern | CHEMBL176385 | 0.860947 | 352.0 | * |
| AP_bits | CHEMBL176329 | 0.626628 | 5.8 | * |
| TT_bits | CHEMBL176329 | 0.450000 | 5.8 | |
| FP2 | CHEMBL176329 | 0.715556 | 5.8 | * |
| hybridization | CHEMBL176329 | 0.722222 | 5.8 | * |
| substructure | CHEMBL150497 | 0.833333 | 230.0 | |
| graph | CHEMBL176016 | 0.703971 | 32000.0 | |
| pubchem | CHEMBL176385 | 0.834951 | 352.0 | * |
| cdk_maccs | CHEMBL176329 | 0.763889 | 5.8 | |
| klekota_roth | CHEMBL176329 | 0.549618 | 5.8 | |

*** ic50 ACTIVITY *** value prediction
based on 8 locally validated fgps ---> 148.231
["Pattern", "AP_bits", "MFP1", "pubchem", "FP2", "FeatMFP1", "RDKit7", "hybridization"]

10 rank

Lysosomal Pro-X carboxypeptidase : Homo sapiens

score: 5.605 on ChEMBL2335 based on 8 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|---------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL1256273 | 0.542857 | 850.0 | |
| MFP1 | CHEMBL1256277 | 0.454545 | 240.0 | |
| RDKit7 | CHEMBL1259114 | 0.742291 | 300.0 | * |
| Pattern | CHEMBL1256278 | 0.866856 | 570.0 | * |
| AP_bits | CHEMBL1256278 | 0.600291 | 570.0 | * |
| TT_bits | CHEMBL1259131 | 0.509804 | 5000.0 | * |
| FP2 | CHEMBL1259114 | 0.753555 | 300.0 | * |
| hybridization | CHEMBL1259114 | 0.743760 | 300.0 | * |
| substructure | CHEMBL1256277 | 0.640000 | 240.0 | |
| graph | CHEMBL1259114 | 0.773946 | 300.0 | * |
| pubchem | CHEMBL1259175 | 0.799107 | 4370.0 | |
| cdk_maccs | CHEMBL1256277 | 0.684932 | 240.0 | |
| klekota_roth | CHEMBL1256277 | 0.614815 | 240.0 | * |

*** ic50 ACTIVITY *** value prediction

based on 8 locally validated fgps ---> 2054.221

["TT_bits", "Pattern", "AP_bits", "klekota_roth", "graph", "FP2", "RDKit7", "hybridization"]

11 rank

Tryptase beta-1 : Homo sapiens

score: 4.476 on ChEMBL2617 based on 7 fingerprints

| Fingerprint type | Ligand | Tanimoto Similarity | activity | Valid fg |
|------------------|--------------|---------------------|----------|----------|
| FeatMFP1 | CHEMBL178315 | 0.656250 | 9090.0 | |
| MFP1 | CHEMBL178315 | 0.576923 | 9090.0 | * |
| RDKit7 | CHEMBL127185 | 0.705224 | 2.0 | * |
| Pattern | CHEMBL178315 | 0.809651 | 9090.0 | |
| AP_bits | CHEMBL361835 | 0.500597 | 12400.0 | * |
| TT_bits | CHEMBL178315 | 0.544554 | 9090.0 | * |
| FP2 | CHEMBL127185 | 0.675926 | 2.0 | * |
| hybridization | CHEMBL127185 | 0.708819 | 2.0 | * |
| substructure | CHEMBL127185 | 0.800000 | 2.0 | |
| graph | CHEMBL127185 | 0.752852 | 2.0 | |
| pubchem | CHEMBL127185 | 0.754902 | 2.0 | |
| cdk_maccs | CHEMBL178315 | 0.783784 | 9090.0 | |
| klekota_roth | CHEMBL178315 | 0.763780 | 9090.0 | * |

*** ic50 ACTIVITY *** value prediction

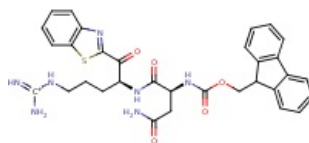
based on 7 locally validated fgps ---> 4628.473
["TT_bits", "AP_bits", "MFP1", "klekota_roth", "FP2", "RDKit7",
"hybridization"]

SwissTargetPrediction report:

Reference:

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

Query Molecule



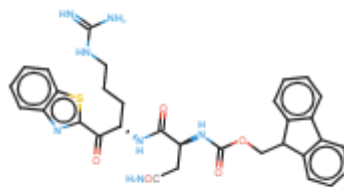
Frequency of Target Class

| Target | Uniprot ID | Gene code | ChEMBL ID | Probability | # sim. cmpds (3D / 2D) | Target Class |
|---|------------|-----------|---------------|------------------------|------------------------|-----------------|
| Activation peptide fragment 1 | P00734 | F2 | CHEMBL204 | <div><div></div></div> | 1464 / 332 | Serine Protease |
| Alpha-trypsin chain 1 (<i>by homology</i>) | P07477 | PRSS1 | CHEMBL209 | <div><div></div></div> | 622 / 132 | Serine Protease |
| Trypsin-3 (<i>by homology</i>) | P35030 | PRSS3 | CHEMBL4551 | <div><div></div></div> | 622 / 132 | Serine Protease |
| Trypsin-2 (<i>by homology</i>) | P07478 | PRSS2 | CHEMBL3159 | <div><div></div></div> | 622 / 132 | Serine Protease |
| Coagulation factor IXa heavy chain (<i>by homology</i>) | P00740 | F9 | CHEMBL2016 | <div><div></div></div> | 1257 / 152 | Serine Protease |
| Factor X light chain | P00742 | F10 | CHEMBL244 | <div><div></div></div> | 1257 / 152 | Serine Protease |
| Coagulation factor VII | P08709 | F7 | CHEMBL3991 | <div><div></div></div> | 1241 / 152 | Serine Protease |
| Plasmin light chain B | P00747 | PLG | CHEMBL1801 | <div><div></div></div> | 268 / 8 | Serine Protease |
| Apolipoprotein(a) (<i>by homology</i>) | P08519 | LPA | | <div><div></div></div> | 268 / 8 | Serine Protease |
| Transmembrane protease serine 11D non-catalytic chain | O60235 | TMPRSS11D | CHEMBL1795138 | <div><div></div></div> | 33 / 1 | Enzyme |
| Transmembrane protease serine 11A (<i>by homology</i>) | Q6ZMR5 | TMPRSS11A | | <div><div></div></div> | 33 / 1 | Enzyme |
| Transmembrane protease serine 11F (<i>by homology</i>) | Q6ZWK6 | TMPRSS11F | | <div><div></div></div> | 33 / 1 | Enzyme |
| Transmembrane protease serine 11B (<i>by homology</i>) | Q86T26 | TMPRSS11B | | <div><div></div></div> | 33 / 1 | Enzyme |
| Transmembrane protease serine 11E (<i>by homology</i>) | Q9UL52 | TMPRSS11E | | <div><div></div></div> | 33 / 1 | Enzyme |
| Urokinase-type plasminogen activator long chain A | P00749 | PLAU | CHEMBL3286 | <div><div></div></div> | 181 / 2 | Serine Protease |

Polypharmacology Browser 2 Prediction:

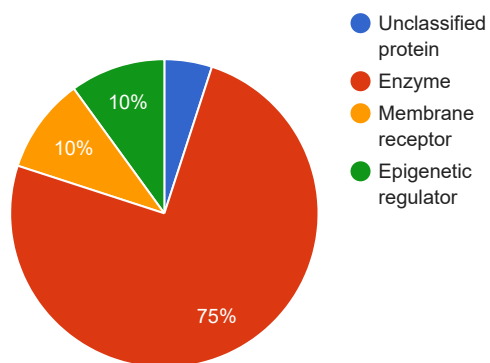
Targets predicted using NN(ECfp4) + NB(ECfp4).

Save Table



Query molecule

Target class overview



| Rank | ChEMBL ID | Common name | Nearest neighbours |
|------|---|--------------------------------------|--------------------|
| 1 | CHEMBL3018 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3018) | Matriptase | Show NN |
| 2 | CHEMBL209 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL209) | Trypsin I | Show NN |
| 3 | CHEMBL1795139 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1795139) | Transmembrane protease serine 6 | Show NN |
| 4 | CHEMBL204 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL204) | Thrombin | Show NN |
| 5 | CHEMBL244 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL244) | Coagulation factor X | Show NN |
| 6 | CHEMBL3991 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3991) | Coagulation factor VII | Show NN |
| 7 | CHEMBL2617 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2617) | Tryptase beta-1 | Show NN |
| 8 | CHEMBL270 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL270) | Mu opioid receptor | Show NN |
| 9 | CHEMBL325 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL325) | Histone deacetylase 1 | Show NN |
| 10 | CHEMBL2079849 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2079849) | Serine protease hepsin | Show NN |
| 11 | CHEMBL3351190 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3351190) | Hepatocyte growth factor activator | Show NN |
| 12 | CHEMBL3286 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL3286) | Urokinase-type plasminogen activator | Show NN |
| 13 | CHEMBL2000 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2000) | Plasma kallikrein | Show NN |
| 14 | CHEMBL2820 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL2820) | Coagulation factor XI | Show NN |
| 15 | CHEMBL4777 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4777) | Neuropeptide Y receptor type 1 | Show NN |
| 16 | CHEMBL1801 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1801) | Plasminogen | Show NN |
| 17 | CHEMBL1865 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL1865) | Histone deacetylase 6 | Show NN |
| 18 | CHEMBL333 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL333) | Matrix metalloproteinase-2 | Show NN |

| | | | |
|----|--|----------------------------|---------|
| 19 | CHEMBL4822 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL4822) | Beta-secretase 1 | Show NN |
| 20 | CHEMBL332 (https://www.ebi.ac.uk/chembl/target/inspect/CHEMBL332) | Matrix metalloproteinase-1 | Show NN |