Supporting Information

Promiscuous Ligands from Experimentally Determined Structures, Binding Conformations, and Protein Family Dependent Interaction Hotspots

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### Supplementary Table S1

**Table S1. Multifamily ligands.**

| PDB_ID | family assignment                                                                 | affinity [nM]                                                                 | classification |
|--------|----------------------------------------------------------------------------------|------------------------------------------------------------------------------|----------------|
| 006    | enzyme_transferase-Gag-Pol polyprotein, enzyme_protease-Plasmepsin-1              | Ki=11.0, Kd=0.14, IC50=690.0                                                   | IV             |
| 03M    | nuclear_other-E3 ubiquitin-protein ligase Mdm2, unclassified-Protein Mdm4        | IC50=33.0, Kd=78.0                                                            | IV             |
| 04J    | membrane_receptor, unclassified-Folate receptor beta, enzyme_reductase-Bifunctional dihydrofolate reductase-thymidylate synthase | Kd=144.0                                                                     | IV             |
| 006    | cytosolic_other-E3 ubiquitin-protein ligase XIAP, enzyme_unclassified-Baculoviral IAP repeat-containing protein 2 | IC50=25.4, IC50=5.4                                                           | III            |
| 0WE    | enzyme_unclassified-Enoyl-[acyl-carrier-protein] reductase [NADPH] FabI, enzyme_reductase-Enoyl-[acyl-carrier-protein] reductase [NADH] FabI | IC50=14.0                                                                     | III            |
| 128    | enzyme_hydrolase-Sarcoplasmic/endoplasmic reticulum calcium ATPase 1, ion_channel_Ligic_p2x-P2X purinoceptor 3 | Ki=100.0, Kd=2.1, Kd=12260.0, Kd=1200.0                                      | II             |
| 198    | transcription_factor-Androgen receptor, secreted-?                                | Ki=76.0                                                                       | I              |
| 1AQ    | enzyme_unclassified-Baculoviral IAP repeat-containing protein 2, cytosolic_other-E3 ubiquitin-protein ligase XIAP | IC50=200.0, IC50=1.3                                                          | III            |
| 1E8    | enzyme_kinase-Epidermal growth factor receptor, enzyme_unclassified-?, enzyme_kinase-Tyrosine-protein kinase BTK | Kd=180.0                                                                      | III            |
| 1M3    | epigenetic_regulator_reader_brkd-Bromodomain-containing protein 4, enzyme_kinase-Tyrosine-protein kinase JAK2 | IC50=130.0                                                                    | IV             |
| 1QK    | epigenetic_regulator-Bromodomain-containing protein 4, enzyme_kinase-Cyclin-dependent kinase 2, epigenetic_regulator-Bromodomain testis-specific protein | Kd=210.0, IC50=19000.0, IC50=37000.0                                         | IV             |
| 2LC    | cytosolic_other-Heat shock protein HSP 90-alpha, membrane_other_?-?-?-?-Endoplasmin | Ki=375.0, Ki=3.0                                                              | IV             |
| 35G    | enzyme_phosphodiesterase-cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A, enzyme_kinase-cGMP-dependent protein kinase 2 | Kd=10.0                                                                       | IV             |
| 3VU    | enzyme_unclassified-Beta-lactamase OXA-10, enzyme_hydrolase-Beta-lactamase       | IC50=3100.0, IC50=360.0                                                       | III            |
| 4IP    | enzyme_kinase-Tyrosine-protein kinase BTK, enzyme_kinase-3-phosphoinositide-dependent protein kinase 1, unclassified-Cytohesin-3, enzyme_kinase-RAC-alpha serine/threonine-protein kinase, enzyme_unclassified-Inositol | Kd=440.0, Kd=87.0, Kd=40.0, Ki=300.0, Kd=43.0                                 | II             |
| Protein Name | Description | IC Values | Kinase Type |
|-------------|-------------|-----------|-------------|
| trisphosphate 3-kinase A | | | III |
| 4K4 | enzyme_kinase-Serine/threonine-protein kinase Chk1, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4 | IC50=5380.0, Ki=28.5, Ki=27.7, Ki=20.0 | III |
| 4WG | enzyme_kinase-Mitogen-activated protein kinase 7, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4 | IC50=98.0 | IV |
| 5GP | enzyme_unclassified-Histidine triad nucleotide-binding protein 1, enzyme_unclassified-Xanthine phosphoribosyltransferase, enzyme_unclassified-Hypoxanthine-guanine phosphoribosyltransferase, unclassified-Disks large homolog 4, DNA-?, enzyme_unclassified-Ribonuclease pancreatic, enzyme_phosphodiesterase-cGMP-specific 3',5'-cyclic phosphodiesterase, enzyme_transf erase-Guanylate kinase, enzyme_hydrolase-Guanylate binding protein 1, enzyme_hydrolase-2'-deoxyxynucleoside 5'-phosphate N-hydrolyase 1, enzyme_phosphodiesterase-cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A, enzyme_transf erase-Genome polyprotein [Cleaved into: Capsid protein C, enzyme_unclassified-Cytosolic purine 5'-nucleotidase, enzyme_phosphodiesterase-High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A, enzyme_kinase-Phosphatidylinositol 5-phosphate 4-kinase type-2 beta, unclassified-Nucleoprotein | IC50=3800.0, IC50=67.0, Kd=165.0, Kd=34.3, Ki=526000.0, Ki=20800.0, Kd=7100.0, Kd=663.0, Kd=1.91E7, Kd=1.84E7, Kd=6130000.0 | II |
| 5ID | enzyme_kinase-Mitogen-activated protein kinase 3, enzyme_kinase-Casein kinase I isoform gamma-2, enzyme_kinase-Serine/threonine-protein kinase haspin, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase, H3 lysine-79 specific, enzyme_kinase-Dual specificity protein kinase CLK1 | IC50=1200.0, IC50=900.0 | IV |
| 5UJ | epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 4A, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5B | IC50=80.0 | III |
| 5VW | enzyme_hydrolase-Beta-lactamase, enzyme_protease-Penicillin-binding protein 1B | Kd=5300.0, Kd=11.0 | IV |
| 6XH | epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, epigenetic_regulator_reader_brd-CREB-binding protein | IC50=13000.0, IC50=20.0 | IV |
| 7F9 | enzyme_kinase-[Pyruvate dehydrogenase, cytosolic_other-Heat shock protein HSP 90-alpha | Ki=2170.0 | IV |
| 7FA | enzyme_transf erase-Fatty acid synthase, enzyme_unclassified-Cytosolic phospholipase A2 delta | Ki=6360.0 | IV |
| 83A | membrane_receptor_unclassified-Folate receptor alpha, enzyme_ligase-Trifunctional purine biosynthetic protein adenosine-3 [Includes: | IC50=3.04, Ki=59.0 | IV |
| Gene  | Description                                                                 | Kd/Ki    | Classification |
|-------|------------------------------------------------------------------------------|----------|----------------|
| 8OG   | DNA-?, enzyme_unclassified-N-glycosylase/DNA ligase [Includes: 8-oxoguanine DNA glycosylase, enzyme_isomerase-DNA topoisomerase 1, enzyme_unclassified-DNA polymerase beta, enzyme_unclassified-DNA polymerase kappa, enzyme_unclassified-DNA polymerase iota, enzyme_unclassified-7,8-dihydro-8-oxoguanine triphosphatase, enzyme_unclassified-DNA polymerase eta, enzyme_unclassified-DNA polymerase lambda] | Kd=52.0  | II             |
| 8PR   | enzyme_kinase-Rhodopsin kinase, enzyme_unclassified-Cytochrome P450 2B4, transporter_electrochemical_slc-Sodium-dependent serotonin transporter | Kd=431.0, Kd=13000.0 | IV             |
| 919   | enzyme_kinase-Tyrosine-protein kinase ABL1, enzyme_kinase-Cyclin-dependent kinase 16, enzyme_unclassified-Serine/threonine-protein kinase PRP4 homolog | IC50=4.0, IC50=0.8 | III            |
| 99E   | epigenetic_regulator_reader_brd-CREB-binding protein, epigenetic_regulator_reader_brd-Histone acetyltransferase p300 | Kd=470.0, Kd=230.0 | IV             |
| A1Z   | enzyme_reductase-Egl nine homolog 1, enzyme_unclassified-Hypoxia-inducible factor 1-alpha inhibitor | IC50=29000.0, IC50=29.0 | IV             |
| A3P   | enzyme_unclassified-Non-secretory ribonuclease, enzyme_unclassified-Ribonuclease pancreatic, enzyme_unclassified-Estrogen sulfotransferase, testis isoform, enzyme_isomerase-DNA topoisomerase 1, enzyme_unclassified-Bile salt sulfotransferase, enzyme_unclassified-Estrogen sulfotransferase, enzyme_unclassified-Sulfotransferase 1A1, enzyme_unclassified-Sulfotransferase family cytosolic 2B member 1, enzyme_unclassified-Sulfotransferase 1A2, enzyme_unclassified-Sulfotransferase 1A3, enzyme_unclassified-Sulfotransferase 1C4, enzyme_unclassified-Sulfotransferase family cytosolic 1B member 1, enzyme_unclassified-Protein-tyrosine sulfotransferase 2, enzyme_unclassified-Sulfotransferase 1C2 | Ki=32000.0, Ki=5000.0, Kd=14000.0, Kd=4200.0 | II             |
| ACD   | auxiliary_transport_protein-Fatty acid-binding protein, adipocyte, secreted-?, enzyme_reductase-Prostaglandin G/H synthase 2, enzyme_unclassified-Prostaglandin G/H synthase 1, enzyme_reductase-Arachidonate 5-lipoxygenase, unclassified-Ferritin light chain, enzyme_unclassified-Ectonucleotide pyrophosphatase/phosphodiesterase family member 2 | Kd=91.0, Kd=13.0, Kd=13.0, Kd=10.0, Kd=4400.0 | II             |
| ACR   | enzyme_hydrolase-Maltase-glucoamylase, intestinal [Includes: Maltase, enzyme_unclassified- | Kd=288.0, Ki=81400.0 | IV             |
| ADP | Glucosyltransferase-SI, enzyme_hydrolase-Lysosomal alpha-glucosidase | Ki=62000.0, Ki=6680.0, Ki=150.0, Kd=248000.0, Kd=2900.0, Ki=600000.0 |
| enzyme_unclassified-Serine/threonine-protein kinase/endoribonuclease IRE1, cytosolic_other-Heat shock cognate 71 kDa protein, unclassified-Endoplasmic reticulum chaperone BiP, transporter_ntpase_errt-Transitional endoplasmic reticulum ATPase, cytosolic_other-ATP-dependent molecular chaperone HSP82, enzyme_kinase-[Pyruvate dehydrogenase, cytosolic_other-Heat shock 70 kDa protein 1A, membrane_other_-?-?-?-?-?-Endoplasm, enzyme_unclassified-Nucleoside diphosphate kinase A, enzyme_kinase-Rhodopsin kinase, enzyme_unclassified-Ribonuclease pancreatic, enzyme_kinase-Neuronal proto-oncogene tyrosine-protein kinase Src, enzyme_unclassified-Non-secretory ribonuclease, enzyme_unclassified-Phosphoglycerate kinase, glycosomal, cytosolic_other-Kinesin-1 heavy chain, cytosolic_other-Heat shock protein HSP 90-alpha, enzyme_unclassified-Hexokinase-1, enzyme_transferase-Thymidylate kinase, enzyme_unclassified-Vancomycin/teicoplanin A-type resistance protein VanA, enzyme_unclassified-2-aminobutyric acid hydroxymethyl-4-hydroxy-6-hydroxymethylpyridoxine pyrophosphokinase, enzyme_ligase-Glutamine synthetase, enzyme_unclassified-Protein RecA, enzyme_reductase-3-hydroxy-3-methylglutaryl-coenzyme A reductase, ion_channel_vgc_trp-Transient receptor potential cation channel subfamily M member 7, cytosolic_other-Kinesin-like protein KIF11, enzyme_unclassified-D-alanine-D-alanine ligase B, enzyme_kinase-Glycogen synthase kinase-3 beta, enzyme_unclassified-Polynucleotide kinase, enzyme_kinase-Focal adhesion kinase 1, enzyme_kinase-Aurora kinase A, enzyme_unclassified-Glutamate dehydrogenase 1, mitochondrial, enzyme_kinase-MAP kinase-activated protein kinase 2, enzyme_unclassified-S-adenosylmethionine synthase isoform type-1, enzyme_transferase-Thymidine kinase, enzyme_unclassified-Deoxyctididine kinase, enzyme_kinase-Mast/stem cell growth factor receptor Kit, enzyme_kinase-cAMP-dependent protein kinase catalytic subunit alpha, enzyme_unclassified-Ribokinase, enzyme_unclassified-Pantothenate kinase, | Kd=4610.0, Kd=620.0, Kd=270.0, Kd=230.0, Kd=110.0, Kd=100.0, Kd=24.0, Kd=20.0, Kd=15.0, Kd=10.0, Kd=5.0, Kd=4.55, IC50=38000.0, Ki=92000.0, Ki=92000.0, Ki=30000.0, Ki=18000.0, Ki=11000.0, Ki=1200.0, Kd=1195000.0, Kd=568000.0, Kd=219000.0, Kd=125000.0, Kd=100000.0, Kd=77500.0, Kd=75000.0, Kd=72000.0, Kd=51300.0, Kd=29000.0, Kd=20400.0, Kd=18000.0, Kd=17000.0, Kd=11000.0, Kd=10600.0, Kd=7100.0, Kd=6000.0, Kd=5800.0, Kd=5800.0, Kd=5630.0, Kd=5000.0, Kd=4370.0, Kd=4200.0, Kd=4000.0, Kd=3300.0, Kd=3300.0, Kd=3230.0, |
enzyme_unclassified-Large T antigen , unclassified-Centromere-associated protein E ,
enzyme_hydrolase-Sarcoplasmic/endoplasmic reticulum calcium ATPase 1 , enzyme_unclassified-
Inositol-trisphosphate 3-kinase A ,
enzyme_unclassified-Creatine kinase M-type ,
enzyme_unclassified-Uridine-cytidine kinase 2 ,
enzyme_ligase-Dihydropyrimidinase.synthase/folypolyglutamate synthase ,
unclassified-Apoptotic protease-activating factor 1 ,
enzyme_unclassified-Nucleoside diphosphate kinase 3 , enzyme_isomerase-DNA topoisomerase 2-alpha ,
enzyme_unclassified-6-phosphofructo-2-
kinase/fructose-2,6-bisphosphatase 3 ,
enzyme_unclassified-RuvB-like 1 ,
enzyme_unclassified-Choline kinase alpha ,
enzyme_kinase-Serine/threonine-protein kinase Chk2 ,
enzyme_kinase-Tyrosine-protein kinase ABL1 ,
cytosolic_other-Kinesin-like protein KIF2C ,
enzyme_kinase-Ephrin type-B receptor 2 ,
enzyme_kinase-Threonine/serine-protein phosphatase 2A activator ,
enzyme_unclassified-UDP-N-acetylmuramoylalanine--D-glutamate ligase ,
enzyme_reductase-Aldehyde dehydrogenase ,
mitochondrial , enzyme_unclassified-Inositol-
tetrakisphtose 1-kinase , enzyme_unclassified-
Uridine-cytidine kinase 1 , enzyme_unclassified-
ATP-dependent DNA helicase Q1 , enzyme_kinase-
Death-associated protein kinase 1 , enzyme_kinase-
Serine/threonine-protein kinase Nek2 ,
enzyme_reductase-Succinate-semialdehyde dehydrogenase ,
mitochondrial , enzyme_kinase-
Serine/threonine-protein kinase Nek7 ,
enzyme_unclassified-4-diphosphocytidyl-2-C-
 methyl-D-erythritol kinase , enzyme_unclassified-
Phosphoglycerate kinase 1 , enzyme_unclassified-
 Peroxisomal bifunctional enzyme ,
cytosolic_other-
?, enzyme_kinase-Serine/threonine-protein kinase 24 ,
enzyme_unclassified-Creatine kinase B-type ,
cytosolic_other-Kinesin-like protein KIF3B ,
cytosolic_other-Kinesin-like protein KIF22 ,
enzyme_kinase-Tyrosine-protein kinase Mer ,
enzyme_kinase-PAS domain-containing serine/threonine-protein kinase ,
enzyme_kinase-Dual specificity mitogen-activated protein kinase 1 ,
enzyme_unclassified-Serine/threonine-protein kinase PknB ,
cytosolic_other-Heat shock 70 kDa protein 6 ,
enzyme_unclassified-Choline/ethanolamine kinase ,
enzyme_kinase-Bone morphogenetic protein receptor type-2 ,
enzyme_unclassified-Pyruvate kinase PKM ,
cytosolic_other-Heat shock-related 70 kDa protein 2 ,
enzyme_kinase-Serine/threonine-protein kinase
| Protein                  | Type                        | Subunit | Kd  |
|-------------------------|-----------------------------|---------|-----|
| mTOR                    | enzyme_unclassified         | Genome  | 77000.0 |
| ALK tyrosine kinase     | enzyme_unclassified         | receptor| 780.0 |
| Shikimate kinase        | enzyme_unclassified         | 6-phosphofructokinase, muscle type| 620.0 |
| binding cassette sub-family B member 6 | enzyme_unclassified-ATP-dependent | 6-phosphofructokinase, muscle type | 130.0 |
| RuvB-like 2             | enzyme_unclassified         |         | 70.0 |
| Sphingosine kinase 1    | enzyme_unclassified         |         | 60.0 |
| Tau-tubulin kinase 1    | enzyme_unclassified         |         | 20.0 |
| Bloom syndrome protein  | enzyme_unclassified         |         |     |
| Poly (ADP-ribose) kinase 14 | enzyme_unclassified-ADP-ribos polymerase 14 |         |     |
| Mitogen-activated protein kinase 1 | enzyme_kinase-Mitogen-activated protein kinase 1 |         |     |
| Non-receptor tyrosine-protein kinase TYK2 | enzyme_unclassified-Polypeptide tyrosine kinase 2 |         |     |
| Phosphatidylinositol 4-kinase type 2-alpha | enzyme_unclassified-Phosphatidylinositol 4-kinase type 2-alpha |         |     |
| Serine/threonine-protein kinase PRP4 homolog | enzyme_unclassified-Serine/threonine-protein kinase PRP4 homolog |         |     |
| Tyrosine-protein kinase ITK/TSK | enzyme_kinase-Tyrosine-protein kinase ITK/TSK |         |     |
| 2-5A-dependent ribonuclease | enzyme_kinase-2-5A-dependent ribonuclease |         |     |
| Serine/threonine-protein kinase RIO1 | enzyme_kinase-Serine/threonine-protein kinase RIO1 |         |     |
| DNA gyrase subunit B, enzyme_unclassified-ATP-dependent RNA helicase | DDX3X |         |     |
| Serine/threonine-protein kinase BUB1 | enzyme_kinase-Serine/threonine-protein kinase BUB1 |         |     |
| mitotic checkpoint serine/threonine-protein kinase | enzyme_kinase-Mitotic checkpoint serine/threonine-protein kinase |         |     |
| Serine/threonine-protein kinase MRCK beta | enzyme_kinase-Serine/threonine-protein kinase MRCK beta |         |     |
| phosphofructokinase, platelet type | enzyme_kinase-Phosphofructokinase, platelet type |         |     |
| 6-phosphofructokinase, platelet type | enzyme_kinase-6-phosphofructokinase, platelet type |         |     |
| PknG                      | enzyme_unclassified         | DNA polymerase theta | 77000.0 |
| Casein kinase II subunit alpha | enzyme_kinase-Casein kinase II subunit alpha |         |     |
| Carbamoyl-phosphate synthase | enzyme_ligase-Carbamoyl-phosphate synthase | [ammonia], mitochondrial | 780.0 |
| Pantothenate kinase 2, mitochondrial | enzyme_kinase-Pantothenate kinase 2, mitochondrial |         |     |
| Tyrosine-protein kinase JAK1 | enzyme_kinase-Tyrosine-protein kinase JAK1 |         |     |
| Histidine triad nucleotide-binding protein 1, cytosolic other-Kinesin-like protein KIFC1 | enzyme_kinase-Histidine triad nucleotide-binding protein 1, cytosolic other-Kinesin-like protein KIFC1 |         |     |
| inward rectifier potassium channel 11 | ion_channel_vgc_k-ATP-sensitive inward rectifier potassium channel 11 |         |     |
| Serine/threonine-protein kinase PAK 3 | enzyme_kinase-Serine/threonine-protein kinase PAK 3 |         |     |

| Protein                  | Type                        | Subunit | Kd  |
|-------------------------|-----------------------------|---------|-----|
| transporter_ntpase_ert  | Transitional endoplasmic reticulum ATPase, unclassified-Synapsin-1, enzyme_unclassified-6-phosphofructokinase, muscle type, fructose-2,6-bisphosphatase 1, enzyme_unclassified-Protein RecA, enzyme_unclassified-Serine/threonine-protein kinase Pkn8, enzyme_kinase-Tyrosine-protein kinase ABL1, enzyme_kinase-Serine/threonine-protein kinase |         |     |
| Synapsin-1              | unclassified-Synapsin-1     |         | 77000.0 |
| enzyme_unclassified-6-phosphofructokinase, muscle type | enzyme_unclassified-6-phosphofructokinase, muscle type |         | 780.0 |
| fructose-2,6-bisphosphatase 1 | enzyme_unclassified-fructose-2,6-bisphosphatase 1 |         | 620.0 |
| Protein RecA             | enzyme_unclassified-Protein RecA |         | 130.0 |
| enzyme_unclassified-Serine/threonine-protein kinase Pkn8 | enzyme_unclassified-Serine/threonine-protein kinase Pkn8 |         | 130.0 |
| enzyme_kinase-Tyrosine-protein kinase ABL1 | enzyme_kinase-Tyrosine-protein kinase ABL1 |         | 70.0 |
| enzyme_kinase-Serine/threonine-protein kinase | enzyme_kinase-Serine/threonine-protein kinase |         | 60.0 |
| enzyme_kinase-Serine/threonine-protein kinase | enzyme_kinase-Serine/threonine-protein kinase |         | 20.0 |
| Enzyme/Protein Name                                                                 | IC50/Ki/Kd (nM)             |
|-----------------------------------------------------------------------------------|----------------------------|
| Protein kinase Nek2, enzyme_kinase-Proto-oncogene tyrosine-protein kinase Src  | IC50=129000.0              |
| enzyme_kinase-Dual specificity mitogen-activated protein kinase kinase 1         | IC50=1300.0, IC50=440.0    |
| enzyme_kinase-Protein-tyrosine kinase 2-beta, cytosolic_other-Heat shock protein HSP 90-alpha | Ki=590000.0, Ki=260000.0   |
| Glucokinase, enzyme_kinase-Serine/threonine-protein kinase N2                     | Ki=94000.0, Ki=63800.0    |
| enzyme_kinase-Mitogen-activated protein kinase kinase 14                          | Ki=55000.0, Ki=46000.0    |
| enzyme_kinase-Serine/threonine-protein kinase PknG                                | Kd=440000.0, Kd=194000.0  |
| enzyme_kinase-Non-receptor tyrosine-protein kinase TYK2, enzyme_kinase-Ephrin type-A receptor 2 | Kd=110000.0, Kd=55000.0   |
| enzyme_kinase-Protein-tyrosine kinase tousled-like 2                               | Kd=10600.0, Kd=7600.0     |
| enzyme_unclassified-Fructose-1,6-bisphosphatase 1, enzyme_unclassified-Glycogen phosphorylase, muscle form | Kd=3300.0, Kd=3000.0      |
| enzyme_unclassified-Histidine triad nucleotide-binding protein 1, enzyme_unclassified-Ribonuclease pancreatic, DNA-? | Kd=423.0, Kd=6000.0    |
| enzyme_unclassified-Glycogen phosphorylase, liver form, enzyme_unclassified-NH, enzyme_ligase-Glutamine synthetase, enzyme_unclassified-Adenylosuccinate synthetase isozyme 1, enzyme_unclassified-ATP | Kd=8000000.0, Kd=4990000.0 |
| enzyme_kinase-Non-receptor tyrosine-protein kinase TYK2, enzyme_kinase-Ephrin type-A receptor 2 | Kd=250000.0 |
| AMP                                                                              |                            |
| enzyme_unclassified-Fructose-1,6-bisphosphatase 1, enzyme_unclassified-Glycogen phosphorylase, muscle form |                            |
| enzyme_unclassified-Histidine triad nucleotide-binding protein 1, enzyme_unclassified-Ribonuclease pancreatic, DNA-? |                            |
| enzyme_unclassified-Glycogen phosphorylase, liver form, enzyme_unclassified-NH, enzyme_ligase-Glutamine synthetase, enzyme_unclassified-Adenylosuccinate synthetase isozyme 1, enzyme_unclassified-ATP |                            |
| enzyme_unclassified-Fructose-1,6-bisphosphatase 1, enzyme_unclassified-Glycogen phosphorylase, muscle form |                            |
| enzyme_unclassified-Histidine triad nucleotide-binding protein 1, enzyme_unclassified-Ribonuclease pancreatic, DNA-? |                            |
| enzyme_unclassified-Glycogen phosphorylase, liver form, enzyme_unclassified-NH, enzyme_ligase-Glutamine synthetase, enzyme_unclassified-Adenylosuccinate synthetase isozyme 1, enzyme_unclassified-ATP |                            |
| Enzyme/Protein Name | IC50/Ki/Kd Values |
|---------------------|-------------------|
| kinase Src, enzyme_unclassified-Choline/ethanolamine kinase, enzyme_unclassified-Fructose-1,6-bisphosphatase isozyme 2, enzyme_kinase-G protein-coupled receptor kinase 6, unclassified-?, enzyme_kinase-Phosphatidylinositol 5-phosphate 4-kinase type-2 beta, enzyme_kinase-Mitogen-activated protein kinase 10, unclassified-Nucleoprotein, enzyme_unclassified-Luciferin 4-monooxygenase, enzyme_unclassified-Glycogen phosphorylase, brain form | IC50=155000.0, IC50=395000.0, Ki=10000.0, Kd=520000.0, Kd=256000.0, Kd=220000.0, Kd=150000.0, Kd=37000.0, Kd=115000.0, Kd=8300.0, Kd=6800.0, Kd=240.0, Ki=400000.0, Ki=100000.0 |
| enzyme_kinase-Serine/threonine-protein kinase PLK1, enzyme_kinase-Tyrosine-protein kinase SYK, enzyme_kinase-Tyrosine-protein kinase HCK, enzyme_kinase-Mitogen-activated protein kinase 12, enzyme_kinase-Casein kinase II subunit alpha, enzyme_transferase-Thymidylate kinase, enzyme_isomerase-DNA gyrase subunit B, enzyme_unclassified-Pantothenate kinase, ion_channel_vgc_trp-Transient receptor potential cation channel subfamily M member 7, enzyme_kinase-Death-associated protein kinase 1, enzyme_kinase-Insulin receptor, enzyme_kinase-Glycogen synthase kinase-3 beta, enzyme_kinase-Mitogen-activated protein kinase 10, enzyme_kinase-Ephrin type-B receptor 2, enzyme_kinase-Insulin-like growth factor 1 receptor, enzyme_kinase-Ephrin type-A receptor 2, cytosolic_other-Heat shock cognate 71 kDa protein, enzyme_unclassified-DNA topoisomerase 2, enzyme_unclassified-Hexokinase-1, enzyme_kinase-Tyrosine-protein kinase Lck, enzyme_isomerase-DNA topoisomerase 4 subunit B, enzyme_unclassified-Inositol-trisphosphate 3-kinase A, enzyme_unclassified-Galactokinase, enzyme_unclassified-Protein RecA, enzyme_kinase-Serine/threonine-protein kinase pim-1, enzyme_isomerase-DNA topoisomerase 2-alpha, enzyme_kinase-G protein-coupled receptor kinase 6, enzyme_unclassified-Pyridoxal kinase, enzyme_kinase-Aurora kinase A, enzyme_kinase-[Pyrurate dehydrogenase, cytosolic_other-Heat shock 70 kDa protein 1A, enzyme_kinase-Epidermal growth factor receptor, enzyme_unclassified-Ketohexokinase, membrane_other_-?_-?-Endoplasmin, enzyme_kinase-Interleukin-1 receptor-associated kinase 4, enzyme_kinase-Tyrosine-protein kinase ZAP-70, enzyme_kinase-Tyrosine-protein kinase Mer, unclassified-?, enzyme_unclassified-Inositol-tetrakisphosphate 1-kinase, enzyme_kinase-Ephrin type-A receptor 3, enzyme_kinase-Serine/threonine-protein kinase Sgg1, |
enzyme_kinase-Proto-oncogene tyrosine-protein kinase Src, enzyme_kinase-Serine/threonine-protein kinase OSR1, cytosolic_other-Heat shock protein HSP 90-alpha, enzyme_kinase-Tyrosine-protein kinase Lyn, enzyme_kinase-Dual specificity mitogen-activated protein kinase kinase 4, transporter_ntpase_errt-Transitional endoplasmic reticulum ATPase, enzyme_unclassified-Ectonucleoside triphosphate diphosphohydrolase 2, enzyme_kinase-Serine/threonine-protein kinase PLK4, enzyme_unclassified-Glucokinase, enzyme_unclassified-Ribosomal protein S6 kinase alpha-3, enzyme_unclassified-Ubiquitin-like modifier-activating enzyme 5, cytosolic_other-Kinesin-like protein KIF11, enzyme_unclassified-?-Receptor tyrosine-protein kinase erbB-3, enzyme_kinase-Ribosomal protein S6 kinase alpha-5, unclassified-Endoplasmic reticulum chaperone BIP, enzyme_unclassified-Peripheral plasma membrane protein CASK, enzyme_kinase-Dual specificity mitogen-activated protein kinase kinase 1, enzyme_kinase-Protein kinase C beta type, enzyme_kinase-Macrophage-stimulating protein receptor, enzyme_kinase-Serine/threonine-protein kinase PAK 1, enzyme_unclassified-ATP-dependent RNA helicase SUPV3L1, mitochondrial, enzyme_kinase-Phosphatidylinositol 5-phosphate 4-kinase type-2 beta, enzyme_kinase-Maternal embryonic leucine zipper kinase, unclassified-Myosin-7, enzyme_kinase-Serine/threonine-protein kinase PAK 4, enzyme_kinase-Mitogen-activated protein kinase 1, enzyme_unclassified-Bifunctional glutamate/proline--tRNA ligase, enzyme_unclassified-Serine/threonine-protein kinase PRP4 homolog, enzyme_unclassified-Proline--tRNA ligase, enzyme_kinase-Serine/threonine-protein kinase 24, enzyme_kinase-Mitogen-activated protein kinase 8, enzyme_kinase-G protein-coupled receptor kinase 5, enzyme_kinase-Mitogen-activated protein kinase kinase kinase 2, enzyme_kinase-Mitogen-activated protein kinase kinase 3, cytosolic_other-Heat shock protein 75 kDa, mitochondrial, enzyme_unclassified-ATP-dependent RNA helicase DDX3X, enzyme_kinase-TGF-beta receptor type-2, unclassified-DNA repair protein RAD51 homolog 1, enzyme_kinase-LIM domain kinase 1, enzyme_unclassified-Atypical kinase COQ8A, mitochondrial, enzyme_unclassified-Pantothenate kinase 3, enzyme_kinase-Serine/threonine-protein kinase WNK3, enzyme_kinase-Serine/threonine-protein kinase Chk1, enzyme_kinase-
| Gene     | Description                                                                                       | Ki/Kd (μM)          |
|----------|---------------------------------------------------------------------------------------------------|---------------------|
| APC      | Serine/threonine-protein kinase WNK1, enzyme_kinase-Fibroblast growth factor receptor 2           | Kd=388000.0, Kd=18000.0, Kd=320.0, Kd=230.0, Ki=850000.0 |
| APR      | enzyme_unclassified-2-amino-4-hydroxy-6-hydroxymethylidihydropteridine pyrophosphokinase, enzyme_unclassified-NH, enzyme_unclassified-Pantothenate synthetase, enzyme_unclassified-T7 RNA polymerase, enzyme_unclassified-Adenylate cyclase, enzyme_unclassified-Adenylate cyclase type 10, enzyme_hydrolase-Ectonucleotide pyrophosphatase/phosphodiesterase family member 3 | Kd=192000.0, Kd=29160.0, Kd=5000.0, Kd=3900.0, Kd=2950.0, Ki=180000.0 |
| AR6      | enzyme_unclassified-Poly [ADP-ribose] polymerase 14, cytosolic_other-Elongation factor 2, enzyme_unclassified-NAD-dependent protein deacetylase HST2, epigenetic_regulator_eraser_hdac-NAD-dependent protein deacetylase sirtuin-5, mitochondrial, enzyme_unclassified-Alcohol dehydrogenase class-3, enzyme_unclassified-ADP-ribose cyclase/cyclic ADP-ribose hydrolase 1, enzyme_unclassified-p-hydroxybenzoate hydroxylase, epigenetic_regulator_eraser_hdac-NAD-dependent protein deacetylase sirtuin-6, epigenetic_regulator_eraser_hdac-NAD-dependent protein deacetylase sirtuin-3, mitochondrial, epigenetic_regulator_eraser_hdac-NAD-dependent protein deacetylase sirtuin-1, enzyme_unclassified-Alcohol dehydrogenase E chain | Kd=6400.0, Kd=6000.0, Kd=1900.0, Kd=1300.0, Kd=130.0 |
| ATM      | enzyme_transferase-Thymidylate kinase, enzyme_unclassified-5', enzyme_transferase-Gag-Pol polyprotein | Ki=10000.0          |
| ATP      | enzyme_kinase-Tyrosine-protein kinase JAK2, transporter_ntpase_atp-Multidrug resistance-associated protein 1, enzyme_kinase-Cyclin-dependent kinase 2, ion_channel_lgic_p2x-P2X purinoreceptor 3, enzyme_unclassified-Adenylate cyclase type 10, ion_channel_other_chloride-Cystic fibrosis transmembrane conductance regulator, unclassified-Endoplasmic reticulum chaperone BiP, enzyme_unclassified-Ribonuclease pancreatic, enzyme_unclassified-Pyruvate kinase PKM, enzyme_unclassified-2-amino-4-hydroxy-6- | Ki=860.0, Kd=780.0, Kd=450.0, Kd=250.0, Kd=180.0, Kd=125.0, Kd=20.0, Kd=20.0, Kd=3.3, Kd=2.8, Ki=1026000.0, |
hydroxymethylidihydropteridine pyrophosphokinase, enzyme_transferase-Thymidylate kinase, enzyme_unclassified-NH, enzyme_kinase-Mitogen-activated protein kinase 1, enzyme_kinase-3-phosphoinositide-dependent protein kinase 1, cytosolic_other-Heat shock cognate 71 kDa protein, enzyme_unclassified-Mevalonate kinase, enzyme_hydrolase-Sodium/potassium-transporting ATPase subunit alpha-1, enzyme_unclassified-S-adenosylmethionine synthase isoform type-1, enzyme_kinase-Aurora kinase A, enzyme_kinase-cAMP-dependent protein kinase catalytic subunit alpha, enzyme_kinase-Dual specificity mitogen-activated protein kinase 2, enzyme_kinase-Dual specificity mitogen-activated protein kinase 1, enzyme_unclassified-Large T antigen, membrane_other_-?-?-?-?-? ENDOPLASMIN, enzyme_kinase-Cyclin-dependent kinase 7, enzyme_unclassified-Pantothenate synthetase, enzyme_kinase-[Pyruvate dehydrogenase, enzyme_unclassified-Non-secretory ribonuclease, enzyme_transferase-Gag-Pol polyprotein, enzyme_kinase-Focal adhesion kinase 1, ion_channel_vgc_trp-Transient receptor potential cation channel subfamily V member 1, enzyme_ligase-Trifunctional purine biosynthetic protein adenosine-3 [Includes: Phosphoribosylamine--glycine ligase, enzyme_unclassified-Phosphoglycerate kinase 1, enzyme_unclassified-Cytosolic purine 5'-nucleotidase, enzyme_unclassified-Pyridoxal kinase, enzyme_kinase-Serine/threonine-protein kinase 24, enzyme_kinase-Protein kinase C iota type, enzyme_hydrolase-Sarcoplasmic/endoplasmic reticulum calcium ATPase 1, enzyme_unclassified-Lysine--tRNA ligase, enzyme_kinase-Rhodopsin kinase, enzyme_kinase-Hepatocyte growth factor receptor, enzyme_unclassified-ATP-dependent 6-phosphofructokinase, enzyme_unclassified-DNA polymerase iota, enzyme_unclassified-Ubiquitin-like modifier-activating enzyme 5, enzyme_kinase-Dual specificity protein kinase TTK, enzyme_reductase-Ribonucleoside-diphosphate reductase large subunit, enzyme_unclassified-Pyruvate kinase, enzyme_unclassified-DNA polymerase kappa, enzyme_unclassified-Protein-glutamine gamma-glutamyltransferase 2, transporter_nmpase_atp-ATP-binding cassette subfamily B member 6, mitochondrial, enzyme_unclassified-ATP-dependent 6-phosphofructokinase, muscle type.

Ki=129000.0, Ki=29000.0, Kd=338000.0, Kd=288000.0, Kd=172000.0, Kd=170000.0, Kd=149000.0, Kd=149000.0, Kd=140000.0, Kd=118000.0, Kd=100000.0, Kd=67000.0, Kd=36000.0, Kd=28000.0, Kd=180000.0, Kd=100000.0, Kd=9600.0, Kd=4600.0, Kd=4400.0, Kd=4370.0, Kd=4000.0, Kd=3000.0, Kd=2500.0, Kd=1930.0, Kd=1700.0, Kd=1400.0, Kd=1380.0, Kd=1380.0, Kd=1000.0, Kd=1000.0, Kd=840.0, Kd=840.0, Kd=745.0, Kd=380.0, Kd=310.0, Kd=280.0, Kd=254.0, Kd=120.0, Ki=200000.0, Ki=200000.0, Ki=8.0E7, Kd=2029999.999999998, Kd=400000.0, Kd=286000.0, Kd=263000.0, Kd=90000.0, Kd=70000.0
| Gene Name                                                                 | Description                                                                 | IC50/Ki/Kd (nM) | Class |
|--------------------------------------------------------------------------|------------------------------------------------------------------------------|-----------------|-------|
| enzyme_unclassified-Phosphoglycerate kinase                              |                                                                              |                 |       |
| enzyme_kinase-Serine/threonine-protein kinase PAK 1                      |                                                                              |                 |       |
| enzyme_unclassified-Sensor histidine kinase WAK                          |                                                                              |                 |       |
| cytosolic_other-Heat shock protein HSP 90-alpha                          |                                                                              |                 |       |
| enzyme_unclassified-Tau-tubulin kinase 1                                 |                                                                              |                 |       |
| enzyme_unclassified-D-alanine--D-alanine ligase B                         |                                                                              |                 |       |
| ion_channel_vgc_trp-Transient receptor potential cation channel subfamily V member 4 |                                                                              |                 |       |
| enzyme_kinase-Calcium/calmodulin-dependent protein kinase type 1         |                                                                              |                 |       |
| enzyme_unclassified-ATP-dependent 6-phosphofructokinase, platelet type   |                                                                              |                 |       |
| enzyme_unclassified-Phosphatidylinositol 4-kinase beta                   |                                                                              |                 |       |
| cytosolic_other-Heat shock 70 kDa protein 1A                              |                                                                              |                 |       |
| enzyme_kinase-Casein kinase II subunit alpha                             |                                                                              |                 |       |
| enzyme_unclassified-DNA polymerase eta                                   |                                                                              |                 |       |
| enzyme_unclassified-6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase 2 |                                                                              |                 |       |
| transporter_ntpase_atp-Multidrug resistance protein 1A, DNA-?            |                                                                              |                 |       |
| unclassified-DNA repair protein RAD51 homolog 1                           |                                                                              |                 |       |
| enzyme_unclassified-DNA polymerase beta                                   |                                                                              |                 |       |
| enzyme_unclassified-ATP phosphoribosyltransferase                        |                                                                              |                 |       |
| transporter_ntpase_atp-Multidrug resistance protein 1                     |                                                                              |                 |       |
| enzyme_kinase-Penicillin-binding protein 1B                               |                                                                              |                 |       |
| enzyme_unclassified-DNA polymerase Toho-1                                 |                                                                              |                 |       |
| epigenetic_regulator_eraser_hdac-Histone deacetylase 8                   |                                                                              |                 |       |
| enzyme_hydrolase-Acetylpolyamine amidohydrolase                          |                                                                              |                 |       |
| epigenetic_regulator_eraser_hdac-Histone deacetylase, enzyme_protease-Leukotriene A-4 hydrolase |                                                                              |                 |       |
| enzyme_kinase-Tyrosine-protein kinase BTK                                 |                                                                              |                 |       |
| enzyme_kinase-Tyrosine-protein kinase HCK                                 |                                                                              |                 |       |
| enzyme_unclassified-?                                                    |                                                                              |                 |       |
| transcription_factor-Thyroid hormone receptor beta, secreted-Transthyretin, transcription_factor-Thyroid hormone receptor alpha |                                                                              |                 |       |
| enzyme_unclassified-Peptide deformylase                                  |                                                                              |                 |       |
| enzyme_protease-Aminopeptidase N                                          |                                                                              |                 |       |
| enzyme_unclassified-Peptide deformylase 1A, chloroplastic/mitochondrial, enzyme_unclassified-Peptide deformylase, mitochondrial |                                                                              |                 |       |

**Class**
- **IV**: Very high affinity
- **III**: High affinity
- **II**: Moderate affinity
- **I**: Low affinity

**Ki**: IC50 or Ki,
**IC50**: 50% inhibition concentration,
**Kd**: Dissociation constant (KD)
| | Enzyme/Protein Complex | IC50/Kd/Ki (nm) |
|---|---|---|
| **BCD** | unclassified-Alpha-hemolysin, enzyme_kinase-5'-AMP-activated protein kinase subunit beta-1, enzyme_cytochrome-Lanosterol 14-alpha demethylase, cytosolic_other-Type 1 fimbrin D-mannose specific adhesin | IC50=20.0, Kd=146000.0, Kd=38000.0, Kd=1800.0, Kd=1200.0, Kd=700.0, Kd=480.0 |
| **BES** | enzyme_protease-Leukotriene A-4 hydrolase, enzyme_protease-Aminopeptidase N, enzyme_protease-Bacterial leucyl aminopeptidase, enzyme_unclassified-M17 leucyl aminopeptidase, enzyme_protease-M1 family aminopeptidase, enzyme_protease-Glutamyl aminopeptidase, enzyme_protease-Endoplasmic reticulum aminopeptidase 1 | IC50=49.9, IC50=7.0, Kd=478.2, Kd=25.0, Kd=18.0, Kd=0.5, IC50=4200.0, Kd=75000.0 |
| **BEY** | enzyme_unclassified-M17 leucyl aminopeptidase, enzyme_protease-M1 family aminopeptidase | Ki=79.0, Ki=13.0 |
| **BIG** | enzyme_hydrolase-5'-methylthioadenosine/S-adenosylhomocysteine nucleosidase, enzyme_unclassified-S-methyl-5'-thioadenosine phosphorylase | Kd=0.208 |
| **BK5** | enzyme_unclassified-?, enzyme_kinase-Proto-oncogene tyrosine-protein kinase Src | Ki=2.5 |
| **BMF** | epigenetic_regulator_reader_phd-Peregrin, epigenetic_regulator_reader_brd-Bromodomain-containing protein 9, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, epigenetic_regulator_reader_brd-Transcription initiation factor TFIID subunit 1-like | Kd=42.7, Kd=41.8, Kd=41.7, Kd=270.0 |
| **BZ1** | enzyme_unclassified-Carbonic anhydrase 4, enzyme_lyase-Carbonic anhydrase 2 | IC50=45.3, Ki=36.0, Ki=3.2 |
| **CB3** | enzyme_transferase-Thymidylate synthase, enzyme_unclassified-?, enzyme_unclassified-Pteridine reductase 1, enzyme_reductase-Bifunctional dihydrofolate reductase-thymidylate synthase | Ki=90.0 |
| **CB4** | enzyme_hydrolase-Beta-lactamase, enzyme_unclassified-Beta-lactamase SHV-1, enzyme_hydrolase-Beta-lactamase TEM | Ki=20.0, Ki=2200.0, Ki=15.0 |
| **CBD** | enzyme_transferase-Hematopoietic prostaglandin D synthase, enzyme_unclassified-NAD, enzyme_unclassified-Glutathione S-transferase P | IC50=40.4 |
| **CBI** | enzyme_protease-Lactotransferrin, enzyme_unclassified-Endoglucanase-5 | Kd=115000.0, Kd=6000.0, Ki=1.01E8, Ki=4500000.0 |
| **CBP** | enzyme_protease-Collagenase 3, enzyme_hydrolase-Collagenase 3 | Ki=0.17 |
| **CDP** | enzyme_unclassified-2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase, enzyme_unclassified-Phosphoglycerate kinase 1, enzyme_reductase- | Kd=110.0 |
| | Ribonucleoside-diphosphate reductase large subunit | |  |
|---|---|---|---|
| **CEL** | enzyme_lyase-Carbonic anhydrase 2, enzyme_unclassified-Prostaglandin G/H synthase 1, enzyme_reductase-Prostaglandin G/H synthase 2, enzyme_protease-Lactotransferrin | IC50=21.0 | IV |
| | enzyme_unclassified-Alcohol dehydrogenase S chain, unclassified-Ferrochelatase, mitochondrial, DNA-?, transcription_factor-Estrogen-related receptor gamma, enzyme_unclassified-Phospholipase A2, major isoenzyme, enzyme_unclassified-Liver carboxylesterase 1, enzyme_lyase-Carbonic anhydrase 2, epigenetic_regulator_writer_hat-Nuclear receptor coactivator 2 | Kd=415000.0, Kd=2500.0 | II |
| **CLR** | transcription_factor-Nuclear receptor ROR-alpha, transporter_unclassified-NPC intracellular cholesterol transporter 1, unclassified-Apolipoprotein A-I, membrane_receptor_7tm1_peptide_short_peptide_-Mu-type opioid receptor, transporter_electrochemical_slc-Sodium-dependent serotonin transporter, membrane_receptor_7tm1_peptide_chemokine_receptor_-C-C chemokine receptor type 9, surface_antigen-CD81 antigen | Kd=300.0 | IV |
| **CMP** | enzyme_kinase-cGMP-dependent protein kinase 1, ion_channel_vgc_c-gmp-Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2, enzyme_unclassified-Adenylate cyclase type 10, ion_channel_vgc_c-gmp-?, unclassified-?, enzyme_phosphodiesterase-cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A, enzyme_phosphodiesterase-cAMP-specific 3',5'-cyclic phosphodiesterase 4D, ion_channel_vgc_c-gmp-Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 1, enzyme_kinase-cAMP-dependent protein kinase 2, enzyme_kinase-cAMP-dependent protein kinase type I-alpha regulatory subunit, enzyme_unclassified-RNA polymerase sigma factor RpoD | Kd=27.0, Kd=6.0, Kd=1.2, Kd=280000.0, Kd=205100.0, Kd=6820.0, Kd=5500.0, Kd=3600.0, Kd=830.0, Kd=800.0, Kd=240.0, Kd=5.42E7 | II |
| **CPB** | enzyme_unclassified-Glycogen phosphorylase, muscle form, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4 | Kd=6.4, IC50=18000.0, IC50=2500.0, IC50=1000.0, Ki=1240.0 | IV |
| **CTP** | enzyme_unclassified-Glucose-1-phosphate cytidylyltransferase, enzyme_unclassified-DNA polymerase I, enzyme_unclassified-Uridine-cytidine kinase 2, enzyme_unclassified-2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase | Ki=110000.0, Ki=35000.0, Kd=17200.0, Kd=410.0 | II |
| DCM | enzyme_transferase-Thymidylate synthase, enzyme_unclassified-Deoxycytidine kinase, DNA-? | Kd=160000.0, Kd=2800.0, Kd=490.0 | IV |
| DM2 | enzyme_protease-Botulinum neurotoxin type B, DNA-?, transporter-Multidrug efflux pump subunit AcrB, enzyme_unclassified-Ribosydihydronicotinamide dehydrogenase [quinone], enzyme_reductase-Sorcin | Kd=10.0, Kd=9400.0 | IV |
| DSH | enzyme_unclassified-Spermidine synthase, epigenetic_regulator_writer_pmt-Histone-arginine methyltransferase CARM1 | Kd=1100.0 | IV |
| DTP | unclassified-Endoplasmic reticulum chaperone BiP, enzyme_unclassified-DNA polymerase beta, enzyme_unclassified-Protein RecA, enzyme_unclassified-Deoxyguanosine kinase, mitochondrial, enzyme_unclassified-DNA polymerase kappa, enzyme_reductase-Ribonucleoside-diphosphate reductase large subunit, enzyme_unclassified-Cytosolic purine 5'-nucleotidase, enzyme_unclassified-DNA polymerase iota, enzyme_transferase-Gag-Pol polyprotein, enzyme_unclassified-DNA polymerase lambda, ion_channel_other_chloride-Cystic fibrosis transmembrane conductance regulator | Kd=750000.0, Kd=19000.0, Kd=1500.0 | II |
| E64 | enzyme_protease-Calpain-1 catalytic subunit, enzyme_protease-Cathepsin K, enzyme_unclassified-Streptopain, enzyme_protease-? | IC50=225.0, IC50=98.0, IC50=76.25, Kd=10.0, IC50=100000.0, Kd=27000.0 | III |
| E67 | epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase EHMT1, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 7A | Kd=244.0, Ki=2500.0 | IV |
| EPA | transcription_factor-Peroxisome proliferator-activated receptor delta, enzyme_unclassified-Prostaglandin G/H synthase 1, enzyme_reductase-Prostaglandin G/H synthase 2 | IC50=4000.0 | IV |
| EPU | enzyme_transferase-UDP-N-acetylglucosamine 1-carboxyvinyltransferase, enzyme_unclassified-UDP-N-acetylenolpyruvoylglucosamine reductase | Ki=900.0 | IV |
| ET | unclassified-Multidrug efflux pump subunit AcrB, enzyme_unclassified-Ribosydihydronicotinamide dehydrogenase [quinone] | Kd=215400.0, Kd=14600.0, Kd=2900.0, Kd=1180.0, | IV |
| Gene | Description | Kd/Ki/IC50 Values | Subcellular Location |
|------|-------------|-------------------|---------------------|
| F89  | enzyme transferase-Thymidylate synthase, enzyme unclassified-? | Kd=990.0 | III |
| FKS  | enzyme isomerase-Peptidyl-prolyl cis-trans isomerase FKBP1A, enzyme unclassified-Peptidyl-prolyl cis-trans isomerase FKBP3, enzyme unclassified-Peptidyl-prolyl cis-trans isomerase FKBP5, enzyme unclassified-Peptidyl-prolyl cis-trans isomerase FKBP4 | IC50=160.0, Ki=200.0, Kd=55.0, Kd=0.4 | III |
| FMN  | enzyme unclassified-NADPH--cytochrome P450 reductase, enzyme reductase-Dihydroorotate dehydrogenase, enzyme unclassified-Oxygen-insensitive NAD, DNA-?, enzyme unclassified-Flavin reductase, enzyme unclassified-Pyridoxine-5'-phosphate oxidase, enzyme unclassified-Chorismate synthase, enzyme unclassified-Hydroxyacid oxidase 2, enzyme unclassified-Nitric oxide synthase, brain, enzyme unclassified-Hydroxyacid oxidase 1, enzyme unclassified-2-nitropropane dioxygenase, enzyme unclassified-Ribosylhydronicotinamide dehydrogenase [quinone], enzyme unclassified-tRNA-dihydrouridine | Kd=90.0, Kd=1.0, Kd=0.43, Kd=120000.0, Kd=170.0 | IV |
| FOL  | membrane receptor unclassified-Folate receptor alpha, membrane receptor unclassified-Folate receptor beta, enzyme reductase-Dihydrofolate reductase, enzyme unclassified-?, enzyme reductase-Bifunctional dihydrofolate reductase-thymidylate synthase | Kd=29.8, Kd=2.7, Kd=0.19, Kd=9510.0 | IV |
| FPP  | enzyme transferase-Farnesyl pyrophosphate synthase, enzyme unclassified-Geranylgeranyl pyrophosphate synthase, enzyme unclassified-Isoprenyl transferase | Kd=94.0, Kd=10.0, Kd=6000.0 | II |
| FT2  | secreted-Transferrin, enzyme unclassified-Enoyl-ACP reductase | IC50=850.0 | I |
| FUA  | secreted-?, enzyme unclassified-Multidrug efflux pump subunit AcrB | Ki=5400.0 | I |
| FUN  | secreted-Thyroxine-binding globulin, enzyme lyase-Carbonic anhydrase 2 | Ki=65.0, Kd=205.0, Ki=560.0 | IV |
| G24  | transcription factor-Thyroid hormone receptor beta, secreted-Transferrin | Kd=0.33, Kd=1200.0, Kd=1000.0 | I |
| G93  | enzyme kinase-RAC-beta serine/threonine-protein kinase, enzyme unclassified-Serine/threonine-protein kinase PknB | Ki=4.0 | III |
| GCP  | cytosolic other-GTPase HRas, enzyme unclassified-Phosphoenolpyruvate carboxykinase, cytosolic [GTP], unclassified-Cell division control protein 42 homolog, enzyme unclassified-Dynamin-1, enzyme unclassified-GTPase KRas | Kd=25700.0, Kd=11500.0, Kd=1850.0 | II |
| GDM  | cytosolic other-ATP-dependent molecular | Kd=24500.0, | III |
| Protein/Enzyme Description                                                                 | KD Values                                       |
|------------------------------------------------------------------------------------------|------------------------------------------------|
| chaperone HSP82, cytosolic_other-Heat shock protein HSP 90-alpha, membrane_other_-?-?-?-?-Endoplasmin | Kd=8620.0, Kd=8060.00000001, Kd=1270.0, Kd=1200.0, Kd=1200.0 |
| unclassified-Ras-related C3 botulinum toxin substrate 1, membrane_other_-?-?-?-?-?-Guanine nucleotide-binding protein G, cytosolic_other-Elongation factor 2, enzyme_unclassified-Nucleoside diphosphate kinase B, unclassified-Cell division control protein 42 homolog, cytosolic_other-GTPase HRas, DNA-?, unclassified-Transforming protein RhoA, unclassified-, enzyme_unclassified-Protein-glutamine gamma-glutamyltransferase 2, enzyme_unclassified-Adenylosuccinate synthetase isozyme 1, cytosolic_other-?, enzyme_unclassified-Bifunctional, unclassified-GTP-binding protein Rheb, enzyme_transferase-Guanylate kinase, enzyme_hydrolase-Guanylate-binding protein 1, unclassified-Ras-related C3 botulinum toxin substrate 3, unclassified-Ras-related protein Rab1A, unclassified-RhoA-related GTP-binding protein RhoB, unclassified-Rho-related GTP-binding protein RhoC, enzyme_unclassified-Phosphoenolpyruvate carboxykinase, cytosolic [GTP], enzyme_unclassified-Adenylosuccinate synthetase isozyme 2, unclassified-Ras-related C3 botulinum toxin substrate 2, enzyme_unclassified-Dynamin-1, enzyme_kinase-Leucine-rich repeat serine/threonine-protein kinase 2, unclassified-GTPase NRas, unclassified-GTP-binding nuclear protein Ran, enzyme_reductase-Ribonucleoside-diphosphate reductase large subunit, unclassified-GTPase KRas | Kd=630.0, Kd=364.0, Kd=24.0, Kd=5.6, Kd=1.6, Kd=22300.0, Kd=169000.0, Kd=146000.0, Kd=146000.0, Kd=45700.0, Kd=41000.0, Kd=36500.0, Kd=18900.0, Kd=14800.0, Kd=14800.0, Kd=11800.0, Kd=11630.0, Kd=11000.0, Kd=10000.0, Kd=9300.0, Kd=8000.0, Kd=5710.0, Kd=5200.0, Kd=4900.0, Kd=3900.0, Kd=3800.0, Kd=3800.0, Kd=3500.0, Kd=1800.0, Kd=1300.0, Kd=1200.0, Kd=1000.0, Kd=1000.0, Kd=640.0, Kd=640.0, Kd=520.0, Kd=500.0, Kd=460.0, Kd=360.0, Kd=350.0, Kd=340.0, Kd=330.0, Kd=260.0, Kd=240.0, Kd=200.0, Kd=190.0, Kd=80.0 |
|        | Kd=30.0 |        |        |        |        |
|--------|---------|--------|--------|--------|--------|
| **GDS** | enzyme_unclassified-Glutathione S-transferase Mu 2, enzyme_reductase-Glutathione reductase, mitochondrial, enzyme_unclassified-Glutathione S-transferase, enzyme_unclassified-Glutathione S-transferase omega-1 | Kd=330000.0, Kd=12900.0, Kd=12200.0, Kd=3090.0, Kd=940.0, Kd=540.0, Kd=530.0 | IV     |
| **GNP** | unclassified-Ras-related C3 botulinum toxin substrate 1, cytosolic_other-GTPase HRas, enzyme_kinase-Casein kinase II subunit alpha, enzyme_hydrolase-Guanylate-binding protein 1, unclassified-Transforming protein RhoA, unclassified-GTP-binding protein RhoB, unclassified-Rho-related GTP-binding protein RhoC, unclassified-Ras-related C3 botulinum toxin substrate 3, unclassified-?, unclassified-GTPase KRas, enzyme_kinase-Phosphatidylinositol 4-kinase type-2 beta, enzyme_unclassified-Ectonucleoside triphosphate diphosphohydrolase 2, unclassified-GTPase NRas | Kd=2256.0, Kd=1574.0, Kd=1574.0, Kd=27.6, Kd=9600.0, Kd=9000.0, Kd=5770.0, Kd=4700.0, Kd=4100.0, Kd=1200.0, Kd=110.0, Kd=250000.0 | II     |
| **GSH** | enzyme_transferase-Hematopoietic prostaglandin D synthase, enzyme_unclassified-Glutathione S-transferase P, enzyme_reductase-Glutathione reductase, mitochondrial, enzyme_unclassified-Glutathione S-transferase omega-1, enzyme_lyase-Carbonic anhydrase 3, enzyme_unclassified-Maleylacetoacetate isomerase, enzyme_unclassified-Glutathione S-transferase A1, unclassified-Triggering receptor expressed on myeloid cells 1, enzyme_unclassified-Hydroxyacylglutathione hydrolase, mitochondrial, enzyme_unclassified-Glutathione S-transferase A3, enzyme_unclassified-Trypanothione reductase, surface_antigen-Major prion protein, enzyme_unclassified-Glutathione S-transferase Mu 2, enzyme_unclassified-Glutathione S-transferase Mu 1, enzyme_protease-Coagulation factor XI, enzyme_unclassified-Glutathione reductase, enzyme_unclassified-Leukotriene C4 synthase, enzyme_unclassified-Glutathione S-transferase A2, enzyme_unclassified-Thioredoxin glutathione reductase, transcription_factor-Peroxisome proliferator-activated receptor gamma, enzyme_unclassified-Carbonyl reductase [NADPH] 1, enzyme_unclassified-Prostaglandin E synthase, enzyme_unclassified-Glutathione S-transferase, enzyme_transferase-Thymidylate synthase, enzyme_protease-Suppressor of tumorigenicity 14 protein, enzyme_unclassified-Glutathione S-transferase omega-2, enzyme_unclassified-6-phosphofructo-2-kinase/fructose-2,6- | Kd=5.0, IC50=261500.0, Kd=668000.0, Kd=90000.0, Kd=23000.0, Kd=22000.0, Kd=6500.0, Kd=5200.0, Kd=3000.0, Kd=3000.0, Ki=1600.0, Ki=7000000.0, Kd=70000.0 | II     |
| Symbol | Description |
|--------|-------------|
| GSP    | unclassified-Transforming protein RhoA, cytosolic_other-?, unclassified-Rho-related GTP-binding protein RhoC, unclassified-?, unclassified-GTPase KRas, unclassified-Ras-related C3 botulinum toxin substrate 1 | Kd=5400.0, Kd=3400.0, Kd=690.0 |
| GTA    | nuclear_other-Eukaryotic translation initiation factor 4E, enzyme_unclassified-m7GpppX diphosphatase, nuclear_other-Eukaryotic translation initiation factor 4E-binding protein 1 | Ki=170.0, IC50=1700000.0 |
| GTG    | nuclear_other-Eukaryotic translation initiation factor 4E-binding protein 1, enzyme_unclassified-m7GpppX diphosphatase | Kd=4000.0, Kd=470.0, Kd=1370000.0 |
| GTP    | enzyme_unclassified-Genome polyprotein [Cleaved into: Core protein p21, DNA-?, enzyme_unclassified-Adenylosuccinate synthetase isozyme 1, unclassified-?, cytosolic_other-GTPase HRas, enzyme_unclassified-T7 RNA polymerase, enzyme_protease-Genome polyprotein [Cleaved into: P1; Capsid protein VP0, unclassified-GTP-binding protein Rheb, enzyme_unclassified-Phosphoenolpyruvate carboxykinase, cytosolic [GTP], unclassified-Ras-related C3 botulinum toxin substrate 2, enzyme_transferase-Genome polyprotein [Cleaved into: Core protein p21, enzyme_unclassified-ADP-ribose cyclase/cyclic ADP-ribose hydrolase 1, enzyme_unclassified-Glutamate dehydrogenase 1, mitochondrial, unclassified-Ras-related protein Rab-1A, enzyme_unclassified-Protein-glutamine gamma-glutamyltransferase 2, unclassified-DNA primase large subunit, cytosolic_other-?, ion_channel_other_chloride-Cystic fibrosis transmembrane conductance regulator, unclassified-GTPase KRas, enzyme_unclassified-RNA polymerase sigma factor RpoD | Kd=124.0, Kd=124.0, Kd=40.0, IC50=220.0, Kd=465000.0, Kd=115000.0, Kd=90100.0, Kd=17000.0, Kd=14100.0, Kd=2120.0, Kd=400.0, Kd=360.0, Kd=2260000.0 |
| H1S    | membrane_receptor_7tm1_peptide_chemokine_receptor_C-C motif chemokine 5, secreted-Stromal cell-derived factor 1, enzyme_hydrolase-Palmitoleoyl-protein carboxylesterase NOTUM | Kd=330.0 |
| HD2    | enzyme_protease-Bifunctional epoxide hydrolase 2 [Includes: Cytosolic epoxide hydrolase 2, enzyme_unclassified-Corticosteroid 11-beta-dehydrogenase isozyme 1 | IC50=22.0 |
| HXA    | auxiliary_transport_protein-Fatty acid-binding protein, brain, transcription_factor-Peroxisome proliferator-activated receptor gamma, enzyme_reductase-Prostaglandin G/H synthase 2 | Kd=53.4 |
| I3P    | ion_channel_lgc_ip3-Insitol 1,4,5-trisphosphate receptor type 1, enzyme_unclassified-1 | Kd=210.0, Kd=2.82, |
| #  | Gene Name                                      | Description                                                                 | Kd/Ki Values                           | IC50/Ki | IV  |
|----|-----------------------------------------------|-----------------------------------------------------------------------------|----------------------------------------|---------|-----|
| I76| enzyme_kinase-Proto-oncogene tyrosine-protein kinase Src, enzyme_unclassified-? |                             | IC50=800.0, Ki=2.8                     | IV      | I76 |
| IBI| enzyme_kinase-Serine/threonine-protein kinase PLK1, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, epigenetic_regulator_reader_brd-Bromodomain testis-specific protein |                             | IC50=0.87                              | IV      | IBI |
| IHP| secreted-Fibroblast growth factor 1, cytosolic_other-Synaptotagmin-1, enzyme_hydrolase-Toxin A, enzyme_kinase-Casein kinase II subunit alpha |                             | Kd=238.0, Kd=85.0, Kd=57.0, Ki=4000.0, Kd=22700.0, Kd=1300.0, Kd=180.0 | II      | IHP |
| IM2| enzyme_hydrolase-Beta-lactamase TEM, enzyme_hydrolase-Beta-lactamase, enzyme_protease-D-alanyl-D-alanine carboxypeptidase DacA, enzyme_protease-D-alanyl-D-alanine carboxypeptidase |                             | Kd=62.1                                | IV      | IM2 |
| IMN| transcription_factor-Peroxisome proliferator-activated receptor gamma, enzyme_unclassified-Basic phospholipase A2 VRV-PL-VIIa, enzyme_unclassified-Lactoylglutathione lyase, enzyme_unclassified-Aldo-keto reductase family 1 member C3, secreted-?, enzyme_hydrolase-Lactotransferrin, enzyme_unclassified-Lactoperoxidase, enzyme_reductase-Prostaglandin G/H synthase 2, secreted-Transthryretin, enzyme_unclassified-Aldo-keto reductase family 1 member C2, secreted-Thyroxine-binding globulin |                             | IC50=21300.0, Kd=18000.0, Kd=9730.0, Kd=1300.0, IC50=1000000.0 | IV      | IMN |
| IX6| enzyme_protease-Genome polyprotein [Cleaved into: Core protein p21, enzyme_transferase-Genome polyprotein [Cleaved into: Core protein p21 |                             | Kd=80.0, Kd=2.3                        | III     | IX6 |
| K17| enzyme_kinase-Casein kinase II subunit alpha, enzyme_unclassified-Ribosyldihydronicotinamide dehydrogenase [quinone] |                             | Ki=300.0                               | IV      | K17 |
| K25| enzyme_kinase-Casein kinase II subunit alpha, enzyme_unclassified-Ribosyldihydronicotinamide dehydrogenase [quinone] |                             | Ki=40.0                                | IV      | K25 |
| KDH| enzyme_unclassified-Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1, cytosolic_other-Troponin C, slow skeletal and cardiac muscles, secreted-Transthryretin |                             | IC50=1900.0, Kd=21600.0                | IV      | KDH |
| KTL| enzyme_hydrolase-Maltase-glucoamylase, intestinal [Includes: Maltase, enzyme_unclassified-Sucrase-isomaltase, intestinal [Cleaved into: |                             | Ki=600.0, Ki=190.0                     | IV      | KTL |
| Gene | Description | IC50/Ki | Stage |
|------|-------------|---------|-------|
| Sucrase | ion_channel_other_misc-Bcl-2-like protein 1, cytosolic_other-Induced myeloid leukemia cell differentiation protein Mcl-1 | IC50=4.4, IC50=610.0 | III |
| LOC | epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, unclassified-Neutrophil gelatinase-associated lipocalin | Ki=1800.0, Kd=20000.0 | IV |
| LP5 | surface_antigen-Lymphocyte antigen 96, enzyme_protease-Lactotransferrin | Kd=1.6 | IV |
| LQT | epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5B, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5A | IC50=19.0 | III |
| LY2 | enzyme_kinase-Serine/threonine-protein kinase pim-1, epigenetic_regulator_reader_brd-Bromodomain-containing protein 4 | IC50=68000.0, IC50=4000.0 | IV |
| LYA | membrane_receptor_unclassified-Folate receptor beta, enzyme_transferase-Thymidylylate synthase, enzyme_transferase-Thymidylylate synthase ThyA, DNA-? | Ki=109.0, Kd=54.0 | IV |
| M0N | enzyme_transferase-Farnesyl pyrophosphate synthase, enzyme_unclassified-Geranylgeranyl pyrophosphate synthase | IC50=3.0, Ki=130.0 | III |
| M2P | enzyme_unclassified-Fructose-bisphosphate aldolase A, enzyme_protease-Lactotransferrin, enzyme_unclassified-Fructose-bisphosphate aldolase | IC50=8000.0 | IV |
| M7G | nuclear_other-Eukaryotic translation initiation factor 4E, enzyme_unclassified-m7GpppX diphosphatase | Kd=83.9, Kd=68.0, Kd=26800.0, Kd=240.0 | II |
| MAL | ion_channel_igic_p2x-P2X purinoceptor 3, enzyme_hydrolase-Pancreatic alpha-amylase, enzyme_protease-Lactotransferrin, enzyme_unclassified-Glucosyltransferase-SI, unclassified-C-type lectin domain family 4 member K, transporter_electrochemical_slc-Solute carrier family 2, facilitated glucose transporter member 3, enzyme_unclassified-Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1 | Kd=110.0, Kd=6800.0, Kd=1500.0, Ki=1.0E8, Kd=1.045E7, Kd=3050000.0 | III |
| MER | enzyme_unclassified-Beta-lactamase SHV-1, enzyme_hydrolase-Beta-lactamase, enzyme_unclassified-Beta-lactamase | IC50=20.0 | III |
| MGP | enzyme_hydrolase-Poly, nuclear_other-Eukaryotic translation initiation factor 4E, ion_channel_other_chloride-Cystic fibrosis transmembrane conductance regulator | Kd=32.1, Kd=6940.0 | II |
| MIX | enzyme_unclassified-Serine/threonine-protein kinase PknB, DNA-?, enzyme_isomerase-DNA topoisomerase 2-beta, enzyme_kinase-Serine/threonine-protein kinase pim-1 | IC50=800.0 | IV |
| MLK | unclassified-?, ion_channel_igic_ach-Neuronal | Ki=41.0 | III |
| Code | Compound Name | Ki/Kd Values | Classification |
|------|---------------|--------------|----------------|
| MLR  | acetylcholine receptor subunit alpha-9 | Kd=2.8, Ki=10.0 | IV |
|      | unclassified-Pulmonary surfactant-associated protein D, enzyme_hydrolase-Pancreatic alpha-amylase | Kd=550.0, Kd=48000.0, Kd=1000.0, IC50=940000.0, Kd=1040000.0 | IV |
| MMK  | epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5C, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5B, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 5A, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 4C, epigenetic_regulator_eraser_kdm-Lysine-specific demethylase 4A | IC50=13.0, IC50=4.0, Kd=52.0 | III |
| MOF  | transcription_factor-Progesterone receptor, epigenetic_regulator_writer_hat-Nuclear receptor coactivator 2 | Ki=0.7 | IV |
| MTX  | enzyme_reductase-Dihydrofolate reductase, membrane_receptor_unclassified-Folate receptor beta, enzyme_transferase-Thymidylate synthase, enzyme_unclassified-Pteridine reductase 1, enzyme_reductase-Bifunctional dihydrofolate reductase-thymidylate synthase | IC50=12.2, Ki=21.0, Kd=281.0, Kd=55.0, Kd=40.0, Kd=4.0, Kd=0.13, Ki=13000.0, Kd=6000.0 | IV |
| MXF  | enzyme_hydrolase-Beta-lactamase, enzyme_unclassified-Beta-lactamase SHV-1 | Ki=4100.0 | III |
| MYC  | enzyme_kinase-Serine/threonine-protein kinase pim-1, enzyme_hydrolase-Pancreatic alpha-amylase, DNA-? | IC50=780.0, Ki=110000.0 | IV |
| NEC  | membrane_receptor_7tm1_smallmol_nucleotide-like_receptor-?, membrane_other_-?-?-?-?-?-Endoplasmin | Ki=430.0, Ki=13.8, Kd=200.0 | IV |
| NGH  | enzyme_protease-Macrophage metalloelastase, enzyme_protease-Stromelysin-2, enzyme_protease-Stromelysin-1, enzyme_unclassified-Matrix metalloproteinase-20 | Kd=10.0 | III |
| NOG  | secreted-Sex hormone-binding globulin, transcription_factor-Progesterone receptor | Kd=1.23 | IV |
| OPO  | enzyme_unclassified-Beta-lactamase Toho-1, enzyme_hydrolase-Beta-lactamase | IC50=271.0, IC50=22.0 | III |
| P6U  | enzyme_protease-Beta-secretase 1, enzyme_cytochrome-Cytochrome P450 2D6 | IC50=69.0 | I |
| PBD  | enzyme_transferase-Glutaminyl-peptide cyclotransferase-like protein, enzyme_unclassified-Glutaminyl-peptide cyclotransferase | Ki=944.0, Ki=944.0, Ki=101.3, Ki=101.3 | III |
| Category | Description | IC50/IC50 | Effect |
|----------|-------------|----------|--------|
| PCG      | enzyme_kinase-cGMP-dependent protein kinase 1 , ion_channel_vgc_c-gmp-Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2 , unclassified-?, enzyme_phosphodiesterase-High affinity cGMP-specific 3',5'-cyclic phosphodiesterase 9A , ion_channel_vgc_c-gmp-?, enzyme_kinase-cGMP-dependent protein kinase 2 , enzyme_kinase-cAMP-dependent protein kinase type I-alpha regulatory subunit | Ki=1817.0, Kd=1731.0, Ki=342.0, Kd=274.0, Ki=134.0, Kd=12.0, Ki=95.0, Kd=10.3 | IV |
| PCQ      | secreted-Transthyretin , enzyme_unclassified-Estrogen sulfotransferase | Kd=3.2 | I |
| PDD      | enzyme_isomerase-Alanine racemase , enzyme_unclassified-Serine racemase | Kd=2400.0 | III |
| PNT      | enzyme_protease-Cationic trypsin , enzyme_unclassified-Amiloride-sensitive amine oxidase [copper-containing] , DNA-? | Ki=290.0, Kd=64000.0, Kd=53000.0, Kd=2360.0 | IV |
| PNU      | enzyme_transferase-Gag-Pol polyprotein , transcription_factor-Nuclear receptor subfamily 1 group I member 2 | IC50=7.0 | IV |
| PVB      | enzyme_unclassified-Cell division control protein 2 homolog , enzyme_kinase-Cyclin-dependent kinase 2 , enzyme_kinase-SRSF protein kinase 2 , enzyme_kinase-Tyrosine-protein kinase ABL1 | IC50=130.0 | IV |
| QPS      | enzyme_hydrolase-Alpha-amylase type A isozyme , enzyme_unclassified-Beta-amylase | Ki=2.0 | III |
| QUE      | enzyme_kinase-Serine/threonine-protein kinase pim-1 , enzyme_unclassified-Glycogen phosphorylase, muscle form , enzyme_protease-Urokinase-type plasminogen activator , enzyme_kinase-Death-associated protein kinase 1 , enzyme_kinase-Tyrosine-protein kinase HCK , enzyme_hydrolase-ATP synthase subunit beta, mitochondrial , enzyme_hydrolase-ATP synthase subunit gamma, mitochondrial , DNA-? , enzyme_hydrolase-3-hydroxyisobutyryl-CoA hydrolase, mitochondrial , enzyme_kinase-Serine/threonine-protein kinase 17B , enzyme_reductase-Xanthine dehydrogenase/oxidase [Includes: Xanthine dehydrogenase , secreted-Transthyretin , enzyme_kinase-Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform , enzyme_reductase-Leucoanthocyanidin dioxygenase , enzyme_reductase-Nitrogenase molybdenum-iron protein alpha chain , enzyme_reductase-Nitrogenase molybdenum-iron | IC50=55.0, IC50=33500.0, IC50=8900.0, IC50=7000.0, IC50=1100.0, Ki=25100.0, Ki=12700.0 | IV |
| Protein/Enzyme | Description | Ki/Kd/IC50/Kd | Category |
|--------------|-------------|----------------|----------|
| RST | enzyme_unclassified-M17 leucyl aminopeptidase, enzyme_protease-M1 family aminopeptidase | Ki=800.0, Ki=30.0 | III |
| RSX | enzyme_unclassified-M17 leucyl aminopeptidase, enzyme_protease-M1 family aminopeptidase | Ki=14.0, Ki=5500.0 | III |
| R78 | epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, enzyme_kinase-Serine/threonine-protein kinase PLK1, enzyme_kinase-Serine/threonine-protein kinase PLK2, epigenetic_regulator_reader_brd-Bromodomain testis-specific protein, enzyme_kinase-Calcium/calmodulin-dependent protein kinase kinase 2 | IC50=25.0, IC50=8.8, IC50=5.0, Kd=37.0 | III |
| RAP | enzyme_isomerase-Peptidyl-prolyl cis-trans isomerase FKB1A, enzyme_unclassified-Peptidyl-prolyl cis-trans isomerase FKB3, enzyme_unclassified-Peptidyl-prolyl cis-trans isomerase FKB1B, DNA-? | Ki=0.9, Kd=0.2, IC50=480.0 | III |
| RDA | membrane_other-?-?-?-?-? Endoplasmin, cytosolic_other-ATP-dependent molecular chaperone HSP82 | Kd=870.0, Kd=520.0 | III |
| RDC | cytosolic_other-Heat shock protein HSP 90-alpha, cytosolic_other-ATP-dependent molecular chaperone HSP82, enzyme_unclassified-Virulence sensor histidine kinase PhoQ, membrane_other-?-?-?-?-? Endoplasmin | Kd=90.0, Kd=19.0, Kd=2.7, IC50=400000.0, Kd=715000.0, Kd=2000.0 | IV |
| REA | cytosolic_other-Cellular retinoic acid-binding protein 1, auxiliary_transport_protein-Cellular retinoic acid-binding protein 2, transcription_factor-Retinoic acid receptor RXR-alpha, unclassified-Beta-lactoglobulin, transcription_factor-Retinoic acid receptor gamma, enzyme_unclassified-Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1, enzyme_unclassified-Aldehyde dehydrogenase family 1 member A3 | Kd=250.0, Kd=120.0, Kd=2.0, Kd=0.4, Ki=280.0, Kd=100.0 | IV |
| REF | enzyme_kinase-Casein kinase II subunit alpha, enzyme_unclassified-Glycogen phosphorylase, muscle form | Ki=20.0 | IV |
| RFP | transcription_factor-Nuclear receptor subfamily 1 group I member 2, unclassified-Multidrug efflux pump subunit AcrB | IC50=12.0, IC50=398000.0, IC50=263000.0, Ki=10000.0 | IV |
| Enzyme/Protein | Kd/Ki | IC50/Ki |
|---------------|-------|---------|
| **RIT** | | |
| enzyme_hydrolase-Endothiapepsin , enzyme_protease-Gag-Pol polyprotein , enzyme_hydrolase-Candidapepsin-2 enzyme_cytochrome-Cytochrome P450 3A4 enzyme_cytochrome-Cytochrome P450 3A5 | Kd=79400.0, Ki=1070000.0 | |
| enzyme_transferase-Gag-Pol polyprotein , enzyme_protease-Endothiapepsin | Ki=48.0, Ki=10.0, Ki=6.0, Ki=4.3, Ki=4.3, Ki=4.3, Ki=3.9, Ki=3.6, Ki=3.3, Ki=2.2, Ki=0.24, Ki=0.12, Kd=176.0, Kd=67.4, Kd=125000.0 | III |
| **ROC** | | |
| enzyme_reductase-Indosine-5’-monophosphate dehydrogenase 2 , enzyme_transferase-Genome polyprotein [Cleaved into: Capsid protein C] | Ki=65.0, Ki=65.0 | IV |
| enzyme_unclassified-7,8-dihydro-8-oxoguanine triphosphatase , membrane_receptor_toll-like_1_2_?_?-Toll-like receptor 8 | IC50=2056.0, Kd=490.0 | IV |
| **RVP** | | |
| enzyme_transferase-Catechol O-methyltransferase , epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase EHMT1 , enzyme_unclassified-?, enzyme_unclassified-Indolethylamine N-methyltransferase , epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase , enzyme_unclassified-Histamine N-methyltransferase , enzyme_unclassified-Phenylethanolamine N-methyltransferase , enzyme_unclassified-Protein-L-isosaprtate, enzyme_transferase-Genome polyprotein [Cleaved into: Capsid protein C] | Kd=697.0, Kd=379.0, IC50=30000.0, IC50=30000.0, IC50=18300.0, Ki=36000.0, Ki=33000.0, Ki=690.0, Ki=3600.0, Ki=2000.0, Ki=320.0, Kd=270.0, Kd=300000.0, Kd=33000.0, Kd=26000.0, Kd=25000.0, Kd=24800.0, Kd=21200.0, Kd=17200.0, Kd=12200.0, Kd=8100.0, Kd=7900.0, Kd=5400.0, Kd=5400.0, Kd=4600.0, Kd=2700.0, Kd=2400.0, Kd=1400.0 | |
| Enzyme/Methyltransferase | Kd (μM) |
|--------------------------|---------|
| CARM1, epigenetic regulator reader brd Histone-lysine N-methyltransferase 2A, enzyme unclassified | 645.0, 600.0, 350.0 |
| Replicase polyprotein 1ab, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase SETMAR, DNA-? | 600.0, 600.0 |
| SMYD3, epigenetic regulator writer pmmt N-lysine methyltransferase SMYD2 |  |  |
| epigenetic regulator writer pmmt Histone-lysine N-methyltransferase SETD2, epigenetic regulator writer pmmt Protein arginine N-methyltransferase 6, epigenetic regulator writer pmmt Protein N-lysine methyltransferase METTL21A |  |  |
| epigenetic regulator writer pmmt Protein arginine N-methyltransferase 8, epigenetic regulator reader phd Histone-lysine N-methyltransferase 2D, epigenetic regulator reader phd Histone-lysine N-methyltransferase 2C |  |  |
| enzyme transferase-Catechol O-methyltransferase, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase SETD7, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase, H3 lysine-79 specific, enzyme unclassified-rRNA adenine N-6-methyltransferase, enzyme unclassified-Phenylethanolamine N-methyltransferase, DNA-, enzyme unclassified-S-adenosylmethionine synthase isoform type-2, epigenetic regulator reader methyl-lysine-Histone-lysine N-methyltransferase SUV39H2, epigenetic regulator writer dnmt-DNA, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase SMYD3, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase, H3 lysine-36 and H4 lysine-20 specific, epigenetic regulator reader brd Histone-lysine N-methyltransferase ASH1L, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase KMT5C, epigenetic regulator writer pmmt N-lysine methyltransferase SMYD2, epigenetic regulator writer pmmt Histone-lysine N-methyltransferase KMT5B, enzyme unclassified-?, epigenetic regulator writer pmmt N-lysine methyltransferase KMT5A, epigenetic regulator writer pmmt Protein-lysine methyltransferase METTL21D, enzyme unclassified-Cystathionine beta-synthase | 68000.0, 52000.0, 44330.0, 43000.0, 41000.0, 37200.0, 21000.0, 20000.0, 18000.0, 13000.0, 11200.0, 7320.0, 6100.0, 5590.0, 5580.0, 2100.0, 1500.0, 290.0 |
| Protein Name                                                                 | IC50/Kd (μM)          | Literature Reference |
|-----------------------------------------------------------------------------|-----------------------|----------------------|
| enzyme_unclassified-DNA adenine methylase, enzyme_unclassified-Replicase polyprotein 1ab, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase NSD2, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase EHMT2, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase EHMT1, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase NSD3 | IC50=6.3, IC50=4600.0 | III |
| SAV epigenetic_regulator_reader_brd-Bromodomain-containing protein 4, enzyme_kinase-Vascular endothelial growth factor receptor 2 |                      | III |
| enzyme_prototease-Prothrombin, secreted-Fibroblast growth factor 23, secreted-Complement factor H, enzyme_phosphatase-Receptor-type tyrosine-protein phosphatase F, enzyme_hydrolase-Palmitoleoyl-protein carboxylesterase NOTUM | Kd=4000.0             | III |
| SFG enzyme_unclassified-Replicase polyprotein 1ab, enzyme_unclassified-rRNA adenine N-6-methyltransferase, epigenetic_regulator_writer_pmt-Histone-arginine methyltransferase CARM1, DNA-?, enzyme_unclassified-Adenosylmethionine-8-amino-7-oxononanoate aminotransferase, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase SMYD3, epigenetic_regulator_writer_dnmnt-DNA, enzyme_unclassified-?, enzyme_transferase-Catechol O-methyltransferase, enzyme_unclassified-DNA adenine methylase, epigenetic_regulator_writer_pmt-Histone-lysine N-methyltransferase SETD2 | IC50=2500.0, IC50=740.0, IC50=700.0, Ki=18000.0, Kd=4200.0, Kd=340.0 | IV |
| SFI transcription_factor-Peroxisome proliferator-activated receptor gamma, enzyme_unclassified-Aldose reductase | IC50=1870.0             | IV |
| SGV enzyme_kinase-G protein-coupled receptor kinase 6, cytosolic_other-Heat shock 70 kDa protein 1A, enzyme_kinase-G protein-coupled receptor kinase 5 | Kd=3300.0, Kd=1000.0 | IV |
| SIS enzyme_prototease-Beta-secretase 1, enzyme_cytochrome-Cytochrome P450 2D6 | IC50=52.0             | I |
| SIA enzyme_prototease-Botulinum neurotoxin type B, enzyme_prototease-Tetanus toxin, adhesion-P-selectin, adhesion-E-selectin, surface_antigen-?, enzyme_unclassified-Liver carboxylesterase 1, enzyme_unclassified-Sialidase, unclassified-Sialic acid-binding Ig-like lectin 7, enzyme_unclassified-Endoglycoceramidase II, cytosolic_other-Galectin-8, cytosolic_other-Galectin-3, cytosolic_other-Galectin-9, enzyme_prototease-Prostate-specific | Kd=24.0, Kd=2.4, Ki=1820000.0, Kd=14000.0, Kd=2.3E7, Kd=8700000.0, Kd=8000000.0 | IV |
| Antigen/Enzyme | Kd/Ki Values | Kd/Ki Values | Kd/Ki Values | Kd/Ki Values |
|---------------|--------------|--------------|--------------|--------------|
| antigen, enzyme_unclassified-Botulinum neurotoxin type C, enzyme_protease-Plasminogen, secreted-Serum amyloid P-component, enzyme_hydrolase-Neuraminidase, enzyme_protease-Prothrombin, surface_antigen-Myeloid cell surface antigen CD33, unclassified-Myelin-associated glycoprotein, adhesion-B-cell receptor CD22 | Kd=6000000.0, Kd=3640000.0 | Kd=6000000.0, Kd=3640000.0 | Kd=6000000.0, Kd=3640000.0 | Kd=6000000.0, Kd=3640000.0 |
| enzyme_protease-Tetanus toxin, enzyme_unclassified-Botulinum neurotoxin type D, enzyme_unclassified-Botulinum neurotoxin type C, enzyme_hydrolase-Neuraminidase | Kd=45.5, Kd=28.0, Kd=19.7, Ki=3.7E7 | Kd=45.5, Kd=28.0, Kd=19.7, Ki=3.7E7 | Kd=45.5, Kd=28.0, Kd=19.7, Ki=3.7E7 | Kd=45.5, Kd=28.0, Kd=19.7, Ki=3.7E7 |
| enzyme_unclassified-?, cytosolic_other-Galectin-1 | Kd=0.39, Kd=56000.0, Kd=1480000.0 | Kd=0.39, Kd=56000.0, Kd=1480000.0 | Kd=0.39, Kd=56000.0, Kd=1480000.0 | Kd=0.39, Kd=56000.0, Kd=1480000.0 |
| enzyme_unclassified-Endoplasmic reticulum mannosyl-oligosaccharide 1,2-alpha-mannosidase, unclassified-? | Kd=755.0, Kd=110000.0 | Kd=755.0, Kd=110000.0 | Kd=755.0, Kd=110000.0 | Kd=755.0, Kd=110000.0 |
| cytosolic_other-E3 ubiquitin-protein ligase XIAP, enzyme_unclassified-Baculoviral IAP repeat-containing protein 2 | IC50=250.0 | IC50=250.0 | IC50=250.0 | IC50=250.0 |
| enzyme_kinase-Tyrosine-protein kinase ABL1, enzyme_kinase-Mast/stem cell growth factor receptor Kit, enzyme_kinase-Epithelial discoidin domain-containing receptor 1, enzyme_kinase-Tyrosine-protein kinase ABL2, enzyme_kinase-Proto-oncogene tyrosine-protein kinase Src, enzyme_kinase-Mitogen-activated protein kinase 14, enzyme_kinase-Tyrosine-protein kinase Lck, enzyme_kinase-Tyrosine-protein kinase SYK, enzyme_unclassified-Ribosylhydronicotinamid dehydrogenase [quinone], enzyme_kinase-Macrophage colony-stimulating factor 1 receptor | IC50=170.0, IC50=100.0, Kd=10.0, Kd=1.9, IC50=370.0, Ki=5000.0, Kd=340000.0, Kd=100000.0, Kd=2000.0, Kd=62.0 | IC50=170.0, IC50=100.0, Kd=10.0, Kd=1.9, IC50=370.0, Ki=5000.0, Kd=340000.0, Kd=100000.0, Kd=2000.0, Kd=62.0 | IC50=170.0, IC50=100.0, Kd=10.0, Kd=1.9, IC50=370.0, Ki=5000.0, Kd=340000.0, Kd=100000.0, Kd=2000.0, Kd=62.0 | IC50=170.0, IC50=100.0, Kd=10.0, Kd=1.9, IC50=370.0, Ki=5000.0, Kd=340000.0, Kd=100000.0, Kd=2000.0, Kd=62.0 |
| transcription_factor-Mineralocorticoid receptor, secreted-Corticosteroid-binding globulin, transcription_factor-Progesterone receptor, enzyme_unclassified-Aldo-keto reductase family 1 member C1, enzyme_cytochrome-Cytochrome P450 3A4, enzyme_unclassified-Aldo-keto reductase family 1 member C2, enzyme_cytochrome-Steroid 17-alpha-hydroxylase/17,20 lyase, enzyme_cytochrome-Steroid 21-hydroxylase, unclassified-? | Ki=5.1, Kd=85.0, Kd=1.0, Kd=0.39, Kd=20000.0 | Ki=5.1, Kd=85.0, Kd=1.0, Kd=0.39, Kd=20000.0 | Ki=5.1, Kd=85.0, Kd=1.0, Kd=0.39, Kd=20000.0 | Ki=5.1, Kd=85.0, Kd=1.0, Kd=0.39, Kd=20000.0 |
| enzyme_kinase-Ribosomal protein S6 kinase alpha-1, enzyme_kinase-Tyrosine-protein kinase Lyn, enzyme_kinase-Serine/threonine-protein kinase pim-1, enzyme_kinase-Tyrosine-protein kinase SYK, enzyme_kinase-Glycogen synthase kinase-3 beta, enzyme_unclassified-Serine/threonine-protein kinase/endothiocellulase IRE1, enzyme_kinase-interleukin-1 receptor-associated kinase 4, enzyme_kinase-Glycogen synthase kinase 3 beta | IC50=55.8, IC50=15.0, IC50=7.0, IC50=7.0, IC50=6.5, IC50=4.8, IC50=4.0, IC50=3.0, | IC50=55.8, IC50=15.0, IC50=7.0, IC50=7.0, IC50=6.5, IC50=4.8, IC50=4.0, IC50=3.0, | IC50=55.8, IC50=15.0, IC50=7.0, IC50=7.0, IC50=6.5, IC50=4.8, IC50=4.0, IC50=3.0, | IC50=55.8, IC50=15.0, IC50=7.0, IC50=7.0, IC50=6.5, IC50=4.8, IC50=4.0, IC50=3.0, |
| Protein Class | Description | IC50/Ki/Kd (μM) |
|---------------|-------------|----------------|
| enzyme_kinase-Serine/threonine-protein kinase 24 | IC50=1.3, IC50=0.3, Ki=8.0, Ki=7.8, Ki=0.33, Kd=30.5, Kd=9.0, IC50=41000.0, IC50=91000.0, IC50=30000.0, IC50=12.0, IC50=10.0, IC50=4.0 |
| enzyme_kinase-Tyrosine-protein kinase Fyn | |
| enzyme_kinase-TGF-beta receptor type-1 | |
| enzyme_kinase-Tyrosine-protein kinase ZAP-70 | |
| enzyme_kinase-3-phosphoinositide-dependent protein kinase 1 | |
| enzyme_kinase-Cyclin-dependent kinase 2 | |
| enzyme_kinase-Dual specificity protein kinase TTK | |
| enzyme_kinase-Protein kinase C theta | |
| enzyme_kinase-Serine/threonine-protein kinase Chk1 | |
| enzyme_kinase-Tyrosine-protein kinase CSK | |
| enzyme_unclassified-Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform | |
| enzyme_kinase-MAP kinase-activated protein kinase 2 | |
| enzyme_kinase-Tyrosine-protein kinase Lck | |
| enzyme_kinase-Tyrosine-protein kinase ITK/TSK | |
| enzyme_kinase-Death-associated protein kinase 1 | |
| enzyme_kinase-Serine/threonine-protein kinase 16 | |
| enzyme_kinase-Mitogen-activated protein kinase kinase 5 | |
| enzyme_kinase-MAP kinase-interacting serine/threonine-protein kinase 2 | |
| enzyme_kinase-Ephrin type-B receptor 4 | |
| enzyme_kinase-Ribosomal protein S6 kinase beta-1 | |
| enzyme_kinase-Tyrosine-protein kinase Fes/Fps | |
| enzyme_kinase-Dual specificity mitogen-activated protein kinase kinase 6 | |
| enzyme_kinase-ALK tyrosine kinase receptor | |
| enzyme_kinase-LIM domain kinase 1 | |
| enzyme_kinase-Serine/threonine-protein kinase 32A | |
| enzyme_kinase-TGF-beta receptor type-2 | |
| enzyme_kinase-Receptor-interacting serine/threonine-protein kinase 2 | |
| enzyme_kinase-Serine/threonine-protein kinase PAK 4 | |

| Protein Class | Description | IC50/Ki/Kd (μM) |
|---------------|-------------|----------------|
| enzyme_protease-Prothrombin | IC50=70.0, IC50=22000.0, IC50=20000.0, IC50=81000.0, Ki=115600.0, Kd=600.0, Kd=440.0 |
| epigenetic_regulator_eraser_hdac-NAD-dependent protein deacylase sirtuin-5, mitochondrial | |
| epigenetic_regulator_reader_methyl-lysine-? | |
| enzyme_unclassified-Pyruvate kinase | |
| SWF | secreted-?, enzyme_cytochrome-Cytochrome P450 2C9 | Kd=2900.0 |
| SY9 | ion_channel_ligic_gly-?, unclassified-? | Ki=38.0, Kd=52.0 |
| T3 | transcription_factor-Thyroid hormone receptor alpha, transcription_factor-Thyroid hormone receptor beta, transcription_factor-Androgen receptor, unclassified-Proliferating cell nuclear antigen | Kd=90.9 |
| T44 | secreted-Transthyretin, secreted-?, transcription_factor-Thyroid hormone receptor beta, secreted-Thyroxine-binding globulin | Kd=2.0, IC50=10500.0, Kd=5720.0 |
| Protein Name                                      | Kd/Ki Values         | Category |
|--------------------------------------------------|----------------------|----------|
| transcription_factor-Thyroid hormone receptor alpha | Kd=4900.0,Kd=2300.0,Kd=260.0,Kd=170.0 |          |
| TDZ                                              | Kd=17.0              | I        |
| TFP                                              | Kd=1000.0            | III      |
| THG                                              | Kd=15.0              | III      |
| TTP                                              | Kd=3270.0            | II       |
| USP                                              | IC50=14000.0,IC50=6900.0,IC50=3800.0,Kd=35000.0,Kd=28200.0,Kd=13000.0 | II       |
| Enzyme/Non-Enzyme | Description | IC50/Ki/Kd (nmol/L) |
|-------------------|-------------|---------------------|
| UDP              | enzyme_hydrolase-Toxin A , enzyme_unclassified-Deoxycytidine kinase , enzyme_unclassified-N-acetyllactosaminide alpha-1,3-galactosyltransferase , enzyme_unclassified-Seminal ribonuclease , enzyme_unclassified-Ribonuclease pancreatic , enzyme_unclassified-Galactosylgalactosylxyllosylprotein 3-beta-galacturonosyltransferase 3 , enzyme_unclassified-UDP-galactose 4-epimerase , enzyme_unclassified-Histo-blood group ABO system transferase , enzyme_unclassified-Galactosylgalactosylxyllosylprotein 3-beta-galacturonosyltransferase 1 , enzyme_hydrolase-Toxin B , unclassified-Polypeptide N-acetylgalactosaminyltransferase 2 , enzyme_unclassified-Beta-1,4-galactosyltransferase 1 , enzyme_unclassified-UDP-3-O-acyl-N-acetylgalactosamine deacetylase , enzyme_transferase-Oleandomycin glycosyltransferase , enzyme_transferase-UDP-N-acetylgalactosamine 1-carboxyvinyltransferase , enzyme_unclassified-UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit , enzyme_unclassified-Galactofuranosyltransferase GifT2 , enzyme_unclassified-UDP-galactopyranose mutase , unclassified-Protein O-linked-mannose beta-1,2-N-acetylgalactosaminyltransferase 1 , enzyme_unclassified-Alpha-1,6-mannosylglycoprotein 2-beta-N-acetylgalactosaminyltransferase | IC50=30000.0, IC50=1800.0, Ki=1046400.00000001, Kd=53000.0, Kd=16000.0, Kd=11400.0, Kd=540.0, Kd=650000.0, Kd=258000.0, Kd=60000.0, Kd=32000.0 |
| UFP              | enzyme_transferase-Thymidylate synthase , DNA-?, enzyme_unclassified-Flavin-dependent thymidylate synthase , enzyme_transferase-Thymidylate synthase ThyA | Ki=14.0 |
| UMP              | enzyme_transferase-Thymidylate synthase , enzyme_unclassified-Putative deoxyuridine triphosphatase , enzyme_reductase-Bifunctional dihydrofolate reductase-thymidylate synthase , enzyme_unclassified-?, enzyme_unclassified-5',DNA-?, enzyme_unclassified-Uridine 5'-monophosphatase synthase , enzyme_transferase-Thymidylate synthase ThyA , enzyme_unclassified-Deoxycytidine kinase | Kd=16000.0, Kd=11000.0, Kd=7500.0, Kd=7300.0, Kd=4000.0, Kd=2700.0, Kd=1700.0, Kd=1600.0, Kd=870.0, Kd=850.0 |
| UMP              | enzyme_kinase-Proto-oncogene tyrosine-protein kinase ROS , enzyme_kinase-ALK tyrosine kinase receptor , enzyme_unclassified-7,8-dihydro-8-oxoguanine triphosphatase , enzyme_kinase-Hepatocyte growth factor receptor | IC50=605.0, IC50=30.0, Ki=8.2, Ki=1.3, Ki=0.88, Ki=0.38, Kd=781.0, Ki=2.0 |
| Ligand | UniProt/ChEMBL Target | IC50/Ki (μM) | Subset Assignment |
|--------|-----------------------|--------------|------------------|
| WY4    | enzyme_hydrolase-Beta-lactamase, enzyme_unclassified-Beta-lactamase SHV-1 | IC50=9.0, IC50=6.2 | III |
| XDI    | transcription_factor-Peroxisome proliferator-activated receptor gamma, enzyme_unclassified-Estrogen sulfotransferase, secreted-Transthyretin | IC50=700.0 | IV |
| XDM    | epigenetic_regulator_reader_brd-CREB-binding protein, epigenetic_regulator_reader_brd-Histone acetyltransferase p300 | Kd=10100.0, Kd=3060.0 | IV |
| ZMR    | enzyme_hydrolase-Neuraminidase, enzyme_unclassified-Sialidase, enzyme_unclassified-Sialidase-2 | IC50=75.7, IC50=1.36, IC50=1.11, IC50=0.5, IC50=0.41, Kd=20.85, Ki=1.9, Ki=1.65, Ki=0.18, IC50=52000.0, IC50=4.0, Ki=720000.0, Ki=170000.0 | III |

All 192 multifamily ligands are listed together with their UniProt/ChEMBL target and family information and their subset assignment (I-IV) according to the text. In addition, for each ligand, all affinity data available in PDBbind were extracted and are reported. Affinity measurements were often not available for all crystallographic targets. However, reported data might also include measurements for targets other than those that are listed. For specific target-affinity assignments of interest, the original PDBbind records of each ligand should be accessed.