Supporting Information

Discovery of New STAT3 Inhibitors as Anticancer Agents Using Docking-Based Ligand-Receptor Contacts Fingerprints and Bioactivity - Classifying Machine Learning

Nour Jamal Jaradat[1], Walhan Alshaer [2], Mamon Hatmal[3], Mutasem Omar Taha[1]*

[1]Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of Jordan, Amman 11492, Jordan.

[2]Cell Therapy Center, the University of Jordan, Amman 11942, Jordan.

[3]Department of Medical Laboratory Sciences, Faculty of Applied Medical Sciences, The Hashemite University, P.O. Box 330127, Zarqa 13133, Jordan

*Corresponding Author.,

Telephone: 00962 6 5355000 ext. 23305.

Fax: 00962 6 5339649.

Email: mutasem@ju.edu.jo

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SM1. Docking

LibDock

The site-feature docking algorithm (LibDock) docks ligands, after the removal of their hydrogen atoms, into the active site guided by the binding hotspots. The ligands' conformations are aligned to polar and nonpolar receptor interaction sites, i.e., hotspots[31, 32]. The following LibDock parameters were implemented in the current study: CAT-CONFIRM module of Discovery Studio 4.5 was utilized to produce a maximum of 255 conformers (not exceeding an energy threshold of 20 kcal/mol from the most stable conformer) for each ligand employing "CAESAR" conformation generation option. A binding site sphere of 12.5 Å radius surrounding the centre of the copied co-crystallized ligand (PDB code: KQV) from the STAT3 crystallographic structure (PDB code: 6NJS) was utilized to locate the binding site. The number of binding site hotspots (polar and apolar) was set to 100. The ligand-to-hotspots matching RMSD tolerance value was set to 0.25 Å. The maximum number of poses saved for each ligand during hotspots matching before final pose minimization = 100. Maximum number of poses to be saved for each ligand in the binding pocket = 100. Minimum LibDock score (poses below this score are not reported) = 100. Maximum number of rigid body minimization steps during the final pose optimization (using BFGS method) = 50. Maximum number of steric clashes allowed before the pose-hotspot alignment is terminated (specified as a fraction of the heavy atom count) = 0.1. Maximum value for nonpolar solvent accessible surface area for a particular pose to be reported as successful = 15.0 $Å^2$. Maximum value for polar solvent accessible solvent area for a particular pose to be reported as successful = 5.0 $Å^2$. Docked poses/conformers were finally energy-minimized using the SMART minimizer option in LibDock. This option performs two minimization steps: Initial 1000 steps of Steepest Descent with an RMS gradient tolerance of three (kcal/mol/Å), followed by a maximum of 1000 steps of

Conjugate Gradient minimization with an RMS gradient tolerance of 0.001 (kcal/mol/Å) and minimization energy change of 0.0 kcal.

CDOCKER

CDOCKER is a CHARMm-based simulated annealing/molecular dynamics methodology that applies rigid receptor for docking [34]. The following CDOCKER parameters were implemented in the current project. A binding site sphere of 12.5 Å radius surrounding the centre of the co-crystallized ligand (PDB code: 6NJS; PDB code of ligand: KQV) was implemented. Starting ligands' conformers were energy-minimized then heated to 1000 K over 1000 molecular dynamics steps to generate 10 starting random conformations for each ligand. Each random conformer was rotated 10 times within the binding pocket for consequent energy refinement. The Van der Waals energies of the resulting conformers/poses were evaluated and those of ≥ 300 kcal/mol were discarded. Surviving conformers/poses were exposed to a cycle of simulated annealing over 2000 heating steps to targeted temperature of 700 K followed by 5000 cooling steps to targeted temperature of 300 K. The docked poses were energy minimized to a final minimization gradient tolerance zero Kcal/mol/Å. Top 100 poses were saved for subsequent scoring.

LigandFit

LigandFit employs Monte-Carlo techniques to create ligand conformations and docks them into the active site utilizing shape-based initial docking[33]. The following LigandFit settings were implemented in the current research. A binding site composed of 8434 grid points (grid spacing of 0.5Å in the X., Y and Z dimensions) surrounding the co-crystallized ligand within STAT3 (PDB code: 6NJS., PDB code of ligand: KQV) was used. Monte Carlo search parameters are as follows:

Number of trials = 30000 and search step for torsions with polar hydrogens = 30.0. The RMS threshold for ligand-to-binding site shape match was set to 2.5 Å., assuming a maximum of three binding site partitions. Interaction energy parameters: The interaction energies were assessed using CFF force field (version 1.02) with a non-bonded cutoff distance of 10.0 Å and distance dependent dielectric. An energy grid extending 3.0 Å from the binding site was implemented. The interaction energy was estimated by a trilinear interpolation value using soft potential energy approximations. Rigid body ligand minimization parameters: 40 steepest descend followed by 80 BFGS minimization iterations were applied to every orientation of the docked ligand. The maximum number of retained poses is 100. Each docked pose/conformer was energy-minimized using the SMART minimizer option in LigandFit., which executes two minimization steps: Initial 1000 steps of Steepest Descent with an RMS gradient tolerance of 3 (kcal/mol/Å)., followed by a maximum of 1000 steps of Conjugate Gradient minimization with an RMS gradient tolerance of 0.001 (kcal/mol/Å) and minimization energy change of 0.0 kcal.

SM2. Machine Learning

Random Forests (RF)

RF is a multipurpose ML strategy for classification based on ensemble of Decision Trees (DTs). Each tree predicts a classification independently and "votes" for the related class. Most of the votes decide the overall RF predictions[21]. We implemented RF Learner node within KNIME Analytics Platform (Version 4.3.3) with the following settings: Splitting criterion is Information Gain Ratio (which normalizes the standard information gain by the split entropy to overcome any unfair preference for nominal splits with many child nodes)., Number of trees = 100. No limitations were imposed on the number of levels or minimum node size.

eXtreme Gradient Boosting (XGBoost)

eXtreme Gradient Boosting (XGBoost., or XGB) relies on the ensemble of weak decision tree (DT) type models to create boosted., DT-type models. This system includes a novel tree learning algorithm., a theoretically justified weighted quantile sketch process with parallel and distributed computing[22]. We implemented the XGBoost Learner node within KNIME Analytics Platform (Version 4.3.3) with the following settings: Tree booster was implemented with depthwise grow policy., boosting rounds = 100., Eta = 0.3., Gamma = 0., maximum depth = 6., minimum child weight = 1., maximum delta step = 0., subsampling rate = 1., column sampling rate by tree = 1., column sampling rate by level = 1., lambda = 1., Alpha = 0., sketch epsilon =0.03., scaled positive weight = 1. Maximum number of bins = 256., Sample type (uniform)., Normalize type (tree)., and Dropout rate = 0.

Naïve Bayes

Naïve Bayes (NB) is a simple classifier whereby class labels are predicted and assigned to external observations based on vectors of descriptors for some limited set of training observations. NB classifier presumes each descriptor to contribute independently to the probability that certain observation (i.e., docked pose) belongs to a particular class (i.e., active, intermediate, or inactive)[23]. The probability of certain observation to belong to certain class is the multiplication of the individual probabilities of that class within each individual descriptor[24].

Probabilistic Neural Network PNN

It is a feed forward neural network used for classification and pattern recognition. PNN is formed by replacing the sigmoid activation function with an exponential function that can compute nonlinear decision boundaries approaching the Bayes optimal. A PNN classifier, having four layers of neural network, can be used to map any input pattern to any number of classification[25, 26]. PNN models were built using the PNN learner node default settings within KNIME Analytics Platform (Version 4.3.3).

k-Nearest Neighbors (kNN)

The kNN classifier depends on a distance learning methodology that calculates the activity value of an unknown member based on the bioactivities of a certain number (k) of nearest neighbors (kNNs) in the training set. In this classifier., the similarity is measured by a distance metric[17]. We implemented kNN Learner node within KNIME Analytics Platform (Version 4.3.3). The value of k was scanned from 3 to 5. The runs were repeated to include all possible combinations (i.e., of k) resulting from allowing the influence of neighbors to be either distance-dependent or distance-independent.

Multilayer perceptron (MLP)

MLP which is a modification of the standard linear perceptron, has a neural network architecture consisting of a layer with several nodes., where each node connects to a subsequent node in another layer. The concept of NN is that each input into the neuron has its own weight., that is adjusted to train the network. In between the inputs and the output layer., there may be several hidden layers[27]. We implemented the MLP learner node in its default settings within the KNIME Analytics Platform (Version 4.3.3).

SM3. Biological evaluation of the captured hits

Cell viability assay (MTT) and IC_{50} determination

Rapid colorimetric test based on mitochondrial dehydrogenase enzymes' capacity to transform 3,-4,5 dimethylthiazol -2,5 diphenyl tetrazolium bromide (MTT) into a purple formazan precipitate. A multi-well plate reader is used to measure the optical density after the formazan crystals have been dissolved. Due to its simplicity and suitability for automation, MTT has thus emerged as the preferred technique for first drug screening in cell lines to assess cell viability[54].

To determine the IC_{50} of NCI hits for cells under study., first; an MTT assay was performed. Approximately 8×10^3 cells per well were seeded into a 96 well plate (Corning., USA) and treated with different concentrations of NCI ligands., Both treated and control cells were incubated at 37 °C in a 5% CO_2 incubator for 72 h after which the old media was aspirated and the MTT assay salt (Bioworld., USA) in 100 µl of fresh media was added to each well. Following that., plates were incubated at 37 °C for 3 h., and then 50 µl of solubilization solution (DMSO) was added to each well. The absorbance of the solution was measured at 570 nm using Glomax plate reader (Promega., USA) to determine cells' viability.

Quantitative Polymerase Chain Reaction (qPCR) analysis

qPCR analysis was performed to determine the expression intensities of target genes (c-Myc and Bcl-xl) at mRNA levels. Cells were lysed by Trizol-hybrid method for RNA extraction using miniRNeasy kit (Qiagen, USA). The extracted RNA was quantified by Nanodrop (Thermofisher, USA). To synthesize cDNA, 0.5 µg total RNA was reverse transcribed using PrimeScript RT Master Mix (Cat No. RR036A, Takara, China) using T100™ Thermal cycler PCR instrument (BioRad, USA). Primers were designed using Primer-BLAST (RRID:SCR_003095) and obtained from IDT (USA) (Table S2).

The qPCR reaction mix was prepared by mixing 25 ng of cDNA with 200 nM of gene-specific forward and reverse primers (IDT), 7.2 µL of nuclease-free water, and 10 µL of SYBR Premix Ex Taq II (Tli RNaseH Plus) (Cat No. RR820L, Takara, China). The amplification was performed on CFX96 C1000 Touch thermal cycler (BioRad, USA) with the following temperature setting: (i) 95 ° C for 3 minutes, (ii) 40 cycles 95 ° C for 5 seconds and 61 ° C for 30 seconds. 18srRNA and actin-β were used as housekeeping reference genes. Each sample was examined in triplicate, and

a mean value was calculated. Data were analyzed according to ΔΔCt method using CFX Maestro™ Software - Bio-Rad.

Table S1. Chemical structures of modeled compounds in SMILE formats and their reported bioactivities

Compound	Chembl ID	SMILES	IC_{50} (nM)
1	CHEMBL156448	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCC(N)=O)C(=O)NCC(=O)N[C@@H](CC(=O)O)C(N)=O)C(C)C	8000
2	CHEMBL405322	CC(=O)N[C@@H](Cc1ccc(C(=O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	6000
3	CHEMBL160849	CC(=O)N[C@@H](Cc1ccc(CP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	8000
4	CHEMBL346370	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	1600
5	CHEMBL160730	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CCC(N)=O)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](C)C(=O)N[C@@H](CCCCN)C(N)=O	6000
6[a]	CHEMBL156168	CC[C@H](C)[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CO)C(=O)N[C@H](C(N)=O)C(C)C	30000
7	CHEMBL157314	CC(=O)N[C@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(=O)O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	6000
8	CHEMBL346706	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CO)C(=O)N[C@@H](CC(=O)O)C(=O)NCC(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](Cc1ccccc1)C(N)=O	150000
9	CHEMBL156407	CC(=O)N[C@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](C)C(=O)N[C@H](C(N)=O)C(C)C	800
10[a]	CHEMBL160658	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@H](CCC(N)=O)C(N)=O	1000
11	CHEMBL156046	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)NC(C)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	4000

12	CHEMBL348612	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@H](CS)C(=O)N[C@H](CN[C@@H](CO)C(N)=O)CC(=O)O	80000
13	CHEMBL2371210	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CO)C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H](Cc1c[nH]cn1)C(N)=O)C(C)C)C(C)C)[C@@H](C)O	>150000
15	CHEMBL348880	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(N)=O	6000
16	CHEMBL2373425	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](Cc1c[nH]cn1)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N1CCC[C@H]1C(N)=O)C(C)C	6000
17	CHEMBL423775	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CS)C(N)=O	60000
18[a]	CHEMBL348181	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@@H](CCCN=C(N)N)C(N)=O)[C@@H](C)O	8000
19[a]	CHEMBL156465	CC(=O)N[C@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	6000
20	CHEMBL348182	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](Cc1c[nH]cn1)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CCC(N)=O)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CC(C)C)C(N)=O	150000
21	CHEMBL158446	CC(=O)N[C@@H](Cc1ccc(-c2nn[nH]n2)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	6000
22[a]	CHEMBL345419	CSCC[C@H](NC(=O)[C@H](C)NC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](CCCN=C(N)N)NC(=O)[C@@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(N)=O	1000
23	CHEMBL160353	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@H](CCC(N)=O)C(=O)N[C@@H](C(N)=O)[C@H](C)O	600
24	CHEMBL433511	CC(=O)N[C@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	2000

25	CHEMBL157727	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@H](CCC(N)=O)C(=O)N[C@@H](C(=O)N[C@H](C)C(=O)O)[C@@H](C)O	400
26	CHEMBL347438	CC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@@H](C)O	6000
27	CHEMBL351757	CSCC[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(N)=O	1500
28[a]	CHEMBL2371211	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCCN)C(=O)N[C@H](C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](Cc1ccccc1)C(N)=O)[C@@H](C)O	20000
29	CHEMBL436427	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCC(=O)O)C(=O)N[C@@H](CO)C(N)=O	6000
30	CHEMBL160733	CSCC[C@H](NC(=O)[C@H](CCC(N)=O)NC(=O)[C@H]1CCCN1C(=O)[C@H](CCCCN)NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N[C@@H](Cc1c[nH]cn1)C(N)=O	400
31	CHEMBL197719	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCN(CC(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)CC1	57100
32	CHEMBL370000	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N1CCCCC1	7000
33	CHEMBL371452	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC[S+](C)[O-])C(=O)N[C@H](C(N)=O)[C@@H](C)O	9870
34[a]	CHEMBL196561	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)NCCCC(N)=O	1780
35	CHEMBL382978	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	600
36	CHEMBL194446	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)NC1CCCC(C(N)=O)C1	9810
37	CHEMBL436319	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	3110

38	CHEMBL197513	CCCC[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	717
39	CHEMBL197580	CCC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	497
40	CHEMBL366244	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N1CCCC(C(N)=O)C1	11800
41	CHEMBL370095	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N1CCCC(C(N)=O)C1	882
42	CHEMBL382709	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N(C)C	1850
43	CHEMBL372758	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	1660
44[a]	CHEMBL370547	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	13400
45	CHEMBL194453	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(=O)N(C)C)C(=O)N[C@H](C(N)=O)[C@@H](C)O	80000
46	CHEMBL193433	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C)c1ccccc1	801
47[a]	CHEMBL425747	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCCC(C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)C1	38600
48	CHEMBL371537	CC[C@H](C)[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	1070
49[a]	CHEMBL371871	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC1CCCCC1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	910
50	CHEMBL372118	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@]1(C)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	1870

51	CHEMBL371705	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	1240
52	CHEMBL196884	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N1CCN(CC(N)=O)CC1	1400
53	CHEMBL382544	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)O	748
54[a]	CHEMBL436479	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N1CCC(CC(N)=O)C1	1690
55	CHEMBL197658	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)C(c1ccccc1)c1ccccc1	>100000
56	CHEMBL372993	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N1CCCC1	2110
57	CHEMBL372429	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1C[C@H](O)C[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	484
58	CHEMBL371056	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC(C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)CC1	34600
59	CHEMBL365749	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)NCCCCCC(N)=O	9780
60	CHEMBL196664	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N(C)[C@H](C(N)=O)[C@@H](C)O	1220
61	CHEMBL370763	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)CCc1ccccc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCc1ccccc1	125
62[a]	CHEMBL370649	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
63	CHEMBL196122	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCS(C)(=O)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	13900

64	CHEMBL425571	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccccc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	814
65	CHEMBL435121	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)OCc1ccccc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	750
66[a]	CHEMBL373124	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N1CCC(C(N)=O)CC1	3020
67	CHEMBL370208	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](C)c1ccccc1	596
68	CHEMBL194855	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCc1ccccc1	409
69	CHEMBL198548	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H](C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)C(C)C	1540
70	CHEMBL442785	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](Cc1ccccc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	1890
71	CHEMBL194427	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N(C)[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
72[a]	CHEMBL197844	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)CCc1ccccc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	276
73	CHEMBL373136	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)Nc1cccc(C(N)=O)c1	36600
74	CHEMBL436504	CNC(=O)CC[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	18100
75	CHEMBL193800	CCN(CC)C(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCN1C(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(C)=O	4220
76[a]	CHEMBL508923	O=C(Cc1ccc2c(c1)OCO2)NCCc1ccc(O)c(O)c1	357000
77	CHEMBL524275	Cc1oc(C)c2c(=O)cc(-c3ccc(O)c(O)c3)cc(O)c12	106000

78[a]	CHEMBL414034	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](COC(N)=O)C(=O)NCc1ccccc1	379
79	CHEMBL267246	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCc1ccccc1	135
80	CHEMBL376795	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](C(=O)NCc1ccccc1)[C@@H](C)OC(N)=O	850
81	CHEMBL398067	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)NCc1ccccc1	800000
82	CHEMBL412549	COc1cccc(NC(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc2ccc(OP(=O)(O)O)cc2)NC(=O)c2ccc(C#N)cc2)c1	31000
83	CHEMBL393817	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)NC1CCCCC1	58000
84	CHEMBL234465	CC(C)CNC(=O)[C@H](CC(C)C)NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1	74000
85[a]	CHEMBL234817	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)NCc1ccncc1	123000
86	CHEMBL234466	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)NCCCO	620000
87	CHEMBL392556	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)O	310000
88	CHEMBL438852	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(OP(=O)(O)O)cc1)NC(=O)c1ccc(C#N)cc1)C(=O)Nc1ccccc1	310000
89	CHEMBL439390	CC(=O)N[C@@H](Cc1ccc(-c2nn[nH]n2)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	800000
90	CHEMBL414897	CC(=O)N[C@@H](Cc1ccc(OCC(=O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	1000
91	CHEMBL231705	CC(=O)N[C@@H](Cc1ccc(OCC(=O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	108000
92	CHEMBL395165	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	9000

93[a]	CHEMBL396939	CC(=O)N[C@@H](Cc1ccc(CP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	138000
94	CHEMBL233355	CC(=O)N[C@@H](Cc1ccc(Cc2nn[nH]n2)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(=O)O)C(C)C)[C@@H](C)O	1000
95	CHEMBL443407	CC(C)C[C@H](NC(=O)c1ccc2cc(OP(=O)(O)O)ccc2c1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
96	CHEMBL471109	CC(C)C[C@H](NC(=O)Cc1c[nH]c2ccc(OP(=O)(O)O)cc12)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
97	CHEMBL505076	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@H](C)O	739
98	CHEMBL454365	CNC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3	269
99	CHEMBL2372260	CC(=O)N1Cc2ccc(OP(=O)(O)O)cc2C[C@H]1C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
100	CHEMBL503765	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H]1CCc2cccc3c2N(C1=O)[C@H](C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)C3	231
101	CHEMBL505207	NC(=O)CC[C@H](NC(=O)[C@@H]1CC[C@H]2CC[C@H](NC(=O)/C=C/c3ccc(OP(=O)(O)O)cc3)C(=O)N12)C(=O)NCc1ccccc1	45700
102	CHEMBL449547	NC(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(=O)NCc1ccccc1	162
103	CHEMBL515762	NC(=O)C1CCN(C(=O)[C@@H]2Cc3cccc4c3N2C(=O)[C@@H](NC(=O)/C=C/c2ccc(OP(=O)(O)O)cc2)CC4)C1	595
104	CHEMBL503946	C[S+]([O-])CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	7600
105	CHEMBL500738	CC(C)C[C@H](NC(=O)/C=C/c1cccc(OP(=O)(O)O)c1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	>100000
106	CHEMBL504218	NC(=O)CC[C@H](NC(=O)[C@H]1CC[C@H]2CC[C@H](NC(=O)/C=C/c3ccc(OP(=O)(O)O)cc3)C(=O)N21)C(=O)NCc1ccccc1	59800

107[a]	CHEMBL508912	NC(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C=C3)C(=O)NCc1ccccc1	195
108	CHEMBL501981	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H]1CCc2ccc3c2N(C1=O)[C@H](C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)C3	1650
109[a]	CHEMBL486267	C[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	25060
110	CHEMBL485921	CC(C)C[C@H](NC(=O)c1cc2cc(OP(=O)(O)O)ccc2[nH]1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	186
111	CHEMBL504633	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1c2ccccc2C[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	4640
112	CHEMBL475488	O=C(O)CCCNC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3	815
113[a]	CHEMBL503365	COC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3	141
114	CHEMBL447460	CC(C)NC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3	815
115[a]	CHEMBL470227	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O	136
116[a]	CHEMBL448296	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H]1CC[C@H]2CC[C@@H](C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)N2C1=O	141
117	CHEMBL502869	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@H]1CC[C@@H]2CC[C@H](C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(N)=O)[C@@H](C)O)N2C1=O	24700
118	CHEMBL510008	NC(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(=O)O	359
119	CHEMBL455671	CS(=O)(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	7030
120	CHEMBL449511	NC(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	233
121	CHEMBL513887	NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3	35600

122	CHEMBL508900	C[C@@H](O)[C@H](NC(=O)[C@H](CCC(N)=O)NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)CCc1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	3240
123	CHEMBL445970	NC(=O)CC[C@H](NC(=O)[C@@H]1CC[C@@H]2CC[C@H](NC(=O)/C=C/c3ccc(OP(=O)(O)O)cc3)C(=O)N21)C(=O)NCc1ccccc1	604
124	CHEMBL452194	NC(=O)CC[C@H](NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)c1cc2cc(OP(=O)(O)O)ccc2[nH]1)CC3)C(=O)NCc1ccccc1	190
125[a]	CHEMBL468082	CCCC[C@H](NC(=O)[C@H](C)NC(=O)[C@@H]1Cc2cccc3c2N1C(=O)[C@@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)CC3)C(N)=O	19200
126[a]	CHEMBL573901	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CC(N)=O)C(=O)NCc1ccccc1	874
127[a]	CHEMBL573930	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)C(C)C	511
128	CHEMBL583726	CC(=O)OC[C@H](CCC(N)=O)NC(=O)[C@@H]1[C@@H]2C[C@@H]2CN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	290
129	CHEMBL573048	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCCC(N)=O	574
130	CHEMBL575513	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)CN(Cc1ccccc1)Cc1ccccc1	1080
131	CHEMBL574844	CC(C)C[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	4900
132	CHEMBL573903	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)Cc1ccc(O)cc1	848
133[a]	CHEMBL575919	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCC#CC(N)=O	1140
134	CHEMBL574636	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCNC(N)=O	131
135[a]	CHEMBL577143	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)NCCCC(N)=O	303
136	CHEMBL573902	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](COCc1ccccc1)COC(N)=O	454
137	CHEMBL583116	CCCC[C@H](CCC(N)=O)NC(=O)[C@@H]1[C@@H]2C[C@@H]2CN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	499
138	CHEMBL573049	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C)CCC(N)=O	1180

139	CHEMBL583756	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](COC(N)=O)[C@@H](C)OCc1ccccc1	6900
140	CHEMBL576590	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCOC(N)=O	360
141	CHEMBL573905	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)CN1CCN(C)CC1	1310
142	CHEMBL577593	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H]1CN[C@H](C(N)=O)C1	3210
143	CHEMBL576785	CCCC[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	1350
144	CHEMBL583727	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)COCc1ccccc1	94
145	CHEMBL575098	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCCC(=O)NN	1830
146[a]	CHEMBL583758	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)[C@@H](C)OCc1ccccc1	272
147	CHEMBL576784	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@H](C)CCC(N)=O	175
148[a]	CHEMBL573068	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H]1CN[C@H](C(N)=O)C1	3600
149	CHEMBL584376	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](C)COC(N)=O	797
150	CHEMBL575497	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCc1ccccc1	68
151	CHEMBL583754	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCC(N)=O)C(=O)NCc1ccccc1	1400
152	CHEMBL578430	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1CCC(N)=O	3310
153	CHEMBL502473	CC(=O)N[C@@H](Cc1ccc(OP(=O)(O)O)cc1)C(=O)N[C@@H](CC(C)C)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@H](C)O	290
154	CHEMBL574202	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NC/C=C\C(N)=O	1110
155	CHEMBL583725	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)[C@@H](C)O	437

156[a]	CHEMBL583138	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCC(=O)NCc1ccccc1	4940
157	CHEMBL574654	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(N)=O	11400
158	CHEMBL578233	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C)C(N)=O	7800
159	CHEMBL575920	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(C)C	1880
160	CHEMBL573904	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)COCc1ccccc1	294
161	CHEMBL583963	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)CN1CCCCC1	1210
162[a]	CHEMBL574875	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCCC(=O)NO	2640
163	CHEMBL576736	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)NCCCS(N)(=O)=O	68200
164	CHEMBL573069	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](C)CNC(N)=O	1350
165	CHEMBL573643	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)COC(N)=O	615
166	CHEMBL584974	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)CN1CCOCC1	1530
167	CHEMBL573980	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](CN)CCC(N)=O	1240
168	CHEMBL575484	CC(C)C[C@H](CCC(N)=O)NC(=O)[C@@H]1[C@@H]2C[C@@H]2CN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	1630
169	CHEMBL573443	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1C[C@H]2C[C@H]2[C@H]1C(=O)N[C@@H](CCC(N)=O)[C@@H](C)OCc1ccccc1	69
170	CHEMBL573442	CC(=O)NC[C@H](CCC(N)=O)NC(=O)[C@@H]1CCCN1C(=O)[C@H](CC(C)C)NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1	589
171	CHEMBL578635	CC(C)C[C@H](NC(=O)/C=C/c1ccc(OP(=O)(O)O)cc1)C(=O)N1CCC[C@H]1C(=O)N[C@H](C)CCC(N)=O	110
172	CHEMBL1290746	Cc1ccc(C(=O)Nc2ccon2)cc1NC(=O)c1cnn(-c2ccccc2F)c1N	10000
173	CHEMBL1687978	O=C(Nc1nnc(-c2ccco2)o1)c1cc(-c2cccc3ccccc23)nc2ccccc12	55000
174	CHEMBL1687967	O=C(Nc1nnc(-c2ccc(Cl)cc2)o1)c1cc(-c2ccccc2)nc2ccccc12	61000

175	CHEMBL1687977	O=C(Nc1nnc(-c2ccco2)o1)c1cc(-c2ccco2)nc2ccccc12	66000
176	CHEMBL1687965	O=C(Nc1nnc(-c2ccoc2)o1)c1cc(-c2ccccc2)nc2ccccc12	72000
177[a]	CHEMBL1687969	O=C(Nc1nnc(-c2ccccc2)o1)c1cc(-c2ccccc2)nc2ccccc12	66000
178	CHEMBL1687966	O=C(Nc1nnc(Cc2ccccc2)o1)c1cc(-c2ccccc2)nc2ccccc12	75000
179	CHEMBL1562195	O=C(Nc1nnc(-c2cccs2)o1)c1cc(-c2ccccc2)nc2ccccc12	75000
180	CHEMBL1687979	O=C(Nc1nnc(-c2ccco2)o1)c1cc(-c2ccccc2)nc2ccccc12	74000
181	CHEMBL1687976	O=C(Nc1nnc(-c2ccco2)o1)c1cc(-c2cccs2)nc2ccccc12	63000
182	CHEMBL2172008	CCN1C(=O)/C(=C/c2ccc(-c3ccc(C(=O)O)cc3)o2)SC1=S	30000
183[a]	CHEMBL2031566	O=C(O)CSc1cc(NS(=O)(=O)c2ccc(C(=O)O)cc2)c2ccccc2c1O	73000
184	CHEMBL2171900	COC(=O)Cc1c(C)c2ccc(OCc3ccc(C(=O)OC)cc3)c(C)c2oc1=O	63000
185	CHEMBL2171898	O=C(O)c1ccc(/C=C/C(=O)c2ccc3c(c2)OCCO3)cc1	91000
186	CHEMBL2171899	CCOc1cc(C=C2C(=O)c3ccccc3C2=O)cc(Cl)c1OCc1cccc(C(=O)O)c1	144000
187	CHEMBL2172009	CCN1C(=O)C(=Cc2ccc(-c3cc(C(=O)O)ccc3Cl)o2)C(=O)N(CC)C1=S	114000
188	CHEMBL187460	C[C@H]1COC2=C1C(=O)C(=O)c1c2ccc2c1CCCC2(C)C	4600
189	CHEMBL207155	C1=Cc2nc1cc1ccc([nH]1)c(-c1ccccc1)c1nc(cc3ccc([nH]3)c2-c2ccccc2)C=C1	280
190	CHEMBL1337170	O=[N+]([O-])c1ccc2c(c1)S(=O)(=O)C=C2	5100
192	CHEMBL2347240	Oc1ccc(NCc2cc(Cl)ccc2OCc2ccc(Cl)cc2)cc1	26680
193	CHEMBL2367507	CC(C)C[C@H](NC(=O)[C@H](Cc1ccc(O)cc1)NC(=O)[C@H]1CCCN1C(=O)CN)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@H](C(=O)N[C@H](C(N)=O)C(C)C)[C@H](C)O	300
194	CHEMBL2431922	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccc(F)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	17600
195	CHEMBL2431990	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2C)cc1	8800
196	CHEMBL2431924	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2cccc(Cl)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	18200
197	CHEMBL2429889	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cc(F)c(F)c(F)c2F)cc1	22200
198	CHEMBL2431991	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(C)c2)cc1	5200
199	CHEMBL2431959	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2cccc(F)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	17800
200	CHEMBL2431977	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccncc2)cc1	46600

201[a]	CHEMBL2431971	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc([N+](=O)[O-])cc2)cc1	11000
202	CHEMBL2431993	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2C(F)(F)F)cc1	2800
203	CHEMBL2431985	CCCN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1ccc(C)cc1	17800
204	CHEMBL2431967	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(OC(F)(F)F)c2)cc1	8000
205[a]	CHEMBL2431975	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccn2)cc1	45200
206[a]	CHEMBL2431995	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(C(F)(F)F)cc2)cc1	9200
207[a]	CHEMBL1829876	CN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	25600
208[a]	CHEMBL2431992	Cc1ccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2ccc(C)cc2)cc1	50000
209	CHEMBL2431932	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2cc(F)c(F)c(F)c2F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	12400
210	CHEMBL2431955	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2C(F)(F)F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	12800
211	CHEMBL2431969	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2[N+](=O)[O-])cc1	10000
212[a]	CHEMBL2431986	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)CC(C)C)cc1	17000
213	CHEMBL2431981	Cc1ccc(S(=O)(=O)NCC(=O)Nc2ccc(C(=O)O)c(O)c2)cc1	300000
214	CHEMBL2431961	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(F)c2)cc1	9000
215	CHEMBL2023989	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)C(=O)OC(C)(C)C)cc1	115000
216	CHEMBL2431974	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(N)cc2)cc1	20800
217	CHEMBL2431984	Cc1ccc(S(=O)(=O)NCC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)cc1	50000
218	CHEMBL2431939	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2c(F)cc(F)c(F)c2F)cc1	15400

219	CHEMBL2431968	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(OC(F)(F)F)cc2)cc1	11800
220	CHEMBL2431988	Cc1ccc(S(=O)(=O)N(CC(N)=O)CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)cc1	50000
221[a]	CHEMBL2431936	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccc3ccccc3c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	21800
222	CHEMBL2431949	CCCN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	20600
223	CHEMBL2431923	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2Cl)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	11000
224[a]	CHEMBL2431925	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccc(Cl)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	13800
225	CHEMBL2431958	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	28000
226	CHEMBL2431946	COC(=O)c1cccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2ccc(C)cc2)c1	18400
227[a]	CHEMBL2431982	Cc1ccc(S(=O)(=O)N(C)CC(=O)Nc2ccc(C(=O)O)c(O)c2)cc1	300000
228[a]	CHEMBL2172013	Cc1ccc(S(=O)(=O)OCC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)cc1	43000
229	CHEMBL2431928	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccc(OC(F)(F)F)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	21600
230	CHEMBL2431979	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(C#N)c2)cc1	12400
231	CHEMBL2431972	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2N)cc1	24000
232	CHEMBL2431989	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2)cc1	14400
233[a]	CHEMBL2431950	CC(C)(C)OC(=O)N(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	27400
234	CHEMBL2431964	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(Cl)c2)cc1	6000
235	CHEMBL2431976	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccnc2)cc1	50000
236	CHEMBL2431941	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2c(F)c(F)c(F)c(F)c2F)cc1	8100

237	CHEMBL2431978	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2C#N)cc1	22600
238	CHEMBL2431951	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	14400
239	CHEMBL2431956	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2cccc(C(F)(F)F)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	9600
240	CHEMBL2431938	COC(=O)c1cccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)c1	30800
241[a]	CHEMBL2431931	N#Cc1ccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	9400
242[a]	CHEMBL2431953	Cc1cccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)c1	14600
243	CHEMBL2431948	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CNS(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	32400
244	CHEMBL2431957	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccc(C(F)(F)F)cc2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	22000
245	CHEMBL2431987	C=CCN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1ccc(C)cc1	50000
246[a]	CHEMBL2431965	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(Cl)cc2)cc1	6200
247	CHEMBL2431927	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2cccc(OC(F)(F)F)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	17800
248	CHEMBL2431934	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2c(F)c(F)cc(F)c2F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	16600
249[a]	CHEMBL2431945	CCOC(=O)c1ccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2ccc(C)cc2)cc1	7600
250[a]	CHEMBL2431942	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc3ccccc3c2)cc1	5000
251	CHEMBL2431966	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2OC(F)(F)F)cc1	7200
252	CHEMBL2431970	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc([N+](=O)[O-])c2)cc1	5000
253	CHEMBL2431983	Cc1ccc(S(=O)(=O)N(CC(=O)Nc2ccc(C(=O)O)c(O)c2)C(=O)OC(C)(C)C)cc1	300000
254	CHEMBL2431943	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(F)cc2C(F)(F)F)cc1	11000

255	CHEMBL2431933	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2c(F)cc(F)c(F)c2F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	17600
256	CHEMBL2431963	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2Cl)cc1	15800
257	CHEMBL2431935	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2c(F)c(F)c(F)c(F)c2F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	11000
258	CHEMBL2431947	COC(=O)c1ccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2ccc(C)cc2)cc1	11600
259	CHEMBL2431954	Cc1ccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1	14400
260	CHEMBL2431994	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(C(F)(F)F)c2)cc1	10200
261[a]	CHEMBL2431937	COC(=O)c1ccccc1CN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	17400
262[a]	CHEMBL1829786	Cc1ccc(S(=O)(=O)N(C)CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)cc1	31000
263	CHEMBL2431952	Cc1ccccc1CN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	11800
264	CHEMBL2431926	O=C(O)c1ccc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2OC(F)(F)F)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)cc1O	10200
265	CHEMBL2431944	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(SC(F)(F)F)cc2)cc1	9600
266	CHEMBL2431940	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2c(F)c(F)cc(F)c2F)cc1	22800
267	CHEMBL2431929	N#Cc1ccccc1CN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(C(=O)O)c(O)c1)S(=O)(=O)c1c(F)c(F)c(F)c(F)c1F	11400
268	CHEMBL2431980	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(C#N)cc2)cc1	8600
269	CHEMBL2431973	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2cccc(N)c2)cc1	12400
270	CHEMBL2431962	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccc(F)cc2)cc1	7600
271[a]	CHEMBL2431960	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)Cc2ccccc2F)cc1	10600
272	CHEMBL477936	Cc1ccc(S(=O)(=O)OCC(=O)Nc2ccc(C(=O)O)c(O)c2)cc1	84000

273	CHEMBL2431930	N#Cc1cccc(CN(CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(C(=O)O)c(O)c2)S(=O)(=O)c2c(F)c(F)c(F)c(F)c2F)c1	19800
274	CHEMBL3126485	CN(C)CCCN1C(=O)c2ccc3c4ccc5c6c(ccc(c7ccc(c2c37)C1=O)c64)C(=O)N(CCCN(C)C)C5=O	4500
275	CHEMBL3133482	O=C(O)c1cc(N(Cc2ccc(Cl)cc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	15000
276	CHEMBL3133484	O=C(O)c1cc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	23300
277[a]	CHEMBL3133490	Cc1ccc(S(=O)(=O)N(C)CC(=O)N(Cc2ccc(C3CCCCC3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	45000
278	CHEMBL3133491	CN(CC(=O)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(O)c(C(=O)O)c1)S(=O)(=O)c1ccc(-c2ccccc2)cc1	32000
279	CHEMBL3133493	CC(C)Cc1ccc(CN(C(=O)CN(C)S(=O)(=O)c2ccc(-c3ccc(Cl)cc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	20000
280	CHEMBL3133487	Cc1ccc(S(=O)(=O)N(C)CC(=O)N(Cc2ccccc2)c2ccc(O)c(C(=O)O)c2)cc1	1000000
281	CHEMBL3133486	CC(C)Cc1ccc(CN(C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	17000
282	CHEMBL3133494	CN(CC(=O)N(Cc1ccc(Cl)cc1)c1ccc(O)c(C(=O)O)c1)S(=O)(=O)c1ccc(-c2ccc(Cl)cc2)cc1	43000
283	CHEMBL3133472	CN(CC(=O)N(Cc1cccc(-c2ccncc2)c1)c1ccc(O)c(C(=O)O)c1)S(=O)(=O)c1ccc(-c2ccccc2)cc1	35300
284	CHEMBL3133488	CN(CC(=O)N(Cc1ccccc1)c1ccc(O)c(C(=O)O)c1)S(=O)(=O)c1ccc(-c2ccccc2)cc1	57000
285	CHEMBL3133468	O=C(O)c1cc(N(Cc2ccc(C3CCNCC3)cc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	300000
286	CHEMBL3133454	COc1ccc(CN(C(=O)c2ccc(Oc3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	118100
287	CHEMBL3133492	CCCCCCCc1ccc(CN(C(=O)CN(C)S(=O)(=O)c2ccc(-c3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	22000
288[a]	CHEMBL3133483	COc1ccc(CN(C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	22000
289	CHEMBL3133467	CCCCCCCc1ccc(CN(C(=O)CN(C)S(=O)(=O)c2ccc(-c3ccc(F)cc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	23000
290	CHEMBL3133459	O=C(O)c1cc(N(Cc2ccc(C3CCCCC3)cc2)C(=O)c2ccc(Oc3ccccc3)cc2)ccc1O	15000

291	CHEMBL3133475	O=C(c1ccc(Oc2ccccc2)cc1)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(CP(=O)(O)O)cc1	28400
292	CHEMBL3133473	O=C(c1ccc(Oc2ccccc2)cc1)N(Cc1ccc(C2CCCCC2)cc1)c1ccc(P(=O)(O)O)cc1	42000
293[a]	CHEMBL3133485	CCCCCCCc1ccc(CN(C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	19000
294	CHEMBL3133466	COc1ccc(CN(C(=O)CN(C)S(=O)(=O)c2ccc(-c3ccc(Cl)cc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	50000
295	CHEMBL3133469	O=C(O)c1cc(N(Cc2cccc(-c3ccncc3)c2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	33500
296	CHEMBL3133489	CN(CC(=O)N(Cc1ccc(Cl)cc1)c1ccc(O)c(C(=O)O)c1)S(=O)(=O)c1ccc(-c2ccccc2)cc1	61000
297	CHEMBL3133460	CCCCCCCc1ccc(CN(C(=O)c2ccccc2)c2ccc(O)c(C(=O)O)c2)cc1	32000
298	CHEMBL3133458	CCCCCCCc1ccc(CN(C(=O)c2ccc(Oc3ccccc3)cc2)c2ccc(O)c(C(=O)O)c2)cc1	12800
299	CHEMBL3133481	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccc(Cl)cc2)c2ccc(O)c(C(=O)O)c2)Cc2ccccc2)cc1	50000
300[a]	CHEMBL3133470	O=C(O)c1cc(N(Cc2ccc(N3CCOCC3)cc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	94700
301[a]	CHEMBL3133461	CCCCCCCc1ccc(CN(C(=O)c2cccc(OC)c2)c2ccc(O)c(C(=O)O)c2)cc1	33300
302	CHEMBL3133456	O=C(O)c1cc(N(Cc2ccc(Cl)cc2)C(=O)c2ccc(Oc3ccccc3)cc2)ccc1O	48000
303[a]	CHEMBL3133496	O=C(O)c1cc(N(Cc2cccc2)C(=O)CN(Cc2ccccc2)S(=O)(=O)c2ccc(-c3ccccc3)cc2)ccc1O	22200
304	CHEMBL3133476	O=C(c1ccc(Oc2ccccc2)cc1)N(Cc1ccc(C2CCCCC2)cc1)c1cccc(CP(=O)(O)O)c1	18900
305	CHEMBL3133495	Cc1ccc(S(=O)(=O)N(CC(=O)N(Cc2ccccc2)c2ccc(O)c(C(=O)O)c2)Cc2ccccc2)cc1	201300
306	CHEMBL3133457	O=C(O)c1cc(N(Cc2ccc(Br)cc2)C(=O)c2ccc(Oc3ccccc3)cc2)ccc1O	52000
307	CHEMBL1241908	O=C(N/N=C/c1coc2ccccc2c1=O)c1cccnc1	180000
308	CHEMBL3218348	O=C(Nc1nonc1-c1ccc(Cl)cc1)c1ccc(C(F)(F)F)cc1	17700
309	CHEMBL3600746	COc1ccc(S(=O)(=O)Nc2ccccc2-c2ccc(C#N)cc2)cc1	440
310	CHEMBL3600853	COc1ccc(S(=O)(=O)N(C(C)=O)c2ccccc2-c2ccc(C#N)cc2)cc1	320
311	CHEMBL3600755	COc1ccc(S(=O)(=O)Nc2ccccc2-c2ccc(F)c(F)c2)cc1	2750
312[a]	CHEMBL3600757	COc1ccc(S(=O)(=O)Nc2ccccc2-c2ccc(C#N)c(F)c2)cc1	200

313	CHEMBL3600744	COc1ccc(S(=O)(=O)Nc2ccccc2-c2ccc(F)cc2)cc1	4020
314	CHEMBL3628691	COc1cc(CNc2nn[nH]n2)cc(Cl)c1OCc1ccc([N+](=O)[O-])cc1	25700
315[a]	CHEMBL4227152	C=C(C)C(=O)N(Cc1ccc(Br)cc1)C(=O)/C=C/c1cc(OC)c(OC)c(OC)c1	10000
316	CHEMBL465843	COc1cc(/C=C/C(=O)N2CCC=CC2=O)cc(OC)c1OC	7000

Table S2: STAT3 complexes in Protein Data Bank (PDB).

Protein Data bank code[a]	Resolution (Å)	Molecular weight of Co-crystallized ligand	Ligand affinity Ki (nM)	Description	Reference
4ZIA	2.7	not found	not found	Crystal Structure of STAT3 N-terminal domain	31
3CWG	3.05	not found	not found	Unphosphorylated mouse STAT3 core fragment	32
6QHD	2.85	not found	not found	Lysine acetylated and tyrosine phosphorylated STAT3 in a complex with DNA	33
4E68	2.59	not found	not found	Unphosphorylated STAT3B core protein binding to dsDNA	34
5U5S	Solution NMR	188.22 N(6)-Acetyl lysine	not found	Solution structures of Brd2 second bromodomain in complex with stat3 peptide	35
6NJS	2.7	835.79 KQV	14 nM	Stat3 Core in complex with compound SD36	36
6NUQ	3.15	835.79 KQV	14 nM	Stat3 Core in complex with compound SI109	36
1BG1	2.25	not found	not found	Transcription Factor Stat3b/DNA Complex	37
6TLC	2.9	not found	not found	Unphosphorylated human STAT3 in complex with MS3-6 monobody	38

[a]Searching the PDB database for STAT3 complexes identified 32 protein structures, out of which only 9 are STAT3 protein structures (listed in the table above), the rest are STAT3-related cellular signaling proteins and were therefore neglected. Two of the nine STAT3 structures are short fragments and unsuitable for docking purposes (namely, 4ZIA and 5U5S, respectively).

Table S3: Cross correlation (R^2) matrix of the 9 docking- scoring functions used in this experiment [a,b].

	LigScore 1	LigScore 2	PLP1	PLP2	Jain	PMF	PMF04	Cdocker energy	Cdocker interaction energy
LigScore 1	1.00								
LigScore 2	0.53	1.00							
PLP1	0.28	0.71	1.00						
PLP2	0.27	0.70	0.97	1.00					
Jain	0.17	0.52	0.80	0.84	1.00				
PMF	0.19	0.50	0.60	0.59	0.47	1.00			
PMF04	0.16	0.49	0.57	0.57	0.44	0.86	1.00		
Cdocker energy	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	
Cdocker interaction energy	0.05	0.28	0.42	0.45	0.48	0.24	0.24	0.00	1.00

[a] A value of 0 implies that there is no linear dependency between the two variables. While a value of 1 indicates the existence of a perfect linear equation connecting the corresponding scoring functions pair.

[b] Cross correlation equation value exceeding 0.9 implies significant linearity between the two variables.

Table S4: Independent samples T-test statistical analysis and related statistical criteria for evaluating the difference between highly potent compounds (IC_{50} < 1.0 μM) and less potent compounds ($IC_{50} \geq 1.0$ μM) within the "active" category in SHAP selected descriptors used for building Hypo-1 and Hypo-2.

	Group Statistical criteria[a]				t-test for equality of means (α = 0.05)
SHAP descriptors	**Group[b,c]**	**Observations (N)**	**Mean**	**Standard deviation**	***p*-value (2-tailed)**
PLP2	$IC_{50} \geq 1.0$ μM	4045	93.84	34.44	0.000
	IC_{50} < 1.0 μM	5384	96.84	35.413	
PMF	$IC_{50} \geq 1.0$ μM	4045	75.62	28.61	0.036
	IC_{50} < 1.0 μM	5384	76.90	30.03	
Cdocker Energy	$IC_{50} \geq 1.0$ μM	4045	$-11.93*10^{13}$	$75.32*10^{14}$	0.318
	IC_{50} < 1.0 μM	5384	$-10.66*10^{11}$	$33.63*10^{12}$	
Cdocker Interaction Energy	$IC_{50} \geq 1.0$ μM	4045	-65.16	145.25	0.031
	IC_{50} < 1.0 μM	5384	-58.53	148.96	
SER 613 HN	$IC_{50} \geq 1.0$ μM	4045	0.28	0.45	0.602
	IC50 < 1.0 μM	5384	0.28	0.45	

[a]Docked poses of all active compounds (training and testing) were considered for the analysis

[b] Docked poses corresponding to active docked compounds with $IC_{50} \geq 1.0$ μM.

[c] Docked poses corresponding to active docked compounds with IC_{50} < 1.0 μM.

Table S5: Forward and reverse primer sequences for STAT3 target genes analyzed in q-PCR

Gene	Forward primer	Reverse primer
c-myc	GGATTCTCTGCTCTCCTCGAC	CTTCTTGTTCCTCCTCAGAGTC
Bcl-XL	CCAGGGTCTTCCCTACCTCA	GACTGGCCCTTCTAGTCAGC

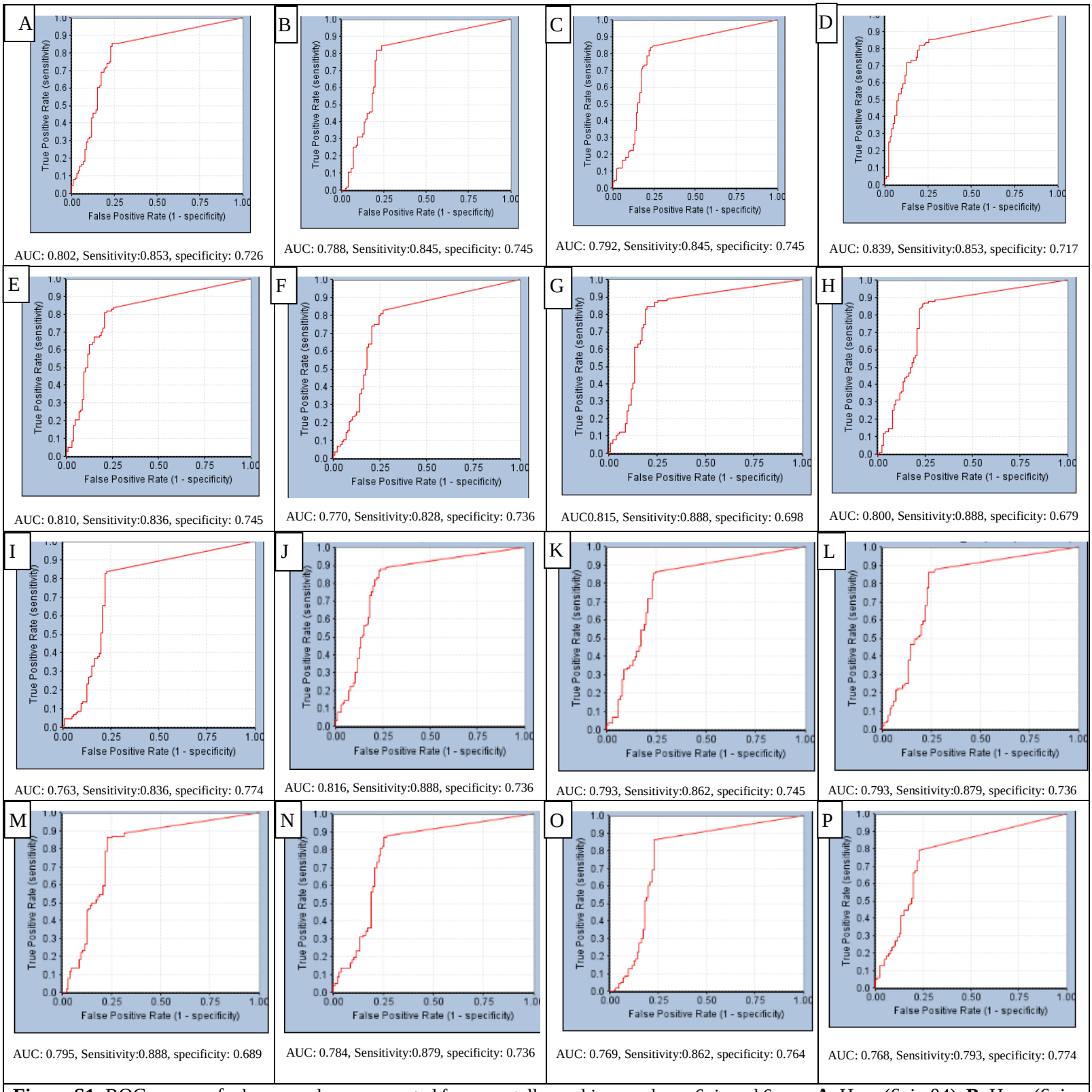


Figure S1: ROC curves of pharmacophores generated from crystallographic complexes 6njs and 6nuq : **A.** Hypo(6njs-04), **B.** Hypo(6njs-05), **C**. Hypo(6njs-06), **D.** Hypo(6njs-08), **E.** Hypo(6njs-09), **F.** Hypo(6njs-10), **G.** Hypo(6nuq-01), **H.** Hypo(6nuq-02), **I.** Hypo(6nuq-03), **J.** Hypo(6nuq-04), **K.** Hypo(6nuq-05), **L.** Hypo(6nuq-06), **M.** Hypo(6nuq-07), **N.** Hypo(6nuq-08), **O.** Hypo(6nuq-09), **P.** Hypo(6nuq-10).

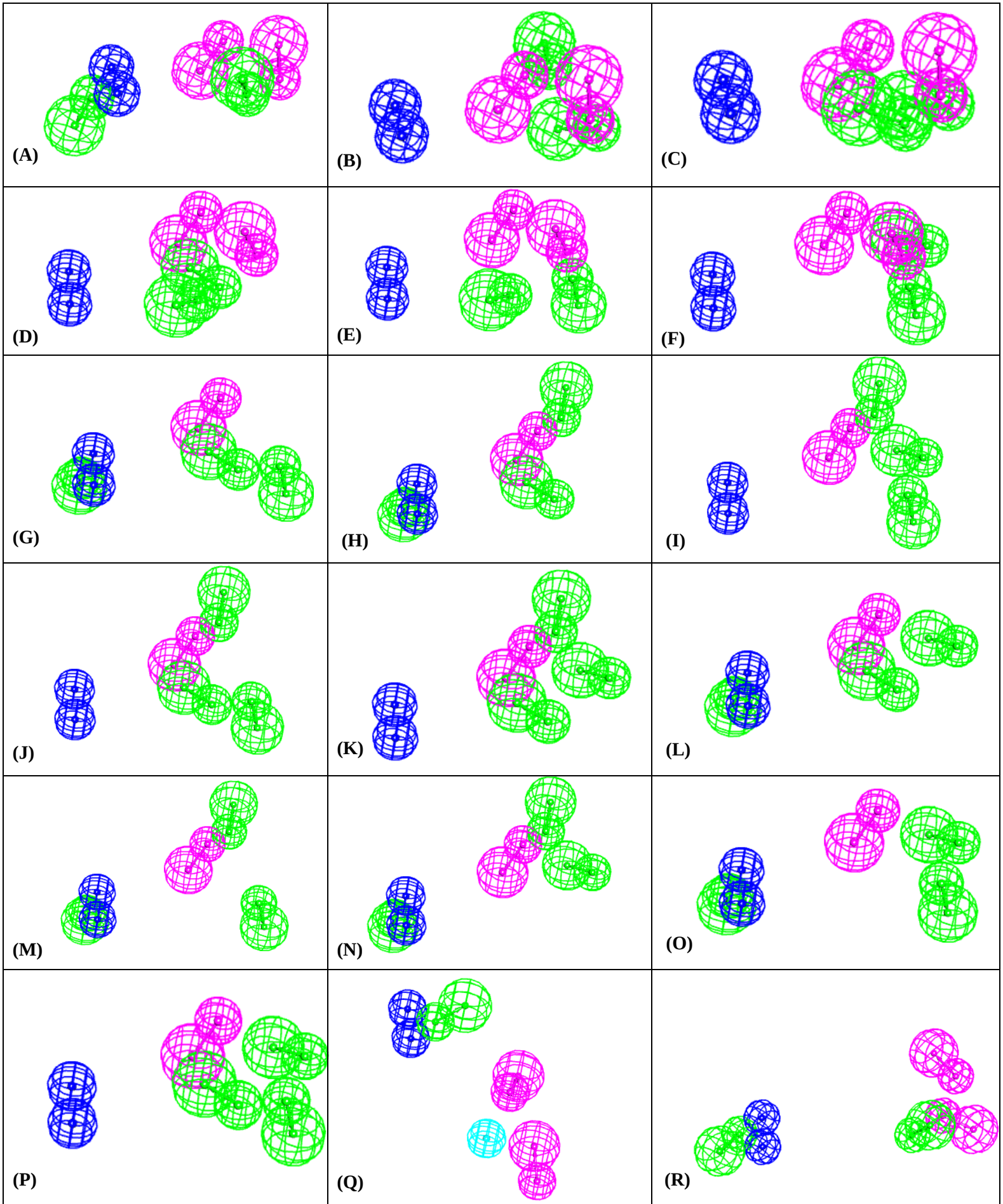
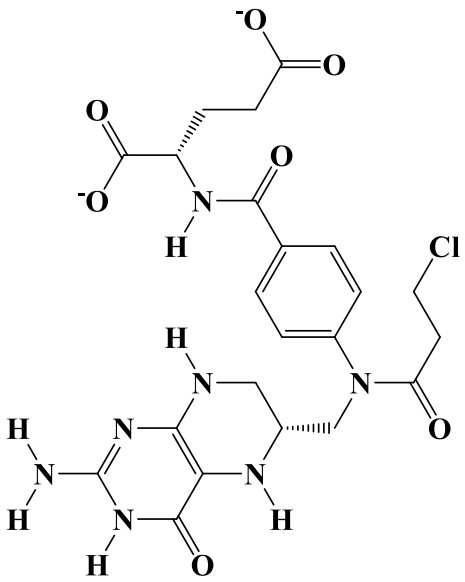
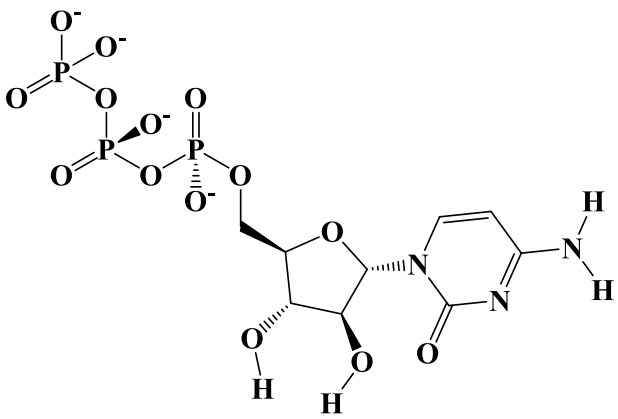


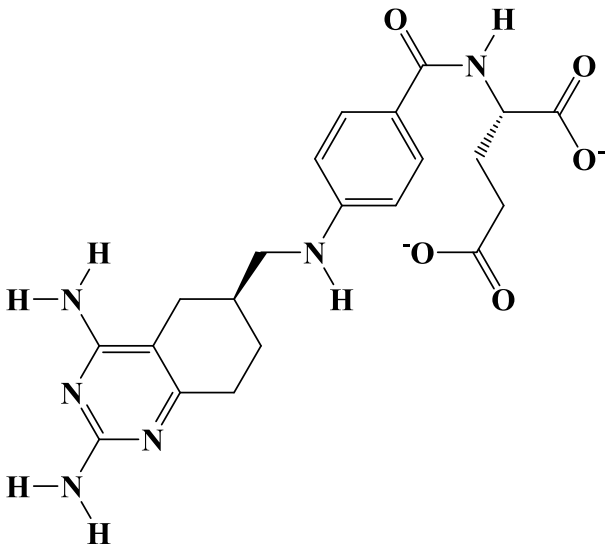
Figure S2: Pharmacophores generated from crystallographic complexes 6njs and 6nuq. **(A)** Hypo(6njs-04), **(B)** Hypo(6njs-05), **(C)** Hypo(6njs-06), **(D)** Hypo(6njs-08), **(E)** Hypo(6njs-09), (F) Hypo(6njs-10), **(G)** Hypo(6nuq-01), **(H)** Hypo(6nuq-02), **(I)** Hypo(6nuq-03), **(J)** Hypo(6nuq-04), **(K)** Hypo(6nuq-05), **(L)** Hypo(6nuq-06), **(M)** Hypo(6nuq-07), **(N)** Hypo(6nuq-08), **(O)** Hypo(6nuq-09), **(P)** Hypo(6nuq-10), **(Q)** Hypo-1 and **(R)** Hypo-2.



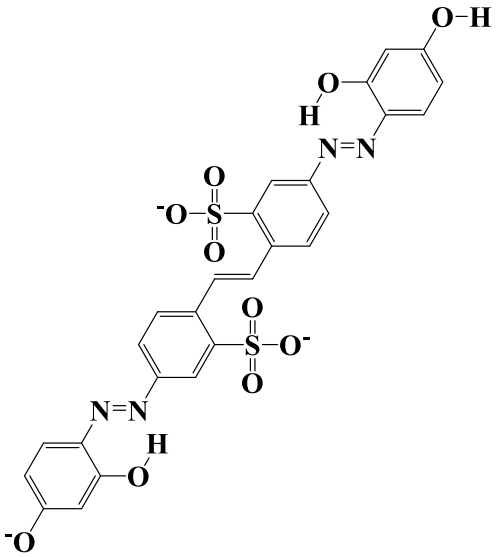
317 (NCI code: 3590)



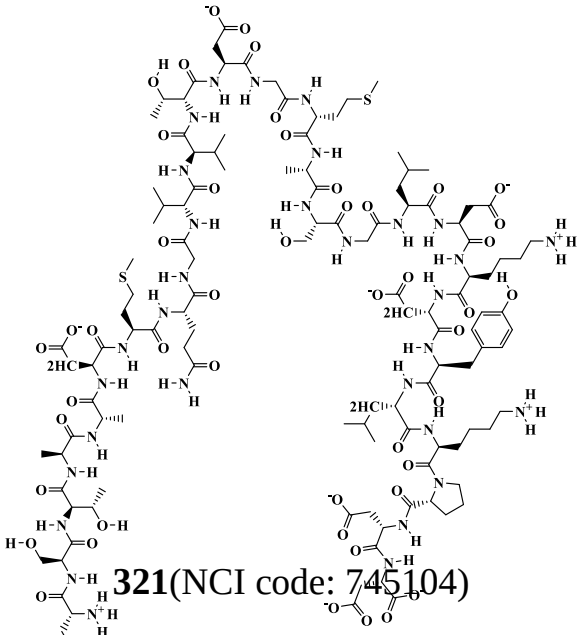
318 (NCI code: 20261)



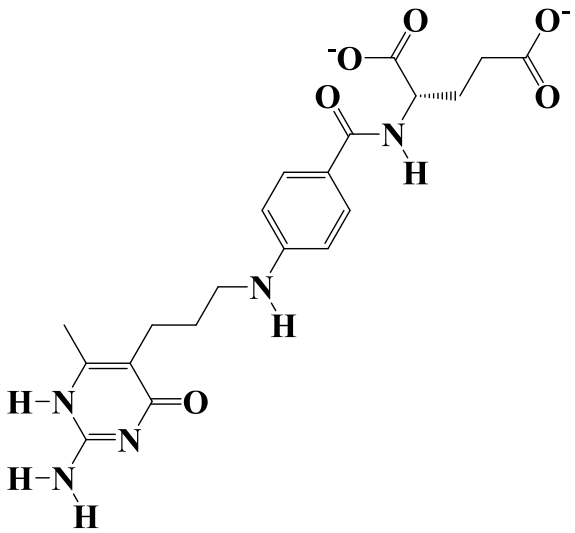
319 (NCI code: 59407)



320 (NCI code:65832)

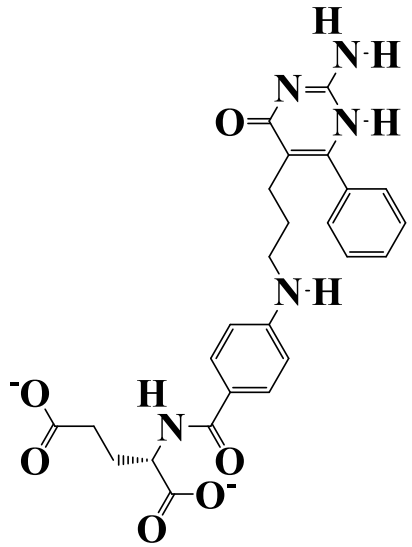


321(NCI code: 745104)

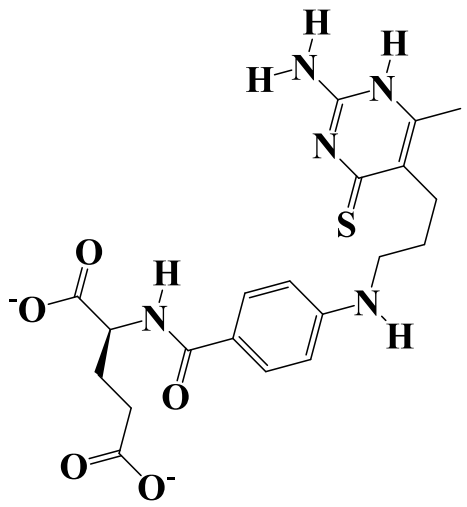


322 (NCI code: 72868)

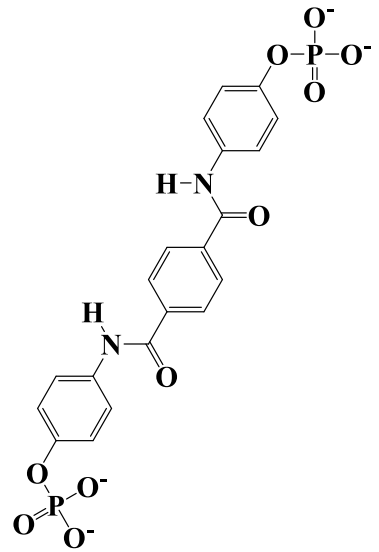
Figure S3. Chemical structures of high-ranking captured hits



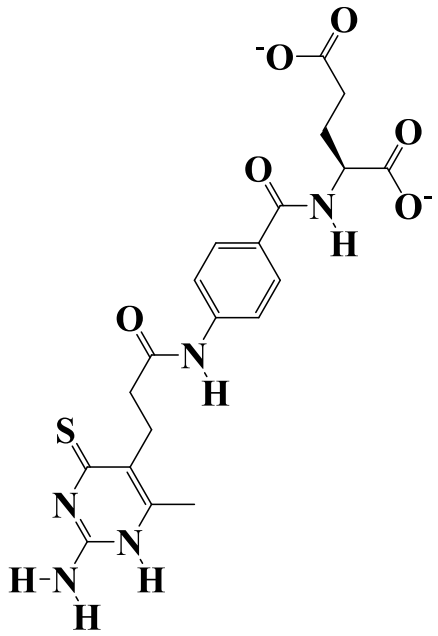
323 (NCI code: 77028)



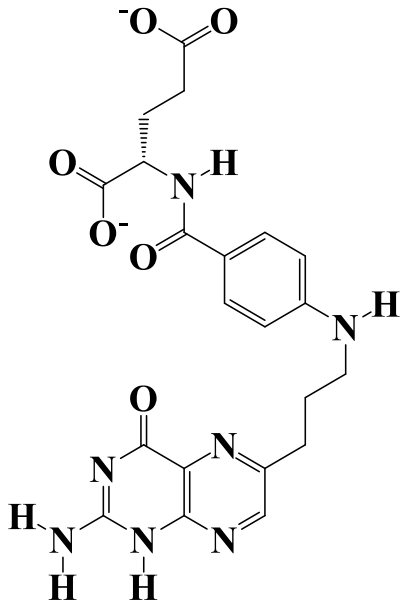
324 (NCI code: 77029)



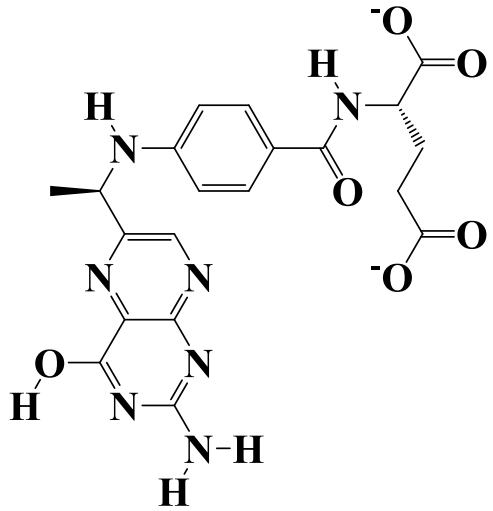
325 (NCI code: 82523)



326 (NCI code: 98711)

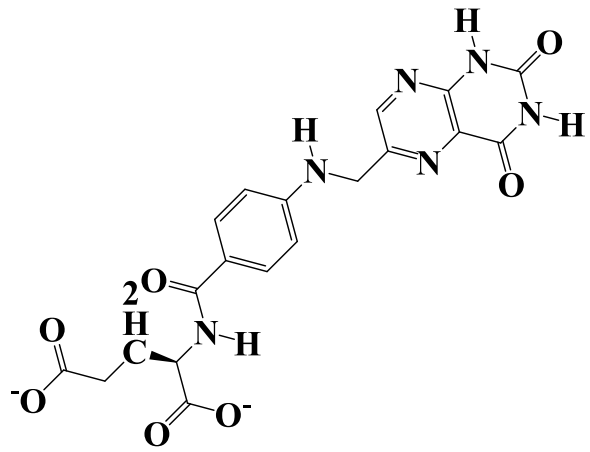


327 (NCI code: 100791)

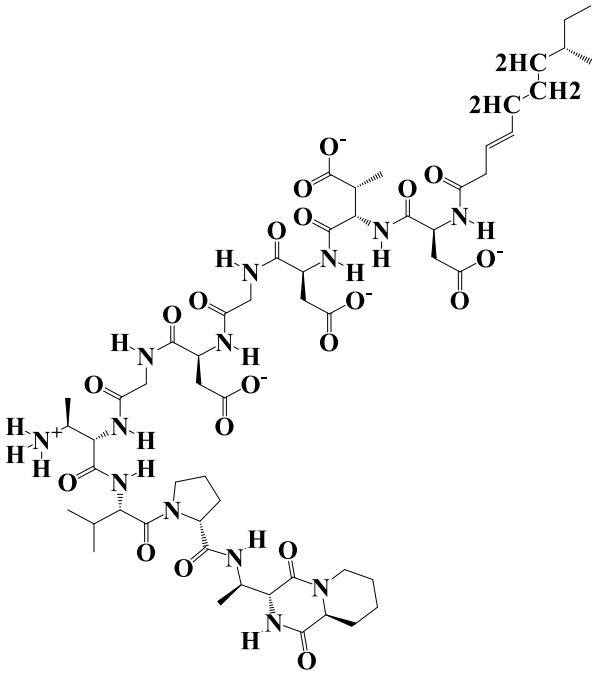


328 (NCI code: 107137)

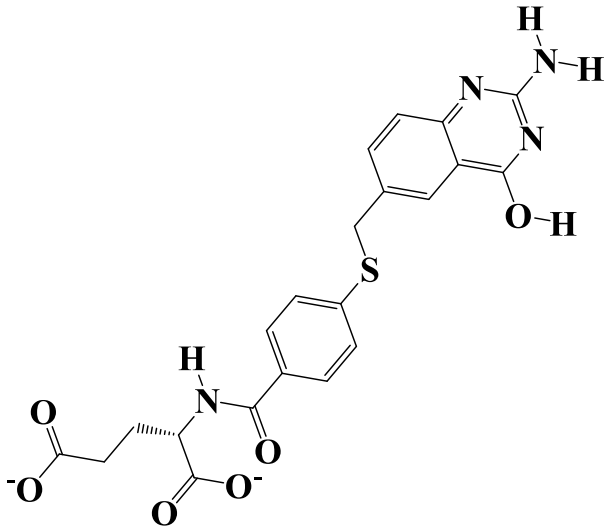
Figure S3. Chemical structures of high-ranking captured hits



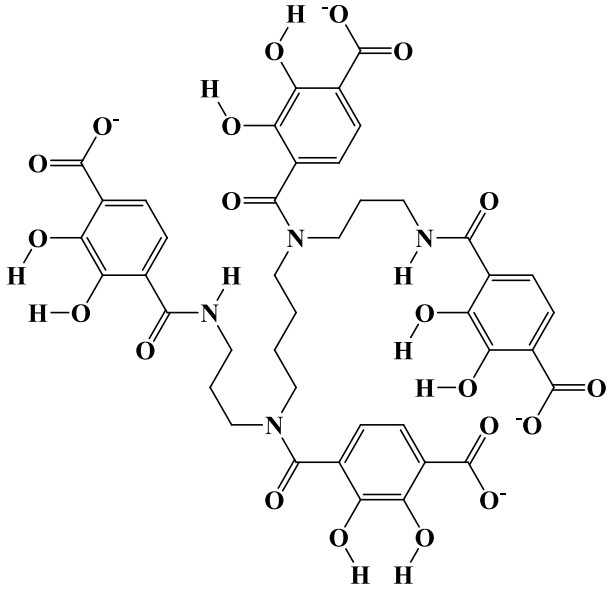
329 (NCI code: 107139)



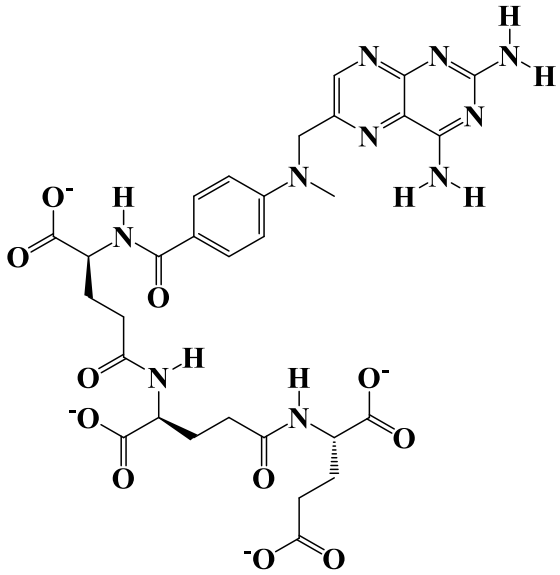
330 (NCI code: 267431)



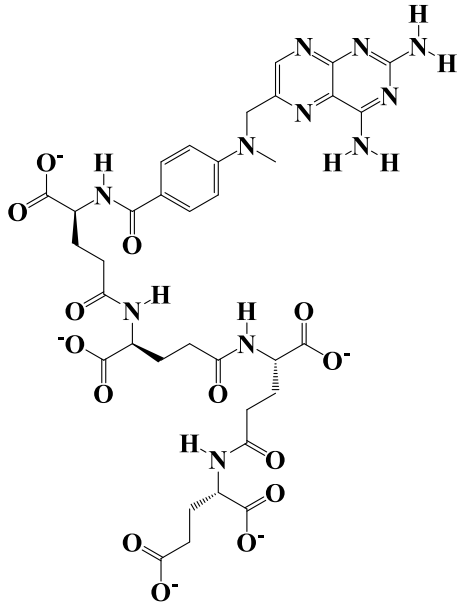
331 (NCI code: 289523)



332 (NCI code: 338310)

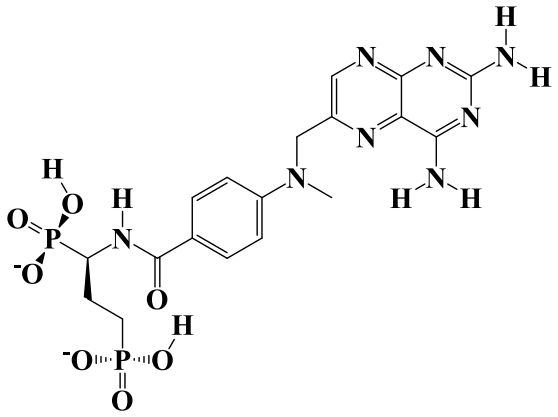


333 (NCI code: 341076)

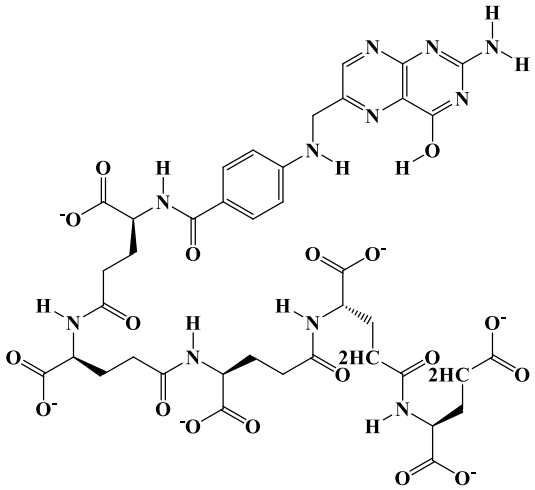


334 (NCI code: 341077)

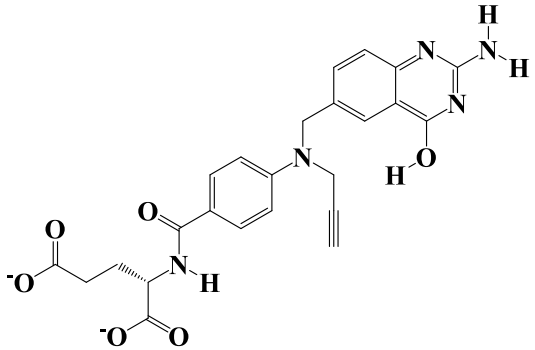
Figure S3. Chemical structures of high-ranking captured hits



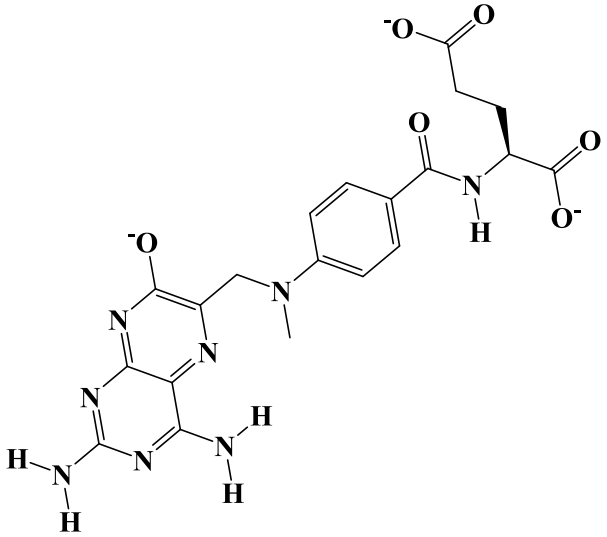
335 (NCI code: 363007)



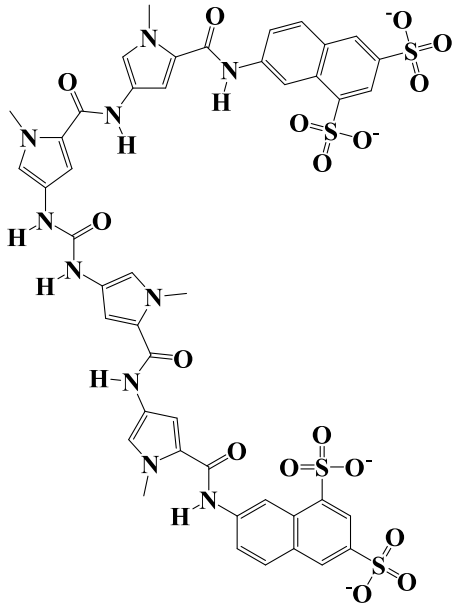
336 (NCI code: 372667)



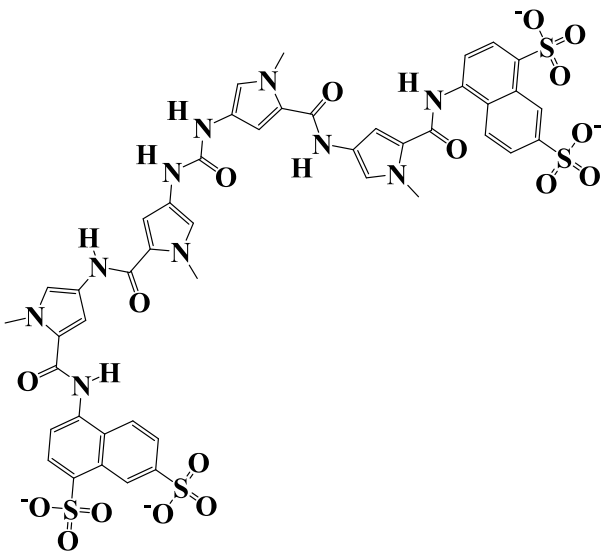
337 (NCI code: 373233)



338 (NCI code: 380962)

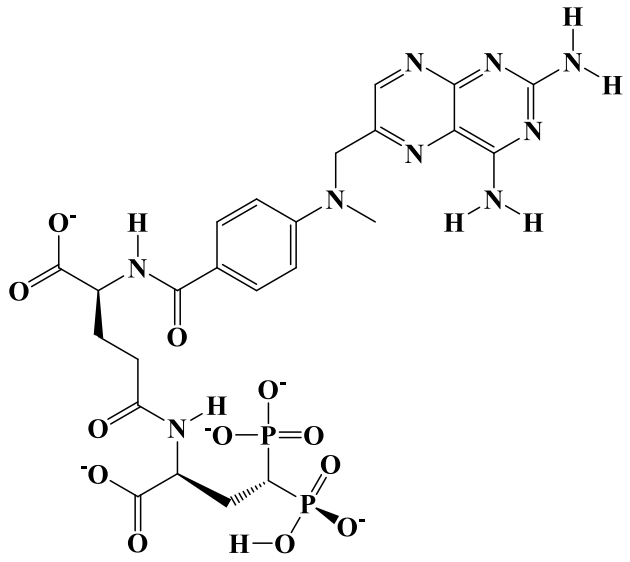


339 (NCI code: 645793)



340 (NCI code: 651016)

Figure S3. Chemical structures of high-ranking captured hits



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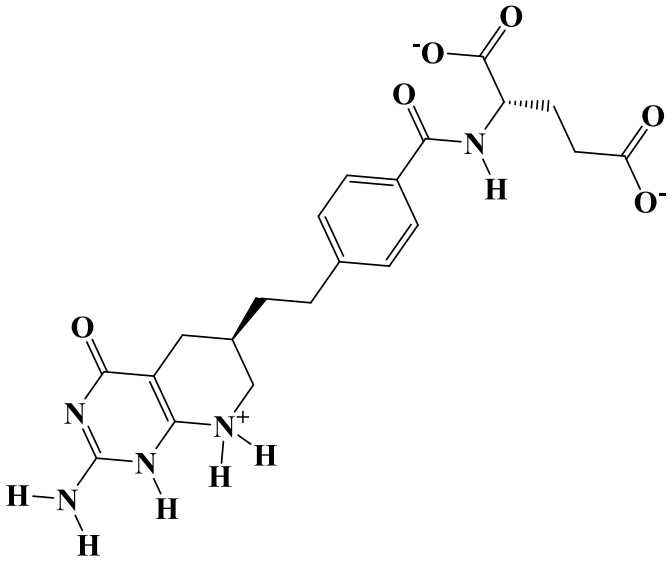

342 (NCI code: 722969)

Figure S3. Chemical structures of high-ranking captured hits