SUPPLEMENTARY MATERIAL:

AntiHIV-Pred: Web-resource for in silico prediction of anti-HIV/AIDS activity

1. Data Selection and Curation

Experimental data for building models of quantitative structure-activity relationships were downloaded from ChEMBL database (version 24) and then analyzed. Data containing about 50 thousand entries were derived from scientific literature turned out to be highly heterogeneous having different experimental conditions and various ligand efficiency indices were measured (Ki, IC50, percent of inhibition etc.). The curation process was realizied according to the pipeline (Figure 1). It corresponds to the "Best QSAR practice" (Tropsha,A., et al. Molecular Informatics, 2010, 29, 476; Fourches,D., et al. Journal of Chemical Information and Modeling, 2016, 56, 1243).
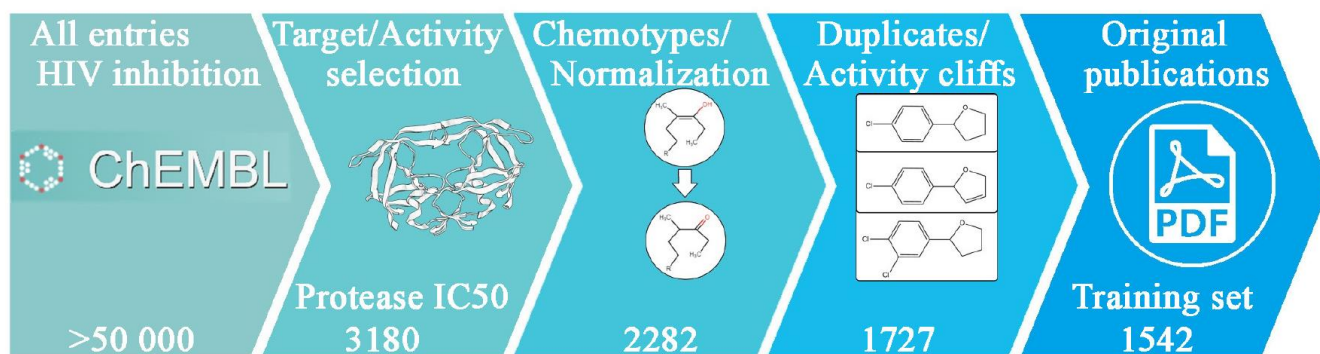

Figure 1. Data curation process pipeline.

The process could be subdivided to two parts – chemical data curation and biological data curation.

Chemical data curation:

- Deletion of incomplete and insufficient entries;
- Deletion of inorganics, metallorganics, rare atom compounds;
- Mixture and salt compunds processing and standartiztion;
- Invalid structures recovery;
- Standartization of structures kekulization;
- Chemical groups normalization;
- Tautomeric data handling;
- Enantiomeric and stereomeric data inspection.

Biological data curation:

- Deletion of entries for mutants, drug-resistant stamps and invalid targets;
- Data split basing on experimental protocols;
- Potential duplicates were checked either for equal compunds with different activity values or for coumppounds having the same set of descriptors. Basing on each case the entries were deleted or the median value was calculated;
- External laboratory error estimation;
- Handling activity cliff data

In addition, the data validity was verified by analysis of the information presented in the original publications. Curated data were used to create training sets for HIV targets.

2. Selected Descriptors

The modelling was accomplished using two types of descriptors – Multilevel Neighborhoods Atoms (MNA) and Quantitative Neighborhoods of Atoms (QNA) descriptors.

MNA descriptors are based on the molecular structure representation, which includes the hydrogen atoms according to the valences and partial charges of other atoms and does not specify the types of bonds. MNA descriptors are generated as recursively defined sequence:

- zero-level MNA descriptor for each atom is the mark A of the atom itself;

any next-level MNA descriptor for the atom is the sub-structure notation $A(D_1, D_2, \ldots, D_i, \ldots)$, where D_i is the previous-level MNA descriptor for i–th immediate neighbor's of the atom A.

The mark of atom may include not only the atomic type but also any additional information about the atom. In particular, if the atom is not included into the ring, it is marked by «-». The neighbor descriptors $D_1, D_2, \ldots, D_i, \ldots$ are arranged in unique manner, e.g., in lexicographic order. Iterative process of MNA descriptors generation can be continued covering first, second, etc. neighborhoods of each atom.

Descriptors for each molecule are generated on the basis of connectivity matrix $\mathbf{C}$ and table of atoms types A. Connectivity matrix contains data on the covalent bonds in a molecule. Various bond types are not specified (topological approximation). All hydrogens based on valences and partial charges of atoms are taken into account. The types of atoms are specified according to the data presented in Table 1.

Table 1. Classification of different atom types used in calculation of descriptors

Class name	Elements
H	H
C	C
N	N
O	O
F	F
Si	Si
P	P
S	S
Cl	Cl
Ca	Ca
As	As
Se	Se
Br	Br
Li*	Li, Na
B*	B, Re
Mg*	Mg, Mn
Sn*	Sn, Pb

Te*	Te, Po
I*	I, At
Os*	Os, Ir
Sc*	Sc, Ti, Zr
Fe*	Fe, Hf, Ta
Co*	Co, Sb, W
Sr*	Sr, Ba, Ra
Pd*	Pd, Pt, Au
Be*	Be, Zn, Cd, Hg
K*	K, Rb, Cs, Fr
V*	V, Cr, Nb, Mo, Tc
Ni*	Ni, Cu, Ge, Ru, Rh, Ag, Bi
In*	In, La, Ce, Pr, Nd, Pm, Sm, Eu
Al*	Al, Ga, Y, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Tl
R*	R, He, Ne, Ar, Kr, Xe, Rn, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr, Db, Jl

Example of structure presentation by zero-, first- and second-levels MNA descriptors for the phenol's molecule is shown in Figure 2.
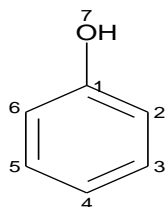
Atom	MNA/0	MNA/1	MNA/2
1	C	C(CC-O)	C(C(CC-H)C(CC-H)-O(C-H))
2	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
3	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
4	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
5	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
6	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
7	-O	-O(C-H)	-O(C(CC-O)-H(-O))
8	-H	-H(C)	-H(C(CC-H))
9	-H	-H(C)	-H(C(CC-H))
10	-H	-H(C)	-H(C(CC-H))
11	-H	-H(C)	-H(C(CC-H))
12	-H	-H(C)	-H(C(CC-H))
13	-H	-H(-O)	-H(-O(C-H))

MNA descriptors for phenol.
MNA/0, MNA/1,MNA/2 - zero, first and second levels
of MNA descriptors.

Figure 2. MNA descriptors of 0, 1, 2 level calculated for an example structure.

QNA descriptors are calculated based on the connectivity matrix C and the standard values of ionization potential IP and electron affinity EA of atoms in a molecule. For any given atom i QNA descriptors are calculated as follow:

$$P_i = B_i \sum_k \left(\mathrm{Exp}\left(-\frac{1}{2}C\right) \right)_{ik} B_k \quad (1)$$

$$Q_i = B_i \sum_k \left(\mathrm{Exp}\left(-\frac{1}{2}C\right) \right)_{ik} B_k A_k \quad (2)$$

where

$$A_k = \frac{1}{2}(IP_k + EA_k) \quad B_k = \frac{1}{2}(IP_k - EA_k)^{-\frac{1}{2}}$$

The values of EA and IP collected from many different sources and used in this work are represented in Table 2.

Table 2. Electron affinity (EA) and first ionization potential (IP), electron volts, and atomic radius (AR), angstroms.

Atom	EA	IP	AR	Atom	EA	IP	AR	Atom	EA	IP	AR
H	0.75	13.60	0.46	Kr	-0.42	14.00	1.98	Lu	0.20	6.15	1.75
He	0.08	24.59	1.22	Rb	0.49	4.18	2.48	Hf	0.33	7.50	1.59
Li	0.62	5.39	1.55	Sr	-0.15	5.69	2.15	Ta	0.40	7.89	1.46
Be	-0.20	9.32	1.13	Y	0.31	6.22	1.81	W	0.67	7.98	1.40
B	0.28	8.30	0.91	Zr	0.33	6.84	1.60	Re	0.23	7.88	1.37
C	1.26	11.26	0.77	Nb	0.51	6.88	1.45	Os	1.44	8.73	1.35
N	0.44	14.53	0.71	Mo	0.68	7.09	1.39	Ir	1.57	9.10	1.35
O	1.46	13.62	0.73	Tc	0.54	7.23	1.36	Pt	1.10	8.96	1.38
F	3.45	17.42	0.71	Ru	1.10	7.37	1.34	Au	1.25	9.23	1.44
Ne	0.00	21.57	1.60	Rh	1.14	7.46	1.34	Hg	-0.19	10.44	1.57
Na	0.55	5.14	1.87	Pd	1.11	8.34	1.37	Tl	0.31	6.11	1.71
Mg	-0.31	7.64	1.60	Ag	1.22	7.58	1.44	Pb	1.39	7.42	1.75
Al	0.30	5.99	1.43	Cd	-0.43	8.99	1.56	Bi	0.97	7.29	1.82
Si	1.39	8.15	1.34	In	0.31	5.79	1.66	Po	1.97	8.42	1.56
P	0.75	10.49	1.30	Sn	1.39	7.34	1.58	At	2.90	9.20	1.48
S	2.00	10.36	1.04	Sb	0.90	8.64	1.61	Rn	-0.15	10.75	2.27
Cl	3.61	12.97	0.99	Te	1.97	9.01	1.70	Fr	0.48	3.98	2.80
Ar	-0.37	15.76	1.92	I	3.23	10.45	1.53	Ra	-0.15	5.28	2.35
K	0.50	4.34	2.36	Xe	-0.25	12.13	2.18	Ac	0.80	5.20	2.03
Ca	-0.19	6.11	1.97	Cs	0.47	3.89	2.66	Th	0.80	6.10	1.80
Sc	0.19	6.56	1.64	Ba	-0.15	5.21	2.23	Pa	0.84	6.00	1.62
Ti	0.33	6.82	1.46	La	0.30	5.59	1.87	U	0.82	6.19	1.53
V	0.53	6.74	1.34	Ce	0.25	5.54	1.83	Np	0.82	6.20	1.50
Cr	0.67	6.77	1.27	Pr	0.20	5.47	1.83	Pu	0.84	6.06	1.62
Mn	-0.17	7.43	1.30	Nd	0.20	5.53	1.82	Am	0.85	6.00	1.70
Fe	0.50	7.90	1.26	Pm	0.20	5.58	1.81	Cm	0.85	6.09	1.55
Co	0.66	7.86	1.25	Sm	0.20	5.64	1.80	Bk	0.82	6.23	1.49
Ni	1.16	7.64	1.24	Eu	0.20	5.67	2.04	Cf	0.84	6.27	1.42
Cu	1.23	7.72	1.28	Gd	0.20	6.15	1.80	Es	0.86	6.47	1.43
Zn	-0.44	9.39	1.39	Tb	0.20	5.86	1.78	Fm	0.86	6.60	1.38
Ga	0.30	6.00	1.39	Dy	0.20	5.94	1.77	Md	0.83	6.68	1.38

Ge	1.39	7.90	1.39	Ho	0.20	6.02	1.78	No	0.79	6.58	1.47
As	0.80	9.79	1.48	Er	0.20	6.11	1.76	Lr	0.85	6.69	1.30
Se	2.02	9.75	1.17	Tm	0.20	6.18	1.75	Db	0.46	6.43	1.14
Br	3.45	11.81	1.14	Yb	0.20	6.25	1.94	Jl	0.50	6.78	1.01

Though the value $\mu(P - Q)$ can be considered by convention as the partial atomic charge, where μ is the chemical potential, in general, the P and Q values are not the estimate of partial atomic charges, hardness or so forth.

QNA describes each of the atoms in a molecule, and, at the same time, each of the P and Q values depends on the whole composition and structure of a molecule (Figure 3).

a) b) c)

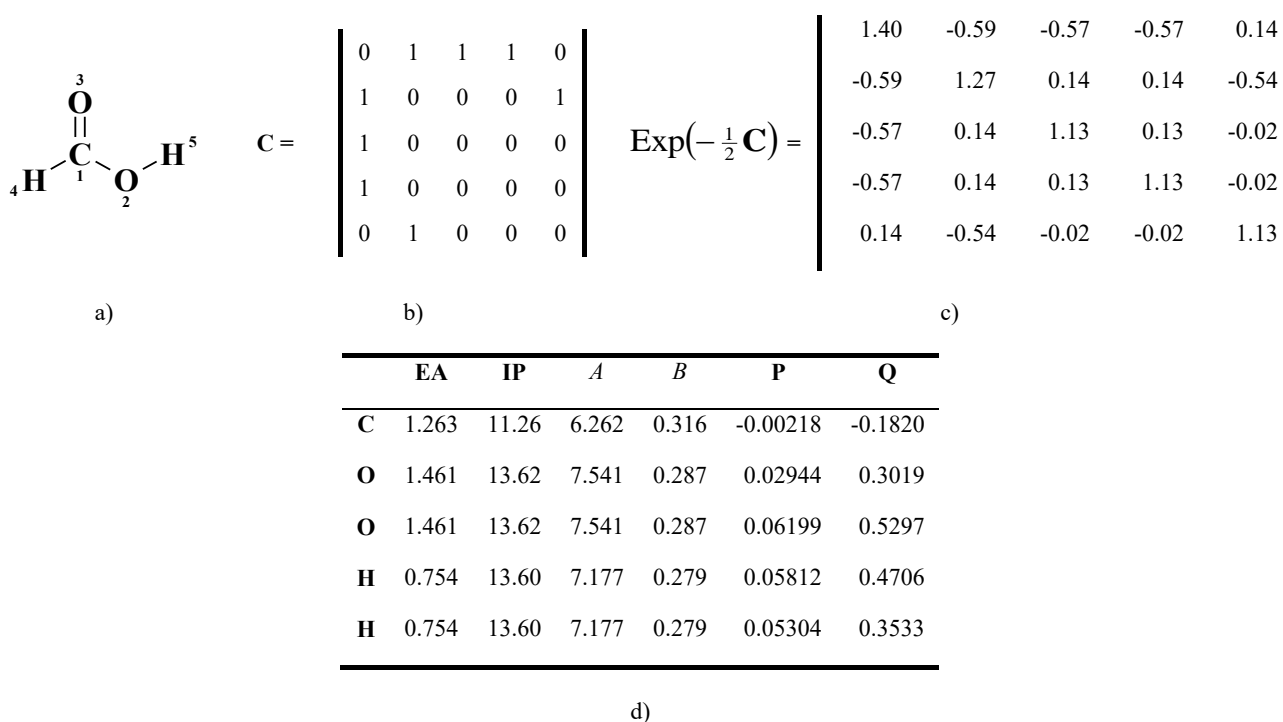|	EA	IP	A	B	P	Q
C	1.263	11.26	6.262	0.316	-0.00218	-0.1820
O	1.461	13.62	7.541	0.287	0.02944	0.3019
O	1.461	13.62	7.541	0.287	0.06199	0.5297
H	0.754	13.60	7.177	0.279	0.05812	0.4706
H	0.754	13.60	7.177	0.279	0.05304	0.3533

d)

Figure 3. Example of QNA description of *formic acid*: (a) structure diagram; (b) connectivity matrix; (c) exponent of the connectivity matrix; (d) electron affinities, ionization potentials, variables of equations (1) and (2), P and Q values for each atom of *formic acid* molecule.

From Figure 3c it is clear that any atom influences the others, though the influence decreases with the increase of the distance between them; *e.g.* components of matrix $\mathrm{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ for atom 1 (C) are: 1.40 for atom 1 itself, -0.59 for its immediate neighbor atom 2 (O), -0.57 for atoms 3 (O) and 4 (H), and 0.14 for atom 5 (H).

The algorithm of QNA descriptor calculation is quite simple due to uselessness of the matrix $\mathrm{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ itself, only product of $\mathrm{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ by vector is necessary, and that matrix $\mathbf{C}$ consists of 0 and 1 only.

3. QSAR Modeling Using GUSAR Program

QNA describe each particular atom of a molecule, at the same time, each P or Q value depends on the total molecule composition and structure. To use this molecule structure representation we have proposed to calculate each $f_i(S)$ function of the structure of a molecule as the average value of $g_i(P, Q)$ function of P and Q variables for those m atoms in a molecule, which have two or more immediate neighbors:

$$f_i(S) = \frac{1}{m} \sum_k g_i(P, Q) \qquad (3)$$

$$y_{pred} = a_0 + \sum_i a_i \frac{1}{m} \sum_k g_i(P, Q) \quad (4)$$

According to the equation (4) the estimate y_{pred} for molecule can be interpreted as an average of values predicted for particular atoms in a molecule. Formally, QNA descriptors represent a molecule structure by two descriptors only (P and Q), in contrast to numerous traditional descriptors used in QSAR. Since P and Q values have different scales (standard deviations are 0.023 and 0.208, respectively), we made the normalization to optimize a family of functions $g_i(P, Q)$.

Normalization has been performed by calculation of the average values (E_P and E_Q), standard deviations (D_P and D_Q) and correlation between P and Q values (R_{PQ}):

$$P' = \frac{P - E_P}{D_P} \qquad Q' = \frac{Q - E_Q}{D_Q} \qquad (5)$$

$$U = \frac{P' + Q'}{\sqrt{2(1 + R_{PQ})}} \qquad V = \frac{P' - Q'}{\sqrt{2(1 - R_{PQ})}} \qquad (6)$$

The orthonormal U and V have zero mean, unit variance and they are uncorrelated.

Chebyshev polynomials were chosen as the family of functions $g_i(P, Q)$, and the orthonormal U and V values have been additionally transformed by using hyperbolic tangent, so, the "normalized QNA" vary from -1 to 1. After this, the functions $g_i(P, Q)$ in equation (4) are represented using Chebyshev polynomials as:

$$g_i(P, Q) = T_{uv}(P, Q) = \text{Cos}\left(u * \text{ArcCos}(\text{TanH}(U))\right) * \text{Cos}\left(v * \text{ArcCos}(\text{TanH}(V))\right) \quad (7)$$

where the integer numbers $u, v = 0, 1, 2 \dots$ define 2-dimesional Chebyshev polynomial degree. The final equation for estimate y_{pred} using QNA descriptors is:

$$y_{pred} = \frac{1}{m} \sum_k \left(a_0 + \sum_{uv} a_{uv} T_{uv}(P, Q) \right) \qquad (8)$$

QNA descriptors and their polynomial transformations (5)-(7) do not provide information on the shape and volume of a molecule although this information may be important for determination of the structure-activity relationships. Therefore, these parameters were added to QNA descriptors. Topological length of a molecule was calculated as the maximal distance between any two atoms and the volume of a molecule – as the sum of each atom's volume,

$\frac{4}{3}\pi R^3$, where R is the atomic radius (see Table 2 (AR)).

The Chebyshev polynomials are arranged in ascending order of their degrees $u + v$. For $u + v = 1$ they are $T_{1,0}$, $T_{0,1}$; for $u + v = 2$ they are $T_{2,0}$, $T_{1,1}$, $T_{0,2}$ etc. The first, second and third power of topological length and volume

of a molecule were used. The number of initial variables equals to the number of Chebyshev polynomials plus the number of the first, second and third power of topological length and volume of a molecule.

The number of initial variables depends on the number of compounds in the training set. If the number of compounds in the training set less than 25, then the initial variables are 24. If the number of compounds in the training set varied from 25 to 100, then the initial variables depends on the following equation:

$$A = (Ln(B) \times 18.755) - 36.37,$$

where A – initial variables and B – the number of compounds in the training set. If the number of compounds in the training set varied from 100 to 2000, then the number of initial variables equal to one-half of the number of compounds in the training set. If the number of compounds in the training set exceeds 2000, then the initial variables are 1000.

GUSAR algorithm uses three procedures described below for generation of different QSAR models based on QNA descriptors.

1) U and V values from (7) are multiplied by value, which are randomly chosen from 0.98 to 1.09.

2) Coefficient before matrix $\mathbf{C}$ is randomly chosen from -0.1 to -0.9.

3) Calculation of QNA descriptors is randomly chosen from two cases. First case is when P and Q values are calculated for all atom types. Second case is when P and Q values are calculated for each atom, which has connection with more than one carbon.

All these procedures are used for creation of each QSAR model based on QNA descriptors. These procedures allow obtaining the different QNA models.

Self-Consistent Regression (SCR)

The classical MLR has a number of limitations. Particularly, the number of objects in the training set should significantly exceed the number of independent variables, and it is important to use the non-collinear variables only. To overcome these limitations, we have employed the approach based on statistical regularization of ill-posed problems. It has resulted in the regularized least-squares method:

$$\boldsymbol{a} = \text{ArgMin}\left[\sum_{i=1}^{n}\left(y_i - \sum_{k=0}^{m}(x_{ik}a_k)\right)^2 + \sum_{k=1}^{m}(v_k a_k{}^2)\right] \quad \textbf{(9)}$$

where $\boldsymbol{a}$ is the regression coefficient, n is the number of objects, y_i is the response value of ith object, m is, here and below, the number of the independent variables, x_{ik} is the value of kth independent variable of ith object, a_k is the kth value of the regression coefficients, v_k is the kth value of the regularization parameters. Equation (9) has the following solution:

$$\boldsymbol{a} = \mathbf{T}\mathbf{X}^T\boldsymbol{y}, \quad \mathbf{T} = (\mathbf{X}^T\mathbf{X} + \mathbf{V})^{-1}$$

where $\mathbf{X}^T$ is the transposed regression matrix $\mathbf{X}$, $\mathbf{V}$ is a diagonal matrix of the regularization parameters. The best regularization $\mathbf{V}$ satisfies to the equations:

$$v_k(a_k{}^2 + s^2 t_k) = s^2, \quad k = 1, \dots, m$$

where s is the standard deviation of residuals, t_k is the kth diagonal element of matrix $\mathbf{T}$.

Use of Nearest Neighbours

Algorithm of GUSAR allows using nearest neighbours for improvement of prediction value obtained from regression model. The corrected value is estimated by taking an average of the three chemicals values in the training set that are the most similar to the chemical under study. Similarity of the any pair of chemical

compounds is estimated as Pirson's coefficient calculated in the space of independent variables obtained after SCR. This function usually increases the prediction accuracy for the external test sets for QSAR models created on the basis of training sets with 500 and more structures. Sometimes the use of this function may lead to decrease of accuracy prediction, which depends on the quality of the training sets.

Consensus method

The predicted value is estimated by taking into account a weighted average of the predicted values from the obtained QSAR models (QSAR models provide the predictions that are within the respective applicability domains). Prediction obtained from each developed model is weighted on its applicability domain values (AD). GUSAR algorithm calculates the similarity value; leverage value and estimation of three nearest neighbours' accuracy of prediction for the applicability domain assessment (see AD description, page 70). Weighting of the predicted value is performed using similarity and leverage values only.

If all predicted values from the obtained QSAR models exceed the similarity threshold and leverage threshold, then the consensus prediction value is calculated from similarity weighted predicted values. If all predicted values from the obtained QSAR models are less than the leverage and similarity thresholds, then the consensus prediction value is calculated from leverage weighted predicted values. If the predicted values from the obtained QSAR models exceed similarity and is less than leverage thresholds, then the consensus prediction value is calculated as average from leverage weighted predicted values and similarity weighted predicted values. If the predicted values from the obtained QSAR models are less than similarity and exceed the leverage thresholds, then the consensus prediction value is calculated as average from all weighted predicted values.

Similarity

Three nearest neighbours from the training set are calculated for each chemical compound under study using similarity estimation. Similarity of the pair of chemical compounds is estimated as Pirson's coefficient calculated in the space of independent variables obtained after SCR. The average similarity of three nearest neighbours is used for assessment of the applicability domain (AD) of the model. If the average similarity exceeds the threshold, then the studied chemical compound falls in AD of the model and vice-versa. The higher value of the threshold was selected, the more similar compounds fell in AD of the model.

Leverage

Hat value of leverage was used for domain applicability assessment. Hat values from the leverage matrix representing the "distance" of the molecule to the model structural space were calculated as:

$$Leverage = x^T (\mathbf{X}^T \mathbf{X})^{-1} x$$

where x is a vector of descriptors of a query compound, and $\mathbf{X}$ is a matrix formed with rows corresponding to the descriptors of molecules from the training set. Hat value of leverage was calculated for each compound of the training set and then a distribution of the obtained values was estimated.

A warning level of hat value was considered as percentile. The end-user could select 99th, 95th and 90th percentile. Therefore, if a chemical compound from the external test set has hat value exceeded this warning level, then this compound is considered as being out of the applicability domain.

Accuracy of three nearest neighbours' predictions

For the assessment of this type of the applicability domain the following equation is used:

$$AD_{value} = \frac{RMSE_{3NN}}{RMSE_{train}}$$

where AD_{value} is the applicability domain value, $RMSE_{3NN}$ is root mean square error of prediction of three most similar compounds from the training set, $RMSE_{train}$ is root mean square error of predictions for the training set.

Three nearest neighbours from the training set are calculated for each studied chemical compound using similarity value. Similarity of the two chemical compounds is estimated as Pirson's coefficient calculated in the space of independent variables obtained by SCR.

If the AD_{value} is less than the threshold , then the studied chemical compound falls into AD of the model and vice-versa. Therefore, any chemical compound, whose three nearest neighbours are predicted worse than the prediction accuracy of the whole training set, is considered as being out of the applicability domain.

Leave-Many-Out procedure

This procedure is used for assessment of external prediction accuracy. The initial data is randomly divided onto the training and the external test sets. End- user could select the following proportions:

10% for the external test set and 90% for the training set;

20% for the external test set and 80% for the training set;

30% for the external test set and 70% for the training set;

50% for the external test set and 50% for the training set.

For obtaining the objective assessment of predictive accuracy and robustness of the developed models each splitting should be repeated many times. End-user could select the following number of repeats: 1, 5, 10 and 20.

Y-randomization procedure

This procedure allows to be ensuring that the developed models do not have the overfitting. In this procedure the dependent-variable vector, Y vector, is randomly shuffled and new QSAR model is developed using the original independent-variable matrix. It is expected that the resulting models should generally have low Q^2 values. This procedure could be repeated many times for each model, and then the average Q^2 value is calculated.

4. PASS (Prediction of Activity Spectra of Substances) Method

In PASS biological activities are described qualitatively (active or inactive). Any property of chemical compounds, which is determined by their structural peculiarities, can be used for prediction by PASS. It is clear, that the applicability of PASS is broader than the prediction of biological activity spectra.

The MNA descriptors (both for predicting the activity spectrum of the compound and for adding substances to SAR Base) are generated only if molecular structure corresponds to the following criteria:

- each of the atoms in a molecule must be presented by atom symbol from the periodic table. Symbols of unspecified atom A, Q, *, or R group labels are not allowed;
- each of the bonds in a molecule must be covalent bond presented by single, double or triple bond types only;
- molecular structure must include three or more carbon atoms;
- molecular structure must include only one component. Single atom parts like HCl, Cl-, OH-, Na+, etc., (hydrogen atoms do not take into account) are excluded from MNA descriptors generation;
- structure (main part, see the previous sentence) must be uncharged;
- the absolute molecular weight of a substance must be less than 1250 Da.

A relevant error will be generated whenever a molecular structure does not correspond to these criteria or input data contains some other errors.

The PASS training sets for HIV-associated comorbidites include about 240,000 thoroughly selected data records about structure and biological activity of organic compounds from the general PASS training set. The knowledgebase SAR Base is created in process of training on the basis of the PASS training set.

The PASS estimations of biological activity spectra of new compounds are based on the Structure-Activity Relationships knowledge-base (SAR Base), which accumulates the results of the training set analysis. SAR Base includes a biological activities dictionary and MNA descriptors dictionary, data and knowledge on the "structure – biological activity" relationships, the database of structure of compounds from the training set with their biological activity spectra. The structure of the compound represented as a set of MNA descriptors. Unfortunately, it is currently impossible to make a large collection of biologically active compounds using only publicly available sources, for which assay results for all types of biological activity were known.

Algorithm of activity spectrum prediction description may be done easy using well known Bayesian approach. For the chemical compound C, which molecular structure is represented by the set $\{D_1, \ldots, D_m\}$ of m MNA descriptors, estimate the probability $P(A|C)$ that the compound C has an activity A. According to the Bayes formula:

$$P(A|C) \ = \ \frac{P(A)P(C|A)}{P(C)} \quad (9)$$

where $P(A)$ is the activity A *prior* probability; $P(C|A)$ is the conditional probability of compound C providing that it has activity A; $P(C)$ is the compound C prior probability.

On the assumption that descriptors $D_1, \ldots, D_m$ are independent one can write the probability $P(C|A)$ as the product of conditional probabilities for particular descriptors:

$$P(C|A) \ \cong \ P(D_1, \ldots, D_m | A) \ = \ \prod_{i=1}^{m} P(D_i | A)$$

This expression is approximately true since the MNA descriptors are a fortiori dependent due to their generation method. However, we have not acceptable alternatives, and we cannot forget about the approximation of obtained formulas.

After simple transformations, we obtain the expression for the log-likelihood ratio of the conditional probabilities $P(A|C)$ for activity A and $P(B|C)$ for activity B as:

$$ln\left[\frac{P(A|C)}{P(B|C)}\right] \cong ln\left[\frac{P(A)}{P(B)}\right] + \sum_{i=1}^{m} \left\{ ln\left[\frac{P(A|D_i)}{P(B|D_i)}\right] - ln\left[\frac{P(A)}{P(B)}\right] \right\}$$

In a particular case, where B is the lack of activity A, we obtain:

$$ln\left[\frac{P(A|C)}{1 - P(A|C)}\right] \cong ln\left[\frac{P(A)}{1 - P(A)}\right] + \sum_{i=1}^{m} \left\{ ln\left[\frac{P(A|D_i)}{1 - P(A|D_i)}\right] - ln\left[\frac{P(A)}{1 - P(A)}\right] \right\}$$

The implication of the expression is quite clear: the logarithm of the posterior likelihood ratio is the sum of the logarithm of the a priori likelihood ratio and the sum of individual descriptors contributions. And, if the activity is not dependent on this descriptor, then $P(A|D_i) = P(A)$ and the such descriptor has no affect on the results and its contribution to the sum is zero. This is the classical result of the probabilistic approach. But, apart from the already marked proximity, this result has another significant, well-known disadvantage: the contribution of some descriptors is too large and suppresses all other terms of the sum for which the conditional probability of activity is too close to 0 or 1, when its present in the structure. The most pronounced effect could be in the situation, when for probabilities $P(A|D_i)$ used frequency estimates based on analysis of the training set and the values 0 and 1 are the rule rather than the exception.

To overcome this problem one can offer many different approaches and they were tested in the PASS development. The best result was obtained by using of so-called Fischer $ArcSin(2p-1)$ conversion instead of $ln[p/(1-p)]$: its shape coincides with the shape of $ln[p/(1-p)]$ for almost all values of p, but $ArcSin(2-1)$ values are bounded by the values $\pm\pi/2$. The accuracy of prediction also improved after changing the sum of descriptor contributions by the their average value, that apparently compensates for the assumption of descriptors independence. Logarithm of the a priori likelihood ratio has little information about a specific predicted organic compound and can be omitted.

Bayesian approach described above explains why PASS prediction algorithm based on the following specific statistics: on the basis of a molecular structure represented by the set $\{D_1, \ldots, D_m\}$ of m MNA descriptors, the B_k values are calculated for each activity A_k:

$$B_k = \frac{S_k - S_{0k}}{1 - S_k \cdot S_{0k}}$$

$$S_k = Sin\left[\sum_i ArcSin(2P(A_k|D_i) - 1)/m\right]$$

$$S_{0k} = 2P(A_k) - 1$$

For each kind of activity, if for all descriptors of molecule $P(A_k|D_i) = 1$, then $B_k = 1$; if for all descriptors of molecule $P(A_k|D_i) = 0$, then $B_k = -1$; if the relationship between descriptors of molecule and activity A_k does not exist and $P(A_k|D_i) \approx P(A_k)$, then $B_k \approx 0$.

The PASS prediction algorithm uses the following data on the "structure-activity" relationships:

N is the total number of compounds in the SAR Base;

N_i is the number of compounds contained descriptor D_i in the structure description;

N_k is the number of compounds contained the activity A_k in the activity spectrum;

N_{ik} is the number of compounds contained both the activity A_k and the descriptor A_k.

The simplest frequency estimations of probabilities $P(A_k)$ и $P(A_k|D_i)$ are given by:

$$P(A_k) = \frac{N_k}{N}, \quad P(A_k|D_i) = \frac{N_{ik}}{N_i}$$

Estimation of PASS prediction accuracy and dependency required for calculation probabilities Pa and Pi on the basis of B statistics, are the end result of the training procedure, which consists in the following. According to the SAR Base, formed on the basis of the training set, for each kind of activity A_k, for each N_k active, and for each $N - N_k$ inactive compound, B statistics values are calculated. Calculations are carried out in the Leave-One-Out Cross-Validation (LOO CV), i.e., after the "exclusion" of the compound from SAR Base, for what is enough to not include it in sum. Smooth estimations of the distribution functions $Pa(B)$ and $Pi(B)$ are based on the obtained sets of B statistics.

The probabilities Pa and Pi are both the measures of belonging to subsets of "active" and "inactive" compounds, and the probabilities of the 1st and 2nd kinds of prediction error, respectively. These two interpretations of the probabilities Pa and Pi are equivalent and can be used for understanding the results of prediction. It allows constructing different critera for analyzing the results of prediction corresponding to the solution of specific practical problems.

An important feature of the PASS prediction algorithm is its robustness to the imperfection of information on the structure and biological activity spectrum of organic compounds in the training set. In a special study was showed that halving the actual well-known information about the structure or activity of organic compounds in the training set only slightly reduces the accuracy of prediction in cross-validation. There's demonstrated that the accuracy base on a LOO CV is even more rigid than for cross-validation.

5. Qualitative Characterstics of the (Q)SAR Models

Here we summarize the information on developed quantitative models for HIV-1 protease, reverse transcriptase, integrase, REV and classification model for TAT.

Number of structures in the training sets, cross-validated determination coefficient (Q^2) and root-mean-square-errors (RMSE) for quantitative models and sensivity, specifity values are shown in Table 3.

Table 3. QSAR models developed in GUSAR program for HIV-1 targets.

Training set	Structures	Q2	RMSE
HIV-1 Protease pIC50:	1440	0.81	0.64
HIV-1 Reverse transcriptase pIC50:	1393	0.68	0.60
HIV-1 Integrase pIC50:	1436	0.83	0.56
HIV-1 REV pIC50:	105	0.55	0.34
Training set	**Structures**	**Sensivity**	**Specifity**
HIV-1 TAT:	2566	0.79	0.82

The following Predicted versus Observed plots (Figures 4-8) correspond to each model. Plots visualize Q^2 and RMSE values and show the studied p(IC50) prediction range and adequate homoscedasticity of prediction results.

Figure 4. Observed versus Predicted plot for pIC50 activities of HIV-1 protease

Figure 5. Observed versus Predicted plot for pIC50 activities of HIV-1 reverse transcriptase
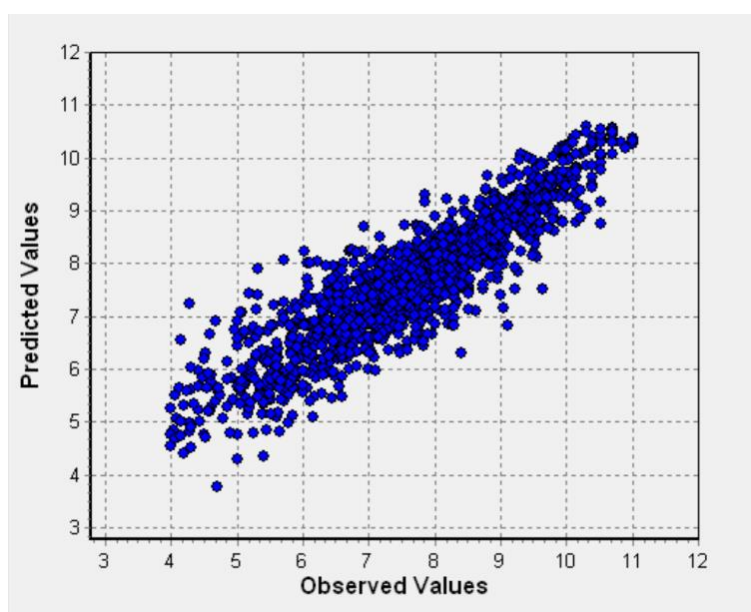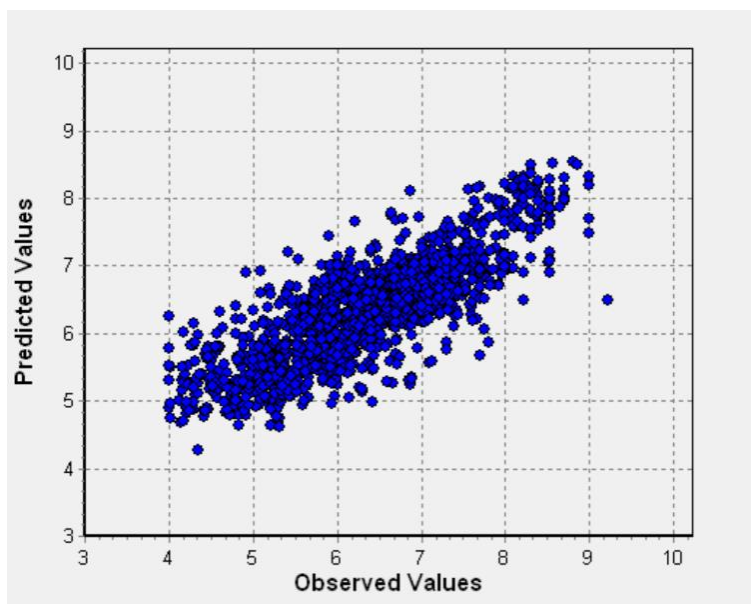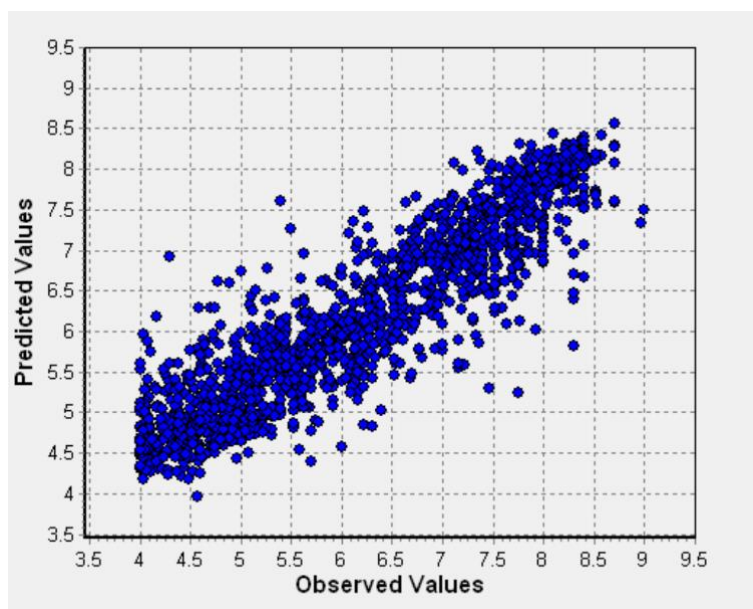

Figure 6. Observed versus Predicted plot for pIC50 activities of HIV-1 integrase
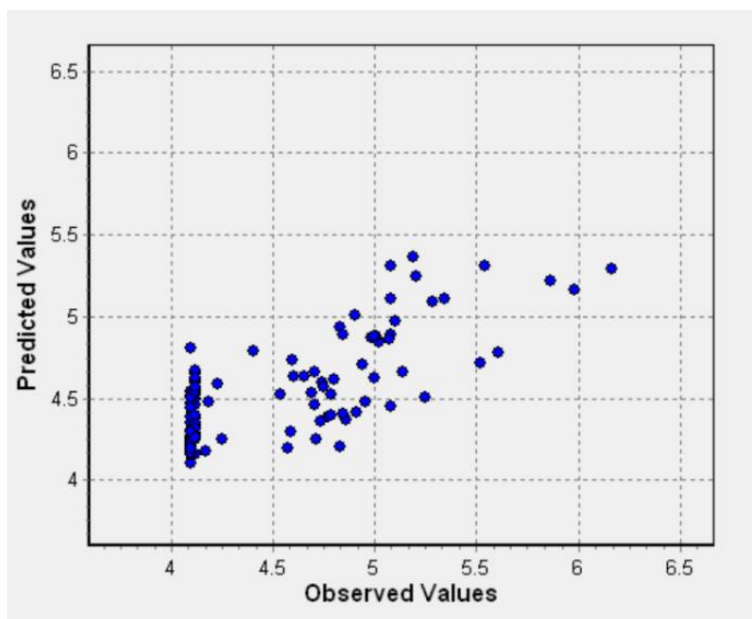
Figure 7. Observed versus Predicted plot for pIC50 activities of HIV-1 REV
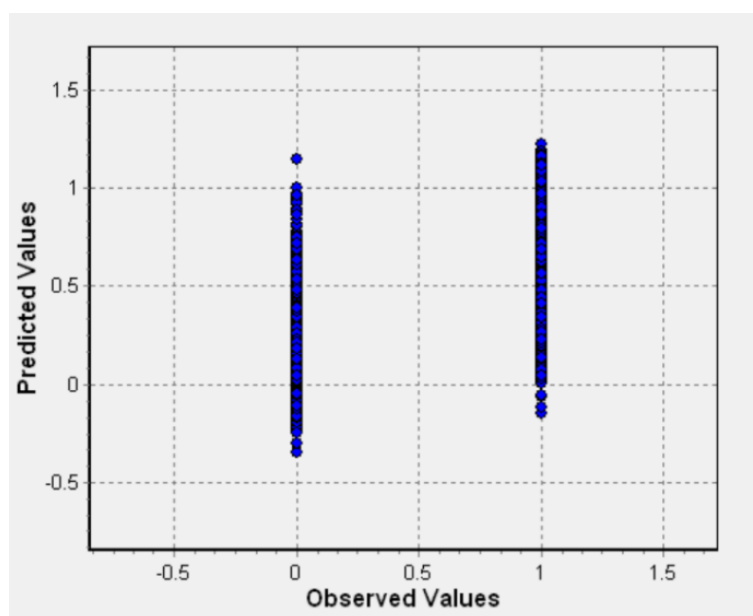
Figure 8. Observed versus Predicted plot for pIC50 activities of TAT (classification model)

6. List of Predicted Activities

List of 81 activities associated with treatment of HIV-associated disorders and deseases is represented in Table 4. For each activity the number of compounds in the training set (N) and invariant accuracy of prediction (IAP) is given (IAP equivalent to AUC ROC value).

Table 4. Activities associated with treatment of HIV-associated disorders and deseases.

HIV-associated comorbidity	N	IAP
Alzheimer's disease treatment	2639	0.9
Amyotrophic lateral sclerosis treatment	463	0.94
Analgesic	16272	0.88
Antiamyloidogenic	284	0.92
Antianorexic	102	0.96
Antiarthritic	13767	0.87
Antidepressant	11164	0.92
Antidiabetic	21403	0.89
Antidiabetic (type 2)	3182	0.94
Antifungal	5074	0.93
Antiinflammatory	9804	0.86
Antileprosy	82	0.94
Antileukemic	5109	0.94
Antimigraine	2172	0.95
Antineoplastic (bladder cancer)	378	0.9
Antineoplastic (brain cancer)	1008	0.9
Antineoplastic (breast cancer)	5668	0.92
Antineoplastic (colorectal cancer)	5740	0.94
Antineoplastic (endocrine cancer)	236	0.88
Antineoplastic (gastric cancer)	635	0.92

Antineoplastic (hematological cancer)	80	0.75
Antineoplastic (liver cancer)	412	0.9
Antineoplastic (lymphocytic leukemia)	2813	0.96
Antineoplastic (lymphoma)	992	0.94
Antineoplastic (melanoma)	1714	0.93
Antineoplastic (multiple myeloma)	208	0.88
Antineoplastic (myeloid leukemia)	133	0.81
Antineoplastic (non-Hodgkin's lymphoma)	83	0.85
Antineoplastic (non-small cell lung cancer)	965	0.91
Antineoplastic (ovarian cancer)	2047	0.95
Antineoplastic (pancreatic cancer)	360	0.89
Antineoplastic (renal cancer)	547	0.9
Antineoplastic (sarcoma)	331	0.92
Antineoplastic (small cell lung cancer)	211	0.87
Antineoplastic (solid tumors)	778	0.88
Antineoplastic antibiotic	1697	0.98
Antineurogenic pain	1162	0.92
Antiobesity	12280	0.91
Antiprotozoal (Leishmania)	1988	0.95
Antismoking	220	0.97
Antiviral (Hepatitis B)	449	0.96
Antiviral (Hepatitis C)	6807	0.97
Antiviral (Papilloma)	77	0.95
Atherosclerosis treatment	4552	0.89
Attention deficit/hyperactivity disorder treatment	676	0.97

Autoimmune disorders treatment	8944	0.88
Biliary tract disorders treatment	97	0.9
Cachexia treatment	265	0.96
Cancer associated disorders treatment	51	0.87
Cocain dependency treatment	235	0.96
Cognition disorders treatment	11383	0.9
Cystic fibrosis treatment	622	0.94
Dependence treatment	2076	0.94
Dermatologic	7173	0.9
Diabetic neuropathy treatment	61	0.81
Endocrine disorders treatment	16	0.84
Female sexual dysfunction treatment	129	0.97
Gastric emptying disorders treatment	99	0.96
Gastrointestinal disorders treatment	305	0.93
Gynecological disorders treatment	1084	0.98
Heart failure treatment	1632	0.94
Immunomodulator	2776	0.91
Immunostimulant	1135	0.92
Immunosuppressant	4252	0.89
Inflammatory Bowel disease treatment	2987	0.91
Lipoprotein disorders treatment	4667	0.95
Macular degeneration treatment	256	0.94
Multiple sclerosis treatment	3001	0.92
Myelodysplastic syndrome treatment	52	0.75
Neuropathy treatment	26	0.89

Pancreatic disorders treatment	400	0.97
Preneoplastic conditions treatment	8	0.87
Prostate cancer treatment	2944	0.93
Psychotropic	32069	0.87
Renal disease treatment	1788	0.95
Rheumatoid arthritis treatment	1925	0.9
Scleroderma treatment	22	0.84
Sickle-cell anemia treatment	55	0.93
Sleep apnea treatment	79	0.95
Sleep disorders treatment	2425	0.96
Wound healing agent	638	0.94

7. Examples of Predictions for the Widely Used Antiretroviral Drugs

Prediction results for FDA approved protease, integrase and non-nucleotide reverse transcriptase inhibitors is represented below. All values are p(IC50) values for molar concentrations (e.g. for p(IC50) = 7.742 IC = 18.11 nM). Prediction results for these inhibitors are close to the average experimental values (even for those which are not in applicability domain).

Protease inhibitors

Amprenavir	8.751	in AD
Atazanavir	7.351	in AD
Darunavir	8.342	in AD
Indinavir	9.035	in AD
Fosamprenavir	8.491	in AD
Lopinavir	7.741	in AD
Nelfinavir	8.074	in AD
Ritonavir	8.946	in AD
Tipranavir	7.158	in AD

NN Reverse trancriptase inhibitors

Efavirenz	7.289	in AD
Etravirine	7.246	not in AD
Delavirdine	6.666	in AD
Doravirine	6.403	not in AD
Nevirapine	6.715	in AD
Rilpivirine	7.095	not in AD

Integrase inhibitors

Dolutegravir	8.522	in AD
Elvitegravir	6.257	in AD
Raltegravir	7.33	in AD

An example of HIV-1 activity prediction for Saquinavir, one of the FDA approved HIV-1 protease inhibitors, is given in Figure 9. The prediction for protease inhibiting activity is close to yje experimental values. The high p(IC50) value for reverse transcriptase inhibiting activity could be ignored because prediction does not correspond to the applicability domain. Prediction of integrase inhibiting activity reflects that Saquinavir is not integrase inhibitor.

HIV TARGETS PREDICTION RESULTS
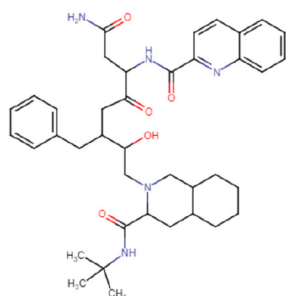
Targets	Value	Prediction	Applicability Domain
Protease (HIV-1):	p(IC50)	8.977	in AD
Reverse Transcriptase (HIV-1):	p(IC50)	7.404	not in AD
Integrase (HIV-1):	p(IC50)	4.604	not in AD

Figure 9. Saquinavir prediction with AntiHIV-Pred.

An example of activity spectra of HIV-1 comorbidities for Lamivudine, one of the FDA approved HIV-1 nucleotide analogue reverse transcriptase inhibitors, is given in Figure 10. The prediction shows four possible activities: antineoplastic, against myelodysplastic syndrome, antiviral (hepatitis B), antileukemic. It was experimentally confirmed that Lamivudine have some activity against hepatitis B (Nabuyuki, T., et al. Hepatology Resarch, 2002, 24, 34).
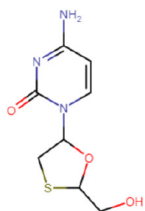
HIV COMORBIDITIES ACTIVITY SPECTRA

Comorbidity	Pa	Pi
Antineoplastic (myeloid leukemia)	0.777	0.007
Myelodysplastic syndrome treatment	0.768	0.005
Antiviral (Hepatitis B)	0.71	0.002
Antileukemic	0.607	0.009

Figure 10. Lamivudine prediction with AntiHIV-Pred.

8. Training Sets

8.1 Protease training set

CHEMBL360212	O[C@@H](C[C@@H](Cc1ocnn1)C(=O)N[C@H]2CCOC[C@H]2O)CN3CCN(Cc4oc(cc4)c5ccc(Cl)cc5)C[C@H]3C(=O)NCC(F)(F)F	0.01	nM
CHEMBL364376	O[C@@H](C[C@@H](Cc1oc(nn1)c2ccccc2)C(=O)N[C@H]3CCOC[C@H]3O)CN4CCN(Cc5oc(cc5)c6ccc(Cl)cc6)C[C@H]4C(=O)NCC(F)(F)F	0.01	nM
CHEMBL361443	Cc1oc(C[C@H](C[C@H](O)CN2CCN(C[C@H]2C(=O)NCC(F)(F)F)C(C)(C)c3oc(cn3)c4ccc(Cl)cc4)C(=O)N[C@H]5CCOC[C@H]5O)nn1	0.01	nM
CHEMBL364409	CCCc1oc(C[C@H](C[C@H](O)CN2CCN(C[C@H]2C(=O)NCC(F)(F)F)C(C)(C)c3oc(cn3)c4ccc(F)cc4)C(=O)N[C@H]5CCOC[C@H]5O)nn1	0.01	nM
CHEMBL116954	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccc6cccnc56	0.01	nM
CHEMBL433165	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2cncc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccc6cccnc56	0.02	nM
CHEMBL373039	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2cc3cnccc3s2)C(=O)N[C@@H]4[C@H](O)COc5ccccc45)[C@@H](C1)C(=O)NCC(F)(F)F)c6oc(cn6)c7ccc(Cl)cc7	0.02	nM
CHEMBL364407	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ocnn2)C(=O)N[C@H]3CCOC[C@H]3O)[C@@H](C1)C(=O)NCC(F)(F)F)c4oc(cn4)c5ccc(F)cc5	0.02	nM
CHEMBL321814	O[C@@H](C[C@@H](Cc1cccnc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc6c(Cl)cccc6c5)C[C@H]4C(=O)NCC(F)(F)F	0.02	nM
CHEMBL435095	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2oc(nn2)c3ccccc3)C(=O)N[C@H]4CCOC[C@H]4O)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc(cn5)c6ccc(F)cc6	0.02	nM
CHEMBL3706622	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc(cn5)c6cnccc6Cl	0.02	nM
CHEMBL364404	Cc1oc(C[C@H](C[C@H](O)CN2CCN(C[C@H]2C(=O)NCC(F)(F)F)C(C)(C)c3oc(cn3)c4ccc(F)cc4)C(=O)N[C@H]5CCOC[C@H]5O)nn1	0.02	nM
CHEMBL3706615	COc1cncc(c1)c2oc(nc2)C(C)(C)N3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)COc6ccccc56)[C@@H](C3)C(=O)NCC(F)(F)F	0.02	nM
CHEMBL381630	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2oc3cnccc3c2)C(=O)N[C@@H]4[C@H](O)COc5ccccc45)[C@@H](C1)C(=O)NCC(F)(F)F)c6oc(cn6)c7ccc(Cl)cc7	0.02	nM
CHEMBL3085527	CC[C@H](C)[C@@H](NC(=O)[C@H](C\C=C\c1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)NCc3nc4ccccc4[nH]3	0.03	nM
CHEMBL96352	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccnc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccc6cccnc56	0.03	nM
CHEMBL3706623	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cc5)c6cccnc6)C[C@H]4C(=O)NCC(F)(F)F	0.03	nM
CHEMBL52669	Cc1cccc(Cl)c1CNC(=O)[C@@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.03	nM
CHEMBL421568	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc(Br)cs2)CCN1C[C@@H](O)C[C@@H](Cc3cccnc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.03	nM
CHEMBL439513	Cc1ccncc1c2oc(C[C@H](C[C@H](O)CN3CCN(Cc4oc(cn4)c5ccc(Cl)cc5)C[C@H]3C(=O)NCC(F)(F)F)C(=O)N[C@@H]6[C@H](O)COc7ccccc67)cc2	0.03	nM
CHEMBL419396	O[C@@H](C[C@@H](Cc1cccnc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(CC5=CC6C=CSC6S5)C[C@H]4C(=O)NCC(F)(F)F	0.03	nM

CHEMBL321260	O[C@@H](C[C@@H](Cc1ccncc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc6c(Cl)cccc6c5)C[C@H]4C(=O)NCC(F)(F)F	0.03	nM
CHEMBL197493	O[C@@H](C[C@@H](Cc1cc2cnccc2s1)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)CN5CCN(Cc6oc(cc6)c7ccc(Cl)cc7)C[C@H]5C(=O)NCC(F)(F)F	0.03	nM
CHEMBL372527	Cc1ccncc1c2oc(C[C@H](C[C@H](O)CN3CCN(C[C@H]3C(=O)NCC(F)(F)F)C(C)(C)c4ncc(s4)c5ccc(Cl)cc5)C(=O)N[C@@H]6[C@H](O)COc7ccccc67)cc2	0.03	nM
CHEMBL2062160	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)[C@H](Cc4ccccc4)NC(=O)OC5CCOC5	0.03	nM
CHEMBL370179	Cc1ccncc1c2oc(C[C@H](C[C@H](O)CN3CCN(Cc4ccc(s4)c5ccc(Cl)cc5)C[C@H]3C(=O)NCC(F)(F)F)C(=O)N[C@@H]6[C@H](O)COc7ccccc67)cc2	0.04	nM
CHEMBL298189	Cc1cccc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.04	nM
CHEMBL433270	CC1(C)SCN([C@@H]1C(=O)NCc2c(Cl)cccc2Cl)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.04	nM
CHEMBL3706621	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc(cn5)c6ccccn6	0.04	nM
CHEMBL326796	O[C@@H](C[C@@H](Cc1ccncc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cc5)c6ccccc6)C[C@H]4C(=O)NCC(F)(F)F	0.04	nM
CHEMBL300140	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc(s4)c5cccs5)C[C@H]3C(=O)NC(C)(C)C	0.04	nM
CHEMBL324461	O[C@@H](C[C@@H](Cc1cccnc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc6ccccc6c5)C[C@H]4C(=O)NCC(F)(F)F	0.04	nM
CHEMBL3706613	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc(cn5)c6cccnc6	0.04	nM
CHEMBL382951	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2cc3cnccc3s2)C(=O)N[C@@H]4[C@H](O)COc5ccccc45)[C@@H](C1)C(=O)NCC(F)(F)F)c6ncc(s6)c7ccc(Cl)cc7	0.04	nM
CHEMBL295414	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CC(Cc2ccc(OCC(=O)O)cc2)C(=O)NC3[C@H](O)Cc4ccccc34	0.04	nM
CHEMBL300754	Cc1nsc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.05	nM
CHEMBL3706619	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cc5)c6ccccn6)C[C@H]4C(=O)NCC(F)(F)F	0.05	nM
CHEMBL100310	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCC(O)CO	0.05	nM
CHEMBL199209	O[C@@H](C[C@@H](Cc1cc2cnccc2s1)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)CN5CCN(Cc6ccc(s6)c7ccc(Cl)cc7)C[C@H]5C(=O)NCC(F)(F)F	0.05	nM
CHEMBL370736	O[C@@H](C[C@@H](Cc1oc2cnccc2c1)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)CN5CCN(Cc6oc(cc6)c7ccc(Cl)cc7)C[C@H]5C(=O)NCC(F)(F)F	0.05	nM
CHEMBL3706620	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc(cc5)c6ccncc6	0.05	nM
CHEMBL96697	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3sccc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccncc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.05	nM
CHEMBL96100	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3ccsc3s2)CCN1C[C@@H](O)C[C@@H](Cc4ccncc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.06	nM
CHEMBL75904	CN(C)c1ncc(nc1Cl)C(=O)N[C@@H]([C@H]2CCOC2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.06	nM

CHEMBL326600	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccc(Br)cc2S)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.06	nM
CHEMBL3085503	CC[C@H](C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3	0.06	nM
CHEMBL49768	COCCOCOCCCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	0.07	nM
CHEMBL197039	O[C@@H](C[C@@H](Cc1cc2cnccc2s1)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)CN5CCN(Cc6csc(n6)c7ccc(cc7)C(F)(F)F)C[C@H]5C(=O)NCC(F)(F)F	0.07	nM
CHEMBL297720	Cc1onc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.07	nM
CHEMBL52645	Cc1ccccc1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.07	nM
CHEMBL314510	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@H](C(=O)NCc3nc4ccccc4[nH]3)c5ccccc5	0.07	nM
CHEMBL326849	O[C@@H](C[C@@H](Cc1ccncc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(CC5=CC6C=CSC6S5)C[C@H]4C(=O)NCC(F)(F)F	0.07	nM
CHEMBL79236	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)F)c5oc6ccncc6c5	0.07	nM
CHEMBL295442	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(OCCN3CC[S+]([O-])CC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.07	nM
CHEMBL310924	CN1CCN(CC1)c2ncc(nc2Cl)C(=O)N[C@@H]([C@H]3CCOC3)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)CN5C[C@H]6CCCC[C@H]6C[C@H]5C(=O)NC(C)(C)C	0.07	nM
CHEMBL312238	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34C(C)(C)c5oc6ccncc6c5	0.08	nM
CHEMBL297294	COC(CCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1)OC	0.08	nM
CHEMBL416082	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(OCCN3CCS(=O)(=O)CC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.08	nM
CHEMBL198531	Cc1ccncc1c2oc(C[C@H](C[C@H](O)CN3CCN(Cc4oc(cc4)c5ccc(Cl)cc5)C[C@H]3C(=O)NCC(F)(F)F)C(=O)N[C@@H]6[C@H](O)COc7ccccc67)cc2	0.08	nM
CHEMBL114756	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cc5)c6ccncc6)C[C@H]4C(=O)NCC(F)(F)F	0.08	nM
CHEMBL295549	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(OCCO)cc2)C(=O)NC3[C@H](O)Cc4ccccc34	0.09	nM
CHEMBL316454	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3sccc3s2)CCN1C[C@@H](O)C[C@@H](Cc4cccnc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.09	nM
CHEMBL298393	Cc1cccc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.09	nM
CHEMBL95611	CC(C)(C)NC(=O)[C@H]1CN(CCN1C[C@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccs5	0.1	nM
CHEMBL293992	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5ccccc5s4)C[C@H]3C(=O)NC(C)(C)C	0.1	nM
CHEMBL325829	O[C@@H](C[C@@H](Cc1ccncc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc6ccccc6c5)C[C@H]4C(=O)NCC(F)(F)F	0.1	nM
CHEMBL3706617	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cn5)c6ccncc6)C[C@H]4C(=O)NCC(F)(F)F	0.1	nM
CHEMBL44489	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(CCCO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.1	nM
CHEMBL294392	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5ccsc5s4)C[C@H]3C(=O)NC(C)(C)C	0.11	nM
CHEMBL331155	Cc1c(CN2CCN(CC(O)CC(Cc3ccccc3)C(=O)NC4C(O)Cc5ccccc45)C(C2)C(=O)NC(C)(C)C)oc6ccccc16	0.11	nM

CHEMBL197114	Cc1ccncc1c2oc(C[C@H](C[C@H](O)CN3CCN(Cc4csc(n4)c5ccc(F)cc5)C[C@H]3C(=O)NCC(F)(F)F)C(=O)N[C@@H]6[C@H](O)COc7ccccc67)cc2	0.11	nM
CHEMBL73934	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)C4=CC(=O)c5ccccc5O4)[C@H]6CCOC6	0.11	nM
CHEMBL113845	CC(C)(C)NC(=O)C1CN(Cc2cc3cccnc3s2)CCN1CC(O)CC(Cc4ccccc4)C(=O)NC5C(O)Cc6ccccc56	0.11	nM
CHEMBL318777	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc(Br)cs2)CCN1C[C@@H](O)C[C@@H](Cc3ccncc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.11	nM
CHEMBL96645	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cc3ccsc3s2)CCN1C[C@@H](O)C[C@@H](Cc4cccnc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.12	nM
CHEMBL307918	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4cnc5ccccc5n4)[C@H]6CCOC6	0.12	nM
CHEMBL211715	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)OCc1ccccn1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.12	nM
CHEMBL301571	Cc1cccnc1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.13	nM
CHEMBL3706614	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cn5)c6ccccn6)C[C@H]4C(=O)NCC(F)(F)F	0.13	nM
CHEMBL149166	Cn1nc(cc1c2ccc(CN3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C)s2)C(F)(F)F	0.13	nM
CHEMBL333828	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)C(=O)C5=Cc6ccccc6OC5=O	0.13	nM
CHEMBL297066	COCCCOCOCCc1ccc(C[C@@H](C[C@@H](O)[C@@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	0.13	nM
CHEMBL326336	Cc1nn(C)c2ncc(CN3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C)c(Cl)c12	0.14	nM
CHEMBL325951	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cnc3ccccc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.14	nM
CHEMBL3706616	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)COc3ccccc23)CN4CCN(Cc5oc(cn5)c6ccccnc6)C[C@H]4C(=O)NCC(F)(F)F	0.14	nM
CHEMBL311953	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC(F)(F)C(F)(F)F)c5oc6ccncc6c5	0.14	nM
CHEMBL318525	CC(C)(C)NC(=O)[C@@H]1CN(Cc2c(F)cccc2F)CCN1C[C@@H](O)C[C@@H](Cc3cccnc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.14	nM
CHEMBL78876	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)C(C)(C)c5oc6ccncc6c5	0.15	nM
CHEMBL309175	CC(C)[C@H](NC(=O)C1=CC(=O)c2ccccc2O1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.15	nM
CHEMBL431999	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCC(O)CO	0.15	nM
CHEMBL299884	Cc1ccnc(C)c1CNC(=O)[C@H]2N(CSC2(C)C)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.16	nM
CHEMBL306974	COC(=O)c1nc(Cl)c(N[C@@H]([C@H]2CCOC2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C)nc1N	0.16	nM
CHEMBL291196	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(CCO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.16	nM
CHEMBL116628	Cc1nc(c(C)s1)S(=O)(=O)N2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C	0.16	nM
CHEMBL295471	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2c	0.17	nM

	cc(cc2)S(=O)(=O)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34		
CHEMBL408413	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cnc3ccoc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.17	nM
CHEMBL46114	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CO)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.17	nM
CHEMBL47610	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](CCc2cnc3ccccc3n2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.17	nM
CHEMBL295530	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](C\C=C\c2ccc(O)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.17	nM
CHEMBL292193	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc(Br)cs4)C[C@H]3C(=O)NC(C)(C)C	0.18	nM
CHEMBL116052	CC(C)(C)NC(=O)C1CN(Cc2oc3ncc(CO)cc3c2)CCN1CC(O)CC(Cc4cccc4)C(=O)NC5C(O)Cc6ccccc56	0.18	nM
CHEMBL45451	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCc3ccccc3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.18	nM
CHEMBL47480	CC(C)C[C@H](NC(=O)[C@H](C\C=C\c1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	0.19	nM
CHEMBL77786	CC(C)C1(CCc2csc(CO)c2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.19	nM
CHEMBL325013	Cc1cc2oc(CN3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C)cc2cn1	0.19	nM
CHEMBL326337	CC(C)(C)NC(=O)C1CN(Cc2csc3ncccc23)CCN1CC(O)CC(Cc4ccccc4)C(=O)NC5C(O)Cc6ccccc56	0.2	nM
CHEMBL297673	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCC(=O)N3CCOCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.2	nM
CHEMBL276447	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3	0.2	nM
CHEMBL46274	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc(OCC[N+]3([O-])CCOCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.2	nM
CHEMBL318114	Cc1cc(O)cc(C)c1CNC(=O)[C@@H](C[C@@H](O)CN2CCN(C[C@@H]2C(=O)NC(C)(C)C)S(=O)(=O)c3ccc4N(CCc4c3)c5ncccn5)Cc6ccccc6	0.2	nM
CHEMBL44578	CN1CCN(CCOc2ccc(C[C@H](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C)C(=O)NC4[C@H](O)Cc5ccccc45)cc2)CC1	0.2	nM
CHEMBL95228	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4cccc5cccnc45)NC(=O)C(F)(F)F	0.21	nM
CHEMBL297189	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cccc(O)c2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.21	nM
CHEMBL295357	CSc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	0.22	nM
CHEMBL358139	CN(C)c1ccc2ccc(cc2n1)S(=O)(=O)N3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C	0.22	nM
CHEMBL98954	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc(F)cc4)NS(=O)(=O)C	0.22	nM
CHEMBL81840	CC(C)(C)NC(=O)[C@@H]1CN(Cc2oc3ccncc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.22	nM
CHEMBL297045	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(O)cc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	0.23	nM
CHEMBL413515	CN(C)c1ccc(CNC(=O)[C@@H](NC(=O)c2ccccc2c3ccccc3)[C@@H]4N[C@@H](C(=O)NCCNC(=O)[C@@H]5N[C@H](SC5(C)C)[C@H](NC(=O)c6ccccc6c7ccccc7)C(=O)NCc8ccc(cc8)N(C)C)C(C)(C)S4)cc1	0.23	nM
CHEMBL329750	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccc3	0.24	nM
CHEMBL432924	CN(C)c1nc(N)c(nc1Cl)C(=O)N[C@@H]([C@H]2CCOC2)C(=O)N[C	0.24	nM

	@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C		
CHEMBL434342	COc1cncc(c1)c2oc(nc2)C(C)(C)N3CCN(C[C@@H](O)C[C@@H](Cc4ocnn4)C(=O)N[C@H]5CCOC[C@H]5O)[C@@H](C3)C(=O)NCC(F)(F)F	0.24	nM
CHEMBL378044	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)Cc1cccnc1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.24	nM
CHEMBL52670	CC1(C)SCN([C@@H]1C(=O)NCc2c(F)cccc2F)C(=O)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45	0.24	nM
CHEMBL77497	CC(C)C1(CCc2cncs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.24	nM
CHEMBL410311	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc(Br)s4)C[C@H]3C(=O)NC(C)(C)C	0.25	nM
CHEMBL268765	CC(=O)N[C@@H](C[S+]([O-])c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)Cc4ccccc4C(=O)NC(C)(C)C	0.25	nM
CHEMBL1790766	CC[C@H](C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NC(=O)C(N)Cc3ccccc3	0.25	nM
CHEMBL325181	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cnc3occc3c2Cl)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.25	nM
CHEMBL112257	CSc1ncccc1CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C	0.26	nM
CHEMBL358228	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ncc(s2)c3ccccc3)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.26	nM
CHEMBL432633	CCOC(=O)c1cnc2oc(CN3CCN(CC(O)CC(Cc4ccccc4)C(=O)NC5C(O)Cc6ccccc56)C(C3)C(=O)NC(C)(C)C)cc2c1	0.27	nM
CHEMBL297620	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@@H](Cc2ccc(cc2)C(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.27	nM
CHEMBL48565	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C(C)C	0.28	nM
CHEMBL305814	CC(C)C1(CCc2cc[nH]n2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.28	nM
CHEMBL275237	CC(=O)N[C@@H](CS(=O)(=O)c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)Cc4ccccc4C(=O)NC(C)(C)C	0.29	nM
CHEMBL295924	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@@H](C\C=C\c2ccc(CCN3CCOCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.29	nM
CHEMBL1233940	CC(C)(C)NC(=O)[C@@H]1CN(Cc2oc3ccccc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.3	nM
CHEMBL325885	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)S(=O)(=O)c5cccnc5	0.3	nM
CHEMBL324084	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.3	nM
CHEMBL326764	O[C@@H]1[C@@H](O)[C@@H](OCc2cncs2)[C@@H](Cc3ccccc3)S(=O)(=O)[C@H](Cc4ccccc4)[C@@H]1OCc5cncs5	0.3	nM
CHEMBL98710	Cc1c(O)cccc1C(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	0.3	nM
CHEMBL277985	CC(=O)N[C@H](CS(=O)(=O)c1ccc2ccccc2c1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)Cc4ccccc4C(=O)NC(C)(C)C	0.31	nM
CHEMBL326543	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccc(F)cc2F)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.31	nM
CHEMBL366293	CCCc1oc(C[C@H](C[C@H](O)CN2CCN(C[C@H]2C(=O)NCC(F)(F)F)C(C)(C)c3oc(cn3)c4cncc(OC)c4)C(=O)N[C@H]5CCOC[C@H]5O)nn1	0.32	nM
CHEMBL301269	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc5sccc5s4)C[C@H]3C(=O)NC(C)(C)C	0.32	nM
CHEMBL324516	CC(C)(C)NC(=O)C1CN(Cc2oc3ncccc3c2)CCN1CC(O)CC(Cc4ccccc4)	0.32	nM

	C(=O)NC5C(O)Cc6ccccc56		
CHEMBL101560	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23)[C@H](Cc4ccccc4)NC(=O)OC5CCCC5	0.33	nM
CHEMBL381583	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccc(c(O)c1)[N+](=O)[O-])C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.33	nM
CHEMBL274186	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)c3ccc(Cl)cc3)NS(=O)(=O)C	0.34	nM
CHEMBL78261	CC(C)C1(CCc2cocc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.34	nM
CHEMBL2062139	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)C(=O)OCc5ccccc5	0.35	nM
CHEMBL2062137	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cnc3occc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	0.35	nM
CHEMBL115080	Cc1nn(C)c2ncc(CN3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C)cc12	0.35	nM
CHEMBL77431	CC(C)C1(CCc2cccs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.35	nM
CHEMBL291195	CC(C)C[C@H](NC(=O)[C@H](CCCc1ccccc1)C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	0.36	nM
CHEMBL82245	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NC5CCCC5)c6oc7ccncc7c6	0.37	nM
CHEMBL11421	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](C[S+]([O-])c3ccc(F)cc3)NS(=O)(=O)C	0.38	nM
CHEMBL113826	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccncc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.39	nM
CHEMBL384210	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)OCc1ccncc1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.39	nM
CHEMBL74472	CC(C)[C@H](NC(=O)c1cnc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.39	nM
CHEMBL325354	CC(C)(C)NC(=O)[C@@H]1CN(Cc2oc3cnccc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.39	nM
CHEMBL364552	COc1cncc(c1)c2oc(nc2)C(C)(C)N3CCN(C[C@@H](O)C[C@@H](Cc4oc(C)nn4)C(=O)N[C@H]5CCOC[C@H]5O)[C@@H](C3)C(=O)NCC(F)(F)F	0.4	nM
CHEMBL378134	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cccc(O)c1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.4	nM
CHEMBL310417	CC(C)CNC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)C(C)(C)c5oc6ccncc6c5	0.4	nM
CHEMBL377826	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cnccc1N)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.4	nM
CHEMBL378829	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cnccc1C)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.4	nM
CHEMBL49002	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](C[S+]([O-])c4ccc5ccccc5c4)NS(=O)(=O)C	0.4	nM
CHEMBL208879	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cccnc1C)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.4	nM
CHEMBL441528	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)OC(C)(C)C)C(c1ccccc1)c2ccccc2)S(=O)(=O)c3ccc(N)cc3	0.4	nM
CHEMBL265975	CC(C)C1(CCc2cscc2C)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.41	nM
CHEMBL99357	CC(=O)N[C@H](CS(=O)(=O)c1cccc2cccnc12)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCS[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.42	nM
CHEMBL298788	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccc(cc2)c3ccccc3)C(=O)N[C@@H](Cc4ccccc4)C(=O)N	0.43	nM
CHEMBL379751	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccc[nH]1)C(	0.43	nM

28

	c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4		
CHEMBL49544	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2cc c(CCCN3CCOCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.43	nM
CHEMBL378557	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)C1CC1)C(c2cc ccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.43	nM
CHEMBL95413	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(= O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCO	0.44	nM
CHEMBL202345	O[C@@H](C[C@]1(Cc2ccccc2)N=CC(=C1O)C3C4OC(=O)N[C@H]4c5ccccc35)[C@H](Cc6ccccc6)NC(=O)O[C@H]7CCOC7	0.44	nM
CHEMBL11143	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C @H](CS(=O)(=O)c3cccc4ccccc34)NS(=O)(=O)C	0.44	nM
CHEMBL379162	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)N(C)C)C(c1cc ccc1)c2ccccc2)S(=O)(=O)c3ccc(N)cc3	0.44	nM
CHEMBL296137	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2c cc(F)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	0.44	nM
CHEMBL11116	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C @H](C[S+]([O-])c3cccc4ccccc34)NS(=O)(=O)C	0.45	nM
CHEMBL306963	CC(C)C1(CCc2nc(C)cs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.45	nM
CHEMBL98129	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCO	0.46	nM
CHEMBL205968	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccccn1)C(c2 ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.46	nM
CHEMBL97253	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(= O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCN	0.46	nM
CHEMBL114834	CC(C)(C)NC(=O)[C@@H]1CN(Cc2nc3ccccc3[nH]2)CCN1C[C@@H] (O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.47	nM
CHEMBL47712	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2c cc(OCCN3CCSCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	0.47	nM
CHEMBL98289	Cc1cc(O)cc(C)c1CNC(=O)[C@@H](C[C@@H](O)CN2CCN(C[C@@ H]2C(=O)NC(C)(C)C)S(=O)(=O)c3cccs3)Cc4ccccc4	0.47	nM
CHEMBL60697	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2cccc c2)[C@H](O)CN3CCN(Cc4csc5ccc(Cl)cc45)C[C@H]3C(=O)NC(C)(C) C	0.47	nM
CHEMBL361062	COc1cncc(c1)c2oc(nc2)C(C)(C)N3CCN(C[C@@H](O)C[C@@H](Cc4 oc(nn4)c5ccccc5)C(=O)N[C@H]6CCOC[C@H]6O)[C@@H](C3)C(=O)NCC(F)(F)F	0.48	nM
CHEMBL377192	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)OCc1cccnc1)C (c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.48	nM
CHEMBL319053	CC(C)(C)NC(=O)[C@@H]1CN(Cc2c(F)cccc2F)CCN1C[C@@H](O)C [C@@H](Cc3ccncc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.48	nM
CHEMBL116107	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccc(Cl)nc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.49	nM
CHEMBL98096	Cc1c(O)cccc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4C CS[C@H]4C[C@H]3C(=O)NC(C)(C)C	0.5	nM
CHEMBL379272	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cnccc1O)C(c 2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.5	nM
CHEMBL209023	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](N)C(c1ccccc1)c2ccccc 2)S(=O)(=O)c3ccc(N)cc3	0.5	nM
CHEMBL432550	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCC5CC5)c6oc7ccncc 7c6	0.5	nM
CHEMBL100089	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@ H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc5ccccc5c 4)NS(=O)(=O)C	0.5	nM
CHEMBL209452	COc1cc(ccc1O)C(=O)N[C@H](C(c2ccccc2)c3ccccc3)C(=O)NCCCC[C @@H](CO)N(CC(C)C)S(=O)(=O)c4ccc(N)cc4	0.5	nM

CHEMBL316694	CC(=O)N[C@H](CS(=O)(=O)c1ccc2ccccc2c1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCS[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.5	nM
CHEMBL47465	C[S+]([O-])c1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	0.51	nM
CHEMBL207077	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)N1CCOCC1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.51	nM
CHEMBL380545	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)N1CCNCC1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.52	nM
CHEMBL54182	Cc1ccccc1CNC(=O)[C@H]2N(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)COc5ccccc45)CSC2(C)C	0.52	nM
CHEMBL438249	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccc(O)cc1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.53	nM
CHEMBL326493	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccc2S)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.54	nM
CHEMBL285759	CC(C)[C@]1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.54	nM
CHEMBL324881	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccn3)C(=O)NCc4ccccc4)[C@H](NC(=O)Cc5ccccn5)C(=O)NCc6ccccc6	0.55	nM
CHEMBL378194	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccc(O)c(c1)[N+](=O)[O-])C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.56	nM
CHEMBL76040	CC(C)C1(CCc2nccs2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.57	nM
CHEMBL77041	CC(C)C1(CCc2ccc(CO)s2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.58	nM
CHEMBL301260	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(CCc4cccs4)C[C@H]3C(=O)NC(C)(C)C	0.59	nM
CHEMBL299821	COCCCN(CCCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1)CCOC	0.59	nM
CHEMBL317793	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](C[S+]([O-])c4ccc(F)cc4)NS(=O)(=O)C	0.6	nM
CHEMBL81811	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NC5CC5)c6oc7ccncc7c6	0.6	nM
CHEMBL52868	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@@H](CC(=O)OC(C)(C)C)Cc1ccccc1)Cc2ccccc2)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	0.6	nM
CHEMBL262300	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NC(=O)C(N)Cc3ccccc3	0.6	nM
CHEMBL323814	O[C@@H]1[C@@H](O)[C@@H](OCc2ccccc2)[C@@H](Cc3ccccc3)S(=O)(=O)[C@H](Cc4ccccc4)[C@@H]1OCc5ccccc5	0.6	nM
CHEMBL57566	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cccs4)C[C@H]3C(=O)NC(C)(C)C	0.6	nM
CHEMBL416814	CN(C)CCCc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	0.6	nM
CHEMBL311514	CCNC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)C(C)(C)c5oc6ccncc6c5	0.61	nM
CHEMBL333607	Cc1ccc(CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C)cn1	0.62	nM
CHEMBL77281	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccncc3	0.62	nM
CHEMBL384211	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccccc1O)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.63	nM
CHEMBL316717	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	0.63	nM
CHEMBL208724	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ccncc1)C(c2	0.65	nM

	ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4		
	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCc5cccs5)c6oc7ccncc7c6		
CHEMBL78514		0.65	nM
CHEMBL261952	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1cccnc1)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.68	nM
CHEMBL325946	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cnc3OCCc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.68	nM
CHEMBL327564	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3cccnc3	0.69	nM
CHEMBL75082	CC(C)[C@H](NC(=O)c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	0.7	nM
CHEMBL282654	CCC(C)C(NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccc3	0.71	nM
CHEMBL263423	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4cccc5cccnc45)NS(=O)(=O)C	0.71	nM
CHEMBL308615	CC(C)C1(CCc2c[nH]c3ccccc23)CC(=O)C(=C(O)O1)Sc4cc(C)c(CO)cc4C(C)(C)C	0.72	nM
CHEMBL327565	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccn3	0.75	nM
CHEMBL115	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	0.76	nM
CHEMBL301193	CCc1ccc(CCN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C)C)s1	0.76	nM
CHEMBL276656	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)c3ccc(F)cc3)NS(=O)(=O)C	0.77	nM
CHEMBL311555	CC(C)C1(CCc2occc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.78	nM
CHEMBL73875	CCCC[C@H](CN[C@H](CCCC)C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)[C@@H](C)O)[C@@H](C)CC	0.78	nM
CHEMBL2374440	COC(=O)N[C@H](Cc1ccccc1c2ccccc2)C(=O)NCCCC[C@@H](CO)N(CC(C)C)S(=O)(=O)c3ccc(N)cc3	0.79	nM
CHEMBL75070	CC(C)c1ncsc1CCC2(CC(=O)C(=C(O)O2)Sc3cc(C)c(CO)cc3C(C)(C)C)C(C)C	0.8	nM
CHEMBL115176	CC(C)(C)NC(=O)[C@@H]1CN(CC(=O)OC(C)(C)C)CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	0.81	nM
CHEMBL100271	CC(C)[C@@H]1SCC[C@@H]1OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	0.82	nM
CHEMBL97825	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ncc[nH]3	0.88	nM
CHEMBL95116	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCC(O)CN3CCOCC3	0.88	nM
CHEMBL295482	COCCN(CCOC)CCOc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)NC3[C@H](O)Cc4ccccc34)cc1	0.9	nM
CHEMBL102664	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccc6	0.9	nM
CHEMBL98355	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@H](C(=O)N)c3ccccc3	0.9	nM
CHEMBL72386	CC(C)[C@H](NC(=O)c1ccc2ccccc2c1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4CC5CCCCC5C[C@H]4C(=O)NC(C)(C)C	0.9	nM
CHEMBL209878	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)c1ncccc1O)C(c2ccccc2)c3ccccc3)S(=O)(=O)c4ccc(N)cc4	0.9	nM
CHEMBL433072	[I-].CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc	0.91	nM

	2ccc(CCC[N+](C)(C)C)cc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34		
CHEMBL99336	C[C@@H]1OCC[C@@H]1OC(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	0.92	nM
CHEMBL262714	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)c3ccc4ccccc4n3)NS(=O)(=O)C	0.92	nM
CHEMBL45457	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(OCCN2CCOCC2)cc1)[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	0.92	nM
CHEMBL74508	CC(C)C1(CCc2cccnc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.94	nM
CHEMBL151080	CC(C)(C)NC(=O)[C@@H]1CN(Cc2oc3ccc(F)cc3c2)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	0.94	nM
CHEMBL72497	CCCCc1cc(CN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C)C)cc(CCCC)n1	0.95	nM
CHEMBL78327	CC(C)C1(CCc2csc(N)n2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	0.95	nM
CHEMBL306932	CC(C)C1(CCc2ccc3[nH]ccc3c2)CC(=O)C(=C(O)O1)Sc4cc(C)c(CO)cc4C(C)(C)C	0.98	nM
CHEMBL46062	CN(C)CCOc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)NC3[C@H](O)Cc4ccccc34)cc1	1	nM
CHEMBL432806	CC(C)[C@@H](NC(=O)N(C)Cc1nccs1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N(C)Cc4nccs4)C(C)C	1	nM
CHEMBL116	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)O[C@H]2CCOC2)S(=O)(=O)c3ccc(N)cc3	1	nM
CHEMBL307582	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N4CCN(C)CC4)cc3C(C)(C)C	1	nM
CHEMBL324071	Nc1cccc(CO[C@@H]2[C@H](O)[C@@H](O)[C@@H](OCc3cccc(N)c3)[C@@H](Cc4ccccc4)S(=O)(=O)[C@@H]2Cc5ccccc5)c1	1	nM
CHEMBL45928	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CCCN3CCSCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1	nM
CHEMBL324260	CC(C)(C)NC(=O)[C@@H]1CN(CCOCc2ccccc2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	1.03	nM
CHEMBL95419	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N	1.1	nM
CHEMBL72399	CCCc1cc(CN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C)C)ccn1	1.1	nM
CHEMBL163045	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](CSc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	1.1	nM
CHEMBL337283	CC(C)(C)NC(=O)[C@@H]1CCCN1C(=O)[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	1.1	nM
CHEMBL277579	CC(C)[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=O)(=O)C(C)(C)C)C(=O)NCP(=O)(O)CNC(=O)[C@@H](NC(=O)[C@H](Cc3cccc4ccccc34)CS(=O)(=O)C(C)(C)C)C(C)C	1.1	nM
CHEMBL323882	COc1ncccc1CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C	1.1	nM
CHEMBL352273	CC(=O)N[C@@H](CC(=O)N)C(=O)N[C@@H](CSc1ccc2ccccc2c1)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	1.1	nM
CHEMBL98228	COC(=O)[C@@H](NC(=O)[C@@H](C[C@H](O[Si](C)(C)C(C)(C)C)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(C)C	1.1	nM
CHEMBL37383	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccc(Cl)c(Cl)c2)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1.1	nM
CHEMBL295777	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(CN3CCOCC3)cc2)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1.15	nM
CHEMBL310459	CC(C)(C)CNC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)C(C)(C)C)c5oc6ccncc	1.16	nM

6c5

CHEMBL311979	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2c cccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)C(C)(C)c5ccnc5	1.16	nM
CHEMBL359236	CC(C)(C)NC(=O)[C@@H]1CN(Cc2noc3ccccc23)CCN1C[C@@H](O) C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	1.17	nM
CHEMBL346120	CC(C)c1nc(CN(C)C(=O)NCCC(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OCc4cncs4)cs1	1.2	nM
CHEMBL71153	CNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C(C)C) cc1C)C(C)(C)C	1.2	nM
CHEMBL2374439	COC(=O)N[C@H](Cc1ccc2ccccc2c1)C(=O)NCCCC[C@@H](CO)N(C C(C)C)S(=O)(=O)c3ccc(N)cc3	1.2	nM
CHEMBL371085	COc1cc(CN2[C@H](Cc3ccccc3)[C@H](O)CN(N(Cc4ccc(O)c(OC)c4) C2=O)C(=O)CCc5ccncc5)ccc1O	1.2	nM
CHEMBL359237	CC(C)(C)NC(=O)[C@@H]1CN(Cc2nc3ccccc3s2)CCN1C[C@@H](O) C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	1.2	nM
CHEMBL406991	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C @H](CSc3cccc4ccccc34)NS(=O)(=O)C	1.2	nM
CHEMBL320126	CC(C)[C@@H](NC(=O)c1cc2ccccc2[nH]1)C(=O)N[C@@H](Cc3cccc c3)C(O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)c5cc6ccccc6[nH] 5)C(C)C	1.2	nM
CHEMBL75118	CC(C)C1(CCc2ccccn2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C) C	1.2	nM
CHEMBL307966	CCC(C)c1cc(CN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C @@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C) C)ccn1	1.2	nM
CHEMBL154831	CCCN(Cc1csc(n1)C(C)C)C(=O)NCC(=O)N[C@H](C[C@H](O)[C@H] (Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	1.2	nM
CHEMBL431455	CC(=O)N[C@H](CS(=O)(=O)c1ccc(F)cc1)C(=O)N[C@@H](Cc2ccccc 2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	1.2	nM
CHEMBL295345	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2cccc3ccccc23)C(=O)N[C@@H](Cc4ccccc4)C(=O) N	1.2	nM
CHEMBL147227	CC(C)(C)NC(=O)[C@@H]1CN(Cc2oc3ccccc3n2)CCN1C[C@@H](O) C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	1.2	nM
CHEMBL98885	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3cc ccc23)[C@H](Cc4ccccc4)NC(=O)OC5CCOCC5	1.22	nM
CHEMBL306073	CC(C)C1(CCc2ccsc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	1.22	nM
CHEMBL94991	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccn3	1.3	nM
CHEMBL168525	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O) c4ccc(cc4)C#N)cc3C(C)(C)C	1.3	nM
CHEMBL53107	CC(C)C[C@]1(N=CC(=C1O)[C@@H](Cc2ccccc2)C(=O)N)C3=C(O)[C@@](C[C@H](O)[C@@H](CC(=O)OC4CCOC4)Cc5ccccc5)(Cc6ccc cc6)N=C3	1.3	nM
CHEMBL77498	CC(C)C1(CCc2cscn2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	1.3	nM
CHEMBL78209	CC(C)C1(CCc2ncsc2C)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C) C	1.3	nM
CHEMBL304805	CC(C)C[C@]1(N=CC(=C1O)[C@@H](Cc2ccccc2)C(=O)N)C3=C(O)[C@@](C[C@H](O)[C@H](Cc4ccccc4)NC(=O)O[C@@H]5CCOC5)(C c6ccccc6)N=C3	1.3	nM
CHEMBL90751	O[C@@H](C[C@H](Cc1ccccc1)NC(=O)c2ccc(O)cc2Cl)[C@H](Cc3cc ccc3)NC(=O)OCc4ccccc4	1.3	nM
CHEMBL46061	CN(C)Cc1ccc(C[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C) (C)C)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)cc1	1.4	nM
CHEMBL333906	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(OCCO)cc4)c(cc1CO)C(C)(C)C	1.4	nM
CHEMBL307091	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2cccc	1.4	nM

33

	c2)[C@H](O)CN3CCN(Cc4ccnc(C)c4)C[C@H]3C(=O)NC(C)(C)C		
CHEMBL93589	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(O)cc2Cl)Cc3ccccc3	1.4	nM
CHEMBL320322	CC(C)[C@@H](NC(=O)N1CCN(CC1)c2ccccc2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)[C@H](O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)N5CCN(CC5)c6ccccc6)C(C)C	1.4	nM
CHEMBL282041	CC(C)CC(NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccc3	1.4	nM
CHEMBL327599	CC(C)(C)NC(=O)[C@@H]1CCCC[C@H]1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	1.4	nM
CHEMBL308786	CC(C)C1(CCc2nc3ccccc3s2)CC(=O)C(=C(O)O1)Sc4cc(C)c(CO)cc4C(C)(C)C	1.4	nM
CHEMBL306570	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4ccc5ccccc5n4)[C@H]6CCSC6	1.41	nM
CHEMBL318129	C[C@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	1.44	nM
CHEMBL351726	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)S(=O)(=O)c4ccccc4	1.5	nM
CHEMBL275969	Cc1cc(S[C@@H]2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)COc4c(C)cccc4C)[C@@H](C2)C(=O)NC(C)(C)C)nc(C)n1	1.5	nM
CHEMBL433704	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4	1.5	nM
CHEMBL164158	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](CSc2ccc3ccccc3c2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc4ccccc4	1.5	nM
CHEMBL97299	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NC(CO)Cc3ccccc3	1.5	nM
CHEMBL308410	CCc1cc(CN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C)C)ccn1	1.5	nM
CHEMBL168270	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4ccccc4)C(C)(C)C	1.5	nM
CHEMBL208907	CC(C)CN([C@H](CO)CCCCNC(=O)[C@@H](NC(=O)C)C(c1ccccc1)c2ccccc2)S(=O)(=O)c3ccc(N)cc3	1.5	nM
CHEMBL306534	CC(C)C1(CCc2ccncc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	1.5	nM
CHEMBL324916	CC(C)[C@@H](NC(=O)CCc1cccnc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CCc4cccnc4)C(C)C	1.5	nM
CHEMBL351145	CC(C)C(NC(=O)N(C)Cc1csc(n1)C(C)C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OCc4cnc(s4)C(C)C	1.5	nM
CHEMBL81974	CC(C)(N1CCN(C[C@@H](O)C[C@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCCC(F)(F)F)c5oc6ccncc6c5	1.6	nM
CHEMBL57238	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(CCc4ccsc4)C[C@H]3C(=O)NC(C)(C)C	1.6	nM
CHEMBL291203	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@@H](Cc2ccc(OCCN3CCCCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	1.6	nM
CHEMBL267571	Cc1cccc(C)c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)Sc4ccncc4	1.6	nM
CHEMBL432101	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)S(=O)(=O)C	1.6	nM
CHEMBL324747	CC(C)[C@@H](NC(=O)c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)C(O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)c5ccc6ccccc6n5)C(C)C	1.6	nM
CHEMBL432784	CC(=O)N[C@H](CS(=O)(=O)c1ccc2ccccc2c1)C(=O)N[C@@H](Cc3cc	1.6	nM

34

	ccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C		
	CC(C)c1nc(CCC2(CC(=O)C(=C(O)O2)Sc3cc(C)c(CO)cc3C(C)(C)C)C(C)C)cs1		
CHEMBL74787	CC(C)[C@@H](NC(=O)N(C)Cc1cccnc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N(C)Cc4cccnc4)C(C)C	1.6	nM
CHEMBL331363	Cc1c(O)cccc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)C[C@H](Cc3cccc3)NC(=O)OC(C)(C)C	1.6	nM
CHEMBL93718	CC(C)CN(Cc1csc(n1)C(C)C)C(=O)NCC(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	1.6	nM
CHEMBL155636	CN(C)S(=O)(=O)Oc1cc(c(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)cc1C)C(C)(C)C	1.6	nM
CHEMBL70386	CC(C)[C@@H](NS(=O)(=O)CCc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NS(=O)(=O)CCc4ccccn4)C(C)C	1.6	nM
CHEMBL112930	CC(C)[C@@H](NC(=O)N(C)Cc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N(C)Cc4ccccn4)C(C)C	1.66	nM
CHEMBL113575	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)c4ccccc4)c(cc1CO)C(C)(C)C	1.7	nM
CHEMBL121545	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3cccnc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1.7	nM
CHEMBL317926	Cc1cccc(C)c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)SCc4cccnc4	1.7	nM
CHEMBL13011	CC(=O)N[C@H](CS(=O)(=O)c1cccc2cccnc12)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	1.7	nM
CHEMBL415318	Cc1ccc(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)c(c1)C(=O)NC(C)(C)C	1.7	nM
CHEMBL58043	CC(C)(C)NC(=O)C1CN(Cc2c[nH]c3ccccc23)CCN1CC(O)CC(Cc4ccccc4)C(=O)NC5C(O)Cc6ccccc56	1.7	nM
CHEMBL325395	CCNS(=O)(=O)Nc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C(C)C)cc1C)C(C)(C)C	1.7	nM
CHEMBL172271	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)C(=O)c5cnc6occc6c5	1.7	nM
CHEMBL116845	CC(C)(C)NC(=O)C1CN(Cc2ccc3occc3c2)CCN1CC(O)CC(Cc4ccccc4)C(=O)NC5C(O)Cc6ccccc56	1.7	nM
CHEMBL332498	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)C[C@@H](Cc3ccncc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1.7	nM
CHEMBL313876	CNCCNC(=O)[C@@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(C)C	1.73	nM
CHEMBL95516	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSc3ccc4ccccc4c3)NS(=O)(=O)C	1.8	nM
CHEMBL11050	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)O)(CC2=O)c3ccccc3	1.8	nM
CHEMBL350861	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCN3CCCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	1.8	nM
CHEMBL295609	Cc1cccc(C)c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)SCc4ccncc4	1.8	nM
CHEMBL13217	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@@H](Cc4ccccc34)C(=O)N	1.8	nM
CHEMBL20546	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccccc4)cc3C(C)(C)C	1.8	nM
CHEMBL287361	CC(=O)N[C@H](CS(=O)(=O)c1ccc(F)cc1)C(=O)N[C@@H](CSc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	1.8	nM
CHEMBL328205	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc5ccccc5c	1.8	nM
CHEMBL317160			

	4)NC(=O)C(F)(F)F		
CHEMBL72385	CCc1cc(CN2CCN(C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)[C@@H]4C(C)C)[C@@H](C2)C(=O)NC(C)(C)C)cc(CC)n1	1.8	nM
CHEMBL357039	O[C@@H](C[C@]1(Cc2ccccc2)CCN([C@@H]3CS(=O)(=O)Cc4ccccc34)C1=O)[C@H](Cc5ccccc5)NC(=O)O[C@H]6CCOC6	1.8	nM
CHEMBL71440	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1OS(=O)(=O)N)C(C)(C)C	1.8	nM
CHEMBL321778	CC(C)[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCS[C@H]4C[C@H]3C(=O)NC(C)(C)C	1.84	nM
CHEMBL316608	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccccc3)NC(=O)O[C@@H]4CCS(=O)(=O)C4	1.84	nM
CHEMBL431387	CC(C)[C@@H]1NC(=O)CCCCCCCOc2ccc(C[C@H](NC1=O)[C@H](O)CN3CC4CCCCC4C[C@H]3C(=O)NC(C)(C)C)cc2	1.84	nM
CHEMBL37037	CC(C)[C@]1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	1.9	nM
CHEMBL348147	CC(C)C(NC(=O)N(Cc1csc(n1)C(C)C)C2CC2)C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)C[C@H](Cc4ccccc4)NC(=O)OCc5cncs5	1.9	nM
CHEMBL71334	CCCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2cnc3ccccc3n2)C(C)(C)C	1.9	nM
CHEMBL11137	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](C[S+]([O-])c3ccccc3)NS(=O)(=O)C	1.9	nM
CHEMBL171434	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)Cn4ccnc4)C(C)(C)C	1.9	nM
CHEMBL169878	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	1.9	nM
CHEMBL21041	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)[C@H](N)c4ccccc34	1.9	nM
CHEMBL346943	CC(C)C(NC(=O)OCc1nc(cs1)C(C)C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OCc4cncs4	1.9	nM
CHEMBL322804	CC(C)[C@@H](NC(=O)OCc1ccncc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccncc4)C(C)C	1.98	nM
CHEMBL45474	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccc(OCCCN3CCOCC3)cc2)C(=O)NC4[C@H](O)Cc5ccccc45	2	nM
CHEMBL75310	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc(C)nc4)C[C@H]3C(=O)NC(C)(C)C	2	nM
CHEMBL202110	O[C@@H](C[C@]1(Cc2ccccc2)N=CC(=C1O)[C@@H]3[C@H](O)Cc4ccccc34)[C@H](Cc5ccccc5)NC(=O)O[C@H]6CCOC6	2	nM
CHEMBL382463	NC(=O)O[C@@H]1Cc2ccccc2[C@@H]1C3=C(O)[C@@](C[C@H](O)[C@H](Cc4ccccc4)NC(=O)O[C@H]5CCOC5)(Cc6ccccc6)N=C3	2	nM
CHEMBL169256	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1OS(=O)(=O)Cn4ccnc4)C(C)(C)C	2	nM
CHEMBL318668	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc(F)cc4)NS(=O)(=O)C	2	nM
CHEMBL274569	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)c3ccc(cc3)C(F)(F)F)NS(=O)(=O)C	2	nM
CHEMBL178421	CC(C)CN([C@@H](CCCCNC(=O)OCC1c2ccccc2c3ccccc13)C(=O)O)S(=O)(=O)c4ccc(N)cc4	2.1	nM
CHEMBL200296	COc1cc(CN2[C@H](Cc3ccccc3)[C@H](O)CN(N(Cc4ccc(O)c(OC)c4)C2=O)C(=O)CCCCN5CCOCC5)ccc1O	2.1	nM
CHEMBL168369	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4ccc(cc4)C#N)C(C)(C)C	2.1	nM
CHEMBL318285	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](C[S+]([O-])c2ccc3ccccc3c2)NS(=O)(=O)C)C(=O)NC(C)(C)C	2.1	nM
CHEMBL98284	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(	2.1	nM

	=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCO		
CHEMBL276833	Cn1nnnc1[S+]([O-])C[C@H](NS(=O)(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	2.1	nM
CHEMBL421330	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)NCc5ccccc5)c6oc7ccncc7c6	2.19	nM
CHEMBL86226	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	2.2	nM
CHEMBL66399	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)C(C)(C)C	2.2	nM
CHEMBL351994	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccn2)S(=O)(=O)c3ccccc3	2.2	nM
CHEMBL113626	CC(C)[C@@H](NC(=O)\C=C\c1cccnc1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)\C=C\c4cccnc4)C(C)C	2.2	nM
CHEMBL171229	CCCC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	2.2	nM
CHEMBL356205	CN1C=C(CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C)C=CC1=O	2.2	nM
CHEMBL169391	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccc(cc4)C#N)cc3C(C)(C)C	2.2	nM
CHEMBL166757	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)C)cc3C(C)(C)C	2.2	nM
CHEMBL66460	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c2cnc3ccccc3n2)C(C)C)C(C)(C)C	2.2	nM
CHEMBL71472	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)cc1C)C(C)(C)C	2.3	nM
CHEMBL418528	CC(C)(C)NC(=O)c1ccccc1[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](C[S+]([O-])c3ccc(cc3)C(F)(F)F)NS(=O)(=O)C	2.3	nM
CHEMBL306772	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc(nc(c4)C(C)C)C(C)C)C[C@H]3C(=O)NC(C)(C)C	2.3	nM
CHEMBL347824	CCN(CCc1csc(n1)C(C)C)C(=O)NC(C)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	2.3	nM
CHEMBL3351098	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](O)[C@@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)C(=O)N[C@@H](Cc5ccccc5)C(=O)OC	2.3	nM
CHEMBL104118	CCNC(=O)[C@@H](NC(=O)CCc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)CCc4ccccc4)C(=O)NCC)C(C)(C)S2	2.4	nM
CHEMBL383732	NC(=O)C[C@H]1CC(C2=C(O)[C@@](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4)(Cc5ccccc5)N=C2)c6ccccc16	2.4	nM
CHEMBL170162	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	2.4	nM
CHEMBL266398	COc1ccc(cc1)S(=O)(=O)C[C@H](NS(=O)(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	2.4	nM
CHEMBL123229	Cc1cc(SC2=C(O)OC(CCc3cccc(O)c3)(CC2=O)c4ccccc4)c(cc1CO)C(C)(C)C	2.5	nM
CHEMBL419072	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc(C)nc(C)c4)C[C@H]3C(=O)NC(C)(C)C	2.5	nM
CHEMBL377274	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccccc3)N=CC(=C2O)C4C5OC(=O)N[C@@H]5c6ccccc46	2.5	nM
CHEMBL304086	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c2ccc3ccccc3n2)C(C)C)C(C)(C)C	2.5	nM
CHEMBL169714	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccccn4)cc3C(C)(C)C	2.6	nM

CHEMBL90090	Cc1c(N)cccc1C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C	2.6	nM
CHEMBL307926	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4ccc5ccccc5n4)C6CCCC6	2.6	nM
CHEMBL265588	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)COc2c(C)cccc2C)S(=O)(=O)c3ccc(N)cc3	2.6	nM
CHEMBL354867	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4cccnc4)cc3C(C)(C)C	2.6	nM
CHEMBL302289	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N4CCOCC4)cc3C(C)(C)C	2.6	nM
CHEMBL97847	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N	2.7	nM
CHEMBL38268	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	2.7	nM
CHEMBL29259	Cc1ccc(C(=O)NC(C)(C)C)c(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)c1	2.73	nM
CHEMBL265026	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4cnccn4)[C@H]5CCOC5	2.83	nM
CHEMBL289195	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	2.9	nM
CHEMBL96996	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCCN3CCOCC3	2.9	nM
CHEMBL69062	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)OCc2ccccc2)C(C)C)C(C)(C)C	2.9	nM
CHEMBL106633	CCNC(=O)[C@@H](NC(=O)\C=C/c1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)\C=C/c4ccccc4)C(=O)NCC)C(C)(C)S2	2.9	nM
CHEMBL336684	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3	3	nM
CHEMBL169381	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4cccn4)cc3C(C)(C)C	3	nM
CHEMBL98002	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)Cc4ccccc4	3	nM
CHEMBL109371	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccn4)C(C)C	3	nM
CHEMBL354829	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	3	nM
CHEMBL1790508	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c2cnc3ccccc3n2)[C@H](C)O)C(C)(C)C	3	nM
CHEMBL105695	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)N)[C@H](NC(=O)Cc4ccccc4)C(=O)N	3	nM
CHEMBL430891	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C(C)C	3	nM
CHEMBL70444	CCCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C(C)C)cc1C)C(C)(C)C	3	nM
CHEMBL263540	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cccc(O)c3C	3	nM
CHEMBL72474	CC(C)[C@H](NC(=O)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN2CC3CCCCC3C[C@H]2C(=O)NC(C)(C)C	3	nM
CHEMBL99616	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)C(=O)NC(C)(C)C	3	nM
CHEMBL315121	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(cn4)C#N	3	nM

	)c3C(=O)O1)O		
CHEMBL123287	Cc1cc(SC2=C(O)OC(CCc3ccc(N)cc3)(CC2=O)c4ccccc4)c(cc1CO)C(C)(C)C	3.1	nM
CHEMBL71509	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N4CCN(C)CC4)cc3C(C)(C)C	3.1	nM
CHEMBL3349509	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](CC(=O)N)NC(=O)OCc3ccccc3)C(=O)N[C@@H](C(C)C)C(=O)OC	3.1	nM
CHEMBL121706	Cc1cc(SC2=C(O)OC(CCc3ccc(N)cc3)(CC2=O)C4CCCC4)c(cc1CO)C(C)(C)C	3.2	nM
CHEMBL93540	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(O)cc2)Cc3ccccc3	3.3	nM
CHEMBL318217	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccccc3)NC(=O)OCc4ccccc4	3.3	nM
CHEMBL327611	COc1cc(ccc1O)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C	3.3	nM
CHEMBL93566	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cc(N)ccc2Cl)Cc3ccccc3	3.3	nM
CHEMBL169074	CCNS(=O)(=O)Nc1cc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)C(C)C)cc1C)C(C)(C)C	3.3	nM
CHEMBL312293	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N(C)C)cc3C(C)(C)C	3.4	nM
CHEMBL93481	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cc(N)cc2Cl)Cc3ccccc3	3.4	nM
CHEMBL58522	CC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCCN(C)C	3.4	nM
CHEMBL101962	COc1cc(CC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)Cc4cc(OC)c(OC)c(OC)c4)C(C)C)cc(OC)c1OC	3.4	nM
CHEMBL273562	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(O)c2)Cc3ccccc3	3.4	nM
CHEMBL325267	CCOc1ccc(CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C)cn1	3.4	nM
CHEMBL265095	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)C)cc3C(C)(C)C	3.4	nM
CHEMBL288033	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	3.45	nM
CHEMBL171786	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4cccnc4)cc3C(C)(C)C	3.5	nM
CHEMBL36608	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)C)cc3C(C)(C)C	3.5	nM
CHEMBL353086	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccnc4)cc3C(C)(C)C	3.5	nM
CHEMBL77671	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)[C@H](CCC(=O)N)NC(=O)[C@@H](CO)NC(=O)[C@@H](N)C(C)C)C(=O)N[C@@H](C(C)C)C(=O)O	3.5	nM
CHEMBL354616	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4ccc(Cl)cc4)C(C)(C)C	3.5	nM
CHEMBL273368	CC(C)(C)NC(=O)c1ccccc1[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](C[S+]([O-])c3ccc4ccccc4c3)NS(=O)(=O)C	3.5	nM
CHEMBL29312	CC(C)(C)NC(=O)c1c(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)ccc5ccccc15	3.5	nM
CHEMBL378214	COC(=O)N[C@@H](C(c1ccccc1)c2ccccc2)C(=O)NCCCC[C@H](CO)N(CC(C)C)S(=O)(=O)c3ccc(N)cc3	3.54	nM
CHEMBL433616	CC(C)CC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)Cn4ccnc4)cc3C(C)(C)C	3.6	nM
CHEMBL1790509	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)c2ccc3ccccc3n2)[C@H](C)O)C(C)(C)C	3.6	nM

CHEMBL168269	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CC4)c(cc1NS(=O)(=O)c5ccccc5)C(C)(C)C	3.6	nM
CHEMBL351155	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccs4)cc3C(C)(C)C	3.6	nM
CHEMBL56247	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccsc4)C[C@H]3C(=O)NC(C)(C)C	3.6	nM
CHEMBL354783	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)N(C)C)cc3C(C)(C)C	3.6	nM
CHEMBL170117	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4cc(F)cc4)C(C)(C)C	3.7	nM
CHEMBL123042	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(OCCO)cc4)c(cc1O)C(C)(C)C	3.7	nM
CHEMBL69755	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)C(C)(C)C	3.8	nM
CHEMBL104576	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)Nc3nc4ccccc4[nH]3)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccc6	3.8	nM
CHEMBL290442	CCCC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	3.8	nM
CHEMBL198734	COc1cc(CN2[C@H](Cc3ccccc3)[C@H](O)CN(N(Cc4ccc(O)c(OC)c4)C2=O)C(=O)CCCN5CCOCC5)ccc1O	3.8	nM
CHEMBL330565	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CC(C4)c5ccccc5	3.8	nM
CHEMBL306421	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N(C)C)cc3C(C)(C)C	3.9	nM
CHEMBL68032	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)N4CCN(C)CC4)cc3C(C)(C)C	3.9	nM
CHEMBL305458	CC(C)[C@@H](N[C@@H](C)C(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)[C@H](C)NC(=O)OCc4ccccc4)C(C)C	4	nM
CHEMBL13134	CC(C)[C@H](NC(=O)c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4CC[C@H](C[C@H]4C(=O)NC(C)(C)C)OCc5ccncc5	4	nM
CHEMBL123022	Cc1cc(SC2=C(O)OC(CCc3cccc(N)c3)(CC2=O)c4ccccc4)c(cc1CO)C(C)(C)C	4	nM
CHEMBL87092	CC(C)(C)OC(=O)NC(Cc1ccccc1)C(=O)C(F)(F)C(=O)NCc2ccccc2	4	nM
CHEMBL352964	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)C)cc3C(C)(C)C	4	nM
CHEMBL3350878	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3)C(=O)N[C@@H](Cc4ccccc4)C(=O)OC	4	nM
CHEMBL113627	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4cccnc4)C(C)C	4	nM
CHEMBL35271	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CC4)c(cc1N)C(C)(C)C	4.1	nM
CHEMBL332868	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCC4)c(cc1CO)C(C)(C)C	4.1	nM
CHEMBL157673	CCCN(CCc1csc(n1)C(C)C)C(=O)NC(C)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3cncs3)Cc4ccccc4	4.1	nM
CHEMBL274534	CC(C)(C)OC(=O)CNC(=O)[C@@H](NC(=O)c1ccccc1c2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)c5ccccc5c6ccccc6)C(=O)NCC(=O)OC(C)(C)C)C(C)(C)S3	4.1	nM
CHEMBL167243	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4cccnc4)cc3C(C)(C)C	4.1	nM
CHEMBL328531	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2c	4.1	nM

	cc(O)c(O)c2)Cc3ccccc3		
	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)		
CHEMBL171720	c4ccc(F)cc4)cc3C(C)(C)C	4.1	nM
CHEMBL122847	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1CO)C(C)(C)C	4.3	nM
	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(N)cc3)(CC2=O)C(C)		
CHEMBL305204	C)cc1C)C(C)(C)C	4.3	nM
	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C		
CHEMBL11426	@H](CSc3ccc(F)cc3)NS(=O)(=O)C	4.4	nM
	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](S		
	C2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCC(F)(F)F)[C@H](NC(=O		
CHEMBL432962	)Cc4ccccc4)C(=O)NCC(F)(F)F	4.4	nM
	CCCCC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C		
CHEMBL38384	)C	4.4	nM
	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@		
	H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4ccc5ccccc5n4)[C		
CHEMBL76352	@H]6CCS(=O)(=O)C6	4.42	nM
	CC(C)(C)NC(=O)C1CCCCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=		
CHEMBL3350611	O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	4.47	nM
	COCc1cc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(OCCO)cc4)cc1		
CHEMBL122802	C)C(C)(C)C	4.5	nM
	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2c		
CHEMBL91600	cccc2)Cc3ccccc3	4.5	nM
	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)		
CHEMBL168839	c4ccc(cc4)C#N)cc3C(C)(C)C	4.5	nM
	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)		
CHEMBL58277	N[C@@H]3[C@H](O)Cc4ccccc34	4.7	nM
	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2cccc		
CHEMBL90313	c2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CC4	4.8	nM
	CC(C)[C@@H](NC(=O)OCc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)C(		
CHEMBL106486	O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccn4)C(C)C	4.8	nM
	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CC		
CHEMBL306297	CCC4)cc1C)C(C)(C)C	4.8	nM
	CC[C@H](C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccc		
	cc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)[C		
CHEMBL90174	@@H](C)CC	4.9	nM
	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C(C)		
CHEMBL70986	C)cc1C)C(C)(C)C	4.9	nM
	CC(C)CN([C@@H](CCCCNC(=O)OCC1c2ccccc2c3ccccc13)C(=O)O)		
CHEMBL359756	S(=O)(=O)c4ccc(C)cc4	5	nM
	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4cc		
CHEMBL37597	c(cc4)C#N)cc3C(C)(C)C	5	nM
	CC(C)C1(CCC2CCCO2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C		
CHEMBL78217	)C	5	nM
	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)		
CHEMBL139538	NC(=O)c3ccccc3C	5	nM
	CC1(C)S[C@@H](N[C@H]1C(=O)NCC(O)CNC(=O)[C@@H]2N[C@		
	H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)[C@H](N		
CHEMBL317882	C(=O)Cc5ccccc5)C(=O)NCc6ccccc6	5	nM
	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)		
CHEMBL169535	c4ccccn4)cc3C(C)(C)C	5	nM
	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](		
CHEMBL317933	CC(=O)N)NC(=O)c2ccc3ccccc3n2)CC4CCCC4	5	nM
	CCCC[C@H](CC(O)C[C@@H](CCCC)C(=O)N[C@@H](C(C)C)C(=		
	O)N[C@@H](C(C)C)C(=O)OC)C(=O)N[C@@H](C(C)C)C(=O)N[C@		
CHEMBL39130	@H](C(C)C)C(=O)OC	5	nM
CHEMBL125448	OC(=O)CCCCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	5	nM
CHEMBL281439	COC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@@H](CC(O)C[C@	5	nM

	@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](C(C)C)C(=O)OC)Cc2ccccc2)C(C)C)C(C)C		
CHEMBL38154	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4ccncc4)cc3C(C)(C)C	5.08	nM
CHEMBL418978	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CSc4ccc5ccccc5c4)NS(=O)(=O)C	5.1	nM
CHEMBL432665	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4cccnc4)cc3C(C)(C)C	5.1	nM
CHEMBL322285	CN(C)C(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4ccccc4)C(=O)N(C)C)C(C)(C)S2	5.2	nM
CHEMBL99016	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](C3CCCCC3)C(=O)N	5.2	nM
CHEMBL169543	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccc(Cl)cc4)cc3C(C)(C)C	5.3	nM
CHEMBL111957	CC(C)[C@@H](NC(=O)\C=C\c1cccnc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)\C=C\c4cccnc4)C(C)C	5.3	nM
CHEMBL94078	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2	5.3	nM
CHEMBL93323	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cccc(N)c2Cl)Cc3ccccc3	5.3	nM
CHEMBL91610	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4Cc5ccccc5C4	5.3	nM
CHEMBL429036	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)OCc3ccccc3)NS(=O)(=O)C	5.4	nM
CHEMBL55586	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cc(C)nc(Cl)c4)C[C@H]3C(=O)NC(C)(C)C	5.4	nM
CHEMBL319400	CCNC(=O)[C@@H](NC(=O)c1c(C)onc1c2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)C4N[C@H](SC4(C)C)[C@H](NC(=O)c5c(C)onc5c6ccccc6)C(=O)NCC)C(C)(C)S3	5.4	nM
CHEMBL315253	NC(=O)CC(NC(=O)c1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	5.4	nM
CHEMBL274912	CC(C)[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=O)(=O)C(C)(C)C)C(=O)NCP(=O)(N)CNC(=O)[C@@H](NC(=O)[C@H](Cc3cccc4ccccc34)CS(=O)(=O)C(C)(C)C)C(C)C	5.5	nM
CHEMBL305466	CC(C)[C@@H]1NC(=O)c2cc3ccccc3cc2OCCCOc4ccc(C[C@H](NC1=O)[C@H](O)CN5CC6CCCCC6C[C@H]5C(=O)NC(C)(C)C)cc4	5.5	nM
CHEMBL314753	O[C@@H](C[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	5.6	nM
CHEMBL300812	O[C@@H](C[C@]1(Cc2ccccc2)N=CC(=C1O)C3CNC(=O)c4ccccc34)[C@H](Cc5ccccc5)NC(=O)O[C@H]6CCOC6	5.7	nM
CHEMBL267092	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)c3ccccc3)NS(=O)(=O)C	5.7	nM
CHEMBL17788	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	5.74	nM
CHEMBL319013	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@H](C(=O)NCc3ccccc3)c4ccccc4	5.8	nM
CHEMBL77819	CC(C)c1scnc1CCC2(CC(=O)C(=C(O)O2)Sc3cc(C)c(CO)cc3C(C)(C)C)C(C)C	5.8	nM
CHEMBL344233	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3Cl	6	nM
CHEMBL99081	CC(=O)N[C@H](CSCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	6	nM
CHEMBL342367	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cccc(N)c3C	6	nM

CHEMBL430445	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccc(O)cc3)N=CC(=C2O)C4[C@H](O)Cc5ccccc45	6	nM
CHEMBL3143353	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)CC(C)(C)C)Cc2ccccc2)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	6	nM
CHEMBL74166	CC(C)[C@H](NC(=O)[C@H](Cc1ccc(O)cc1)NC(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C(=O)N[C@H]3Cc4ccc(OCCCNC(=O)[C@@H](NC3=O)C(C)C)cc4	6	nM
CHEMBL58406	CC(C)(C)NS(=O)(=O)c1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	6	nM
CHEMBL305463	CCCCCCC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN2CC3CCCCC3C[C@H]2C(=O)NC(C)(C)C	6	nM
CHEMBL45953	CC(C)C[C@H](NC(=O)[C@H](C)[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)C(=O)N[C@@H](Cc2ccccc2)C(=O)N	6	nM
CHEMBL91657	Nc1ccc(C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3)Cc4ccccc4)c(Cl)c1	6.1	nM
CHEMBL333610	CCN1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)[C@@H](C1)C(=O)NC(C)(C)C	6.1	nM
CHEMBL38236	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4ccccn4)cc3C(C)(C)C	6.1	nM
CHEMBL347662	Cc1ccc(cc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C)C(=O)N4CCc5ccccc5C4	6.1	nM
CHEMBL434190	COc1cc(CN2[C@H](Cc3ccccc3)[C@H](O)CN(N(Cc4ccc(O)c(OC)c4)C2=O)C(=O)CN5CCNCC5)ccc1O	6.1	nM
CHEMBL308889	CCCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)cc1C)C(C)(C)C	6.2	nM
CHEMBL98229	CCN(CC)CC(O)CNC(=O)[C@@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(C)C	6.3	nM
CHEMBL169871	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4ccc(cc4)c5cccs5)C(C)(C)C	6.3	nM
CHEMBL333211	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(OCCO)cc4)c(cc1OCCO)C(C)(C)C	6.4	nM
CHEMBL37668	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1O)C(C)(C)C	6.5	nM
CHEMBL2374444	COC(=O)N(C)[C@H](Cc1ccccc1)C(=O)NCCCC[C@@H](CO)N(CC(C)C)S(=O)(=O)c2ccc(N)cc2	6.5	nM
CHEMBL407999	CC(C)[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=O)(=O)C(C)(C)C)C(=O)N[C@H](Cc3ccccc3)P(=O)(O)[C@@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)[C@H](Cc5cccc6ccccc56)CS(=O)(=O)C(C)(C)C)C(C)C	6.52	nM
CHEMBL99875	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	6.6	nM
CHEMBL331412	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c(cc1CO)C(C)(C)C	6.6	nM
CHEMBL149053	CC1=CSC2C(CN3CCN(C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56)[C@@H](C3)C(=O)NC(C)(C)C)N=CN12	6.7	nM
CHEMBL354615	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4cccn4)cc3C(C)(C)C	6.7	nM
CHEMBL151824	Cn1cc(CN2CCN(C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45)[C@@H](C2)C(=O)NC(C)(C)C)c6ccccc16	6.7	nM
CHEMBL112186	CC(C)[C@@H](NC(=O)OCc1cccnc1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4cccnc4)C(C)C	6.8	nM
CHEMBL333427	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c(cc1OCCO)C(C)(C)C	6.8	nM
CHEMBL106748	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)N4CCCCC4)[C@H](NC(=O)Cc5ccccc5)C(=O)N6CCCCC6	6.9	nM
CHEMBL272599	Cc1cccc(C)c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	7	nM

43

CHEMBL108960	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@](C)(Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	7	nM
CHEMBL70388	CC(C)[C@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C(=O)N[C@H]3Cc4ccc(OCCCNC(=O)[C@@H](NC3=O)C(C)C)cc4	7	nM
CHEMBL94266	C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N	7	nM
CHEMBL70502	CN1CCN(CC1)S(=O)(=O)Oc2cc(c(SC3=C(O)OC(C)(CCc4ccc(O)cc4)CC3=O)cc2C)C(C)(C)C	7.1	nM
CHEMBL419580	CC(C)[C@@H](NC(=O)C1Cc2ccccc2CN1)C(=O)N[C@@H](Cc3ccccc3)C(O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)C5Cc6ccccc6CN5)C(C)C	7.1	nM
CHEMBL97362	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCN(C)C	7.1	nM
CHEMBL105880	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccn3)C(=O)NCc4ccc(Cl)cc4)[C@H](NC(=O)Cc5ccccn5)C(=O)NCc6ccc(Cl)cc6	7.5	nM
CHEMBL112846	CC(C)[C@@H](NC(=O)CN1CCOCC1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CN4CCOCC4)C(C)C	7.5	nM
CHEMBL441065	COc1cc(ccc1N)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C	7.5	nM
CHEMBL439366	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)c3ccccc3c4ccccc4)C(=O)NCc5ccccc5)[C@H](NC(=O)c6ccccc6c7ccccc7)C(=O)NCc8ccccc8	7.5	nM
CHEMBL38269	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	7.5	nM
CHEMBL90139	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(O)c(N)c2)Cc3ccccc3	7.6	nM
CHEMBL347500	CC(C)(C)NC(=O)[C@@H]1CN(CC2(CC2)c3ccccc3)CCN1C[C@@H](O)C[C@@H](Cc4ccccc4)C(=O)NC5[C@H](O)Cc6ccccc56	7.7	nM
CHEMBL36448	CCCCCC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	7.7	nM
CHEMBL2092982	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@@H](O)Cc4ccccc34	7.72	nM
CHEMBL113825	CC(C)(C)NC(=O)[C@@H]1CC2CCCCC2CN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	7.8	nM
CHEMBL318700	CCC(C)[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCCN(C)C	7.9	nM
CHEMBL370853	COc1cc(CN2[C@H](Cc3ccccc3)[C@H](O)CN(N(Cc4ccc(O)c(OC)c4)C2=O)C(=O)CN5CCCC5)ccc1O	7.9	nM
CHEMBL306897	CC(C)[C@@H]1NC(=O)c2ccccc2OCCCOc3ccc(C[C@H](NC1=O)[C@H](O)CN4CC5CCCC5C[C@H]4C(=O)NC(C)(C)C)cc3	8	nM
CHEMBL407052	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)NCc3ccc4ccccc4n3)NS(=O)(=O)C	8	nM
CHEMBL169490	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCCC4)c(cc1OS(=O)(=O)Cn5ccnc5)C(C)(C)C	8	nM
CHEMBL1790510	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)OCc2ccccc2)[C@H](C)O)C(C)(C)C	8.2	nM
CHEMBL328233	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CCSC4	8.3	nM
CHEMBL330915	CC(C)[C@@H](NC(=O)N1CCN(Cc2ccccc2)CC1)C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)[C@@H](O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)N5CCN(Cc6ccccc6)CC5)C(C)C	8.38	nM
CHEMBL12900	Cc1cccc(C)c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	8.4	nM
CHEMBL327194	CCCCCCCCN1CCN(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@@	8.4	nM

	@H]3CCS(=O)(=O)[C@@H]3C(C)C)[C@@H](C1)C(=O)NC(C)(C)C		
CHEMBL17600	CC[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	8.41	nM
CHEMBL323203	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)[C@@H](NC(=O)C)C(C)C	8.5	nM
CHEMBL275123	CC(C)[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=O)(=O)C(C)(C)C)C(=O)NCP(=O)(CNC(=O)[C@@H](NC(=O)[C@H](Cc3cccc4ccccc34)CS(=O)(=O)C(C)(C)C)C(C)C)NN	8.5	nM
CHEMBL163243	CN(Cc1ccccn1)C(=O)c2ccc(C)c(c2)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C	8.6	nM
CHEMBL169278	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCC4)c(cc1NS(=O)(=O)c5ccccc5)C(C)(C)C	8.6	nM
CHEMBL104683	CCNC(=O)[C@@H](NC(=O)CC(C)C)[C@@H]1N[C@@H](C(=O)NCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)CC(C)C)C(=O)NCC(C)(C)S1	8.7	nM
CHEMBL354803	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4cccs4)cc3C(C)(C)C	8.7	nM
CHEMBL67867	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)C(C)C)cc1C)C(C)(C)C	8.9	nM
CHEMBL414648	CC(C)[C@H]1SCC[C@H]1OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	9	nM
CHEMBL112412	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCCN4CCOCC4)C(C)C	9	nM
CHEMBL94797	CC(C)[C@H](NC(=O)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)[C@@H](NC(=O)C)C(C)C	9	nM
CHEMBL3350608	CC(C)C[C@H](NC(=O)[C@H](Cc1ccccc1)CP(=O)(O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	9	nM
CHEMBL169037	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccc(cc4)C#N)cc3C(C)(C)C	9.1	nM
CHEMBL155588	CC(C)c1nc(CN(C2CC2)C(=O)NC(C)C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)C[C@H](Cc4ccccc4)NC(=O)OCc5cncs5)cs1	9.4	nM
CHEMBL342037	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(N)cc3C	9.49	nM
CHEMBL90699	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(N)c(N)c2)Cc3ccccc3	9.6	nM
CHEMBL103783	CC(C)[C@H](NC(=O)CC1NC(=O)NC1=O)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CC4NC(=O)NC4=O)C(C)C	9.6	nM
CHEMBL354216	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4ccc(F)cc4)cc3C(C)(C)C	9.6	nM
CHEMBL354173	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)C)C(C)(C)C	9.7	nM
CHEMBL71662	CN1CCN(CC1)S(=O)(=O)Oc2cc(c(SC3=C(O)OC(CCc4ccc(O)cc4)(CC3=O)C5CCCC5)cc2C)C(C)(C)C	9.7	nM
CHEMBL172622	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1OS(=O)(=O)c4cccc4)C(C)(C)C	9.8	nM
CHEMBL405969	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4	9.83	nM
CHEMBL107748	CCNC(=O)[C@@H](NC(=O)c1ccccc1c2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)c5ccccc5c6ccccc6)C(=O)NCC)C(C)(C)S3	9.9	nM
CHEMBL121995	CCC(C)c1ccccc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	10	nM
CHEMBL343108	CCc1ccccc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN(CC(C)C)S(=O)(=O)c3ccc(OC)cc3	10	nM
CHEMBL70140	CC(C)C[C@]1(N=CC(=C1O)[C@@H](Cc2ccccc2)C(=O)N)C3=C(O)[	10	nM

	C@@](C[C@H](O)[C@H](Cc4ccccc4)NC(=O)OC(C)(C)C)(Cc5ccccc5)N=C3		
CHEMBL430863	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](CS(=O)(=O)c2ccc(F)cc2)NS(=O)(=O)C)C(=O)NC(C)(C)C	10	nM
CHEMBL114192	CC(C)[C@@H](NC(=O)NCc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)NCc4ccccn4)C(C)C	10	nM
CHEMBL302958	CC(C)[C@H](NC(=O)[C@H](Cc1c[nH]c2ccccc12)NC(=O)C)C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)C(=O)N[C@H]4Cc5ccc(OCCCNC(=O)[C@@H](NC4=O)C(C)C)cc5	10	nM
CHEMBL317204	CC(C)CN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)OCc2ccccc2)C(C)C)NC(=O)[C@@H](NC(=O)OCc3ccccc3)C(C)C	10	nM
CHEMBL431534	CC(C)C[C@]1(N=CC(=C1O)[C@@H](Cc2ccccc2)C(=O)N)C3=C(O)[C@@](C[C@H](O)[C@@H](CC(=O)OC(C)(C)C)Cc4ccccc4)(Cc5ccccc5)N=C3	10	nM
CHEMBL354502	OCc1ccc(CN2[C@H](COc3ccccc3)[C@H](O)[C@@H](O)[C@@H](COc4ccccc4)N(Cc5ccc(CO)cc5)C2=O)cc1	10	nM
CHEMBL288163	CC(C)[C@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc1ccccc1)C(=O)N[C@@H](C(C)C)C(=O)NCc2nc3ccccc3[nH]2)Cc4ccccc4)C(=O)NCc5nc6ccccc6[nH]5	10	nM
CHEMBL70787	CC(C)(C)NC(=O)[C@@H]1CC2CCCCC2CN1C[C@@H](O)[C@@H]3Cc4ccc(OCCCOc5cc6ccccc6cc5C(=O)N[C@@H](CC(=O)N)C(=O)N3)cc4	10	nM
CHEMBL290900	COC(=O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)OC)Cc4ccccc4)C(C)C	10	nM
CHEMBL71961	C[C@@H](N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C(=O)N[C@H]2Cc3ccc(OCCCNC(=O)[C@@H](NC2=O)C(C)C)cc3)NC(=O)OCc4ccccc4	10	nM
CHEMBL347671	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)c3ccc(Cl)cc3	10	nM
CHEMBL99878	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2SCC[C@@H]2CN1C[C@@H](O)[C@H](CSc3ccccc3)NC(=O)[C@@H](CS(=O)(=O)c4ccc(F)cc4)NC(=O)C(F)(F)F	10	nM
CHEMBL353812	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4ccccc4)cc3C(C)(C)C	10.4	nM
CHEMBL191849	COc1cc(ccc1N)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3)Cc4ccccc4	10.5	nM
CHEMBL2115250	CC(C)(C)NC(=O)[C@@H]1CCCC[C@@H]1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3	10.68	nM
CHEMBL59522	CC(C)(C)c1c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)sc5ccccc15	10.91	nM
CHEMBL88255	CC(C)[C@@H](NC(=O)C)C(=O)N[C@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)C(C)C)C(C)C	10.95	nM
CHEMBL289799	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCCC4)c(cc1N)C(C)(C)C	10.95	nM
CHEMBL37813	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c(cc1N)C(C)(C)C	11	nM
CHEMBL91443	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccc(N)c(O)c2)Cc3ccccc3	11	nM
CHEMBL105879	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccn4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccn6	11	nM
CHEMBL150003	CCCNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)N(C)CCN(C)C(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4ccccc4)C(=O)NCC)C(C)(C)S2	11	nM
CHEMBL35088	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(cc3C(C)(C)C)N(C)C	11	nM

46

CHEMBL17494	CCC[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	11.16	nM
CHEMBL37755	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1N)C(C)(C)C	11.17	nM
CHEMBL112578	CC(C)[C@@H](NS(=O)(=O)CCc1ccncc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NS(=O)(=O)CCc4ccncc4)C(C)C	11.7	nM
CHEMBL278416	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCS(=O)(=O)[C@H]4C5CCC5	11.84	nM
CHEMBL291974	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccccc3)N=CC(=C2O)C4[C@H](O)Cc5ccccc45	11.9	nM
CHEMBL276431	Cc1c(O)cccc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	12	nM
CHEMBL331829	CC(C)[C@@H](NC(=O)CCc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CCc4ccccn4)C(C)C	12	nM
CHEMBL91601	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cc(O)ccc2Cl)Cc3ccccc3	12	nM
CHEMBL331724	Cc1ccc(c(SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4)c1)C(C)(C)C	12	nM
CHEMBL119488	Cc1ccc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(OCCO)cc4)c1)C(C)(C)C	12	nM
CHEMBL2374441	COC(=O)N[C@H](Cc1ccccc1)C(=O)NCCCC[C@@H](CO)N(CC(C)C)S(=O)(=O)c2ccc(N)cc2	12	nM
CHEMBL321514	CC(C)[C@H](NC(=O)Cc1csc(N)n1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)Cc4csc(N)n4)C(C)C	12	nM
CHEMBL36600	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4ccc(cc4)C(F)(F)F)cc3C(C)(C)C	12.1	nM
CHEMBL263268	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1NS(=O)(=O)c4ccc(cc4)C(F)(F)F)C(C)(C)C	12.3	nM
CHEMBL273827	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](C[S+]([O-])c3ccccn3)NS(=O)(=O)C	12.35	nM
CHEMBL323955	CC(C)[C@@H](NC(=O)N(C)CCc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N(C)CCc4ccccn4)C(C)C	12.7	nM
CHEMBL72487	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccncc4)C[C@H]3C(=O)NC(C)(C)C	12.95	nM
CHEMBL312909	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(N)cn4)c3)C(=O)O1)O	13	nM
CHEMBL430995	CC(C)[C@@H]1NC(=O)[C@H](Cc2ccc(OCCCNC1=O)cc2)NC(=O)C(=O)C(Cc3ccccc3)NC(=O)OC(C)(C)C	13	nM
CHEMBL99725	CC(C)[C@H](NC(=O)c1sc(C)nc1C)C(=O)N[C@@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)c3sc(C)nc3C)C(C)C)Cc4ccccc4	13	nM
CHEMBL90449	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccccn4)c3)C(=O)O1)O	13	nM
CHEMBL431754	CC(C)(C)NC(=O)[C@@H]1CC2CCCCC2CN1C[C@@H](O)[C@@H]3Cc4ccc(OCCOc5cc6ccccc6cc5C(=O)N[C@@H](CC(=O)N)C(=O)N3)cc4	13	nM
CHEMBL113264	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCC4CCCN(C)C4)C(C)C	13	nM
CHEMBL77685	CC(C)C1(CCc2csc(C)n2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	13	nM
CHEMBL100039	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)C(=O)NC(C)(C)C	13	nM
CHEMBL72129	CC(C)[C@H](NC(=O)N[C@@H](C)S(=O)(=O)c1ccc(C)cc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C(=O)N[C@H]3Cc4ccc(OCCCNC(=O)[C@@H](NC3=O)C(C)C)cc4	13	nM

CHEMBL99607	Cc1c(O)cccc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	13	nM
CHEMBL321377	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3)C(=O)N[C@@H](C(C)C)C(=O)OC	13	nM
CHEMBL35664	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4ccccc4)cc3C(C)(C)C	13.2	nM
CHEMBL249788	CC(C)CC(NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCc3ccccc3	13.42	nM
CHEMBL113268	CC(C)[C@@H](NC(=O)OCc1ccncc1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCc4ccncc4)C(C)C	13.49	nM
CHEMBL287118	CC(C)CC1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(N)cc3C(C)(C)C	13.5	nM
CHEMBL305063	CC(C)[C@@H]1NC(=O)\C=C/CCCCCOc2ccc(C[C@H](NC1=O)[C@H](O)CN3CC4CCCC4C[C@H]3C(=O)NC(C)(C)C)cc2	13.51	nM
CHEMBL91085	CCCN1CCN(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@@H]3CS(=O)(=O)[C@@H]3C(C)C)[C@@H](C1)C(=O)NC(C)(C)C	13.7	nM
CHEMBL82490	CC(C)(N1CCN(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)COc4ccccc34)[C@@H](C1)C(=O)Nc5ccccc5)c6oc7ccncc7c6	13.8	nM
CHEMBL3706748	Cc1ccc(cc1C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C)C(=O)N5CCc6ccccc6C5	13.8	nM
CHEMBL354499	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4ccnc4)cc3C(C)(C)C	14	nM
CHEMBL269252	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccn3)C(=O)NCc4ccc(Cl)cc4Cl)[C@H](NC(=O)Cc5ccccn5)C(=O)NCc6ccc(Cl)cc6Cl	14	nM
CHEMBL73308	O[C@@H](CC[C@H](Cc1ccccc1)NC(=O)c2ccccc2NC(=O)OCc3ccccn3)[C@H](Cc4ccccc4)NC(=O)c5ccccc5NC(=O)OCc6ccccn6	14	nM
CHEMBL307001	CC(C)(C)[C@@H](CC(=O)Nc1ccccc1)C(=O)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3	14	nM
CHEMBL308167	CC(C)C1(CCc2ccsc2CO)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	14	nM
CHEMBL284341	CC(C)C1(CCc2ccccc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4ccc(cc4)C#N)cc3C(C)(C)C	14	nM
CHEMBL121855	CC(C)c1ccc(C(C)C)c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c1	14	nM
CHEMBL348282	O[C@@H](CN(CC1CCCCC1)S(=O)(=O)c2ccccc2)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	14	nM
CHEMBL78185	CC(C)c1csc(CCC2(CC(=O)C(=C(O)O2)Sc3cc(C)c(CO)cc3C(C)(C)C)C(C)C)n1	14	nM
CHEMBL159378	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](CSc2ccccc2)NC(=O)[C@@H](CC(=O)N)NC(=O)OCc3ccccc3	14	nM
CHEMBL141046	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3	14	nM
CHEMBL112569	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCCN4CCCC4)C(C)C	14	nM
CHEMBL146361	C[C@@H]1CC[C@@H](O)[C@H]1N2CC[C@](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C)(Cc4ccccc4)C2=O	14	nM
CHEMBL139444	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(O)cc3C	14.14	nM
CHEMBL430153	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSCc3ccccc3)NS(=O)(=O)C	14.7	nM
CHEMBL276203	CC(=O)N[C@@H](CSc1ccc2ccccc2n1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)Cc4ccccc4C(=O)NC(C)(C)C	14.7	nM
CHEMBL436252	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H]4CCCS(=O)(=O)C4	14.7	nM

48

CHEMBL109500	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CO)NC(=O)C)C(=O)N[C@@H](C(C)C)C(=O)OC	14.87	nM
CHEMBL276077	C[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	14.93	nM
CHEMBL34008	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)c4cccc(c4)C#N)cc3C(C)(C)C	15	nM
CHEMBL105459	CNC(=O)[C@@H](NC(=O)[C@H](OCc1ccccc1)[C@H](O)[C@@H](O)[C@@H](OCc2ccccc2)C(=O)N[C@@H](C(C)C)C(=O)NC)C(C)C	15	nM
CHEMBL116677	CC(C)C)NC(=O)[C@@H]1C[C@@H](CN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34)Oc5ccc6ccccc6c5	15	nM
CHEMBL423189	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccc(C)cc3	15	nM
CHEMBL69134	CCC(CC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)C(C)(C)C	15	nM
CHEMBL107393	CCNC(=O)[C@@H](NC(=O)Cc1cccs1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4cccs4)C(=O)NCC)C(C)(C)S2	15	nM
CHEMBL89038	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(cc4)C#N)c3)C(=O)O1)O	15	nM
CHEMBL331458	COc1cc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)cc1C)C(C)(C)C	15	nM
CHEMBL276671	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cc(C)cc(C)c3	15	nM
CHEMBL21145	OCc1ccc(CN2[C@H](Cc3ccccc3)[C@H](O)[C@@H](O)[C@@H](Cc4ccccc4)N(Cc5ccc(CO)cc5)C2=O)cc1	15	nM
CHEMBL75833	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cccnc4)C[C@H]3C(=O)NC(C)(C)C	15	nM
CHEMBL151617	CC(C)(C)NC(=O)[C@@H]1CN(CCCC(F)(F)F)CCN1C[C@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	15.3	nM
CHEMBL83768	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4CO[C@@H]5OCC[C@H]45	15.41	nM
CHEMBL413390	CC(C)[C@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=O)(=O)C(C)(C)C)C(=O)N[C@H](Cc3ccccc3)P(=O)(N)[C@@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)[C@H](Cc5cccc6ccccc56)CS(=O)(=O)C(C)(C)C)C(C)C	15.81	nM
CHEMBL316767	CC(C)[C@H](NC(=O)CSc1ncccn1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CSc4ncccn4)C(C)C	16	nM
CHEMBL20930	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3CCCc4ccccc34	16	nM
CHEMBL324398	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(CC(C)C)NC(=O)[C@@H](NC(=O)OC)C(C)C	16	nM
CHEMBL321165	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(OC)cc2)NC(=O)[C@@H](NC(=O)OC)C(C)C	16	nM
CHEMBL357009	CC(C)(CO)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)CO	16	nM
CHEMBL11287	COc1ccc(SC[C@H](NS(=O)(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C)cc1	16	nM
CHEMBL168384	Cc1cc(SC2=C(O)OC(C)(CCc3ccc(O)cc3)CC2=O)c(cc1OS(=O)(=O)c4cc(F)cc4)C(C)(C)C	16.9	nM
CHEMBL326913	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2cccs2)NC(=O)[C@@H](NC(=O)OC)C(C)C	17	nM
CHEMBL263995	CC(C)(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccccc3	17	nM
CHEMBL146875	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccccc3)CCN([C@@H]4CS(=O)(=O)Cc5ccccc45)C2=O	17	nM
CHEMBL126058	CC(C)c1ccc(C)cc1SC2=C(O)C=C(OC2=O)c3ccccc3	17	nM

CHEMBL125506	CCC(C)c1ccccc1SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4	17	nM
CHEMBL74275	CC(C)C1(CCc2cncnc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	17	nM
CHEMBL275792	Cn1nnnc1SC[C@H](NS(=O)(=O)C)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	17.5	nM
CHEMBL124555	CC(C)(C)c1ccccc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	17.66	nM
CHEMBL93082	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3	18	nM
CHEMBL431976	CC(C)C1(CCc2csc(NC(=O)C)n2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	18	nM
CHEMBL324657	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(O)cc2)NC(=O)[C@@H](NC(=O)OC)C(C)C	18	nM
CHEMBL171873	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NS(=O)(=O)c4ccc(cc4)C(F)(F)F)cc3C(C)(C)C	18.3	nM
CHEMBL169247	CC(C)C1(CCc2ccc(N)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O)c4cccs4)cc3C(C)(C)C	18.5	nM
CHEMBL418511	Cc1ccc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c1)C(C)(C)C	18.71	nM
CHEMBL353815	CC(C)C[C@H]1[C@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	18.97	nM
CHEMBL17852	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)C4CO[C@@H]5CCS(=O)(=O)[C@@H]5C4	18.97	nM
CHEMBL69651	CC(C)(C)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)C(C)(C)C	19	nM
CHEMBL77621	CC(C)[C@H](NC(=O)[C@@H](NC(=O)[C@@H]1CCCN1C[C@H](Cc2ccccc2)NC(=O)[C@H](C)NC(=O)[C@H](C)NC(=O)[C@@H](N)CO)C(C)C)C(=O)N	19	nM
CHEMBL324377	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(C)cc2)NC(=O)[C@@H](NC(=O)OC)C(C)C	19	nM
CHEMBL423648	CC(=O)N[C@@H](CC(=O)N)C(=O)N[C@@H](CSc1ccccc1)[C@H](O)Cc2ccccc2C(=O)NC(C)(C)C	19	nM
CHEMBL74654	CC(C)C1(CCc2ncc(C)s2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	19	nM
CHEMBL432787	CCNC(=O)[C@@H](NC(=O)Cc1ccccn1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4ccccn4)C(=O)NCC)C(C)(C)S2	19	nM
CHEMBL98302	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)Cc4ccncc4	19	nM
CHEMBL329068	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)Cc3ccccc3	19	nM
CHEMBL71852	CC(C)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)C(C)(C)C	19	nM
CHEMBL273424	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CS(=O)(=O)Cc3ccccc3)NS(=O)(=O)C	19.4	nM
CHEMBL325107	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3CCc4ccccc34	19.97	nM
CHEMBL333611	CC(C)[C@@H](NC(=O)OCCN1CCOCC1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCCN4CCOCC4)C(C)C	20	nM
CHEMBL71980	CN(C)S(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCC4)cc1C)C(C)(C)C	20	nM
CHEMBL445105	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(OCc2ccccc2)cc1)C(=O)N3CCC(=O)[C@@H]3Sc4ccccc4	20	nM
CHEMBL275960	CC(=O)N[C@@H](CS(=O)(=O)c1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	20	nM
CHEMBL274128	CC(Oc1c(C)cccc1C)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	20	nM

CHEMBL201918	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccc cc3)N=CC(=C2O)C4C[C@H](CC(=O)N)c5ccccc45	20.5	nM
CHEMBL125719	Cc1ccc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(O)cc4)c1)C(C)(C) C	20.98	nM
CHEMBL106991	CC(C)(C)OC(=O)CNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC (=O)Cc4ccccc4)C(=O)NCC(=O)OC(C)(C)C)C(C)(C)S2	21	nM
CHEMBL122402	CC(C)(C)NC(=O)[C@H]1N(CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)CSC1(C)C	21	nM
CHEMBL171404	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCCC4)c(cc1OS(= O)(=O)c5ccc(cc5)C#N)C(C)(C)C	21	nM
CHEMBL282787	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C @H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	21.17	nM
CHEMBL169142	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(OS(=O)(=O) c4cccs4)cc3C(C)(C)C	21.8	nM
CHEMBL279279	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2c ccc2)C(=O)NC3Cc4ccccc34	22	nM
CHEMBL13136	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(Cl)c(Cl)c3	22	nM
CHEMBL109220	CC(C)[C@@H](NC(=O)CCc1cccnc1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CCc4ccnc4)C(C)C	22	nM
CHEMBL273437	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C @H](CS(=O)(=O)c3ccccn3)NS(=O)(=O)C	22	nM
CHEMBL90510	Nc1ccc(cc1O)C(=O)N[C@H](C[C@H](O)[C@H](Cc2ccccc2)NC(=O) OCc3ccccc3)Cc4ccccc4	22	nM
CHEMBL97512	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@ @H](O)CN(Cc3ccc(F)cc3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C(C) C	22	nM
CHEMBL88964	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(cn4)C(F) (F)F)c3)C(=O)O1)O	22.36	nM
CHEMBL427631	CC1(C)S[C@@H](N[C@H]1C(=O)NC[C@@H](O)[C@H](O)CNC(= O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NC c4ccccc4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccc6	22.45	nM
CHEMBL139237	CC(C)(C)OC(=O)[C@@H]1CCCN1C[C@@H](O)[C@H](Cc2ccccc2) NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	23	nM
CHEMBL263236	CC(C)C[C@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)NCCCN(C)C	23	nM
CHEMBL109699	CC(C)[C@@H](NC(=O)CCN1CCOCC1)C(=O)N[C@@H](Cc2ccccc2) [C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)CC N4CCOCC4)C(C)C	23	nM
CHEMBL541982	COc1cccc(c1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)C[C@H](Cc3c cccc3)NC(=O)OC(C)(C)C	23	nM
CHEMBL121920	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@ H](O)CNC(=O)[C@@H]3N[C@H](SC3(C)C)C(NC(=O)Cc4ccccc4)C(=O)N	23	nM
CHEMBL324630	COC(=O)NC(C(C)C)C(=O)NN(CC(C)C)C[C@H](O)[C@H](Cc1ccccc 1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2	23	nM
CHEMBL12714	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(Cl)c3	23	nM
CHEMBL124892	CC(C)c1ccccc1SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4	23	nM
CHEMBL95462	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@ @H](O)CN(Cc3ccc(cc3)C#N)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C (C)C	24	nM
CHEMBL99774	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@ H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](CSc4ccc(F)cc4)NS(=O)(=O)C	24	nM
CHEMBL356947	CCCNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCC(CO)NC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4c cccc4)C(=O)NCC)C(C)(C)S2	25	nM

CHEMBL302902	CC(C)(C)OC(=O)N[C@@H](Cc1ccc(O)cc1)C(=O)N2CCC(=O)[C@@H]2Sc3ccccc3	25.5	nM
CHEMBL12224	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cc(Cl)cc(Cl)c3	26	nM
CHEMBL333982	CN(C)c1ccc(CNC(=O)C(NC(=O)Cc2ccccc2)[C@@H]3N[C@@H](C(=O)NC[C@H](O)CN4C[C@H]5CCCC[C@H]5C[C@H]4C(=O)NC(C)(C)C)C(C)(C)S3)cc1	26	nM
CHEMBL329974	CN(C)CCCNC(=O)[C@@H](NC(=O)[C@@H](C[C@H](O)[C@@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)c3ccccc3	26	nM
CHEMBL164570	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)NCc3ccccc3)(CC2=O)c4ccccc4	26	nM
CHEMBL324989	CCC(C)[C@H](NC(=O)C[C@H](O)[C@H](CC1CCCCC1)NC(=O)CC2CCCN3N2C(=O)C(CN)CCC3=O)C(=O)N[C@@H](Cc4ccccc4)C(=O)N	26	nM
CHEMBL71218	CCNS(=O)(=O)Oc1cc(c(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)c4ccccc4)cc1C)C(C)(C)C	26	nM
CHEMBL279372	CCCC[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	26.12	nM
CHEMBL322119	COC(=O)NC(C(C)C)C(=O)NN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)CC4CCCCC4	27	nM
CHEMBL224483	CC(C)(C)[C@H](NC(=O)OCc1ccccc1)C(=O)NC(Cc2ccccc2)C(=O)C(F)(F)C(=O)NCc3ccccc3	27	nM
CHEMBL154952	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)S(=O)(=O)C	27	nM
CHEMBL341697	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cccc(C)c3	27	nM
CHEMBL91995	CC(C)CN1CCN(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@@H]3CCS(=O)(=O)[C@@H]3C(C)C)[C@@H](C1)C(=O)NC(C)(C)C	27.1	nM
CHEMBL331846	Cc1ccc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccc(N)cc4)c1)C(C)(C)C	27.71	nM
CHEMBL122426	CC(C)c1ccc(C)cc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	27.93	nM
CHEMBL61755	CCc1c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)sc5ccccc15	28	nM
CHEMBL405134	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccc(c2)C(C)(C)NC(=O)OC(C)(C)C)CCN1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)NC4[C@H](O)Cc5ccccc45	28	nM
CHEMBL411507	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N4CCN(C)CC4)C(C)C	28	nM
CHEMBL29010	Cc1cccc(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)c1C(=O)NC(C)(C)C	28	nM
CHEMBL320671	CC(C)[C@@H](NC(=O)C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)CN(Cc2ccc(F)cc2)NC(=O)[C@@H](NC(=O)C)C(C)C	28	nM
CHEMBL98150	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)CC3CCCCC3	29	nM
CHEMBL355735	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCCC4)c(cc1OS(=O)(=O)c5ccc(F)cc5)C(C)(C)C	29	nM
CHEMBL97423	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](Cc3ccccc3)C(=O)N	29	nM
CHEMBL291773	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(COC(=O)N3CCOCC3)cc2)NC(=O)OC(C)(C)C	30	nM
CHEMBL2114445	CC[C@H](C)[C@@H](NC(=O)[C@@H](C[C@@H](O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)Cc3ccccc3)C(=O)NCc4nc5ccccc5[nH]4	30	nM
CHEMBL290163	COC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(C)C)NC(=O)[C@@H](CC(O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)OC)Cc4ccccc4	30	nM
CHEMBL94497	CC(C)[C@@H](NC(=O)C)C(=O)NN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)C)C(C)C)Cc2ccccc2	30	nM

CHEMBL415896	CC[C@H](C)[C@H](NC(=O)[C@H](CC(C)C)CC(O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)C(=O)NCc3nc4ccccc4[nH]3	30	nM
CHEMBL40829	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1CCCCC1C(=O)NC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3	30	nM
CHEMBL91102	O[C@@H](C[C@H](Cc1ccccc1)NC(=O)c2ccccc2)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	31	nM
CHEMBL93120	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2c(Cl)ccc(N)c2Cl)Cc3ccccc3	31	nM
CHEMBL320783	COC(=O)NC(C(C)C)C(=O)NN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)Cc4ccc(OC)cc4	31	nM
CHEMBL330980	CCNC(=O)C(NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCC(O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C)C(C)(C)S2	31	nM
CHEMBL158358	CC(C)c1nc(CN(C2CC2)C(=O)NCCC(=O)N[C@@H](Cc3ccccc3)[C@@H](O)C[C@H](Cc4ccccc4)NC(=O)OCc5cncs5)cs1	31.97	nM
CHEMBL122320	OC1=C(Sc2ccccc2C3CCCCC3)C(=O)CC(CCc4ccccc4)(O1)c5ccccc5	32	nM
CHEMBL339407	Cc1cc(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c(cc1O)C(C)(C)C	33	nM
CHEMBL280464	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(cc2)C(F)(F)F)NC(=O)[C@@H](NC(=O)OC)C(C)C	33	nM
CHEMBL97547	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)NN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)OCc3ccccc3)C(C)C)Cc4ccccc4	33	nM
CHEMBL325561	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(OC)c(OC)c2OC)NC(=O)[C@@H](NC(=O)OC)C(C)C	34	nM
CHEMBL276097	CC(C)OC(=O)c1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	34	nM
CHEMBL292264	CC(C)(C)c1cc2CCCc2cc1SC3=C(O)OC(CCc4ccccc4)(CC3=O)c5ccccc5	34.21	nM
CHEMBL88757	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CCOCC4	34.6	nM
CHEMBL297633	CC[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23	34.7	nM
CHEMBL90768	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CCCC4	35	nM
CHEMBL148090	CC(C)[C@@H](CO)N1CC[C@](C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)(Cc3ccccc3)C1=O	35	nM
CHEMBL12768	CCOC(=O)c1ccc(cc1)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	35	nM
CHEMBL325800	CCNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@@H](CNC(=O)Cc4ccccc4)SC3(C)C)C(C)(C)S2	35	nM
CHEMBL143470	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)CO	35	nM
CHEMBL124789	CC(C)c1ccccc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	36.85	nM
CHEMBL140653	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3C(F)(F)F	37	nM
CHEMBL325778	CC(C)CN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)NC(=O)C(NC(=O)OCc4ccccc4)C(C)C	37	nM
CHEMBL430701	CC(C)(C)NC(=O)[C@@H]1CNCCN1C[C@@H](O)C[C@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	38	nM
CHEMBL12421	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(c3)c4ccccc4	38	nM
CHEMBL122480	CC(C)c1ccc(C)cc1SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4	38	nM
CHEMBL386631	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)c3ccccc3c4ccccc4)C(=O)NCC(=O)O)[C@H](NC(=O)c5ccccc5c6ccccc6)C(=O)NCC(=O)O	39	nM
CHEMBL107310	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCC(=O)O)[C@H](NC(=O)Cc4ccccc4)C(=O)NCC(=O)O	39	nM
CHEMBL68267	CCCC(CCC)NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)C(C)(C)C	39	nM

CHEMBL273317	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCS(=O)(=O)C4	39.77	nM
CHEMBL345868	OC(C[C@@H](Cc1ccccc1)C(=O)N[C@H]2CCCC[C@@H]2NC(=O)c3ccc4ccccc4n3)C[C@@H](Cc5ccccc5)C(=O)N[C@H]6CCCC[C@@H]6NC(=O)c7ccc8ccccc8n7	40	nM
CHEMBL60782	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCN3CCOC3=O)cc2)NC(=O)OC(C)(C)C	40	nM
CHEMBL2374443	COC(=O)N[C@H](CCc1ccccc1)C(=O)NCCCC[C@@H](CO)N(CC(C)C)S(=O)(=O)c2ccc(N)cc2	40	nM
CHEMBL301046	CN(C)C(=O)OCCOc1ccc(C[C@H](NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)cc1	40	nM
CHEMBL326679	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCCO[C@H](NC(=O)Cc4ccccc4)C(=O)NCCO	40	nM
CHEMBL320050	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCC4CCCCC4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCC6CCCCC6	40	nM
CHEMBL108807	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(CC(C)C)NC(=O)[C@@H](NC(=O)OC)C(C)C	41	nM
CHEMBL111259	CC(C)C(NC(=O)OCc1ccccc1)C(=O)NN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)CC5CCCCC5	41	nM
CHEMBL418527	CC(=O)N[C@@H](CSc1ccc2ccccc2c1)C(=O)N[C@@H](Cc3ccccc3)[C@H](O)Cc4ccccc4C(=O)NC(C)(C)C	42	nM
CHEMBL108102	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(F)cc2)NC(=O)[C@@H](NC(=O)OC)C(C)C	42	nM
CHEMBL341237	OC1=C(Sc2ccccc2C3CCCC3)C(=O)CC(O1)(c4ccccc4)c5ccccc5	42.17	nM
CHEMBL113554	CC(C)[C@@H](NC(=O)N(C)Cc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N(C)Cc4ccccn4)C(C)C	43	nM
CHEMBL322964	CC(C)[C@@H](NC(=O)N1CCOCC1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)N4CCOCC4)C(C)C	43	nM
CHEMBL355811	CC(C)(C)NC(=O)c1ccccc1OC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4C(=O)c5ccccc5S(=O)(=O)c4c3	44	nM
CHEMBL10777	CC(C)(C)NC(=O)c1ccccc1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSc3ccccc3)NS(=O)(=O)C	44	nM
CHEMBL368352	CC(C)(C)NC(=O)c1ccccc1OC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	45	nM
CHEMBL292161	COc1cc(Oc2ccccc2)ccc1C[C@@H](O)C[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	45	nM
CHEMBL97189	CC(C)CN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)C)C(C)C)NC(=O)[C@@H](NC(=O)C)C(C)C	45	nM
CHEMBL276704	CC(=O)N[C@@H](CSSc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	45	nM
CHEMBL348047	OC(C[C@@H](Cc1ccccc1)C(=O)N[C@H]2CCCC[C@@H]2NC(=O)c3cc4ccccc4cn3)C[C@@H](Cc5ccccc5)C(=O)N[C@H]6CCCC[C@@H]6NC(=O)c7cc8ccccc8cn7	45	nM
CHEMBL285836	CC(C)CN1CC(O)(CNC(=O)[C@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)C[C@@H]1C(=O)NC(C)(C)C	45.83	nM
CHEMBL122547	CC(C)c1ccc(c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)c1)C(C)(C)C	47	nM
CHEMBL217396	CN(C)c1ccc(CNC(=O)[C@@H](NC(=O)Cc2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccc(cc6)N(C)C)C(C)(C)C)S3)cc1	47	nM
CHEMBL330739	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(CC(C)(C)C)C[C@H]3C(=O)NC(C)(C)C	48	nM
CHEMBL293860	CC(C)(C)c1c(oc2ccccc12)SC3=C(O)OC(CCc4ccccc4)(CC3=O)c5ccccc5	48.06	nM

CHEMBL53979	CC(O)COc1ccc(C[C@H](NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)cc1	49	nM
CHEMBL139309	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3C(C)C	49	nM
CHEMBL325815	COc1ccc(CN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3)NC(=O)C(NC(=O)OCc5ccccc5)C(C)C)cc1	49	nM
CHEMBL341294	CC(C)(C)c1ccccc1SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4	49	nM
CHEMBL59706	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCc3ccccn3)cc2)NC(=O)OC(C)(C)C	50	nM
CHEMBL59667	COCCCCCOc1ccc(C[C@H](NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)cc1	50	nM
CHEMBL120090	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3cccc(c3)C(=O)N4CCc5ccccc5C4	50	nM
CHEMBL327752	CC(C)[C@H](NC(=O)C)C(=O)N[C@@H](Cc1ccccc1)[C@@H](O)CN(Cc2ccc(cc2)C#N)NC(=O)[C@@H](NC(=O)C)C(C)C	50	nM
CHEMBL98709	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](CSc2ccc3ccccc3c2)NS(=O)(=O)C)C(=O)NC(C)(C)C	50	nM
CHEMBL323425	CC(C)C(NC(=O)OCC=C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OCC=C)C(C)C	51	nM
CHEMBL91062	CC(C)(C)OC(=O)N[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cc(O)cc(O)c2)Cc3ccccc3	51	nM
CHEMBL268605	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)OCc3ccccc3)NC(=O)N	51	nM
CHEMBL340811	OC1=C(SCCc2ccccc2)C(=O)CC(CCc3ccccc3)(O1)c4ccccc4	51	nM
CHEMBL316975	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)C(O)CNC(=O)Cc3ccccc3)[C@H](NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	53	nM
CHEMBL310485	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4ccc5ccccc5c4)C[C@H]3C(=O)NC(C)(C)C	54	nM
CHEMBL122641	COC(=O)C(NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NC[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C)C(C)(C)S2	54	nM
CHEMBL12950	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(O)cc3	54	nM
CHEMBL320637	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)NCCCO)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	54	nM
CHEMBL354884	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)C4=CCCS(=O)(=O)C4	54.7	nM
CHEMBL2062145	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@]2(Cc3ccccc3)CCN([C@@H]4[C@H](O)Cc5ccccc45)C2=O	56.41	nM
CHEMBL88755	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C(C)C	57	nM
CHEMBL9726	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	57.97	nM
CHEMBL107015	CCNC(=O)[C@@H](NS(=O)(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NS(=O)(=O)Cc4ccccc4)C(=O)NCC)C(C)(C)S2	58	nM
CHEMBL71741	CC(C)C(NC(=O)C[C@@H](C(=O)NC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)C(C)(C)C)C(C)C	58	nM
CHEMBL12257	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(C)cc3	59	nM
CHEMBL34479	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)CC(C)(C)C)cc3C(C)(C)C	60	nM
CHEMBL421622	OC1=C(SCc2ccccc2)C(=O)CC(CCc3ccccc3)(O1)c4ccccc4	60	nM
CHEMBL292653	CN1CCN(CCOc2ccc(C[C@H](NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C)cc2)C1=O	60	nM
CHEMBL61670	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCOc3ccnc3)cc2)NC(=O)OC(C)(C)C	60	nM

CHEMBL262764	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](Cc3cc4ccccc4[nH]3)C(=O)N	60	nM
CHEMBL10725	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSc3ccc4ccccc4n3)NS(=O)(=O)C	60	nM
CHEMBL177011	CC(C)(C)NC(=O)c1c(OC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4C(=O)c5ccccc5S(=O)(=O)c4c3)ccc6ccccc16	60	nM
CHEMBL104525	COC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4ccccc4)C(=O)OC)C(C)(C)S2	60	nM
CHEMBL333738	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@H](O)CNC(=O)[C@@H]3N[C@H](SC3(C)C)C(NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	60.66	nM
CHEMBL172724	CC(C)(C)NC(=O)c1ccccc1OC[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4C(=O)c5ccccc5C(=O)c4c3	60.75	nM
CHEMBL50382	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C3(O)CCCC3(C)C	61.24	nM
CHEMBL292791	CC(C)(C)c1oc2ccccc2c1SC3=C(O)OC(CCc4ccccc4)(CC3=O)c5ccccc5	61.63	nM
CHEMBL273234	COC(=O)c1cc(ccc1O)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	62	nM
CHEMBL175385	CC(C)(C)NC(=O)c1c(OC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](CC(=O)N)NC(=O)c3ccc4C(=O)c5ccccc5C(=O)c4c3)ccc6ccccc16	62	nM
CHEMBL323161	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C(O)CN(Cc2ccc(cc2)C#N)NC(=O)[C@@H](NC(=O)OC)C(C)C	62	nM
CHEMBL302532	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCCC[C@H]3C(=O)NC(C)(C)C	62	nM
CHEMBL105851	CCNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)Cc4ccccc4)C(=O)NCC)C(C)(C)S2	62.45	nM
CHEMBL297349	C[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)C(=O)N[C@@H]2[C@H](O)Cc3ccccc23	62.7	nM
CHEMBL110603	CC(C)[C@@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCC4CCCCN4C)C(C)C	63	nM
CHEMBL95467	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](CC3CCCCC3)C(=O)N	64	nM
CHEMBL61188	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCO)cc2)NC(=O)OC(C)(C)C	64	nM
CHEMBL327087	COCCOC(=O)NC(C(C)C)C(=O)NC(Cc1ccccc1)C(O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OC)C(C)C	64.45	nM
CHEMBL97146	CC(C)[C@@H](NC(=O)c1ccc2ccccc2n1)C(=O)NN(C[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4ccc5ccccc5n4)C(C)C)Cc6ccccc6	65	nM
CHEMBL87806	CCCC1(CCc2ccccc2)OC(=C(C(CC)c3cccc(NS(=O)(=O)c4ccc(cn4)[N+](=O)[O-])c3)C(=O)O1)O	65	nM
CHEMBL322995	CCOC(=O)NC(C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OC)C(C)C	65.24	nM
CHEMBL275937	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(c3)[N+](=O)[O-]	67	nM
CHEMBL92272	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2c(Cl)cccc2Cl)Cc3ccccc3	67	nM
CHEMBL320343	COCCOCCOC(=O)NC(C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OCCOCCOC)C(C)C	67	nM
CHEMBL418902	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4ccc5ccccc5n4)C6CCOCC6	67.9	nM
CHEMBL275560	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(cc3)C(=O)O	68	nM
CHEMBL2111802	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)C(=O)O	68.96	nM

	c5ccccc5		
CHEMBL308845	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@H](Cc2cccc2)[C@H](O)CN3CCN(Cc4cc(Cl)cc(Cl)c4)C[C@H]3C(=O)NC(C)(C)C	69	nM
CHEMBL412878	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1CC(O)C[C@@H](Cc3ccccc3)C(=O)N[C@H]4CCCC[C@@H]4NC(=O)c5cc6ccccc6cn5	70	nM
CHEMBL291155	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1CC(O)C[C@@H](Cc3ccccc3)C(=O)N[C@H]4CCCC[C@@H]4NC(=O)c5ccc6ccccc6n5	70	nM
CHEMBL305845	CC(C)C1(CCc2c[nH]cn2)CC(=O)C(=C(O)O1)Sc3cc(C)c(CO)cc3C(C)(C)C	70	nM
CHEMBL290749	CC[C@H](C)[C@H](NC(=O)[C@H](Cc1ccccc1)CC(O)(CO)CN2C[C@H]3CCCC[C@H]3C[C@H]2C(=O)NC(C)(C)C)C(=O)NCc4nc5ccccc5[nH]4	70	nM
CHEMBL321789	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@@H](COC(=O)c3ccccc3)NC(=O)Cc4ccccc4)[C@@H](COC(=O)c5ccccc5)NC(=O)Cc6ccccc6	70	nM
CHEMBL159658	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)NCCc3ccccc3)(CC2=O)c4ccccc4	71	nM
CHEMBL292276	COCCOc1ccc(C[C@H](NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)cc1	72	nM
CHEMBL106282	CCNC(=O)[C@@H](NC(=O)c1ccccc1Cc2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)c5ccccc5Cc6ccccc6)C(=O)NCC)C(C)(C)S3	72	nM
CHEMBL339426	Cc1ccccc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	73	nM
CHEMBL266620	CCC(=O)N[C@@H](CC(=O)OCc1ccccc1)C(=O)N[C@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	73	nM
CHEMBL64513	Cc1c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)sc5ccccc15	74	nM
CHEMBL106623	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)OCc4ccccc4)[C@H](NC(=O)Cc5ccccc5)C(=O)OCc6ccccc6	75	nM
CHEMBL41965	CCCC[C@H](CC(O)C[C@@H](CCCC)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)OC)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)OC	75	nM
CHEMBL12600	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(c3)C(F)(F)F	76	nM
CHEMBL275730	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(Cl)cc3	76	nM
CHEMBL76338	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2cccc2)[C@H](O)CN3CCN(Cc4cc(C)cc(C)c4)C[C@H]3C(=O)NC(C)(C)C	78	nM
CHEMBL415758	CC(C)(C)NC(=O)c1ccccc1OC[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3cnc4ccccc4n3	79.37	nM
CHEMBL57069	COc1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	80	nM
CHEMBL289928	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1CCC[C@@H]1C(=O)NC(C)(C)C)Cc2ccccc2)C(=O)NCc3nc4ccccc4[nH]3	80	nM
CHEMBL293777	CC(C)(C)NC(=O)[C@@H]1CCCCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	80	nM
CHEMBL293727	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCCN3CCOCC3=O)cc2)NC(=O)OC(C)(C)C	80	nM
CHEMBL13067	COC(=O)c1cccc(c1)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	80	nM
CHEMBL171148	O[C@@H]1[C@@H](O)[C@@H](COc2ccccc2)N(Cc3ccccc3)C(=O)N(Cc4ccccc4)[C@@H]1COc5ccccc5	80	nM
CHEMBL159602	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)NCc3ccccc3)(CC2=O)c4ccccc4	81	nM
CHEMBL440834	COc1ccc(cc1)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	83	nM
CHEMBL170804	OC1=C(C(CC2CC2)SCc3ccccc3)C(=O)C=C(O1)c4ccccc4	84	nM
CHEMBL347431	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=	84.85	nM

57

	O)(=O)c3ccccc3		
CHEMBL64701	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(CCC(=O)N3CCOCC3)cc2)NC(=O)OC(C)(C)C	85	nM
CHEMBL11193	CC(=O)N[C@@H](CC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	85	nM
CHEMBL330620	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](CSc2ccc(F)cc2)NS(=O)(=O)C)C(=O)NC(C)(C)C	85	nM
CHEMBL62133	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCCN3CCOCC3)cc2)NC(=O)OC(C)(C)C	86	nM
CHEMBL122031	CCCCCCCNC(=O)C(NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCC(O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C)C(C)(C)S2	86	nM
CHEMBL430984	CC(C)(C)NC(=O)[C@@H]1CC2CCCCC2CN1C[C@@H](O)[C@@H]3Cc4ccc(OCCCCOc5cc6ccccc6cc5C(=O)N[C@@H](CC(=O)N)C(=O)N3)cc4	88	nM
CHEMBL164110	CCCCCC1(CC(=O)C(=C(O)O1)Sc2ccccc2C(C)C)c3ccccc3	88	nM
CHEMBL170195	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H]4CCCSC4	88.01	nM
CHEMBL340472	Cc1ccc(c(SC2=C(O)C=C(OC2=O)c3ccccc3)c1)C(C)(C)C	88.86	nM
CHEMBL12408	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(O)c3	89	nM
CHEMBL63717	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)C(=O)N2CCC(=O)[C@@H]2Sc3ccccc3	89.44	nM
CHEMBL355533	CC(C)(C)NC(=O)c1ccccc1SC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	90	nM
CHEMBL304249	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCC(=O)N3CCCCC3)cc2)NC(=O)OC(C)(C)C	90	nM
CHEMBL304231	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCn3ccnc3)cc2)NC(=O)OC(C)(C)C	90	nM
CHEMBL35215	CCCC[C@H](CC(O)C[C@@H](CCCC)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)OC)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc2ccccc2)C(=O)OC	90	nM
CHEMBL423628	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)Nc3ccccc3)(CC2=O)c4ccccc4	91	nM
CHEMBL286861	CC(C)C1(CCc2ccc(O)cc2)CC(=O)C(=C(O)O1)Sc3cc(C)c(NC(=O)OC(C)(C)C)cc3C(C)(C)C	91	nM
CHEMBL156424	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)c3cccc(Cl)c3	92	nM
CHEMBL163941	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)N)(CC2=O)c3ccccc3	92	nM
CHEMBL174803	CC(C)(C)NC(=O)c1ccccc1NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4n3	94	nM
CHEMBL18031	C[C@@H]1OCC[C@@H]1OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	94.1	nM
CHEMBL322171	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)CN(CC3CCCCC3)NC(=O)[C@@H](NC(=O)OCc4ccccc4)C(C)C	95	nM
CHEMBL57987	CSc1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	95	nM
CHEMBL325764	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)NCC(O)CO[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	95	nM
CHEMBL320243	CC(C)[C@@H](NS(=O)(=O)N(C)Cc1ccccn1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NS(=O)(=O)N(C)Cc4ccccn4)C(C)C	95.5	nM
CHEMBL201216	CC(C)(C)CC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@]2(Cc3ccccc3)N=CC(=C2O)C4C5OC(=O)N[C@@H]5c6ccccc46	96	nM
CHEMBL123513	CC(C)CCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	96	nM
CHEMBL127754	CCCCCCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	96.99	nM

CHEMBL58701	CC(C)COc1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	97	nM
CHEMBL124841	CC(C)CCC1(CC(=O)C(=C(O)O1)SCc2ccccc2)c3ccccc3	98	nM
CHEMBL93113	CCC(CC)N1CCN(C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@@H]3CCS(=O)(=O)[C@@H]3C(C)C)[C@@H](C1)C(=O)NC(C)(C)C	98.6	nM
CHEMBL435594	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC3(CO)CCC3	100	nM
CHEMBL294635	O=C(N[C@@H](Cc1ccccc1)C(=O)N2CCC(=O)C2Sc3ccccc3)c4ccnc4	100	nM
CHEMBL61118	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCN3CCOCC3)cc2)NC(=O)OC(C)(C)C	100	nM
CHEMBL321398	CC(C)(C)NC(=O)C1CC2CCCCC2CN1C[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)OCc4ccccc4	100	nM
CHEMBL48805	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)C(Cc2ccc(O)cc2)NC(=O)OC(C)(C)C	100	nM
CHEMBL59705	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCC(=O)N3CCOCC3)cc2)NC(=O)OC(C)(C)C	100	nM
CHEMBL154252	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)S(=O)(=O)C	100	nM
CHEMBL162922	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N)(CC2=O)c3ccccc3	101	nM
CHEMBL74862	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccc2O)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	102	nM
CHEMBL74629	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccc2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	102	nM
CHEMBL17571	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)OC4CS(=O)(=O)C4	104	nM
CHEMBL430674	CC(C)(C)NC(=O)N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)Cc3ccncc3	105	nM
CHEMBL58606	COc1ccc(C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34)c(OC)c1	105	nM
CHEMBL123428	OC1=C(SCc2ccccc2)C(=O)CC(CC3CCCC3)(O1)c4ccccc4	109.8	nM
CHEMBL62046	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCC(O)c3ccccn3)cc2)NC(=O)OC(C)(C)C	110	nM
CHEMBL341006	OC1=C(Sc2ccccc2)C(=O)CC(O1)(c3ccccc3)c4ccccc4	110	nM
CHEMBL356749	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)C[C@]2(Cc3ccccc3)CCN([C@@H]4CSCc5ccccc45)C2=O	111	nM
CHEMBL12884	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(c3)N(C)C	114	nM
CHEMBL3349554	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OC(C)(C)C)C(=O)N[C@@H](C(C)C)C(=O)OC	116.62	nM
CHEMBL124529	CC(C)c1ccc(C(C)C)c(SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4)c1	119	nM
CHEMBL12449	Cc1ccccc1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	120	nM
CHEMBL291506	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCC(C)(C)O)cc2)NC(=O)OC(C)(C)C	120	nM
CHEMBL333043	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1CC(O)CNC(=O)[C@@H]3N[C@H](SC3(C)C)C(NC(=O)Cc4ccccc4)C(=O)NCCNC(=O)CCCC[C@@H]5SC[C@@H]6NC(=O)N[C@H]56	120	nM
CHEMBL122388	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)c4ccc(O)cc4)c(cc1CO)C(C)(C)C	120	nM
CHEMBL45699	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(C)(O)C(C)(C)CO	120	nM
CHEMBL68721	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CNC(=O)[C@H](CC(=O)NC(C)(C)C)C(C)(C)C	120.62	nM
CHEMBL279323	C[C@@H]1CS(=O)(=O)C[C@@H]1OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	122.96	nM
CHEMBL330615	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@	123.91	nM

	H](O)[C@H](Cc3ccccc3)NC(=O)O[C@@H]4COCC=C4		
CHEMBL275301	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(F)cc3	124	nM
CHEMBL274027	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N3CCN(CC3)C(=O)OC(C)(C)C)(CC2=O)c4ccccc4	124	nM
CHEMBL110557	CCOC(=O)NC(C(C)C)C(=O)NN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)CC4CCCCC4	126	nM
CHEMBL100034	CCCCNC(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2	126	nM
CHEMBL317103	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	127	nM
CHEMBL162769	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)N3CCN(CC3)C(=O)OC(C)(C)C)(CC2=O)c4ccccc4	127	nM
CHEMBL309582	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(Cc4cccc(O)c4)C[C@H]3C(=O)NC(C)(C)C	127	nM
CHEMBL343727	C[C@H](O)C(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	129.61	nM
CHEMBL339288	OC1=C(Sc2ccccc2)C(=O)CC(CCc3ccccc3)(O1)c4ccccc4	130	nM
CHEMBL41789	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)Cc3ccccc3)C(=O)NCCc4nc5ccccc5[nH]4	130	nM
CHEMBL294261	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc3ncccc3c2)NC(=O)OC(C)(C)C	130	nM
CHEMBL45699	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(C)(O)C(C)(C)CO	130	nM
CHEMBL355438	Cc1cc(SC2=C(O)OC(CCc3ccc(O)cc3)(CC2=O)C4CCCCC4)c(cc1OS(=O)(=O)c5ccccc5)C(C)(C)C	131	nM
CHEMBL308837	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)C(=O)c4ccncc4	132	nM
CHEMBL331232	CC(C)(C)NC(=O)C1N(C[C@H](O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)C(C)(C)SC1(C)C	132.93	nM
CHEMBL422408	CC(C)(C)[C@@H](CC(=O)NC1CCCCC1)C(=O)NC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3	135	nM
CHEMBL273732	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(cc3)C(=O)N	135	nM
CHEMBL353836	CC(C)CC(SC1CCCCC1)C2=C(O)C=C(OC2=O)c3ccccc3	136.24	nM
CHEMBL40291	CC[C@H](C)[C@H](NC(=O)[C@H](Cc1ccccc1)CC(O)(CO)CN(CC2CCCCC2)CC(=O)NC(C)(C)C)C(=O)NCc3nc4ccccc4[nH]3	140	nM
CHEMBL63319	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2cccc(OCc3ccccc3)c2)NC(=O)OC(C)(C)C	140	nM
CHEMBL308693	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CNC(=O)C3CCCC[C@H]3C(=O)NC(C)(C)C	140	nM
CHEMBL107250	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@@H](CO)NC(=O)Cc3ccccc3)[C@@H](CO)NC(=O)Cc4ccccc4	140	nM
CHEMBL2112563	CCC[C@]1(CCc2ccccc2)CC(=O)C(=C(O)O1)[C@H](CC)c3cccc(NS(=O)(=O)c4ccc(cn4)C(F)(F)F)c3	140	nM
CHEMBL107701	CCOC(=O)NC(C(C)C)C(=O)NN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)C(NC(=O)OCCOC)C(C)C)CC2CCCCC2	141.77	nM
CHEMBL91557	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2ccccc2O)Cc3ccccc3	145	nM
CHEMBL334057	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)NCc3ccccc3)C(NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	145.46	nM
CHEMBL163390	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)NCc3ccccc3)(CC2=O)c4ccccc4	146	nM
CHEMBL13036	CCOC(=O)c1cc(ccc1O)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	148	nM
CHEMBL28462	CC(C)(C)NC(=O)c1cc2ccccc2cc1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4	149	nM

CHEMBL293525	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCC(=O)O)cc2)NC(=O)OC(C)(C)C	150	nM
CHEMBL43739	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)Cc3ccccc3)C(=O)NCc4ccccn4	150	nM
CHEMBL318814	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@@H](CO)Cc2ccccc2)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	150	nM
CHEMBL13037	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3cccc(c3)C(=O)O	151	nM
CHEMBL115292	CC(C)(C)OC(=O)[C@@H]1CCCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3	151.49	nM
CHEMBL124731	OC1=C(SCCc2ccccc2)C(=O)CC(O1)(c3ccccc3)c4ccccc4	152	nM
CHEMBL74699	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccc(O)cc2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	153	nM
CHEMBL419595	CC(C)CCCC1(CC(=O)C=C(O)O1)SCCc2ccccc2)c3ccccc3	155	nM
CHEMBL125827	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1CC(O)CNC(=O)[C@@H]3N[C@H](SC3(C)C)C(NC(=O)Cc4ccccc4)C(=O)NCCNC(=O)OC(C)(C)C	160	nM
CHEMBL106965	CCNC(=O)[C@@H](NC(=O)c1ccccc1Oc2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)c5ccccc5Oc6ccccc6)C(=O)NCC)C(C)(C)S3	160	nM
CHEMBL316766	CC(C)[C@H](NC(=O)C(O)(c1ccccc1)c2ccccc2)C(=O)N[C@H](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)C(O)(c4ccccc4)c5ccccc5)C(C)C)Cc6ccccc6	160	nM
CHEMBL12844	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccccc3	160.93	nM
CHEMBL108429	COCCOC(=O)NC(C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OCCOC)C(C)C	164	nM
CHEMBL354379	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)C4=CCCSC4	167.4	nM
CHEMBL276653	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSc3ccc(cc3)C(F)(F)F)NS(=O)(=O)C	170	nM
CHEMBL277725	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCSC4	170.41	nM
CHEMBL124672	OC1=C(SCc2ccccc2)C(=O)CC(COc3ccccc3)(O1)c4ccccc4	172	nM
CHEMBL72784	CC(C)(C)NC(=O)[C@@H]1CN(CCCc2ccccc2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	175	nM
CHEMBL97544	CC(C)C[C@@H](NC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2)C(=O)N	176.07	nM
CHEMBL432252	CCOC(=O)NC(C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)C(NC(=O)OCC)C(C)C	177	nM
CHEMBL316959	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)N[C@H](CO)c3ccccc3)[C@H](NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	179.72	nM
CHEMBL325847	CC(C)[C@@H](NC(=O)OCCN1CCOCC1)C(=O)N[C@@H](Cc2ccccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)OCCN4CCOCC4)C(C)C	180	nM
CHEMBL123324	CC(C)CCCC1(CC(=O)C=C(O)O1)SCc2ccccc2)c3ccccc3	183	nM
CHEMBL163633	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N3CCOCC3)(CC2=O)c4ccccc4	186	nM
CHEMBL606565	CN([C@@H]1[C@H](O)Cc2ccccc12)C(=O)[C@@H](C[C@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C)Cc4ccccc4	186	nM
CHEMBL288759	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@](C)(O)C(C)(C)C	189.74	nM
CHEMBL15053	CC(C)(C)NC(=O)c1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	190	nM
CHEMBL154197	O[C@H](CN(Cc1ccccc1)S(=O)(=O)c2ccccc2)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	190	nM
CHEMBL141398	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3OC	190	nM

CHEMBL12671	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(cc3)[N+](=O)[O-]	191	nM
CHEMBL318595	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)N[C@H](CO)Cc3ccccc3)[C@H](NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	193.39	nM
CHEMBL162317	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)N3CCOCC3)(CC2=O)c4ccccc4	195	nM
CHEMBL62390	Cc1ccsc1SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4	195	nM
CHEMBL354169	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H]4CCS(=O)(=O)C4	196.47	nM
CHEMBL71514	CC(C)C(NC(=O)OCc1ccccc1)C(=O)N[C@H](CC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(NC(=O)OCc3ccccc3)C(C)C)Cc4ccccc4	200	nM
CHEMBL130998	O[C@@H]1[C@@H](O)[C@@H](COc2ccccc2)N(Cc3ccccc3)S(=O)(=O)N(Cc4ccccc4)[C@@H]1COc5ccccc5	200	nM
CHEMBL356345	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)CCO	200	nM
CHEMBL121005	OC(C(COCc1ccccc1F)OCc2ccc(F)cc2)C(O)C(COCc3ccccc3F)OCc4ccc(F)cc4	200	nM
CHEMBL292423	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2cccc(O)c2)NC(=O)OC(C)(C)C	200	nM
CHEMBL142990	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(CO)CO	200	nM
CHEMBL170517	O[C@@H]1[C@@H](O)[C@@H](CCc2ccccc2)N(Cc3ccccc3)S(=O)(=O)N(Cc4ccccc4)[C@@H]1CCc5ccccc5	200	nM
CHEMBL125097	CCCCCC1(CC(=O)C(=C(O)O1)SCc2ccccc2)c3ccccc3	201.37	nM
CHEMBL12485	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(cc3)C#N	205	nM
CHEMBL405657	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	205.75	nM
CHEMBL267553	Cc1ccccc1COC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	210	nM
CHEMBL3349988	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)OCc3ccccc3	210	nM
CHEMBL155051	CCCS(=O)(=O)N(CCC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2	210	nM
CHEMBL71913	CC(C)[C@H](NC(=O)[C@H](Cc1ccc(O)cc1)NC(=O)[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)[C@H](Cc3ccc(O)cc3)NC(=O)C)C(C)C)C(=O)N	212	nM
CHEMBL351243	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N(C)CCc3ccccc3)(CC2=O)c4ccccc4	216	nM
CHEMBL141265	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)c3ccccc3	219.09	nM
CHEMBL11008	CC(=O)N[C@@H](CSc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	220	nM
CHEMBL273775	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@]3(O)CCN(C3)[C@@H](Cc4ccccc4)C(=O)N[C@@H]5[C@H](O)Cc6ccccc56	220	nM
CHEMBL353679	OC1=C(C(SC2CCCC2)C3CCCC3)C(=O)C=C(O1)c4ccccc4	225	nM
CHEMBL12707	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccccc3Cl	225	nM
CHEMBL143415	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCCO	230	nM
CHEMBL2111769	CCC[C@@]1(CCc2ccccc2)CC(=O)C(=C(O)O1)[C@@H](CC)c3cccc(NS(=O)(=O)c4ccc(cn4)C#N)c3	232.16	nM
CHEMBL423618	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)N3CCNCC3)(CC2=O)c4ccccc4	234	nM
CHEMBL90645	CC(C)[C@@H]1[C@@H](CCS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CCN(C[C@H]3C(=O)NC(C)(C)C)C4CCSCC4	238	nM
CHEMBL14889	OC1=C(SCc2ccccc2C(=O)OC3CCCC3)C(=O)C=C(O1)c4ccccc4	244.95	nM

CHEMBL99317	CC(C)CN(C[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)c2ccc3ccccc3n2)C(=O)NC(C)(C)C	244.95	nM
CHEMBL48917	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](O)C(C)(C)C	244.95	nM
CHEMBL42366	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1CCCCC1C(=O)NC(C)(C)C)Cc2ccccc2)C(=O)NCc3ccccn3	250	nM
CHEMBL93389	CC(C)(C)OC(=O)N[C@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)c2cc(N)cc(N)c2)Cc3ccccc3	250	nM
CHEMBL14437	Cc1cc(cc(C)c1O)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	250	nM
CHEMBL319188	CCCCC(CO)NC(=O)[C@@H]1N[C@H](SC1(C)C)[C@H](NC(=O)Cc2ccccc2)C(=O)NCc3ccccc3	250	nM
CHEMBL71646	CC(C)[C@@H]1NC(=O)[C@H](Cc2ccc(OCCCNC1=O)cc2)NC(=O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)OC(C)(C)C	251	nM
CHEMBL174527	CC(C)(C)NC(=O)c1ccccc1OC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3cnnc4ccccc34	254.95	nM
CHEMBL76460	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)C(=O)c4ccccn4	257	nM
CHEMBL295472	OP1(=O)C(Cc2ccccc2)N(Cc3ccc4ccccc4c3)C(=O)N(Cc5ccc6ccccc6c5)C1Cc7ccccc7	260	nM
CHEMBL13205	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)OCc4ccncc4	260	nM
CHEMBL317077	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)C(=O)NC(C)C	260	nM
CHEMBL14751	Cc1cc(C)cc(c1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	260	nM
CHEMBL171551	CC(C)CC(SCc1ccccc1)C2=C(O)C=C(OC2=O)c3ccccc3	260	nM
CHEMBL125948	OC1=C(SCc2ccccc2)C(=O)CC(O1)(c3ccccc3)c4ccccc4	262	nM
CHEMBL12229	CCc1cccc(c1)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	262	nM
CHEMBL342585	CC(C)(C)NC(=O)[C@@H]1CCCN1C(=O)[C@H](O)[C@@H]2Cc3ccc(OCCCOc4cc5ccccc5cc4C(=O)N[C@@H](CC(=O)N)C(=O)N2)cc3	268.7	nM
CHEMBL126166	OC(=O)CCCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	270	nM
CHEMBL123561	CCCCC1(CC(=O)C(=C(O)O1)SCc2ccccc2)c3ccccc3	270	nM
CHEMBL2092978	CCC[C@]1(CCc2ccccc2)CC(=O)C(=C(O)O1)[C@@H](CC)c3cccc(NS(=O)(=O)c4cn(C)cn4)c3	274.59	nM
CHEMBL324788	CC1=C(CCC(=O)O)c2cc3[nH]c(cc4[nH]c(cc5nc(cc1n2)c(C)c5CCOC(=O)C6=CC6)C(=C4CCOC(=O)C7=CC7)c(C)c3CCC(=O)O	275	nM
CHEMBL292691	COCOc1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	276	nM
CHEMBL301401	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCCCc3oc4ccccc4n3)cc2)NC(=O)OC(C)(C)C	280	nM
CHEMBL174342	OC1=C(C(CC2CC2)SC3CCCC3)C(=O)C=C(O1)c4ccccc4	282.01	nM
CHEMBL163435	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N3CCSCC3)(CC2=O)c4ccccc4	285	nM
CHEMBL338010	CCCC1(CC(=O)C(=C(O)O1)SCc2ccccc2)c3ccccc3	290	nM
CHEMBL417238	OC1=C(Sc2cccs2)C(=O)CC(CCc3ccccc3)(O1)c4ccccc4	290	nM
CHEMBL59022	NS(=O)(=O)c1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	290	nM
CHEMBL12573	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccc(O)c(c3)C(=O)O	292	nM
CHEMBL308574	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccncc2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	293	nM
CHEMBL309507	CC(C)(C)OC(=O)NC(CC(=O)N)C(=O)N[C@@H](Cc1ccccc1)C(O)CN[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	295	nM
CHEMBL45838	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(O)C(F)(F)F	296.65	nM
CHEMBL107758	COC(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN(CC2CCCCC2)NC(=O)[C@@H](NC(=O)OC)C(C)C	298.4	nM

CHEMBL291802	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCc3ccccc3)cc2)NC(=O)OC(C)(C)C	300	nM
CHEMBL125720	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@H](O)CNC(=O)[C@@H]3N[C@H](SC3(C)C)C(NC(=O)Cc4ccccc4)C(=O)NCC5CCCCC5	300	nM
CHEMBL59816	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2O)NC(=O)OC(C)(C)C	300	nM
CHEMBL170802	CC(C)(C)CC(SC1CCCCC1)C2=C(O)C=C(OC2=O)c3ccccc3	300	nM
CHEMBL431043	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC(=O)NCCc3ncc[nH]3)[C@H](NC(=O)Cc4ccccc4)C(=O)NCc5ccccc5	300	nM
CHEMBL299475	CS(=O)(=O)c1ccccc1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	314	nM
CHEMBL49773	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](O)c3ccccc3	320	nM
CHEMBL413271	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccc(OCc3oc4ccccc4n3)cc2)NC(=O)OC(C)(C)C	320	nM
CHEMBL11142	CCCC(=O)N[C@@H](CC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)Cc3ccccc3C(=O)NC(C)(C)C	323	nM
CHEMBL98533	CCNC(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2	330	nM
CHEMBL120342	OC(C(COCc1c(F)cccc1F)OCc2ccc(F)cc2)C(O)C(COCc3c(F)cccc3F)OCc4ccc(F)cc4	330	nM
CHEMBL125597	NC(=O)CCCCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	338	nM
CHEMBL40760	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc1ccccc1)C(=O)N[C@@H]([C@@H](C)CC)C(=O)NCc2nc3ccccc3[nH]2)Cc4ccccc4)C(=O)NCc5nc6ccccc6[nH]5	346.41	nM
CHEMBL326288	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	347	nM
CHEMBL327277	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCCOC4	347.47	nM
CHEMBL3138267	CC(C)CCCC(C)[C@H]1CC[C@H]2[C@@H]3CCC4CC(=C(c5cc(Cl)c(O)c(c5)C(=O)O)c6cc(Cl)c(O)c(c6)C(=O)O)CC[C@]4(C)[C@H]3CC[C@]12C	350	nM
CHEMBL156839	OC(C[C@@H](Cc1ccccc1)C(=O)N[C@H]2CCCC[C@@H]2NC(=O)c3ccncc3)C[C@@H](Cc4ccccc4)C(=O)N[C@H]5CCCC[C@@H]5NC(=O)c6ccncc6	350	nM
CHEMBL94335	CC(C)[C@@H](NC(=O)Cc1ccccc1)C(=O)NN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)Cc3ccccc3)C(C)C)Cc4ccccc4	360	nM
CHEMBL429193	C[C@@H]1C[C@@H](CS1(=O)=O)OC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3C[C@H]4CCCC[C@H]4C[C@H]3C(=O)NC(C)(C)C	362.22	nM
CHEMBL62158	OC1=C(Sc2cc3ccccc3s2)C(=O)CC(CCc4ccccc4)(O1)c5ccccc5	363	nM
CHEMBL141281	OC(=O)c1cc(cc(Cl)c1O)C(=CCC23CC4CC(CC(C4)C2)C3)c5cc(Cl)c(O)c(c5)C(=O)O	370	nM
CHEMBL308771	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)C(=O)c4cccnc4	371	nM
CHEMBL303444	CC(C)(C)OC(=O)N[C@H](CC[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2	380	nM
CHEMBL154600	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)c3ccccc3Cl	380	nM
CHEMBL338554	Cc1ccccc1SC2=C(O)OC(CC2=O)(c3ccccc3)c4ccccc4	388	nM
CHEMBL176742	CC(C)(C)NC(=O)c1ccccc1SC[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3ccc4ccccc4c3	390	nM
CHEMBL3138268	CC(CCC=C(c1cc(Cl)c(O)c(c1)C(=O)O)c2cc(Cl)c(O)c(c2)C(=O)O)[C@H]3CC[C@H]4[C@@H]5CC[C@@H]6CC(F)(F)CC[C@]6(C)[C@H]5CC[C@]34C	390	nM
CHEMBL320268	CCNC(=O)[C@@H](NC(=O)c1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3N[C@H](SC3(C)C)[C@H](NC(=O)c4ccccc4)C(	390	nM

=O)NCC)C(C)(C)S2

CHEMBL170981	CC(C)CCC(Sc1ccccc1)C2=C(O)C=C(OC2=O)c3ccccc3	390	nM
CHEMBL319872	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@@H](O)CC(=O)N)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	394.72	nM
CHEMBL153845	OC(C[C@@H](Cc1ccccc1)C(=O)N[C@H]2CCCC[C@@H]2NC(=O)c3ccccn3)C[C@@H](Cc4ccccc4)C(=O)N[C@H]5CCCC[C@@H]5NC(=O)c6ccccn6	400	nM
CHEMBL12413	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3)OCc4ccncc4	400	nM
CHEMBL299054	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccncc2)NC(=O)OC(C)(C)C	400	nM
CHEMBL20303	CCCC[C@H](CC1(C[C@@H](CCCC)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc2ccccc2)C(=O)OC)CO1)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc3ccccc3)C(=O)OC	400	nM
CHEMBL300492	CC(C)(C)NC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	400	nM
CHEMBL122565	CCCCC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3	400	nM
CHEMBL170421	CC(C)CC(Sc1ccccc1)C2=C(O)C=C(OC2=O)c3ccccc3	410	nM
CHEMBL369369	CC(C)(C)NC(=O)c1ccccc1OC[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)c3cc(O)c4ccccc4n3	410	nM
CHEMBL371457	CC(C)C[C@@H](C[C@@H](O)[C@H](Cc1cccc(Br)c1)NC(=O)COc2c(C)cccc2C)S(=O)(=O)c3ccc(F)cc3	412.31	nM
CHEMBL73723	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)C(=O)c4ccccc4	414	nM
CHEMBL265333	Cc1cccc(C)c1COC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	420	nM
CHEMBL115376	CC[C@H](C)[C@H](NC(=O)[C@@H]1CCCN1CC(O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NC(=O)[C@H](CC(C)C)NC(=O)[C@H](CO)NC(=O)C)C(=O)OC	420	nM
CHEMBL344953	COCC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	420	nM
CHEMBL368994	CC(C)(C)NC(=O)c1ccccc1OC[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CC(=O)N)NS(=O)(=O)c3ccc4ccccc4c3	425	nM
CHEMBL159387	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)Nc3ccccc3)(CC2=O)c4ccccc4	429	nM
CHEMBL317881	CC(C)CNC(=O)C[C@H](O)[C@@H](Cc1ccccc1)NC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	439.55	nM
CHEMBL122292	CC(C)CC1(CC(=O)C(=C(O)O1)SCc2ccccc2)c3ccccc3	440	nM
CHEMBL46020	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(C)(C)O	450	nM
CHEMBL302486	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)[C@@H]2Cc3ccc(OCCOc4cc5ccccc5cc4C(=O)N[C@@H](CC(=O)N)C(=O)N2)cc3	450	nM
CHEMBL287984	CC[C@H](C)[C@@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc1ccccc1)C(=O)N[C@@H]([C@@H](C)CC)C(=O)NCc2ccccn2)Cc3ccccc3)C(=O)NCc4ccccn4	450	nM
CHEMBL331645	CC(C)(C)NC(=O)[C@@H]1CSCN1CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	450	nM
CHEMBL428686	CC(C)CCNC(=O)[C@@H](C[C@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2	470	nM
CHEMBL355133	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)[C@H]4CCSC4	471.49	nM
CHEMBL306598	CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@H](O)[C@H](Cc2ccccc2)NC(=O)O[C@H]3CCOC3)C(=O)OCc4ccccc4	476.24	nM
CHEMBL73662	CC(C)(C)NC(=O)[C@@H]1CN(CCc2ccccc2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	478	nM
CHEMBL366779	OC1=C(C(SC2CCCCC2)c3ccccc3)C(=O)C=C(O1)c4ccccc4	480	nM
CHEMBL171802	OC1=C(C(SCc2ccccc2)c3ccccc3)C(=O)C=C(O1)c4ccccc4	480	nM

CHEMBL75270	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccc(O)c2)CCN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	482	nM
CHEMBL277060	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccc4OCOc4c3	490	nM
CHEMBL94271	CC(C)[C@@H](NC(=O)Cc1cccnc1)C(=O)NN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)Cc3cccnc3)C(C)C)Cc4ccccc4	500	nM
CHEMBL48891	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)C(CCc2ccccc2)NC(=O)OC(C)(C)C	500	nM
CHEMBL163563	Cc1cc(cc(c1)C(=O)N2CCc3ccccc3C2)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)Cc5ccccc5C(=O)NC(C)(C)C	500	nM
CHEMBL291354	CC(C)(C)n1c(SC2=C(O)OC(CCc3ccccc3)(CC2=O)c4ccccc4)nc5ccccc15	505	nM
CHEMBL333568	OC1=C(SCCc2ccccc2)C(=O)CC(CC3CCCC3)(O1)c4ccccc4	510	nM
CHEMBL99934	CCCNC(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2	518	nM
CHEMBL313250	COc1ccccc1CCCCC2=C(O)Oc3cc(O)ccc3C2=O	520	nM
CHEMBL382924	CNc1ccc(cc1)S(=O)(=O)[C@@H](CC(C)C)C[C@@H](O)[C@H](Cc2cccc(Br)c2)NC(=O)COc3c(C)cccc3C	530	nM
CHEMBL436266	CC1(C)S[C@@H](N[C@H]1C(=O)NCCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccc6	530	nM
CHEMBL318844	CC1(C)S[C@@H](N[C@H]1C(=O)NCCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)[C@H](NC(=O)Cc5ccccc5)C(=O)NCc6ccccc6	540	nM
CHEMBL319126	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NCC(=O)N	550	nM
CHEMBL422197	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N3CCNCC3)(CC2=O)c4ccccc4	564	nM
CHEMBL163539	CC(C)c1ccccc1SC2=C(O)OC(CCCCC(=O)N3CCSCC3)(CC2=O)c4ccccc4	583	nM
CHEMBL3351009	CC(C)[C@H](N)C(=O)N[C@@H](Cc1ccccc1)C(O)[C@H](Cc2ccccc2)NC(=O)[C@@H](N)C(C)C	590	nM
CHEMBL278499	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccccc(c3)C(F)(F)F	600	nM
CHEMBL345630	OC(C[C@@H](Cc1ccccc1)C(=O)N[C@H]2CCCC[C@@H]2NC(=O)c3cccnc3)C[C@@H](Cc4ccccc4)C(=O)N[C@H]5CCCC[C@@H]5NC(=O)c6cccnc6	600	nM
CHEMBL95316	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](CO)C(=O)N	606	nM
CHEMBL15217	CC(C)COC(=O)c1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	619	nM
CHEMBL354917	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N(C)c3ccccc3)(CC2=O)c4ccccc4	624	nM
CHEMBL274046	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3cc(cc(c3)C(F)(F)F)C(F)(F)F	630	nM
CHEMBL124123	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CN1CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)OCc5ccccc5	650	nM
CHEMBL163616	Cc1ccc(cc1C(=O)N2CCc3ccccc3C2)C(=O)N[C@@H](Cc4ccccc4)[C@H](O)Cc5ccccc5C(=O)NC(C)(C)C	670	nM
CHEMBL91025	OC1=C(CCCOc2cccc(c2)C#N)C(=O)Oc3ccccc13	670	nM
CHEMBL159290	CC(C)c1ccccc1SC2=C(O)OC(CCCC(=O)N(C)Cc3ccccc3)(CC2=O)c4ccccc4	676	nM
CHEMBL420379	CC(C)(C)NC(=O)[C@@H]1CN(Cc2cccnc2)CCN1C[C@@H](O)[C@@H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	676	nM
CHEMBL370663	O[C@H](C[C@H](CCc1ccc(Cl)cc1Cl)S(=O)(=O)c2ccc(F)cc2)[C@@H](Cc3cccc(Br)c3)NC(=O)[C@H]4CCCO4	689.93	nM
CHEMBL14692	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccc(O)cc3	690	nM
CHEMBL14759	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3cccc(Cl)c3	690	nM
CHEMBL354897	NC(=O)OC[C@@H]1CCCOC1	694	nM

CHEMBL51366	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)SC(C)(C)C	700	nM
CHEMBL408667	CC1=C(C(COC(=O)C2=CCC2)OC(=O)C3=CCC3)c4cc5[nH]c(cc6[nH]c(cc7nc(cc1n4)c(C)c7CCC(=O)O)c(CCC(=O)O)c6C)C(=C5C)C(COC(=O)C8=CCC8)OC(=O)C9=CCC9	700	nM
CHEMBL333259	CCNC(=O)C(NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCC(O)CN(C)[C@@H](CC3CCCCC3)C(=O)NC(C)(C)C)C(C)(C)S2	710	nM
CHEMBL14298	COc1ccc(cc1C)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	740	nM
CHEMBL94316	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)N[C@@H](Cc3ncc[nH]3)C(=O)N	770	nM
CHEMBL49305	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C(O)(CO)C(C)(C)C	774.6	nM
CHEMBL326831	CC1=C(C(COC(=O)C2=CC2)OC(=O)C3=CC3)c4cc5[nH]c(cc6[nH]c(cc7nc(cc1n4)c(C)c7CCC(=O)O)c(CCC(=O)O)c6C)C(=C5C)C(COC(=O)C8=CC8)OC(=O)C9=CC9	774.6	nM
CHEMBL173361	OC1=C(C(Sc2ccccc2)c3ccccc3)C(=O)C=C(O1)c4ccccc4	780	nM
CHEMBL421475	OC1=C(SCCc2ccccc2)C(=O)CC(O1)(c3ccccc3)c4ccncc4	790	nM
CHEMBL383583	CC(C)C[C@@H](C[C@@H](O)[C@H](Cc1cccc(Br)c1)NC(=O)COc2c(C)cccc2C)S(=O)(=O)c3ccc(cc3)N(C)C	790	nM
CHEMBL14578	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccc4OCCOc4c3	790	nM
CHEMBL334149	Cc1ccccc1COC(COCc2ccccc2F)C(O)C(O)C(COCc3ccccc3F)OCc4ccccc4C	800	nM
CHEMBL48302	CC(C)(C)OC(=O)NC(CC1CCCCC1)[C@H](O)CNC[C@@H](O)C(CC2CCCCC2)NC(=O)OC(C)(C)C	800	nM
CHEMBL447834	CCNC(=O)[C@@H](NC(=O)Cc1ccc2ccccc2c1)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)Cc5cc6ccccc6c5)C(=O)NCC)C(C)(C)S3	820	nM
CHEMBL316755	CN(Cc1ccccc1)C(=O)[C@@H](NC(=O)Cc2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)Cc5ccccc5)C(=O)N(C)Cc6ccccc6)C(C)(C)S3	820	nM
CHEMBL325546	CC1(C)S[C@@H](N[C@H]1C(=O)NCCNC(=O)[C@@H]2N[C@H](SC2(C)C)[C@H](NC(=O)Cc3ccccc3)C(=O)N(CCO)CCO)[C@H](NC(=O)Cc4ccccc4)C(=O)N(CCO)CCO	840	nM
CHEMBL173704	CC(C)CC(SCC1CCCCC1)C2=C(O)C=C(OC2=O)c3ccccc3	848	nM
CHEMBL41063	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc1ccccc1)C(=O)N[C@@H]([C@@H](C)CC)C(=O)NCCN2CCOCC2)Cc3ccccc3)C(=O)NCCN4CCOCC4	850	nM
CHEMBL14792	Cc1cccc(c1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	860	nM
CHEMBL318387	CC(C)[C@H](NC(=O)c1sc(C)nc1C)C(=O)N[C@@H](Cc2ccccc2)[C@@H](O)[C@H](O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NC(=O)c4sc(C)nc4C)C(C)C	860	nM
CHEMBL290872	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)Cc3ccccc3)C(=O)OC	870	nM
CHEMBL46067	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)C3(O)COCC3(C)C	877.5	nM
CHEMBL139346	COc1ccc(cc1)S(=O)(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)c3ccccc3O	900	nM
CHEMBL304369	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)[C@@H]2Cc3ccc(OCCCCOc4cc5ccccc5cc4C(=O)N[C@@H](CC(=O)N)C(=O)N2)cc3	900	nM
CHEMBL48175	CC(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@@H](Cc2ccccc2)NC(=O)OC(C)C	900	nM
CHEMBL11424	CC(C)(C)NC(=O)c1ccccc1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@H](CSc3ccccn3)NS(=O)(=O)C	910	nM
CHEMBL99015	CCCCNC(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2	940	nM
CHEMBL275161	COP(=O)(CNC(=O)[C@@H](NC(=O)[C@H](Cc1cccc2ccccc12)CS(=	950	nM

	O)(=O)C(C)(C)C)C(C)C)CNC(=O)[C@@H](NC(=O)[C@H](Cc3cccc4 cccc34)CS(=O)(=O)C(C)(C)C)C(C)C		
CHEMBL73804	CC(C)(C)NC(=O)[C@@H]1CN(Cc2ccccn2)CCN1C[C@@H](O)[C@ H](Cc3ccccc3)NC(=O)O[C@H]4CCOC4	957	nM
CHEMBL14828	COc1cccc(c1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	990	nM
CHEMBL14934	COC(=O)c1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	1000	nM
CHEMBL122233	CCNC(=O)C(NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCC(O) CN[C@@H](CC3CCCCC3)C(=O)NC(C)(C)C)C(C)(C)S2	1000	nM
CHEMBL17704	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@ H](O)[C@H](Cc3ccccc3)NC(=O)OCCS(=O)(=O)C	1030	nM
CHEMBL432178	OCc1ccc(CN2C(Cc3ccccc3)P(=O)(O)C(Cc4ccccc4)N(Cc5ccc(CO)cc5) C2=O)cc1	1073.31	nM
CHEMBL421410	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](Cc2ccccc2)[C@H](O)CC (=O)NCCO)[C@H](NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	1100	nM
CHEMBL309402	NC(CC(=O)N)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN[C@@H](C c2ccccc2)C(=O)NC3[C@H](O)Cc4ccccc34	1100	nM
CHEMBL12705	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@@H](O)[C@H](C c2ccccc2)NC(=O)COc3ccccc3)OCc4ccncc4	1100	nM
CHEMBL348226	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)CCCO	1100	nM
CHEMBL439833	CC(C)c1ccccc1SC2=C(O)OC(CCC(=O)N3CCSCC3)(CC2=O)c4ccccc4	1103	nM
CHEMBL161954	CC(C)c1ccccc1SC2=C(O)OC(CCC(=O)N3CCNCC3)(CC2=O)c4ccccc4	1106	nM
CHEMBL52153	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@@H](Cc2ccccc2)NC(=O)OC(C)(C)C	1118.03	nM
CHEMBL15182	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3cccc(O)c3	1190	nM
CHEMBL339998	OC(=O)CCC1(CC(=O)C=C(O)O1)SCCc2ccccc2)c3ccccc3	1200	nM
CHEMBL121976	CC(C)CC1(CC(=O)C=C(O)O1)SCCc2ccccc2)c3ccccc3	1200	nM
CHEMBL37465	CC[C@H](C)[C@H](NC(=O)[C@@H](CC(O)C[C@@H](Cc1ccccc1) C(=O)N[C@@H]([C@@H](C)CC)C(=O)NCC2CCc3ccccc3N2)Cc4ccc cc4)C(=O)NCC5CCc6ccccc6N5	1200	nM
CHEMBL58998	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@@H]2[C@H](O)Cc3cc ccc23)Cc4ccccc4	1200	nM
CHEMBL340206	OCCCCC1(CC(=O)C=C(O)O1)SCc2ccccc2)c3ccccc3	1260	nM
CHEMBL353796	CC(C)c1ccccc1SC2=C(O)OC(CCC(=O)N3CCN(CC3)C(=O)OC(C)(C) C)(CC2=O)c4ccccc4	1270	nM
CHEMBL325673	CC(C)[C@@H](NS(=O)(=O)N(C)Cc1ccccn1)C(=O)N[C@@H](Cc2cc ccc2)C(O)[C@H](Cc3ccccc3)NC(=O)[C@@H](NS(=O)(=O)N(C)Cc4c cccn4)C(C)C	1300	nM
CHEMBL122797	OC1=C(SCCc2ccccc2)C(=O)CC3(CCCc4ccccc34)O1	1300	nM
CHEMBL121837	NC(=O)CCCC1(CC(=O)C=C(O)O1)SCCc2ccccc2)c3ccccc3	1300	nM
CHEMBL104471	CC(CCC=C(C)C)C1=C(O)C(CCc2ccccc2)(OC1=O)C(=O)NC(C)(C)C	1300	nM
CHEMBL48993	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)[C@](C)(O)c3ccccc3	1300	nM
CHEMBL331664	OC(C(COCc1ccc(F)cc1)OCc2ccccc2)C(O)C(COCc3ccc(F)cc3)OCc4cc ccc4	1322.88	nM
CHEMBL12484	CC(C)c1ccccc1SC2=C(O)C=C(OC2=O)c3ccccc3C	1345	nM
CHEMBL99211	CC(C)CN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)C(=O)NC(C)(C)C	1374.77	nM
CHEMBL328732	CCOC(=O)c1cccc(OCCCC2=C(O)Oc3ccccc3C2=O)c1	1400	nM
CHEMBL327912	OC1=C(CCCOc2cccc(Cl)c2)C(=O)Oc3ccccc13	1400	nM
CHEMBL274291	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@@H](O)[C@H](C c2ccccc2)NC(=O)CCc3ccccc3)OCc4ccncc4	1400	nM
CHEMBL435401	CC(C)CCC1(CC(=O)C=C(O)O1)Sc2ccccc2)c3ccccc3	1400	nM
CHEMBL12797	COc1ccccc1C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	1418	nM
CHEMBL119968	OC(C(COCc1ccccc1)OCc2c(F)cccc2F)C(O)C(COCc3ccccc3)OCc4c(F)	1453.27	nM

	cccc4F		
CHEMBL306640	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)C2(O)CCN(CC2)[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1460	nM
CHEMBL121287	OC(C(COCc1ccccc1F)OCc2ccccc2)C(O)C(COCc3ccccc3F)OCc4ccccc4	1489.97	nM
CHEMBL69781	CC(C)C(NC(=O)OCc1ccccc1)C(=O)N[C@H](CC(C[C@H](Cc2ccccc2)NC(=O)C(NC(=O)OCc3ccccc3)C(C)C)[N+](=O)[O-])Cc4ccccc4	1500	nM
CHEMBL99527	CNC(=O)N(CC(C)C)C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2	1500	nM
CHEMBL3138187	CC(C)CCCC(C)[C@H]1CC[C@H]2[C@@H]3CCC4C[C@H](CCC=C(c5cc(Cl)c(O)c(c5)C(=O)O)c6cc(Cl)c(O)c(c6)C(=O)O)CC[C@]4(C)[C@H]3CC[C@]12C	1500	nM
CHEMBL346860	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)CNC=O	1500	nM
CHEMBL3137943	CC(CCC=C(c1cc(Cl)c(O)c(c1)C(=O)O)c2cc(Cl)c(O)c(c2)C(=O)O)[C@H]3CC[C@H]4[C@@H]5CC[C@@H]6CCCC[C@]6(C)[C@H]5CC[C@]34C	1500	nM
CHEMBL122261	CC(C)(C)NC(=O)[C@@H]1C[C@H](CN1CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4)OC(C)(C)C	1600	nM
CHEMBL330840	OC(C(COCc1ccc(F)cc1)OCc2ccc(F)cc2)C(O)C(COCc3ccc(F)cc3)OCc4ccc(F)cc4	1600	nM
CHEMBL291732	O[C@@H](C[C@@H](Cc1ccccc1)C(=O)N[C@H]2[C@H](O)Cc3ccccc23)Cc4ccccc4O	1600	nM
CHEMBL274011	COc1ccc(cc1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	1630	nM
CHEMBL120214	OC(C(COCc1ccccc1)OCc2cccc(F)c2)C(O)C(COCc3ccccc3)OCc4cccc(F)c4	1643.17	nM
CHEMBL14930	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccccc3	1700	nM
CHEMBL89444	COc1ccccc1CCCCC2=C(O)Oc3ccccc3C2=O	1700	nM
CHEMBL68528	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@]2(O)CCN(C2)[C@@H](Cc3ccccc3)C(=O)N[C@@H]4[C@H](O)Cc5ccccc45	1897.37	nM
CHEMBL18086	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@@H](O)[C@H](Cc3ccccc3)NC(=O)O[C@H]4CCCS(=O)(=O)C4	1899.65	nM
CHEMBL48996	CCCC[C@@H](CN[C@@H](CCCC)C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CCCNC(=N)N)C(=O)N)NC(=O)[C@@H](NC(=O)[C@@H](NC(=O)C)[C@@H](C)O)[C@@H](C)CC	1900	nM
CHEMBL280520	OC(=O)c1ccc(CSC2=C(O)C=C(OC2=O)c3ccccc3)cc1	1917.19	nM
CHEMBL12622	CCOC(=O)c1cccc(c1)C2=CC(=C(Sc3ccccc3C(C)C)C(=O)O2)O	1934	nM
CHEMBL38501	CCCC[C@H](CC(O)(CO)C[C@@H](CCCC)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)OC)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc2ccccc2)C(=O)OC	2000	nM
CHEMBL324640	CC(C1=C(O)C(CCc2ccccc2)(OC1=O)C(=O)NC(C)(C)C)c3ccccc3	2000	nM
CHEMBL327985	CC(C)[C@@H](NC(=O)N1CCOCC1)C(=O)NN(C[C@H](O)[C@H](Cc2ccccc2)NC(=O)[C@@H](NC(=O)N3CCOCC3)C(C)C)Cc4ccccc4	2000	nM
CHEMBL15246	CCc1cccc(c1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	2040	nM
CHEMBL332603	OC1=C(SCCc2ccccc2)C(=O)CC(O1)c3ccccc3	2100	nM
CHEMBL441952	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3cccc(OC(F)(F)F)c3	2140	nM
CHEMBL122464	CC(C)(C)NC(=O)[C@@H]1CCCN1CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	2156.39	nM
CHEMBL123370	CN(CC1(CC(=O)C(=C(O)O1)SCCc2ccccc2)c3ccccc3)c4ccccc4	2280	nM
CHEMBL88443	OC1=C(CCCOc2ccccc2)C(=O)Oc3ccccc13	2300	nM
CHEMBL314852	OCc1cccc(OCCCC2=C(O)Oc3ccccc3C2=O)c1	2300	nM
CHEMBL334126	OC1=C(SCc2ccccc2)C(=O)CC3(CCCc4ccccc34)O1	2300	nM
CHEMBL12906	Cc1cccc(C)c1CCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	2400	nM

CHEMBL118872	O[C@H]([C@@H](COCc1ccccc1)OCc2ccccc2)[C@H](O)[C@@H](COCc3ccccc3)OCc4ccccc4	2400	nM
CHEMBL69604	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN[C@@H](Cc2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	2418.68	nM
CHEMBL414635	CC(C)c1ccccc1SC2=C(O)OC(CCC(=O)N3CCOCC3)(CC2=O)c4ccccc4	2440	nM
CHEMBL173655	OC1=C(C(Sc2ccccc2)C3CCCCC3)C(=O)C=C(O1)c4ccccc4	2440	nM
CHEMBL172909	OC1=C(C(Sc2ccc3ccccc3c2)c4ccccc4)C(=O)C=C(O1)c5ccccc5	2450	nM
CHEMBL45627	C\C=C\C\C=C\CCC(=O)[C@H]1O[C@H]1C(=O)N	2500	nM
CHEMBL13075	Cc1ccccc1CCC(=O)N[C@@H](Cc2ccccc2)[C@H](O)CN3CC[C@H](C[C@H]3C(=O)NC(C)(C)C)OCc4ccncc4	2500	nM
CHEMBL14707	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccccc3Cl	2540	nM
CHEMBL3084791	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)CC3(C[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)OCc5ccccc5)C(C)C)CCC(=O)N3	2700	nM
CHEMBL422928	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)C[C@@H](Cc2ccccc2)C(=O)NCCc3ccccc3	2800	nM
CHEMBL2113708	CC(C)(C)OC(=O)N[C@H](CCNC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OC(C)(C)C)Cc2ccccc2	2900	nM
CHEMBL356524	OC1=C(C(C=C)c2ccccc2)C(=O)CC3(CCCC3)O1	3000	nM
CHEMBL439641	CC(=O)N[C@H]1CCCC[C@@H]1NC(=O)[C@@H](CC(O)C[C@@H](Cc2ccccc2)C(=O)N[C@H]3CCCC[C@@H]3NC(=O)C)Cc4ccccc4	3000	nM
CHEMBL141176	CCC(C1=C(O)OC2(CCCCCCC2)CC1=O)c3ccccc3	3000	nM
CHEMBL9409	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)C(O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	3000	nM
CHEMBL310487	OC1=C(Sc2ccccc2)C(=O)C=C(O1)c3ccccc3	3049.59	nM
CHEMBL121035	OC(C(COCc1ccc(cc1)C#N)OCc2ccc(cc2)C#N)C(O)C(COCc3ccc(cc3)C#N)OCc4ccc(cc4)C#N	3100	nM
CHEMBL154798	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)C	3200	nM
CHEMBL16796	OC(C(COCc1ccc(Cl)cc1)OCc2ccccc2)C(O)C(COCc3ccc(Cl)cc3)OCc4ccccc4	3224.9	nM
CHEMBL92492	COc1ccc2C(=C(CCCCc3ccccc3OC)C(=O)Oc2c1)O	3300	nM
CHEMBL332379	OC(C(COCc1ccc(F)cc1F)OCc2ccccc2)C(O)C(COCc3ccc(F)cc3F)OCc4ccccc4	3304.54	nM
CHEMBL121243	Cc1ccc(COCC(OCc2ccccc2)C(O)C(O)C(COCc3ccc(C)cc3)OCc4ccccc4)cc1	3331.67	nM
CHEMBL48147	O[C@H](CNC[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)[C@H](Cc3ccccc3)NC(=O)OCc4ccccc4	3400	nM
CHEMBL14342	OC1=C(SCc2ccc3OCCOc3c2)C(=O)C=C(O1)c4ccccc4	3420	nM
CHEMBL121327	OCc1ccc(COC(COCc2ccccc2)C(O)C(O)C(COCc3ccccc3)OCc4ccc(CO)cc4)cc1	3464.1	nM
CHEMBL120694	OC(C(COCc1ccccc1)OCc2ccc(Br)cc2)C(O)C(COCc3ccccc3)OCc4ccc(Br)cc4	3549.65	nM
CHEMBL314409	OP1(=O)C(Cc2ccccc2)N(Cc3ccc(CBr)cc3)C(=O)N(Cc4ccc(CBr)cc4)C1Cc5ccccc5	3549.65	nM
CHEMBL91773	NC(=O)c1cccc(OCCCC2=C(O)Oc3ccccc3C2=O)c1	3900	nM
CHEMBL298572	CC(C)(C)CC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C	4000	nM
CHEMBL69731	O[C@@H]1[C@@H](O)[C@@H](CCc2ccccc2)N(Cc3ccccc3)C(=O)N(Cc4ccccc4)[C@@H]1CCc5ccccc5	4000	nM
CHEMBL88511	OC1=C(CCCOc2cccc(c2)[N+](=O)[O-])C(=O)Oc3ccccc13	4000	nM
CHEMBL90188	OC1=C(CCOCc2ccccc2)C(=O)Oc3ccccc13	4000	nM
CHEMBL120747	COC(=O)c1ccc(COC(COCc2ccccc2)C(O)C(O)C(COCc3ccccc3)OCc4cc(cc4)C(=O)OC)cc1	4098.78	nM
CHEMBL12886	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@@H](O)[C@H](C	4200	nM

	c2ccccc2)NC(=O)CSc3ccccc3)OCc4ccncc4		
CHEMBL161243	COC(=O)[C@@H](\N=C(/S)\[C@@H](NC(=O)[C@H](Cc1ccccc1)NC(=O)[C@H](Cc2ccccc2)NC(=O)[C@H](C)NC(=O)[C@H](C)NC(=O)OC(C)(C)C)C(C)(C)C)C(C)C	4500	nM
CHEMBL46316	CC[C@@H](C)C(NC(=O)OC(C)(C)C)[C@H](O)CNC[C@@H](O)C(NC(=O)OC(C)(C)C)[C@@H](C)CC	4500	nM
CHEMBL382513	COc1cc(Br)c(cc1OC)C(=O)N[C@@H](Cc2cccc(Br)c2)[C@H](O)C[C@H](CCc3ccc(Cl)cc3Cl)S(=O)(=O)c4ccc(F)cc4	4500	nM
CHEMBL419560	CCNC(=O)[C@@H](NC(=O)c1ccccc1Nc2ccccc2)[C@@H]3N[C@@H](C(=O)NCCNC(=O)[C@@H]4N[C@H](SC4(C)C)[C@H](NC(=O)c5ccccc5Nc6ccccc6)C(=O)NCC)C(C)(C)S3	4800	nM
CHEMBL120466	OC(C(COCc1ccccc1)OCc2ccc(cc2)C#N)C(O)C(COCc3ccccc3)OCc4ccc(cc4)C#N	4818.71	nM
CHEMBL113559	CC(C)CN(C[C@@H](O)[C@@H](NC(=O)O[C@@H]1CCOC1)Sc2ccccc2)S(=O)(=O)c3ccc(N)cc3	4835.29	nM
CHEMBL2111673	C[C@H](C1=C(O)[C@](CCc2ccccc2)(OC1=O)C(=O)NCc3ccc(cc3)C(C)(C)C)c4ccccc4	4983.97	nM
CHEMBL124434	COC(=O)[C@@H](NC(=O)[C@H](OCc1ccccc1)[C@H](O)[C@@H](O)[C@@H](OCc2ccccc2)C(=O)N[C@@H](C(C)C)C(=O)OC)C(C)C	5000	nM
CHEMBL302877	O=C(N[C@@H](Cc1ccccc1)C(=O)N2CCC(=O)C2Sc3ccccc3)c4ccc5ccccc5n4	5000	nM
CHEMBL121923	CC(C)(C)NC(=O)[C@@H]1C[C@@H](O)CN1CC(O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	5100	nM
CHEMBL125639	CCCC1(CC(=O)C=C(O)O1)SCCc2ccccc2)c3ccccc3	5100	nM
CHEMBL278942	Cc1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	5370	nM
CHEMBL315189	OC1=C(CCCN(c2ccccc2)c3ccc(F)cc3)C(=O)Oc4ccccc14	5500	nM
CHEMBL607102	C[C@H](N(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)[C@H](CC(=O)N)NC(=O)OCc2ccccc2)C(=O)NC(C)(C)C)c3ccccc3	5757.6	nM
CHEMBL305289	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)[C@@H]2Cc3ccc(OCCCOc4cc5ccccc5cc4C(=O)N[C@@H](CC(=O)N)C(=O)N2)cc3	6000	nM
CHEMBL49341	CC(C)(C)COC(=O)N[C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCC(C)(C)C	6000	nM
CHEMBL120693	OC(C(COCc1ccc(cc1)C(F)(F)F)OCc2ccc(cc2)C(F)(F)F)C(O)C(COCc3ccc(cc3)C(F)(F)F)OCc4ccc(cc4)C(F)(F)F	6000	nM
CHEMBL14620	OC1=C(SCc2ccccc2)C(=O)C=C(O1)c3ccccc3O	6000	nM
CHEMBL14855	OC(=O)c1cccc(CSC2=C(O)C=C(OC2=O)c3ccccc3)c1	6150	nM
CHEMBL331741	C[C@H](N(CC(O)CNC(=O)[C@@H]1N[C@H](SC1(C)C)C(NC(=O)Cc2ccccc2)C(=O)NCc3ccccc3)CC4CCCC4)C(=O)NC(C)(C)C	6400	nM
CHEMBL92171	Nc1cccc(OCCCC2=C(O)Oc3ccccc3C2=O)c1	6400	nM
CHEMBL322644	CC(C)[C@H](NC(=O)C(O)(c1ccccc1)c2ccccc2)C(=O)N[C@@H](Cc3ccccc3)[C@@H](O)[C@H](O)[C@H](Cc4ccccc4)NC(=O)[C@@H](NC(=O)C(O)(c5ccccc5)c6ccccc6)C(C)C	6400	nM
CHEMBL273621	CC(C)(C)NC(=O)[C@@H]1CCCCN1C[C@@H](O)CNC(=O)[C@@H]2N[C@H](SC2(C)C)C(NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	6500	nM
CHEMBL3349992	CC(C)(C)OC(=O)[C@@H]1CCCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OCc3ccccc3	6500	nM
CHEMBL261987	Cc1ccc(COCC(OCc2ccc(C)cc2)C(O)C(O)C(COCc3ccc(C)cc3)OCc4ccc(C)cc4)cc1	7000	nM
CHEMBL442513	CN(C)c1ccc(cc1)C(=O)OCC(OC(=O)c2ccc(cc2)N(C)C)C3=C(C)c4cc5[nH]c(cc6[nH]c(cc7nc(cc3n4)c(C)c7C(COC(=O)c8ccc(cc8)N(C)C)OC(=O)c9ccc(cc9)N(C)C)c(c)c6CCC(=O)O)C(=C5C)CCC(=O)O	7000	nM
CHEMBL96857	CC(C)(C)NC(=O)c1cc(ccc1CCC(O)Cc2ccc(cc2C(=O)NC(C)(C)C)C(C)(C)C)C(C)(C)C	7000	nM
CHEMBL90889	OC(=O)c1cccc(OCCCC2=C(O)Oc3ccccc3C2=O)c1	7000	nM
CHEMBL120261	OC(C(COCc1ccccc1)OCc2ccc(cc2)C(F)(F)F)C(O)C(COCc3ccccc3)OCc4ccc(cc4)C(F)(F)F	7071.07	nM

CHEMBL14931	Cc1ccc(cc1)C2=CC(=C(SCc3ccccc3)C(=O)O2)O	7493.38	nM
CHEMBL107001	CC1(C)S[C@H](CNC(=O)Cc2ccccc2)N[C@H]1C(=O)NCCNC(=O)[C@@H]3N[C@@H](CNC(=O)Cc4ccccc4)SC3(C)C	7800	nM
CHEMBL352550	OC1=C(C(Sc2ccccc2)c3ccc4ccccc4c3)C(=O)C=C(O1)c5ccccc5	7820	nM
CHEMBL171235	COC(=O)c1ccc(CN2[C@H](COc3ccccc3)[C@H](O)[C@@H](O)[C@@H](COc4ccccc4)N(Cc5ccc(cc5)C(=O)OC)C2=O)cc1	8000	nM
CHEMBL67968	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)[C@H](O)CNC(=O)CCC(=O)NC(C)(C)C	8250	nM
CHEMBL299429	CN([C@@H](Cc1ccccc1)[C@H](O)CNC[C@@H](O)[C@H](Cc2ccccc2)NC(=O)OC(C)(C)C)C(=O)OC(C)(C)C	8500	nM
CHEMBL15001	Cc1cccc(CSC2=C(O)C=C(OC2=O)c3ccccc3)c1	8540	nM
CHEMBL2115206	CC(C)(C)OC(=O)N[C@@H](Cc1cccccc1)[C@H](O)CNC(C(O)c2ccccc2)C(=O)N[C@@H]3[C@H](O)Cc4ccccc34	8549.85	nM
CHEMBL326249	CCNC(=O)[C@@H](NC(=O)Cc1ccccc1)[C@@H]2N[C@@H](C(=O)NCCNC(=O)[C@@H]3NCSC3(C)C)C(C)(C)S2	8800	nM
CHEMBL124921	OC1=C(SCc2ccccc2)C(=O)CC(O1)c3ccccc3	8900	nM
CHEMBL290349	CC(C)CN1C[C@@](O)(C[C@H]1C(=O)NC(C)(C)C)[C@H](CC2CCCC2)NC(=O)CC(C)(C)C	9000	nM
CHEMBL21296	OC1[C@H](Cc2ccccc2)N(CC3CC3)C(=O)N(CC4CC4)[C@H]1Cc5ccccc5	9000	nM
CHEMBL369126	[O-][N+](=O)c1ccc2c(c1)C(=O)Oc3ccc(CBr)cc23	10000	nM
CHEMBL355782	O[C@@H]1[C@@H](O)[C@@H](CCCc2ccccc2)N(Cc3ccccc3)C(=O)N(Cc4ccccc4)[C@@H]1CCCc5ccccc5	10000	nM
CHEMBL419513	CC(C)(C)NC(=O)[C@@H]1CCCN1C[C@@H](O)CCc2ccccc2C(=O)NC(C)(C)C	10000	nM
CHEMBL62621	COc1ccc(C[C@H](NC(=O)OC(C)(C)C)C(=O)N2CCC(=O)[C@@H]2Sc3ccccc3)cc1	10000	nM
CHEMBL436088	O[C@H](C[C@H](CCc1ccc(Cl)cc1Cl)S(=O)(=O)c2ccc(F)cc2)[C@H](Cc3cccc(Br)c3)NC(=O)COc4ccc(Cl)cc4Cl	10000	nM
CHEMBL155260	CC(C)CCN(C[C@@H](O)[C@H](Cc1ccccc1)NC(=O)OCc2ccccc2)S(=O)(=O)Cc3ccccc3	10000	nM
CHEMBL12161	CC(C)(C)NC(=O)[C@@H]1C[C@@H](CCN1C[C@@H](O)[C@H](Cc2ccccc2)NC(=O)\C=C\c3ccccc3)OCc4ccncc4	11000	nM
CHEMBL121586	OC(C(COCc1ccccc1)OCc2ccc(cc2)C(=O)O)C(O)C(COCc3ccccc3)OCc4ccc(cc4)C(=O)O	11401.75	nM
CHEMBL125816	OC1=C(SCc2ccccc2)C(=O)CC3(CCc4ccccc34)O1	11800	nM
CHEMBL313331	OC1=C(CCCN(Cc2ccccc2)c3ccccc3)C(=O)Oc4ccccc14	13000	nM
CHEMBL70657	COC(=O)[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)[C@@H](Cc2c[nH]c3ccccc23)NC(=O)C)C(C)C	14000	nM
CHEMBL217693	CC1=C(C(COC(=O)c2ccccc2)OC(=O)c3ccccc3)c4cc5nc(cc6[nH]c(cc7[nH]c(cc1n4)C(=C7CCC(=O)O)C)c(CCC(=O)O)c6C)c(C(COC(=O)c8ccccc8)OC(=O)c9ccccc9)c5C	14000	nM
CHEMBL384612	CC1=C(C(COC(=O)c2ccc3ccccc3c2)OC(=O)c4ccc5ccccc5c4)c6cc7nc(cc8[nH]c(cc9[nH]c(cc1n6)C(=C9CCC(=O)O)C)c(CCC(=O)O)c8C)c(C(COC(=O)c%10ccc%11ccccc%11c%10)OC(=O)c%12ccc%13ccccc%13c%12)c7C	14000	nM
CHEMBL14698	Cc1ccccc1C2=CC(=C(SCc3ccccc3)C(=O)O2)O	14160	nM
CHEMBL142248	OC[C@@]12C3N(Cc4ccccc4)C5[C@]6(CO)C(N(Cc7ccccc7)C1[C@@]3(CO)[C@H]6c8ccccc8)[C@@]5(CO)[C@@H]2c9ccccc9	16100	nM
CHEMBL348791	COC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc1ccccc1)\N=C(/S)\[C@H](Cc2ccccc2)NC(=O)[C@H](C)NC(=O)[C@H](C)NC(=O)OC(C)(C)C)C(C)C)C(C)C	18000	nM
CHEMBL14373	COC(=O)c1cccc(CSC2=C(O)C=C(OC2=O)c3ccccc3)c1	19330	nM
CHEMBL331444	NC(=O)c1ccc(COC(COCc2ccccc2)C(O)C(O)C(COCc3ccccc3)OCc4ccc(cc4)C(=O)N)cc1	20000	nM
CHEMBL161488	OC1(CCN(CC#CC(=O)c2ccccc2)CC1)c3ccc(Cl)cc3	20000	nM

	CCC(C)[C@H](NC(=O)C[C@H](O)[C@H](CC(C)C)NC(=O)CC1C=C CN2N1C(=O)C(CNCc3ccccc3)CCC2=O)C(=O)N[C@@H](Cc4ccccc4)		
CHEMBL325180	C(=O)N	21000	nM
CHEMBL315009	OP1(=O)C(Cc2ccccc2)N(Cc3ccccc3)C(=O)N(Cc4ccccc4)C1Cc5ccccc5	21000	nM
CHEMBL89166	OC1=C(SCCOc2ccccc2)C(=O)Oc3ccccc13	24000	nM
CHEMBL14675	OC(=O)c1ccccc1CSC2=C(O)C=C(OC2=O)c3ccccc3	24760	nM
CHEMBL94703	CC(C)(C)NC(=O)c1ccccc1SCC(O)Cc2ccc3ccccc3c2C(=O)NC(C)(C)C	25000	nM
	CC1(C)S[C@@H](N[C@H]1C(=O)N[C@H](CO)CCc2ccccc2)[C@H](		
CHEMBL319004	NC(=O)Cc3ccccc3)C(=O)NCc4ccccc4	25495.1	nM
CHEMBL88778	OC1=C(CCCSc2ccccc2)C(=O)Oc3ccccc13	26000	nM
	CC(C)C[C@H](N1CCC(O)(CC1)[C@H](Cc2ccccc2)NC(=O)[C@@H](		
CHEMBL69243	NC(=O)OCc3ccccc3)C(C)C)C(=O)NC(C)(C)C	26700	nM
	NCc1ccc(COC(COCc2ccccc2)C(O)C(O)C(COCc3ccccc3)OCc4ccc(CN		
CHEMBL122655	)cc4)cc1	27000	nM
CHEMBL278187	NC1C(OCc2ccccc2)OC(COC(=O)Nc3ccccc3)C(OCc4ccccc4)C1N	28000	nM
	O[C@@H]1Cc2ccccc2[C@@H]1NC(=O)[C@H](Cc3ccccc3)N4CCC(		
CHEMBL69250	O)(CC4)[C@H](Cc5ccccc5)NC(=O)O[C@H]6CCOC6	29700	nM
CHEMBL160413	OC1(CC[N+]([O-])(C\C=C\C(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3	30000	nM
CHEMBL91457	OC1=C(CCCOC2CCCCC2)C(=O)Oc3ccccc13	32000	nM
	COC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc1ccccc1)NC(		
	=O)N[C@H](Cc2ccccc2)NC(=O)[C@H](C)NC(=O)[C@H](C)N)C(C)		
CHEMBL187239	C)C(C)C	32400	nM
	COc1ccc(cc1)[C@@H]2[C@@]3(CO)C4N(Cc5ccccc5)C6[C@@]7(CO		
CHEMBL142249	)C(N(Cc8ccccc8)C3[C@]4(CO)[C@H]7c9ccc(OC)cc9)[C@]26CO	33000	nM
	CC(C)(C)NC(=O)[C@H](CC1CCCCC1)N2CC[C@](O)(C2)[C@H](Cc		
CHEMBL304135	3ccccc3)NC(=O)OC(C)(C)C	37000	nM
	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)C(O)CNC(Cc2ccccc2)C(=O)		
CHEMBL431023	NC(CO)c3ccccc3	38000	nM
CHEMBL313167	OC1=C(CCCOCc2ccccc2)C(=O)Oc3ccccc13	38000	nM
	CC(C)[C@H](NC(=O)OCc1ccccc1)C(=O)N[C@@H](Cc2ccccc2)C3(O		
CHEMBL69362	)CCN(CCc4ccccc4)CC3	38700	nM
CHEMBL89631	COc1ccccc1OCCCC2=C(O)Oc3ccccc3C2=O	44000	nM
CHEMBL182831	Cc1ccc2OC(=O)c3cc(ccc3c2c1)[N+](=O)[O-]	50000	nM
CHEMBL182782	Nc1ccc2c(c1)C(=O)Oc3ccc(CBr)cc23	50000	nM
	CC(C)(C)OC(=O)N[C@@H](Cc1ccccc1)[C@@H](O)CN(Cc2ccccc2)		
CHEMBL330438	NC(=O)OC(C)(C)C	50000	nM
	COC(=O)[C@@H](NC(=O)[C@@H](NC(=O)[C@H](Cc1ccccc1)NC(		
	=O)[C@H](Cc2ccccc2)\N=C(/S)\[C@H](C)NC(=O)[C@H](C)NC(=O)		
CHEMBL434478	OC(C)(C)C)C(C)C)C(C)C	51000	nM
	CC(C)[C@@H](NC(=O)OC(C)(C)C)C(=O)NN(C[C@H](O)[C@H](Cc		
CHEMBL415698	1ccccc1)NC(=O)[C@@H](NC(=O)OC(C)(C)C)C(C)C)Cc2ccccc2	52000	nM
CHEMBL22057	OC1[C@H](Cc2ccccc2)N(CC=C)C(=O)N(CC=C)[C@H]1Cc3ccccc3	53000	nM
CHEMBL88855	OC1=C(CCOc2ccccc2)C(=O)Oc3ccccc13	53000	nM
CHEMBL113197	CCCCCC=C(c1cc(Cl)c(O)c(c1)C(=O)NO)c2cc(Cl)c(O)c(c2)C(=O)NO	58000	nM
CHEMBL159191	OC1(CCN(CC#CC(=O)c2cccc(c2)c3ccccc3)CC1)c4ccc(Cl)cc4	63000	nM
	N[C@@H](Cc1ccccc1)C(O)CN[C@@H](Cc2ccccc2)C(=O)NC3[C@H		
CHEMBL313367	](O)Cc4ccccc34	63000	nM
	CC(C)N1CCC(=C(C1)C(=O)NC(C)(C)C)CC(O)CCc2ccccc2C(=O)NC(		
CHEMBL328536	C)(C)C	70000	nM
	COC(=O)[C@H](O)[C@H](Cc1ccccc1)NC(=O)[C@@H](NC(=O)[C@		
CHEMBL419630	H](Cc2ccc(O)cc2)NC(=O)C)C(C)C	71000	nM
CHEMBL89376	O\N=C(\CCC1=C(O)Oc2ccccc2C1=O)/c3ccccc3	71000	nM
CHEMBL142907	CCC(C1=C(O)OC(CC(C)C)(CC(C)C)CC1=O)c2ccccc2	75000	nM
CHEMBL159101	OC1(CCN(C\C=C\C(=O)c2ccc(F)cc2)CC1)c3ccc(Cl)cc3	80000	nM

CHEMBL444869	OC1=C(CSc2ccccc2)C(=O)C=C(O1)c3ccccc3	84300	nM
CHEMBL88145	OCCCC1=C(O)Oc2ccccc2C1=O	86000	nM
CHEMBL21291	OC1[C@H](Cc2ccccc2)N(Cc3ccccc3)C(=O)N(Cc4ccccc4)[C@H]1Cc5ccccc5	89000	nM
CHEMBL91766	OC1=C(CCC(=O)c2ccccc2)C(=O)Oc3ccccc13	90000	nM
CHEMBL182348	Cc1ccc2OC(=O)c3cc(N)ccc3c2c1	100000	nM
CHEMBL329047	CC(C)(C)NC(=O)C1CCCCN1CC(O)CCc2ccccc2C(=O)NC(C)(C)C	100000	nM
CHEMBL161613	OC1(CCN(CC#CC(=O)c2ccc(cc2)c3ccccc3)CC1)c4ccc(Cl)cc4	100000	nM

8.2 Reverse training set

CHEMBL338099	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4ccnc4	0.6	nM
CHEMBL88677	Fc1cccc(F)c1CC\N=C(/S)\Nc2ccc(Br)cn2	1	nM
CHEMBL132756	COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1C#N	1	nM
CHEMBL135380	Clc1ccc(NC(=S)NCCN2C(=O)c3ccccc3C2=O)nc1	1	nM
CHEMBL253186	COc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1F	1	nM
CHEMBL37835	CCOc1ccc(Cl)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F	1.4	nM
CHEMBL37024	CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F	1.55	nM
CHEMBL37762	Fc1cccc(F)c1[C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3	2	nM
CHEMBL38341	COc1ccc(OC)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1F	2	nM
CHEMBL103706	Fc1cc(F)c(CC\N=C(/S)\Nc2ccc(Cl)cn2)c(F)c1	2	nM
CHEMBL436376	CCOc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1C#N	2	nM
CHEMBL341201	Clc1ccc(NC(=S)NCCN2C(=O)c3c(Cl)ccc(Cl)c3C2=O)nc1	2	nM
CHEMBL436177	CCOc1ccc(Cl)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1F	2	nM
CHEMBL162118	CCN1c2nc(Cl)cc(C)c2NC(=O)c3cc(CSc4ccncc4)cnc13	2.2	nM
CHEMBL133658	CCOc1ccc(Cl)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1F	2.7	nM
CHEMBL287317	COc1ccc(OC)c(CCNC(=O)Nc2ccc(Cl)cn2)c1F	3	nM
CHEMBL36930	Fc1cccc(F)c1CCNC(=O)Nc2ccc(Cl)cn2	3	nM
CHEMBL85110	CCC1=C(Sc2ccccc2)N(COCCOCc3ccccc3)C(=O)NC1=O	3	nM
CHEMBL328258	COc1ccccc1C(=O)CC\N=C(/S)\Nc2ccc(Br)cn2	3	nM
CHEMBL88840	Clc1ccc(NC(=S)NCCc2ccccc2)nc1	3	nM
CHEMBL91624	Fc1cccc(F)c1C(=O)CC\N=C(/S)\Nc2ccc(Br)cn2	3	nM
CHEMBL435600	COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(cn2)C#N)c1C#N	3	nM
CHEMBL133195	Brc1ccc(NC(=S)NCCn2nc3ccccc3n2)nc1	3	nM
CHEMBL334983	COc1ccc(F)c(F)c1CC\N=C(/S)\Nc2ccc(Br)cn2	3	nM
CHEMBL381134	Cc1ccc(c(Br)c1)n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]	3	nM
CHEMBL382553	Cc1c(Cl)cccc1n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]	3	nM
CHEMBL207839	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]	3	nM
CHEMBL207512	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3Cl)C(=O)N	3	nM
CHEMBL206522	NS(=O)(=O)c1ccc(NC(=O)CSc2nnnn2c3cc(Cl)ccc3Cl)c(Cl)c1	3	nM
CHEMBL398766	Cc1ccc(NC(=S)NCCc2c(F)cccc2F)nc1	3	nM
CHEMBL79339	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4c[nH]c5ncccc45	3.1	nM
CHEMBL133559	CC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Br)cn3)c1O	3.5	nM
CHEMBL36424	CCOc1ccc(F)c(CCNC(=O)Nc2ccc(Br)cn2)c1Cl	4	nM
CHEMBL91332	Fc1ccccc1C(=O)CC\N=C(/S)\Nc2ccc(Br)cn2	4	nM
CHEMBL134630	Fc1ccoc1CC\N=C(/S)\Nc2ccc(Cl)cn2	4	nM
CHEMBL379722	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3Cl)S(=O)(=O)N	4	nM
CHEMBL205152	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(Cl)cc3[N+](=O)[O-]	4	nM
CHEMBL206962	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3c(Cl)cccc3Cl	4	nM
CHEMBL207929	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3cc(Cl)ccc3Cl	4	nM

CHEMBL252964	CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F	4	nM
CHEMBL253169	COCc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F	4	nM
CHEMBL38318	CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(cn3)C#N)c1Cl	4.15	nM
CHEMBL421841	CCN1c2nccc(C)c2NC(=O)c3cc(CSc4cc(C)nc(C)c4)cnc13	4.2	nM
CHEMBL134026	CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Br)cn3)c1O	4.27	nM
CHEMBL399976	CCOc1cccc(F)c1CCNC(=S)Nc2ccc(C)cn2	4.5	nM
CHEMBL134278	CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(Cl)cn3)c1O	4.93	nM
CHEMBL135259	CCOc1ccc(F)c(CC\N=C(/S)\N[n+]2ccc(Cl)cn2)c1Cl	5	nM
CHEMBL135254	COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Cl)cn2)c1C#N	5	nM
CHEMBL377010	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccccc3Cl	5	nM
CHEMBL207900	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3cccc4ccccc34	5	nM
CHEMBL207920	CN(C)CCCNC(=O)c1ccc(NC(=O)CSc2nnnn2c3c(C)cc(C)cc3C)c(Cl)c1	5	nM
CHEMBL400547	CCc1csc(NC(=S)NCCc2c(F)cccc2F)n1	5	nM
CHEMBL429488	CCOc1ccc(F)c(CCNC(=S)Nc2ccc(cn2)C#N)c1Cl	5	nM
CHEMBL253822	COc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1	5	nM
CHEMBL402265	CCOc1ccc(F)c(F)c1CCNC(=S)Nc2ccc(Br)cn2	5	nM
CHEMBL399503	CCOc1ccc(OC)c(CCNC(=S)Nc2ccc(Cl)cn2)c1F	5	nM
CHEMBL131972	CCOc1ccc(Cl)c(C2CC2NC(=O)Nc3cc(Cl)cnn3)c1F	5.2	nM
CHEMBL135105	CC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1O	5.3	nM
CHEMBL129	CC1=CN([C@H]2C[C@H](N=[N+]=[N-])[C@@H](CO)O2)C(=O)NC1=O	6	nM
CHEMBL436546	CC(C)C1=C(Cc2ccccc2)N(COCc3ccccc3)C(=O)NC1=O	6	nM
CHEMBL88710	Fc1cccc(F)c1C(=O)CC\N=C(/S)\Nc2ccc(Cl)cn2	6	nM
CHEMBL351728	CCN1c2nc(Cl)cc(C)c2NC(=O)c3cc(CSc4nc(C)cc(C)n4)cnc13	6	nM
CHEMBL252137	Fc1cccc(Cl)c1CCNC(=S)Nc2nccs2	6	nM
CHEMBL254007	Fc1cccc(F)c1CCNC(=S)Nc2nc(cs2)C#N	6	nM
CHEMBL253369	CCOc1cccc(F)c1CCNC(=S)Nc2ccc(Br)cn2	6	nM
CHEMBL398890	COc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F	6	nM
CHEMBL253170	CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Cl)cn2)c1Cl	6	nM
CHEMBL132425	CCC(=O)c1ccc(F)c(C2CC2NC(=O)Nc3ccc(cn3)C#N)c1O	6.8	nM
CHEMBL162383	CCN1c2nc(F)cc(C)c2NC(=O)c3cc(CSc4cc(C)nc(C)c4)cnc13	6.9	nM
CHEMBL37834	CCOc1ccc(OC)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Br)cn3)c1F	7	nM
CHEMBL137111	COc1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1OC	7	nM
CHEMBL164261	CCN1c2nc(Cl)cc(C)c2NC(=O)c3cc(CSc4cc(C)nc(C)c4)cnc13	7	nM
CHEMBL381513	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccccc3Br	7	nM
CHEMBL443063	CN(C)c1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F	7	nM
CHEMBL100980	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CSc4ccncc4)cnc13	7.75	nM
CHEMBL37025	CCOc1ccc(F)c([C@H]2C[C@H]2NC(=O)Nc3ccc(Cl)cn3)c1Cl	8	nM
CHEMBL35729	CCOc1ccc(OC)c(CCNC(=O)Nc2ccc(Cl)cn2)c1F	8	nM
CHEMBL83412	CCc1cc(NCc2cc(C)c(C)cc2OC)c(O)nc1C	8	nM
CHEMBL88729	Brc1ccc(NC(=S)N[C@@H]2C[C@@H]2c3ccccc3)nc1	8	nM
CHEMBL135808	CN(C)c1ccc(CC\N=C(/S)\Nc2ccc(Br)cn2)c(F)c1C#N	8	nM
CHEMBL422371	CCN1c2ncc(CSc3oc4ccccc4n3)cc2C(=O)Nc5c(C)cc(Cl)nc15	8	nM
CHEMBL252963	CN(C)c1ccc(F)c(CCNC(=S)Nc2ccc(Cl)cn2)c1F	8	nM
CHEMBL253171	CCOc1ccc(F)c(CCNC(=S)Nc2ccc(I)cn2)c1Cl	8	nM
CHEMBL84621	CCc1cc(NCc2cc(C)c(C)nc2OC)c(O)nc1C	9	nM
CHEMBL319224	Fc1ccc(C#N)c(F)c1CC\N=C(/S)\Nc2ccc(Cl)cn2	9	nM
CHEMBL383088	NS(=O)(=O)c1ccc(NC(=O)CSc2nnnn2c3cccc(Cl)c3Cl)c(Cl)c1	9	nM
CHEMBL78882	Clc1ccc2NC(=O)NC(C#Cc3occc3)(C4CC4)c2c1	9.2	nM
CHEMBL88397	Clc1ccccc1C(=O)CCNC(=S)Nc2ccc(Br)cn2	10	nM

CHEMBL142837	CCN1c2ncccc2C(=O)Nc3c(C)cc(Cl)nc13	10	nM
CHEMBL144744	CCN1c2nc(cc(C)c2NC(=O)c3cccnc13)N(C)CCO	10	nM
CHEMBL366017	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc13	10	nM
CHEMBL381888	CC1CN(C2C[C@H](CO)C(C2)N=[N+]=[N-])C(=O)NC1=O	10	nM
CHEMBL205764	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3cc(F)ccc3Cl	10	nM
CHEMBL250438	COc1cccc(F)c1CCNC(=S)Nc2nccs2	10	nM
CHEMBL438146	CCOc1cccc(F)c1CCNC(=S)Nc2nccs2	10	nM
CHEMBL252136	Fc1cccc(F)c1CCNC(=S)Nc2nccs2	10	nM
CHEMBL81227	Clc1ccc2NC(=O)NC(C#Cc3ccccc3C#N)(C4CC4)c2c1	10.8	nM
CHEMBL79526	Clc1ccc2NC(=O)NC(C#Cc3nccs3)(C4CC4)c2c1	10.9	nM
CHEMBL162272	CCN1c2ncc(CSc3ccncc3C)cc2C(=O)Nc4c(C)cc(Cl)nc14	11	nM
CHEMBL171919	CCc1cc(SCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	11	nM
CHEMBL99235	CCc1cc(CCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	11.59	nM
CHEMBL106783	Oc1ncccc1C(OCc2ccccc2)(C#Cc3ccccc3)C(F)(F)F	11.69	nM
CHEMBL320282	Oc1ncccc1C(OCc2ccccc2)(C#CC3CC3)C(F)(F)F	11.82	nM
CHEMBL350538	Cc1cc(SCc2cnc3N(C4CC4)c5nc(Cl)cc(C)c5NC(=O)c3c2)cc(C)n1	12	nM
CHEMBL207105	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3cccc(Cl)c3Cl	12	nM
CHEMBL398891	CCOc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1Cl	12	nM
CHEMBL82764	[O-][N+](=O)c1ccccc1C#CC2(NC(=O)Nc3ccc(Cl)cc23)C4CC4	12.8	nM
CHEMBL368116	CCc1cc(CCc2oc3cccc(F)c3n2)c(S)nc1C	13	nM
CHEMBL377820	CN(C)CCCOc1ccc(NC(=O)CSc2nnnn2c3c(C)cc(C)cc3C)c(Cl)c1	13	nM
CHEMBL192231	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc5cc(ccc5c4)C(=O)O)cnc13	14	nM
CHEMBL336237	CCc1c(C)nc(O)c(N)c1Sc2cc(C)cc(C)c2	15	nM
CHEMBL176362	CCc1cc(CCc2oc3cccc(F)c3n2)c(O)nc1C	15	nM
CHEMBL175162	CCc1cc(CCc2oc3c(F)ccc(F)c3n2)c(S)nc1C	15	nM
CHEMBL191163	CCN1c2ncc(CCOc3ccc(cc3C)C(=O)O)cc2C(=O)N(C)c4ccc(OC)nc14	15	nM
CHEMBL189942	CCN1c2nc(F)ccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc13	15	nM
CHEMBL133772	CCOC(=O)NCCC=C(c1cc(C)c(OC)c(c1)C(=O)OC)c2cc(C)c(OC)c(c2)C(=O)OC	16	nM
CHEMBL336426	CCOc1ccc(F)c(C2CC2NC(=O)Nc3cc(Cl)cnn3)c1Cl	16	nM
CHEMBL320379	Oc1ncccc1C(OCc2ccccc2)(\C=C\C3CC3)C(F)(F)F	16.68	nM
CHEMBL192530	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc13	17	nM
CHEMBL80064	Clc1ccc2NC(=O)NC(C#Cc3ccccc3)(C4CC4)c2c1	17.7	nM
CHEMBL57995	Oc1ncc2c(F)c(F)ccc2n1	18	nM
CHEMBL342771	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccccn4	18	nM
CHEMBL192790	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(cc4Br)C(=O)O)cnc13	18	nM
CHEMBL382454	Cc1cccc(c1C)n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]	18	nM
CHEMBL55445	CCN1C(=O)c2cccnc2Oc3cc(C)cc(C#N)c13	19	nM
CHEMBL85947	CC(C)Sc1nc(O)c(C)c(n1)C(C)c2c(F)cccc2F	19	nM
CHEMBL86109	CCc1cc(CNc2cc(CC)c(C)nc2O)c(OC)nc1C	19	nM
CHEMBL189423	CCN1c2nc(C)ccc2N(C)C(=O)c3cc(CCOc4ccc(cc4C)C(=O)O)cnc13	19	nM
CHEMBL189928	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(cc4CC)C(=O)O)cnc13	19	nM
CHEMBL314012	CN1C(=O)Nc2ccc(Cl)cc2C1(C#Cc3ccccn3)C4CC4	19.6	nM
CHEMBL37803	CCc1cc(NCc2oc3c(C)ccc(C)c3n2)c(O)nc1C	20	nM
CHEMBL433489	CN1C(=O)c2cc(N)ccc2Oc3cc(C)cc(C)c13	20	nM
CHEMBL85946	CCC(C)Sc1nc(O)c(C)c(n1)C(C)c2c(F)cccc2F	20	nM
CHEMBL310803	CSc1nc(O)c(C)c(n1)C(C)c2c(F)cccc2F	20	nM
CHEMBL102113	CCN1c2ncc(CCc3ccnc(N)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	20	nM
CHEMBL101845	CCN1c2ncc(CCc3ccc4ccccc4c3)cc2C(=O)N(C)c5ccc(F)nc15	20	nM
CHEMBL102166	CCN1c2ncccc2N(C)C(=O)c3cc(COc4ccncc4)cnc13	20	nM

CHEMBL103386	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CSc4ccccc4)cnc13	20	nM
CHEMBL316796	S=C(NCCc1ccccc1)Nc2ccccn2	20	nM
CHEMBL99896	CN(C)c1cc(F)c(CC\N=C(/S)\Nc2ccc(Cl)cn2)c(F)c1	20	nM
CHEMBL338047	CCC1=C(C)NC(=O)C(=C1Cc2cc(C)cc(C)c2)N(C)C	20	nM
CHEMBL343007	Cc1cc(Cl)nc2N(C3CC3)c4ncccc4C(=O)Nc12	20	nM
CHEMBL145199	CCN1c2ncccc2C(=O)Nc3c(C)cc(F)nc13	20	nM
CHEMBL145237	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4cn[nH]c4	20	nM
CHEMBL144326	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)N4CCCC4	20	nM
CHEMBL342103	CCN1c2ncccc2C(=O)Nc3c(C)cc(C)nc13	20	nM
CHEMBL356744	CCN1c2nc(SC)cc(C)c2NC(=O)c3cccnc13	20	nM
CHEMBL212448	COC(=O)CCC\C=C(/c1cc(C)c2OC(=O)N(C)c2c1)\c3cc(C)c(OC)c(c3)C(=O)OC	20	nM
CHEMBL135509	Brc1ccc(NC(=S)NCCC2=NC3C=CC=CC3N2)nc1	21	nM
CHEMBL398837	CCOc1c(Cl)cc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1Cl	21	nM
CHEMBL83622	CCc1cc(CCc2oc3ccccc3n2)c(O)nc1C	21.45	nM
CHEMBL298607	COC(=O)c1cc(C)cc2Oc3ncccc3C(=O)N(C)c12	22	nM
CHEMBL364043	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(CCC(=O)O)cc4C)cnc13	22	nM
CHEMBL204993	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3Cl)[N+](=O)[O-]	22	nM
CHEMBL29274	FC(F)(F)[C@]1(NC(=O)Nc2ccc(Cl)cc12)\C=C\C3CC3	23	nM
CHEMBL56051	CN1C(=O)c2cccnc2Oc3cc(C)cc(c13)[N+](=O)[O-]	23	nM
CHEMBL87765	CCc1cc(NCc2cc(C)ccc2OC)c(O)nc1C	23	nM
CHEMBL317574	CNC(=O)c1ccc(F)c(CC\N=C(/S)\Nc2ccc(Br)cn2)c1F	23	nM
CHEMBL339203	Cc1nc(O)c(NCc2oc3c(Cl)ccc(Cl)c3n2)cc1C=C	23	nM
CHEMBL370699	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(CC(=O)O)cc4C)cnc13	23	nM
CHEMBL207527	Cc1ccc(Cl)cc1n2nnnc2SCC(=O)Nc3ccccc3[N+](=O)[O-]	23	nM
CHEMBL172861	CCc1cc(CCc2oc3ccccc3n2)c(S)nc1C	24	nM
CHEMBL106694	Oc1ncccc1C(Oc2cccc(Oc3ccccc3)c2)(C#CC4CC4)C(F)(F)F	24.34	nM
CHEMBL223228	FC(F)(F)[C@]1(OC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	24.49	nM
CHEMBL283950	NC(=O)c1[nH]c2ccc(Cl)cc2c1S(=O)(=O)c3ccccc3	25	nM
CHEMBL39665	CN(C)c1ccc(F)c(CCNC(=O)Nc2ccc(Br)cn2)c1F	25	nM
CHEMBL329720	CCc1cc(CCc2oc3c(C)ccc(C)c3n2)c(O)nc1C	25.38	nM
CHEMBL106997	Oc1ncccc1C(OCc2cccnc2)(C#CC3CC3)C(F)(F)F	25.56	nM
CHEMBL104349	Oc1ncccc1C(OCc2ccccn2)(C#CC3CC3)C(F)(F)F	26	nM
CHEMBL162629	CCN1c2nc(Cl)cc(C)c2NC(=O)c3cc(CSc4cncnc4)cnc13	26	nM
CHEMBL294171	CCN1C(=O)c2cc(N)cnc2Oc3cc(C)cc(C)c13	27	nM
CHEMBL162905	CCN1c2ncc(CSc3ccnc(C)c3)cc2C(=O)Nc4c(C)cc(Cl)nc14	27	nM
CHEMBL79338	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4c[nH]c5ccccc45	28	nM
CHEMBL440860	CCN1C(=O)c2cccnc2Oc3cc(C)cc(C)c13	29	nM
CHEMBL174130	CCc1cc(CCc2oc3c(Cl)cccc3n2)c(S)nc1C	29	nM
CHEMBL416107	CCc1c(C)nc(O)c(c1Sc2cc(C)cc(C)c2)[N+](=O)[O-]	30	nM
CHEMBL301222	CN1C(=O)c2cc(N)ccc2Oc3cc(C)ccc13	30	nM
CHEMBL100445	CCN1c2ncc(COc3ccnc(C)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	30	nM
CHEMBL319091	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccncc4)cnc13	30	nM
CHEMBL318002	CCN1c2ncc(COc3cc[n+]([O-])cc3)cc2C(=O)N(C)c4ccc(F)nc14	30	nM
CHEMBL100981	CCN1c2ncc(CSc3ncccn3)cc2C(=O)N(C)c4ccc(Cl)nc14	30	nM
CHEMBL103953	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccnc(C)c4)cnc13	30	nM
CHEMBL108396	COc1ccc(cc1)C(=O)CSC2=NC(=C(C(C)C)C(=O)N2)Cc3cccc4ccccc34	30	nM
CHEMBL144852	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)N4CC=CC4	30	nM
CHEMBL144522	CN1C(=O)c2cccnc2N(C3CC3)c4nc(Br)ccc14	30	nM
CHEMBL147749	S\C(=N/CCc1ccccc1N=[N+]=[N-])\Nc2nccs2	30	nM

CHEMBL172311	CCc1cc(CCc2oc3c(Cl)ccc(Cl)c3n2)c(S)nc1C	30	nM
CHEMBL174419	CCc1cc(CCc2oc3cccc(Cl)c3n2)c(S)nc1C	30	nM
CHEMBL366402	CC1=C(Cc2c(F)cccc2F)N=C(NC3CCCC3)NC1=O	30	nM
CHEMBL252135	COc1ccc(Br)cc1CCNC(=S)Nc2nccs2	30	nM
CHEMBL398765	Cc1ccc(NC(=S)NCCc2ccccc2)nc1	30	nM
CHEMBL291763	CCN1C(=O)c2cccnc2Oc3cc(C)cc(c13)[N+](=O)[O-]	31	nM
CHEMBL85059	Cc1cc(C)cc(c1)S(=O)(=O)c2c([nH]c3ccc(Cl)cc23)C(=O)N	31	nM
CHEMBL205999	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccccc3I	31	nM
CHEMBL81319	CCN1c2ccccc2C(=O)N(C)c3ccc(nc13)c4cc[nH]c4	31.46	nM
CHEMBL36995	CCOCN1C(=O)NC(=O)C(=C1Sc2ccccc2)CC	32	nM
CHEMBL82798	CCc1ccc(OC)c(CNc2cc(CC)c(C)nc2O)c1	32	nM
CHEMBL87676	CCc1cc(NCc2ccc(C)cc2OC)c(O)nc1C	32	nM
CHEMBL83635	CCc1cc(CNc2cc(CC)c(C)nc2O)c(OC)cc1C	33	nM
CHEMBL177016	CCc1cc(CCc2oc3cccc(C)c3n2)c(O)nc1C	33	nM
CHEMBL84933	CCc1cc(NCc2cc3ccccc3nc2OC)c(O)nc1C	34	nM
CHEMBL176957	CCCc1cc(CCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	34	nM
CHEMBL83888	CCc1cc(NCc2cc3CCCCc3nc2OC)c(O)nc1C	35	nM
CHEMBL368172	CC(C1=C(C)C(=O)NC(=N1)NC2CCCC2)c3c(F)cccc3F	35	nM
CHEMBL70629	CCN1c2ccc(C)c(C)c2N(C)C(=O)c3cccnc13	36	nM
CHEMBL105863	Oc1nc2ccccc2cc1C(OCc3ccccc3)(C#CC4CC4)C(F)(F)F	36.01	nM
CHEMBL84900	Cc1cc(C)cc(c1)C23SCCN2C(=O)c4ccccc34	36.66	nM
CHEMBL367052	CCc1cc(CCc2oc3c(F)cccc3n2)c(O)nc1C	37	nM
CHEMBL307220	CCN1c2cccc(C)c2NC(=O)c3cccnc13	38	nM
CHEMBL309674	CC(C1=CC(=O)NC(=N1)SC2CCCC2)c3c(F)cccc3F	38.73	nM
CHEMBL64233	CC(C)C#C[C@@]1(NC(=O)Nc2ccc(F)cc12)C(F)(F)F	39	nM
CHEMBL308907	CCN1c2ccccc2C=Cc3cccnc13	40	nM
CHEMBL439943	CCN1c2cc(C)c(C)cc2N(C)C(=O)c3cccnc13	40	nM
CHEMBL314883	CCc1cc(NCc2cc3CCCc3cc2OC)c(O)nc1C	40	nM
CHEMBL101946	CCN1c2ccccc2N(C)C(=O)c3cc(CCc4cccc(N)c4)cnc13	40	nM
CHEMBL99747	CCN1c2ncc(COc3ccnc(c3)C(F)(F)F)cc2C(=O)N(C)c4ccc(Cl)nc14	40	nM
CHEMBL328848	CCN1c2ccccc2N(C)C(=O)c3cc(CCc4nccs4)cnc13	40	nM
CHEMBL145397	CCN1c2nc(OC)ccc2N(C)C(=O)c3cccnc13	40	nM
CHEMBL144851	CCN1c2nc(cc(C)c2NC(=O)c3cccnc13)N4CCC(O)C4	40	nM
CHEMBL144145	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccc(N)cc4	40	nM
CHEMBL344289	CCN1c2ccccc2C(=O)N(C)c3ccc(nc13)c4cocc4	40	nM
CHEMBL177201	CC(C1=CC(=O)NC(=N1)NC2CCCC2)c3c(F)cccc3F	40	nM
CHEMBL176443	CCc1cc(CCc2oc3c(C)cccc3n2)c(O)nc1C	40	nM
CHEMBL254201	COc1ccccc1CCNC(=S)Nc2nccs2	40	nM
CHEMBL362936	CCN1c2ccccc2N(C)C(=O)c3cc(CCOc4ccc(C(=O)O)c5ccccc45)cnc13	40.25	nM
CHEMBL325343	CCc1cc(c(O)nc1C)C(OCc2c(Cl)cccc2Cl)(C#CC3CC3)C(F)(F)F	41.1	nM
CHEMBL280752	CC(Sc1nc(N)cc(Cl)n1)c2cc3ccoc3cn2	41.23	nM
CHEMBL125336	CCc1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(S)nc1C	42	nM
CHEMBL291987	CCN1C(=O)c2cc(N)ccc2Oc3cc(C)cc(C)c13	43	nM
CHEMBL338263	CSc1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	43	nM
CHEMBL172583	CCc1cc(CCc2oc3c(F)cccc3n2)c(S)nc1C	43	nM
CHEMBL313404	CCc1cc(NCc2nc3CCCCc3cc2OC)c(O)nc1C	43.36	nM
CHEMBL322004	Oc1ncccc1C(OCc2ccccc2)(\C=C\c3ccccc3)C(F)(F)F	43.89	nM
CHEMBL81441	CCN1c2ccccc2C(=O)N(C)c3ccc(nc13)c4c[nH]c5cnccc45	44	nM
CHEMBL56501	CC(C)N1C(=O)c2cc(N)cnc2Oc3cc(C)c(C)cc13	45	nM
CHEMBL440706	CCc1c(O)nc(SCC(=O)c2ccc(OC)cc2)nc1Cc3cccc4ccccc34	45	nM

CHEMBL400708	CC(=O)NCc1ccc(F)c(CCNC(=S)Nc2ccc(Br)cn2)c1F	45	nM
CHEMBL31977	CC1OC(\C=C\C2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	46	nM
CHEMBL56500	CN1C(=O)c2cc(N)cnc2Oc3cc(C)cc(C)c13	46	nM
CHEMBL431868	CC(C)c1c(O)nc(SCC(=O)c2ccccc2)nc1Cc3cccc4ccccc34	46	nM
CHEMBL89195	Fc1ccc(cc1)C(=O)CC\N=C(/S)\Nc2ccc(Br)cn2	47	nM
CHEMBL135760	CCOc1ccc(F)c(CC\N=C(/S)\Nc2nc(cs2)C(F)(F)F)c1Cl	47	nM
CHEMBL176594	CC(C)c1cc(CCc2oc3ccccc3n2)c(O)nc1C	48	nM
CHEMBL38679	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccccc3	50	nM
CHEMBL54900	CN1C(=O)c2cc(ccc2Oc3cc(C)cc(C)c13)C#N	50	nM
CHEMBL303089	Fc1ccc2NC(=O)N[C@@](C#CC3CC3)(c2c1)C(F)(F)F	50	nM
CHEMBL87393	CCC(C)Sc1nc(O)cc(Cc2c(F)cccc2F)n1	50	nM
CHEMBL87451	CC(C)SC1=NC(=CC(=O)N1)Cc2c(F)cccc2F	50	nM
CHEMBL87235	CCC(C)Sc1nc(O)c(C)c(Cc2c(F)cccc2F)n1	50	nM
CHEMBL83140	CC(C)SC1=NC(=C(C)C(=O)N1)Cc2c(F)cccc2F	50	nM
CHEMBL101412	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccccc4)cnc13	50	nM
CHEMBL330416	CCN1c2ncc(CCc3ccnc(c3)C(=O)N)cc2C(=O)N(C)c4ccc(Cl)nc14	50	nM
CHEMBL102192	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4ccccc4)cnc13	50	nM
CHEMBL100833	CCN1c2nc(F)ccc2N(C)C(=O)c3cc(CCc4ccncc4)cnc13	50	nM
CHEMBL100352	CCN1c2ncccc2N(C)C(=O)c3cc(CO)cnc13	50	nM
CHEMBL102034	CCN1c2nc(F)ccc2N(C)C(=O)c3cc(COc4ccncc4)cnc13	50	nM
CHEMBL101091	CCN1c2ncc(COc3cccc(N)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	50	nM
CHEMBL317180	CCN1c2ncc(CSc3[nH]cnc4nncc34)cc2C(=O)N(C)c5ccc(Cl)nc15	50	nM
CHEMBL341350	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)N4CCCC4	50	nM
CHEMBL142659	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccc(N)nc4	50	nM
CHEMBL444080	CCN1c2nc(OC)cc(CO)c2NC(=O)c3cccnc13	50	nM
CHEMBL422123	CN1C(=O)c2cccnc2N(C3CC3)c4nc(ccc14)c5cc[nH]c5	50	nM
CHEMBL196274	COC(=O)CCC\C=C(\c1cc(C)c2ON(C)C(=O)c2c1)/c3cc(Cl)ccc3OC	50	nM
CHEMBL400546	Cc1ccc(NC(=S)NCCc2ccccn2)nc1	50	nM
CHEMBL268871	CCc1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	51.96	nM
CHEMBL173575	CCc1cc(CCc2oc3c(C)ccc(C)c3n2)c(S)nc1C	52	nM
CHEMBL62104	CCC#C[C@@]1(NC(=O)Nc2ccc(F)cc12)C(F)(F)F	54	nM
CHEMBL68137	Oc1c(Cl)ccc2NC(=O)NC(C#CC3CC3)(c12)C(F)(F)F	54	nM
CHEMBL88966	Fc1ccccc1C(=O)CCNC(=O)Nc2ccc(Br)cn2	54	nM
CHEMBL208057	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3C)S(=O)(=O)N	54	nM
CHEMBL56052	CN1C(=O)c2cccnc2Oc3cc(C)cc(C#N)c13	55	nM
CHEMBL99992	CCc1cc(NCc2oc3c(C)cccc3n2)c(O)nc1C	55	nM
CHEMBL207746	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3C)C(=O)N	55	nM
CHEMBL56110	CN1C(=O)c2ccccc2Oc3cc(C)cc(C)c13	57	nM
CHEMBL123636	CCc1cc(NCc2oc3c(Cl)ccc(Cl)c3c2)c(O)nc1C	57	nM
CHEMBL125232	CCc1cc(N(C)Cc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	58	nM
CHEMBL176463	CCc1cc(CCC2=NC3CCCCC3O2)c(O)nc1C	58	nM
CHEMBL59458	Fc1ccc2NC(=O)N[C@@](C#CC3CC3)(c2c1Cl)C(F)(F)F	59	nM
CHEMBL292608	CCN1C(=O)c2cc(N)ccc2Oc3cccc(C)c13	60	nM
CHEMBL100136	CCN1c2ncc(CCc3ccnc(C)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	60	nM
CHEMBL100934	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4cccc(NC(=O)N)c4)cnc13	60	nM
CHEMBL322869	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccc(N)cc4)cnc13	60	nM
CHEMBL329728	CCN1c2ncc(CNc3cccc(N)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	60	nM
CHEMBL123959	CCN(CC)C(=O)\C=C\CSc1nc(N)cc(Cl)n1	60	nM
CHEMBL335202	Clc1ccc(NC(=S)NCCc2occc2C#N)nc1	60	nM
CHEMBL142853	CN1C(=O)c2cccnc2N(C3CC3)c4nc(ccc14)c5cn[nH]c5	60	nM

CHEMBL157741	CCC(C)Sc1nc(O)c(C)c(Cc2c(Cl)cccc2Cl)n1	60	nM
CHEMBL253994	Fc1ccccc1CCNC(=S)Nc2nccs2	60	nM
CHEMBL254414	CCOc1cccc(CCNC(=S)Nc2nccs2)c1	60	nM
CHEMBL336635	CCc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	61	nM
CHEMBL64722	Fc1cccc2NC(=O)N[C@@](C#CC3CC3)(c12)C(F)(F)F	62	nM
CHEMBL70719	CCN1c2cc(Cl)c(Cl)cc2N(C)C(=O)c3cccnc13	62	nM
CHEMBL176972	CCc1cc(CCc2oc3cccc(Cl)c3n2)c(O)nc1C	62	nM
CHEMBL300608	CN1C(=O)c2cc(O)ccc2Oc3cc(C)cc(C)c13	63	nM
CHEMBL372241	CCN1c2ccccc2N(C)C(=O)c3cc(CCOc4ccc5c(cccc5c4)C(=O)O)cnc13	63	nM
CHEMBL309462	Clc1ccc2NC(=O)NC(C#Cc3cccnc3)(C4CC4)c2c1	64.5	nM
CHEMBL82856	CCc1cc(CCc2cc(CC)c(C)nc2OC)c(O)nc1C	65	nM
CHEMBL339090	CCc1cc(NCc2oc3c(Cl)cccc3n2)c(O)nc1C	65	nM
CHEMBL60545	Fc1ccc2NC(=O)N[C@@](C#Cc3cccn3)(c2c1F)C(F)(F)F	68	nM
CHEMBL15411	Cc1cc(C)c2NC(=O)c3cccnc3N(C4CC4)c2n1	70	nM
CHEMBL66947	COc1c(Cl)ccc2NC(=O)NC(C#CC3CC3)(c12)C(F)(F)F	70	nM
CHEMBL85574	CCc1cc(NCc2nc(C)c(C)cc2OC)c(O)nc1C	70	nM
CHEMBL315290	CCc1cc(NCc2nc(CC)c(C)cc2OC)c(O)nc1C	70	nM
CHEMBL99624	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4ccncc4)cnc13	70	nM
CHEMBL103808	CCN1c2ncc(C[S+]([O-])c3ccccc3)cc2C(=O)N(C)c4ccc(Cl)nc14	70	nM
CHEMBL330180	CCN1c2ncc(CSc3[nH]cnc4ncnc34)cc2C(=O)N(C)c5ccc(Cl)nc15	70	nM
CHEMBL436200	CCc1cc(NCc2oc3c(F)ccc(F)c3n2)c(O)nc1C	70	nM
CHEMBL135804	Cn1cccc1CC\N=C(/S)\Nc2ccc(cn2)C#N	70	nM
CHEMBL145322	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)N(C)C	70	nM
CHEMBL144035	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccc(O)cc4	70	nM
CHEMBL343883	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4cccc(N)c4	70	nM
CHEMBL357221	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccc[nH]4	70	nM
CHEMBL156340	Cc1c(O)nc(SC2CCCCC2)nc1Cc3c(F)cccc3F	70	nM
CHEMBL173790	Fc1cccc(F)c1CC2=CC(=O)NC(=N2)NC3CCCC3	70	nM
CHEMBL236161	CC(C1=C(C)C(=O)NC(=N1)SC2CCCC2)c3c(F)cccc3F	70.71	nM
CHEMBL293332	CCN1C(=O)c2cc(N)cnc2Oc3cc(C)c(C)cc13	71	nM
CHEMBL299334	CSCCN1C(=O)c2ccccc2Oc3nc(Cl)ccc13	72	nM
CHEMBL293037	FC(F)(F)[C@]1(NC(=O)Nc2cccc(Cl)c12)C#CC3CC3	72	nM
CHEMBL84217	Cc1ccc(cc1)S(=O)(=O)c2c([nH]c3ccc(Cl)cc23)C(=O)N	72	nM
CHEMBL300087	CCOC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	72.87	nM
CHEMBL62039	Fc1ccc2NC(=O)N[C@@](C#CC3CC3)(c2c1F)C(F)(F)F	74	nM
CHEMBL292711	CCC#C[C@@]1(NC(=O)Nc2ccc(F)c(F)c12)C(F)(F)F	74	nM
CHEMBL105859	COC(=O)CCC\C=C(\c1ccc(OC)c(OC)c1)/c2cc(C)c(OC)c(c2)C(=O)OC	74	nM
CHEMBL64521	CC(C)C#C[C@@]1(NC(=O)Nc2ccc(F)c(Cl)c12)C(F)(F)F	78	nM
CHEMBL107180	CCc1c(O)nc(SCC(=O)c2ccc(F)cc2)nc1Cc3cccc4ccccc34	78	nM
CHEMBL324237	CC(C)c1c(O)nc(SCC(=O)c2ccc(F)cc2)nc1Cc3cccc4ccccc34	78	nM
CHEMBL417394	Fc1ccc2NC(=O)N[C@@](C#Cc3ccccn3)(c2c1Cl)C(F)(F)F	80	nM
CHEMBL82630	Clc1cccc2C(=O)N3CCSC3(c4ccccc4)c12	80	nM
CHEMBL309899	CC1=C(Cc2c(F)cccc2F)N=C(NC1=O)SC3CCCC3	80	nM
CHEMBL312874	Fc1cccc(F)c1CC2=CC(=O)NC(=N2)SC3CCCC3	80	nM
CHEMBL313998	COc1cccc(c1)C(=O)CC\N=C(/S)\Nc2ccc(Br)cn2	80	nM
CHEMBL318952	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4cccc(c4)N=[N+]=[N-])cnc13	80	nM
CHEMBL321544	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4ccncc4)cnc13	80	nM
CHEMBL103593	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccccc4N)cnc13	80	nM
CHEMBL421210	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccc5ccccc5c4)cnc13	80	nM

CHEMBL320663	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CNc4ccccc4)cnc13	80	nM
CHEMBL125446	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4cccc4	80	nM
CHEMBL445136	CCNc1ccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)cc1	80	nM
CHEMBL254207	Cc1ccccc1CCNC(=S)Nc2nccs2	80	nM
CHEMBL1203237	Cl.CSc1ccc2c(C)nc(CCCCCCC(=O)c3ccccc3)n2n1	80	nM
CHEMBL173589	CCCc1cc(CCc2oc3ccccc3n2)c(O)nc1C	83	nM
CHEMBL317992	Fc1ccc2NC(=O)OC(C#CC3CC3)(c2c1F)C(F)(F)F	84	nM
CHEMBL339067	Nc1cc(Cl)nc(SCc2cc3OCOc3cc2Cl)n1	85	nM
CHEMBL176631	CCc1cc(OCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	88	nM
CHEMBL292188	CCN1C(=S)c2cccnc2Oc3cc(C)cc(C)c13	90	nM
CHEMBL303446	FC(F)(F)C12NC(=O)Nc3ccc(Cl)c(OC(=C1)C4CC4)c23	90	nM
CHEMBL101501	CCN1c2ncccc2N(C)C(=O)c3cc(CCC(=O)OC)cnc13	90	nM
CHEMBL318982	CCN1c2nc(I)ccc2N(C)C(=O)c3cc(CCc4ccncc4)cnc13	90	nM
CHEMBL103946	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccc(c4)C(=O)O)cnc13	90	nM
CHEMBL122343	CN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4N C5CC5	90	nM
CHEMBL135179	Cn1cccc1CC\N=C(/S)\Nc2ccc(Cl)cn2	90	nM
CHEMBL422659	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)n4cccc4	90	nM
CHEMBL144820	CN1C(=O)c2cccnc2N(C3CC3)c4nc(Cl)ccc14	90	nM
CHEMBL358947	CCN1c2nc(CC)cc(C)c2NC(=O)c3cccnc13	90	nM
CHEMBL343625	CCN1c2ncccc2C(=O)Nc3c(C)cc(NCCCO)nc13	90	nM
CHEMBL341847	CCN1c2nc(NCCO)cc(C)c2NC(=O)c3cccnc13	90	nM
CHEMBL156255	Oc1cc(Cc2c(F)cccc2F)nc(SC3CCCCC3)n1	90	nM
CHEMBL156637	CC(C)CSc1nc(O)c(C)c(Cc2c(F)cccc2F)n1	90	nM
CHEMBL160869	CCCCSc1nc(O)c(C)c(Cc2c(F)cccc2F)n1	90	nM
CHEMBL191910	Ic1ccc(NC(=S)OCCN2C(=O)c3ccccc3C2=O)cc1	90	nM
CHEMBL400685	COc1cccc(OC)c1CCNC(=S)Nc2nccs2	90	nM
CHEMBL62179	CC(C)C#C[C@@]1(NC(=O)Nc2ccc(F)c(F)c12)C(F)(F)F	91	nM
CHEMBL312896	CCc1cc(CNc2cc(CC)c(C)nc2O)c(O)nc1C	91	nM
CHEMBL125299	CCc1cc(NCc2oc3c(F)cccc3n2)c(O)nc1C	92	nM
CHEMBL37842	CCN1c2nccc(Cl)c2NC(=O)c3cccnc13	95	nM
CHEMBL193125	CCN1c2ncccc2N(C)C(=O)c3cc(CCOc4ccc(cc4)C(=O)O)cnc13	95	nM
CHEMBL174364	Cc1cc(CCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	97	nM
CHEMBL336807	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4 CC	98	nM
CHEMBL57733	CCc1c(C)nc(O)c(N)c1Cc2cc(C)cc(C)c2	100	nM
CHEMBL99793	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccc(OC)c4)cnc13	100	nM
CHEMBL323072	CCN1c2ncc(CS(=O)(=O)c3ccccc3)cc2C(=O)N(C)c4ccc(Cl)nc14	100	nM
CHEMBL433172	CCN1c2ncc(COc3cc[n+]([O-])c(C)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	100	nM
CHEMBL318635	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccc(C)cc4)cnc13	100	nM
CHEMBL100903	CCN1c2ncc(COc3ccccc3O)cc2C(=O)N(C)c4ccc(Cl)nc14	100	nM
CHEMBL434441	Cc1cncn1c2ccc3c(C)nc(CCCCCCC(=O)c4ccccc4)n3n2	100	nM
CHEMBL125532	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4cncn4	100	nM
CHEMBL128931	CCc1c(C)nc(O)c(N)c1C(=O)c2cc(C)cc(C)c2	100	nM
CHEMBL140532	Cc1cc(C)cc(Sc2c(C)cnc(O)c2N)c1	100	nM
CHEMBL357183	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4nccs4	100	nM
CHEMBL146550	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ccsc4	100	nM
CHEMBL144653	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4cccc(O)c4	100	nM
CHEMBL359195	Nc1ccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)cc1	100	nM
CHEMBL154913	CCC(C)Sc1nc(O)cc(Cc2c(Cl)cccc2Cl)n1	100	nM
CHEMBL240416	COc1ccc(OC)c(CCNC(=S)Nc2ccc(Br)cn2)c1	100	nM

CHEMBL254628	Cc1csc(NC(=S)NCCc2ccccc2)n1	100	nM
CHEMBL98159	CCc1cc(CCc2oc3ccccc3c2)c(O)nc1C	100.05	nM
CHEMBL305345	Fc1c(Cl)ccc2NC(=O)N[C@@](C#CC3CC3)(c12)C(F)(F)F	102	nM
CHEMBL124430	CCc1cc(N(C)Cc2oc3c(C)ccc(C)c3n2)c(O)nc1C	103	nM
CHEMBL40562	COc1ccc(C(=O)C)c(F)c1CCNC(=O)Nc2ccc(Cl)cn2	104.4	nM
CHEMBL104658	CCCOC(C#CC1CC1)(c2cc(CC)c(C)nc2O)C(F)(F)F	105	nM
CHEMBL122293	CCc1cc(NCc2oc3c(Cl)ccc(F)c3n2)c(O)nc1C	105	nM
CHEMBL29171	FC(F)(F)C1(OCC(=O)Nc2ccc(Cl)cc12)\C=C\C3CC3	108	nM
CHEMBL49316	CC(C)OC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	108	nM
CHEMBL37343	CCN1c2ncccc2N(C)C(=O)c3cccnc13	108.17	nM
CHEMBL48628	COc1ccc2NC(=O)C(C#CC3CC3)(N(CC4CC4)c2c1)C(F)(F)F	109	nM
CHEMBL593	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	109.54	nM
CHEMBL288336	CCN1c2ncccc2C(=O)N(C)c3ccc(Cl)nc13	109.54	nM
CHEMBL39792	CCN1c2ncccc2C(=O)N(C)c3c(CC)ccnc13	110	nM
CHEMBL293894	CCC#C[C@@]1(NC(=O)Nc2ccc(Cl)cc12)C(F)(F)F	110	nM
CHEMBL102163	CCN1c2ncc(CCc3cccc(C)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	110	nM
CHEMBL319277	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4ccccc4)cnc13	110	nM
CHEMBL319032	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4cccc(C)c4)cnc13	110	nM
CHEMBL124786	CCc1cc(NCc2oc3cccc(F)c3n2)c(O)nc1C	110	nM
CHEMBL145273	CCN1c2nc(O)cc(COCc3ccccc3)c2NC(=O)c4cccnc14	110	nM
CHEMBL356998	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ocnc4	110	nM
CHEMBL144652	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4occc4	110	nM
CHEMBL144061	C=Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	110	nM
CHEMBL420519	Cc1nc(O)c(NCc2oc3c(Cl)ccc(Cl)c3n2)c4Cc14	113	nM
CHEMBL317130	CCN1c2ncccc2N(C)C(=O)c3cc(N)cnc13	114.02	nM
CHEMBL126634	COc1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	115	nM
CHEMBL330597	CCN1c2ncccc2N(C)C(=O)c3cc(CCCc4ccccc4)cnc13	120	nM
CHEMBL318720	CCN1c2ncccc2N(C)C(=O)c3cc(Cc4ccccc4)cnc13	120	nM
CHEMBL100056	CCN1c2ncc(CCc3cccc(N)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	120	nM
CHEMBL102960	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4cccc(F)c4)cnc13	120	nM
CHEMBL413252	CCN1c2ncc(COc3cc[n+]([O-])c(c3)C(F)(F)F)cc2C(=O)N(C)c4ccc(Cl)nc14	120	nM
CHEMBL144642	O=C1Nc2c(COc3ccccc3)ccnc2N(C4CC4)c5ncccc15	120	nM
CHEMBL143107	COc1ccc2N(C)C(=O)c3cccnc3N(C4CC4)c2n1	120	nM
CHEMBL297897	CCOC(=O)N1c2cc(F)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	121	nM
CHEMBL69005	FC(F)(F)C12NC(=O)Nc3ccc(Cl)c(OC(=C1)c4cccnc4)c23	122	nM
CHEMBL99018	CCc1cc(NCc2oc3cccc(C)c3n2)c(O)nc1C	122.47	nM
CHEMBL48376	COc1ccc2NC(=O)C(C#CC3CC3)(N(CC=C)c2c1)C(F)(F)F	123	nM
CHEMBL295606	Fc1ccc2NC(=O)C(C#CC3CC3)(N(CC=C)c2c1)C(F)(F)F	124	nM
CHEMBL64467	COc1ccc2NC(=O)N[C@@](C#CC3CC3)(c2c1)C(F)(F)F	124	nM
CHEMBL430601	Fc1ccc2NC(=O)N[C@@](C#Cc3ccccn3)(c2c1)C(F)(F)F	126	nM
CHEMBL299394	CCOC(=O)N1c2cc(Cl)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	127	nM
CHEMBL287650	CC1OC(\C=C\C2CC2)(c3cc(F)ccc3NC1=O)C(F)(F)F	129	nM
CHEMBL57113	FC(F)(F)[C@@]1(C#CC2CC2)[C@@H](OCc3ccncc3)C(=O)Nc4ccc(Cl)cc14	129	nM
CHEMBL302622	FC(F)(F)[C@]1(NC(=O)Nc2ccc(Cl)cc12)C#Cc3ccccn3	129	nM
CHEMBL107693	CCCCOC(C#CC1CC1)(c2cc(CC)c(C)nc2O)C(F)(F)F	129	nM
CHEMBL431936	CC(C)OC(=O)N1c2cc(F)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	130	nM
CHEMBL53451	CCCN1C(=O)c2cc(N)ccc2Oc3cc(C)ccc13	130	nM
CHEMBL293736	FC(F)(F)[C@]1(CC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	130	nM

CHEMBL312397	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4c[nH]c5ccncc45	130	nM
CHEMBL310306	Clc1ccc2NC(=O)NC(C#Cc3ncccn3)(C4CC4)c2c1	130	nM
CHEMBL101944	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4cccnc4)cnc13	130	nM
CHEMBL101979	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccc(c4)C(=O)N)cnc13	130	nM
CHEMBL99845	CCN1c2ncc(COc3cccc(O)c3)cc2C(=O)N(C)c4ccc(Cl)nc14	130	nM
CHEMBL126107	CCCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	130	nM
CHEMBL132770	CCCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4CC	130	nM
CHEMBL356779	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ncc[nH]4	130	nM
CHEMBL198276	COC(=O)c1cc(cc(C)c1OC)\C(=C/CCN2CCOC2=O)\c3cc(F)cc(c3)C(F)(F)F	130	nM
CHEMBL254413	[O-][N+](=O)c1ccccc1CCNC(=S)Nc2nccs2	130	nM
CHEMBL79403	C[C@@H]1Cn2c(S)nc3cccc(CN1CC=C(C)C)c23	130.77	nM
CHEMBL97653	COc1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	131	nM
CHEMBL299495	CCN1C(=O)c2cccnc2Oc3cc(C)cc(N)c13	132	nM
CHEMBL432763	Cc1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	133	nM
CHEMBL133779	Oc1ccc(F)c(C2CC2NC(=O)Nc3ccc(Cl)cn3)c1Cl	135	nM
CHEMBL58596	CC(C)C#CC1(NS(=O)(=O)Nc2ccc(Cl)cc12)C(C)C	137	nM
CHEMBL305996	COc1c(Cl)ccc2NC(=O)NC(C#Cc3cccnc3)(c12)C(F)(F)F	139	nM
CHEMBL87303	O=C1N2CCSC2(c3ccccc13)c4cccc5ccccc45	139.64	nM
CHEMBL317356	Brc1ccc(NC(=S)NCCc2ccccc2)nc1	139.64	nM
CHEMBL73015	CCCCN1c2ccccc2N(C)C(=O)c3cccnc13	140	nM
CHEMBL74690	CCN1c2cc(ccc2N(C)C(=O)c3cccnc13)N=[N+]=[N-]	140	nM
CHEMBL327938	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4cccc(NS(=O)(=O)C)c4)cnc13	140	nM
CHEMBL262633	CCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NC(=O)N5CCN(C)CC5)ccc4[nH]3	140	nM
CHEMBL331911	CCN(C1CCN(CC1)C(=O)c2cc3cc(NC(=O)N4CCN(C)CC4)ccc3[nH]2)c5ncccc5NC(C)C	140	nM
CHEMBL132491	COCc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	140	nM
CHEMBL134106	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4COC	140	nM
CHEMBL145193	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4cccs4	140	nM
CHEMBL358292	O=C1Nc2c(Cc3ccccc3)ccnc2N(C4CC4)c5nccc15	140	nM
CHEMBL344288	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)C#C	140	nM
CHEMBL2114369	C[C@@H]1O[C@@](C#CC2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	142.89	nM
CHEMBL304028	Fc1ccc2NC(=O)N[C@@](C#Cc3ccccc3)(c2c1)C(F)(F)F	143	nM
CHEMBL304938	COc1c(Cl)ccc2NC(=O)NC(C#Cc3ccccc3)(c12)C(F)(F)F	144	nM
CHEMBL293077	CCN1C(=O)c2cc(N)ccc2Oc3ccccc13	145	nM
CHEMBL299978	FC(F)(F)C1(C#CC2CC2)N(C(=O)OCC=C)c3ccccc3NC1=O	147	nM
CHEMBL101938	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4ccnc(c4)C(=O)OC)cnc13	150	nM
CHEMBL125715	CCCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4NCC	150	nM
CHEMBL124526	CCc1cc(NCc2oc3cccc(Cl)c3n2)c(O)nc1C	150	nM
CHEMBL135662	Cc1cc2nn(CC\N=C(/S)\Nc3ccc(Br)cn3)nc2cc1C	150	nM
CHEMBL435030	CCN1c2nc(cc(C)c2NC(=O)c3cccnc13)N4CCSCC4	150	nM
CHEMBL355918	CN1C(=O)c2cccnc2N(C3CC3)c4nc(ccc14)c5ccncc5	150	nM
CHEMBL145049	O=C1Nc2c(CNc3ccccc3)ccnc2N(C4CC4)c5nccc15	150	nM
CHEMBL144290	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4cccc(OC)c4	150	nM
CHEMBL253995	Fc1cccc(CCNC(=S)Nc2nccs2)c1	150	nM
CHEMBL400733	COc1cccc(CCNC(=S)Nc2nccs2)c1	150	nM

CHEMBL2114381	CCN1c2cc(C)c(C)nc2N(C)C(=O)c3cc(N)cnc13	150	nM
CHEMBL30752	CCC1OC(\C=C\C2CC2)(c3cc(F)ccc3NC1=O)C(F)(F)F	151	nM
CHEMBL42906	CCN1c2ncccc2c3ncc(C)n3c4ccc(OC)nc14	156	nM
CHEMBL297851	CC(C)OC(=O)N1c2cc(Cl)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	160	nM
CHEMBL295893	CC(C)C(I)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	160	nM
CHEMBL327744	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4ccnc(CO)c4)cnc13	160	nM
CHEMBL330602	CCN1c2ncc(CCc3ccc(N)cc3)cc2C(=O)N(C)c4ccc(Cl)nc14	160	nM
CHEMBL125203	CN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4N C5(C)CC5	160	nM
CHEMBL116350	Brc1ccc(NC(=S)NCCc2c[nH]c3ccccc23)nc1	164.32	nM
CHEMBL59140	CCCN1C(=O)c2cc(N)ccc2Oc3cc(C)c(C)cc13	165	nM
CHEMBL377310	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3C)[N+](=O)[O-]	165	nM
CHEMBL59917	FC(F)(F)[C@]1(NC(=O)Nc2ccc(Cl)c(Cl)c12)C#CC3CC3	166	nM
CHEMBL50664	CC(=C)OC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	169	nM
CHEMBL305965	CCN1c2ccc(Cl)cc2N(C)C(=O)c3cccnc13	170	nM
CHEMBL316922	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccc(c4)[N+](=O)[O-])cnc13	170	nM
CHEMBL103399	CCN1c2ncc(COc3ccccc3F)cc2C(=O)N(C)c4ccc(Cl)nc14	170	nM
CHEMBL331790	CC(C)Nc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccc(CO)cc4[nH]3	170	nM
CHEMBL132122	COc1ccc2N=C(S)C(CSC)N(C(=O)OC(C)C)c2c1	170	nM
CHEMBL426396	Cc1cc(CCc2oc3ccccc3n2)c(O)nc1C	170	nM
CHEMBL177256	CCc1cc(CCc2oc3cc(C)ccc3n2)c(O)nc1C	172	nM
CHEMBL57	Cc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	172.92	nM
CHEMBL281230	CC1OC(\C=C\C2CC2)(c3c(F)c(F)ccc3NC1=O)C(F)(F)F	173	nM
CHEMBL177191	CCc1cnc(O)c(CCc2oc3ccccc3n2)c1	177	nM
CHEMBL35033	CCOCN1C(=O)NC(=O)C(=C1Cc2ccccc2)C(C)C	178.89	nM
CHEMBL301370	CC[C@@H]1N(C(=O)OC(C)C)c2cc(F)ccc2NC1=O	179	nM
CHEMBL50550	FC(F)(F)C1(C#CC2CC2)N(CC3CC3)c4ccccc4NC1=O	179.25	nM
CHEMBL301022	CN1C(=O)c2cc(N)ccc2Oc3ccccc13	180	nM
CHEMBL539427	Brc1ccc(NC(=N)N[C@@H]2C[C@@H]2c3ccccc3)nc1	180	nM
CHEMBL110625	Cc1c(O)nc(SCC(=O)c2ccc(F)cc2)nc1Cc3cccc4ccccc34	180	nM
CHEMBL125437	CNC(=O)Nc1ccc2[nH]c(cc2c1)C(=O)N3CCC(CC3)N(C)c4ncccc4NC(C)C	180	nM
CHEMBL127564	CCc1cc(NCc2oc3cccc(OC)c3n2)c(O)nc1C	180	nM
CHEMBL145736	CN1C(=O)c2cccnc2N(C3CC3)c4nc(ccc14)c5cccnc5	180	nM
CHEMBL144773	CCN1c2nc(\C=C\C(=O)OC)ccc2N(C)C(=O)c3cccnc13	180	nM
CHEMBL254237	CCOc1ccc(OCC)c(CCNC(=S)Nc2ccc(Br)cn2)c1	180	nM
CHEMBL302861	Fc1ccc2NC(=O)N[C@@](C#Cc3ccccc3)(c2c1F)C(F)(F)F	181	nM
CHEMBL131518	CCOC(=O)CCCC=C(c1cc(C)c(OC)c(c1)C(=O)OC)c2cc(C)c(OC)c(c2) C(=O)OC	181	nM
CHEMBL49733	CC(=C)OC(=O)N1c2cc(F)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	183	nM
CHEMBL321174	CCOC(C#CC1CC1)(c2cc(CC)c(C)nc2O)C(F)(F)F	183	nM
CHEMBL284065	CCC1OC(\C=C\C2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	185	nM
CHEMBL105400	CCc1cc(c(O)nc1C)C(OCC2CC2)(C#CC3CC3)C(F)(F)F	188	nM
CHEMBL71311	CCN1c2ccc(C)cc2N(C)C(=O)c3cccnc13	190	nM
CHEMBL94725	Fc1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	190	nM
CHEMBL441072	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccnc4)cnc13	190	nM
CHEMBL102056	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccccn4)cnc13	190	nM
CHEMBL339279	CCCN(C1CCN(CC1)C(=O)c2cc3cc(NC(=O)N4CCN(C)CC4)ccc3[nH]2)c5ncccc5NC(C)C	190	nM
CHEMBL124594	CSc1cc(NCc2oc3ccccc3n2)c(O)nc1C	190	nM
CHEMBL340381	Nc1cc(Cl)nc(SC\C=C\c2ccccc2)n1	190	nM

CHEMBL147800	Oc1ccccc1Cc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23	190	nM
CHEMBL342068	CCN1c2nc(NC)ccc2N(C)C(=O)c3cccnc13	190	nM
CHEMBL2115336	CCN1c2cc(C)c(C)nc2N(C)C(=O)c3cccnc13	190	nM
CHEMBL174311	CCc1cc(OCc2oc3ccccc3n2)c(O)nc1C	191	nM
CHEMBL31771	CC1OC(C#CC2CC2)(c3c(F)c(F)ccc3NC1=O)C(F)(F)F	193	nM
CHEMBL35434	C[C@H]1C(Cl)n2c(S)nc3cccc(CN1CC=C(C)C)c23	200	nM
CHEMBL41694	Cc1ccccc1C(OCCn2c(C)ncc2[N+](=O)[O-])c3ccccc3	200	nM
CHEMBL70483	CC(C)N1c2ccccc2N(C)C(=O)c3cccnc13	200	nM
CHEMBL311356	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4c[nH]c5ccc(OC)cc45	200	nM
CHEMBL83401	CSc1nc(O)cc(n1)C(C)c2c(F)cccc2F	200	nM
CHEMBL319762	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4ccccc4C)cnc13	200	nM
CHEMBL333128	CN(C)C(=O)\C=C\CSc1nc(N)cc(Cl)n1	200	nM
CHEMBL338936	CCC1=C(C)NC(=O)C(=C1Cc2cc(C)cc(C)c2)NC=O	200	nM
CHEMBL135235	C[C@]1(Cl)CC2=C(CCC(=O)C2)[C@H]3CC[C@@]4(C)[C@@H](CC[C@@]4(O)C#C)[C@H]13	200	nM
CHEMBL358143	Cc1ccc(Cc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)c(O)c1	200	nM
CHEMBL148106	S=C(NCCc1ccccc1)Nc2nc(cs2)C#N	200	nM
CHEMBL145709	S=C(NCCc1ccccn1)Nc2nccs2	200	nM
CHEMBL147099	S=C(NCCc1ccccc1)Nc2nc3ccccc3s2	200	nM
CHEMBL345190	CCCCSc1nc(O)cc(Cc2c(F)cccc2F)n1	200	nM
CHEMBL347823	CC(C)CSc1nc(O)cc(Cc2c(F)cccc2F)n1	200	nM
CHEMBL157028	CSc1nc(O)c(C)c(Cc2c(F)cccc2F)n1	200	nM
CHEMBL381286	Cc1cc(C)c(c(C)c1)n2nnc2SCC(=O)Nc3cccc(c3)[N+](=O)[O-]	200	nM
CHEMBL254415	CCCOc1cccc(CCNC(=S)Nc2nccs2)c1	200	nM
CHEMBL401167	COc1ccc(OC)c(CCNC(=S)Nc2nccs2)c1	200	nM
CHEMBL254839	CC(C)c1csc(NC(=S)NCCc2ccccc2)n1	200	nM
CHEMBL398764	CCOC(=O)c1csc(NC(=S)NCCc2ccccc2)n1	200	nM
CHEMBL176637	CCc1cc(c(O)nc1C)S(=O)(=O)Cc2oc3c(Cl)ccc(Cl)c3n2	205	nM
CHEMBL294211	CCCN1C(=O)c2ccccc2Oc3nc(Cl)ccc13	210	nM
CHEMBL318646	CCN1c2ncccc2N(C)C(=O)c3cc(CCC#N)cnc13	210	nM
CHEMBL103437	CCN1c2ncccc2N(C)C(=O)c3cc(COc4cc[n+]([O-])cc4)cnc13	210	nM
CHEMBL101293	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(cnc13)N(C)C(=O)c4ccccc4	210	nM
CHEMBL99644	CCN1c2ncc(COc3ccc(O)cc3)cc2C(=O)N(C)c4ccc(Cl)nc14	210	nM
CHEMBL43308	Cc1ccnc2N(C3CC3)c4ncccc4c5nccn5c12	217	nM
CHEMBL291662	COc1ccc2NC(=O)N[C@@](C#Cc3ccccc3)(c2c1)C(F)(F)F	219	nM
CHEMBL84705	COC(=O)[C@H]1CSC2(N1C(=O)c3ccccc23)c4ccccc4	220	nM
CHEMBL125478	CCN(C1CCN(CC1)C(=O)c2cc3cc(NC(=O)N4CCN(C)CC4)ccc3[nH]2)c5ncccc5NC(C)(C)C	220	nM
CHEMBL342056	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4occn4	220	nM
CHEMBL132259	COc1c(CCNC(=O)Nc2ccc(Cl)cn2)c(F)ccc1C(=O)C	224	nM
CHEMBL37628	CCN1c2nccc(C)c2NC(=O)c3cccnc13	229.13	nM
CHEMBL308686	CCCN1c2ccccc2N(C)C(=O)c3cccnc13	230	nM
CHEMBL308248	CCN1c2cc(ccc2N(C)C(=O)c3cccnc13)C(F)(F)F	230	nM
CHEMBL101670	CCN1c2ncc(CCc3ccc(C)cc3)cc2C(=O)N(C)c4ccc(Cl)nc14	230	nM
CHEMBL319425	CCN1c2ncc(COc3cc[n+]([O-])cc3)cc2C(=O)N(C)c4ccc(Cl)nc14	230	nM
CHEMBL436392	CC(C)Nc1cccnc1N(C2CC2)C3CCN(CC3)C(=O)c4cc5cc(NS(=O)(=O)C)ccc5[nH]4	230	nM
CHEMBL121820	Cc1nc(CCCCCCC(O)c2ccccc2)n3nc(ccc13)n4ccnc4	230	nM
CHEMBL359187	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccccc4	230	nM
CHEMBL144378	CCNc1ccc2N(C)C(=O)c3cccnc3N(CC)c2n1	230	nM
CHEMBL204735	[O-][N+](=O)c1ccccc1NC(=O)CSc2nnnn2c3ccc(Cl)c(Cl)c3	230	nM

CHEMBL129835	CCOC(=O)CCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	233	nM
CHEMBL31285	FC(F)(F)CC1OC(C#CC2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	235	nM
CHEMBL316785	CCc1cc(NCc2oc3ccccc3c2)c(O)nc1C	235	nM
CHEMBL292790	COc1ccc2NC(=O)N[C@@](C#Cc3ccccn3)(c2c1)C(F)(F)F	237	nM
CHEMBL55391	CCN1C(=O)c2cc(N)ccc2Oc3ccc(C)cc13	240	nM
CHEMBL305521	CCN1c2cccc(C)c2N(C)C(=O)c3cccnc13	240	nM
CHEMBL70850	CCN1c2nc(C)c(C)cc2N(C)C(=O)c3cccnc13	240	nM
CHEMBL108360	CC(C)c1c(O)nc(SCC(=O)c2ccc(C)cc2)nc1Cc3cccc4ccccc34	240	nM
CHEMBL108647	CC(C)c1c(O)nc(SCC(=O)c2ccc(C)cc2C)nc1Cc3cccc4ccccc34	240	nM
CHEMBL125112	CCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)N5CCN(C)CC5)ccc4[nH]3	240	nM
CHEMBL340822	CCCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4NC(C)C	240	nM
CHEMBL145796	CCN1c2nc(OC)cc(C=O)c2NC(=O)c3cccnc13	240	nM
CHEMBL294720	Nc1ccc(CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F)cc1F	241	nM
CHEMBL68353	FC(F)(F)C12NC(=O)Nc3ccc(Cl)c(OC(=C1)c4ccccc4)c23	244	nM
CHEMBL297982	CCN1c2ncccc2c3nccn3c4c(C)ccnc14	245	nM
CHEMBL56383	CN1C(=O)c2cc(N)cnc2Oc3cc(C)ccc13	250	nM
CHEMBL329653	CCC1(Oc2ccccc2n3cccc3C1=O)c4ccccc4	250	nM
CHEMBL100629	CCN1c2ncccc2N(C)C(=O)c3cc(\C=C/c4ccccc4)cnc13	250	nM
CHEMBL331330	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4NC(C)C	250	nM
CHEMBL130177	COC(=O)c1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	250	nM
CHEMBL143976	CCN1c2nc(\C=C\C(=O)N)ccc2N(C)C(=O)c3cccnc13	250	nM
CHEMBL39999	Brc1ccc(NC(=S)NCCc2ccccn2)nc1	251	nM
CHEMBL57697	CCCN1C(=O)c2cc(N)ccc2Oc3cccc(C)c13	260	nM
CHEMBL328168	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(NCc4ccccc4)cnc13	260	nM
CHEMBL108581	CCc1c(O)nc(SCC(=O)c2ccc(Cl)cc2)nc1Cc3cccc4ccccc34	260	nM
CHEMBL124726	CCc1cc(NCc2oc3c(CC)cccc3n2)c(O)nc1C	260	nM
CHEMBL299073	Fc1ccc2NC(=O)C(C#CC3CC3)(N(CC4CC4)c2c1)C(F)(F)F	263	nM
CHEMBL314061	CCc1cc(NCc2ccccc2OC)c(O)nc1C	265	nM
CHEMBL82481	Clc1ccc2NC(=O)NC(C#Cc3cnccn3)(C4CC4)c2c1	270	nM
CHEMBL341512	CN(C)c1ccc2c(C)nc(CCCCCC(=O)c3ccccc3)n2n1	270	nM
CHEMBL132883	CCCc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	270	nM
CHEMBL341667	O=C1Nc2c(COCc3ccccc3)ccnc2N(C4CC4)c5ncccc15	270	nM
CHEMBL150424	CC(C)OC(=O)c1cccn1S(=O)(=O)c2cc(Cl)ccc2N	270	nM
CHEMBL291400	FC(F)(F)[C@]1(NC(=O)Nc2ccc(Cl)cc12)C#Cc3ccccc3	277	nM
CHEMBL56628	CN1C(=O)c2cc(ccc2Oc3cc(C)ccc13)C#N	280	nM
CHEMBL317080	CCN1c2ncc(COc3ccc(F)cc3)cc2C(=O)N(C)c4ccc(Cl)nc14	280	nM
CHEMBL338992	CCc1cc(NCc2oc3CCCCc3n2)c(O)nc1C	280	nM
CHEMBL123779	Cc1cccc(CSc2nc(N)cc(Cl)n2)c1	280	nM
CHEMBL339354	Nc1cc(nc(SCc2ccc3ccccc3c2)n1)C(F)(F)F	280	nM
CHEMBL2115325	CCN1c2cccnc2N(C)C(=O)c3cc(N)cnc13	280	nM
CHEMBL416853	CC(C)C#C[C@@]1(NC(=O)Nc2ccc(Cl)cc12)C(F)(F)F	281	nM
CHEMBL70255	CCN1c2cc(cc(Cl)c2N(C)C(=O)c3cccnc13)C(F)(F)F	290	nM
CHEMBL144872	Cc1ccccc1OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23	290	nM
CHEMBL2115328	CN1C(=O)c2cccnc2N(C3CC3)c4ncc(Cl)cc14	290	nM
CHEMBL39021	Cc1cccc(c1)C(OCCn2c(C)ncc2[N+](=O)[O-])c3ccccc3	300	nM

86

CHEMBL40632	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3cccc(c3)[N+](=O)[O-]	300	nM
CHEMBL301055	Nc1cccc(c1C#N)S(=O)(=O)c2cc(Cl)ccc2Cl	300	nM
CHEMBL69855	C1CC1N2c3ncccc3C=Cc4cccnc24	300	nM
CHEMBL100844	CCN1c2ncccc2N(C)C(=O)c3cc(CCCO)cnc13	300	nM
CHEMBL124557	CCc1cc(NCc2ccc3ccccc3c2)c(S)nc1C	300	nM
CHEMBL339406	CC(C)Nc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccc(OCCOCCOCCO)cc4[nH]3	300	nM
CHEMBL124149	CC(=O)c1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	300	nM
CHEMBL357411	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)N4CCCCC4	300	nM
CHEMBL347403	CCC(C)Sc1nc(O)cc(Cc2ccccc2[N+](=O)[O-])n1	300	nM
CHEMBL157137	CCC(C)Sc1nc(O)cc(Cc2cccc(c2)[N+](=O)[O-])n1	300	nM
CHEMBL155689	CCC(C)Sc1nc(O)cc(Cc2ccccc2F)n1	300	nM
CHEMBL262184	CCN1c2ncc(COc3ccc4[nH]ccc4c3)cc2C(=O)N(C)c5ccc(Cl)nc15	310	nM
CHEMBL144866	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)n4cccn4	310	nM
CHEMBL174953	Cc1nc(O)c(CCc2oc3ccccc3n2)cc1C#N	310	nM
CHEMBL46008	CC(=C)OC(=O)N1c2cc(Cl)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	315	nM
CHEMBL320702	CCc1c(O)nc(SCC(=O)c2ccc(C)cc2)nc1Cc3cccc4ccccc34	320	nM
CHEMBL316773	CC(C)c1c(O)nc(SCC(=O)c2ccc(Cl)cc2)nc1Cc3cccc4ccccc34	320	nM
CHEMBL133250	COc1ccc2[nH]cc(CC\N=C(/S)\Nc3ccc(Br)cn3)c2c1	320	nM
CHEMBL418104	CN1C(=O)c2cc(N)cnc2Oc3cc(C)c(C)cc13	322	nM
CHEMBL49531	FC(F)(F)C1(C#CC2CC2)N(CC3CC3)c4cc(Cl)ccc4NC1=O	329	nM
CHEMBL100951	CCN1c2ncc(COc3cccc4[nH]ccc34)cc2C(=O)N(C)c5ccc(Cl)nc15	330	nM
CHEMBL101834	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(CCc4ccc(NS(=O)(=O)C)cc4)cnc13	330	nM
CHEMBL125928	COC(=O)c1cccc(CSc2nc(N)cc(Cl)n2)c1	330	nM
CHEMBL342342	CCN1c2nc(cc(C=O)c2NC(=O)c3cccnc13)c4cccc(OC)c4	330	nM
CHEMBL311050	Clc1ccc2NC(=O)N[C@@](C#Cc3ccccn3)(C4CC4)c2c1	334.07	nM
CHEMBL123553	CCc1cc(NCc2oc3c(Cl)cccc3c2)c(O)nc1C	335	nM
CHEMBL48286	FC(F)(F)C1(C#CC2CC2)N(CCC3CC3)c4ccccc4NC1=O	340	nM
CHEMBL56567	CC(C)N1C(=O)c2ccccc2Oc3ccccc13	340	nM
CHEMBL125205	Clc1ccc2cnc(CCCCCCC(=O)c3ccccc3)n2n1	340	nM
CHEMBL357250	CCN1c2nc(O)cc(Cc3ccccc3)c2NC(=O)c4cccnc14	340	nM
CHEMBL293785	CCN1C(=O)c2cccnc2Oc3cccc(c13)[N+](=O)[O-]	343	nM
CHEMBL37067	CC1=C(Sc2ccccc2)N(COCc3ccccc3)C(=O)NC1=O	346.41	nM
CHEMBL288305	CCN1c2ncccc2C(=O)N(C)c3ccc(C)nc13	346.41	nM
CHEMBL306032	CCN1c2ccccc2N(C)C(=O)c3cccnc13	350	nM
CHEMBL85142	CCOc1ccccc1CNc2cc(CC)c(C)nc2O	350	nM
CHEMBL124610	CCC(C)(C)Nc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	350	nM
CHEMBL254206	COc1ccc(CCNC(=S)Nc2nccs2)cc1	350	nM
CHEMBL399069	CCCc1csc(NC(=S)NCCc2ccccc2)n1	350	nM
CHEMBL340869	CCOC(=O)CCCC=C(c1cc(Br)c(OC)c(c1)C(=O)OC)c2cc(Br)c(OC)c(c2)C(=O)OC	359	nM
CHEMBL309574	CCN1c2ncccc2N(C(=O)C)C(=O)c3cccnc13	360	nM
CHEMBL121827	CC(C)Nc1ccc(Cl)nc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	360	nM
CHEMBL95426	CCc1cc(CCc2nc3ccccc3s2)c(O)nc1C	370	nM
CHEMBL107606	COc1ccc(cc1)C(=O)CSc2nc(O)c(C)c(Cc3cccc4ccccc34)n2	370	nM
CHEMBL56451	CCCN1C(=O)c2ccccc2Oc3ccccc13	375	nM
CHEMBL58542	CCCCCC=C(c1cc(Br)c(OC)c(c1)C(=O)OC)c2cc(Br)c(OC)c(c2)C(=O)OC	380	nM
CHEMBL70312	CCN1C(=O)c2cccnc2N(CC)c3ccccc13	380	nM

CHEMBL73845	CCN1c2ccccc2NC(=O)c3cccnc13	380	nM
CHEMBL340556	CCNc1cccnc1N(C(C)C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	380	nM
CHEMBL332675	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)N4CCN(C)CC4)ccc3[nH]2)c5ncccc5NC(C)C	380	nM
CHEMBL125084	Cc1nc(CCCCCCC(O)c2ccccc2)n3nc(Cl)ccc13	380	nM
CHEMBL358564	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4cncs4	380	nM
CHEMBL173635	CCc1cc(CCc2oc(cn2)c3ccccc3)c(O)nc1C	385	nM
CHEMBL315990	Cc1ccc(cc1C)C23SCCN2C(=O)c4ccccc34	390	nM
CHEMBL144561	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccn[nH]4	390	nM
CHEMBL345006	CCN1c2nc(N\C=C\C)ccc2N(C)C(=O)c3cccnc13	390	nM
CHEMBL285510	CCC1OC(C#CC2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	391	nM
CHEMBL295978	CCN1c2ccccc2c3nccn3c4cccc(OC)nc14	392.79	nM
CHEMBL43293	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccccc3F	400	nM
CHEMBL299714	CCOC(=O)c1cccn1S(=O)(=O)c2cc(Cl)ccc2N	400	nM
CHEMBL55258	CCCN1C(=O)c2ccccc2Sc3ccccc13	400	nM
CHEMBL71927	CCN1c2cc(ccc2N(C)C(=O)c3cccnc13)[N+](=O)[O-]	400	nM
CHEMBL83641	CCc1cc(CCc2cc(CC)c(C)nc2O)c(O)nc1C	400	nM
CHEMBL91942	CCOc1ccc(F)c(CC\N=C(/N)\Nc2ccc(Br)cn2)c1Cl	400	nM
CHEMBL93822	Brc1ccc(NC(=S)NCCC2=CCCCC2)nc1	400	nM
CHEMBL340453	CCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)CC)ccc4[nH]3	400	nM
CHEMBL341931	CCc1c(C)nc(O)cc1Sc2cc(C)cc(C)c2	400	nM
CHEMBL145295	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)N4CCOCC4	400	nM
CHEMBL356611	CCCOC(=O)c1cccn1S(=O)(=O)c2cc(Cl)ccc2N	400	nM
CHEMBL349806	Oc1cc(Cc2c(Cl)cccc2Cl)nc(SC3CCCCC3)n1	400	nM
CHEMBL155864	CCC(C)Sc1nc(O)c(C)c(Cc2ccccc2Cl)n1	400	nM
CHEMBL351121	CCC(C)Sc1nc(O)c(C)c(Cc2cccc(c2)[N+](=O)[O-])n1	400	nM
CHEMBL170942	COc1cccc(CC\N=C(/S)\Nc2ccc(Br)cn2)c1	400	nM
CHEMBL254416	CC(C)Oc1cccc(CCNC(=S)Nc2nccs2)c1	400	nM
CHEMBL60513	COc1ccc2NC(=O)N[C@@](C#CC(C)C)(c2c1)C(F)(F)F	401	nM
CHEMBL300721	CC(C)CN1c2cc(Cl)ccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	404	nM
CHEMBL311349	CCN1c2ncccc2C(=O)Nc3cc(C)c(C)nc13	410	nM
CHEMBL321980	CC(C)c1c(O)nc(SCC(=O)C)nc1Cc2ccccc3ccccc23	410	nM
CHEMBL336318	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4CC(C)C	410	nM
CHEMBL146828	O=C1Nc2c(COc3ccc(cc3)C#N)ccnc2N(C4CC4)c5ncccc15	410	nM
CHEMBL348086	CCC(C)Sc1nc(O)c(C)c(Cc2ccccc2F)n1	410	nM
CHEMBL57216	Nc1ccc(CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F)cc1	412	nM
CHEMBL70930	CN1C(=O)c2cccnc2N(C(=O)C)c3cc(C)c(C)cc13	420	nM
CHEMBL143250	CCN1c2nc(O)cc(CO)c2NC(=O)c3cccnc13	420	nM
CHEMBL434122	O=C1Nc2c(COCCc3ccccc3)ccnc2N(C4CC4)c5ncccc15	420	nM
CHEMBL283614	CC(C)C#CC1(OCC(=O)Nc2ccc(Cl)cc12)C(F)(F)F	423	nM
CHEMBL42132	CCN1c2ncccc2c3ncc(C)n3c4cccnc14	425	nM
CHEMBL2114370	C[C@@H]1O[C@@](C#CC2CC2)(c3cc(F)ccc3NC1=O)C(F)(F)F	429.3	nM
CHEMBL70077	Oc1c(Cl)ccc2NC(=O)NC(C#Cc3ccccc3)(c12)C(F)(F)F	430	nM
CHEMBL424046	O=C1Nc2cccnc2N(C3CCC3)c4ncccc14	430	nM
CHEMBL321765	CCN1c2ncccc2N(C)C(=O)c3cc(CCO)cnc13	430	nM
CHEMBL124453	CCSc1cc(NCc2oc3ccccc3n2)c(O)nc1C	430	nM
CHEMBL32290	FC(F)(F)C1(OCC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	432	nM

CHEMBL59215	FC(F)(F)[C@@]1(C#CC2CC2)[C@@H](OCc3cccnc3)C(=O)Nc4ccc(Cl)cc14	438	nM
CHEMBL291024	CCN1c2ncccc2NC(=O)c3cccnc13	440	nM
CHEMBL58970	FC(F)(F)[C@@]1(C#CC2CC2)[C@@H](OCc3ccccc3)C(=O)Nc4ccc(Cl)cc14	440	nM
CHEMBL123778	CCc1cc(NCc2oc3cccc(O)c3n2)c(O)nc1C	440	nM
CHEMBL2114371	CC[C@@H]1O[C@@](C#CC2CC2)(c3cc(F)ccc3NC1=O)C(F)(F)F	441.52	nM
CHEMBL94526	Fc1cc2NC(=O)OC(C#CC3CC3)(c2c(F)c1F)C(F)(F)F	442	nM
CHEMBL177898	CCc1cc(CCc2oc3cc(F)ccc3n2)c(O)nc1C	442	nM
CHEMBL127283	CCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	444.75	nM
CHEMBL289816	O=C1Nc2cccnc2N(C3CC3)c4ncccc14	450	nM
CHEMBL290957	CCCN1c2ncccc2N(C)C(=O)c3cccnc13	450	nM
CHEMBL79696	Clc1ccc2NC(=O)NC(C#Cc3ccncc3)(C4CC4)c2c1	450	nM
CHEMBL122460	CCNc1cccnc1N(CC)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C(C)C)ccc4[nH]3	450	nM
CHEMBL144136	CC(C\N=C(/S)\Nc1nccs1)c2ccccc2	450	nM
CHEMBL151896	COC(=O)c1cccn1S(=O)(=O)c2cc(Cl)ccc2N	450	nM
CHEMBL101998	CCN1c2ncc(CCc3ccncc3)cc2C(=O)N(C)c4ccc(nc14)C#N	460	nM
CHEMBL127456	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4nc(F)ccc4NC(C)C	460	nM
CHEMBL124494	Nc1cc(Cl)nc(SCc2ccc3ccccc3c2)n1	460	nM
CHEMBL145158	Oc1ccccc1OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23	460	nM
CHEMBL301443	C=CCN1C(=O)c2ccccc2Oc3ccccc13	465	nM
CHEMBL125397	CCc1cc(NCc2oc3ccc(F)cc3n2)c(O)nc1C	470	nM
CHEMBL146169	CCN1c2ncccc2C(=O)N(C)c3ccc(O)nc13	470	nM
CHEMBL316083	FC(F)(F)C1(OC(=O)Nc2ccccc12)C#CC3CC3	478	nM
CHEMBL125324	CCCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4NC(C)(C)C	480	nM
CHEMBL124279	Nc1cc(Cl)nc(SCc2ccc(Cl)c(Cl)c2)n1	490	nM
CHEMBL145893	CCN1c2nc(cc(COc3ccccc3)c2NC(=O)c4cccnc14)c5cccc(OC)c5	490	nM
CHEMBL131761	COC(=O)c1cc(cc(Br)c1OC)C(=CCCN2CCOC2=O)c3cc(Br)c(OC)c(c3)C(=O)OC	499	nM
CHEMBL37056	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(NS(=O)(=O)C)cc4[nH]3	500	nM
CHEMBL416617	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3cccc(Cl)c3	500	nM
CHEMBL288629	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3cccc(F)c3	500	nM
CHEMBL305010	CCN1c2ccccc2C(=O)N(C)c3cccnc13	500	nM
CHEMBL91891	CCC1(Oc2ccccc2n3cccc3C1=O)c4ccc5ccccc5c4	500	nM
CHEMBL156083	CCCCSc1nc(O)cc(Cc2c(Cl)cccc2Cl)n1	500	nM
CHEMBL199090	CC(C)CC(=O)c1c(O)c(CC(=C(C)C)O)c2OC(=O)C=C(c3ccccc3)c2c1O	500	nM
CHEMBL297103	COC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	504	nM
CHEMBL82904	CCc1ccc(CNc2cc(CC)c(C)nc2O)c(OC)c1	510	nM
CHEMBL133469	CC(C)Cc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	510	nM
CHEMBL340193	CN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4NCC5CC5	520	nM
CHEMBL313695	CCc1cc(NCc2ccccc2[N+](=O)[O-])c(O)nc1C	530	nM
CHEMBL330990	CN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4nc(F)ccc4NC(C)(C)C	530	nM
CHEMBL100968	CCN1c2ncccc2N(C)C(=O)c3cc(CCc4cncnc4)cnc13	540	nM
CHEMBL85446	Cc1cccc(c1)C23SCCN2C(=O)c4ccccc34	547.72	nM
CHEMBL107200	COC(=O)CCCC=C(c1cc(Br)c(OC)c(c1)C(=O)OC)c2cc(Br)c(OC)c(c2)	547.72	nM

	C(=O)OC		
CHEMBL106661	Cc1c(O)nc(SCC(=O)c2ccc(Cl)cc2)nc1Cc3cccc4ccccc34	550	nM
CHEMBL127427	Cc1cn(cn1)c2ccc3c(C)nc(CCCCCCC(=O)c4ccccc4)n3n2	550	nM
CHEMBL410771	FC(F)(F)c1csc(NC(=S)NCCc2ccccc2)n1	550	nM
CHEMBL2115335	CCN1c2cc(Br)cnc2N(C)C(=O)c3cccnc13	550	nM
CHEMBL299710	CCN1C(=O)c2ccccc2Oc3ccccc13	560	nM
CHEMBL340248	Cc1nc(CCCCCCC(=O)c2ccccc2)n3ncccc13	560	nM
CHEMBL312340	CCN1c2ccc(C)cc2C(=O)N(C)c3cccnc13	580	nM
CHEMBL356313	Cc1ccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)cc1	580	nM
CHEMBL71023	CC(C)N1c2ncccc2NC(=O)c3cccnc13	590	nM
CHEMBL314633	Clc1cc(Cl)cc(c1)C23SCCN2C(=O)c4ccccc34	590	nM
CHEMBL103716	CCN1c2nc(ccc2N(C)C(=O)c3cc(CCc4ccccc4)cnc13)C5=CCC=N5	590	nM
CHEMBL102735	CCN1c2ncc(CN(C)c3ccccc3)cc2C(=O)N(C)c4ccc(Cl)nc14	590	nM
CHEMBL32038	CC(C)C1OC(C#CC2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	597	nM
CHEMBL288535	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccccc3Cl	600	nM
CHEMBL295585	Fc1ccccc1CC\N=C(/S)\Nc2ccc(Br)cn2	600	nM
CHEMBL298405	CN1C(=O)c2ccccc2Oc3cc(C)ccc13	600	nM
CHEMBL69952	Brc1ccc(NC(=S)NCCN2CCCCC2)nc1	600	nM
CHEMBL102957	Clc1ccccc1CCNC(=S)Nc2nccs2	600	nM
CHEMBL415716	CCc1c(C)nc(O)c(NCc2oc3ccccc3n2)c1C	600	nM
CHEMBL357409	CCOC(=O)c1c(O)nc(C)c(CC)c1Sc2cc(C)cc(C)c2	600	nM
CHEMBL156380	CC(C)CSc1nc(O)cc(Cc2c(Cl)cccc2Cl)n1	600	nM
CHEMBL346023	CCC(C)Sc1nc(O)cc(Cc2cccc(F)c2)n1	600	nM
CHEMBL254836	CCc1csc(NC(=S)NCCc2ccccc2)n1	600	nM
CHEMBL46209	FC(F)(F)C1(C#CC2CC2)N(CC=C)c3ccccc3NC1=O	601	nM
CHEMBL413751	CCc1cc(c(O)nc1C)C(OCc2c(F)cccc2F)(C#CC3CC3)C(F)(F)F	613	nM
CHEMBL317072	CCN1c2ncccc2N(C)C(=O)c3cc(CCC(=O)N)cnc13	620	nM
CHEMBL191146	CCCC1=C(SC2CCCCC2)c3cc(Cl)ccc3NC1=O	621.61	nM
CHEMBL190170	CC(C)C1=C(OC2CCCCC2)c3cc(Cl)ccc3NC1=O	630	nM
CHEMBL55610	CN1C(=O)c2cc(O)ccc2Oc3cc(C)ccc13	640	nM
CHEMBL69657	CCOCCOCN1C(=O)NC(=O)C2=C1Sc3ccccc3NC2	640	nM
CHEMBL435017	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4ccnn4	640	nM
CHEMBL144591	O=C1Nc2c(CC3=CCNC3)ccnc2N(C4CC4)c5ncccc15	640	nM
CHEMBL1203236	Cl.COc1ccc2c(C)nc(CCCCCCC(=O)c3ccccc3)n2n1	640	nM
CHEMBL48629	FC(F)(F)C1(C#CC2CC2)N(CC=C)c3cc(Cl)ccc3NC1=O	650	nM
CHEMBL303466	CN1C(=O)c2cccnc2N(C#C)c3ccccc13	650	nM
CHEMBL302931	CCN1C(=O)c2cccc(C)c2N(CC)c3ncccc13	650	nM
CHEMBL359410	S=C(NCCc1occc1)Nc2nccs2	650	nM
CHEMBL126214	CCN(Cc1oc2c(Cl)ccc(Cl)c2n1)c3cc(CC)c(C)nc3O	654	nM
CHEMBL294848	CCCN1C(=O)c2cc(N)ccc2Oc3cccc(C)c(C)c13	670	nM
CHEMBL321026	Cc1ccc(cc1)C(=O)CSc2nc(O)c(C)c(Cc3cccc4ccccc34)n2	670	nM
CHEMBL301986	CCCCOC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	672	nM
CHEMBL198050	COC(=O)CCC\C=C(/c1cccc(c1)C#N)\c2cc(C)c(OC)c(c2)C(=O)OC	673.5	nM
CHEMBL85533	CCc1cc(NCc2cccnc2OC)c(O)nc1C	680	nM
CHEMBL133010	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCC(=O)N(C)C)c2cc(Cl)c(OC)c(c2)C(=O)OC	687	nM
CHEMBL70562	CCN1C(=O)c2ccccc2N(CC)c3ncccc13	690	nM
CHEMBL40631	Clc1ccccc1CCNC(=S)Nc2ccc(Br)cn2	700	nM
CHEMBL40625	Fc1cccc(CC\N=C(/S)\Nc2ccc(Br)cn2)c1	700	nM
CHEMBL103235	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4cccc(c4)C(=O)OC)cnc13	700	nM

CHEMBL114559	Brc1ccc(NC(=S)NCCc2ccc3OCOc3c2)nc1	700	nM
CHEMBL421246	CC(C)Nc1cccnc1N(C2CC2)C3CCN(CC3)C(=O)c4cc5ccccc5[nH]4	700	nM
CHEMBL356278	O=C1Nc2c(CN3CCCC3)ccnc2N(C4CC4)c5ncccc15	700	nM
CHEMBL215724	COC(=O)CCC\C=C(\c1ccc(cc1)C#N)/c2cc(C)c3onc(OC)c3c2	700	nM
CHEMBL80118	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4c[nH]c5ccc(F)cc45	706	nM
CHEMBL187718	CCCC1=C(OC2CCCCC2)c3cc(Cl)ccc3NC1=O	710	nM
CHEMBL134227	C[C@H]1Oc2c3C=CC(C)(C)Oc3c4C(=CC(=O)Oc4c2[C@@H](OC(=O)C)[C@@H]1C)c5ccccc5	720	nM
CHEMBL283619	FC(F)(F)[C@]1(NC(=O)Nc2ccc(Cl)cc12)C#CC3CC3	725.95	nM
CHEMBL123478	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4nc(F)ccc4NC(C)(C)C	730	nM
CHEMBL121881	CC(C)Nc1ccnnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	740	nM
CHEMBL42656	CCN1c2ccncc2N(C)C(=O)c3cccnc13	748.33	nM
CHEMBL100942	CCN1c2nccccc2N(C)C(=O)c3cc(C)cnc13	750	nM
CHEMBL198425	COC(=O)CCC\C=C(/c1cccc(c1)C#N)\c2cc(Cl)c(OC)c(c2)C(=O)OC	750	nM
CHEMBL37789	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(CO)cc4[nH]3	760	nM
CHEMBL39950	CCN1c2ncc(C)cc2N(C)C(=O)c3cccnc13	760	nM
CHEMBL340593	Nc1cc(Cl)nc(SCc2cccc(Br)c2)n1	760	nM
CHEMBL2115334	CN1C(=O)c2cccnc2N(C3CC3)c4cc(Cl)cnc14	760	nM
CHEMBL313175	Cc1ccc(cc1)C23SCCN2C(=O)c4ccccc34	770	nM
CHEMBL106646	CCc1cc(c(O)nc1C)C(OC)(C#CC2CC2)C(F)(F)F	770	nM
CHEMBL85425	CCc1cc(NCc2ccccc2C#N)c(O)nc1C	790	nM
CHEMBL125896	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)N4CCN(C)CC4)ccc3[nH]2)c5ncccc5NC(C)(C)C	790	nM
CHEMBL94779	Fc1ccc(F)c2c1NC(=O)OC2(C#CC3CC3)C(F)(F)F	796	nM
CHEMBL283630	CCCC1OC(C#CC2CC2)(c3cc(Cl)ccc3NC1=O)C(F)(F)F	799	nM
CHEMBL314572	CCC(c1cc(O)nc(SC(C)C)n1)c2cccc3ccccc23	800	nM
CHEMBL317765	Fc1cc(F)c2NC(=O)OC(C#CC3CC3)(c2c1F)C(F)(F)F	800	nM
CHEMBL100394	CCN1c2nc(Cl)ccc2N(C)C(=O)c3cc(COc4ccc(cc4)C(=O)OC)cnc13	800	nM
CHEMBL116474	Brc1ccc(NC(=S)NCCc2cccs2)nc1	800	nM
CHEMBL145279	CCN1c2nc(OC)cc(C3OCCCO3)c2NC(=O)c4cccnc14	800	nM
CHEMBL157777	CSc1nc(O)cc(Cc2c(F)cccc2F)n1	800	nM
CHEMBL94550	CN(C)c1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	816	nM
CHEMBL145004	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ccccc4OC	820	nM
CHEMBL331684	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)N4CCN(C)CC4)ccc3[nH]2)c5nc(F)ccc5NC(C)(C)C	830	nM
CHEMBL351375	O=C1N2CCS[C@@H](c3ccccc23)c4ccccc14	830	nM
CHEMBL290410	CSCN1c2ncccc2N(C)C(=O)c3cccnc13	850	nM
CHEMBL310490	CN1C(=O)c2cccnc2N(CC=C)c3ncccc13	850	nM
CHEMBL70743	CCN1c2nc(N)c(Cl)cc2N(C)C(=O)c3cccnc13	850	nM
CHEMBL142478	COc1ccc(O)c(Cc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)c1	850	nM
CHEMBL280527	CCNc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(OC)ccc4[nH]3	853.23	nM
CHEMBL305416	CCN1c2cc(ccc2N(C)C(=O)c3cc(Br)cnc13)[N+](=O)[O-]	890	nM
CHEMBL57178	Fc1ccc(CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F)cc1	899	nM
CHEMBL33981	S=C(NCCc1ccccc1)Nc2nccs2	900	nM
CHEMBL54977	CCCN1C(=O)c2cc(N)ccc2Oc3c(C)cc(C)cc13	900	nM
CHEMBL83362	O=C1N2CCSC2(c3ccccc13)c4c5ccccc5cc6ccccc46	900	nM
CHEMBL314884	O=C1N2CCSC2(c3cccc4CCCc34)c5ccccc15	900	nM
CHEMBL149275	Nc1ccc(Cl)cc1S(=O)(=O)n2ccccc2C(=O)OCC=C	900	nM
CHEMBL345908	CCC(C)Sc1nc(O)c(C)c(Cc2cccc(Cl)c2)n1	900	nM

CHEMBL170810	COc1ccc(CC\N=C(/S)\Nc2ccc(Br)cn2)cc1	900	nM
CHEMBL372175	COC(=O)CCC\C=C(/c1cc(F)cc(c1)C(F)(F)F)\c2cc(C)c3onc(OC)c3c2	900	nM
CHEMBL357664	CCN1c2ncccc2C(=O)Nc3c(COCc4ccccc4)cc(OC)nc13	920	nM
CHEMBL187438	CCCc1c(O)nc2ccc(Cl)cc2c1[S+]([O-])C3CCCCC3	951	nM
CHEMBL281239	CCC#CC1(OCC(=O)Nc2ccc(Cl)cc12)C(F)(F)F	964	nM
CHEMBL262374	Cc1ccc(C)c(c1)C23SCCN2C(=O)c4ccccc34	970	nM
CHEMBL338872	CCc1cc(NC(C)c2oc3ccccc3c2)c(O)nc1C	970	nM
CHEMBL334129	COc1cccc(CSc2nc(N)cc(Cl)n2)c1	980	nM
CHEMBL37518	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(N)ccc4[nH]3	1000	nM
CHEMBL433487	CN1C(=O)c2cccnc2Oc3cc(C)cc(N)c13	1000	nM
CHEMBL419629	CN1C(=O)c2cccnc2N(CCF)c3ccccc13	1000	nM
CHEMBL313273	Cc1ccnc(c1)C23SCCN2C(=O)c4ccccc34	1000	nM
CHEMBL335768	CCCCCC=C(c1cc(C)c(OC)c(c1)C(=O)OC)c2cc(C)c(OC)c(c2)C(=O)OC	1000	nM
CHEMBL144949	CCN1c2nc(cc(C)c2NC(=O)c3cccnc13)C(C)C	1000	nM
CHEMBL141323	CCC(=O)CCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	1000	nM
CHEMBL355333	COc1ccccc1CC\N=C(/S)\Nc2ccc(Br)cn2	1000	nM
CHEMBL171920	CCc1cc(CCc2oc3c(Cl)cccc3n2)c(O)nc1C	1000	nM
CHEMBL198551	COC(=O)c1cc(cc(C)c1OC)\C(=C/CCN2CCOC2=O)\c3ccc(OC)c(OC)c3	1000	nM
CHEMBL253996	Fc1ccc(CCNC(=S)Nc2nccs2)cc1	1000	nM
CHEMBL2115323	CN1C(=O)c2cccnc2N(C3CC3)c4ccc(Cl)nc14	1000	nM
CHEMBL294840	COC(=O)CCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	1002.5	nM
CHEMBL61152	Nc1ccccc1CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F	1019	nM
CHEMBL86015	CC(c1cc(O)nc(SC2CCCC2)n1)c3cccc4ccccc34	1019.8	nM
CHEMBL357187	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCCN=[N+]=[N-])c2cc(Cl)c(OC)c(c2)C(=O)OC	1019.8	nM
CHEMBL318562	CCN1c2ncc(CCc3ccc4ccccc4c3)cc2C(=O)N(C)c5ccc(Cl)nc15	1020	nM
CHEMBL340403	CCN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4nc(Cl)ccc4NC(C)(C)C	1020	nM
CHEMBL422839	O=C1Nc2c(CN3CCOCC3)ccnc2N(C4CC4)c5ncccc15	1030	nM
CHEMBL145730	O=C1Nc2c(CSc3ccccc3)ccnc2N(C4CC4)c5ncccc15	1030	nM
CHEMBL357877	COc1ccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)cc1	1040	nM
CHEMBL124338	CC(C)Nc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	1048.81	nM
CHEMBL124556	CC(O)c1cc(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	1050	nM
CHEMBL124992	CCc1cc(N(C)Cc2oc3c(Cl)ccc(Cl)c3c2)c(O)nc1C	1050	nM
CHEMBL294406	CCCO[C@H]1C(=O)Nc2ccc(Cl)cc2[C@@]1(C#CC3CC3)C(F)(F)F	1051	nM
CHEMBL337029	C[C@H]1Oc2c3C=CC(C)(C)Oc3c4C(=CC(=O)Oc4c2[C@@H](O)[C@@H]1C)c5ccccc5	1067.71	nM
CHEMBL109389	CCC(C)Sc1nc(O)c(C)c(Cc2ccccc2)n1	1095.45	nM
CHEMBL288062	CCN1c2ncccc2c3ncc(C)n3c4ccc(nc14)N(C)C	1100	nM
CHEMBL418885	CCN1c2ccc(cc2N(C)C(=O)c3cccnc13)C(=O)OC	1100	nM
CHEMBL85697	CCc1cccc(c1)C23SCCN2C(=O)c4ccccc34	1100	nM
CHEMBL420460	CCN1c2ncccc2N(C)C(=O)c3cc(NC(=O)N)cnc13	1100	nM
CHEMBL121834	CCc1cc(NCC2=COc3ccccc3C2=O)c(O)nc1C	1100	nM
CHEMBL142664	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4ccc(O)nc4	1100	nM
CHEMBL147375	S=C(NCCc1cccc(Oc2ccccc2)c1)Nc3nccs3	1100	nM
CHEMBL149055	CC(C)Oc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	1100	nM

CHEMBL351323	CC(C)CSc1nc(O)c(C)c(Cc2c(Cl)cccc2Cl)n1	1100	nM
CHEMBL174267	Cc1nc(O)c(CCc2oc3ccccc3n2)cc1c4ccccc4	1100	nM
CHEMBL400684	Oc1ccccc1CCNC(=S)Nc2nccs2	1100	nM
CHEMBL106204	CC(=O)CSc1nc(O)c(C)c(Cc2cccc3ccccc23)n1	1120	nM
CHEMBL124991	CCc1cc(NC(C)c2ccc3ccccc3c2)c(O)nc1C	1130	nM
CHEMBL141443	[O-][N+](=O)c1ccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)cc1	1130	nM
CHEMBL1807294	Brc1ccccc1c2nc3ccccn3c2NC4CCCCC4	1140.18	nM
CHEMBL439929	CC(C)COC(=O)N1c2ccccc2NC(=O)C1(C#CC3CC3)C(F)(F)F	1142	nM
CHEMBL125666	Cc1nc(O)c(NCc2oc3ccccc3n2)cc1S(=O)(=O)C	1150	nM
CHEMBL345580	CC(C)Sc1nc(O)c(C)c(Cc2c(Cl)cccc2Cl)n1	1150	nM
CHEMBL156636	CCCCSc1nc(O)c(C)c(Cc2c(Cl)cccc2Cl)n1	1150	nM
CHEMBL264587	CNC(=O)CCCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	1159.31	nM
CHEMBL37080	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(O)cc4[nH]3	1200	nM
CHEMBL289969	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	1200	nM
CHEMBL292339	C[C@@H](\N=C(/S)\Nc1ccc(Cl)cn1)c2ccccc2	1200	nM
CHEMBL294743	C[C@@H](\N=C(/S)\Nc1ccc(Br)cn1)C2CCCCC2	1200	nM
CHEMBL322898	CCC(C)Sc1nc(O)cc(Cc2ccc(cc2)[N+](=O)[O-])n1	1200	nM
CHEMBL112886	CCC(C)Sc1nc(O)cc(Cc2cccc(C)c2)n1	1200	nM
CHEMBL114598	Brc1ccc(NC(=S)NCCc2occc2)nc1	1200	nM
CHEMBL145287	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ccc(OC)nc4	1200	nM
CHEMBL145897	S=C(NCc1ccccc1)Nc2nccs2	1200	nM
CHEMBL215542	COC(=O)CCC\C=C(\c1ccc(cc1)C#N)/c2cc(C)c3OC(=O)N(C)c3c2	1200	nM
CHEMBL96328	FC(F)(F)Oc1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	1249	nM
CHEMBL291113	O=C1Nc2c(ccnc2N(C3CC3)c4ncccc14)C#N	1250	nM
CHEMBL85945	CCc1cc(NCc2cccc(OC)c2)c(O)nc1C	1250	nM
CHEMBL124186	CCc1cc(NCc2oc3cc(F)ccc3n2)c(O)nc1C	1250	nM
CHEMBL338658	CCc1cc(NCc2oc3ccc(C)cc3n2)c(O)nc1C	1250	nM
CHEMBL175089	CCc1cc(CNc2oc3ccccc3n2)c(O)nc1C	1250	nM
CHEMBL208008	Cc1cc(C)c(c(C)c1)n2nnnc2SCC(=O)Nc3ccc(cc3)S(=O)(=O)N	1252	nM
CHEMBL443996	Fc1ccccc1CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F	1296	nM
CHEMBL289304	COc1ccc2cc([nH]c2c1)C(=O)N3CCN(CC3)c4ncccc4NC(C)C	1300	nM
CHEMBL38068	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(O)ccc4[nH]3	1300	nM
CHEMBL298243	CCN1c2cccnc2N(C)C(=O)c3cccnc13	1300	nM
CHEMBL86178	CCc1cc(NCc2c(C)cccc2OC)c(O)nc1C	1300	nM
CHEMBL338415	Cc1nc(CCCCCC(=O)c2ccccc2)n3nc(ccc13)n4nccn4	1300	nM
CHEMBL433925	CCOCc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	1300	nM
CHEMBL2115326	CCN1c2ncccc2N(C)C(=O)c3cc(Br)cnc13	1300	nM
CHEMBL338339	Cc1nc(CCCCCOC(=O)c2ccccc2)n3nc(Cl)ccc13	1319.85	nM
CHEMBL105630	CCc1cc(c(O)nc1C)C(OCc2ccccc2)(C#CC3CC3)C(F)(F)F	1348	nM
CHEMBL313481	O=C1N2CCSC2(c3occc3)c4ccccc14	1350	nM
CHEMBL330537	Clc1ccc(NC(=S)NCCC2=CCCCC2)nc1	1360.15	nM
CHEMBL71766	CCN1c2ncccc2N(C)C(=O)c3cc(Cl)cnc13	1374.77	nM
CHEMBL38129	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(C=O)cc4[nH]3	1400	nM
CHEMBL41458	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccc(Cl)cc3Cl	1400	nM
CHEMBL302866	C[C@@H](\N=C(/S)\Nc1ccc(Cl)cn1)C2CCCCC2	1400	nM
CHEMBL72535	C=CCN1C(=O)c2cccnc2Nc3ccccc13	1400	nM
CHEMBL314925	CCC(c1cc(O)nc(SC2CCCCC2)n1)c3cccc4ccccc34	1400	nM
CHEMBL86261	CCc1cc(NCc2ccccc2F)c(O)nc1C	1400	nM

CHEMBL144794	CCN1c2ncccc2C(=O)N(C)c3ccc(nc13)c4ccc(OC)cc4	1400	nM
CHEMBL151955	CC(C)Oc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	1400	nM
CHEMBL176814	CCc1cc([S+]([O-])Cc2oc3c(Cl)ccc(Cl)c3n2)c(O)nc1C	1400	nM
CHEMBL320056	CCOC(=O)CSc1nc(O)c(C(C)C)c(Cc2cccc3ccccc23)n1	1410	nM
CHEMBL358782	C=CCOCc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	1410	nM
CHEMBL58408	FC(F)(F)[C@@]1(C#CC2CC2)[C@@H](OCC3CC3)C(=O)Nc4ccc(Cl)cc14	1434	nM
CHEMBL86215	[O-][S+]1CCN2C(=O)c3ccccc3C12c4ccccc4	1450	nM
CHEMBL85829	CCc1cc(NCc2ccccc2Cl)c(O)nc1C	1450	nM
CHEMBL292468	Nc1cccc(CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F)c1	1455	nM
CHEMBL112949	Cc1c(O)nc(SC2CCCC2)nc1Cc3ccccc3	1466.29	nM
CHEMBL83524	Clc1cccc(c1)C23SCCN2C(=O)c4ccccc34	1469.69	nM
CHEMBL1807340	Cc1cccc2nc(c(NC3CCCCC3)n12)c4ccccc4Cl	1488.79	nM
CHEMBL41119	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccc(cc3)C(C)(C)C	1500	nM
CHEMBL309696	Clc1ccc2NC(=O)NC(C#Cc3cncnc3)(C4CC4)c2c1	1500	nM
CHEMBL87284	CCc1cc(NCc2ccccc2SC)c(O)nc1C	1500	nM
CHEMBL318343	CCN1c2ncc(CCc3ccnc(c3)C(=O)O)cc2C(=O)N(C)c4ccc(Cl)nc14	1500	nM
CHEMBL317866	CN(\C(=N\CCc1ccccc1)\S)c2nccs2	1500	nM
CHEMBL156208	CC(C)Sc1nc(O)cc(Cc2c(Cl)cccc2Cl)n1	1500	nM
CHEMBL160781	CCC(C)Sc1nc(O)c(C)c(Cc2cccc(F)c2)n1	1500	nM
CHEMBL315689	CCc1cc(NCc2ncccc2OC)c(O)nc1C	1550	nM
CHEMBL291970	FC(F)(F)[C@@]1(C#CC2CC2)[C@@H](OCc3ccccn3)C(=O)Nc4ccc(Cl)cc14	1572	nM
CHEMBL58607	Cc1cccc2c1nc(c3c(F)cccc3F)n2Cc4ccccc4	1600	nM
CHEMBL432526	C[C@@H](\N=C(/S)\Nc1ccc(Br)cn1)c2ccccc2	1600	nM
CHEMBL157349	CCC(C)Sc1nc(O)cc(Cc2ccccc2Cl)n1	1600	nM
CHEMBL111153	CCC(C)Sc1nc(O)cc(Cc2ccccc2)n1	1643.17	nM
CHEMBL313366	Cc1cccc(c1C)C23SCCN2C(=O)c4ccccc34	1650	nM
CHEMBL125504	CCc1cc(NCc2oc3cc(C)ccc3n2)c(O)nc1C	1650	nM
CHEMBL175531	CCc1cc(CCc2oc3ccc(F)cc3n2)c(O)nc1C	1700	nM
CHEMBL195108	OC(=O)c1ccccc1C(=O)NCCO\C(=N/c2ccc(I)cc2)\S	1700	nM
CHEMBL284241	Cc1cccc(Cc2nc(SC3CCCCC3)nc(O)c2C)c1	1749.29	nM
CHEMBL123966	CCOC(=O)c1cc(NCc2oc3ccccc3n2)c(O)nc1C	1750	nM
CHEMBL46961	C[C@H]1CN2C(=S)Nc3cccc(CN1CC=C(C)C)c23	1754.99	nM
CHEMBL2115322	CCN1c2ccc(C)nc2N(C)C(=O)c3cccnc13	1760	nM
CHEMBL59059	Fc1cccc(CO[C@H]2C(=O)Nc3ccc(Cl)cc3[C@@]2(C#CC4CC4)C(F)(F)F)c1	1776	nM
CHEMBL36835	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NC(=O)C)ccc4[nH]3	1800	nM
CHEMBL323573	CCC(C)Sc1nc(O)c(C)c(Cc2ccc(cc2)[N+](=O)[O-])n1	1800	nM
CHEMBL356163	CC(C)Oc1cccnc1N2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	1800	nM
CHEMBL49030	FC(F)(F)C1(C#CC2CC2)N(CC#C)c3ccccc3NC1=O	1807	nM
CHEMBL84717	O=C1N2CCSC2(c3cccc(c3)C#N)c4ccccc14	1810	nM
CHEMBL301996	FC(F)(F)C1(C#CC2CC2)N(Cc3ccccc3)c4ccccc4NC1=O	1818	nM
CHEMBL106659	CCc1cc(c(O)nc1C)C(OCC#N)(C#CC2CC2)C(F)(F)F	1842	nM
CHEMBL177192	CN(C)c1cc(CCc2oc3ccccc3n2)c(O)nc1C	1850	nM
CHEMBL289429	CCN1c2ncccc2C(=O)N(C)c3c(C)ccnc13	1900	nM
CHEMBL73672	CCN1c2nccc(CC)c2NC(=O)c3cccnc13	1900	nM
CHEMBL124838	CCc1cc(NCc2oc3cccnc3n2)c(O)nc1C	1900	nM
CHEMBL144130	Cn1cccc1CC\N=C(/S)\Nc2nccs2	1900	nM

CHEMBL144420	S=C(NCCc1ccccc1)Nc2nncs2	1900	nM
CHEMBL151173	CCOc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	1900	nM
CHEMBL422001	CCC(C)Sc1nc(O)cc(Cc2cccc(Cl)c2)n1	1900	nM
CHEMBL96591	FC(F)(F)C1(OC(=O)Nc2cc3ccccc3cc12)C#CC4CC4	1909	nM
CHEMBL335037	CCOC(=O)NCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	1930	nM
CHEMBL125120	CCc1cc(NCc2oc3ccccc3c2C)c(O)nc1C	1950	nM
CHEMBL321786	CCc1cc(c(O)nc1C)C(OCc2c(F)cccc2OC)(C#CC3CC3)C(F)(F)F	1951	nM
CHEMBL94541	CC(C)c1ccc2NC(=O)OC(C#CC3CC3)(c2c1)C(F)(F)F	1958	nM
CHEMBL357658	CCNC(=O)OCCCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	1959.59	nM
CHEMBL316151	COc1cccc(c1)C23SCCN2C(=O)c4ccccc34	1969.77	nM
CHEMBL155936	OC1(CC1)C#CC2(OC(=O)Nc3ccc(Cl)cc23)C(F)(F)F	1983	nM
CHEMBL36656	CCNc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(O)ccc4[nH]3	2000	nM
CHEMBL123514	CCc1nc(CCCCCCC(=O)c2ccccc2)n3nc(Cl)ccc13	2000	nM
CHEMBL358754	CC(C)Oc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	2000	nM
CHEMBL151565	CC(C)Nc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	2000	nM
CHEMBL166126	Clc1ccc(cc1)N(C(=S)OCCN2C(=O)c3ccccc3C2=O)C(=O)c4ccnc(Cl)c4	2000	nM
CHEMBL379813	COc1ccc(cc1OC2CCCC2)[C@@H]3CN(C(=O)C3)c4cccc(N)c4	2000	nM
CHEMBL212394	COC(=O)CCC\C=C(/c1cc(C)c(OC)c(c1)C(=O)OC)\c2cc(C)c3ON(C)C(=O)c3c2	2000	nM
CHEMBL126811	Cc1nc(CCCCCCCC(=O)c2ccccc2)n3nc(Cl)ccc13	2007.98	nM
CHEMBL38744	Cc1ccc(cc1)C(OCCn2c(C)ncc2[N+](=O)[O-])c3ccccc3	2100	nM
CHEMBL71310	CCN1c2ccc(OC)cc2N(C)C(=O)c3cccnc13	2100	nM
CHEMBL440879	CC(C)c1cccc(c1)C23SCCN2C(=O)c4ccccc34	2100	nM
CHEMBL315287	CC(c1ccccc1)c2cc(O)nc(SC3CCCC3)n2	2100	nM
CHEMBL356173	CCOc1cccnc1N2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	2100	nM
CHEMBL177174	COCc1cc(CCc2oc3ccccc3n2)c(O)nc1C	2100	nM
CHEMBL301109	CCN1c2ncccc2c3ncc(C)n3c4ccc(nc14)N5CCCC5	2186.09	nM
CHEMBL43324	CCN1c2ncccc2c3nccn3c4cccc(nc14)N(C)C	2190	nM
CHEMBL114292	Oc1cc(Cc2ccccc2)nc(SC3CCCCC3)n1	2190.89	nM
CHEMBL36776	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(OS(=O)(=O)C)cc4[nH]3	2200	nM
CHEMBL299002	CCCN1C(=S)c2ccccc2Oc3ccccc13	2200	nM
CHEMBL312172	O=C1N2CCCSC2(c3ccccc3)c4ccccc14	2200	nM
CHEMBL85830	CCc1cc(NCc2ccccc2C)c(O)nc1C	2200	nM
CHEMBL322539	CC(C)CSc1nc(O)c(C)c(Cc2ccccc2)n1	2200	nM
CHEMBL145272	O=C1Nc2c(Cn3cccn3)ccnc2N(C4CC4)c5ncccc15	2200	nM
CHEMBL343149	COC(=O)CC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	2200	nM
CHEMBL424141	CCNc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	2200	nM
CHEMBL48427	Cc1cccc(n1)N2C(SCC2=O)c3c(Cl)cccc3Cl	2240	nM
CHEMBL43348	Cc1ncc([N+](=O)[O-])n1CCOC(c2ccccc2)c3ccc(F)cc3	2300	nM
CHEMBL85368	CC(C)Sc1nc(O)cc(n1)C(C)c2ccccc2	2300	nM
CHEMBL87569	CCC(c1ccccc1)c2cc(O)nc(SC(C)C)n2	2300	nM
CHEMBL435216	Cc1nc(CCCCCOCc2ccccc2)n3nc(Cl)ccc13	2300	nM
CHEMBL355113	Clc1ccc(cc1)N(C(=S)OCCN2C(=O)c3ccccc3C2=O)C(=O)c4occc4	2300	nM
CHEMBL1309	Oc1cc(Cl)cc2c1NC(=O)O[C@]2(C#CC3CC3)C(F)(F)F	2341	nM
CHEMBL125052	CCc1cc(NCc2oc(cn2)c3ccccc3)c(O)nc1C	2350	nM
CHEMBL132489	COC(=O)NCCC=C(c1cc(Br)c(OC)c(c1)C(=O)OC)c2cc(Br)c(OC)c(c2)C(=O)OC	2390	nM
CHEMBL101348	Clc1cnc(NC(=S)NCCc2ccccc2)s1	2400	nM

CHEMBL342794	Cc1cccc(OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23)c1	2430	nM
CHEMBL346356	Oc1cc2NC(=O)OC(C#CC3CC3)(c2cc1Cl)C(F)(F)F	2450	nM
CHEMBL173529	CCc1cc(CCc2ccc3ccccc3n2)c(O)nc1C	2450	nM
CHEMBL49334	CCN1c2ncccc2c3ncc(CC)n3c4cccnc14	2488.57	nM
CHEMBL415871	COC(=O)Nc1ccc2[nH]c(cc2c1)C(=O)N3CCN(CC3)c4ncccc4NC(C)C	2500	nM
CHEMBL301449	CC(C)c1ccc(cc1)S(=O)(=O)n2ccc(c2)C(O)c3ccc(Cl)cc3Cl	2500	nM
CHEMBL109551	CC(C)Sc1nc(O)c(C)c(Cc2ccccc(C)c2)n1	2500	nM
CHEMBL110007	CSc1nc(O)c(C)c(Cc2ccccc(C)c2)n1	2500	nM
CHEMBL110857	CC(C)Sc1nc(O)c(C)c(Cc2ccccc2)n1	2500	nM
CHEMBL123202	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4ccnc4C	2500	nM
CHEMBL338826	CCc1cc(NCc2nc(O)c3ccccc3n2)c(O)nc1C	2500	nM
CHEMBL350396	Clc1ccc(cc1)N(C(=S)OCCN2C(=O)c3ccccc3C2=O)C(=O)c4cccs4	2500	nM
CHEMBL197069	CC(C)C(=O)c1c(O)c(CC=C(C)C)c2OC(=O)C=C(c3ccccc3)c2c1O	2500	nM
CHEMBL254840	CCCCc1csc(NC(=S)NCCc2ccccc2)n1	2500	nM
CHEMBL31455	FC(F)(F)C1(OCC(=O)Nc2ccc(Cl)cc12)C#Cc3cocc3	2510	nM
CHEMBL151716	Oc1ccc(CCOC(=O)c2cc(O)c(O)c(O)c2)cc1O	2533.77	nM
CHEMBL110008	Cc1cccc(Cc2cc(O)nc(SC3CCCC3)n2)c1	2600	nM
CHEMBL126216	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4cnnc4	2600	nM
CHEMBL293498	C[C@H]1CN2C(=S)Nc3cc(Cl)cc(CN1CC=C(C)C)c23	2607.68	nM
CHEMBL85312	O=C1N2CCSC2(c3cccs3)c4ccccc14	2650	nM
CHEMBL105826	CCc1cc(c(O)nc1C)C(OCc2ccc(Cl)cc2Cl)(C#CC3CC3)C(F)(F)F	2696	nM
CHEMBL32469	CCC(C)Sc1nc(O)c(C)c(Cc2ccccc(C)c2)n1	2700	nM
CHEMBL124328	CCc1cc(NCc2oc3ccc4ccccc4c3n2)c(O)nc1C	2700	nM
CHEMBL151192	CCNc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	2700	nM
CHEMBL297115	CCN1c2ncccc2c3nc(C)cn3c4cccnc14	2750	nM
CHEMBL49441	CCN1c2ncccc2c3nccn3c4ccc(nc14)N5CCCC5	2792.85	nM
CHEMBL50019	Cc1ccnc(c1)N2C(SCC2=O)c3c(F)cccc3F	2840	nM
CHEMBL124946	Cc1cc(C)c(NCc2oc3c(Cl)ccc(Cl)c3n2)c(O)n1	2850	nM
CHEMBL359315	Cc1cccc(n1)N2C(SCC2=O)c3c(C)cccc3F	2850	nM
CHEMBL393003	Fc1cccc(F)c1CN2C(=O)Nc3ccc(Cl)cc23	2860	nM
CHEMBL347244	Cc1c(O)nc(SC2CCCCC2)nc1Cc3c(Cl)cccc3Cl	2886.17	nM
CHEMBL37722	CN1C(=O)c2cccnc2N(CCF)c3ncccc13	2900	nM
CHEMBL296589	Cc1cccc(n1)N2C(SCC2=O)c3c(F)cccc3F	2900	nM
CHEMBL306079	CCN1c2ccccc2N(C)C(=O)c3ccc(F)nc13	2900	nM
CHEMBL111368	CC(C)Sc1nc(O)cc(Cc2cccc(C)c2)n1	2900	nM
CHEMBL3143764	COCCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	2900	nM
CHEMBL313212	[O-][N+](=O)c1cccc(c1)C23SCCN2C(=O)c4ccccc34	2932.58	nM
CHEMBL48637	CCN1c2ncccc2c3nccn3c4cccnc14	2946.18	nM
CHEMBL133393	COC(=O)c1cc(cc(C)c1OC)C(=CCCNC(=O)OCC(C)C)c2cc(C)c(OC)c(c2)C(=O)OC	2950	nM
CHEMBL39343	OCc1ccnc2N(C3CC3)c4ncccc4C(=O)Nc12	3000	nM
CHEMBL99844	CCN1c2ncccc2N(C)C(=O)c3cc(\C=C\c4ccncc4)cnc13	3000	nM
CHEMBL338823	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(N)ccc13	3000	nM
CHEMBL345252	CC(=O)NC1=CC(=O)c2ccc(nc2C1=O)c3[nH]c(cc4c5ccccc5nc34)C(=O)OCCOP(=O)(O)O	3000	nM
CHEMBL156109	CSc1nc(O)cc(Cc2c(Cl)cccc2Cl)n1	3000	nM
CHEMBL3143760	COC(=O)CN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	3000	nM
CHEMBL144476	Clc1ccccc1OCc2ccnc3N(C4CC4)c5ncccc5C(=O)Nc23	3050	nM

CHEMBL338435	CN(C1CCN(CC1)C(=O)c2cc3cc(NS(=O)(=O)C)ccc3[nH]2)c4ncccc4N C(C)(C)C	3100	nM
CHEMBL211582	CN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C) C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	3100	nM
CHEMBL3143768	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(= O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCO)C1=O	3100	nM
CHEMBL3143792	CNC(=O)CN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C) C	3100	nM
CHEMBL63497	CCCCCC=C(c1ccc(OC)c(c1)C(=O)OC)c2ccc(OC)c(c2)C(=O)OC	3200	nM
CHEMBL147224	CCOc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	3200	nM
CHEMBL32460	FC(F)(F)C1(OCC(=O)Nc2ccc(Cl)cc12)C#Cc3ccccc3	3300	nM
CHEMBL305840	CCN1C(=O)c2ccccc2N(C)c3nc(Cl)ccc13	3300	nM
CHEMBL310070	O=C1N2CCS[C@]2(c3ccccc3)c4ccccc14	3329.86	nM
CHEMBL124271	CNc1ccc2c(C)nc(CCCCCCC(=O)c3ccccc3)n2n1	3400	nM
CHEMBL338302	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)n4cccn4	3400	nM
CHEMBL151316	CCOc1cccnc1N(C)C2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	3400	nM
CHEMBL367204	Cc1nc(O)c(CCc2oc3ccccc3n2)cc1CO	3400	nM
CHEMBL84486	O=C1N2CCSC2(c3ccccc3)c4ncccc14	3450	nM
CHEMBL1807342	Clc1ccccc1c2nc3cccc(C#N)n3c2NC4CCCCC4	3470	nM
CHEMBL313676	S=C1N2CCSC2(c3ccccc3)c4ccccc14	3500	nM
CHEMBL3143793	CN(C)C(=O)CN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C) (C)C	3500	nM
CHEMBL53554	Fc1cccc(F)c1C2SCc3nc4ccccc4n23	3505	nM
CHEMBL63150	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCCO)c2cc(Cl)c(OC)c(c2)C(=O)OC	3600	nM
CHEMBL82439	CCCc1cc(CCN2C(=O)c3ccccc3C2=O)c(O)nc1C	3700	nM
CHEMBL86062	CCC(c1ccccc1)c2cc(O)nc(SC3CCCC3)n2	3700	nM
CHEMBL358555	CCN1c2nc(ccc2N(C)C(=O)c3cccnc13)c4cnc[nH]4	3700	nM
CHEMBL3142918	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(= O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCOP(=O)(O)C(=O)O)C1=O	3700	nM
CHEMBL84821	CCc1cc(NCc2ccccc(C)c2OC)c(O)nc1C	3800	nM
CHEMBL177271	CCc1cc(CCc2oc3c(F)ccc(F)c3n2)c(O)nc1C	3800	nM
CHEMBL263515	CC(C)[C@H](N)C(=O)NCC(=O)NCCCN1C(=O)N(C=C(C)C1=O)C2O C(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C) (C)C	3800	nM
CHEMBL3142919	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(= O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCOP(=O)(O)C(=O)OCc4ccccc4)C1=O	3800	nM
CHEMBL107899	CCc1cc(c(O)nc1C)C(OCc2cc(OC)cc(OC)c2)(C#CC3CC3)C(F)(F)F	3843	nM
CHEMBL38088	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(cc4[nH]3)C#N	3900	nM
CHEMBL320902	S=C(NCCc1ccccc1)Nc2cnccn2	3900	nM
CHEMBL332351	Cc1nc(CCCCCC(=O)Cc2ccccc2)n3nc(Cl)ccc13	3900	nM
CHEMBL7483	CCNc1cccnc1N2CCN(CC2)C(=O)c3cc4ccccc4[nH]3	4000	nM
CHEMBL84260	Clc1ccc(cc1)C23SCCN2C(=O)c4ccccc34	4000	nM
CHEMBL82751	Clc1ccc(cc1Cl)C23SCCN2C(=O)c4ccccc34	4000	nM
CHEMBL92810	FC(F)(F)c1ccc(\N=C(/S)\NCCC2=CCCCC2)nc1	4000	nM
CHEMBL344562	CCN1c2nc(OC)cc(COc3ccccc3)c2NC(=O)c4cccnc14	4000	nM
CHEMBL151411	CCOC(=O)c1cccn1S(=O)(=O)c2cc(C)ccc2N	4000	nM
CHEMBL213257	CC1=CN(C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCNC(=O)[C@@H]4CCCN4C(=O)[C	4000	nM

@@H](N)CC(=O)N)C1=O

CHEMBL85783	Cc1cccc(n1)C23SCCN2C(=O)c4ccccc34	4100	nM
CHEMBL151152	Cc1ccnc(c1)N2C(SCC2=O)c3c(F)cccc3Cl	4120	nM
CHEMBL150025	Cc1cc(C)nc(c1)N2C(SCC2=O)c3c(F)cccc3F	4120	nM
CHEMBL176587	CCc1cc(\C=C/c2oc3ccccc3n2)c(O)nc1C	4207.14	nM
CHEMBL417331	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(OCc5ccccc5)ccc4[nH]3	4300	nM
CHEMBL58711	C[C@H]1CN2C(=S)Nc3ccc(Cl)c(CN1CC=C(C)C)c23	4300	nM
CHEMBL108944	CC(C)SC1=N\C(=C\c2ccccc2)\C(C)(C)C(=O)N1	4300	nM
CHEMBL320735	CCC(C)SC1=N\C(=C\c2ccccc2)\C(C)(C)C(=O)N1	4300	nM
CHEMBL87799	FC(F)(F)c1cccc(c1)C23SCCN2C(=O)c4ccccc34	4311.03	nM
CHEMBL1807345	Clc1ccccc1c2nc3cccc(Cl)n3c2NC4CCCCC4	4384.47	nM
CHEMBL1807291	Clc1ccccc1c2nc3ccccn3c2NC4CCCCC4	4390	nM
CHEMBL286325	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(F)cc4[nH]3	4400	nM
CHEMBL212339	CC(C)[C@H](N)C(=O)N1CCC[C@H]1C(=O)N[C@@H](C(C)C)C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(=O)C=C4N)C3O[Si](C)(C)C(C)(C)C	4400	nM
CHEMBL133678	COC(=O)NCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OCc2cc(Cl)c(OC)c(c2)C(=O)OC	4430	nM
CHEMBL63515	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCN=[N+]=[N-])c2cc(Cl)c(OC)c(c2)C(=O)OC	4449.72	nM
CHEMBL82461	Clc1cc2C(=O)N3CCSC3(c4ccccc4)c2cc1Cl	4480	nM
CHEMBL107562	COC(=O)CSc1nc(O)c(C(C)C)c(Cc2cccc3ccccc23)n1	4490	nM
CHEMBL70324	CCN1c2cc(N)ccc2N(C)C(=O)c3cccnc13	4500	nM
CHEMBL145260	S=C(NCCCc1ccccc1)Nc2nccs2	4500	nM
CHEMBL343398	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCC=O)c2cc(Cl)c(OC)c(c2)C(=O)OC	4536.52	nM
CHEMBL86268	Nc1cccc(c1)C23SCCN2C(=O)c4ccccc34	4549.73	nM
CHEMBL144654	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCCBr)c2cc(Cl)c(OC)c(c2)C(=O)OC	4571.65	nM
CHEMBL314103	Cc1ccnc(c1)C23SCCN2C(=O)c4cccnc34	4600	nM
CHEMBL85476	CCc1cc(NCc2ccccc2O)c(O)nc1C	4600	nM
CHEMBL111088	CC(C)CSC1=N\C(=C\c2ccccc2)\C(C)(C)C(=O)N1	4600	nM
CHEMBL111118	CC(C)CSc1nc(O)c(C)c(Cc2cccc(C)c2)n1	4600	nM
CHEMBL378037	CC(C)C[C@H](NC(=O)[C@@H](N)C(C)C)C(=O)NCCCN1C(=O)N(C=C(C)C1=O)C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C	4600	nM
CHEMBL1807347	Clc1ccccc1c2nc3cccc(Br)n3c2NC4CCCCC4	4620	nM
CHEMBL58865	CC(C)C#CC1(NS(=O)(=O)Nc2ccc(Cl)cc12)C3CC3	4627	nM
CHEMBL294602	Cc1ccc(cc1)C(O)c2ccn(c2)S(=O)(=O)c3ccc(C)cc3	4700	nM
CHEMBL380211	CC1=CN(C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCNC(=O)[C@@H]4CCCN4C(=O)[C@@H](N)CCCCN)C1=O	4700	nM
CHEMBL3142917	[Na+].COC(=O)P(=O)([O-])OCCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	4700	nM
CHEMBL110328	CCc1c(O)nc(SCC(=O)OC)nc1Cc2cccc3ccccc23	4720	nM
CHEMBL313518	OC(=O)c1cc(Br)ccc1NC(=O)CCCCC(=O)Nc2ccc(Br)cc2C(=O)O	4757.1	nM
CHEMBL35655	CSCSc1nc(O)c(C(C)C)c(Cc2cc(C)cc(C)c2)n1	4800	nM
CHEMBL148532	CC(C)(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C)ccc4[nH]3	4800	nM
CHEMBL345128	CCC(C)Sc1nc(O)cc(Cc2ccc(Cl)cc2)n1	4800	nM
CHEMBL214795	CC(C)[C@H](N)C(=O)N1C[C@H](O)[C@H](O)[C@H]1C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(	4800	nM

	=O)C=C4N)C3O[Si](C)(C)C(C)(C)C		
CHEMBL151315	Oc1cc(O)c2CC(COc2c1)OC(=O)c3cc(O)c(O)c(O)c3	4853.86	nM
CHEMBL109721	CSc1nc(O)c(C)c(Cc2ccccc2)n1	4900	nM
CHEMBL432812	Brc1ccc(NC(=S)NCCN2CCCC2)nc1	4900	nM
CHEMBL387370	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCO)C1=O	4929.5	nM
CHEMBL130316	COC(=O)NCCC=C(c1cc(C)c(OC)c(c1)C(=O)OC)c2cc(C)c(OC)c(c2)C(=O)OC	4930	nM
CHEMBL316094	CC1(Sc2ccccc2n3cccc3C1=O)c4ccccc4	5000	nM
CHEMBL327832	CCC1(CC=C)Oc2ccccc2n3cccc3C1=O	5000	nM
CHEMBL151077	CCOC(=O)c1cccn1S(=O)(=O)c2cc(C)ccc2[N+](=O)[O-]	5000	nM
CHEMBL370921	Oc1nc2ccc(Cl)cc2n1Cc3ccc4ccccc4c3	5200	nM
CHEMBL125213	COC(=O)\C=C\CSc1nc(N)cc(Cl)n1	5250	nM
CHEMBL1460	OC[C@@H]1CC[C@@H](O1)n2cnc3C(=O)NC=Nc23	5370	nM
CHEMBL1807339	Cc1ccc2nc(c(NC3CCCCC3)n2c1)c4ccccc4Cl	5390	nM
CHEMBL172773	CCc1cc(CCC(=O)Nc2ccccc2O)c(O)nc1C	5400	nM
CHEMBL383894	CC(C)[C@H](N)C(=O)N[C@@H](C)C(=O)NCCCN1C(=O)N(C=C(C)C1=O)C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C	5400	nM
CHEMBL37888	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(OS(=O)(=O)C)ccc4[nH]3	5500	nM
CHEMBL34542	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(ccc4[nH]3)N(C)S(=O)(=O)C	5600	nM
CHEMBL40642	CSCSc1cc(Cc2ccccc2)c(C(C)C)c(O)n1	5600	nM
CHEMBL63982	CCCCCC1OC1(c2cc(Br)c(OC)c(c2)C(=O)OC)c3cc(Br)c(OC)c(c3)C(=O)OC	5600	nM
CHEMBL130336	COC(=O)c1cc(cc(C)c1OC)C(=CCCCC(=O)N(C)C)c2cc(C)c(OC)c(c2)C(=O)OC	5650	nM
CHEMBL198201	COC(=O)CCC\C=C(/c1cccc(c1)C#N)\c2cc(C)c3onc(OC)c3c2	5700	nM
CHEMBL288626	Brc1ccc(NC(=S)NCN2CCCCC2)nc1	5800	nM
CHEMBL58119	C[C@H]1Cn2c(S)nc3ccc(F)c(CN1CC=C(C)C)c23	5800	nM
CHEMBL86289	CC(C)Sc1nc(O)cc(n1)C(C)c2cccc3ccccc23	5800	nM
CHEMBL153896	CCCCOC(=O)c1cc2c3ccccc3[nH]c2c(n1)c4ccc5C(=O)C=C(NC(=O)CCC)C(=O)c5n4	5800	nM
CHEMBL314558	O=C1N2CCSC2(c3ccccn3)c4ccccc14	5850	nM
CHEMBL147069	Oc1ccc(CCOC(=O)c2cc(O)c(O)c(O)c2)cc1	5962.38	nM
CHEMBL325757	COC(=O)c1cc(cc(Br)c1OC)C(=CCCCC#C)c2cc(Br)c(OC)c(c2)C(=O)OC	6000	nM
CHEMBL104738	CCc1cc(c(O)nc1C)C(OCc2c(F)cccc2Cl)(C#CC3CC3)C(F)(F)F	6093	nM
CHEMBL35755	CSCSc1nc(O)c(C(C)C)c(Cc2ccccc2)n1	6100	nM
CHEMBL313729	O=C1N2CCOC2(c3ccccc3)c4ccccc14	6100	nM
CHEMBL111523	CSC1=N\C(=C\c2ccccc2)\C(C)(C)C(=O)N1	6100	nM
CHEMBL147336	Oc1cc(cc(O)c1O)C(=O)OC2COc3ccccc3C2	6100	nM
CHEMBL433258	CCN1c2ncccc2c3ncc(C)n3c4ccc(O)nc14	6248.2	nM
CHEMBL85280	Cc1ccccc1C23SCCN2C(=O)c4ccccc34	6300	nM
CHEMBL3142914	CCOC(=O)P(=O)(O)OCCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	6300	nM
CHEMBL287978	Fc1ccc(CC\N=C(/S)\Nc2ccc(Br)cn2)cc1	6400	nM
CHEMBL46562	CCN1c2cnccc2C(=O)N(C)c3cccnc13	6400	nM
CHEMBL60866	CC(C)(C)c1ccc(cc1)S(=O)(=O)n2ccc(c2)C(O)c3ccc(Cl)cc3Cl	6400	nM
CHEMBL98394	CCc1cc(NCc2nc3ccccc3[nH]2)c(O)nc1C	6400	nM
CHEMBL308549	CSCN1c2ccccc2N(C)C(=O)c3cccnc13	6600	nM

CHEMBL82909	Cc1cccc(n1)C23SCCN2C(=O)c4cccnc34	6600	nM
CHEMBL1807341	Clc1ccccc1c2nc3ccc(cn3c2NC4CCCCC4)C#N	6600	nM
CHEMBL3143767	CN(C)CCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	6600	nM
CHEMBL124578	Nc1cc(Cl)nc(SCc2ccccc2)n1	6660	nM
CHEMBL262415	Cc1nc(CCCCCCC(=O)c2ccccc2)n3nc(ccc13)N4CCCCC4	6700	nM
CHEMBL385844	CC(C)[C@H](N)C(=O)NCCCN1C(=O)N(C=C(C)C1=O)C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C	6700	nM
CHEMBL445417	CC(C)[C@H](N)C(=O)N[C@@H](Cc1ccccc1)C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(=O)C=C4N)C3O[Si](C)(C)C(C)(C)C	6800	nM
CHEMBL83356	CCc1ccccc1CNc2cc(CC)c(C)nc2O	6900	nM
CHEMBL198873	CC(C)CC(=O)c1c(O)cc(O)c2C(=CC(=O)Oc12)c3ccccc3	6900	nM
CHEMBL108196	COC(=O)CSc1nc(O)c(C)c(Cc2cccc3ccccc23)n1	6990	nM
CHEMBL290312	CSCSc1cc(Cc2cc(C)cc(C)c2)c(C(C)C)c(O)n1	7000	nM
CHEMBL108605	CCOC(=O)CSc1nc(O)c(C)c(Cc2cccc3ccccc23)n1	7000	nM
CHEMBL156598	CCCCCCCCOC(=O)c1cc2c3ccccc3[nH]c2c(n1)c4ccc5C(=O)C=C(NC=O)C(=O)c5n4	7100	nM
CHEMBL264639	COC(=O)c1cc(cc(C)c1OC)C(=CCCCC(=O)N2CCCCC2)c3cc(C)c(OC)c(c3)C(=O)OC	7120	nM
CHEMBL142532	COC(=O)CCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	7200	nM
CHEMBL405279	CC1=CN(C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCNC(=O)[C@@H]4CCCN4C(=O)[C@@H](N)CC(=O)O)C1=O	7200	nM
CHEMBL290125	CCC(C)Sc1nc(O)cc(Cc2ccc3ccccc3c2)n1	7400	nM
CHEMBL415703	CCC(C)Sc1nc(O)cc(Cc2ccc(F)cc2)n1	7400	nM
CHEMBL85745	CCc1cc(NCc2ccc(OC)cc2)c(O)nc1C	7500	nM
CHEMBL192976	Oc1nc2ccc(Cl)cc2n1Cc3c(Cl)cccc3Cl	7500	nM
CHEMBL1807350	Clc1ccccc1c2nc3ccc4ccccc4n3c2NC5CCCCC5	7520	nM
CHEMBL194923	COC(=O)CCC\C=C(/c1cccc(c1)C#N)\c2cc(Cl)ccc2OC	7580	nM
CHEMBL72272	CCN1c2ccccc2N(C)C(=O)c3cc(Cl)cnc13	7600	nM
CHEMBL387003	COc1noc2c(C)cc(cc12)\C(=C/CCN3CCOC3=O)\c4cc(C)c5ON(C)C(=O)c5c4	7600	nM
CHEMBL290204	Cc1nnc2c3cccnc3N(C4CC4)c5ncccc5n12	7820	nM
CHEMBL302957	CCN1C(=O)c2cccnc2N(CC)c3cccc(C)c13	8000	nM
CHEMBL84266	Cc1cccc2c1C(=O)N3CCSC23c4ccccc4	8000	nM
CHEMBL174899	Cc1nc(O)c(CCc2oc3ccccc3n2)cc1C(=O)N	8000	nM
CHEMBL151791	COc1cc(OC)c2CC(COc2c1)OC(=O)c3cc(O)c(O)c(O)c3	8094.44	nM
CHEMBL144209	COC(=O)c1cc(cc(Cl)c1OC)C(=CCC2OCCO2)c3cc(Cl)c(OC)c(c3)C(=O)OC	8099.38	nM
CHEMBL417311	CCC(C)Sc1nc(O)cc(Cc2cccc3ccccc23)n1	8100	nM
CHEMBL380100	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCN)C1=O	8100	nM
CHEMBL379994	CC1=CN(C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCNC(=O)[C@@H]4CCCN4C(=O)[C@@H](N)Cc5ccc(O)cc5)C1=O	8100	nM
CHEMBL107946	Oc1ncccc1C(OCc2ccncc2)(C#CC3CC3)C(F)(F)F	8115	nM
CHEMBL36479	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NS(=O)(=O)C(F)(F)F)ccc4[nH]3	8300	nM
CHEMBL326205	CCCOC(=O)CCCC=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	8300	nM
CHEMBL419025	CC(C)CSc1nc(O)cc(Cc2cccc(C)c2)n1	8400	nM

CHEMBL175235	CCc1cc(CCc2ccc3ccccc3c2)c(O)nc1C	8400	nM
CHEMBL88591	OC(=O)c1cc(I)ccc1NC(=O)CCCC(=O)Nc2ccc(I)cc2C(=O)O	8500	nM
CHEMBL347255	CCC(C)Sc1nc(O)c(C)c(Cc2ccc(Cl)cc2)n1	8500	nM
CHEMBL386338	COC(=O)CCC\C=C(\c1cccc(c1)C#N)/c2cc(C)c3OC(=O)N(C)c3c2	8597.67	nM
CHEMBL163536	O=C1c2ccccc2C34CC=CC[C@@]13c5ccccc5C4=O	8700	nM
CHEMBL89524	OC(=O)c1cc(Cl)ccc1NC(=O)CCCC(=O)Nc2ccc(Cl)cc2C(=O)O	8848.73	nM
CHEMBL73568	CN1C(=O)c2cccnc2N(Cc3ccccc3)c4ccccc14	9000	nM
CHEMBL134252	C[C@H]1Oc2c3C=CC(C)(C)Oc3c4C(=CC(=O)Oc4c2C=C1C)c5ccccc5	9000	nM
CHEMBL323016	CCCOC(=O)CCCC=C(c1cc(Br)c(OC)c(c1)C(=O)OC)c2cc(Br)c(OC)c(c2)C(=O)OC	9150	nM
CHEMBL109213	CC(C)CSc1nc(O)cc(Cc2ccccc2)n1	9400	nM
CHEMBL132790	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCN2CCOC2=O)c3cc(Cl)c(OC)c(c3)C(=O)OC	9470	nM
CHEMBL157342	O[C@@H]1[C@@H](O)[C@H](Oc2cc(Cl)cc3c2NC(=O)O[C@]3(C#CC4CC4)C(F)(F)F)O[C@@H]([C@H]1O)C(=O)O	9489	nM
CHEMBL338873	CCc1cc(NCC2CCCc3ccccc23)c(O)nc1C	9500	nM
CHEMBL36031	CCc1c(O)nc(SCSC)nc1Cc2ccccc2	9700	nM
CHEMBL215346	COC(=O)c1cc(cc(C)c1OC)\C(=C/CCN2CCOC2=O)\c3cc(C)c4ON(C)C(=O)c4c3	9860	nM
CHEMBL82628	O=C1N2CCSC2(c3ccccc3)c4cc5ccccc5cc14	10000	nM
CHEMBL83640	CC(C)c1ccc(cc1)C23SCCN2C(=O)c4ccccc34	10000	nM
CHEMBL82621	CCc1cc(NCc2cnccc2OC)c(O)nc1C	10000	nM
CHEMBL91318	CC1(Oc2ccccc2n3cccc3C1=O)c4ccccc4	10000	nM
CHEMBL88213	CCCC1(CC)Oc2ccccc2n3cccc3C1=O	10000	nM
CHEMBL340658	CCc1cc(NCc2oc3cc4ccccc4cc3n2)c(O)nc1C	10000	nM
CHEMBL131432	CCCCCC=C(c1cc(F)c(OC)c(c1)C(=O)OC)c2cc(F)c(OC)c(c2)C(=O)OC	10000	nM
CHEMBL145842	CCC1(CCCC=C(c2cc(Cl)c(OC)c(CO)c2)c3cc(Cl)c(OC)c(CO)c3)OCCO1	10055.84	nM
CHEMBL88463	COc1ccc(NC(=O)CCCC(=O)Nc2ccc(OC)O)c(c1)C(=O)O	10600	nM
CHEMBL1807337	Cc1cccn2c(NC3CCCCC3)c(nc12)c4ccccc4Cl	10681.3	nM
CHEMBL39505	CN1C(=O)c2cccnc2N(c3ncccc13)C(C)(C)C	11000	nM
CHEMBL305535	CCCCCC=C(c1cc(I)c(OC)c(c1)C(=O)OC)c2cc(I)c(OC)c(c2)C(=O)OC	11000	nM
CHEMBL122978	CCC1=C(C)N(C)C(=O)C(=C1)NCc2ccc3ccccc3c2	11000	nM
CHEMBL3142920	COC(=O)P(=O)(OC)OCCCN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	11000	nM
CHEMBL3143763	[I-].CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CCC[N+](C)(C)C)C1=O	11000	nM
CHEMBL363624	CC(=CCc1c(O)cc(O)c2C(=CC(=O)Oc12)c3ccccc3)C	11200	nM
CHEMBL1807343	Fc1ccc2nc(c(NC3CCCCC3)n2c1)c4ccccc4Cl	11280	nM
CHEMBL410036	CC(=O)OCCOCN1C(=O)NC(=O)C2=C1Sc3ccccc3NC2	11500	nM
CHEMBL89674	OC(=O)c1cc(ccc1NC(=O)CCCC(=O)Nc2ccc(cc2C(=O)O)C(F)(F)F)C(F)(F)F	12000	nM
CHEMBL408333	CC(C)[C@H](N)C(=O)N1CCC[C@@H]1C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(=O)C=C4N)C3O[Si](C)(C)C(C)(C)C	12049.9	nM
CHEMBL1807346	Clc1ccccc1c2nc3ccc(Br)cn3c2NC4CCCCC4	12200	nM
CHEMBL76986	CCCON1C(=O)NC(=O)C(=C1Sc2cc(C)cc(C)c2)C(C)C	12300	nM
CHEMBL83301	CCc1cc(NCc2ccccc2C(F)(F)F)c(O)nc1C	12500	nM
CHEMBL312160	Oc1cccc(c1)C23SCCN2C(=O)c4ccccc34	12700	nM
CHEMBL152355	CC(=O)NC1=CC(=O)c2ccc(nc2C1=O)c3[nH]c(cc4c5ccccc5nc34)C(=O	12700	nM

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CHEMBL362924	Oc1nc2ccc(Cl)cc2n1Cc3cccc4ccccc34	12700	nM
CHEMBL48690	CCN1c2ncccc2c3nccn3c4ccc(O)nc14	12915.96	nM
CHEMBL417737	C[C@@H](\N=C(/S)\Nc1nccs1)C2CCCCC2	13000	nM
CHEMBL316466	CCC(C)Sc1nc(O)c(C)c(Cc2ccc(F)cc2)n1	13000	nM
CHEMBL213365	CC1=CN(C2OC(CO[Si](C)(C)C(C)(C)C)C3(OS(=O)(=O)C=C3N)C2O[Si](C)(C)C(C)(C)C)C(=O)N(CCCNC(=O)[C@@H]4CCCN4C(=O)CN)C1=O	13000	nM
CHEMBL346794	CC(=O)NC1=CC(=O)c2ccc(nc2C1=O)c3[nH]c(cc4c5ccccc5nc34)C(=O)O	13300	nM
CHEMBL177074	CCc1cc(CCc2oc3ccncc3c2)c(O)nc1C	13500	nM
CHEMBL59279	C[C@H]1Cn2c(S)nc3ccc(C)c(CN1CC=C(C)C)c23	13600	nM
CHEMBL89744	Cc1ccc(NC(=O)CCCCC(=O)Nc2ccc(C)cc2C(=O)O)c(c1)C(=O)O	14000	nM
CHEMBL341238	Cc1nc(CCCCCCCc2ccccc2)n3nc(Cl)ccc13	14000	nM
CHEMBL1807344	Clc1ccc2nc(c(NC3CCCCC3)n2c1)c4ccccc4Cl	14470	nM
CHEMBL625	c1ccc2[nH]c(nc2c1)c3cscn3	14600	nM
CHEMBL67095	CN1CC2=C(Sc3ccccc13)N(COCCOC(=O)C)C(=O)NC2=O	14700	nM
CHEMBL82454	O=C1N2CCCC2(c3ccccc3)c4ccccc14	15000	nM
CHEMBL314121	OC(=O)c1cc(Br)ccc1NC(=O)CCCCC(=O)Nc2ccc(Br)cc2	15000	nM
CHEMBL88458	OC(=O)c1cc(Br)ccc1NC(=O)Cc2ccccc2)C(=O)Nc3ccc(Br)cc3C(=O)O	15000	nM
CHEMBL313804	CCC1(Sc2ccccc2n3cccc3C1=O)c4ccccc4	15000	nM
CHEMBL379599	CC1=CN([C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C)C(=O)N(CC(=O)O)C1=O	15000	nM
CHEMBL347211	COC(=O)c1[nH]c(c2ccc3C(=O)C=C(NC(=O)C)C(=O)c3n2)c4nc5ccccc5c4c1C	15100	nM
CHEMBL290781	CN1C(=O)c2cccnc2N(C(=O)C)c3ncccc13	15300	nM
CHEMBL57772	Fc1cccc(F)c1Cn2c(nc3ccccc23)c4ccccc4	16000	nM
CHEMBL63680	COC(=O)C=C(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	16000	nM
CHEMBL72920	CCOC(=O)CN1c2ccccc2N(C)C(=O)c3cccnc13	16000	nM
CHEMBL340145	Nc1cc(Cl)nc(SCC2=CCCc3ccccc23)n1	16000	nM
CHEMBL176982	CCc1cc(CCCc2oc3ccccc3n2)c(O)nc1C	16000	nM
CHEMBL379485	CC(C)[C@H](N)C(=O)N1C[C@H](O)C[C@H]1C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(=O)C=C4N)C3O[Si](C)(C)C(C)(C)C	16000	nM
CHEMBL192499	CC(C)c1ccc(Cn2c(O)nc3ccc(Cl)cc23)cc1	16200	nM
CHEMBL347273	Oc1ccc2CC(COc2c1)OC(=O)c3cc(O)c(O)c(O)c3	16609.64	nM
CHEMBL59133	OC(c1ccn(c1)S(=O)(=O)c2ccc(Cl)cc2)c3ccc(Cl)cc3Cl	17000	nM
CHEMBL309921	O=C1N2CCSC2(c3ccccc3)c4cnccc14	17000	nM
CHEMBL301913	Cc1ccc(cc1)S(=O)(=O)n2ccc(c2)C(O)c3ccc(Cl)cc3Cl	18000	nM
CHEMBL132691	Fc1cccc(F)c1c2nc3ccccc3n2Cc4ccccc4	18600	nM
CHEMBL32386	CSCSc1nc(O)c(C)c(Cc2ccccc2)n1	18800	nM
CHEMBL90333	CSc1ccc(NC(=O)CCCCC(=O)Nc2ccc(SC)cc2C(=O)O)c(c1)C(=O)O	19000	nM
CHEMBL85069	OC(=O)c1cc(Br)ccc1NC(=O)c2cccc(c2)C(=O)Nc3ccc(Br)cc3C(=O)O	19000	nM
CHEMBL151175	Oc1cc(cc(O)c1O)C(=O)OC2COc3cccc(O)c3C2	19895.98	nM
CHEMBL192310	Fc1cccc(F)c1CN2C(=O)Oc3ccc(Cl)cc23	20000	nM
CHEMBL154000	NC(=O)c1cc2c3ccccc3[nH]c2c(n1)c4ccc5C(=O)C=C(NC=O)C(=O)c5n4	20500	nM
CHEMBL315784	OC(=O)c1ccccc1NC(=O)CCCCC(=O)Nc2ccccc2C(=O)O	21000	nM
CHEMBL1807331	Clc1ccc(c(Cl)c1)c2nc3ccccn3c2NC4CCCCC4	21760	nM
CHEMBL59226	CCc1ccc(cc1)S(=O)(=O)n2ccc(c2)C(O)c3ccc(Cl)cc3Cl	22000	nM

CHEMBL123839	Cc1nc(CCCCCOC(=O)C2CCCC2)n3nc(Cl)ccc13	22000	nM
CHEMBL197138	COc1c(C(=O)CC(C)C)c(O)c(CC=C(C)C)c2OC(=O)C=C(c3ccccc3)c12	22200	nM
CHEMBL151146	Oc1cc(cc(O)c1O)C(=O)OCCc2ccccc2	22427.88	nM
CHEMBL301973	CCN1c2ncccc2c3nnnn3c4c(C)ccnc14	22464.91	nM
CHEMBL33311	CCC(C)Sc1nc(O)c(C)c(Cc2cccc3ccccc23)n1	22500	nM
CHEMBL314443	O=C1N2CCSC2(c3ccccn3)c4ncccc14	23000	nM
CHEMBL123864	CCc1cc(NCc2oc3cccc(c3n2)[N+](=O)[O-])c(O)nc1C	24500	nM
CHEMBL299935	Fc1ccc2NS(=O)(=O)NC(C#CC3CC3)(c2c1F)C(F)(F)F	24667	nM
CHEMBL328235	C=CCC1(Oc2ccccc2n3cccc3C1=O)c4ccccc4	25000	nM
CHEMBL304269	COC(=O)c1cc(cc(Br)c1OC)C(=CC)c2cc(Br)c(OC)c(c2)C(=O)OC	26000	nM
CHEMBL85270	O=C1N2CCSC2(c3ccccc3)c4c1ccc5ccccc45	26000	nM
CHEMBL34010	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(NC(=O)C(F)(F)F)ccc4[nH]3	27000	nM
CHEMBL57709	Cc1ccccc1S(=O)(=O)n2ccc(c2)C(O)c3ccc(Cl)cc3Cl	27000	nM
CHEMBL305503	CCN1c2ccc(cc2N(C)C(=O)c3cccnc13)C(=O)N	27000	nM
CHEMBL313308	O=C1N2CCSC2(c3cccnc3)c4ccccc14	28000	nM
CHEMBL83300	CCc1cc(NCc2ccccc2N)c(O)nc1C	28000	nM
CHEMBL378646	CC(C)[C@H](N)C(=O)N1C[C@@H](C[C@H]1C(=O)NCCCN2C(=O)N(C=C(C)C2=O)C3OC(CO[Si](C)(C)C(C)(C)C)C4(OS(=O)(=O)C=C4N)C3O[Si](C)(C)C(C)(C)C)OCc5ccccc5	28000	nM
CHEMBL292808	OC(c1ccn(c1)S(=O)(=O)c2ccccc2)c3ccccc3Cl	29500	nM
CHEMBL58811	C[C@H]1Cn2c(S)nc3ccc(C#C)c(CN1CC=C(C)C)c23	29500	nM
CHEMBL287025	CCC(C)Sc1nc(O)c(C)c(Cc2ccc3ccccc3c2)n1	29700	nM
CHEMBL106414	CCCOC(=O)CCCC=C(c1cc(C)c(OC)c(c1)C(=O)OC)c2cc(C)c(OC)c(c2)C(=O)OC	29700	nM
CHEMBL3143797	COC(=O)\C=C\CN1C(=O)N(C=C(C)C1=O)[C@@H]2O[C@H](CO[Si](C)(C)C(C)(C)C)[C@@]3(OS(=O)(=O)C=C3N)[C@H]2O[Si](C)(C)C(C)(C)C	30000	nM
CHEMBL333862	C[S+]([O-])c1cc(NCc2oc3ccccc3n2)c(O)nc1C	31500	nM
CHEMBL65776	COC(=O)c1cc(cc(Br)c1OC)C(=CCCO)c2cc(Br)c(OC)c(c2)C(=O)OC	31600	nM
CHEMBL144509	CCC1(CCC\C=C(\c2cc(Cl)c(OC)c(CO)c2)/c3cc(Cl)c(OC)c(C=O)c3)OCCO1	31600	nM
CHEMBL334946	C[C@H]1Oc2c3C=CC(C)(C)Oc3c4C(=CC(=O)Oc4c2C(=O)[C@@H]1C)c5ccccc5	31622.78	nM
CHEMBL383592	CC(C)C(=O)c1c(O)c(CC=C(C)C)c(O)c2C(=CC(=O)Oc12)c3ccccc3	31900	nM
CHEMBL198546	CC(C)C(=O)c1c(O)c2C(=CC(=O)Oc2c3C=CC(C)(C)Oc13)c4ccccc4	32100	nM
CHEMBL32690	Oc1cc(Cc2ccc3ccccc3c2)nc(SC4CCCCC4)n1	33100	nM
CHEMBL298981	CCN1c2ncccc2c3nnc(CC)n3c4cccnc14	33813.02	nM
CHEMBL433931	COc1ccc2NC(=S)N3C[C@H](C)N(CC=C(C)C)Cc1c23	33900	nM
CHEMBL287924	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4cc(C)ccc4[nH]3	34000	nM
CHEMBL89319	OC(=O)c1cc(Br)ccc1NC(=O)c2ccc(nc2)C(=O)Nc3ccc(Br)cc3C(=O)O	35000	nM
CHEMBL314003	CCc1cc(NCc2ccccc2COC)c(O)nc1C	35500	nM
CHEMBL58552	Clc1ccc2NS(=O)(=O)NC(C#CC3CC3)(C4CC4)c2c1	35870	nM
CHEMBL37994	CC(C)Nc1cccnc1N2CCN(CC2)C(=O)c3cc4ccc(OCc5ccccc5)cc4[nH]3	37000	nM
CHEMBL355912	Oc1cc(O)c2CC(COc2c1)OC(=O)c3ccc(O)c(O)c3	37200	nM
CHEMBL86243	C[C@@H]1CN2C(=O)c3ccccc3C2(O1)c4ccccc4	37600	nM
CHEMBL299555	CCN1c2ncccc2c3nnc(C)n3c4cccnc14	38900	nM
CHEMBL85459	O=C1N2Cc3ccccc3SC2(c4ccccc4)c5ccccc15	40000	nM
CHEMBL346225	Cc1ccc(nc1)N2C(SCC2=O)c3c(C)cccc3Cl	42400	nM
CHEMBL52500	CCN1c2ncccc2c3nncn3c4c(C)ccnc14	44500	nM
CHEMBL286313	Cc1c(O)nc(SC2CCCC2)nc1Cc3cccc4ccccc34	45000	nM
CHEMBL144096	Nc1ccc2c(cc(c(N)c2c1O)S(=O)(=O)O)S(=O)(=O)O	45000	nM

CHEMBL367515	CCc1cc(Cc2oc3ccccc3n2)c(O)nc1C	45000	nM
CHEMBL334861	C[C@H]1Oc2c3C=CC(C)(C)Oc3c4C(=CC(=O)Oc4c2[C@H]([C@H]1 C)C(=O)c5ccc(Br)cc5)c6ccccc6	46000	nM
CHEMBL36019	Oc1cc(Cc2cccc3ccccc23)nc(SC4CCCC4)n1	48700	nM
CHEMBL214489	COC(=O)CCC\C=C(/c1cc(C)c2OC(=O)N(C)c2c1)\c3cc(C)c4ON(C)C(=O)c4c3	49200	nM
CHEMBL212395	COC(=O)CCC\C=C(\c1cccc(c1)C#N)/c2cc(C)c3ON(C)C(=O)c3c2	49600	nM
CHEMBL444789	Nc1cc(c2ccccc2c1N)S(=O)(=O)O	50000	nM
CHEMBL353328	CCc1cc(CCc2ccccc2)c(O)nc1C	50000	nM
CHEMBL366202	Oc1nc2ccc(Cl)cc2n1CC3CCCCC3	50000	nM
CHEMBL302788	CCOCN1C(=O)NC(=O)C2=C1Sc3ccccc3NC2	50200	nM
CHEMBL316043	O=C1N2CCCOC2(c3ccccc3)c4ccccc14	51000	nM
CHEMBL84743	C[C@H]1COC2(N1C(=O)c3ccccc23)c4ccccc4	54037.02	nM
CHEMBL194649	COC(=O)CCC\C=C(/c1cc(C)c(OC)c(c1)C(=O)OC)\c2cc(F)cc(c2)C(F)(F)F	55300	nM
CHEMBL58506	C[C@H]1Cn2c(S)nc3ccc(C#N)c(CN1CC=C(C)C)c23	56300	nM
CHEMBL357261	Clc1cccc(Cl)c1C2SCC(=O)N2c3ccc(Br)cn3	56600	nM
CHEMBL312872	NC(=O)[C@H]1CSC2(N1C(=O)c3ccccc23)c4ccccc4	59000	nM
CHEMBL191692	Oc1nc2cc(Cl)ccc2n1Cc3c(F)cccc3F	60000	nM
CHEMBL323276	COC(=O)c1cc(cc(C)c1OC)C(=CCCCC(=O)OC(C)C)c2cc(C)c(OC)c(c2)C(=O)OC	60400	nM
CHEMBL357713	Fc1cccc(F)c1C2SCC(=O)N2c3ccc(Br)cn3	61400	nM
CHEMBL296773	CCN1c2ncccc2c3nnc(C(C)C)n3c4cccnc14	62600	nM
CHEMBL63394	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCN)c2cc(Cl)c(OC)c(c2)C(=O)OC	63000	nM
CHEMBL133842	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCNC(=O)OCC(C)C)c2cc(Cl)c(OC)c(c2)C(=O)OC	65400	nM
CHEMBL315961	OC(=O)c1cc(Br)ccc1NC(=O)c2ccnc(c2)C(=O)Nc3ccc(Br)cc3C(=O)O	66000	nM
CHEMBL339425	CCc1cc(NCc2oc3cccc(N)c3n2)c(O)nc1C	67000	nM
CHEMBL150149	Fc1cccc(F)c1C2SCC(=O)N2c3ccc(Cl)cn3	67000	nM
CHEMBL335955	C[C@H]1Oc2c([C@@H](O)[C@H]1C)c3OC(=O)C=C(c4ccccc4)c3c5O[C@H]6[C@@H](c25)C6(C)C	70000	nM
CHEMBL144121	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCCCl)c2cc(Cl)c(OC)c(c2)C(=O)OC	70000	nM
CHEMBL323259	COC(=O)c1cc(cc(Br)c1OC)C(=CCCCC(=O)OC(C)C)c2cc(Br)c(OC)c(c2)C(=O)OC	70800	nM
CHEMBL295165	CCN1c2ncccc2c3nncn3c4cccnc14	72800	nM
CHEMBL85514	O=C1N2CCCCC2(c3ccccc3)c4ccccc14	75500	nM
CHEMBL418686	COC(=O)c1cc(cc(Br)c1OC)C(=CCCN=[N+]=[N-])c2cc(Br)c(OC)c(c2)C(=O)OC	94000	nM
CHEMBL63229	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCOS(=O)(=O)C)c2cc(Cl)c(OC)c(c2)C(=O)OC	96000	nM
CHEMBL347272	Oc1cc(O)cc(c1)C(=O)OC2COc3cc(O)cc(O)c3C2	96300	nM
CHEMBL196121	COc1ccc(cc1OC)\C(=C/CCN2CCOC2=O)\c3cc(F)cc(c3)C(F)(F)F	97800	nM
CHEMBL108267	COC(=O)c1cc(cc(Br)c1OC)C(=CCCCC=C)c2cc(Br)c(OC)c(c2)C(=O)OC	99000	nM
CHEMBL32718	O=C1C(Sc2ccccc2n3cccc13)c4ccccc4	100000	nM
CHEMBL63988	COC(=O)c1cc(cc(Cl)c1OC)C(=CCCCC(=O)O)c2cc(Cl)c(OC)c(c2)C(=O)OC	100000	nM
CHEMBL330735	CCC1Oc2ccccc2n3cccc3C1=O	100000	nM
CHEMBL359242	COC(=O)CCCCC(c1cc(Cl)c(OC)c(c1)C(=O)OC)c2cc(Cl)c(OC)c(c2)C(=O)OC	100000	nM
CHEMBL367850	CCC1=C(C)NC(N)C(=C1)CCc2oc3ccccc3n2	100000	nM

8.3 Integrase training set

CHEMBL1917873	CC(C)N1C(=O)C(=C(O)c2ncccc12)C(=O)NCc3ccc(F)cc3	1	nM
CHEMBL3806067	NC(=O)c1c2[C@H]3CCCCN3C(=O)c2c(O)c4ncc(Cc5cccc(Cl)c5F)cc14	1.1	nM
CHEMBL454633	Oc1c(nc(N2CCCCS2(=O)=O)c3cccnc13)c4oc(Cc5ccc(F)cc5)nn4	2	nM
CHEMBL492465	CN(C)C1(CCOCC1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	2	nM
CHEMBL549422	CC1(C)N(Cc2nnn[nH]2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	2	nM
CHEMBL556894	Cn1cc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)nn1	2	nM
CHEMBL2316125	C[C@H](O)CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	2	nM
CHEMBL2403116	OC1=C2N(C[C@@H]3OCCCN3C2=O)C=C(C(=O)NCc4ccc(F)cc4)C1=O	2	nM
CHEMBL1213165	[Na+].C[C@@H]1CCO[C@H]2CN3C=C(C(=O)NCc4ccc(F)cc4F)C(=O)C(=C3C(=O)N12)[O-]	2.7	nM
CHEMBL1229211	C[C@@H]1CCO[C@H]2CN3C=C(C(=O)NCc4ccc(F)cc4F)C(=O)C(=C3C(=O)N12)O	2.7	nM
CHEMBL1773312	ON1CCc2c(ncc3c2ccn3Cc4ccc(F)cc4)C1=O	2.9	nM
CHEMBL492464	CN1C(=O)C(=C(N=C1C(C)(C)N2CCOCC2)C(=O)NCc3ccc(F)cc3)O	3	nM
CHEMBL559395	CC1(C)N(Cc2cocn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	3	nM
CHEMBL550051	CC1(C)N(CCN2CCOCC2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	3	nM
CHEMBL2316116	CC(C)(CO)NC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	3	nM
CHEMBL2403238	C[C@H]1CO[C@@H]2CN3C=C(C(=O)NCc4ccc(F)cc4F)C(=O)C(=C3C(=O)N12)O	3	nM
CHEMBL3310085	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC4CC4	3	nM
CHEMBL3360113	CSC1COCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	3	nM
CHEMBL3360128	COCCCN1CCN(C1=O)c2cc(F)ccc2CNC(=O)C3=C(O)C(=O)N(C)C(=N3)C4CCOC4	3	nM
CHEMBL2316126	C[C@@H](CO)CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	3.46	nM
CHEMBL242926	CN(C)CC(=O)N1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	4	nM
CHEMBL412149	COc1cc(\C=C/2\C(=NN(C2=O)c3nnn[nH]3)C)cc(Cl)c1OC	4	nM
CHEMBL429327	CCOc1cc(\C=C/2\C(=NN(C2=O)c3nnn[nH]3)C)cc(Cl)c1OCC	4	nM
CHEMBL522802	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	4	nM
CHEMBL491336	CCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	4	nM
CHEMBL491347	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	4	nM
CHEMBL480904	COc1ccccc1CCN2CC(=C(O)C2=O)C(=O)NCc3ccc(F)cc3	4	nM
CHEMBL522374	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)C(=O)O)C(=O)NCc2ccc(F)cc2)O	4	nM
CHEMBL517428	CN(C)C(=O)C(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2S(=O)(=O)C	4	nM
CHEMBL517136	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2nnc(C)[nH]2)C(=O)NCc3ccc(F)cc3)O	4	nM
CHEMBL549592	CN1CCN(CC1(C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)C	4	nM
CHEMBL558051	CC1(C)N(Cc2ocnc2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	4	nM
CHEMBL1914460	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCc4ccc(F)cc4	4	nM
CHEMBL2316111	CN(CCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O)S(=O)(=O)C	4	nM

CHEMBL2316118	CC(C)(CO)CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	4	nM
CHEMBL2316136	OC1=C(C(=O)NCCCN2CCCC2=O)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	4	nM
CHEMBL3310087	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N(C)C)C1=O	4	nM
CHEMBL3360111	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3)O	4	nM
CHEMBL3360121	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3n4cncn4)O	4	nM
CHEMBL2311585	C[C@H](O)CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	4.24	nM
CHEMBL3309906	CCN(CC)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC	4.4	nM
CHEMBL3310078	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC4CC4)C1=O	4.4	nM
CHEMBL2316114	C[C@H](CO)NC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	4.47	nM
CHEMBL3310413	COCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N4CCCCC4)C1=O	4.7	nM
CHEMBL1256978	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCO	4.93	nM
CHEMBL406595	Nc1c2C=C(C(=O)O)C(=O)Nc2sc1C(=O)Nc3ccc(Cl)c(Cl)c3	5	nM
CHEMBL407352	OC(=O)CSc1nnc(c2occc2)c(n1)c3occc3	5	nM
CHEMBL272420	COc1ccc(\C=C/2\C(=NN(C2=O)c3nnn[nH]3)C)cc1OCc4ccccc4Cl	5	nM
CHEMBL492188	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	5	nM
CHEMBL481094	OC1=C(CN(CCCc2ccccc2)C1=O)C(=O)NCc3ccc(F)cc3	5	nM
CHEMBL563502	CC1(C)N(Cc2ccccc2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	5	nM
CHEMBL559537	CC1(C)N(Cc2ccn[nH]2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	5	nM
CHEMBL560387	CC1=C(C=C2C(CCC(CC#N)C2(C)C)C1=C)C(=C)CCc3ccc(C)cc3	5	nM
CHEMBL550985	Cn1nnnc1CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O	5	nM
CHEMBL552065	CC1(C)NC(=O)CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL554284	Cc1oc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)nn1	5	nM
CHEMBL557854	CC(=O)N1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL558641	CC1(C)N(CC(=O)N)CCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL2315830	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCN4CCNC4=O	5	nM
CHEMBL2315831	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCNC(=O)C	5	nM
CHEMBL2315832	CN(CCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O)S(=O)(=O)C	5	nM
CHEMBL2316113	CSCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	5	nM
CHEMBL2316119	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCC(F)F	5	nM
CHEMBL2316120	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCCO	5	nM
CHEMBL2316129	CC(C)CCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	5	nM
CHEMBL2316132	OCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	5	nM
CHEMBL2403118	C[C@@H]1CCN2[C@H](CN3C=C(C(=O)NCc4ccc(F)cc4)C(=O)C(=C3C2=O)O)O1	5	nM
CHEMBL3360114	CN1C(=O)C(=C(N=C1C2(C)CCCO2)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL3360115	CN1C(=O)C(=C(N=C1C2(C)CCCS2)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL3360116	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3)O	5	nM
CHEMBL2042548	OC(=O)\C(=C\C(=O)C1=CC(=CN(Cc2ccc(F)cc2F)C1=O)Cc3ccc(F)cc3F)\O	5.5	nM
CHEMBL2316121	C[C@H](CO)NC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(C)C1=O	5.66	nM
CHEMBL3310084	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NOC)C1=O	5.7	nM
CHEMBL3310086	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCO	5.7	nM

CHEMBL521793	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	6	nM
CHEMBL519936	Cc1cccc(CN2CC(=C(O)C2=O)C(=O)NCc3ccc(F)cc3)c1	6	nM
CHEMBL462045	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2c[nH]cn2)C(=O)NCc3ccc(F)cc3)O	6	nM
CHEMBL560251	Cn1nncc1CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O	6	nM
CHEMBL561467	CC1(C)N(Cc2cnccn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	6	nM
CHEMBL560322	CC1(C)N(Cc2cnn[nH]2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	6	nM
CHEMBL550784	Cc1onc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)n1	6	nM
CHEMBL564212	CN(C)C(=O)C(=O)N1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	6	nM
CHEMBL549831	Cn1nnc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)n1	6	nM
CHEMBL559306	CN1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	6	nM
CHEMBL1914553	COc1ccccc1CNC(=O)C2=C(O)c3ncc(Cc4ccc(F)cc4)cc3NC2=O	6	nM
CHEMBL1917874	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(C3CCCC3)c4cccnc14	6	nM
CHEMBL1917876	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	6	nM
CHEMBL2043144	OC(=O)\C(=C\C(=O)C1=CC(=CN(Cc2ccccc2F)C1=O)Cc3ccc(F)cc3F)\O	6	nM
CHEMBL2316123	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC(C)(C)CO	6	nM
CHEMBL2316128	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCCN4CCCC4	6	nM
CHEMBL3360112	CN1C(=O)C(=C(N=C1C2COCC2O)C(=O)NCc3ccc(F)cc3)O	6	nM
CHEMBL3360124	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3c4ncnn4C)O	6	nM
CHEMBL3360127	CN1CCN(C1=O)c2cc(F)ccc2CNC(=O)C3=C(O)C(=O)N(C)C(=N3)C4CCOC4	6	nM
CHEMBL3360132	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3n4cncn4)O	6	nM
CHEMBL3360137	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3N4CC(C)(C)N(C)S4(=O)=O)O	6	nM
CHEMBL3310092	C[C@@H](O)CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N(C)C)C1=O	6.14	nM
CHEMBL3310409	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC(C)C)C1=O	6.2	nM
CHEMBL3310090	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC(C)(C)CO	6.5	nM
CHEMBL3310082	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCCOC)C1=O	6.8	nM
CHEMBL3310079	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC(C)(C)C)C1=O	6.9	nM
CHEMBL243151	CN1CCN(CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)S(=O)(=O)c4ccccc4	7	nM
CHEMBL246744	CNC(=O)Cc1ccccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	7	nM
CHEMBL492667	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)C)C(=O)NCc2ccc(F)cc2)O	7	nM
CHEMBL518491	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2ncccn2)C(=O)NCc3ccc(F)cc3)O	7	nM
CHEMBL460771	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2ocnc2)C(=O)NCc3ccc(F)cc3)O	7	nM
CHEMBL561729	CC1(C)N(CC(=O)N2CCOCC2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	7	nM
CHEMBL561987	CC1(C)NS(=O)(=O)CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	7	nM
CHEMBL557646	CC1(C)N(Cc2cn[nH]c2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	7	nM
CHEMBL557308	CC1(C)N(CC(=O)N2CCCC2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	7	nM

	Cn1nccc1CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O		
CHEMBL558121		7	nM
CHEMBL1914551	COc1ccc(CNC(=O)C2=C(O)c3ncc(Cc4ccc(F)cc4)cc3NC2=O)cc1	7	nM
CHEMBL2316124	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC4(CO)CCCC4	7	nM
CHEMBL2316137	OC1=C(C(=O)NCCN2CCOCC2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	7	nM
CHEMBL518520	[K+].CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2oc(C)nn2)C(=O)NCc3cc c(F)cc3)[O-]	7.04	nM
CHEMBL3310081	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCC(F)(F)F)C1= O	7.1	nM
CHEMBL3310097	COCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC4CC4)C 1=O	7.3	nM
CHEMBL3309903	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N)C1=O	7.6	nM
CHEMBL3310414	COCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N4CCOCC4)C1=O	7.6	nM
CHEMBL3310095	COCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N)C1=O	7.7	nM
CHEMBL3310077	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC(C)C)C1=O	7.8	nM
CHEMBL3310088	C[C@H](CO)NC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N(C) C)C1=O	7.81	nM
CHEMBL524164	CN1C(=O)C(=C(N=C1C(C)(C)NS(=O)(=O)C)C(=O)NCc2ccc(F)cc2)O	8	nM
CHEMBL460977	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2cscn2)C(=O)NCc3ccc(F)cc3) O	8	nM
CHEMBL562327	CC1(C)N(CC(=O)O)CCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3) O	8	nM
CHEMBL563631	Cc1oc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)n c1	8	nM
CHEMBL550997	CN(C)S(=O)(=O)N1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	8	nM
CHEMBL551808	CN(C)C(=O)CN1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)c c3)O	8	nM
CHEMBL1914554	COc1ccc(CNC(=O)C2=C(O)c3ncc(Cc4ccc(F)cc4)cc3NC2=O)cc1OC	8	nM
CHEMBL1914564	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(CC(=O)N3CCOCC3)c4cc(Cc5 ccc(F)cc5)cnc14	8	nM
CHEMBL2316138	OC1=C(C(=O)NCCCN2CCOCC2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	8	nM
CHEMBL3310080	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCC4CC4)C1=O	8	nM
CHEMBL3360129	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3S(=O)(=O)C) O	8	nM
CHEMBL3360133	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3n4ncnc4C)O	8	nM
CHEMBL3309268	CCNC(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC	8.2	nM
CHEMBL3310098	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NC4CCC4) C1=O	8.5	nM
CHEMBL3310094	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCC N4CCOCC4	8.6	nM
CHEMBL1773408	CC(C)(O)CCc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	8.8	nM
CHEMBL461405	CN(C)C(=O)C(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc (F)c(Cl)c2	9	nM
CHEMBL523678	CC1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	9	nM
CHEMBL564823	CC1(C)N(Cc2cscn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4) O	9	nM
CHEMBL552202	CC1(C)N(Cc2ccccn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4) O	9	nM
CHEMBL552264	Cn1ccc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O) n1	9	nM
CHEMBL2316112	OC1=C(C(=O)NC2CCS(=O)(=O)CC2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc1 3	9	nM
CHEMBL2316130	CCOCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	9	nM

108

CHEMBL2316131	CC(C)OCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	9	nM
CHEMBL3310096	CNC(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCOC	9	nM
CHEMBL3360118	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3S(=O)(=O)C)O	9	nM
CHEMBL3360120	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3N4CCCCS4(=O)=O)O	9	nM
CHEMBL3360135	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3c4ncnn4C)O	9	nM
CHEMBL3310076	CCCNC(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC	9.2	nM
CHEMBL3309904	CNC(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC	9.3	nM
CHEMBL3309905	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N(C)C)C1=O	9.3	nM
CHEMBL3805726	NC(=O)c1c2C[C@H]3CCCN3C(=O)c2c(O)c4ncc(Cc5cccc(Cl)c5F)cc14	9.49	nM
CHEMBL32865	Oc1c(ncc2cccnc12)C(=O)c3cc(CN4CCCS4(=O)=O)cc(Cc5ccccc5)c3	10	nM
CHEMBL216874	Oc1nc(nc(C(=O)NCc2ccc(F)cc2)c1O)c3cccs3	10	nM
CHEMBL232226	Oc1nc(nc(C(=O)Nc2cc3ccccc3s2)c1O)c4cccs4	10	nM
CHEMBL232446	Oc1nc(nc(C(=O)NCc2ccc(Cl)c(Cl)c2)c1O)c3cccs3	10	nM
CHEMBL240692	CCOC(=O)c1cn2CCN(Cc3ccc(Cl)c(Cl)c3)C(=O)c2c1O	10	nM
CHEMBL428565	OC(=O)c1cn2CCN(Cc3cccc(Cl)c3)C(=O)c2c1O	10	nM
CHEMBL246535	Oc1c(nc(N2CCCCS2(=O)=O)c3cccnc13)C(=O)NCc4ccccc4	10	nM
CHEMBL245519	NS(=O)(=O)c1cc(F)ccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	10	nM
CHEMBL245719	CNC(=O)c1cc(F)ccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	10	nM
CHEMBL407651	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2)O	10	nM
CHEMBL259573	CCOc1ccccc1CNC(=O)c2nc(nc(O)c2O)C(C)(C)C	10	nM
CHEMBL259779	CC(C)(C)c1nc(O)c(O)c(n1)C(=O)NCc2cccc3cc[nH]c23	10	nM
CHEMBL259780	CC(C)(C)c1nc(O)c(O)c(n1)C(=O)NCc2ccc(F)cc2	10	nM
CHEMBL495331	CN(C)C(=O)C(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	10	nM
CHEMBL457616	CC(C)N1C[C@H](C)n2c3C=NN(Cc4ccc(F)cc4)C(=O)c3c(O)c2C1=O	10	nM
CHEMBL456356	CC(C)N1C[C@H](C)n2c3C(=NN(Cc4ccc(F)cc4)C(=O)c3c(O)c2C1=O)C	10	nM
CHEMBL554737	CC1(C)N(CCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O)S(=O)(=O)C	10	nM
CHEMBL1088058	Oc1nc(nc(C(=O)NCc2cc3ccccc3s2)c1O)c4cccs4	10	nM
CHEMBL1914552	COc1cccc(CNC(=O)C2=C(O)c3ncc(Cc4ccc(F)cc4)cc3NC2=O)c1	10	nM
CHEMBL2171671	OC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	10	nM
CHEMBL3360117	CN1C(=O)C(=C(N=C1C2CCCCO2)C(=O)NCc3ccc(F)cc3)O	10	nM
CHEMBL3360119	CN(C)S(=O)(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C3CCOC3	10	nM
CHEMBL3360123	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3n4nncc4C)O	10	nM
CHEMBL3360126	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3N4CC(C)(C)N(C)S4(=O)=O)O	10	nM
CHEMBL3582062	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2F)c3ccccc3C1=O)\O	10	nM
CHEMBL452588	Oc1c(nc(N2CCCCS2(=O)=O)c3cccnc13)c4nnc(Cc5ccc(F)cc5)[nH]4	11	nM
CHEMBL1773322	ON1CCc2c(ncc3c2c(CN4CCC(F)(F)C4)cn3Cc5ccc(F)cc5)C1=O	11	nM
CHEMBL1773324	ON1CCc2c(ncc3c2c(COCc4ccccn4)cn3Cc5ccc(F)cc5)C1=O	11	nM
CHEMBL2316133	OCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	11	nM
CHEMBL2316139	CN1CCN(CCCNC(=O)C2=C(O)c3ncc(Cc4ccc(F)cc4)cc3NC2=O)CC1	11	nM
CHEMBL3310410	COCCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCC(F)(F)F)C1=O	11	nM
CHEMBL3360131	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3N4CCCCS4(=O)=O)O	11	nM
CHEMBL242924	CN1CCN(CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)	12	nM

	c4ccccc4		
CHEMBL493295	CN(C)S(=O)(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	12	nM
CHEMBL521567	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cccc(F)c2F)c3cccc(OC)c13)\O	12	nM
CHEMBL551325	CC1(C)N(CCc2ccccn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	12	nM
CHEMBL1773323	ON1CCc2c(ncc3c2c(COCCc4ccccn4)cn3Cc5ccc(F)cc5)C1=O	12	nM
CHEMBL3360122	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3n4ncnc4C)O	12	nM
CHEMBL3360130	CN(C)S(=O)(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C3CCOCC3	12	nM
CHEMBL243365	CN(C)S(=O)(=O)N1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	12.65	nM
CHEMBL272194	CC1=NN(C(=O)/C/1=C\c2cc(Cl)c(O)c(Cl)c2)c3nnn[nH]3	13	nM
CHEMBL552177	Cc1noc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)n1	13	nM
CHEMBL1773405	ON1CCc2c(ncc3c2c(CCC(=O)O)cn3Cc4ccc(F)cc4)C1=O	13	nM
CHEMBL1773406	ON1CCc2c(ncc3c2c(CCCN4CCOCC4)cn3Cc5ccc(F)cc5)C1=O	13	nM
CHEMBL1773410	ON1CCc2c(ncc3c2c(CCC(F)(F)F)cn3Cc4ccc(F)cc4)C1=O	13	nM
CHEMBL1773413	CN(C)S(=O)(=O)c1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	13	nM
CHEMBL1917872	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)Nc3cccnc13	13	nM
CHEMBL1917875	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)Nc3cc(Cc4ccccc4)cnc13	13	nM
CHEMBL2315829	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCN4CCOCC4	13	nM
CHEMBL3309907	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N4CCCC4)C1=O	13	nM
CHEMBL3360134	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3n4nncc4C)O	13	nM
CHEMBL394786	CN1CCN(CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)C	13.86	nM
CHEMBL394251	CN(C)C(=O)Cc1ccccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	14	nM
CHEMBL476564	CCN1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	14	nM
CHEMBL461259	COc1c2CNC(=O)c2c(O)c3ncc(Cc4ccc(F)cc4)cc13	14	nM
CHEMBL563757	CC(=O)N1CCCCC1(C)C2=NC(=C(O)C(=O)N2)C(=O)NCc3cccc(F)cc3	14	nM
CHEMBL1773401	ON1CCc2c(ncc3c2c(COCC4CCOCC4)cn3Cc5ccc(F)cc5)C1=O	14	nM
CHEMBL1773403	ON1CCc2c(ncc3c2c(COCCCc4ccccn4)cn3Cc5ccc(F)cc5)C1=O	14	nM
CHEMBL1773407	CN(CCCc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13)C(=O)C	14	nM
CHEMBL1773409	ON1CCc2c(ncc3c2c(CCCOC4CCOCC4)cn3Cc5ccc(F)cc5)C1=O	14	nM
CHEMBL1914562	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(CCN3CCCC3=O)c4cc(Cc5ccc(F)cc5)cnc14	14	nM
CHEMBL2316134	OC1=C(C(=O)NCCN2CCCCC2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	14	nM
CHEMBL3125979	ON1C(=O)C(=Cc2cccnc12)C(=O)NCc3ccc(F)c(Cl)c3	14	nM
CHEMBL497501	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cccc(cc3C1=O)C(=O)\C=C(/O)\C(=O)O)\O	14.28	nM
CHEMBL389829	CN1C(=O)C(=C(N=C1C2COCCN2C(=O)C)C(=O)NCc3cccc(F)cc3)O	15	nM
CHEMBL495332	COC(=O)C(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	15	nM
CHEMBL493920	CN(C)C(=O)C(=O)N(C)C(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	15	nM
CHEMBL460770	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2cccnn2)C(=O)NCc3ccc(F)cc3)O	15	nM
CHEMBL550108	CCNC(=O)N1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	15	nM
CHEMBL1773318	CN(CCO)Cc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	15	nM
CHEMBL1773319	ON1CCc2c(ncc3c2c(CN4CCCCC4)cn3Cc5ccc(F)cc5)C1=O	15	nM
CHEMBL2236599	OC(=O)\C(=C\C(=O)C1=CN(Cc2cccc(F)c2)c3cccccc3C1=O)\O	15	nM

CHEMBL550394	CC1(C)NCCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	16	nM
CHEMBL1773404	ON1CCc2c(ncc3c2c(COCc4ccccc4F)cn3Cc5ccc(F)cc5)C1=O	16	nM
CHEMBL2315828	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCCCN4CCCC4=O	16	nM
CHEMBL3360125	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3N4CCN(C(C)(C)C)S4(=O)=O)O	16	nM
CHEMBL3582057	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2F)c3ccccc3C1=O)\O	16	nM
CHEMBL406596	Cc1ccc(cc1NC(=O)CSc2nc3ccccc3s2)C(=O)O	17	nM
CHEMBL558661	OC(=O)C(=O)CC(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(cc3C1=O)C(=O)CC(=O)C(=O)O	17	nM
CHEMBL1773316	ON1CCc2c(ncc3c2ccn3Cc4ccc(F)c(Cl)c4C#N)C1=O	17	nM
CHEMBL1773402	CC(C)OCCOCc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	17	nM
CHEMBL1914556	CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NCc4ccc(F)cc4	17	nM
CHEMBL3125980	ON1C(=O)C(=Cc2cccnc12)C(=O)NCc3ccc(F)c(F)c3	17	nM
CHEMBL3360136	CN1C(=O)C(=C(N=C1C2CCOCC2)C(=O)NCc3ccc(F)cc3N4CCN(C(C)(C)C)S4(=O)=O)O	17	nM
CHEMBL564267	CN1CCN(CC1(C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)S(=O)(=O)C	17.32	nM
CHEMBL261833	OC(=O)c1ccccc1NC(=O)c2ccccc2S(=O)(=O)Nc3ccc(Oc4ccccc4)cc3	18	nM
CHEMBL481296	OC1=C(C2CCCCN2C1=O)C(=O)NCc3ccc(F)cc3	18	nM
CHEMBL505332	CN(C)C(=O)NC(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	18	nM
CHEMBL492930	OC1=C(N=C2N(C=CC=C2NC(=O)c3ccccc3)C1=O)C(=O)NCc4ccc(F)cc4	18	nM
CHEMBL494944	CCCN(C(=O)C(=O)N(C)C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	18	nM
CHEMBL523833	CCN(C(=O)c1oncc1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	18	nM
CHEMBL1773314	ON1CCc2c(ncc3c2ccn3Cc4ncc(F)cc4F)C1=O	18	nM
CHEMBL1914557	CCCN1C(=O)C(=C(O)c2ncc(Cc3ccccc3)cc12)C(=O)NCc4ccc(F)cc4	18	nM
CHEMBL2171670	COC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	18	nM
CHEMBL3352894	CN1C(=O)C(=C(N=C1C2CCOC2)C(=O)NCc3ccc(F)cc3c4nncn4C)O	18	nM
CHEMBL3582070	OC(=O)\C(=C\C(=O)C1=CN(Cc2cccc(Cl)c2F)c3ccccc3C1=O)\O	18	nM
CHEMBL243150	CN1CCN(CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)S(=O)(=O)C	18.17	nM
CHEMBL244863	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3cccc(Br)c3	19	nM
CHEMBL492538	CCN(CC)C(=O)C(=O)N(CC)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	19	nM
CHEMBL1914563	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(CC(=O)N3CCCCC3)c4cc(Cc5ccc(F)cc5)cnc14	19	nM
CHEMBL2236601	OC(=O)\C(=C\C(=O)C1=CN(Cc2c(F)cccc2F)c3ccccc3C1=O)\O	19	nM
CHEMBL3360110	CN1C(=O)C(=C(N=C1C2=CCOC2)C(=O)NCc3ccc(F)cc3)O	19	nM
CHEMBL3415853	OC(=O)\C(=C\C(=O)c1cc(cn1Cc2ccc(F)cc2)c3ccccc3)\O	19	nM
CHEMBL199145	Oc1c(ncc2cccnc12)C(=O)NCc3ccc(F)cc3	19.9	nM
CHEMBL226916	Oc1nc(nc(C(=O)NCCc2ccccc2)c1O)c3cccs3	19.95	nM
CHEMBL232228	Oc1nc(nc(C(=O)NCc2c[nH]c3ccccc23)c1O)c4cccs4	19.95	nM
CHEMBL232444	Oc1nc(nc(C(=O)NCc2ccc(Cl)cc2)c1O)c3cccs3	19.95	nM
CHEMBL388908	CN1C[C@@H](F)C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	20	nM
CHEMBL243377	CN1C(=O)C(=C(N=C1C2COCCN2C(=O)OC(C)(C)C)C(=O)NCc3ccc(F)cc3)O	20	nM
CHEMBL237728	OC1=C(C#N)C(=O)N2CCN(Cc3ccc(F)cc3)C(=O)C2=C1O	20	nM
CHEMBL237942	OC1=C(I)C(=O)N2CCN(Cc3ccc(F)cc3)C(=O)C2=C1O	20	nM
CHEMBL240481	CCOC(=O)c1cn2CCN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O	20	nM

CHEMBL258681	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2C(=O)N)O	20	nM
CHEMBL258682	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2S(=O)(=O)C)O	20	nM
CHEMBL411299	CNC(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)C	20	nM
CHEMBL260665	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2c3onc(C)n3)O	20	nM
CHEMBL408075	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2cccc3cc[nH]c23)O	20	nM
CHEMBL259125	CCOc1ccccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)C	20	nM
CHEMBL262067	Cc1noc(n1)c2cc(F)ccc2CNC(=O)c3nc(nc(O)c3O)C(C)(C)C	20	nM
CHEMBL408076	CNC(=O)c1cc(F)ccc1CNC(=O)c2nc(nc(O)c2O)C(C)(C)C	20	nM
CHEMBL510093	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)C(=O)N2CCOCC2)C(=O)NCc3ccc(F)cc3)O	20	nM
CHEMBL461406	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2ccccn2)C(=O)NCc3ccc(F)cc3)O	20	nM
CHEMBL476357	CN1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	20	nM
CHEMBL523901	COc1cccc2c1c(cn2Cc3ccc(F)cc3F)C(=O)\C=C(/O)\C(=O)O	20	nM
CHEMBL499475	COc1cccc2c1c(cn2Cc3cc(F)ccc3F)C(=O)\C=C(/O)\C(=O)O	20	nM
CHEMBL456326	ON1C(=O)Cc2ccc(NC(=O)Cc3ccc(F)cc3)cc2C1=O	20	nM
CHEMBL565220	CC1(CCCCN1)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	20	nM
CHEMBL550202	Cc1nc(C)c(s1)C(=O)N2CCCCC2(C)C3=NC(=C(O)C(=O)N3)C(=O)NCc4ccc(F)cc4	20	nM
CHEMBL550674	CC(=O)N1CCC[C@@]1(C)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	20	nM
CHEMBL563898	CC(=O)N1CCCCC1C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	20	nM
CHEMBL563270	CC1(C)NCCCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	20	nM
CHEMBL562595	CN(C)S(=O)(=O)N1CCN(C)C(C)(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	20	nM
CHEMBL572902	CC(=O)N1CCN(CC1)c2cc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	20	nM
CHEMBL573605	CN(C(=O)C)c1cc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13	20	nM
CHEMBL1222998	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4ncc(Cc5ccc(F)cc5)s4	20	nM
CHEMBL1914555	CC(NC(=O)C1=C(O)c2ncc(Cc3ccccc3)cc2NC1=O)c4ccccc4	20	nM
CHEMBL243265	CN1CC[C@@H](O)C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	21	nM
CHEMBL394353	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)c(F)c3	21	nM
CHEMBL461652	COc1cccc(CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)NC(=O)C(=O)N(C)C)c1OC	21	nM
CHEMBL492329	CCN(C(=O)c1ccccn1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL494945	CC(C)N(C(=O)C(=O)N(C)C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	21	nM
CHEMBL495145	CCN(C(=O)c1cscn1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL492350	CCN(C(=O)C(=O)N1CCCC1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL492543	CCN(C(=O)C(=O)N1CCN(C)CC1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL560185	CN1CCN(CC1)C(=O)CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL551402	CNC(=O)CN1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	21	nM
CHEMBL552327	CC1(C)N(Cc2ocnn2)CCN3C(=O)C(=C(N=C13)C(=O)NCc4ccc(F)cc4)O	21	nM
CHEMBL3360109	CN1C(=O)C(=C(N=C1c2occc2)C(=O)NCc3ccc(F)cc3)O	21	nM
CHEMBL499184	OC1=C(N=C2C=CC=CN2C1=O)C(=O)NCc3ccc(F)cc3	22	nM
CHEMBL1773414	ON1CCc2c(ncc3c2c(cn3Cc4ccc(F)cc4)S(=O)(=O)N5CCCC5)C1=O	22	nM
CHEMBL3310083	CNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCCN(C)C)C1=	22	nM

O

CHEMBL3415843	OC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)cc1c3ccccc3)\O	22	nM
CHEMBL272642	Cc1ccc2nc(sc2c1)c3ccc(NC(=O)\C=C\C(=O)O)cc3	23	nM
CHEMBL492932	CCN(C(=O)CN1CCOCC1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	23	nM
CHEMBL2316135	OC1=C(C(=O)NCCCN2CCCC2)C(=O)Nc3cc(Cc4ccc(F)cc4)cnc13	23	nM
CHEMBL3310091	CN(C)C(=O)CN1C(=O)C(=C(O)c2ncc(Cc3ccc(F)cc3)cc12)C(=O)NC4(CO)CCCC4	23	nM
CHEMBL492526	OC1=C(N=C2N(C=CC=C2CNC(=O)c3ccccc3)C1=O)C(=O)NCc4ccc(F)cc4	24	nM
CHEMBL514836	Oc1c(nc(C2CNC(=O)C2)c3cccnc13)C(=O)NCc4ccc(F)cc4	24	nM
CHEMBL3415845	OC(=O)\C(=C\C(=O)c1ccn(Cc2ccc(F)cc2)c1)\O	24	nM
CHEMBL550590	Cn1cnc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)n1	25	nM
CHEMBL48573	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)cc2	26	nM
CHEMBL492682	CN1CCN(CC1)C(=O)C(=O)NC(C)(C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	26	nM
CHEMBL492537	CN(C)C(=O)C(=O)N(C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	26	nM
CHEMBL514555	CCN1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3S(=O)(=O)C)c(O)c4ncccc24	26	nM
CHEMBL1773320	COCCN(C)Cc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	26	nM
CHEMBL3125970	ON1C(=O)C(=C(O)c2cccnc12)C(=O)NCc3ccc(F)c(Cl)c3	27	nM
CHEMBL414850	O\C(=N/Cc1ccc(F)cc1)\c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	27.39	nM
CHEMBL394610	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)c(Cl)c3	28	nM
CHEMBL513189	CN(c1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14)S(=O)(=O)C	28	nM
CHEMBL1914559	Nc1ccc(CN2C(=O)C(=C(O)c3ncc(Cc4ccccc4)cc23)C(=O)NCc5ccc(F)cc5)cc1	28	nM
CHEMBL1914560	CS(=O)(=O)c1ccc(CN2C(=O)C(=C(O)c3ncc(Cc4ccccc4)cc23)C(=O)NCc5ccc(F)cc5)cc1	28	nM
CHEMBL3310415	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N4CCN(C)CC4)C1=O	28	nM
CHEMBL209591	Oc1c(ccc2cccnc12)C(=O)NCc3ccc(F)cc3	30	nM
CHEMBL216683	CN1CCOCC1c2nc(O)c(O)c(n2)C(=O)NCc3ccc(F)cc3	30	nM
CHEMBL242561	CN1C[C@H](C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)NS(=O)(=O)C	30	nM
CHEMBL244520	CN1CC(F)(F)C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	30	nM
CHEMBL394905	OC1=C(Br)C(=O)N2CCN(Cc3ccc(F)cc3)C(=O)C2=C1O	30	nM
CHEMBL240479	CCOC(=O)c1cn2CCN(Cc3cccc(Cl)c3)C(=O)c2c1O	30	nM
CHEMBL247570	CN(C)S(=O)(=O)c1cc(F)ccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	30	nM
CHEMBL260185	COc1ccc(OC)c2c1c(cn2Cc3ccc(F)cc3)C(=O)\C=C(/O)\C(=O)O	30	nM
CHEMBL525898	COc1cccc2c1c(cn2Cc3cccc(F)c3)C(=O)\C=C(/O)\C(=O)O	30	nM
CHEMBL560944	CN1CCN(C(C1)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3)C(=O)C	30	nM
CHEMBL554745	CN1CN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	30	nM
CHEMBL562899	OC(=O)C(=O)CC(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(Br)cc3C1=O	30	nM
CHEMBL575207	CN(CCNc1cc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13)C(=O)C	30	nM
CHEMBL1213723	COc1cccc2c1c(cn2Cc3cccc(Cl)c3)C(=O)\C=C(/O)\C(=O)O	30	nM
CHEMBL1213788	COc1cccc2c1c(cn2Cc3cccc(Cl)c3F)C(=O)\C=C(/O)\C(=O)O	30	nM
CHEMBL1770430	OC(=O)\C=C\c1ccc2N(Cc3ccc(F)cc3)C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c2c1	30	nM
CHEMBL1770431	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(Br)cc3C1=O)\O	30	nM

CHEMBL2407280	ON1C(=O)C(C(=O)NCc2ccccc2)c3ccccc3C1=O	30	nM
CHEMBL1087940	Oc1nc(nc(C(=O)Nc2ccc3ccccc3c2)c1O)c4cccs4	30.2	nM
CHEMBL3805585	Oc1c2C(=O)N3CCCN3Cc2c(C#N)c4cc(Cc5cccc(Cl)c5F)cnc14	30.22	nM
CHEMBL498697	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(F)ccc3C1=O)\O	31.62	nM
CHEMBL563963	CC1(C)NC(=O)N2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	32	nM
CHEMBL1773313	ON1CCc2c(ncc3c2ccn3Cc4ccc(F)cn4)C1=O	32	nM
CHEMBL1914550	OC1=C(C(=O)NCc2ccc(F)cc2C(F)(F)F)C(=O)Nc3cc(Cc4ccccc4)cnc13	32	nM
CHEMBL1914561	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(CCN3CCCC3=O)c4cc(Cc5cccc5)cnc14	32	nM
CHEMBL243366	CCN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	33	nM
CHEMBL478239	CN(C)C(=O)CN1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	33	nM
CHEMBL272448	OC(=O)C1CCCCC1C(=O)Nc2ccc(Oc3cccc4ccccc34)cc2	34	nM
CHEMBL1914558	OC1=C(C(=O)NCc2ccc(F)cc2)C(=O)N(CC3CC3)c4cc(Cc5ccccc5)cnc14	34	nM
CHEMBL3582056	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2)c3ccccc3C1=O)\O	34	nM
CHEMBL386710	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	34.64	nM
CHEMBL1258726	OC1=C(N=C2N(C=C(C=C2N3CCOC3=O)N4CCOCC4)C1=O)c5ncc(Cc6ccc(F)cc6)[nH]5	35	nM
CHEMBL1773321	CN(CC1CC1)Cc2cn(Cc3ccc(F)cc3)c4cnc5C(=O)N(O)CCc5c24	35	nM
CHEMBL1917877	OC1=C(C(=O)NCc2ccc(F)cc2Cl)C(=O)Nc3cc(Cc4ccccc4)cnc13	35	nM
CHEMBL493335	CCNC1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	36	nM
CHEMBL522534	CCN(C(=O)C(=O)N(C)C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	36	nM
CHEMBL1222997	OC1=C(N=C2N(C=C(C=C2N3CCCS3(=O)=O)N4CCOCC4)C1=O)c5ncc(Cc6ccc(F)cc6)s5	36	nM
CHEMBL1773415	CC1CCN(CC1)S(=O)(=O)c2cn(Cc3ccc(F)cc3)c4cnc5C(=O)N(O)CCc5c24	36	nM
CHEMBL389566	CN1CC[S+]([O-])CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	37	nM
CHEMBL2236588	COc1ccccc1CN2C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c3ccccc23	38	nM
CHEMBL232629	Cc1cccc(CNC(=O)c2nc(nc(O)c2O)c3cccs3)c1	39.81	nM
CHEMBL36070	Oc1c(ncc2cccnc12)C(=O)c3cccc(Cc4ccccc4)c3	40	nM
CHEMBL209854	Oc1c2C(=O)N(Cc3ccc(F)cc3)Cc2c(C(=O)N4CCOCC4)c5cccnc15	40	nM
CHEMBL237725	OC1=CC(=O)N2C=CN(Cc3ccc(F)cc3)C(=O)C2=C1O	40	nM
CHEMBL237726	OC1=CC(=O)N2CCN(Cc3ccccc(Cl)c3)C(=O)C2=C1O	40	nM
CHEMBL237727	OC1=CC(=O)N2CCN(Cc3ccc(F)c(Cl)c3)C(=O)C2=C1O	40	nM
CHEMBL239413	CCOC(=O)c1cn2CCN(Cc3ccc(F)cc3)C(=O)c2c1O	40	nM
CHEMBL240058	CCOC(=O)c1cn2CCN(Cc3ccc(Cl)cc3)C(=O)c2c1O	40	nM
CHEMBL236409	CNC(=O)c1cn2CCN(Cc3ccc(Cl)c(Cl)c3)C(=O)c2c1O	40	nM
CHEMBL476565	CC(C)N1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	40	nM
CHEMBL497605	COc1cccc2c1c(cn2Cc3ccccc3F)C(=O)\C=C(/O)\C(=O)O	40	nM
CHEMBL563628	CC(=O)N1CCCC1C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	40	nM
CHEMBL572901	CN1CCN(CC1)c2cc(C(=O)NCc3ccc(F)cc3)c(O)c4ncccc24	40	nM
CHEMBL572448	CN(C)C(=O)C(=O)N(C)c1cc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13	40	nM
CHEMBL3125971	ON1C(=O)C(=C(O)c2cccnc12)C(=O)NCc3ccc(F)c(F)c3	40	nM
CHEMBL394537	CN1CCN(CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)OC(C)(C)C	41	nM
CHEMBL3125981	ON1C(=O)C(=Cc2cccnc12)C(=O)NCc3ccc(F)cc3F	41	nM
CHEMBL491150	Oc1c(ncc2cccnc12)c3oc(Cc4ccc(F)cc4)nn3	42	nM
CHEMBL1222999	OC1=C(N=C2N(C=C(C=C2Br)N3CCOCC3)C1=O)c4ncc(Cc5ccc(F)cc5)s4	42	nM
CHEMBL3087617	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)cc2F	42	nM

CHEMBL3310412	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)N4CCCC4)C1=O	42	nM
CHEMBL260960	COc1cccc(NC(=O)c2sc3NC(=O)C(=Cc3c2N)C(=O)O)c1	43	nM
CHEMBL1773411	ON1CCc2c(ncc3c2c(cn3Cc4ccc(F)cc4)S(=O)(=O)N5CCOCC5)C1=O	43	nM
CHEMBL3415846	N\C(=C/C(=O)c1cn(Cc2ccc(F)cc2)cc1c3ccccc3)\C(=O)O	43	nM
CHEMBL270717	OC(=O)C1=CNc2ccc(Cc3cccc(Cl)c3F)cc2C1=O	43.5	nM
CHEMBL390027	C[C@H]1C[C@H](N(C)C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	43.59	nM
CHEMBL395819	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)c(Br)c3	44	nM
CHEMBL437940	CNS(=O)(=O)c1cc(F)ccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	45	nM
CHEMBL491538	NC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2NC1=O	45	nM
CHEMBL1258050	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4ncc(Cc5ccc(F)cc5)[nH]4	45	nM
CHEMBL3310411	COCCNC(=O)C1=C(O)c2ncc(Cc3ccc(F)cc3)cc2N(CC(=O)NCCN(C)C)C1=O	45	nM
CHEMBL497688	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(Cl)ccc3C1=O)\O	45.72	nM
CHEMBL272419	OC(C(O)c1nc2cc3ccccc3cc2[nH]1)C(=O)O	46	nM
CHEMBL3805532	Oc1c2C(=O)N3CCCN3Cc2cc4cc(Cc5cccc(Cl)c5F)cnc14	46.65	nM
CHEMBL1258727	OC1=C(N=C2N(C=C(C=C2N3CCCC3=O)N4CCOCC4)C1=O)c5ncc(Cc6ccc(F)cc6)[nH]5	47	nM
CHEMBL2206768	Oc1cc(c2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O)S(=O)(=O)N4CCOCC4	47	nM
CHEMBL2401912	O[C@@H]1CCC[C@H]1NC(=O)C(=O)\C=C(/O)\C2=CC(=CN(Cc3ccccc3F)C2=O)Cc4ccc(F)cc4F	48	nM
CHEMBL512195	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccccc3C1=O)\O	48.99	nM
CHEMBL498713	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(Cl)c(Cl)cc3C1=O)\O	49.75	nM
CHEMBL35842	Oc1c(ccc2cccnc12)C(=O)c3cccc(Cc4ccccc4)c3	50	nM
CHEMBL209440	COc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14	50	nM
CHEMBL386515	CN(C)C(C)(C)c1nc(O)c(O)c(n1)C(=O)NCc2ccc(F)cc2	50	nM
CHEMBL430194	CN1CC(=O)N(C)CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	50	nM
CHEMBL394782	CN1C(=O)C(=C(N=C1C2COCCN2)C(=O)NCc3ccc(F)cc3)O	50	nM
CHEMBL232227	Oc1nc(nc(C(=O)Nc2csc3ccccc23)c1O)c4cccs4	50	nM
CHEMBL492328	CCN(C(=O)c1ccncc1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	50	nM
CHEMBL495144	CCN(C(=O)c1oc(C)nn1)C2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O	50	nM
CHEMBL559493	Cc1nc(C)c(s1)C(=O)N2CCCCC2C3=NC(=C(O)C(=O)N3)C(=O)NCc4cc(F)cc4	50	nM
CHEMBL1770428	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(OCc4ccc(F)cc4)cc3C1=O)\O	50	nM
CHEMBL1773315	ON1CCc2c(ncc3c2ccn3Cc4ccc(F)cc4C#N)C1=O	50	nM
CHEMBL3582069	Cc1cc(C)cc(CN2C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c3ccccc23)c1	50	nM
CHEMBL438113	COc1cccc(CNC(=O)c2nc(nc(O)c2O)c3cccs3)c1	50.12	nM
CHEMBL232630	Oc1nc(nc(C(=O)NCc2cccc(c2)c3ccccc3)c1O)c4cccs4	50.12	nM
CHEMBL1088059	Oc1nc(nc(C(=O)NCc2csc3ccccc23)c1O)c4cccs4	50.12	nM
CHEMBL246774	CNC(=O)c1cc(F)ccc1CNC(=O)c2ncc3cccnc3c2O	51	nM
CHEMBL394781	CCNC(=O)N1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	52	nM
CHEMBL272418	CCOc1cc(CNc2nn[nH]n2)cc(Cl)c1OCc3ccc(Cl)cc3	52	nM
CHEMBL3087618	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(F)ccc2F	52	nM
CHEMBL498698	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3c(F)cccc3C1=O)\O	53.67	nM
CHEMBL2206761	CCN(CC)S(=O)(=O)c1cc(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	54	nM
CHEMBL3125972	ON1C(=O)C(=C(O)c2cccnc12)C(=O)NCc3ccc(F)cc3F	55	nM

CHEMBL499273	OC(=O)\C(=C\C(=O)c1cccn1Cc2ccc(F)cc2)\O	57	nM
CHEMBL2206770	CN(CC(=O)O)S(=O)(=O)c1cc(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	58	nM
CHEMBL260096	CCOc1cc(\C=C/2\C(=NN(C2=O)c3nnn[nH]3)C)ccc1OC	59	nM
CHEMBL1258049	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4oc(Cc5ccc(F)cc5)cn4	59	nM
CHEMBL3087616	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(F)c2F	59	nM
CHEMBL236408	CNC(=O)c1cn2CCN(Cc3ccc(Cl)cc3)C(=O)c2c1O	60	nM
CHEMBL259336	CC(C)(C)c1nc(O)c(O)c(n1)C(=O)NCc2ccc(F)cc2S(=O)(=O)C	60	nM
CHEMBL405927	OC(=O)CSc1nc(cc(c2ccc(Cl)cc2)c1C#N)c3ccccc3	60	nM
CHEMBL559494	CN1CCN(C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)c4cnccn4	60	nM
CHEMBL1213726	COc1cccc2c1c(cn2Cc3ccc(F)cc3Cl)C(=O)\C=C(/O)\C(=O)O	60	nM
CHEMBL244700	CN1C[C@H](C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)NC(=O)C	61	nM
CHEMBL243655	CN1CC[C@H](C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)OCc4ccccc4	62	nM
CHEMBL244651	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3cccc(F)c3	62	nM
CHEMBL389142	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3cccc(Cl)c3	62	nM
CHEMBL560265	CN(C)CCN1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	62	nM
CHEMBL552176	Cc1cc(CN2CCN3C(=O)C(=C(N=C3C2(C)C)C(=O)NCc4ccc(F)cc4)O)on1	62	nM
CHEMBL3415847	OC(=O)\C(=C\C(=O)\C=C\c1cc(cn1Cc2ccccc2)C(=O)c3ccc(F)cc3)\O	63	nM
CHEMBL272193	CCOc1cc(ccc1\C=C/2\C(=NN(C2=O)c3nnn[nH]3)C)N(CC)CC	65	nM
CHEMBL428570	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccccc3	66	nM
CHEMBL409315	OC(=O)CN1C(=O)\C(=C\2/SC(=S)N(C(Cc3ccccc3)C(=O)O)C2=O)\c4ccccc14	66	nM
CHEMBL1773412	COCCN(C)S(=O)(=O)c1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	66	nM
CHEMBL3415850	OC(=O)\C(=C\C(=O)\C=C\c1cc(cn1Cc2ccc(F)cc2)c3ccccc3)\O	66	nM
CHEMBL562760	CN(C)[C@@H]1CCCN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	69	nM
CHEMBL211634	Oc1c2C(=O)N(Cc3ccc(F)cc3)Cc2cc4cccnc14	70	nM
CHEMBL244904	CN1CCSCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	70	nM
CHEMBL430049	CCCNC(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)C	70	nM
CHEMBL408938	CCNC(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)C	70	nM
CHEMBL261703	OC(=O)[C@@H](Cc1cc(O)c(O)cc1[N+](=O)[O-])OC(=O)\C=C\c2cc(O)c(O)cc2[N+](=O)[O-]	70	nM
CHEMBL493531	CN(C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	70	nM
CHEMBL496380	CCOC(=O)\C(=C\C(=O)c1cn(Cc2c(F)cccc2F)c3cccc(OC)c13)\O	70	nM
CHEMBL1214536	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)c(Cl)c2)c3cccc(OC)c13)\O	70	nM
CHEMBL1258617	CN1CCN(C2=CC(=CN3C(=O)C(=C(N=C23)c4ncc(Cc5ccc(F)cc5)[nH]4)O)N6CCOCC6)S1(=O)=O	70	nM
CHEMBL2042382	OC(=O)\C(=C\C(=O)C1=CC(=CN(Cc2ccccc2)C1=O)Cc3ccccc3)\O	70	nM
CHEMBL277754	Cc1ccc(CNC(=O)c2nc(nc(O)c2O)c3cccs3)cc1	70.79	nM
CHEMBL398211	Oc1nc(nc(C(=O)NCc2cccc(F)c2)c1O)c3cccs3	70.79	nM
CHEMBL496454	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(ccc3C1=O)N4CCCC4)\O	70.99	nM
CHEMBL428215	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCCc3ccccc3	71	nM
CHEMBL551401	CCN(CC)CCN1CCN2C(=O)C(=C(N=C2C1(C)C)C(=O)NCc3ccc(F)cc3)O	76	nM
CHEMBL254316	CN1C(=O)C(=C(N=C1C(C)(C)NC(=O)c2oc(C)nn2)C(=O)NCc3ccc(F)cc3)O	77.07	nM
CHEMBL244963	CN1CCCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	78.74	nM
CHEMBL212921	COc1c2C(=O)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14	80	nM

CHEMBL240694	OC(=O)c1cn2CCN(Cc3ccccc3)C(=O)c2c1O	80	nM
CHEMBL396890	CNC(=O)c1cn2CCN(Cc3ccc(F)cc3)C(=O)c2c1O	80	nM
CHEMBL495540	COc1cccc2c1c(cn2Cc3c(F)cccc3F)C(=O)\C=C(/O)\C(=O)O	80	nM
CHEMBL459382	CN(c1c2CN(C)C(=O)c2c(O)c3ncc(Cc4ccc(F)cc4)cc13)S(=O)(=O)C	80	nM
CHEMBL554522	C[C@]1(CCCN1)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	80	nM
CHEMBL2206769	OC(=O)CNS(=O)(=O)c1cc(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	80	nM
CHEMBL3238130	CC(=O)N1CCN(CC1)c2ccc3C(=O)C(=CN(Cc4ccc(F)cc4)c3c2)C(=O)\C=C(/O)\C(=O)O	80	nM
CHEMBL234707	Oc1nc(nc(C(=O)Nc2cccc3ccccc23)c1O)c4cccs4	80.09	nM
CHEMBL1773317	CN(C)Cc1cn(Cc2ccc(F)cc2)c3cnc4C(=O)N(O)CCc4c13	81	nM
CHEMBL2407281	Cc1ccc(CNC(=O)C2C(=O)N(O)C(=O)c3ccccc23)cc1	84	nM
CHEMBL437708	Oc1nc(nc(C(=O)NCc2ccccc2)c1O)c3cccs3	85.11	nM
CHEMBL244236	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)c(C)c3	86	nM
CHEMBL386055	COc1cnc2c(O)c3C(=O)N(Cc4ccc(F)cc4)Cc3c(OC)c2c1	90	nM
CHEMBL260913	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2C(=O)NCC(F)(F)F)O	90	nM
CHEMBL260082	CC(C)NC(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)C	90	nM
CHEMBL549798	CN1CCC[C@@]1(C)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	90	nM
CHEMBL1213791	COc1cccc2c1c(cn2Cc3cc(Cl)ccc3F)C(=O)\C=C(/O)\C(=O)O	90	nM
CHEMBL232435	COc1ccccc1CNC(=O)c2nc(nc(O)c2O)c3cccs3	91.2	nM
CHEMBL226764	CN1CCCC1c2nc(O)c(O)c(n2)C(=O)NCc3ccc(F)cc3	91.65	nM
CHEMBL480531	OC1=C(CN(Cc2ccccn2)C1=O)C(=O)NCc3ccc(F)cc3	94	nM
CHEMBL1258504	OC1=C(N=C2N(C=C(C=C2N3CCCS3(=O)=O)N4CCOCC4)C1=O)c5ncc(Cc6ccc(F)cc6)[nH]5	95	nM
CHEMBL3582072	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(Cl)c2)c3c(Cl)cccc3C1=O)\O	96	nM
CHEMBL2407287	ON1C(=O)C(C(=O)NCc2ccc(F)cc2)c3ccccc3C1=O	99	nM
CHEMBL242137	CN1C[C@H](O)C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	100	nM
CHEMBL244754	CN1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	100	nM
CHEMBL388419	Oc1nc(nc(C(=O)Nc2cccs2)c1O)c3cccs3	100	nM
CHEMBL237724	OC1=CC(=O)N2CCN(Cc3ccc(F)cc3)C(=O)C2=C1O	100	nM
CHEMBL481279	OC1=C(CN(Cc2ccccc2)C1=O)C(=O)NCc3ccc(F)cc3	100	nM
CHEMBL498202	COc1cccc2c1c(cn2Cc3cc(F)c(F)c(F)c3)C(=O)\C=C(/O)\C(=O)O	100	nM
CHEMBL512021	ON1C(=O)Cc2ccc(NC(=O)Cc3ccccc3)cc2C1=O	100	nM
CHEMBL460632	COc1c2CN(C)C(=O)c2c(O)c3ncc(Cc4ccc(F)cc4)cc13	100	nM
CHEMBL516025	OC(=O)\C(=C\C(=O)c1cc(OCc2ccccc2)cc(OCc3ccccc3)c1)\O	100	nM
CHEMBL559492	CN1CCN(C(=O)C)C(C)(C1)C2=NC(=C(O)C(=O)N2)C(=O)NCc3ccc(F)cc3	100	nM
CHEMBL551942	CN1CCN(C(=O)c2cnccn2)C(C)(C1)C3=NC(=C(O)C(=O)N3)C(=O)NCc4ccc(F)cc4	100	nM
CHEMBL557899	Oc1ccc2CN(Cc3ccc(Cl)c(Cl)c3)C(=O)c2c1O	100	nM
CHEMBL1088620	Oc1nc(nc(C(=O)NCc2cccs2)c1O)c3cccs3	100	nM
CHEMBL496652	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cccc(Cl)cc3C1=O)\O	105.83	nM
CHEMBL232437	Cc1ccccc1CNC(=O)c2nc(nc(O)c2O)c3cccs3	109.65	nM
CHEMBL240272	CCOC(=O)c1cn2CCN(Cc3cccc(F)c3)C(=O)c2c1O	110	nM
CHEMBL245717	CN(C)C(=O)c1cc(F)ccc1CNC(=O)c2nc(N3CCCCS3(=O)=O)c4cccnc4c2O	110	nM
CHEMBL2206762	Oc1cc(c2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O)S(=O)(=O)NCCCBr	110	nM
CHEMBL2407278	ON1C(=O)C(C(=O)Nc2cccc(F)c2)c3ccccc3C1=O	110	nM
CHEMBL3415854	O\C(=C/C(=O)c1cccn1Cc2ccc(F)cc2)\c3nc[nH]n3	110	nM
CHEMBL3582064	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(F)c2)c3ccccc3C1=O)\O	110	nM

CHEMBL390433	Oc1nc(nc(C(=O)N[C@H]2CCc3ccccc23)c1O)c4cccs4	110.91	nM
CHEMBL562366	Oc1ccc2C(=O)N(Cc3ccc(F)c(F)c3)C(=O)c2c1O	118.32	nM
CHEMBL495952	COc1cccc2c1c(cn2Cc3cccc(F)c3F)C(=O)\C=C(/O)\C(=O)O	120	nM
CHEMBL564984	OC1=C(N=C(NC1=O)C2CCCN2)C(=O)NCc3ccc(F)cc3	120	nM
CHEMBL559753	CCOC(=O)C(=O)CC(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(Br)cc3C1=O	120	nM
CHEMBL550776	Oc1ccc2C(=O)N(Cc3ccc(Cl)c(Cl)c3)C(=O)c2c1O	120	nM
CHEMBL1213789	COc1cccc2c1c(cn2Cc3ccc(F)c(Cl)c3)C(=O)\C=C(/O)\C(=O)O	120	nM
CHEMBL2206760	CNS(=O)(=O)c1cc(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	120	nM
CHEMBL478452	CN1CC(CC1=O)c2nc(C(=O)NCc3ccc(F)cc3S(=O)(=O)C)c(O)c4nccc24	123	nM
CHEMBL2407273	COc1ccc(CCNC(=O)C2C(=O)N(O)C(=O)c3ccccc23)cc1OC	126	nM
CHEMBL389093	Oc1nc(nc(C(=O)NCc2ccccc2c3ccccc3)c1O)c4cccs4	128.82	nM
CHEMBL3805531	Oc1c2C(=O)N3CCC[C@@H]3c2c(C#N)c4cc(Cc5cccc(Cl)c5F)cnc14	128.84	nM
CHEMBL227497	Oc1nc(nc(C(=O)NCc2ccc(F)cc2)c1O)C3CCCCN3	130	nM
CHEMBL389332	CN1C[C@@H](C[C@H]1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)OCc4ccccc4	130	nM
CHEMBL242609	CC(C)N1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	130	nM
CHEMBL455437	Oc1c(ncc2cccnc12)c3noc(Cc4ccc(F)cc4)n3	130	nM
CHEMBL522630	Oc1c(ncc2cccnc12)c3nnc(Cc4ccc(F)cc4)[nH]3	130	nM
CHEMBL523974	Oc1c(ncc2cccnc12)c3oc(Cc4ccccc4)nn3	130	nM
CHEMBL492727	CNC1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	130	nM
CHEMBL584772	OC(=O)\C(=C\C(=O)c1csc(Cc2ccccc2)c1)\O	130	nM
CHEMBL1213787	COc1cccc2c1c(cn2Cc3c(F)cccc3Cl)C(=O)\C=C(/O)\C(=O)O	130	nM
CHEMBL2171665	COCCNC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	130	nM
CHEMBL3582073	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2F)c3c(Cl)cccc3C1=O)\O	130	nM
CHEMBL3805269	Oc1c2C(=O)N3CCCC[C@@H]3c2c(C#N)c4cc(Cc5cccc(Cl)c5F)cnc14	138.56	nM
CHEMBL397268	CN1CCS(=O)(=O)CC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	140	nM
CHEMBL244235	COc1cccc(CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C3COCCN3C)c1	140	nM
CHEMBL573637	COc1cccc(Cc2cccc(c2)C(=O)\C=C(/O)\C(=O)O)c1	140	nM
CHEMBL2236603	COc1cccc(CN2C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c3ccccc23)c1	140	nM
CHEMBL2297147	CC(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	140	nM
CHEMBL1289430	CN(O)C(=O)c1cc2c(CO)cn(Cc3ccc(F)cc3)c2cn1	145	nM
CHEMBL572414	COc1ccc(Cc2cccc(c2)C(=O)\C=C(/O)\C(=O)O)cc1	150	nM
CHEMBL3087619	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2c(F)cccc2F	150	nM
CHEMBL437361	C[C@H](NC(=O)c1nc(nc(O)c1O)c2cccs2)c3ccc4ccccc4c3	156.67	nM
CHEMBL253342	Oc1ccc2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O	160	nM
CHEMBL526283	COc1cccc2c1c(cn2Cc3c(F)ccc(F)c3F)C(=O)\C=C(/O)\C(=O)O	160	nM
CHEMBL232445	Oc1nc(nc(C(=O)NCc2ccccc2F)c1O)c3cccs3	162.18	nM
CHEMBL50605	OC(=O)C(=O)CC(=O)c1cccn1Cc2ccc(F)cc2	164.32	nM
CHEMBL492524	OC1=C(N=C2N(C=CC=C2CN3CCOCC3)C1=O)C(=O)NCc4ccc(F)cc4	170	nM
CHEMBL559284	Oc1ccc2C(=O)N(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O	170	nM
CHEMBL1258167	OC1=C(N=C2N(C=C(C=C2I)N3CCOCC3)C1=O)c4oc(Cc5ccc(F)cc5)cn4	170	nM
CHEMBL3087330	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2c(Cl)cccc2Cl	170	nM
CHEMBL3087628	Cc1ccccc1Cn2cccc2\C=C\C(=O)CC(=O)C(=O)O	170	nM
CHEMBL389141	CN1CCOCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccccc3F	175	nM
CHEMBL3805498	Oc1c2C(=O)N3CCC[C@@H]3Cc2c(C#N)c4cc(Cc5cccc(Cl)c5F)cnc14	178.27	nM
CHEMBL389331	CO[C@@H]1C[C@H](N(C)C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	180	nM
CHEMBL410444	CN(C)C(=O)c1cc(F)ccc1CNC(=O)C2=C(O)C(=O)N(C)C(=N2)C(C)(C)	180	nM

C

CHEMBL572471	OC(=O)\C(=C\C(=O)C1C=CSC1Cc2ccccc2)\O	180	nM
CHEMBL492525	CC(=O)N1CCN(CC2=CC=CN3C(=O)C(=C(N=C23)C(=O)NCc4ccc(F)cc4)O)CC1	185	nM
CHEMBL494946	CCN(C(=O)CN(C)C)C1=CC=CN2C(=O)C(=C(N=C12)C(=O)NCc3ccc(F)cc3)O	185	nM
CHEMBL211110	Oc1c2C(=O)N(Cc3ccc(F)cc3)Cc2c(C(=O)NCc4ccccn4)c5cccnc15	190	nM
CHEMBL261714	COc1cccc2c(cn(Cc3ccc(F)cc3)c12)C(=O)\C=C(/O)\C(=O)O	190	nM
CHEMBL2206767	NCCN1CCN(CC1)S(=O)(=O)c2cc(O)c(O)c3C(=O)N(Cc4ccc(F)c(Cl)c4)Cc23	190	nM
CHEMBL2206773	CC(C)c1c(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc2c1S(=O)(=O)N(C)C	190	nM
CHEMBL3582071	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(Cl)c2)c3ccccc3C1=O)\O	190	nM
CHEMBL3736106	CCOC(=O)C1=C(C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1Cc3ccccc3	190	nM
CHEMBL1088621	Oc1nc(nc(C(=O)NCc2nccs2)c1O)c3cccs3	199.53	nM
CHEMBL242353	CCO[C@@H]1C[C@H](N(C)C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	200	nM
CHEMBL427698	CN1CCNCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	200	nM
CHEMBL232025	Oc1nc(nc(C(=O)Nc2nccs2)c1O)c3cccs3	200	nM
CHEMBL458279	OCCN1C=C(C(=O)O)C(=O)c2cc(Cc3ccc(Cl)cc3Cl)ccc12	200	nM
CHEMBL559852	Oc1ccc2C(=O)N(Cc3cccc(F)c3F)C(=O)c2c1O	200	nM
CHEMBL2180587	Oc1c(nc(NCCCCCCNC=O)c2cccnc12)C(=O)NCc3ccc(F)cc3	200	nM
CHEMBL2407272	ON1C(=O)C(C(=O)NCCc2ccc(F)cc2)c3ccccc3C1=O	200	nM
CHEMBL234922	CN(C(=O)c1nc(nc(O)c1O)c2cccs2)c3cccc4ccccc34	210	nM
CHEMBL427715	Oc1ccc(cc1O)S(=O)(=O)N(N2Cc3ccc(O)c(O)c3C2=O)S(=O)(=O)c4ccc(O)c(O)c4	210	nM
CHEMBL407451	CN1CCCCC1c2nc(O)c(O)c(n2)C(=O)NCc3ccc(F)cc3	220	nM
CHEMBL240057	CCOC(=O)c1cn2CCN(Cc3ccccc3)C(=O)c2c1O	220	nM
CHEMBL261541	COc1ccc2c(cn(Cc3ccc(F)cc3)c2c1)C(=O)\C=C(/O)\C(=O)O	220	nM
CHEMBL573644	OC(=O)\C(=C\C(=O)c1cccn1Cc2ccccc2)\O	220	nM
CHEMBL3582065	OC(=O)\C(=C\C(=O)C1=CN(Cc2cc(F)cc(F)c2)c3ccccc3C1=O)\O	220	nM
CHEMBL1257823	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4nnc(Cc5ccc(F)cc5)s4	225	nM
CHEMBL237083	OC1=CC(=O)N2CCN(Cc3ccccc3)C(=O)C2=C1O	230	nM
CHEMBL261106	CN1C(=O)C(=C(N=C1C(C)(C)C)C(=O)NCc2ccc(F)cc2C(=O)N3CCCC3)O	230	nM
CHEMBL493291	CN(C)C(C)(C)C1=NC(=C(O)C(=O)N1C)C(=O)NCc2ccc(F)cc2	230	nM
CHEMBL564147	Oc1ccc2C(=O)N(Cc3cc(F)ccc3F)C(=O)c2c1O	230	nM
CHEMBL524066	COc1cccc2c1c(cn2Cc3cc(F)cc(F)c3)C(=O)\C=C(/O)\C(=O)O	240	nM
CHEMBL2203322	CN(C)CCCNS(=O)(=O)c1cc(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	240	nM
CHEMBL1289543	COCc1cn(Cc2ccc(F)cc2)c3cnc(cc13)C(=O)N(C)O	242	nM
CHEMBL2180590	C[C@@H](CO)Nc1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13	244.95	nM
CHEMBL214371	CN(C)S(=O)(=O)Oc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14	250	nM
CHEMBL394536	CCN1CCN(C)C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	250	nM
CHEMBL549309	CN1CCCCC1(C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	250	nM
CHEMBL572473	OC(=O)\C(=C\C(=O)c1cccc(Cc2cccc(F)c2)c1)\O	250	nM
CHEMBL567841	CN(O)C(=O)c1cc2ccn(Cc3ccc(F)cc3)c2cn1	250	nM
CHEMBL578867	CN(O)C(=O)c1cc2ccn(Cc3ccc(F)cc3F)c2cn1	250	nM
CHEMBL1213790	COc1cccc2c1c(cn2Cc3cc(F)cc(Cl)c3)C(=O)\C=C(/O)\C(=O)O	250	nM
CHEMBL2206228	CN(C)S(=O)(=O)c1ccc(cc1)c2c(O)c(O)c3C(=O)N(Cc4ccc(F)c(Cl)c4)Cc3c2S(=O)(=O)N(C)C	250	nM
CHEMBL2236600	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2c(F)cccc2F)c3ccccc3C1=O)\O	250	nM
CHEMBL1289757	CC(C)NC(=O)c1cn(Cc2ccc(F)cc2)c3cnc(cc13)C(=O)N(C)O	251	nM

CHEMBL2407283	COc1ccc(CNC(=O)C2C(=O)N(O)C(=O)c3ccccc23)c(OC)c1	254	nM
CHEMBL2407286	ON1C(=O)C(C(=O)NCc2ccc(O)c(O)c2)c3ccccc3C1=O	258	nM
CHEMBL206604	CC(C)[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12	259.31	nM
CHEMBL2206227	CN(C)S(=O)(=O)c1c(O)c(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	260	nM
CHEMBL517854	CN(c1c2CN(C)C(=O)c2c(O)c3ncc(Cc4ccc(F)c(Cl)c4)cc13)S(=O)(=O)C	265	nM
CHEMBL409643	COc1ccc2c(c1)c(cn2Cc3ccc(F)cc3)C(=O)\C=C(/O)\C(=O)O	270	nM
CHEMBL1213727	COc1cccc2c1c(cn2Cc3cc(F)ccc3Cl)C(=O)\C=C(/O)\C(=O)O	270	nM
CHEMBL3582067	OC(=O)\C(=C\C(=O)C1=CN(Cc2c(Cl)cccc2Cl)c3ccccc3C1=O)\O	270	nM
CHEMBL2407277	COc1ccc(NC(=O)C2C(=O)N(O)C(=O)c3ccccc23)cc1Cl	277	nM
CHEMBL521569	COc1cccc2c1c(cn2Cc3ccc(F)c(F)c3F)C(=O)\C=C(/O)\C(=O)O	280	nM
CHEMBL3582039	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2F)c3ccccc3C1=O)\O	280	nM
CHEMBL204656	COc1cc2N(C=C(C(=O)O)C(=O)c2cc1Cc3cccc(Cl)c3F)[C@H](CO)C(C)C	293.94	nM
CHEMBL2407274	ON1C(=O)C(C(=O)NCCc2ccc(O)c(O)c2)c3ccccc3C1=O	296	nM
CHEMBL497672	OC(=O)\C=C\c1ccc(O)c2OC3C(C(=O)c4cc(O)c(O)cc34)c12	300	nM
CHEMBL564630	Oc1ccc2C(=O)N(Cc3cccc(F)c3)C(=O)c2c1O	300	nM
CHEMBL552566	Oc1ccc2C(=O)N(Cc3ccc(F)cc3F)C(=O)c2c1O	300	nM
CHEMBL563256	Oc1ccc2CN(Cc3cc(F)cc(F)c3)C(=O)c2c1O	300	nM
CHEMBL2171666	OCCNC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	300	nM
CHEMBL2180589	OCCNc1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13	300	nM
CHEMBL2407285	COc1ccc(CNC(=O)C2C(=O)N(O)C(=O)c3ccccc23)cc1OC	307	nM
CHEMBL1289651	CCOCCOCc1cn(Cc2ccc(F)cc2)c3cnc(cc13)C(=O)N(C)O	308	nM
CHEMBL551568	Oc1ccc2C(=O)N(Cc3cc(Cl)ccc3F)C(=O)c2c1O	310	nM
CHEMBL1257699	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4oc(Cc5ccc(F)cc5)nn4	310	nM
CHEMBL2206764	Oc1cc(c2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O)S(=O)(=O)NCCN4CCNCC4	310	nM
CHEMBL3087332	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(Cl)c2	310	nM
CHEMBL3087337	CCOc1ccccc1Cn2cccc2\C=C\C(=O)CC(=O)C(=O)O	310	nM
CHEMBL1289542	CN(O)C(=O)c1cc2c(COC3CCOCC3)cn(Cc4ccc(F)cc4)c2cn1	313	nM
CHEMBL1289756	CN(O)C(=O)c1cc2c(cn(Cc3ccc(F)cc3)c2cn1)C(=O)N4CCC[C@@H]4CO	319	nM
CHEMBL2206763	Oc1cc(c2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O)S(=O)(=O)NCCN4CCOCC4	320	nM
CHEMBL379382	Oc1c2C(=O)N(Cc3ccc(F)cc3)Cc2c(c4c(F)cccc4F)c5cccnc15	330	nM
CHEMBL564495	OC(=O)\C(=C\C(=O)c1cccc(CN=[N+]=[N-])c1)\O	330	nM
CHEMBL1289864	CN(O)C(=O)c1cc2c(CCCO)cn(Cc3ccc(F)cc3)c2cn1	340	nM
CHEMBL524807	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3c(Cl)cccc3C1=O)\O	342.49	nM
CHEMBL378395	CCOC(=O)c1ccccc1c2c3CN(Cc4ccc(F)cc4)C(=O)c3c(O)c5ncccc25	350	nM
CHEMBL492770	OC(=O)\C(=C\C(=O)c1cccc(OCc2ccccc2)c1)\O	350	nM
CHEMBL455438	Oc1c(ncc2cccnc12)c3nnc(Cc4ccccc4)[nH]3	360	nM
CHEMBL504621	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(F)cc3C1=O)\O	365.24	nM
CHEMBL268633	OC1=CC(=O)N2CCN(Cc3ccccc3Cl)C(=O)C2=C1O	370	nM
CHEMBL2206765	Oc1cc(c2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c1O)S(=O)(=O)NCc4ccccn4	370	nM
CHEMBL389930	OC(=O)C(=O)CC(=O)c1cc2ccccc2c3ccccc13	380	nM
CHEMBL394890	OC1=CC(=O)N2CCN(Cc3ccc(Cl)cc3)C(=O)C2=C1O	380	nM
CHEMBL2171667	NC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	380	nM
CHEMBL1289431	COCCOCc1cn(Cc2ccc(F)cc2)c3cnc(cc13)C(=O)N(C)O	382	nM
CHEMBL1289200	CN(O)C(=O)c1cc2c(CN3CCNC(=O)C3)cn(Cc4ccc(F)cc4)c2cn1	388	nM
CHEMBL550494	Oc1ccc2C(=O)N(Cc3ccccc3)C(=O)c2c1O	394.97	nM
CHEMBL496379	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(F)ccc2F)c3cccc(OC)c13)\O	400	nM

CHEMBL560644	Oc1ccc2C(=O)N(Cc3cc(Cl)c(F)cc3F)C(=O)c2c1O	400	nM
CHEMBL549966	Oc1ccc2C(=O)N(Cc3cccc(Cl)c3)C(=O)c2c1O	400	nM
CHEMBL569375	Oc1ccc2C(=O)N(Cc3cccc(Br)c3)C(=O)c2c1O	400	nM
CHEMBL551559	Oc1ccc2C(=O)N(Cc3cc(F)cc(F)c3)C(=O)c2c1O	400	nM
CHEMBL2206759	CN(C)S(=O)(=O)c1ccc(cc1)c2cc3CN(Cc4ccc(F)c(Cl)c4)C(=O)c3c(O)c2O	400	nM
CHEMBL2206766	CN1CCN(CC1)S(=O)(=O)c2cc(O)c(O)c3C(=O)N(Cc4ccc(F)c(Cl)c4)Cc23	400	nM
CHEMBL3582082	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc3ccccc3n2)c4ccccc4C1=O)\O	400	nM
CHEMBL541369	COc1c2CCc3cc4C=NN(C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15)c7ccccc7	410	nM
CHEMBL2206774	CC(C)c1c(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc2c1S(=O)(=O)N4CCOCC4	410	nM
CHEMBL3415832	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)cc1c3ccccc3)\O	420	nM
CHEMBL216389	CN1CCCCC1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	440	nM
CHEMBL1257700	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)c4noc(Cc5ccc(F)cc5)n4	450	nM
CHEMBL3087621	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(F)ccc2F	450	nM
CHEMBL3582059	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(O)cc2)c3ccccc3C1=O)\O	450	nM
CHEMBL574315	OC(=O)\C(=C\C(=O)c1cc(CN=[N+]=[N-])cc(CN=[N+]=[N-])c1)\O	460	nM
CHEMBL3741323	COc1ccc(cc1)C2=Cc3ccc(cc3C(CC(=O)C)N2c4ccc(F)cc4)[N+](=O)[O-]	460	nM
CHEMBL401801	CN1CCN(CC1)C(=O)c2cc(F)ccc2CNC(=O)C3=C(O)C(=O)N(C)C(=N3)C(C)(C)C	490	nM
CHEMBL3087624	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(F)cc(F)c2	490	nM
CHEMBL403574	Oc1cccc(C(=O)NNC(=O)c2ccccc2O)c1O	500	nM
CHEMBL560202	Oc1ccc2CN(Cc3ccc(F)cc3F)C(=O)c2c1O	500	nM
CHEMBL563552	Oc1ccc2C(=O)N(Cc3cc(F)c(F)cc3F)C(=O)c2c1O	500	nM
CHEMBL582913	OC(=O)\C(=C\C(=O)c1cccn1CCCc2ccccc2)\O	500	nM
CHEMBL573874	OC(=O)\C(=C\C(=O)c1ccc(Cc2ccccc2)s1)\O	500	nM
CHEMBL2180599	Oc1c(nc(Br)c2cccnc12)C(=O)NCc3ccc(F)cc3	500	nM
CHEMBL3334637	Cc1ccc(CNC(=O)C2=C(O)C(=O)NC(=N2)c3ccc(F)cc3)cc1C	500	nM
CHEMBL1289652	CN(O)C(=O)c1cc2c(cn(Cc3ccc(F)cc3)c2cn1)C(=O)NCCN4CCOCC4	503	nM
CHEMBL1289312	CN(O)C(=O)c1cc2c(CN3CCC[C@@H]3C(=O)N)cn(Cc4ccc(F)cc4)c2cn1	509.93	nM
CHEMBL3415841	CCOC(=O)\C(=C\C(=O)c1cccn1Cc2ccc(F)cc2)\O	510	nM
CHEMBL3582060	COc1ccc(CN2C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c3ccccc23)cc1	510	nM
CHEMBL1214587	COc1cccc2c1c(cn2Cc3ccccc3Cl)C(=O)\C=C(/O)\C(=O)O	520	nM
CHEMBL225681	OC(=O)C(=O)CC(=O)c1ccc2ccc3cccc4ccc1c2c34	530	nM
CHEMBL3087336	COc1ccccc1Cn2ccccc2\C=C\C(=O)CC(=O)C(=O)O	530	nM
CHEMBL3087790	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(F)c2F	530	nM
CHEMBL3125976	ON1C(=O)C(=Cc2cccc(O)c12)C(=O)NCc3ccc(F)c(Cl)c3	530	nM
CHEMBL1289199	CN(O)C(=O)c1cc2c(CN3CCN(C)CC3)cn(Cc4ccc(F)cc4)c2cn1	534	nM
CHEMBL2171669	CN(C)C(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	540	nM
CHEMBL3582058	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(Cl)cc2)c3ccccc3C1=O)\O	540	nM
CHEMBL458064	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccccc3C1=O)\O	542.95	nM
CHEMBL232436	COc1ccc(CNC(=O)c2nc(nc(O)c2O)c3cccs3)cc1	549.54	nM
CHEMBL562482	CN1CCCCC1(C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	550	nM
CHEMBL573873	OC(=O)\C(=C\C(=O)c1ccn(Cc2ccccc2)c1)\O	550	nM
CHEMBL1289981	COCCOCCCc1cn(Cc2ccc(F)cc2)c3cnc(cc13)C(=O)N(C)O	552	nM
CHEMBL1289863	CN(O)C(=O)c1cc2c(CCCN3CCOCC3)cn(Cc4ccc(F)cc4)c2cn1	559	nM
CHEMBL2407284	ON1C(=O)C(C(=O)NCc2ccc(O)cc2O)c3ccccc3C1=O	572	nM
CHEMBL1213724	COc1cccc2c1c(cn2Cc3ccc(Cl)cc3)C(=O)\C=C(/O)\C(=O)O	590	nM

CHEMBL3415848	OC(=O)\C(=C\C(=O)\C=C\c1cc(cn1c2ccccc2)C(=O)c3ccc(F)cc3)\O	590	nM
CHEMBL240506	Oc1c(\C=N\Nc2nc(Nc3ccccc3)nc(Nc4ccccc4)n2)cc(Br)cc1[N+](=O)[O-]	600	nM
CHEMBL253394	Oc1ccc2CN(N3C(=O)c4ccc(O)c(O)c4C3=O)C(=O)c2c1O	600	nM
CHEMBL495960	COc1cccc2c1c(cn2Cc3ccc(F)c(F)c3)C(=O)\C=C(/O)\C(=O)O	600	nM
CHEMBL522229	OCCCCN1C=C(C(=O)O)C(=O)c2cc(Cc3ccc(Cl)cc3Cl)ccc12	600	nM
CHEMBL459381	COc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncc(Cc5ccc(F)cc5)cc14	600	nM
CHEMBL572334	Oc1ccc2C(=O)N(Cc3cc(F)c(F)c(F)c3)C(=O)c2c1O	600	nM
CHEMBL3087623	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)c(F)c2	600	nM
CHEMBL3334633	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(F)cc3	600	nM
CHEMBL3415856	CCOC(=O)\C(=C\C(=O)\C=C\c1cccn1Cc2ccc(F)c(F)c2)\O	600	nM
CHEMBL3740792	COc1ccc(cc1)C2=Cc3ccc(cc3C(CC(=O)C)N2c4ccc(C)cc4)[N+](=O)[O-]	600	nM
CHEMBL523303	Oc1c(ncc2cccnc12)c3nnc(Cc4ccc(Cl)cc4)[nH]3	640	nM
CHEMBL3582061	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(cc2)[N+](=O)[O-])c3ccccc3C1=O)\O	640	nM
CHEMBL3736051	CCOC(=O)C1=C(CC)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccccc3	640	nM
CHEMBL260398	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3c(OC)ccc(OC)c13)\O	660	nM
CHEMBL496580	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2F)c3cccc(OC)c13)\O	670	nM
CHEMBL241924	CC1CCC(N1C)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	690	nM
CHEMBL36640	COc1cc(\C=C\c2ccc3ccc(C(=O)O)c(O)c3n2)cc(O)c1O	700	nM
CHEMBL539708	Oc1ccc2CN(Cc3cccc(F)c3F)C(=O)c2c1O	700	nM
CHEMBL549298	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(Br)cc3	700	nM
CHEMBL549299	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3cccc(Br)c3	700	nM
CHEMBL1631331	[Na+].COc1cc(\C=C\c2ccc3ccc(C(=O)[O-])c(O)c3n2)cc(O)c1O	700	nM
CHEMBL2180585	CS(=O)(=O)NCCCN(c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13)S(=O)(=O)C	700	nM
CHEMBL2180586	CS(=O)(=O)NCCCCCCN(c1nc(C(=O)NCc2ccc(F)cc2)c(O)c3ncccc13)S(=O)(=O)C	700	nM
CHEMBL3397851	COC1=C(N=C(Cc2ccc(O)cc2)N(C)C1=O)C(=O)N3CCN(CCNC(=O)c4cc(O)c(O)c(O)c4)CC3	700	nM
CHEMBL3582038	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2)c3ccccc3C1=O)\O	700	nM
CHEMBL3739466	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(C[N+](=O)[O-])N2c4ccc(Cl)cc4	700	nM
CHEMBL373761	Oc1nc(nc(C(=O)NCC2CCCCC2)c1O)c3cccs3	707.11	nM
CHEMBL3334635	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(Br)cc3	707.11	nM
CHEMBL244051	CC1CCN(C)C1C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3	710	nM
CHEMBL496565	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccccc2F)c3cccc(OC)c13)\O	720	nM
CHEMBL578595	Oc1ccc2C(=O)N(Cc3cccc4ccccc34)C(=O)c2c1O	720	nM
CHEMBL524273	OC(=O)\C=C\c1ccc(O)c(O)c1\C(=C\c2ccc(O)c(O)c2)\C(=O)O	730	nM
CHEMBL1214417	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccccc2Cl)c3cccc(OC)c13)\O	730	nM
CHEMBL2407276	ON1C(=O)C(C(=O)Nc2ccccc2)c3ccccc3C1=O	730	nM
CHEMBL3415852	OC(=O)\C(=C\C(=O)\C=C\c1cn(Cc2ccc(F)cc2)cc1c3ccccc3)\O	730	nM
CHEMBL443502	Oc1ccc2CN(Cc3cccc4ccccc34)C(=O)c2c1O	740	nM
CHEMBL1214535	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cccc(Cl)c2F)c3cccc(OC)c13)\O	740	nM
CHEMBL572472	OC(=O)\C(=C\C(=O)c1cccc(Cc2ccc(Cl)cc2)c1)\O	750	nM
CHEMBL3087334	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(c2)C#N	750	nM
CHEMBL210396	CN(C)C(=O)Oc1c2CN(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14	760	nM
CHEMBL1257580	OC1=C(N=C2C=CC(=CN2C1=O)N3CCOCC3)C(=O)NCc4ccc(F)cc4	775	nM
CHEMBL1928170	Cc1c(nnn1Cc2cccc(F)c2)C(=O)\C=C(/O)\c3cc(O)c(O)c(O)c3	780	nM
CHEMBL3125977	ON1C(=O)C(=Cc2cccc(O)c12)C(=O)NCc3ccc(F)c(F)c3	780	nM
CHEMBL3415842	CCOC(=O)\C(=C\C(=O)c1cc(cn1Cc2ccc(F)cc2)c3ccccc3)\O	790	nM

CHEMBL550574	Cc1cc(CN2C(=O)c3ccc(O)c(O)c3C2=O)ccc1F	800	nM
CHEMBL553173	Oc1ccc2C(=O)N(Cc3ccc(F)c(F)c3F)C(=O)c2c1O	800	nM
CHEMBL568970	Oc1ccc2CN(Cc3ccc4ccccc4c3)C(=O)c2c1O	800	nM
CHEMBL402709	Oc1ccc2CN(N3C(=O)c4cc(O)c(O)cc4C3=O)C(=O)c2c1O	810	nM
CHEMBL498204	CCOC(=O)\C(=C\C(=O)c1cn(Cc2c(F)ccc(F)c2F)c3cccc(OC)c13)\O	820	nM
CHEMBL3739970	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)CO)N2c4ccc(cc4)[N+](=O)[O-]	820	nM
CHEMBL456580	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(F)cc3C1=O)\O	830.66	nM
CHEMBL49201	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2	843.21	nM
CHEMBL3735829	CCOC(=O)C1=C(CC)N(Cc2ccc(Cc3cccc(c3)C(=O)\C=C(/O)\C(=O)O)cc2)C(=O)N=C1c4ccccc4	850	nM
CHEMBL2206232	Oc1c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc2cc1c4ccccc4	870	nM
CHEMBL1214584	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(Cl)ccc2F)c3cccc(OC)c13)\O	890	nM
CHEMBL464215	CN1C(=O)C(=C(O)c2cc(Cc3ccc(F)cc3)ccc12)C(=O)O	900	nM
CHEMBL444646	ON1C(=O)Cc2ccc(Br)cc2C1=O	900	nM
CHEMBL563507	Oc1ccc2CN(Cc3ccc(F)c(F)c3)C(=O)c2c1O	900	nM
CHEMBL561770	Cc1cc(CN2Cc3ccc(O)c(O)c3C2=O)ccc1F	900	nM
CHEMBL569376	Oc1ccc2C(=O)N(Cc3ccc(Cl)c(F)c3)C(=O)c2c1O	900	nM
CHEMBL556071	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(F)cc3	900	nM
CHEMBL563783	Oc1ccc2C(=O)N(Cc3ccc(F)c(Br)c3)C(=O)c2c1O	900	nM
CHEMBL2297144	Oc1ccc(\C=C\S(=O)(=O)CS(=O)(=O)\C=C\c2ccc(O)c(O)c2O)c(O)c1O	900	nM
CHEMBL3397844	COC1=C(N=C(Cc2ccccc2)N(C)C1=O)C(=O)N3CCN(CCCNC(=O)c4cc(O)c(O)c(O)c4CC3	900	nM
CHEMBL3087631	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(F)c2	920	nM
CHEMBL3735630	CCOC(=O)c1c(CC)nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)nc1c3ccc(F)cc3	920	nM
CHEMBL510677	Oc1c(ncc2cccnc12)c3noc(Cc4ccccc4)n3	950	nM
CHEMBL574570	OC(=O)c1cc2ccn(Cc3cccc(Cl)c3F)c2cn1	950	nM
CHEMBL579040	Oc1ccc2C(=O)N(Cc3ccc4ccccc4c3)C(=O)c2c1O	960	nM
CHEMBL3087331	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(Cl)cc(Cl)c2	970	nM
CHEMBL3087630	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2F	980	nM
CHEMBL373760	Oc1nc(nc(C(=O)Nc2ccccc2)c1O)c3cccs3	1000	nM
CHEMBL241597	OC1=C(C(=O)NNC(=O)c2cccc(c2)[N+](=O)[O-])C(=O)Nc3ccccc13	1000	nM
CHEMBL572338	Oc1ccc2C(=O)N(Cc3ccccc(I)c3)C(=O)c2c1O	1000	nM
CHEMBL557898	Oc1ccc2CN(Cc3ccc(F)c(Br)c3)C(=O)c2c1O	1000	nM
CHEMBL2180588	Oc1c(nc(NCCc2c[nH]c3ccccc23)c4cccnc14)C(=O)NCc5ccc(F)cc5	1000	nM
CHEMBL3085796	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)cc2F	1000	nM
CHEMBL3087632	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2F	1000	nM
CHEMBL3334636	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(F)c(F)c3	1000	nM
CHEMBL3334647	OC1=C(N=C(NC1=O)c2ccccc2)C(=O)NCc3ccc(F)cc3	1000	nM
CHEMBL3334652	OC1=C(N=C(NC1=O)c2cccc(F)c2)C(=O)NCc3ccc(F)cc3	1000	nM
CHEMBL490971	Oc1c(ncc2cccnc12)c3nnc(Cc4cccc(Cl)c4)[nH]3	1030	nM
CHEMBL2407282	COc1ccc(CNC(=O)C2C(=O)N(O)C(=O)c3ccccc23)cc1	1030	nM
CHEMBL236241	OC1=CC(=O)N2CCCN(Cc3ccc(F)cc3)C(=O)C2=C1O	1040	nM
CHEMBL3582052	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cccc(Cl)c2F)c3ccccc3C1=O)\O	1080	nM
CHEMBL507259	OC(=O)Cc1c(O)c(O)ccc1\C=C\C(=O)O	1090	nM
CHEMBL3735944	CCOC(=O)C1=C(CC)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(F)cc3	1100	nM
CHEMBL2407279	ON1C(=O)C(C(=O)Nc2ccc(F)cc2)c3ccccc3C1=O	1120	nM
CHEMBL496346	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)c(F)c2F)c3cccc(OC)c13)\O	1150	nM
CHEMBL574571	OC(=O)c1cc2ccn(Cc3c(F)cc(Cl)cc3F)c2cn1	1190	nM

CHEMBL49363	Cc1ccc(Cn2cccc2\C=C\C(=O)CC(=O)C(=O)O)cc1	1200	nM
CHEMBL377693	CCOc1ccc(cc1)c2c3CN(Cc4ccc(F)cc4)C(=O)c3c(O)c5ncccc25	1200	nM
CHEMBL252570	Oc1ccc2CN(N3Cc4ccc(O)c(O)c4S3(=O)=O)C(=O)c2c1O	1200	nM
CHEMBL550838	Oc1ccc2CN(Cc3cc(Cl)ccc3F)C(=O)c2c1O	1200	nM
CHEMBL1214534	CCOC(=O)\C(=C\C(=O)c1cn(Cc2c(F)cccc2Cl)c3cccc(OC)c13)\O	1200	nM
CHEMBL3087328	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(F)cc(F)c2	1200	nM
CHEMBL3415836	CCOC(=O)\C(=C\C(=O)\C=C\c1cc(cn1c2ccccc2)C(=O)c3ccc(F)cc3)\O	1200	nM
CHEMBL3735286	CCOC(=O)c1c(nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)nc1c3ccc(OC)cc3)c4ccccc4	1200	nM
CHEMBL458275	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(F)ccc3C1=O)\O	1249	nM
CHEMBL3334634	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(Cl)cc3	1264.91	nM
CHEMBL458280	OCCCN1C=C(C(=O)O)C(=O)c2cc(Cc3ccc(Cl)cc3Cl)ccc12	1300	nM
CHEMBL564499	Oc1ccc2C(=O)N(Cc3ccc(F)cc3Cl)C(=O)c2c1O	1300	nM
CHEMBL560769	Oc1ccc2C(=O)N(Cc3c(F)c(F)c(F)c(F)c3F)C(=O)c2c1O	1300	nM
CHEMBL557046	CCOc1ccc(NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2)cc1	1300	nM
CHEMBL2171668	CNC(=O)C1=C(O)C(=O)C(=CN1)C(=O)NCc2ccc(F)cc2	1300	nM
CHEMBL3087629	Cc1cccc(Cn2cccc2\C=C\C(=O)CC(=O)C(=O)O)c1	1300	nM
CHEMBL3582051	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cc(C)cc(C)c2)c3ccccc3C1=O)\O	1300	nM
CHEMBL3735397	CCOC(=O)C1=C(C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(F)cc3	1300	nM
CHEMBL3736042	CCOC(=O)C1=C(N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3cc(C)cc(C)c3)c4ccccc4	1300	nM
CHEMBL2236589	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccccc2OC)c3ccccc3C1=O)\O	1400	nM
CHEMBL3334640	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3cccc(Cl)c3	1400	nM
CHEMBL3334644	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3cccc(Cl)c3F	1400	nM
CHEMBL3582041	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(O)cc2)c3ccccc3C1=O)\O	1400	nM
CHEMBL497394	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(F)c(F)c(F)c2)c3cccc(OC)c13)\O	1410	nM
CHEMBL1289080	CN(O)C(=O)c1cc2c(CN3CCC(O)C3)cn(Cc4ccc(F)cc4)c2cn1	1421	nM
CHEMBL562196	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(F)c(F)c3	1500	nM
CHEMBL549713	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccccc3	1500	nM
CHEMBL2206233	Oc1cc2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c(O)c1O	1500	nM
CHEMBL496142	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)c(F)c2)c3cccc(OC)c13)\O	1560	nM
CHEMBL497661	CCN1C=C(C(=O)O)C(=O)C2=C1C(=O)C=C(Sc3ccccc3)C2=O	1600	nM
CHEMBL560002	CC(=O)Oc1cc(cc(OC(=O)C)c1OC(=O)C)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccccc3	1600	nM
CHEMBL549995	CC(=O)Oc1cc(cc(OC(=O)C)c1OC(=O)C)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccccc3C	1600	nM
CHEMBL3087338	Cc1cc(C)cc(Cn2cccc2\C=C\C(=O)CC(=O)C(=O)O)c1	1600	nM
CHEMBL3087620	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)c(F)c2	1600	nM
CHEMBL3415833	CCOC(=O)\C(=C\C(=O)c1ccn(Cc2ccc(F)cc2)c1)\O	1600	nM
CHEMBL19977	OC(=O)C(=O)CC(=O)c1cc(OCc2ccccc2)cc(OCc3ccccc3)c1	1641.65	nM
CHEMBL226490	OC(=O)C(=O)CC(=O)c1c2ccccc2cc3ccccc13	1700	nM
CHEMBL562335	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(Cl)c(Cl)c3	1700	nM
CHEMBL3087335	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(cc2)C#N	1700	nM
CHEMBL3087626	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2c(Cl)cccc2Cl	1700	nM
CHEMBL36303	Oc1ccccc1C(=O)NNC(=O)c2ccccc2O	1800	nM
CHEMBL252700	COc1cccc(CN(Cc2cccc(OC)c2)c3ccc4nc(N)[nH]c4c3)c1	1800	nM
CHEMBL549415	Oc1ccc2C(=O)N(Cc3c(F)ccc(F)c3F)C(=O)c2c1O	1800	nM
CHEMBL556473	Oc1ccc2C(=O)N(Cc3cccc(Cl)c3F)C(=O)c2c1O	1843.91	nM
CHEMBL557770	OC(=O)C(=O)CC(=O)c1ccc(NC(=O)c2ccccc2)s1	1900	nM
CHEMBL3736096	CCOC(=O)C1=C(N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(OC)cc3)c4ccccc4	1900	nM

CHEMBL388276	COc1cccc(\C=C\C(=O)c2ccccc2)c1O	2000	nM
CHEMBL562273	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)NCc3ccc(Cl)cc3	2000	nM
CHEMBL559681	Cc1ccccc1NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2	2000	nM
CHEMBL561709	Oc1ccc2C(=O)N(Cc3ccccc3F)C(=O)c2c1O	2000	nM
CHEMBL561593	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)NCc3ccc(F)cc3	2000	nM
CHEMBL564228	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(Cl)cc3	2000	nM
CHEMBL549886	Oc1ccc2CN(Cc3cccc(Cl)c3F)C(=O)c2c1O	2000	nM
CHEMBL551560	Oc1ccc2C(=O)N(Cc3c(F)cccc3F)C(=O)c2c1O	2000	nM
CHEMBL557865	NS(=O)(=O)c1ccc(NC(=O)c2cc(O)c(O)c(O)c2)cc1	2000	nM
CHEMBL1223974	CC1(C)Oc2ccc3C(=O)C(=C(O)C(=O)c3c2C=C1)C4=C(C(=O)c5ccccc5C4=O)C6=C(O)C(=O)c7c8C=CC(C)(C)Oc8ccc7C6=O	2000	nM
CHEMBL1813126	CCOC(=O)CC(=O)Nc1ccc(cc1)C(=O)O	2000	nM
CHEMBL3334638	COc1ccc(CNC(=O)C2=C(O)C(=O)NC(=N2)c3ccc(F)cc3)cc1	2000	nM
CHEMBL3334650	OC1=C(N=C(NC1=O)c2ccccc2F)C(=O)NCc3ccc(F)cc3	2000	nM
CHEMBL3735322	CCOC(=O)C1=C(N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccccc3)c4ccccc4	2000	nM
CHEMBL211275	CCOC(=O)c1cccc(c1)c2c3CN(Cc4ccc(F)cc4)C(=O)c3c(O)c5ncccc25	2100	nM
CHEMBL252905	NC(=N)c1ccc2cc(ccc2c1)C#Cc3cccc(OCc4ccccc4)c3	2100	nM
CHEMBL497490	CCN1C=C(C(=O)O)C(=O)C2=C1C(=O)C=C(Nc3ccc(F)c(Cl)c3)C2=O	2100	nM
CHEMBL473489	O\C(=C/C(=O)c1c[nH]c2ccc(Cl)cc12)\c3nnn[nH]3	2100	nM
CHEMBL555736	COc1c2CCc3cc(\C=N\Nc4ccc(cc4)[N+](=O)[O-])c(C(=O)O)c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	2200	nM
CHEMBL3582044	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2F)c3ccccc3C1=O)\O	2200	nM
CHEMBL3735665	CCOC(=O)c1c(CC)nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)nc1c3cccc3	2230	nM
CHEMBL495970	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cccc(F)c2)c3cccc(OC)c13)\O	2260	nM
CHEMBL3735583	CCOC(=O)c1c(CC)nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)nc1c3ccc(OC)cc3	2270	nM
CHEMBL2206772	CCCCc1c(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc2c1S(=O)(=O)N(C)C	2300	nM
CHEMBL3582066	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(Cl)cc2Cl)c3ccccc3C1=O)\O	2300	nM
CHEMBL3735455	CCOC(=O)C1=C(C(C)C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccccc3	2300	nM
CHEMBL259012	OC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3ccccc13)\O	2330	nM
CHEMBL1673089	OC(=O)\C(=C\C(=O)c1cn(Cc2ccccc2)c3ccccc13)\O	2330	nM
CHEMBL260619	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3cc(OC)ccc13)\O	2340	nM
CHEMBL212320	CN(C)C(=O)Oc1c2C(=O)N(Cc3ccc(F)cc3)C(=O)c2c(O)c4ncccc14	2400	nM
CHEMBL491149	Oc1c(ncc2cccnc12)c3nnc(CCc4ccccc4)[nH]3	2400	nM
CHEMBL574316	OC(=O)\C(=C\C(=O)C(=O)c1cccc(c1)C(=O)c2ccccc2)\O	2400	nM
CHEMBL1270317	ON1C(=O)C=C(c2cccc(c2)c3ccccc3)c4cccnc14	2400	nM
CHEMBL3238122	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(ccc3C1=O)N4CCN(CC)CC4)\O	2400	nM
CHEMBL3397845	COC1=C(N=C(Cc2ccc(Cl)cc2)N(C)C1=O)C(=O)N3CCN(CCCNC(=O)c4cc(O)c(O)c(O)c4)CC3	2400	nM
CHEMBL3734837	CCOC(=O)C1=C(C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccccc3	2400	nM
CHEMBL3734908	CCOC(=O)C1=C(N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(F)cc3)c4ccccc4	2400	nM
CHEMBL3116306	NC(Cc1ccc(Cl)c(Cl)c1)(P(=O)(O)O)P(=O)(O)O	2449.49	nM
CHEMBL456365	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(ccc3C1=O)N4CCCC4)\O	2491.99	nM
CHEMBL388420	Oc1nc(nc(C(=O)Nc2cncs2)c1O)c3cccs3	2500	nM
CHEMBL561646	Oc1ccc2CN(Cc3ccc(F)cc3Cl)C(=O)c2c1O	2500	nM
CHEMBL556642	CCCCc1ccc(NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2)cc1	2500	nM

CHEMBL557319	Cc1cc(C)cc(NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2)c1	2500	nM
CHEMBL564494	OC(=O)\C(=C\C(=O)c1cccc(Br)c1)\O	2500	nM
CHEMBL1223975	COc1ccc2C(=O)C(=C(C(=O)c2c1)C3=C(O)C(=O)c4c5C=CC(C)(C)Oc5ccc4C3=O)C6=C(O)C(=O)c7c8C=CC(C)(C)Oc8ccc7C6=O	2500	nM
CHEMBL3397850	COC1=C(N=C(Cc2ccc(F)cc2)N(C)C1=O)C(=O)N3CCN(CCNC(=O)c4cc(O)c(O)c(O)c4)CC3	2500	nM
CHEMBL3415838	CCOC(=O)\C(=C\C(=O)\C=C\c1cc(cn1Cc2ccc(F)cc2)c3ccccc3)\O	2500	nM
CHEMBL1087929	Oc1nc(nc(C(=O)NCc2cncs2)c1O)c3cccs3	2511.89	nM
CHEMBL1214481	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2Cl)c3cccc(OC)c13)\O	2560	nM
CHEMBL254727	CC(C)S(=O)(=O)Nc1ccc2nc(N)[nH]c2c1	2600	nM
CHEMBL1928167	Cc1c(nnn1Cc2ccc(F)cc2)C(=O)\C=C(/O)\c3cc(O)c(O)c(O)c3	2600	nM
CHEMBL496455	CCOC(=O)\C(=C\C(=O)C1=CNc2ccc(Cl)cc2C1=O)\O	2632.49	nM
CHEMBL405652	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3c(OC)cccc13)\O	2640	nM
CHEMBL456158	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(Cl)c(Cl)cc3C1=O)\O	2649.53	nM
CHEMBL555734	CCOC(=O)CN1N=Cc2cc3CCc4c(OC)c5C(=O)c6c(O)c(C)c(O)cc6C(=O)c5c(O)c4c3c(O)c2C1=O	2670	nM
CHEMBL569135	Oc1ccc2CN(Cc3ccc(F)c(F)c3F)C(=O)c2c1O	2700	nM
CHEMBL496143	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(F)cc(F)c2)c3cccc(OC)c13)\O	2740	nM
CHEMBL490972	COc1cccc(Cc2nnc([nH]2)c3ncc4cccnc4c3O)c1	2800	nM
CHEMBL2206771	CN(C)S(=O)(=O)c1c(C)c(O)c(O)c2C(=O)N(Cc3ccc(F)c(Cl)c3)Cc12	2800	nM
CHEMBL3735239	CCOC(=O)c1c(nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C=O)O)nc1c3ccc(F)cc3)c4ccccc4	2800	nM
CHEMBL254632	Oc1cccc(C(=O)NNC(=O)c2cccc(O)c2O)c1O	2828.43	nM
CHEMBL1214478	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cccc(Cl)c2)c3cccc(OC)c13)\O	2890	nM
CHEMBL3740311	COc1ccc(cc1)C2=Cc3ccc(cc3C(CC(=O)C)N2c4ccc(cc4)C#N)[N+](=O)[O-]	2900	nM
CHEMBL1214533	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(F)ccc2Cl)c3cccc(OC)c13)\O	2940	nM
CHEMBL30922	COC(=O)[C@H](COC(=O)\C=C\c1ccc(OC(=O)C)c(OC(=O)C)c1)NC(=O)\C=C\c2ccc(OC(=O)C)c(OC(=O)C)c2	3000	nM
CHEMBL226484	Cc1ccc2cc(ccc2c1)C(=O)CC(=O)C(=O)O	3000	nM
CHEMBL249349	Cc1ccc(cc1)n2c(SCC(=O)NNC(=O)c3ccccc3O)nnc2c4ccccc4O	3000	nM
CHEMBL457779	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccc4ccccc4c3)cc1Cl	3000	nM
CHEMBL458228	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3ccc(Br)cc3)cc1Cl	3000	nM
CHEMBL564594	Oc1ccc2CN(Cc3cccc(Br)c3)C(=O)c2c1O	3000	nM
CHEMBL552413	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(cc3)[N+](=O)[O-]	3000	nM
CHEMBL558132	Oc1cc(cc(O)c1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccc(F)c(F)c3F	3000	nM
CHEMBL1223978	CC1(C)Oc2ccc3C(=O)C(=C(O)C(=O)c3c2C=C1)C4=C(C(=O)c5c6C=CC(C)(C)Oc6ccc5C4=O)C7=C(O)C(=O)c8c9C=CC(C)(C)Oc9ccc8C7=O	3000	nM
CHEMBL2216808	Oc1ccc(NC(=O)C(=S)NN2C(=S)S\C(=C\c3cc(I)cc(I)c3O)\C2=O)cc1	3000	nM
CHEMBL3334642	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3cccc(F)c3	3000	nM
CHEMBL562425	COc1c2CCc3cc4C=NN(C(=N)N)C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	3020	nM
CHEMBL3582053	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(Cl)c2)c3ccccc3C1=O)\O	3100	nM
CHEMBL3740012	[O-][N+](=O)CC1N(C(=Cc2ccc(cc12)[N+](=O)[O-])c3ccccc3)c4ccc(Cl)cc4	3100	nM
CHEMBL562741	COc1c2CCc3cc(\C=N\NC(=N)N)c(C(=O)O)c(O)c3c2c(O)c4C(=O)c5cc(O)c(C)c(O)c5C(=O)c14	3150	nM
CHEMBL1214583	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cc(F)cc(Cl)c2)c3cccc(OC)c13)\O	3170	nM
CHEMBL565676	OC(=O)c1cc2ccn(Cc3cc(Cl)cs3)c2cn1	3200	nM
CHEMBL3582063	OC(=O)\C(=C\C(=O)C1=CN(Cc2cc(F)ccc2F)c3ccccc3C1=O)\O	3200	nM
CHEMBL3736464	CCOC(=O)C1=C(C(C)C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O	3300	nM

126

	)N=C1c3ccc(OC)cc3		
CHEMBL1774045	OC1=C2C(=O)N(Cc3ccc(F)c(Cl)c3)C(=O)C2=C4CCCCN4C1=O	3304.54	nM
CHEMBL1214585	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(Cl)cc2F)c3cccc(OC)c13)\O	3320	nM
CHEMBL404423	CC(C)(C)C1CCC(CC1)C2=NCCc3ccc(cc23)[C@H]4CC4c5ccc6cc(ccc6c5)C(=N)N	3400	nM
CHEMBL540405	COc1c2CCc3cc4C=NN(C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15)c7ccc(cc7)C(=O)O	3450	nM
CHEMBL523302	Oc1c(ncc2cccnc12)c3nnc(Cc4cccnc4)[nH]3	3500	nM
CHEMBL562110	Oc1ccc2C(=O)N(Cc3c(F)cccc3Cl)C(=O)c2c1O	3500	nM
CHEMBL568050	OC(=O)c1cc2ccn(Cc3ccc(F)cc3F)c2cn1	3500	nM
CHEMBL3397847	COC1=C(N=C(Cc2ccc(C)cc2)N(C)C1=O)C(=O)N3CCN(CCCNC(=O)c4cc(O)c(O)c(O)c4)CC3	3500	nM
CHEMBL3582078	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc3ccccc3n2)c4ccccc4C1=O)\O	3500	nM
CHEMBL3116308	OP(=O)(O)C(Cc1ccc(Cl)c(Cl)c1)(Cc2ccc(Cl)c(Cl)c2)P(=O)(O)O	3577.71	nM
CHEMBL226485	OC(=O)C(=O)CC(=O)c1ccc2ccc3ccccc3c2c1	3600	nM
CHEMBL3735086	CCOC(=O)C1=C(C(C)C)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(F)cc3	3600	nM
CHEMBL576026	OC(=O)c1cc2ccn(Cc3ccc(F)c(F)c3F)c2cn1	3690	nM
CHEMBL260778	OC(=O)[C@@H](Cc1cc(O)c(O)cc1[N+](=O)[O-])OC(=O)\C=C\c2ccc(O)c(O)c2	3700	nM
CHEMBL550086	Oc1ccc2CN(Cc3cc(F)c(F)cc3F)C(=O)c2c1O	3700	nM
CHEMBL3582045	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cc(F)ccc2F)c3ccccc3C1=O)\O	3700	nM
CHEMBL242139	CN1CCN(C(C1)C2=NC(=C(O)C(=O)N2C)C(=O)NCc3ccc(F)cc3)C(=O)C	4000	nM
CHEMBL241397	OC(=O)c1cc(ccc1Cl)c2oc(\C=N\Nc3nc4nonc4nc3Nc5ccccc5F)cc2	4000	nM
CHEMBL506605	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5ccc6c(C[C@@H](NC(=O)C(=O)c7cc(Cl)c(O)c(Cl)c7)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C@@H](C1=O)c8cc(Cl)c(O)c(Cl)c8)c9cc(Cl)c(O)c(Cl)c9)c[nH]c6c5)cc2)C(=O)N[C@@H](C(=O)O)c%10ccc(O)cc%10	4000	nM
CHEMBL461996	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cc(sc3C(=O)N2Cc4ccccc4)C(C)(C)C	4000	nM
CHEMBL459890	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cc(sc3C(=O)N2Cc4ccccc4)c5ccc(Cl)cc5	4000	nM
CHEMBL561849	Oc1ccc2CN(Cc3cc(F)c(F)c(F)c3)C(=O)c2c1O	4000	nM
CHEMBL560706	Oc1ccc2CN(Cc3cccc(I)c3)C(=O)c2c1O	4000	nM
CHEMBL550978	Oc1ccc2C(=O)N(Cc3c(F)ccc(F)c3Cl)C(=O)c2c1O	4000	nM
CHEMBL540719	Oc1ccc2CN(Cc3cccc(Cl)c3)C(=O)c2c1O	4000	nM
CHEMBL576652	Oc1ccc2C(=O)N(C3Cc4ccccc4C3)C(=O)c2c1O	4000	nM
CHEMBL1223981	CC1(C)Oc2ccc3C(=O)C(=C(O)C(=O)c3c2C=C1)C4=C(C(=O)N(Cc5ccccc5)C4=O)C6=C(O)C(=O)c7c8C=CC(C)(C)Oc8ccc7C6=O	4000	nM
CHEMBL3087622	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2c(F)cccc2F	4000	nM
CHEMBL3334639	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCCc3ccc(F)cc3	4000	nM
CHEMBL3334645	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(F)c(Cl)c3	4000	nM
CHEMBL552100	COc1c2CCc3cc4C=NNC(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	4060	nM
CHEMBL46032	COc1ccc(Cn2ccccc2\C=C\C(=O)CC(=O)C(=O)O)cc1	4100	nM
CHEMBL299873	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(Cl)cc2	4100	nM
CHEMBL1761475	CCC1=C(N(COCCc2ccc(F)cc2)C(=O)N(O)C1=O)C(=O)c3ccccc3	4100	nM
CHEMBL131784	Cc1cc(c(S)cc1Cl)S(=O)(=O)Nc2nnc3c4scc(C)c4ncn23	4260	nM
CHEMBL3415835	CCOC(=O)\C(=C\C(=O)\C=C\c1cc(cn1Cc2ccccc2)C(=O)c3ccc(F)cc3)\O	4300	nM
CHEMBL555979	Oc1ccc2CN(Cc3cc(Cl)c(F)cc3F)C(=O)c2c1O	4400	nM
CHEMBL562871	COc1ccc(NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2)cc1	4500	nM

CHEMBL1213850	COc1cccc2c1c(cn2Cc3ccc(Cl)c(F)c3)C(=O)\C=C(/O)\C(=O)O	4580	nM
CHEMBL366861	Cc1cc(O)c(C=O)c2Oc3c(C)c(C(=O)O)c(O)c(COC(=O)\C=C\C(=O)O)c3OC(=O)c12	4600	nM
CHEMBL490970	Oc1c(ncc2cccnc12)c3nnc(Cc4ccncc4)[nH]3	4600	nM
CHEMBL564339	COc1c2CCc3cc4C=NN(CC(=O)O)C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	4620	nM
CHEMBL565954	Oc1ccc2C(=O)N([C@H]3CCc4ccccc34)C(=O)c2c1O	4647.58	nM
CHEMBL453488	CC(C)C(=C)CC[C@@H](C)[C@H]1CC=C2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)CC[C@H](OS(=O)(=O)O)C(C)(C)[C@@H]4CC3	4800	nM
CHEMBL472374	Cc1cc(c(S)cc1Cl)S(=O)(=O)Nc2nc(N)n[nH]2	4900	nM
CHEMBL1631332	[Na+].COc1cc(\C=C\c2ccc3ccc(C(=O)[O-])c(O)c3n2)cc(OC)c1O	4900	nM
CHEMBL2236598	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cccc(F)c2)c3ccccc3C1=O)\O	4900	nM
CHEMBL3087329	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(Cl)cc2Cl	4900	nM
CHEMBL250975	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(c3ccc(Cl)cc3)n2c4ccccc4	5000	nM
CHEMBL525803	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5cccc6c(C[C@@H](NC(=O)C(=O)c7cc(Cl)c(O)c(Cl)c7)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C@@H](C1=O)c8cc(Cl)c(O)c(Cl)c8)c9cc(Cl)c(O)c(Cl)c9)c[nH]c56)cc2)C(=O)N[C@@H](C(=O)O)c%10ccc(O)cc%10	5000	nM
CHEMBL511191	CCCCCN1C(=O)C(=C(O)c2cc(Cc3ccc(F)cc3)ccc12)C(=O)O	5000	nM
CHEMBL1223976	CCCOc1ccc2C(=O)C(=C(C(=O)c2c1)C3=C(O)C(=O)c4c5C=CC(C)(C)Oc5ccc4C3=O)C6=C(O)C(=O)c7c8C=CC(C)(C)Oc8ccc7C6=O	5000	nM
CHEMBL1813504	Oc1cc(cc(C(=O)NCc2ccc(F)cc2)c1O)S(=O)(=O)N3CCCCC3	5000	nM
CHEMBL551241	Oc1ccc2C(=O)N(Cc3ccc(F)cc3)C(=O)c2c1O	5147.82	nM
CHEMBL3742287	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(cc4)[N+](=O)[O-]	5200	nM
CHEMBL2206231	CC(C)c1cc2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c(O)c1O	5400	nM
CHEMBL565266	OC(=O)c1cc2ccn(Cc3cccc(Cl)c3Cl)c2cn1	5420	nM
CHEMBL1270108	OC(=O)C1=NN(C(=O)/C/1=C\c2ccc(O)c(OCc3ccc(F)cc3)c2)c4cccc(c4)[N+](=O)[O-]	5477.23	nM
CHEMBL3582046	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(F)c2)c3ccccc3C1=O)\O	5500	nM
CHEMBL1213849	COc1cccc2c1c(cn2Cc3ccc(Cl)cc3F)C(=O)\C=C(/O)\C(=O)O	5520	nM
CHEMBL454134	C[C@H](CCC1(CO)C(C)(C)C)O)[C@H]2CC[C@H]3C4=C([C@@H](O)[C@H](OC(=O)C)[C@]23C)[C@@]5(C)C[C@H](OC(=O)CCCCCCCCCCCO)[C@H](OS(=O)(=O)O)C(C)(C)[C@@H]5CC4	5600	nM
CHEMBL561619	OC[C@H](C1CCCCC1)N2C=C(C(=O)O)C(=O)c3cc(Cc4cccc(Cl)c4F)ccc23	5600	nM
CHEMBL2407275	CN(C(=O)C1C(=O)N(O)C(=O)c2ccccc12)c3ccccc3	5600	nM
CHEMBL3735646	CCOC(=O)C1=C(CC)N(Cc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)C(=O)N=C1c3ccc(OC)cc3	5600	nM
CHEMBL583059	OC(=O)\C(=C\C(=O)c1ccccc1Cc2ccccc2)\O	5670	nM
CHEMBL550220	COc1cc2N(C=C(C(=O)O)C(=O)c2cc1Cc3cccc(Cl)c3F)[C@H](CO)C(C)(C)C	5800	nM
CHEMBL550080	CCC[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)c(OC)cc12	5800	nM
CHEMBL250367	COc1ccccc1n2c(SCC(=O)NNC(=O)c3ccccc3O)nnc2c4ccccc4O	6000	nM
CHEMBL400055	Oc1cccc(C(=O)NN2Cc3ccc(O)c(O)c3C2=O)c1O	6000	nM
CHEMBL448564	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5cccc6c(C[C@@H](N)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C@@H](C1=O)c7cc(Cl)c(O)c(Cl)c7)c8cc(Cl)c(O)c(Cl)c8)c[nH]c56)cc2)C(=O)O	6000	nM
CHEMBL461997	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cc(sc3C(=O)N2Cc4ccccc4)c5ccccc5	6000	nM
CHEMBL459891	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cc(sc3C(=O)N2Cc4occc4)c5ccsc5	6000	nM

CHEMBL464212	CN1C(=O)C(=C(O)c2cc(Cc3ccccc3)ccc12)C(=O)O	6000	nM
CHEMBL565125	CC(C)(C)[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12	6000	nM
CHEMBL540720	Oc1ccc2CN(Cc3ccc(Cl)c(F)c3)C(=O)c2c1O	6000	nM
CHEMBL1223980	CC1(C)CCc2c(O1)ccc3C(=O)C(=C(C(=O)c23)C4=C(O)C(=O)c5c6C=CC(C)(C)Oc6ccc5C4=O)C7=C(O)C(=O)c8c9C=CC(C)(C)Oc9ccc8C7=O	6000	nM
CHEMBL3087333	OC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2C#N	6000	nM
CHEMBL3087634	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(Cl)c2	6000	nM
CHEMBL3334641	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccc(O)cc3	6000	nM
CHEMBL538448	COc1c2CCc3cc(\C=N\NC(=O)c4ccccc4O)c(C(=O)O)c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	6090	nM
CHEMBL3735570	CCOC(=O)c1c(nc(SCc2ccc(cc2)C(=O)\C=C(/O)\C(=O)O)nc1c3ccccc3)c4ccccc4	6100	nM
CHEMBL239057	CCOc1ccc(cc1)c2c(C#N)c(N)nc(SCC(=O)C3=Cc4cc(Br)cc(Br)c4OC3=O)c2C#N	6196.77	nM
CHEMBL554095	COc1c2CCc3cc4C=NN(CCOC(=O)C)C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	6280	nM
CHEMBL523468	COc1ccc(Cc2nnc([nH]2)c3ncc4cccnc4c3O)cc1OC	6300	nM
CHEMBL557286	CCCN1N=Cc2cc3CCc4c(OC)c5C(=O)c6c(O)c(C)c(O)cc6C(=O)c5c(O)c4c3c(O)c2C1=O	6340	nM
CHEMBL3739763	COc1ccc(cc1)C2=Cc3ccc(cc3C(CC(=O)C)N2c4ccc(O)cc4)[N+](=O)[O-]	6600	nM
CHEMBL560836	COc1cc2N(C=C(C(=O)O)C(=O)c2cc1Cc3cccc(Cl)c3F)[C@H](CO)C4CCCCC4	6700	nM
CHEMBL567591	Oc1ccc2C(=O)N(CCc3ccccc3)C(=O)c2c1O	6800	nM
CHEMBL2206230	CCCCc1cc2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c(O)c1O	6800	nM
CHEMBL236066	Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3cccc(Cl)c3)c4ncc(s4)S(=O)(=O)c5ccc(cc5)[N+](=O)[O-]	6985.7	nM
CHEMBL226434	COC(=O)c1ccccc1c2ccc(cc2[N+](=O)[O-])C(=O)CC(=O)C(=O)O	7000	nM
CHEMBL375956	OC(=O)C(=O)CC(=O)c1ccc2ccccc2c1	7000	nM
CHEMBL457778	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccc(Cl)c(Cl)c3)cc1Cl	7000	nM
CHEMBL458432	Cc1cc(Cl)cc2SC(=NS(=O)(=O)c12)C(=O)c3ccc4ccccc4c3	7000	nM
CHEMBL1761476	CCC1=C(N(COCCc2ccc(F)cc2)C(=O)N(O)C1=O)C(=O)c3cc(C)cc(C)c3	7000	nM
CHEMBL3334643	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3ccccc3F	7000	nM
CHEMBL3582068	Cc1ccc(CN2C=C(C(=O)\C=C(/O)\C(=O)O)C(=O)c3ccccc23)c(C)c1	7000	nM
CHEMBL456791	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3cc(Cl)ccc3C1=O)\O	7099.3	nM
CHEMBL3125975	OC1=C(C(=O)NCc2ccc(F)cc2F)C(=O)Nc3ncccc13	7100	nM
CHEMBL477328	O=C(CN1CCCC1)Nc2ccc(Cc3ccc(NC(=O)CN4CCCC4)cc3)cc2	7290	nM
CHEMBL585005	OC(=O)c1cc2ccn(Cc3ccc(F)cc3)c2cn1	7350	nM
CHEMBL129147	Cc1cc2nc3nc(N)nc(NS(=O)(=O)c4cc(C)c(Cl)cc4S)n3c2cc1C	7410	nM
CHEMBL573623	OC(=O)\C(=C\C(=O)c1cccn1Cc2ccc(cc2)c3ccccc3)\O	7500	nM
CHEMBL406929	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3ccc(OC)cc13)\O	7550	nM
CHEMBL3739984	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)CO)N2c4ccc(cc4)C#N	7600	nM
CHEMBL550839	COc1c2CCc3cc4C(O)N(N(C)C)C(=O)c4c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	7700	nM
CHEMBL1270510	NCc1ccc(cc1)c2ccccc2C3=CC(=O)N(O)c4ncccc34	7800	nM
CHEMBL3125973	OC1=C(C(=O)NCc2ccc(F)c(Cl)c2)C(=O)Nc3ncccc13	7800	nM
CHEMBL491685	Cn1nc(nc1Cc2ccc(F)cc2)c3ncc4cccnc4c3O	7900	nM
CHEMBL3742037	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(F)cc4	7900	nM
CHEMBL457850	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3ccc(Cl)cc3C1=O)\O	7937.25	nM
CHEMBL385951	Oc1nc(nc(C(=O)NCc2ccccc2)c1O)c3ccccc3	8000	nM

CHEMBL250777	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(Cc3ccccc3)n2c4cccc(Cl)c4	8000	nM
CHEMBL254853	COc1cccc(C(=O)NNC(=O)c2cc3ccccc3cc2O)c1O	8000	nM
CHEMBL507121	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5cccc6c(C[C@@H](NC(=O)C(=O)c7cc(Cl)c(O)c(Cl)c7)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C@@H](C1=O)c8cc(Cl)c(O)c(Cl)c8)c9cc(Cl)c(O)c(Cl)c9)c[nH]c56)cc2)C(=O)O	8000	nM
CHEMBL475854	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)c2cc(cc(c2O)[N+](=O)[O-])[N+](=O)[O-])c1)\O	8000	nM
CHEMBL458653	Clc1ccc2c(SC(=NS2(=O)=O)C(=O)c3ccc4ccccc4c3)c1	8000	nM
CHEMBL562442	Oc1ccc2CN(Cc3c(F)c(F)c(F)c(F)c3F)C(=O)c2c1O	8000	nM
CHEMBL551736	Cc1ccc(NS(=O)(=O)c2ccc(NC(=O)c3cc(O)c(O)c(O)c3)cc2)cc1C	8000	nM
CHEMBL1813506	CC(C)(C)NS(=O)(=O)c1cc(O)c(O)c(c1)C(=O)NCc2ccc(F)cc2	8000	nM
CHEMBL3087627	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(Cl)cc(Cl)c2	8000	nM
CHEMBL3087792	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(C)c2	8000	nM
CHEMBL3334646	OC1=C(N=C(NC1=O)c2ccc(F)cc2)C(=O)NCc3cc(F)c(F)c(F)c3	8000	nM
CHEMBL1270511	NCc1ccc(cc1)c2ccccc(CC3=CC(=O)N(O)c4ncccc34)c2	8100	nM
CHEMBL3125974	OC1=C(C(=O)NCc2ccc(F)c(F)c2)C(=O)Nc3ncccc13	8100	nM
CHEMBL563677	CCC[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12	8200	nM
CHEMBL1214479	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(Cl)cc2)c3cccc(OC)c13)\O	8260	nM
CHEMBL399581	Oc1cccc(\C=N\NC(=O)c2cccc(O)c2O)c1O	8378.54	nM
CHEMBL2297149	NNS(=O)(=O)c1cccc(OCC(=O)O)c1	8700	nM
CHEMBL569371	Oc1ccc2CN(Cc3c(F)ccc(F)c3Cl)C(=O)c2c1O	8900	nM
CHEMBL398969	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(c3ccccc3O)n2Cc4ccccc4	9000	nM
CHEMBL250574	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(c3ccccc3)n2Cc4ccccc4	9000	nM
CHEMBL464213	CCCCCN1C(=O)C(=C(O)c2ccccc12)C(=O)Nc3cc(ccc3O)[N+](=O)[O-]	9000	nM
CHEMBL446297	CC(C)C(=C)CC[C@@H](C)[C@H]1CC=C2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)C[C@@H](O)[C@H](OS(=O)(=O)O)C(C)(C)[C@@H]4CC3	9000	nM
CHEMBL549816	CC[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12	9000	nM
CHEMBL583869	C[C@@H](C1CCCc2ccccc12)N3Cc4ccc(O)c(O)c4C3=O	9000	nM
CHEMBL1223979	CC1(C)CCc2c(O1)ccc3C(=O)C(=C(O)C(=O)c23)C4=C(C(=O)c5c6CCC(C)(C)Oc6ccc5C4=O)O	9000	nM
CHEMBL3087635	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2C#N	9000	nM
CHEMBL1270417	NCc1cccc(c1)c2ccccc(c2)C3=CC(=O)N(O)c4ncccc34	9100	nM
CHEMBL462081	Clc1ccc2c(SC(NS2(=O)=O)C(=O)c3ccc4ccccc4c3)c1	9165.15	nM
CHEMBL1214480	CCOC(=O)\C(=C\C(=O)c1cn(Cc2cccc(F)c2Cl)c3cccc(OC)c13)\O	9200	nM
CHEMBL396335	CC1(C)OC(=O)C2([C@H](CC(=O)C[C@H]2c3c[nH]c4ccccc34)c5occc5)C(=O)O1	9600	nM
CHEMBL557891	OC[C@@H](N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12)c4ccccc4	9800	nM
CHEMBL253138	Oc1ccc2CN(Cc3ccc(F)cc3)C(=O)c2c1O	10000	nM
CHEMBL254527	OC(=O)\C(=C(/C#N)\c1cn(c2ccc(F)cc2)c3ccccc13)\O	10000	nM
CHEMBL457536	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3ccc(Cl)c(Cl)c3)cc1Cl	10000	nM
CHEMBL456024	Clc1ccc(cc1)C(=O)C2NS(=O)(=O)c3ccc(Cl)cc3S2	10000	nM
CHEMBL1223983	COc1ccc2C(=O)C(=C(O)C(=O)c2c1)C3=C(C(=O)c4ccccc4C3=O)C5=C(O)C(=O)c6cc(OC)ccc6C5=O	10000	nM
CHEMBL1224084	COc1cc2C(=O)C(=C(C(=O)c2cc1OC)C3=C(C(=O)c4cc(OC)c(OC)cc4C3=O)C5=C(O)C(=O)c6cc(OC)c(OC)cc6C5=O)O	10000	nM
CHEMBL2297143	Cc1ccc(cc1)n2ncnc2c3nc4ccccc4nc3NS(=O)(=O)c5cc(C(=O)Nc6ccccc6)c(Cl)cc5S	10000	nM
CHEMBL3334648	OC1=C(N=C(Cc2ccc(F)cc2)NC1=O)C(=O)NCc3ccc(F)cc3	10000	nM
CHEMBL576837	C[C@H](N1Cc2ccc(O)c(O)c2C1=O)c3ccc4ccccc4c3	10507.14	nM

CHEMBL3741789	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(C)cc4	10600	nM
CHEMBL1774044	OC1=C2C(=O)N(Cc3ccc(F)c(Cl)c3)C(=O)C2=C4CCCN4C1=O	10900	nM
CHEMBL401049	Oc1ccc(Br)cc1\C=N\Nc2nc3nonc3nc2Nc4ccc(F)cc4	11000	nM
CHEMBL252775	Oc1ccc2CN(N3C(=O)c4cccc(O)c4C3=O)C(=O)c2c1O	11000	nM
CHEMBL478246	CN(C)c1ccc(\C=C\C(=O)C2=C(O)C=C(C)OC2=O)s1	11000	nM
CHEMBL1269999	COc1ccc(\C=C\2/C(=O)N(N=C2C(=O)O)c3cccc(c3)[N+](=O)[O-])cc1Cc4ccc(F)cc4	11000	nM
CHEMBL1270406	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc1Cc4ccc(F)cc4	11000	nM
CHEMBL1813508	Oc1cc(cc(C(=O)NCc2ccc(cc2)C(F)(F)F)c1O)S(=O)(=O)N3CCCCC3	11000	nM
CHEMBL3087633	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(F)c2	11000	nM
CHEMBL3582047	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cc(F)cc(F)c2)c3ccccc3C1=O)\O	11000	nM
CHEMBL457106	Clc1ccc2c(SC(NS2(=O)=O)C(=O)c3ccc(Cl)c(Cl)c3)c1	11180.34	nM
CHEMBL573638	OC(=O)\C(=C\C(=O)c1ccc(Oc2ccccc2)cc1)\O	11400	nM
CHEMBL443983	CC(C)C(=C)CC[C@@H](C)[C@H]1CC=C2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)C[C@@H](OC(=O)CN)[C@H](OC(=O)CN)C(C)(C)[C@@H]4CC3	11500	nM
CHEMBL2206229	Cc1cc2CN(Cc3ccc(F)c(Cl)c3)C(=O)c2c(O)c1O	11500	nM
CHEMBL444733	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3ccccc3)cc1Cl	11618.95	nM
CHEMBL514422	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3c(F)cccc3C1=O)\O	11627.55	nM
CHEMBL3742275	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(Cl)cc4	11800	nM
CHEMBL239485	Oc1cc2ccccc2cc1C(=O)NNC(=O)COc3ccc4ccccc4c3	12000	nM
CHEMBL401050	O=C(CSc1nc(SCC(=O)NCc2occc2)nc(SCC(=O)NCc3occc3)n1)NCc4occc4	12000	nM
CHEMBL241495	CN(C)[C@H]1[C@@H]2C[C@H]3C(=C(O)[C@]2(O)C(=O)C(=C1O)C(=O)NCN4CCN(CC4)c5cc6N(C=C(C(=O)O)C(=O)c6cc5F)C7CC7)C(=O)c8c(O)cccc8[C@@]3(C)O	12000	nM
CHEMBL396688	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCN(CNC(=O)C4=C(O)[C@H]([C@@H]5[C@@H](O)[C@H]6C(=C(O)[C@]5(O)C4=O)C(=O)c7c(O)cccc7[C@@]6(C)O)N(C)C)CC3	12000	nM
CHEMBL250977	Cc1ccc(cc1)n2c(SCC(=O)NNC(=O)c3ccccc3O)nnc2c4ccccc4	12000	nM
CHEMBL506797	CC(C)C(=C)CC[C@@H](C)[C@H]1CC=C2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)C[C@@H](O)[C@H](OC(=O)CCC(=O)O)C(C)(C)[C@@H]4CC3	12000	nM
CHEMBL391925	CC(C)C(=C)CC[C@@H](C)[C@H]1CC=C2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)C[C@@H](OC(=O)CCC(=O)O)[C@H](O)C(C)(C)[C@@H]4CC3	12000	nM
CHEMBL449723	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccccc3)cc1Cl	12000	nM
CHEMBL559410	Oc1ccc(\C=C\C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccccc3)cc1O	12000	nM
CHEMBL1223984	COc1cc2C(=O)C(=C(C(=O)c2cc1OC)C3=C(C(=O)c4ccccc4C3=O)C5=C(O)C(=O)c6cc(OC)c(OC)cc6C5=O)O	12000	nM
CHEMBL1270908	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cc(Cl)cc(Cl)c3)cc1OCc4ccc(F)cc4	12000	nM
CHEMBL1813496	Oc1cccc(C(=O)NCc2cccs2)c1O	12000	nM
CHEMBL3087788	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2OCC	12000	nM
CHEMBL3741160	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C)N2c4ccc(O)cc4	12000	nM
CHEMBL3116307	OP(=O)(O)C(Cc1ccc(Cl)c(Cl)c1)P(=O)(O)O	12247.45	nM
CHEMBL253137	Oc1ccc2CN(Cc3ccccc3)C(=O)c2c1O	12300	nM
CHEMBL524869	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5ccc6c(NC(=O)C6(O)C[C@@H](NC(=O)C(=O)c7cc(Cl)c(O)c(Cl)c7)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C@@H](C1=O)c8cc(Cl)c(O)c(Cl)c8)c9cc(Cl)c(O)c(Cl)c9)c5)cc2)C(=O)N[C@@H](C(=O)O)c%10ccc(O)cc%10	12500	nM
CHEMBL524665	CN1[C@@H](Cc2ccc(Oc3cc4cc(c3O)c5ccc6C(C[C@@H](NC(=O)C(=O)c7cc(Cl)c(O)c(Cl)c7)C(=O)N[C@@H](C(=O)N[C@H]4C(=O)N[C	12500	nM

131

	@@H](C1=O)c8cc(Cl)c(O)c(Cl)c8)c9cc(Cl)c(O)c(Cl)c9)C(=O)Nc6c5)c2)C(=O)N[C@@H](C(=O)O)c%10ccc(O)cc%10		
CHEMBL561566	CO\N=C\c1cc2CCc3c(OC)c4C(=O)c5c(O)c(C)c(O)cc5C(=O)c4c(O)c3c2c(O)c1C(=O)O	12500	nM
CHEMBL510036	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3ccc(Cl)cc3)cc1Cl	12649.11	nM
CHEMBL1213725	COc1cccc2c1c(cn2Cc3cccc(F)c3Cl)C(=O)\C=C(/O)\C(=O)O	12740	nM
CHEMBL1224051	Oc1cc(cc(O)c1O)C(=O)NCCCN2CCN(CC2)C(=O)\C=C\c3ccccc3	12830	nM
CHEMBL456991	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)cc2)c3c(Cl)cccc3C1=O)\O	12899.61	nM
CHEMBL226489	OC(=O)C(=O)CC(=O)c1ccc2cc3ccccc3cc2c1	13000	nM
CHEMBL241359	COc1ccc(Nc2nc(NCc3occc3)nc(N\N=C\c4ccc(Br)cc4)n2)cc1	13000	nM
CHEMBL396907	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(cc12)N3CCN(CNC(=O)C4=C(O)[C@H]([C@@H]5C[C@H]6C(=C(O)[C@]5(O)C4=O)C(=O)c7c(O)cccc7[C@@]6(C)O)N(C)C)CC3	13000	nM
CHEMBL398846	Oc1ccc2CN(Cc3cccc(CBr)c3)C(=O)c2c1O	13000	nM
CHEMBL1223982	COc1cccc2C(=O)C(=C(C(=O)c12)C3=C(C(=O)c4ccccc4C3=O)C5=C(O)C(=O)c6cccc(OC)c6C5=O)O	13000	nM
CHEMBL1224083	OC1=C(C(=O)c2ccccc2C1=O)C3=C(C(=O)c4ccccc4C3=O)C5=C(O)C(=O)c6ccccc6C5=O	13000	nM
CHEMBL1813507	Oc1cc(cc(C(=O)NCc2occc2)c1O)S(=O)(=O)N3CCCCC3	13000	nM
CHEMBL2180600	CS(=O)(=O)Oc1c(nc(Br)c2cccnc12)C(=O)NCc3ccc(F)cc3	13000	nM
CHEMBL2311867	COc1cc(Br)cc(\C=N\NC(=O)c2ccccn2)c1O	13000	nM
CHEMBL3087785	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cccc(c2)C#N	13000	nM
CHEMBL554301	COc1c2CCc3cc(C(=O)O)c(C(=O)O)c(O)c3c2c(O)c4C(=O)c5cc(O)c(C)c(O)c5C(=O)c14	13200	nM
CHEMBL34249	OC(Cc1ccc(Cl)c(Cl)c1)(P(=O)(O)O)P(=O)(O)O	13416.41	nM
CHEMBL392565	COc1c(N2CCN(CNC(=O)C3=C(O)[C@H]([C@@H]4[C@@H](O)[C@H]5C(=C(O)[C@]4(O)C3=O)C(=O)c6c(O)cccc6[C@@]5(C)O)N(C)C)C(C)C2)c(F)cc7C(=O)C(=CN(C8CC8)c17)C(=O)O	13500	nM
CHEMBL427703	CC1(C)OC(=O)C2([C@H](CC(=O)C[C@H]2c3occc3)c4occc4)C(=O)O1	13700	nM
CHEMBL565985	C[C@H](N1Cc2ccc(O)c(O)c2C1=O)c3cccc4ccccc34	13899.64	nM
CHEMBL464216	CN1C(=O)C(=C(O)c2cc(Oc3ccccc3)ccc12)C(=O)O	14000	nM
CHEMBL501254	C[C@H](CCC1(CO1)C(C)(C)O)[C@H]2CC=C3C4=C([C@@H](O)[C@H](OC(=O)C)[C@]23C)[C@@]5(C)C[C@@H](OC(=O)CCCCCCCCCCCCCCCO)[C@H](OS(=O)(=O)O)C(C)(C)[C@@H]5CC4	14000	nM
CHEMBL453267	Cc1cc(Cl)cc2SC(NS(=O)(=O)c12)C(=O)c3ccc(Cl)cc3	14000	nM
CHEMBL456030	Cc1cc(Cl)cc2SC(NS(=O)(=O)c12)C(=O)c3ccc(Cl)c(Cl)c3	14000	nM
CHEMBL1270000	COc1ccc(\C=C\2/C(=O)N(N=C2C(=O)O)c3cccc(c3)[N+](=O)[O-])cc1OCc4ccc(F)cc4	14000	nM
CHEMBL1813512	CC(=O)Nc1cc(O)c(O)c(c1)C(=O)NCc2ccc(F)cc2	14000	nM
CHEMBL3582077	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccncc2)c3ccccc3C1=O)\O	14000	nM
CHEMBL2297148	O=C1NC(=S)SC1NS(=O)(=O)c2ccc(cc2)N=Nc3ncccn3	14120	nM
CHEMBL538878	COc1c2CCc3cc(\C=N\NC(=O)c4ccccc4)c(C(=O)O)c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	14600	nM
CHEMBL48381	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2	15000	nM
CHEMBL503991	CC(C)C(=C)CC[C@@H](C)[C@H]1CC[C@H]2C3=C([C@@H](O)[C@H](OC(=O)C)[C@]12C)[C@@]4(C)C[C@@H](O)[C@H](OS(=O)(=O)O)C(C)(C)[C@@H]4CC3	15000	nM
CHEMBL462288	Clc1ccc(cc1Cl)C(=O)C2NS(=O)(=O)c3ccccc3S2	15000	nM
CHEMBL1269478	ON1C(=O)C=Cc2cccnc12	15000	nM
CHEMBL1270213	COc1cc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc(OC)c1OC	15000	nM
CHEMBL1813497	Oc1cccc(C(=O)NCc2occc2)c1O	15000	nM
CHEMBL2311873	Oc1ccc(Br)cc1\C=N\NC(=O)C2=NNC3CCCCC23	15000	nM

CHEMBL3741987	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)CO)N2c4ccc(C)cc4	15100	nM
CHEMBL1224124	Oc1cccc(\C=C\C(=O)N2CCN(CCCNC(=O)c3cc(O)c(O)c(O)c3)CC2)c1	15410	nM
CHEMBL3116305	OC(Cc1ccc(Cl)cc1)(P(=O)(O)O)P(=O)(O)O	15874.51	nM
CHEMBL197014	CC(C)CN1C(=O)C(=C(O)c2ccccc12)C(=O)Nc3ccccc3S(=O)(=O)N	16000	nM
CHEMBL225682	Cc1ccc2Oc3nc(C)c(cc3C(=O)c2c1)C(=O)CC(=O)C(=O)O	16000	nM
CHEMBL240547	COc1ccc(cc1)C(=O)Nc2ccccc2C(=O)NC(C(C)C)C(=O)NNC(=O)c3cccc3O	16000	nM
CHEMBL1270602	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(c3)c4ccccc4)cc1OCc5ccc(F)cc5	16000	nM
CHEMBL2236602	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2cccc(OC)c2)c3ccccc3C1=O)\O	16000	nM
CHEMBL3582081	OC(=O)\C(=C\C(=O)C1=CN(Cc2ccncc2)c3ccccc3C1=O)\O	16000	nM
CHEMBL526642	COCCN1C=C(C(=O)O)C(=O)c2cc(Cc3ccc(Cl)cc3Cl)ccc12	16500	nM
CHEMBL232024	Oc1nc(nc(C(=O)NCc2ccncc2)c1O)c3cccs3	16595.87	nM
CHEMBL1084126	Oc1nc(nc(C(=O)NCn2ccnc2)c1O)c3cccs3	16982.44	nM
CHEMBL392160	CCN1C(=O)C(=C(O)c2ccccc12)C(=O)NNC(=O)c3cccc(c3)[N+](=O)[O-]	17000	nM
CHEMBL239176	CN(C)[C@H]1[C@@H]2[C@@H](O)[C@H]3C(=C(O)[C@]2(O)C(=O)C(=C1O)C(=O)NCN4CCN(CC4)c5cc6N(C=C(C(=O)O)C(=O)c6cc5F)C7CC7)C(=O)c8c(O)cccc8[C@@]3(C)O	17000	nM
CHEMBL398970	COc1ccc(cc1)n2c(Cc3ccccc3)nnc2SCC(=O)NNC(=O)c4ccccc4O	17000	nM
CHEMBL250779	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(Cc3ccccc3)n2C4CCCCC4	17000	nM
CHEMBL456482	COc1ccc(cc1)C(=O)C2NS(=O)(=O)c3cc(C)c(Cl)cc3S2	17000	nM
CHEMBL565527	C[C@H](N1Cc2ccc(O)c(O)c2C1=O)c3ccc(F)cc3	17182.55	nM
CHEMBL1224052	Cc1ccc(\C=C\C(=O)N2CCN(CCCNC(=O)c3cc(O)c(O)c(O)c3)CC2)cc1	17470	nM
CHEMBL456031	Cc1cc(Cl)cc2SC(NS(=O)(=O)c12)C(=O)c3ccc4ccccc4c3	17492.86	nM
CHEMBL3739597	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)CO)N2c4ccc(Cl)cc4	17900	nM
CHEMBL394650	Oc1ccccc1C(=O)NNC(=O)COc2ccc3ccccc3c2	18000	nM
CHEMBL241804	COc1ccc(cc1)C(=O)NNC(=O)c2cc3ccccc3cc2O	18000	nM
CHEMBL239177	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(N3CCN(CNC(=O)C4=C(O)[C@H]([C@@H]5C[C@@H]6Cc7c(ccc(O)c7C(=O)C6=C(O)[C@]5(O)C4=O)N(C)C)N(C)C)C(C)C3)c(F)c12	18000	nM
CHEMBL475828	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)\C=C\c2ccc(Cl)cc2)c1)\O	18000	nM
CHEMBL561848	Oc1ccc2CN(Cc3c(F)cccc3Cl)C(=O)c2c1O	18000	nM
CHEMBL1270416	NCc1ccccc1c2ccccc(c2)C3=CC(=O)N(O)c4ncccc34	18000	nM
CHEMBL1813501	Oc1cccc(C(=O)NCC2CCCCC2)c1O	18000	nM
CHEMBL1978342	OC1=C(C(C2=C(O)c3ccccc3OC2=O)c4ccc(cc4)C(=O)c5ccccc5)C(=O)Oc6ccccc16	18000	nM
CHEMBL3125978	ON1C(=O)C(=Cc2cccc(O)c12)C(=O)NCc3ccc(F)cc3F	18000	nM
CHEMBL511508	OCCN1C=C(C(=O)O)C(=O)c2cc(Sc3ccccc3)ccc12	18500	nM
CHEMBL3397849	COC1=C(N=C(Cc2ccccc2)N(C)C1=O)C(=O)N3CCN(CCNC(=O)c4cc(O)c(O)c(O)c4)CC3	18600	nM
CHEMBL3397846	COC1=C(N=C(Cc2ccc(F)cc2)N(C)C1=O)C(=O)N3CCN(CCCNC(=O)c4cc(O)c(O)c(O)c4)CC3	18900	nM
CHEMBL1269893	COc1ccc(\C=C\2/C(=O)N(N=C2C(=O)O)c3cccc(Br)c3)cc1OCc4ccc(F)cc4	19000	nM
CHEMBL1270700	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(c3)[N+](=O)[O-])cc1OCc4ccc(F)cc4	19000	nM
CHEMBL1813509	Oc1cc(cc(C(=O)NCC2CCCCC2)c1O)S(=O)(=O)N3CCCCC3	19000	nM
CHEMBL3087789	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2cc(C)cc(C)c2	19000	nM
CHEMBL1224122	Oc1cc(cc(O)c1O)C(=O)NCCCN2CCN(CC2)C(=O)\C=C\c3ccccc3Cl	19270	nM
CHEMBL3125968	ON1C(=O)C(=Cc2ccccc12)C(=O)NCc3ccc(F)cc3F	19700	nM
CHEMBL252551	COc1cccc(C(=O)NNC(=O)c2cccc(O)c2O)c1O	19899.75	nM
CHEMBL459074	COc1ccc(cc1)C(=O)C2=NS(=O)(=O)c3cc(C)c(Cl)cc3S2	19899.75	nM

CHEMBL235417	COc1ccc(OC)c(c1)C(=O)C2=C(O)C(=O)N(CCCCCC(=O)O)C2c3ccc(Cl)cc3	20000	nM
CHEMBL239696	CCN1C(=O)C(=C(O)c2ccccc12)C(=O)NNC(=O)c3ccc(cc3)[N+](=O)[O-]	20000	nM
CHEMBL240752	NC(=O)NN=C1c2cc(ccc2c3ccc(cc13)S(=O)(=O)NCc4occc4)S(=O)(=O)NCc5occc5	20000	nM
CHEMBL468656	CCCC[C@@H](C)C1=C(O)C(=O)[C@@H]2C[C@H](C)C[C@@H]([C@H]2[C@]1(C)C(=O)CCO)C(=O)O	20000	nM
CHEMBL512638	CCCCCC[C@@H](C)C1=C(O)C(=O)[C@@H]2[C@H](O)[C@H](C)C[C@H](O)[C@H]2[C@]1(C)C(=O)\C=C/O	20000	nM
CHEMBL560218	Oc1ccc2CN(Cc3c(F)cccc3F)C(=O)c2c1O	20000	nM
CHEMBL554975	COc1c2CCc3cc4C5SCC(N5C(=O)c4c(O)c3c2c(O)c6C(=O)c7cc(O)c(C)c(O)c7C(=O)c16)C(=O)O	20000	nM
CHEMBL1813514	CN(C)Cc1ccc(C(=O)NCc2ccc(F)cc2)c(O)c1O	20000	nM
CHEMBL1214586	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(Cl)c(F)c2)c3cccc(OC)c13)\O	20350	nM
CHEMBL235847	CCOC(=O)c1sc(nc1C)N2C(C(=C(O)C2=O)C(=O)c3ccccc3)c4ccc(F)cc4	21000	nM
CHEMBL438489	OC1=C(C(N(C1=O)c2nc3ccccc3s2)c4ccc5OCOc5c4)C(=O)c6ccccc6	21000	nM
CHEMBL399559	COc1ccc(cc1OC)c2nnc(SCC(=O)NNC(=O)c3ccccc3O)n2c4ccccc4	21000	nM
CHEMBL252161	Oc1ccc2CN(NS(=O)(=O)c3ccc(F)cc3)C(=O)c2c1O	21000	nM
CHEMBL561164	Oc1ccc2CN(Cc3cccc(F)c3)C(=O)c2c1O	21000	nM
CHEMBL1761473	CCC1=C(N(COCc2ccc(F)cc2)C(=O)N(O)C1=O)C(=O)c3cc(C)cc(C)c3	21000	nM
CHEMBL1813498	Oc1cccc(C(=O)NCc2ccc(cc2)c3cccs3)c1O	21000	nM
CHEMBL430776	[Na+].COc1ccc(cc1O)c2c3c4cc(OC)c(OS(=O)(=O)[O-])cc4OC(=O)c3n5ccc6cc(OC)c(OC)cc6c25	22000	nM
CHEMBL254852	COc1cccc(C(=O)NNC(=O)c2cccc(OC)c2O)c1O	22000	nM
CHEMBL505948	COc1ccc(cc1O)c2c3c4cc(OC)c(OS(=O)(=O)O)cc4OC(=O)c3n5ccc6cc(OC)c(OC)cc6c25	22000	nM
CHEMBL475819	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)\C=C\c2ccc(F)cc2)c1)\O	22000	nM
CHEMBL538947	COc1c2CCc3cc(\C=N\NS(=O)(=O)c4ccc(C)cc4)c(C(=O)O)c(O)c3c2c(O)c5C(=O)c6cc(O)c(C)c(O)c6C(=O)c15	22000	nM
CHEMBL1270308	Oc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc1OCc4ccc(F)cc4	22000	nM
CHEMBL1813513	Oc1cc(cc(C(=O)NCc2ccc(F)cc2)c1O)C#N	22000	nM
CHEMBL3741049	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)CO)N2c4ccc(O)cc4	22100	nM
CHEMBL3740456	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(cc4)C#N	22200	nM
CHEMBL3397848	COC1=C(N=C(Cc2ccc(Cl)c(Cl)c2)N(C)C1=O)C(=O)N3CCN(CCCNC(=O)c4cc(O)c(O)c(O)c4)CC3	22400	nM
CHEMBL428588	Oc1cccc(C(=O)NNC(=O)c2cc3ccccc3cc2O)c1O	22627.42	nM
CHEMBL389881	OC(=O)C(=O)CC(=O)c1ccc(cc1)N2CCOCC2	23000	nM
CHEMBL445242	CC1=CC(=C(C(=O)\C=C\c2ccc(Br)s2)C(=O)O1)O	23000	nM
CHEMBL586817	Oc1ccc2CN(C3Cc4ccccc4C3)C(=O)c2c1O	23000	nM
CHEMBL1813386	Oc1cccc(C(=O)NCc2ccc(F)c(F)c2)c1O	23000	nM
CHEMBL3087787	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2OC	23000	nM
CHEMBL563525	C[C@@H](CO)N1C=C(C(=O)O)C(=O)c2cc(Cc3cccc(Cl)c3F)ccc12	23808.4	nM
CHEMBL145	OC(=O)\C=C\c1ccc(O)c(O)c1	24000	nM
CHEMBL1270501	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(c3)C(F)(F)F)cc1OCc4ccc(F)cc4	24000	nM
CHEMBL1270611	NCc1ccc(cc1)c2ccc(CC3=CC(=O)N(O)c4ncccc34)cc2	24000	nM
CHEMBL1813493	Oc1cccc(C(=O)NCc2ccc3[nH]ccc3c2)c1O	24000	nM
CHEMBL497505	CN(C)CCN1C=C(C(=O)O)C(=O)c2cc(Cc3ccc(Cl)cc3Cl)ccc12	24100	nM
CHEMBL568462	C[C@H](C1CCc2ccccc12)N3Cc4ccc(O)c(O)c4C3=O	24372.12	nM
CHEMBL1224053	Oc1cc(cc(O)c1O)C(=O)NCCCN2CCN(CC2)C(=O)\C=C\c3ccc(Cl)cc3	24940	nM

CHEMBL240543	Oc1ccc(C(=O)CSc2nnc([nH]2)c3ccncc3)c(O)c1	25000	nM
CHEMBL456475	Cc1cc(Cl)cc2SC(=NS(=O)(=O)c12)C(=O)c3ccc(Cl)cc3	25000	nM
CHEMBL456476	Cc1cc(Cl)cc2SC(=NS(=O)(=O)c12)C(=O)c3ccc(Cl)c(Cl)c3	25000	nM
CHEMBL565197	Oc1ccc2CN(Cc3c(F)ccc(F)c3F)C(=O)c2c1O	25000	nM
CHEMBL554974	Oc1ccc2CN(Cc3ccccc3F)C(=O)c2c1O	25000	nM
CHEMBL1270909	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3ccc(Br)cc3)cc1OCc4ccc(F)cc4	25000	nM
CHEMBL1761472	CCC1=C(N(COCc2ccc(F)cc2)C(=O)N(O)C1=O)C(=O)c3ccccc3	25000	nM
CHEMBL492335	OC(=O)\C(=C\C(=O)C1=CNc2cc(Cl)ccc2C1=O)\O	25079.87	nM
CHEMBL3582054	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc(F)c(Cl)c2)c3c(Cl)cccc3C1=O)\O	25080	nM
CHEMBL3741857	COc1ccc(cc1)C2=Cc3ccc(F)cc3C(CC(=O)C(C)O)N2c4ccc(O)cc4	25200	nM
CHEMBL235418	COc1ccc(cc1OC)C2N(C(=O)C(=C2C(=O)c3ccc(Br)cc3)O)c4cccc(c4)C(F)(F)F	26000	nM
CHEMBL391411	Oc1ccc(\C=N\NC(=O)c2ccccc2O)cc1O	26000	nM
CHEMBL516404	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)\C=C\c2ccc(O)cc2)c1)\O	26000	nM
CHEMBL1813385	Oc1cccc(C(=O)NCc2cccc3ccccc23)c1O	26000	nM
CHEMBL3415851	OC(=O)\C(=C\C(=O)\C=C\c1ccn(Cc2ccc(F)cc2)c1)\O	26000	nM
CHEMBL226433	COC(=O)C(=O)CC(=O)c1ccc(c2ccccc2C(=O)OC)c(c1)[N+](=O)[O-]	27000	nM
CHEMBL251378	Cc1cc(C)nc(SCc2nnc(SCC(=O)NNC(=O)c3ccccc3O)n2c4ccccc4)n1	27000	nM
CHEMBL512205	ONC(=O)c1cc(on1)c2cccc(OCc3ccccc3)c2	27000	nM
CHEMBL561565	Oc1ccc2CN(Cc3cc(F)ccc3F)C(=O)c2c1O	27000	nM
CHEMBL1271215	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3nc4ccccc4s3)cc1OCc5ccc(F)cc5	27000	nM
CHEMBL241598	OC1=C(C(=O)NNC(=O)c2ccccc2)C(=O)Nc3ccccc13	28000	nM
CHEMBL252831	Oc1ccc2CN(CCc3ccccc3)C(=O)c2c1O	28000	nM
CHEMBL458229	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3cccc(c3)[N+](=O)[O-])cc1Cl	28000	nM
CHEMBL576828	Oc1ccc2C(=O)N([C@H]3CCCc4ccccc34)C(=O)c2c1O	28460.5	nM
CHEMBL391519	COc1cc(cc(\C=N\Nc2nc(Nc3ccccc3)nc(Nc4ccccc4)n2)c1O)[N+](=O)[O-]	29000	nM
CHEMBL518799	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3ccsc3C(=O)N2Cc4ccccc4	29000	nM
CHEMBL430168	CCOc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(O)c(OC)c3)c4nccs4	30000	nM
CHEMBL239482	CCN1C(=O)C(=C(O)c2ccccc12)C(=O)NNC(=O)c3ccccc3[N+](=O)[O-]	30000	nM
CHEMBL395448	OC1=C(C(=O)NNC(=O)c2ccccc2F)C(=O)Nc3ccccc13	30000	nM
CHEMBL506796	COc1ccc(\C=C\C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O)cc1	30000	nM
CHEMBL510455	Cc1cc2c(SC(NS2(=O)=O)C(=O)c3ccc4ccccc4c3)cc1Cl	30000	nM
CHEMBL513773	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccc(Br)cc3)cc1Cl	30000	nM
CHEMBL1270214	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc1OCc4cccc(Cl)c4F	30000	nM
CHEMBL1270805	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Cl)c3)cc1OCc4ccc(F)cc4	30000	nM
CHEMBL399560	Oc1ccccc1C(=O)NNC(=O)CSc2nnc(c3ccncc3)n2c4ccc(F)cc4	31000	nM
CHEMBL399480	Oc1cccc(C(=O)NCCCNC(=O)c2cccc(O)c2O)c1O	31000	nM
CHEMBL462344	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cscc3C(=O)N2Cc4ccccc4	31000	nM
CHEMBL2094513	Oc1ccc(\C=N\N2CCN(CC2)c3ccccc3)cc1O	31000	nM
CHEMBL2180601	Cc1ccc(cc1)S(=O)(=O)Oc2c(nc(Br)c3cccnc23)C(=O)NCc4ccc(F)cc4	31000	nM
CHEMBL1224123	Oc1cc(cc(O)c1O)C(=O)NCCCN2CCN(CC2)C(=O)\C=C\c3ccccc3[N+](=O)[O-]	31310	nM
CHEMBL241606	OC(=O)c1ccccc1NC(=O)c2ccc(cc2)C(=O)Nc3ccccc3C(=O)O	32000	nM
CHEMBL1928169	Cc1c(nnn1Cc2cccc(F)c2)C(=O)\C=C(/O)\c3ccc(O)c(O)c3	32000	nM
CHEMBL3087791	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccccc2C	32000	nM
CHEMBL3582049	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2c(Cl)cccc2Cl)c3ccccc3C1=O)\O	32000	nM

CHEMBL3582076	CCOC(=O)\C(=C\C(=O)C1=CN(Cc2ccc3ccccc3c2)c4ccccc4C1=O)\O	32000	nM
CHEMBL235848	CCOC(=O)c1sc(nc1C)N2C(C(=C(O)C2=O)C(=O)c3ccc(C)cc3)c4ccc(F)cc4	33000	nM
CHEMBL240329	COc1cccc(c1)C(=O)NNC(=O)c2ccc3ccccc3c2O	33000	nM
CHEMBL400246	Oc1ccc2CN(N(S(=O)(=O)c3ccc(F)cc3)S(=O)(=O)c4ccc(F)cc4)C(=O)c2c1O	33000	nM
CHEMBL471327	Cc1cc(c(SCc2ccccc2)cc1Cl)S(=O)(=O)NC3=Nc4cc(Cl)ccc4C(=O)N3	33000	nM
CHEMBL1237046	CN(C)[C@H]1[C@@H]2C[C@H]3C(=C(O)[C@]2(O)C(=O)C(=C1O)C(=O)NCN4CCCC4)C(=O)c5c(O)cccc5[C@@]3(C)O	34000	nM
CHEMBL1270106	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc1OC	34000	nM
CHEMBL1813511	CS(=O)(=O)Nc1cc(O)c(O)c(c1)C(=O)NCc2ccc(F)cc2	34000	nM
CHEMBL254646	COc1cccc(\C=N\NC(=O)c2cccc(O)c2O)c1OC	34985.71	nM
CHEMBL389931	Cc1nc2Oc3ccccc3C(=O)c2cc1C(=O)CC(=O)C(=O)O	35000	nM
CHEMBL252553	Oc1cccc(C(=O)NCc2ccc(F)cc2)c1O	35000	nM
CHEMBL462561	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cc(sc3C(=O)N2N)C(C)(C)C	35000	nM
CHEMBL1270806	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(I)c3)cc1OCc4ccc(F)cc4	35000	nM
CHEMBL264109	CCOC(=O)C1=C(O)CCC2([C@H]1c3occc3)C(=O)OC(C)(C)OC2=O	35700	nM
CHEMBL240334	Oc1ccc(C(=O)N\N=C/2\C(=O)Nc3ccccc23)c(O)c1	36000	nM
CHEMBL479537	Clc1cc(SCc2ccccc2)c(cc1C(=O)Nc3ccccc3)S(=O)(=O)NC4=Nc5ccccc5C(=O)N4	36000	nM
CHEMBL247961	COc1ccc(cc1)[C@@H]2CC(=O)C[C@H](c3occc3)C24C(=O)OC(C)(C)OC4=O	36300	nM
CHEMBL240513	CNc1nc(N\N=C\c2oc(cc2)c3ccc(cc3OC)[N+](=O)[O-])nc(Nc4ccccc4)n1	37000	nM
CHEMBL552987	COc1c2CCc3cc(\C=N\C45CC6CC(CC(C6)C4)C5)c(C(=O)O)c(O)c3c2c(O)c7C(=O)c8cc(O)c(C)c(O)c8C(=O)c17	37000	nM
CHEMBL1761471	CCC1=C(N(COCc2ccccc2)C(=O)N(O)C1=O)C(=O)c3ccccc3	37000	nM
CHEMBL182653	COc1ccc(\C=C\C(=O)c2ccc(O)cc2O)cc1	39000	nM
CHEMBL235639	Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(Cl)cc3)c4nccs4	39000	nM
CHEMBL518478	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3sc(C)c(c3C(=O)N2N	39000	nM
CHEMBL490818	COc1ccc(\C=C\C=C\C(=O)C2=C(O)C=C(C)OC2=O)cc1	39000	nM
CHEMBL1813515	CN(C)Cc1ccc(C(=O)NCc2occc2)c(O)c1O	39000	nM
CHEMBL131063	CC(C)Cn1cnnc1NS(=O)(=O)c2cc(C(=O)Nc3ccc(Cl)cc3)c(Cl)cc2S	39810	nM
CHEMBL468459	CC(C)C(=C)CC[C@@H](C)[C@H]1CC(=O)C2=C3CC[C@H]4C(C)(C)[C@@H](O)[C@H](O)C[C@]4(C)C3=C[C@H](OC(=O)C)[C@]12C	40000	nM
CHEMBL538879	COc1c2CCc3cc(C4NCc5ccccc5N4)c(C(=O)O)c(O)c3c2c(O)c6C(=O)c7cc(O)c(C)c(O)c7C(=O)c16	40000	nM
CHEMBL1270307	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(Br)c3)cc1OCc4ccc(F)cc4	40000	nM
CHEMBL1909979	COc1ccc(CCN2C(C(=C(O)C2=O)C(=O)c3ccccn3)c4cccc(Cl)c4)cc1	40000	nM
CHEMBL1928166	Cc1c(nnn1Cc2ccc(F)cc2)C(=O)\C=C(/O)\c3ccc(O)c(O)c3	40000	nM
CHEMBL253609	Oc1ccc2CN(N3Cc4ccc(O)c(O)c4C3=O)C(=O)c2c1O	41000	nM
CHEMBL513386	CCCCCC[C@H]1OC(=O)C2=C1[C@@H](O)[C@@H]3O[C@@H]3[C@@H]2O	41000	nM
CHEMBL475853	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)c2ccccc2O)c1)\O	41000	nM
CHEMBL1271008	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3ccc(cc3)C(=O)O)cc1OCc4ccc(F)cc4	41000	nM
CHEMBL1761474	CCC1=C(N(COCc2ccccc2)C(=O)N(O)C1=O)C(=O)c3cc(C)cc(C)c3	41000	nM
CHEMBL417356	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(Cl)cc2	42000	nM
CHEMBL392358	COc1ccc(cc1OC)C(=O)C2=C(O)C(=O)N(CCc3ccccc3)C2c4ccc(Br)cc4	42000	nM
CHEMBL518513	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3ccccc3C(=O)N2Cc4occc4	42000	nM
CHEMBL475661	COc1cc(\C=C\C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O)ccc1O	42000	nM

CHEMBL1813127	CCOC(=O)CC(=O)Nc1ccc2cccc(O)c2n1	42000	nM
CHEMBL2297146	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccc(F)cc3)cc1Cl	42000	nM
CHEMBL235637	COc1ccc(cc1OC)C2N(C(=O)C(=C2C(=O)c3ccc(Br)cc3)O)c4cc(on4)C(C)(C)C	43000	nM
CHEMBL392359	CC(C)(C)c1ccc(cc1)C2N(C(=O)C(=C2C(=O)c3ccc(F)cc3)O)c4nncs4	43000	nM
CHEMBL240299	Nc1ccc(cc1)C(=O)CC(=O)Nc2cc(cc2)C(=O)O)C(=O)O	43000	nM
CHEMBL459879	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3cscc3C(=O)N2N	43000	nM
CHEMBL396686	CCN1C=C(C(=O)O)C(=O)c2cc(F)c(N3CCN(CNC(=O)C4=C(O)[C@H]([C@@H]5C[C@H]6C(=C(O)[C@]5(O)C4=O)C(=O)c7c(O)cccc7[C@@]6(C)O)N(C)C)C(C)C3)c(F)c12	44000	nM
CHEMBL1813505	CNS(=O)(=O)c1cc(O)c(c(c1)C(=O)NCc2ccc(F)cc2	44000	nM
CHEMBL1813510	Oc1cc(cc(C(=O)NCc2cccs2)c1O)S(=O)(=O)N3CCCCC3	44000	nM
CHEMBL1909981	OC1=C(C(N(C1=O)c2cccccc2)c3ccc(cc3)[N+](=O)[O-])C(=O)c4ccccc4	44000	nM
CHEMBL394249	COc1cccc([C@@H]2CC(=O)C[C@H](c3occc3)C24C(=O)OC(C)(C)OC4=O)c1OC	44200	nM
CHEMBL505739	CN[C@@H](Cc1ccc(Oc2cc3cc(c2O)c4cccc5c(C[C@@H](N)C(=O)N[C@@H](C(=O)N[C@H]3C(=O)N[C@@H](C(=O)O)c6cc(Cl)c(O)c(Cl)c6)c7cc(Cl)c(O)c(Cl)c7)c[nH]c45)cc1)C(=O)O	45000	nM
CHEMBL1909980	COc1ccc(CCN2C(C(=C(O)C2=O)C(=O)c3ccccc3)c4ccccc4)cc1	45000	nM
CHEMBL241596	OC1=C(C(=O)NNC(=O)c2ccccc2[N+](=O)[O-])C(=O)Nc3ccccc13	46000	nM
CHEMBL148472	Oc1ccc(C(=O)\C=C\c2ccccc2O)c(O)c1	47000	nM
CHEMBL240330	CCCN1C(=O)C(=C(O)c2ccccc12)C(=O)NNC(=O)CC(=O)OCC	48000	nM
CHEMBL474027	Cc1cccc(C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O)c1O	48000	nM
CHEMBL239274	[O-][N+](=O)c1ccc2N(C3=NC(=O)NC(=O)C3=Cc2c1)c4ccc(Cl)cc4	49000	nM
CHEMBL399272	Oc1cccc(C(=O)NCCNC(=O)c2cccc(O)c2O)c1O	50000	nM
CHEMBL457777	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3cccc(c3)[N+](=O)[O-])cc1Cl	50000	nM
CHEMBL559409	Oc1ccc(cc1O)C(=O)Nc2ccc(cc2)S(=O)(=O)Nc3ccccc3	50000	nM
CHEMBL1456957	CCOC(=O)CC(=O)Nc1ccc(C)cc1	50000	nM
CHEMBL398210	Oc1nc(nc(C(=O)NCc2ccc(cc2)c3ccccc3)c1O)c4cccs4	50118.72	nM
CHEMBL1085426	Oc1nc(nc(C(=O)NCn2cncn2)c1O)c3cccs3	50118.72	nM
CHEMBL479348	Clc1ccc(NC(=O)c2cc(c(SCc3ccccc3)cc2Cl)S(=O)(=O)NC4=Nc5ccccc5C(=O)N4)cc1	52000	nM
CHEMBL2311887	Cc1sc2ncnc(N\N=C\c3c(O)ccc4ccccc34)c2c1C	52000	nM
CHEMBL241396	CC(C)CN1C2C(N=C1N\N=C\c3cc(Br)ccc3O)N(C)C(=O)NC2=O	53000	nM
CHEMBL404420	Oc1ccc2CN(N3C(=O)c4ccc(F)cc4C3=O)C(=O)c2c1O	53000	nM
CHEMBL516661	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3ccsc3C(=O)N2N	53000	nM
CHEMBL460943	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3ccsc3C(=O)N2Cc4occc4	53000	nM
CHEMBL253395	Oc1cccc(\C=N\N2Cc3ccc(O)c(O)c3C2=O)c1O	54000	nM
CHEMBL1682052	COc1ccc(\C=C\C(=O)c2cc(Br)cc(C(=O)O)c2O)cc1OC3CCCC3	55000	nM
CHEMBL500308	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)Cc2ccccc2)c1)\O	56000	nM
CHEMBL497314	OC(=O)\C(=C\C(=O)C1=CNc2ccc(Cl)cc2C1=O)\O	56000	nM
CHEMBL549679	COc1c2CCc3cc4C5NCCCN5C(=O)c4c(O)c3c2c(O)c6C(=O)c7cc(O)c(C)c(O)c7C(=O)c16	56000	nM
CHEMBL1813502	CNC(=O)Cc1ccccc1CNC(=O)c2cccc(O)c2O	56000	nM
CHEMBL394683	Oc1ccccc1C(=O)N\N=C\2/C(=O)Nc3ccccc23	57000	nM
CHEMBL510239	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)c2cccc(Cl)c2)c1)\O	57000	nM
CHEMBL1271426	COc1ccc(\C=C/2\C(=NN(C2=O)c3cccc(Br)c3)COC(=O)C)cc1OCc4ccc(F)cc4	57000	nM
CHEMBL240546	CCCC1=Nc2ccccc2C(=O)N1NC(=O)C3=C(O)c4cccc5CCCN(C3=O)c45	58000	nM
CHEMBL251172	Cn1c(SCC(=O)NNC(=O)c2ccccc2O)nnc1c3ccccc3	58000	nM
CHEMBL1813495	Oc1cccc(C(=O)Nc2ccc3[nH]ccc3c2)c1O	58000	nM

137

CHEMBL498504	CCN1C=C(C(=O)O)C(=O)C2=C1C(=O)C=CC2=O	58700	nM
CHEMBL399006	Oc1ccccc1C(=O)NNC(=O)CSC2=Nc3ccccc3C(=O)N2CC4CCCO4	60000	nM
CHEMBL239244	CCCOc1ccc(\C=N\NC2=NC(CC(=N2)c3ccccc3)c4ccccc4O)c(O)c1	60000	nM
CHEMBL1270701	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3cccc(F)c3)cc1OCc4ccc(F)cc4	60000	nM
CHEMBL398558	Oc1ccc(C(=O)NNC(=O)CSc2nnnn2c3ccccc3)c(O)c1	61000	nM
CHEMBL3706873	O=C1Nc2ccc(cc2c3ccccc13)N(Cc4ccc(cc4)C#N)Cc5ccc(cc5)C#N	62000	nM
CHEMBL226374	OC(=O)C(=O)CC(=O)c1ccc2c(NC(=O)c3ccccc23)c1	65000	nM
CHEMBL457554	Cc1cc2c(SC(=NS2(=O)=O)C(=O)c3ccc(Cl)cc3)cc1Cl	65000	nM
CHEMBL239056	CCCN1C(=O)C(=C(O)c2ccccc12)C(=O)NNC(=O)c3ccccc3	66000	nM
CHEMBL237537	Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(CCCn3ccnc3)C2c4ccc(Cl)cc4	67000	nM
CHEMBL458494	OC(=O)c1cc(on1)c2cccc(OCc3ccccc3)c2	68000	nM
CHEMBL1086442	CC(C)C[C@H](N)C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CCC(=O)N)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1ccccc1)C(=O)O	68000	nM
CHEMBL235200	Cc1ccc(cc1)C2N(CC(=O)O)C(=O)C(=C2C(=O)c3ccc(Cl)cc3)O	69000	nM
CHEMBL474862	COc1cccc(c1)C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O	69000	nM
CHEMBL1271007	COc1ccc(\C=C\2/C(=O)N(N=C2C(F)(F)F)c3ccc(I)cc3)cc1OCc4ccc(F)cc4	69000	nM
CHEMBL2180593	OCCNc1c(nc(Br)c2cccnc12)C(=O)NCc3ccc(F)cc3	69000	nM
CHEMBL496412	OC(=O)c1ccc(cc1O)c2oc(C=C3C(=O)NC(=S)NC3=O)cc2	69160	nM
CHEMBL239484	O\C(=C/C(=O)c1ccc(Cl)cc1)\C(=O)Nc2nccs2	70000	nM
CHEMBL391423	COc1ccc(NC(=O)c2cccc(c2)S(=O)(=O)Nc3ccc(cc3)C(=O)O)cc1	70000	nM
CHEMBL471330	Cc1cc(c(SCc2ccccc2)cc1Cl)S(=O)(=O)NC3=Nc4ccsc4C(=O)N3	70000	nM
CHEMBL572179	C[C@H](N1Cc2ccc(O)c(O)c2C1=O)c3ccccc3	70000	nM
CHEMBL239483	Cc1cc(C)cc(OCC(=O)NNC(=O)C2=Cc3ccccc3OC2=O)c1	72000	nM
CHEMBL474861	COc1ccccc1C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O	73000	nM
CHEMBL2311881	Cc1occc1C(=O)NN\C=C/2\C(=O)N(C(=O)c3ccccc23)c4ccccc4Cl	75000	nM
CHEMBL240331	Oc1ccc(cc1O)C(=O)CSc2nc(O)c3ccccc3n2	77000	nM
CHEMBL479347	Cc1ccc(NC(=O)c2cc(c(SCc3ccccc3)cc2Cl)S(=O)(=O)NC4=Nc5ccccc5C(=O)N4)cc1	77000	nM
CHEMBL225669	Brc1ccc2NC(=O)c3ccccc3c2c1	78000	nM
CHEMBL235846	Cc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(F)cc3)c4nccs4	78000	nM
CHEMBL513058	Cc1cc(c(SCc2ccccc2)cc1Cl)S(=O)(=O)NC3=Nc4cscc4C(=O)N3	78000	nM
CHEMBL2407289	Fc1ccc(CNC(=O)C2C(=O)NC(=O)c3ccccc23)cc1	79000	nM
CHEMBL241183	CCCn1c(N\N=C\c2cc(Br)ccc2O)nc3N(C)C(=O)NC(=O)c13	80000	nM
CHEMBL2311882	COCCN1C(=S)NC(=O)\C(=C\NNC(=O)c2cc(Cl)ccc2O)\C1=O	80000	nM
CHEMBL240542	CCOc1cc(Br)cc(\C=N\c2ncccc2O)c1O	81000	nM
CHEMBL459878	Cc1cc(c(S)cc1Cl)S(=O)(=O)NC2=Nc3scc(C)c3C(=O)N2N	81000	nM
CHEMBL501858	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)c2ccc(O)cc2)c1)\O	81000	nM
CHEMBL455820	OC(=O)c1onc(c1)c2cccc(OCc3ccccc3)c2	81000	nM
CHEMBL429082	OC1=C(C(N(C1=O)c2nc3ccccc3s2)c4ccccn4)C(=O)c5ccc(Cl)cc5	83000	nM
CHEMBL240333	Oc1ccc(cc1O)c2csc(Nc3ncccn3)n2	83000	nM
CHEMBL513057	Cc1cc(c(SCc2ccccc2)cc1Cl)S(=O)(=O)NC3=Nc4ccccc4C(=O)N3	83000	nM
CHEMBL240511	Cc1ccc(NC(=O)CN2C(=O)\C(=C/NC(=O)c3ccc4ccccc4n3)\c5ccccc25)cc1	84000	nM
CHEMBL577062	ONC(=O)c1cc2ccn(Cc3ccc(F)cc3F)c2cn1	84000	nM
CHEMBL240548	CC(C)Cc1c(C#N)c(SCC(=O)c2ccc(O)c(O)c2)nc(C)c1C(=O)N	85000	nM
CHEMBL452658	C[C@H](CCC(O)C(C)(C)O)[C@H]1CC[C@@]2(C)C3=C(CC[C@]12C)[C@@]4(C)C[C@@H](OC(=O)CC(C)(O)CC(=O)O)C(=O)C(C)(C)[C@@H]4CC3	85000	nM
CHEMBL1813382	ONC(=O)c1cc(OCc2ccc(F)cc2)ccc1O	85000	nM

138

CHEMBL448271	CN([C@@H](Cc1ccc(Oc2cc3cc(c2O)c4cccc5c(C[C@@H](N)C(=O)N[C@@H](C(=O)N[C@H]3C(=O)O)c6cc(Cl)c(O)c(Cl)c6)c[nH]c45)cc1)C(=O)O)C(=O)[C@H](N)c7cc(Cl)c(O)c(Cl)c7	86000	nM
CHEMBL1269892	CCC(=O)OC1=NN(C(=O)/C/1=C\c2ccc(OC)c(OCc3ccc(F)cc3)c2)c4cccc(Br)c4	88000	nM
CHEMBL238632	O=C(Nc1cccc(\C=C\C(=O)c2ccccc2)c1)c3cccs3	89000	nM
CHEMBL240544	Nc1cc(O)nc(SCC(=O)c2ccc(O)c(O)c2)n1	89000	nM
CHEMBL391949	CCOc1ccc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(OC)cc3)c4nccs4	90000	nM
CHEMBL236067	OC1=C(C(N(C1=O)c2nc3ccccc3s2)c4cccnc4)C(=O)c5ccc(Cl)cc5	90000	nM
CHEMBL239275	CCCC(=O)NC(c1ccc(OC)c(OC)c1)c2cc(Cl)c3cccnc3c2O	90000	nM
CHEMBL472204	CN1C(=NC(=O)c2ccccc12)NS(=O)(=O)c3cc(C)c(Cl)cc3SCc4ccccc4	90000	nM
CHEMBL512918	Clc1ccc(cc1)C(=O)C2=NS(=O)(=O)c3ccc(Cl)cc3S2	90000	nM
CHEMBL3415839	CCOC(=O)\C(=C\C(=O)\C=C\c1ccn(Cc2ccc(F)cc2)c1)\O	90000	nM
CHEMBL1774052	OC1=C2C(=O)N(Cc3cccc4ccccc34)C(=O)C2=C5CCCCCN5C1=O	90500	nM
CHEMBL247960	COc1ccc(cc1OC)[C@@H]2CC(=O)C[C@H](c3occc3)C24C(=O)OC(C)(C)OC4=O	91500	nM
CHEMBL238633	O=C(Oc1ccccc1\C=C\C(=O)c2ccccc2)C3=Cc4ccccc4OC3=O	92000	nM
CHEMBL474035	OC(=O)\C(=C\C(=O)c1cccc(NC(=O)c2ccccc2Cl)c1)\O	92000	nM
CHEMBL1682034	OC(=O)c1cc(Cl)cc(C(=O)\C=C\c2cccc(Cl)c2Cl)c1O	92000	nM
CHEMBL263887	CCOC(=O)\C(=C\C(=O)c1cn(Cc2ccc(F)cc2)c3cccc(OC)c13)\O	92300	nM
CHEMBL455050	COc1ccc(NC(=O)c2cc(c(SCc3ccccc3)cc2Cl)S(=O)(=O)NC4=Nc5ccccc5C(=O)N4)cc1	93000	nM
CHEMBL474034	COc1ccc(cc1)C(=O)Nc2cccc(c2)C(=O)\C=C(/O)\C(=O)O	95000	nM
CHEMBL541701	COc1c2CCc3cc4C5Sc6ccccc6N5C(=O)c4c(O)c3c2c(O)c7C(=O)c8cc(O)c(C)c(O)c8C(=O)c17	96000	nM
CHEMBL450074	OC(=O)c1cc(on1)c2ccc(cc2)[N+](=O)[O-]	97000	nM
CHEMBL1813383	ONC(=O)c1c(O)cccc1OCc2ccc(F)cc2	97000	nM
CHEMBL246950	COc1ccc(cc1)[C@H]2CC(=O)CCC23C(=O)OC(C)(C)OC3=O	97500	nM
CHEMBL498635	OC(=O)c1ccc(cc1O)c2oc(\C=C\3/SC(=S)NC3=O)cc2	97720	nM
CHEMBL45578	CCOC(=O)C(=O)CC(=O)\C=C\c1cccn1Cc2ccc(F)cc2	98000	nM
CHEMBL3415855	CCOC(=O)\C(=C\C(=O)\C=C\c1cccn1Cc2ccc(F)cc2)\O	98000	nM
CHEMBL387679	Clc1ccc2NC(=O)c3ccccc3c2c1	100000	nM
CHEMBL399412	CN1C(=O)c2c3CCCc3sc2N=C1SCC(=O)NNC(=O)c4cccc(O)c4	100000	nM
CHEMBL240974	Oc1cccc(NC(=O)c2cc(cc(c2)C(=O)Nc3cccc(O)c3)N4C(=O)c5ccccc5C4=O)c1	100000	nM
CHEMBL241184	CCc1nc2sc3CCCCc3c2c4nnc(SCC(=O)NNC(=O)c5ccc(OC)cc5)n14	100000	nM
CHEMBL241185	CCc1cccc2c(SCC(=O)NNC(=O)c3ccccc3[N+](=O)[O-])nc(nc12)c4ccc(F)cc4	100000	nM
CHEMBL490208	COc1ccc(Br)cc1\C=C\C(=O)C2=C(O)C=C(OC2=O)\C=C\c3ccc(cc3)N(C)C	100000	nM
CHEMBL455952	OC(=O)c1cc([nH]n1)c2cccc(OCc3ccccc3)c2	100000	nM
CHEMBL1271425	COc1ccc(\C=C/2\C(=NN(C2=O)c3cccc(Br)c3)OC(=O)C)cc1OCc4ccc(F)cc4	100000	nM
CHEMBL1813381	ONC(=O)c1ccc(OCc2ccc(F)cc2)cc1O	100000	nM
CHEMBL1813494	Oc1cccc(C(=O)NCCc2c[nH]c3ccccc23)c1O	100000	nM
CHEMBL1813503	CNC(=O)c1cc(F)ccc1CNC(=O)c2cccc(O)c2O	100000	nM
CHEMBL1909977	COc1ccc(CCN2C(C(=C(O)C2=O)C(=O)c3ccccc3)c4ccc(O)cc4)cc1	100000	nM
CHEMBL2311878	Oc1c(Br)cc(Br)cc1\C=N\NC(=O)CP(=O)(c2ccccc2)c3ccccc3	100000	nM
CHEMBL2311902	OC1=Cc2ccccc2\C(=N/Nc3ccc(Cl)cc3)\C1=O	100000	nM

8.4 Rev training set

CHEMBL1374066	Nc1ccc2nonc2c1[N+](=O)[O-]	690.35	nM
CHEMBL2000619	CN(C)c1ccc(cc1)\N=C\2/C(=O)N(C)c3cccc4c(O)c5ccccc5c2c34	1047	nM
CHEMBL1864348	Oc1ccc(\C=N\Nc2cc(nc(n2)N3CCCC3)N4CCCC4)cc1	1364	nM
CHEMBL1378470	CCOc1cc(ccc1N)c2ccc(N)c(OCC)c2	2471	nM
CHEMBL1410045	CN(C)c1ccc(\C=C/2\C(=O)ON=C2C)cc1	2861	nM
CHEMBL1517523	[O-][N+](=O)\C=C\1/SCC(=O)N1c2ccccc2	3035	nM
CHEMBL1527986	CCOC(=O)CN1C(=O)C(=Nc2ccccc12)c3cc(Br)ccc3N	4534	nM
CHEMBL1391213	Nc1cccc(c1)C(=O)OCC(=O)Nc2cccc3C(=O)c4ccccc4C(=O)c23	5219	nM
CHEMBL1303557	[I-].CC[n+]1c(oc2ccccc12)\C=C\Nc3ccccc3	5664	nM
CHEMBL1579180	COc1ccc(NS(=O)(=O)c2ccc(Cl)s2)cn1	6301	nM
CHEMBL1460312	CCCCN1C(=O)Nc2nc3cc(NC(=O)C)ccc3nc2C1=O	6497	nM
CHEMBL1411766	CCCCN(C(=O)c1oc(cc1)[N+](=O)[O-])C2=C(N)N(CC(C)C)C(=O)NC2=O	7261	nM
CHEMBL269410	Nc1cccc2C(=O)N(C(=O)c12)c3ccccc3	7863	nM
CHEMBL282433	Cc1ccccc1NC(=N)Nc2ccccc2C	8312	nM
CHEMBL1555842	CC(CCC(C)C(C)(C)C)[C@@H]1CC[C@H]2C3C[C@H](OS(=S)(=S)O)[C@H]4C[C@H](OS(=S)(=S)O)[C@H](C[C@]4(C)[C@H]3CC[C@]12C)OS(=S)(=S)O	8337	nM
CHEMBL1357473	CC(C)CCN(C(=O)CCCSc1nc2ccccc2[nH]1)C3=C(N)N(Cc4ccccc4)C(=O)NC3=O	8380	nM
CHEMBL1493286	CN(C1CCCCC1)C(=O)CN2C(=O)c3cccc(N)c3C2=O	8386	nM
CHEMBL3211323	Cc1nnc(C)n1\N=C\c2cccc(CC=C)c2O	8387	nM
CHEMBL1553837	OCCN(CCO)c1cccc2C(=O)c3ccccc3C(=O)c12	8440	nM
CHEMBL274921	Nc1cc2nc3ccccc3nc2cc1N	9529	nM
CHEMBL166209	OC(=O)c1ccc2C(=O)c3ccccc3c4ncnc1c24	9783	nM
CHEMBL1469144	Cc1ccc2C(=O)c3ccccc3c4cccc1c24	10093	nM
CHEMBL1425966	Cc1ccc[n+](c1)c2nc([O-])sc2C=NNc3ccc(cc3)[N+](=O)[O-]	10098	nM
CHEMBL1378107	[O-][N+](=O)c1ccccc1\C=C(/C#N)\C(=O)NCC=C	10447	nM
CHEMBL1308993	COCCOC(=O)C1=C(N)N(CCOC)C(=S)S1	11141	nM
CHEMBL1568292	COc1ccc(NC(=O)Nc2cc(C)cc(C)c2)cn1	11406	nM
CHEMBL1478947	COC(=O)c1cc2c(C)cc3ccc(C)cn3c2c1C(=O)OC	12248	nM
CHEMBL68500	O=C1NC(=O)c2nc3ccccc3nc2N1	12395	nM
CHEMBL1446983	OC1=CC(=O)c2ccccc3cccc1c23	13868	nM
CHEMBL1494927	Cc1c(O)ccc2C=C(C(=O)Oc12)S(=O)(=O)c3ccccc3	14216	nM
CHEMBL1456904	CN1C(=O)C=C2c3ccccc3C(=O)c4c(ccc1c24)N5CCCCC5	14250	nM
CHEMBL1560136	COc1ccc2nc(N3CCCCC3)c(cc2c1)C#N	14753	nM
CHEMBL1354016	CC(=O)Nc1ccc2nc3ccccc3nc2c1	14833	nM
CHEMBL1585268	CC(=O)N1CCN(CC1)C2=Nc3cccc4cccc2c34	15785	nM
CHEMBL1391235	COc1cc(O)cc2cc3OC(C)(O)CC(=O)c3c(O)c12	16241	nM
CHEMBL1566518	COc1ccc(NC(=O)c2oc(cc2)c3ccc(cc3)C(=O)C)cn1	16416	nM
CHEMBL1365400	CCN1C\C(=C\c2cccs2)\c3nc4ccccc4c(C(=O)O)c3C1	16969	nM
CHEMBL1574146	Nc1cccc2C(=O)N(Cc3cccc(Cl)c3)C(=O)c12	17851	nM
CHEMBL1549677	CC1CN(CC(C)O1)C2=Nc3cccc4cccc2c34	18230	nM
CHEMBL1378413	COC(=O)[C@@]1(C#N)[C@@H]2C=CC(=CN2[C@H]([C@@H]1c3ccc(F)cc3)C(=O)N)C(=O)C	18291	nM
CHEMBL1332240	COc1ccc(cc1)c2oc(C)c(C[S+]([O-])CC(=O)NCc3ccccn3)n2	19371	nM
CHEMBL1385436	Cc1ccc(cc1)N2CCN(CC2)c3ccc(NCc4nc5ccccc5n4C)cc3	19597	nM
CHEMBL1575084	CCn1c(CSc2nccn2C)nc3cc(ccc13)C(=O)O	19748	nM
CHEMBL1437954	CCOc1ccc2nc(N3CCCN(CC3)C(=O)Nc4ccccc4C)c(cc2c1)C#N	20324	nM

CHEMBL1442125	OC(=O)c1ccccc1N=Nc2ccc(O)cc2	22020	nM
CHEMBL1998429	Cc1oc(cc1)C(=O)N\N=C\c2oc(cc2)c3ccc(Br)cc3[N+](=O)[O-]	25109	nM
CHEMBL1549136	COc1ccc(NC(=O)Cc2ccccc2)cn1	25171	nM
CHEMBL1541803	ClC1=CCC2C(C1)C(=O)N(CC(=O)NCc3ccccc3)C2=O	25752	nM
CHEMBL1578982	Cc1ccc(cc1)S(=O)(=O)N[C@H](C(=O)Oc2ccc3C(=CC(=O)Oc3c2)C(F)(F)F)c4ccccc4	26862	nM
CHEMBL1470560	C1CN(CCO1)C2=Nc3cccc4cccc2c34	29228	nM
CHEMBL1436090	CCCN1C(=O)NC(=O)C(=C1N)N(CCOC)C(=O)Cc2ccc(s2)S(=O)(=O)N3CCOCC3	39575	nM
CHEMBL3190665	COc1ccc(\C=N\c2c(nc3ccccn23)c4occc4)cc1OC	56122	nM
CHEMBL1415258	CCc1ccc2nc3nc(C)cc(C)c3c(N)c2c1	58820	nM
CHEMBL1415985	FC(F)(F)C1=CC(=O)Oc2cc(OC(=O)CN3C(=O)NC4(CCCCC4)C3=O)ccc12	65306	nM
CHEMBL1445765	COc1ccc2nc(N3CCC(O)CC3)c(cc2c1)C#N	67576	nM
CHEMBL1981093	Nc1nnnn1\N=C\c2cc(Cl)ccc2O	75326	nM
CHEMBL1546264	COc1ccc(\C=C(/CC(=O)O)\c2nc3ccccc3s2)cc1O	75365	nM
CHEMBL1573564	OCCCN1C(=O)C2=C(SCCS2)C1=O	75380	nM
CHEMBL1523792	CCOC(=O)c1[nH]cnc1N=Nc2c(O)ccc3ccccc23	75386	nM
CHEMBL1495503	Cc1ccc(cc1)S(=O)(=O)Nc2cc3c(C(=O)Nc4ccccc4)c(C)oc3c5ccccc25	75403	nM
CHEMBL1601851	CCOC(=O)c1cc2c(ccn2C)n1CC(=O)N(Cc3ccccc3)c4ccccc4	75403	nM
CHEMBL1442453	COc1ccc(Nc2nnc(SCC3=CC(=O)N4C=CSC4=N3)s2)cc1	75409	nM
CHEMBL41286	CC(=O)Oc1cccc2C(=O)c3cc(cc(OC(=O)C)c3C(=O)c12)C(=O)O	75411	nM
CHEMBL1362550	CCOc1cc(cc(Br)c1O)C2C(=CN(C=C2C(=O)OC)C3CCCC3)C(=O)OC	75412	nM
CHEMBL11475	CC1=CC(=O)c2c(O)ccc(O)c2C1=O	75414	nM
CHEMBL456295	COc1cc2C(=O)c3nccc4c(OC)c(OC)c(OC)c(c2cc1OC)c34	75418	nM
CHEMBL1503865	CCN(CC)S(=O)(=O)c1ccc(N2CCCC2)c(NS(=O)(=O)c3ccc(F)cc3)c1	75418	nM
CHEMBL88326	Nc1ccc(O)c2C(=O)c3ccccc3C(=O)c12	75421	nM
CHEMBL1337685	COC(=O)c1ccc2N=C3CCCC(=C3Sc2c1)O	75421	nM
CHEMBL1381318	Nc1c(O)ccc2C(=O)c3ccccc3C(=O)c12	75421	nM
CHEMBL1987546	Clc1ccc(\C=N\c2c(nc3ccccn23)c4occc4)cc1	75421	nM
CHEMBL1421995	Cc1c(O)ccc(c1O)c2[nH]nc(C(=O)O)c2c3nc4ccccc4s3	75423	nM
CHEMBL1587496	CCOC(=O)c1cc2c(ccn2C)n1CC(=O)N(Cc3ccccc3)c4ccc(F)cc4	75425	nM
CHEMBL1376371	CN1CC2=Cc3ccccc3OC24Oc5ccccc5C=C4C1	75427	nM
CHEMBL1537049	CCOC(=O)c1cc2c(ccn2C)n1CC(=O)N3CCN(CC3)c4cccc(c4)C(F)(F)F	75427	nM
CHEMBL294264	Oc1cc(O)c2C(=O)c3ccccc3C(=O)c2c1O	75434	nM
CHEMBL1419027	COc1ccc(N2CCCC2)c(NC(=O)c3oc(Br)cc3)c1	75442	nM
CHEMBL1502839	CCn1c(CSc2nnc3ccccn23)nc4cc(ccc14)C(=O)O	75449	nM
CHEMBL1397154	CC(OC(=O)\C(=C\c1ccc(cc1)N(C)C)\C#N)C(=O)NCc2occc2	75472	nM
CHEMBL1469407	Oc1nc2cc3ccccc3cc2nc1C(F)(F)F	75487	nM
CHEMBL1312914	Nc1c(nc2ccccn12)c3cccc(c3)[N+](=O)[O-]	75502	nM
CHEMBL539676	COc1ccc(Nc2nc(N)nc(CN(C)C3CCCCC3)n2)cc1	79370	nM
CHEMBL546344	[Cl-].[N+]c1nc(Nc2ccc(Cl)cc2)nc3ccccc13	79370	nM
CHEMBL1299250	COc1ccc(CCNC(C)CCc2ccc(OC)cc2)cc1	79370	nM
CHEMBL1311876	[Cl-].[N+]CCCC(=O)N1c2ccccc2[S]c3ccccc13	79370	nM
CHEMBL1349146	COc1ccc(\C=C\C2=[N+](C)OC(=C2)c3ccc(C)cc3)cc1.[Cl-]	79370	nM
CHEMBL1369795	CNCCCOc1ccc(cc1)C(C)(C)c2ccccc2	79370	nM
CHEMBL1382621	Cc1nc(Nc2ccncc2)c3oc4ccccc4c3n1	79370	nM
CHEMBL1385794	[Br-].C[n+]1c2SCC(=Nn2c3ccccc13)c4ccc(Cl)cc4	79370	nM
CHEMBL1386820	CC(C)COc1ccc(Cc2cnc(N)nc2N)cc1	79370	nM
CHEMBL1401938	Cc1ccc(cc1)C(=O)NNC(=O)CSc2n[nH]c3c4cc(F)ccc4nc3n2	79370	nM
CHEMBL1405895	CC1=NN(C(=O)C1N=Nc2ccc(N)cc2)c3ccccc3	79370	nM

CHEMBL1418879	[Cl-].CC([N+]Cc1ccc(cc1)N(C)C)C2CC3CCC2C3	79370	nM
CHEMBL1485867	COc1ccccc1NC2=NC(=NC(N2)c3ccc(Cl)cc3)N	79370	nM
CHEMBL1503307	COc1cccc(OC)c1c2nn3c(nnc3s2)c4cc([nH]n4)c5ccccc5	79370	nM
CHEMBL1508313	CCOC(=O)c1c(C)n(C)c2ccc(O)c(CN(C)C)c12	79370	nM
CHEMBL1540598	[Br-].Brc1ccc(cc1)C(=O)C[N+]2C3=NCCN3c4ccccc24	79370	nM
CHEMBL1557351	[Cl-].CCN(CC)CC[N+]C1=NCCN2C1=CC3=CC(OC)=CC=C23	79370	nM
CHEMBL1572144	[Cl-].COc1ccc(cc1)C2N=C(N)N=C([N+])N2c3ccc(C)cc3	79370	nM
CHEMBL1587299	COc1cccc(Nc2nc(N)nc(n2)c3oc4ccccc4c3C)c1	79370	nM
CHEMBL1599483	[Cl-].COC(=O)c1c(C(=O)OC)n(CCC[N+])c2ccc(C)cc12	79370	nM
CHEMBL1603067	CC(C)C[NH+]=C1C=C(Oc2ccc(Cl)cc12)c3ccccc3.[Cl-]	79370	nM
CHEMBL1603229	CN(C)CC(O)COc1ccc(cc1)c2ccc(cc2)C#N	79370	nM
CHEMBL1704267	Fc1ccc(\C=N\NC(=O)c2cc(nc3ccccc23)c4occc4)cc1	79370	nM
CHEMBL1706577	Fc1cccc(\C=N\NC(=O)c2cc(nc3ccccc23)c4occc4)c1	79370	nM

8.5 TAT training set

CHEMBL1553368	O.Cl.COC(=O)c1ccccc1C2=C3C=CC(=N)C=C3Oc4cc(N)ccc24	190	nM
CHEMBL1536556	COc1ccc(O)c(c1)C(=O)C2N(C(=O)c3ccccc23)c4ccc(C)cc4	303	nM
	O[C@H]1[C@H]2[C@H](CC(=O)O)C(=O)O[C@@H]3C(COC(=O)c4		
	cc(O)c(O)c(O)c4)O[C@@H](OC(=O)c5cc(O)c(O)c(O)c5)[C@@H](OC		
CHEMBL1391063	(=O)c6cc(O)c(O)c(OC1=O)c26)[C@H]3OC(=O)c7cc(O)c(O)c(O)c7	556	nM
CHEMBL1398964	OC(=O)c1cc(ccc1Cl)N2N=C(\C(=C\C=C\c3occc3)\C2=O)C(F)(F)F	615	nM
CHEMBL1600422	COc1cccc(c1)C2CC(c3ccccc3OC)n4nc(N)nc4N2	686	nM
CHEMBL1527520	OC(=O)C1Nc2c(O)cccc2C3C=CCC13	702	nM
CHEMBL1334586	Cc1ccc(C)n1NC2=NC(=O)CS2	881	nM
CHEMBL1455440	CC1(C)OC(=C(C(=O)O1)C2=NCCC2)O	881	nM
	Cc1cccc(c1)N2C(=O)NC(=O)\C(=C\c3cc4OCOc4cc3[N+](=O)[O-		
CHEMBL1420548	])\C2=O	906	nM
CHEMBL1504655	Cc1ccc(C)n1c2sccc2C(=O)O	908	nM
CHEMBL1405834	O=C1NC(=S)S/C/1=C\c2oc(SCc3occc3)cc2	926	nM
CHEMBL1546396	Nc1c(sc2nc3\C(=C/c4occc4)\CCc3c(c5occc5)c12)C(=O)NC6CC6	937	nM
CHEMBL1453703	CNC(=O)c1ccccc1NC(=O)c2ccc(C)c(c2)S(=O)(=O)N3CCCCC3	968	nM
CHEMBL1346508	CCOC(=O)c1ccc(NS(=O)(=O)c2ccc3N(C)C(=O)Oc3c2)cc1	995	nM
CHEMBL1405604	Sc1nnc(COc2ccc3OCOc3c2)n1c4ccccc4	1029	nM
CHEMBL1446786	Cc1ccccc1Cc2c(C)nc3c(cnn3c2C)C(=O)NCc4ccc5OCOc5c4	1058	nM
CHEMBL1375570	CCN(C(=O)C1=COC(=O)C(=C1)Br)c2ccc3OCOc3c2	1170	nM
	Fc1ccc(NC(=O)C(N2CCN(CC2)S(=O)(=O)c3ccc4ccccc4c3)c5ccccc5)c		
CHEMBL1409647	c1	1234	nM
CHEMBL1575767	OC(=O)C(Cc1ccccc1)N2C(=S)S\C(=C/C=C/c3occc3)\C2=O	1259	nM
CHEMBL1324208	Clc1ccc(cc1)S(=O)(=O)N2CCN(CC(=O)Nc3ccc4OCCOc4c3)CC2	1306	nM
CHEMBL1508847	OC(=O)CC(N1C(=S)S\C(=C/C=C/c2occc2)\C1=O)C(=O)O	1334	nM
CHEMBL1402056	CC1=C(C#N)C(=O)N(C2CCS(=O)(=O)C2)C(=O)/C/1=C\c3oc(C)cc3	1347	nM
CHEMBL1710520	[O-][N+](=O)c1ccc(cc1)c2oc(\C=N\c3c(nc4ccccn34)c5occc5)cc2	1400	nM
CHEMBL257359	CC(C)C(N1C(=S)S\C(=C/C=C/c2occc2)\C1=O)C(=O)O	1404	nM
CHEMBL1423980	COc1cc(NC(=O)CS(=O)(=O)c2ccc(C)cc2)cc(OC)c1OC	1416	nM
CHEMBL3188788	COC(=O)CSc1nnc(CNC(=O)Cc2ccccc2)n1C	1433	nM
CHEMBL1541610	CCn1cc(Br)c(n1)C(=O)Nc2ccccc(SC)c2	1434	nM
CHEMBL1583518	COCc1cc(C)nc(NCCCO)c1C#N	1439	nM
CHEMBL1312986	CCOC(=O)CNc1ccc2OCOc2c1	1469	nM
CHEMBL1412911	CCN1CCN(CC1)C2=NC(=O)\C(=C\c3oc(C)cc3)\S2	1469	nM
CHEMBL1524916	CN(C)c1ncc(s1)C2=C(Cl)C(=O)C(=C(Cl)C2=O)N3CCCC3	1536	nM

CHEMBL255881	CC(N1C(=S)S\C(=C/C=C/c2occc2)\C1=O)C(=O)O	1541	nM
CHEMBL1331134	O=C1CC(=O)N(Cc2occc2)C(=S)N1	1564	nM
CHEMBL1375860	CCOC1(OCC)N=C(N)C2(C#N)C(c3cccc(OC)c3OC)C12C#N	1593	nM
CHEMBL1544334	CC(C)CN1C(=O)c2ccccc2N=C1SCC(=O)NC(=O)Nc3ccc4OCCOc4c3	1619	nM
CHEMBL1430473	OC(=O)C1Nc2c(O)cc(Cl)c(c2C3C=CCC13)[N+](=O)[O-]	1639	nM
CHEMBL6246	Oc1cc2C(=O)Oc3c(O)c(O)cc4C(=O)Oc(c1O)c2c34	1669	nM
CHEMBL1411862	OCCNC(=O)Nc1ccc2nc(c3occc3)c(nc2c1)c4occc4	1756	nM
CHEMBL196072	NCCCC[C@H](COC(=O)N)NC(=O)CN(CCCCN)C(=O)OC[C@@H](N)CCCN=C(N)N	1799	nM
CHEMBL1335321	O=C(NC1CC1)Nc2ccc3nc(c4occc4)c(nc3c2)c5occc5	1833	nM
CHEMBL3392033	NC1=C(C#N)C2=C(CCCCC2)C(=S)S1	1842	nM
CHEMBL1528814	COc1cccc2C3C=CCC3C(Nc12)C(=O)O	1870	nM
CHEMBL1492764	CCC(N(CCCO)Cc1cc2cc(C)cc(C)c2nc1O)c3nnnn3C(C)(C)CC	1879	nM
CHEMBL1595235	C=CCSC1=N\C(=C/C=C/c2occc2)\C(=O)S1	1889	nM
CHEMBL1399331	OC(=O)C1Nc2c(cccc2C(=O)O)C3C(Cl)C(CC13)Sc4ccccc4[N+](=O)[O-]	1906	nM
CHEMBL1576095	CCCN1C(=O)S\C(=C/c2ccc(cc2C)N3CCOCC3)\C1=O	1918	nM
CHEMBL1493158	CC(C)OC(=O)c1cccc(n1)C(=O)O	1924	nM
CHEMBL1597042	O=C1NC(=O)\C(=C/C=C/c2occc2)\C(=O)N1Cc3occc3	1953	nM
CHEMBL1373961	CCOC(=O)C1CCN(CC1)C(c2cccs2)c3sc4nc(C)nn4c3O	1957	nM
CHEMBL1542128	CCCC1=NN2C(=N)\C(=C/c3oc(SCc4occc4)cc3)\C(=O)N=C2S1	1976	nM
CHEMBL1464853	ClC1=C(N2CCCCC2)C(=O)C(=C(C1=O)c3cnc(s3)N4CCCCC4)Cl	1991	nM
CHEMBL1482883	Oc1ccc(cc1)N2C(=O)S\C(=C/C=C/c3occc3)\C2=O	1998	nM
CHEMBL1374242	OCCCNC(=O)Nc1ccc2nc(c3occc3)c(nc2c1)c4occc4	2009	nM
CHEMBL1526171	CCOC(=O)C1CCN(CC1)C(=O)Nc2ccc3nc(c4occc4)c(nc3c2)c5occc5	2009	nM
CHEMBL1335699	OC(=O)\C=C\C(=O)Nc1cccnc1	2016	nM
CHEMBL213432	Cc1ccc(C)n1c2cccc(c2)C(=O)O	2069	nM
CHEMBL1371777	Clc1ccccc1CSc2nnc(c3occc3)c(n2)c4occc4	2074	nM
CHEMBL1310699	O=C(NC1CCCC1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	2080	nM
CHEMBL1523317	Cc1cc2c(N)cccc2nn1	2080	nM
CHEMBL1506682	OC1C(O)C(OC2=C(Oc3cc(O)cc(O)c3C2=O)c4ccc(O)c(O)c4)OC(C1O)C(=O)O	2123	nM
CHEMBL1457427	COc1ccc(NC(=O)c2cccc(c2)S(=O)(=O)Nc3ccc(Br)cc3)cn1	2154	nM
CHEMBL1366915	NC(=O)c1cc(N)ccc1N2CCCC2	2165	nM
CHEMBL1501132	COCCNC(=O)Nc1ccc2nc(c3occc3)c(nc2c1)c4occc4	2168	nM
CHEMBL1505467	Cc1nc2cc(nn2c(O)c1Cl)c3ccsc3n4c(C)ccc4C	2172	nM
CHEMBL1384172	o1cccc1c2nc(c3occc3)c(nc2c4occc4)c5occc5	2184	nM
CHEMBL1584917	CN=C1C=CC=CC(=C1O)c2ccc3cc4OCOc4cc3n2	2221	nM
CHEMBL1334684	OC(=O)C1Nc2ccc(cc2C3C=CCC13)C(=O)OC4CCCCC4	2264	nM
CHEMBL2001337	Cc1ccc(cn1)C(=O)N\N=C/c2oc(Br)c(Br)c2	2343	nM
CHEMBL1470525	CCN(CC)C(=O)c1oc(CS(=O)(=O)c2ccc(OC)cc2)cc1	2346	nM
CHEMBL458328	CCCCCC#CCC#CCC#CCC#CCCCC(=O)O	2378	nM
CHEMBL1424486	Nc1nc(c2occc2)c(s1)c3occc3	2391	nM
CHEMBL1504113	CN(C)[C@H]1C2CC3C(=C(O)[C@]2(O)C(=C(C(=O)NCN4CCCC4)C1=O)O)C(=O)c5c(O)cccc5[C@@]3(C)O	2462	nM
CHEMBL1567396	CC(=O)c1ccc2NC(C3CC=CC3c2c1)C(=O)O	2472	nM
CHEMBL1416439	O=C1N(NS(=O)(=O)c2ccccc2)C(=S)S/C/1=C\C=C/c3occc3	2483	nM
CHEMBL1302827	N=C1N2N=CSC2=NC(=O)/C/1=C/c3oc(SCc4occc4)cc3	2486	nM
CHEMBL1698517	COc1cc2Cc3cc(N)ccc3c2cc1N	2509	nM
CHEMBL1482554	O=C(CSc1ncnc2sccc12)Nc3oc(c4occc4)c(c5occc5)c3C#N	2524	nM
CHEMBL1587849	O=C(Nc1nc(c2occc2)c(s1)c3occc3)C4CCC4	2648	nM

CHEMBL3199404	CCCOc1ccc(CC2=NN3C(=O)\C(=C\c4occc4)\SC3=NC2=O)cc1	2675	nM
CHEMBL1401747	O=C(NN1C(=S)S\C(=C/C=C/c2occc2)\C1=O)c3ccncc3	2692	nM
CHEMBL1402117	Oc1nc(S)nc2Oc3nc(S)nc(O)c3C(c4ccc(Br)cc4)c12	2719	nM
CHEMBL1566266	Cc1ccccc1NC(=O)CSc2nnc(c3occc3)c(n2)c4occc4	2733	nM
CHEMBL69612	[O-][N+](=O)c1oc(\C=C\C=C\2/SC(=S)NC2=O)cc1	2758	nM
CHEMBL1416218	OC(=O)c1ccc(Cl)c2NC(C3CC=CC3c12)c4ccccn4	2814	nM
CHEMBL1452952	Cc1occc1c2nnc3sc(nn23)c4cc(oc4C)c5ccc(Cl)cc5	2865	nM
CHEMBL1548317	CC1(OCCO1)c2ccc3noc(c4ccccc4)c3c2	2870	nM
CHEMBL1497651	CC1=C(C#N)C(=O)N(C2CCS(=O)(=O)C2)C(=O)/C/1=C\c3occc3	2882	nM
CHEMBL1573365	Cl.CCN(CC)c1ccc2NCCCc2c1	2886	nM
CHEMBL1304024	FC(F)(F)C1=Nc2c(C=O)ccc3cccc(N1)c23	2914	nM
CHEMBL1609454	Cc1cc(\C=C\2/C(=O)NC(=O)N(C2=O)c3cccc(F)c3)c(C)n1c4cc(cc(c4)C(=O)O)C(=O)O	2947	nM
CHEMBL1378036	CCOC1=CC=CC(=O)c2c(C)n(Cc3occc3)c(C)c12	2954	nM
CHEMBL3196373	Oc1ccccc1\C=N\c2c(nc3ccccn23)c4occc4	2965	nM
CHEMBL1586326	Cc1oc(\C=C\C2=Cc3c(C#N)c(NC(=O)CSc4n[nH]c(N)n4)sc3C(C)(C)C2)cc1	3043	nM
CHEMBL1589300	CCCSC1=N\C(=C/C=C/c2occc2)\C(=O)S1	3052	nM
CHEMBL1364967	COC1=CC=CC(=O)c2c(C)n(c(C)c12)c3ccc(cc3)C(=O)O	3059	nM
CHEMBL1305450	COc1ccc2nc(c3occc3)c(nc2c1)c4occc4	3131	nM
CHEMBL1872442	O=C1CC(SC(=S)C2CCCC2=O)C(=O)N1	3212	nM
CHEMBL1487717	COc1ccc(NC(=O)N2c3ccc(OC)cc3C(=CC2(C)C)C)cc1	3286	nM
CHEMBL1326606	Oc1ccccc1C=Nc2ccc(F)c3c(O)[nH]nc23	3295	nM
CHEMBL1477236	CCOC1=CC=CC(=O)c2c(C)n(c(C)c12)c3ccc(cc3)C(=O)O	3303	nM
CHEMBL1334484	Nc1ncnc2oc(c3occc3)c(c4occc4)c12	3362	nM
CHEMBL1723511	OC(=O)c1cccc2cccc(C3=C4C=CC(=O)C(=C4Oc5c(O)c(O)ccc35)O)c12	3379	nM
CHEMBL1443088	Clc1ccc(cc1)N2C(=O)NC(=O)\C(=C\c3oc(Sc4nc5ccccc5[nH]4)cc3)\C2=O	3404	nM
CHEMBL1504429	CC(=O)OCCCNc1cc(Sc2nc3ccccc3s2)c4nonc4c1[N+](=O)[O-]	3414	nM
CHEMBL3199921	CCOC(=O)C1=C(N)N2C(=O)\C(=C\c3occc3)\SC2=C(C1c4occc4)C(=O)OC(C)C	3450	nM
CHEMBL408994	Cc1ccc(C)n1Cc2ccc(cc2)C(=O)O	3451	nM
CHEMBL1506843	COc1ccc(cc1)S(=O)(=O)c2c(N)n(Cc3occc3)c4nc5ccccc5nc24	3462	nM
CHEMBL1699836	OCC1=C(CO)C(=O)c2c(O)ccc(O)c2C1=O	3482	nM
CHEMBL1566165	O=C(Nc1ccc2nc(c3occc3)c(nc2c1)c4occc4)N5CCCCC5	3560	nM
CHEMBL1409603	OCCCNC(=O)c1ccc2nc(c3occc3)c(nc2c1)c4occc4	3584	nM
CHEMBL1312212	COc1cccc(NS(=O)(=O)c2ccc3NC(C4CC=CC4c3c2)c5ccc(cc5)C(=O)O)c1	3585	nM
CHEMBL1309430	OC(=O)CCCNc1cc(N2CCC3(CC2)OCCO3)c4noc5c6ccccc6C(=O)c1c45	3590	nM
CHEMBL1423705	Cc1oc(C)c(c1)c2nc3c4c5CCCc5sc4nc(O)n3n2	3658	nM
CHEMBL201289	OC(=O)C1Nc2ccc(Br)cc2C3C=CCC13	3730	nM
CHEMBL1376870	Cc1ccc2NC(C3CC=CC3c2c1)C(=O)O	3753	nM
CHEMBL1609550	O=C1N(C(=S)S/C/1=C\c2occc2)c3cccnc3	3901	nM
CHEMBL1995275	O=C(N\N=C\C=C/c1occc1)c2cccnc2	3913	nM
CHEMBL1568631	CC1C\C(=C\c2occc2)\C(=O)\C(=C\c3occc3)\C1	3915	nM
CHEMBL66953	OC1=CC=Cc2cc(O)c(O)c(O)c2C1=O	3958	nM
CHEMBL1493956	Cc1oc(CN2C(=S)Nc3ccc(cc3C2=O)N4CCOCC4)cc1	3984	nM
CHEMBL1449836	C(Sc1nnc(c2occc2)c(n1)c3occc3)c4ccccc4	4045	nM
CHEMBL1527833	Cc1oc(cc1)[C@@H]2C3COCC=C3C(=C(N)C2(C#N)C#N)C#N	4055	nM
CHEMBL1507864	CC1=C(C(C(C2=C(O)CC(CC2=N1)c3ccccc3)c4ccsc4)C(=O)Nc5ccccc5F	4055	nM

CHEMBL1394046	CCN1C(=S)NC(=O)\C(=C\c2ccc(s2)[N+](=O)[O-])\C1=O	4071	nM
CHEMBL1980204	CCOC(=O)c1c(C)oc2c3ccccc3c(O)c(\C=N\Cc4ccccn4)c12	4146	nM
CHEMBL1351226	CCOc1cccc(OCC)c2c(C)[n+](CC3CCCO3)c(C)c12.[O-]Cl(=O)(=O)=O	4163	nM
CHEMBL1383746	O=C(N1CCC2(CC1)OCCO2)c3ccc4nc(c5occc5)c(nc4c3)c6occc6	4259	nM
CHEMBL1422059	C(N1CCCc2ccccc12)c3nnc4CCCCCn34	4289	nM
CHEMBL1549687	Oc1ccc2C(=O)\C(=C\c3occc3)\Oc2c1CN4CCCCC4	4297	nM
CHEMBL1586973	COc1ccc(CCNC(=O)c2ccc3nc(c4occc4)c(nc3c2)c5occc5)cc1OC	4318	nM
CHEMBL1451059	CCN(CC)Cc1cc(O)c(CN(CC)CC)cc1O	4364	nM
CHEMBL1347567	CN=C1C=CC=CC=C1S	4407	nM
CHEMBL1469243	Cc1cc(C(=O)CSc2oc(nn2)c3occc3)c(C)n1Cc4occc4	4408	nM
CHEMBL1320230	Oc1ccccc1C(=O)NN2C(=S)S\C(=C/C=C/c3occc3)\C2=O	4462	nM
CHEMBL1446668	O=C(NCc1ccccc1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	4552	nM
CHEMBL1424878	CC(=O)c1sc2nc(ccc2c1N)c3occc3	4641	nM
CHEMBL1577840	Cc1ccc(C=C2C(=C(Cl)C(=C2Cl)Cl)Cl)cc1	4671	nM
CHEMBL195705	CCOC(=O)C(=O)NCc1oc(\C=C/2\N=C(C)C(=C2O)C(=O)OCC)cc1	4710	nM
CHEMBL1997195	CCCCN1C2=C(C=C(C#N)/C/1=N\C(=O)c3cccnc3)C(=O)N4C=CC=C(C)C4=N2	4743	nM
CHEMBL1346172	O=C(NCc1ccccn1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	4750	nM
CHEMBL3193785	CN(C)c1ccc(cc1)\N=C/2\C(=C(C#N)C(=O)N(C)C2=O)C	4768	nM
CHEMBL1350637	CC1CCN(Cc2c(O)ccc3C(=O)\C(=C\c4occc4)\Oc23)CC1	4794	nM
CHEMBL1409184	CC(=O)NN1C(=S)S\C(=C\c2oc(Br)cc2)\C1=O	4816	nM
CHEMBL1586235	BrC1CCc2c(sc3N=C4CCCCCN4C(=O)c23)C1=O	4818	nM
CHEMBL210208	OC1=C2Oc3c(O)c(O)ccc3C(=C2C=CC1=O)c4ccccc4S(=O)(=O)O	4836	nM
CHEMBL1340288	BrC1=CC(=COC1=O)C(=O)N2CCCc3ccccc23	4842	nM
CHEMBL1527832	CC(=O)c1sc(C(=O)O)c(c2occc2)c1c3occc3	4862	nM
CHEMBL3193134	Oc1ccc(\C=N\NC(=O)CCN2CCN(CC2)c3ccccc3)c(O)c1O	4869	nM
CHEMBL1406770	COC(=O)c1ccccc1NC(=O)C2CCCC2	4920	nM
CHEMBL1414222	CC(C)C1Nc2ccc(cc2C3C=CC13)C(=O)O	4932	nM
CHEMBL1527095	Oc1nc(cc(c2occc2)c1C#N)c3ccccc3	5005	nM
CHEMBL1459161	O=C(N1CCCc2ccccc12)C3=COC(=O)C=C3	5018	nM
CHEMBL1537686	O=C1N(C2CCS(=O)(=O)C2)C(=S)S/C/1=C\c3occc3	5051	nM
CHEMBL1431490	O=C(CSc1nnc(c2occc2)c(n1)c3occc3)Nc4ccccc4	5156	nM
CHEMBL3190370	O=C1N=C2S\C(=C/c3occc3)\C(=O)N2N=C1Cc4ccccc4	5206	nM
CHEMBL1257092	CC(C)NC[C@@H](O)c1ccc(O)c(O)c1.OC(C(O)C(=O)O)C(=O)O	5209	nM
CHEMBL3197320	CCN(CC)c1ccc(\C=N\N2C(=CC(=CC2=O)C)C)cc1	5266	nM
CHEMBL3190112	Sc1nnc(c2cccnc2)n1\N=C\C=C\c3occc3	5300	nM
CHEMBL1441847	COc1ccccc1n2c(S)nnc2c3cc([nH]n3)c4occc4	5362	nM
CHEMBL1477510	CCOc1ccc(cc1)N(CC(=O)NC(C)(C)C)S(=O)(=O)c2c(C)onc2C	5370	nM
CHEMBL3193845	CC1CCCC(=C1O)\C=N\c2ccc(C(=O)O)c(O)c2	5373	nM
CHEMBL1613571	CN1c2ccsc2C(=C(C(=Nc3ccc(F)c(Cl)c3)S)S1(=O)=O)O	5378	nM
CHEMBL1566203	Cc1oc(\C=C\2/SC(=S)N(C2=O)c3cccnc3)cc1	5441	nM
CHEMBL1379164	NC1=C(C#N)C(C#N)(C#N)C2CCCC(=C12)N3CCCC3	5444	nM
CHEMBL2132953	CC\C(=N/c1ccc(N)cc1)\C2=C(O)C(C(=O)OC)C(C)(C)CC2=O	5480	nM
CHEMBL1505704	Cl.Cc1cc(c(C)n1CC=C)c2csc(N)n2	5491	nM
CHEMBL1502381	Cl.COc1ccc(O)c(N)c1	5503	nM
CHEMBL1555752	CCN(CC)C(=O)c1ccc2NC(C3CC(Sc4ccccc4[N+](=O)[O-])C(Cl)C3c2c1)C(=O)O	5544	nM
CHEMBL1465392	O=C(C1CCCO1)N2CCC3(CC2)OCCO3	5547	nM
CHEMBL1460695	OC(=O)c1cccc(c1)n2ccccc2\C=C\[N+](=O)[O-]	5566	nM
CHEMBL3190368	Cc1cc(\C=N\Nc2ccc(cn2)[N+](=O)[O-])c(C)n1c3ccc(cc3)C(=O)O	5575	nM
CHEMBL1532547	CC1CCCN(Cc2c(O)ccc3C(=O)\C(=C\c4occc4)\Oc23)C1	5598	nM

CHEMBL3199451	Oc1ccc(\C=N/Nc2nccs2)cc1[N+](=O)[O-]	5683	nM
CHEMBL1517799	CCCCCC(=O)N1CC2(C[C@H]1C(=O)N)CC(=NO2)c3cccc(NC(=O)C(=C)C)c3	5758	nM
CHEMBL1415665	Cc1oc(cc1)C2C3=C(OC(=C2C#N)N)C(=O)C=C(CO)O3	5769	nM
CHEMBL1517227	CCN1CCN(CC1)c2cc(N3CCN(CC3)C(=O)c4occc4)c5C(=O)c6ccccc6c7onc2c57	5774	nM
CHEMBL1559731	Cc1cc(ccc1n2c(C)ccc2C)C(=O)O	5778	nM
CHEMBL2003564	CSc1ccc(\C=N\Nc2cccc(c2)C(=O)O)cc1	5808	nM
CHEMBL1419637	CCC1=CC(=O)Oc2cc(C)c(CN3CCCC3)c(O)c12	5838	nM
CHEMBL33864	OC(=O)CCCCC1CCSS1	5891	nM
CHEMBL377295	CCOC(=O)C1=C(O)\C(=C/c2oc(CNC(=O)C(=O)Nc3ccccc3)cc2)\N=C1C	5896	nM
CHEMBL1706619	CC1=C(C(N2C(=N1)S\C(=C/c3occc3)\C2=O)c4oc(C)cc4)C(=O)Nc5ccccc5	5901	nM
CHEMBL1449334	CSc1nnc(c2occc2)c(n1)c3occc3	6067	nM
CHEMBL1548822	FC(F)(F)c1cccc(NC(=O)c2ccc3nc(c4occc4)c(nc3c2)c5occc5)c1	6072	nM
CHEMBL1371637	Cc1nc2ncccn2c1c3csc(NCc4occc4)n3	6083	nM
CHEMBL1387545	Cc1ccc(c(Br)c1)n2c(S)nnc2c3cc([nH]n3)c4occc4	6085	nM
CHEMBL1340344	NC1=NC(=O)\C(=C/c2occc2)\S1	6087	nM
CHEMBL1385808	Cl.CN(C)[C@@H]1C2CC3Cc4c(ccc(O)c4C(=C3C(=O)[C@@]2(O)C(=C(C(=O)N)C1=O)O)O)N(C)C	6138	nM
CHEMBL1459370	COc1ccc(cc1OC)C2=CC(c3ccc(Cl)cc3)n4cnnc4N2	6187	nM
CHEMBL1978236	CN(C)c1ccc(cc1)\N=C/2\C(=C(C#N)C(=O)N(CCO)C2=O)C	6234	nM
CHEMBL1368432	CCOC(=O)c1cc2cc(F)ccc2nc1C	6243	nM
CHEMBL1598935	OC(=O)c1ccc2NC(C3CC(Sc4ccccc4[N+](=O)[O-])C(Cl)C3c2c1)c5cccc(c5)[N+](=O)[O-]	6298	nM
CHEMBL1421993	Cc1nc2ccccc2n3c(O)c(CC(=O)O)cc13	6318	nM
CHEMBL1364584	COc1ccc(NC2=NC(=O)\C(=C/C=C/c3occc3)\S2)cc1	6323	nM
CHEMBL1399979	CN(C1CCS(=O)(=O)C1)C(=O)COC(=O)c2cc(nc3ccccc23)c4occc4	6355	nM
CHEMBL1457676	OC(=O)c1ccc2NC(C3CC=CC3c2c1)c4ccncc4	6368	nM
CHEMBL1581251	Cc1cccc(C)c1NC(=O)CSc2nnc(c3occc3)c(n2)c4occc4	6432	nM
CHEMBL1331573	CCOC(=O)C(C(=O)OCC)c1cc(Br)c2noc3c4ccccc4C(=O)c1c23	6439	nM
CHEMBL305978	o1cccc1c2nc3ccccc3nc2c4occc4	6440	nM
CHEMBL3192690	Oc1cccc(\C=N\Cc2ccccc2)c1O	6464	nM
CHEMBL1323674	OC(=O)c1ccc(NN=C2C(=O)CCCC2=O)cc1	6468	nM
CHEMBL1987546	Clc1ccc(\C=N\c2c(nc3ccccn23)c4occc4)cc1	6483	nM
CHEMBL1478565	CN(C)c1c(F)c(F)c2c(C)c3ccccc3nc2c1F	6507	nM
CHEMBL1478395	O=C1NC(=S)SC1=C2CCCC2	6589	nM
CHEMBL1427047	CC(=O)c1ccc(NC(=O)CSc2nnc(c3occc3)c(n2)c4occc4)cc1	6605	nM
CHEMBL1574133	Cc1onc(c2ccccc2Cl)c1C(=O)NCc3occc3	6654	nM
CHEMBL1432884	CNC1=CC=CC=C(C(=O)\C=C\c2ccccc2OC)C1=O	6693	nM
CHEMBL1418568	CN1CCN(CC1)C2=C(Cl)C(=O)C=C(Cl)C2=O)c3cnc(s3)N4CCCCC4	6714	nM
CHEMBL1571110	Brc1ccc(cc1)C2=N\C(=C\c3occc3)\C(=O)N2	6780	nM
CHEMBL1340515	O=C1CC(=Nc2ccccc2N1)\C=C\c3occc3	6837	nM
CHEMBL1348345	CCCCNC(=O)c1ccc2nc(c3occc3)c(nc2c1)c4occc4	6844	nM
CHEMBL3196552	CCC\C(=N/c1ccc(N)cc1)\C2=C(O)C(C(=O)OC)C(C)(C)CC2=O	6876	nM
CHEMBL1421346	Cc1noc(\C=C\c2occc2)c1S(=O)(=O)N3CCC(CC3)C(=O)NCc4occc4	6925	nM
CHEMBL1981008	CC(\N=C\c1cccc(O)c1O)c2ccccc2	6963	nM
CHEMBL1408103	COc1ccc(NC(=O)CC2Nc3cccc4cccc(NC2=O)c34)cc1	7032	nM
CHEMBL1413495	CC(C)(C)C1C\C(=C\c2occc2)\C(=O)\C(=C\c3occc3)\C1	7084	nM
CHEMBL1391547	OC(=O)c1ccc2N[C@H]([C@H]3CC=C[C@H]3c2c1)c4ccccn4	7096	nM
CHEMBL3197343	Oc1ccc(\C=N\NC(=O)\C(=C\c2ccc(cc2)[N+](=O)[O-	7168	nM

146

	])\NC(=O)c3ccccc3)c(O)c1O		
	Cc1oc(\C=C\C(=O)Nc2ccc(c(NC(=O)\C=C\c3oc(C)cc3)c2)[N+](=O)[O-])cc1	7203	nM
CHEMBL1509648			
CHEMBL1584828	O=C(N1CCN(CC1)c2ncccn2)c3ccc4nc(c5occc5)c(nc4c3)c6occc6	7279	nM
CHEMBL1310375	CCCCC1=CC2=CC(=O)C(C)(OC(=O)c3cnc4ccccc4n3)C(=O)C2=CO1	7297	nM
CHEMBL1401798	Clc1ccc(Cl)c(NC=C2C(=O)CC(CC2=O)c3occc3)c1	7328	nM
CHEMBL1334452	OCCNC(=O)c1ccc2nc(c3occc3)c(nc2c1)c4occc4	7343	nM
CHEMBL1584646	NC1=C(C#N)C(C2=C(O1)\C(=C/c3cocc3)\CCC2)c4cocc4	7351	nM
CHEMBL1429570	CCCSC1=N\C(=C/c2oc(cc2)[N+](=O)[O-])\C(=O)S1	7367	nM
CHEMBL1972037	NS(=O)(=O)c1ccc(N\N=C\c2ccc(O)c(O)c2O)c(c1)[N+](=O)[O-]	7443	nM
CHEMBL1370375	COC\C=C\C1=CC2=CC(=O)C(C)(OC(=O)c3occc3)C(=O)C2=CO1	7470	nM
CHEMBL1414317	CC(=O)C1=C(C)N(CC=C)C(=S)N=C1N2CCN(CC2)c3ccccc3	7511	nM
CHEMBL1450458	CC1CCCCC1NC(=O)COC(=O)c2c3CC\C(=C/c4occc4)\c3nc5ccccc25	7581	nM
CHEMBL463175	CC1CC(=O)c2c(O)c3c(O)cc(O)c(c4c(O)cc(O)c5c(O)c6C(=O)CC(C)Oc6cc45)c3cc2O1	7617	nM
CHEMBL1446626	O=C(Nc1ccccc1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	7630	nM
CHEMBL1604074	COC(=O)C1=COC(C)C2CN3CCc4c([nH]c5ccccc45)C3CC12	7634	nM
CHEMBL1558113	CCOC(=O)N1CCN(CC1)C(=O)c2ccc3c(SCC(=O)O)c4CCCc4nc3c2	7654	nM
CHEMBL371627	NCCCC[C@H](COC(=O)N)NC(=O)CN(CCCCN)C(=O)OC[C@@H](N)CCC\N=C/1\C(=C(O)C1=N)O	7699	nM
CHEMBL1500600	CC(=O)c1ccc(NC(=O)c2ccc3nc(c4occc4)c(nc3c2)c5occc5)cc1	7730	nM
CHEMBL1539325	CC1(C)CCCN(C1)C(=O)C2=COC(=O)C(=C2)Br	7768	nM
CHEMBL1346055	OC(=O)c1ccc(cc1)n2cccc2\C=C/3\NC(=O)N(C3=O)c4cccc(Cl)c4	7846	nM
CHEMBL1981770	CCOC(=O)C1=C(N)N2C(=O)\C(=C\c3occc3)\SC2=C(C1c4occc4)C(=O)OCC	7852	nM
CHEMBL1423852	O=C(\C=C\c1occc1)N(c2ccccn2)c3ccccn3	7904	nM
CHEMBL1387355	O=C(CCCN1C(=S)S\C(=C\c2occc2)\C1=O)Nc3cccc4ccccc34	7924	nM
CHEMBL3191622	CN1\C(=N/c2cccc(c2)C(=O)O)\S\C(=C/c3occc3)\C1=O	7933	nM
CHEMBL1338027	CNC1=CC=C(Br)C=C(C(=O)\C=C\c2cccc(OC)c2OC)C1=O	7998	nM
CHEMBL1432333	O=C(NC(=S)Nc1cccc(c1)S(=O)(=O)NC2=NCCC2)c3cc(nc4ccccc34)c5occc5	8036	nM
CHEMBL1507308	CCNC(=O)COC(=O)c1cc(nc2ccccc12)c3occc3	8092	nM
CHEMBL1358059	COC\C=C\C1=CC2=CC(=O)C(C)(OC(=O)CCC(=O)OC)C(=O)C2=CO1	8103	nM
CHEMBL3190665	COc1ccc(\C=N\c2c(nc3ccccn23)c4occc4)cc1OC	8154	nM
CHEMBL3192197	O=C(Cc1cccs1)N\N=C\C=C\c2occc2	8220	nM
CHEMBL3191661	C\C(=C/c1occc1)\C=N\n2c(S)nnc2c3ccncc3	8220	nM
CHEMBL1378817	O=C1C2C3CCCC3=C4CCCC4C2C(=O)N1c5ccccc5	8279	nM
CHEMBL1342716	CCOC(=O)COc1nc(cc(c2occc2)c1C#N)c3occc3	8336	nM
CHEMBL1532407	Sc1nc2CCCCc2c(c3occc3)c1C#N	8343	nM
CHEMBL3197060	CN(C)c1ccc(cc1)\N=C/2\C(=C(C#N)C(=O)N(CCCO)C2=O)C	8435	nM
CHEMBL1348610	[O-][n+]1c2CCCc2[n+]([O-])c3cc(Br)ccc13	8442	nM
CHEMBL2007057	Br\C(=C/c1ccccc1)\C=N\NC(=O)c2cc([nH]n2)c3occc3	8533	nM
CHEMBL1417070	Cc1c(Cl)cccc1NS(=O)(=O)c2ccc3NC(C4CC=CC4c3c2)c5ccc(cc5)C(=O)O	8536	nM
CHEMBL504791	Oc1ccc(cc1)\N=C\c2ccc(s2)c3cccs3	8645	nM
CHEMBL1389990	C\C(=C/c1occc1)\C=C/2\SC(=S)N(CC(=O)O)C2=O	8804	nM
CHEMBL1406195	Oc1ccc(cc1O)C(=O)CSc2nc3ccccc3n2CCc4ccccc4	8815	nM
CHEMBL1516515	Cc1nn(c2CCC(Br)C(=O)c12)c3ccccn3	8819	nM
CHEMBL1255778	Cl.NC(CO)C(=O)NNCc1ccc(O)c(O)c1O	8835	nM
CHEMBL1305385	Cc1ccccc1NC(=O)c2c(C)nc(S)c(C#N)c2c3occc3	8909	nM
CHEMBL1410381	Oc1c(cc(CN2CCCC2)c3cccnc13)[N+](=O)[O-]	8940	nM

CHEMBL1570659	OC(=O)C1Nc2c(cccc2C(=O)N3CCOCC3)C4C=CCC14	8990	nM
CHEMBL1311222	COc1cc(CN(C(=O)c2occc2)c3ccc(C)cc3)ccc1O	9048	nM
CHEMBL1723399	COc1cccc(CNC(=O)CCNS(=O)(=O)c2cccs2)c1	9048	nM
CHEMBL1380684	Cl.CN1CCc2cccc3c2[C@@H]1Cc4ccc(O)c(O)c34	9078	nM
CHEMBL212827	Cc1ccc(C)n1c2ccc(cc2)C(=O)O	9092	nM
CHEMBL1400828	Cc1cc(C(=O)COC(=O)c2cc(O)c3ccccc3c2O)c(C)n1CC4CCCO4	9140	nM
CHEMBL1463326	CNC1=CC=C(Br)C=C(C(=O)\C=C\c2ccc(OC)cc2)C1=O	9153	nM
CHEMBL1501573	Brc1cccc(c1)C2=N\C(=C/c3occc3)\C(=O)N2	9199	nM
CHEMBL1427289	O=C(NC1CC1)c2cc(nc3ccccc23)c4occc4	9273	nM
CHEMBL1604163	o1cccc1\C=C\c2ccc3ccccc3n2	9388	nM
CHEMBL1342736	CSc1nc(NCCOCCO)c2sc3nc(c4CCCc4c3c2n1)c5occc5	9422	nM
CHEMBL1522155	NS(=O)(=O)c1ccc(cc1)N=Nc2cnc(O)c(O)c2	9469	nM
CHEMBL1416382	CN=C1C=CC(=CC(=C1O)C(=O)\C=C\c2ccc(Cl)cc2Cl)Br	9564	nM
CHEMBL1408802	Clc1cc(Cl)cc(NC=C2C(=O)CC(CC2=O)c3occc3)c1	9578	nM
CHEMBL1576254	Cl.Nc1ccc(cc1)N(CCO)CCO	9623	nM
CHEMBL1463595	O=C1N(C(=S)S/C/1=C/c2occc2)c3ccccc3	9641	nM
CHEMBL1301164	CNC1=CC=C(Br)C=C(C(=O)\C=C\c2cc(OC)ccc2OC)C1=O	9748	nM
CHEMBL1981675	CCOC(=O)C1=C(N)N2C(=O)\C(=C/c3occc3)\SC2=C(C1c4occc4)C(=O)OC	9783	nM
CHEMBL1445785	Cl.COc1cc(CNCCc2ccc(F)cc2)ccc1OCc3ccc(Cl)nc3	9799	nM
CHEMBL1339797	CC1=CC2=C(C(C(=C(N)O2)C#N)c3oc(cc3)[N+](=O)[O-])C(=O)O1	9958	nM
CHEMBL1543190	NS(=O)(=O)c1ccc2NC(C3CCC=CC3)C4CC=CC4c2c1	9982	nM
CHEMBL1300569	CN(C)c1ccc(cc1)N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	9991	nM
CHEMBL1364109	CC1Cc2ccccc2N1CC3=CC(=O)N4C=CSC4=N3	10044	nM
CHEMBL1509350	COc1cccc(c1)n2c(Cc3cc(O)nc(O)n3)nnc2SCC(=O)NC4CCCC4	10125	nM
CHEMBL1382279	CCNC1=CC=C(Br)C=C(C(=O)\C=C\c2ccc(OCC)cc2)C1=O	10157	nM
CHEMBL1980184	O=C(N\N=C\C=C\c1occc1)c2ccncc2	10178	nM
CHEMBL1341340	OC(COc1ccc(cc1)S(=O)(=O)N2CCOCC2)CN3CCC(Cc4ccccc4)CC3	10328	nM
CHEMBL3198038	C\C(=N/c1cccc(O)c1)\C=C(/O)\c2ccc(C)cc2	10369	nM
CHEMBL1428997	CS(=O)(=O)c1ccc2N3C(=NC(=O)\C(=C\c4occc4)\C3=N)Sc2c1	10374	nM
CHEMBL3195505	o1cccc1\C=C\C=N\n2cnnc2	10410	nM
CHEMBL1526580	CC(=O)Oc1cccc(c1)N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	10460	nM
CHEMBL1453783	COC\C=C\C1=CC2=CC(=O)C(C)(OC(=O)C3CCCC3)C(=O)C2=CO1	10521	nM
CHEMBL3193859	C\C(=C\c1occc1)\C=N\NC(=O)Cc2cccn2C	10699	nM
CHEMBL1337304	[O-][N+](=O)c1ccc(\C=C/2\C(=O)NC(=O)N(C2=O)c3ccccc3)s1	10713	nM
CHEMBL1352170	CN1N(C(=O)C(=C1C)N=C2C=C(Br)C(=O)C(=C2)Br)c3ccccc3	10962	nM
CHEMBL47986	Oc1ccc(O)c(\C=C\NC=O)c1	10970	nM
CHEMBL1334633	CCOC(=O)c1ccc2NC(C3CC=CC3c2c1)C(=O)O	10981	nM
CHEMBL1414652	COc1ccc2C(=NN(C)c3ccccc1c23)C	11063	nM
CHEMBL1360529	COC(=O)CCC(=O)OC1(C)C(=O)C=C2C=C3CCCN3C=C2C1=O	11100	nM
CHEMBL1579407	[O-][n+]1c2CCCCc2[n+]([O-])c3cc(F)c(F)cc13	11139	nM
CHEMBL1478258	COC(=O)c1oc(CC(=O)c2c(C)cc(O)cc2O)cc1	11178	nM
CHEMBL1547446	CN1C(=S)NC(=O)\C(=C/C=C/c2occc2)\C1=O	11218	nM
CHEMBL1604283	CO[C@H]1C=CO[C@@]2(C)Oc3c(C)c(O)c4c(O)c(NC(=O)C(=CC=C[C@H](C)[C@H](O)[C@@H](C)[C@@H](O)[C@@H](C)[C@H](OC(=O)C)[C@@H]1C)C)c(C=NN5CCN(C)CC5)c(O)c4c3C2=O	11234	nM
CHEMBL1546048	OC(=O)CC(N1C(=S)S\C(=C/c2oc(cc2)c3nc4ccccc4s3)\C1=O)C(=O)O	11286	nM
CHEMBL1528757	Nc1cc(N)c(OCC(F)(F)F)cc1OCC(F)(F)F	11389	nM
CHEMBL1330585	O=C1CC(Nc2ccc(cc2)N3CCOCC3)C(=O)N1C4CCCCC4	11573	nM
CHEMBL1974521	O=C(N\N=C\C=C\c1occc1)c2cccs2	11607	nM
CHEMBL1479103	Oc1cc2CC3(O)COc4c(O)c(O)ccc4C3c2cc1O	11696	nM

CHEMBL6640	NCCc1c[nH]c2ccccc12	11752	nM
CHEMBL601952	Cl.Nc1ccc(cc1)N2CCCCC2	11781	nM
CHEMBL1256958	CNC[C@H](O)c1ccc(O)c(O)c1.OC(C(O)C(=O)O)C(=O)O	11807	nM
CHEMBL605747	CC1=CC=CN2C(=O)C3=C(N=C12)N(CCc4ccccc4)C(=N)C(=C3)C(=O)NCc5occc5	11809	nM
CHEMBL1468476	CN1C(=O)\C(=C/NNc2ccc(C)c(C)c2)\C(=C(C#N)C1=O)C	11852	nM
CHEMBL1442048	O=C1N=C(S/C/1=C\c2occc2)N3CCN(CC3)c4ccccc4	11857	nM
CHEMBL1407274	O=C1OC(=Nc2sc3CCCc3c12)\C=C\c4occc4	11917	nM
CHEMBL1609186	NC(=O)\C(=C\c1occc1)\C(=S)N	12031	nM
CHEMBL1373655	CC1=NN(C(=O)/C/1=C\C=C\c2occc2)c3cccc(c3)C(=O)O	12042	nM
CHEMBL1446904	Cc1cc(C)c(C(=O)\C=C\c2occc2)c(O)n1	12134	nM
CHEMBL1412282	OC(=O)CSc1c2CCCCc2nc3cc(ccc13)C(=O)N4CCOCC4	12165	nM
CHEMBL1425000	COc1cccc(C2C(=C(N)OC3=C2C(=O)CC(C3)c4occc4)C#N)c1OCc5ccc(F)cc5	12209	nM
CHEMBL1486503	CC1=CN2C(=NC(=O)\C(=C/c3oc(cc3)[N+](=O)[O-])\C2=N)S1	12235	nM
CHEMBL1601846	OC1=CC2=C(OC1=O)c3c(O)c(O)c(O)cc3C(=O)O2	12259	nM
CHEMBL1412617	COc1ccc(N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O)c(OC)c1	12371	nM
CHEMBL1716317	Oc1cc(cc2cc(Nc3ccccc3)ccc12)S(=O)(=O)O	12487	nM
CHEMBL1488898	CCN=C1C=CC(=CC(=C1O)C(=O)\C=C\c2ccc(Cl)cc2)Br	12533	nM
CHEMBL1508080	CCC1C\C(=C\c2occc2)\C(=O)\C(=C\c3occc3)\C1	12553	nM
CHEMBL1560617	Cn1nc(c2ccc(Cl)cc2)c3cc(sc13)C(=O)N4CCN(CC4)c5ccccc5	12597	nM
CHEMBL1340633	COc1cc(ccc1Nc2ccccc2C(=O)O)c3ccc(Nc4ccccc4C(=O)O)c(OC)c3	12655	nM
CHEMBL1349278	CCc1cc(O)n2nc(C)c(c3ccccc3OC)c2n1	12721	nM
CHEMBL1568791	Fc1ccccc1N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	12854	nM
CHEMBL3194876	Oc1ccc(\C=N\NC(=S)Nc2cccnc2)c(O)c1O	12905	nM
CHEMBL1523510	COC(=O)CCC(=O)OC1(C)C(=O)C(=C2C=C(OC=C2C1=O)c3ccc(OC)cc3)Br	13025	nM
CHEMBL1586096	COc1cc(cc(OC)c1O)C2Nc3cccc4cccc(N2)c34	13117	nM
CHEMBL1712631	Cc1nc2C(=O)NC(=S)Nc2nc1O	13177	nM
CHEMBL1408143	OC(=O)c1c2CCCc2nc3ccc(Cl)cc13	13210	nM
CHEMBL3196071	Oc1c(\C=N\Cc2ccncc2)c3c4CCCCc4oc3cc1[N+](=O)[O-]	13357	nM
CHEMBL1982713	Cc1oc(\C=C\2/Sc3nc(nn3C2=O)c4cccs4)cc1	13568	nM
CHEMBL1452185	OC(=O)c1cccc(NN=C2C(=O)CCCC2=O)c1	13660	nM
CHEMBL1415169	CC(=O)N1CCN(CC1)c2ccc(NCc3ccccc3)cc2	13679	nM
CHEMBL1341061	COc1ccc(N=C(S)NCCc2ccccc2OC)c(OC)c1	13703	nM
CHEMBL1430005	O.C[n+]1cccc2cccc([O-])c12	13712	nM
CHEMBL2007178	OC(=O)c1ccc(cc1)n2cccc2\C=N/NC(=O)c3oc4ccc(Br)cc4c3	13827	nM
CHEMBL1991599	Oc1ccc(\C=N\N2CCOCC2)c(O)c1O	14003	nM
CHEMBL1569952	CCOC(=O)N1CCN(CC1)c2ccc(O)cc2	14028	nM
CHEMBL1423121	CCN(CC(=O)Nc1c([nH]c2ccccc12)C(=O)OC)c3ccc4OCOc4c3	14279	nM
CHEMBL1570323	CC[C@H](C)\C=C(/C)\C=C\C1=CC2=CC(=O)[C@]3(C)OC(=O)[C@H]([C@@H]3C2=CO1)C(=O)C	14355	nM
CHEMBL3190976	CN1N(C(=O)C(=C1C)\N=C\2/C=CC(=O)C(=C2)C)c3ccccc3	14504	nM
CHEMBL1313956	Clc1ccccc1OCC(=O)c2ccc[nH]2	14626	nM
CHEMBL1403497	O=C1CC(=O)N(Cc2occc2)C(=O)N1	14648	nM
CHEMBL3189657	Oc1ccc(\C=N\N2C(=O)c3ccccc3C2=O)c(O)c1O	14745	nM
CHEMBL1342528	CCOc1cc(N2CCOCC2)c(OCC)cc1NS(=O)(=O)c3ccc(Cl)s3	14902	nM
CHEMBL1543330	CCC1S\C(=C(/C#N)\C(=O)NCc2occc2)\N(C1=O)c3ccc(F)cc3	14916	nM
CHEMBL1093246	Oc1ccc(cc1)\N=C\c2ccc(O)c(O)c2	14957	nM
CHEMBL1981446	Oc1cc(O)cc(c1)C(=O)N\N=C\c2cn(Cc3cccc(F)c3)c4ccccc24	14961	nM
CHEMBL1402539	[Br-].Cc1cccc2cc(c3ccccc3)c(c[n+]12)c4ccccc4	14969	nM

CHEMBL1562537	Fc1ccccc1NC(=O)C2=COC(=O)C(=C2)Br	14985	nM
CHEMBL1546136	Cc1cccc(NC(=O)CSc2nnc(c3occc3)c(n2)c4occc4)c1C	15030	nM
CHEMBL1577453	COc1ccc(cc1)c2cc(nc(O)c2C#N)c3occc3	15075	nM
CHEMBL1457755	CCOC(=O)N1CC=C2[C@H](C1)[C@@H](c3cccs3)C(C#N)(C#N)C(=C2C#N)N	15255	nM
CHEMBL1304584	CC1=CC(C)(C)Nc2ccc(OC(=O)CN3C(=O)c4cccc5cccc(C3=O)c45)cc12	15289	nM
CHEMBL3191022	CCn1c(C)nc2cc(ccc12)C(=O)N\N=C\c3ccc(O)c(O)c3O	15294	nM
CHEMBL1584173	OC(=O)\C(=C\c1occc1)\NC(=O)c2ccccc2	15314	nM
CHEMBL1308302	CN(C)N1C(=C(C#N)C(C2=C1CCCC2=O)c3ccnc3)N	15324	nM
CHEMBL383041	O=C1CC(Nc2ccc(cc2)N3CCOCC3)C(=O)N1Cc4ccccc4	15440	nM
CHEMBL1340051	NC(=O)CN1C(=O)N(Cc2occc2)C(=O)c3c4CCCCCc4sc13	15488	nM
CHEMBL3210868	C\C(=N/Nc1ccc(cc1[N+](=O)[O-])[N+](=O)[O-])\C2=Cc3c(OC2=O)ccc4ccccc34	15623	nM
CHEMBL1561729	OC(=O)c1ccc(cc1)n2cccc2\C=C/3\NC(=O)N(C3=O)c4ccccc4	15662	nM
CHEMBL1448387	Oc1cc2C[C@]3(O)COc4c(O)c(O)ccc4[C@@H]3c2cc1O	15711	nM
CHEMBL1562824	Oc1c(cc(CN2CCOCC2)c3cccnc13)[N+](=O)[O-]	15777	nM
CHEMBL2028186	[Na+].[Na+].Oc1ccc(Cl)cc1N=Nc2c(O)c3c(O)cc(cc3cc2S(=O)(=O)[O-])S(=O)(=O)[O-]	15919	nM
CHEMBL1580335	Cc1oc(\C=C\C(=O)Nc2ncc(C)s2)cc1	15966	nM
CHEMBL1449261	CC(C)N1C(=O)CC(Nc2ccc(cc2)N3CCOCC3)C1=O	16015	nM
CHEMBL1303019	NC(=S)\C(=C/c1oc(Br)cc1)\C#N	16044	nM
CHEMBL1723023	O=C1N(C(=S)N/C/1=C/c2occc2)c3ccccc3	16122	nM
CHEMBL1420119	CCOC(=O)c1sc2nc(CC(=O)OC)nc(NCc3occc3)c2c1C	16139	nM
CHEMBL1328733	O=C1NC(=S)N(C(=O)/C/1=C/c2occc2)c3ccccc3	16200	nM
CHEMBL1711538	Cc1ccc(NC(=O)COc2ccc(\C=N\NC(=O)CSc3ccccc3)cc2)cc1	16288	nM
CHEMBL1455912	CCOc1ccccc1N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	16336	nM
CHEMBL1464373	O=C(COC(=O)c1ccc(NS(=O)(=O)c2cccs2)cc1)NCc3occc3	16369	nM
CHEMBL1525725	FC(F)(F)c1cc(NC(=O)CCCCN2C(=O)CCC2=O)ccc1Cl	16378	nM
CHEMBL523200	[O-][N+](=O)c1ccc(Sc2oc3ccccc3n2)c(c1)[N+](=O)[O-]	16429	nM
CHEMBL1486335	OCCCNc1cc(SCc2occc2)c3nonc3c1[N+](=O)[O-]	16538	nM
CHEMBL1497208	ClC1=C(N2CCOCC2)C(=O)N(C1=O)c3ccccc3	16572	nM
CHEMBL1348852	Cc1cc(c(C)n1Cc2occc2)c3csc(NC(=O)c4ccc(cc4)C#N)n3	16658	nM
CHEMBL3196993	Oc1ccc(\C=N\NC(=O)Cc2csc(n2)N3CCOCC3)c(O)c1O	16715	nM
CHEMBL1531750	CCCC1=CC(=O)Oc2cc(C)c(CN3CCCC3)c(O)c12	16949	nM
CHEMBL518575	Cn1cccc1\C=C\2/CCC\C(=C/c3cccn3C)\C2=O	17045	nM
CHEMBL3194107	CN1C(=O)N(C)c2ncn(CC(=O)N\N=C\C=C\c3occc3)c2C1=O	17128	nM
CHEMBL1509377	CC(=C)C(=O)Nc1cccc(c1)C2=NOC3(C[C@@H](N(C3)C(=O)COc4ccc(Cl)cc4)C(=O)N)C2	17335	nM
CHEMBL1359359	CNCc1ccccc1Sc2cc(O)ccc2O.OC(=O)\C=C/C(=O)O	17504	nM
CHEMBL1533230	CC(C)(CS(=O)(=O)[O-])NC(=O)CC[N+](C)(C)CCO	17509	nM
CHEMBL1605099	O=C1N(Cc2ccccc2)C(=S)S/C/1=C/c3occc3	17542	nM
CHEMBL1425725	COc1ccccc1N2C(=O)NC(=O)\C(=C\c3ccc(s3)[N+](=O)[O-])\C2=O	17553	nM
CHEMBL1449846	Cc1sc2ncnc(SCc3occc3)c2c1C	17604	nM
CHEMBL1446502	CCCCNC(=O)CSC1=Nc2scc(c3occc3)c2C(=O)N1CC=C	17774	nM
CHEMBL1598904	Cc1ccc(cc1)c2ccc(CCC(=O)O)n2N=C(N)S	17820	nM
CHEMBL1381017	CC1=NNC(=S)N(NC(=O)\C=C\C(=O)NN2C(=S)NN=C(C)C2=O)C1=O	18161	nM
CHEMBL567531	O=C(COC(=O)c1cc(nc2ccccc12)c3occc3)NCc4ccc5OCOc5c4	18179	nM
CHEMBL3191675	CC\C(=N/c1ccc(O)cc1)\C=C(/O)\c2ccncc2	18275	nM
CHEMBL1560775	Oc1ccc(NC2=NC(=O)\C(=C\C=C\c3occc3)\S2)cc1	18287	nM
CHEMBL1599175	N=C1S\C(=C/c2occc2)\C(=O)N1c3ccc4OCOc4c3	18390	nM

CHEMBL1501577	COC(=O)c1ccccc1NC(=O)CCS(=O)(=O)c2ccc(Br)cc2	18402	nM
CHEMBL3189351	Cc1cc([nH]n1)c2nnc(S)n2\N=C\C=C\c3occc3	18553	nM
CHEMBL1384137	CCOC1=CC=CC(=O)c2c(C)n(CC(=O)c3ccccc3)c(C)c12	18607	nM
CHEMBL1301589	O=C(N1CCN(CC1)c2ccccc2)c3cc(on3)c4occc4	18614	nM
CHEMBL1446243	COc1ccc(CCN2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O)cc1OC	18846	nM
CHEMBL1562928	Oc1cc(c2CCCc2n1)c3ccccc3Cl	18847	nM
CHEMBL1256708	O.Cl.CN1CCc2cccc3c2[C@H]1Cc4ccc(O)c(O)c34	19071	nM
CHEMBL1349676	COC(=O)CCC(=O)OC1(C)C(=O)C(=C2C=C(N(CCCOC(C)C)C=C2C1=O)c3ccc(OC)cc3)Br	19073	nM
CHEMBL1493191	Oc1ccc(cc1)N2C(=S)S\C(=C/C=C/c3occc3)\C2=O	19113	nM
CHEMBL1706454	Cl.OCCN1CCN(CC1)C2=C(Cl)C(=O)c3c(O)ccc(O)c3C2=O	19262	nM
CHEMBL1402286	COc1ccc(NC(=O)c2cc(nc3ccccc23)c4occc4)cc1S(=O)(=O)N5CCOCC5	19303	nM
CHEMBL1730401	Nc1cccc2c(O)cc(cc12)S(=O)(=O)O	19312	nM
CHEMBL179024	Cc1oc(cc1)C(=O)Nc2ccc(O)c(c2)C(=O)O	19380	nM
CHEMBL117966	[O-][N+](=O)c1oc(\C=C(/C#N)\c2nc3ccccc3[nH]2)cc1	19583	nM
CHEMBL1336400	O=C1CCC/C/1=C/Nc2ccc3OCOc3c2	19679	nM
CHEMBL1526514	COc1ccccc1N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	20063	nM
CHEMBL1575100	Cc1cccc(NC(=S)NC(=O)\C=C\c2occc2)c1	20153	nM
CHEMBL1510832	FC(F)(F)c1cnc(NC(=O)COC(=O)\C=C\c2occc2)c(Cl)c1	20166	nM
CHEMBL1417290	CCN(CC)c1ccc2OC(=O)C(=Nc2c1)C	20244	nM
CHEMBL1364651	CN1N(C(=O)C(=C1C)n2c(C)cc(C(=O)CCl)c2C)c3ccccc3	20310	nM
CHEMBL1505471	COC(=O)c1ccc(O)c2nc3c(C=O)c(O)cc(O)c3nc12	20342	nM
CHEMBL1271266	Oc1cc(cc2ccc(Nc3ccccc3)cc12)S(=O)(=O)O	20505	nM
CHEMBL1996233	OC1=C(\C=N\c2cc(Cl)ccc2O)C(=O)CC(C1)c3occc3	20511	nM
CHEMBL1473059	[O-][N+](=O)c1cnc(NC(=O)COC(=O)c2ccccc2)s1	20534	nM
CHEMBL1566010	Cc1oc(cc1)c2c3CCCCc3nc(S)c2C#N	21214	nM
CHEMBL1437977	Cc1ccn2cc(cc2c1)c3nonc3C	21370	nM
CHEMBL1992547	C\C(=N/Nc1ccc(Cl)c(c1)C(=O)O)\c2ccc[nH]2	21390	nM
CHEMBL1569992	CC(=C)C(=O)Nc1ccc2OCCOCCOCCOc2c1	21624	nM
CHEMBL1421172	CCCCN1C(=S)NC(=O)\C(=C/C=C/c2occc2)\C1=O	21699	nM
CHEMBL1571597	CNc1c(ccc2C(=O)c3ccccc3C(=O)c12)C(=O)O	21860	nM
CHEMBL1508001	Cc1ccc[n+](c1)C2=C(SC(=O)[N-]2)C=NNC(=O)c3ccccc3O	22059	nM
CHEMBL1346425	Fc1ccc(CN2CCNC(=O)C2CC(=O)NCCN3CCCc4ccccc34)cc1	22113	nM
CHEMBL1452551	COC\C=C\C1=CC2=CC(=O)C(C)(OC(=O)c3cnc4ccccc4n3)C(=O)C2=CN1c5ccccc5	22256	nM
CHEMBL1700270	Oc1ccc(N=Nc2cc(Cl)cc(c2O)S(=O)(=O)O)c(O)c1	22502	nM
CHEMBL195455	COC(=O)C1=C(O)\C(=C/c2oc(CNC(=O)C(=O)Nc3ccc(C)cc3)cc2)\N=C1C	22526	nM
CHEMBL1519796	CCOC1=CC=CC(=O)c2c(C)oc(C)c12	22563	nM
CHEMBL1318848	Cl.CC(C)CC(N1CCN(C)CC1)c2nnnn2CS(=O)(=O)c3ccc(C)cc3	22634	nM
CHEMBL1559159	COC1=CC(=CC(=O)c2c(C)oc(C)c12)c3cccs3	22671	nM
CHEMBL1342436	CCCN=C1C(=C(O)C2=C(C(COC(=O)N)[C@]3(OC)C4NC4CN23)C1=O)C	22678	nM
CHEMBL1449868	CCCCN1C(=O)c2cc(ccc2N=C1SCC(=O)NCc3occc3)N4CCOCC4	22759	nM
CHEMBL1611654	Oc1ccc2OC3(CCCC3c2c1)N4CCOCC4	23136	nM
CHEMBL1586339	COc1ccc(Nc2ccc(OC)cc2)cc1	23170	nM
CHEMBL1505755	Clc1ccc(CNC(=O)CN2CCN(CC2)S(=O)(=O)c3ccc(Cl)s3)cc1	23222	nM
CHEMBL3192541	CN(C)S(=O)(=O)c1cccc(NC(=S)N\N=C\c2ccc(O)c(O)c2O)c1	23245	nM
CHEMBL1569215	OC(=O)c1cccc(c1)c2oc(\C=C/3\C(=O)NN(C3=O)c4ccc(Cl)cc4)cc2	23406	nM
CHEMBL1545983	Cc1cc2ccccc2n1CCNC(=O)C3CCCCC3	23461	nM
CHEMBL1451156	Clc1cc(Cl)cc(NC(=O)C2=COC(=O)C(=C2)Br)c1	23493	nM

CHEMBL1612606	Cc1cc(cs1)C(=O)Nc2sc3CCCCCc3c2C#N	23639	nM
CHEMBL1567271	Fc1ccccc1\C=C\2/CCCC3=C2Nc4ncnn4C3c5ccccc5F	23721	nM
CHEMBL1413743	Brc1c(CSc2oc(nn2)c3occc3)nc4ccccn14	23935	nM
CHEMBL1541353	CCC1=NC2=C(C(=O)N1Cc3occc3)C(=O)c4ccc(OC)cc4O2	23969	nM
CHEMBL1365518	Cc1onc(c1)C(=O)NCCCN2CCCC2=O	24002	nM
CHEMBL1548022	COc1cc2[nH]c(Cl)c(c2cc1OC)[N+](=O)[O-]	24283	nM
CHEMBL1340117	CC\C=C\C(=O)N1CC2(C[C@H]1C(=O)N)CC(=NO2)c3cccc(NC(=O)C(=C)C)c3	24549	nM
CHEMBL1607313	COc1ccc2[nH]c3c4C(=O)C=CC(=O)c4ccc3c2c1	24724	nM
CHEMBL2140249	CC(=O)Nc1ccc(C=C(C#N)c2ccc(C)cc2)cc1	24744	nM
CHEMBL1610414	Cc1ccc(SCCN2C(=O)NC(C)(C)C2=O)cc1	24814	nM
CHEMBL1538976	CCOc1ccc2nc(O)c(CN(Cc3nnnn3Cc4occc4)C5CCCCC5)cc2c1	24925	nM
CHEMBL1452254	Fc1ccc(cc1)N2C(=S)NC(=O)\C(=C\c3cocc3)\C2=O	25000	nM
CHEMBL3197750	Oc1ccc(\C=N\NC2=NCCCCC2)c(O)c1	25092	nM
CHEMBL1566545	Cc1ccc(cc1)n2nc(C)c(C3C(=C(N)OC4=C3C(=O)Oc5ccccc45)C#N)c2Cl	25242	nM
CHEMBL3199328	Oc1ccc(\C=N\NP(=S)(c2ccccc2)c3ccccc3)c(O)c1O	25258	nM
CHEMBL1324111	Cc1c(Br)c(O)c(Br)c2SC(=O)Oc12	25288	nM
CHEMBL1496732	CCc1ccc(CNc2ccc(O)cc2)cc1	25359	nM
CHEMBL1500249	Oc1cc(cc(O)c1O)C(=O)OCC2O[C@@H](OC(=O)c3cc(O)c(O)c(O)c3)[C@@H](OC(=O)c4cc(O)c(O)c4)[C@@H](OC(=O)c5cc(O)c(O)c(O)c5)[C@@H]2OC(=O)c6cc(O)c(O)c(O)c6	25388	nM
CHEMBL1438567	Cc1ccc(CNc2ccc(O)cc2)cc1	25510	nM
CHEMBL1423479	Oc1ccc(NCN2C(=O)C3C4CC(C=C4)C3C2=O)cc1	25701	nM
CHEMBL1538100	O=C(NC(=S)Nc1ccccc1N2CCOCC2)\C=C\c3occc3	25777	nM
CHEMBL1564253	O=C1Oc2c3CCCN4CCCc(cc2S1)c34	25970	nM
CHEMBL1384502	C\C(=C/c1ccccc1)\C=C\2/SC(=S)N(CCCC(=O)Nc3ccc(C(=O)O)c(O)c3)C2=O	26013	nM
CHEMBL3198517	C\C(=C/C(=O)c1cccnc1)\Nc2ccc(O)cc2	26183	nM
CHEMBL1419712	CCc1ccccc1NC(=O)c2cccc(NC(=O)\C=C\c3occc3)c2	26582	nM
CHEMBL1493529	COc1cc(CC(=O)OCC(=O)Nc2cccc(c2)[N+](=O)[O-])cc(OC)c1OC	26638	nM
CHEMBL1598092	CN(C(=Nc1cccnc1)S)c2ccc(O)cc2	26983	nM
CHEMBL1597115	Clc1ccccc1CNC(=O)c2csc3CCCCCc23	27215	nM
CHEMBL3191565	O\N=C/1\C(\CCC1)=C\c2occc2	27219	nM
CHEMBL1517543	CCN(CC)c1ccc(NC2CC(=O)N(CCc3ccc(OC)cc3)C2=O)cc1	27329	nM
CHEMBL1541890	OC(=O)Cc1ccc(cc1)N=Nc2c(O)c(cc3ccccc23)C(=O)O	27546	nM
CHEMBL1488004	Cc1cccc(N(C(C(=O)NCc2occc2)c3ccncc3)C(=O)Cn4nnc5ccccc45)c1C	27590	nM
CHEMBL1437464	CCOC(=O)C1CCCN(C1)C(=O)c2cc(nc3ccccc23)c4occc4	27780	nM
CHEMBL1343300	CC(C)Sc1nnc(Cc2cc(O)nc(O)n2)n1c3cccc(C)c3	28238	nM
CHEMBL1605431	COC(=O)COc1ccc(cc1)S(=O)(=O)Nc2cc(OC)ccc2OC	28244	nM
CHEMBL1571047	CC1(C)Cc2nc3sc(C(=O)O)c(N)c3cc2CS1	28300	nM
CHEMBL1500799	Brc1ccc(NN=C(Nc2ccccc2)P(=O)(N3CCOCC3)N4CCOCC4)cc1	28355	nM
CHEMBL1470303	FC(F)(F)c1cc(nc(NCc2occc2)n1)c3occc3	28538	nM
CHEMBL1352145	COC(=O)C1=C(C)NC(=O)/C/1=C\c2cc(C)n(c2C)c3ccccc3C	28654	nM
CHEMBL1976046	[O-][N+](=O)c1cc(ccc1Cl)c2oc(\C=N\c3nc4ccccn4c3c5occc5)cc2	28680	nM
CHEMBL1480305	CN(c1c(C)cc(C)c(c1C)S(=O)(=O)N2CCCCC2)S(=O)(=O)c3ccc(Cl)cc3	29008	nM
CHEMBL1340514	CCN=C1C=CC(=CC(=C1O)C(=O)\C=C\c2ccc3OCOc3c2)Br	29067	nM
CHEMBL3209184	COC(=O)\C(=N\Nc1ccccc1C)\N2CCCc3ccccc23	29237	nM
CHEMBL1518604	CC(=C)C(=O)Nc1cccc(c1)C2=NOC3(C[C@H](N(C3)C(=O)CC(c4ccccc4)c5ccccc5)C(=O)N)C2	29299	nM
CHEMBL1456730	CCCCC1=CC2=C(C(=O)C(C)(OC(=O)c3ccc(OC)cc3)C(=O)C2=CN1CCCCO)c4occc4	29309	nM

CHEMBL1561303	Cc1ccc2cc(CN(CC3CCCO3)Cc4nnn4Cc5occc5)c(O)nc2c1C	29378	nM
CHEMBL1558288	FC(F)(F)c1cccc(c1)N2C(=O)CC(Nc3ccc(cc3)N4CCOCC4)C2=O	29455	nM
CHEMBL1564810	CC(=O)NC1=NC(=O)\C(=C\c2cc(C)n(c2C)c3cccc(c3)C(=O)O)\S1	29719	nM
CHEMBL1299853	Cc1ccc(C(CC(=O)NCc2occc2)c3ccccc3)c(O)c1	30042	nM
CHEMBL1387187	Brc1ccccc1C(=O)Nc2ccn(n2)c3ccccc3	30155	nM
CHEMBL1479899	CCc1c(C)sc(NC(=O)OC)c1C(=O)N2CCCCC2	30235	nM
CHEMBL52347	O=C1C=Cc2ccccc2C1=O	30461	nM
CHEMBL1575442	Cc1oc(cc1)c2cc(c3ccc4OCOc4c3)c(C#N)c(N)n2	30478	nM
CHEMBL1981464	Cc1ccsc1\C=N\c2ccc(O)cc2	30533	nM
CHEMBL1733621	CCC(C)C(NC(=O)[C@@H](NC(=O)c1ccccc1F)C(C)C)C(=O)OC	30708	nM
CHEMBL3199408	CC1CCCC(=C1O)\C=N\c2ccc(O)cc2	30796	nM
CHEMBL399293	COc1cc(OC)c2c(O)c3CO[C@@H](C)[C@@H](O)c3c(c4c5[C@H](O)[C@H](C)OCc5c(O)c6c(OC)cc(OC)cc46)c2c1	30829	nM
CHEMBL1389450	O=C1NC(=O)\C(=C\C=C\c2occc2)\C(=O)N1Cc3ccccc3	30878	nM
CHEMBL1535216	O=C1NC(=O)C(=Cc2oc(SC3CCCCC3)cc2)C(=O)N1	30888	nM
CHEMBL1710057	OC(=O)C1=NN(C(=O)C1)c2cc(Cl)c(cc2Cl)S(=O)(=O)O	30944	nM
CHEMBL1373855	CC(=O)Nc1cccc(Oc2ncnc3scc(c4ccccc4)c23)c1	31028	nM
CHEMBL3198782	CC(C)CNC1=CC(=O)CC(C1)c2occc2	31255	nM
CHEMBL175266	CC1=C2C=C(O)C(=O)C=C2Oc3cc(O)c(O)cc13	31297	nM
CHEMBL1576952	CCOC(=O)C1=C(C)N=C2SC(=CC(=O)N2C1c3cc(OC)c(OC)c(OC)c3)C(=O)OC	31407	nM
CHEMBL1398855	Nc1ccc(Nc2ccccc2)c(c1)S(=O)(=O)O	31412	nM
CHEMBL1536118	Brc1ccc(NC(=O)\C=C\c2cccs2)nc1	31412	nM
CHEMBL3190186	Nc1ccccc1NC2=CC(=O)CC(C2)c3occc3	31565	nM
CHEMBL1459778	CC(=C)C(=O)Nc1cccc(c1)C2=NOC3(C[C@@H](N(C3)C(=O)C(c4ccccc4)c5ccccc5)C(=O)N)C2	31746	nM
CHEMBL3191714	Cc1ncc(CO)c(\C=N\NC(=O)c2cc(O)c(O)c(O)c2)c1O	32123	nM
CHEMBL1400929	CC(=O)Nc1ccc(cc1)S(=O)(=O)Nc2nc3ccccc3nc2Nc4ccc(C(=O)O)c(O)c4	32163	nM
CHEMBL1386695	FC(F)(F)C1CCN(CC1)c2ccc(NC(=O)Nc3ccc(Cl)cc3)cn2	32459	nM
CHEMBL1319656	CCCCN1C(=O)NC(=O)\C(=C(\CC)/NCCN2CCCCC2)\C1=O	32493	nM
CHEMBL1347633	CC(CNc1ccccc1O)C(=O)O	32717	nM
CHEMBL3196704	CCOC(=O)C1=C(N=C2S\C(=C/c3occc3)\C(=O)N2C1c4cccs4)c5ccccc5	32790	nM
CHEMBL1448985	O=C(NCCc1ccccc1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	33139	nM
CHEMBL1312576	OC(=O)c1ccc(cc1)n2ccccc2C=C(C#N)C#N	33284	nM
CHEMBL1539384	Oc1ccc(NCc2nnc(O)c3ccccc23)cc1	33726	nM
CHEMBL1479292	CC(C)c1ccc(\C=C\C(=O)N2CCc3ccccc3C2)cc1	33743	nM
CHEMBL2006418	Oc1ccc(\C=N\Nc2ccc(cc2S(=O)(=O)N3CCOCC3)[N+](=O)[O-])c(O)c1O	33991	nM
CHEMBL1374511	CCOc1cc(CNc2ccc(O)cc2)ccc1OCc3ccc(Cl)cc3Cl	33999	nM
CHEMBL1509980	CC(C)c1ccc(cc1)N2C(=O)NC(=O)\C(=C/C=C/c3occc3)\C2=O	34175	nM
CHEMBL1549172	COc1cccc(c1)N2C(=O)NC(=O)\C(=C\c3ccc(s3)[N+](=O)[O-])\C2=O	34347	nM
CHEMBL1429677	COCCCNC(=O)\C(=C\c1ccc(OCC(=O)O)c(OC)c1)\C#N	34408	nM
CHEMBL1496473	CC1=CC2(O)OCCN(CCO)C2=CC1=O	34498	nM
CHEMBL1360102	COc1cc(CNc2ccc(O)cc2)cc(Br)c1OCc3ccccc3	34537	nM
CHEMBL1382847	[O-][N+]1=C(C(=O)N(OCc2ccccn2)c3ccccc13)c4oc5ccccc5c4	34537	nM
CHEMBL1447034	Cc1ccc2C3C=CCC3C(Nc2c1C)C(=O)O	34670	nM
CHEMBL1720594	Clc1ccccc1N=Nc2ccccn2	35035	nM
CHEMBL1578372	Cc1cc(C(=O)CSc2nnnn2c3ccccc3)c(C)n1CC4CCCO4	35041	nM
CHEMBL1378258	FC(F)(F)c1cc(nc(SCC(=O)N2CCc3ccccc3C2)n1)c4occc4	35210	nM
CHEMBL1995550	Oc1ccc(\C=N\N=C(\C(=O)c2ccccc2)/c3ccccc3)c(O)c1O	35242	nM

CHEMBL1379060	COCCNC(=O)COC(=O)c1[nH]c(C)c(C(=O)C)c1C	35420	nM
CHEMBL1968789	Oc1ccc(\C=N\N2\C(=N\CC=C)\SC=C2c3occc3)c(O)c1O	35444	nM
CHEMBL1391625	CCOc1cc(N2CCOCC2)c(OCC)cc1NC(=O)CSc3nc[nH]n3	35656	nM
CHEMBL1717355	O=C1NC(=S)NC1=Cc2occc2	35684	nM
CHEMBL1410964	COc1cc(cc(OC)c1OC)C(=O)NCc2oc(SCC(=O)Nc3nc4ccc(C)cc4s3)nn2	35858	nM
CHEMBL1310907	Cc1ccc(NC(=O)CN2C(=O)N\C(=C\c3occc3)\C2=O)cc1	35970	nM
CHEMBL3197651	Cc1cccc(N\N=C\c2ccc(O)c(O)c2O)c1	35995	nM
CHEMBL1407877	Cc1ccc(cc1)N2C(=S)S\C(=C\c3occc3)\C2=O	36020	nM
CHEMBL592184	CC(=O)NN1C(=S)S\C(=C/c2oc(Br)cc2)\C1=O	36195	nM
CHEMBL1557235	O=C(CN1C(=O)NC2(CCCCCCC2)C1=O)NCc3cccs3	36458	nM
CHEMBL1393622	Cc1cnnc2ccc3c(no[n+]3[O-])c12	36541	nM
CHEMBL1373732	CC(=O)c1ccc2NC(C3CC=CC3c2c1)c4ccncc4	36569	nM
CHEMBL484640	Cc1c(O)cc2OC(CC(=O)c2c1O)c3ccc(O)cc3	37149	nM
CHEMBL1735496	NC(=S)N=Nc1c(O)cc(O)c2nc(O)ccc12	37205	nM
CHEMBL1501325	Cn1cnnc1SC\C(=C(/C#N)\c2nc3ccccc3[nH]2)\O	37446	nM
CHEMBL1571187	O=C1CCCC(=O)C1=NNc2ccc(cc2)S(=O)(=O)N3CCOCC3	37636	nM
CHEMBL1434555	CN(CC(=O)Nc1ccc(C)cc1)C(=O)c2cccc(c2)n3cccc3	38005	nM
CHEMBL1484657	O=C1N(Cc2occc2)C(=S)Nc3ccc(cc13)N4CCOCC4	38652	nM
CHEMBL3195481	Cc1nccn1CC(=O)N\N=C\c2ccc(O)c(O)c2	39009	nM
CHEMBL1577182	CCc1cc2cc(C)cc(C)c2nc1SCC(=O)N3CCN(CC3)C(=O)c4occc4	39280	nM
CHEMBL1373183	Cc1ccc(C)c2nc(O)c(CN(Cc3ccc4OCOc4c3)Cc5nnnn5Cc6occc6)cc12	39572	nM
CHEMBL1464727	COC(=O)C1=C(C)NC(=O)/C/1=C\c2occc2	39663	nM
CHEMBL1163377	CN1CCN(CC1)C2=C(Cl)C(=O)c3ccccc3C2=O	40018	nM
CHEMBL1580917	Cc1nn(c2cccc2)c3sc(cc13)C(=O)N4CCc5ccccc5C4	40133	nM
CHEMBL426	CN(Cc1cnc2nc(N)nc(N)c2n1)c3ccc(cc3)C(=O)NC(CCC(=O)O)C(=O)O	40141	nM
CHEMBL1335040	CCC(NC(=O)Nc1ccc(O)cc1)C(F)(F)F)C(F)(F)F	40216	nM
CHEMBL1564066	CN=C1C=CC(=CC(=C1O)C(=O)\C=C\c2ccc3OCOc3c2)Br	40729	nM
CHEMBL1555191	CN(CC(=O)Nc1cccc(F)c1)C(=O)c2cccc(c2)n3cccc3	40924	nM
CHEMBL1422858	O=C1CCCC/C/1=C/Nc2ccc3OCOc3c2	41299	nM
CHEMBL1507759	Oc1ccc2ccccc2c1C3Nc4cccc5cccc(N3)c45	41650	nM
CHEMBL11417	COC1=C(N)C(=O)c2nc(ccc2C1=O)c3nc(C(=O)O)c(C)c(c3N)c4ccc(OC)c(OC)c4O	42129	nM
CHEMBL1520425	COC(=O)Cn1c(CCC(=O)O)ccc1c2ccccc2	42288	nM
CHEMBL1307692	Fc1ccc(CN2C(=O)NC(=O)\C(=C\C=C\c3occc3)\C2=O)cc1	42342	nM
CHEMBL1503776	Cc1cc(C)cc(Nc2ncc3C(=O)CC(Cc3n2)c4occc4)c1	42685	nM
CHEMBL1524408	[O-][n+]1c2CCCCc2[n+]([O-])c3cc(Cl)ccc13	42904	nM
CHEMBL1428153	Cc1cccc(NC2=Nc3ccccc3N4C(c5ccc(O)c(O)c5)c6c(C)nn(c7ccccc7)c6N=C24)c1	42949	nM
CHEMBL1433261	CCn1cc(CNC(=O)c2ccc(Cl)c(c2)[N+](=O)[O-])c(C)n1	42964	nM
CHEMBL2094422	Oc1cc(CC(=O)N\N=C\C=C\c2ccccc2)n[nH]1	43057	nM
CHEMBL1549311	CC(=O)Nc1ccc(cc1)S(=O)(=O)Nc2nc3ccccc3nc2Nc4ccc(N)cc4	43283	nM
CHEMBL1373753	COc1cc(ccc1O)C2C(=C(N)N(C3=C2C(=O)CCC3)c4cccnc4)C#N	43357	nM
CHEMBL1341268	CCn1c2ccccc2c3cc(NC(=O)c4ccccc4[N+](=O)[O-])ccc13	43803	nM
CHEMBL1361845	CC(C)(C)NC(=O)C(N(C(=O)CNC(=O)c1occc1)c2ccc3OCOc3c2)c4ccncc4	44052	nM
CHEMBL1723523	CN(CCc1ccccc1)C(=O)c2ccc(NC(=O)Cc3ccc(NC(=O)C4CCN(CC4)C(=O)CCc5ccccc5)cc3)cc2	44272	nM
CHEMBL1332241	CN1C(=S)NC(=O)\C(=C/c2cccn2c3ccc4ccccc4c3)\C1=O	44469	nM
CHEMBL1488190	CCC(=O)NNc1ncnc2ccccc12	44509	nM
CHEMBL1482715	CC1(CCl)[N+](=C2CCCCC2=[N+]1[O-])[O-]	44600	nM
CHEMBL1701585	CN(C)C(=O)c1nc2ccc(Cl)cn2c1CN3CCCC(C3)OCc4ccccc4	44612	nM

CHEMBL1715550	COc1cc(\C=C\C=C/2\CC\C(=C\C=C\c3ccc(O)c(OC)c3)\C2=O)ccc1O	44779	nM
CHEMBL1533336	CC(NC(=O)Nc1ccc(O)cc1)(C(F)(F)F)C(F)(F)F	44783	nM
CHEMBL1487660	O=S(=O)(N1CCOCC1)c2ccc3nc(c4occc4)c(nc3c2)c5occc5	44849	nM
CHEMBL1461309	C=CCNc1nc2ccccc2nc1NS(=O)(=O)c3cccs3	44952	nM
CHEMBL1424746	CCc1ccc(cc1)N2C(=O)NC(=O)\C(=C/C=C/c3occc3)\C2=O	45025	nM
CHEMBL1521203	[O-][N+](=O)c1ccccc1S(=O)(=O)NC2CCCC2	45032	nM
CHEMBL1489590	CC1(OC(=O)C2CCCC2)C(=O)C=C3C=C(OC=C3C1=O)c4ccsc4	45427	nM
CHEMBL1462735	OC(=O)CCc1ccc(c2cccs2)n1c3ccc(cc3)C(=O)O	45608	nM
CHEMBL1386686	CCOC(=O)c1cnn2c(N)c(nnc12)C#N	45710	nM
CHEMBL1407135	COC(=O)C1=C(C)N(CC=C)C(=O)/C/1=C\c2occc2	45865	nM
CHEMBL1445447	Sc1nnc(C2CC2)n1Cc3occc3	45896	nM
CHEMBL1456035	OC(=O)C1Nc2c(Cl)cc(Cl)c(Cl)c2C3C=CCC13	45923	nM
CHEMBL1539623	O=C(CCN1C(=S)S\C(=C/c2cccs2)\C1=O)NC3=NCCS3	45987	nM
CHEMBL1430931	COC(=O)c1ccc(COc2ccccc2\C=C(/C#N)\C(=O)Nc3c(C)cc(C)cc3C)cc1	46228	nM
CHEMBL1563532	COc1ccc2OCc3ccccc3C(=O)c2c1	46311	nM
CHEMBL1551448	COc1ccc(NC(=O)CN(C)C(=O)c2cc(nc3ccccc23)c4occc4)cc1	46350	nM
CHEMBL1599024	Cc1ccc2cc(C(N3CCc4ccccc34)c5nnnn5Cc6ccccc6)c(O)nc2c1	46437	nM
CHEMBL1371301	CCN(CC)c1ccc(NC(=O)CCS(=O)(=O)c2ccc(Br)cc2)c(C)c1	46486	nM
CHEMBL1438907	COc1ccc(Br)cc1CNc2ccc(O)cc2	46687	nM
CHEMBL1985664	COc1ccc(\C=N\NC(=O)c2cc(O)c(O)c(O)c2)cc1Cn3cc(cn3)[N+](=O)[O-]	46702	nM
CHEMBL1405178	O=C(C1CCCN1S(=O)(=O)c2cccc3cccnc23)N4CCN(CC4)c5ccccc5	46817	nM
CHEMBL1400666	Cc1cc(C)cc(Nc2ccc(cc2N)C(=O)O)c1	47139	nM
CHEMBL1568805	CC1=CC(=O)c2c(O)c(O)ccc2O1	47371	nM
CHEMBL1535453	CN(C)c1ccc(NC(=O)CSC2=Nc3ccccc3C(=O)N2C4CCCCC4)cc1	47439	nM
CHEMBL2000670	Oc1ccc(cc1)\N=C\c2ccc(OCc3ccccc3)cc2	47519	nM
CHEMBL1366516	CC(C)N1CCC2(CC1)C(=C(N)NC(=C2C#N)S)C#N	47631	nM
CHEMBL1374754	O=S(=O)(Nc1nccs1)c2ccc(Nc3nnc(c4ccccc4)c5ccccc35)cc2	47706	nM
CHEMBL1330736	CCOC(=O)C1=C(O)\C(=C\c2oc(CNC(=O)C(=O)Nc3ccc(C)cc3)cc2)\N=C1C	47835	nM
CHEMBL220259	Nc1ccc2c(O)cc(cc2c1)S(=O)(=O)O	47954	nM
CHEMBL1382979	O=C(CCCN1C(=S)S\C(=C\c2occc2)\C1=O)Nc3ccc4ccccc4c3	48281	nM
CHEMBL1374657	O=C(NCCc1c[nH]c2ccccc12)c3ccc(cc3)S(=O)(=O)NCc4occc4	48319	nM
CHEMBL1703645	Cc1cc(cc2C3C=CCC3C(Nc12)c4ccccn4)[N+](=O)[O-]	49134	nM
CHEMBL1466563	Cc1cc(C(=O)CSc2nc(O)c3ccccc3n2)c(C)n1C	49178	nM
CHEMBL1506938	Cc1ccc(Nc2ccc(N)cc2S(=O)(=O)O)cc1	49333	nM
CHEMBL1706128	CCOC(=O)C(=O)Cc1cccnn1	49486	nM
CHEMBL1390729	O=C(NCC1CCCO1)c2cc(nc3ccccc23)c4occc4	49502	nM
CHEMBL3191780	C\N=C\1/SC=C(C)N1\N=C\c2ccc(O)c(O)c2O	49829	nM
CHEMBL1307209	Cn1c(SCC(=O)c2cc(Cl)c(Cl)s2)nnc1c3occc3	49999	nM
CHEMBL1312802	Cc1nc2cc(NN=C3C(=O)CCCC3=O)ccc2s1	49999	nM
CHEMBL1347346	[Na+].CCC(C)CN1C(=CC2=NN(C(=O)C2=C1C)c3nc4ccccc4s3)[O-]	49999	nM
CHEMBL1539086	COc1cc(CNc2ccc3[nH]c(O)nc3c2)cc(Cl)c1OCC(=O)NC(C)(C)C	50510	nM
CHEMBL1321176	Brc1ccc(cc1)S(=O)(=O)CCC(=O)NC2CCCC2	50819	nM
CHEMBL1457086	Cc1ccc(cc1)S(=O)(=O)N2CCC(CC2)C(=O)Nc3nnc(s3)c4occc4	51066	nM
CHEMBL1320455	CCCCC(=O)NC(=S)Nc1cc(ccc1Cl)C(=O)O	51158	nM
CHEMBL1735454	Oc1ccc(N=Nc2c(O)cc(c3ccccc23)S(=O)(=O)O)c(O)c1	51339	nM
CHEMBL1398921	Clc1ccc(OCc2nn3c(nnc3s2)c4occc4)c(Cl)c1	51481	nM
CHEMBL1465049	Oc1ccc(NCc2ccccc2OCc3ccccc3)cc1	51562	nM
CHEMBL1403572	CN1C(=S)NC(=O)\C(=C/NNC(=O)c2ccncc2)\C1=O	51822	nM
CHEMBL3392035	CCOC(=O)C1=C(N)SC(=S)C2=C1CCC2	52030	nM

CHEMBL1390647	CNC1=CC=C(Br)C=C(C(=O)\C=C\c2ccc(OC)cc2OC)C1=O	52035	nM
CHEMBL1523543	COc1ccc2c(c1)[n+]([O-])c3CCCc3[n+]2[O-]	52109	nM
CHEMBL175266	CC1=C2C=C(O)C(=O)C=C2Oc3cc(O)c(O)cc13	52180	nM
CHEMBL1447514	COC(=O)C1=C(N)OC2=C(C1c3cccs3)C(=O)CCC2	52219	nM
CHEMBL1430855	CCc1c(C)sc(NC(=O)c2cc(on2)c3occc3)c1C#N	52375	nM
CHEMBL1353369	CC(=C)C(=O)Nc1cccc(c1)C2=NOC3(C[C@H](N(C3)C(=O)c4cc(cc(c4)[N+](=O)[O-])[N+](=O)[O-])C(=O)N)C2	52944	nM
CHEMBL1522218	OC(=O)COc1ccc2C(=O)\C(=C\c3occc3)\Oc2c1	53108	nM
CHEMBL1524927	Oc1cccc(\C=N\c2c(nc3ccccn23)c4occc4)c1	53259	nM
CHEMBL1558644	CCCCC1=CC2=CC(=O)C(C)(OC(=O)C3CCCC3)C(=O)C2=CO1	53638	nM
CHEMBL1578768	Brc1oc(\C=C\2/C(=O)N=C3SC(=NN3C2=N)CC(=O)N4CCCC4)cc1	53730	nM
CHEMBL1583808	CC(C)CC(=O)Nc1nnc(s1)c2occc2	53787	nM
CHEMBL1546820	Cc1ccc(C)n1c2ccc(s2)c3nnc4CCCCCn34	54190	nM
CHEMBL3195177	CC\N=C\1/SC=C(C)N1\N=C\c2ccc(O)c(o)c2O	54379	nM
CHEMBL3195484	COC(=O)C1C(O)C(C)C(O)C(C)(O)\C=C/C=C(\C)/C(=O)Nc2c(C)c(OC(=O)C)c3C4=C(OCOC4=C(C)C(=O)c3c2O)\C(=C\C(C)(O)C(O)C(C)C1O)\C	54617	nM
CHEMBL1509389	CN(C)c1ccc(cc1)N2C(=O)CSC2=S	54638	nM
CHEMBL1724282	OC(=O)CC1=C(C(=O)O)C(=O)C(=CC=C1)O	54748	nM
CHEMBL1343718	CCOC1=CC=CC(=O)c2c(C)n(C)c(C)c12	55219	nM
CHEMBL1576094	[O-][N+](=O)c1oc(\C=C(/C#N)\C(=O)Nc2ccc(F)cc2)cc1	55645	nM
CHEMBL578585	Cc1onc(NC(=O)Cc2cccs2)c1	55861	nM
CHEMBL1538773	OC(=O)CSc1c2CCCCc2nc3cc(ccc13)C(=O)Nc4cccc(c4)C(F)(F)F	56199	nM
CHEMBL1548829	COC(=O)\C(=C(/C=C/C=C/C=C/N(C)C)\N(C)C)\C(=O)C	56319	nM
CHEMBL1400903	CCOC(=O)CSc1nncc2ccc(OC)c(OC)c12	56583	nM
CHEMBL1711432	COc1cc(NCCCCCCN)c2ncccc2c1OC	56674	nM
CHEMBL1873953	Oc1c(O)c2ccccc2cc1[N+](=O)[O-]	56760	nM
CHEMBL1468142	CC1CC2=C(S1)C(=O)N(C)C(=N2)SCC(=O)Nc3cc(C)cc(C)c3	56948	nM
CHEMBL1352279	Cc1ccc(Cl)cc1N2CCN(CC2)C(=O)COc3ccc4CCCc4c3	57190	nM
CHEMBL1324051	CSc1nc(N(CCO)CCO)c2sc3nc(c4CCCc4c3c2n1)c5occc5	57328	nM
CHEMBL3198658	Cc1cc(C)c(cc1c2oc(\C=N\c3c(nc4ccccn34)c5occc5)cc2)[N+](=O)[O-]	57460	nM
CHEMBL1523651	CC1=NC(=C(C#N)C(/C/1=C(\O)/OCC=C)c2occc2)SCC(=O)Nc3ccccc3	57515	nM
CHEMBL1479248	COc1ccccc1NCCC(=O)OCC(=O)NCc2occc2	58030	nM
CHEMBL1475596	Cn1cnnc1SCC(=O)Nc2ncc(s2)[N+](=O)[O-]	58218	nM
CHEMBL1539362	NC(=O)c1c2CCCCCc2sc1NC(=O)c3ccc(cc3)S(=O)(=O)N4CCOCC4	58277	nM
CHEMBL1391120	O=C(CSc1nnnn1c2ccccc2)Nc3ncc4C(=O)CC(Cc4n3)c5occc5	58452	nM
CHEMBL1504445	Cc1cccc(c1)n2c(Cc3cc(O)nc(O)n3)nnc2SCC(=O)NCC4CCCO4	58457	nM
CHEMBL1447615	CC(=O)N1CCN(CC1)c2nc(c3CSC(C)(C)Cc3c2C#N)c4occc4	58829	nM
CHEMBL1390770	CCN(CC)c1nc(NCc2ccccc2)c(C#N)c3CCN(CC)Cc13	59403	nM
CHEMBL1547422	Cl.CCCOc1ccc(N)cc1N	59538	nM
CHEMBL1359999	Brc1oc(cc1)C(=O)Nc2ccccc2N3CCCC3	59629	nM
CHEMBL1559207	Cc1onc(c1C(=O)Nc2nnc(s2)C3CC3)c4c(F)cccc4Cl	60686	nM
CHEMBL1500840	COc1ccc(NC(=O)\C(=C/c2oc(Br)cc2)\C#N)cc1	60788	nM
CHEMBL1529201	CC1(C)[N+](=C2C=CC(=CC2=[N+]1[O-])[N+](=O)[O-])[O-].NO	61277	nM
CHEMBL1416649	COc1ccc(\C=C(/NC(=O)c2ccc(OCC(C)C)cc2)\C(=O)OCc3occc3)cc1	61465	nM
CHEMBL3195461	Oc1ccc(cc1)\N=C\c2sc3ccccc3c2Cl	62279	nM
CHEMBL1997568	COC(=O)c1ccc(COc2ccc(\C=N\Nc3cccc(c3)C(=O)O)cc2)cc1	62412	nM
CHEMBL1462509	COc1ccc(cc1)n2c(C)cc(C(=O)CSC3=NN4C(=NN=C(C4=O)C(C)(C)C)S3)c2C	62698	nM
CHEMBL1898589	NN=C1C(=C(Cl)C(=C1Cl)Cl)Cl	62872	nM
CHEMBL1367262	CCOc1cccc(CNc2ccc(O)cc2)c1OCc3ccccc3Cl	63039	nM

CHEMBL1582403	CCC1=NN2C(=NC(=O)\C(=C\c3oc(SCc4occc4)cc3)\C2=N)S1	63258	nM
CHEMBL1454531	Cc1cccc(NC(=O)CNC(=O)c2cccc(c2)n3cccc3)c1C	63294	nM
CHEMBL1311036	Cl.CN(C1CCN(C)CC1)C(=O)COc2ccccc2c3ccccc3	63707	nM
CHEMBL1365054	Cc1ccc(cc1)N(CC(=O)NCCSCc2occc2)S(=O)(=O)c3ccc(F)cc3	63739	nM
CHEMBL1333464	C(SC1CCCCC1)c2cn3ccsc3n2	63775	nM
CHEMBL1732255	O=C1C(=Cc2occc2)CCCC1=Cc3occc3	63899	nM
CHEMBL213017	Cc1cc(\C=N\Nc2ccc(cn2)[N+](=O)[O-])c(C)n1c3cccc(C(=O)O)c3C	63954	nM
CHEMBL1588892	o1cccc1c2nn3c(nnc3s2)c4cccnc4	63954	nM
CHEMBL1509369	OC(=O)C1=C(CSC2C(NC(=O)Cc3ccccc3)C(=O)N12)C=C	64157	nM
CHEMBL3196561	CN(C)c1ccc(cc1)\N=C\C=C/2\N(C)c3ccccc3C2(C)C	64399	nM
CHEMBL1893341	COC(=O)c1ccc(C(=O)OC)c(NC(=O)Cc2cccs2)c1	64765	nM
CHEMBL1419581	CCOc1ccc(NCC2CCOC(C)(C)C2)cc1	64789	nM
CHEMBL1511058	COC(=O)c1ccc(C)c(NC(=O)CCSc2ccccc2)c1	65056	nM
CHEMBL1989690	CCOC(=O)C1CCCN(C1)C(=O)c2ccc(C\N=C/3\C(=O)C(=C3N4CCC(C)CC4)O)cc2	65277	nM
CHEMBL1350188	COc1cc(OC)c2C(=O)CC(Oc2c1O)c3ccccc3	65404	nM
CHEMBL1487945	CC1(OC(=O)CCc2ccccc2)C(=O)C=C3C=C(OC=C3C1=O)c4ccsc4	65776	nM
CHEMBL1378801	CC(=O)Nc1ccc(cc1)S(=O)(=O)NCCSCc2occc2	65798	nM
CHEMBL1417382	COc1ccccc1NC(=O)CSc2nnc(Cc3cc(O)nc(O)n3)n2c4ccccc4	66484	nM
CHEMBL1408535	Oc1ccc(NCc2cccc(OCc3ccccc3)c2)cc1	66736	nM
CHEMBL1584278	Cn1cccc1\C=C/2\C(=O)NC(=O)N(Cc3ccccc3)C2=O	66994	nM
CHEMBL1455108	CCOC(=O)Cn1nnnc1C(C(C)C)N(Cc2cc3c(C)cc(C)cc3nc2O)C4CCCC4	67647	nM
CHEMBL602807	COc1ccc2ccccc2c1C3CC(=O)N4CN(Cc5occc5)CSC4=C3C#N	67667	nM
CHEMBL1234578	Nc1cccc2cc(ccc12)S(=O)(=O)O	67864	nM
CHEMBL1468124	COC(=O)c1cnn2c(cc(nc12)c3occc3)C(F)(F)F	68089	nM
CHEMBL1356373	OC(=O)CCc1ccc(cc1)S(=O)(=O)Nc2cc(ccc2N3CCCC3)C(F)(F)F	68191	nM
CHEMBL1306571	Cc1oc(cc1)C2SCC(=O)N2Cc3cn4ccsc4n3	68491	nM
CHEMBL1546783	CCN(C(=O)CN1CCN(CC1)c2ccc(O)cc2)C3=C(N)N(Cc4ccccc4)C(=O)NC3=O	68533	nM
CHEMBL1305813	CN(C)C(CNC(=O)c1cccnc1Sc2ccccc2)c3occc3	68679	nM
CHEMBL1609070	Oc1ccc(NCc2cccc(OCc3ccc(F)cc3)c2)cc1	68747	nM
CHEMBL1603474	CN(CC(=O)Nc1ccc(C)cc1)C(=O)c2cc(nc3ccccc23)c4occc4	69167	nM
CHEMBL1430463	COc1cccc(NC(=O)CSc2nnc(c3occc3)c(n2)c4occc4)c1	69298	nM
CHEMBL1524564	OC(=O)c1[nH]c2ccc(Cl)cc2c1CC(=O)N3CCN(CC3)C(=O)c4occc4	69516	nM
CHEMBL1485262	O=C(Nc1ccccc1)C2=C(CC(CC2=O)c3occc3)Nc4ccccc4	70291	nM
CHEMBL3213843	CC1SC(=NC1=O)N\N=C\c2occc2	70298	nM
CHEMBL1465739	CCN1C(=O)c2c3CCCc3sc2N=C1SC(C)C(=O)O	70403	nM
CHEMBL1361743	CCCC(=O)N(CCc1ccc(OC)cc1)Cc2nc(O)c3ccccc3n2	71828	nM
CHEMBL1613004	Oc1ccc(cc1O)c2cn3CCSc3n2	71879	nM
CHEMBL1900570	C1CN(CCN1c2cnccn2)c3ncccn3	71936	nM
CHEMBL1968376	Cl.Cc1cc(C)nc(N\N=C\C2=C(N3CCOCC3)\C(=C/c4ccc(Cl)cc4)\CC2)n1	72388	nM
CHEMBL1389080	Cc1cc(C)nc(n1)N2CCC(CC2)C(=O)O	72773	nM
CHEMBL1331081	[I-].CC[n+]1ccc(C)c2cc(ccc12)P(=O)(c3ccccc3)c4ccccc4	72913	nM
CHEMBL1313485	CCOC(=O)c1oc(CC(=O)c2ccc(O)c(O)c2O)cc1	74005	nM
CHEMBL1503182	CC(=O)c1ccc(cc1)S(=O)(=O)Nc2cccc(c2)n3cnnn3	74240	nM
CHEMBL1571640	CCN1CCCc2cc(CN(CCN3CCOCC3)C(=O)Nc4ccc(CC)cc4)ccc12	74458	nM
CHEMBL234338	Oc1ccc(cc1)C2=CC(=O)c3c(O)c(O)c(O)c(O)c3O2	74865	nM
CHEMBL1566068	CCOc1ccc(CNc2ccc(cc2)N3CCCC3)cc1	75252	nM
CHEMBL477936	Cc1ccc(cc1)S(=O)(=O)OCC(=O)Nc2ccc(C(=O)O)c(O)c2	75277	nM
CHEMBL1710608	CCN(CC(=O)Nc1c(F)cccc1F)C(=O)CSC(=S)N2CCCC2	75584	nM

CHEMBL1522695	CN1C(=C(C(=O)COC(=O)C2CCCCC2)C(=O)N(C)C1=O)N	76227	nM
CHEMBL1727409	CC(C)Sc1nnc(Cc2cc(O)nc(O)n2)n1c3cc(C)ccc3C	76994	nM
CHEMBL1976219	Oc1c(Br)cc(cc1\C=N\c2ccc(cc2)N3CCOCC3)[N+](=O)[O-]	77469	nM
CHEMBL1559616	Brc1ccc(NC=C2C(=O)CC(CC2=O)c3occc3)cc1	77615	nM
CHEMBL1707498	CCOc1ccccc1C(O)C2=CC(=O)c3ccccc3C2=O	77680	nM
CHEMBL1332702	Cl.CCCN1C(=N)N(CC(O)c2occc2)c3ccccc13	78162	nM
CHEMBL1460044	COC(=O)CCCC(=O)Nc1c(F)c(F)c(F)c(F)c1F	78229	nM
CHEMBL1900407	CCCCN1C2CCCC1CC(C2)NC(=O)c3ccc(OC)c(OC)c3	78291	nM
CHEMBL1565385	Cc1nc2c(Cl)cccc2c(O)c1CN3CCCC3	78327	nM
CHEMBL1576106	CCOC(=O)Cc1cc(O)n2nc(C)cc2n1	78346	nM
CHEMBL1349942	CCOc1cc(N2CCOCC2)c(OCC)cc1NC(C)C(=O)N3CCN(CC)CC3.OC(=O)C(=O)O	78805	nM
CHEMBL1367133	O=C1N(Cc2occc2)C(Nc3ccccc3)c4ncccc14	79168	nM
CHEMBL1403524	BrC1=CC(=COC1=O)C(=O)Nc2ccc(Br)cn2	79525	nM
CHEMBL1339808	COC(=O)C1=C(C)N(Cc2ccccc2)C(=O)/C/1=C\c3occc3	79695	nM
CHEMBL2133196	CCN1C[C@@H]2[C@H]3[C@H](C(=O)N(Cc4ccccc4)C3=O)[C@@](C)(N2/C/1=N/C5CCCCC5)C(=O)OC.OC(=O)C(F)(F)F	79756	nM
CHEMBL1722566	CN(CCC#N)C(=O)COC(=O)c1c2CC\C(=C\c3occc3)\c2nc4ccccc14	79769	nM
CHEMBL1586657	OC(=O)[C@@H]1CC[C@@H](CC1)NC(=O)OCc2ccccc2	79770	nM
CHEMBL1350226	CN1CCc2c(C)sc3c2c(NCc4occc4)nc5nnnn35	79810	nM
CHEMBL1446929	CCC(=O)NC1=C(Cl)C(=O)C(=C(Cl)C1=O)NC(=O)CC	79821	nM
CHEMBL1339888	OC(=O)c1cc2cccc(c2cc1O)S(=O)(=O)N3CCOCC3	80304	nM
CHEMBL610508	COc1ccc2C(CC(=O)c3ccc(O)c(O)c3)OC(=O)c2c1OC	80536	nM
CHEMBL576353	Cc1cc(O)ccc1c2cnc3ccccc3n2	80768	nM
CHEMBL1890961	O=C1C=C(N2CC2)c3ccccc3C1=O	80943	nM
CHEMBL1527971	CCOC(=O)c1ccc(NC(=O)CSCc2occc2)cc1	81621	nM
CHEMBL1427517	COc1ccc2nc3ccccc3nc2c1N	81646	nM
CHEMBL1492200	CCN1C(=C(C(=O)OC)\C(=C\c2occc2)\C1=O)C	81829	nM
CHEMBL1421238	CCOC(=O)C1CCN(CC1)C(=O)COc2ccc(cc2)S(=O)(=O)NC(C)C	81829	nM
CHEMBL1309683	Cc1oc(C)c2C3=C(C=CC(=O)c12)C(C(=C(N)O3)C#N)c4ccccc4	81859	nM
CHEMBL1433062	COc1ccc(OC)c(c1)N2C(=O)[C@H]3ON=C([C@H]3C2=O)c4ccccc4Cl	82129	nM
CHEMBL3193853	O=C(N\N=C\1/CCCC(=O)C1)c2ccc(COc3cccc4cccnc34)cc2	82296	nM
CHEMBL1595597	COc1ccc(cc1OC)C2=NCC(=O)N(CC(=O)NCc3occc3)c4sc5CCCCc5c24	82338	nM
CHEMBL1402642	Cc1oc(cc1)C(=O)C2=C(O)C(=O)N(C2c3ccc(F)cc3)c4ncccn4	82749	nM
CHEMBL1328778	COc1ccc(OC)c(c1)S(=O)(=O)Nc2ccc(O)c3ccccc23	83040	nM
CHEMBL1561738	Cc1occ(c1)c2cc(nc(N)c2C#N)c3ccc(Cl)cc3	83569	nM
CHEMBL1380806	Cl.CCOc1cccc(CNCCNC(=O)c2nonc2N)c1	84171	nM
CHEMBL1432334	COc1ccccc1C2C=C(Nc3nnnn23)c4ccc(C)cc4	84418	nM
CHEMBL1363465	Cc1cccc(C)c1NC(=O)COC(=O)c2cc(nc3ccccc23)c4cccnc4	84606	nM
CHEMBL1498126	Cc1cc(C(=O)CSc2nnnn2C)c(C)n1CCc3ccc(Cl)cc3	84609	nM
CHEMBL1966984	OC1CC(CC(O)C1OC(=O)\C=C\c2ccc(O)c(O)c2)(OC(=O)\C=C\c3ccc(O)c(O)c3)C(=O)O	85194	nM
CHEMBL1728065	CN(C)c1ccc(CC2=Cc3c(O)ccc(O)c3C=C(Cc4ccc(cc4)N(C)C)C2=O)cc1	85420	nM
CHEMBL1456026	Cc1cccc(c1)n2nc3CSCc3c2NC(=O)c4oc(Br)cc4	85925	nM
CHEMBL1596115	CCOc1cccc(CNc2ccc(O)cc2)c1OCc3ccc(Cl)cc3	86022	nM
CHEMBL1362933	CN(C)c1cc(Cl)c2nonc2c1N	87225	nM
CHEMBL1900368	OC1=C2C(=CC=CC(=O)C2=O)CC(=O)O1	87659	nM
CHEMBL1536718	ClC(Cl)(Cl)C(NC(=O)Cc1ccccc1)Nc2ccccc2	87821	nM
CHEMBL1546569	CC(=O)OC1COC(C(OC(=O)C)C1OC(=O)C)n2ccc3ccccc23	88133	nM
CHEMBL1470983	BrC1=CC(=COC1=O)C(=O)NCc2ccccn2	88328	nM

CHEMBL1366858	CCOC(=O)NC1(NC2CCCCC2)Oc3ccccc3O1	88377	nM
CHEMBL1595607	CCC(=O)N1N=C(CC1c2ccc(C)cc2)c3ccc(NS(=O)(=O)C)cc3	88764	nM
CHEMBL1301323	Cc1oc(\C=C\C(=O)Nc2cccc(c2)S(=O)(=O)N3CCOCC3)cc1	89133	nM
CHEMBL1731349	Fc1ccc(\C=C/2\CN(C\C(=C\c3ccc(F)cc3)\C2=O)C(=O)C=C)cc1	89470	nM
CHEMBL1527565	Cc1cc(O)c(cc1O)c2cc(O)c(C)cc2O	89682	nM
CHEMBL1737002	CN(C)c1ccc2cc(cc(O)c2c1)S(=O)(=O)O	89990	nM
CHEMBL1381289	Cc1ccc(cc1)N2C(=S)NC(=O)\C(=C/c3oc(CN(CCC#N)S(=O)(=O)C)cc3)\C2=O	90018	nM
CHEMBL1416184	OCCNc1cc(Sc2nc3ccccc3s2)c4nonc4c1[N+](=O)[O-]	90119	nM
CHEMBL1579003	OC(=O)c1oc(COc2c(F)c(F)c(F)c(F)c2F)cc1	90615	nM
CHEMBL1542330	Clc1ccc(cc1Cl)c2cn3cccnc3n2	90898	nM
CHEMBL1321516	CC(=O)C1=C(C)NC(=C(C1c2cccs2)C(=O)C)C	91400	nM
CHEMBL1505865	C\C(=C\C(=O)O)\C=C\c1oc(Cl)cc1	92029	nM
CHEMBL3192400	CCN(CC)S(=O)(=O)c1cccc(c1)C(=O)N\N=C\c2ccc(O)c(O)c2O	92720	nM
CHEMBL1505758	CCOc1ccc(cc1)n2c(Cc3cc(O)nc(O)n3)nnc2SC(C)C(=O)OC	92868	nM
CHEMBL1523154	COc1cc(ccc1OCc2c(C)onc2C)C(=O)NCC(N3CCCC3)c4occc4	93528	nM
CHEMBL1502881	Cc1cc(NC(=O)CCNS(=O)(=O)c2cc(Br)cnc2N)ccc1Br	93660	nM
CHEMBL1419195	Fc1ccc(OCc2nnc(SCC(=O)NC(=O)NCc3occc3)n2CC=C)cc1	93790	nM
CHEMBL1413554	COCCCn1nnnc1C(N2CCN(CC2)c3ccc(O)cc3)c4cc5cc(OC)c(OC)cc5nc4O	94264	nM
CHEMBL1363824	OC(=O)C1Nc2c(Cl)cc(Cl)cc2C3C=CC13	94367	nM
CHEMBL1472381	CC1CCN(CC1)S(=O)(=O)c2ccc(cc2)C(=O)NCc3ccc4OCOc4c3	95660	nM
CHEMBL3199579	CC(C)N1C2=C(C=C(C#N)/C/1=N\C(=O)c3occc3)C(=O)N4C=CC=CC4=C2	95912	nM
CHEMBL1420642	COc1cc(\C=C/2\C(=O)c3cccc(c3C2=O)[N+](=O)[O-])c(Br)cc1O	96529	nM
CHEMBL1334980	Cc1cccc(\C=C(/C(=O)O)\c2ccc(s2)S(=O)(=O)N3CCCC3)c1	98015	nM
CHEMBL3198496	C\N=C\1/SC=C(N1\N=C\c2ccc(O)c(O)c2O)c3cccs3	98143	nM
CHEMBL1504221	Fc1cccc(c1)\C(=C/c2oc(cc2)N3CCCCCC3)\C#N	98433	nM
CHEMBL1541522	O=C(Nc1nnc(s1)C2CCCO2)c3cccs3	98826	nM
CHEMBL1371777	Clc1ccccc1CSc2nnc(c3occc3)c(n2)c4occc4	98960	nM
CHEMBL1314823	CC1=NN(C(=S)N)C(=O)C1N=Nc2cccc(c2)[N+](=O)[O-]	99228	nM
CHEMBL3189793	COc1ccc(c(OC)c1)c2cc(C(=O)N\N=C\c3ccc(OC)c(COCC(F)(F)C(F)F)c3)c4ccccc4n2	99392	nM
CHEMBL1524798	COc1cccc(c1)c2cn3nc4CCCCc4nc3n2	99986	nM
CHEMBL3189877	Cc1ccc(cc1)c2nc3S\C(=C/c4occc4)\C(=O)n3n2	100000	nM
CHEMBL1386036	CCCn1cnc2cc(NCc3ccccn3)ccc12	100000	nM
CHEMBL1386272	COc1ccc(cc1)C2CC(c3ccccc3)n4nc(NC(=O)c5cccs5)nc4N2	100000	nM
CHEMBL1342384	CN(C)c1ccc(NC(=O)Cn2cc3CCCCc3n2)cc1	100000	nM
CHEMBL1975523	CCN(CC)c1ccc(\C=N\c2ccc(cc2)N(C)C)c(O)c1	100000	nM
CHEMBL1212972	CC1OC(CC(=O)O)CC2=C1C(=O)c3c(O)cccc3C2=O	100000	nM
CHEMBL1429930	Cc1c(CCc2ccncc2)n3ccccc3c1C(=O)Nc4ccc(Cl)cc4	100000	nM
CHEMBL1414027	Cc1oc(CCC(=O)Nc2ccc(cc2)S(=O)(=O)N)cc1	100000	nM
CHEMBL1529824	CC(c1ccccc1)c2cc(C)c(C)c(CN3CCOCC3)c2O	100000	nM
CHEMBL1370669	OC(=O)CCc1oc(cc1)c2ccc(Br)cc2	100000	nM
CHEMBL1518296	CCOc1ccc(Nc2nc3ccccc3n4nnnc24)cc1	100000	nM
CHEMBL1486598	COC(=O)C1=C(C)NC(=O)/C/1=C\c2cccs2	100000	nM
CHEMBL1307104	COc1ccccc1\C=C(\CC(=O)NCc2ccccc2)/c3nc4ccccc4s3	100000	nM
CHEMBL1600987	CCOc1ccc(cc1OCC)c2nnn(CC(=O)c3ccc4OCCOc4c3)n2	100000	nM
CHEMBL1300285	CCc1ccc2nc(N3CCN(C)CC3)c(cc2c1)C#N	100000	nM
CHEMBL1383536	CCOC(=O)c1cc(NC(=O)N2CCCc3ccccc23)c(C)nc1C	100000	nM
CHEMBL1497978	Cc1ccn2cc(CNS(=O)(=O)c3ccc(Cl)s3)nc2c1	100000	nM

CHEMBL1731995	O=C(COC(=O)c1c2CC\C(=C\c3occc3)\c2nc4ccccc14)NC5CCCC5	100000	nM
CHEMBL1323320	OC(=O)c1cccc(c1)n2ccccc2\C=C/3\SC(=O)N(Cc4ccccc4C#N)C3=O	100000	nM
CHEMBL1604171	CC(C)(C)NC(=O)\C(=C\c1occc1)\c2ccccc2	100000	nM
CHEMBL1560978	CCC(C)(C)n1nnnc1C(N2CCN(CC2)c3ccc(O)cc3)c4ccc5ncccc5c4	100000	nM
CHEMBL1517216	O=C(N1CCN(CC1)S(=O)(=O)c2ccccc2)c3cccc(c3)n4cccc4	100000	nM
CHEMBL1492213	COc1ccc(cc1)N2C3=C(CC4=C2CCCC4=O)C(=O)CCC3	100000	nM
CHEMBL1706291	OC(=O)c1cc(nn1c2ccc(F)cc2F)c3ccc(cc3)N4CCOCC4	100000	nM
CHEMBL1454994	COc1ccc(cc1)C2CC(=O)Oc3cc(OC)ccc23	100000	nM
CHEMBL1304345	Cc1c(C)n(C(=O)CSc2nc3ccccc3[nH]2)c4ccccc14	100000	nM
CHEMBL1537344	Cl.CN(C)[C@H]1[C@@H]2CC3C(=C(O)C[C@]2(O)C(=C(C(=O)N)C1=O)O)C(=O)c4c(O)ccc(Cl)c4[C@@]3(C)O	100000	nM
CHEMBL1344700	COC(=O)\C(=C(\F)/SCC(=O)C)\C(F)(F)F	100000	nM
CHEMBL1328241	O=C1C(Cc2ccccc12)Sc3oc(nn3)c4ccccn4	100000	nM
CHEMBL1541295	Cc1cccc(c1)N2C(=S)NC(=O)\C(=C/c3oc(CN(CCC#N)S(=O)(=O)C)cc3)\C2=O	100000	nM
CHEMBL1383388	CN1C(=O)C(=C(C)CC1(C)C)C#N	100000	nM
CHEMBL1492858	COc1cc2CCN(C3CC4(C=CC(=O)C=C4)c(c1OC)c23)C(=O)CCC(=O)O	100000	nM
CHEMBL1548690	CCOC(=O)C1=NN(C(=N)C(=C1C)C#N)c2ccc(Cl)cc2Cl	100000	nM
CHEMBL1543104	Cc1ccc(cc1)N2C(=O)[C@@H]3[C@H]4C=CC=NN4[C@@H]([C@@H]3C2=O)C(=O)Nc5ccc(Cl)cc5	100000	nM
CHEMBL1884136	CC(C)(C)OC(=O)N(Cc1ccccc1)Cc2cccc(OCc3cccc(NC(=O)c4ccccc4)c3)c2	100000	nM
CHEMBL1352461	COCC(C)n1c(C)cc(C(=O)CSC2=Nc3sc(C)c(C)c3C(=O)N2CC=C)c1C	100000	nM
CHEMBL1431126	Oc1nc2ccccc2n3c(nnc13)c4ccccc4	100000	nM
CHEMBL1562255	Cc1cccc(C)c1NC(=O)CCS(=O)(=O)c2cccc3nsnc23	100000	nM
CHEMBL3210787	COc1ccc(cc1)\N=C/2\S\C(=C/c3oc(C)cc3)\C(=O)N2CC(C)C	100000	nM
CHEMBL1362225	CNC(=O)[C@@H]1C[C@H]1[C@@H](NC(=O)OCc2ccccc2)c3ccccc3	100000	nM
CHEMBL1985649	CC1=CC(C)(C)N2C(=O)\C(=N\c3ccc(O)cc3)\c4cccc1c24	100000	nM
CHEMBL1487668	C(Nc1nc(cs1)c2cccnc2)c3occc3	100000	nM
CHEMBL1517511	CC(=O)N(\C=C/C=C/C=C/1\Sc2ccccc2C1=O)c3ccccc3	100000	nM
CHEMBL1349645	CC1CCCN(C1)C(=O)CN2CCN(CC2)C(=O)c3occc3	100000	nM
CHEMBL1495281	C(CNc1ccc2nnc(c3ccccc3)n2n1)CN4CCN(Cc5ccccc5)CC4	100000	nM
CHEMBL1473579	CN(CC(=O)Nc1ccc(F)cc1)C(=O)c2cc(nc3ccccc23)c4occc4	100000	nM
CHEMBL1598620	Cc1cc(ccc1n2cnnn2)S(=O)(=O)N(Cc3occc3)Cc4ccccn4	100000	nM
CHEMBL3198411	CCSC1=C(C#N)C(\C(=C(/O)\OC)\C(=N1)C)c2cccs2	100000	nM
CHEMBL3211848	COc1ccc(cc1)C(=O)N\N=C\c2cccnc2	100000	nM
CHEMBL1318116	CCCCN1C(=O)NC(=O)C(=C1N)N(CCOC)C(=O)c2cc(nc3ccccc23)c4occc4	100000	nM
CHEMBL1435484	O=C(Nc1nc(c2occc2)c(s1)c3occc3)c4occc4	100000	nM
CHEMBL1393731	CCOc1ccc2nc(O)c(CN(Cc3occc3)C(=O)c4ccc(Br)cc4)cc2c1	100000	nM
CHEMBL1368322	Nc1ccc(cc1)C(=C2C=CC(=N)C=C2)c3ccc(N)cc3	100000	nM
CHEMBL1363924	CCn1c(SCC(=O)Nc2cc(C)on2)nnc1c3cccnc3	100000	nM
CHEMBL1352809	CCOc1ccc(cc1)n2c(Cc3cc(O)nc(O)n3)nnc2SCC(=O)NC4CCCC4	100000	nM
CHEMBL1498201	NC(=O)c1ccc(N2CCN(CC2)c3ccc(O)cc3)c(c1)[N+](=O)[O-]	100000	nM
CHEMBL1323006	Cc1onc(C)c1COc2ccc(cc2)C(=O)OCC(=O)N3c4ccccc4NC(=O)C3(C)C	100000	nM
CHEMBL1325311	COc1ccc2cc(C3C(=C(N)OC(=C3C(=O)C)C)C#N)c(Cl)nc2c1	100000	nM
CHEMBL1598069	COc1ccc2nc(O)c(CN(Cc3occc3)C(C(C)C)c4nnnn4Cc5ccccc5)cc2c1	100000	nM
CHEMBL1585469	CCCCN1C(=O)NC(=O)C2(Cc3ccccc3N4CCOCC24)C1=O	100000	nM
CHEMBL1428889	CCc1nc(OCc2occc2)c3sc4nc5CC(C)(C)OCc5cc4c3n1	100000	nM
CHEMBL1574497	CC1Cc2ccccc2N1C(=O)C3CCN(CC3)S(=O)(=O)c4c(C)noc4\C=C\c5occc5	100000	nM
CHEMBL1419169	COc1cccc(C(C#N)N2CCCCC2)c1O	100000	nM

CHEMBL1556882	CC1(C)Cc2nc3sc4c(SCC(=O)NCc5occc5)ncnc4c3cc2CO1	100000	nM
CHEMBL3193682	O=C(N\N=C\c1ccc[nH]1)c2cccnc2	100000	nM
CHEMBL1388553	O.Cl.Nc1ccc(cc1)N2CCN(CCCCN3C(=O)C4CCCN4C3=O)CC2	100000	nM
CHEMBL1375390	CN1C(=O)N(C)C(=O)C2(Cc3cc4cc(C)ccc4nc3N5CCCCC25)C1=O	100000	nM
CHEMBL1311134	CCOC(=O)N1CCC(CC1)NC(=O)c2ccc(OC)c(CN3CC(=O)N4CCCC4C3=O)c2	100000	nM
CHEMBL1200567	O.Cl.CCO.C[C@@H]1[C@H]2[C@H](O)[C@H]3[C@H](N(C)C)C(=C(C(=O)N)C(=O)[C@@]3(O)C(=C2C(=O)c4c(O)cccc14)O)O	100000	nM
CHEMBL1351621	CN1N(C(=O)C(=C1C)NC(=O)CN2CCN(CC2)c3ccc(O)cc3)c4ccccc4	100000	nM
CHEMBL1419335	COc1ccc(OC)c(Nc2nc(cs2)c3ccc(O)c(O)c3)c1	100000	nM
CHEMBL1392444	O=C(NC(=S)N1CCCc2ccccc12)c3ccccc3	100000	nM
CHEMBL1533621	O=C1C=C(Nc2cccc3cccnc23)c4ccccc4C1=O	100000	nM
CHEMBL1502275	COc1ccc(cc1)n2c(Cc3cccn3C)nnc2SCC(=O)N	100000	nM
CHEMBL1462570	Cc1cc(O)c(Oc2cc(C)cc(O)c2O)c(O)c1	100000	nM
CHEMBL1310730	COc1ccc(NS(=O)(=O)c2cccc(c2)C(=O)NNC(=O)c3cccn3C)cc1	100000	nM
CHEMBL1587966	OP(=O)(CN1CCCCC1)CN2CCCCC2	100000	nM
CHEMBL1416437	Cc1cc(c(C)n1C)c2csc(NC(=O)c3oc4ccccc4c3)n2	100000	nM
CHEMBL1871358	C[C@@H](CO)N1C[C@@H](C)[C@H](CN(C)C(=O)Nc2ccc(cc2)C(F)(F)F)OCCCC[C@H](C)Oc3ccc(NC(=O)Nc4ccccc4)cc3C1=O	100000	nM
CHEMBL1519669	CC(=O)c1cccc(NC(=O)CN2C(=O)NC3(CCCCCCC3)C2=O)c1	100000	nM
CHEMBL1503314	COc1ccc(CCNC(=O)CN2CCCc3ccccc23)cc1OC	100000	nM
CHEMBL1337299	NC(=O)c1c2CCCc2sc1NC(=O)Cc3cccs3	100000	nM
CHEMBL1549834	O=C(N1CCN(CC1)C(c2ccccn2)c3nnnn3C4CCCC4)c5occc5	100000	nM
CHEMBL1369848	O=C(NCCN1CCN(CC1)c2ccccc2)C3CCN(CC3)S(=O)(=O)c4cccc5nonc45	100000	nM
CHEMBL1350464	CCc1ccccc1N(CC(=O)NCCSCc2occc2)S(=O)(=O)C	100000	nM
CHEMBL1720147	Cl.CN1CCc2nc3ccc(Cl)cc3c(c2C1)c4ccccc4Cl	100000	nM
CHEMBL1324188	CN(C1CCCCC1)C2=NN3C(=Nc4ccccc4C3=O)C=C2	100000	nM
CHEMBL1318963	Cc1cc(C(=O)CSc2nnc(c3ccccc3)n2Cc4ccc5OCOc5c4)c(C)n1C	100000	nM
CHEMBL1593348	Cc1oc(C)c(c1)C(=O)NNC(=O)\C=C\c2occc2	100000	nM
CHEMBL1594813	COC(=O)C(C)Sc1nnc(Cc2cc(O)nc(O)n2)n1c3cc(C)ccc3C	100000	nM
CHEMBL1570840	OC1=CC(=O)NC(=S)N1c2ccc(F)cc2	100000	nM
CHEMBL1562157	Cc1cc(O)cc(O)c1C(=O)Cc2cnn(c2)c3ccccc3	100000	nM
CHEMBL1409063	OC(=O)C(Cc1c[nH]c2ccccc12)NC(=O)c3ccccc3NC(=O)c4occc4	100000	nM
CHEMBL1555494	CCCn1c(CNc2ccccc2O)nc3ccccc13	100000	nM
CHEMBL1404083	O=C1NC(=O)C(=CN2CCc3ccccc23)C(=O)N1	100000	nM
CHEMBL1442147	CC\C(=C/1\C(=O)NC(=O)N(CC=C)C1=O)\NCCN2CCOCC2	100000	nM
CHEMBL1557913	COc1ccccc1C2=Nc3cccc4cccc(N2)c34	100000	nM
CHEMBL1490479	COc1ccc(NC(=NNc2ccc(cc2)[N+](=O)[O-])P(=O)(N3CCOCC3)N4CCOCC4)cc1	100000	nM
CHEMBL1979957	COCC\N=C\1/SC=C(N1\N=C\c2ccc(O)c(O)c2O)c3cccs3	100000	nM
CHEMBL1312190	Oc1ccc(cc1O)C(=O)CN2CCN(CC2)S(=O)(=O)c3ccc(F)cc3	100000	nM
CHEMBL1446088	CCN(CC(=O)Nc1c(F)cccc1F)C(=O)c2cccc(c2)n3cccc3	100000	nM
CHEMBL1422946	CCc1ccc(CC)c(c1)S(=O)(=O)Nc2ccc(C(=O)O)c(O)c2	100000	nM
CHEMBL1364567	CN(CC(=O)Nc1c(Cl)cccc1Cl)C(=O)c2cccc(c2)n3cccc3	100000	nM
CHEMBL1458390	COc1ccc(cc1OC)c2ccc(C#N)c(SCC(=O)Nc3sc4CCCc4c3C#N)n2	100000	nM
CHEMBL1450538	Cc1occc1c2nnc(SCC(=O)N3CCN(CC3)c4ccccc4)n2C	100000	nM
CHEMBL3193326	COc1ccc(\C=N/NC(=O)c2cc(O)c(O)c(O)c2)cc1CN3CCN(CC3)c4ccc(F)cc4	100000	nM
CHEMBL1548347	CN1CCN(CC1)C(=O)CSc2nc(ccc2C#N)c3cccs3	100000	nM
CHEMBL1533464	OC(=O)c1ccc(cc1)n2nc(c3CCc4occc4c23)C(F)(F)F	100000	nM
CHEMBL1608918	O=C(NC1CCCC1)C(N(Cc2ccccc2)C(=O)c3csnn3)c4occc4	100000	nM

CHEMBL1313583	NC1=CC=CC2=[N+]([O-])C3(CCCCC3)N=C12	100000	nM
CHEMBL1299528	CCOc1ccc(cc1)n2c(Cc3cc(O)nc(O)n3)nnc2SCC(=O)N	100000	nM
CHEMBL1432345	CC(=O)N1CCN(CC1)c2ccc(NCc3ccc(F)cc3)cc2	100000	nM
CHEMBL1425459	CC(C)CN(C1CCS(=O)(=O)C1)C(=O)COC(=O)c2cc(C)n(c2C)c3ccc(C)cc3	100000	nM
CHEMBL1416702	Cc1cc(C)cc(NCc2cc3OCOc3cc2[N+](=O)[O-])c1	100000	nM
CHEMBL2003964	C\N=C\1/SC=C(N1\N=C\c2ccc(O)c(O)c2)c3occc3	100000	nM
CHEMBL1346640	CCOc1cccc(CNc2ccc(O)cc2)c1OCc3ccc(Cl)cc3Cl	100000	nM
CHEMBL1333695	CCC(=O)Nc1cc(C)c(NC(=O)C23CC4CC(CC(C4)C2)C3)cn1	100000	nM
CHEMBL1480652	COCCCNC(=O)C1=CC=CN2C(=O)c3cc4ccccc4cc3N=C12	100000	nM
CHEMBL1301692	Clc1cccc(c1)n2nc(cc2C(=O)N3CCCCC3)c4occc4	100000	nM
CHEMBL1306765	COCCNC(=O)c1oc(CS(=O)(=O)c2c(Cl)cccc2Cl)cc1	100000	nM
CHEMBL1451078	Oc1ccc(CC2NC3([C@H]4[C@@H]2C(=O)N(C4=O)c5ccc(F)cc5)C(=O)Nc6ccc(F)cc36)cc1	100000	nM
CHEMBL1535798	CC(C)(Oc1ccc(Cl)cc1)C(=O)NCc2occc2	100000	nM
CHEMBL1364286	Cc1ccc(cc1)N2CCN(C2c3ccccn3)c4ccc(C)cc4	100000	nM
CHEMBL1463665	CC(=O)C1=C(O)C(=O)N(Cc2occc2)C1c3ccc(F)cc3	100000	nM
CHEMBL1612609	COc1ccc(cc1)C2=NC3=C(C(=O)N2Cc4occc4)C(=O)c5ccc(OC)cc5O3	100000	nM
CHEMBL1531315	CSc1oc(nc1S(=O)(=O)c2ccccc2)c3occc3	100000	nM
CHEMBL1863612	CCN1CCN(CC1)C(=O)CN(C)S(=O)(=O)c2ccc(OC)c(C)c2	100000	nM
CHEMBL1735497	COCOC1CCC2C3CCC4=CC(=O)CCC4=C3C=CC12C	100000	nM
CHEMBL1608044	Nc1ccc(Oc2ncccn2)cc1	100000	nM
CHEMBL1585044	COc1ccccc1NC(=O)CN(Cc2occc2)C(=O)c3cccs3	100000	nM
CHEMBL3195986	CC(C)Nc1nnc(SC\C(=C(\C#N)/C(=N)C)\O)s1	100000	nM
CHEMBL1542333	S=C(Nc1ccc2OCCOc2c1)Nc3ccc4OCOc4c3	100000	nM
CHEMBL1372650	Clc1ccc(cc1)C(=O)CSc2nc(ccc2C#N)c3occc3	100000	nM
CHEMBL1463037	CC(C)CN(C(=O)CN1CCN(CC1)c2ccc(O)cc2)C3=C(N)N(CC(C)C)C(=O)NC3=O	100000	nM
CHEMBL1423709	Cn1cccc1\C=C/2\C(=O)NC(=S)N(Cc3ccc(F)cc3)C2=O	100000	nM
CHEMBL1408125	[O-][N+](=O)c1cc(Br)c(c(Br)c1)c2oc(\C=C/3\NC(=S)NC3=O)cc2	100000	nM
CHEMBL1545501	COc1ccc(OC)c(N\C(=C\C(=O)c2oc(C)cc2)\C)c1	100000	nM
CHEMBL1400510	CC1=Nc2cccc3cccc(N1)c23	100000	nM
CHEMBL1381306	COc1ccc2c(c1)C(=O)Oc3cc(OCC(=O)N4CCC(C)CC4)ccc23	100000	nM
CHEMBL1373289	[O-][N+](=O)c1oc(\C=C\2/C=C(OC2=O)c3ccc(F)cc3)cc1	100000	nM
CHEMBL1612931	COCCCNc1nnc(SC(C)C(=O)Nc2ccc(cc2)c3nc4ccc(C)cc4s3)s1	100000	nM
CHEMBL1301260	CC(C)C[C@H](NC(=O)c1[nH]cnc1C(=O)N2CCN(CC2)c3ccccc3)C(=O)OC(C)(C)C	100000	nM
CHEMBL1423492	Cc1cc(Cl)cc2c1NC(=O)[C@]23[C@H]4[C@@H]([C@@H]5CCCN35)C(=O)N(Cc6ccccc6)C4=O	100000	nM
CHEMBL1534745	CCOC(=O)\C=C\1/SCC(=O)N1CC(=O)NC(C)c2ccc(F)cc2	100000	nM
CHEMBL1338730	CCOC(=O)C1=C(COC(=O)\C=C\c2occc2)NC(=O)NC1C	100000	nM
CHEMBL1486316	CC(=O)Nc1ccc(NC(=O)CSCc2cnn(c3ccccc3)c2n4cccc4)cc1	100000	nM
CHEMBL1325883	COc1ccc(NC(=O)CCCSc2ccccc2)cc1	100000	nM
CHEMBL1452930	COc1ccc(cc1)S(=O)(=O)Cc2oc(cc2)C(=O)N3CCN(CC3)c4ccccc4	100000	nM
CHEMBL1439414	Clc1cccc(c1)N2C(=O)NC(=O)\C(=C\c3oc(Sc4nc5ccccc5[nH]4)cc3)\C2=O	100000	nM
CHEMBL82134	[I-].CCN1\C(=C\C=C\C=C\C=C\c2sc3ccccc3[n+]2CC)\Sc4ccccc14	100000	nM
CHEMBL1345135	Cc1oc(cc1)c2cc(C(=O)Nc3ccc(C)cn3)c4ccccc4n2	100000	nM
CHEMBL1703976	Oc1c(ccc2cccc12)C3(OC(=O)c4ccccc34)c5ccc6ccccc6c5O	100000	nM
CHEMBL1412418	COc1cc(\C=C(/CC(=O)O)\c2nc3ccccc3s2)cc(OC)c1O	100000	nM
CHEMBL1370087	Cc1cc(C(=O)CN2C(=O)c3ccccc3S2(=O)=O)c(C)n1CC4CCCO4	100000	nM
CHEMBL1707215	[O-][N+](=O)c1ccc(c(c1)[N+](=O)[O-	100000	nM

162

	])S(=O)(=O)Nc2ccccc2C(=O)N3O[C@H]4C[C@@H]3C=C4		
CHEMBL1447076	NS(=O)(=O)c1ccc(cc1)N2N=C(CC2c3ccc(F)cc3)c4ccc(Br)cc4	100000	nM
CHEMBL1408354	Cc1cc(C)c(c(C)c1)S(=O)(=O)NCC2CCC(CC2)C(=O)N3CCC4(CC3)O CCO4	100000	nM
CHEMBL1549607	Cc1ccc(cc1)N2CSC3=C(C#N)C(CC(=O)N3C2)c4cccs4	100000	nM
CHEMBL1528749	Cl.CC(=O)N1CCN(CC1)c2ccc(NCc3ccc(C)s3)cc2	100000	nM
CHEMBL1473982	COc1ccc(NC(=O)CN(C)C(=O)c2cccc(c2)n3cccc3)cc1	100000	nM
CHEMBL1539953	COc1ccc(CCNC(=O)\C=C\c2occc2)cc1	100000	nM
CHEMBL1887584	CC(C)CCN1CCN(Cc2cccn2c3cccnc3)CC1CCO	100000	nM
CHEMBL1874279	COc1cc(NCCCNC(C)C)c2nccc(C)c2c1	100000	nM
CHEMBL1712082	CC1=C(O)C(=O)C=C2C1=CC=C3C2(C)CCC4(C)C5CC(C)(CCC5(C)C CC34C)C(=O)O	100000	nM
CHEMBL1602613	FC(F)(F)C1CC(Nc2cc(nn12)C(=O)N3CCc4ccccc4C3)c5occc5	100000	nM
CHEMBL1576463	O=C(CSc1nnc(C2CCCCC2)n1Cc3ccccc3)NCc4occc4	100000	nM
CHEMBL1414980	CC(C)CC(NC(=O)\C(=C\c1occc1)\NC(=O)c2oc(Br)cc2)C(=O)O	100000	nM
CHEMBL1392313	CC(C)c1ccc(cc1)N2C(=O)Cc3c2nc4N=C(C)Nc5nc(N6CCCCC6)c(C#N)c3c45.CN(C)C=O	100000	nM
CHEMBL1536196	CNCc1ccccc1Sc2ccc(O)c(O)c2.OC(=O)\C=C/C(=O)O	100000	nM
CHEMBL1512376	CN(CC(=O)Nc1cc(C)ccc1C)C(=O)c2cccc(c2)n3cccc3	100000	nM
CHEMBL1347904	CCCCn1cnc2cc(NCc3ccncc3)ccc12	100000	nM
CHEMBL1727678	COc1cc(ccc1C=C2c3ccccc3n4c2cc(c5ccccc5)[n+]4C)N(C)C.[O-]S(=O)(=O)C(F)(F)F	100000	nM
CHEMBL1597571	COc1ccc(OC)c(c1)C2C(=C(C)Nc3nc(CCCO)nn23)C(=O)Nc4ccc(F)cc4	100000	nM
CHEMBL1419228	CC1OC(OCC2OC(OC3=C(Oc4cc(O)cc(O)c4C3=O)c5ccc(O)cc5)C(O) C(O)C2O)C(O)C(O)C1O	100000	nM
CHEMBL3184468	NC(=O)\C(=C\1/C=CC2=NC34CCCCC3CC5=C(CCCC5)N4C2=C1)\C #N	100000	nM
CHEMBL1997370	CN1C(=O)\C(=N/C(=O)C)\c2c3ccccc3c(O)c4cccc1c24	100000	nM
CHEMBL1361703	COc1ccccc1CNC(=O)COC(=O)c2cc(nc3ccccc23)c4occc4	100000	nM
CHEMBL1736432	[O-][N+](=O)c1cc2no[n+]([O-])c2cc1N3CCCCC3	100000	nM
CHEMBL1350960	CCn1c(SCC(=O)NCc2occc2)nnc1c3cccs3	100000	nM
CHEMBL1333071	FC(F)(F)c1cc(nc(NCc2cccnc2)n1)c3occc3	100000	nM
CHEMBL1328884	CCC(N(Cc1ccccc1OC)Cc2cc3cc(C)ccc3nc2O)c4nnnn4Cc5occc5	100000	nM
CHEMBL1303512	CCCOC(=O)Nc1sc2CCCc2c1C(=O)OCC	100000	nM