Biointerface Research in Applied Chemistry
Platinum Open Access Journal (ISSN: 2069-5837)

Article
Volume 12, Issue 3, 2022, 2905 - 2957
https://doi.org/10.33263/BRIAC123.29052957

Ester-Functionalized Imidazolium- and Pyridinium-Based Ionic Liquids: Design, Synthesis and Cytotoxicity Evaluation

Diana Hodyna [1,*], Vasyl Kovalishyn [1], Ivan Semenyuta [1], Sergiy Rogalsky [2], Olena Trokhimenko [3], Anastasiia Gryniukova [1], Larysa Metelytsia [1]

[1] Department of Medical and Biological Researches, V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Science of Ukraine, Kyiv, 02094, Ukraine
[2] Laboratory of Modification of Polymers, V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Science of Ukraine, Kyiv, 02094, Ukraine
[3] Department of Virology, Shupyk National Healthcare University of Ukraine, Kyiv, 04112, Ukraine
* Correspondence: dianahodyna@gmail.com (D.H.);

Scopus Author ID 56897133500
Received: 9.06.2021; Revised: 15.07.2021; Accepted: 20.07.2021; Published: 8.08.2021

Abstract: The QSAR model for the prediction of cytotoxicity of Ionic liquids (ILs) was developed using a data set of 1195 compounds. The Artificial Neural Networks learning technique was used. The predictive ability of the models was tested by means of cross-validation; the q^2 value was 0.76 for the regression model. The prediction for the external evaluation set afforded high predictive power (q^2 =0.75 for 239 compounds). The developed QSAR models evaluated the anticancer activity of a small set of virtual compounds and 6 compounds were selected for synthesis and biological testing. It was found that imidazolium and pyridinium ILs with C_{12} and C_{10} alkyl chain length exhibited significant cytotoxicity, particularly, compounds 3 and 6 were identified as the most potent anticancer agents with IC_{50} values 0.18 μM and 5.75 μM against Hep-2 cell line and different acute toxicity levels to cladoceran *Daphnia magna*. Molecular docking showed that the high cytotoxic activity of imidazolium and pyridinium ILs with C_{12} alkyl chain length may be associated with specific DNA binding in the region of CG nucleotides.

Keywords: ionic liquids; QSAR; cytotoxicity; molecular docking; acute toxicity.

1. Introduction

It is known that the increase in the incidence of various types of cancer creates a constant need to develop new anticancer drugs, including synthetic compounds of different chemical classes, possessing cytotoxic properties [1-5].

Today the Ionic liquids (ILs) are the actual topics of study by researchers in the pharmaceutical industry in their search for new therapeutic agents [6-8]. Apart from the physicochemical features of ILs, their high biological activity attracts significant attention from medical scientists, biochemists, and ecologists. It is now clearly established that ILs have an impact on different levels of life, from single proteins to higher multicellular organisms. In addition to the use of ILs as antibacterial and antifungal agents [9-11], several studies have reported using different ILs in biomedical applications as therapeutic agents, namely as antitumor cytotoxic agents [8,12,13]. The cancerous cells of invertebrate and vertebrate species were investigated, including insects *Drosophila melanogaster* S2 cell culture [13], channel

catfish ovary cell line CCO [14], mouse fibroblasts 3T3 [15], rat glial cells C6 [16], promyelocytic leukemia IPC-81 [17], pheochromocytoma PC12 [18], lung carcinoma A431 [19], squamous carcinoma CaCo-2 [20], colon carcinoma HaCaT [21], embryonic kidney HeLa [16], cervical cancer HepG2 [22], hepatocyte carcinoma HT-29 [23], colon carcinoma MCF-7 [20], breast cancer T98G [24], brain cancer U937 [25] and others.

It is established that the cytotoxicity of ILs depends on their structure and has a wide range of values from micromolar to millimolar. The preliminary structure-activity relationship (SAR) showed that the chain length of alkyl chains on the cations plays a crucial role in the anti-tumor activity and cytotoxicity of ILs [20]. The nature of the cation also affects the activity of ILs. So, cholinium ILs demonstrated lower cytotoxicity than imidazolium- and pyridinium-based ILs. A number of potential anticancer agents with high cytostatic and low cytotoxic activity among imidazolium, phosphonium, and ammonium ILs was identified in 60 human tumor cell line tests [20,26]. In general, phosphonium-based ILs were identified as more active and less cytotoxic as compared to ammonium and imidazolium salts. Guanidinium tetrafluoroborate with long alkyl chains and the entered natural amino acids showed very high cytotoxicity toward several tumor cell lines [27]. The authors assumed that such an increase in cytotoxicity can be connected with the enhancement of transport of the toxic anion into the cells [28]. Short-chain ILs, triethylammonium sulfate, triethylammonium phosphate, 1-methylimidazolium chloride, and 1-butyl-3-methylimidazolium chloride were found to have poor anti-tumor activity and were less toxic toward nonmalignant HEK (human embryonic kidney) cells as compared to T98G brain cancer cells [25].

Accumulated information about mechanisms of ILs cytotoxicity demonstrates that ILs disturb the lipid bilayers of the cell membrane, and cation hydrophobicity and lipophilicity correlate with the cytotoxic effect [29-32]. 1-alkylquinolinium ILs caused cell membrane disruption in the 3T3 cells culture [33]. Imidazolium ILs induced mitochondrial failure, oxidative stress, and apoptosis in malignant and normal cells [20,34-36]. The expression of cytochrome P450 genes, which products were involved in the metabolism of drugs and other exogenous substances, were induced by1-octyl-3-methylimidazolium chloride in the mammary carcinoma cells EMT6 of mouse [37]. A number of studies of the anticancer activity of ionic liquids based on imidazolium and pyridinium deserve special attention [38-40]. The authors associate this activity with their specific interaction with the cellular DNA.

It is worth noting that the long-chain ILs commonly demonstrate cytotoxicity to both normal and cancer cell lines that is one of the main problems limiting their practical applications [19,20,41]. However, the major advantage of ILs are in tuning their toxicity while tailoring pharmacological properties necessary for desired therapeutic applications [26,42]. The hydrophobic interaction between the lipophilic tails of cationic biocides and phospholipids of eukaryote cell membranes plays a major role in forming biocide-cell binding and consequently toxic impact [43]. From this point of view, introducing polar functional groups into the hydrocarbon chains of ILs may retard their penetration through the cell membrane due to reduced lipophilicity [44]. Thus, long-chain pyridinium-based ILs, comprising the polar ester group in the hydrocarbon radical, were found to have dramatically reduced acute toxicity towards *Danio rerio* model freshwater hydrobiont as compared to common long-chain ILs [45]. However, the anti-tumor activity of ester-functionalized ILs has not yet been studied.

Several attempts to create a prediction model for assessing ILs cytotoxicity *in silico* have been made [46-50] however, at the moment, there is no possibility to distinguish the cytotoxicity of ILs only by their structure because it also strongly depends on the external

factors, such as the cell type. Despite active investigations in the ILs anticancer properties area, this problem remains open for further scientific finds.

The cytotoxic activity and acute toxicity of a number of ionic liquids are presented in this study using the created QSAR models, biological testing, and docking analysis.

2. Materials and Methods

2.1. QSAR modeling.

2.1.1. Composition of training and test sets and calculation of molecular descriptors.

The data for our analysis consisted of 1195 compounds cytotoxic against Hep-2 cells that were obtained from the ChEMBL database [51]. The activity of compounds was expressed as IC_{50} ranging from 0.0002 to 5000 μM (Supplementary material).

Biological data obtained as inhibitory concentration (IC_{50}) were converted to $lg(1/IC_{50})$ and used as a dependent variable in the subsequent QSAR studies. In this work, external testing was performed using a test set that was formed using the method of Kennard-Stone Design (KSD) [52]. In this case, 20-25% of compounds were selected in the test set, while the remaining compounds from the general data set were used to build QSAR models [53]. Thus, the initial sample was divided into a test set that included 239 (20%) compounds, while the remaining 956 compounds were used as a training data sample.

Each molecule was modeled using ChemAxon Standardizer [54]. The 2D coordinates of the atoms were recalculated, ions and salts were removed from the molecular structure, the molecules were reduced to neutral, 3D structures were optimized and saved in SDF format.
The molecular descriptors' calculation was done using the DRAGON package [55] as the original variables, including molecular properties topological, geometrical, constitutional descriptors, atom-centered fragments, and many others [56]. The descriptors with coefficients with variance less than 5% and constants were deleted. In addition, if any of the two descriptors were at least 99% correlated, one of them was deleted.

Detailed information about the descriptors can be found on the Talete website [55]. As a result, the 1016 descriptors were selected.

2.1.2. Machine learning methods.

In this work, data analysis and selection of descriptors were performed using Batch Pruning Algorithm (BPA) [57]. This algorithm is a combination of the Associative Neural Network (ASNN) method [58], Self-Organized Map (SOM) of Kohonen [59], and the descriptor selection methods [60,61], used together. The Kohonen network was used to analyze the similarity of molecular descriptors, while ASNN was used to construct predictive models.

ASNN consists of an ensemble of Back Propagation Neural Networks (BPNN) and the method of k-nearest neighbors (k-NN) [58]. Traditional BPNNs are memoryless networks, i.e., after learning neural networks, the input data is no longer needed, and all the information needed to predict the properties of the new data is stored using weights. On the contrary, the k-Nearest Neighbours (k-NN) method maintains a memory of all training samples, and predictions are based on a local approximation of the stored data [62]. ASNN uses the k-NN method in the space of ensemble residuals. After learning ASNN, all compounds are represented as vectors of neural network predictions by the neural network ensemble. The nearest neighbor method uses the correlation between these vectors to measure the distance

between the analyzed cases. Thus, this approach increases the accuracy of the forecast by adjusting the source data based on information about the input data [58].

For data analysis, we used neural networks consisting of three levels. The number of input neurons was equal to the number of descriptors. One hidden layer with five neurons was used. Weights were initialized with random numbers within [-0.5; +0.5] for each of the 200 networks in the ensemble. This initialization allows the ASNN to avoid local minima and speeds up the ensemble learning procedure [63]. A bias neuron was also presented in both the input and hidden layers. One output neuron was used for regression tasks, and the output activity values $lg(1/IC_{50})$ were linearly scaled between 0.1 and 0.9 [63]. An algorithm known as the SuperSAB algorithm [64] was used for training. All the networks had the same architecture. Cross-validation techniques were used to strictly control the possibility of overfitting the data known as the Early Stopping over Ensemble (ESE) [63]. Research manuscripts reporting large datasets that are deposited in a publicly available database should specify where the data have been deposited and provide the relevant accession numbers. If the accession numbers have not yet been obtained at the time of submission, please state that they will be provided during review. They must be provided prior to publication.

2.1.3. Statistical coefficients.

The prediction statistics for the models are given in Table 1 (section Results and Discussion). The generally used measures of a regression QSAR model performance are the root mean square error (RMSE), the mean absolute error (MAE), the squared correlation coefficient R^2 [65], and cross-validated coefficient q^2 [66]. ASNN calculates these statistical parameters for both the training and the validation sets.

2.2. Synthesis of ionic liquids.

Following chemicals were used for the synthesis of ionic liquids: pyridine (99%), chloroacetyl chloride (98%), 1-octanol, 1-decanol, 1-dodecanol (98%), 1-methylimidazole (for synthesis), benzene, hexane, ethyl acetate (98%). All chemicals were purchased from Sigma-Aldrich and used without further purification.

Proton Nuclear Magnetic Resonance (1H NMR) spectroscopy was used to confirm the structure of synthesized compounds. The spectra were recorded on a Varian Gemini-2000 (400 MHz) NMR spectrometer.

2.2.1. Synthesis of long-chain alkyl esters of chloroacetic acid.

Alkyl esters of chloroacetic acid (1-octyl chloroacetate, 1-decyl chloroacetate, and 1-dodecyl chloroacetate) were synthesized as follows (Scheme 1).

Chloroacetyl chloride (13.5 g, 0.12 mol) was added dropwise to the stirred mixture of corresponding alcohol (0.1 mol) and potassium carbonate (14 g, 0.1 mol) in dry benzene (100 mL). The reaction was carried out for 6 h at room temperature. After completion of the reaction, the reactionary mixture was washed with water (3x200 mL). The organic layer was separated and dried overnight over calcium chloride. Benzene was distilled, the residual solvent was removed in a vacuum 10 mbar at 60 °C.

$$ClCH_2COCl + ROH \xrightarrow[K_2CO_3]{C_6H_6} ClCH_2COOR \qquad R = C_8H_{17}, C_{10}H_{21}, C_{12}H_{25}$$

Scheme 1. Synthesis of long-chain esters of chloroacetic acid.

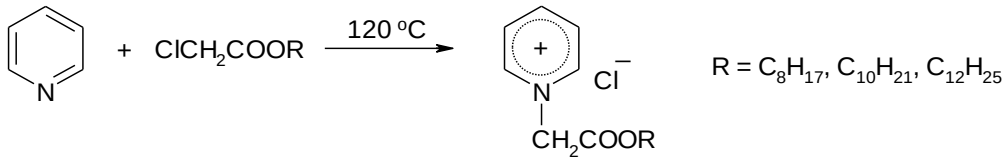
Octyl chloroacetate - 1H NMR (400 MHz, $CDCl_3$): δ = 0.88 (t, 3H, CH_3), 1.27 (m, 10H, $CH_3(CH_2)_5$), 1.66 (m, 2H, OCH_2CH_2), 4.05 (s, 2H, $COCH_2$), 4.18 (t, 2H, OCH_2);

Decyl chloroacetate - 1H NMR (400 MHz, $CDCl_3$): δ = 0.89 (t, 3H, CH_3), 1.27 (m, 14H, $CH_3(CH_2)_7$), 1.67 (m, 2H, OCH_2CH_2), 4.07 (s, 2H, $COCH_2$), 4.19 (t, 2H, OCH_2);

Dodecyl chloroacetate - 1H NMR (400 MHz, $CDCl_3$): δ = 0.89 (t, 3H, CH_3), 1.28 (m, 18H, $CH_3(CH_2)_9$), 1.66 (m, 2H, OCH_2CH_2), 4.06 (s, 2H, $COCH_2$), 4.18 (t, 2H, OCH_2);

2.2.2. Synthesis of ester-functionalized pyridinium ILs.

Long-chain ester-functionalized pyridinium ILs were synthesized by the following method (Scheme 2). The mixture of pyridine and corresponding alkyl chloroacetate (10% molar excess) was stirred at 120 °C for 2 h. After cooling to room temperature, the solid products were obtained. They were purified by recrystallizing from ethyl acetate ($PyrCH_2COOC_{12}$-Cl) or washed with a hexane-ethyl acetate mixture (3:1, v/v).



Scheme 2. Synthesis of ester-functionalized pyridinium ILs.

1-octyloxycarbonylmethylpyridinium chloride ($PyrCH_2COOC_8$-Cl) **(1)**

Amorphous solid of light brown color (m. p. 59 °C)

1H NMR (400 MHz, $CDCl_3$): δ = 0.82 (t, 3H, CH_3), 1.21 (m, 14H, $CH_3(CH_2)_7$), 1.58 (m, 2H, OCH_2CH_2), 4.12 (t, 2H, OCH_2), 6.26 (s, 2H, NCH_2), 8.05 (t, 2H, C_3-H, C_5-H), 8.49 (t, 1H, C_4-H), 9.46 (d, 2H, C_2-H, C_6-H).

1-decyloxycarbonylmethylpyridinium chloride ($PyrCH_2COOC_{10}$-Cl) **(2)**

White solid (m. p. 89-91 °C)

1H NMR (400 MHz, DMSO-D_6): δ = 0.86 (t, 3H, CH_3), 1.27 (m, 14H, $CH_3(CH_2)_7$), 1.61 (m, 2H, OCH_2CH_2), 4.17 (t, 2H, OCH_2), 5.8 (s, 2H, NCH_2), 8.26 (t, 2H, C_3-H, C_5-H), 8.72 (t, 1H, C_4-H), 9.18 (d, 2H, C_2-H, C_6-H).

1-dodecyloxycarbonylmethylpyridinium chloride ($PyrCH_2COOC_{12}$-Cl) **(3)**

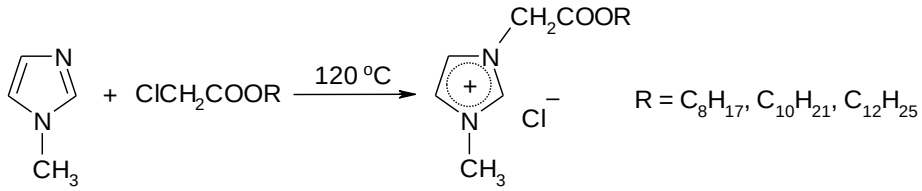
White solid (m. p. 70-73 °C)

1H NMR (400 MHz, DMSO-D_6): δ = 0.85 (t, 3H, CH_3), 1.25 (m, 18H, $CH_3(CH_2)_9$), 1.61 (m, 2H, OCH_2CH_2), 4.17 (t, 2H, OCH_2), 5.9 (s, 2H, NCH_2), 8.26 (t, 2H, C_3-H, C_5-H), 8.74 (t, 1H, C_4-H), 9.27 (d, 2H, C_2-H, C_6-H).

2.2.3. Synthesis of ester-functionalized imidazolium ILs.

Long-chain ester-functionalized imidazolium ILs were synthesized according to Scheme 3.

The mixture of 1-methylimidazole and alkyl chloroacetate (10% molar excess) was stirred at 120 °C for 2 h. After cooling, the solid products were obtained. They were purified by recrystallizing from ethyl acetate ($IMC_1CH_2COOC_{12}$-Cl) or washed with a hexane-ethyl acetate mixture (3:1, v/v).



Scheme 3. Synthesis of ester-functionalized imidazolium ILs.

1-octyl-3-methylimidazolium chloride ($IMC_1CH_2COOC_8$-Cl) **(4)**

1H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, 3H, CH_3), 1.22 (m, 14H, $(CH_2)_7$), 1.6 (m, 2H, $COOCH_2CH_2$), 4.04 (s, 3H, NCH_3), 4.13 (t, 2H, $COOCH_2$), 5.44 (s, 2H, NCH_2CO), 7.52 (d, 1H, C_4-H), 7.59 (d, 1H, C_5-H), 10.35 (s, 1H, C_2-H).

White solid (m. p. 42-45 °C)

1-decyl-3-methylimidazolium chloride ($IMC_1CH_2COOC_{10}$-Cl) **(5)**

1H NMR (400 MHz, $CDCl_3$): δ = 0.83 (t, 3H, CH_3), 1.22 (m, 14H, $(CH_2)_7$), 1.61 (m, 2H, $COOCH_2CH_2$), 4.04 (s, 3H, NCH_3), 4.13 (t, 2H, $COOCH_2$), 5.43 (s, 2H, NCH_2CO), 7.53 (d, 1H, C_4-H), 7.58 (d, 1H, C_5-H), 10.18 (s, 1H, C_2-H).

White solid (m. p. 74-77 °C)

1-dodecyl-3-methylimidazolium chloride ($IMC_1CH_2COOC_{12}$-Cl) **(6)**

White solid (m. p. 56-58 °C)

1H NMR (400 MHz, $CDCl_3$): δ = 0.86 (t, 3H, CH_3), 1.24 (m, 18H, $(CH_2)_9$), 1.63 (m, 2H, $COOCH_2CH_2$), 4.06 (s, 3H, NCH_3), 4.16 (t, 2H, $COOCH_2$), 5.45 (s, 2H, NCH_2CO), 7.47 (d, 1H, C_4-H), 7.54 (d, 1H, C_5-H), 10.24 (s, 1H, C_2-H).

2.3. Biological evaluation.

2.3.1. *In vitro* cytotoxic activity study.

The cytotoxic activity of studied compounds was evaluated in vitro using the throat cancer Hep-2 cell lines as a test object. The cells were cultivated in RPMI-1640 medium (Sigma, USA) supplemented with cow embryos serum (5%) and antibiotics at 37 °C for 72 h. The cytotoxic activity test was carried out in polystyrene 96-well culture plates (Sarstedt, Germany). 100 µL of cell suspension in a growth medium at cell density ranging 5 x 10^5 cells/mL was introduced into wells of culture plates and cultured at 37 °C in an atmosphere of 5% CO_2 for 24 h until complete cellular monolayer formation.

Studied compounds dissolved in distilled water or 1.5% DMSO to the final concentration of 2000 µg/mL. In a separate plate, serial two-fold and ten-fold dilutions of the studied compounds were prepared. The content of compounds was equal to the concentrations for two-fold dilutions: 1000; 500; 250; 125; 62.5; 32.25; 15.63; 7.81; 3.91; 1.95; µg/mL and for ten-fold dilutions: 200.00, 20.00, 2.00, 0.20, and 0.02 µg/mL. The studied compounds were brought into cultural plate holes with the cell culture in a volume of 100 µL. Cytotoxic effect of compounds was conducted after 24, 48, and 72 h of incubation with the cellular culture at 37 °C under 5% CO_2 using the inverted microscope. The cytotoxic parameter, that is, IC_{50} expressed as the amount of compound (µM) which causes cell degeneration in half of the test objects. The cellular degeneration was determined with reference to the control values (without test compound). Cisplatin [67], as a chemotherapy medication used to treat a number of cancers, was tested as the positive control. DMSO (1.5%) used in our study as a known solvent was tested as the negative control.

2.3.2. *In vivo* acute toxicity assessment.

The acute toxicity test of the investigated compounds to freshwater organism *Daphnia magna* was estimated by calculating the lethal concentration (LC_{50}), which is the concentration of a chemical that kills 50% of the tested organisms. The *D. magna* tests were performed according to the procedures set out in the Organization for Economic Co-operation and Development Guideline 202 [68] in a light incubator with the 22±1°C temperature and 16:8-h light:dark photoperiod. *D. magna* neonates (6-24 h-old) were used for the controls and for the geometric series of concentrations of each test compound according to the 48-h acute toxicity test procedure without food or organic extract. Five neonates were randomly taken and placed in a glass beaker (50mL) containing the test solution (30 mL). The mortality of the neonates in each beaker was observed after 48 h that is the endpoint for effect calculation. Animals that were not able to swim within 15 s after gentle agitation of the test vessel were considered to be immobilized. The sensitivity of the *D. magna* to the reference toxicant potassium dichromate ($K_2Cr_2O_7$) was determined as well.

All experiments were run in triplicate. The LC_{50} values in mg/L with their 95% confidence intervals (CI) were determined using Statistica 7 program. The degree of toxicity of the studied compounds was determined by D.R. Passino with co-authors classification [69].

2.4. Molecular docking.

IL docking was performed using the DNA dodecamer (PDB ID: 1BNA) [70] as a known model structure for studying DNA-oriented biologically active compounds. AutoDock Tools (ADT) 1.5.6 [71] was used to prepare DNA fragments and studied ligands for docking. All polar hydrogens were added to the DNA oligomer by ADT. The Gasteiger method was used for the calculation and addition of partial charges. The prepared DNA-dodecamer was saved in PDBQT format. The ChemAxon Marvin Sketch 5.3.735 program [54] was used to make, optimize, and save the ligand structures in Mol2 format. The ligands energy minimization was conducted by the MOPAC 2016 program [72]. The prepared DNA dodecamer and ligands were used for molecular docking using AutoDock Vina 1.1.2 [73]. A grid box of 30*30*30 points was used with a grid spacing of 1 Å. The analysis and visualization of DNA-ligand interactions were performed by Accelrys DS [74].

3. Results and Discussion

3.1. Results of QSAR modeling.

The initial set of 1196 compounds was split into training (956 compounds) and test (239 compounds) sets following the Kennard-Stone algorithm described in Materials and Methods. The initial number of descriptors was submitted to an additional reduction procedure, as follows: descriptors with constant values were removed, and a pairwise correlation analysis was then performed, whereby a given descriptor was eliminated if its correlation coefficient with another descriptor was equal to or greater than 0.99. As a result of this process, 1016 descriptors were selected.

In the second stage, the descriptors' contribution to the analyzed activity was evaluated, and the number of descriptors was pruned using our Batch Pruning Algorithm [57]. As a result of descriptors pruning, the BPA selected 66 best fitting descriptors out of 1016.

Table 1 summarizes the statistical parameters obtained for the final QSAR model. The full computational details of the proposed approach, including the methods used to analyze the results, can be found elsewhere (section Materials and methods) [57].

QSAR model was first developed based on the training set only, and their accuracy was estimated using the cross-validation techniques (Materials and methods). The q^2 coefficient for the training set was 0.76, RMSE=0.42, MAE=32. In the external test set the compounds were predicted with the accuracy, q^2 = 0.75, RMSE=0.42, MAE=0.32 (Table 1). Deviation of coefficients ensemble did not exceed 0.01.

Table 1. Statistical coefficients calculated using ASNN for series of compounds possessing cytotoxicity against throat cancer Hep-2 cell lines.

Molecule numbers	Amount of descriptors	Data set	q^2	RMSE[a]	MAE[b]
956	66	Training set	0.76±0.01	0.42	0.32
239		Test set	0.75±0.01	0.42	0.32

[a]RMSE – Root Mean Squared Error
[b]MAE – Mean Absolute Error

The results of predictions for ASNN for the training and test set are given in Figure 1. A good correlation between the predicted and the observed values for the test set indicates that the obtained model can be used for predicting the $lg(1/IC_{50})$ within the applicability domain for compounds similar to those in the training and the test sets. In the training set, 97% of predicted values do not differ from the experimental values by more than 1 lg unit. In the test set, also 98% of chemicals have residuals between the experimental and predicted $lg(1/IC_{50})$ lower than 1 lg unit. This result supports the robustness of the proposed model (Figure 1, Table 1).

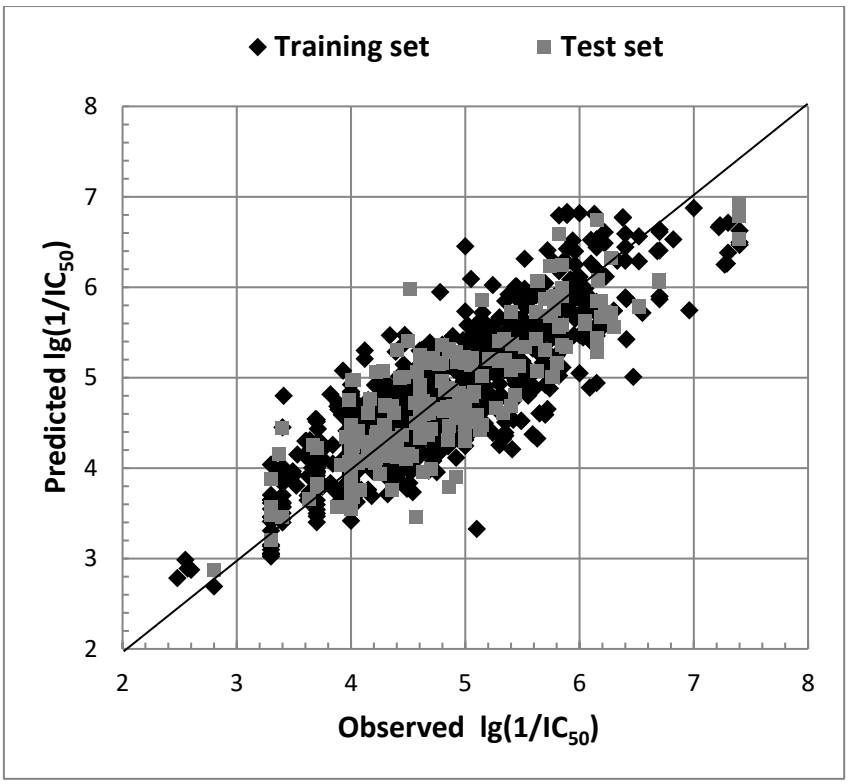


Figure 1. Plots of experimental versus predicted values for the QSAR model data set.

In the present study, we generated virtual sets of drug-like molecules in order to screen potential inhibitors of throat cancer Hep-2 cells. The activity of 12 virtual compounds was predicted using the proposed QSAR model (Supplementary material). The cytotoxic activity

of 6 compounds was predicted lower than 50 µM, and the rest compounds were predicted in the range 50 and 100 µM. The 6 compounds predicted as more active were selected for synthesis and testing. The results of the biological testing confirmed the most QSAR predictions (Table 2).

3.2. Biological evaluation.

3.2.1. *In vitro* evaluating of cytotoxic activity.

Synthesized compounds **1-6** were evaluated *in vitro* toward the throat cancer Hep-2 cell lines. The results of cytotoxic activity of each water-soluble and DMSO-soluble compound are presented in Table 2.

Table 2. Predicted and experimental cytotoxic activity of studied compounds.

№	Compounds	Predicted activity		Biological testing of cytotoxic activity by IC_{50} (µM) values after incubation time (hours)		
		lg(1/IC_{50})	IC_{50} (µM)	24	48	72
1	PyrCH_2COOC_8-Cl	4.31	48.9	3898.85*	1949.4	734.37
				359.43**	**139.54**	**139.54**
2	PyrCH_2COOC_{10}-Cl	4.78	16.6	739.14	297.48	34.13
				122.82	**20.54**	**20.54**
3	PyrCH_2COOC_{12}-Cl	4.88	13.2	ND[a]	ND	ND
				0.181	**0.181**	**0.181**
4	IM$C_1CH_2COOC_8$-Cl	4.55	28.2	472.79	302.22	302.22
				411.58	**263.64**	**263.64**
5	IM$C_1CH_2COOC_{10}$-Cl	4.43	37.1	502.65	412.67	263.5
				80.98	**67.93**	**67.93**
6	IM$C_1CH_2COOC_{12}$-Cl	4.45	35.5	ND	ND	ND
				5.75	**5.75**	**5.75**
7	Cisplatin	ND	ND	44.8	44.8	44.8
				39.77	**39.77**	**39.77**

* – IC_{50} of water-soluble compounds
** – IC_{50} of DMSO-soluble compounds
[a]ND – not determined

The obtained results indicated the highest cytotoxic activity of ester-functionalized pyridinium- and imidazolium ILs with C_{12} alkyl chains. Compounds **3** and **6** dissolved in DMSO have the highest cytotoxic activity with IC_{50} of 0.181 and 5.75 µM for 72 h, respectively, compared with standard anticancer agent cisplatin (IC_{50}=39.77 µM). Moreover, these effects persisted for 24, 48, and 72 hours of the observed experiment.

It is evident from the dose screening data that compound **5** dissolved in DMSO with alkyl chain length C_{10} was more active with imidazolium cation (IC_{50} value of 67.93 µM) than the same compound **4** with C_8 alkyl chain length (IC_{50} value of 263.64 µM).

The same pattern is observed in cytotoxic effects of the pyridinium salts dissolved in DMSO with alkyl chain lengths C_8 and C_{10}. The IC_{50} value of pyridinium salt **1** with C_8 alkyl chain length was 139.54 µM, and the IC_{50} value of pyridinium salt with C_{10} alkyl chain length was 20.54 µM.

Also, it is worth mentioning that compound **2** with alkyl chain length C_{10} and pyridinium cation dissolved in H_2O showed cytotoxicity for 72 h indicated by IC_{50}=34.13 µM. All other compounds dissolved in H_2O do not show any improvement in cytotoxic activity.

3.2.2. In vivo acute toxicity tests.

A series of toxicity tests of the studied compounds was carried out, taking into account the promising results of their biological activity.

The results of toxicological effects of studied compounds on *D. magna* assessed by measuring their lethal effect after 48 hours are presented in Table 3.

Table 3. Acute toxicity of the studied compounds on the mortality of *D. magna.*

№	Compounds	LC_{50} (48h, mg/L)	95% CI
1	$PyrCH_2COOC_8$-Cl	13.02 ± 01.71	9.49-16.55
2	$PyrCH_2COOC_{10}$-Cl	5.82 ± 0.63	4.51-7.14
3	$PyrCH_2COOC_{12}$-Cl	0.57 ± 0.11	0.33-0.79
4	$IMC_1CH_2COOC_8$-Cl	2.13 ± 0.63	0.85-3.40
5	$IMC_1CH_2COOC_{10}$-Cl	0.83 ± 0.20	0.42-1.24
6	$IMC_1CH_2COOC_{12}$-Cl	0.074 ± 0.018	0.037-0.11
7	Cisplatin	0.15 ± 0.03	0.082-0.22

The acute toxicity results of tested ILs toward *D. magna* indicated the dependence of toxicity level on ILs structure (Table 2). The increase of the alkyl chain length from C_8 to C_{12} of all compounds led to the gradual increase of the toxicity level. Thus, the acute toxicity of compounds with C_8 species increased from LC_{50} values 13.02 and 2.13 mg/L to LC_{50} values 0.57 and 0.074 mg/L of compounds with C_{12} species, respectively. It should be noted that ILs based on pyridinium cation turned out to be the least toxic in contrast with ILs based on imidazolium cation. Generally, according to classification D.R. Passino and S.B. Smith studied ILs in the *D. magna* tests were slightly toxic with LC_{50}=13.02 mg/L (IL **1**), moderately toxic with the range of LC_{50} from 2.13 to 5.82 mg/L (IL **2** and IL **4**), highly toxic with LC_{50}=0.57-0.83 mg/L (IL **3** and IL **5**) and extremely toxic with LC_{50} 0.074 mg/L (IL **6**) compared to highly toxic cisplatin (LC_{50}=0.15 mg/L).

3.3. Docking study.

To analyze the potential interaction mechanisms of the most active ligands **3** and **6**, molecular docking was performed in two different regions of the DNA-oligomer 1BNA (Figure 2,3). The features of the formed DNA ligand complexes are presented in Table 4.

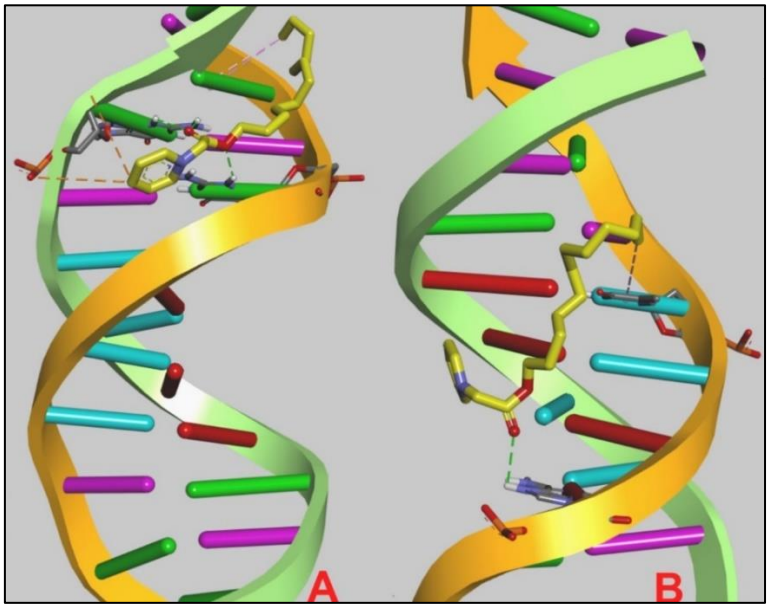


Figure 2. Docking of ligand **3** into the (**A**) CG; (**B**) AT base pair regions of DNA oligonucleotide.

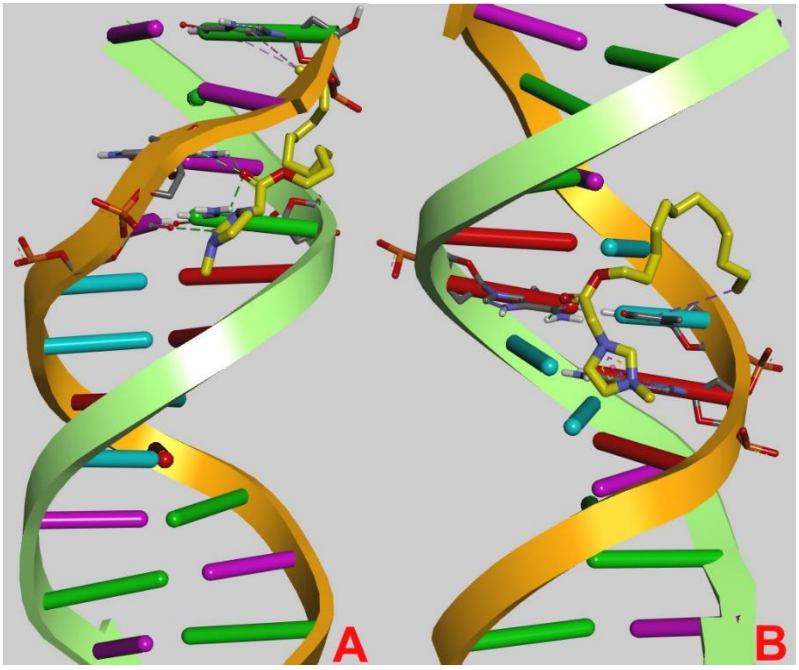


Figure 3. Docking ligand **6** into the (**A**) CG; (**B**) AT base pair regions of DNA oligonucleotide.

Table 4. Comparative characteristics of the ligands' interactions with different DNA base pairs.

Compound /region DNA	ΔG, (kcal/mol)	Hydrogen bonds	Electrostatic interaction	Hydrophobic interactions
3/A	− 6.8	DG10 (2.46Å) DG10 (2.07Å) DG16 (2.25Å)	DG10 (5.44Å) DC11 (5.47Å)	DG14 (5.22Å) DG14 (5.30Å)
3/B	− 5.1	DA17 (2.92Å)		DT20 (5.48Å)
6/A	− 6.7	DG10 (2.21Å) DG10 (2.68Å) DG16 (2.24Å) DG9 (3.54Å)		DG12 (5.38Å) DG12 (5.00Å)
6/B	− 5.0	DA6 (2.38Å)		DA18 (4.81Å) DT19 (4.89Å)

The docking results indicate that the CG region of the DNA-oligonucleotide is the most energetically favorable for the complexation of the studied ligands (Figure 2,3 and Table 4). The formation of ligand-DNA complexes is accompanied by estimated binding energies in the ranges from −6.7 to −6.8 kcal/mol (CG base pair region) and from −5.0 to −5.1 kcal/mol (AT base pair region). Also, the ligand-DNA complexes in the CG region stabilize by multiple hydrogen bonds (2.07− 2.46Å), electrostatic (5.44− 5.47Å) and hydrophobic (5.00− 5.38Å) interactions. At the same time, the ligand-DNA complexes in the AT region were stabilized by only hydrogen bonds (2.38−2.92Å) and hydrophobic (4.81−5.48Å) interactions. The key role in complexation in the CG base pair region belongs to DG9, DG10, DC11, DG12, DG14, DG16 nucleotide bases of DNA.

4. Conclusions

In this study, long-chain pyridinium- and imidazolium-based ionic liquids, comprising polar ester groups in the alkyl substituents, have been designed, synthesized, and evaluated *in vitro* and *in vivo* as potential anticancer agents. The preliminary prediction of cytotoxic activity of ionic liquids by constructed regression QSAR model revealed the most active compounds from a small set of virtual compounds for synthesis and *in vitro* testing. The obtained results indicated that most studied compounds showed a significant cytotoxic effect on the human

Hep-2 cell line. Ester-functionalized ILs based on imidazolium and pyridinium cation with C_{12} and C_{10} alkyl chain length demonstrated high cytotoxic potential on Hep-2 cell line and different acute toxicity levels to aquatic commonly used model organism *D. magna*. It should be noted that salts **3** and **6** (IC_{50} = 0.181 µM and 5.75 µM) showed extremely potent cytotoxicity compared to cisplatin (IC_{50}=39.77 µM). The acute toxicity results of tested ILs displayed that in *D. magna* tests in contrast to highly toxic cisplatin, compounds **1-5** were less toxic (slightly toxic, moderately toxic, and highly toxic) except extremely toxic compound **6** according to classification D.R. Passino and S.B. Smith. The established ILs properties are associated with their structural features. The degree of hydrophobicity of the alkyl chain and cationic type of functionalized salts are important in their activity potential as highly active and low toxic anticancer agents with specific DNA binding mechanisms associated with the CG base pair region.

Funding

This research received no external funding.

Acknowledgments

This research has no acknowledgment.

Conflicts of Interest

The authors declare no conflict of interest

References

1. Pucci, C.; Martinelli, C.; Ciofani, G. Innovative approaches for cancer treatment: Current perspectives and new challenges. *Ecancermedicalscience* **2019**, *13*, 961, https://doi.org/10.3332/ecancer.2019.961.
2. Chikara, S.; Nagaprashantha, L.D.; Singhal, J.; Horne, D.; Awasthi, S.; Singhal, S.S. Oxidative stress and dietaryphytochemicals: Role in cancer chemoprevention and treatment. *Cancer Lett.* **2018**, *413*, 122-134, https://doi.org/10.1016/j.canlet.2017.11.002.
3. Kurzrock, R.; Kantarjian, H.M.; Kesselheim, A.S.; Sigal, E.V. New drug approvals in oncology. *Nature Reviews Clinical Oncology* **2020**, *17*, 140-146, https://doi.org/10.1038/s41571-019-0313-2.
4. Wan, M.; Zhang, L.; Chen, Y.; Li, Q.; Fan, W.; Xue, Q.; Yan, F.; Song, W. Synthesis and Anticancer Activity Evaluation of Novel Phenanthridine Derivatives. *Front. Oncol.* **2019**, *9*, 274, https://doi.org/10.3389/fonc.2019.00274.
5. Haq, S.H.; Al-Ruwaished, G.; Al-Mutlaq, M.A.; Naji, S.A.; Al-Mogren, M.; Al-Rashed, S.; Ain, Q.T.; Al-Amro, A.A.; Al-Mussallam, A. Antioxidant, Anticancer Activity and Phytochemical Analysis of Green Algae, Chaetomorpha Collected from the Arabian Gulf. *Sci. Rep.* **2019**, *9*, 18906, https://doi.org/10.1038/s41598-019-55309-1.
6. Pedro, S.N.; Freire, C.S.R.; Silvestreand, AJ.D.l Freire M.G. The Role of Ionic Liquids in the Pharmaceutical Field:An Overview of Relevant Applications. *Int. J. Mol. Sci.* **2020**, *21*, 8298, https://doi.org/10.3390/ijms21218298.
7. Shamshina, J.L.; Berton, P.; Wang, H.; Zhou, X.; Gurau, G.; Rogers, RD. Ionic Liquids in Pharmaceutical Industry. *Green Techniques for Organic Synthesis and Medicinal Chemistry* **2018**, https://doi.org/10.1002/9781119288152.ch20.
8. Amaral, M.; Pereiro, A.B.; Gaspar, M.M;. Reis, C.P. Recent advances in ionic liquids and nanotechnology for drug delivery. *Nanomedicine (Lond)* **2021**, *16*, 63-80, https://doi.org/10.2217/nnm-2020-0340.
9. Ferraz, R.; Silva, D.; Dias, A.; Dias, V.; Santos, M.M.; Pinheiro, L.; Prudêncio, C.; Noronha, J.; Petrovski, Ž.; Branco, L. Synthesis and Antibacterial Activity of Ionic Liquids and Organic Salts Based on Penicillin G and Amoxicillin hydrolysate Derivatives against Resistant Bacteria. *Pharmaceutics* **2020**, *12*, https://doi.org/10.3390/pharmaceutics12030221.

10. Karaman, M.;Vraneš, M.; Tot, A.; Papović, S.; Miljaković, D.; Gadžurić, S.; Ignjatov, M. Ionic liquids as potentially new antifungal agents against Alternaria species. *RSC Advances* **2020**, *10*, 22318-22323, https://doi.org/10.1039/D0RA02475A.
11. Kiran Kumar Reddy, G.; Nancharaiah, Y.V. Alkylimidazolium Ionic Liquids as Antifungal Alternatives: Antibiofilm Activity Against Candida albicans and Underlying Mechanism of Action. *Frontiers in Microbiology* **2020**, *11*, https://doi.org/10.3389/fmicb.2020.00730.
12. Jovanović-Šanta, S. Anticancer and antimicrobial properties of imidazolium based ionic liquids with salicylate anion. *J. Serb. Chem. Soc*. **2020**, *85*, 291-303, https://doi.org/10.2298/JSC190717098J.
13. Rahman, M.; O'Donnell, J.M.; Brazel, C.S. Cytotoxicity of Plasticizers and Ionic Liquids Using Drosophila melanogaster S2 Cell Culture. *Chem. Eng. Technol*. **2011**, *34*, 429–438, https://doi.org/10.1002/ceat.201000199.
14. Radošević, K.; Železnjak, J.; Cvjetko Bubalo, M.; Radojčić Redovniković, I.; Slivac, I.; Gaurina Srček, V. Comparative In Vitro Study of Cholinium-Based Ionic Liquids and Deep Eutectic Solvents toward Fish Cell Line. *Ecotoxicol. Environ. Saf.* **2016**, *131*, 30-36, https://doi.org/10.1016/j.ecoenv.2016.05.005.
15. Egorova, K.S.; Seitkalieva, M.M.; Posvyatenko, A.V.; Ananikov, V.P. An Unexpected Increase of Toxicity of Amino Acid-Containing Ionic Liquids. *Toxicol. Res*. **2015**, *4*, 152-159, https://doi.org/10.1039/C4TX00079J.
16. Yu, J.; Zhang, S.; Dai, Y.; Lu, X.; Lei, Q.; Fang, W. Antimicrobial Activity and Cytotoxicity of Piperazinium- and Guanidinium-Based Ionic Liquids *J. Hazard. Mater*. **2016**, *307*, 73-81, https://doi.org/10.1016/j.jhazmat.2015.12.028.
17. Steudte, S.; Stepnowski, P.; Cho, C.W.; Thöming, J.; Stolte, S. (Eco)toxicity of Fuoro-Organic and Cyano-Based Ionic Liquid Anions. *Chem. Commun.* **2012**, *48*, 9382-9384, https://doi.org/10.1039/c2cc34955h.
18. Li, X.Y.; Jing, C.Q.; Zang, X.Y.; Yang, S.; Wang, J.J. Toxic Cytological Alteration and Mitochondrial Dysfunction in PC12 Cells Induced by 1-octyl-3-methylimidazolium Chloride. *Toxicol. In Vitro*. **2012**, *26*, 1087–1092, https://doi.org/10.1016/j.tiv.2012.07.006.
19. Malhotra, S.V.; Kumar, V.A. Profile of the In vitro Anti-Tumor Activity of Imidazolium-Based Ionic Liquids. *Bioorg. Med. Chem. Lett*. **2010**, *20*, 581-585, https://doi.org/10.1016/j.bmcl.2009.11.085.
20. Malhotra, S.V.; Kumar, V.; Velez, C.; Zayas, B. Imidazolium-Derived Ionic Salts Induce Inhibition of Cancerous Cell Growth through Apoptosis. *MedChemComm*. **2014**, *5*, 1404-1409, https://doi.org/10.1039/C4MD00161C.
21. Egorova, K.S.; Seitkalieva, M.M.; Posvyatenko, A.V.; Khrustalev, V.N.; Ananikov, V.P. Cytotoxic Activity of Salicylic Acid-Containing Drug Models with Ionic and Covalent Binding ACS Med. *Chem. Lett*. **2015**, *6*, 1099-1104, https://doi.org/10.1021/acsmedchemlett.5b00258.
22. Gouveia, W.; Jorge, T.F.; Martins, S.; Meireles, M.; Carolino, M.; Cruz, C.; Almeida, T.V.; Araújo, M.E.M. Toxicity of ionic liquids prepared from biomaterials. *Chemosphere* **2014**, *104*, 51-56, https://doi.org/10.1016/j.chemosphere.2013.10.055.
23. Messali, M.; Almtiri, M.N.; Abderrahman, B.; Salghi, R.; Aouad, M.R.; Alshahateet, S.F.; Ali, A.A.S. New pyridazinium-based ionic liquids: An eco-friendly ultrasound-assisted synthesis, characterization and biological activity. *S. Afr. J. Chem.* **2015**, *68*, 219-225, https://doi.org/10.17159/0379-4350/2015/v68a30.
24. Wang, C.L.; Zhu, X.W.; Liu, S.S. Toxicity Studies of Ionic Liquids and Heavy Metal Compounds to MCF-7 and Photobacteria Q67. *Adv. Mater. Res*. **2013**, *610-613*, 721-724, https://doi.org/10.4028/www.scientific.net/AMR.610-613.721.
25. Kaushik, N.K.; Attri, P.; Kaushik, N.; Choi, E.H. Synthesis and Antiproliferative Activity of Ammonium and Imidazolium Ionic Liquids against T98G Brain Cancer Cells. *Molecules* **2012**, *17*, 13727-13739, https://doi.org/10.3390/molecules171213727.
26. Kumar, V.; Malhotra, S.V. Study on the Potential Anti-Cancer Activity of Phosphonium and Ammonium-Based Ionic Liquids. *Bioorg. Med. Chem. Lett*. **2009**, *19*, 4643-4646, https://doi.org/10.1016/j.bmcl.2009.06.086.
27. Flieger, J.; Flieger, M. Ionic Liquids Toxicity-Benefits and Threats. *Int J Mol Sci*. **2020**, *21*, 6267, https://doi.org/10.3390/ijms21176267.
28. Egorova, K.S.; Seitkalieva, M.M.; Posvyatenko, A.V.; Ananikov, V.P. An Unexpected Increase of Toxicity of Amino Acid-Containing Ionic Liquids. *Toxicol. Res*. **2015**, *4*, 152-159, https://doi.org/10.1039/C4TX00079J.
29. Pérez, S.A.; Montalbán, M.G.; Carissimi, G.; Licence, P.; Víllora, G. *In vitro* cytotoxicity assessment of monocationic and dicationic pyridinium-based ionic liquids on HeLa, MCF-7, BGM and EA.hy926 cell lines. *Journal of Hazardous Materials* **2020**, *385*, 121513, https://doi.org/10.1016/j.jhazmat.2019.121513.
30. Gal, N.; Malferrari, D.; Kolusheva, S.; Galletti, P.; Tagliavini, E.; Jelinek, R. Membrane Interactions of Ionic Liquids: Possible Determinants for Biological Activity and Toxicity. *Biochim. Biophys. Acta* **2012**, *1818*, 2967-2974, https://doi.org/10.1016/j.bbamem.2012.07.025.

31. Jing, B.; Lan, N.; Qiu, J.; Zhu, Y. Interaction of Ionic Liquids with a Lipid Bilayer: A Biophysical Study of Ionic Liquid Cytotoxicity. *J. Phys. Chem. B* **2016**, *120*, 2781-2789, https://doi.org/10.1021/acs.jpcb.6b00362.
32. Benedetto, A.; Ballone, P. Room Temperature Ionic Liquids Interacting with Bio-Molecules: An Overview of Experimental and Computational Studies. *Philos. Mag*. **2016**, *96*, 870-894, https://doi.org/10.1080/14786435.2015.1119323.
33. McLaughlin, M.; Earle, M.J.; Gîlea, M.A.; Gilmore, B.F.; Gorman, S.P.; Seddon, K.R. Cytotoxicity of 1-Alkylquinolinium Bromide Ionic Liquids in Murine Fibroblast NIH 3T3 Cells. *Green Chem*. **2011**, *13*, 2794-2800, https://doi.org/10.1039/c0gc00813c.
34. Li, X.Y.; Jing, C.Q.; Lei, W.L.; Li, J.; Wang, J.J. Apoptosis Caused by Imidazolium-Based Ionic Liquids in PC12 Cells. *Ecotoxicol. Environ. Saf.* **2012,** *83*, 102-107, https://doi.org/10.1016/j.ecoenv.2012.06.013.
35. Wang, X.; Ohlin, C.A.; Lu, Q.; Fei, Z.; Hu, J.; Dyson, P.J. Cytotoxicity of Ionic Liquids and Precursor Compounds towards Human Cell Line HeLa. *Green Chem*. **2007**, *9*, 1191-1197, https://doi.org/10.1039/b704503d.
36. Li, X.; Ma, J.; Wang, J. Cytotoxicity, Oxidative Stress, and Apoptosis in HepG2 Cells Induced by Ionic Liquid 1-methyl-3-octylimidazolium Bromide. *Ecotoxicol. Environ. Saf.* **2015**, *120*, 342-348, https://doi.org/10.1016/j.ecoenv.2015.06.018.
37. Li, X.; Ma, J.; Jing, C.; Wang, J. Expression Alterations of Cytochromes P4501A1, 2E1 and 3A, and Their Receptors AhR and PXR Caused by 1-Octyl-3-methylimidazolium Chloride in Mouse Mammary Carcinoma Cells. *Chemosphere* **2013**, *93*, 2488-2492, https://doi.org/10.1016/j.chemosphere.2013.08.092.
38. Rezki, N.; Al-Blewi, F.F.; Al-Sodies, S.A.; Alnuzha, A.K.; Messali, M.; Ali, I.; Aouad, M.R. Synthesis, Characterization, DNA Binding, Anticancer, and Molecular Docking Studies of Novel Imidazolium-Based Ionic Liquids with Fluorinated Phenylacetamide Tethers. *ACS Omega* **2020**, *10*, 4807-4815, https://doi.org/10.1021/acsomega.9b03468.
39. Bonsignore, R.; Notaro, A.; Salvo, A.M.P.; Spinello, A.; Fiasconaro, G.; Terenzi, A.; Giacalone, F.; Keppler, B.K.; Giuliano, M.; Gruttadauria, M.; Barone, G. DNA-Binding and Anticancer Activity of Pyrene-Imidazolium Derivatives. *ChemistrySelect* **2016**, *1*, 6755-6761, https://doi.org/10.1002/slct.201601502.
40. Al-Sodies, S.; Aouad, M.; Ihmaid, S.; Aljuhani, A.; Messali, M.; Ali, I.; Rezki, N. Microwave and conventional synthesis of ester based dicationic pyridinium ionic liquids carrying hydrazone linkage: DNA binding, anticancer and docking studies. *J. Mol. Struct*. **2020**, *1207*, 127756, https://doi.org/10.1016/j.molstruc.2020.127756.
41. Chen, H-L.; Kao, H-F.; Wang, J-Y.; Wei, G-T. Cytotoxicity of imidazole ionic liquids in human lung carcinoma A549 cell line. *J. Chin. Chem. Soc*. **2014**, *61*, 763-769, https://doi.org/10.1002/jccs.201300632.
42. Marrucho, I.M.; Branco, L.C.; Rebelo, L.P.N. Ionic liquids in pharmaceutical applications. *Annu. Rev. Chem. Biomol. Eng*. **2014**, *5*, 527-546, https://doi.org/10.1146/annurev-chembioeng-060713-040024.
43. Przestalski, S.; Sarapuk, J.; Kleszczyńska, H.; Gabrielska, J.; Hładyszowski, J.; Trela, Z.; Kuczera, J. Influence of amphiphilic compounds on membranes. *Acta Biochim Pol*. **2000**, *47*, 627-638.
44. Stolte, S.; Matzke, M.; Arning, J.; Böschen, A.; Pitner, W.-R.; Welz-Biermann, U.; Jastorff, B.; Ranke, J. Effects of different head groups and functionalised side chains on the aquatic toxicity of ionic liquids. *Green Chem.* **2007**, *9*, 1170-1179, https://doi.org/10.1039/B711119C.
45. Trush, M.; Metelytsia, L.; Semenyuta, I.; Kalashnikova, L.; Papeykin, O.; Venger, I.; Tarasyuk, O.; Bodachivska, L.; Blagodatnyi, V.; Rogalsky, S. Reduced ecotoxicity and improved biodegradability of cationic biocides based on ester-functionalized pyridinium ionic liquids. *Environmental Science and Pollution Research* **2019**, *26*, 4878-4889, https://doi.org/10.1007/s11356-018-3924-8.
46. Torrecilla, J.S.; Garcia, J.; Rojo, E.; Rodriguez, F. Estimation of Toxicity of Ionic Liquids in Leukemia Rat Cell Line and Acetylcholinesterase Enzyme by Principal Component Analysis, Neural Networks and Multiple Lineal Regressions. *J. Hazard. Mater*. **2009**, *164*, 182-194, https://doi.org/10.1016/j.jhazmat.2008.08.022.
47. Fatemi, M.H.; Izadiyan, P. Cytotoxicity Estimation of Ionic Liquids Based on Their Effective Structural Features. *Chemosphere* **2011**, *84*, 553-563, https://doi.org/10.1016/j.chemosphere.2011.04.021.
48. Paternò, A.; D'Anna, F.; Musumarra, G.; Noto, R.; Scirè, S. A Multivariate Insight into Ionic Liquids Toxicities. *RSC Adv*. **2014**, *4*, 23985-24000, https://doi.org/10.1039/c4ra03230f.
49. Sosnowska, A.; Barycki, M.; Zaborowska, M.; Rybinska, A.; Puzyn, T. Towards Designing Environmentally Safe Ionic Liquids: the Influence of the Cation Structure. *Green Chem*. **2014**, *16*, 4749-4757, https://doi.org/10.1039/C4GC00526K.
50. De Melo, E.B. A Structure-Activity Relationship Study of the Toxicity of Ionic Liquids Using an Adapted Ferreira-Kiralj Hydrophobicity Parameter Phys. *Chem. Chem. Phys*. **2015**, *17*, 4516-4523, https://doi.org/10.1039/C4CP04142A.
51. ChEMBL. https://www.ebi.ac.uk/chembl/ (accessed on 12 January **2021**).
52. Kennard, R.W.; Stone, L.A. Computer aided design of experiments. *Technometrics* **1969**, *11*, 137-147, https://doi.org/10.2307/1266770.

53. Kovalishyn, V.; Kopernyk, I.; Chumachenko, S.; Shablykin, O.; Kondratyuk, K.; Pil'o, S.; Prokopenko, V.; Brovarets, V.; Metelytsia, L. QSAR studies, design, synthesis and antimicrobial evaluation of azole derivatives. *Comput. Biol. Bioinfor* **2014**, *2*, 25-32, https://doi.org/10.11648/j.cbb.20140202.12.
54. ChemAxon. https://www.chemaxon.com/ (accessed on 12 January **2021**).
55. Talete SRL. http://www.talete.mi.it/products/dragon_description.htm (accessed on 1 April **2020**).
56. Todeschini, R.; Consonni, V. Handbook of Molecular Descriptors. Weinheim: Wiley-VCH Verlag GmbH; **2008**.
57. Kovalishyn, V.; Poda, G. Efficient Variable Selection Batch Pruning Algorithm for Artificial Neural Networks. *Int. Lab. Sys*. **2015**, *149*, 10-16, https://doi.org/10.1016/j.chemolab.2015.10.005.
58. Tetko, I.V. Neural network studies. 4. Introduction to associative neural network. *J. Chem. Inf. Comput. Sci*. **2002**, *42*, 717–728, https://doi.org/10.1021/ci010379o.
59. Kohonen, T. Self-Organizing Maps. Berlin: Springer-Verlag; **2001**; 501, http://dx.doi.org/10.1007/978-3-642-56927-2.
60. Tetko, I.V.; Villa, A.E.P.; Livingstone, D.J. Neural network studies. 2. Variable selection. *J. Chem. Inf. Comput. Sci*. **1996**, *36*, 794-803, https://doi.org/10.1021/ci950204c.
61. Kovalishyn, V.V.; Tetko, I.V.; Luik, A.I.; Kholodovych, V.V.; Villa, A.E.P.; Livingstone, D.J. Neural network studies. 3. Variable selection in the cascade-correlation learning architecture. *J. Chem. Inf. Comput. Sci*. **1998**, *38*, 651-659, https://doi.org/10.1021/ci980325n.
62. Dasarathy, B.V. Nearest neighbor (NN) norms: NN pattern classification techniques. Washington: *IEEE Computer Society Press*; **1991**, 447.
63. Tetko, I.V.; Livingstone, D.J.; Luik, A.I. Neural Network Studies. 1. Comparison of Overfitting and Overtraining. *J. Chem. Inf. Comput. Sci*. **1995**, *35*, 826-833, https://doi.org/10.1021/ci00027a006.
64. Tollenaere, T. Super SAB: Fast adaptive back propagation with good scaling properties. *Neural Networks*. **1990**, *3*, 561–573, https://doi.org/10.1016/0893-6080(90)90006-7.
65. Johnson, J.L.; Leone, F.C. Statistic and Experimental Design in Engineering and the Physical Sciences. New York: *John Wiley & Sons*; **1977**.
66. Cramer, R.D.; Patterson, D.E.; Bunce, J.D. Comparative molecular field analysis (CoMFA). 1. Effect of shape on binding of steroids to carrier proteins. *J Am Chem Soc*. **1988**, *110*, 5959-67, https://doi.org/10.1021/ja00226a005.
67. Aldossary S.A. Review on Pharmacology of Cisplatin: Clinical Use, Toxicity and Mechanism of Resistance of Cisplatin. *Biomed Pharmacol J* **2019**, *12*, https://dx.doi.org/10.13005/bpj/1608.
68. OECD. OECD Guidelines for the testing of chemicals, Section 2: Effects on Biotic Systems. Test No. 202: Daphnia sp. Acute Immobilisation Test. **2004**, https://doi.org/10.1787/20745761.
69. Passino, D.R.; Smith, S.B. Acute bioassays and hazard evaluation of representative contaminants detected in Great Lakes fish. *Environ Toxicol Chem*. **1987**, *6*, 901-7, https://doi.org/10.1002/etc.5620061111.
70. Protein Data Bank. http://www.rcsb.org/structure/1BNA (accessed on 1 February **2021**).
71. Sanner, M.F. Python: A programming language for software integration and development. *J. Mol. Graph. Model*. **1999**, *17*, 57-61.
72. Stewart, J.J.P. MOPAC2016. Stewart Computational Chemistry. Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2016). (accessed on 1 February **2021**).
73. Trott, O.; Olson, A.J. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. *J. Comput. Chem*. **2010**, *31*, 455-461, https://doi.org/10.1002/jcc.21334.
74. Dassault Systèmes BIOVIA. Discovery Studio Visualizer, v4.0.100.13345. San Diego: Dassault Systèmes; **2020**.

Supplementary materials

Table S1. Initial data set.

NAME	SMILE	lg(1/IC50)
1	ONC(=O)NC(C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1	4,08
2	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,21
3	CCC(C)C(NC(=O)NO)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,45
4	O=C(NC1CCCC1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,02
5	ONC(=O)NC(C(=O)NCC1=CC=CC=C1)C1=CC=CC=C1	4,49
6	O=C(NC(C1=CC=CC=C1)C1=CC=CC=C1)C(NC(=O)N1N=NC2=CC=CC=C12)C1=CC=CC=C1	4,23
7	CC(C)C(NC(=O)NO)C(=O)NC1CCCC1	4,48
8	O=C(NC(C(=O)N1CCCCC1)C1=CC=CC=C1)N1N=NC2=C1C=CC=C2	4
9	CC(C)C1NC(=O)N(C2CCCC2)C1=O	4,01
10	O=C1NC(C(=O)N1CC1=CC=CC=C1)C1=CC=CC=C1	4,08
11	O=C(NC(CC1=CC=CC=C1)C(=O)N1CCCC1)N1N=NC2=CC=CC=C12	4
12	ONC(=O)NC(C(=O)N1CCCCC1)C1=CC=CC=C1	4
13	O=C(NCC1=CC=CC=C1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,09
14	CC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCCC1	4,22
15	O=C(NC(C1=CC=CC=C1)C1=CC=CC=C1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,39
16	O=C1NC(C(=O)N1C1CCCC1)C1=CC=CC=C1	4
17	CCC(C)C(NC(=O)NO)C(=O)NC1CCCCC1	4
18	O=C(NC1CCCCC1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,19
19	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC1CCCCC1	4,03
20	CCC(C)C(NC(=O)NO)C(=O)NC1CCCC1	4
21	ONC(=O)NC(CC1=CC=CC=C1)C(=O)N1CCCC1	4
22	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,26
23	O=C(NC1CCCCC1)C(NC(=O)N1N=NC2=C1C=CC=C2)C1=CC=CC=C1	4,16
24	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCCC1	4,24
25	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCC1	4,25
26	CCC(C)C1NC(=O)N(C2CCCCC2)C1=O	4,16
27	CC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCC1	4,22
28	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC1CCCC1	4
29	CC(C)C(NC(=O)NO)C(=O)NC1CCCCC1	4
30	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NCC1=CC=CC=C1	4
31	O=C(NCC1CCCCC1)C(NC(=O)N1N=NC2=C1C=CC=C2)C1=CC=CC=C1	4,16
32	ONC(=O)NC(C(=O)NC1=CC=CC=C1)C1=CC=CC=C1	4
33	CCC(C)C(NC(=O)NO)C(=O)NCC1=CC=CC=C1	4
34	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NCC1=CC=CC=C1	4
35	CC(C)C1NC(=O)N(C2CCCCC2)C1=O	4
36	CCC(C)C1NC(=O)N(C2CCCC2)C1=O	4
37	CCC(C)C1NC(=O)N(CC2=CC=CC=C2)C1=O	4,33
38	CC(C)\N=C(\N)C1=CC=C2N=C(O)C3=C(C4=C(S3)C=C(C=C4)C#N)C2=C1	4
39	CC1=CC=C(NC(=O)C2=C(Cl)C3=CC=C(C=C3S2)C#N)C=C1	4
40	COC(=O)C1=CC=C2N=C(O)C3=C(C4=C(S3)C=C(C=C4)C(=N)NC(C)C)C2=C1	4,01
41	CC(C)\N=C(\N)C1=CC=C(NC(=O)C2=C(Cl)C3=CC=CC=C3S2)C=C1	4,82
42	ClC1=C(SC2=CC=CC=C12)C(=O)NC1=CC=C(C=C1)C#N	5,19
43	CC(C)\N=C(\N)C1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=C(C)C=C3)C=C1	5,4
44	COC(=O)C1=CC=C(NC(=O)C2=C(Cl)C3=CC=C(C=C3S2)C#N)C=C1	4,23
45	CC(C)\N=C(\N)C1=CC=C2C(SC(C(=O)NC3=CC=CC=C3)=C2Cl)=C1	4,62
46	COC1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=C(C=C3)C#N)C=C1	4,32
47	CC(C)\N=C(\N)C1=CC=C2N=C(O)C3=C(C4=C(S3)C=C(C)C=C4)C2=C1	5,07
48	CC(C)\N=C(\N)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=CC=C12	4,68
49	COC1=CC=C2C(Cl)=C(SC2=C1)C(=O)NC1=CC=C(C=C1)C(=N)NC(C)C	5,59
50	CC(C)\N=C(\N)C1=CC2=C(C=C1)N=C(O)C1=C2C2=CC=C(C=C2S1)C(\N)=N/C(C)C	4
51	COC1=CC=C2C(SC3=C2C2=C(C=CC(=C2)C(=N)NC(C)C)N=C3O)=C1	4,46
52	CC(C)\N=C(\N)C1=CC=C(NC(=O)C2=C(Cl)C3=CC=C(C=C3S2)C(\N)=N/C(C)C)C=C1	4,17
53	CC(C)\N=C(\N)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=C(Br)C=C12	5,01
54	CC(C)\N=C(\N)C1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=C(Br)C=C3)C=C1	5,63
55	CC(C)\N=C(\N)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=C(C)C=C12	5,07
56	COC(=O)C1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=CC=C3)C=C1	4
57	COC(=O)C1=CC=C2C(Cl)=C(SC2=C1)C(=O)NC1=CC=CC=C1	4
58	CC(C)\N=C(\N)C1=CC=C2N=C(O)C3=C(C4=C(S3)C=CC=C4)C2=C1	4,78
59	COC(=O)C1=CC=C2C(Cl)=C(SC2=C1)C(=O)NC1=CC=C(C=C1)C(=N)NC(C)C	5,27
60	CC(C)\N=C(\N)C1=CC=C2N=C(O)C3=C(C4=C(S3)C=C(Br)C=C4)C2=C1	5,16
61	CC(C)\N=C(\N)C1=CC=C(NC(=O)C2=C(Cl)C3=CC=C(C=C3S2)C#N)C=C1	4,68
62	COC1=CC=C(NC(=O)C2=C(Cl)C3=CC=C(C=C3S2)C(=N)NC(C)C)C=C1	5,01
63	COC(=O)C1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=C(C=C3)C(=N)NC(C)C)C=C1	5,09
64	CC(C)\N=C(\N)C1=CC=C2C(Cl)=C(SC2=C1)C(=O)NC1=CC=C(Br)C=C1	5,5
65	CC(C)\N=C(\N)C1=CC=C2C(SC(C(=O)NC3=CC=C(C)C=C3)=C2Cl)=C1	5,53
66	ClC1=C(SC2=CC(=CC=C12)C#N)C(=O)NC1=CC=C(Br)C=C1	4
67	COC(=O)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=C(C=C12)C(=N)NC(C)C	4,34
68	ClC1=C(SC2=CC(=CC=C12)C#N)C(=O)NC1=CC=CC=C1	6,16
69	CC(=O)OCCON1C=NC2=C(S)N=C(N)N=C12	5,31
70	CC(=O)OCCON1C=NC2=C(Cl)N=C(N)N=C12	3,3
71	CC(O)N1C=NC2=C(Cl)N=C(I)N=C12	3,3

NAME	SMILE	lg(1/IC50)
72	CC(OC(C)=O)N1C=NC2=C(S)N=C(N)N=C12	5
73	CC(OC(C)=O)N1C=NC2=C(S)N=C(F)N=C12	3,7
74	CC(O)N1C=NC2=C(N)N=C(I)N=C12	3,3
75	CC(O)CN1C=NC2=C1N=C(N)N=C2F	4,2
76	OCCON1C=NC2=C(S)N=C(F)N=C12	3,3
77	NC1=C2N=CN(OCCO)C2=NC(I)=N1	3,3
78	CC(=O)OCCON1C=NC2=C(S)N=C(F)N=C12	3,3
79	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(F)N=C12	5
80	CC(O)N1C=NC2=C(S)N=C(F)N=C12	3,3
81	COC1=C2N=CN(OCCO)C2=NC(I)=N1	3,3
82	CC(OC(C)=O)N1C=NC2=C(N)N=C(I)N=C12	3,3
83	CC(=O)OCCON1C=NC2=C(Cl)N=C(I)N=C12	4,25
84	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(I)N=C12	5,2
85	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(N)N=C12	3,3
86	CCOC(=O)NC1=CC(NC(C2=CC=CC=C2)C2=CC=CC=C2)=C(N)C(N)=N1	6,59
87	CC1=CN([C@H]2C[C@H](O)[C@@H](CO)S2)C(=O)NC1=O	6,85
88	OC[C@H]1S[C@H](C[C@@H]1O)N1C=CC(=O)NC1=O	5,68
89	CC1=CN([C@@H]2C[C@H](O)[C@@H](CO)S2)C(=O)NC1=O	4,6
90	NC1=NC(=O)N(C=C1)[C@H]1C[C@H](O)[C@@H](CO)S1	6,7
91	NC1=NC(=O)N(C=C1)C1C[C@H](O)[C@@H](CO)S1	6,7
92	NC1=NC(Cl)=NC2=C1N=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	5,52
93	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@@H]3F)C2=NC(Cl)=N1	7,92
94	NC1=C2N=CN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC(Cl)=N1	7,52
95	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3F)C2=NC(Br)=N1	6,66
96	NC1=C2N=CN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC(F)=N1	6,7
97	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@@H]3F)C2=NC(F)=N1	6,47
98	NC1=NC(Br)=NC2=C1N=CN2C1O[C@H](CO)[C@@H](O)[C@H]1O	5,4
99	NC1=NC(F)=NC2=C1N=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	5,05
100	NC1=C2N=CN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC(Br)=N1	7,7
101	CC(Br)C(=O)NCC1OC(CC1O)N1C=C(C)C(=O)NC1=O	4,3
102	CC1=CN(C2CC(O)C(CNC(=O)CCBr)O2)C(=O)NC1=O	4,3
103	CC1=CN([C@H]2C[C@H](O)[C@@H](CNC(=O)CBr)O2)C(=O)NC1=O	5,1
104	CCOC(=O)C(=O)NCC1OC(CC1O)N1C=C(C)C(=O)NC1=O	4,22
105	CC1=CN(C2CC(O)C(CNC(=O)CI)O2)C(=O)NC1=O	5,1
106	CC1=CN(C2CC(O)C(CNC(=O)CCl)O2)C(=O)NC1=O	4,6
107	CC1=CN(C2CC(O)C(CNS(=O)(=O)CBr)O2)C(=O)NC1=O	4,3
108	CC1=CN(C2CC(O)C(CC(=O)OCBr)O2)C(=O)NC1=O	5,52
109	CC1=CN(C2CC(O)C(CNC(=O)C3=CC=CC(=C3)S(F)(=O)=O)O2)C(=O)NC1=O	4,3
110	OC[C@H]1O[C@H]([C@H](O)[C@@H]1O)C1NN=C(C(=O)CN=N)C1=N	5,7
111	CC1=CN(C2CC(O)C(CNC(=O)N(CCCl)N=O)O2)C(=O)NC1=O	5
112	CN(N=O)C(=O)NC1=CC=C(NC(=O)C2OC(C(O)C2O)N2C=CC(=O)NC2=O)C=C1	4,48
113	OC1CC(OC1CNC(=O)N(CCCl)N=O)N1C=CC(=O)NC1=O	4,85
114	CC1=CN(C2CC(O)C(O2)C(=O)NCCN(N=O)C(=O)NC2=CC=CC=C2)C(=O)NC1=O	4,05
115	CCN(N=O)C(=O)NCC1OC(CC1O)N1C=C(C)C(=O)NC1=O	4,06
116	CN(N=O)C(=O)NC1=CC=C(NC(=O)C2OC(CC2O)N2C=C(C)C(=O)NC2=O)C=C1	4,34
117	NC1=C2N=CN(C3O[C@H](CO)[C@H](O)[C@H]3Cl)C2=NC(Cl)=N1	3,92
118	NC1=C2N=CN(C3O[C@H](CO)[C@H](O)[C@H]3N=[N+]=[N-])C2=NC(F)=N1	4,54
119	NC1=C2N=CN(C3O[C@H](CO)[C@H](O)[C@H]3Cl)C2=NC(F)=N1	4
120	NC1=NC(Cl)=NC2=C1N=CN2C1O[C@H](CO)[C@H](O)[C@H]1Br	3,96
121	NC1=C2N=CN(C3O[C@H](CO)[C@H](O)[C@H]3I)C2=NC(Cl)=N1	4
122	N[C@@H]1[C@@H](O)[C@@H](CO)OC1N1C=NC2=C(N)N=C(F)N=C12	4,92
123	N[C@@H]1[C@@H](O)[C@@H](CO)OC1N1C=NC2=C(N)N=C(Cl)N=C12	4,1
124	NC1=C2N=CN(C3O[C@H](CO)[C@H](O)[C@H]3N=[N+]=[N-])C2=NC(Cl)=N1	3,92
125	CCOC(=O)CCCCC\N=C(/S)N1C(CNC2=CC=C(C=C2)C(=O)NC(CCC(O)=O)C(O)=O)CNC2=NC(N)=NC(O)=C12	4,6
126	CCOC(=O)CCCCCCC\N=C(/S)N1C(CNC2=CC=C(C=C2)C(=O)NC(CCC(O)=O)C(O)=O)CNC2=NC(N)=NC(O)=C12	4,6
127	CCOC(=O)CCCCCC\N=C(/S)N1C(CNC2=CC=C(C=C2)C(=O)NC(CCC(O)=O)C(O)=O)CNC2=NC(N)=NC(O)=C12	4,6
128	CCOC(=O)CCCCCCCCC\N=C(/S)N1C(CNC2=CC=C(C=C2)C(=O)NC(CCC(O)=O)C(O)=O)CNC2=NC(N)=NC(O)=C12	4,6
129	NC1=NC2=C(F)N=CN=C2N1C1O[C@H](CO)[C@@H](O)[C@H]1O	5,74
130	OC1CC(OC1CNC(=O)CBr)N1C=C(F)C(=O)NC1=O	4,8
131	OC1CC(OC1CNC(=O)CBr)N1C=CC(=O)NC1=O	4,96
132	CCC1=CN(C2CC(O)C(CNC(=O)CBr)O2)C(=O)NC1=O	6
133	OC1CC(OC1CNC(=O)CBr)N1C=C(I)C(=O)NC1=O	5,7
134	OC1CC(OC1CNC(=O)CI)N1C=CC(=O)NC1=O	4,55
135	CC(Br)C(=O)NCC1OC(CC1O)N1C=CC(=O)NC1=O	4,26
136	OC1CC(OC1CNC(=O)C1=CC=C(C=C1)S(F)(=O)=O)N1C=CC(=O)NC1=O	5
137	OC1CC(OC1CNC(=O)CBr)N1C=C(Br)C(=O)NC1=O	6
138	CC1=CN([C@H]2C[C@H](O)[C@@H](CNC(=O)CBr)O2)C(=O)NC1=O	5,1
139	CCOC1=NC(N)=C2N=NN(C3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	4,12
140	NC1=C2N=NN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC(F)=N1	4,15
141	NC1=NC(F)=NC2=NN(N=C12)C1O[C@H](CO)[C@@H](O)[C@H]1O	4,12
142	NC1=NC(O)=C2NN=NC2=N1	5,7

NAME	SMILE	lg(1/IC50)
143	NC1=C2N=NN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC=N1	4,6
144	NC1=C2N=NN(C3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC(F)=N1	5,7
145	NC1=C2N=NN([C@H]3C[C@H](O)[C@@H](CO)O3)C2=NC=N1	5
146	NC1=NC(O)=NC2=NN(N=C12)C1O[C@H](CO)[C@@H](O)[C@H]1O	4,12
147	CSC1=NC(N)=C2N=NN(C3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	3,89
148	NC1=NC2=NN(N=C2C(N)=N1)C1O[C@H](CO)[C@@H](O)[C@H]1O	4,12
149	NC1=NC(N)=C2N=NN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	6,15
150	NC1=NC(N)=C2N=NN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	4,7
151	CSC1=NC2=NN(N=C2C(N)=N1)C1O[C@H](CO)[C@@H](O)[C@H]1O	4,6
152	CS(=O)(=O)C1=NC(N)=C2N=NN(C3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	4,85
153	CSC1=NC2=NN(N=C2C(SC)=N1)[C@@H]1O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H]1OC(C)=O	6,1
154	NC1=NC(O)=C2N=NN(C3O[C@H](CO)[C@@H](O)[C@H]3O)C2=N1	5,7
155	CS(=O)(=O)C1=NC2=NN(N=C2C(N)=N1)C1O[C@H](CO)[C@@H](O)[C@H]1O	4,66
156	NC1=C2N=NN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1	7,7
157	NC1=C2N=NN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1	6,15
158	NC1=C2N=CN([C@@H]3C[C@H](CO)[C@H](O)C3O)C2=CC=N1	6,22
159	NC1=C2C=CN([C@@H]3C[C@H](CO)[C@H](O)C3O)C2=NC=N1	5,85
160	NC1=C2N=CN=C2C=CN1	5,15
161	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1	4,7
162	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=NC=N1	6,15
163	NC1=NC=NC2=C1C=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	5,52
164	NC1=NC=NC2=C1C=CN2[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	8,7
165	NC1=C2C=CNC2=NC=N1	4,15
166	NC1=C2N=CN([C@@H]3O[C@H](CO)[C@@H](O)[C@H]3O)C2=CC=N1	5,7
167	CC1=CN(C2CC(O)C(CCC(=O)CI)O2)C(=O)NC1=O	4,77
168	CC1=CN(C2CC(O)C(O2)C(=O)NC2=CC=C(C=C2)C(=O)CBr)C(=O)NC1=O	4,92
169	CC1=CN(C2CC(O)C(O2)C(=O)NC2=CC=C(C=C2)C(=O)CI)C(=O)NC1=O	4,54
170	CC1=CN(C2CC(O)C(CCC(=O)CCl)O2)C(=O)NC1=O	4,6
171	CC1=CN(C2CC(O)C(CCC(=O)CBr)O2)C(=O)NC1=O	4,26
172	CC1=CN(C2CC(O)C(O2)C(=O)NC2=CC=C(C=C2)C(=O)CCl)C(=O)NC1=O	4,52
173	CC1=CN(C2CC(O)C(CNC(=O)C3=CC=C(C=C3)C(=O)CBr)O2)C(=O)NC1=O	4,4
174	NC1=NC(O)=C2N=CN(C3CC(O)C(C3)OCP(O)(O)=O)C2=N1	5,62
175	NC1=NC(O)=C2N=CN([C@H]3C[C@H](O)[C@@H](CO)C3)C2=N1	4,02
176	COC1=NC(N)=C(C(=N1)C(Br)Br)[N+]([O-])=O	2,8
177	COC1=NC(OC)=C(C(=N1)C(Br)Br)[N+]([O-])=O	2,6
178	COC1=NC(OC)=C(C(=N1)C(Br)Br)[N+]([O-])=O	2,57
179	COC1=NC(C(Br)Br)=C(C(=N1)N1CCOCC1)[N+]([O-])=O	2,8
180	COC1=NC(C(Br)Br)=C(C(=N1)N1CCOCC1)[N+]([O-])=O	2,55
181	COC1=NC(N)=C(C(=N1)C(Br)Br)[N+]([O-])=O	2,48
182	NC1=NC(O)=C2N=CN(COC(CO)CO)C2=N1	2,48
183	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,92
184	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,7
185	C[C@@H]1O[C@@H](O[C@H]2[C@H](OC(=O)\C=C\C3=CC=C(O)C(O)=C3)[C@@H](COC(C)=O)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2OC(C)=O)[C@H](OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	4,5
186	NC(=O)C1=NN(C=N1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	3,99
187	NC(=O)C1=NN(C=N1)[C@@H]1O[C@H](CO)[C@@H](O)[C@H]1O	3,84
188	NC1=NC(O)=C2N=CN(COCCO)C2=N1	3,53
189	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O[C@@H]3OC[C@](O)(CO)[C@@H]3O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](COC(C)=O)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	3,65
190	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	4,08
191	C[C@@H]1O[C@@H](O[C@H]2[C@H](OC(C)=O)[C@@H](COC(=O)\C=C\C3=CC=C(OC(C)=O)C(OC(C)=O)=C3)O[C@@H](OCCC3=CC=C(OC(C)=O)C(OC(C)=O)=C3)[C@@H]2OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	4,95
192	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](CO)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	4,15
193	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O[C@@H]2OC[C@](O)(CO)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,92
194	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O[C@@H]2OC[C@](O)(CO)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,91
195	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	4,36
196	C[C@@H]1O[C@@H](O[C@H]2[C@H](OC(=O)\C=C\C3=CC=C(OC(C)=O)C(OC(C)=O)=C3)[C@@H](COC(C)=O)O[C@@H](OCCC3=CC=C(OC(C)=O)C(OC(C)=O)=C3)[C@@H]2OC(C)=O)[C@H](OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	4,47
197	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](CO)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	3,76

NAME	SMILE	lg(1/IC50)
198	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O[C@@H]2OC[C@](O)(CO)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,62
199	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	4,32
200	COC1=CC(\C=C\C(=O)OC[C@H]2O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@H](O[C@@H]3OC[C@](O)(CO)[C@@H]3O)[C@@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)[C@@H]2O)=CC=C1O	3,37
201	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	3,85
202	C[C@@H]1O[C@@H](O[C@H]2[C@H](OC(C)=O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2OC(C)=O)[C@H](OC(C)=O)[C@H](OC(C)=O)[C@H]1OC(C)=O	4,72
203	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](CO)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	3,94
204	NC1=NC(O)=C2N=CN(COCCO)C2=N1	4,35
205	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O[C@@H]3OC[C@](O)(CO)[C@@H]3O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](COC(C)=O)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	4,02
206	COC1=CC(\C=C\C(=O)OC[C@H]2O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@H](O[C@@H]3OC[C@](O)(CO)[C@@H]3O)[C@@H](O[C@@H]3O[C@@H](C)[C@H](O)[C@@H](O)[C@H]3O)[C@@H]2O)=CC=C1O	3,61
207	C[C@@H]1O[C@@H](O[C@H]2[C@H](O)[C@@H](COC(=O)\C=C\C3=CC=C(O)C(O)=C3)O[C@@H](OCCC3=CC=C(O)C(O)=C3)[C@@H]2O[C@@H]2OC[C@](O)(CO)[C@@H]2O)[C@H](O)[C@H](O)[C@H]1O	4,05
208	NC1=NC(O)=C2N=CN(COC(CO)CO)C2=N1	3,41
209	COC(=O)C1=CO[C@@H](O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H]2[C@@H]1[C@@H](C[C@]2(C)OC(C)=O)OC(=O)\C=C\C1=CC=C(O)C=C1	4,15
210	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](OCCC3=CC=C(O)C(O)=C3)O[C@H](CO)[C@H]2OC(=O)\C=C\C2=CC=C(O)C(O)=C2)[C@H](O)[C@H](O)[C@H]1O	3,91
211	COC(=O)C1=CO[C@@H](O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H]2[C@@H]1[C@@H](C[C@]2(C)OC(C)=O)OC(=O)\C=C/C1=CC=C(O)C=C1	4,15
212	BrC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,05
213	O=C1O\C(=C/CN2C=NC3=C2N=CN=C3N2C=CC=C2)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4
214	O=C1O\C(=C/CN2C=CC(=O)NC2=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4,4
215	ClC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,7
216	ClC1=NC=NC2=C1N=CN2C\C=C1/OC(=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4,22
217	ClC1=NC=NC2=C1N(C\C=C1\OC(=O)C(OCC3=CC=CC=C3)=C1OCC1=CC=CC=C1)C=N2	4,22
218	FC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,7
219	FC(F)(F)C1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,4
220	IC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	5
221	CC1=CC(=O)C2=C(CO)CC[C@@H]3C[C@]12OC(=O)C3=C	5,96
222	CC1=CC(=O)C2=C(CO)CC[C@@H]3C[C@]12OC(=O)C3=C	5,89
223	CC1=CC(=O)C2=C(CO)CC[C@H](C[C@]12O)C(=C)C(=O)O[C@@H]1[C@@H](O)[C@H](O)[C@@H](OCC2=C3C(=O)C=C(C)[C@@]33C[C@@H](CC2)C(=C)C(=O)O3)O[C@H]1CO	6,1
224	CC1=CC(=O)C2=C(CO)CC[C@@H]3C[C@]12OC(=O)C3=C	5,82
225	C[C@@H]1C[C@H]2OC(=O)C(=C)[C@H]2[C@H](O)[C@@]2(C)[C@H]1C=CC2=O	6,05
226	CC1=CC(=O)C2=C(CO)CC[C@H](C[C@]12O)C(=C)C(=O)O[C@@H]1[C@@H](O)[C@H](O)[C@@H](OCC2=C3C(=O)C=C(C)[C@@]33C[C@@H](CC2)C(=C)C(=O)O3)O[C@H]1CO	6,15
227	CC1=CC(=O)C2=C(CO)CC[C@H](C[C@]12O)C(=C)C(=O)O[C@@H]1[C@@H](O)[C@H](O)[C@@H](OCC2=C3C(=O)C=C(C)[C@@]33C[C@@H](CC2)C(=C)C(=O)O3)O[C@H]1CO	6,22
228	C[C@@H]1C[C@H]2OC(=O)C(=C)[C@H]2[C@H](O)[C@@]2(C)[C@H]1C=CC2=O	6,1
229	CN(C)CCCOC1=NC=CC(=N1)C1=CC=C(S1)C1=CC=CS1	4,5
230	CN(C)CCOC1=NC=CC(=N1)C1=CC=CS1	3,7
231	CN(C)CCOC1=NC=CC(=N1)C1=CC=C(S1)C1=CC=CS1	4,32
232	CN(C)CCSC1=NC=CC(=N1)C1=CC=CS1	3,72
233	CN(C)CCSC1=NC=CC(=N1)C1=CC=C(S1)C1=CC=CS1	3,84
234	CN(C)CCCOC1=NC=CC(=N1)C1=CC=CS1	3,72
235	CC(=O)NC1=CC2=NC3=CC=CC=C3OC2=CC1=O	5,85
236	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	8,4
237	CC(=O)C1=C2N=C3C(OC2=CC=C1)=CC(=O)C(N)=C3C(C)=O	5,82
238	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	7,4
239	O=C1C=CC2=NC3=CC=CC=C3OC2=C1	4,85
240	O=C1C=C2OC3=CC=CC=C3N=C2C2=CC=CN=C12	7,4
241	NC1=CC2=NC3=CC=CC=C3OC2=CC1=O	5,74
242	O=C1C=C2SC3=CC=CC=C3N=C2C2=CC=CN=C12	7
243	O=C1C=C2OC3=CC=C(C=C3N=C2C2=CC=CN=C12)C#N	7,7
244	[O-][N+](=O)C1=CC=C2OC3=CC(=O)C4=NC=CC=C4C3=NC2=C1	6,4
245	O=C1C=C2OC3=CC=CC=C3N=C2C2=NC=CC=C12	5,92
246	CC1=CC=CC2=C1OC1=CC(=O)C3=NC=CC=C3C1=N2	6,7
247	ClC1=CC=C2OC3=CC(=O)C4=NC=CC=C4C3=NC2=C1	6,7
248	CC1=CC=C2OC3=CC(=O)C4=NC=CC=C4C3=NC2=C1	6,52

NAME	SMILE	lg(1/IC50)
249	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	7,4
250	O=C1C=C2OC3=CC=CC=C3N=C2C2=CC=CC=C12	5,85
251	[O-][N+](=O)C1=CC=CC2=C1N=C1C(O2)=CC(=O)C2=NC=CC=C12	7,3
252	O=C1C=C2OC3=CC=CC=C3N=C2C2=CC=CN=C12	7,4
253	[O-][N+](=O)C1=CC=C2N=C3C(OC2=C1)=CC(=O)C1=NC=CC=C31	5,96
254	CC1=CC=C2N=C3C(OC2=C1)=CC(=O)C1=NC=CC=C31	6,7
255	O=C1C=C2OC3=CC=CC=C3N=C2C2=CC=NC=C12	5,05
256	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	8,4
257	O=C1C=C2OC3=CC=CC=C3N=C2C2=CN=CC=C12	5,05
258	[O-][N+](=O)C1=CC=CC2=C1OC1=CC(=O)C3=NC=CC=C3C1=N2	6,15
259	CC1=CC=CC2=C1N=C1C(O2)=CC(=O)C2=NC=CC=C12	6,22
260	COC1=CC=C2C(SC3=C2C2=CC=CC=C2N(CCCN(C)C)C3=O)=C1	5,53
261	CN(C)CCCN1C(=O)C2=C(C3=C(S2)C=C(C=C3)[N+]([O-])=O)C2=CC=CC=C12	5,45
262	CN(C)CCCN1C(=O)C2=C(C3=C(S2)C=C(C)C=C3)C2=CC=CC=C12	5,44
263	CN(C)CCCN1C(=O)C2=C(C3=C(S2)C=C(C=C3)C(=O)NC2=CC=CC=C2)C2=CC=CC=C12	5,75
264	CN(C)CCCN1C(=O)C2=C(C3=C(S2)C=CC=C3)C2=CC=CC=C12	5,44
265	CN(C)CCCNC(=O)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=CC=C12	5,18
266	CN(C)CCCN1C(=O)C2=C(C3=C(S2)C=C(F)C=C3)C2=CC=CC=C12	5,5
267	CN(C)CCCN(C(=O)C1=CC2=C(C=C1)C1=C(S2)C(O)=NC2=CC=CC=C12)C1=CC=CC=C1	5,5
268	COC(=O)C1=CC=C2C(SC3=C2C2=CC=CC=C2N(CCCN(C)C)C3=O)=C1	6,19
269	CC(=O)OCCON1C=NC2=C(S)N=C(N)N=C12	5,31
270	CC(=O)OCCON1C=NC2=C(Cl)N=C(N)N=C12	3,3
271	CC(O)N1C=NC2=C(Cl)N=C(I)N=C12	3,3
272	CC(OC(C)=O)N1C=NC2=C(S)N=C(N)N=C12	5
273	CC(OC(C)=O)N1C=NC2=C(S)N=C(F)N=C12	3,7
274	CC(O)N1C=NC2=C(N)N=C(I)N=C12	3,3
275	CC(O)CN1C=NC2=C1N=C(N)N=C2F	4,2
276	OCCON1C=NC2=C(S)N=C(F)N=C12	3,3
277	NC1=C2N=CN(OCCO)C2=NC(I)=N1	3,3
278	CC(=O)OCCON1C=NC2=C(S)N=C(F)N=C12	3,3
279	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(F)N=C12	5
280	CC(O)N1C=NC2=C(S)N=C(F)N=C12	3,3
281	COC1=C2N=CN(OCCO)C2=NC(I)=N1	3,3
282	CC(OC(C)=O)N1C=NC2=C(N)N=C(I)N=C12	3,3
283	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(N)N=C12	3,3
284	CC(=O)OCCON1C=NC2=C(Cl)N=C(I)N=C12	4,25
285	CC(OC(C)=O)N1C=NC2=C(Cl)N=C(I)N=C12	5,2
286	C[C@@H](CCC(=O)NCCNC(=O)CC[C@@H](C)[C@H]1CCC2C3CCC4C[C@H](O)CC[C@]4(C)C3C[C@@H](O)[C@]12C)[C@H]1CCC2C3CCC4C[C@H](O)CC[C@]4(C)C3C[C@@H](O)[C@]12C	5,66
287	C[C@@H](CCC(=O)NCCNCCNC(=O)CC[C@@H](C)[C@H]1CCC2C3CCC4C[C@H](O)CC[C@]4(C)C3C[C@@H](O)[C@]12C)[C@H]1CCC2[C@]1(C)C1CCC3C(CCC4C[C@H](O)CC[C@]34C)[C@]21O	5
288	NC1=NC=CC(=N1)C1=CNC2=CC=C(Br)C=C12	5,01
289	NC1=NC=CC(=N1)C1=CNC2=CC(Br)=CC(O)=C12	5,77
290	NC1=NC=CC(=N1)C1=CNC2=CC(Br)=C(Br)C=C12	5,74
291	NC1=NC=CC(=N1)C1=CNC2=CC(Br)=CC=C12	5,14
292	NC1=NC=CC(=N1)C1=CNC2=C(Br)C=CC(O)=C12	5,96
293	CNC1=CC=CC=C1C(=O)NC(=O)NC1=CC=C(OC2=NC=C(Br)C=N2)C(C)=C1	6
294	CN(C(=O)NC1=CC=CC=C1C(=O)N(C)C(=O)NC1=CC=C(OC2=NC=C(Br)C=N2)C(C)=C1)C(=O)C1=CC=CC=C1N	5,3
295	CN(C(=O)NC1=CC=C(OC2=NC=C(Br)C=N2)C(C)=C1)C(=O)C1=CC=CC=C1N	5,3
296	ONC(=O)NC(C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1	4,08
297	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,21
298	CCC(C)C(NC(=O)NO)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,45
299	O=C(NC1CCCC1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,02
300	ONC(=O)NC(C(=O)NCC1=CC=CC=C1)C1=CC=CC=C1	4,49
301	O=C(NC(C1=CC=CC=C1)C1=CC=CC=C1)C(NC(=O)N1N=NC2=CC=CC=C12)C1=CC=CC=C1	4,23
302	CC(C)C(NC(=O)NO)C(=O)NC1CCCC1	4,48
303	O=C(NC(C(=O)N1CCCCC1)C1=CC=CC=C1)N1N=NC2=C1C=CC=C2	4
304	CC(C)C1NC(=O)N(C2CCCC2)C1=O	4,01
305	O=C1NC(C(=O)N1CC1=CC=CC=C1)C1=CC=CC=C1	4,08
306	O=C(NC(CC1=CC=CC=C1)C(=O)N1CCCC1)N1N=NC2=CC=CC=C12	4
307	ONC(=O)NC(C(=O)N1CCCCC1)C1=CC=CC=C1	4
308	O=C(NCC1=CC=CC=C1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,09
309	CC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCCC1	4,22
310	O=C(NC(C1=CC=CC=C1)C1=CC=CC=C1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,39
311	O=C1NC(C(=O)N1C1CCCC1)C1=CC=CC=C1	4
312	CCC(C)C(NC(=O)NO)C(=O)NC1CCCCC1	4
313	O=C(NC1CCCCC1)C(CC1=CC=CC=C1)NC(=O)N1N=NC2=CC=CC=C12	4,19
314	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC1CCCCC1	4,03
315	CCC(C)C(NC(=O)NO)C(=O)NC1CCCC1	4
316	ONC(=O)NC(CC1=CC=CC=C1)C(=O)N1CCCC1	4
317	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC(C1=CC=CC=C1)C1=CC=CC=C1	4,26

NAME	SMILE	lg(1/IC50)
318	O=C(NC1CCCCC1)C(NC(=O)N1N=NC2=C1C=CC=C2)C1=CC=CC=C1	4,16
319	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCCC1	4,24
320	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCC1	4,25
321	CCC(C)C1NC(=O)N(C2CCCCC2)C1=O	4,16
322	CC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NC1CCCC1	4,22
323	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NC1CCCC1	4
324	CC(C)C(NC(=O)NO)C(=O)NC1CCCCC1	4
325	ONC(=O)NC(CC1=CC=CC=C1)C(=O)NCC1=CC=CC=C1	4
326	O=C(NCC1CCCCC1)C(NC(=O)N1N=NC2=C1C=CC=C2)C1=CC=CC=C1	4,16
327	ONC(=O)NC(C(=O)NC1=CC=CC=C1)C1=CC=CC=C1	4
328	CCC(C)C(NC(=O)NO)C(=O)NCC1=CC=CC=C1	4
329	CCC(C)C(NC(=O)N1N=NC2=CC=CC=C12)C(=O)NCC1=CC=CC=C1	4
330	CC(C)C1NC(=O)N(C2CCCCC2)C1=O	4
331	CCC(C)C1NC(=O)N(C2CCCC2)C1=O	4
332	CCC(C)C1NC(=O)N(CC2=CC=CC=C2)C1=O	4,33
333	ON(C(=O)C12CC3CC(CC(C3)C1)C2)C1=CC=C(Cl)C=C1	4
334	ON(C(=O)CCC1CCCC1)C1=CC=C(Cl)C=C1	4,7
335	ON(C(=O)CCC1CCCCC1)C1=CC=C(Cl)C=C1	4,52
336	ON(C(=O)CC1CCCCC1)C1=CC=C(Cl)C=C1	5,05
337	ON(C(=O)C1CC1)C1=CC=C(Cl)C=C1	4
338	ON(C(=O)CC1CCCCC1)C1=CC=CC=C1	4
339	ON(C(=O)C1CCCCC1)C1=CC=C(Cl)C=C1	4,4
340	[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Zn].[O-]C(=O)C1=CC(=CC(OC2=CC3=C4NC(\N=C5/N=C(/N=C6\N\C(=N/C7=N/C(=N/4)/C4=CC(OC8=CC(=CC(=C8)C([O-])=O)C([O-])=O)C([O-])=O)=C(OC8=CC(=CC(=C8)C([O-])=O)C([O-])=O)C=C74)C4=CC(OC7=CC(=CC(=C7)C([O-])=O)C([O-])=O)=C(OC7=CC(=CC(=C7)C([O-])=O)C([O-])=O)C=C64)C4=CC(OC6=CC(=CC(=C6)C([O-])=O)C([O-])=O)=C(OC6=CC(=CC(=C6)C([O-])=O)C([O-])=O)C=C54)=C3C=C2OC2=CC(=CC(=C2)C([O-])=O)C([O-])=O)=C1)C([O-])=O	5,35
341	[Zn++].OC(=O)C1=CC(=CC(OC2=CC3=C4[N-]C(\N=C5/N=C(/N=C6\[N-]\C(=N/C7=N/C(=N/4)/C4=CC(OC8=CC(=CC(=C8)C(O)=O)C(O)=O)=C(OC8=CC(=CC(=C8)C(O)=O)C(O)=O)C=C74)C4=CC(OC7=CC(=CC(=C7)C(O)=O)C(O)=O)=C(OC7=CC(=CC(=C7)C(O)=O)C(O)=O)C=C64)C4=CC(OC6=CC(=CC(=C6)C(O)=O)C(O)=O)=C(OC6=CC(=CC(=C6)C(O)=O)C(O)=O)C=C54)=C3C=C2OC2=CC(=CC(=C2)C(O)=O)C(O)=O)=C1)C(O)=O	5,35
342	[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Na+].[Zn++].OC(=O)C1=CC(=CC(OC2=CC3=C4NC(\N=C5\N=C(\N=C6/N\C(=N/C7=N/C(=N\4)/C4=CC(OC8=CC(=CC(=C8)C([O-])=O)C(O)=O)=C(OC8=CC(=CC(=C8)C([O-])=O)C(O)=O)C=C74)C4=CC(OC7=CC(=CC(=C7)C(O)=O)C([O-])=O)=C(OC7=CC(=CC(=C7)C([O-])=O)C([O-])=O)C=C64)C4=CC(OC6=CC(=CC(=C6)C([O-])=O)C([O-])=O)=C(OC6=CC(=CC(=C6)C([O-])=O)C([O-])=O)C=C54)=C3C=C2OC2=CC(=CC(=C2)C([O-])=O)C([O-])=O)=C1)C([O-])=O	5,35
343	CN(C)CCCN1C(=O)NC2(CSC3=C2C(=O)C2=CC=CC=C2C3=O)C1=O	6,77
344	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	7,23
345	COC1=CC(=CC(OC)=C1OC)C(=O)\C=C\C1=CC=C(F)C=C1	5
346	COC1=CC=C(C=C1)C(=O)\C=C\C1=CC(OC)=C(OC)C(OC)=C1	5,06
347	COC1=CC=C(C=C1)C1NN=C(C1O)C1=CC(OC)=C(OC)C(OC)=C1	5,11
348	COC1=CC(=CC(OC)=C1OC)C(=O)\C=C\C1=CC=C2OCOC2=C1	5
349	COC1=CC(=CC=C1OC(C)=O)C(=O)\C=C\C1=CC(OC)=C(OC)C(OC)=C1	5,16
350	COC1=CC=C(C=C1)C1=NNC(=C1)C1=CC(OC)=C(OC)C(OC)=C1	6,09
351	COC1=CC(\C=C\C(=O)C2=CC=C(OC(C)=O)C=C2)=CC(OC)=C1OC	4,88
352	COC1=CC(=CC(OC)=C1OC)C1=NNC(C1O)C1=CC=C2OCOC2=C1	4,4
353	COC1=CC(=CC(OC)=C1OC)C1=NN(C(C)=O)C(=C1OC(C)=O)C1=CC=C2OCOC2=C1	4,21
354	COC1=CC(=CC(OC)=C1OC)C(=O)\C=C\C1=CC=CC=C1	5,12
355	COC1=CC(=CC=C1O)C(=O)\C=C\C1=CC(OC)=C(OC)C(OC)=C1	5,22
356	COC1=CC(=CC(OC)=C1OC)C(=O)\C=C\C1=CC=C(Cl)C=C1	4,92
357	COC1=CC=C(C=C1OC)C1=NNC(=C1)C1=CC(OC)=C(OC)C(OC)=C1	5,08
358	COC1=CC=CC(=C1)C(=O)\C=C\C1=CC(OC)=C(OC)C(OC)=C1	4,86
359	COC1=CC(\C=C\C(=O)C2=CC(OC)=C(OC)C(OC)=C2)=CC(OC)=C1OC	5,11
360	COC1=CC(=CC(OC)=C1OC)C1=CC(=NN1)C1=CC(OC)=C(OC)C(OC)=C1	5,19
361	COC1=CC=C(C=C1)C1=NNC(=C1)C1=CC(OC)=C(OC)C(OC)=C1	4,9
362	COC1=CC(=CC(OC)=C1OC)C1=NNC(=C1)C1=CC=C2OCOC2=C1	4,47
363	COC1=CC(\C=C\C(=O)C2=CC=CC=C2)=CC(OC)=C1OC	4,93
364	COC1=CC(=CC(OC)=C1OC)C1=NNC(=C1)C1=CC=C(F)C=C1	5,42
365	COC1=CC=C(\C=C\C(=O)C2=CC(OC)=C(OC)C(OC)=C2)C=C1OC	5,21
366	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
367	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,64
368	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,63
369	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](C[C@@H](O)[C@@H]4[C@@]5(C)[C@H](O)C[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,66
370	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,63
371	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)C=CC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,63

NAME	SMILE	lg(1/IC50)
372	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)[C@@H](O)C[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
373	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](C[C@@H](O)[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,64
374	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](C[C@@H](O)[C@@H]4[C@@]5(C)CC[C@@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,66
375	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5[C@H](O)C[C@@]34C)[C@@H]12	4,66
376	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)C=CC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C=O	4,64
377	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
378	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)C=CC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,64
379	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5[C@H](O)C[C@@]34C)[C@@H]12)C(O)=O	4,67
380	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5[C@H](O)C[C@@]34C)[C@@H]12	4,66
381	CC(C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)CC[C@H](OC(=O)\C=C\C6=CC=C(O)C(O)=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,77
382	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)[C@H](O)CC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,64
383	CC(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)[C@@H](O)C[C@@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
384	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	5,17
385	CC(=O)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
386	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OC(=O)\C=C\C6=CC=C(O)C(O)=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,78
387	CC(=C)[C@@H]1CC[C@@]2(C)[C@H]1[C@@H]1CC[C@@H]3[C@@]4(C)CCC(=O)C(C)(C)[C@@H]4[C@H](O)C[C@@]3(C)[C@]1(C)C[C@@H]2O	4,66
388	CC1(C)[C@@H]2CC[C@]3(C)[C@H](CC[C@H]4[C@H]5[C@@H](CC[C@]5(CO)CC[C@@]34C)C(=C)CO)[C@@]2(C)CCC1=O	4,81
389	CC1=CC[C@]2(CC1)C(=C)C[C@H](O)[C@H](Br)C2(C)C	4,17
390	CC(=O)O[C@H]1CC(=C)[C@]2(CCC(C)=CC2)C(C)(C)[C@H]1Br	4,24
391	CC(=O)O[C@H]1CC(=C)[C@]2(CCC(C)=C(Cl)C2)C(C)(C)[C@H]1Br	4,55
392	CC(=O)O[C@@H]1C[C@@H](Br)C(C)(C)O[C@]1(C)[C@H]1CC[C@](C)(Cl)[C@@H](Br)C1	4,38
393	CC1(C)O[C@@](C)([C@H](O)C[C@H]1Br)[C@H]1CC[C@](C)(Cl)[C@@H](Br)C1	4,34
394	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	6,72
395	CC1=C(Cl)C[C@]2(CC1)C(=C)C[C@H](O)[C@H](Br)C2(C)C	5,62
396	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	8,22
397	CC1=C(Cl)C[C@]2(CC1)C(=C)C[C@H](O)[C@H](Br)C2(C)C	5,7
398	CC(=O)O[C@H]1CC(=C)[C@]2(CCC(C)=C(Cl)C2)C(C)(C)[C@H]1Br	4,65
399	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCN=C(N)N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)CNC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C(N2)\C(=C2\C=CC\1=N2)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C(N)=O	5,82
400	NCCCC[C@H](NC(=O)[C@H](CCCN=C(N)N)NC(=O)CNC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C(N2)\C(=C2\C=CC\1=N2)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@@H]1C(=O)N[C@@H](CCC(N)=O)C(N)=O	4,52
401	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCN=C(N)N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)CNC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C(N2)\C(=C2\C=CC\1=N2)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C(N)=O	4,05
402	NC(=N)NCCC[C@H](NC(=O)CNC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C(N2)\C(=C2\C=CC\1=N2)C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCN=C(N)N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCN=C(N)N)C(O)=O	4,12
403	CC1=CC2=C(C=C1C)N=C1C(O2)=CC(=O)C2=NC=CC=C12	6,1
404	O=C1C=C2OC3=CC=CC=C3N=C2C2=CC=CN=C12	7,4
405	O=C1C=C2OC3=CC=C4CCCCC4=C3N=C2C2=CC=CN=C12	5,72
406	O=C1C=C2OC3=C4CCCCC4=CC=C3N=C2C2=CC=CN=C12	5,74
407	CC1=CC=C(C)C2=C1OC1=CC(=O)C3=NC=CC=C3C1=N2	6,4
408	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	7,4
409	CC1=CC(C)=C2OC3=CC(=O)C4=NC=CC=C4C3=NC2=C1	5,96
410	CC1=CC=C2N=C3C(OC2=C1C)=CC(=O)C1=NC=CC=C31	6,4

NAME	SMILE	lg(1/IC50)
411	O=C1C=C2OC3=C(C=CC4=C3C=CC=C4)N=C2C2=CC=CN=C12	7,22
412	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	8,4
413	O=C1C=C2OC3=CC4=C(CCCC4)C=C3N=C2C2=CC=CN=C12	5,77
414	O=C1C=C2OC3=CC4=C(C=CC=C4)C=C3N=C2C2=CC=CN=C12	7,3
415	CC1=CC=C2OC3=CC(=O)C4=NC=CC=C4C3=NC2=C1C	5,89
416	CC1=CC(C)=C2N=C3C(OC2=C1)=CC(=O)C1=NC=CC=C31	6,52
417	O=C1C=C2OC3=CC=C4C=CC=CC4=C3N=C2C2=CC=CN=C12	7,4
418	CC(C)=CCC\C(C)=C\CCC(CC(=O)C1=CC(O)=CC=C1O)C(O)=O	4,2
419	CC(C)=CCCC1=CC(OC1=O)C1=CC(O)=CC=C1O	3,96
420	COC1(OC(=O)C(CC\C=C(/C)CCC=C(C)C)=C1)C1=CC(O)=CC=C1O	4,39
421	C=CC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,85
422	OC1=C(O)\C(OC1=O)=C\CN1C=C(C2=CC=CS2)C(=O)NC1=O	4
423	BrC1=CC=C(O1)C1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,55
424	O=C1O\C(=C/CN2C=C(C(=O)NC2=O)C2=CC=CC=C2)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4,66
425	Br\C=C\C1=C(Br)N(C\C(Br)=C2\OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,66
426	O=C1O\C(=C/CN2C=C(C3=CC=CO3)C(=O)NC2=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	5,66
427	OC1=C(O)\C(OC1=O)=C/CN1C=C(C#CC2=CC=CC=C2)C(=O)NC1=O	5,52
428	OC1=C(O)\C(OC1=O)=C\CN1C=C(C#C)C(=O)NC1=O	4,92
429	OC1=C(O)\C(OC1=O)=C\CN1C=C(C(=O)NC1=O)C1=CC=CC=C1	4
430	CC#CC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	6,15
431	CC(C)=CCC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	5,59
432	OC1=C(O)\C(OC1=O)=C\CN1C=C(C=C)C(=O)NC1=O	4,34
433	Br\C=C\C1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4,4
434	OC1=C(O)\C(OC1=O)=C\CN1C=C(C2=CC=CO2)C(=O)NC1=O	4
435	O=C1O\C(=C/CN2C=C(C#C)C(=O)NC2=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	5,34
436	C=C=CC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4
437	O=C1O\C(=C/CN2C=C(C3=CC=CS3)C(=O)NC2=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4,74
438	ClC1=CC=C(O1)C1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	4
439	O=C1O\C(=C/CN2C=C(C#CC3=CC=CC=C3)C(=O)NC2=O)C(OCC2=CC=CC=C2)=C1OCC1=CC=CC=C1	4
440	C=CCC1=CN(C\C=C2/OC(=O)C(OCC3=CC=CC=C3)=C2OCC2=CC=CC=C2)C(=O)NC1=O	5,33
441	[Br-].[Br-].C(C/C1=C/NC2=CC=CC=C2\N=C\C(\CCC[N+]2=CC=C(C=C2)C2=CC=NC=C2)=C/NC2=CC=CC=C2\N=C\1)C[N+]1=CC=C(C=C1)C1=CC=NC=C1	4
442	[Br-].[Br-].C(C/C1=C/NC2=CC=CC=C2\N=C\C(\CCC[N+]2=CC=CC=C2)=C/NC2=CC=CC=C2\N=C\1)C[N+]1=CC=CC=C1	4,96
443	[Br-].[Br-].C[N+]1=CC=C(CCC(=O)OCCC/C2=C/NC3=CC=CC=C3\N=C\C(\CCCOC(=O)CCC3=CC=[N+](C)C=C3)=C/NC3=CC=CC=C3\N=C\2)C=C1	4,42
444	COC1=CC=C(C=C1OC(C)C)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	4,04
445	COC1=CC=C(C=C1)C1=C(C(=O)C(C1)O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	4,46
446	COC1=CC=C(C=C1F)C1=C(C(=O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	5,63
447	COC1=CC=C(C=C1)C1=C(\C(CC1OC(C)=O)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	5,15
448	COC1=CC=C(C=C1[N+]([O-])=O)C1=C(CC(O)C1=O)C1=CC(OC)=C(OC)C(OC)=C1	3,62
449	COC1=CC=C(C=C1)C1=C(\C(=N/O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	3,63
450	COC1=CC=C(C=C1)C1=C(C(=O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	4,36
451	COC1=CC=C(C=C1Cl)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,62
452	COC1=CC(=CC(OC)=C1OC)C1=C(C(CC1=O)O[SiH2]C(C)(C)C)C1=CC=CC=C1	3,63
453	[Na+].COC1=CC=C(C=C1C([O-])=O)C1=C(C(=O)CC1C)C1=CC(OC)=C(OC)C(OC)=C1	3,64
454	COC1=CC=C(C=C1O)C1=C(\C(CC1OC(C)=O)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	3,65
455	COC1=CC=C(C=C1N)C1=C(CC(O)C1=O)C1=CC(OC)=C(OC)C(OC)=C1	4,38
456	COC1=CC=C(C=C1O)C1=C(C(=O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	3,63
457	COC1=CC=C(C=C1Cl)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,61
458	COC1=CC=C(OC)C(=C1)C1=C(C(=O)CC1O)C1=CC(OC)=C(OC)C(OC)=C1	3,6
459	COC1=CC=C(C=C1Cl)C1=C(C(=O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	5,65
460	COC1=CC=C(C=C1OC(C)C)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	3,63
461	COC1=CC(=CC(OC)=C1OC)C1=C(C(CC1=O)O[SiH2]C(C)(C)C)C1=CC(C)=C(OC)C(C)=C1	4,27
462	COC1=CC=C(C=C1O)C1=C(C(=O)CC1O)C1=CC(OC)=C(OC)C(OC)=C1	5,59
463	COCOC1=CC(=CC=C1OC)C1=C(\C(CC1O[SiH2]C(C)(C)C)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	4,59
464	COC1=CC=C(C=C1F)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,59
465	COC1=CC=C(C=C1OCC=C)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	3,63
466	COC1=CC(=CC(OC)=C1OC)C1=C(CC(O[SiH2]C(C)(C)C)C1=O)C1=CC=C(SC)C=C1	3,67
467	COC1=CC(=CC(OC)=C1OC)C1=C(C(=O)C(C1)O[SiH2]C(C)(C)C)C1=CC=C(OC)C(=C1)[N+]([O-])=O	3,7
468	COC1=CC=C(C=C1F)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,61
469	COC1=CC=C(C=C1)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,57
470	COC1=CC=C(C=C1OC(C)C)C1=C(C(=O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	3,67
471	COC1=CC=C(C=C1OCC=C)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	3,64
472	COC1=CC=C(C=C1Cl)C1=C(\C(=N/O)C(C1)OC(C)=O)C1=CC(OC)=C(OC)C(OC)=C1	5,66
473	COC1=CC(=CC(OC)=C1OC)C1=C(C(O)CC1=O)C1=CC(C)=C(OC)C(C)=C1	3,6
474	COC1=CC=C(OC)C(=C1)C1=C(\C(CC1O[SiH2]C(C)(C)C)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	4,86
475	COC1=CC=C(C=C1)C1=C(C(=O)CC1O)C1=CC(OC)=C(OC)C(OC)=C1	3,57
476	COC1=CC=C(C=C1)C1=C(\C(CC1OC(C)=O)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	5,63
477	COC1=CC=C(C=C1NC(=O)C1=CC=CC=C1)C1=C(C(=O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	3,69

NAME	SMILE	lg(1/IC50)
478	COC1=CC(=CC(OC)=C1OC)C1=C(C(CC1=O)OC(C)=O)C1=CC(C)=C(OC)C(C)=C1	3,64
479	COC1=CC=C(C=C1O)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	4,3
480	COC1=CC=C(C=C1O)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	4,51
481	COC1=CC=C(C=C1OC(C)C)C1=C(C(=O)C(C1)O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	4,86
482	COC1=CC=C(C=C1OC)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	3,69
483	COC1=CC=C(C=C1)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	3,66
484	COC1=CC=C(C=C1O)C1=C(\C(CC1O)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	5,6
485	COC1=CC=C(C=C1)C1=C(\C(CC1O)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	3,59
486	COC1=CC=C(C=C1)C1=C(\C(=N/O)C(O)C1)C1=CC(OC)=C(OC)C(OC)=C1	5,59
487	O\N=C1\CC(O)C(=C1C1=CC=CC=C1)C1=CC=CC=C1	3,42
488	COC1=CC=C(\C=C/C2=CC(OC)=C(OC)C(OC)=C2)C=C1O	4,8
489	CC(C)(C)[SiH2]OC1CC(=O)C(=C1C1=CC=CC=C1)C1=CC=CC=C1	4,92
490	COC1=CC=C(OC)C(=C1)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	4,41
491	COC1=CC(=CC(OC)=C1OC)C1=C(C(C\C1=N\O)OC(C)=O)C1=CC(C)=C(OC)C(C)=C1	3,66
492	[Na+].COC1=CC(=CC(OC)=C1OC)C1=C(C(O)CC1=O)C1=CC=C(OCC([O-])=O)C=C1	3,64
493	CC(=O)OC1C\C(=N\O)C(=C1C1=CC=CC=C1)C1=CC=CC=C1	3,49
494	COC1=CC=C(C=C1OC)C1=C(\C(CC1O[SiH2]C(C)(C)C)=N/O)C1=CC(OC)=C(OC)C(OC)=C1	4,2
495	COCOC1=CC(=CC=C1OC)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	4,63
496	COC1=CC(=CC(OC)=C1OC)C1=C(CC(O)\C1=N\O)C1=CC=C(SC)C=C1	5,6
497	COC(=O)C1=CC(=CC=C1OC)C1=C(C(=O)CC1O[SiH2]C(C)(C)C)C1=CC(OC)=C(OC)C(OC)=C1	3,71
498	CCOC(=O)COC1=CC=C(C=C1)C1=C(C(=O)CC1O)C1=CC(OC)=C(OC)C(OC)=C1	3,65
499	CCOC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO)C(=O)C2=C1OCC	6,07
500	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(SCCO)C(=O)C2=C1OC	5,76
501	CC1=CC(O)=C2C(=O)C=C(C(=O)C2=C1)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1O	5,45
502	CCOC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OCC	5,62
503	COC1=CC(C)=CC2=C1C(=O)C1OC1(C2=O)C1=C(C)C=C2C(=O)C3OC3C(=O)C2=C1OC	6,68
504	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OC	6,41
505	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO)C(=O)C2=C1OC	5,85
506	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	6,38
507	CCOC1=C2C(O)=CC(=C(O)C2=CC(C)=C1)C1=C(C)C=C2C(O)=CC=C(O)C2=C1OCC	5,78
508	CN1CCN(\C=C2/OC3=CC=CC=C3C2=O)C(C1)C1=CC=CC=C1	4,3
509	O=C1\C(OC2=CC=CC=C12)=C\N1CCN(CC1)C1=CC=CC=C1	4,56
510	O=C1C(SC2=NC3=CC=CC=C3O2)=COC2=CC=CC=C12	4,53
511	CC1=CC(C)=NC(SC2=COC3=CC=CC=C3C2=O)=N1	4,3
512	O=C1C(SC2=NC3=CC=CC=C3N2)=COC2=CC=CC=C12	4,37
513	O=C1\C(OC2=CC=CC=C12)=C\N1CCN(CC2=CC=CC=C2)CC1	5,24
514	FC1=CNC(=O)NC1=O	3,89
515	CC1=NN=C(O1)SC1=COC2=CC=CC=C2C1=O	4,3
516	NC1=NN=C(SC2=COC3=CC=CC=C3C2=O)S1	4,32
517	O=C1\C(OC2=CC=CC=C12)=C\N1CCCCC1	4,3
518	CC1=NN=C(SC2=COC3=CC=CC=C3C2=O)S1	4,4
519	FC1=CC=C(C=C1)C(CN1CCN(CC1)\C=C1/OC2=CC=CC=C2C1=O)C1=CC=C(F)C=C1	5,33
520	CN1CCN(CC1)\C=C1/OC2=CC=CC=C2C1=O	4,3
521	O=C1C(SC2=NC3=CC=CC=C3S2)=COC2=CC=CC=C12	4,5
522	COC1=CC(CC(C)(O)C(F)(F)F)=NC(OC)=N1	3,7
523	COC1=CC(CC(C)(CF)OC(C)=O)=NC(OC)=N1	4,75
524	COC1=NC(CC(C)(O)C(F)(F)F)=C(C2=CC=CC=C2)C(OC)=N1	4,72
525	CC(=O)OC(C)(CF)CC1=CC(O)=NC(O)=N1	3,7
526	COC1=NC(CBr)=C(Br)C(OC)=N1	5,15
527	COC1=CC(\C=C(\O)C(F)(F)F)=NC(OC)=N1	3,7
528	COC1=CC(\C=C(/O)C(F)(F)C(F)(F)F)=NC(OC)=N1	4,26
529	COC1=CC(CC(C)(O)C2=CC=C(F)C=C2)=NC(OC)=N1	4
530	COC1=NC(CC(C)(O)C2=CC=C(F)C=C2)=C(C)C(OC)=N1	4,37
531	COC1=NC(C)=C(Br)C(OC)=N1	4
532	COC1=NC(C)=C(C2=CC=CC=C2)C(OC)=N1	4
533	CC(=O)OC(C)(CC1=CC(O)=NC(O)=N1)CC1=CC=CC=C1F	3,7
534	CC(O)(CF)CC1=CC(O)=NC(O)=N1	3,7
535	COC1=CC(CC(C)(O)CF)=NC(OC)=N1	3,7
536	COC1=CC(CC(C)(O)CC2=CC=CC=C2F)=NC(OC)=N1	3,7
537	COC1=NC(OC)=C(Br)C(=N1)C(Br)Br	5,7
538	COC1=CC(\C=C(/C)C2=CC=C(F)C=C2)=NC(OC)=N1	4,7
539	COC1=CC(\C=C(\O)C2=CC=C(F)C=C2)=NC(OC)=N1	4
540	COC1=CC(CC(O)(C2=CC=C(F)C=C2)C2=CC=C(F)C=C2)=NC(OC)=N1	4
541	CC(O)(CC1=CC(O)=NC(O)=N1)C(F)(F)F	4
542	C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@@H](O)[C@@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]2[C@]1(C)O)C(O)=O	3,98
543	Cl.CC(C)NC(=N)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1Cl	4,52
544	Cl.NC(=N)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1Cl	4,54
545	Cl.CC(C)NC(=N)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1	4
546	Cl.C1CN=C(N1)C1=CC=C2N=C3C=CC4=C(C=CC=C4)N3C2=C1	5,7
547	Cl.CC(C)NC(=N)C1=CC=C2C=CC3=NC4=C(C=CC=C4)N3C2=C1	5,8
548	Cl.ClC1=CC=CC=C1\C=C/C1=NC2=CC=C(C=C2N1)C(=N)NN1CCOCC1	5,05
549	Cl.ClC1=CC=CC=C1\C=C\C1=NC2=CC=C(C=C2N1)C1=NCCN1	4,8

NAME	SMILE	lg(1/IC50)
550	Cl.CC(C)NC(=N)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1	4,09
551	Cl.N=C(NN1CCOCC1)C1=CC=C2C=CC3=NC4=C(C=CC=C4)N3C2=C1	5,33
552	C1=CC2=C(C=C1)N1C(C=CC3=CC=CC=C13)=N2	4,82
553	Cl.CC(C)NC(=N)C1=CC2=C(C=C1)N=C1C=CC3=CC=CC=C3N21	5,4
554	Cl.NC(=N)C1=CC=C2C=CC3=NC4=C(C=CC=C4)N3C2=C1	5,4
555	Cl.N=C(NN1CCOCC1)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1	4,21
556	Cl.ClC1=CC=CC=C1\C=C\C1=NC2=CC=C(C=C2N1)C(=N)NN1CCOCC1	5
557	Cl.C1CN=C(N1)C1=CC=C2C=CC3=NC4=C(C=CC=C4)N3C2=C1	5,62
558	Cl.NC(=N)C1=CC2=C(C=C1)N=C1C=CC3=CC=CC=C3N21	4,89
559	Cl.N=C(NN1CCOCC1)C1=CC=C2N=C3C=CC4=C(C=CC=C4)N3C2=C1	5,7
560	Cl.NC(=N)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1	4
561	Cl.NC(=N)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1	4,96
562	Cl.C1CN=C(N1)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1	4,8
563	Cl.ClC1=CC=CC=C1\C=C/C1=NC2=CC=C(C=C2N1)C1=NCCN1	4
564	Cl.N=C(NN1CCOCC1)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1	4,89
565	Cl.CC(C)NC(=N)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1Cl	4,15
566	Cl.NC(=N)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CC=C1Cl	4,64
567	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	7,4
568	Cl.C1CN=C(N1)C1=CC=C2N=C(NC2=C1)\C=C/C1=CC=CC=C1	4,57
569	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC=C3)N=N2)C2=CC3=C(OCO3)C=C12	5,33
570	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC=C3C)N=N2)C2=CC3=C(OCO3)C=C12	5,04
571	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC=C3)N=N2)C2=CC3=C(OCO3)C=C12	5,53
572	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC=C3C)N=N2)C2=CC3=C(OCO3)C=C12	5,82
573	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC=C3Cl)N=N2)C2=CC3=C(OCO3)C=C12	5,9
574	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC(Cl)=C3)N=N2)C2=CC3=C(OCO3)C=C12	5,91
575	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](O[C@@H]2O[C@@H]3CO[C@@H](C)O[C@H]3[C@H](O)[C@H]2O)C2=CC3=C(OCO3)C=C12	5,67
576	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC(=C3)[N+]([O-])=O)N=N2)C2=CC3=C(OCO3)C=C12	5,44
577	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@@H](O)C2=CC3=C(OCO3)C=C12	5,85
578	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=C(C)C=C3)N=N2)C2=CC3=C(OCO3)C=C12	5,49
579	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC(=C3)[N+]([O-])=O)N=N2)C2=CC3=C(OCO3)C=C12	5,39
580	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CNC3=CC=CC(Cl)=C3)N=N2)C2=CC3=C(OCO3)C=C12	5,86
581	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	6,38
582	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(Cl)C=C3)C(=O)C2=C1OC	6,19
583	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCC3=CC=CC=C3)C(=O)C2=C1OC	5,58
584	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OC	6,41
585	CCOC(=O)CNC1=CC(=O)C2=CC(C)=C(C(OC)=C2C1=O)C1=CC(=O)C2=C(OC)C=C(C)C=C2C1=O	6,07
586	CCOC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OCC	5,62
587	COC1=CC(C)=CC2=C1C(=O)C(N)=C(C2=O)C1=C(C)C=C2C(=O)C=C(N)C(=O)C2=C1OC	5,63
588	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC(C)=O)C(=O)C2=C1OC	6,04
589	CC1=CC(O)=C2C(=O)C=C(C(=O)C2=C1)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1O	5,45
590	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(N)C(=O)C2=C1OC	5,45
591	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C4C=CC=CC4=C3)C(=O)C2=C1OC	5,69
592	CCN(CC)C1=CC=C(\C=N\NC(=S)NC2=CC=CC=C2)C(O)=C1	6,52
593	CCN(CC)C1=CC=C(\C=N\NC(N)=S)C(O)=C1	6,05
594	OC1=CC=CC=C1\C=N\NC(=S)NC1=CC=CC=C1	5,62
595	COC1=CC=CC(\C=N\NC(=S)NC2=CC=CC=C2)=C1O	5,8
596	OC1=CC=C2C=CC=CC2=C1\C=N\NC(=S)NC1=CC=CC=C1	6,15
597	COC1=CC=CC(\C=N\NC(N)=S)=C1O	5,85
598	NC(=S)N\N=C\C1=C(O)C=CC2=C1C=CC=C2	6,7
599	NC(=S)N\N=C\C1=CC=CC=C1O	5,3
600	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCNC(N)=N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H]1CCCN1C(=O)[C@H](C)NC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2\C=CC(=N2)\C(=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C\1N2)C1=CC=CC=C1)C1=CC=CC=C1)\C1=CC=CC=C1)C(=O)N[C@@H](CCC(O)=O)C(=O)N[C@@H](CC(O)=O)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCC(O)=O	5,12
601	CC(C)[C@H](NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCNC(N)=N)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@H](CCCCN)NC(=O)[C@@H]1CCCN1C(=O)[C@@H]1CCCN1C(=O)[C@H](C)	4,47

NAME	SMILE	lg(1/IC50)
	NC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2\C=CC(=N2)\C(=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C\1N2)C1=CC=CC=C1)C1=CC=CC=C1)\C1=CC=CC=C1)C(=O)N[C@@H](CCC(O)=O)C(=O)N[C@@H](CC(O)=O)C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCC(N)=O)C(=O)NCC(O)=O	
602	CC[C@H](C)[C@H](NC(=O)[C@H](CCC(N)=O)NC(=O)[C@H](CCCNC(N)=N)NC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2\C=CC(=N2)\C(=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C\1N2)C1=CC=CC=C1)C1=CC=CC=C1)\C1=CC=CC=C1)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H]([C@@H](C)CC)C(=O)N[C@@H](CC1=CNC2=CC=CC=C12)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](C)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](C(C)C)C(=O)NCC(O)=O	4,28
603	CC[C@H](C)[C@H](NC(=O)[C@H](CCC(N)=O)NC(=O)[C@H](CCCNC(N)=N)NC(=O)COCCOCCOCCOCCOCCOCCNC(=O)COCC(=O)NC1=CC=C(C=C1)C1=C2\C=CC(=N2)\C(=C2/N\C(\C=C2)=C(/C2=N/C(/C=C2)=C(\C2=CC=C\1N2)C1=CC=CC=C1)C1=CC=CC=C1)\C1=CC=CC=C1)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H]([C@@H](C)CC)C(=O)N[C@@H](CC1=CNC2=CC=CC=C12)C(=O)N[C@@H](CC1=CC=CC=C1)C(=O)N[C@@H](CCC(N)=O)C(=O)N[C@@H](CC(N)=O)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCSC)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CC1=CNC2=CC=CC=C12)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](C)C(=O)N1CCC[C@H]1C(=O)N1CCC[C@H]1C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](CCCNC(N)=N)C(=O)N[C@@H](CCCCN)C(=O)N[C@@H](C(C)C)C(=O)NCC(O)=O	5,03
604	Cl.NC(=N)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CO1	4,72
605	Cl.C1CN=C(N1)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CS1	4,96
606	Cl.C1CN=C(N1)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CO1	4,17
607	Cl.N=C(NC1CCCCC1)C1=CC=C2N=C(NC2=C1)\C=C\C1=CC=CO1	4,19
608	CC1=CC=C(C=C1)[C@H]1OC(=O)[C@@H]2C=C3[C@](C)(CCCC3(C)C)[C@H]12	4
609	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=CO1	4,01
610	COC1=CC=C(C=C1)[C@H]1OC(=O)[C@@H]2C=C3[C@](C)(CCCC3(C)C)[C@H]12	4
611	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=C(Br)C=C1	4
612	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=CC=C1	4
613	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=C(Cl)C=C1	4
614	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=C(C=C1)C#N	4
615	C[C@]12CCCC(C)(C)C1=C[C@@H]1[C@H]2[C@H](OC1=O)C1=CC=C(F)C=C1	4
616	CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC=C4)N=C13)C2=O	7,24
617	C[C@H]1C(=O)O[C@H]2[C@@H](Cl)C(=C)\C=C\[C@H](OC(C)=O)[C@@]3(C)[C@@H](OC(C)=O)[C@H](CC(=C)[C@@H]3[C@H](OC(C)=O)[C@]12O)OC(C)=O	4,46
618	CC(C)CC(=O)OCC(=O)O[C@H]1\C=C/C(=C)[C@H](Cl)[C@@H]2OC(=O)[C@H](C)[C@@]2(O)[C@@H](OC(C)=O)[C@H]2C(=C)CC[C@H](OC(C)=O)[C@]12C	4,49
619	C[C@H]1C(=O)O[C@H]2[C@@H](Cl)C(=C)[C@@]3(O)C[C@H](OC(C)=O)[C@@]4(C)[C@@H](OC(C)=O)[C@H](CC(=C)[C@@H]4[C@H](OC(C)=O)[C@]12O3)OC(C)=O	4,48
620	CCC(=O)O[C@@H]1C[C@H](OC(C)=O)[C@@]2(C)[C@@H]([C@H](OC(C)=O)[C@]3(O)[C@@H](C)C(=O)O[C@H]3\C=C(C)/CC[C@@H]2OC(C)=O)C1=C	4,45
621	C[C@H]1C(=O)O[C@H]2\C=C(C)/CC[C@H](OC(C)=O)[C@@]3(C)[C@@H](OC(C)=O)[C@H](CC(=C)[C@@H]3[C@H](OC(C)=O)[C@]12O)OC(C)=O	4,44
622	C[C@H]1C(=O)O[C@H]2[C@@H](Cl)C(=C)\C=C\[C@H](OC(C)=O)[C@@]3(C)[C@@H](OC(C)=O)[C@H](C[C@]4(CO4)[C@@H]3[C@H](OC(C)=O)[C@]12O)OC(C)=O	4,48
623	CC(C)CC(=O)OCC(=O)O[C@H]1\C=C/C(=C)[C@H](Cl)[C@@H]2OC(=O)[C@H](C)[C@@]2(O)[C@@H](OC(C)=O)[C@H]2[C@@]3(CO3)CC[C@H](OC(C)=O)[C@]12C	4,51
624	CC(=O)O[C@H]1C[C@H]2CC[C@@](C)(OC(=O)C2=C)[C@@H](CC[C@@](C)(O)[C@@H]2CC[C@@]1(C)O2)OC(C)=O	4,35
625	CC(=O)O[C@H]1C[C@H]2CC[C@@](C)(OC(=O)C2=C)C(=O)CC[C@@](C)(O)[C@@H]2CC[C@@]1(C)O2	4,31
626	CC(=O)O[C@@H]1CC[C@@](C)(O)[C@@H]2CC[C@@](C)(O2)[C@@H](O)C[C@H]2CC[C@@]1(C)OC(=O)C2=C	4,31
627	CC(=O)O[C@H]1CC[C@@]2(C)O[C@]1(C)CCC(=O)[C@@]1(C)CC[C@H](C[C@@H]2O)C(=C)C(=O)O1	4,31
628	C[C@]12CC[C@H](O1)[C@](C)(O)CCC(=O)[C@@]1(C)CC[C@H](C[C@@H]2O)C(=C)C(=O)O1	4,26
629	C[C@]12CC[C@H](O1)[C@](C)(O)CC[C@@H](O)[C@@]1(C)CC[C@H](C[C@@H]2O)C(=C)C(=O)O1	4,27
630	CC(=O)O[C@@H]1CCC(=C)[C@@H]2CC[C@@](C)(O2)[C@@H](O)C[C@H]2CC[C@@]1(C)OC(=O)C2=C	4,29
631	CC(=O)O[C@H]1C[C@H]2CC[C@@](C)(OC(=O)C2=C)[C@@H](CCC(=C)[C@@H]2CC[C@@]1(C)O2)OC(C)=O	4,34
632	CC[C@]1(O)C[C@H]2CN(C1)CCC1=C(NC3=CC=CC=C13)[C@@](C2)(C(=O)OC)C1=CC2=C(C=C1OC)N(C=O)[C@@H]1[C@]22CCN3CC=C[C@](CC)([C@@H]23)[C@@H](OC(C)=O)[C@]1(O)C(=O)OC	8,44
633	C[C@H](OC(C)=O)[C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H](OC(C)=O)\C=C/[C@H]1CC=CC(=O)O1	4,66
634	C[C@H](OC(C)=O)[C@@H](C[C@H](OC(C)=O)\C=C/[C@H]1CC=CC(=O)O1)OC(C)=O	4,77
635	CC1=C2NC3=C(C=CC=C3)C2=C(C)C2=C1C=CN=C2	5,79
636	CC1=CC=NC(NC2=NC3=CC=C(C=C3S2)C#N)=C1	5,15
637	ClC1=CC=C(NC2=NC3=CC=C(C=C3S2)C#N)N=C1	5

NAME	SMILE	lg(1/IC50)
638	N#CC1=CC=C2N=C(NC3=NC=CC=N3)SC2=C1	5,3
639	CC1=CC=CC(NC2=NC3=CC=C(C=C3S2)C#N)=N1	5
640	CC1=CC=C(NC2=NC3=CC=C(C=C3S2)C#N)N=C1	5
641	N#CC1=CC=C(NC2=NC3=CC=C(C=C3S2)C#N)C=C1	5
642	CC1=CC=CN=C1NC1=NC2=CC=C(C=C2S1)C#N	5
643	[Br-].CC(=O)CC1=CC=C(C=C1)N1C=C[N+](CC(=O)C2=CC=CC=C2)=C1	3,7
644	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C1=CC=C(C=C1)[N+]([O-])=O	4,38
645	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(CCC2=CC=C(OC)C(OC)=C2)C=C1	4,21
646	[Br-].O=C(C[N+]1=CN(C=C1)C12CC3CC(CC(C3)C1)C2)C1=CC=CC=C1	4,03
647	[Br-].CC(C)(C)N1C=C[N+](CC(=O)C2=CC=CC=C2)=C1	3,7
648	[Br-].CC1=C(C)[N+](CC(=O)C2=CC=C3C=CC=CC3=C2)=CN1C1=C(C)C=C(C)C=C1C	5,72
649	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C1=CC=C(CC(C)=O)C=C1	4,07
650	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C3=CC=C(Br)C=C3)=C2)C(C)=C1	4,66
651	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C3=CC=CC=C3)=C2)C(C)=C1	4,01
652	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C1=C(C)C=C(C)C=C1C	5,82
653	[Br-].O=C(C[N+]1=CN(C=C1)C12CC3CC(CC(C3)C1)C2)C1=CC=C2C=CC=CC2=C1	6,1
654	[Br-].CC(C)C1=CC=CC(C(C)C)=C1N1C=C[N+](CC(=O)C2=CC=C3COCC3=C2)=C1	4,94
655	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C1=C(C=CC=C1C(C)C)C(C)C	5,55
656	[Br-].CC(C)C1=CC=CC(C(C)C)=C1N1C=C[N+](CC(=O)C2=CC=C3C=CC=CC3=C2)=C1	5,46
657	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C3=CC=C4C=CC=CC4=C3)=C2)C(C)=C1	6,15
658	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C12CC3CC(CC(C3)C1)C2	5,15
659	[Br-].COC1=CC=C(CCN2C=C[N+](CC(=O)C3=CC=C4C=CC=CC4=C3)=C2)C=C1OC	4,11
660	[Br-].CC(C)C1=CC=CC(C(C)C)=C1N1C=C[N+](CC(=O)C2=CC=C(Br)C=C2)=C1	5,04
661	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C3=CC=C4COCC4=C3)=C2)C(C)=C1	4,91
662	[Br-].COC1=CC=C(C=C1)C(=O)C[N+]1=CN(C=C1)C(C)(C)C	3,93
663	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C(C)(C)C)=C2)C(C)=C1	3,88
664	O=C(CCC1=NC(=NO1)C1=CC=CC=C1)OCC#C	3,71
665	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=CC=C2C)N=N1	4,11
666	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=C(C)C=C2)N=N1	4,11
667	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=CC=C2)N=N1	4,1
668	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=C(Cl)C=C2)N=N1	4,12
669	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=CC(C)=C2)N=N1	4,11
670	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=C(Br)C=C2)N=N1	4,15
671	CC(=O)OC[C@H]1O[C@H]([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(COC(=O)CCC2=NC(=NO2)C2=CC=C(C=C2)[N+]([O-])=O)N=N1	4,13
672	CC1=CC=C2C(=O)C(CSC(=S)N3CCCC3)=COC2=C1	5,44
673	CC1=CC=C2C(=O)C(CSC(=S)N3CCOCC3)=COC2=C1	5,4
674	O=C1C(CSC(=S)N2CCOCC2)=COC2=CC=CC=C12	5,36
675	CCN(CC)C(=S)SCC1=CC(=O)C2=CC=C(Cl)C=C2O1	5,06
676	CC(C)N(C(C)C)C(=S)SCC1=CC(=O)C2=CC=CC=C2O1	4,87
677	CC1=CC=C2C(=O)C(CSC(=S)N3CCCCC3)=COC2=C1	6,05
678	CC(C)N(C(C)C)C(=S)SCC1=COC2=CC=CC=C2C1=O	5,52
679	COC1=CC=C2OC=C(CSC(=S)N3CCOCC3)C(=O)C2=C1	5,32
680	O=C1C(SC(=S)N2CCCC2)=COC2=CC=CC=C12	5,13
681	COC1=CC=C2OC=C(CSC(=S)N3CCCCC3)C(=O)C2=C1	5,37
682	O=C1C(CSC(=S)N2CCN(CC2)C2=CC=CC=C2)=COC2=CC=CC=C12	4,78
683	CN(C(=S)SCC1=COC2=CC=CC=C2C1=O)C1=CC=CC=C1	4,6
684	CC(C)N(C(C)C)C(=S)SCC1=CC(=O)C2=CC=C(Cl)C=C2O1	4,64
685	O=C1C(CSC(=S)N2CCCCC2)=COC2=CC=CC=C12	6,41
686	ClC1=C(CSC(=S)N2CCCCC2)OC2=CC=CC=C2C1=O	6,03
687	ClC1=CC=C2C(=O)C=C(CSC(=S)N3CCOCC3)OC2=C1	4,69
688	ClC1=CC=C2C(=O)C=C(CSC(=S)N3CCCC3)OC2=C1	4,4
689	FC1=CC=C(C=C1)C(N1CCN(CC1)C(=S)SCC1=COC2=CC=CC=C2C1=O)C1=CC=C(F)C=C1	5,02
690	O=C1C=C(CSC(=S)N2CCOCC2)OC2=CC=CC=C12	4,6
691	O=C1C(SC(=S)N2CCCCC2)=COC2=CC=CC=C12	5,24
692	COC1=CC=C2OC(CSC(=S)N3CCCCC3)=CC(=O)C2=C1	5,82
693	ClC1=C(CSC(=S)N2CCCC2)OC2=CC=CC=C2C1=O	6,22
694	COC1=CC=C2OC=C(CSC(=S)N3CCCC3)C(=O)C2=C1	5,51
695	CC(C)N(C(C)C)C(=S)SCC1=COC2=CC(Cl)=CC=C2C1=O	5,38
696	CN1CCN(CC1)C(=S)SCC1=COC2=CC=CC=C2C1=O	5,62
697	O=C1C=C(CSC(=S)N2CCCC2)OC2=CC=CC=C12	5,04
698	O=C1C=C(CSC(=S)N2CCCCC2)OC2=CC=CC=C12	4,92
699	ClCCN(CCCl)C(=S)SCC1=CC(=O)C2=CC=CC=C2O1	4,81
700	ClC1=CC=C2OC=C(SC(=S)N3CCCCC3)C(=O)C2=C1	4,91
701	ClC1=CC=C2C(=O)C(CSC(=S)N3CCCCC3)=COC2=C1	6,55
702	COC1=CC=C2OC(CSC(=S)N(C(C)C)C(C)C)=CC(=O)C2=C1	5,12
703	CCOC(=O)C1=CC(=O)C2=CC(CSC(=S)N3CCOCC3)=CC=C2O1	4,6
704	CCOC(=O)C1=CC(=O)C2=CC(CSC(=S)N(C(C)C)C(C)C)=CC=C2O1	4,8
705	O=C1C(CSC(=S)N2CCCC2)=COC2=CC=CC=C12	5,44

NAME	SMILE	lg(1/IC50)
706	CC(C)N(C(C)C)C(=S)SCC1=C(Cl)C(=O)C2=CC=CC=C2O1	4,7
707	ClC1=C(CSC(=S)N2CCOCC2)OC2=CC=CC=C2C1=O	5,05
708	CCOC(=O)C1=CC(=O)C2=CC(CSC(=S)N3CCCCC3)=CC=C2O1	5,47
709	CC1=CC=C2C(OC=C(CSC(=S)N(CCCl)CCCl)C2=O)=C1	5,1
710	ClC1=CC=C2C(=O)C(CSC(=S)N3CCCC3)=COC2=C1	5,68
711	ClC1=CC=C2OC=C(SC(=S)N3CCCC3)C(=O)C2=C1	4,59
712	O=C1C(CSC(=S)N2CCN(CC3=CC=CC=C3)CC2)=COC2=CC=CC=C12	5,54
713	COC1=CC=C2OC=C(CSC(=S)N(C(C)C)C(C)C)C(=O)C2=C1	5,05
714	COC1=CC=C2OC(CSC(=S)N3CCOCC3)=CC(=O)C2=C1	5,52
715	ClC1=CC=C2C(=O)C=C(CSC(=S)N3CCN(CC3)C3=CC=CC=C3)OC2=C1	4,8
716	CCOC(=O)C1=CC(=O)C2=CC(CSC(=S)N3CCCC3)=CC=C2O1	5,05
717	ClC1=CC=C2C(=O)C=C(CSC(=S)N3CCCCC3)OC2=C1	5,8
718	CC(C)N(C(C)C)C(=S)SCC1=COC2=CC(C)=CC=C2C1=O	6,15
719	ClC1=CC=C2C(=O)C(CSC(=S)N3CCOCC3)=COC2=C1	6,05
720	[O-][Cl](=O)(=O)=O.CC1=C\C(=C\C2=[N+](C)C3=CC=CC=C3O2)N=C2SC3=CC(OCCO)=CC=C3N12	5,17
721	[O-][Cl](=O)(=O)=O.CC1=C\C(=C\C2=[N+](C)C3=CC=CC=C3S2)N=C2SC3=CC(OCCO)=CC=C3N12	6,03
722	[O-][Cl](=O)(=O)=O.CC1=C\C(=C\C2=[N+](C)C3=CC=CC=C3O2)C(C#N)=C2SC3=CC=CC=C3N12	5,26
723	[O-][Cl](=O)(=O)=O.CCOC1=CC=C2N3C(SC2=C1)=N\C(=C/C1=[N+](C)C2=CC=CC=C2O1)C=C3C	6,3
724	[O-][Cl](=O)(=O)=O.COC1=CC=C2N3C(SC2=C1)=N\C(=C/C1=[N+](C)C2=CC=CC=C2O1)C=C3C	6,15
725	[O-][Cl](=O)(=O)=O.CC1=C\C(=C\C2=[N+](C)C3=CC=CC=C3O2)N=C2SC3=CC(Cl)=CC=C3N12	5,15
726	[O-][Cl](=O)(=O)=O.COC1=CC=C2N3C(SC2=C1)=N\C(=C/C1=[N+](C)C2=CC=CC=C2S1)C=C3C	6,3
727	[O-][Cl](=O)(=O)=O.CC1=C\C(=C\C2=[N+](C)C3=CC=CC=C3S2)N=C2C=CC=CN12	5,44
728	COC(=O)C1=C2C=C(COC2(O)[C@H]2OC(=O)[C@@]11CCCC(C)(C)[C@H]21)C(C)C	4,22
729	CC(C)C1=CC2=C[C@H]3OC(=O)[C@@]4(CCCC(C)(C)[C@H]34)C2=C(O)C1=O	4,49
730	SC1=NC=NC2=C1NC=N2	3,5
731	C[C@H]1COC2=C(O)C3=C(C=C12)[C@@H]1C[C@H]2C(C)(C)CCC[C@]32C(=O)O1	4,22
732	C[C@H]1COC2=C1C(=O)C1=C(C2=O)[C@@]23CCCC(C)(C)[C@@H]2C[C@@H]1OC3=O	4,4
733	C[C@H]1COC2=C1C(=O)C1=C(C2=O)[C@@]23CCCC(C)(C)[C@@H]2C[C@@H]1OC3=O	4,23
734	CO[C@@H]1[C@H]2OC(=O)[C@@]3(CCCC(C)(C)[C@H]23)C2=C1C=C(C(C)C)C(=O)C2=O	4,37
735	CC(C)C1=CC2=C[C@H]3OC(=O)[C@@]4(CCCC(C)(C)[C@H]34)C2=C(O)C1=O	4,72
736	CC(C)C1=CC2=C(C(O)=C1O)[C@]1(CCCC(C)(C)[C@@H]1C[C@H]2SC1=CC=CC=C1)C(O)=O	4,82
737	CC(C)C1=CC2=C(C(=O)C1=O)[C@@]13CCCC(C)(C)[C@@H]1[C@@H](O)[C@@H]2OC3=O	4,41
738	CC(C)C1=CC2=C(C(=O)C1=O)[C@@]13CCCC(C)(C)[C@@H]1[C@@H](O)[C@@H]2OC3=O	4,4
739	CC(C)C1=CC2=C(C(=O)C1=O)[C@@]13CCCC(C)(C)[C@@H]1C[C@@H]2OC3=O	4,22
740	SC1=NC=NC2=C1NC=N2	3,37
741	C[C@@H](COC(C)=O)C1=C(OC(C)=O)C(O)C2=C([C@@H]3C[C@H]4C(C)(C)CCC[C@]24C(=O)O3)C1=O	4,35
742	CC(C)C1=CC2=C(C(O)=C1O)[C@]1(CCCC(C)(C)[C@@H]1C[C@H]2SC1=CC=CC=C1)C(O)=O	4,72
743	CO[C@@H]1[C@H]2OC(=O)[C@@]3(CCCC(C)(C)[C@H]23)C2=C1C=C(C(C)C)C(=O)C2=O	4,22
744	ClC1=CC=C2C(OC=C(C3SSC(=N3)C3=CC=CC=C3)C2=O)=C1	4
745	FC1=CC2=C(OC=C(C3SSC(=N3)C3=CC=CC=C3)C2=O)C=C1Cl	4,01
746	FC1=CC=C2OC=C(C(=S)NC3=CC=CC=C3)C(=O)C2=C1	4
747	ClC1=CC=C2C(=O)C(=COC2=C1)C(=S)NC1=CC=CC=C1	4
748	O=C1C(=COC2=CC=CC=C12)C1SSC(=N1)C1=CC=CC=C1	4
749	CC1=CC=C2OC=C(C3SSC(=N3)C3=CC=CC=C3)C(=O)C2=C1	4
750	FC1=CC=C2OC=C(C3SSC(=N3)C3=CC=CC=C3)C(=O)C2=C1	4,01
751	O=C1C(=COC2=CC=CC=C12)C(=S)NC1=CC=CC=C1	4
752	ClC1=CC=C2OC=C(C3SSC(=N3)C3=CC=CC=C3)C(=O)C2=C1	4,13
753	CO[C@]12[C@H]3N[C@H]3CN1C1=C([C@H]2COC(N)=O)C(=O)C(N)=C(C)C1=O	5,82
754	ClC1=CC2=C(C=C1Cl)C(=O)C(=CO2)C(=S)NC1=CC=CC=C1	4
755	ClC1=CC2=C(C=C1Cl)C(=O)C(=CO2)C1SSC(=N1)C1=CC=CC=C1	4,01
756	Cl.Cl.NC(=N)C1=CC=C2N=C(SC2=C1)C1=CC=C(S1)C1=NC2=CC=C(C=C2S1)C(N)=N	6,33
757	Cl.Cl.C1CN=C(N1)C1=CC=C(C=C1)C1=CC=C(S1)C1=NC2=CC=C(C=C2S1)C1=NCCN1	6,82
758	Cl.Cl.C1CN=C(N1)C1=CC=C2N=C(SC2=C1)C1=CC=C(S1)C1=NC2=CC=C(C=C2S1)C1=NCCN1	6,77
759	Cl.Cl.CC(C)NC(=N)C1=CC=C(C=C1)C1=CC=C(O1)C1=NC2=CC=C(C=C2S1)C(=N)NC(C)C	4,29
760	Cl.Cl.C1CN=C(N1)C1=CC=C(C=C1)C1=CC=C(O1)C1=NC2=CC=C(C=C2S1)C1=NCCN1	6,43
761	Cl.Cl.C1CN=C(N1)C1=CC=C2N=C(SC2=C1)C1=CC=C(O1)C1=NC2=CC=C(C=C2S1)C1=NCCN1	4
762	Cl.Cl.NC(=N)C1=CC=C2N=C(SC2=C1)C1=CC=C(O1)C1=NC2=CC=C(C=C2S1)C(N)=N	4
763	Cl.Cl.CC(C)NC(=N)C1=CC=C(C=C1)C1=CC=C(S1)C1=NC2=CC=C(C=C2S1)C(=N)NC(C)C	4,51
764	[Br-].CC1=CC(C)=C(N2C=C[N+](CC(=O)C3=CC=C4C=CC=CC4=C3)=C2)C(C)=C1	6,16
765	CC1=CC=C(NC(=O)C2=C(C(=NN2C2=CC=CC=C2)C2=CC=CC=C2)C2=CC=C(Cl)C=C2)C=C1	5,76
766	O=C(NC1=CC=CC=C1)C1=C(C(=NN1C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1	5,44
767	O=C(N1C(=S)NC2=CC=CC=C12)C1=C(C(=NN1C1=CC=CC=C1)C1=CC=CC=C1)C1=CC=CC=C1	4,82
768	ClC1=CC=C(C=C1)C1=C(N(N=C1C1=CC=CC=C1)C1=CC=CC=C1)C(=O)NC1=CC=CC=C1	5,78
769	CC1=CC=C(NC(=O)C2=C(C(=NN2C2=CC=CC=C2)C2=CC=C(Cl)C=C2)C2=CC=CC=C2)C=C1	5,58
770	CC1=CC=C(NC(=O)C2=C(C(=NN2C2=CC=CC=C2)C2=CC=CC=C2)C2=CC=CC=C2)C=C1	5,55
771	ClC1=CC=C(C=C1)C1=C(N(N=C1C1=CC=CC=C1)C1=CC=CC=C1)C(=O)N1C(=S)NC2=CC=CC=C12	5,52
772	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	6,13
773	COC1=CC=C(C=C1)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	6,28
774	COC(=O)NNC(=O)C(=C\C1=CC=C2C=CC=CC2=C1)\C1=CC(OC)=C(OC)C(OC)=C1	7,27
775	COC(=O)NNC(=O)C(=C\C1=CC=C2C=CC=CC2=C1)\C1=CC(OC)=C(OC)C(OC)=C1	7,29
776	COC1=CC=C(C=C1F)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	5,93
777	COC1=CC=C(\C=C/C2=CC(OC)=C(OC)C(OC)=C2)C=C1O	8,28

NAME	SMILE	lg(1/IC50)
778	COC1=CC=C(\C=C/C2=CC(OC)=C(OC)C(OC)=C2)C=C1O	8,26
779	COC1=CC=C(C=C1)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	6,21
780	COC1=CC=C(C=C1F)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	6,16
781	COC1=CC=C(C=C1O)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	6,15
782	COC1=CC=C(C=C1O)C1=C(C(=O)NN1)C1=CC(OC)=C(OC)C(OC)=C1	5,94
783	OC(=O)C1=C(NC2=CC=CC=C2C1=O)C1=CC=CN1	3,41
784	CC1(C)CC[C@H](O)[C@]23CO[C@@](O)([C@@H](O)[C@H]12)[C@@]12[C@H](O)[C@@H](CC[C@@H]31)C(=C)C2=O	4,43
785	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO)C(=O)C2=C1OC	5,85
786	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(SCCO)C(=O)C2=C1OC	5,77
787	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](COC(C)=O)[C@H](OC(C)=O)[C@H](OC(C)=O)[C@H]4OC(C)=O)C=C3)C(=O)C2=C1OC	6,05
788	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OC	6,4
789	CCOC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1OCC	5,62
790	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](CO)[C@@H](O)[C@H](O)[C@H]4O)C=C3)C(=O)C2=C1OC	5,74
791	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](CO)[C@@H](O)[C@H](O)[C@@H]4O)C=C3)C(=O)C2=C1OC	6,52
792	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO[C@H]3O[C@H](COC(C)=O)[C@@H](OC(C)=O)C=C3)C(=O)C2=C1OC	6,15
793	CC(=O)OC[C@H]1OC(OC2=CC(C)=CC3=C2C(=O)C=C(C3=O)C2=C(C)C=C3C(=O)C=CC(=O)C3=C2O)[C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O	5,38
794	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](CO)[C@H](O)[C@H](O)[C@H]4O)C=C3)C(=O)C2=C1OC	5,35
795	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO[C@@H]3O[C@H](COC(C)=O)[C@@H](OC(C)=O)C=C3)C(=O)C2=C1OC	6
796	COC1=CC(C)=CC2=C1C(=O)C(N)=C(C2=O)C1=C(C)C=C2C(=O)C=C(N)C(=O)C2=C1OC	5,64
797	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(N)C(=O)C2=C1OC	5,46
798	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCC3=CC=CC=C3)C(=O)C2=C1OC	5,59
799	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H](OC(C)=O)[C@H]4OC(C)=O)C=C3)C(=O)C2=C1OC	6,3
800	COC1=CC(C)=CC2=C1C(=O)C1OC1(C2=O)C1=C(C)C=C2C(=O)C3OC3C(=O)C2=C1OC	6,7
801	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C4C=CC=CC4=C3)C(=O)C2=C1OC	5,7
802	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC(C)=O)C(=O)C2=C1OC	6,05
803	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(OC4O[C@H](COC(C)=O)[C@@H](OC(C)=O)[C@H](OC(C)=O)[C@@H]4OC(C)=O)C=C3)C(=O)C2=C1OC	5,54
804	CCOC1=C2C(O)=CC(=C(O)C2=CC(C)=C1)C1=C(C)C=C2C(O)=CC=C(O)C2=C1OCC	5,77
805	CC1=CC(O)=C2C(=O)C=C(C(=O)C2=C1)C1=C(C)C=C2C(=O)C=CC(=O)C2=C1O	5,44
806	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NC3=CC=C(Cl)C=C3)C(=O)C2=C1OC	6,15
807	CCOC(=O)CNC1=CC(=O)C2=CC(C)=C(C(OC)=C2C1=O)C1=CC(=O)C2=C(OC)C=C(C)C=C2C1=O	6,05
808	CCOC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCO)C(=O)C2=C1OCC	6,05
809	COC1=CC(C)=CC2=C1C(=O)C=C(C2=O)C1=C(C)C=C2C(=O)C=C(NCCOC3O[C@H](COC(C)=O)[C@@H](OC(C)=O)C=C3)C(=O)C2=C1OC	5,24
810	FC1=CC=C(C=C1)C(=O)NC\C=C/CN1C=CC(=O)NC1=O	4
811	FC1=CN(C\C=C/CNC(=O)C2=CC=CC=C2)C(=O)NC1=O	4,06
812	FC(F)(F)C1=CN(C\C=C/CNC(=O)C2=CC=CC=C2)C(=O)NC1=O	4
813	NC1=NC(=O)N(C\C=C/CNC(=O)C2=CC=CC=C2)C=C1F	4
814	NC1=C2N=CN(C\C=C/CNC(=O)C3=CC=CC=C3)C2=NC=N1	4
815	NC1=NC(=O)N(C\C=C/CNC(=O)C2=CC=C(F)C=C2)C=C1F	4,49
816	NC1=NC(=O)N(C\C=C/CNC(=O)C2=CC=CC=C2)C=C1	4
817	CC1=CN(C\C=C/CNC(=O)C2=CC=C(F)C=C2)C(=O)NC1=O	4
818	CC1=CN(C\C=C/CNC(=O)C2=CC=CC=C2)C(=O)NC1=O	4
819	NC1=NC(=O)N(C\C=C/CNC(=O)C2=CC=C(F)C=C2)C=C1	4
820	O=C(NC\C=C/CN1C=CC(=O)NC1=O)C1=CC=CC=C1	4
821	OC1=CC=C2C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)=CC(=O)OC2=C1	4
822	OC1=CC=C2OC(=O)C=C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)C2=C1	4
823	CC1=CC=C2C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)=CC(=O)OC2=C1	4
824	ClC1=CC=C2C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)=CC(=O)OC2=C1	4
825	[O-][N+](=O)C1=CC=C2C(CC3=C4C=CC=CC4=NC4=C3C=CC=C4)=CC(=O)OC2=C1	4
826	ClC1=CC=C2OC(=O)C=C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)C2=C1	4
827	CC1=CC=C2OC(=O)C=C(CC3=C4C=CC=CC4=NC4=CC=CC=C34)C2=C1	4
828	O=C1OC2=CC=CC=C2C(CC2=C3C=CC=CC3=NC3=C2C=CC=C3)=C1	4
829	ClCCN(CCCl)P1(=O)NCCCO1	4
830	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC3=C(C=CC4=CC=CC=C34)C3=CC=CC=C23)C2=CC3=C(OCO3)C=C12	8
831	CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC=C4)N=C13)C2=O	6,15
832	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=C(C=C2)C(=O)C2=CC=C(F)C=C2)C2=CC3=C(OCO3)C=C12	5,15
833	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=C3C=CC4=CC=CC5=CC=C2C3=C45)C2=CC3=C(OCO3)C=C12	9,7
834	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=C3C=C4C=CC=CC4=CC3=CC=C2)C2=CC3=C(OCO3)C=C12	5,17

NAME	SMILE	lg(1/IC50)
835	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=CC3=C2CC2=CC=CC=C32)C2=CC3=C(OCO3)C=C12	5,52
836	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC3=C(C=CC4=CC=CC=C34)C3=CC=CC=C23)C2=CC3=C(OCO3)C=C12	8,7
837	FC1=CNC(=O)NC1=O	6,52
838	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=C(C=C2)C(=O)C2=CC=C(F)C=C2)C2=CC3=C(OCO3)C=C12	5,89
839	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=C3C=C4C=CC=CC4=CC3=CC=C2)C2=CC3=C(OCO3)C=C12	5,07
840	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=C(C=C2)C(=O)C2=CC=C(C=C2)N(CCCl)CCCl)C2=CC3=C(OCO3)C=C12	6,05
841	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](NC2=CC=CC3=C2CC2=CC=CC=C32)C2=CC3=C(OCO3)C=C12	6
842	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](O[C@@H]2O[C@@H]3CO[C@@H](C)O[C@H]3[C@H](O)[C@H]2O)C2=CC3=C(OCO3)C=C12	6,05
843	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(N3C=CC4=CC=CC=C34)C(OC)=C2)=CC=C1N1C=CC2=CC=CC=C12	4
844	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(C(N)=O)C(OC)=C2)=CC=C1C(N)=O	4
845	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(N3C=CN=C3)C(OC)=C2)=CC=C1N1C=CN=C1	4
846	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(O)C(OC)=C2)=CC=C1O	4,24
847	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(N3C=NC4=CC=CC=C34)C(OC)=C2)=CC=C1N1C=NC2=CC=CC=C12	4
848	CNC1=CC=C(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(NC)C(OC)=C2)C=C1OC	4
849	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(I)C(OC)=C2)=CC=C1I	4
850	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(NC(C)=O)C(OC)=C2)=CC=C1NC(C)=O	4
851	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(N3C=CC=N3)C(OC)=C2)=CC=C1N1C=CC=N1	4
852	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(Br)C(OC)=C2)=CC=C1Br	4
853	COC1=CC(\C=C\C(\O)=C\C(=O)\C=C\C2=CC=C(N)C(OC)=C2)=CC=C1N	4
854	ClC1=CC=C(C=C1)N1C(=O)N(CC2=CC=CC=C2)C(=N)C1=S	5
855	COC1=CC=C(N2C(=O)N(C(=N)C2=S)C2=CC=C(C)C=C2)C(OC)=C1	4,7
856	COC1=CC=C(N2C(=O)N(C(=N)C2=S)C2=CC=C(SC)C=C2)C(OC)=C1	4,51
857	COC1=CC=C(C=C1)N1C(=O)N(C(=S)C1=N)C1=CC=C(OC)C=C1OC	4,98
858	CCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	4,68
859	CCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	7,3
860	CCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,8
861	COC1=CC(=CC(OC)=C1OC)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CO)N=N2)C2=CC3=C(OCO3)C=C12	7,22
862	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](O[C@@H]2O[C@@H]3CO[C@@H](C)O[C@H]3[C@H](O)[C@H]2O)C2=CC3=C(OCO3)C=C12	5,67
863	CCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	7,22
864	CCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,11
865	CCCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	4,74
866	CCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	4
867	CCCCCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	4,72
868	COC1=CC(=CC(OC)=C1O)[C@H]1[C@@H]2[C@H](COC2=O)[C@H](N2C=C(CO)N=N2)C2=CC3=C(OCO3)C=C12	5,17
869	CCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,02
870	CCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	4,77
871	CCCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,42
872	CCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5
873	CCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,01
874	CCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,54
875	CCCCCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(OC)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,24
876	CCCCCCCC1=CN(N=N1)[C@H]1[C@H]2COC(=O)[C@@H]2[C@H](C2=CC(OC)=C(O)C(OC)=C2)C2=CC3=C(OCO3)C=C12	5,22
877	[O-][N+](=O)C1=CC=C(Cl)C(\C=C\C2=NC3=NC=CC=C3N2)=C1	4,31
878	[O-][N+](=O)C1=CC=C(Cl)C(\C=C\C2=NC3=NC=C(Br)C=C3N2)=C1	6,04
879	NC1=CC=C2N3C(C=CC2=C1)=NC1=C3C=C(Br)C=N1	4,85
880	ClC1=CC=CN=C1\C=C\C1=NC2=NC=CC=C2N1	4
881	[O-][N+](=O)C1=CC=C2N3C(C=CC2=C1)=NC1=C3C=CC=N1	4
882	C1=CC2=C(N=C3C=CC4=NC=CC=C4N23)N=C1	4

NAME	SMILE	lg(1/IC50)
883	Cl.NC1=CC=C2N3C(C=CC2=C1)=NC1=C3C=CC=N1	4,57
884	N#CC1=CC=C2C=CC3=NC4=C(C=CC=N4)N3C2=C1	4,33
885	ClC1=CC=CC=C1\C=C\C1=NC2=NC=CC=C2N1	4,53
886	[I-].C[N+]1=CC=CC2=C1N=C1C=CC3=CC=CC=C3N21	4,88
887	BrC1=CN=C2N=C(NC2=C1)\C=C\C1=CC=C(C=C1)C#N	5,24
888	Cl.C1CN=C(N1)C1=CC=C2C=CC3=NC4=C(C=CC=N4)N3C2=C1	6,57
889	Cl.BrC1=CC2=C(N=C3C=CC4=CC=C(C=C4N23)C2=NCCN2)N=C1	5,4
890	[O-][N+](=O)C1=CC=C2N3C(C=CC2=C1)=NC1=C3C=C(Br)C=N1	4,51
891	FC1=CNC(=O)NC1=O	4
892	[I-].C[N+]1=CC=CC2=C1N=C1C=CC3=CC(=CC=C3N21)[N+]([O-])=O	4,5
893	N1C(\C=C\C2=CC=CC=C2)=NC2=NC=CC=C12	5,41
894	Cl.NC1=CC=C2N3C(C=CC2=C1)=NC1=C3C=C(Br)C=N1	4,67
895	C1=CC2=C(N=C3C=CC4=CC=CC=C4N23)N=C1	4,28
896	NC1=CC=C2N3C(C=CC2=C1)=NC1=C3C=CC=N1	4,41
897	N#CC1=CC=C(\C=C\C2=NC3=NC=CC=C3N2)C=C1	4,07
898	O=C(NC1=CC=C(C=C1)C#N)C1=CC=C(O1)C(=O)NC1=CC=C(C=C1)C#N	4
899	Cl.Cl.CC(C)NC(=N)C1=CC=C(NC(=O)C2=CC=C(O2)C(=O)NC2=CC=C(C=C2)C(=N)NC(C)C)C=C1	5,3
900	O=C(NC1=CC=C(C=C1)C#N)C1=CC=CO1	4
901	Cl.CC(C)NC(=N)C1=CC=C(NC(=O)C2=CC=CO2)C=C1	4
902	Cl.Cl.CC(C)NC(=N)C1=CC=C(NC(=O)C2=CC=CC(=N2)C(=O)NC2=CC=C(C=C2)C(=N)NC(C)C)C=C1	4,52
903	Cl.Cl.NC(=N)C1=CC=C(NC(=O)C2=CC=C(O2)C(=O)NC2=CC=C(C=C2)C(N)=N)C=C1	4,96
904	Cl.Cl.NC(=N)C1=CC=C(NC(=O)C2=CC=CC(=N2)C(=O)NC2=CC=C(C=C2)C(N)=N)C=C1	4,33
905	Cl.NC(=N)C1=CC=C(NC(=O)C2=CC=CO2)C=C1	4
906	Cl.Cl.CC(C)NC(=N)C1=CC=C(C=C1)C(=O)NC1=CC=CC(NC(=O)C2=CC=C(C=C2)C(=N)NC(C)C)=N1	4,42
907	Cl.Cl.NC(=N)C1=CC=C(C=C1)C(=O)NC1=CC=CC(NC(=O)C2=CC=C(C=C2)C(N)=N)=N1	4,68
908	CC(=O)N(\N=N\C1=CC=C(C=C1Cl)[N+]([O-])=O)C1=CC=C(C=C1Cl)[N+]([O-])=O	6,21
909	NC1=NC=CC(=N1)C1=CNC2=CC=CC(O)=C12	4
910	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)N[C@@H](CC(O)=O)C(O)=O)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	3,43
911	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)NCCC(=O)N[C@@H](CC(O)=O)C(O)=O)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	3,42
912	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(O)=O)=C(N1)\C(CC(O)=O)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(O)=O	4,68
913	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)N[C@@H](CCCCN)C(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	4,54
914	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)N[C@@H](CC(O)=O)C(O)=O)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	3,55
915	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)NCCNC(=O)[C@@H](N)CCCCN)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	3,57
916	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)N[C@@H](CCCCN)C(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	3,4
917	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)N[C@@H](CC(O)=O)C(O)=O)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	5,4
918	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)NCCNC(=O)[C@@H](N)CCCCN)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	5,87
919	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(O)=O)=C(N1)\C(CC(O)=O)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(O)=O	3,4
920	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)N[C@@H](CCCCN)C(=O)OC	3,4
921	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)OC)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)N[C@@H](CCCCN)C(=O)OC	4,58
922	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)N[C@@H](CC(O)=O)C(O)=O)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	6,21
923	CCC1=C(C)C2=N\C1=C/C1=C(C)C(C(=O)NCCC(=O)N[C@@H](CC(O)=O)C(O)=O)=C(N1)\C(CC(=O)OC)=C1/N=C(/C=C3/NC(=C2)C(C=C)=C3C)[C@@H](C)[C@@H]1CCC(=O)OC	6,09
924	CC1=NNC(=O)\C1=C\C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1	5,1
925	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	5,06
926	ClC1=CC=C2NC(=C(C=C3C(=O)NC(=S)NC3=O)C2=C1)C1=CC=CC=C1	4,34
927	O=C1NC(=S)NC(=O)C1=CC1=CNC2=CC=CC=C12	4
928	O=C1NC(=O)C(=CC2=CNC3=CC=CC=C23)C(=O)N1	4
929	CC1=CC=C2NC(=C(\C=C3/SC(=O)NC3=O)C2=C1)C1=CC=CC=C1	4
930	O=C1NC(=O)\C(S1)=C\C1=CNC2=CC=CC=C12	4
931	CC1=NNC(=O)\C1=C\C1=CNC2=CC=CC=C12	5,92
932	ClC1=CC=C2NC(=C(C=C3C(=O)NC(=O)NC3=O)C2=C1)C1=CC=CC=C1	4
933	CC1=CC=C2NC(=C(C=C3C(=O)NC(=S)NC3=O)C2=C1)C1=CC=CC=C1	4
934	CC1=NNC(=O)\C1=C\C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1	4,58
935	CC1=CC=C2NC(=C(C=C3C(=O)NC(=O)NC3=O)C2=C1)C1=CC=CC=C1	4
936	ClC1=CC=C2NC(=C(\C=C3/SC(=O)NC3=O)C2=C1)C1=CC=CC=C1	4,92
937	CC1C(CCC1(C)\C=C\C1=CC=C(O)C=C1)C(C)(C)O	4,72
938	COC1=CC=C(\C=C\[C@@](C)(CCC=C(C)C)\C=C\C2=CC=C(O)C=C2)C=C1	4,85
939	CC(C)=CCC[C@@](C)(C=C)\C=C\C1=CC=C(OC(C)=O)C=C1	4,7
940	CC(C)(O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O)[C@@H]1CC[C@@]2(C)CCC=C(CO)[C@@H]2C1	5
941	CC(C)(O)[C@@H]1C[C@@H]2[C@@]3(C)C[C@H]3C[C@@]2(C)C[C@@H]1O	5,37

NAME	SMILE	lg(1/IC50)
942	CO[C@@H]1O[C@@]2(CO)CC[C@@]11CC[C@]3(C)[C@H](C[C@@H](O)[C@@H]4[C@@]5(C)CC[C@H](O)[C@](C)(CO)[C@@H]5CC[C@@]34C)[C@@H]1[C@]2(C)O	5,26
943	CC1(C)CC[C@]2(C)CC[C@]3(C)[C@H](CC[C@H]4[C@@]3(C)CC[C@H]3C(C)(C)[C@@H](O)C[C@H](O)[C@]43C)C2=C1	5,27
944	CC(C)(O)[C@@H]1C[C@@H]2[C@@]3(C)C[C@H]3C[C@@]2(C)C[C@H]1O	5
945	CC(C)(O)[C@@H]1C[C@@H]2[C@@]3(C)C[C@H]3C[C@@]2(C)CC1=O	5,28
946	C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@@H](O)[C@@H](O)[C@@](C)(CO)[C@@H]5CC[C@@]34C)[C@@H]2[C@H]1C)C(=O)O[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O	5
947	C\C=C(\C)C(=O)O[C@H]1[C@H](O)[C@@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)O[C@@H](O[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC=C3[C@@H]5CC(C)(C)[C@@H](O)[C@H](O)[C@]5(CO[C@@H]5O[C@H](CO[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6O)[C@@H](O)[C@H](O)[C@H]5O)C(=O)C[C@@]43C)C2(C)C)[C@@H]1O	4
948	C\C=C(\C)C(=O)O[C@@H]1[C@@H](O)[C@H](O[C@H]2[C@H](O)[C@]3(COC(C)=O)[C@H](O)C[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@@H]([C@@H](O)[C@H](O)[C@H]7O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)C(O)=O)[C@](C)(CO)[C@@H]6CC[C@@]45C)[C@@H]3CC2(C)C)O[C@H](C)[C@@H]1OC(C)=O	4
949	CC1(C)C[C@H]2C3=CC[C@@H]4[C@@]5(C)CC[C@H](O[C@@H]6O[C@H](CO[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)[C@@H](O)[C@H](O)[C@H]6O[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6O)C(C)(C)[C@@H]5CC[C@@]4(C)[C@]3(C)CC(=O)[C@@]2(CO[C@@H]2O[C@H](CO[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O	4
950	C[C@@H]1O[C@@H](O[C@@H]2[C@@H](O)[C@H](O)[C@@H](CO[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)O[C@H]2OC[C@@]23CC[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@H](CO[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O)[C@@H](O)[C@H](O)[C@H]7O)C(C)(C)[C@@H]6CC[C@@]45C)[C@@H]2CC(C)(C)[C@@H](O)[C@@H]3O)[C@H](O)[C@H](O)[C@H]1O	4
951	FC1=CNC(=O)NC1=O	4,61
952	C\C=C(\C)C(=O)O[C@@H]1[C@@H](O)[C@H](O[C@H]2[C@H](OC(C)=O)[C@]3(CO)[C@H](O)C[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@@H]([C@@H](O)[C@H](O)[C@H]7O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)C(O)=O)[C@](C)(CO)[C@@H]6CC[C@@]45C)[C@@H]3CC2(C)C)O[C@H](C)[C@@H]1OC(C)=O	4,75
953	C\C=C(\C)C(=O)O[C@H]1[C@@H](C)O[C@@H](O[C@H]2[C@H](OC(C)=O)[C@]3(CO)[C@H](O)C[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@@H]([C@@H](O)[C@H](O)[C@H]7O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)C(O)=O)[C@](C)(CO)[C@@H]6CC[C@@]45C)[C@@H]3CC2(C)C)[C@H](O)[C@H]1OC(=O)C(\C)=C/C	5,33
954	CC1(C)C[C@H]2C3=CC[C@@H]4[C@@]5(C)CC[C@H](O[C@@H]6O[C@H](CO[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)[C@@H](O)[C@H](O)[C@H]6O)C(C)(C)[C@@H]5CC[C@@]4(C)[C@]3(C)CC[C@@]2(CO[C@@H]2O[C@H](CO[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O	4
955	CC1(C)C[C@H]2C3=CC[C@@H]4[C@@]5(C)CC[C@H](O[C@@H]6O[C@H](CO[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)[C@@H](O)[C@H](O)[C@H]6O)C(C)(C)[C@@H]5CC[C@@]4(C)[C@]3(C)CC(=O)[C@@]2(CO[C@@H]2O[C@H](CO[C@@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@@H](O)[C@@H]1O	4
956	C\C=C(\C)C(=O)O[C@H]1[C@H](O)[C@@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)O[C@@H](O[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC=C3[C@@H]5CC(C)(C)[C@@H](O)[C@H](O)[C@]5(CO[C@@H]5O[C@H](CO[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6O)[C@@H](O)[C@H](O)[C@H]5O)CC[C@@]43C)C2(C)C)[C@@H]1O	4
957	C\C=C(\C)C(=O)O[C@H]1[C@@H](C)O[C@@H](O[C@H]2[C@H](O)[C@]3(COC(C)=O)[C@H](O)C[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@@H]([C@@H](O)[C@H](O)[C@H]7O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)C(O)=O)[C@](C)(CO)[C@@H]6CC[C@@]45C)[C@@H]3CC2(C)C)[C@H](O)[C@H]1OC(=O)C(\C)=C/C	4
958	C\C=C(\C)C(=O)O[C@@H]1[C@@H](O)[C@H](O[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC=C3[C@@H]5CC(C)(C)[C@@H](O)[C@H](O)[C@]5(CO[C@@H]5O[C@H](CO[C@@H]6O[C@H](CO)[C@@H](O)[C@H](O)[C@H]6O)[C@@H](O)[C@H](O)[C@H]6O)[C@@H](O)[C@H](O)[C@H]5O)[C@@H]5O[C@H](CO)[C@@H](O)[C@H](O)[C@H]5O)CC[C@@]43C)C2(C)C)O[C@H](CO[C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)[C@H]1OC(C)=O	4
959	C\C=C(\C)C(=O)O[C@H]1[C@@H](C)O[C@@H](O[C@H]2[C@H](OC(C)=O)[C@]3(CO)[C@H](O)C[C@]4(C)C(=CC[C@@H]5[C@@]6(C)CC[C@H](O[C@@H]7O[C@@H]([C@@H](O)[C@H](O)[C@H]7O[C@@H]7O[C@H](CO)[C@@H](O)[C@H](O)[C@H]7O)C(O)=O)C(C)(C)[C@@H]6CC[C@@]45C)[C@@H]3CC2(C)C)[C@H](O)[C@H]1OC(=O)C(\C)=C/C	5,3
960	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=CC=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
961	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(O)C=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4,4
962	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC=C(Br)C=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4,19
963	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC(Cl)=CC=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	4
964	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(C=C4)[N+]([O-])=O)[C@@H]3CC[C@@]2(C)C=CC1=O	4
965	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(Br)C(F)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4,48
966	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC(Cl)=CC=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	4
967	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC=C(C=C4)[N+]([O-])=O)[C@@H]3CC[C@@]2(C)C=CC1=O	4,85
968	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC=C(F)C(Br)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4

NAME	SMILE	lg(1/IC50)
969	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC(F)=CC(F)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
970	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC=CC(=C4)[N+]([O-])=O)[C@@H]3CC[C@@]2(C)C=CC1=O	4
971	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=C5C=CC=CC5=CC=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
972	COC1=CC=C(C=C1)C1=NOC2(C1)[C@@H]1CC[C@@]3(C)C=CC(=O)C(C)=C3[C@H]1OC2=O	4
973	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC(F)=CC(F)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
974	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC=C(C=C4)[N+]([O-])=O)[C@@H]3CC[C@@]2(C)C=CC1=O	4
975	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=CC(F)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
976	COC1=CC=C(C=C1Br)C1=NOC2(C1)[C@@H]1CC[C@@]3(C)C=CC(=O)C(C)=C3[C@H]1OC2=O	4
977	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=CC=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	5,14
978	COC1=CC=C(C=C1Br)[C@H]1CC2(ON1C1=CC=CC=C1)[C@@H]1CC[C@@]3(C)C=CC(=O)C(C)=C3[C@H]1OC2=O	4
979	COC1=CC=C(C=C1Br)[C@@H]1CC2(ON1C1=CC=CC=C1)[C@@H]1CC[C@@]3(C)C=CC(=O)C(C)=C3[C@H]1OC2=O	4
980	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=C5C=CC=CC5=CC=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
981	FC1=CNC(=O)NC1=O	5,35
982	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=C(Cl)C=CC=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	4,82
983	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(Br)C=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
984	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC=C(F)C(Br)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	5,43
985	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(F)C=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
986	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C(Cl)C=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	4,54
987	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=CC=C5C=CC=CC5=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
988	CC1=C2[C@H]3OC(=O)C4(CC(=NO4)C4=C5C=CC=CC5=CC5=CC=CC=C45)[C@@H]3CC[C@@]2(C)C=CC1=O	4,3
989	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC=C(Br)C=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
990	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC(Cl)=CC=C4Cl)[C@@H]3CC[C@@]2(C)C=CC1=O	6,22
991	CC1=C2[C@H]3OC(=O)C4(C[C@H](N(O4)C4=CC=CC=C4)C4=CC(F)=CC(F)=C4)[C@@H]3CC[C@@]2(C)C=CC1=O	4
992	CC1=C2[C@H]3OC(=O)C4(C[C@@H](N(O4)C4=CC=CC=C4)C4=CC=CC(=C4)[N+]([O-])=O)[C@@H]3CC[C@@]2(C)C=CC1=O	4
993	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=CC=C6C#N)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,92
994	COC1=CC(=CC(OC)=C1OC)N1C=C(CO[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC[C@@H]3[C@H]5[C@@H](CC[C@@]5(CC[C@@]43C)C(O)=O)C(C)=C)C2(C)C)N=N1	4,3
995	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=C7C=CC=C(O)C7=CC=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,89
996	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=CC(I)=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	5,42
997	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=CC=C6CO)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,85
998	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C(C=C6)C#N)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,49
999	CC(=O)OC[C@H]1OC([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@H]1OC(C)=O)N1C=C(CO[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC[C@@H]3[C@H]5[C@@H](CC[C@@]5(CC[C@@]43C)C(O)=O)C(C)=C)C2(C)C)N=N1	4,4
1000	CC(=O)OC[C@H]1OC([C@H](OC(C)=O)[C@@H](OC(C)=O)[C@@H]1OC(C)=O)N1C=C(CO[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC[C@@H]3[C@H]5[C@@H](CC[C@@]5(CC[C@@]43C)C(O)=O)C(C)=C)C2(C)C)N=N1	4,3
1001	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C(CC#N)C=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,89
1002	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,8
1003	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C(C=C6)C(=O)C6=CC=CC=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,3
1004	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C7OCOC7=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,59
1005	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C(Cl)C=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,36
1006	COC1=CC=C(C=C1)N1C=C(CO[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC[C@@H]3[C@H]5[C@@H](CC[C@@]5(CC[C@@]43C)C(O)=O)C(C)=C)C2(C)C)N=N1	4,64
1007	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=C(C=C6)[N+]([O-])=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,82
1008	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC=CC(CO)=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	5,1
1009	COC1=CC=CC(=C1)N1C=C(CO[C@H]2CC[C@@]3(C)[C@@H](CC[C@]4(C)[C@@H]3CC[C@@H]3[C@H]5[C@@H](CC[C@@]5(CC[C@@]43C)C(O)=O)C(C)=C)C2(C)C)N=N1	4,54
1010	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC(I)=CC=C6C)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,3

NAME	SMILE	lg(1/IC50)
1011	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@H](OCC6=CN(N=N6)C6=CC(C)=CC(O)=C6)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	4,3
1012	OC1=CC=C(Br)C=C1\C=N\CC1=CC=CS1	5,42
1013	CC1=NC2=NC(SCC3=NN=C(SCC4=CC(=O)OC5=CC(O)=CC(C)=C45)S3)=NN2C(C)=C1	4,6
1014	COC(=O)NC1=CC=C2C(CSC3=NN=C(CSC4=NC(C)=CC(C)=N4)S3)=CC(=O)OC2=C1	5,68
1015	NC1=NN=C(SCN2C=NC3=CC=CC=C3C2=O)S1	4,6
1016	O=C1N(CSC2=NC3=CC=CC=C3O2)C=NC2=CC=CC=C12	4,6
1017	ClC1=CC=CC2=C1N=CN(CSC1=NC3=CC=CC=C3O1)C2=O	4,6
1018	ClC1=CC=CC2=C1N=CN(CSC1=NC3=CC=CC=C3S1)C2=O	4,6
1019	ClC1=CC=CC2=C1N=CN(CSC1=CC(=O)C3=CC=CC=C3S1)C2=O	4,6
1020	CC1=NC2=NC(SCC3=CC(=O)C4=CC(Cl)=CC=C4O3)=NN2C(C)=C1	4,6
1021	CC1=NN=C(O1)SCC1=COC2=CC=CC=C2C1=O	5,42
1022	CC1=NN=C(SCC2=CC(=O)C3=CC(C)=CC=C3O2)S1	4,6
1023	CC1=CC(C)=NC(SCN2C=NC3=CC=CC=C3C2=O)=N1	4,6
1024	CC1=CC=C2OC(CSC3=NC4=CC=CC=C4S3)=CC(=O)C2=C1	4,6
1025	CC1=CC=C2OC(CSC3=NC(C)=CC(C)=N3)=CC(=O)C2=C1	4,6
1026	NC1=NN=C(SCC2=COC3=CC=CC=C3C2=O)S1	5,82
1027	O=C1C(CSC2=NC3=CC=CC=C3O2)=COC2=CC=CC=C12	5,57
1028	CC1=NC2=NC(SCC3=NN=C(SCC4=COC5=CC=CC=C5C4=O)S3)=NN2C(C)=C1	5,28
1029	NC1=NN=C(SCC2=CC(=O)C3=CC=CC=C3O2)S1	4,6
1030	O=C1C=C(CSC2=NC3=CC=CC=C3S2)OC2=CC=CC=C12	4,6
1031	CC1=CC(C)=NC(SCC2=CC(=O)C3=CC=CC=C3O2)=N1	4,6
1032	CC1=NN=C(O1)SCC1=CC(=O)C2=CC(C)=CC=C2O1	4,6
1033	OC1=CC=C2C(CSC3=NC4=CC=CC=C4O3)=CC(=O)OC2=C1O	4,6
1034	O=C1C=C(SCN2C=NC3=CC=CC=C3C2=O)SC2=CC=CC=C12	5,23
1035	CC1=CC(C)=NC(SCN2C=NC3=C(Cl)C=CC=C3C2=O)=N1	4,6
1036	CC1=CC=C2OC(CSC3=NN=C(N)S3)=CC(=O)C2=C1	4,6
1037	CC1=NC2=NC(SCC3=NN=C(O3)SCC3=CC(=O)C4=CC=CC=C4O3)=NN2C(C)=C1	4,6
1038	CC1=NC2=NC(SCC3=NN=C(SCC4=CC(=O)C5=CC=CC=C5O4)N3N)=NN2C(C)=C1	4,6
1039	CC1=CC(O)=CC2=C1C(CSC1=NC3=CC=CC=C3O1)=CC(=O)O2	4,6
1040	O=C1N(CSC2=NC3=CC=CC=C3S2)C=NC2=CC=CC=C12	4,6
1041	CC1=NC2=NC(SCN3C=NC4=CC=CC=C4C3=O)=NN2C(C)=C1	4,6
1042	CC1=NN=C(O1)SCC1=CC(=O)C2=CC(Cl)=CC=C2O1	4,6
1043	CC1=NN=C(SCC2=CC(=O)C3=CC(Cl)=CC=C3O2)S1	4,6
1044	CC1=CC(C)=NC(SCC2=CC(=O)C3=CC(Cl)=CC=C3O2)=N1	4,6
1045	CC1=NN=C(O1)SCC1=CC(=O)C2=CC=CC=C2O1	4,6
1046	CC1=NN=C(O1)SC1=C(C)OC2=CC=CC=C2C1=O	4,3
1047	CC1=NC2=NC(SCC3=NN=C(SCC4=CC(=O)OC5=C6C=CC=CC6=CC=C45)S3)=NN2C(C)=C1	4,6
1048	CC1=NC2=NC(SCC3=NN=C(SCN4C=NC5=C(Cl)C=CC=C5C4=O)S3)=NN2C(C)=C1	4,6
1049	O=C1C=C(SCC2=COC3=CC=CC=C3C2=O)SC2=CC=CC=C12	5,85
1050	CC1=NN=C(SCC2=CC(=O)C3=CC=CC=C3O2)S1	4,6
1051	CC1=NC2=NC(SCC3=NN=C(SCC4=CC(=O)C5=CC=CC=C5O4)S3)=NN2C(C)=C1	4,6
1052	CC1=NN=C(SC2=COC3=CC=CC=C3C2=O)S1	4,3
1053	FC1=CNC(=O)NC1=O	3,89
1054	NC1=NN=C(SCC2=CC(=O)OC3=C4C=CC=CC4=CC=C23)S1	4,6
1055	CC1=CC(O)=CC2=C1C(CSC1=NC3=CC=CC=C3S1)=CC(=O)O2	4,6
1056	CC1=CC(O)=CC2=C1C(CSC1=NC3=CC=CC=C3N1)=CC(=O)O2	4,6
1057	COC(=O)NC1=CC=C2C(CSC3=NC(C)=CC(C)=N3)=CC(=O)OC2=C1	5,1
1058	CC1=NC2=NC(SCC3=NN=C(SCC4=COC5=CC=CC=C5C4=O)N3N)=NN2C(C)=C1	5,15
1059	CC1=NN=C(O1)SCC1=COC2=CC=C(Cl)C=C2C1=O	5,19
1060	CC1=NC2=NC(SCC3=NN=C(SCC4=CC(=O)C5=CC=CC=C5O4)N3C3=CC=CC=C3)=NN2C(C)=C1	4,6
1061	CC1=CC=C2OC(CSC3=NN4C(=N3)N=C(C)C=C4C)=CC(=O)C2=C1	4,6
1062	CC1=NN=C(SCC2=COC3=CC=CC=C3C2=O)S1	5,54
1063	NC1=NC(SCC2=COC3=CC=CC=C3C2=O)=NN1	4,67
1064	CC1=NC2=NC(SCC3=CC(=O)C4=CC=CC=C4O3)=NN2C(C)=C1	4,6
1065	CC1=NN=C(SCC2=COC3=CC=C(Cl)C=C3C2=O)S1	5,38
1066	CC1=NC2=NC(SCN3C=NC4=C(Cl)C=CC=C4C3=O)=NN2C(C)=C1	4,6
1067	NC1=NN=C(SCC2=CC(=O)C3=CC(Cl)=CC=C3O2)S1	4,6
1068	ClC1=CC=C2OC(CSC3=NC4=CC=CC=C4S3)=CC(=O)C2=C1	4,6
1069	CC1=CC(C)=NC(SCC2=COC3=CC=CC=C3C2=O)=N1	4,26
1070	CC1=NC2=NC(SCC3=NN=C(SCC4=COC5=CC=CC=C5C4=O)N3C3=CC=CC=C3)=NN2C(C)=C1	4,66
1071	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=CS1	4
1072	COC1=CC(=CC(OC)=C1)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	5,4
1073	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(Br)C=C1	4,55
1074	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=CS1	3,4
1075	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(S1)C1=CC=C(Br)S1	5,1
1076	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=C(F)C(F)=C(F)C(F)=C1F	3,7
1077	COC(=O)C1=CC=C(C=C1)C1=C2C(C)=CC(C)=[N+]2[B-](F)(F)N2C(C)=CC(C)=C12	4
1078	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=C(S1)C1=CC=CS1	4
1079	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=C(S1)C1=CC=CS1	3,4
1080	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=CC=C1	3,4
1081	COC(=O)C1=CC=C(C=C1)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	3,4
1082	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(Br)S1	3,7
1083	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=C(F)C(F)=C(F)C(F)=C1F	3,4

NAME	SMILE	lg(1/IC50)
1084	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(S1)C1=CC=CS1	3,4
1085	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=C(S1)C1=CC=C(Br)S1	4,09
1086	COC1=CC=C(C=C1OC)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	3,4
1087	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=CS1	3,52
1088	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=CS1	4,85
1089	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(S1)C1=CC=CS1	3,7
1090	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(S1)C1=CC=C(Br)S1	5,46
1091	CC1=CC(C)=C2N1[B-](F)(F)[N+]1=C(C)C=C(C)C1=C2C1=CC=C(S1)C1=CC=C(Br)S1	3,52
1092	COC1=CC(=CC(OC)=C1)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	3,4
1093	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC(=CC(=C1)C(C)(C)C)C(C)(C)C	3,7
1094	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(Br)C=C1	3,4
1095	COC(=O)C1=CC=C(C=C1)C1=C2C(C)=CC(C)=[N+]2[B-](F)(F)N2C(C)=CC(C)=C12	3,4
1096	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=CC=C1	4,57
1097	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC(=CC(=C1)C(C)(C)C)C(C)(C)C	3,4
1098	COC1=CC=C(C=C1OC)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	5,12
1099	COC(=O)C1=CC=C(C=C1)C1=C2C(C)=C(I)C(C)=[N+]2[B-](F)(F)N2C(C)=C(I)C(C)=C12	3,7
1100	CC1=C(I)C(C)=C2N1[B-](F)(F)[N+]1=C(C)C(I)=C(C)C1=C2C1=CC=C(Br)S1	3,4
1101	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	6,77
1102	CC(C)[C@H]1NC(=O)[C@@H](NC(=O)C2=C3N=C4C(OC3=C(C)C=C2)=C(C)C(=O)C(N)=C4C(=O)N[C@H]2[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]3CCCN3C(=O)[C@H](NC2=O)C(C)C)[C@@H](C)OC(=O)[C@H](C(C)C)N(C)C(=O)CN(C)C(=O)[C@@H]2CCCN2C1=O	8,21
1103	CC1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)C1=CC2=O	4,15
1104	CC(CO)C1=CC2=C(C(O)=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,15
1105	CC(CO)C1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,37
1106	CC(C)C1=CC=C2C(C[C@@H](O)[C@H]3C(C)(C)CCC[C@]23C)=C1O	4,33
1107	CC(C)C1=CC2=C(C(O)=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,34
1108	CC(C)C1=CC2=C(C(O)=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,31
1109	CC1C(=O)OC2=C(O)C3=C(CC[C@H]4C(C)(C)CCC[C@]34C)C=C12	4,42
1110	CC(CO)C1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,27
1111	CC1C(=O)OC2=C(O)C3=C(CC[C@H]4C(C)(C)CCC[C@]34C)C=C12	4,38
1112	CC1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@]11O[C@H]1C2=O	4,63
1113	CC1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@]11O[C@H]1C2=O	4,15
1114	CC(C)C1=CC=C2C(C[C@@H](O)[C@H]3C(C)(C)CCC[C@]23C)=C1O	4,41
1115	CC1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,24
1116	CC1=CC2=C(C=C1O)[C@@]1(C)CCCC(C)(C)[C@@H]1CC2=O	4,79
1117	COC1=CC=CC=C1NCOC1=CC=C2OC(=O)C=C(C)C2=C1	5,27
1118	CC1=CC(=O)OC2=CC=C(OCNC3=CC=C(F)C=C3)C=C12	5,44
1119	CC1=CC(=O)OC2=CC=C(OCNC3=CC=CC=C3O)C=C12	5,38
1120	C[C@@H]1CC[C@@]2(O)[C@@H](C[C@@H](O)C2(C)C)C(=O)[C@@]1(C)CCC1=CC(=O)OC1	5
1121	C[C@@H]1C[C@H]2C(=O)C(C)(C)[C@H](O)CC[C@]2(O)[C@@]1(C)CCC1=CC(=O)OC1	5
1122	C[C@@H]1CC[C@]2(O)[C@H](C[C@@H](O)C2(C)C)C(=O)[C@@]1(C)CCC1=CC(=O)OC1	5
1123	C[C@@H]1C[C@H]2C(=O)C(C)(C)[C@@H](CC[C@]2(O)[C@@]1(C)CCC1=CC(=O)OC1)OC=O	5
1124	COC1=C(C=CC2=C1C(=O)OCC1=CC(C)=CC(O)=C1O2)[C@@H](O)CC(C)C	5,17
1125	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	5,82
1126	OC1=CC=C2NC=C(C2=C1)C1=CN=C(C=N1)C1=CNC2=CC=C(O)C=C12	3,82
1127	COC1=CC=C(C=C1)C1=C(SC#N)C2=CC=CC=C2N1C	4,66
1128	CC1=CC=C(C=C1)C1=C(SC#N)C2=CC=CC=C2N1	4,99
1129	CN1C=C(SC#N)C2=CC(=CC=C12)C1=CC=C(C)C=C1	4,62
1130	ClC1=CC=C(C=C1)C1=C(SC#N)C2=CC=CC=C2N1	5,06
1131	N1C=CC2=CC=CC=C12	4,3
1132	CN1C2=CC=CC=C2C(SC#N)=C1C1=CC=C(Cl)C=C1	5,55
1133	N#CSC1=C(NC2=CC=CC=C12)C1=CC=CC=C1	5,3
1134	CN1C=CC2=C1C=CC=C2	4,3
1135	CN1C=C(SC#N)C2=CC=CC=C12	4,45
1136	COC1=CC=C(C=C1)N1C=C(SC#N)C2=CC=CC=C12	4,97
1137	BrC1=CC=C2NC=C(SC#N)C2=C1	4,7
1138	CN1C(=CC2=CC=CC=C12)C1=CC=C(Cl)C=C1	4,3
1139	ClC1=CC=C(C=C1)N1C=C(SC#N)C2=CC=CC=C12	5,07
1140	FC(F)(F)C1=CC=CC(=C1)C1=C(SC#N)C2=CC=CC=C2N1	5,39
1141	N#CSC1=CN(C2=CC=CC=C12)C1=CC=CC=C1	5,55
1142	CN1C2=CC=CC=C2C(SC#N)=C1C1=CC=CC=C1	5,09
1143	CC1=CC=C(C=C1)C1=CC=C2NC=C(SC#N)C2=C1	4,8
1144	N#CSC1=CNC2=CC=C(C=C12)C#N	4,92
1145	N#CSC1=CNC2=CC=CC=C12	4,72
1146	CN1C2=CC=CC=C2C(SC#N)=C1C1=CC=C(C)C=C1	5,44
1147	COC1=CC=C2NC=C(SC#N)C2=C1	4,39
1148	CN1C2=CC=CC=C2C(SC#N)=C1C1=CC=CC(=C1)C(F)(F)F	4,43
1149	COC1=CC=C(C=C1)C1=C(SC#N)C2=CC=CC=C2N1	5,04
1150	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	5,89
1151	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC6=C(N=NC(C)=[N+]6[O-])C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12)C(O)=O	5,82

NAME	SMILE	lg(1/IC50)
1152	CC(=O)OC[C@]12CC[C@H]([C@@H]1[C@H]1CC[C@@H]3[C@@]4(C)CC5=NN(N=C5C(C)(C)[C@@H]4CC[C@@]3(C)[C@]1(C)CC2)C(C)=O)C(C)=C	4,75
1153	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@H]4[C@@]3(C)CC[C@H]3C(C)(C)C5=C(N=C(C)O5)C(=O)[C@]43C)[C@@H]12	4,71
1154	CC(=O)NC1=C[C@@]2(C)[C@@H](CC[C@]3(C)[C@@H]2CC[C@@H]2[C@H]4[C@@H](CC[C@]4(CO)CC[C@@]32C)C(C)=C)C(C)(C)C1=O	4,98
1155	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC6=C(N=NC(C)=[N+]6[O-])C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	5,35
1156	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)C\C(=N/O)C(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4
1157	CC(=O)OC[C@]12CC[C@H]([C@@H]1[C@H]1CC[C@H]3[C@@](C)(CC[C@H]4C(C)(C)C(=O)C5=NOC(C)=C5[C@]34C)[C@]1(C)CC2)C(C)=C	4,66
1158	CC(=C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC6=NN(N=C6C(C)(C)[C@@H]5CC[C@@]34C)C(C)=O)[C@@H]12)C=O	4
1159	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC6=NN(N=C6C(C)(C)[C@@H]5CC[C@@]34C)C(C)=O)[C@@H]12	5,13
1160	CC(=O)NC1=C[C@@]2(C)[C@@H](CC[C@]3(C)[C@@H]2CC[C@@H]2[C@H]4[C@@H](CC[C@]4(COC(C)=O)CC[C@@]32C)C(C)=C)C(C)(C)C1=O	4,66
1161	CC(=O)OC[C@]12CC[C@H]([C@@H]1[C@H]1CC[C@H]3[C@@](C)(CC[C@H]4C(C)(C)C5=C(N=C(C)O5)C(=O)[C@]34C)[C@]1(C)CC2)C(C)=C	4,4
1162	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@H]4[C@@]3(C)CC[C@H]3C(C)(C)C(=O)C5=NOC(C)=C5[C@]43C)[C@@H]12	4,51
1163	CC[C@@]1(O)C(=O)OCC2=C1C=C1N(CC3=CC4=C(C=CC=C4)N=C13)C2=O	5,52
1164	CC(=C)[C@@H]1CC[C@]2(CO)CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CCC(=O)C(C)(C)[C@@H]5CC[C@@]34C)[C@@H]12	4,65
1165	C[C@H](OC(=O)\C=C\C1=CC=C(O)C=C1)[C@@H]1CC[C@@H](O1)[C@H](O)[C@H]1CC=CC(=O)O1	5
1166	COC1=CC=C(\C=C\C(=O)O[C@@H](C)[C@@H]2CC[C@@H](O2)[C@H](O)[C@H]2CC=CC(=O)O2)C=C1	5,24
1167	C[C@H](OC(=O)\C=C\C1=CC=C(O)C(O)=C1)[C@@H]1CC[C@@H](O1)[C@H](O)[C@H]1CC=CC(=O)O1	5,03
1168	C[C@H](OC(=O)\C=C/C1=CC=C(O)C=C1)[C@@H]1CC[C@@H](O1)[C@H](O)[C@H]1CC=CC(=O)O1	5,11
1169	COC1=CC=C(\C=C/C(=O)O[C@@H](C)[C@@H]2CC[C@@H](O2)[C@H](O)[C@H]2CC=CC(=O)O2)C=C1	5
1170	CC[C@]1(O)C[C@H]2CN(C1)CCC1=C(NC3=CC=CC=C13)[C@@](C2)(C(=O)OC)C1=CC2=C(C=C1OC)N(C)[C@@H]1[C@]22CCN3CC=C[C@](CC)([C@@H]23)[C@@H](OC(C)=O)[C@]1(O)C(=O)OC	8,15
1171	OC[C@H]1O[C@H](OC2CCCC2)C=CC1=O	5,1
1172	OC[C@H]1O[C@H](OCCC#C)C=CC1=O	5,15
1173	OC[C@H]1O[C@H](OC2CCCCC2)C=CC1=O	5,12
1174	OC[C@H]1O[C@H](OCC=C)C=CC1=O	4,58
1175	OC[C@H]1O[C@H](OCC#C)C=CC1=O	4,81
1176	CCCO[C@H]1O[C@H](CO)C(=O)C=C1	4,87
1177	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	5,89
1178	COCCOCCOCCO[C@H]1O[C@H](CO)C(=O)C=C1	4,49
1179	CC(C)O[C@H]1O[C@H](CO)C(=O)C=C1	4,46
1180	OC[C@H]1O[C@H](OCC2=CC=CC=C2)C=CC1=O	5,07
1181	CCO[C@H]1O[C@H](CO)C(=O)C=C1	5,24
1182	Cl.COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	6
1183	OC1=C2C=CC(Cl)=CC2=NC=C1	4,3
1184	Cl.NCCCNC(=O)C1=CN(CC2=CC=CC=C2)C2=CC(Cl)=CC=C2C1=O	5,08
1185	Cl.CCCCN1C=C(C(=O)NCCCN)C(=O)C2=CC=C(Cl)C=C12	4,66
1186	Cl.NCCCNC(=O)C1=CN(CC=C)C2=CC(Cl)=CC=C2C1=O	4,44
1187	Cl.NCCCNC(=O)C1=CN(CCCC2=CC=CC=C2)C2=CC(Cl)=CC=C2C1=O	5,49
1188	Cl.CCN1C=C(C(=O)NCCCN)C(=O)C2=CC=C(Cl)C=C12	4,55
1189	COC(=O)[C@H](NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1)C(C)C	4,3
1190	COC(=O)[C@H](CO)NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1	4,3
1191	COC(=O)[C@H](C)NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1	4,3
1192	O=C1N(C(=O)C2=CC=CC=C12)C1=CC=C(C=C1)C1=CC=CC=C1	4,39
1193	CC(=O)N1CC(C(=N1)C1=CC=C2C=CC=CC2=C1)C1=CC=C2OCOC2=C1	6
1194	COC1=CC(=CC(OC)=C1OC)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	6,28
1195	COC1=CC=C(C=C1O)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,99
1196	O=CCN1N=C(CC1C1=CC=CO1)C1=CC=C2C=CC=CC2=C1	4,72
1197	COC1=CC=CC2=C1C(=O)C1=C(O)C3=C(C[C@](O)(C[C@@H]3O[C@H]3C[C@H](N)[C@H](O)[C@H](C)O3)C(=O)CO)C(O)=C1C2=O	5,06
1198	ClC1=CC=C(C=C1)N1C(=O)C2=CC=CC=C2C1=O	3,75
1199	COC1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=C(Br)C=C1	4,75
1200	CC(=O)N1N=C(CC1C1=CC=CC=C1)C1=CC=CC(=C1)[N+]([O-])=O	5,05
1201	CC(=O)N1N=C(CC1C1=CC=CC(O)=C1)C1=CC=CO1	5
1202	CC(=O)N1N=C(CC1C1=CC=C(Cl)C=C1)C1=CC=CO1	4,24
1203	COC1=CC(=CC(OC)=C1OC)C1CC(=NN1C(C)=O)C1=CC=CO1	4,67
1204	COC1=CC=C(C=C1OC)C1CC(=NN1C(C)=O)C1=CC=CO1	5
1205	CC1=NNC(=O)C1C(C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1)C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1	4,84
1206	NC1=CC=CC(=C1)N1C(=O)C2C(C3CCC2C=C3)C1=O	4,27

NAME	SMILE	lg(1/IC50)
1207	COC1=CC=C(C=C1)N1C(=O)C2C(C3CCC2C=C3)C1=O	3,7
1208	SC1=CC=C(C=C1)N1C(=O)C2=CC=CC=C2C1=O	3,7
1209	COC1=CC=C(C=C1OC)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	6
1210	CC(=O)N1N=C(CC1C1=CC=CC=C1)C1=CC=CC=C1	4,93
1211	O=C1N(C(=O)C2=CC=CC=C12)C1=CC=CC=C1	3,7
1212	COC1=CC(=CC=C1O)C1CC(=NN1C(C)=O)C1=CC=CC=C1	5,3
1213	COC1=CC(=CC=C1O)C1CC(=NN1C(C)=O)C1=CC=CO1	5
1214	CC(=O)N1N=C(CC1C1=CC=C2OCOC2=C1)C1=CC=CO1	4,7
1215	COC(=O)[C@H](CC1=CN=CN1)NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1	4,3
1216	COC1=CC=C(C=C1)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,49
1217	O=CCN1N=C(CC1\C=C\C1=CC=CC=C1)C1=CC=C2C=CC=CC2=C1	4,7
1218	ClC1=CC=CC(C2CC(=NN2CC=O)C2=CC=C3C=CC=CC3=C2)=C1Cl	4,9
1219	COC1=CC=C(OC)C(=C1)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,96
1220	BrC1=CC=CC(=C1)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,06
1221	CC(=O)N1N=C(CC1C1=CC=C2OCOC2=C1)C1=CC=CC=C1	5,18
1222	CC(=O)N1N=C(CC1C1=CC=C(C)C=C1)C1=CC=CO1	4,71
1223	CC(=O)O[C@@H]1C2=C(C)[C@H](C[C@@](O)([C@@H](OC(=O)C3=CC=CC=C3)[C@@H]3[C@@]4(CO[C@@H]4C[C@H](O)[C@@]3(C)C1=O)OC(C)=O)C2(C)C)OC(=O)[C@H](O)[C@@H](NC(=O)C1=CC=CC=C1)C1=CC=CC=C1	6,96
1224	OC1=CC=C2NC=C(C3=C\C(C(=O)N3)=C3/C(=O)NC4=CC=CC=C34)C2=C1	5,66
1225	CC(=O)N1N=C(CC1C1=CC=CC(Cl)=C1Cl)C1=CC=CC=C1	4,62
1226	COC1=CC=C(C=C1OC)C1CC(=NN1C(C)=O)C1=CC=C(Br)C=C1	5,05
1227	COC1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=CC(=C1)[N+]([O-])=O	5,09
1228	COC1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=C2C=CC=CC2=CC=C1	5,43
1229	COC1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=CO1	4,81
1230	CC1=NNC(=O)C1C(C1=C(NC2=CC=CC=C12)C1=CC=CC=C1)C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1	4,38
1231	CC1=NNC(=O)C1C(C1=CNC2=CC=CC=C12)C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1	4
1232	CC1=NNC(=O)C1C(C1=CNC2=CC=CC=C12)C1=C(NC2=CC=CC=C12)C1=CC=CC=C1	5,17
1233	CC1=NNC(=O)C1C(C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1)C1=C(NC2=CC=C(Cl)C=C12)C1=CC=CC=C1	4,49
1234	COC(=O)[C@@H](NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1)C(C)C	4,3
1235	COC(=O)CNC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1	4,3
1236	ClC1=CC=C(N=C1)N1C(=O)C2C(C3CCC2C=C3)C1=O	3,7
1237	CC1=CC=C2C(=O)N(C(=O)C2=C1)C1=CC=C(C=C1)C1=CC=CC=C1	3,98
1238	NC1=CC=CC(=C1)N1C(=O)C2=CC=CC3=CC=CC(C1=O)=C23	3,83
1239	COC1=CC(=CC(OC)=C1OC)C1CC(=NN1C(C)=O)C1=CC=CC=C1	5,45
1240	CC(=O)N1N=C(CC1C1=CC=C2OCOC2=C1)C1=CC=C(Br)C=C1	5,06
1241	CC(=O)N1N=C(CC1C1=CC=CC=C1)C1=C2C=CC=CC2=CC=C1	4,95
1242	COC1=CC(=CC=C1O)C1CC(=NN1C(C)=O)C1=C2C=CC=CC2=CC=C1	5,95
1243	CC(=O)N1N=C(CC1C1=CC=CC(Cl)=C1Cl)C1=C2C=CC=CC2=CC=C1	4,78
1244	CC(=O)N1N=C(CC1C1=CC=CC(=C1)[N+]([O-])=O)C1=CC=CO1	4,52
1245	COC1=CC(OC)=C(C=C1OC)C1CC(=NN1C(C)=O)C1=CC=CO1	5,17
1246	COC1=CC=C2NC(=C(C(C3C(=O)NN=C3C)C3=C(NC4=CC=C(Cl)C=C34)C3=CC=CC=C3)C2=C1)C1=CC=CC=C1	5,21
1247	CC1=NNC(=O)C1C(C1=C(NC2=CC=CC=C12)C1=CC=CC=C1)C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1	4
1248	COC(=O)[C@H](CC(C)C)NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1	4,37
1249	CC[C@H](C)[C@H](NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1)C(=O)OC	4,3
1250	NC1=CC=C(C=C1)N1C(=O)C2=CC=CC3=CC=CC(C1=O)=C23	4,36
1251	CC1=CC=C2C(=O)N(C(=O)C2=C1)C1=CC=C(C=C1)\N=N/C1=CC=CC=C1	3,98
1252	O=C1N(C(=O)C2=CC=CC=C12)C1=CC=CC=C1N1C(=O)C2=CC=CC=C2C1=O	4,25
1253	O=CCN1N=C(CC1C1=CC=C2C=CC=CC2=C1)C1=CC=C2C=CC=CC2=C1	6,77
1254	CC(=O)N1N=C(CC1\C=C\C1=CC=CC=C1)C1=C2C=CC=CC2=CC=C1	4,68
1255	COC1=CC=C(C2CC(=NN2CC=O)C2=CC=C3C=CC=CC3=C2)C(OC)=C1OC	6,23
1256	O=C1C2C(C3CCC2C=C3)C(=O)N1C1=CC=CC=C1	4,39
1257	ClC1=CC=C(N=C1)N1C(=O)C2=CC=CC=C2C1=O	4,25
1258	COC1=CC=C(C=C1)N1C(=O)C2=CC=CC=C2C1=O	3,7
1259	FC1=CNC(=O)NC1=O	5,7
1260	CC(=O)N1N=C(CC1C1=CC=C2OCOC2=C1)C1=CC=CC(=C1)[N+]([O-])=O	5,12
1261	CC(=O)N1N=C(CC1C1=CC=CC(=C1)[N+]([O-])=O)C1=C2C=CC=CC2=CC=C1	5,39
1262	CC(=O)N1N=C(CC1C1=CC=CC(Br)=C1)C1=C2C=CC=CC2=CC=C1	5,01
1263	COC1=CC=C(OC)C(=C1)C1CC(=NN1C(C)=O)C1=C2C=CC=CC2=CC=C1	5,88
1264	CC(=O)N1N=C(CC1C1=CC=CC=C1[N+]([O-])=O)C1=CC=CO1	4,32
1265	CC(=O)N1N=C(CC1C1=CC=CC(Cl)=C1Cl)C1=CC=CO1	4,36
1266	[O-][N+](=O)C1=CC=CC(=C1)N1C(=O)C2=CC=CC=C2C1=O	3,75
1267	CC1=NNC(=O)C1C(C1=CNC2=CC=CC=C12)C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1	5,49
1268	COC(=O)C[C@H](NC(=O)\C=C\C=C\C1=CC=C2OCOC2=C1)C(=O)OC	4,3
1269	ClC1=CN=C(N2C(=O)C3C(C4CCC3C=C4)C2=O)C(Cl)=C1	3,7
1270	BrC1=CC=C(N=C1)N1C(=O)C2C(C3CCC2C=C3)C1=O	3,82
1271	CC1=CC=C2C(=O)N(C(=O)C2=C1)C1=CC=C(C=N1)[N+]([O-])=O	3,76
1272	O=C1N(C(=O)C2=CC=CC=C12)C1=CC=CC=C1C#N	3,7
1273	COC1=CC(=CC(OC)=C1OC)C1CC(=NN1C(C)=O)C1=CC=C(Br)C=C1	5,34
1274	CN(C)C1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=CC=C1	4,84
1275	CC(=O)N1N=C(CC1C1=CC=CC(Cl)=C1Cl)C1=CC=C(Br)C=C1	4,3

NAME	SMILE	lg(1/IC50)
1276	COC1=CC=C(C=C1OC)C1CC(=NN1C(C)=O)C1=CC=CC(=C1)[N+]([O-])=O	5,11
1277	CC(=O)N1N=C(CC1C1=CC=C(C=C1)[N+]([O-])=O)C1=CC=CO1	4,66
1278	COC1=CC=C(OC)C(=C1)C1CC(=NN1C(C)=O)C1=CC=CO1	4,87
1279	CC1=NNC(=O)C1C(C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1)C1=C(NC2=CC=C(C)C=C12)C1=CC=CC=C1	4
1280	COC1=CC=C2NC(=C(C(C3C(=O)NN=C3C)C3=C(NC4=CC=C(C)C=C34)C3=CC=CC=C3)C2=C1)C1=CC=CC=C1	5,46
1281	NC1=CC=CC=C1N1C(=O)C2C(C3CCC2C=C3)C1=O	4,49
1282	O=CCN1N=C(CC1C1=CC=CC=C1)C1=CC=C2C=CC=CC2=C1	5,08
1283	[O-][N+](=O)C1=CC=CC(=C1)C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,41
1284	[O-][N+](=O)C1=CC=CC=C1C1CC(=NN1CC=O)C1=CC=C2C=CC=CC2=C1	5,44
1285	O=C1N(C(=O)C2=CC=CC=C12)C1=CC=CC=N1	4,18
1286	COC1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=CC=C1	4,97
1287	CC(=O)N1N=C(CC1C1=CC=CC=C1)C1=CC=C(Br)C=C1	4,56
1288	CC(=O)N1N=C(CC1C1=CC=CC(Cl)=C1Cl)C1=CC=CC(=C1)[N+]([O-])=O	4,56
1289	CC(=O)N1N=C(CC1C1=CC=CC=C1[N+]([O-])=O)C1=C2C=CC=CC2=CC=C1	5,4
1290	COC1=CC=C(C=C1OC)C1CC(=NN1C(C)=O)C1=C2C=CC=CC2=CC=C1	5,99
1291	CC(=O)N1N=C(CC1C1=CC=C2OCOC2=C1)C1=C2C=CC=CC2=CC=C1	5,97
1292	CC(=O)N1N=C(CC1C1=CC=C2C=CC=CC2=C1)C1=C2C=CC=CC2=CC=C1	6,72
1293	CC(=O)N1N=C(CC1C1=CC=CC=C1)C1=CC=CO1	4,49
1294	CC(=O)N1N=C(CC1C1=CC=C(Br)C=C1)C1=CC=CO1	4,29
1295	COC1=CC=C2NC(=C(C(C3C(=O)NN=C3C)C3=CNC4=CC=CC=C34)C2=C1)C1=CC=CC=C1	5,28
1296	COC1=CC=C(C=C1OC)C1CC(=NN1C(C)=O)C1=CC=CC=C1	5,11
1297	NC1=CC=C(C=C1)N1C(=O)[C@H]2[C@H](C3CCC2C=C3)C1=O	3,7
1298	O=C1C2C(C3CCC2C=C3)C(=O)N1C1=CC=C(C=C1)C1=CC=CC=C1	4,33
1299	CC(=O)N1N=C(CC1C1=CC=CO1)C1=C2C=CC=CC2=CC=C1	4,77
1300	COC1=CC=C(C2CC(=NN2C(C)=O)C2=C3C=CC=CC3=CC=C2)C(OC)=C1OC	5,89
1301	O=C1N(C2=CC=CC=C2)C(=O)C2=C3C(C=CC=C13)=CC=C2	4,35
1302	O=C(\C=C\C=C\C1=CC=C2OCOC2=C1)N1CCCCC1	4,15
1303	COC1=CC(=CC(OC)=C1OC)C1CC(=NN1C(C)=O)C1=C2C=CC=CC2=CC=C1	6
1304	CN(C)C1=CC=C(C=C1)C1CC(=NN1C(C)=O)C1=CC=CO1	4,8
1305	COC1=CC=C(C=C1)N1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,46
1306	ClC1=CC=C(CN2C(=O)C3=CC(Cl)=CC=C3N=C2C2=CC=CC=C2)C=C1	3,88
1307	FC1=CC=C(C=C1Cl)N1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,79
1308	ClC1=CC=CC(=C1)N1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,77
1309	ClC1=CC=C(C=C1)N1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,17
1310	CN(C)CCN1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,2
1311	FC1=CC=C(CN2C(=O)C3=CC(Cl)=CC=C3N=C2C2=CC=CC=C2)C=C1	4,53
1312	FC1=CC=C(C=C1)N1C(=O)C2=CC(Cl)=CC=C2N=C1C1=CC=CC=C1	4,51

Table S2. QSAR model data set.

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
1	4,08	4,1919	0,1119	2	4,21	4,058	0,152
3	4,45	4,0524	0,3976	7	4,48	4,0954	0,3846
4	4,02	4,2518	0,2318	12	4	4,1443	0,1443
5	4,49	4,0839	0,4061	17	4	4,0981	0,0981
6	4,23	4,1548	0,0752	22	4,26	4,1827	0,0773
8	4	3,9325	0,0675	27	4,22	4,1145	0,1055
9	4,01	4,1433	0,1333	32	4	4,0606	0,0606
10	4,08	4,0397	0,0403	37	4,33	4,1298	0,2002
11	4	3,9238	0,0762	43	5,4	5,0837	0,3163
13	4,09	4,2823	0,1923	48	4,68	4,612	0,068
14	4,22	4,1175	0,1025	54	5,63	5,0693	0,5607
15	4,39	4,0589	0,3311	61	4,68	4,7117	0,0317
16	4	4,3354	0,3354	66	4	4,2925	0,2925
18	4,19	4,1208	0,0692	72	5	4,605	0,395
19	4,03	4,0614	0,0314	77	3,3	3,2029	0,0971
20	4	4,1206	0,1206	82	3,3	3,8825	0,5825
21	4	4,0606	0,0606	90	6,7	6,0787	0,6213
23	4,16	4,2092	0,0492	99	5,05	5,1989	0,1489
24	4,24	4,246	0,006	105	5,1	4,5823	0,5177
25	4,25	4,2104	0,0396	110	5,7	5,3092	0,3908
26	4,16	4,0096	0,1504	115	4,06	4,4084	0,3484
28	4	4,235	0,235	120	3,96	4,3481	0,3881
29	4	4,0332	0,0332	125	4,6	4,919	0,319
30	4	4,2195	0,2195	130	4,8	5,3634	0,5634
31	4,16	4,2444	0,0844	136	5	4,2974	0,7026
33	4	4,1474	0,1474	146	4,12	4,2837	0,1637
34	4	4,1396	0,1396	152	4,85	4,8802	0,0302
35	4	4,0194	0,0194	159	5,85	6,2429	0,3929

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
36	4	4,1587	0,1587	168	4,92	4,5909	0,3291
38	4	4,5374	0,5374	173	4,4	4,2391	0,1609
39	4	4,501	0,501	179	2,8	2,8764	0,0764
41	4,82	5,2375	0,4175	185	4,5	5,4048	0,9048
42	5,19	4,8508	0,3392	190	4,08	3,7541	0,3259
44	4,23	4,5333	0,3033	195	4,36	3,7541	0,6059
45	4,62	5,3064	0,6864	200	3,37	4,1575	0,7875
46	4,32	4,2647	0,0553	205	4,02	3,6769	0,3431
47	5,07	4,4844	0,5856	210	3,91	4,0382	0,1282
49	5,59	5,3225	0,2675	215	4,7	4,4256	0,2744
50	4	4,7343	0,7343	220	5	4,4558	0,5442
51	4,46	4,8926	0,4326	225	6,05	5,5897	0,4603
53	5,01	4,997	0,013	230	3,7	3,8204	0,1204
55	5,07	4,6395	0,4305	235	5,85	5,3639	0,4861
58	4,78	4,7788	0,0012	241	5,74	5,6819	0,0581
59	5,27	5,359	0,089	247	6,7	6,0543	0,6457
60	5,16	5,6232	0,4632	252	7,4	6,529	0,871
62	5,01	5,2601	0,2501	258	6,15	6,7434	0,5934
63	5,09	5,0527	0,0373	263	5,75	5,6846	0,0654
64	5,5	4,963	0,537	268	6,19	5,6706	0,5194
65	5,53	5,0733	0,4567	273	3,7	3,7928	0,0928
67	4,34	5,4685	1,1285	278	3,3	3,567	0,267
69	5,31	4,6067	0,7033	283	3,3	3,4796	0,1796
70	3,3	3,4103	0,1103	289	5,77	5,8918	0,1218
71	3,3	3,6447	0,3447	294	5,3	5,4031	0,1031
73	3,7	3,9601	0,2601	299	4,02	4,2427	0,2227
74	3,3	3,0439	0,2561	304	4,01	4,115	0,105
75	4,2	4,5115	0,3115	309	4,22	4,1594	0,0606
76	3,3	3,5453	0,2453	314	4,03	4,0509	0,0209
78	3,3	3,702	0,402	319	4,24	4,2634	0,0234
79	5	4,3116	0,6884	324	4	4,0176	0,0176
80	3,3	3,1363	0,1637	329	4	4,1252	0,1252
81	3,3	3,0558	0,2442	334	4,7	3,9914	0,7086
83	4,25	4,7782	0,5282	340	5,35	5,1923	0,1577
84	5,2	4,7882	0,4118	346	5,06	5,2194	0,1594
85	3,3	3,6132	0,3132	351	4,88	4,8657	0,0143
88	5,68	5,2412	0,4388	358	4,86	5,3134	0,4534
91	6,7	5,8662	0,8338	363	4,93	5,1719	0,2419
92	5,52	5,369	0,151	368	4,63	4,7359	0,1059
97	6,47	5,0087	1,4613	373	4,64	4,6779	0,0379
98	5,4	5,292	0,108	378	4,64	4,5963	0,0437
101	4,3	4,9549	0,6549	383	4,65	4,6364	0,0136
102	4,3	4,4071	0,1071	388	4,81	4,6352	0,1748
103	5,1	4,9621	0,1379	395	5,62	5,428	0,192
104	4,22	4,6695	0,4495	400	4,52	5,9764	1,4564
106	4,6	4,8031	0,2031	406	5,74	6,2311	0,4911
107	4,3	4,7564	0,4564	412	8,4	7,5945	0,8055
108	5,52	4,9645	0,5555	417	7,4	6,9296	0,4704
109	4,3	4,2264	0,0736	422	4	4,4249	0,4249
111	5	4,7856	0,2144	429	4	4,3215	0,3215
112	4,48	4,1868	0,2932	436	4	4,4744	0,4744
113	4,85	4,7506	0,0994	442	4,96	4,6754	0,2846
114	4,05	4,5142	0,4642	447	5,15	4,4698	0,6802
116	4,34	4,1743	0,1657	455	4,38	4,3296	0,0504
117	3,92	4,5889	0,6689	460	3,63	3,6584	0,0284
118	4,54	3,7337	0,8063	466	3,67	4,253	0,583
119	4	4,8088	0,8088	474	4,86	4,4669	0,3931
121	4	4,4009	0,4009	481	4,86	3,7924	1,0676
122	4,92	4,8375	0,0825	489	4,92	3,9043	1,0157
123	4,1	4,6448	0,5448	495	4,63	3,9533	0,6767
124	3,92	4,0864	0,1664	500	5,76	5,0057	0,7543
126	4,6	4,6758	0,0758	505	5,85	5,9854	0,1354
127	4,6	4,8835	0,2835	510	4,53	4,133	0,397
128	4,6	4,496	0,104	515	4,3	4,2759	0,0241
129	5,74	5,6401	0,0999	521	4,5	4,1538	0,3462
131	4,96	4,8722	0,0878	526	5,15	5,022	0,128

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
133	5,7	4,5911	1,1089	531	4	3,9837	0,0163
134	4,55	4,4912	0,0588	536	3,7	4,2166	0,5166
135	4,26	4,9713	0,7113	542	3,98	4,7515	0,7715
138	5,1	4,959	0,141	547	5,8	5,1646	0,6354
139	4,12	5,2996	1,1796	552	4,82	4,8645	0,0445
141	4,12	4,4567	0,3367	557	5,62	5,7189	0,0989
144	5,7	5,3029	0,3971	562	4,8	4,9581	0,1581
148	4,12	4,6966	0,5766	567	7,4	6,7819	0,6181
149	6,15	4,9417	1,2083	572	5,82	5,5553	0,2647
150	4,7	5,3341	0,6341	577	5,85	5,5811	0,2689
151	4,6	4,6461	0,0461	582	6,19	5,842	0,348
154	5,7	4,9211	0,7789	587	5,63	6,071	0,441
155	4,66	4,4833	0,1767	592	6,52	5,7852	0,7348
157	6,15	5,7082	0,4418	597	5,85	5,9066	0,0566
158	6,22	5,6017	0,6183	602	4,28	5,0745	0,7945
162	6,15	5,5783	0,5717	608	4	4,0562	0,0562
165	4,15	3,7598	0,3902	613	4	4,2126	0,2126
166	5,7	6,0439	0,3439	620	4,45	4,369	0,081
167	4,77	4,3702	0,3998	625	4,31	4,1276	0,1824
169	4,54	4,6883	0,1483	630	4,29	4,4708	0,1808
170	4,6	4,7069	0,1069	635	5,79	5,908	0,118
171	4,26	4,9668	0,7068	640	5	5,1621	0,1621
172	4,52	4,6736	0,1536	646	4,03	4,9695	0,9395
175	4,02	4,3615	0,3415	651	4,01	4,9775	0,9675
176	2,8	2,692	0,108	657	6,15	5,4412	0,7088
177	2,6	2,8753	0,2753	663	3,88	3,5714	0,3086
178	2,57	2,8895	0,3195	668	4,12	4,0742	0,0458
180	2,55	2,9848	0,4348	673	5,4	5,73	0,33
181	2,48	2,783	0,303	678	5,52	5,3385	0,1815
183	3,92	3,7823	0,1377	683	4,6	5,2445	0,6445
184	3,7	3,799	0,099	688	4,4	5,3039	0,9039
186	3,99	4,0337	0,0437	693	6,22	5,7232	0,4968
187	3,84	4,0481	0,2081	698	4,92	5,2847	0,3647
188	3,53	4,1498	0,6198	703	4,6	5,2155	0,6155
189	3,65	3,7045	0,0545	708	5,47	5,1226	0,3474
191	4,95	4,9162	0,0338	713	5,05	5,1419	0,0919
192	4,15	4,0351	0,1149	718	6,15	5,2845	0,8655
193	3,92	3,6538	0,2662	723	6,3	5,5567	0,7433
194	3,91	3,6495	0,2605	728	4,22	5,0657	0,8457
196	4,47	4,9307	0,4607	733	4,23	4,403	0,173
197	3,76	4,0894	0,3294	738	4,4	4,125	0,275
198	3,62	3,696	0,076	743	4,22	4,3549	0,1349
199	4,32	3,7099	0,6101	748	4	3,8729	0,1271
201	3,85	3,7628	0,0872	753	5,82	6,5853	0,7653
202	4,72	4,8503	0,1303	761	4	4,2254	0,2254
203	3,94	4,0714	0,1314	768	5,78	5,7619	0,0181
204	4,35	3,9346	0,4154	773	6,28	5,7082	0,5718
206	3,61	4,2988	0,6888	780	6,16	6,0824	0,0776
207	4,05	3,6251	0,4249	786	5,77	5,0057	0,7643
208	3,41	4,7991	1,3891	791	6,52	5,7869	0,7331
209	4,15	4,7513	0,6013	796	5,64	6,071	0,431
211	4,15	4,4751	0,3251	801	5,7	5,8692	0,1692
212	4,05	4,5071	0,4571	806	6,15	5,842	0,308
213	4	4,5247	0,5247	811	4,06	4,0579	0,0021
214	4,4	4,491	0,091	816	4	4,1913	0,1913
216	4,22	4,5218	0,3018	821	4	3,8495	0,1505
217	4,22	4,2554	0,0354	826	4	4,0991	0,0991
218	4,7	4,8559	0,1559	832	5,15	5,8615	0,7115
219	4,4	4,2969	0,1031	842	6,05	5,6218	0,4282
221	5,96	6,2497	0,2897	847	4	3,5505	0,4495
222	5,89	6,2726	0,3826	853	4	4,2086	0,2086
223	6,1	6,5232	0,4232	858	4,68	5,1638	0,4838
224	5,82	6,1787	0,3587	867	4,72	5,2128	0,4928
226	6,15	6,5304	0,3804	872	5	5,1742	0,1742
227	6,22	6,4857	0,2657	877	4,31	4,1769	0,1331
228	6,1	5,401	0,699	883	4,57	4,4947	0,0753

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
229	4,5	4,3733	0,1267	889	5,4	4,6831	0,7169
231	4,32	3,9888	0,3312	894	4,67	4,3611	0,3089
232	3,72	4,3034	0,5834	900	4	3,7698	0,2302
233	3,84	4,2566	0,4166	905	4	4,1352	0,1352
234	3,72	4,1188	0,3988	916	3,4	4,4414	1,0414
236	8,4	7,3712	1,0288	927	4	3,9504	0,0496
237	5,82	5,2787	0,5413	933	4	4,0594	0,0594
239	4,85	5,2105	0,3605	938	4,85	4,3099	0,5401
240	7,4	6,469	0,931	943	5,27	4,6658	0,6042
242	7	6,8761	0,1239	948	4	4,4107	0,4107
244	6,4	6,5901	0,1901	953	5,33	4,6075	0,7225
245	5,92	6,0852	0,1652	958	4	4,1596	0,1596
246	6,7	6,6123	0,0877	963	4	4,3673	0,3673
248	6,52	6,5624	0,0424	968	4	4,0631	0,0631
249	7,4	6,6261	0,7739	973	4	4,0763	0,0763
250	5,85	6,2774	0,4274	978	4	4,0421	0,0421
251	7,3	6,3823	0,9177	983	4	4,1102	0,1102
253	5,96	6,095	0,135	989	4	4,017	0,017
254	6,7	6,6357	0,0643	995	4,89	4,6842	0,2058
255	5,05	6,0916	1,0416	1000	4,3	4,6988	0,3988
256	8,4	7,3709	1,0291	1005	4,36	4,6853	0,3253
259	6,22	6,6077	0,3877	1010	4,3	4,6876	0,3876
260	5,53	5,6151	0,0851	1015	4,6	4,9172	0,3172
261	5,45	5,2003	0,2497	1020	4,6	4,3909	0,2091
262	5,44	5,4275	0,0125	1025	4,6	4,6271	0,0271
264	5,44	5,4368	0,0032	1031	4,6	4,3312	0,2688
265	5,18	5,3719	0,1919	1036	4,6	4,8436	0,2436
266	5,5	5,3948	0,1052	1041	4,6	4,6031	0,0031
267	5,5	5,1834	0,3166	1046	4,3	4,2756	0,0244
269	5,31	4,8118	0,4982	1051	4,6	4,5182	0,0818
270	3,3	3,4602	0,1602	1056	4,6	4,5609	0,0391
271	3,3	3,6489	0,3489	1061	4,6	4,5888	0,0112
272	5	4,3421	0,6579	1066	4,6	4,856	0,256
274	3,3	3,0974	0,2026	1071	4	3,6921	0,3079
275	4,2	4,5178	0,3178	1078	4	3,7875	0,2125
276	3,3	3,4591	0,1591	1083	3,4	3,4556	0,0556
277	3,3	3,308	0,008	1089	3,7	3,8031	0,1031
279	5	4,49	0,51	1096	4,57	3,4567	1,1133
280	3,3	3,1511	0,1489	1103	4,15	4,1547	0,0047
281	3,3	3,0217	0,2783	1108	4,31	4,2968	0,0132
282	3,3	4,0374	0,7374	1113	4,15	4,6026	0,4526
284	4,25	4,8023	0,5523	1118	5,44	4,8023	0,6377
285	5,2	4,6915	0,5085	1123	5	4,6779	0,3221
287	5	6,4531	1,4531	1128	4,99	5,2304	0,2404
288	5,01	4,7937	0,2163	1133	5,3	5,1814	0,1186
290	5,74	4,8814	0,8586	1138	4,3	4,4343	0,1343
291	5,14	5,2942	0,1542	1143	4,8	5,1657	0,3657
292	5,96	5,8749	0,0851	1148	4,43	4,9906	0,5606
293	6	5,0482	0,9518	1154	4,98	4,5569	0,4231
295	5,3	5,2513	0,0487	1159	5,13	4,4195	0,7105
296	4,08	4,1974	0,1174	1164	4,65	4,6985	0,0485
297	4,21	4,0524	0,1576	1169	5	4,5817	0,4183
298	4,45	4,0397	0,4103	1174	4,58	5,0653	0,4853
300	4,49	4,1098	0,3802	1179	4,46	5,0042	0,5442
301	4,23	4,1595	0,0705	1184	5,08	4,8375	0,2425
302	4,48	4,0568	0,4232	1189	4,3	4,3056	0,0056
303	4	3,9639	0,0361	1194	6,28	6,322	0,042
305	4,08	4,0264	0,0536	1200	5,05	4,5068	0,5432
306	4	3,9114	0,0886	1205	4,84	4,6725	0,1675
307	4	4,1684	0,1684	1210	4,93	4,5642	0,3658
308	4,09	4,2989	0,2089	1215	4,3	4,4208	0,1208
310	4,39	4,0717	0,3183	1220	5,06	4,799	0,261
311	4	4,3598	0,3598	1225	4,62	4,6896	0,0696
312	4	4,1117	0,1117	1230	4,38	4,6106	0,2306
313	4,19	4,1247	0,0653	1235	4,3	4,2206	0,0794
315	4	4,1088	0,1088	1241	4,95	4,8249	0,1251

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
316	4	4,0424	0,0424	1246	5,21	5,2068	0,0032
317	4,26	4,1837	0,0763	1251	3,98	4,0666	0,0866
318	4,16	4,2014	0,0414	1257	4,25	3,9278	0,3222
320	4,25	4,1532	0,0968	1263	5,88	5,3386	0,5414
321	4,16	4,0108	0,1492	1268	4,3	4,4737	0,1737
322	4,22	4,1247	0,0953	1273	5,34	5,4273	0,0873
323	4	4,2262	0,2262	1278	4,87	4,8627	0,0073
325	4	4,2401	0,2401	1283	5,41	5,3696	0,0404
326	4,16	4,2364	0,0764	1288	4,56	4,7234	0,1634
327	4	4,0504	0,0504	1294	4,29	4,4239	0,1339
328	4	4,1555	0,1555	1299	4,77	5,1454	0,3754
330	4	4,0073	0,0073	1304	4,8	4,6577	0,1423
331	4	4,1656	0,1656	1309	4,17	4,7664	0,5964
332	4,33	4,0562	0,2738				
333	4	4,2914	0,2914				
335	4,52	3,955	0,565				
337	4	3,8891	0,1109				
338	4	4,0316	0,0316				
339	4,4	3,92	0,48				
341	5,35	4,5078	0,8422				
342	5,35	5,5051	0,1551				
344	7,23	6,6851	0,5449				
345	5	4,9077	0,0923				
347	5,11	5,5764	0,4664				
348	5	5,7318	0,7318				
349	5,16	4,9877	0,1723				
350	6,09	4,889	1,201				
354	5,12	5,0753	0,0447				
355	5,22	5,5212	0,3012				
356	4,92	5,0911	0,1711				
357	5,08	5,1619	0,0819				
359	5,11	5,3618	0,2518				
360	5,19	5,2011	0,0111				
361	4,9	5,1656	0,2656				
362	4,47	5,3819	0,9119				
364	5,42	5,1595	0,2605				
365	5,21	5,3616	0,1516				
366	4,65	4,9337	0,2837				
367	4,64	4,7114	0,0714				
369	4,66	4,6173	0,0427				
370	4,63	4,7123	0,0823				
371	4,63	4,7545	0,1245				
372	4,65	4,7331	0,0831				
374	4,66	4,6901	0,0301				
375	4,66	4,8438	0,1838				
376	4,64	4,711	0,071				
377	4,65	4,7438	0,0938				
379	4,67	4,7801	0,1101				
380	4,66	4,7171	0,0571				
381	4,77	4,6838	0,0862				
382	4,64	4,655	0,015				
384	5,17	4,6508	0,5192				
385	4,65	4,4988	0,1512				
386	4,78	4,6058	0,1742				
387	4,66	4,3544	0,3056				
390	4,24	4,5809	0,3409				
391	4,55	4,3733	0,1767				
392	4,38	4,3583	0,0217				
393	4,34	4,7461	0,4061				
396	8,22	7,3873	0,8327				
397	5,7	5,2595	0,4405				
398	4,65	4,357	0,293				
399	5,82	5,4069	0,4131				
402	4,12	5,2089	1,0889				
403	6,1	6,2604	0,1604				
404	7,4	6,4972	0,9028				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
405	5,72	6,4075	0,6875				
407	6,4	6,4433	0,0433				
409	5,96	6,3978	0,4378				
410	6,4	6,2936	0,1064				
411	7,22	6,6654	0,5546				
413	5,77	6,2846	0,5146				
414	7,3	6,7128	0,5872				
415	5,89	6,4242	0,5342				
416	6,52	6,2856	0,2344				
418	4,2	4,2332	0,0332				
419	3,96	4,4111	0,4511				
420	4,39	4,5602	0,1702				
421	4,85	4,5918	0,2582				
423	4,55	4,0716	0,4784				
424	4,66	4,6889	0,0289				
427	5,52	4,9853	0,5347				
428	4,92	5,1501	0,2301				
432	4,34	4,7513	0,4113				
433	4,4	4,3076	0,0924				
434	4	4,0035	0,0035				
435	5,34	5,0818	0,2582				
437	4,74	5,0181	0,2781				
438	4	4,2667	0,2667				
440	5,33	4,3205	1,0095				
441	4	4,9231	0,9231				
443	4,42	4,7362	0,3162				
444	4,04	4,6681	0,6281				
445	4,46	3,8135	0,6465				
446	5,63	4,3271	1,3029				
448	3,62	3,644	0,024				
450	4,36	4,3436	0,0164				
452	3,63	3,9175	0,2875				
453	3,64	4,3066	0,6666				
456	3,63	4,1889	0,5589				
457	5,61	4,8878	0,7222				
458	3,6	4,1342	0,5342				
459	5,65	4,6039	1,0461				
461	4,27	3,9875	0,2825				
463	4,59	4,2161	0,3739				
464	5,59	4,3728	1,2172				
465	3,63	4,1338	0,5038				
467	3,7	3,6449	0,0551				
470	3,67	4,1899	0,5199				
472	5,66	5,2514	0,4086				
473	3,6	4,2984	0,6984				
477	3,69	4,5427	0,8527				
478	3,64	3,8962	0,2562				
479	4,3	4,5497	0,2497				
480	4,51	3,8346	0,6754				
482	3,69	4,0061	0,3161				
483	3,66	4,0021	0,3421				
487	3,42	3,864	0,444				
488	4,8	4,9677	0,1677				
490	4,41	3,9519	0,4581				
492	3,64	3,7397	0,0997				
493	3,49	3,9631	0,4731				
494	4,2	4,5537	0,3537				
496	5,6	5,0564	0,5436				
497	3,71	3,8665	0,1565				
498	3,65	3,6816	0,0316				
499	6,07	5,7922	0,2778				
501	5,45	6,0076	0,5576				
502	5,62	5,9103	0,2903				
503	6,68	6,3991	0,2809				
504	6,41	5,873	0,537				
506	6,38	6,7688	0,3888				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
507	5,78	5,8971	0,1171				
508	4,3	4,6551	0,3551				
509	4,56	4,9404	0,3804				
511	4,3	4,038	0,262				
512	4,37	4,0725	0,2975				
513	5,24	4,6979	0,5421				
514	3,89	4,6467	0,7567				
516	4,32	4,5163	0,1963				
517	4,3	4,1094	0,1906				
518	4,4	4,2901	0,1099				
520	4,3	4,6553	0,3553				
522	3,7	4,1284	0,4284				
523	4,75	3,9548	0,7952				
524	4,72	4,08	0,64				
525	3,7	4,1015	0,4015				
527	3,7	3,8834	0,1834				
528	4,26	4,2971	0,0371				
529	4	4,1929	0,1929				
530	4,37	4,237	0,133				
532	4	4,2876	0,2876				
533	3,7	4,0947	0,3947				
534	3,7	3,5385	0,1615				
535	3,7	3,8506	0,1506				
538	4,7	4,169	0,531				
539	4	4,1005	0,1005				
540	4	4,0377	0,0377				
541	4	3,4176	0,5824				
543	4,52	4,3687	0,1513				
544	4,54	4,5853	0,0453				
545	4	4,3631	0,3631				
546	5,7	5,5422	0,1578				
548	5,05	4,5625	0,4875				
549	4,8	4,865	0,065				
550	4,09	4,2715	0,1815				
551	5,33	5,1947	0,1353				
553	5,4	5,1145	0,2855				
554	5,4	5,4099	0,0099				
555	4,21	4,9187	0,7087				
556	5	4,7854	0,2146				
558	4,89	5,4589	0,5689				
559	5,7	5,1062	0,5938				
560	4	4,1814	0,1814				
561	4,96	4,6848	0,2752				
563	4	4,6085	0,6085				
564	4,89	4,6598	0,2302				
565	4,15	4,4467	0,2967				
566	4,64	4,517	0,123				
568	4,57	4,8561	0,2861				
569	5,33	5,4267	0,0967				
570	5,04	5,3667	0,3267				
571	5,53	5,7795	0,2495				
573	5,9	5,721	0,179				
574	5,91	5,8723	0,0377				
575	5,67	5,5526	0,1174				
576	5,44	4,9303	0,5097				
578	5,49	5,6538	0,1638				
579	5,39	5,1915	0,1985				
580	5,86	5,444	0,416				
581	6,38	6,7729	0,3929				
583	5,58	5,9505	0,3705				
584	6,41	5,8693	0,5407				
585	6,07	5,9141	0,1559				
586	5,62	5,9468	0,3268				
588	6,04	5,7434	0,2966				
589	5,45	5,9968	0,5468				
590	5,45	5,8851	0,4351				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
591	5,69	5,915	0,225				
593	6,05	5,9851	0,0649				
594	5,62	5,5611	0,0589				
595	5,8	5,6917	0,1083				
596	6,15	6,195	0,045				
598	6,7	5,8987	0,8013				
599	5,3	5,6662	0,3662				
600	5,12	5,2779	0,1579				
601	4,47	5,4715	1,0015				
603	5,03	5,171	0,141				
604	4,72	4,5381	0,1819				
605	4,96	4,7534	0,2066				
607	4,19	4,299	0,109				
609	4,01	4,3066	0,2966				
610	4	4,4768	0,4768				
611	4	4,175	0,175				
612	4	4,0343	0,0343				
614	4	4,8013	0,8013				
615	4	4,3783	0,3783				
617	4,46	4,5781	0,1181				
618	4,49	4,2671	0,2229				
621	4,44	4,4346	0,0054				
622	4,48	4,5777	0,0977				
623	4,51	4,3525	0,1575				
624	4,35	4,7404	0,3904				
626	4,31	4,2531	0,0569				
627	4,31	4,8276	0,5176				
628	4,26	4,4023	0,1423				
629	4,27	4,5461	0,2761				
631	4,34	4,5114	0,1714				
632	8,44	7,2294	1,2106				
633	4,66	4,6663	0,0063				
634	4,77	4,7482	0,0218				
636	5,15	5,7182	0,5682				
637	5	5,0544	0,0544				
638	5,3	4,9287	0,3713				
639	5	4,9458	0,0542				
641	5	4,5326	0,4674				
642	5	5,0097	0,0097				
643	3,7	3,9466	0,2466				
644	4,38	4,2715	0,1085				
647	3,7	4,5134	0,8134				
648	5,72	4,6527	1,0673				
649	4,07	3,9819	0,0881				
650	4,66	4,8071	0,1471				
652	5,82	5,0957	0,7243				
654	4,94	4,7487	0,1913				
655	5,55	4,8016	0,7484				
656	5,46	4,9676	0,4924				
658	5,15	5,112	0,038				
660	5,04	4,4557	0,5843				
661	4,91	5,2367	0,3267				
662	3,93	5,077	1,147				
664	3,71	4,4331	0,7231				
665	4,11	4,1412	0,0312				
666	4,11	4,0781	0,0319				
667	4,1	4,0512	0,0488				
669	4,11	4,0347	0,0753				
670	4,15	4,1021	0,0479				
671	4,13	4,4391	0,3091				
672	5,44	5,6696	0,2296				
674	5,36	5,6411	0,2811				
675	5,06	5,1566	0,0966				
676	4,87	4,8388	0,0312				
677	6,05	5,5185	0,5315				
679	5,32	5,4248	0,1048				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
680	5,13	4,8269	0,3031				
681	5,37	5,2489	0,1211				
682	4,78	5,9471	1,1671				
684	4,64	5,0628	0,4228				
685	6,41	5,4242	0,9858				
686	6,03	5,4448	0,5852				
687	4,69	5,3871	0,6971				
689	5,02	5,5821	0,5621				
690	4,6	5,2986	0,6986				
691	5,24	4,7365	0,5035				
692	5,82	5,1049	0,7151				
694	5,51	5,1537	0,3563				
695	5,38	5,92	0,54				
696	5,62	5,6396	0,0196				
697	5,04	5,275	0,235				
699	4,81	4,8123	0,0023				
700	4,91	4,4977	0,4123				
701	6,55	5,717	0,833				
702	5,12	5,0661	0,0539				
704	4,8	5,2118	0,4118				
705	5,44	5,5952	0,1552				
706	4,7	5,2125	0,5125				
707	5,05	5,3277	0,2777				
709	5,1	5,0324	0,0676				
710	5,68	6,039	0,359				
711	4,59	4,5833	0,0067				
712	5,54	5,4767	0,0633				
714	5,52	5,0329	0,4871				
715	4,8	5,3632	0,5632				
716	5,05	5,3144	0,2644				
717	5,8	5,1528	0,6472				
719	6,05	5,8317	0,2183				
720	5,17	5,4786	0,3086				
721	6,03	5,8973	0,1327				
722	5,26	5,6007	0,3407				
724	6,15	5,4609	0,6891				
725	5,15	5,4769	0,3269				
726	6,3	5,7371	0,5629				
727	5,44	5,9285	0,4885				
729	4,49	4,5513	0,0613				
730	3,5	3,924	0,424				
731	4,22	4,7177	0,4977				
732	4,4	4,4324	0,0324				
734	4,37	4,3419	0,0281				
735	4,72	4,5349	0,1851				
736	4,82	4,6142	0,2058				
737	4,41	4,1102	0,2998				
739	4,22	4,3751	0,1551				
740	3,37	3,9518	0,5818				
741	4,35	4,4852	0,1352				
742	4,72	4,7025	0,0175				
744	4	3,8247	0,1753				
745	4,01	3,7926	0,2174				
746	4	4,0927	0,0927				
747	4	4,1815	0,1815				
749	4	3,8736	0,1264				
750	4,01	3,8095	0,2005				
751	4	4,1012	0,1012				
752	4,13	4,234	0,104				
754	4	4,4344	0,4344				
755	4,01	4,1037	0,0937				
756	6,33	6,2934	0,0366				
757	6,82	6,5277	0,2923				
762	4	4,0763	0,0763				
765	5,76	5,4368	0,3232				
766	5,44	5,6223	0,1823				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
767	4,82	5,0806	0,2606				
769	5,58	5,5653	0,0147				
770	5,55	5,4313	0,1187				
771	5,52	4,9278	0,5922				
772	6,13	6,8122	0,6822				
774	7,27	6,2511	1,0189				
775	7,29	6,2621	1,0279				
776	5,93	6,0417	0,1117				
779	6,21	5,5699	0,6401				
781	6,15	6,4397	0,2897				
782	5,94	6,517	0,577				
784	4,43	4,7411	0,3111				
785	5,85	5,9569	0,1069				
787	6,05	5,7686	0,2814				
788	6,4	5,8861	0,5139				
789	5,62	5,9246	0,3046				
790	5,74	5,875	0,135				
792	6,15	5,7959	0,3541				
793	5,38	5,5422	0,1622				
794	5,35	5,8465	0,4965				
795	6	5,9001	0,0999				
797	5,46	5,8643	0,4043				
798	5,59	5,9237	0,3337				
799	6,3	5,741	0,559				
800	6,7	6,4057	0,2943				
802	6,05	5,7222	0,3278				
803	5,54	5,8248	0,2848				
804	5,77	5,8383	0,0683				
805	5,44	6,0073	0,5673				
807	6,05	5,9308	0,1192				
808	6,05	5,8098	0,2402				
809	5,24	6,0236	0,7836				
810	4	3,9176	0,0824				
812	4	3,9638	0,0362				
813	4	4,83	0,83				
814	4	3,7072	0,2928				
815	4,49	4,7034	0,2134				
817	4	4,0438	0,0438				
818	4	3,9871	0,0129				
819	4	4,2267	0,2267				
820	4	4,1086	0,1086				
822	4	3,9888	0,0112				
823	4	3,9508	0,0492				
824	4	4,6903	0,6903				
825	4	3,9267	0,0733				
827	4	3,9184	0,0816				
828	4	3,9029	0,0971				
829	4	4,3997	0,3997				
831	6,15	5,8368	0,3132				
835	5,52	6,3135	0,7935				
838	5,89	5,7825	0,1075				
840	6,05	5,875	0,175				
841	6	6,0211	0,0211				
843	4	3,8404	0,1596				
844	4	4,0019	0,0019				
845	4	4,1377	0,1377				
846	4,24	4,0039	0,2361				
848	4	4,7523	0,7523				
849	4	3,8596	0,1404				
850	4	3,6571	0,3429				
852	4	3,9016	0,0984				
854	5	4,2461	0,7539				
855	4,7	4,6302	0,0698				
856	4,51	4,8652	0,3552				
857	4,98	5,4134	0,4334				
860	5,8	5,2426	0,5574				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
862	5,67	5,534	0,136				
864	5,11	5,2308	0,1208				
865	4,74	5,0982	0,3582				
868	5,17	5,4009	0,2309				
869	5,02	5,2687	0,2487				
870	4,77	5,2688	0,4988				
871	5,42	4,7444	0,6756				
873	5,01	5,1655	0,1555				
874	5,54	5,0872	0,4528				
875	5,24	5,4627	0,2227				
876	5,22	5,1431	0,0769				
879	4,85	4,2393	0,6107				
880	4	3,9943	0,0057				
881	4	4,2302	0,2302				
882	4	4,2464	0,2464				
884	4,33	4,5239	0,1939				
885	4,53	4,7201	0,1901				
886	4,88	4,3797	0,5003				
887	5,24	4,388	0,852				
890	4,51	4,0415	0,4685				
891	4	4,6313	0,6313				
892	4,5	4,1924	0,3076				
893	5,41	4,2085	1,2015				
895	4,28	4,5018	0,2218				
896	4,41	4,5466	0,1366				
897	4,07	4,6937	0,6237				
898	4	3,8738	0,1262				
901	4	4,1431	0,1431				
902	4,52	4,4267	0,0933				
903	4,96	4,2953	0,6647				
904	4,33	4,3553	0,0253				
906	4,42	5,015	0,595				
907	4,68	5,0572	0,3772				
912	4,68	3,9715	0,7085				
913	4,54	4,4086	0,1314				
919	3,4	4,4499	1,0499				
921	4,58	4,6073	0,0273				
924	5,1	4,6142	0,4858				
926	4,34	3,8754	0,4646				
928	4	4,0327	0,0327				
929	4	4,6928	0,6928				
930	4	4,3015	0,3015				
932	4	4,1914	0,1914				
934	4,58	4,6945	0,1145				
935	4	4,1252	0,1252				
936	4,92	4,1144	0,8056				
937	4,72	4,7208	0,0008				
939	4,7	4,2984	0,4016				
940	5	4,7492	0,2508				
941	5,37	5,121	0,249				
942	5,26	5,0399	0,2201				
944	5	5,2615	0,2615				
945	5,28	5,2096	0,0704				
946	5	4,786	0,214				
947	4	4,0917	0,0917				
949	4	3,9361	0,0639				
950	4	4,035	0,035				
951	4,61	4,5278	0,0822				
952	4,75	4,5599	0,1901				
954	4	4,1706	0,1706				
955	4	3,9553	0,0447				
956	4	4,3701	0,3701				
957	4	4,7091	0,7091				
959	5,3	4,2546	1,0454				
960	4	4,1183	0,1183				
961	4,4	4,0674	0,3326				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
962	4,19	3,9663	0,2237				
964	4	4,5959	0,5959				
965	4,48	4,0526	0,4274				
966	4	4,584	0,584				
967	4,85	4,3304	0,5196				
969	4	3,8766	0,1234				
970	4	3,8716	0,1284				
971	4	4,2137	0,2137				
972	4	4,1065	0,1065				
974	4	4,4884	0,4884				
975	4	4,0763	0,0763				
976	4	4,1059	0,1059				
977	5,14	4,4794	0,6606				
979	4	4,0657	0,0657				
980	4	4,1376	0,1376				
981	5,35	4,3591	0,9909				
982	4,82	4,397	0,423				
985	4	4,1438	0,1438				
986	4,54	4,4916	0,0484				
987	4	4,2072	0,2072				
988	4,3	4,3967	0,0967				
991	4	3,8501	0,1499				
992	4	3,7758	0,2242				
993	4,92	4,51	0,41				
994	4,3	4,7059	0,4059				
996	5,42	4,5343	0,8857				
997	4,85	4,5099	0,3401				
998	4,49	4,6736	0,1836				
999	4,4	4,8866	0,4866				
1001	4,89	4,8016	0,0884				
1002	4,8	4,7843	0,0157				
1003	4,3	4,8222	0,5222				
1004	4,59	4,5318	0,0582				
1006	4,64	4,732	0,092				
1007	4,82	4,5572	0,2628				
1008	5,1	4,6277	0,4723				
1009	4,54	4,7297	0,1897				
1011	4,3	4,5426	0,2426				
1012	5,42	5,5547	0,1347				
1013	4,6	4,5225	0,0775				
1014	5,68	5,1682	0,5118				
1016	4,6	4,8935	0,2935				
1017	4,6	4,97	0,37				
1018	4,6	4,691	0,091				
1019	4,6	5,1419	0,5419				
1021	5,42	5,5248	0,1048				
1022	4,6	4,6028	0,0028				
1023	4,6	4,8353	0,2353				
1024	4,6	4,636	0,036				
1026	5,82	5,0217	0,7983				
1028	5,28	5,1349	0,1451				
1029	4,6	4,8023	0,2023				
1030	4,6	4,6135	0,0135				
1032	4,6	4,827	0,227				
1033	4,6	4,8444	0,2444				
1034	5,23	5,138	0,092				
1035	4,6	4,6788	0,0788				
1037	4,6	4,2865	0,3135				
1038	4,6	4,7295	0,1295				
1039	4,6	4,1331	0,4669				
1040	4,6	5,0486	0,4486				
1042	4,6	4,6496	0,0496				
1043	4,6	4,6499	0,0499				
1044	4,6	4,3463	0,2537				
1045	4,6	4,6046	0,0046				
1047	4,6	4,9466	0,3466				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
1048	4,6	4,849	0,249				
1049	5,85	5,1119	0,7381				
1050	4,6	4,5693	0,0307				
1052	4,3	4,2888	0,0112				
1053	3,89	4,7101	0,8201				
1054	4,6	4,8772	0,2772				
1055	4,6	4,7866	0,1866				
1057	5,1	4,8049	0,2951				
1058	5,15	4,9408	0,2092				
1059	5,19	5,3785	0,1885				
1060	4,6	4,6034	0,0034				
1062	5,54	5,5583	0,0183				
1063	4,67	4,6714	0,0014				
1064	4,6	4,579	0,021				
1065	5,38	5,2762	0,1038				
1067	4,6	4,5185	0,0815				
1068	4,6	4,4308	0,1692				
1069	4,26	4,0615	0,1985				
1070	4,66	4,9092	0,2492				
1074	3,4	3,5664	0,1664				
1075	5,1	3,3264	1,7736				
1076	3,7	3,4665	0,2335				
1077	4	3,5962	0,4038				
1079	3,4	3,9503	0,5503				
1080	3,4	3,4423	0,0423				
1081	3,4	3,5023	0,1023				
1082	3,7	3,5962	0,1038				
1084	3,4	3,8313	0,4313				
1085	4,09	3,759	0,331				
1086	3,4	4,0137	0,6137				
1087	3,52	3,8069	0,2869				
1092	3,4	3,5734	0,1734				
1093	3,7	3,4015	0,2985				
1094	3,4	3,6197	0,2197				
1095	3,4	3,6987	0,2987				
1097	3,4	3,3994	0,0006				
1099	3,7	3,4987	0,2013				
1100	3,4	3,6106	0,2106				
1102	8,21	7,3668	0,8432				
1104	4,15	4,5414	0,3914				
1105	4,37	4,424	0,054				
1106	4,33	4,3674	0,0374				
1107	4,34	4,3289	0,0111				
1109	4,42	4,545	0,125				
1110	4,27	4,441	0,171				
1111	4,38	4,5649	0,1849				
1112	4,63	4,6334	0,0034				
1114	4,41	4,3667	0,0433				
1115	4,24	4,238	0,002				
1116	4,79	4,191	0,599				
1117	5,27	5,2302	0,0398				
1119	5,38	5,0603	0,3197				
1120	5	4,6512	0,3488				
1121	5	4,73	0,27				
1122	5	4,5875	0,4125				
1124	5,17	5,1007	0,0693				
1125	5,82	6,7948	0,9748				
1126	3,82	4,8155	0,9955				
1127	4,66	5,2748	0,6148				
1129	4,62	5,2983	0,6783				
1130	5,06	5,1976	0,1376				
1131	4,3	4,2297	0,0703				
1132	5,55	5,0782	0,4718				
1134	4,3	4,1698	0,1302				
1135	4,45	4,8724	0,4224				
1136	4,97	5,2921	0,3221				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
1137	4,7	4,3472	0,3528				
1139	5,07	5,0337	0,0363				
1140	5,39	4,7353	0,6547				
1141	5,55	5,076	0,474				
1142	5,09	5,062	0,028				
1144	4,92	4,567	0,353				
1145	4,72	4,7296	0,0096				
1146	5,44	4,9639	0,4761				
1147	4,39	5,286	0,896				
1149	5,04	5,1531	0,1131				
1150	5,89	6,7998	0,9098				
1152	4,75	4,4084	0,3416				
1153	4,71	4,6904	0,0196				
1155	5,35	4,393	0,957				
1156	4	4,551	0,551				
1157	4,66	4,5364	0,1236				
1158	4	4,4499	0,4499				
1160	4,66	4,4955	0,1645				
1161	4,4	4,6121	0,2121				
1162	4,51	4,6317	0,1217				
1163	5,52	5,9816	0,4616				
1165	5	4,6919	0,3081				
1166	5,24	4,7273	0,5127				
1167	5,03	4,6823	0,3477				
1168	5,11	4,731	0,379				
1170	8,15	7,1452	1,0048				
1171	5,1	5,4388	0,3388				
1172	5,15	5,0236	0,1264				
1173	5,12	4,8103	0,3097				
1175	4,81	5,1387	0,3287				
1176	4,87	5,2943	0,4243				
1177	5,89	6,8317	0,9417				
1178	4,49	4,8202	0,3302				
1180	5,07	4,422	0,648				
1181	5,24	5,2046	0,0354				
1182	6	6,8195	0,8195				
1183	4,3	3,9156	0,3844				
1185	4,66	4,9112	0,2512				
1186	4,44	4,9875	0,5475				
1187	5,49	4,5238	0,9662				
1188	4,55	5,0764	0,5264				
1190	4,3	4,495	0,195				
1191	4,3	4,3509	0,0509				
1192	4,39	4,0217	0,3683				
1193	6	5,4722	0,5278				
1195	5,99	5,9447	0,0453				
1196	4,72	4,9278	0,2078				
1198	3,75	3,797	0,047				
1199	4,75	5,0322	0,2822				
1201	5	4,5748	0,4252				
1202	4,24	4,4123	0,1723				
1203	4,67	5,1895	0,5195				
1204	5	4,9938	0,0062				
1206	4,27	4,0159	0,2541				
1207	3,7	4,0141	0,3141				
1208	3,7	3,9988	0,2988				
1209	6	6,1147	0,1147				
1211	3,7	4,5349	0,8349				
1212	5,3	5,112	0,188				
1213	5	4,997	0,003				
1214	4,7	4,9734	0,2734				
1216	5,49	4,9093	0,5807				
1217	4,7	4,8377	0,1377				
1218	4,9	5,0939	0,1939				
1219	5,96	5,6505	0,3095				
1221	5,18	5,1224	0,0576				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
1222	4,71	4,2744	0,4356				
1223	6,96	5,7443	1,2157				
1224	5,66	5,4457	0,2143				
1226	5,05	5,4594	0,4094				
1227	5,09	4,763	0,327				
1228	5,43	5,4015	0,0285				
1229	4,81	4,7769	0,0331				
1231	4	4,8463	0,8463				
1232	5,17	4,4963	0,6737				
1233	4,49	4,5863	0,0963				
1234	4,3	4,3654	0,0654				
1236	3,7	3,9611	0,2611				
1237	3,98	4,3182	0,3382				
1239	5,45	5,5773	0,1273				
1240	5,06	5,1427	0,0827				
1242	5,95	5,4688	0,4812				
1243	4,78	4,9661	0,1861				
1244	4,52	4,4807	0,0393				
1245	5,17	4,8905	0,2795				
1247	4	4,6538	0,6538				
1248	4,37	4,0486	0,3214				
1249	4,3	4,3317	0,0317				
1250	4,36	4,8756	0,5156				
1252	4,25	3,9684	0,2816				
1254	4,68	5,0208	0,3408				
1255	6,23	6,1173	0,1127				
1256	4,39	3,9213	0,4687				
1258	3,7	4,0713	0,3713				
1260	5,12	5,2194	0,0994				
1261	5,39	5,2381	0,1519				
1262	5,01	4,5341	0,4759				
1264	4,32	4,7888	0,4688				
1265	4,36	4,632	0,272				
1266	3,75	3,7977	0,0477				
1267	5,49	4,522	0,968				
1269	3,7	3,9179	0,2179				
1270	3,82	3,8323	0,0123				
1271	3,76	4,217	0,457				
1272	3,7	3,9668	0,2668				
1274	4,84	4,6442	0,1958				
1275	4,3	4,6248	0,3248				
1276	5,11	5,3352	0,2252				
1277	4,66	4,7381	0,0781				
1279	4	4,679	0,679				
1280	5,46	5,1437	0,3163				
1281	4,49	3,7718	0,7182				
1282	5,08	4,9225	0,1575				
1284	5,44	5,5868	0,1468				
1285	4,18	3,6916	0,4884				
1286	4,97	5,0119	0,0419				
1287	4,56	4,4782	0,0818				
1289	5,4	5,0393	0,3607				
1290	5,99	6,077	0,087				
1291	5,97	5,6842	0,2858				
1293	4,49	4,3734	0,1166				
1295	5,28	5,4841	0,2041				
1296	5,11	5,6057	0,4957				
1297	3,7	4,1705	0,4705				
1298	4,33	4,0526	0,2774				
1300	5,89	5,891	0,001				
1301	4,35	4,1521	0,1979				
1302	4,15	4,4084	0,2584				
1303	6	6,0046	0,0046				
1305	4,46	5,1463	0,6863				
1306	3,88	4,6824	0,8024				
1307	4,79	4,4955	0,2945				

Training set		ASNN		Test set			
NAME	lg(1/IC50)	Predicted	delta	NAME	lg(1/IC50)	Predicted	x delta
1308	4,77	4,645	0,125				
1310	4,2	4,2451	0,0451				
1311	4,53	4,4926	0,0374				
1312	4,51	4,6186	0,1086				

Table S3. Test new data.

New set		
NAME	SMILE	lg(1/IC50)
1t	CCCCCCCCCCOC(=O)CN1C=CN=C1	4,26
2t	[Cl-].CCCCCCCCCC[N+]1=CC=CC=C1	4,09
3t	[Cl-].CCCCCCCCCCC[N+]1=CC=CC=C1	4,29
4t	[Cl-].CCCCCCCCCCCC[N+]1=CC=CC=C1	4,22
5t	[Cl-].CCCCCCCCOC(=O)C[N+]1=CC=CC=C1	4,31
6t	[Cl-].CCCCCCCCCCOC(=O)C[N+]1=CC=CC=C1	4,78
7t	[Cl-].CCCCCCCCCCCCOC(=O)C[N+]1=CC=CC=C1	4,88
8t	[Cl-].CCCCCCCCOC(=O)CN1C=C[N+](C)=C1	4,55
9t	[Cl-].CCCCCCCCCCOC(=O)CN1C=C[N+](C)=C1	4,43
10t	[Cl-].CCCCCCCCCCCCOC(=O)CN1C=C[N+](C)=C1	4,45
11t	[Cl-].CCCCCCCCOC(=O)C[N+]1=CSC(CCO)=C1C	4,07
12t	[Cl-].CCCCCCCCCCOC(=O)C[N+]1=CSC(CCO)=C1C	4,18