FABP4 inhibitors 3D-QSAR model and isosteric replacement of BMS309403 datasets

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Data article

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FABP4 inhibitors 3D-QSAR model and isosteric replacement of BMS309403 datasets

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Abstract

The data have been obtained from FABP4 inhibitor molecules previously published. The 120 compounds were used to build a 3D-QSAR model. The development of the QSAR model has been undertaken with the use of Forge software using the PM3 optimized structure and the experimental IC\textsubscript{50} of each compound. The QSAR model was also employed to predict the activity of 3000 new isosteric derivatives of BMS309403. The isosteric replacement was also validated by the synthesis and the biological screening of three new compounds reported in the related research article “3D-QSAR assisted identification of FABP4 inhibitors: An effective scaffold hopping analysis/QSAR evaluation”[1].

Specifications Table

| Subject area         | Computational Chemistry |
|----------------------|-------------------------|
More specific subject area | Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) modeling
---|---
Type of data | Tables, figures
How data was acquired | Statistical modeling and online databases
Data format | Raw and analyzed
Experimental factors | The whole dataset consists of 120 FABP4 ligands and 3000 isosteric derivatives of BMS309403
Experimental features | The 3D-QSAR model has been developed using Forge as software. Chemical structure descriptors and pIC$_{50}$ were used as variables. Spark was used for the isosteric replacement
Data source location | Department of Drug Sciences, University of Catania, Italy
Data accessibility | Data is with this article
Related research article | G. Floresta, A. Cilibrizzi, V. Abbate, A. Spampinato, C. Zagni, A. Rescifina, 3D-QSAR assisted identification of FABP4 inhibitors: An effective scaffold hopping analysis/QSAR evaluation, Bioorganic Chemistry, 84 (2019) 276-284 [1].

Value of the data
- FABP4 recently demonstrated an interesting molecular target for the treatment of type 2 diabetes, other metabolic diseases and some type of cancers.
- QSAR modeling data was generated to provide a method useful in finding or repurposing novel FABP4 ligands.
- The model has also been used to predict the activity of 3000 isosteric derivatives of BMS309403.
- The data can be used by others to build their own model.
- The data can be used for the synthesis of some potent suggested compounds.

Data
FABP4 recently demonstrated an interesting molecular target for the treatment of type 2 diabetes, other metabolic diseases and some type of cancers [2-10]. Recently, a variety of effective FABP4 inhibitors have been developed [11], but unfortunately, none of them is currently in the clinical research phases. CAMD shows a promising and effective tool for the identification of FABP4 inhibitors [12-15]. In line with our recent interest in the development of QSAR models and related applications [16-24], in order to identify novel hit compounds, herein we report the dataset and the parameter used to build a 3D-QSAR model for FABP4. This dataset is reported in Tables 2 and 3, were the molecules used in the training set (96) and in the test set (24) are reported, respectively. Information for the building of the 3D-QSAR model is reported in Figures 1–9. Moreover, the 3D-QSAR model was also used to predict the biological activity of 3000 new isosteric derivatives of BMS309403 derived from a scaffold-hopping analysis, the analyzed areas of the selected compounds and the Spark’s parameters used for the isosteric replacement are reported in Figures 8 and 9. The results of the isosteric replacement of different portion of BMS309403 are reported in Tables 4–9.

Experimental Design, Materials and Methods

Compounds alignments
With the aim to generate a plausible and consistent set of alignment molecules, before running the regression analysis, we evaluated two different types of alignment (Fig. 1).

First, we evaluated a structure-based alignment, based on the docking of the different ligands on the active site of the protein. All 120 structures, optimized at the PM3 level of theory [25-27], have been converted into pdbqt format using Babel,[28] and subsequently docked in the active site of FABP4. Molecular docking was performed using the three-dimensional crystal structures of substrate-free fatty acid binding protein 4 in complex with BMS309403 (PDB ID: 2NNQ) obtained from the Protein Data Bank (PDB, http://www.rcsb.org/pdb). AutoDock Vina (version 1.1.2)[29], was used for all docking experiments. The default values of the docking parameters in AutoDock Vina were all maintained, except for "exhaustiveness" that was set to 15. A grid box of 18 Å × 18 Å × 18 Å was used, encompassing the inhibitor binding cavity of FABP4 and centered on the ligand. The binding modes were clustered through the root mean square deviation among the Cartesian coordinates of the ligand atoms. The docking results were ranked based on the binding free energy. After the calculations with AutoDock Vina, all the generated structures were manually checked, in order to ensure a correct positioning within the binding site. Then the generated structures were imported into Forge [30] to build the Structure-based 3D-QSAR model. A classic ligand-based alignment is the second type of alignment that was evaluated. This was carried out with the same software used for the building of the model. All the optimized structures, together with their respective IC₅₀ values, were imported into Forge (10.4.2, Cresset, Luton, Cambridgeshire, UK, http://www.cresset-group.com/forge) [30-34] for setting-up the field-based 3D-QSAR model. Eight different molecules were chosen as a template for the calculations of field points and as a template for the alignment. These eight molecules were selected since they are present in crystallized forms with FABP4 (PDB IDs: 2NNQ, 3FR2, 3FR4, 3FR5, 4NNS, 4NNT, 1TOU and 1TOW, Table 1) [35-38]. The structures, small protein, and inhibitors, were first downloaded from the Protein Data Bank (PDB); the amino acid sequence was then superposed and aligned with YASARA (version 17.8.15) to get also the ligands in the binding site aligned and superposed, thus the eight molecules were imported on Forge (Fig. 2 and 3).

The XED (eXtended Electron Distribution) force field was used to generate the field point. The compounds in the training set were aligned to the reference compound by maximum common substructure using a customized set-up for the conformation hunt:

- Max number of conformations: 500.
- RMS cut-off for duplicate conformers: 0.5 Å.
- Gradient cut-off for conformer minimization: 0.1 kcal/mol.
- Energy window: 2.5 kcal/mol.

The RMS cut-off for duplicate conformers parameter controls the similarity threshold below which two conformers are assumed identical. Conformations that gave a minimized energy outside the energy window were discarded.

All the alignments were manually checked to ensure the best possible model. All the field points of the training set were used to derive a gauge invariant set of sampling points, which reduced the number of descriptors that needed to be taken into account, with a distance of 1 Å between the sample points.
Sample values were calculated, ensuring that all areas around the molecule (and possibly contributing to the activity) are properly described.

**Statistical analysis**

For the validation of the QSAR model, the leave-one-out method was used. 20 was the maximum number of components to extract from the PLS regression. 50 was the number of Y scrambles to use. The threshold of the sample point minimum distance was set to 1 Å. The Leave-one-out method was used during the validation of the QSAR model. The regression method used in Forge was PLS (SIMPLS algorithm) [39-43]. All the parameters for the QSAR model are resumed in Figures 4–6.

The predictive ability of the generated QSAR model was confirmed by several statistical tests. The cross-validation regression coefficient ($q^2$) was calculated based on the PRESS (Prediction error sum of squares) and SSY (Sum of squares of deviation of the experimental values from their mean):

$$q^2 = 1 - \frac{\text{PRESS}}{\text{SSY}} = 1 - \frac{\sum_{i=1}^{n}(Y_{\text{exp}} - Y_{\text{pred}})^2}{\sum_{i=1}^{n}(Y_{\text{exp}} - Y_{\text{mean}})^2}$$

$Y_{\text{exp}}$ = experimental activity of training set compound  
$Y_{\text{pred}}$ = predicted activity of training set compound  
$Y_{\text{mean}}$ = mean values of the activity of training set compound

The derived ligand-based approach results to be more reliable ($r^2 = 0.92$, $q^2 = 0.64$) than the structure-based alignment ($r^2 = 0.90$, $q^2 = 0.38$). The ligand-based 3D-QSAR align model was further validated with a set of external compounds (i.e. test set). Out of 120 molecules, we randomly choose 96 molecules (covering the whole range of activities of the compounds) as a training set to build the model, while the remaining 24 compounds served as a test set to evaluate the model. The statistical reliability of this model was also validated by the determination of the $r^2_{\text{test}}$, using the following equation:

$$r^2_{\text{test}} = 1 - \frac{\sum_{i=1}^{n}(Y_{\text{pred test}} - Y_{\text{test}})^2}{\sum_{i=1}^{n}(Y_{\text{test}} - Y_{\text{mean}})^2}$$

$Y_{\text{pred test}}$ = predicted activity of test set compound by QSAR equation  
$Y_{\text{test}}$ = experimental activity of test set compound  
$Y_{\text{mean}}$ = mean values of the activity of training set compound

The 11-components model (Fig. 7) shows both good predictive and descriptive capability as it is shown by the good $r^2$ (0.99) and $q^2$ (0.69) [44] values for the training and the cross-validated training sets. The plot of experimental vs. predicted activity for the compounds, in both the training set and the cross-validated training set ($q^2 = 0.69$), shows a reasonable distribution of the values. The plot of experimental vs. predicted activity for the compounds in the test set is still reasonably good with only few outliers and a good cross-validated $r^2$ of 0.73.
Isosteric replacement

The isosteric replacement was performed using Spark as a software (10.4.0, Cresset, Litlington, Cambridgeshire, UK, http://www.cresset-group.com/forge) [30-34]. As reported in Fig. 8, different portions of the BMS309403 were replaced. Then, the newly designed molecules were aligned with the 3D-QSAR model and evaluated. The replacement was performed through the same 178,558 fragments for each part, which derive from ChEMBL and Zinc databases (Fig. 9) [45, 46]. Five hundred compounds were generated for each substitution producing 3,000 hits (reported in Tables 4–9). There of the suggested molecules were synthesized and tested as reported in the related research article [1].

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Preferred alignment protocols

**Structure-based Autodock Vina Docking**
- AutoDock Vina 1.1.2
- Retain 8 poses per ligand
- Manually select preferred poses
- Tweak and refine inconsistent poses

**Ligand-based Forge**
- Substructure alignment, protein present, no constraints
- Use most accurate conformation hunt
- Tweak and refine inconsistent groups
- Use 8 different references to align ligands

**Fig. 1.** Comparison of alignment methods.

**Fig. 2.** Schematic representation of the process adopted to obtain the template compounds for the ligand-based alignment.

**Table 1**

PDB codes and molecules used as reference compounds for ligand-based alignment.

| PDB code | 2D structure | PDB code | 2D structure |
|----------|--------------|----------|--------------|
| 2NNQ     | ![2NNQ 2D structure](image) | 4NNT     | ![4NNT 2D structure](image) |
Fig. 3. A) Protein and inhibitors aligned. B) Aligned inhibitors imported to Forge for ligand-based alignment.

Fig. 4. Forge’s parameters used for conformation hunt.
**Fig. 5.** Forge’s parameters used for alignment.

**Fig. 6.** Forge’s parameters used to build the QSAR model.
Fig. 7. Model statistics for FABP4 model.

| Comp | $R^2$ | $Q^2$ | Test $R^2$ | RMSE | RMSEP | Tau  | Tau-pred |
|------|-------|-------|------------|-------|-------|------|----------|
| 0    | -0.044| -0.023| -0.001     | 1.093 | 1.096 | 0.494| -0.510   |
| 1    | 0.620 | 0.598 | 0.841      | 0.866 | 0.767 | 0.587| 0.492    |
| 2    | 0.781 | 0.541 | 0.625      | 0.501 | 0.740 | 0.675| 0.514    |
| 3    | 0.697 | 0.595 | 0.718      | 0.347 | 0.711 | 0.707| 0.573    |
| 4    | 0.948 | 0.618 | 0.745      | 0.244 | 0.681 | 0.855| 0.568    |
| 5    | 0.988 | 0.636 | 0.743      | 0.192 | 0.663 | 0.855| 0.598    |
| 6    | 0.983 | 0.635 | 0.772      | 0.142 | 0.651 | 0.920| 0.594    |
| 7    | 0.900 | 0.711 | 0.746      | 0.110 | 0.631 | 0.929| 0.621    |
| 8    | 0.993 | 0.673 | 0.757      | 0.088 | 0.629 | 0.947| 0.621    |
| 9    | 0.896 | 0.683 | 0.744      | 0.068 | 0.619 | 0.958| 0.633    |
| 10   | 0.997 | 0.687 | 0.733      | 0.059 | 0.616 | 0.957| 0.626    |
| 11   | 0.998 | 0.680 | 0.731      | 0.044 | 0.615 | 0.969| 0.626    |
| 12   | 0.999 | 0.683 | 0.729      | 0.037 | 0.619 | 0.969| 0.618    |
| 13   | 0.999 | 0.880 | 0.726      | 0.030 | 0.622 | 0.976| 0.618    |
| 14   | 1.000 | 0.679 | 0.731      | 0.015 | 0.623 | 0.982| 0.613    |
| 15   | 1.000 | 0.670 | 0.728      | 0.015 | 0.624 | 0.980| 0.616    |
| 16   | 1.000 | 0.678 | 0.728      | 0.011 | 0.625 | 0.988| 0.615    |
| 17   | 1.000 | 0.677 | 0.730      | 0.008 | 0.625 | 0.991| 0.615    |
| 18   | 1.000 | 0.770 | 0.728      | 0.006 | 0.625 | 0.993| 0.616    |
| 19   | 1.000 | 0.777 | 0.728      | 0.005 | 0.625 | 0.995| 0.616    |

Preferred number of components: 11

Fig. 8. The studied position for the bioisosteric replacement of BMS309403 are highlighted in bold.
### Table 2

SMILES, experimental and predicted pIC$_{50}$ values of the molecules in the training set.

| N° | SMILES                                                                 | Exp. | Pred. |
|----|------------------------------------------------------------------------|------|-------|
| 1  | FC(F)(F)[C@H]1CCc2c(C1)c(c(n2)C3CCCCC3)C=4[N-]N=NN4)-c5ccnc(c5)C       | 8.0  | 8.0   |
| 2  | CC1(CCCCC1)c2c(c(n3)[n2]CCCCC3)-c4ccnc(c4)C=C5[N-]N=NN5                | 8.0  | 8.0   |
| 3  | Clc1c(F)c2cc(c(c(N(CC))C)n2)C=3[N-]N=NN3)-c4ccccc5)C1                 | 7.9  | 7.9   |
| 4  | Clc1c(F)c2cc(c(c(n2)C(CCC)C)C=3[N-]N=NN3)-c4ccccc4)c1                 | 7.8  | 7.8   |
| 5  | OCCI1(CCCCC1)c2c(c(c3)[n2]CCCCC3)-c4ccnc(c4)C=C5[N-]N=NN5              | 7.7  | 7.7   |
| 6  | CCCCC[C@H]1CCc2c(C1)c(c(c2)C3(CCCC3)CC0C)=4[N-]N=NN4)-c5ccccc5        | 7.7  | 7.7   |
| 7  | FC(F)c1ccccc2(c(c(c(N3CCCCC3)n2)C=4[N-]N=NN4)-c5ccccc5)c1             | 7.5  | 7.5   |
| 8  | Clc1ccc2c(c(c(n2)C3CC3)C(O-)=O)-c4cccc4)c1                            | 7.4  | 7.4   |
| 9  | Clc1ccc2c(c(c(c(N(CC))C)n2)C=3[N-]N=NN3)-c4ccccc4)c1                 | 7.3  | 7.4   |
| 10 | Clc1cc(C)c(c(nc(NC)=O)NC2)(CCCCC2)C(O-)=O)=(c1-c3cccc3)              | 7.3  | 7.3   |
| 11 | Clc1c(F)c2c(c(c(NC)=O)NC2)(CCCCC2)C(O-)=O)=(c1-c3cccc3)              | 7.0  | 7.0   |
| 12 | O=c(N)c1cccc1Cn2c3c(ccc3c4CCCCCCc42)C(O-)=O                            | 7.0  | 7.0   |
| 13 | n1c2c(CCCCCC3)c(c(c1C3CCCCC3)C=4[N-]N=NN4)-c5ccccc5                  | 7.0  | 6.9   |
| 14 | Clc1ccc2c(c(NC)=O)NC2)(CCCCC2)C(O-)=O)=(c1-c3cccc(F)c3                | 6.9  | 6.9   |
| 15 | FC(F)c1ccccc1Cn2c3c(ccc3c4CCCCC42)C(O-)=O                              | 6.4  | 6.5   |
| 16 | Fc1ccc(-c2c(c(c(n2)-C3cccc3-c4cccc(c(OC(O-O)=O)C4)CC)-c5ccccc5)cc1  | 6.5  | 6.5   |
| 17 | [O-]C]=O)c1cccc2c3CCCCC3n(c12)Cc4cccc4                                 | 6.2  | 6.3   |
| 18 | Fc1cccc1Cn2c3c(ccc3c4CCCCC42)C(O-)=O                                 | 6.4  | 6.3   |
| 19 | Fc1ccc3(Gn2c3c(cccc3c4CCCCC42)C(O-)=O)c1                              | 6.4  | 6.3   |
| SMILES                                                                 | Exp. | Pred. |
|----------------------------------------------------------------------|------|-------|
| FC(F)(F)c1ccc2c(c(c(c(N(CC)CC)n2)C=3[N\-N=NN3]-c4cccc4)c1            | 7.6  | 7.8   |
| Clc1cc(-c2cc(nn2-c3cccc3)-c4cccc40CCCCCCC9([O\-])=O)c1               | 4.5  | 4.5   |
| FC(F)(F)c1cc(O)nc(NCc2ccncc2)n1                                     | 4.4  | 4.4   |
| Clc1ccc(-c2cc(nn2-c3cccc3)-c4cccc40CCCCCCC9([O\-])=O)c1               | 4.1  | 4.2   |
| O=C(N)c1cccc(Cn2c3c(cccc3c4CCCCCc42)C([O\-])=O)c1                    | 7.2  | 7.2   |
| [O\-]C(=O)c1ccc2c(n(S=O)(=O)c3c(C(C)C)cc(C(C)C)cc3C(C)C)n2)c1       | 6.8  | 6.5   |
| FC(F)(F)c1cc(O)nc(n1)NCc2ccc(-c3cccc3)c2                             | 4.0  | 4.0   |
| Clc1ccc(-c2cc(nn2-c3cccc3)-c4cccc40CCCCC9([O\-])=O)c1                | 4.0  | 4.0   |
| FC(F)(F)c1cc(O)nc(n1)CCc2cccc2                                     | 4.0  | 4.0   |
| Clc1ccc(-c2cc(nn2-c3cccc3)-c4cccc40CCCCC9([O\-])=O)c1                | 2.0  | 2.0   |

Table 3

SMILES, experimental, and predicted pIC\(_{50}\) values of the molecules in the test set.
| N° | SMILES                                                                 | Pred pIC50 |
|----|------------------------------------------------------------------------|------------|
| 1  | [O-]C(=O)COc1ccc(-c2cccc2-n3c(c(n3)-c4c(c(c(s4)c(C)c-c5cccc5)CC)c1)       | 6.1        |
| 2  | [O-]C(=O)COc1cccc(-c2cccc2-n3c(c(n3)C4CCCCCC4-c5cccc5)CC)c1)             | 6.0        |
| 3  | [O-]C(=O)COc1ccc(-c2cccc2-n3c(c(n3)-c4cn(c(c4)c(C)c-c5cccc5)CC)c1)       | 6.0        |
| 4  | Clc1cc(O)c1c1-c2c(cl(n2)-c3cccc3-c4cccc(OCC([O-])=O)c4)C-c5cccc5         | 6.0        |
| 5  | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)cc5)-6cccc6)CC)c1           | 5.9        |
| 6  | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)cc5)-6cccc6)CC)c1           | 5.9        |
| 7  | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)cc5)-6cccc6)CC)c1           | 5.9        |
| 8  | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)cc5)-6cccc6)CC)c1           | 5.9        |
| 9  | Clc1cc(=c2c(n(n2)-c3cccc3-c4cccc(0CC([O-])=O)c4)C-c5cccc5)cc10          | 5.9        |
| 10 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)CC)C-c5cccc5)CC)c1          | 5.9        |
| 11 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(nH)c5s4)-6cccc6)CC)c1          | 5.9        |
| 12 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)CC)C-c5cccc5)CC)c1          | 5.9        |
| 13 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)CC)C-c5cccc5)CC)c1          | 5.9        |
| 14 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)NC)-5cccc5)CC)c1           | 5.8        |
| 15 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(s4)NC)-5cccc5)CC)c1           | 5.8        |
| 16 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(nH)NC)-5cccc5)CC)c1           | 5.8        |
| 17 | Oc1cc(c1c1=c2c(c(n2)-c3cccc3-c4cccc(0CC([O-])=O)c4)C-c5cccc5)CC)Cc1     | 5.8        |
| 18 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(nH)NC)-5cccc5)CC)c1           | 5.8        |
| 19 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(nH)NC)-5cccc5)CC)c1           | 5.8        |
| 20 | [O-]C(=O)COc1cc(-c2cccc2-n3c(c(n3)-c4cc5c(nH)NC)-5cccc5)CC)c1           | 5.8        |

Table 4

SMILE and predicted pIC50 values for Series 1 derivatives.
| 241 | Oc1cc(-c2c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 242 | Oc1c(O)ccc(-c2c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 243 | [O-]c(=O)OCo1cccc(-c2ccccc2-n3c(c(n3)-c4cc(0c4)C)\-c5cccc5)CC)c1 | 5.4 |
| 244 | C1c1cc1c(O)c1\-c2c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 245 | Fc1ccc1cc1c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 246 | [O-]c(=O)OCo1cccc(-c2ccccc2-n3c(c(n3)-c4cc(0c4)C)\-c5cccc5)CC)c1 | 5.4 |
| 247 | Sc1cccc(-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 248 | Oc1cc(c(O)c1\-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 249 | Fc1ccnc1cc1c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 250 | Oc1cc(c1cc1c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 251 | Fc1ccc(-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 252 | [O-]c(=O)OCo1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 253 | Sc1cc(-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 254 | [O-]c(=O)OCo1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 255 | Sc1cccc(-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 256 | [O-]c(=O)OCo1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 257 | Sc1cc(cc1c\-c2c(c(n(n2)-c3cccc3-c4cccc(OCC[O-]=O)c4)CC)\-c5cccc5ccc1C | 5.4 |
| 258 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 259 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 260 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 261 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 262 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 263 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 264 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 265 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 266 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 267 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 268 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 269 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 270 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 271 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 272 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 273 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 274 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 275 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 276 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 277 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 278 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 279 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 280 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 281 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 282 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 283 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| 284 | FC1cc1cccc(-c2ccccc2-n3c(c(n3)-c4cccc4c4CC)c1 | 5.4 |
| Line | Reaction |
|------|----------|
| 373  | ONc1ccc(c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)c1 | 5.2 |
| 374  | Fe1ccc(F)c1-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 375  | Clc1cc(F)c1-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)c1 | 5.2 |
| 376  | Clc1cc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)c1C | 5.2 |
| 377  | Clc1cc(c(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)c1)C | 5.2 |
| 378  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(CO5)c4)-c6ccccc6)CC)c1 | 5.2 |
| 379  | Fc(F)F1ecc(s1)-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 380  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)C=C(C4)CC)-c5cccc5)CC)c1 | 5.2 |
| 381  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce4(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 382  | OCC1ccccc(-c2ccccc2-n3c(c(n3)-c4cccccc(OCC([O-])=O)c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 383  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce4(C(C)(C)c4)-c5cccc5)CC)c1 | 5.2 |
| 384  | Fe1cc(c(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1OCC | 5.2 |
| 385  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)[C@H]([O]c4)C(=O)c5)CC)-c5cccc5)CC)c1 | 5.2 |
| 386  | Fe1cc(O)c1ccc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 387  | Fe1cc(O)c1ccc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 388  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(CC)c4)-c5cccc5)CC)c1 | 5.2 |
| 389  | Fe1cc(N)c1cc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 390  | Ooc1ccccc(OCC([O-])=O)c1-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 391  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)C=C(C4)CC)-c5cccc5)CC)c1 | 5.2 |
| 392  | Clc1cc(c(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 393  | Fe1cc(O)c1ccc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 394  | Clc1cc(c(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1C | 5.2 |
| 395  | Fe1cc(N)c1cc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 396  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 397  | Clc1cc(c(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1C | 5.2 |
| 398  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 399  | Fe1cc(O)c1cc(ccc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1C | 5.2 |
| 400  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 401  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 402  | Fe1cc(F)c1ccc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.2 |
| 403  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(c4)CC)-c5cccc5)CC)c1 | 5.2 |
| 404  | FCCcc1cc(c(n(n1)-c2ccccc2-c3cccccc(OCC([O-])=O)c3)CC)-c4cccce4 | 5.1 |
| 405  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccccc4(c4)C(=O)c5)CC)-c5cccc5)CC)c1 | 5.1 |
| 406  | Clc1cc(c1ccccc1-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.1 |
| 407  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccccc4(CN)=C(c5)CC)-c5cccc5)CC)c1 | 5.1 |
| 408  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccccc4(c4)CC)-c5cccc5)CC)c1 | 5.1 |
| 409  | Fe1cc(F)c1cc(-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1O | 5.1 |
| 410  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccccc4(c4)CC)-c5cccc5)CC)c1 | 5.1 |
| 411  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)C=C(C4)CC)-c5cccc5)CC)c1 | 5.1 |
| 412  | Fe1cc(F)c1cc(cc1-c2c(n(n2)-c3cccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5 | 5.1 |
| 413  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)C=C(C4)CC)-c5cccc5)CC)c1 | 5.1 |
| 414  | Fe1cc(O)c1cccc(-c2c(n(n2)-c3ccccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)cc1 | 5.1 |
| 415  | [O-]C(O)c1ccccc(-c2ccccc2-n3c(c(n3)-c4ccce5(CO5)c4)-c5cccc5)CC)c1 | 5.1 |
| 416  | Oc1ccccc(-c2c(n(n2)-c3ccccc3-c4ccccc(OCC([O-])=O)c4)CC)-c5cccc5)c1C | 5.1 |
| SMILE | pIC<sub>50</sub> | Predicted pIC<sub>50</sub> |
|-------|----------------|-----------------------------|
| [O-][n+1]c1ccc1-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)c5cccc5 | 4.9 | 4.9 |
| [O-]C(=O)Oc1ccccc(2c2cccc2-n3c(c(3)c4=C(OCC4)C)-c5cccc5)CC)c1 | 4.9 | 4.9 |
| [O-]C(=O)Oc1ccccc(2c2cccc2-n3c(c(N4CSCC4)n3)-c5cccc5)CC)c1 | 4.9 | 4.9 |
| [O-]C(=O)Oc1ccccc(2c2cccc2-n3c(c(C)(C)-c4cccc4)CC)c1 | 4.9 | 4.9 |
| Oc1c(OC)cc(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)cc1N | 4.9 | 4.9 |
| Fe1c(F)(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)cc1OC | 4.9 | 4.9 |
| Clc1cccn1-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5 | 4.9 | 4.9 |
| Fe1cc(c(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)c1)C | 4.9 | 4.9 |
| Fe1cc(c(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)c1)C | 4.9 | 4.9 |
| Fe1cc(O)c(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)cc1C | 4.9 | 4.9 |
| Clc1ccc(c1-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)c1N | 4.9 | 4.9 |
| Oc1ccc(c1-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)CC)c1 | 4.9 | 4.9 |
| Oc1ccccc(-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)cc1C | 4.9 | 4.9 |
| Clc1ccc(c1-c2cc(n(2)-c3cccc3-c4cccc(OCC([O-]=O)c4)CC)-c5cccc5)CC)c1 | 4.9 | 4.9 |

Table 5

SMILE and predicted pIC<sub>50</sub> values for Series 2 derivatives.
| N° | SMILES                                                                 | PredPIC50 |
|----|------------------------------------------------------------------------|-----------|
| 1  | Oc1c(OC)ccc1cc-c2c(nn(c2CC))-c3cccccc3-c4ccccc(OC(O)(=O))=c4)-c5cccccc5 | 6.0       |
| 2  | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5c(nH)=c5CCc1        | 5.9       |
| 3  | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5c(nH)=c5CCc1        | 5.9       |
| 4  | Oc1c(N)ccc(-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.9       |
| 5  | Oc1c(nn(c1)[n+1])-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5 | 5.9       |
| 6  | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5c(nC)=c5(C)(C)C)c1  | 5.8       |
| 7  | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(-c4cccccc(NCC)=c4)(c(n3)=c5cccccc5)CC)c1 | 5.8       |
| 8  | Fe1cccccc(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5   | 5.8       |
| 9  | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(-c4cccccc5(c4)(c(nH)=c5CC)c1          | 5.8       |
| 10 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5cccccc(NC)=c5CCc1     | 5.8       |
| 11 | C1c1c(N)ccc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.8       |
| 12 | Oc1c(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5       | 5.8       |
| 13 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5cccccc5(NC)=c5CCc1  | 5.8       |
| 14 | Sc1c(N)ccc(-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.8       |
| 15 | Oc1c(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5      | 5.8       |
| 16 | Oc1ccc(-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5         | 5.8       |
| 17 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(-c4cccccc5(c4)(c(nH)=c5CC)c1          | 5.7       |
| 18 | FC(F)c1cccc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5   | 5.7       |
| 19 | Oc1ccccc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5        | 5.7       |
| 20 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5cccccc5(NN)=c5CCc1  | 5.7       |
| 21 | Br1cc(-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5         | 5.7       |
| 22 | Br1ccc([nH]=1)-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5  | 5.7       |
| 23 | Oc1c(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5       | 5.7       |
| 24 | Clc1ccccc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.7       |
| 25 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)-c5cccccc5(CS)=c5CCc1 | 5.7       |
| 26 | Clc1cccc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5         | 5.7       |
| 27 | Fc1cc(-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5        | 5.7       |
| 28 | Oc1ccnncc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.7       |
| 29 | Oc1ccnncc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5     | 5.7       |
| 30 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(-c4cccccc5CCNc54)(c(n3)=c6cccccc6)=c5CCc1 | 5.7       |
| 31 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc4)(c5cc(N)=c5CC)=c5CCc1 | 5.7       |
| 32 | Fc1cc(nn(c2CC)=c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5           | 5.7       |
| 33 | Oc1cc(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5 | 5.7       |
| 34 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 35 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 36 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 37 | [O=C]([=O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 38 | Clc1ccnncc1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5 | 5.7       |
| 39 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 40 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 41 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(n3)=c4cccccc5c4nn(nH)=c5cc(cc)=c6cccccc6)=c5CCc1 | 5.7       |
| 42 | [O=C]([O])OC1cccccc-c2cccccc2-n3c(c(-c4cccccc(N)=c4CC)(c(n3)=c5cccccc5)=c5CCc1 | 5.7       |
| 43 | Oc1cc(O)c1-c2c(nn(c2CC))-c3cccccc3-c4cccccc(OC(O)(=O))=c4)-c5cccccc5 | 5.7       |
| Number | Chemical Structure | Description |
|--------|-------------------|-------------|
| 132    | Clc1cccc1-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5cccc5)c1 | 5.5 |
| 133    | [O-]C(OCC1cccc1(-c2cccc2-13nc(c(c3)-c4cccc4)-c5cccc5N(C)CC)c1 | 5.5 |
| 134    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 135    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5c(S)c5CC)c1 | 5.5 |
| 136    | Oc1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5cccc5CCC)c1 | 5.5 |
| 137    | [O-]C(OCC1cccc1(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 138    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 139    | Oc1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccc4-c5ccccc5CC)c1 | 5.5 |
| 140    | [O-]C(OCC1cccc1(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 141    | Fc1c1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5ccccc5C | 5.5 |
| 142    | [O-]C(OCC1cccc1(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 143    | Oc1cc1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccc4-c5ccccc5CC)c1 | 5.5 |
| 144    | Fc1cc1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5ccccc5C | 5.5 |
| 145    | Fc1ccccc1-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5ccccc5C | 5.5 |
| 146    | [O-]C(OCC1cccc1(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 147    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 148    | FCC1ccccc1-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5ccccc5C | 5.5 |
| 149    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 150    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 151    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 152    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 153    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 154    | Fc1ccccc1-c2(nc(n(c2CC)-c3cccc3-c4cccc(OCC((O--)=O)c4)-c5ccccc5C | 5.5 |
| 155    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 156    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 157    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 158    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 159    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 160    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 161    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 162    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 163    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 164    | C1ccc1cc1(-c2(nc(n(c2CC)-c3cccc3-c4cccccc0(OCC((O--)=O)c4)-c5ccccc5)C | 5.5 |
| 165    | OC1c1ccc1(-c2(nc(n(c2CC)-c3cccc3-c4cccccc0(OCC((O--)=O)c4)-c5ccccc5)C | 5.5 |
| 166    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 167    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 168    | Clc1ccccc(-c2(nc(n(c2CC)-c3cccc3-c4ccccccCC(0CC((O--)=O)c4)-c5ccccc5CC | 5.5 |
| 169    | Fc1ccccc1(-c2(nc(n(c2CC)-c3cccc3-c4ccccccCC(0CC((O--)=O)c4)-c5ccccc5CC | 5.5 |
| 170    | Oc1ccccc1(-c2(nc(n(c2CC)-c3cccc3-c4ccccccCC(0CC((O--)=O)c4)-c5ccccc5CC | 5.5 |
| 171    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 172    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 173    | Fc1ccccc1(-c2(nc(n(c2CC)-c3cccc3-c4ccccccCC(0CC((O--)=O)c4)-c5ccccc5CC | 5.5 |
| 174    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
| 175    | [O-]C(OCC1ccccc(-c2cccc2-13nc(c(c3)-c4cccc4)-c5ccccc5CC)c1 | 5.5 |
532  Fc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OC(O-))=O)c4)-c5cccc5)c1N  5.3
533  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)C)OC)c1  5.3
534  Cc1c(cc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cC(cc5)cc1C  5.3
535  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc6s5)C)CC)c1  5.3
536  OCc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
537  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
538  Fc(F)(F)F1ccsc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
539  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
540  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
541  O[@@H][c1ccc(s1)-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4]-c5cccc5)c1  5.3
542  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)C)CC)c1  5.3
543  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
544  Fc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1NN  5.3
545  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)C)CC)c1  5.3
546  Fc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1N  5.3
547  FC(F)(F)F1ccsc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
548  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)C)CC)c1  5.3
549  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
550  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc4)-c5cC(cc5)CC)c1  5.3
551  Cc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
552  Sc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
553  Sc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
554  Sc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
555  Br1c[nH](c(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
556  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
557  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
558  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
559  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
560  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
561  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
562  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
563  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
564  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
565  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
566  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
567  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
568  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
569  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
570  [O-](c=O)OC1cccc(-c2cccc2-n3c(c(c3)-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.2
571  Cc1ccccc(-c2(nn(c2CC)-c3cccc3-c4cccc5cC(OCC(O-))=O)c4)-c5cccc5)c1  5.3
572  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
573  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
574  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
575  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
576  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
577  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
578  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
579  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
580  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
581  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
582  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
583  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
584  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
585  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
586  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
587  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
588  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
589  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
590  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
591  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
592  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
593  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
594  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
595  [O-](c=O)OC(c)=O)-c5cC(cc5)C)CC)c1  5.3
| N°  | SMILES                                                                 | Pred pIC5  |
|-----|------------------------------------------------------------------------|------------|
| 1   | [O-][O]+=O)c1ccccc(-c2ccccc2-n3c(c(nc(c34)c4c5cccc5)c5cccc5)c1           | 6.5        |
| 2   | [O-][O]+=O)c1ccccc(-c2ccccc2-n3c(c(nc(c34)c4c5cccc5)c5cccc5)c1           | 6.3        |
| 3   | Clc1nc(nc1-c2cccccc2-e3ccccc(OCC(O-)=O)c3-e4cccccc4-e5cccccc5)          | 6.3        |
| 4   | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c(nc(c34)c4c5cccccc5)c5cccccc5)c1       | 6.3        |
| 5   | Fc1nc(nc1-c2cccccc2-e3ccccc(OCC(O-)=O)c3-e4cccccc4-e5cccccc5)           | 6.2        |
| 6   | [O-][O]+=O)c1ccccc(-c2cccccc2/C=N/Oc3cccccc3)c4cccccc4c5cccccc5)        | 6.1        |
| 7   | Occo1c1(c(nc1-c2cccccc2-e3cccccc(OCC(O-)=O)c3-e4cccccc4-e5cccccc5)      | 6.0        |
| 8   | [O-][O]+=O)c1ccccc(-c2ccccc2-n3c4c(c(n34)c5cccccc5)(n34)=6cccccc6)c1     | 6.0        |
| 9   | [O-][O]+=O)c1ccccc(-c2ccccc2OC[C@H](Nc3cccccc3)bco4cccccc4)            | 6.0        |
| 10  | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c([H3]-c4cccccc4)-c5cccccc5)c1         | 6.0        |
| 11  | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c([H3]-c4cccccc4)-c5cccccc5)c1         | 6.0        |
| 12  | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c([H3]-c4cccccc4)-c5cccccc5)c1         | 6.0        |
| 13  | [O-][O]+=O)c1ccccc(-c2ccccc2-n3c(c(c34)c4c5cccccc5)3c5cccccc5)c1        | 6.0        |
| 14  | O=c[O][C@H](Nc3cccccc3)c2cccccc2c3cccccc3-e4cccccc(OCC(O-)=O)c4         | 5.9        |
| 15  | Clc1nc(OCC(O-)=O)c1ccccc2-c3ccccc(OCC(O-)=O)c3-e4cccccc4-e5cccccc5      | 5.9        |
| 16  | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c([H3]-c4cccccc4)-c5cccccc5)(OCC(O-)=O)c5 | 5.9        |
| 17  | [O-][O]+=O)c1ccccc(-c2ccccc2-n3c4c(c(c(o4)-c5cccccc5)-6cccccc6)c(n3)c1   | 5.9        |
| 18  | [O-][O]+=O)c1ccccc(-c2ccccc2-c3c(c(n34)c4c5cccccc4)-c5cccccc5)c1        | 5.9        |
| Line | Chemical Structure                                                                 | Coordinate | Score |
|------|-----------------------------------------------------------------------------------|------------|-------|
| 283  | O=C(O)c1ccccc(-c2ccc=cc2-n3c(OC)c(c(n3)-c4ccc=cc4)-c5cccc5)c1                       | 5.3        |       |
| 284  | O=C(OC)c1ccc(2ccccc3-c4cccc4(OC)(O)=O)c4                                            | 5.3        |       |
| 285  | FeCl(c(c(F)(c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4)c5cccc5)                      | 5.2        |       |
| 286  | O=N(c1cccc1)C(C(=O)c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4                           | 5.2        |       |
| 287  | 5.2 | O=C(O)c1ccc(-c2ccc=cc2-n3c(OC)c(c(n3)-c4ccc=cc4)-c5cccc5)c1                       | 5.3        |       |
| 288  | O=C(OC)c1ccc(2ccccc3-c4cccc4(OC)(O)=O)c4                                            | 5.3        |       |
| 289  | FeCl(c(c(F)(c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4)c5cccc5)                      | 5.2        |       |
| 290  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 291  | O=C(O)c1ccc(2ccccc3-c4cccc4(OC)(O)=O)c4                                            | 5.3        |       |
| 292  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 293  | FeCl(c(c(F)(c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4)c5cccc5)                      | 5.2        |       |
| 294  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 295  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 296  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 297  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 298  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 299  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 300  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 301  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 302  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 303  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 304  | O=C(O)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 305  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 306  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 307  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 308  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 309  | C=3[Nc1c(1-c2ccc=CC-c3ccc(OCC(O))=O)=c3)c4ccccc4(OC(O))=O)c5                        | 5.2        |       |
| 310  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 311  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 312  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 313  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 314  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 315  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 316  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 317  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 318  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 319  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 320  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 321  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 322  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 323  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 324  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 325  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| 326  | O=C(OC)c1ccc(-c2ccc=CC-c3ccc(OCC(O))=O)c4                                            | 5.3        |       |
| Line | Chemical Structure | Time   |
|------|-------------------|--------|
| 327  | OC[O](H)[C@@H](C(=NN1c2cccccc2-c3cccc(c(OCC([O-])=O)c3)c4cccccc4)c5cccccc5) | 5.2    |
| 328  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3N)-c4cccccc4)-c5cccccc5)c1 | 5.2    |
| 329  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3N)-c4cccccc4)-c5cccccc5)c1 | 5.2    |
| 330  | O=C1N(C(=O)cc2ccc2=C(C1H)[C@@H](N([N3J]c4cccccc4)c5cccccc5)c1 | 5.2    |
| 331  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3N)-c4cccccc4)-c5cccccc5)c1 | 5.2    |
| 332  | O=C1(n1-c2cccccc2-c3cccccc3)-c4cccccc4-c5cccccc5(OCC([O-])=O)c5C | 5.2    |
| 333  | [O-C](=O)C0c1cccc(-c2cccccc2-c3cc(c(n3)-c4cccccc4)-c5cccccc5)[C@@H]c1 | 5.2    |
| 334  | [O-C](=O)C0c1cccc(-c2cccccc2/N=C/[C@@H](Cc3cccccc3)c4cccccc4)c1 | 5.2    |
| 335  | [O-C](=O)C0c1cccc(-c2cccccc2/C=C([C@@H](N([N3J]c4cccccc4)c5cccccc5)c1 | 5.1    |
| 336  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(s3)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 337  | [O-C](=O)C0c1cccc(-c2cccccc2/C[H]3/C[H](OC)(C)[C@@H]([C@H])(O3)c4cccccc4)c5cccccc5)c1 | 5.1    |
| 338  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3C)(C)c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 339  | [O-C](=O)C0c1cccc(-c2cccccc2C3=NN([C@@H])(O3)c4cccccc4)c5cccccc5)c1 | 5.1    |
| 340  | [O-][N+]=[O]c1(c(c(n1-c2cccccc2-c3cccccc(OCC([O-])=O)c3)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 341  | FC1cl(-c2cccccc2-c3cccccc(OCC([O-])=O)c3)cc(c1-c4cccccc4)-c5cccccc5 | 5.1    |
| 342  | [O-C](=O)C0c1cccc(-c2cccccc22C[O@@H](Cc3cccccc3)c4cccccc4) | 5.1    |
| 343  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3COC)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 344  | [O-C](=O)C0c1cccc(-c2cccccc2/C=C([C@@H])(O3)c4cccccc4)c5cccccc5)c1 | 5.1    |
| 345  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3C4CCCCC4)-c5cccccc5)-c6cccccc6)c1 | 5.1    |
| 346  | FC1cl(-c2cccccc2-c3cccccc(OCC([O-])=O)c3)cc(c1-c4cccccc4)-c5cccccc5)C | 5.1    |
| 347  | Sc1cc(-c2cccccc2-c3cccccc(OCC([O-])=O)c3)cc(c1-c4cccccc4)-c5cccccc5 | 5.1    |
| 348  | [O-C](=O)C0c1cccc(-c2cccccc22N3C=C([C@@H])(Cc4cccccc4)-C3]c5cccccc5)c1 | 5.1    |
| 349  | [O-C](=O)C0c1cccc(-c2cccccc2/C=N/[C@@H](Cc3cccccc3)c4cccccc4)c1 | 5.1    |
| 350  | O1c1(nc(c(n1-c2cccccc2-c3cccccc3)-c4cccccc4-c5cccccc5)(OCC([O-])=O)c5) | 5.1    |
| 351  | [O-C](=O)C0c1cccc(-c2cccccc2-c3cc(c(c3NCC)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 352  | FC1(F)[C@@H]([O@@H][C@@H]1c2cccccc23cccccc3)c4cccccc4-c5cccccc5(OCC([O-])=O)c5 | 5.1    |
| 353  | [O-C](=O)C0c1cccc(-c2cccccc2C[C@@H](Cc3cccccc3)c4cccccc4) | 5.1    |
| 354  | O=C(N)Cc1c(nc1(c-2cccccc2-c3cccccc3)-c4cccccc4-c5cccccc5(OCC([O-])=O)c5 | 5.1    |
| 355  | O=C(N)Cc1c(nc1(c-2cccccc2-n3c(-n4cnc(c4JC))c(n1-c5cccccc5)-c6cccccc6)c1 | 5.1    |
| 356  | O1c1(c(-c2cccccc2-c3cccccc(OCC([O-])=O)c3)cc(c1-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 357  | O=C(N([C@@H])(Cc1ccccc1-c2ccccccOCC([O-])=O)c2)C(c3cccccc3)c4cccccc4 | 5.1    |
| 358  | [O-C](=O)C0c1cccc(-c2cccccc22OCC[C@@H][Oc3cccccc3)c4cccccc4)c1 | 5.1    |
| 359  | O=C1(C[C@@H](C[N1c2cccccc2-3cccccc(OCC([O-])=O)c3])c4cccccc4)c5cccccc5 | 5.1    |
| 360  | O=C1N(C=C1C[N1c2cccccc2-3cccccc3]c4cccccc4-c5cccccc5(OCC([O-])=O)c5 | 5.1    |
| 361  | O=C1(N[C@@H](CC[C@H]1c2cccccc2)c3cccccc3-c4cccccc4-c5cccccc5)c1 | 5.1    |
| 362  | O=S([O])NC1(C[C@H][C[N1c2cccccc2-3cccccc(OCC([O-])=O)c3])c4cccccc4)c5cccccc5 | 5.1    |
| 363  | [O-C](=O)C0c1cccc(-c2cccccc2-n3c(N[C])c(c(n3)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 364  | FC1cc(nc1-c2cccccc2-3cccccc(OCC([O-])=O)c3)-c4cccccc4)-c5cccccc5 | 5.1    |
| 365  | Clc1c(nc1-c2cccccc2-3cccccc(OCC([O-])=O)c3)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 366  | [O-C](=O)C0c1cccc(-c2cccccc2-[n+]3cc(c(n3C)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 367  | [O-C](=O)C0c1cccc(-c2cccccc2-c3nc(c(n3C)(C(c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 368  | FC1cc(-c2(nc(c-3cccccc3)-c4cccccc4-c5cccccc5)-c6cccccc5(OCC([O-])=O)c6)c1 | 5.1    |
| 369  | [O-C](=O)C0c1cccc(-c2cccccc2-c3cc(Cc(c(n3)-c4cccccc4)-c5cccccc5)c1 | 5.1    |
| 370  | O=C(O)C1c(nc1(c-2cccccc2)-3cccccc3)c4cccccc4-c5cccccc5(OCC([O-])=O)c5 | 5.1    |
Table 7
SMILE and predicted pIC$_{50}$ values for Series 4 derivatives.

| N° | SMILES | PredpIC$_{50}$ |
|----|---------|---------------|
| 1  | [O-][C(=O)Cc1cn(nn1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.3 |
| 2  | [O-][C(=O)Nc1cc2_cn1cccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc2 | 6.3 |
| 3  | Fc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1[[@H](O)C([O-])=O | 6.3 |
| 4  | O=C(N1CCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc21)]CC([O-])=O | 6.3 |
| 5  | O=C(OCC([O-])=O[N1CC][@H]1Cc12cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.3 |
| 6  | O=C(N1([@H])CC[[@H]](C1)Cc12cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCCC([O-])=O | 6.2 |
| 7  | O=C(c1c(cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1)]CC([O-])=O | 6.2 |
| 8  | Fc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.1 |
| 9  | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.1 |
| 10 | Oc1cc(c(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.1 |
| 11 | [O-][C(=O)Cn1cc2(c(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCcc2cn1 | 6.1 |
| 12 | O=S([@O])CC([O-])=O]c1nc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCcs1 | 6.1 |
| 13 | Oc1cc(s([@O])=O]c1cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.1 |
| 14 | O=C(Nc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc11NC([O-])=O | 6.1 |
| 15 | Clc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc10CC([O-])=O | 6.1 |
| 16 | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.0 |
| 17 | Oc1cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 18 | O=C(Nc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 19 | Clc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 20 | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.0 |
| 21 | Oc1cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 22 | O=C(SC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1 | 6.0 |
| 23 | Fc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 24 | Fc1cc(c)(cc1-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 25 | O=C1ccOc2cccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc221CC([O-])=O | 6.0 |
| 26 | [O-][C(=O)]CC([@H])1Cc12cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 6.0 |
| 27 | O=C(N1CCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc21)]CC([O-])=O | 6.0 |
| 28 | O=C(N1CCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc21)]CC([O-])=O | 6.0 |
| 29 | O=C(N1CCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc21)]CC([O-])=O | 6.0 |
| 30 | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 6.0 |
| 31 | O=C1ccCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc221CC([O-])=O | 6.0 |
| 32 | Fc1ccc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc10CC([O-])=O | 6.0 |
| 33 | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 5.9 |
| 34 | O=C(c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 35 | Clc1ccc(SC([O-])=O]c1cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CC | 5.9 |
| 36 | O=S([@O])NC([O-])=O]c1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 37 | O=C1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 38 | O=C1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 39 | Fc1ccCc2ccc(-c3cccccc3-n4c(c(n4)-c5cccccc5)-c6cccccc6)]CCc2 | 5.9 |
| 40 | O=C1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 41 | O=C1cc(c(s1)-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
| 42 | Fc1cc(-c2cccccc2-n3c(c(n3)-c4cccccc4)-c5cccccc5)]CCc1CC([O-])=O | 5.9 |
[O]C(=O)COC[=O][H][C(1)cccc1-n2c(c(n2)-c3cccc3)-c4cccc4]CC

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OCC[=O][H][C(1)cccc1-n2c(c(n2)-c3cccc3)-c4cccc4]CC

Fc1cc(-c2cccc2-n3c(c(n3)-c4cccc4)-c5cccc5)CC)c(cCC(C)(O)C)c1

Fc1cc(F)c(c1cccc1-n2c(c(n2)-c3cccc3)-c4cccc4)CC

O=C(=O)COC[=O][H][C(1)cccc1-n2c(c(n2)-c3cccc3)-c4cccc4]CC

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

O=C(=O)COC[=O][H][C(1)cccc1-n2c(c(n2)-c3cccc3)-c4cccc4]CC

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O

[O]C(=O)OC1c1(nc(c(c(n3)-c4cccc4)-c5cccc5)CC)c(CC(C)(O)C)c1

O=S(=O)(Nc1ccc(c(c(n3)-c4cccc4)-c5cccc5)CC)C[=O][=O]=O
| N  | SMILES                                                                 | PredpIC<sub>50</sub> |
|----|------------------------------------------------------------------------|----------------------|
| 1  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.7                  |
| 2  | [O-]C=OClc1cc(nn2)C(NCCc1ccccc1-n2cc(c(n2)-c3ccc3c3)-c4ccccc4)CC)c1     | 6.5                  |
| 3  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.4                  |
| 4  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.4                  |
| 5  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.3                  |
| 6  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.3                  |
| 7  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 8  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 9  | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 10 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 11 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 12 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 13 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 14 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 15 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 16 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 17 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| 18 | O=C(NC[O-])=O(COC=O)Clc1cc(-c2cccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1 | 6.2                  |
| Line | Chemical Structure | Value |
|------|--------------------|-------|
| 459  | [O-][C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 460  | O=S(O)N[C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 461  | O=S(O)N[C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 462  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 463  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 464  | Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.7   |
| 465  | O=S(O)N[C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 466  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 467  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 468  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 469  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 470  | Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.7   |
| 471  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 472  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 473  | Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.7   |
| 474  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.7   |
| 475  | Brccccc1-c1cc1c(c(n1)-c2cccc2-n3c(c(n3)-c4cccc4)-c5cccc5)CC| 4.6   |
| 476  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 477  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 478  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 479  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 480  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 481  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 482  | Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.6   |
| 483  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 484  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.6   |
| 485  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.5   |
| 486  | Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.5   |
| 487  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.5   |
| 488  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.5   |
| 489  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.5   |
| 490  | Fc1ccc(C=N][+][C@][H]([C]C)Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.5   |
| 491  | [C@][H]([C]C)Clc1ccc(-n2c(c(n2)-c3cccc3)-c4cccc4)CC| 4.5   |
| 492  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 493  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 494  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 495  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 496  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 497  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.4   |
| 498  | O=C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)[N+]C(=O)] | 4.2   |

Table 9
SMILE and predicted pIC₅₀ values for Series 6 derivatives.

| N° | SMILES                                                                 | PredpIC₅₀ |
|----|------------------------------------------------------------------------|-----------|
| 1  | [O-][C]([SC1=[N+]([C@]([C@@]2(Nc3cccccc3N12)c4cccccc4)(c5cccccc5)C)=O]   | 7.3       |
| 2  | O=C(N(C([O-])=O)C([O-])=O)[C@H][Cc1cccccc1c2cccccc2]C(=O)             | 7.2       |
| 3  | S=NC(N1c1cccccc1)c2cccccc2CCCC([O-])=O                                 | 6.6       |
| 4  | S=NC(N=C(Cc1cccccc1)C2cccccc2)CC([O-])=O                               | 6.5       |
| 5  | O=C(N[C@H][1][C@H][O][C@H][1](c2cccccc2)C=3cccccc3)[C@H][OC][O-]=O   | 6.5       |
| 6  | O=C(O[C][O-]=O)CS[C@H][1][C@H][O][C@H][1][C][C@H][C]=2cccccc2c3cccccc3 | 6.5       |
| 7  | [O-][C]=O)NCC[C@H][1]c1cccccc1CCOc2cccccc2                           | 6.4       |
| 8  | [O-][C]=O)CC[C@H][1][C@H][C][C@H](c1cccccc1)C=2cccccc2(C)             | 6.4       |
| 9  | [O-][C]=O)O[C@H][1][C@H][OC][C@H][O]1[C@H][C2cccccc2][C3cccccc3]OC    | 6.4       |
| 10 | O=C(N(C1c1cccccc1)C2cccccc2)[C@H][CC([O-])=O]                          | 6.4       |
| 11 | O=C1[C@H][1]N2C=[O-][O][C@H][1][C@H][3CCCN13]C4cccccc4)(c5cccccc5)CC([O-])=O | 6.3       |
| 12 | [O-][C]=O)C=C(C[C@H][1]c1cccccc1)C=2cccccc2                           | 6.3       |
| 13 | O=C1[C@H][1][C@H][C][C@H][C]=1c2cccccc2)c=C(=O)C(C)                  | 6.3       |
| 14 | [O-][C]=O)O[C@H][1][C@H][CC][C@H](=C)C[C@H][C]=2cccccc2(C)             | 6.2       |
| 15 | O=C1[C@H][1][C@H][C][C@H][C]=1cc1cccccc1)(C=2cccccc2)[C=2cccccc2]C(=O) | 6.2       |
| 16 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 17 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 18 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 19 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 20 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 21 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 22 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 23 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 24 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 25 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 26 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 27 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 28 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 29 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 30 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 31 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 32 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 33 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 34 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 35 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 36 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 37 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 38 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 39 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 40 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
| 41 | O=C1[C@H][1]C[O-C@H][1][C@H][C][C@H][C]=1cc1cccccc1)C=2cccccc2(C)     | 6.2       |
75
\[O=C(N[@H]|([@H]|(c1ccccc1)C)c2ccccc2)|@H]|(C)|C([O-])=O\]
6.0
76
\[O=C(OC([O-])=O)|@H]|(Cc1ccccc1)c2ccccc2\]
6.0
77
\[[O-]|C=O)|C|H]|([@H]|(Cc2ccccc2)|3c3ccc3|C)|C([O-])=O\]
6.0
78
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
6.0
79
\[O=C(OC([O-])=O)|C|H]|([@H]|(Cc2ccccc2)|3c3ccc3|C)|C([O-])=O\]
6.0
80
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
6.0
81
\[O=C(GG([O-])=O)|C|H]|([@H]|(Cc2ccccc2)|3c3ccc3|C)|C([O-])=O\]
6.0
82
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
5.8
83
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
5.8
84
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
5.8
85
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
5.8
86
\[O=C(GG([O-])=O)|@H]|(C)c2ccccc2\]
5.8
[O-]C(=O)CC([@H]1)(CCC([@H]1)c2cccccc2)c3ccccc3
176 [O-]C([O][C@H]1)(C@H)3(C@H)[(c2cccccc2)C=CO1)c3ccccc3]=O
177 [O-][C6H]1c1ccce(o1)[C@H]1[N(C2CCCCC2)3c3ccccc3]c4cccccc4
178 [O-][C6H]1c1ccce(n1)-c2cccccc2-c3ccccc3
179 [C@H]1[C@H][O[C@H][C@H]1c2cccccc2)c3ccccc3]C=O([O-])=O
180 [O-][C6H]1COC([O][C@H]1[C@H]2[C=CO1][O]](c2cccccc2)c3ccccc3]C=O([O-])=O
181 [O-][C6H]1C(C@H)1[C@H][C@H][O1]c2cccccc2)c3ccccc3
182 [O-][C6H]1COC([@H]1c1cccccc1)c2cccccc2
183 [O-][C6H]1C@H1CC([@H]1][O1])c2cccccc2)c3ccccc3
184 [O-][C6H]1C@H1C1CCN12=C([@H]2)c4ccccc4S3)c5ccccc5)c6cccccc6
185 [O-][n1Cnc2c1C@H][O1C2c3ccccc3])c4ccccc4]C([O-])=O
186 S([O][C@H]1C@H1C1c1cccccc1)c2cccccc2]CC([O-])=O
187 [O-][C6H]1COC([@H]1Sc1cccccc1)c2cccccc2
188 S=[CNC([@H]1C1c1cccccc1)c2cccccc2])C([O-])=O
189 O=C1C([@H]1C1c12C0([O][C@H]1c2CC([O-])=O)=c3ccccc3)c4cccccc4
190 Br([C@H]1)[C([@H]1][C@H]2C([O-])=O]=c3ccccc3)c4cccccc4
191 [O-][C6H]1C1nc1nc(N([@H]1c2cccccc2)c3ccccc3)n1C
192 O[C6H]1C1c1cccccc1)c2cccccc2]CC([O-])=O
193 [O-][C6H]1CC([@H]1OC([@H]1c2cccccc2)c3ccccc3]C([O-])=O
194 O=S([O])=N1CC[C@H]1c2cccccc2]C([@H]1c3ccccc3)C([O-])=O
195 O=C([O][C@H]1c1cccccc1)c2cccccc2]CC([O-])=O
196 F([C@H]1)[C@H]1NC([@H]1CC([O-])=O]=c2cccccc2)c3ccccc3
197 O[C@H]1C@H1OC([O][C@H]1c2cccccc2)c3ccccc3]C([O-])=O
198 O=C([O][C@H]1c1cccccc1]C2=N([@H]1SS2)c3ccccc3]C([O-])=O
199 O=C([O][C@H]1c1cccccc1)C([O1][C@H]1c2cccccc2)c3ccccc3]CC([O-])=O
200 O=C([O][C@H]1c1cccccc1)C((OCC([O-])=O]=c2cccccc2
201 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
202 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
203 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
204 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
205 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
206 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
207 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
208 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
209 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
210 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
211 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
212 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
213 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
214 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
215 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
216 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
217 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
218 O=C([O][C@H]1c1cccccc1)c2cccccc2]C([@H]1c3ccccc3]C44(CCC4)C([O-])=O
| Line | Chemical Structure |
|------|---------------------|
| 395  | [O-]C(=O)O[O[O[O[O]C@H]1[C@H]2OC[C@H]((O2)[C@H]((C@H)1c3cccccc3)c4cccccc4)5.1 |
| 396  | O[C@H]1[C@H][O][C@H]([O[O[O[O]C@H]1c2cccccc2)]C(=O)c3cccccc3)CC([O-])=O 5.1 |
| 397  | [O-]C(=O)1noc(n1)C[C@H]((C2cccccc2)c3cccccc3)5.1 |
| 398  | [O-]C(=O)[C@H][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.1 |
| 399  | Fe1ccc([C@H]([C@H]([C@H]c2cccccc2)c3cccccc3)Cc1Cc([O-])=O 5.1 |
| 400  | S=C1(N=N1)(O)[O[C@H]((C2cccccc2)c3cccccc3)5.1 |
| 401  | O=C([C@H]1CCCC1c2cccccc2)c3cccccc3)CC([O-])=O 5.1 |
| 402  | O=S(O)[N(c1ccccc1)Cc2ccccc2)c3cccccc3)5.1 |
| 403  | O=C(=O)[C@H][O][C@H]([C@H]1Cc2ccccc2)c3cccccc3)5.1 |
| 404  | O=C([C@H][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.1 |
| 405  | O=C1Cc(n1)s1)[C@H]((C2cccccc2)c3cccccc3)C15.0 |
| 406  | O=C([C@H][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)CC([O-])=O 5.1 |
| 407  | O=C([C@H][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)CC([O-])=O 5.1 |
| 408  | O=C([O[C@H]][C[C@H]1(C[C@H]c1cccccc1)c2cccccc2)CC([O-])=O 5.1 |
| 409  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C5.1 |
| 410  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C15.1 |
| 411  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.0 |
| 412  | O=C([C@H][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)CC([O-])=O 5.1 |
| 413  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C3cccccc3)5.0 |
| 414  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C3cccccc3)C5.0 |
| 415  | O=S([O[C@H]][C[C@H]1CCCC1c2cccccc2)C5.0 |
| 416  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.0 |
| 417  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.0 |
| 418  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C3cccccc3)C5.0 |
| 419  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C3cccccc3)C5.0 |
| 420  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C3cccccc3)C5.0 |
| 421  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C5.0 |
| 422  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.0 |
| 423  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)OC([O-])=O 5.0 |
| 424  | O=C([O[C@H]][C[N+]=C(N1)[C@H]((C2cccccc2)c3cccccc3)C5.0 |
| 425  | O=C1CC([O@H][C@H]1)[C@H]1Cc2ccccc2)c3cccccc3)C([O-])=O 5.0 |
| 426  | O=C([O[C@H]][C[C@H]1CCCC1c2cccccc2)C5.0 |
| 427  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 428  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 429  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 430  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 431  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 432  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 433  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 434  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 435  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 436  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 437  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
| 438  | O=C([O[C@H]][C[N+]=C(N1)[C@H]1c2cccccc2)CCS([O-])=O)c3cccccc3 5.0 |
85  O[C@@]1[C(N+)]CC[C@H]1c2cccccc2CC(=O-)=O)c3cccccc3  4.7
484  O=C1[C@H]([C@@]1)[C@H]1(=O)C(=O)c3cccccc3  4.6
485  [O-][C]=O)CC1CCCC1CC(=O)c3cccccc3  4.6
486  O=C1[C@H]1CCN1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.6
487  O=CC1CC1[C@H]1c2cccccc2NCCN1C)C  4.6
488  O=C1[C@H]1CC1CCCC1CC(=O-)=O)c3cccccc3  4.6
489  [O-][C]=O)CC1CC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.6
490  [O-][C]=O)[C@@]1(C[N+])([C@@]H)(Cc2cccccc2)c3cccccc3)CCN1C)C  4.6
491  [O-][C]=O)[C@@]1(C[N+])1(c2cccccc2)C(c3cccccc3)C  4.6
492  [O-][C]=O)[C@@]1(C[N+])1(Cc1cccccc1)(c2cccccc2)C(c3cccccc3)C  4.5
493  O=C1[C@H]1CC1CCCC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.5
494  O=C1CC1[C@H]1c2cccccc2NCCN1C)C  4.5
495  O=C1[C@H]1CC1CCCC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.5
496  [O-][C]=O)[C@@]1(C[N+])1(c2cccccc2)C(c3cccccc3)C  4.4
497  [O-][C]=O)[C@@]1CC1CCCC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.4
498  O=C1CC1[C@H]1CC1CCCC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.4
499  [O-][C]=O)[C@@]1(C[N+])1(Cc2cccccc2)c3cccccc3CC[N+1]C)C  4.3
500  O=C1CC1CC1[C@H]1CC1CCCC1CC(=O-)=O)(Cc2cccccc2)c3cccccc3  4.2