Stratified-bagging models for the prediction of ACE2 allosteric Inhibitors

The jupyter notebook for the prediction of ACE2 allosteric Inhibitors using Stratified Bagging models and Morgan fingerprints.

Installation and dependencies Anaconda (<https://docs.anaconda.com/anaconda/navigator/install/>) >= 1.9.12; Python >= 3.7.7; Pandas >= 1.0.3; numpy >= 1.18.1

Usage

1. From the anaconda navigator, start the jupyter notebook and load the file ‘ACE2\_allosteric\_Prediction\_StratifiedBagging.ipynb’ available under the folder ‘ACE2\_StratifiedBagging’
2. Calculate the Morgan fingerprint for the test compounds (sample knime workflow provided under the folder ‘knime\_workflow\_descriptor\_calculation’).
3. Place the generated file with the calculated descriptor in the folder ‘test\_data’. A sample file is available (sample\_test\_file\_morgan.csv).
4. In the jupyter notebook ‘ACE2\_allosteric\_Prediction\_StratifiedBagging.ipynb’, change the name of the test file (3rd cell; #Path to the test file)
5. Execute the notebook.
6. The ACE2 allosteric Inhibitor’s prediction using Stratified Bagging models and Morgan fingerprints will be saved in the ‘output\_predictions’ folder.

The folder ‘SB\_models’ also contains Stratified Bagging models generated for Avalon Fingerprint and RDKit descriptors (physicochemical properties).

The folder ‘knime\_workflow\_descriptor\_calculation’ contains the knime workflow to generate the descriptor files for Morgan Fingerprint, Avalon Fingerprint and RDKit descriptors (physicochemical properties). This workflow takes input a .csv file with columns: ‘Molecule name’; ‘smiles’

The folder ‘pharmacophore\_models’ contains Ligand-based pharmacophore models generated for the virtual screening.