

Blog Topics

Workflow

1. ChEMBL - Bioactivity - IC50 - Why is it important - SMILES
2. Why Prediction of Bioactivity is important
3. Which Methods?
4. QSAR - what are the methods that are being used
5. Structural Similarity and types (Tanimoto coefficient)
6. Importance of Normalization and its types
7. Chemical Descriptors- why important and types
8. Molecular Fingerprints - importance and type
9. RDKit and PaDELPy
10. AI/ML - importance in Prediction
11. Study the different regressors and evaluation matrices
12. Linear and Ensemble regressors
13. Hyperparameter tuning
14. Exhaustive search GridsearchCV
15. Visualisation and Understanding (Better R-squared and less errors)