

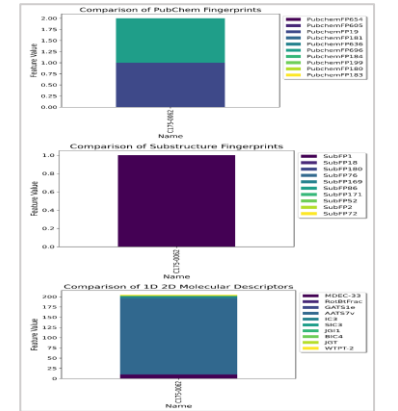
MAO-B-pred app

MAO-B-pred allows users to predict bioactivity of a query molecule against the MAO-B target protein.

Application Description

This module of MAO-B-Pred (<https://github.com/RatulBhowmik/MAO-B>) has been built to predict bioactivity and identify potent inhibitors against MAO-B using robust machine learning algorithms.

Predict bioactivity of molecules against MAO-B using pubchemfingerprints



- Conclusion
- Developed ML-QSAR models using fingerprints and molecular descriptors to predict MAO-B inhibitor activity
 - Created a web application (MAO-B-pred) for rapid bioactivity prediction.
 - Screened 8812 compounds and identified **C175-0062** as the top MAO-B inhibitor
 - Findings support potential for new MAO-B inhibitors in Parkinson's disease, pending experimental validation

Kumar, Sunil, Ratul Bhowmik, Jong Min Oh, Mohamed A. Abdelgawad, Mohammed M. Ghoneim, Rasha Hamed Al-Serwi, Hoon Kim, and Bijo Mathew. "Machine learning driven web-based app platform for the discovery of monoamine oxidase B inhibitors." *Scientific Reports* 14, no. 1 (2024): 4868.