

GUI for Chiral Descriptors Calculation

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ChiralDescriptorCalculator is a PyQt6 desktop application for the computation and machine learning-based processing of chiral molecular descriptors. Two complementary descriptor types are implemented: chiral atom-centered scalar triple products (cSTP) and delta fingerprints (Δ FP). cSTP descriptors encode absolute configuration geometrically — their sign flips between enantiomers by construction — while Δ FP descriptors cancel all achiral information from Morgan fingerprints, retaining only the chirality signal.

The application provides an end-to-end workflow covering 3D conformer generation (ETKDG or molecular dynamics), descriptor calculation, and model training using Random Forest and Decision Tree classifiers. Enantiomer-aware GroupKFold cross-validation prevents data leakage that would otherwise inflate validation metrics.

cSTP descriptors were evaluated on four published datasets for predicting enantiomer elution order in chiral HPLC, outperforming standard Morgan fingerprints across most datasets. Additional features include leave-one-pair-out cross-validation, out-of-bag scoring, interactive decision tree visualisation, and single-molecule prediction by SMILES input.

ChiralDescriptorCalculator makes chiral descriptor-based QSER modelling accessible to non-programming users, with applications in chiral chromatography, assignment of absolute configurations, prediction of enantioselective biological activity, and VCD spectra prediction.