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FragFEATURE: Knowledge-based Fragment Binding Prediction using Unsupervised Machine Learning

FragFEATURE is a data-driven computational method for fragment binding prediction. It predicts small molecule fragments preferred by a protein structure using a knowledge base of all previously observed protein-fragment interactions. For an evaluated protein structure, predicted fragments correspond to native ligands of the protein or in other cases drugs that target the protein. Predicted fragments can therefore aid in identifying promising drug-like compounds to evaluate in the drug discovery pipeline.

Applications

- Drug Discovery
- Fragment-based drug design
- Virtual Screening

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