Ligand-based Virtual screening using Fuzzy Correlation Coefficient

Abstract

Selection and identification of a subset of compounds from libraries or databases, which are likely to possess a desired biological activity is the main target of ligand-based virtual screening approaches. The main challenge of such approaches is achieving of high recall of active molecules. In this paper we presented fuzzy correlation coefficients (FCC), which is used as a
similarity coefficient. The new approach is based on mutually dependent between molecular features, while most common approaches (Tanimoto, Bayesian and other coefficients) based on mutually independent between features. Our experiments have shown that the new coefficient increases the recall of active molecules in high diversity database compared with other correlation coefficients and Tanimoto.

Reference

- Pipeline Pilot; Accelrys Software Inc.: San Diego, CA, 2008.

Index Terms

Computer Science               Information Retrieval

Key words

Correlation coefficients               fingerprint features
similarity search

similarity coefficients

virtual screening