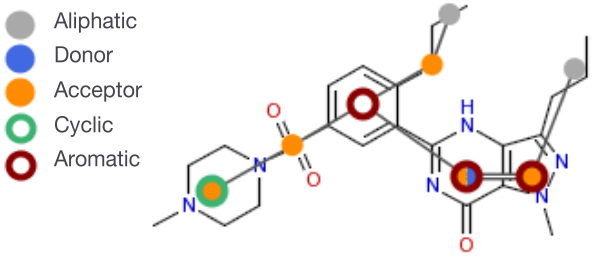
Pharmacophore Graph

Discngine Chemistry Collection for Accelrys Enterprise Platform

Introduction

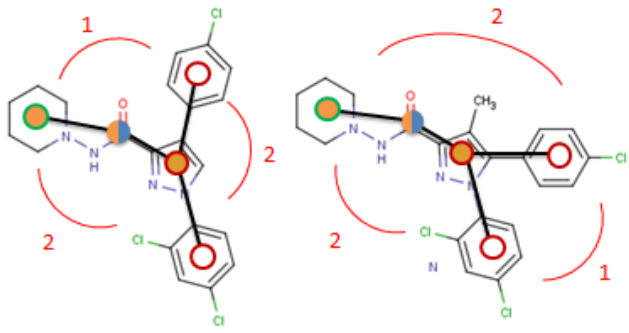
A **Pharmacophore Graph** is an object encoding molecular structures into simplified, typed molecular graph.



A pharmacophore graph is obtained by grouping atoms into fragments, connecting the fragments to each other using the original molecular graph, and assigning pharmacophore features to the resulting graph vertices based on the pharmacophoric fragment properties.

Several reduction level are available depending on fragment definition rules. Moreover, pharmacophore graph can be computed on the entire molecule, or using different definition of molecular scaffold.

The pharmacophore graph matching procedure is highly configurable, and can be setup to perform similarity search at various fuzziness levels. For example, connectivity between attachment points at each node can be optionally taken into account.



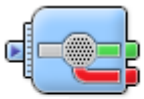
Business cases

Pharmacophore graph finds its use in compound similarity search, compound clustering, molecular structure alignment, etc… It is particularly well suited for **lead hopping** strategies to identify structurally dissimilar molecules displaying similar shape and pharmacophore spatial arrangement.

Component collection

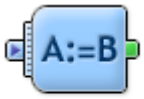
Generate Pharmacophore Graph

Converts a molecule to a pharmacophore graph using one of the available encoding schemes. The graph is added to the molecule or output in replacement of it.



Match Pharmacophore Graphs

Pharmacophore graph matching compares and score a set of target compounds to one or several reference compounds using a MCS-based search procedure.



Add Node Constraints

Features or SMARTS **constraints** can be added at a specific graph position in order to fine tune the note compatibility rules and account for mandatory features for activity.

Ph4Graph Fingerprint

Several fingerprint schemes are available: nodes, edges and connectivity, extended connectivity, doublets and triplets.

Canvas Graph Display

Intuitive and customizable representation of pharmacophore graphs can be generated and integrated in pipeline pilot reports.

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