What is JKlustor

JKlustor is a ChemAxon module for diversity calculation and clustering integrated into JChem. Although the users of JChem are mainly chemists, JKlustor can be used for other objects too.

Currently JKlustor offers the following command-line tools for clustering:

- GenerateMD generates various molecular descriptors including chemical hashed and pharmacophore fingerprints for molecules, which may be used for structural diversity computations and clustering.
- Jarp performs variable-length Jarvis-Patrick clustering.
- Ward clusters molecules using Ward's hierarchic clustering method applying the RNN approach.
- LibMCS clusters molecules by maximum common substructures in a hierarchical manner. It can be applied to focused set profiling and diversity analysis.
- CreateView composes an SDfile that contains both structures and calculation results using the input SDfile of GenerateMD and a table containing the ordinal number of compounds from the SDfile and other data to be viewed. Such table can be created for example by Compr, Jarp or Ward. The generated SDfiles can be displayed by MarvinView or other SDF viewer.

You can also find all ChemAxon's clustering methods grouped below:

Hierarchical clustering

Maximum Common Substructure (MCS) Search

Library MCS (LibMCS) clustering

Ward clustering

Non-hierarchical clustering

Bemis-Murcko clustering

Diverse Set Selection

Jarvis-Patrick clustering

K-means clustering

Sphere exclusion clustering