Structural Complexity Estimation

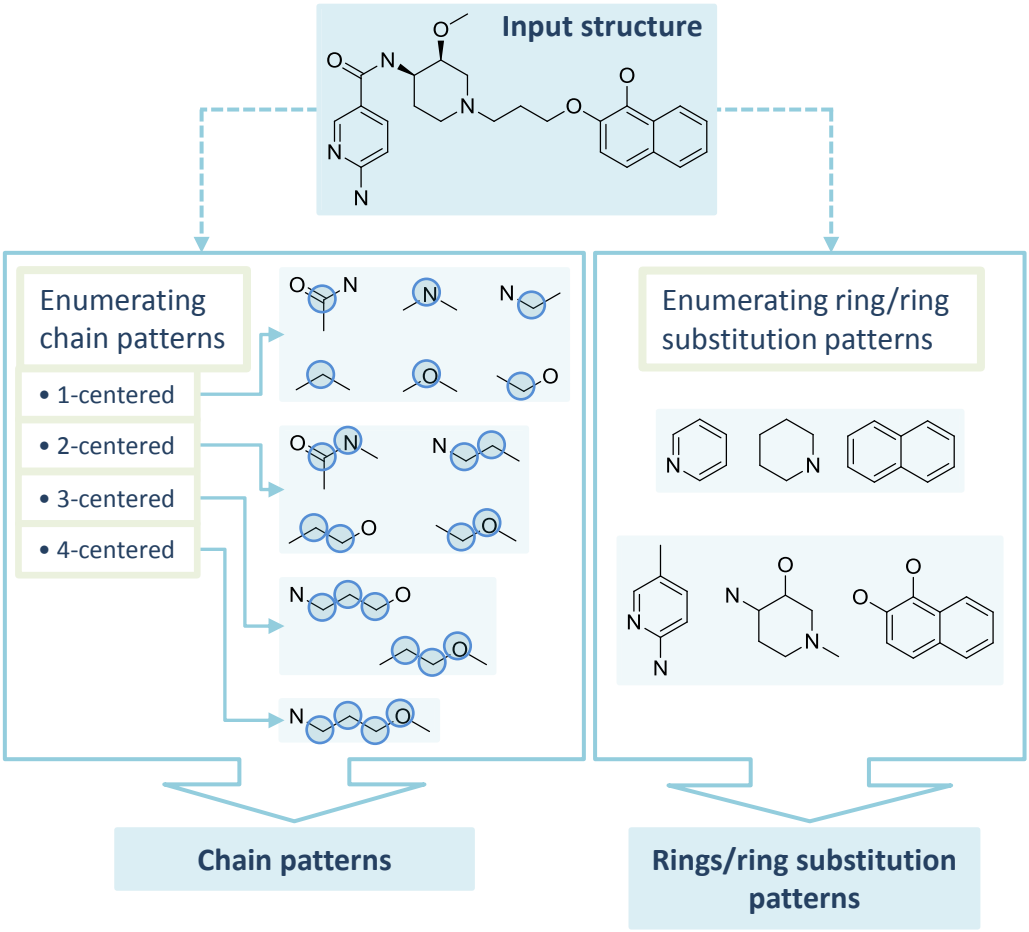
Keymodule Ltd.

TopoPlex

Estimate structural complexity

TopoPlex[1] is a software tool for estimating molecular structure complexity based on a user-provided starting material database. The structural complexity analysis performed by TopoPlex provides a rapid and effective ranking technique which can be used for estimating synthetic accessibility, or for the elimination of structures with unfeasible molecular motifs.

The method is based upon the common assumption that a structure has low structural complexity [drug-like properties] if it contains chain and ring structural motifs (patterns) which frequently occur in commercially available starting materials [existing drugs].



The enumeration of chain and ring patterns of an input structure in TopoPlex

1. K. Boda and A. P. Johnson: Molecular Complexity Analysis of de Novo Designed Ligands. *J. Med. Chem*. **2006**, 49, 5869 – 5879

About Keymodule

Keymodule Ltd. is a chemoinformatics software company which specializes in the development of toolkits and applications for chemical and pharmaceutical research.

www.keymodule.co.uk | info@keymodule.co.uk | Tel: +44 113 343 6595

Synthetic Feasibility Estimation

Keymodule Ltd.

CAESA

Estimate synthetic accessibility

CAESA (**C**omputer **A**ssisted **E**stimation of **S**ynthetic **A**ccessibility) automatically ranks sets of molecules according to their ease of synthesis and displays the synthesis route.

Input structure

Expert system

1. Select potential starting materials
2. Identify the structural features that make the input structure difficult to synthesize
3. Establish synthetic routes
4. Assess the length and quality of each route
5. Select the best routes

Database of available starting materials

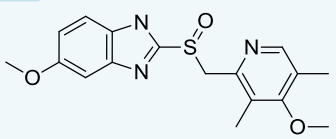
Synthetic Knowledge Base reactions described in PATRAN

1. **Estimation of synthetic accessibility** (percentage)
2. **Synthetic routes**
3. **Potential starting materials**

Workflow of CAESA

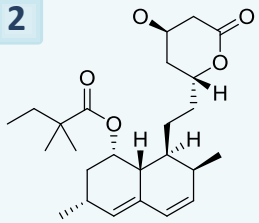
Examples

1



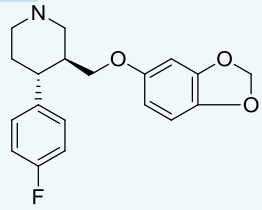
CAESA: **96.4%**
TopoPlex: **14.38**

2



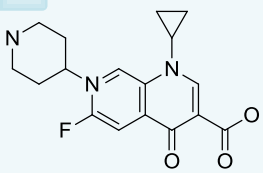
CAESA: **81.3%**
TopoPlex: **24.14**

3



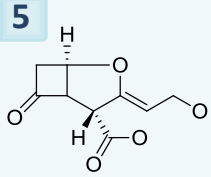
CAESA: **66.6%**
TopoPlex: **17.72**

4



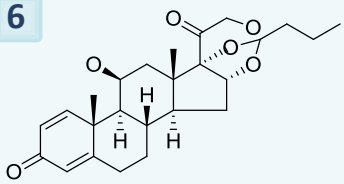
CAESA: **59.6%**
TopoPlex: **40.49**

5



CAESA: **39.3%**
TopoPlex: **52.10**

6



CAESA: **9.0%**
TopoPlex: **18.78**