

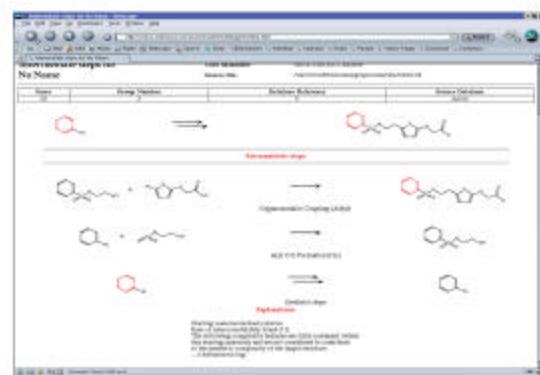
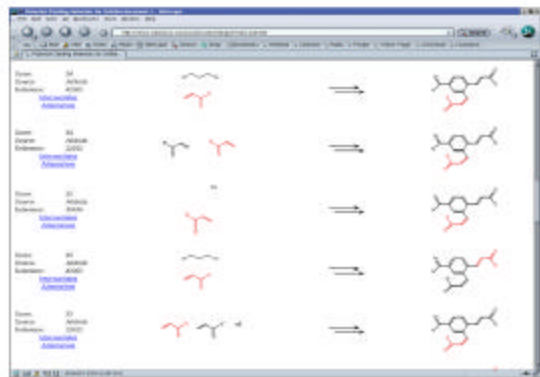
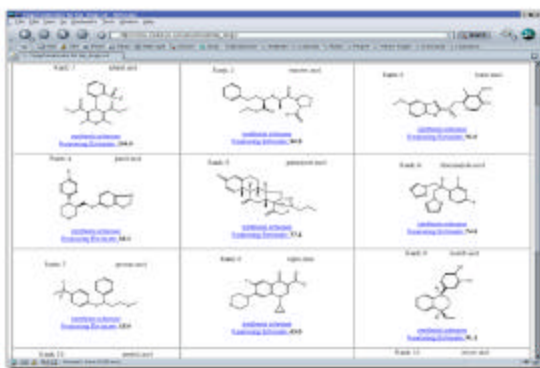
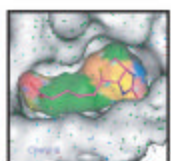
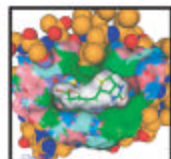
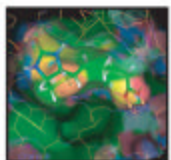
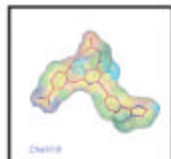
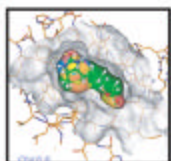
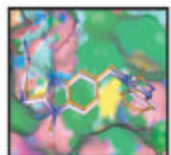
CAESA

Molecular structure synthesis ranking software



OVERVIEW

CAESA uses the technology of expert systems to emulate methods of an experienced synthetic chemist to estimate the ease of synthesis of a particular compound.



Potential starting materials are selected from databases of available compounds and the structural features that make a compound difficult to synthesise are identified. The combination of these two types of information provides a realistic estimate of the likely ease of synthesis.

CAESA comprises of a set of modules which estimate a structure's synthetic accessibility using a knowledge based approach.

FEATURES

Productivity

The program establishes which compounds could be synthesised via quick and efficient synthetic routes.

Explanation

Exactly how the estimate was calculated is displayed within the interface. The selected starting materials are displayed along with all the structural features which contribute to the difficulty of synthesising the compound. A network of the reasoning used to explain how the estimate was calculated alongside a textual description.

Input Data

Structures are entered into the program in the form of MDL molfiles and the program can be easily used with a variety of external structure generation programs.

Usability

The results are displayed within an easy to use interactive, graphical interface.