SYLVIA

Fast Estimation of Synthetic Accessibility

SYLVIA rapidly evaluates the ease of synthesis of organic compounds. **SYLVIA** can prioritize thousands of structures, e.g., generated by de novo design experiments or retrieved from large virtual compound libraries, according to their synthetic complexity. Thus, **SYLVIA** bridges the areas of computer-aided molecular design, chemoinformatics and synthetic chemistry.

SYLVIA ranks chemical compounds on a scale that reflects whether a structure can be synthesized by a straightforward synthesis route or whether it is a complex, challenging synthesis target. The scoring function is based on the following criteria:

- Structure-based criteria:
  molecular graph, ring and stereo-chemical complexity
- Starting material-based criterion:
  synthetic similarity to available chemicals
- Reaction-based criterion:
  frequency analysis on the presence of strategic bonds that are extracted from reaction databases

Key Features

- Visualization of chemical structures, synthetic accessibility scores and read-in information
- Extension or replacement of starting material database by in-house chemicals
- Output of individual contributions of structure- and reaction-based components to total synthetic accessibility score
- Adjustable color-coding for low, medium and high synthetic accessibility scores
- Highly interactive and intuitive, wizard driven graphical user interface
- Applicable to a broad range of organic chemistry

Areas of Application

- Filtering of results of *de novo* design or virtual screening experiments
- Prioritization and screening of compound libraries and collections
- Lead identification and prioritization, *e.g.*, of structures proposed from inverse QSAR/QSPR
- Compound profiling of in-house substance databases or databases of chemical suppliers
- Synthesis design and planning

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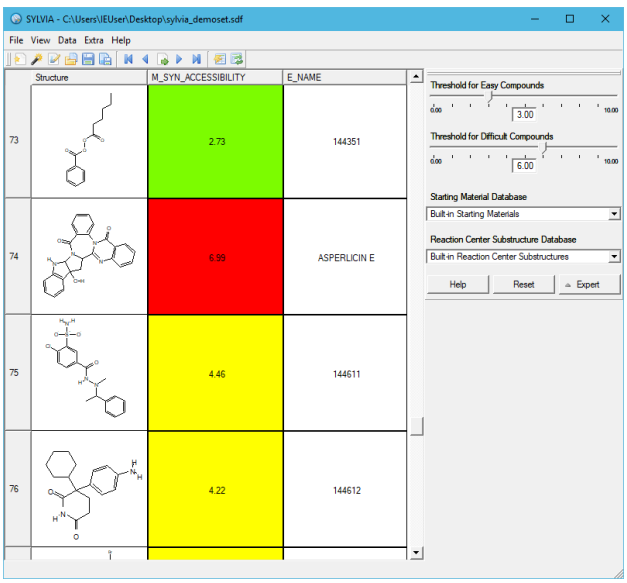
SYLVIA assists scientists in analyzing organic chemical structures from the synthetic chemist's point of view to make better decisions about which chemical compounds to prioritize for the next steps in a research and development project.

In its calculation process, **SYLVIA** assesses various structural and chemical features of the target molecule that are typically considered when chemists intellectually evaluate the synthetic accessibility of a set of compounds. The calculated synthetic accessibility scores agree with the values proposed by chemists to an extent that compares well with how individual chemists agree with each other.

Due to the fast calculation process, **SYLVIA** can effectively be incorporated into virtual screening tools or de novo design systems to rank huge amounts of structures according to their synthetic complexity.



Technical Features

- Graphical user interface, optional batch mode execution and daemon mode
- Interface for integration into internal IT environments and workflows
- Through consultation available as component for BIOVIA Pipeline Pilot®

References

- K. Boda, T. Seidel, J. Gasteiger. Structure and reaction based evaluation of synthetic accessibility. *J. Comp.-Aided. Mol. Des.* **2007**, *21*, 311-325.
- J. Gasteiger. Cheminformatics: Computing target complexity. *Nature Chemistry* **2015**, *7*, 619-620.

System Requirements

SYLVIA is available for Microsoft® Windows® (7/8/10, 32bit).

Evaluation

A 30 days evaluation copy of **SYLVIA** is available free of charge in the Download Area of the web site of MN-AM at mn-am.com.

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