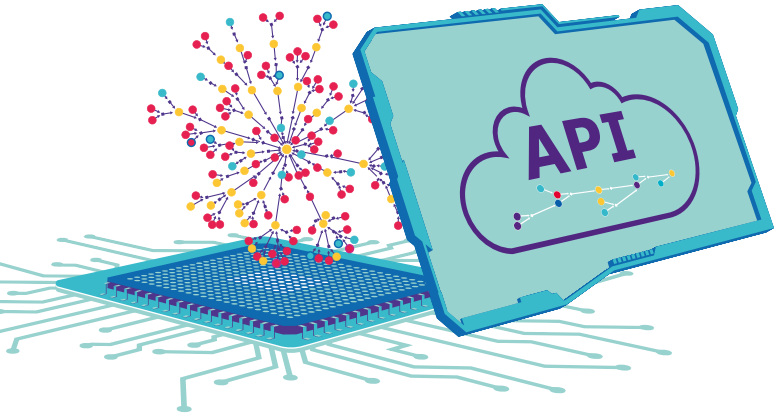
SYNTHIA™ API

Expedite *in silico* drug discovery

Connect SYNTHIA™ with your preferred cheminformatics software for high-throughput pathway design & molecular synthesis assessment



SYNTHIA™
Application Programming Interface

Our Application Programming Interface (API) allows you to incorporate SYNTHIA™ Retrosynthesis Software with your preferred cheminformatics tools to streamline retrosynthetic analysis for promising leads and assess synthetic accessibility scores (SAS) of thousands of virtual molecules in minutes.

The result: a customized, fully integrated retrosynthesis experience that greatly expedites *in silico* drug discovery.

- **Seamless integration** with your existing software
- **Automation** of retrosynthesis planning accelerates workflows
- **Customization** to your specific needs and workflows
- **Scalability** to meet your growing retrosynthesis requirements
- **Enhanced efficiency** due to automated, interconnected workflows
- **Data security** with ISO 27001 certification to protect your work

Two Types of SYNTHIA™ API

Synthia	Output	Speed	Basis
Full Retro API	Reaction SMILES and names, references, prices and CAS numbers of starting materials, pathway scores	20 molecules per hour	Entire SYNTHIA™ engine
Synthetic Accessibility Score (SAS) API	SAS (0 to 10)	Up to 100,000 molecules per hour	AI model trained on SYNTHIA™ expert-coded rules

How It Works

Use SYNTHIA™ API to easily launch the analysis. Our software integrates seamlessly with your drug discovery platform, and displays results in your existing workflow (e.g., Knime, Pipeline Pilot, Jupyter Notebook, etc.).

Ask us for a Docker image to run SYNTHIA™ SAS API on your organization's infrastructure:
www.synthiaonline.com/contact-us/

SYNTHIA™ Full Retro API

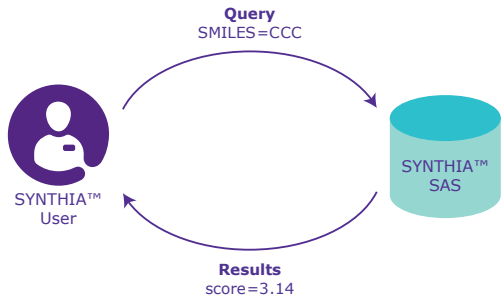
The Full Retro API is based on a completely automated retrosynthesis search mode that allows you to design customized pathways, starting from commercially available or known building blocks. Simply query multiple molecules at once, and begin.

The default settings are suitable for most searches, or you can tailor the search criteria to suit your project needs. The detailed output data includes reaction SMILES and names, illustrative literature references, prices and CAS numbers of starting materials, as well as pathway scores.

SYNTHIA™ SAS API

Our Synthetic Accessibility Score (SAS) API combines deep-learning model with data from our retrosynthesis software to predict molecule complexity in terms of number of synthetic steps, starting from small, commercially available building blocks.

For every molecule entered, the software generates a SAS score ranging from 0 to 10. The lower the score, the easier it should be to synthesize the molecule. The service allows you to analyze thousands of molecules in minutes, greatly accelerating molecule selection prior to synthesis.



Users can enter molecules individually or as a batch in the SMILES text format, and the software returns a score for each molecule.

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