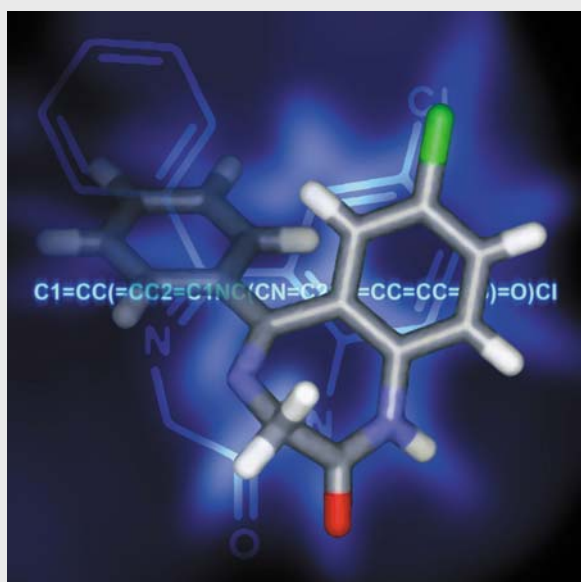


CORINA

Fast Generation of High-Quality 3D Molecular Models

CORINA is a fast and powerful 3D structure generator for small and medium sized, organic molecules. **CORINA** matured through a series of versions during the past decades and has become the recognized world-wide standard in industry and academia to generate 3D molecular models of high quality.



CORINA has been designed to efficiently and reliably handle massive volumes of structures and its scope, robustness, speed and performance makes **CORINA** a perfect application to convert large chemical datasets or databases.

CORINA delivers structures of high quality. The RMS deviation of **CORINA** built models from published X-ray structures is among the best of all commercially available conversion programs.

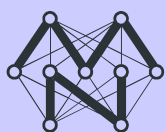
CORINA is extremely fast and performs with excellent conversion rates of higher than 99.5% for small and medium sized, organic molecules.

Key Features

- Applicable to a broad range of organic chemistry and many organometallic compounds
- No upper limits to the size of molecules or size of ring systems
- Generation of low-energy conformations
- Consideration of stereochemical information
- Generation of stereoisomers (tetrahedral chiral centers and *E/Z* double bonds)
- Generation of multiple ring conformations
- Several options to influence the 3D structure generation process

Areas of Application

- 3D database generation
- Lead discovery and lead optimization, *e.g.*, for pharmacophore searches, ligand docking studies and similarity searches
- Quantitative structure activity and property relationships (QSAR and QSPR)
- Spectra prediction and structure elucidation
- Prediction of chemical reactivity
- Input to quantum-mechanical and force field calculations



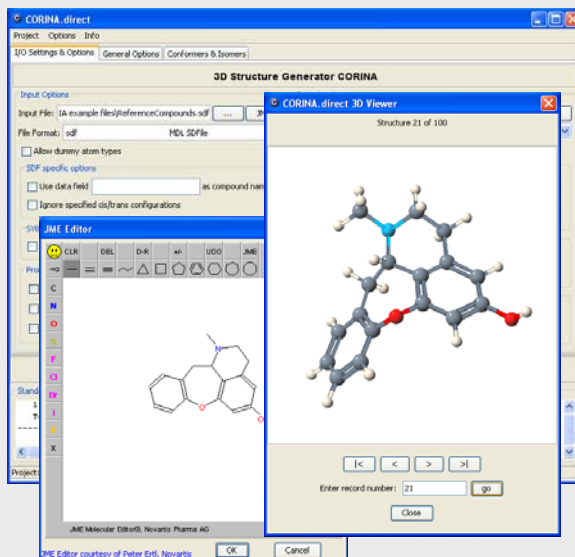
CORINA

Fast Generation of High-Quality 3D Molecular Models

The standard version of **CORINA** is a command line program for batch mode execution. In addition, the graphical user interface **CORINA.direct** is available that can be regarded as a graphical front-end to the standard version of **CORINA**.

CORINA.direct triggers the standard version of **CORINA** and executes the 3D structure generation process in the background of the system. All options and settings of program parameters that are provided by the command line version can be comfortably selected with **CORINA.direct**.

Furthermore, **CORINA.direct** provides an integrated molecule editor and a viewer to browse the generated 3D models as well as the typical robust and reliable **CORINA** performance.



Technical Features

- Batch mode execution and optional graphical user interface
- Interface for integration into internal IT environments and workflows
- Interface to ligand docking program FlexX
- Also available as component for SciTegic® Pipeline Pilot®

System Requirements

CORINA is available for Microsoft® Windows®, x86 Linux (32 and 64 bit), SGI® Irix® 6.5 and Sun™ Solaris™ 9 platforms and operating systems.

Reference

- J. Sadowski, J. Gasteiger
Chemical Reviews **1993**, *93*, 2567-2581.
- J. Sadowski, J. Gasteiger, G. Klebe
J. Chem. Inf. Comput. Sci. **1994**, *34*, 1000-1008.

Test Version

CORINA can be tested free of charge online on the web server of Molecular Networks at www.molecular-networks.com/online_demos. A 30 days evaluation copy of **CORINA** is available free of charge in the Download Area of the web server of Molecular Networks at www.molecular-networks.com.



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