CORINA Classic

Fast Generation of High-Quality 3D Molecular Models

CORINA Classic is a fast and powerful 3D structure generator for small and medium sized, organic molecules. **CORINA Classic** 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 Classic has been designed to efficiently and reliably handle massive volumes of structures and its scope, robustness, speed and performance makes **CORINA Classic** a perfect application to convert large chemical datasets or databases.

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

CORINA Classic 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 including natural products and many organometallic compounds
- No upper limits to the size of molecules or size of ring systems
- Generation of low-energy conformations
- Consideration of stereo-chemical information
- Generation of stereo-isomers (tetrahedral chiral centers, E/Z double bonds, and atropisomers)
- Generation of multiple ring conformations
- Several options to influence the 3D structure generation process
- Robust performance with high conversion rates

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
- Input for refinement of experimentally determined structures (*e.g.*, X-ray geometries)

Contacts Molecular Networks GmbH, Neumeyerstr. 22-34, 90411 Nuremberg, Germany
Altamira LLC, 470 West Broad Street, Columbus, OH 43215, USA
www.mn-am.com
Phone +49 (0)911 597 424 00
Phone +1 614 824 4586
info@mn-am.com

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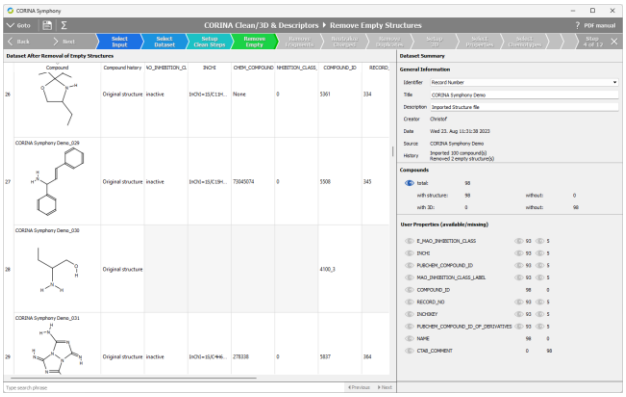
The standard version of **CORINA Classic** is a command line program for batch mode execution. In addition, **CORINA Classic** is integrated in the CORINA Clean/3D workflow in the GUI application **CORINA Symphony**. This interactive workflow provides the main functionalities of **CORINA Classic** for chemical structure clean-up and standardization and 3D structure generation.

Furthermore, a Python module is available to integrate **CORINA Classic** into new or existing applications, workflows, scripts, and various ecosystems using the familiar Python syntax. Interactive computation support for Jupyter notebooks is also provided.

CORINA Clean/3D processes molecular structures in a well-designed workflow routinely employed for generating 3D molecular representations and preparing datasets for modelling. Containing much of the **CORINA Classic** functionality, this workflow can be used to remove counter ions or small fragments, neutralize, add hydrogens, apply preferred orientations, and detect/remove duplicates. Input to the process may include structure files, SMILES, or database records.



Technical Features

- Batch mode execution
- Intuitive and interactive workflow-based user interface
- Python module for integration into internal IT environments and workflows
- Interface to ligand docking program FlexX
- Through consultation available as component for KNIME

References

- J. Sadowski. 3D Structure Generation. In *Handbook of Chemoinformatics – From Data to Knowledge*. J. Gasteiger, J.; Engel, T., Eds., Wiley-VCH: Weinheim, 2003, pp. 231-261.
- C.H. Schwab. Conformations and 3D pharmacophore searching. *Drug Discovery Today: Technologies*, Volume 7, Issue 4, Winter **2010**, e245-e253.

System Requirements

CORINA Classic is available for Microsoft® Windows® (10/11) and for x86-64 Linux platforms and operating systems (RHEL 6/7). The Python module is available for x86-64 RHEL7 and Python versions 3.8 to 3.11.

Evaluation

CORINA Classic can be tested free of charge online at mn-am.com/demos.

An evaluation copy of **CORINA Classic** is available from MN-AM on request.

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