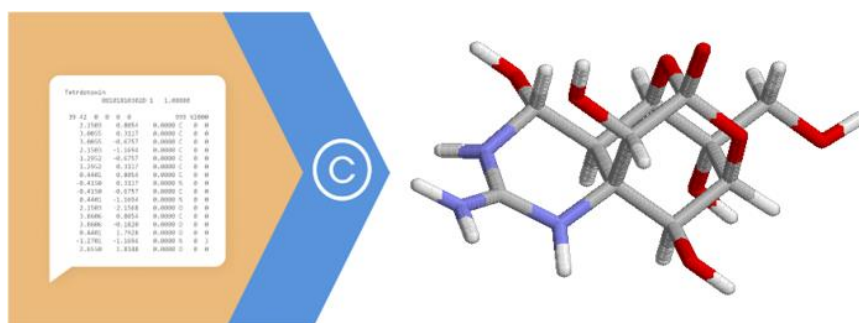August 24, 2023

CORINA Classic Version 5.0.0 – What's New?

New features

- Module for integration into Python environments
- Support of x86-64 Linux platforms (RHEL7) and Python versions 3.8, 3.9, 3.10, and 3.11
- GitHub repository with example Python scripts and use cases at https://github.com/mn-am

Benefits

- Integration of CORINA Classic into inhouse applications, workflows, scripts, and various ecosystems using the familiar Python syntax
- Deployment and usage of CORINA Classic directly in Python tool kits for machine learning and artificial intelligence applications in chemoinformatics projects
- Interactive computation support for Python and Jupyter notebooks

Comparison with version 4.4.0

- Test set of 225,735 structures (subset from Open NCI Database, release 4, May 2012)
- All 3D structures converted by version 5.0.0 have an RMSD (all non-hydrogen atoms) 0 Å compared to 3D structures generated by version 4.4.0, *i.e.*, are identical conformations

Further information

- Please visit the CORINA Classic product page at www.mn-am.com/products/corina or contact us at info@mn-am.com