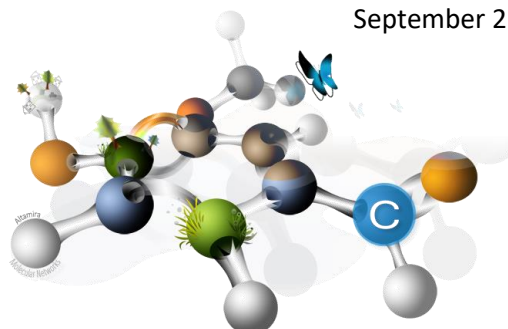


September 27, 2021



CORINA Classic Version 4.4.0 – What's New

Improvements

- Option to preserve configuration at defined *E/Z* double bonds during stereoisomer enumeration
- Detection of prochiral centers and preservation of positions of substituents for 3D input structures
- Enhanced flexibility for restraint parameter settings in CIF output files

Benefits

- Improved handling of stereochemistry and generation of stereoisomers
- Improved accuracy of reproduction of input 3D geometries, *e.g.*, when using it for structure elucidation purposes
- Improved flexibility for handling of crystallographic information

Comparison with version 4.3.0

- Test set of 245,710 structures (subset from Open NCI Database, release 4, May 2012)
- 99.6% of 3D structures converted by version 4.4.0 have an RMSD (all non-hydrogen atoms) of less than 0.3 Å compared to 3D structures generated by version 4.3.0, *i.e.*, can be considered as 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