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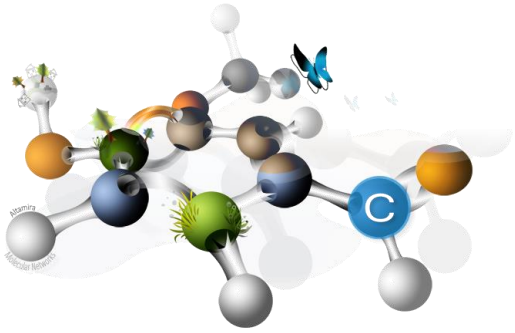
October 30, 2019



CORINA Classic Version 4.3.0 – What's New

Improvements

- Improved handling and support of stereochemical information
  - Accurate interpretation to generate racemic mixtures or pure enantiomers
- Enhanced flexibility for restraint parameters in CIF output files
- Extended unique atom labelling in PDB, CIF, MacroModel and Maestro output files

Benefits

- More robust and reliable support of stereochemistry including atropisomerism
- More flexibility for handling of crystallographic information and compound meta data

Comprehensive robustness test

- Conversion of the PubChem Database (https://pubchem.ncbi.nlm.nih.gov) with 96 million chemicals with an error rate of 0.3%

Comparison with version 4.2.0

- Test set of 245,710 structures (subset from Open NCI Database, release 4, May 2012)
- Almost 94% of 3D structures converted by version 4.3.0 have an RMSD (all non-hydrogen atoms) of less than 0.3 Å to the 3D structures generated by version 4.2.0, *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