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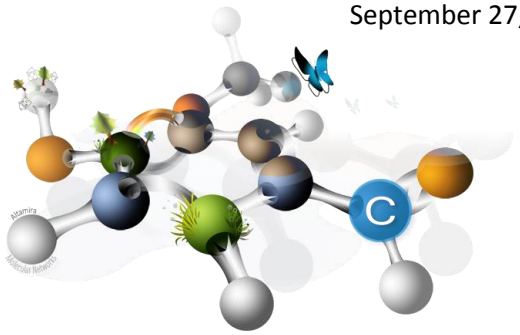

CORINA Classic Version 4.2.0 – What's New

Improvements

- Support of atropisomerism and generation of defined atropisomers (if specified in input)
  - Optional enumeration of atropisomers with stereo isomer generation module
- Enhanced flexibility for processing multi-column text input files containing SMILES or InChI
- Enhanced flexibility for restraint parameter settings in CIF output files
- Improvement of generation of large ring systems (≥ 10 ring atoms)

Benefits

- Support of stereochemistry including atropisomerism
- More flexibility for handling of compound *meta* information and for file format interconversion
- Higher conversion rate and speed

Comprehensive robustness test

- Conversion of the PubChem Database (https://pubchem.ncbi.nlm.nih.gov) with 91 million chemicals with an error rate of 0.3%

Comparison with version 4.1.0

- Test set of 245,706 structures (subset from Open NCI Database, release 4, May 2012)
- 89% of 3D structures converted by version 4.2.0 have an RMSD (all non-hydrogen atoms) of less than 0.3 Å compared to 3D structures generated by version 4.1.0, *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
- 30 days evaluation copies of CORINA Classic can be downloaded free of charge in our Download Area (after registration)