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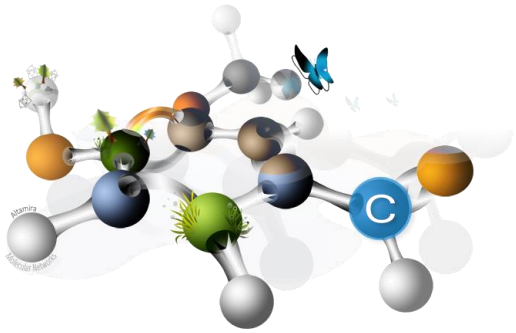

CORINA Classic Version 4.1.0 – What's New

Improvements

- Internal and automatic canonicalization of the input structure's connection table
  - Original atom and bond ordering from input file is preserved in output file
- Few changes and corrections to improve the general stability of the program

Benefits

- Deterministic behavior for a broader range of chemical compounds
- Higher conversion rates of up to 27%

Comprehensive robustness tests

- Conversion of the GDB13 database (http://gdb.unibe.ch) of 971 million organic molecules with up to 13 atoms (C, N, S, O, Cl) with a conversion rate of 99.0%
- Conversion of the PubChem Database (https://pubchem.ncbi.nlm.nih.gov) with 91 million chemicals with a conversion rate of 99.6%

Comparison of version 4.1.0 with version 4.0

- Test set of 245,712 structures (subset derived from Open NCI Database, version May 2012)
- 77% of 3D structures converted by version 4.1.0 have an RMSD (all non-hydrogen atoms) of less than 0.3 Å compared to 3D structures converted by version 4.0
- 100% of 3D structures converted by version 4.1.0 have an RMSD of less than 0.1 Å, if version 4.0 is used with optional internal canonicalization (driver option "canon")

Further information

- Please visit the 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)