CORINA Symphony

Manage and Profile Your Molecular Datasets

CORINA Symphony is a cheminformatics application to manage, manipulate and profile molecular data sets for *in silico* discovery and optimization, with a focus on toxicity applications.

CORINA Symphony assists scientists in creating, preparing and exploring chemical structures for predictive model building, classification and categorization, grouping and filtering based on physicochemical effects and properties, structural features of molecules and the powerful chemotype profiling approach.

CORINA Symphony consists of workflows that can be used independently or combined.

- CORINA Clean/3D workflow for reliable and efficient molecular structure processing and standardization
- CORINA Descriptors workflow for structural and physicochemical descriptor calculation

CORINA Symphony provides a database backend for the storage of chemical data sets and associated information. It supports the visual managing and exploration of imported or calculated data in table views with sorting functionality and editable table cells, including *copy-and-paste* to external spreadsheet applications.

Key Features

- Applicable to a broad range of chemical compound classes
- Provides functionalities for structure clean-up and standardization
- Fast and reliable conversion of molecules into uniform descriptors encoding structural and physicochemical features
- Provides global molecular, shape- and size-related descriptors, surface properties and quantum mechanical parameters
- Houses the ToxPrint chemotypes (fragment) library for profiling and fingerprinting
- Database backend to efficiently store and manage chemical and associated data

Areas of Application

- Predictive model building, *e.g.*, quantitative structure activity and property relationships (QSAR and QSPR) studies
- Drug design and optimization
- Predictive and computational toxicology
- Risk and safety assessment of chemical substances
- Profiling, classification and clustering of chemical data sets, databases and inventories
- Development of chemical categories for read-across applications

1455 Candlewood Dr.
Columbus, OH 43235
USA

www.mn-am.com

MN-AM

Neumeyerstr. 28
90411 Nuremberg
Germany

info@mn-am.com

CORINA Symphony

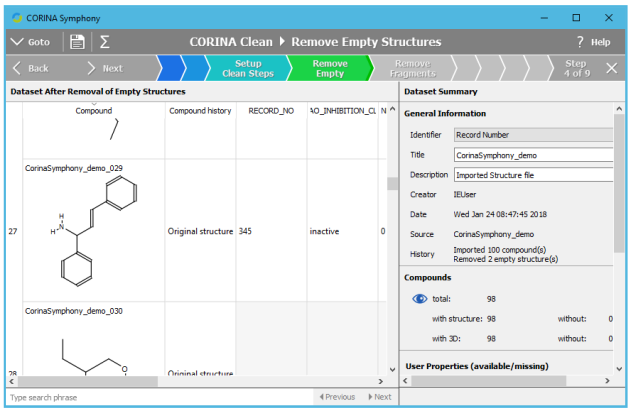
Manage and Profile Your Molecular Datasets

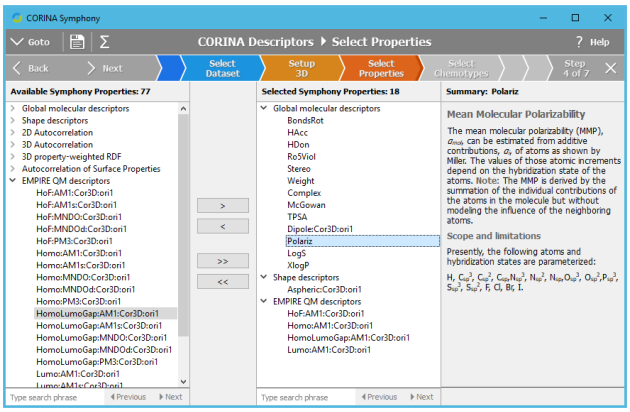
The **CORINA Symphony Clean/3D** workflow processes molecular structures in a well-designed workflow routinely employed for generating 3D molecular representations and preparing datasets for modelling.

Containing much of the **CORINA Classic** functionality, this workflow can be used to remove counter ions or small fragments, neutralize, add hydrogens, apply preferred orientations, and detect/remove duplicates. Input to the process may include structure files, SMILES, or database records.

The **CORINA Symphony Descriptors** workflow allows reliable and efficient calculation of 6 different types of descriptors, including (i) global molecular, (ii) shape and size descriptors, (iii) surface properties, (iv) property-weighted 2D/3D autocorrelation, (v) property-weighted RDF and (vi) quantum mechanical parameters.

The chemotype approach (ToxPrint) captures fragment-based structural features of molecules that may exhibit similar biologically-related initiating events on a molecular level.





Technical Features

- Graphical user interface and optional command line version
- Interface for integration into internal IT environments and workflows

References

- C. Yang *et al. J. Chem. Inf. Model.* **2015**, *55*, 510-528 (DOI: 10.1021/ci500667v)
- A.M. Richard *et al. Chem. Res. Toxicol.* **2016**, *29*, 1225-1251 (DOI: 10.1021/acs.chemrestox.6b00135)

System Requirements

CORINA Symphony is available for Microsoft® Windows® (7, 10)

Evaluation

An evaluation license of **CORINA Symphony** for Windows platforms can be requested from MN-AM

1455 Candlewood Dr.
Columbus, OH 43235
USA

www.mn-am.com

Neumeyerstr. 28
90411 Nuremberg
Germany

info@mn-am.com