Performance improvements, new functionalities and applications of the 3D structure generator CORINA Classic

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Support for Shape and size descriptors
Placement
Structure clean
Process all rotatable bonds
Chemotype approach to capture fragment

Background
- The power of any in silico tool for chemistry/toxicity prediction depends on the accuracy of the representation of molecular structures, so that they can be correctly interpreted and handled by the software used to compute molecular descriptors.
- The three-dimensional (3D) structures of chemical compounds are closely related to their chemical, physical and biological properties.

CORINA Classic
- Fast and powerful “on-the-fly” based tool for generating 3D-coordinates of molecules and for processing chemical structures to derive computational forms
- Maturated over the past 20 years to become the world-wide standard in industry/academia to generate 3D molecular structures of high quality

GUI Application
- CORINA Symphony combines features of CORINA Classic with interactive graphical workflows: ChemIn/3D (for structures preprocessing and 3D coordinates generating) and DESCRIPTORS (for descriptors calculating)
- CORINA Symphony has additional features to store, manage, manipulate and profile molecular data sets for in silico discovery and optimization with a focus on applications in computational toxicity

Objectives
- Present the computational performance and new features of CORINA Classic V4, including support of 3D/RO V3000 for structure input and output, as well as of Standard InChI for structure input
- Demonstrate a range of CORINA Classic applications within MN-AM’s chemoinformatics platform, illustrating the importance and impact of 3D coordinates on metabolism and toxicity prediction results

Conclusions
- CORINA Classic can efficiently and reliably handle massive volumes of structures (over 100 million per day), including large molecules, ring systems (with no upper size limits), and metal complexes
- The high quality 3D representation of chemical compounds is essential for metabolism and toxicity prediction. We demonstrated that CORINA/ROVIB Classic can be used for generating possible conformations of chemical compounds, and ROVIB and CORINA 3D Descriptors can successfully capture the differences between individual conformers, which can influence metabolism and QSAR model predictions
- The ability of CORINA-Classic and CORINA-Symphony to generate high quality 3D structures as well as its workflows for structure clean-up, standardization and descriptors calculation make it an invaluable tool for in silico discovery and optimization experiments, as well as for the development of high quality computational structures, which can be broadly applied for safety evaluation, risk assessment, and med-chem