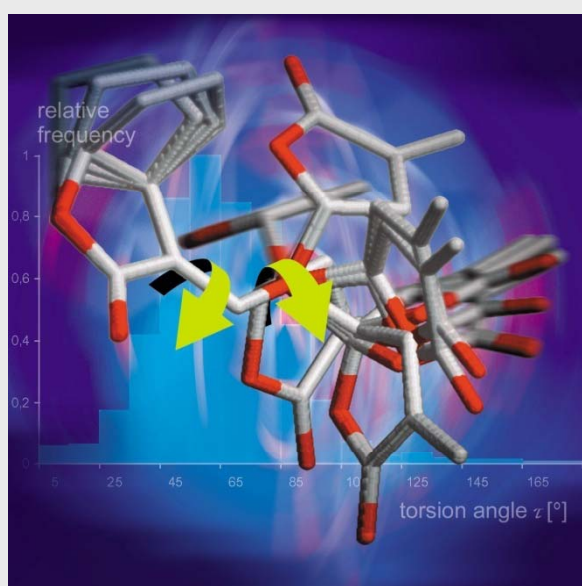


# ROTATE

## Generation of Sets of Diverse Conformations

**ROTATE** generates diverse and user controlled sets of molecular conformations starting from a given 3D model. **ROTATE** has been specifically designed for small to medium sized, typically drug-like molecules and generates conformations of biological relevance, *i.e.*, conformations that are close to the geometry when the structure is bound to its biological receptor.



**ROTATE** provides several methods to the user to fully or partially explore the conformational space in order to influence the number of output conformations by retaining a maximum of structural diversity and ensuring a balanced sampling of the conformational space.

**ROTATE** generates conformations by applying a set of rules that resulted from a statistical analysis on the conformational preferences of experimentally determined molecular structures of small molecules.

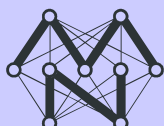
**ROTATE** is robust and powerful in order to process large datasets of chemical structures.

### Key Features

- Applicable to a broad range of organic chemistry
- Generation of observed conformations rather than sampling local energy minima or generating conformations randomly
- Generation of biologically relevant conformations (*bioactive* conformations)
- Classification of conformations with user-defined thresholds for a scalable and diverse sampling of the conformational space
- Generation of conformations within a user-defined energy window

### Areas of Application

- Lead discovery and lead optimization, *e.g.*, for flexible pharmacophore searches, ligand docking studies, similarity searches and ligand-based virtual screening experiments
- Generation of conformational ensembles for 3D databases
- Quantitative structure activity and property relationships (QSAR and QSPR)
- Prediction of chemical reactivity



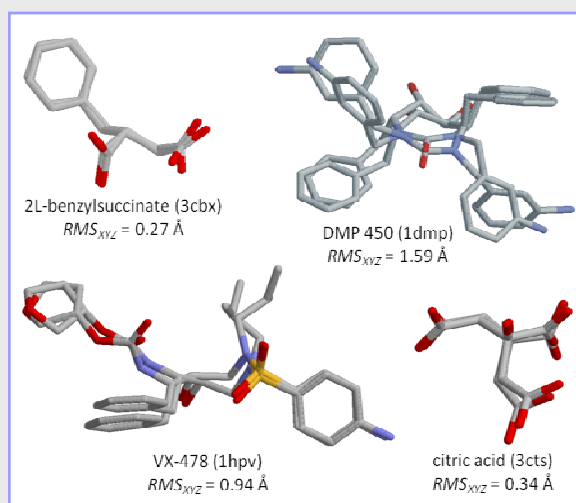
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In a recent study, **ROTATE** was found to be successful in finding conformations that are close to the "bioactive" one, although the conformation space was only searched to a limited extent regarding the number of rotatable bonds of the molecules that were processed and the relatively coarse search grid that was applied.

Furthermore, **ROTATE** performed with good quality and acceptable CPU time compared to other conformer generator packages and methods tested.

In addition, **ROTATE** can be seamlessly interfaced to the 3D structure generator **CORINA** (also available from Molecular Networks). The combination of both programs systems **CORINA** and **ROTATE** allows for a fast and efficient generation of conformational ensembles of the molecules under investigation even starting from 2D or linear string representations.



### Technical Features

- Batch mode execution
- Interface for integration into internal IT environments and workflows

### System Requirements

**ROTATE** is available for x86 Linux (32 and 64 bit), SGI® Irix® 6.5 and Sun™ Solaris™ 9 platforms and operating systems.

### Reference

S. Renner, C.H. Schwab, G. Schneider, J. Gasteiger  
*J. Comp. Inf. Model.* **2006**, *46*, 2324-2332.

### Test Version

A 30 days evaluation copy of **ROTATE** is available free of charge in the Download Area of the web server of Molecular Networks at [www.molecular-networks.com](http://www.molecular-networks.com).



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