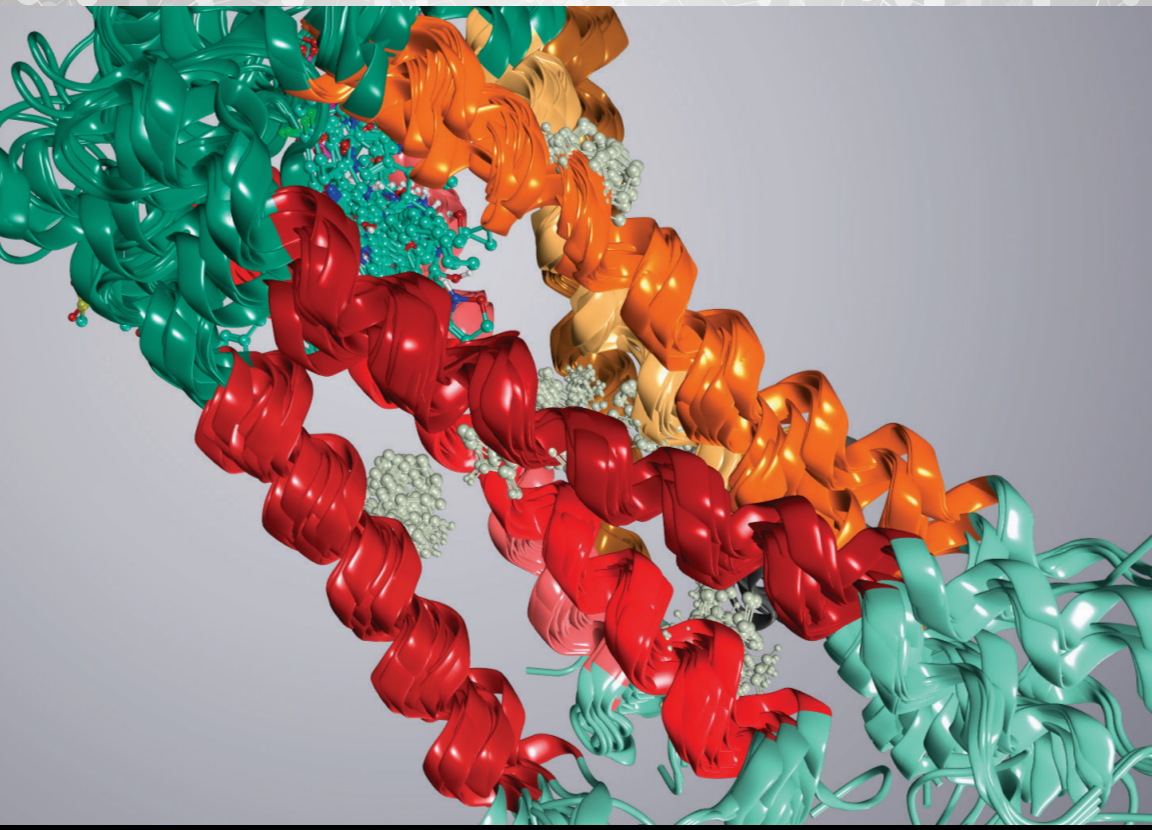
MOE
MOLECULAR OPERATING ENVIRONMENT



The Integrated Drug Discovery Software Platform

- Structure-Based Drug Design
- Ligand- and Fragment-Based Drug Design
- Pharmacophore Screening
- Protein, Antibody and Peptide Modeling
- Molecular Modeling and Simulations
- Cheminformatics and QSAR
- Methods Development and Deployment

Chemical Computing Group

The Molecular Operating Environment (MOE) is a leading drug discovery software platform that integrates visualization, modeling and simulations, as well as methodology development, in a single package. MOE scientific applications are used by medicinal chemists, biologists, crystallographers and computational chemists in pharmaceutical, biotechnology and academic research.

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The Integrated Drug Discovery Software Platform

Structure-Based Drug Design
- Active Site Visualization and Analysis
- Molecular Surfaces and Property Maps
- Interactive Ligand Design in the Pocket
- Ligand-Receptor Docking with Induced Fit
- Water Placement and Energetics

Ligand- and Fragment-Based Drug Design
- Conformation Generation and Clustering
- Flexible Molecular Alignments
- Web Application for SAR Analysis
- Scaffold Replacement - Grow, Link and Transform
- Pharmacophore Screening and Descriptor Filtering

Pharmacophore Screening
- Ligand- and Structure-Based Query Editor
- Boolean Expressions and Custom Features
- Partial Matches, Constraints and Shape Filters
- High-Throughput Conformation Generation
- Pharmacophore Elucidation and Search

Protein, Antibody and Peptide Modeling
- Multimer Homology Modeling
- Loop and Linker Modeling
- Ala, Cys, SNP, Residue Scanning
- Protein Property Descriptors
- Patch Analysis for Property Modulation

Molecular Modeling and Simulations
- AMBER10:EHT, MMFF94x, CHARMM Forcefields
- Explicit and Implicit Solvent Models
- LowModeMD Conformational Search
- Molecular Mechanics and Dynamics
- Quantum and Semi-Empirical Calculations

Cheminformatics and QSAR
- 400+ 2D and 3D Descriptors
- Similarity, Diversity and Fingerprints
- PLS, PCR, and Binary QSAR
- pKa Prediction and Protomer Generation
- Pipeline Tools and Components

Methods Development and Deployment
- Automated Protocol for Organizing SBDD Data
- Relational Database Connectivity
- SOAP Server and KNIME Nodes
- MOE/web: Web Browser Application Framework
- Cluster Computing

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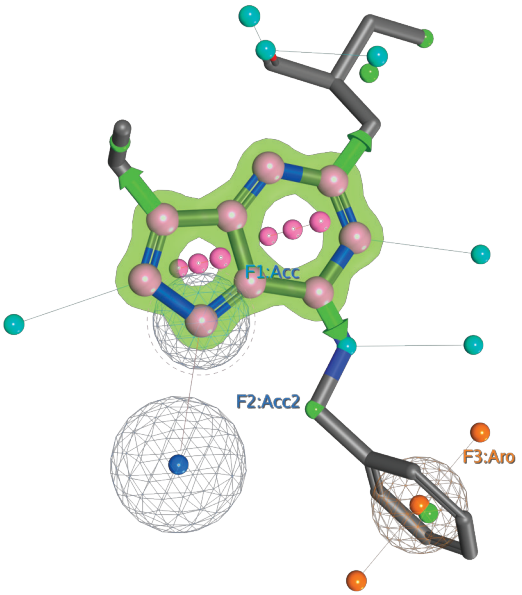

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