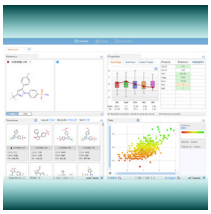
NEW IN MOE 2016.08

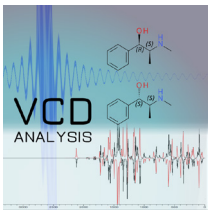
MOE 2016.08

NEW IN VERSION 2016.08



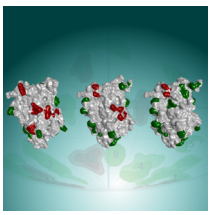
MOEsaic: Web-Application for Ligand Analytics

- Profile R-groups and analyze Matched Molecular Pairs
- Track design ideas and ligand modifications with property models
- Produce correlation plots to visualize structure, property, and activity relationships



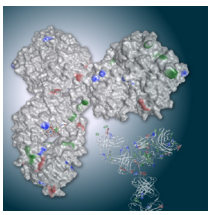
Spectral Analysis for Structure Determination

- Analyze NMR chemical shifts and coupling constants for any NMR active nuclei
- Compare calculated and experimental VCD spectra to determine absolute configuration
- Generate NMR/VCD spectral reports for determining stereoisomers



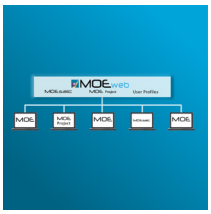
Enhanced Protein Patch Analyzer

- Visualize hydrophobic and charged protein surface to study aggregation prone regions
- Manage and analyze protein patches through an enhanced workflow oriented interface
- Calculate descriptors for quantitative property prediction



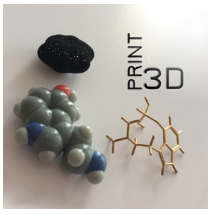
Integrated Antibody Project Database and Antibody Homology Modeler

- Automatically align and superpose antibody structures using the MOE Project protocol
- Generate and search advanced antibody queries with the Project Search application
- Build full length Ig structures including bispecifics with the Antibody Homology Modeler



Small Footprint MOE to Facilitate Large Scale Deployments

- Use MOE/web to offload MOE Project databases and reduce disk space
- Streamline deployment of project data, MOEsaic, and external tools using web server
- Customize MOE for different end users using user profiles for themes, menus and functionality



Physical and Virtual Rendering of Structures

- Export molecules in VRML, X3D or STL format
- Print in 3D virtual proteins and molecules
- Visualize MOE generated structures on web pages and PowerPoint by embedding MOE scenes

To learn more about MOE, please visit: chemcomp.com

About MOE

MOE is a leading drug discovery software platform that integrates visualization, modeling and simulations, as well as methodology development, in one package. MOE scientific applications are used by biologists, medicinal chemists and computational chemists in pharmaceutical, biotechnology and academic research. MOE runs on Windows, Linux, Unix, and MAC OS X.

MAIN APPLICATION AREAS

- Structure-Based Design
- Fragment-Based Design
- Pharmacophore Discovery
- Medicinal Chemistry Applications
- Biologics Applications
- Protein and Antibody Modeling
- Molecular Modeling and Simulations
- Cheminformatics & QSAR

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