NEW IN MOE 2018.01

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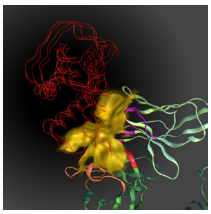
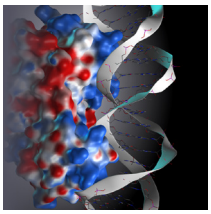


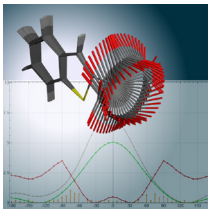
Epitope Mapping and Analysis

- Identify epitopes automatically during protein-protein docking
- Analyze and cluster Protein-Protein Interaction Fingerprints
- Visualize annotated epitope sequences and browse through associated protein poses



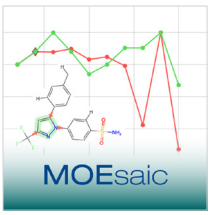
RNA/DNA Builder

- Build, edit, align and superpose DNA and RNA polynucleotide sequences
- Mutate and explore nucleotide conformations
- Introduce non-natural nucleobases for synthetic polynucleotide design



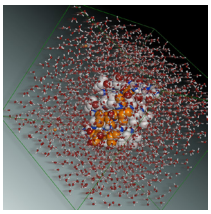
Torsion Scanning and Analysis

- Calculate bond torsions and plot energy curves using MM and QM
- Generate ligand conformers and identify optimal conformations and torsion angles
- Browse and compare QM torsion energy plots against Mogul statistics



MOEsaic – SAR and MMP Analysis

- Calculate and plot R-group contributions to molecular properties
- Search and filter matched molecular pair lists to find activity cliffs
- Improved plot capabilities



Unified Molecular Dynamics Interface to AMBER

- Launch AMBER for MD simulations using a streamlined interface
- Generate and convert parameters automatically through MOE
- Run MD on parallel clusters or GPU and analyze trajectories in MOE

MOE/web Enhancements

- Update client machines with new or customized SVL applications
- Build and deploy custom project and user profiles across client computers
- Run remote Scaffold Replacement searches against large fragment databases

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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