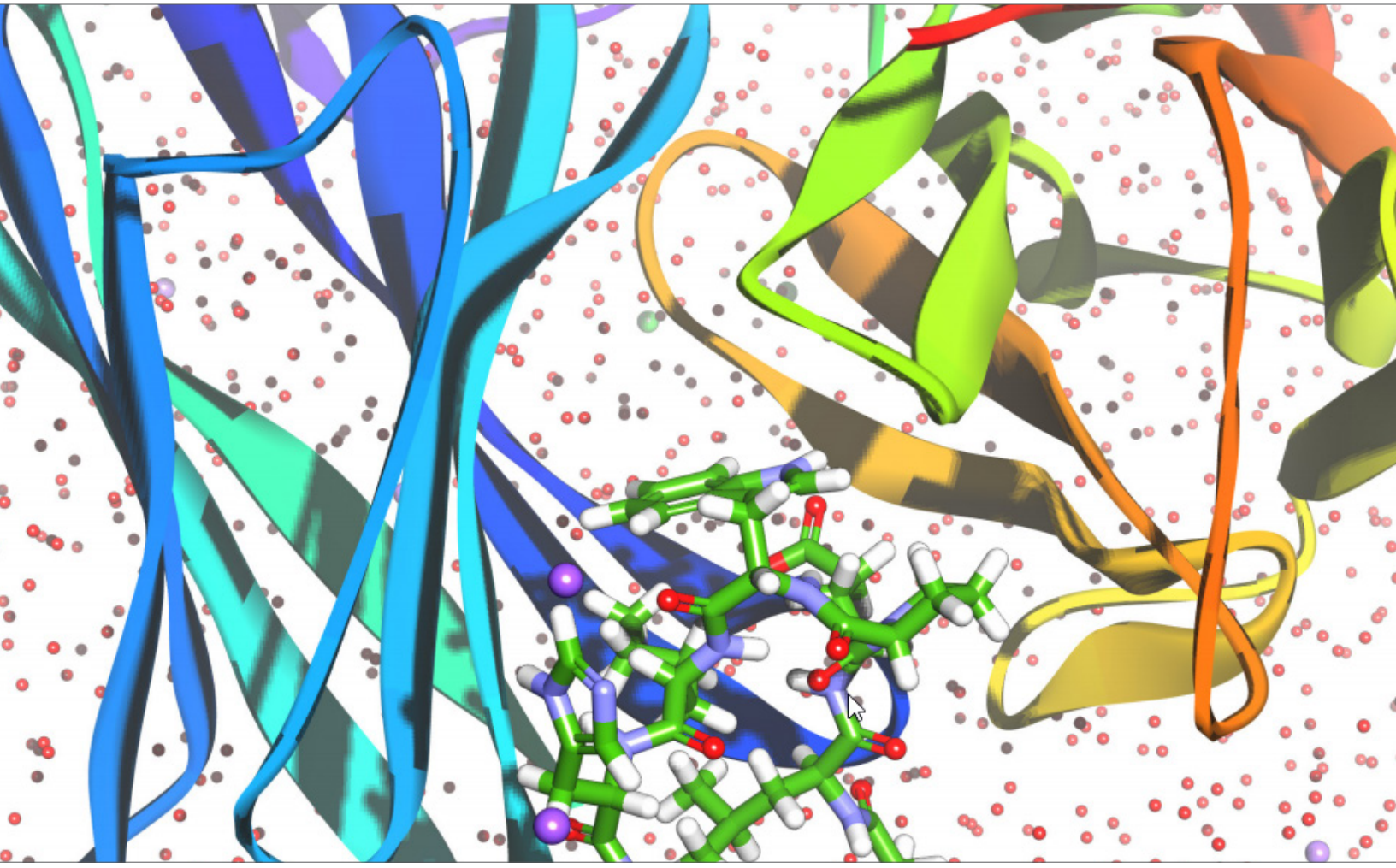
DASSAULT SYSTEMES

BIOVIA

MOLECULAR SIMULATIONS WITH BIOVIA DISCOVERY STUDIO®

DATASHEET



MATURE VALIDATED SCIENCE

Interactions between molecules such as proteins, ligands and ions are fundamental to all biomolecular processes. For example, simulating a small molecule as it binds into a protein, or an antibody binding to an antigen, can provide insight into the energetics that contribute to these processes. Simulations in BIOVIA Discovery Studio are founded on the **CHARMm** molecular mechanics and molecular dynamics forcefield engine, delivering over 30 years of peer-reviewed validated science. Integrated with both industry-standard macromolecule design and ligand design tools, BIOVIA Discovery Studio delivers a comprehensive, scalable portfolio of molecular simulation tools.

BIOVIA DISCOVERY STUDIO (DS) AND CHARMM

BIOVIA Discovery Studio delivers best-in-class forcefield simulations using the **CHARMM*** Molecular Mechanics simulation program

- **CHARMm**: Version c41b1
- DS supports a broad range of force fields, including CGenFF, charmm36, charmm27, charmm22, CHARMm, CHARMm-polarH, CFF, MMFF and more
- Automatic atom typing is built-in for small molecules, peptides, and macromolecules including enzymes, receptors, antibodies, DNA and RNA
- Full support of CHARMM patching mechanism and custom improper definition support
- Simulations methods include: Single point energy calculations with entropy estimation, Molecular Mechanics (MM) minimizations, Molecular Dynamics (MD)

QUANTUM MECHANICS (QM) SIMULATIONS

BIOVIA Discovery Studio includes full ***ab initio*** DFT-based QM, semi empirical and hybrid QM/MM methods:

- QM Density Functional Theory: **BIOVIA Discovery Studio DMol³** version 2017 R2
- QM semi-empirical simulations: **BIOVIA Discovery Studio VAMP** version 2017 R2

MULTI-PROCESSOR AND GRID ENGINE SUPPORT

- Simulations and Docking protocols include support for multiple processors and grid computers with fine-grained or coarsegrained options

MODEL PREPARATION AND REFINEMENT

BIOVIA Discovery Studio combines **CHARMM** with **MODELER** to yield a best in class suite of homology modeling tools

- Generate starting conformations for missing loops with **LOOPER** and rank using **CHARMm**
- Systematically search for co-compatible side-chain conformation using **Chi-Rotor**, based on **CHARMm**
- Quick and accurate protein ionization and residue pKs using a **CHARMm** Generalized-Born (GB) solvent model
- Fast explicit aqueous solvation method with optional counterions suitable for very large molecular systems

FORCEFIELD-BASED SIMULATIONS

Perform a range of simulations, including receptor-ligand complexes and protein-protein binding studies.

- **Simulate Receptor-Ligand complexes**
  - Perform pose optimization of multiple ligands in the context of a receptor with a static or flexible receptor
  - Perform ligand docking with the robust CHARMm based **CDOCKER** method
  - Score binding interactions with explicit solvent ***in situ*** MM-PBSA or MM-GBSA **CHARMm**-based methods
  - Compute single point energies or perform minimizations or receptor-ligand complexes using hybrid QM/MM
- **Simulate macromolecule structures**
  - Perform either implicit GB solvent- or explicit solvent-based Molecular Mechanics minimizations
  - Perform either implicit GB solvent- or explicit solvent-based MD simulations using **CHARMm**
  - Alternatively, launch a **NAMD†** calculation and perform production MD simulations with explicit waters
  - Accurately predict relative ligand binding energy using free energy perturbation (FEP)
  - Study the conformational detailed of ligand unbinding, or protein unfolding using Steered Molecular Dynamics (SMD)
  - **Add an implicit membrane to a protein structure to represent membrane bound models in simulations**
- **Molecular Dynamics analysis**
  - Select frames from across multiple DCD files and select subset of atoms for analysis
  - Plot temperature versus time, or energy versus time for easy analysis and save the energy data as CSV file
  - Calculate RMSD against a reference structure, or RMS fluctuations (RMSF) for all or selected frames

*** CHARMM information is available at http://www.charmm.org**

† NAMD is available from the University of Illinois at Urbana-Champaigniciliae

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Dassault Systèmes Corporate
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

BIOVIA Corporate Americas
BIOVIA
5005 Wateridge Vista Drive,
San Diego, CA
92121
USA

BIOVIA Corporate Europe
BIOVIA
334 Cambridge Science Park,
Cambridge CB4 0WN
England