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
- QM semi-empirical simulations: BIOVIA Discovery Studio

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

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