

Simulate biological molecules with a range of powerful components.

Apply for molecular mechanics and molecular dynamics simulations of proteins, protein-ligand complexes and small molecules.

Access all stand-alone CHARMM functionality with a custom component.

CHARMm Component Collection

The CHARMM[®] Component Collection offers a powerful set of components for simulating biological molecules based on the well validated CHARMM engine. This collection of components extends standard capabilities of Pipeline Pilot[™] to include stable and accurate molecular mechanics and molecular dynamics simulation of proteins, nucleic acids, small molecules, and protein-ligand complexes.

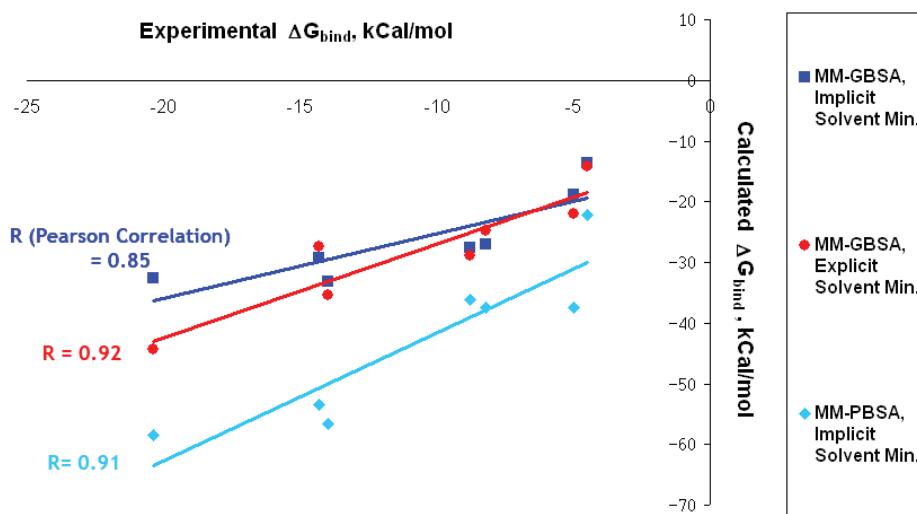
With these enhancements, you can create customized simulation workflows that incorporate different methods:

- Assign forcefield types and parameters
- Score docked ligands using the Molecular Mechanics-Poisson Boltzmann with Surface Area (MM-PBSA) or Molecular Mechanics-Generalized Born with Surface Area (MM-GBSA) method
- Dock ligands using the CDOCKER method
- Run customized scripts created with the CHARMM scripting language
- Perform molecular mechanics and molecular dynamics on proteins or protein-ligand complexes using a variety of forcefields, methods and solvent models

CHARMm Component Collection Applications and Workflows

The following applications and workflows, critical for a computational drug discovery research environment, are all possible with the CHARMM Component Collection:

- Perform physics-based scoring using CHARMM for much more accurate rank ordering of vHTS results
- Completely automated ligand preparation and virtual screening in a single protocol
- Create sophisticated CHARMM protocols without knowledge of the complex CHARMM scripting language
- Publish your protocols (via email) to all non-expert users in your organization
- Point any compound library into existing protocols, or replace one component with another, for true "Plug and Play" capabilities



Physics-based scoring of biotin analogs (docked to avidin) using different solvation models.

Included Components

Assign Forcefield Types Most of the forcefields supported by CHARMM are available: CHARMM, CHARMM-polarH, cff, charmm22, charmm and charmm27

Explicit Solvation Spherical boundary with harmonic restraint or periodic boundary conditions (latter supports cubic, orthorhombic and truncated octahedron cell shapes)

CDOCKER CDOCKER is a CHARMM-based MD simulation scheme for docking ligands in a receptor binding site. Random ligand orientations generated from a high-temperature MD are first translated into the binding site. The binding poses are searched using random rigid-body rotations, followed by simulated annealing with a grid potential. A final minimization with full forcefield potential is used to refine the ligand poses.

Binding Energy Binding free energies between a ligand and a receptor can be calculated with the MM-PBSA or MM-GBSA method. Several GB solvation models are available: Generalized Born approximation, Generalized Born with molecular volume (GBMV), and Generalized Born with simple switching (GBSW)

Standard CHARMM Tasks Individual components are available for energy calculation, minimization, heating, equilibration, production, and optimizing hydrogens (HBUILD)

Run Any CHARMM Script File Users who are experts of the CHARMM scripting language can stream any CHARMM script using a customized component

Manipulators Components are available for removing specific chains, waters and hetero-atoms for the molecular system. You can calculate the geometric center of molecule or a chain based on a select selection.

Prerequisites

- Discovery Studio® 1.7 CHARMM
- Pipeline Pilot Server 6.0 (Windows or Linux)
- Pipeline Pilot Professional Client 6.0 license with Chemistry Collection
- Integration collection is strongly recommended
- DS Visualizer Pro is strongly recommended

