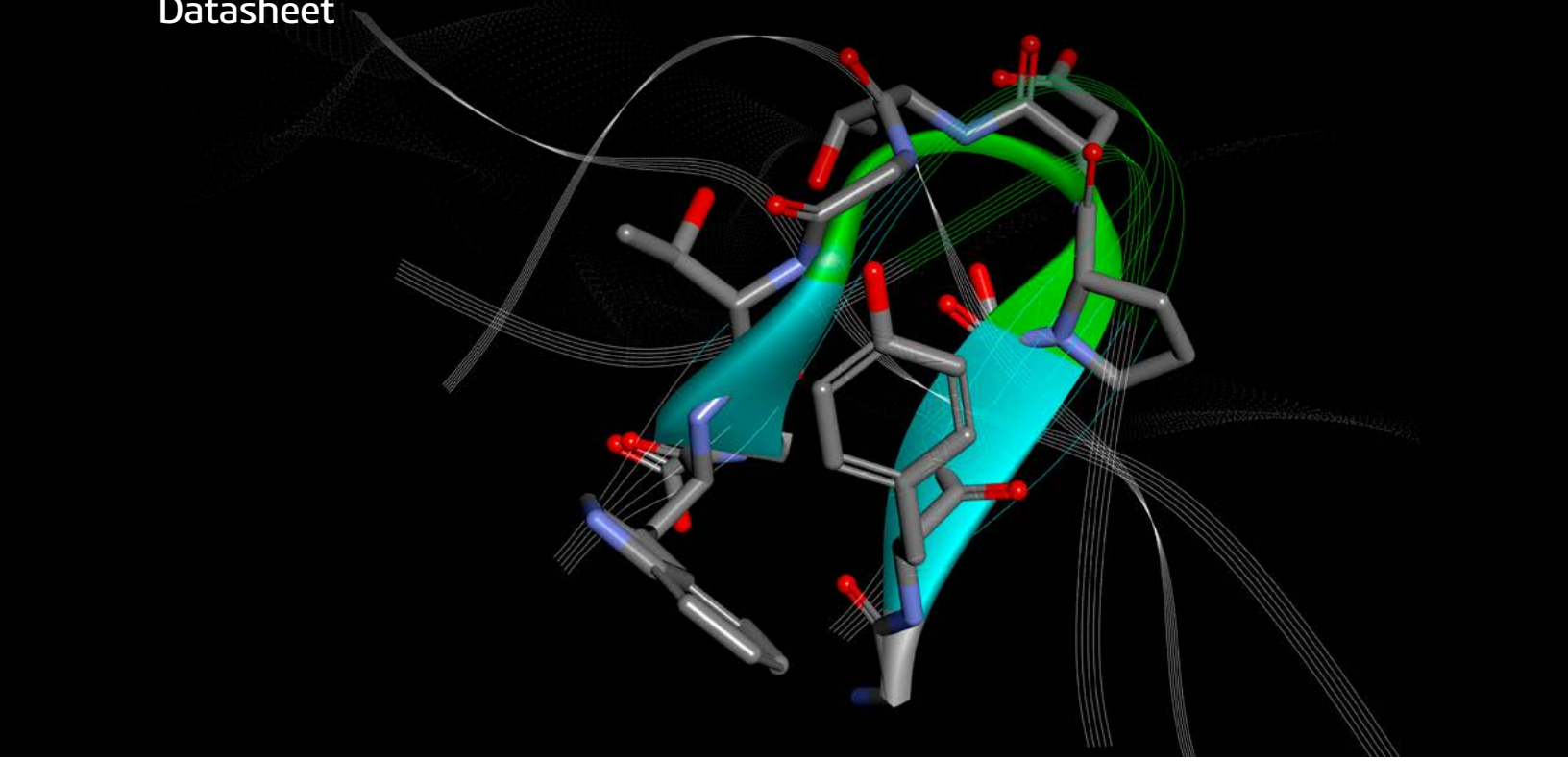
BIOVIA DISCOVERY STUDIO® 2023 SP1
COMPREHENSIVE MODELING AND SIMULATIONS FOR LIFE SCIENCES

Datasheet



DELIVERING NEW SCIENCE

Molecular simulations are essential to modeling and understanding complex biomolecular systems. The latest release of BIOVIA's predictive science application, Discovery Studio®, includes Gaussian accelerated Molecular Dynamics to enhance simulations. Built on BIOVIA Pipeline Pilot™, Discovery Studio® is uniquely positioned as the most comprehensive, collaborative modeling and simulation application for Life Sciences discovery research.

DISCOVERY STUDIO 2023 SP1

Part of the 2023 BIOVIA product release series, Discovery Studio 2023 SP1 continues to deliver scientific developments in the areas of biotherapeutics, simulations, and small molecule research.

ENHANCED SCIENCE

New! Machine Learning humanization model.

- The **Predict Humanizing Mutations** protocol now contains a new published machine learning method[1] to better distinguish between human and murine sequences, using classifiers built on a large-scale antibody sequence database.

Enhanced! Protein modeling.

- The **Predict Humanizing Mutations** protocol has been improved:
  - Uses a larger new residue frequency data set.
  - Humanized sequences now display a 'humanness' score and the identity/similarity to the query sequence.
  - Easier identification of the positions of VL/VH interface and Vernier residues.
  - Chain breaks have been added to the sequences in the Residue Substitutions alignment to match the Query sequence.
- Protein-protein docking and analysis protocols have enhanced performance; 10-30% faster depending on settings, and support for larger systems.
- The Antibody Database is updated with 6711 antibody structures from the PDB database release of July 2022.
- Several protein modeling protocols, **Prepare Protein, Calculate Protein Ionization and Residue pK, Calculate Mutation Energy (Binding), Calculate Mutation Energy (Stability)**, and **Calculate Protein Formulation Properties** now support the charmm36 forcefield.

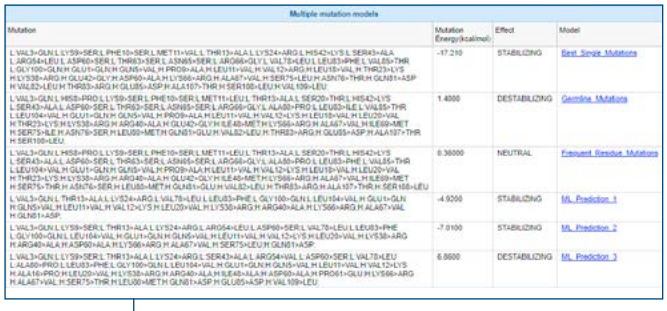


Figure 1. Multiple humanized mutation models generated by the Predict Humanizing Mutations protocol.

New! Gaussian accelerated Molecular Dynamics[2] (GaMD) for simultaneous unconstrained enhanced sampling and free energy calculations.

- A new protocol, **GaMD Equilibration**, configures and runs a Gaussian accelerated Molecular Dynamics equilibration, automatically parametrizing the boost potentials needed.
- A new protocol, **GaMD Production**, allows you to run and restart Gaussian accelerated Molecular Dynamics simulations.

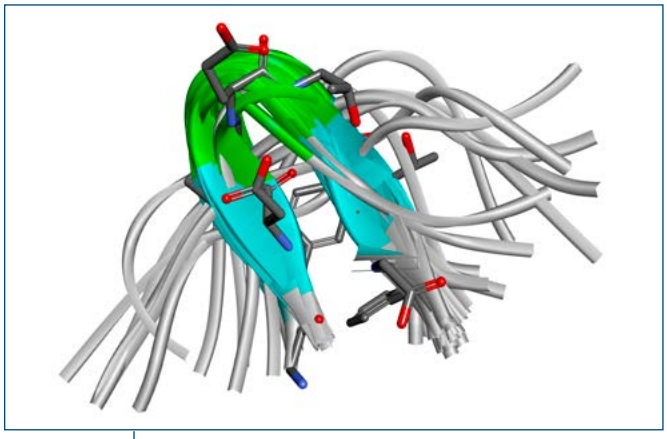


Figure 2. Clustered conformation of a GaMD simulation overlaid on a reference structure.

- A new protocol, **Estimate Free Energy Landscape**, estimates a free energy landscape from a set of molecular dynamics trajectories; it also allows for statistical reweighting of GaMD simulations.
- A new protocol, **Measure Trajectory Features**, measures time-series features (such as SASA, RMSD, dihedrals) from molecular dynamics trajectories for further analysis.
- A new protocol, **Cluster Conformations**, generates conformational states from simulation trajectories based on features such as SASA, RMSD, dihedrals, intermolecular or intramolecular residue contacts and distances.
- A larger chemical space can now be typed with the **Assign Forcefield** and **Type Ligands with MATCH (Prototype)** protocols, with options for assigning charges through a new ML model trained on ESP-fit QM data, and torsion parameters generated by fitting to QM data.

Enhanced! Free energy simulations.

- The **MSLD Bias Optimization and Production** protocol is updated to use the Basic Lambda Dynamics Engine (BLaDE[3]), giving a 3x improvement in performance.

New! PharmaDB protocols.

- A new protocol, **PharmaDB Filter**, filters the PharmaDB by properties based on the ligand (molecular weight, HET codes, etc.), binding site (for example, percentage of polar sites for example), or RCSB database (for example, publication date).
- A new protocol, **PharmaDB Profiler**, maps a set of ligands against the filtered pharmacophores from the PharmaDB Filter protocol and supports scalability by using parallelization based on pharmacophores.

Enhanced! Various pharmacophore modeling enhancements.

- The PharmaDB is updated based on the scPDB release 2022[4], and now contains over 37,000 entries.
- The **Ligand Profiler** protocol now adds shape similarity properties to the output ligands.

Enhanced! Small molecules protocols.

- The **Filter by SMARTS** protocol has a new option to filter ligands by PAINS (Pan Assay Interference Compounds) substructures.
- The **Dock Ligands (GOLD)** protocol performance is improved by reducing the docking logs.

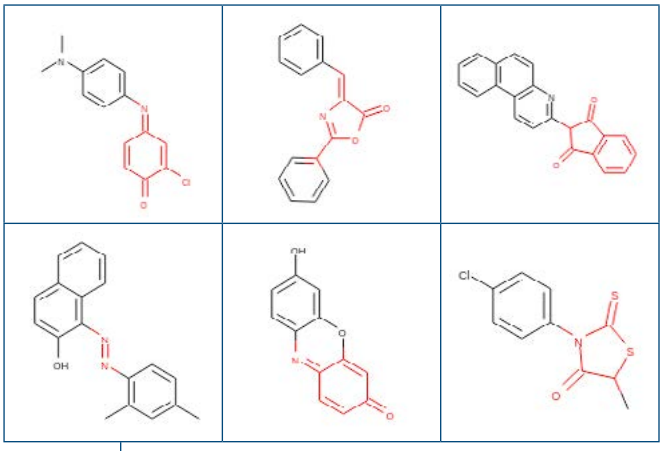


Figure 4. PAIN substructures shown colored in red.

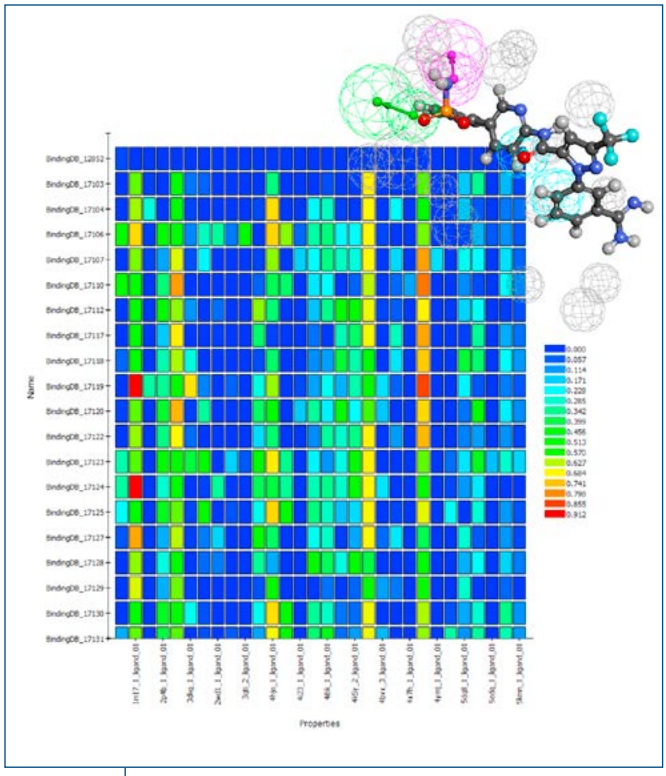


Figure 3. Heatmap simply displays ligand hits that map to filtered PharmaDB models.

Enhanced! Client functionality enhancements.

- The trajectory animation toolbar has been enhanced to give more control of playback with a slider bar and frame number identification.

PARTNER SCIENCE

- **CHARMm**: Incorporates the academic CHARMM version c47b1[5].
- **NAMD**: Distributed with both CPU and GPU editions, version 2.13.
- **MODELER**: Incorporates the academic MODELLER version 9.24[6].
- **BLAST+**: Incorporates BLAST+ version 2.11.0.
- **GOLD**: Supports GOLD 2023.1.

COMPATIBILITY

Discovery Studio 2023 SP1 is built on BIOVIA Pipeline Pilot 2023 SP1.

REFERENCES

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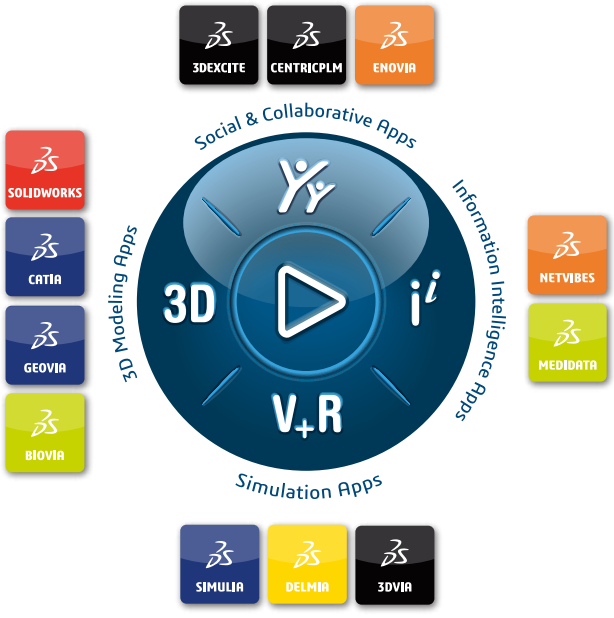
3. Hayes R. L., Buckner J., Brooks III C. L., *J. Chem. Theory Comp.*, **2021**, 17, 6799–6807
4. http://bioinfo-pharma.u-strasbg.fr/scPDB
5. Brooks B. R., Brooks III C. L., Mackerell A. D., Karplus M., *et al, J. Comp. Chem.*, **2009**, 30, 1545-1615.
6. Eswar N., Marti-Renom M. A. Webb B., Madhusudhan M. S., Eramian D., Shen M., Pieper U., Sali A., *Current Protocols in Bioinformatics*, John Wiley & Sons, Inc., **2006**, Supplement 15, 5.6.1-5.6.30.



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