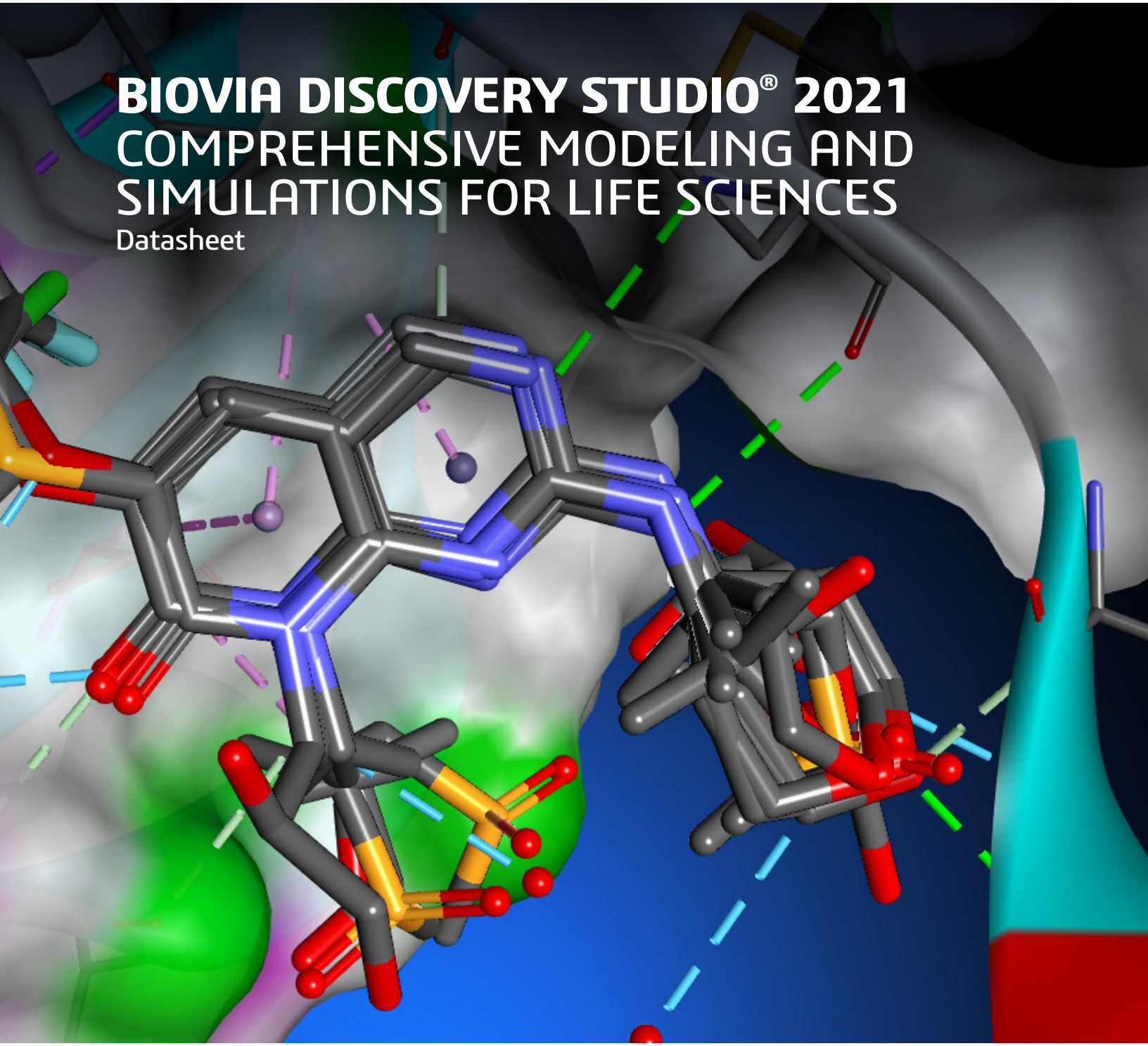
BIOVIA

3DEXPERIENCE®

BIOVIA DISCOVERY STUDIO® 2021
COMPREHENSIVE MODELING AND SIMULATIONS FOR LIFE SCIENCES

Datasheet



DASSAULT SYSTEMES

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®, improves the Multi-Site Lambda Dynamics workflow and accelerates science with more GPU-enabled platforms. 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 2021

Part of the 2021 BIOVIA product release series, Discovery Studio 2021 continues to deliver scientific developments in the areas of biotherapeutics, simulations and small molecule research.

NEW AND ENHANCED SCIENCE

New! Multi-Site Lambda Dynamics[1] workflow.

- A single protocol, **MSLD Bias Optimization and Production**, combines three protocols for a simplified and enhanced user-experience with CHARMm on GPUs.
- Calculate relative binding free energies for an entire combinatorial library in a single simulation, mimicking a competitive binding assay.
- Large scale[2] validation establishes the accuracy of the science to explore large congeneric chemistry space in early lead optimization.
- Up to 20 times more efficient than FEP.

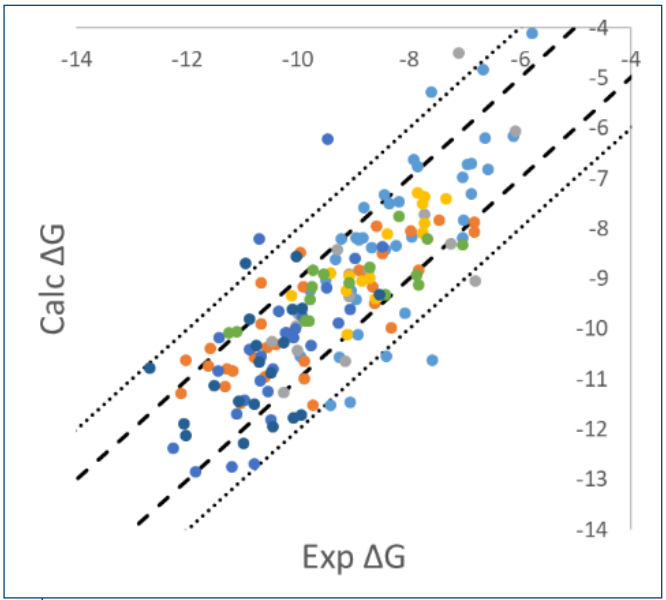


Figure 1: MSLD validation[2] with seven protein targets and 165 ligands, with average unassigned error (AUE) = 0.76 kcal/mol.

New! Free Energy Perturbation with CHARMm-DOMDEC.

- A new **CHARMm Relative FEP Calculations** protocol allows FEP calculations of multiple systems on GPU (Linux).
- Forward and Reverse estimates of free energy.
- Custom lambda schedule with narrower windows near the end states to improve accuracy.

New and Enhanced! Atom typer and force field parameters.

- More accurate and consistent small molecule hierarchical atom typing scheme with CGenFF.
- Extended and improved force field bond and angle parameters, significantly expanding CGenFF chemical space.

Enhanced! Viscosity and Aggregation prediction for biologics.

- Calculate Protein Formulation Properties protocol automatically generates Charge Map[3] and Aggregation Scores[3] surfaces.

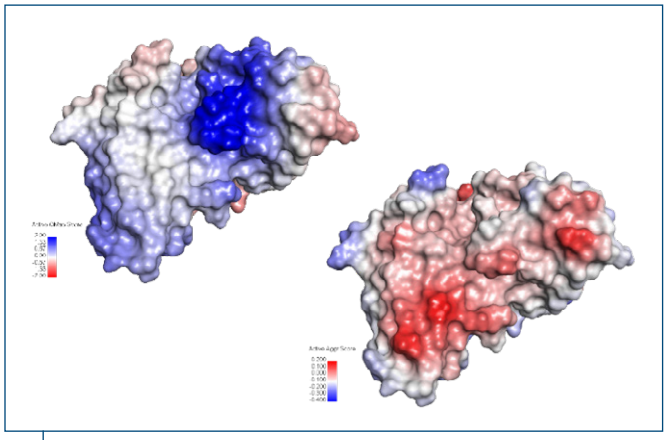


Figure 2: Charge QMap (left) and Aggregation Scores (right) surfaces on an antibody structure.

Enhanced! Various protein modeling enhancements.

- **RCSB Structure Search**: Rewritten to support new JSON queries, as previous search APIs were retired November 2020.
- **BLAST Search (NCBI Server)**: Improved performance and robustness.
- **Analyze Protein-Ligand Complexes**: Allows multiple proteins as input.
- **Predict Humanizing Mutations**: Improved performance and loads germline files more easily.
- **Retrieve Antibody Templates from Database**: New example protocol available to retrieve specified antibody templates from the database.
- BLAST PDB and Swiss-Prot databases automatically installed.

Enhanced! Various pharmacophore modeling enhancements.

- Non-bond pharmacophore features supported in the ligand-based pharmacophore protocols, and the Edit and Cluster Features tool panel.
- PharmaDB scPDB[4] receptor-ligand targets updated with non-bond pharmacophore features.
- Full PharmaDB database now included in default installation; the disk space has reduced from ~10 GB to 0.27GB.

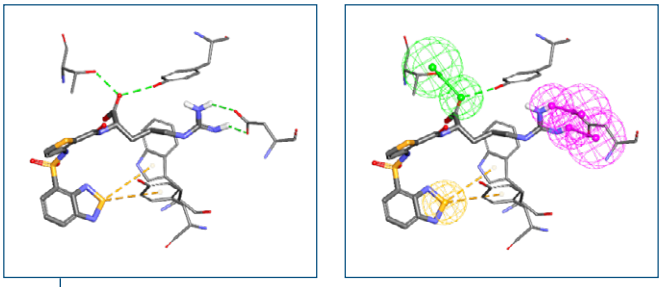


Figure 3: Interactions pharmacophores harmonize with non-bond feature perception.

New! GPU- enabled protocols to accelerate calculations.

- **Dock Proteins (ZDOCK)**: Up to 13x faster than CPU.
- **Dynamics (NAMD)** and **Solvate with Explicit Membrane**: 1 GPU is 7-10x faster than 8 CPUs.
- **MSLD Bias Optimization and Production**: Runs on both grid and non-grid servers.
- **CHARMm Relative FEP Calculations (GPU)**: FEP Calculations now supported with DOMDEC-GPU.

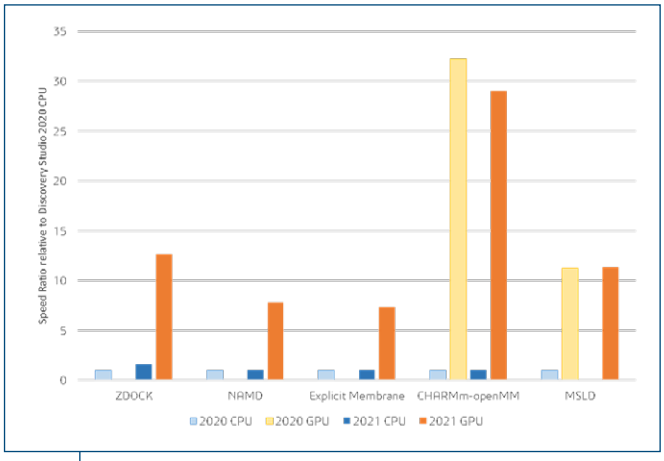


Figure 4: Performance improvements of 2021 GPU-enabled protocols relative to 2020 CPU versions.

PARTNER SCIENCE

- **CHARMm**: Incorporates the latest release of the academic CHARMM, version c44b2[5].
- **NAMD**: Distributed with both CPU and GPU editions, version 2.13.
- **MODELER**: Incorporates the latest release of the academic MODELLER, version 9.24[6].
- **BLAST+**: The BLAST+ version in Discovery Studio has been updated to version 2.10.1.
- **GOLD**: Supports GOLD 2020.

COMPATIBILITY

Discovery Studio 2021 is built on BIOVIA Pipeline Pilot 2021.

DATABASES

- The ANTIBODY database has been updated to include the latest antibody template structures from the PDB (based on PDB release July 2020).
- PDB and PDB_nr95 BLAST databases have been updated (based on PDB data July 2020).
- Swiss-Prot BLAST database has been updated (based on Uni-Prot from July 2020).
- The RCSB Structure Search protocol ligand database has been updated (July 2020, 32,522 entries).

REFERENCES

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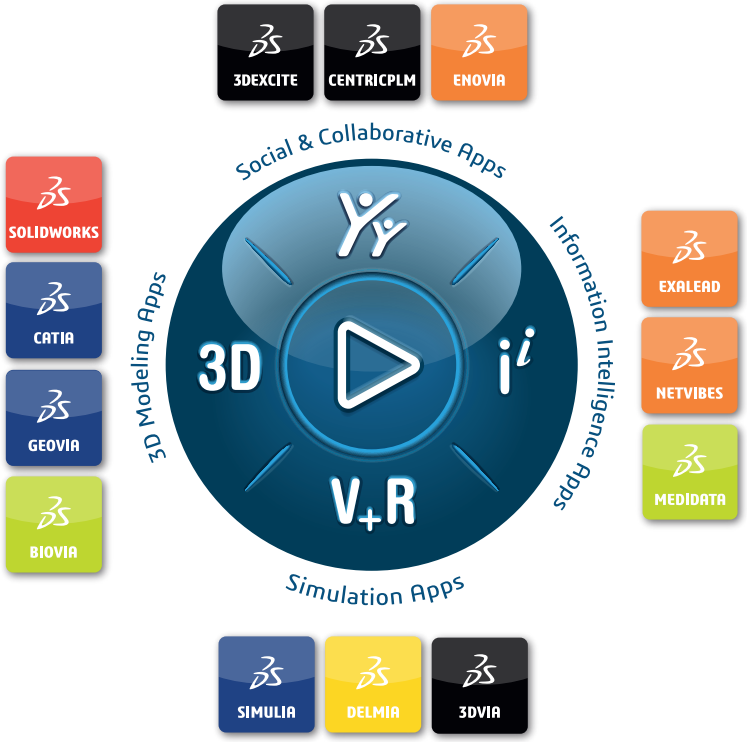
6. Eswar N., Marti-Renom M. A. Webb B., Madhusudhan M. S., Eramian D., Shen M., Pieper U., Sali A., *Current Protocols in Bioinformatics*, John Wiley & Sons, Inc., **2006**, Supplement 15, 5.6.1-5.6.30.



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