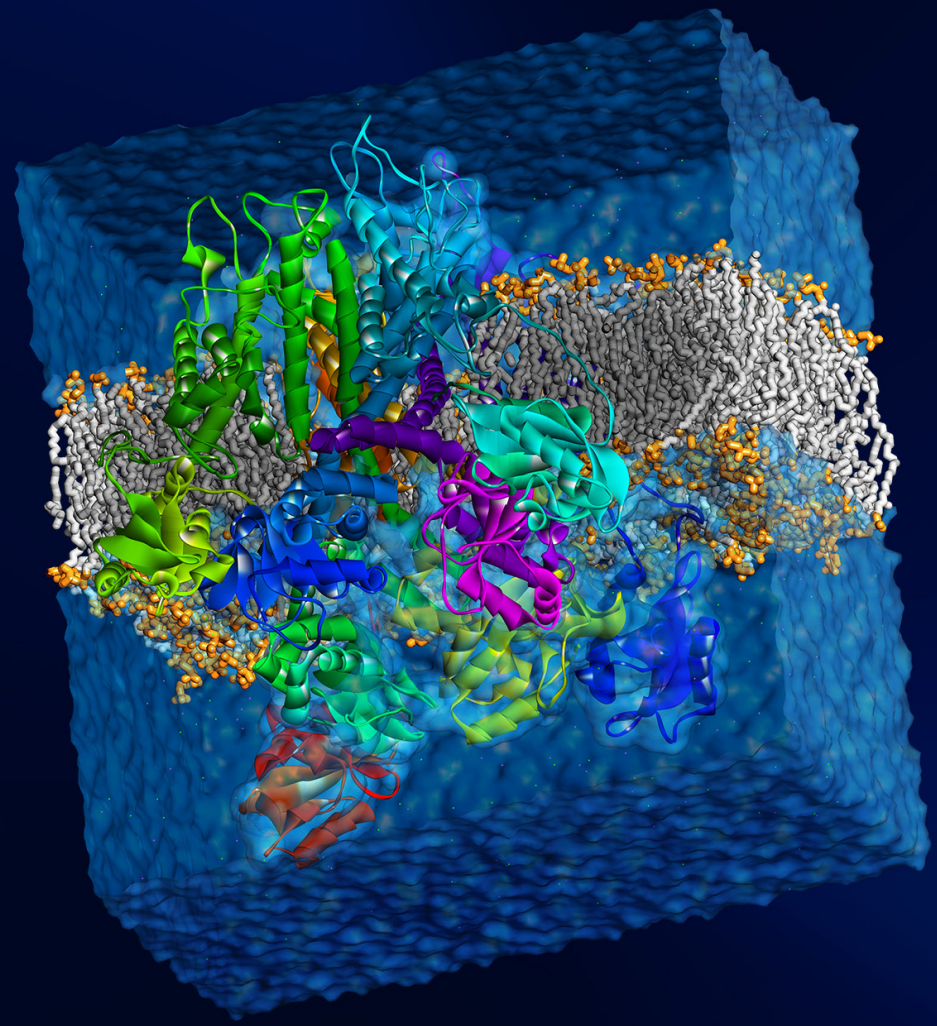
BIOVIA

3DEXPERIENCE®

BIOVIA DISCOVERY STUDIO® 2020
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®, introduces several new scientific features including the first commercial implementation of Multi-Site Lambda Dynamics. 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 2020

Part of the 2020 BIOVIA product release series, Discovery Studio 2020 delivers major new scientific developments in the areas of biotherapeutics, simulations and small molecule research.

NEW AND ENHANCED SCIENCE

New! Multi-Site Lambda Dynamics[1] via CHARMm-DOMDEC for both GPU and CPU, for exploring large congeneric chemistry space in early lead optimization.

- Calculate relative binding free energies for multiple ligands in a single simulation, mimicking a competitive binding assay.
- Up to 20 times more efficient than FEP.
- New user-friendly interface for easy set-up, running and analyzing results.

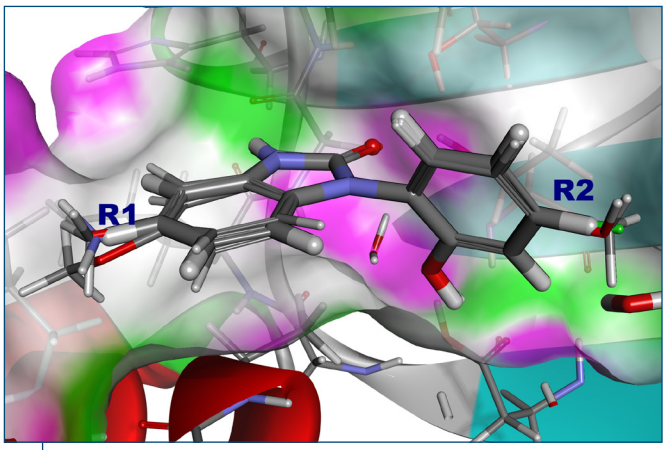


Figure 1: Combinatorial library defined with a core and two sites within the Hsp90 binding site for MSLD simulation.

New! Solubility and Viscosity prediction for biologics.

- **Calculate Protein Formulation Properties**: A new protocol to calculate the protein Developability Index (DI), antibody viscosity (in-licensed from MIT SCM[2] algorithm), and protein solubility.

New! Explicit membrane-based MD simulations.

- **Solvate with Explicit Membrane**: A new protocol that adds an explicit bilayer of lipids, water and counterions to a trans-membrane protein.
- Supports a number of prepared equilibrated homogenous membranes, as well as complex custom membranes.

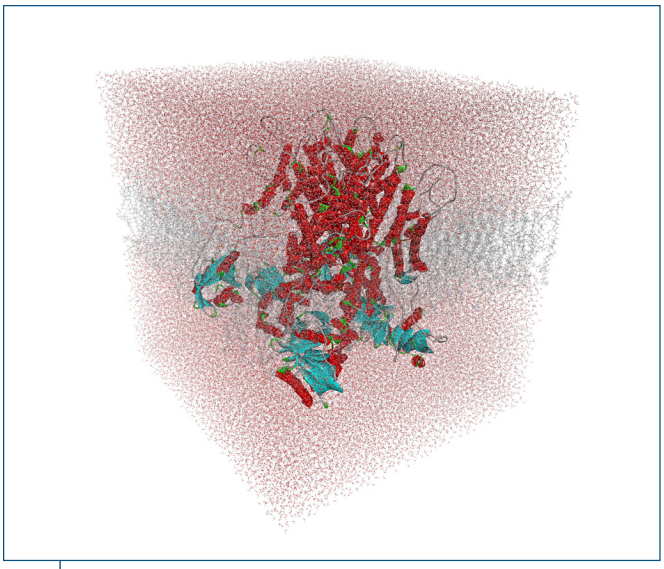


Figure 2: Solvated hERG ion channel within a POPC explicit membrane.

Enhanced! Various protein modeling and simulation enhancements.

- **Prepare Proteins**: Can now take multiple protein molecules as input and runs in parallel.
- **Predict Humanizing Mutations**: V and J genes can be specified for both the H and L chains.
- BLAST Search and PSI-BLAST Search protocols now support both NCBI nr and nr_v5 databases. They also support the UniRef90 database available from UniProt.
- Bond and forcefield information is now read from a CHARMm Structure PSF file and a paired CRD or PDB file to construct a fully typed molecule.

New! Pharmacophore generation methods.

- **Ensemble Pharmacophore Generation**: A new protocol to generate ensemble pharmacophores from large sets of active and inactive ligands, with detailed confusion matrices and ROC metrics for easy analysis.
- **Interaction Pharmacophore Generation**: A new protocol to generate and validate pharmacophores from ligand-receptor non-bond interactions.

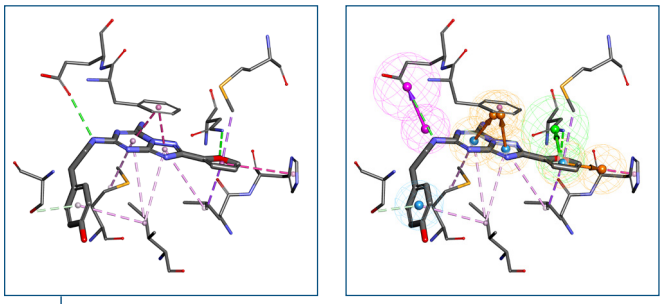


Figure 3: Interactions pharmacophores harmonize with non-bond feature perception.

- Optimized FitValue cut-offs in ensemble pharmacophores provide the best discrimination of active ligands from inactive ligands based on balanced accuracy.

Enhanced! Various pharmacophore modeling enhancements.

- **PharmaDB**: Updated to the latest version based on scPDB release 2017. It now contains over 250,000 pharmacophore models with 16,034 entries, 4782 proteins and 6326 ligands.
- **3D QSAR Pharmacophore Generation**: The ligand mappings for the validation set are now retained.
- **Ligand Profiler**: The protocol result tables are now sortable.

Enhanced!

- **Dock Ligands (GOLD)**: Now supports covalent ligand docking.

Enhanced! Various pharmacophore modeling enhancements.

- The 2D binding sites diagram can now also be used with nucleic acid-ligand complexes.
- The non-bond interactions tools now use a more sophisticated method to determine hydrophobic regions on ligands.
- The Discovery Client can now reconnect to interrupted jobs, for example due to network errors.

PARTNER SCIENCE

- **CHARMm**: Incorporates the latest release of the academic CHARMM, version c43b2[3].
- **NAMD**: Distributed with the CPU edition, version 2.12.
- **MODELER**: Incorporates the latest release of the academic MODELLER, version 9.22[4].
- **BLAST+**: The BLAST+ version in Discovery Studio has been updated to version 2.9.
- **GOLD**: Supports GOLD 2019 (version 5.7).

COMPATIBILITY

Discovery Studio 2020 is built on BIOVIA Pipeline Pilot 2020.

DATABASES

- The ANTIBODY database has been updated to include the latest antibody template structures from the PDB (based on PDB release July 2019).
- PDB and PDB_nr95 BLAST databases have been updated (based on PDB data July 2019).
- Swiss-Prot BLAST database has been updated based on Uni-Prot from August 2019.
- The RCSB Structure Search protocol database has been updated (August 2019, 29,815 entries).

REFERENCES

1. Hayes R. L., Armacost K. A., Vilseck J. Z., Brooks III C. L., *J Phys Chem B.*, **2017**, 121, 3626-3635.
2. Agrawal N. J., Helk B., Kumar S., Mody N., Sathish H. A., Samra H. S., Buck P. M., Li L., Trout B. *L., MAbs.*, **2016**; 8, 43-8.
3. Brooks B. R., Brooks III C. L., Mackerell A. D., Karplus M., *et al, J. Comp. Chem.*, **2009**, 30, 1545-1615.
4. 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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