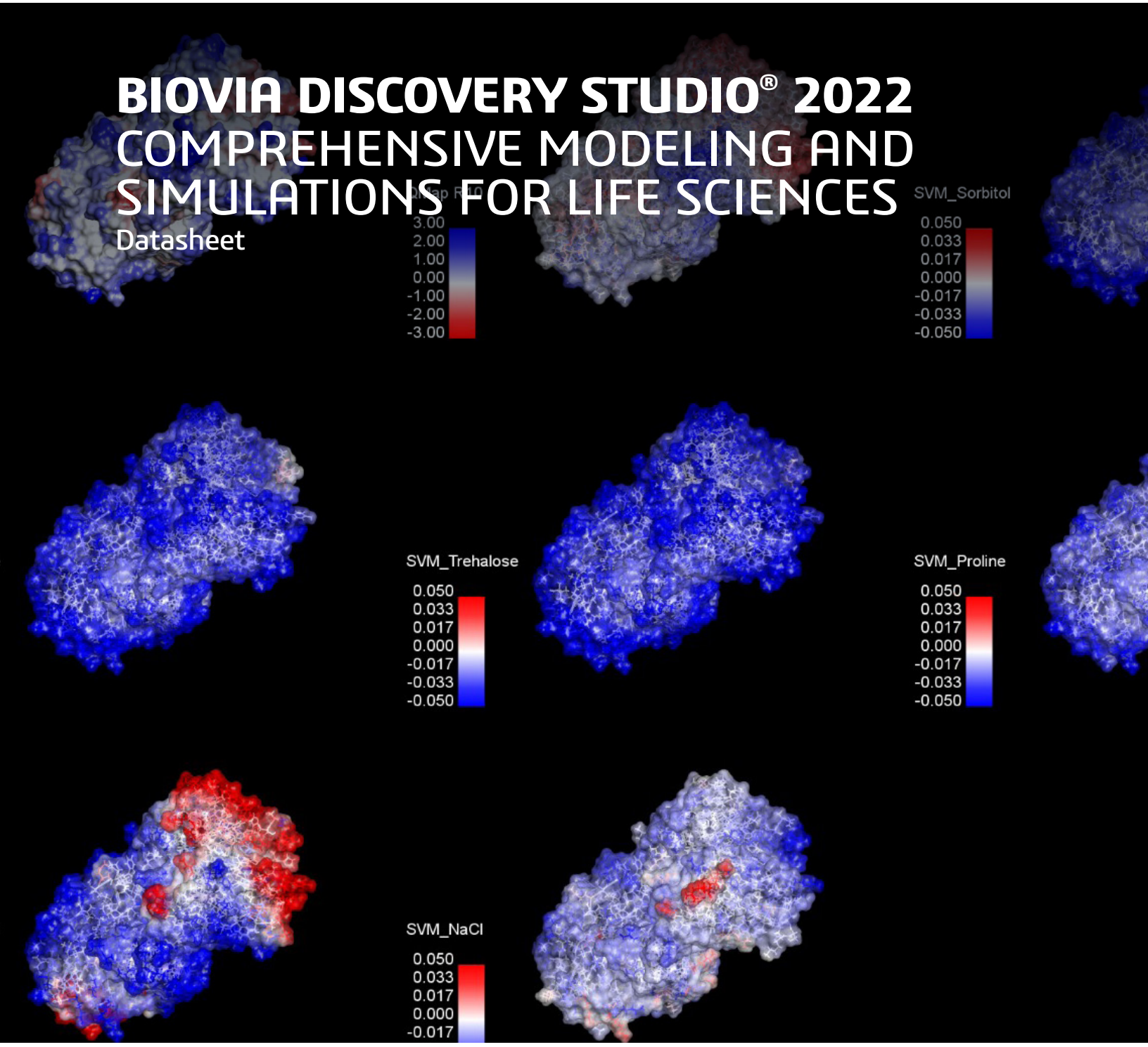
BIOVIA

3DEXPERIENCE®

BIOVIA DISCOVERY STUDIO® 2022
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®, includes antibody excipient interactions prediction to enhance biotherapeutics formulations. 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 2022

Part of the 2022 BIOVIA product release series, Discovery Studio 2022 continues to deliver scientific developments in the areas of biotherapeutics, simulations, and small molecule research.

NEW AND ENHANCED SCIENCE

New! Excipient Interactions Prediction.

- A new protocol, **Predict Excipient Interactions**, predicts the preferential interaction of common excipients with antibody surface residues for antibody formulation[1].
- Support Vector Machine and Elastic Net machine learning models generated from molecular dynamics simulations predict molecular interactions for 6 formulation excipients – sorbitol, sucrose, trehalose, proline, arginine·HCl and NaCl.
- Protein surfaces colored by Γ_{23} values (preferential interaction coefficients) show interactions of local excipient molecules compared to local water molecules.
- Used with existing aggregation and viscosity prediction tools, this enables formulation design earlier in the development process.

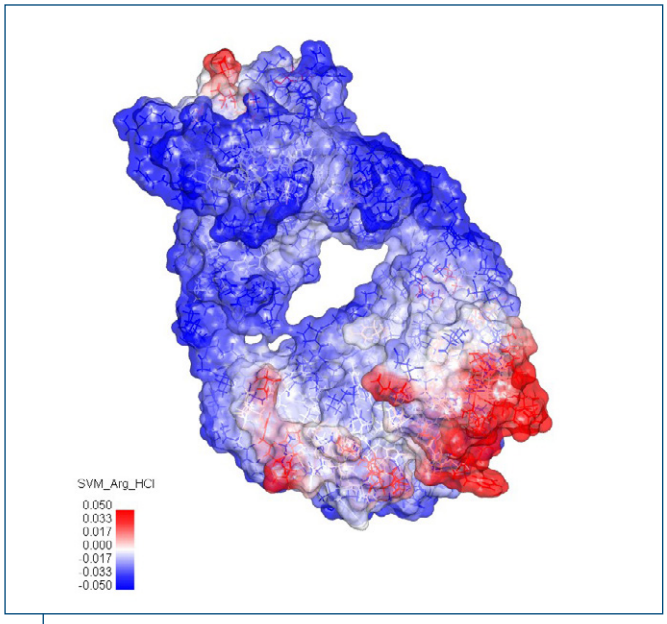


Figure 1: Positive values in red indicate higher Γ_{23} values, corresponding to more local excipient molecules, while negative values in blue correspond to more local water molecule interactions with the antibody.

New! Feature Generation Components.

- **Calculate Protein Features** and **Calculate Sequence Descriptors** components calculate structure- and sequence-based descriptors for machine learning.
- New scripting APIs to support standard and specialized feature calculations, e.g., a specific interatomic distance for a particular residue type.

Enhanced! Protein modeling.

- **Calculate Protein Formulation Properties** protocol now automatically creates aggregation sites and surfaces for analysis with the View Aggregation Sites tools.
- Positively and negatively charged areas in the Charge Map are available as Site groups.

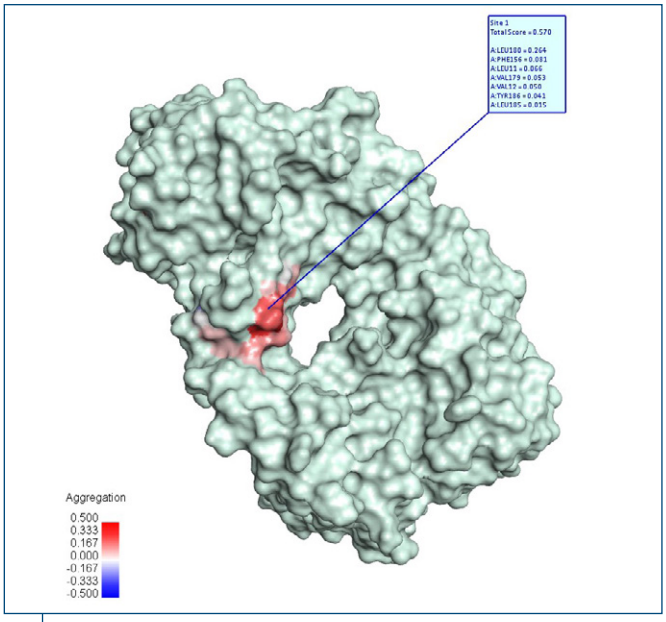


Figure 2: View the details of aggregation sites.

- Substructure search for ligand query added to the **RCSB Structure Search** protocol, as well all available match types from the RCSB server.

Enhanced! Simulation enhancements.

- Reduced the memory usage of large solvated systems when running simulations.
- **Assign Forcefield** protocol now works with RNA and DNA templates from custom RTF files.

Enhanced! Various pharmacophore modeling enhancements.

- Nucleic acids supported in the **Interaction Pharmacophore Generation** protocol.
- Pharmacophores from a receptor-ligand complex that have more than 50 non-bond interactions can be built with the **Interaction Pharmacophore Generation** protocol.

- **Ligand Profiler** protocol includes an option to maximize the number of features or maximize the pharmacophore fit when selecting the best fit.
- **Screen Library** protocol includes an option to report only the highest fitting pharmacophore for each molecule.

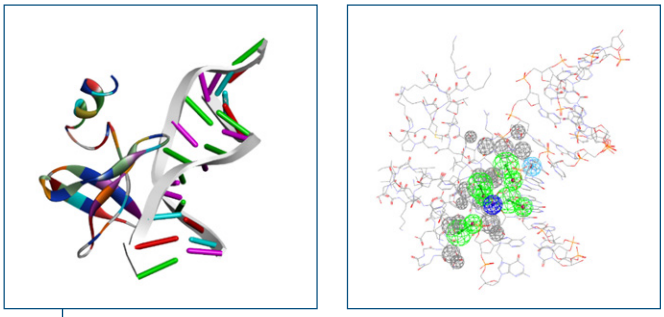


Figure 3: Nucleic acid interaction pharmacophore.

Enhanced! Client functionality enhancements.

- Access the AlphaFold Protein Structure Database from the Open URL dialog.
- Color proteins from the AlphaFold Protein Structure Database based on the per-residue confidence score.
- Calculate RMSD and similarity properties without alignment.
- Analyze reports with sortable tables without an active server.

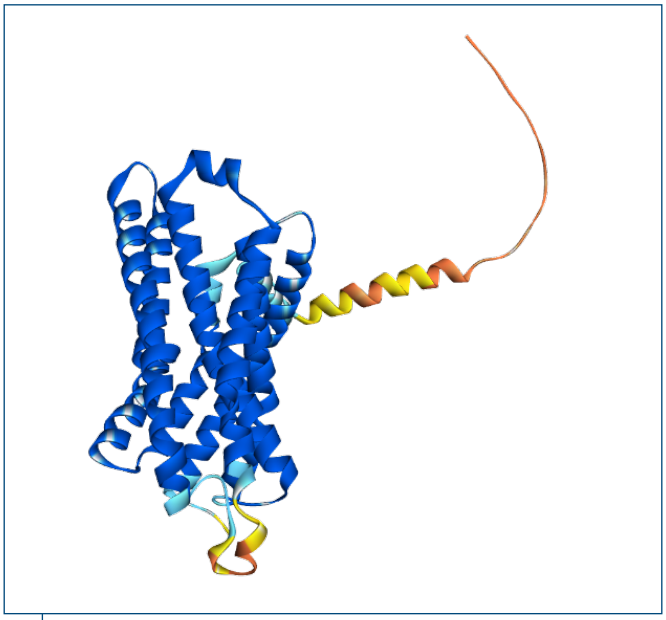


Figure 4: A protein from the AlphaFold Protein Structure Database colored by the per-residue confidence score.

PARTNER SCIENCE

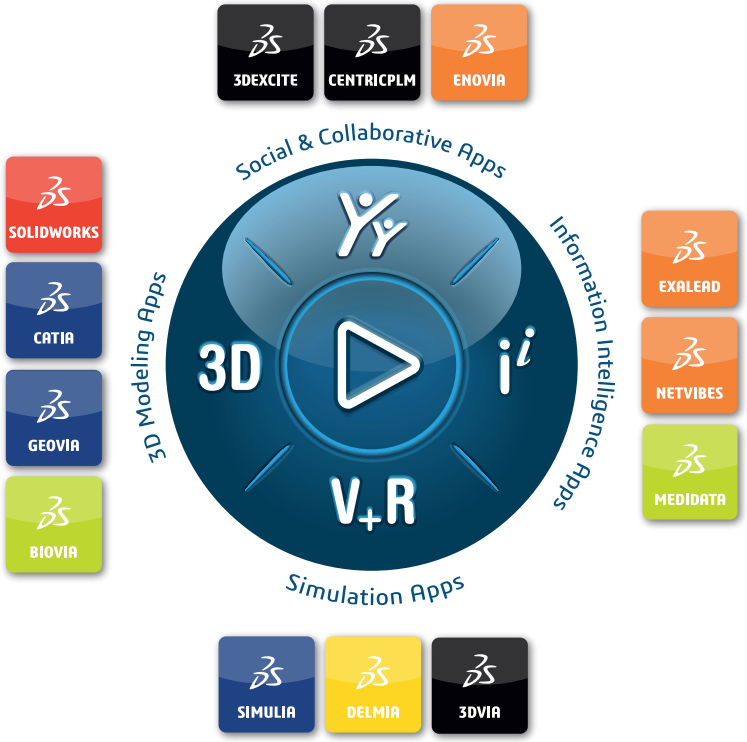
- **CHARMm**: Incorporates the academic release CHARMM, version c44b2[2].
- **NAMD**: Distributed with both CPU and GPU editions, version 2.13.
- **MODELER**: Incorporates the latest release of the academic MODELLER, version 9.24[3].
- **BLAST+**: The BLAST+ version 2.10.1.
- **GOLD**: Supports GOLD 2021.

COMPATIBILITY

Discovery Studio 2022 is built on BIOVIA Pipeline Pilot 2022.

REFERENCES

1. Cloutier T. K., Sudrik C., Mody N., Sathish H. A., Trout B. L., Molecular Pharmaceutics, **2020**, 17, 3589-3599.
2. Brooks B. R., Brooks III C. L., Mackerell A. D., Karplus M., *et al, J. Comp. Chem.*, **2009**, 30, 1545-1615.
3. 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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