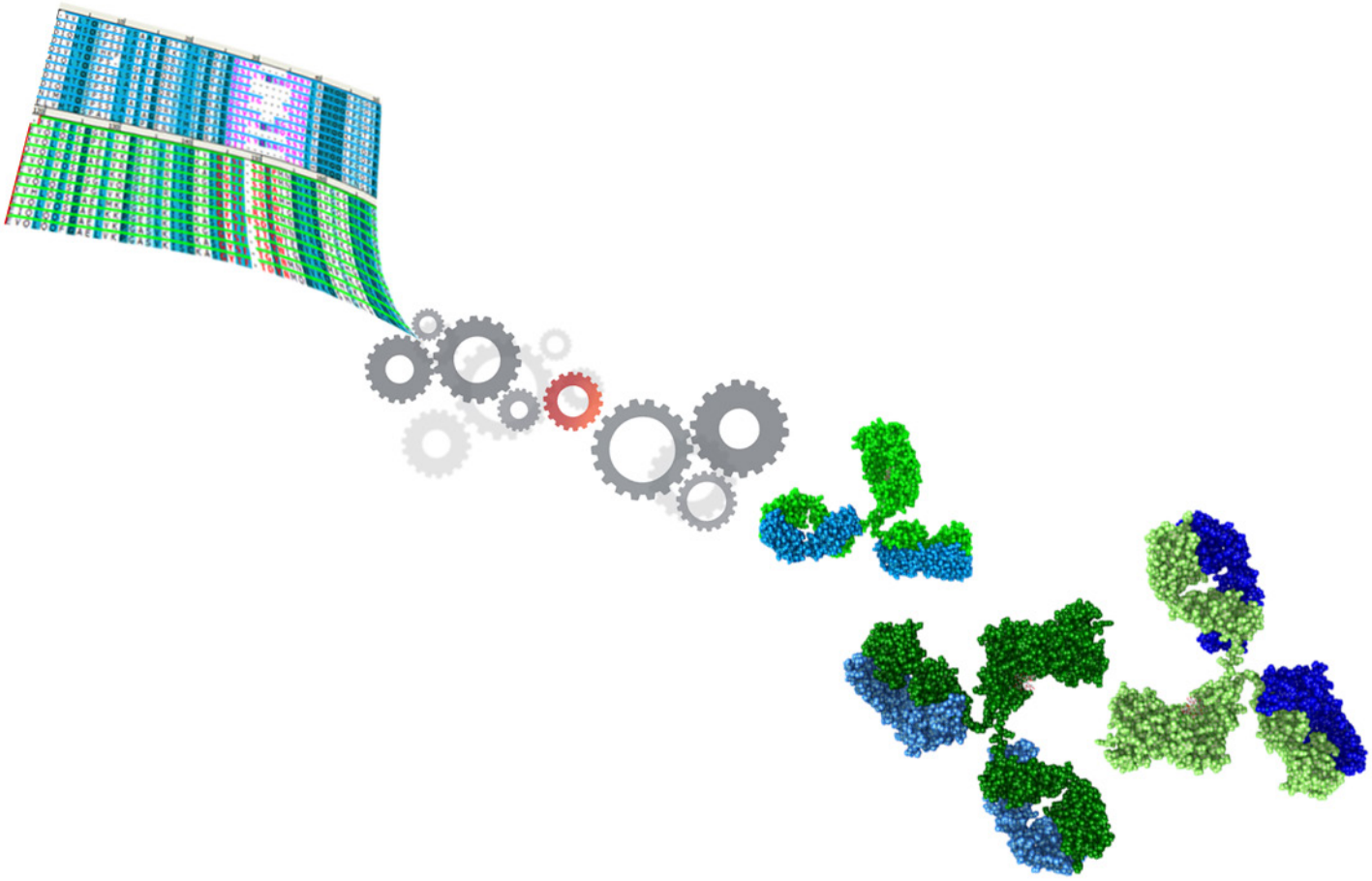
DASSAULT SYSTEMES

BIOVIA

BIOVIA DISCOVERY STUDIO® 4.5

COMPREHENSIVE MODELING AND SIMULATIONS FOR LIFE SCIENCES

Datasheet



AUTOMATED PROFILING OF ANTIBODIES

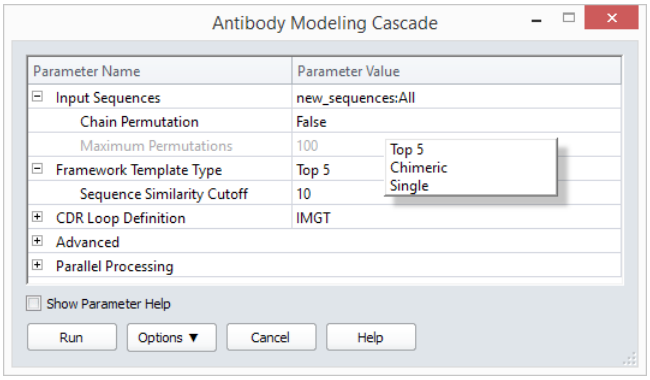
Drug discovery is a multi-objective optimization. Scientists have to optimize both biochemical potency and characteristics such as ADME and toxicity. The latest release of BIOVIA's predictive science application, Discovery Studio®, continues the evolution of new science in its market-leading biological simulation tools and enhancements to its small molecule design suite. Built on BIOVIA Foundation™, Discovery Studio® is uniquely positioned as the most comprehensive, collaborative modeling and simulation application for Life Sciences discovery research.

DISCOVERY STUDIO 4.5

Building on versions 4.0 & 4.1, the new release continues the theme of new science and performance improvements.

NEW AND ENHANCED SCIENCE

- **New! Antibody Modeling Cascade**: Developed and validated as part of the Antibody Modeling Assessment challenge[1,2], the protocol enables the easy and automatic generation of robust high quality 3D antibody Fab or Fv models



  - Three methods based on blind studies over three years
  - Supports combined or separate light and heavy chains and single chain antibody sequences
  - Automatic recognition of light/heavy chains
  - Use BIOVIA Pipeline Pilot and combine the results with the Post Translational Modification and Developability Index protocols to enable high throughput prediction of critical manufacturability profiles
- **Updated** 'Annotate Antibody Sequence' protocol
  - Ability to add Chothia Canonical Loop Type and identify Antibody Germline Sequences
- **New! Assign Forcefield Types (Prototype):** Uses BIOVIA Pipeline Pilot substructure matching to assign atom types for charmm36, charmm27 and charmm22 forcefields
  - Ability to import and assign custom atom types and parameters
  - Improved typing for many chemical functional groups, including carbohydrates, lipids and ligands
  - Handles modified amino acid residues such as glycosylated asparagine
- **Protein Ionization and Residue pK**: Enhanced protocol that calculates the protein ionization and residue pKs
  - New features to calculate mean atomic charges, average dipole moment, net charge, electrostatic contribution to the solvation energy as a function of pH
  - Useful in studying protein solubility and viscosity, protein-protein docking and enzyme activity

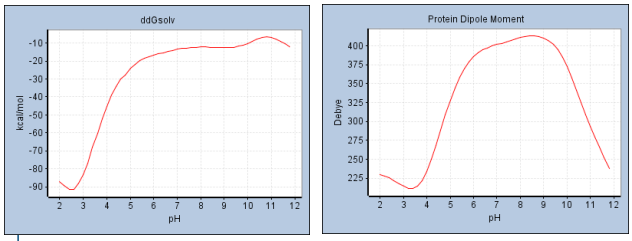


Figure 2: Charts of $\Delta\Delta G_{solv}$ and protein dipole moment as a function of pH.

VISUALIZATION

- **New! 3D WebGL component (Prototype)**: Our next generation web viewer is a Pipeline Pilot component which requires no client-side plug-ins, offering new opportunities to embed interactive 3D objects into a wide range of supported web browsers

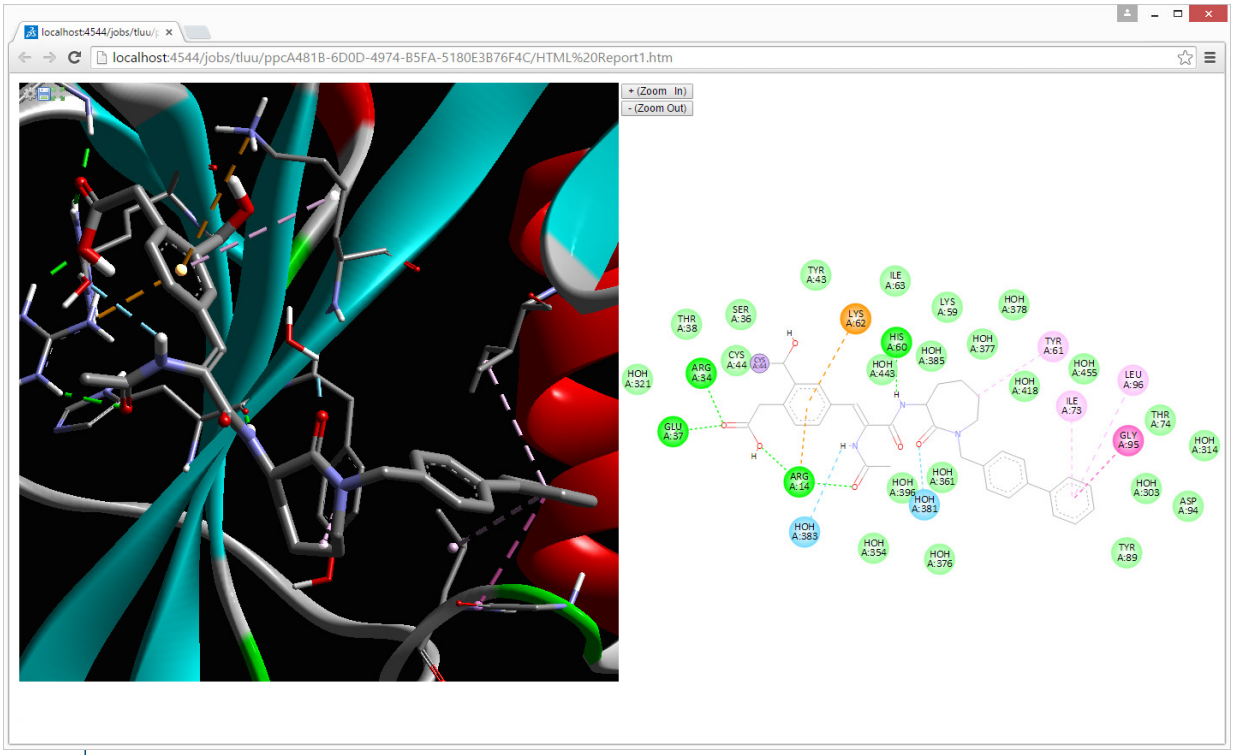


Figure 1: 3D web viewer interactively linked to a 2.5D view of receptor-ligand interactions.

- **2D Ligand Interaction Diagram**: Now includes full support for the extended library of non-bond interaction types
  - Available via scripting and as a Pipeline Pilot component

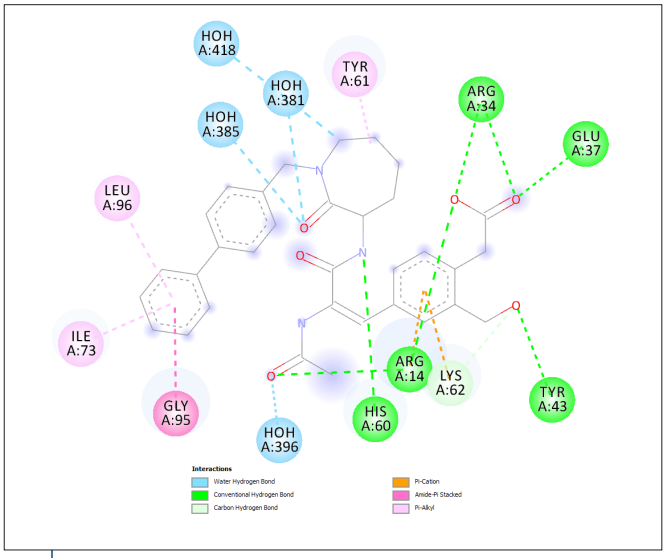


Figure 3: 2D receptor-ligand interactions of an inhibitor bound to the SH2 domain of (pp60)Src (1043.pdb).

PLATFORM

- **Compatibility**: Discovery Studio 4.5 is built on and supports the latest release of BIOVIA Foundation, version 9.5

PARTNER SCIENCE

- **CHARMm**: Incorporates the latest release of the academic CHARMM, version 39b1
- **GOLD Support**: Dock Ligands (GOLD) now includes support for the latest release of CCDC GOLD, version 5.3
- **NAMD**: Distributed with the CPU edition, version 2.9
- **MODELER**: Incorporates the latest release of the academic MODELLER, version 9.14[6]

DATABASES

- **BLAST** databases are updated for PDB_nr95, PDB, UniRef90, Swiss-Prot, and NR
- **ANTIBODY** has been updated to include the latest antibody template structures from the PDB

REFERENCES

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2. Almagro J.C., Teplyakov A., Luo J., Sweet R.W., Kodangattil S., Hernandez-Guzman F., Gilliland G.L., Second Antibody Modeling Assessment (AMA-II). *Proteins*, **2014**, 82, 1553
3. Brooks B. R., Brooks III C. L., Mackerell A. D., Karplus M., et al, *J. Comp. Chem.*, **2009**, 30, 1545-1615
4. GOLD is available from the Cambridge Crystallographic Data Centre: http://www.ccdc.cam.ac.uk/products/life_sciences/gold/ A valid GOLD license is required to run GOLD and GOLDscore
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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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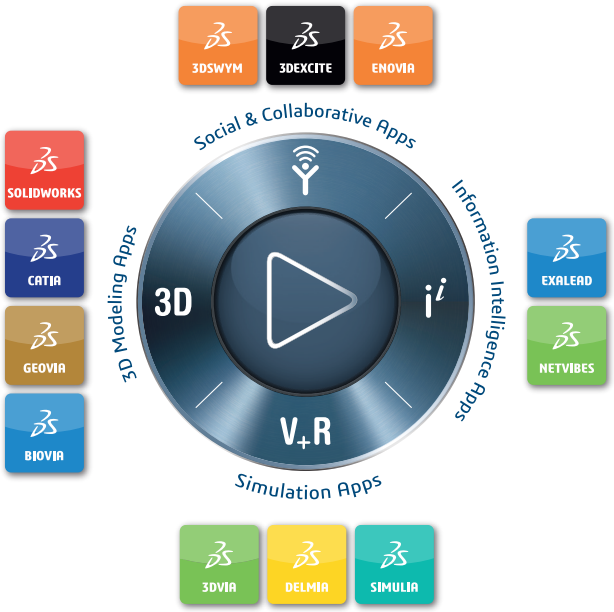

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Dassault Systèmes Corporate
Dassault Systèmes
175 Wyman Street
Waltham, Massachusetts
02451-1223
USA

BIOVIA Corporate Americas
BIOVIA
5005 Wateridge Vista Drive,
San Diego, CA
92121
USA

BIOVIA Corporate Europe
BIOVIA
334 Cambridge Science Park,
Cambridge CB4 0WN
England