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<sup>1,2</sup>, 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

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.](image1)

![Figure 2: Charts of ΔΔG<sub>solv</sub> and protein dipole moment as a function of pH.](image2)
**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.

**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.

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

**REFERENCES**
4. GOLD is available from the Cambridge Crystallographic Data Centre: [http://www.ccdc.cam.ac.uk/products/life_sciences/gold/](http://www.ccdc.cam.ac.uk/products/life_sciences/gold/). A valid GOLD license is required to run GOLD and GOLDscore.

**Our 3DEXPERIENCE® platform powers our brand applications, serving 12 industries, and provides a rich portfolio of industry solution experiences.**

Dassault Systèmes, the 3DEXPERIENCE® Company, provides business and people with virtual universes to imagine sustainable innovations. Its world-leading solutions transform the way products are designed, produced, and supported. Dassault Systèmes’ collaborative solutions foster social innovation, expanding possibilities for the virtual world to improve the real world. The group brings value to over 190,000 customers of all sizes in all industries in more than 140 countries. For more information, visit [www.3ds.com](http://www.3ds.com).