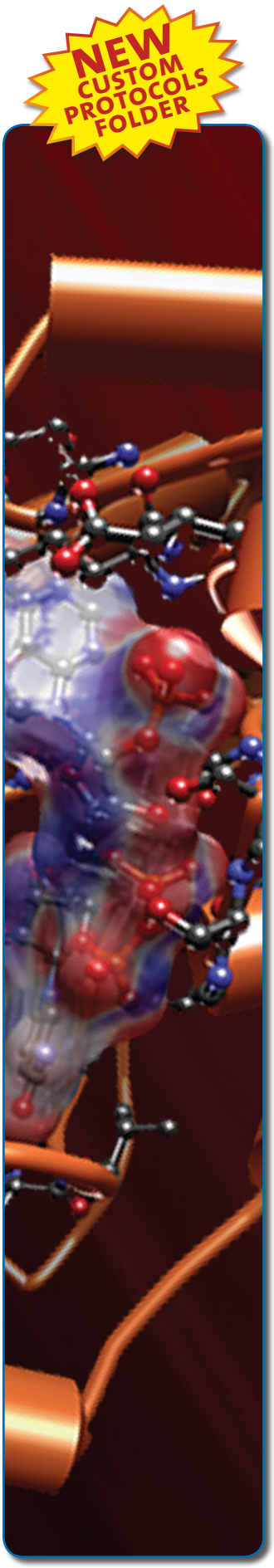
accelrys®



What's New in Discovery Studio 1.6

Discovery Studio® 1.6 includes several enhancements in the areas of visualization, protein modeling, simulations and analysis, structure-based design, and Pipeline Pilot integration.

Visualization

Discovery Studio Visualizer Pro Enhancements

- Save and re-use forcefield files.
- Gain further insight about your structure by calculating molecular properties.
- Identify similarities by superimposing structures based on molecular overlay.
- Explore several possible conformations and refine them with Dreiding minimization.
- Simplify your workflow by dragging and dropping files from the desktop or file explorer windows into Discovery Studio Visualizer Pro.*
- Maximize your working area by splitting, docking and dragging windows.*
- Enhance 3D structure appearance by applying materials enhancements (e.g. metallic, chalk, plastic, rubber).*
- Incorporate your own data by adding and editing attributes (e.g. values, text) to a molecule, atom, residue, etc. in the molecular data table.*
- View monitors (e.g., H-bonds, bumps) both on your structure and in a text window.*

* Enhancements also made in Discovery Studio Visualizer, the free commercial-grade visualizer that is an ideal solution for those who need to view, share and analyze protein and modeling data, but don't require access to the expert level tools in Discovery Studio.

Discovery Studio is a powerful drug discovery research environment that provides:

- all the software you'll need from project conception to lead optimization
- an easy-to-use interface that can be customized with your own preferred layout and default settings (e.g. define PDB download location)
- enhanced team collaboration through the ability to share and reuse protocols and exchange feedback within each other's results

Protein Modeling, Simulations, and Analysis

Updated Server Codes

- Perform automated homology model generation with MODELER 8.2.
- Access CHARMm 32b1 for energy minimization and molecular dynamics.

New Profile Alignment Protocol

- Improve sequence alignment results for low homology sequences by using a new profile alignment protocol in MODELER 8.2 that lets you include sequence profiles in the alignment.

X-ray Enhancements in Biopolymer

- Fit ligands into electron density maps with X-LIGAND technology.
- Build protein models into electron density maps with X-BUILD technology.

Pick the Platform You Prefer

Linux:

- Red Hat Enterprise Linux WS 3.0 with updates 4-7
- Red Hat Enterprise Linux WS 4.0 with updates 1-3
- GNOME desktop on Linux

Windows:

- Windows 2000 Professional SP4 Rollup 1
- Windows XP Professional SP1 or SP2
- Windows 2003 SP 1 (server support only)

Graphics Cards:

- Nvidia Quadro FX 1100
- Nvidia Quadro FX 1400
- Nvidia Quadro FX540
- ATI Fire Mobility GL graphics cards provided on IBM T42p Thinkpads

Structure-Based Design

New Small Molecule Docking Methods

- Launch jobs and analyze results with a new interface to the CHARMm-based docking refinement program CDOCKER.
- Set up and run GOLD, a genetic algorithm-based docking program from the Cambridge Crystallographic Data Centre (separate license for GOLD required).

General Structure-based Design Enhancements

- Perform rigid-body minimization after a LigandFit docking experiment.
- Specify interaction filters for docking jobs (with both LigandFit and GOLD docking).
- Inspect ligand poses with flexible receptor hydrogens (for GOLD results).
- Explore large binding sites by combinatorial fusion of site partitions.

Pipeline Pilot Integration

- Quickly access Discovery Studio protocols for protein modeling, receptor-ligand interactions, and simulation through either the Discovery Studio or Pipeline Pilot interface.
- Easily access protocols edited in Pipeline Pilot via the Discovery Studio "user" protocol folder.
- Use Discovery Studio to visualize and analyze results after running a protocol, and then export results in different file formats.
- Utilize centralized computational resources with new Linux cluster support.

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