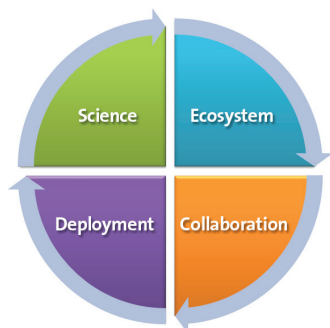


# WHAT'S NEW IN DISCOVERY STUDIO® 3.1

From project conception, through to candidate selection, Discovery Studio delivers a comprehensive portfolio of validated scientific technologies that address the modeling challenges faced by research scientists. Packaged into a single, easy-to-use client interface, Discovery Studio can be readily accessed from both Windows® and Linux environments. Furthermore, built on Accelrys' market leading Pipeline Pilot™ platform technology, Discovery Studio enables scientists to rapidly integrate third party applications, automate routine tasks and even deploy models out to research colleagues. Together, these provide a highly-effective and comprehensive modeling environment.

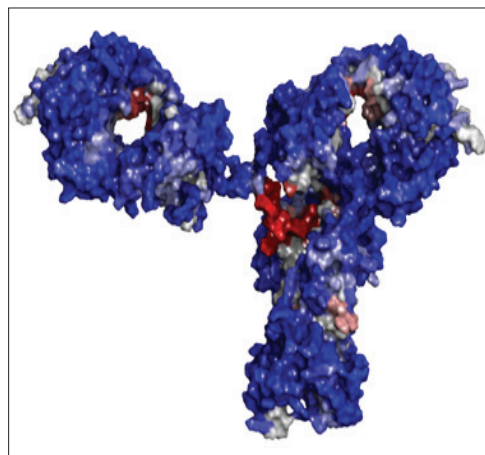


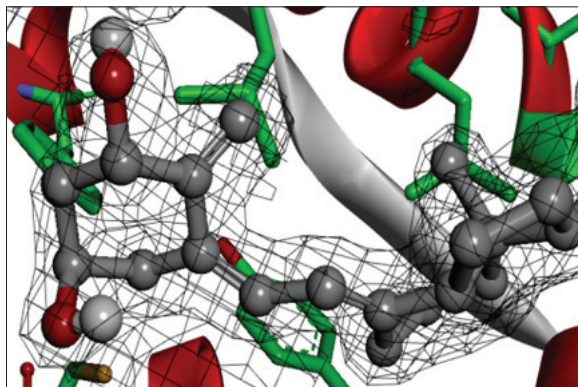
This release of Discovery Studio (DS) provides support for the latest release of Pipeline Pilot. It also includes a number of new features and enhancements:

- **Science:** New spatial aggregation propensity algorithm to predict sites of protein-protein aggregation in biological therapeutics
- **Ecosystem:** Updated support for GOLD (5.0.1) and NAMD (2.7)
- **Collaboration:** DS3.1 can now save 3D molecules directly to .html and .PPTx slides. Accordingly, our free 3D plug-in, DS ActiveX control, has been updated to support DS3.1
- **Deployment:** DS3.1 is fully compatible with the latest release of Pipeline Pilot 8.5 and exploits the latest enhancements to Cluster and Grid support.

## NEW AND UPDATED SCIENCE:

- **New! Spatial Aggregation Propensity algorithm:** Identify the size and location of regions on antibodies prone to aggregation, and then predict mutations leading to improved stability. Uses the experimentally validated spatial aggregation propensity algorithm licensed from Massachusetts Institute of Technology and developed by Professor Bernhard Trout, Ph.D. [Trout et al, 2010; Trout et al 2009, WO 2009/155518 A1]





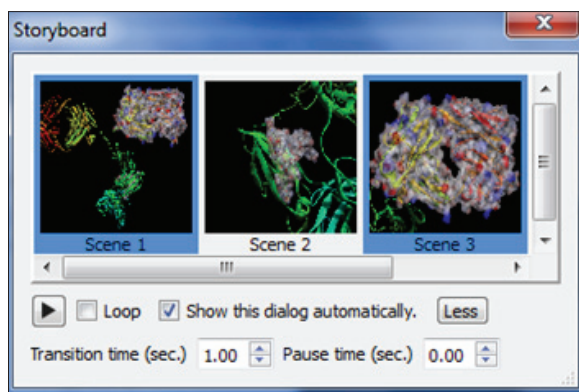
- **HT-X PIPE:**

Added functionality for complete structure determination of protein-ligand complexes with an automated pipeline for phasing by molecular replacement, ligand placement, structure refinement and solvent placement. An option for CHARMm ligand minimization prior to placement is also available.

### DS3.1: ENHANCED COLLABORATION

Sharing and communicating results is even easier in DS3.1. The Storyboard tool has been enhanced, and you can now save to PowerPoint and Html files directly.

- **Storyboard playback and timings:** Storyboards can now be played as a movie, with options for setting transition and pause times. You can also set the dialog to open automatically whenever a .DSV file containing a storyboard is opened.
- **Export as movie:** Storyboards can now be exported using the open, royalty-free, media file format .WebM ([www.webmproject.org](http://www.webmproject.org)).



- **Save as html:** Save 3D molecules directly into a single html file. Easily share or upload to websites and Microsoft™ SharePoint™
- **Save as PPT slide:** Simplify the process of creating presentations containing your 3D molecules by directly creating a Microsoft PowerPoint™ slide

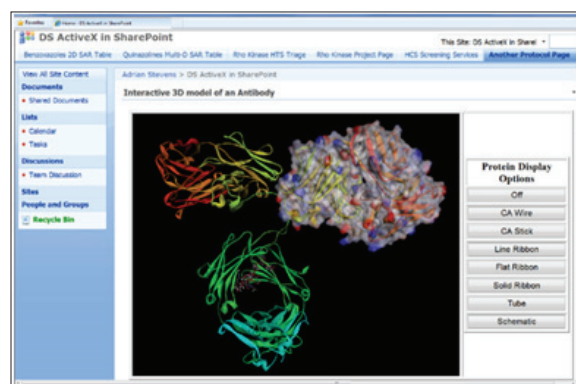
### DS3.1: SUPPORTS PIPELINE PILOT 8.5

- **Parallelization:** Improved handling of long running jobs on Cluster/Grid systems.
- **Support:** SUSE 11 64-bit OS.
- **Enhanced performance:** Improvements to job pooling and caching to both reduce latency and increase job request throughput.

### DS3.1 ACTIVEX CONTROL:

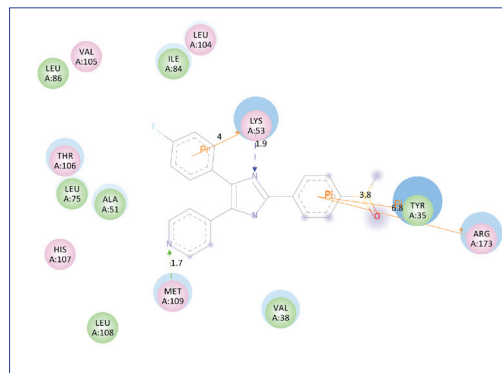
Our free 3D molecular web tool has been completely revised and updated. New features include:

- **Storyboard support:** Incorporates all of the scene transition, timing and auto-play features.
- **DSV file support:** Now fully supports the latest release of the Accelrys DSV file format.
- **Graphics support:** Supports the latest enhancements to depth blur, and also direct and ambient shading.

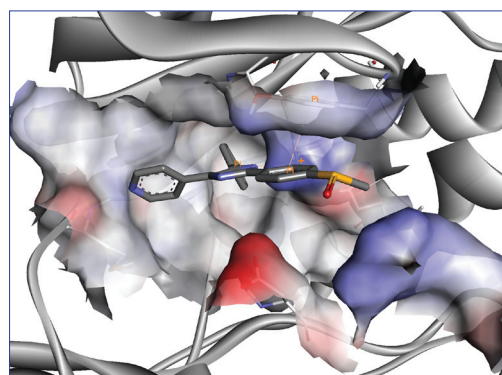


## OTHER NOTABLE ENHANCEMENTS:

- **CHARMm:** CHARMm [Karplus *et al* 2009; 1983] has been upgraded to the latest release version c35b5 (released in August, 2010).
- **NAMD:** Updated support to version 2.7 [Phillips *et al* 2005].
- **CCDC GOLD:** Updated support for v5.0.1 [Taylor *et al*, 2005; Jones *et al*, 1997].
- **Sequence:** Report residue propensity at a given multiple sequence alignment position.
- **Protein Docking:** Support to use ZRANK as a scoring function for poses generated by third party software.
- **2D Ligand Plot:** Improvements have been made to the default display style.
- **Pharmacophore:** Enhancements in active/inactive validation testing with pharmacophore generation tools.
- **Pharmacophore:** Improvements to use of databases and spreadsheets as input files for pharmacophore generation and screening protocols.
- **Improved support for databases as inputs:** Reduced size of intermediate files when a large database is used as input.
- **Modal/Amodal parameter window:** Improvements to simplify switching between floating and docked job parameter window.
- **Surfaces:** Default surface type has been changed to "Open".
- **Graphics hardware acceleration:** Updated system checking tools to test for supported graphics hardware and driver versions.



A 2D ligand plot demonstrating the new display enhancements



Example of an "open" surface on a protein active site

To learn more about Discovery Studio, go to:  
[accelrys.com/discovery-studio](http://accelrys.com/discovery-studio)

## REFERENCES:

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