Schrödinger Suite 2009 Update 2 – List of Major Improvements

The Schrödinger Suite 2009 Update 2 release includes a number of bug fixes and usability enhancements to all our products – below is a list of just the major improvements

Canvas 1.2.211

A new standalone graphical interface now accompanies the Canvas computing suite. The interface is a highly intuitive and responsive tool for cheminformatics project work, providing chemical structure storage, data analysis and visualization, and access to a wide range of scientific applications. Key features include:

- Runs on Linux and Windows
- Binary fingerprints
- Charting
- Chemical & property filtering
- Clustering (hierarchical, leader-follower, k-means)
- Cluster dendrograms
- Custom views
- Diverse compound selection with hole filling
- Heat maps
- High performance 2D chemical spreadsheet
- Input/output of standard file types
- Maximum common substructure
- Molecular property calculations
- Multiple linear regression
- Naïve Bayes classification
- Neural networks
- Partial least-squares regression
- Principal components analysis & regression
- Row partitions
- Self-organizing maps
- Similarity searching
- Statistics
- Substructure searching

Desmond 2.2.736

- Improvements to glue to better support visualization of complexes as indivisible units within the periodic system

Epik 2.0.211

- Fixes for a number of problems with misprotonation or deprotonation of cyclic amines (piperidine and imidazolidine) and anilines

Force Field OPLS_2005

- Improved equilibrium structures for nitroguanidines, N-arylimides, and 2-pyrimidyl-piperazines

Glide 5.5.211

- Improved performance when docking large numbers of ligands through use of many subjobs
- Fixed bug that was causing Glide to generate invalid files for analysis via the XP visualizer in some circumstances
- Fixed bug that was causing failure to dock ligands in mol2 format in some circumstances
- Added ability to perform post-docking minimization for SP rigid docking

Jaguar 7.6.211

- Now possible to use PBF solvation for TDDFT calculations

Job Control and Infrastructure

- Improved stability for massively distributed jobs, for example, on the Cloud
- License availability is checked prior to a job being submitted to a compute node when using PBS Pro (as is currently done with SGE and LSF)

KNIME Extensions 1.2.207

- Windows support
- Better support for flow variables and looping constructs
  - Ability to use flow variables in the Chemistry External Tool
  - Variable based Glide Grid Reader
  - Row iterator loop start
- New options for Glide, LigPrep and PhaseShape
- New Protein Preparation Wizard node
- New Unique Title Check node to ensure uniqueness of compound titles
- Additional example workflow

Liaison 5.5.211

- New driver with greatly improved remote job submission, monitoring and recovery capabilities

LigPrep 2.3.211

- Fixed bug that prevented ligparse from running on Windows
- Added support for compressed SD files

Maestro 9.0.211

- New Multiple Sequence Viewer
- Seamless integration with PyMOL
- Significant improvements to plotting tool
- Now possible to download PDB files directly from the web
- Position of the Project Table scroll bar configurable by user
- Fixed problems with file browsers not updating on NFS
- Options now available directly in Import and Export dialogs
- Redesigned Custom Property Family feature

MCPRO+ 2.6.211

- Fixed bug that was causing missing atomtype parameters for angles and dihedral terms with dummy atoms in some circumstances
- Improved robustness of protein z-matrix generation workflow

Phase 3.1.211

- Addressed several stability issues on Windows
- Consensus shape creation from multiple structures
- Database duplicate elimination based on unique SMILES
- Database subset creation from a list of property values
- Partial matching applied to site groupings

Prime 2.1.211

- Addressed issues preventing certain jobs from running on Windows
- Updated Find Homologs table

PrimeX 1.6.211

- Improved handling of input parameters and output data for Ligand Placement
- Resolved timing issue that interfered with incorporation of some jobs into Maestro

Python Scripts (available at the Script Center)

- Significant enhancements to R-Group Analysis, including heatmap display