

Schrödinger Suite 2009 – Major New Features Added Since Last Release

In addition to the major new features listed below, minor enhancements have been implemented in nearly all products

CombiGlide 2.5.007

- New interactive enumerate and dock graphical interface
 - Supports designing, enumerating and docking of combinatorial libraries from a convenient 2D interface
 - Works stand-alone but can also interact with the Maestro project table and workspace
 - Uses Schrödinger- or user-supplied fragment files
 - Includes a 2D interface for building fragment files from a Schrödinger- or user-supplied "palette" of molecular structures
- Now runs on Windows
- Linux x86 64-bit platform support

ConfGen 2.1.108

- Better sampling of ring systems

Converter Utilities

- Automatic import support for V3000 SD file format; files can be written in this format with "sdconvert -v3"
- More robust support of mol2 files

Desmond 2.2.623

- Extensive improvements to the graphical interface
- Better methods for setting up and relaxing membrane systems, in particular GPCRs
- Support for replica exchange (REMD) calculations
- Support for simulated annealing calculations
- Checkpointing and restarting of multisim jobs
- Custom multisim job stages coded in Python
- New script to translate Amber input files into a Desmond input structure file
- Script to adjust simulation parameters for correctness and good performance
- Langevin thermostat and barostat
- Improvements in FEP calculations of absolute and relative solvation free energies
- Improved support for multiprocessor jobs on LSF queuing systems
- Linux x86 64-bit platform support

Epik 2.0.109

- More accurate pKa predictions
- New option for preparing ligands appropriate for docking into metalloproteins
- Linux x86 64-bit platform support

Force Field OPLS_2005

- Updated charges for [Fe^{+3/+2}][heme] moieties. In particular [S⁻] coordinated ligands can now be used in modeling cytochrome P450s (CYPs).

Glide 5.5.108

- Improved performance in virtual screening via inclusion of Epik ionization and tautomeric penalties in Glide scoring function
- Sampling of user-selected protein hydroxyl torsions during docking
- Increase in the maximum number of ligand atoms for docking to 300 and number of rotatable bonds to 50
- Significantly faster generation of grids for docking
- Computation of RMSD between a docked pose and its input structure
- Linux x86 64-bit platform support

Glide XPVisualizer 5.5.108

None

Impact 5.5.108

- Linux x86 64-bit platform support

Induced Fit Docking (IFD)

- Windows platform support
- Linux x86 64-bit platform support

Jaguar 7.6.108

- Second derivative calculations for M05 and M06 classes of density functionals
- Semiempirical QM support via MOPAC (command line; graphical interface on ScriptCenter)
- Surface maps for average local ionization potential
- Replacement of MPICH-1 with OpenMPI for parallel calculations
- Distributed counterpoise calculations using counterpoise.py
- Improvements to geometry optimizer to reduce the number of 'stuck' jobs and reduce the number of steps to converge systems with flat potential energy surfaces
- Availability of Linux x86 64-bit executables, which are about 30% faster than the x86 32-bit executables when run on the same machine
- SM8 solvation model

Job Control and Infrastructure

- Numerous changes to enhance robustness of file transfer
- Better performance of workflows on Windows
- Support for license checking when running the LSF queuing system
- Support for the LoadLeveler queuing system

KNIME Extensions 1.2.120

- Support for KNIME 2.0.2 the latest version of the KNIME workbench available from knime.org; major improvements in KNIME 2.0 include:
 - More than 20 new nodes (not counting 70 new nodes in the WEKA extension)
 - A newly defined database API for performing operations on databases
 - Improved meta node handling
 - Optimized workflow management
 - Many improvements on the user interface to ease workflow assembly and data inspection
 - New support for workflow variables and workflow loops
 - PMML support for some of the data mining nodes
- High-quality 2D molecular rendering (via CambridgeSoft's coordinate generation library) from Mae, SD, and SMILES input formats
- Additional Canvas functionality
 - Maximum common substructure (MCS)
 - Fingerprint similarity search
- Support for Phase Shape
- Streamlined installation through KNIME update site
- Improved scalability, stability, and robustness

Liaison 5.5.108

- Linux x86 64-bit platform support
- Support for mol2 files

Ligand- & Structure-Based Descriptors (LSBD)

None

LigPrep 2.3.108

- Preparation of ligands for docking into metalloproteins using Epik
- Improved Ligand Filtering graphical interface to remove structures with undesirable properties
- Improved templating for ring systems
- Simplified input files
- SMILES input with associated molecular properties using CSV files
- Linux x86 64-bit platform support

MacroModel 9.7.108

- Restraining of ligand atoms in Embrace calculations
- Extension to the support for simplified input files
- Serial Energy calculations available in Maestro
- Linux x86 64-bit platform support

Maestro 9.0.108

- Large number of significant usability enhancements throughout the graphical interface
- Native Windows support
 - Improved 3D graphics performance
 - Windows look and feel
 - Windows-style file selectors
 - Copy and paste Workspace images to Microsoft Office and other Windows applications
 - Copy and paste text from Maestro to other applications and vice versa
 - Relocate and tear-off toolbars
- 2D structures in the Project Table
- Support for sending structures from Maestro directly to PyMOL v1.2
- Several panels in Maestro are now able to be docked into the main window to reduce panel clutter
- New Workspace Style toolbar
 - provides quick methods for setting the graphical display for protein ligand complexes
 - styles can be reapplied when the Workspace changes
 - single-click generation of binding site surfaces
 - single click to display ligand/receptor contacts and H-bonds
- Atom labels now allow user selection from a much greater range of fonts, sizes, and styles
- Support for horizontal interlaced stereo monitors (e.g., Zalman Trimon 3D monitors)

MCPRO+ 2.6.108

- Per-lambda point minimization prior to MC sampling for FEP calculations
- Improved robustness of several workflows and restart machinery

Phase 3.1.108

- New "Generate 3D Database" graphical workflow that prepares structures via LigPrep, filters according to QikProp, then runs phasedb_manage and phasedb_confsites to build or append to a Phase database
- Duplicate checking in Phase databases using a uniquely-valued property
- Significantly faster database conversion/merging using phasedb_convert
- Database subset creation from a list of titles
- New environment variable for output level in phasedb_confsites and phase_fileSearch
- Excluded volumes surrounding only a portion of a structure
- New utility to investigate alternate atom numbering schemes in order to identify 180° ring twists and other symmetry operations that may reduce RMSD
- New utility flex_align for generating multi-ligand alignments using the Phase Shape technology
- 2 GB limit on Phase Match files removed
- Looping over n, n-1, ... sites in Find Common Pharmacophores jobs
- Automatic "retry" mechanism for phasedb_confsites,
- Elimination of excessive memory usage in Score Actives jobs
- Windows support for Develop Pharmacophore, Find Matches, and Generate 3D Database
- Linux x86 64-bit platform support

PrimeX 1.6.108

- Improved accuracy of ligand placement
- Separate control of electron density weight in energy and scoring for ligand placement
- Kicked omit maps
- Improved grouped B-factor refinement, limited by Bmin and Bmax
- Direct calculation of summary geometry statistics using the Engh & Huber standard
- Linux x86 64-bit platform support

Prime 2.1.108

- Homology Modeling
 - More responsive sequence viewer
 - Faster and more reliable loop building
- Refinement
 - More robust/accurate long-loop prediction through use of a sequence-dependent backbone rotamer library
 - Restarting of extended loop sampling jobs
 - Spatial constraints during loop predictions (command line)
 - Pairwise atom constraints for all Refine Structure job types (command line)
 - Helix building during loop predictions (command line)
- Docking
 - New graphical interface in Maestro for Covalent Docking
- Windows support for Homology Modeling, Refinement, and Covalent Docking
- Linux x86 64-bit platform support for Homology Modeling, Refinement, and Covalent Docking

Protein Preparation Wizard

- Automatic filling of missing loops with Prime
- Generation of all reasonable phosphate and sulfate protonation states
- Automatic detection and highlighting of overlapping atoms

QikProp 3.2.108

- Linux x86 64-bit platform support

QM-Polarized Ligand Docking (QLPD)

None

QSite 5.5.108

- Second derivative calculations for M05 and M06 classes of density functionals
- Replacement of MPICH-1 with OpenMPI for parallel calculations
- Improvements to geometry optimizer to reduce the number of 'stuck' jobs and reduce the number of steps to converge systems with flat potential energy surfaces
- Linux x86 64-bit executables, which are up to 30% faster than the x86 32-bit executables
- Writing of IRC points to output .mae file for visualization

SiteMap 2.3.108

None

Strike 1.8.108

None

Virtual Screening Workflow (VSW)

- Inclusion of Epik state penalties in the GlideScore.
- Larger number of Glide Grids (up to 100)
- Prime MM-GBSA run after any docking stage
- Post-docking minimization
- Selection of constraint atoms in the Workspace when picked
- Choice of force field for docking
- Distributed QikProp stage
- Windows platform support