

Major New Features/Improvements in Schrödinger Suite 2011

Visualization & Automation

Maestro 9.2

- Significant improvement in 3D graphics
- Improved performance of projects with large numbers of small molecules and properties
- Smaller Project file size
- Ability to completely configure mouse button assignments
- Workspace highlighting and annotation features
- 2D Sketcher for structure input and modification
- Reorganized Preferences panel
- Toolbar enhancements: Main toolbar broken into smaller user-configurable toolbars; ability to show icon, icon+text, or just text
- Task-based view of Applications menu
- Presets for graphics quality and appearance
- Option to use transparent background when saving images
- Support for importing structure files in SMILES format
- Ability to import structures from an existing project
- Interactive Python shell
- Job monitoring enhancements: workspace job status indicator; enhanced monitor panel; faster job database
- Ability to color surfaces by cavity depth
- Interface for editing and defining color schemes, including those based on arbitrary atom properties
- Significant improvements to the Prime user interface
- Ability to specify the color ramp (and range) for ESP surface color scheme
- Many additional usability enhancements
- Improvements to Protein Preparation Wizard
 - H-bond assignment at variable pH
 - Option to minimize hydrogens in H-bond assignment
 - Option to build biological unit when importing structure
 - Ability to directly add side chains with missing density (uses Prime)
 - Use of OPLS_2005 force field for minimization
- Improvements to Glide XP Visualizer
 - Improved performance
 - Improved look and feel

Job Control

- Much faster and better organized job control database (indexed and hierarchical)
- Faster job launch on all platforms, in particular on Windows
- WinHPC: crucial bug fix for runaway multiple jproxies

PyMOL 1.4

- New 64-bit MacPyMOL allows Mac users to access more than 4 GB of memory
- Volume visualization for unique display of volumetric data and simultaneous visualization of multiple iso-surfaces
- Electron density map generation from reflection data
- Stereochemical labeling
- New "ligalign" function for rigid and flexible ligand alignment, conserved residue detection and more
- OpenGL Shaders (GLSL) for improved on-screen rendering (cartoons, sticks, surfaces, volumes)
- Dynamic measurements (distances, bond angles and dihedral angles)
- File > Save Molecule now allows saving of multiple files, multi-state PDBs to a single file, and multi-state PDBs to multiple files
- Improved State Handling makes operations on multi-state objects easier
- Built using Schrödinger-compatible distribution of Python (v2.7)
- PyMOL Web GUI (PWG)
- Several bug fixes

JyMOL 1.1

- New functions added: mplay, feedback, rock, get_names, map_new, turn, bg_rgb
- Support for quad-buffered stereoscopic 3D
- Updates to infrastructure:
 - JOGL version 2.0
 - Conversion of proprietary JAVA-to-C interface to SWIG; makes it easier to add functionality to JyMOL and simplifies API of some functions
 - Added GLEW to allow JyMOL to be able to use GLSL shaders
- Bug fixes

KNIME Extensions 1.4

- Canvas 2D renderer on 64 bit KNIME workbench
- Windows installers
- Desmond nodes (System builder and Molecular dynamics, Extract frames)
- Node for running Phase queries on files
- Canvas model building and prediction (PLS and Bayes classification) nodes
- Canvas nodes for filtering structures based on an ASL expression, and calculating properties
- Prime homology model node – added option to include ligands and cofactors
- Run Maestro node enhancements: import as groups, read hypotheses, and specify a project to which structures are added
- New start-up script options to pass user/machine/OS-specific parameters (memory limit, temporary directory)
- Various usability and stability enhancements

Structure-Based Lead Discovery, Lead Optimization & ADME/Tox Prediction

Glide 5.7

- Ability to enhance planarity of conjugated groups during docking
- NOE constraints for HTVS/SP/XP docking – behaves like positional constraints, but specified by a range rather than a specific radius; includes support for visualization
- Switched default force field to OPLS_2005
- Greater user control in specifying residues for use in computing per-residue interaction terms

QM-Polarized Ligand Docking (QPLD)

- Minor bug fixes

CombiGlide 2.7

- Sketcher to build fragments for interactive enumeration and docking
- Bug fixes

Virtual Screening Workflow (VSW)

- Ability to save a list of ligands filtered for each filtering criteria
- Minor enhancements and bug fixes

P450 SOM Prediction 1.0

- New P450 Site of Metabolism prediction (see [whitepaper](#))

Induced Fit Docking (IFD)

- Option to return XP descriptors
- New job distribution mechanism
- Improved speed of Compile Residue List stage
- Control over which docking stage H-bond constraints are applied
- New options to control ligand sampling:
 - Option for rigid ligand docking
 - Option to enable/disable ring conformational sampling, as well as ability to set the energy window
 - Options for controlling sampling of amide bonds

Prime MM-GBSA 3.0

- Increased minimizer controls
- User-specified restraints on subset of ligand atoms
- Greater control of residues to minimize
- More detailed energy breakdown

SiteMap 2.5

- Minor bug fixes

Liaison 5.7

- Minor bug fixes

Protein Modeling & Refinement

Prime Homology Modeling & Refinement 3.0

Protein Refinement:

- New energy model for greatly improved accuracy of side-chain and loop prediction
- Significantly improved robustness and less sensitivity to issues with input structures
- Improved controls for setting up membranes
- New constraint to prevent loop building from entering membrane
- New constraint types (command line only): angle restraints, torsional restraints, solvent exposure/burial restraints
- New output property indicating status of pair-wise constraints
- Allow use of Maestro-file partial charges for both ligand and protein

Homology Modeling:

- Homo- and hetero-multimer building
- Consensus model building
- User-specified pair-wise residue and disulfide constraints during model building
- Support for DNA/RNA during model building
- Variety of speed and usability enhancements to the user interface
- Coloring and property setting in output model indicating residue conservation status

PrimeX 1.8

- REFMAC-style dictionary files improved to better suit CCP4-compatible programs
- Windows version of PrimeX introduced
- Report number of steric clashes in PrimeX geometry summary
- Write mtz phased reflection files for omit maps from command line

Ligand-Based & Pharmacophore Modeling

Phase 3.3

- Phase GUI Features:
 - Distance, angle, and dihedral constraints in Find Matches to Hypothesis
 - Exclude specific ligand sites from common pharmacophore perception
 - Create groupings of actives from tautomers, ionic states, etc., and treat as a single ligand for common pharmacophore perception
 - Require specific actives/active groups to match common pharmacophores
- Phase Command Line/Backend Features:
 - Options to investigate additional atom mappings to find better superpositions (phase_shape)
 - Create Canvas properties when extracting (phasedb_props)
 - Create and manage Phase databases in new, more compact format. Replaces phasedb_manage, phasedb_confsites, phasedb_props, phasedb_convert, and phasedb_export (phase_database)
 - Searches files, command line projects, and databases created using phase_database. Replaces phase_dbsearch, phase_fileSearch, phase_gridSearch, phasedb_findmatches and pharm_align_mol (phase_find_matches)

Core Hopping 1.1

- Support for GPGPU – screen ~170 cores/sec (see [GPGPU roadmap](#) for more details)
- Support for receptor constraints if receptor is present
- Filter results based on H-bond matching of cores against template
- Evaluate overlap of new core with original template core
- Pre-filtering of cores to be screened based on need to meet donor/acceptor criteria
- Corefinder program to prepare SQLite database
- Expanded core library
- User-specified attachment sites
- Synthesizability scoring
- Donor/acceptor matching with template structure
- Dynamic results viewer - view results while program is running

QikProp 3.4.015

- Minor bug fixes

Cheminformatics & QSAR

Canvas 1.4

- R-Group Analysis via new Scripts menu (see R-Group Analysis in Medicinal Chemistry Applications)
- Scripts menu and Python APIs for custom applications
- Grid view of spreadsheet structures
- Automatic creation of a new view for each imported file
- Run substructure queries on external read-only projects
- Duplicate detection/elimination
- Ensemble recursive partitioning
- 3D structure generation and minimization via LigPrep
- 3D shape screening
- Measure diversity and similarity of compound collections
- Partitions with custom bins
- Plot partition class values
- Create ordinary property from partition
- Redesigned Substructure Query

Seurat

- Please visit <http://www.schrodinger.com/products/14/33/>

R-Group Analysis (Maestro and Canvas)

- Better overall panel organization
- Activity-cliff analysis
- R-group families
- Importance analysis
 - Importance measure for R-group positions
 - Drill down to get insight into R groups at important positions

Strike 2.0

- Minor bug fixes

Medicinal Chemistry Applications

Maestro Elements 1.2

- 2D Sketcher for structure input and modification
- Mouse button operations customizable
- Option to display text under toolbar icons, making it easier for new users to get started
- Customizable toolbars
- Faster startup and job launching
- Improved conformer generation with ConfGen
- Usability enhancements
 - Job monitor panel is hidden unless the user opens it
 - Electrostatic surface potential: ability to specify the color ramp and new "fast" surface option
 - Flexible Ligand Alignment: align to workspace structure
 - MacroModel Ligand Designer: simplified panel and added on-line Help
 - Glide Ligand Designer: automatically run SAR analysis of results
 - Ligand Interaction Diagram supports π -cation interactions

R-Group Analysis (Maestro and Canvas)

- See in *Cheminformatics & QSAR*

Canvas 1.4

- See in *Cheminformatics & QSAR*

PyMOL 1.4

- See in *Visualization & Automation*

Core Hopping 1.1

- See in *Ligand-Based & Pharmacophore Modeling*

MacroModel 9.9

- Improvements to the script for creating user-defined ring templates
- Enhanced sampling of macrocycles
- New, more efficient support for distributed processing using the 'bmin' command

LigPrep 2.5

- New, more efficient support for distributed processing using the 'ligprep' command
- Automatic variation of unspecified cis/trans ring conformations
- Improvements in ring templating (see ConfGen)

Epik 2.2

- Improved pK_a accuracy
- Reduced production of high-energy protonation states
- Improvements in the way that acid_base groups are encoded
- New, more efficient support for distributed processing using the 'epik' command

ConfGen 2.3

- Conformation generation using OPLS_2005 by default – permits searching of compounds containing B and Si
- Additional Fast (CF) mode based on the work described in [J. Chen and N. Foloppe, J. Chem. Info. Model. 2010, 50, 822](#)
- Improvements in ring templating – more ring templates including some for macrocycles, also able to specify the location of custom templates using an environment variable, templates containing double bonds instead of amide bonds may be used when an exact match is not found
- Option to reward hydrogen bonds that complete 5- or 6-membered pseudo-rings
- Option to enhance coplanarity of bonded sp² atoms
- New, more efficient distributed processing

QSite 5.7

- Visualization of non-covalent interactions
- Improved geometry optimization

MCPRO+ 2.8

- Minor bug fixes

Jaguar and Jaguar pKa 7.8

- Calculation of vibrational circular dichroism (VCD) for determining chirality
- Visualization of non-covalent interactions
- pK_a prediction of oximes
- Calculation of the electrostatic potential at the nuclei

Desmond 3.0

- GUI support for launching and analyzing metadynamics simulations
- Support for non-power of 2 processor topologies in standard workflows
- Script to support using custom charges in FEP calculations
- Maestro related improvements:
 - Improved speed of trajectory viewer
 - Improvements to trajectory analysis: atom-based root mean square fluctuations (RMSFs) relative to a reference structure; calculate RMSD for all pairwise combinations of frames in a trajectory
 - Can align on helices when building a membrane system
 - Simulation event analysis can display statistics in a table
 - Lambda Hopping for Relative Free Energy Perturbation calculations to increase intramolecular conformational sampling
- Enhancements to 'multisim':
 - Support for metadynamics
 - Support for internal restraints including flat bottomed potentials
 - Optional GCMC equilibration for FEP jobs
 - Automated FEP analysis

Impact 5.7

- Bug fixes

Semiempirical NDDO Library (Maestro)

- Based on the public domain version of MOPAC 7.1
- Provides RM1, AM1, PM3, MNDO, and MNDO/d semiempirical methods for treating electronic structure
- Visualization of molecular orbitals, electron density, electrostatic potential, average local ionization energy and electron affinity
- Faster calculation of ESP charges
- Graphical interface is provided in Maestro

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