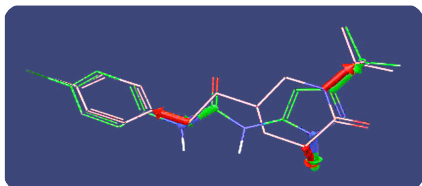


Major New Features in Schrödinger Suite 2010

Core Hopping 1.0 (new)

New product for core/scaffold hopping – provides three modes:

- Receptor-based core hopping – accounts for interactions with the receptor
- Shape-based core hopping – accounts for shape and atom property similarity between new cores and the current core
- Attachment-based core hopping – accounts for compatibility of attachment points on cores with fixed ligand side chains; supports automatic addition of linkers; uses multi-threading technology to take advantage of multiple cores on Windows and Linux



Canvas 1.3

- Editable spreadsheet
- Append new rows and columns
- Copy/paste operations on structure cells, including
 - Cell to cell
 - ISIS/Draw to cell
 - Cell to external SMILES
 - External SMILES to cell
- Create new properties from mathematical expressions
- Highlighting of substructure matches
- Master View state persists between sessions
- Access to job control (e.g., host, number of CPUs)
- Cloning of jobs to allow rapid submission of similar jobs and to review the settings used in a particular job
- Use of partitions to define training and test set memberships
- 3D Pharmacophore fingerprints

CombiGlide 2.6

- Minor bug fixes

ConfGen 2.2

- New confgen command
 - easy launching of standard ConfGen jobs without setting up a search parameter file
 - supports distributed processing
 - supports and distributes combined jobs that use more than one of the standard search modes
- Major improvements in ring templating (see ring templating under LigPrep)

Converter Utilities

- Many minor bug fixes
- Support for compressed pdb files (.pdb.gz)
- New script (structcat) for merging/converting structure files

Desmond 2.4

- Maestro enhancements for Desmond
 - Structural waters retained as part of the solvent
 - More water models for membrane systems
 - Automatically generated temperature schedule for replica exchange
 - Centering of solutes and dynamic selection of nearby atoms in trajectory viewing
 - Jobs can be submitted to remote Linux machines from Windows
- The cfg and msj file syntax has been simplified to make them more user friendly
- Changes to multisim behavior
 - solvate_pocket for equilibrating water in buried regions of the system
 - lambda_hopping for enhancing sampling during FEP calculations
 - the 'LOCAL' command line option now applies to subjobs as well as the master multisim process
- Enhanced sampling/meta dynamics is now supported from the command line
- More types of restraints, including distance, angle, and dihedral are now supported
 - Restraints now have flat-bottom variants
 - New types of restraints can function over much longer distances
- Changes to support for analysis of simulation trajectories
 - RMSD calculations are faster
 - FEP trajectories can now be analysed
- New script, trajectory_extract_frame, to extract system configurations from a trajectory

Epik 2.1

- More than 200 changes/additions have been made to the Hammett and Taft parameters used in pKa predictions
- The number of types of tautomerization explicitly encoded has increased to more than 900 (an increase by more than a factor of two)

Glide 5.6

- Optionally constrain torsions in docked ligands
- Improve speed of pre- and post-docking steps; important when docking large numbers of ligands (>50,000) in a single job
- Hydrogen-bond constraint symmetry can be turned off to, for example, allow a constraint to only one O atom of a carboxylate
- Improved docking accuracy and enrichments for metalloproteins – entails modification of the input file to set required options, which have not yet been exposed in the graphical interface
- Support for up to 90,000 atoms

Glide XP Visualizer 5.6

- Minor bug fixes

Impact 5.6

- Support for up to 90,000 atoms

Induced Fit Docking (IFD)

- Reduction in disk space usage via compressed files and file cleanup
- Support compressed input .mae files
- Option to write Glide XP descriptors for use in the Glide XP Visualizer
- Option to automatically perform side-chain trimming (Ala mutation) based on B-factors
- Automatically use multiple input ligand conformations during redocking stage to improve accuracy

Jaguar 7.7

- Analytic electric dipole derivatives and IR intensities for DFT
- Analysis of the electrostatic potential on the molecular surface
- Calculation and display of Fukui functions

Job Control and Infrastructure

- Changes to management of job-control records, which has led to speed up of Maestro startup
- More efficient and robust file transfer, particularly when there are large numbers of jobs
- Windows HPC support of Glide and LigPrep
- Some changes made for AFS compatibility will be made available to AFS customers via special builds
- Significant improvements in robustness and performance on Windows
- New graphical wizard for configuring Windows desktops for submitting jobs to remote Linux machines

KNIME Extensions 1.3

- Updates to KNIME 2.1.2, including the following:
 - Support for groups in the Workflow project repository
 - Undo/Redo functionalities
 - Workflow global variables
 - New time series nodes
 - New Hilite collector, double to integer, row splitter nodes
 - New Find & Find Next in Interactive table node
 - Webservice client and Perl nodes (in Labs)
- New KNIME web page for easy access to the latest KNIME workflows
- New nodes:
 - CombiGlide reagent preparation and library enumeration
 - ConfGen standard
 - MacroModel coordinate scan
 - Prime side chain sampling
- New options to existing nodes:
 - Glide ligand docking positional constraints
 - Control over additional parameters for Induced-Fit Docking
 - Prime MM-GBSA protein flexibility
 - Fingerprint generation advanced options and jobcontrol tab
 - Conformational search high throughput mode
 - Molecule reader control over the order the files are read
 - Split by molecule option puts all the water molecules in the same row

Liaison 5.6

- Windows support

Ligand- & Structure-Based Descriptors (LSBD)

- Support distributed Embrace calculations for faster throughput

LigPrep 2.4

- para_ligprep enhancements
 - Better documentation of failed subjobs
 - Supported on Windows
 - Ability to run the master process and the subjobs on different hosts/queues
- New ligprep -run_from option to continue interrupted LigPrep runs from a specified stage
- Major improvements in ring templating
 - Approximately 500 more ring templates
 - For molecules containing multiple ring systems, lack of a template for any of them does not prevent sampling of the rest
 - Incidents of distorted 3 and 4 membered rings connected to flexible ring via a spirocenter have been significantly reduced
- The number of types of tautomerization explicitly encoded has increased to more than 900 (an increase by more than a factor of two)
- Lower rates of dropped structures when generating structures from SMILES strings
- More robust handling of misdrawn sulfone and nitro functional groups

MacroModel 9.8

- para_bmin jobs can now run the master job on a different host/queue than the subjobs
- para_bmin jobs can now be run on Windows
- Progress of MacroModel conformational searches and molecular dynamics jobs expressed as the percent of the calculation completed can now be tracked in Maestro's monitor panel
- Flat-bottom restraints can be applied using ASL commands

Maestro 9.1

- R-group analysis
 - Now in the Maestro Workflows menu
 - SAR Table added
 - Better core perception when MCS gives multiple matches
 - Enhancements to display of results
 - Usability enhancements to graphical interface
- Workspace can be copied to PowerPoint for interactive 3D figures (via ActiveX control)
- New skin (simplified mode) specifically for medicinal chemists
- Copy structures from ChemDraw and ISIS/Draw and paste into Maestro
- Tiling is now a mode that creates multiple workspaces
- Support two thicknesses of tubes
- Conversion of aliphatic ring substituents between axial and equatorial
- New Find toolbar in the main Maestro window
- Ribbon rendering for DNA, RNA, etc
- Ribbons pass through the alpha carbons
- Allow "Starring" of Entries
- Lock entries in PT to prevent editing of structure
- New Find toolbar in the Project Table panel
- Support multiple "snapshots" (Scenes) of the Workspace and Project state
- Support saving of multiple Workspace views (new Views toolbar)
- Graphical interface for customization of menus and shortcuts
- Edit any atom-level property
- Improvements to Workspace Style toolbar
- A number of performance enhancements
- Support for Linux-x86_64

MCPro+ 2.7

- Support for Linux-x86_64

MOPAC 1.9

- Calculation of electrophilic, nucleophilic, and radical superdelocalizabilities, electrophilic and nucleophilic frontier electron densities, and atom polarizabilities (useful for building QSAR models)
- Windows support

Phase 3.2

- Improvements to Shape Screening
 - Supports remote Phase database searching
 - Weights of selected atoms may be set to a single value
 - Checkpoint directory may be specified to allow command line restart
 - Can force alignment on one or more substructures
- Edit Features contains "Workspace" and "Ligands" columns that indicate whether a given SMARTS pattern is present in the applicable structures
- Specific sites may be excluded from Find Common Pharmacophores by using the command line workaround \$PHARMA_EXEC/exclude_sites
- Find Matches to Hypothesis allows users to define site groups and require one or more sites from each group to be matched
- Generate Phase Database supports duplicate skipping and automatically creates and updates a searchable property database
- A new Manage Phase Database application is available from the Applications > Phase menu. Provides access to individual database records and all imported properties, and supports creation of subsets from selected records, from matching titles, or at random
- Ligands in command line projects may be grouped by title.
- phasedb_manage automatically adds a unique SMILES property to each structure before storing in the database
- Support for distance, angle, and dihedral constraints among ordinary sites and two-point vector features when searching for matches to a hypothesis

Prime 2.2

- Support for web-based BLAST searches, eliminating the need for maintaining local sequence databases
- Major overhaul of memory intensive core, significantly reducing memory usage and greatly increasing maximum system size
- Conversion of all jobs and workflows to compressed .mae files, greatly reducing disk usage
- Graphical interface for setting up pairwise, spatial, and helical constraints during refinement
- Preliminary support for building homology models from the Multiple Sequence Viewer
- Optional C β (CB) sampling during side-chain prediction
- Mini-loop sampling during side-chain prediction
- Improved backbone torsional parameters to increase loop prediction accuracy
- Improvements to Protein Structure Alignment results
- Speed improvements, particularly for large systems
- Improved robustness and error reporting

Virtual Screening Workflow (VSW)

- One-step selection of multiple grid files for ensemble docking
- Phase database can be used as input for docking
- Additional tabs for cleaner layout
- Strain corrections can be performed in each docking stage
- Enabled rigid docking for HTVS and XP
- Automatically enumerate water combinations for ensemble docking
- Receptors can be aligned before docking

PrimeX 1.7

- Ability added to generate REFMAC-style dictionary files in cif format
- Support added for the use of external electron density maps for ligand placement
- Memory management improved to support up to 5000 protein residues plus 5000 water residues
- Simulated annealing enhanced to include full NCS restraints and fine control of relative planarity restraints
- Method enhanced for command line jobs, preventing water placement in electron density belonging to a larger molecule
- Number of poses returned may be specified for command line ligand placement jobs
- Maps may be exported as phased reflection files for command line jobs
- Method improved to fix any portion of a structure in both real- and reciprocal-space operations
- Post-refinement processing of structures streamlined to reduce time requirements

Protein Preparation Wizard

- Interface redesigned to improve usability
- Structural assessment tools: View Problems, Protein Reports, Ramachandran Plot

PyMOL 1.3

- Release of official A \times PyMOL product
- New movie_quality setting for controlling movie output quality
- New label_anchor setting
- Dynamic distances
- Improvements to the fetch command
 - now fetches electron density maps (if present)
 - fetch_host setting to fetch from the US, European or Japanese PDB servers
- New structure alignment algorithm based on the CE method (<http://cl.sdsc.edu/>)
- New command, 'obscure', to artistically hide proprietary data (e.g., structure of molecule bound to a protein) for public presentations
- Improvements to JyMOL 0.91 – built on new Java platform (v1.6)
- Next generation APBS plugin
- Updated FreeMOL with APBS v1.2 and PDB2PQR v1.6

QikProp 3.3

- Added support for compressed Maestro and mol input/output files

QM-Polarized Ligand Docking (QPLD)

- Supports use of MOPAC for calculating charges

QSite 5.6

- NDDO methods (RMI, AM1, PM3, MNDO) may now be used to model the QM region for free ligands and for hydrogen-capped regions
- Automatic handling of MM regions of up to 90,000 atoms
- Property calculation from new Property tab in QSite panel

SiteMap 2.4

None

Strike 1.9

None

