SCIGRESS Release Notes

SCIGRESS 2.9 (3.4)

- General-purpose quantum-chemical package niedoida available on Windows, Linux and MacOS. New methods implemented:
  - *Ab initio*: HF, MP2.
  - DFT: SVWN, BLYP, B3LYP, B3LYP5, B2PLYP, PW91, PBE, PBE0.
  - Basis sets: CNDO, STO-2G, STO-3G, STO-6G, 3-21G, 4-31G, 6-31G, 6-311G, 6-31G*, 6-31G**, 6-311G*, 6-311G**, 6-31+G*, 6-311+G*, 6-31++G**, 6-311++G**, 6-311++G(2d,2p), 6-311++G(3df,3pd), DZVP-DFT-orbital, FPGA, DF-Ahlrichs, DF-DeMon, DF-DeGauss-A1, DF-DeGauss-A2, DF-Weigend, Def2-SVP, Def2-SVPD, Def2-TZVP, Def2-TZVPD, Def2-TZVPP, Def2-TZVPPD, Def2-QZVP, Def2-QZVPD, Def2-QZVPP, def2-QZVPPD, Poisson-MP2-standard-DZ, Poisson-MP2-DZ, G94-Poisson-MP2-DZ.
  - Population analysis: Mulliken, Löwdin, Hirshfeld, Voronoi, Bader.
  - Bond order analysis: Nalewajski-Mrozek, Mayer, Gopinathan-Jug.
- Parallelized DFT, semi-empirical and molecular dynamics calculation on Windows, Linux and MacOS.
- Calculation of larger systems (64-bit support) for DFT, semi-empirical and molecular dynamics.
- Performance improvement of Spreadsheet.
- Improved parallelization for non-MPI LAMMPS for Windows.
- External validation set support in QSAR.
- Bugfixing.

SCIGRESS 2.8.1 (3.3)

- Improved MD-ME potentials selection wizard.
- Prepare receptor for docking - step by step docking input preparation.
- Interface to Autodock Vina.
- Improved protein cleaning using PDB data (missing atoms and residues).
- Solvate molecule wizard.
- Analyze docking results visualization method.
- Support of 3D displays for stereographic molecule representation.
- Molecule animation for geometry optimization with MO-G and MM simulations.
- Improved energy and gradient graph for MO-G, MM and MD-ME simulations.
- NMR spectra from DGauss simulations.
- Improved keyboard shortcuts for "on the fly" atom change.
- Improvement of automatic QSAR functionality.
- LAMMPS Minimize support.
- Support of MOPAC2016.
- Autodock Vina spreadsheet procedure.
- Enhancement of installation/deinstallation process.
- Improved online SCIGRESS licensing mechanism.
- Bugfixing.

SCIGRESS

SCIGRESS 2.7 (3.2)

- Automated QSAR analysis (Enhanced Replacement Method and Genetic Algorithm).
    - Automated QSAR in SCIGRESS builds linear regression models for molecules in the Spreadsheet. Linear regression models are easy to interpret and quantify.
- LAMMPS interface for all supported platforms.
    - SCIGRESS can now create input files and run LAMMPS Molecular Dynamics Simulator experiments. LAMMPS is open source classical molecular dynamics software.
- Transparent handling of calculations on cloud and grid computing systems (currently PL-Grid, more coming).
    - SCIGRESS has now possibility of running experiments on academic supercomputers. Currently this functionality is limited to Poland. Please contact our support if you think that we should add new public computing center to our supported servers.
- Protein cleaning (missing atoms, residues, loops) function.
    - An automated tool for repairing common problems with PDB files. Helps preparing input structures for docking and quantum calculations.
- GAMESS support on Mac OS X.
- Batch procedures for SCIGRESS calculations.
    - User can prepare calculations and run them sequentially overnight or during weekend.
- Fastdock code optimization (Grid pre-calculation).
- The common calculations for all the ligands have been separated and are executed before screening procedure starts.
- Fastdock default genetic algorithm parameters optimization.
- NMR spectra from DGauss calculations.
- Windows 10 support.
- Various bug fixes.

SCIGRESS 2.6 (3.1.8)

- Mac OS X version of SCIGRESS client.
- Single-node server with very simple procedure of installation.
- Implemented animation of IR transitions.
- Continuous update of atom coordinates during geometry optimization in Mechanics.
- Displays contours on the plane through surfaces (molecular orbitals, electrostatic isopotentials, etc.).
- PubChem search directly from Workspace and Spreadsheet.
- Update of MO-G source code.
- New potentials for molecular dynamics calculations.
- Handle monomer angle when building a polymer.
- Export option of multiple molecules from Project Explorer.
- Implemented massive import of files.
- Implemented word search for text view (text documents).
- Update of documentation.
- Partial charges and UV-VIS spectra from GAMESS calculations.
- UV-VIS spectra from Gaussian calculations.

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- Bug fixing.

SCIGRESS 2.5 (3.1.6)

- MOPAC2012 support.
- 64-bits Windows version of SCIGRESS client.
- IA installer project file update - enable console and silent mode of installer for massive installations.

SCIGRESS 2.5 (3.1.4)

- New potentials for molecular dynamics calculations.
- pKa estimation is available in MO-G.
- Parameter optimization of MM correction in MO-G.
- CGDMS convergence and calculation speed improved.
- Fragment Library became editable.
- Improved import of SDF.
- CONFLEX7 support.
- ADF2013 support.
- GAMESS I/F new features:
    - Transition state geometry optimization.
    - Vibrational spectrum.
    - Potential energy surface (gas-phase model, one or two distance labels are supported only).
    - Intrinsic reaction coordinate.
- Windows 8 supported.
- Implemented authorization in client-server communication.
- Implemented billing.log on server.
- Multiple bug fixes.

SCIGRESS 2.4 (3.1)

- Implemented quantum semiempirical docking: both local and on server. Can check partial results. Can detach client from calculations being performed on server. Can check status of detached calculations, re-attach and download results.
- Implemented “Create Docking Spreadsheet” wizard.
- Implemented conformer generation with LocalSCF, implemented selection of unique conformers.
- Conformer generation merged into “Create Docking Object”.
- Server-side Phase calculations can be easily parallelized directly from SCIGRESS client.
- Selection of cells to be evaluated extends automatically when additional samples are created during evaluation.
- Return output files of failed experiments.
- Added option to specify a non-default name of a document being created in a wizard.
- Added new versions of bioexercises consistent with updated Teaching with SCIGRESS e-book.

- Desktop version for Linux (Ubuntu, OpenSUSE, Debian, Centos) 32&64 bit, KDE and GNOME released as public BETA.

SCIGRESS 2.4 (3.0)

- General:
  - Complete redesign of GUI, including menu system for better productivity.
  - New 3D molecular graphics with improved appearence and performance.
  - PubChem query functionality.
  - Export of presentation-quality graphics.
  - Compounds library featuring drag & drop.
  - ProjectExplorer and project handling functionality including dependencies between samples, calculation results and analyses.
  - Demo mode.
  - Teaching with SCIGRESS pdf book for beginners and students.
  - Reduced memory, CPU and disk usage by chemical samples.
  - Fixed performance and stability issues.
  - Improved ModelExplorer functionality.
  - Improved molecule drawing and manipulation tools.
  - Improved and simplified tools for building advanced periodic systems.
  - Improved protein sequence handling.
  - Improved Chemical Spreadsheet functionality.

- Calculations:
  - Potential Parameter Optimization for Molecular Dynamics.
  - Potential Editor for Molecular Dynamics.
  - EEM method for partial charge calculations during Molecular Dynamics calculations.
  - Improved docking engine.
  - RM1 added to MO-G semiempirical engine.
  - Redesigned Procedure Library.
  - Run Single compute Engine functionality for advanced users.
  - Simplified wavefunction analysis tools.

SCIGRESS 2.1

- User-defined elements: Workspace now allows you to define and use your own chemical elements for MD-ME calculations.
- Variable-charge potential: The variable-charge potential is now available for MD-ME potential assignment.
- Extension of library: The ME Mol files and ME's infinite chain unit cell files are newly added to the Fragment Library.
- Support for ME Mol file format: Workspace now enables importing ME Mol files and saving as CSF files.
- Common Data folder: The files stored in the Common Data folder can be used as component data in model builders.
- Mouse/keyboard-based view transform: Workspace now enables you to rotate,translate and scale a displayed model using only mouse buttons (and wheel) and key modifiers.

- Dipole moment display: Workspace now enables displaying a dipole moment graphically.
- Statistics information on chart: Workspace now enables you to obtain statistics information between two specified plot points on a chart of MAP file.
- Quick view of physical properties of MD-ME results: Workspace now allows you to quickly obtain physical properties such as static dielectric constant, isothermal compressibility, etc.
- PM6 method support: The new hamiltonian PM6 is now available in the MO-G compute engine.

SCIGRESS 2.0

- Project centric user interface for superior management of projects and data.
- Materials Science features:
    - Model builders including builders for polymers, dendrimers, interfaces, and layers.
    - Molecular dynamic engine.
    - Comprehensive molecular dynamics analysis.
- Chemical database interfaces to CambridgeSoft ChemFinder.
- Interface to latest version of MOPAC.
- Latest version of CONFLEX.
- Interface to GAMESS.
- Improved performance and stability of SCIGRESS application and compute engines.

SCIGRESS 1.0

SCIGRESS is molecular design modeling software currently available for Microsoft Windows XP or Vista. A state-of-the-art molecular builder and visualizer enables the researcher to import experiment structures using a variety of industry standard formats, or to build novel structures using a multi-function tool palette. SCIGRESS integrates Scigress Explorer (former **CAChe**) and Materials Explorer into one powerful suite.

Tools available to the researcher for analyzing molecular structure and properties include the following (compute engines or interfaces required to evaluate properties are shown in parentheses):

- Reaction mechanism determination via determination of reaction transitions states and evaluation and visualization of intrinsic reaction coordinates (MO-G)
- Determination of low energy conformations (CONFLEX)
- Vibrational analysis including visualization of IR spectra and normal modes of vibration
- Interactions with radiation including visualization of UV-visible spectra, and identification of molecular orbitals responsible for orbitals electronic transitions (ZINDO, MO-S)
- 3D-visualization of electronic surfaces including orbitals, electron densities, and electrostatic surfaces (Huckel MO-G, ZINDO)
- Visualization of experimental crystal and protein structures (Workspace, SequenceView)
- Molecular mechanics and dynamics (Mechanics)

ADDITIVE
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