



SCiGRESS

| Release Notes |



SCIGRESS 2.0

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Overview description

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.

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)

What's new in Version 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 Dynamics engine
 - Comprehensive Molecular dynamics analysis
- Chemical database interfaces to CambridgeSoft ChemFinder
- Interface to latest versions of MOPAC
- Latest version of CONFLEX
- Interface to GAMESS
- Improved performance and stability of SCIGRESS application and compute engines

System requirements

Supported operating systems are Windows® XP (service pack 2) and Windows® Vista. For proper function of SCIGRESS it is recommended that on the installed platform one's system has a minimum of 1Gb of RAM and OpenGL accelerated graphics hardware. A minimum of 250Mb of hard disk space is required to install SCIGRESS.

Calculation methods

- **CONFLEX:** CONFLEX generates low energy conformers of a molecule of any shape. Use CONFLEX to compute optimum geometries, conformations and potential energy maps.
- **Dynamics:** Dynamics methods use classical, empirical force fields to approximate the movement of atoms. The dynamics application uses the same force fields (MM2 and MM3) as the Mechanics application. Use dynamics to visualize conformations that occur as a result of molecular motion; discover information regarding the structure-energy relationships of the molecule; investigate conformational space occupied by the system at varying temperatures.
- **Huckel:** Extended Huckel is a semiempirical quantum mechanical method used for calculating the electronic wavefunction to determine electron densities, molecular orbitals, electrostatic potentials, partial charges and bond orders.
- **Mechanics:** Mechanics is used by Scigress to optimize molecular structures using an augmented version of Allenger's standard MM2 and MM3 classical force field.
- **MO-G:** MO-G is a general-purpose semi-empirical molecular orbital package. Use MO-G to calculate the vibrational spectra, thermodynamic quantities, isotopic substitution effects and force constants for molecules, radicals, ions, and polymers. For studying chemical reactions a transition state location routine is also available. The MO-G user guide is located in the *Product Literature* folder of the SCIGRESS installation folder.
- **MO-S:** MO-S is a semi-empirical program with advanced methods (configuration interactions and random phase approximation) for evaluation of UV-visible electronic absorption spectra. Use MO-S for the evaluation and interpretation of electronic structure transitions. The MO-S user guide is located in the *Product Literature* folder of the SCIGRESS installation folder.
- **ZINDO:** ZINDO computes semi-empirical quantum mechanical values for molecular properties and spectra of molecules. ZINDO uses theoretically-based INDO parameterization and therefore contains parameters for more elements than does the experimentally-based MO-G or MO-S. However, because MO-G has been specifically parameterized for ground-state heats of formations MO-G is the better method for computing molecule structures and energetics. Use ZINDO to carry out calculations of electronic UV-visible absorptions spectra.
- **MD-ME:** MD-ME is an advanced molecular dynamics program and can be used to study the molecular dynamics of model systems including crystals, polymers,

dendrimers, etc. The program implements a wide variety of force fields that can be used with organic and non-organic models.

- **MOPAC2007** [Interface Only]: MOPAC2007 is developed and released by Stewart Computational Chemistry. Please refer to www.openmopac.net for details on how to obtain the program. Details on how to configure and use the SCIGRESS MOPAC2007 interface can be found in the file ***MOPAC2007_IF_User_Manual.pdf*** located in the *Product Literature* folder of the SCIGRESS installation folder.
- **ADF** [Interface Only]: ADF is developed and released by Scientific Computing & Modelling NV (SCM). Please refer to www.scm.com for more information. Details on how to configure and use the SCIGRESS ADF interface can be found in the file ***ADF_IF_User_Manual.pdf*** located in the *Product Literature* folder of the SCIGRESS installation folder.
- **CONFLEX6** [Interface Only]: CONFLEX is developed and released by CONFLEX Corporation. Details on how to configure and use the SCIGRESS CONFLEX6 interface can be found in the file ***CONFLEX6_IF_User_Manual.pdf*** located in the *Product Literature* folder of the SCIGRESS installation folder.
- **Advance/PHASE** [Interface Only]: Advance/PHASE is developed and released by AdvanceSoft Corporation. Please refer to www.advancesoft.jp for more information. Details on how to configure and use the SCIGRESS Advance/PHASE interface can be found in the file ***PHASE_IF_User_Manual.pdf*** located in the *Product Literature* folder of the SCIGRESS installation folder.
- **GAMESS** [Interface Only]: GAMESS is developed and released by the Gordon Group at Iowa State University. Please refer to www.msg.chem.iastate.edu/gamess for details on how to obtain the program. Details on how to configure and use the SCIGRESS GAMESS interface can be found in the file ***GAMESS_Interface_User_Manual.pdf*** located in the *Product Literature* folder of the SCIGRESS installation folder.

Please refer to the SCIGRESS User Guide and the respective program manuals for details on how to use calculation methods.

Graphics performance and display issues

On some hardware configurations (e.g. Intel® integrated graphics cards) SCIGRESS might experience graphics performance and display issues. If you experience such problems we recommend that you update the graphics drivers for your hardware. Please contact your hardware vendor for more details on performing updates to system drivers.

In some cases disabling graphics hardware acceleration can actually improve the stability of the application. If you continue to experience problems after updating to use the latest drivers for your graphics hardware try to adjust the hardware acceleration used by the graphics card. To do this:

- Open the Display control panel or right click on the Windows desktop and select Properties
- Select the Setting tab in the Display Properties dialog box
- Click the Advanced button to display the properties dialog for the monitor
- Select the Troubleshoot tab
- The Hardware acceleration can now be set manually

On some configurations running Windows Vista display problems might be resolved by changing certain OpenGL settings, in particular changing the “OpenGL depth buffer bit” from default to “16 bit”.

Please refer to the manual for the graphics card on your system for details on how to disable OpenGL acceleration specific to the graphics hardware or change the OpenGL settings.

Troubleshooting

- Interface becomes sluggish: Should you experience sluggish behavior in the application you may free unused memory allocated by the program by clicking on the wastepaper basket icon in the lower, right-hand corner of the interface.
- Energy maps or other graphical displays are completely gray: If you encounter this condition try upgrading the driver for your video card. This is a known problem with some of the older Intel® video card drivers.

Contact Information

United States and Canada

Fujitsu America

Computers_Biosciences_Support

@us.fujitsu.com

Europe/South America/Africa

Fujitsu Kyushu Systems

ccs@fqspl.pl

Japan and Asia

Fujitsu Limited

biochem-info@ml.css.fujitsu.com