



Green Chemistry Expert System (GCES) Version 0.99

The Green Chemistry Expert System (GCES) is a stand-alone computer program that can be used to select green chemicals and reactions. Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. This new approach to pollution prevention is the central focus of the U.S. Environmental Protection Agency's (EPA's) Green Chemistry Program, an initiative under the EPA Design for the Environment Program.

How Does GCES Assist Users?

- Identifies opportunities to eliminate or reduce the use or generation of hazardous substances during chemical manufacture.
- Suggests molecular modifications to minimize toxicity and provides techniques that might reduce hazards to human health and the environment.
- Presents technical information on green synthesis, solvent systems, reaction conditions, and chemical products.
- Provides a database of useful green chemistry references.
- Prints results in an easy-to-read format.

How Does GCES Work?

The five GCES modules help users build a green chemical process, design a green chemical, or survey the field of green chemistry. The system is equally useful for new or existing chemicals and their synthetic processes. It includes extensive system documentation describing each of the features and how to use them.

- The Synthetic Methodology Assessment for Reduction Techniques (SMART) module quantifies and categorizes the hazardous substances used in or generated by a chemical reaction based on information provided by the user. Reactions can be modified and reevaluated to optimize their green nature.
- The Green Synthetic Reactions module provides technical information on green synthetic methods of making chemicals.
- The Designing Safer Chemicals module describes how chemical substances can be modified to make them safer; it is organized by chemical class, properties, and use.
- The Green Solvents/Reaction Conditions module includes technical information on green alternatives to traditional solvent systems and allows users to search for green solvents based on physicochemical properties.
- The Green Chemistry References module allows the user to obtain additional information using a number of search strategies as well as add references to the module.





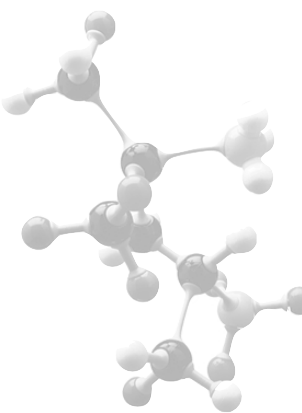
What Information Do I Need to Use GCES?

For the SMART Module:

- The quantity of each chemical used and generated in a manufacturing process.
- The role each chemical plays in the reaction (e.g., product, feedstock, catalyst, solvent, etc.).
- Basic reaction data, including batches per year, product yield, and annual production volume.

For the other modules, technical information on a chemical product or its manufacturing process might be required; the user also can browse each of these modules without entering any specific information.

How Can GCES Output Be Used?



The expert system selects chemicals and reactions that eliminate or minimize the use and production of hazardous chemicals. EPA uses GCES to identify pollution prevention opportunities for the synthesis of new and existing chemicals. Users should find the output valuable for any chemical manufacturing process or green chemistry initiative.

- The SMART module calculates the theoretical amount and hazard of each reaction component on an individual chemical basis and then points users to other modules for information on developing a green alternative.
- The Green Synthetic Reactions module provides a searchable list of green synthetic processes including descriptions, keywords, and references.
- The Designing Safer Chemicals module leads the user through a series of questions and then identifies molecular modifications to minimize hazard.
- The Green Solvents/Reaction Conditions module provides details on green solvents and techniques that can be used to design green reactions.
- The Green Chemistry References module provides references to additional information.

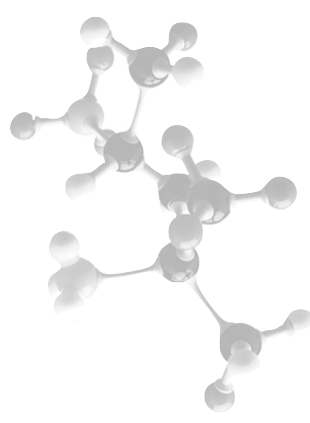


What Type of Computer System Do I Need?

Hardware: IBM-compatible computer running Windows 3.x, Windows 95, or Windows 98.

- For a complete installation: 20 MB free hard drive disk space.
- For a partial installation: 5 MB free hard disk space and 15 MB on another disk, such as a removable-media drive, for the GCES external databases.

Software: GCES is completely self-contained and requires no additional software. Some advanced features, such as running QSAR estimation software from within GCES (e.g., ECOSAR), require the installation of other EPA or commercially available software packages.



How Can I Obtain a Copy of GCES?

GCES is available for download at www.epa.gov/greenchemistry. There is no charge for this program.

How Can I Get More Information?

Technical Contact: Richard Engler
U.S. Environmental Protection Agency
1200 Pennsylvania Ave., NW (7406M)
Washington, DC 20460
Phone: 202 564-8740
Fax: 202 564-8679
E-Mail: engler.richard@epa.gov
www.epa.gov/greenchemistry

