

New Tools to Improve Access to Green Chemistry and Engineering Resources

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**Green
Chemistry
Institute**



Green Chemistry Institute

- ❑ Founded in 1997 as an independent, nonprofit organization to promote green chemistry through research, education, industrial implementation, information dissemination, conferences and symposia
- ❑ Formed an alliance with the American Chemical Society in 2001
- ❑ Headquarters staff located in Washington D.C.
- ❑ Worldwide network of technical expertise



Green
Chemistry
Institute

Green Chemistry Institute

□ Mission:

To advance the implementation of green chemistry principles into all aspects of the chemical enterprise.



Green
Chemistry
Institute

Green Chemistry Institute

- Research
- Education
- Industrial Implementation
- International Cooperation
- Policy Advocacy
- Conferences & Awards

Effective dissemination of Green Chemistry information
is central to each of these endeavors



Spreading the Information

- After 10+ years of work from all sectors, there now exists a great deal of good information about green chemistry:
 - Alternative chemicals
 - Alternative processes
 - Ground-breaking research
 - Industrial success stories

But, that information is scattered and not readily accessible



GCI Website

- GCI is upgrading its website to become a powerful green chemistry and green engineering information resource:

www.greenchemistryinstitute.org



Spreading the Information

- GCI is beginning several database projects to bring together green chemistry information, and make it readily available for use by:
 - Chemists, engineers, and leaders throughout the chemical enterprise as well as people outside of it
 - Academia
 - Industry
 - Government
 - NGO's
 - Supply chain
 - Consumers



Two Information Databases being Developed at GCI

- Protocol Database addresses:
 - What is green chemistry? What are the Principles?
 - How do I use green chemistry in my own process or synthesis?
 - What are the opportunities for using green chemistry and green engineering in my work?
 - What green chemistry information resources exist and how do I find them?
- Catalog of Examples Database addresses:
 - What are proven examples of green chemistry and engineering? What are some academic, small business, industrial, or government examples?
 - Are there examples that are similar to my work/field?



Information Database Projects at GCI

Protocol Database

An interactive tool that lets chemists & engineers identify opportunities for applying green chemistry to their work:

- Users walk through a survey
- Tool generates a list of potential opportunities
- Tool provides a list of resources including websites, programs, literature references, keywords, etc.

Catalog of Examples Database

An online search tool where users can access info. on:

- Who's doing green chemistry
- New chemicals & processes
- Chemicals being replaced
- Industries affected by green chemistry work



Flow of the Protocol Database

Survey

- A survey completed by the user
- Based on principles of green chemistry and green engineering
- Identifies opportunities for using green chemistry or engineering

*Based on the user's responses in the **Survey**,
an **Opportunity Assessment Report** is generated*

Opportunity Assessment Report

- Summarizes the opportunities
- Highlights potential benefits
- Includes brief case study examples

*The user is linked to green chemistry and green
engineering **Resources** relevant to their work*

Framework of Resources

- Contains information resources including websites, programs, models, databases, literature references, keywords, etc.



Protocol Survey is based on Green Chemistry Principles, sorted by Focus Areas

Focus Area I:
Alternative
synthetic
pathways

- Maximize atom economy
- Design less hazardous chemical syntheses
- Use renewable feedstocks
- Avoid chemical derivatives
- Use catalysts, not stoichiometric reagents

Focus Area II:
Alternative reaction
conditions or
processing

- Prevent waste (*see example on slides 13-14*)
- Use safer solvents and reaction conditions (*example on slides 15-16*)
- Increase energy efficiency
- Analyze in real time to prevent pollution
- Minimize the potential for accidents

Focus Area III:
Safer product

- Design safer chemicals and products (*example on slides 17-18*)
- Design chemicals and products that degrade after use

Abbreviated Principles based on: Anastas, P. T. and Warner, J. C.

Green Chemistry: Theory and Practice, Oxford University Press: New York, 2000.



Protocol Survey is also based on Principles of Green Engineering

Abbreviated List:

- 1) All material/energy inputs/outputs are inherently nonhazardous
- 2) Prevent waste
- 3) Separation/purification should minimize energy/materials
- 4) Maximize mass, energy, space, and time efficiency
- 5) Should be output pulled rather than input pushed
- 6) Consider entropy/complexity for recycling/reuse/disposal
- 7) Target durability not immortality
- 8) Don't design for unnecessary capacity or capability
- 9) Minimize material diversity for disassembly and value retention
- 10) Integration and interconnectivity with available energy and materials
- 11) Design for performance in a commercial afterlife
- 12) Renewable material and energy inputs



Representative Content of Protocol Database: *Waste Reduction*

- Survey*
 - Can the process or synthetic route be redesigned to reduce or eliminate **waste**?
- Opportunity Assessment Report
 - Identifies that waste can be reduced or eliminated
 - Describes **benefits** (such as cost savings) and a case study **example** (Imation's DryView™ Imaging Systems, 1997 PGCC Award Winner)
- Framework of Resources*
 - **Links** to tools that can aid the user in assessing, managing, minimizing, and reducing waste, such as the **EPA Waste Reduction Model**
<http://yosemite.epa.gov/oar/globalwarming.nsf/content/ActionsWasteWarm.html>

* the actual survey contains a series of questions and the framework contains multiple resources



EPA's Waste Reduction Model

<http://yosemite.epa.gov/oar/globalwarming.nsf/content/ActionsWasteWarm.html>

Global Warming - Waste

U.S. Environmental Protection Agency

WARM Online

(Version 7, 8/05)

EPA created WARM to help solid waste planners and organizations track and voluntarily report greenhouse gas emissions reductions and energy savings from several different waste management practices. WARM Online was last updated August 2005.

Use this worksheet to describe the baseline and alternative MSW management scenarios that you want to compare. Please follow the steps below to enter your material tonnage information in the input boxes in the tables, and select appropriate landfill and waste transport characteristics.

Tips:

- If the listed material is not generated in your community/organization or you do not want to analyze it, leave it blank or enter 0.
- Make sure that the total quantity generated equals the total quantity managed.
- If you have any questions, consult the [WARM User's Guide](#).

Step 1. Baseline Scenario

Please describe your current (or baseline) waste management scenario by entering the tons of each material type that is generated and disposed.

Material	Tons Generated	Tons Recycled	Tons Landfilled	Tons Combusted	Tons Composted
Corrugated Cardboard	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	N/A
Office Paper	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	N/A
Mixed Metals	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	N/A
Mixed Plastics	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	N/A
Mixed Recyclables	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	N/A
Mixed Organics	<input type="text"/>	N/A	<input type="text"/>	<input type="text"/>	<input type="text"/>

Selected lines from the table...Model continues on the website...



Representative Content of Protocol Database: *Use Safer Solvents/Conditions*

- Survey*
 - Can a **less volatile** solvent be used?
- Opportunity Assessment Report
 - Identifies that a less volatile solvent can be used
 - Describes **benefits** (such as cost savings for regulations and safety) and a case study **example** (use of supercritical carbon dioxide as a solvent, 1997, 2002 and 2004 PGCC Award Winners)
- Framework of Resources*
 - **Links** to tools that can aid the user in selecting alternative solvents, such as the **NCMS Solv-DB** (*National Center for Manufacturing Sciences Solvent Database*) <http://solvdb.ncms.org>

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NCMS Solvent Database

<http://solvdb.ncms.org/solvdb.htm>



SOLV-DB[®]

Choose Solvent Lookup Criteria:(How to use these selections.)

Solvent Name	Select By Solvent Name
Chemical Abstracts Number	Select By Chemical Abstracts Number
Sax Number	Select By Sax Number
Chemical Formula	Select By Chemical Formula
Select By Chemical Category	Select By Chemical Category
Select By Property Range	Select By Property Range
Select By Matching Text	Select By Matching Text
Select By Synonym	Select By Solvent Synonym



Representative Content of Protocol Database: *Design Safer Chemicals*

- Survey*
 - Can the chemical structure be modified to create a **less toxic** chemical?
- Opportunity Assessment Report
 - Identifies that less toxic products can be designed
 - Describes **benefits** (such as cost savings for regulations and safety) and a case study **example** (Bayer's Baypure™ CX non-toxic chelating agent, 2001 PGCC Award Winner)
- Framework of Resources*
 - **Links** to tools that can aid the user in assessing and minimizing toxicity, such as the **EPA EPI Suite™ software models**
<http://www.epa.gov/opptintr/exposure/docs/episuite.htm>

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EPA's EPI Suite™

<http://www.epa.gov/opptintr/exposure/docs/episuite.htm>

Exposure Assessment Tools and Models

U.S. Environmental Protection Agency

Estimation Program Interface (EPI) Suite

Estimation Program Interface (EPI) Suite

What Does EPI Suite™ Do?

- The EPI (Estimation Programs Interface) Suite™ is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite™ uses a single input to run the following estimation models: KOWWIN™, AOPWIN™, HENRYWIN™, MPBPWIN™, BIOWIN™, PCKOCWIN™, WSKOWWIN™, BCFWIN™, HYDROWIN™, and STPWIN™, WVOLWIN™, and LEV3EPI™. EPI Suite™ was previously called EPIWIN.

What's New?

- [Description of Updates for EPI Suite Version 3.12 \(November 30, 2004\)](#)
- [Description of Updates for EPI Suite Version 3.11 \(June 10, 2003\)](#)

[Download EPI 3.12](#)

More information available on the website...



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Catalog of Examples: Search Topics

Each Catalog entry is matched to multiple search topics and sub-topics, so the user can easily find entries.

□ Industry Sectors:

- Agriculture/food/forestry
- Automotive
- Biotechnology
- Coatings
- Construction
- etc.

□ Materials/Chemicals:

- Adhesives and sealants
- Bulk and commodity chemicals
- Catalysts
- Colorants
- Fine chemicals
- etc.

□ Green Chemistry Keywords:

- Green feedstocks
- Green reagents
- Green solvents
- Designing safer chemicals
- Green synthetic pathway design

Text searching is also an option.



Samples of Entries in the Catalog of Examples Database

2005 Presidential Green Chemistry Challenge Award Winners:

Title: A Platform Strategy Using Ionic Liquids to Dissolve and Process Cellulose for Advanced New Materials

Sponsor: Professor Robin D. Rogers, The University of Alabama

Search Topic Matches in Catalog: **Industry Sectors:** automotive, biotechnology, nanotechnology, pulp and paper, textiles/fabrics/fibers; **Chemicals/Materials:** plastics/polymers/resins; **Green Chemistry Keywords:** ionic liquids, renewable feedstocks.

Title: NovaLipid: Low *Trans* Fats and Oils Produced by Enzymatic Interesterification of Vegetable Oils Using Lipozyme

Sponsor: Archer Daniels Midland Company / Novozymes

Search Topic Matches in Catalog: **Industry Sectors:** ag/food/forestry; **Chemicals/Materials:** fine and specialty chemicals; **Green Chemistry Keywords:** bio-catalysis/enzyme, hazardous chemical reduction/elimination, waste quantity reduction.

Additional 2005 winners: Metabolix, Inc., Merck & Co., Inc., BASF Corporation, Archer Daniels Midland Co.



GCI Projects: Future Expansion

- Catalog of Examples and Protocol Databases are seeds for future efforts; we anticipate the Catalog of Examples to be internet-accessible *by the end of 2005*.
- These tools will be built with expansion in mind, to provide an ideal way for GCI to fulfill its catalyst role:
 - Use the initial tools as the foundations for ever-growing resources on green chemistry.
 - GCI will partner with other groups to add their data to the pool.
 - The GCI resource becomes the mechanism by which a diverse and ever-growing amount of green chemistry data is made available.



Acknowledgements

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- U.S. EPA's Design for the Environment (DfE) – Catalog of Examples Database
- PRF – Protocol Database

Personnel

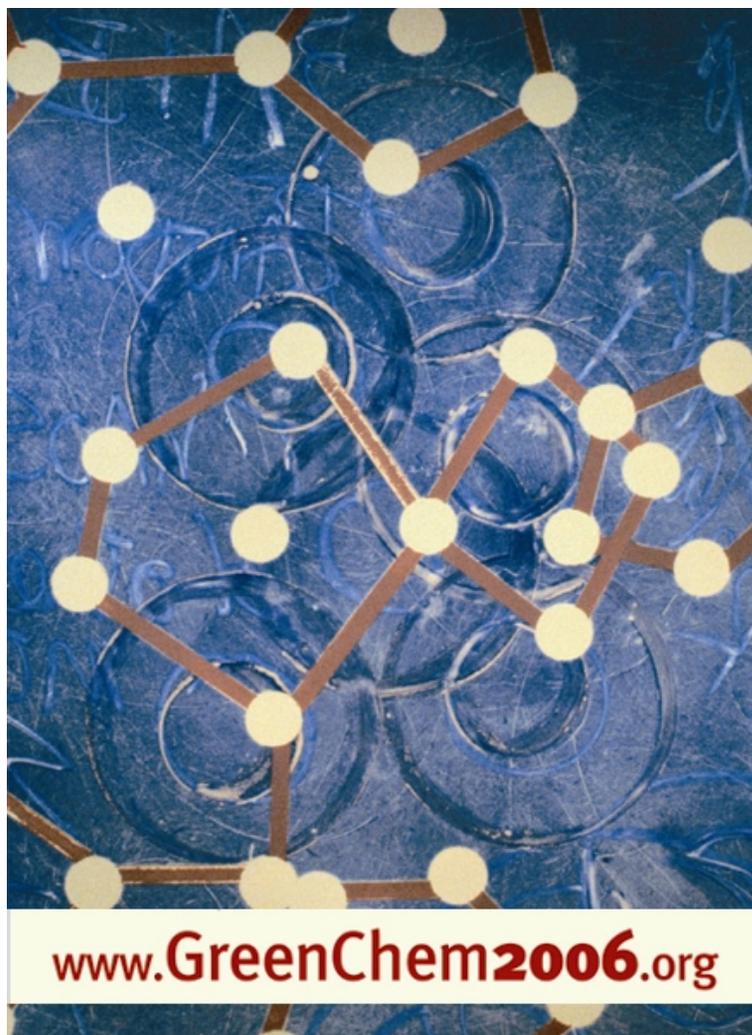
- James Rea
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- Alita Jones
 - Investigating the Green Engineering aspects for the Protocol Database
- Eric Chang
 - Contributing to Catalog of Examples Database

www.greenchemistryinstitute.org



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Mark Your Calendar!



MARK YOUR CALENDAR

10th Annual Green Chemistry & Engineering Conference

› *Designing for a
Sustainable Future*

June 26–29, 2006

WASHINGTON, DC





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