Green Chemistry Education Webinar Series
April 17, 2014

The 12 Principles of Green Chemistry: Sustainability at the Molecular Level
What is the GC3?

A cross sectoral, B-2-B network of more than 70 companies and other organizations formed in 2005 with a mission to promote green chemistry and design for environment (DfE), nationally and internationally.
The 12 Principles of Green Chemistry: Sustainability at the Molecular Level: Speakers

Amy Cannon, Ph.D., Executive Director, Beyond Benign

John C. Warner, President and Chief Technology Officer, Warner Babcock Institute for Green Chemistry, LLC
Ground Rules

• Due to the number of participants on the Webinar, all lines will be muted.

• If you wish to ask a question or make a comment, please type in the Q&A box located in the drop down control panel at the top of the screen

• Questions will be answered at the end of the presentation.
Upcoming Events
http://www.greenchemistryandcommerce.org/

The Coop Story: How a leading Danish Retailer is working to eliminate endocrine disrupting chemicals from its products, Wednesday, April 30, 1pm est/10am pst

And....
THANK YOU!
The 12 Principles of Green Chemistry: Sustainability at the Molecular Level

Amy S. Cannon
Executive Director
Beyond Benign

John C. Warner
President and Chief Technology Officer
Warner Babcock Institute for Green Chemistry, LLC
Disclaimer
Today’s Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI
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Green Chemistry is the *design* of chemical products and processes that reduce or eliminate the *use* and/or *generation* of hazardous substances.
# The Twelve Principles of Green Chemistry

1. **Prevention.** It is better to prevent waste than to treat or clean up waste after it is formed.

2. **Atom Economy.** Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

3. **Less Hazardous Chemical Synthesis.** Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

4. **Designing Safer Chemicals.** Chemical products should be designed to preserve efficacy of the function while reducing toxicity.

5. **Safer Solvents and Auxiliaries.** The use of auxiliary substances (solvents, separation agents, etc.) should be made unnecessary whenever possible and, when used, innocuous.

6. **Design for Energy Efficiency.** Energy requirements should be recognized for their environmental and economic impacts and should be minimized. Synthetic methods should be conducted at ambient temperature and pressure.

7. **Use of Renewable Feedstocks.** A raw material or feedstock should be renewable rather than depleting whenever technically and economically practical.

8. **Reduce Derivatives.** Unnecessary derivatization (blocking group, protection/deprotection, temporary modification of physical/chemical processes) should be avoided whenever possible.

9. **Catalysis.** Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

10. **Design for Degradation.** Chemical products should be designed so that at the end of their function they do not persist in the environment and instead break down into innocuous degradation products.

11. **Real-time Analysis for Pollution Prevention.** Analytical methodologies need to be further developed to allow for real-time in-process monitoring and control prior to the formation of hazardous substances.

12. **Inherently Safer Chemistry for Accident Prevention.** Substance and the form of a substance used in a chemical process should be chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires.
Green Chemistry

- More environmentally benign than alternatives
- Perform better than alternatives
- More economical than alternatives
Green Chemistry

- Safety
- Green Chemistry
- Performance
- Cost
Of all the products and processes...

Maybe 10% are benign...

Maybe 25% have alternatives available...

65% Still have to be invented!
How does Green Chemistry fit into the big picture of Sustainability.
Green Chemistry is also known as sustainable chemistry.
Today’s Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI
Product Design

1. Identify and prioritize key attributes
2. Design/plan metrics and tools to evaluate
3. Identify possible existing materials
4. Measure/Quantify performance of materials
   - If acceptable materials are not found -> Invent new technology
   - If acceptable materials are found -> Make Product

This will happen less than 25% of the time.
Performance and Cost

1. Identify and prioritize key attributes
   - Industry Standards
   - Voice of Customer
   - Business Economics
   - Color stability in light
   - Stability to cold and heat
   - Cost

2. Design/plan metrics and tools to evaluate
   - ASTM Tests
   - In-house historical
   - Customer Supplied
   - Z% fading in Y amount of time under X amount of intensity
   - < W number of cracks > V mm in length after U hours at T °C
   - Less that S$/gallon

3. Identify possible existing materials
   - Pre-existing supplier relationships
   - Product development intelligence
   - Supply chain sales and marketing
   - Material A
   - Material B
   - Material C

4. Measure/Quantify performance of materials
   - In house testing
   - Supplier testing
   - 3rd Party testing
   - Material C: S”, T”, U”, V”, W”, X”, Y”, Z”

5. If acceptable materials are not found -> Invent new technology
   - In house R&D
   - Supplier R&D
   - University/Government
   - 3rd Party R&D
Performance, Cost, Safety and Sustainability

Identify and prioritize key attributes
- Industry Standards
- Voice of Customer
- Business Economics
- Regulatory Agencies
- NGOs
- ASTM Tests
- In-house historical
- Customer Supplied
- Government Agencies
- 3rd Party Organizations

Design/plan metrics and tools to evaluate
- Pre-existing supplier relationships
- Product development intelligence
- Supply chain sales and marketing
- Alternatives Assessment

Identify possible existing materials
- In house testing
- Supplier testing
- 3rd Party testing
- Government Labs

Measure/Quantify performance of materials
- Material A
- Material B
- Material C

If acceptable materials are not found -> Invent new technology
- In house R&D
- Supplier R&D
- University/Government
- 3rd Party R&D

Color stability in light
- Stability to cold and heat
- Cost
- Safety (Mutagenicity, Endocrine Activity, Hepatotoxicity...)
- Sustainability (Energy Usage, Renewables Usage...)
- Z% fading in Y amount of time under X amount of intensity
- < W number of cracks > V mm in length after U hours at T °C
- Less that S$/gallon
- > R mg/kg on Ames Test
- > Q mg/kg on Tier three TiPED assay
- < P% mitochondrial damage with CM-H2DCFDA probe
- < N BTU per manufactured unit
- > M % Biobased Carbon (ASTM D6866)

A deliverable attribute must be:

**Quantifiable**

Color doesn’t fade.

**Achievable**

Color NEVER fades (IS NOT achievable)  
Color only fades a little over a certain period of time (IS achievable)

**Measurable**

Optical density decreases by less than 10% after 48 hours with 20000 lumens solar simulator.
Today’s Talk:

- Green Chemistry
- Product Design
- Zero and Big Numbers
- How it fits together
- Examples from WBI
Lets talk about nothing:

There are two issues with the use of “free” and “zero”:

(1) What does “chemical free” mean?
“BPA Free”:

(2) Can we ever have an “anything” free product?

BPA in cash register receipts....

No BPA added in the coating...

Unavoidable trace amounts of BPA in the paper!!!!

So what does “BPA-Free” mean?

Is it achievable?
TiPED
Tiered Protocol for Endocrine Disruption

DOI: 10.1039/c2gc35055f
“Nothing” and Big Numbers:

55 Gal Drum water  
6.97 x 10^{27} Molecules of water

Teaspoon of sugar  
7.93 x 10^{21} Molecules of sugar  1.14 ppm

Grain of sugar  
5.22 x 10^{17} Molecules of sugar  50.6 ppt

Nanogram of sugar  
1.76 x 10^{12} Molecules of sugar  176 Billion molecules of sugar

Amedeo Avogadro
Today’s Talk:

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The ability to invent & design solutions to a problem is directly proportional to the quality of the description of success.

Quantifiable
Achievable
Measurable
Safety and Sustainability

1. Identify and prioritize key attributes
   - Industry Standards
   - Voice of Customer
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Chemicals Policy

Toxicology and Environmental Health Sciences

Alternatives Assessment

Green Chemistry
We can’t sit on our hands waiting for all the criteria to be sorted out.

While zero may not be achievable from a regulatory perspective...

From an innovation and design perspective, it will always point us in the right direction.
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- Examples from WBI
John Warner  Amy Cannon

Jim Babcock  Joe Pont, CEO

100 Research Drive
Wilmington, MA 01887
**Science**

- **Explore**
  - Observe and define structure and dynamics.
- **Basic Research**
- **Understand**
  - Identify and characterize impact of changes of structure on dynamics and dynamics on structure.
- **Parameterize**
  - Design alterations in structure and/or dynamics to purposefully control response.
- **Create**
  - Create a potentially useful prototype.

**Business**

- **Explore**
  - Observe and define a product and market.
- **Market Analysis**
- **Understand**
  - Identify and characterize market history and likely future trends.
- **Parameterize**
  - Design potential products and assess potential markets and parameters for success.
- **Commercialize**
  - Commercialize a successful product.

**Technology Greenhouse**
**Technology Incubator**
Business Sectors at WBI

Pharmaceuticals, Agriculture and Biotechnology

Chemical Sciences, Development and Manufacturing

Textiles, Materials and Coatings

Energy, Natural Resources and Environment

Cosmetics, Personal Care and Consumer
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Cosmetics, Personal Care and Consumer
Alzheimer’s Disease Therapeutic

Lead Development History (Bis ANS)

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<td>Aggregation EC50 (uM)</td>
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<td>47</td>
<td>64</td>
<td>81</td>
<td>89</td>
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<tr>
<td>Disaggregation EC50 (uM)</td>
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Log [EC50 (M)]
Parkinson’s Disease Therapeutic

CuATSM

H N N Cu N N Cu
H C S S C H C
H C N N N N N H
H C S S C H C

PARKINSON’S FUNDED GRANT

Lead Optimization for a Parkinson’s Disease Therapeutic.

GRANT ABSTRACT

Objective/rationale: CuII(CO3) has the potential to delay disease progression in Parkinson’s disease, based on extensive pre-clinical modal data. CuII(CO3) has been shown to significantly improve motor function in standard models of Parkinson’s disease. The observed motor improvement correlates with preservation of dopaminergic neurons in the brain and biomarkers of neuronal health and function.

Project Description: CuII(CO3) is sparingly soluble and requires formulation for oral administration prior to entering human clinical development. Procypta will pursue two parallel approaches to develop a proprietary oral formulation: (1) Procypta will work with the Warner Babcock Institute for Green Chemistry to develop a proprietary formulation of CuII(CO3) incorporating GRAT (Generally Regarded As Safe) excipients; and (2) Procypta will evaluate the solubility of proprietary CuII(CO3) analogues. The utility of these formulations will be evaluated using standard solubility and bioavailability assays and efficacy will be compared to the parent formulation in the MPTP toxic lesion preclinical model of Parkinson’s disease.

Relevance to Diagnosis/Treatment of Parkinson’s Disease: CuII(CO3) has the potential to delay disease progression in Parkinson’s disease. Successful clinical development of an optimized formulation of CuII(CO3) would provide Parkinson’s disease patients, on diagnosis, the opportunity to delay the progression of their disease and maintain their quality of life for a much extended period of time.

Related news

Recording Brain Activity Could Lead to Personalized Deep Brain Stimulation

How Fast Your Eyes Move Could Predict Cognitive Impairment

University of Melbourne enters agreement to develop therapy for Parkinson's disease

11 October 2013
Business Sectors at WBI

Pharmaceuticals, Agriculture and Biotechnology

Chemical Sciences, Development and Manufacturing

Textiles, Materials and Coatings

Energy, Natural Resources and Environment

Cosmetics, Personal Care and Consumer
Non-Toxic Natural Hair Color Restoration

3:45 PM (Before)
4:45 PM (After)
Business Sectors at WBI

Pharmaceuticals, Agriculture and Biotechnology

Chemical Sciences, Development and Manufacturing

Textiles, Materials and Coatings

Energy, Natural Resources and Environment

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Chemistry to increase use of recycled asphalt pavement and shingles
Paving with recycled asphalt and shingles
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9th Annual GC3 Innovators Roundtable
MAY 28-30 2014
St. Paul, Minnesota
Hosted by 3M
THANK YOU!