EMPLOYING DOZN™ 2.0
THE QUANTITATIVE GREENER ALTERNATIVE EVALUATOR IN ACADEMIC SETTINGS FOR SAFER LABS

Prof. Irv Levy
Chemistry Professor, Simmons University
GCC Director, Beyond Benign

Dr. Ettigounder Ponnusamy
Fellow and Global Manager
Green Chemistry MilliporeSigma
Welcome to the
Green Chemistry Connections
Webinar Series

Host:
Natalie O’Neil, Ph.D.
Higher Education Program Manager, Beyond Benign
@natjoneil
Submit questions in the Control/Chat box on the Control Panel

Recording and supporting documents will be available: https://www.beyondbenign.org/he-webinars/
The **Green Chemistry Commitment** (GCC) is a consortium program that unites the green chemistry community around shared goals and a common vision to:

- expand the community of **green chemists**
- **grow** departmental resources
- share **best practices** in green chemistry education
- affect systemic and lasting **change** in chemistry education

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Juliana Vidal
Communications Intern
Beyond Benign
@juliana_lvidal
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DOZN'2.0—A QUANTITATIVE GREEN CHEMISTRY EVALUATOR

BEYOND BENIGN WEBINAR, APRIL 29, 2020

Samy Ponnusamy
Fellow & Global Manager – Green Chemistry
Outline

• How the DOZN™ 2.0 System works?
• Applying DOZN™ 2.0 System
• Product Examples
• Advantages of DOZN™ 2.0
• DOZN™ 2.0 Demo
The 12 Principles of Green Chemistry

**Prevention**
It is better to prevent waste than to treat or clean up waste after it has been created.

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

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

**Reduce Derivatives**
Unnecessary derivatization (use of blocking groups, protection/deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.

**Less Hazardous Chemical Syntheses**
Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

**Designing Safer Chemicals**
Chemical products should be designed to affect their desired function while minimizing their toxicity.

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

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

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

**Design for Energy Efficiency**
Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.

**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.

**Inherently Safer Chemistry for Accident Prevention**
Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fires.
THE THREE GROUPS
Greener Products and Solutions
Re-engineering: DOZN™

An industry first, DOZN™ 2.0 is our proprietary Quantitative Green Chemistry Evaluator that enables us to consistently evaluate different products and processes against the 12 Principles of Green Chemistry—clarifying what’s “greener” about our greener alternatives.

To evaluate products and processes using DOZN™, we group the 12 Principles of Green Chemistry into three major groups:

1. Improved Resource Use
2. Increased Energy Efficiency
3. Reduced Human and Environmental Hazards

Then, an aggregate score on a scale of 0-100 is given, with 0 being the most desired.
Group 1: Improved Resource Use

\[ \Sigma \text{Principles } 1, 2, 7, 8, 9, \text{ & } 11 \]
\[ \frac{6}{6} \]

Group 1 is aimed at improving the material efficiency of the chemical or process.
Group 2: Increased energy efficiency

Group 2 = Principle 6

Group 2 acknowledges that there is more than just raw material input that contributes to greenness and is aimed at improving the energy efficiency of the chemical or process.
Group 3: Reduced human and environmental hazards

\[ \sum \text{Principles 3, 4, 5, 10, &12} \]

\[ \frac{5}{5} \]

Group 3 aims at improving the safety of humans and the environment by minimizing potential risks.
The Aggregate score

\[ \sum_{Group\ 1,\ 2,\ 3} \frac{\text{score}}{50} \]

- The Aggregate score gives greenness, a quick summary of the 12 principles
- The Aggregate score is on a scale of 0-100 with 0 being the most desired
- The DOZN™ system was verified and validated by third party
APPLYING THE DOZN² 2.0
Analysis

Procedural Run-through and Data Gathering

Matrix Data Entry

Score Calculation
PRODUCT EXAMPLES
Greener Products and Solutions
DOZN™ in Action: β-Amylase

β-Amylase—an enzyme commonly found in sweet potatoes—hydrolyzes starch into sugar.

6,000 lbs of sweet potatoes

1,900 gallons of acetone

No solvent required

2,000 lbs of sweet potatoes

Significant use of electricity

Minimal electricity use
**β-AMYLASE**

An enzyme commonly found in sweet potatoes—hydrolyzes starch into sugar

<table>
<thead>
<tr>
<th>Resource Used</th>
<th>12 Principles of Green Chemistry</th>
<th>Percentage of Improvement</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atom Economy</td>
<td>93%</td>
<td>Increased yield. Used less raw materials.</td>
<td></td>
</tr>
<tr>
<td>Waste Prevention</td>
<td>97%</td>
<td>Eliminated use of organic solvents. Reduced waste.</td>
<td></td>
</tr>
<tr>
<td>Reduce Derivatives</td>
<td>N/A</td>
<td>More efficient sweet potato use. Reduced auxiliary chemicals.</td>
<td></td>
</tr>
<tr>
<td>Renewable Feedstocks Use</td>
<td>96%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Real-Time Pollution Prevention</td>
<td>N/A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Catalyst</td>
<td>N/A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Energy Efficiency Design</td>
<td>100%</td>
<td>Eliminated need for elevated temperature and pressure.</td>
<td></td>
</tr>
<tr>
<td>Safer Chemical Design</td>
<td>N/A</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Safer Solvents and Auxiliaries</td>
<td>100%</td>
<td>Eliminated all organic solvents.</td>
<td></td>
</tr>
<tr>
<td>Design for Degradation</td>
<td>No Change</td>
<td>No increased impact with new procedure.</td>
<td></td>
</tr>
<tr>
<td>Inherently Safer Chemical for Accident Prevention</td>
<td>96%</td>
<td>Eliminated flammability and reactivity dangers.</td>
<td></td>
</tr>
</tbody>
</table>

**TOTAL PERCENT IMPROVEMENT** 98%  
**AGGREGATE SCORE** 57/100 (Re-engineered Score)
Re-engineered Products DOZN™ Scores

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Old Score</th>
<th>New Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-Aminobenzotriazole</td>
<td>100</td>
<td>44</td>
</tr>
<tr>
<td>1,3,5-Tris(4-Iodophenyl)benzene</td>
<td>100</td>
<td>4</td>
</tr>
<tr>
<td>(DHQD)2 PHAL</td>
<td>13</td>
<td>3</td>
</tr>
<tr>
<td>N-Benzyol-L-threonine methyl ester</td>
<td>21</td>
<td>4</td>
</tr>
<tr>
<td>Tetramethyl tin</td>
<td>15</td>
<td>5</td>
</tr>
<tr>
<td>(S)-(−)-3-Chloro-1-phenyl-1-propanol</td>
<td>55</td>
<td>5</td>
</tr>
<tr>
<td>5β-Pregnane-3α,20α-diol</td>
<td>83</td>
<td>7</td>
</tr>
<tr>
<td>N-Maleoyl-β-alanine</td>
<td>17</td>
<td>6</td>
</tr>
<tr>
<td>β-Nicotinamide adenine dinucleotide hydrate</td>
<td>57</td>
<td>1</td>
</tr>
<tr>
<td>4-Nitrophenyl β-D-xylopyranoside</td>
<td>100</td>
<td>49</td>
</tr>
</tbody>
</table>
Advantages of DOZN™ 2.0

- Measurement: Ability to use on-hand data sources or establish straightforward data collection programs
- Calculations: Ability to utilize well-defined metrics to calculate the benefits of the 12 principles of green chemistry
- Communication: Ability to transparently communicate greener alternatives to customers
- Data privacy—users can evaluate their processes and products in a secure manner
- This free web-based tool enables customers to choose more environmentally friendly approaches for their research/manufacturing projects to promote overall sustainability
- The DOZN™ system was verified and validated by third party and also published (https://pubs.acs.org/doi/pdf/10.1021/acssuschemeng.6b02399)

For more information visit www.sigmaaldrich.com/greener
The DOZN™ 2.0 DEMO Video can be accessed once you create a DOZN™ 2.0 Account
Employing the DOZN™ 2.0 tool in the Undergraduate Curriculum

Irv Levy, Simmons University, Beyond Benign
Wrestling with social distancing

- How to teach labs
- Virtual vs. simulated vs. marathon vs. “next” semester
- At home labs
- Creative moment for new possibilities that are not currently in the curriculum
Here’s where DOZN™ 2.0 comes in

- A new experience for students who will gain
  - Deeper appreciation of green chemistry
    - Including ability to discern greener approaches and key areas for improvement of a process
  - Better understanding of the value of an SDS
  - Familiarity with a genuine industrial tool
Benefits to using DOZN™ 2.0

- Freely available after registration at https://bioinfo.milliporesigma.com/dozn/
- Showcases to your students that your personal focus on green chemistry is not isolated
- Significant, non-trivial, team-amenable experience that can be facilitated in Zoom breakout rooms
The problem with a very green lab curriculum

- Can it be improved?
- Do students understand the green development work that you have done?
Case study, Synthesis of benzaldehyde
Classic 1978 synthesis

- Semi-macro scale; 500 mL RBF; 100 mmol
Many Greener Alternatives

- The green and effective oxidation of alcohols to carboxylic acids with molecular oxygen via biocatalytic reaction
- Green and Efficient: Iron-Catalyzed Selective Oxidation of Olefins to Carbonyls with $O_2$
- Selective oxidation of alcohols and aldehydes over supported metal nanoparticles
- Ionic Liquids in Selective Oxidation: Catalysts and Solvents.
- Silver catalysts for liquid-phase oxidation of alcohols in green chemistry: Challenges and outlook
- The green and effective oxidation of alcohols to carboxylic acids with molecular oxygen via biocatalytic reaction
Our choice


- Pedagogical advantages:
  - Novel catalyst; compared to 50% stoichiometric excess of PCC Tetrakis(benzyltriethylammonium) octamolybdate ($\text{C}_{13}\text{H}_{22}\text{N})_4\text{[Mo}_8\text{O}_{26}$]
    - Demonstrates organometallic synthesis
  - Uses benign 3% hydrogen peroxide as oxidizer (cf. paper 15%)
Walkthrough of benzaldehyde analysis

- To begin – collect data from the Experimental Method (use the template)
  - Substance
  - Supplier, catalog #
  - Amount (mass) may require calculations
  - SDS files
Substances, classic method, begin with product

Benzaldehyde

Synonym: Bitter almond

Linear Formula: C₆H₅CHO | Molecular Weight: 106.12 | CAS Number: 100-52-7

- 418099 purified by redistillation, ≥99.5%
- B1334 ReagentPlus®, ≥99%
- 09143 analytical standard
- 8.01756 for synthesis
- PHR1203 Pharmaceutical Secondary Standard; Certified Reference Material

Show All 11 Results
B score – Biohazard score

Locate the SDS and check section 10.6 for hazardous decomposition products. If there is no data, then use the B score for the material; otherwise, check section 12 of the SDS and use the info to determine the B score. If you would arrive at different B scores for different degradation products, use the higher number for the DOZN B score. Remember that, for the B Score, higher number is a more hazardous substance.

<table>
<thead>
<tr>
<th>element</th>
<th>GHS Category 1</th>
<th>GHS Category 2</th>
<th>GHS Category 3</th>
<th>GHS Category 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute aquatic toxicity</td>
<td>≤ 1.00mg / L</td>
<td>&gt; 1.00 but</td>
<td>&gt; 10.00 but</td>
<td>&gt; 100 mg/ L</td>
</tr>
<tr>
<td></td>
<td></td>
<td>≤ 10.0 mg/L</td>
<td>≤ 100.0 mg/L</td>
<td></td>
</tr>
<tr>
<td>Chronic aquatic toxicity, NOEC</td>
<td>≤ 1.00mg / L</td>
<td>&gt; 1.00 but</td>
<td>&gt; 10.00 but</td>
<td>&gt; 100 mg/ L</td>
</tr>
<tr>
<td>(fish, daphnia)</td>
<td></td>
<td>≤ 10.0 mg/L</td>
<td>≤ 100.0 mg/L</td>
<td></td>
</tr>
<tr>
<td>B Score</td>
<td>4</td>
<td>3</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>
SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

- Flammable liquids (Category 4), H227
- Acute toxicity, Oral (Category 4), H302
- Acute toxicity, Inhalation (Category 4), H332
- Eye irritation (Category 2A), H319
- Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
- Short-term (acute) aquatic hazard (Category 2), H401

For the full text of the H-Statements mentioned in this Section, see Section 16.

- Acute aquatic GHS category 2; B score = 3
- Hint: Levy’s Rule of Five
Reactants, Pyridinium Chlorochromate

**Pyridinium chlorochromate**

1 Product Result | Match Criteria: Product Name, Property

- **Synonym:** PCC
- **Linear Formula:** C₅H₆NClCrO₃
- **Molecular Weight:** 215.56
- **CAS Number:** 26299-14-9

- **190144**
  - 98%

[Sigma-Aldrich](#)
SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

- Oxidizing solids (Category 2), H272
- Skin sensitisation (Category 1), H317
- Carcinogenicity (Category 1B), H350
- Short-term (acute) aquatic hazard (Category 1), H400
- Long-term (chronic) aquatic hazard (Category 1), H410

- Acute/chronic aquatic GHS Category 1; B score = 4
Solvents, methylene chloride

- 170 mL per run (1978 method); need density to calculate mass (typical sources including section 9 in SDS)
- 226 g CH₂Cl₂
**SECTION 2: Hazards identification**

2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

- Skin irritation (Category 2), H315
- Eye irritation (Category 2A), H319
- Carcinogenicity (Category 2), H351
- Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336

• Necessary info is not in section 2; on to 12.1
## SECTION 12: Ecological information

### 12.1 Toxicity

<table>
<thead>
<tr>
<th>Toxicity to fish</th>
<th>flow-through test LC50 - Pimephales promelas (fathead minnow) - 193.00 mg/l - 96 h Remarks: (ECHA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toxicity to daphnia and other aquatic invertebrates</td>
<td>static test LC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h (US-EPA)</td>
</tr>
</tbody>
</table>

- Daphnia between 10 and 100 mg / L; therefore, B Score = 2
Solvents, diethyl ether (250 mL!)
<table>
<thead>
<tr>
<th>Substance</th>
<th>Amount (mL)</th>
<th>Density</th>
<th>Amount (g)</th>
<th>MW</th>
<th>Mol</th>
<th>Company</th>
<th>Catalog #</th>
<th>B-score</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCC</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Sigma-Aldrich</td>
<td>190144</td>
<td>4</td>
<td>pick the first</td>
</tr>
<tr>
<td>Methylene chloride</td>
<td>170</td>
<td>1.33</td>
<td>226.1</td>
<td></td>
<td></td>
<td>Sigma-Aldrich</td>
<td>M1550000</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Benzyl alcohol</td>
<td>10.8</td>
<td></td>
<td>108.14</td>
<td>99.87</td>
<td></td>
<td>Sigma-Aldrich</td>
<td>305197</td>
<td>1</td>
<td>100-1000</td>
</tr>
<tr>
<td>Diethyl ether</td>
<td>250</td>
<td>0.71</td>
<td>177.5</td>
<td></td>
<td></td>
<td>Sigma-Aldrich</td>
<td>296082</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Alumina</td>
<td>10.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Sigma-Aldrich</td>
<td>199974</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Benzoaldehyde (30-80%)</td>
<td>7.418</td>
<td>106.12</td>
<td>69.91</td>
<td></td>
<td></td>
<td>Sigma-Aldrich</td>
<td>418099</td>
<td>3</td>
<td>short term aquatic: 2</td>
</tr>
</tbody>
</table>

120 min total, swirl or magnetic stirring

Fractional distillation - 90 min?

Calculated 70% yield
Now enter the data into DOZN™ 2.0

- Enter the product information first
- Reaction conditions for various “phases” of the process; with their own temperature or pressure.
Reaction Conditions

Default Unit (Applies to each individual reaction condition)

*Time Unit
- min
- hr

*Pressure Unit
- Torr
- mBar
- atm

*Temperature Unit
- °C
- °F
- K

Reaction Condition #1

Name of Synthesis Step: Addition, stirring, extraction

Time: 120.0
Time Unit: min

Pressure Input Method: Exact
Pressure Score: No mention of vacuum or press.

Temperature Input Method: Exact
Temperature Score: Room temperature

Reaction Condition #2

Name of Synthesis Step: Fractional distillation

Time: 90.0
Time Unit: min

Pressure Input Method: Exact
Pressure Score: No mention of vacuum or press.

Temperature Input Method: Exact
Temperature Score: Hot oil or electrical heating
Tips on answering Raw Materials queries in DOZN™ 2.0

Waste?

- Only if it is discarded wholly in the process. If it is *incorporated* into the product in any way, or is an acid or base used to change the pH of the *product*, then it is not waste. (yes for catalysts unless reused? Yes for oxidizing agents)

- Categories (students must develop ability to make good, defensible choices. This will be very uncomfortable for some at first)
  - Semi-solid; containment/land disposal
  - Semi-solid; incinerated (e.g. organic solvents) ; most common choice
  - Solid; non-hazardous (e.g. drying agents)
  - Waste water; semi-hazardous (i.e. aqueous acids, bases and salts)
Tips on answering Raw Materials queries in DOZN™ 2.0

Is it renewable?

- Select Yes only if using a renewably sourced product, e.g. ethanol from fermentation (Yes) vs. from petroleum (No); a material that meets the USDA definition of “biobased product” as described by the biopreferred program. E.g. Cyrene; look for the symbol
Tips on answering Raw Materials queries in DOZN™ 2.0

Is it solvent?
- Yes only for organic solvents not water,

Is it monitored?
- Yes if automated analytical methods were used to monitor the process in real time to alert of a spill or formation of hazardous chemicals
Tips on answering Raw Materials queries in DOZN™ 2.0

Used as

- **Reactant**: Integral reagent that is incorporated into product, or an acid or base used to change the pH of the product (includes oxidizers, unrecovered catalysts)

- **Recovered reactant**: a reagent that is recovered and reused (catalysts if recovered for reuse)

- **Auxiliary**: anything besides a reactant e.g. water, wash solutions, and non-reacting solvents

- **Recovered Auxiliary**: an auxiliary that is recovered and reused
### Raw Materials

#### Weight Unit (Applies to each individual raw material)
- **Unit**: g, kg

#### Raw Material #1
- **Product Name**: Benzyl alcohol
- **Product Number**: 305197
- **Brand**: SIGMA-ALDRICH
  - **Is Solvent?**: Yes, No
  - **B Score**: 1
- **Mass**: 10.8 g
- **Is Waste?**: Yes, No
- **Is Renewable?**: Yes, No
- **Used As**: Reactant
- **Reaction Conditions**: Addition, stirring, extraction
- **Fractional distillation**

#### Raw Material #2
- **Product Name**: PCC
- **Product Number**: 190144
- **Brand**: SIGMA-ALDRICH
  - **Is Solvent?**: Yes, No
  - **Is Renewable?**: Yes, No
- **Mass**: 32.3 g
- **Is Waste?**: Yes, No
- **Waste Severity**: Semi-solid waste
- **Is Derivative?**: Yes, No
- **Reaction Conditions**: Addition, stirring, extraction
- **Auxiliary**: Fractional distillation
Ready to save and calculate!

Process Information

*B score of Product
3

*Mass used for B score of Product
7.42 g

*Number of Catalytic Steps
0

*Number of Synthesis Steps
1

Is Monitored?
Yes No

SAVE SAVE & CALCULATE
Aggregate score: 8 (0-100 scale)

<table>
<thead>
<tr>
<th>Groups</th>
<th>Principles</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1 Improved Resource Use</td>
<td>1, 2, 7, 8, 9, 11</td>
<td>60.46</td>
</tr>
<tr>
<td>#2 Increased Energy Efficiency</td>
<td>6</td>
<td>244.77</td>
</tr>
<tr>
<td>#3 Reduced Human and Environmental Hazards</td>
<td>3, 4, 5, 10, 12</td>
<td>78.14</td>
</tr>
</tbody>
</table>

**Note:** The intent of the DOZN tool is to compare relative “greenness” for similar products or processes, as indicated by a lower DOZN score.
<table>
<thead>
<tr>
<th>Principle</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1 Prevention</td>
<td>263.80</td>
</tr>
<tr>
<td>#2 Atom Economy</td>
<td>61.55</td>
</tr>
<tr>
<td>#3 Less Hazardous Chemical Synthesis</td>
<td>165.71</td>
</tr>
<tr>
<td>#4 Designing Safer Chemicals</td>
<td>3.65</td>
</tr>
<tr>
<td>#5 Safer Solvents and Auxiliaries</td>
<td>56.83</td>
</tr>
<tr>
<td>#6 Design for Energy Efficiency</td>
<td>244.77</td>
</tr>
<tr>
<td>#7 Use of Renewable Feedstocks</td>
<td>61.55</td>
</tr>
<tr>
<td>#8 Reduce Derivatives</td>
<td>0.00</td>
</tr>
<tr>
<td>#9 Catalysis</td>
<td>1.00</td>
</tr>
<tr>
<td>#10 Design for Degradation</td>
<td>4.71</td>
</tr>
<tr>
<td>#11 Real-time analysis for Pollution Prevention</td>
<td>1.00</td>
</tr>
<tr>
<td>#12 Inherently Safer Chemistry for Accident Prevention</td>
<td>159.79</td>
</tr>
</tbody>
</table>
Same analysis on the octamolybdate method

- Preparation of the catalyst
- Reaction and distillation
Preparation of the catalyst

<table>
<thead>
<tr>
<th>Groups</th>
<th>Principles</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1 Improved Resource Use</td>
<td>1, 2, 7, 8, 9, 11</td>
<td>1.77</td>
</tr>
<tr>
<td>#2 Increased Energy Efficiency</td>
<td>6</td>
<td>0.88</td>
</tr>
<tr>
<td>#3 Reduced Human and Environmental Hazards</td>
<td>3, 4, 5, 10, 12</td>
<td>3.32</td>
</tr>
</tbody>
</table>

Note: The intent of the DOZN tool is to compare relative “greenness” for similar products or processes, as indicated by a lower DOZN score.

- Compared to 60.46; 244.77; 78.14
Synthesis and isolation

- Recall that the catalyst prep is 2.77; 0.88; 3.32
- Compared to 60.46; 244.77; 78.14

<table>
<thead>
<tr>
<th>Groups</th>
<th>Principles</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1 Improved Resource Use</td>
<td>1, 2, 7, 8, 9, 11</td>
<td>1.77</td>
</tr>
<tr>
<td>#2 Increased Energy Efficiency</td>
<td>6</td>
<td>0.88</td>
</tr>
<tr>
<td>#3 Reduced Human and Environmental Hazards</td>
<td>3, 4, 5, 10, 12</td>
<td>3.32</td>
</tr>
</tbody>
</table>

Note: The intent of the DOZN tool is to compare relative “greenness” for similar products or processes, as indicated by a lower DOZN score.
Agreggate scores

- Classic method, one step
  - Score: 8
- Greener method, two steps
  - Scores: 1; 2 (clearly greener choice)
Not being critical of the classic authors

- From a different time 40 years ago – labs were different!
- Before microscale
- Before green chemistry
And even green chemists did funny things once upon a time

- Anastas & Warner, 1998
And even green chemists did funny things once upon a time

The Wittig Reaction in the Undergraduate Organic Laboratory

John C. Warner, Paul T. Anastas, and Jean-Pierre Anselme
University of Massachusetts at Boston, Harbor Campus, Boston, MA 02125

Excellent student project after walking through the aldehyde synthesis

Synthesizing Stilbene by Olefin Metathesis Reaction Using Guided Inquiry To Compare and Contrast Wittig and Metathesis Methodologies

Timothy J. Bannin, Partha P. Datta, Elizabeth T. Kiesewetter and Matthew K. Kiesewetter*

Questions?

Dr. Ettigounder Ponnusamy
Fellow & Global Manager
Green Chemistry
MilliporeSigma

Professor Irv Levy
Simmons University
Director of the GCC, Beyond Benign

Submit questions in the Control/Chat box on the Control Panel

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