

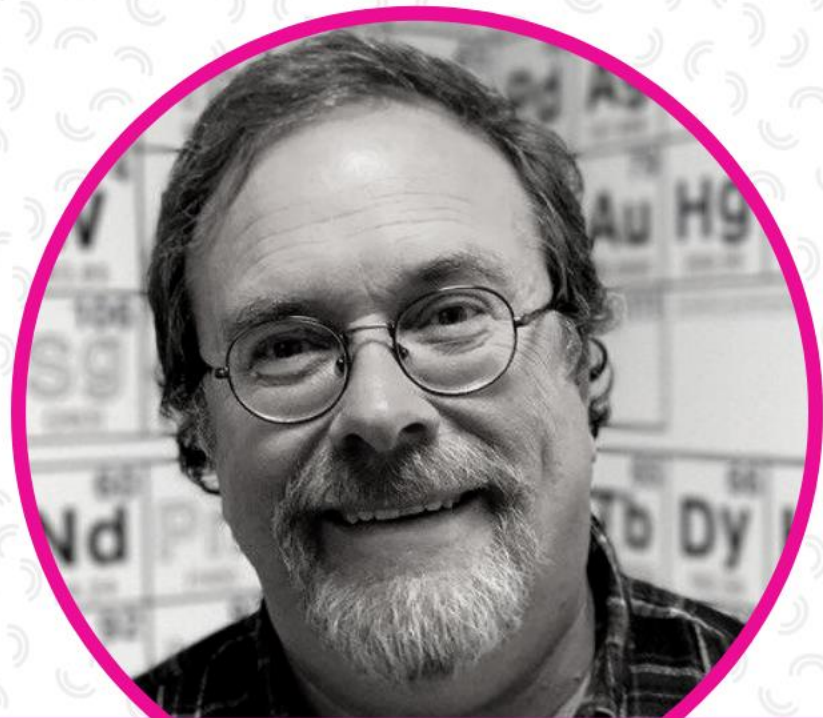


DOZN™

Quantitative **Green** Chemistry Evaluator

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:

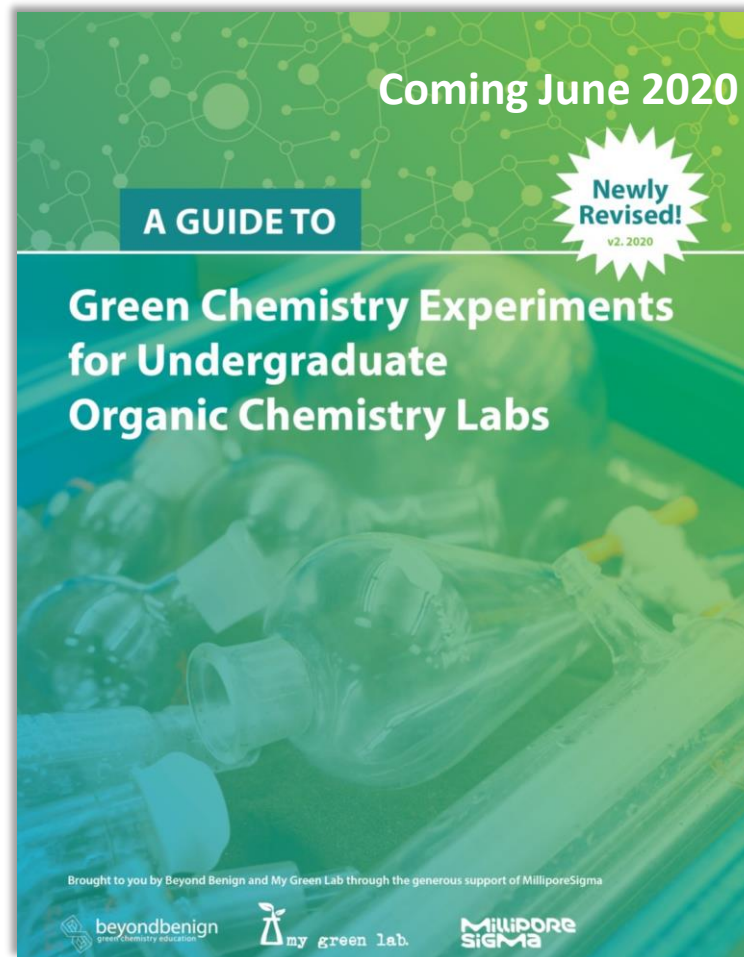
Natalie O'Neil, Ph.D.

Higher Education Program Manager, **Beyond Benign**

@natjoneil



Natalie O'Neil, Ph.D.
Program Manager, Higher Education
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/>



What is the GCC?

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

<https://www.beyondbenign.org/he-green-chemistry-commitment/>



Join the conversation online!



@beyondbenign
#GreenChemistry



<https://www.facebook.com/beyondbenign/>



Juliana Vidal
Communications Intern
Beyond Benign
@juliana_lvidal

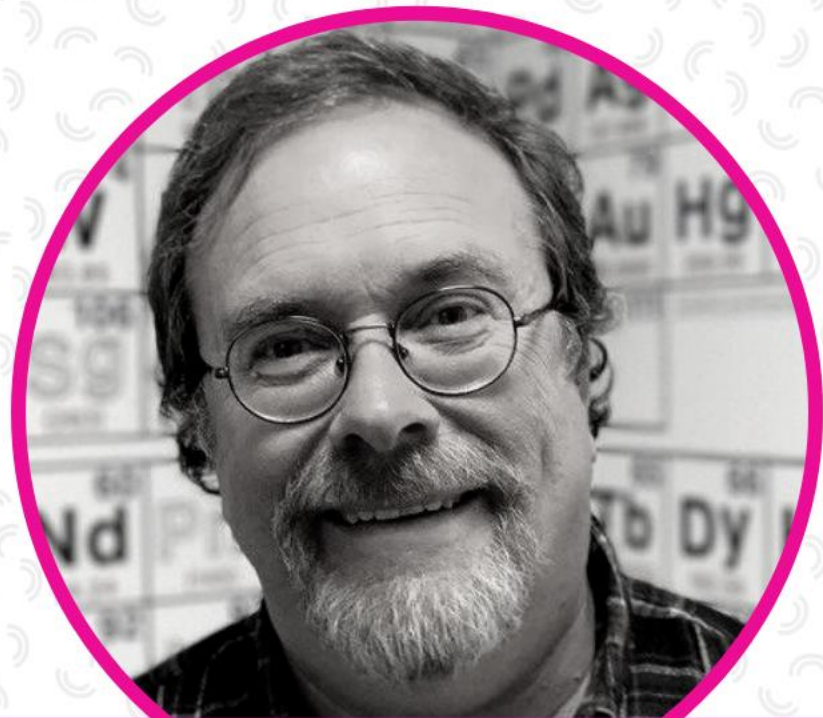


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beyondbenign
green chemistry education

Millipore
Sigma

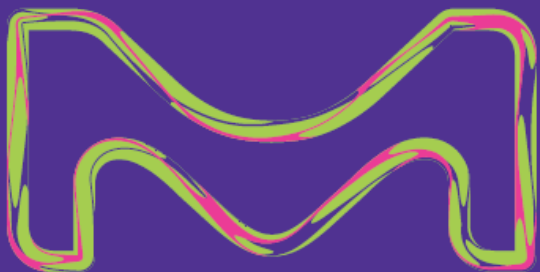


DOZN[®] 2.0 – A QUANTITATIVE GREEN CHEMISTRY EVALUATOR

BEYOND BENIGN WEBINAR, APRIL 29, 2020

Samy Ponnusamy

Fellow & Global Manager – Green Chemistry



**Millipore
Sigma**

MilliporeSigma is a
business of Merck KGaA,
Darmstadt, Germany

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.

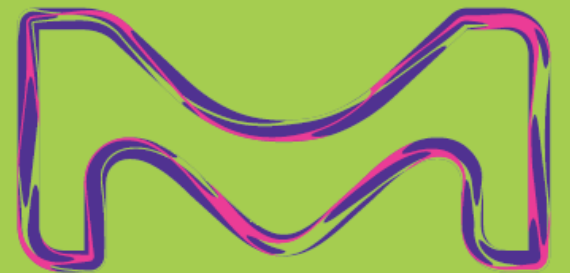


Inherently Safer Chemistry for Accident Prevention

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



$$\frac{\sum \text{Principles 1, 2, 7, 8, 9, \& 11}}{6}$$



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



$$\frac{\sum \textit{Principles 3, 4, 5, 10, \&12}}{5}$$



Group 3 aims at improving the safety of humans and the environment by minimizing potential risks



The Aggregate score



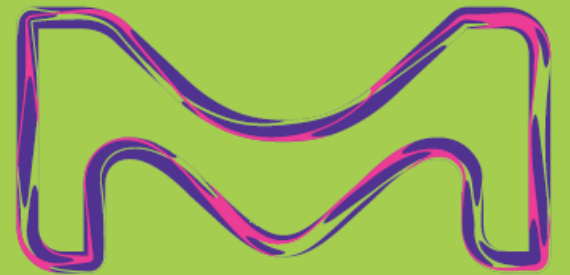
$$\frac{\sum \text{Group 1, 2, 3}}{50}$$



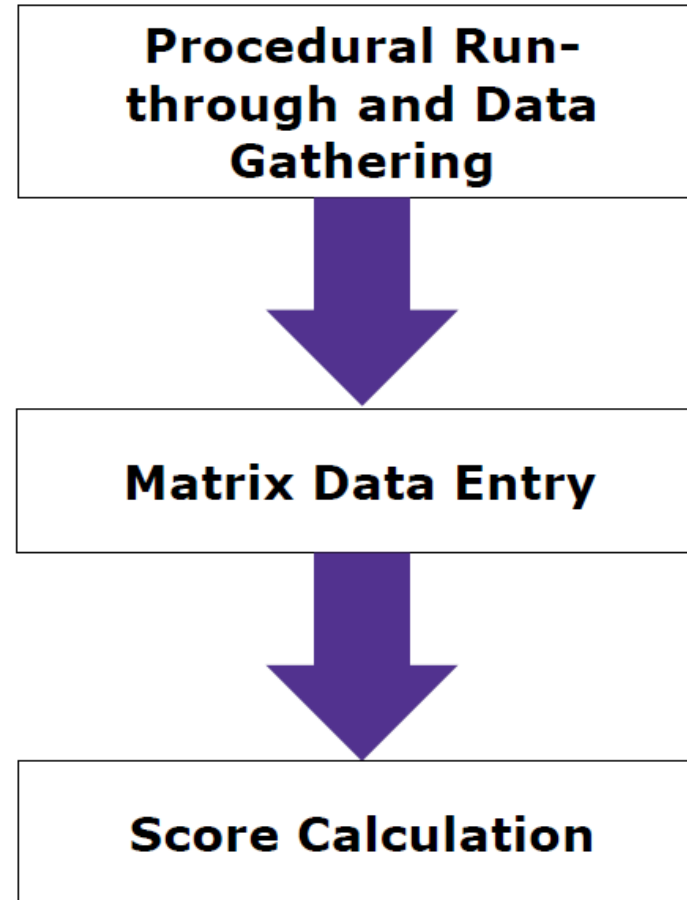
- The Aggregate score gives greenness, a quick summary of the 12 principles
- The Aggregate score is on a scale of 0-100 with 0 being the most desired
- The DOZNTM system was verified and validated by third party



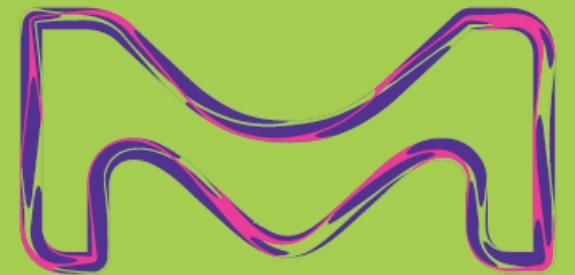
APPLYING THE DOZN[™] 2.0



Analysis



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



**Significant
use**

of electricity



2,000 lbs

of sweet potatoes



**No solvent
required**



**Minimal
electricity use**



β-AMYLASE

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

	12 Principles of Green Chemistry	Percentage of Improvement	Results
Resource Used	Atom Economy	93%	Increased yield. Used less raw materials.
	Waste Prevention	97%	Eliminated use of organic solvents. Reduced waste.
	Reduce Derivatives	N/A	
	Renewable Feedstocks Use	96%	More efficient sweet potato use. Reduced auxiliary chemicals.
	Real-Time Pollution Prevention	N/A	
	Catalyst	N/A	
Human & Environmental Hazards Reduction	Energy Efficiency Design	100%	Eliminated need for elevated temperature and pressure.
	Less Hazardous Chemical Synthesis	95%	Water-based solutions replaced organic solvents. Removed toxic filtering agents.
	Safer Chemical Design	N/A	
	Safer Solvents and Auxiliaries	100%	Eliminated all organic solvents.
	Design for Degradation	No Change	No increased impact with new procedure.
	Inherently Safer Chemical for Accident Prevention	96%	Eliminated flammability and reactivity dangers.

TOTAL PERCENT IMPROVEMENT

98%

AGGREGATE SCORE

0= Most Desirable



Re-engineered Products DOZN[™] Scores

Product Name	Old Score	New Score
1-Aminobenzotriazole	100	44
1,3,5-Tris(4-Iodophenyl)benzene	100	4
(DHQD)2 PHAL	13	3
N-Benzoyl-L-threonine methyl ester	21	4
Tetramethyl tin	15	5
(S)-(-)-3-Chloro-1-phenyl-1-propanol	55	5
5 β -Pregnane-3 α ,20 α -diol	83	7
N-Maleoyl- β -alanine	17	6
β -Nicotinamide adenine dinucleotide hydrate	57	1
4-Nitrophenyl β -D-xylopyranoside	100	49



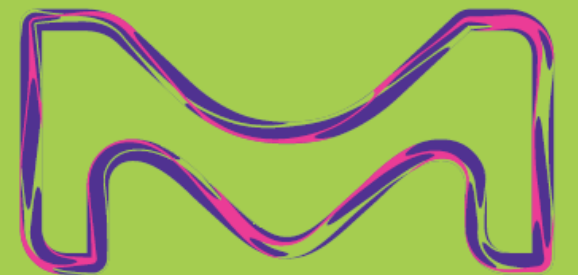
Advantages of DOZN™ 2.0

- 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>)

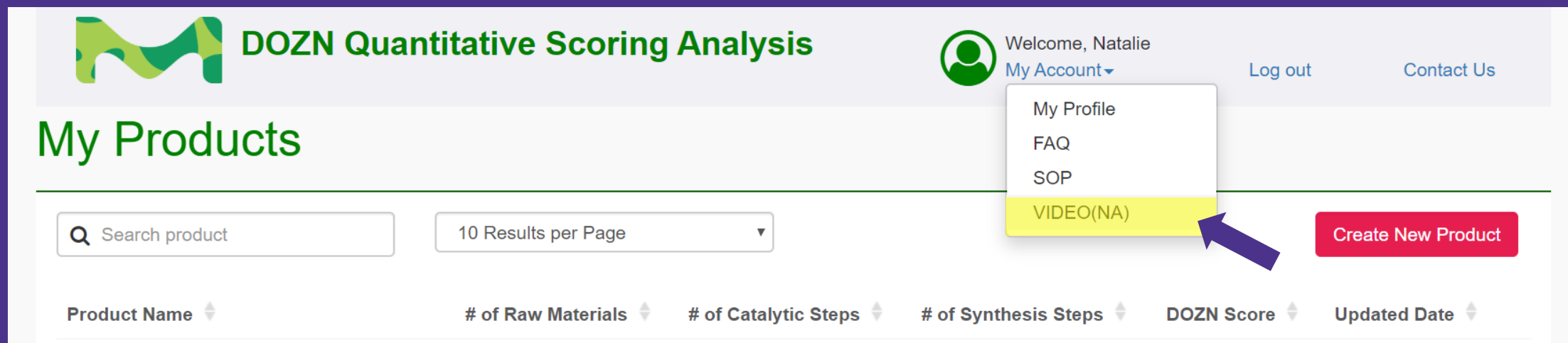
For more information visit www.sigmaaldrich.com/greener



DOZNTM 2.0
DEMO



The DOZN™ 2.0 DEMO Video can be accessed once you create a DOZN™ 2.0 Account



The screenshot displays the DOZN Quantitative Scoring Analysis web application. At the top, the logo is followed by the title "DOZN Quantitative Scoring Analysis". On the right, a user profile section for "Natalie" includes a "My Account" dropdown menu, "Log out", and "Contact Us" links. The dropdown menu is open, showing options: "My Profile", "FAQ", "SOP", and "VIDEO(NA)", with a blue arrow pointing to the last option. Below the header, the "My Products" section features a search bar, a "10 Results per Page" selector, and a "Create New Product" button. A table header is visible at the bottom with columns: "Product Name", "# of Raw Materials", "# of Catalytic Steps", "# of Synthesis Steps", "DOZN Score", and "Updated Date".

DOZN Quantitative Scoring Analysis

Welcome, Natalie
My Account ▾
Log out
Contact Us

My Profile
FAQ
SOP
VIDEO(NA)

My Products

Q Search product 10 Results per Page ▾

Create New Product

Product Name ◆ # of Raw Materials ◆ # of Catalytic Steps ◆ # of Synthesis Steps ◆ DOZN Score ◆ Updated Date ◆



Irv Levy, Simmons University, Beyond Benign

Employing the DOZN™ 2.0 tool in the Undergraduate Curriculum

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

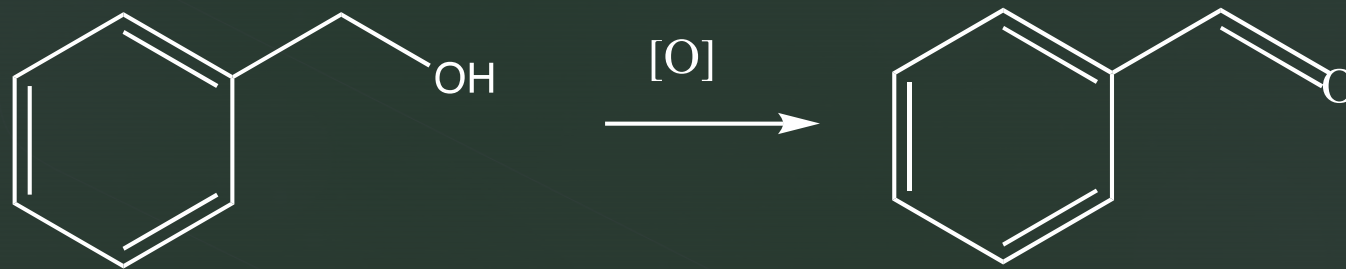
- Freely available after registration at <https://bioinfo.milliporesigma.com/dozn/>
- Showcases to your students that your personal focus on green chemistry is not isolated
- Significant, non-trivial, team-amenable experience that can be facilitated in Zoom breakout rooms



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

- Glaros, G. The Oxidation of Primary Alcohol to Aldehydes with Pyridinium Chlorochromate. *J. Chem. Educ.* **1978**, 55, 410.
- Semi-macroscale; 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 O₂
- 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

- Ming-Lin, G.; Hui-Zhen, L. Selective oxidation of benzyl alcohol to benzaldehyde with hydrogen peroxide over tetra-alkylpyridinium octamolybdate catalysts. *Green Chem.* **2007**, 9, 421-423.
- Pedagogical advantages:
 - Novel catalyst; compared to 50% stoichiometric excess of PCC
Tetrakis(benzyltriethylammonium) octamolybdate
 $(C_{13}H_{22}N)_4[Mo_8O_{26}]$
 - Demonstrates organometallic synthesis
 - Uses benign 3% hydrogen peroxide as oxidizer (cf. paper 15%)

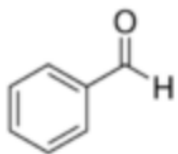
Walkthrough of benzaldehyde analysis

- 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

11 Product Results | Match Criteria: Product Name, Property, Description



Synonym: **Bitter almond**

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

<input type="checkbox"/> 418099	purified by redistillation, ≥99.5%	Sigma-Aldrich	❖ SDS	Pricing	▼
<input type="checkbox"/> B1334	ReagentPlus®, ≥99%	Sigma-Aldrich	❖ SDS	Pricing	▼
<input type="checkbox"/> 09143	analytical standard	Supelco	❖ SDS	Pricing	▼
<input type="checkbox"/> 8.01756	for synthesis	Sigma-Aldrich		Pricing	▼
<input type="checkbox"/> PHR1203	Pharmaceutical Secondary Standard; Certified Reference Material	Supelco	❖ SDS	Pricing	▼

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.

element	GHS Category 1	GHS Category 2	GHS Category 3	GHS Category 4
Acute aquatic toxicity	$\leq 1.00\text{mg / L}$	> 1.00 but $\leq 10.0 \text{ mg/L}$	> 10.00 but $\leq 100.0 \text{ mg/L}$	$> 100 \text{ mg/ L}$
Chronic aquatic toxicity, NOEC (fish, daphnia)	$\leq 1.00\text{mg / L}$	> 1.00 but $\leq 10.0 \text{ mg/L}$	> 10.00 but $\leq 100.0 \text{ mg/L}$	$> 100 \text{ mg/ L}$
B Score	4	3	2	1

Using the SDS

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

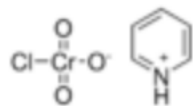
For the full text of the H-Statements mentioned in this Section, see Section 16.

- 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: **C₅H₆NCrO₃** | Molecular Weight: **215.56** | CAS Number: **26299-14-9**

☐ **190144**

98%

Sigma-Aldrich

 **SDS** **Pricing** 

B score: 4

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

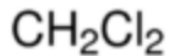
Long-term (chronic) aquatic hazard (Category 1), H410

- Acute/chronic aquatic GHS Category 1; B score = 4

Solvents, methylene chloride

Methylene chloride

2 Product Results | Match Criteria: Product Name



Synonym: **Dichloromethane, Methylene chloride**

Empirical Formula (Hill Notation): **CH₂Cl₂** | Molecular Weight: **84.93** | CAS Number: **75-09-2**

☐ **M1550000**

European Pharmacopoeia (EP) Reference Standard

Sigma-Aldrich

[SDS](#) [Pricing](#) [▼](#)

☐ **PHR1557**

Pharmaceutical Secondary Standard; Certified
Reference Material

Supelco

[SDS](#) [Pricing](#) [▼](#)

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

B Score

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

B Score

SECTION 12: Ecological information

12.1 Toxicity

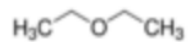
Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 193.00 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia magna (Water flea) - 27 mg/l - 48 h (US-EPA)

- Daphnia between 10 and 100 mg / L; therefore, B Score = 2

Solvents, diethyl ether (250 mL!)

Diethyl ether

18 Product Results | Match Criteria: Product Name, Description



Synonym: **Ether, Ethyl ether**

Linear Formula: **(CH₃CH₂)₂O** | Molecular Weight: **74.12** | CAS Number: **60-29-7**

☐ **296082**

contains 1 ppm BHT as inhibitor, anhydrous, ≥99.7%

Sigma-Aldrich

 **SDS**

Pricing 

☐ **1.00921**

for analysis EMSURE® ACS,ISO,Reag. Ph Eur

Supelco

Pricing 

- 178 g diethyl ether

Continue to gather data

substance	amount (mL)	density	amount (g)	FW	mmol	Company	catalog #	B-score	comments
PCC			32.3	215.56		Sigma-Aldrich	190144	4	pick the first
methylene chloride	170	1.33	226.1			Sigma-Aldrich	M1550000	2	
benzyl alcohol			10.8	108.14	99.87	Sigma-Aldrich	305197	1	100-1000
	120 min total, swirl or magnetic stirring								
diethyl ether	250	0.71	177.5			Sigma-Aldrich	296082	1	
alumina			10			Sigma-Aldrich	199974	1	
	fractional distillation - 90 min?								
benzaldehyde (30-80%)			7.418	106.12	69.91	Sigma-Aldrich	418099	3	short term aquatic: 2
			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

[Remove](#)

Name of Synthesis Step

Addition, stirring, extraction

Time

120.0

Time Unit

min

Pressure Input Method

☐

Exact
Value

☒

General
Conditions

Pressure Score 

No mention of vacuum or pres

Temperature Input Method

☐

Exact
Value

☒

General
Conditions

Temperature Score 

Room temperature

Reaction Condition #2

[Remove](#)

Name of Synthesis Step

Fractional distillation

Time

90.0

Time Unit

min

Pressure Input Method

☐

Exact
Value

☒

General
Conditions

Pressure Score 

No mention of vacuum or pres

Temperature Input Method

☐

Exact
Value

☒

General
Conditions

Temperature Score 

Hot oil or electrical heating

ADD A REACTION CONDITION

Tips on answering Raw Materials queries in DOZN™ 2.0

Waste?

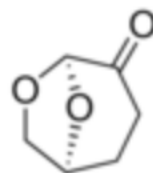
- Only if it is discarded wholly in the process. If it is *incorporated* into the product in any way, or is an acid or base used to change the pH of the *product*, then it is not waste. (yes for catalysts unless reused? Yes for oxidizing agents)
- Categories (students must develop ability to make good,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

Cyrene™
1 Product Result | Match Criteria: Product Name, Description



Empirical Formula (Hill Notation): **C₆H₈O₃**

☐ **807796**

BioRenewable 

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

[Remove](#)

*Product Name

Benzyl alcohol

*Product Number

305197

*Brand

SIGMA-ALDRICH

*Mass

10.8

Is Waste? ?

☐ Yes ☒ No

Is Renewable? ?

☐ Yes ☒ No

Is Solvent? ?

☐ Yes ☒ No

B Score ?

1

Used As ?

Reactant

Reaction Conditions ?

☒ Addition,
stirring,
extraction

☐ Fractional
distillation

Raw Material #2

[Remove](#)

*Product Name

PCC

*Product Number

190144

*Brand

SIGMA-ALDRICH

*Mass

32.3

Is Waste? ?

☒ Yes ☐ No

Waste Severity ?

Semi-solid waste

Is Derivative? ?

☐ Yes ☒ No

Is Renewable? ?

☐ Yes ☒ No

Is Solvent? ?

☐ Yes ☒ No

B Score ?

4

Used As ?

Auxiliary

Reaction Conditions ?

☒ Addition,
stirring,
extraction

☐ Fractional
distillation

Raw Material #3 Remove

*Product Name

methylene chloride

*Product Number

M1550000

*Brand

SIGMA-ALDRICH

*Mass

226.1

Is Waste?

☒ Yes ☐ No

Waste Severity

Semi-solid wa

Is Derivative?

☐ Yes ☒ No

Is Renewable?

☐ Yes ☒ No

Is Solvent?

☒ Yes ☐ No

B Score

2

Used As

Auxiliary

Reaction Conditions

☒ Addition, stirring, extraction ☒ Fractional distillation

Raw Material #4 Remove

*Product Name

diethyl ether

*Product Number

296082

*Brand

SIGMA-ALDRICH

*Mass

177.5

Is Waste?

☒ Yes ☐ No

Waste Severity

Semi-solid wa

Is Derivative?

☐ Yes ☒ No

Is Renewable?

☐ Yes ☒ No

Is Solvent?

☒ Yes ☐ No

B Score

1

Used As

Auxiliary

Reaction Conditions

☒ Addition, stirring, extraction ☒ Fractional distillation

Raw Material #5 Remove

*Product Name

alumina

*Product Number

199974

*Brand

SIGMA-ALDRICH

*Mass

10.0

Is Waste?

☒ Yes ☐ No

Waste Severity

Solid waste, n

Is Derivative?

☐ Yes ☒ No

Is Renewable?

☐ Yes ☒ No

Is Solvent?

☐ Yes ☒ No

B Score

1

Used As

Auxiliary

Reaction Conditions

☒ Addition, stirring, extraction ☐ Fractional distillation

ADD A RAW MATERIAL

Ready to save and calculate!

Process Information

*B score of Product 

3

*Mass used for B score of Product

7.42

*Unit

g

*Number of Catalytic Steps

0

*Number of Synthesis Steps

1

Is Monitored? 

☐

Yes

☒

No

SAVE

SAVE & CALCULATE

Aggregate score: 8 (0-100 scale)

Groups	Principles	Score
#1 Improved Resource Use	1, 2, 7, 8, 9, 11	60.46
#2 Increased Energy Efficiency	6	244.77
#3 Reduced Human and Environmental Hazards	3, 4, 5, 10, 12	78.14

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

Aggregate Score



Scoring Matrix



Principle

Score

#1 Prevention	263.80
#2 Atom Economy	61.55
#3 Less Hazardous Chemical Synthesis	165.71
#4 Designing Safer Chemicals	3.65
#5 Safer Solvents and Auxiliaries	56.83
#6 Design for Energy Efficiency	244.77
#7 Use of Renewable Feedstocks	61.55
#8 Reduce Derivatives	0.00
#9 Catalysis	1.00
#10 Design for Degradation	4.71
#11 Real-time analysis for Pollution Prevention	1.00
#12 Inherently Safer Chemistry for Accident Prevention	159.79

Same analysis on the octamolybdate method

- Preparation of the catalyst
- Reaction and distillation

Preparation of the catalyst

Groups	Principles	Score
#1 Improved Resource Use	1, 2, 7, 8, 9, 11	1.77
#2 Increased Energy Efficiency	6	0.88
#3 Reduced Human and Environmental Hazards	3, 4, 5, 10, 12	3.32

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

Groups	Principles	Score
#1 Improved Resource Use	1, 2, 7, 8, 9, 11	1.77
#2 Increased Energy Efficiency	6	0.88
#3 Reduced Human and Environmental Hazards	3, 4, 5, 10, 12	3.32

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

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

Agreggate scores

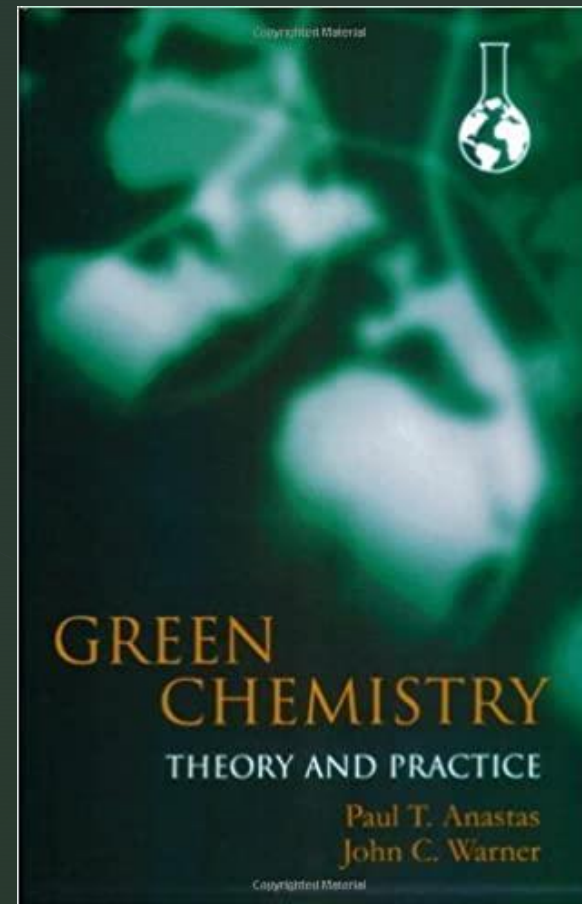
- Classic method, one step
- Score: 8
- Greener method, two steps
- Scores: 1; 2 (clearly greener choice)

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 Anselme¹

University of Massachusetts at Boston, Harbor Campus, Boston, MA 02125

- *J. Chem. Educ.* **1985**, 62, 346.

Excellent student project after walking through the aldehyde synthesis

JOURNAL OF
CHEMICAL EDUCATION

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*

- Bannin T. J.; Datta, P. P.; Kiesewetter, E. T.; Kiesewetter*, M.K. Synthesizing Stilbene by Olefin Metathesis Reaction Using Guided Inquiry To Compare and Contrast Wittig and Metathesis Methodologies. *J. Chem. Educ.* **2019**, 96, 143-147.



Questions?



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

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