Green Chemistry

Introduction and Project

Green Chemistry

The utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture, and application of chemical product.

Paul T. Anastas and John Warner, 1990s

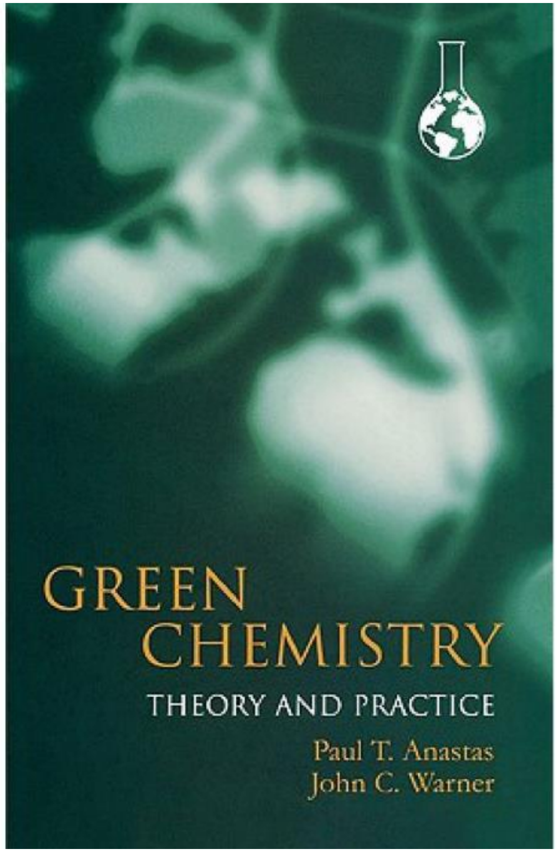
What is Green Chemistry?

Introduction to Green Chemistry (video 1:57)

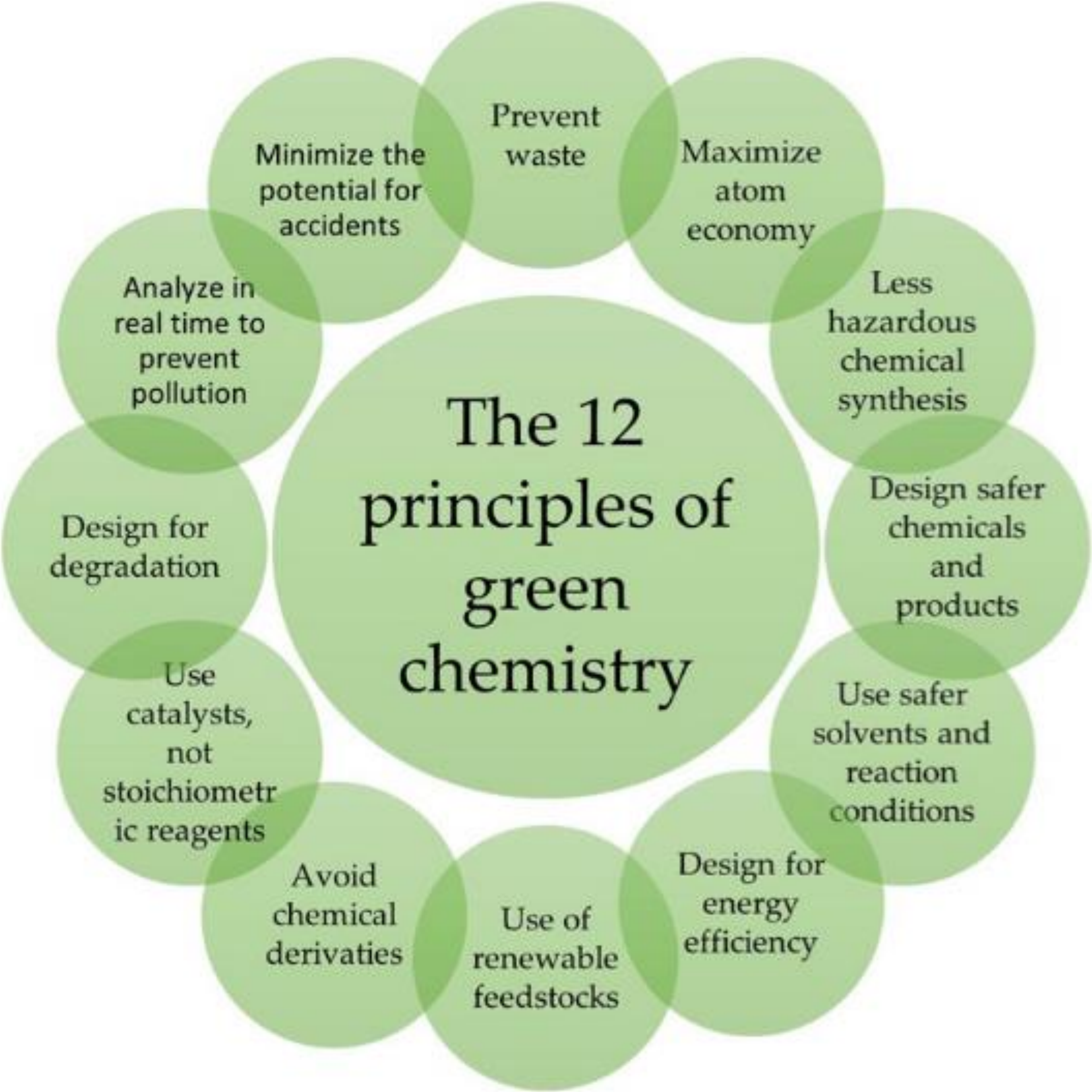
Green Chemistry at UC Berkeley (video 5:28)

The 12 Principles of Green Chemistry

1. Waste Prevention
2. Atom Economy
3. Less Hazardous Chemical Synthesis
4. Designing Safer Chemicals
5. Safer Solvents and Auxiliaries
6. Design for Energy Efficiency
7. Use of Renewable Feedstocks
8. Reduce Derivatives
9. Catalysis
10. Design for Degradation
11. Real-time Analysis for Pollution Prevention
12. Inherently Safer Chemistry for Accident Prevention



Anastas, P. T., Warner, J. C. (2000). Green chemistry: Theory and Practice. New York; Oxford University Press.

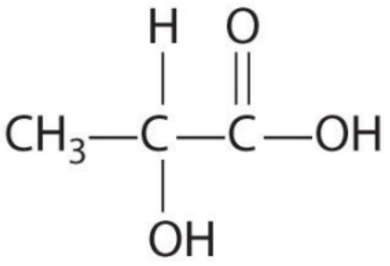

The 12 principles of green chemistry
Prevent waste
Maximize atom economy
Less hazardous chemical synthesis
Design safer chemicals and products
Use safer solvents and reaction conditions
Design for energy efficiency
Use of renewable feedstocks
Avoid chemical derivaties
Use catalysts, not stoichiometr ic reagents
Design for degradation
Analyze in real time to prevent pollution
Minimize the potential for accidents

Key Concepts

Reduce toxicity	Using water as a solvent
Renewable feedstocks	Renewable resources as reactants
Design safer products	Non-toxic
Biodegradable products	Break down at end of life
Reduce energy needs	Operate at lower temperatures
Increase efficiency	Reduces # of steps and generate less waste

Comparative Analysis: Production of Lactic Acid

- Lactic acid ($C_3H_6O_3$) or 2-hydroxypropanoic acid:



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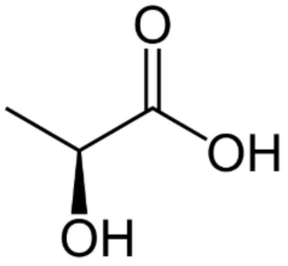


- Commercially and industrially useful molecule.
- Used to make a wide variety of products (Figure 1 next slide).
- ~370 000 metric tons (= 3.7 x 10^8 kg) produced in 2017.
- Demand increasing 5-8% per year (Krishna, et.al.)

Comparative Analysis, continued

Plastics

- Polylactic acid (PLA)

Food Industry

- Preservatives
- Flavoring agents
- Fermented foods

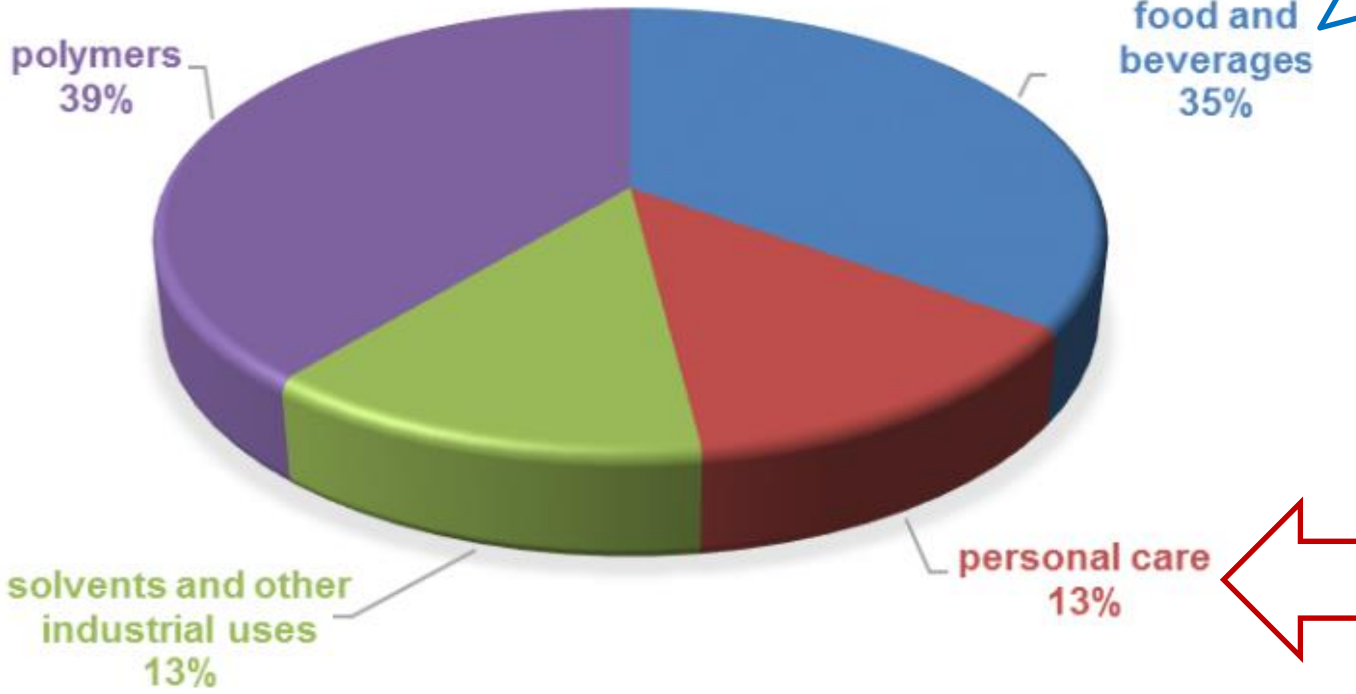


Fig. 1. Uses and demands of lactic acid

Chemical Industry

- Cleaning agents
- Green solvents
- pH regulators

Cosmetic Industry

- Moisturizers
- Anti-acne agents

Comparative Analysis, continued

Production of Lactic acid:

(1) Chemical Synthesis

(2) Biochemical Synthesis

(1) Chemical Synthesis:

- **Starting material:** petroleum products
- **Process**:
  - Uses hydrogen cyanide, catalysts, and sulfuric acid.
  - Operates at high temperature and high pressure.
- **Produces** mixture of optical stereoisomers that needs to be separated.

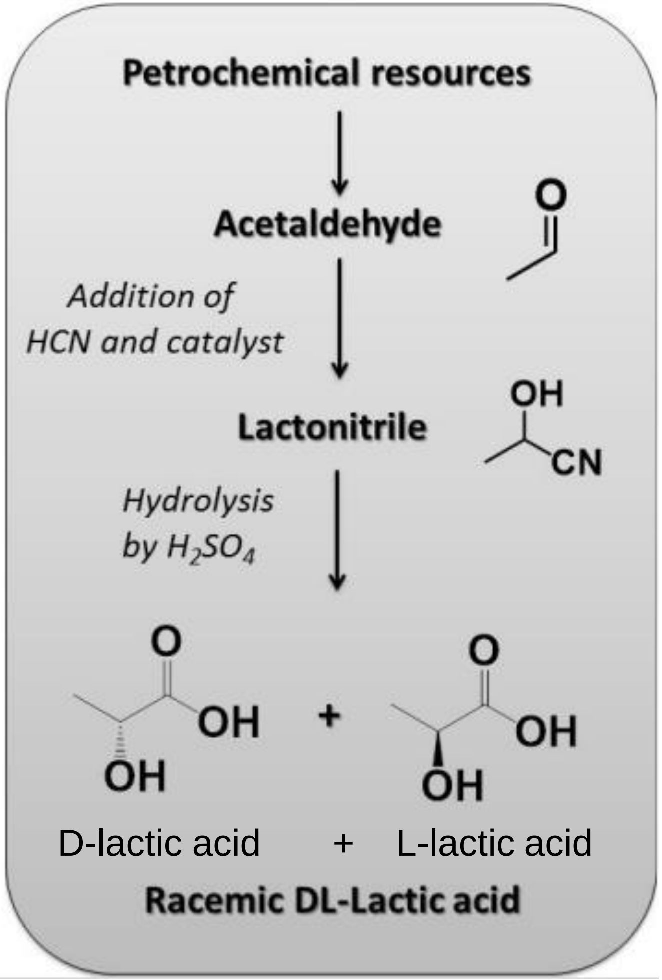


Fig.2. Chemical synthesis of lactic acid

(2) Biochemical Synthesis:

» **Starting material**: Carbohydrates

» **Process**:

- Acid hydrolysis and/or saccharification (SSF*) breaks down complex carbohydrates.
- Bacterial fermentation.
- Operates at low temperature.

» **Produces** pure lactic acid (no need for separation).

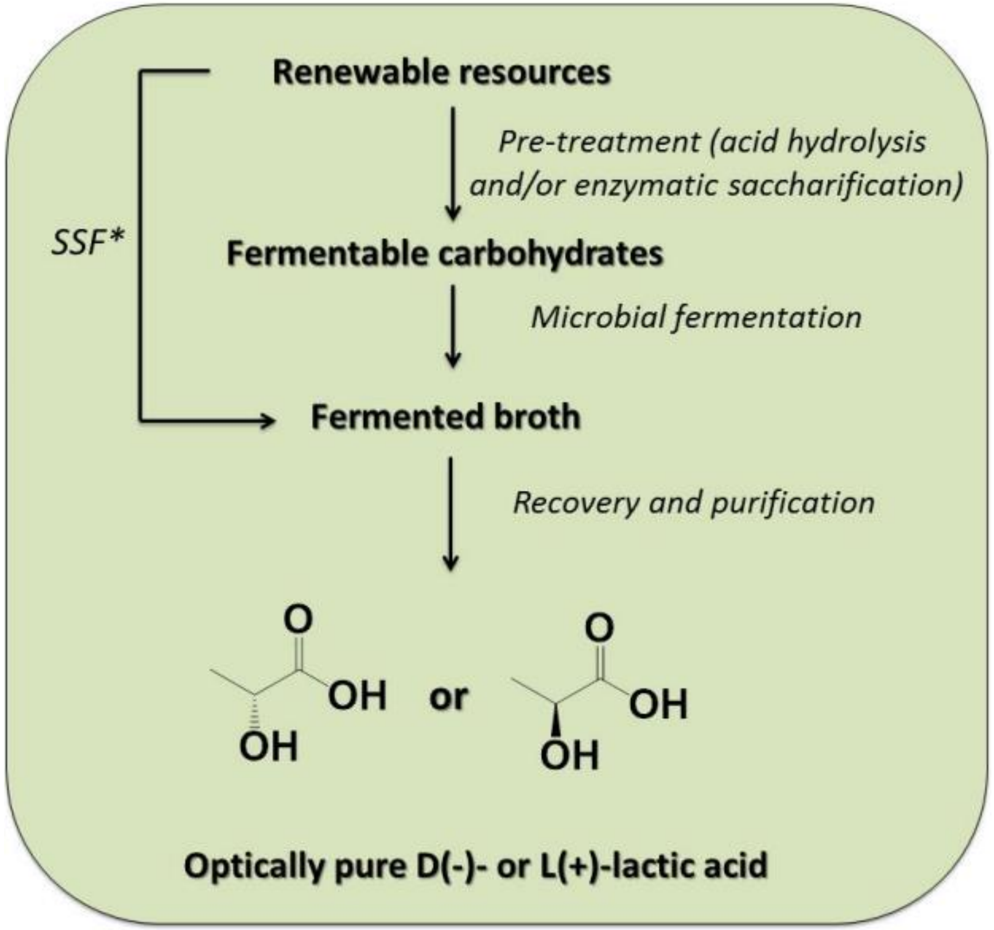


Fig 3. Microbial fermentation production of lactic acid
(SSF*: simultaneous saccharification and fermentation)

Comparative Analysis: Dihydropyrimidone (Pharmaceutical compound)

» **Uses:**

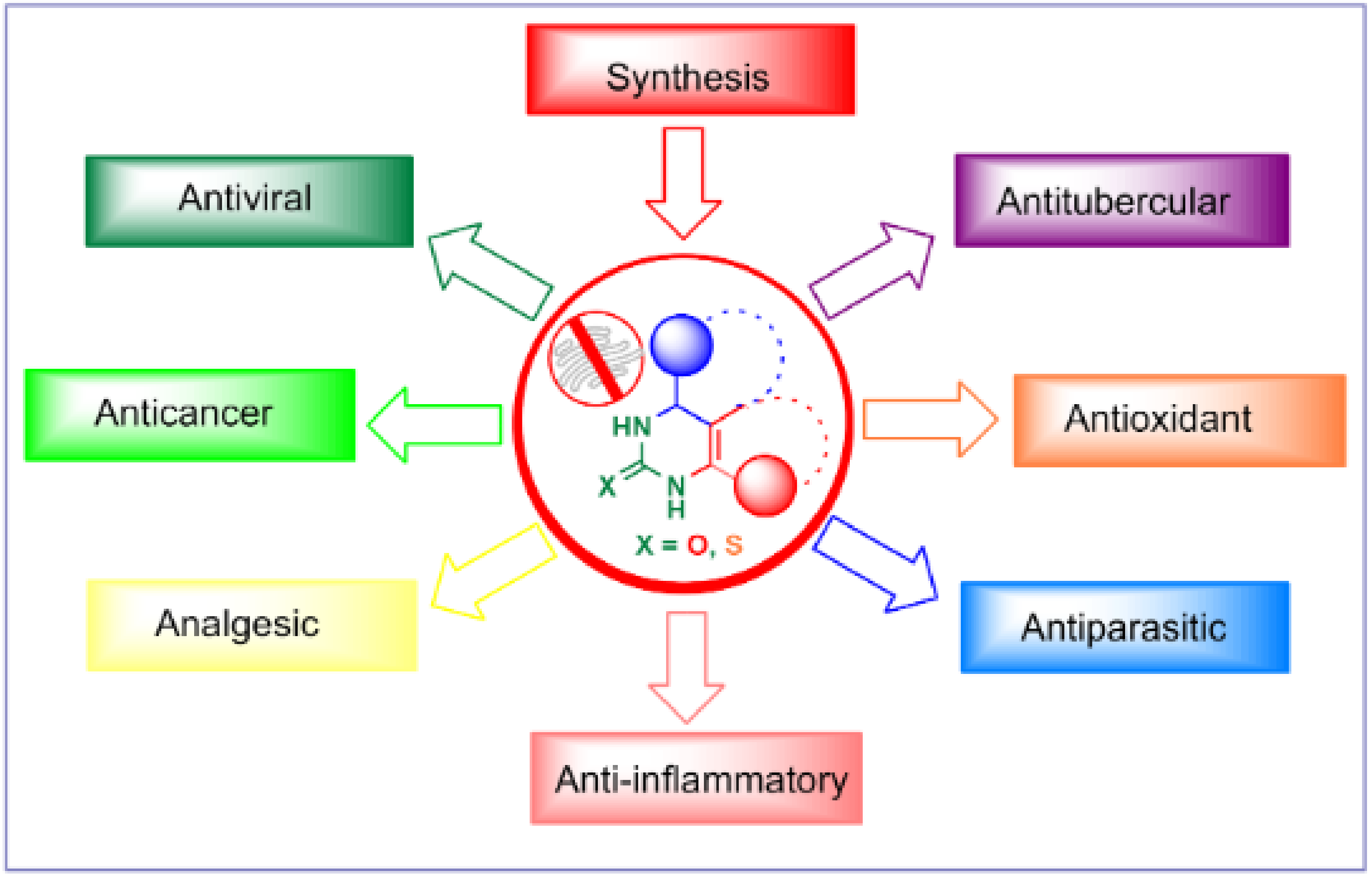
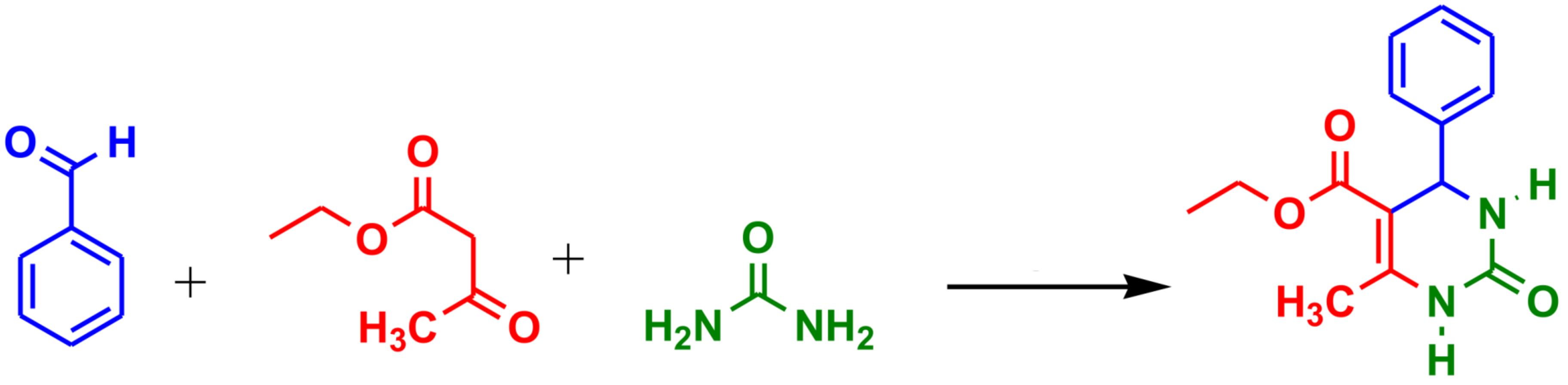


Fig. 4. Therapeutic properties of pyrimidine compounds

Dihydropyrimidone Synthesis



Benzaldehyde
(C_6H_5CHO)

Ethyl
acetylacetate
($C_6H_{10}O_3$)

Urea
($CO(NH_2)_2$)

Dihydropyrimidone
(DHPMs)

Dihydropyrimidone Synthesis, continued

The following 2 pathways result in the production of Dihydropyrimidone.

(1) Analyse each using the 12 principles of Green Chemistry.

(2) Compare all aspects of each reaction.

(3) Determine which pathway is "greener"?

	Synthesis Pathways	
Conditions	**1**	**2**
Catalyst	HCl (2 drops)	$ZnCl_2$ (25 mol%)
Solvent	Ethanol (10 mL)	None
Temperature	80°C	70-80°C
Time	3 hours	15 minutes
Yield	58%	90%

Green Chemistry Is About…

- Design
- Innovation
- Efficiency
- Costs
- Performance
- Intrinsic Hazard
- Shifting roles
- Changing education

Real-World Analysis of Green Chemistry

- 5-minute Powerpoint presentation
- Teams of 2
- Presentations weeks of November 6, 13, and 20.

- Themes presented one week before.
- Submit Powerpoint on Moodle 24-hours before presentation.
- Student and teacher evaluations

Real-World Analysis of Green Chemistry

• Introduce topic
• Summarize the chemistry - reactions, chemicals, conditions, etc.
• Analysis: - Advantages* - Disadvantages* - Feasibility
• Conclusion: Is this option green?
• References

*Address the 12 principles, economy, efficiency, health, environment, etc.

Real-World Analysis of Green Chemistry

- **Evaluation:**
  - Clarity, visual support (slides), and language.
  - Students present equally (time; level of difficulty)

  - Was the topic properly introduced?
  - Were green principles integrated?
  - Was the position on how green the process/product is clearly stated?
  - Citations

  - What did you learn?
  - Best aspect of the presentation and an aspect to improve

Week 8 Oct. 16	● Introduction to Green Chemistry Project
Week 9 Oct. 23	• Lab 4
Week 10 Oct. 30	● Open themes to present next week - 5 pairs ● Midterm
Week 11 Nov. 6	● Presentations (in lab time) - Submit powerpoint on moodle no later than 24 hours before. ● Open themes to present next week - 5 pairs
Week 12 Nov. 13	● Presentations (in lab time) - Submit powerpoint on moodle no later than 24 hours before. ● Open themes to present next week – 4 pairs
Week 13 Nov. 20	● Presentations (in lab time) - Submit powerpoint on moodle no later than 24 hours before.

Image Source: https://pixabay.com/en/hands-keep-globe-protection-earth-1080792/