Green Chemistry

Production of Ibuprofen

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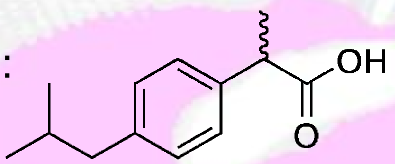
Introduction

- Anti-inflammatory drug
- Two ways of synthesis: Boot’s synthesis and Green synthesis
- Structure of Ibuprofen:



Green chemistry

- Based on reducing health and environmental damage

- 12 principles:

I. Prevention
II. Atom economy
III. Less hazardous synthesis
IV. Designing safer chemicals
V. Safer auxiliary substances

Green chemistry

VI. Energy efficiency
VII. Use of renewable resources
VIII. Reducing derivatives
IX. Catalysis
X. Design for degradation
XI. Use real-time analysis for pollution
XII. Accident prevention

Boot's synthesis

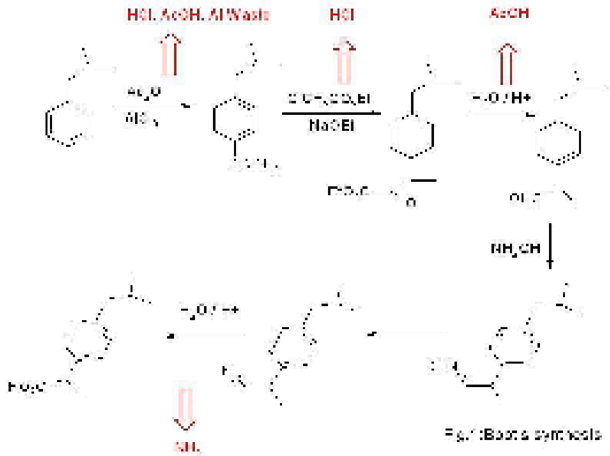


Fig. 1 :Boot's synthesis

Green synthesis

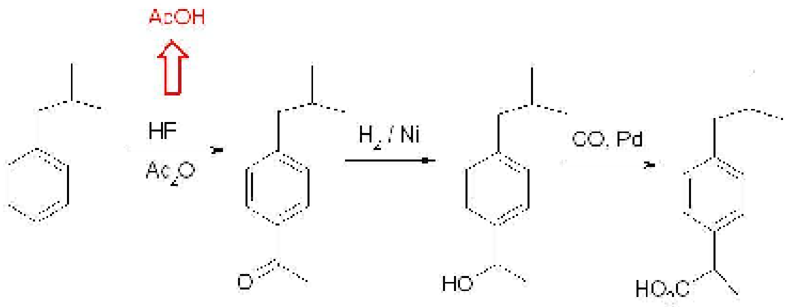


Fig. 2: Green synthesis

Prevention

- Boot's synthesis:
  - HCl, C_2H_5COOH, NH_3 and Al as waste
- Green synthesis:
  - AcOH as the only waste
- No need to clean it up!

Atom economy and Reducing derivatives

- Atom
- Perc
  synth

[illegible]	Formula mass
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[illegible]	[illegible]
[illegible]	[illegible]
[illegible]	[illegible]
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[illegible]	Formula mass
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$\times 100$

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Atom economy and Reducing derivatives

How about green synthesis? Let's calculate!

Atom economy and Reducing derivatives

$$\frac{Molecular\ Weight\ of\ desired\ product}{Molecular\ Weight\ of\ all\ reactants} \times 100$$

[illegible]	[illegible]
[illegible]	[illegible]
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Atom economy and Reducing derivatives

- Percentage atom economy of Green synthesis:

77%!

Atom economy and Reducing derivatives

- Green synthesis: With a higher percentage atom economy → efficient!
- Environmentally friendly → less unwanted materials!
- Unnecessary derivatives are **eliminated**!

Less hazardous synthesis and Designing safer chemicals

Boot's synthesis:

Hydrochloric acid	I) Corrosive II) Body damage (skin burn, eye damage) III) Chlorine gas may be produced(OA)
Ammonia	I) Toxic to fish and amphibians II) Pungent smell
Acetic acid	Same as hydrochloric acid except (III)
Al waste	I) Not degradable II) Pollution to soil

Less hazardous synthesis and Designing safer chemicals

- Green synthesis: The only side product — acetic acid!
- Reduction of by-products → Effective synthesis!

Energy efficiency

- Boot's synthesis: Six steps reaction → Heating → much energy requirement
- Green synthesis: Three steps reaction → Fewer steps, less energy required → expenditure on energy reduced

Use of renewable resources

Green synthesis are catalysts that can be recovered and reused repeatedly.

- Hydrogen fluoride

  Produced by treatment of the mineral fluorite (CaF_2) with concentrated sulfuric acid

  $$CaF_2 + H_2SO_4 \rightarrow 2\ HF + CaSO_4$$

Use of renewable resources

- Raney nickel

  A solid catalyst of a nickel-aluminium alloy
  - Porous structure, increasing surface area

$$2\ Al + 2\ NaOH + 6\ H_2O \rightarrow 2\ Na[Al(OH)_4] + 3\ H_2$$

Use of renewable resources

- Palladium

  A silvery-white metal
  - Commonly used in catalytic converters, which can be recycled

Safer auxiliary substances

- Boot's synthesis:

I) Aluminium trichloride
II) Hydroxylamine
III) 2-chlorobutyl ester ($ClCH_2CO_2Et$)
IV) Sodium ethoxide (NaOEt)

However, they are not safe enough!

Catalysis

Boot's synthesis: aluminium trichloride in Friedel-Crafts acetylation of isobutylbenzene

- not a true catalyst
- only hydrated, has to be disposed
- a waste by-product which has to be landfilled

Catalysis

Green synthesis: hydrogen fluoride

- A true catalyst
- Can be recovered and reused with over 99.9% efficiency
- Generates no waste
- Used as the solvent

Design for degradation

Ibuprofen

- A very weak photosensitising agent
  Reason:

I) Only one single phenyl moiety

II) No bond conjugation in it

→Resulting in a very weak chromophore system and a very weak absorption spectrum

- Half life between 1.9 and 2.2 hours

→Photolytic degradation of ibuprofen