

SF₄ as a deoxofluorinating reagent. Is it green or hazardous?

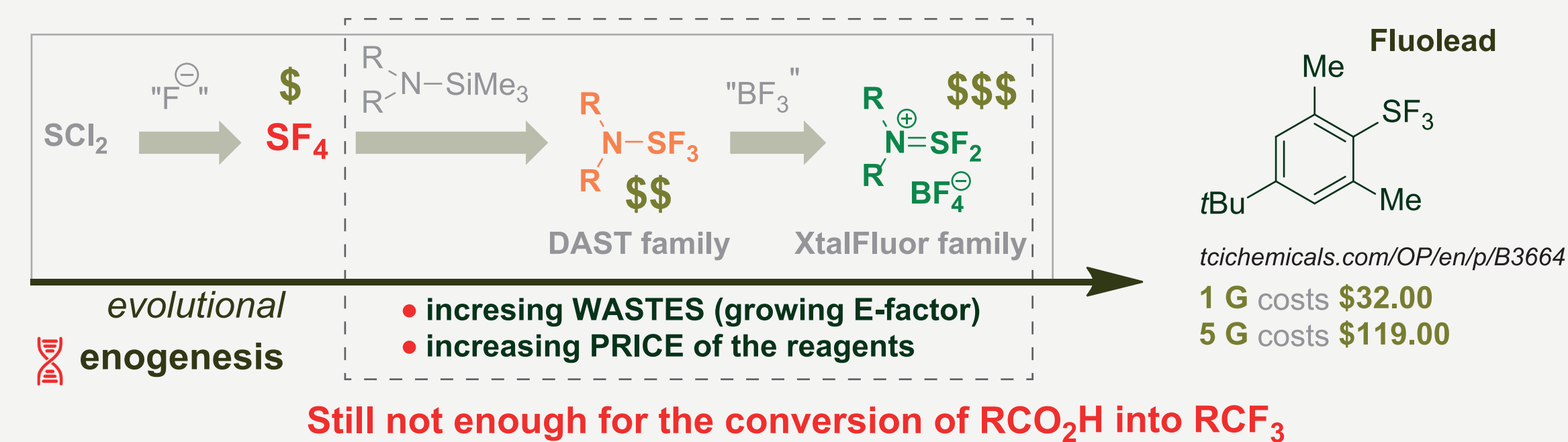
Dmytro M.Volochnyuk, Serhii A.Trofimchuk, Serhiy V.Ryabukhin

Background and synthetic strategy

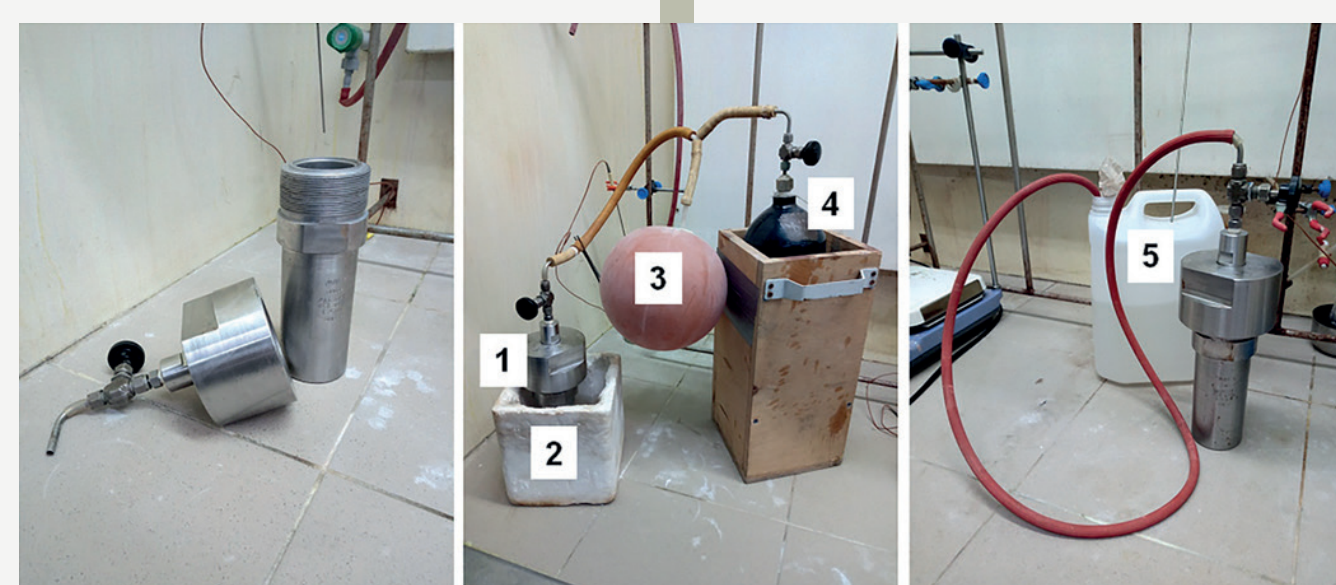
STATUS QUO



- colorless gas, bp -38 °C, mp -121°C
- soluble in nonpolar solvents
- a strong irritant and a corrosive agent
- very toxic LD₅₀ = 19 ppm (86 mg/m³, 4 h, rats)
- Industrial production ~2,000 t annually
 - Agrochemistry – 50%
 - Pharm – 21%
 - Others – 29% (10% liquid crystals)



WORK
SAFELY!



Loading of SF₄ to the vacuum autoclave from the balloon through the damper chamber

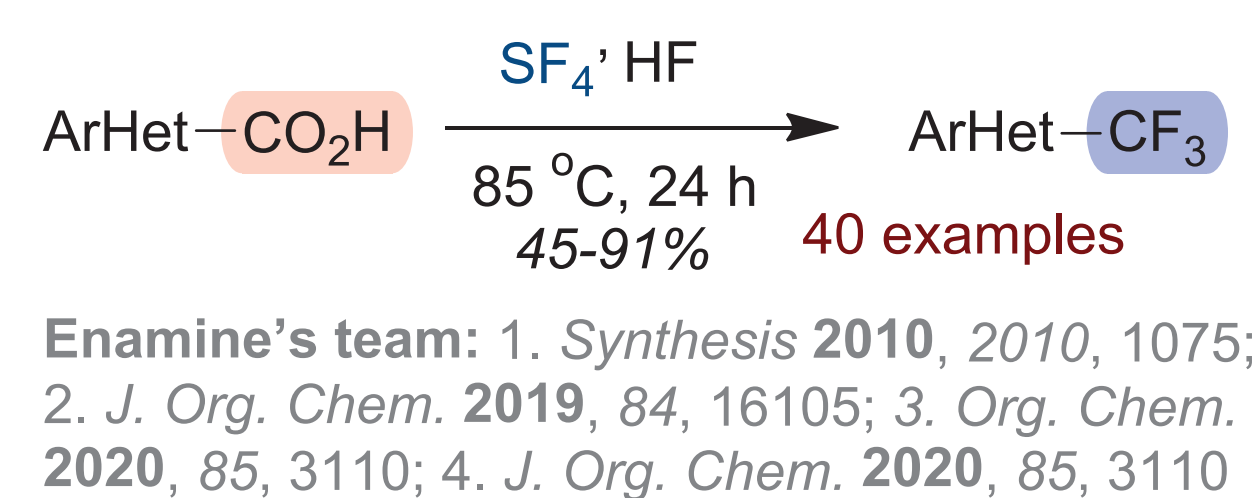
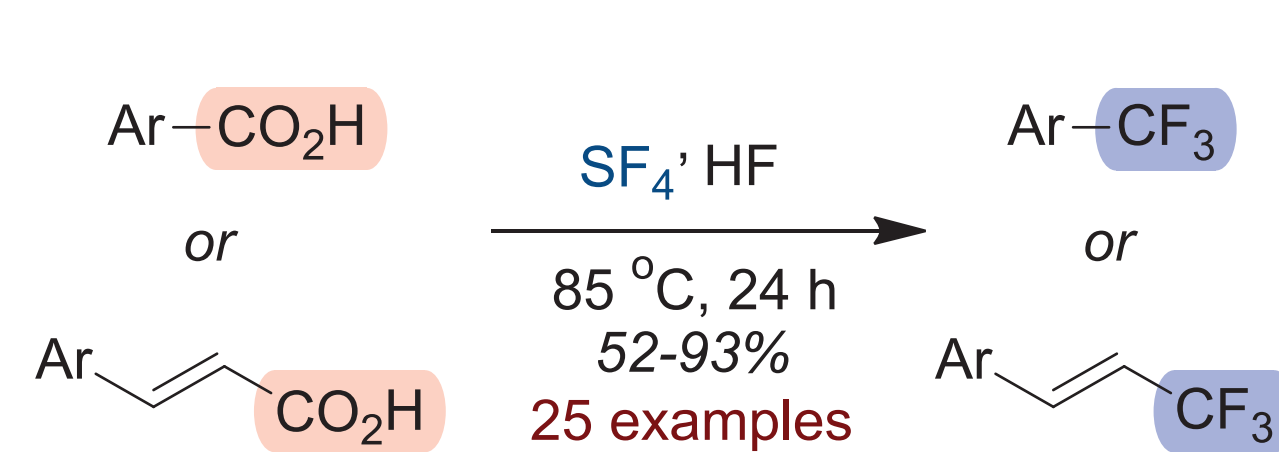
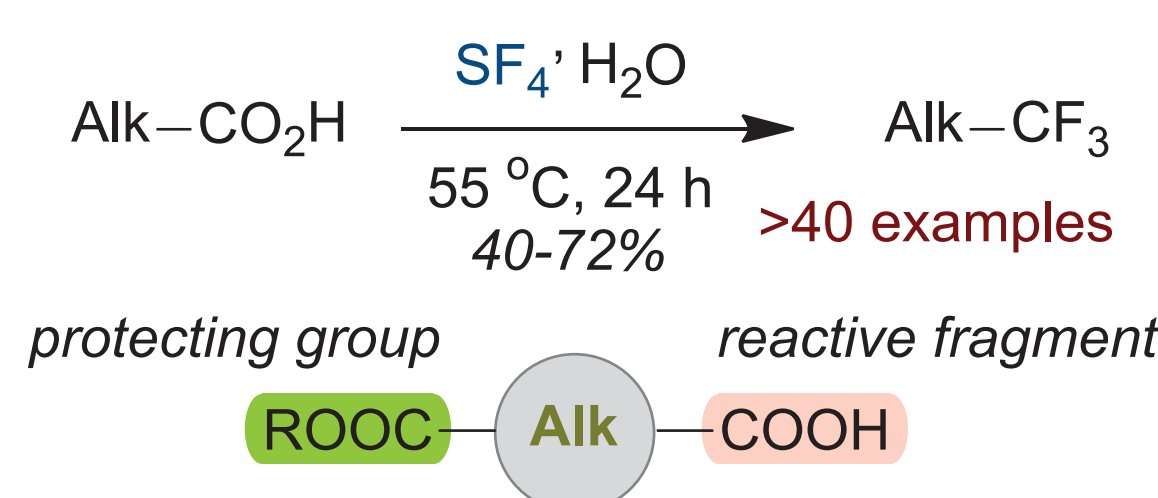
Release of the excess SF₄ and gaseous by-products into the KOH solution

Opened Hastelloy autoclave 1200 mL

[PRECAUTIONS]

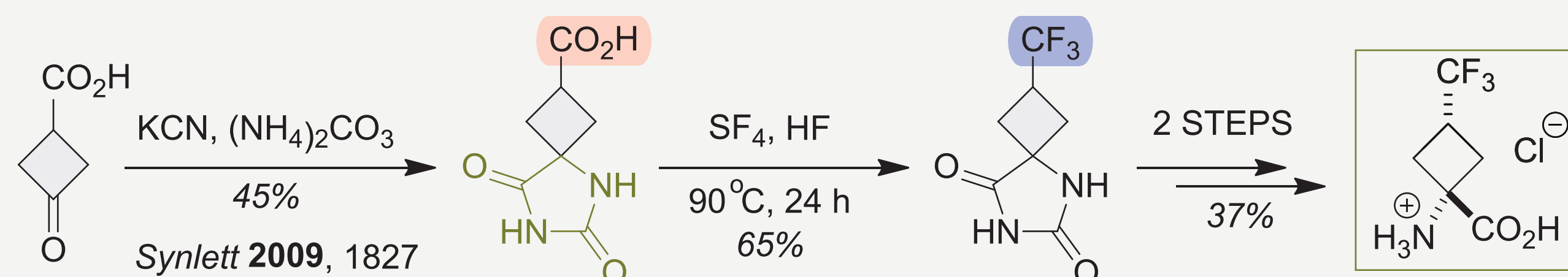
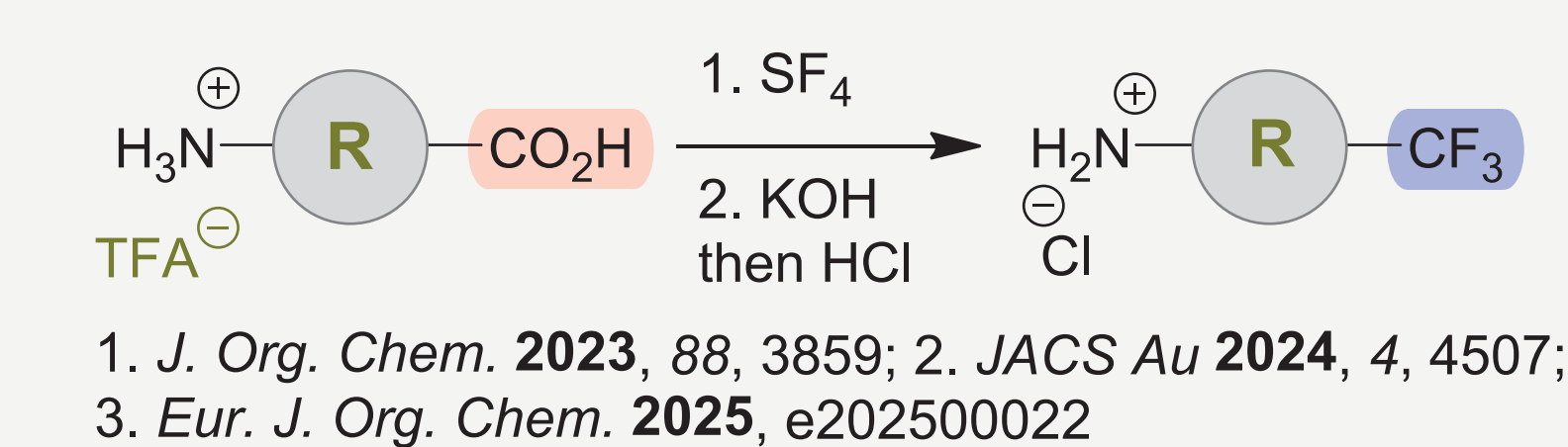
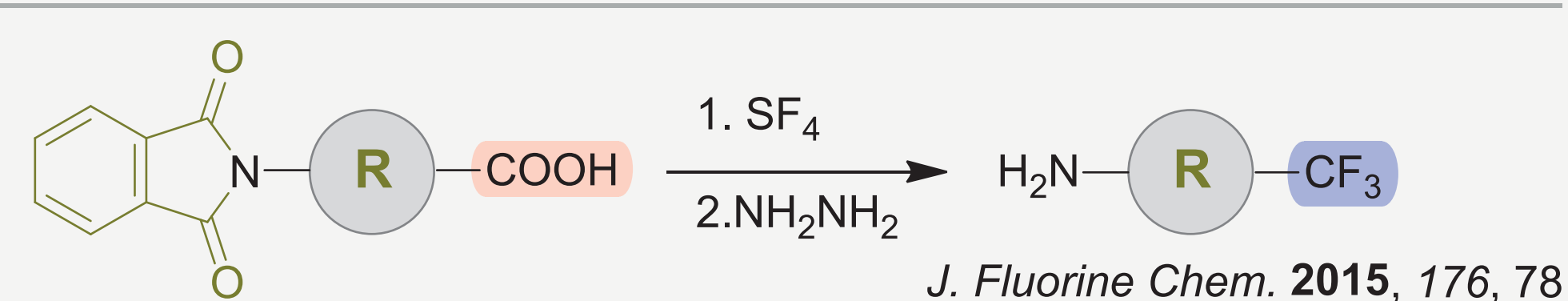
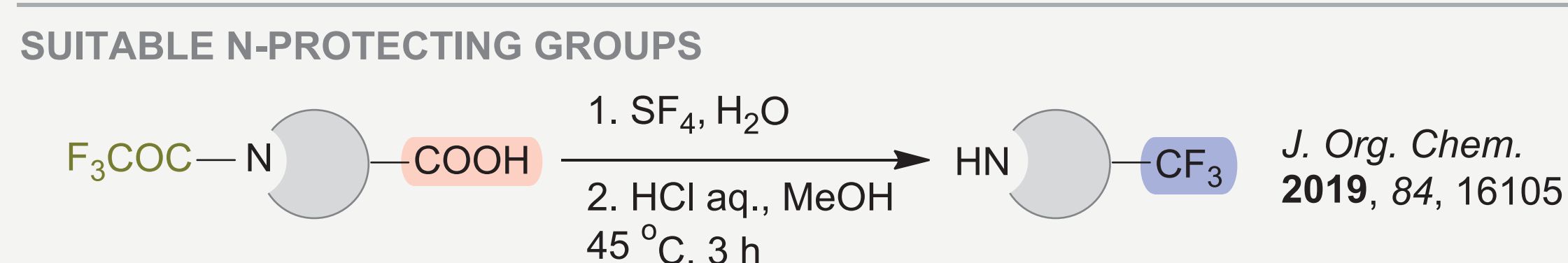
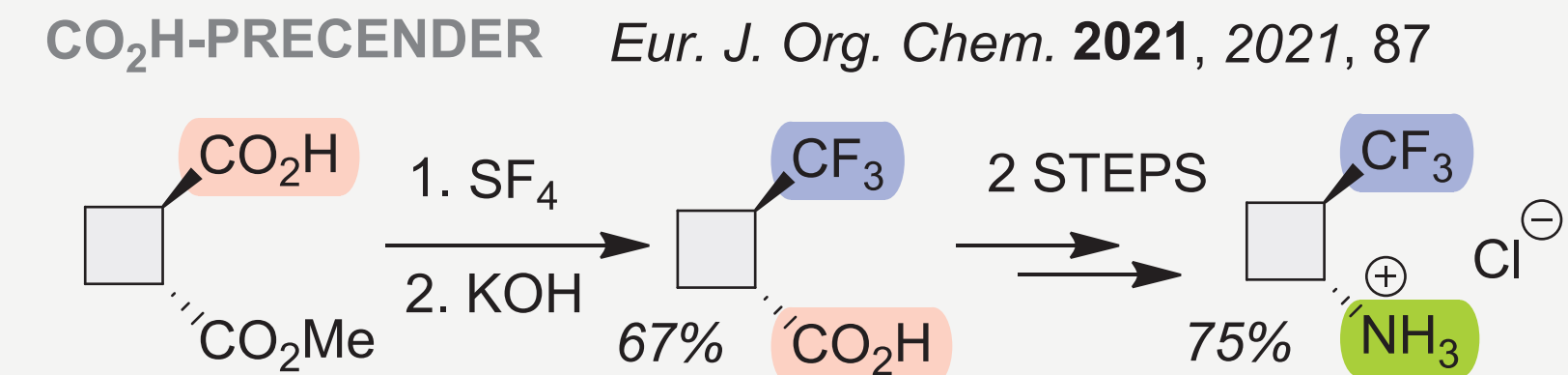
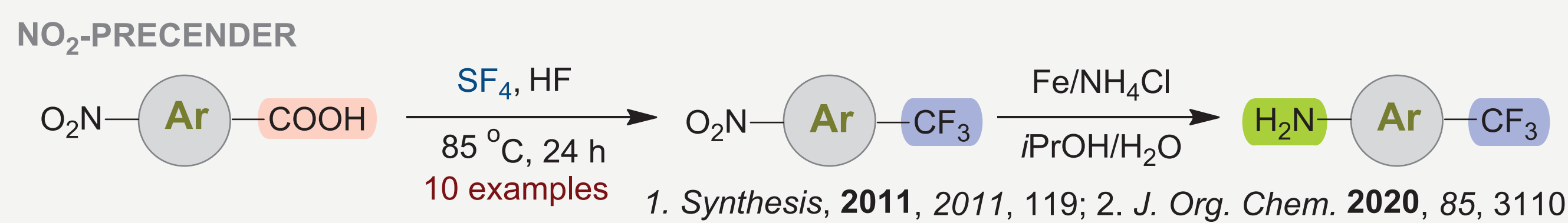
- a separate well-ventilated laboratory
- strictly limited staff access
- the personal-protection equipment including single-filter, full-face masks during operation
- the damper technique applied for loading of SF₄ into the autoclave

Deoxofluorination of CO₂H with SF₄ – an efficient way to CF₃ functionality

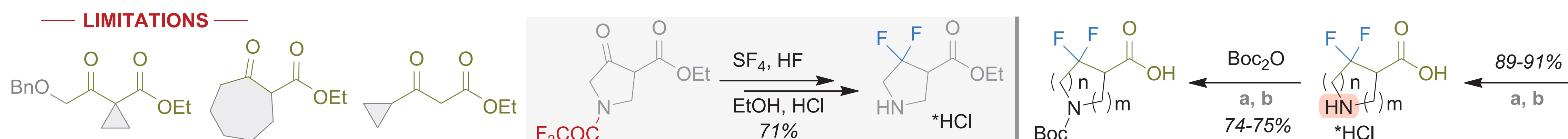
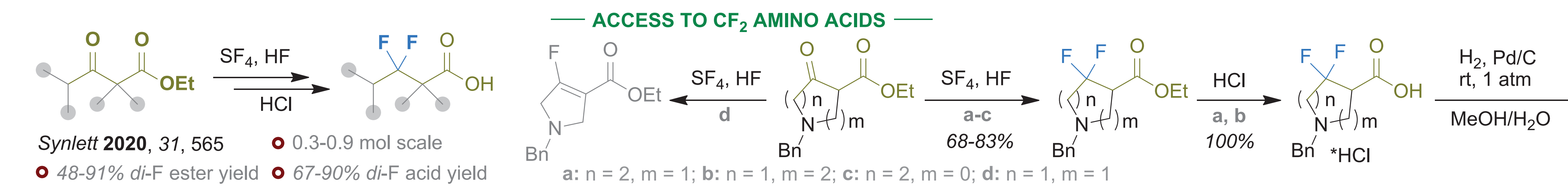


- racemization-free
- epimerization-free
- HF-free
- metal-free
- 1°, 2°, and 3° acids
- gram scale
- 5-/6-memb. Het

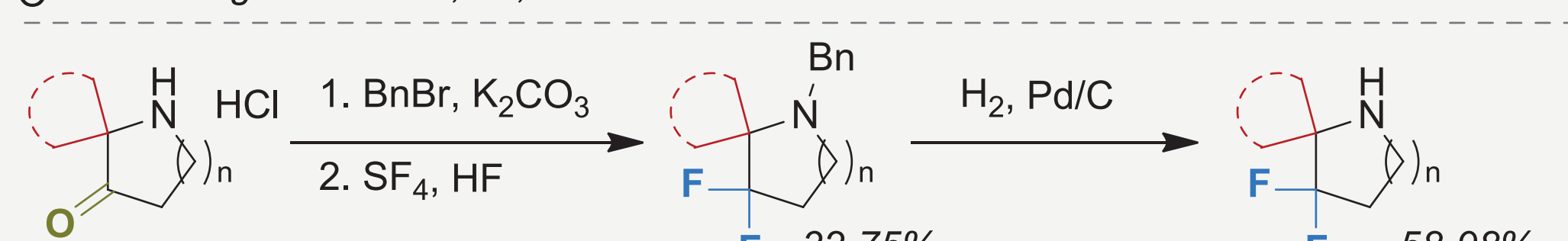
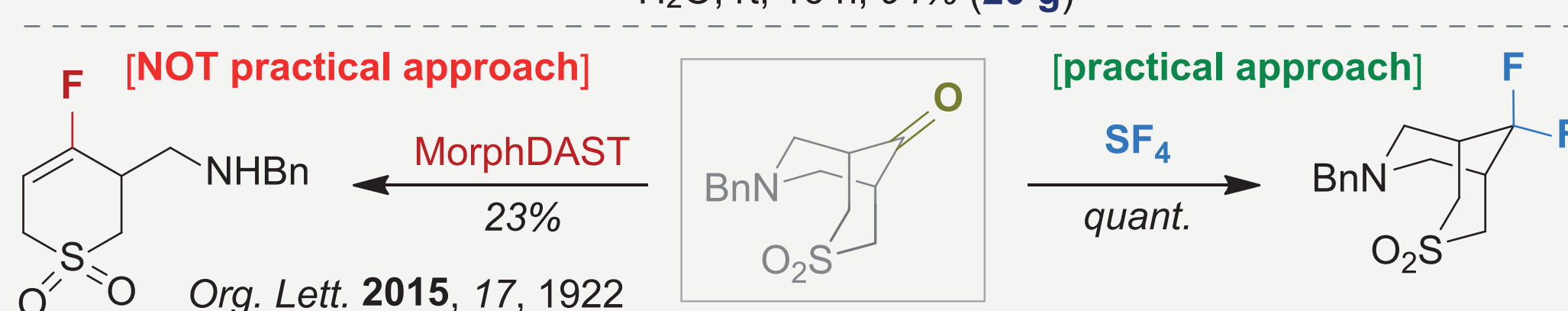
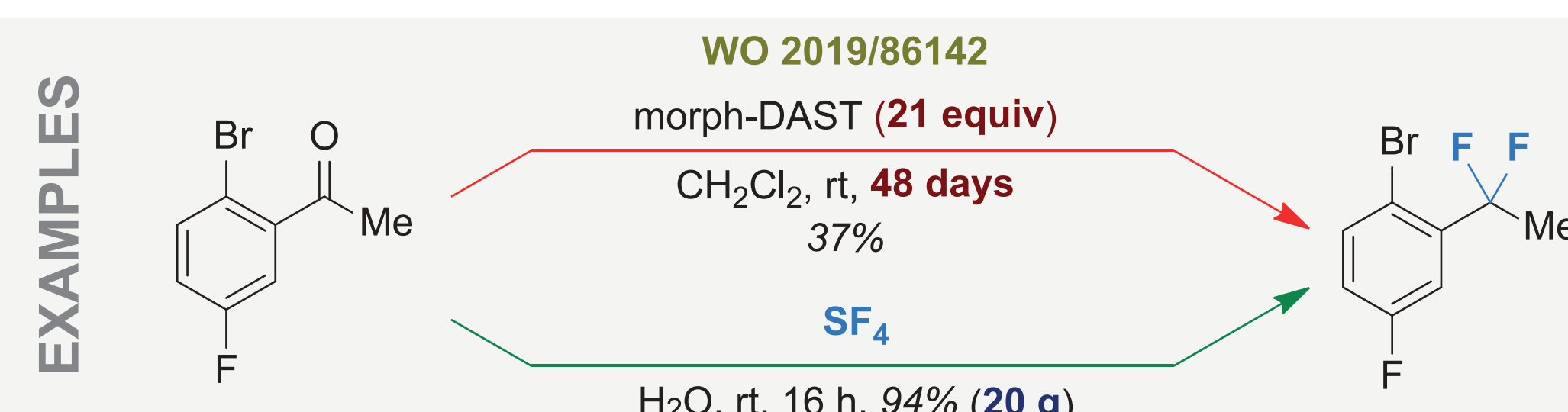
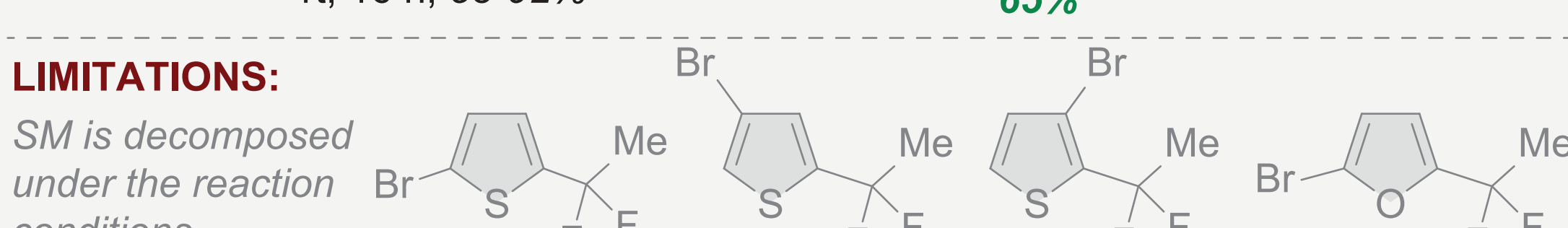
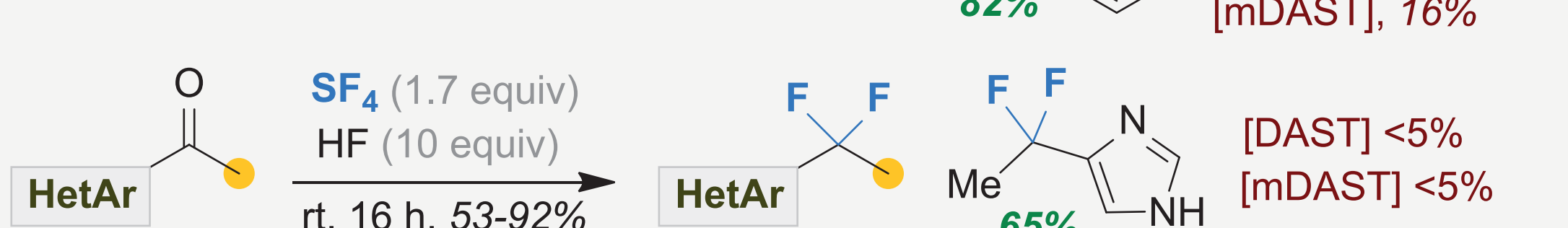
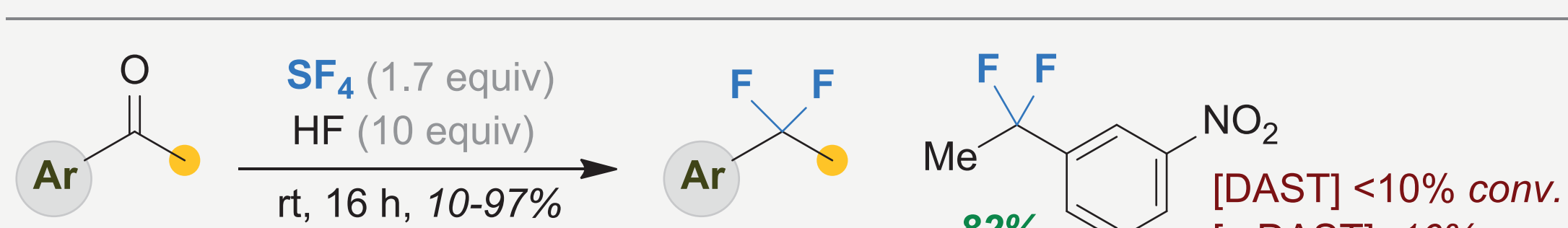
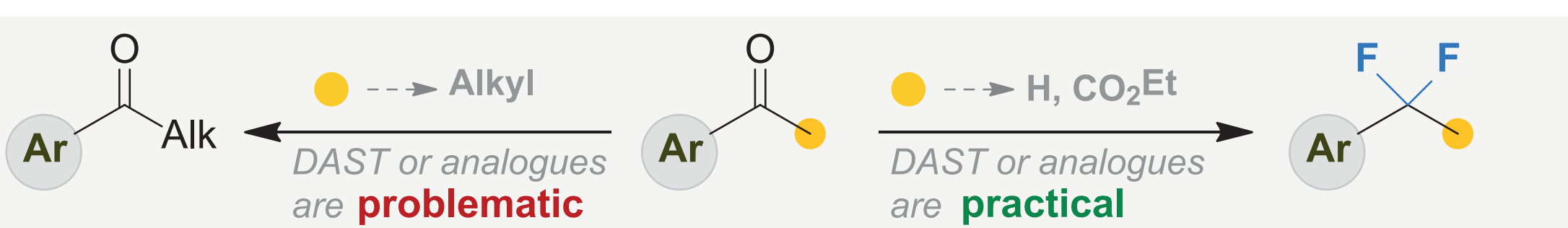
STRATEGIES TO
CF₃-CONTAINING AMINES



SF₄ supported fluorination of ketones



HINDERED
KETONES



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