

Honors Cup Synthetic Proposal

Section: 211

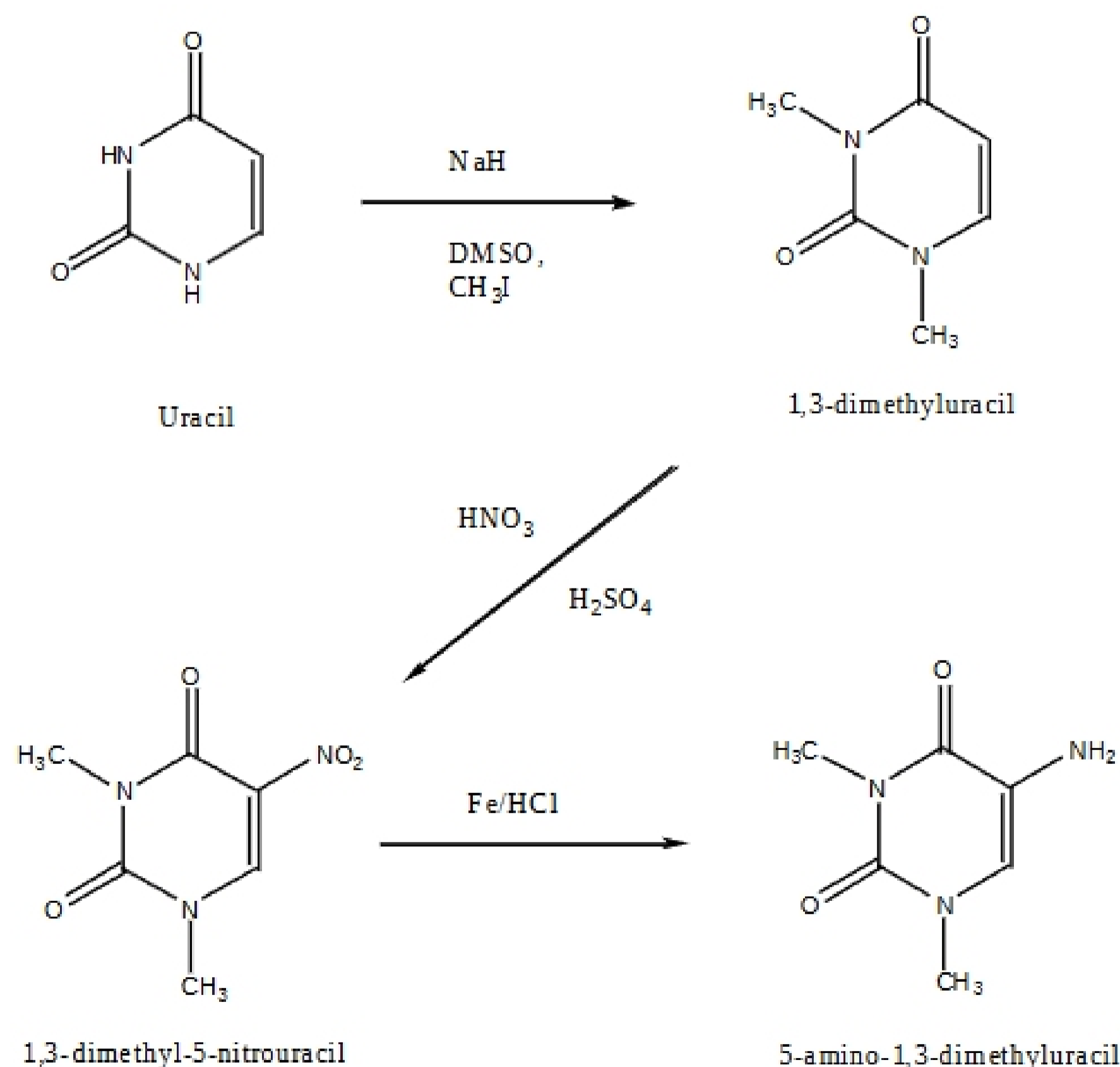
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Title: Synthesis of 5-Amino-1,3-dimethyluracil (Precursor to Caffeine)

Introduction: (what makes your target interesting?)

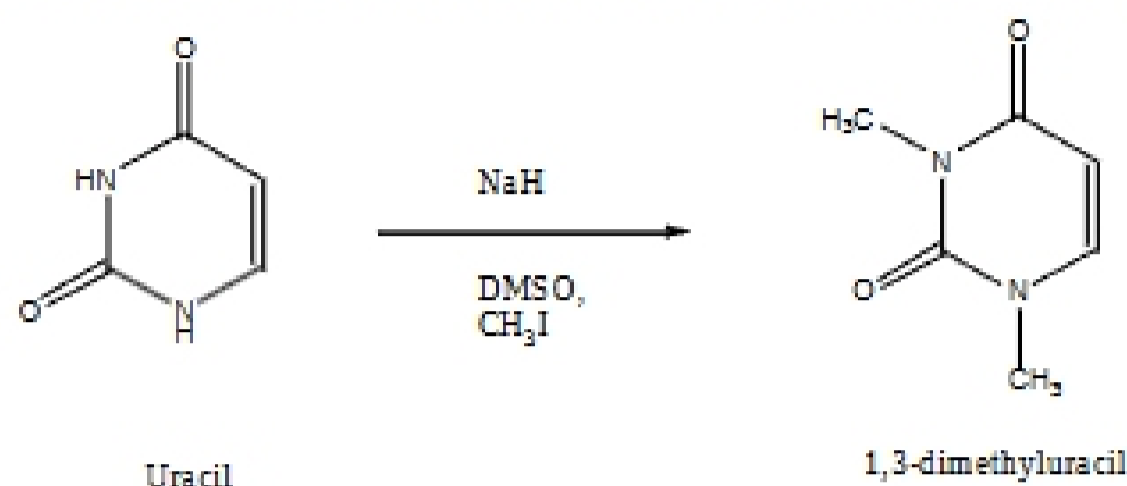
Although caffeine occurs naturally in at least sixty-three different plant species, it has been manufactured and used because of its unique effects on our bodies. It is found mainly in beverages, but is also used in several types of prescription medications, diuretics, and pain relievers. Caffeine is sought by many for its abilities to increase alertness and energy. As energy drinks such as Red Bull™ and Amp™ become more and more popular, caffeine continues to stretch its influence. 5-Amino-1,3-dimethyluracil is a precursor to caffeine and has many of the same functional groups. Here we produce it in a three-step synthesis.

Overall synthetic reaction scheme: (a Chemdraw or similar drawing of all three steps)



Step 1

Synthetic transformation 1: (Chemdraw picture of first transformation)



Experimental 1 (notes if this transformation is not exactly the one reported in literature (e.g. on a different scale) and how it was modified):

- 6.0 g (.053 mol) of uracil were stirred for a week (changed from “overnight”) in 300 mL of DMSO at room temperature.
- 5.1 g (.265 mol) of sodium hydride were added carefully to the solution of uracil.
- 37.6 g (.265 mol) of methyl iodide were added slowly over a period of ten minutes.
- The mixture was stirred for forty minutes and then diluted with 100 mL of water to remove excess of hydride.
- Concentrated HCl was added to the solution until it reached a pH of 1-2.
- The product was then extracted with methylene chloride and washed with saturated bicarbonate solution until neutral.
- After removing the dichloromethane, 1,3-dimethyl-uracil should be left behind.
- HNMR peaks: 3.29 (s, 3H), 3.37 (s, 3H), 5.65 (d, $J = 15$ Hz, 1H, HC=), 7.1 (d, $J = 15$ Hz, 1H, HC=)

Notes:

- The reaction mixture was stirred for a week instead of overnight because we cannot come to lab every day (it’s a darn shame...).

Expected yield: 61% , 8.6 g

Safety, disposal and green issues 1:

Uracil

- Minimize contact

Sodium Hydride (NaH)

- Reacts violently with water
- Incompatible with water, acids, alcohols, and strong oxidizing agents
- Dispose of correctly

