

Supporting Information

Improved Chemical Syntheses of 5,6-Dihydro-5-fluorouracil

Andrew L. LaFrate and John A. Katzenellenbogen*

Department of Chemistry, University of Illinois at Urbana-Champaign,
600 S. Mathews Ave, Urbana, Illinois, 61820

jkatzene@uiuc.edu

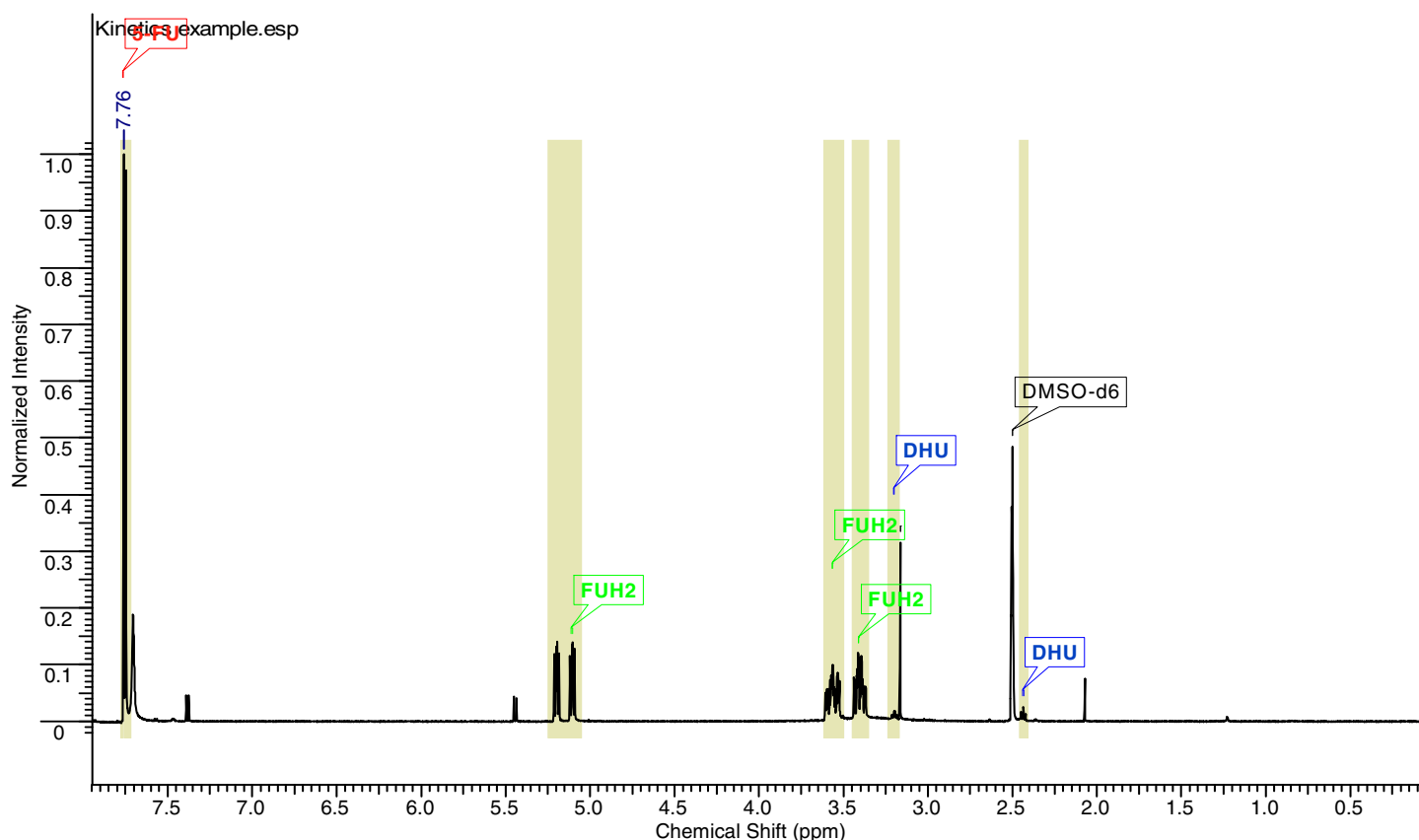
Table of contents

General considerations	S2
NMR Spectra of 3 (^1H and ^{13}C)	S3
NMR Spectra of 4 (^1H and ^{13}C)	S4
NMR Spectra of 5 (^1H and ^{13}C)	S5
NMR Spectra of 5-DHFU (^1H and ^{13}C)	S6

General Considerations

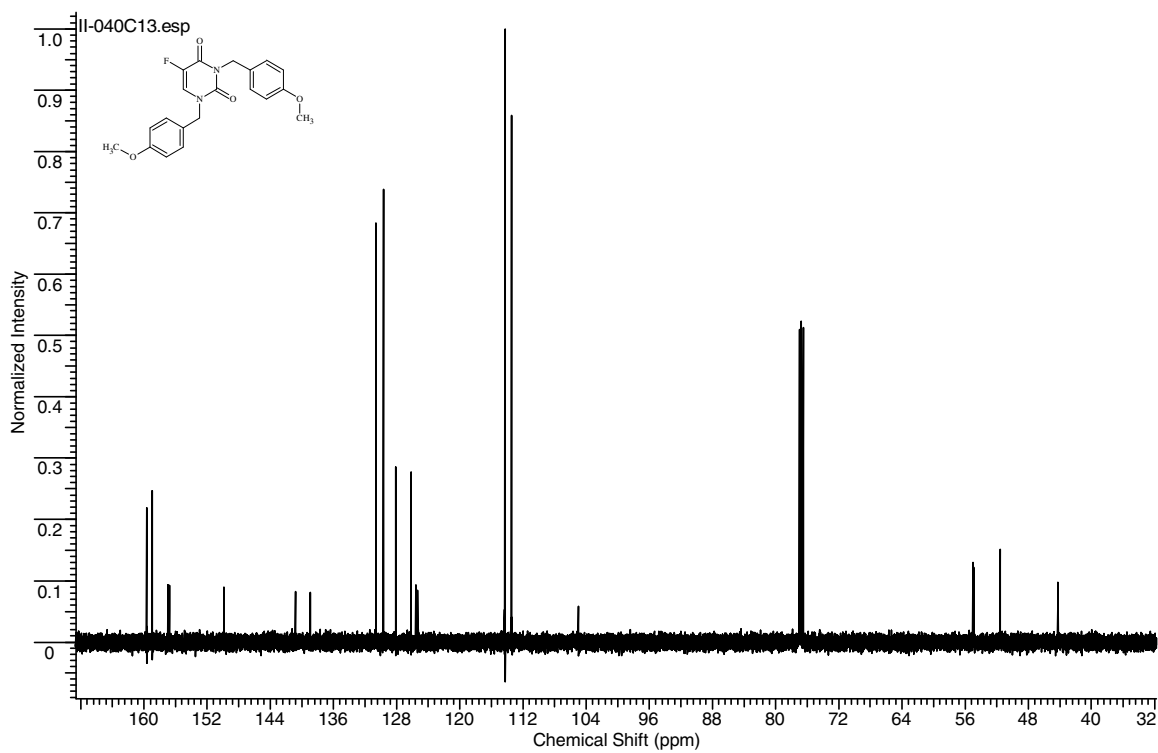
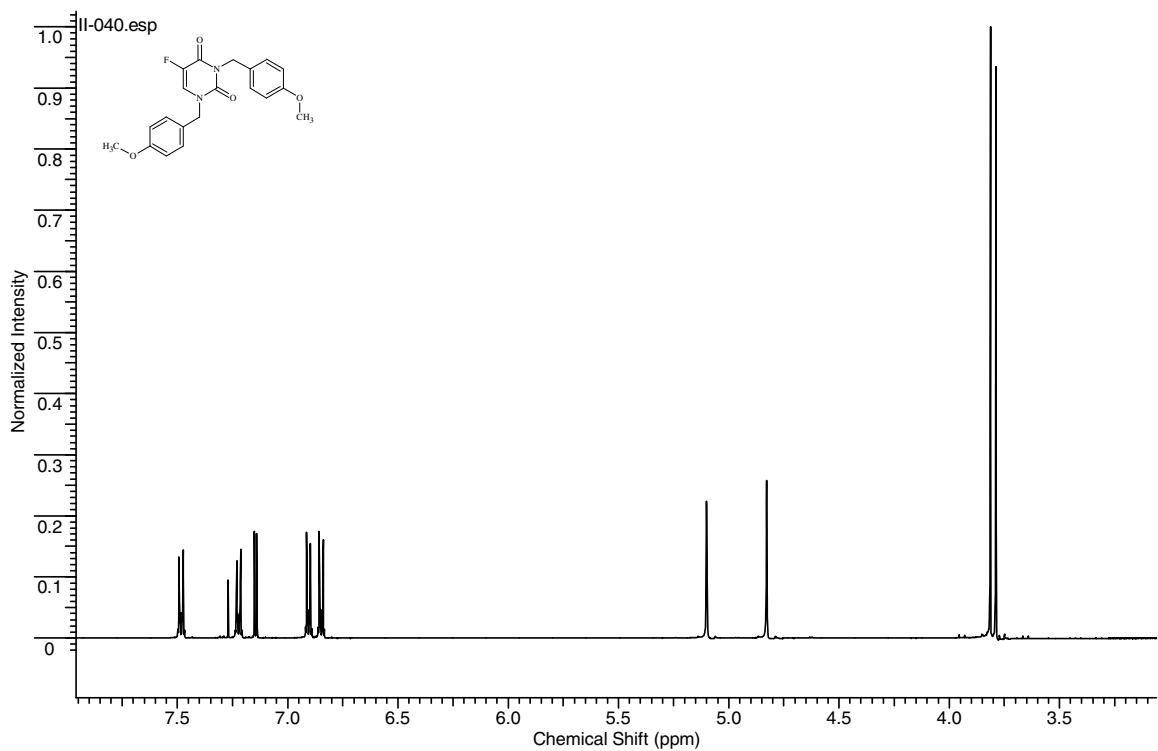
All reagents were purchased from commercial suppliers and were used without further purification. Anhydrous THF was obtained from an anhydrous solvent dispensing system,¹ and anhydrous DMF was obtained by distillation over molecular sieves. For specified reactions, all glassware was oven-dried overnight and cooled under vacuum, then purged with argon; all of these reactions were conducted under argon. ¹H NMR spectra were recorded on either a 400 or 500 MHz instrument, and ¹³C NMR were recorded at either 100 or 125 MHz on the same instruments. NMR spectra are reported in ppm and were referenced to the solvent peak. EI mass spectra were recorded at 70 eV.

Sample NMR Spectrum from 5-FU Hydrogenation Kinetics Study

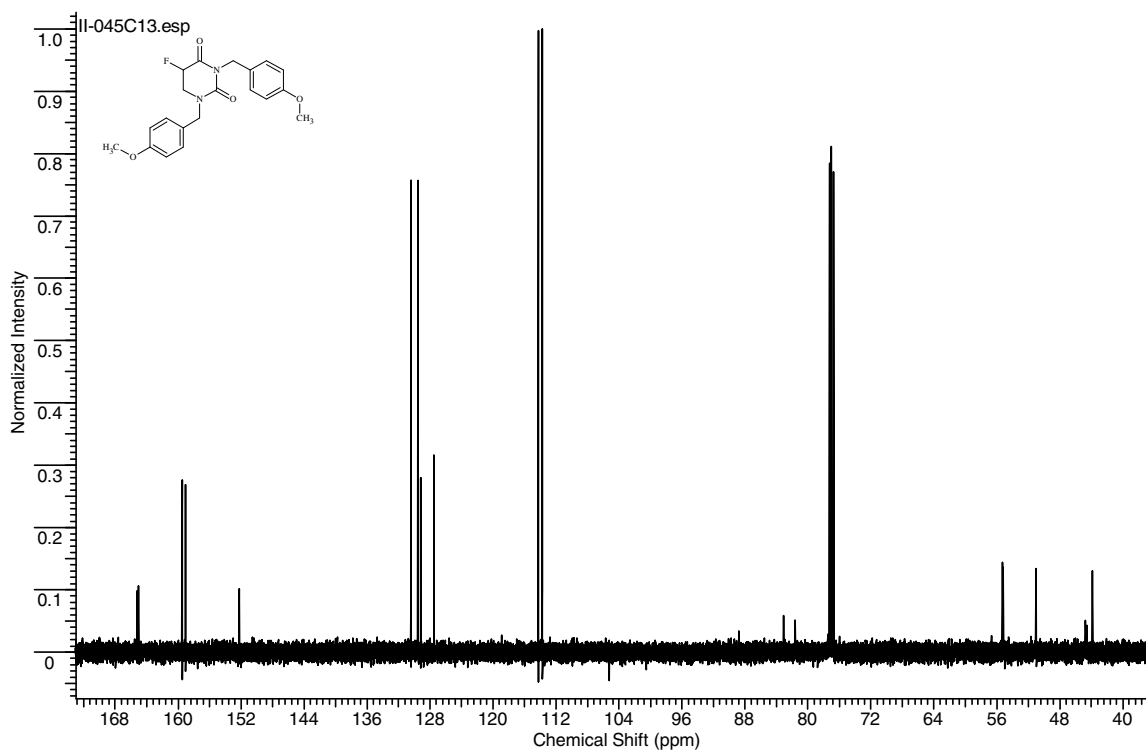
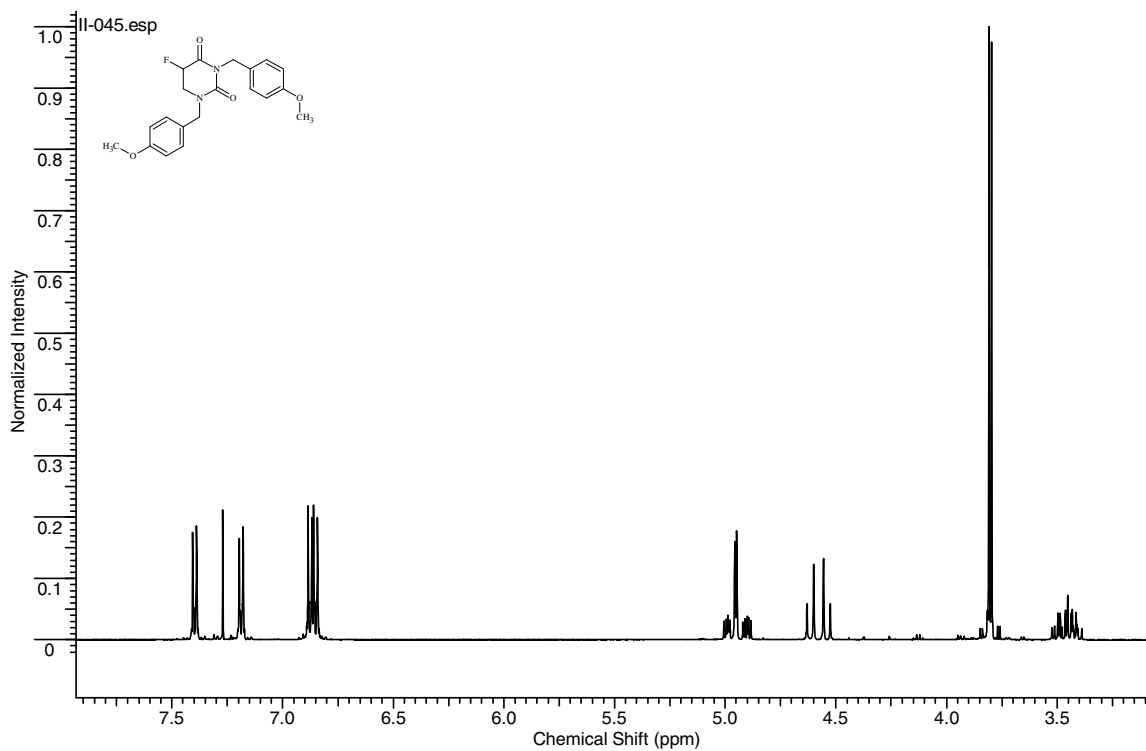


¹ Pangborn, A.B., Giardello, M.A., Grubbs, R.H., Rosen, R.K., and Timmers, F.J. *Organometallics*, **1996** *15*, 1518-1520.

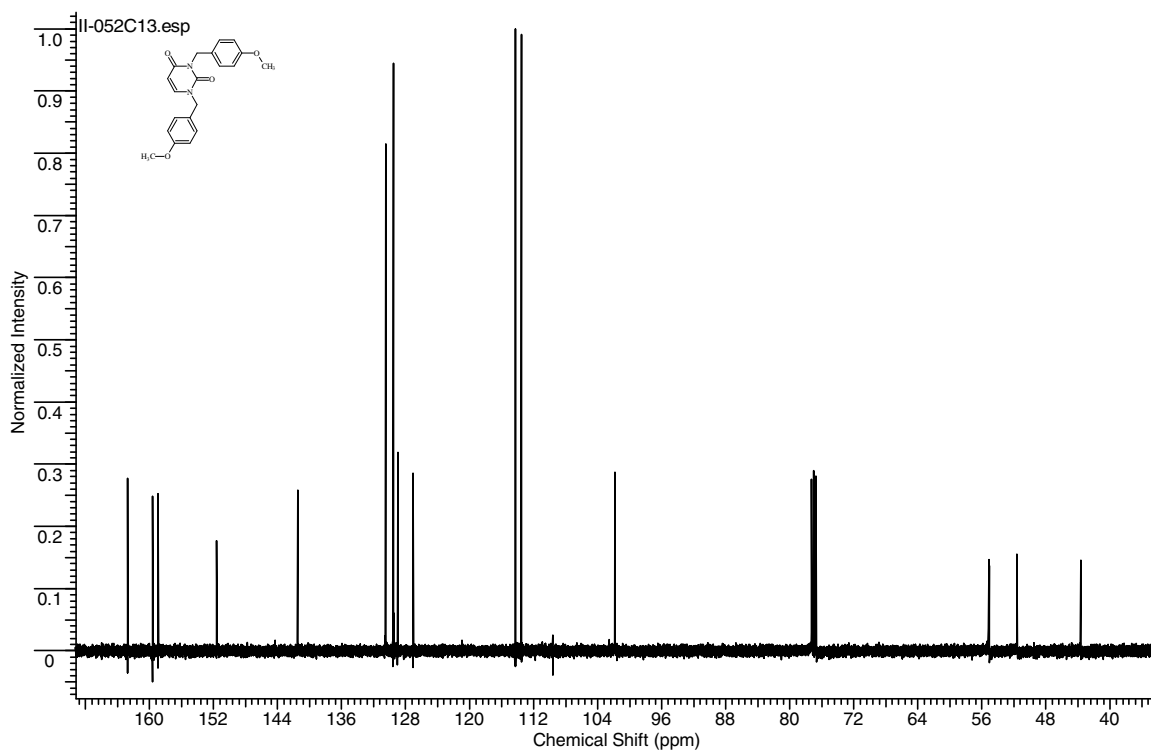
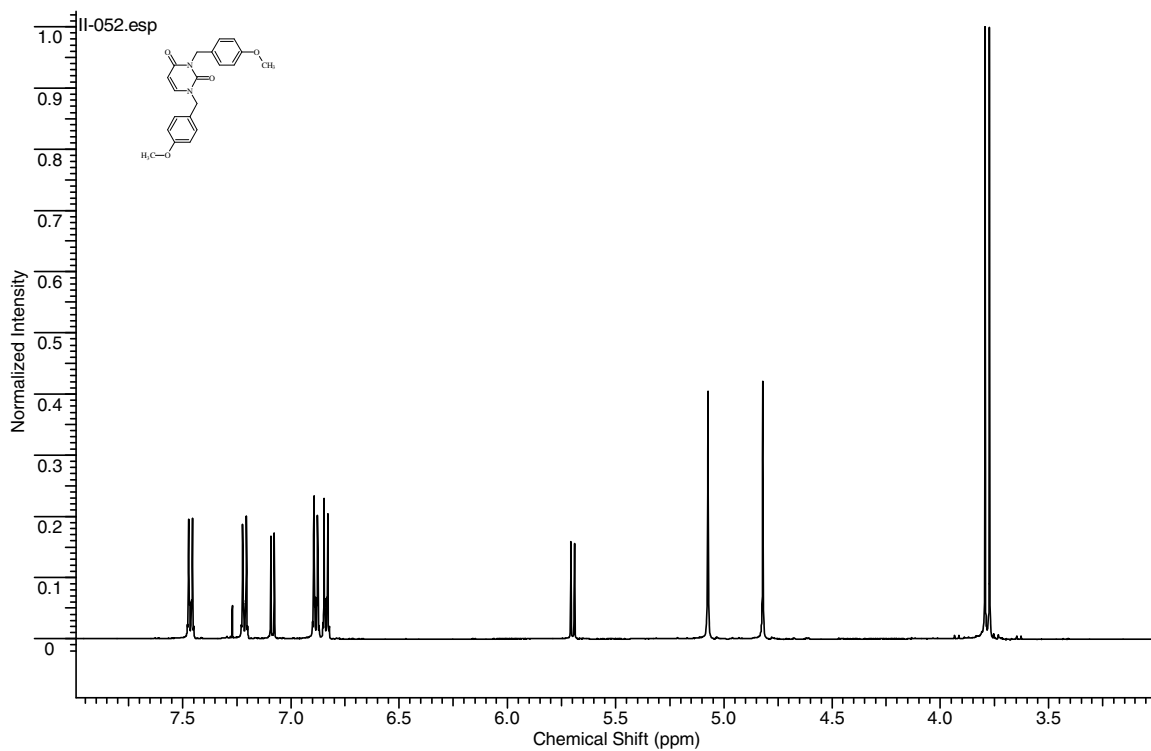
NMR Spectra of 1,3-Bis-(4-methoxybenzyl)-5-fluorouracil (**3**)



NMR Spectra of 1,3-Bis-(4-methoxybenzyl)-5,6-dihydro-5-fluorouracil (4)



NMR Spectra of 1,3-Bis-(4-methoxybenzyl)-uracil (**5**)



NMR Spectra of 5,6-Dihydro-5-fluorouracil (**5-DHFU**)

