

Dehydrogenation of a β -Ketoester to a Phenol Using a Recyclable Oxoammonium Salt

Fabrizio Politano, William P. Brydon, Jyoti Nandi, and Nicholas E. Leadbeater*

Department of Chemistry, University of Connecticut, 55 North Eagleville Road, Storrs, CT 06269-3060, USA

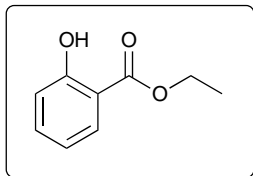
* Correspondence: nicholas.leadbeater@uconn.edu

SUPPORTING INFORMATION

<i>Product Characterization</i>	S2
¹ H-NMR (400 MHz CDCl ₃).....	S3
¹³ C-NMR (101 MHz CDCl ₃).....	S4
GC-MS	S5

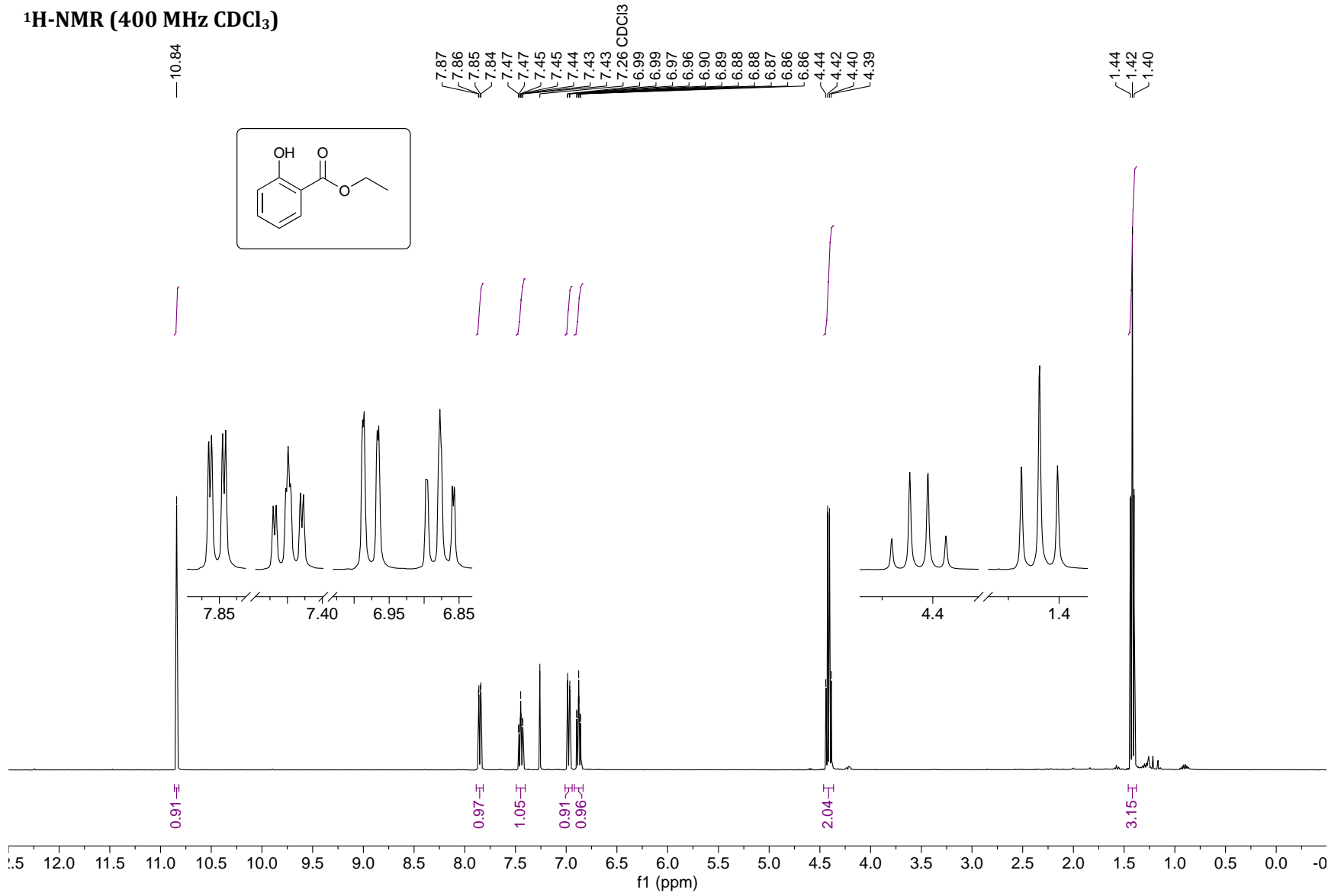
Product Characterization

2-Ethyl-7-nitro-1H-benzimidazole3-oxide (3). ¹H NMR: (400 MHz, CDCl₃) δ ppm 10.84 (s, 1H), 7.85 (dd, J = 8.0, 1.8 Hz, 1H), 7.45 (ddd, J = 8.8, 7.2, 1.8 Hz, 1H), 6.98 (dd, J = 8.4, 1.1 Hz, 1H), 6.88 (ddd, J = 8.2, 7.2, 1.1 Hz, 1H), 4.41 (q, J = 7.1 Hz, 2H), 1.42 (t, J = 7.1 Hz, 3H). ¹³C NMR: (101 MHz, CDCl₃) δ ppm 170.36, 161.83, 135.73, 130.05, 119.22, 117.70, 112.79, 77.48, 77.16, 76.84, 61.55, 14.33. **GC-MS:** (EI), m/z (relative intensity, %), 166 ([M]⁺, 39), 121 (28), 120 (100), 92 (37), 65 (11). Spectral data for this compound is consistent with that previously reported.¹



1. Magano, J.; Chen, M. H.; Clark, J. D.; Nussbaumer, T. *J. Org. Chem.*, 2006, **71**, 7103-7105.

¹H-NMR (400 MHz CDCl₃)



¹³C-NMR (101 MHz CDCl₃)

— 170.36

— 161.83

— 135.73

— 130.05

— 119.22

— 117.70

— 112.79

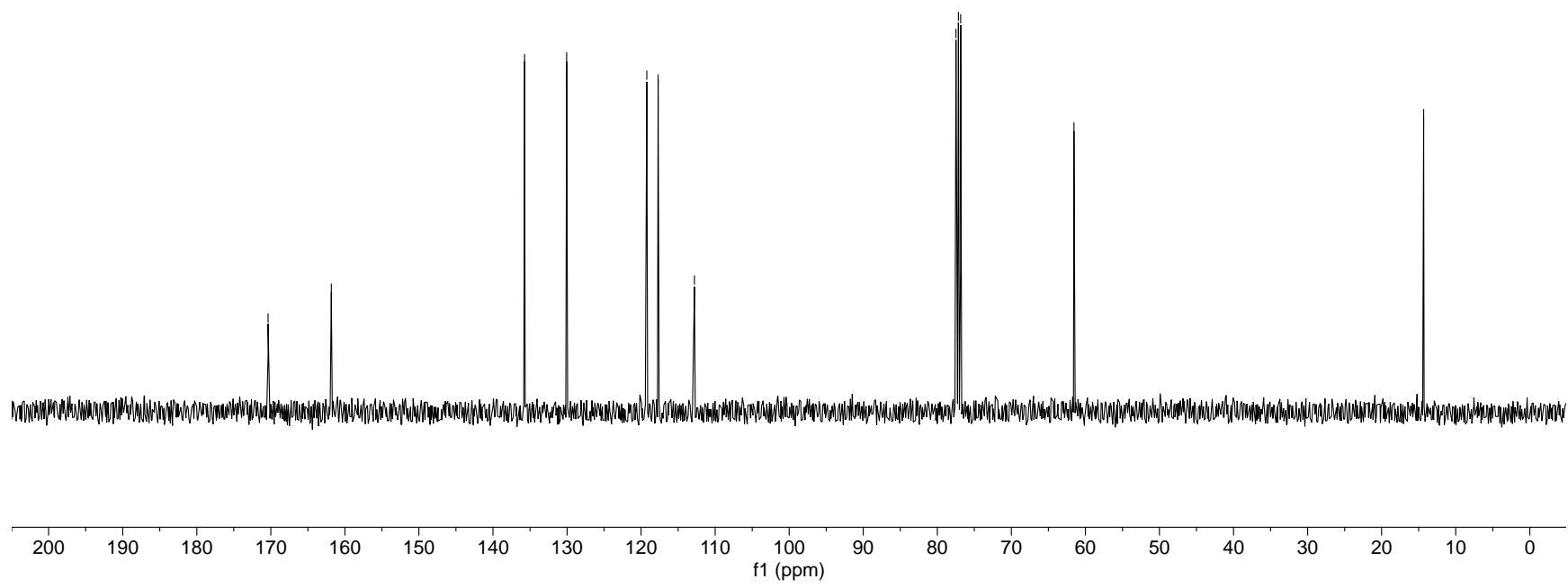
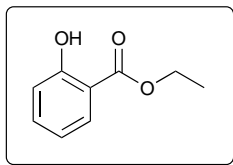
77.48 CDCl₃

77.16 CDCl₃

76.84 CDCl₃

— 61.55

— 14.33



GC-MS

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Misc Info :
Vial Number: 22

