

3-(4-(benzyloxy)-3-methoxyphenyl)-[1,2,4]triazolo[4,3-*a*]pyridine

Katrina E. Doherty, Arturo León Sandoval, Ethan T. Mercier and Nicholas E. Leadbeater*

Department of Chemistry, University of Connecticut, 55 North Eagleville Road, Storrs, Connecticut 06269-3060, United States

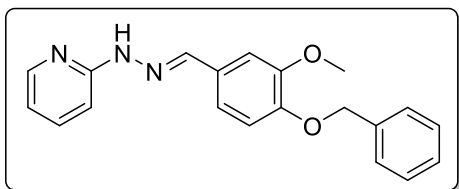
* Correspondence e-mail: nicholas.leadbeater@uconn.edu

SUPPORTING INFORMATION

<i>Characterization of N-[(3-methoxy-4-phenylmethoxyphenyl)methylideneamino]pyridin-2-amine (1)</i>	S2
¹ H-NMR Spectrum (400 MHz CDCl ₃).....	S3
¹³ C-NMR Spectrum(101 MHz CDCl ₃).....	S4
IR Spectrum.....	S5
<i>Characterization of 3-(4-(benzyloxy)-3-methoxyphenyl)-[1,2,4]triazolo[4,3-<i>a</i>]pyridine (2)</i>	S6
¹ H-NMR Spectrum (400 MHz CDCl ₃).....	S7
¹³ C-NMR Spectrum(101 MHz CDCl ₃).....	S8
IR Spectrum.....	S9

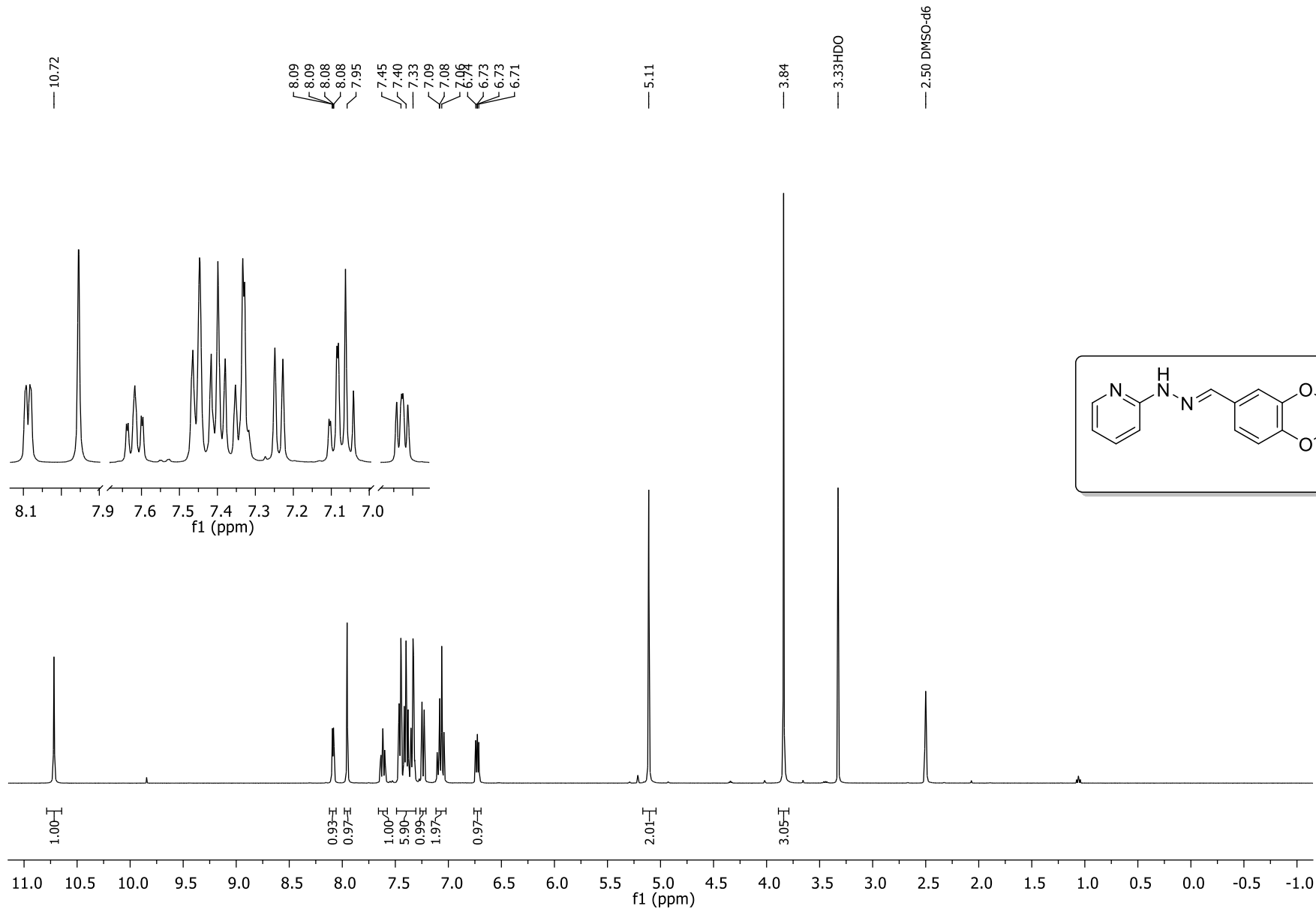
Product Characterization

***N*-[(3-methoxy-4-phenylmethoxyphenyl)methylideneamino]pyridin-2-amine (1):** ¹H NMR (400 MHz, DMSO)

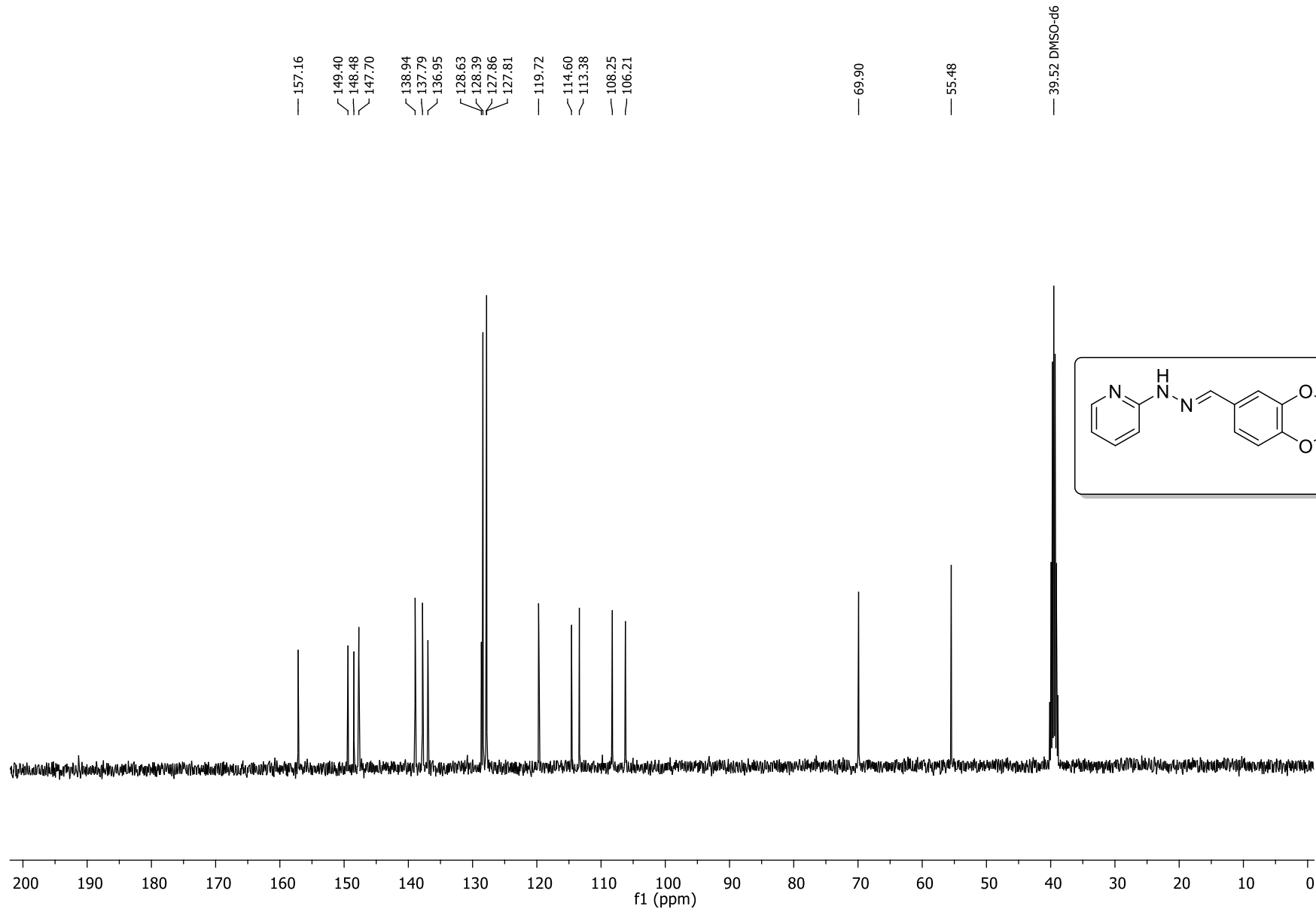


δ 10.72 (s, 1H), 8.09 (dd, $J = 4.8, 0.9$ Hz, 1H), 7.95 (s, 1H), 7.66 – 7.58 (m, 1H), 7.49 – 7.31 (m, 6H), 7.24 (d, $J = 8.4$ Hz, 1H), 7.12 – 7.02 (m, $J = 15.9, 5.0$ Hz, 2H), 6.73 (dd, $J = 6.5, 5.2$ Hz, 1H), 5.11 (s, 2H), 3.84 (s, 3H). ¹³C NMR (101 MHz, DMSO) δ 157.16, 149.40, 148.48, 147.70, 138.94, 137.79, 136.95, 128.63, 128.39, 127.86, 127.81, 119.72, 114.60, 113.38, 108.25, 106.21, 69.90, 55.48. **HRMS (ESI)** m/z calculated for C₂₀H₂₀N₃O₂ [M + H]⁺ 334.1556, found 334.1553 **MP:** 175-176 °C.

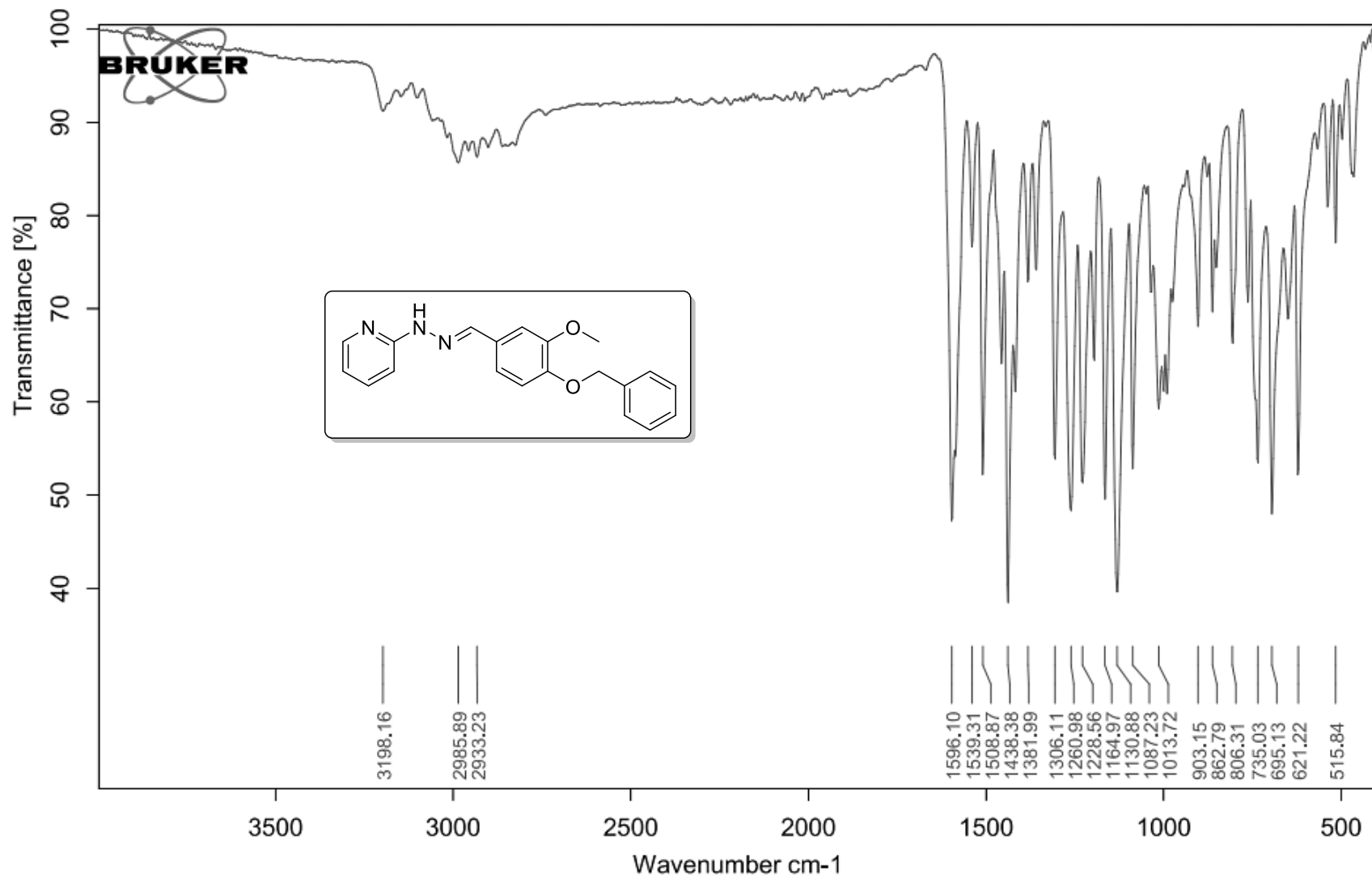
¹H-NMR Spectrum (400 MHz CDCl₃)



¹³C-NMR Spectrum 101 MHz CDCl₃)

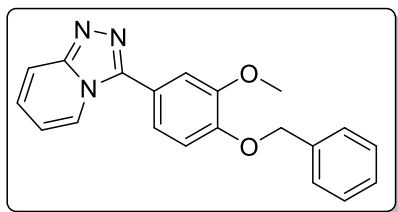


IR Spectrum



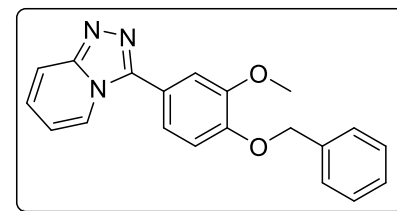
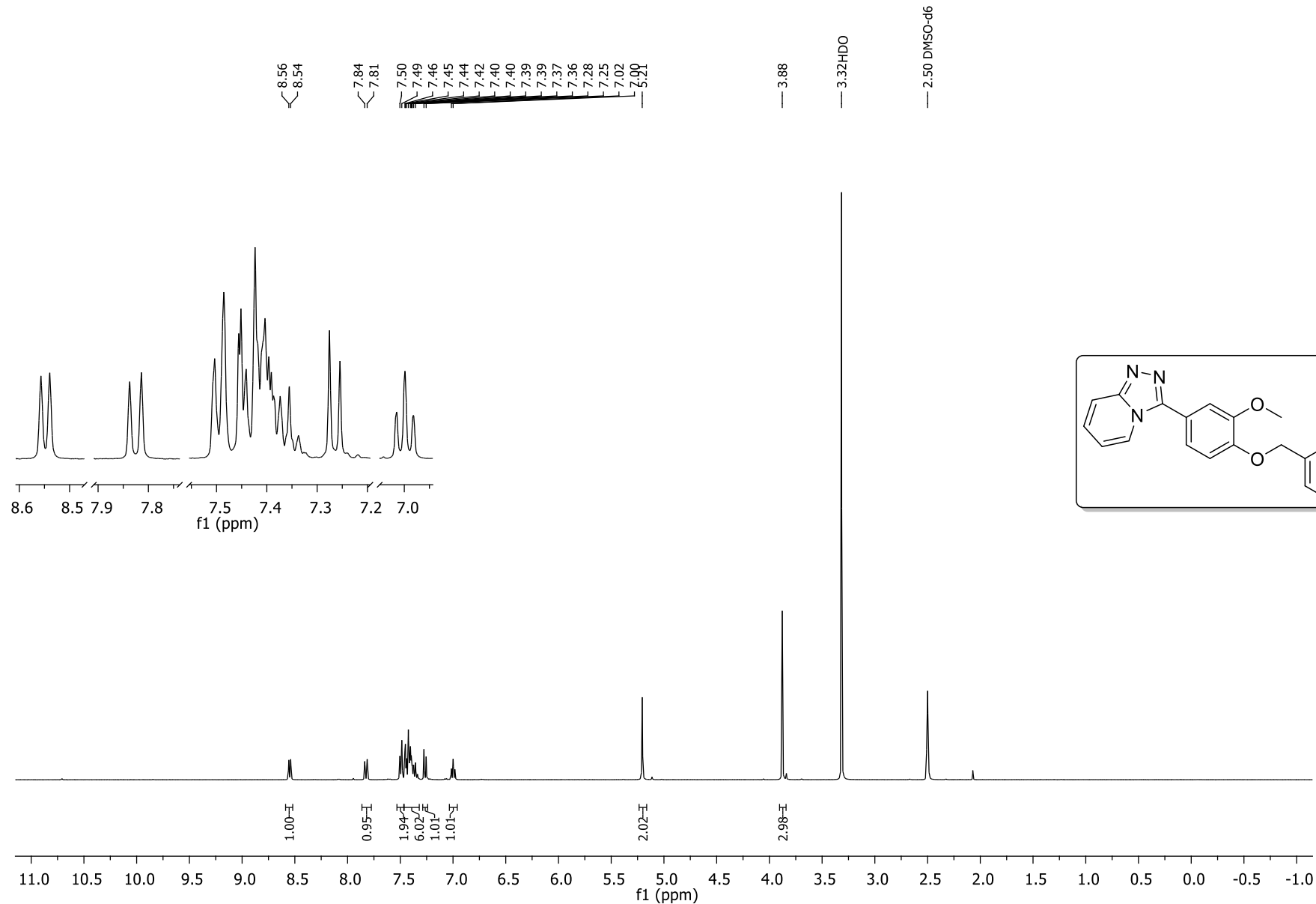
Product Characterization

***N*-(4-(benzyloxy)-3-methoxyphenyl)-[1,2,4]triazolo[4,3-*a*]pyridine (2):** $^1\text{H NMR}$ (400 MHz, DMSO) δ

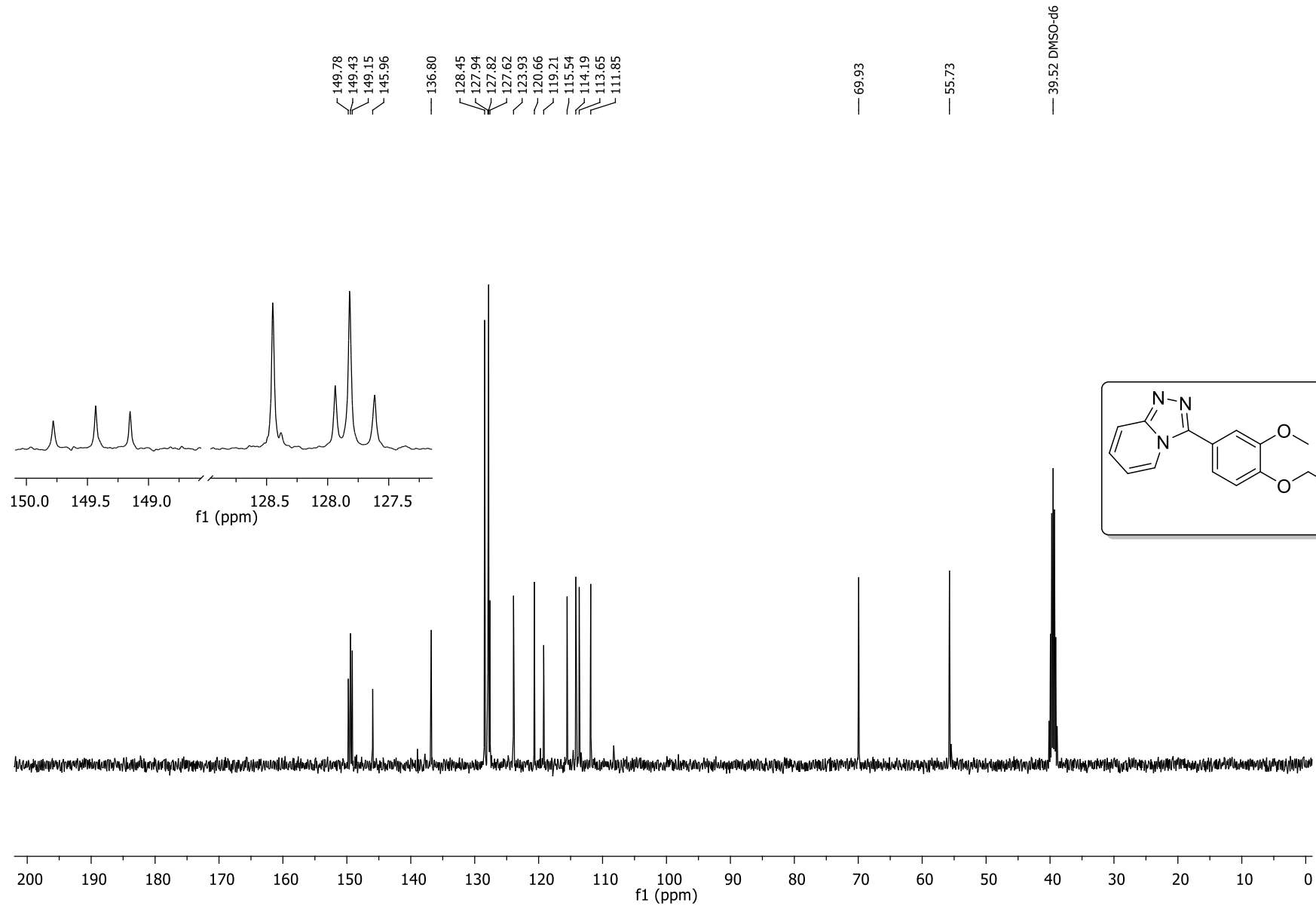


8.55 (d, $J = 7.0$ Hz, 1H), 7.83 (d, $J = 9.3$ Hz, 1H), 7.53 – 7.47 (m, $J = 7.2$ Hz, 2H), 7.46 – 7.32 (m, 6H), 7.27 (d, $J = 8.3$ Hz, 1H), 7.00 (t, $J = 6.6$ Hz, 1H), 5.21 (s, 2H), 3.88 (s, 3H). $^{13}\text{C NMR}$ (101 MHz, DMSO) δ 149.78, 149.43, 149.15, 145.96, 136.80, 128.45, 127.94, 127.82, 127.62, 123.93, 120.66, 119.21, 115.54, 114.19, 113.65, 111.85, 69.93, 55.73. **HRMS (ESI)** m/z calculated for $\text{C}_{20}\text{H}_{18}\text{N}_3\text{O}_2$ $[\text{M} + \text{H}]^+$ 332.1399, found 332.1402. **MP:** 136-139 °C.

¹H-NMR Spectrum (400 MHz CDCl₃)



¹³C-NMR Spectrum 101 MHz CDCl₃)



IR Spectrum

