

Supporting Information
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Scandium-Catalyzed intramolecular Friedel-Crafts reactions of 2-[(2-Alkyl-1H-indol-3-yl)methylene]malonates

Supporting Information

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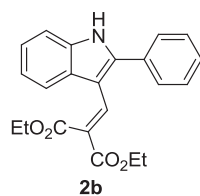
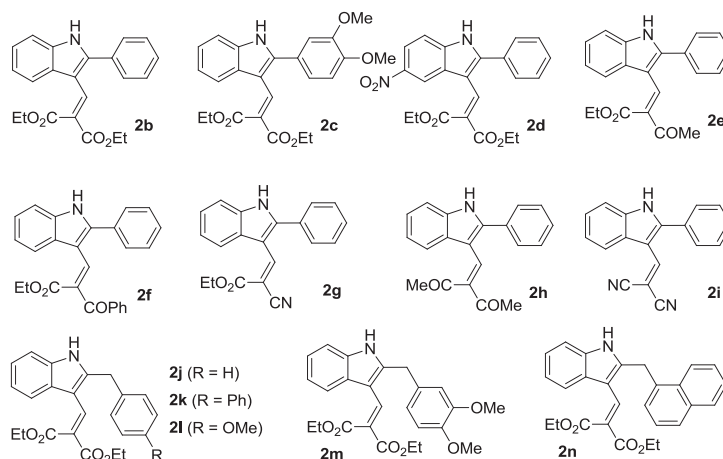
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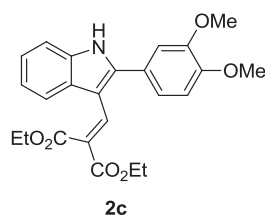
General: All chemicals were purchased from Aldrich Chemical Co. All solvents were reagent grade. Reactions were normally carried out under argon atmosphere in flame-dried glasswares. Merck silica gel 60 (partial size 0.04-0.063 mm) was employed for flash chromatography. NMR spectra of samples in CDCl₃ with TMS as the internal standard were recorded on a Varian-400 spectrometer (400 MHz, ¹H; 100 MHz, ¹³C). HRMS-ESI data were collected on a TOF mass spectrometer made by Micromass Inc. In this supporting information, we supplied spectral data of **2b-2n**.



¹H NMR (400 MHz, CDCl₃) δ 8.56 (s, 1H), 8.02 (s, 1H), 7.59-7.44 (m, 6H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H), 1.08 (t, *J* = 7.2 Hz, 3H)

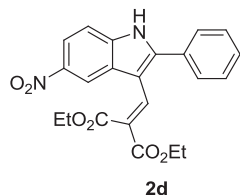
¹³C NMR (100 MHz, CDCl₃) δ 167.41, 165.72, 142.00, 139.90, 136.26, 131.31,

129.21, 129.14, 129.11, 126.81, 123.46, 122.82, 121.41, 120.58, 111.52, 109.21, 61.39, 61.32, 14.38, 13.89.



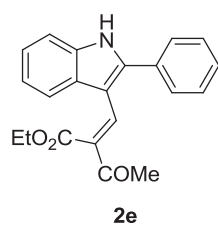
¹H NMR (400 MHz, CDCl₃) δ 8.88 (s, 1H), 8.05 (s, 1H), 7.95 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.21-7.13 (m, 2H), 7.03-6.99 (m, 2H), 6.91 (d, *J* = 8.0 Hz, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 4.20 (q, *J* = 7.2 Hz, 2H), 3.92 (s, 3H), 3.86 (s, 3H), 1.31 (t, *J* = 6.8 Hz, 3H), 1.14 (t, *J* = 6.8 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 167.80, 165.90, 149.85, 149.05, 142.92, 140.44, 136.33, 126.51, 123.81, 123.10, 122.24, 121.15, 121.07, 120.22, 111.91, 111.56, 111.38, 108.32, 61.47, 61.22, 55.97, 55.90, 14.31, 13.86.



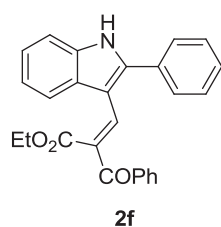
¹H NMR (400 MHz, CDCl₃) δ 9.30 (s, 1H), 8.43 (s, 1H), 7.97 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.88 (s, 1H), 7.46-7.47 (m, 3H), 7.41-7.40 (m, 2H), 7.26 (s, 1H), 4.34 (dq, *J* = 8.8, 7.2 Hz, 4H), 1.38 (dt, *J* = 8.8, 7.2 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 167.67, 165.06, 143.91, 142.62, 139.40, 138.17, 129.91, 129.80, 129.16, 128.82, 125.71, 125.39, 118.93, 116.89, 111.74, 109.76, 62.50, 61.72, 14.35.



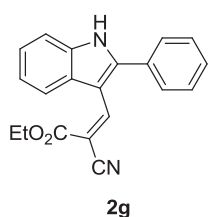
¹H NMR (400 MHz, CDCl₃) δ 8.73 (s, 1H), 7.95 (s, 1H), 7.55-7.47 (m, 6H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.19 (t, *J* = 7.2 Hz, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.03 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 195.7, 168.8, 143.0, 139.8, 138.8, 136.4, 131.3, 130.7, 129.6, 129.4, 129.3, 123.7, 121.7, 120.8, 111.7, 61.4, 28.1, 13.9.



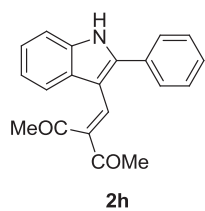
¹H NMR (400 MHz, CDCl₃) δ 8.88 (s, 1H), 8.23 (s, 1H), 7.88 (d, *J* = 7.2 Hz, 2H), 7.49-7.37 (m, 6H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 1H), 4.16 (q, *J* = 7.6 Hz, 2H), 1.08 (t, *J* = 7.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 195.9, 166.8, 143.0, 139.8, 138.1, 136.3, 133.1, 131.3, 129.3, 129.1, 128.4, 127.1, 126.1, 123.3, 121.5, 121.3, 111.4, 109.2, 61.1, 14.1.



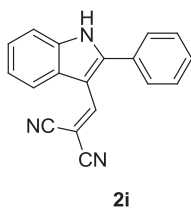
¹H NMR (400 MHz, DMSO) δ 8.28 (s, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 7.65-7.60 (m, 5H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.34 (t, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.26 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, DMSO) δ 163.9, 149.7, 148.9, 137.4, 130.2, 129.9, 129.1, 124.9, 123.9, 122.6, 121.8, 117.9, 112.8, 108.0, 94.3, 61.6, 14.2.



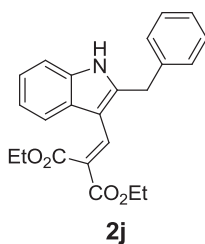
^1H NMR (400 MHz, CDCl_3) δ 9.04 (s, 1H), 7.92 (s, 1H), 7.50-7.46 (m, 5H), 7.44 (d, J = 8.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 1H), 7.25 (t, J = 8.0 Hz, 1H), 7.19 (t, J = 7.6 Hz, 1H), 2.36 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 205.3, 196.7, 142.5, 138.9, 138.5, 136.4, 131.1, 129.6, 129.3, 129.2, 126.9, 123.8, 122.0, 120.8, 111.7, 109.1, 31.6, 27.9.

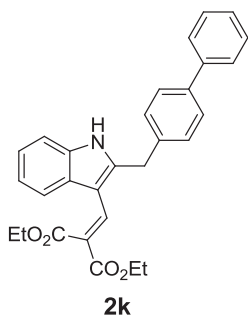


^1H NMR (400 MHz, CDCl_3) δ 8.96 (s, 1H), 8.26 (m, 1H), 7.81 (s, 1H), 7.62-7.60 (m, 3H), 7.52-7.47 (m, 3H), 7.41 (t, J = 4.0 Hz, 2H).

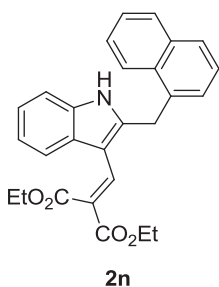
^{13}C NMR (100 MHz, CDCl_3) δ 168.2, 166.2, 144.5, 138.9, 135.7, 125.6, 122.6, 121.2, 120.0, 118.8, 108.5, 62.1, 52.3, 52.1, 28.9, 25.8, 18.1.



^1H NMR (400 MHz, CDCl_3) δ 8.90 (s, 1H), 8.08 (s, 1H), 7.47-7.45 (m, 1H), 7.25-7.06 (m, 8H), 4.28 (q, J = 7.2 Hz, 2H), 4.25 (q, J = 7.2 Hz, 2H), 3.84 (s, 2H), 1.32 (s, J = 7.2 Hz, 3H), 1.16 (s, J = 7.2 Hz, 3H).



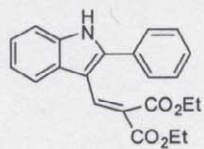
^1H NMR (400 MHz, CDCl_3) δ 8.16 (s, 1H), 8.15 (s, 1H), 7.59-7.56 (m, 3H), 7.46-7.28 (m, 8H), 7.17-7.13 (m, 2H), 4.32 (q, J = 7.2 Hz, 2H), 4.25 (1, J = 7.2 Hz, 2H), 4.22 (s, 2H), 1.54 (t, J = 7.2 Hz, 3H), 1.14 (t, J = 7.2 Hz, 3H).



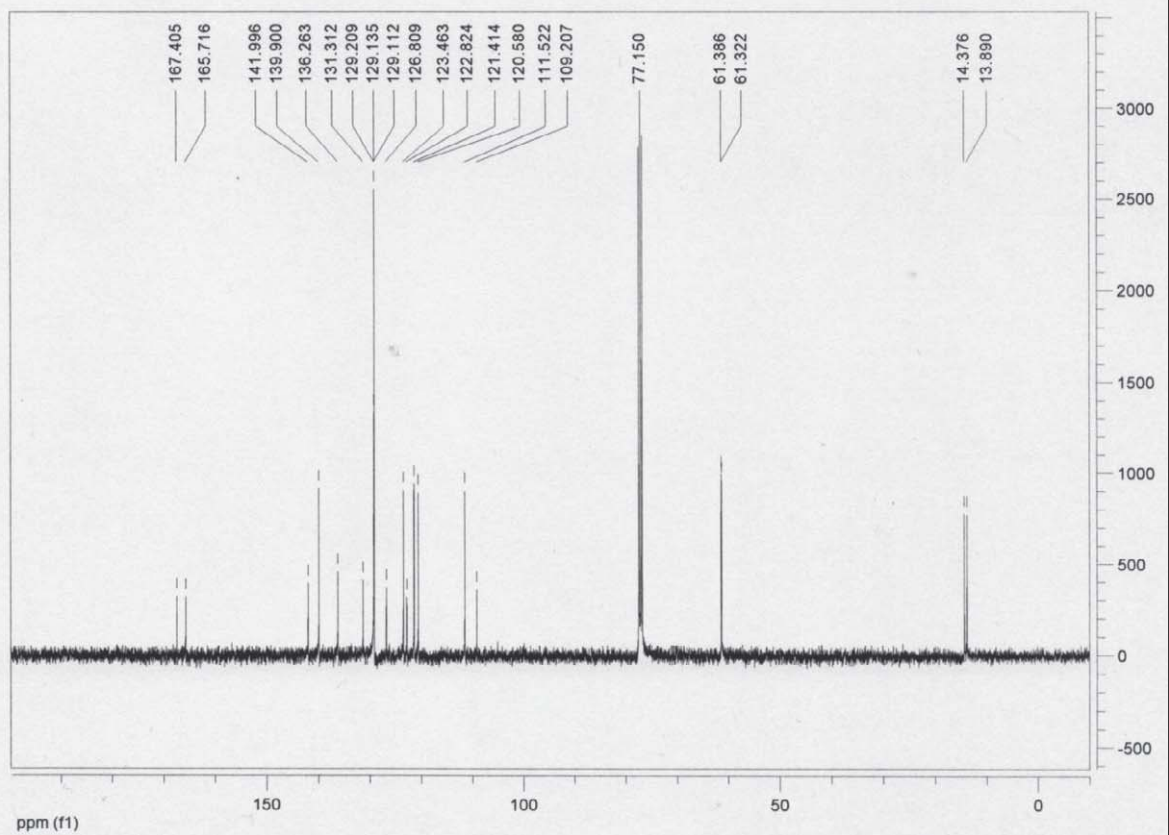
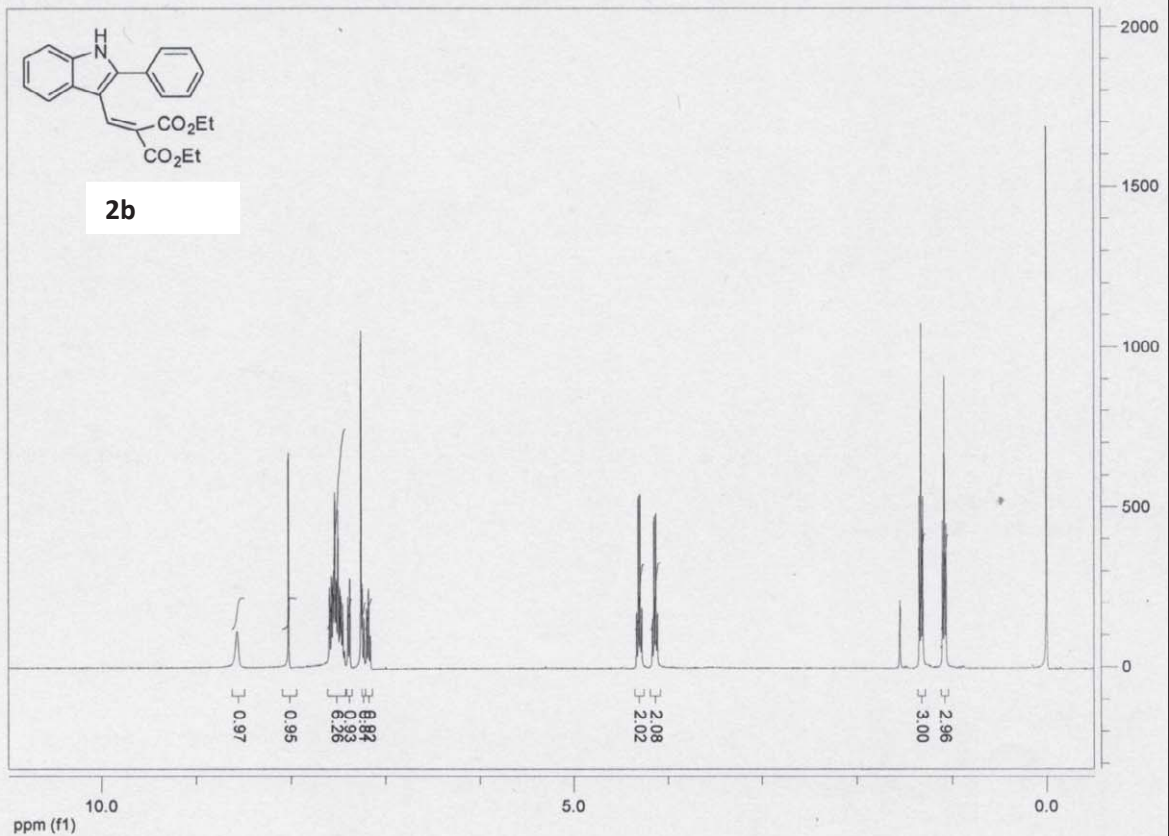
^1H NMR (400 MHz, CDCl_3) δ 8.29 (s, 1H), 8.19 (s, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.79 (t, J = 8.4 Hz, 2H), 7.52 (d, J = 6.8 Hz, 1H), 7.49-7.39 (m, 3H), 7.25 (d, J = 4.8 Hz, 1H), 7.16-7.06 (m, 3H), 4.38 (s, 2H), 4.32-4.19 (m, 4H), 1.33 (t, J = 6.8 Hz, 3H), 1.14 (t, J = 6.8 Hz, 3H).

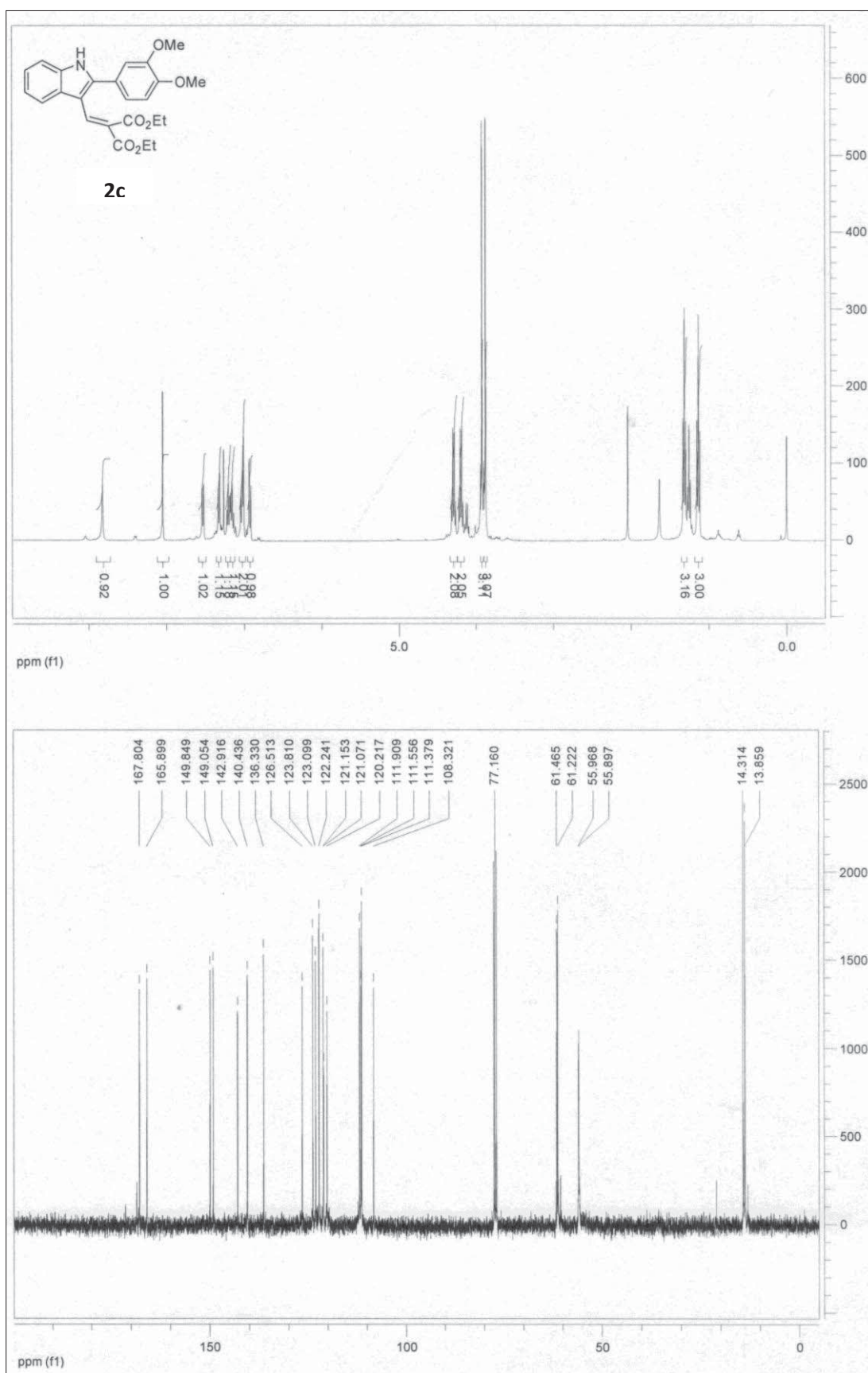
^{13}C NMR (100 MHz, CDCl_3) δ 167.9, 165.8, 142.7, 138.1, 135.8, 134.0, 132.6, 131.9, 128.9, 128.3, 127.6, 126.8, 126.4, 126.2, 125.7, 123.6, 122.5, 121.2, 121.1,

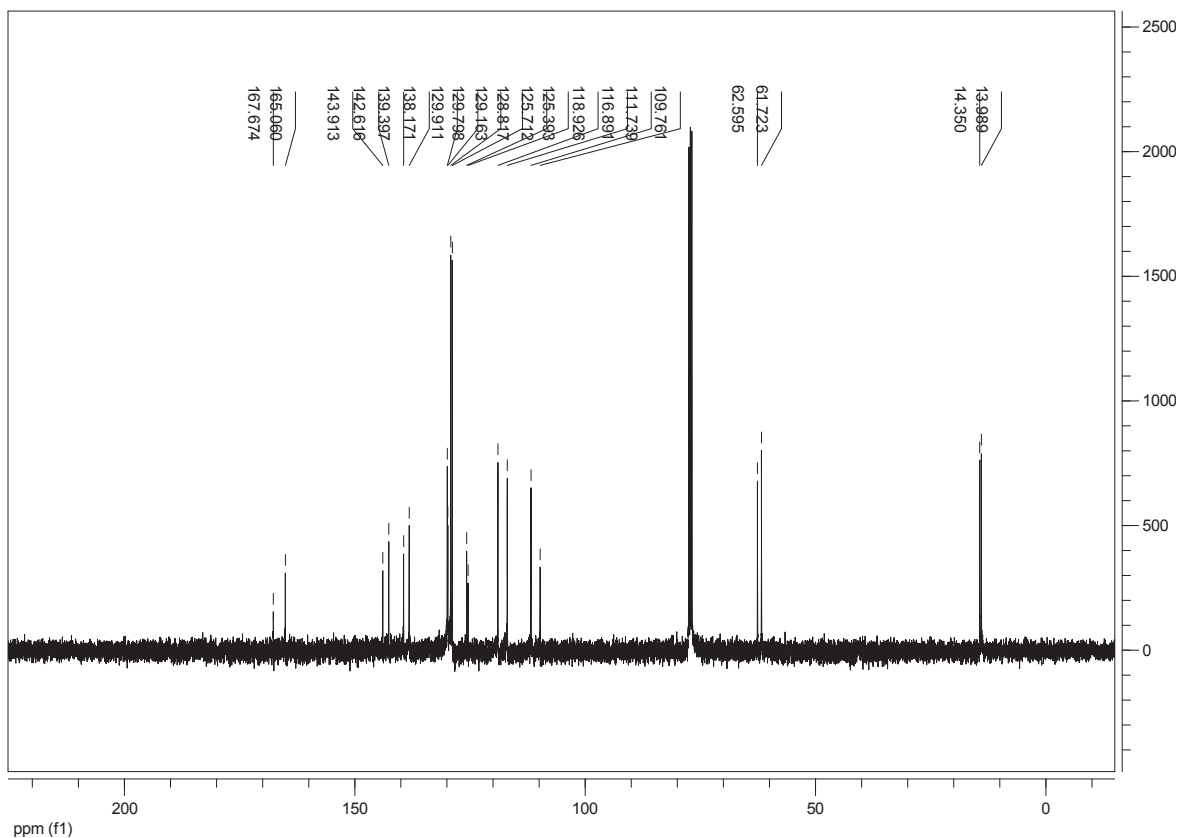
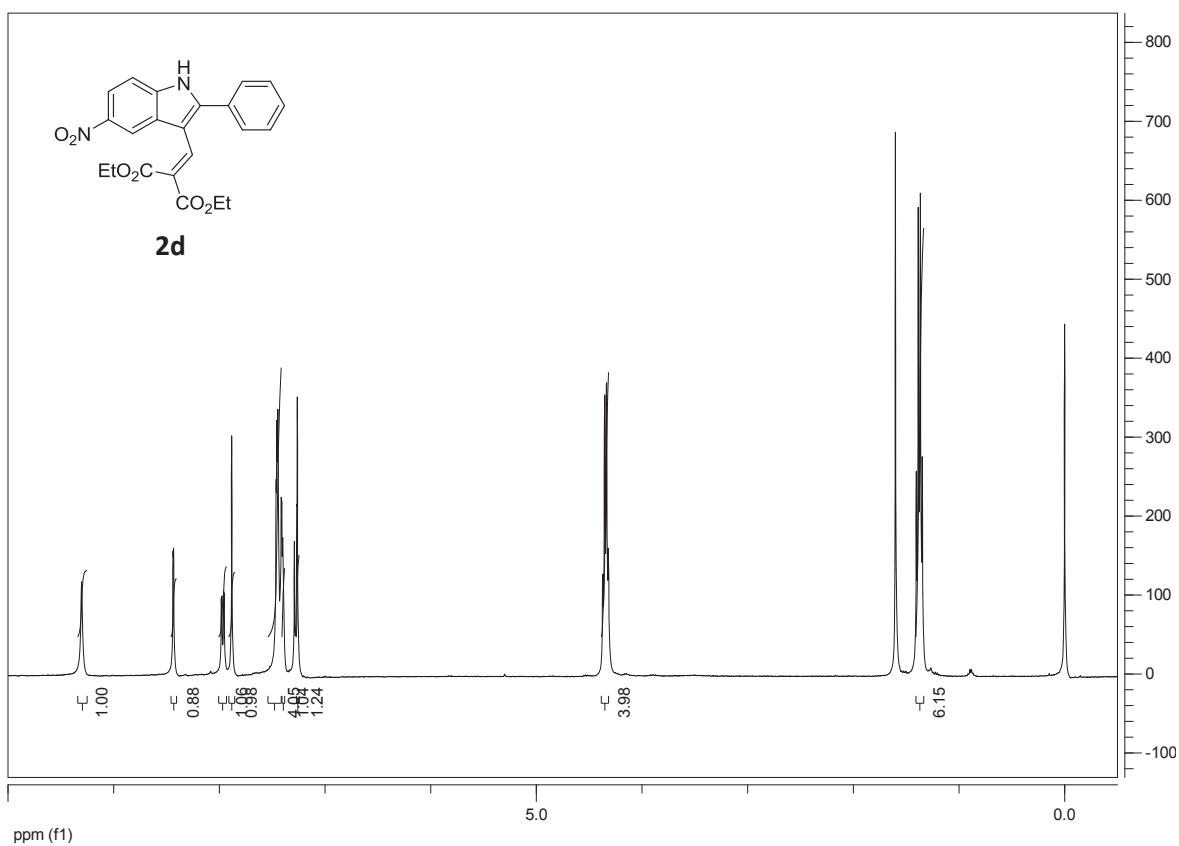
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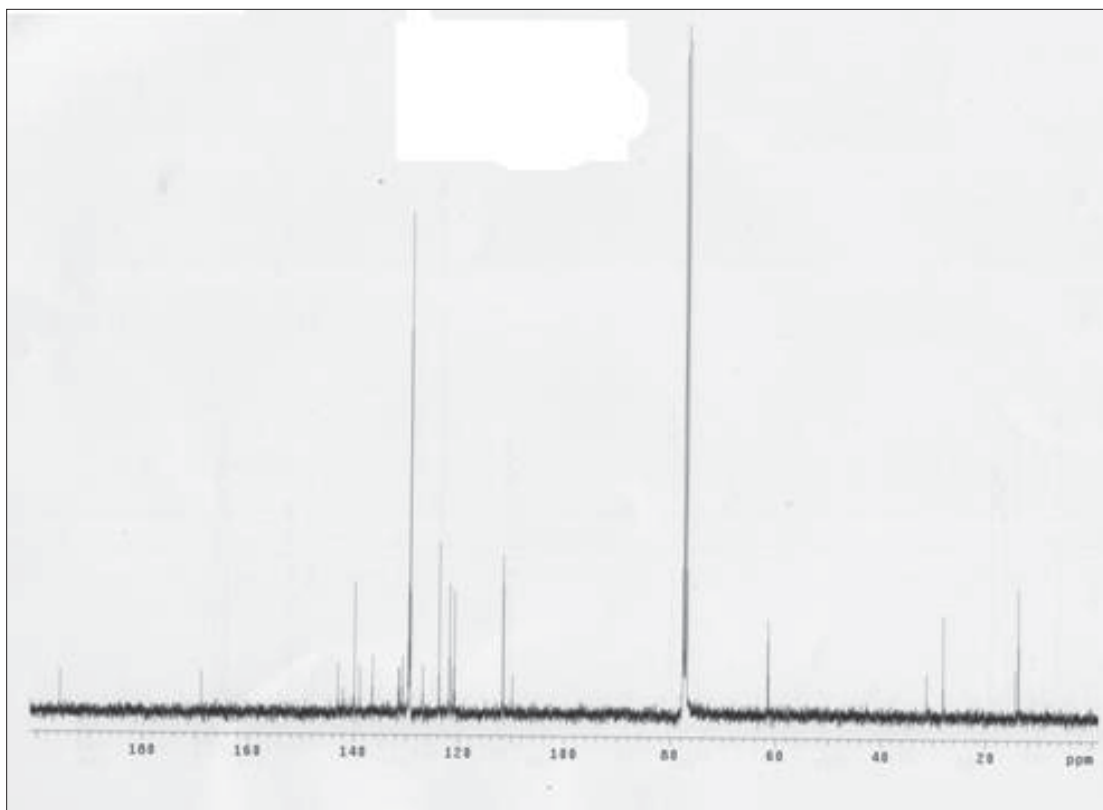
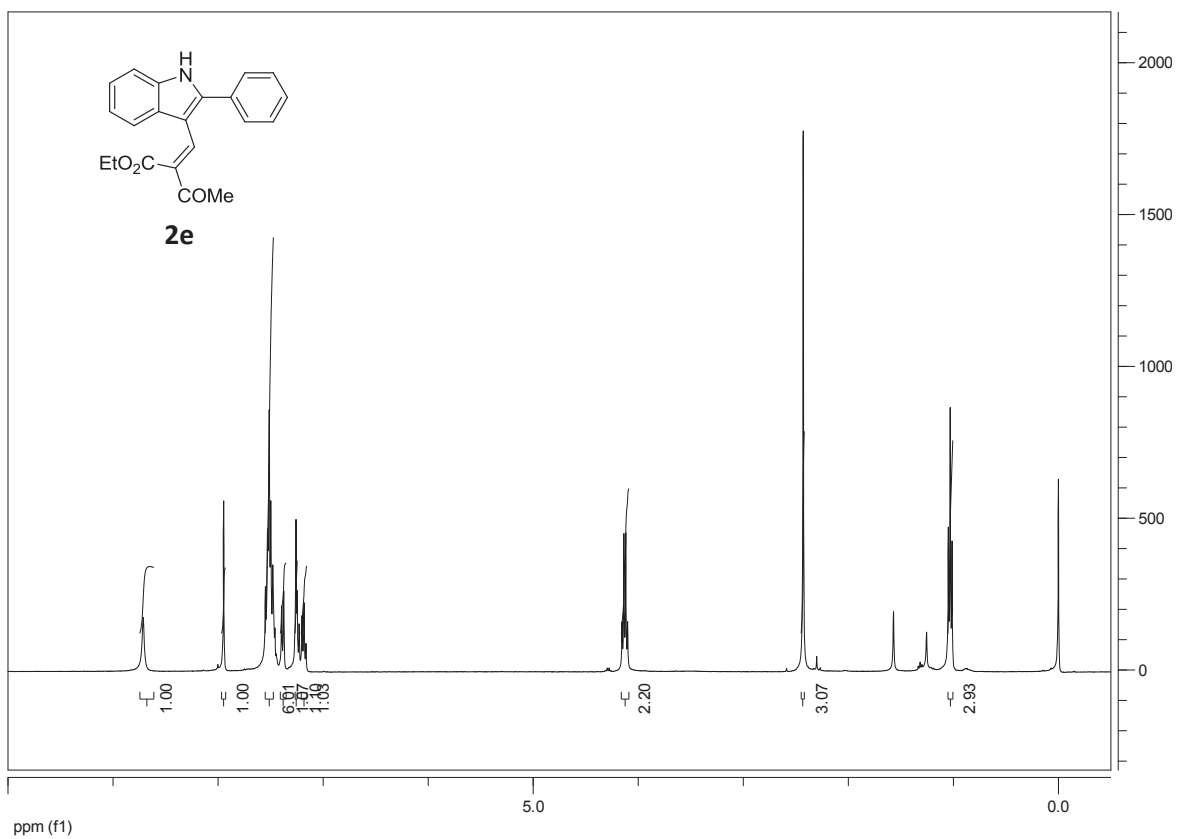


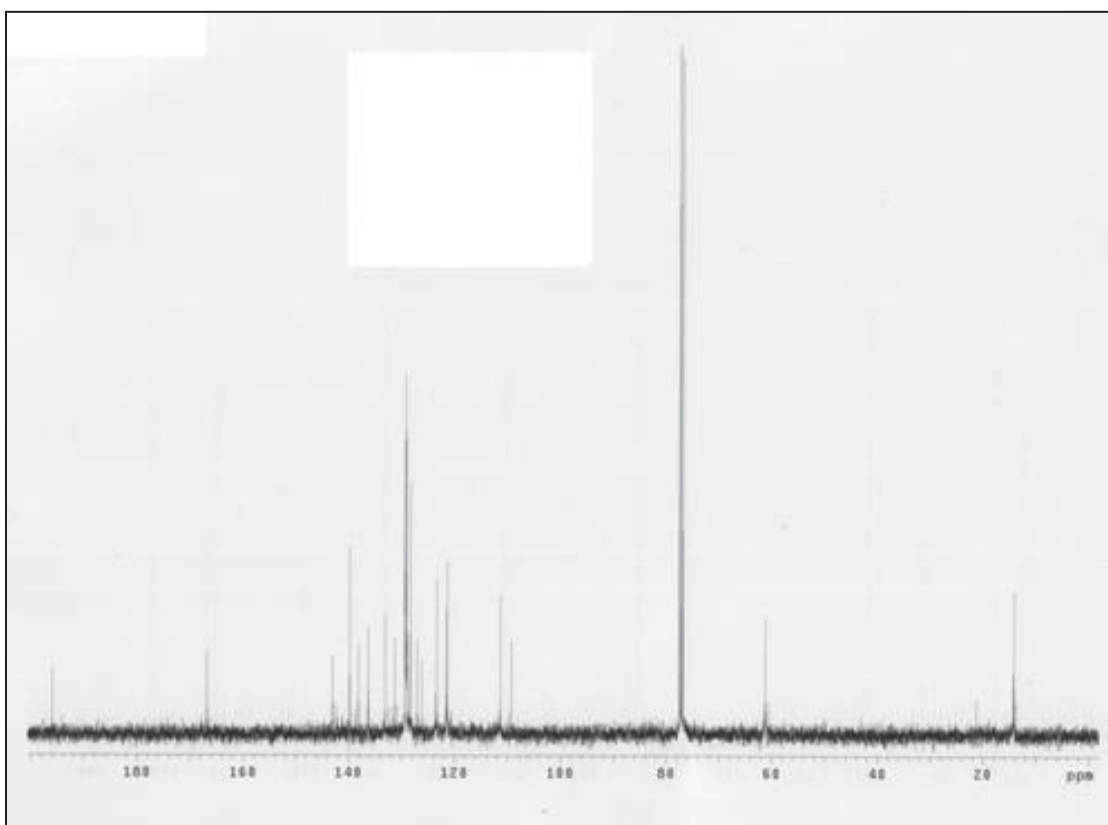
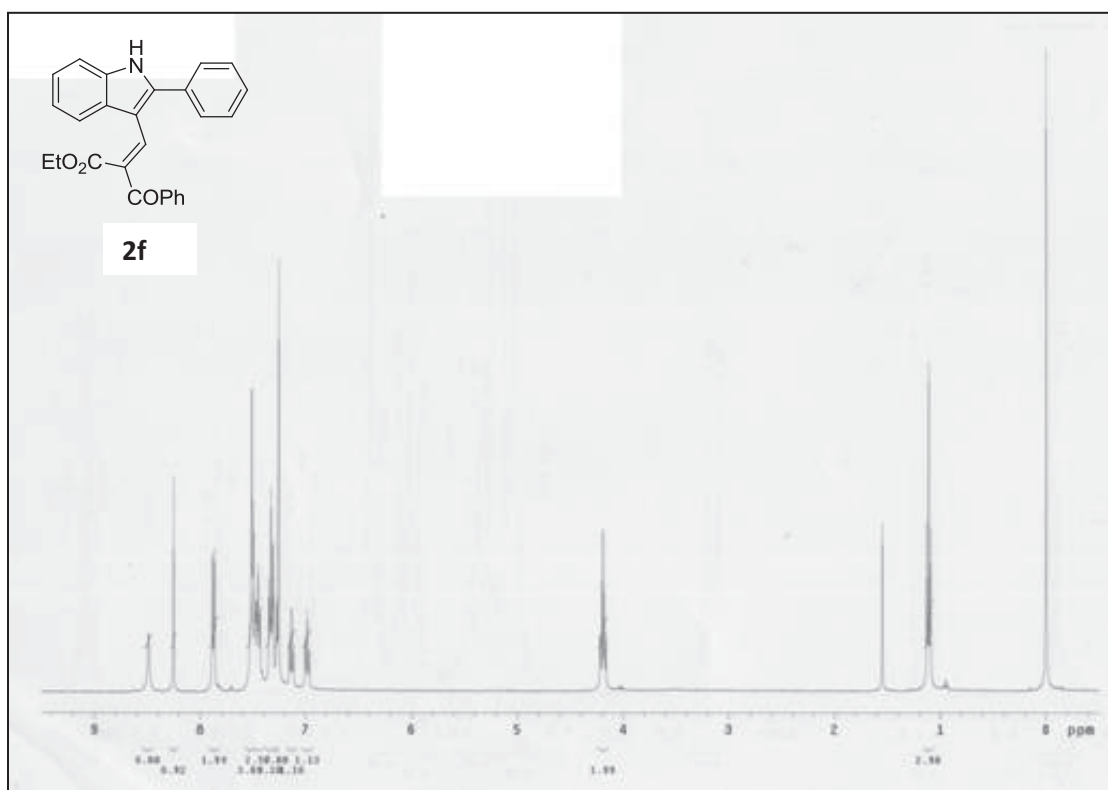
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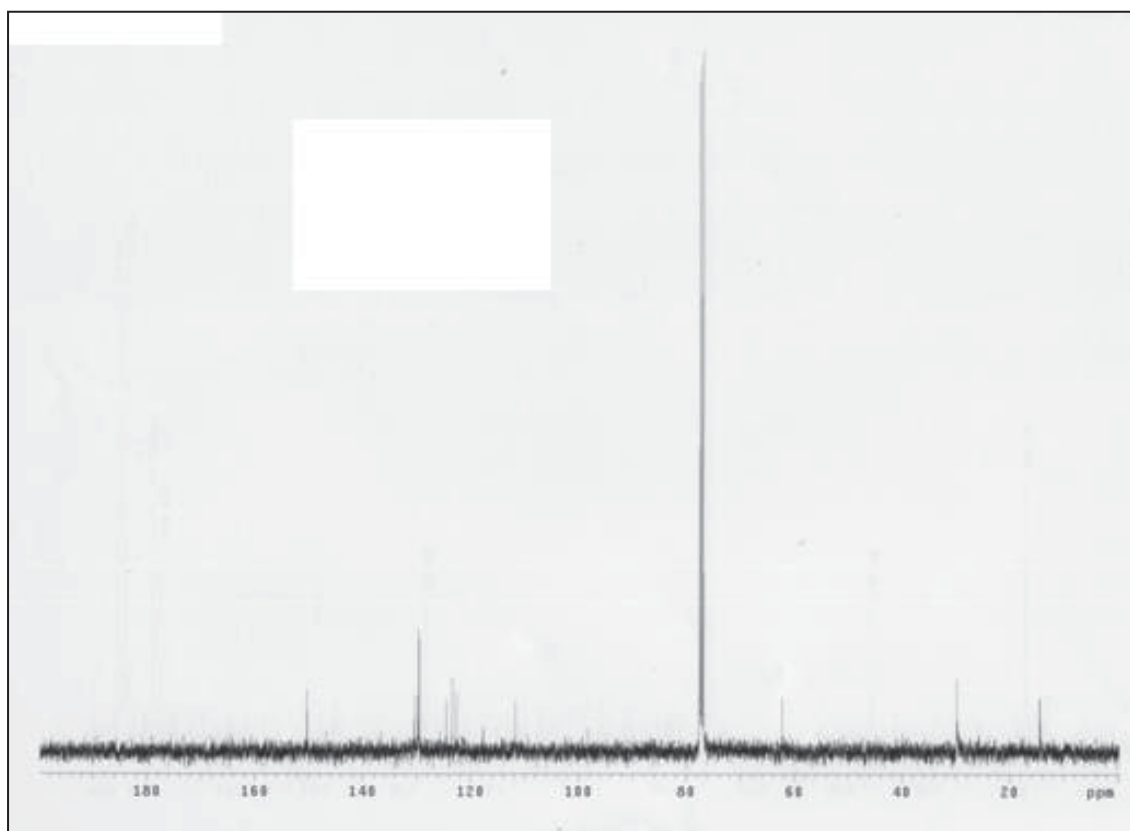
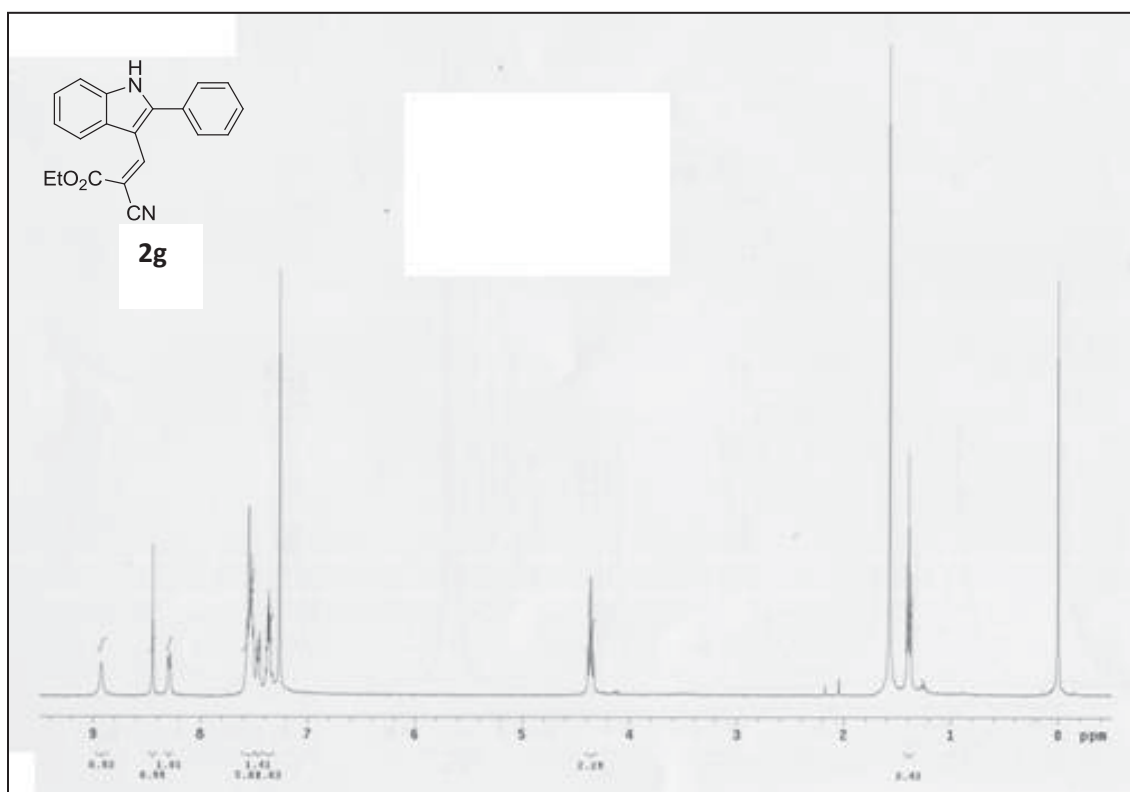


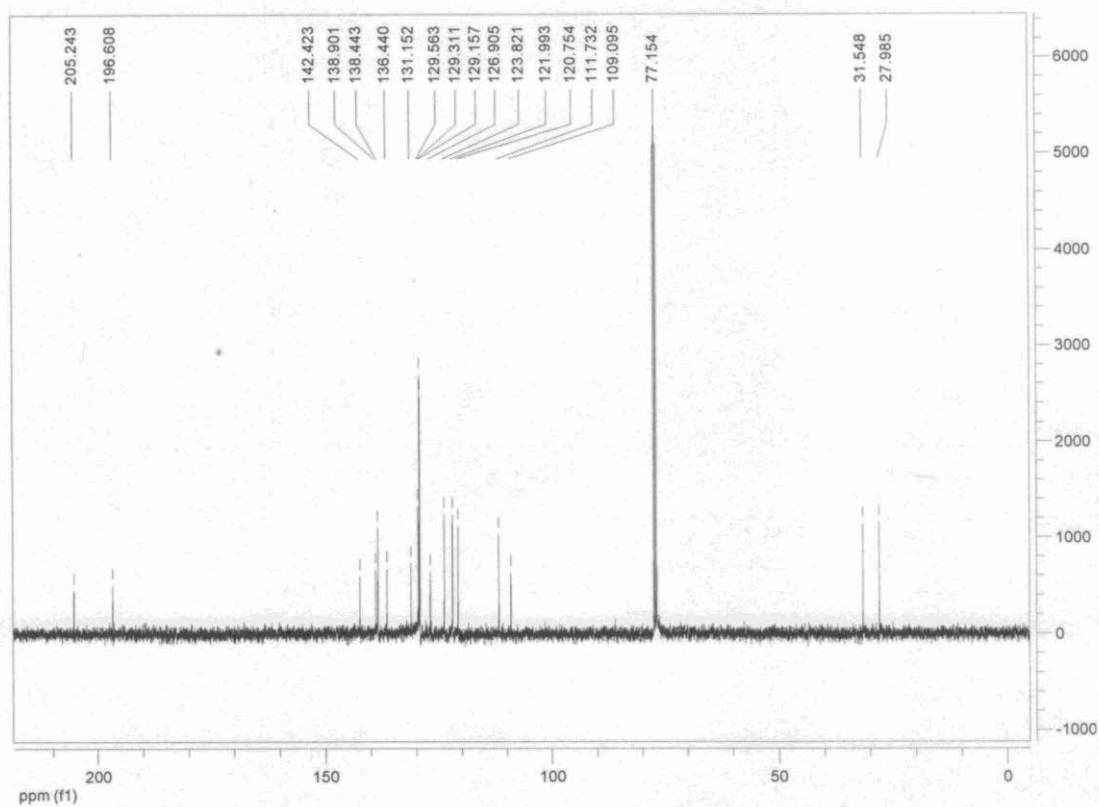
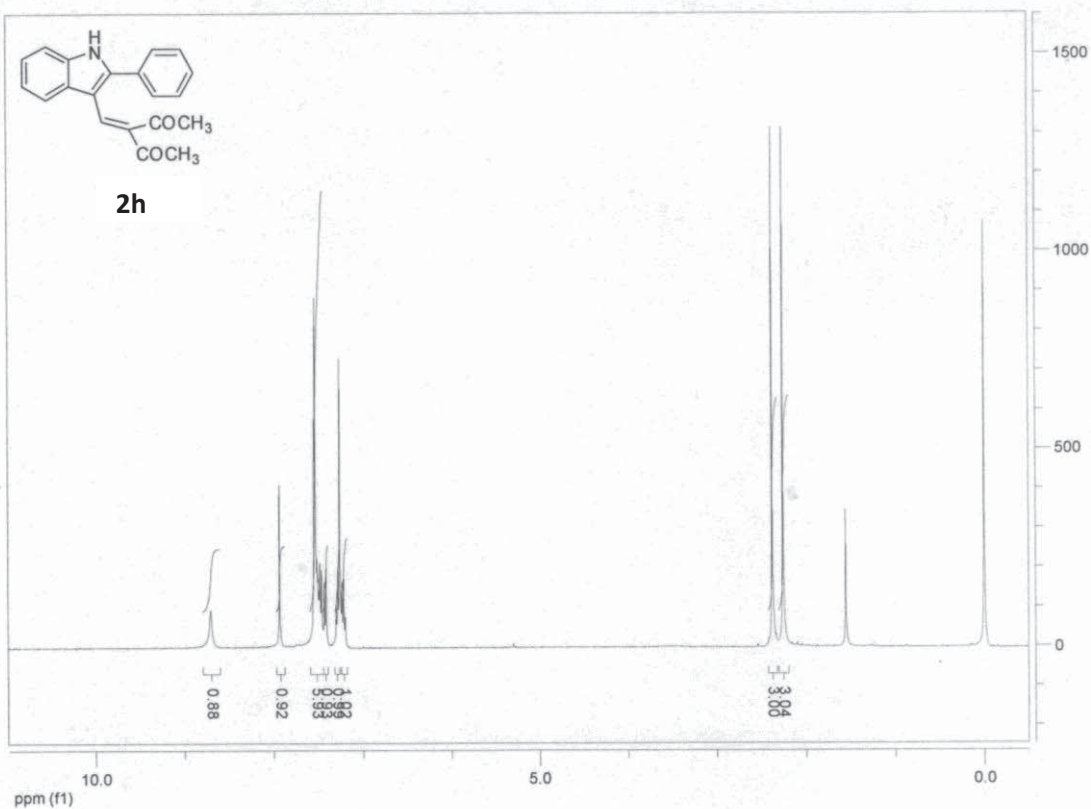


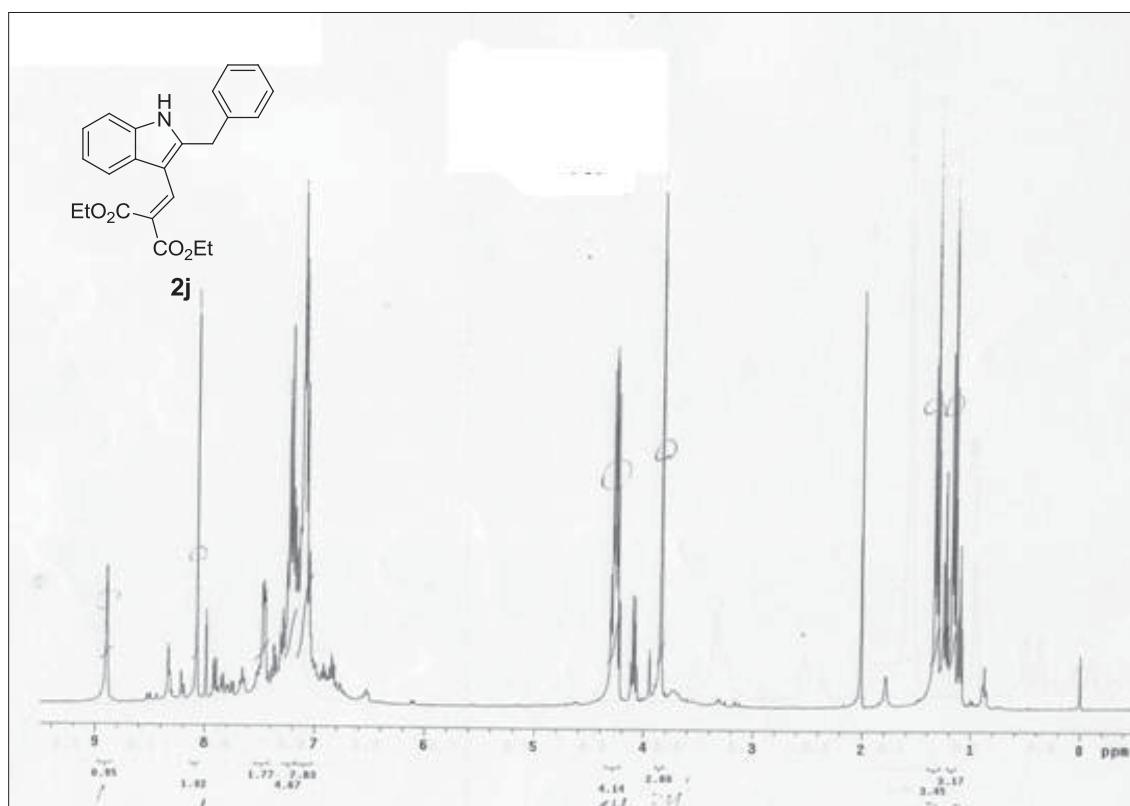
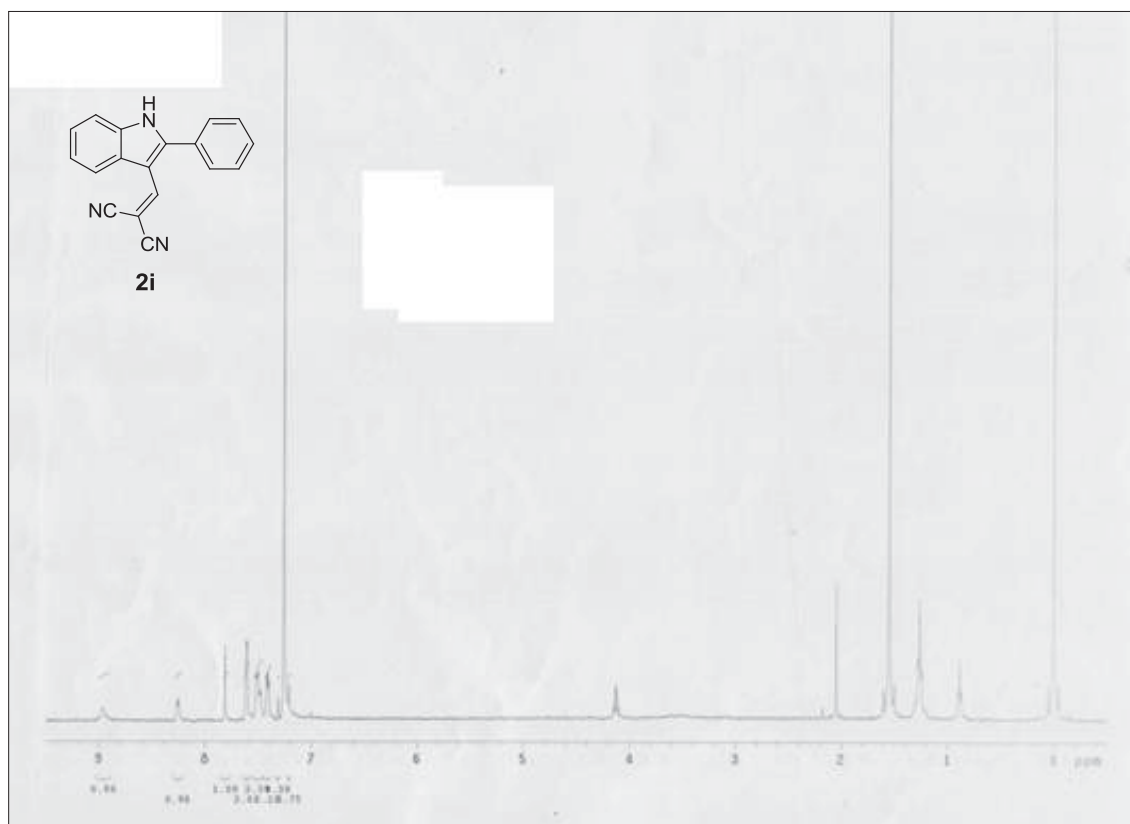


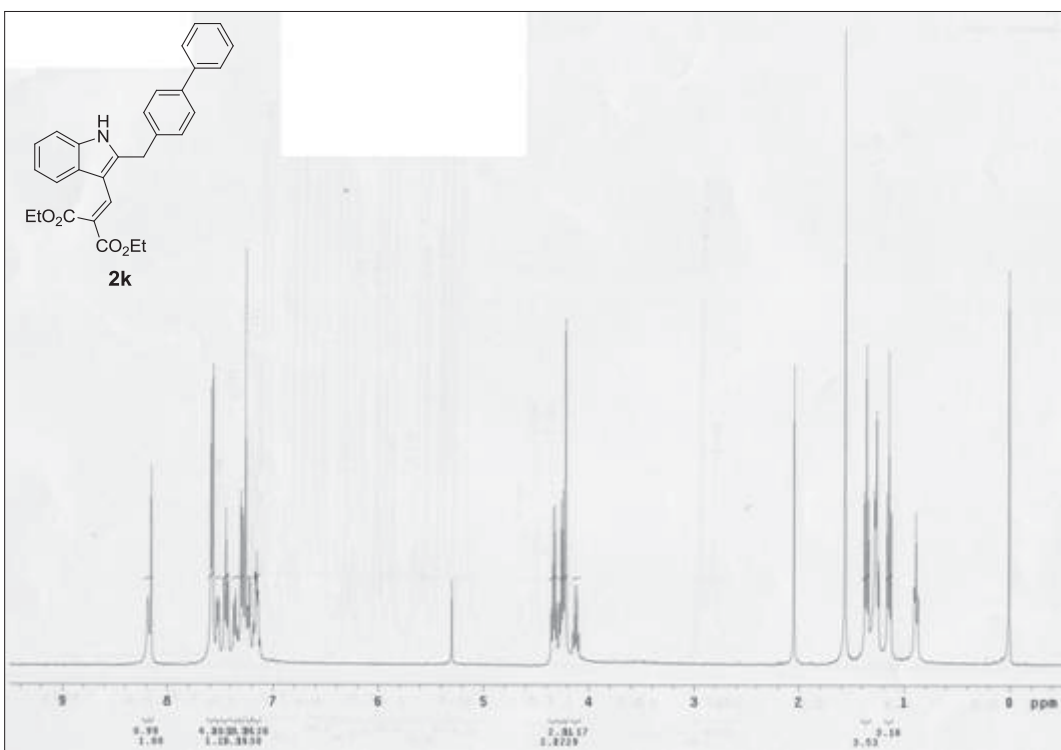


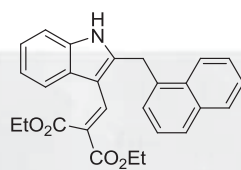












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