Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting information

$AlCl_3$-Catalyzed *O*-Alkylative Passerini Reaction of Isocyanides, Cinnamaldehydes and Various Aliphatic Alcohols for Accessing α-Alkoxy-β,γ-Enamides

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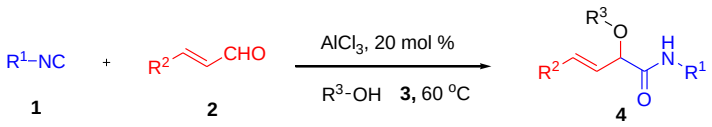
Table of Contents

General information

Material and instrumentation

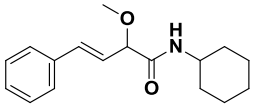
NMR Spectra were recorded on a Bruker DPX-400 or DPX-500 spectrometer at 400 MHz or 500 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR in $CDCl_3$. Chemical shifts are reported in δ (ppm) referenced to an internal tetramethylsilane (TMS) standard or the residual deuterated solvent peaks and coupling constants (J) were expressed in Hz. High resolution mass spectra (HRMS) were recorded on a LC-TOF spectrometer. ESI-HRMS data were acquired using a Thermo LTQ Orbitrap XL Instrument equipped with an ESI source. All chemicals were purchased from Acros, Alfa Aesar and TCI, and used as received.

General procedure for the synthesis of α-alkoxy-β,γ-enamides (Table 2 and 3).



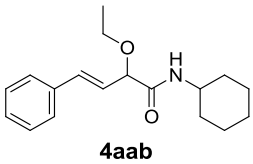
To a solution of $AlCl_3$ (0.2 mmol, 0.20 eq) in indicated alcohols (4 mL) in a sealed vial were added cinnamaldehyde 2 (1mmol, 1.0 eq) and isocyanides 1 (1.5 mmol, 1.5 eq) in sequence. Then the result mixtures were stirred at 60 ^{o}C for indicated time. After the reactions were completed, the solvent was removed under reduced pressure. The residues were chromatographed on silica gel with petroleum ether-ethyl acetate (6:1–1:1) as eluent to afford the desired products in 51–91% yields (Table 2 and 3).

Analytic data for the products in table 2 and 3.



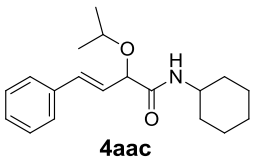
4aaa

4aaa was obtained in 85 % yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.24 (m, 5H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.48 (d, *J* = 7.5 Hz, 1H), 6.17 (dd, *J* = 16.0, 6.5 Hz, 1H), 4.25 (d, *J* = 6.5 Hz, 1H), 3.83 – 3.77 (m, 1H), 3.45 (s, 3H), 1.96 – 1.90 (m, 2H), 1.75 – 1.70 (m, 2H), 1.64 – 1.61 (m, 1H), 1.44 – 1.32 (m, 2H), 1.26 – 1.14 (m, 3H).^{13}C NMR (126 MHz, $CDCl_3$) δ 169.30, 136.28, 133.34, 128.50, 127.90, 126.70, 125.01, 82.83, 77.22, 76.97, 76.72, 57.35, 47.71, 33.13, 33.03, 25.54, 24.79, 24.77. HRMS (ESI) calcd for $C_{17}H_{23}NO_2$ $(M+H)^+$ 274.1807, found 274.1791.



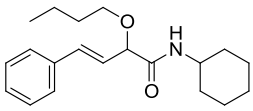
4aab

4aab was obtained in 63 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.22 (m, 5H), 6.71 (d, *J* = 16.0 Hz, 1H), 6.54 (d, *J* = 8.3 Hz, 1H), 6.20 (dd, *J* = 16.0, 6.2 Hz, 1H), 4.35 (dd, *J* = 6.2, 1.4 Hz, 1H), 3.84 – 3.73 (m, 1H), 3.67 (dq, *J* = 9.3, 7.0 Hz, 1H), 3.56 (dq, *J* = 9.4, 7.0 Hz, 1H), 1.91 (m, 2H), 1.70 (m, 2H), 1.44 – 1.37 (m, 2H), 1.28 (m, 4H), 1.24 – 1.13 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.77, 136.28, 132.68, 128.52, 127.87, 126.70, 125.50, 80.93, 77.34, 77.03, 76.71, 65.53, 47.68, 33.14, 33.01, 25.52, 24.78, 15.30. HRMS (ESI) calcd for $C_{18}H_{25}NO_2$ $(M+H)^+$ 288.1964, found 288.1952.



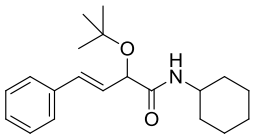
4aac

4aac was obtained in 64 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.14 (m, 5H), 6.70 (d, *J* = 16.0, 1H), 6.59 (d, *J* = 8.3 Hz, 1H), 6.25 (dd, *J* = 16.0, 5.6 Hz, 1H), 4.45 (dd, *J* = 5.6, 1.6 Hz, 1H), 3.84 – 3.69 (m, 2H), 1.94 – 1.86 (m, 2H), 1.66 – 1.55 (m, 2H), 1.41 – 1.31 (m, 2H), 1.24 (t, *J* = 6.2 Hz, 6H), 1.22 – 1.10 (m, 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.36, 136.42, 131.70, 128.51, 127.76, 126.67, 126.26, 78.69, 77.35, 77.03, 76.71, 71.78, 47.64, 33.12, 32.98, 25.52, 24.73, 22.54, 22.24. HRMS (ESI) calcd for $C_{19}H_{27}NO_2$ $(M+H)^+$ 302.2120, found 302.2107.



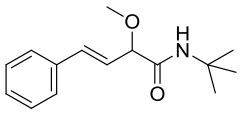
4aad

4aad was obtained in 61 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.19 (m, 5H), 6.71 (dd, *J* = 16.0, 1.0 Hz, 1H), 6.54 (d, *J* = 8.3 Hz, 1H), 6.21 (dd, *J* = 16.0, 6.1 Hz, 1H), 4.34 (dd, *J* = 6.1, 1.4 Hz, 1H), 3.89 – 3.69 (m, 1H), 3.62 (m, 1H), 3.49 (m, 1H), 1.95 – 1.87 (m, 2H), 1.75 – 1.56 (m, 5H), 1.48 – 1.32 (m, 4H), 1.24 – 1.13 (m, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.80, 136.31, 132.51, 128.52, 127.85, 126.69, 125.52, 81.07, 77.37, 77.05, 76.73, 69.97, 47.63, 33.12, 33.01, 31.81, 25.51, 24.75, 19.45, 13.92. HRMS (ESI) calcd for $C_{20}H_{29}NO_2$ $(M+H)^+$ 316.2277, found 316.2277.



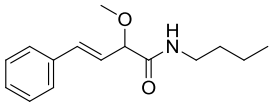
4aae

4aae was obtained in 53 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.3 Hz, 2H), 7.32 (dd, *J* = 10.3, 4.7 Hz, 2H), 7.27 – 7.20 (m, 1H), 6.72 (dd, *J* = 15.9, 1.7 Hz, 1H), 6.65 (d, *J* = 8.4 Hz, 1H), 6.38 (dd, *J* = 15.9, 4.7 Hz, 1H), 4.60 (dd, *J* = 4.7, 1.7 Hz, 1H), 3.90 – 3.71 (m, 1H), 1.97 – 1.86 (m, 2H), 1.76 – 1.67 (m, 2H), 1.66 – 1.60 (m, 1H), 1.46 – 1.35 (m, 2H), 1.29 (s, 9H), 1.24 – 1.14 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.25, 136.69, 130.14, 128.48, 127.83, 127.54, 126.60, 73.48, 47.53, 33.09, 32.97, 29.71, 28.02, 27.73, 25.52, 24.76. HRMS (ESI) calcd for $C_{20}H_{29}NO_2$ $(M+H)^+$ 316.2277, found 316.2272.



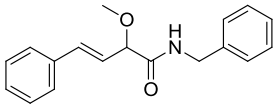
4baa

4baa was obtained in 81 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.18 (m, 5H), 6.70 (d, *J* = 16.0, 1H), 6.44 (s, 1H), 6.15 (dd, *J* = 16.0, 6.6 Hz, 1H), 4.14 (dd, *J* = 6.6, 1.3 Hz, 1H), 3.42 (s, 3H), 1.37 (s, 9H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.51, 136.20, 133.50, 128.53, 127.95, 126.72, 124.96, 83.14, 77.39, 77.07, 76.75, 57.31, 50.92, 28.77. HRMS (ESI) calcd for $C_{15}H_{21}NO_2$ $(M+H)^+$ 248.1651, found 248.1653.



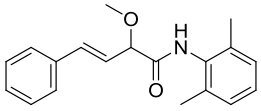
4caa

4caa was obtained in 82 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 – 7.18 (m, 5H), 6.72 (d, *J* = 16.0 Hz, 1H), 6.61 (s, 1H), 6.17 (dd, *J* = 16.0, 6.5 Hz, 1H), 4.27 (dd, *J* = 6.5, 1.2 Hz, 1H), 3.45 (s, 3H), 3.30 (m, 2H), 1.52 (m, 2H), 1.43 – 1.32 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.30, 136.12, 133.52, 128.55, 128.00, 126.72, 124.78, 82.77, 77.35, 77.04, 76.72, 57.43, 38.78, 31.65, 29.71, 20.07, 13.76. HRMS (ESI) calcd for $C_{15}H_{21}NO_2$ $(M+H)^+$ 248.1651, found 248.1651.



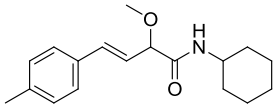
4daa

4daa was obtained in 75 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.19 (m, 5H), 6.94 (s, 1H), 6.75 (d, *J* = 15.9 Hz, 1H), 6.20 (dd, *J* = 15.9, 6.6 Hz, 1H), 4.49 (qd, *J* = 14.8, 5.9 Hz, 2H), 4.34 (dd, *J* = 6.6, 1.2 Hz, 1H), 3.44 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.36, 138.00, 136.06, 133.86, 128.76, 128.58, 128.08, 127.83, 127.58, 126.75, 124.56, 82.72, 77.35, 77.03, 76.72, 57.42, 43.12, 29.72. HRMS (ESI) calcd for $C_{18}H_{19}NO_2$ $(M+H)^+$ 282.1494, found 282.1482.



4eaa

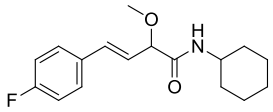
4eaa was obtained in 72 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.55 – 7.00 (m, 10H), 6.85 (dt, *J* = 7.6, 3.8 Hz, 1H), 6.30 (dd, *J* = 16.0, 6.2 Hz, 1H), 4.49 (dd, *J* = 6.2, 1.4 Hz, 1H), 3.60 (s, 3H), 2.24 (s, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.84, 136.14, 135.29, 133.53, 132.97, 128.64, 128.27, 128.11, 127.37, 126.74, 124.63, 83.15, 77.35, 77.04, 76.72, 57.83, 18.48. HRMS (ESI) calcd for $C_{19}H_{21}NO_2$ $(M+H)^+$ 296.1650, found 296.1637.



5aba

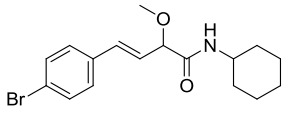
5aba was obtained in 85 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.07 (m, 5H), 6.68 (d, *J* = 15.9 Hz, 1H), 6.48 (d, *J* = 8.2 Hz, 1H), 6.09 (dd, *J* = 15.9, 6.6 Hz, 1H), 4.22 (dd, *J* = 6.6, 1.2 Hz, 1H), 3.88 – 3.71 (m, 1H), 3.43 (s, 3H), 2.33 (s, 3H), 2.01 – 1.82 (m, 2H), 1.74 – 1.69 (m, 2H), 1.65 – 1.55 (m, 1H), 1.44 – 1.30 (m, 2H), 1.25 – 1.10 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.47, 137.86,

133.52, 133.40, 129.23, 126.63, 123.77, 82.84, 77.35, 77.03, 76.72, 57.27, 47.69, 33.15, 33.05, 25.52, 24.83, 21.22. HRMS (ESI) calcd for $C_{18}H_{25}NO_2$ $(M+H)^+$ 288.1964, found 288.1966.



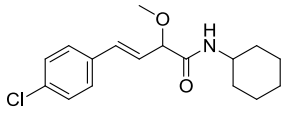
5aca

5aca was obtained in 64 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 – 7.28 (m, 2H), 7.11 – 6.93 (m, 2H), 6.67 (d, *J* = 15.9 Hz, 1H), 6.49 (d, *J* = 7.9 Hz, 1H), 6.07 (dd, *J* = 15.9, 6.5 Hz, 1H), 4.22 (dd, *J* = 6.5, 1.3 Hz, 1H), 3.85 – 3.71 (m, 1H), 3.44 (s, 3H), 1.96 – 1.87 (m, 2H), 1.73 – 1.71 (m, 2H), 1.65 – 1.63 (s, 1H), 1.44 – 1.31 (m, 2H), 1.27 – 1.13 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.28, 132.29, 128.31, 128.23, 124.62, 115.58, 115.37, 82.65, 57.42, 47.74, 33.15, 33.04, 25.51, 24.81. HRMS (ESI) calcd for $C_{17}H_{22}FNO_2$ $(M+H)^+$ 292.1713, found 292.1710.



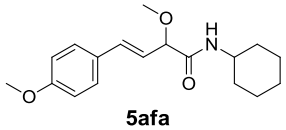
5ada

5ada was obtained in 76 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.28 – 7.24 (m, 3H), 6.65 (d, *J* = 15.9 Hz, 1H), 6.48 (d, *J* = 7.6 Hz, 1H), 6.16 (dd, *J* = 16.0, 6.4 Hz, 1H), 4.22 (dd, *J* = 6.4, 1.3 Hz, 1H), 3.89 – 3.71 (m, 1H), 3.44 (s, 3H), 1.96 – 1.87 (m, 2H), 1.73– 1.70 (m, 2H), 1.64 – 1.62 (m, 1H), 1.43 – 1.31 (m, 2H), 1.26 – 1.12 (m, 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.09, 135.13, 132.07, 131.67, 128.22, 125.77, 121.79, 82.58, 77.34, 77.22, 77.02, 76.70, 57.54, 47.76, 33.14, 33.03, 25.50, 24.81. HRMS (ESI) calcd for $C_{17}H_{22}BrNO_2$ $(M+H)^+$ 352.0912, found 352.0909.



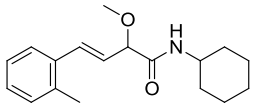
5aea

5aea was obtained in 73 % yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.29 (d, 2H), 7.29 – 7.25 (m, 4H), 6.66 (d, *J* = 16.0 Hz, 1H), 6.48 (d, *J* = 7.7 Hz, 1H), 6.14 (dd, *J* = 16.0, 6.4 Hz, 1H), 4.23 (dd, *J* = 6.4, 1.4 Hz, 1H), 3.83 – 3.72 (m, 1H), 3.44 (s, 3H), 2.03 (m, 2H), 1.91 (m, 2H), 1.75 – 1.70 (m, 1H), 1.43 – 1.33 (m, 2H), 1.22 – 1.11 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.15, 134.68, 133.61, 132.07, 128.72, 127.92, 125.62, 82.58, 57.53, 47.76, 33.16, 33.05, 25.50, 24.82. HRMS (ESI) calcd for $C_{17}H_{22}C_lNO_2$ $(M+H)^+$ 308.1417, found 308.1423.



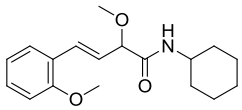
5afa

5afa was obtained in 91 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.27 (d, *J* = 8.8 Hz,2H), 6.91 – 6.76 (d, *J* = 8.8 Hz,2H), 6.65 (d, *J* = 15.8 Hz, 1H), 6.48 (d, *J* = 8.1 Hz, 1H), 5.99 (dd, *J* = 15.9, 6.8 Hz, 1H), 4.20 (dd, *J* = 6.8, 1.2 Hz, 1H), 3.80 (s, 3H), 3.42 (s, 3H), 2.00 – 1.84 (m, 2H), 1.76 – 1.67 (m, 2H), 1.65 – 1.56 (m, 1H), 1.36 (m, 2H), 1.26 – 1.12 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.56, 159.50, 133.26, 128.97, 127.96, 122.53, 113.93, 82.90, 77.36, 77.04, 76.72, 57.20, 55.29, 47.69, 33.15, 33.05, 25.52, 24.82. HRMS (ESI) calcd for $C_{18}H_{25}NO_3$ $(M+H)^+$ 304.1913, found 304.1910.



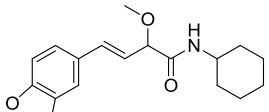
5aga

5aga was obtained in 80 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.45 (m, 1H), 7.22 – 7.09 (m, 3H), 6.93 (dd, *J* = 15.8, 1.0 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 1H), 6.03 (dd, *J* = 15.8, 6.6 Hz, 1H), 4.25 (dd, *J* = 6.6, 1.3 Hz, 1H), 3.89 – 3.72 (m, 1H), 3.44 (s, 3H), 2.36 (s, 3H), 2.00 – 1.85 (m, 2H), 1.73 – 1.66 (m, 2H), 1.66 – 1.58 (m, 1H), 1.44 – 1.30 (m, 2H), 1.26 – 1.12 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.42, 135.66, 135.33, 131.46, 130.28, 127.86, 126.15, 126.08, 125.89, 82.94, 77.36, 77.04, 76.72, 57.26, 47.71, 33.13, 33.05, 25.52, 24.83, 19.84. HRMS (ESI) calcd for $C_{18}H_{25}NO_2$ $(M+H)^+$ 288.1964, found 288.1966.



5aha

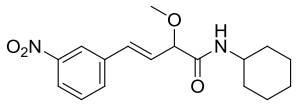
5aha was obtained in 83 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.42 (m, 1H), 7.25 – 7.17 (m, 1H), 7.04 (d, *J* = 16.1 Hz, 1H), 6.96 – 6.80 (m, 2H), 6.48 (d, *J* = 8.2 Hz, 1H), 6.18 (dd, *J* = 16.1, 6.7 Hz, 1H), 4.24 (dd, *J* = 6.7, 1.3 Hz, 1H), 3.91 – 3.75 (m, 4H), 3.43 (s, 3H), 1.99 – 1.85 (m, 2H), 1.78 – 1.66 (m, 2H), 1.66 – 1.57 (m, 1H), 1.46 – 1.29 (m, 2H), 1.18 – 1.11 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.58, 156.90, 129.02, 128.55, 127.19, 125.23, 125.16, 120.55, 110.87, 83.21, 77.36, 77.04, 76.72, 57.26, 55.44, 47.67, 33.16, 33.04, 25.53, 24.84. HRMS (ESI) calcd for $C_{18}H_{25}NO_3$ $(M+H)^+$ 304.1913, found 304.1903.



5aia

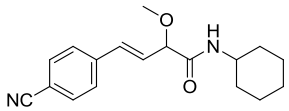
5afa was obtained in 75 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 – 6.73 (m, 3H), 6.72 (d, *J* = 16.0 Hz, 1H), 6.48 (d, *J* = 7.9 Hz, 1H), 6.02 – 5.87 (m, 3H), 4.20 (dd, *J* = 6.7, 1.2 Hz, 1H), 3.77 (m, 1H), 3.42 (s, 3H), 1.90 (m, 2H), 1.78 – 1.67 (m, 2H), 1.61 (m, 1H), 1.36 (m, 2H), 1.27 – 1.09 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 169.45, 147.99, 147.53, 133.32, 130.65, 123.02, 121.60, 108.23,

105.95, 101.11, 82.76, 77.35, 77.03, 76.71, 57.27, 47.71, 33.15, 33.05, 25.52, 24.82. HRMS (ESI) calcd for $C_{18}H_{23}NO_4$ $(M+H)^+$ 318.1705, found 318.1706.



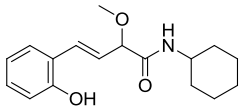
5aja

5aja was obtained in 58 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (t, *J* = 1.8 Hz, 1H), 8.11 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 6.79 (dd, *J* = 16.0, 0.9 Hz, 1H), 6.54 (d, *J* = 8.2 Hz, 1H), 6.36 (dd, *J* = 16.0, 6.1 Hz, 1H), 4.30 (dd, *J* = 6.1, 1.4 Hz, 1H), 3.85 – 3.74 (m, 1H), 3.49 (s, 3H), 2.00 – 1.86 (m, 2H), 1.77 – 1.72 (m, 2H), 1.68 – 1.61 (m, 1H), 1.44 – 1.33 (m, 2H), 1.26 – 1.13 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.73, 148.54, 137.98, 132.47, 130.59, 129.51, 128.48, 122.51, 121.36, 82.27, 77.37, 77.26, 77.05, 76.74, 57.82, 47.85, 33.14, 33.02, 25.48, 24.81. HRMS (ESI) calcd for $C_{17}H_{22}N_2O_4$ $(M+H)^+$ 319.1658, found 319.1650.



5aka

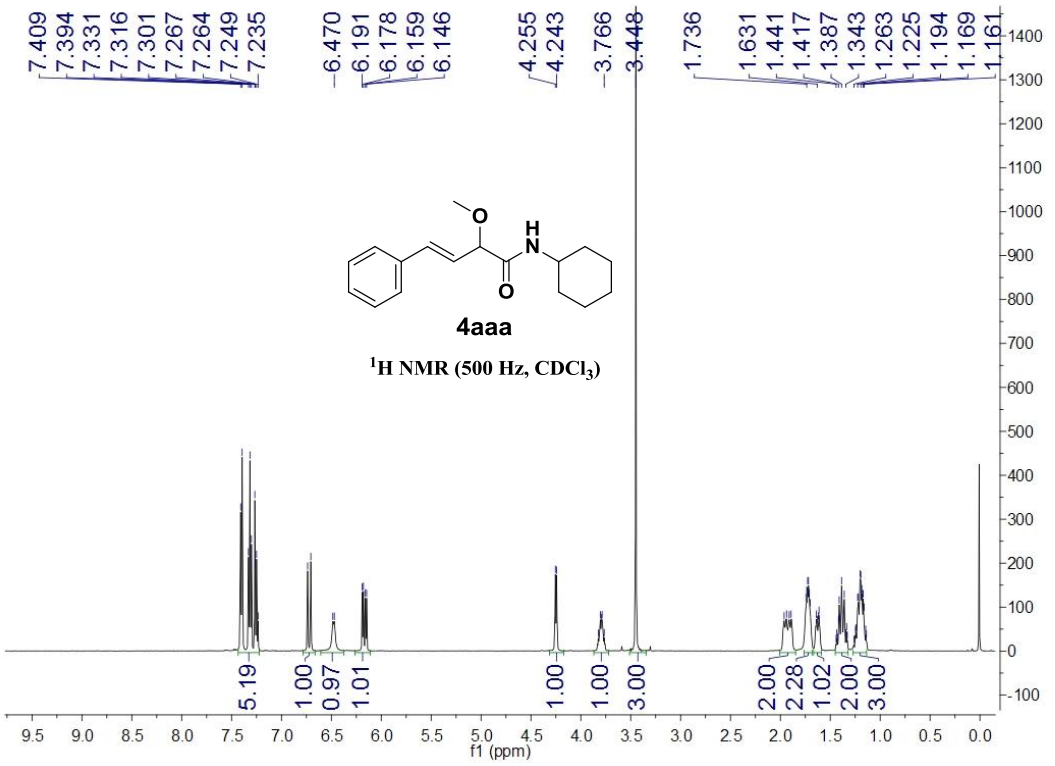
5aka was obtained in 56 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 6.73 (dd, *J* = 16.0, 1.0 Hz, 1H), 6.52 (d, *J* = 8.3 Hz, 1H), 6.34 (dd, *J* = 16.0, 6.0 Hz, 1H), 4.28 (dd, *J* = 6.0, 1.0 Hz, 1H), 3.85 – 3.72 (m, 1H), 3.47 (s, 3H), 1.97 – 1.84 (m, 2H), 173 – 1.63 (m, 2H), 1.66 – 1.59 (m, 1H), 1.44 – 1.30 (m, 2H), 1.23 – 1.12 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 168.68, 140.66, 132.40, 131.02, 129.18, 127.18, 118.89, 111.11, 82.30, 77.42, 77.30, 77.10, 76.78, 57.87, 47.85, 33.12, 32.99, 25.46, 24.80. HRMS (ESI) calcd for $C_{18}H_{22}N_2O_2$ $(M+H)^+$ 299.1760, found 299.1752.



5ala

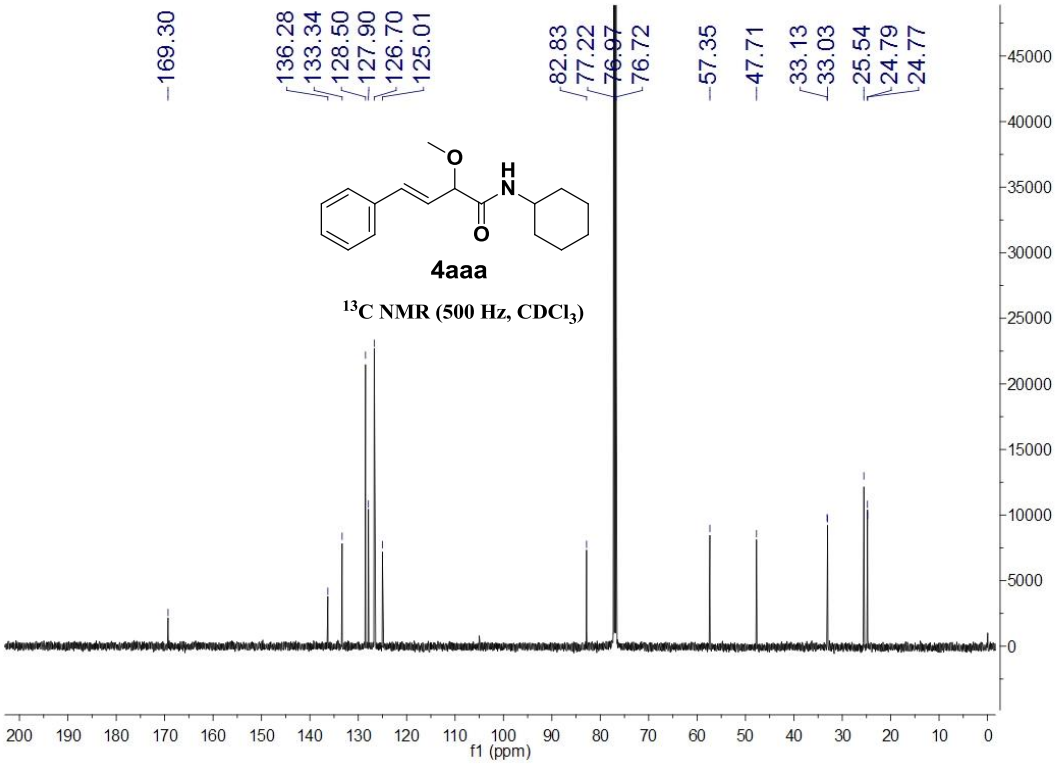
5ala was obtained in 70 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.32 (d, *J* = 7.7, 1H), 7.19 – 7.04 (m, 2H), 6.86 (dd, *J* = 8.1, 0.9 Hz, 1H), 6.77 (m, 1H), 6.72 (d, *J* = 8.3 Hz, 1H), 6.00 (dd, *J* = 16.0, 8.0 Hz, 1H), 4.27 (d, *J* = 8.0, 1H), 3.86 – 3.79 (m, 1H), 3.41 (s, 3H), 2.06 – 1.95 (m, 2H), 1.80 – 169 (m, 2H), 1.67 – 1.59 (m, 1H), 1.47 – 1.35 (m, 2H), 1.27 – 1.14 (m, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 170.81, 154.76, 131.50, 129.01, 126.76, 123.12, 122.99, 119.52, 116.24, 83.27, 77.39, 77.07, 76.75, 56.69, 48.07, 32.98, 32.91, 25.50, 24.80. HRMS (ESI) calcd for $C_{17}H_{23}NO_3$ $(M+H)^+$ 290.1756, found 290.1750.

Copies of ^{1}H, ^{13}C spectra in table 2 and 3.



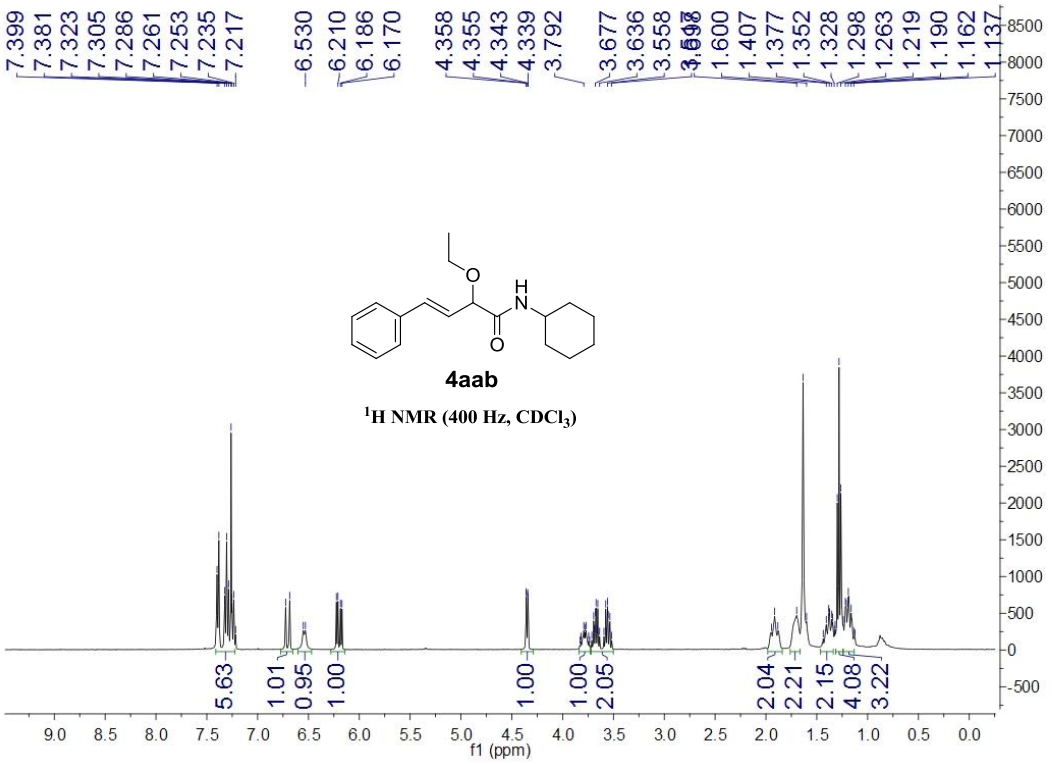
4aaa

^{1}H NMR (500 Hz, $CDCl_3$)



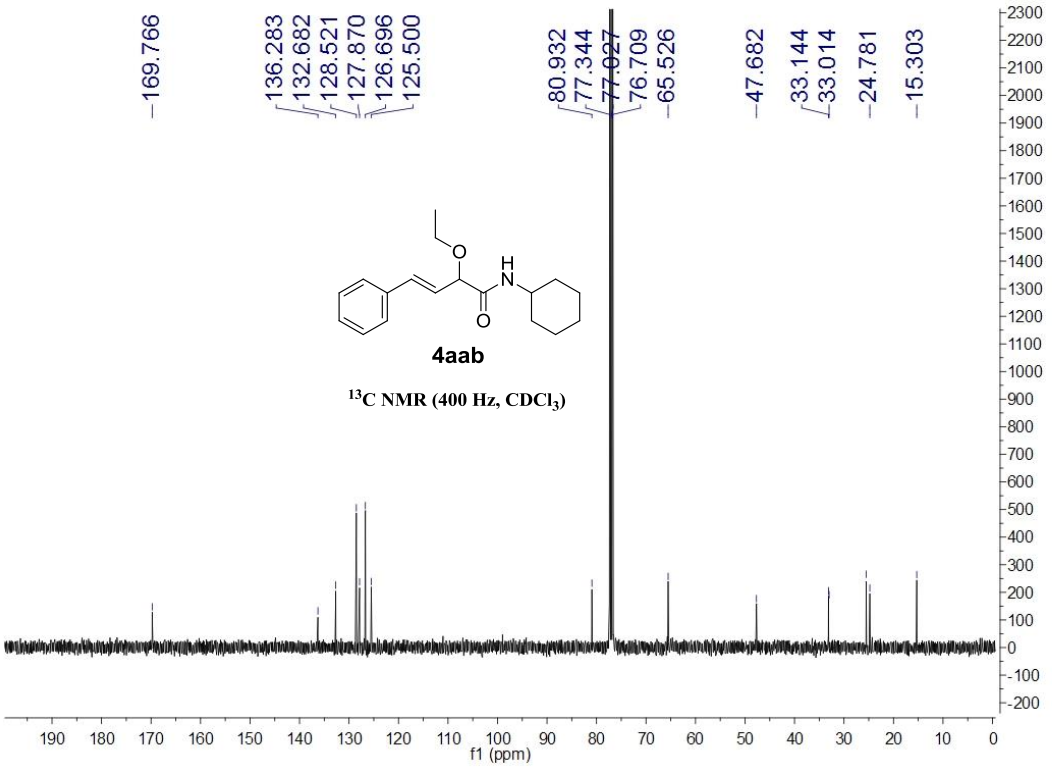
4aaa

^{13}C NMR (500 Hz, $CDCl_3$)



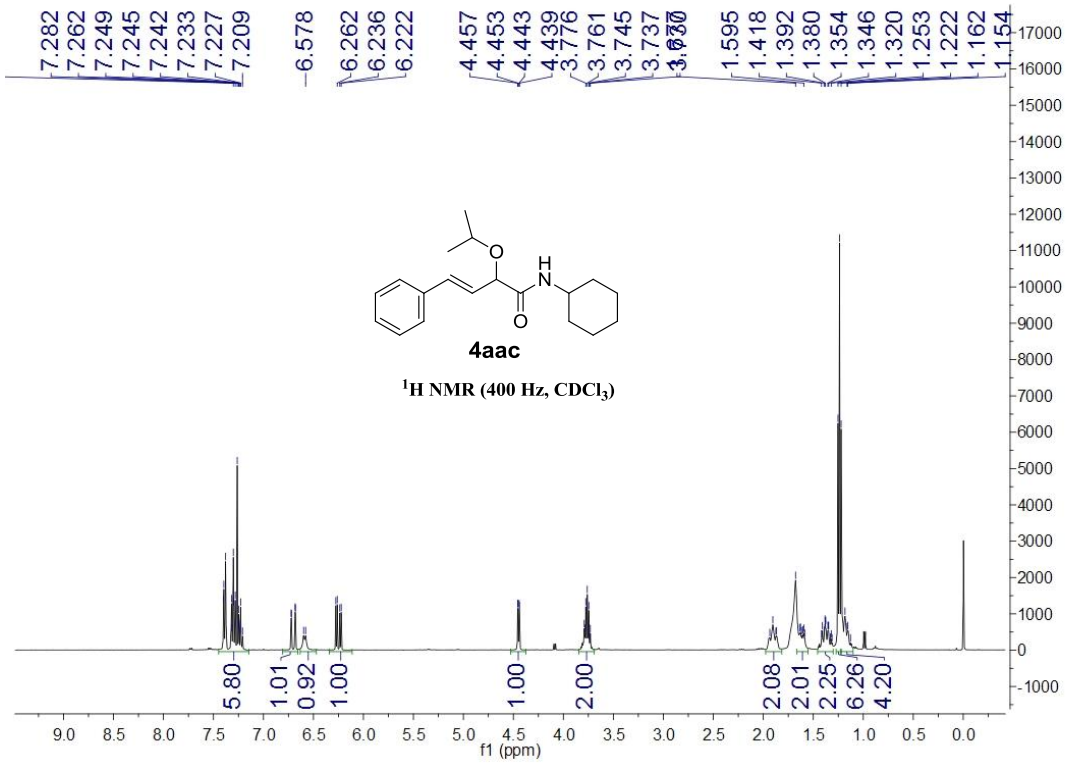
4aab

^{1}H NMR (400 Hz, $CDCl_3$)



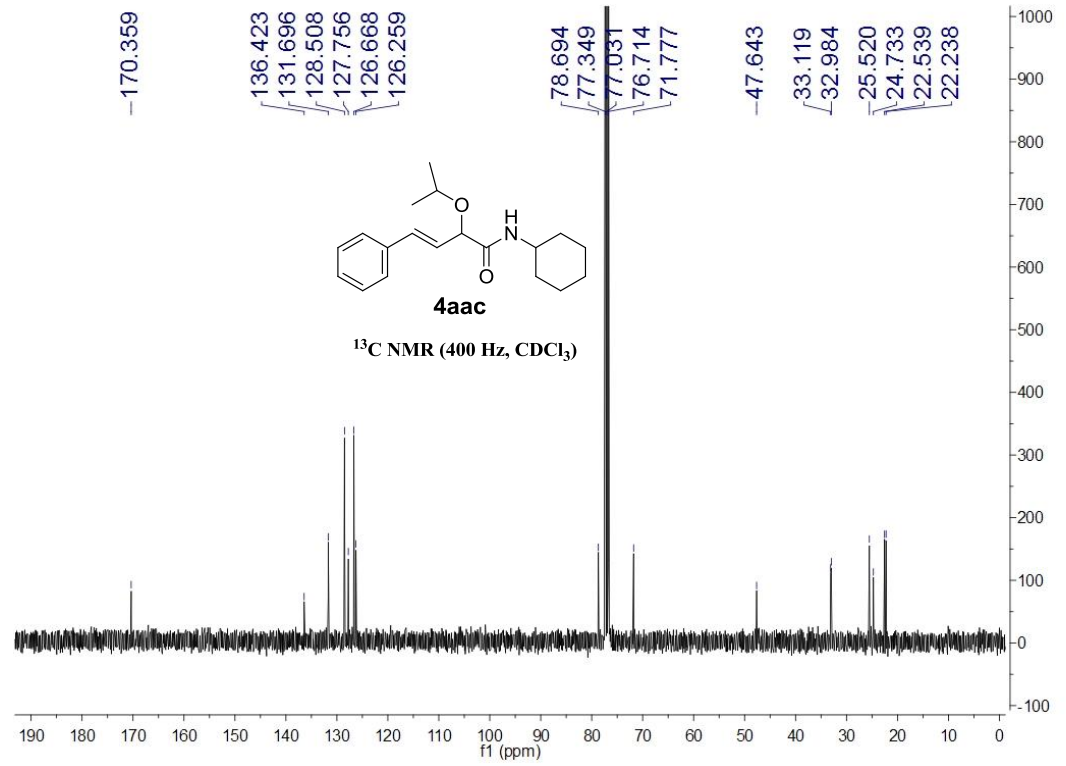
4aab

^{13}C NMR (400 Hz, $CDCl_3$)



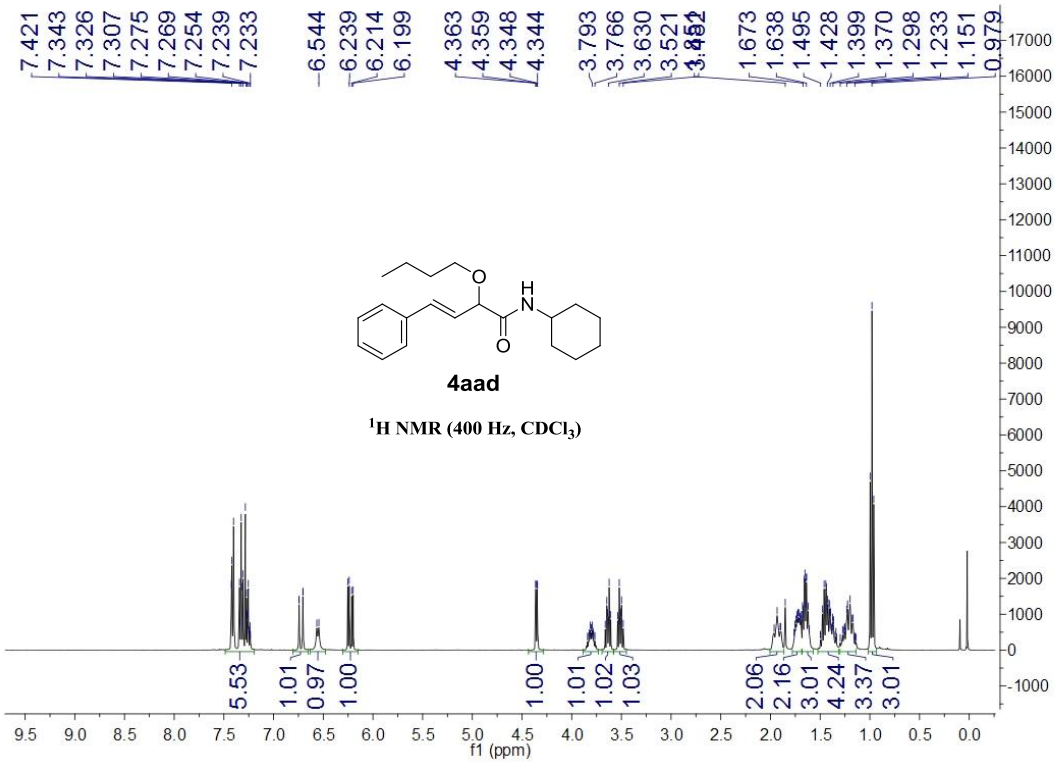
4aac

^{1}H NMR (400 Hz, $CDCl_3$)



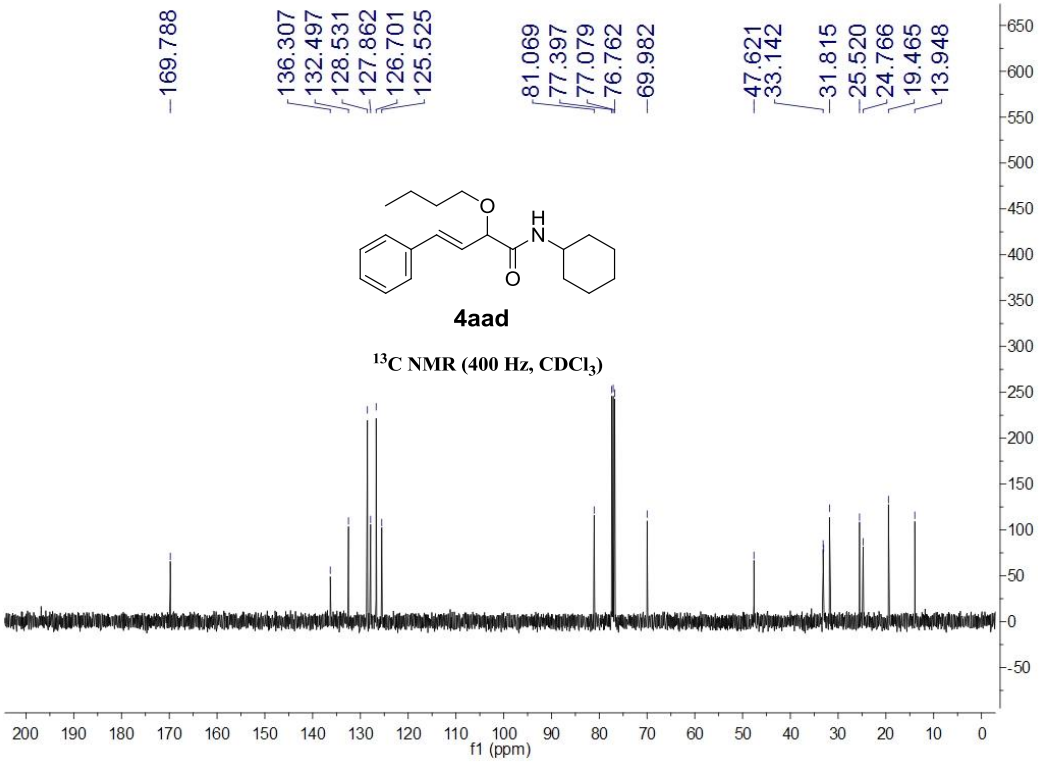
4aac

^{13}C NMR (400 Hz, $CDCl_3$)



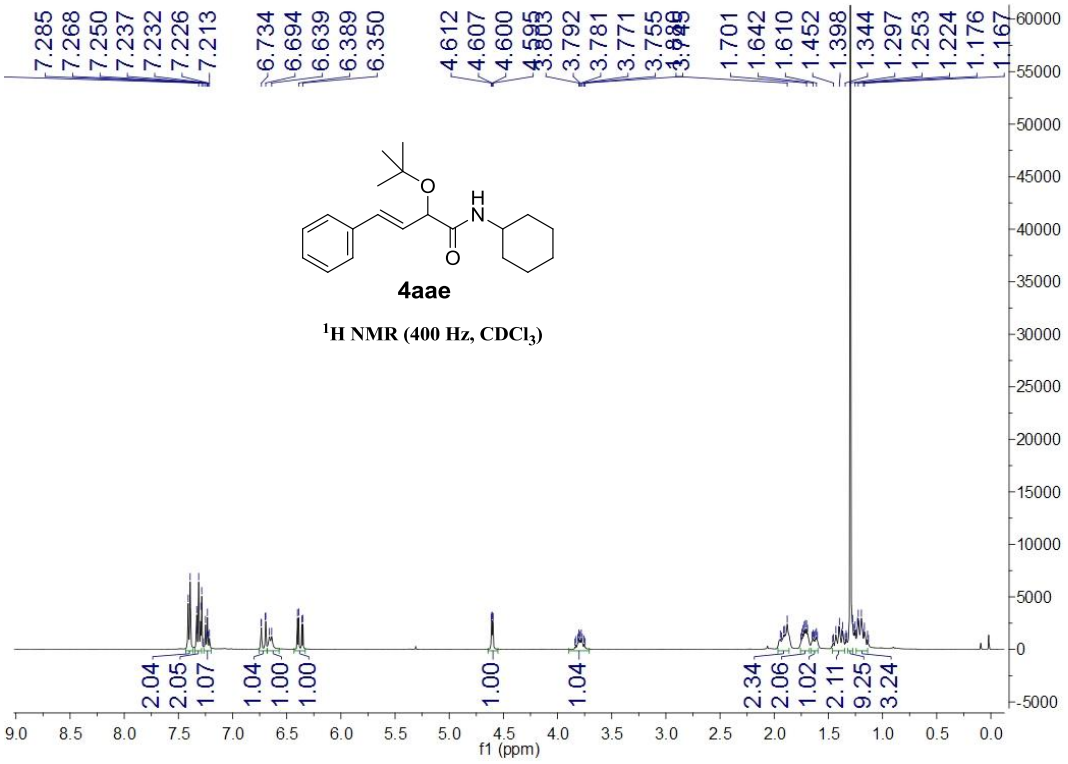
4aad

^{1}H NMR (400 Hz, $CDCl_3$)



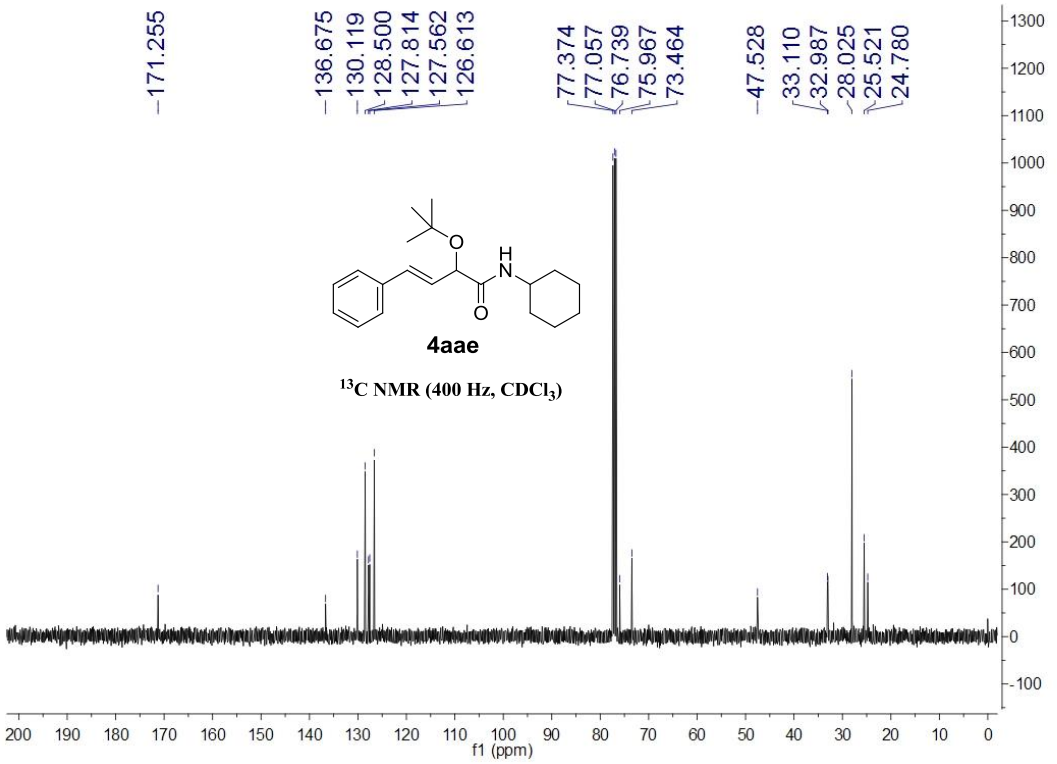
4aad

^{13}C NMR (400 Hz, $CDCl_3$)



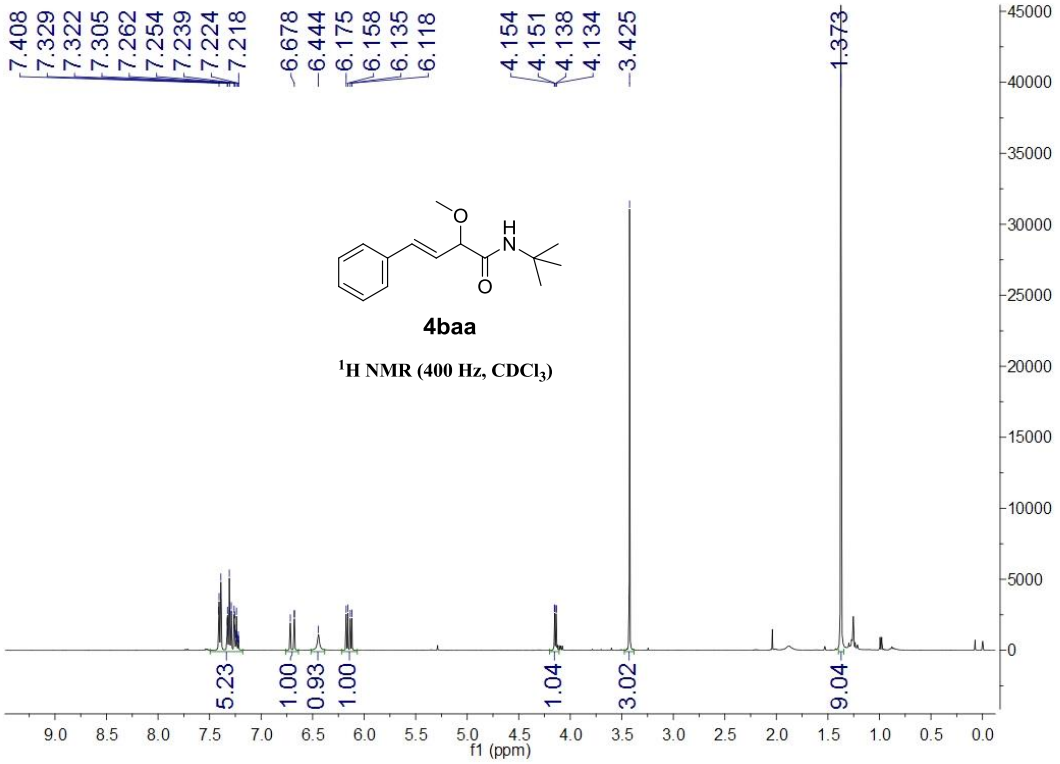
4aae

^{1}H NMR (400 Hz, $CDCl_3$)



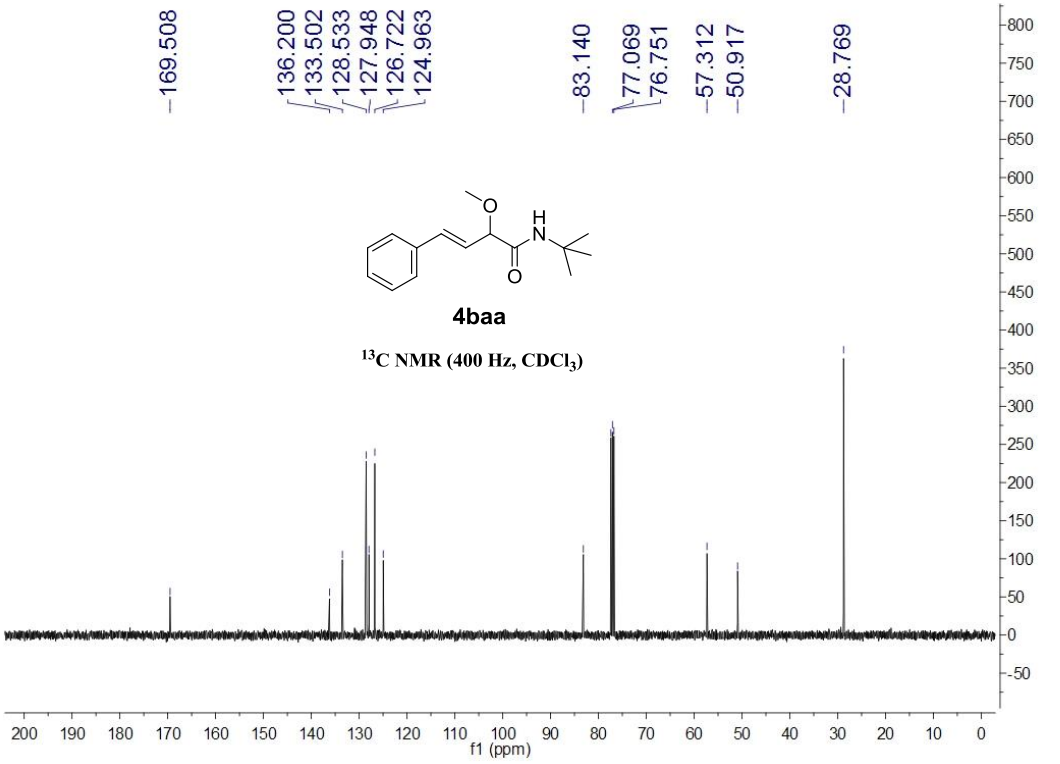
4aae

^{13}C NMR (400 Hz, $CDCl_3$)



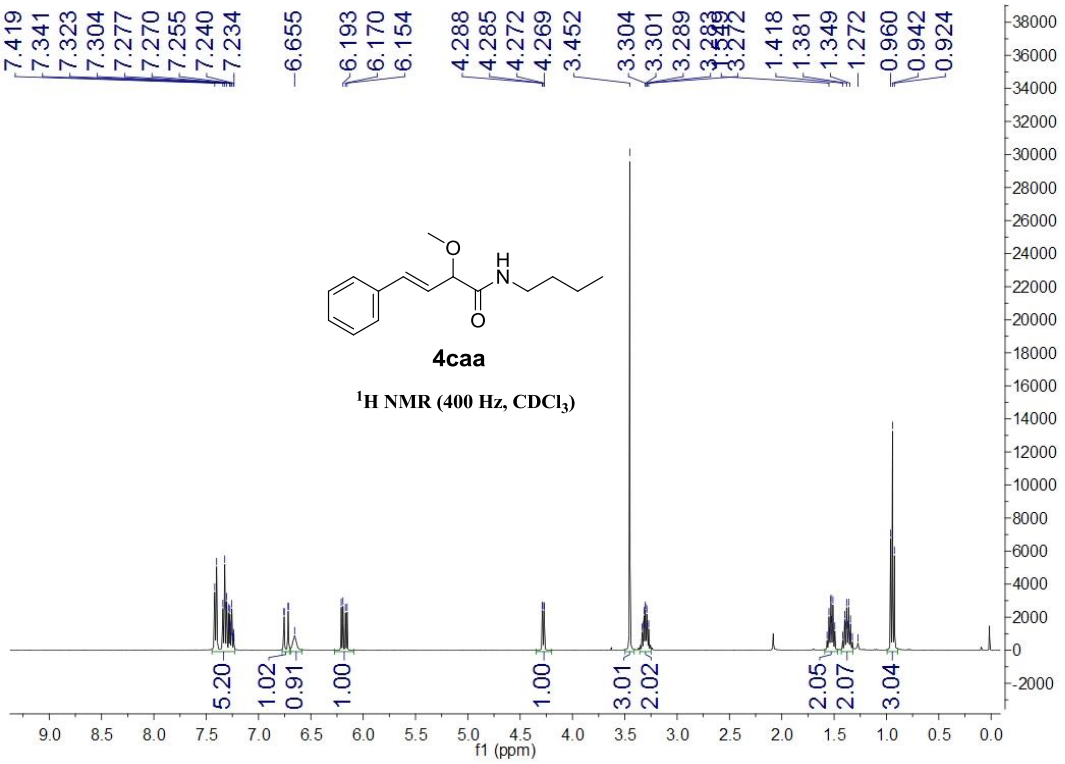
4baa

^{1}H NMR (400 Hz, $CDCl_3$)



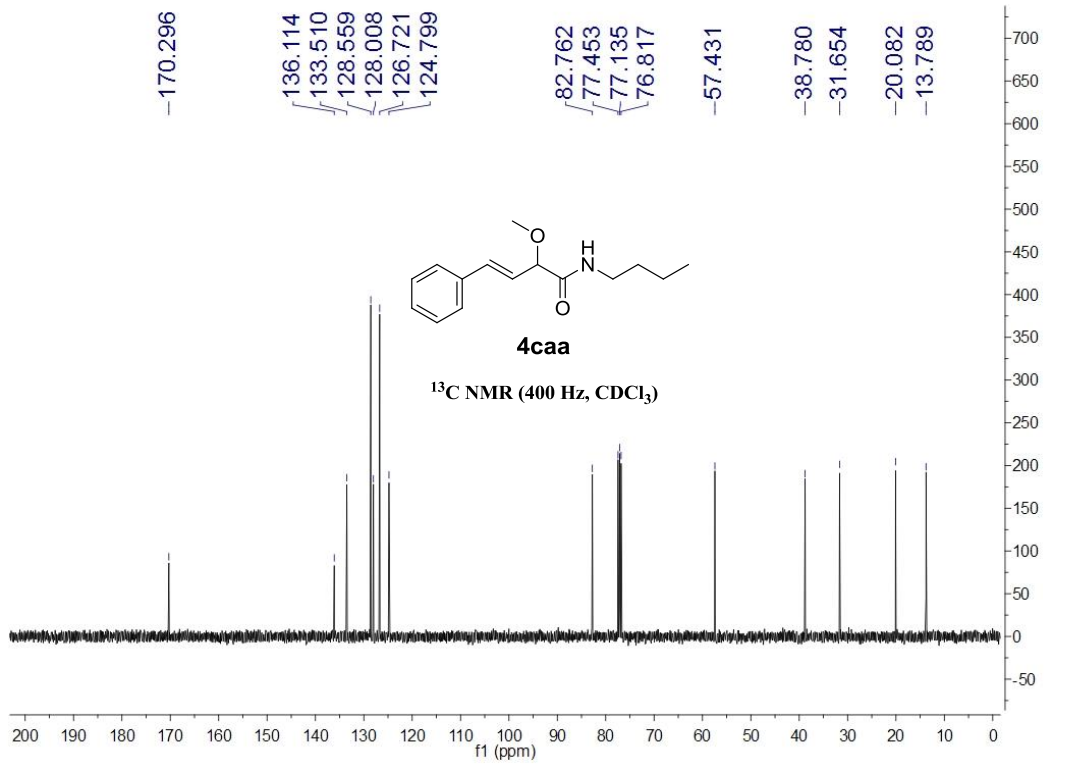
4baa

^{13}C NMR (400 Hz, $CDCl_3$)



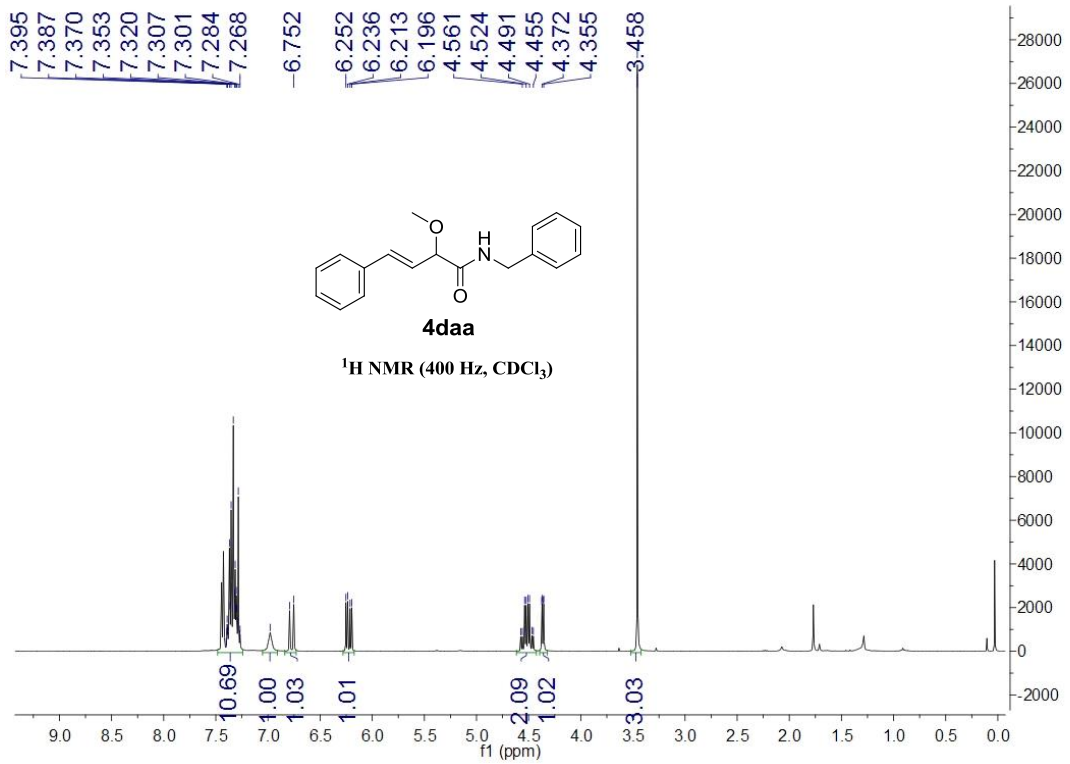
4caa

^{1}H NMR (400 Hz, $CDCl_3$)



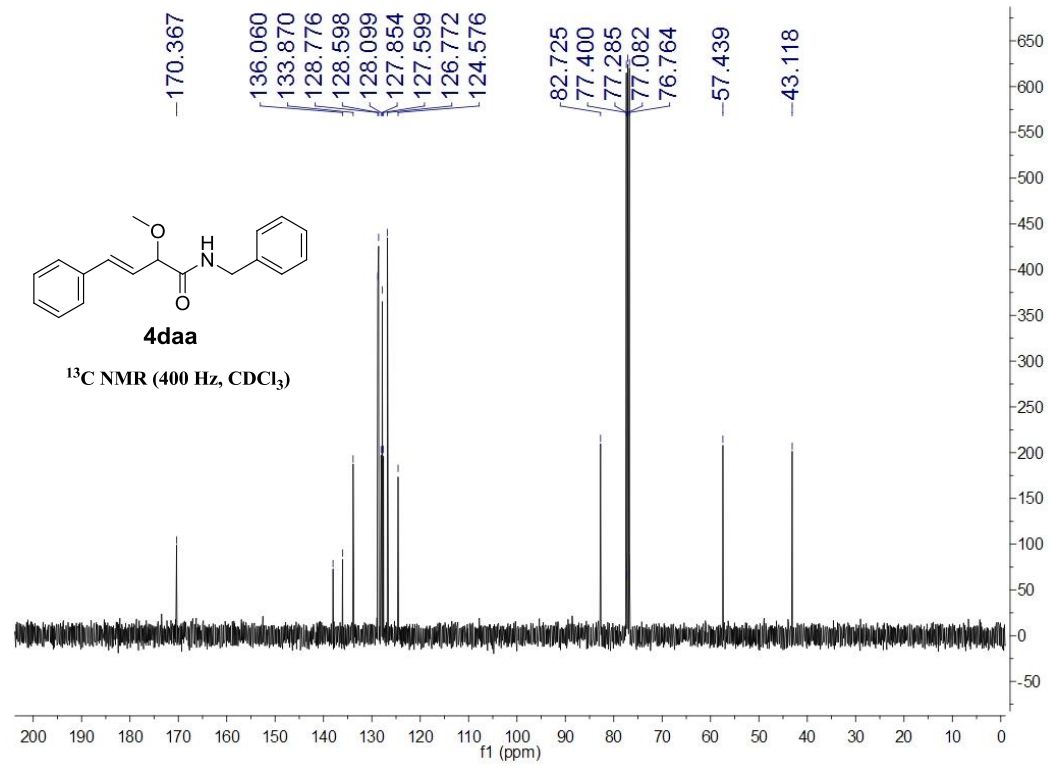
4caa

^{13}C NMR (400 Hz, $CDCl_3$)



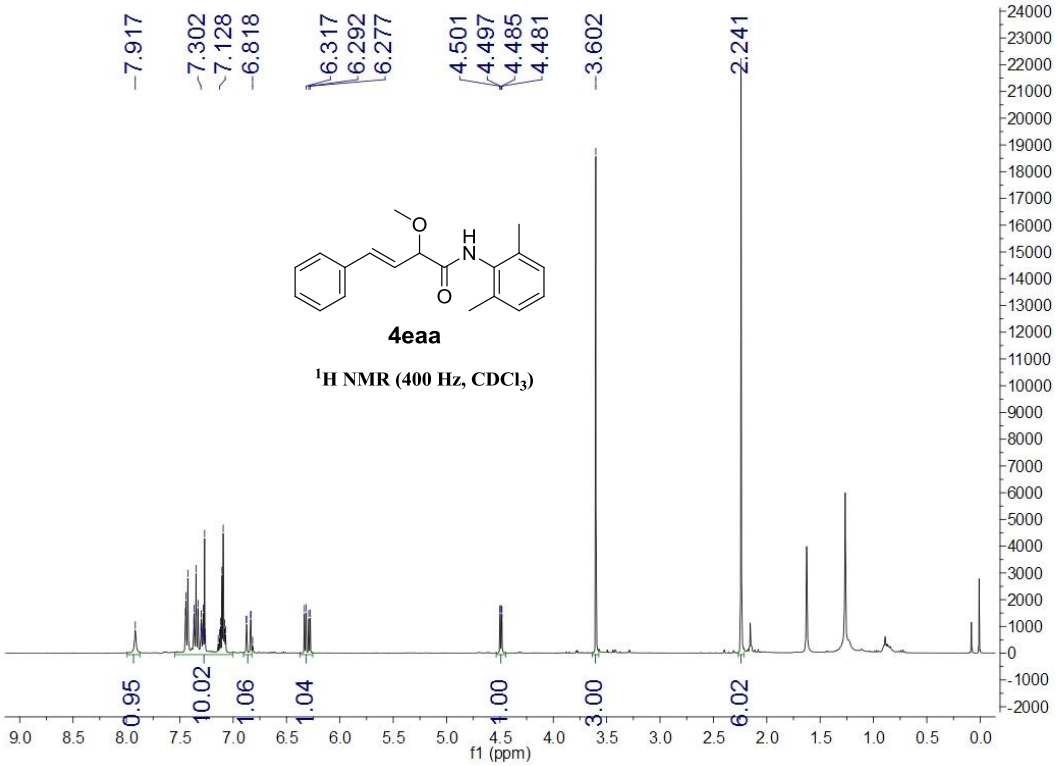
4daa

^{1}H NMR (400 Hz, $CDCl_3$)



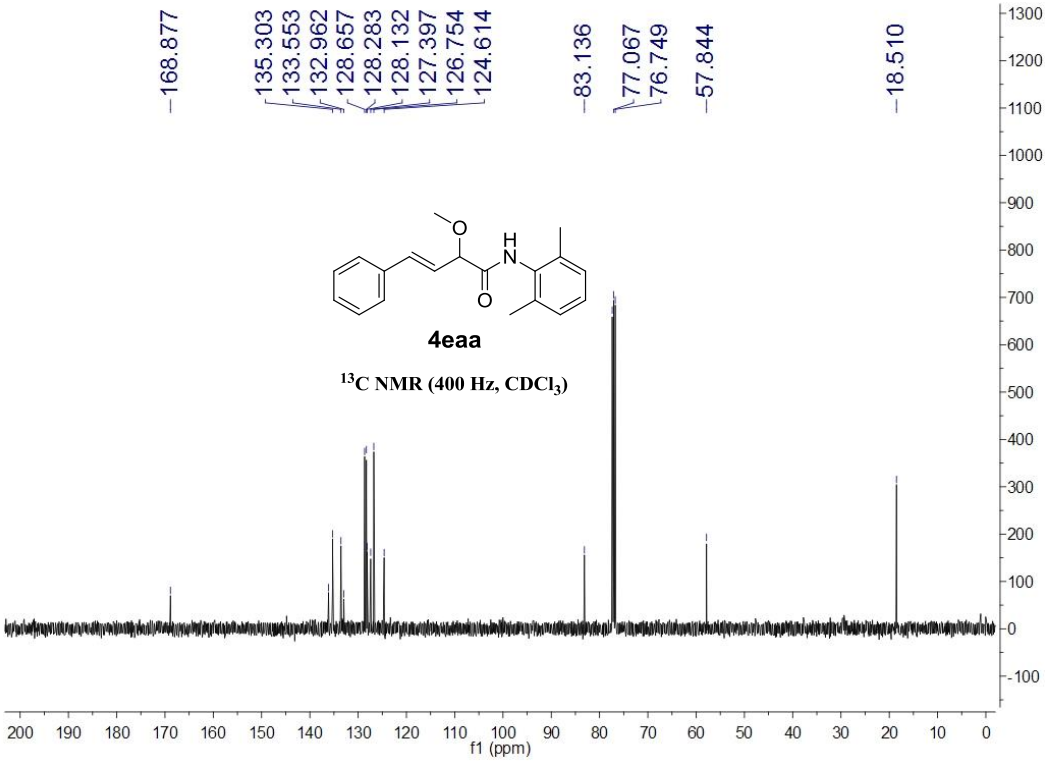
4daa

^{13}C NMR (400 Hz, $CDCl_3$)



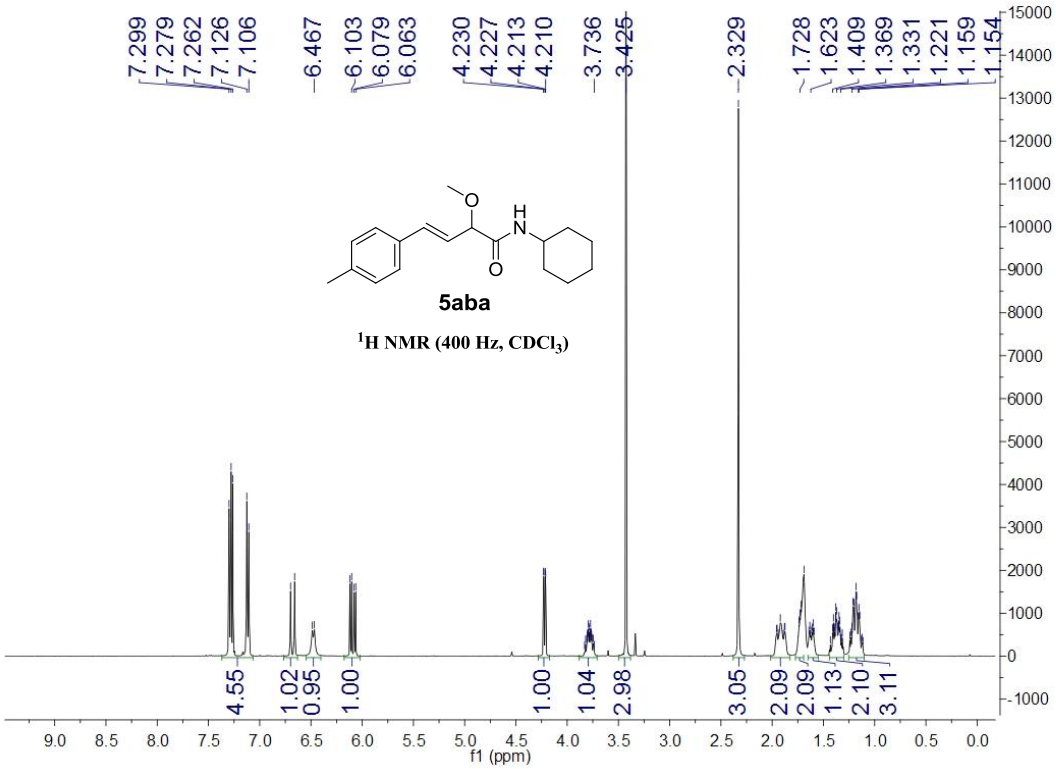
4eaa

^{1}H NMR (400 Hz, $CDCl_3$)



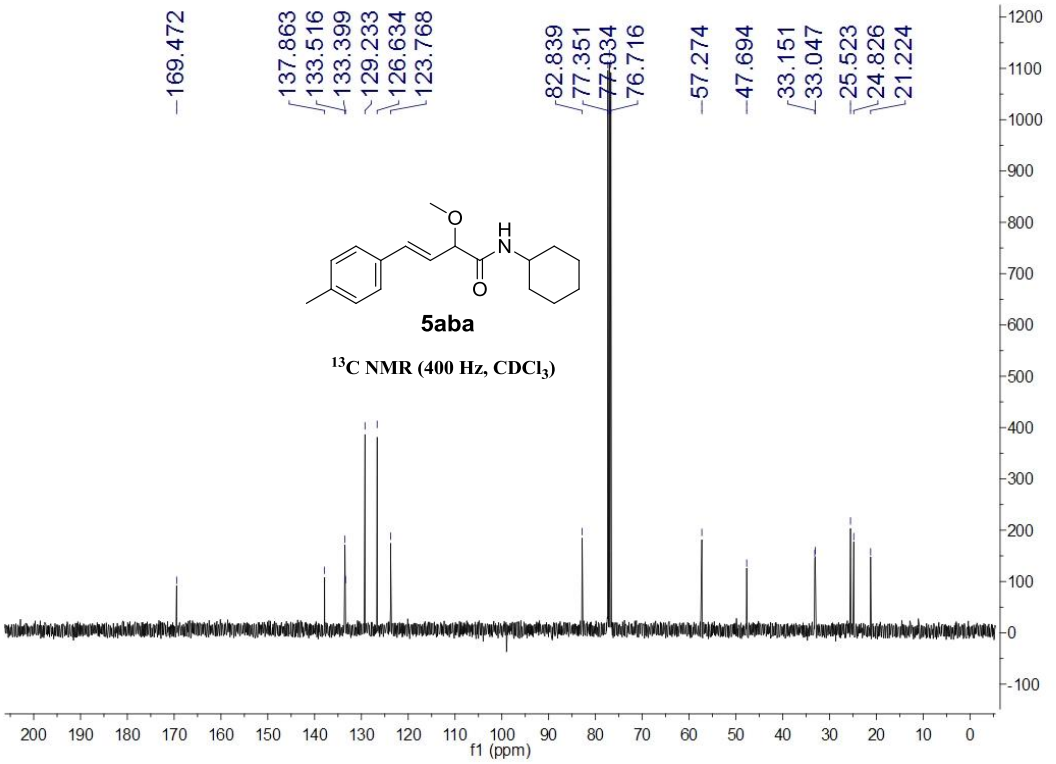
4eaa

^{13}C NMR (400 Hz, $CDCl_3$)



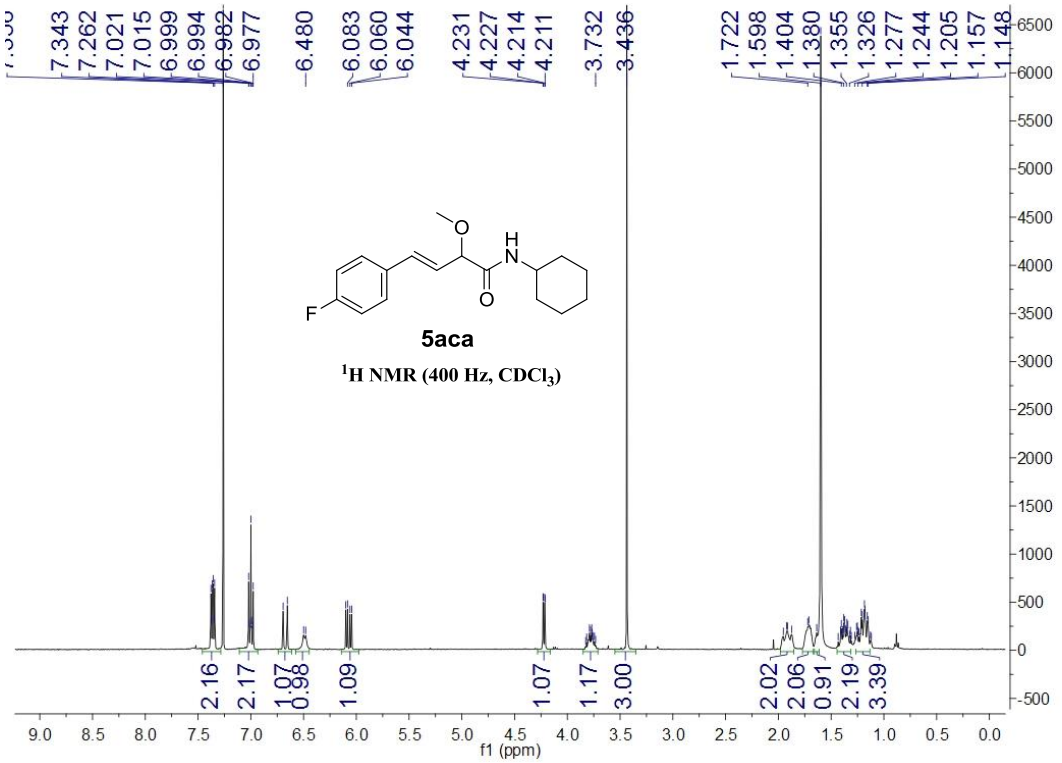
5aba

^{1}H NMR (400 Hz, $CDCl_3$)



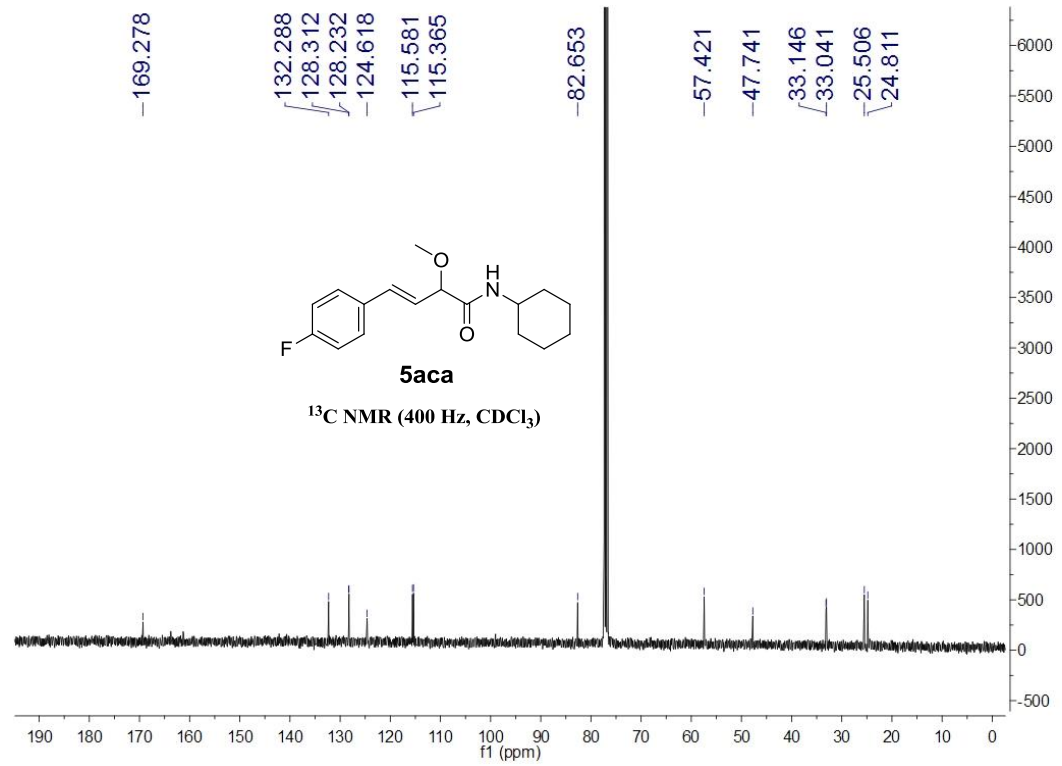
5aba

^{13}C NMR (400 Hz, $CDCl_3$)



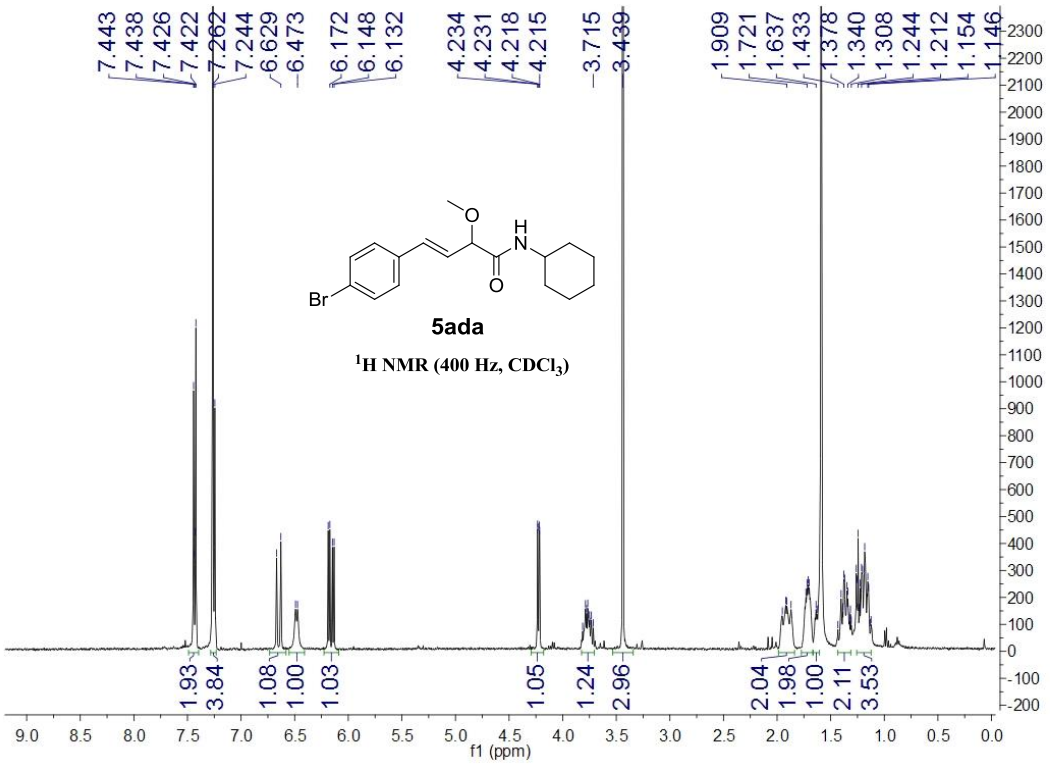
5aca

^{1}H NMR (400 Hz, $CDCl_3$)



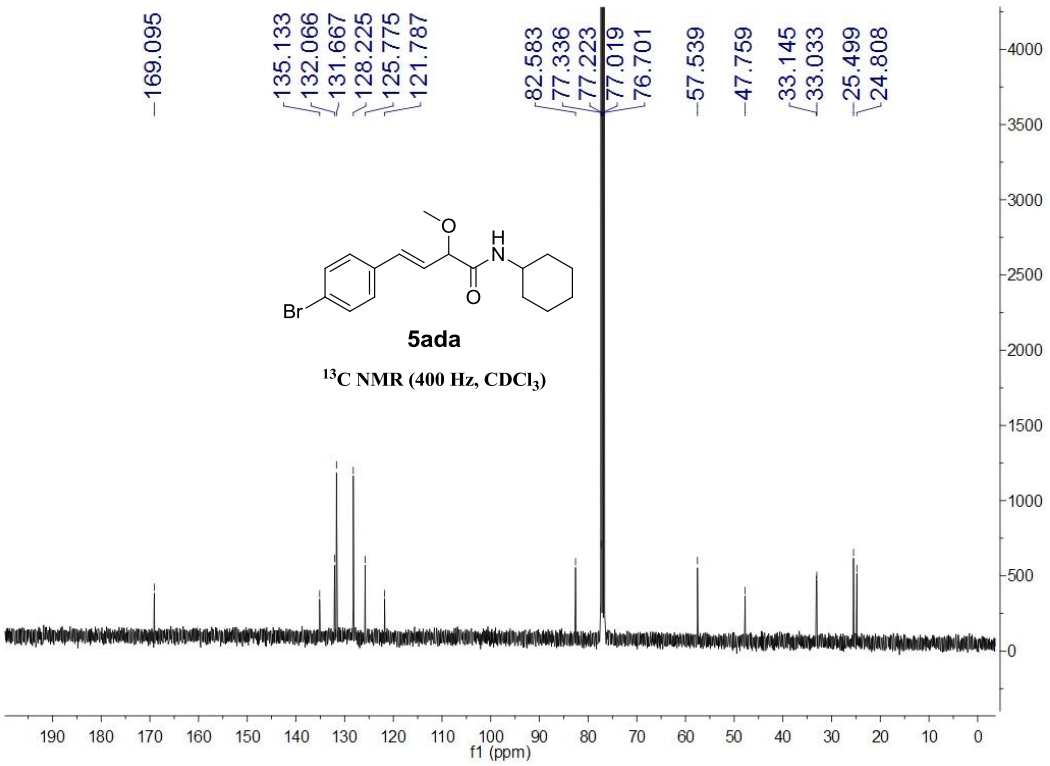
5aca

^{13}C NMR (400 Hz, $CDCl_3$)



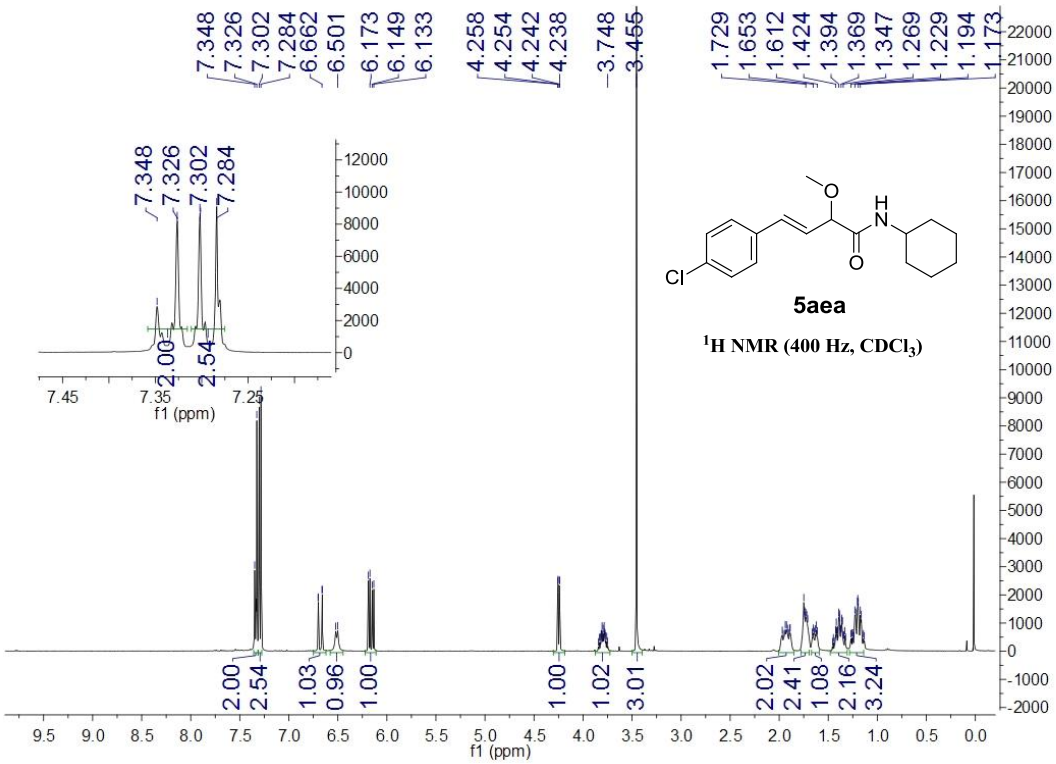
5ada

^{1}H NMR (400 Hz, $CDCl_3$)



5ada

^{13}C NMR (400 Hz, $CDCl_3$)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6.501
6.173
6.149
6.133
4.258
4.254
4.242
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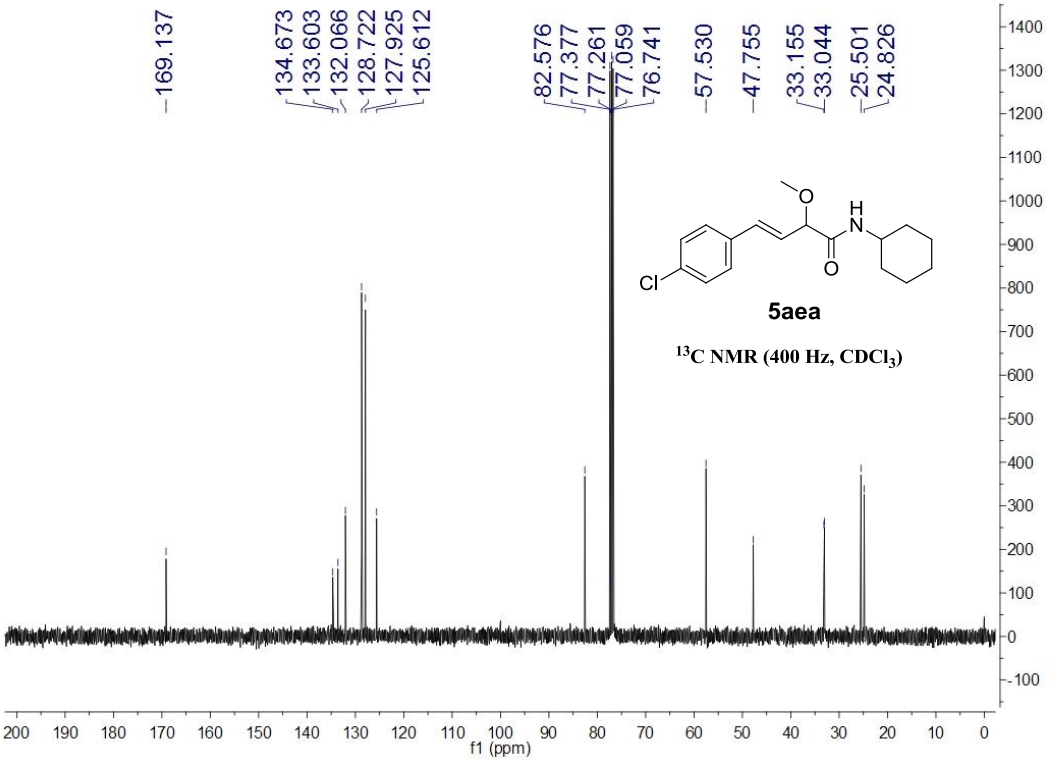
3.748
3.455
1.729
1.653
1.612
1.424
1.394
1.369
1.347
1.269
1.229
1.194
1.173
2.00
2.54
1.03
0.96
1.00
1.00
1.02
3.01
2.02
2.41
1.08
2.16
3.24
f1 (ppm)
Cl
O
H
N
O
5aea
^{1}H NMR (400 Hz, $CDCl_3$)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132.066
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127.925
125.612
82.576
77.377
77.261
77.059
76.741
57.530
47.755
33.155
33.044
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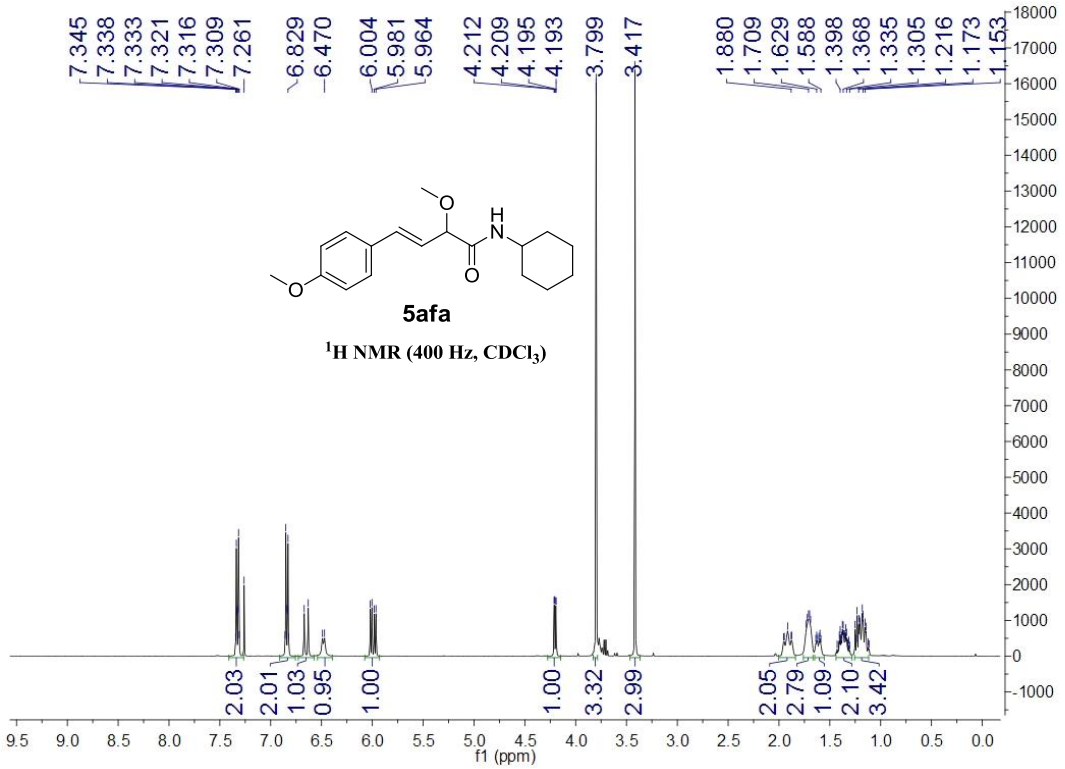
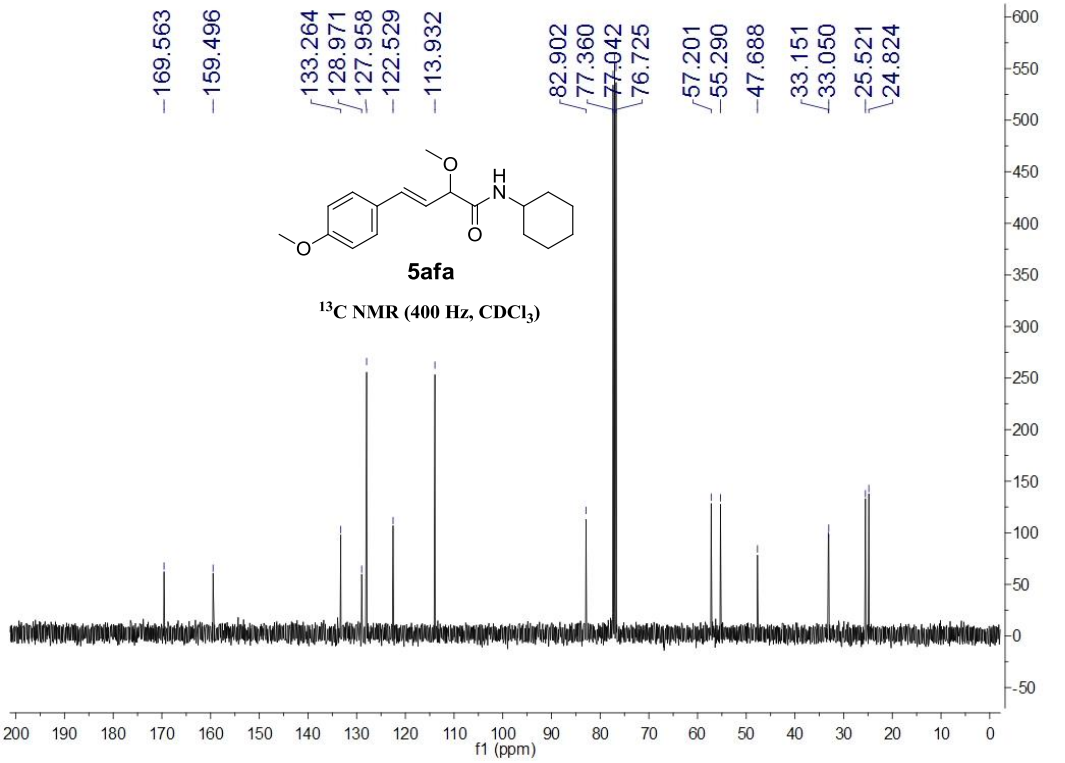
24.826
f1 (ppm)
Cl
O
H
N
O
5aea
^{13}C NMR (400 Hz, $CDCl_3$)



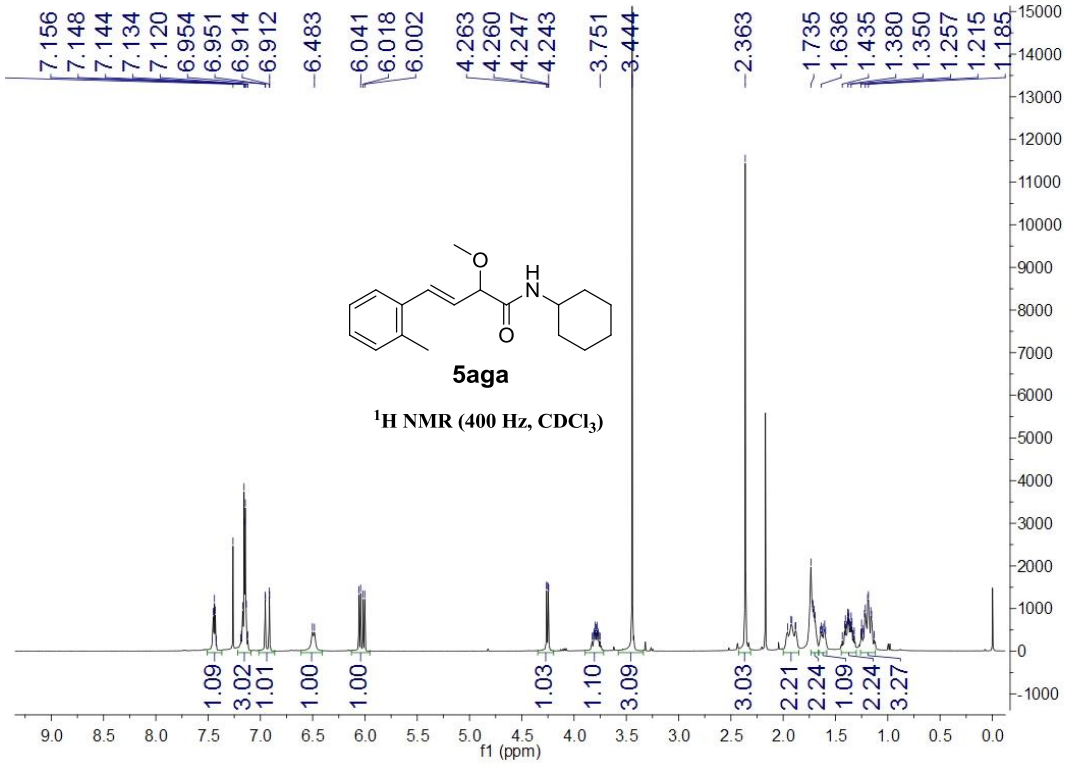
5afa

^{1}H NMR (400 Hz, $CDCl_3$)



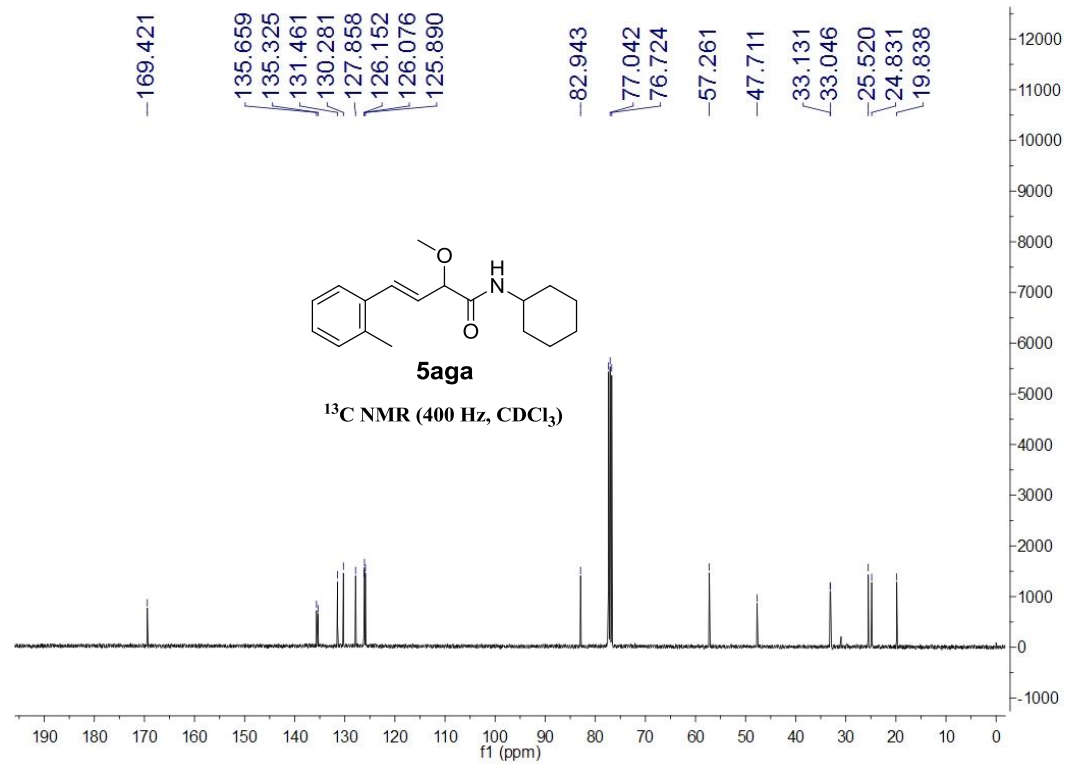
5afa

^{13}C NMR (400 Hz, $CDCl_3$)



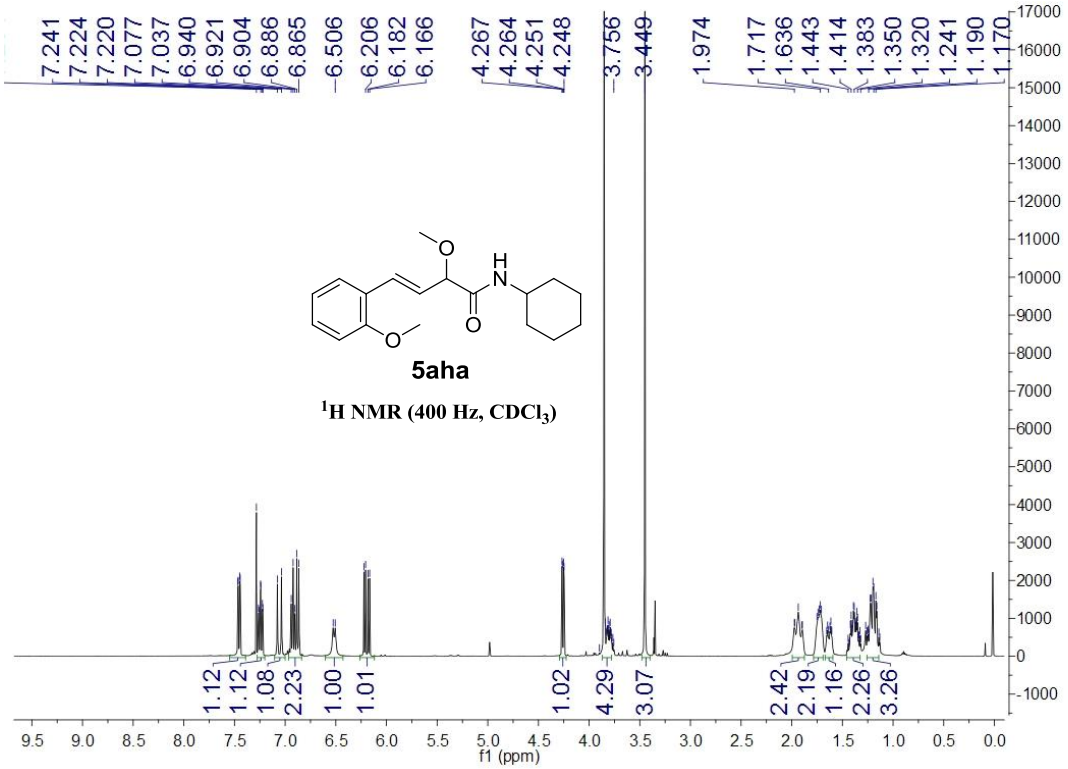
5aga

^{1}H NMR (400 Hz, $CDCl_3$)



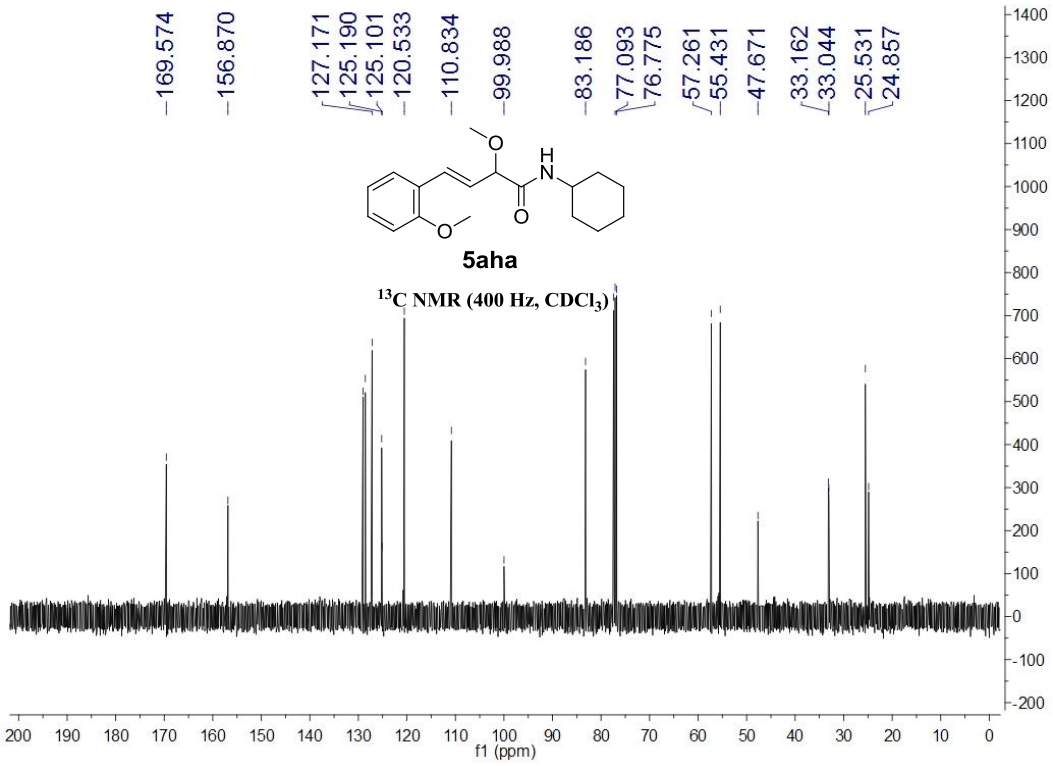
5aga

^{13}C NMR (400 Hz, $CDCl_3$)



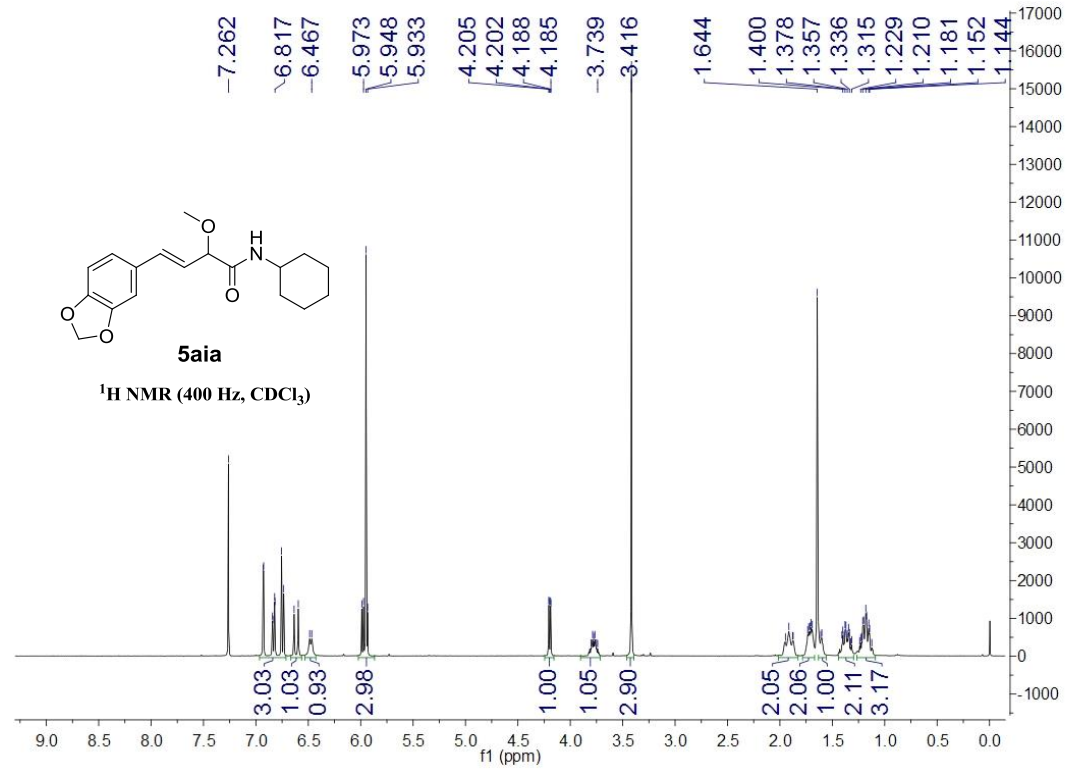
5aha

^{1}H NMR (400 Hz, $CDCl_3$)



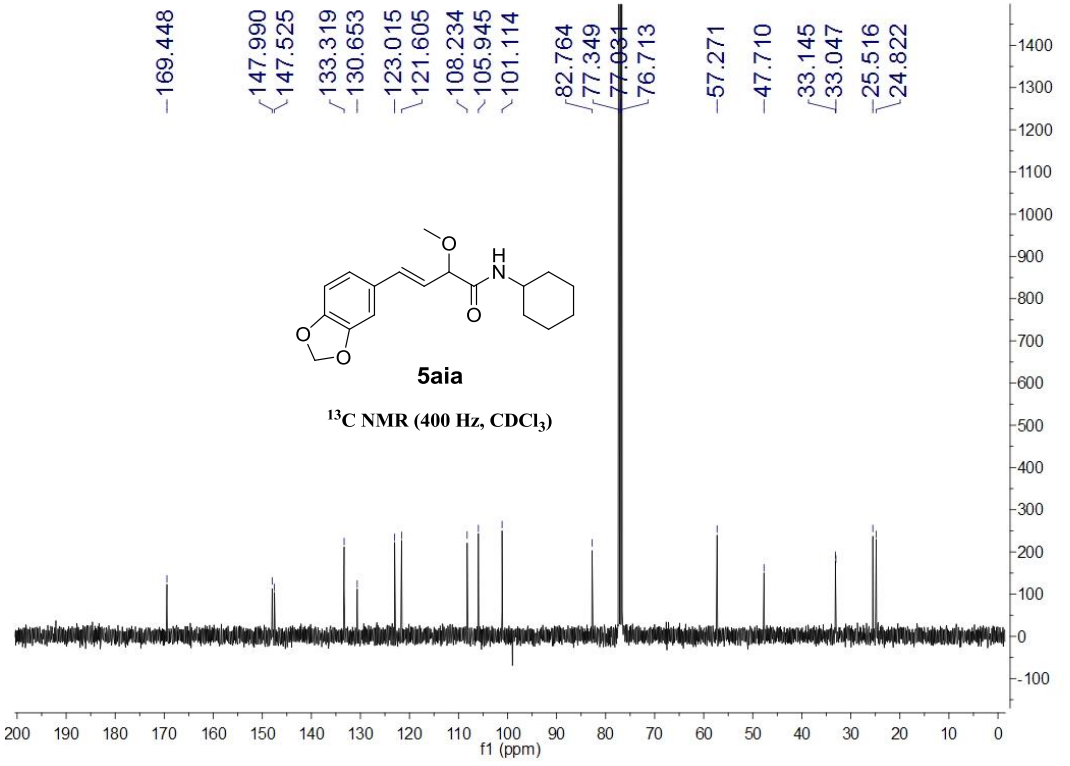
5aha

^{13}C NMR (400 Hz, $CDCl_3$)



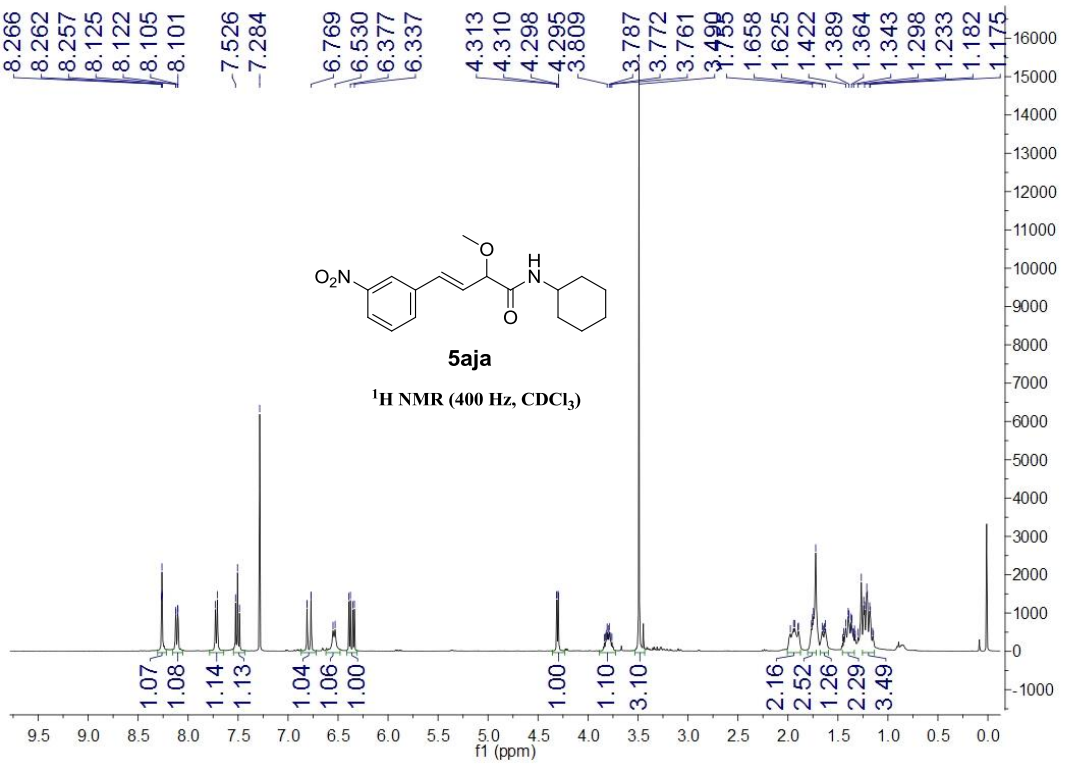
5aia

^{1}H NMR (400 Hz, $CDCl_3$)



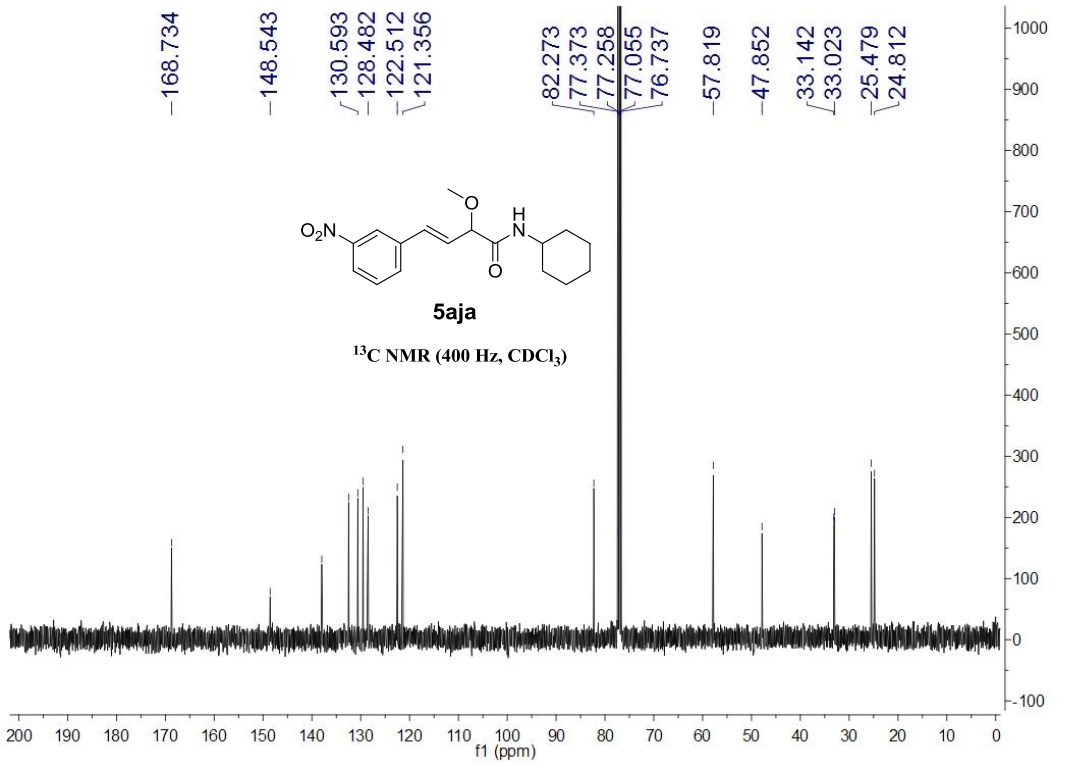
5aia

^{13}C NMR (400 Hz, $CDCl_3$)



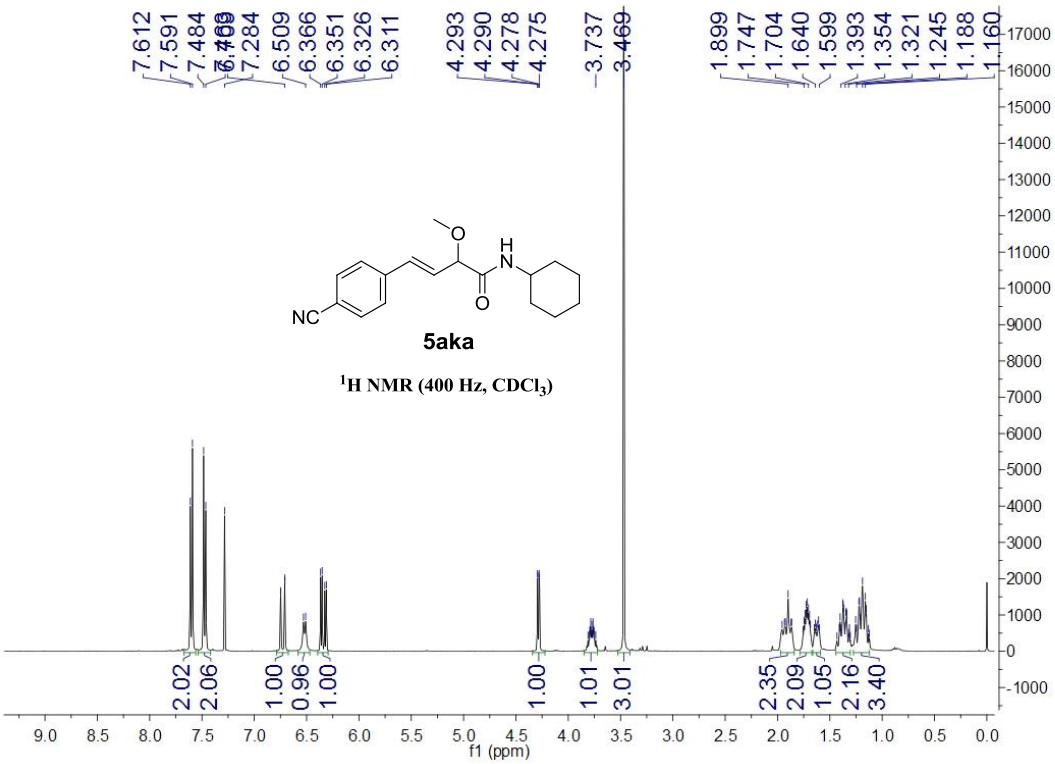
5aja

^{1}H NMR (400 Hz, $CDCl_3$)



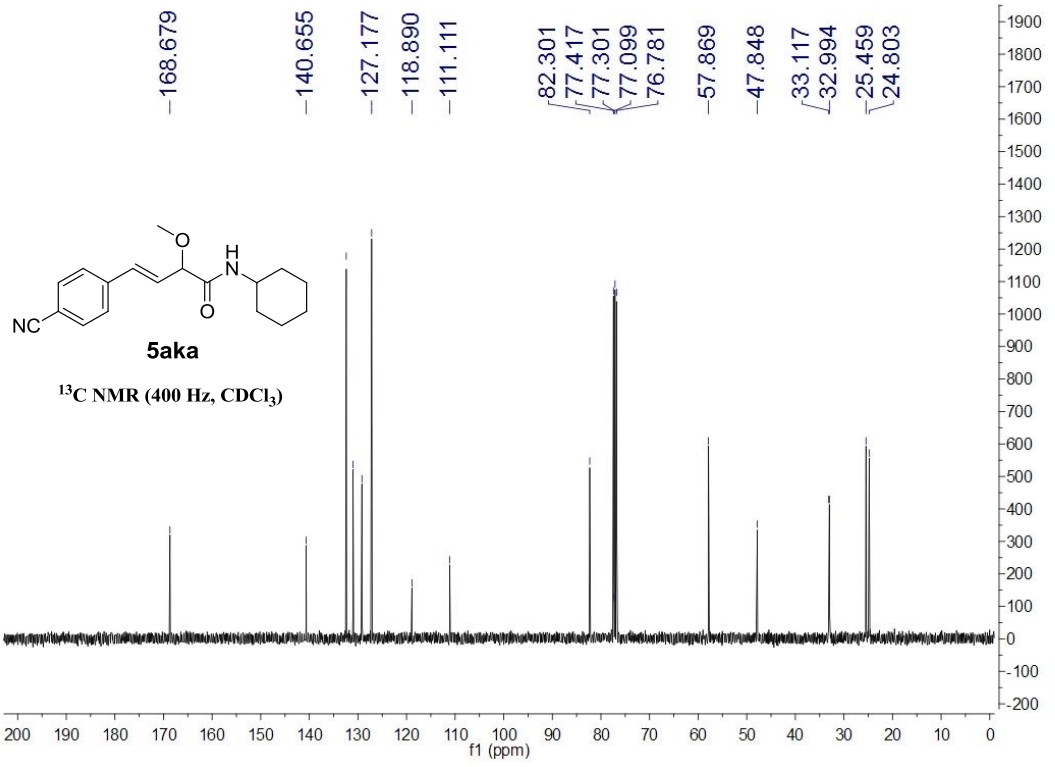
5aja

^{13}C NMR (400 Hz, $CDCl_3$)



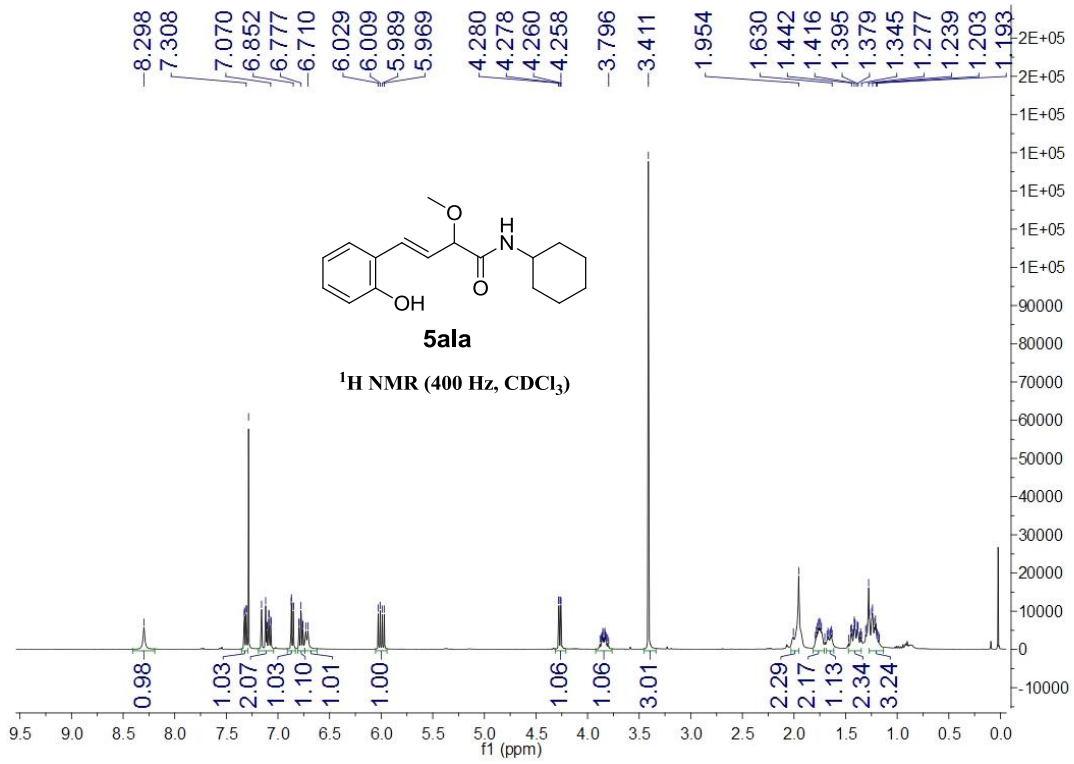
5aka

^{1}H NMR (400 Hz, $CDCl_3$)



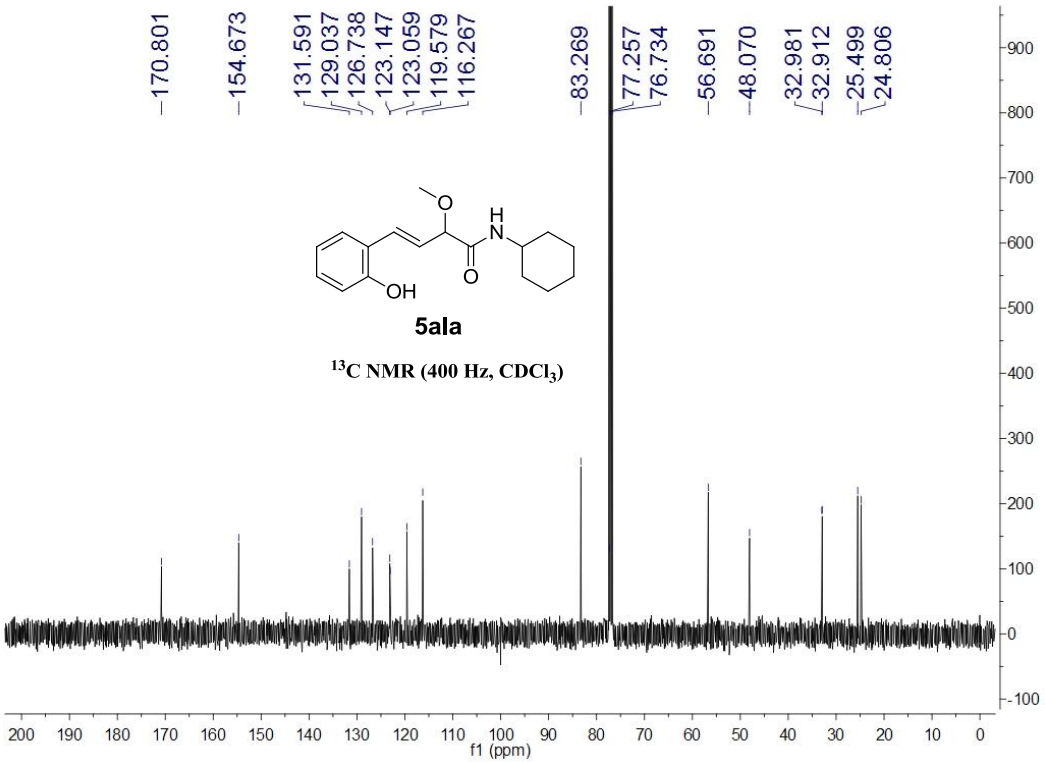
5aka

^{13}C NMR (400 Hz, $CDCl_3$)



5ala

^{1}H NMR (400 Hz, $CDCl_3$)



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^{13}C NMR (400 Hz, $CDCl_3$)