Electronic Supplementary Information for

Cyanodifluorosulfonium ion: an efficient reagent for the deoxyfluorination of cinnamic acids into vinyl acyl fluorides intermediate

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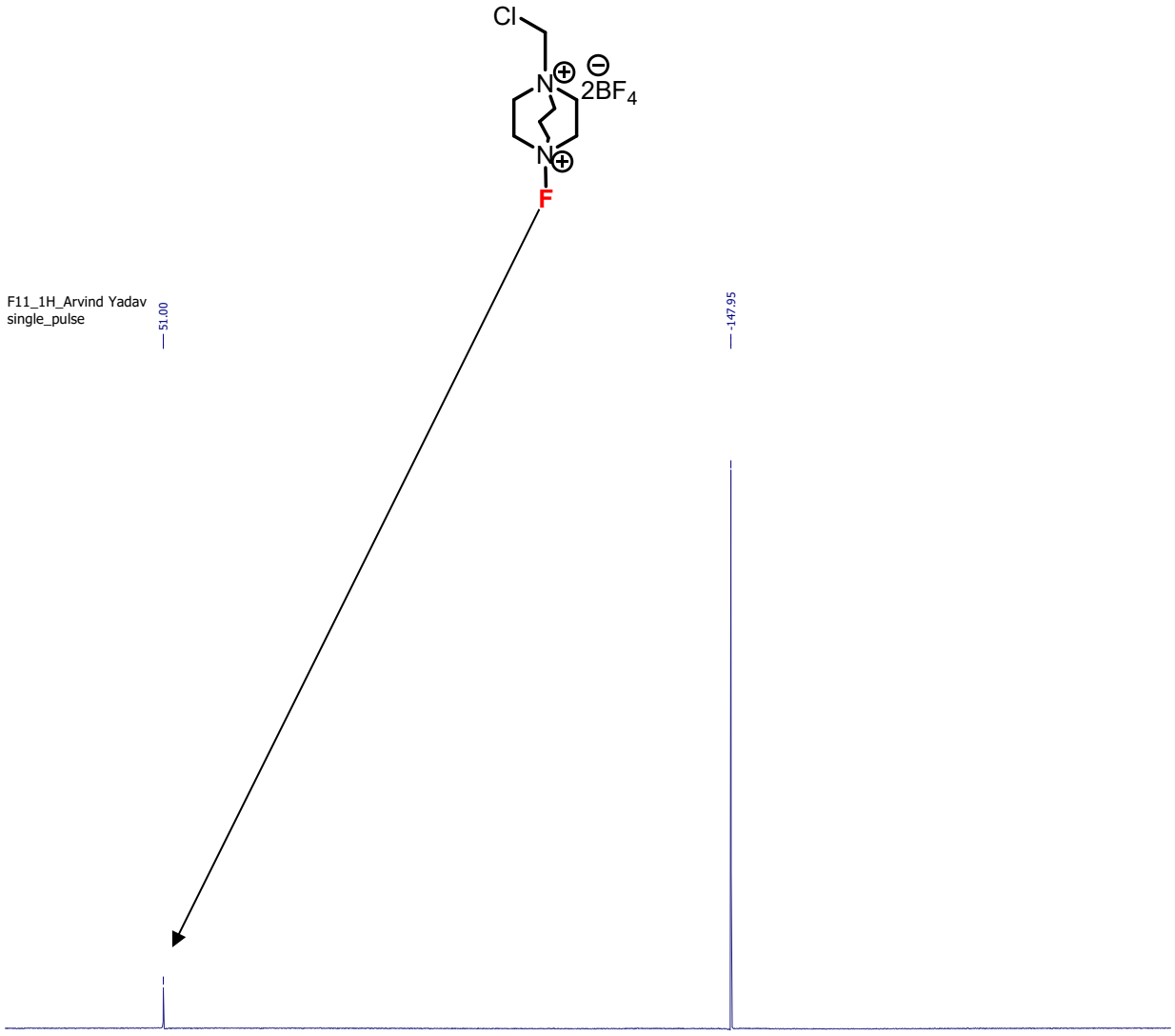
I. General Information: Unless otherwise stated, all reactions were carried out under an air atmosphere in oven-dried screw-cap reaction tubes. All commercially available reagents were used without further purification unless otherwise specified by a reference. Cinnamic acids were purchased from TCI. Selectfluor and KSCN were purchased from Sigma-Aldrich and TCI. Solvents were obtained from Merck and TCI; freshly opened, sealed bottles were used without further purification. Organic solutions of reaction mixture were concentrated using a Buchi rotary evaporator. Column chromatography was carried out over silica gel (Merck 100–200 mesh) and TLC was performed using silica gel GF254 (Merck) plates. ^{1}H (600 MHz), ^{13}C (151 MHz) NMR spectra were recorded on a Bruker AVII spectrometer in $CDCl_3$ using TMS as internal reference. ^{19}F NMR (470 MHz) spectra recorded by 500 MHz Bruker AVII spectrometer of the crude reaction mixtures were performed using fluorobenzene or hexafluorobenzene as internal standards. All chemical shifts are reported in δ/ppm and coupling constants (*J*) in Hertz (Hz). High-resolution mass spectrometry (HRMS (QTOF) was recorded on an electron impact ionization mass spectrometer.

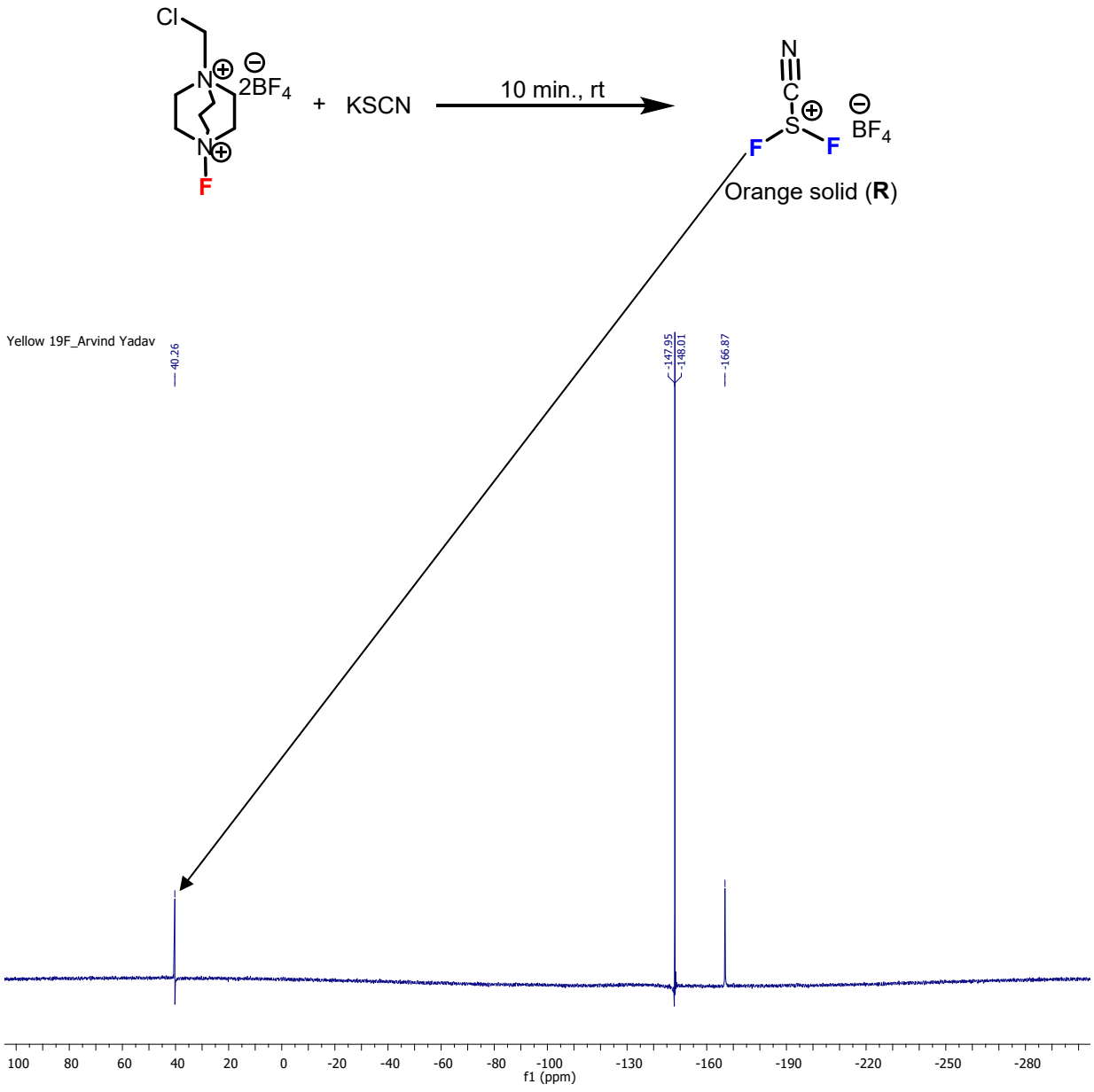
Safety note: The use of Selectfluor and KSCN is not without risk. Selectfluor may be harmful if swallowed, may cause severe skin and eye damage and KSCN is harmful on inhalation/in contact with skin. All operations should be conducted in a well-ventilated fume hood while wearing appropriate personal protective equipment (lab coat, gloves, and safety goggles).

(ii) Spectroscopy evidence in support of acyl fluorides intermediate and formation of the reagent (R):

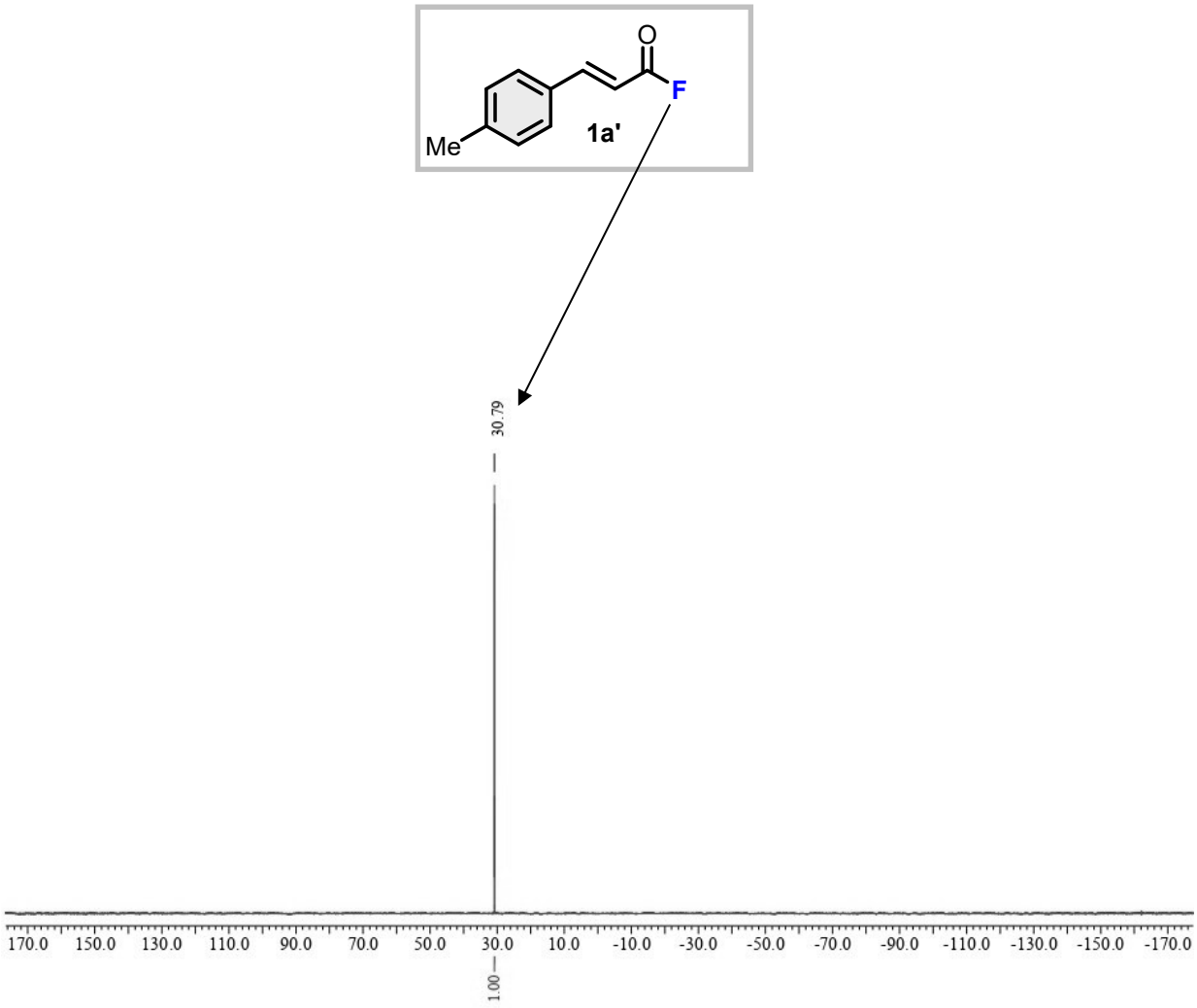
^{19}F NMR Spectrum of the Selectfluor (w.r.t. C_6F_6):



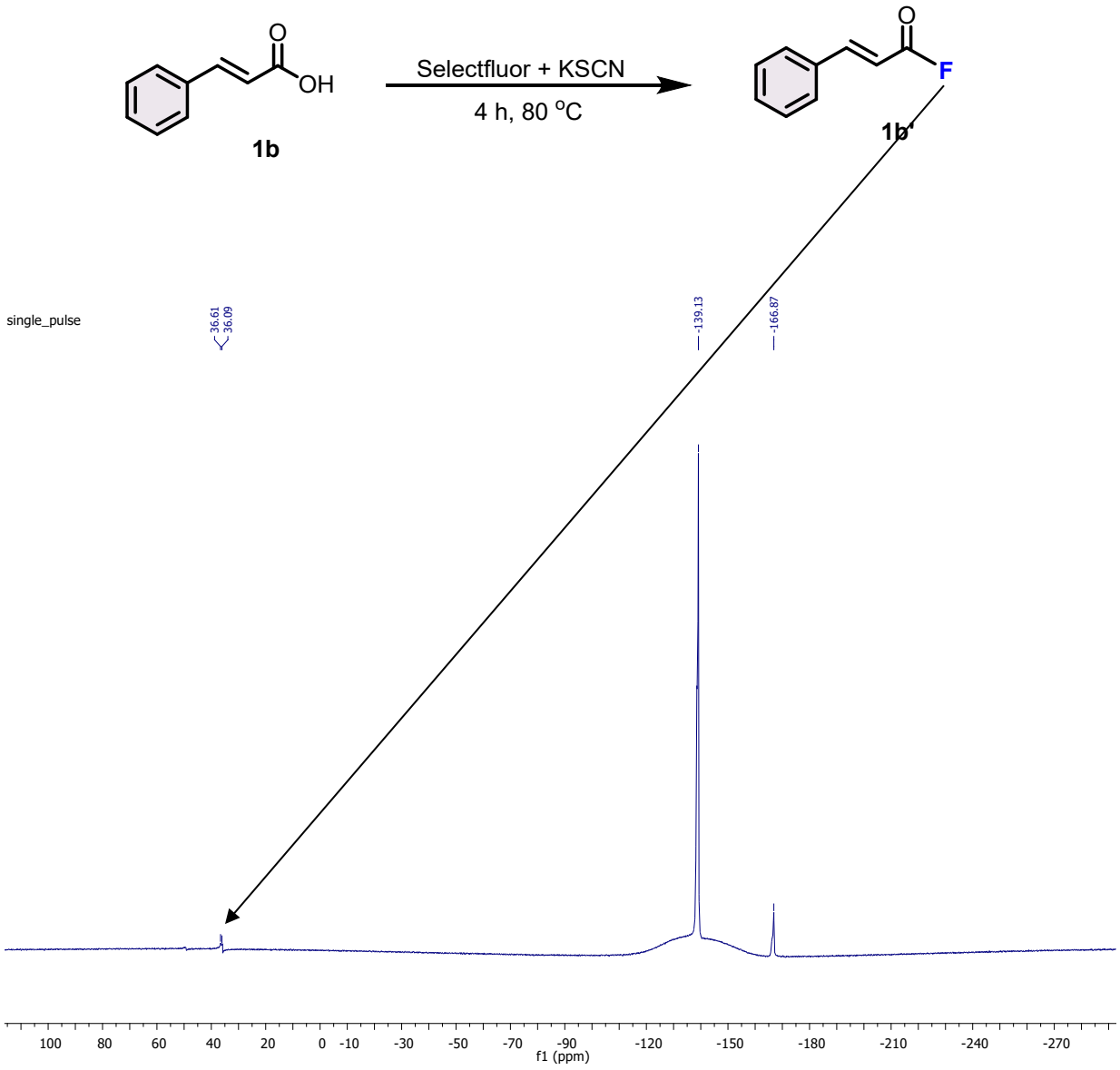
^{19}F NMR Spectrum of the Orange Solid reagent (R) (w.r.t. C_6F_6):



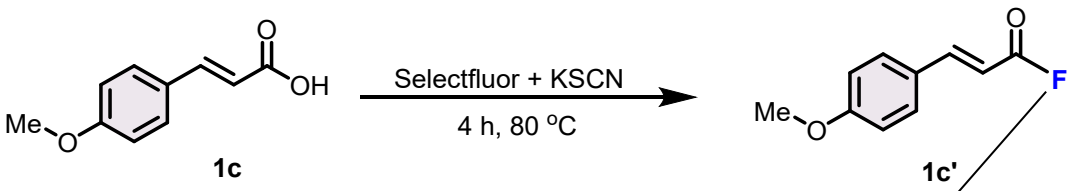
^{19}F NMR Spectrum of the intermediate (*E*)-3-(*p*-tolyl)acryloyl fluoride (1a') (w.r.t. C_6F_6):

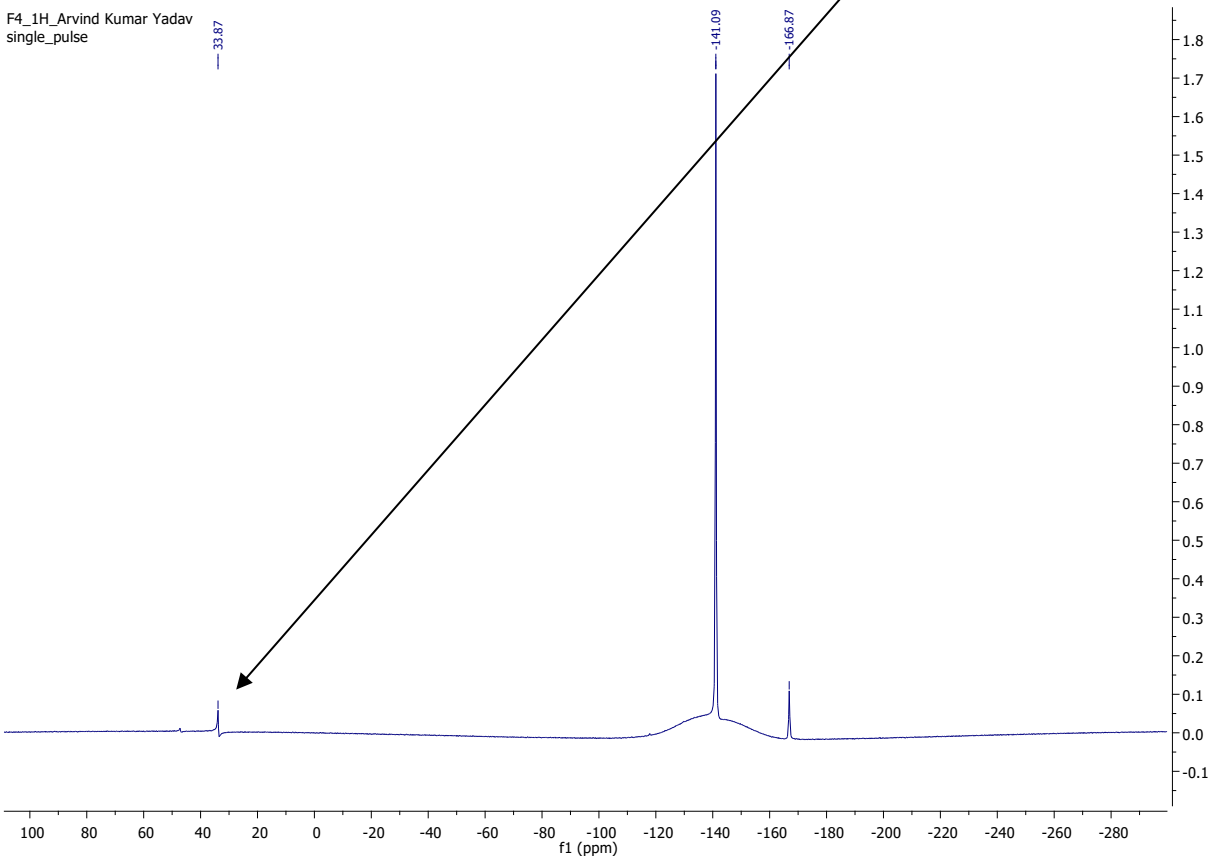


^{19}F NMR Spectrum of the reaction mixture 1b (w.r.t. C_6F_6):

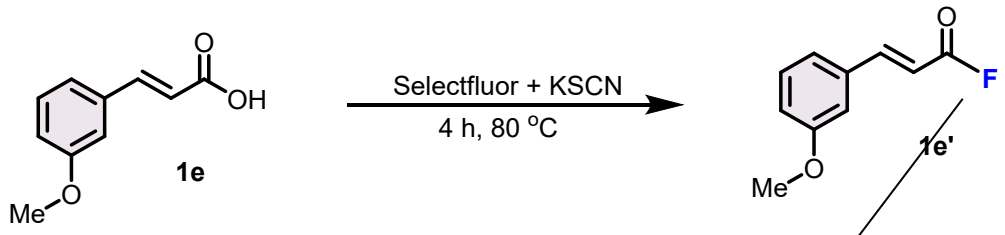


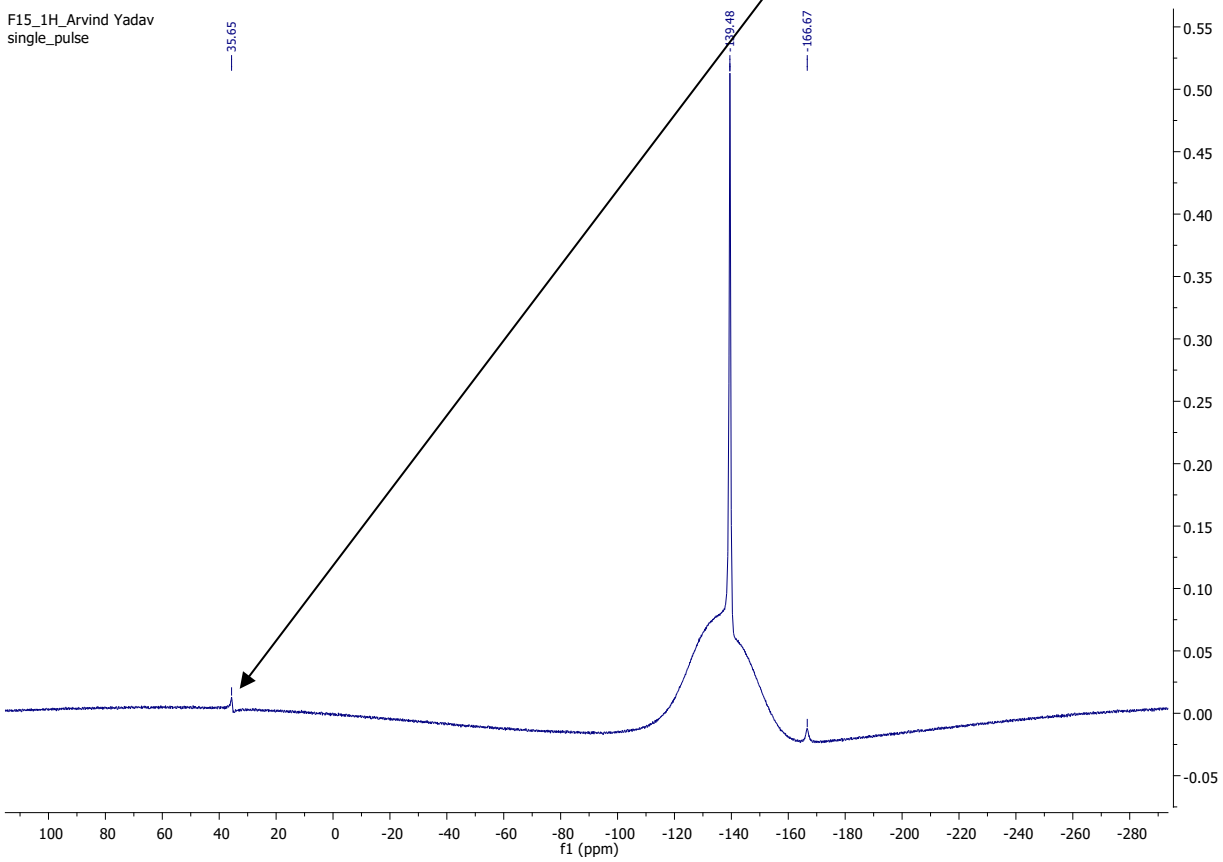
^{19}F NMR Spectrum of the reaction mixture 1c (w.r.t. C_6F_6):



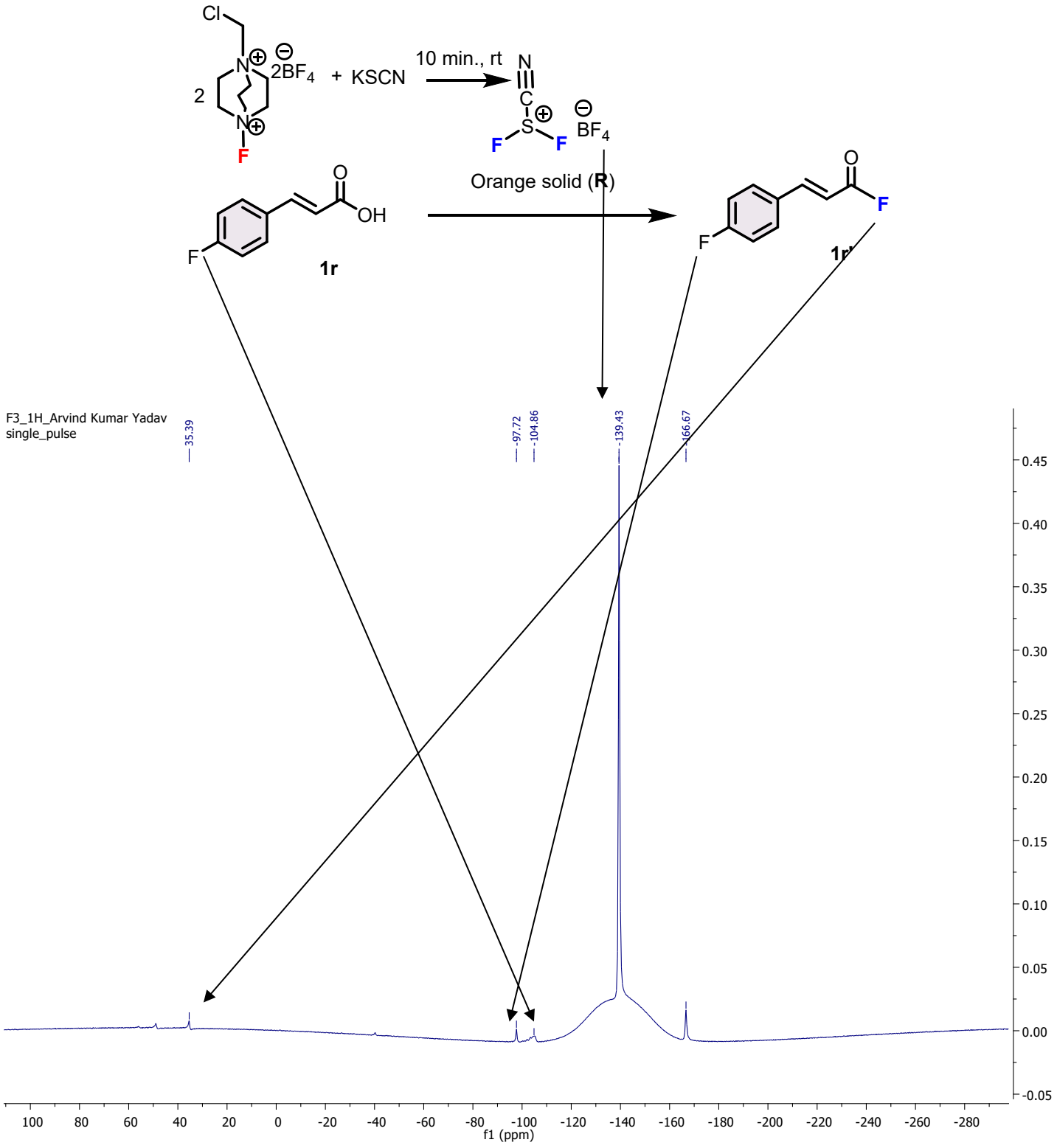


^{19}F NMR Spectrum of the reaction mixture 1e (w.r.t. C_6F_6):

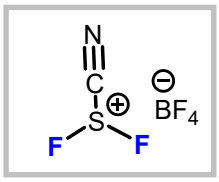




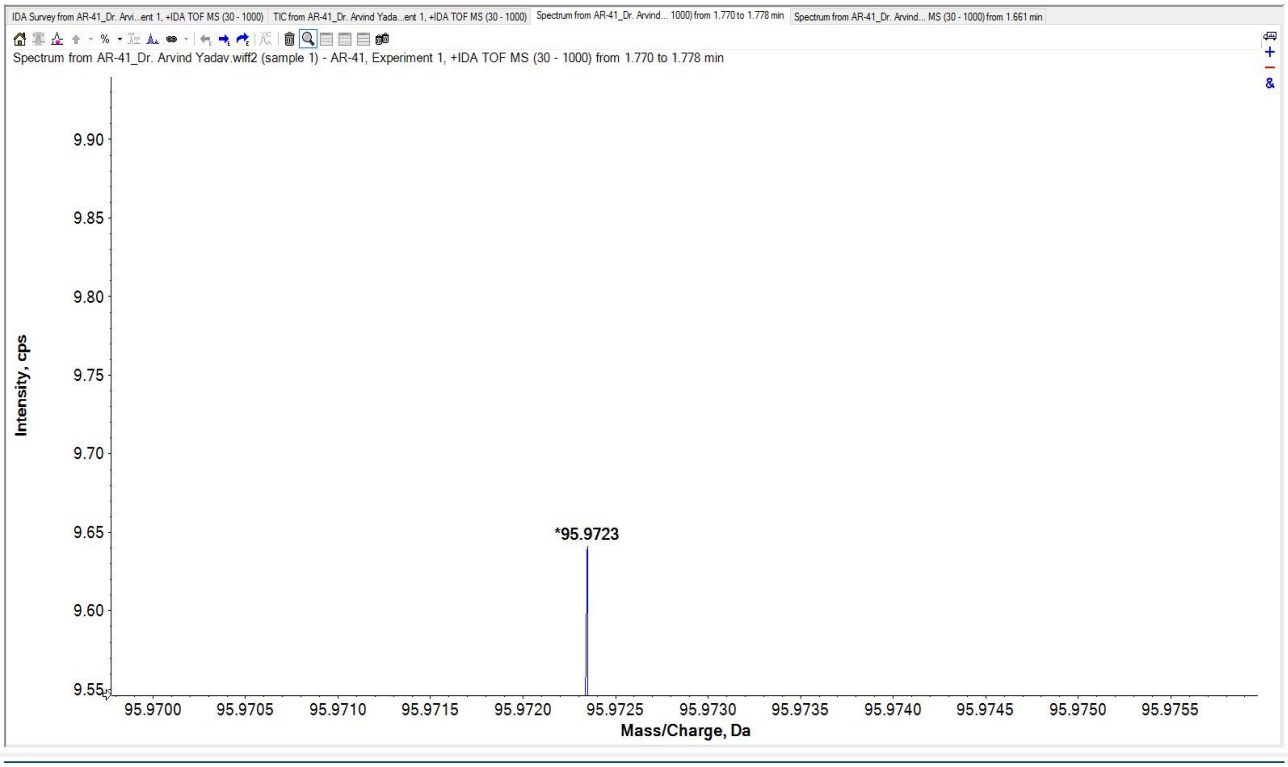
^{19}F NMR Spectrum of the reaction mixture 1r (w.r.t. C_6F_6) after 2h:



HRMS Spectrum of the reagent R:



(M+) Calculated: 95.9714, found 95.9723



EDAX Spectrum of the reagent R:

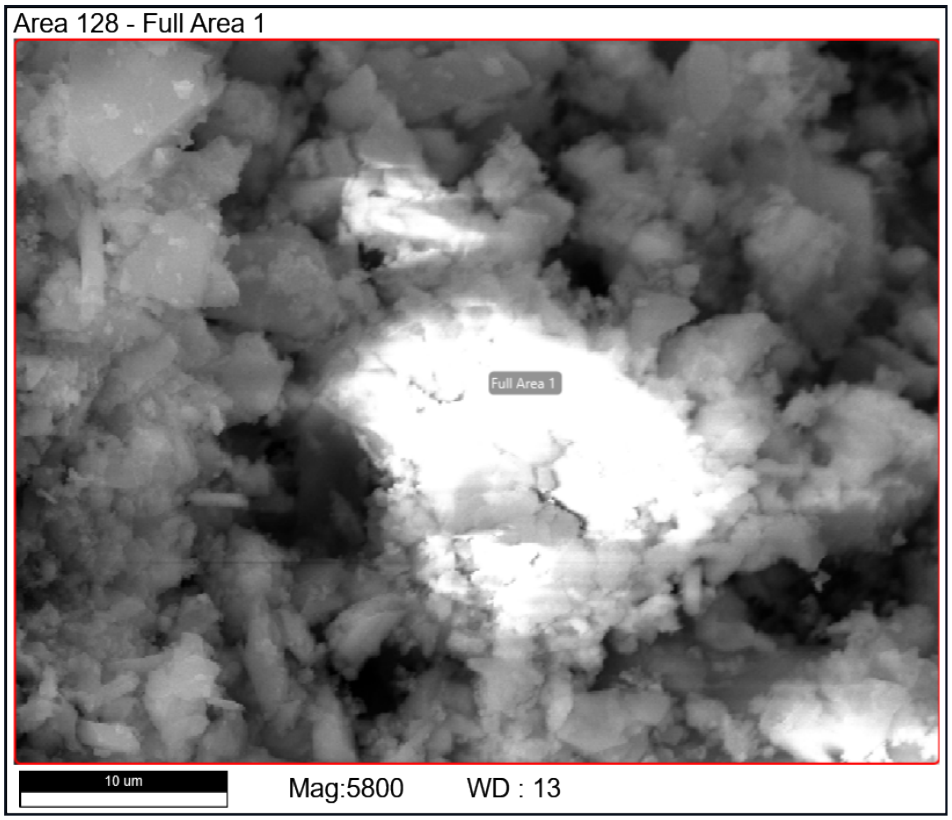
EDAX APEX

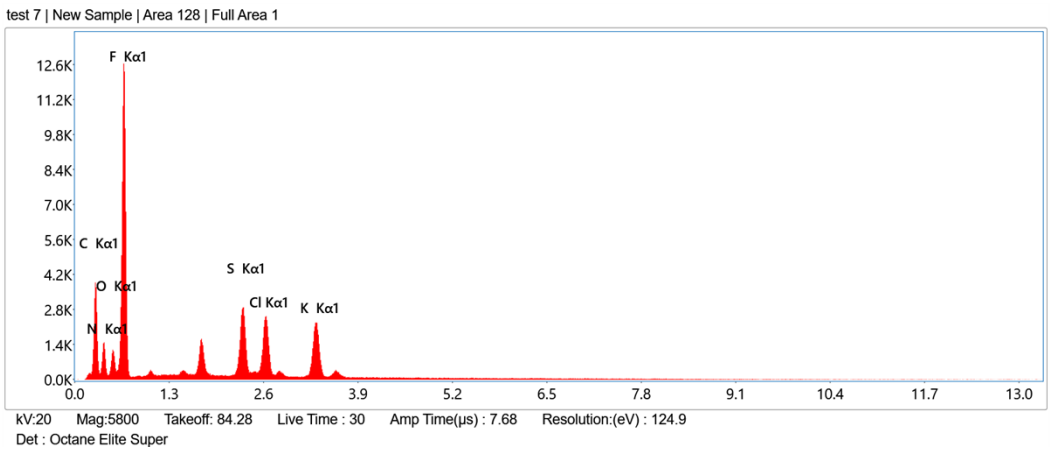
test 7

Author: User Apex

Creation: 12/10/2025 3:39:57 PM

Sample Name: New Sample

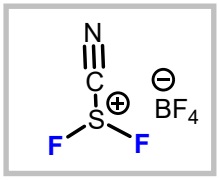


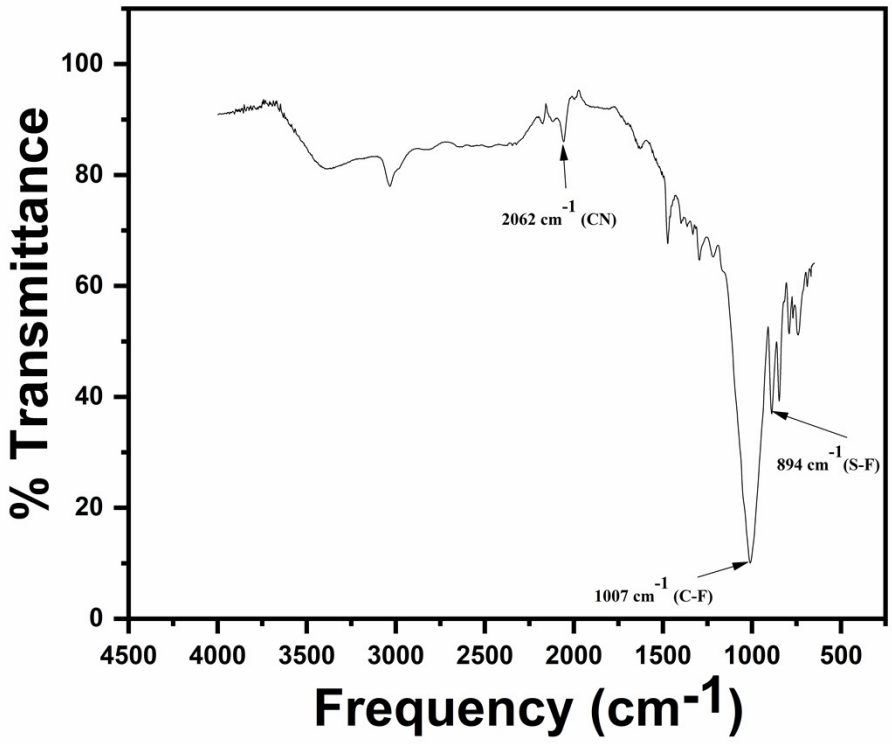


eZAF Quant Result - Analysis Uncertainty: 99.00 %

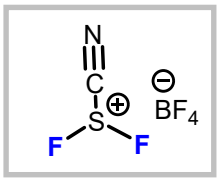
Element	Weight %	Atomic %
C K	38.2	51.1
N K	10.2	11.7
O K	4.2	4.2
F K	29.4	24.8
S K	5.2	2.6
Cl K	5.6	2.5
K K	7.2	3.0

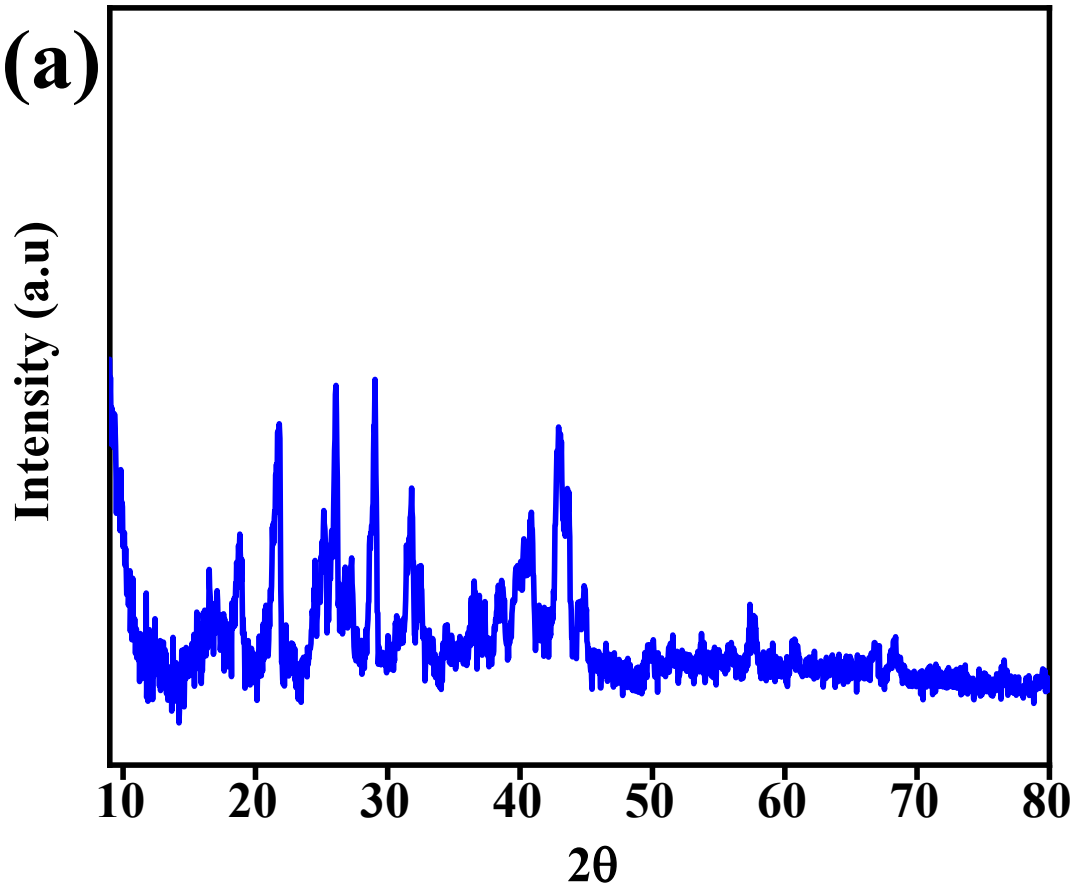
FTIR Spectrum of reagent R:





XRD Spectrum of the reagent R:





III. General procedure for the synthesis of the products 3: A mixture of KSCN (1.0 equiv.),

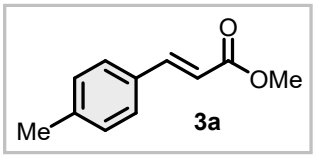
Selectfluor (2.0 equiv.) and CH_3CN (3 mL) was taken in a closed vessel, the content was stirred at room temperature for 10 minute until the formation of orange ppt appear, then cinnamic acids **1** (0.5 mmol) was added and stirred at 80 °C for 4 h. After the completion of reaction (as indicated by TLC) alcohols/amines **2** (1.5 equiv.) & triethyl amine (1.5 equiv.) were added successively by syringe and stirred for 2 h at 80 °C to room temperature, then it was quenched with water (5 mL) and extracted with ethyl acetate (3 × 5 mL). The combined organic phase was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure to yield the crude product, which was purified by silica gel column chromatography using a mixture of EtOAc-Hexane in appropriate ratio (1:9) to give the pure products **3**.

The structures of the products were confirmed by the comparison of ^1H and ^{13}C NMR data with those reported in the literature.

Spectral data of compounds **3** are summarised below with relevant references:

IV. Spectral data of the products 3:

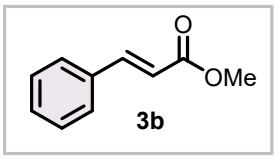
(1) Methyl(*E*)-3-(*p*-tolyl)acrylate (3a):[1]



3a

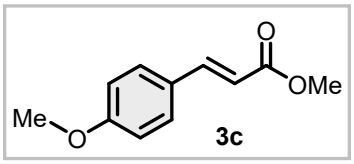
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.68 (d, *J* = 12 Hz, 1H), 7.42 (d, *J* = 6 Hz, 2H), 7.19 (d, *J* = 6 Hz, 2H), 6.41 (d, *J* = 18 Hz, 1H), 3.80 (s, 3H), 2.34 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.66, 144.90, 140.74, 131.66, 129.63, 128.08, 116.70, 51.65, 21.47. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_2$, 177.0916; Found 177.0913.

(2) Methyl cinnamate (3b, *E*/*Z*:1/0.7):[1]



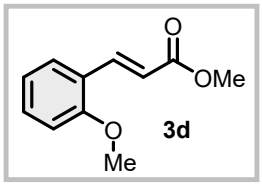
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 12 Hz, 1H), 7.53 (d, *J* = 6 Hz, 3H) 7.38 (d, *J* = 6 Hz, 5H), 6.86 (d, *J* = 18 Hz, 1H) 3.74 (s, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.64, 144.47, 143.29, 135.14, 134.72, 130.06, 129.78, 128.86, 128.85, 128.07, 127.80, 119.93, 116.53, 77.24, 77.03, 76.82, 66.94, 66.24, 44.68, 43.64. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{10}H_{11}O_2$, 163.0759; Found 163.0760.

(3) Methyl (*E*)-3-(4-methoxyphenyl)acrylate (**3c**):[1]



^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.66 (d, *J* = 24 Hz, 1H), 7.47 (d, *J* = 6 Hz, 2H), 6.90 (d, *J* = 12 Hz, 2H), 6.31 (d, *J* = 18 Hz, 1H), 3.83 (s, 3H), 3.78 (s, 3H). **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_3$, 193.0865; Found 193.00869.

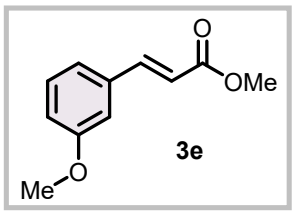
(4) Methyl (*E*)-3-(2-methoxyphenyl)acrylate (**3d**):[1]



^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.01 (d, *J* = 18 Hz, 1H) 7.51 (d, *J* = 6 Hz, 1H), 7.36 (t, *J* = 6 Hz, 1H), 6.97(t, *J* = 6 Hz, 1H), 6.92 (d, *J* = 6 Hz, 1H) 6.54 (d, *J* = 12 Hz, 1H), 3.89 (s, 3H), 3.80 (s, 3H). **^{13}C NMR**

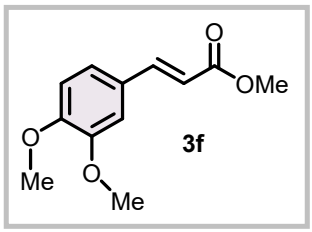
(151 MHz, $CDCl_3$): δ = 167.97, 158.36, 140.30, 131.50, 128.93, 123.38, 120.71, 118.33, 111.15, 55.47, 51.60. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_3$, 193.0865; Found 193.0864.

(5) Methyl (*E*)-3-(3-methoxyphenyl)acrylate (3e):[1]



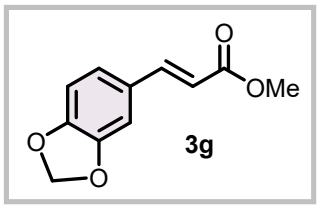
^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 (d, *J* = 18 Hz, 1 H), 7.24(t, *J* = 6 Hz, 1H), 7.05 (d, *J* = 6 Hz, 1H), 6.97(s, 1H), 6.87 (d, *J* = 12 Hz, 1H), 6.37 (d, *J* = 18 Hz, 1H), 3.76 (s, 3H), 3.73 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.99, 158.38, 140.32, 131.51, 128.95, 123.40, 120.74, 118.34, 111.16, 55.49, 51.62. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_3$, 193.0865; Found 193.0865.

(6) Methyl (*E*)-3-(3,4-dimethoxyphenyl)acrylate (3f) (CAS No.: 5396-64-5):



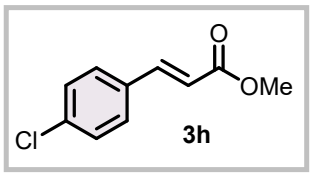
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.65 (d, J = 12 Hz, 1H), 7.11 (d, *J* = 6 Hz, 1H), 7.05 (s, 1H), 6.87 (d, *J* = 6 Hz, 1 H), 6.33 (d, *J* = 18 Hz, 1H), 3.91 (s, 3H), 3.80 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.69, 151.15, 149.22, 144.81, 127.37, 122.62, 115.49, 111.04, 109.64, 55.98, 55.89, 51.63. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{12}H_{15}O_4$, 223.0970; Found 223.0973.

(7) Methyl (*E*)-3-(benzo[d][1,3]dioxol-5-yl)acrylate (3g) (CAS No.: 40918-96-5)**:**



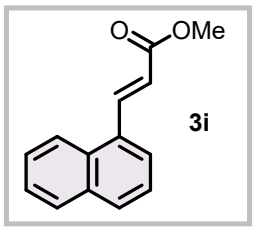
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.61 (d, *J* = 12 Hz, 1H), 7.03 (s, 1H), 7.01 (d, *J* = 6 Hz, 1H), 6.82(d, *J* = 12 Hz, 1H), 6.28 (d, *J* = 18 Hz, 1H), 6.01 (s, 2H), 3.79 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$):** δ = 167.64, 149.63, 148.36, 144.59, 128.83, 124.45, 115.74, 108.56, 106.50, 101.57, 51.64. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{11}O_4$, 207.0657; Found 207.0657.

(8) Methyl (*E*)-3-(4-chlorophenyl)acrylate (**3h**)**:**[1]



^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.65 (d, *J* = 12 Hz, 1H), 7.46 (d, *J* = 6 Hz, 2H), 7.37 (d, *J* = 12 Hz, 2H), 6.43 (d, *J* = 18 Hz, 1H), 3.81 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.21, 143.44, 136.23, 132.88, 129.20, 118.39, 51.81. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{10}H_{10}ClO_2$, 197.0369; Found 197.0365.

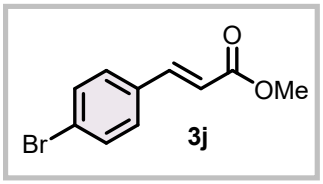
(9) Methyl (*E*)-3-(naphthalen-1-yl)acrylate (**3i**):[1]



^{1}H NMR (600 MHz, $CDCl_3$): δ = 9.26 (d, *J* = 6 Hz, 1H), 8.55 (d, *J* = 12 Hz, 1H), 8.21 (d, *J* = 12 Hz, 1H), 8.12 (d, *J* = 12 Hz, 1H), 8.01(m, 1H), 7.71 (m, 1H), 6.55 (d, *J* = 12 Hz, 1H), 3.86 (s, 3H). **^{13}C NMR (151**

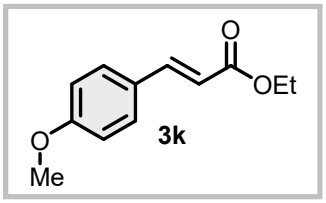
MHz, $CDCl_3$): δ = 167.36, 141.94, 136.69, 135.33, 130.55, 129.10, 128.49, 126.97, 126.25, 125.47, 124.90, 123.40, 120.47, 51.81. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{13}O_2$, 213.0916; Found 213.0915.

(10) Methyl(E)-3-(4-bromophenyl)acrylate (**3j**) (CAS No.: 3650-78-0):



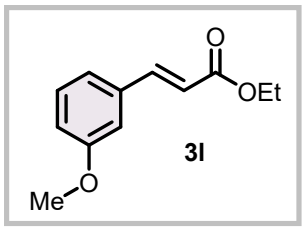
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.63 (d, *J* = 12 Hz, 1H), 7.52 (d, *J* = 6 Hz, 2H), 7.39 (d, *J* = 12Hz, 2H), 6.44(d, *J* = 18 Hz, 1H), 3.81 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.17, 143.49, 133.29, 132.15, 129.44, 124.56, 118.49, 51.81. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{10}H_{10}BrO_2$, 240.9864; Found 240.9861.

(11) Ethyl (*E*)-3-(4-methoxyphenyl)acrylate (**3k**):[2]



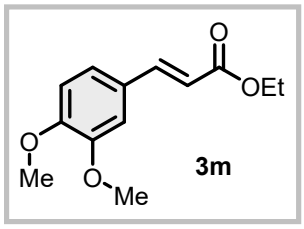
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.66 (d, *J* = 18 Hz, 1H), 7.48 (d, *J* = 6 Hz, 2H), 6.91 (d, *J* = 6 Hz, 2H), 6.32 (d, *J* = 18 Hz, 1H), 4.27 (q, *J* = 6 Hz, 2H), 3.84 (s, 3H), 1.34 (t, *J* = 6 Hz, 3H). **^{13}C NMR (151MHz, $CDCl_3$)**: δ = 167.38, 161.34, 144.26, 129.70, 127.22, 115.77, 114.39, 60.34, 55.38, 14.36. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{12}H_{15}O_3$, 207.1021; Found 207.1025.

(12) Ethyl (*E*)-3-(3-methoxyphenyl)acrylate (**3l**):[3]



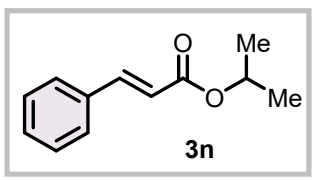
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.66 (d, *J* = 12 Hz, 1H), 7.31 (t, *J* = 6 Hz, 1H), 7.12 (d, *J* = 6Hz, 1H), 7.04 (s, 1H), 6.94 (d, *J* = 12 Hz, 1H), 6.44 (t, *J* = 18 Hz, 1H), 4.28 (q, *J* = 6 Hz, 2H), 3.83 (s, 3H), 1.35(t, *J* = 6 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$):** δ = 166.98, 159.90, 144.53, 135.84, 129.88, 120.78, 118.58, 116.13, 112.89, 60.55, 55.30, 14.33. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{12}H_{15}O_3$, 207.1021; Found 207.1020.

(13) Ethyl (*E*)-3-(3,4-dimethoxyphenyl)acrylate (**3m**) (CAS No.: 20583-78-2):



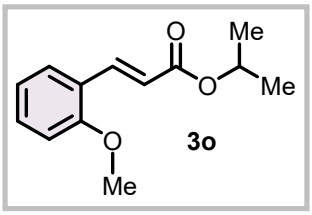
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.64 (d, *J* = 6 Hz, 1H), 7.11 (dd, *J* = 6 Hz, 1H), 7.06 (d, *J* = 6 Hz, 1H), 6.88 (d, *J* = 12 Hz, 1H), 6.33 (d, *J* = 18 Hz, 1H), 4.28, (q, *J* = 6 Hz, 1H), 3.91 (s, 6H), 1.35 (t, *J* = 6 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.27, 151.08, 149.21, 144.53, 127.46, 122.58, 115.97, 111.03, 109.58, 60.39, 55.97, 55.88, 14.36. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{17}O_4$, 237.1127; Found 237.1131.

(14) Isopropyl cinnamate (**3n**) (CAS No.: 7780-06-5):



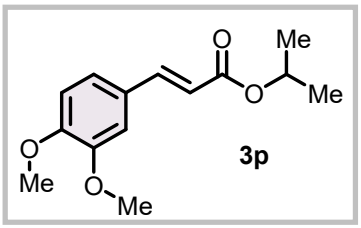
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.68 (d, *J* = 18 Hz, 1H), 7.53 (d, *J* = 6 Hz, 2H), 7.38 (m, 3H), 6.43 (d, *J* = 18 Hz, 1H), 5.17 (sept. *J* = 6 Hz, 1H), 1.32 (d, *J* = 6 Hz, 6 H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.56, 144.33, 134.55, 130.15, 128.87, 128.03, 118.82, 67.83, 21.95. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{12}H_{15}O_2$, 191.1072; Found 191.1070.

(15) Isopropyl (*E*)-3-(2-methoxyphenyl)acrylate (**3o**):



^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.91 (d, *J* = 18 Hz, 1H), 7.44 (d, *J* = 6 Hz, 1H), 7.28 (d, *J* = 6 Hz, 1H), 6.90 (t, *J* = 6 Hz, 1H), 6.87 (t, *J* = 6 Hz, 1H), 6.45 (d, *J* = 18 Hz, 1H), 5.10 (sept., *J* = 6 Hz, 1H), 3.82 (s, 3H), 1.25 (d, *J* = 6 Hz, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.05, 157.28, 138.72, 130.18, 127.90, 122.51, 119.64, 118.33, 110.07, 66.54, 54.43, 20.94. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{17}O_3$, 221.1178; Found 221.1175.

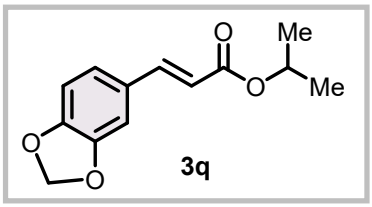
(16) Isopropyl (*E*)-3-(3,4-dimethoxyphenyl)acrylate (**3p**):



^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.62 (d, *J* = 6 Hz, 1H), 7.11 (d, *J* = 12 Hz, 1H), 7.06 (s, 1H), 6.87 (d, *J* = 6 Hz, 1H), 6.31 (d, *J* = 18 Hz, 1H), 5.17 (sept., *J* = 6 Hz, 1H), 3.91 (s, 6H), 1.32 (d, *J* = 6 Hz, 1H). **^{13}C NMR (151 MHz, $CDCl_3$)**: **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.78, 151.01, 149.19, 144.26, 127.53,

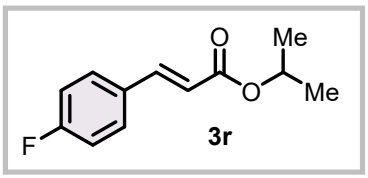
122.56, 116.51, 111.02, 109.53, 67.64, 55.97, 55.87, 21.99. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{19}O_4$, 251.1283; Found 251.1282.

(17) Isopropyl (*E*)-3-(benzo[d][1,3]dioxol-5-yl)acrylate (**3q**):



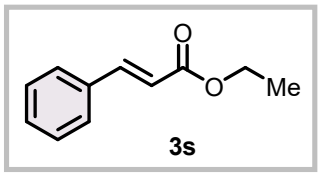
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.58 (d, *J* = 6 Hz, 1H), 7.03 (s, 1H), 7.01 (d, *J* = 12 Hz, 1H), 6.81 (d, *J* = 6 Hz, 1H), 6.25 (d, *J* = 12 Hz, 1H), 5.16(septet, *J* = 6 Hz, 1H), 1.31 (d, *J* = 6 Hz, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.73, 149.49, 148.32, 144.02, 128.99, 124.31, 116.78, 108.53, 106.49, 101.52, 67.68, 21.97. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{15}O_4$, 235.0970; Found 235.0970.

(18) Isopropyl (*E*)-3-(4-fluorophenyl)acrylate (**3r**):



^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.64 (d, *J* = 18 Hz, 1H), 7.52 (m, 2H), 7.08 (t, *J* = 6 Hz, 2H), 6.35 (d, *J* = 6 Hz, 1H), 5.16 (q, *J* = 6 Hz, 1H), 1.32 (d, *J* = 6 Hz, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.42, 164.66 (d, $J_{C\text{-}F}$ = 250.66 Hz), 143.01, 130.80, 129.89, 129.84, 118.58, (d, $J_{C\text{-}F}$ = 157.04 Hz), 67.90, 21.94. **^{19}F NMR Spectrum (376 MHz, $CDCl_3$)**: δ = -117.40 (s, 1F). **HRMS (QTOF) m/z:** [M+H] calcd for $C_{12}H_{14}FO_2$, 209.0978; Found 209.0980.

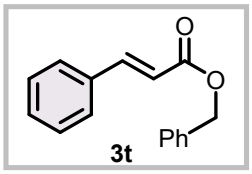
(19) Ethyl cinnamate (**3s**):[3]



3s

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 12 Hz, 1H), 7.53 (d, *J* = 6 Hz, 2H), 7.38 (s, 3H), 6.45 (d, *J* = 12 Hz, 1H), 4.29 (q, *J* = 12 Hz, 2H), 1.35 (t, *J* = 6 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.04, 144.61, 134.49, 130.23, 128.89, 128.06, 118.29, 60.53, 14.33. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_2$, 177.0916; Found 177.0920.

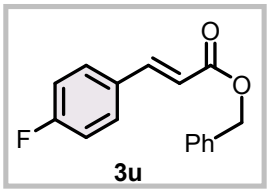
(20) Benzyl cinnamate (**3t**):[4]



3t

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.67 (d, *J* = 18 Hz, 1H), 7.45-7.44 (m, 2H), 7.35-7.33 (m, 2H), 7.33-7.18 (m, 5H), 6.43 (d, *J* = 18 Hz, 1H), 5.18 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.84, 145.22, 136.07, 134.38, 130.30, 128.92, 128.62, 128.30, 128.28, 128.13, 117.89, 77.25, 77.04, 76.83, 66.39. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{16}H_{15}O_2$, 239.1072; Found 239.1070.

(21) Benzyl(*E*)-3-(4-fluorophenyl)acrylate (**3u**):

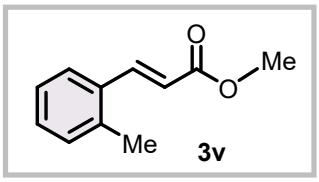


3u

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 18 Hz, 1H), 7.51-7.49 (m, 2H), 7.44-7.35 (m, 5H), 7.08 (t, *J* = 6 Hz, 2H), 6.42 (d, *J* = 18 Hz, 1H), 5.25 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$):** δ = 166.71, 164.79 (d, *J* = 252 Hz), 143.89, 140.88, 136.01, 129.97, 128.63, 128.31, 127.01, 117.65, 116.15 (d, *J* = 22 Hz), 66.44.

^{19}F NMR Spectrum (376 MHz, $CDCl_3$): δ = -123.90 (s, 1F). **HRMS (QTOF) m/z:** [M+H] calcd for $C_{16}H_{14}FO_2$, 257.0978; Found 257.0978.

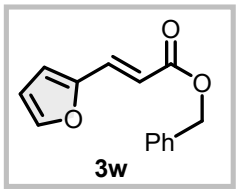
(22) Methyl(*E*)-3-(*o*-tolyl)acrylate (**3v**):[1]



3v

^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.00 (d, *J* = 18 Hz, 1H), 7.55 (d, *J* = 6 Hz, 1H), 7.29 (t, *J* = 12 Hz, 1H), 7.22(t, *J* = 6 Hz, 2H), 6.38 (d, *J* = 18 Hz, 1H), 3.81 (s, 3H), 2.44 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.52, 142.58, 137.68, 133.38, 130.81, 130.05, 126.41, 126.35, 118.85, 51.71, 19.81. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{11}H_{13}O_2$, 177.0916; Found 177.0915.

(23) Benzyl (*E*)-3-(furan-2-yl)acrylate (**3w**):[4]

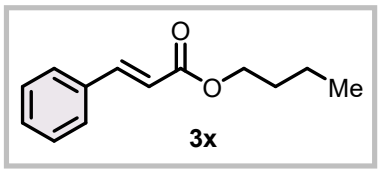


3w

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.48-7.36 (m, 6 H), 7.34(t, *J* = 6 Hz, 1H), 6.61 (s, 1H), 6.46 (s, 1H), 6.38 (d, *J* = 18 Hz, 1H), 5.23 (s, 2H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 166.89, 150.89, 144.84,

136.12, 131.49, 128.58, 128.21, 115.52, 114.94, 112.30, 66.30. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{13}O_3$, 229.0865; Found 229.0861.

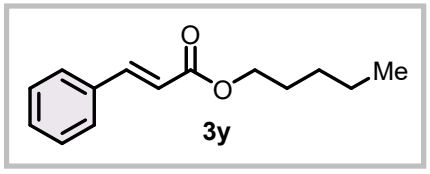
(24) Butyl cinnamate (**3x**):[5]



3x

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.70 (d, *J* = 18 Hz, 1H), 7.53(d, *J* = 6 Hz, 2H), 7.39 (d, *J* = 6 Hz, 3H), 6.46 (d, *J* = 18 Hz, 1H), 4.22 (t, *J* = 6 Hz, 2H), 1.72- 1.67 (m, 2H), 1.47-1.41 (m, 2H), 0.98 (t, *J* = 6 Hz, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.14, 144.57, 134.49, 130.22, 128.88, 128.06, 118.31, 64.46, 30.79, 19.21, 13.76. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{17}O_2$, 205.1229; Found 205.1225.

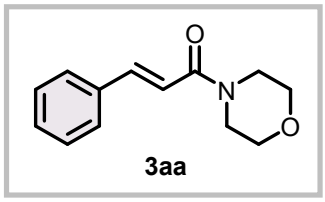
(25) Pentyl cinnamate (**3y**) (CAS 3487-99-8):



3y

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.61 (d, *J* = 12 Hz, 1H), 7.45 (d, *J* = 6 Hz, 2H), 7.29 (s, 3H), 6.37 (d, *J* = 12 Hz, 1H), 4.17-3.92 (m, 2H), 1.73-1.65 (m, 1H), 1.54 (q, *J* = 6 Hz, 1H), 1.45-1.13 (m, 1H), 0.90- 0.85 (m, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 167.11, 144.57, 134.49, 130.22, 128.88, 128.07, 118.32, 69.22, 63.24, 37.45, 34.27, 26.11, 25.14, 22.52, 16.47, 11.27. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{19}O_2$, 219.1385; Found 219.1383.

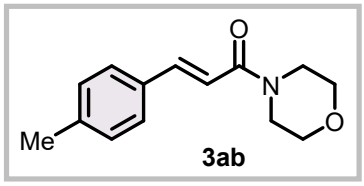
(26) (*E*)-1-Morpholino-3-phenylprop-2-en-1-one (**3aa**) (CAS No. 16619-19-5):



3aa

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.71 (d, *J* = 6 Hz, 1H), 7.66 (d, *J* = 12 Hz, 0.6 H), 7.53 (d, *J* = 12 Hz, 3H), 7.38 (d, *J* = 12 Hz, 5H), 6.86 (d, *J* = 18 Hz, 1H), 6.49 (d, *J* = 18 Hz, 1 H), 3.81-3.74 (m, 8H), 3.71-3.70 (m, 8 H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.64, 144.47, 143.29, 135.14, 134.72, 130.06, 129.78, 128.86, 128.07, 127.80, 119.93, 116.53, 66.89, 66.24, 44.68, 43.64. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{16}NO_2$, 218.1181; Found 218.1180.

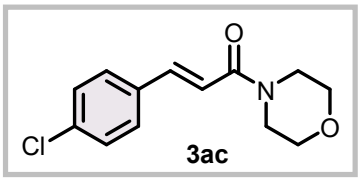
(27) (*E*)-1-Morpholino-3-(*p*-tolyl)prop-2-en-1-one (**3ab**):



3ab

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.69 d, *J* = 18 Hz, 1H), 7.43 (d, *J* = 12 Hz, 2H), 7.19 (d, *J* = 6 Hz, 2H), 6.81 (d, *J* = 18 Hz, 1H), 3.73-3.70 (m, 8 H), 2.37 (s, 3H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.80, 143.28, 140.10, 132.38, 129.56, 127.79, 115.39, 66.89, 43.64, 21.43. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{18}NO_2$, 232.1338; Found 231.1337.

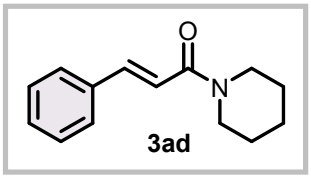
(28) (*E*)-3-(4-Chlorophenyl)-1-morpholinoprop-2-en-1-one (**3ac**):



3ac

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.66 (d, *J* = 18 Hz, 1H), 7.46 (d, J = 12 Hz, 2H), 7.35 (d, *J* = 6 Hz, 2H), 6.83 (d, *J* = 18 Hz, 1H), 3.73-3.65 (m, 8H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.30, 141.87, 135.60, 133.62, 129.10, 128.97, 117.09, 66.85, 46.28, 42.53. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{13}H_{14}ClNO_2$, 251.0713; Found 251.0712.

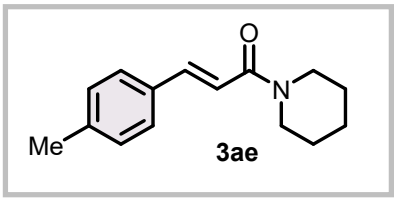
(29) (*E*)-3-Phenyl-1-(piperidin-1-yl)prop-2-en-1-one (**3ad**) (CAS No.: 27845-72-3):



3ad

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.65 (d, *J* = 12 Hz, 1H), 7.52 (d, *J* = 6 Hz, 2H), 7.38-7.32 (m, 3H), 6.92 (d, *J* = 18 Hz, 1H), 3.67 (d, *J* = 48 Hz, 4H), 1.72-1.62 (m, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.38, 142.14, 135.52, 129.41, 128.76, 127.69, 117.78, 47.04, 43.36, 26.77, 25.62, 24.66. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{14}H_{18}NO$, 216.1388; Found 216.1391.

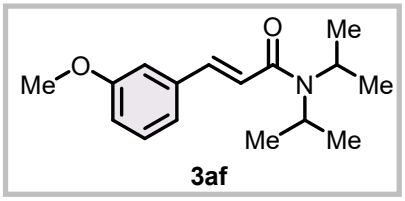
(30) (*E*)-1-(Piperidin-1-yl)-3-(*p*-tolyl)prop-2-en-1-one (3ae):



3ae

^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.63 (d, *J* = 12 Hz, 1H), 7.42 (d, *J* = 6 Hz, 2H), 7.18 (d, *J* = 12 Hz, 2H), 6.87 (d, *J* = 18 Hz, 1H), 3.66 (d, *J* = 48 Hz, 4H), 2.36 (s, 3H), 1.68-1.62 (m, 6H). **^{13}C NMR (151 MHz, $CDCl_3$)**: δ = 165.56, 142.18, 139.65, 132.76, 129.48, 127.67, 116.64, 47.02, 43.35, 26.77, 25.63, 24.68, 21.40. **HRMS (QTOF) m/z:** [M+H] calcd for $C_{15}H_{20}NO$, 230.1545; Found 230.1545.

(31) (*E*)-*N*,*N*-Diisopropyl-3-(3-methoxyphenyl)acrylamide (**3af**):



3af

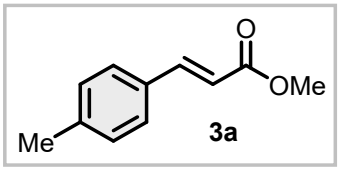
^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.50 (d, *J* = 18 Hz, 1H), 7.23 (t, *J* = 12 Hz, 1H), 7.04 (d, *J* = 6 Hz, 1H), 6.96 (s, 1H), 6.82 (d, *J* = 6 Hz, 1H), 6.75 (d, *J* = 12 Hz, 1H), 4.10-3.95 (m, 1H), 3.76 (s, 3H), 3.58 (d, *J* = 3 Hz, 1H), 1.33-1.22 (m, 12H). **HRMS (QTOF) m/z:** [M+H] calcd for $C_{16}H_{24}NO_2$, 262.1807; Found 262.1805.

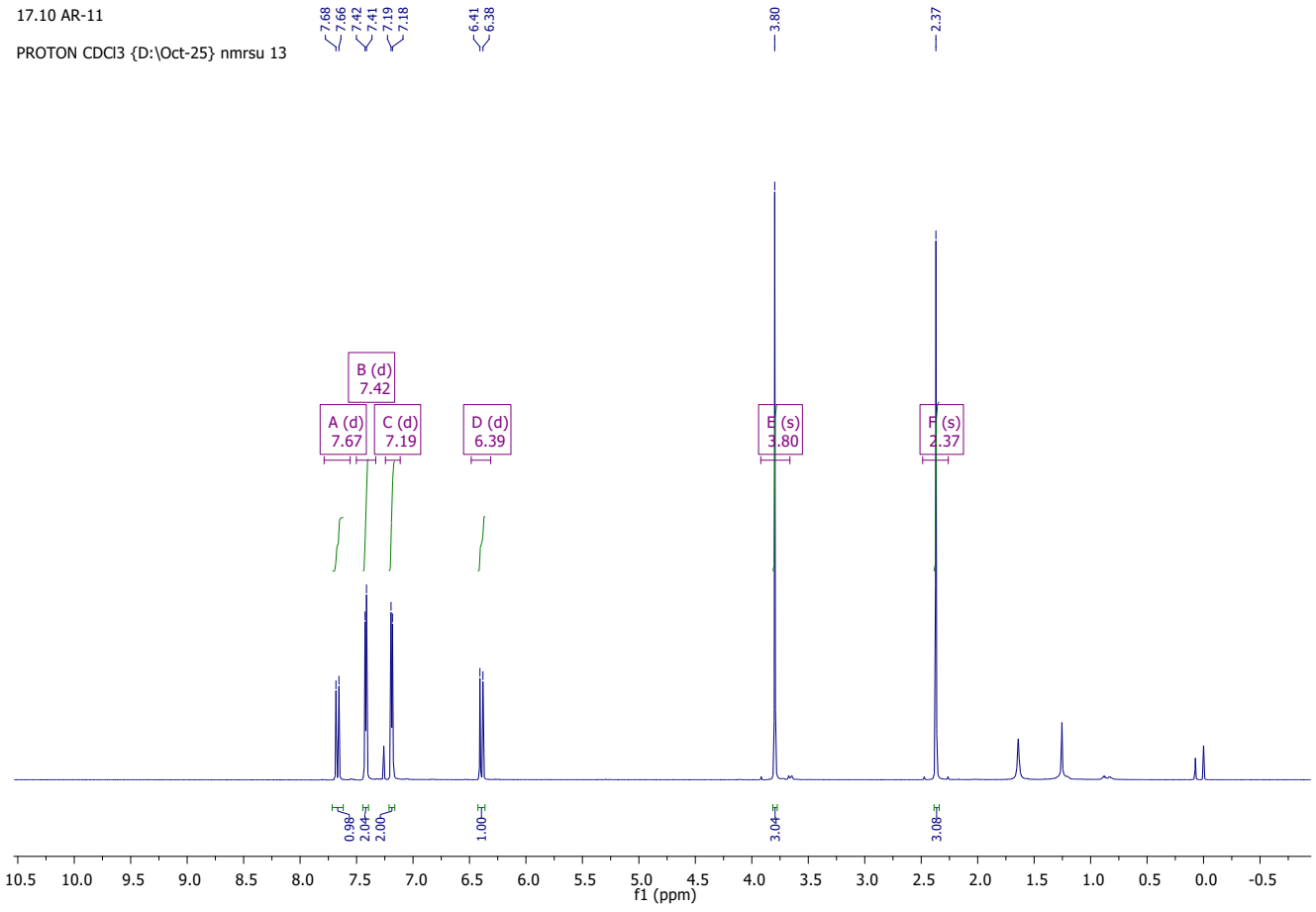
V. References:

1. P. Sun, Y. Zhu, H. Yang, H. Yan, L. Lu, X. Zhang and J. Mao, *Org. Biomol. Chem.*, 2012, **10**, 4512.
2. S. Hegde, A. Nizam and A. Vijayan, *New J. Chem.*, 2024, **48**, 1121.
3. L. Li, Z. Ma, C. Li, G. Chen and T. Gao, *New J. Chem.*, 2024, **48**, 16642.
4. A. R. Katritzky, S. Zhang, A. Soares and M. Wang, *ARKIVOC*, 2001, 54-57.
5. S. Liu, T. Fukuyama, M. Sato, I. Ryu, *Org. Proc. Res. Dev.*, 2004, **8**, 477.

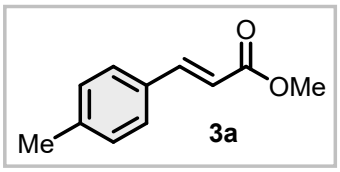
VI. Copies of ^{1}H, ^{13}C & ^{19}F NMR spectra of the Products 3.

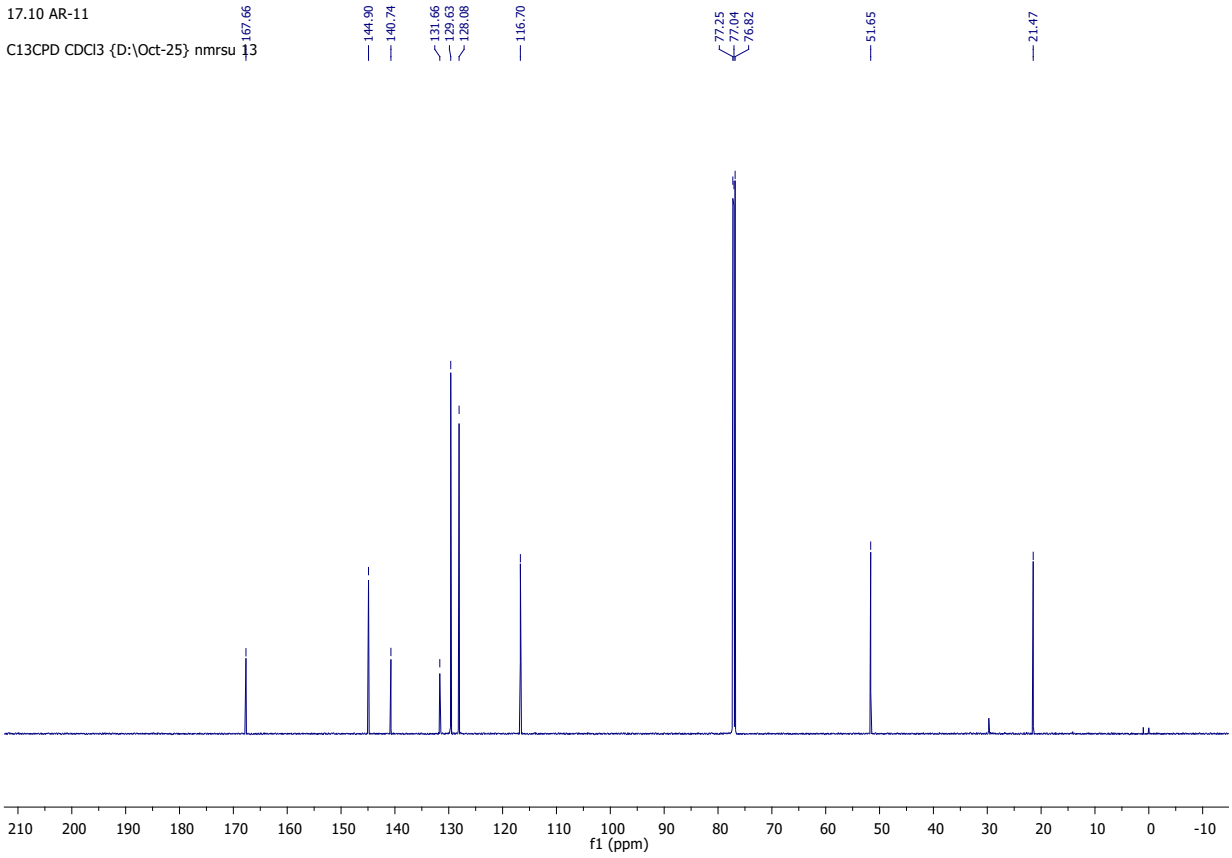
Compound 3a. ^{1}H NMR Spectrum ($CDCl_3$).



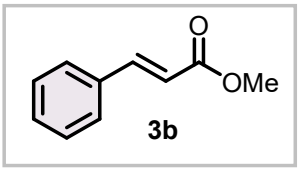


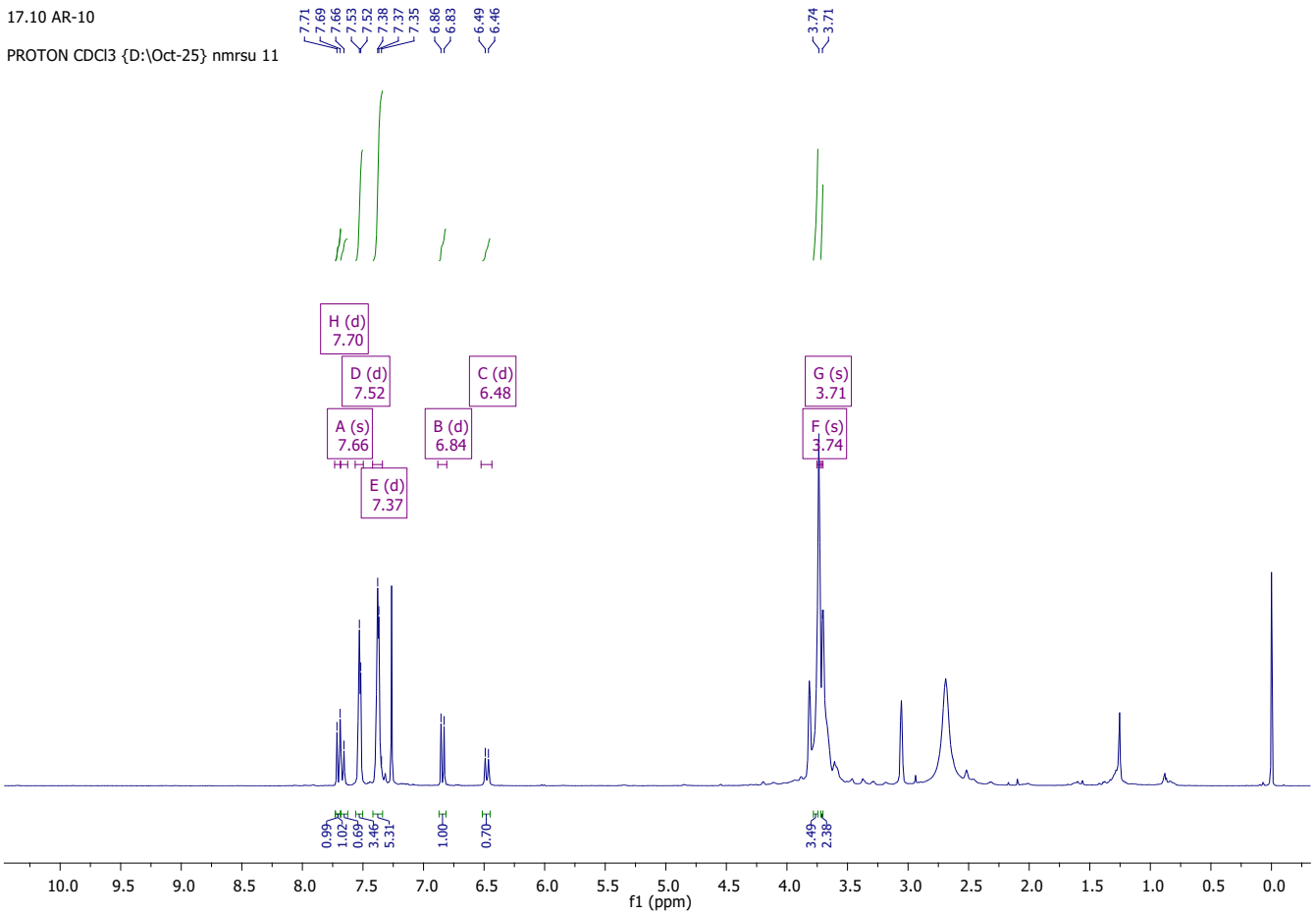
Compound 3a. ^{13}C NMR Spectrum ($CDCl_3$).



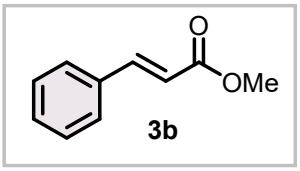


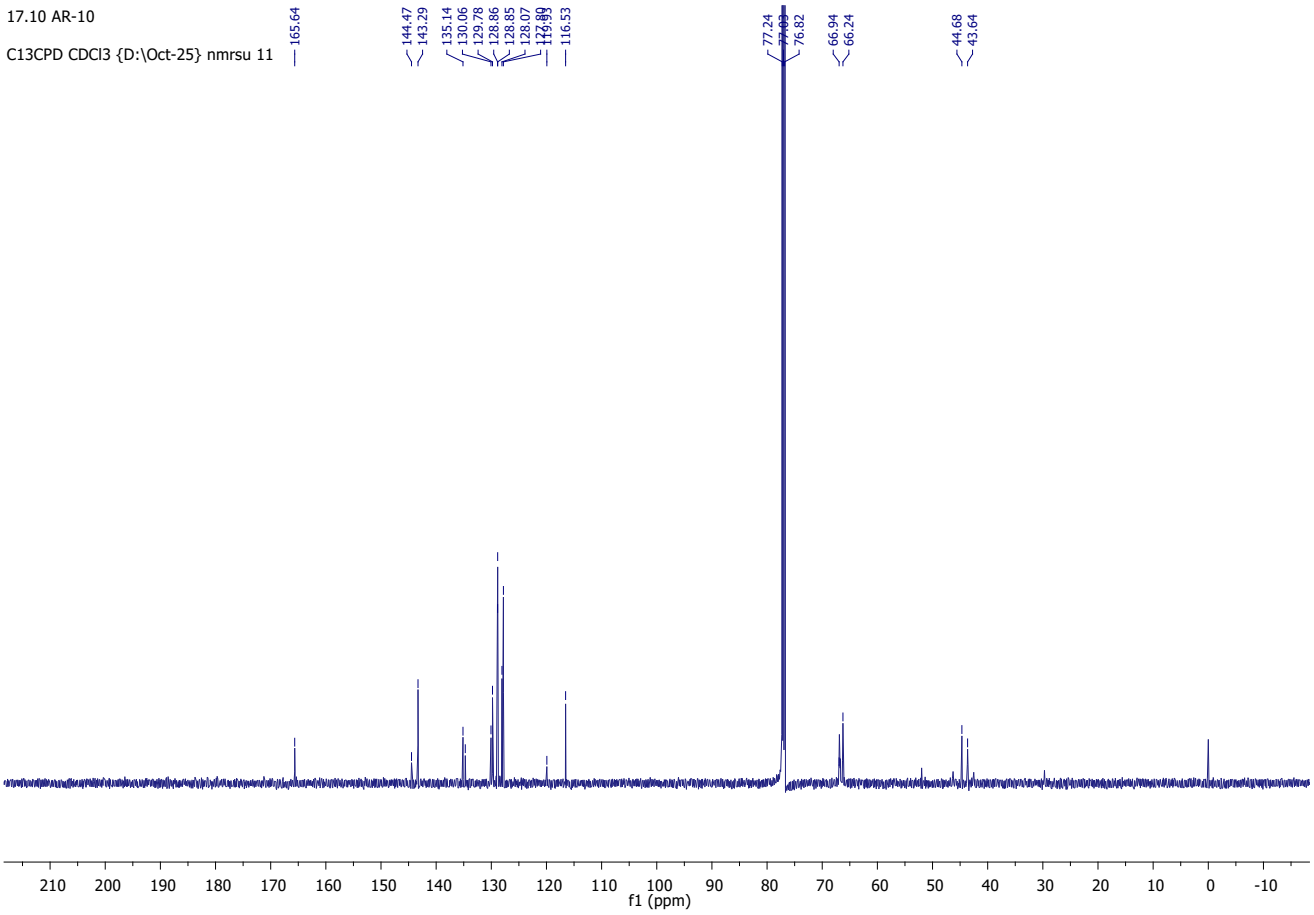
Compound 3b. ^{1}H NMR Spectrum ($CDCl_3$).



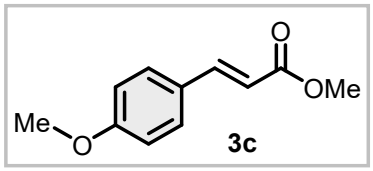


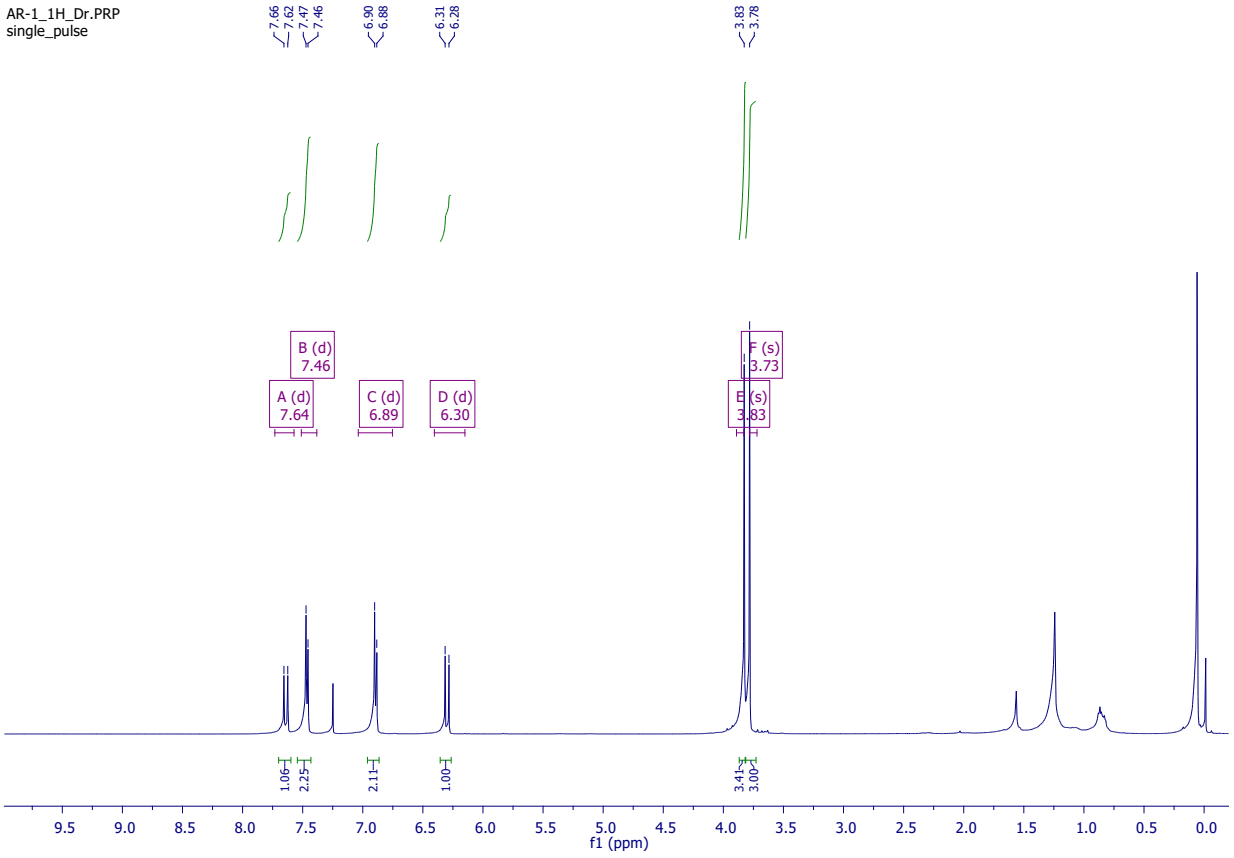
Compound 3b. ^{13}C NMR Spectrum ($CDCl_3$).



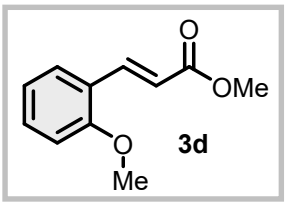


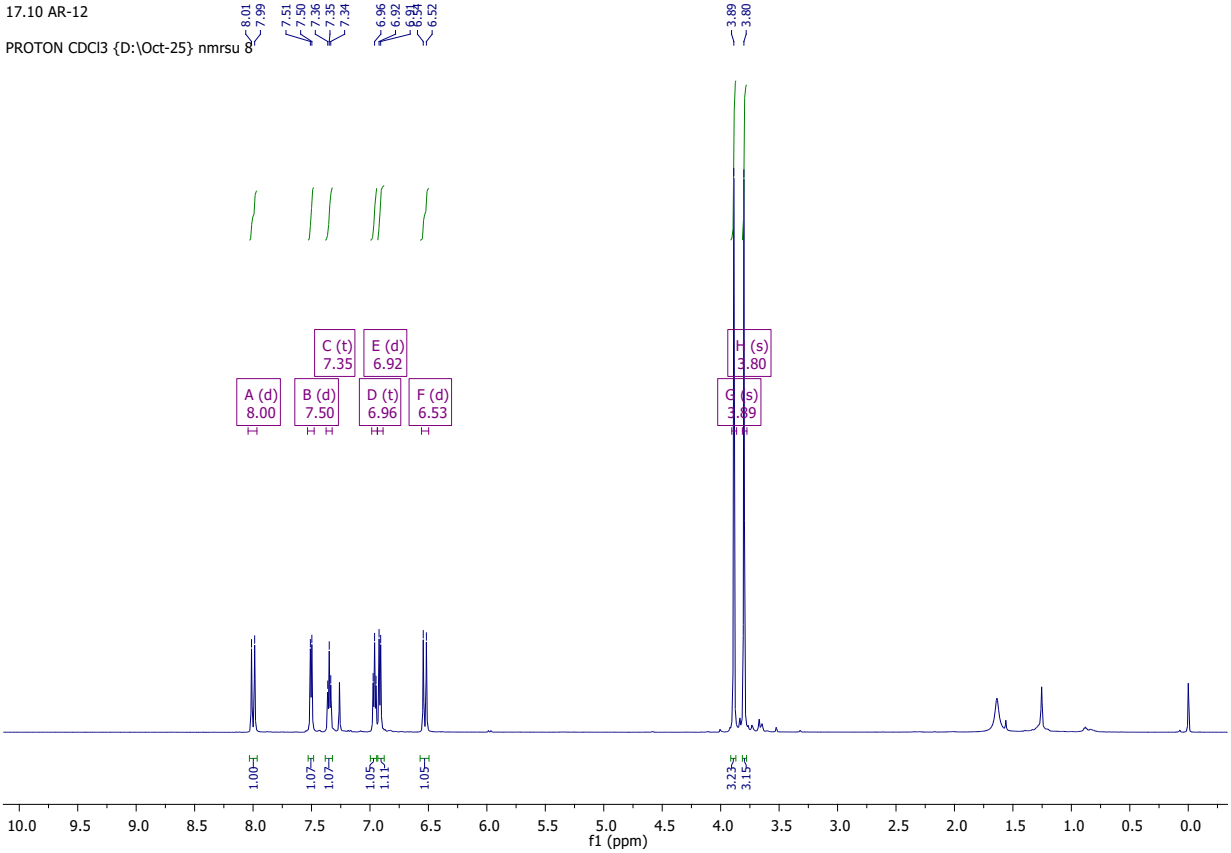
Compound 3c. ^{1}H NMR Spectrum ($CDCl_3$).



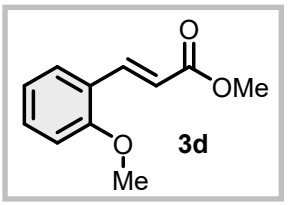


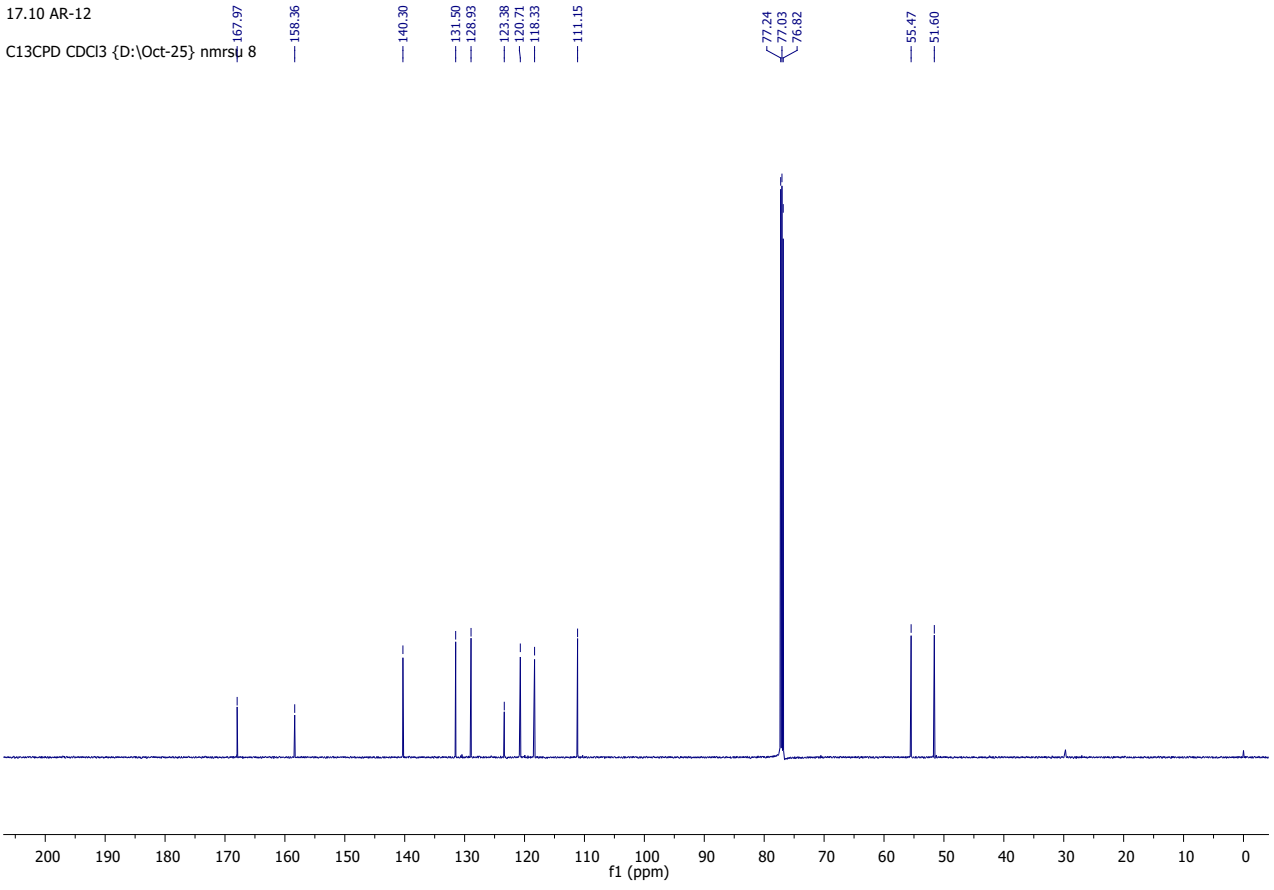
Compound 3d. ^{1}H NMR Spectrum ($CDCl_3$).



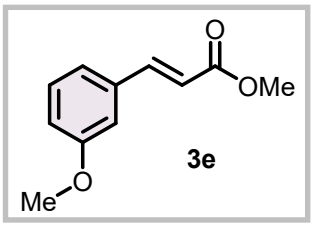


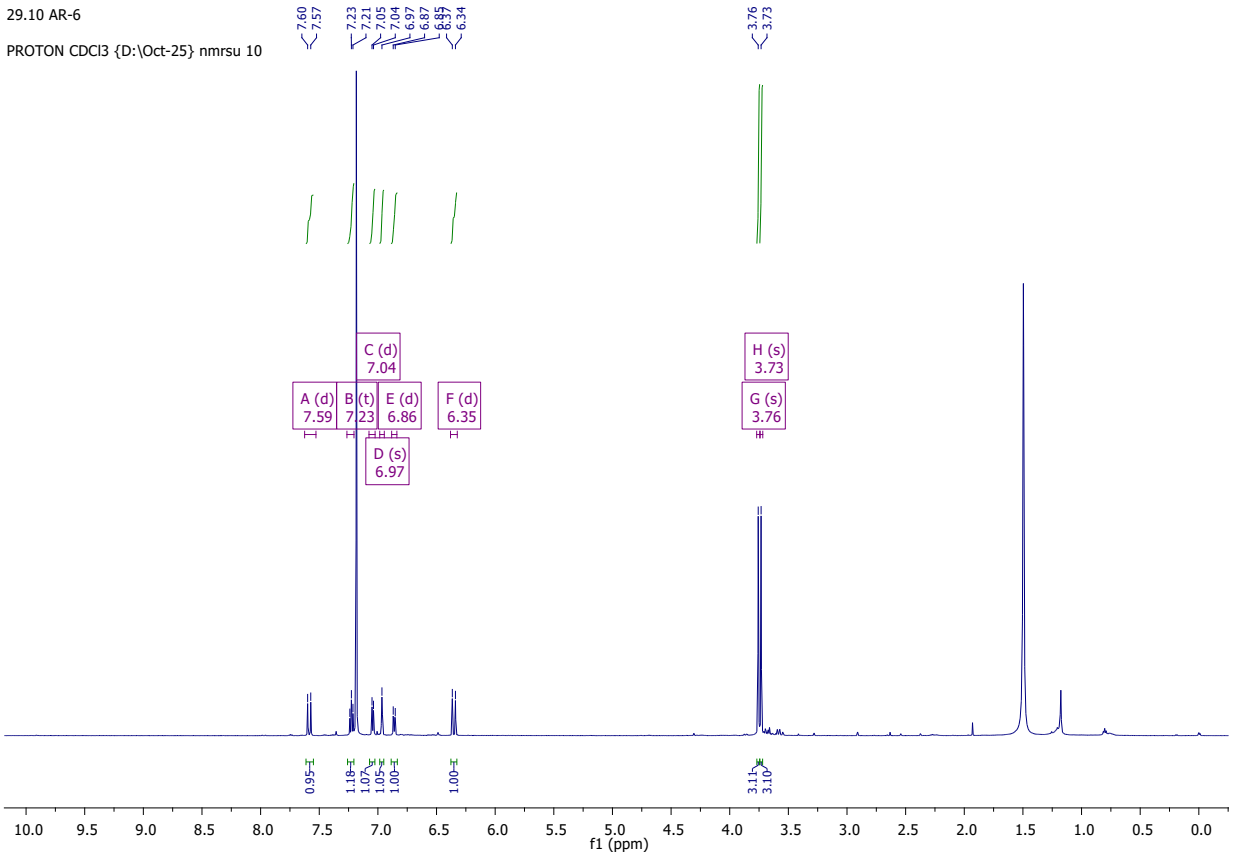
Compound 3d. ^{13}C NMR Spectrum ($CDCl_3$).



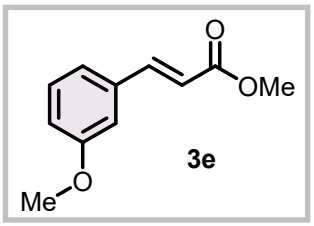


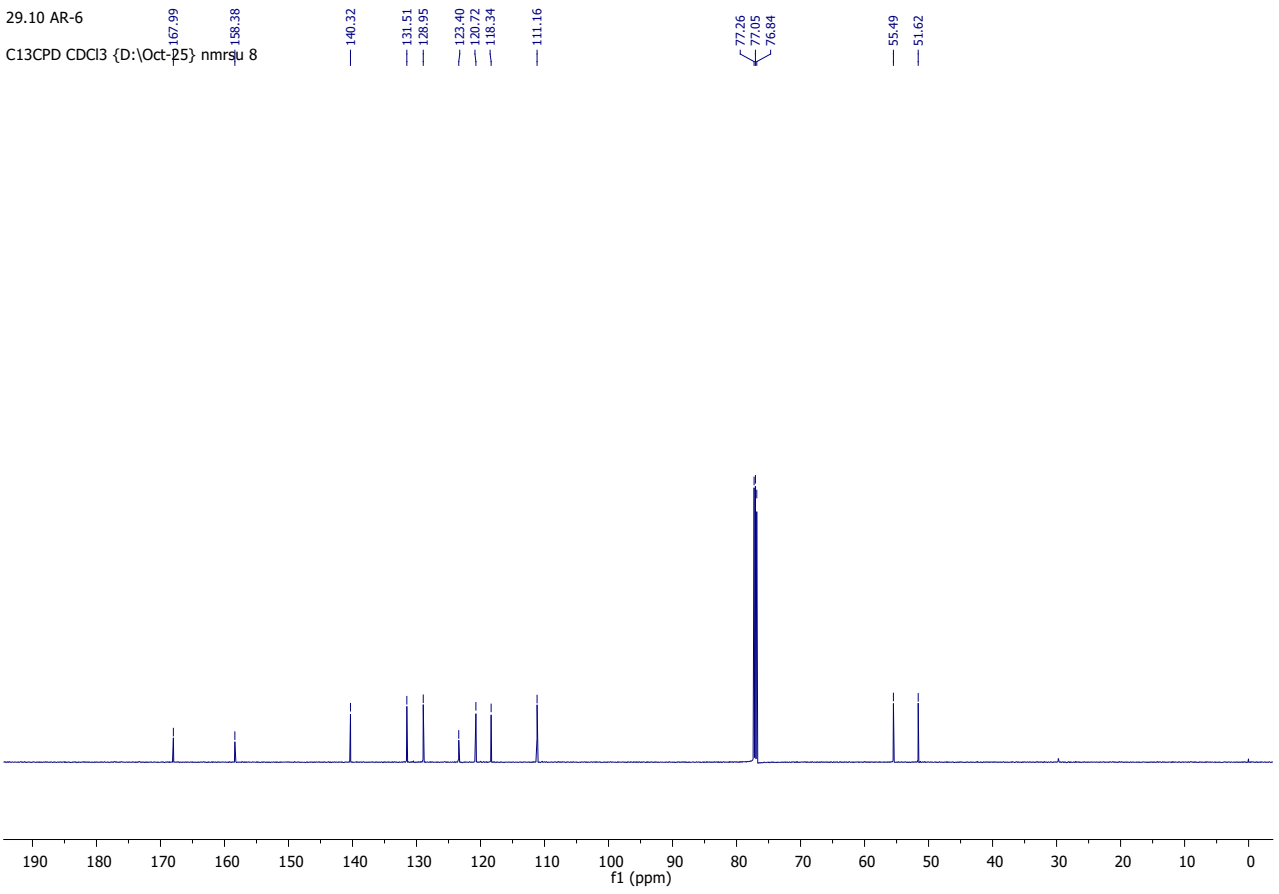
Compound 3e. ^{1}H NMR Spectrum ($CDCl_3$).



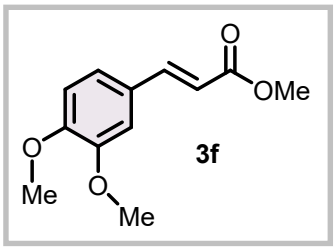


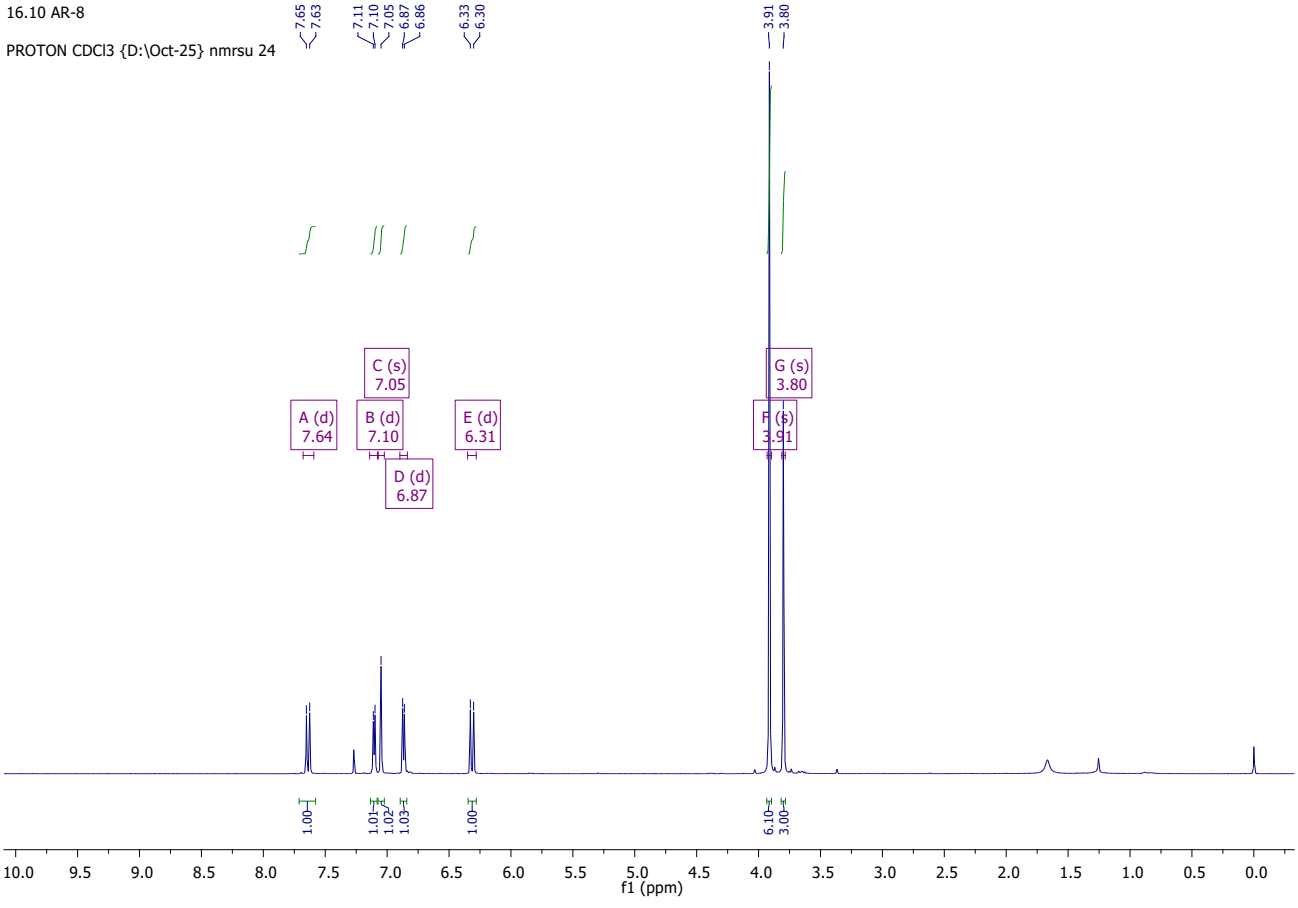
Compound 3e. ^{13}C NMR Spectrum ($CDCl_3$).



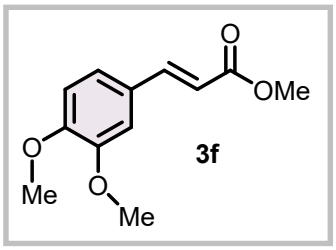


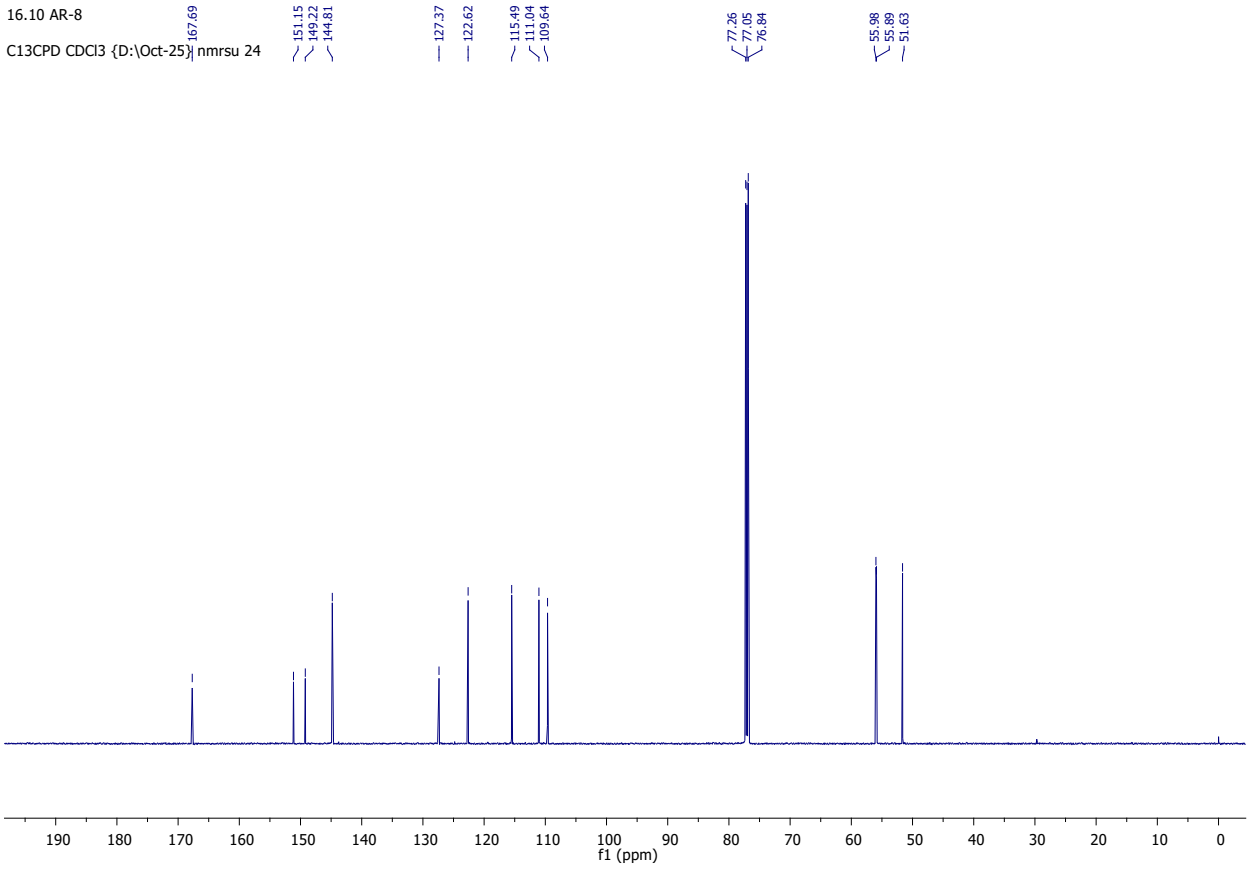
Compound 3f. ^{1}H NMR Spectrum ($CDCl_3$).



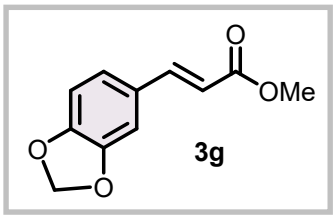


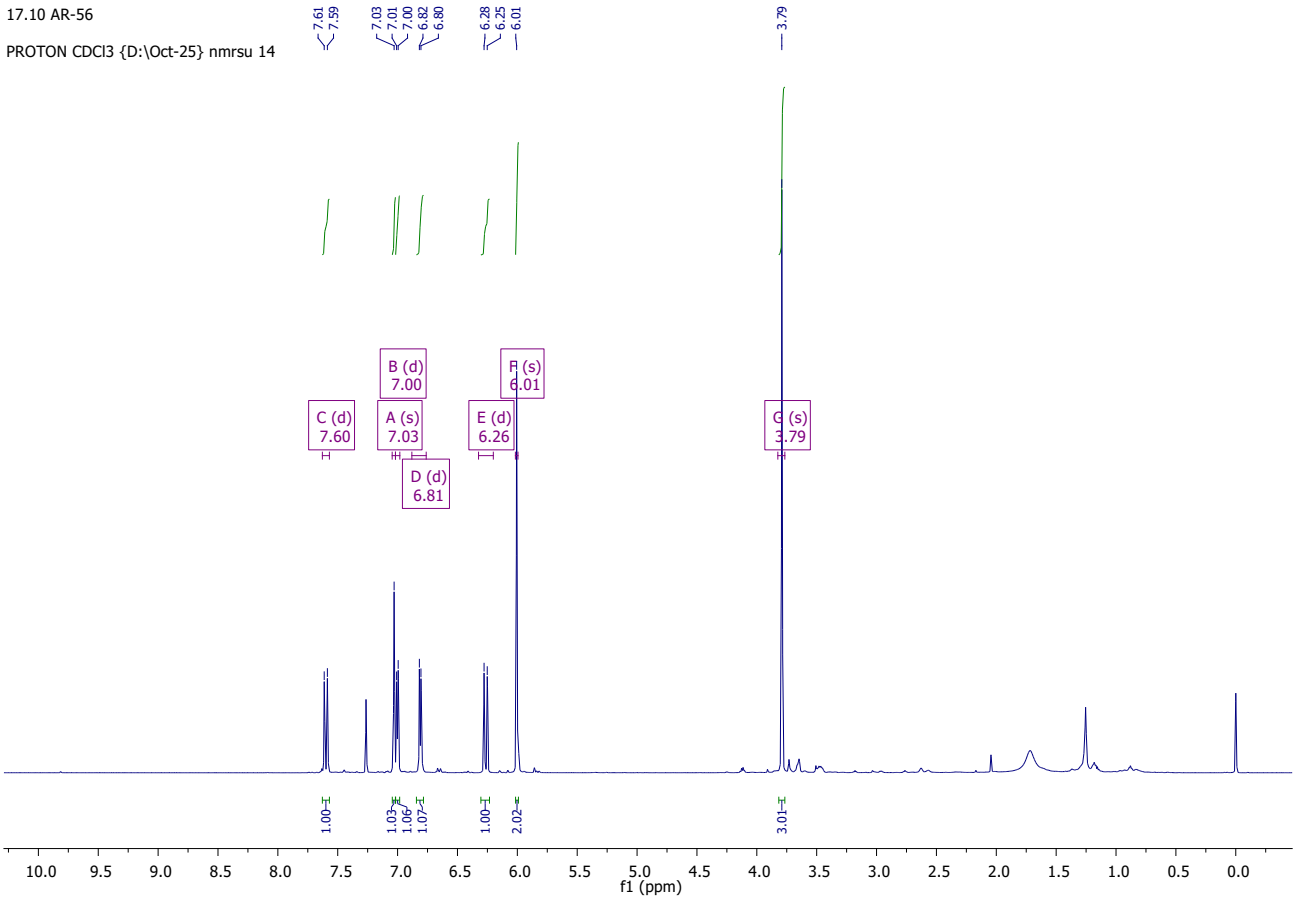
Compound 3f. ^{13}C NMR Spectrum ($CDCl_3$).



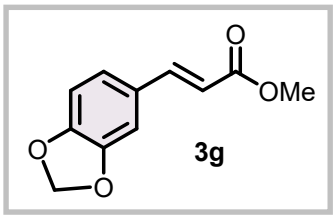


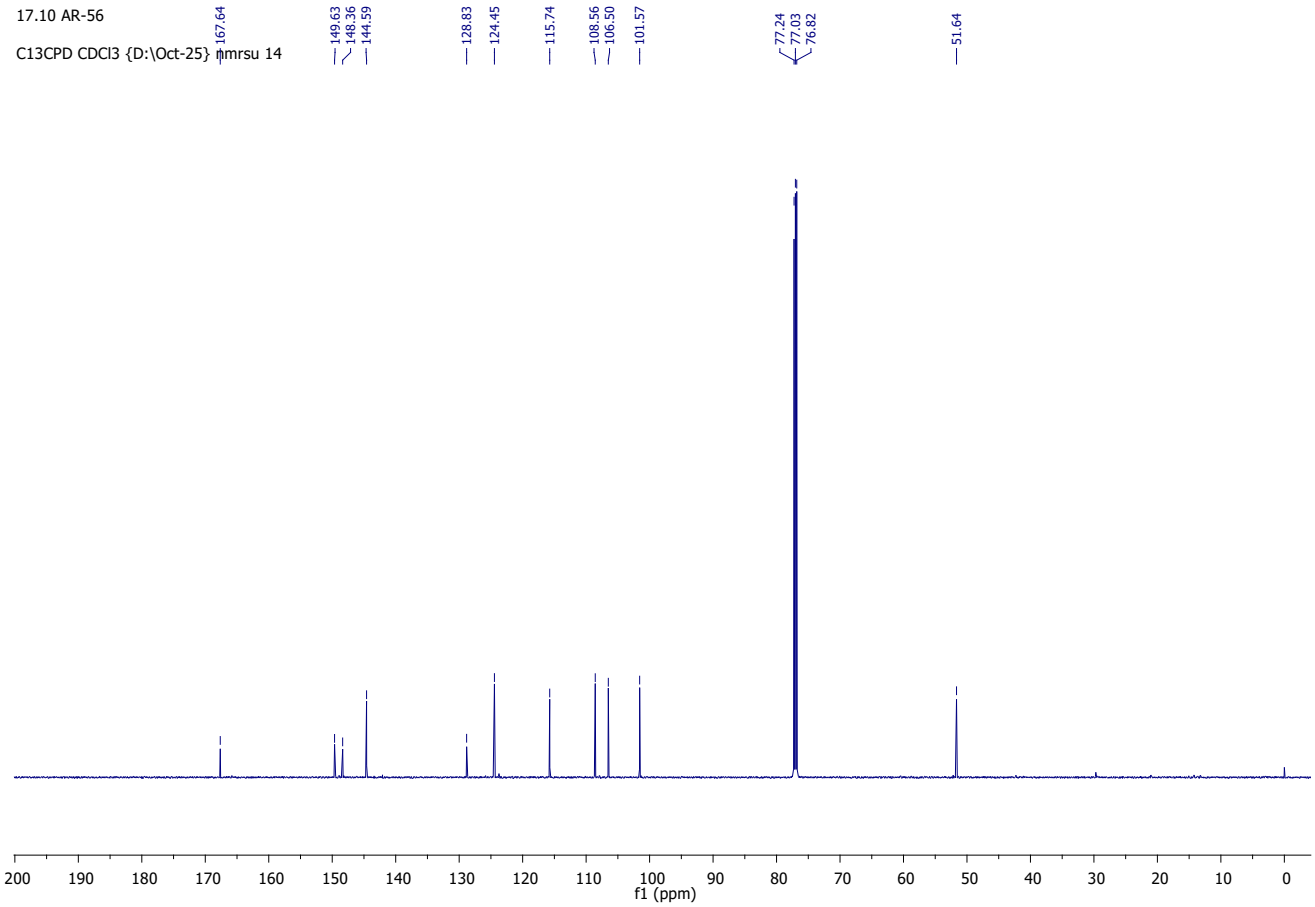
Compound 3g. ^{1}H NMR Spectrum ($CDCl_3$).



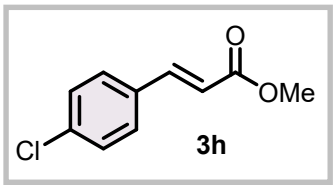


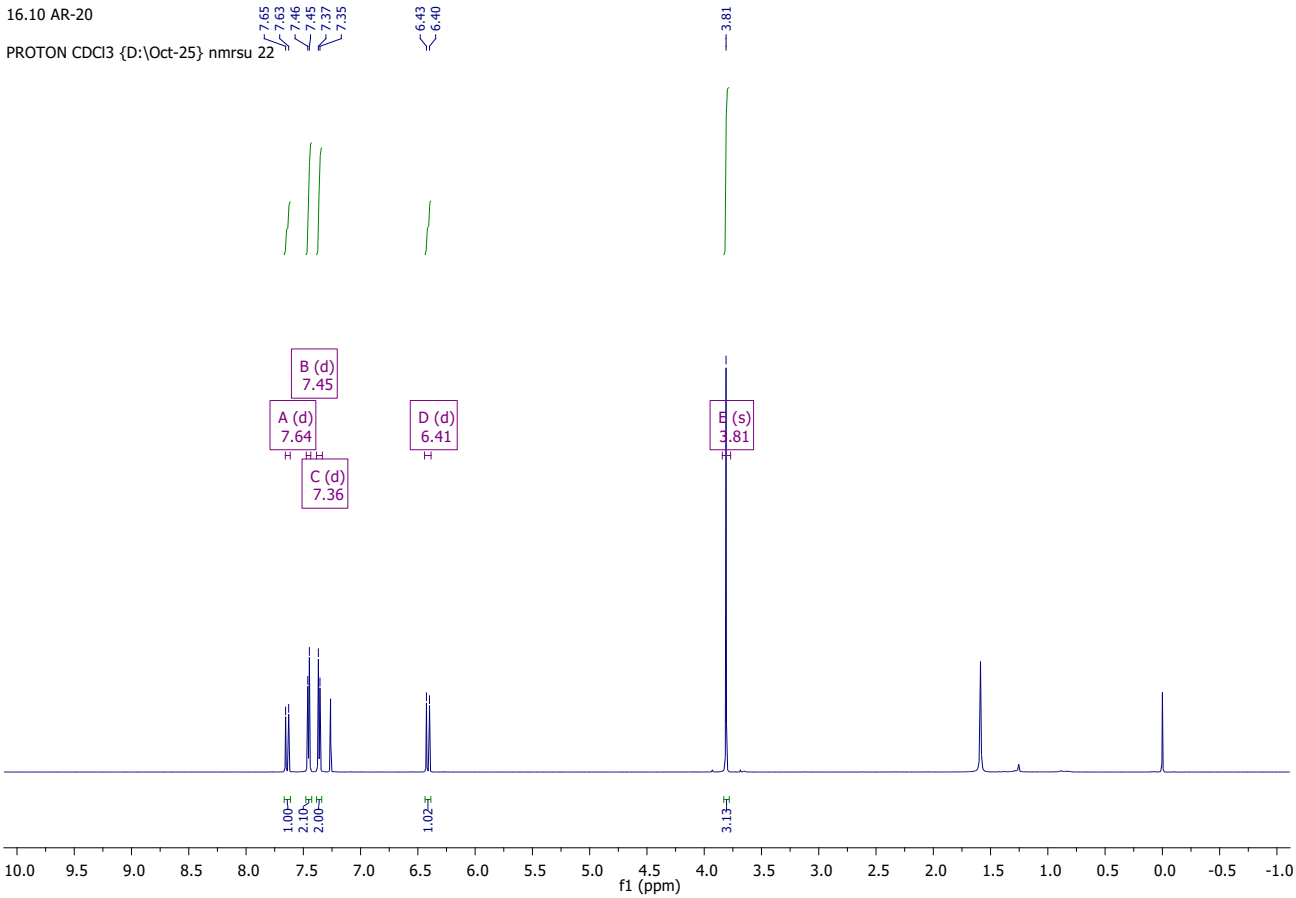
Compound 3g. ^{13}C NMR Spectrum ($CDCl_3$).



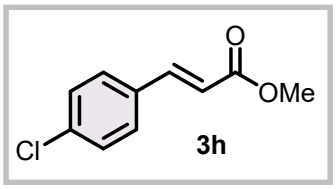


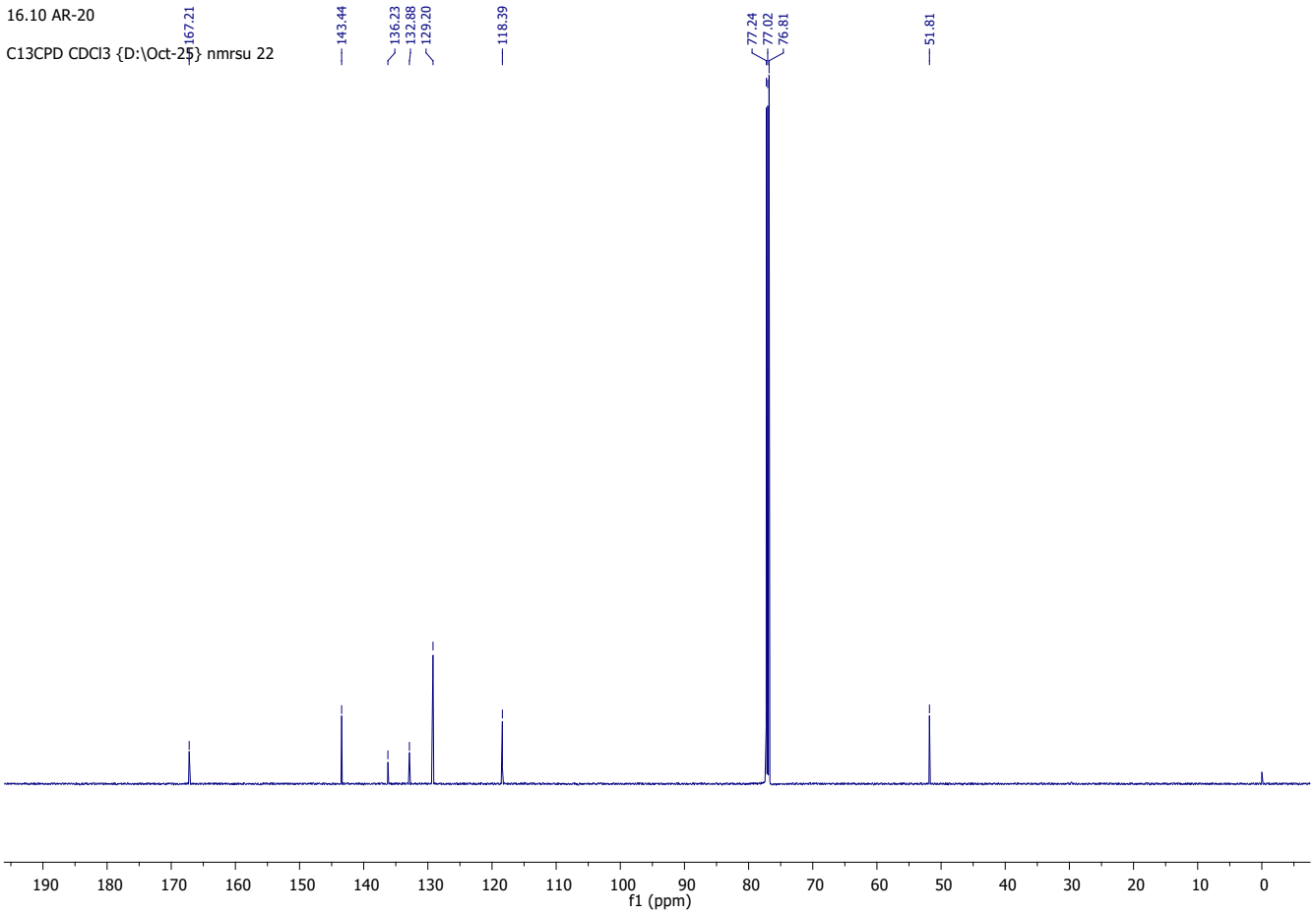
Compound 3h. ^{1}H NMR Spectrum ($CDCl_3$).



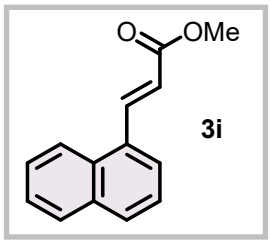


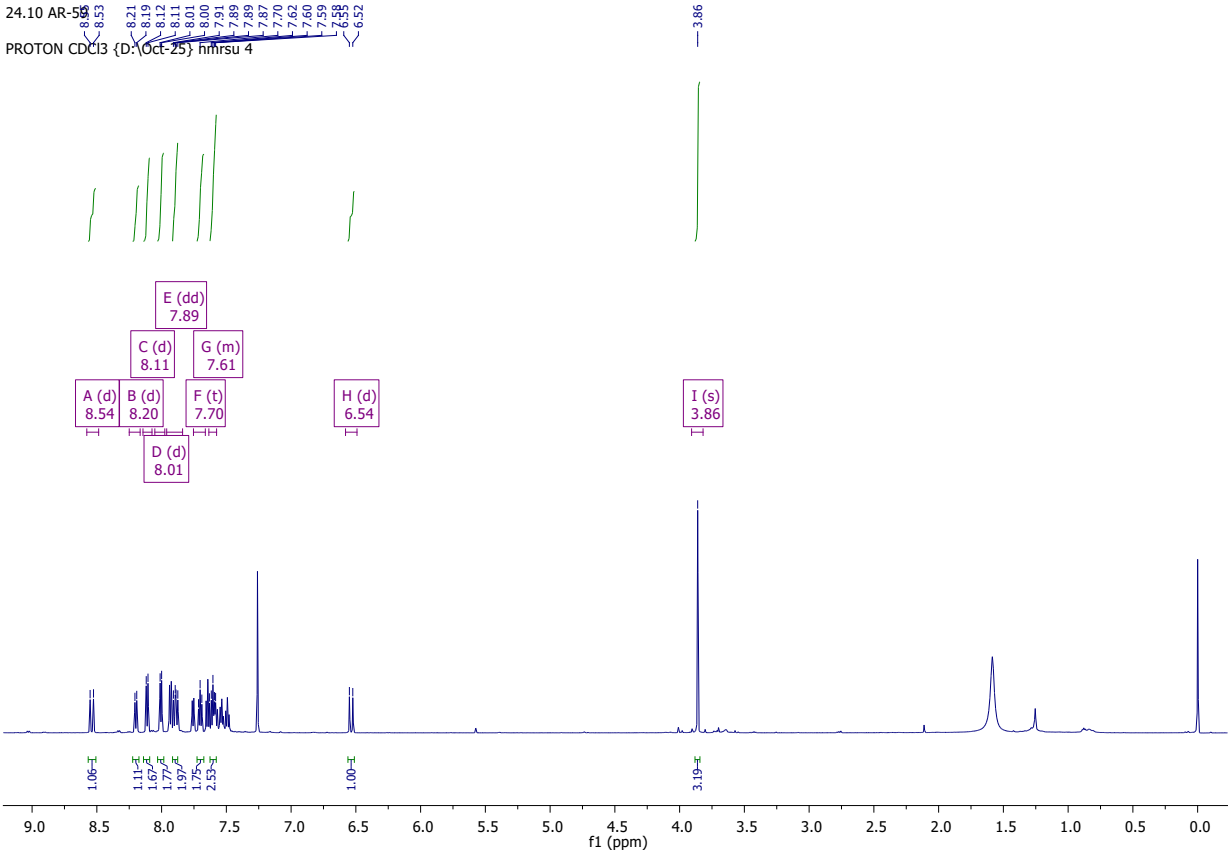
Compound 3h. ^{13}C NMR Spectrum ($CDCl_3$).



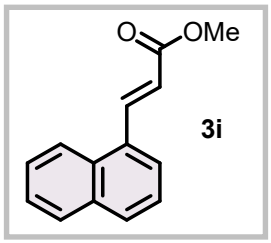


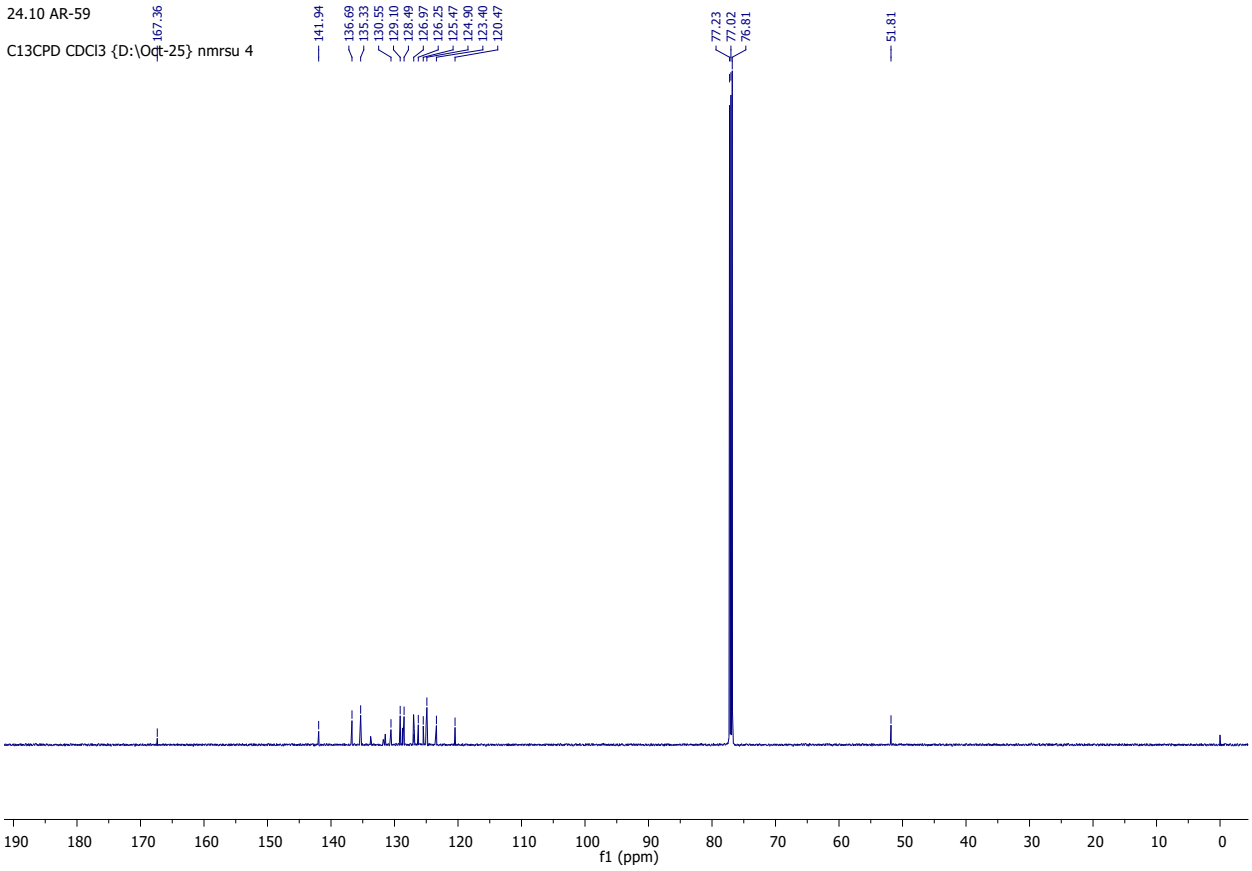
Compound 3i. ^{13}C NMR Spectrum ($CDCl_3$).



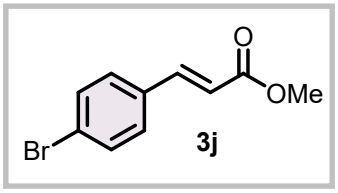


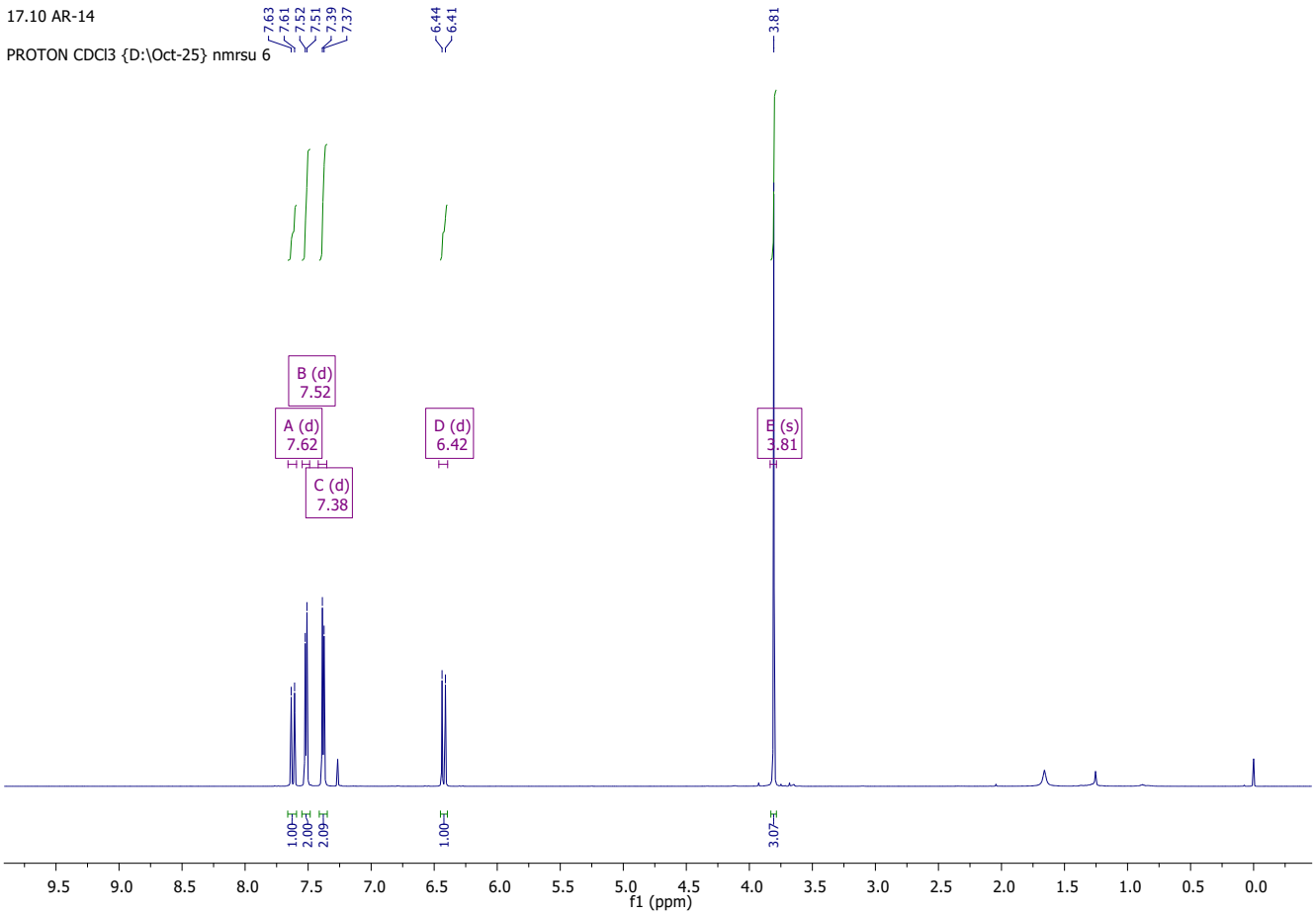
Compound 3i. ^{13}C NMR Spectrum ($CDCl_3$).



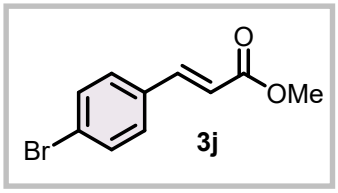


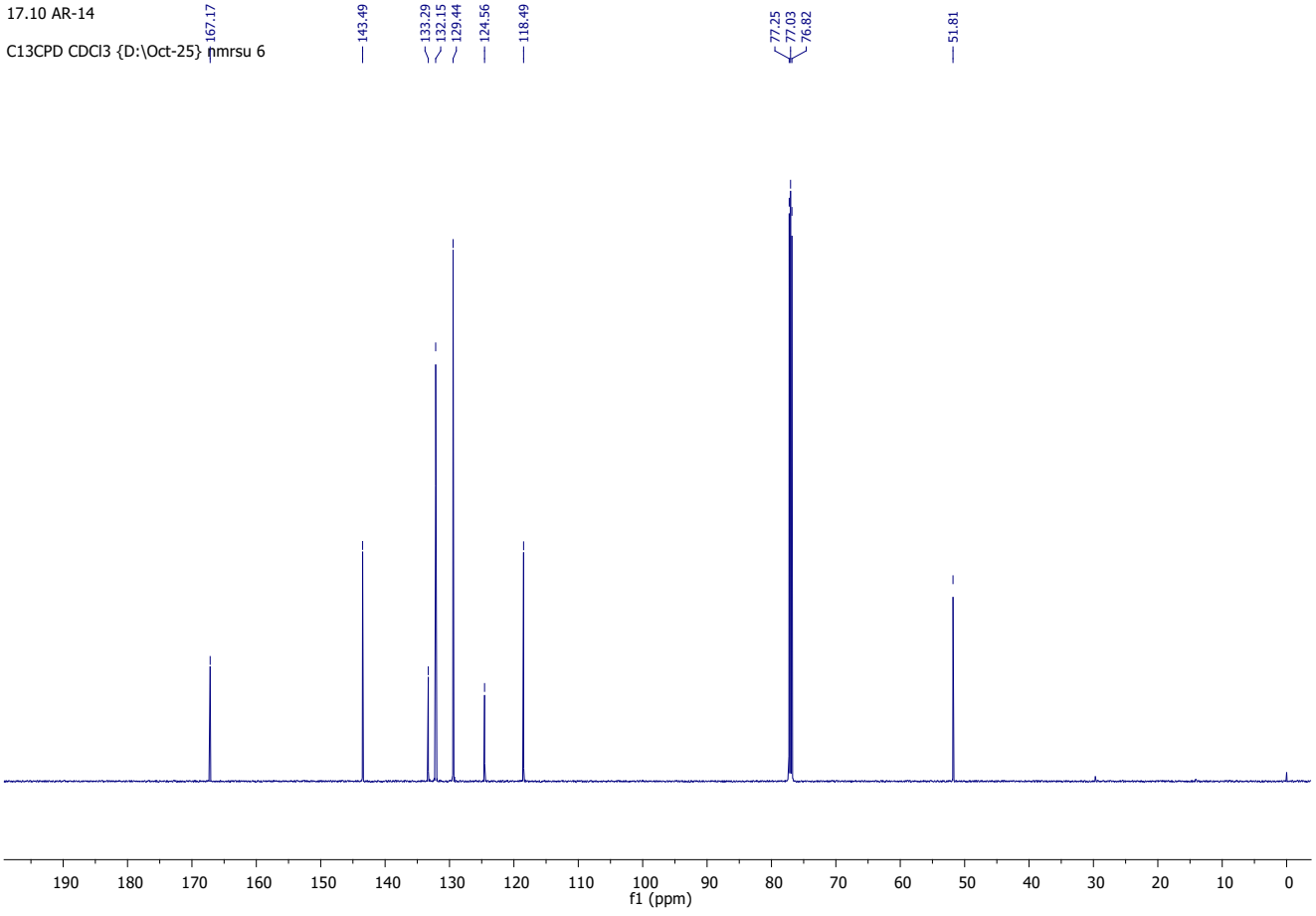
Compound 3j. ^{1}H NMR Spectrum ($CDCl_3$).



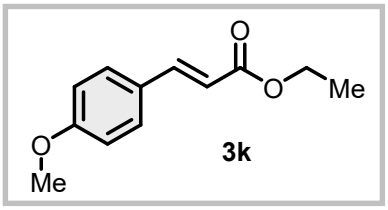


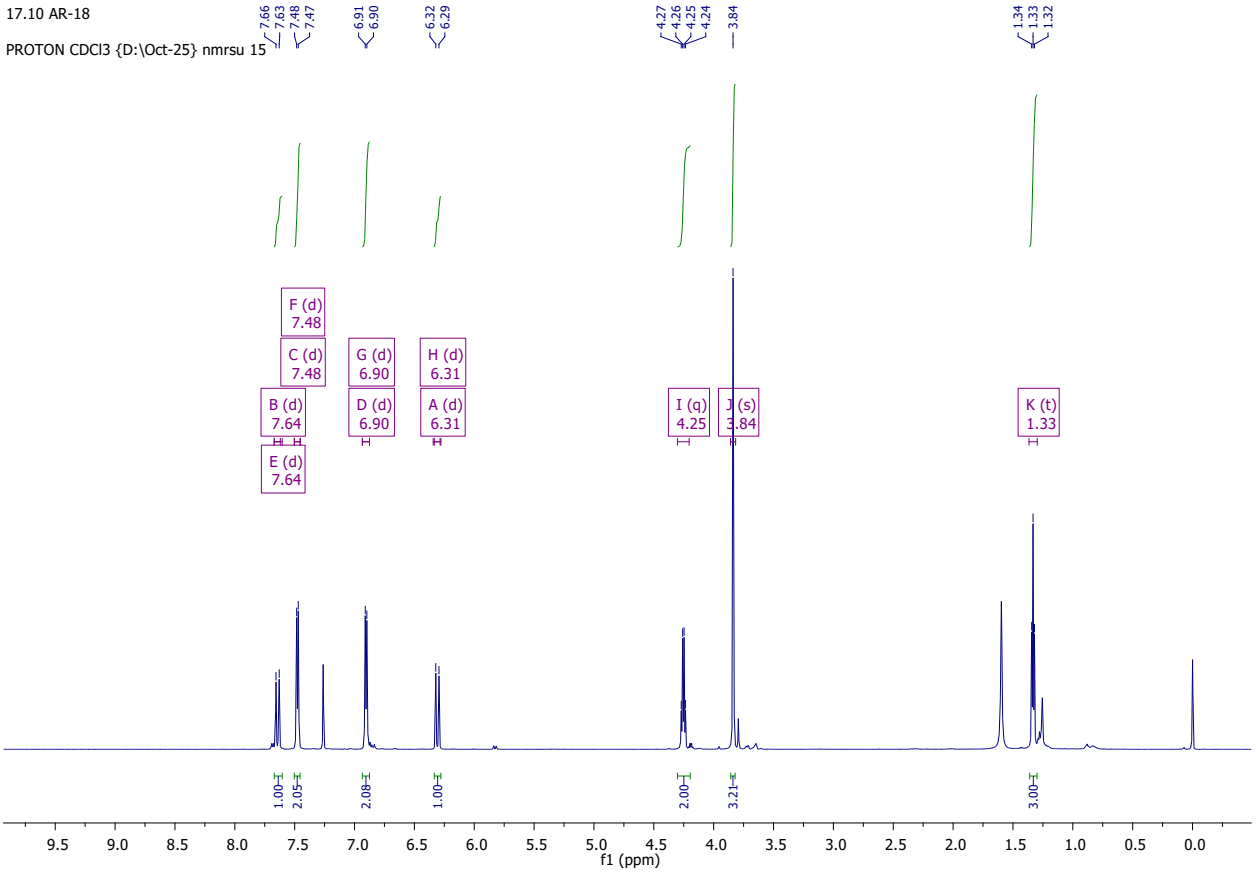
Compound 3j. ^{13}C NMR Spectrum ($CDCl_3$).



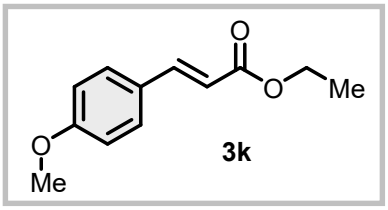


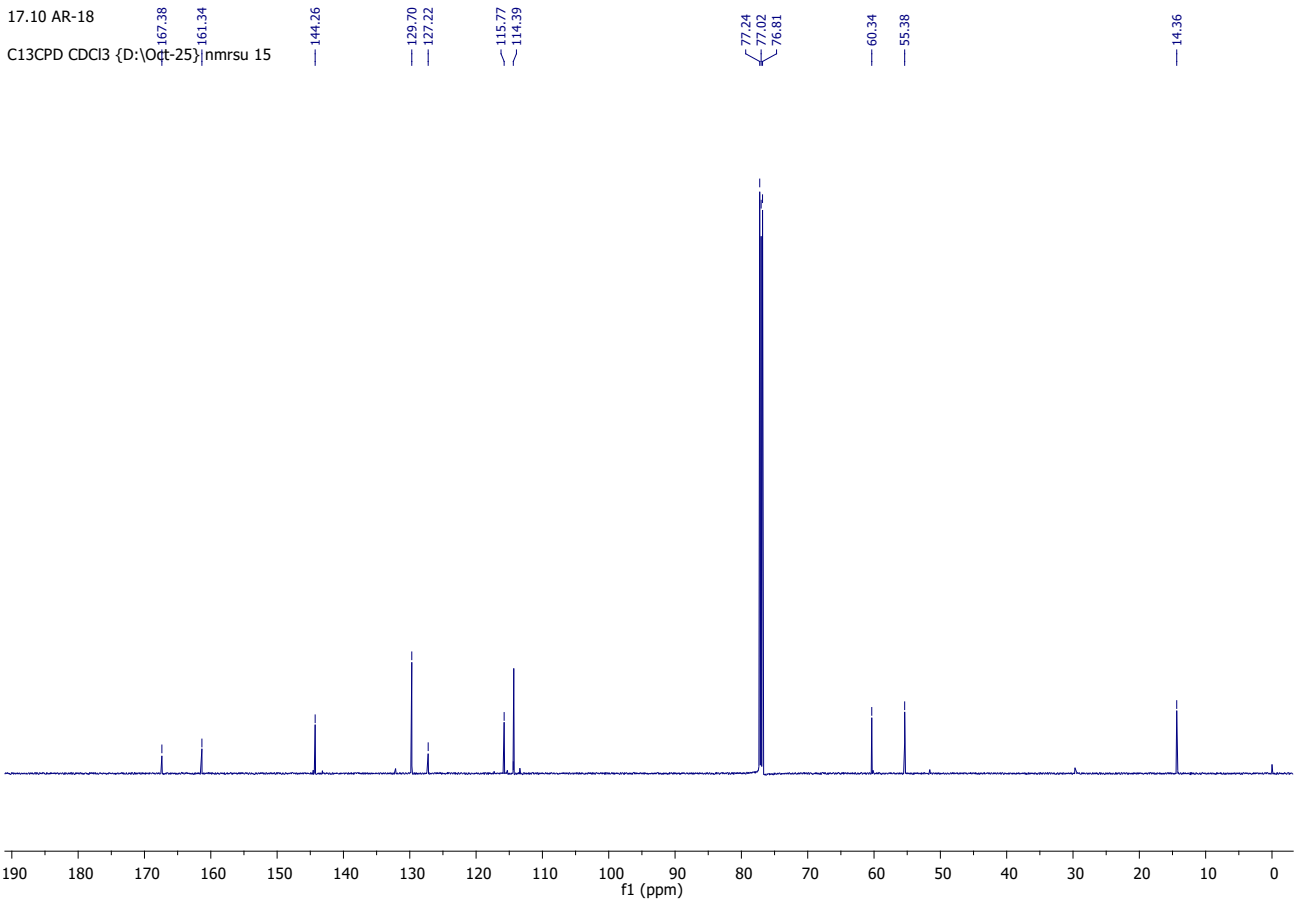
Compound 3k. ^{1}H NMR Spectrum ($CDCl_3$).



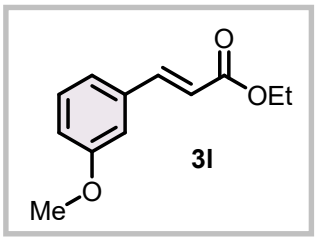


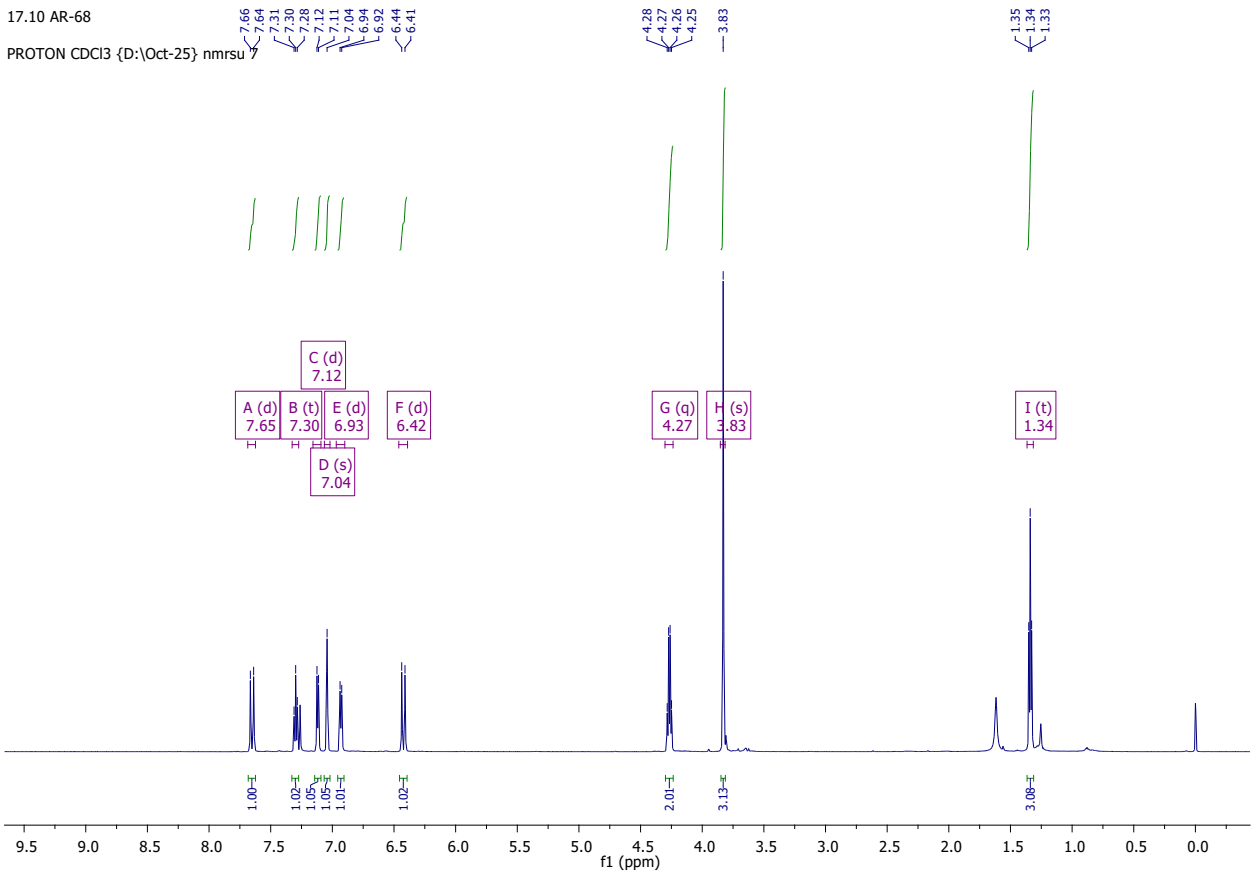
Compound 3k. ^{13}C NMR Spectrum ($CDCl_3$).



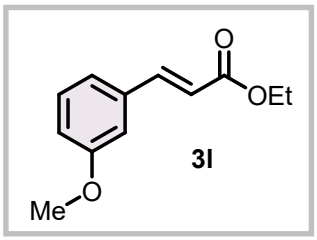


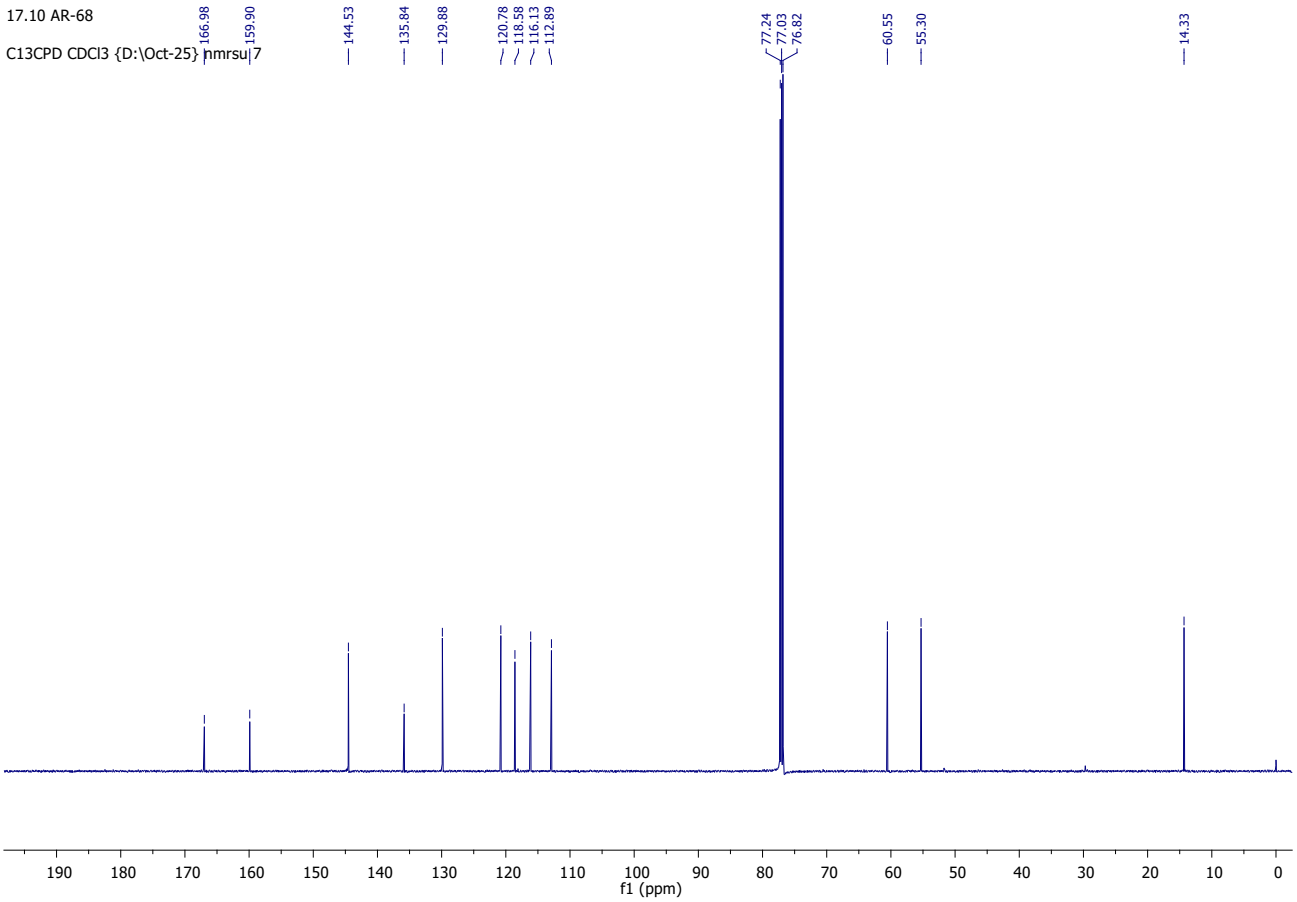
Compound 3l. ^{1}H NMR Spectrum ($CDCl_3$).



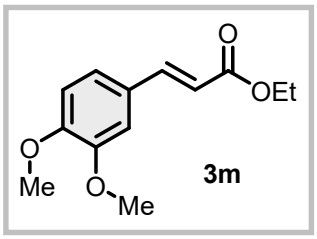


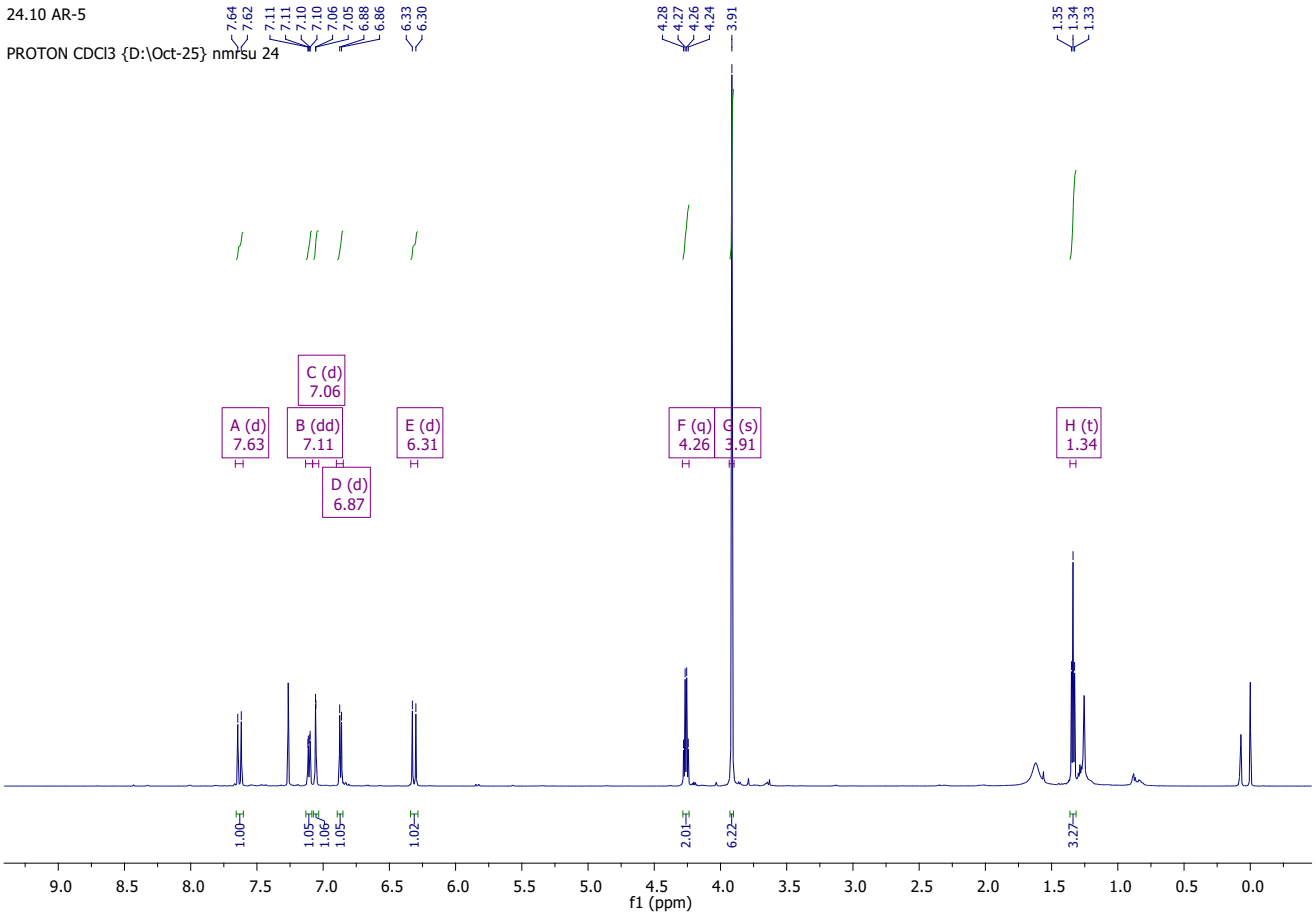
Compound 3l. ^{13}C NMR Spectrum ($CDCl_3$).



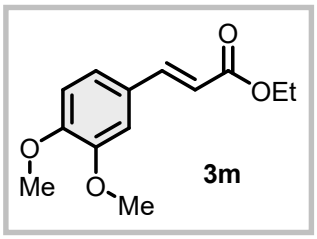


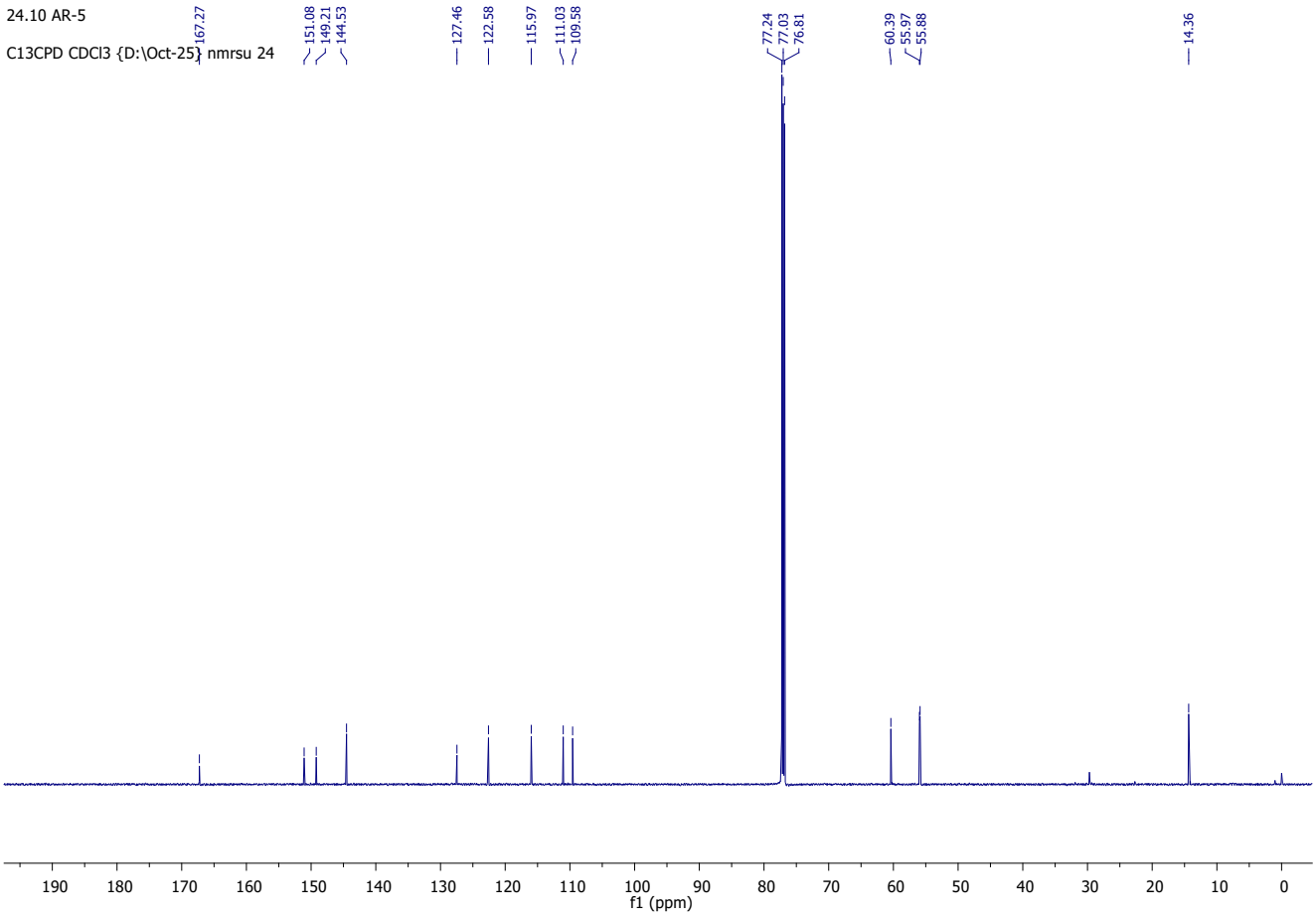
Compound 3m. ^{1}H NMR Spectrum ($CDCl_3$).



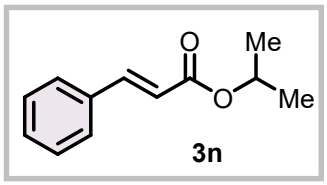


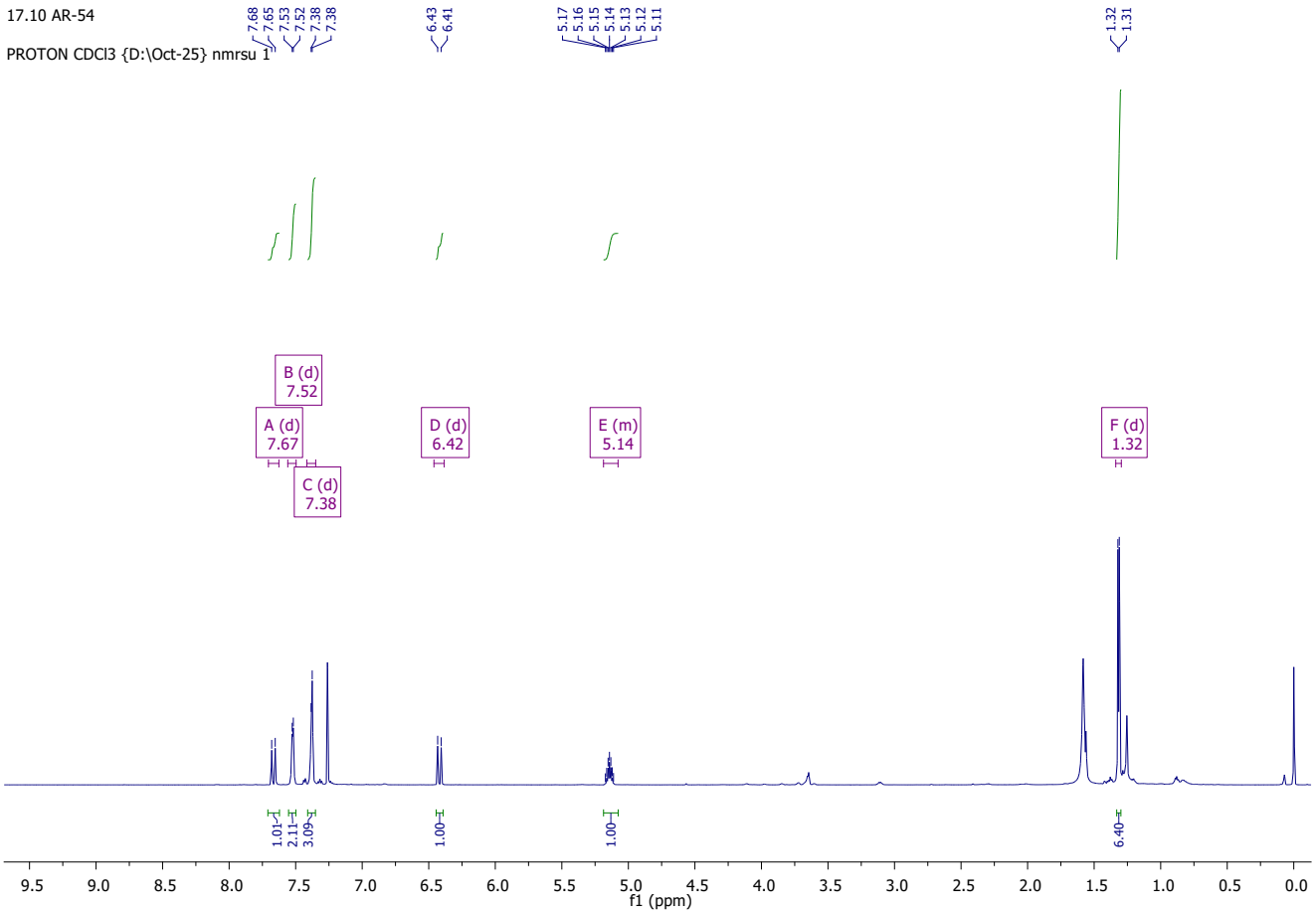
Compound 3m. ^{13}C NMR Spectrum ($CDCl_3$).



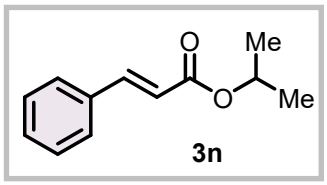


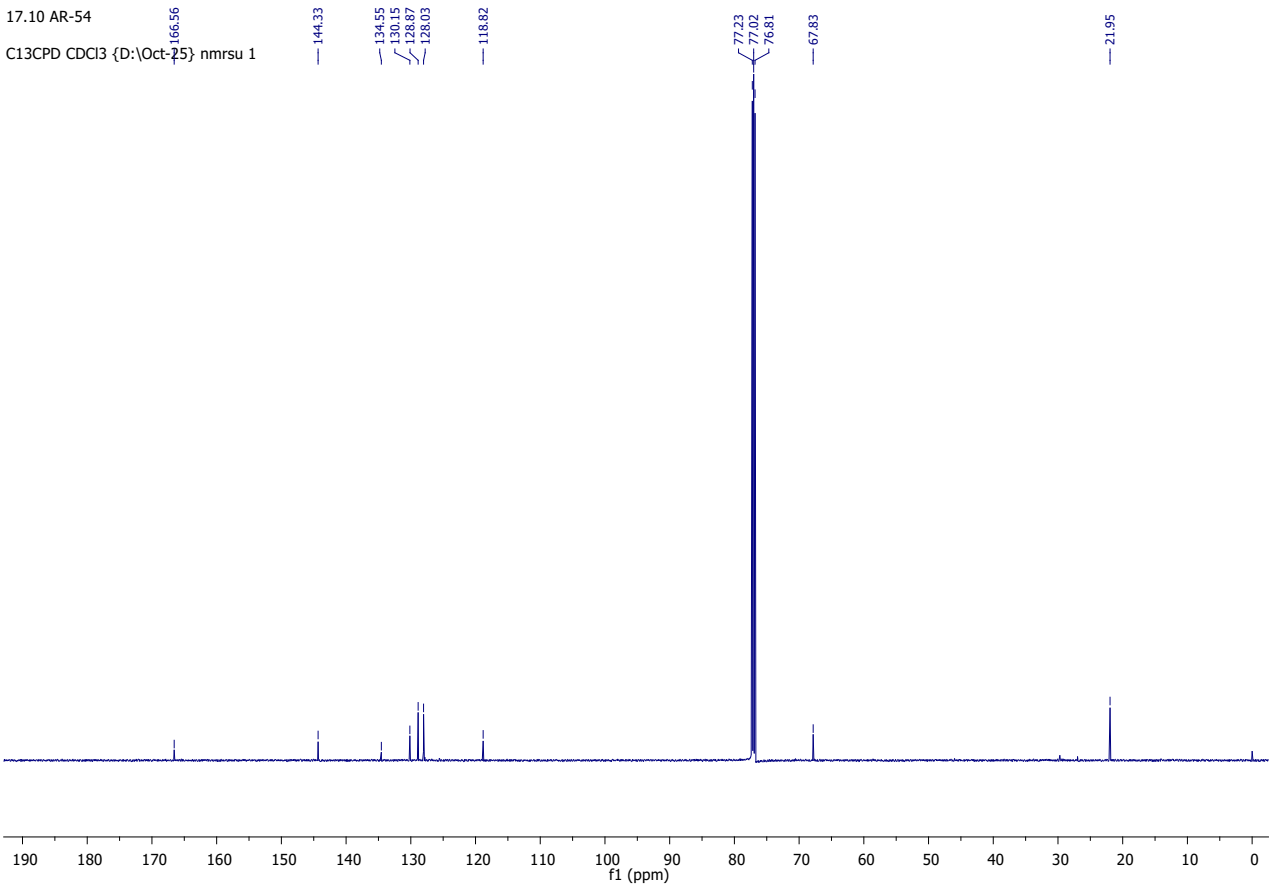
Compound 3n. ^{1}H NMR Spectrum ($CDCl_3$).



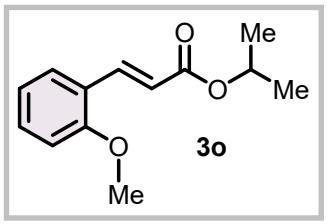


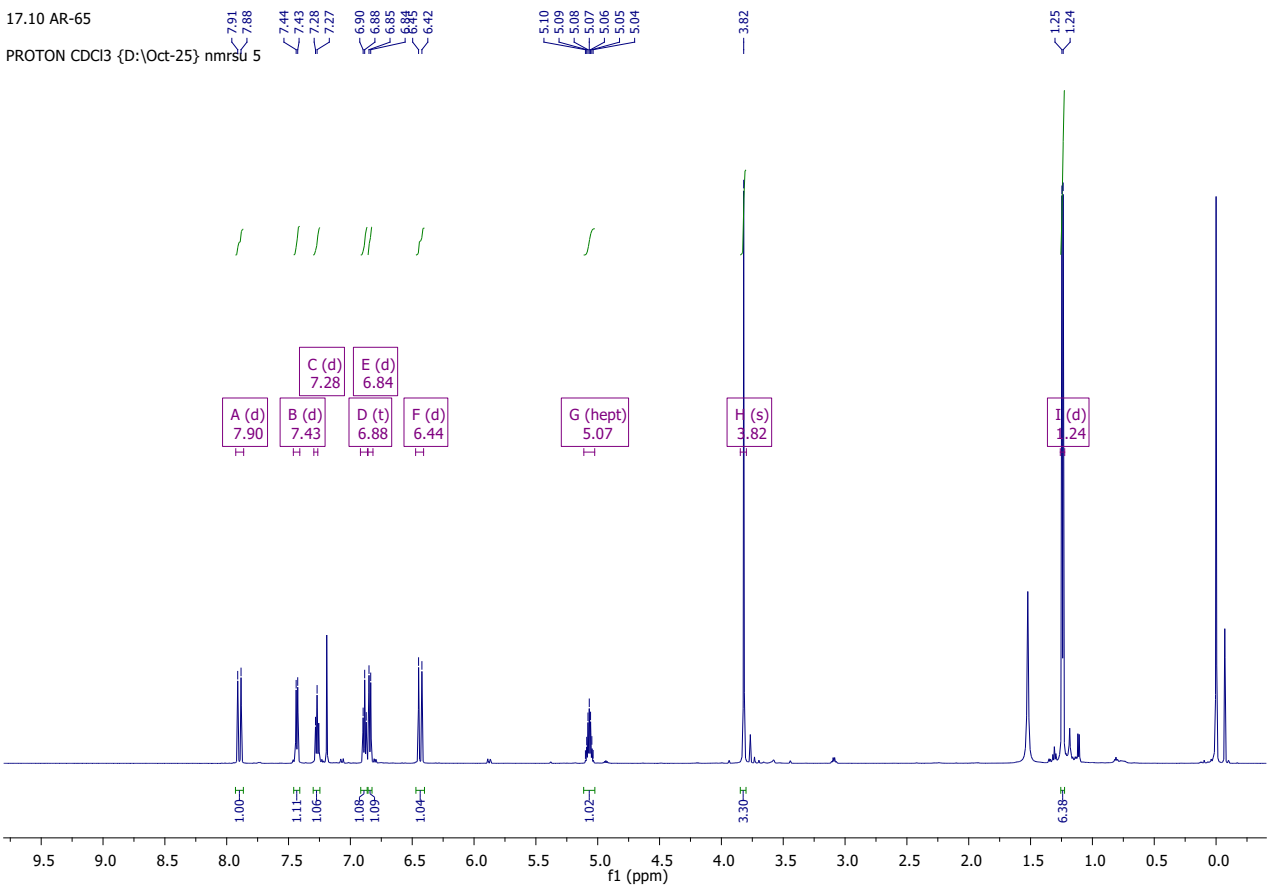
Compound 3n. ^{13}C NMR Spectrum ($CDCl_3$).



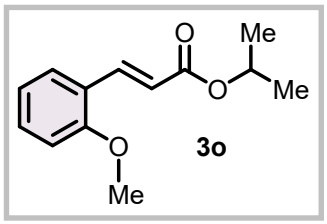


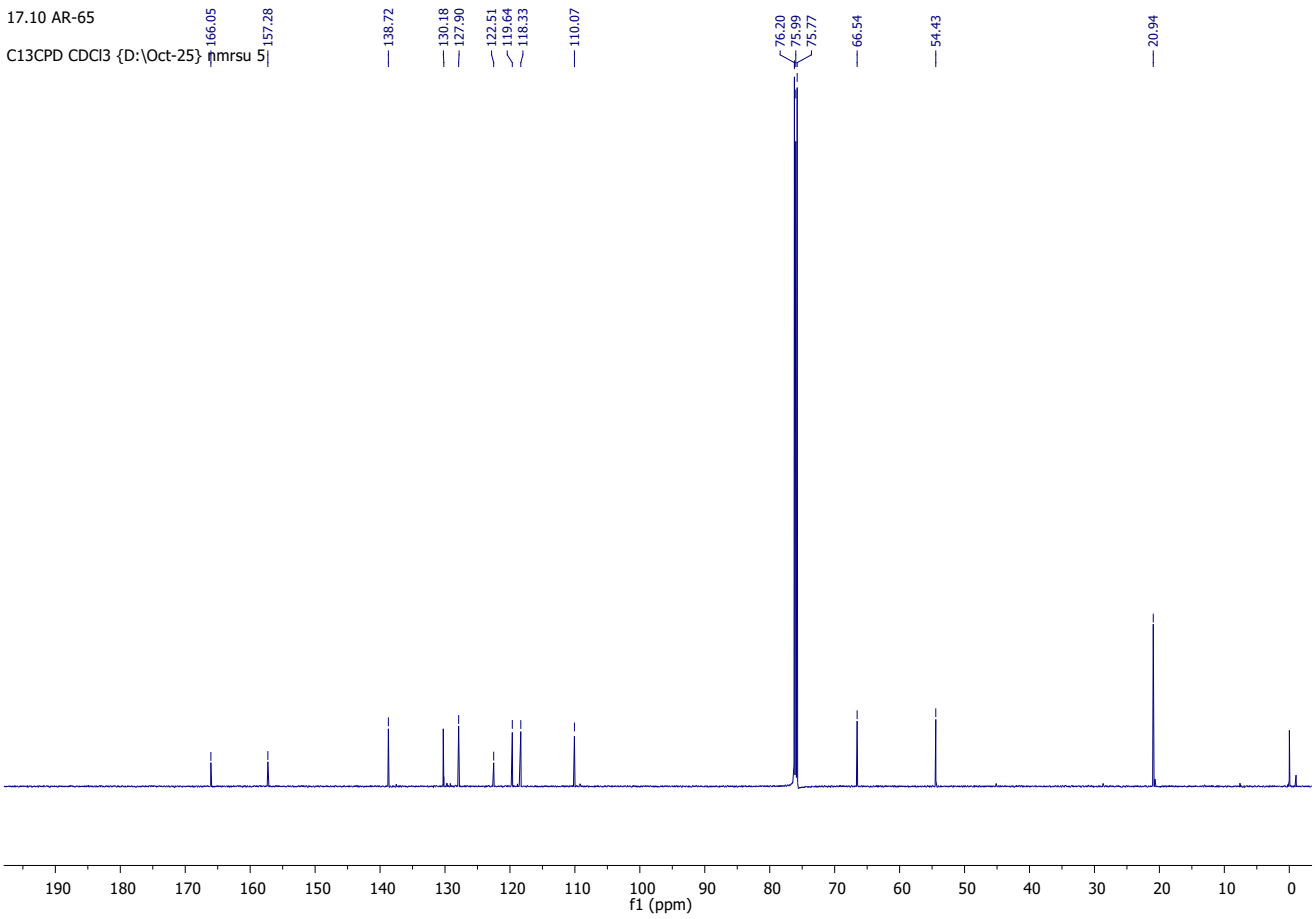
Compound 3o. ^{1}H NMR Spectrum ($CDCl_3$).



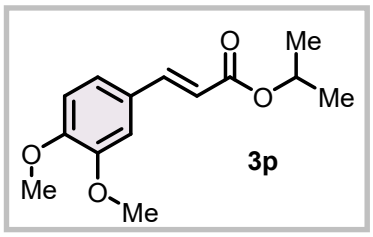


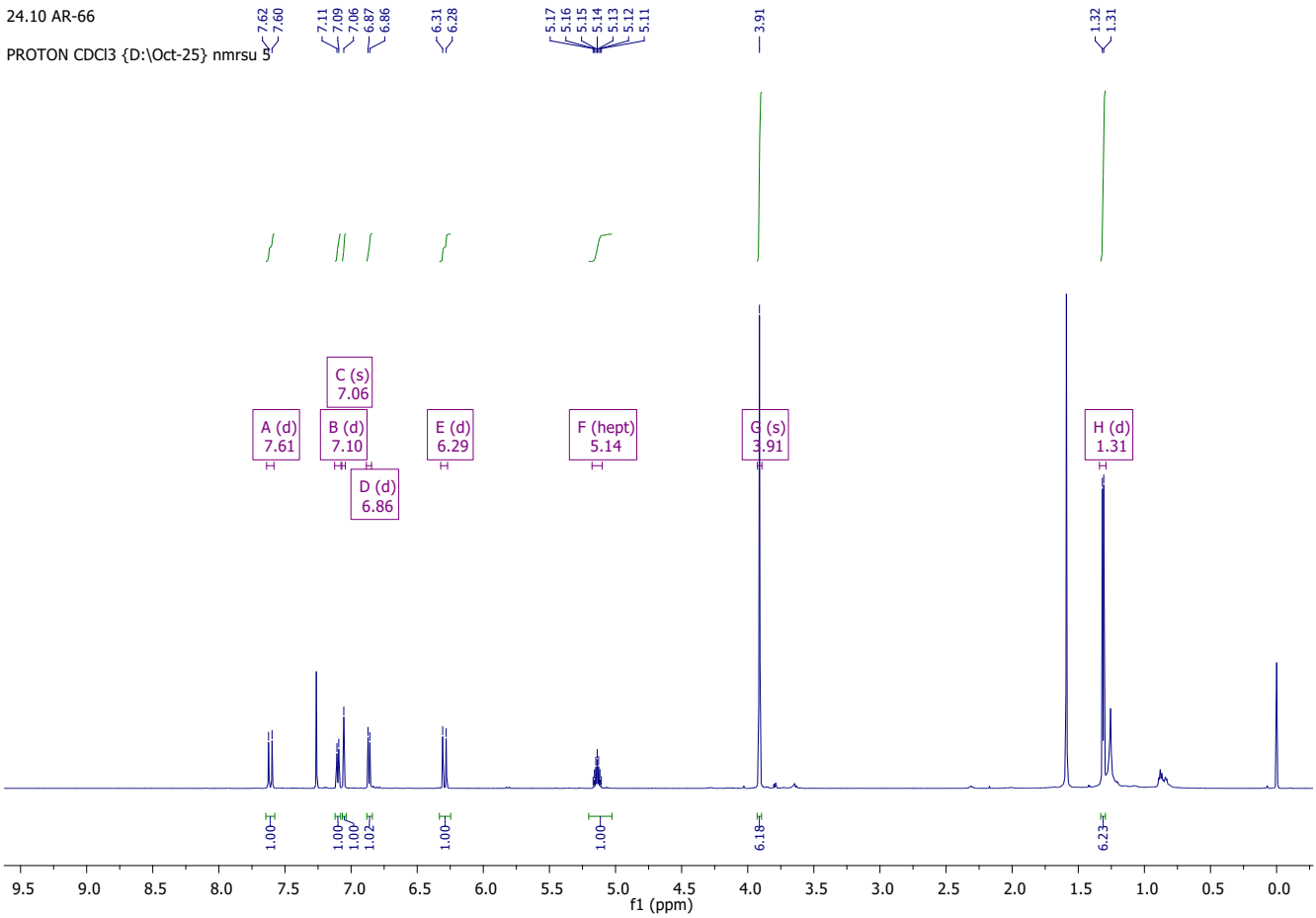
Compound 3o. ^{13}C NMR Spectrum ($CDCl_3$).



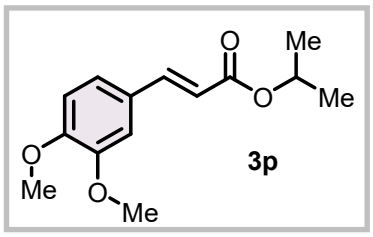


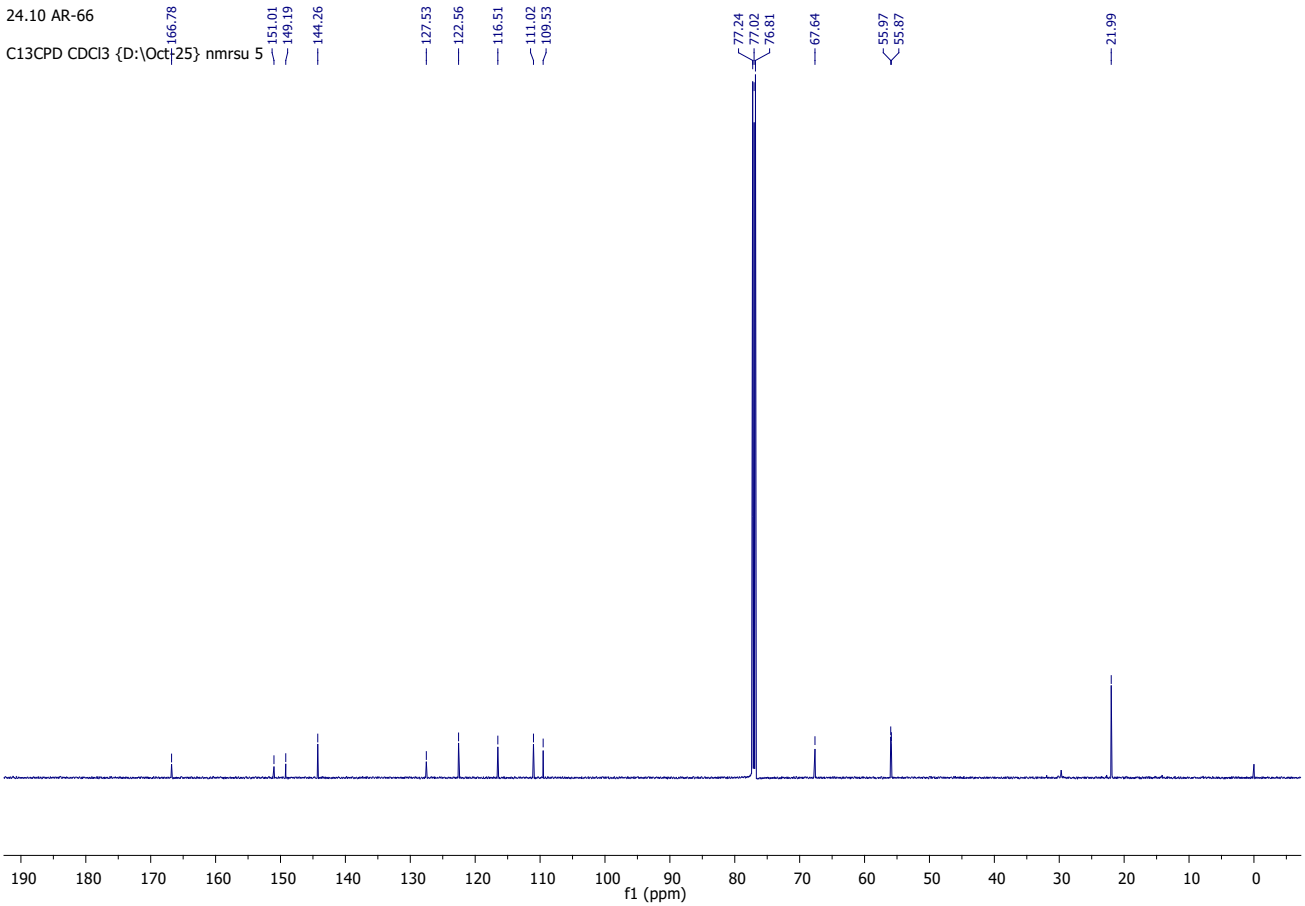
Compound 3p. ^{1}H NMR Spectrum ($CDCl_3$).



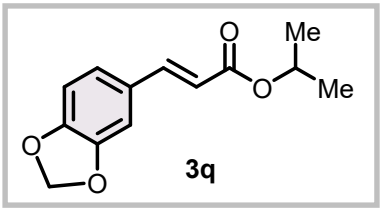


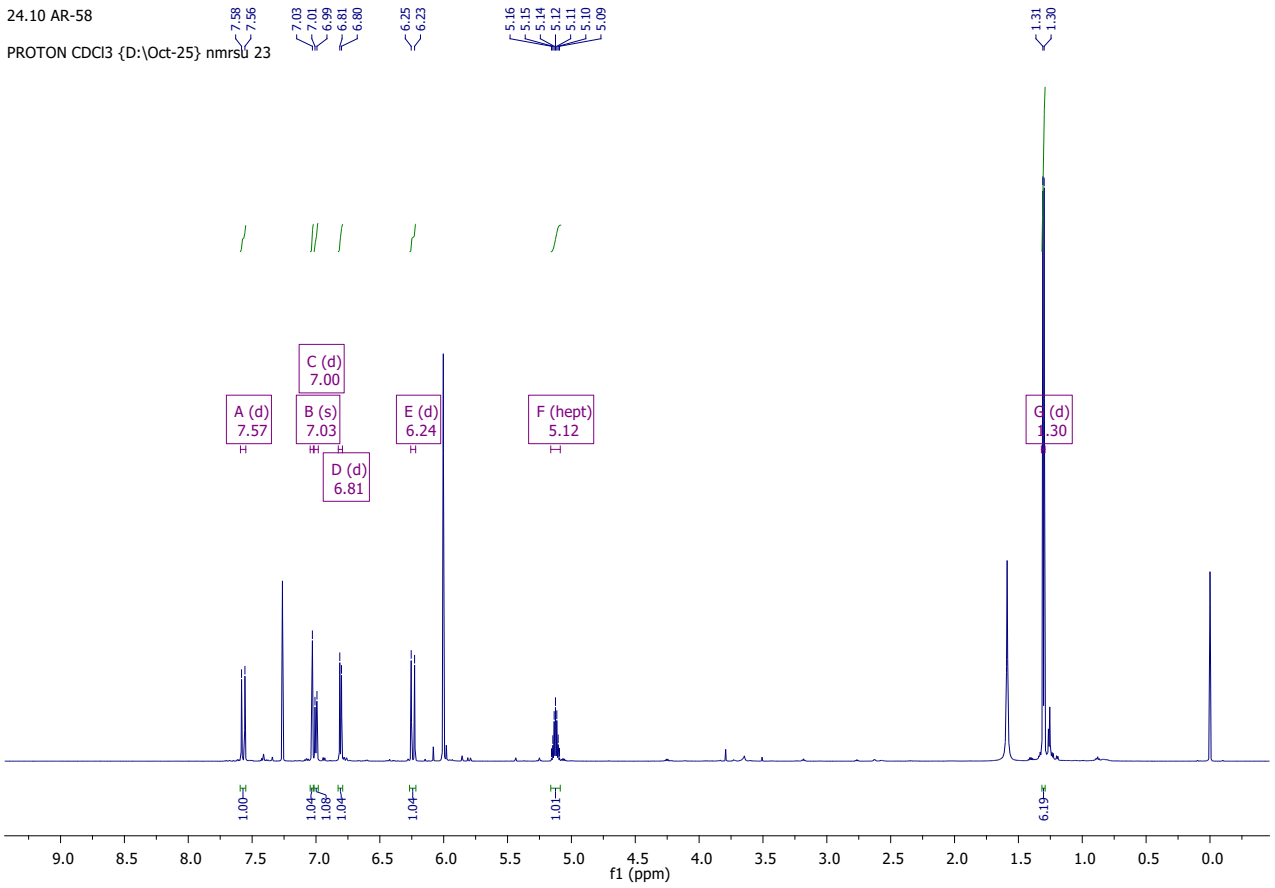
Compound 3p. ^{13}C NMR Spectrum ($CDCl_3$).



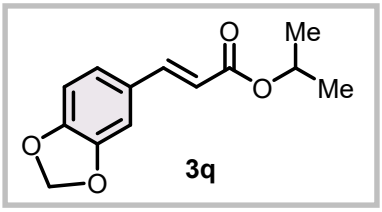


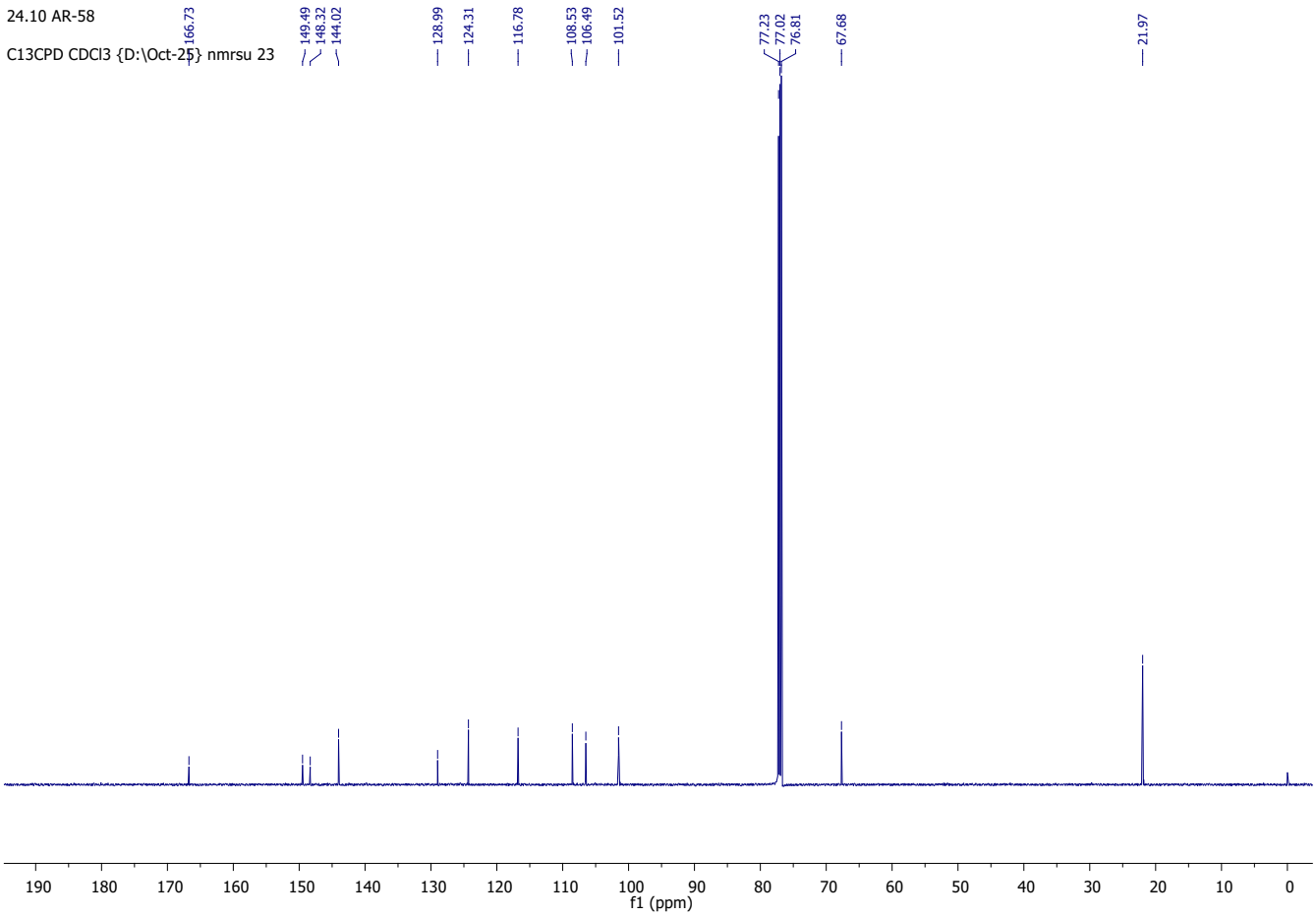
Compound 3q. ^{1}H NMR Spectrum ($CDCl_3$).



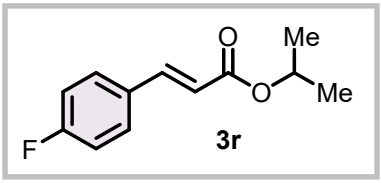


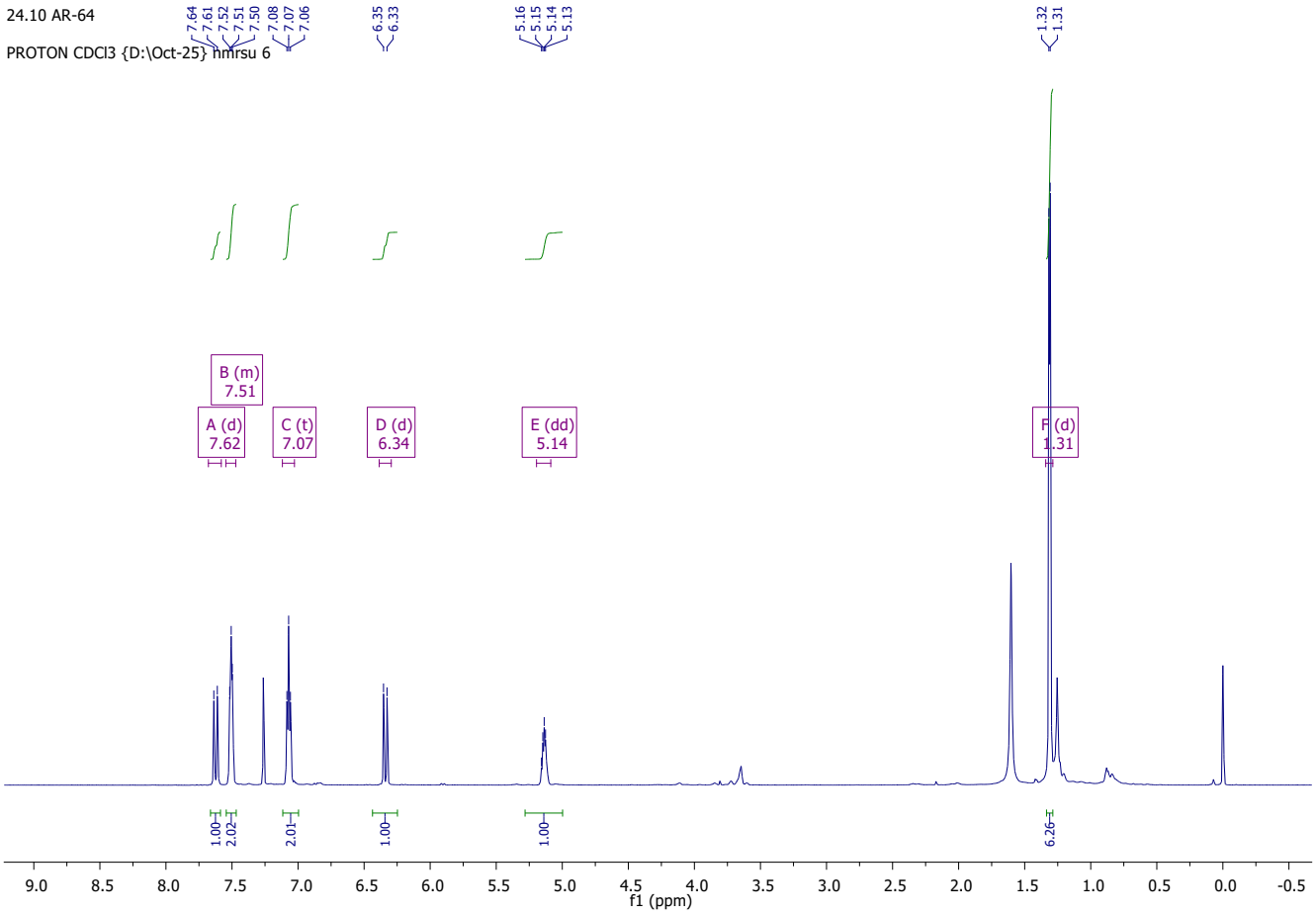
Compound 3q. ^{13}C NMR Spectrum ($CDCl_3$).



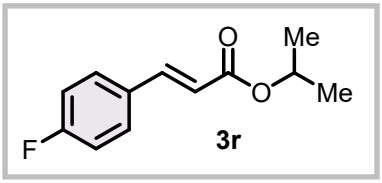


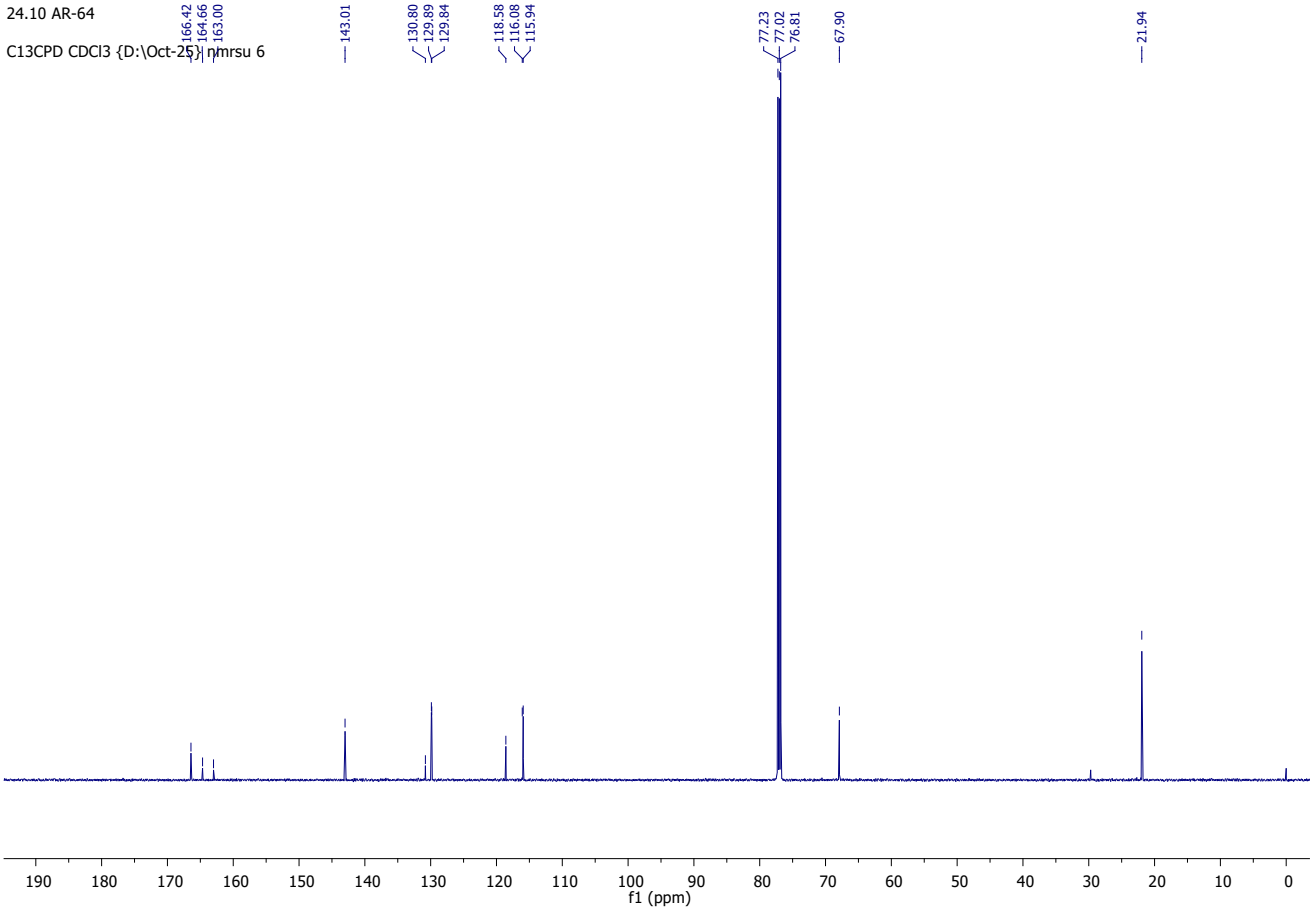
Compound 3r. ^{1}H NMR Spectrum ($CDCl_3$).



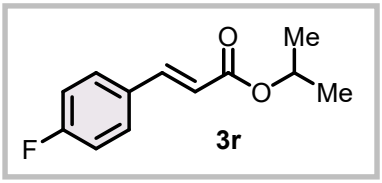


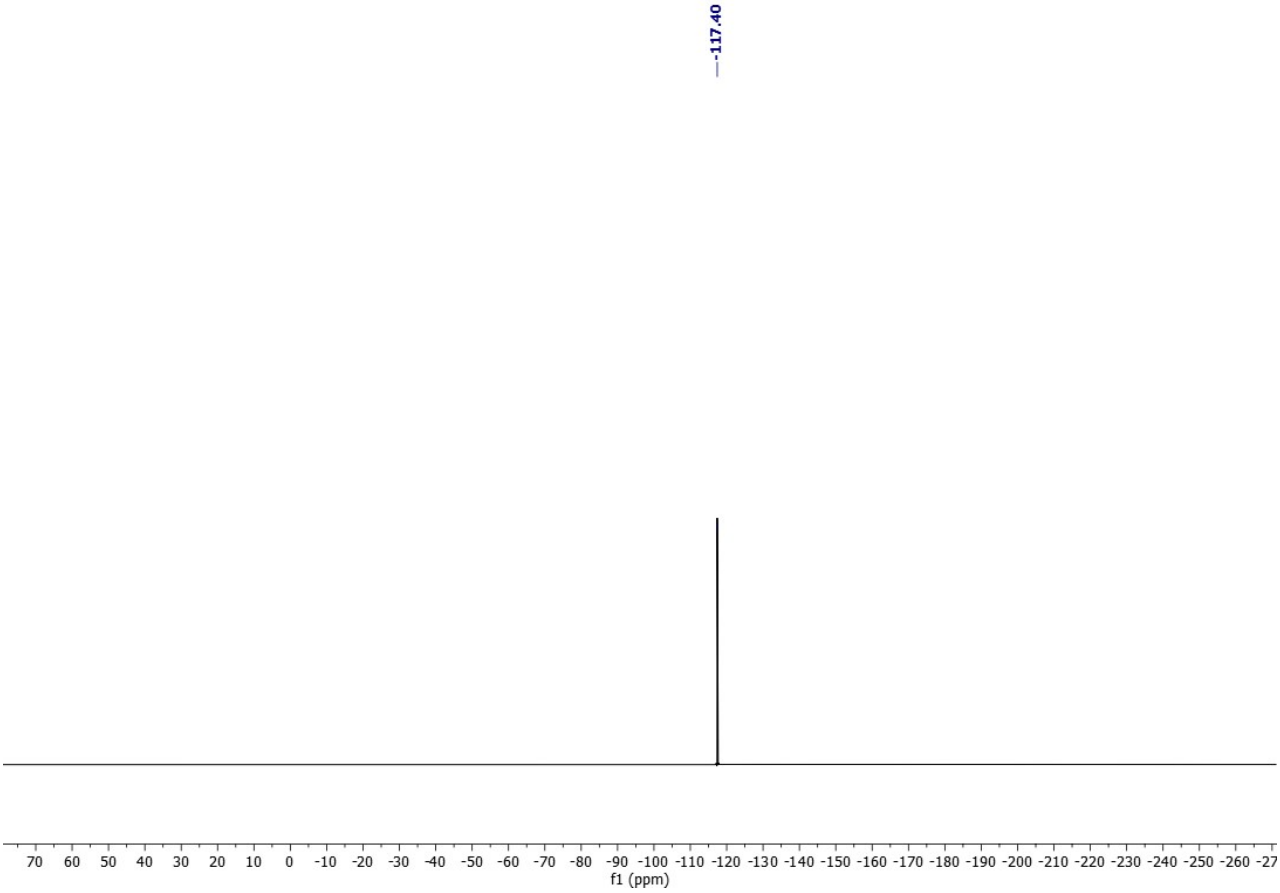
Compound 3r. ^{13}C NMR Spectrum ($CDCl_3$).



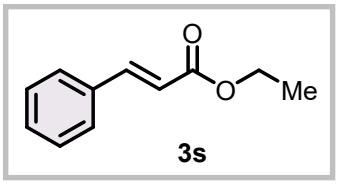


Compound 3r. ^{19}F NMR Spectrum ($CDCl_3$).

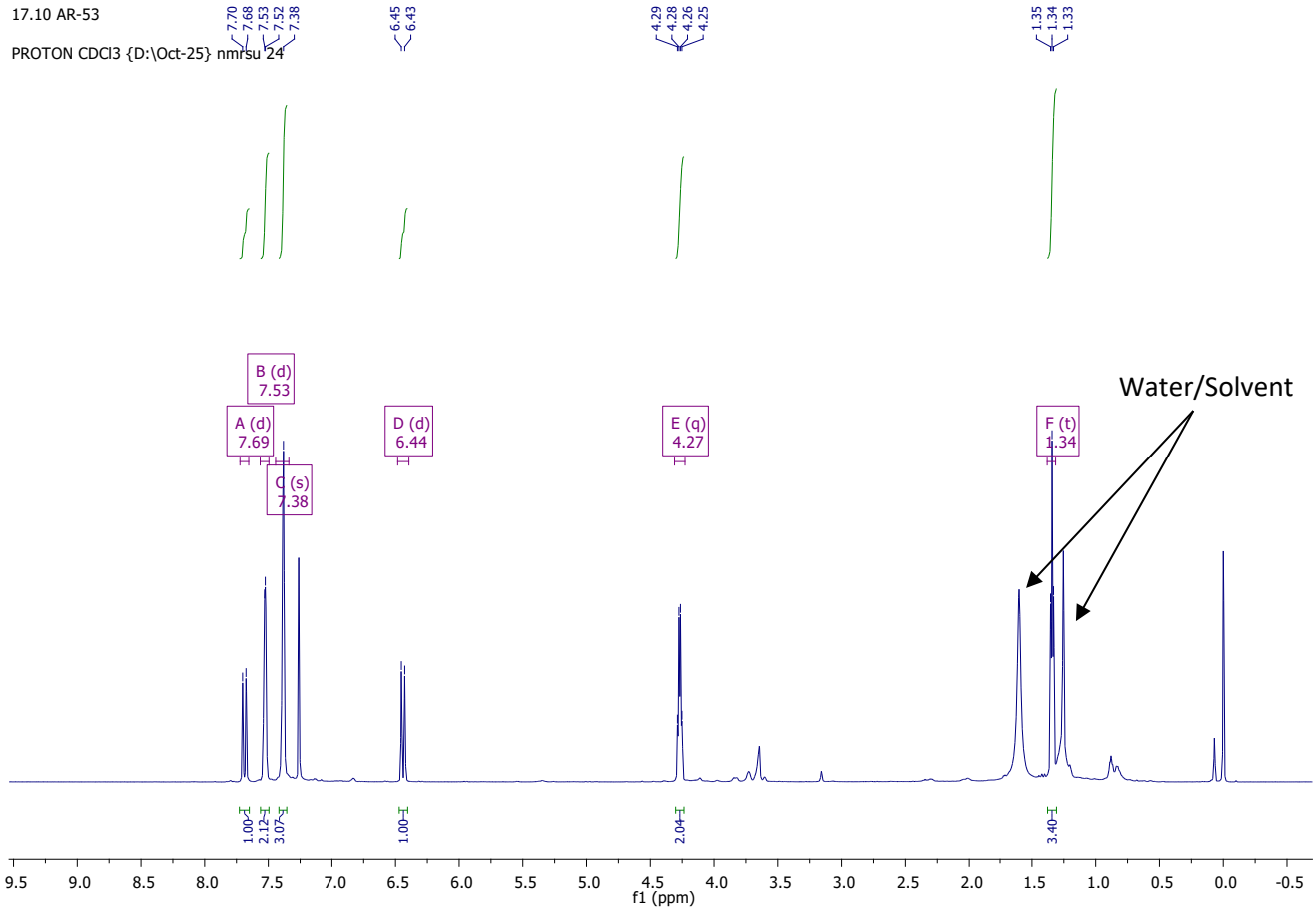




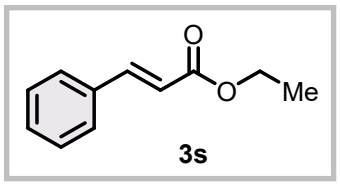
Compound 3s. ^{1}H NMR Spectrum ($CDCl_3$).



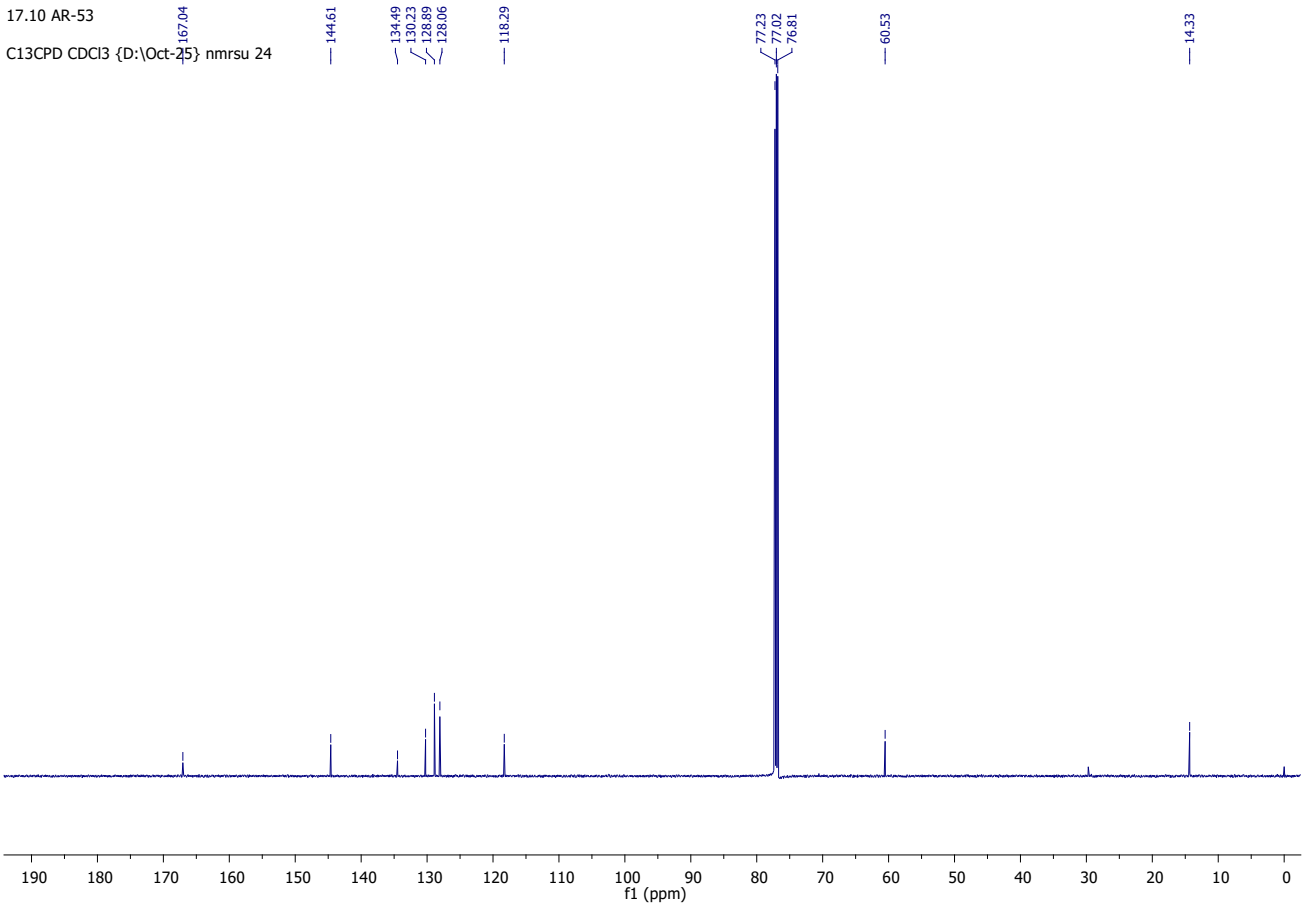
3s



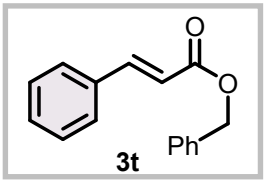
Compound 3s. ^{13}C NMR Spectrum ($CDCl_3$).

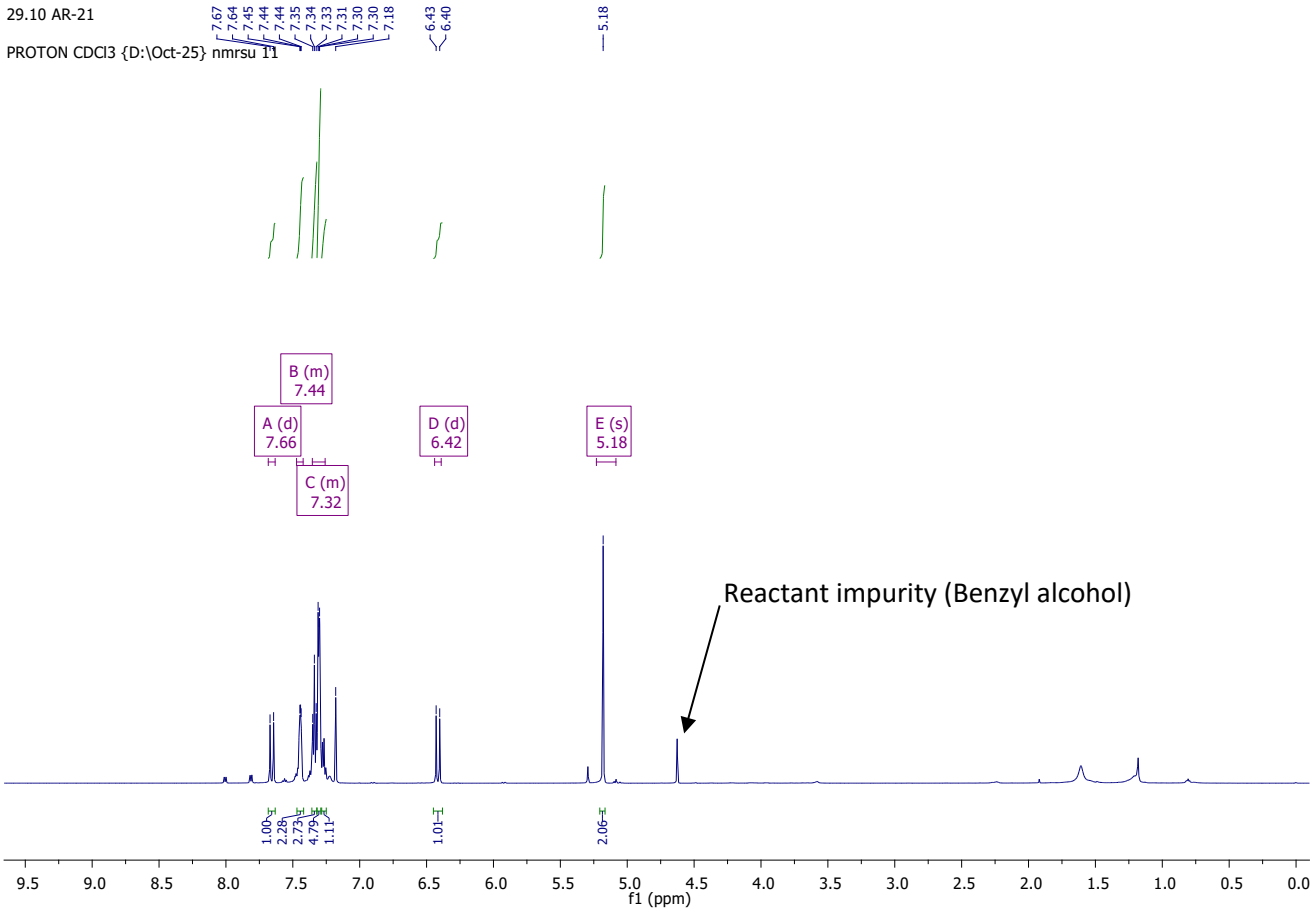


3s

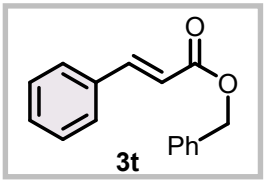


Compound 3t. ^{1}H NMR Spectrum ($CDCl_3$).





Compound 3t. ^{1}H NMR Spectrum ($CDCl_3$).



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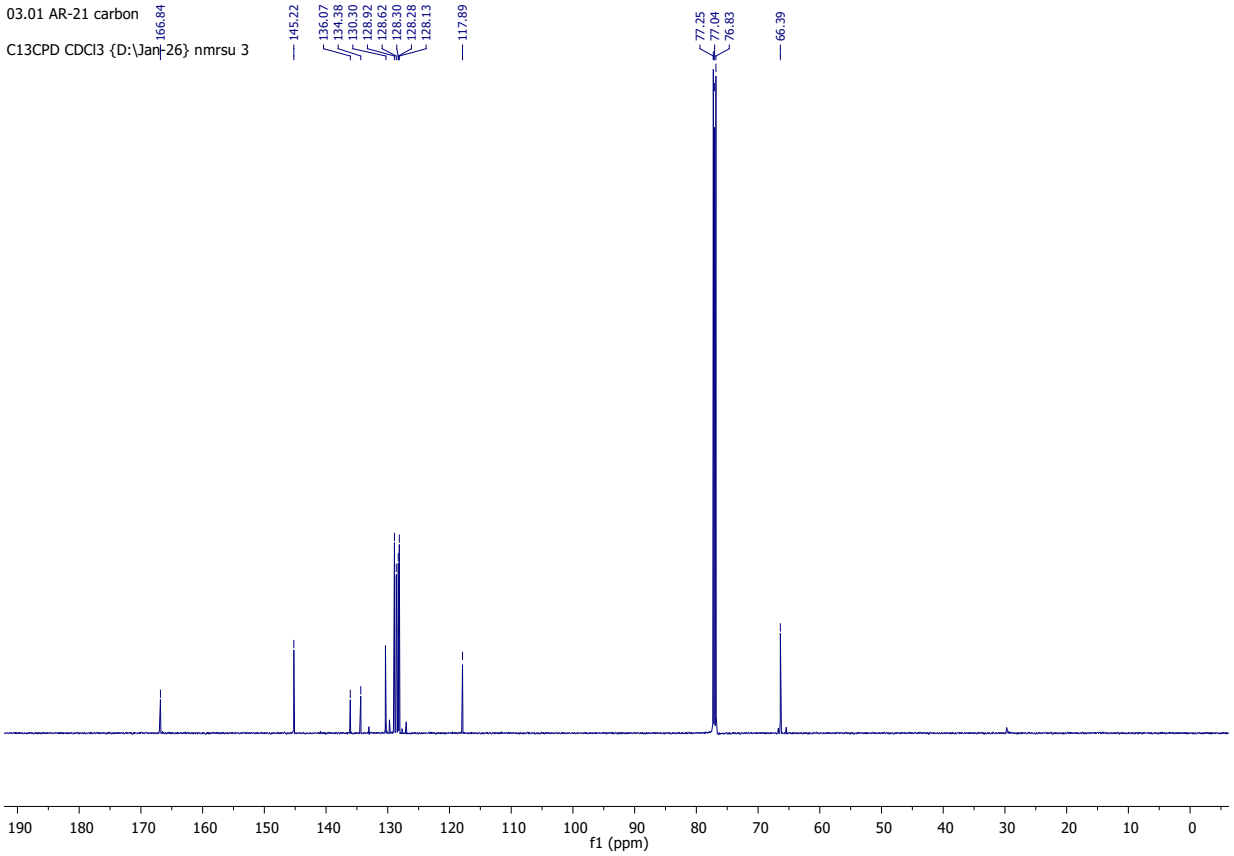
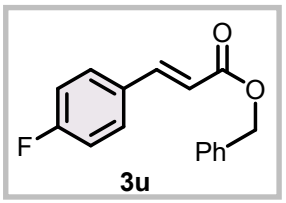


Compound 3u. ^{1}H NMR Spectrum ($CDCl_3$).



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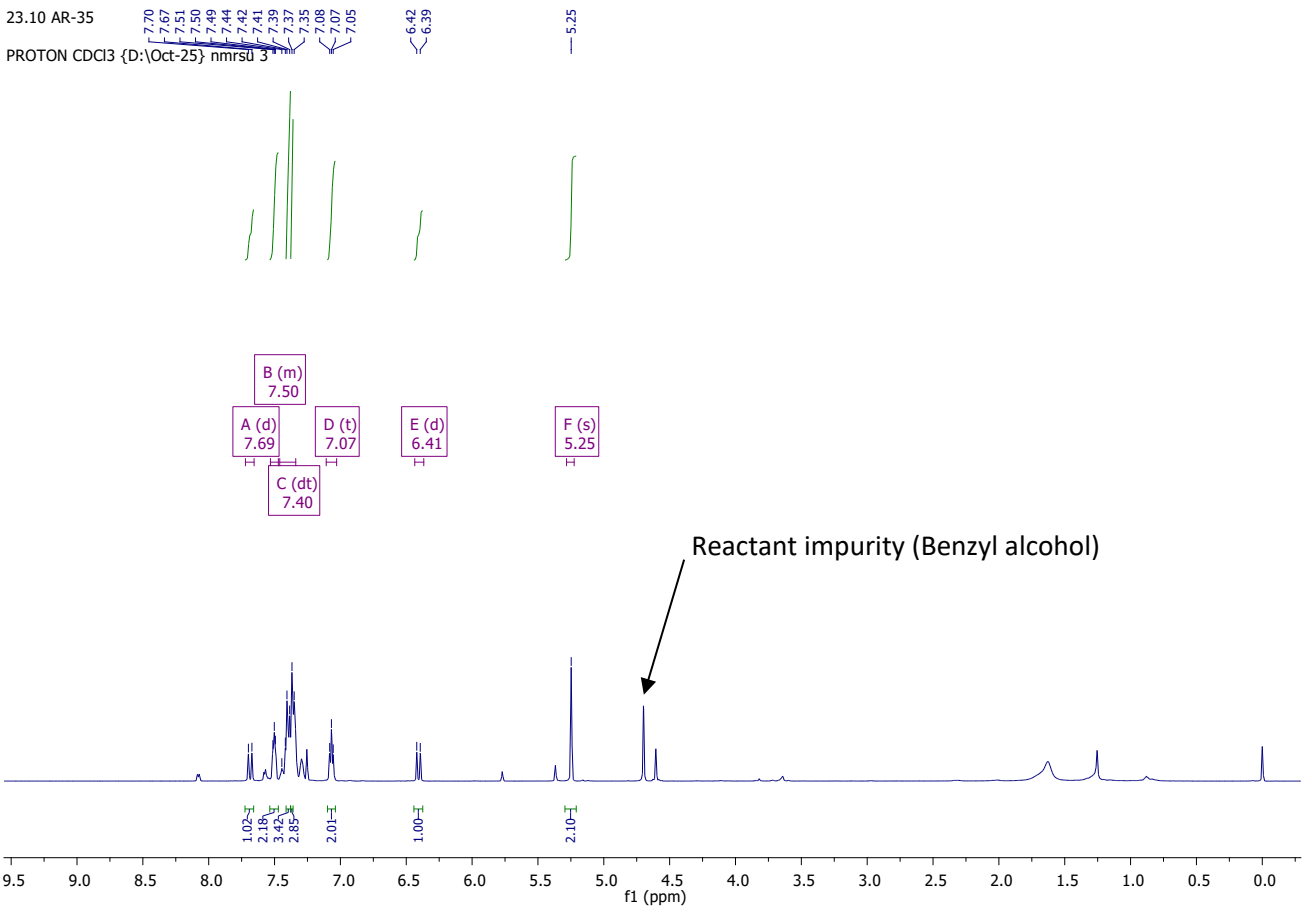
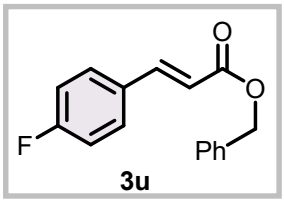


Compound 3u. ^{13}C NMR Spectrum ($CDCl_3$).



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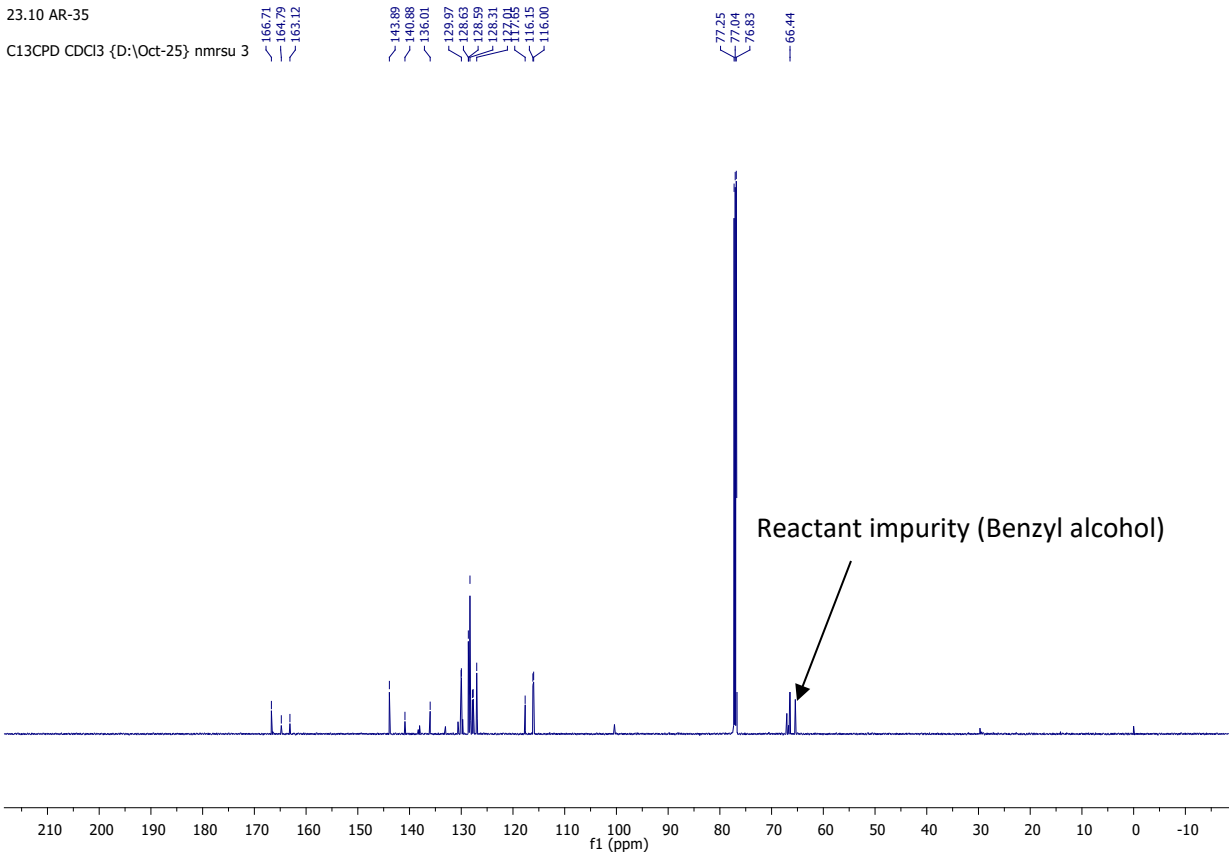
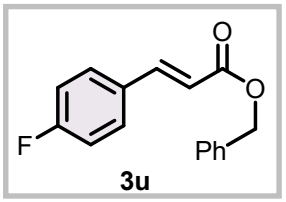


Compound 3u. ^{19}F NMR Spectrum ($CDCl_3$).



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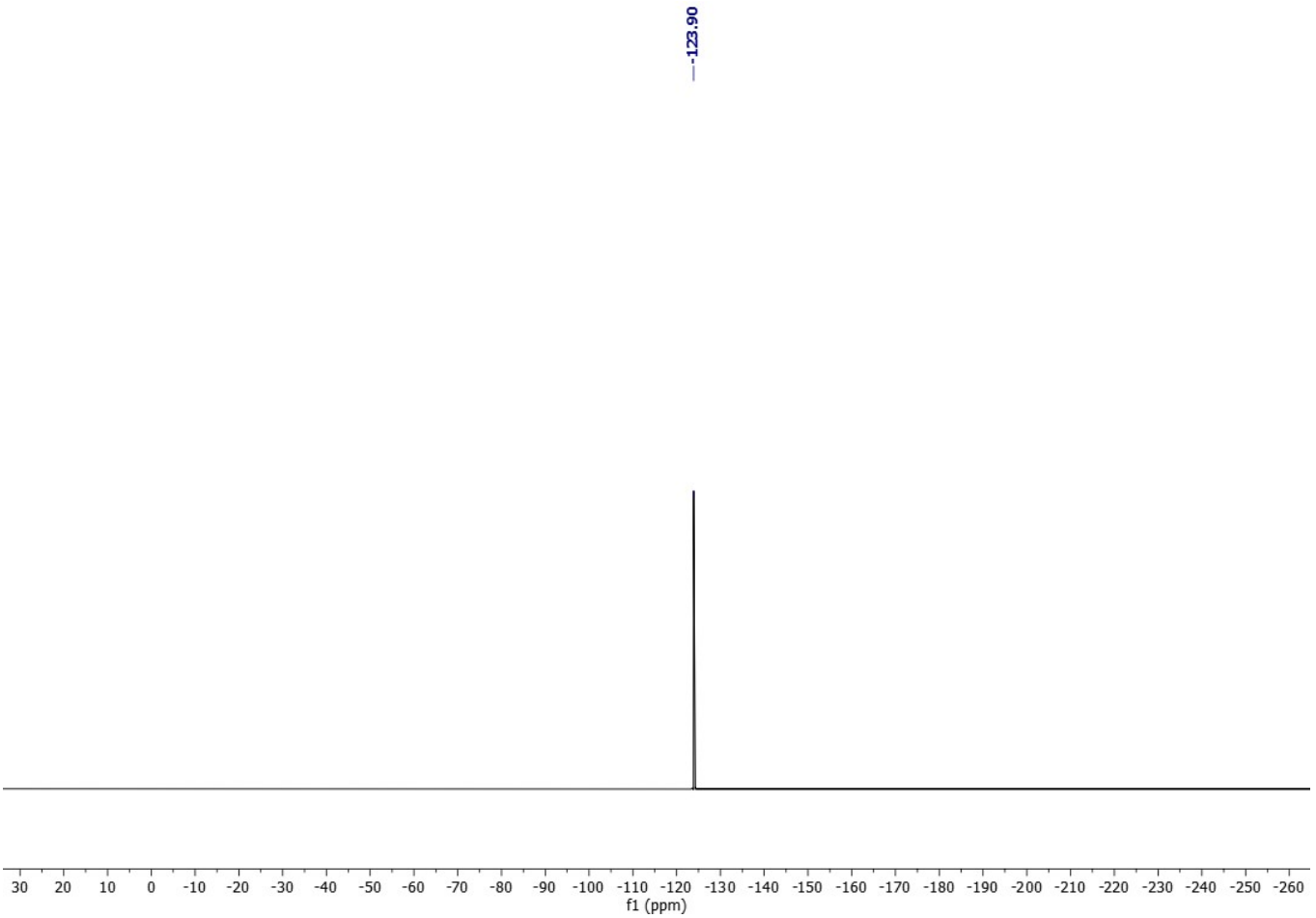
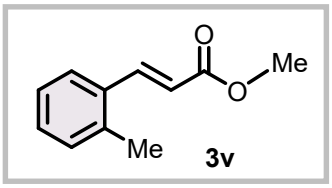
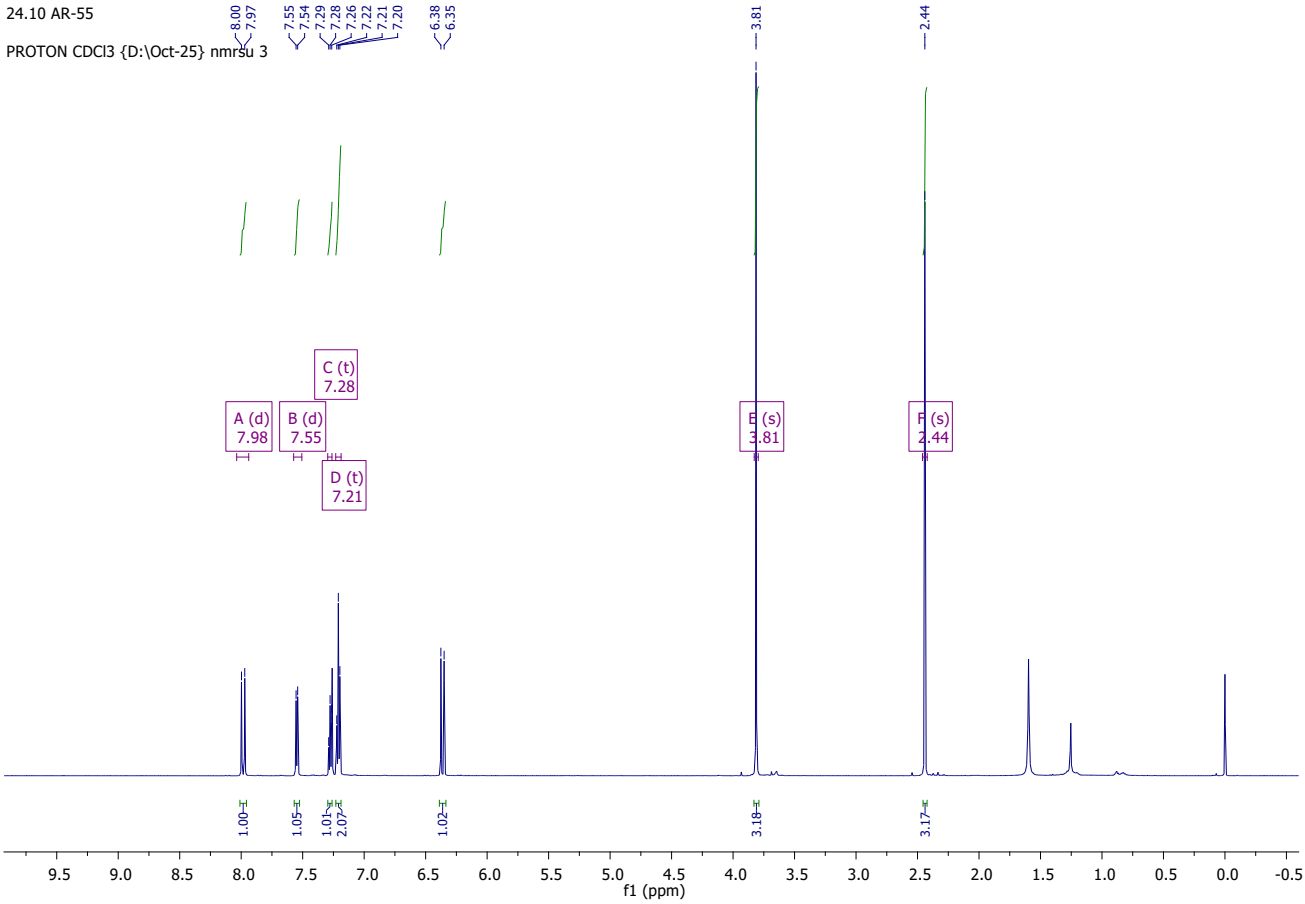
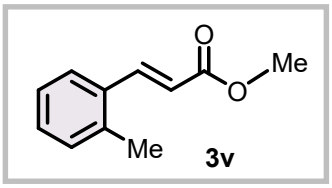


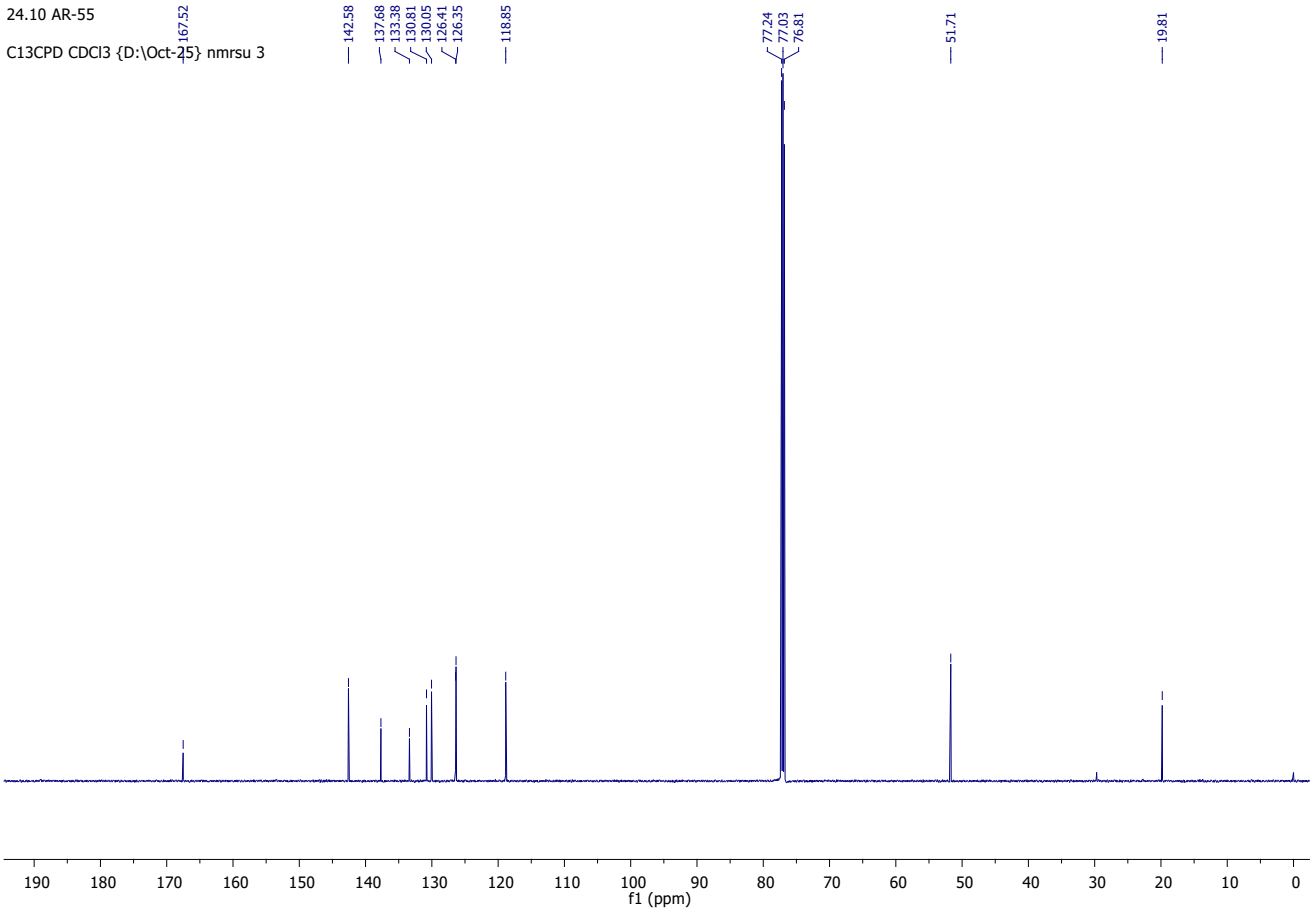
Compound 3v. ^{1}H NMR Spectrum ($CDCl_3$).



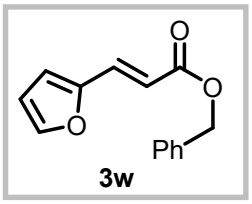


Compound 3v. ^{13}C NMR Spectrum ($CDCl_3$).

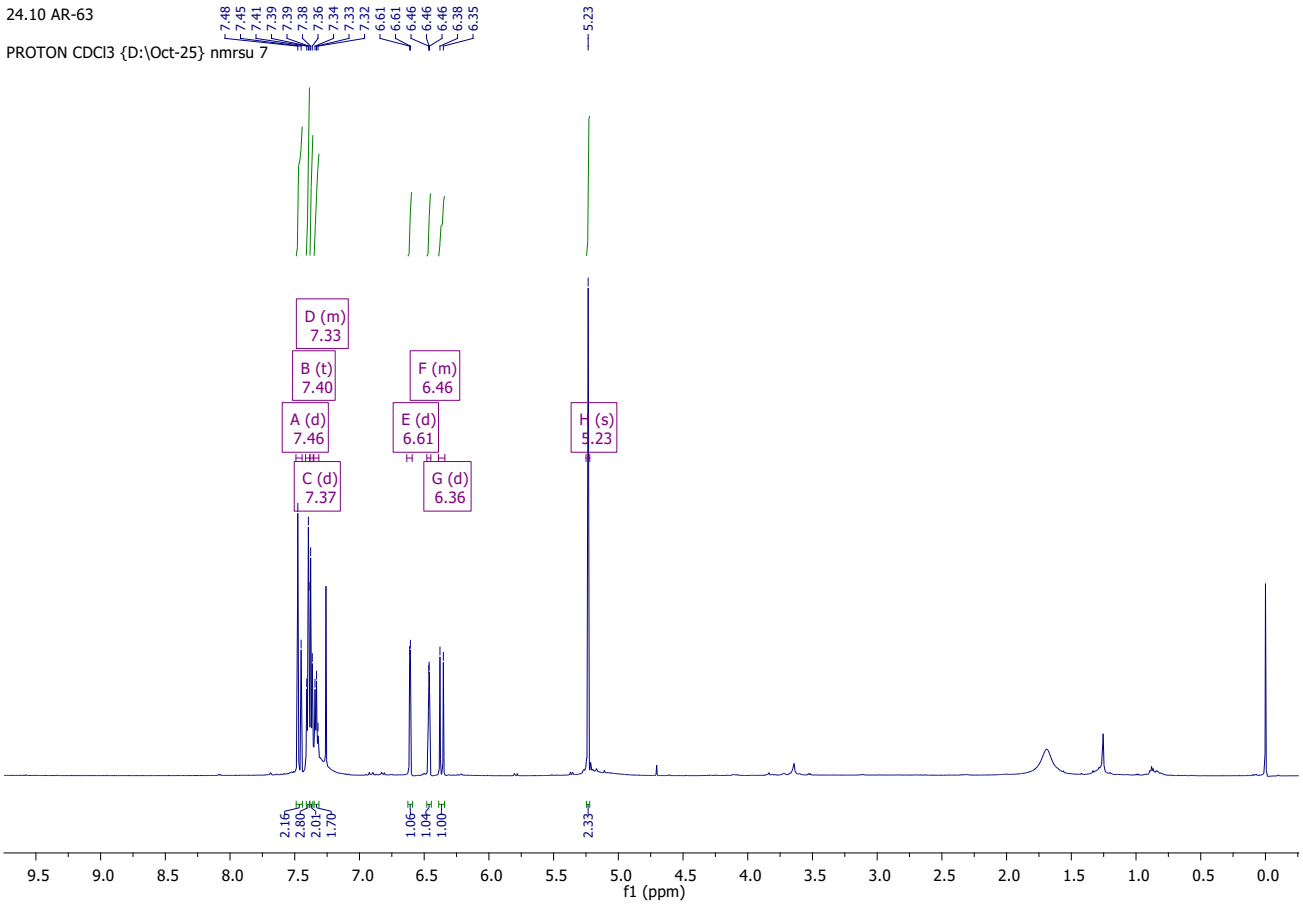




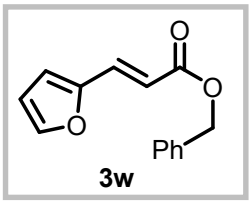
Compound 3w. ^{1}H NMR Spectrum ($CDCl_3$).



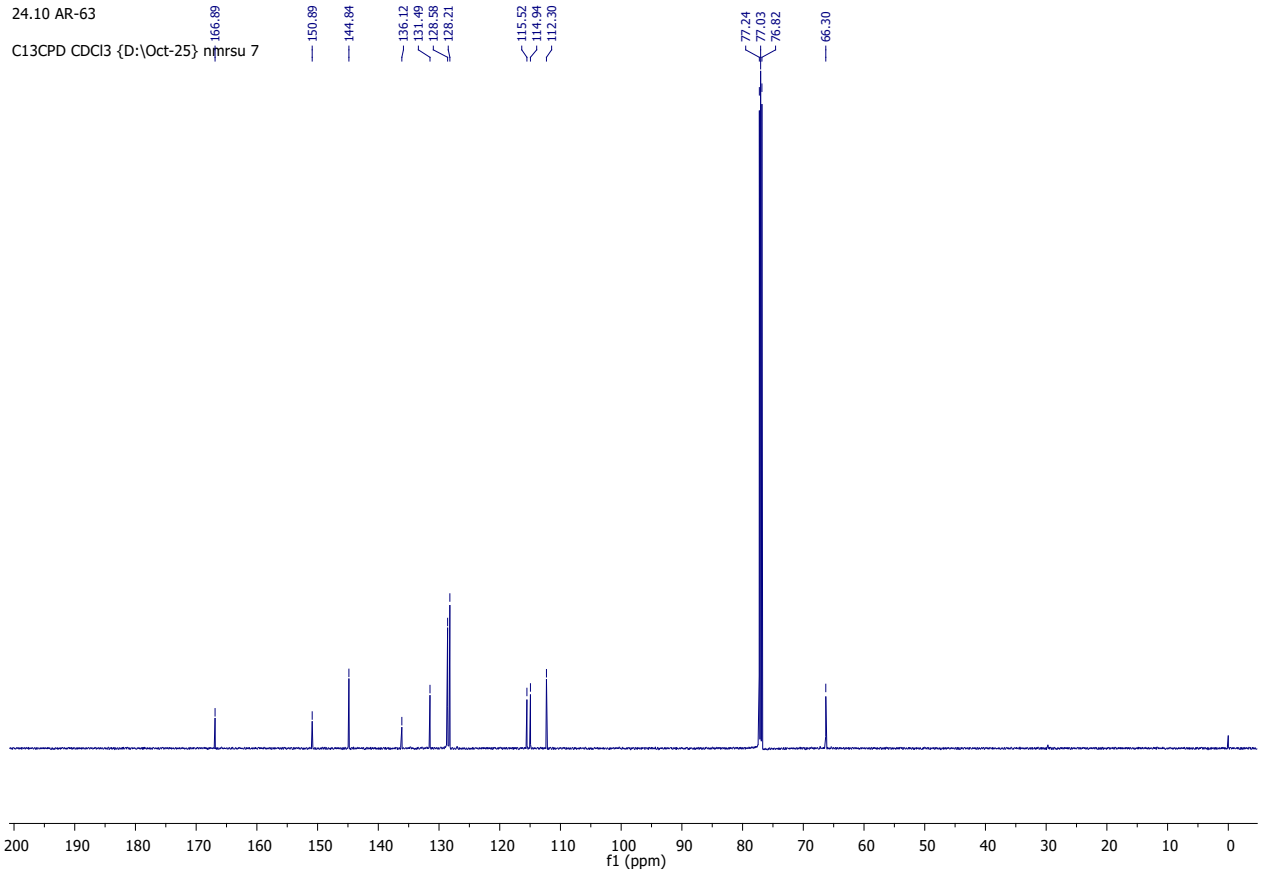
3w



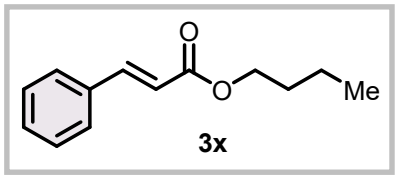
Compound 3w. ^{13}C NMR Spectrum ($CDCl_3$).



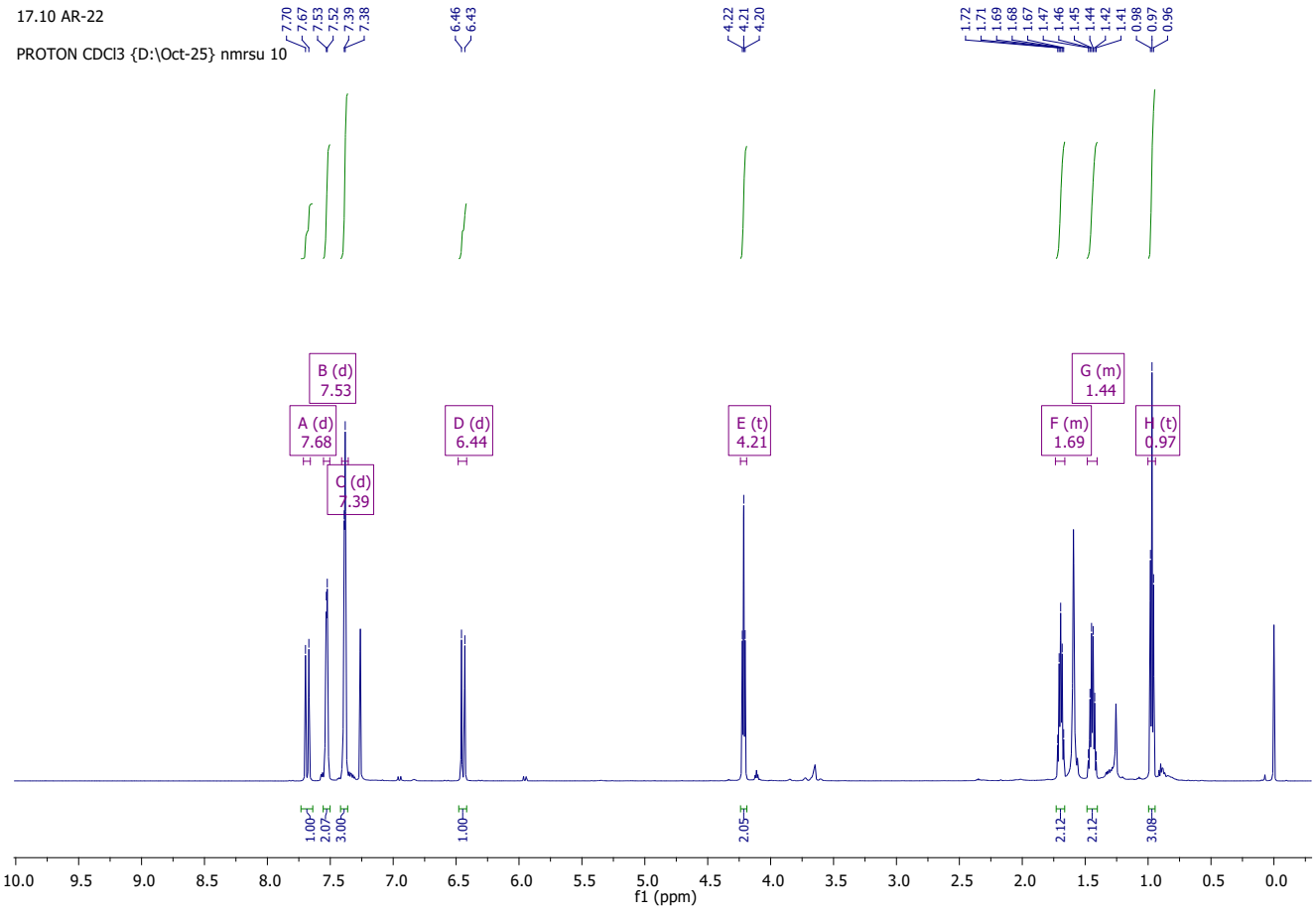
3w



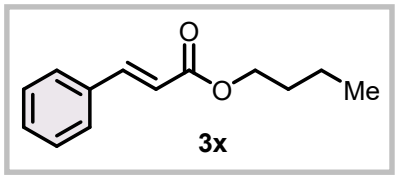
Compound 3x. ^{1}H NMR Spectrum ($CDCl_3$).



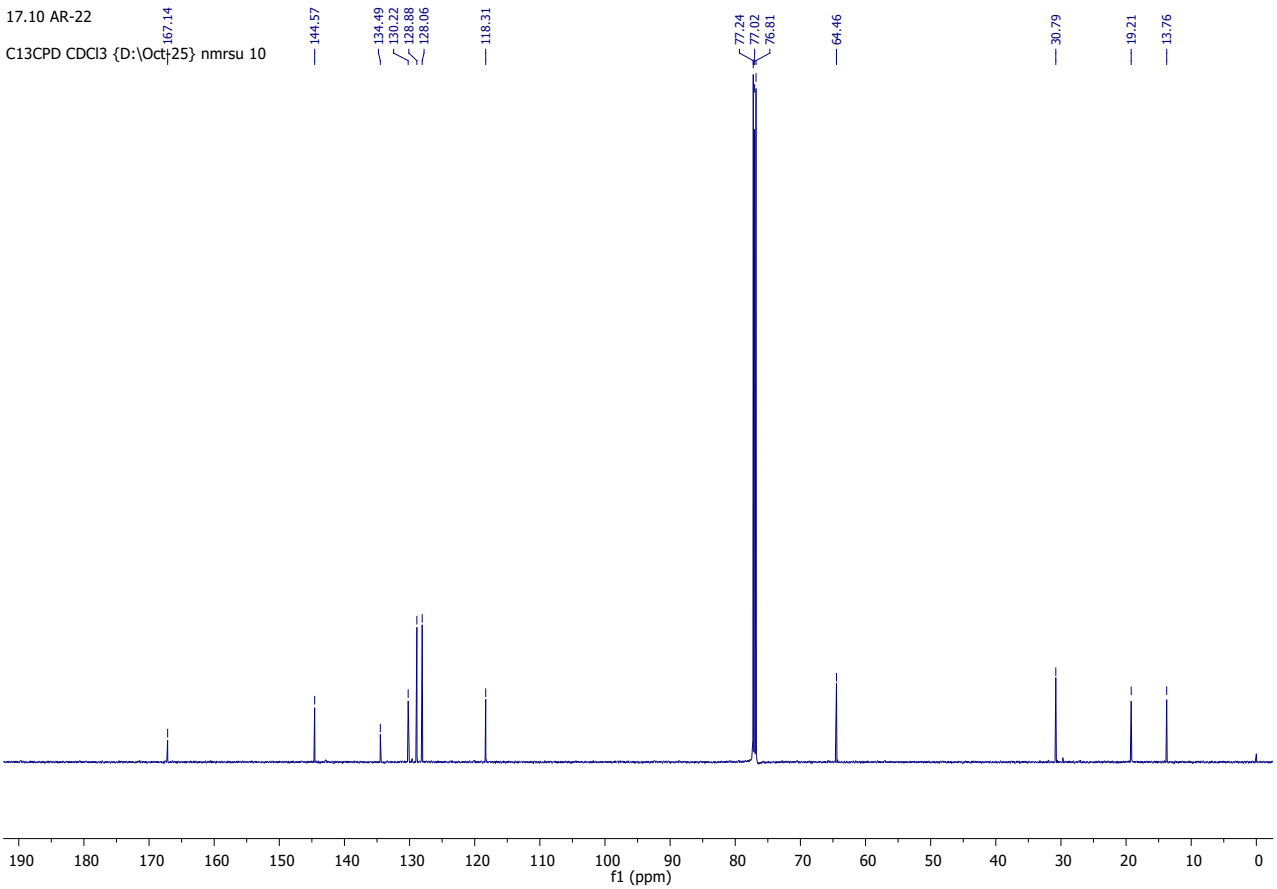
3x



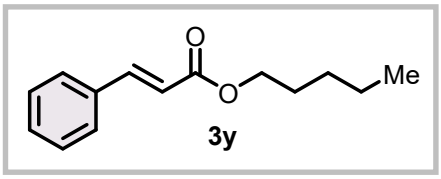
Compound 3x. ^{13}C NMR Spectrum ($CDCl_3$).



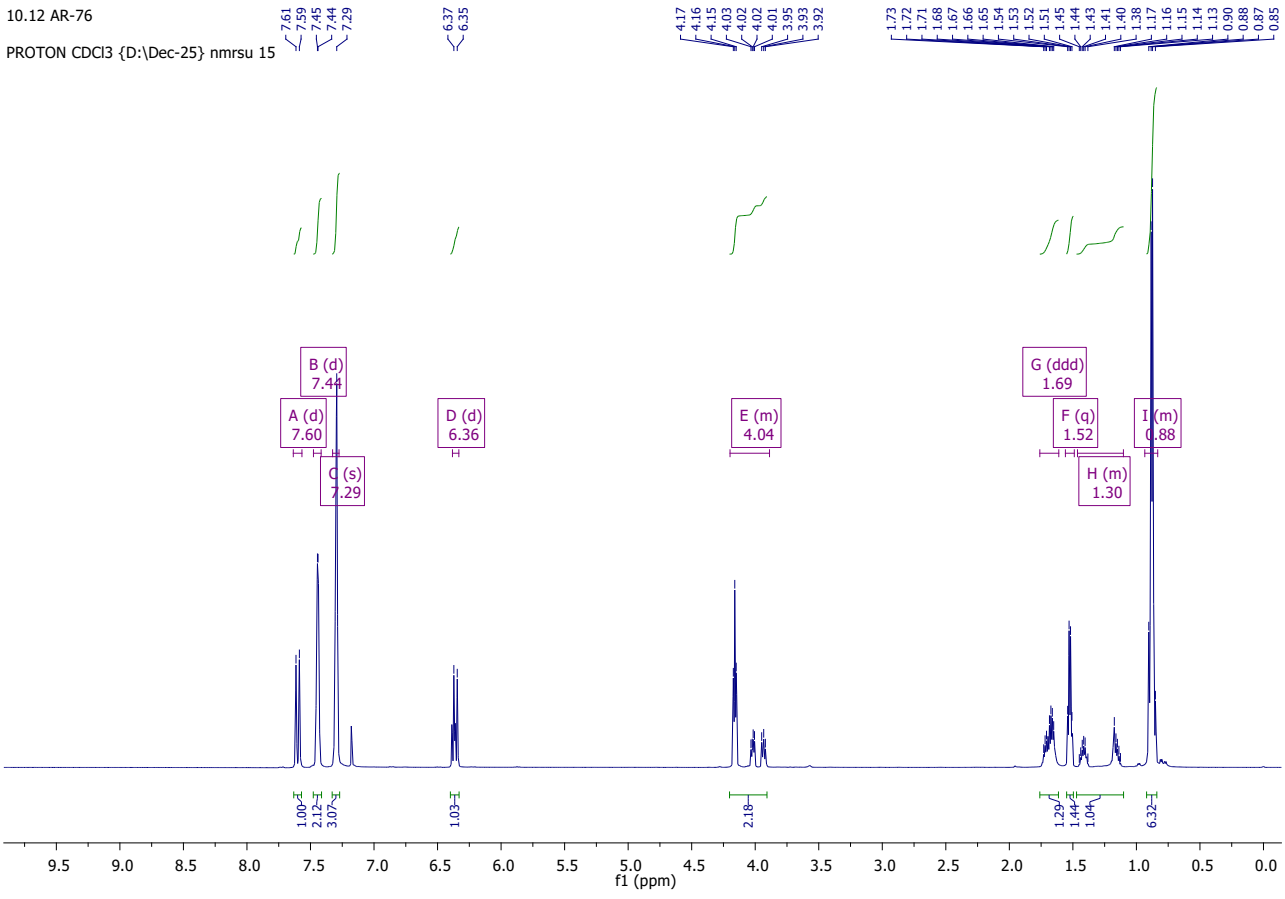
3x



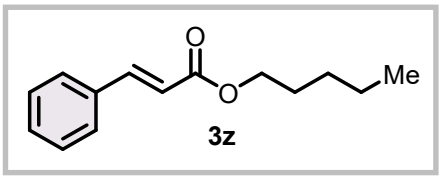
Compound 3y. ^{1}H NMR Spectrum ($CDCl_3$).



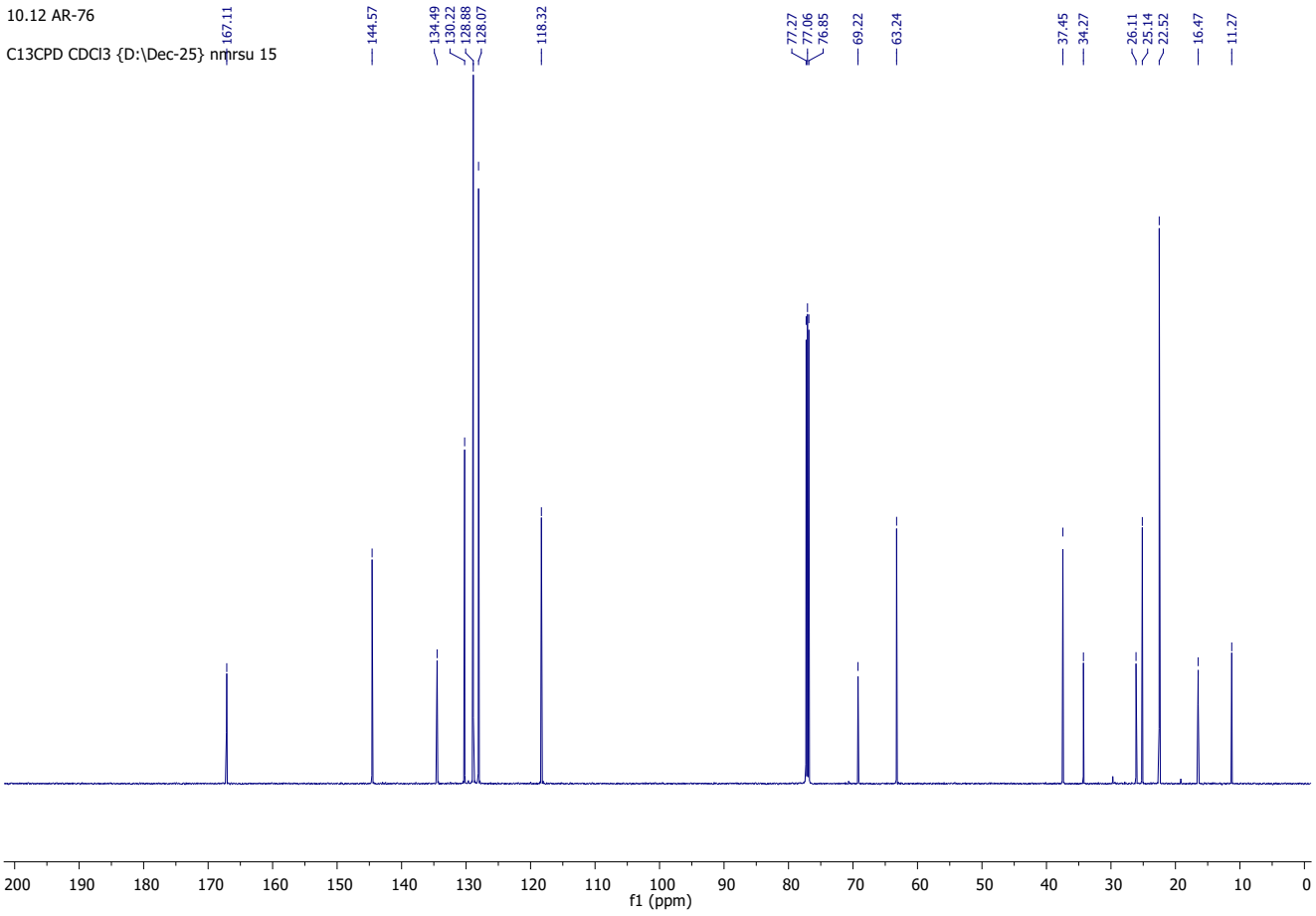
3y



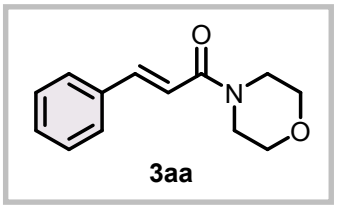
Compound 3z. ^{13}C NMR Spectrum ($CDCl_3$).



3z



Compound 3aa. ^{1}H NMR Spectrum ($CDCl_3$).



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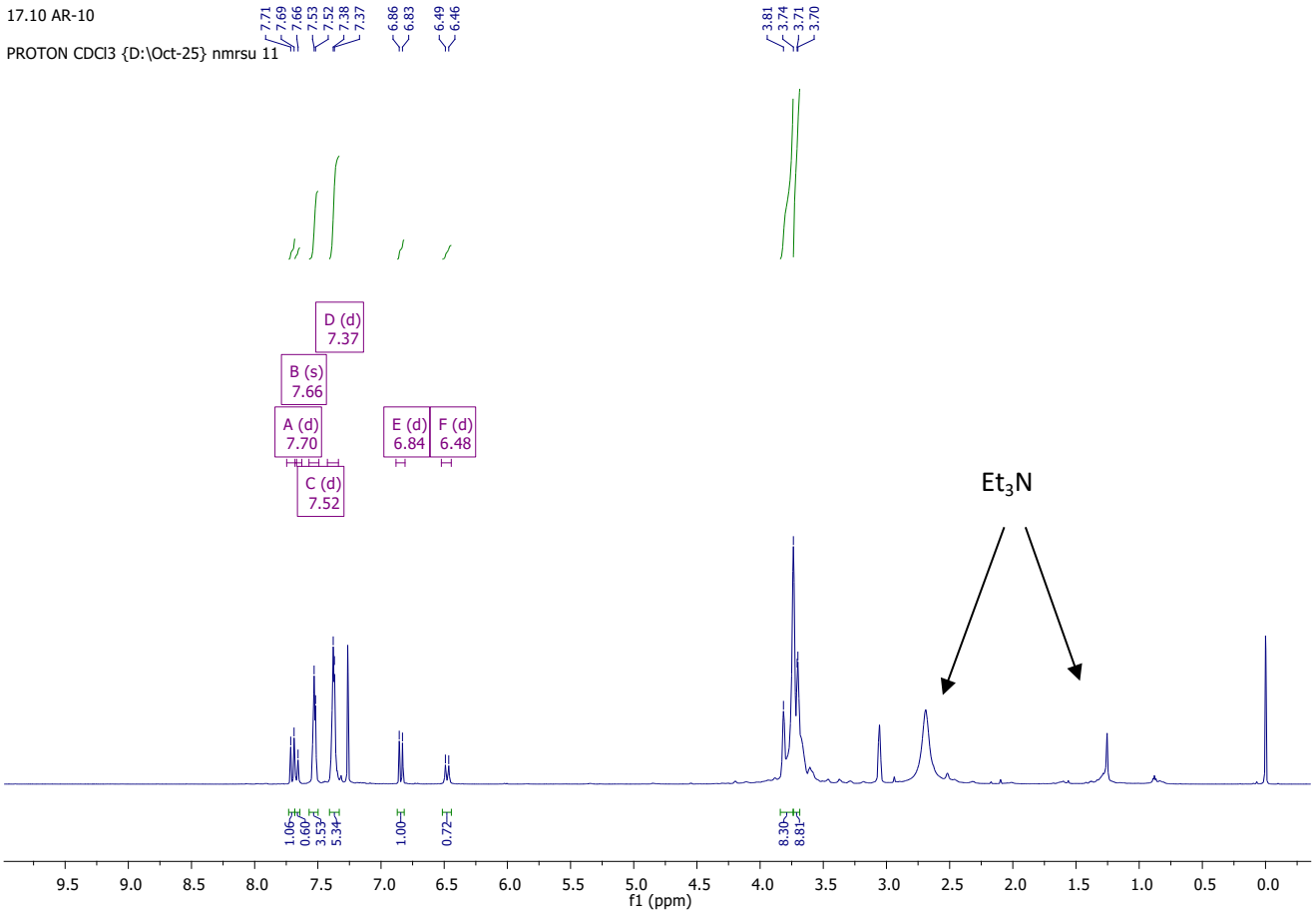
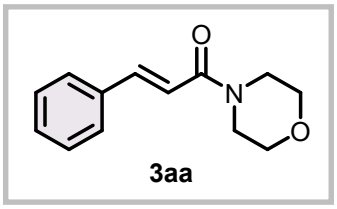
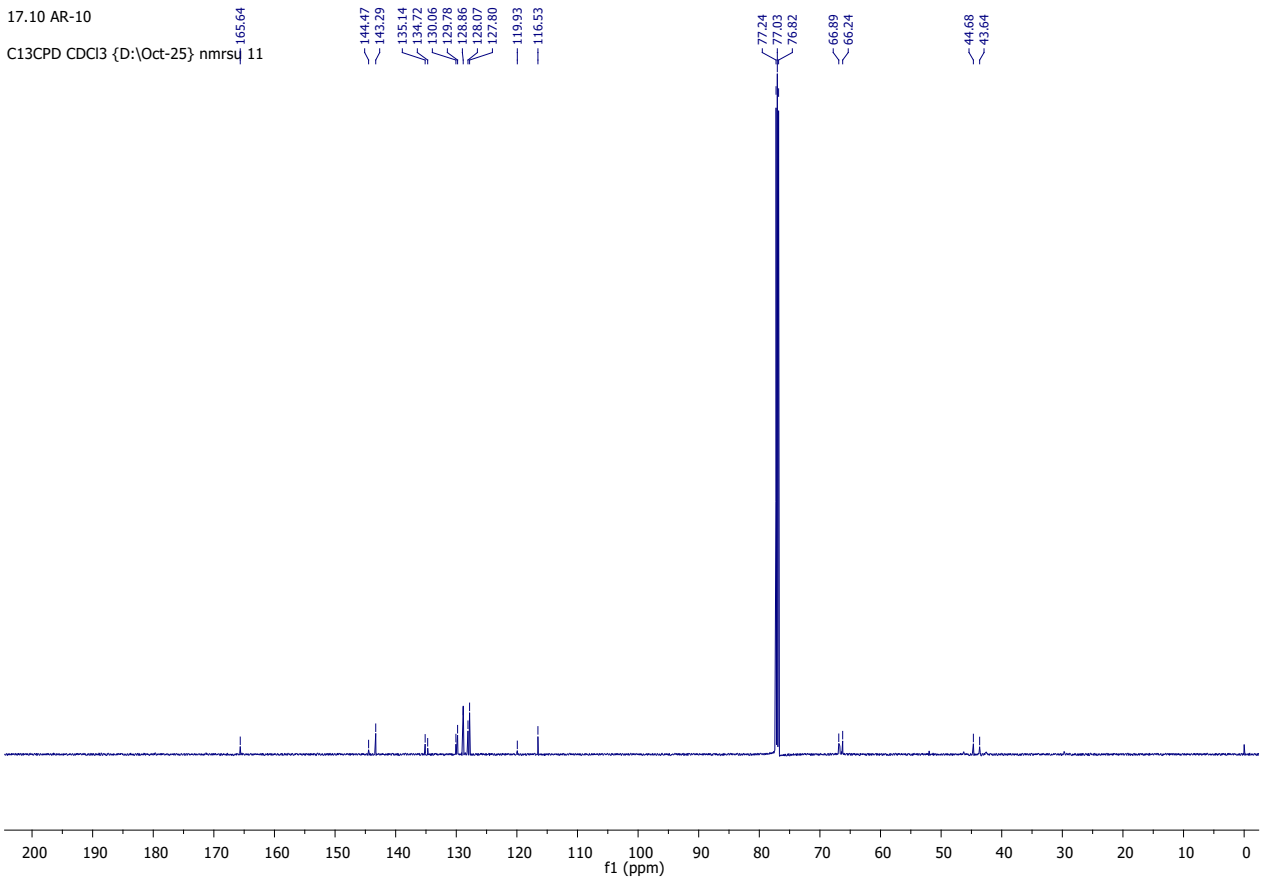


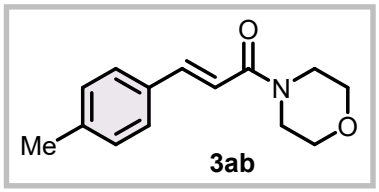
Compound 3aa. ^{13}C NMR Spectrum ($CDCl_3$).



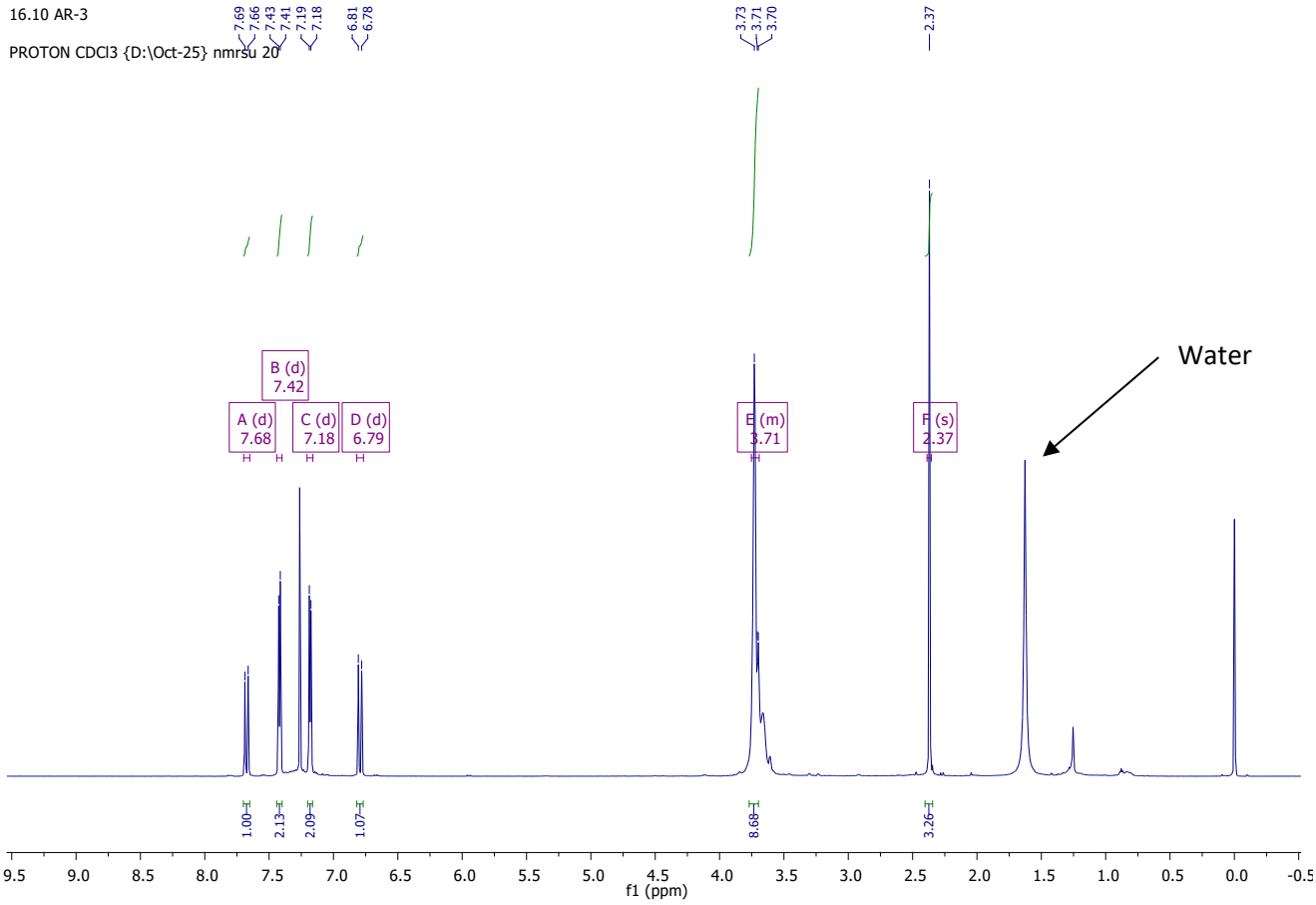
3aa



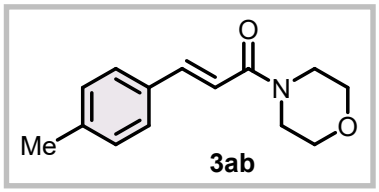
Compound 3ab. ^{1}H NMR Spectrum ($CDCl_3$).



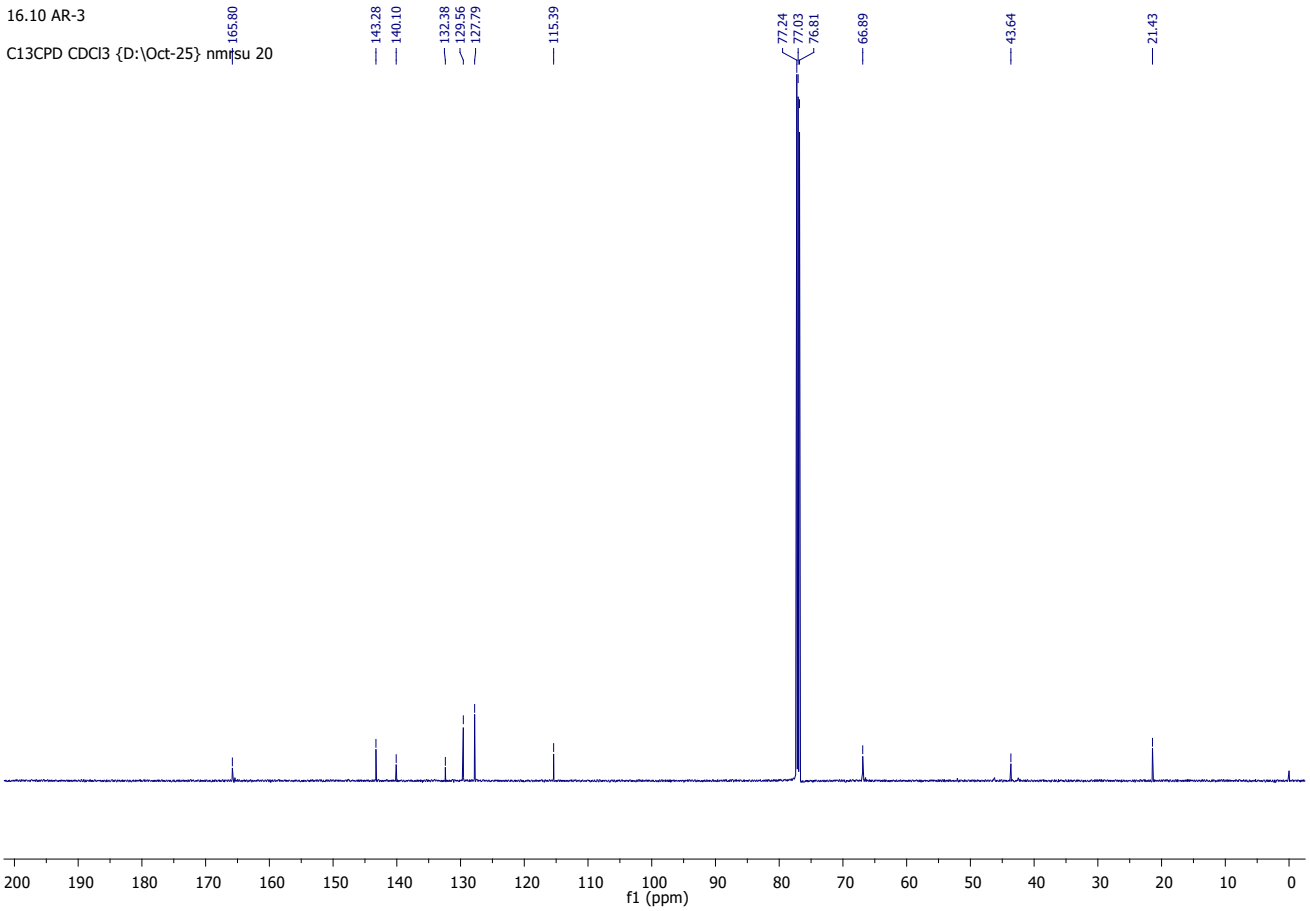
3ab



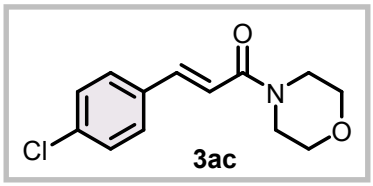
Compound 3ab. ^{13}C NMR Spectrum ($CDCl_3$).

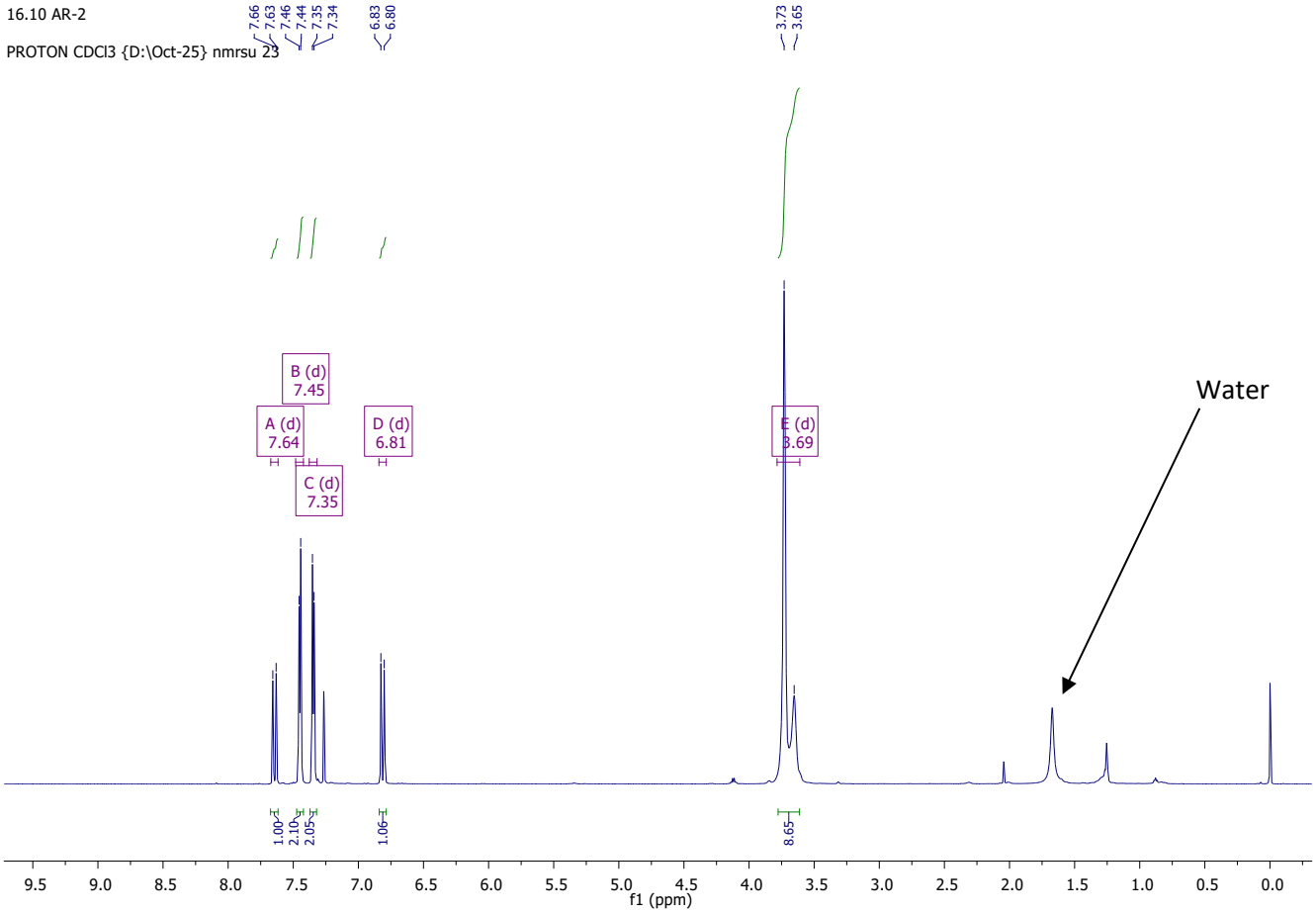


3ab

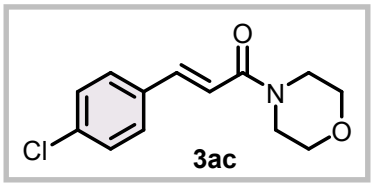


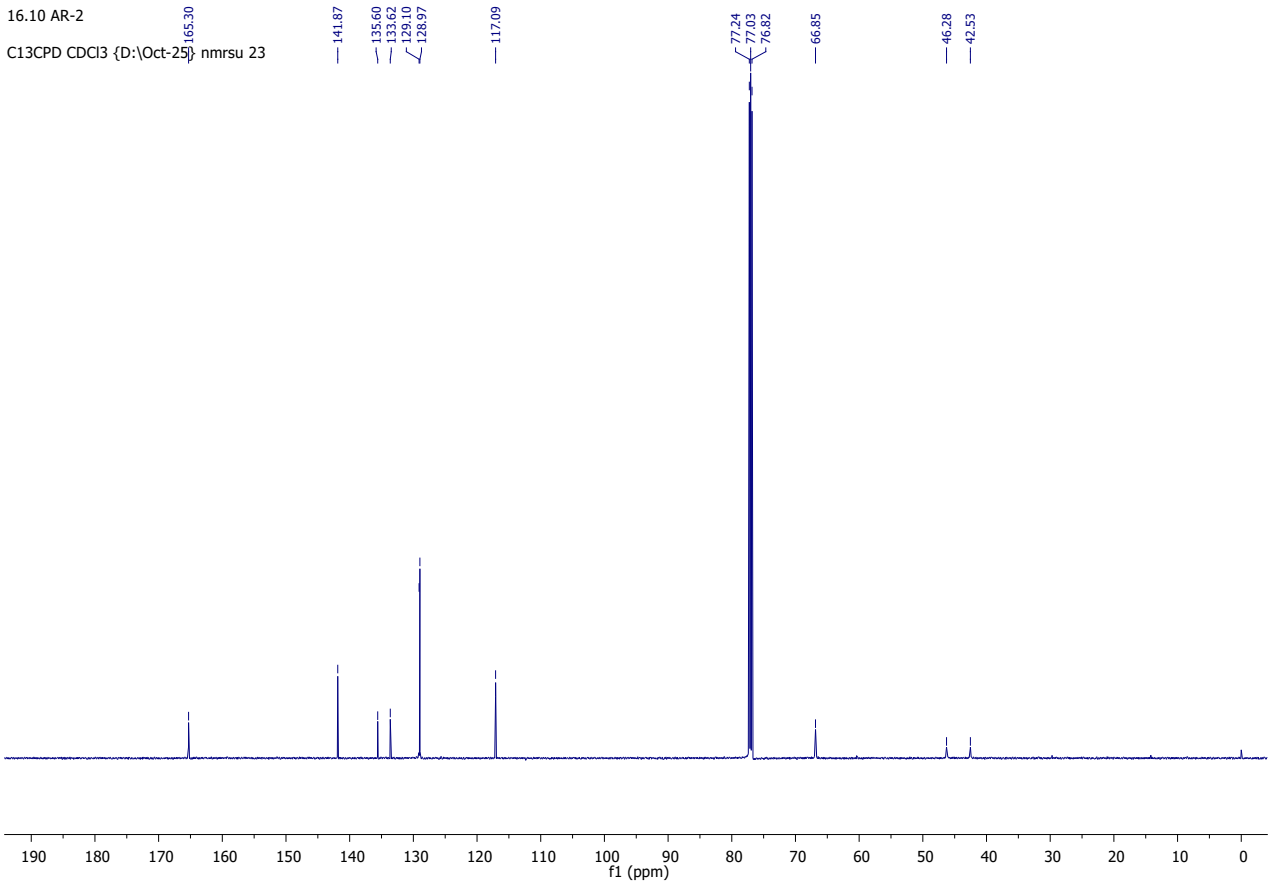
Compound 3ac. ^{1}H NMR Spectrum ($CDCl_3$).



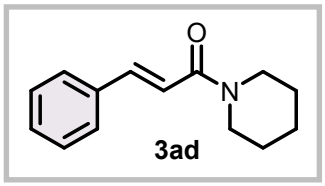


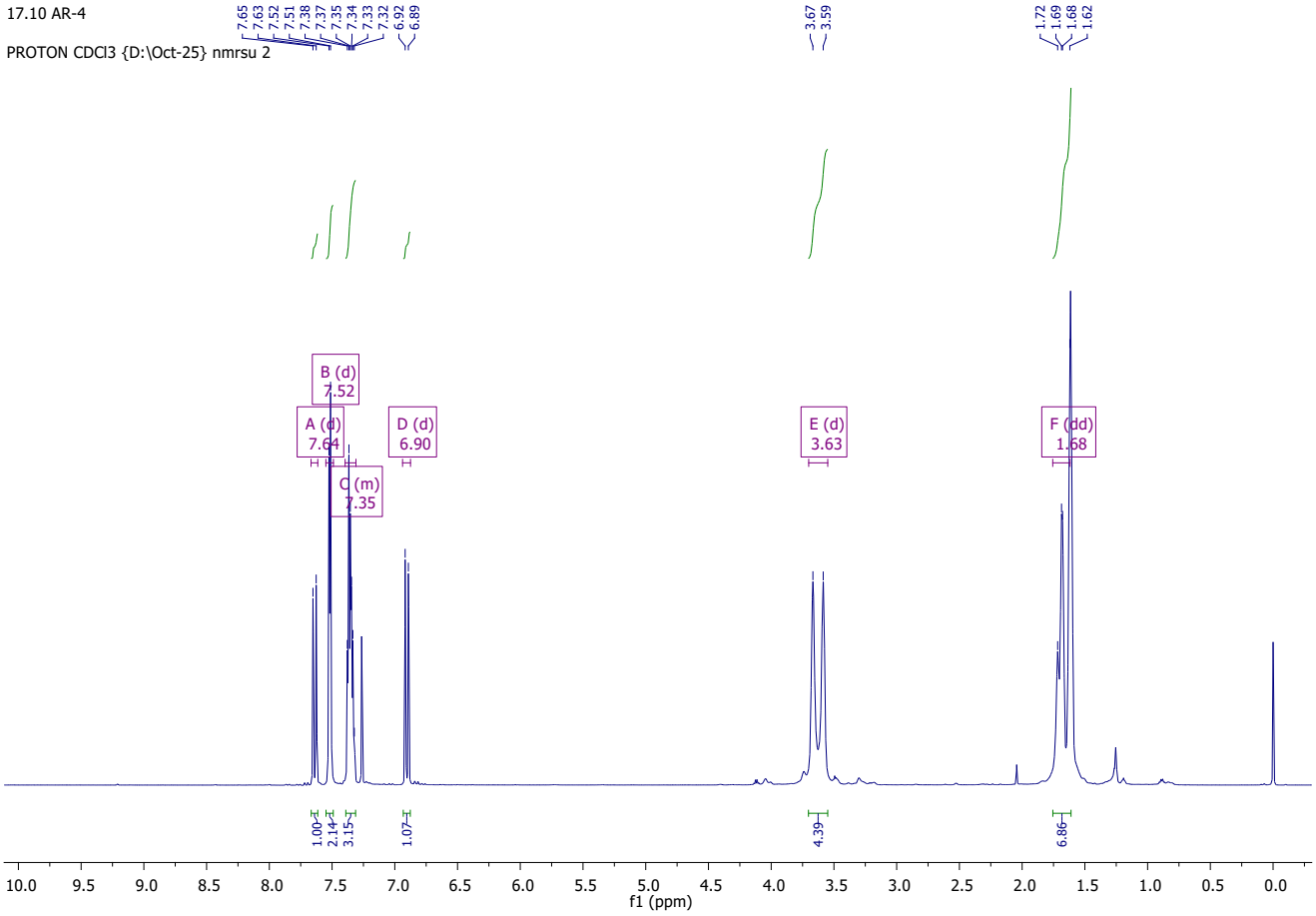
Compound 3ac. ^{13}C NMR Spectrum ($CDCl_3$).



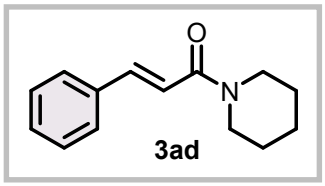


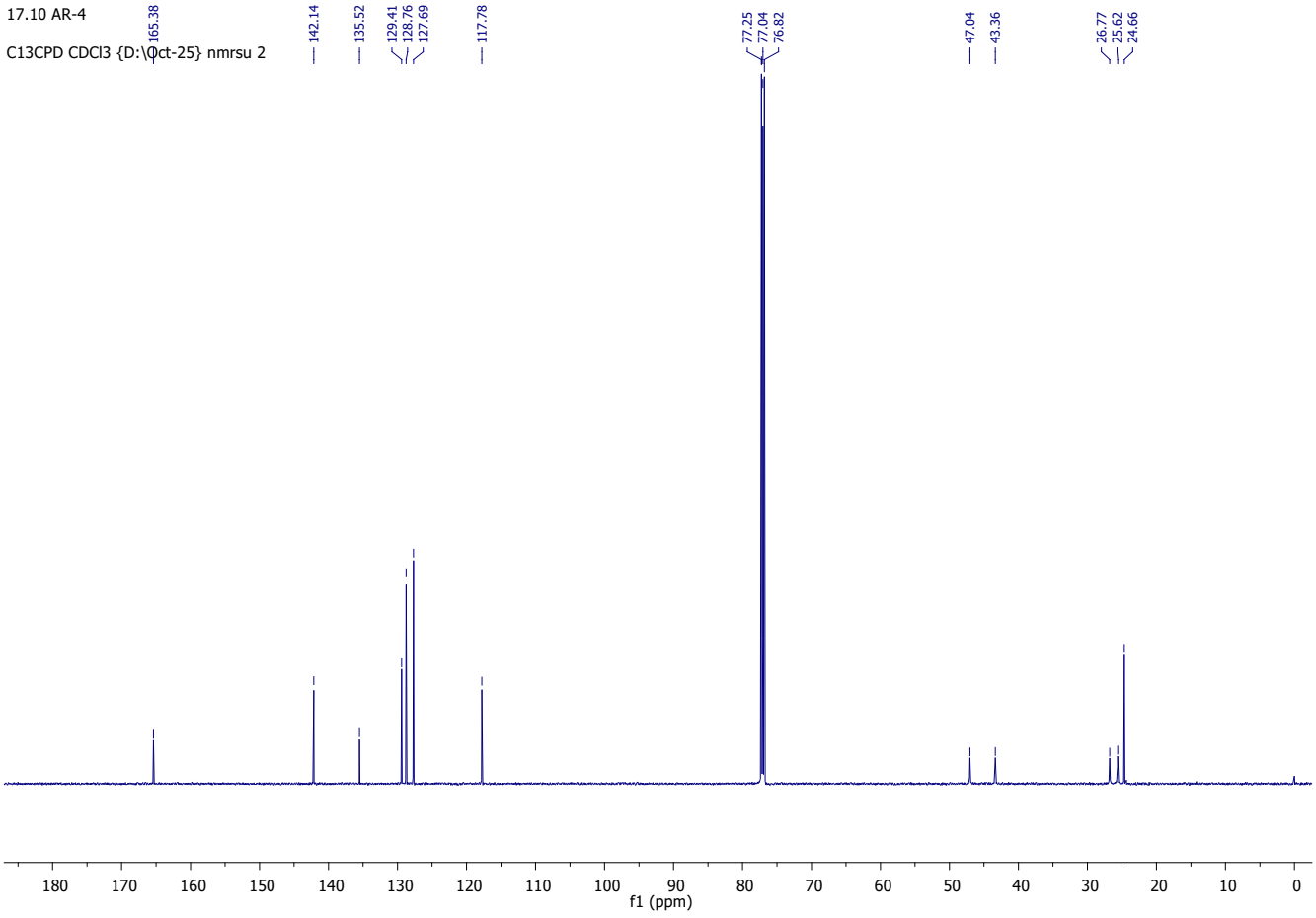
Compound 3ad. ^{1}H NMR Spectrum ($CDCl_3$).



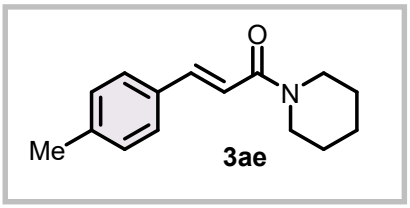


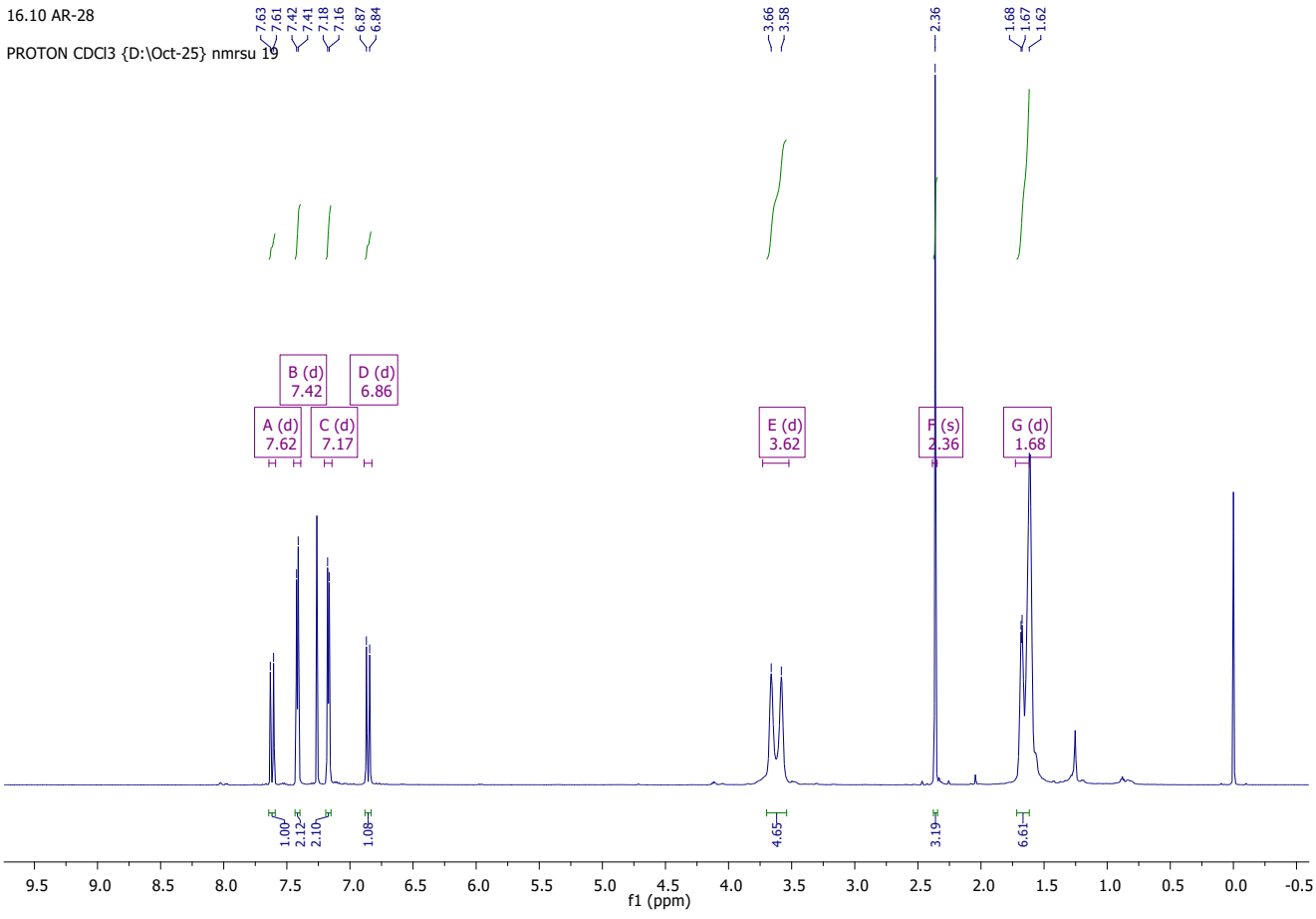
Compound 3ad. ^{13}C NMR Spectrum ($CDCl_3$).



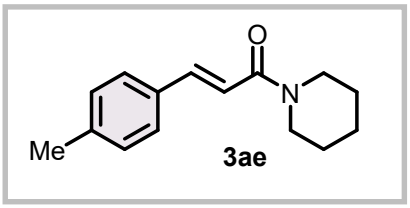


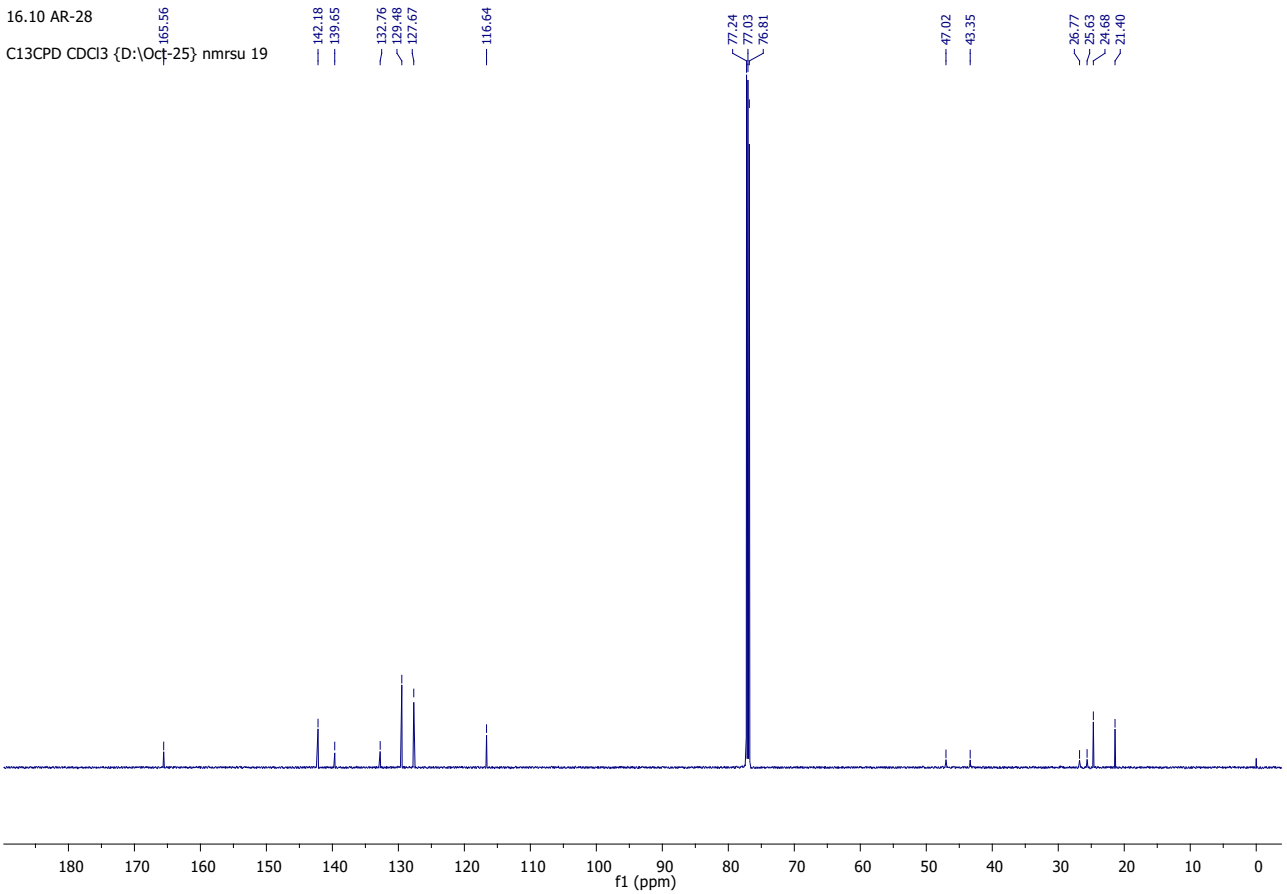
Compound 3ae. ^{1}H NMR Spectrum ($CDCl_3$).



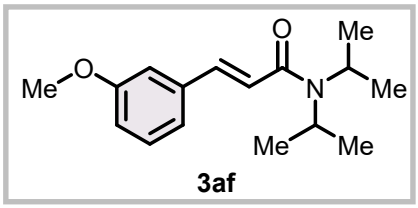


Compound 3ae. ^{13}C NMR Spectrum ($CDCl_3$).





Compound 3af. ^{1}H NMR Spectrum ($CDCl_3$).



3af