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Supporting Information

Oxygen as Single Oxidant for Two Steps: Base-Free One-Pot Pd(II)-Catalyzed Alcohol Oxidation & Arylation to Halogen-Intact β-Aryl α,β-Enones

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Table of Contents

Serial No.	Description	Page No.
1.1	General Experimental	S2
1.2	General Experimental Procedure	S2
1.3	Analytical Data	S3-S16
1.4	References	S17
1.5	^{1}H NMR and ^{13}C NMR Spectra	S18-S51

1.1 General Experimental Details:

All solvents and reagents were used, as received from the suppliers. TLC was performed on Merck Kiesel gel 60, F_{254} plates with the layer thickness of 0.25 mm. Column chromatography was performed on silica gel (100-200 mesh) using a gradient of ethyl acetate and hexane as mobile phase. Melting points were determined on a Fisher John's melting point apparatus and are uncorrected. IR spectra were recorded on a Bruker Alpha Spectrometer FT-IR system. ^{1}H NMR spectral data were collected at 300 (AVANCE & JCAMP), 400 (INOVA) & 500 (INOVA & AVANCE) MHz, while ^{13}C NMR were recorded at 75, 100 & 125 MHz. ^{1}H NMR spectral data are given as chemical shifts in ppm followed by multiplicity (s- singlet; d- doublet; t- triplet; q- quartet; m- multiplet), number of protons and coupling constants. ^{13}C NMR chemical shifts are expressed in ppm. HRMS (ESI) spectral data were collected using Q-star & ORBITRAP High Resolution Mass Spectrometer. Starting materials were prepared as previously reported [1-(4-Methoxyphenyl)prop-2-en-1-ol,[1a] 1-Phenylprop-2-en-1-ol,[1a] 1-*p*-Tolylprop-2-en-1-ol,[1a] 1-(4-Bromophenyl)prop-2-en-1-ol,[1b] 1-(Naphthalen-1-yl)prop-2-en-1-ol,[1a] 1-(4-Chlorophenyl)prop-2-en-1-ol,[1c] 5-Methylhex-1-en-3-ol,[1d] (*E*)-1-Phenylpenta-1,4-dien-3-ol[1e]]. But-3-en-2-ol and Pent-1-en-3-ol were purchased from Alfa Aesar. Oct-1-en-3-ol and Cyclohex-2-enol were purchased from Aldrich.

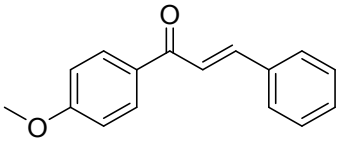
1.2 General Procedure for Synthesis of β-Aryl α,β-Enones from Allyl Alcohols

A solution of allylic alcohol (1.0 mmol) and $Pd(OAc)_2$ (0.022 g, 0.1 mmol) in DMF (3.0 mL) was taken in a 10.0 mL RB flask, which was then attached to an oxygen balloon (1atm. pressure). The mixture was vigorously stirred at 90 °C for 4 h. The RB flask was opened. After adding 2,9-dimethyl-1,10-phenanthroline (0.042 g, 0.20 mmol) and organoboronic acid (1.2 mmol) to the reaction mixture, the RB flask was again attached to the oxygen balloon (1atm. pressure) and the stirring continued for18 h at 90 °C. After cooling

to room temperature, the reaction mixture was partitioned between ethyl acetate (25.0 mL) and water (25.0 mL) in a separatory funnel. The organic layer was washed with water, and brine, dried over anhydrous Na_2SO_4 (s) and concentrated *in vacuo*. The residue was purified by column chromatography using a gradient of hexane and ethyl acetate (eluent system) to afford the pure product.

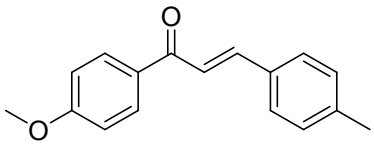
1.3 Analytical data for products

(*E*)-1-(4-Methoxyphenyl)-3-phenylprop-2-en-1-one (1)[2]



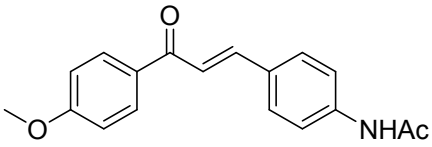
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.231 g, 97%). M.p. 90-92 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, J = 8.9 Hz, 2H), 7.80 (d, J = 15.7 Hz, 1H), 7.63 (dd, J = 6.4, 3.0 Hz, 2H), 7.54 (d, J = 15.7 Hz, 1H), 7.43 – 7.37 (m, 3H), 6.97 (d, J = 8.9 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.7, 163.5, 144.0, 135.1, 131.1, 130.9, 130.4, 129.0, 128.4, 121.8, 113.9, 55.5; (IR, Neat): 3061, 1690, 1657, 1598, 1450, 1216, 764, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{15}O_2]^+$ 239.10666; Found 239.10722.

(*E*)-1-(4-Methoxyphenyl)-3-*p*-tolylprop-2-en-1-one (2)[2]



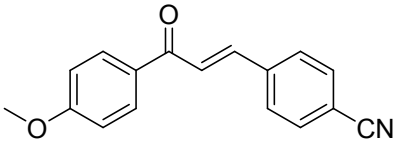
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.229 g, 91%). M.p. 123-125 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, J = 8.8 Hz, 2H), 7.79 (d, J = 15.6 Hz, 1H), 7.54 (d, J = 6.6 Hz, 2H), 7.50 (d, J = 14.3 Hz, 1H), 7.21 (d, J = 7.9 Hz, 2H), 6.97 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.8, 163.4, 144.1, 140.8, 132.4, 131.3, 130.8, 129.7, 128.4, 120.9, 113.8, 55.5, 21.5; (IR, Neat): 2933, 1651, 1594, 1567, 1414, 1171, 807, 606 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{17}O_2]^+$ 253.12231; Found 253.12251.

(*E*)-*N*-(4-(3-(4-Methoxyphenyl)-3-oxoprop-1-enyl)phenyl)acetamide (3)[4]



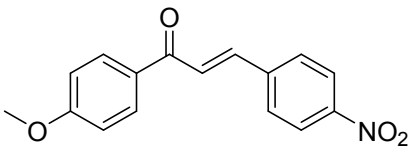
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 20% ethyl acetate in hexane as the eluent) to afford the title product as a light brown solid (0.248 g, 84%). M.p. 148-150 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.9 Hz, 2H), 7.84 (s, 1H), 7.75 (d, J = 15.6 Hz, 2H), 7.62 – 7.56 (m, 3H), 7.52 – 7.47 (m, 1H), 7.42 (d, J = 17.9 Hz, 1H), 6.98 (d, J = 8.9 Hz, 2H), 3.89 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$+DMSO-d_6) δ 186.8, 167.8, 167.0, 142.1, 140.2, 129.4, 128.4, 128.0, 120.3, 118.8, 118.2, 113.9, 54.2, 22.6; (IR, Neat): 3307, 2943, 1654, 1597, 1512, 1412, 1221, 1020, 750 cm^{-1}; HRMS (ESI): Calculated for $[C_{18}H_{19}O_3N]^+$ 296.12812; Found 296.12873.

(*E*)-4-(3-(4-Methoxyphenyl)-3-oxoprop-1-enyl)benzonitrile (4)[5]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.242 g, 92%). M.p. 165-167 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 15.7 Hz, 1H), 7.69 (dd, J = 8.3, 2.0 Hz, 4H), 7.61 (d, J = 15.7 Hz, 1H), 6.99 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 187.8, 163.8, 141.2, 139.4, 132.6, 130.9, 130.5, 128.6, 125.0, 118.4, 114.0, 113.2, 55.6; (IR, Neat): 3016, 2219, 1656, 1596, 1507, 1415, 1221, 811, 603 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{14}NO_2]^+$ 264.10191; Found 264.10266.

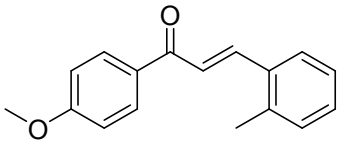
(*E*)-1-(4-Methoxyphenyl)-3-(4-nitrophenyl)prop-2-en-1-one (5)[5]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 15 % ethyl acetate in hexane as the eluent) to

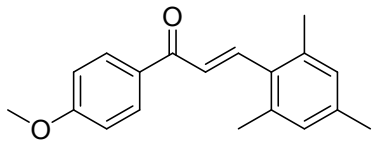
afford the title product as a yellow solid (0.240 g, 85%). M.p. 178-180 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, J = 8.8 Hz, 2H), 8.06 (d, J = 8.9 Hz, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.78 (d, J = 8.8 Hz, 2H), 7.66 (d, J = 15.7 Hz, 1H), 7.01 (d, J = 8.9 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.8, 163.9, 148.4, 141.3, 140.7, 131.0, 130.4, 128.9, 125.6, 124.2, 114.1, 55.6; (IR, Neat): 3018, 1657, 1596, 1513, 1342, 1225, 825, 756 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{14}NO_4]^+$ 284.09173; Found 284.09262.

(*E*)-1-(4-Methoxyphenyl)-3-*o*-tolylprop-2-en-1-one (6)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.204 g, 81%). M.p. 98-100 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, J = 15.6 Hz, 1H), 8.05 (d, J = 8.9 Hz, 2H), 7.69 (d, J = 7.8 Hz, 1H), 7.47 (d, J = 15.5 Hz, 1H), 7.30 – 7.21 (m, 3H), 6.98 (d, J = 8.9 Hz, 2H), 3.88 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.7, 163.5, 141.6, 138.2, 134.2, 131.2, 130.9, 130.8, 130.1, 126.4, 126.3, 123.1, 113.9, 55.5, 19.9; (IR, Neat): 3014, 1656, 1591, 1569, 1483, 1214, 738, 673 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{17}O_2]^+$ 253.12231; Found 253.12285.

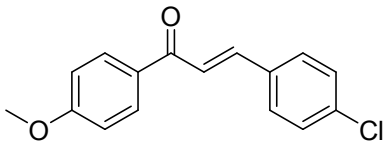
(*E*)-3-Mesityl-1-(4-methoxyphenyl)prop-2-en-1-one (7)[5]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.224 g, 80%). M.p. 77-79 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, J = 8.9 Hz, 2H), 7.94 (d, J = 16.0 Hz, 1H), 7.16 (d, J = 16.0 Hz, 1H), 6.97 (d, J = 8.9 Hz, 2H), 6.92 (s, 2H), 3.88 (s, 3H), 2.39 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.8, 163.4, 142.5, 138.4, 137.1, 131.1, 130.9, 130.2, 129.3, 127.2, 113.9, 55.5, 21.3, 21.1; (IR, Neat): 2935, 1658, 1597, 1459, 1167, 748, 666 cm^{-1}; HRMS (ESI): Calculated for

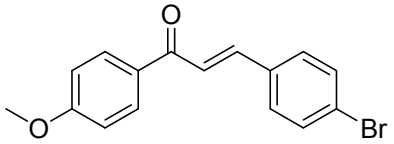
$[C_{19}H_{21}O_2]^+$ 281.15361; Found 281.15390.

(*E*)-3-(4-Chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (8)[3]



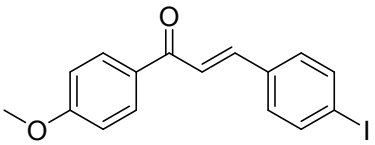
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.247 g, 91%). M.p. 128-130 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 (d, J = 8.8 Hz, 2H), 7.72 (d, J = 15.6 Hz, 1H), 7.54 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 15.9 Hz, 1H), 7.35 (d, J = 8.4 Hz, 2H), 6.96 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (125 Hz, $CDCl_3$) δ 188.3, 163.5, 142.4, 136.2, 133.6, 130.9, 130.8, 129.5, 129.2, 122.3, 113.9, 55.5; (IR, Neat): 3018, 1659, 1605, 1491, 1215, 743, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{14}O_2Cl]^+$ 273.06768; Found 273.06839.

(*E*)-3-(4-Bromophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (9)[3]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.294 g, 93%). M.p. 146-148 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.9 Hz, 2H), 7.72 (d, J = 15.6 Hz, 1H), 7.51 (dd, J = 15.4, 8.6 Hz, 5H), 6.97 (d, J = 8.9 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.2, 163.5, 142.4, 133.9, 132.1, 130.8, 129.6, 124.4, 122.3, 113.8, 55.4; (IR, Neat): 3010, 1656, 1601, 1483, 1219, 810, 746, 671 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{14}O_2Br]^+$ 317.01717; Found 317.01798.

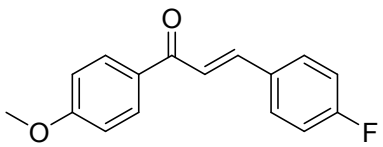
(*E*)-3-(4-Iodophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (10)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.323 g, 89%). M.p. 179-181 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J

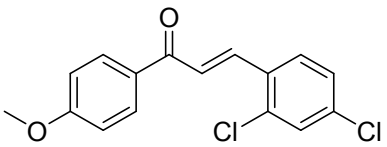
= 8.9 Hz, 2H), 7.74 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 15.7 Hz, 1H), 7.54 (d, J = 15.6 Hz, 1H), 7.48 (d, J = 8.9 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.9, 163.7, 143.1, 138.1, 137.4, 134.4, 130.9, 129.8, 122.3, 113.9, 96.7, 55.5; (IR, Neat): 2924, 1657, 1600, 1484, 1220, 772, 635 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{14}O_2I]^+$ 365.00330; Found 365.00475.

(*E*)-3-(4-Fluorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (11)[3]



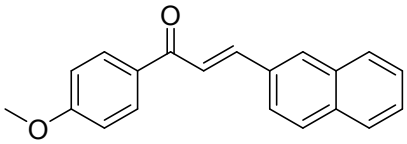
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.225 g, 88%). M.p. 113-115 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, J = 8.8 Hz, 2H), 7.76 (d, J = 15.6 Hz, 1H), 7.63 (dd, J = 8.6, 5.5 Hz, 2H), 7.47 (d, J = 15.6 Hz, 1H), 7.10 (dd, J = 8.6 Hz, 2H), 6.98 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.4, 165.6, 162.3, 142.6, 130.8, 130.3, 130.2, 121.6, 116.2, 115.9, 113.9, 55.5; (IR, Neat): 3010, 1654, 1596, 1503, 1417, 1171, 811, 746 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{14}O_2F]^+$ 257.09723; Found 257.09776.

(*E*)-3-(2,4-Dichlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (12)[3]



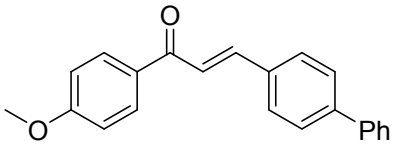
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.263 g, 86%). M.p. 136-138 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, J = 15.8 Hz, 1H), 8.02 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 8.5 Hz, 1H), 7.47 (d, J = 16.4 Hz, 1H), 7.44 (s, 1H), 7.28 (d, J = 8.9 Hz, 1H), 6.97 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.2, 163.6, 138.4, 136.2, 135.9, 132.1, 130.9, 130.7, 130.1, 128.5, 127.5, 124.9, 113.9, 55.5; (IR, Neat): 2996, 1651, 1594, 1573, 1464, 1216, 816, 748 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{13}O_2Cl_2]^+$ 307.02871; Found 307.02957.

(*E*)-1-(4-Methoxyphenyl)-3-(naphthalen-2-yl)prop-2-en-1-one (13)[6]



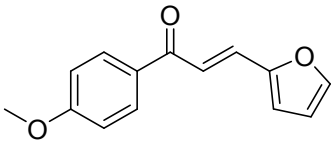
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.233 g, 81%). M.p. 140-142 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, J = 8.8 Hz, 2H), 8.00 – 7.95 (m, 2H), 7.83 (d, J = 8.5 Hz, 2H), 7.78 – 7.72 (m, 2H), 7.65 (d, J = 15.6 Hz, 1H), 7.51 – 7.48 (m, 2H), 6.97 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 163.6, 144.5, 131.0, 130.7, 129.7, 128.7, 128.7, 127.8, 127.7, 127.3, 126.8, 126.4, 123.7, 123.3, 121.9, 113.9, 55.5; (IR, Neat): 2925, 1652, 1592, 1437, 1211, 771, 665 cm^{-1}; HRMS (ESI): Calculated for $[C_{20}H_{17}O_2]^+$ 289.12231; Found 289.12314.

(*E*)-3-(Biphenyl-4-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (14)[5]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.260 g, 83%). M.p. 150-152 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, J = 8.7 Hz, 2H), 7.85 (d, J = 15.6 Hz, 1H), 7.73 – 7.59 (m, 6H), 7.52 (d, J = 21.7 Hz, 1H), 7.41 (dt, J = 25.7, 7.2 Hz, 3H), 6.99 (d, J = 8.7 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.6, 163.4, 143.5, 143.1, 140.2, 134.0, 131.1, 130.8, 128.9, 128.9, 127.9, 127.6, 127.0, 121.7, 113.9, 55.5; (IR, Neat): 2962, 1661, 1598, 1485, 1221, 771, 692 cm^{-1}; HRMS (ESI): Calculated for $[C_{22}H_{19}O_2]^+$ 315.13796; Found 315.13792.

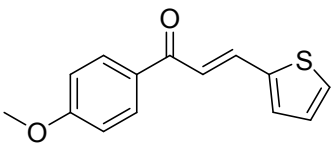
(*E*)-3-(Furan-2-yl)-1-(4-methoxyphenyl)prop-2-en-1-one (15)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a

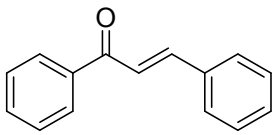
light brown solid (0.180 g, 79%). M.p. 85-87 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 2H), 7.61 – 7.43 (m, 3H), 6.97 (d, J = 8.9 Hz, 2H), 6.69 (d, J = 3.2 Hz, 1H), 6.52 – 6.48 (m, 1H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.1, 163.4, 151.8, 144.7, 131.1, 130.8, 130.0, 119.2, 115.8, 113.8, 112.6, 55.5; (IR, Neat): 2943, 1655, 1603, 1419, 1018, 753, 665 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{13}O_3]^+$ 229.08592; Found 229.08592.

(*E*)-1-(4-Methoxyphenyl)-3-(thiophen-2-yl)prop-2-en-1-one (16)[6]



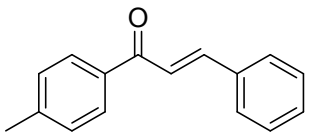
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a light brown solid (0.200 g, 82%). M.p. 105-107 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.9 Hz, 2H), 7.94 (d, J = 15.3 Hz, 1H), 7.44 – 7.31 (m, 3H), 7.09 (dd, J = 5.0, 3.7 Hz, 1H), 6.98 (d, J = 8.9 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.1, 163.4, 140.6, 136.4, 131.8, 130.7, 128.4, 128.3, 120.6, 113.8, 55.5; (IR, Neat): 3007, 1652, 1585, 1508, 1419, 1237, 821, 707 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{13}O_2S]^+$ 245.06308; Found 245.06370.

(*E*)-1,3-Diphenylprop-2-en-1-one (17)[8]



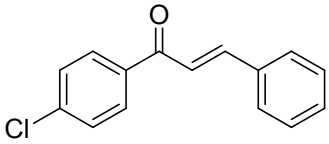
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.189 g, 91%). M.p. 54-56 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 2H), 7.81 (d, J = 15.7 Hz, 1H), 7.63 (dd, J = 6.7, 2.8 Hz, 2H), 7.57 (dd, J = 14.3, 6.8 Hz, 2H), 7.50 (dd, J = 12.9, 5.1 Hz, 2H), 7.41 (dd, J = 4.9, 1.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.3, 144.6, 138.0, 134.7, 132.6, 130.4, 128.8, 128.5, 128.4, 128.3, 121.9; (IR, Neat): 3059, 1661, 1641, 1573, 1448, 1210, 975, 742, 684 cm^{-1}; HRMS (ESI): Calculated for $[C_{15}H_{13}O]^+$ 209.09609; Found 209.09664.

(*E*)-3-Phenyl-1-*p*-tolylprop-2-en-1-one (18)[8]



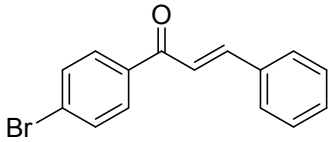
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.197 g, 89%). M.p. 78-80 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, J = 8.2 Hz, 2H), 7.80 (d, J = 15.7 Hz, 1H), 7.64 (dd, J = 6.5, 3.0 Hz, 2H), 7.53 (d, J = 15.7 Hz, 1H), 7.41 (dd, J = 5.1, 2.0 Hz, 3H), 7.30 (d, J = 8.0 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.0, 144.4, 143.7, 135.6, 135.0, 130.4, 129.4, 128.9, 128.7, 128.4, 122.1, 21.7; (IR, Neat): 3028, 1659, 1596, 1448, 1177, 754, 668 cm^{-1}; HRMS (ESI) Calculated for $[C_{16}H_{15}O]^+$ 223.11174; Found 223.11232.

(*E*)-1-(4-Chlorophenyl)-3-phenylprop-2-en-1-one (19)[8]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.218 g, 90%). M.p. 95-98 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, J = 8.6 Hz, 2H), 7.82 (d, J = 15.7 Hz, 1H), 7.64 (dd, J = 6.2, 3.3 Hz, 2H), 7.50 (d, J = 7.3 Hz, 1H), 7.46 (s, 2H), 7.44 – 7.41 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.2, 145.3, 139.2, 136.5, 134.7, 130.7, 129.9, 129.0, 128.9, 128.5, 121.5; (IR, Neat): 3060, 1659, 1589, 1489, 1212, 977, 760, 691 cm^{-1}; HRMS (ESI) Calculate for $[C_{15}H_{12}OCl]^+$ 243.05712; Found 243.05783.

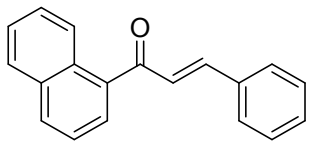
(*E*)-1-(4-Bromophenyl)-3-phenylprop-2-en-1-one (20)[8]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.263 g, 92%). M.p. 90-92 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (d, J =

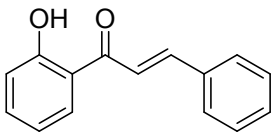
8.4 Hz, 2H), 7.81 (d, J = 15.7 Hz, 1H), 7.64 (dd, J = 8.2, 1.9 Hz, 4H), 7.47 (d, J = 15.7 Hz, 1H), 7.44 – 7.40 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.4, 145.4, 136.9, 134.7, 132.0, 130.8, 130.1, 129.0, 128.6, 127.9, 121.4; (IR, Neat): 3019, 1687, 1656, 1581, 1479, 1285, 753, 690 cm^{-1}; HRMS (ESI): Calculated for $[C_{15}H_{12}BrO]^+$ 287.00660; Found 287.00726.

(*E*)-1-(Naphthalen-1-yl)-3-phenylprop-2-en-1-one (21)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 6% ethyl acetate in hexane as the eluent) to afford the title product as a light brown liquid (0.222 g, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, J = 7.8 Hz, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.85 (d, J = 7.9 Hz, 1H), 7.73 (d, J = 7.1 Hz, 1H), 7.59 (d, J = 15.5 Hz, 1H), 7.55 – 7.45 (m, 5H), 7.34 (s, 3H), 7.28 (d, J = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.7, 145.9, 136.9, 134.5, 133.7, 131.5, 130.6, 130.4, 130.0, 128.9, 128.4, 127.4, 127.1, 127.0, 126.4, 125.6, 124.4; (IR, Neat): 3016, 1695, 1636, 1449, 1215, 744, 666 cm^{-1}; HRMS (ESI): Calculated for $[C_{19}H_{15}O]^+$ 259.11174; Found 259.11155.

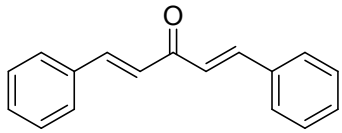
(*E*)-1-(2-Hydroxyphenyl)-3-phenylprop-2-en-1-one (22)[11b,12]



A solution of 2-(1-Hydroxyallyl)phenol (5.00 g, 33.00 mmol) {prepared as per the literature protocol[11a]} and $Pd(OAc)_2$ (0.739 g, 3.3 mmol) in DMF (25.0 mL) was taken in a 100.0 mL RB flask, which was then attached to an oxygen balloon (1atm. pressure). The mixture was vigorously stirred at 90 °C for 4 h. The RB flask was opened. After adding 2,9-dimethyl-1,10-phenanthroline (1.373 g, 6.6 mmol) and phenylboronic acid (4.831g, 39.6 mmol), to the reaction mixture, the RB flask was again attached to the oxygen balloon (1atm. pressure) and the stirring continued for18 h at 90 °C. After cooling to room temperature, the reaction mixture was partitioned between ethyl acetate (50.0 mL) and water (50.0 mL) in a separatory funnel. The organic layer was washed with water, and brine, dried over anhydrous Na_2SO_4 (s) and

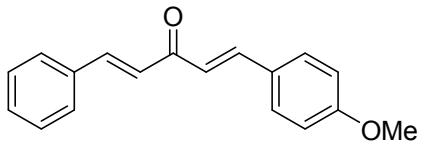
concentrated *in vacuo*. The residue was purified by column chromatography (silica gel 100-200 mesh, 15% ethyl acetate in hexane as eluent) to afford the title product as a yellow solid (6.420 g, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.85 (s, 1H), 7.92 – 7.86 (m, 2H), 7.65 – 7.59 (m, 3H), 7.46 (t, J = 7.7 Hz, 1H), 7.41 – 7.38 (m, 3H), 7.01 (d, J = 8.3 Hz, 1H), 6.92 (t, J = 7.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.7, 163.6, 145.5, 136.4, 134.6, 131.0, 129.7, 129.1, 128.7, 120.1, 120.0, 118.9, 118.7; (IR, Neat): 3361, 3059, 1637, 1570, 1483, 1152, 734, 662 cm^{-1}; HRMS (ESI) Calculate for $[C_{15}H_{13}O_2]^+$ 225.09101; Found 225.09110.

(1*E*,4*E*)-1,5-Diphenylpenta-1,4-dien-3-one (23)[9]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.199 g, 85%). M.p. 119-121 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, J = 16.0 Hz, 2H), 7.60 (dd, J = 6.5, 2.7 Hz, 3H), 7.39 (d, J = 2.7 Hz, 5H), 7.27 (dd, J = 4.9, 3.0 Hz, 2H), 7.08 (d, J = 15.9 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.1, 143.5, 134.8, 130.6, 129.0, 128.5, 125.5; (IR, Neat): 3023, 1650, 1592, 1448, 1184, 747, 691 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{15}O]^+$ 235.11174; Found 235.11179.

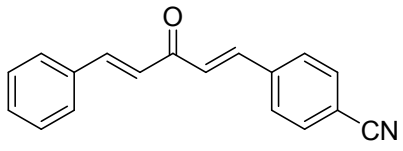
(1*E*,4*E*)-1-(4-Methoxyphenyl)-5-phenylpenta-1,4-dien-3-one (24)[9]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as eluent) to afford the title product as a pale yellow solid (0.229 g, 87%). M.p. 103-105 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (dd, J = 15.9, 4.7 Hz, 2H), 7.63 – 7.60 (m, 2H), 7.57 (d, J = 8.7 Hz, 2H), 7.41 (dd, J = 5.1, 1.9 Hz, 3H), 7.08 (d, J = 15.9 Hz, 1H), 6.97 (d, J = 15.9 Hz, 1H), 6.93 (d, J = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.9, 161.7, 143.2, 142.8, 135.0, 130.4,

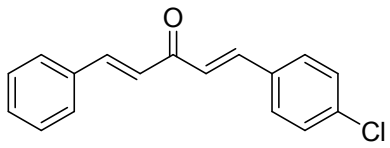
130.2, 128.9, 128.4, 127.5, 125.6, 123.3, 114.5, 55.4; (IR, Neat): 2933, 1648, 1568, 1249, 770, 691 cm^{-1}; HRMS (ESI): Calculated for $[C_{18}H_{17}O_2]^+$ 265.12231; Found 265.12219.

4-((1*E*,4*E*)-3-Oxo-5-phenylpenta-1,4-dienyl)benzonitrile (25)[9]



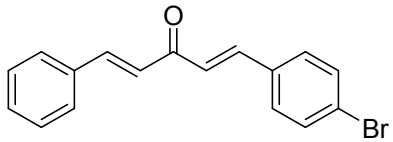
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.230 g, 89%). M.p. 98-100 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.78 (d, J = 16.0 Hz, 2H), 7.70 (d, J = 5.2 Hz, 4H), 7.63 (dd, J = 6.7, 2.8 Hz, 2H), 7.47 – 7.41 (m, 3H), 7.13 (dd, J = 30.6, 16.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.7, 144.7, 140.9, 139.1, 134.2, 132.7, 131.0, 129.1, 128.7, 128.6, 128.0, 125.1, 118.4, 116.4; (IR, Neat): 2924, 2225, 1650, 1602, 1497, 1185, 770, 691 cm^{-1}; HRMS (ESI): Calculated for $[C_{18}H_{14}ON]^+$ 260.10699; Found 260.10722.

(1*E*,4*E*)-1-(4-Chlorophenyl)-5-phenylpenta-1,4-dien-3-one (26)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.236 g, 88%). M.p. 128-130 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, J = 16.0 Hz, 1H), 7.67 (d, J = 15.9 Hz, 1H), 7.60 (dd, J = 6.6, 2.9 Hz, 2H), 7.53 (d, J = 8.5 Hz, 2H), 7.42 – 7.40 (m, 3H), 7.37 (d, J = 8.5 Hz, 2H), 7.05 (dd, J = 15.9, 4.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.6, 143.6, 141.8, 136.4, 134.7, 133.3, 130.6, 129.6, 129.3, 129.0, 128.5, 125.7, 125.4; (IR, Neat): 3019, 1650, 1588, 1489, 1188, 757, 692 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{14}OCl]^+$ 269.07277; Found 269.07287.

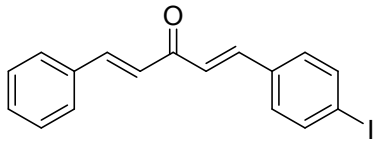
(1*E*,4*E*)-1-(4-Bromophenyl)-5-phenylpenta-1,4-dien-3-one (27)[9]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl

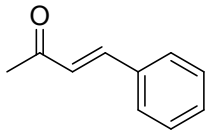
acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.281 g, 90%). M.p. 109-110 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (dd, J = 25.7, 15.9 Hz, 2H), 7.58 (dd, J = 6.5, 2.8 Hz, 2H), 7.51 (d, J = 8.5 Hz, 2H), 7.40 (d, J = 2.3 Hz, 3H), 7.30 (d, J = 8.8 Hz, 2H), 7.06 (d, J = 15.9 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 189.5, 144.4, 142.7, 134.5, 133.5, 132.4, 132.3, 130.9, 129.9, 129.1, 128.6, 125.6, 125.1; (IR, Neat): 2923, 1647, 1581, 1487, 1185, 771, 689 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{14}OBr]^+$ 313.02225; Found 313.02233.

(1*E*,4*E*)-1-(4-Iodophenyl)-5-phenylpenta-1,4-dien-3-one (28)



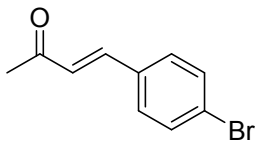
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.309 g, 86%). M.p. 118-120 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.74 (dd, J = 18.2, 10.3 Hz, 2H), 7.62 (dd, J = 5.7, 3.2 Hz, 2H), 7.54 (d, J = 7.0 Hz, 2H), 7.45 – 7.42 (m, 3H), 7.36 (d, J = 8.4 Hz, 2H), 7.09 (dd, J = 15.9, 6.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 188.7, 143.7, 142.1, 138.2, 135.4, 134.6, 129.8, 129.0, 128.4, 128.2, 125.8, 125.3, 96.8; (IR, Neat): 2924, 1689, 1616, 1448, 1177, 770, 666 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{14}OI]^+$ 361.00838; Found 361.00882.

(*E*)-4-Phenylbut-3-en-2-one (29)[10]



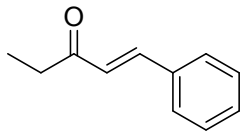
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a light brown liquid (0.124 g, 85%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53 (t, J = 3.3 Hz, 2H), 7.49 (d, J = 10.4 Hz, 1H), 7.40 – 7.36 (m, 3H), 6.70 (d, J = 16.3 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.5, 143.5, 134.4, 130.5, 129.0, 128.3, 127.1, 27.5; (IR, Neat): 3019, 1708, 1600, 1451, 1216, 770, 698 cm^{-1}; HRMS (ESI): Calculated for $[C_{10}H_{11}O]^+$ 147.08044; Found 147.08021.

(*E*)-4-(4-Bromophenyl)but-3-en-2-one (30)



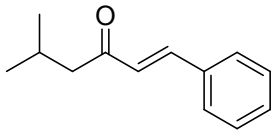
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a colourless solid (0.197 g, 88%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, J = 8.5 Hz, 2H), 7.44 (d, J = 16.3 Hz, 1H), 7.39 (d, J = 8.5 Hz, 2H), 6.69 (d, J = 16.3 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.3, 142.0, 133.3, 132.2, 129.6, 127.5, 124.8, 27.6; (IR, Neat): 2926, 1691, 1668, 1586, 1485, 1217, 975, 749, 664 cm^{-1}; HRMS (ESI): Calculated for $[C_{10}H_{10}OBr]^+$ 224.99095; Found 224.99124.

(*E*)-1-Phenylpent-1-en-3-one (31)[10]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow liquid (0.144 g, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 – 7.52 (m, 3H), 7.38 (dd, J = 6.0, 3.5 Hz, 3H), 6.74 (d, J = 16.2 Hz, 1H), 2.69 (q, J = 7.3 Hz, 2H), 1.17 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.0, 142.2, 134.6, 130.4, 128.9, 128.2, 126.0, 34.1, 8.3; (IR, Neat): 3019, 1692, 1662, 1577, 1451, 1216, 743, 666 cm^{-1}; HRMS (ESI): Calculated for $[C_{11}H_{13}O]^+$ 161.09606; Found 161.09625.

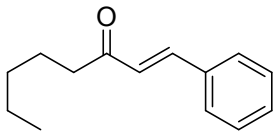
(*E*)-5-Methyl-1-phenylhex-1-en-3-one (32)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow liquid (0.171 g, 91%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 – 7.50 (m, 3H), 7.40 – 7.34 (m, 3H), 6.74 (d, J = 16.2 Hz, 1H), 2.53 (d, J = 7.0 Hz, 2H), 2.31 – 2.17 (m, 1H), 0.98 (d, J = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.4, 142.5, 134.5, 130.4, 128.9, 128.3, 126.5, 49.9, 25.2, 22.7;

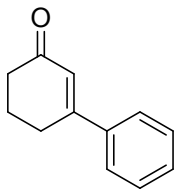
(IR, Neat): 2959, 1688, 1608, 1550, 1450, 1217, 744, 666 cm^{-1}; HRMS (ESI): Calculated for $[C_{13}H_{17}O]^+$ 189.12739; Found 189.12747.

(*E*)-1-Phenyloct-1-en-3-one (33)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow liquid (0.190 g, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, J = 10.5 Hz, 3H), 7.54 (d, J = 5.9 Hz, 5H), 7.39 – 7.36 (m, 6H), 6.74 (d, J = 16.2 Hz, 2H), 2.67 – 2.61 (m, 5H), 1.70 – 1.66 (m, 4H), 1.34 (dd, J = 7.3, 3.7 Hz, 8H), 0.89 (d, J = 7.7 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.7, 142.3, 134.6, 130.4, 129.0, 128.3, 126.3, 41.0, 31.6, 24.1, 22.6, 14.0; (IR, Neat): 2958, 1692, 1609, 1450, 1215, 743, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{19}O]^+$ 203.14304; Found 203.14321.

3-Phenylcyclohex-2-enone (34)[7]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 5% ethyl acetate in hexane as the eluent) to afford the title product as a pale yellow solid (0.149 g, 87%). M.p. 65-67 ^oC; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.51 (m, 2H), 7.40 (d, J = 2.8 Hz, 3H), 6.42 (s, 1H), 2.77 (dd, J = 4.3, 1.3 Hz, 2H), 2.48 (dd, J = 5.7, 4.0 Hz, 2H), 2.15 (dd, J = 11.5, 5.8 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.0, 159.9, 138.8, 130.0, 128.8, 126.1, 125.4, 37.3, 28.1, 22.8; (IR, Neat): 2931, 1661, 1604, 1449, 1216, 744, 665 cm^{-1}; HRMS (ESI): Calculated for $[C_{12}H_{13}O]^+$ 173.09609; Found 173.09612.

1.4 References

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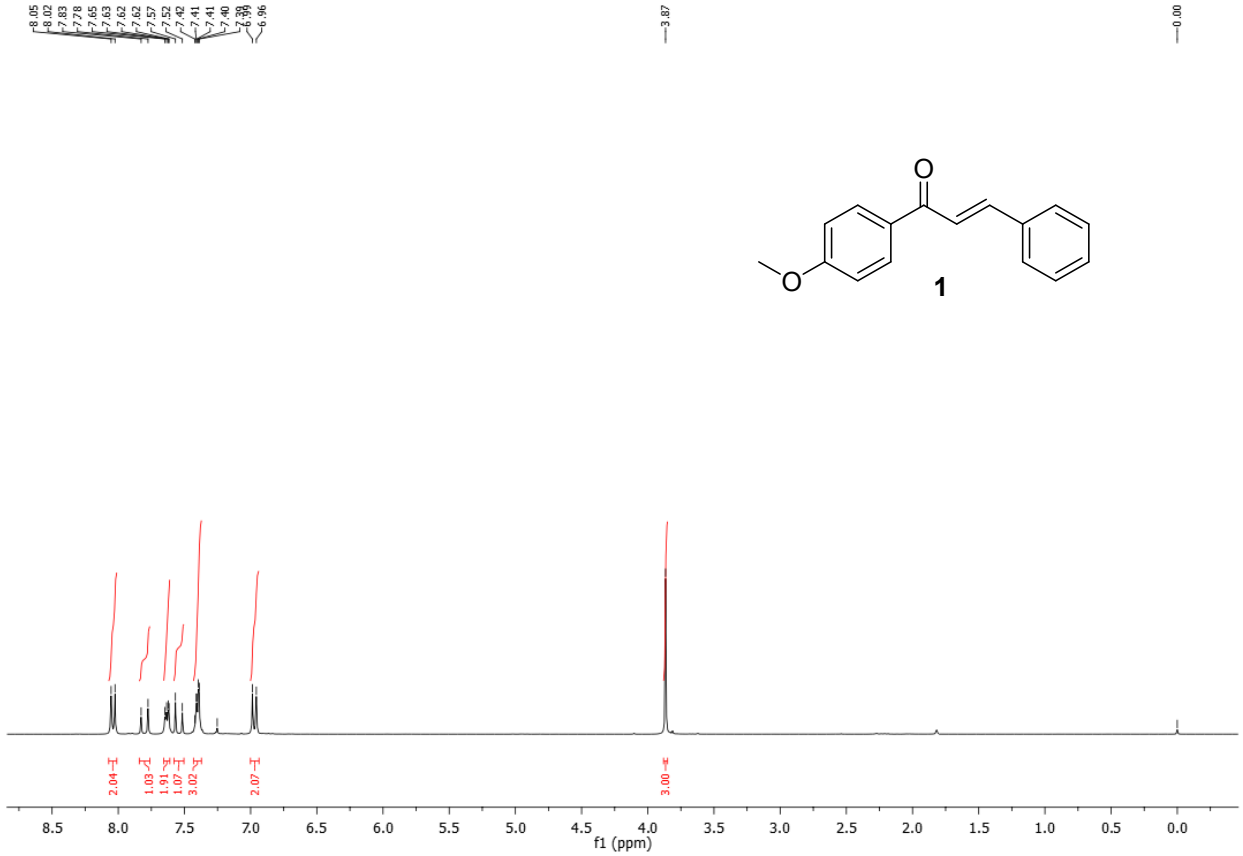
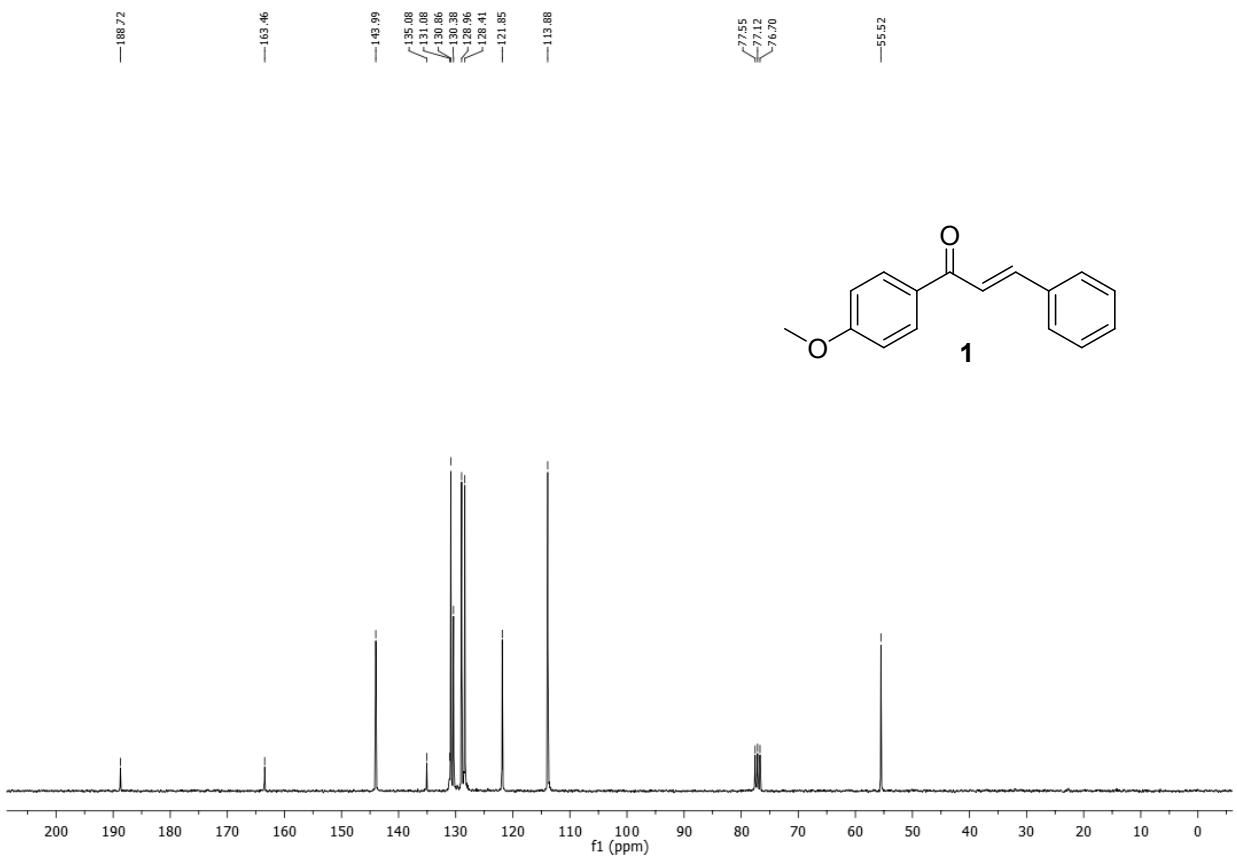
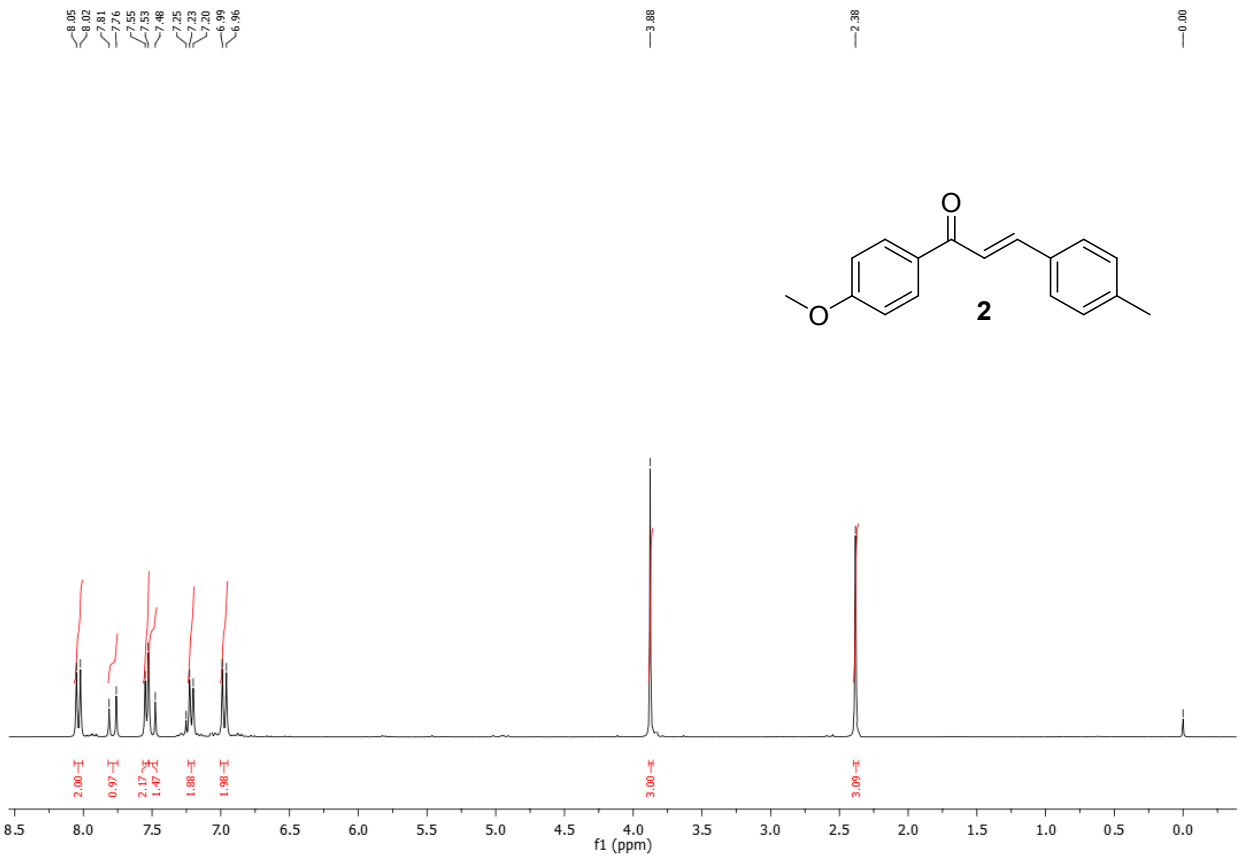
[12] Cabrera, M.; Simoens, M.; Falchi, G.; Lavaggi, M. L.; Piro, O. E.; Castellano, E. E.; Vidal, A.; Azqueta, A.; Monge, A.; Adela, L. C.; Sagrera, G.; Seoane, G.; Cerecetto, H.; Mercedes, G. *Bioorg. Med. Chem.*, **2007**, *15*, 3356.

1.5 ^{1}H and ^{13}C NMR Spectra for compounds (**1-34**)



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7.53
7.48
7.25
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7.20
6.99
6.96
3.88
2.38
0.00
O
O
2
2.00
0.97
2.17
1.47
1.88
1.98
3.00
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
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1.5
1.0
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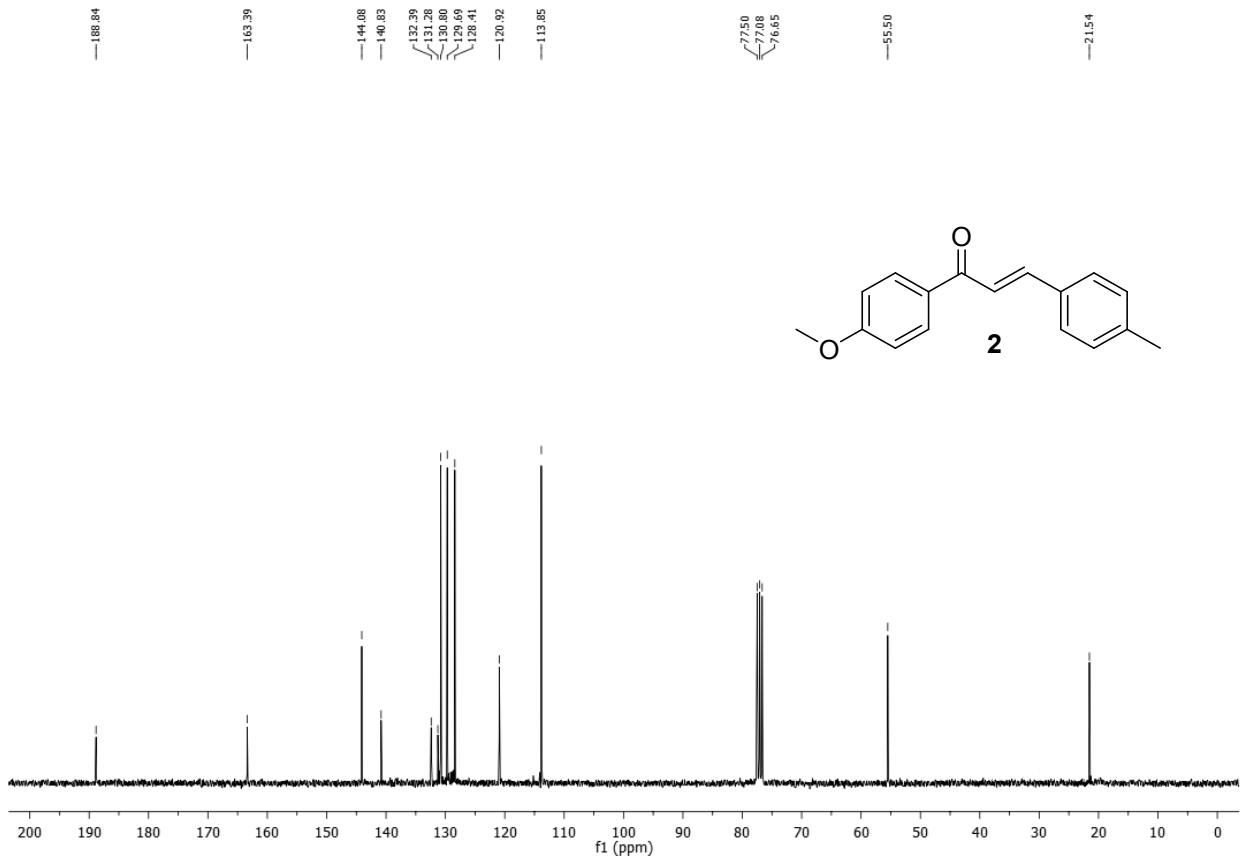
f1 (ppm)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129.69
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120.92
113.85
77.50
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76.65
55.50
21.54
O
O
2
200
190
180
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50
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30
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10
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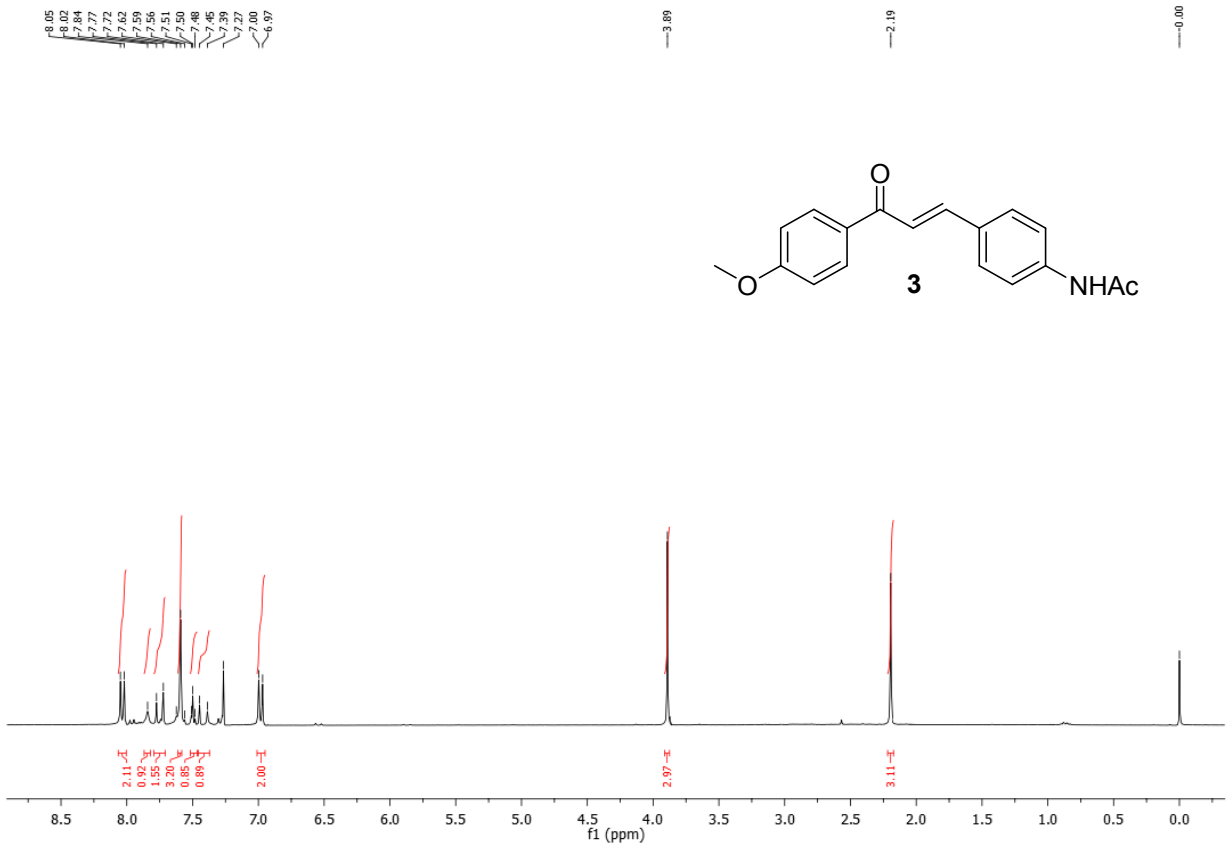
f1 (ppm)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O
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NHAc
2.11
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1.55
3.20
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2.00
2.97
3.11
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8.0
7.5
7.0
6.5
6.0
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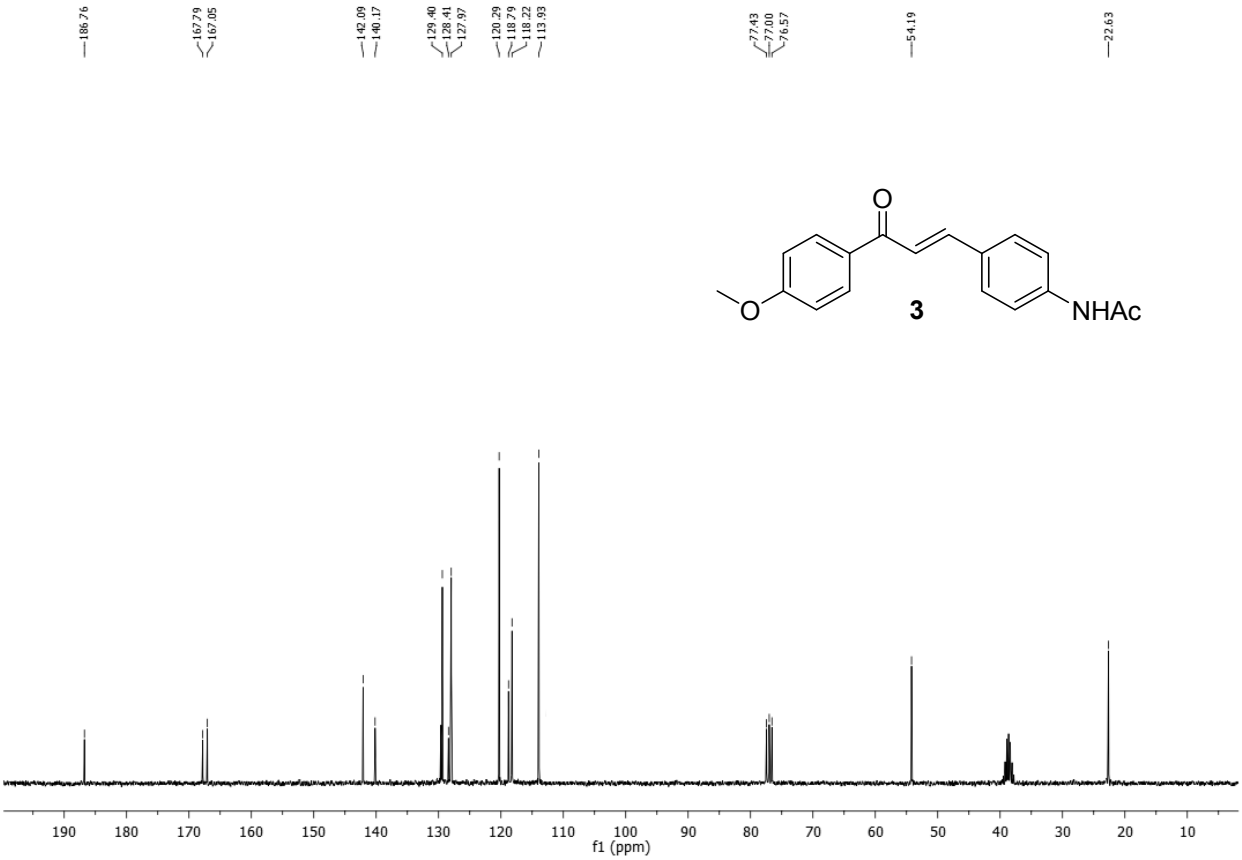
f1 (ppm)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77.43
77.00
76.57
54.19
22.63
O
O
3
NHAc
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110
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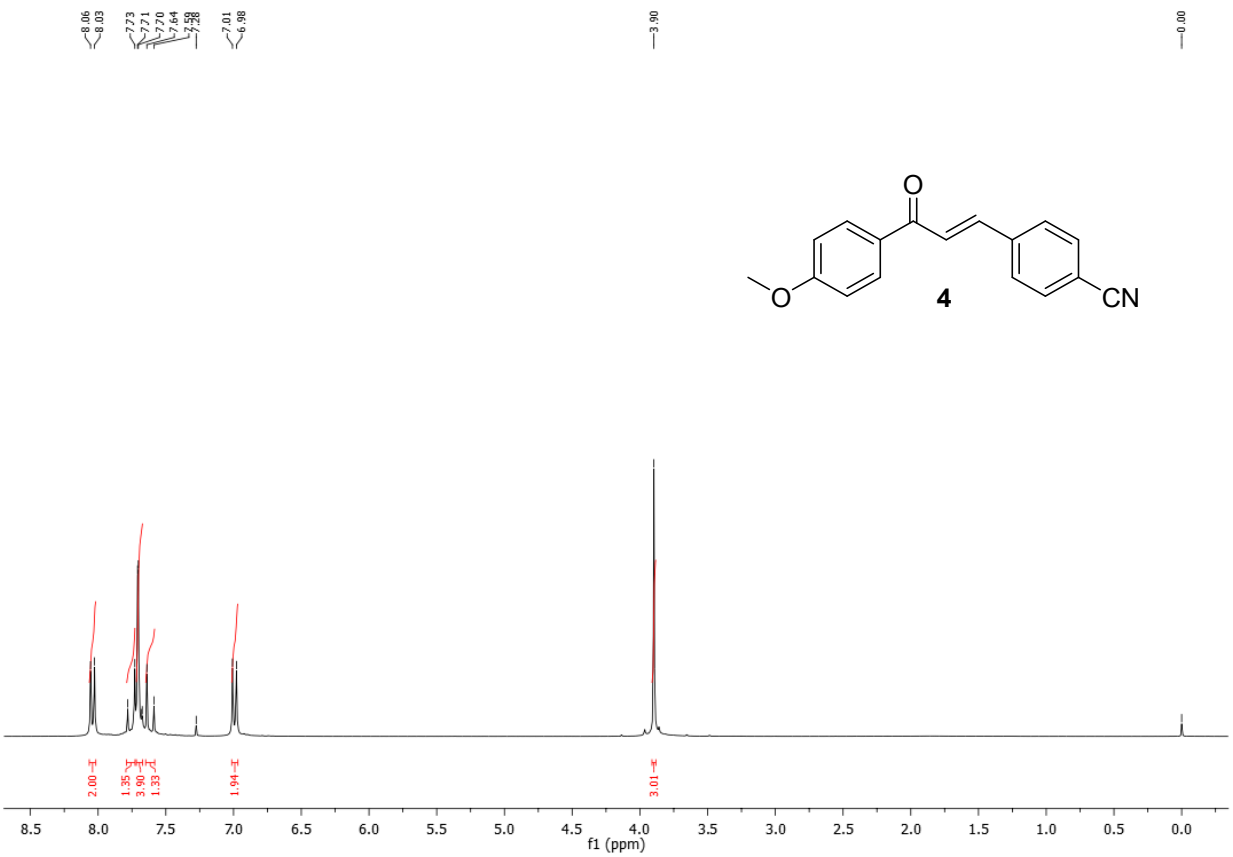
60
50
40
30
20
10
f1 (ppm)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CN
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3.01
8.5
8.0
7.5
7.0
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6.0
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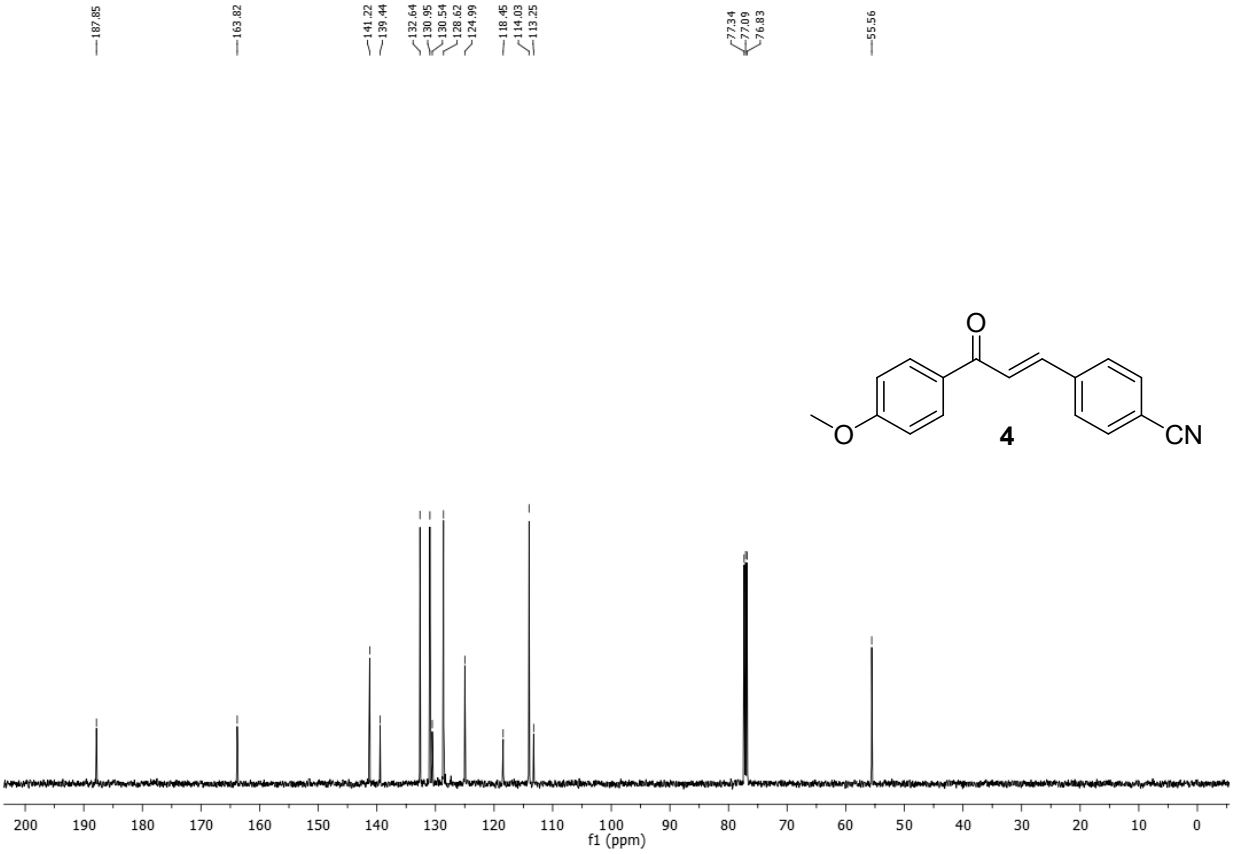
0.0
f1 (ppm)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77.09
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55.56
O
O
CN
4
200
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180
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160
150
140
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110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8.29
8.26
8.07
8.05
7.84
7.80
7.79
7.77
7.69
7.63
7.27
7.02
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0.00
1.98
2.11
1.31
1.91
0.79
2.00
2.99
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

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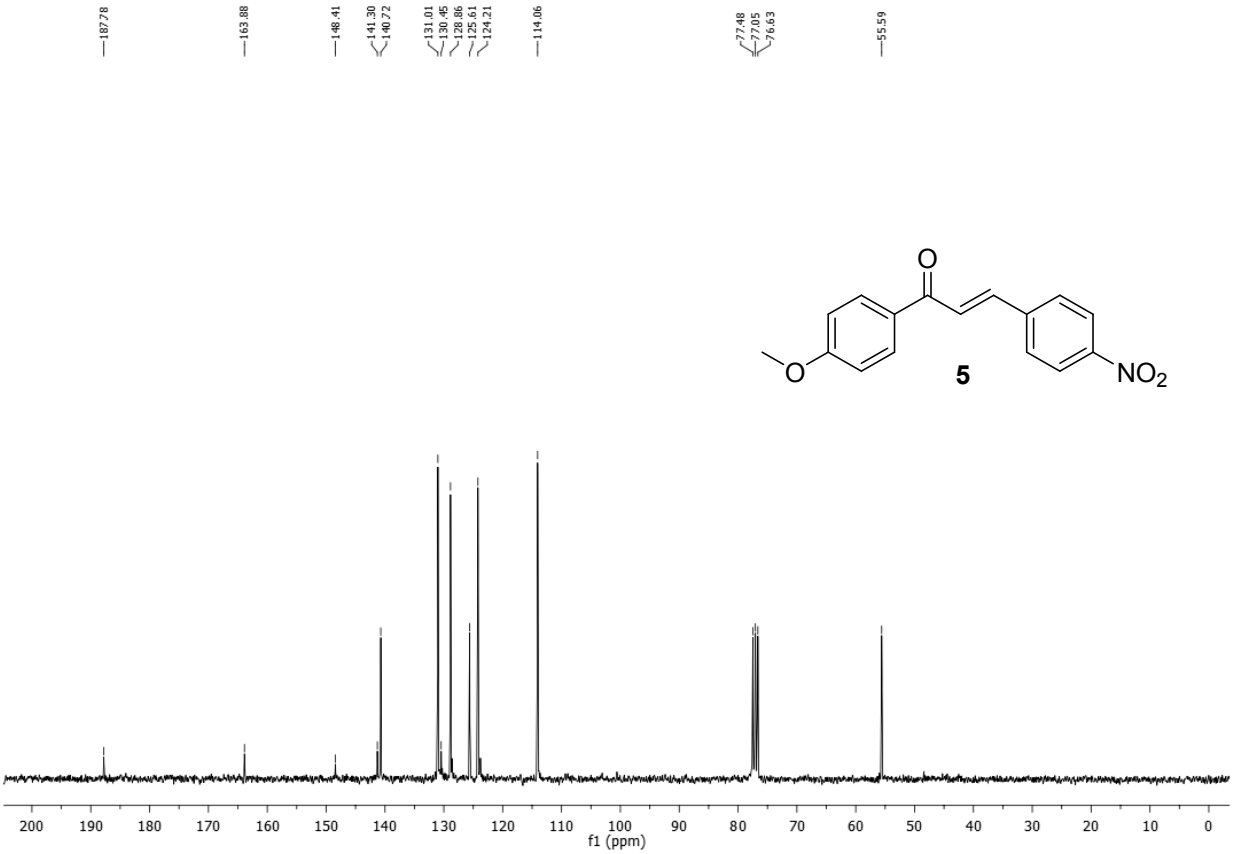
O
NO2
5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180
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150
140
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50
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30
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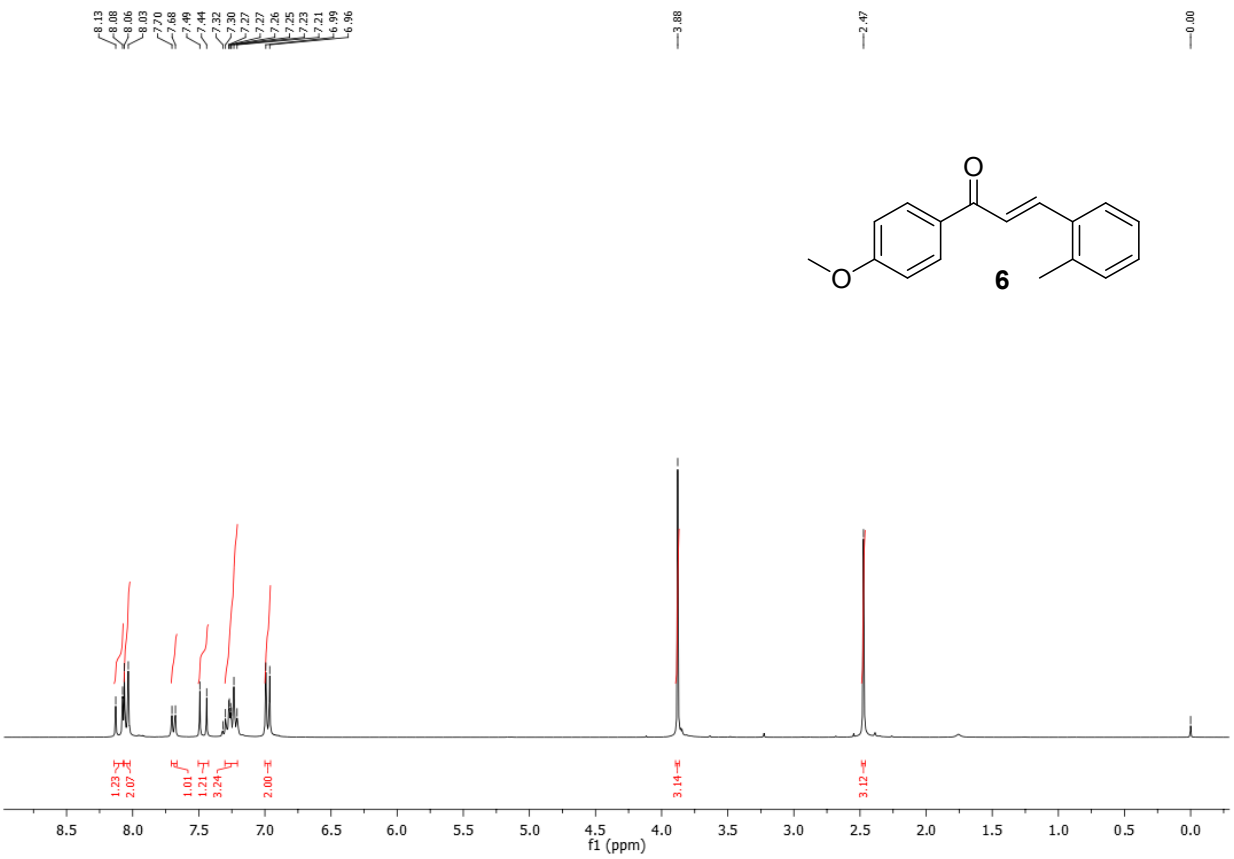
10
0
f1 (ppm)

O
O
NO2
5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7.21
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2.07
1.01
1.21
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7.0
6.5
6.0
5.5
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4.5
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0.5
0.0
f1 (ppm)

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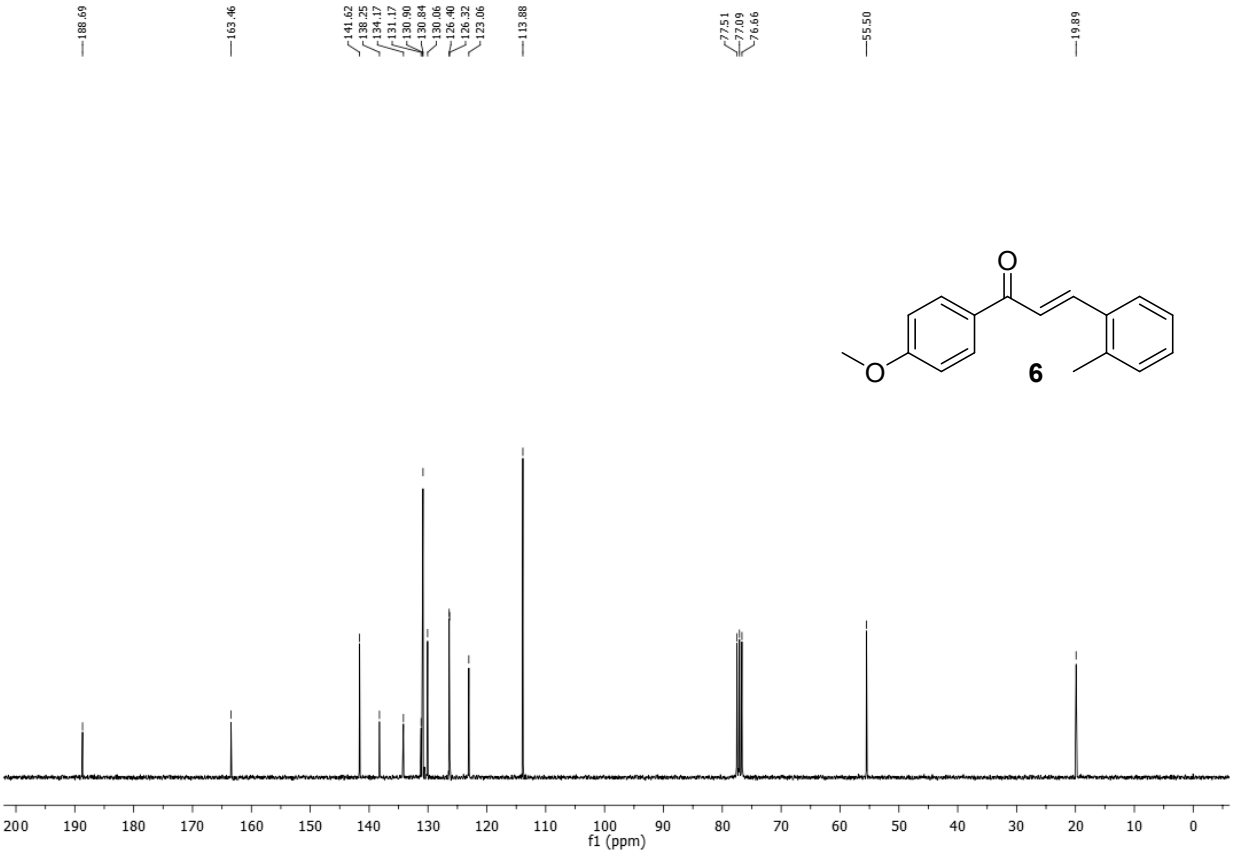
O
6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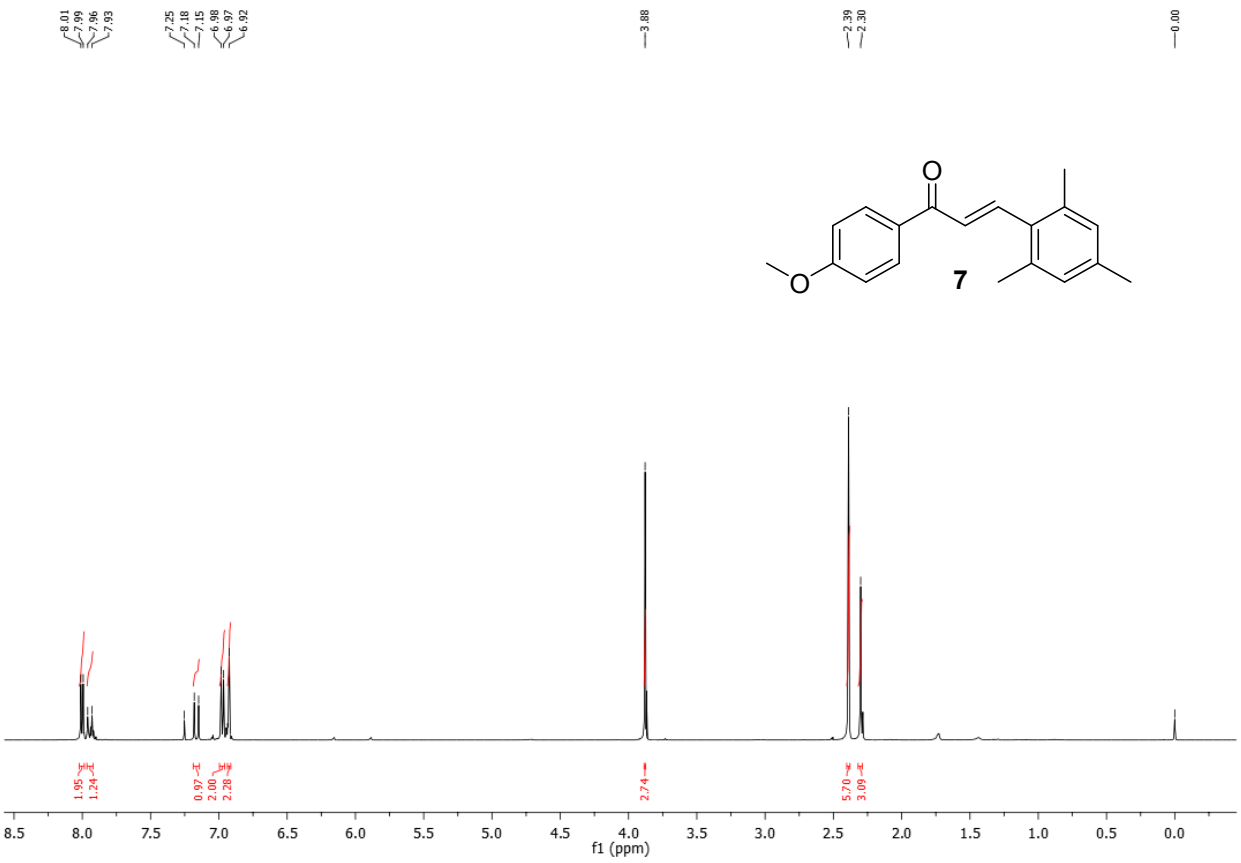
f1 (ppm)

O
O
6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2.5
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1.0
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0.0
f1 (ppm)
188.78
163.44
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138.39
137.10
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129.27
127.21
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77.08
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55.53
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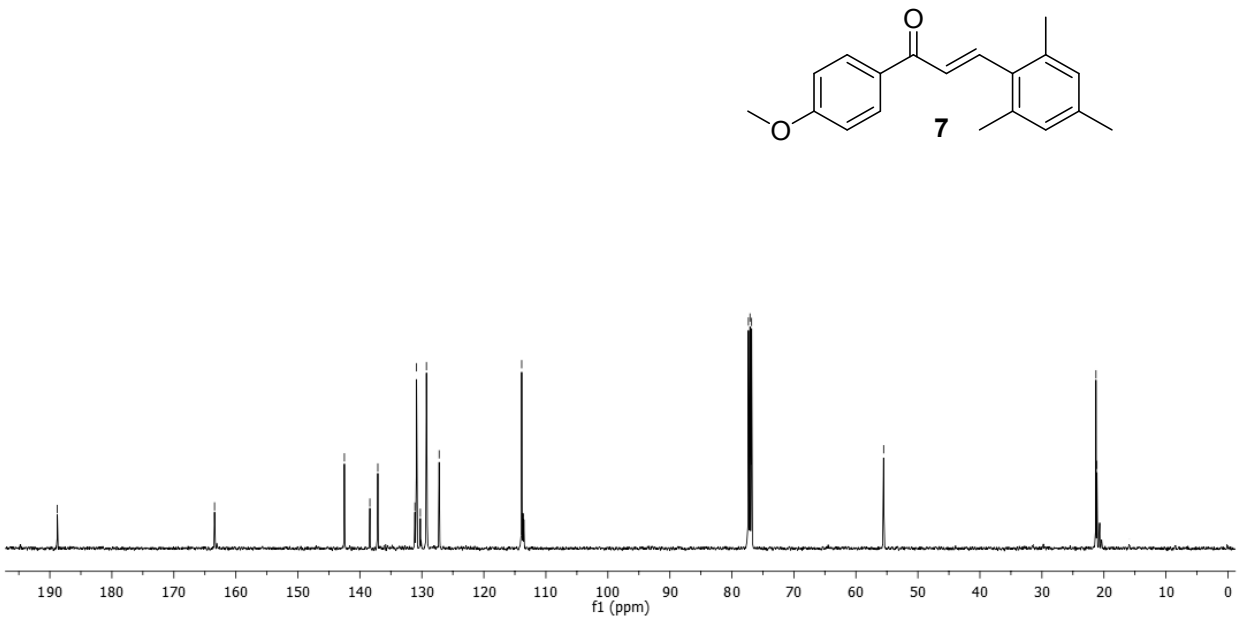
21.13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O
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50
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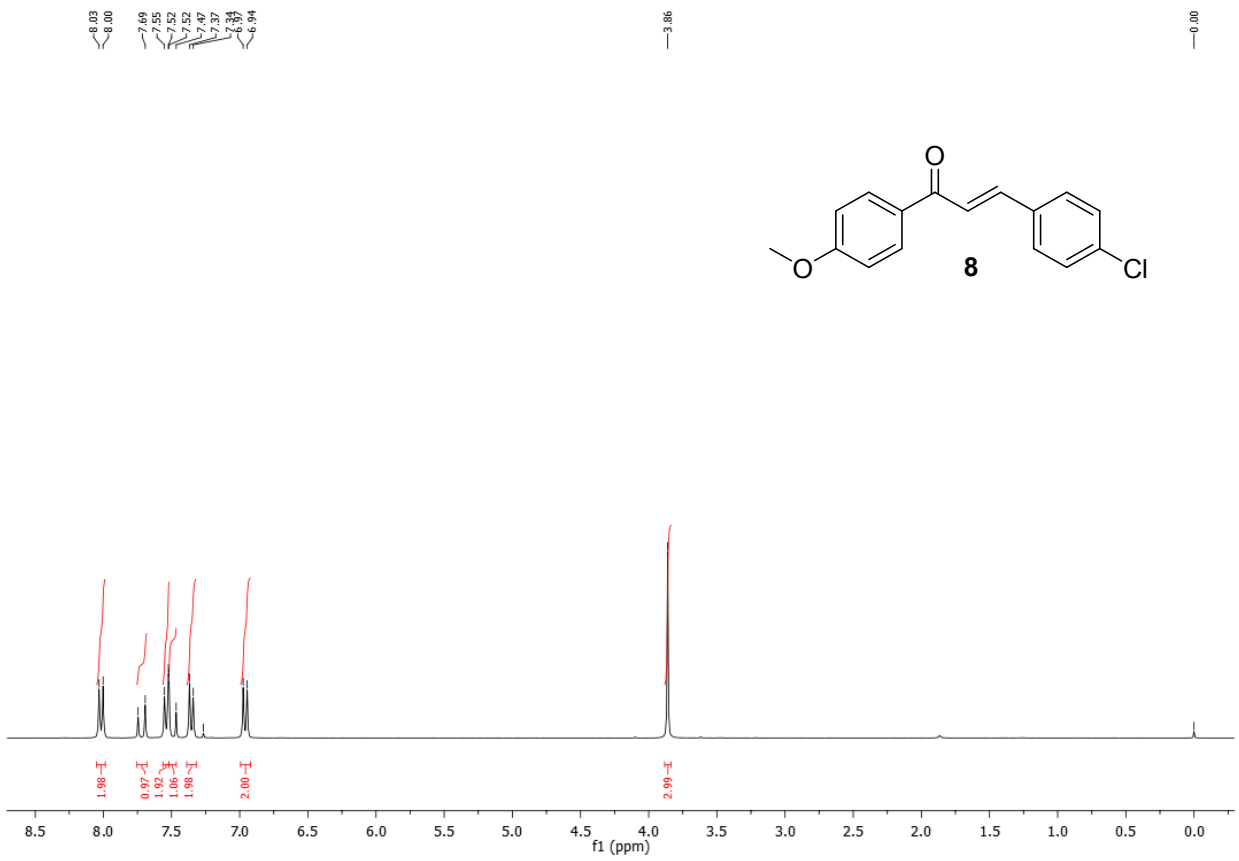
30
20
10
0
f1 (ppm)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8
Cl
1.98
0.97
1.92
1.06
1.98
2.00
2.99
8.5
8.0
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7.0
6.5
6.0
5.5
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2.5
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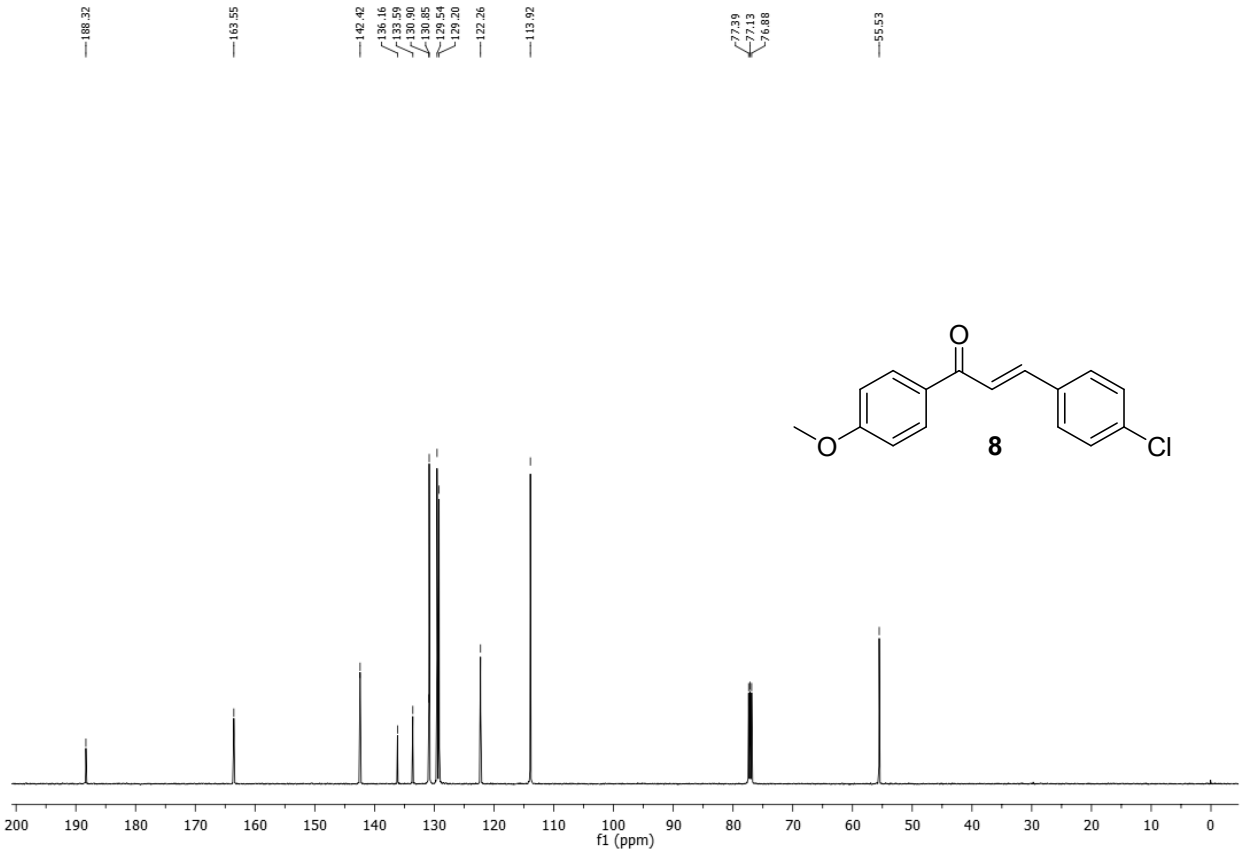
0.5
0.0
f1 (ppm)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113.92
77.39
77.13
76.88
55.53
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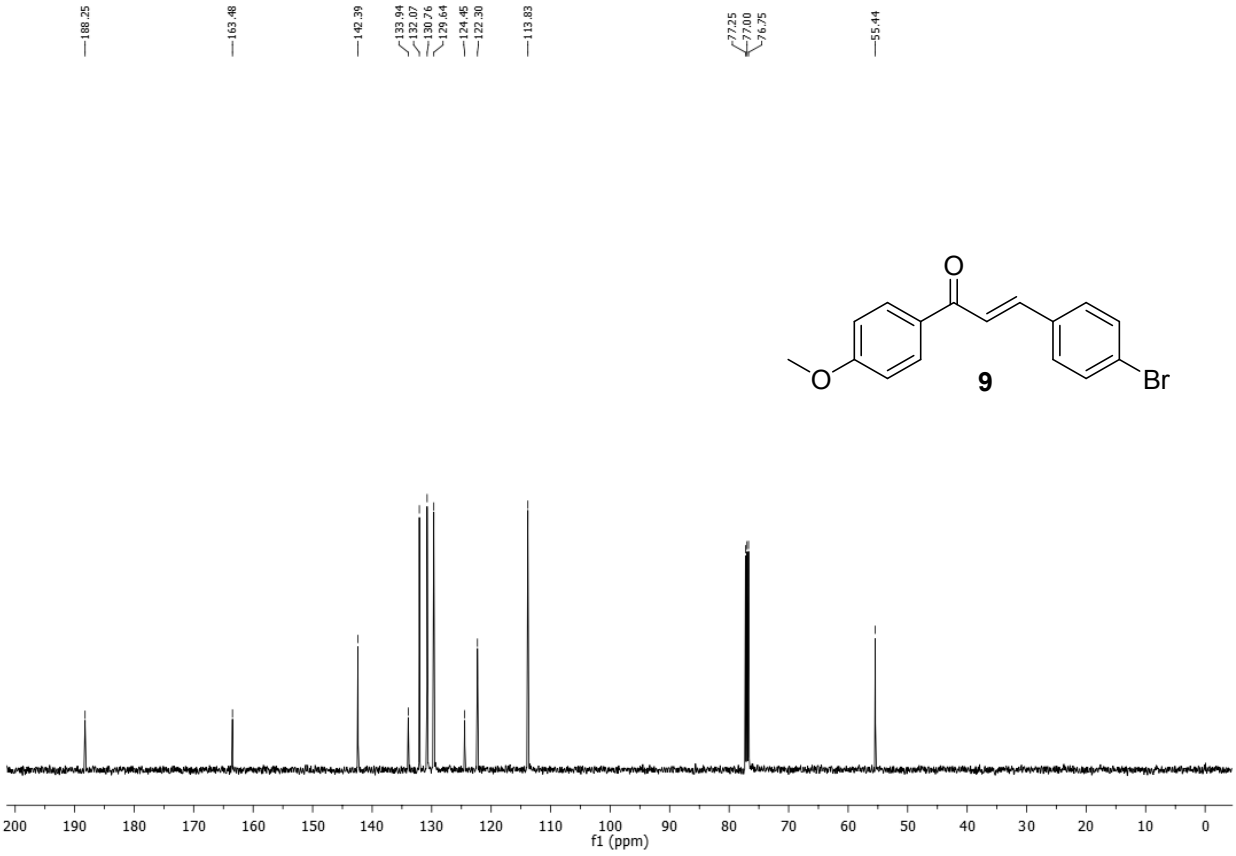
O
8
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8.04
8.01
7.74
7.69
7.55
7.52
7.50
7.47
7.27
6.99
6.96
3.88
0.00
O
O
Br
9
1.92
0.97
5.15
2.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.76
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122.30
113.83
77.25
77.00
76.75
55.44
O
O
Br
9
200
190
180
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130
120
110
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90
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50
40
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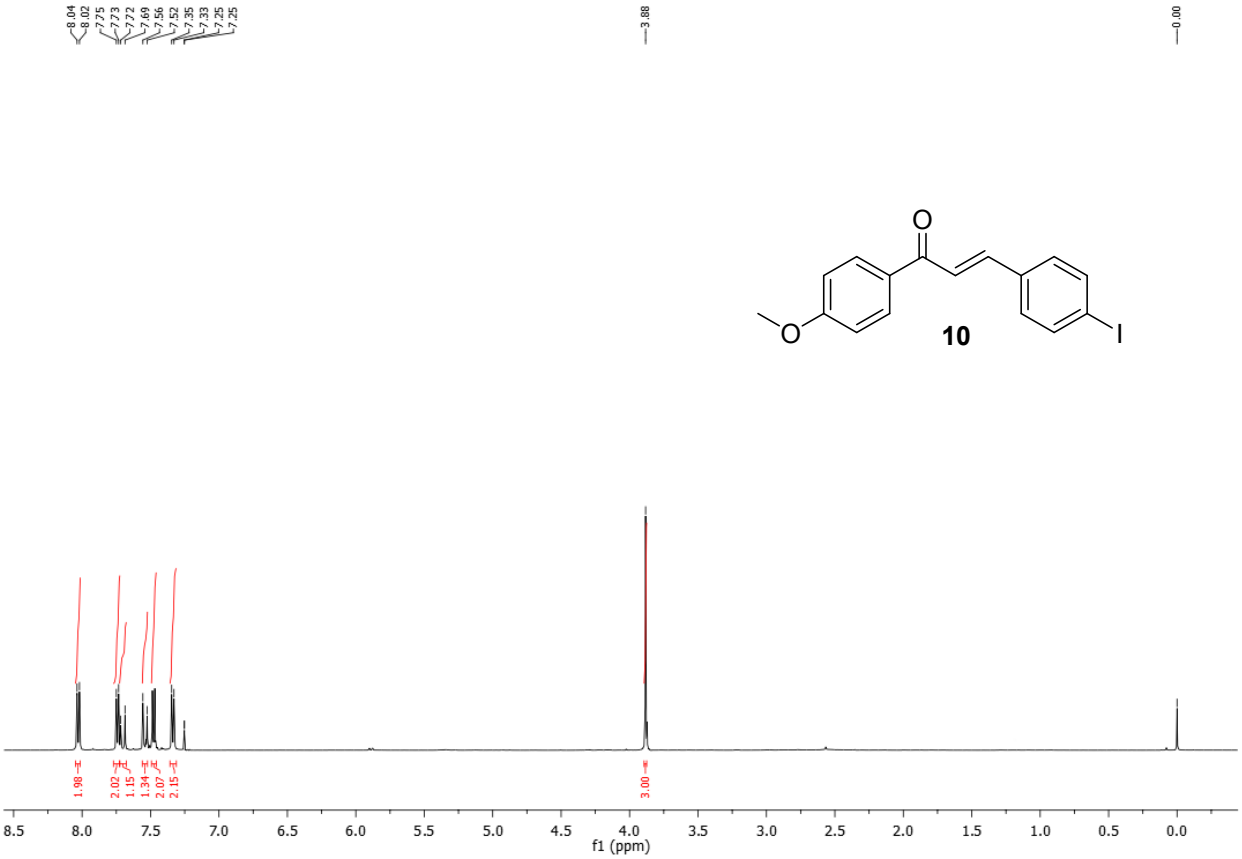
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7.52
7.35
7.33
7.25
7.25
3.88
0.00
O
O
I
10
1.98
2.02
1.15
1.34
2.07
2.15
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
1.5
1.0
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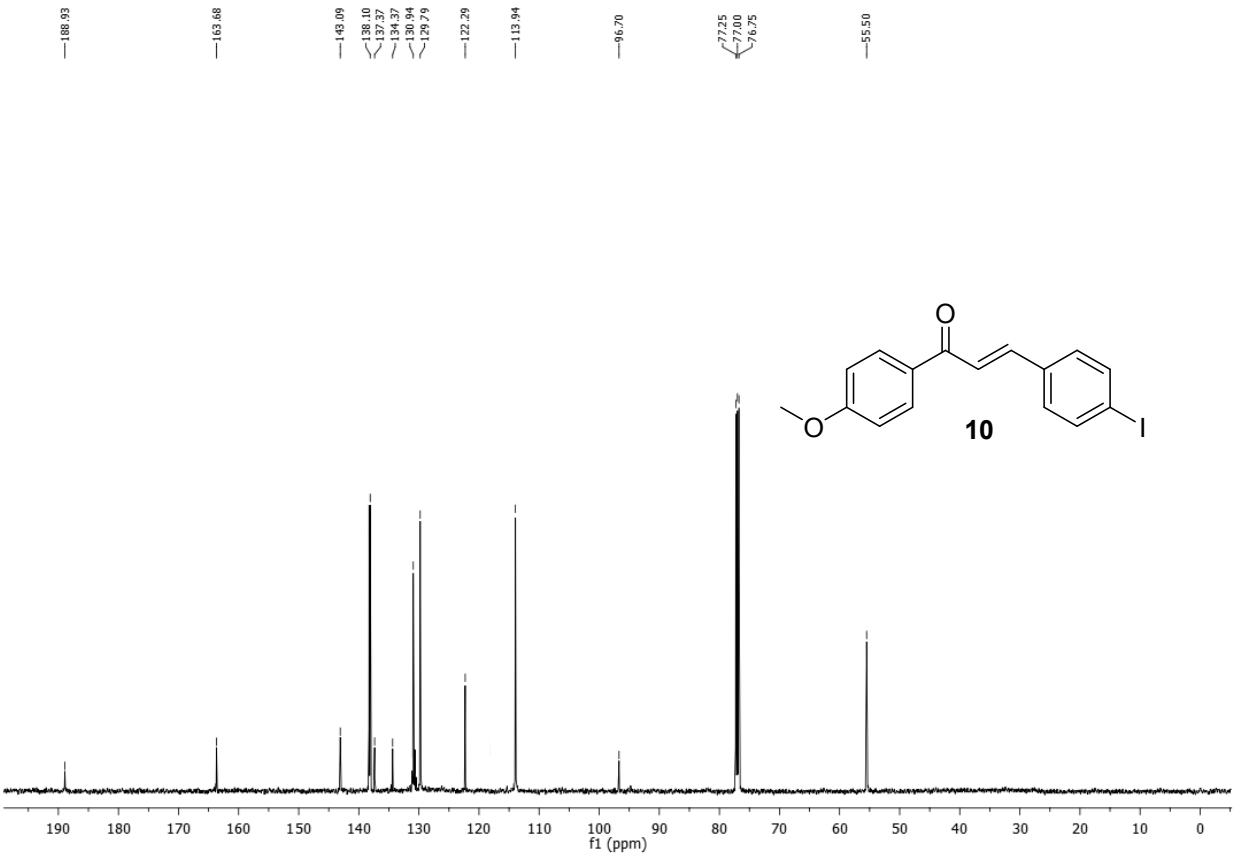
f1 (ppm)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113.94
96.70
77.25
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76.75
55.50
O
O
I
10
190
180
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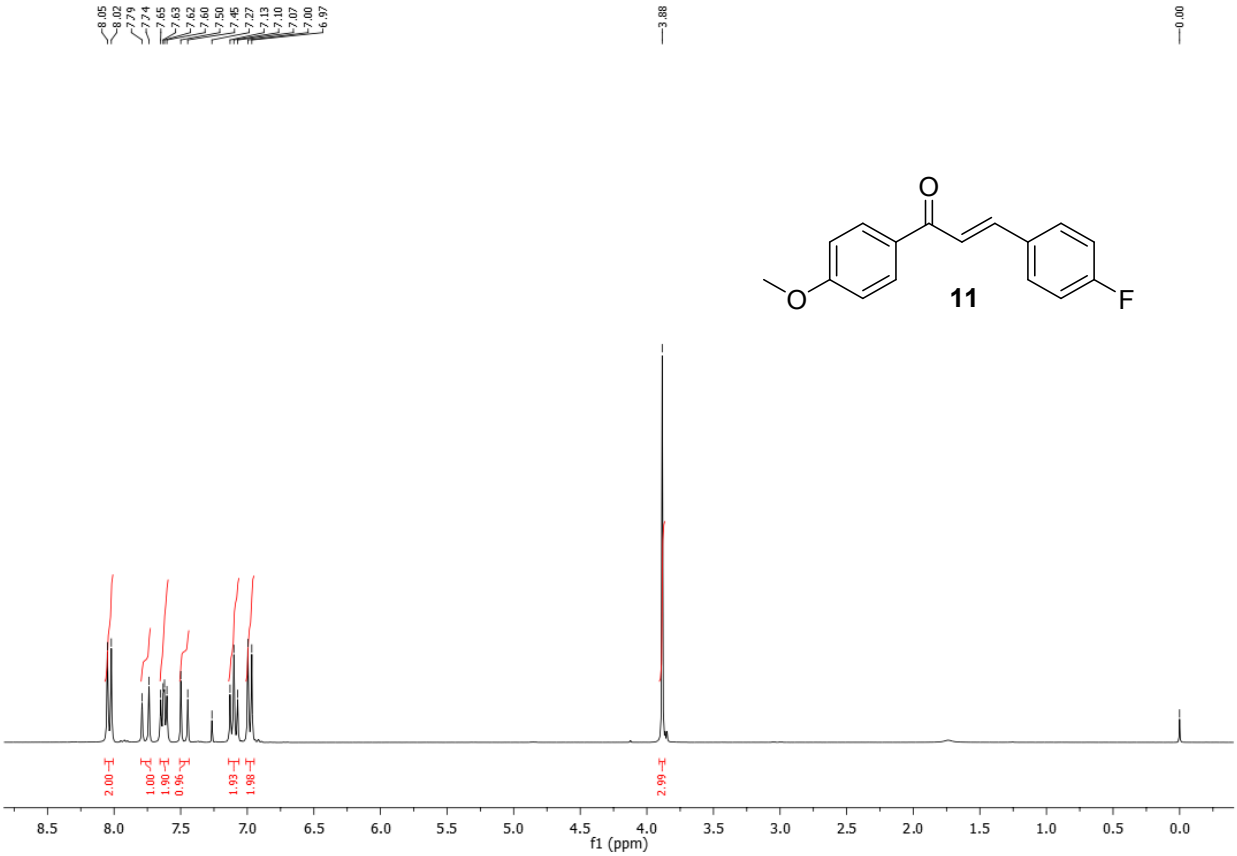
f1 (ppm)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7.60
7.50
7.45
7.27
7.13
7.10
7.07
7.00
6.97
3.88
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O
F
11
2.00
1.00
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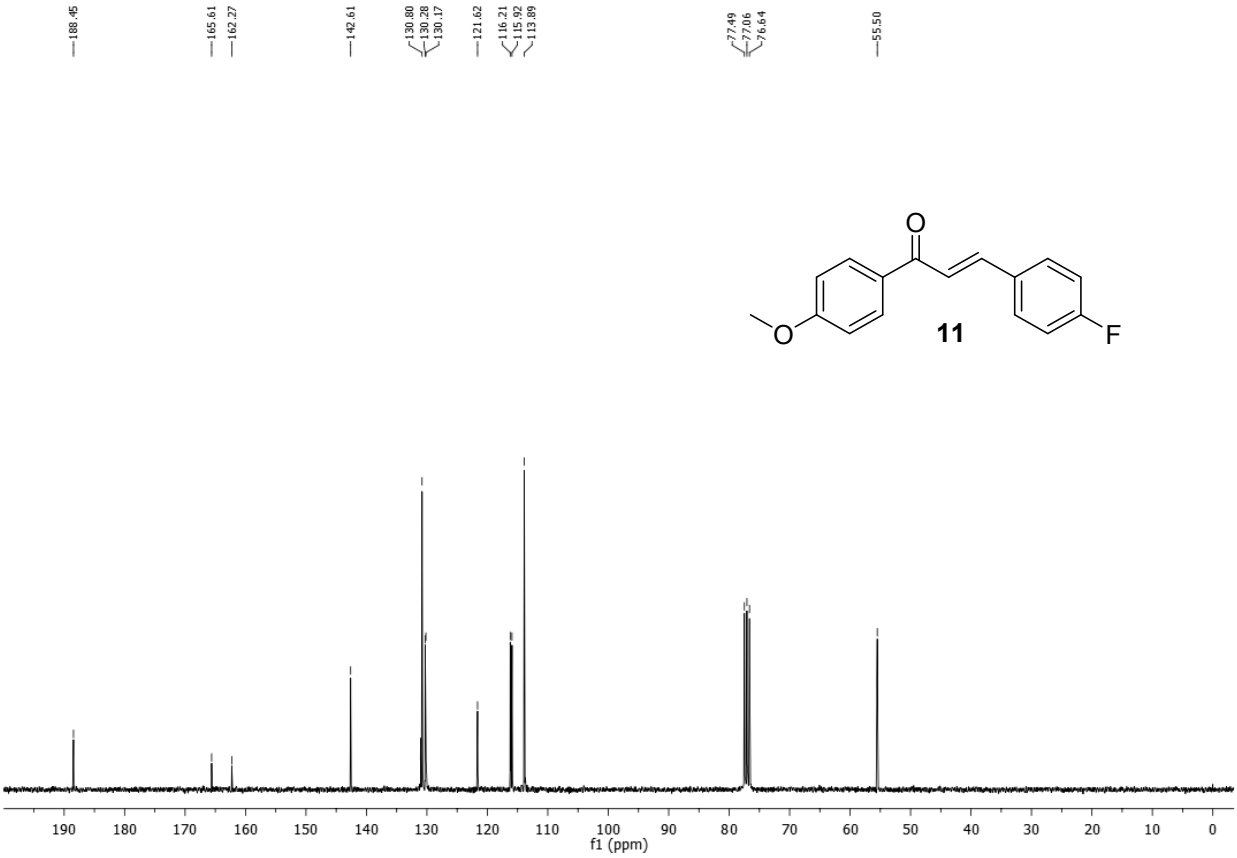
0.96
1.93
1.98
2.99
f1 (ppm)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130.80
130.28
130.17
121.62
116.21
115.92
113.89
77.49
77.06
76.64
55.50
O
O
F
11
f1 (ppm)

8.10
8.05
8.05
8.03
8.00
7.68
7.65
7.50
7.45
7.44
7.30
7.27
6.99
6.96
3.88
0.00
O
O
12
Cl
Cl
0.76
1.94
1.04
1.94
0.89
2.00
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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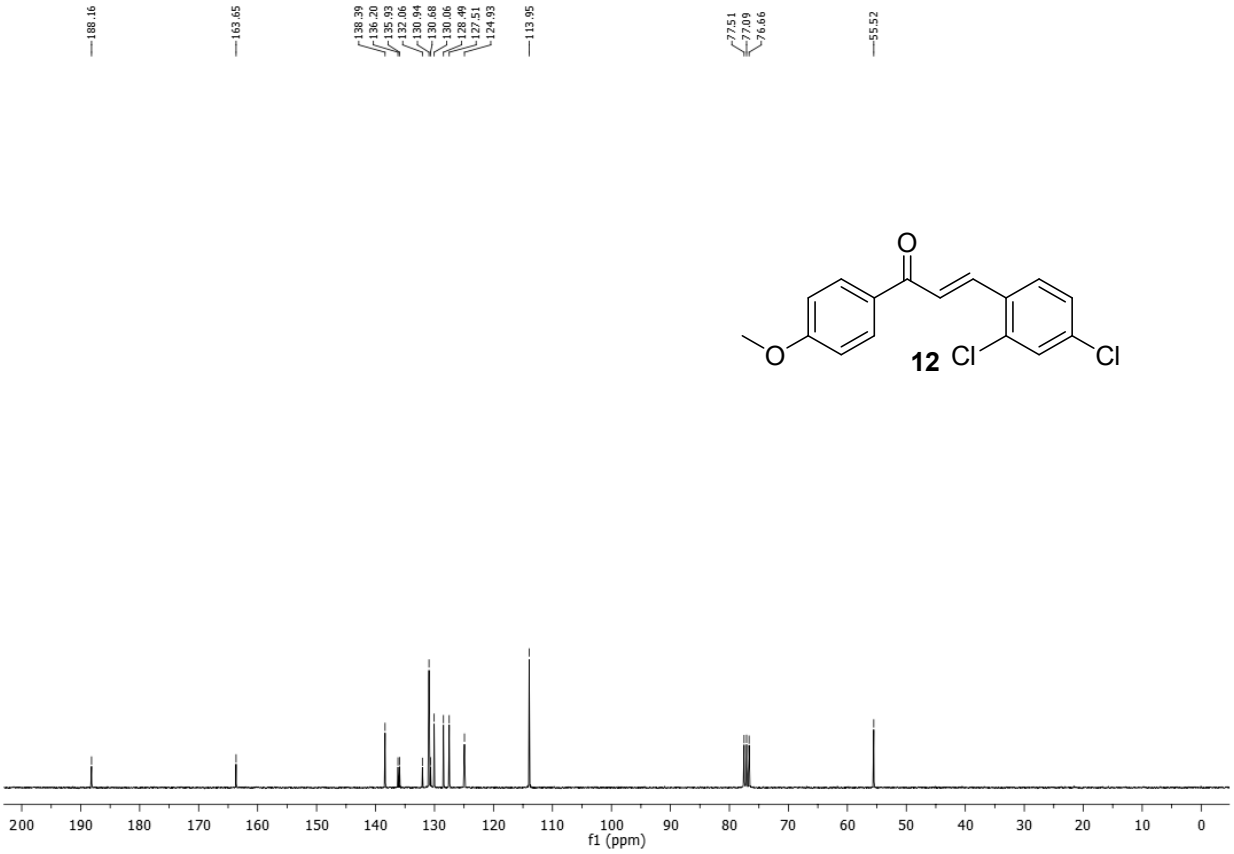
f1 (ppm)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128.49
127.51
124.93
113.95
77.51
77.09
76.66
55.52
O
O
12
Cl
Cl
200
190
180
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150
140
130
120
110
100
90
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70
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50
40
30
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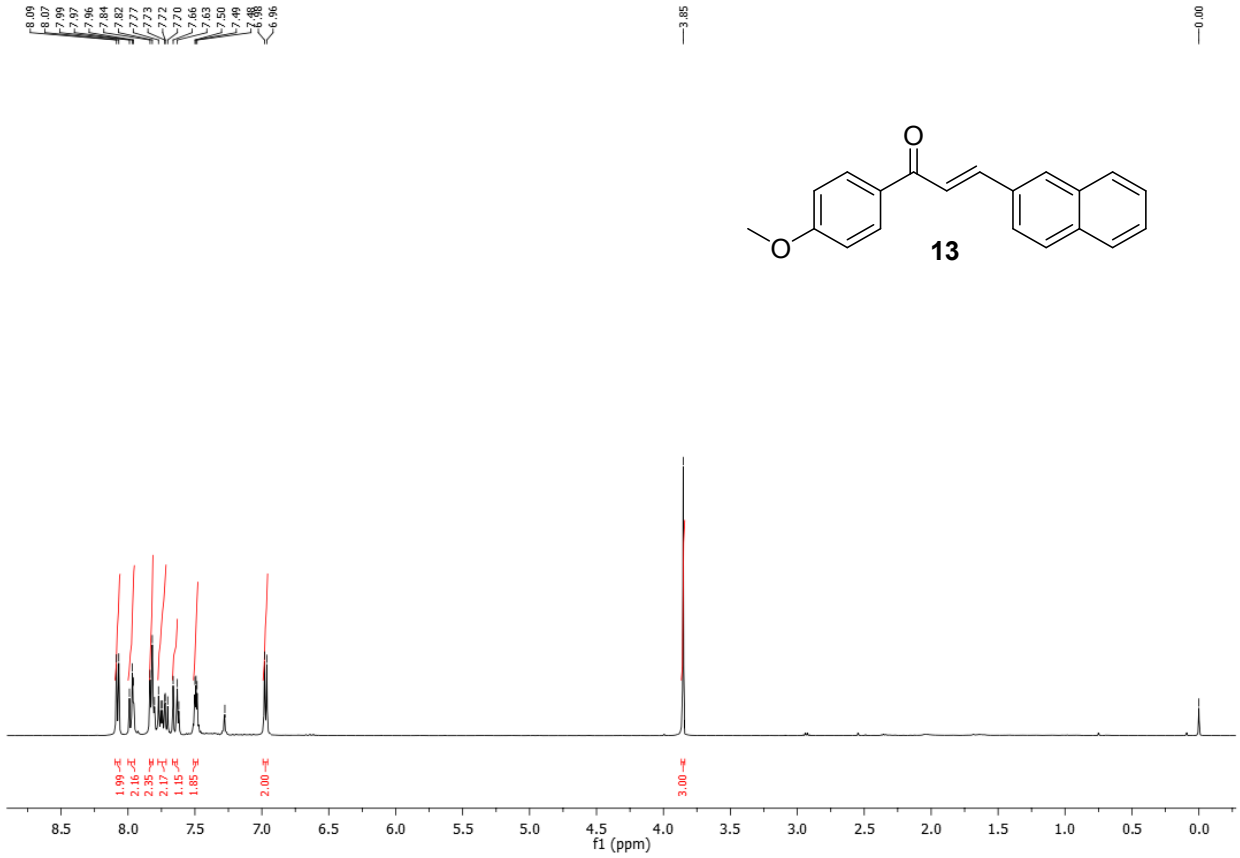
10
0
f1 (ppm)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7.84
7.82
7.77
7.73
7.72
7.70
7.66
7.63
7.50
7.49
6.96
3.85
0.00
O
O
13
1.99
2.16
2.35
2.17
1.15
1.85
2.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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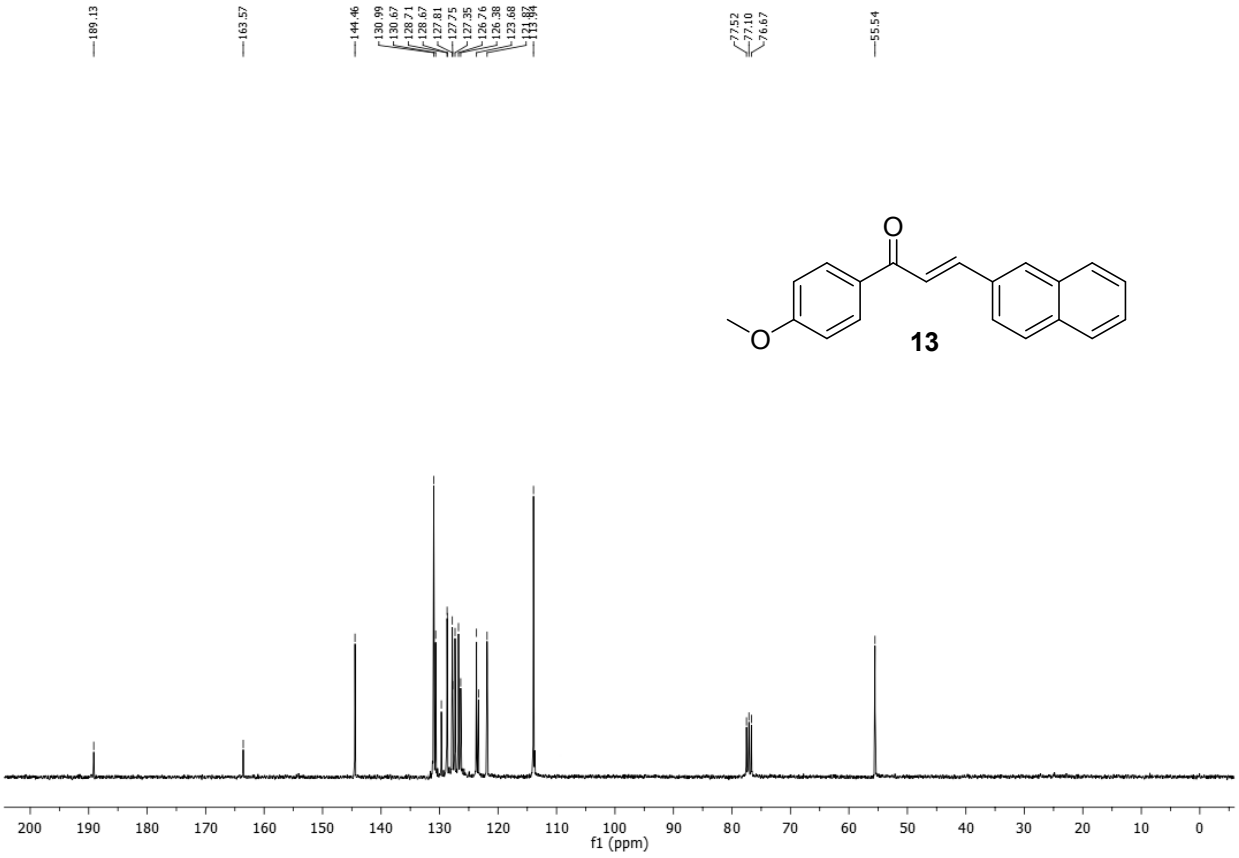
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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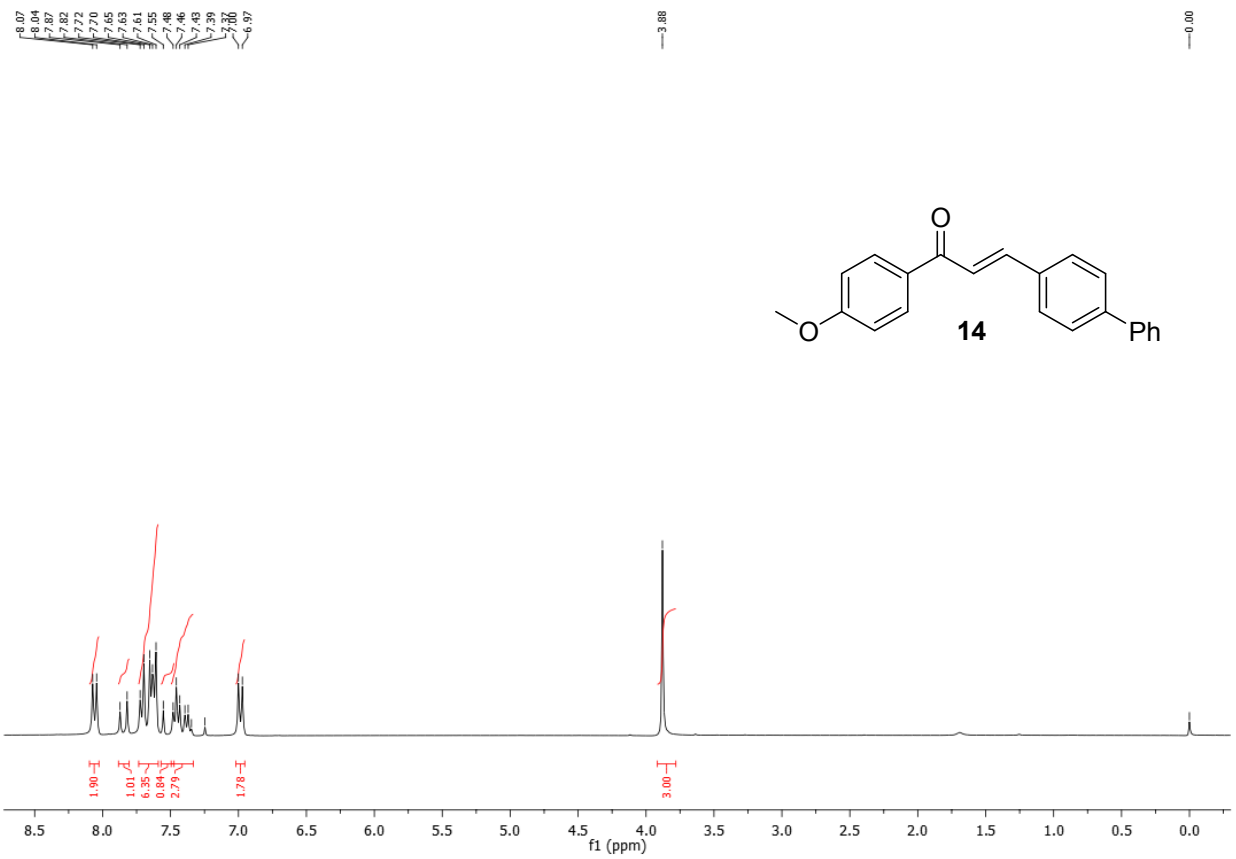
128.67
127.81
127.75
127.35
126.76
126.38
123.68
121.87
113.94
77.52
77.10
76.67
55.54
O
O
13
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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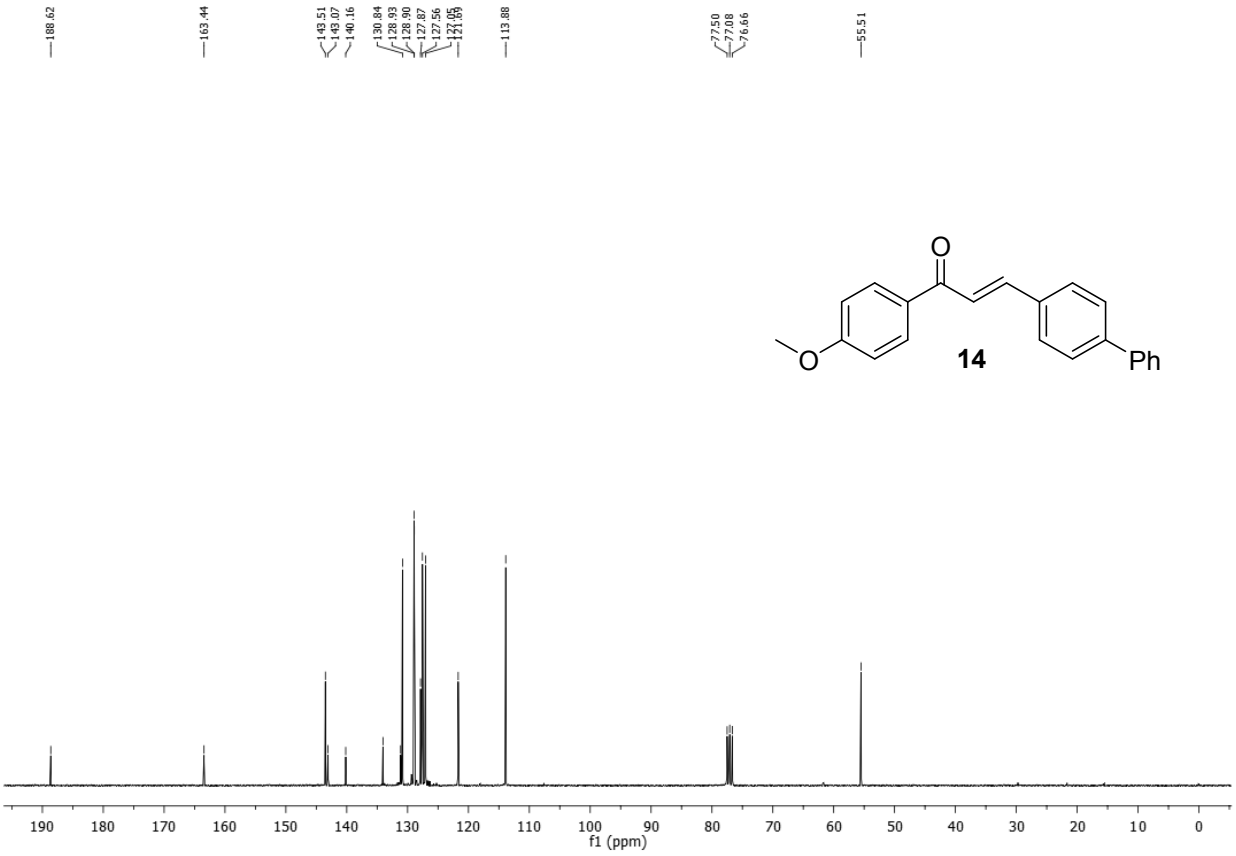
7.82
7.72
7.70
7.65
7.63
7.61
7.55
7.48
7.46
7.43
7.39
7.37
7.00
6.97
3.88
0.00
O
O
14
Ph
1.90
1.01
6.35
0.84
2.79
1.78
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.84
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128.90
127.87
127.56
127.05
121.69
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77.08
76.66
55.51
O
O
14
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
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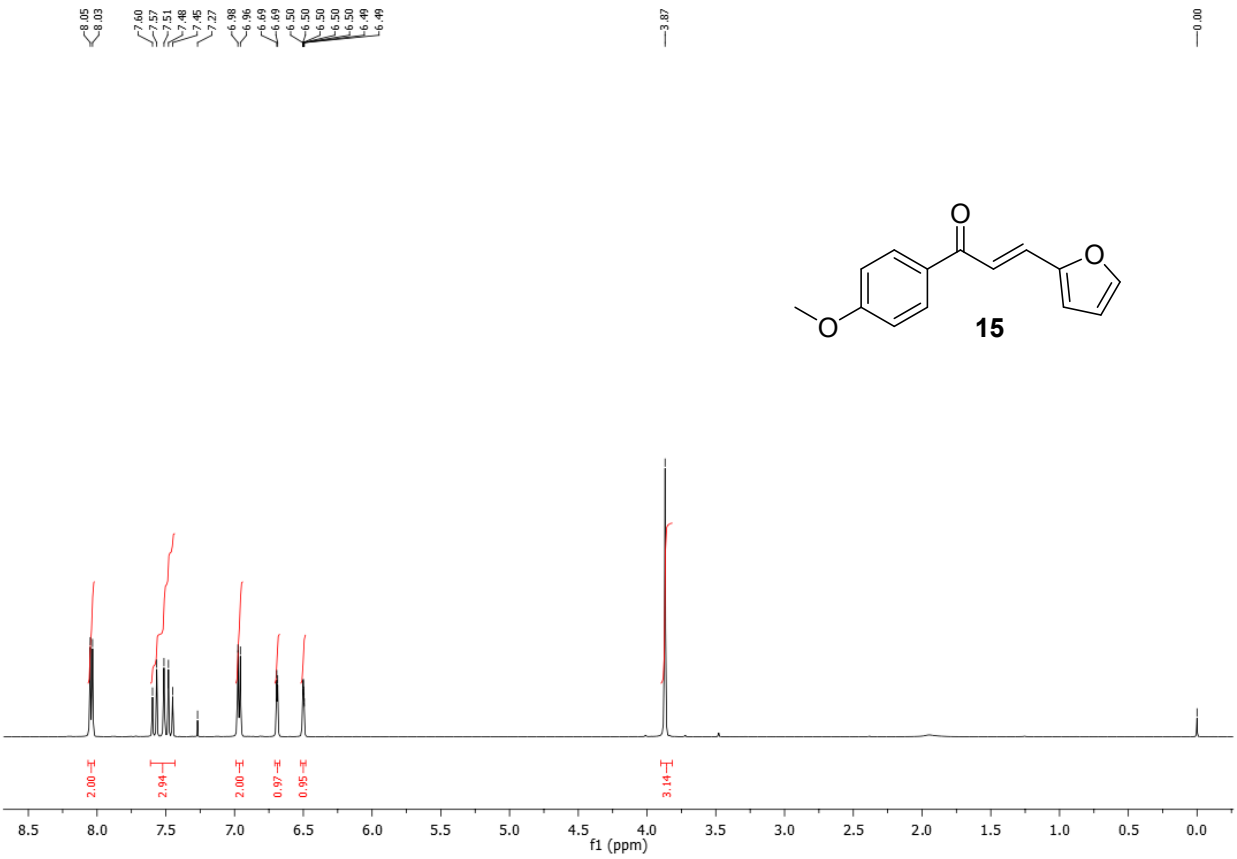
50
40
30
20
10
0
f1 (ppm)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7.27
6.98
6.96
6.69
6.69
6.50
6.50
6.50
6.50
6.49
6.49
3.87
0.00
O
O
O
15
2.00
2.94
2.00
0.97
0.95
3.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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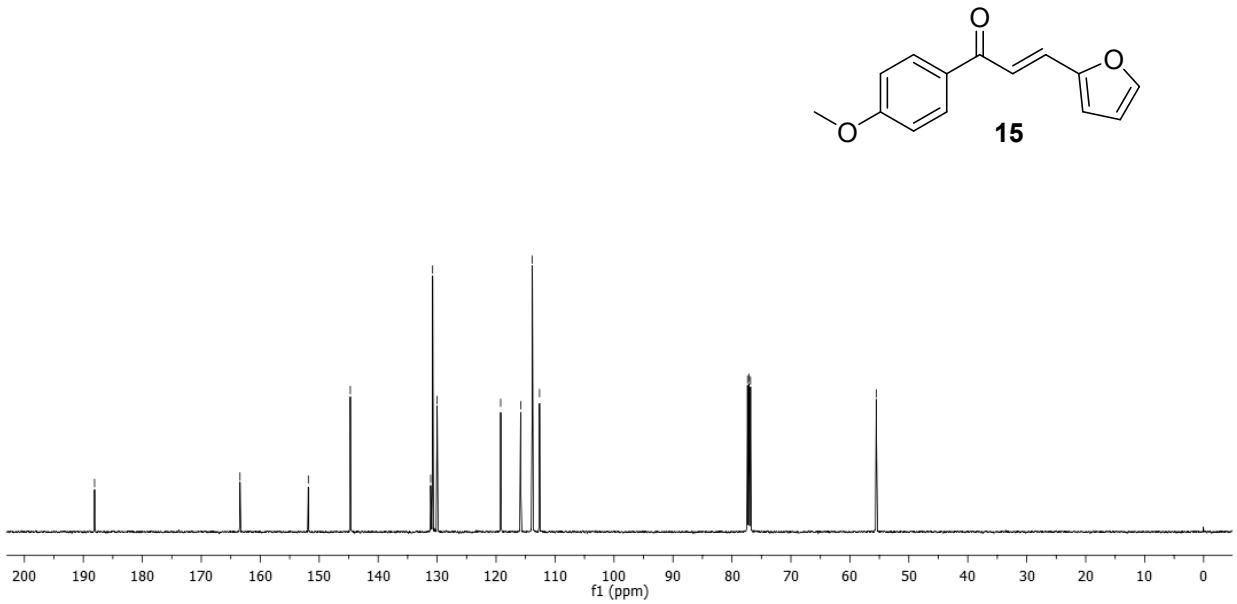
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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151.84
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131.09
130.76
130.00
119.22
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113.85
112.63
77.35
77.10
76.84
55.51
O
O
O
15
200
190
180
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90
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50
40
30
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10
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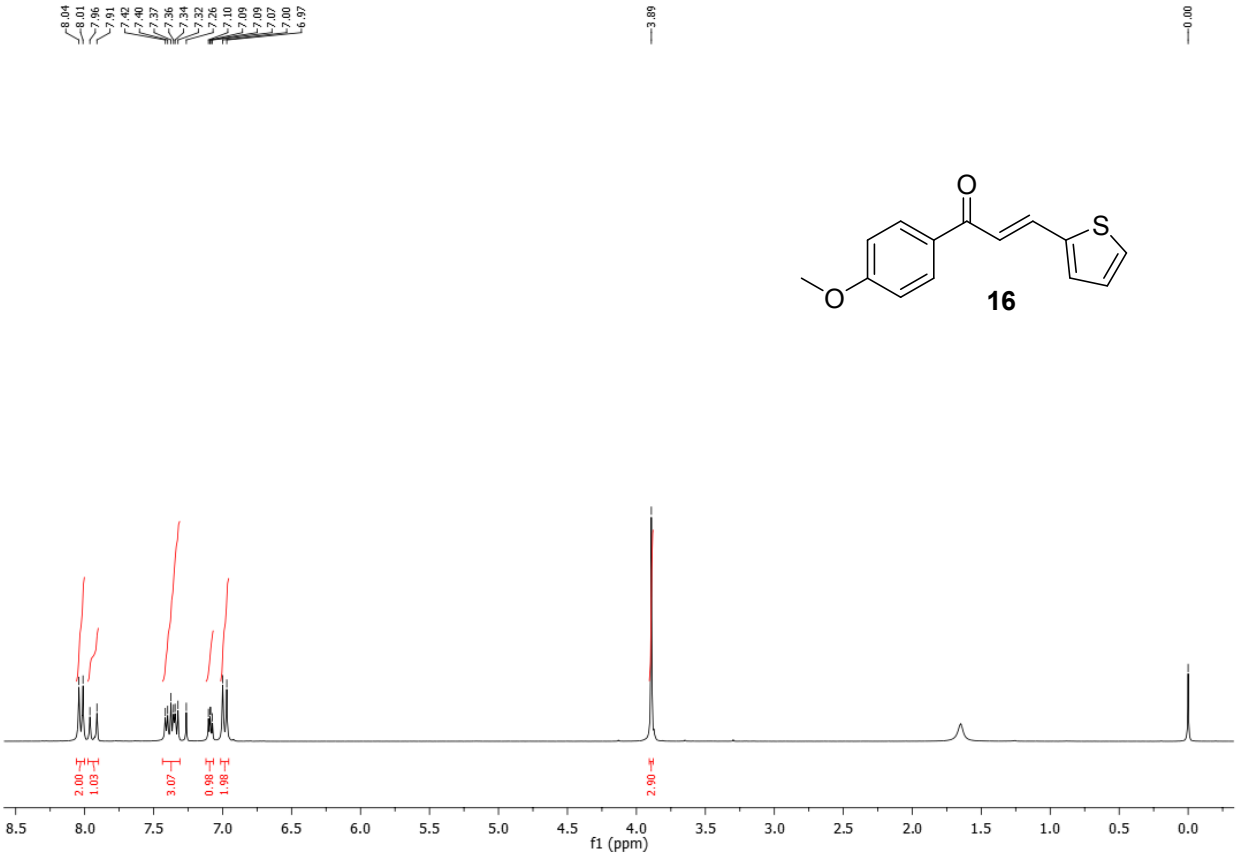
f1 (ppm)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7.32
7.26
7.10
7.09
7.09
7.07
7.00
6.97
3.89
0.00
O
S
O
16
2.00
1.03
3.07
0.98
1.98
2.90
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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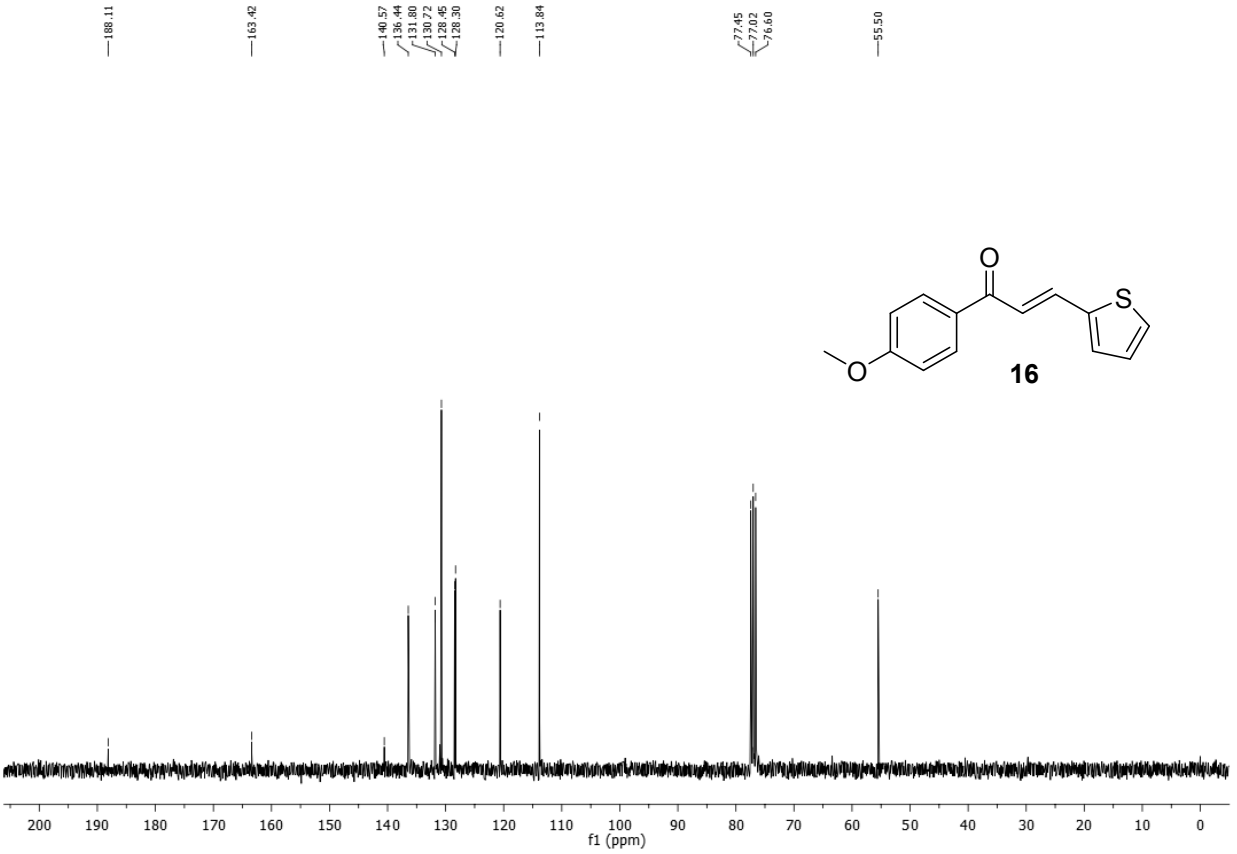
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.30
120.62
113.84
77.45
77.02
76.60
55.50
O
S
O
16
200
190
180
170
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130
120
110
100
90
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70
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50
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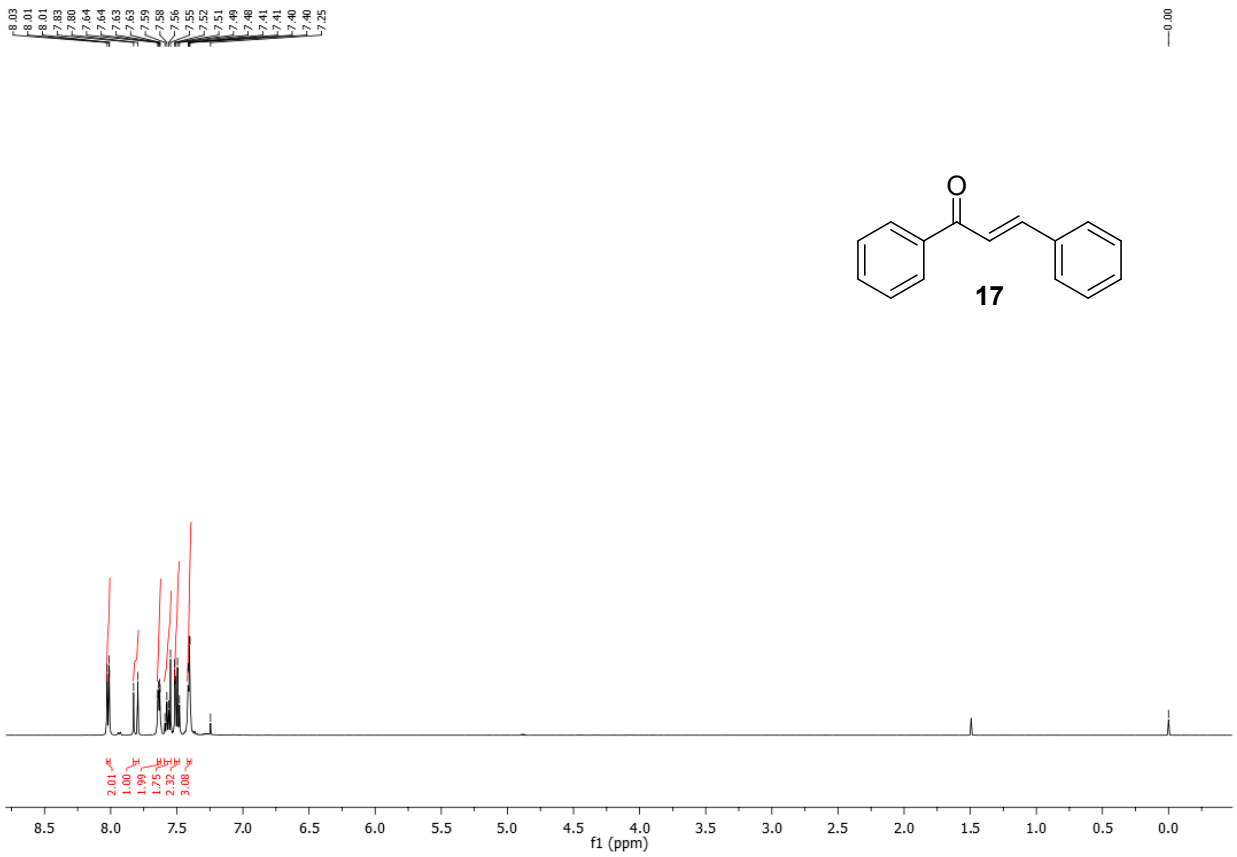
10
0
f1 (ppm)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7.64
7.63
7.63
7.59
7.58
7.56
7.55
7.52
7.51
7.49
7.48
7.41
7.41
7.40
7.40
7.25
0.00
O
17
2.01
1.00
1.99
1.75
2.32
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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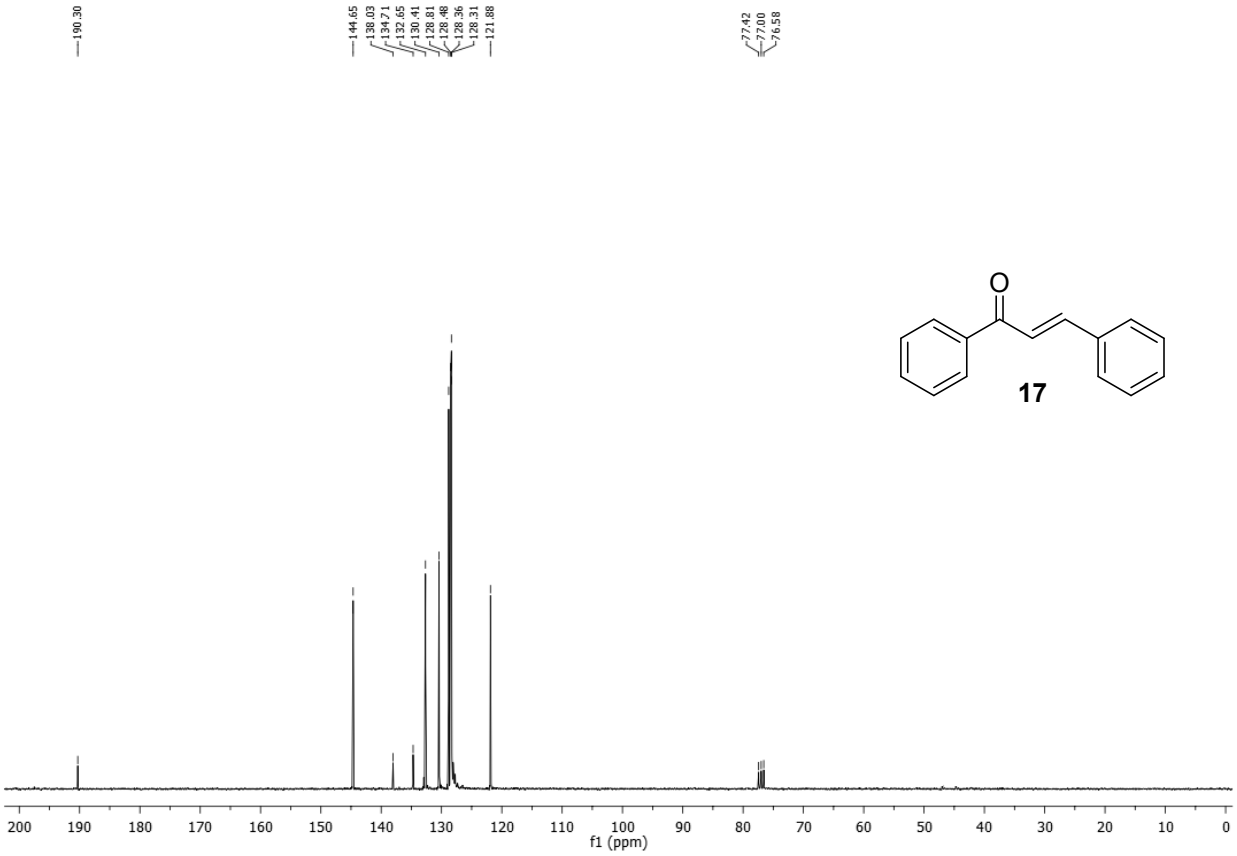
f1 (ppm)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130.41
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128.48
128.36
128.31
121.88
77.42
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76.58
O
17
200
190
180
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150
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130
120
110
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90
80
70
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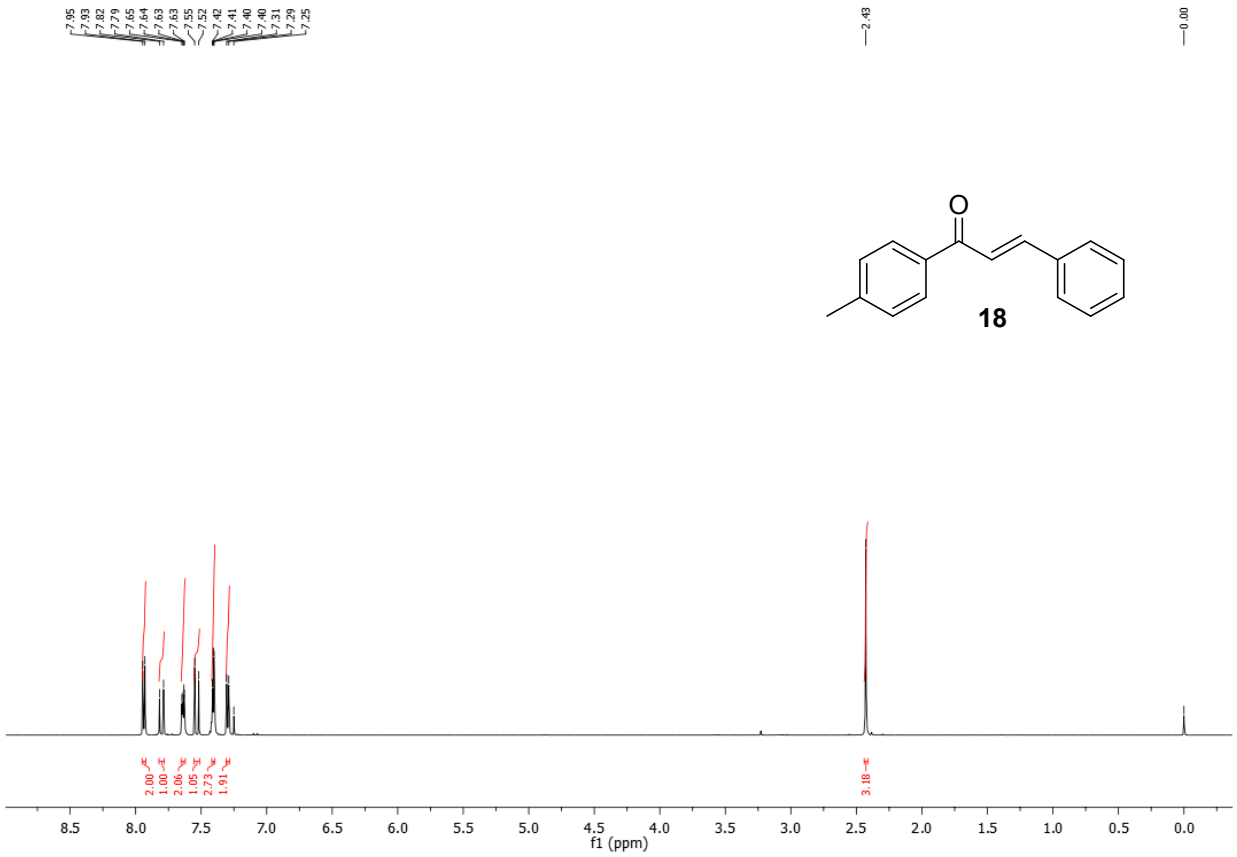
50
40
30
20
10
0
f1 (ppm)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7.63
7.55
7.52
7.42
7.41
7.40
7.40
7.31
7.29
7.25
2.43
0.00
O
18
2.00
1.00
2.06
1.05
2.73
1.91
3.18
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
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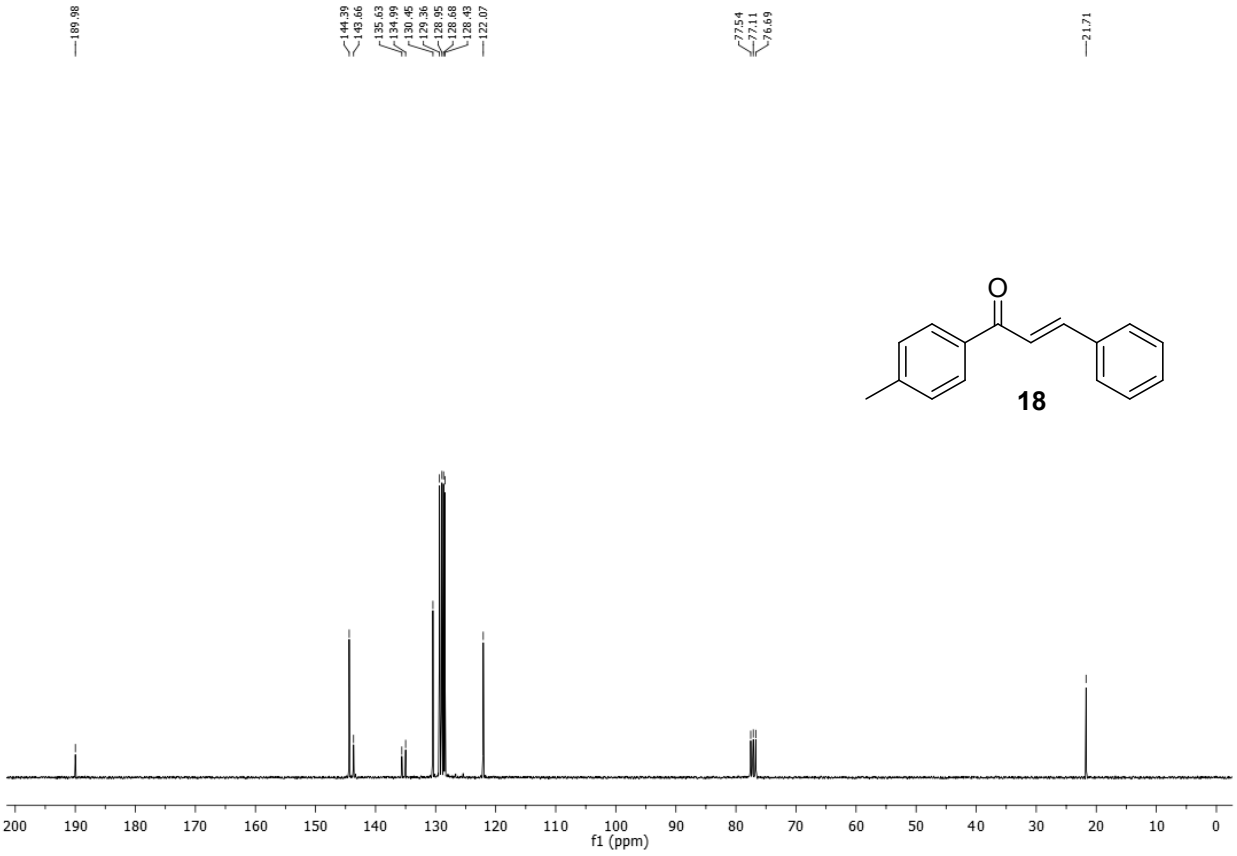
0.0
f1 (ppm)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128.95
128.68
128.43
122.07
77.54
77.11
76.69
21.71
O
18
200
190
180
170
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150
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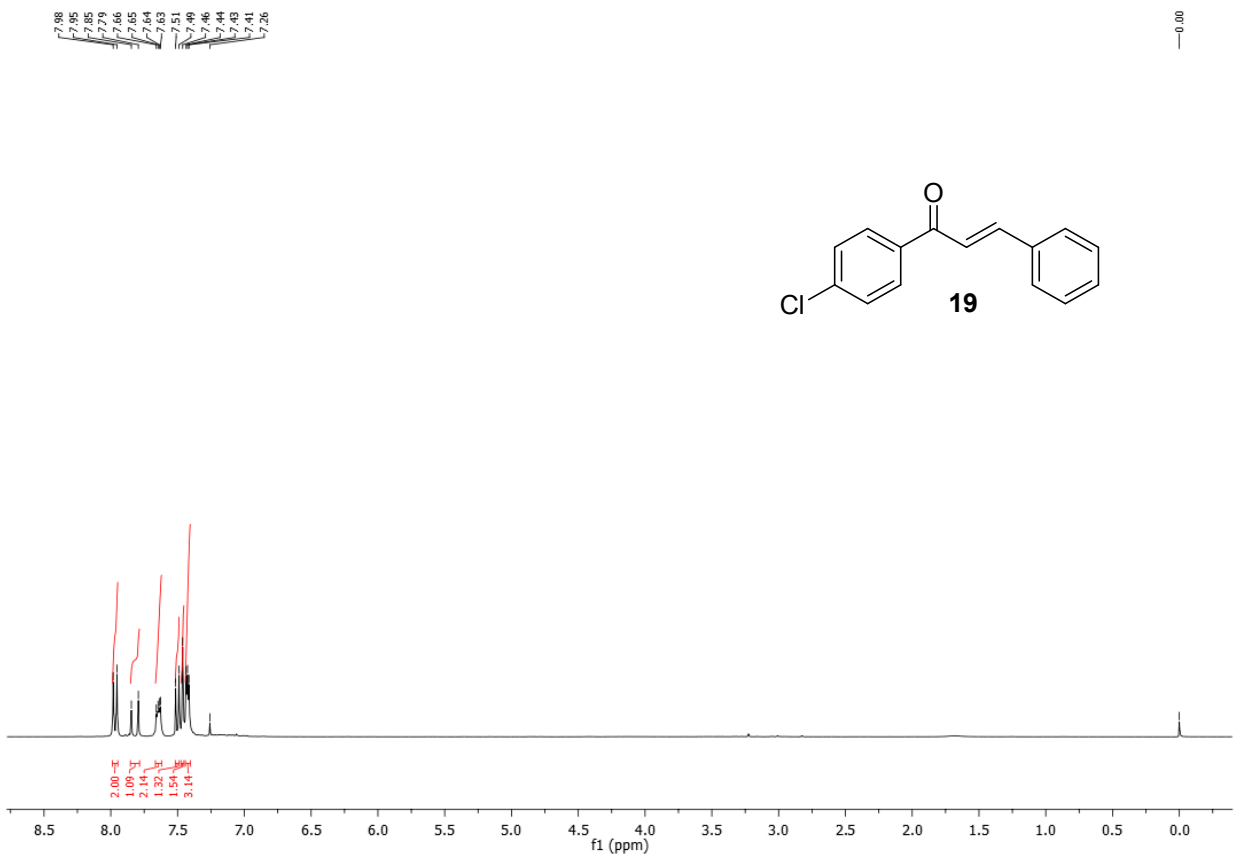
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.64
7.63
7.51
7.49
7.46
7.44
7.43
7.41
7.26
0.00
O
Cl
19
2.00
1.09
2.14
1.32
1.54
3.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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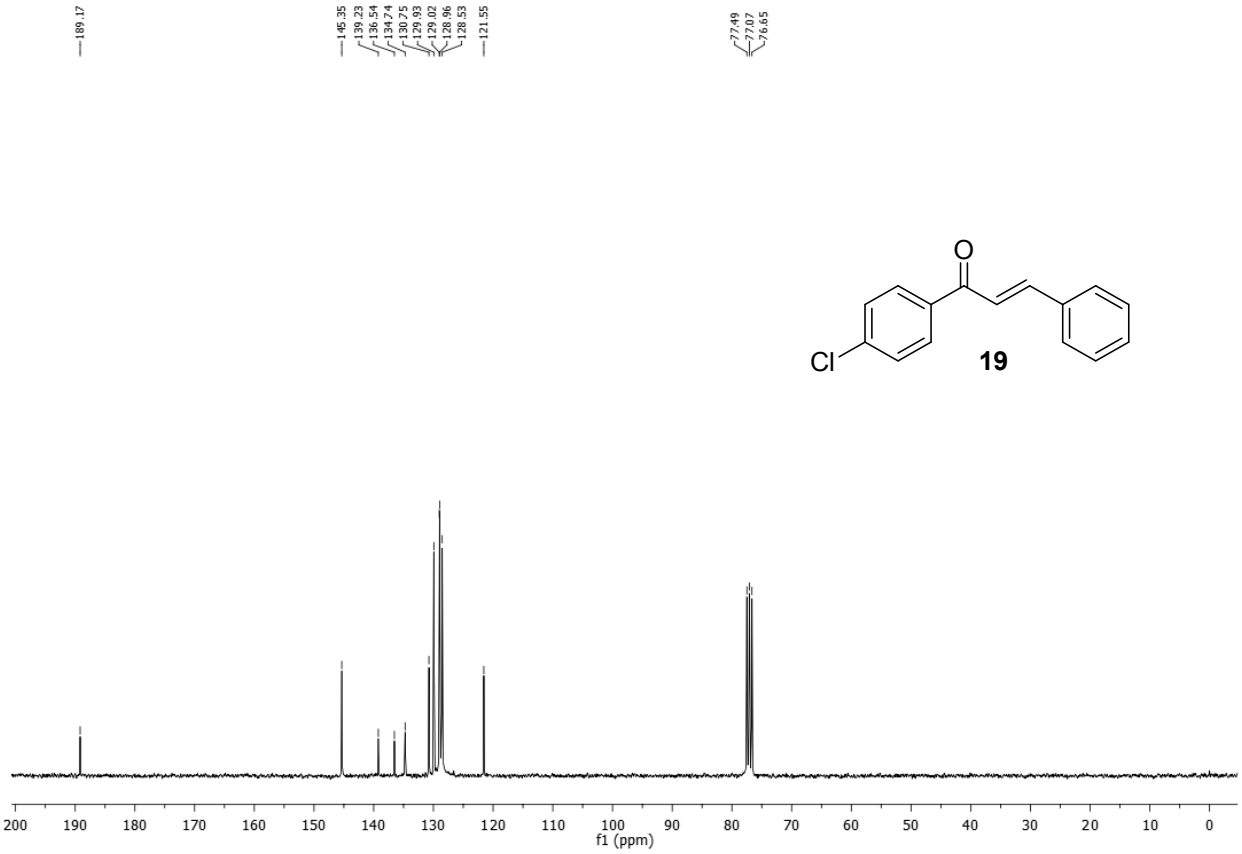
0.0
f1 (ppm)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129.02
128.96
128.53
121.55
77.49
77.07
76.65
O
Cl
19
200
190
180
170
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150
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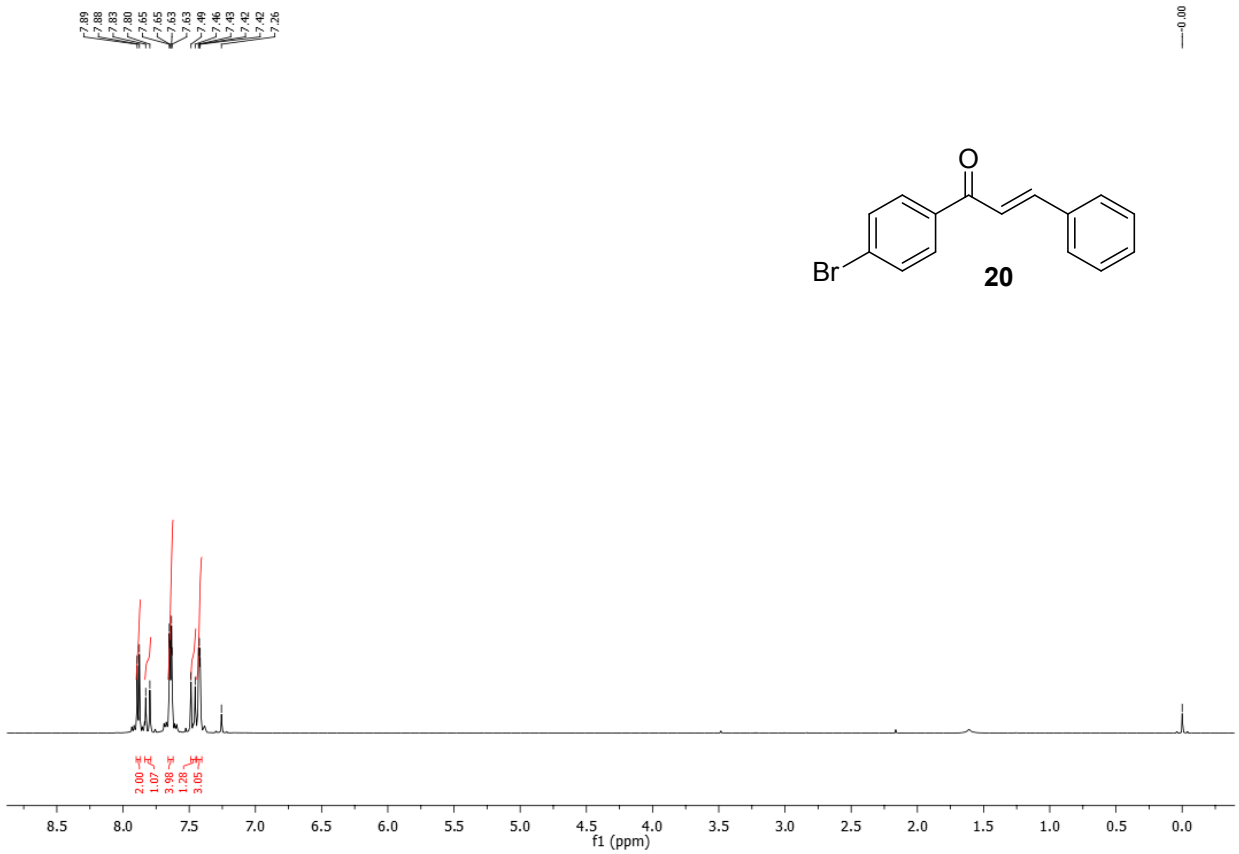
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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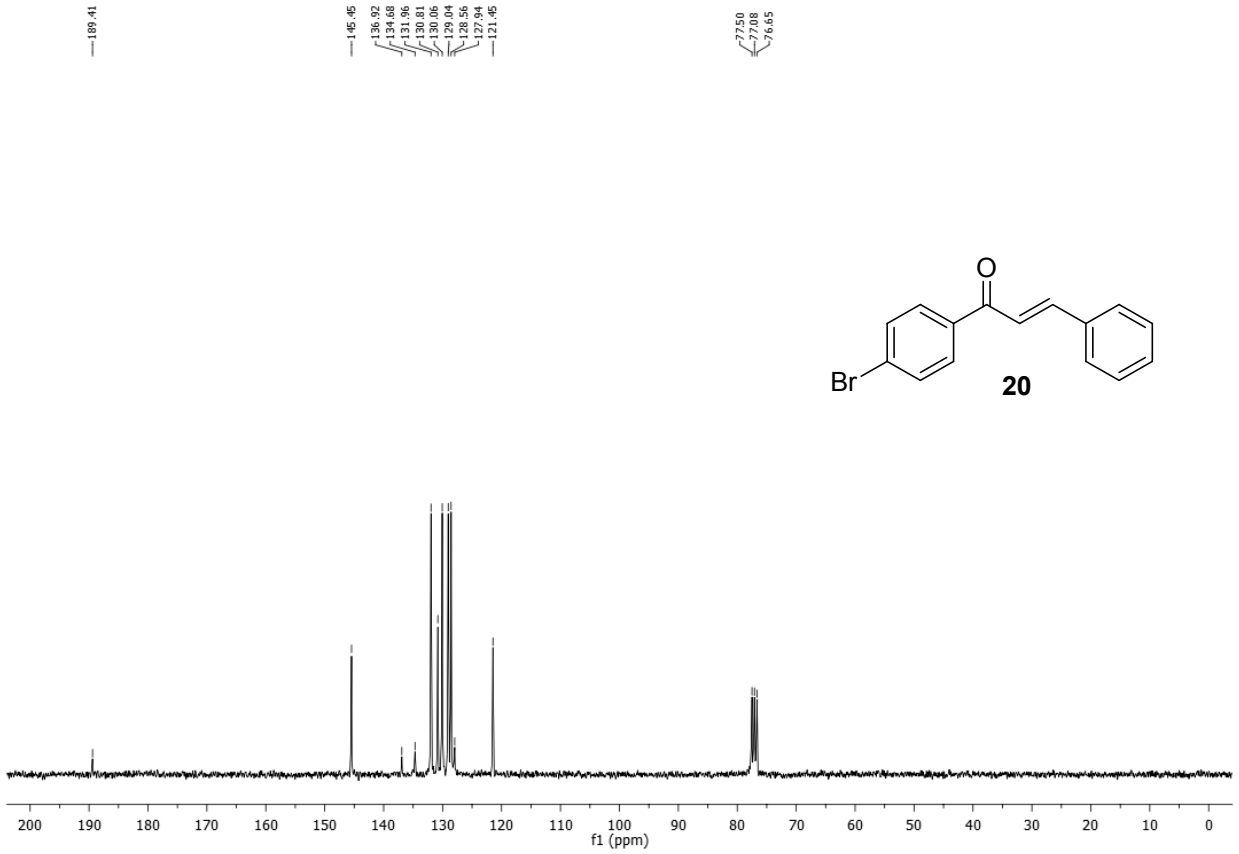
7.63
7.63
7.49
7.46
7.43
7.42
7.42
7.26
0.00
O
Br
20
2.00
1.07
3.98
1.28
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.81
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129.04
128.56
127.94
121.45
77.50
77.08
76.65
O
Br
20
200
190
180
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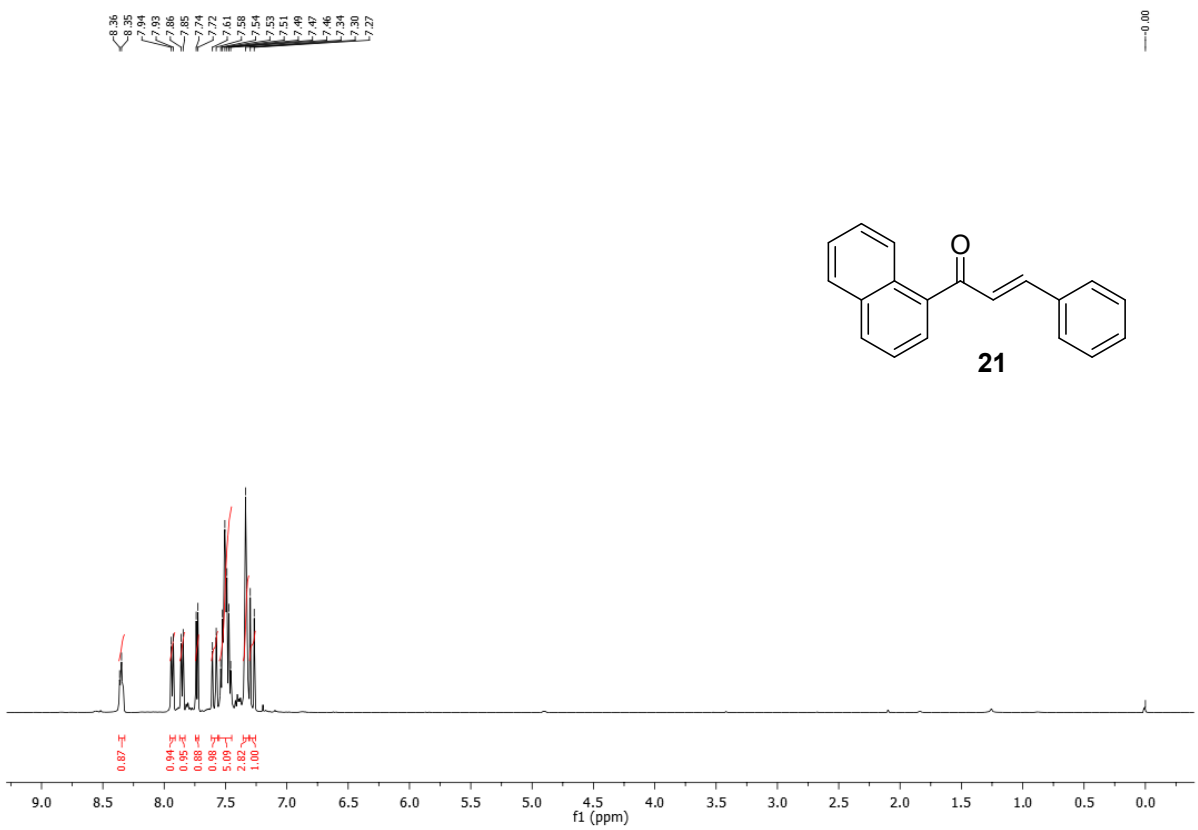
50
40
30
20
10
0
f1 (ppm)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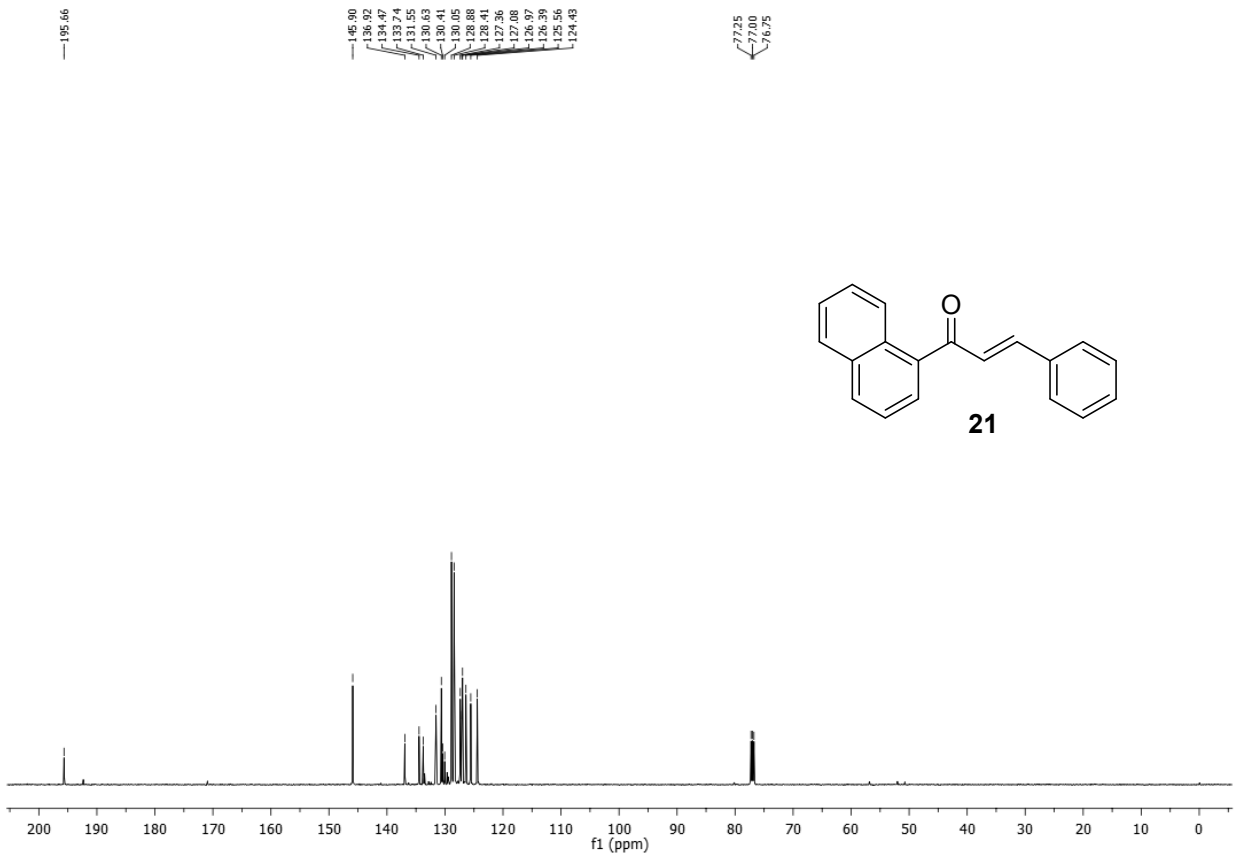
7.72
7.61
7.58
7.54
7.53
7.51
7.49
7.47
7.46
7.34
7.30
7.27
0.00
O
21
0.87
0.94
0.95
0.88
0.98
5.09
2.82
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.74
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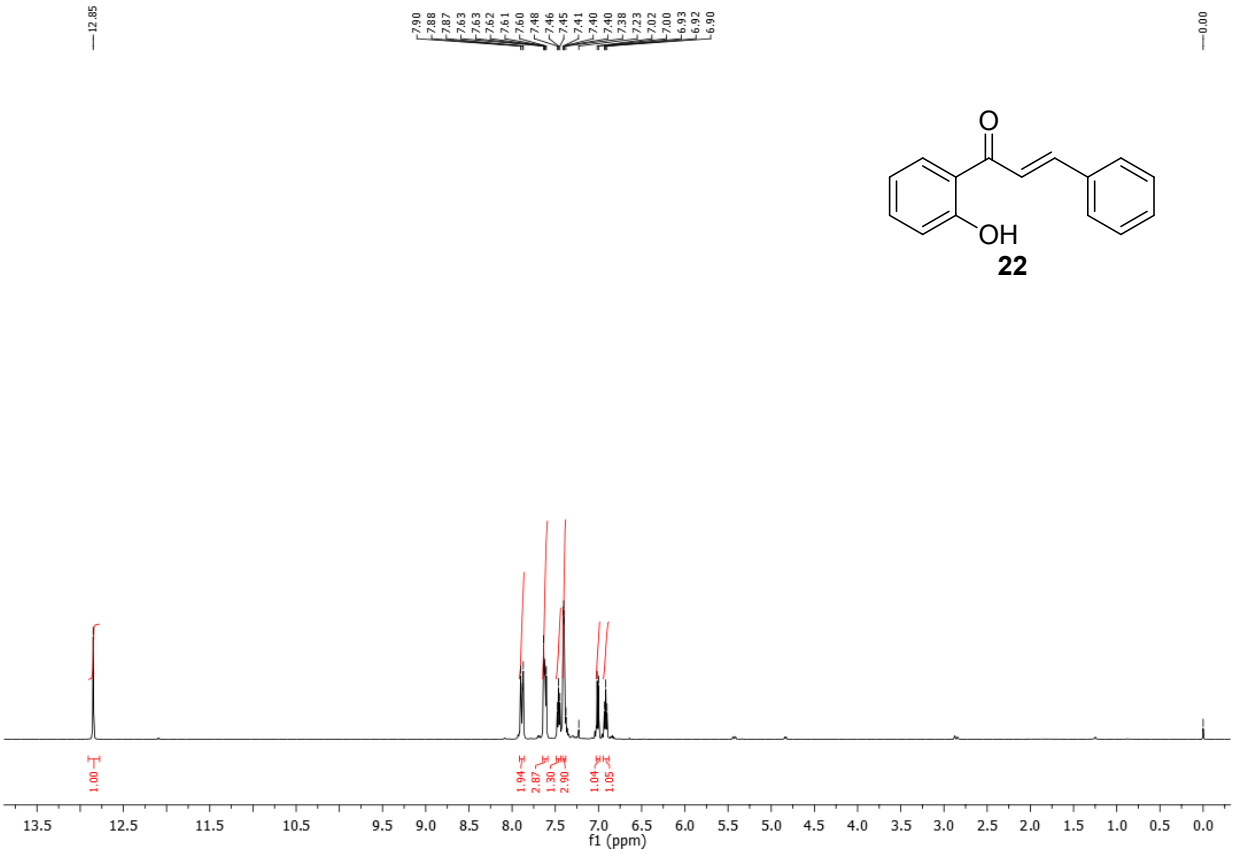
130.41
130.05
128.88
128.41
127.36
127.08
126.97
126.39
125.56
124.43
77.25
77.00
76.75
O
21
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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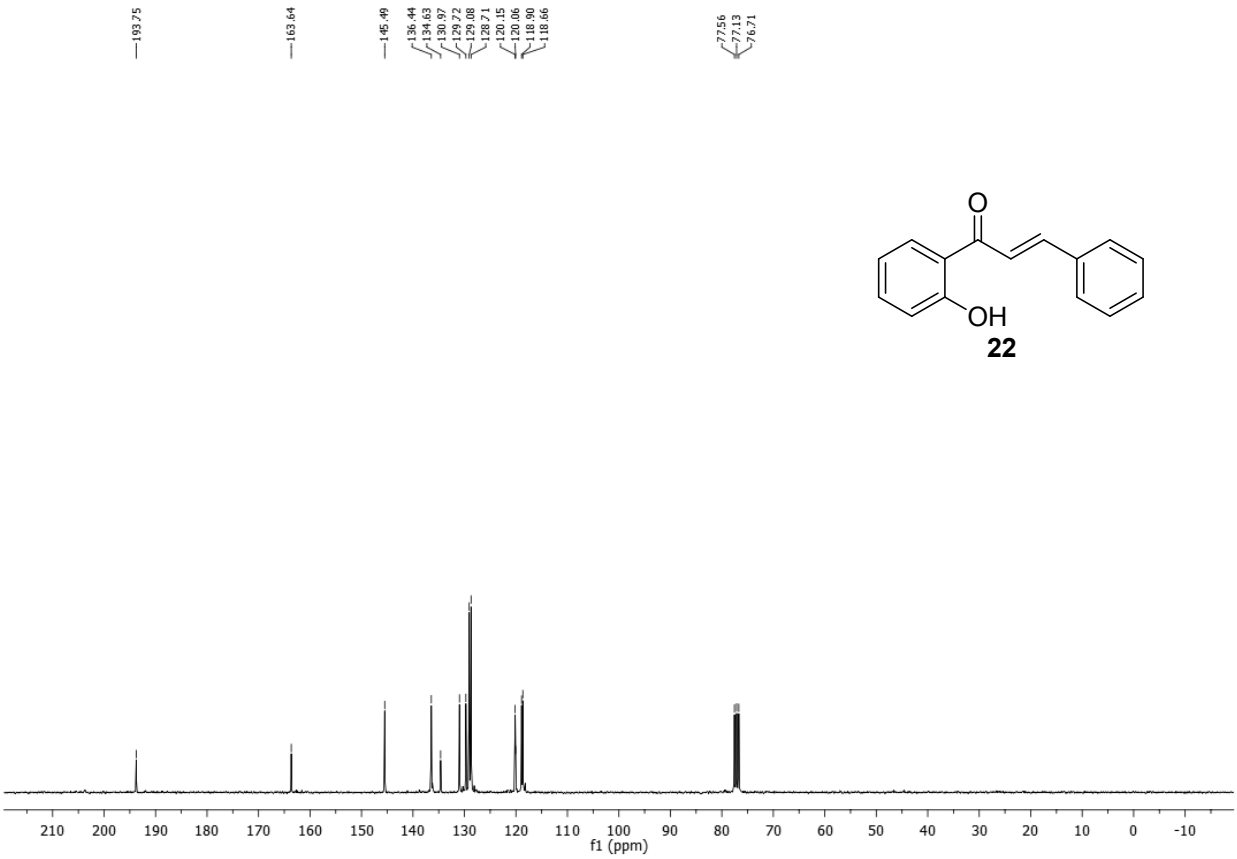
7.61
7.60
7.48
7.46
7.45
7.41
7.40
7.40
7.38
7.23
7.02
7.00
6.93
6.92
6.90
0.00
O
OH
22
1.00
1.94
2.87
1.30
2.90
1.04
1.05
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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163.64
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136.44
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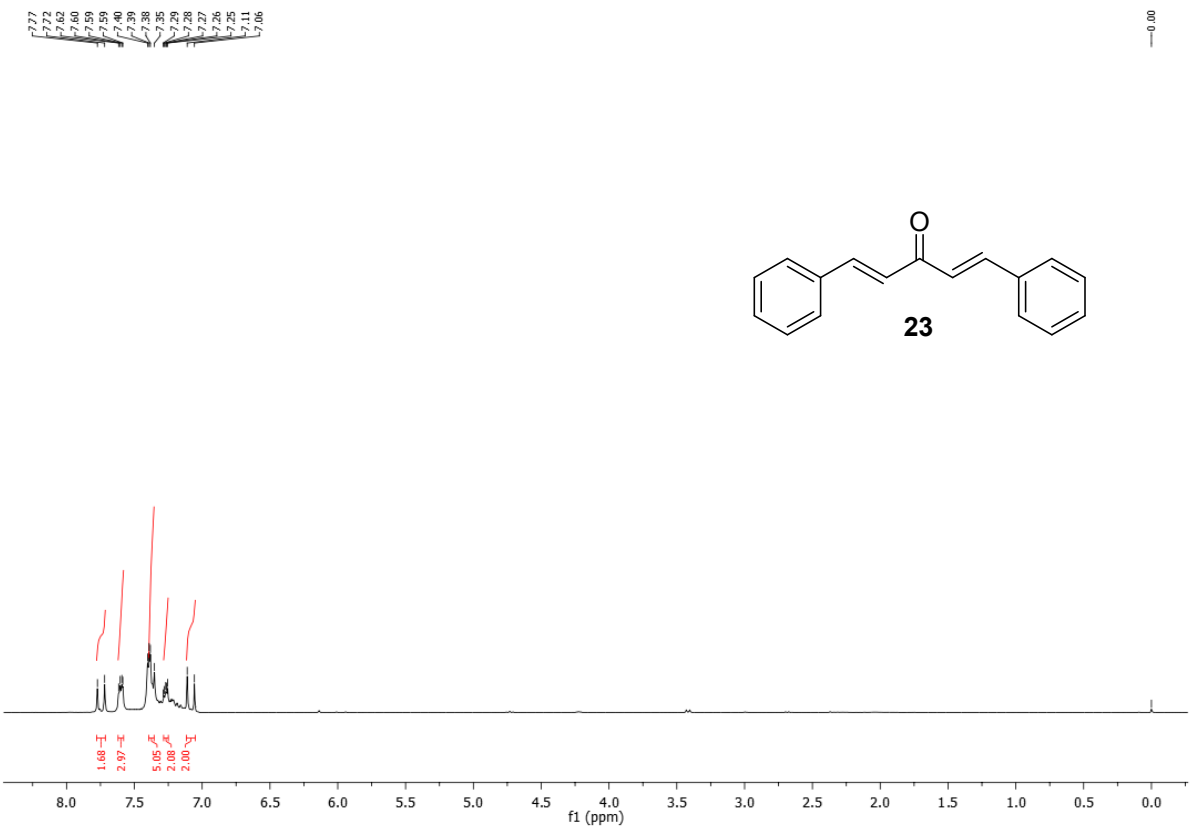
130.97
129.72
129.08
128.71
120.15
120.06
118.90
118.66
77.56
77.13
76.71
O
OH
22
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.39
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7.35
7.29
7.28
7.27
7.26
7.25
7.11
7.06
0.00
O
23
1.68
2.97
5.05
2.08
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
1.0
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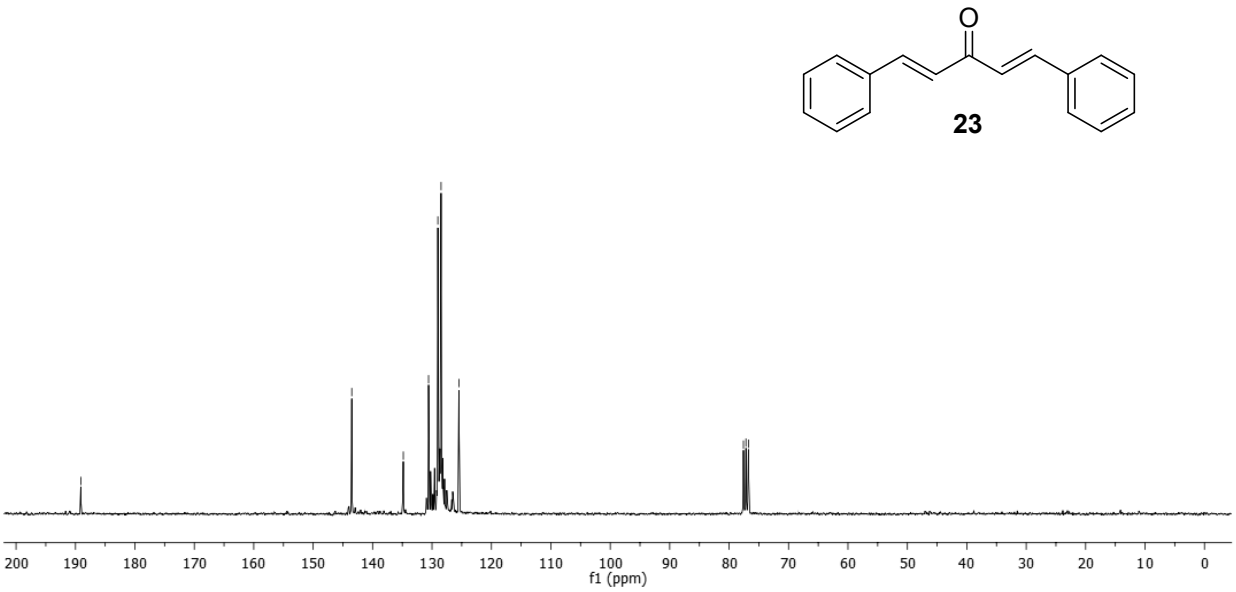
0.0
f1 (ppm)


189.10
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129.02
128.47
125.47
77.59
77.17
76.74
O
23
200
190
180
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90
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50
40
30
20
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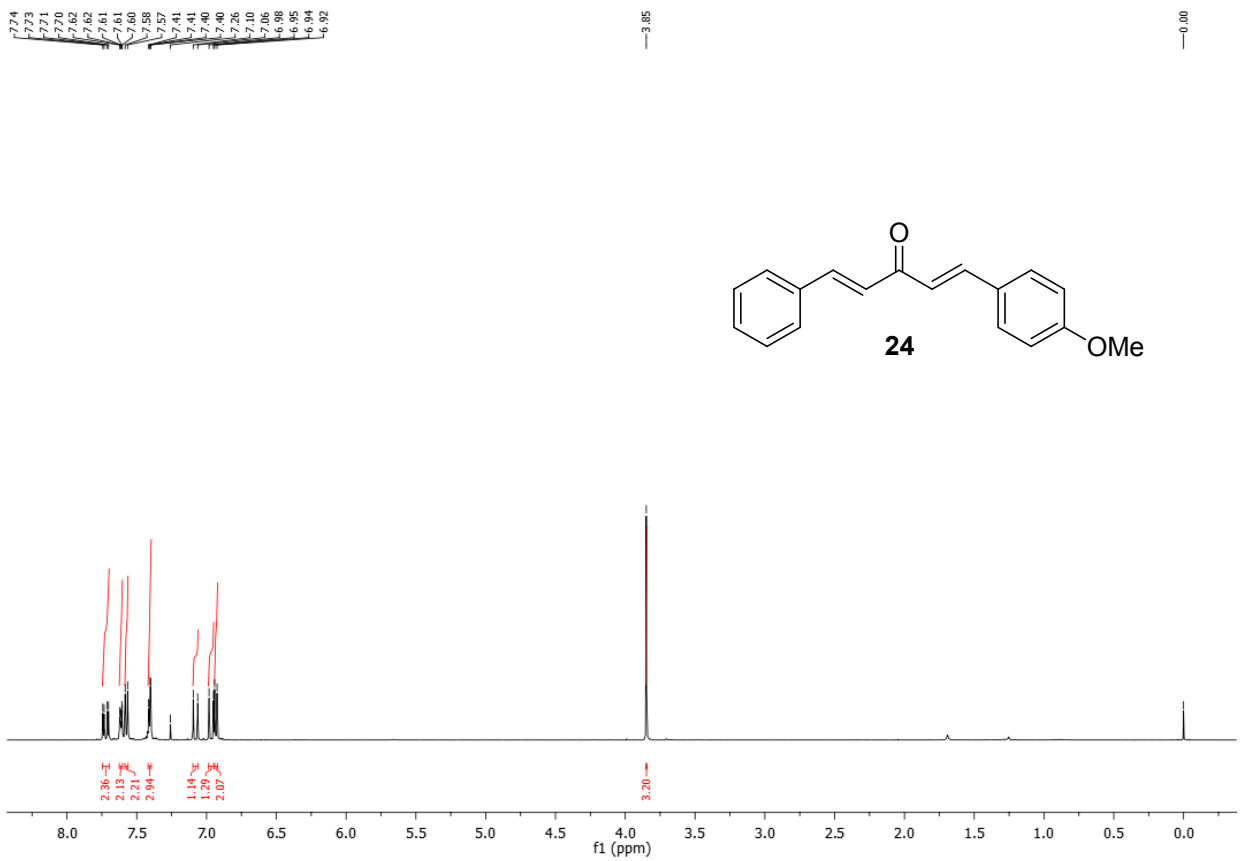
0
f1 (ppm)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7.61
7.61
7.60
7.58
7.57
7.41
7.41
7.40
7.40
7.26
7.10
7.06
6.98
6.95
6.94
6.92
3.85
0.00
O
24
OMe
2.36
2.13
2.21
2.04
1.14
1.29
2.07
3.20
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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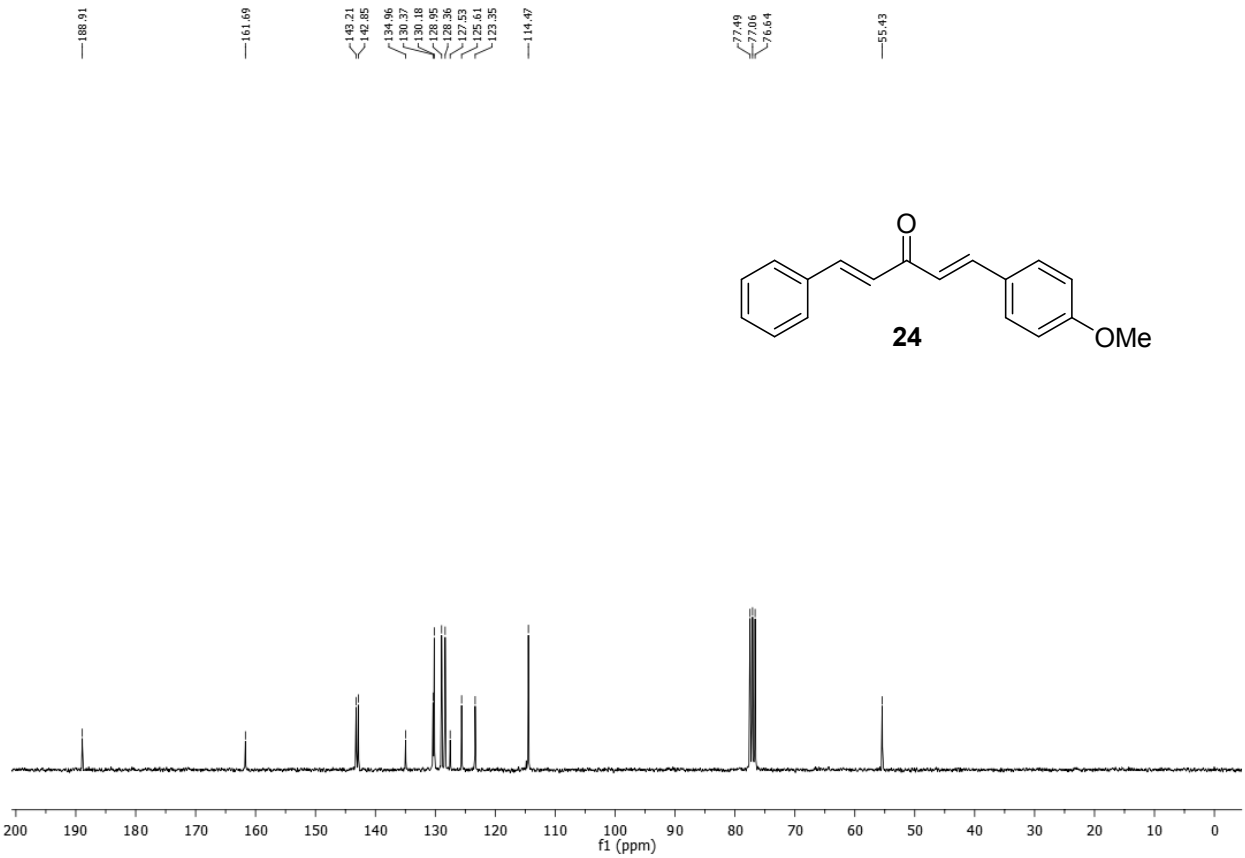
0.0
f1 (ppm)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143.21
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128.95
128.36
127.53
125.61
123.35
114.47
77.49
77.06
76.64
55.43
O
24
OMe
200
190
180
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120
110
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90
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50
40
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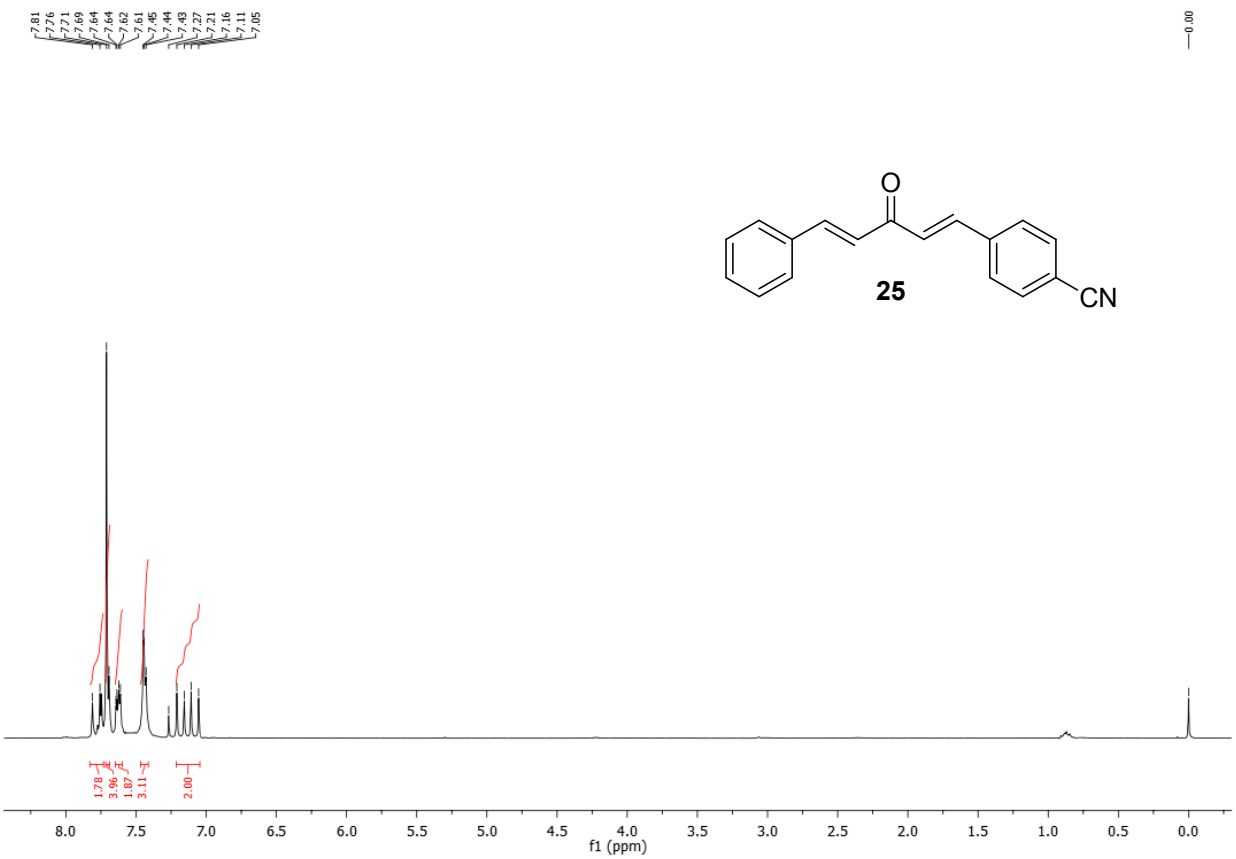
f1 (ppm)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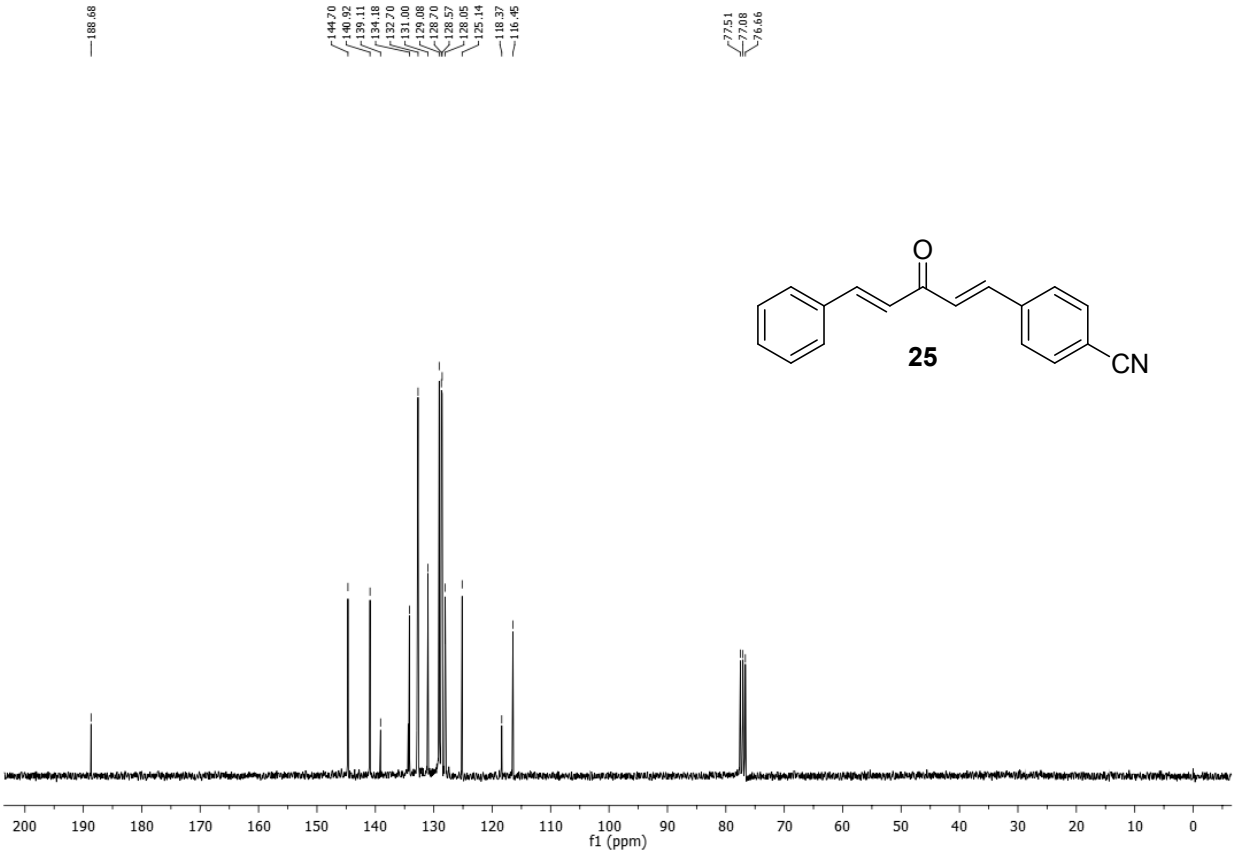
7.71
7.69
7.64
7.64
7.62
7.61
7.45
7.44
7.43
7.27
7.21
7.16
7.11
7.05
0.00
O
25
CN
1.78
3.96
1.87
3.11
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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140.92
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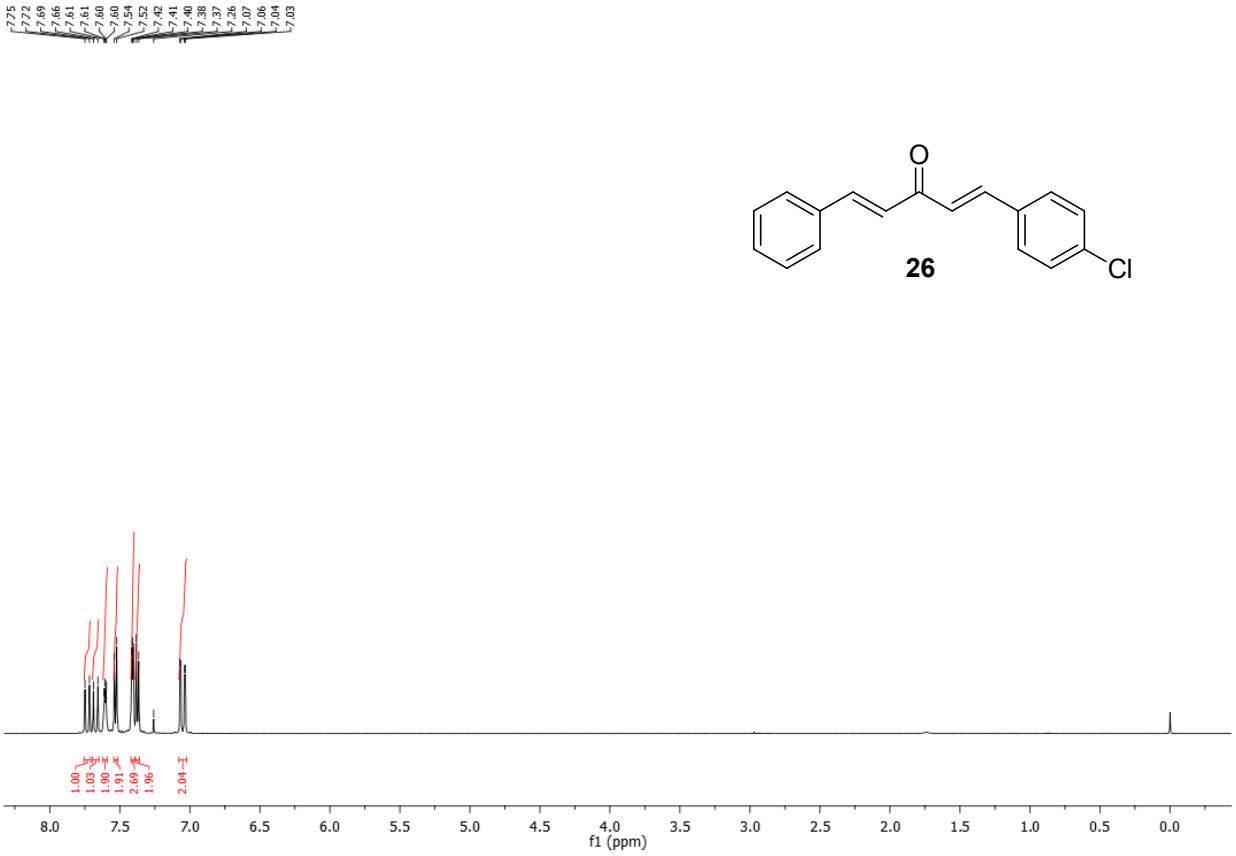
134.18
132.70
131.00
129.08
128.70
128.57
128.05
125.14
118.37
116.45
77.51
77.08
76.66
O
25
CN
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.60
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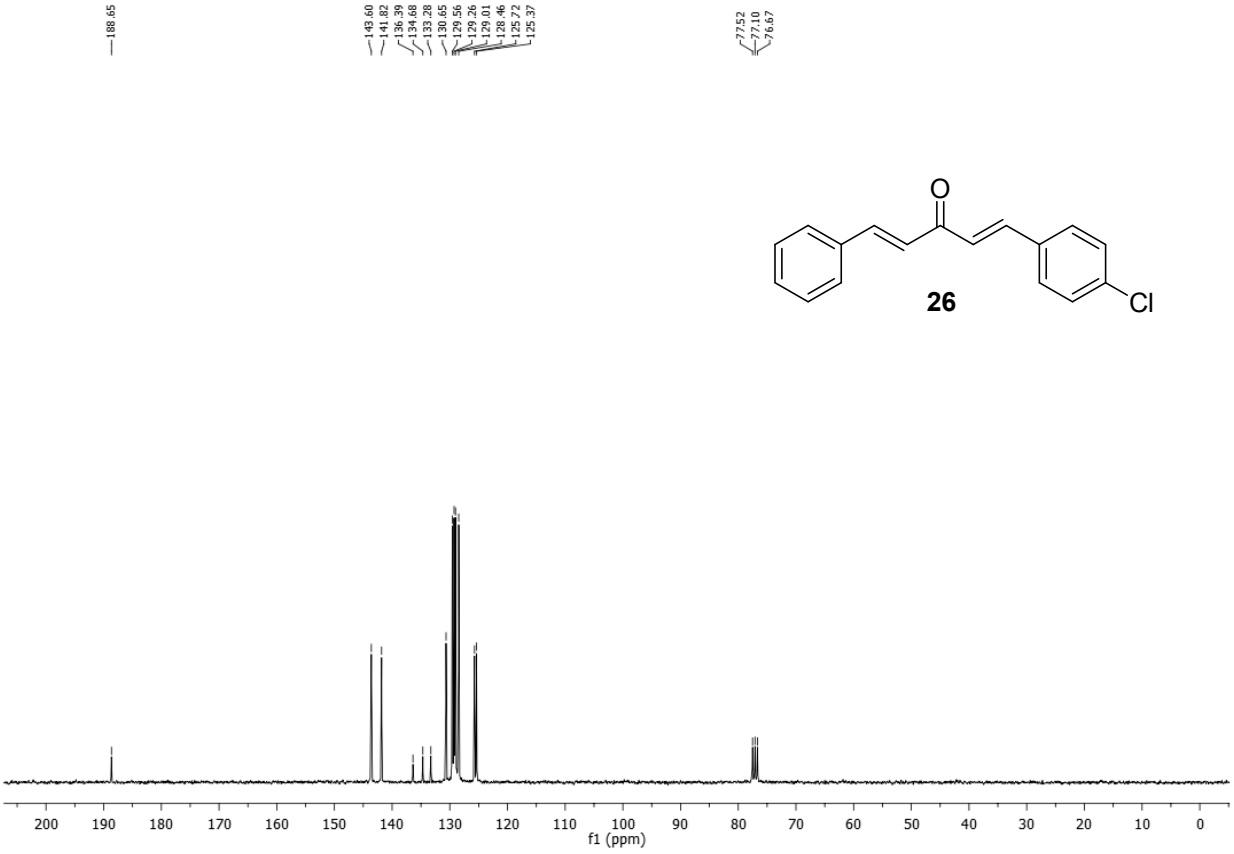
7.52
7.42
7.41
7.40
7.38
7.37
7.26
7.07
7.06
7.04
7.03
O
26
Cl
1.00
1.03
1.00
1.01
2.69
1.96
2.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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143.60
141.82
136.39
134.68
133.28
130.65
129.56
129.26
129.01
128.46
125.72
125.37
77.52
77.10
76.67
O
26
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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50
40
30
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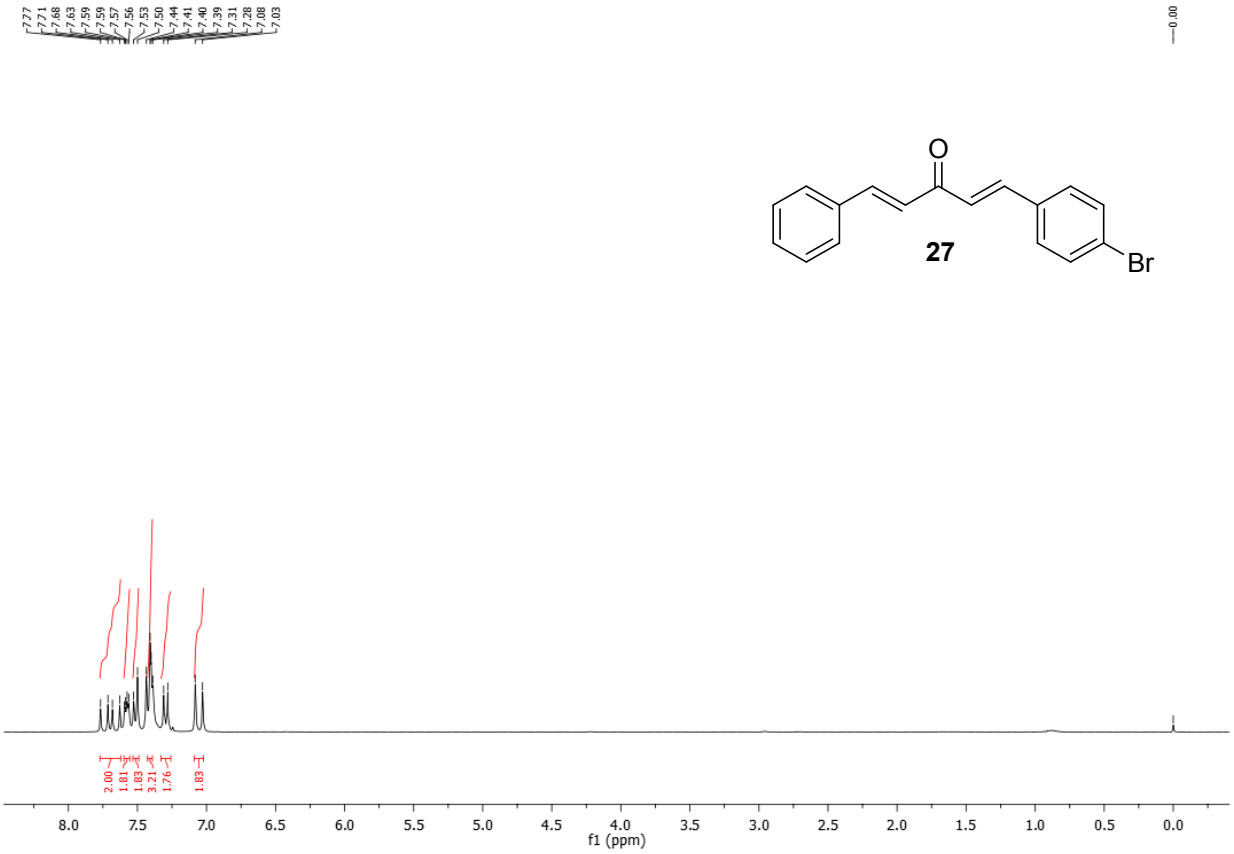
10
0
f1 (ppm)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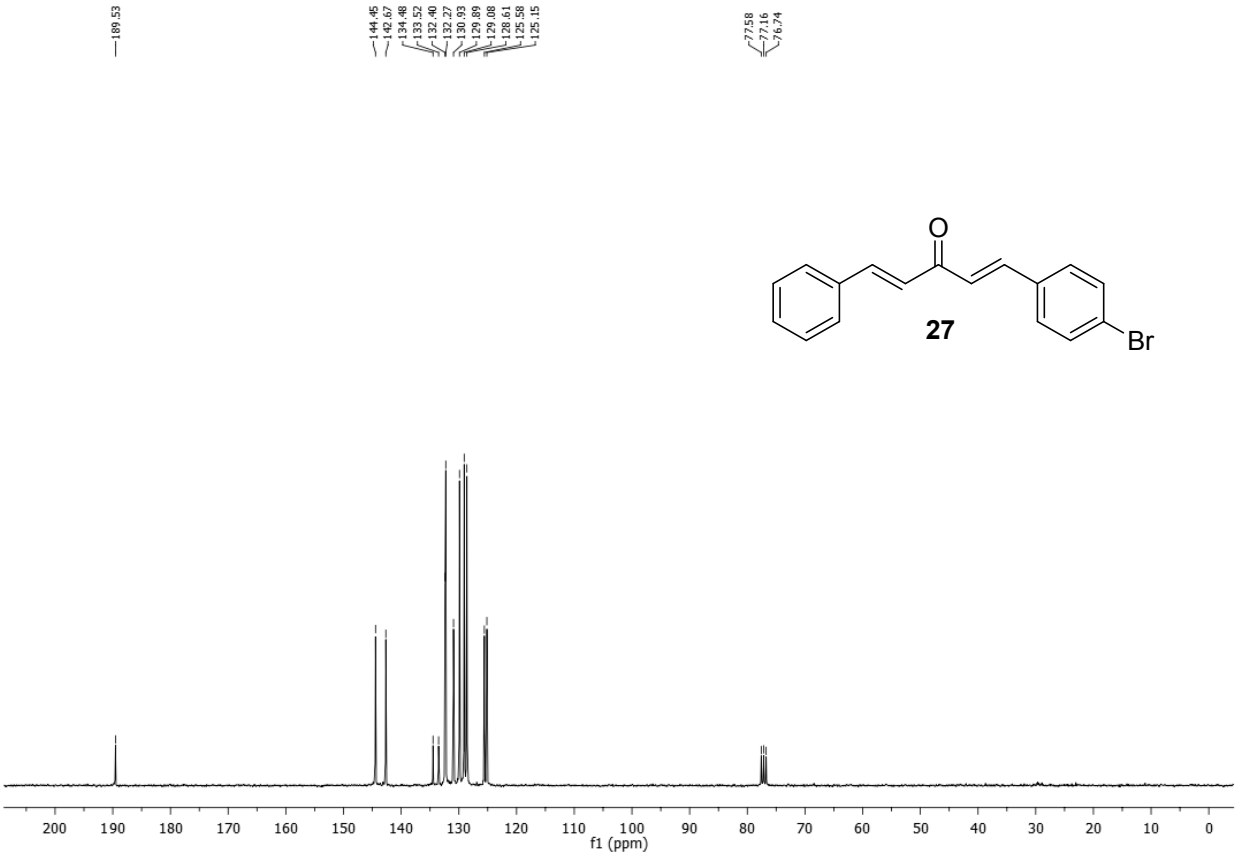
7.59
7.57
7.56
7.53
7.50
7.44
7.41
7.40
7.39
7.31
7.28
7.08
7.03
0.00
O
27
Br
2.00
1.81
1.83
3.21
1.76
1.83
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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132.40
132.27
130.93
129.89
129.08
128.61
125.58
125.15
77.58
77.16
76.74
O
27
Br
200
190
180
170
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130
120
110
100
90
80
70
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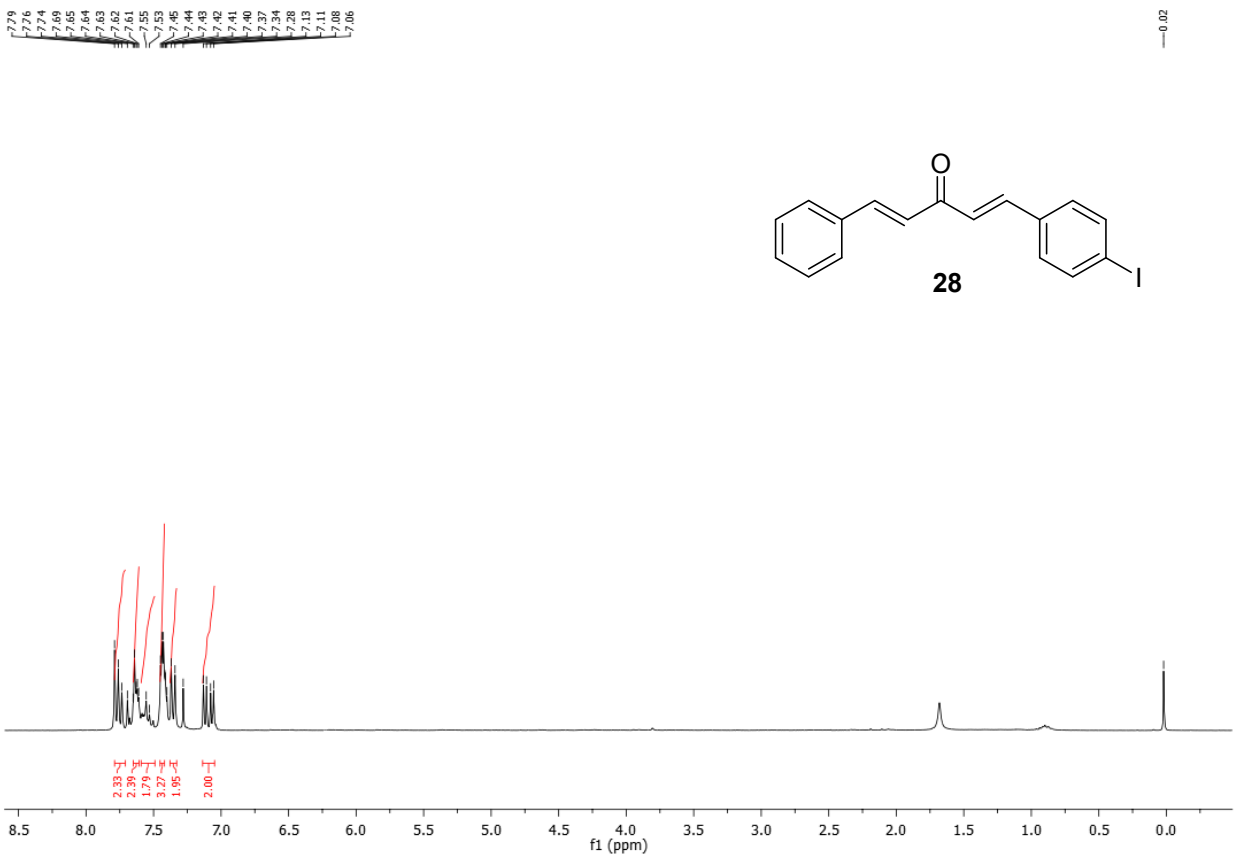
50
40
30
20
10
0
f1 (ppm)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7.62
7.61
7.55
7.53
7.45
7.44
7.43
7.42
7.41
7.40
7.37
7.34
7.28
7.13
7.11
7.08
7.06
0.02
O
I
28
2.33
2.39
1.79
3.27
1.95
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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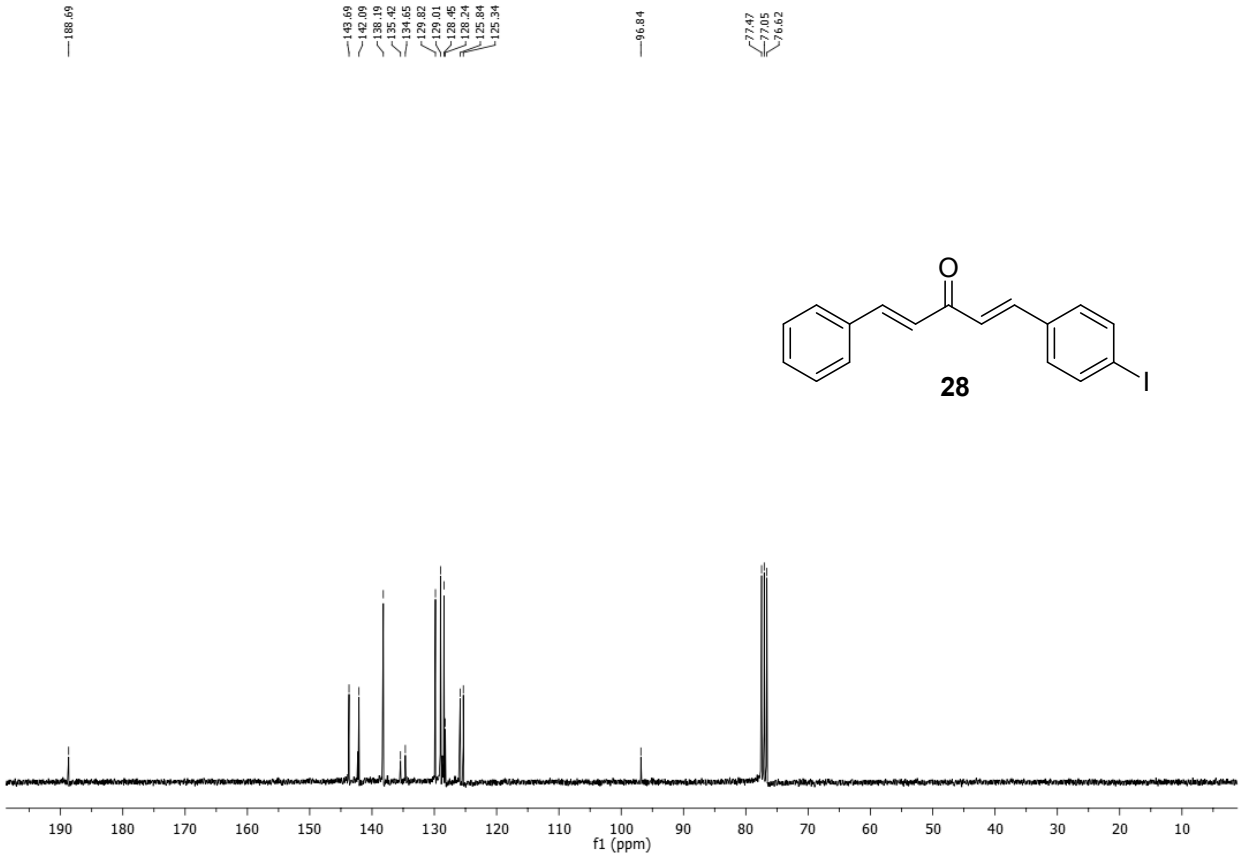
0.0
f1 (ppm)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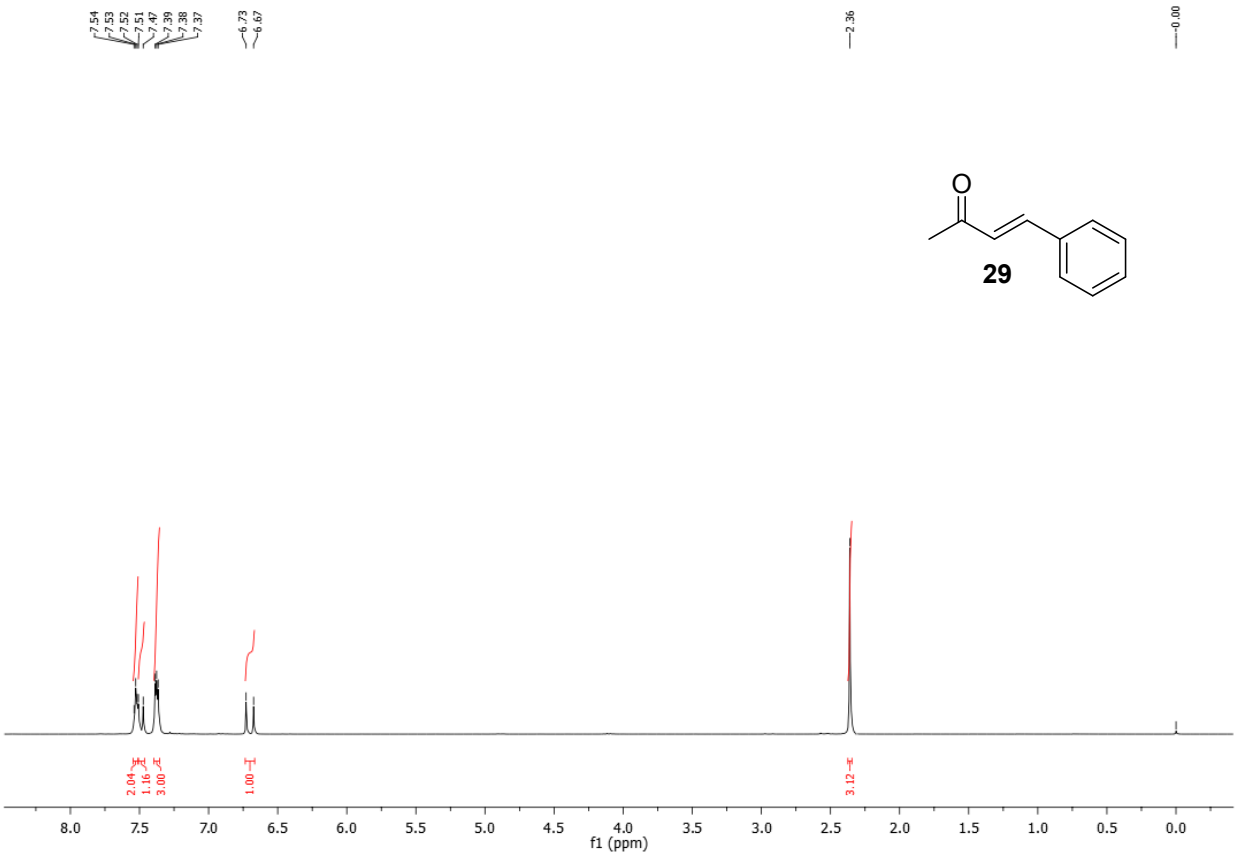
134.65
129.82
129.01
128.45
128.24
125.84
125.34
96.84
77.47
77.05
76.62
O
I
28
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.52
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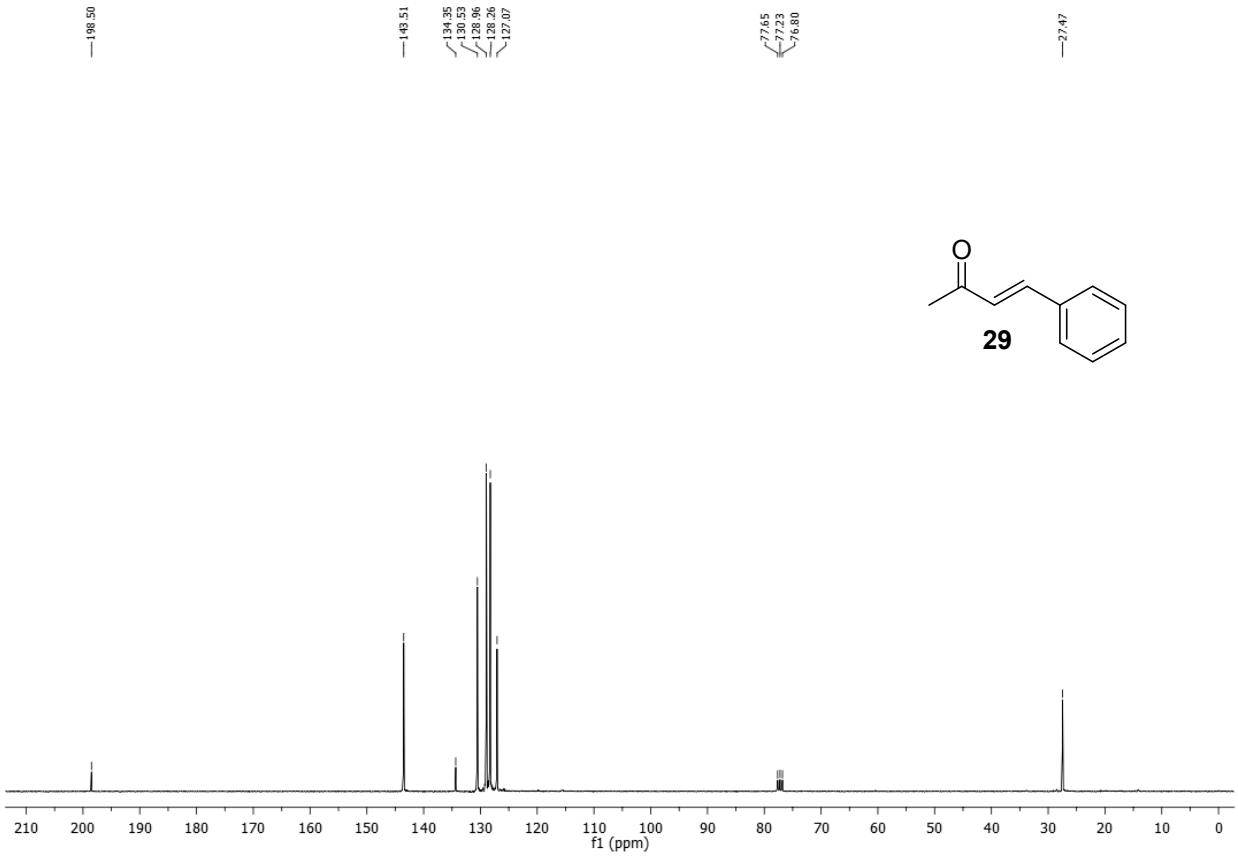
7.47
7.39
7.38
7.37
6.73
6.67
2.36
0.00
2.04
1.16
3.00
1.00
3.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

29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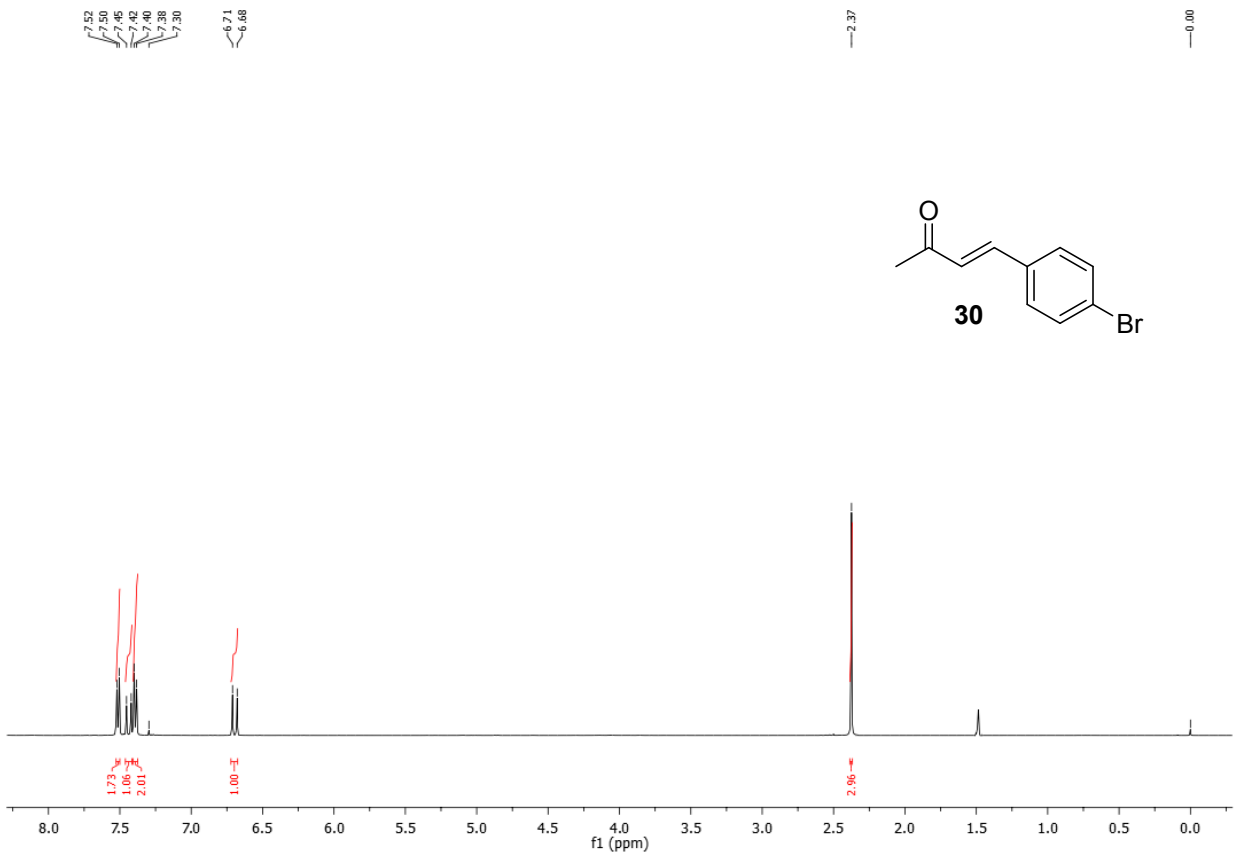
128.26
127.07
77.65
77.23
76.80
27.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

29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7.30
6.71
6.68
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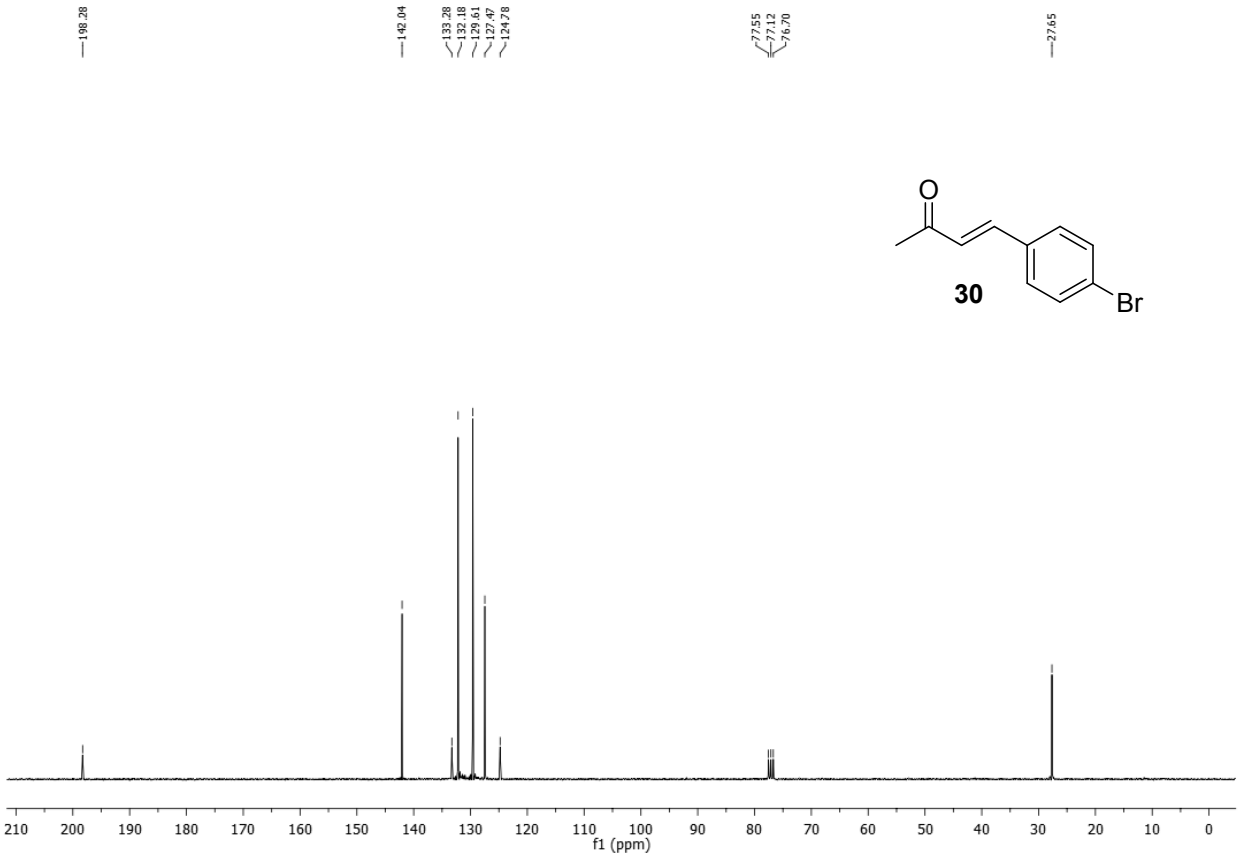
0.00
O
30
Br
1.73
1.06
2.01
1.00
2.96
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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124.78
77.55
77.12
76.70
27.65
O
30
Br
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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50
40
30
20
10
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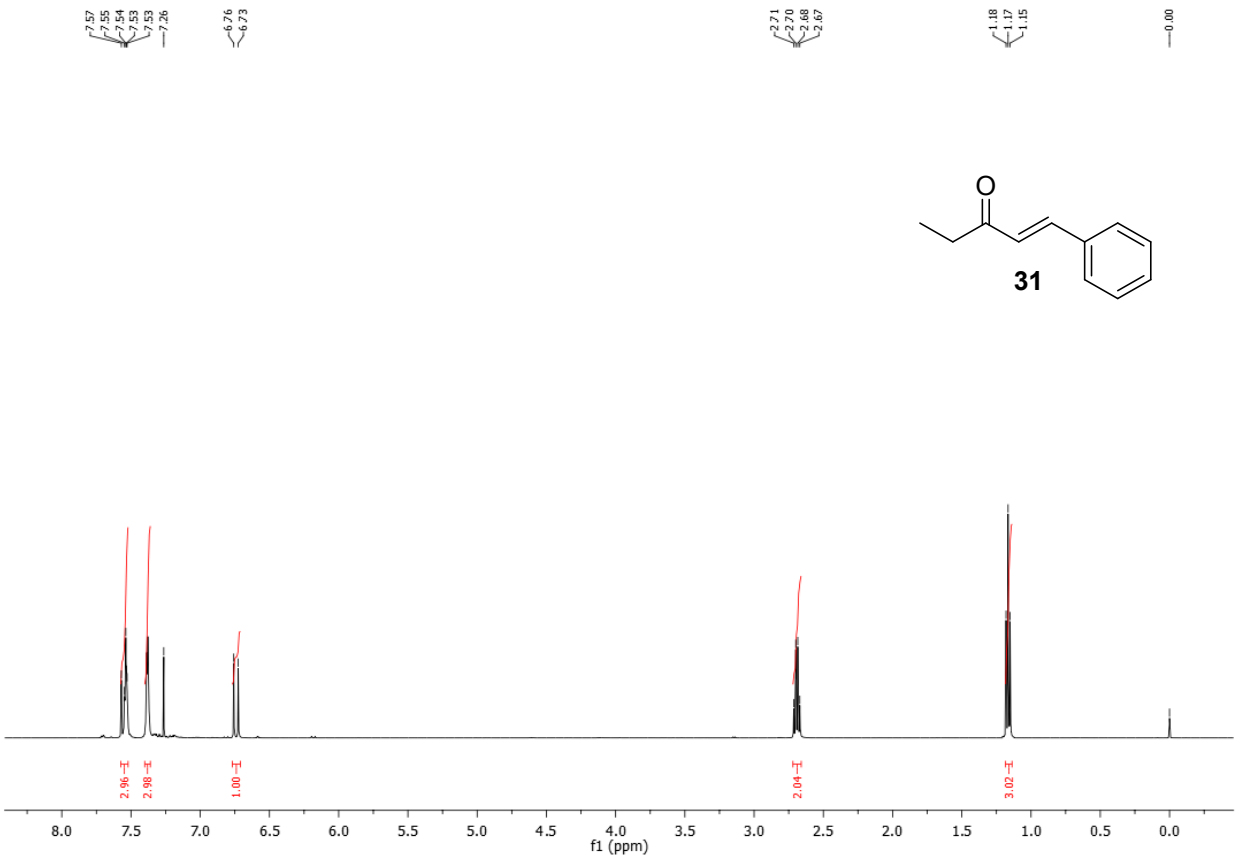
f1 (ppm)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6.73
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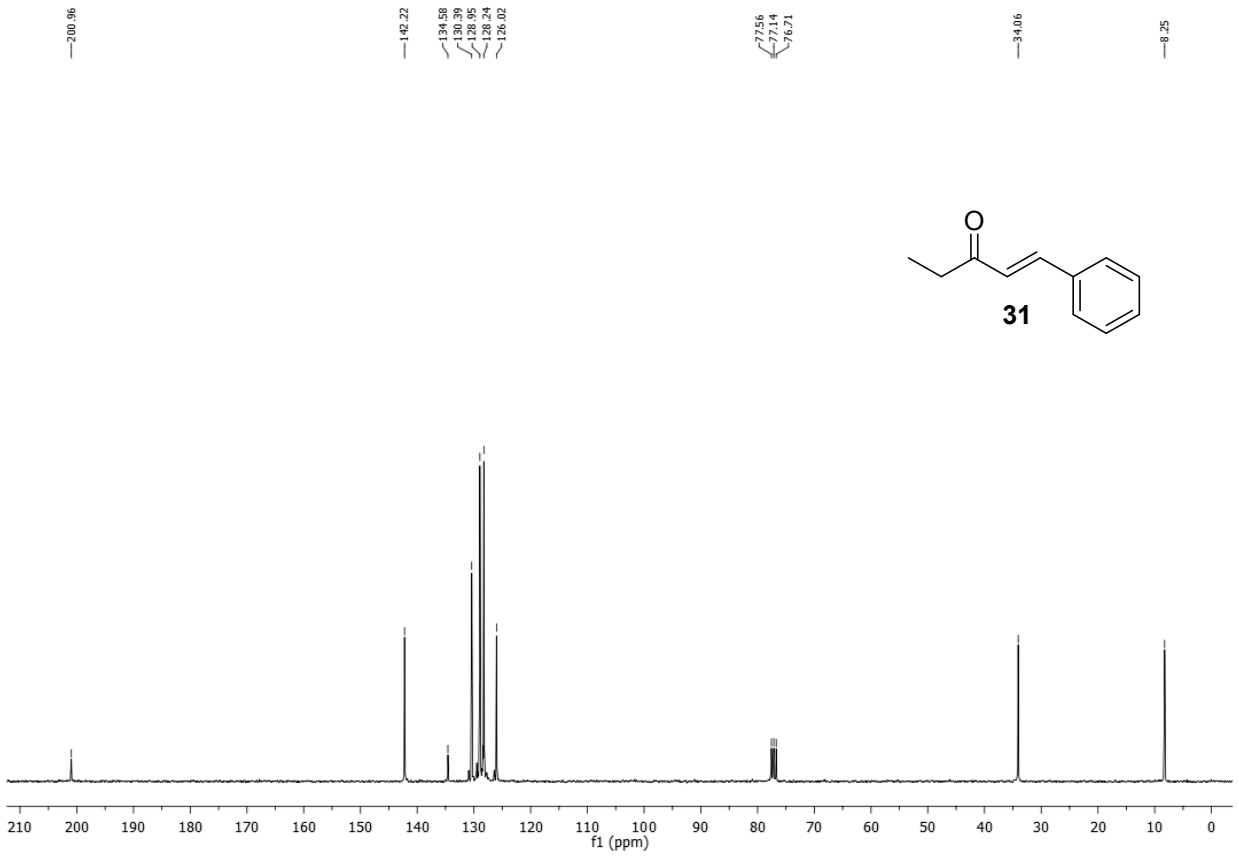
2.70
2.68
2.67
1.18
1.17
1.15
0.00
O
31
2.96
2.98
1.00
2.04
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.24
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77.56
77.14
76.71
34.06
8.25
O
31
210
200
190
180
170
160
150
140
130
120
110
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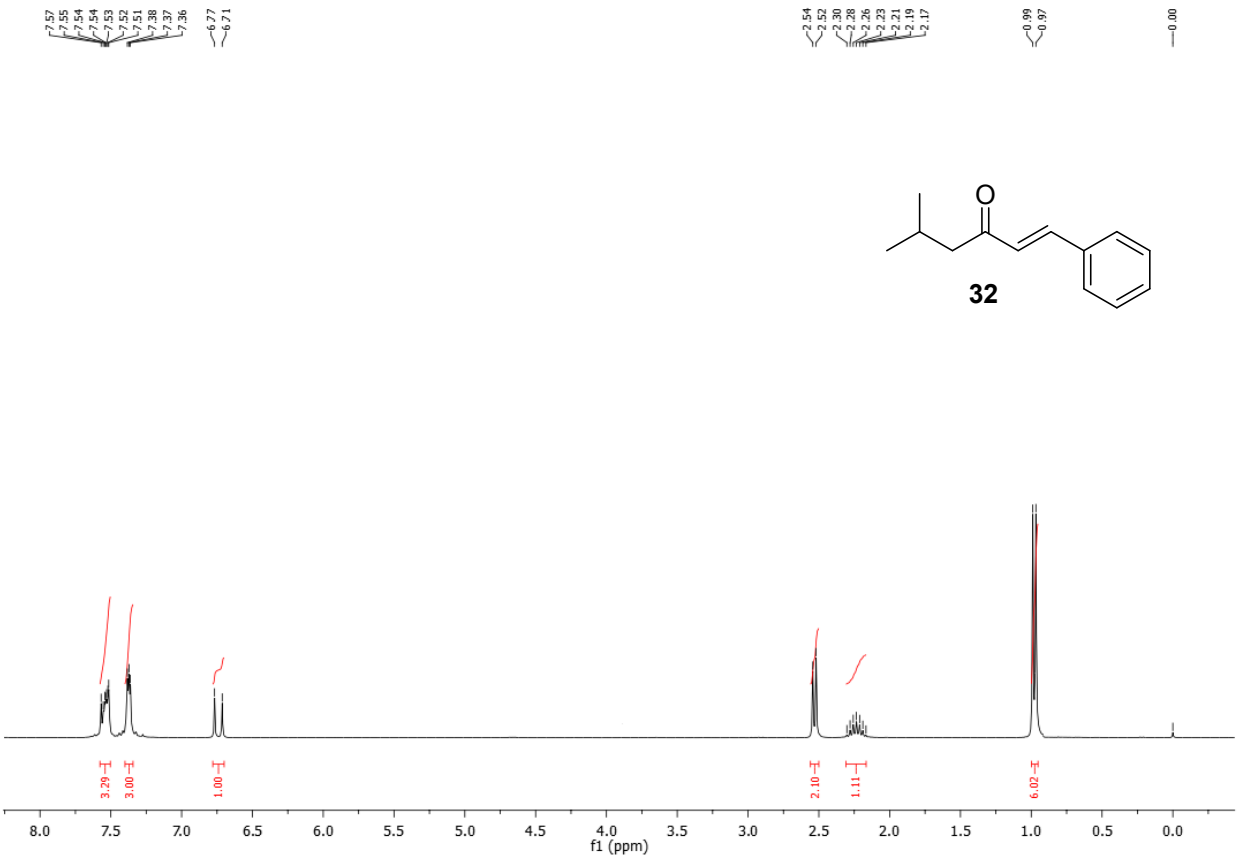
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.51
7.38
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7.36
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6.71
2.54
2.52
2.30
2.28
2.26
2.23
2.21
2.19
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0.00
O
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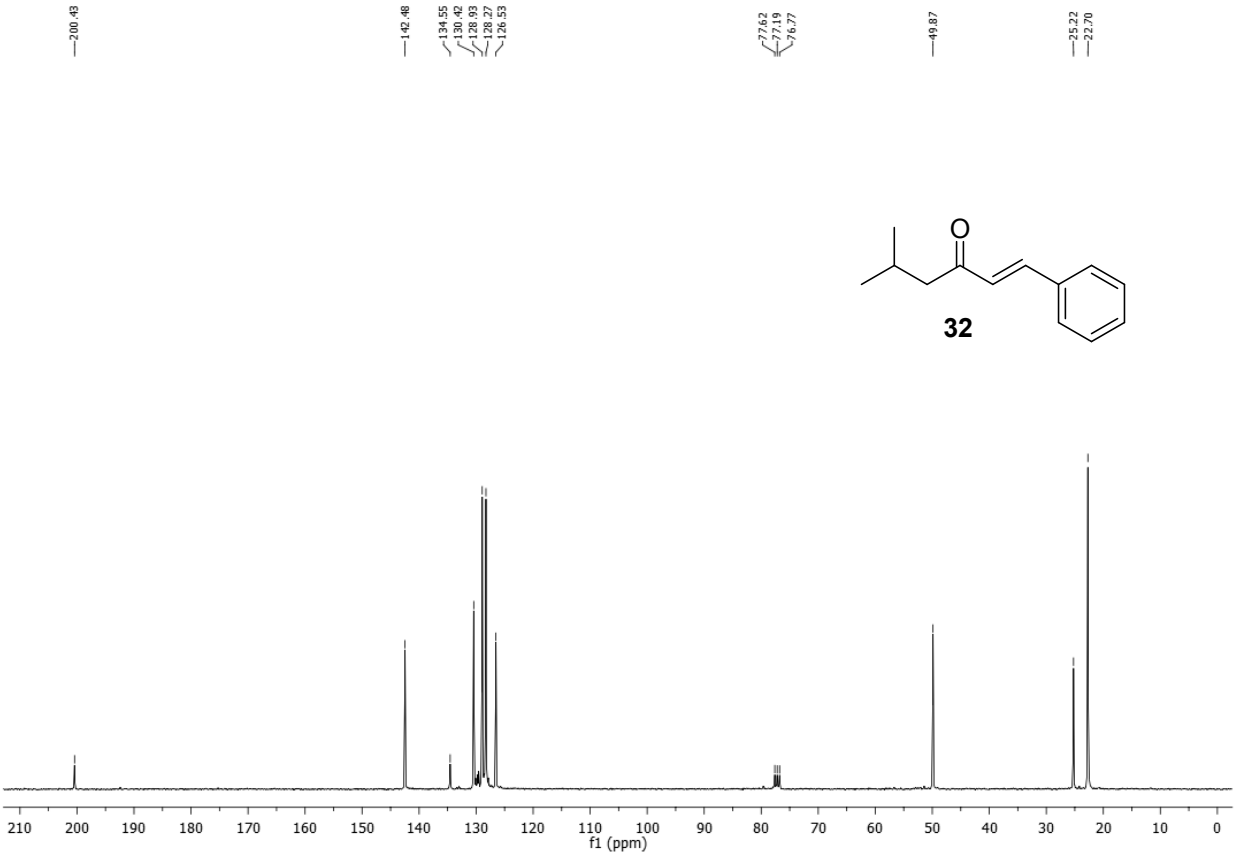
3.29
3.00
1.00
2.10
1.11
6.02
f1 (ppm)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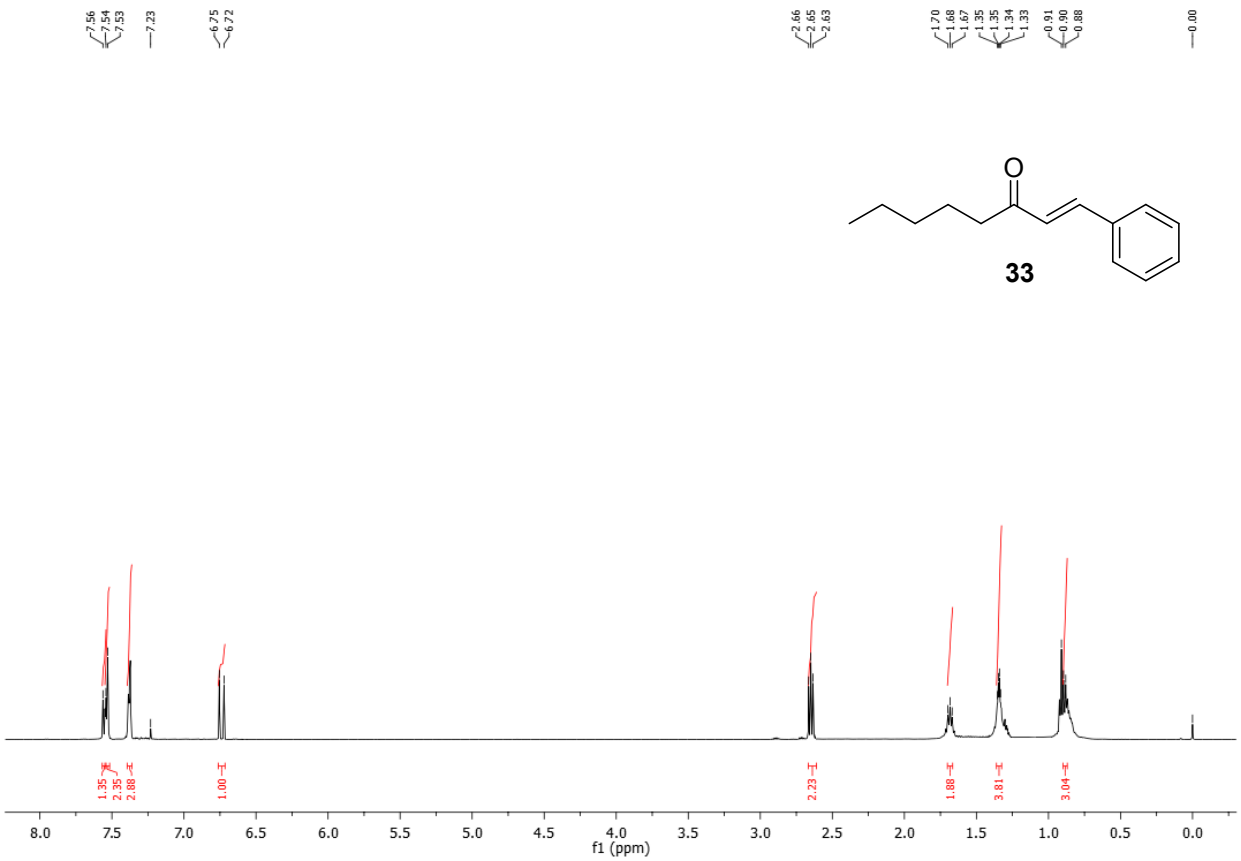
76.77
49.87
25.22
22.70
O
32
f1 (ppm)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6.72
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1.70
1.68
1.67
1.35
1.35
1.34
1.33
0.91
0.90
0.88
0.00
1.35
2.35
2.88
1.00
2.23
1.88
3.81
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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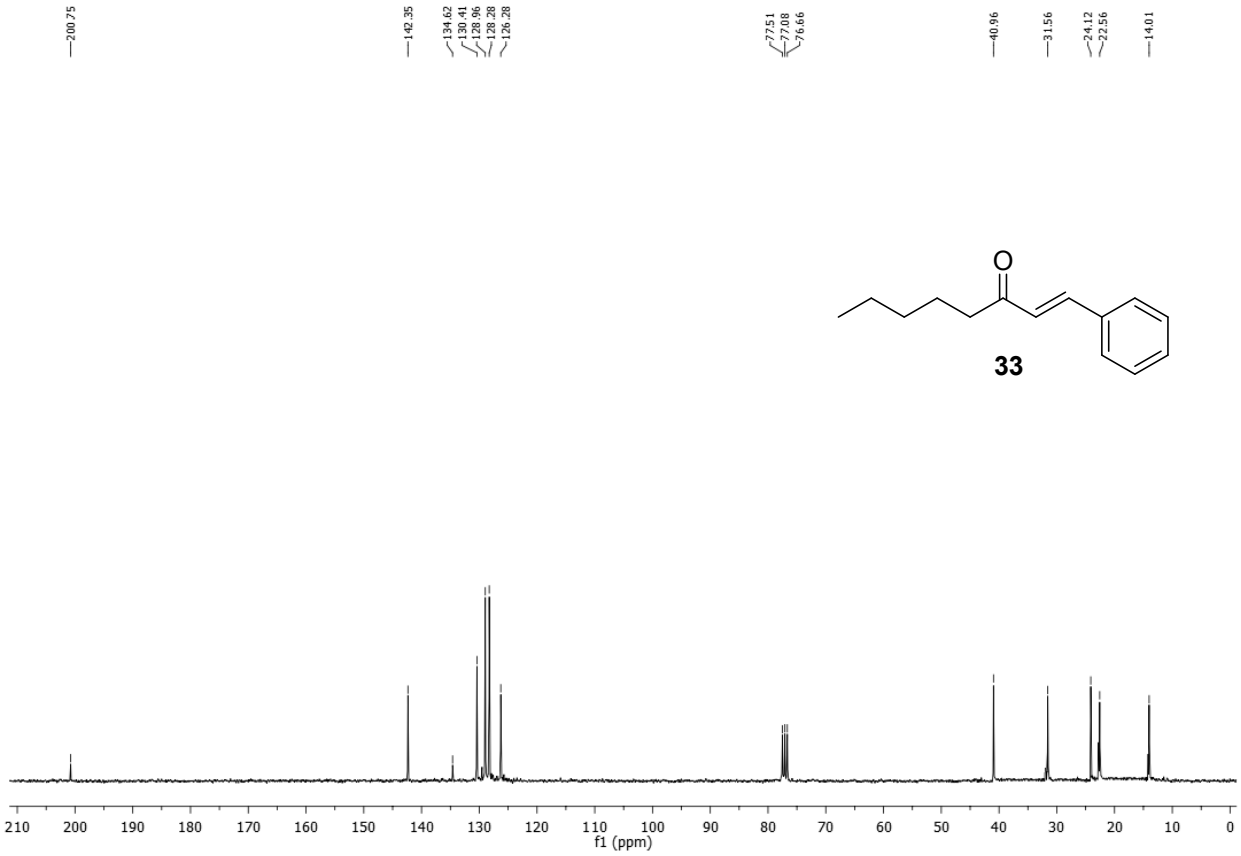
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

O
33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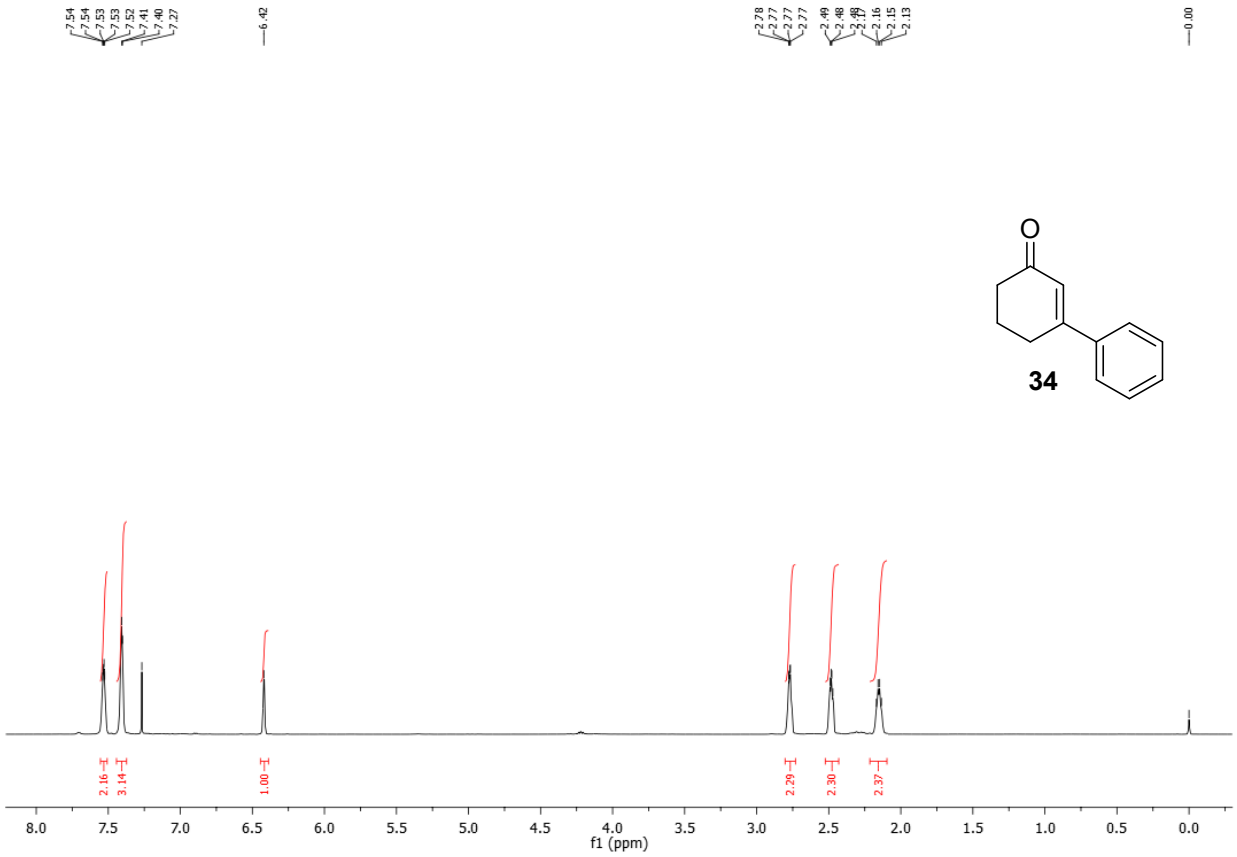
128.28
126.28
77.51
77.08
76.66
40.96
31.56
24.12
22.56
14.01
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

O
33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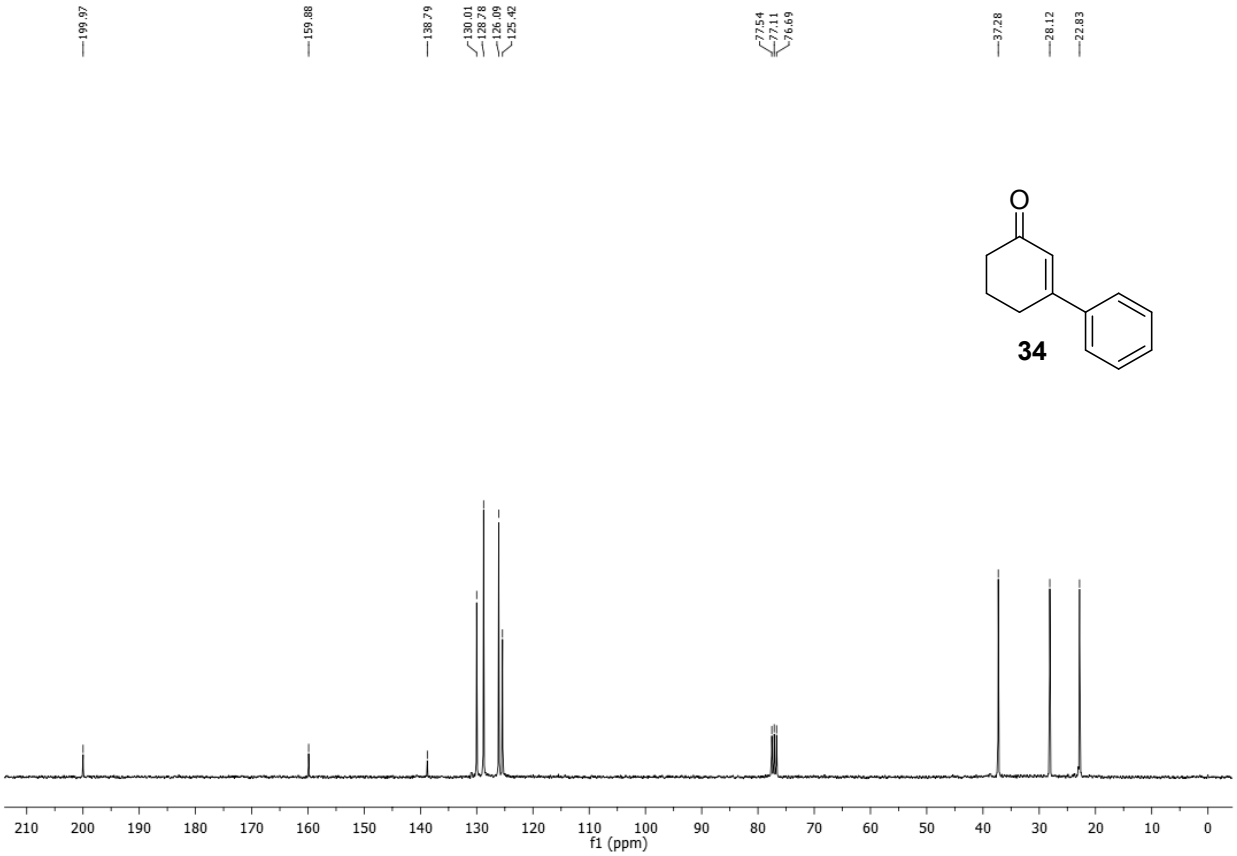
2.77
2.77
2.77
2.49
2.48
2.16
2.15
2.13
0.00
O
34
2.16
3.14
1.00
2.29
2.30
2.37
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


199.97
159.88
138.79
130.01
128.78
126.09
125.42
77.54
77.11
76.69
37.28
28.12
22.83
O
34
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

****