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Supporting Information

Replacing Stoichiometric Silver Oxidant with Air: Ligated Pd(II)-Catalysis to β-Aryl Carbonyl Derivatives with Improved Chemoselectivity

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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 Perkin–Elmer RX-1 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] 4-(1-Hydroxyallyl)benzonitrile,[1c] 1-(Pyridin-3-yl)prop-2-en-1-ol,[1d] 1-(Naphthalen-1-yl)prop-2-en-1-ol,[1a] 4,4-Dimethylpent-1-en-3-ol,[1e] 1-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)prop-2-en-1-ol,[1f] 1-((3a*R*,5*S*,6*S*,6a*R*)-2,2,6-Trimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-5-yl)prop-2-en-1-ol,[1g] (*Z*)-4-(*tert*-butyldimethylsilyloxy)but-2-en-1-ol,[1h] Butyl-2-(hydroxy(phenyl)methyl)acrylate,[1i] Butyl-2-((4-bromophenyl)(hydroxy)methyl)acrylate,[1i] Butyl-2-(hydroxy(4-methoxyphenyl) methyl)acrylate [1i]]. Oct-1-en-3-ol, Prop-2-en-1-ol and Cyclohex-2-enol were purchased from Aldrich.

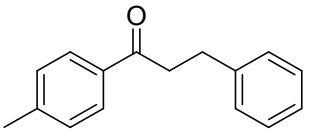
1.2 General Procedure for Synthesis of β-Aryl Carbonyl Compounds from Allyl Alcohols

A mixture of arylboronic acid (1.5 mmol), $Pd(OAc)_2$ (0.022 g, 0.1 mmol), and 2,9-dimethyl-1,10-phenanthroline (0.042 g, 0.20 mmol), CuCl (0.005 g, 0.05 mmol) and allyl

alcohol (1.0 mmol) was dissolved in DMSO (3 mL) in a 10 mL RB flask closed with air balloon (1atm pressure). The mixture was vigorously stirred at 50 °C for 12 h. After cooling to room temperature, the reaction mixture was partitioned between ethyl acetate (25.0 mL) and water (25 mL) and it was transferred to 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.

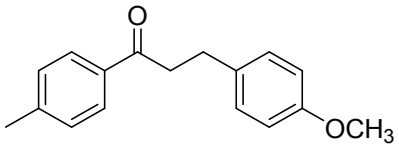
1.3 Analytical data for products

3-Phenyl-1-*p*-tolylpropan-1-one (1)[2a]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.208 g, 93%). M.p. 62-63 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.89 (d, J = 8.1 Hz, 2H), 7.38 – 7.20 (m, 7H), 3.31 (t, J = 7.7 Hz, 2H), 3.09 (t, J = 7.7 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.9, 143.9, 141.4, 134.4, 129.3, 128.6, 128.5, 128.2, 126.1, 40.4, 30.3, 21.7; (IR, Neat): 3060, 1681, 1606, 1451, 1292, 1180, 974, 700 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{16}ONa]^+$ 247.1098; Found 247.1103.

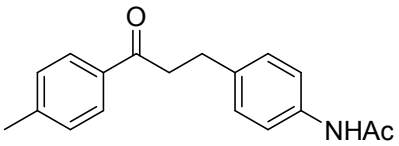
3-(4-Methoxyphenyl)-1-*p*-tolylpropan-1-one (2) [2a]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3-4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.213 g, 84%). M.p. 112-114 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.88 (d, J = 7.9 Hz, 2H), 7.27 (d, J = 7.7 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 6.86 (d, J = 8.3 Hz, 2H), 3.81 (s, 3H), 3.26 (t, J = 7.6 Hz, 2H), 3.02 (t, J = 7.6 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.0, 158.0, 143.8, 134.5, 133.5, 129.4, 129.3, 128.2, 114.0, 55.3, 40.6,

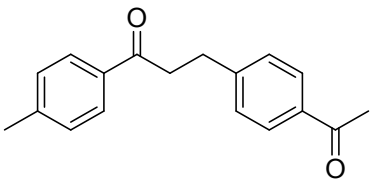
29.4, 21.6; (IR, Neat): 3016, 1678, 1607, 1512, 1216, 746 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{19}O_2]^+$ 255.13796; Found 255.13807.

_N_-(4-(3-Oxo-3-_p_-tolylpropyl)phenyl)acetamide (3)



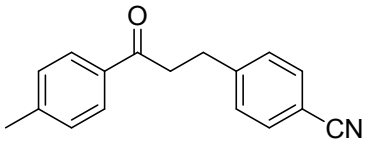
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 10% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.214 g, 76%). M.p. 142-143 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, J = 8.3 Hz, 2H), 7.66 (s, 1H), 7.43 (d, J = 8.5 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 8.3 Hz, 2H), 3.26 (t, J = 7.5 Hz, 2H), 3.02 (t, J = 7.5 Hz, 2H), 2.41 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.1, 168.6, 143.9, 137.4, 136.1, 134.4, 129.3, 128.9, 128.2, 120.3, 40.3, 29.6, 24.4, 21.6; (IR, Neat): 3017, 1674, 1369, 1215, 743 cm^{-1}; HRMS (ESI): Calculated for $[C_{18}H_{19}O_2NNa]^+$ 304.13080; Found 304.13092.

3-(4-Acetylphenyl)-1-_p_-tolylpropan-1-one (4)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 7-8 % ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.205 g, 77%). M.p. 138-140 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.88 (dd, J = 11.0, 8.2 Hz, 4H), 7.35 (d, J = 7.9 Hz, 2H), 7.26 (d, J = 8.0 Hz, 2H), 3.31 (t, J = 7.5 Hz, 2H), 3.13 (t, J = 7.3 Hz, 2H), 2.58 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.3, 197.8, 147.3, 144.1, 135.2, 134.2, 129.3, 128.7, 128.7, 128.1, 39.6, 30.1, 26.6, 21.7; (IR, Neat): 3019, 1679, 1607, 1412, 1215, 743, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{18}H_{19}O_2]^+$ 267.13796; Found 267.13821.

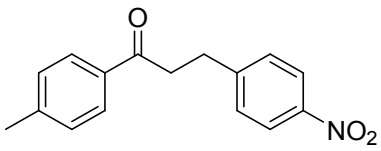
4-(3-Oxo-3-_p_-tolylpropyl)benzonitrile (5)[2b]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl

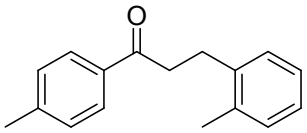
acetate in hexane as eluent) to afford the title product as a colourless solid (0.219 g, 88%). M.p. 130-132 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, J = 8.2 Hz, 2H), 7.59 (d, J = 8.3 Hz, 2H), 7.38 (d, J = 8.2 Hz, 2H), 7.27 (d, J = 7.4 Hz, 2H), 3.34 – 3.29 (m, 2H), 3.14 (t, J = 7.3 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.9, 147.1, 144.2, 134.1, 132.3, 129.4, 129.4, 128.1, 119.0, 110.0, 39.3, 30.1, 21.7; (IR, Neat): 3020, 2223, 1678, 1481, 1214, 742 cm^{-1}; HRMS (ESI): Calculated for $[C_{17}H_{15}NONa]^{+}$ 272.10512; Found 272.10514.

3-(4-Nitrophenyl)-1-*p*-tolylpropan-1-one (6)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4 % ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.234 g, 87%). M.p. 110-112 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.36 (d, J = 8.9 Hz, 2H), 8.14 (d, J = 8.7 Hz, 2H), 7.42 (d, J = 8.7 Hz, 2H), 7.26 (d, J = 6.8 Hz, 2H), 3.33 (t, J = 7.2 Hz, 2H), 3.18 (t, J = 7.1 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 149.3, 144.2, 134.1, 129.4, 128.3, 128.1, 124.4, 123.7, 39.3, 29.8, 21.6; (IR, Neat): 3020, 1679, 1519, 1215, 742 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{16}NO_3]^{+}$ 270.11247; Found 270.11251.

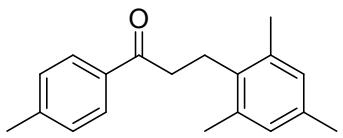
3-*o*-Tolyl-1-*p*-tolylpropan-1-one (7)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.193 g, 81%). M.p. 86-88 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, J = 8.2 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 7.15 (ddd, J = 13.1, 6.3, 3.0 Hz, 4H), 3.20 (t, J = 8.6 Hz, 2H), 3.02 (t, J = 8.4 Hz, 2H), 2.38 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.0, 143.9, 139.5, 136.0, 134.5, 130.4, 129.3, 128.8, 128.2, 126.3, 126.2, 39.0, 27.7, 21.7, 19.4; (IR, Neat): 3018, 1679, 1607, 1570, 1216, 1180, 974, 743 cm^{-1}; HRMS (ESI):

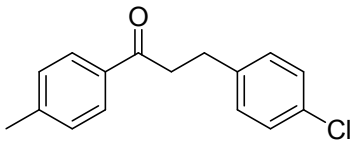
Calculated for $[C_{17}H_{19}O]^+$ 239.14304; Found 239.14325.

3-Mesityl-1-*p*-tolylpropan-1-one (8)



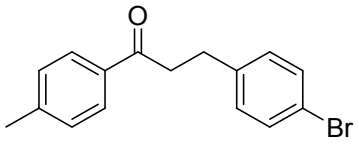
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.210 g, 79%). M.p. 112-114 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.0 Hz, 2H), 6.93 (s, 2H), 3.22 – 3.02 (m, 4H), 2.46 (s, 3H), 2.37 (s, 6H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.9, 148.5, 140.7, 140.1, 139.5, 139.0, 133.9, 133.7, 132.7, 42.4, 28.4, 26.2, 25.4, 24.4; (IR, Neat): 3011, 1677, 1447, 1180, 748, cm^{-1}; HRMS (ESI): Calculated for $[C_{19}H_{23}O]^+$ 267.17434; Found 267.17463.

3-(4-Chlorophenyl)-1-*p*-tolylpropan-1-one (9) [2a]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.230 g, 89%). M.p. 101-102 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.87 (d, J = 8.1 Hz, 2H), 7.32 – 7.17 (m, 6H), 3.27 (t, J = 7.4 Hz, 2H), 3.05 (t, J = 7.5 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.5, 144.0, 139.9, 134.3, 131.8, 129.8, 129.3, 128.6, 128.1, 40.1, 29.5, 21.7; (IR, Neat): 3025, 1668, 1603, 1219, 808, 771 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{16}OCl]^+$ 259.08842; Found 259.08863.

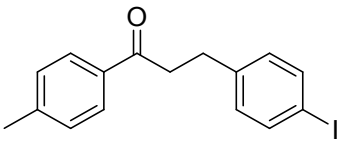
3-(4-Bromophenyl)-1-*p*-tolylpropan-1-one (10)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.284 g, 94%). M.p. 104-106 ^oC; ^1H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 8.3 Hz, 2H), 7.24 (d, J = 7.8 Hz, 2H), 7.12 (d, J = 8.3 Hz, 2H), 3.24

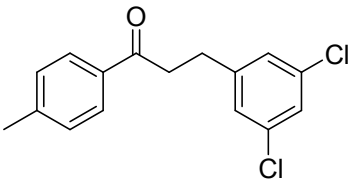
(t, J = 7.5 Hz, 2H), 3.01 (t, J = 7.5 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.4, 144.0, 140.4, 134.3, 131.5, 130.2, 129.3, 128.1, 119.9, 39.9, 29.6, 21.6; (IR, Neat): 3020, 1678, 1214, 747, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{16}OBr]^+$ 303.03790; Found 303.03843.

3-(4-Iodophenyl)-1-*p*-tolylpropan-1-one (11)



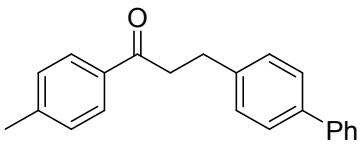
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.312 g, 89%). M.p. 105-106 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, J = 7.9 Hz, 2H), 7.59 (d, J = 7.1 Hz, 2H), 7.24 (d, J = 7.8 Hz, 2H), 7.00 (d, J = 7.9 Hz, 2H), 3.23 (t, J = 7.2 Hz, 2H), 3.00 (t, J = 7.2 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.4, 144.0, 141.1, 137.5, 134.3, 130.6, 129.3, 128.2, 91.2, 39.9, 29.6, 21.7; (IR, Neat): 3018, 1679, 1607, 1447, 1215, 745, 666 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{16}OI]^+$ 351.02403; Found 351.02450.

3-(3,5-Dichlorophenyl)-1-*p*-tolylpropan-1-one (12)



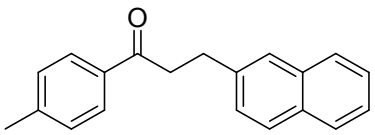
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.228 g, 78%). M.p. 118-119 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 7.18 (d, J = 1.6 Hz, 1H), 7.14 (d, J = 1.6 Hz, 2H), 3.28 – 3.23 (m, 2H), 3.01 (t, J = 7.4 Hz, 2H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 144.9, 144.1, 134.8, 134.1, 129.4, 128.1, 127.1, 126.3, 39.4, 29.4, 21.7; (IR, Neat): 3019, 1680, 1566, 1214, 745, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{16}H_{15}OCl_2]^+$ 293.04945; Found 293.04980.

3-(Biphenyl-4-yl)-1-*p*-tolylpropan-1-one (13)



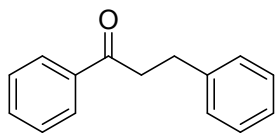
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.246 g, 82%). M.p. 109-110 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, J = 8.1 Hz, 2H), 7.53 (dd, J = 14.4, 8.0 Hz, 4H), 7.40 (t, J = 7.5 Hz, 2H), 7.34 – 7.27 (m, 3H), 7.22 (d, J = 8.1 Hz, 2H), 3.28 (t, J = 7.5 Hz, 2H), 3.08 (t, J = 7.6 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.9, 143.9, 141.0, 140.6, 139.1, 134.4, 129.4, 128.9, 128.8, 128.2, 127.3, 127.2, 127.1, 40.3, 29.9, 21.7; (IR, Neat): 3017, 1601, 1420, 1214, 981, 743 cm^{-1}; HRMS (ESI): Calculated for $[C_{22}H_{21}O]^+$ 301.15869; Found 301.15892.

3-(Naphthalen-2-yl)-1-*p*-tolylpropan-1-one (14)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.225 g, 82%). M.p. 89-90 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (d, J = 8.1 Hz, 2H), 7.77 (t, J = 7.2 Hz, 3H), 7.66 (s, 1H), 7.46 – 7.33 (m, 3H), 7.21 (d, J = 8.0 Hz, 2H), 3.32 (t, J = 8.4 Hz, 2H), 3.20 (t, J = 7.9 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.9, 143.9, 139.0, 134.5, 133.7, 132.2, 129.3, 128.2, 128.1, 127.7, 127.5, 127.2, 126.5, 126.0, 125.3, 40.3, 30.4, 21.7; (IR, Neat): 3018, 1679, 1409, 1215, 742 cm^{-1}; HRMS (ESI): Calculated for $[C_{20}H_{19}O]^+$ 275.14304; Found 275.14341.

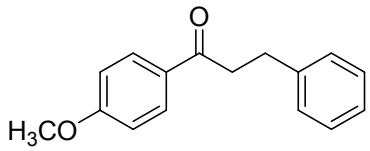
1,3-Diphenylpropan-1-one (15) [2c,4]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.185 g, 88%). M.p. 62-63 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.92 (m, 2H), 7.61 – 7.53 (m, 1H), 7.51 – 7.43 (m, 2H),

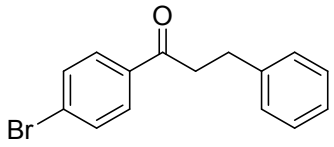
7.35 – 7.22 (m, 5H), 3.32 (t, *J* = 7.5 Hz, 2H), 3.09 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.2, 141.3, 136.8, 133.0, 128.6, 128.5, 128.4, 128.0, 126.1, 40.4, 30.1; (IR, KBr): 3059, 1679, 1593, 1446, 1207, 975, 746, 693 cm^{-1}; HRMS (ESI): Calculated for $[C_{15}H_{14}ONa]^+$ 233.0942; Found 233.0939.

1-(4-Methoxyphenyl)-3-phenylpropan-1-one (16) [2c,3]



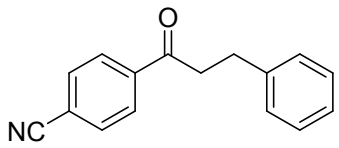
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.226 g, 94%). M.p. 98-99 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.7 Hz, 2H), 7.35 – 7.14 (m, 5H), 6.93 (d, *J* = 8.7 Hz, 2H), 3.86 (s, 3H), 3.25 (t, *J* = 7.9 Hz, 2H), 3.05 (t, *J* = 7.9 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 163.4, 141.5, 130.3, 130.0, 128.5, 128.4, 126.1, 113.7, 55.4, 40.1, 30.3; (IR, KBr): 3003, 1668, 1602, 1450, 1256, 1174, 1026, 841, 660 cm^{-1}; HRMS (ESI) Calculated for $[C_{16}H_{16}O_2Na]^+$ 263.1035; Found 263.1038.

1-(4-Bromophenyl)-3-phenylpropan-1-one (17)



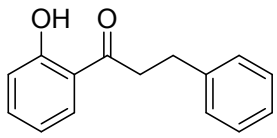
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.268 g, 93%). M.p. 97-98 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 – 7.79 (m, 2H), 7.63 – 7.56 (m, 2H), 7.36 – 7.18 (m, 5H), 3.28 (t, *J* = 7.7 Hz, 2H), 3.07 (t, *J* = 7.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 198.1, 141.0, 135.5, 131.9, 129.5, 128.5, 128.4, 128.2, 126.2, 40.4, 30.0; (IR, KBr): 3054, 1656, 1595, 1483, 1210, 991, 760 cm^{-1}; HRMS (ESI): Calculated for $[C_{15}H_{13}BrONa]^+$ 311.0047; Found 311.0041.

4-(3-Phenylpropanoyl)benzonitrile (18)



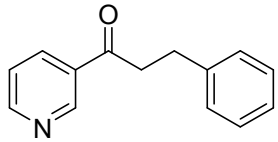
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.212 g, 90%). M.p. 57-58 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 – 8.02 (m, 2H), 7.80 – 7.74 (m, 2H), 7.32 – 7.19 (m, 5H), 3.30 (dd, J = 8.0, 6.7 Hz, 2H), 3.08 (t, J = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 146.6, 132.5, 131.2, 129.1, 128.6, 128.4, 126.4, 121.2, 117.9, 40.7, 29.8; (IR, KBr): 3035, 2224, 1682, 1597, 1402, 1205, 985, 774 cm^{-1}; HRMS (ESI) Calculate for $[C_{16}H_{13}NONa]^+$ 258.0895; Found 258.0923.

1-(2-Hydroxyphenyl)-3-phenylpropan-1-one (19) [5a]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 10% ethyl acetate in hexane as eluent) to afford the title product as a pale yellowish coloured oil (0.201 g, 89%); ^{1}H NMR (300 MHz,) δ 12.30 (s, 1H), 7.70 (d, J = 7.9 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.25 (dt, J = 11.8, 6.4 Hz, 5H), 6.96 (d, J = 8.3 Hz, 1H), 6.84 (t, J = 7.6 Hz, 1H), 3.29 (t, J = 7.6 Hz, 2H), 3.04 (t, J = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 205.3, 162.4, 140.6, 136.2, 129.7, 128.5, 128.3, 126.2, 119.2, 118.8, 118.5, 39.9, 29.9; (IR, Neat): 3358, 2995, 1658, 1450, 1219, 772 cm^{-1}; HRMS (ESI) Calculate for $[C_{15}H_{14}O_2Na]^+$ 249.08860; Found 249.08883.

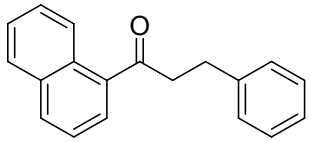
3-Phenyl-1-(pyridin-3-yl)-propan-1-one (20)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 35% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.165 g, 78%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.16 (d, J = 1.7 Hz, 1H), 8.77 (dd, J = 4.7, 1.4 Hz, 1H), 8.22 (dt, J = 7.9, 1.9 Hz, 1H), 7.41 (dd, J = 7.9, 4.8 Hz, 1H), 7.36 – 7.16 (m, 5H), 3.32 (t, J = 7.6 Hz, 2H), 3.09

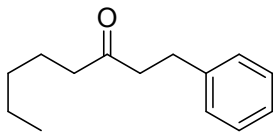
(t, J = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.8, 153.4, 149.6, 140.7, 135.3, 132.1, 128.6, 128.4, 126.3, 123.6, 40.7, 29.8; (IR, Neat): 3028, 1690, 1585, 1495, 1294, 1024, 772 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{14}NO]^+$ 212.1075; Found 212.1071.

1-(Naphthalen-2-yl)-3-phenylpropan-1-one (21)



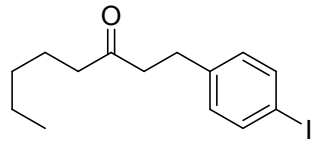
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.208 g, 80%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, J = 8.3 Hz, 1H), 7.98 (d, J = 8.2 Hz, 1H), 7.90 – 7.80 (m, 2H), 7.62 – 7.44 (m, 3H), 7.34 – 7.21 (m, 5H), 3.39 (t, J = 7.7 Hz, 2H), 3.15 (t, J = 7.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.5, 141.1, 135.9, 133.9, 132.5, 128.5, 128.4, 128.4, 127.8, 127.4, 126.4, 126.1, 125.7, 124.3, 43.8, 30.6; (IR, Neat): 3056, 1681, 1597, 1400, 1231, 1098, 776 cm^{-1}; HRMS (ESI): Calculated for $[C_{19}H_{16}ONa]^+$ 283.1098; Found 283.1100.

1-Phenyloctan-3-one (22) [2c]



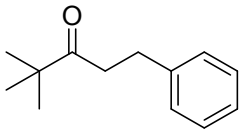
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.200 g, 98%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (t, J = 7.6 Hz, 2H), 7.18 – 7.13 (m, 3H), 2.87 (t, J = 7.6 Hz, 2H), 2.69 (t, J = 7.6 Hz, 2H), 2.34 (t, J = 7.4 Hz, 2H), 1.55 (dt, J = 14.9, 7.4 Hz, 2H), 1.34 – 1.20 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.3, 141.1, 128.4, 128.3, 126.0, 44.2, 43.0, 31.3, 29.7, 23.4, 22.4, 13.9; (IR, Neat): 2955, 1713, 1602, 1456, 1127, 1029, 699 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{20}ONa]^+$ 227.1411; Found 227.1416.

1-(4-Iodophenyl)-octan-3-one (23)



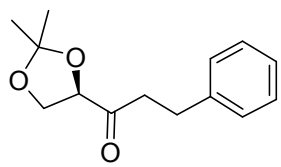
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.314 g, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, J = 8.3 Hz, 2H), 6.93 (d, J = 8.3 Hz, 2H), 2.83 (t, J = 7.5 Hz, 2H), 2.69 (t, J = 7.5 Hz, 2H), 2.36 (t, J = 7.5 Hz, 2H), 1.57 – 1.53 (m, 2H), 1.28 – 1.22 (m, 4H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 205.2, 136.2, 132.8, 125.8, 86.4, 39.1, 38.3, 26.7, 24.5, 18.8, 17.7, 9.2; (IR, Neat): 2925, 1712, 1461, 1218, 771 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{19}OINa]^+$ 353.03728; Found 353.03858.

4,4-Dimethyl-1-phenylpentan-3-one (24) [2c]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.182 g, 96%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24 (dd, J = 8.8, 5.7 Hz, 2H), 7.18 – 7.12 (m, 3H), 2.90 – 2.83 (m, 2H), 2.80 – 2.73 (m, 2H), 1.11 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 214.8, 141.5, 128.4, 127.8, 126.0, 44.0, 38.4, 30.1, 26.3; (IR, Neat): 2966, 1704, 1606, 1454, 1218, 1076, 761, 699 cm^{-1}; HRMS (ESI): Calculated for $[C_{13}H_{18}ONa]^+$ 213.1255; Found 213.1248.

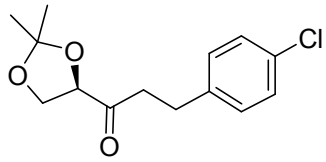
(*R*)-1-(2,2-Dimethyl-1,3-dioxolan-4-yl)-3-phenylpropan-1-one (25)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 10% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.215 g, 92%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 – 7.11 (m, 5H), 4.39 (dd, J = 7.2, 6.0 Hz, 1H), 4.14 (t, J = 8.2 Hz, 1H), 3.90 (dd, J = 8.4, 5.7 Hz, 1H), 3.01 – 2.76 (m, 4H), 1.43 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.9, 140.9, 128.5, 128.3, 126.1, 110.9,

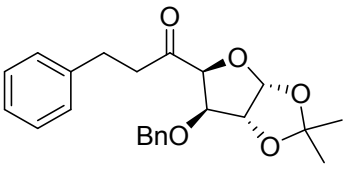
80.3, 66.4, 40.2, 29.0, 26.0, 25.0; (IR, Neat): 3028, 1718, 1495, 1217, 1081, 752, 700 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{18}O_3Na]^+$ 257.1153; Found 257.1143.

(*R*)-3-(4-Chlorophenyl)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-1-one (26)



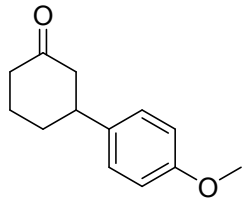
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 10% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.249 g, 93%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.25 (d, J = 8.3 Hz, 2H), 7.14 (d, J = 9.1 Hz, 2H), 4.43 (dd, J = 7.8, 5.5 Hz, 1H), 4.19 (dd, J = 8.6, 7.9 Hz, 1H), 3.94 (dd, J = 8.7, 5.5 Hz, 1H), 2.98 – 2.84 (m, 4H), 1.47 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 209.8, 139.4, 131.9, 129.7, 128.6, 111.0, 80.2, 66.4, 40.0, 28.2, 26.0, 24.9; (IR, Neat): 2988, 1716, 1491, 1374, 1217, 1063, 772 cm^{-1}; HRMS (ESI): Calculated for $[C_{14}H_{18}O_3Cl]^+$ 269.0944; Found 269.0947.

1-((3a*R*,5*S*,6*R*,6a*R*)-6-(Benzyloxy)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-5-yl)-3-phenylpropan-1-one (27)



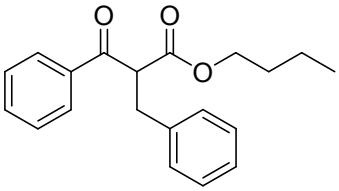
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 15% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.336 g, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, J = 7.8 Hz, 3H), 7.23 – 7.14 (m, 5H), 7.13 – 7.07 (m, 2H), 4.63 (d, J = 3.6 Hz, 1H), 4.56 (d, J = 3.5 Hz, 1H), 4.52 (dd, J = 7.7, 3.9 Hz, 2H), 4.39 (d, J = 11.6 Hz, 1H), 4.24 (d, J = 3.6 Hz, 1H), 2.93 – 2.79 (m, 4H), 1.43 (s, 3H), 1.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 207.7, 141.1, 136.9, 128.5, 128.3, 128.1, 127.7, 126.2, 125.9, 112.3, 105.9, 85.4, 83.7, 81.8, 72.5, 46.7, 44.6, 42.2, 29.7, 28.6, 26.9, 26.3; (IR, Neat): 2928, 1717, 1655, 1454, 1219, 1076, 856 cm^{-1}; HRMS (ESI): Calculated for $[C_{23}H_{26}O_5Na]^+$ 405.1677; Found 405.1692.

3-(4-Methoxyphenyl)-cyclohexanone (28) [5b]



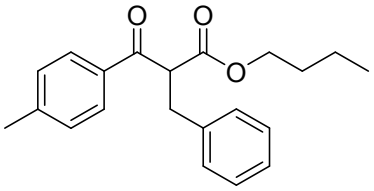
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.177 g, 87%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.10 (d, J = 8.6 Hz, 2H), 6.82 (d, J = 8.7 Hz, 2H), 3.79 (s, 3H), 3.01 – 2.90 (m, 1H), 2.60 – 2.30 (m, 4H), 2.18 – 2.02 (m, 2H), 1.80 (ddd, J = 12.7, 6.5, 2.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.5, 158.3, 136.5, 127.4, 114.0, 96.2, 55.1, 49.2, 44.0, 41.2, 33.1, 29.8, 25.5; (IR, Neat): 2926, 1709, 1608, 1512, 1456, 1251, 1033, 828 cm^{-1}; HRMS (ESI): Calculated for $[C_{13}H_{16}O_2Na]^+$ 227.1047; Found 227.1049.

Butyl 2-benzyl-3-oxo-3-phenylpropanoate (29)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.285 g, 92%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (d, J = 7.3 Hz, 2H), 7.61 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.35 – 7.24 (m, 5H), 4.68 (t, J = 7.3 Hz, 1H), 4.08 (t, J = 6.6 Hz, 2H), 3.38 (d, J = 7.3 Hz, 2H), 1.52 (dd, J = 14.3, 7.5 Hz, 2H), 1.21 (dt, J = 14.6, 7.3 Hz, 2H), 0.85 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.4, 169.3, 138.4, 136.2, 133.4, 128.9, 128.6, 128.6, 128.5, 126.6, 65.3, 56.2, 34.7, 30.4, 18.8, 13.5; (IR, Neat): 2960, 1733, 1685, 1450, 1181, 1078, 772 cm^{-1}; HRMS (ESI): Calculated for $[C_{20}H_{23}O_3]^+$ 311.1641; Found 311.1640.

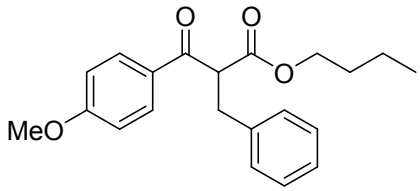
Butyl 2-benzyl-3-oxo-3-*p*-tolylpropanoate (30)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.269 g, 83%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, J = 7.4 Hz, 2H),

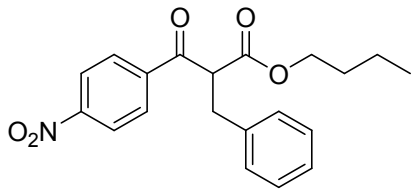
7.59 (t, J = 7.3 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.12 (dd, J = 18.0, 8.0 Hz, 4H), 4.63 (t, J = 7.3 Hz, 1H), 4.06 (t, J = 6.6 Hz, 2H), 3.32 (d, J = 7.3 Hz, 2H), 2.32 (s, 3H), 1.55 – 1.43 (m, 2H), 1.19 (dt, J = 14.7, 7.3 Hz, 2H), 0.84 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 194.5, 169.4, 136.2, 136.1, 135.3, 133.5, 129.2, 128.8, 128.6, 65.3, 56.3, 34.3, 30.4, 21.0, 18.9, 13.5; (IR, Neat): 3021, 1733, 1687, 1515, 1448, 1217, 907, 728 cm^{-1}; HRMS (ESI): Calculated for $[C_{21}H_{24}O_3Na]^+$ 347.1617; Found 347.1609.

Butyl 2-benzyl-3-(4-methoxyphenyl)-3-oxopropanoate (31)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.286 g, 84%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, J = 8.8 Hz, 2H), 7.22 – 7.09 (m, 5H), 6.85 (d, J = 8.8 Hz, 2H), 4.48 (t, J = 7.3 Hz, 1H), 4.03 – 3.95 (m, 2H), 3.82 (s, 3H), 3.26 (dd, J = 7.2, 3.2 Hz, 2H), 1.48 – 1.41 (m, 2H), 1.18 (dq, J = 15.2, 7.4 Hz, 2H), 0.81 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 192.0, 169.2, 163.7, 138.7, 131.0, 129.4, 129.0, 128.5, 126.5, 113.8, 65.0, 56.0, 55.3, 34.8, 30.5, 19.0, 13.7; (IR, KBr): 2959, 1773, 1676, 1420, 1294, 1222, 1026, 840, 698 cm^{-1}; HRMS (ESI): Calculated for $[C_{21}H_{24}O_4Na]^+$ 363.1572; Found 363.1588.

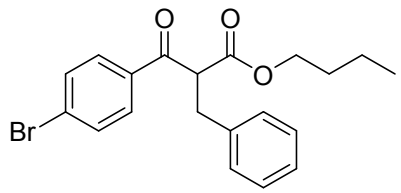
Butyl 2-benzyl-3-(4-nitrophenyl)-3-oxopropanoate (32)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4-5% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.323 g, 91%). M.p. 87-88 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (d, J = 8.8 Hz, 2H), 8.06 (d, J = 8.8 Hz, 2H), 7.28 – 7.18 (m, 5H), 4.62 (t, J = 7.4 Hz, 1H), 4.05 (t, J = 6.6 Hz, 2H), 3.36 (d, J = 7.4 Hz, 2H), 1.55 – 1.36 (m, 2H), 1.27 – 1.08 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.4, 168.6, 150.4, 140.9,

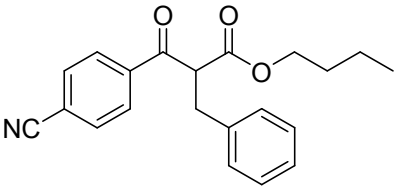
137.8, 129.6, 128.9, 128.7, 126.9, 123.9, 65.8, 56.7, 34.6, 30.4, 18.9, 13.6; (IR, Neat): 3020, 1737, 1696, 1529, 1347, 1215, 667 cm^{-1}; HRMS (ESI): Calculated for $[C_{20}H_{22}NO_5]^+$ 356.14925; Found 356.14947.

Butyl 2-benzyl-3-(4-bromophenyl)-3-oxopropanoate (33)



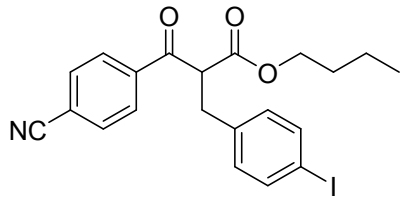
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.334 g, 86%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 8.4 Hz, 2H), 7.31 – 7.21 (m, 5H), 4.59 (t, J = 7.3 Hz, 1H), 4.06 (t, J = 6.6 Hz, 2H), 3.35 (d, J = 7.4 Hz, 2H), 1.55 – 1.43 (m, 2H), 1.20 (dd, J = 15.1, 7.4 Hz, 2H), 0.85 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.5, 169.0, 138.2, 135.0, 132.0, 130.1, 128.8, 128.5, 127.8, 126.7, 65.4, 56.1, 34.6, 30.3, 18.8, 13.5; (IR, Neat): 2958, 1737, 1689, 1488, 1273, 1071, 771 cm^{-1}; HRMS (ESI): Calculated for $[C_{20}H_{22}BrO_3]^+$ 389.0746; Found 389.0752.

Butyl 2-benzyl-3-(4-cyanophenyl)-3-oxopropanoate (34)



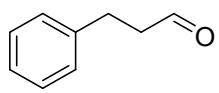
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.298 g, 89%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 (d, J = 8.7 Hz, 2H), 7.75 (d, J = 8.7 Hz, 2H), 7.28 – 7.16 (m, 5H), 4.54 (t, J = 7.4 Hz, 1H), 4.05 (td, J = 6.6, 1.7 Hz, 2H), 3.33 (d, J = 7.3 Hz, 2H), 1.49 (ddd, J = 13.3, 8.7, 6.6 Hz, 2H), 1.25 – 1.17 (m, 2H), 0.87 (t, J = 7.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.4, 168.6, 139.3, 137.8, 132.5, 128.9, 128.8, 128.6, 126.8, 117.7, 116.7, 65.7, 56.4, 34.5, 30.3, 18.8, 13.5; (IR, KBr): 2926, 2232, 1734, 1694, 1373, 1220, 940, 771 cm^{-1}; HRMS (ESI): Calculated for $[C_{21}H_{21}NO_3Na]^+$ 358.1419; Found 358.1420.

Butyl 3-(4-cyanophenyl)-2-(4-iodobenzyl)-3-oxopropanoate (35)



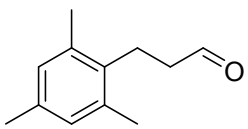
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless solid (0.401 g, 87%). M.p. 89-91 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 8.6 Hz, 2H), 7.75 (d, J = 8.5 Hz, 2H), 7.58 (d, J = 8.3 Hz, 2H), 6.96 (d, J = 8.3 Hz, 2H), 4.54 (t, J = 7.4 Hz, 1H), 4.04 (t, J = 6.6 Hz, 2H), 3.28 (dd, J = 7.4, 2.8 Hz, 2H), 1.47 – 1.42 (m, 2H), 1.19 – 1.13 (m, 2H), 0.82 (t, J = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.0, 168.4, 139.1, 137.7, 137.5, 132.6, 131.0, 129.0, 117.7, 116.9, 92.2, 65.8, 56.2, 33.9, 30.3, 18.9, 13.6; (IR, Neat): 2929, 1734, 1694, 1217, 746 cm^{-1}; HRMS (ESI): Calculated for: $[C_{21}H_{21}NIO_3]^+$ 462.05606; Found 462.05606.

3-Phenylpropanal (36) [3,6a]



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 3% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.118 g, 88%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.81 (s, 1H), 7.32 – 7.18 (m, 5H), 2.95 (t, J = 7.5 Hz, 2H), 2.77 (t, J = 7.5 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.5, 140.3, 128.5, 128.2, 126.2, 45.2, 28.0; (IR, Neat): 3028, 2924, 1704, 1412, 1214, 925, 695 cm^{-1}.

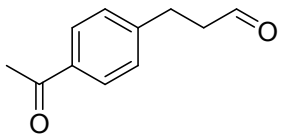
3-Mesitylpropanal (37)



Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.139 g, 79%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.85 (s, 1H), 6.84 (s, 2H), 2.96 – 2.86 (m, 2H), 2.63 – 2.52 (m, 2H), 2.27 (s, 6H), 2.24 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 199.7, 133.9, 133.7, 132.0, 127.1, 121.5, 41.3, 19.6, 18.8, 17.7; (IR, Neat): 2951, 1724, 1448, 1219, 772 cm^{-1}; Calculated for

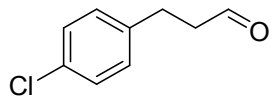
$[C_{12}H_{16}ONa]^+$ 199.1093; Found 199.1099.

3-(4-Acetylphenyl)propanal (38) [6a]



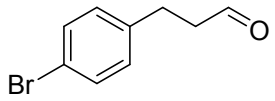
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 20% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.157 g, 89%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 7.9 Hz, 2H), 3.02 (t, J = 7.1 Hz, 2H), 2.83 (t, J = 7.3 Hz, 2H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 200.8, 197.8, 146.1, 135.5, 130.9, 128.8, 128.6, 44.7, 28.0, 26.6; (IR, Neat): 2961, 2933, 1679, 1605, 1359, 1268, 772 cm^{-1}; HRMS (ESI): Calculated for $[C_{11}H_{13}O_2]^+$ 177.0910; Found 177.0916.

3-(4-Chlorophenyl)propanal (39) [6b]



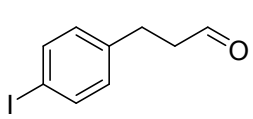
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.146 g, 87%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.83 (s, 1H), 7.92 (d, J = 8.7 Hz, 2H), 7.46 (d, J = 8.7 Hz, 2H), 2.95 (t, J = 7.2 Hz, 2H), 2.79 (t, J = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.1, 138.9, 132.0, 129.7, 128.7, 45.1, 27.4; (IR, Neat): 2923, 1710, 1491, 1219, 1091, 772 cm^{-1}.

3-(4-Bromophenyl)propanal (40) [7a]



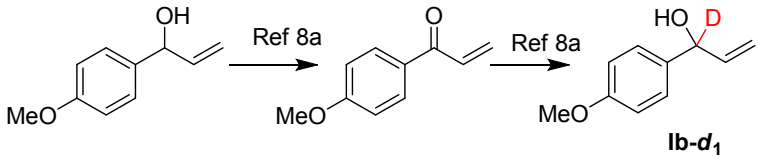
Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.191 g, 90%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.81 (s, 1H), 7.41 (d, J = 8.3 Hz, 2H), 7.09 (d, J = 8.2 Hz, 2H), 2.91 (t, J = 7.5 Hz, 2H), 2.66 (t, J = 7.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.0, 139.1, 131.6, 130.1, 120.2, 35.4, 29.9; (IR, Neat): 2915, 1692, 1432, 1270, 1073, 817 cm^{-1}.

3-(4-Iodophenyl)propanal (41) [7b]

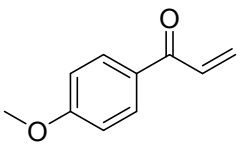


Following the general procedure, the residue was purified by column chromatography (silica gel 100-200 mesh, 4% ethyl acetate in hexane as eluent) to afford the title product as a colourless liquid (0.244 g, 94%). ^{1}H NMR (300 MHz,) δ 9.83 (s, 1H), 7.63 (d, J = 8.3 Hz, 2H), 6.97 (d, J = 8.3 Hz, 2H), 2.92 (t, J = 6.9 Hz, 2H), 2.79 (t, J = 7.0 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 201.0, 140.1, 137.6, 130.4, 91.9, 45.0, 27.5; (IR, Neat): 2922, 1729, 1512, 1219, 1072, 772 cm^{-1}.

Deuterium Labeling Experiment:

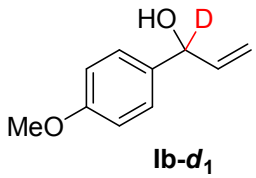


1-(4-methoxyphenyl)prop-2-en-1-one[8a]



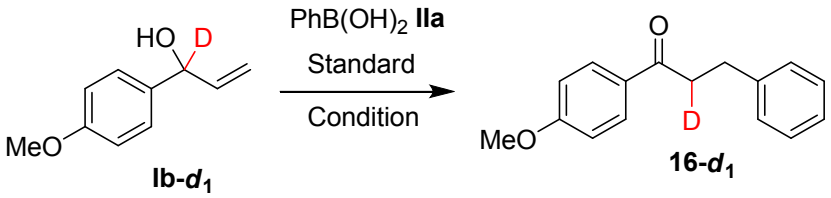
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, J = 9.0 Hz, 2H), 7.17 (dd, J = 17.1, 10.5 Hz, 1H), 6.95 (d, J = 8.9 Hz, 2H), 6.42 (dd, J = 17.1, 1.8 Hz, 1H), 5.86 (dd, J = 10.5, 1.8 Hz, 1H), 3.87 (s, 3H).

1-(4-methoxyphenyl)prop-1-(^{2}H$_1$)-2-en-1-ol (Ib-d_1)[8a]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, J = 8.2 Hz, 2H), 6.87 (d, J = 8.2 Hz, 2H), 6.02 (dd, J = 17.1, 10.3 Hz, 1H), 5.31 (dd, J = 17.1, 1.4 Hz, 1H), 5.17 (dd, J = 10.3, 1.4 Hz, 1H), 3.78 (s, 3H).

1-(4-methoxyphenyl)-3-phenyl-2($^2H_1$)-propan-1-one (16-d_1)[8b]



Ib-d_1 **16-d_1**

A mixture of phenylboronic acid **IIa** (0.183g, 1.5mmol), $Pd(OAc)_2$ (0.022 g, 0.1 mmol), and 2,9-dimethyl-1,10-phenanthroline (0.042 g, 0.20 mmol), CuCl (0.005 g, 0.05 mmol), Deuterium-labelled propenol (**Ib-d_1**) (0.165g, 1.0mmol) {prepared as per the literature procedure[8a]}, was dissolved in DMSO (3 mL) in a 10 mL RB flask closed with air balloon (1atm pressure). The mixture was vigorously stirred at 50 °C for 12 h. After cooling to room temperature, the reaction mixture was partitioned between ethyl acetate (25.0 mL) and water (25 mL) and it was transferred to 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, 4% ethyl acetate in hexane as eluent) to afford the title product **16-d_1** as a colourless solid (0.203 g, 84%). M.p. 100-101 ^oC; ^1H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, J = 8.9 Hz, 2H), 7.30 (dd, J = 10.1, 4.7 Hz, 2H), 7.25 (d, J = 6.5 Hz, 2H), 7.20 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 8.9 Hz, 2H), 3.86 (s, 3H), 3.28 – 3.19 (m, 1H), 3.05 (d, J = 7.9 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.9, 163.5, 141.5, 130.3, 130, 128.5, 128.4, 126.1, 113.8, 77.3, 77.1, 76.8, 55.5, 39.8 (t, J = 38.2 Hz, CHD), 30.3; HRMS (ESI): Calculated for $[C_{16}H_{16}DO_2]^+$ 242.12858; Found 242.12697.

1.4 References

[1] *a*) A. Bartoszewicz and B. Martín-Matute, *Org.Lett*., 2009*,* **11**, 1749 ; b) A. Bouziane, B. Carboni, C. Bruneau, F. Carreaux and J. Renaud, *Tetrahedron*, 2008, **64**, 11745; c) N. Marion, R. Gealageas and S. P. Nolan, *Org.Lett.,* 2007, **9**, 2653; d) G. Zhang, T. Kumamoto, T. Heima and T. Ishikawa, *Tetrahedron Lett*., 2010, **51**, 3927; e) P. D. Hammen, A. C. Braisted and D. L. Northrup, *Synth Commun*, 1991, **21**, 2157; f) J. Nokami, H. Ogawa, S. Miyamoto, T. Mandai, S. Wakabayashi and J. Tsuji, *Tetrahedron Lett*., 1988, **29**, 5181; g) S. D. Markad, N. S. Karanjule, T. Sharma, S. G. Sabharwal, V. G. Puranik and D. D. Dhavale, *Org. Biomol. Chem.,* 2006, **4**, 2549; h) G. Righi, G. Pescatore, F. Bonadies, C. Bonini, *Tetrahedron,* 2001, **57**, 5649; i) Y. Song, H. Ke, N. Wang, L. Wang, G. Zou, *Tetrahedron*, 2009, **65**, 9086.

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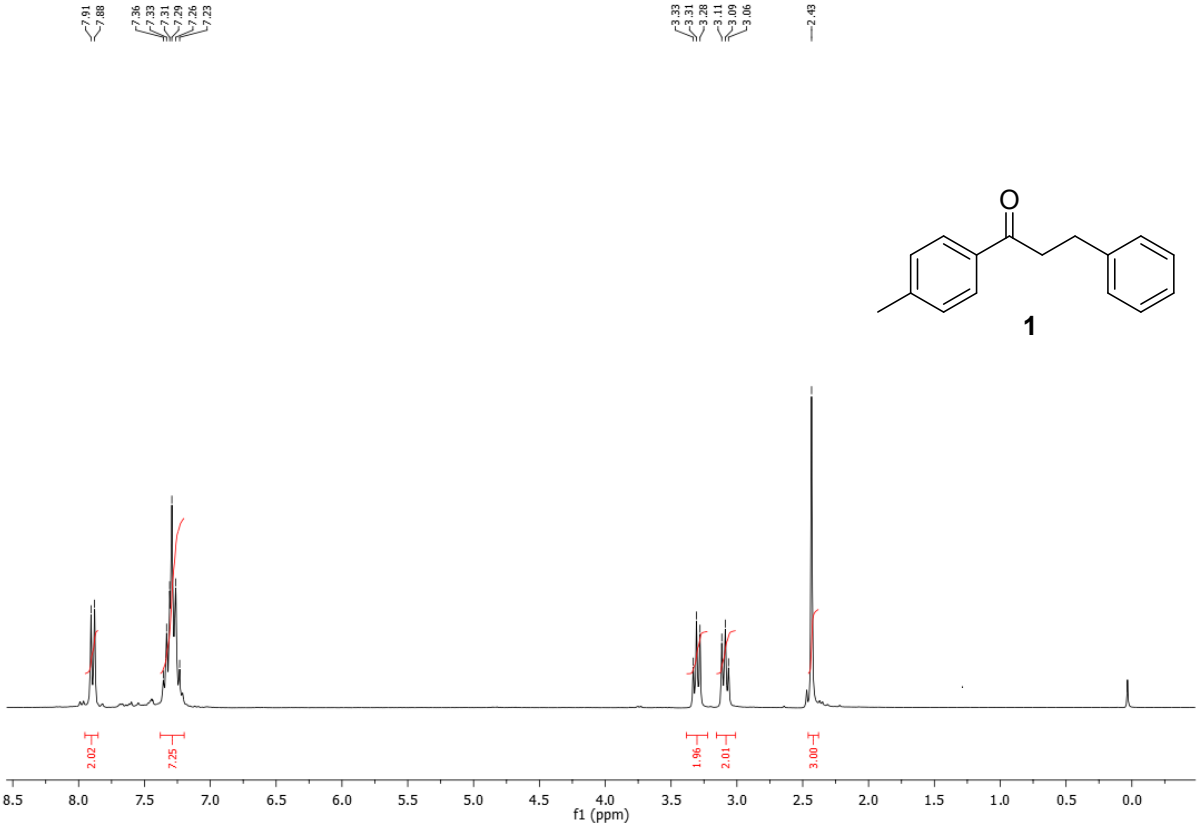
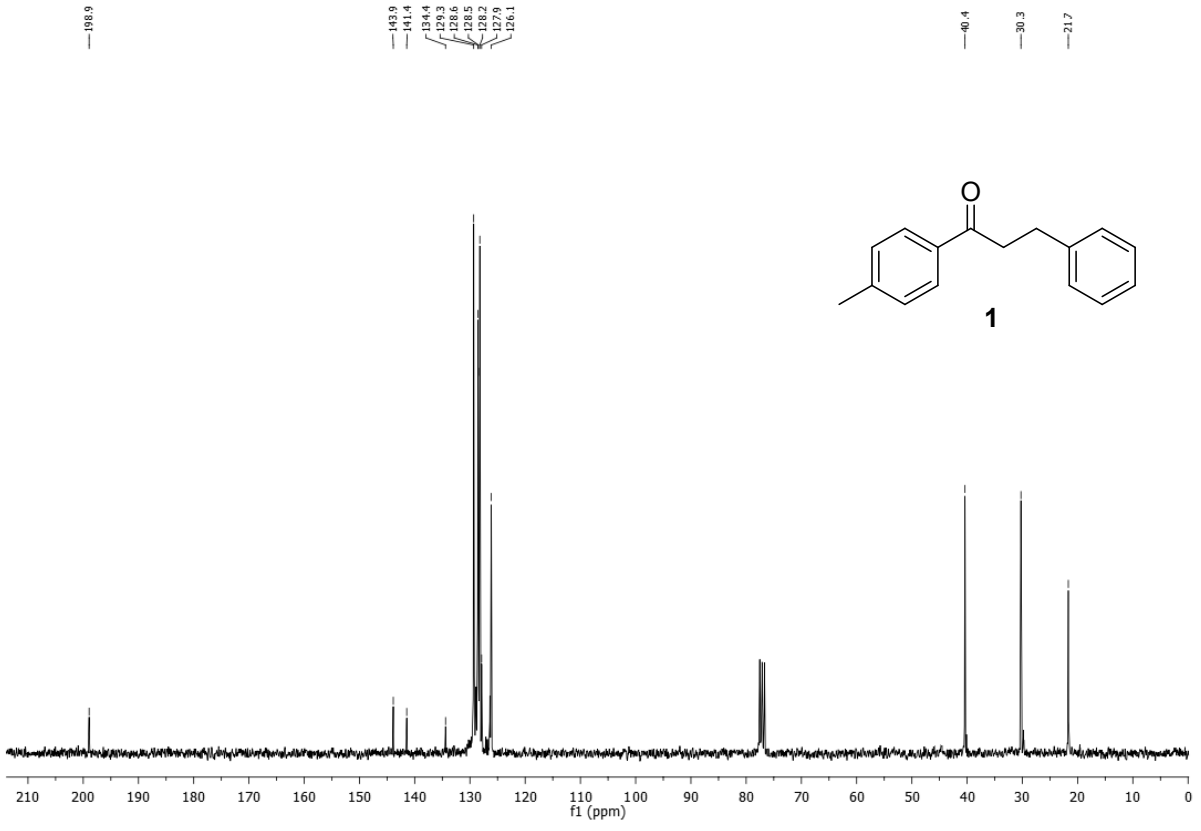
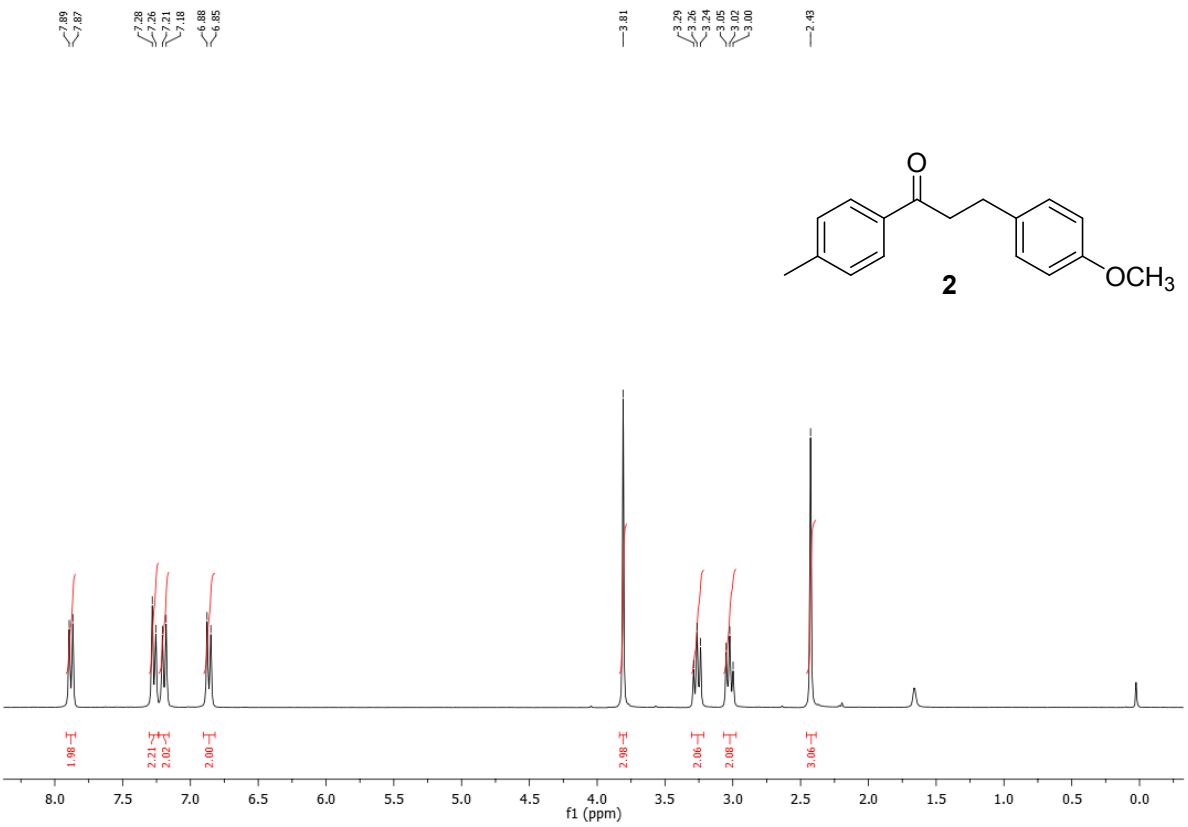
^{1}H and ^{13}C NMR Spectra for compounds (**1-41)**



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7.87
7.28
7.26
7.21
7.18
6.88
6.85
3.81
3.29
3.26
3.24
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3.02
3.00
2.43
O
OCH3
2
1.98
2.21
2.02
2.00
2.98
2.06
2.08
3.06
8.0
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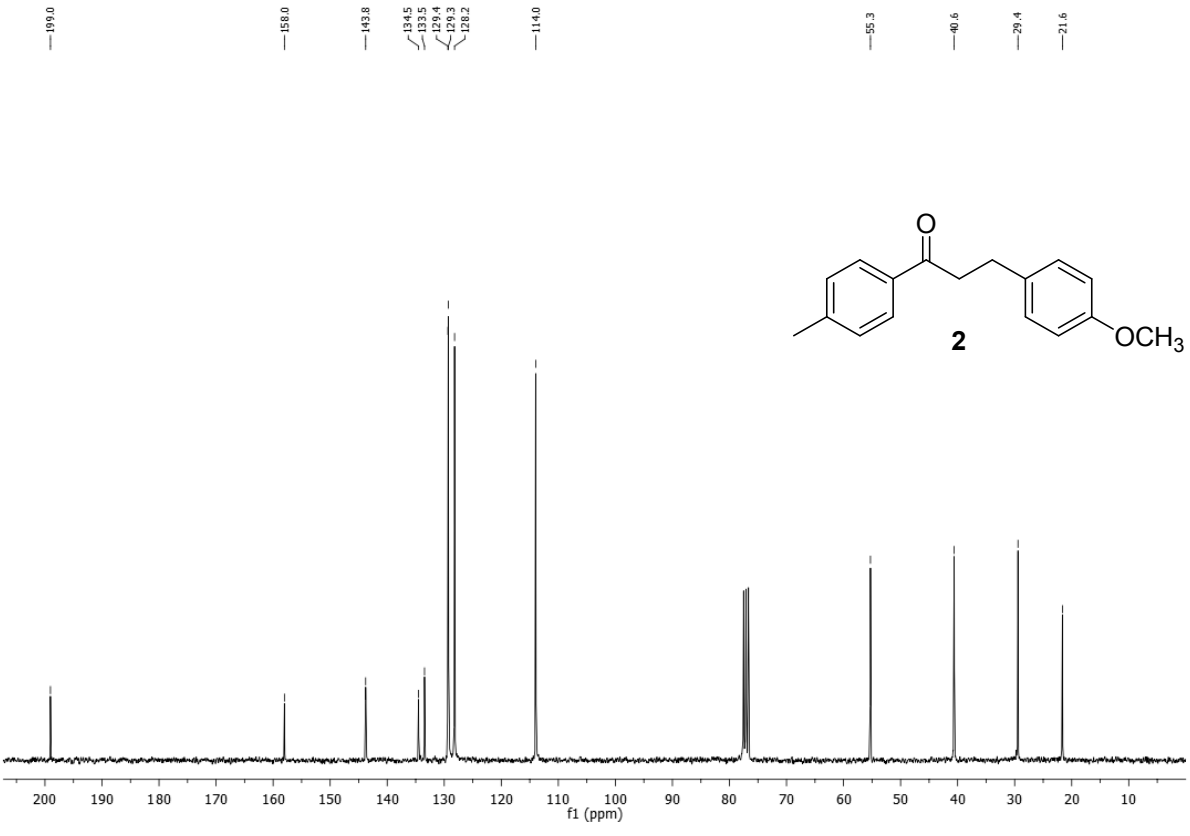
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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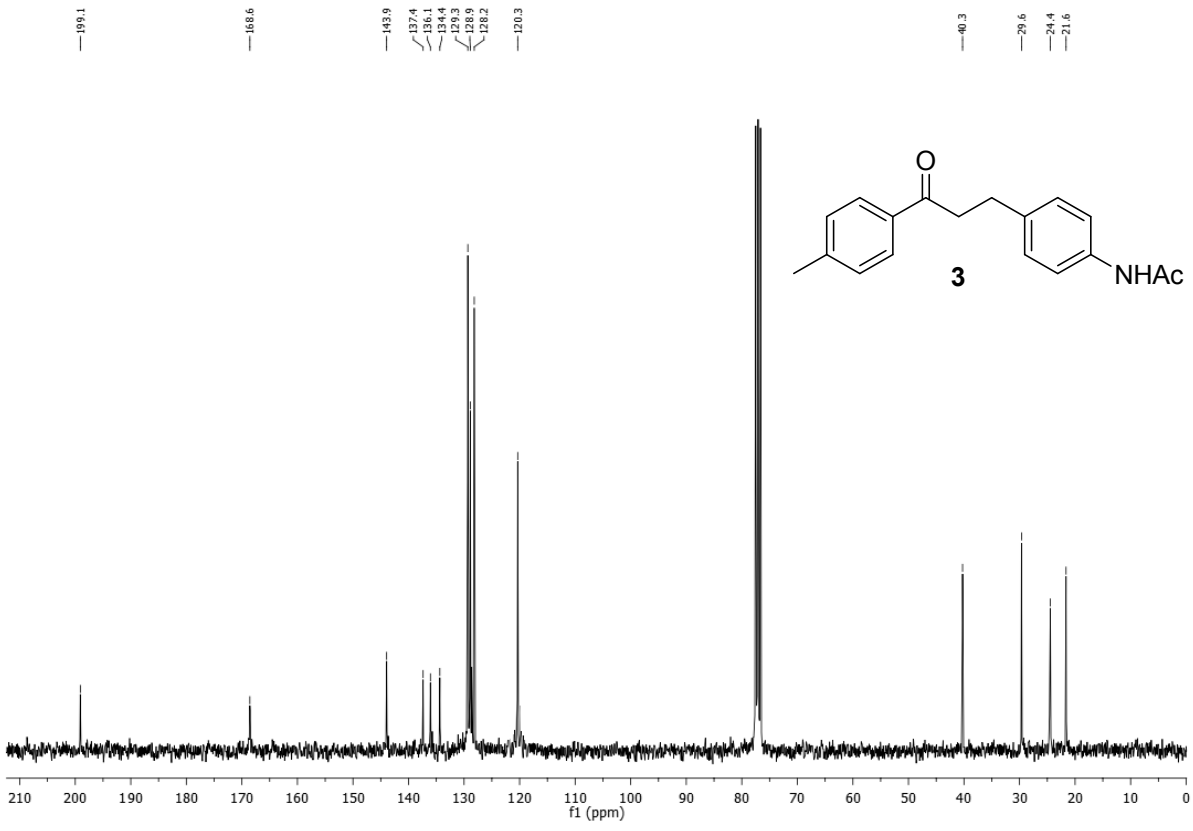
158.0
143.8
134.5
133.5
129.4
129.3
128.2
114.0
55.3
40.6
29.4
21.6
O
OCH3
2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.87
7.85
7.66
7.44
7.42
7.28
7.27
7.25
7.20
7.18
3.28
3.26
3.23
3.05
3.02
3.00
2.41
2.16
O
NHAc
3
1.92
0.64
1.82
2.04
1.80
1.94
2.00
2.99
3.29
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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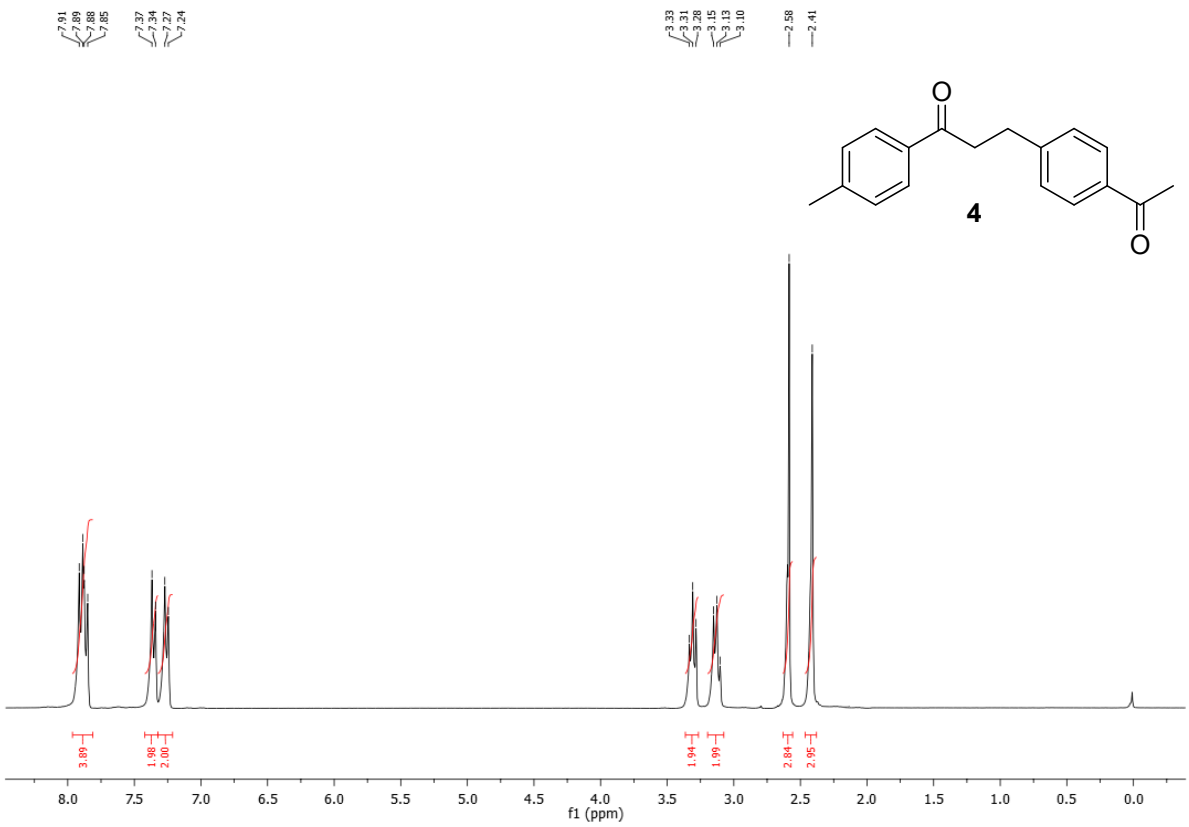
168.6
143.9
137.4
136.1
134.4
129.3
128.9
128.2
120.3
40.3
29.6
24.4
21.6
O
NHAc
3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.89
7.88
7.85
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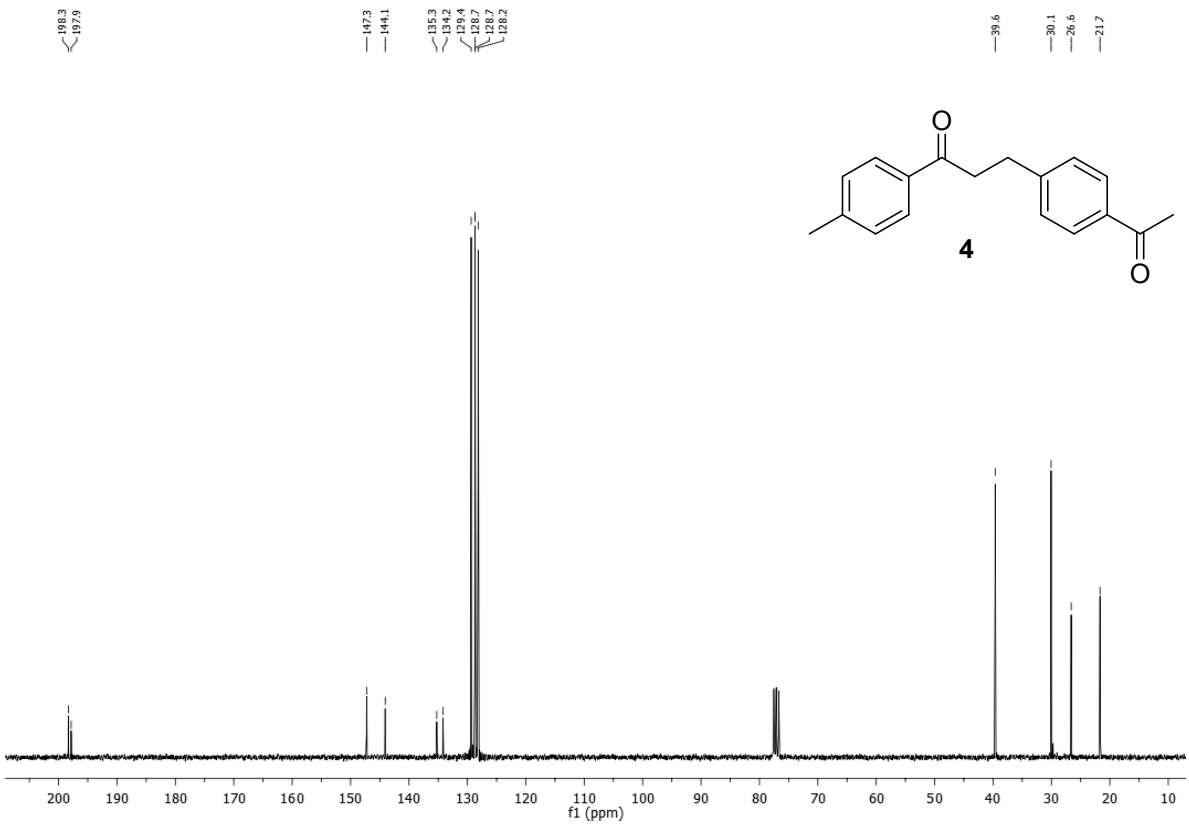
7.34
7.27
7.24
3.33
3.31
3.28
3.15
3.13
3.10
2.58
2.41
O
4
O
3.89
1.98
2.00
1.94
1.99
2.84
2.95
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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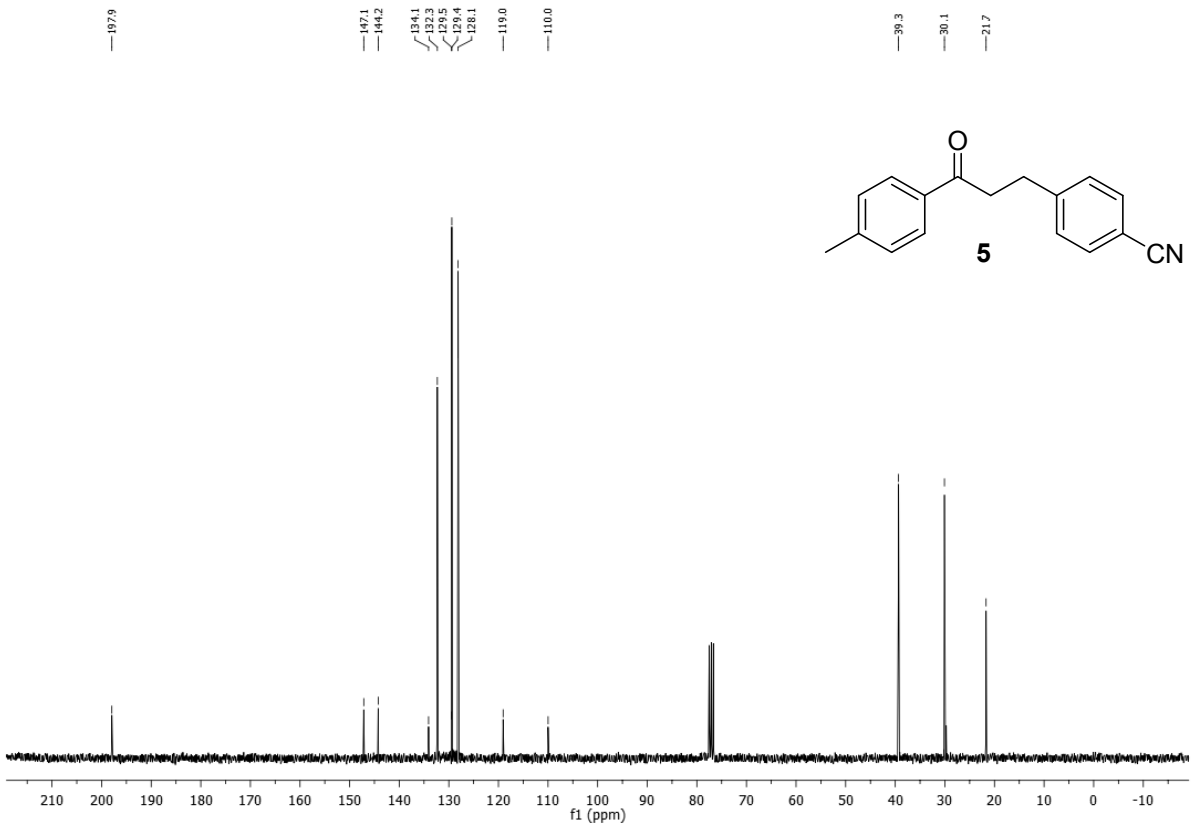
147.3
144.1
135.3
134.2
129.4
128.7
128.7
128.2
39.6
30.1
26.6
21.7
O
4
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.87
7.85
7.60
7.58
7.39
7.36
7.28
7.26
3.34
3.34
3.31
3.29
3.16
3.14
3.12
2.42
O
5
CN
1.98
1.93
1.95
2.11
2.03
2.00
3.00
f1 (ppm)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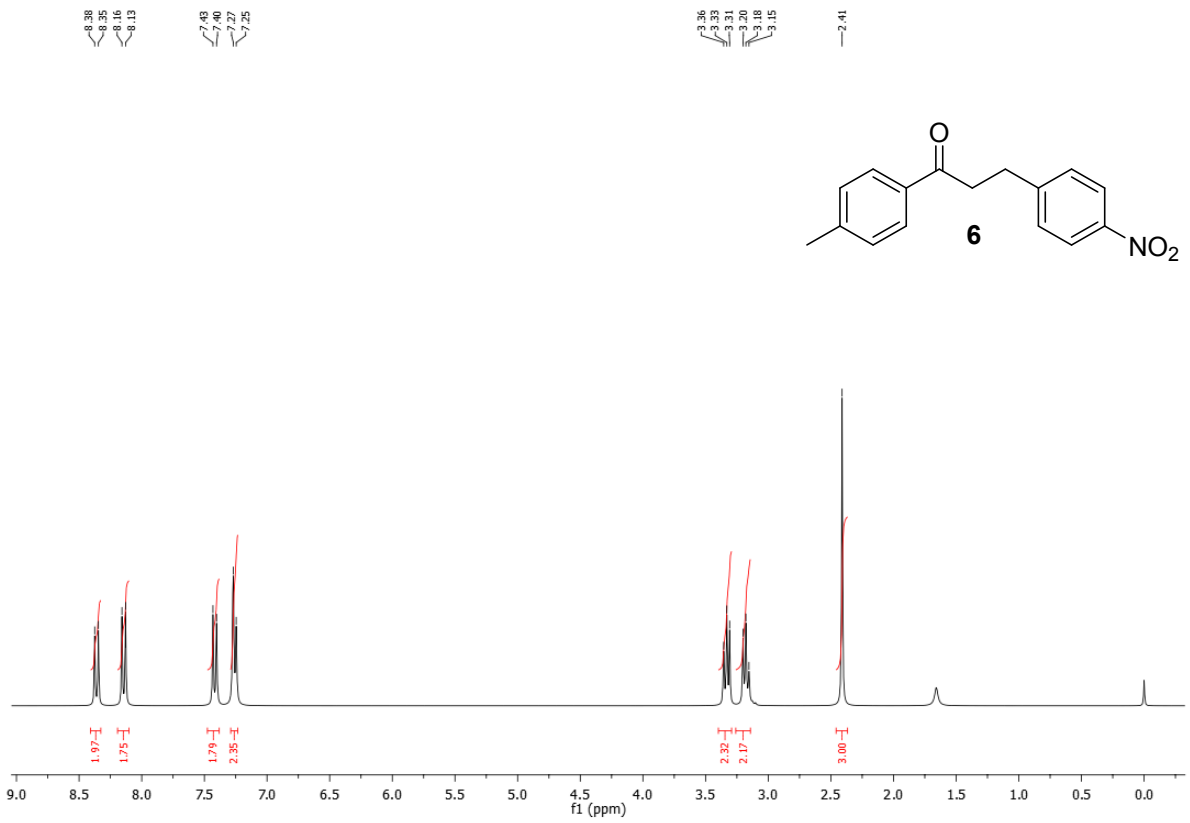
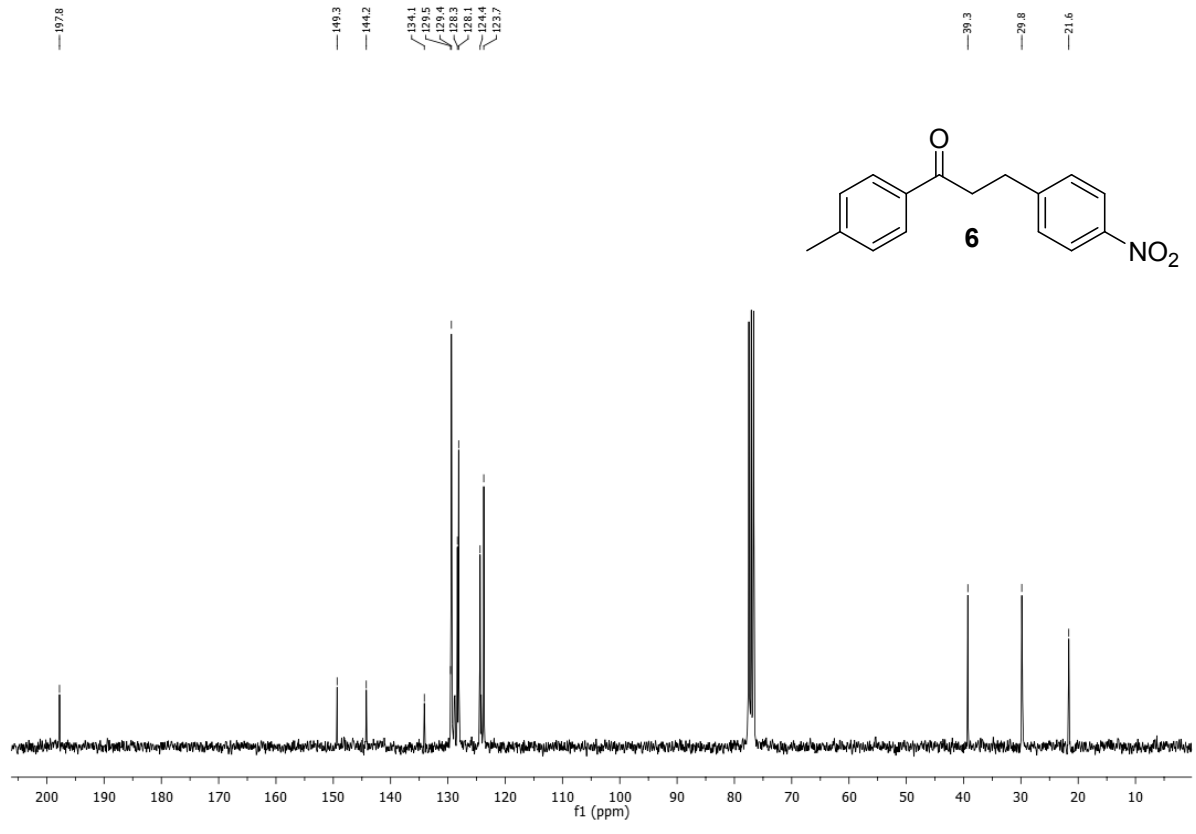
147.1
144.2
134.1
132.3
129.5
129.4
128.1
119.0
110.0
39.3
30.1
21.7
O
5
CN
f1 (ppm)


8.38
8.35
8.16
8.13
7.43
7.40
7.27
7.25
3.36
3.33
3.31
3.20
3.18
3.15
2.41
O
6
NO2
1.97
1.75
1.79
2.35
2.32
2.17
3.00
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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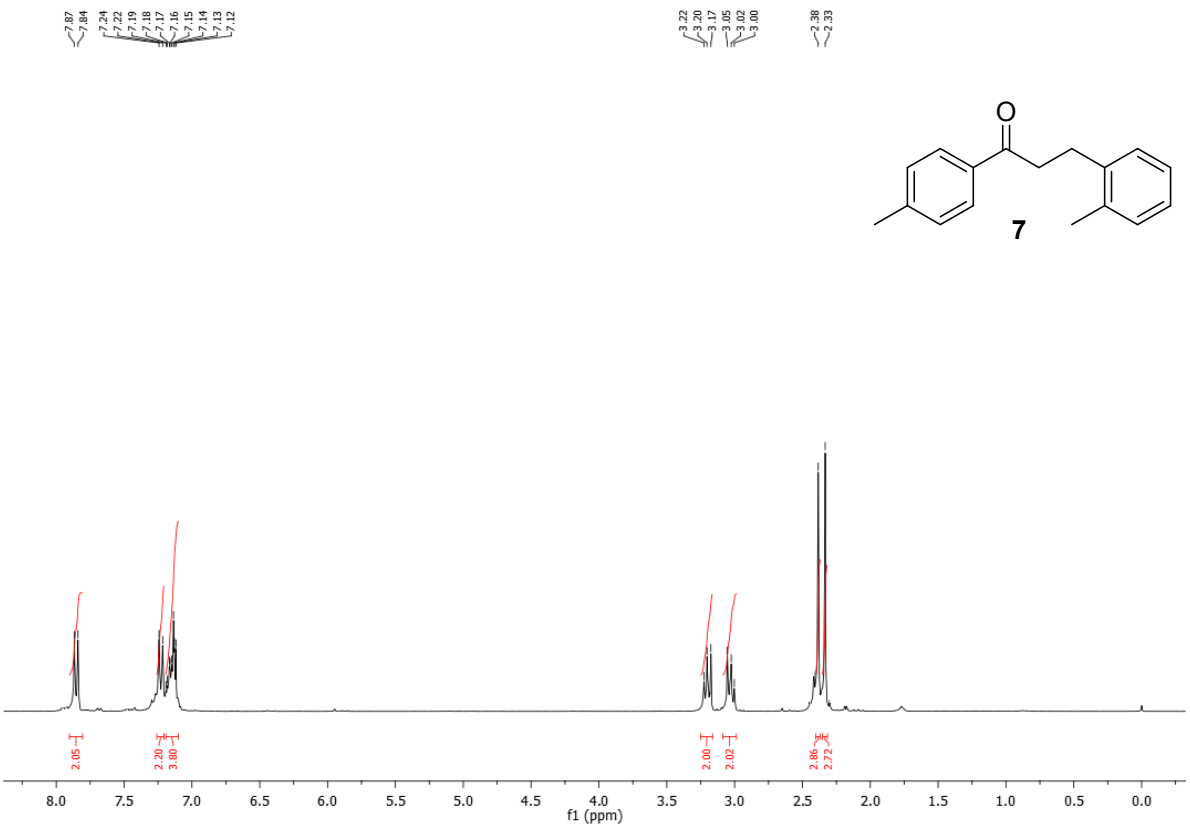
149.3
144.2
134.1
129.5
129.4
128.3
128.1
124.4
123.7
39.3
29.8
21.6
O
6
NO2
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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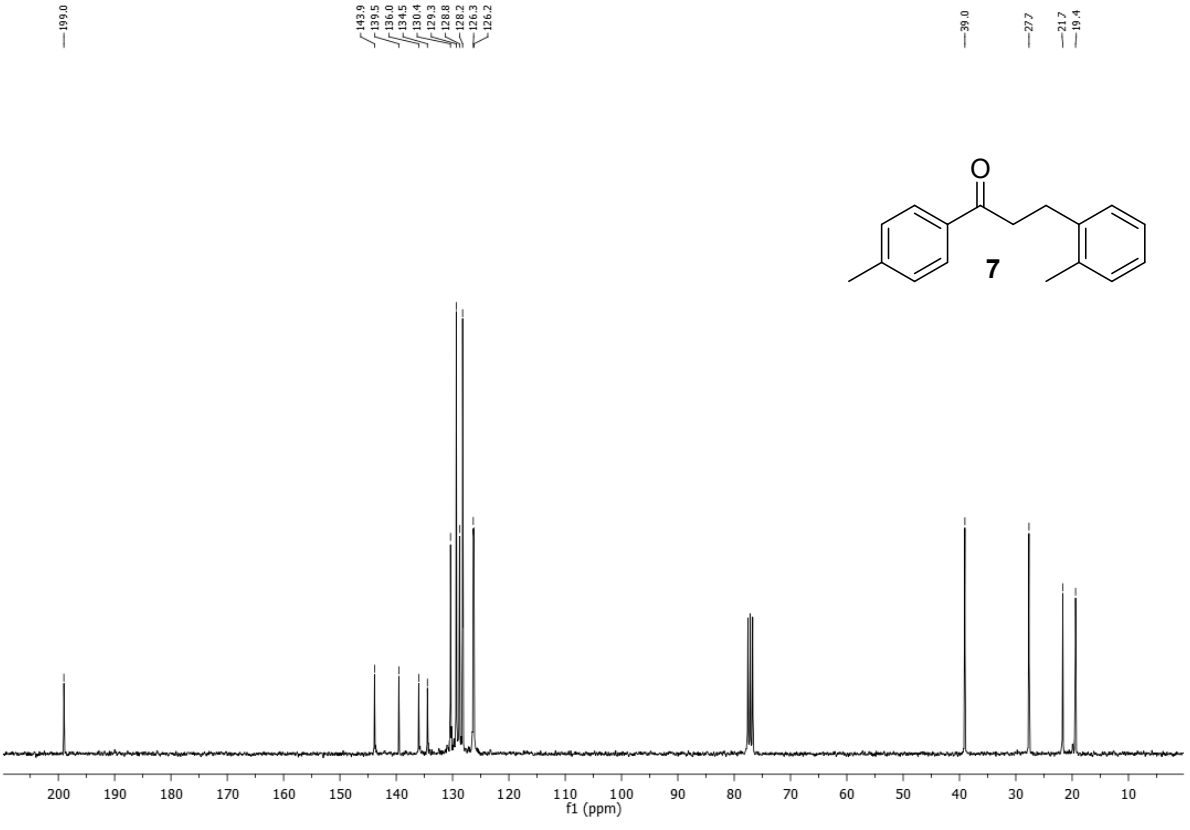
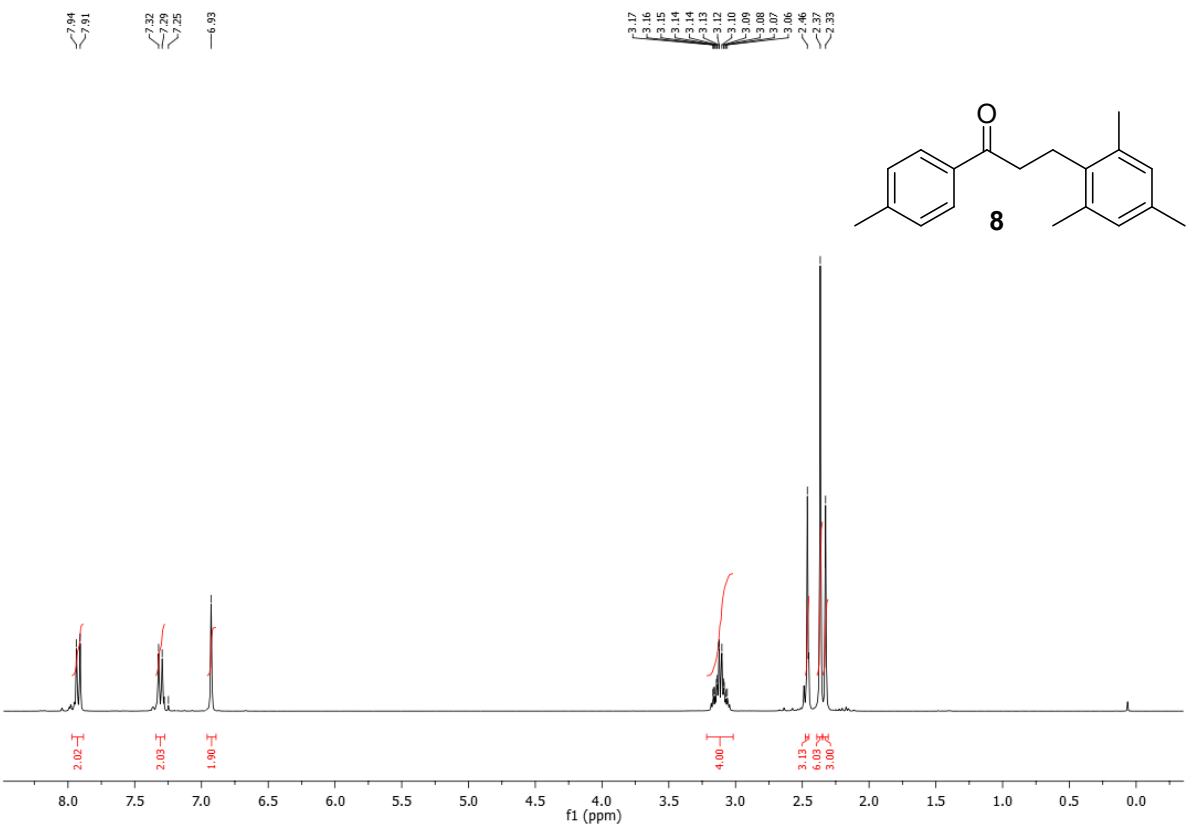
7.84
7.24
7.22
7.19
7.18
7.17
7.16
7.15
7.14
7.13
7.12
3.22
3.20
3.17
3.05
3.02
3.00
2.38
2.33
O
7
2.05
2.20
3.80
2.00
2.02
2.86
2.72
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


199.0
143.9
139.5
136.0
134.5
130.4
129.3
128.8
128.2
126.3
126.2
39.0
27.7
21.7
19.4
O
7
200
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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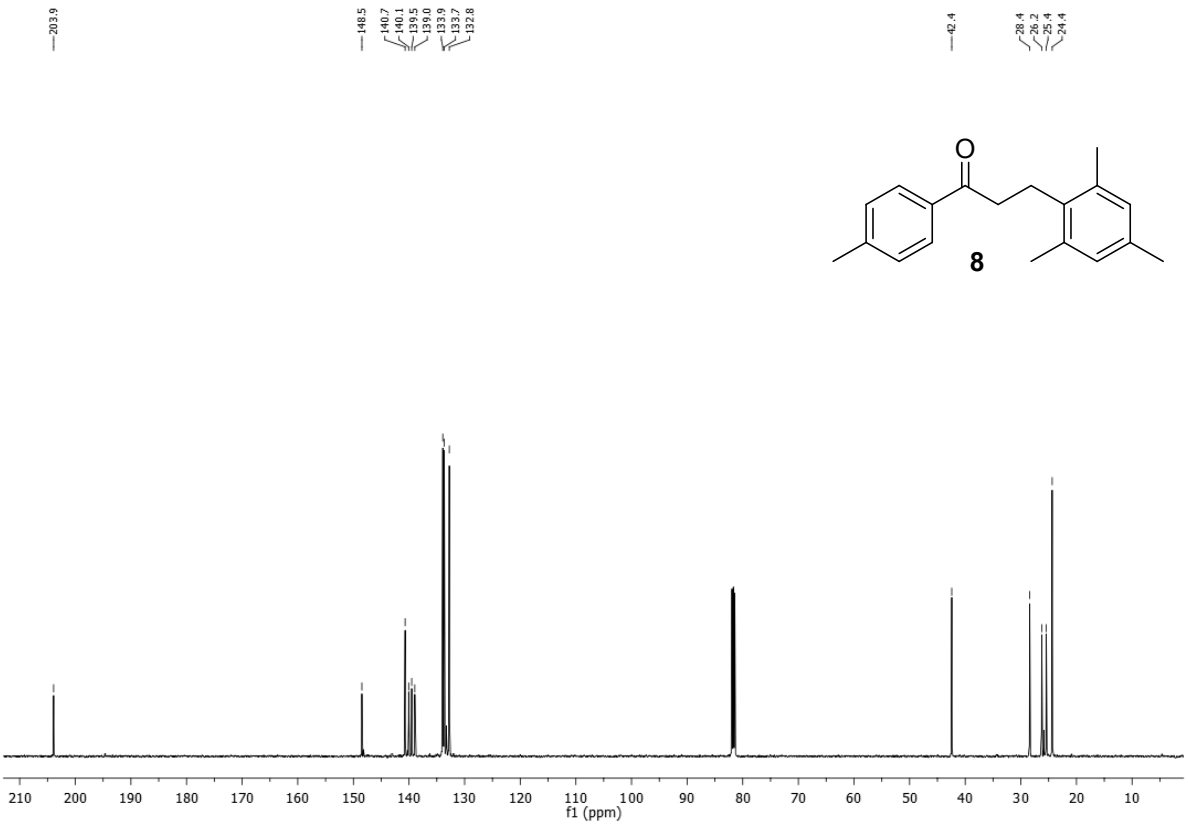
7.91
7.32
7.29
7.25
6.93
3.17
3.16
3.15
3.14
3.14
3.13
3.12
3.10
3.09
3.08
3.07
3.06
2.46
2.37
2.33
O
8
2.02
2.03
1.90
4.00
3.13
6.03
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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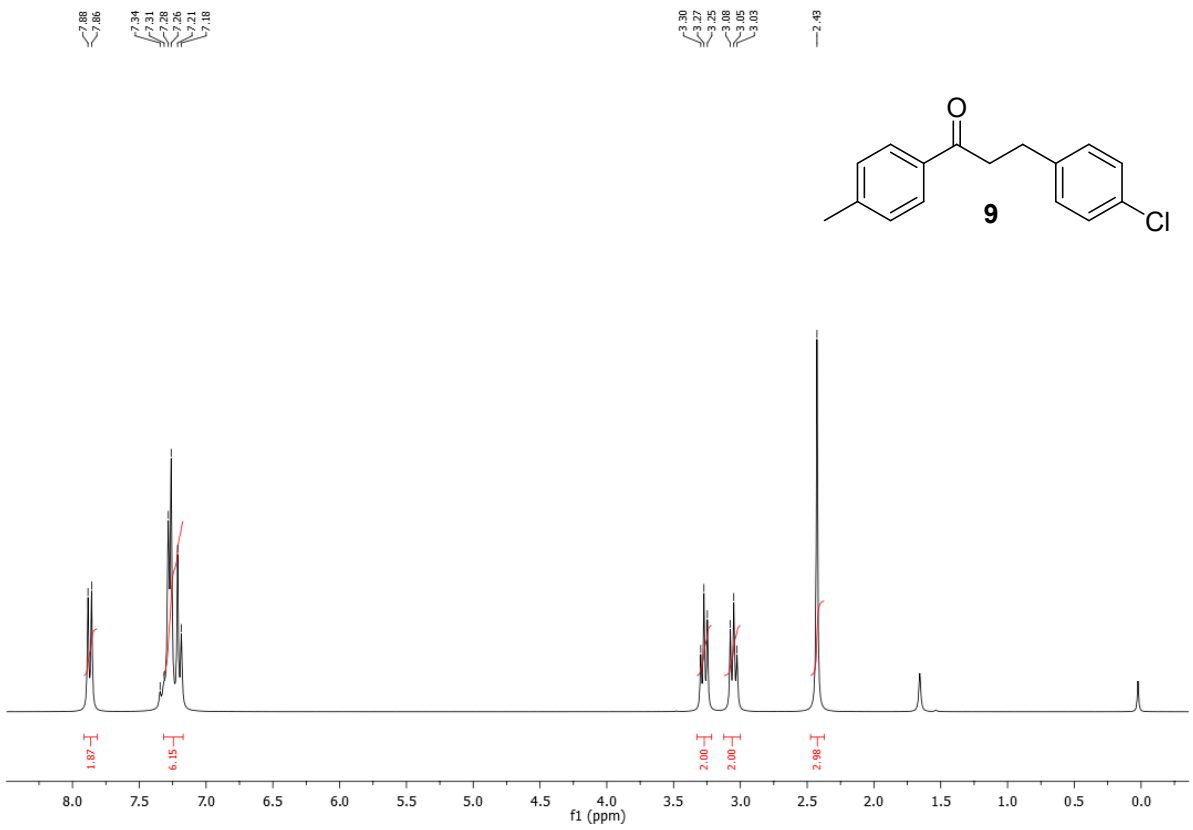
148.5
140.7
140.1
139.5
139.0
133.9
133.7
132.8
42.4
28.4
26.2
25.4
24.4
O
8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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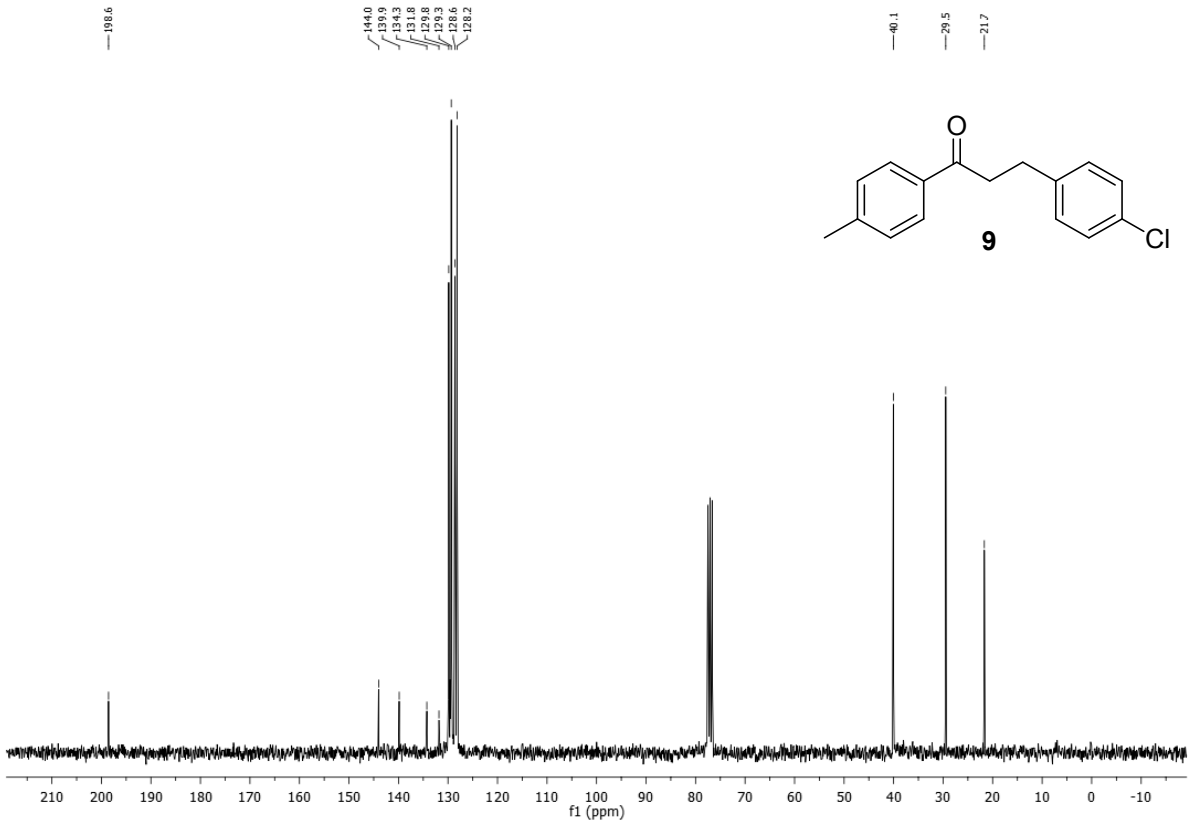
7.86
7.34
7.31
7.28
7.26
7.21
7.18
3.30
3.27
3.25
3.08
3.05
3.03
2.43
O
Cl
9
1.87
6.15
2.00
2.00
2.98
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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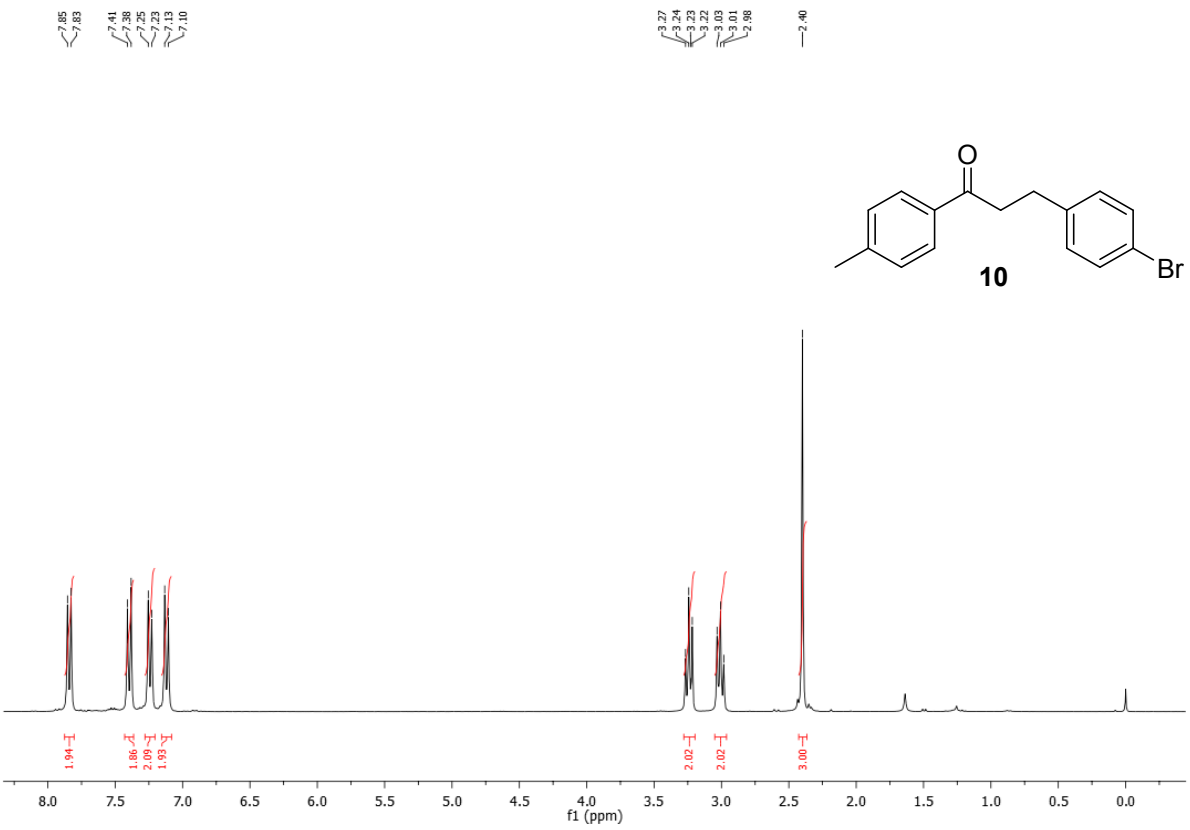
134.3
131.8
129.8
129.3
128.6
128.2
40.1
29.5
21.7
O
Cl
9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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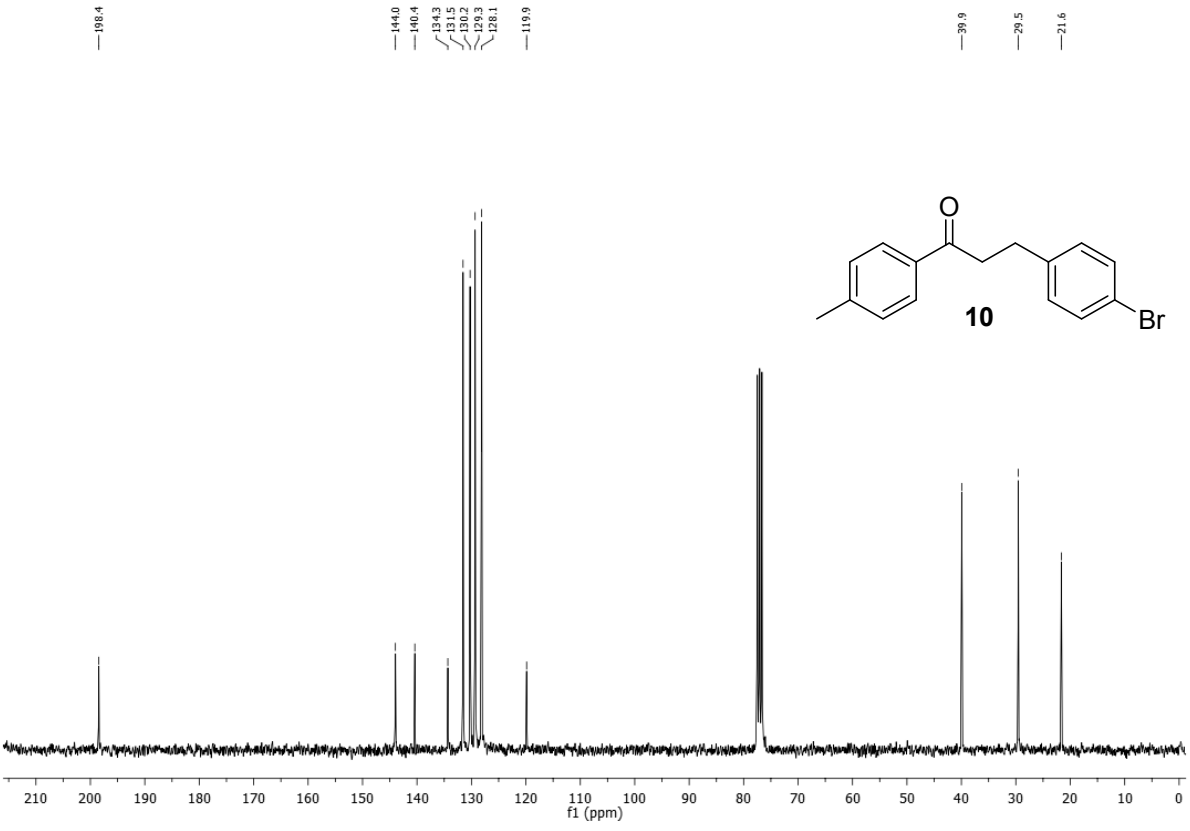
7.83
7.41
7.38
7.25
7.23
7.13
7.10
3.27
3.24
3.23
3.22
3.03
3.01
2.98
2.40
O
Br
10
1.94
1.86
2.09
1.93
2.02
2.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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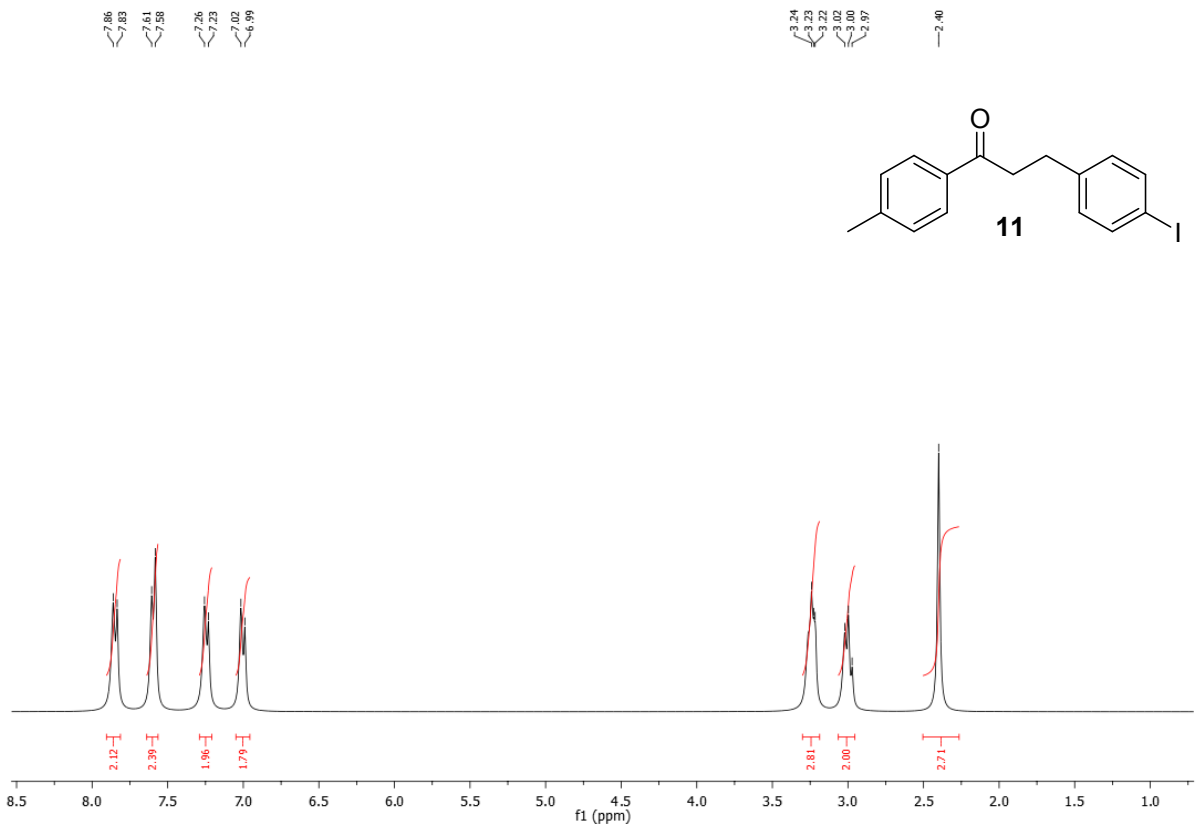
134.3
131.5
130.2
129.3
128.1
119.9
39.9
29.5
21.6
O
Br
10
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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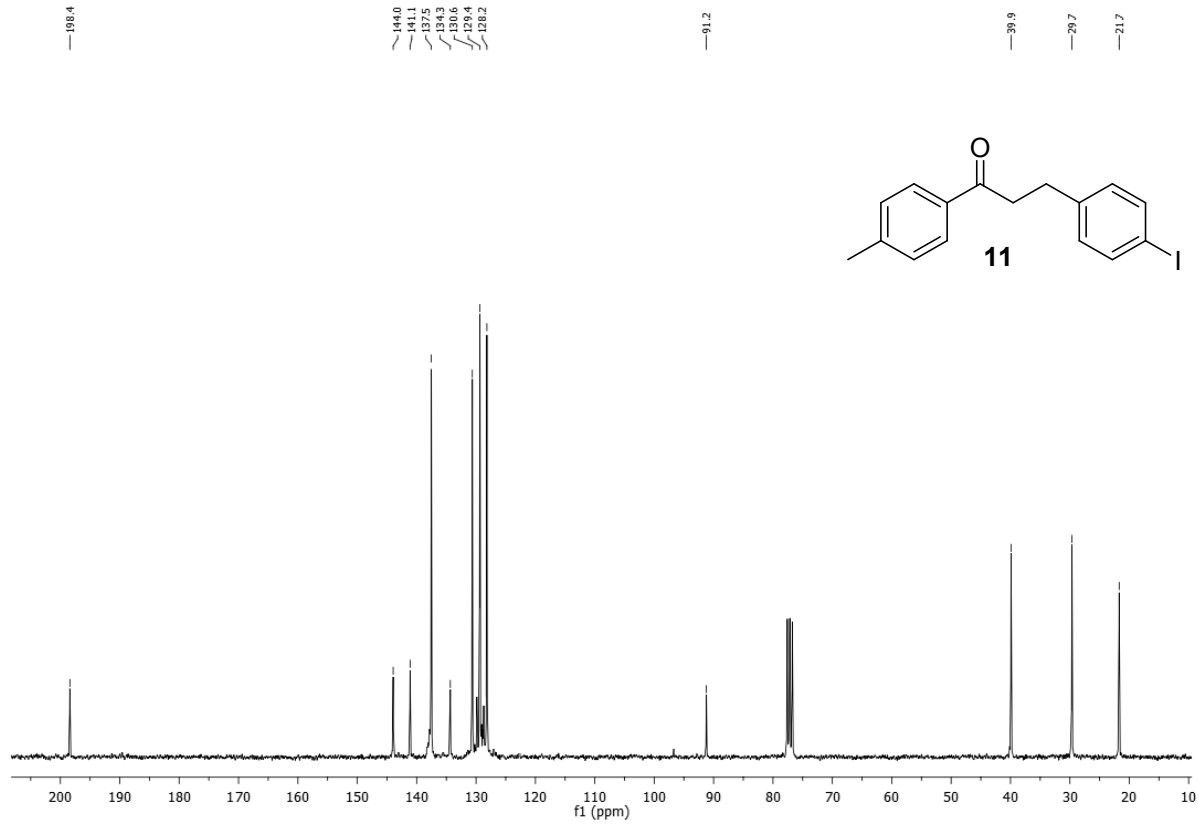
7.83
7.61
7.58
7.26
7.23
7.02
6.99
3.24
3.23
3.22
3.02
3.00
2.97
2.40
O
11
I
2.12
2.39
1.96
1.79
2.81
2.00
2.71
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)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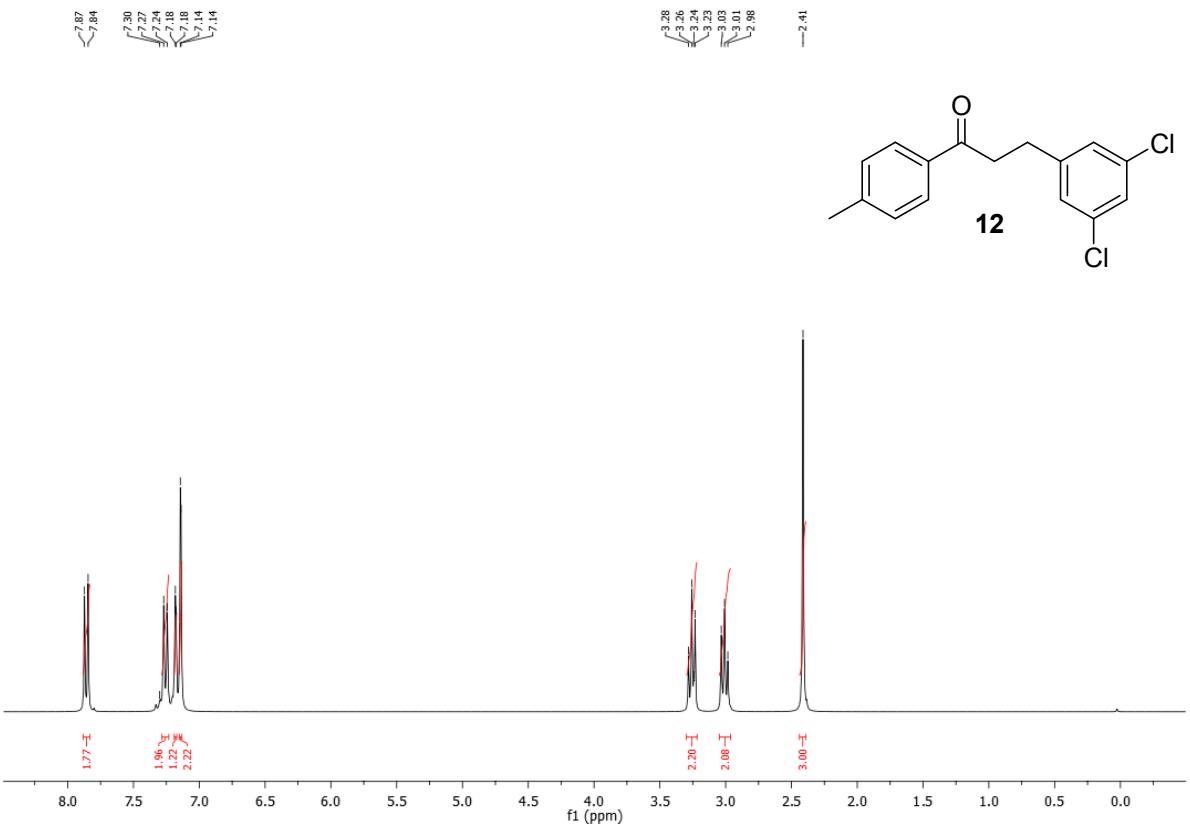
144.0
141.1
137.5
134.3
130.6
129.4
128.2
91.2
39.9
29.7
21.7
O
11
I
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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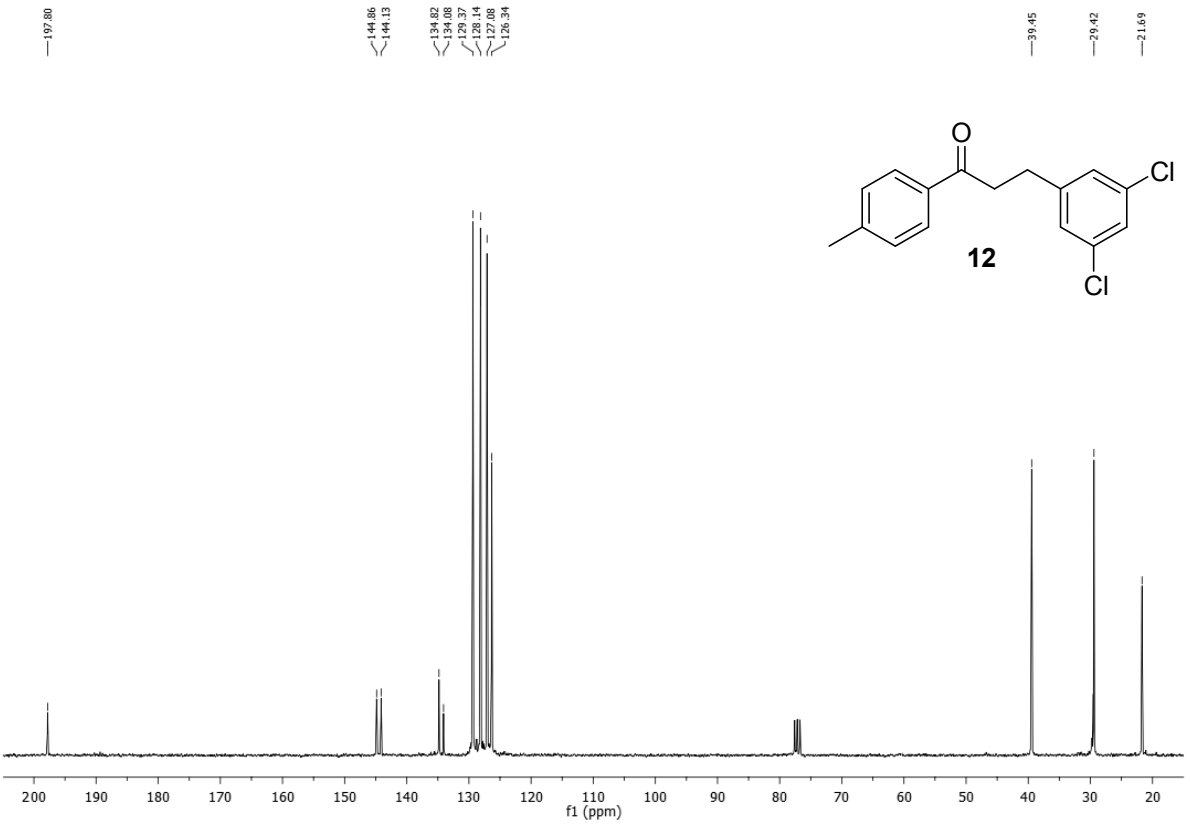
7.84
7.30
7.27
7.24
7.18
7.18
7.14
7.14
3.28
3.26
3.24
3.23
3.03
3.01
2.98
2.41
O
Cl
Cl
12
1.77
1.96
1.22
2.22
2.20
2.08
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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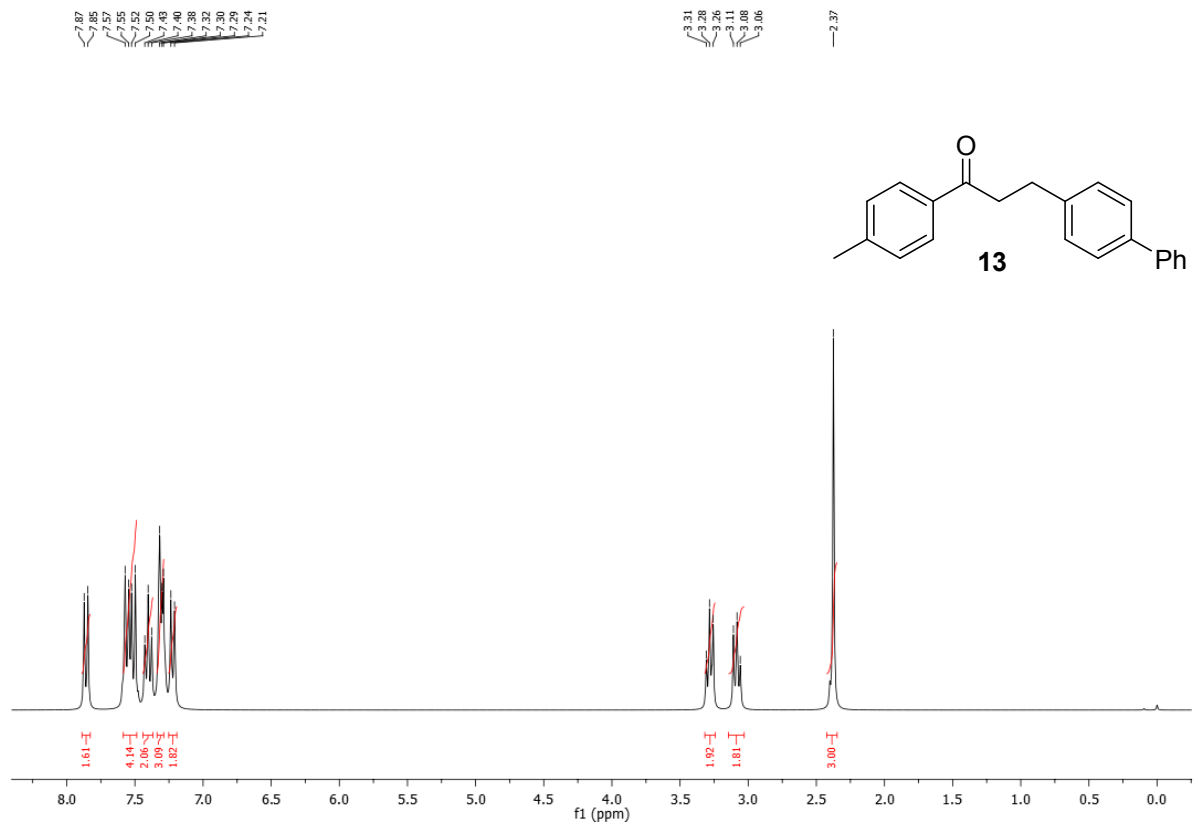
144.86
144.13
134.82
134.08
129.37
128.14
127.08
126.34
39.45
29.42
21.69
O
Cl
Cl
12
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)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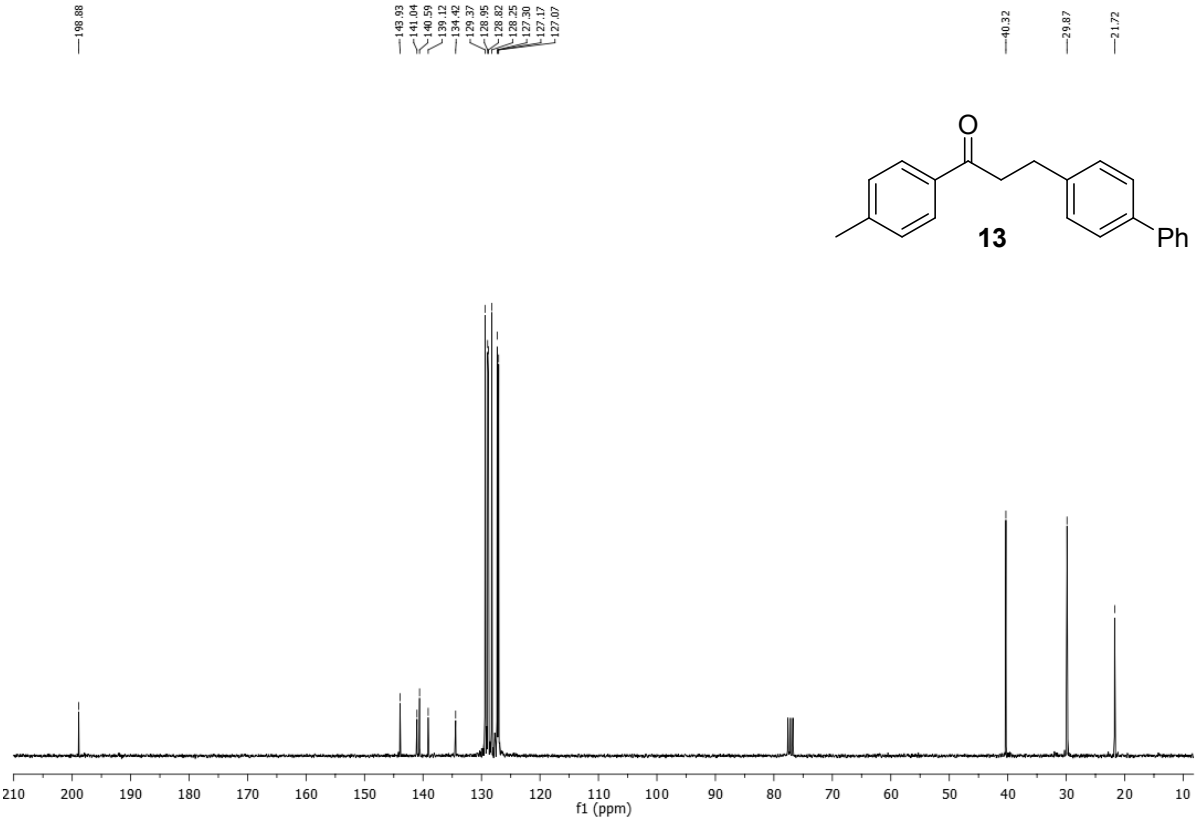
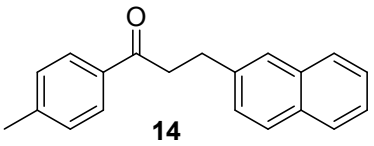
7.50
7.43
7.40
7.38
7.32
7.30
7.29
7.24
7.21
3.31
3.28
3.26
3.11
3.08
3.06
2.37
O
13
Ph
1.61
4.14
2.06
3.09
1.82
1.92
1.81
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


198.88
143.93
141.04
140.59
139.12
134.42
129.37
128.95
128.82
128.25
127.30
127.17
127.07
40.32
29.87
21.72
O
13
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

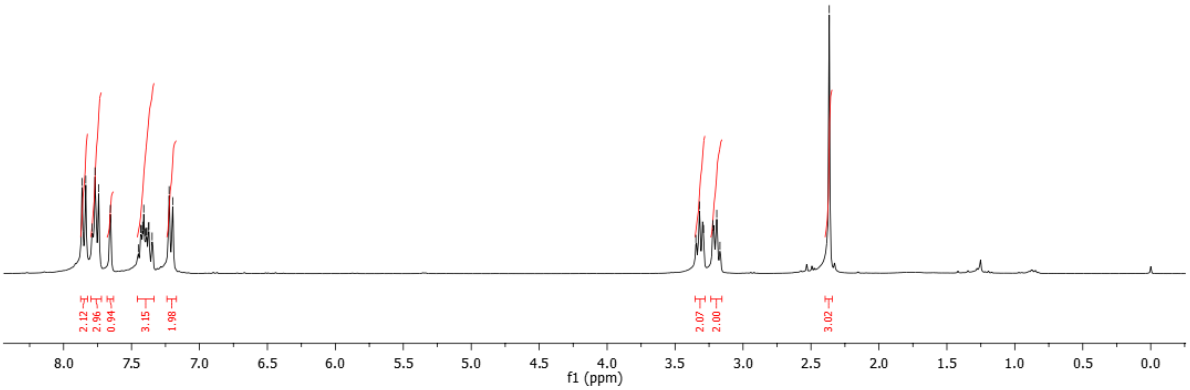

7.86
7.84
7.79
7.77
7.74
7.66
7.45
7.43
7.43
7.42
7.41
7.40
7.39
7.39
7.38
7.37
7.35
7.22
7.20


3.35
3.32
3.29
3.22
3.19
3.17

2.37


O

14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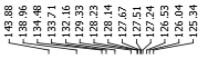
2.96
0.94
3.15
1.98
2.07
2.00
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

198.86


143.88
138.96
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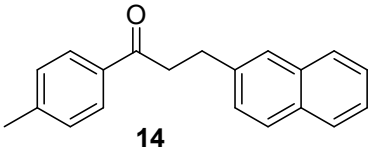
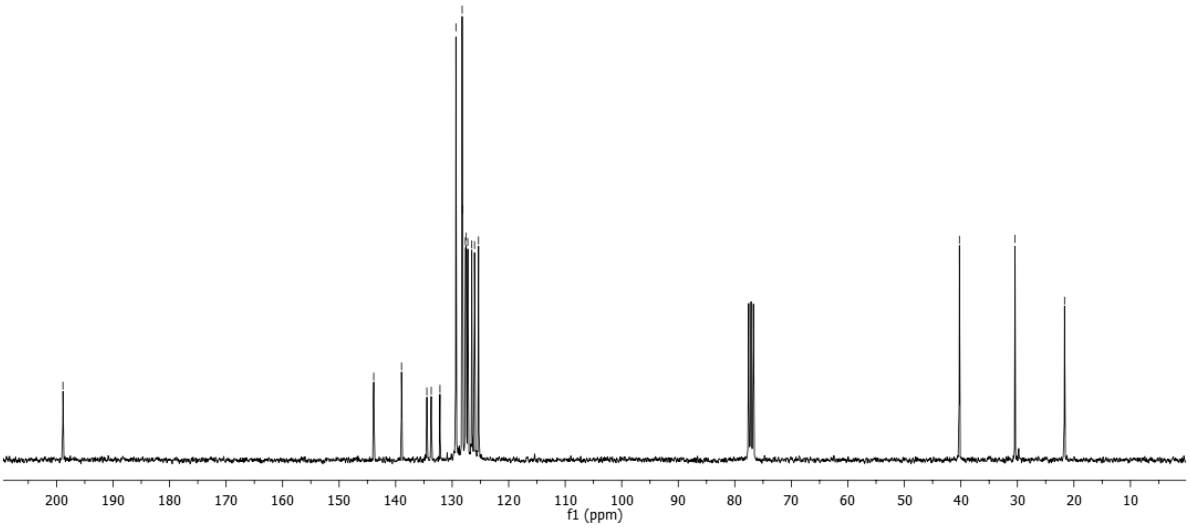
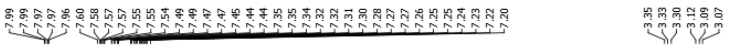
133.71
132.16
129.33
128.23
128.14
127.67
127.51
127.24
126.53
126.04
125.34

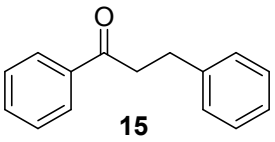

40.26
30.42
21.66


O

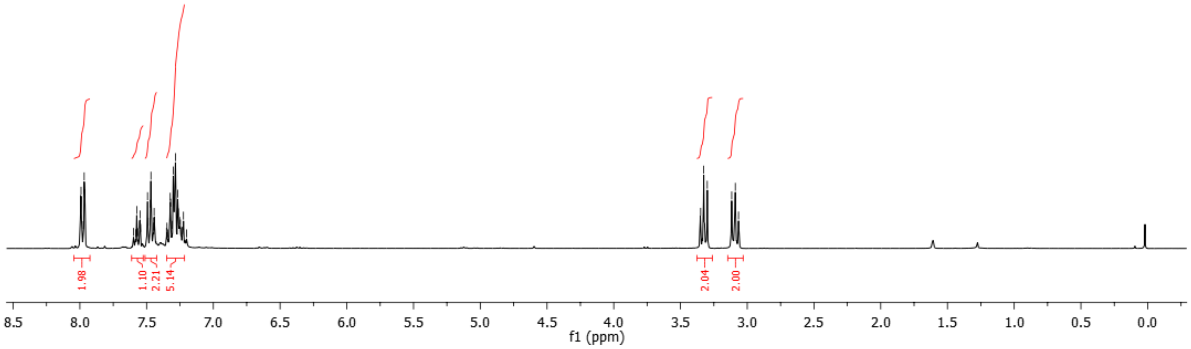
14


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.99
7.99
7.97
7.97
7.96
7.60
7.58
7.57
7.57
7.55
7.55
7.54
7.49
7.49
7.47
7.47
7.45
7.44
7.44
7.35
7.35
7.34
7.32
7.32
7.31
7.30
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.23
7.22
7.20
3.35
3.33
3.30
3.12
3.09
3.07


O

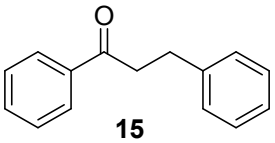
15


1.98
1.10
2.21
5.14
2.04
2.00
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)

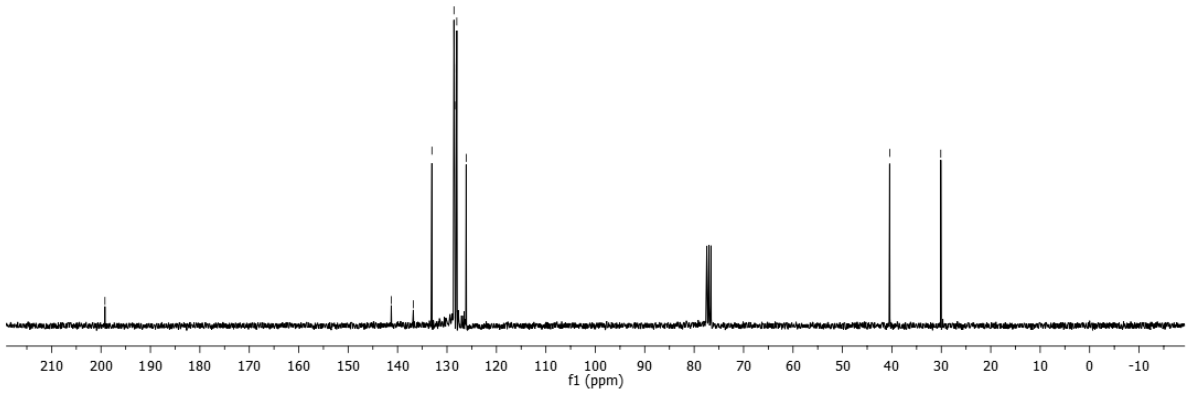

199.21

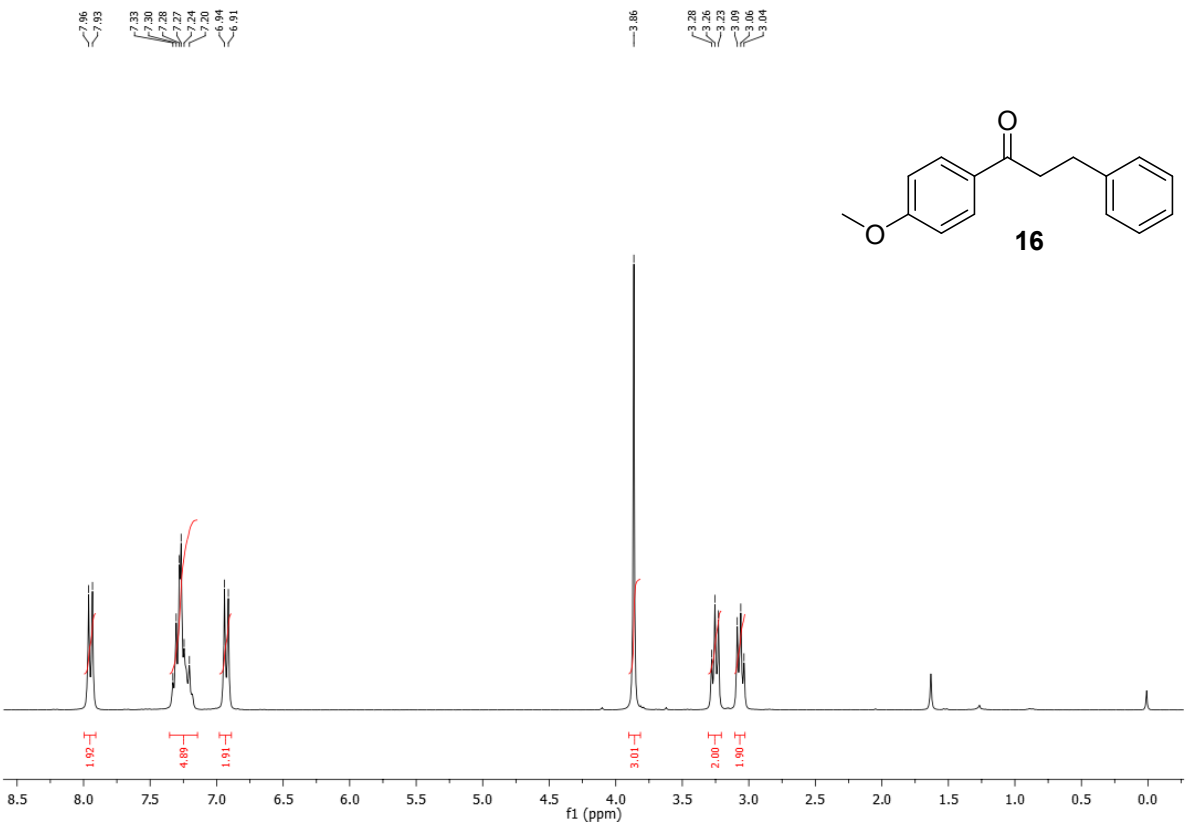
141.27
136.82
133.05
128.59
128.52
128.41
128.02
126.12

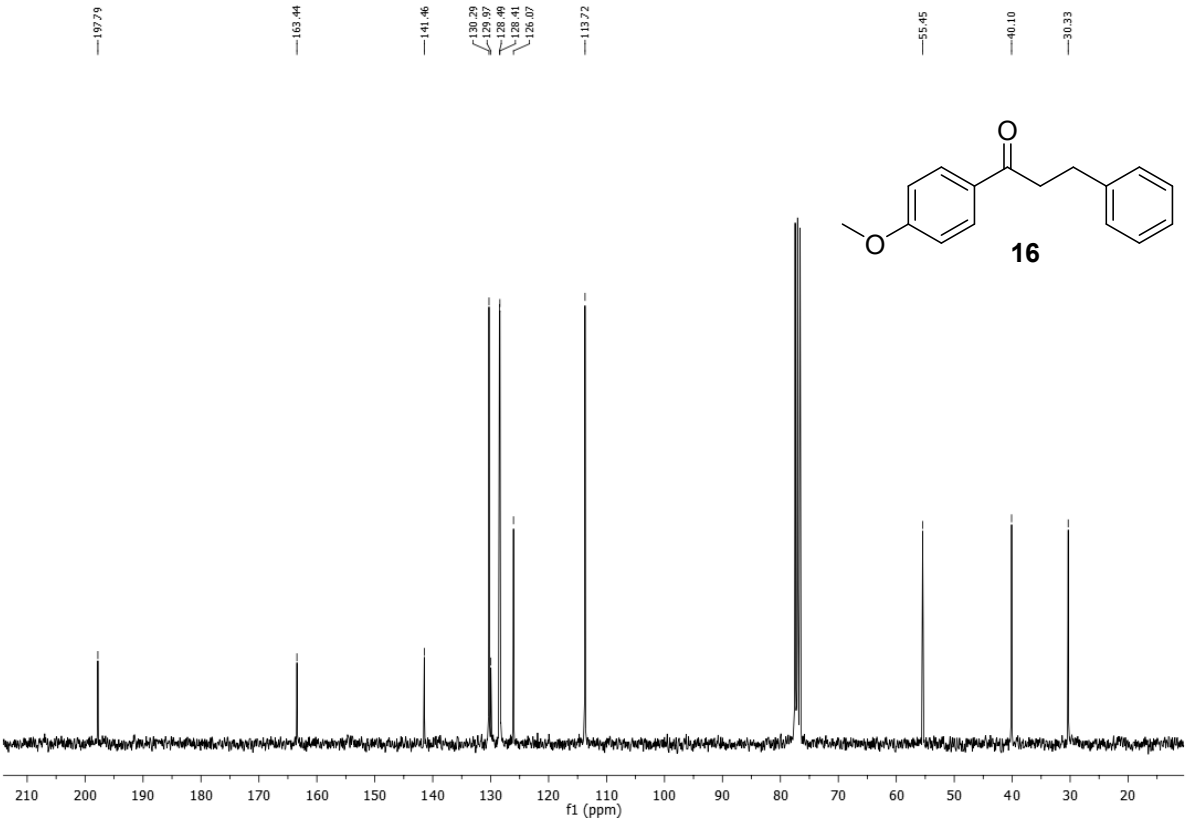

40.45
30.11


O

15

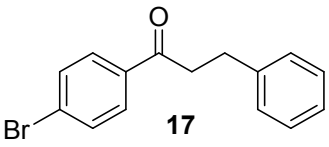

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.96
7.93
7.33
7.30
7.28
7.27
7.24
7.20
6.94
6.91
3.86
3.28
3.26
3.23
3.09
3.06
3.04
O
O
16
1.92
4.89
1.91
3.01
2.00
1.90
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)

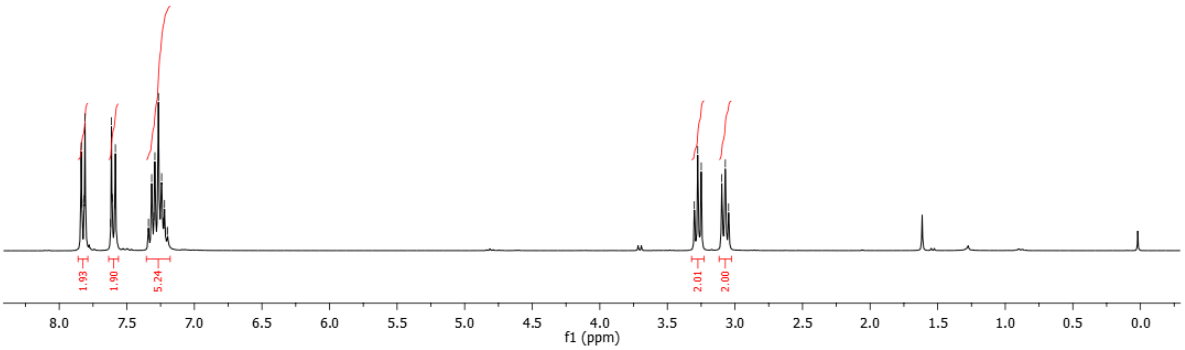

197.79
163.44
141.46
130.29
129.97
128.49
128.41
126.07
113.72
55.45
40.10
30.33
O
O
16
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


7.84
7.83
7.81
7.81
7.62
7.61
7.61
7.59
7.58
7.34
7.34
7.32
7.31
7.30
7.29
7.27
7.24
7.23
7.22
7.21
7.20


3.30
3.28
3.25
3.10
3.07
3.05

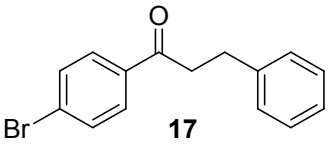

O
Br

17

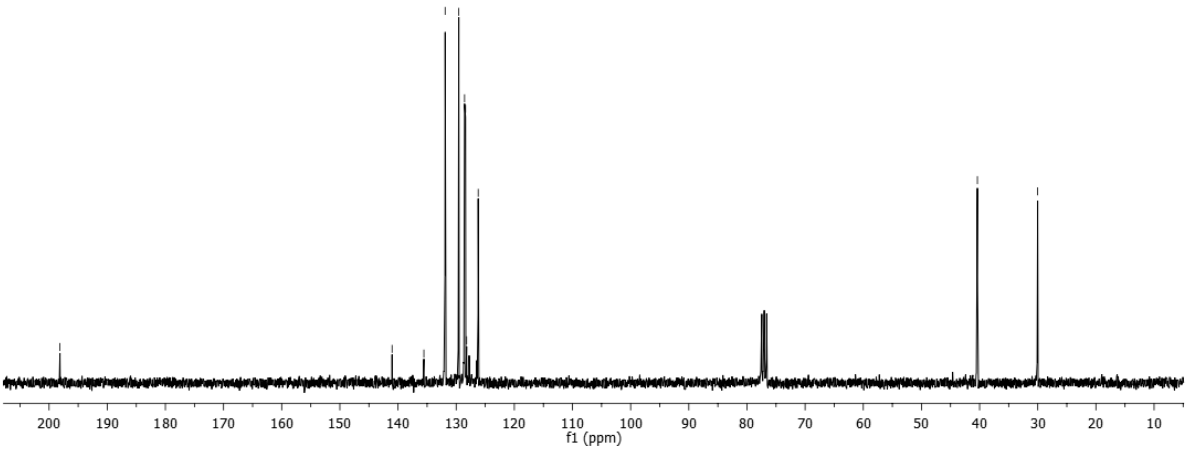

1.93
1.90
5.24
2.01
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

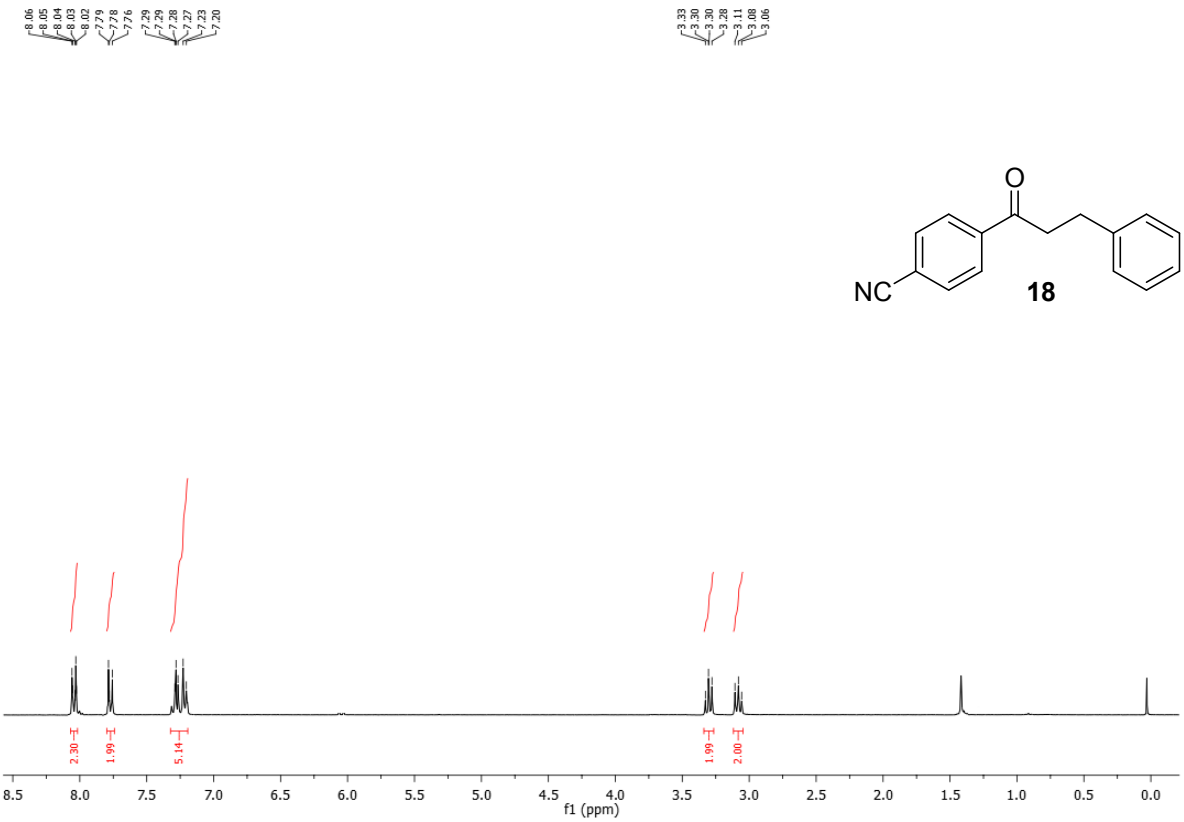

198.13
141.02
135.55
131.90
129.55
128.55
128.39
128.20
126.21

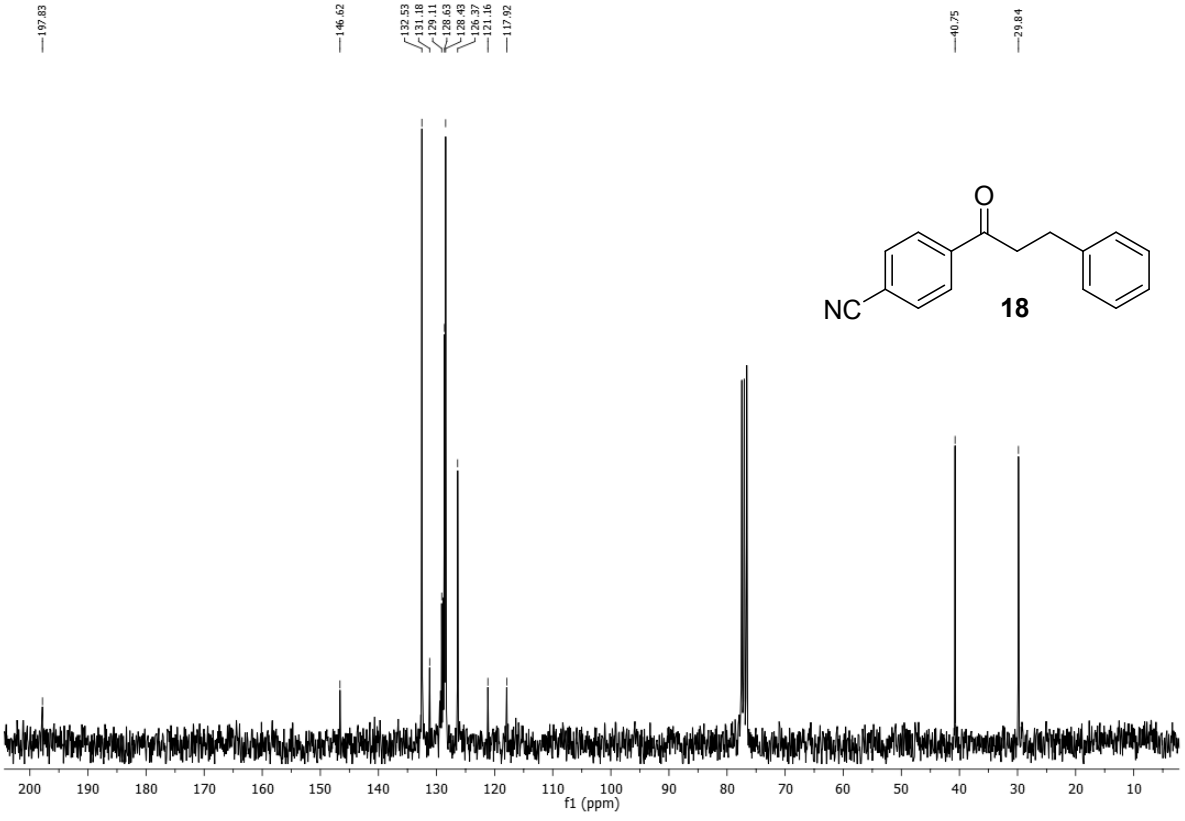

40.38
30.01

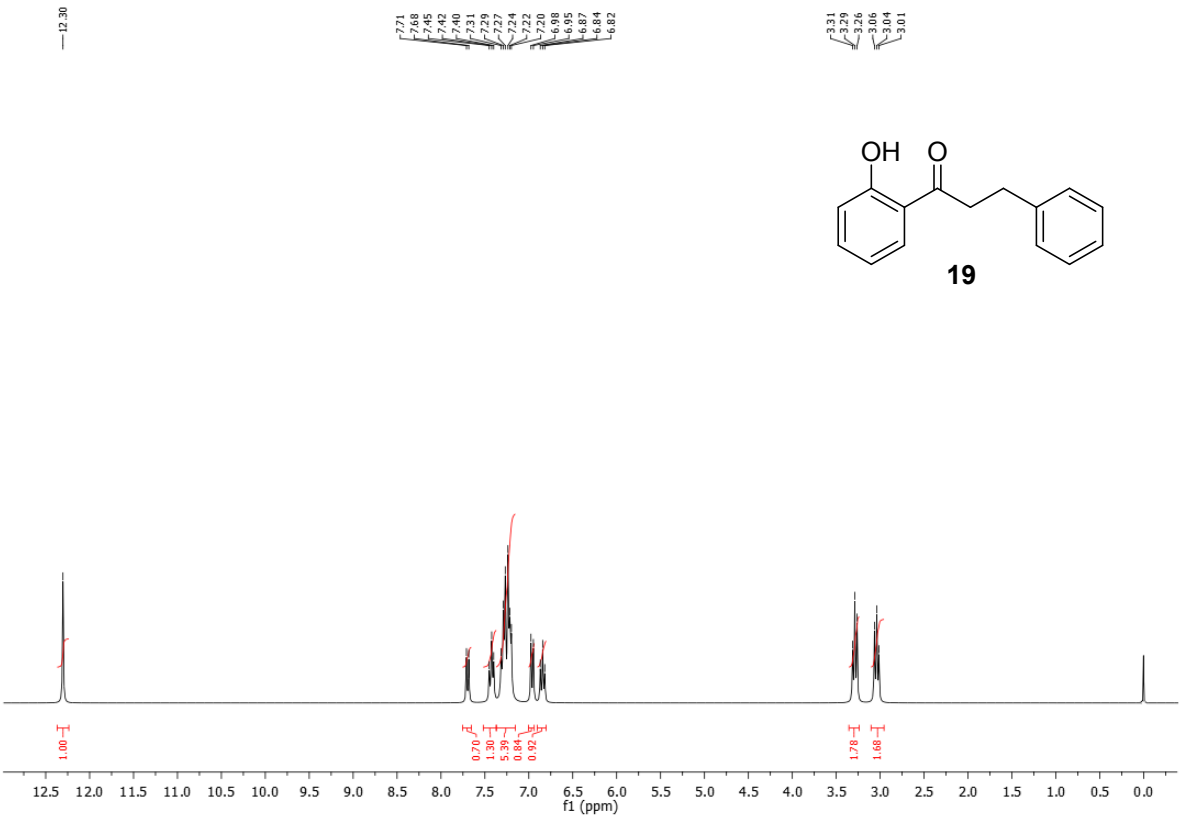

O
Br

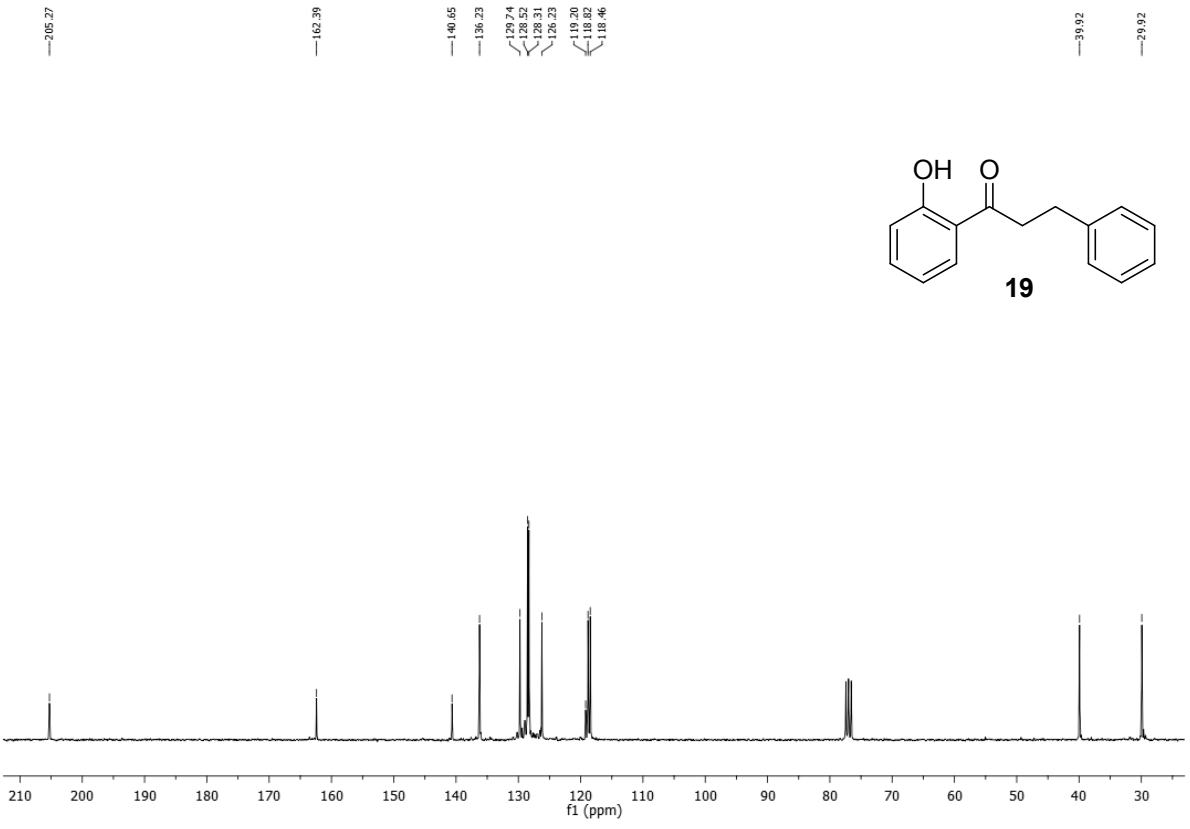
17


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

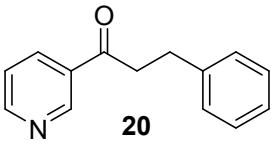

8.06
8.05
8.04
8.03
8.02
7.79
7.78
7.76
7.29
7.29
7.28
7.27
7.23
7.20
3.33
3.30
3.30
3.28
3.11
3.08
3.06
O
NC
18
2.30
1.99
5.14
1.99
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


197.83
146.62
132.53
131.18
129.11
128.63
128.43
126.37
121.16
117.92
40.75
29.84
O
NC
18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

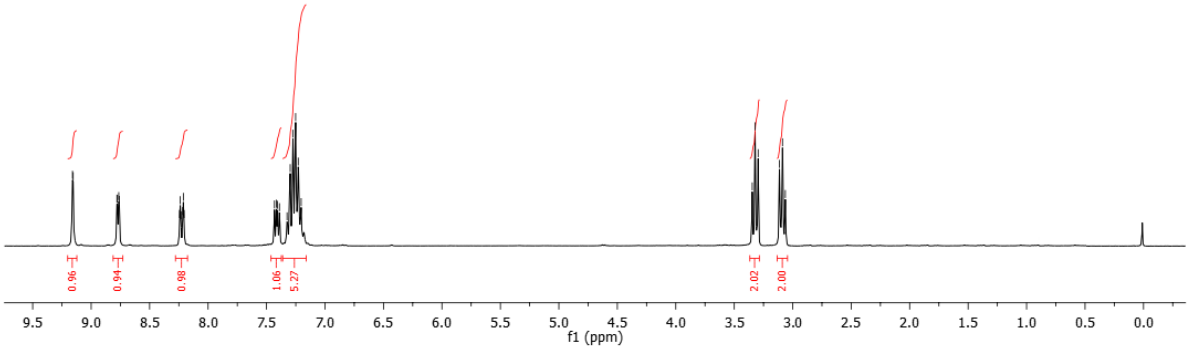

12.30
7.71
7.68
7.45
7.42
7.40
7.31
7.29
7.27
7.24
7.22
7.20
6.98
6.95
6.87
6.84
6.82
3.31
3.29
3.26
3.06
3.04
3.01
OH
O
19
1.00
0.70
1.30
5.39
0.84
0.92
1.78
1.68
f1 (ppm)

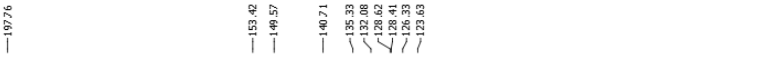

205.27
162.39
140.65
136.23
129.74
129.52
128.31
126.23
119.20
118.82
118.46
39.92
29.92
OH
O
19
f1 (ppm)

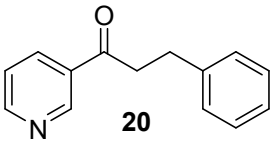

9.16
9.15
8.78
8.77
8.76
8.76
8.24
8.24
8.22
8.21
8.21
7.42
7.41
7.39
7.32
7.30
7.27
7.25
7.23
7.20
3.35
3.32
3.30
3.11
3.09
3.06


O
N

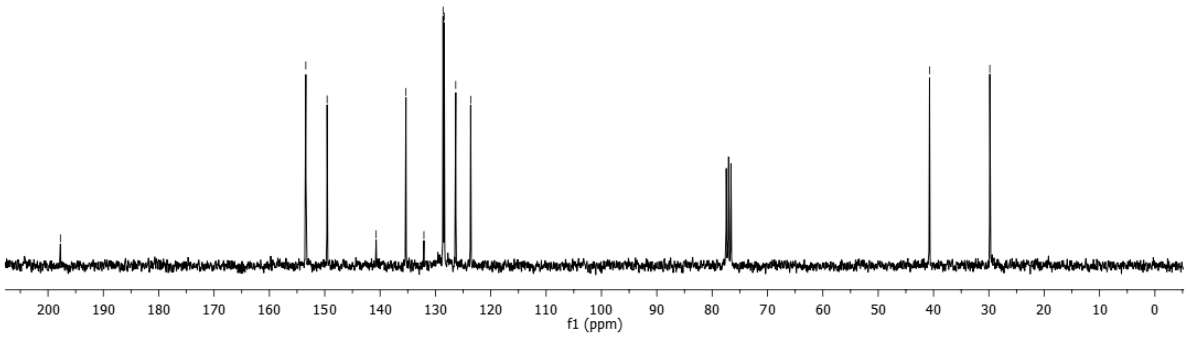
20

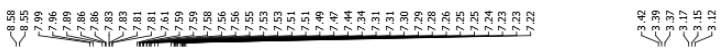

0.96
0.94
0.98
1.06
5.27
2.02
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

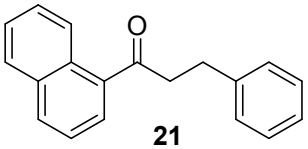

197.76
153.42
149.57
140.71
135.33
132.08
128.62
128.41
126.33
123.63
40.72
29.83


O
N

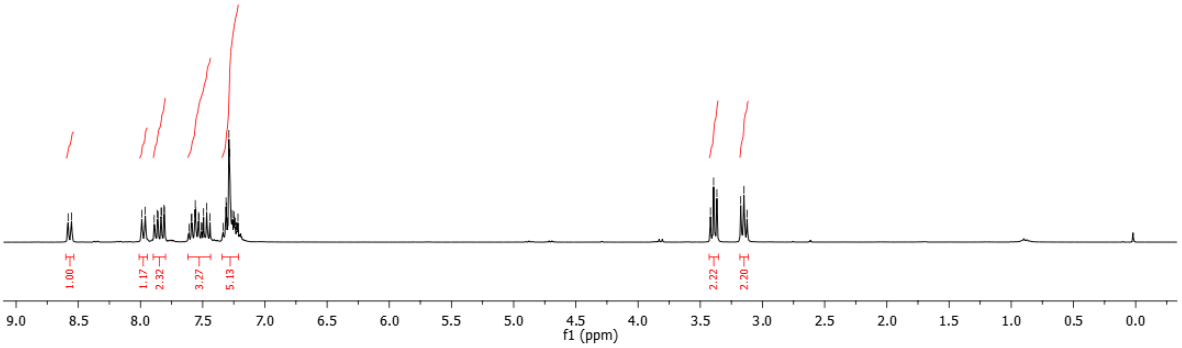
20


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

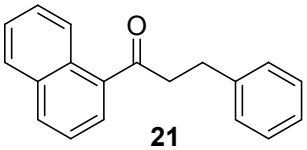

8.58
8.55
7.99
7.96
7.89
7.86
7.86
7.83
7.81
7.81
7.61
7.59
7.59
7.58
7.56
7.56
7.55
7.53
7.53
7.51
7.51
7.49
7.47
7.44
7.34
7.31
7.31
7.30
7.29
7.28
7.26
7.25
7.25
7.24
7.23
7.23
7.22
3.42
3.39
3.37
3.17
3.15
3.12


O

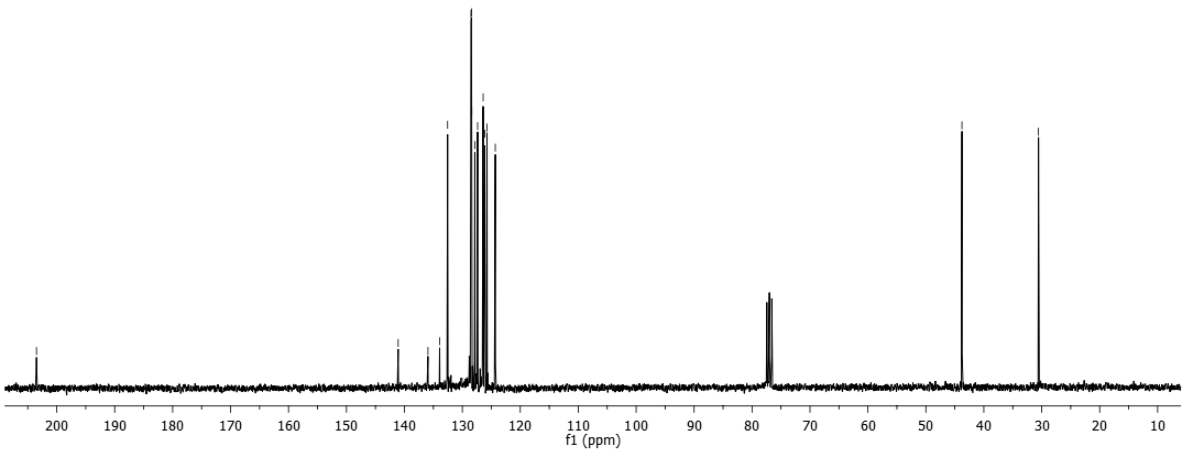
21

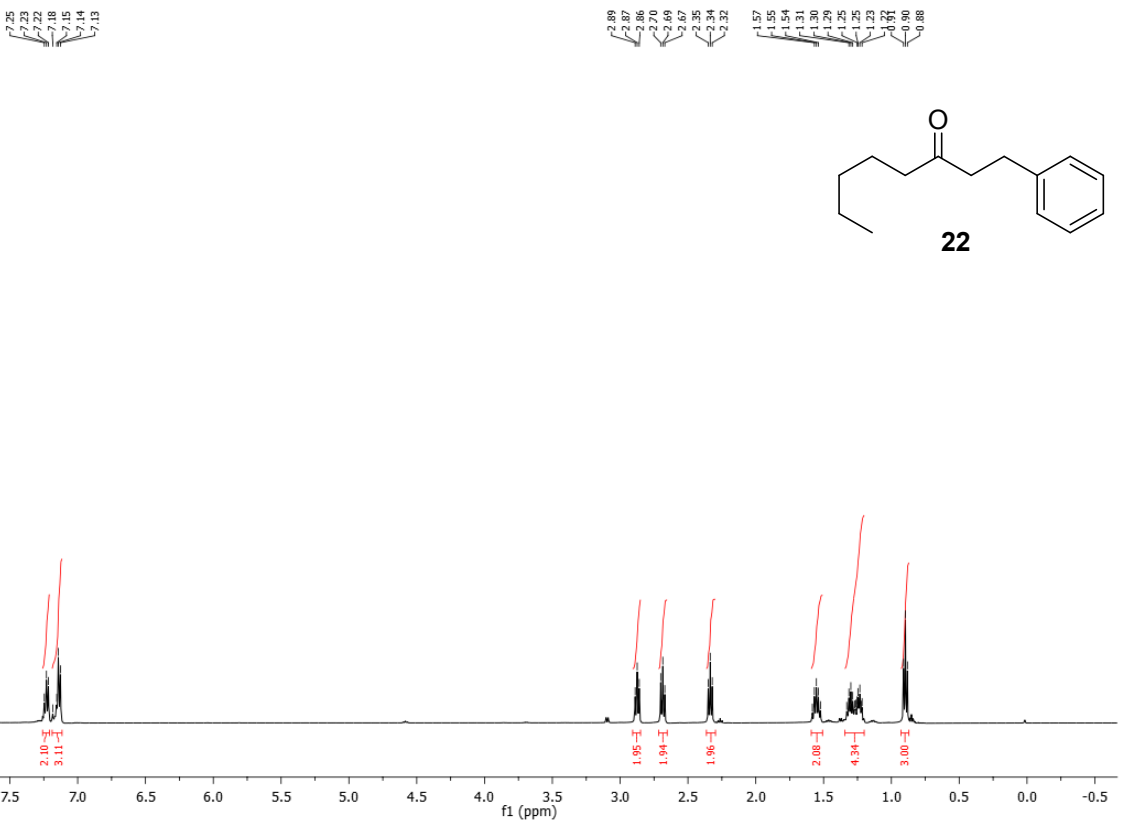

1.00
1.17
2.32
3.27
5.13
2.22
2.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

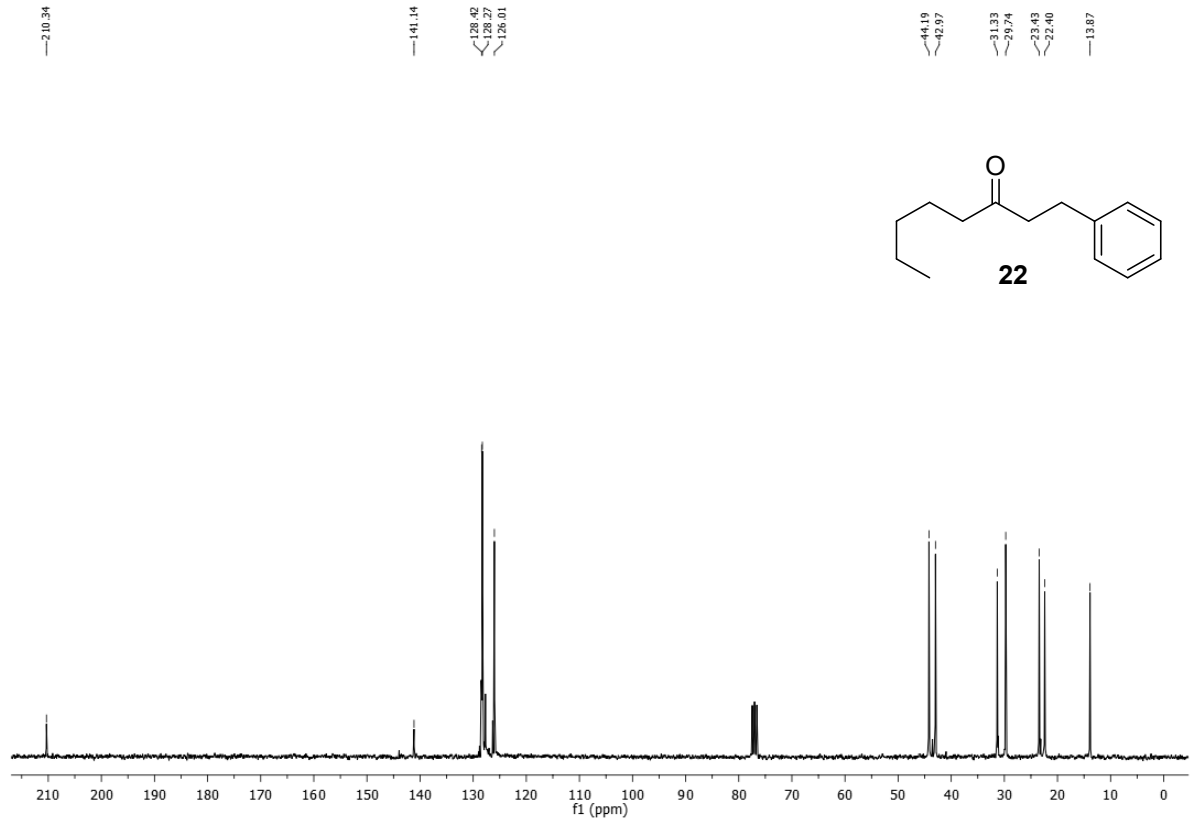

203.50
141.08
135.93
133.92
132.54
128.51
128.43
128.37
127.84
127.36
126.41
126.13
125.74
124.31
43.78
30.56

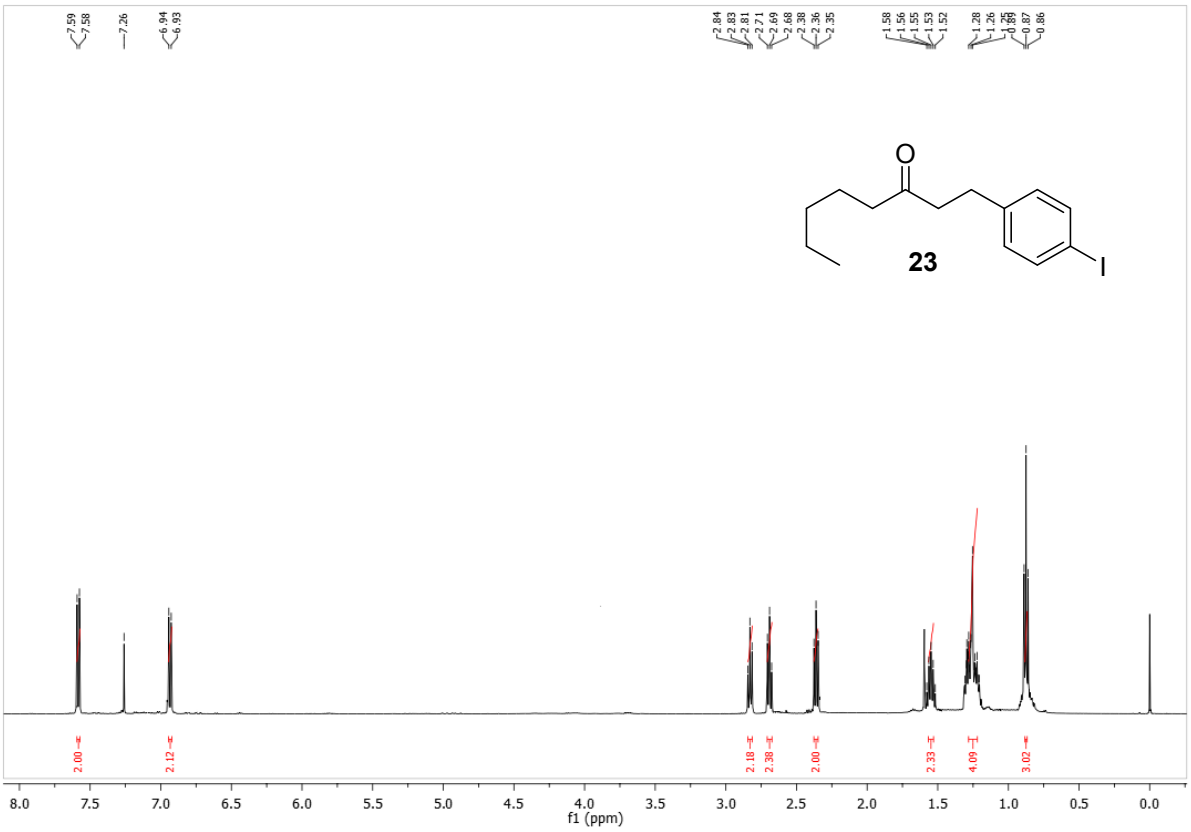

O

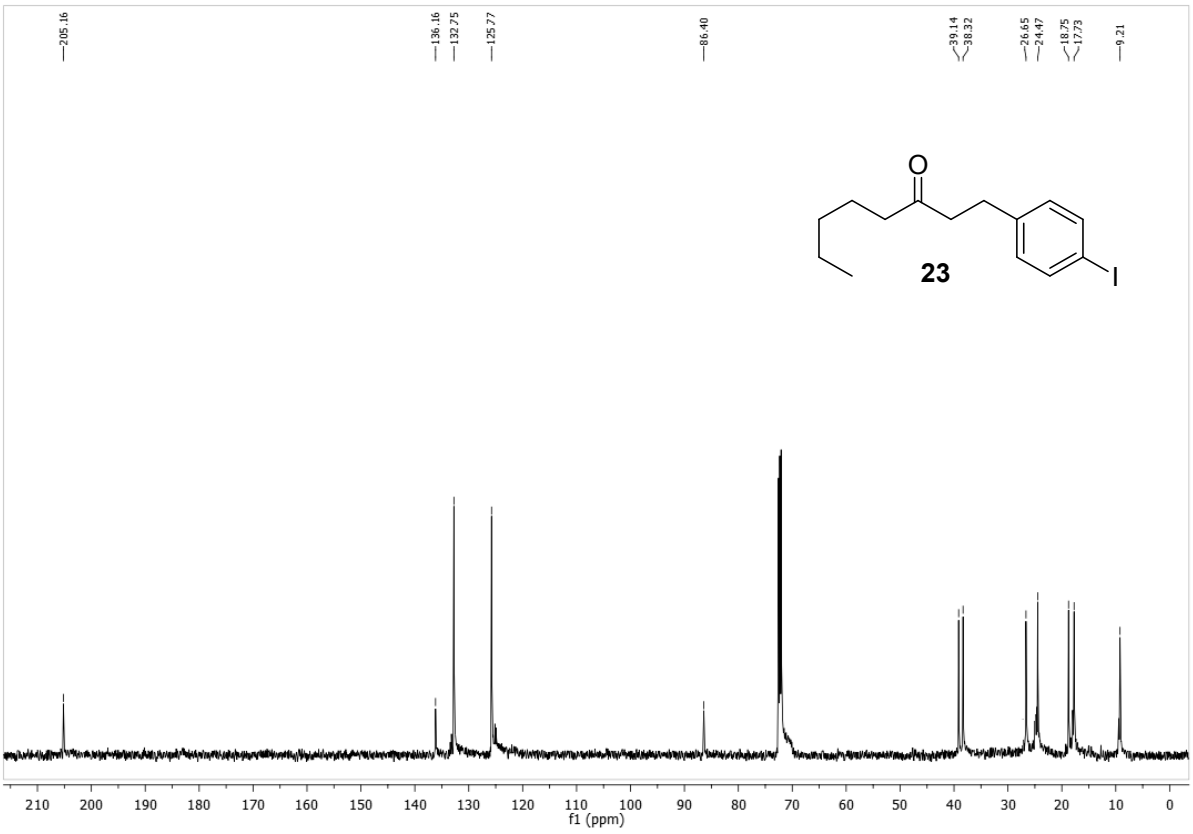
21

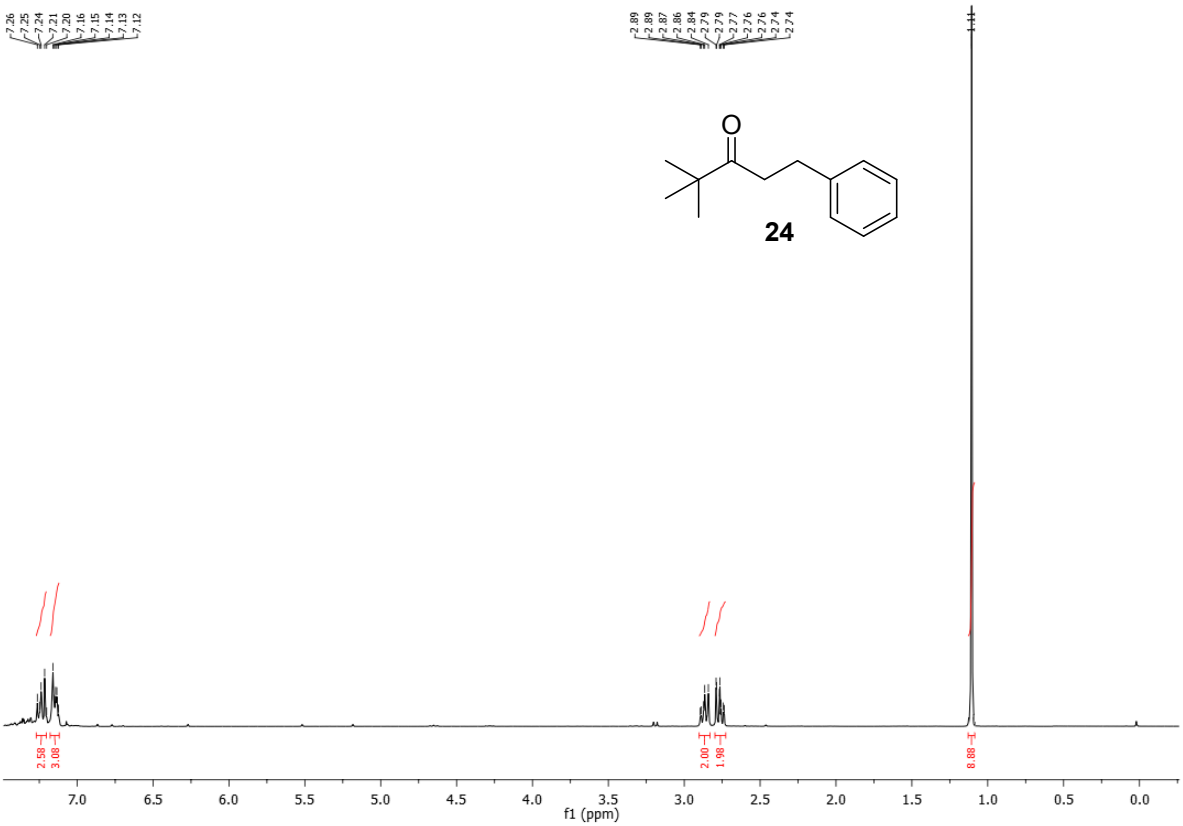

200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

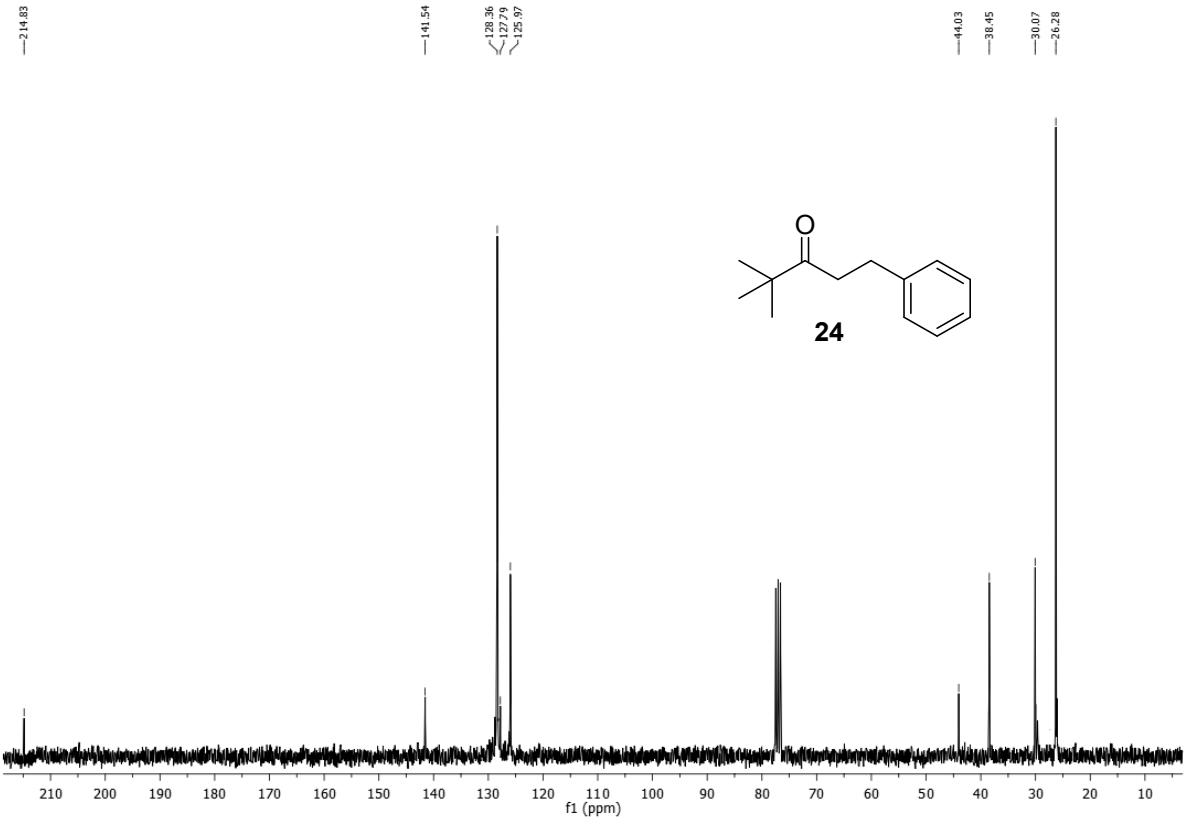

7.25
7.23
7.22
7.18
7.15
7.14
7.13
2.89
2.87
2.86
2.70
2.69
2.67
2.35
2.34
2.32
1.57
1.55
1.54
1.31
1.30
1.29
1.25
1.23
0.92
0.91
0.90
0.88
O
22
2.10
3.11
1.95
1.94
1.96
2.08
4.34
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

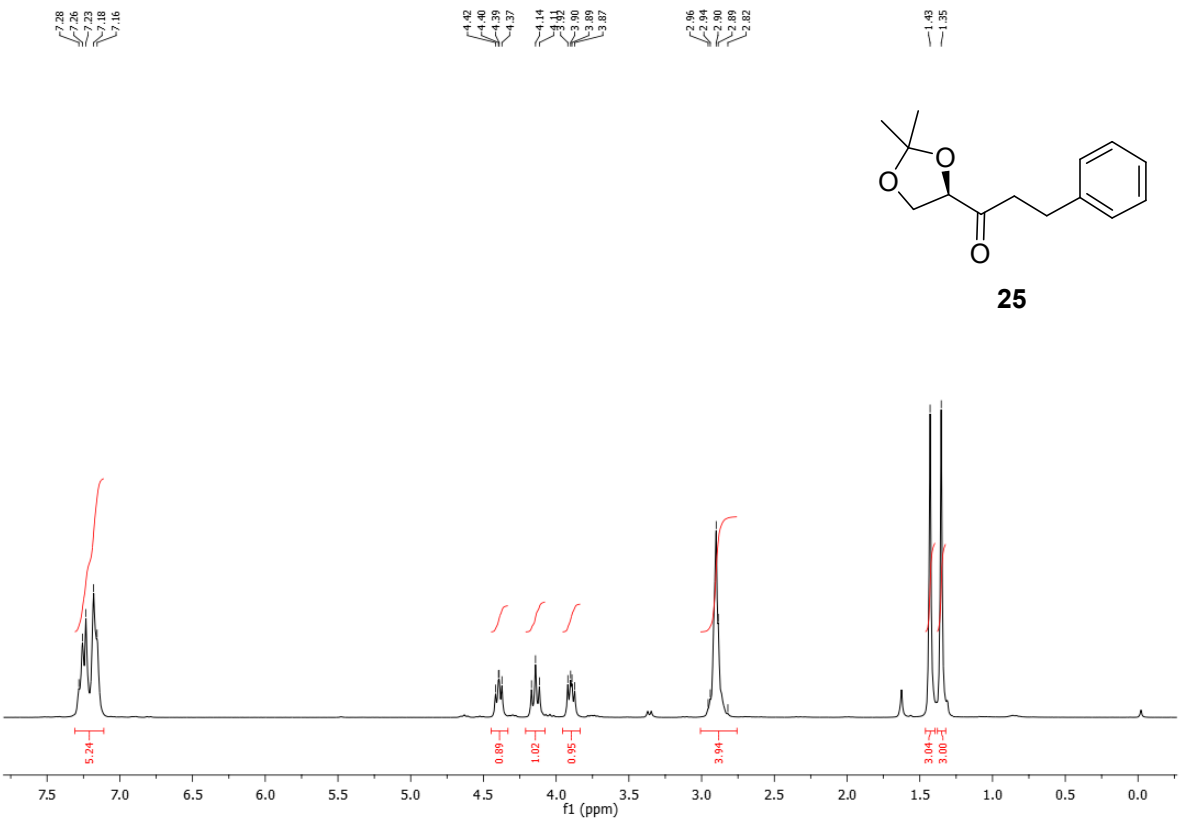

210.34
141.14
128.42
128.27
126.01
44.19
42.97
31.33
29.74
23.43
22.40
13.87
O
22
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.59
7.58
7.26
6.94
6.93
2.84
2.83
2.81
2.71
2.69
2.68
2.38
2.36
2.35
1.58
1.56
1.55
1.53
1.52
1.28
1.26
0.87
0.86
O
I
23
2.00
2.12
2.18
2.38
2.00
2.33
4.09
3.02
f1 (ppm)

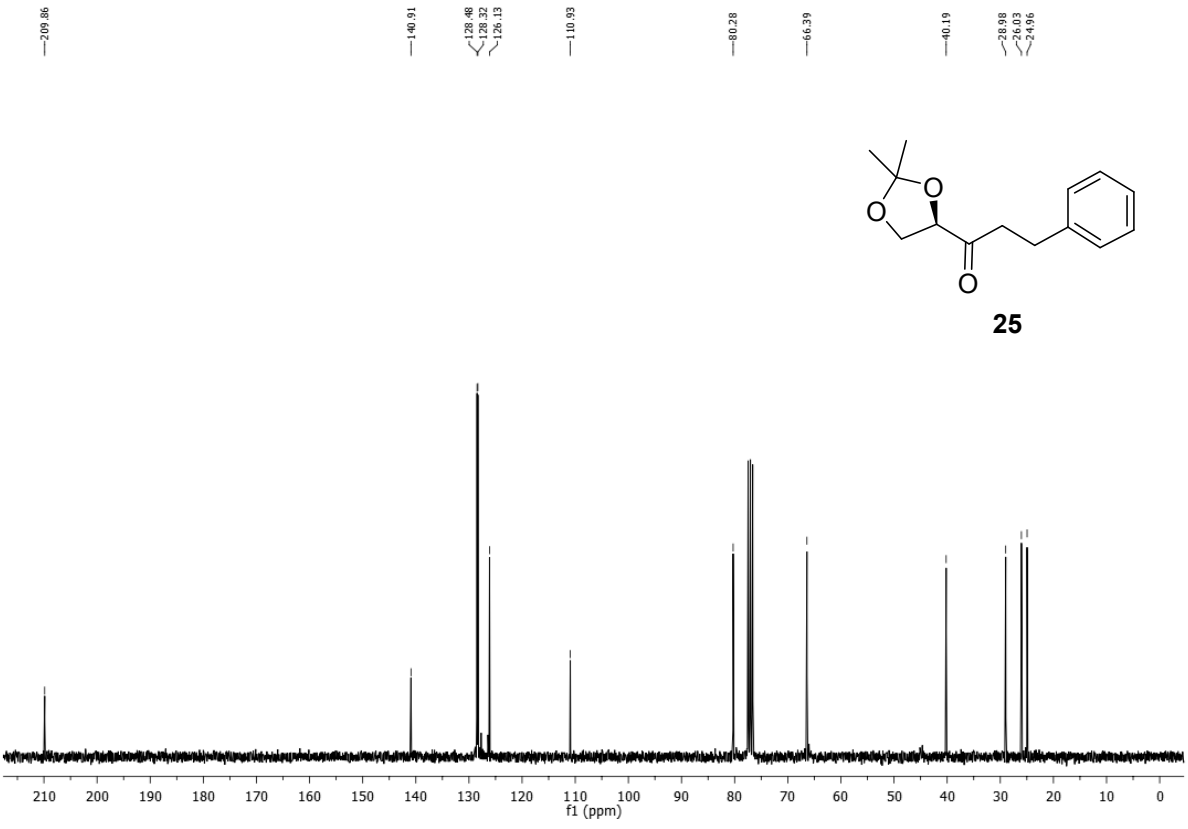

205.16
136.16
132.75
125.77
86.40
39.14
38.32
26.65
24.47
18.75
17.73
9.21
O
I
23
f1 (ppm)


7.26
7.25
7.24
7.21
7.20
7.16
7.15
7.14
7.13
7.12
2.89
2.89
2.87
2.86
2.84
2.79
2.79
2.77
2.76
2.76
2.74
2.74
1.11
O
24
2.58
3.08
2.00
1.98
8.88
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)

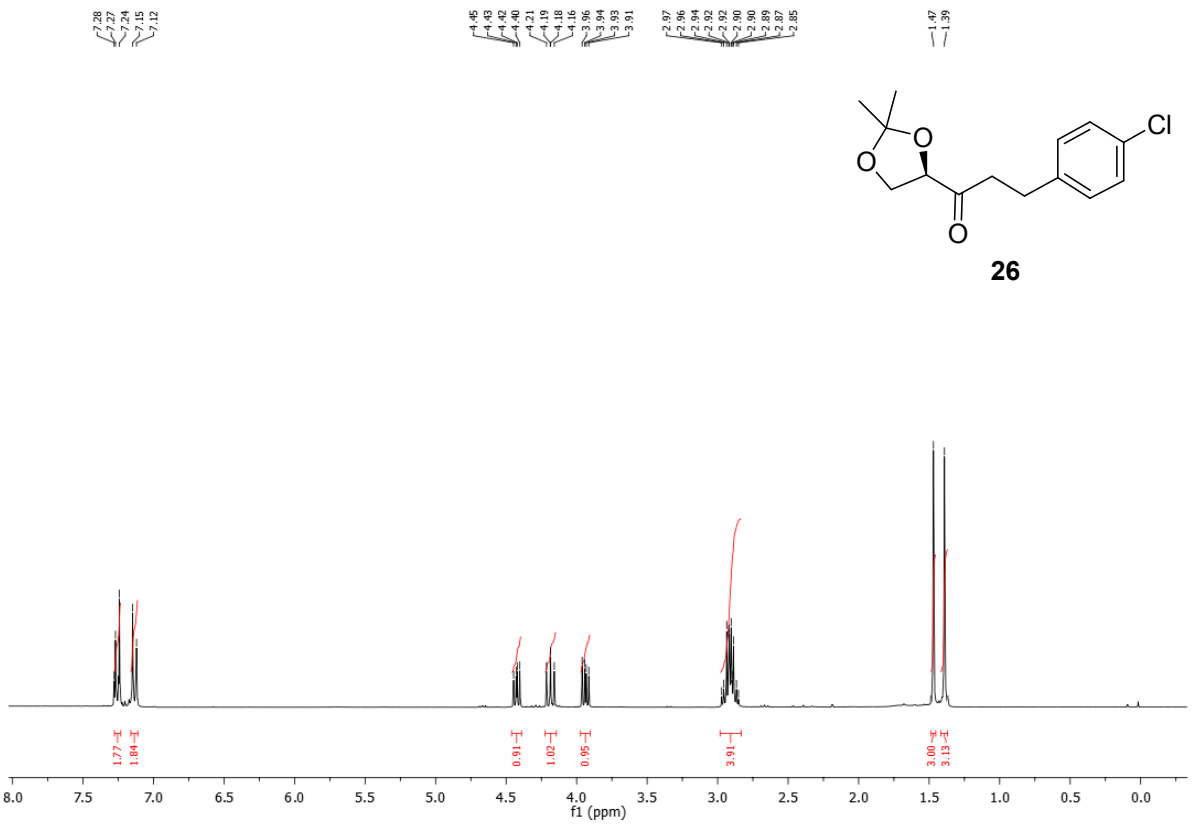

214.83
141.54
128.36
127.79
125.97
44.03
38.45
30.07
26.28
O
24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.28
7.26
7.23
7.18
7.16
4.42
4.40
4.39
4.37
4.14
4.11
3.92
3.90
3.89
3.87
2.96
2.94
2.90
2.89
2.82
1.43
1.35
O
O
O
5.24
0.89
1.02
0.95
3.94
3.04
3.00
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)

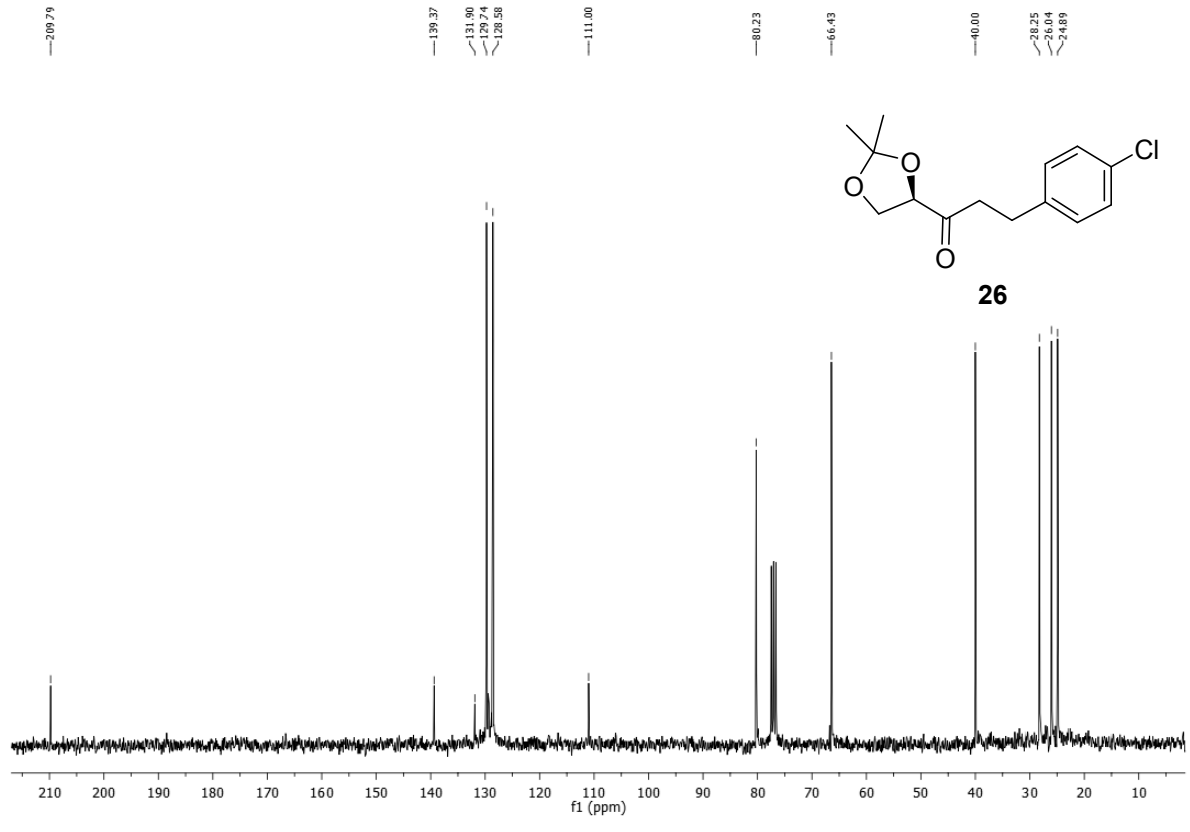
25


209.86
140.91
128.48
128.32
126.13
110.93
80.28
66.39
40.19
28.98
26.03
24.96
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

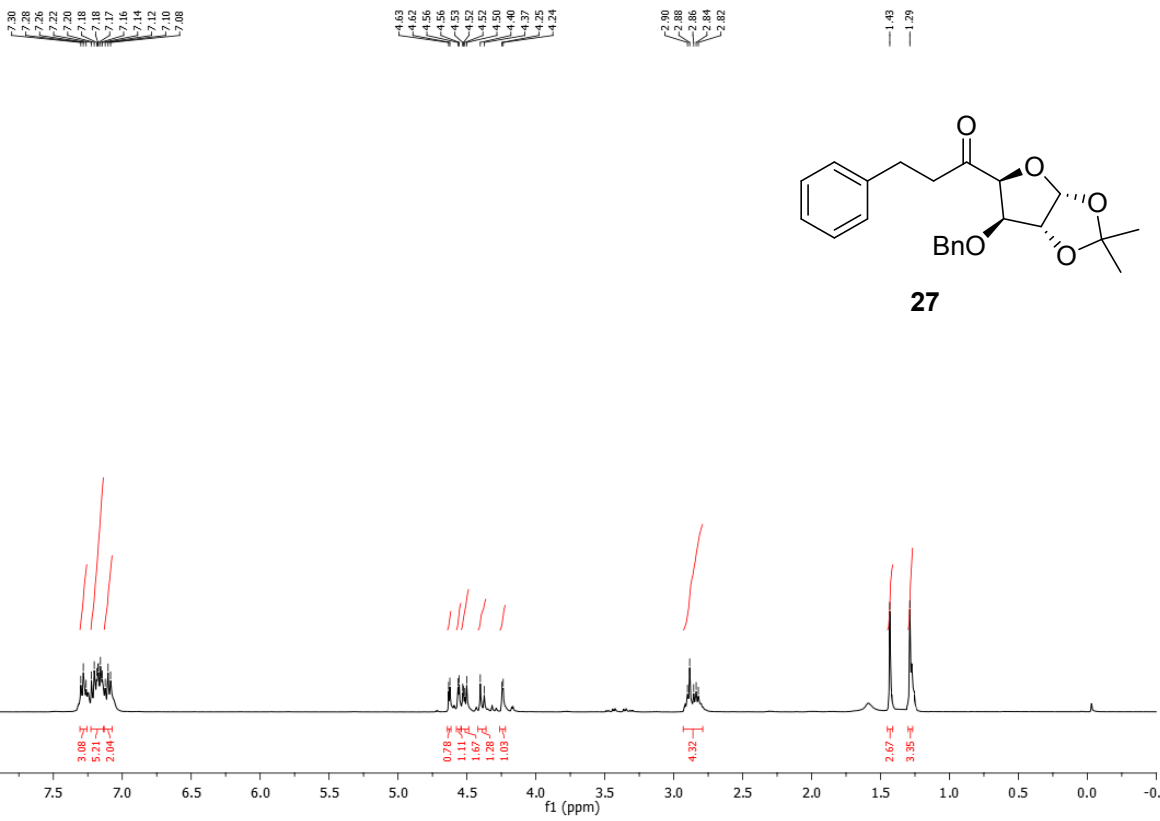
25


7.28
7.27
7.24
7.15
7.12
4.45
4.43
4.42
4.40
4.21
4.19
4.18
4.16
3.96
3.94
3.93
3.91
2.97
2.96
2.94
2.92
2.92
2.90
2.90
2.89
2.87
2.85
1.47
1.39
Cl
O
O
O
1.77
1.84
0.91
1.02
0.95
3.91
3.00
3.13
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)

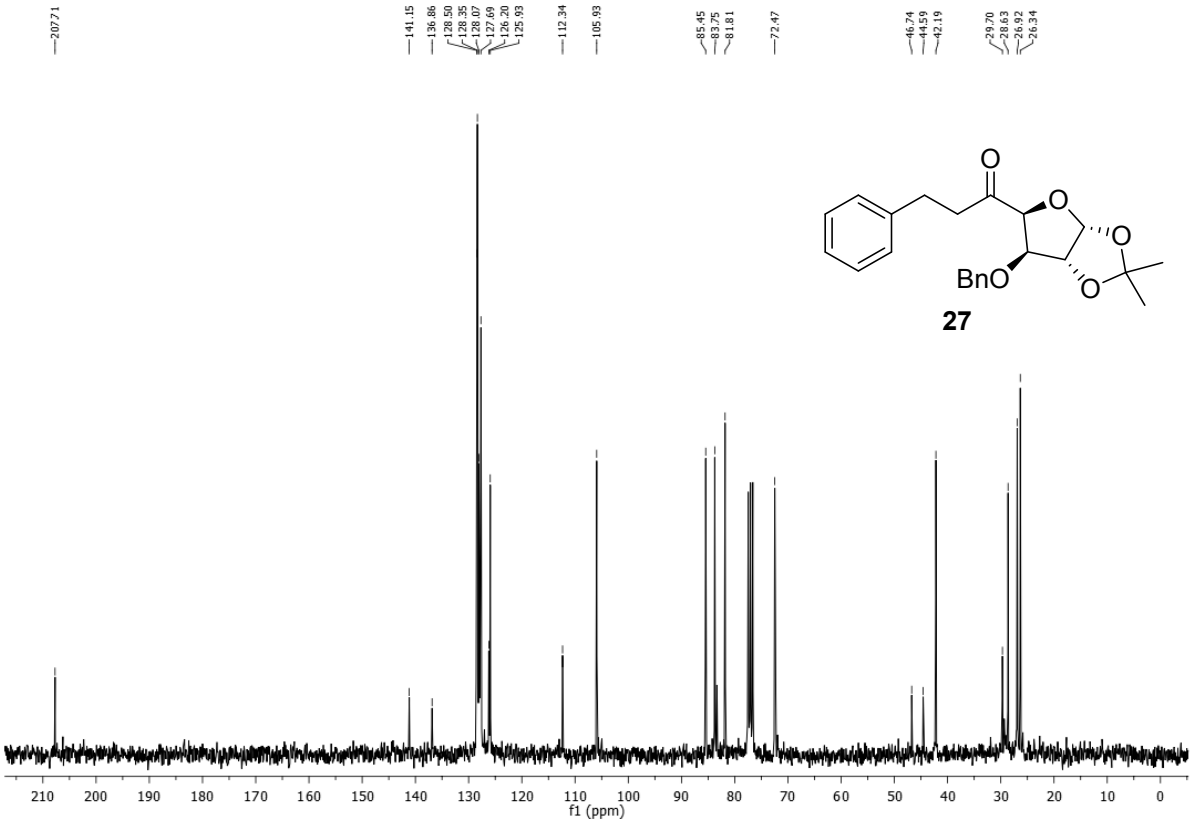
26


209.79
139.37
131.90
129.74
128.58
111.00
80.23
66.43
40.00
28.25
26.04
24.89
Cl
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

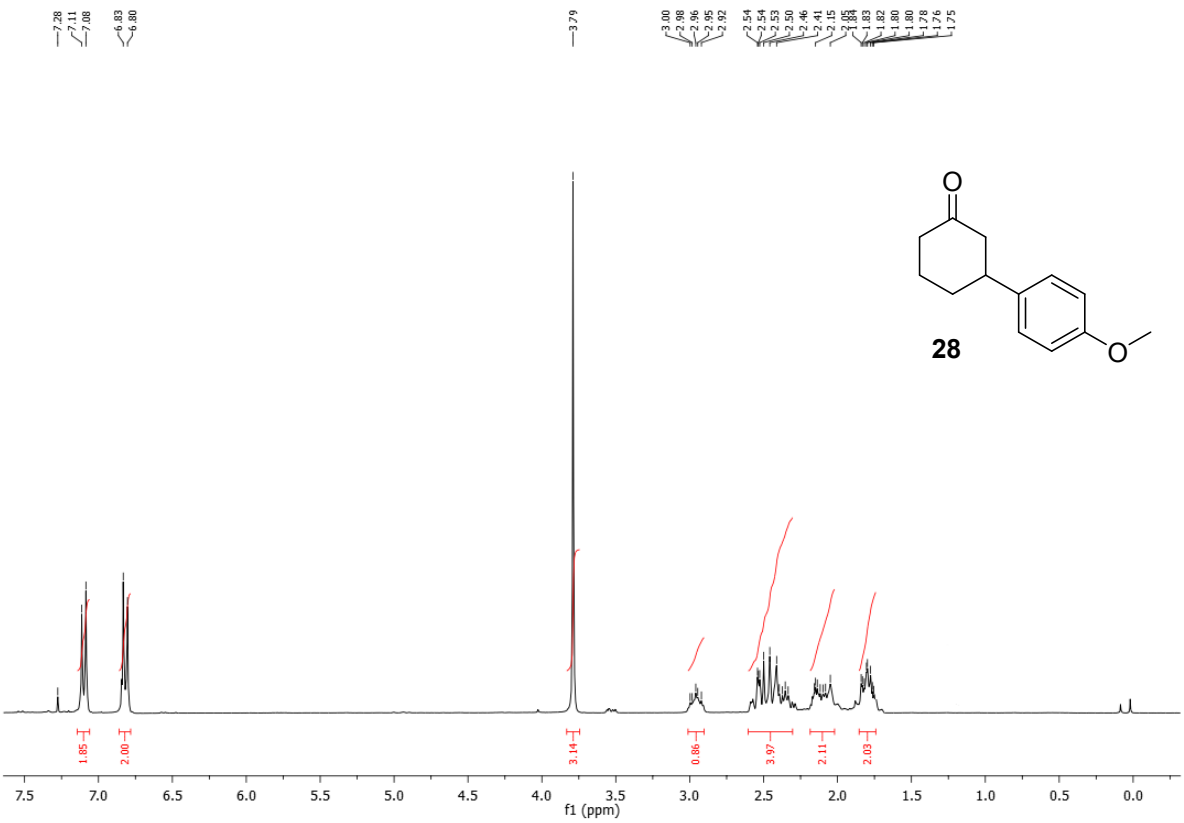
26

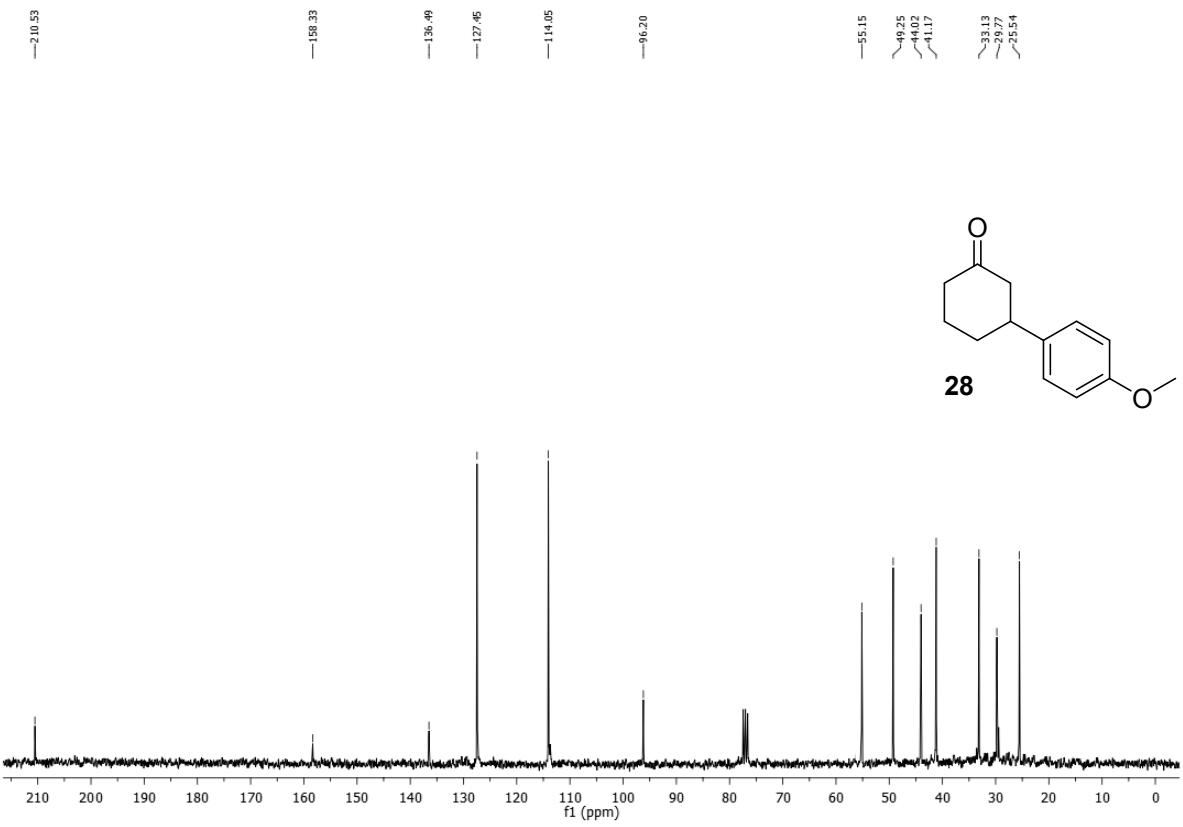

7.30
7.28
7.26
7.22
7.20
7.18
7.17
7.16
7.14
7.12
7.10
7.08
4.63
4.62
4.56
4.56
4.53
4.52
4.52
4.50
4.40
4.37
4.25
4.24
2.90
2.88
2.86
2.84
2.82
1.43
1.29
O
O
O
O
BnO
3.08
5.21
2.04
0.78
1.11
1.67
1.28
1.03
4.32
2.67
3.35
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

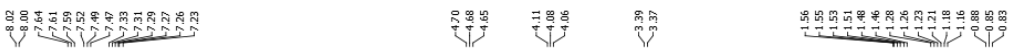
27

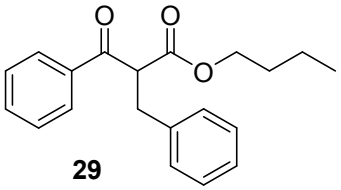

207.71
141.15
136.86
128.50
128.35
128.07
127.69
126.20
125.93
112.34
105.93
85.45
83.75
81.81
72.47
46.74
44.59
42.19
29.70
28.63
26.92
26.34
O
O
O
O
BnO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

27

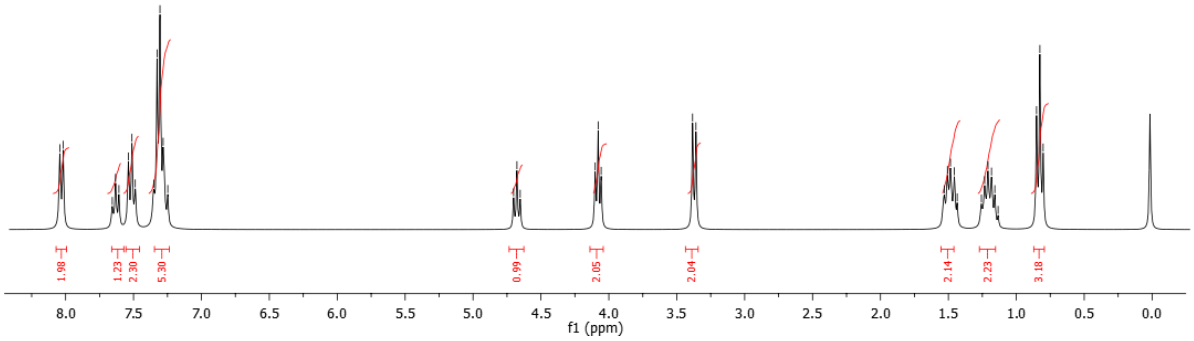

7.28
7.11
7.08
6.83
6.80
3.79
3.00
2.98
2.96
2.95
2.92
2.54
2.54
2.53
2.50
2.46
2.41
2.15
2.05
1.84
1.83
1.82
1.80
1.80
1.78
1.76
1.75
O
O
28
1.85
2.00
3.14
0.86
3.97
2.11
2.03
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


210.53
158.33
136.49
127.45
114.05
96.20
55.15
49.25
44.02
41.17
33.13
29.77
25.54
O
O
28
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

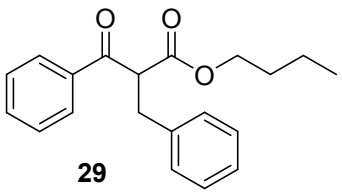

8.02
8.00
7.64
7.61
7.59
7.52
7.49
7.47
7.33
7.31
7.29
7.27
7.26
7.23
4.70
4.68
4.65
4.11
4.08
4.06
3.39
3.37
1.56
1.55
1.53
1.51
1.48
1.46
1.28
1.26
1.23
1.21
1.18
1.16
0.88
0.85
0.83


O
O
O

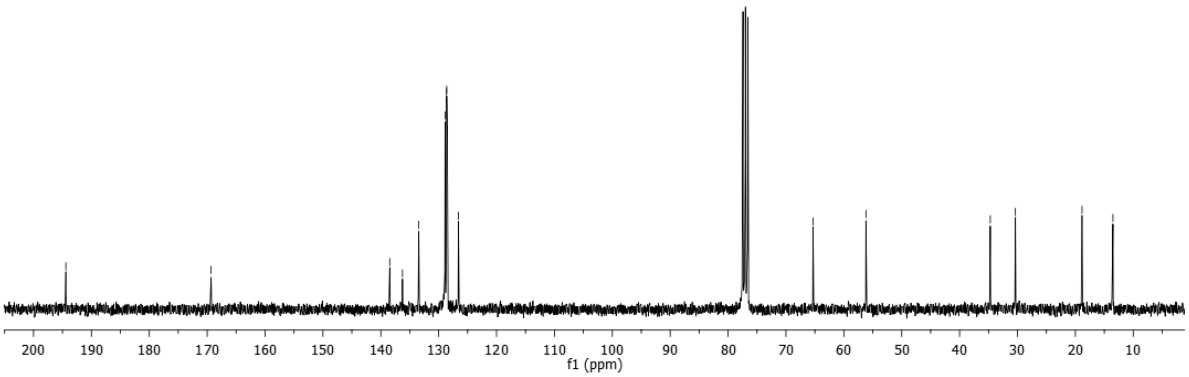
29

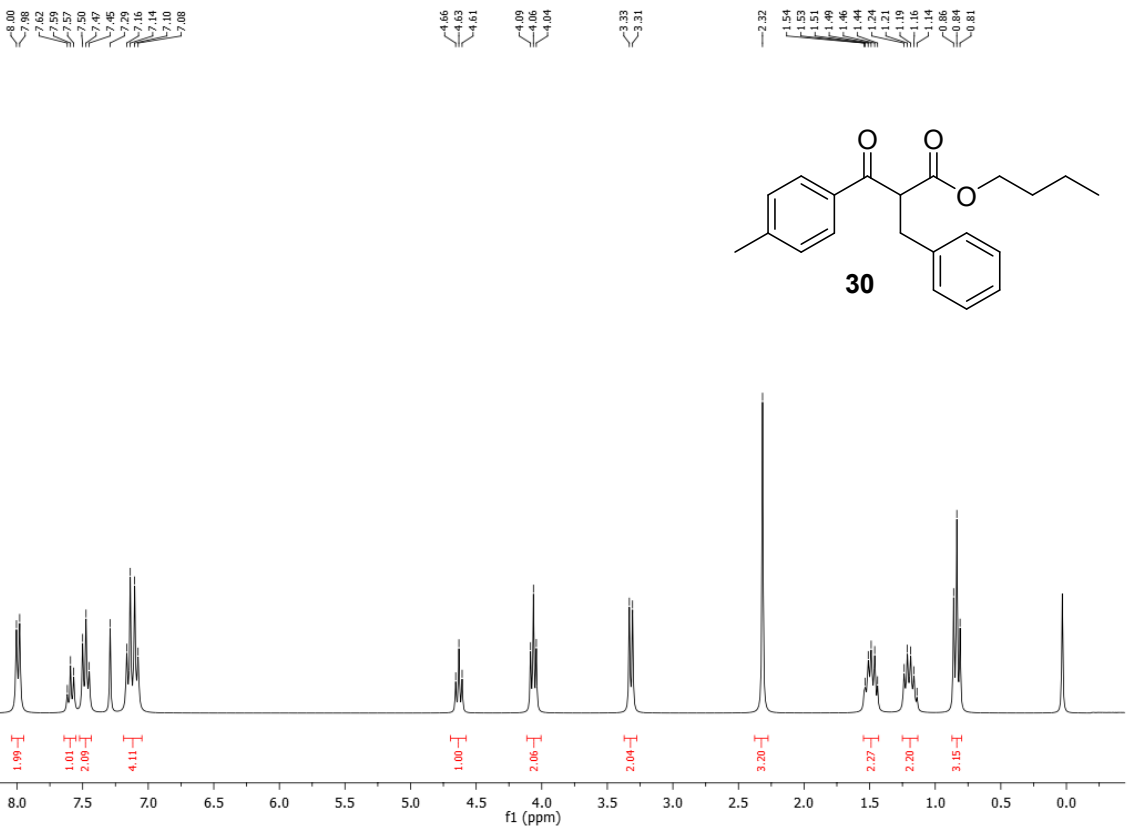

1.98
1.23
2.30
5.30
0.99
2.05
2.04
2.14
2.23
3.18
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

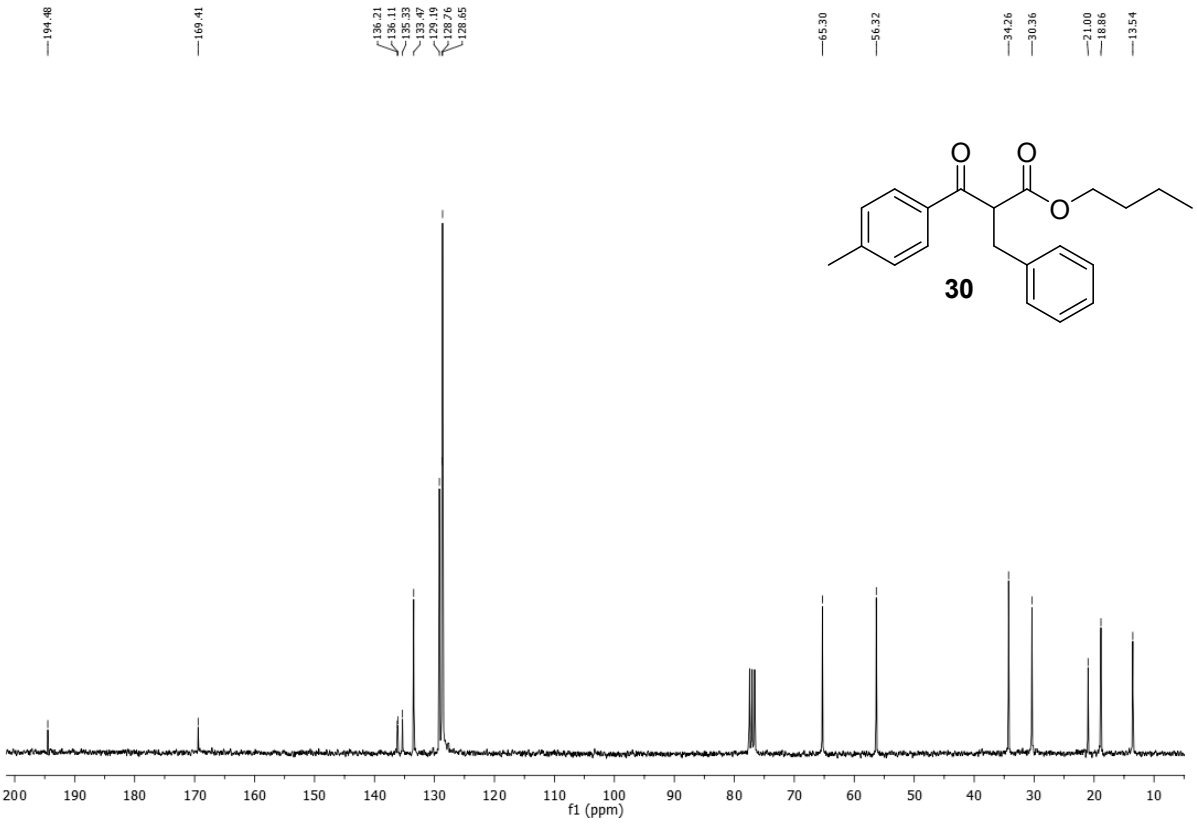

194.41
169.32
138.45
136.25
133.45
128.89
128.64
128.61
128.49
126.59
65.32
56.18
34.69
30.36
18.85
13.50

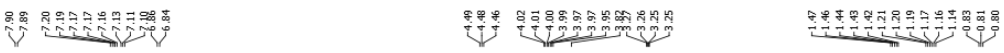

O
O
O

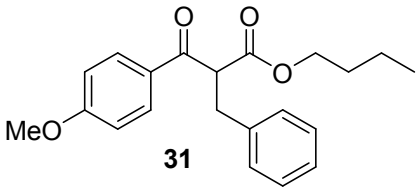
29


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

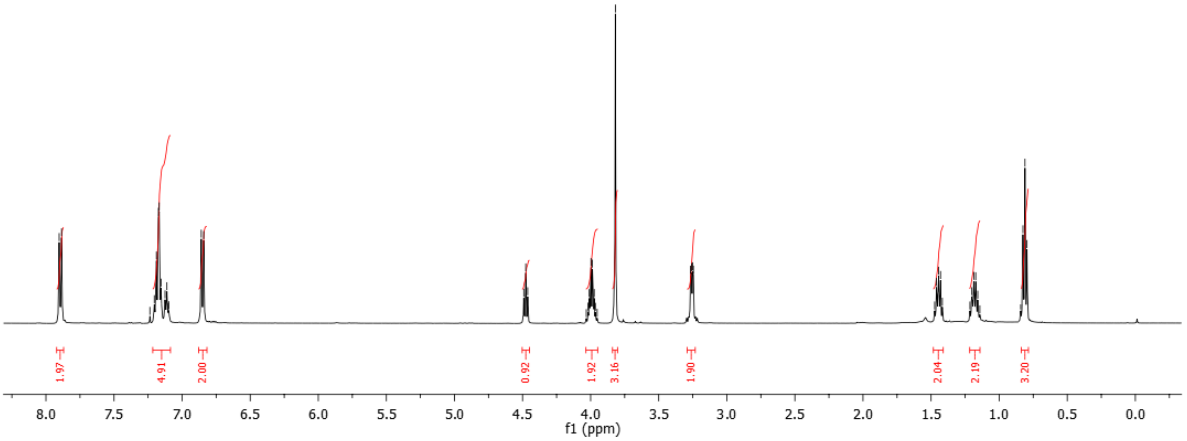

8.00
7.98
7.62
7.59
7.57
7.50
7.47
7.45
7.29
7.16
7.14
7.10
7.08
4.66
4.63
4.61
4.09
4.06
4.04
3.33
3.31
2.32
1.54
1.53
1.51
1.49
1.46
1.44
1.24
1.21
1.19
1.16
1.14
0.86
0.84
0.81
O
O
O
30
1.99
1.01
2.09
4.11
1.00
2.06
2.04
3.20
2.27
2.20
3.15
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

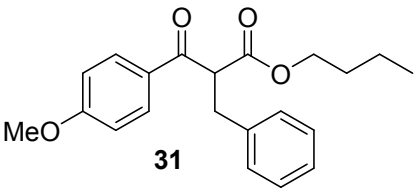

194.48
169.41
136.21
136.11
135.33
133.47
129.19
128.76
128.65
65.30
56.32
34.26
30.36
21.00
18.86
13.54
O
O
O
30
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



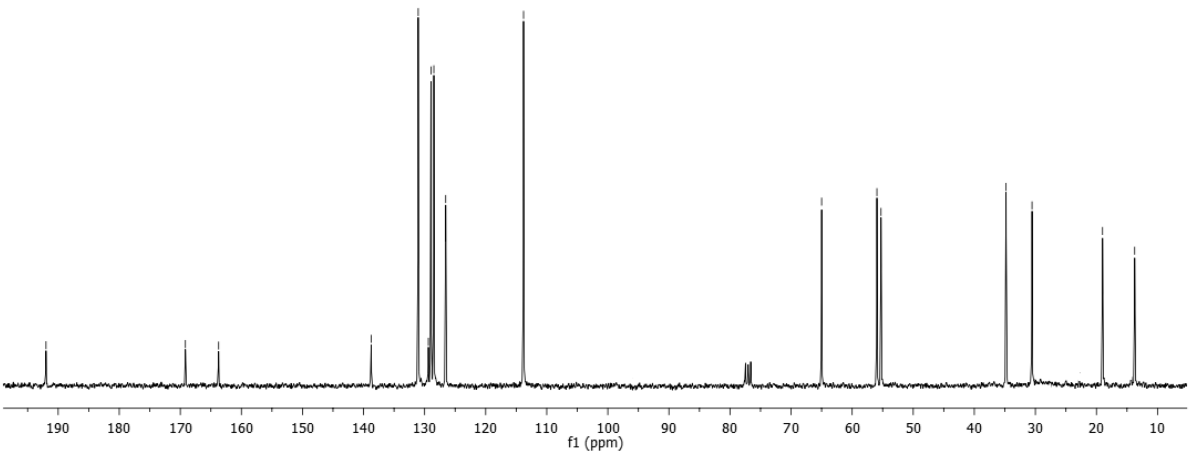

O
O
O
MeO

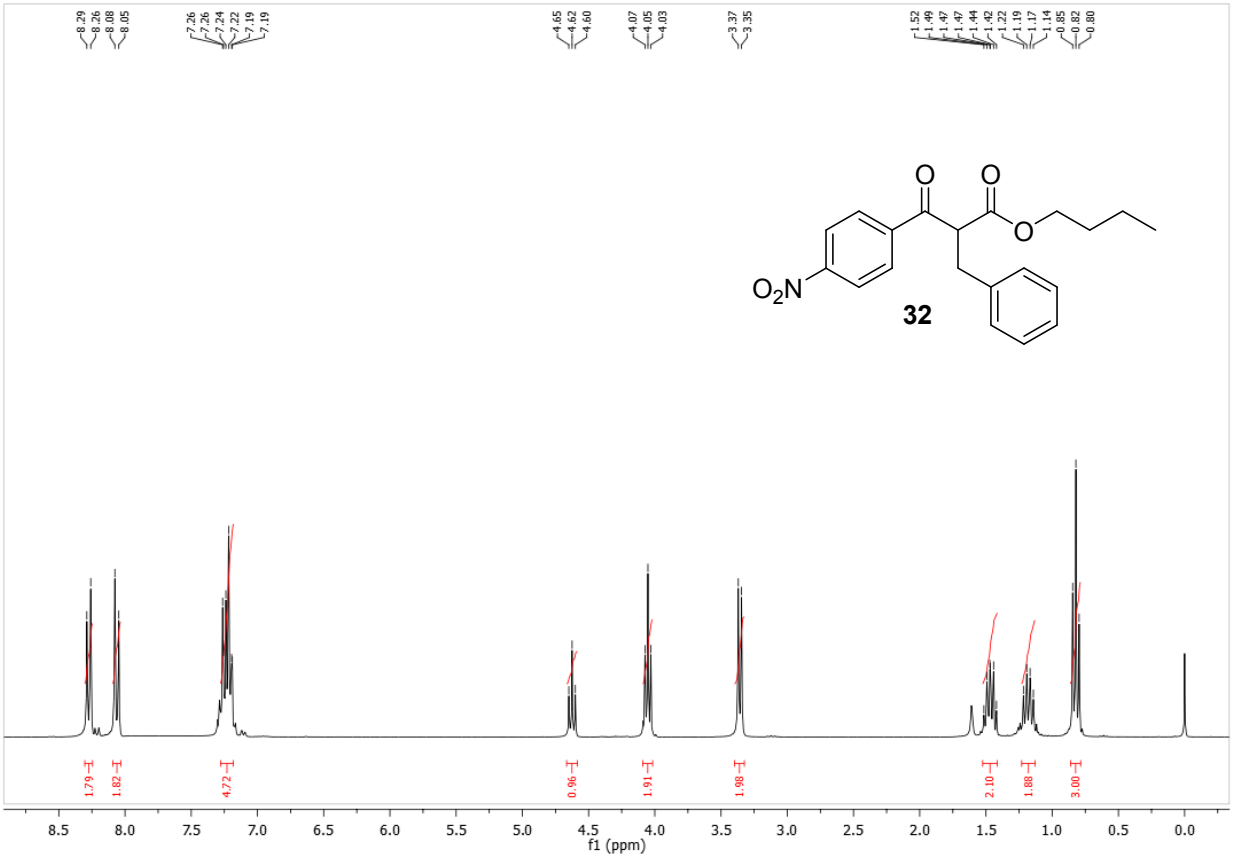
31

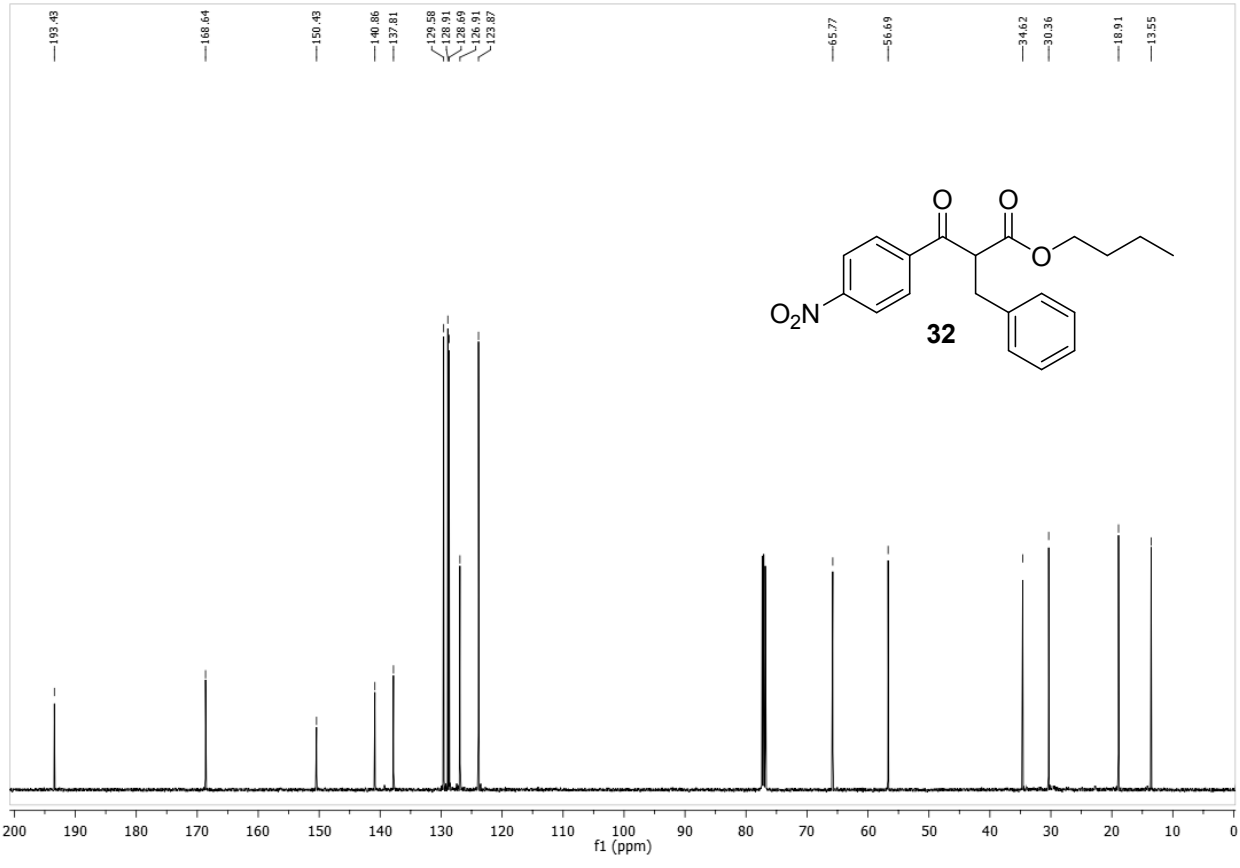

1.97
4.91
2.00
0.92
1.92
3.16
1.90
2.04
2.19
3.20
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

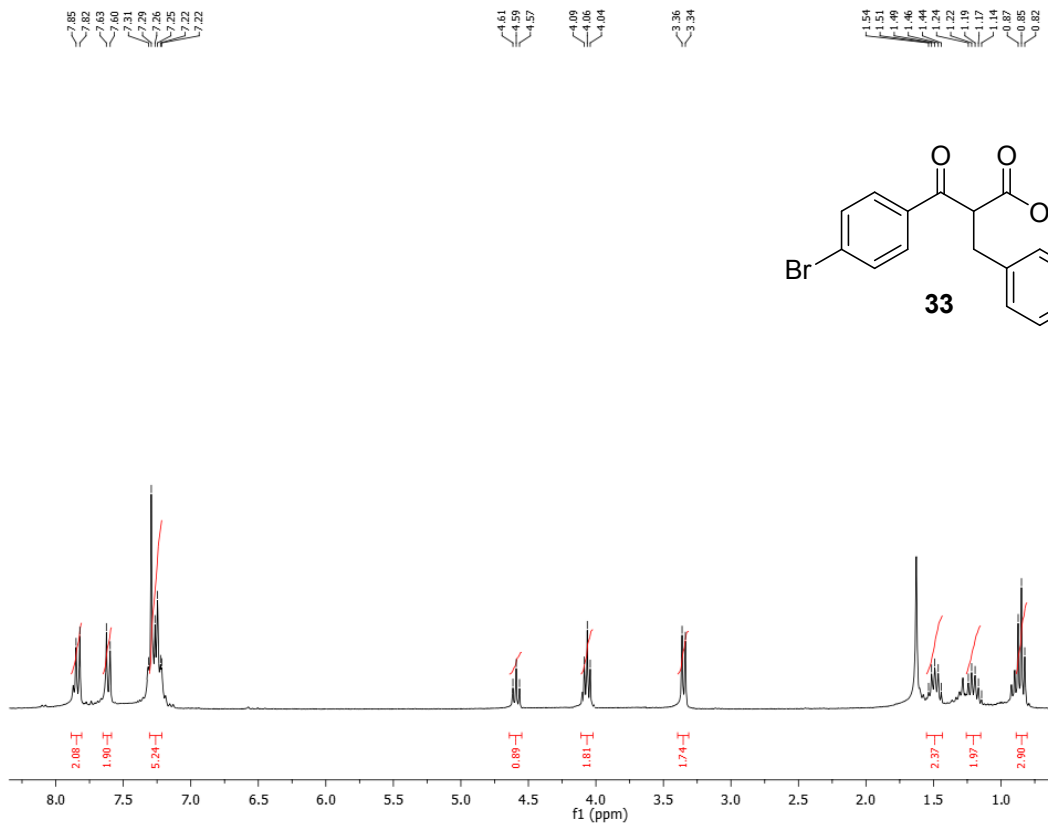

O
O
O
MeO

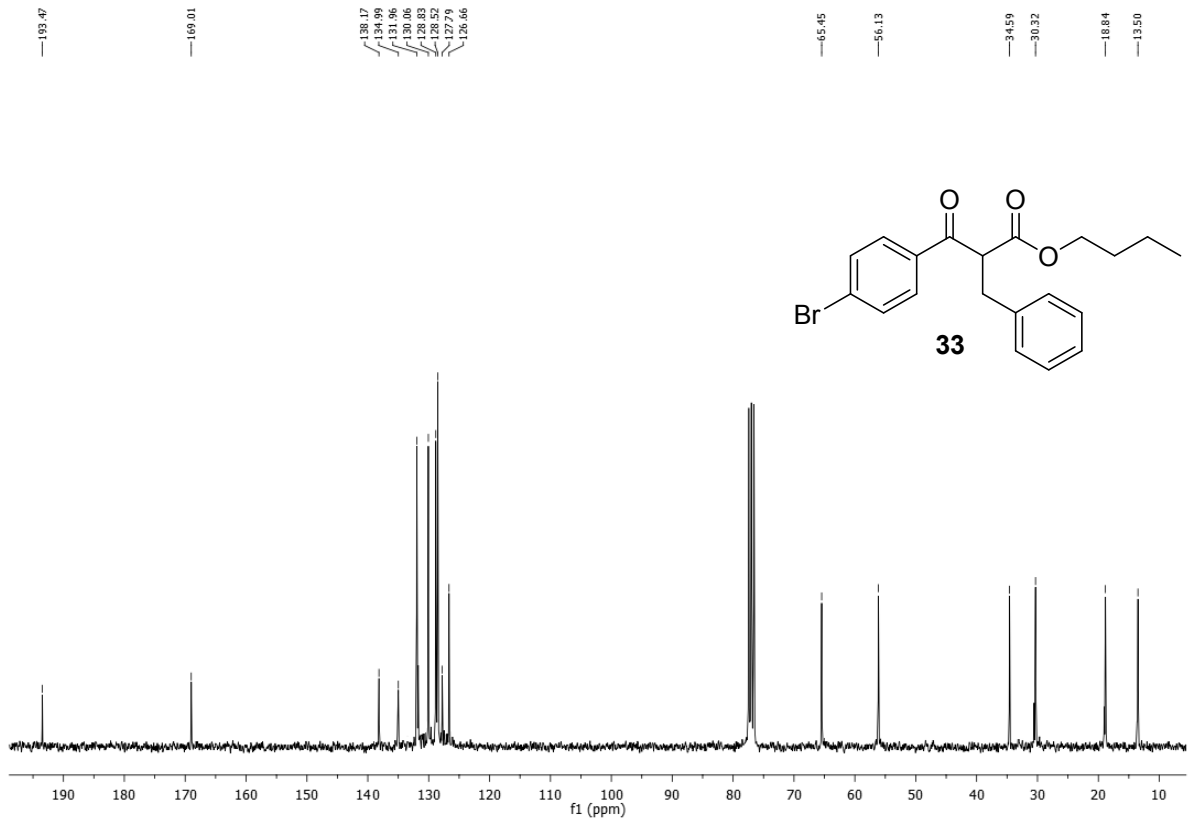
31

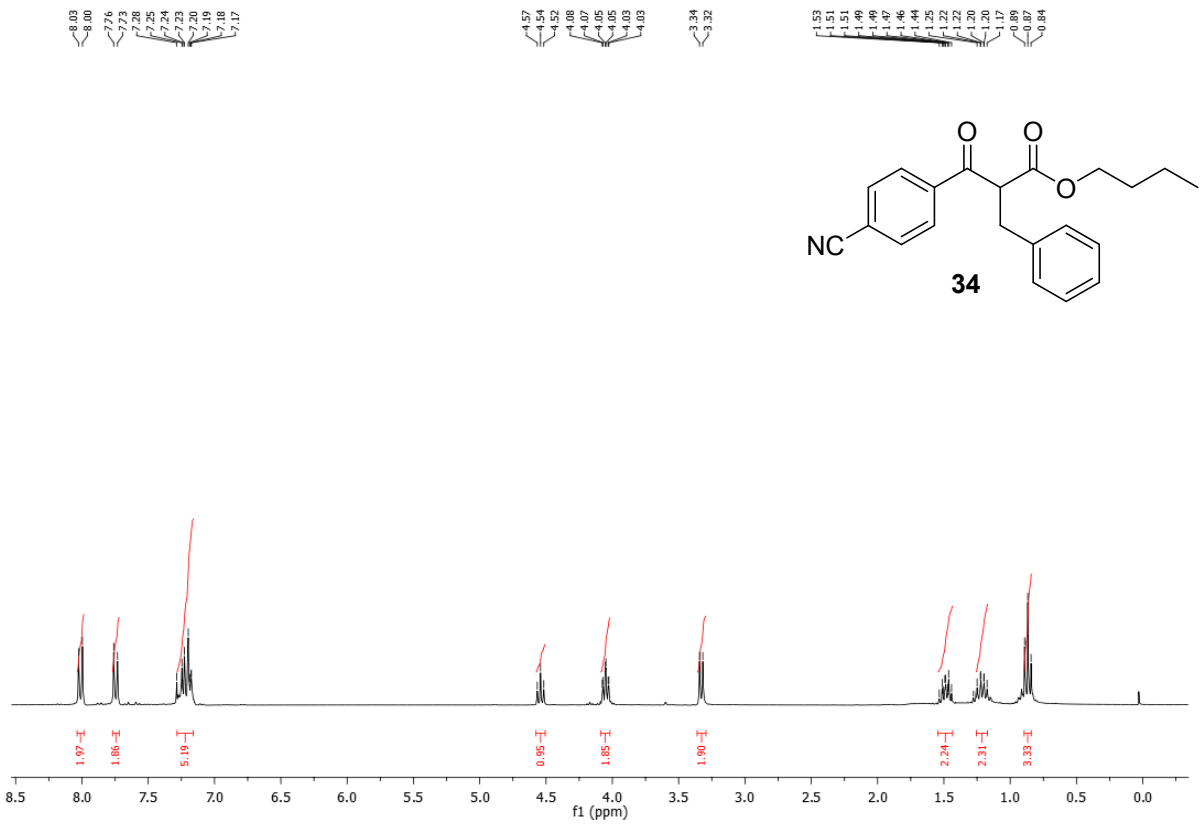

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

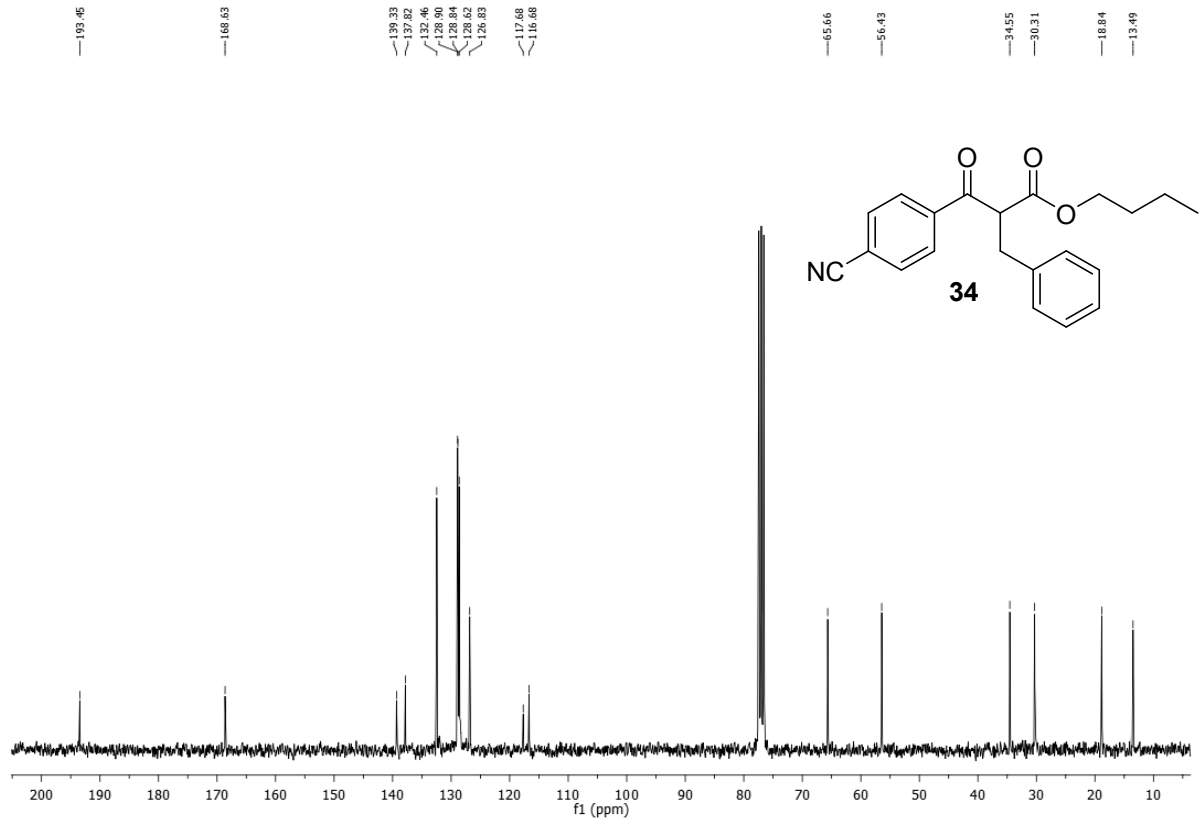

8.29
8.26
8.08
8.05
7.26
7.26
7.24
7.22
7.19
7.19
4.65
4.62
4.60
4.07
4.05
4.03
3.37
3.35
1.52
1.49
1.47
1.47
1.44
1.42
1.22
1.19
1.17
1.14
0.85
0.82
0.80
O
O
O
O2N
32
1.79
1.82
4.72
0.96
1.91
1.98
2.10
1.88
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

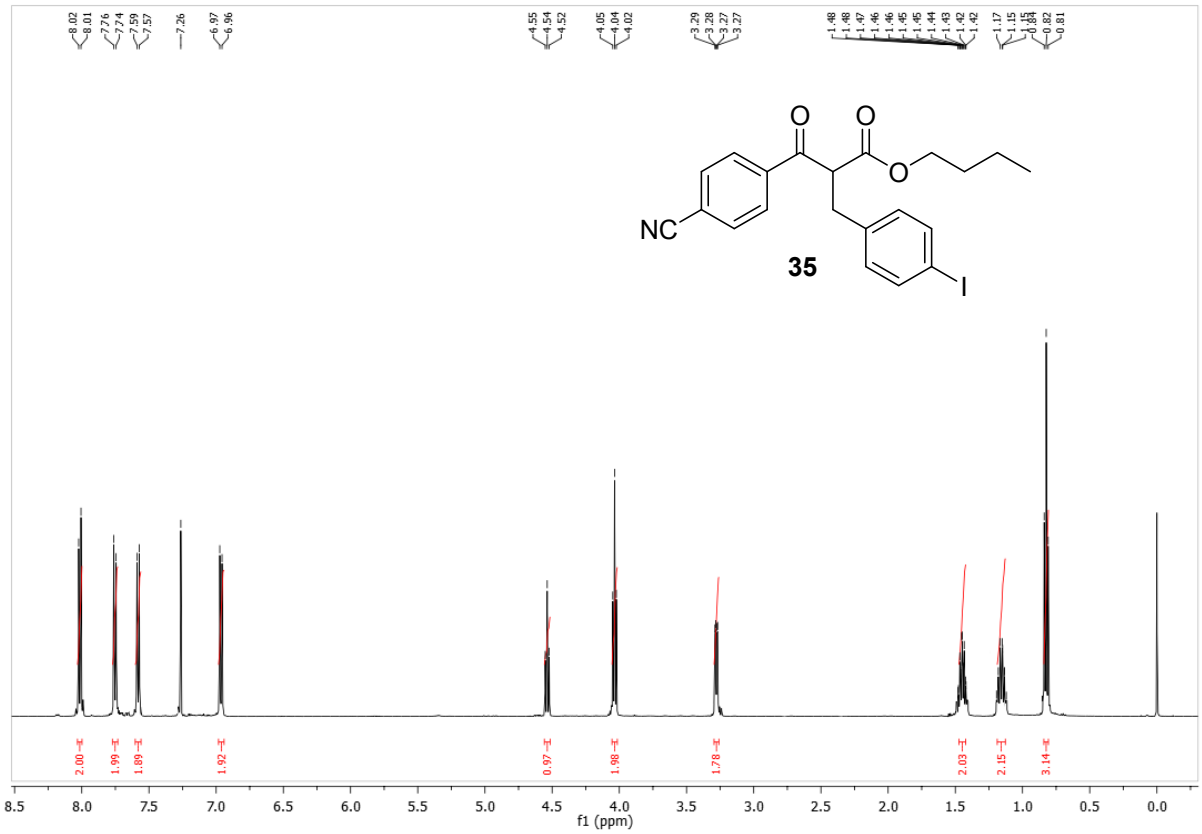

193.43
168.64
150.43
140.86
137.81
129.58
128.91
128.69
126.91
123.87
65.77
56.69
34.62
30.36
18.91
13.55
O
O
O
O2N
32
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

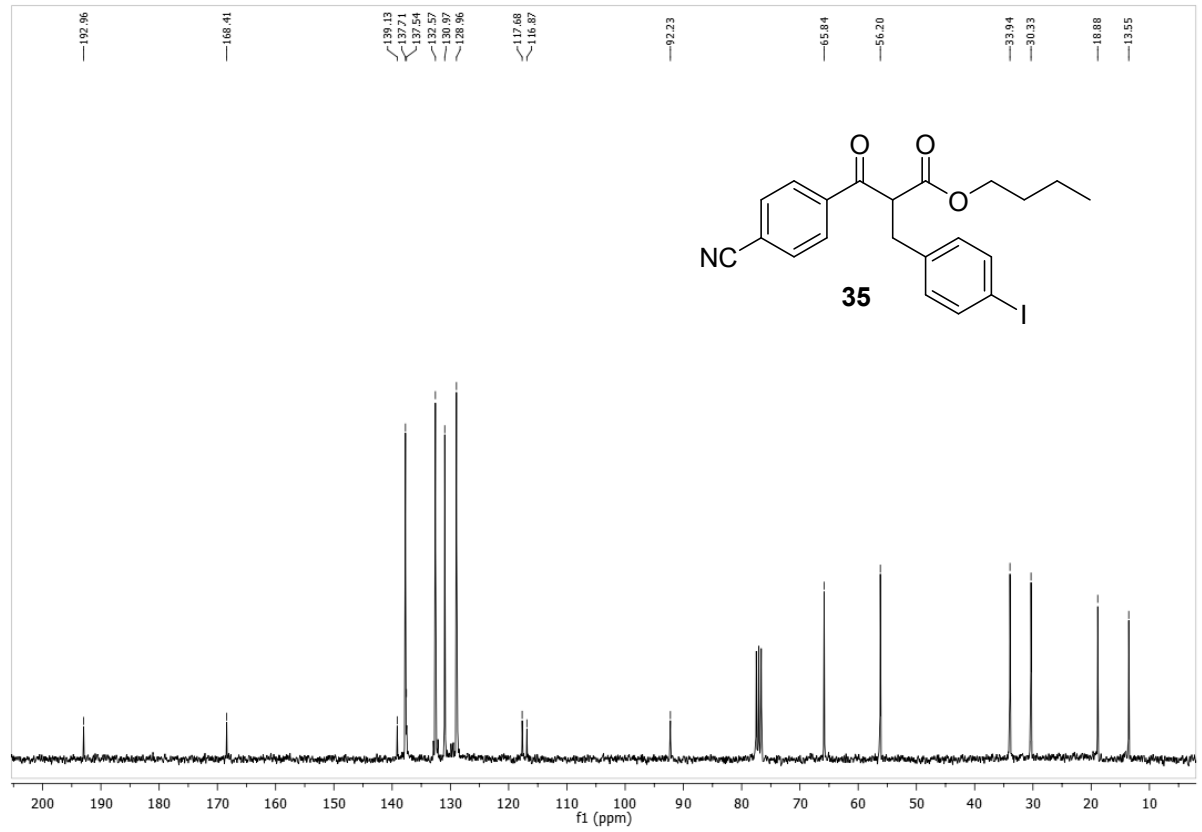

7.85
7.82
7.63
7.60
7.31
7.29
7.26
7.25
7.22
7.22
4.61
4.59
4.57
4.09
4.06
4.04
3.36
3.34
1.54
1.51
1.49
1.46
1.44
1.24
1.22
1.19
1.17
1.14
0.87
0.85
0.82
O
O
O
Br
33
2.08
1.90
5.24
0.89
1.81
1.74
2.37
1.97
2.90
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

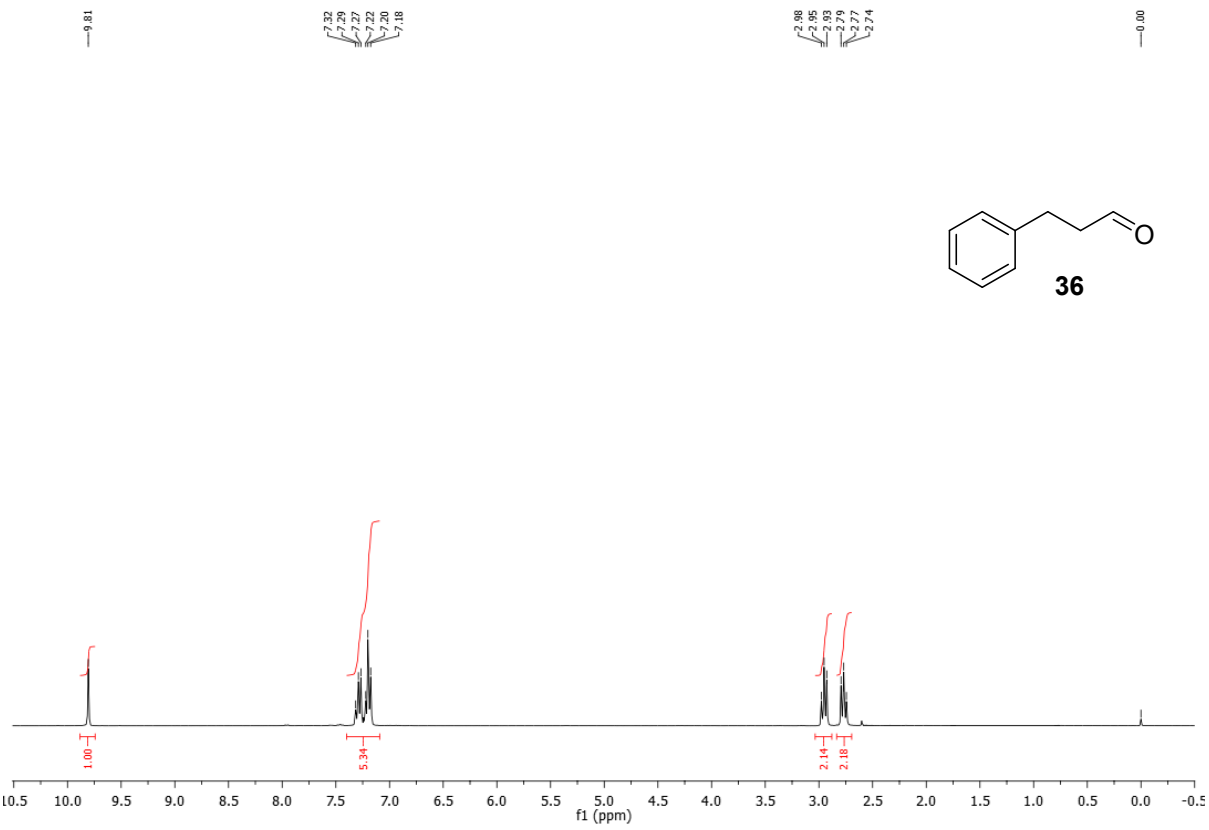

193.47
169.01
138.17
134.99
131.96
130.06
128.83
128.52
127.79
126.66
65.45
56.13
34.59
30.32
18.84
13.50
O
O
O
Br
33
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

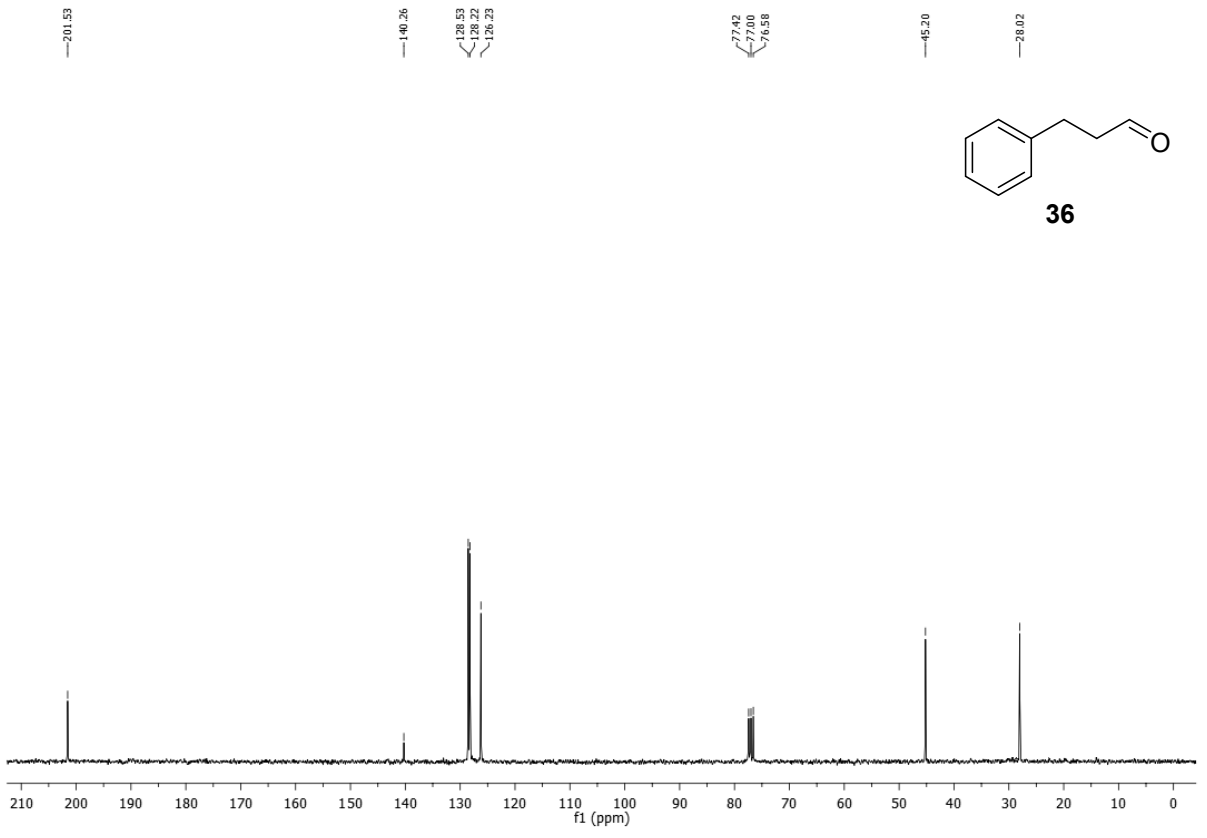

8.03
8.00
7.76
7.73
7.28
7.25
7.24
7.23
7.20
7.19
7.18
7.17
4.57
4.54
4.52
4.08
4.07
4.05
4.05
4.03
4.03
3.34
3.32
1.53
1.51
1.51
1.49
1.49
1.47
1.46
1.44
1.25
1.22
1.22
1.20
1.20
1.17
0.89
0.87
0.84
O
O
O
NC
34
1.97
1.86
5.19
0.95
1.85
1.90
2.24
2.31
3.33
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

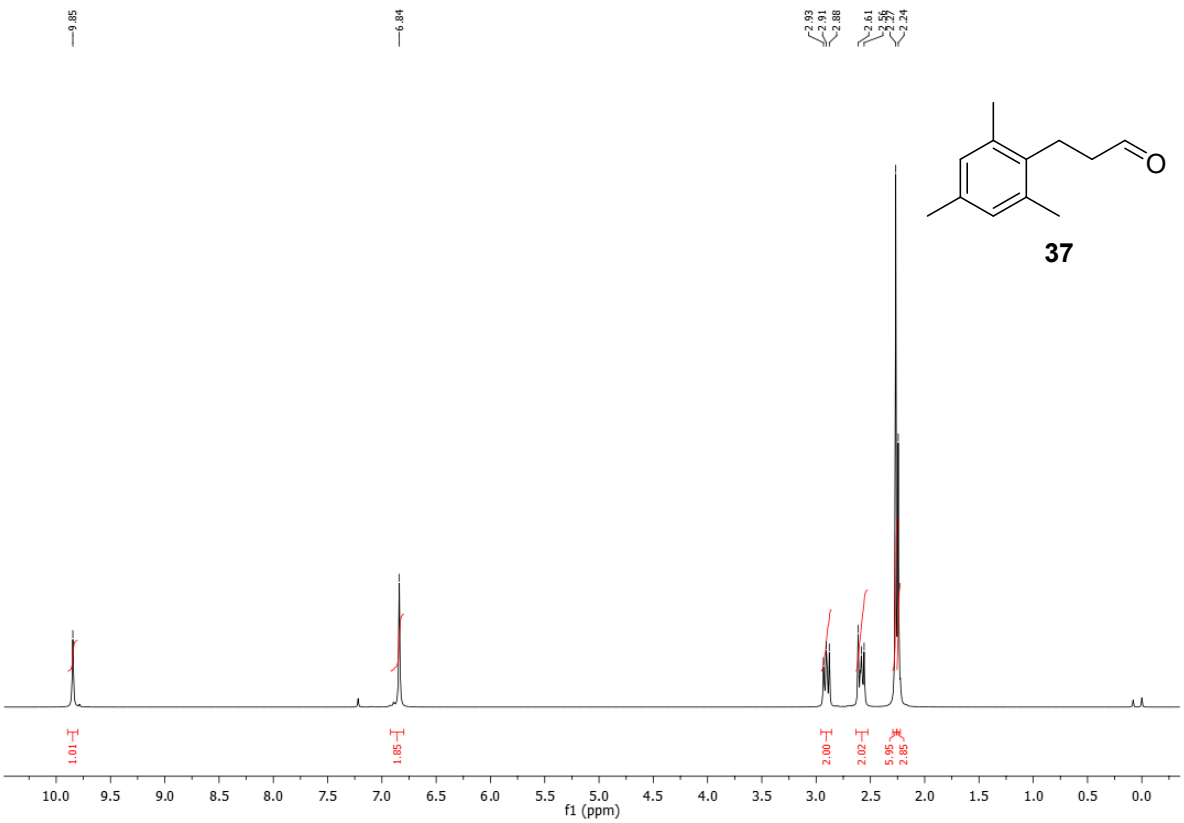

193.45
168.63
139.33
137.82
132.46
128.90
128.84
128.62
126.83
117.68
116.68
65.66
56.43
34.55
30.31
18.84
13.49
O
O
O
NC
34
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

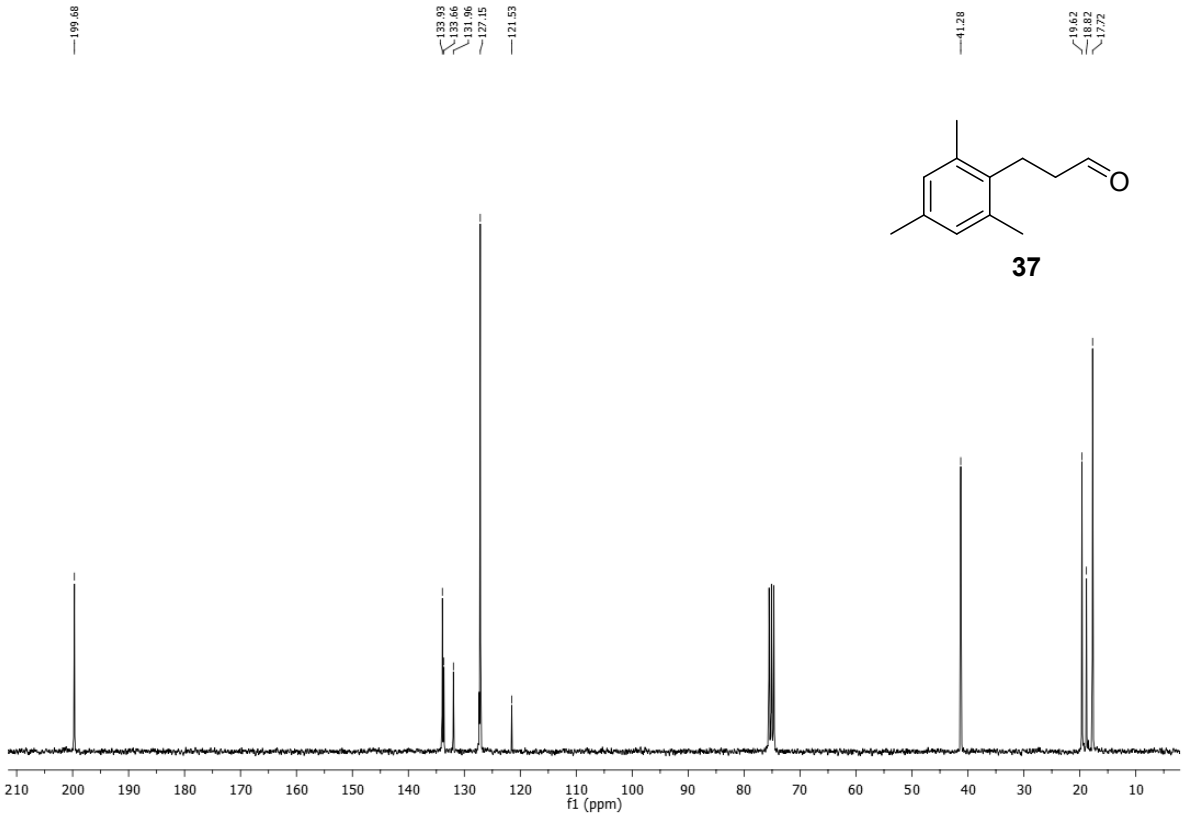

8.02
8.01
7.76
7.74
7.59
7.57
7.26
6.97
6.96
4.55
4.54
4.52
4.05
4.04
4.02
3.29
3.28
3.27
3.27
1.48
1.48
1.47
1.46
1.46
1.45
1.45
1.44
1.43
1.42
1.42
1.17
1.15
0.84
0.82
0.81
O
O
O
NC
35
I
2.00
1.99
1.89
1.92
0.97
1.98
1.78
2.03
2.15
3.14
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

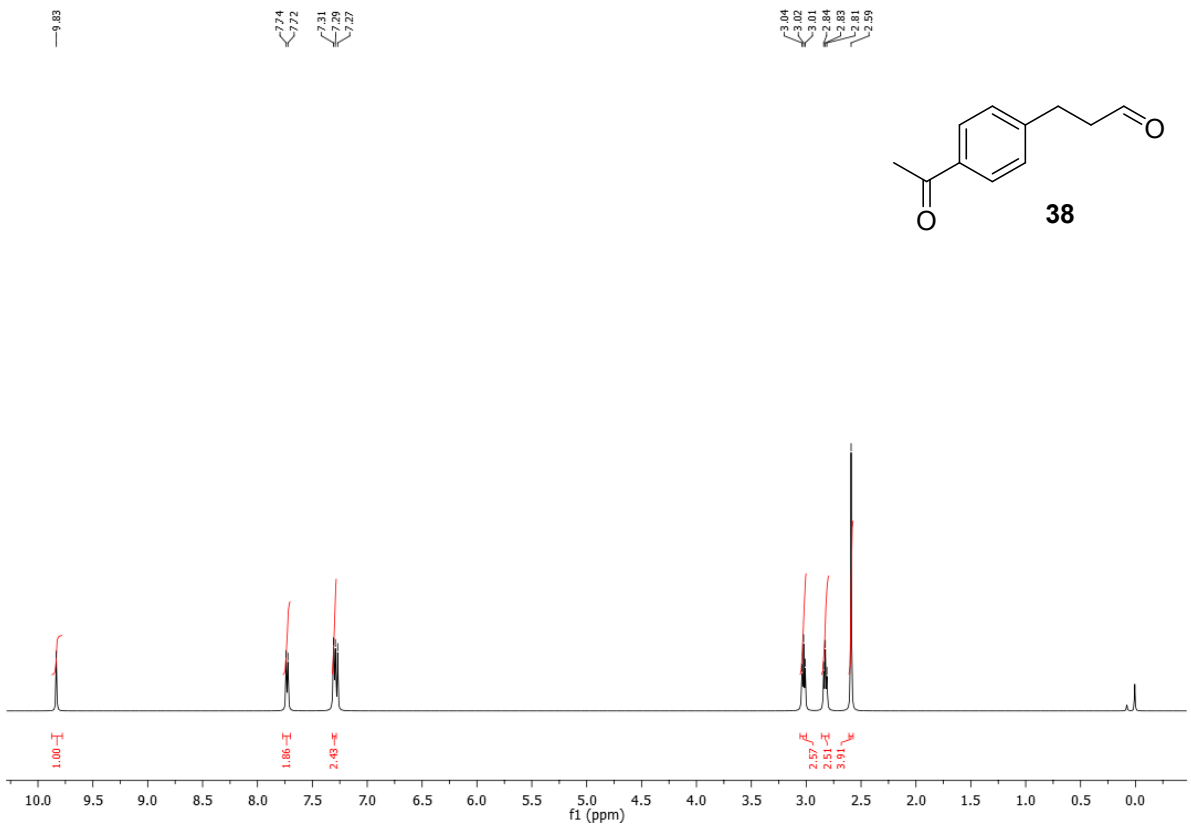

192.96
168.41
139.13
137.71
137.54
132.57
130.97
128.96
117.68
116.87
92.23
65.84
56.20
33.94
30.33
18.88
13.55
O
O
O
NC
35
I
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

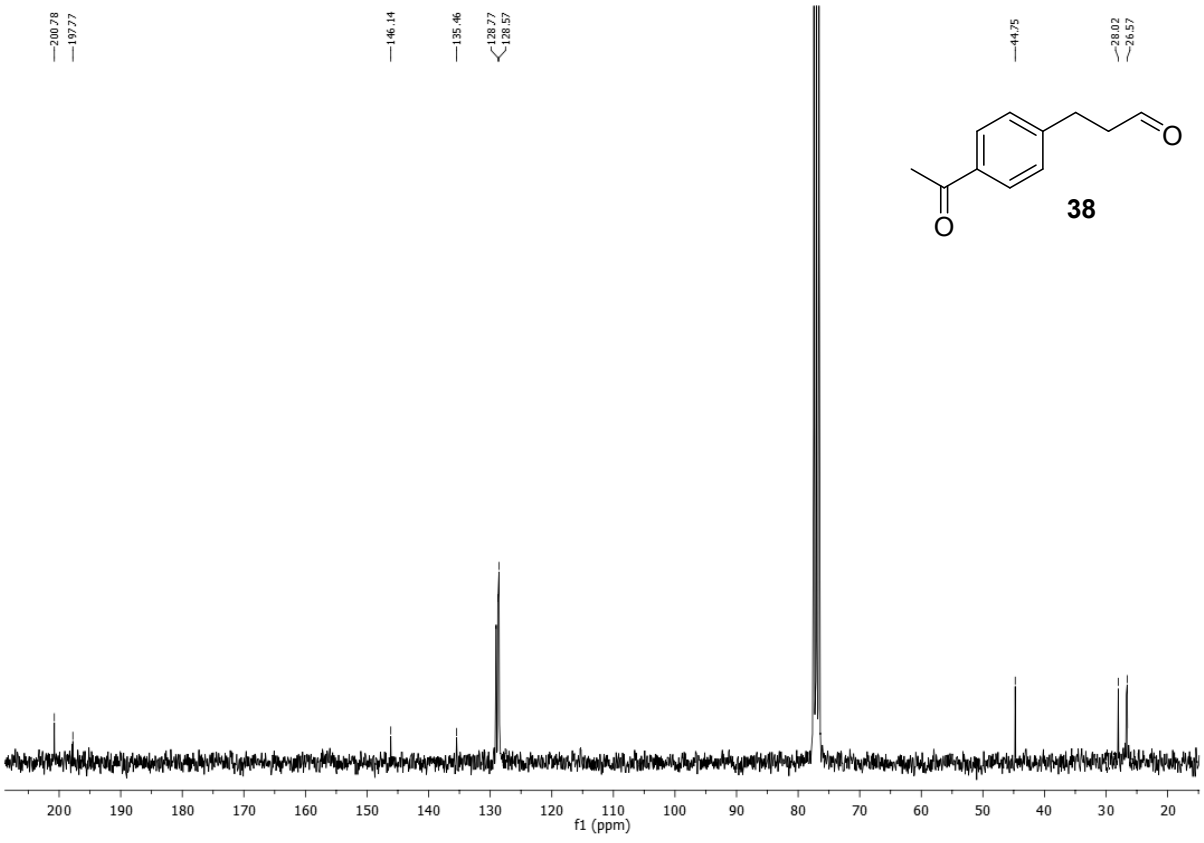

9.81
7.32
7.29
7.27
7.22
7.20
7.18
2.98
2.95
2.93
2.79
2.77
2.74
0.00
O
36
1.00
5.34
2.14
2.18
f1 (ppm)

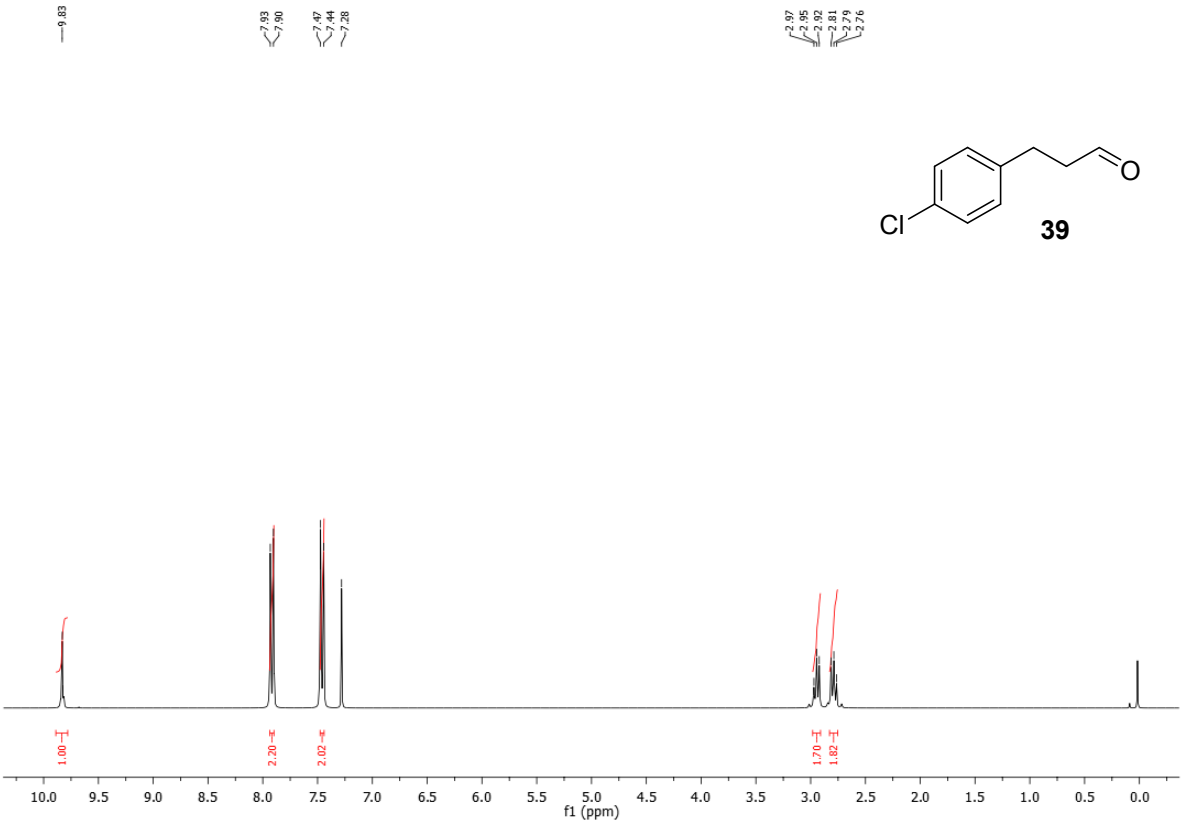

201.53
140.26
128.53
128.22
126.23
77.42
77.00
76.58
45.20
28.02
O
36
f1 (ppm)

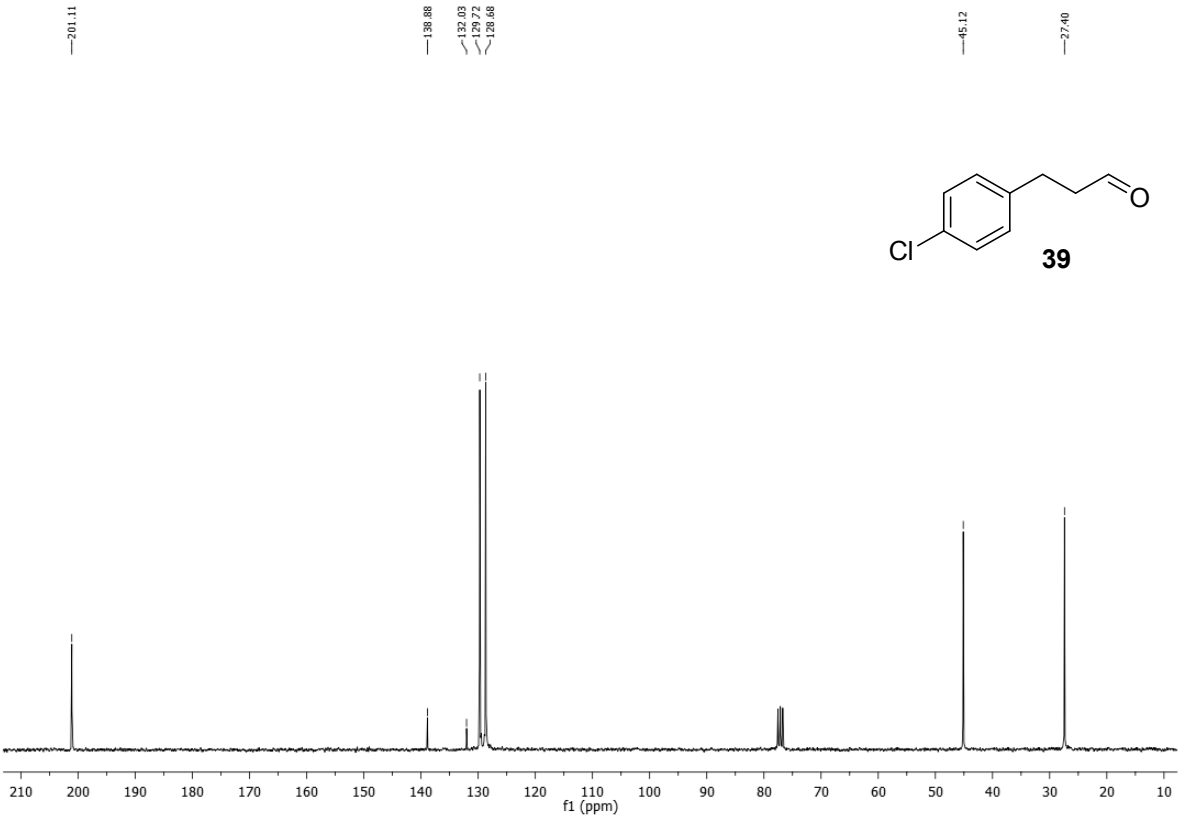

9.85
6.84
2.93
2.91
2.88
2.61
2.59
2.57
2.24
O
37
1.01
1.85
2.00
2.02
5.95
2.85
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

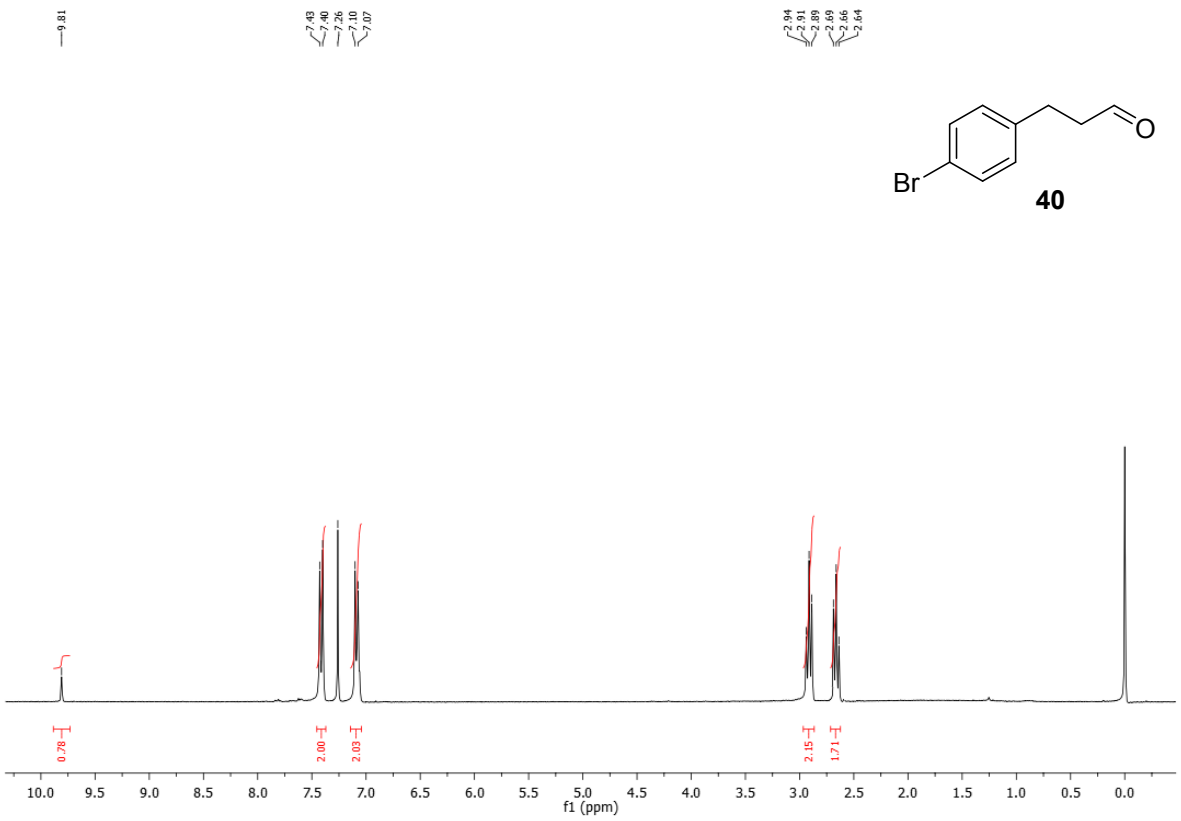

199.68
133.93
133.66
131.96
127.15
121.53
41.28
19.62
18.82
17.72
O
37
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

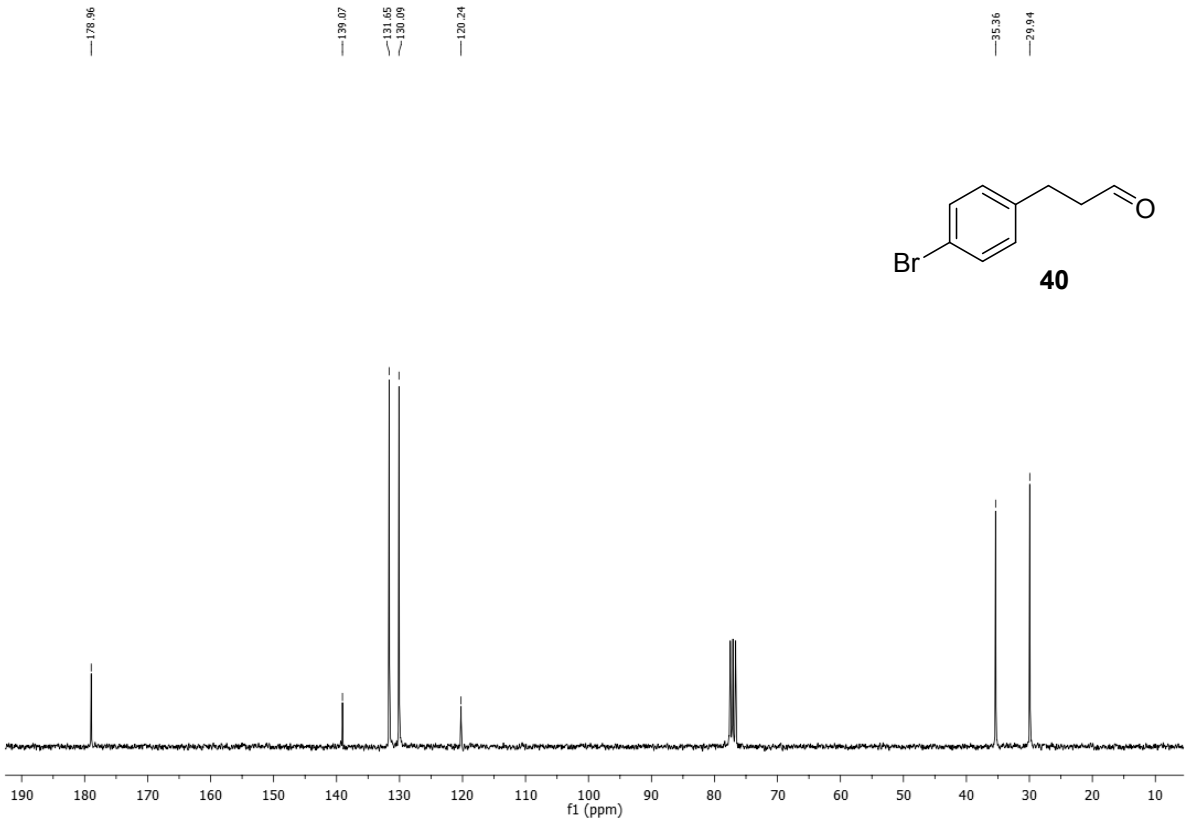

9.83
7.74
7.72
7.31
7.29
7.27
3.04
3.02
3.01
2.84
2.83
2.81
2.59
O
O
38
1.00
1.86
2.48
2.57
2.51
3.91
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

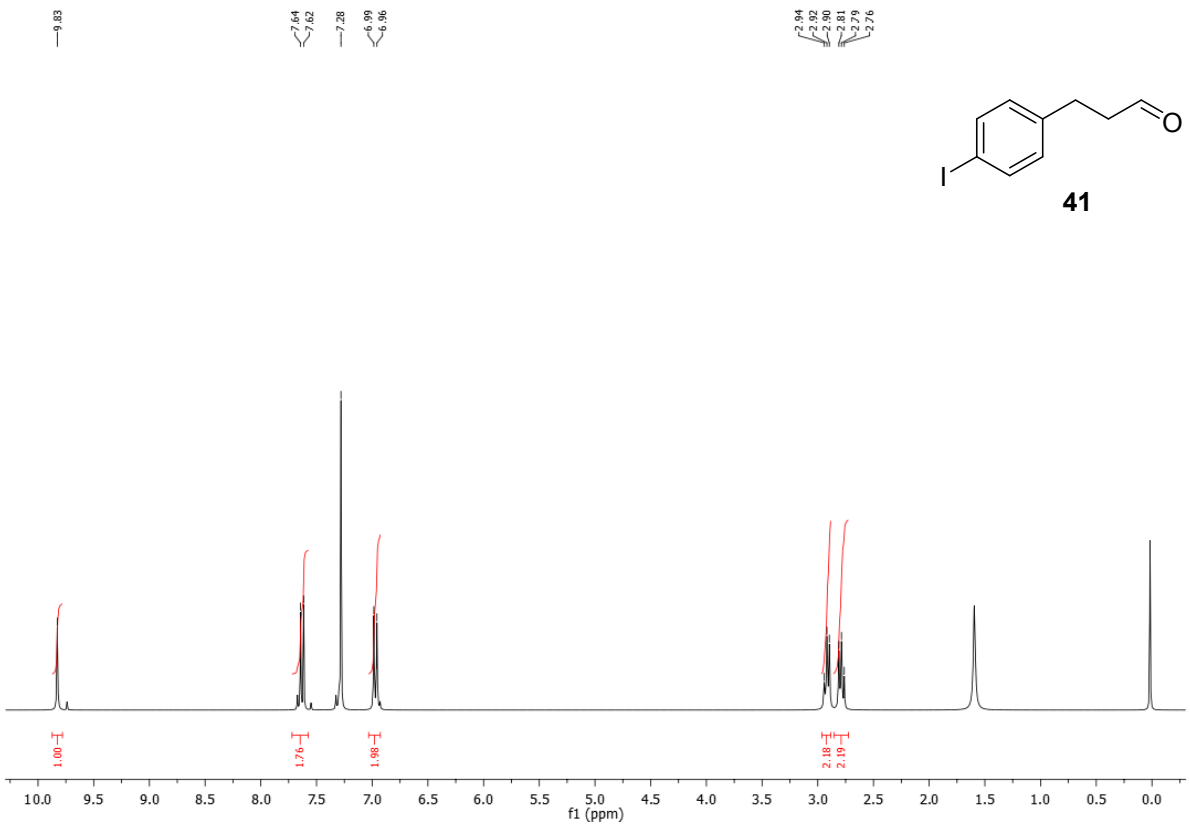

200.78
197.77
146.14
135.46
128.77
128.57
44.75
28.02
26.57
O
O
38
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

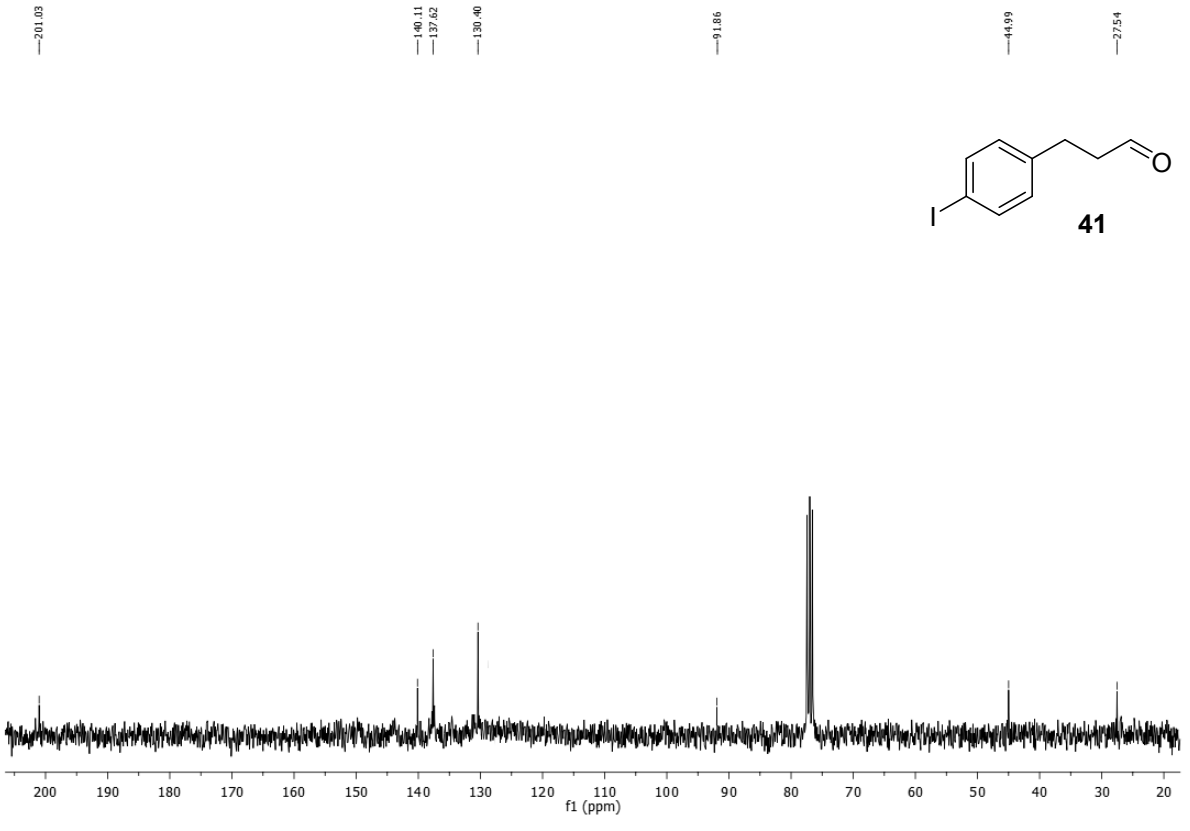

9.83
7.93
7.90
7.47
7.44
7.28
2.97
2.95
2.92
2.81
2.79
2.76
Cl
O
39
1.00
2.20
2.02
1.70
1.82
f1 (ppm)

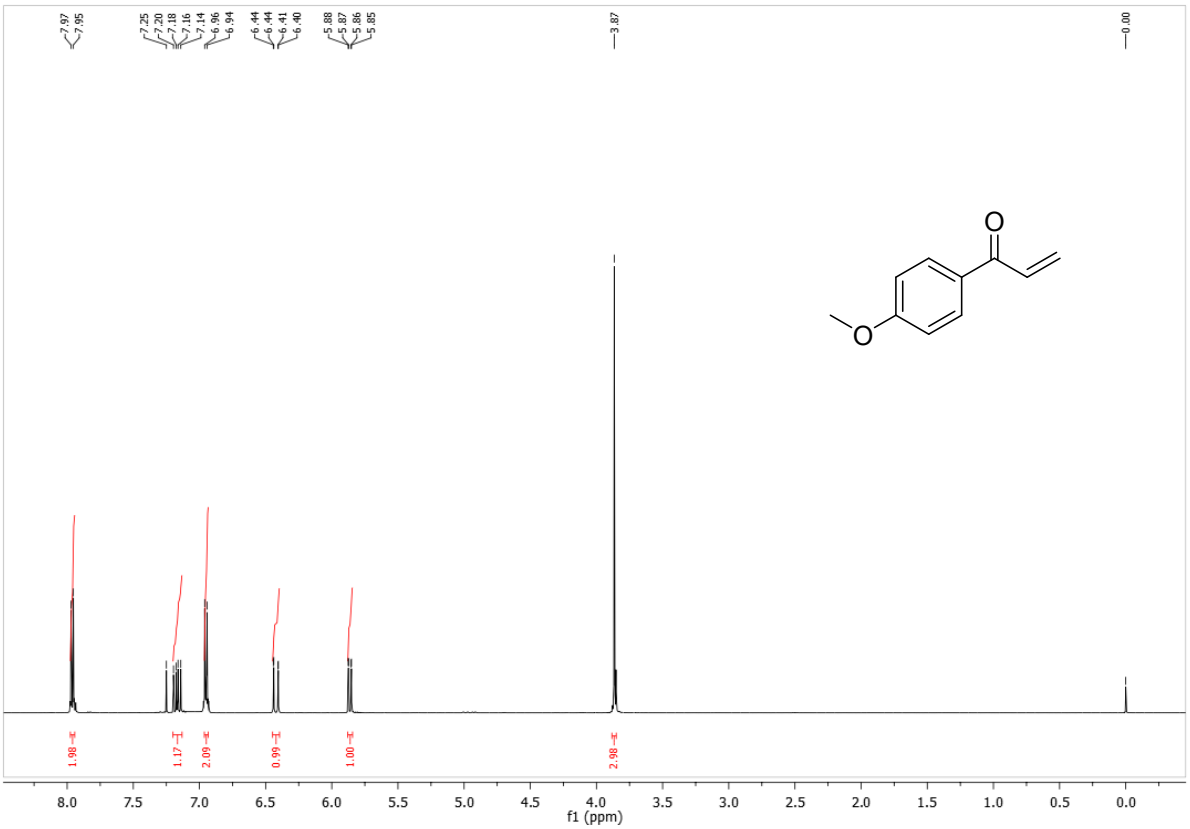

201.11
138.88
132.03
129.72
128.68
45.12
27.40
Cl
O
39
f1 (ppm)

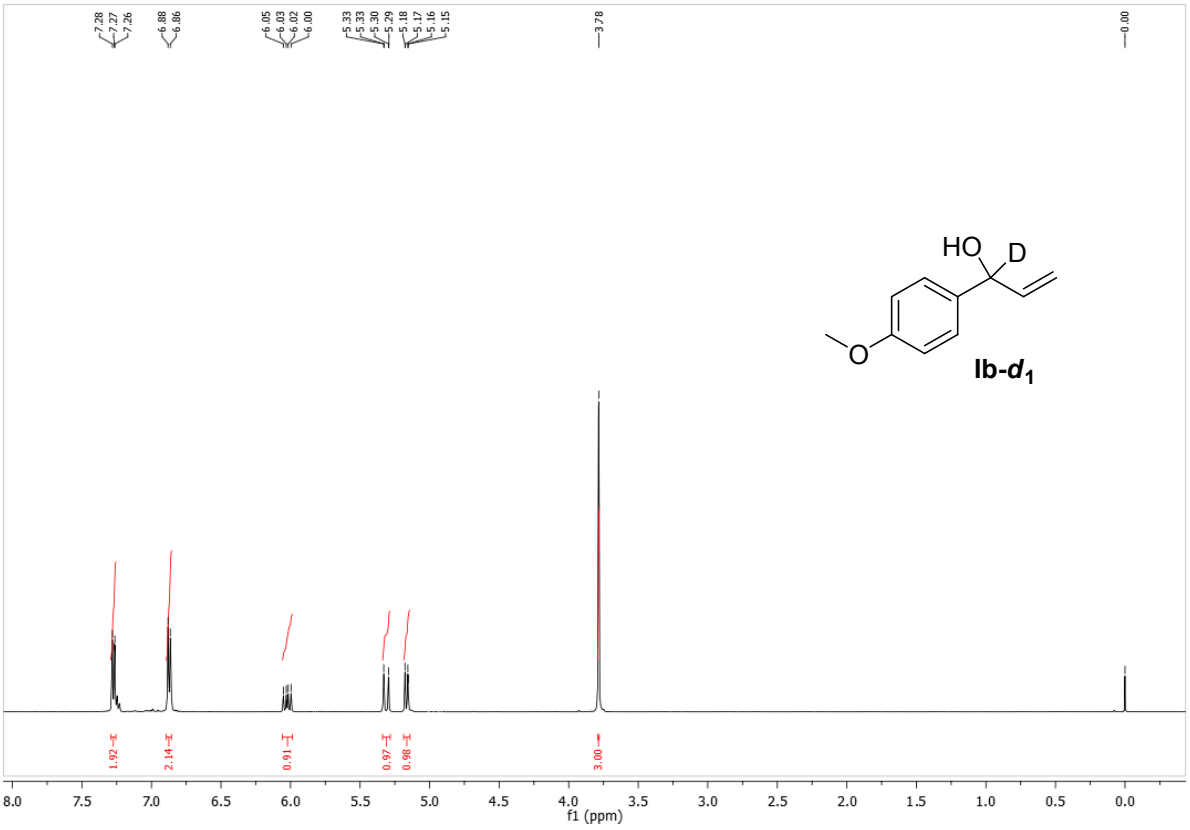

9.81
7.43
7.40
7.26
7.10
7.07
2.94
2.91
2.89
2.69
2.66
2.64
Br
O
40
0.78
2.00
2.03
2.15
1.71
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

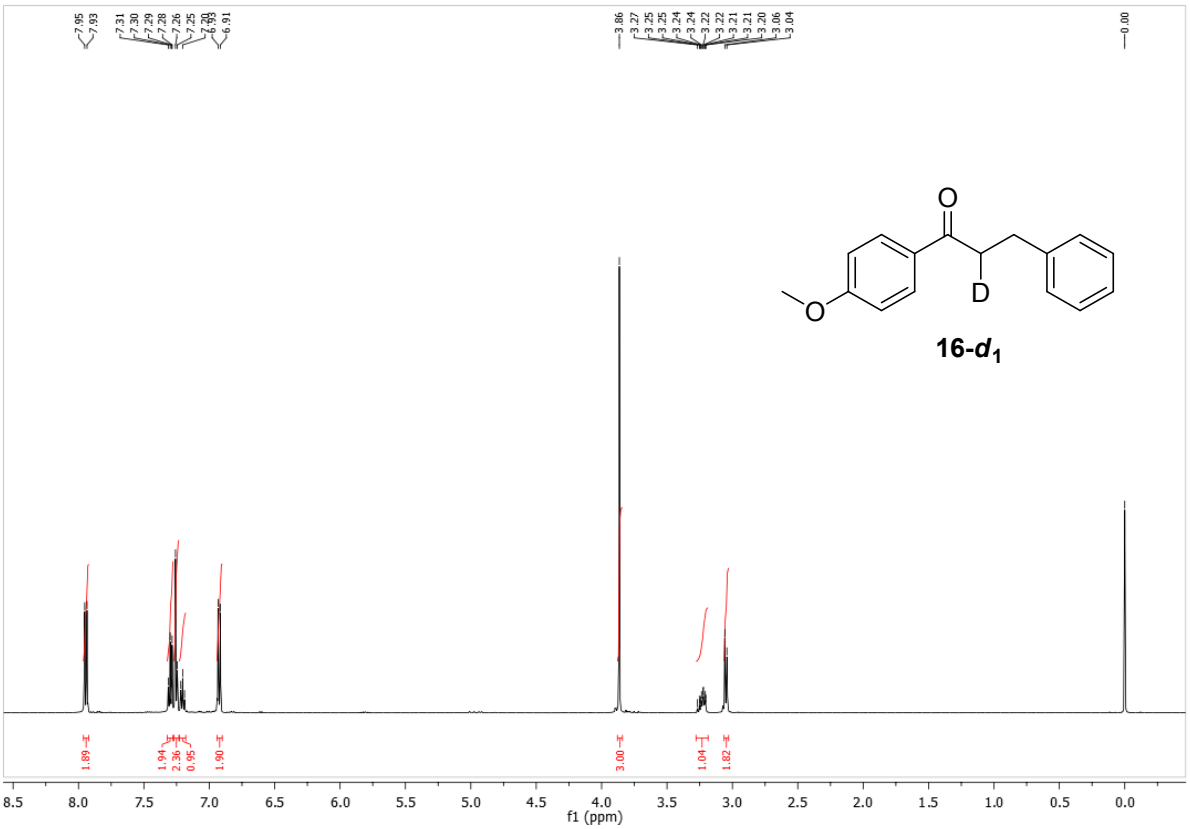

178.96
139.07
131.65
130.09
120.24
35.36
29.94
Br
O
40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

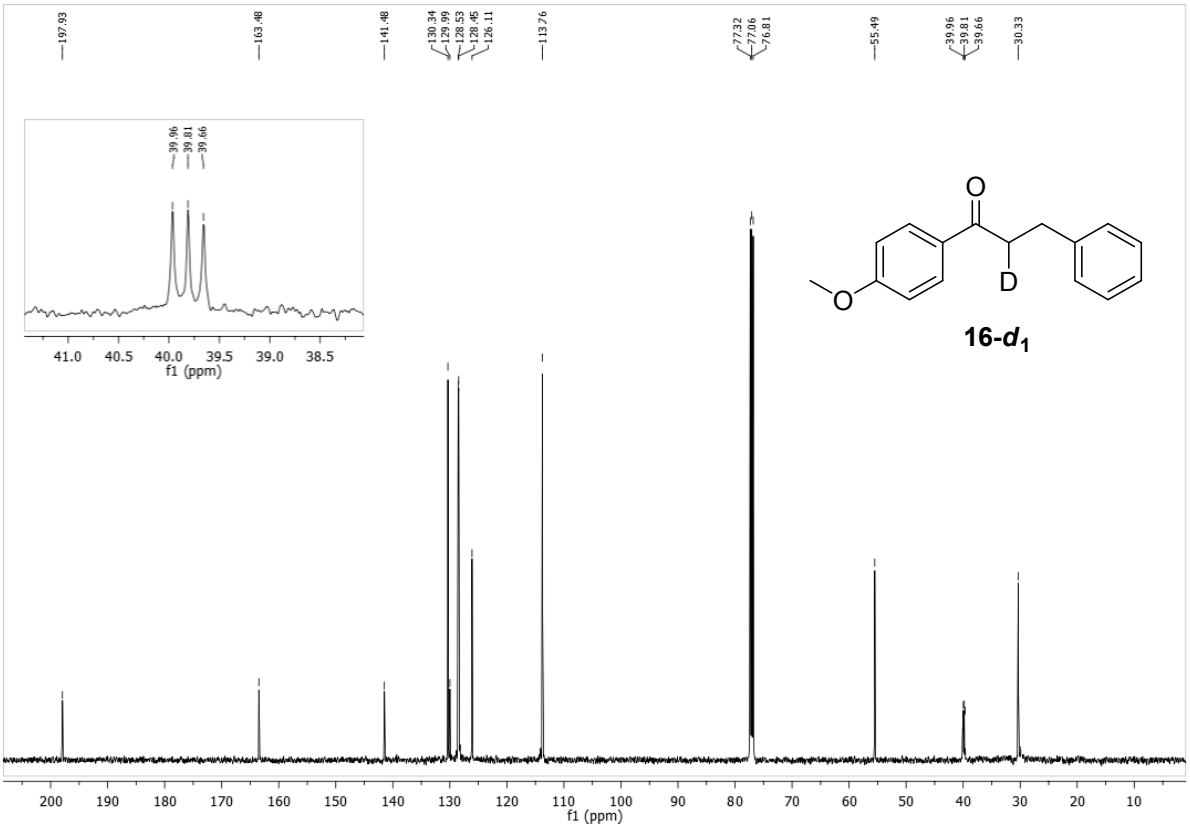

9.83
7.64
7.62
7.28
6.99
6.96
2.94
2.92
2.90
2.81
2.79
2.76
O
I
41
1.00
1.76
1.98
2.18
2.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


201.03
140.11
137.62
130.40
91.86
44.99
27.54
O
I
41
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)


7.97
7.95
7.25
7.20
7.18
7.16
7.14
6.96
6.94
6.44
6.44
6.41
6.40
5.88
5.87
5.86
5.85
3.87
0.00
O
O
1.98
1.17
2.09
0.99
1.00
2.98
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)


7.28
7.27
7.26
6.88
6.86
6.05
6.03
6.02
6.00
5.33
5.33
5.30
5.29
5.18
5.17
5.16
5.15
3.78
0.00
HO
D
O
Ib-d1
1.92
2.14
0.91
0.97
0.98
3.00
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)


7.95
7.93
7.31
7.30
7.29
7.28
7.26
7.25
6.93
6.91
3.86
3.27
3.25
3.25
3.24
3.24
3.22
3.22
3.21
3.21
3.20
3.06
3.04
0.00
O
D
O
16-d_1
1.89
1.94
2.38
0.95
1.90
3.00
1.04
1.82
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)


197.93
163.48
141.48
130.34
129.99
128.53
128.45
126.11
113.76
77.32
77.06
76.81
55.49
39.96
39.81
39.66
30.33
39.96
39.81
39.66
41.0
40.5
40.0
39.5
39.0
38.5
f1 (ppm)
O
D
O
16-d_1
200
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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