Supporting Information

Hydrogen Peroxide and Anhydride Prompted Transformation of Enamides into α-Acyloxy Ketones *via* Acyl Intramolecular Migration Process

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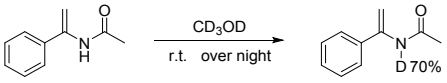
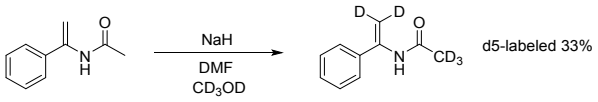
General Remarks

^{1}H-NMR spectra were recorded on Bruker avance III-400 spectrometers. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in CDCl3 as an internal standard. ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. Commercially available reagents and solvents were used without further purification. Unless otherwise noted, the enamides **1** were in all cases prepared from the corresponding ketoximes according to reported literature[1]. Ethyl 2-acetamidoacrylate **1x** was prepared according to the reported literature[2]. N-(1-phenylvinyl)benzamide **1ae** was prepared according to the reported literature[3].

Preparation of deuterated enamide substrates *d*-1a and *d5*-1a[3]



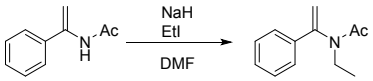
A solution of N-(1-Phenylvinyl)acetamide (**1a**, 322 mg, 2 mmol) in CD_3OD (0.6 mL) was stirred at room temperature for 12 h and then concentrated under reduced pressure to afford the deuterated product *d*-**1a** as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 5 H), 6.98 (m, 0.3 H), 5.86 (m, 1 H), 5.08 (s, 1 H), 2.11 (s, 3 H).



NaH (120 mg, 3 mmol, 1.5 equiv, 60 wt %) was added to the solution of N-(1-Phenylvinyl)acetamide (1a, 322 mg, 2 mmol, 1.0 equiv) in DMF (2 mL) at 0 ^{o}C. The

reaction mixture was warmed to room temperature and stirred overnight. CD_3OD (0.6 mL) was added dropwise and the resulting mixture was stirred for 2 h at room temperature. Then quenched by addition of water (5 mL) and EtOAc (8 mL). The organic layer was separated, washed with water, dried over sodium sulfate, concentrated and purified by column chromatography to afford *d5*-**1a** as white solid. ^1H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 5 H), 6.98 (m, 1 H), 5.89 (s, 0.7 H), 5.09-5.07 (m, 0.7 H), 2.11 (s, 2 H).

Preparation of N-ethyl enamide substrates 1ag[4]



1 mmol (1 equiv) of enamide was dissolved in 5 mL of anhydrous DMF in a screw cap via under argon atmosphere. The solution was cooled to 0 °C and 1.5 mmol (1.5 equiv) of sodium hydride (60% dispersion in mineral oil) was added in portions. The resulting suspension was stirred at the same temperature for 10 min. Iodoethane (2 mmol, 2 equiv) was then added dropwise. The final solution was warmed to room temperature and continued to stir for overnight. The completion of the reaction was confirmed by checking TLC and the excess of sodium hydride was quenched by adding water at 0 °C. The organic layer was extracted with ethyl acetate through stages of extraction with water. The combined organic layers were concentrated under reduced pressure and the pure product was isolated by flash column chromatography (hexane/ethyl acetate) to afford the corresponding product **1ag**.

1. Z. Guan, Z. Zhang, Z. Ren, Y. Wang and X. Zhang, *J. Org. Chem.* **2011**, *76*, 339.

2. B. Li, N. Wang, Y. Liang, S. Xu and B. Wang, *Org. Lett.* **2013**, *15*, 136.

3. N. Hu, G. Zhao, Y. Zhang, X. Liu, G. Li and W. Tang, *J. Am. Chem. Soc.* **2015**, *137*, 6746.

4. M. Wang, X, Zhang, Y. Zhuang, Y. Xu and T. Loh, *J. Am. Chem. Soc.* **2015**, *137*, 1341.

General experimental procedure

A test tube equipped with a magnetic stir bar was charged with enamide **1a** (32.2 mg, 0.2 mmol), H_2O_2 (30% in water) (113.3 mg, 1.0 mmol) and Ac_2O (102.0 mg 1.0 mmol). Then the reaction mixture was stirred at room temperature under air with a water bath. After completion of the reaction (monitored by TLC), the mixture was extracted with ethyl acetate and washed with NaOH (0.4 mol/L, 6 mL) and brine. The organic phase was dried over anhydrous Na_2SO_4 and concentrated in vacuo, the residues were purified by column chromatography, eluting with petroleum ether/EtOAc to give the desired product **2a** as colorless oil**.**

Experimental procedure for Table 1, entry 14

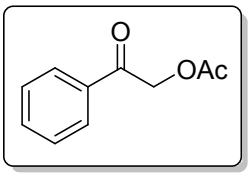
A schlenk tube equipped with a magnetic stir bar was charged with enamide **1a** (32.2 mg, 0.2 mmol), and Ac_2O (102.0 mg, 1.0 mmol). The reaction tube was evacuated and backfilled with N_2 (3 times, balloon), Then H_2O_2 (30% in water) (113.3 mg, 1.0 mmol) was added, and the reaction mixture was stirred at room temperature with a water bath for 10 min, the mixture was extracted with ethyl acetate and washed with NaOH (0.4 mol/L, 6 mL) and brine. The organic phase was dried over anhydrous Na_2SO_4 and concentrated in vacuo the residues were purified by column chromatography, eluting with petroleum ether/EtOAc to give the pure product **2a**.

Experimental procedure for Table 1, entry 15

H_2O_2 (30% in water, 20 mmol) was added to a solution of enamide **1a** (10 mmol) in Ac_2O (20 mmol) at 0 °C under air. The reaction mixture was warmed to room temperature and stirred for 1 h. After completion of the reaction (monitored by TLC), the mixture was extracted with ethyl acetate and washed with NaOH and brine. The organic phase was dried over anhydrous Na_2SO_4 and concentrated in vacuo and purified by column chromatography to afford desired product **2a** as white solid with 83% yield.

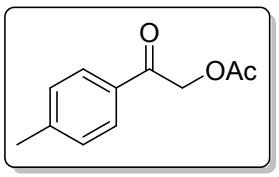
Analytical Data for Products.

2-oxo-2-phenylethyl acetate (**2a**)[5]



Colorless oil (90%, 32.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2 H), 7.63-7.59 (t, *J* = 7.6 Hz, 1 H), 7.50-7.46 (t, *J* = 7.6 Hz, 2 H), 5.34 (s, 2 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.13, 170.41, 134.18, 133.87, 128.84, 127.73, 65.99, 20.55. EI-MS: m/z 178.

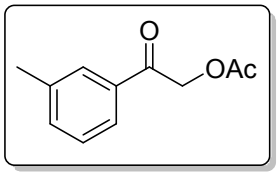
2-oxo-2-(p-tolyl)ethyl acetate (**2b**)[5]



White solid (73%, 28.0 mg), melting point: 80−82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.80 (d, J = 8.0 Hz, 2 H), 7.29-7.27 (d, *J* = 8.0 Hz, 2 H), 5.32 (s, 2 H), 2.42 (s, 3 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.72, 170.43, 144.82, 131.67, 129.48,

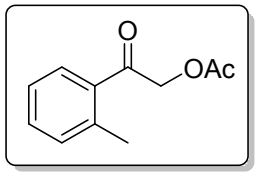
127.80, 65.91, 21.69, 20.54. EI-MS: m/z 192.

2-oxo-2-(m-tolyl)ethyl acetate (**2c**)[6]



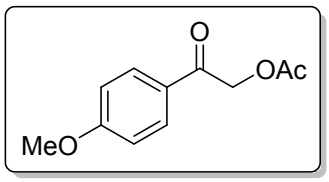
Colorless oil (86%, 33.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.69 (m, 2 H), 7.42-7.34 (m, 2 H), 5.33 (s, 2 H), 2.41 (s, 3 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.27, 170.40, 138.71, 134.61, 134.18, 128.66, 128.21, 124.86, 66.01, 21.26, 20.53. EI-MS: m/z 192.

2-oxo-2-(o-tolyl)ethyl acetate (**2d**)[7]



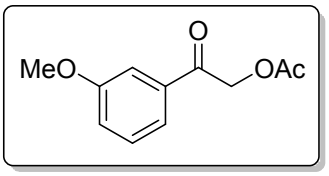
Colorless oil (73%, 27.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.59 (m, 1 H), 7.44-7.40 (m, 1 H), 7.29-7.26 (m, 2 H), 5.18 (s, 2 H), 2.51 (s, 3 H), 2.21 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.75, 170.41, 139.04, 134.32, 132.22, 132.12, 128.00, 125.72, 67.26, 21.07, 20.50. EI-MS: m/z 192.

2-(4-methoxyphenyl)-2-oxoethyl acetate (**2e**)[6]



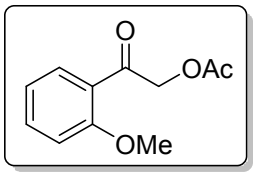
Yellow oil (36%, 15.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.88 (m, 2 H), 6.98-6.94 (m, 2 H), 5.30 (s, 2 H), 3.88 (s, 3 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.58, 170.50, 164.02, 130.04, 127.18, 114.02, 65.73, 55.51, 20.60. EI-MS: m/z 208.

2-(3-methoxyphenyl)-2-oxoethyl acetate (**2f**)[8]



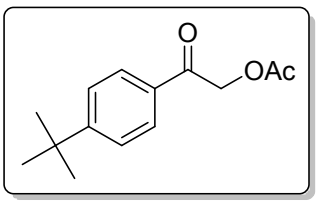
Colorless oil (60%, 25.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.44 (m, 2 H), 7.41-7.37 (m, 1 H), 7.16-7.13 (m, 1 H), 5.32 (s, 2 H), 3.85 (s, 3 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.96, 170.38, 159.93, 135.41, 129.82, 120.36, 120.11, 112.01, 66.05, 55.43, 20.53. EI-MS: m/z 208.

2-(2-methoxyphenyl)-2-oxoethyl acetate (**2g**)[9]



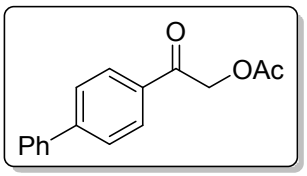
Yellow solid (53%, 22.0 mg), melting point: 58−60 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.92 (m, 1 H), 7.55-7.50 (m, 1 H), 7.06-6.98 (m, 2 H), 5.24 (s, 2 H), 3.94 (s, 3 H), 2.21 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.00, 170.57, 159.46, 134.88, 131.01, 124.30, 121.00, 111.45, 69.96, 55.52, 20.62. EI-MS: m/z 208.

2-(4-(tert-butyl)phenyl)-2-oxoethyl acetate (**2h**)[6]



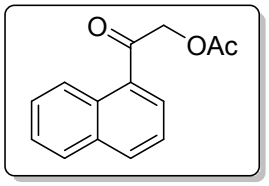
Colorless oil (77%, 36.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.85 (m, 2 H), 7.52-7.49 (m, 2 H), 5.34 (s, 2 H), 2.24 (s, 3 H), 1.34 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.69, 170.43, 157.71, 131.48, 127.65, 125.76, 65.93, 35.16, 30.95, 20.57. EI-MS: m/z 234.

2-([1,1'-biphenyl]-4-yl)-2-oxoethyl acetate (**2i**)[5]



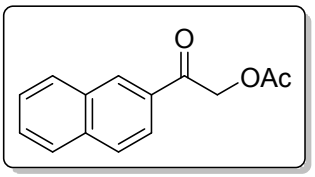
White solid (71%, 36.0 mg), melting point: 96−98 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.97 (m, 2 H), 7.71-7.69 (m, 2 H), 7.63-7.61 (m, 2 H), 7.49-7.45 (m, 2 H), 7.42-7.38 (m, 1 H), 5.36 (s, 2 H), 2.24 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.73, 170.44, 146.56, 139.57, 132.83, 128.97, 128.40, 128.32, 127.43, 127.24, 66.00, 20.56. EI-MS: m/z 254.

2-(naphthalen-1-yl)-2-oxoethyl acetate (**2j**)[5]



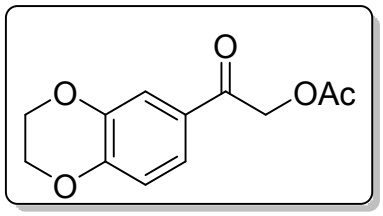
Yellow solid (61%, 27.8 mg), melting point: 88−90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64-8.62 (d, J = 8.4 Hz, 1 H), 8.04-8.02 (d, J = 8.0 Hz, 1 H), 7.89-7.84 (m, 2 H), 7.63-7.48 (m, 3 H), 5.31 (s, 2 H), 2.25 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.07, 170.51, 133.90, 133.51, 132.30, 130.17, 128.44, 128.33, 127.43, 126.75, 125.50, 124.19, 67.46, 20.57. EI-MS: m/z 228.

2-(naphthalen-2-yl)-2-oxoethyl acetate (**2k**)[10]



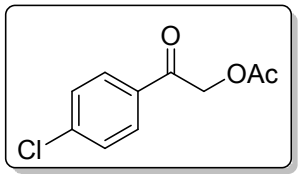
White solid (67%, 30.6 mg), melting point: 68−70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1 H), 7.97-7.86 (m, 4 H), 7.64-7.54 (m, 2 H), 5.47 (s, 2 H), 2.25 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.05, 170.46, 135.83, 132.31, 131.46, 129.51, 129.44, 128.83, 128.78, 127.83, 127.01, 123.21, 66.05, 20.58. EI-MS: m/z 228.

2-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-2-oxoethyl acetate (**2l**)



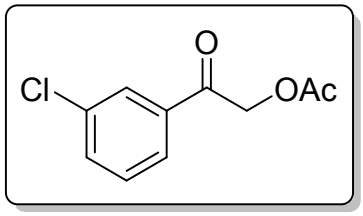
Colorless oil (72%, 34.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.43 (m, 2 H), 6.93-6.91 (m, 1 H), 5.27 (s, 2 H), 4.33-4.31 (m, 2 H), 4.29-4.27 (m, 2 H), 2.22 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.44, 170.39, 148.59, 143.48, 127.77, 121.75, 117.44, 117.17, 65.71, 64.62, 63.99, 20.54. EI-MS: m/z 236.

2-(4-chlorophenyl)-2-oxoethyl acetate (**2m**)[5]



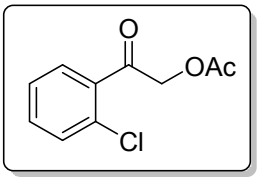
White solid (87%, 36.9 mg), melting point: 70−72 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.83 (m, 2 H), 7.48-7.44 (m, 2 H), 5.30 (s, 2 H), 2.22 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.06, 170.33, 140.33, 132.43, 129.17, 129.11, 65.79, 20.46. EI-MS: m/z 212.

2-(3-chlorophenyl)-2-oxoethyl acetate (**2n**)[6]



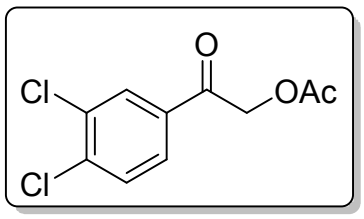
Colorless oil (71%, 30.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.88 (m, 1 H), 7.80-7.78 (m, 1 H), 7.60-7.57 (m, 1 H), 7.46-7.42 (m, 1 H), 5.31 (s, 2 H), 2.24 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.04, 170.35, 135.54, 135.19, 133.82, 130.19, 127.85, 125.77, 65.88, 20.50. EI-MS: m/z 212.

2-(2-chlorophenyl)-2-oxoethyl acetate (**2o**)



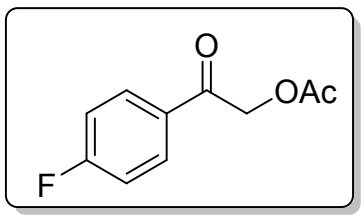
Yellow oil (78%, 33.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.60 (m, 1 H), 7.45-7.43 (m, 2 H), 7.38-7.34 (m, 1 H), 5.20 (s, 2 H), 2.18 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.25, 170.29, 135.77, 132.76, 131.53, 130.54, 129.93, 127.08, 68.23, 20.38. EI-MS: m/z 212.

2-(3,4-dichlorophenyl)-2-oxoethyl acetate (**2p**)



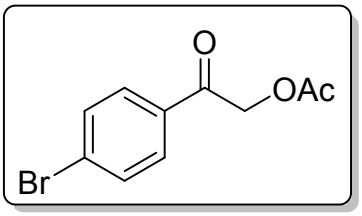
White solid (80%, 39.3 mg), melting point: 68−70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.99 (m, 1 H), 7.75-7.72 (m, 1 H), 7.59-7.57 (m, 1 H), 5.27 (s, 2 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.23, 170.26, 138.53, 133.64, 133.59, 130.99, 129.74, 126.69, 65.72, 20.44. EI-MS: m/z 246.

2-(4-fluorophenyl)-2-oxoethyl acetate (**2q**)[6]



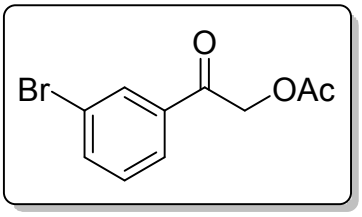
White solid (87%, 34.1 mg), melting point: 48−50 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98-7.92 (m, 2 H), 7.19-7.14 (m, 2 H), 5.30 (s, 2 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.63, 170.33, 167.36-164.81 (d, J = 255 Hz), 130.48, 130.39, 116.17-115.96 (d, J = 21 Hz), 65.76, 20.49. EI-MS: m/z 196.

2-(4-bromophenyl)-2-oxoethyl acetate (**2r**)[5]



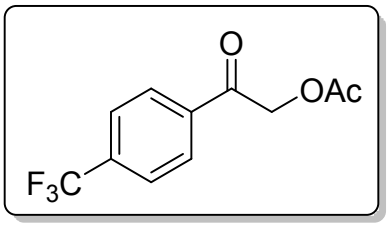
White solid (95%, 48.6 mg), melting point: 72−74 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.76 (m, 2 H), 7.65-7.61 (m, 2 H), 5.29 (s, 2 H), 2.22 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.25, 170.32, 132.78, 132.15, 129.17, 129.08, 65.77, 20.47. EI-MS: m/z 256.

2-(3-bromophenyl)-2-oxoethyl acetate (**2s**)[8]



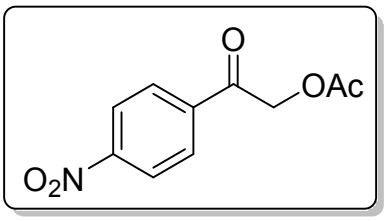
White solid (78%, 40.0 mg), melting point: 60−62 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (m, 1 H), 7.84-7.82 (m, 1 H), 7.75-7.73 (m, 1 H), 7.40-7.36 (m, 1 H), 5.30 (s, 2 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.95, 170.31, 136.71, 135.72, 130.77, 130.41, 126.19, 123.13, 65.83, 20.49. EI-MS: m/z 256.

2-oxo-2-(4-(trifluoromethyl)phenyl)ethyl acetate (**2t**)[7]



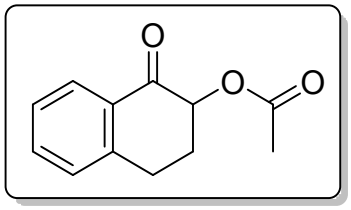
White solid (57%, 28.0 mg), melting point: 76−78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.02 (d, J = 8.0 Hz, 2 H), 7.77-7.75 (d, J = 8.0 Hz, 2 H), 5.34 (s, 2 H), 2.24 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.46, 170.31, 136.83, 135.59-134.62 (q, J = 32 Hz), 128.15, 125.98-125.87 (q, J = 4 Hz), 127.43-119.30 (q, J = 271 Hz), 65.99, 20.45. EI-MS: m/z 246.

2-(4-nitrophenyl)-2-oxoethyl acetate (**2u**)[5]



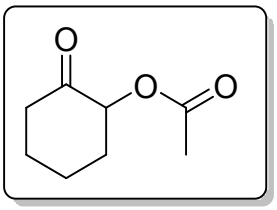
White Solide (49%, 21.8 mg), melting point: 118−120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.33 (m, 2 H), 8.10-8.06 (m, 2 H), 5.34 (s, 2 H), 2.24 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.08, 170.25, 150.73, 138.65, 128.90, 124.07, 66.04, 20.41. EI-MS: m/z 223.

1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl acetate (**2v**)[5]



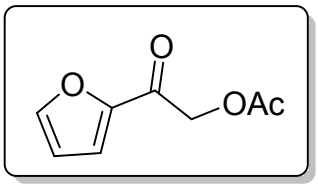
White solide (91%, 37.1 mg), melting point: 74−76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03-8.01 (m, 1 H), 7.52-7.48 (m, 1 H), 7.35-7.25 (m, 2 H), 5.57 (m, 1 H), 3.25-3.17 (m, 1 H), 3.11-3.05 (m, 1 H), 2.43-2.36 (m, 1 H), 2.34-2.26 (m, 1 H), 2.22 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.90, 170.13, 143.01, 133.85, 131.51, 128.58, 127.75, 126.90, 74.52, 29.08, 27.89, 20.80. EI-MS: m/z 204.

2-oxocyclohexyl acetate (**2w**)[5]



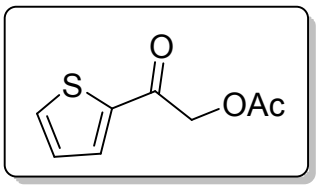
Colorless oil (33%, 10.3 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.19-5.14 (m, 1 H), 2.55-2.49 (m, 1 H), 2.44-2.35 (m, 1 H), 2.33-2.27 (m, 1 H), 2.16 (s, 3 H), 2.14-2.06 (m, 1 H), 2.02-1.93 (m, 1 H), 1.80-1.74 (m, 2 H), 1.68-1.60 (m, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.51, 170.01, 76.53, 40.67, 33.05, 27.13, 23.75, 20.70. EI-MS: m/z 156.

2-(furan-2-yl)-2-oxoethyl acetate (**2y**)[10]



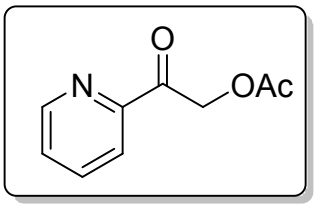
Colorless oil (30%, 10.1 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.61 (m, 1 H), 7.29-7.28 (d, J = 3.6 Hz, 1 H), 6.59-6.58 (dd, J_1 = 3.6 Hz, J_2 = 1.6 Hz, 1 H), 5.19 (s, 2 H), 2.22 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.69, 170.34, 150.53, 146.75, 117.73, 112.49, 65.33, 20.50. EI-MS: m/z 168.

2-oxo-2-(thiophen-2-yl)ethyl acetate (**2z**)[10]



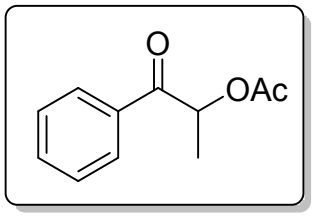
Colorless oil (54%, 19.9 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.76 (dd, J_1 = 4.0 Hz, J_2 = 1.2 Hz, 1 H), 7.72-7.71 (dd, J_1 = 4.8 Hz, J_2 = 1.2 Hz, 1 H), 7.18-7.16 (dd, J_1 = 4.8 Hz, J_2 = 4.0 Hz, 1 H), 5.23 (s, 2 H), 2.23 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.37, 170.31, 140.28, 134.32, 131.94, 128.25, 65.69, 20.51. EI-MS: m/z 184.

2-oxo-2-(pyridin-2-yl)ethyl acetate (**2aa**)[11]



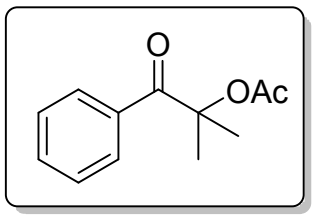
Colorless oil (77%, 27.6 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66-8.65 (m, 1 H), 8.04-8.02 (m, 1 H), 7.88-7.84 (m, 1 H), 7.53-7.50 (m, 1 H), 5.62 (s, 2 H), 2.24 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.42, 170.47, 151.52, 149.02, 137.00, 127.84, 121.83, 66.82, 20.56. EI-MS: m/z 179.

1-oxo-1-phenylpropan-2-yl acetate (**2ab**)[5]



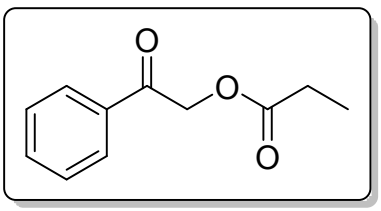
Colorless oil (94%, 36.0 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.93 (m, 2 H), 7.61-7.57 (m, 1 H), 7.50-7.46 (m, 2 H), 6.00-5.94 (q, *J* = 7.2 Hz, 1 H), 2.15 (s, 3 H), 1.54-1.52 (d, *J* = 7.2 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.82, 170.36, 134.27, 133.53, 128.72, 128.38, 71.35, 20.68, 17.09. EI-MS: m/z 192.

2-methyl-1-oxo-1-phenylpropan-2-yl acetate (**2ac**)[12]



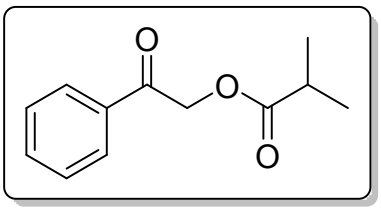
Colorless oil (98%, 40.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02-8.00 (m, 2 H), 7.51-7.48 (m, 1 H), 7.42-7.38 (m, 2 H), 1.93 (s, 3 H), 1.72 (s, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.07, 170.03, 134.56, 132.38, 128.38, 128.31, 84.20, 25.29, 21.31. EI-MS: m/z 206.

2-oxo-2-phenylethyl propionate (**2ad**)[7]



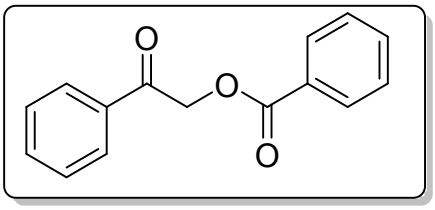
Colorless oil (84%, 32.2 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2 H), 7.63-7.59 (t, *J* = 7.6 Hz, 1 H), 7.51-7.47 (t, *J* = 7.6 Hz, 2 H), 5.35 (s, 2 H), 2.56-2.50 (q, *J* = 7.6 Hz, 2 H), 1.24-1.20 (d, *J* = 7.6 Hz, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.29, 173.88, 134.15, 133.81, 128.79, 127.69, 65.82, 27.17, 9.00. EI-MS: m/z 192.

2-oxo-2-phenylethyl isobutyrate (**2ae**)[13]



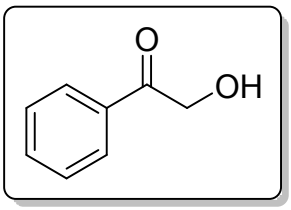
Colorless oil (86%, 35.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.90 (m, 2 H), 7.62-7.58 (m, 1 H), 7.50-7.46 (m, 2 H), 5.34 (s, 2 H), 2.80-2.69 (m, 1 H), 1.28 (s, 3 H), 1.26 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.34, 176.53, 134.20, 133.76, 128.78, 127.68, 65.72, 33.74, 18.93. EI-MS: m/z 206.

2-oxo-2-phenylethyl benzoate (**2af**)[7]



White Solide (66%, 31.7 mg), melting point: 104−106 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.13 (m, 2 H), 7.98-7.95 (m, 2 H), 7.64-7.57 (m, 2 H), 7.52-7.45 (m, 4 H), 5.58 (s, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.07, 166.01, 134.26, 133.86, 133.32, 129.94, 129.37, 128.86, 128.41, 127.80, 66.42. EI-MS: m/z 240.

2-hydroxy-1-phenylethan-1-one (**3a**)[14]



White solide (19%, 5.2 mg), melting point: 54−56 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.92 (m, 2 H), 7.66-7.62 (m, 1 H), 7.53-7.49 (m, 2 H), 4.89-4.88 (d, J = 4.8 Hz, 2 H), 3.52-3.50 (t, J = 4.8 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.38, 134.29, 133.38, 128.97, 127.68, 65.45. EI-MS: m/z 136.

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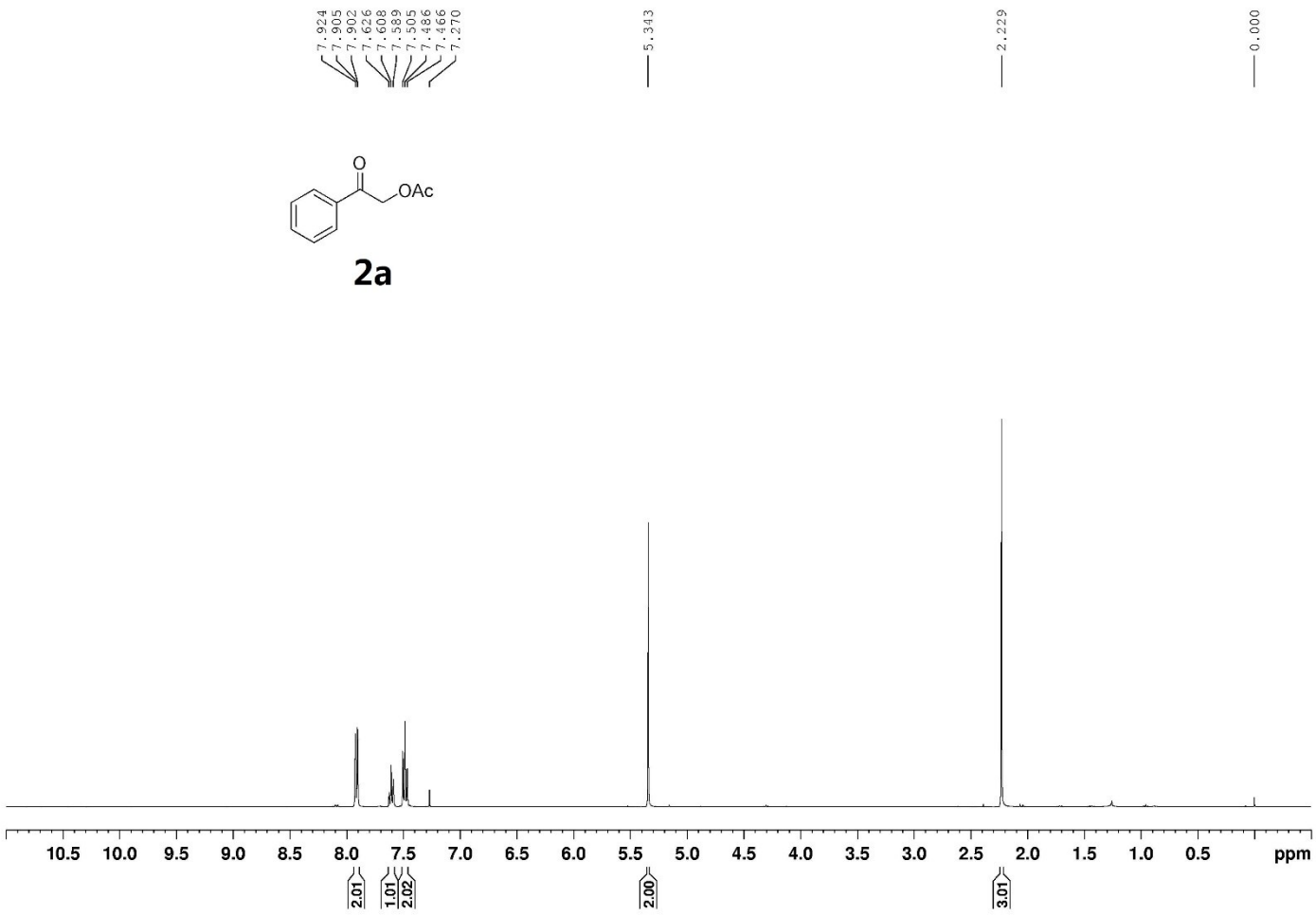
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7.505
7.486
7.466
7.270
5.343
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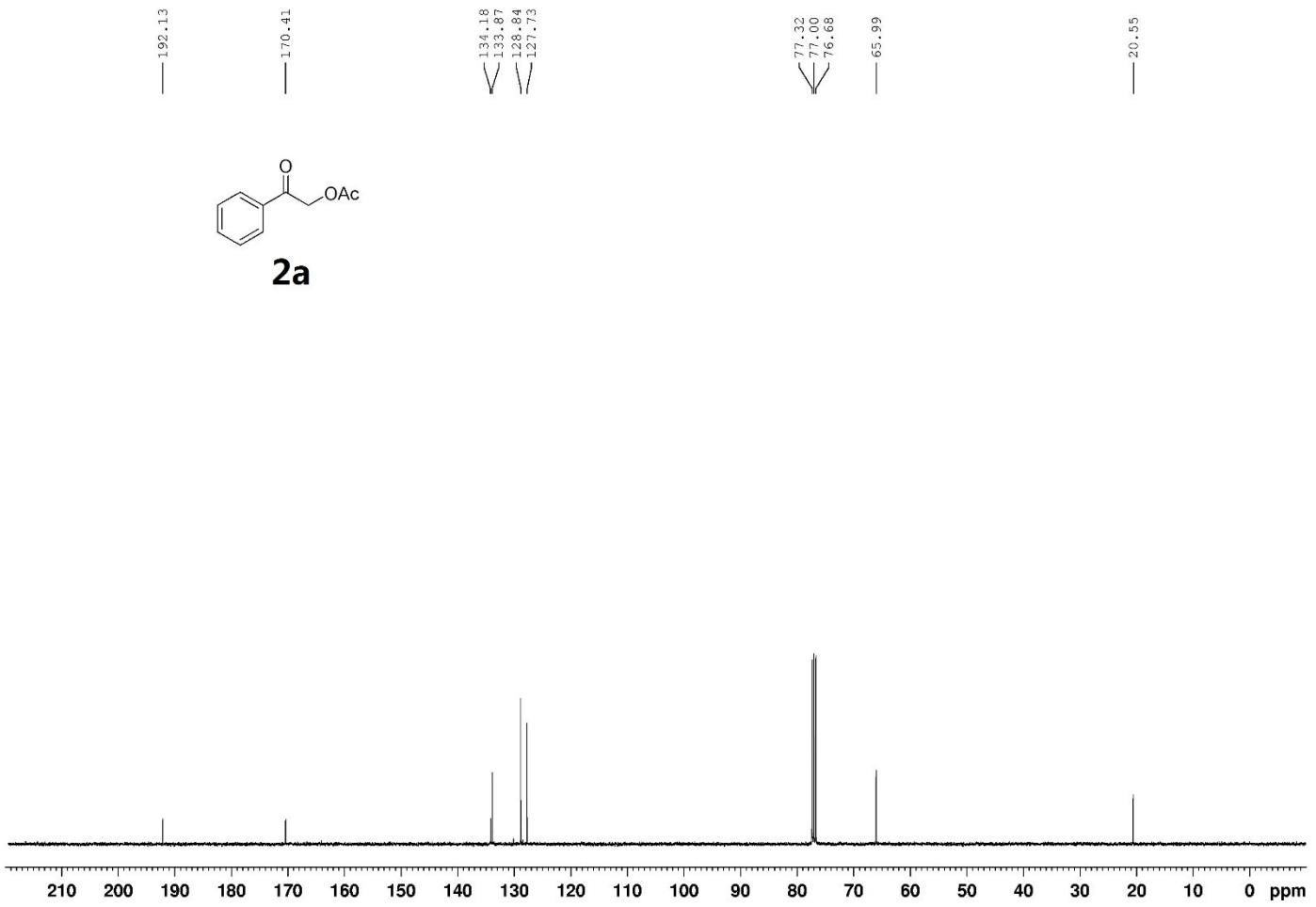
0.000
O
OAc
2a
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.01
1.01
2.02
2.00
3.01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127.73
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76.68
65.99
20.55
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OAc
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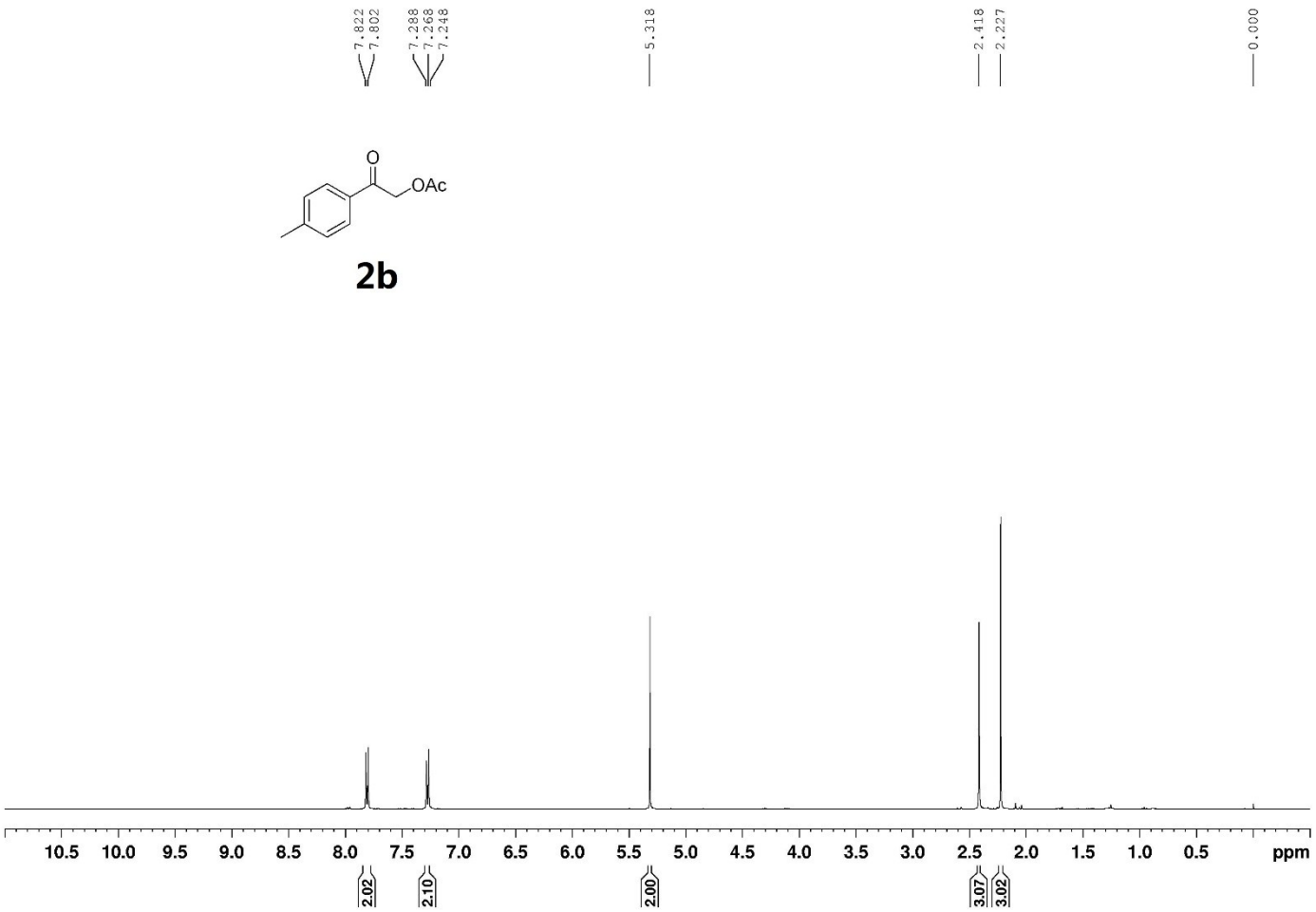
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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9.0
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8.0
7.5
7.0
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6.0
5.5
5.0
4.5
4.0
3.5
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0.5
ppm
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2.10
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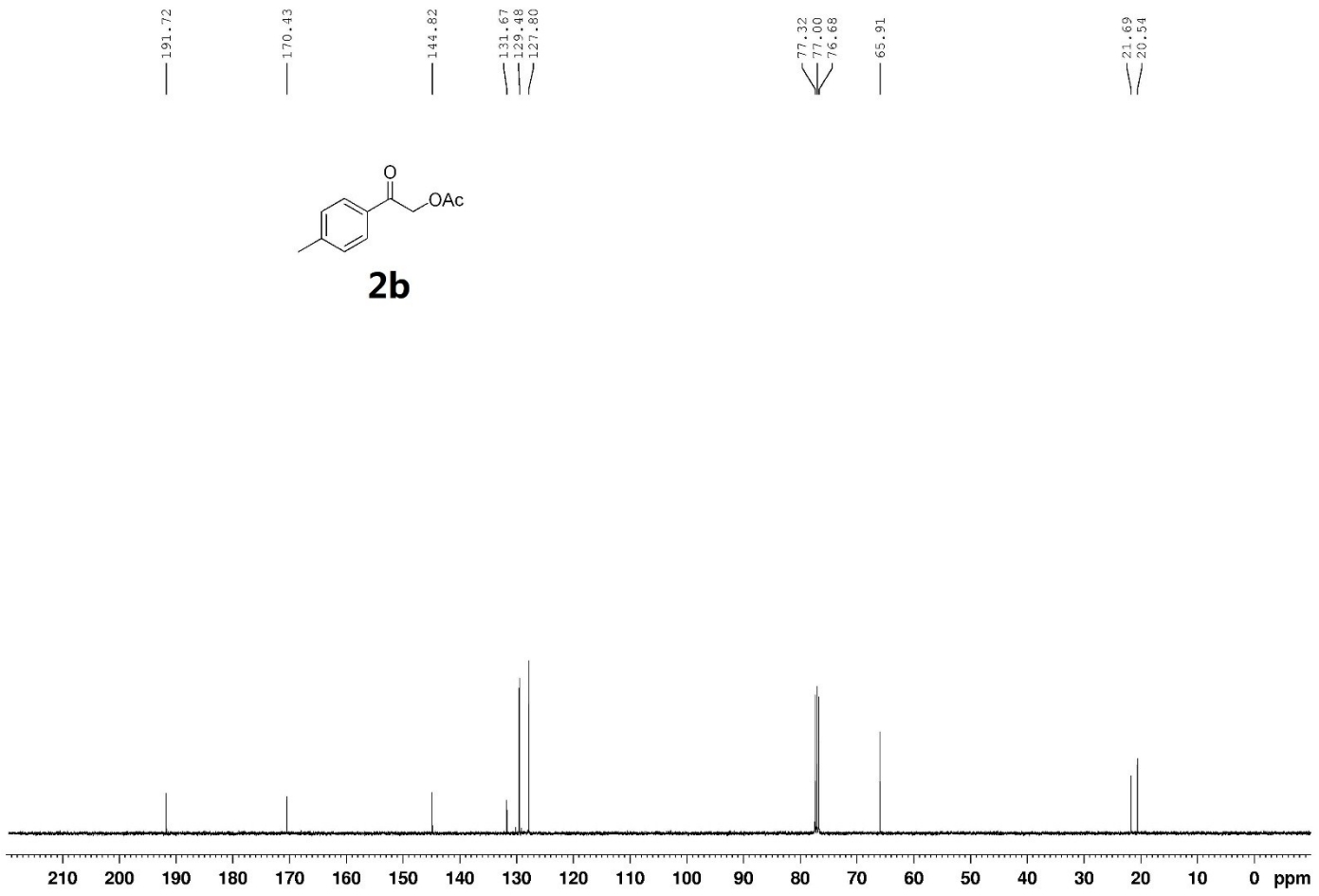
3.07
3.02

2b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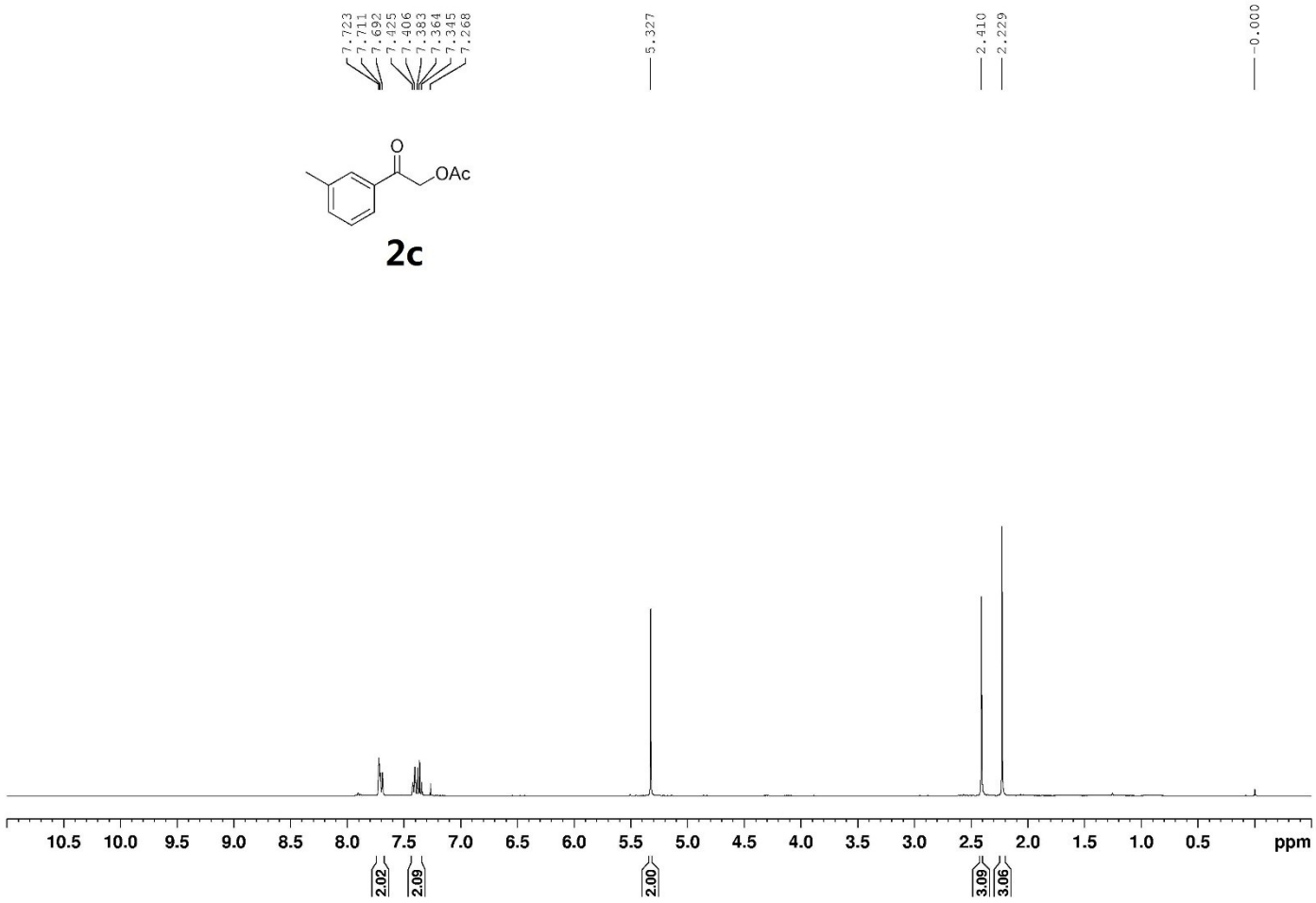
OAc
2b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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O
OAc
2c
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.02
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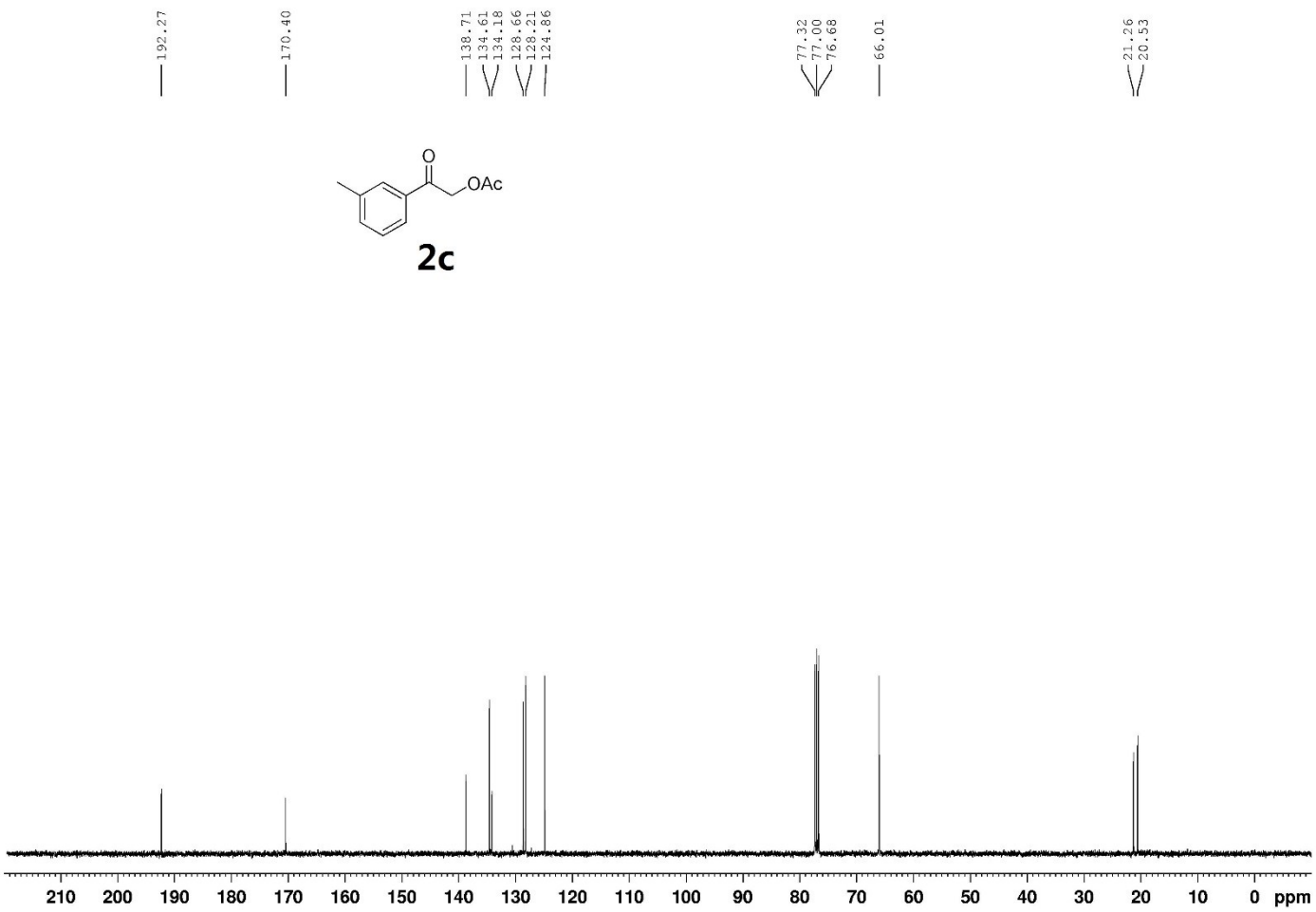
2.00
3.09
3.06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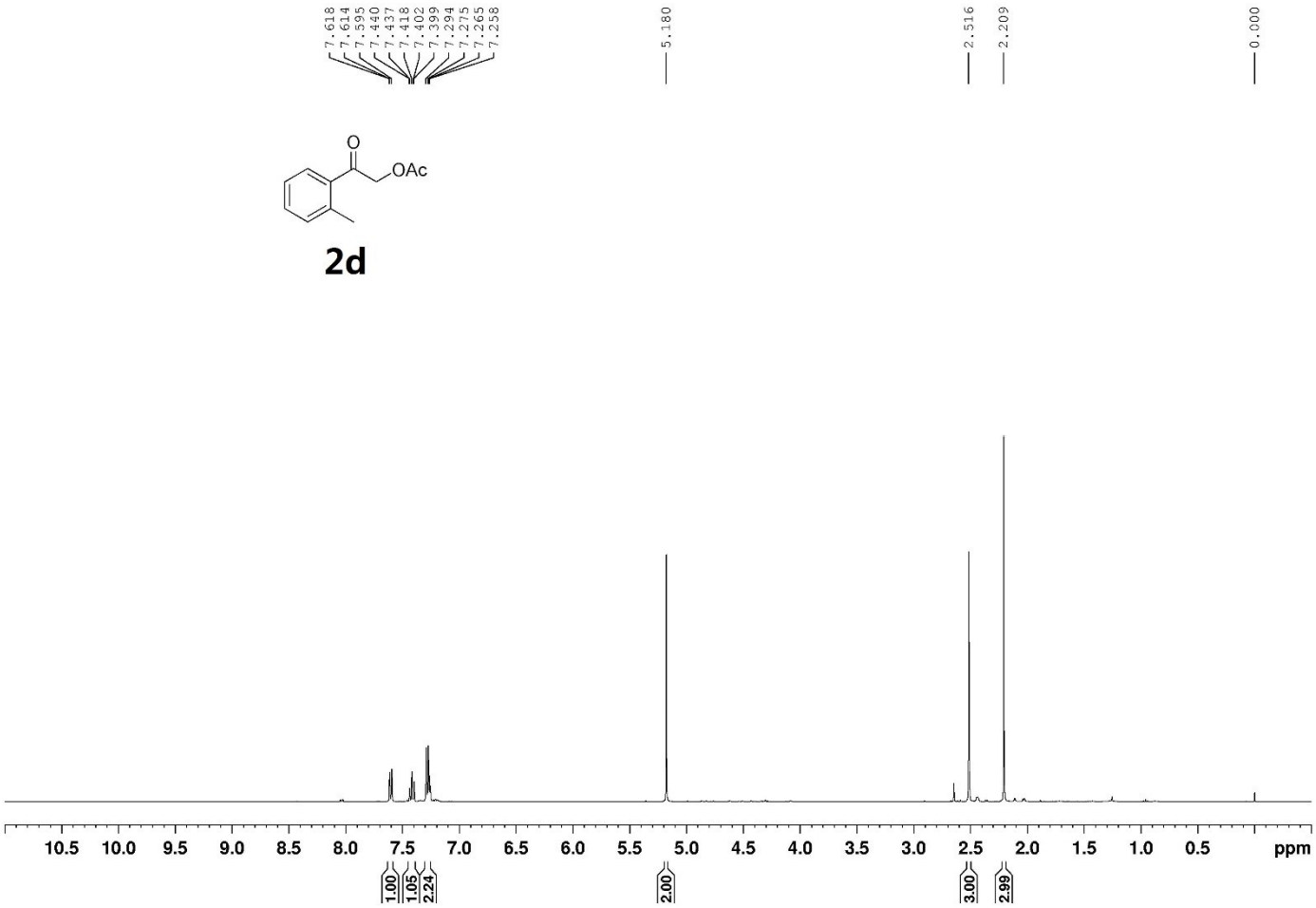
20.53
O
OAc
2c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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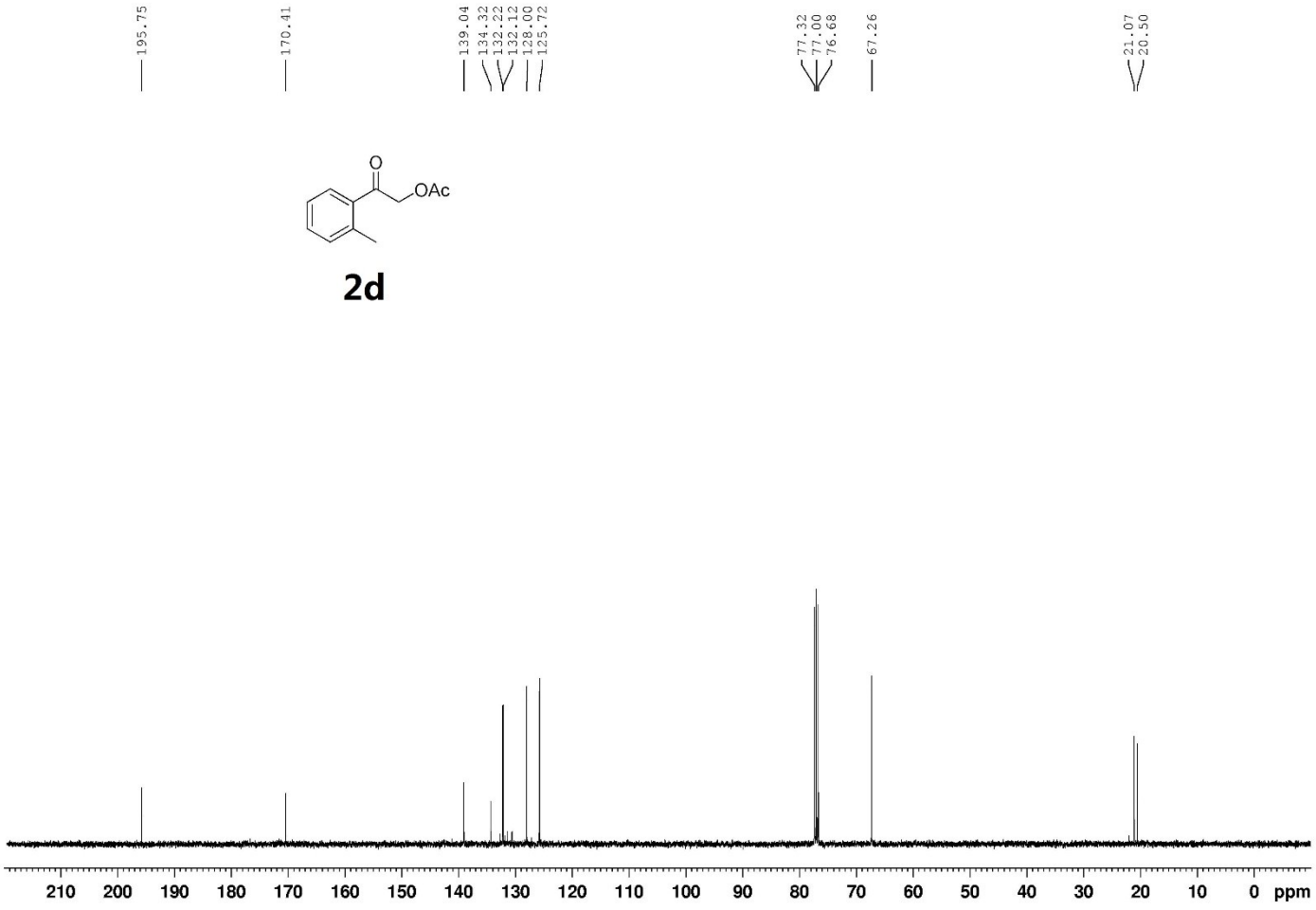
O
OAc
2d
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.05
2.24
2.00
3.00
2.99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132.12
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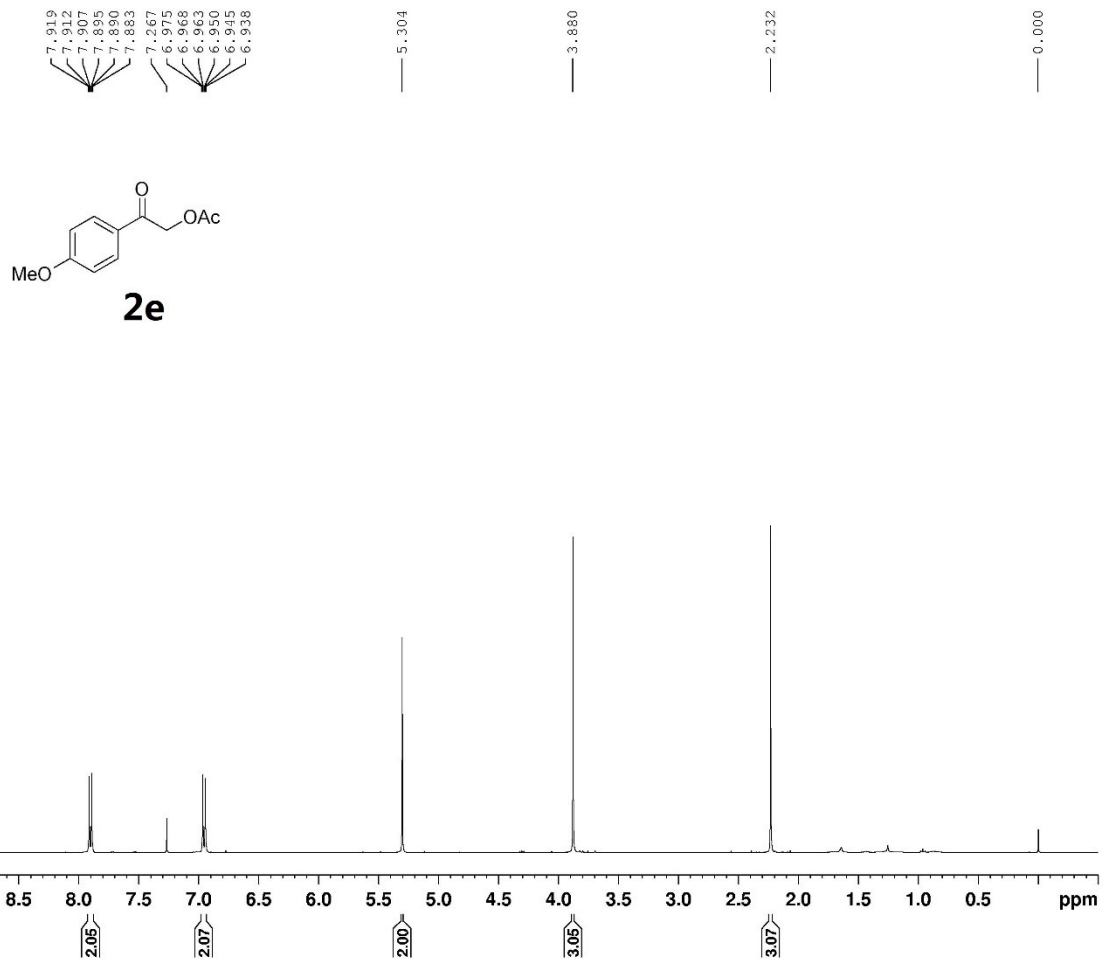
77.00
76.68
67.26
21.07
20.50
O
OAc
2d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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6.945
6.938
5.304
3.880
2.232
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MeO
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8.0
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7.0
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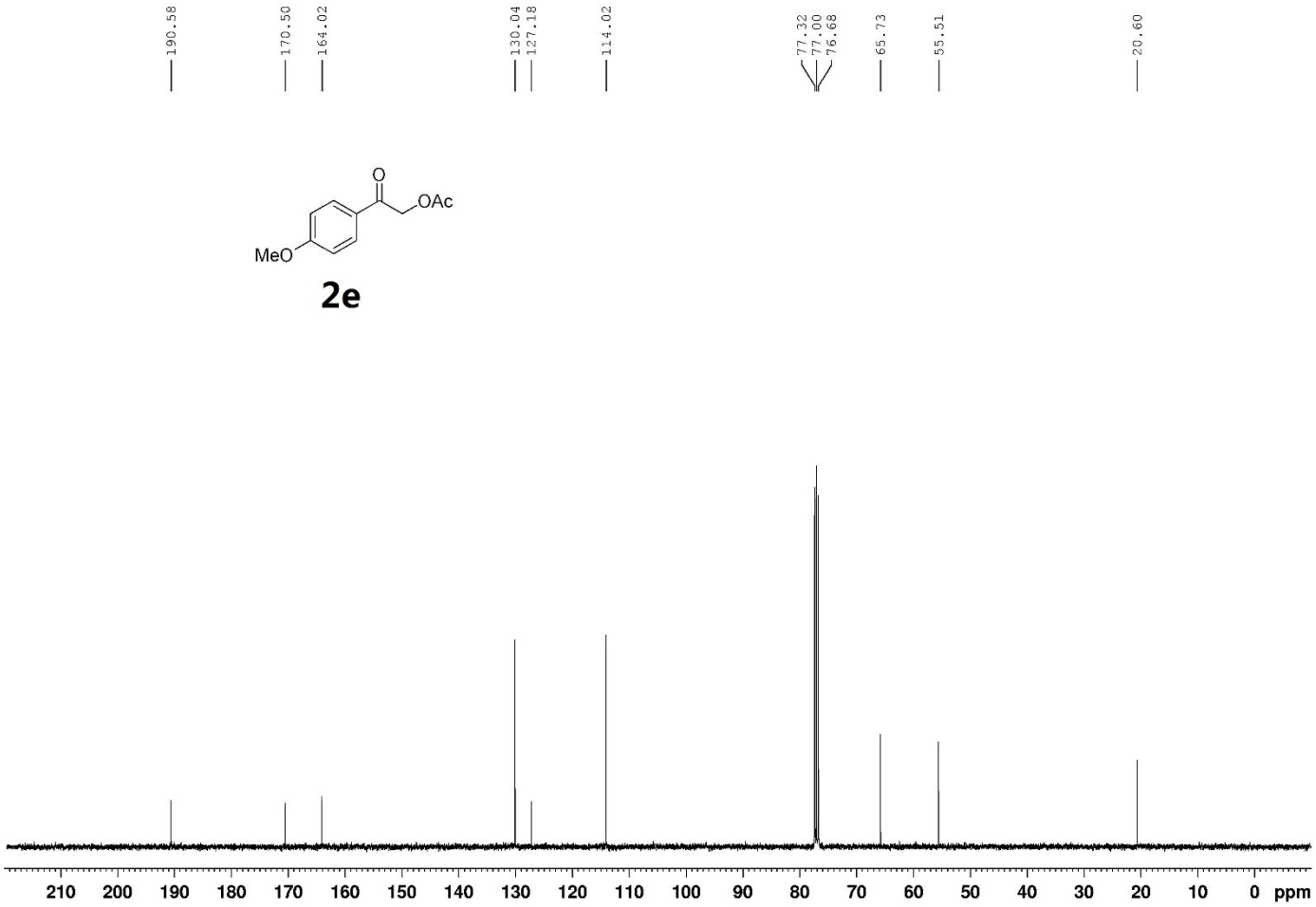
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20.60
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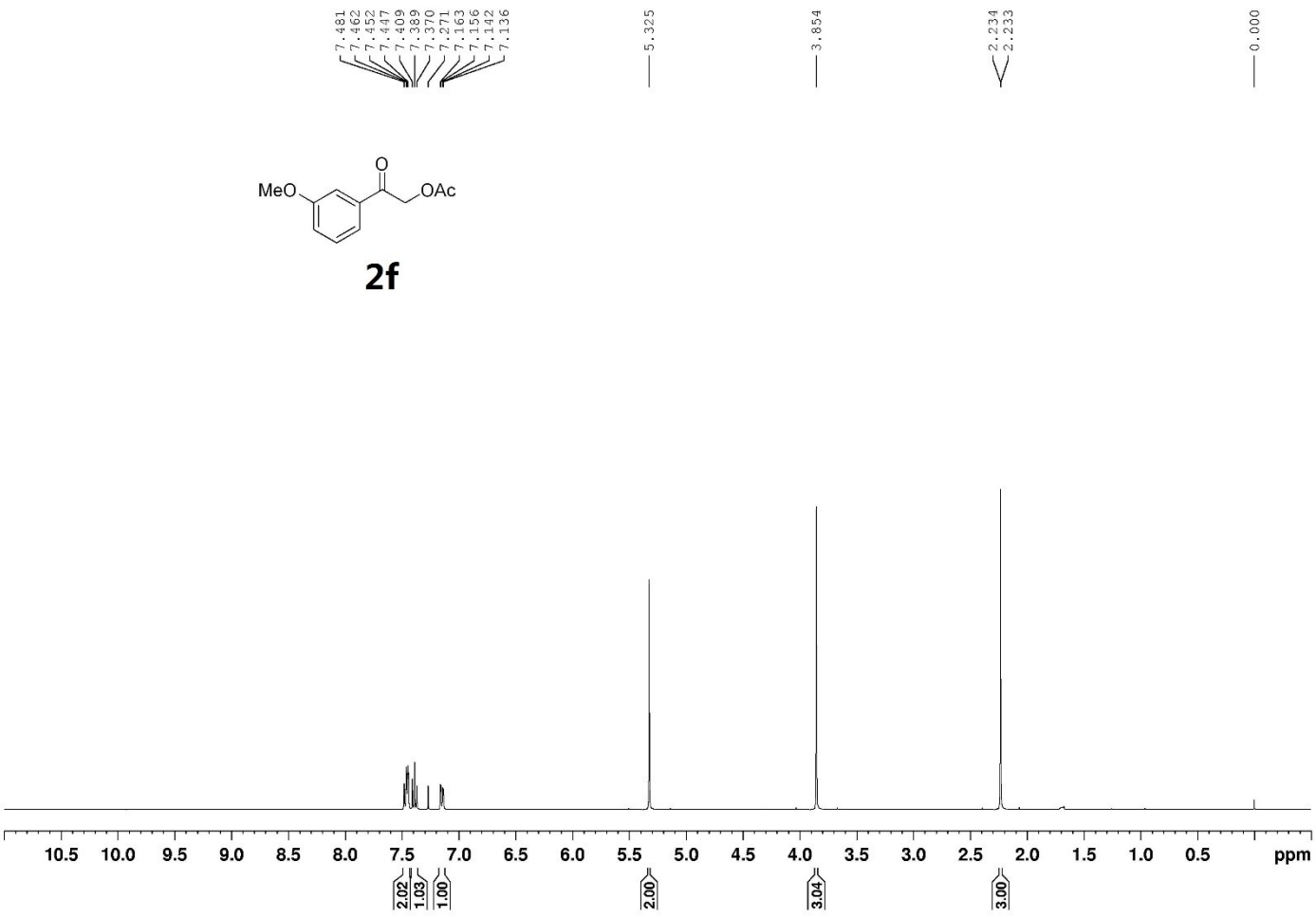
OAc
MeO
2e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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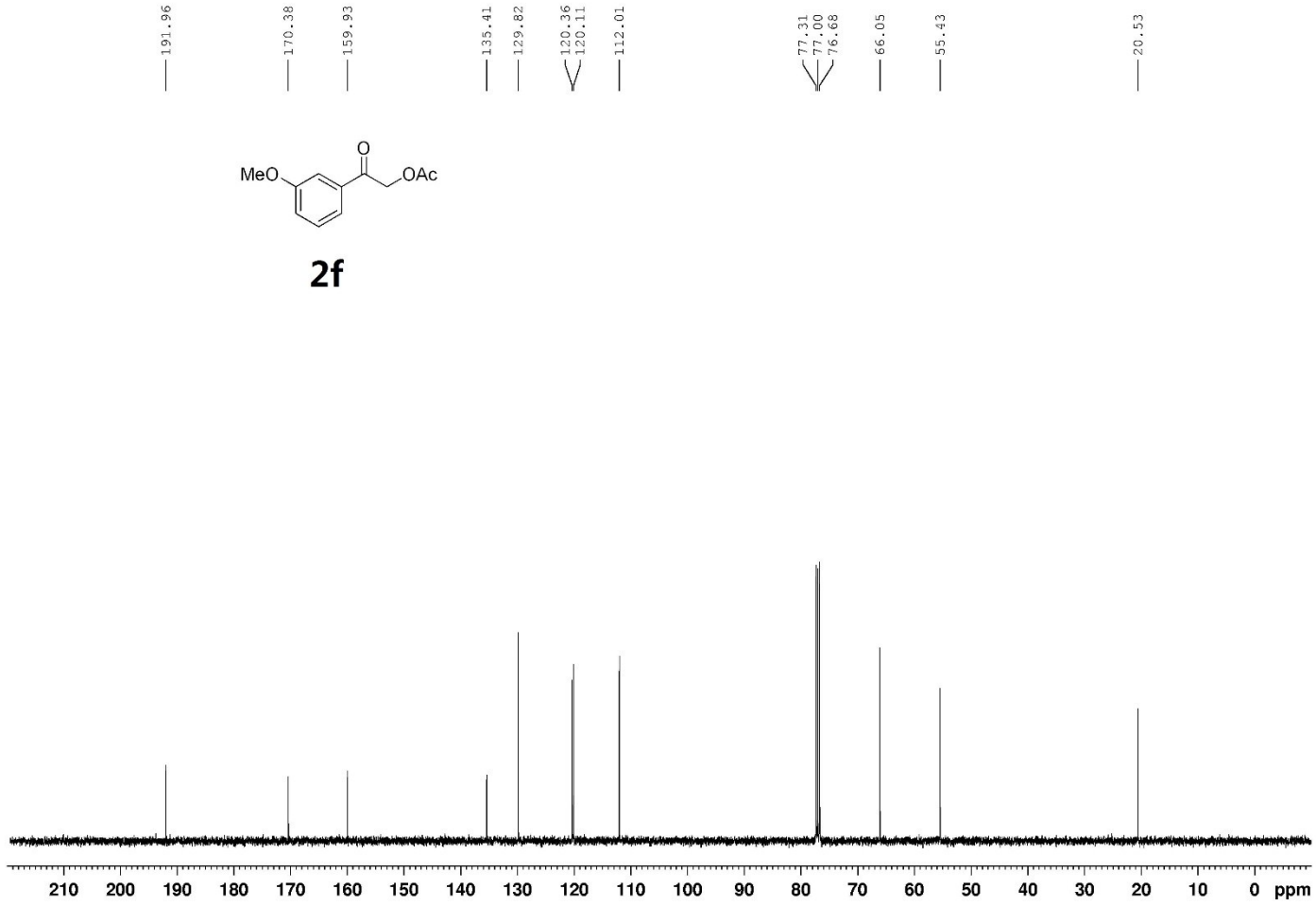
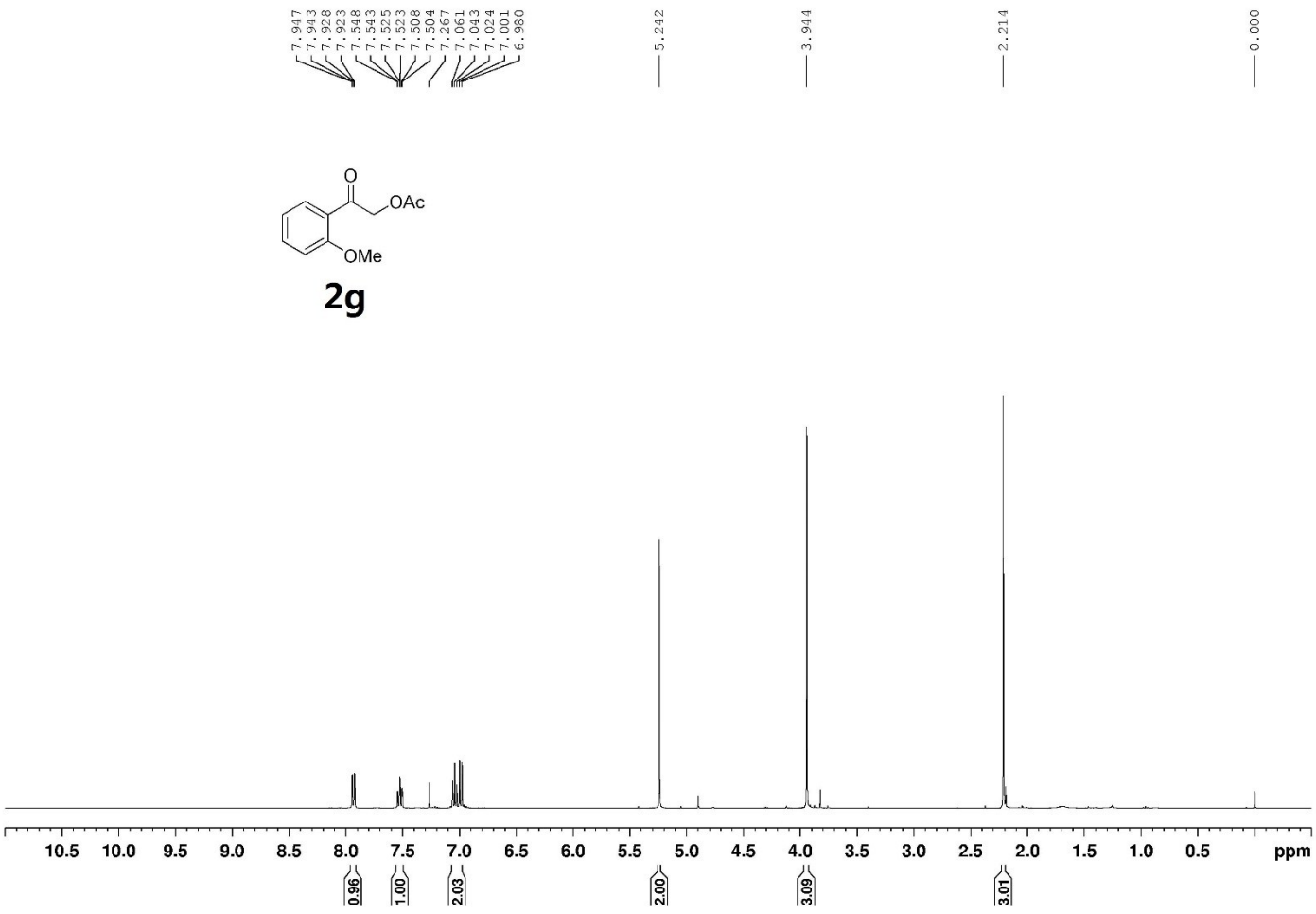
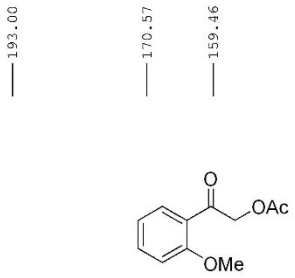
3.04
3.00


191.96
170.38
159.93
135.41
129.82
120.36
120.11
112.01
77.31
77.00
76.68
66.05
55.43
20.53
MeO
O
OAc
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

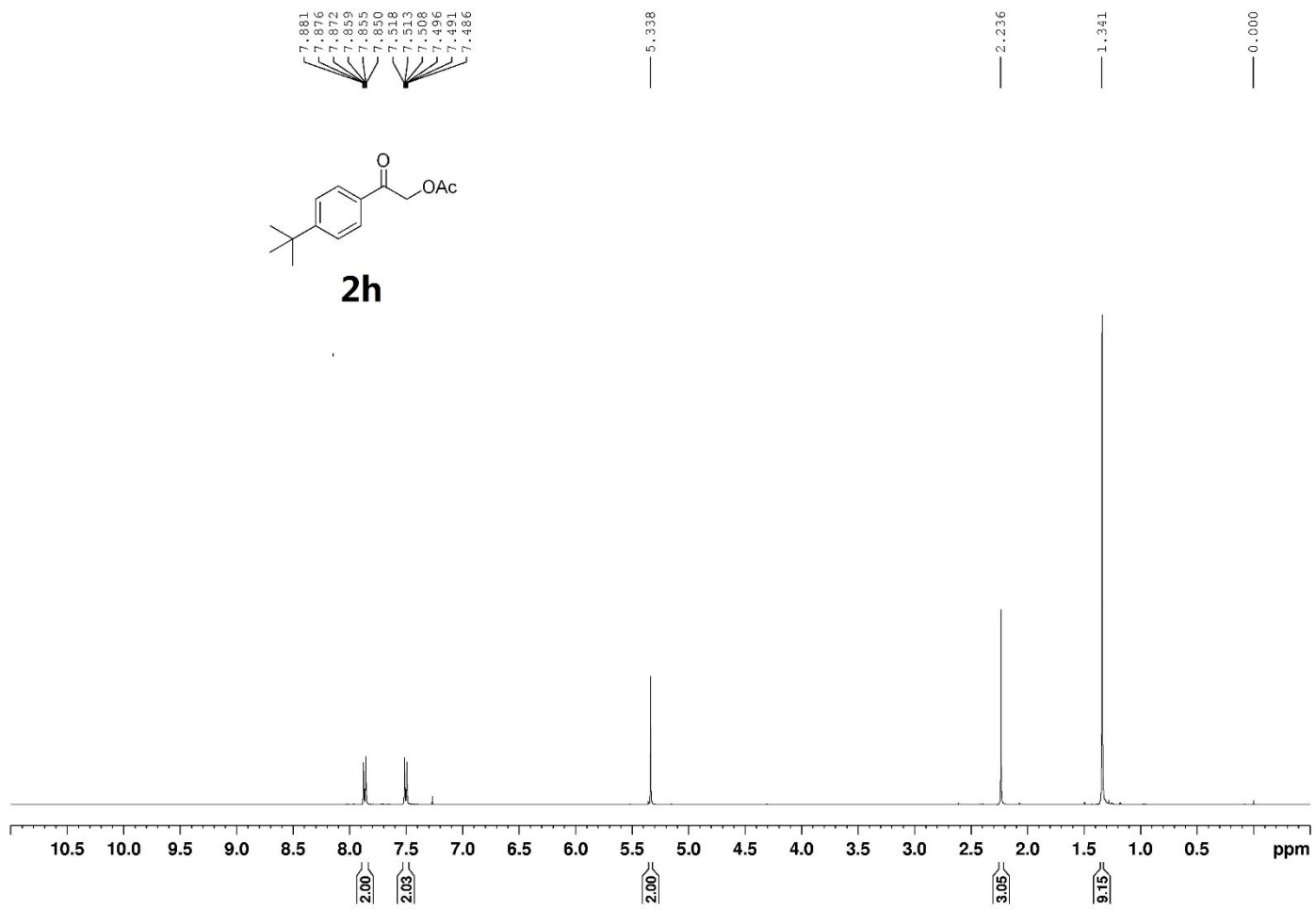
2f

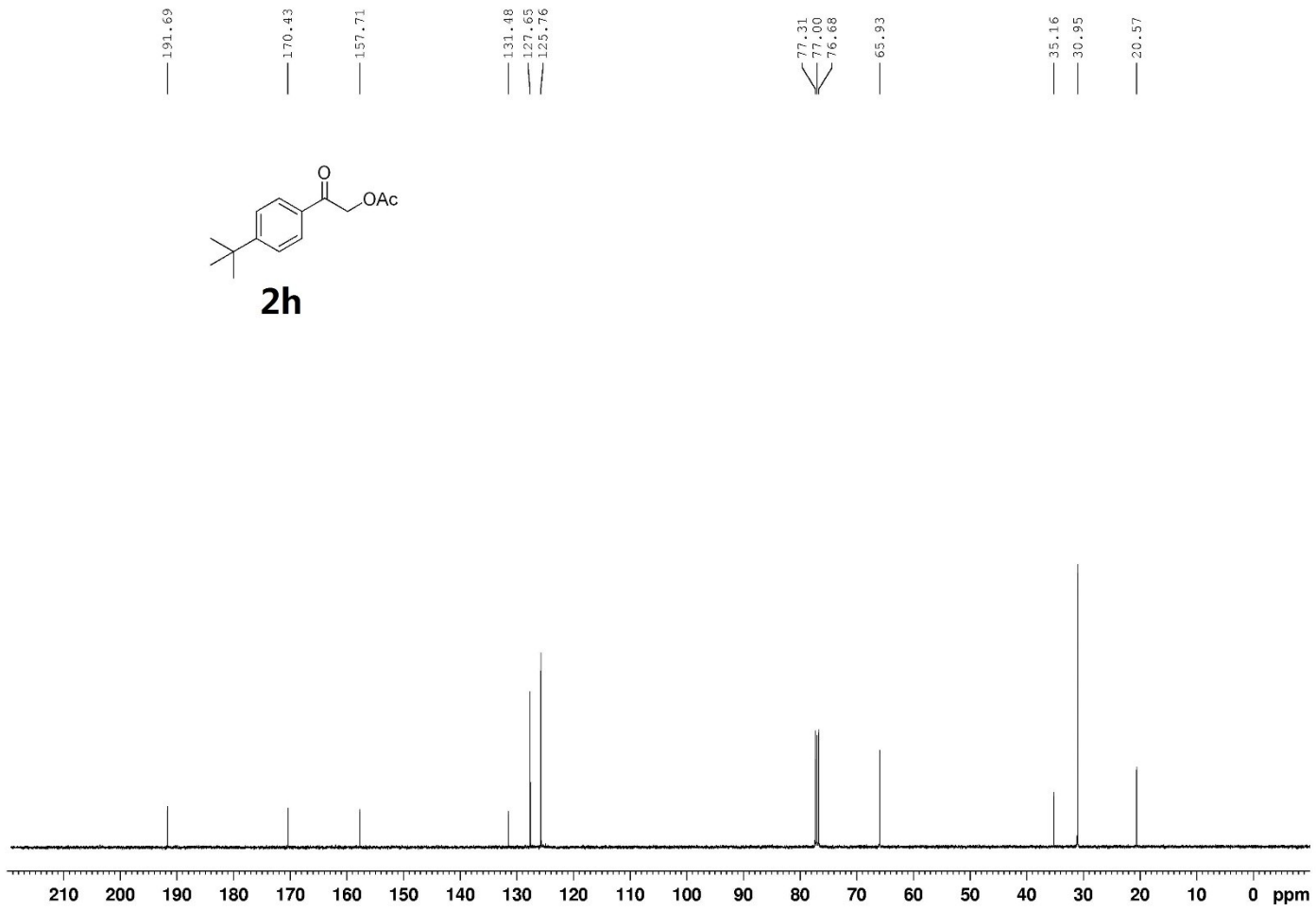

7.947
7.943
7.928
7.923
7.548
7.543
7.525
7.523
7.508
7.504
7.267
7.061
7.043
7.024
7.001
6.980
5.242
3.944
2.214
0.000
O
OAc
OMe
2g
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.96
1.00
2.03
2.00
3.09
3.01

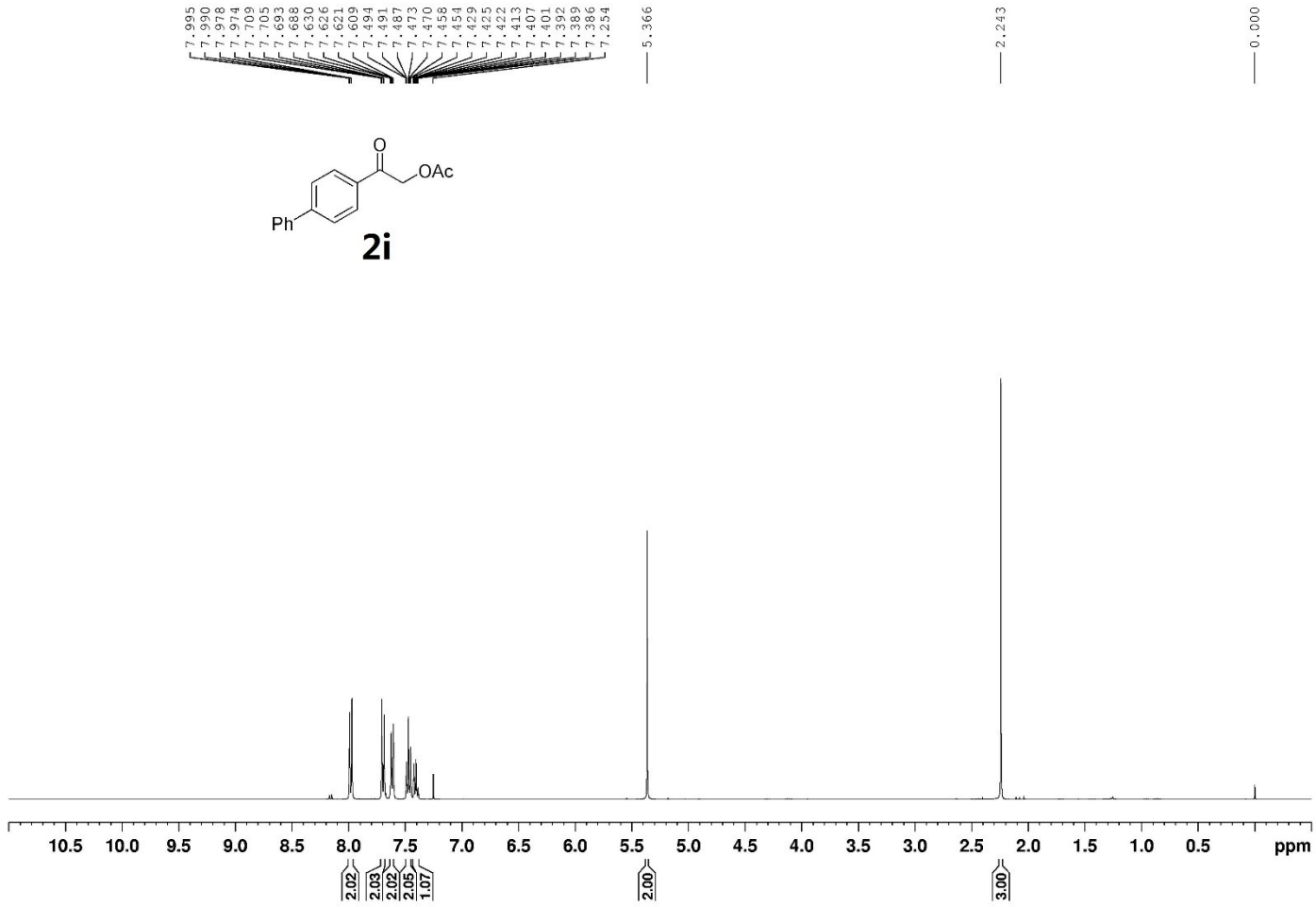

O
OAc
OMe

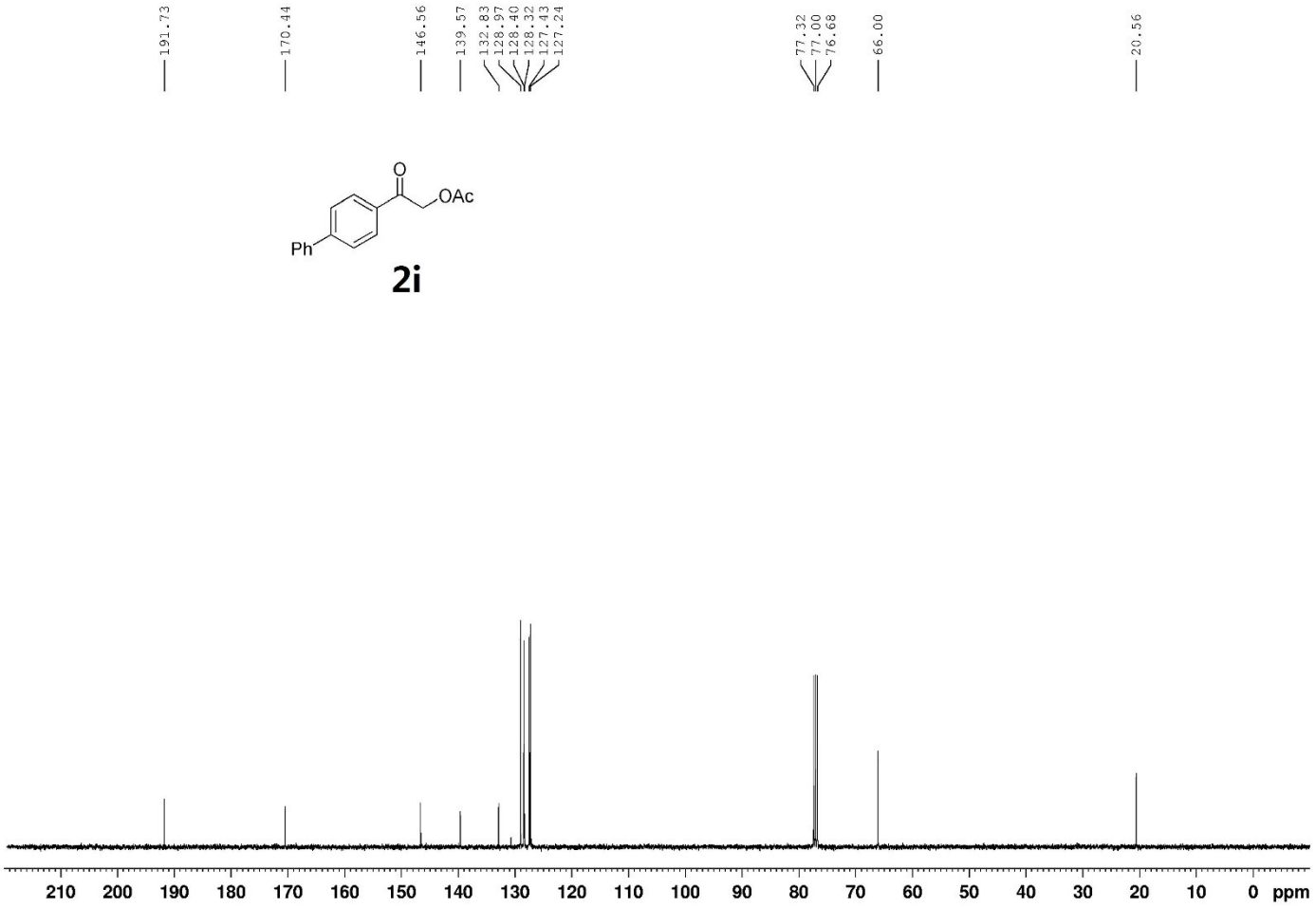
2g

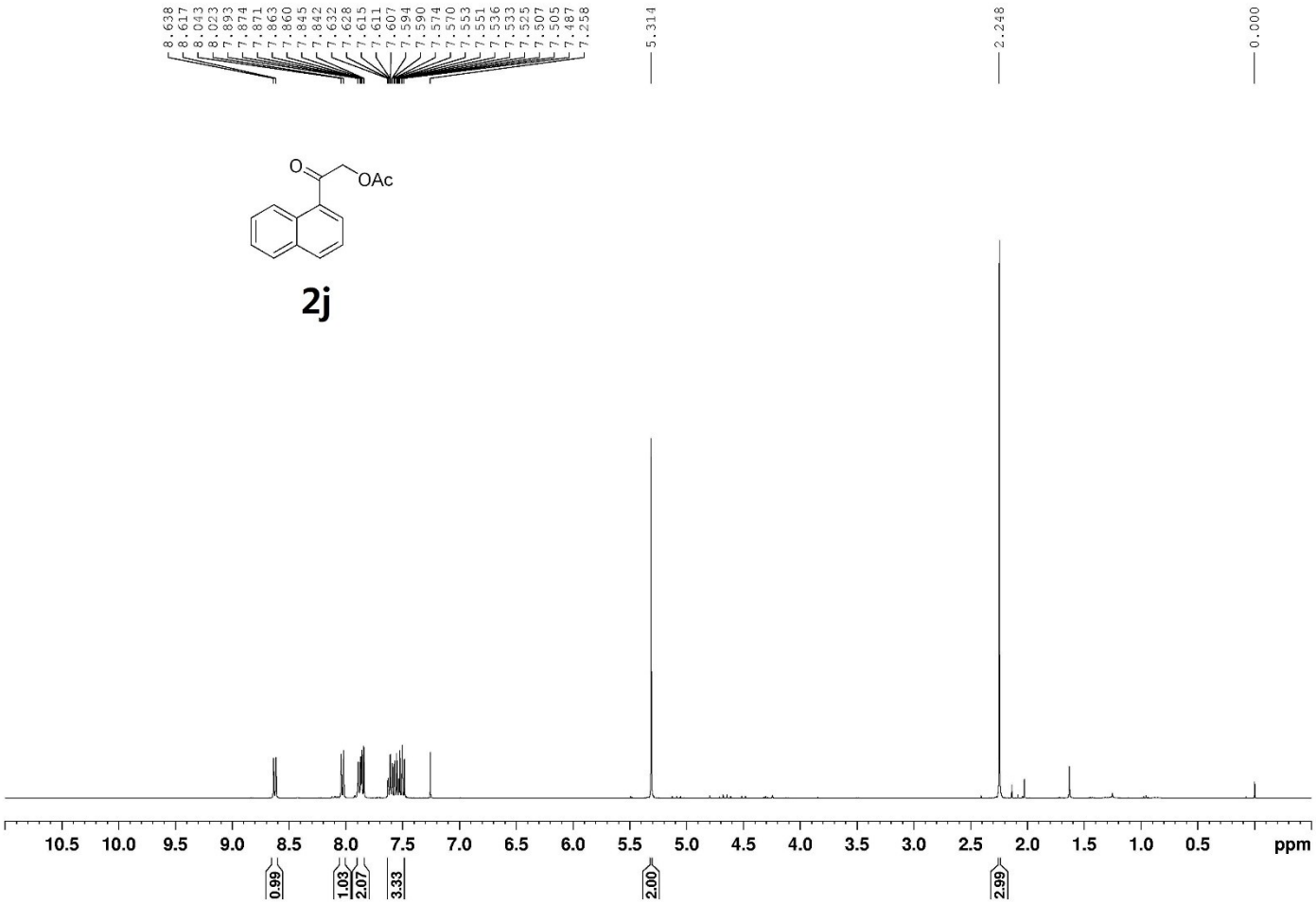
193.00
170.57
159.46
134.88
131.01
124.30
121.00
111.45
77.31
77.00
76.68
69.96
55.52
20.62
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.881
7.876
7.872
7.859
7.855
7.850
7.518
7.513
7.508
7.496
7.491
7.486
5.338
2.236
1.341
0.000
O
OAc
2h
10.5 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 ppm
2.00
2.03
2.00
3.05
9.15

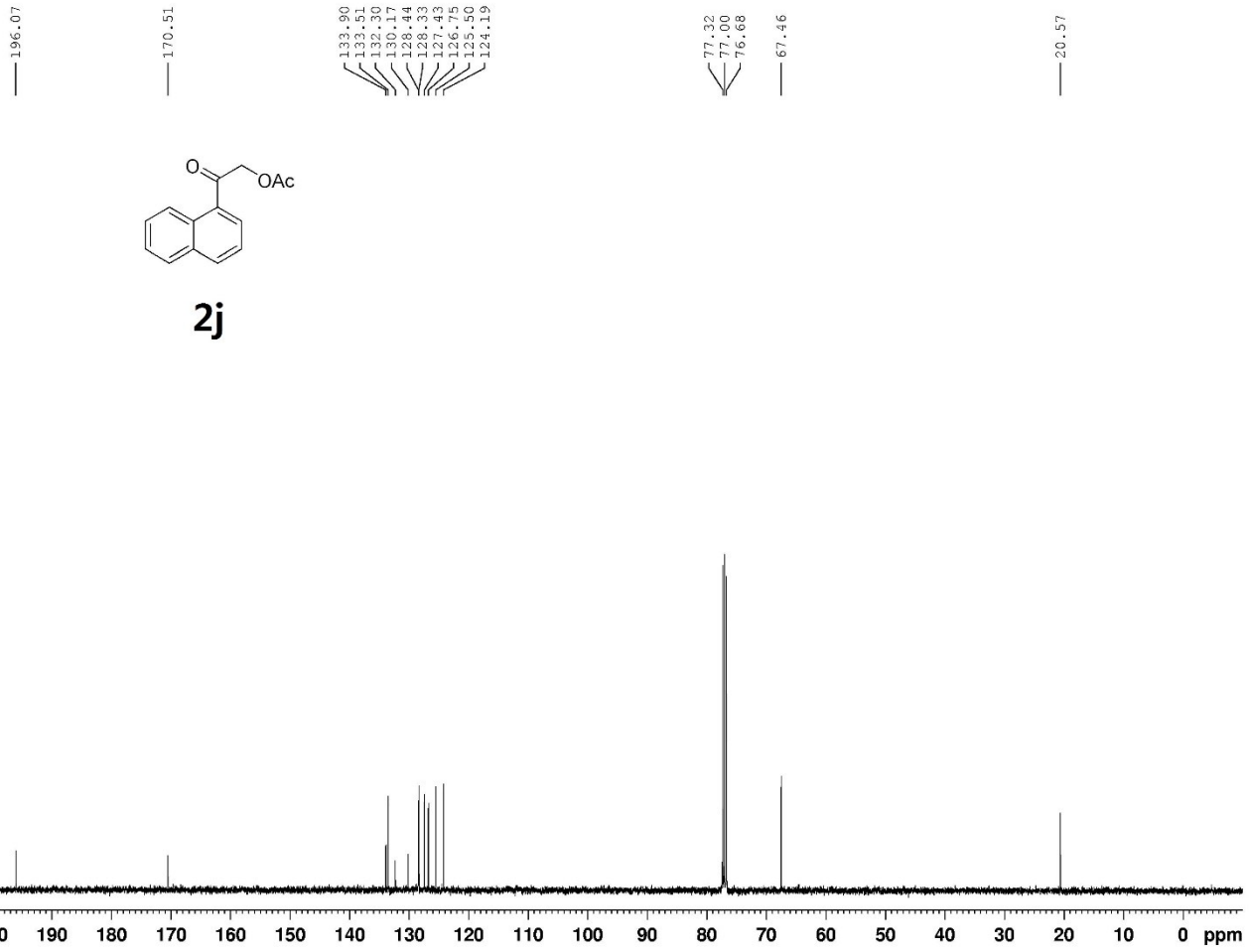

191.69
170.43
157.71
131.48
127.65
125.76
77.31
77.00
76.68
65.93
35.16
30.95
20.57
O
OAc
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

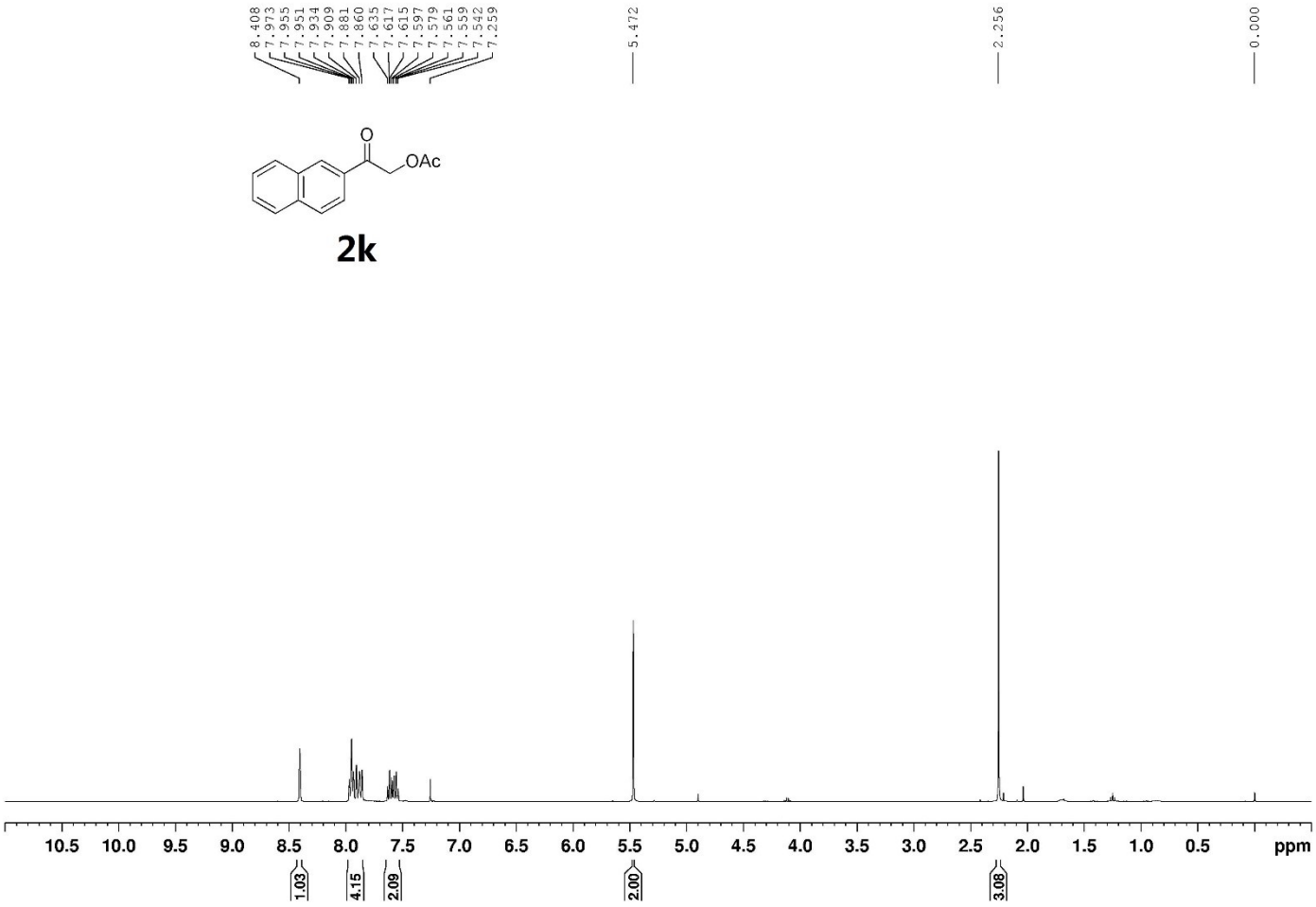

7.995
7.990
7.978
7.974
7.709
7.705
7.693
7.688
7.630
7.626
7.621
7.609
7.494
7.491
7.487
7.473
7.470
7.458
7.454
7.429
7.425
7.422
7.413
7.407
7.401
7.392
7.389
7.386
7.254
5.366
2.243
0.000
O
OAc
Ph
2i
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
2.03
2.02
2.05
1.07
2.00
3.00

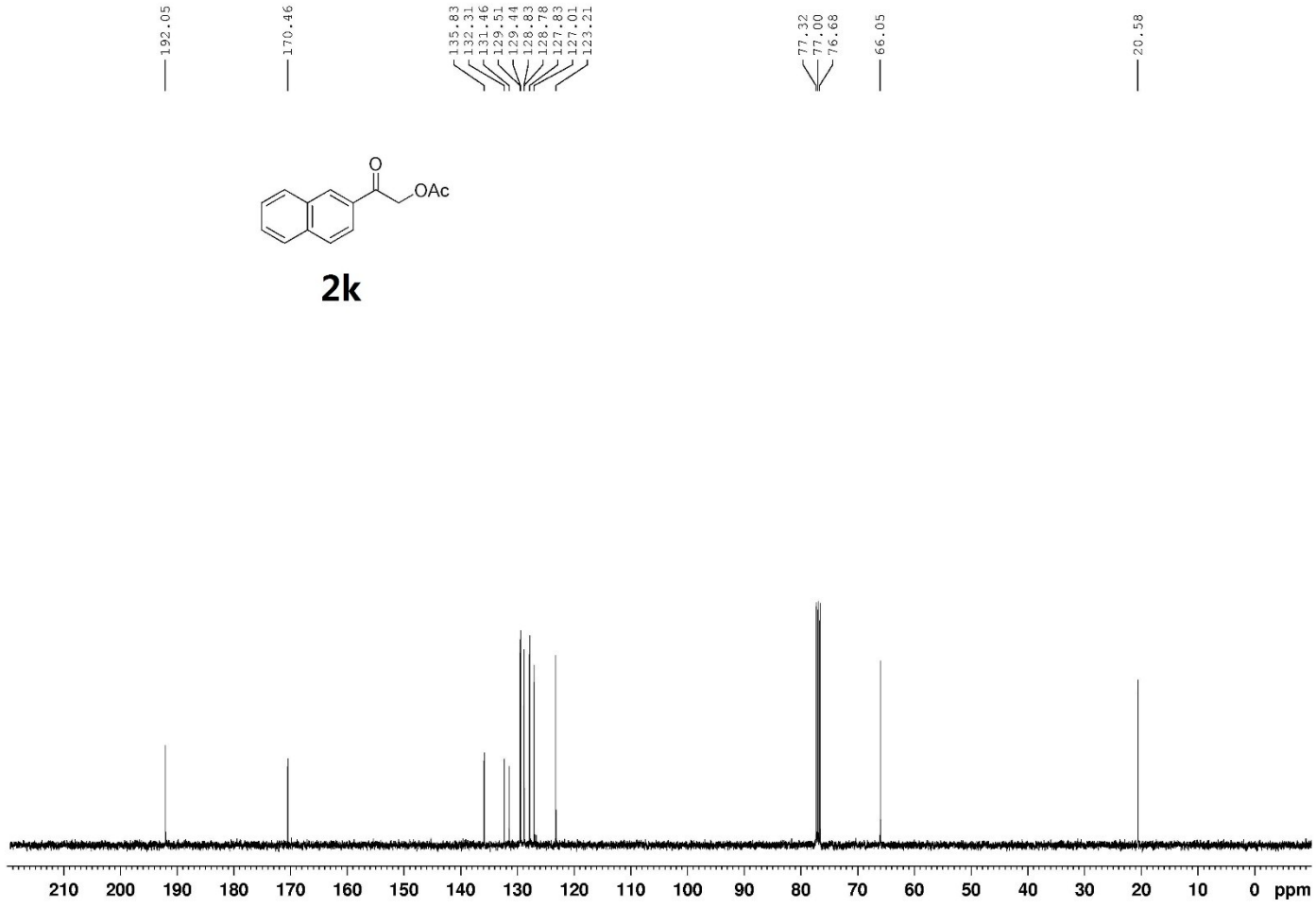

191.73
170.44
146.56
139.57
132.83
128.97
128.40
128.32
127.43
127.24
77.32
77.00
76.68
66.00
20.56
O
OAc
Ph
2i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

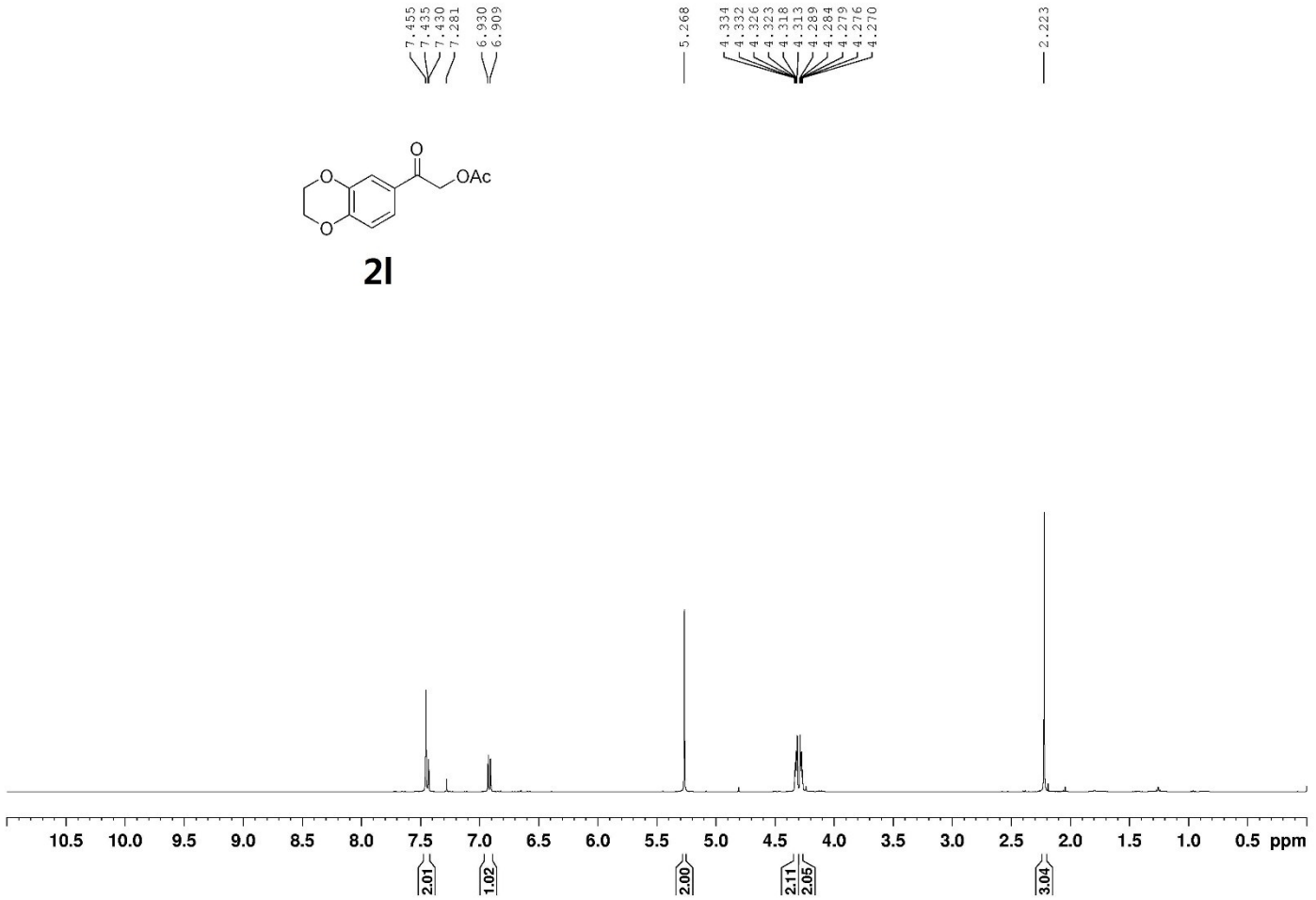

8.638
8.617
8.043
8.023
7.893
7.874
7.871
7.863
7.860
7.845
7.842
7.632
7.628
7.615
7.611
7.607
7.594
7.590
7.574
7.570
7.553
7.551
7.536
7.533
7.525
7.507
7.505
7.487
7.258
5.314
2.248
0.000
O
OAc
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
1.03
2.07
3.33
2.00
2.99

2j

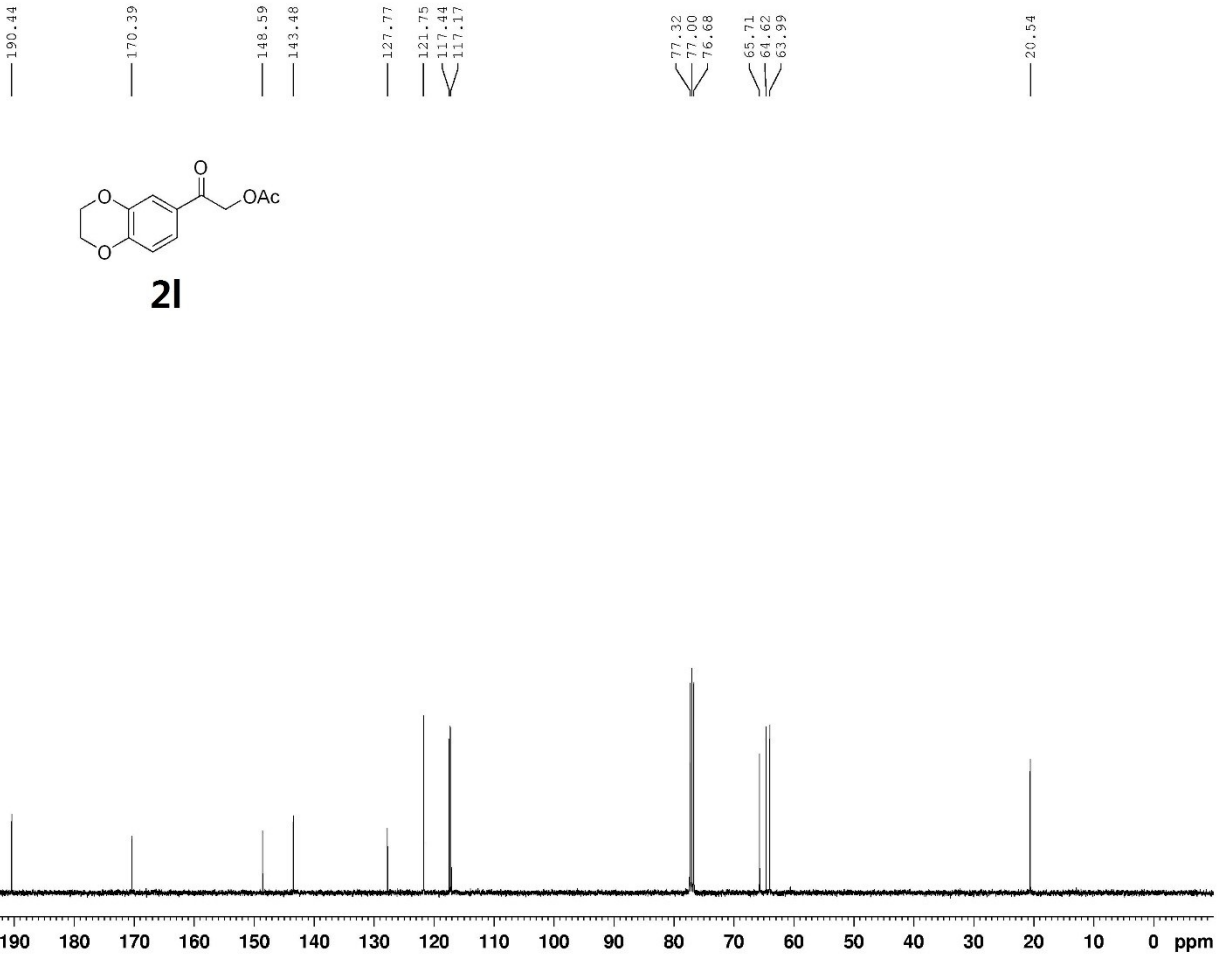

196.07
170.51
133.90
133.51
132.30
130.17
128.44
128.33
127.43
126.75
125.50
124.19
77.32
77.00
76.68
67.46
20.57
O
OAc
2j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.408
7.973
7.955
7.951
7.934
7.909
7.881
7.860
7.635
7.617
7.615
7.597
7.579
7.561
7.559
7.542
7.259
5.472
2.256
0.000
O
OAc
2k
10.5
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
ppm
1.03
4.15
2.09
2.00
3.08

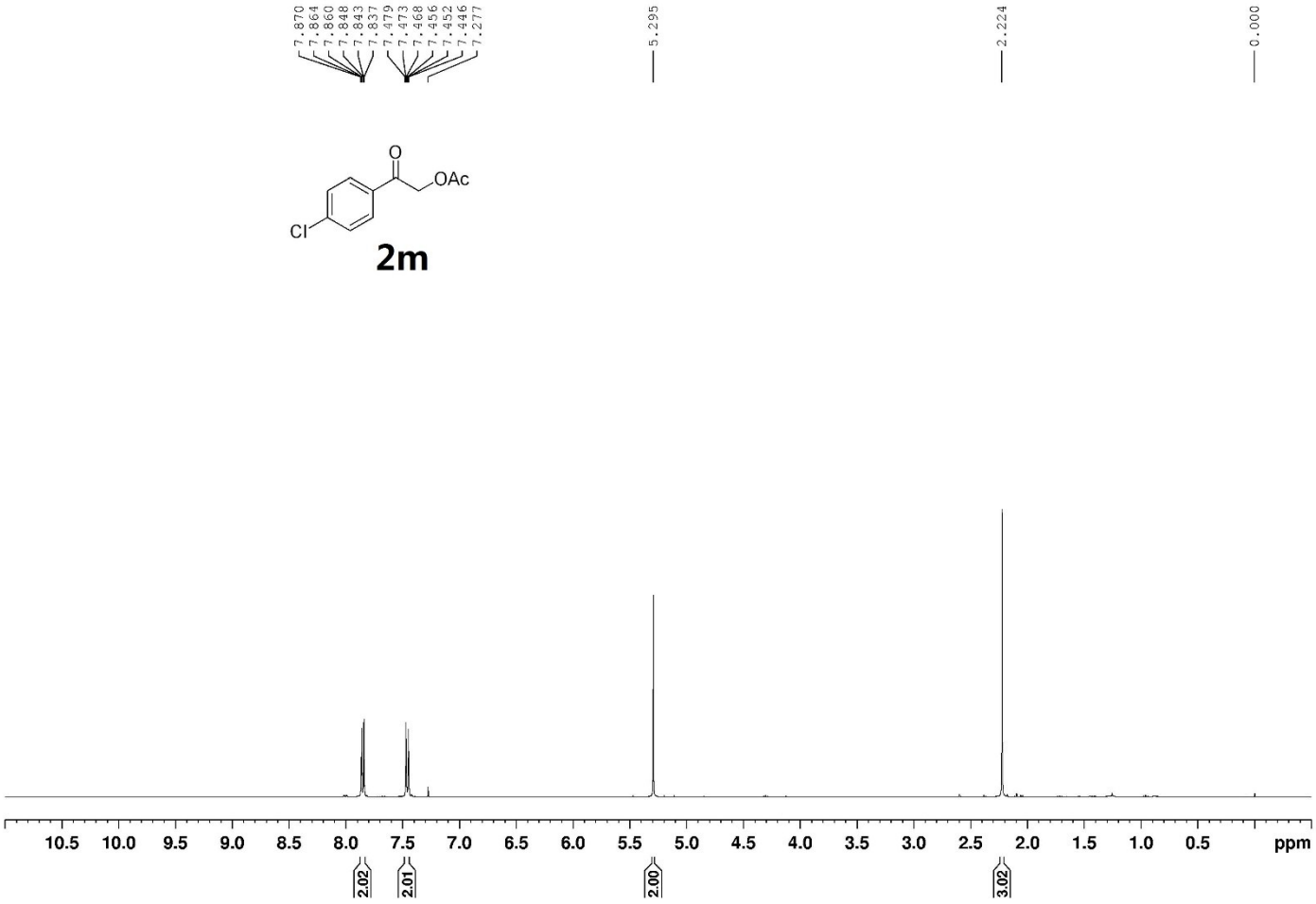

192.05
170.46
135.83
132.31
131.46
129.51
129.44
128.83
128.78
127.83
127.01
123.21
77.32
77.00
76.68
66.05
20.58
O
OAc
2k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

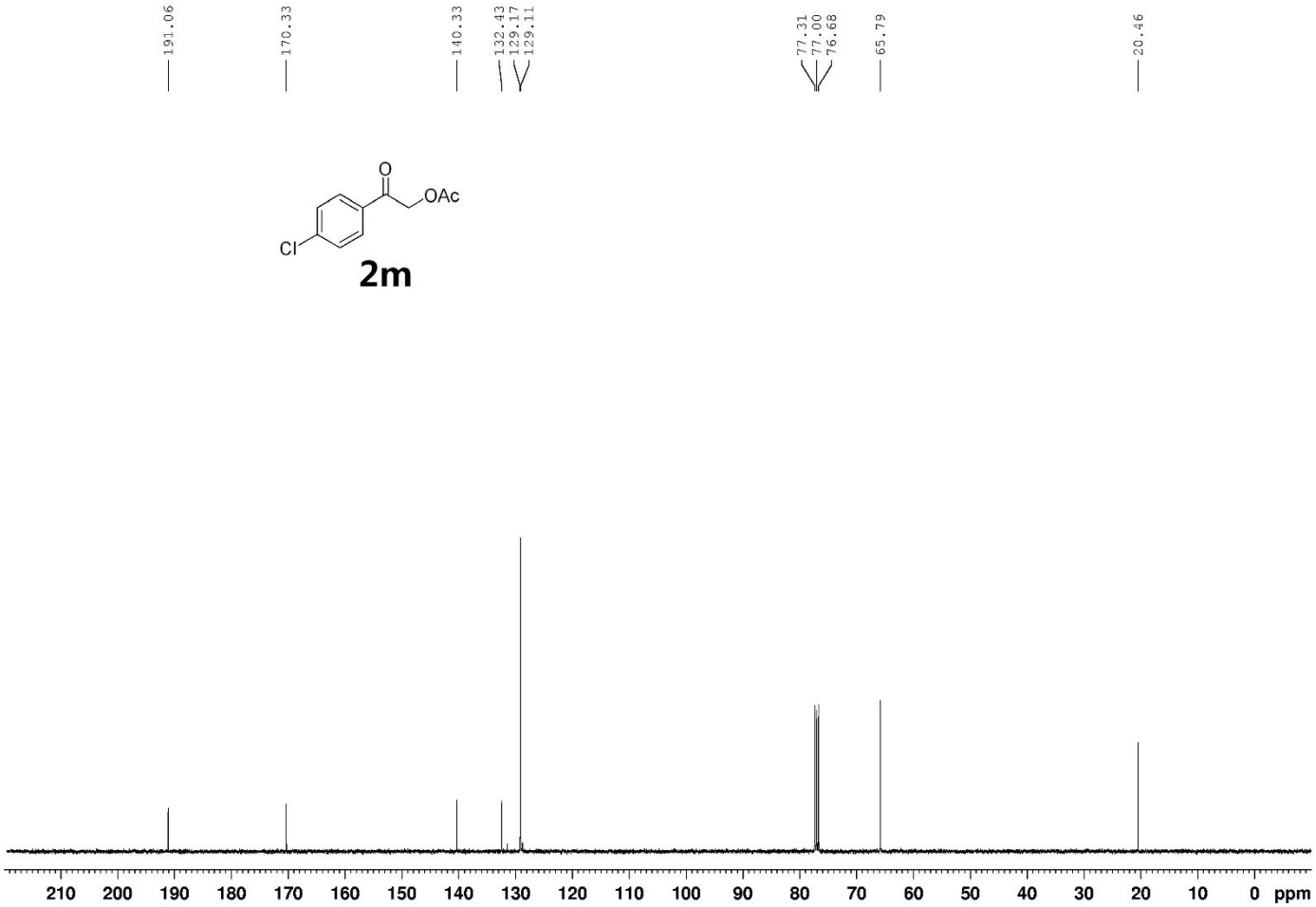

7.455
7.435
7.430
7.281
6.930
6.909
5.268
4.334
4.332
4.326
4.323
4.318
4.313
4.289
4.284
4.279
4.276
4.270
2.223
O
O
O
OAc
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.01
1.02
2.00
2.11
2.05
3.04

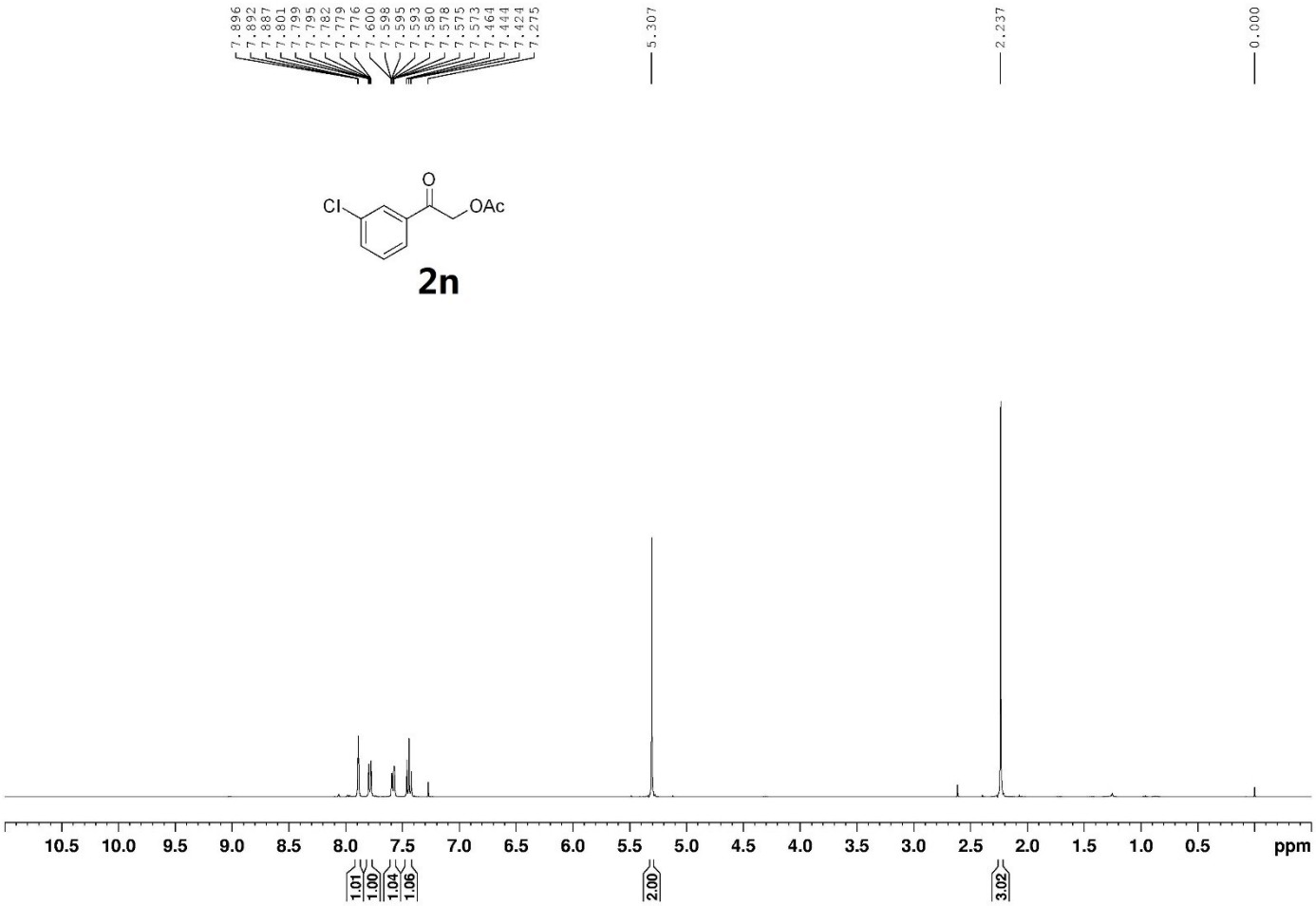
2l

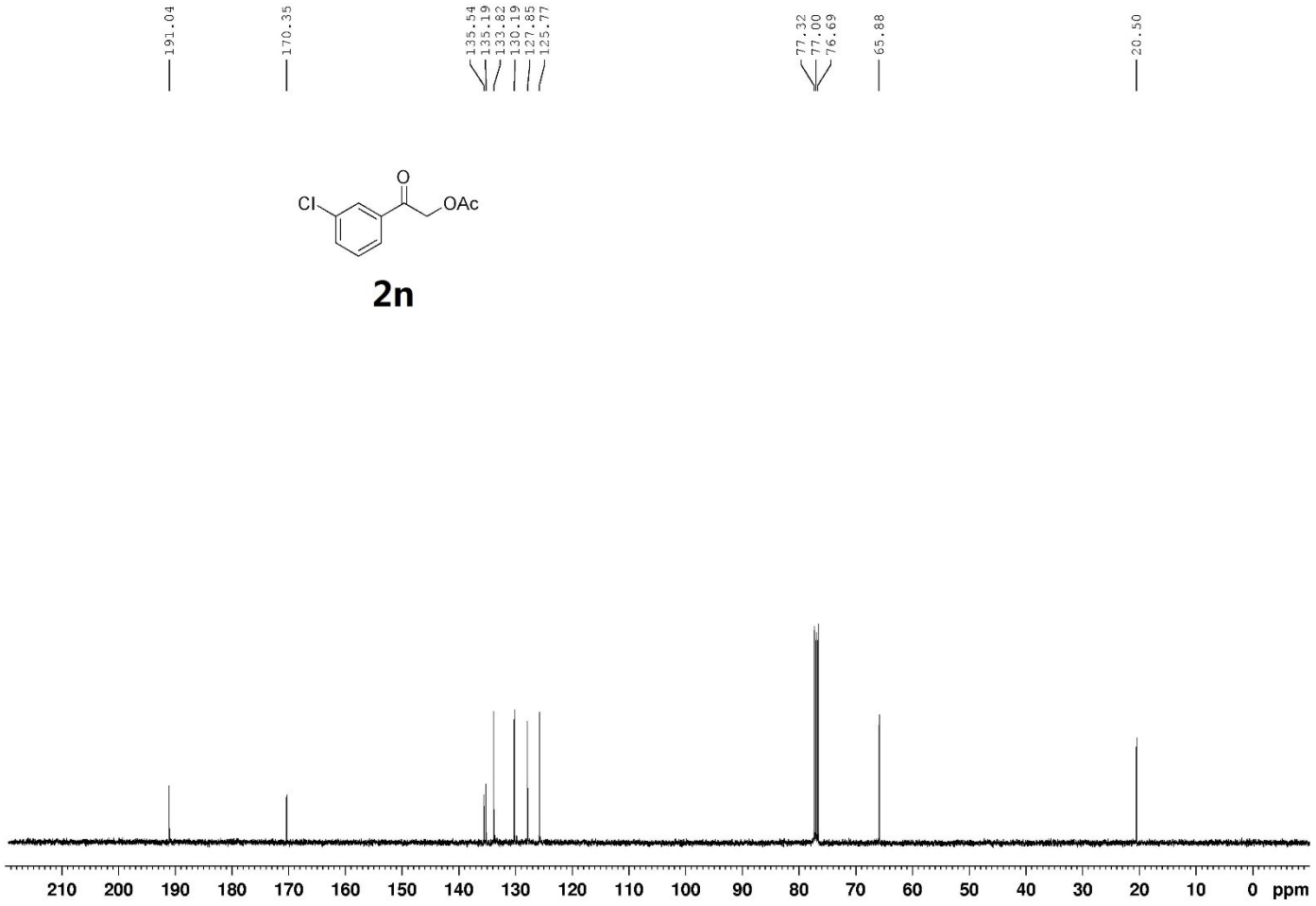

190.44
170.39
148.59
143.48
127.77
121.75
117.44
117.17
77.32
77.00
76.68
65.71
64.62
63.99
20.54
O
OAc
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

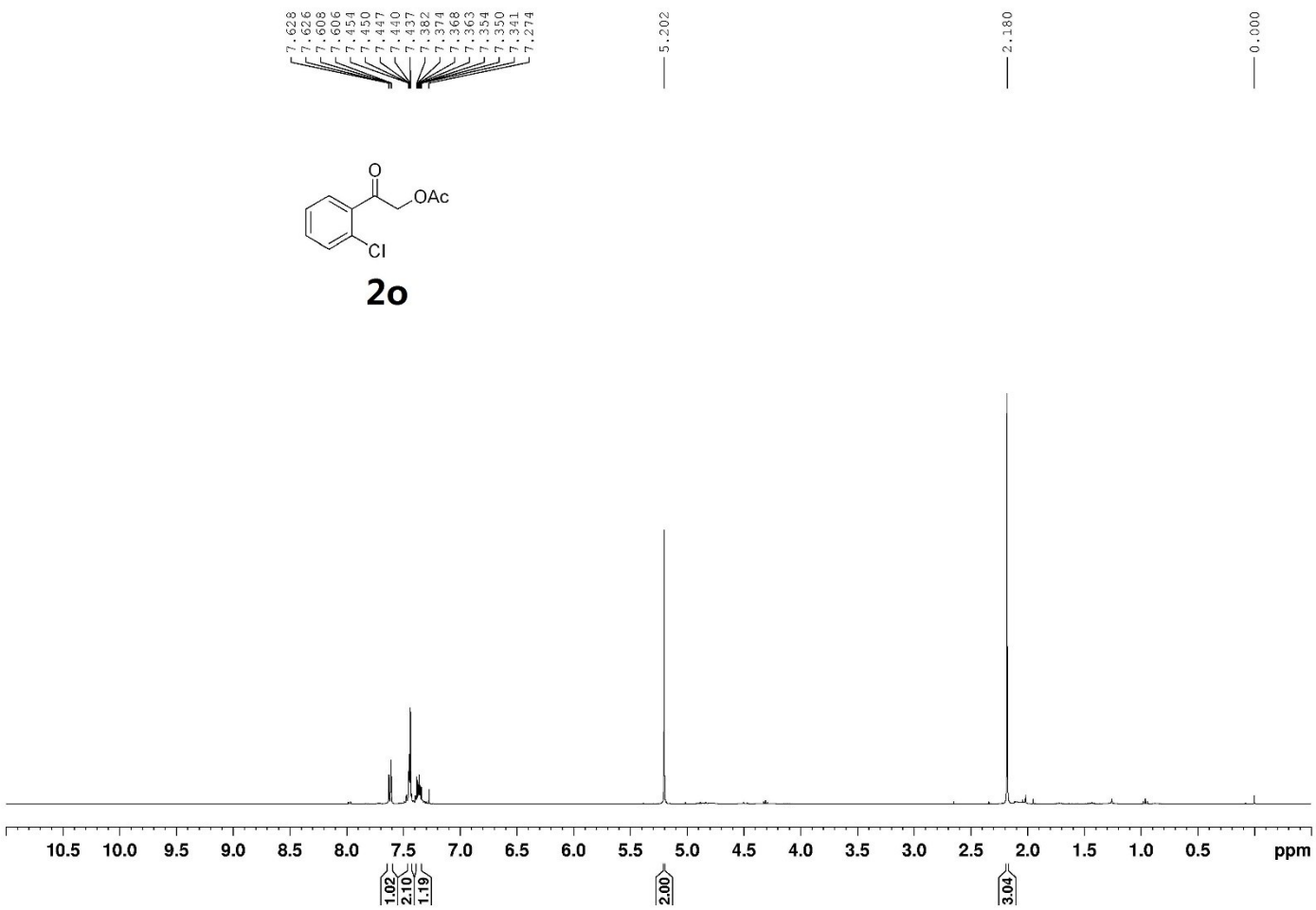
2l

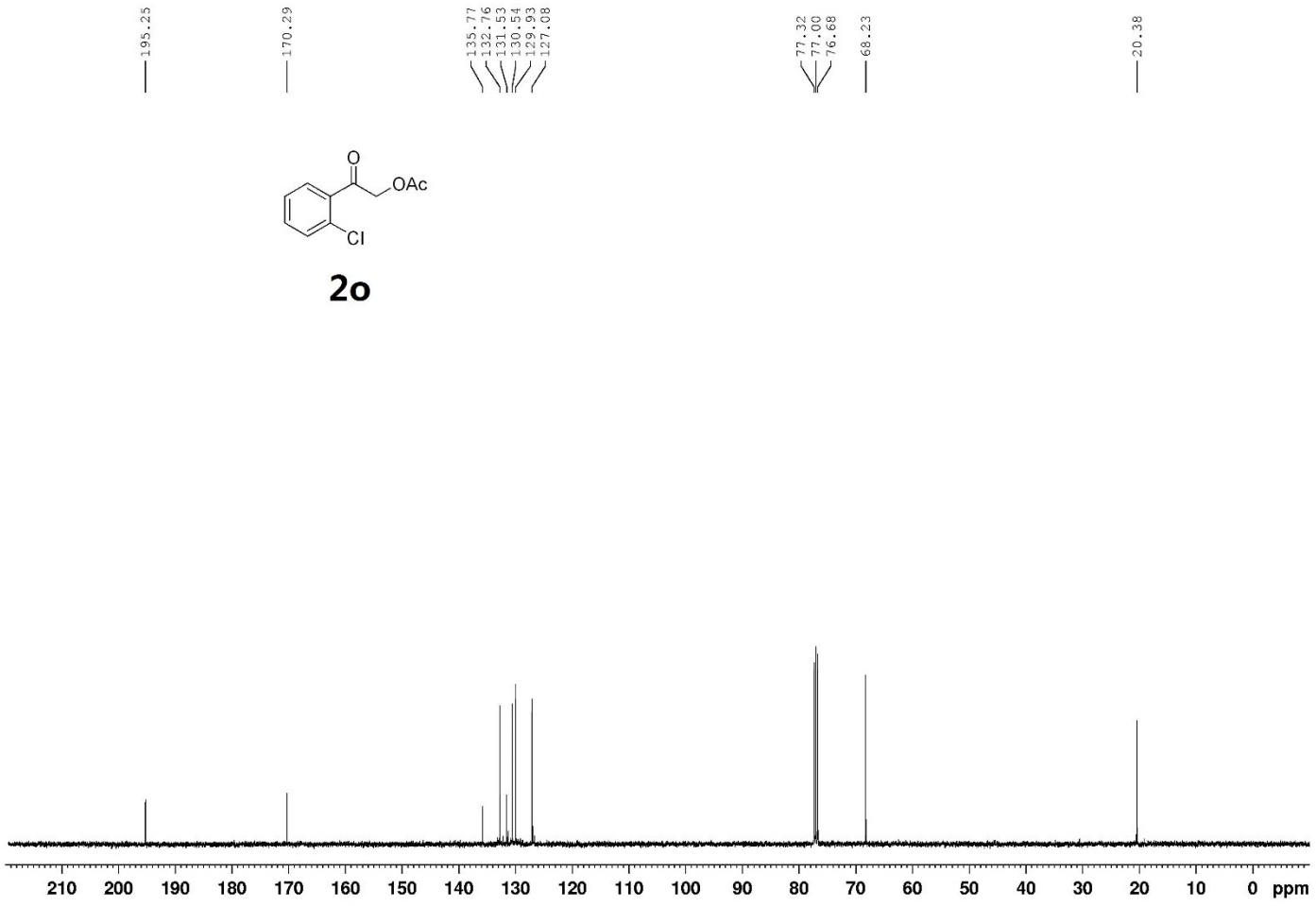

7.870
7.864
7.860
7.848
7.843
7.837
7.479
7.473
7.468
7.456
7.452
7.446
7.277
5.295
2.224
0.000
O
OAc
Cl
2m
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.02
2.01
2.00
3.02


191.06
170.33
140.33
132.43
129.17
129.11
77.31
77.00
76.68
65.79
20.46
O
OAc
Cl
2m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

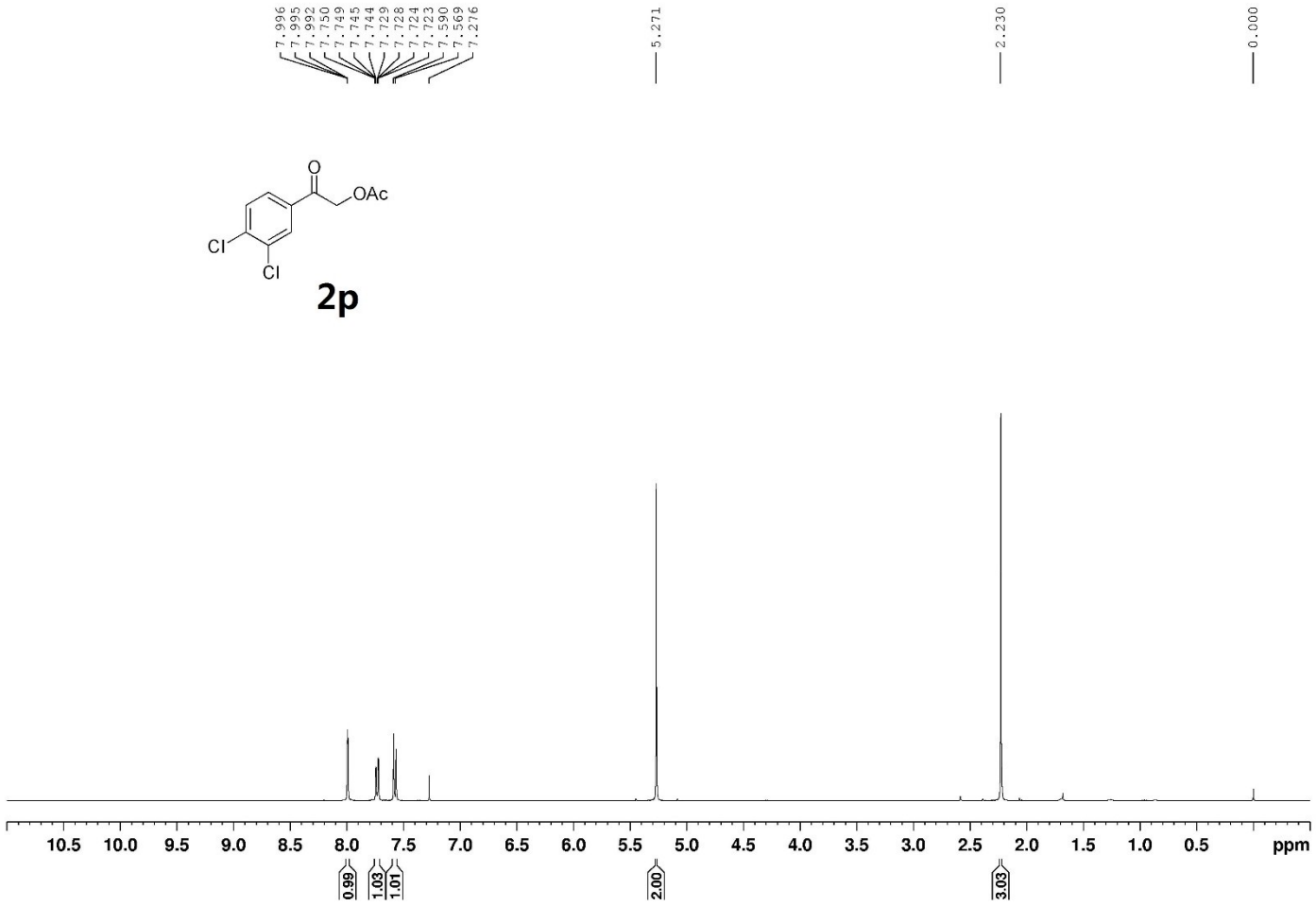

7.896
7.892
7.887
7.801
7.799
7.795
7.782
7.779
7.776
7.600
7.598
7.595
7.593
7.580
7.578
7.575
7.573
7.464
7.444
7.424
7.275
5.307
2.237
0.000
Cl
O
OAc
2n
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.01
1.00
1.04
1.06
2.00
3.02

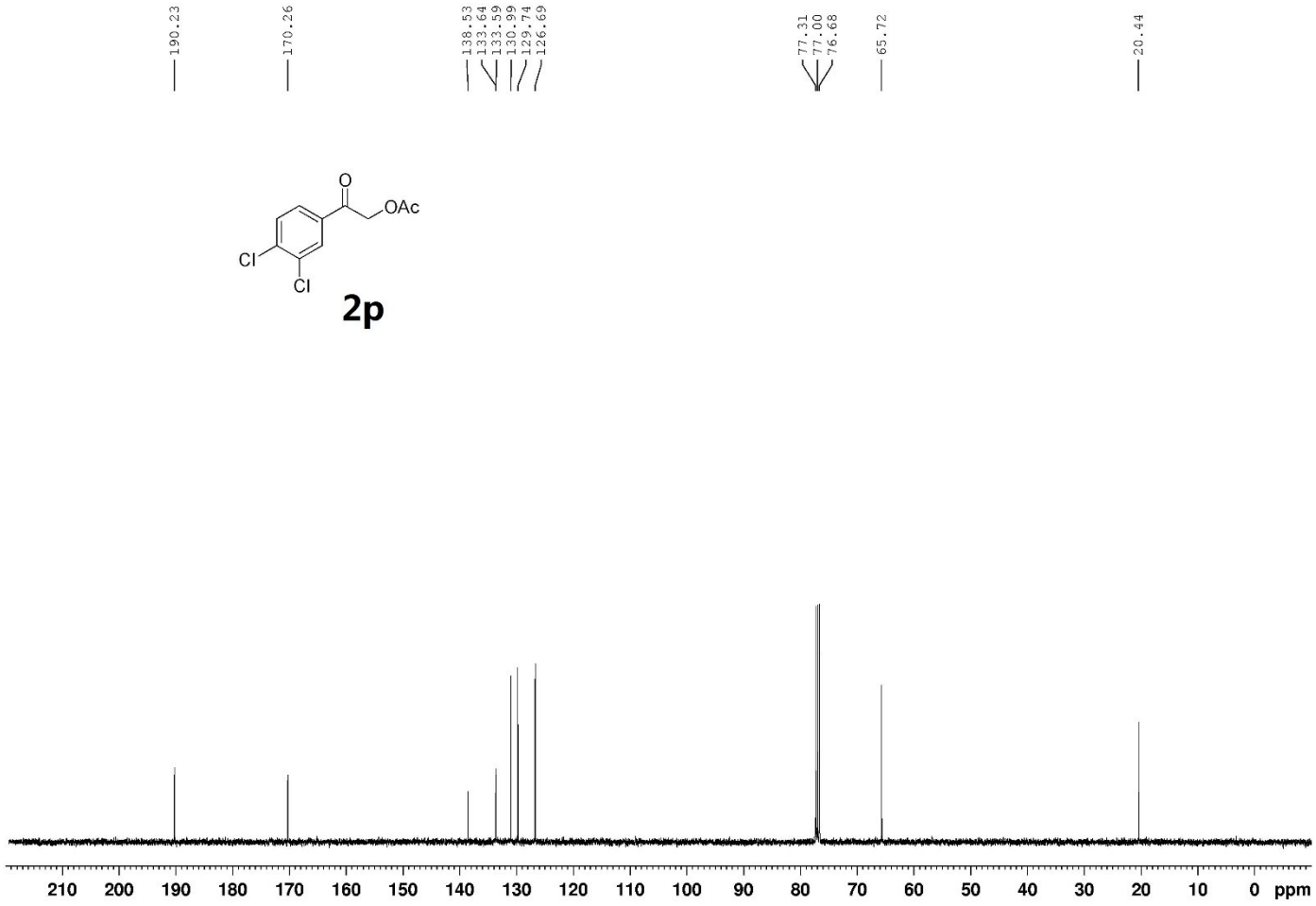

191.04
170.35
135.54
135.19
133.82
130.19
127.85
125.77
77.32
77.00
76.69
65.88
20.50
Cl
O
OAc
2n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

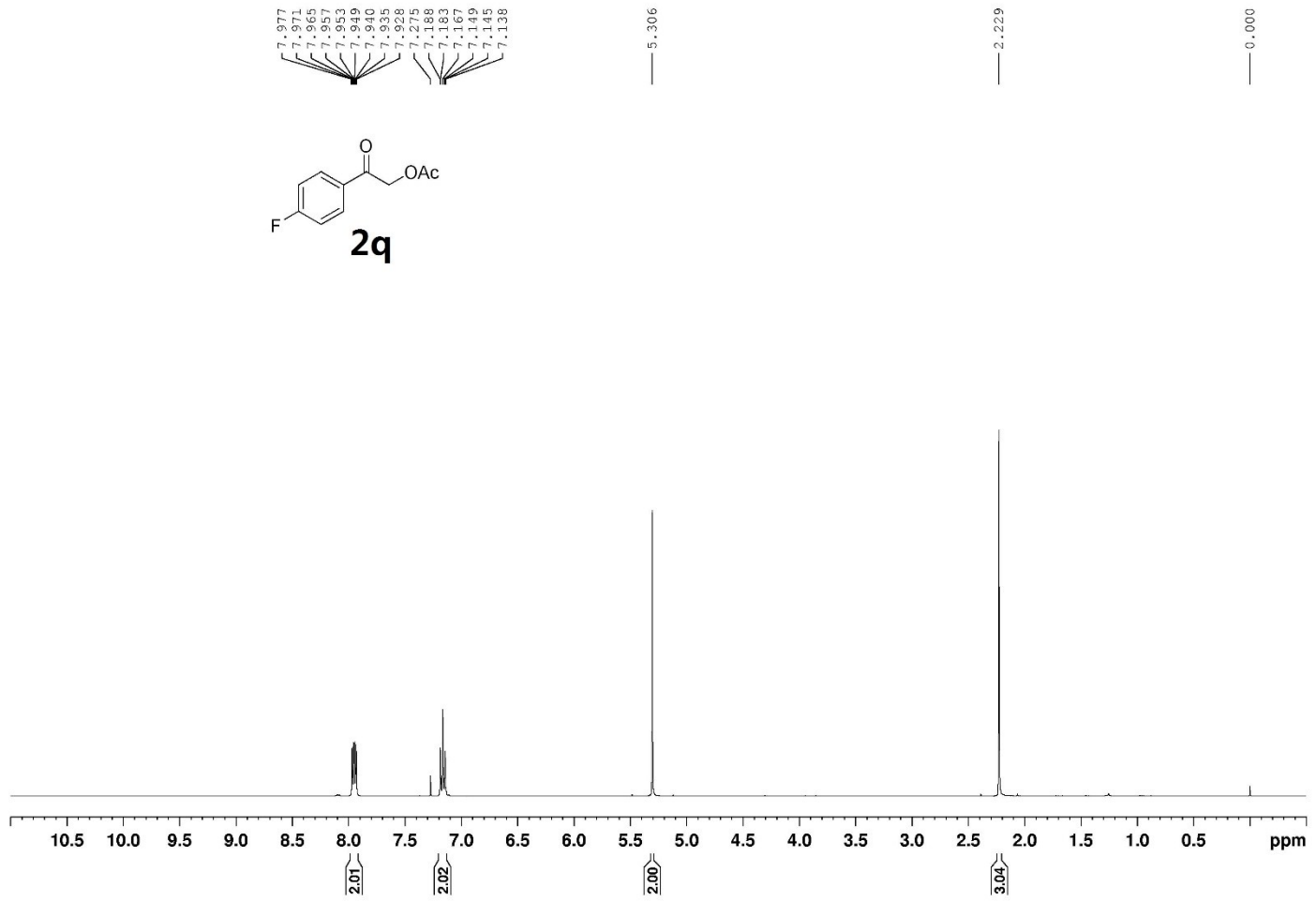

7.628
7.626
7.608
7.606
7.454
7.450
7.447
7.440
7.437
7.382
7.374
7.368
7.363
7.354
7.350
7.341
7.274
5.202
2.180
0.000
O
OAc
Cl
2o
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.02
2.10
1.19
2.00
3.04

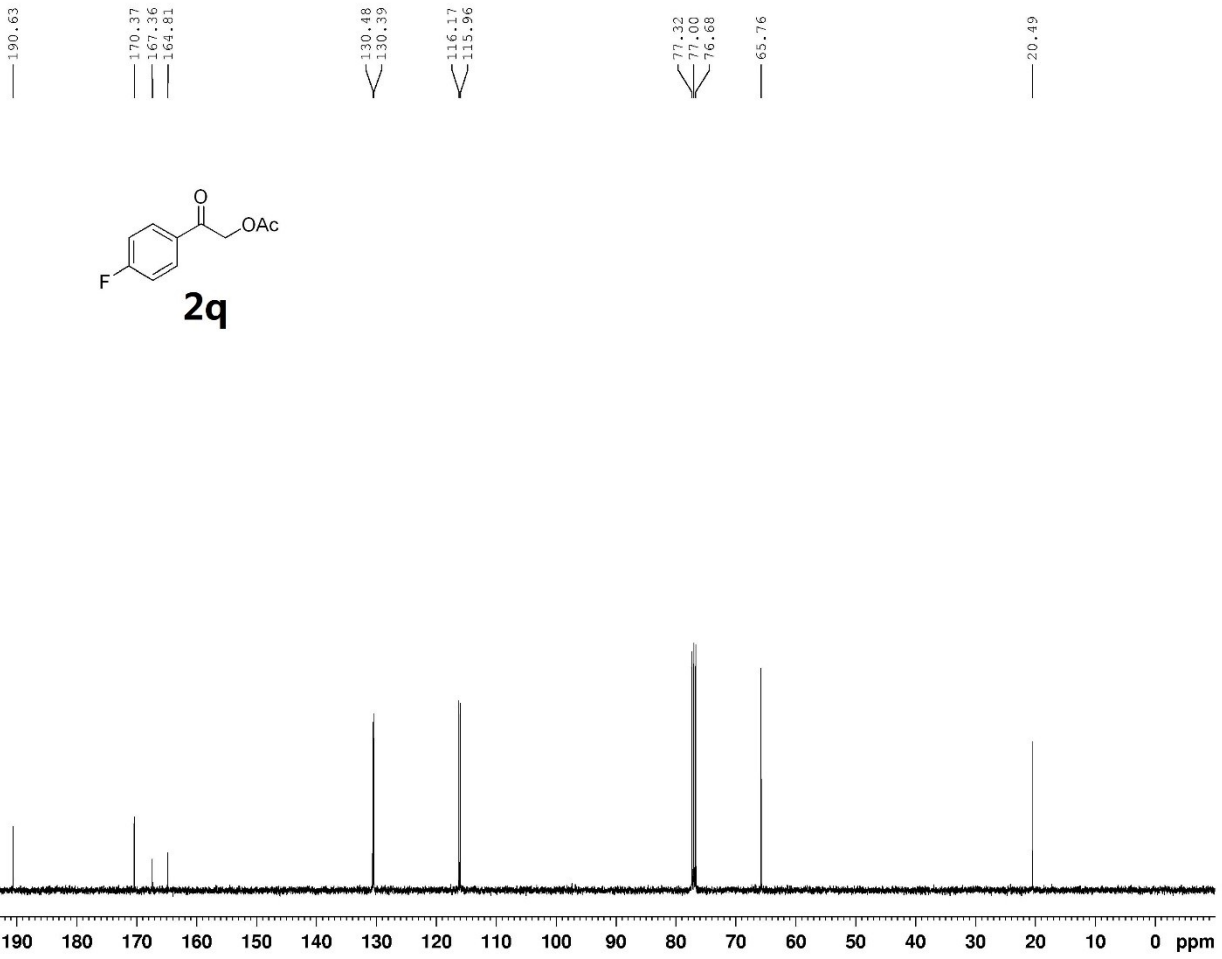

195.25
170.29
135.77
132.76
131.53
130.54
129.93
127.08
77.32
77.00
76.68
68.23
20.38
O
OAc
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

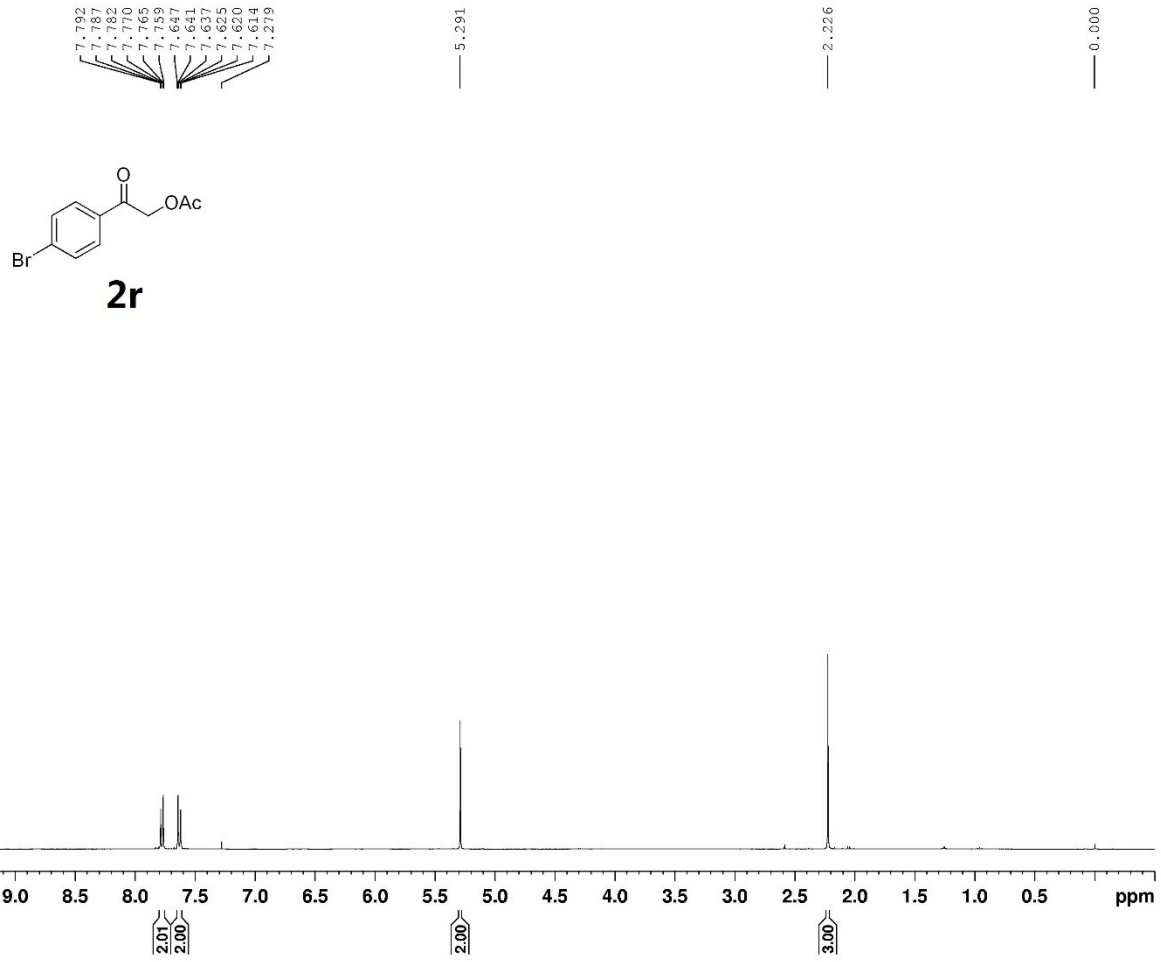
2o

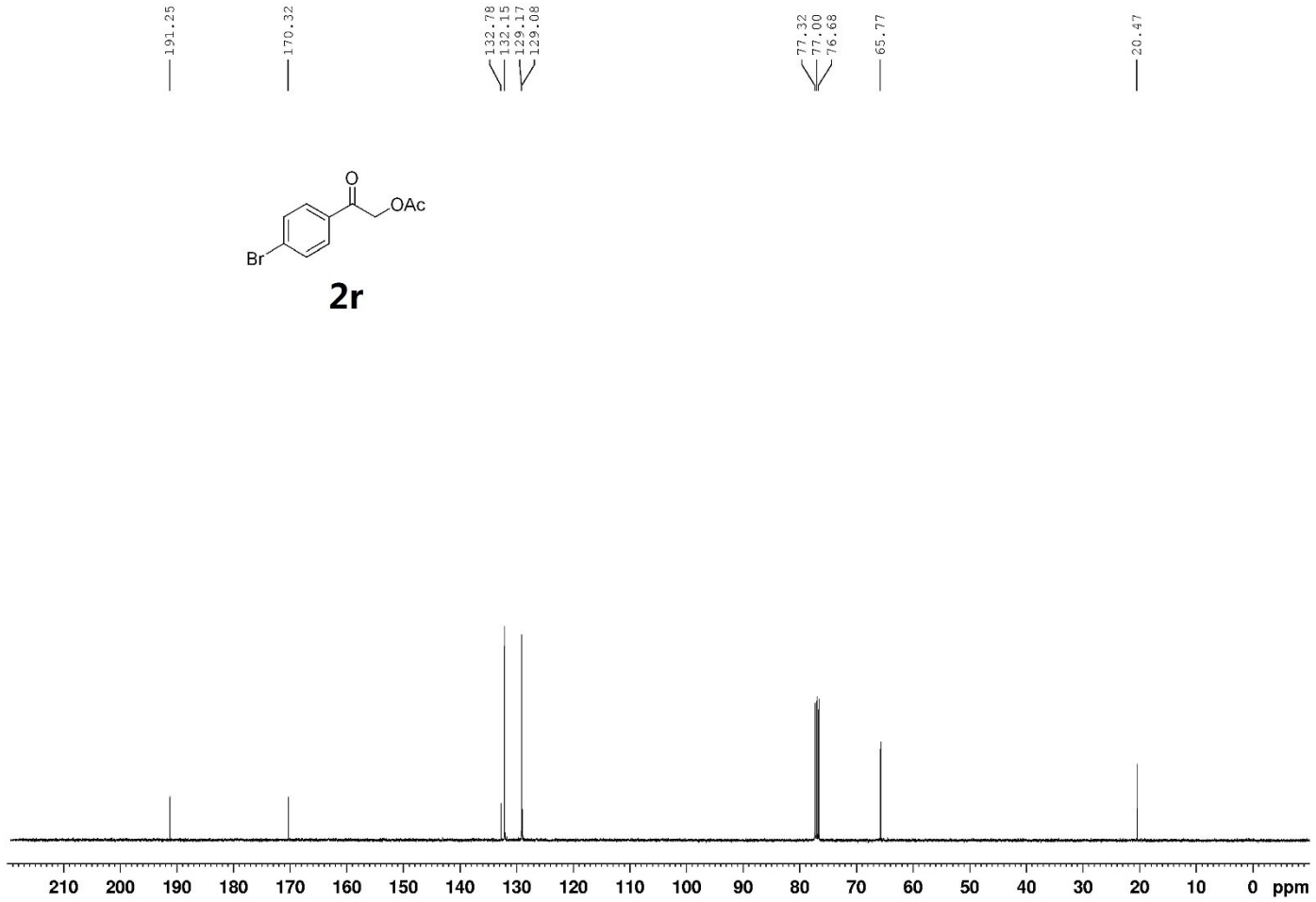

7.996
7.995
7.992
7.750
7.749
7.745
7.744
7.729
7.728
7.724
7.723
7.590
7.569
7.276
5.271
2.230
0.000
O
OAc
Cl
Cl
2p
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
1.03
1.01
2.00
3.03


190.23
170.26
138.53
133.64
133.59
130.99
129.74
126.69
77.31
77.00
76.68
65.72
20.44
O
OAc
Cl
Cl
2p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

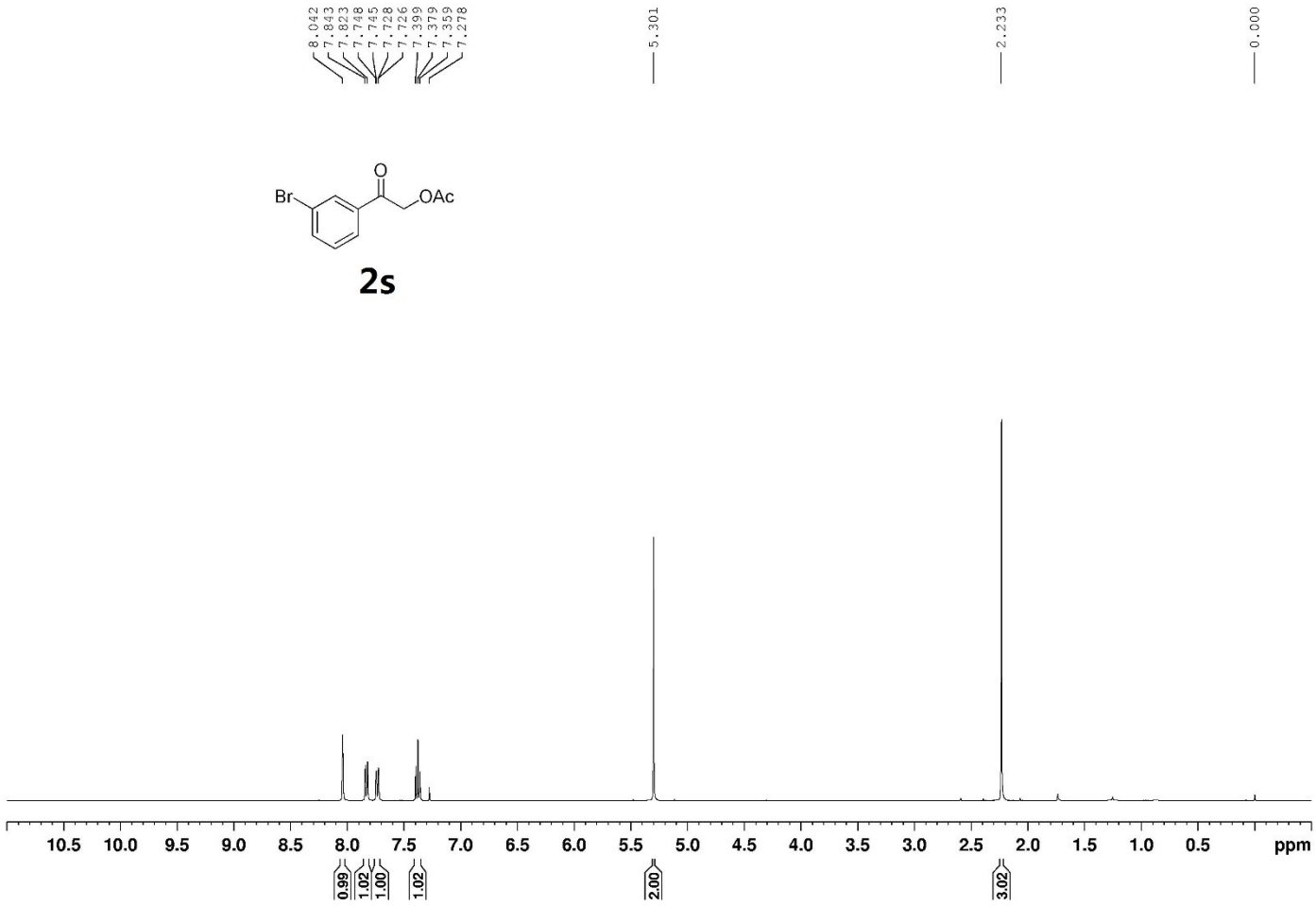

7.977
7.971
7.965
7.957
7.953
7.949
7.940
7.935
7.928
7.275
7.188
7.183
7.167
7.149
7.145
7.138
5.306
2.229
0.000
O
OAc
F
2q
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.01
2.02
2.00
3.04

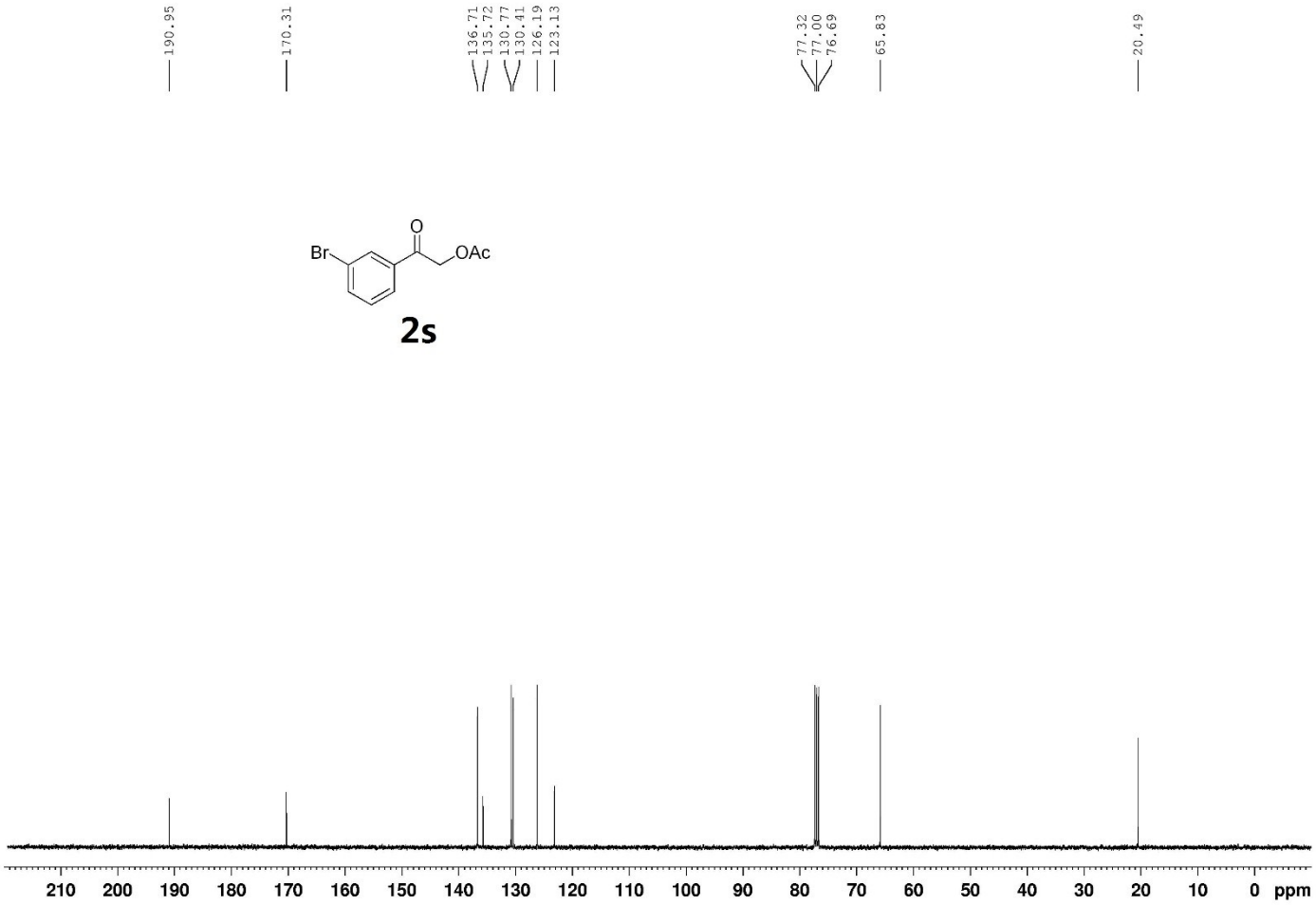

190.63
170.37
167.36
164.81
130.48
130.39
116.17
115.96
77.32
77.00
76.68
65.76
20.49
O
OAc
F
2q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

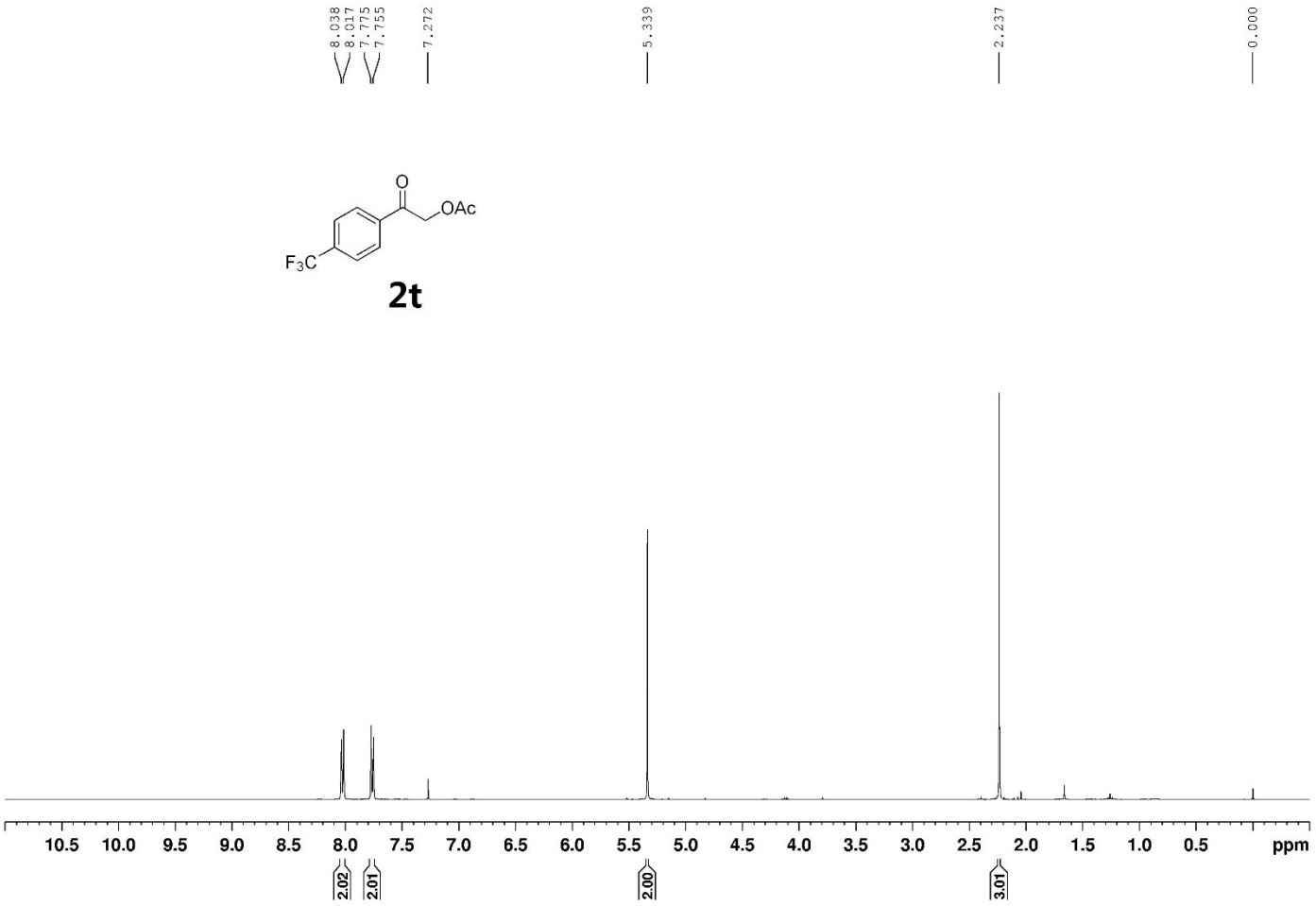

7.792
7.787
7.782
7.770
7.765
7.759
7.647
7.641
7.637
7.625
7.620
7.614
7.279
5.291
2.226
0.000
O
OAc
Br
2r
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.01
2.00
2.00
3.00

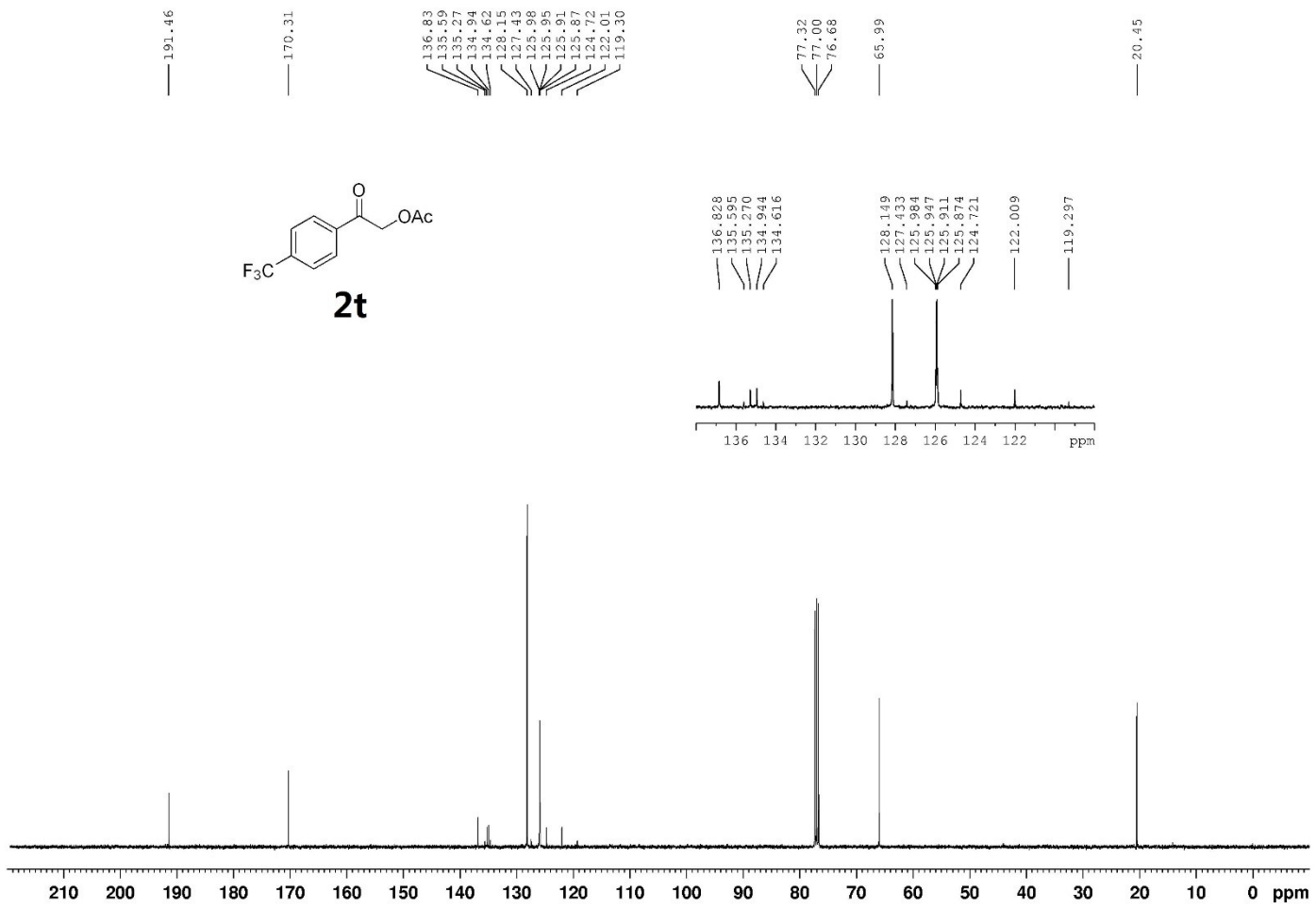

191.25
170.32
132.78
132.15
129.17
129.08
77.32
77.00
76.68
65.77
20.47
O
OAc
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

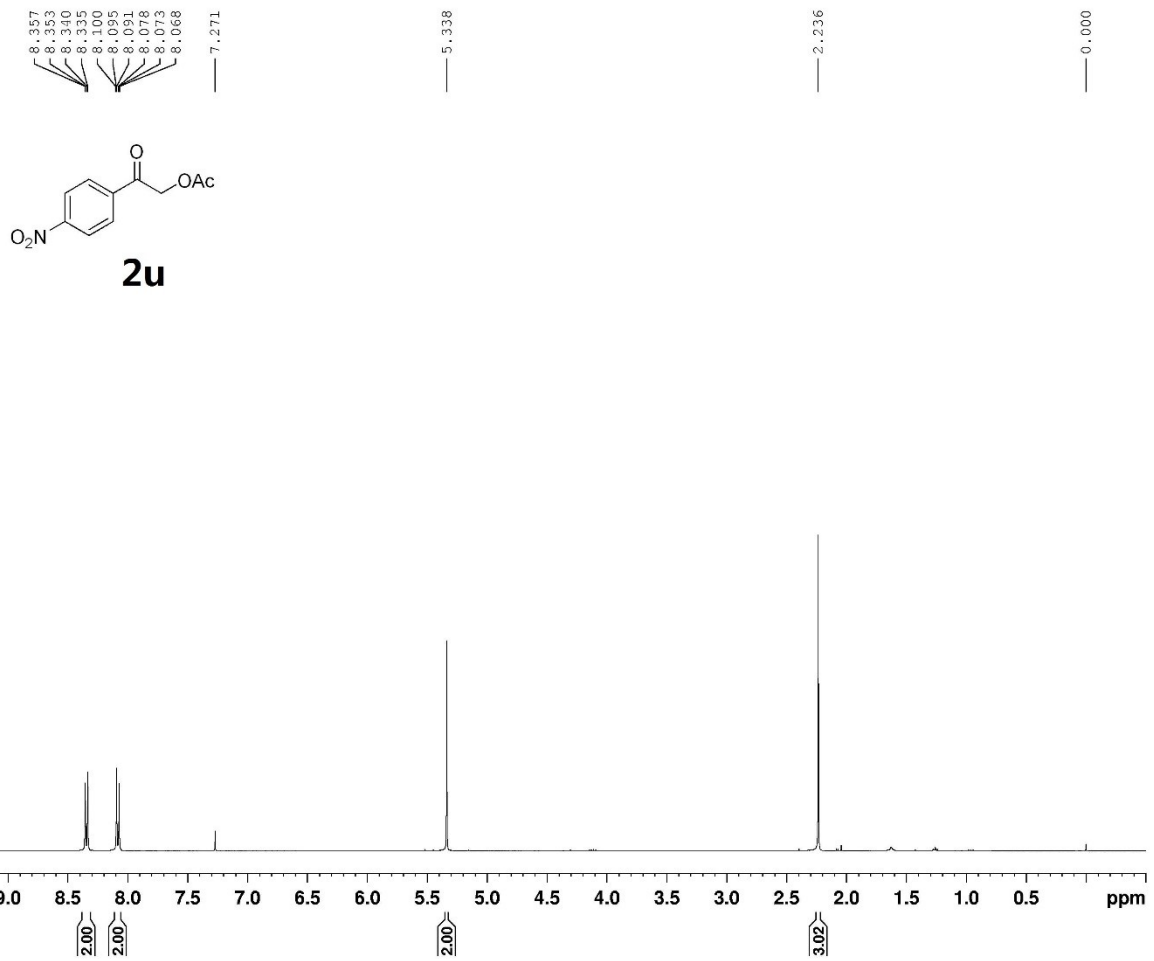
2r

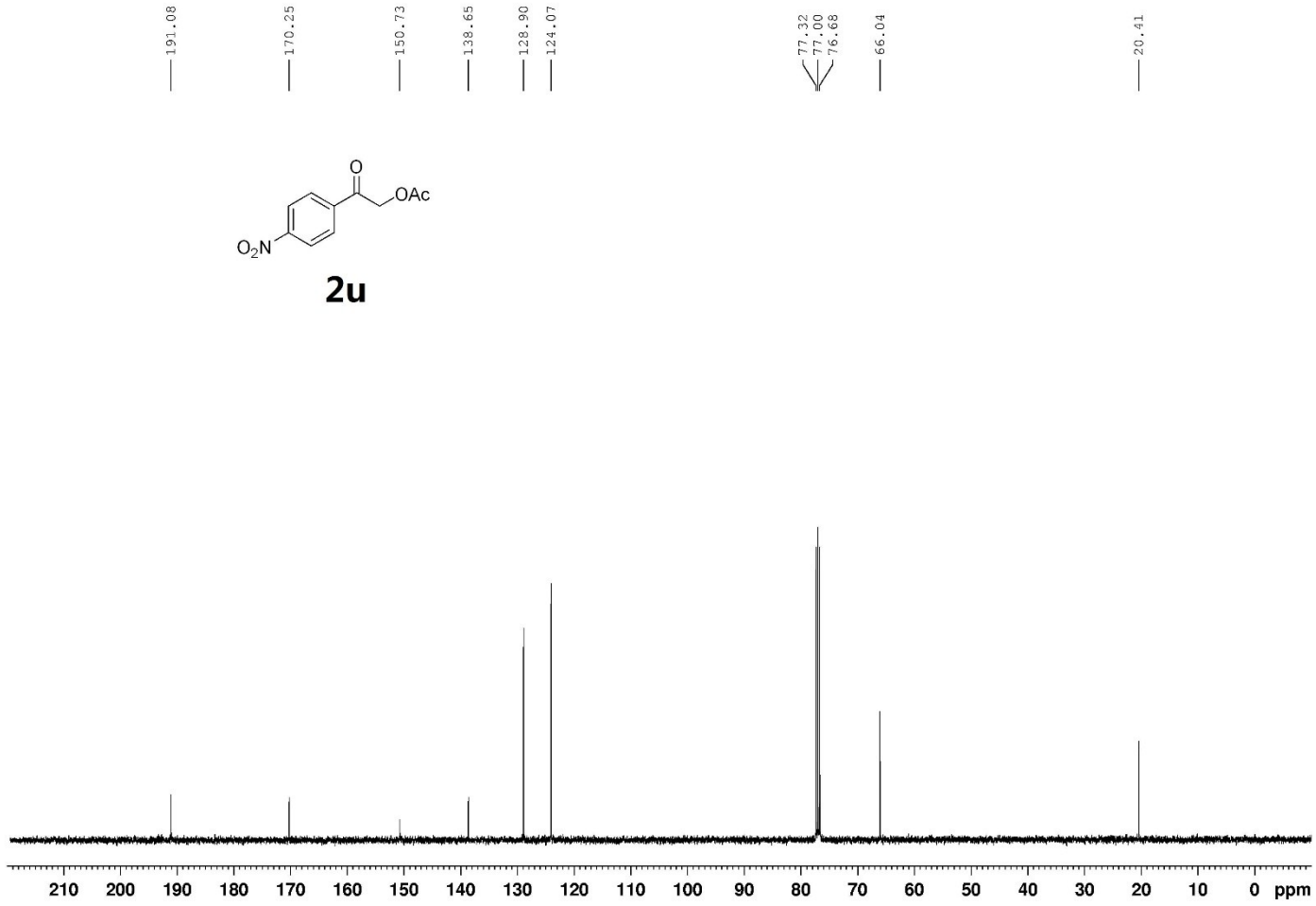

8.042
7.843
7.823
7.748
7.745
7.728
7.726
7.399
7.379
7.359
7.278
5.301
2.233
0.000
Br
O
OAc
2s
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
1.02
1.00
1.02
2.00
3.02


190.95
170.31
136.71
135.72
130.77
130.41
126.19
123.13
77.32
77.00
76.69
65.83
20.49
Br
O
OAc
2s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

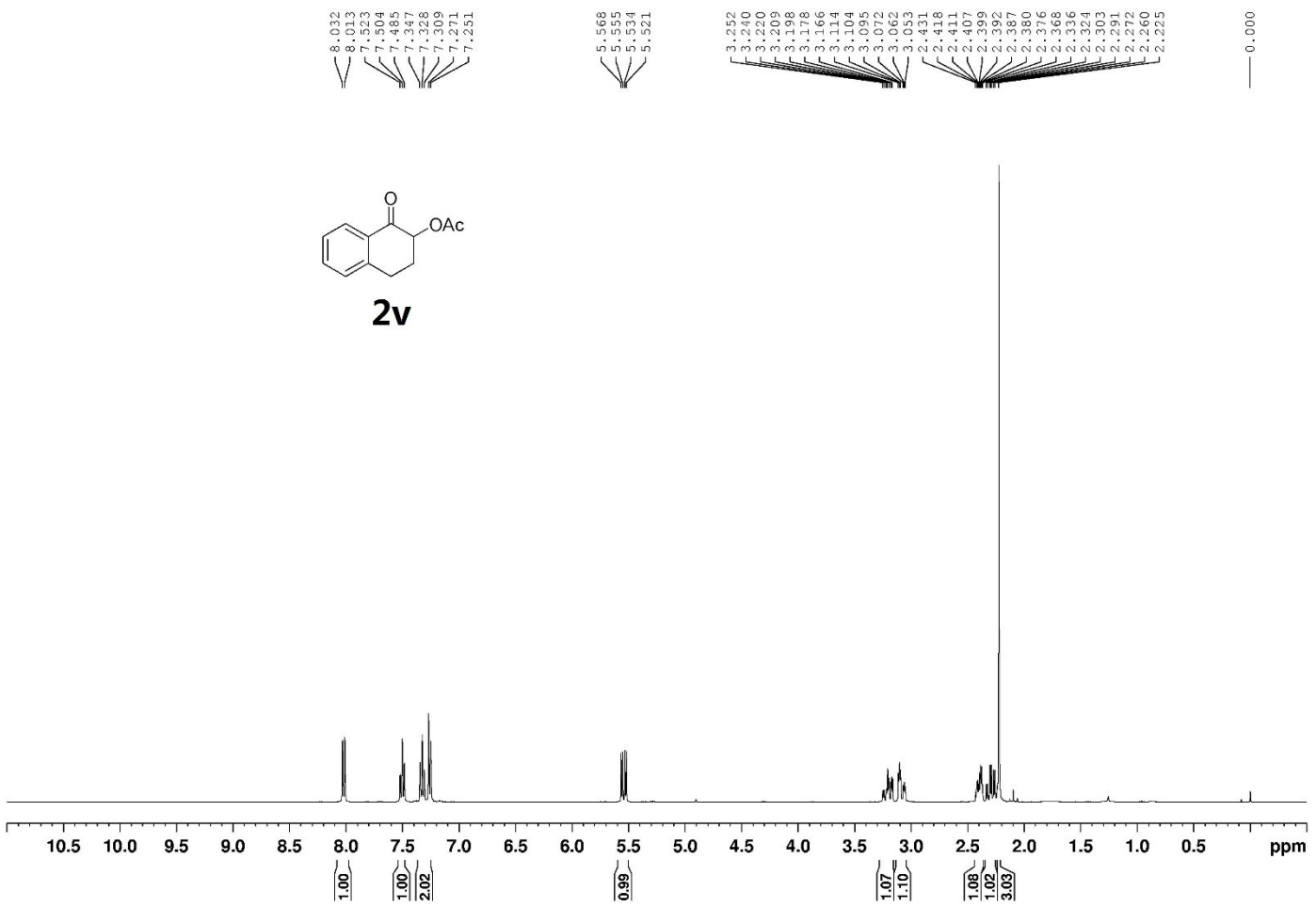

8.038
8.017
7.775
7.755
7.272
5.339
2.237
0.000
O
OAc
F3C
2t
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
2.01
2.00
3.01

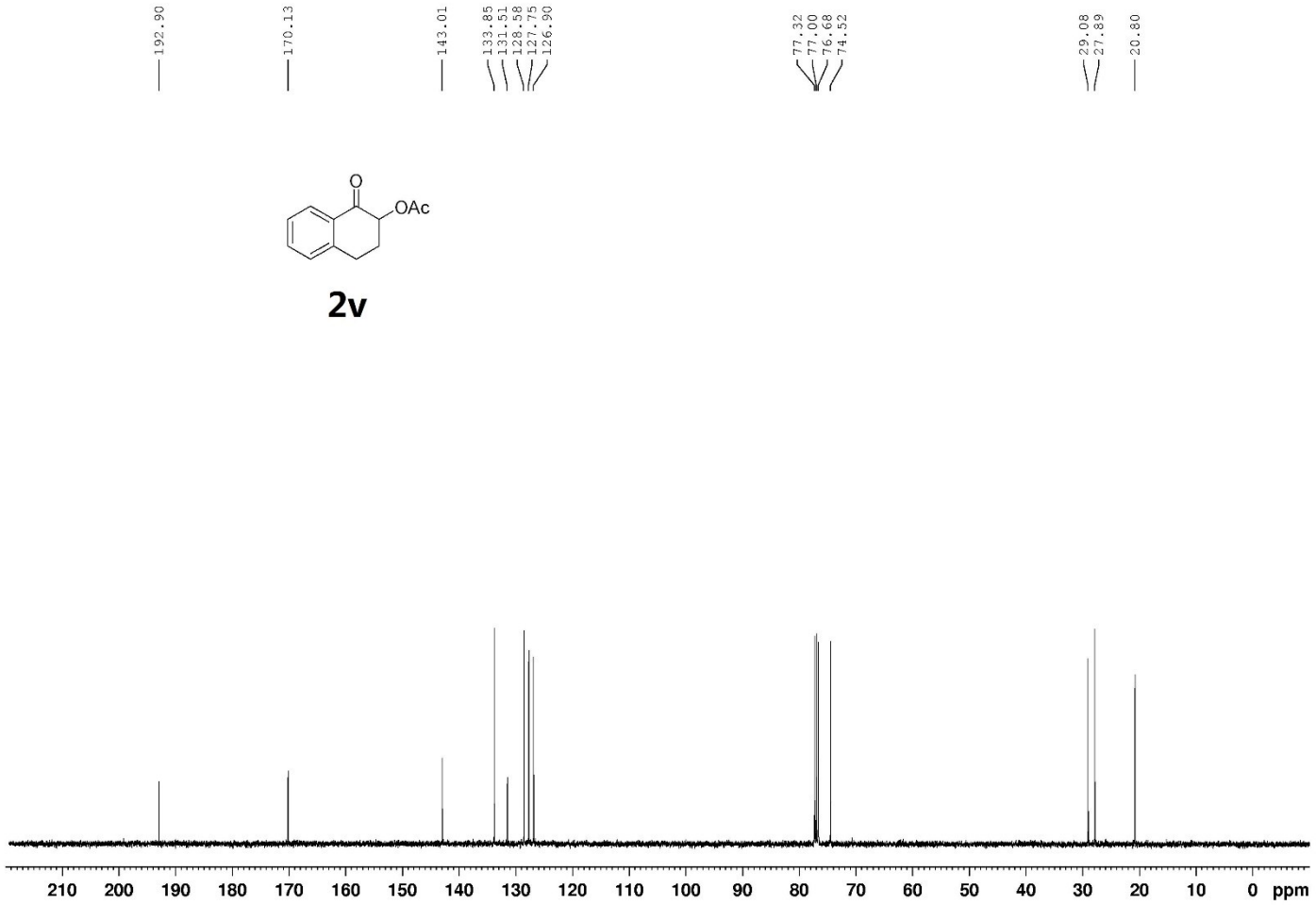

191.46
170.31
136.83
135.59
135.27
134.94
134.62
128.15
127.43
125.98
125.95
125.91
125.87
124.72
122.01
119.30
77.32
77.00
76.68
65.99
20.45
O
OAc
F3C
2t
136.828
135.595
135.270
134.944
134.616
128.149
127.433
125.984
125.947
125.911
125.874
124.721
122.009
119.297
136 134 132 130 128 126 124 122 ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

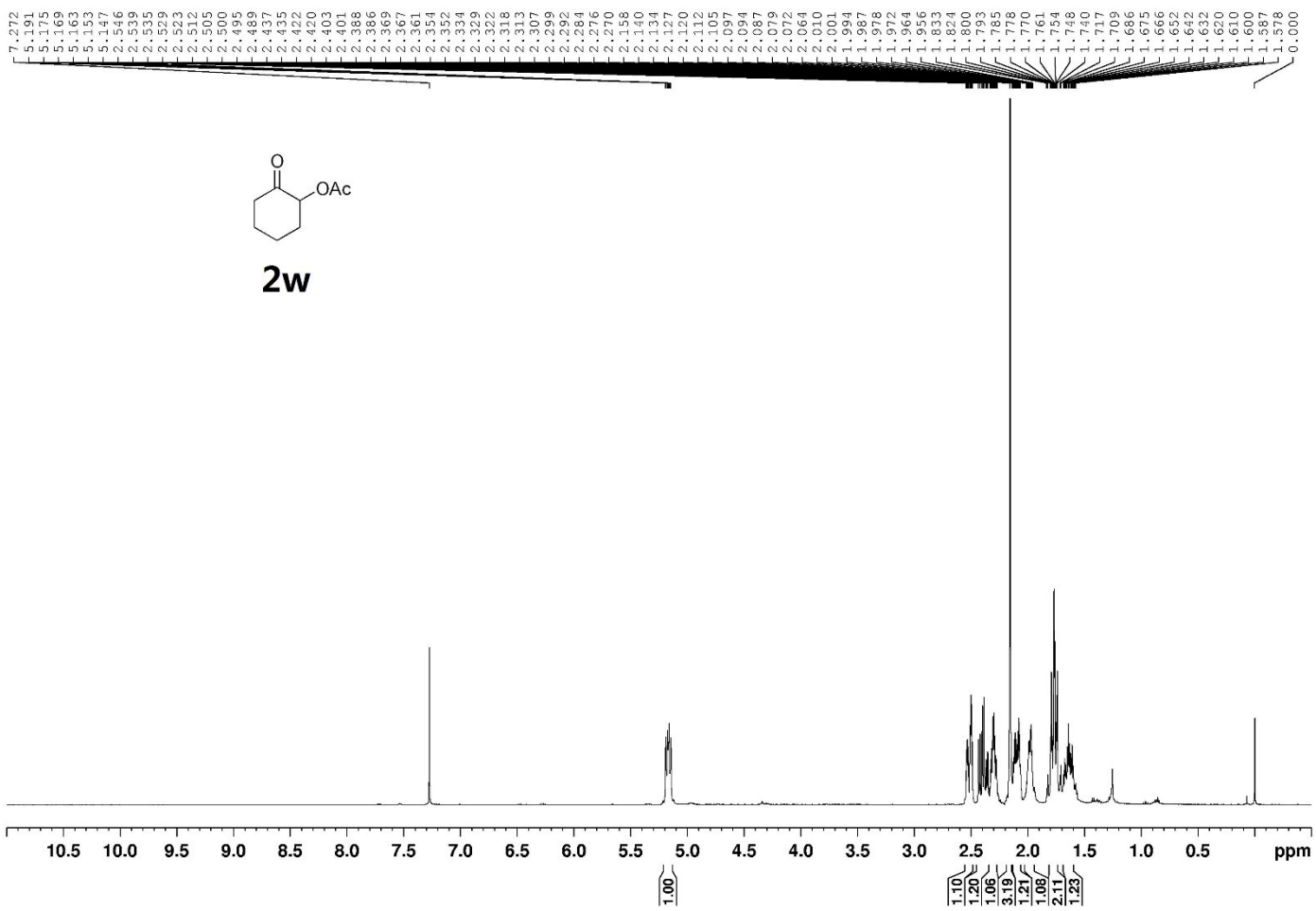

8.357
8.353
8.340
8.335
8.100
8.095
8.091
8.078
8.073
8.068
7.271
5.338
2.236
0.000
O
OAc
O_2N
2u
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.00
2.00
2.00
3.02

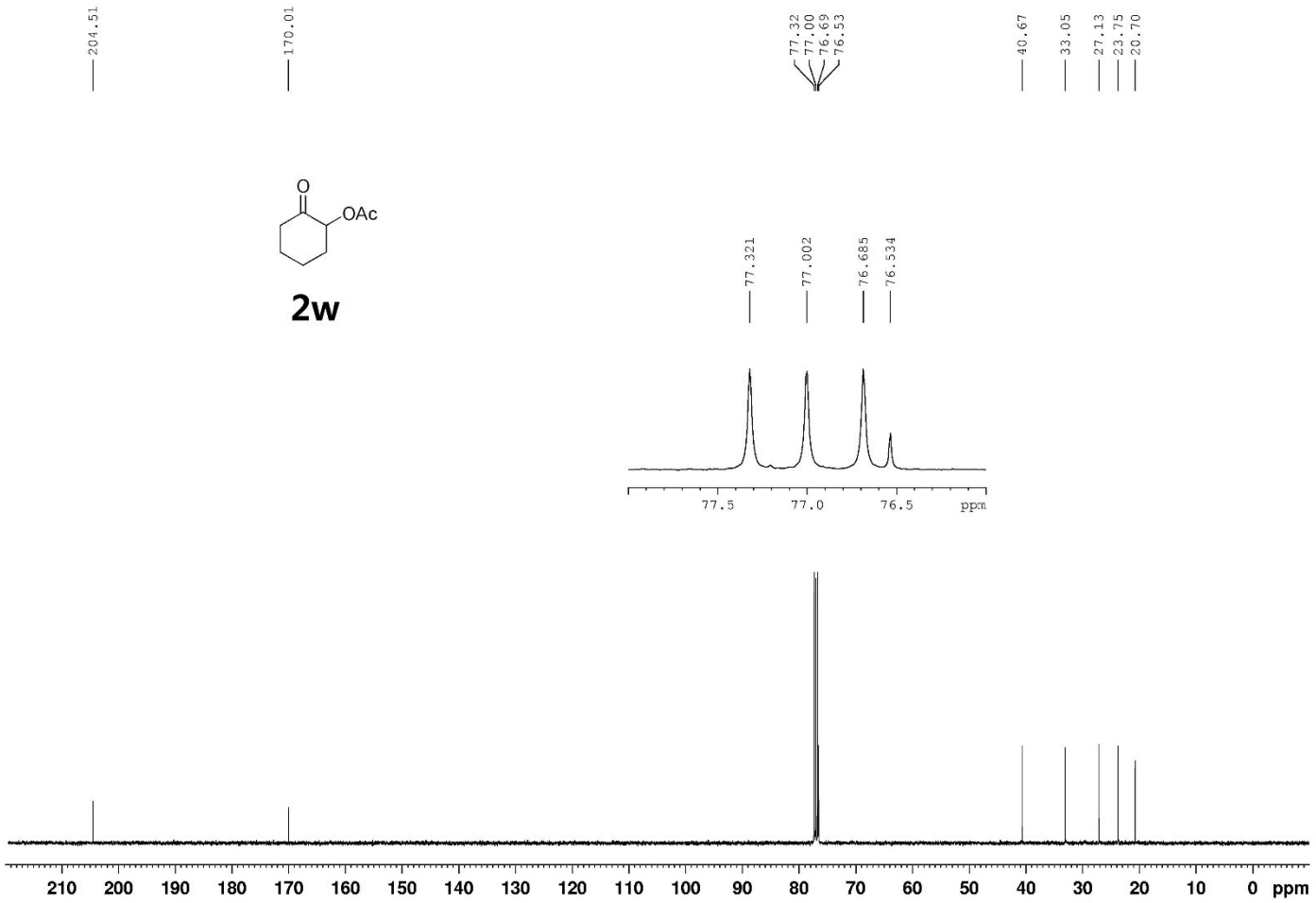

191.08
170.25
150.73
138.65
128.90
124.07
77.32
77.00
76.68
66.04
20.41
O
OAc
O2N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

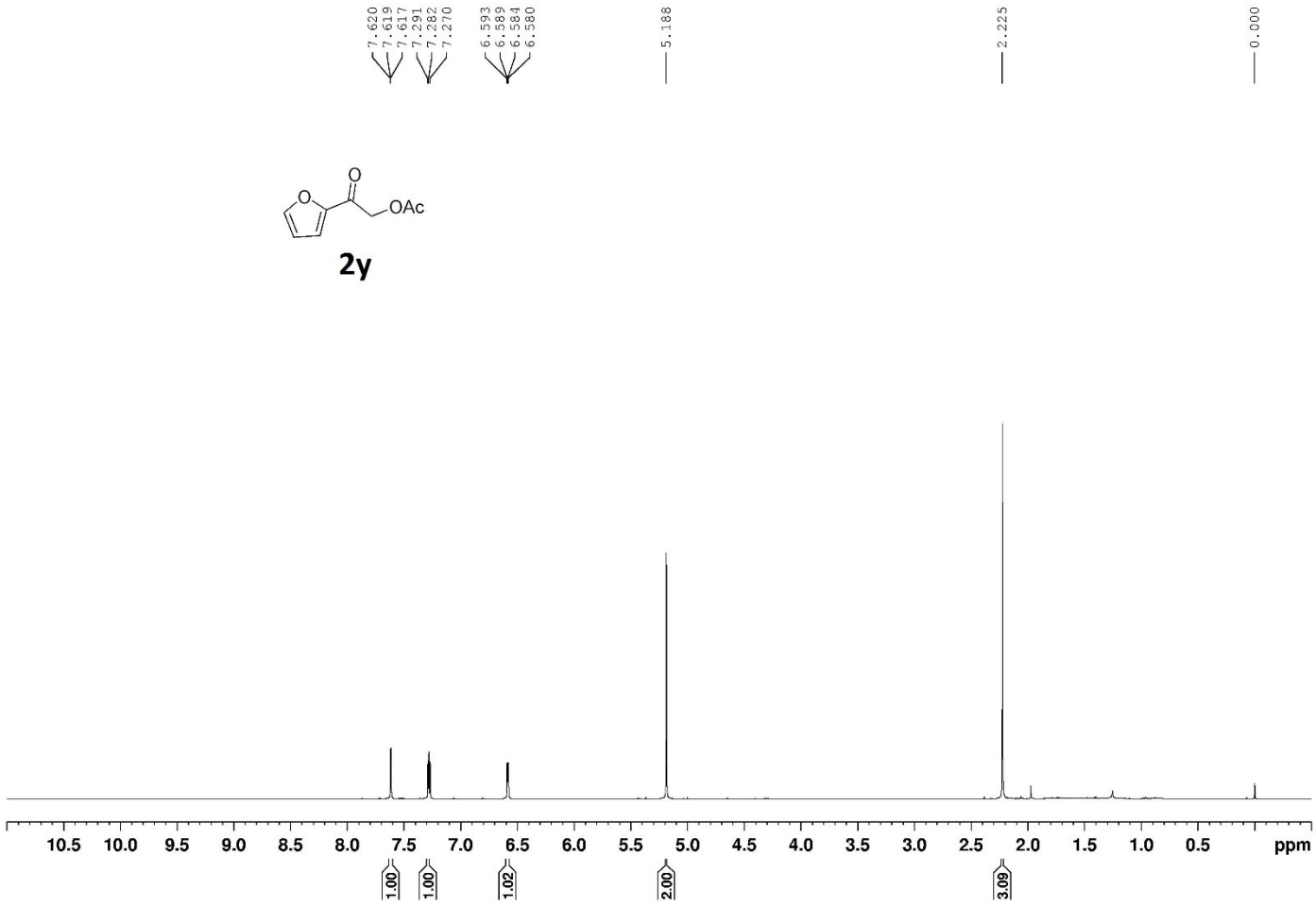
2u


8.032
8.013
7.523
7.504
7.485
7.347
7.328
7.309
7.271
7.251
5.568
5.555
5.534
5.521
3.252
3.240
3.220
3.209
3.198
3.178
3.166
3.114
3.104
3.095
3.072
3.062
3.053
2.431
2.418
2.411
2.407
2.399
2.392
2.387
2.380
2.376
2.368
2.336
2.324
2.303
2.291
2.272
2.260
2.225
0.000
O
OAc
2v
10.5 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 ppm
1.00
1.00
2.02
0.99
1.07
1.10
1.08
1.02
3.03

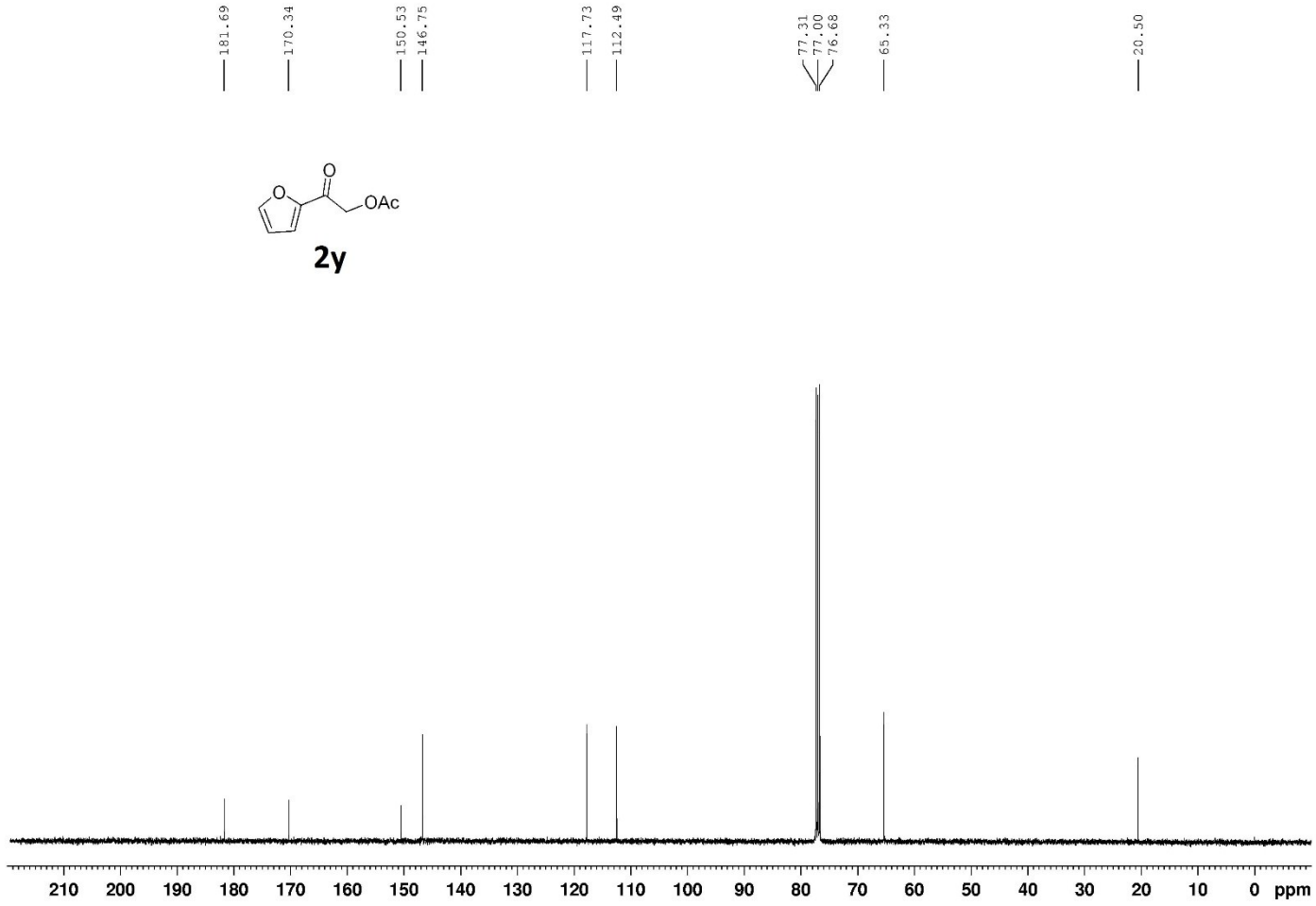

192.90
170.13
143.01
133.85
131.51
128.58
127.75
126.90
77.32
77.00
76.68
74.52
29.08
27.89
20.80
O
OAc
2v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

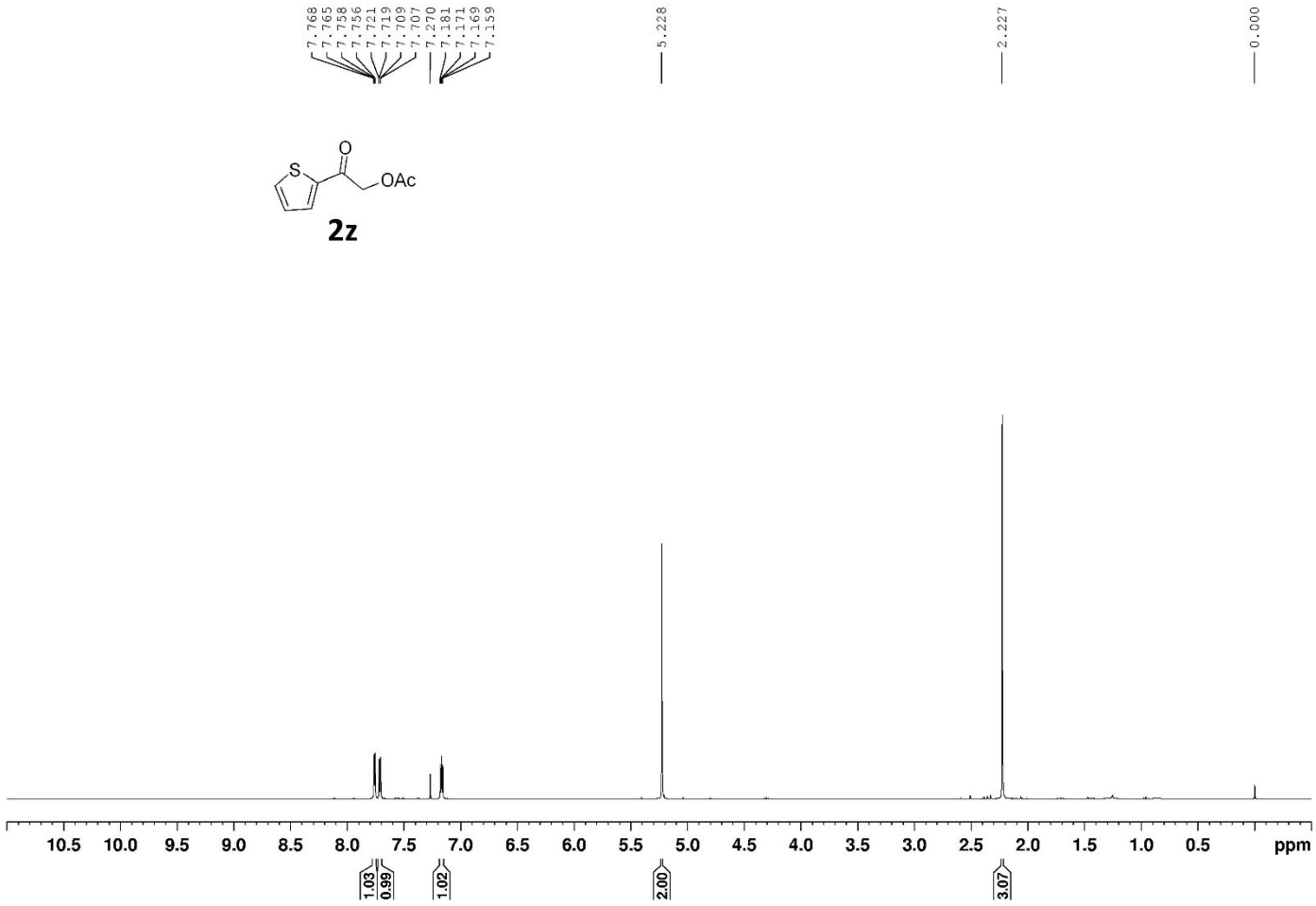

7.272
5.191
5.175
5.169
5.163
5.153
5.147
2.546
2.539
2.535
2.529
2.523
2.512
2.505
2.500
2.495
2.489
2.437
2.435
2.422
2.420
2.403
2.401
2.388
2.386
2.369
2.367
2.361
2.354
2.352
2.334
2.329
2.322
2.318
2.313
2.307
2.299
2.292
2.284
2.276
2.270
2.158
2.140
2.134
2.127
2.120
2.112
2.105
2.097
2.094
2.087
2.079
2.072
2.064
2.010
2.001
1.994
1.987
1.978
1.972
1.964
1.956
1.833
1.824
1.800
1.793
1.785
1.778
1.770
1.761
1.754
1.748
1.740
1.717
1.709
1.686
1.675
1.666
1.652
1.642
1.632
1.620
1.610
1.600
1.587
1.578
0.000
O
OAc
2w
10.5
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
ppm
1.00
1.10
1.20
1.06
3.19
1.21
1.08
2.11
1.23


204.51
170.01
77.32
77.00
76.69
76.53
40.67
33.05
27.13
23.75
20.70
O
OAc
2w
77.321
77.002
76.685
76.534
77.5
77.0
76.5
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

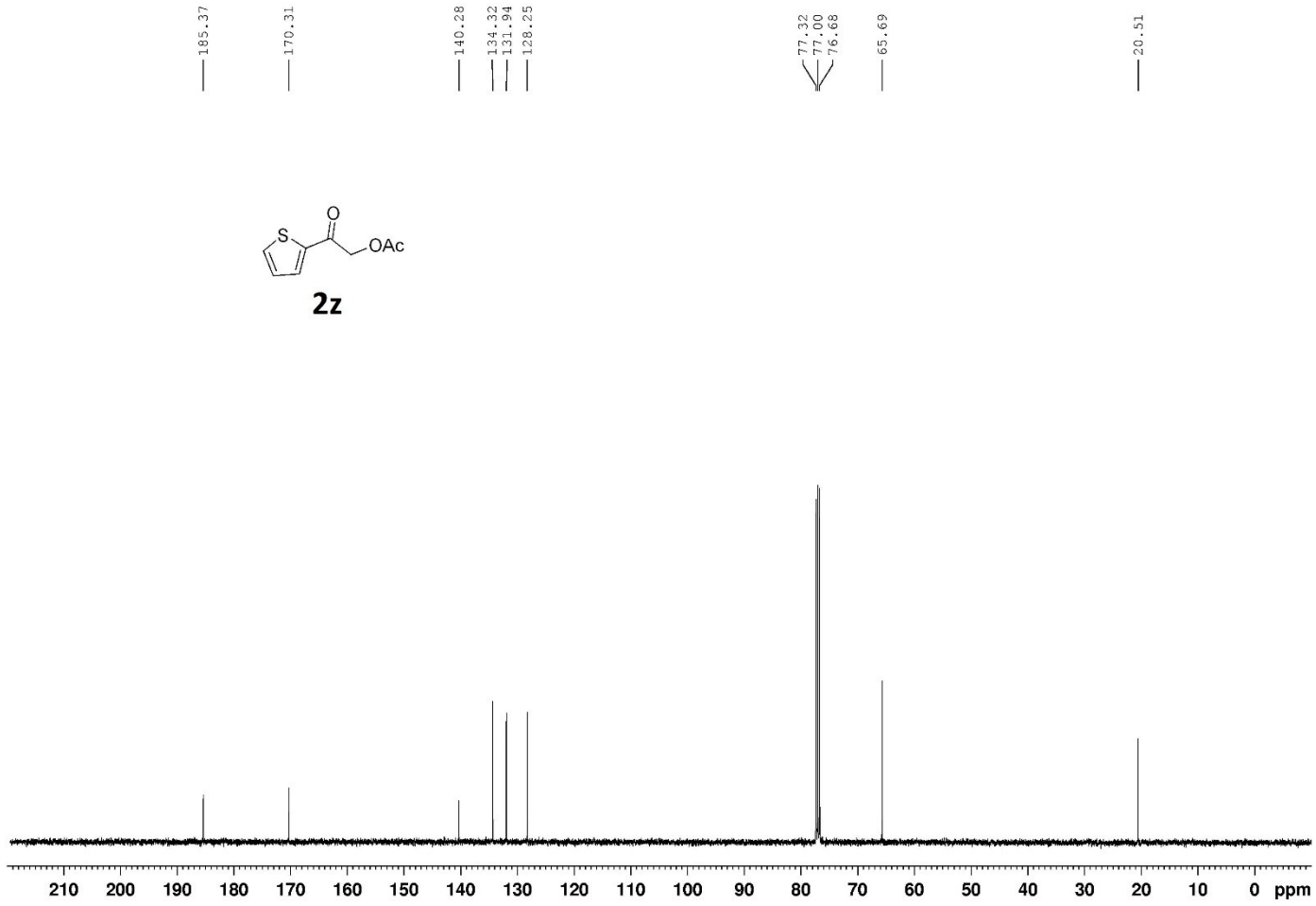

7.620
7.619
7.617
7.291
7.282
7.270
6.593
6.589
6.584
6.580
5.188
2.225
0.000
O
O
OAc
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.00
1.02
2.00
3.09

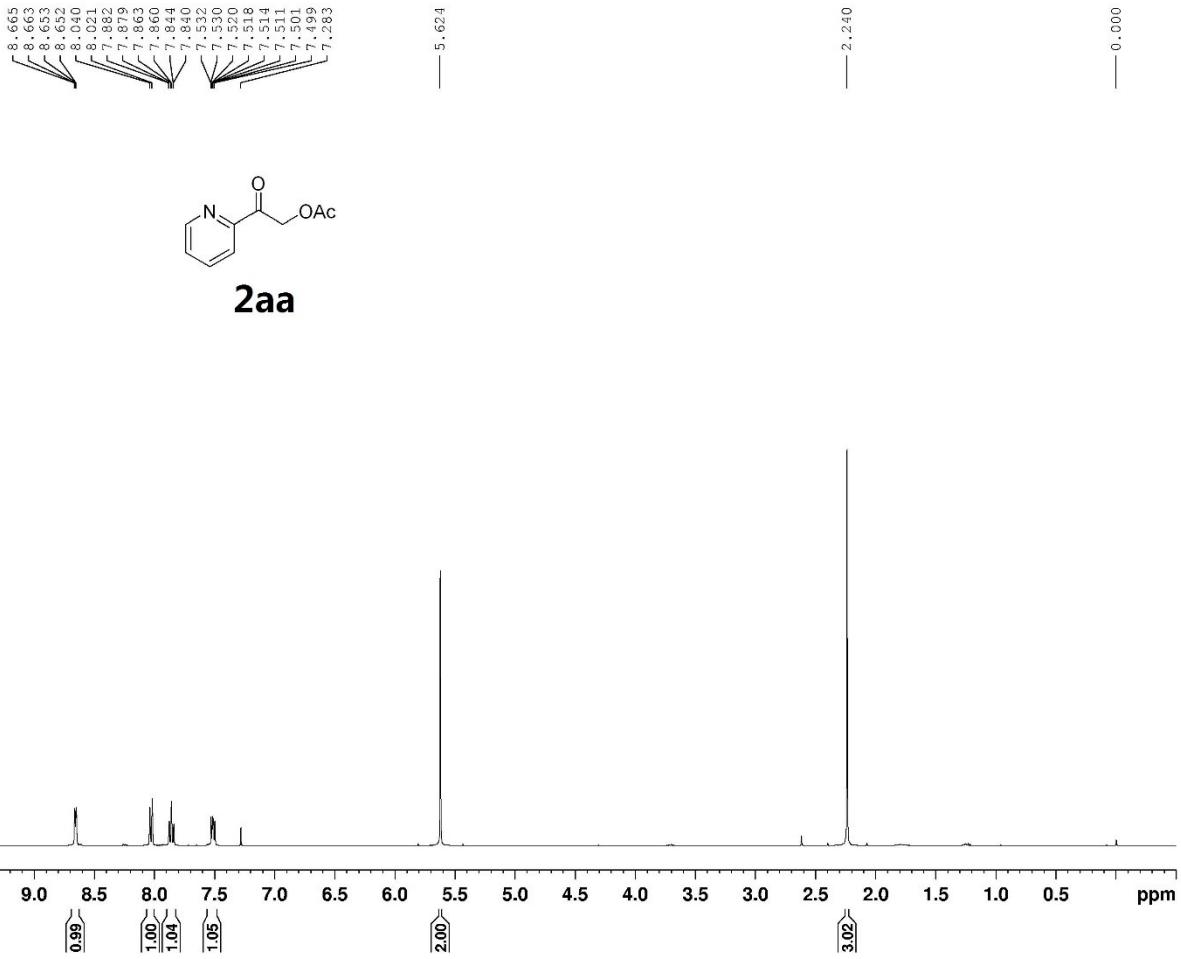
2y


181.69
170.34
150.53
146.75
117.73
112.49
77.31
77.00
76.68
65.33
20.50
O
O
OAc
2y
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

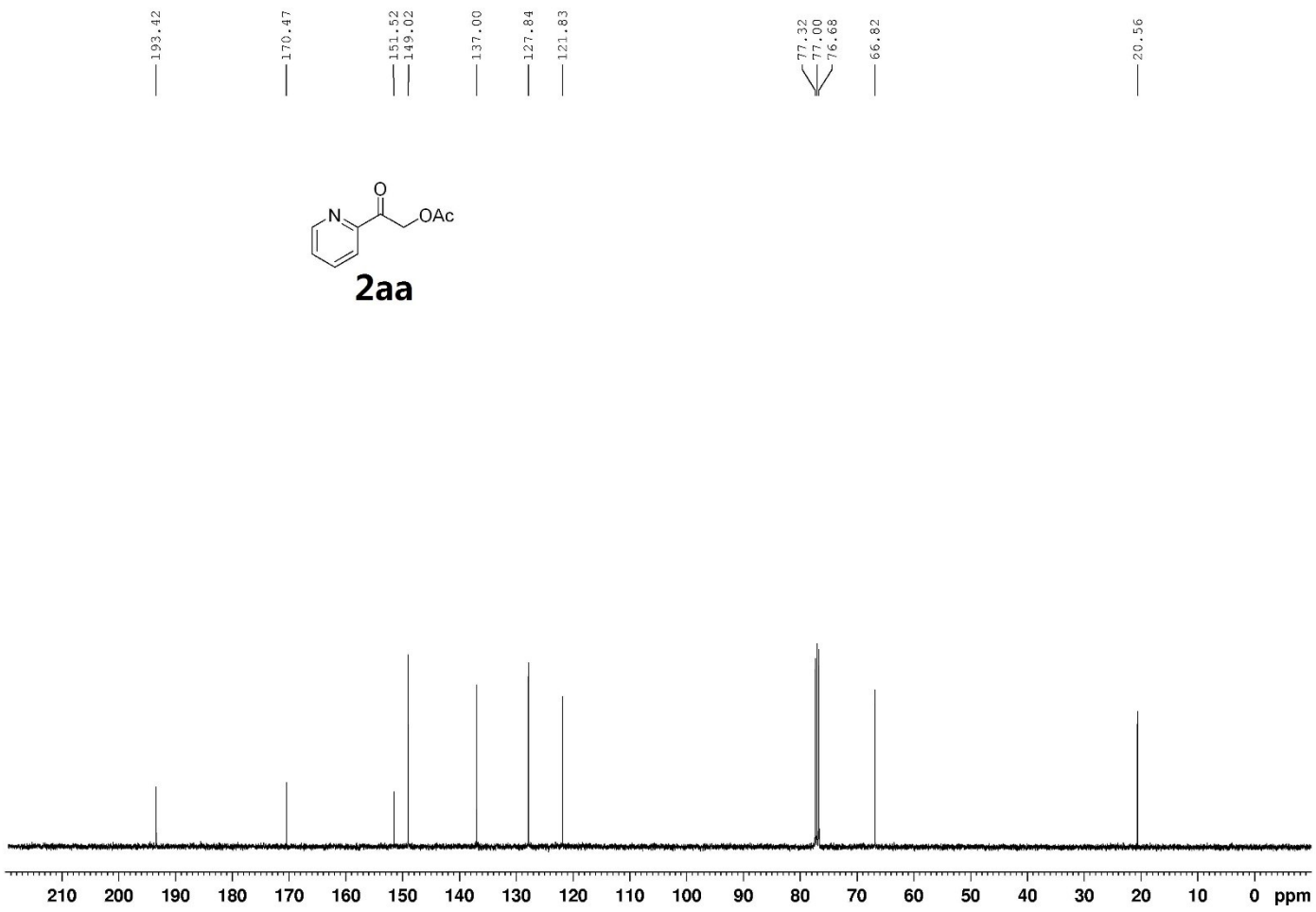

7.768
7.765
7.758
7.756
7.721
7.719
7.709
7.707
7.270
7.181
7.171
7.169
7.159
5.228
2.227
0.000
O
S
OAc
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.03
0.99
1.02
2.00
3.07

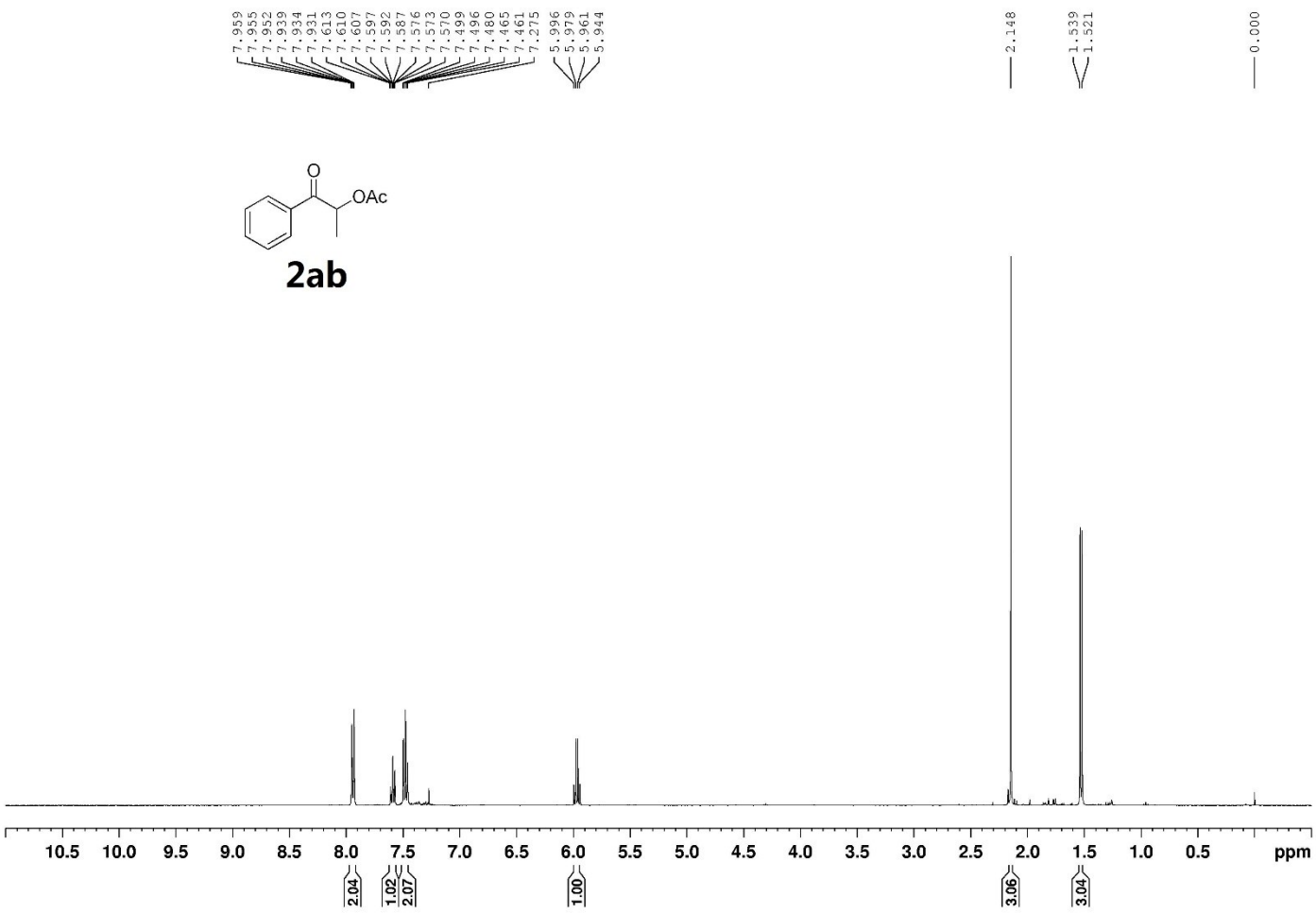
2z

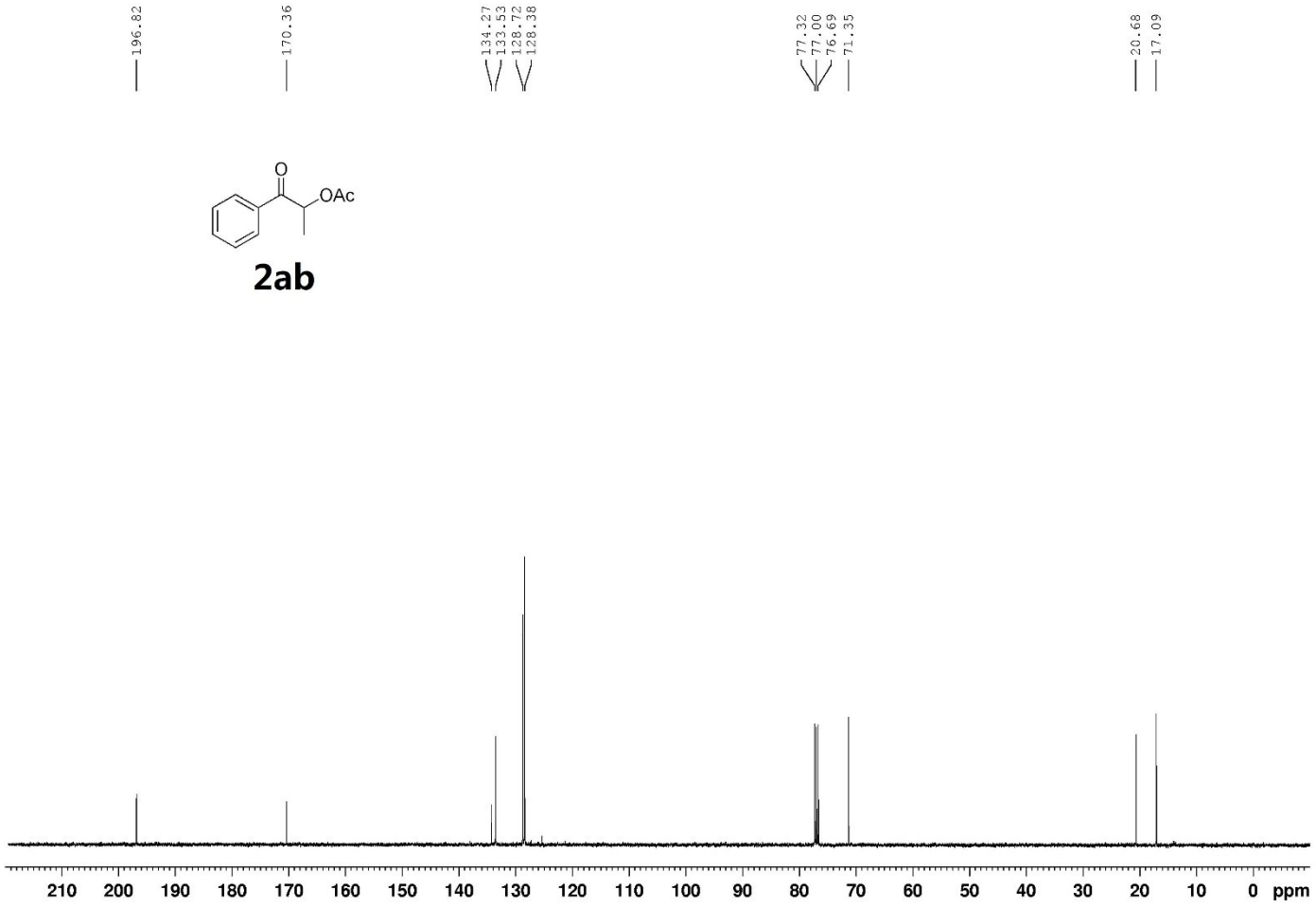

185.37
170.31
140.28
134.32
131.94
128.25
77.32
77.00
76.68
65.69
20.51
O
S
OAc
2z
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

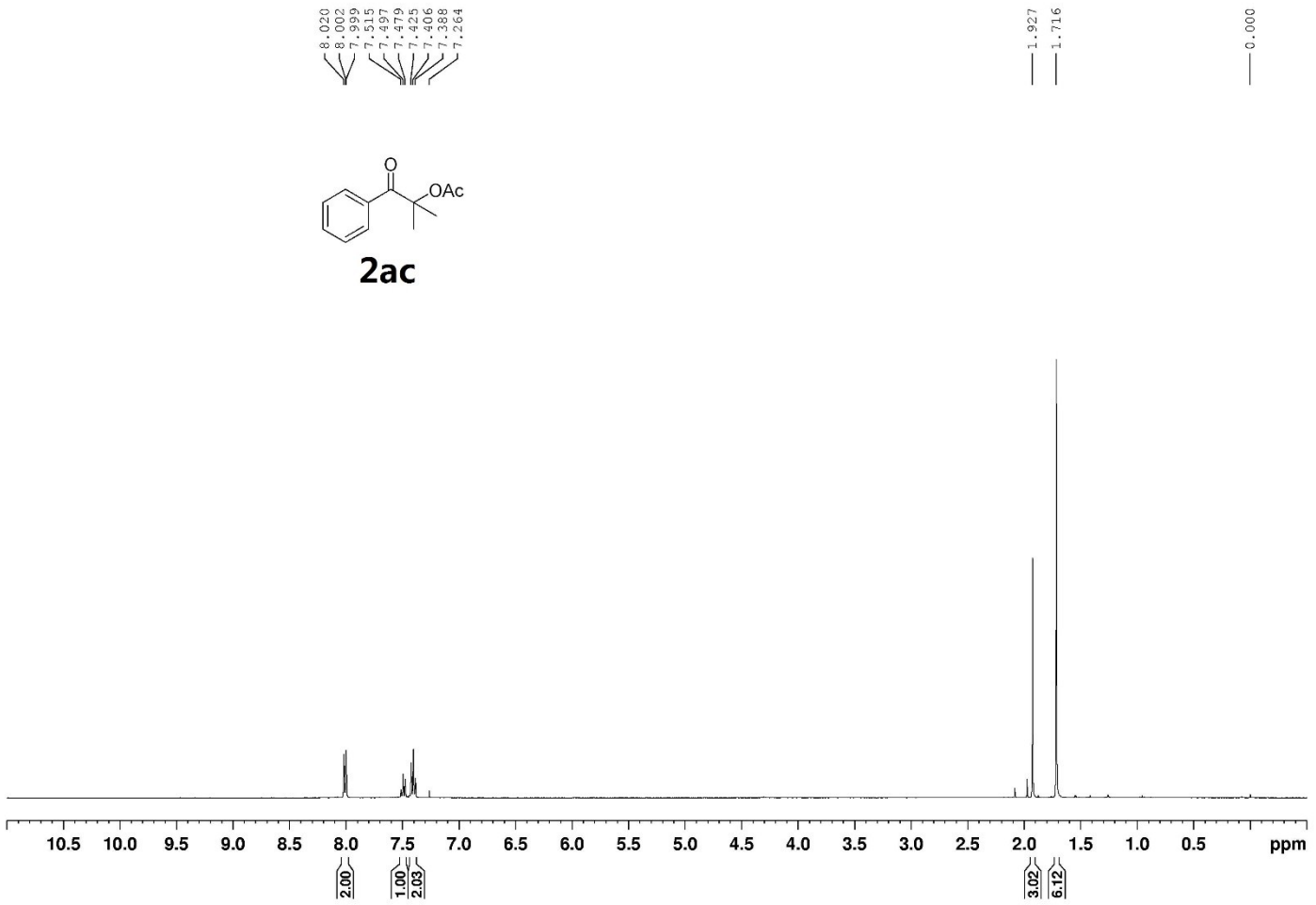

8.665
8.663
8.653
8.652
8.040
8.021
7.882
7.879
7.863
7.860
7.844
7.840
7.532
7.530
7.520
7.518
7.514
7.511
7.501
7.499
7.283
5.624
2.240
0.000
O
N
OAc
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.99
1.00
1.04
1.05
2.00
3.02

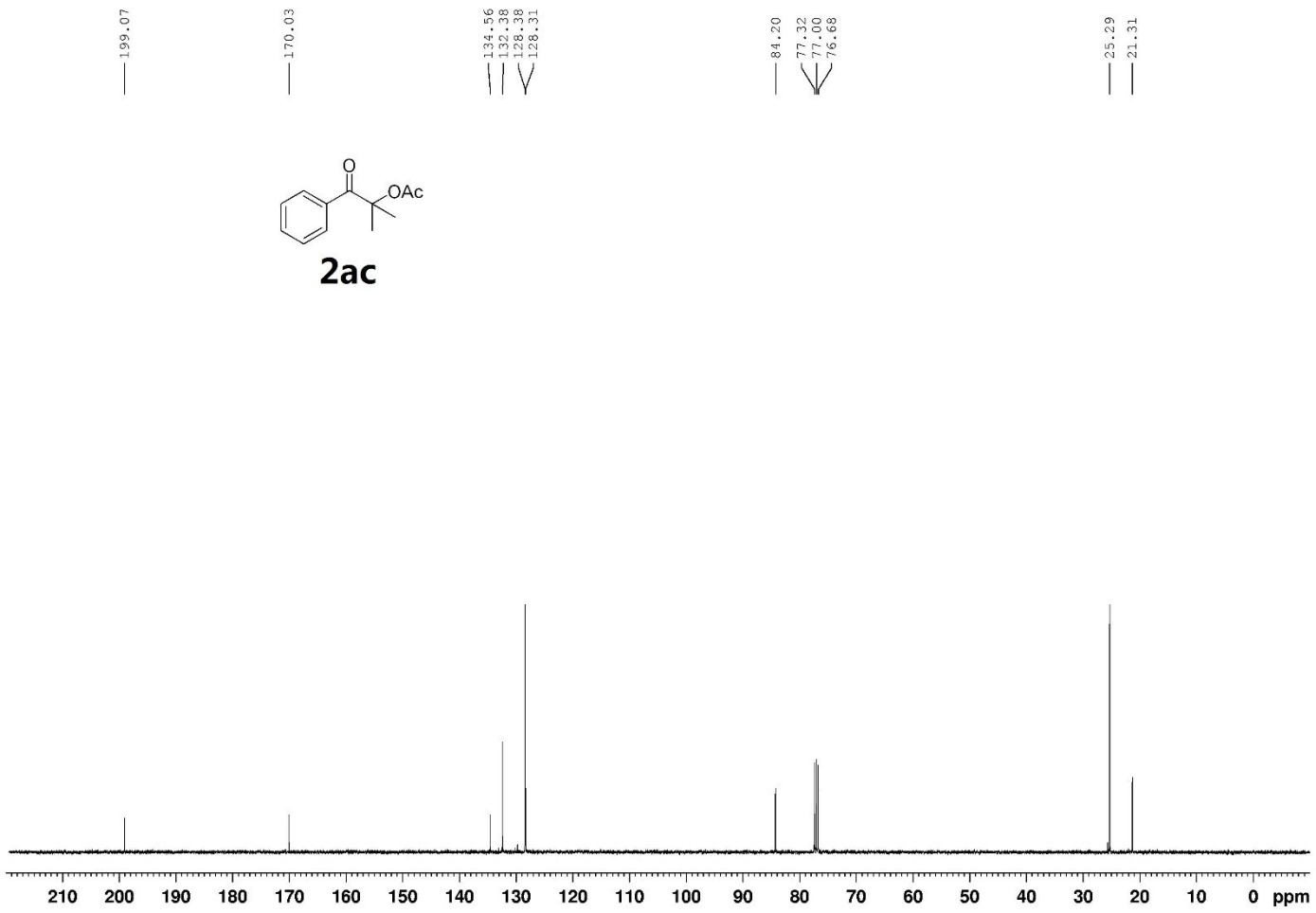
2aa


193.42
170.47
151.52
149.02
137.00
127.84
121.83
77.32
77.00
76.68
66.82
20.56
O
N
OAc
2aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

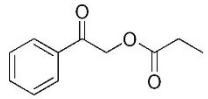

7.959
7.955
7.952
7.939
7.934
7.931
7.613
7.610
7.607
7.597
7.592
7.587
7.576
7.573
7.570
7.499
7.496
7.480
7.465
7.461
7.275
5.996
5.979
5.961
5.944
2.148
1.539
1.521
0.000
O
OAc
2ab
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.04
1.02
2.07
1.00
3.06
3.04


196.82
170.36
134.27
133.53
128.72
128.38
77.32
77.00
76.69
71.35
20.68
17.09
O
OAc
2ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

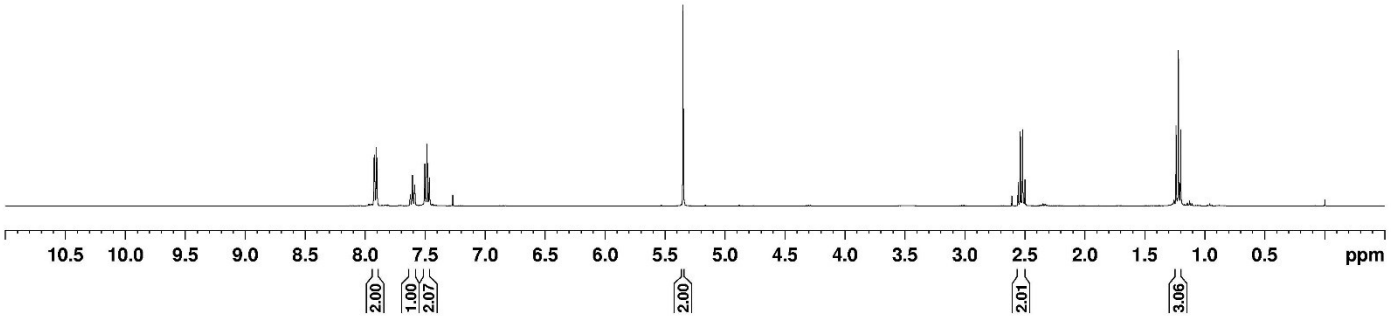

8.020
8.002
7.999
7.515
7.497
7.479
7.425
7.406
7.388
7.264
1.927
1.716
0.000
O
OAc
2ac
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.00
2.03
3.02
6.12

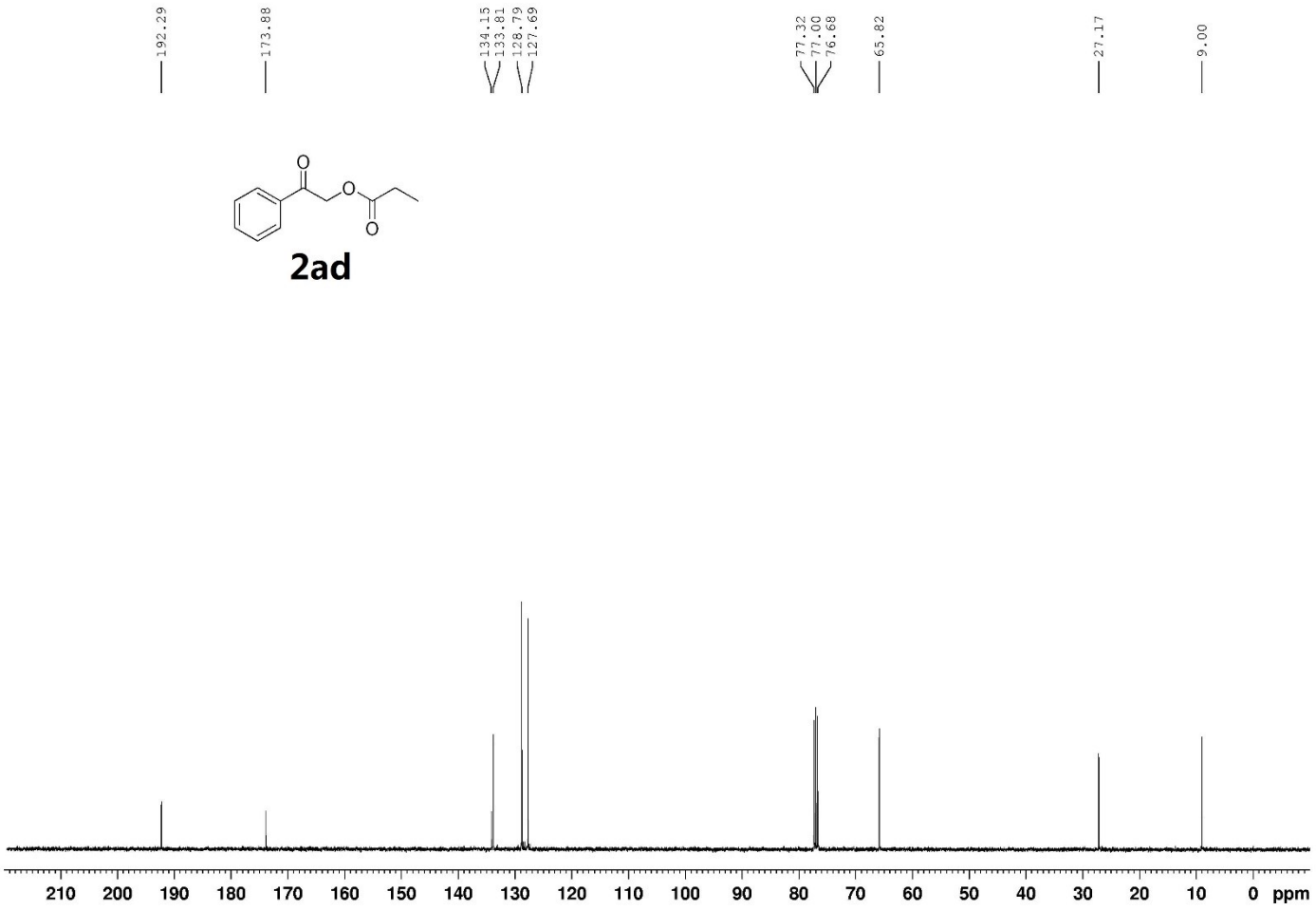

199.07
170.03
134.56
132.38
128.38
128.31
84.20
77.32
77.00
76.68
25.29
21.31
O
OAc
2ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

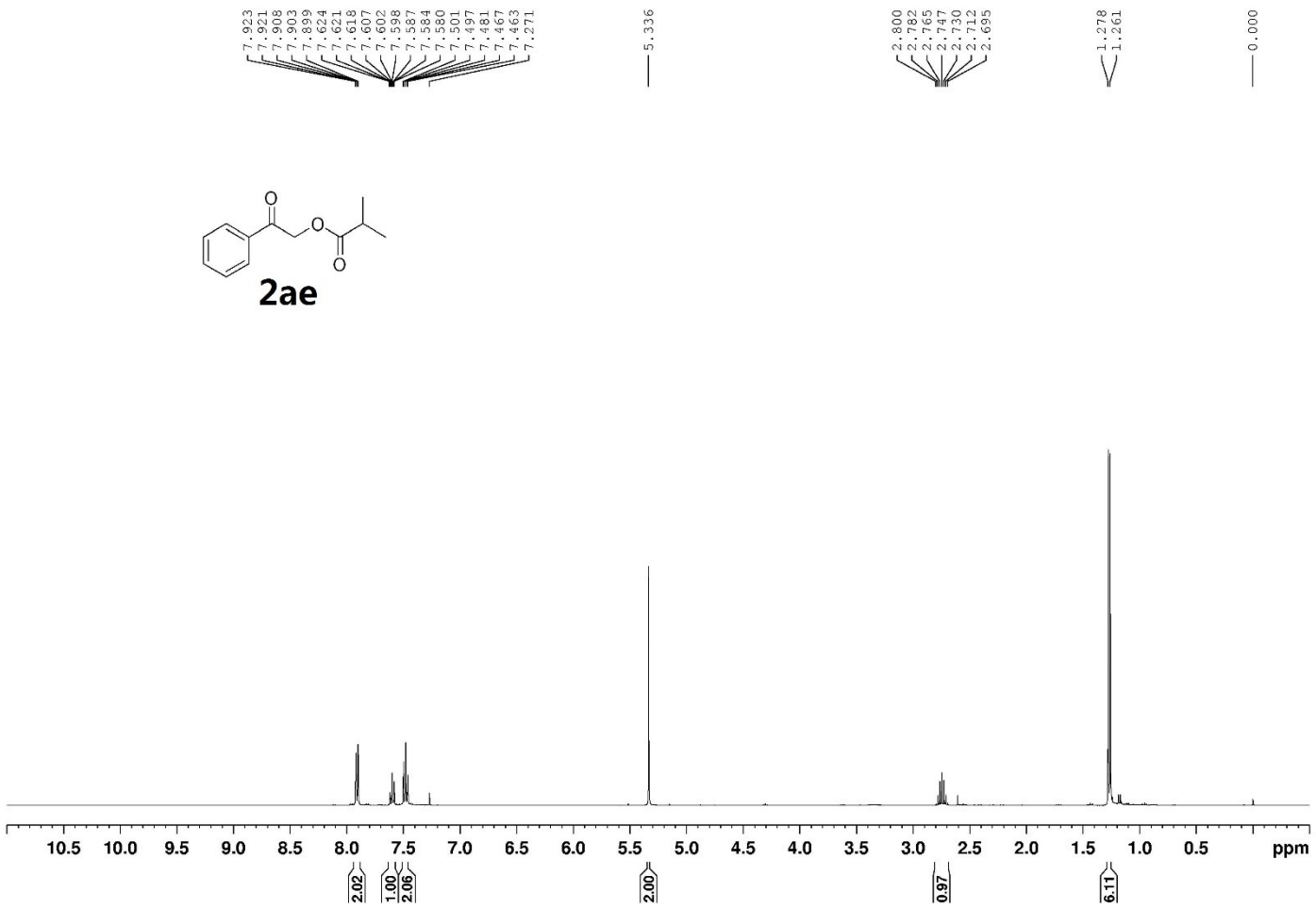

7.925
7.907
7.904
7.626
7.607
7.588
7.505
7.485
7.467
7.272
5.351
2.557
2.539
2.519
2.501
1.240
1.221
1.202
0.000

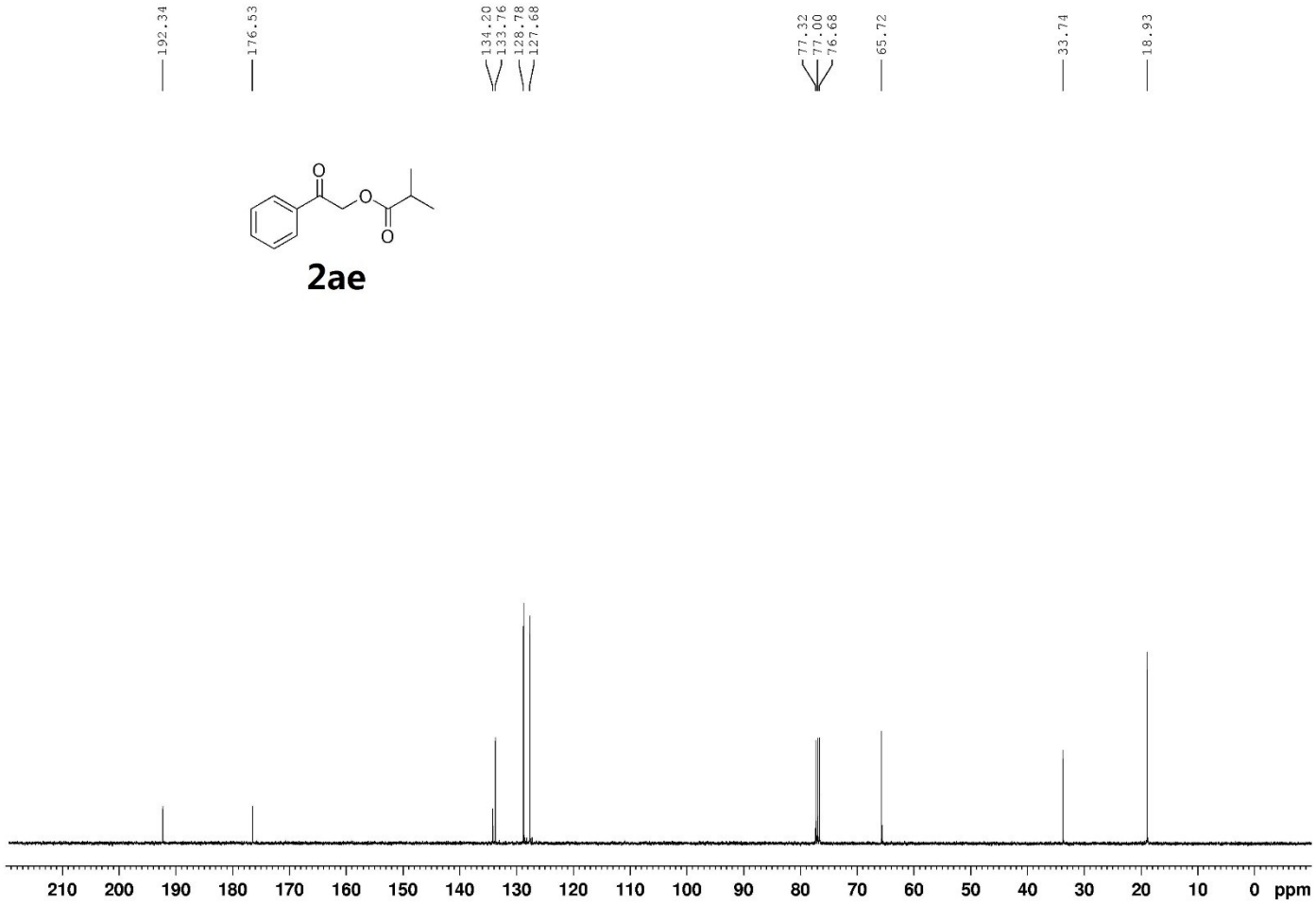


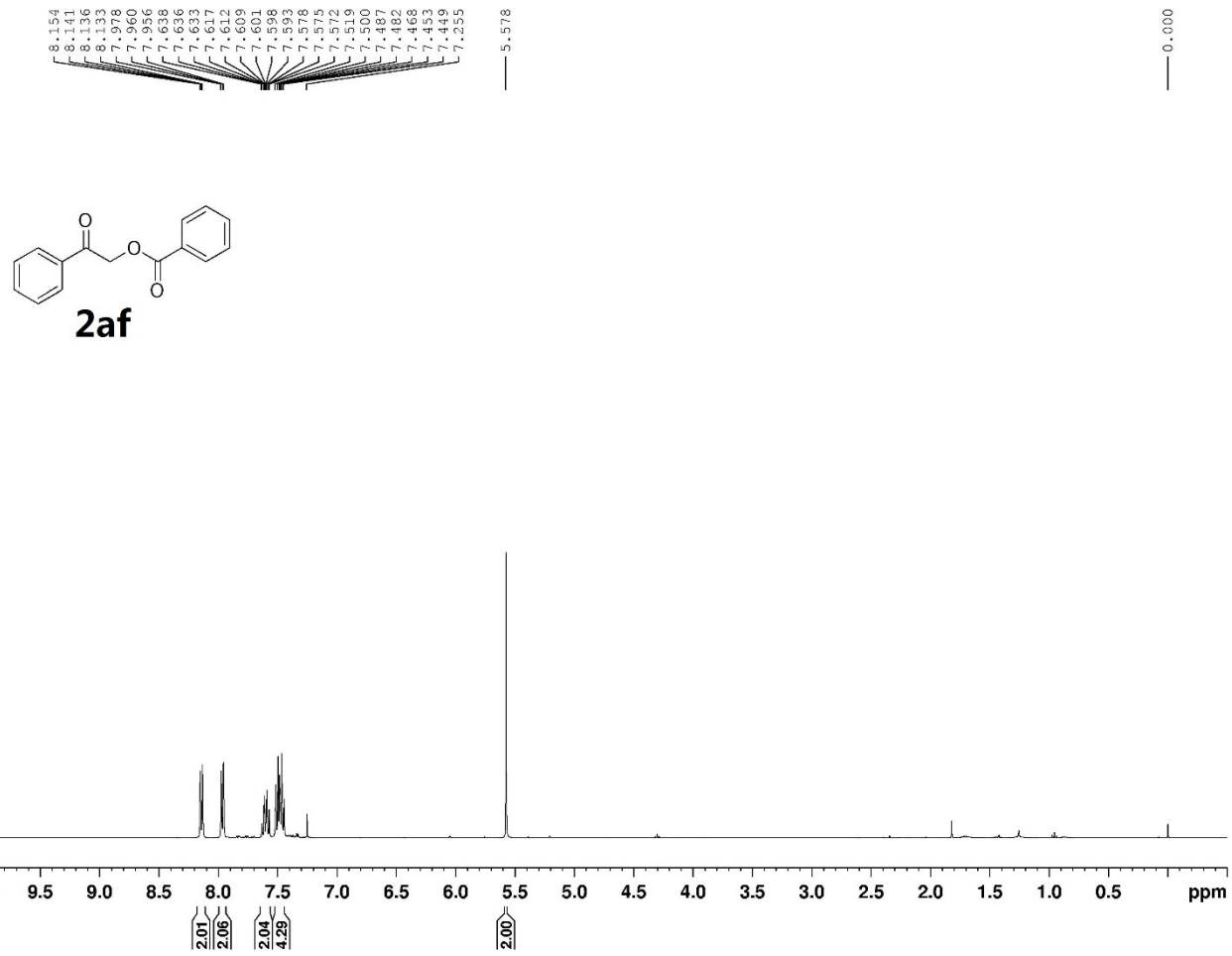
2ad

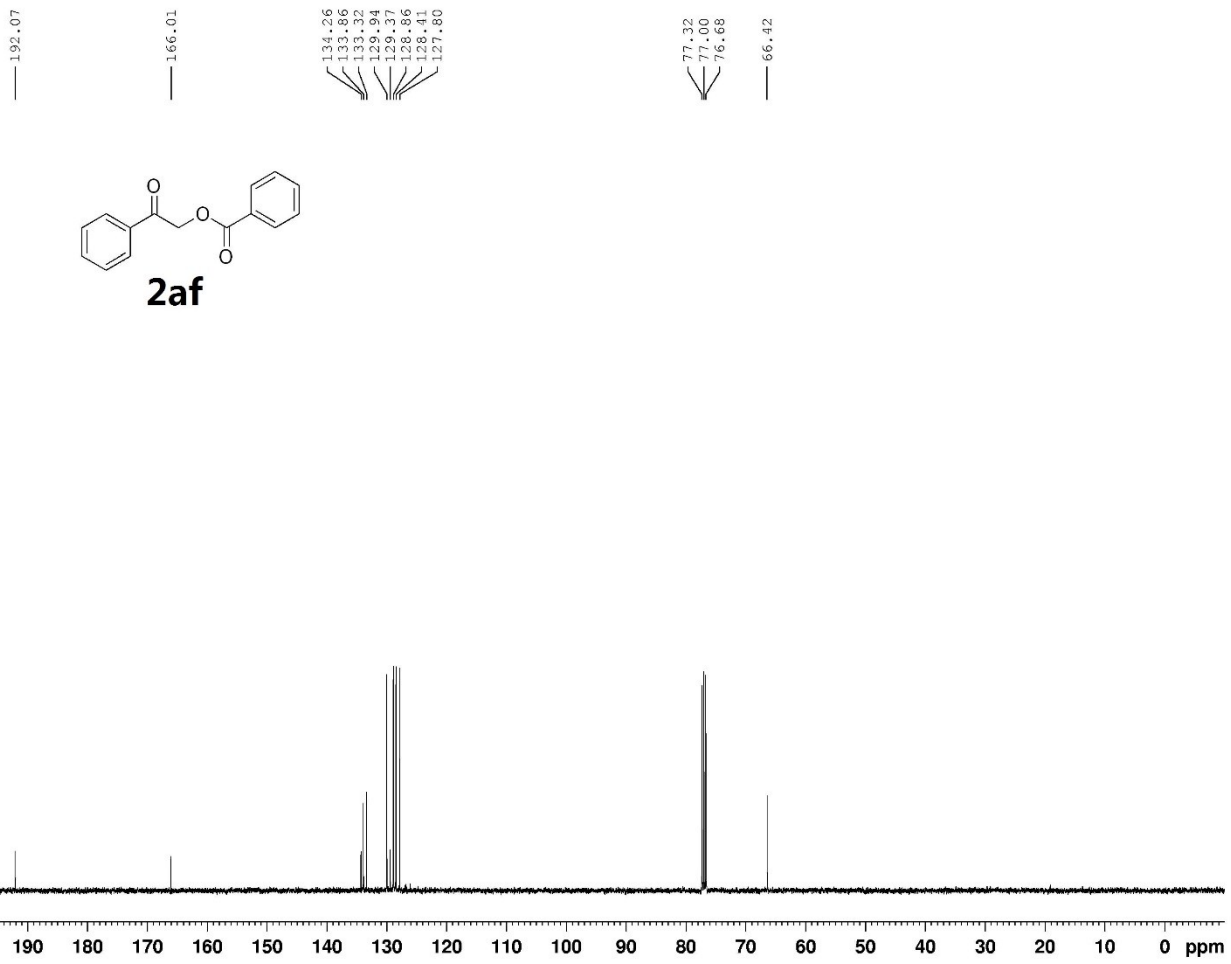

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.00
2.07
2.00
2.01
3.06

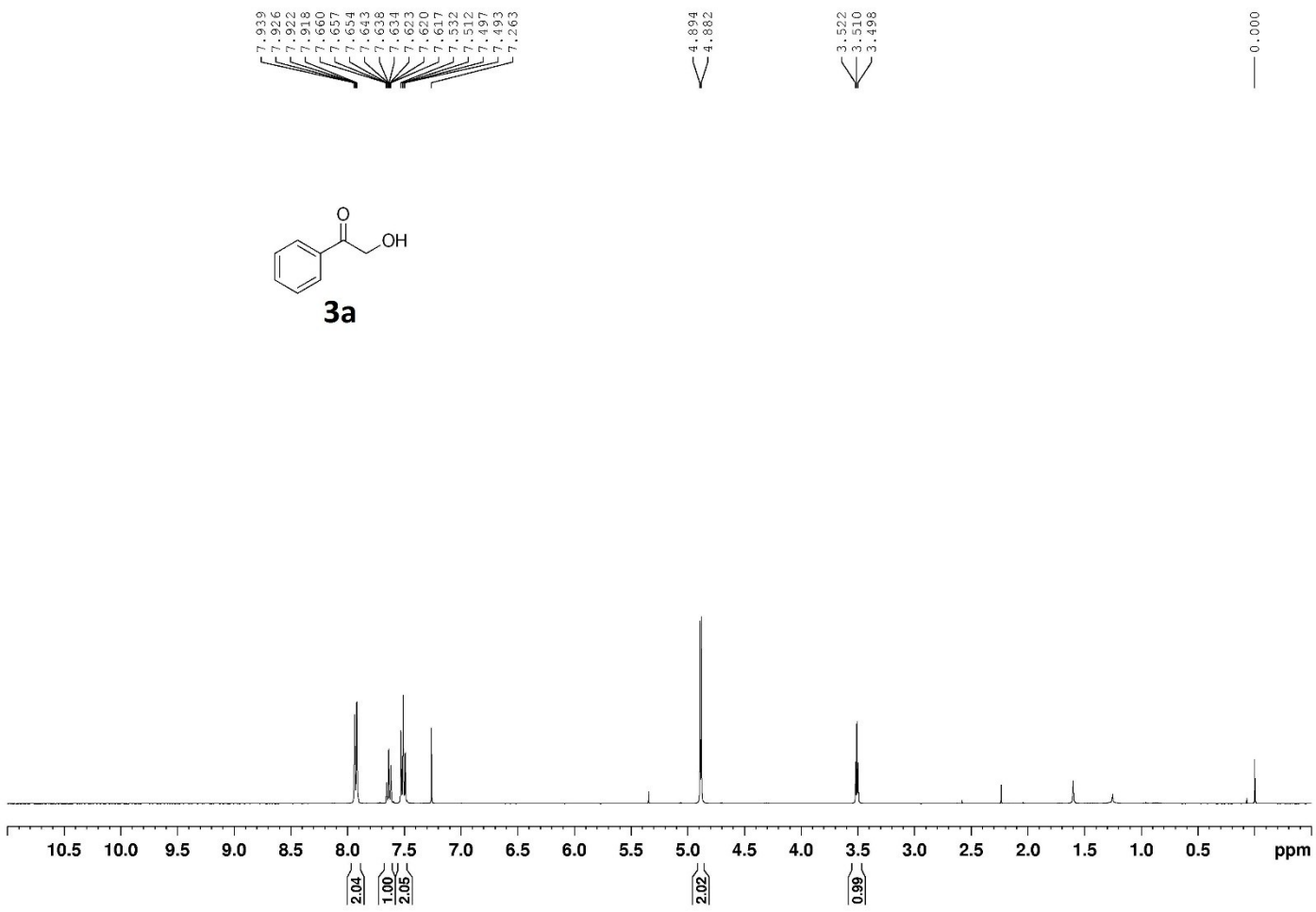

192.29
173.88
134.15
133.81
128.79
127.69
77.32
77.00
76.68
65.82
27.17
9.00
O
O
O
2ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.923
7.921
7.908
7.903
7.899
7.624
7.621
7.618
7.607
7.602
7.598
7.587
7.584
7.580
7.501
7.497
7.481
7.467
7.463
7.271
5.336
2.800
2.782
2.765
2.747
2.730
2.712
2.695
1.278
1.261
0.000
2ae
10.5 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 ppm
2.02
1.00
2.06
2.00
0.97
6.11

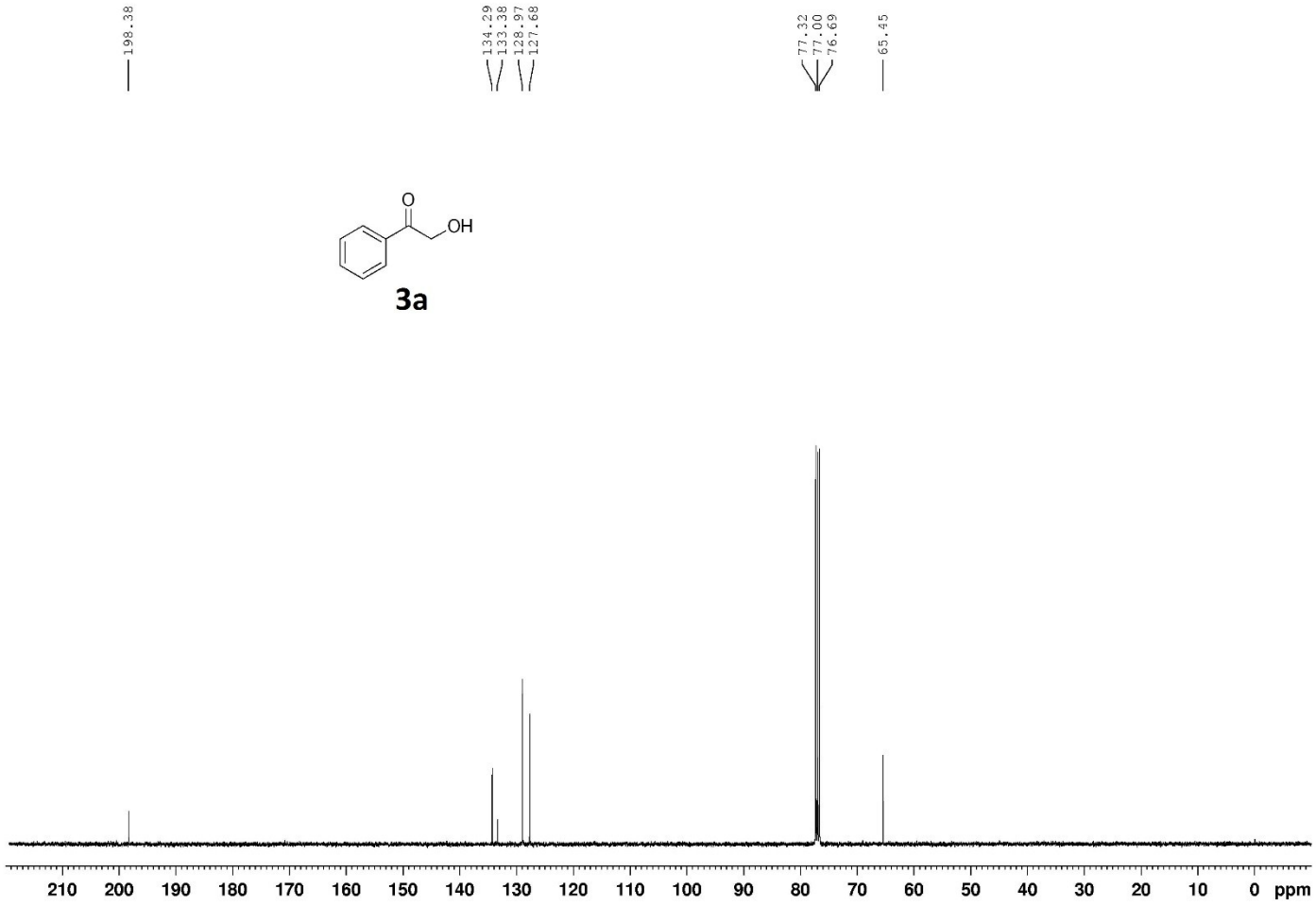

192.34
176.53
134.20
133.76
128.78
127.68
77.32
77.00
76.68
65.72
33.74
18.93
O
O
O
2ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.154
8.141
8.136
8.133
7.978
7.960
7.956
7.638
7.636
7.633
7.617
7.612
7.609
7.601
7.598
7.593
7.578
7.575
7.572
7.519
7.500
7.487
7.482
7.468
7.453
7.449
7.255
5.578
0.000
O
O
O
2af
10.5
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
ppm
2.01
2.06
2.04
4.29
2.00

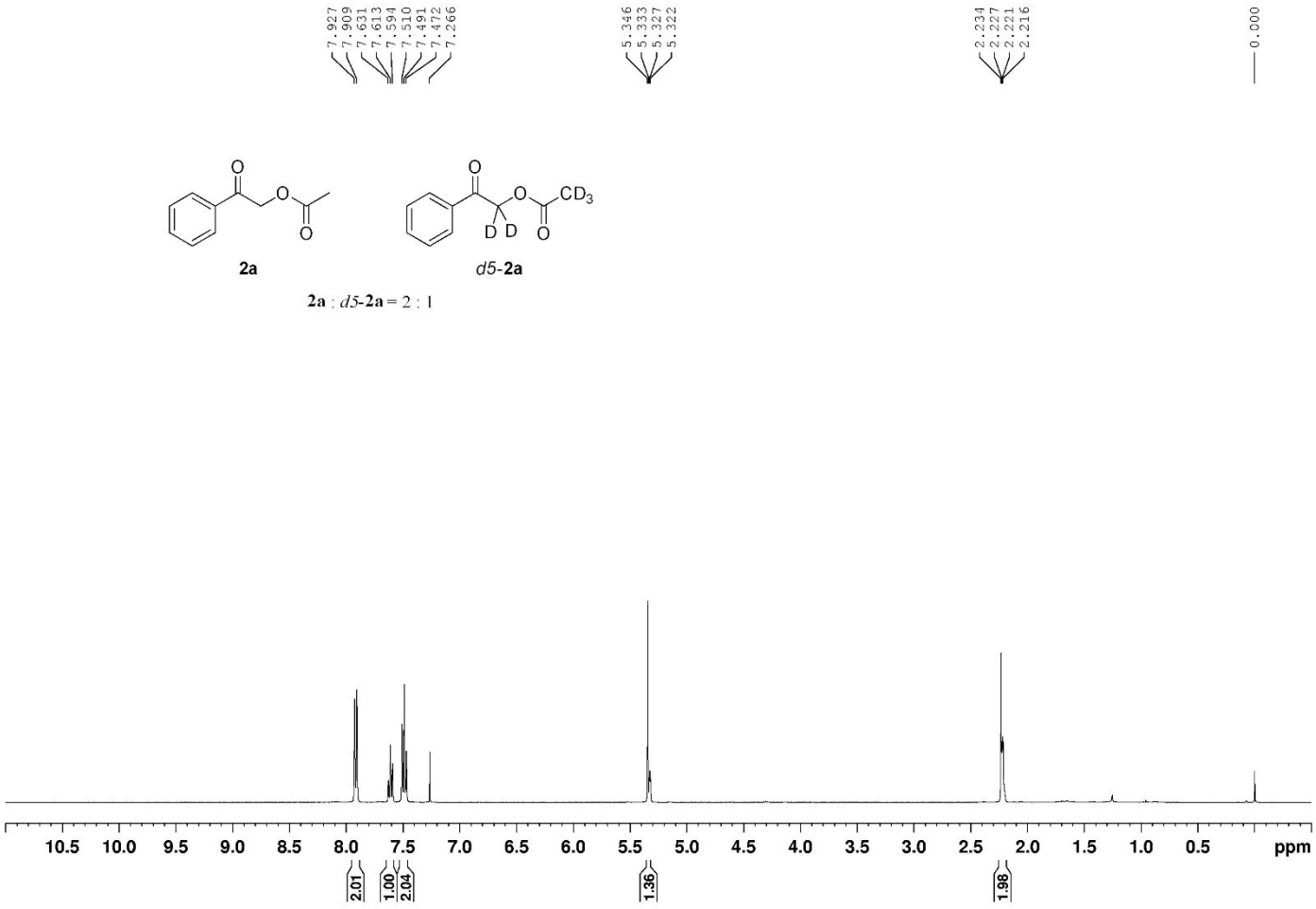

192.07
166.01
134.26
133.86
133.32
129.94
129.37
128.86
128.41
127.80
77.32
77.00
76.68
66.42
O
O
O
2af
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.939
7.926
7.922
7.918
7.660
7.657
7.654
7.643
7.638
7.634
7.623
7.620
7.617
7.532
7.512
7.497
7.493
7.263
4.894
4.882
3.522
3.510
3.498
0.000
O
OH
10.5
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
ppm
2.04
1.00
2.05
2.02
0.99

3a


198.38
134.29
133.38
128.97
127.68
77.32
77.00
76.69
65.45
O
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

3a


7.927
7.909
7.631
7.613
7.594
7.510
7.491
7.472
7.266
5.346
5.333
5.327
5.322
2.234
2.227
2.221
2.216
0.000
O
O
O
2a
O
O
CD3
D D
O
d5-2a
2a : d5-2a = 2 : 1
10.5
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
ppm
2.01
1.00
2.04
1.36
1.98