

Supporting Information

Photocatalytic redox-neutral arylation of cyclopropanols with cyanoarenes via radical-mediated C–C and C–CN bond cleavage

Yue Tong,^{‡a} Na Hao,^{‡a} Long Zhang,^a Jun Wei,^a Zhijie Zhang,^a Qiang Fu,^a Dong Yi,^a Yao Mou,^b
Jun Wang,^a Xianchao Pan,^a Lin Yang,^a Siping Wei,^{*a} Lei Zhong^{*c} and Ji Lu^{*a}

^aSchool of Pharmacy, Southwest Medical University, Luzhou 646000, China. *E-mail:* jilu@swmu.edu.cn; swei1225@swmu.edu.cn

^bDepartment of Pharmacy, the Affiliated Hospital of Southwest Medical University, Luzhou 646000, China

^cDepartment of Pharmacy, Personalized Drug Therapy Key Laboratory of Sichuan Province Sichuan Academy of Medical Sciences & Sichuan Provincial People's Hospital, School of Medicine, University of Electronic Science and Technology of China, Chengdu 610072, China. *E-mail:* zhl7235301@163.com

[‡]These authors contributed equally.

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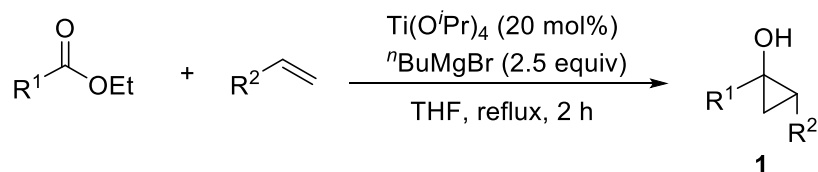
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1. General information

All reagents and starting materials, unless otherwise noted, were purchased from Energy, J&K, TCI, and Adamas-beta® Chemical company as reagent grade and used without further purification. Anhydrous solvents (including DME, CH₂Cl₂, DMF, THF, MeCN, Water < 0.005%) were purchased from Energy, and used as received. Unless otherwise indicated, all syntheses and manipulations were carried out under argon atmosphere.

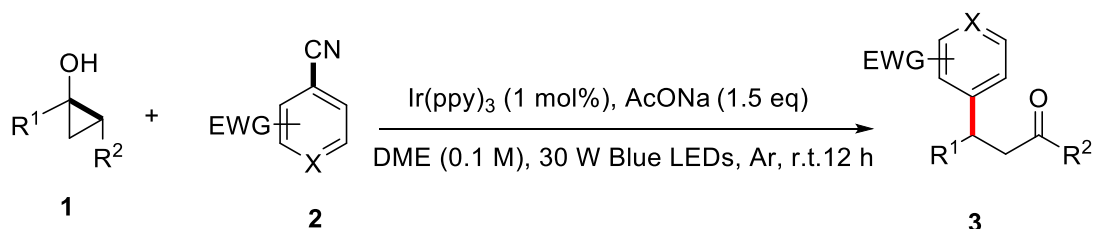
¹H NMR, ¹³C NMR, and ¹⁹F NMR spectra were obtained with a Bruker AV II-400 spectrometer (¹H: 400 MHz, ¹³C: 101 MHz, ¹⁹F: 376 MHz). The chemical shifts were measured with tetramethylsilane as the internal reference. The chemical shifts (δ) were expressed in ppm and *J* values were given in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets, and br = broad. TLC was performed using commercially prepared silica gel plates (GF254), and visualized under UV light 254 nm. Flash column chromatography was performed on silica gel (100-200 mesh). All mixed solvent eluents are reported as v/v solutions. Cyclic voltammetry tests were carried out with a CHI700E electrochemical workstation. Mass analysis data were acquired on a SCIEX UPLC (EXion) –QTOF (X500R). Melting points were measured using a Hanon MP470 apparatus.

2. Synthesis of cyclopropanols



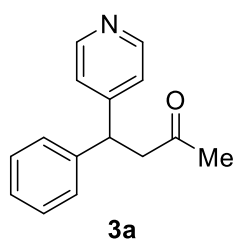
The procedure was followed by previous work^{1a}: To a solution of ester (10 mmol, 1.0 equiv), alkene (11 mmol, 1.1 equiv) and $\text{Ti(O}^i\text{Pr)}_4$ (2 mmol, 0.2 equiv) in 15 mL of anhydrous THF, a solution of $^n\text{BuMgBr}$ (25 mmol, 2.5 equiv) in THF was added dropwise over 1 h, at reflux. The mixture was stirred for an additional 30 min, then was poured into ice-cold 10% sulfuric acid (50 mL). The organic layer was separated and the aqueous layer was extracted with Et_2O (2×20 mL). The combined organic layer extracts were washed with saturated NaHCO_3 , dried over anhydrous Na_2SO_4 , filtered and concentrated under reduced pressure, and the residue was purified by column chromatography on silica gel with a gradient eluent of petroleum ether and ethyl acetate ($\sim 10/1$) to give the desired product **1** (the corresponding cyclopropanols have been reported, see the ref.1).

3. Typical experimental procedure



An oven-dried Schlenk tube (10 mL) containing a stirring bar was charged with the corresponding aromatic nitrile (0.2 mmol, 1.0 equiv), the corresponding cyclopropanol (0.4 mmol, 2.0 equiv), Ir(ppy)_3 (0.002 mmol, 1 mol%), AcONa (0.3 mmol, 1.5 equiv). The Schlenk tube was then connected to a vacuum line where it was evacuated and back-filled with argon for 3 times. Then DME (2 mL) was added under argon flow. Finally, the tube was placed approximately 2 cm from 30 W blue LEDs, and stirred at room temperature for 12 h. After completion, the reaction was quenched with H_2O (2.5 mL) and extracted with EtOAc . The organic layer was dried over anhydrous Na_2SO_4 , filtered and concentrated under reduced pressure, and the residue was purified by silica gel flash chromatography (petroleum ether/ethyl acetate 3/1 \sim 1/1) to afford the corresponding product **3**.

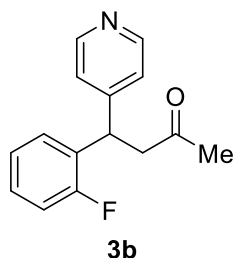
4. Characterization data for products



41.5 mg, 92%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.48 (d, $J = 5.6$ Hz, 2H), 7.32 – 7.28 (m, 2H), 7.24 – 7.21 (m, 1H), 7.20 – 7.18 (m, 2H), 7.15 – 7.13 (m, 2H), 4.57 (t, $J = 7.2$ Hz, 1H), 3.19 (d, $J = 7.6$ Hz, 2H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.0, 152.9, 150.0, 142.2, 129.0, 127.9, 127.2, 123.2, 48.8, 45.2, 30.8.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{16}\text{NO}]^+$: 226.1226, found: 226.1226.

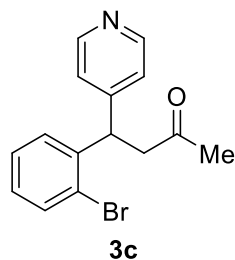


44.4 mg, 91%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.47 (d, $J = 5.6$ Hz, 2H), 7.23 – 7.17 (m, 2H), 7.14 (d, $J = 5.2$ Hz, 2H), 7.08 (t, $J = 7.2$ Hz, 1H), 7.00 (t, $J = 8.8$ Hz, 1H), 4.81 (t, $J = 7.2$ Hz, 1H), 3.28 – 3.16 (m, 2H), 2.13 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.5, 160.6 (d, $J = 247.5$ Hz), 151.7, 150.0, 129.2 (d, $J = 14.1$ Hz), 129.0, 129.0 (d, $J = 12.1$ Hz), 124.5 (d, $J = 3.0$ Hz), 123.1, 116.1 (d, $J = 22.2$ Hz), 47.5 (d, $J = 2.0$ Hz), 39.1 (d, $J = 2.0$ Hz), 30.4.

$^{19}\text{F NMR}$ (376 MHz, CDCl_3) δ -116.15.

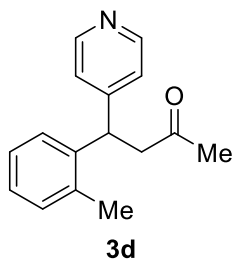
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{15}\text{FNO}]^+$: 244.1132, found: 244.1132.



37.7 mg, 62%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.50 (d, $J = 5.2$ Hz, 2H), 7.60 – 7.54 (m, 1H), 7.30 – 7.27 (m, 1H), 7.16 – 7.14 (m, 2H), 7.13 – 7.08 (m, 2H), 5.07 (t, $J = 7.2$ Hz, 1H), 3.22 – 3.11 (m, 2H), 2.15 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.3, 151.6, 149.9, 141.2, 133.7, 128.8, 128.7, 128.0, 125.0, 123.5, 48.5, 44.1, 30.3.

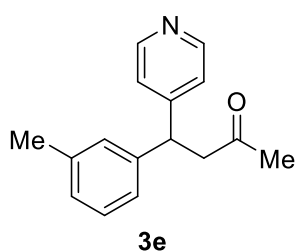
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{15}\text{BrNO}]^+$: 304.0332, found: 304.0331



37.4 mg, 83%; Yellow oil. $^1\text{H NMR}$ (400 MHz, MeOD) δ 8.39 (d, $J = 5.2$ Hz, 2H), 7.28 (d, $J = 7.0$ Hz, 2H), 7.25 (s, 1H), 7.21 – 7.17 (m, 1H), 7.15 – 7.11 (m, 2H), 4.82 (t, $J = 7.2$ Hz, 1H), 3.33 – 3.30 (m, 2H), 2.31 (s, 3H), 2.13 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, MeOD) δ 208.7, 156.0, 150.0, 141.4, 137.4, 131.9, 128.0, 127.8, 127.5, 125.2, 49.3, 42.3, 30.3, 19.9.

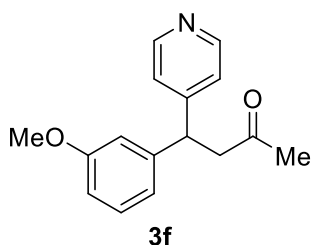
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{18}\text{NO}]^+$: 240.1383, found: 240.1382



38.3 mg, 80%; Yellow solid, m.p. 58.6-62.2 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.48 (d, $J = 6.0$ Hz, 2H), 7.20 – 7.16 (m, 1H), 7.13 (d, $J = 6.0$ Hz, 2H), 7.03 (d, $J = 5.4$ Hz, 1H), 7.00 – 6.99 (m, 2H), 4.53 (t, $J = 7.2$ Hz, 1H), 3.18 (d, $J = 7.6$ Hz, 2H), 2.30 (s, 3H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.1, 153.0, 150.0, 142.1, 138.6, 128.8, 128.7, 127.9, 124.7, 123.1, 48.8, 45.1, 30.8, 21.6.

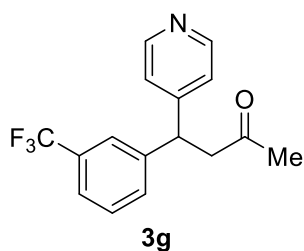
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{18}\text{NO}]^+$: 240.1383, found: 240.1382.



40.7 mg, 80%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.48 (d, $J = 6.0$ Hz, 2H), 7.21 (t, $J = 8.0$ Hz, 1H), 7.12 (d, $J = 6.0$ Hz, 2H), 6.79 – 6.74 (m, 2H), 6.72 – 6.71 (m, 1H), 4.53 (t, $J = 7.6$ Hz, 1H), 3.76 (s, 3H), 3.17 (d, $J = 7.2$ Hz, 2H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.0, 159.9, 152.7, 150.0, 143.8, 130.0, 123.1, 120.1, 114.2, 111.9, 55.3, 48.7, 45.1, 30.8.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{18}\text{NO}_2]^+$: 256.1332, found: 256.1332.



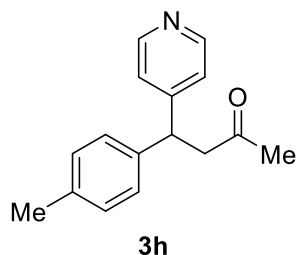
51 mg, 87%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.51 (d, $J = 6.0$ Hz, 2H), 7.49 (d, $J = 7.6$ Hz, 1H), 7.44 (s, 1H), 7.41 (d, $J = 7.6$ Hz, 1H), 7.38 (d, $J = 7.6$ Hz, 1H), 7.12 (d, $J = 6.0$ Hz, 2H), 4.65 (t, $J = 7.2$ Hz, 1H), 3.28 – 3.15 (m, 2H), 2.14 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.2, 151.9, 150.3, 143.3, 131.5,

131.3 (q, $J = 31.3$ Hz), 129.5, 124.5 (q, $J = 4.0$ Hz), 124.1 (q, $J = 4.0$ Hz), 124.0 (q, $J = 272.7$ Hz), 123.1, 48.6, 44.8, 30.7.

^{19}F NMR (376 MHz, CDCl_3) δ -62.58.

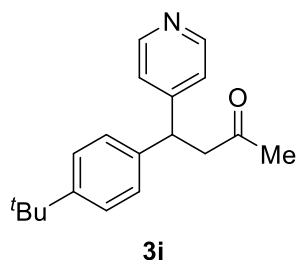
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{15}\text{F}_3\text{NO}]^+$: 294.1100, found: 294.1099.



40.1 mg, 84%; Yellow solid, m.p. 54.9-55.8 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.47 (d, $J = 5.6$ Hz, 2H), 7.13 (d, $J = 5.6$ Hz, 2H), 7.09 – 7.06 (m, 4H), 4.53 (t, $J = 7.2$ Hz, 1H), 3.16 (d, $J = 7.2$ Hz, 2H), 2.29 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.1, 153.1, 150.0, 139.2, 136.8, 129.6, 127.7, 123.1, 48.8, 44.8, 30.7, 21.1.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{18}\text{NO}]^+$: 240.1383, found: 240.1383.

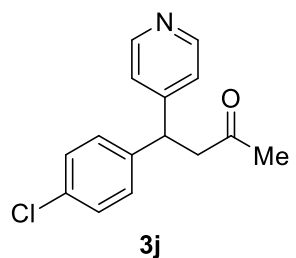


48.4 mg, 86%; Yellow solid, m.p. 97.1-99.6 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.48 (d, $J = 6.0$ Hz, 2H), 7.30 (dd, $J_1 = 1.6$ Hz, $J_2 = 6.0$ Hz, 2H), 7.16 – 7.13 (d, $J = 6.0$ Hz, 2H), 7.10 (d, $J = 6.0$ Hz, 2H), 4.54 (t, $J = 7.2$ Hz, 1H), 3.23-3.12 (m, 2H), 2.11 (s, 3H), 1.27 (s, 9H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.2, 153.1, 150.0, 139.1, 139.1,

127.4, 125.9, 123.2, 49.0, 44.8, 34.5, 31.4, 30.7.

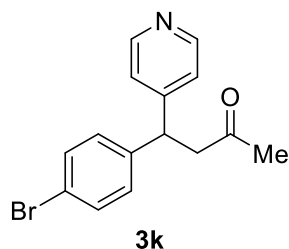
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{19}\text{H}_{24}\text{NO}]^+$: 282.1852, found: 282.1850



43.6 mg, 84%; Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.49 (d, $J = 5.6$ Hz, 2H), 7.27 – 7.25 (m, 2H), 7.12 (d, $J = 5.2$ Hz, 2H), 7.10 (d, $J = 5.6$ Hz, 2H), 4.55 (t, $J = 7.2$ Hz, 1H), 3.16 (d, $J = 7.2$ Hz, 2H), 2.12 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 205.5, 152.4, 150.2, 140.7, 133.0, 129.3, 129.1, 123.1, 48.7, 44.5, 30.7.

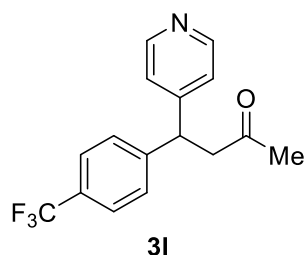
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{15}\text{ClNO}]^+$: 260.0837, found: 260.0837.



57.6 mg, 95%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.48 (dd, $J_1 = 6.0\text{ Hz}$, $J_2 = 1.6\text{ Hz}$, 2H), 7.41 (d, $J = 8.4\text{ Hz}$, 2H), 7.10 (d, $J = 6.0\text{ Hz}$, 2H), 7.06 (d, $J = 8.0\text{ Hz}$, 2H), 4.53 (t, $J = 7.2\text{ Hz}$, 1H), 3.16 (d, $J = 7.2\text{ Hz}$, 2H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.5, 152.3, 150.2, 141.3, 132.1, 129.6, 123.0, 121.1, 48.6, 44.5, 30.7.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{15}\text{BrNO}]^+$: 304.0332, found: 304.0328.

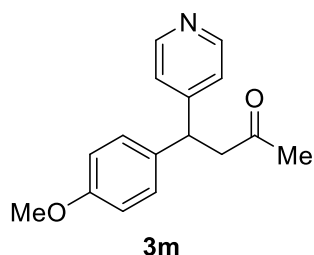


12.2 mg, 21%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.51 (d, $J = 5.6\text{ Hz}$, 2H), 7.55 (d, $J = 8.4\text{ Hz}$, 2H), 7.31 (d, $J = 8.4\text{ Hz}$, 2H), 7.11 (d, $J = 5.6\text{ Hz}$, 2H), 4.65 (t, $J = 7.6\text{ Hz}$, 1H), 3.21 (d, $J = 7.6\text{ Hz}$, 2H), 2.15 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.3, 151.9, 150.3, 146.3, 129.5 (q,

$J = 32.3\text{ Hz}$), 128.3, 125.9 (q, $J = 4.0\text{ Hz}$), 124.1 (q, $J = 273.7\text{ Hz}$), 123.1, 48.5, 44.8, 30.7.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{15}\text{F}_3\text{NO}]^+$: 294.1100, found: 294.1100.

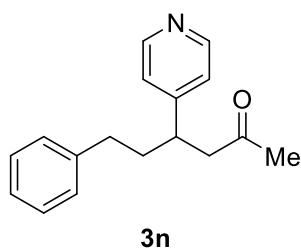


42.4 mg, 83%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.47 (d, $J = 6.0\text{ Hz}$, 2H), 7.12 – 7.09 (m, 4H), 6.82 (dd, $J_1 = 7.2\text{ Hz}$, $J_2 = 1.6\text{ Hz}$, 2H), 4.52 (t, $J = 7.2\text{ Hz}$, 1H), 3.76 (s, 3H), 3.15 (d, $J = 7.2\text{ Hz}$, 2H), 2.11 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.2, 158.6, 153.3, 150.0, 134.2,

128.9, 123.0, 114.3, 55.4, 49.0, 44.4, 30.8.

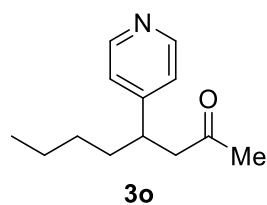
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{16}\text{H}_{18}\text{NO}_2]^+$: 256.1332, found: 256.1331.



24.3 mg, 48%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.54 (d, $J = 5.6\text{ Hz}$, 2H), 7.28 – 7.24 (m, 2H), 7.19 (d, $J = 7.2\text{ Hz}$, 1H), 7.15 (d, $J = 6.0\text{ Hz}$, 2H), 7.07 (d, $J = 7.2\text{ Hz}$, 2H), 3.22 – 3.15 (m, 1H), 2.76 (d, $J = 7.2\text{ Hz}$, 2H), 2.48 – 2.37 (m, 2H), 2.04 (s, 3H), 1.97 – 1.83 (m, 2H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.7, 153.4, 150.1, 141.4, 128.6, 128.4, 126.2, 123.3, 50.0, 39.9, 37.3, 33.5, 30.7.

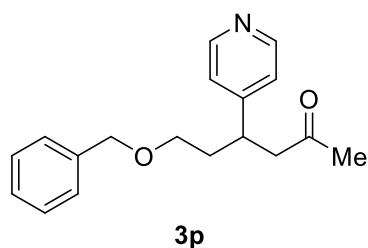
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{17}\text{H}_{20}\text{NO}]^+$: 254.1539, found: 254.1539.



16.0 mg, 39%; Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.49 (d, $J = 6.0$ Hz, 2H), 7.10 (dd, $J_1 = 5.6$ Hz, $J_2 = 1.6$ Hz, 2H), 3.15 – 3.08 (m, 1H), 2.72 (d, $J = 7.2$ Hz, 2H), 2.05 (s, 3H), 1.62 – 1.51 (m, 2H), 1.32 – 1.02 (m, 4H), 0.81 (t, $J = 7.2$ Hz, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.9, 154.0, 150.0, 123.2, 49.9, 40.4, 35.5, 30.7, 29.5, 22.6, 14.0.

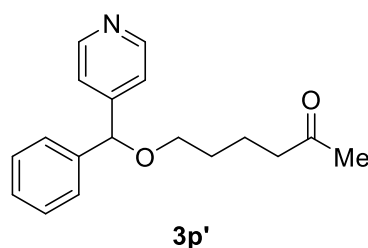
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{13}\text{H}_{20}\text{NO}]^+$: 206.1539, found: 206.1538.



5.1 mg, 9%; Yellow oil. Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.43 (d, $J = 5.6$ Hz, 2H), 7.30 – 7.27 (m, 1H), 7.24 – 7.20 (m, 4H), 7.04 (d, $J = 6.0$ Hz, 2H), 4.38 – 4.30 (m, 2H), 3.36 – 3.26 (m, 2H), 3.21 – 3.15 (m, 1H), 2.77 – 2.66 (m, 2H), 1.98 (s, 3H), 1.96 – 1.90 (m, 1H), 1.76 – 1.73 (m, 1H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.5, 153.4, 150.0, 138.2, 128.5, 127.9, 127.8, 123.2, 73.1, 67.6, 49.6, 37.3, 35.6, 30.6.

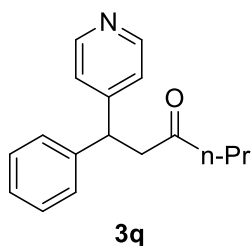
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{18}\text{H}_{22}\text{NO}_2]^+$: 284.1645, found: 284.1640



19.8 mg, 35%; Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 8.53 (d, $J = 5.6$ Hz, 2H), 7.36 – 7.33 (m, 1H), 7.33 – 7.31 (m, 2H), 7.30 – 7.28 (m, 2H), 7.28 – 7.26 (m, 2H), 5.28 (s, 1H), 3.44 (t, $J = 6.0$ Hz, 2H), 2.45 (t, $J = 6.8$ Hz, 2H), 2.12 (s, 3H), 1.71 – 1.62 (m, 4H).

^{13}C NMR (101 MHz, CDCl_3) δ 209.1, 151.5, 149.9, 140.9, 128.8, 128.2, 127.2, 121.7, 82.5, 69.0, 43.4, 30.1, 29.3, 20.6.

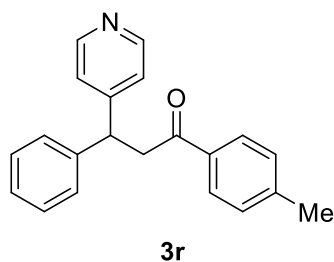
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{18}\text{H}_{22}\text{NO}_2]^+$: 284.1645, found: 284.1644.



40.5 mg, 80%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.47 (d, $J = 6.0$ Hz, 2H), 7.30 – 7.26 (m, 2H), 7.22 – 7.20 (m, 1H), 7.19 – 7.17 (m, 2H), 7.13 (d, $J = 6.0$ Hz, 2H), 4.59 (t, $J = 7.6$ Hz, 1H), 3.15 (d, $J = 7.6$ Hz, 2H), 2.32 (t, $J = 7.2$ Hz, 2H), 1.56 – 1.46 (m, 2H), 0.81 (t, $J = 7.6$ Hz, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 208.3, 153.0, 150.0, 142.3, 128.9, 127.9, 127.1, 123.2, 47.9, 45.5, 45.2, 17.1, 13.7.

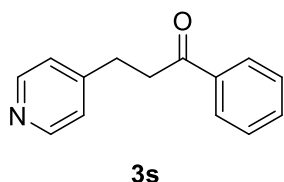
HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{17}\text{H}_{20}\text{NO}]^+$: 254.1539, found: 254.1538.



24.2 mg, 40%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.48 – 8.47 (m, 2H), 7.84 (d, $J = 7.6$ Hz, 2H), 7.33 – 7.28 (m, 2H), 7.26 – 7.25 (m, 5H), 7.19 – 7.18 (m, 2H), 4.81 (t, $J = 6.8$ Hz, 1H), 3.79 – 3.64 (m, 2H), 2.41 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 196.9, 153.2, 150.0, 144.4, 142.7, 134.3, 129.5, 129.0, 128.3, 128.0, 127.1, 123.3, 45.4, 43.9, 21.8.

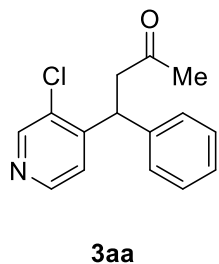
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{21}\text{H}_{20}\text{NO}]^+$: 302.1540, found: 302.1542



10.4 mg, 25%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.51 (brs, 2H), 7.96 (d, $J = 7.2$ Hz, 2H), 7.58 (t, $J = 7.2$ Hz, 1H), 7.47 (t, $J = 7.2$ Hz, 2H), 7.21 (brs, 2H), 3.34 (t, $J = 7.2$ Hz, 2H), 3.08 (t, $J = 6.8$ Hz, 2H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 198.4, 150.5, 149.9, 136.7, 133.5, 128.8, 128.1, 124.1, 39.0, 29.3

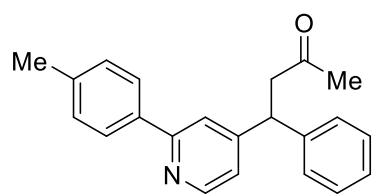
HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{14}\text{H}_{14}\text{NO}]^+$: 212.1070, found: 212.1075.



33.8 mg, 65%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.53 (s, 1H), 8.40 (d, $J = 4.8$ Hz, 1H), 7.32 – 7.28 (m, 2H), 7.24 – 7.22 (m, 1H), 7.22 – 7.20 (m, 2H), 7.13 (d, $J = 5.2$ Hz, 1H), 5.01 (t, $J = 7.6$ Hz, 1H), 3.25 – 3.13 (m, 2H), 2.14 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.4, 150.0, 150.0, 148.0, 140.4, 132.1, 129.0, 128.1, 127.3, 122.9, 48.2, 41.9, 30.4.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{15}\text{H}_{15}\text{ClNO}]^+$: 260.0837, found: 260.0837.

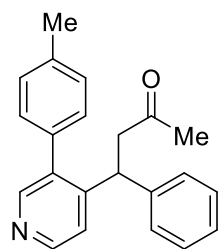


3ab

36.6 mg, 58%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.55 (d, $J = 5.2$ Hz, 1H), 7.83 (d, $J = 8.0$ Hz, 2H), 7.55 (s, 1H), 7.33 – 7.29 (m, 2H), 7.27 – 7.21 (m, 5H), 7.05 (dd, $J_1 = 4.8$ Hz, $J_2 = 1.2$ Hz, 2H), 4.64 (t, $J = 7.6$ Hz, 1H), 3.24 (d, $J = 7.2$ Hz, 2H), 2.40 (s, 3H), 2.13 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.1, 157.9, 153.5, 149.9, 142.3, 139.1, 136.6, 129.6, 129.0, 127.9, 127.1, 127.0, 121.2, 119.9, 48.9, 45.5, 30.8, 21.4.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{22}\text{H}_{22}\text{NO}]^+$: 316.1696, found: 316.1694.

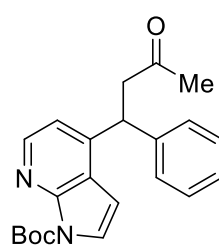


3ac

46.7 mg, 74%; Yellow solid, m.p. 116.3-117.4 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.55 (d, $J = 5.2$ Hz, 1H), 8.43 (s, 1H), 7.28 (d, $J = 6.8$ Hz, 1H), 7.25 – 7.24 (m, 4H), 7.20 – 7.18 (m, 1H), 7.15 – 7.13 (m, 2H), 6.98 (d, $J = 6.8$ Hz, 2H), 4.73 (t, $J = 7.6$ Hz, 1H), 3.18 (dd, $J_1 = 17.2$ Hz, $J_2 = 8.0$ Hz, 1H), 3.09 (dd, $J_1 = 17.2$ Hz, $J_2 = 7.2$ Hz, 1H), 2.42 (s, 3H), 2.02 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.9, 150.9, 149.9, 148.8, 142.1, 138.0, 137.7, 134.5, 129.5, 129.2, 128.7, 127.8, 126.8, 121.4, 49.5, 41.5, 30.3, 21.4.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{22}\text{H}_{22}\text{NO}]^+$: 316.1696, found: 316.1694.

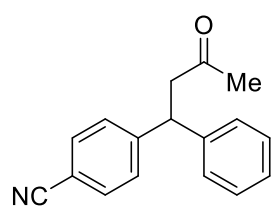


3ad

32 mg, 20%, Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.45 (d, $J = 4.8$ Hz, 1H), 7.56 (d, $J = 4.0$ Hz, 1H), 7.28 – 7.24 (m, 2H), 7.22 – 7.20 (m, 2H), 7.20 – 7.16 (m, 1H), 7.04 (d, $J = 5.2$ Hz, 1H), 6.52 (d, $J = 4.0$ Hz, 1H), 4.97 (t, $J = 7.6$ Hz, 1H), 3.27 (d, $J = 7.2$ Hz, 2H), 2.11 (s, 3H), 1.63 (s, 9H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.2, 148.6, 147.9, 145.6, 145.5, 142.2, 128.9, 127.8, 127.0, 126.3, 122.3, 116.4, 103.1, 84.1, 48.6, 42.7, 30.9, 28.2.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{22}\text{H}_{25}\text{N}_2\text{O}_3]^+$: 365.1860, found: 365.1854.

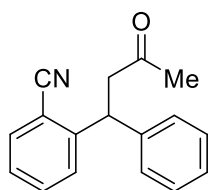


3ae

36.4 mg, 73%; Yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.56 (dd, $J_1 = 6.4$ Hz, $J_2 = 1.6$ Hz, 2H), 7.33 (d, $J = 8.4$ Hz, 2H), 7.29 (d, $J = 7.6$ Hz, 2H), 7.24 – 7.21 (m, 1H), 7.20 – 7.17 (m, 2H), 4.65 (t, $J = 7.6$ Hz, 1H), 3.20 (d, $J = 7.2$ Hz, 2H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.0, 149.6, 142.5, 132.5, 129.0, 128.7, 127.8, 127.1, 118.9, 110.4, 49.1, 45.8, 30.8.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{17}\text{H}_{16}\text{NO}]^+$: 250.1226, found: 250.1222

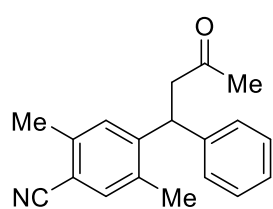


3af

17.5 mg, 35%; Yellow solid, m.p. 98.0-99.1 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.59 (dd, $J_1 = 6.4$ Hz, $J_2 = 1.2$ Hz, 1H), 7.50 (td, $J_1 = 7.6$ Hz, $J_2 = 1.2$ Hz, 1H), 7.34 (d, $J = 8.0$ Hz, 1H), 7.31 – 7.24 (m, 5H), 7.21 – 7.17 (m, 1H), 4.99 (t, $J = 7.6$ Hz, 1H), 3.24 (d, $J = 7.6$ Hz, 2H), 2.12 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 205.6, 147.5, 141.6, 133.6, 133.1, 129.0, 127.9, 127.5, 127.2, 127.1, 118.2, 112.8, 49.1, 44.2, 30.2.

HRMS(ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{17}\text{H}_{16}\text{NO}]^+$: 250.1226, found: 250.1226.

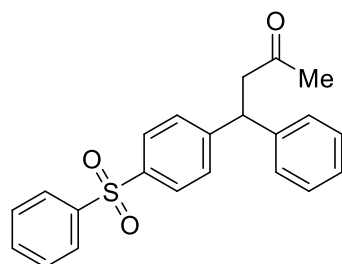


3ag

20.0 mg, 36%; White solid, m.p. 132.0-132.2 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.35 (s, 1H), 7.28 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 7.21 – 7.16 (m, 1H), 7.15 – 7.11 (m, 3H), 4.76 (t, $J = 7.6$ Hz, 1H), 3.16 (d, $J = 7.6$ Hz, 2H), 2.50 (s, 3H), 2.29 (s, 3H), 2.11 (s, 3H).

$^{13}\text{C NMR}$ (101 MHz, CDCl_3) δ 206.2, 147.2, 142.2, 139.6, 135.1, 134.5, 128.9, 128.2, 128.0, 126.9, 118.4, 110.7, 49.6, 41.9, 30.8, 20.5, 19.4.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{19}\text{H}_{20}\text{NO}]^+$: 278.1539, found: 278.1539

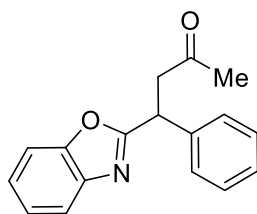


3ah

24.8 mg, 34%; White solid, m.p. 90.8-92.7 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.92 (d, $J = 7.2$ Hz, 2H), 7.84 (d, $J = 8.0$ Hz, 2H), 7.58 – 7.54 (m, 1H), 7.51 – 7.47 (m, 2H), 7.35 (d, $J = 8.8$ Hz, 2H), 7.30 – 7.27 (m, 2H), 7.22 – 7.19 (m, 1H), 7.16 (d, $J = 8.0$ Hz, 2H), 4.64 (t, $J = 7.2$ Hz, 1H), 3.24 – 3.13 (m, 2H), 2.10 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 206.1, 149.9, 142.5, 141.6, 139.7, 133.3, 129.4, 129.0, 128.8, 128.1, 127.8, 127.7, 127.1, 49.2, 45.7, 30.8.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{22}\text{H}_{21}\text{O}_3\text{S}]^+$: 365.1206, found: 365.1200.



3ai

18.0 mg, 34%; Yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.63 – 7.59 (m, 1H), 7.37 – 7.35 (m, 1H), 7.29 – 7.28 (m, 1H), 7.25 – 7.24 (m, 2H), 7.23 – 7.21 (m, 2H), 7.20 – 7.17 (m, 2H), 4.70 (dd, $J_1 = 8.8$ Hz, $J_2 = 1.6$ Hz, 1H), 3.68 (dd, $J_1 = 18.0$ Hz, $J_2 = 8.8$ Hz, 2H), 3.03 (dd, $J_1 = 18.0$ Hz, $J_2 = 5.6$ Hz, 2H), 2.16 (s, 3H).

^{13}C NMR (101 MHz, CDCl_3) δ 205.8, 167.5, 151.1, 141.1, 139.2, 129.1, 128.0, 127.8, 124.9, 124.3, 119.9, 110.8, 48.0, 40.6, 30.5.

HRMS (ESI+): calculated m/z $[\text{M}+\text{H}]^+$ for $[\text{C}_{17}\text{H}_{16}\text{NO}_2]^+$: 266.1176, found: 266.1163.

5. Cyclic voltammetry test for cyclopropanol

Cyclic voltammetry test was performed in a three-electrode cell under argon at room temperature. All cyclic voltammograms were measured using Ag/Ag^+ (0.01 M AgNO_3 in MeCN) reference electrode, platinum (Pt) wire counter electrode, and a glassy carbon working electrode. The conditions of the experiments were as follows: testing compounds are in a solution of 0.1 M hexafluorophosphate ($n\text{Bu}_4\text{NPF}_6$) in MeCN at a scan rate of 50 mV/s; Prior to each measurement, solutions were purged with argon (Ar) for 10 minutes to ensure the oxygen-free conditions.

Measuring the Fc/Fc^+ redox couple afforded $E_{1/2} = +0.11$ V vs. Ag/Ag^+ under our experimental conditions. The obtained value was referenced to Ag/Ag^+ and converted to SCE by subtracting 0.31V, providing a value of +0.42 V for the Fc/Fc^+ couple.² The oxidation half-peak potential of **1a** in MeCN was measured as +0.69 V (vs Ag/Ag^+), and calculated to +1.00 V (vs. SCE).

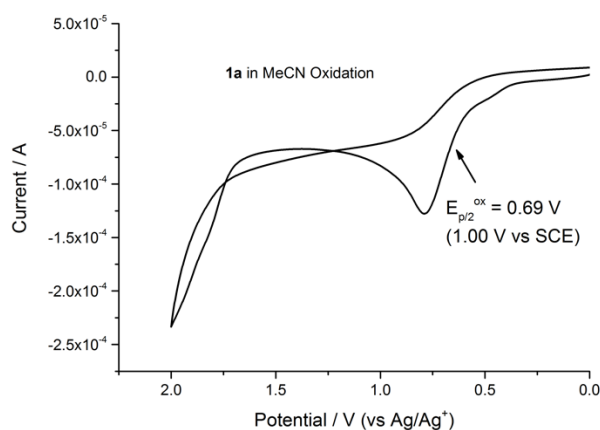
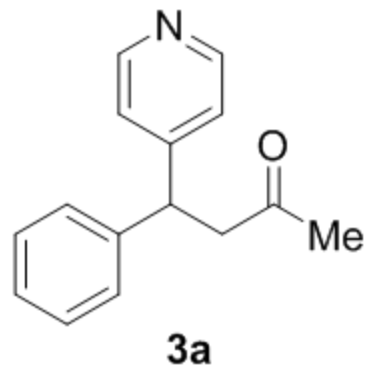


Figure S1. Cyclic voltammetry of **1a** (0.01 M) in MeCN (vs Ag/Ag⁺) with ^tBu₄NPF₆ (0.1 M) under argon at a glassy carbon electrode at a scan rate of 50 mV/s.

6. Reference

- (a) C. Jiang, L. Wang, H. Zhang, P. Chen, Y.-L. Guo and G. Liu, Enantioselective Copper-Catalyzed Trifluoromethylation of Benzylic Radicals via Ring Opening of Cyclopropanols, *Chem*, 2020, **6**, 2407-2419; (b) L. Wu, L. Wang, P. Chen, Y. L. Guo and G. Liu, Enantioselective Copper-Catalyzed Radical Ring-Opening Cyanation of Cyclopropanols and Cyclopropanone Acetals, *Adv. Synth. Catal.*, 2020, **362**, 2189-2194; (c) T. Xie, L. Zhou, M. Shen, J. Li, X. Lv and X. Wang, Diastereoselective synthesis of cis-1,2-disubstituted cyclopropanols and cyclopent-3-enols via SmI₂ mediated C–N(Bt) bond cleavage, *Tetrahedron Lett.*, 2015, **56**, 3982-3987; (d) S. Bloom, D. D. Bume, C. R. Pitts and T. Lectka, Site-Selective Approach to beta-Fluorination: Photocatalyzed Ring Opening of Cyclopropanols, *Chem. –Eur. J.*, 2015, **21**, 8060-8063; (e) D. T. Ziegler, A. M. Steffens and T. W. Funk, Synthesis of α -methyl ketones by a selective, iridium-catalyzed cyclopropanol ring-opening reaction, *Tetrahedron Lett.*, 2010, **51**, 6726-6729; (f) O. G. Kulinkovich and D. G. Kananovich, Advanced Procedure for the Preparation of cis-1,2-Dialkylcyclopropanols – Modified Ate Complex Mechanism for Titanium-Mediated Cyclopropanation of Carboxylic Esters with Grignard Reagents, *Eur. J. Org. Chem.*, 2007, **2007**, 2121-2132; (g) O. L. Epstein, A. I. Savchenko and O. G. Kulinkovich, Titanium(IV) isopropoxide-catalysed reaction of alkylmagnesium halides with ethyl acetate in the presence of styrene. Non-hydride mechanism of ligand exchange in the titanacyclopropanes, *Tetrahedron Lett.*, 1999, **40**, 5935-5938.
- D. Nicewicz, H. Roth and N. Romero, Experimental and Calculated Electrochemical Potentials of Common Organic Molecules for Applications to Single-Electron Redox Chemistry, *Synlett*, 2015, **27**, 714-723.

ty-3-54-2 H1 CDCl3 400 M Hz

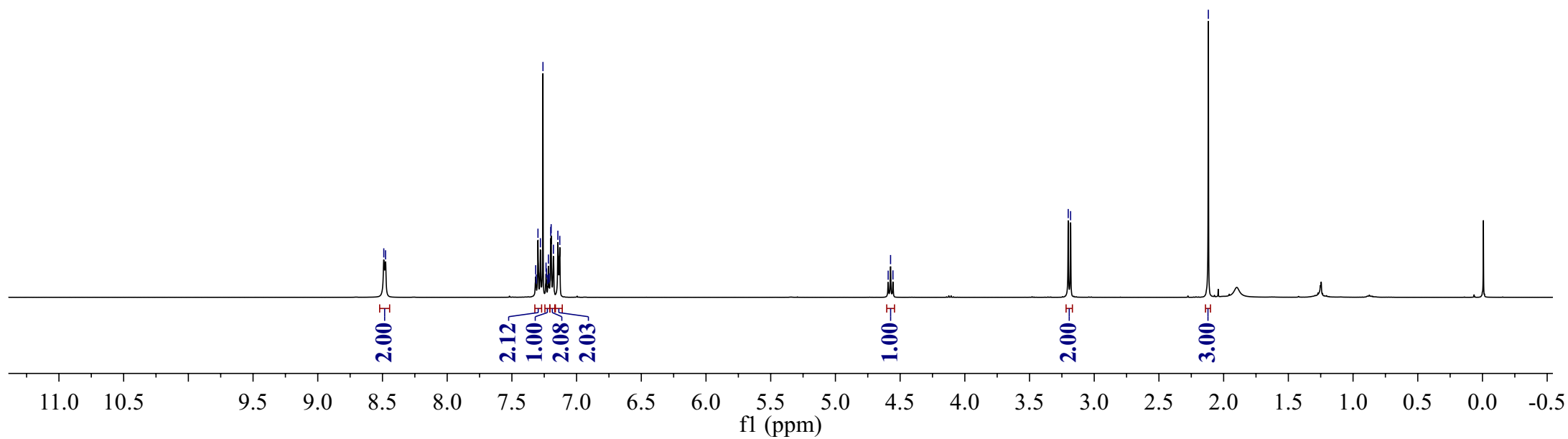


8.490
8.476
7.316
7.312
7.298
7.280
7.260
7.236
7.233
7.223
7.218
7.212
7.200
7.197
7.179
7.145
7.130

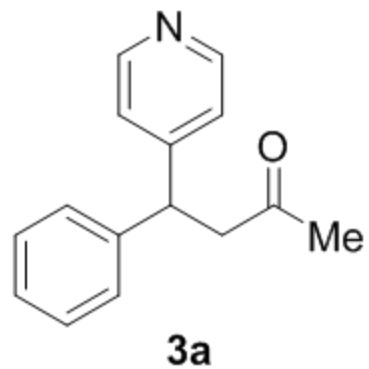
4.592
4.574
4.555

3.201
3.182

-2.118



ty-3-54-2 C13 CDCl3 101 M Hz



—206.00

—152.94

—150.02

—142.20

—128.99

—127.88

—127.18

—123.17

—77.48

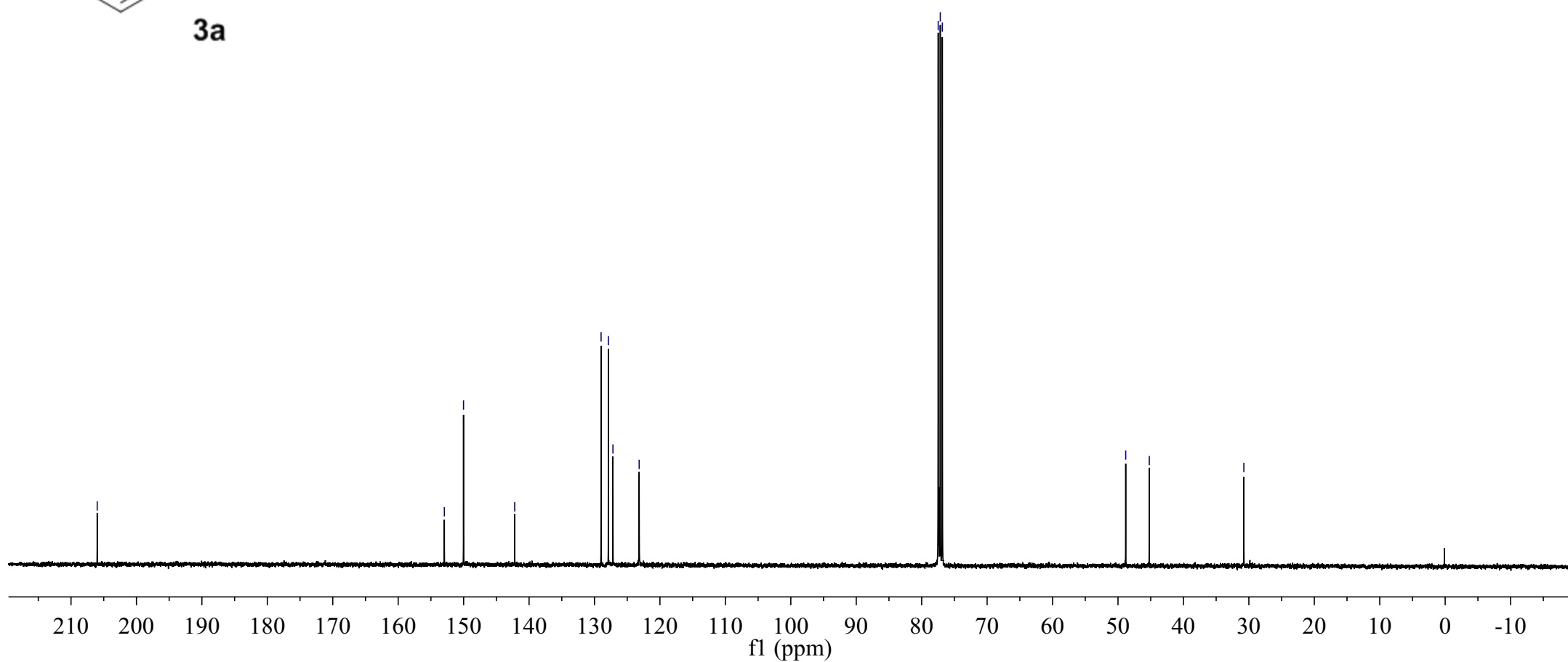
—77.16

—76.84

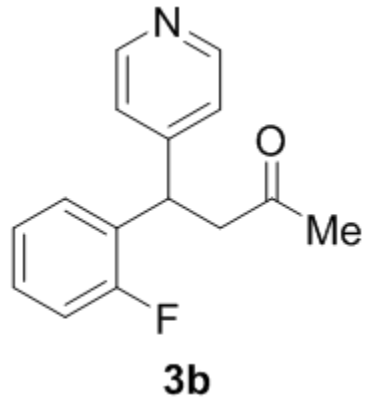
—48.82

—45.22

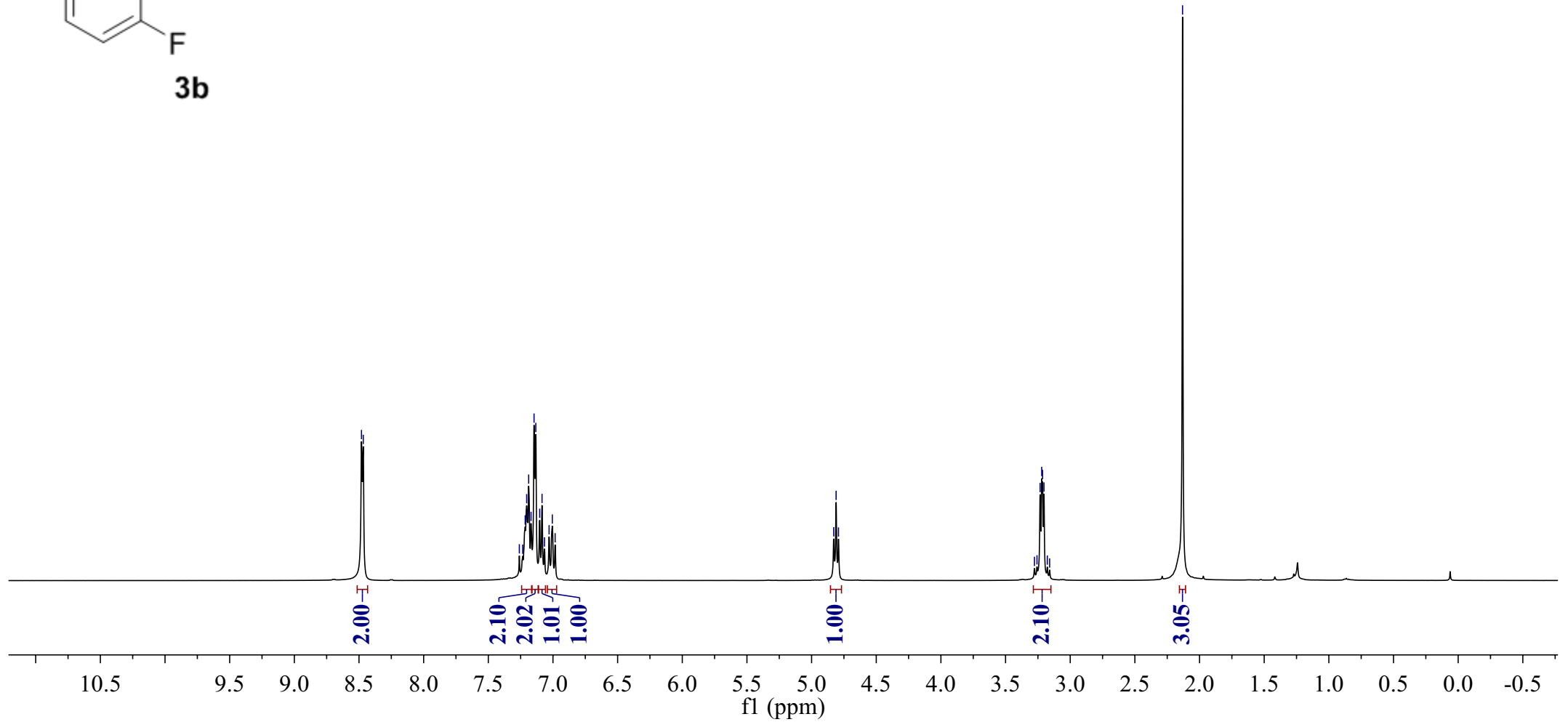
—30.76



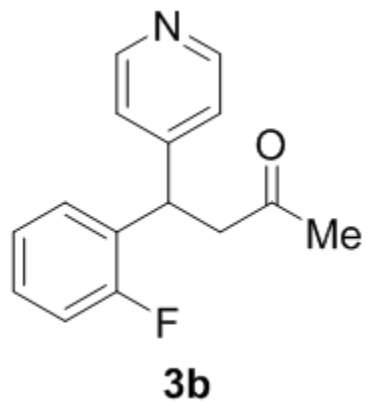
ty-4-61 H1 CDCl3 400 M Hz



8.481
8.467
7.260
7.234
7.215
7.203
7.196
7.188
7.170
7.146
7.133
7.103
7.085
7.066
7.030
7.005
6.983
4.829
4.811
4.792
3.277
3.257
3.233
3.220
3.214
3.203
3.177
3.159
-2.131



ty-4-61 C13 CDCl3 101 M Hz



—205.52

—161.86

—159.41

—151.67

—150.04

129.23

129.09

129.03

128.99

128.91

124.55

124.52

123.05

116.20

115.98

77.48

77.16

76.84

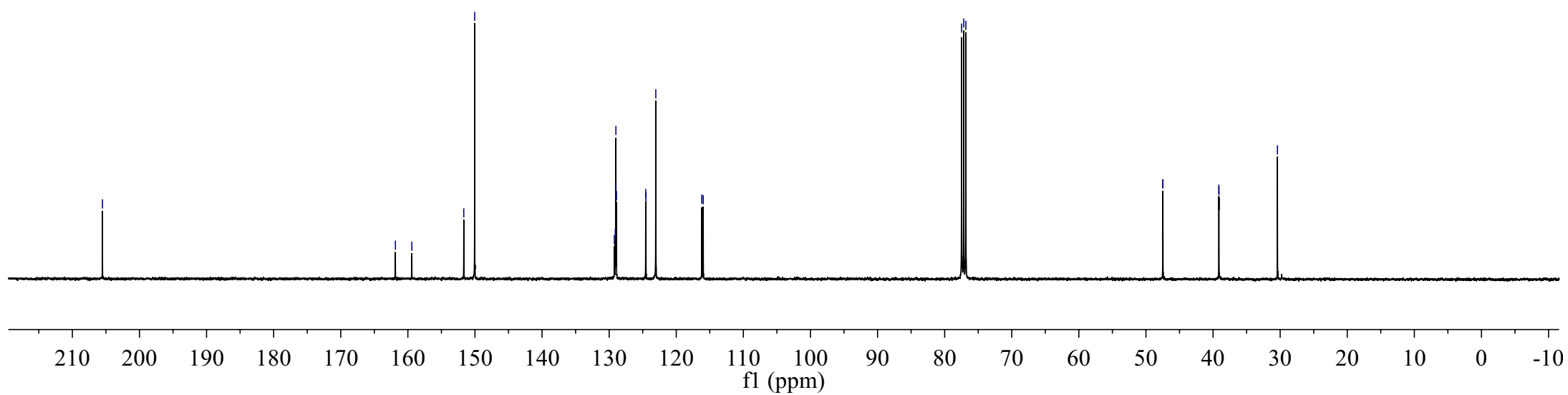
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47.47

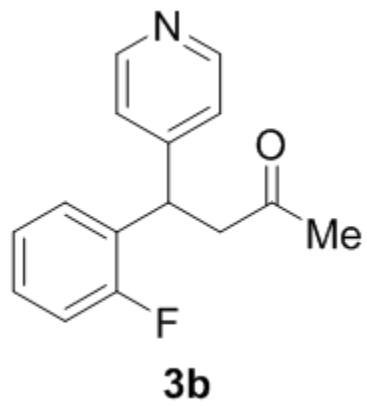
39.14

39.12

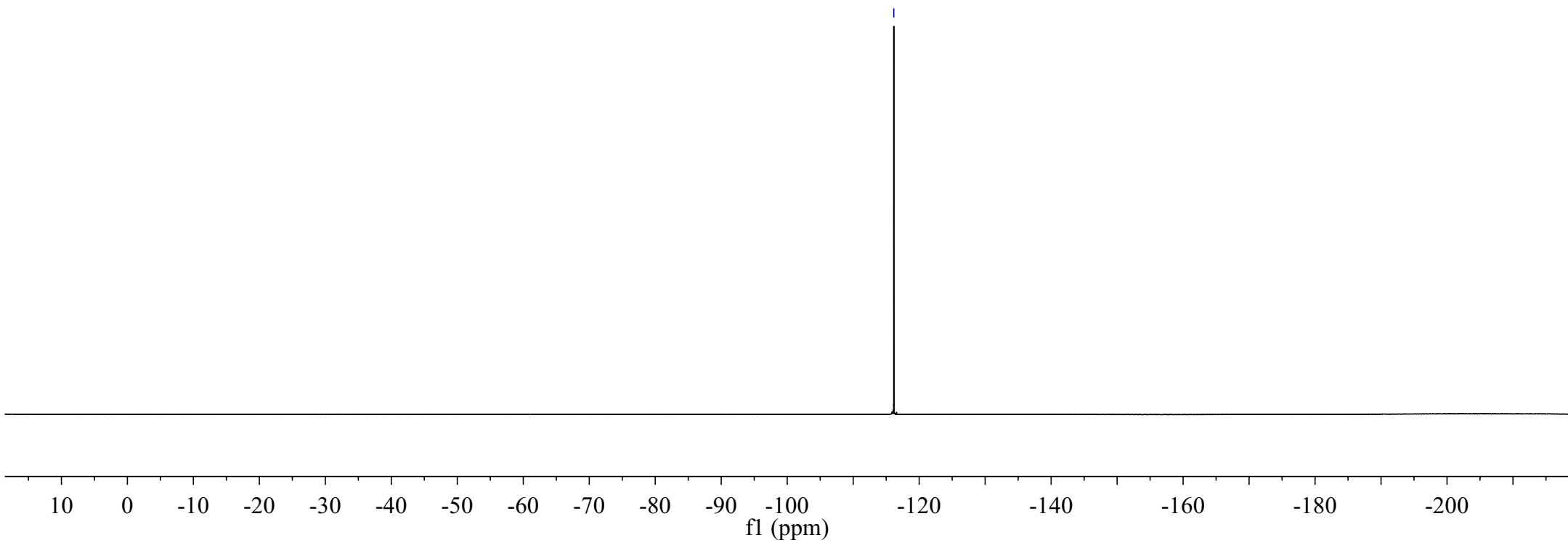
—30.40



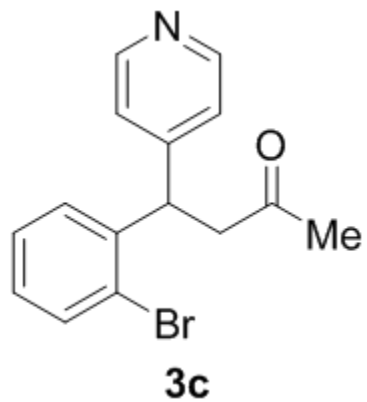
ty-4-61 F19 CDCl3 376 M Hz



--116.15



ty-3-63 H1 CDCl3 400 M Hz



8.502
8.489

7.584

7.581

7.564

7.561

7.278

7.260

7.155

7.150

7.145

7.140

7.129

7.126

5.109

5.074

5.055

3.229

3.208

3.185

3.171

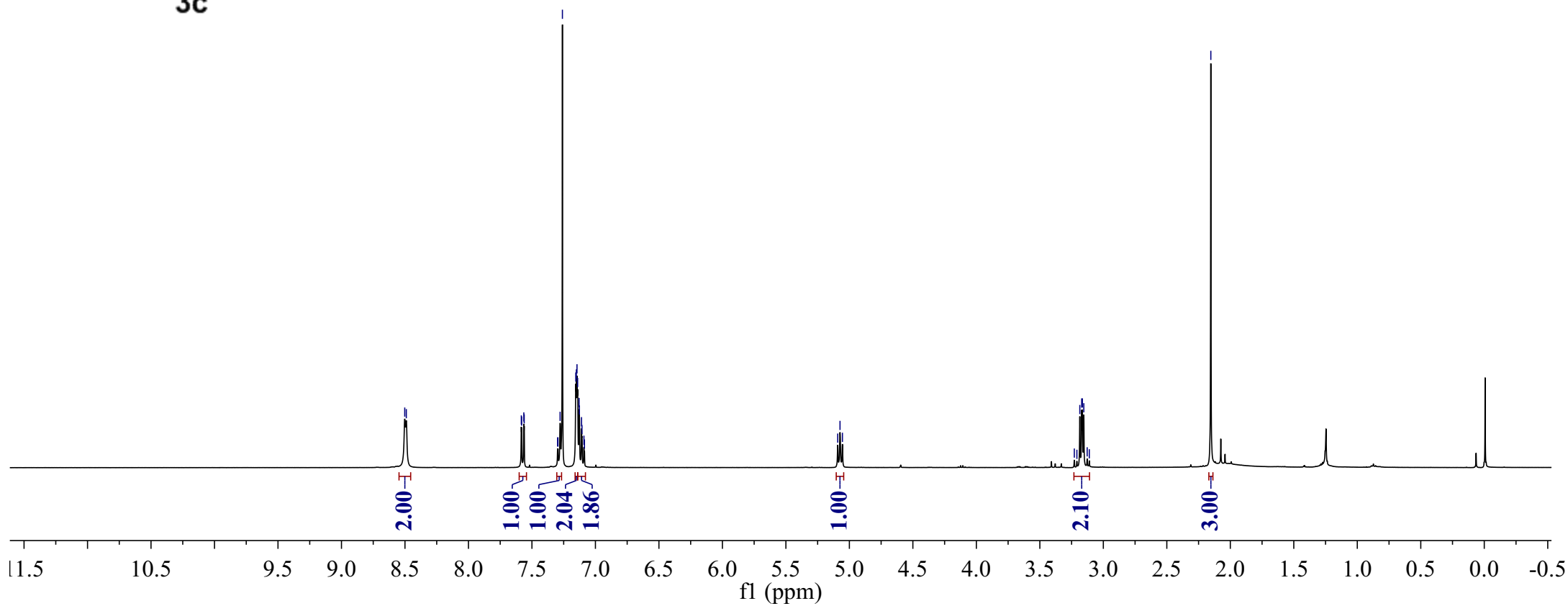
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3.154

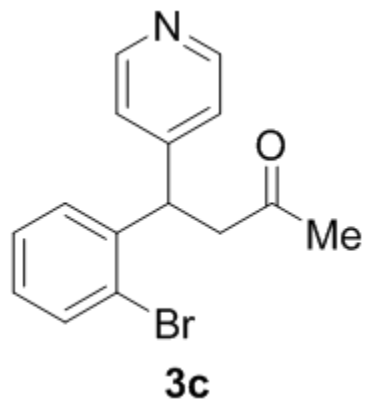
3.127

3.110

2.153



ty-3-63 C13 CDCl3 101 M Hz



—205.34

~151.55

~149.91

~141.16

~133.71

~128.79

~128.72

~127.97

~125.02

~123.51

~77.48

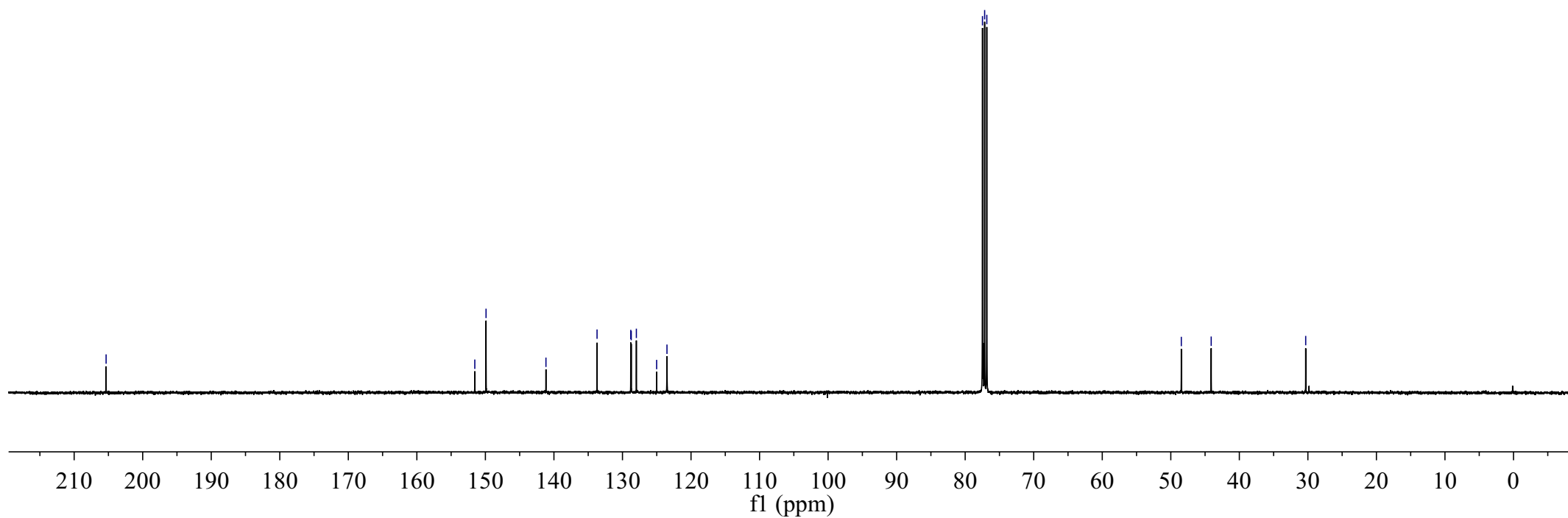
~77.16

~76.84

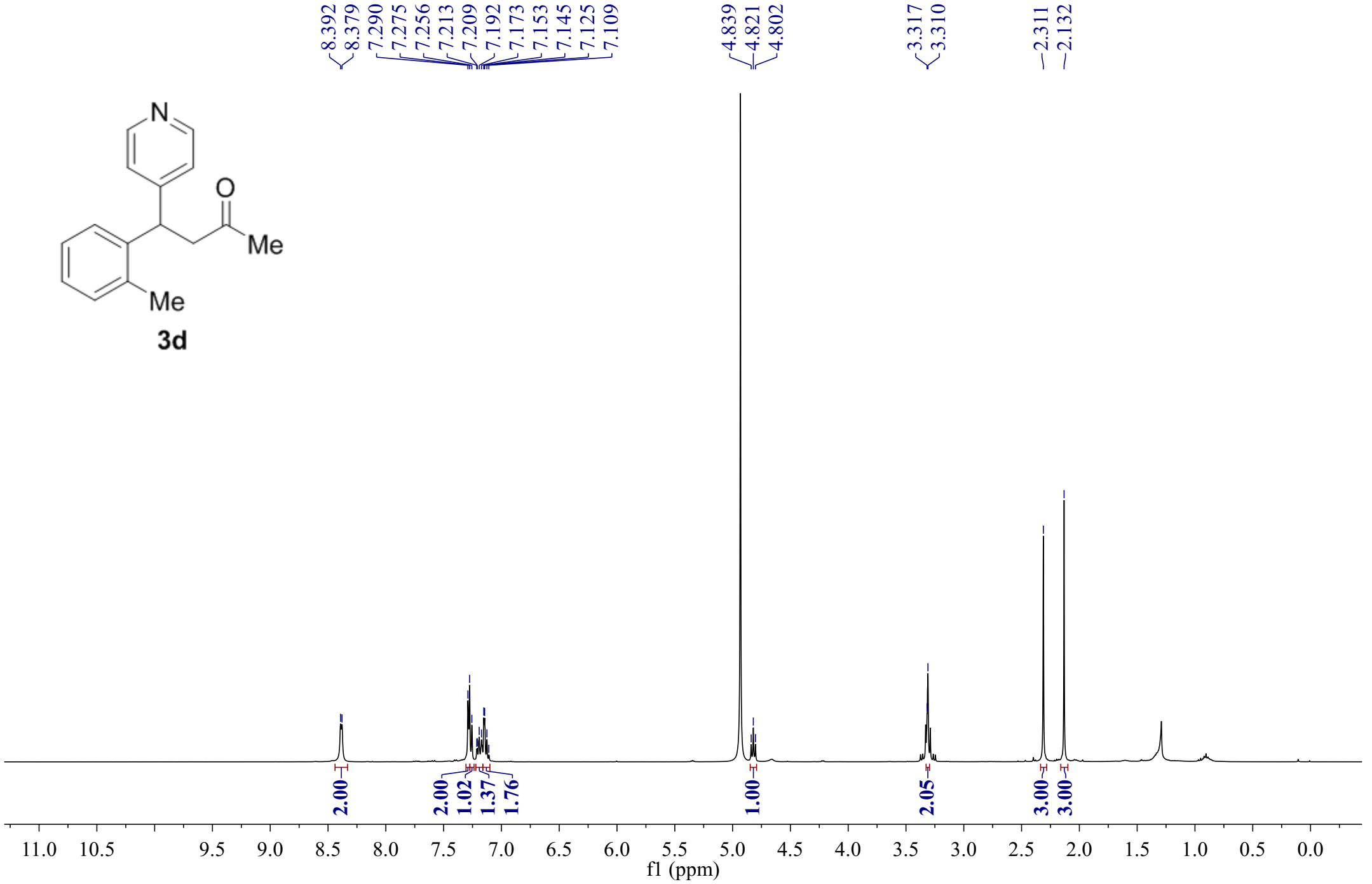
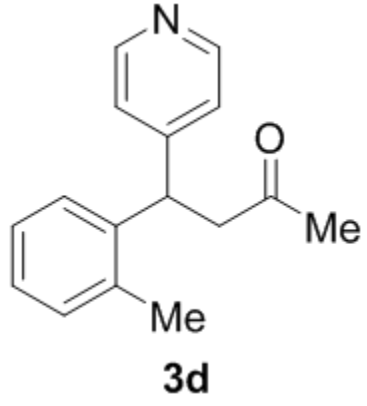
—48.46

—44.11

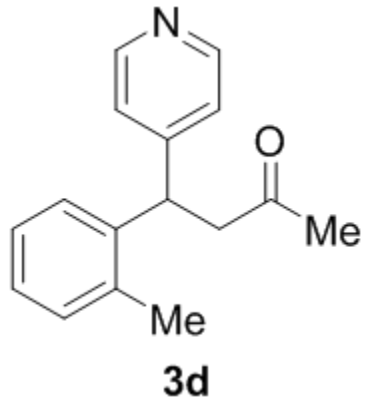
—30.32



ty-3-68-1 H1 MeOD 400 M Hz



ty-3-68-1 C13 MeOD 101 M Hz



—208.73

—155.99

—149.96

141.41

137.43

131.85

127.99

127.77

127.47

125.15

49.64

49.43

49.33

49.21

49.00

48.79

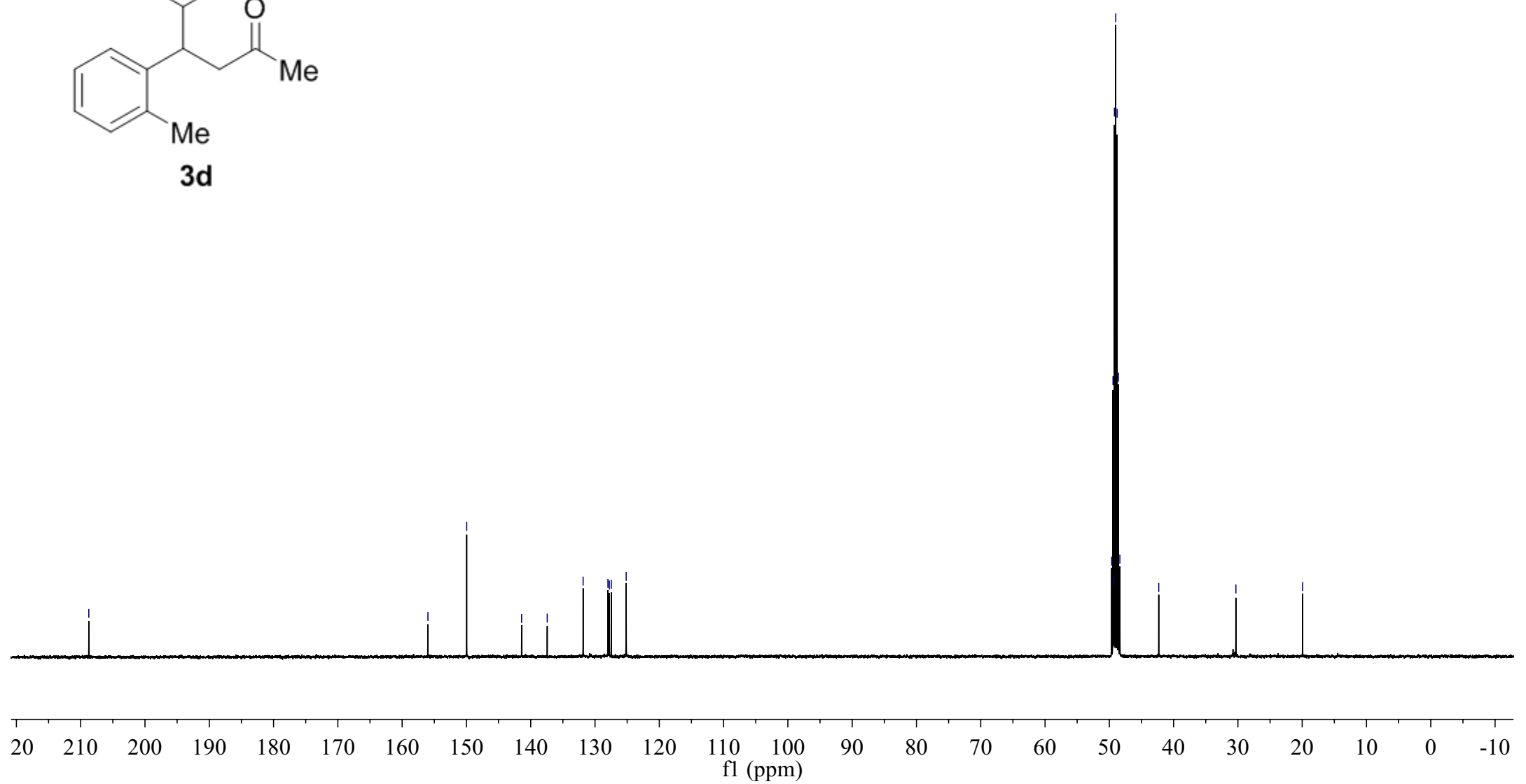
48.57

48.36

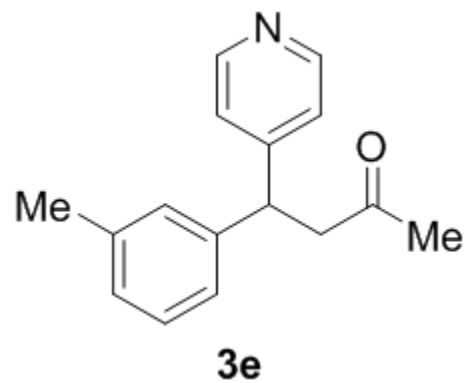
42.31

—30.31

—19.94



ty-4-15 H1 CDCl3 400 M Hz

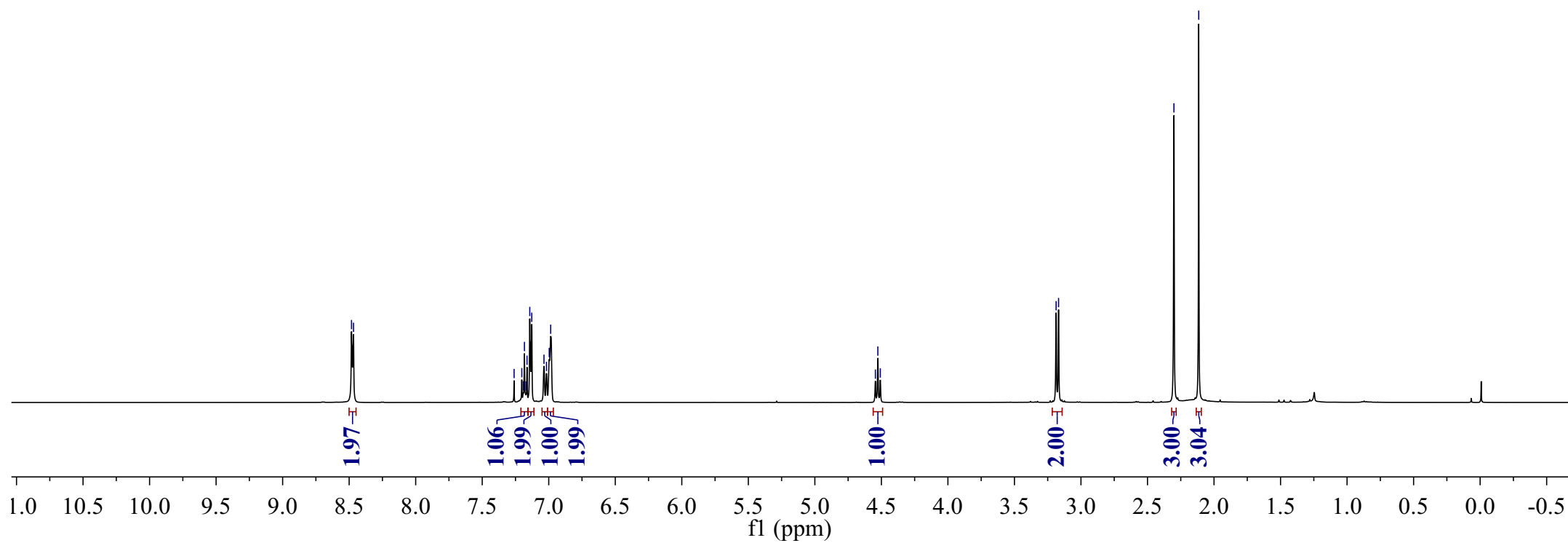


8.482
8.467
7.260
7.202
7.190
7.183
7.170
7.163
7.143
7.128
7.036
7.017
6.996
6.985

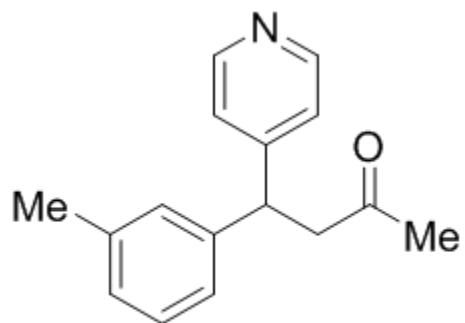
4.545
4.527
4.508

3.187
3.168

2.301
2.115



ty-4-15 C13 CDCl3 101 M Hz



3e

-206.09

-153.00

-149.99

-142.11

-138.62

-128.82

-128.69

-127.91

-124.73

-123.14

77.48

77.16

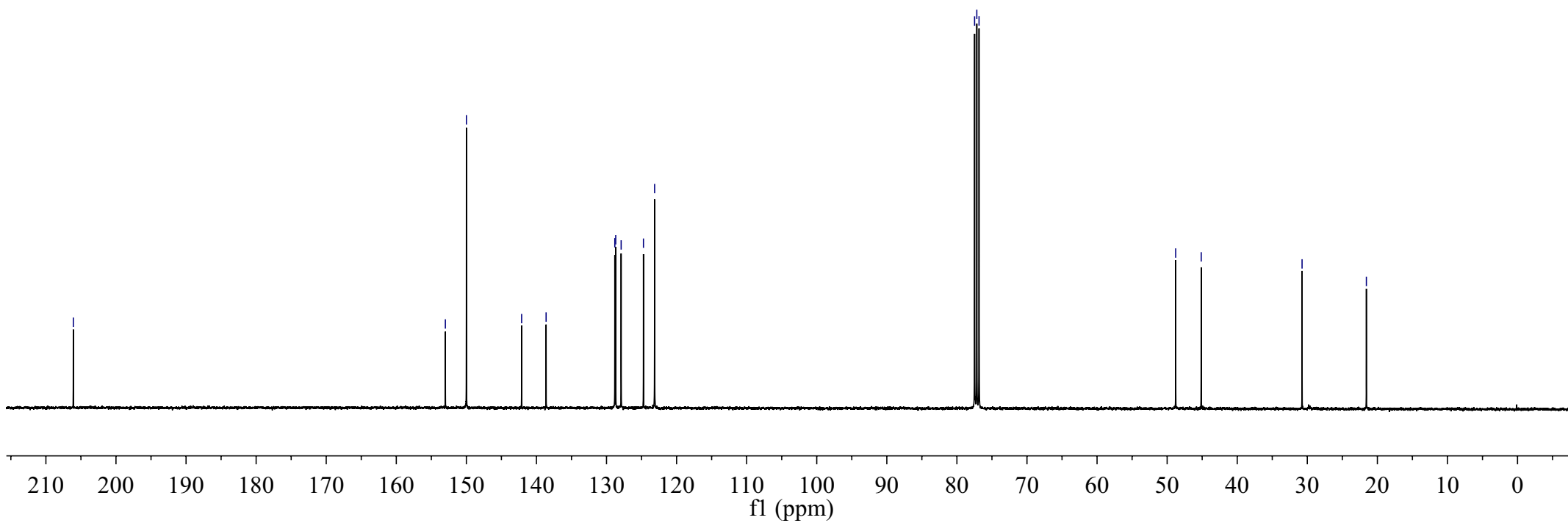
76.84

-48.78

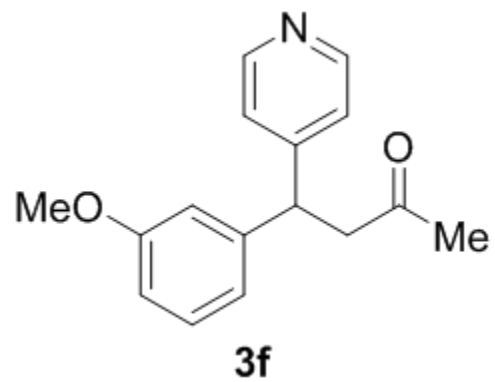
-45.14

-30.75

-21.57



ty-4-28 H1 CDCl3 400 M Hz



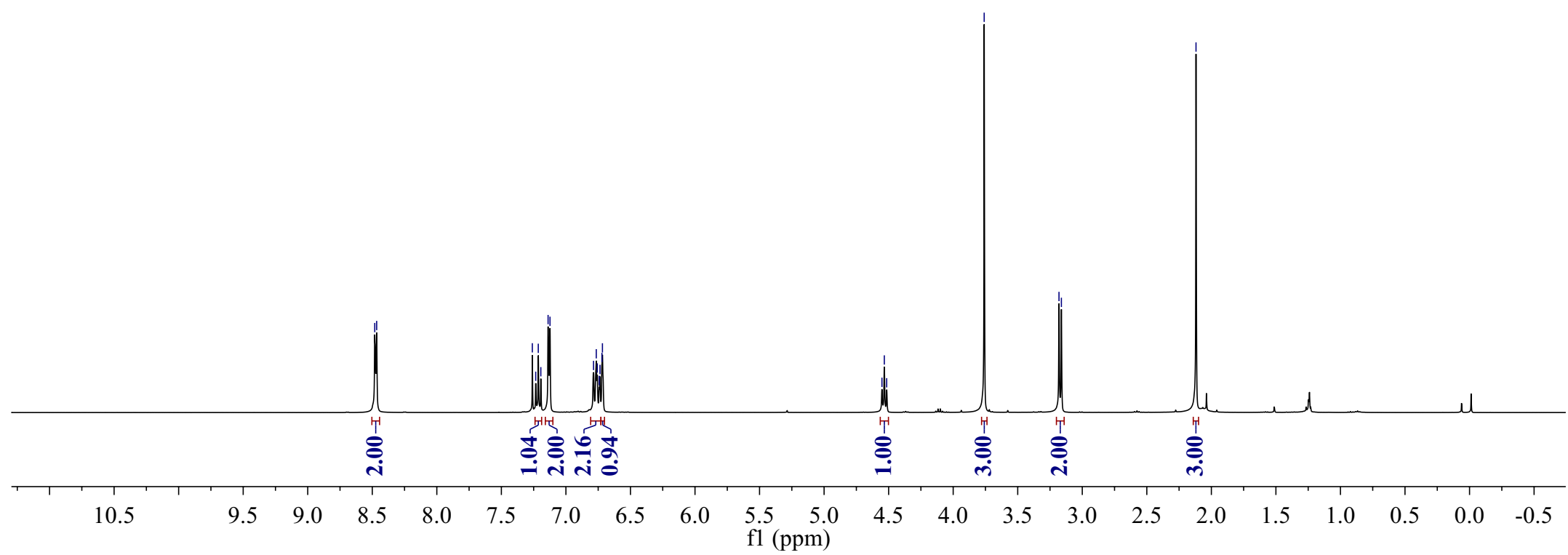
8.481
8.466
7.260
7.234
7.214
7.194
7.138
7.123
6.786
6.765
6.757
6.742
6.736
6.721
6.717

4.552
4.533
4.515

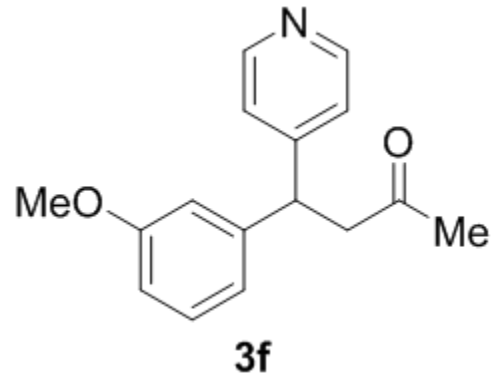
3.760

3.180
3.162

2.119



ty-4-28 C13 CDC13 101 M Hz



—205.98

~159.89

~152.72

~150.04

~143.75

~129.97

~123.09

~120.11

~114.16

~111.86

~77.48

~77.16

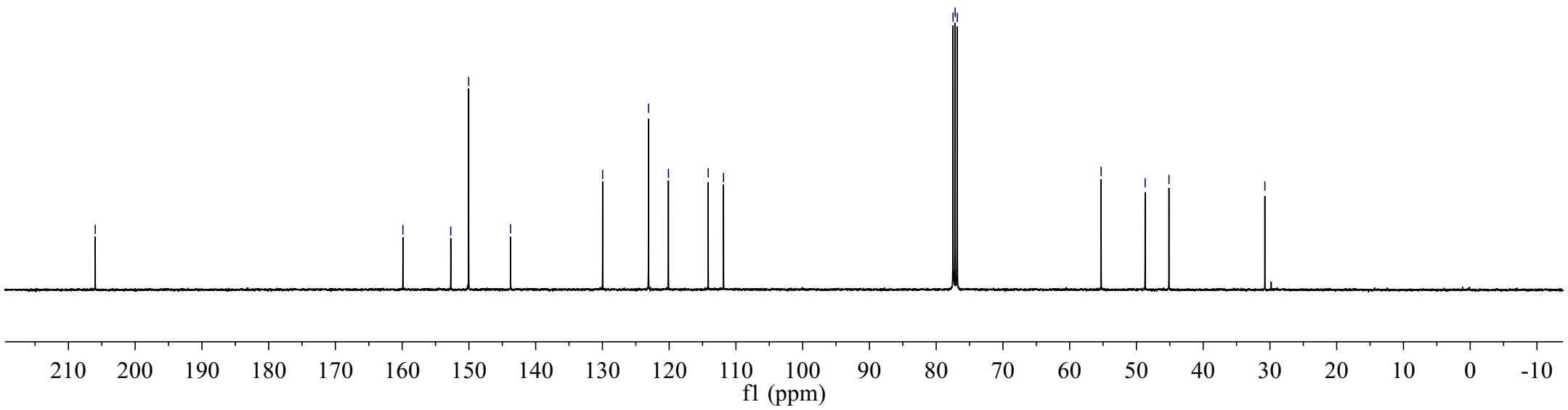
~76.84

~55.29

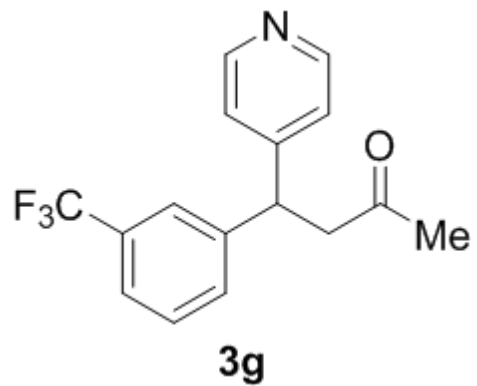
~48.70

~45.13

—30.76



ty-4-71 H1 CDCl3 400 M Hz

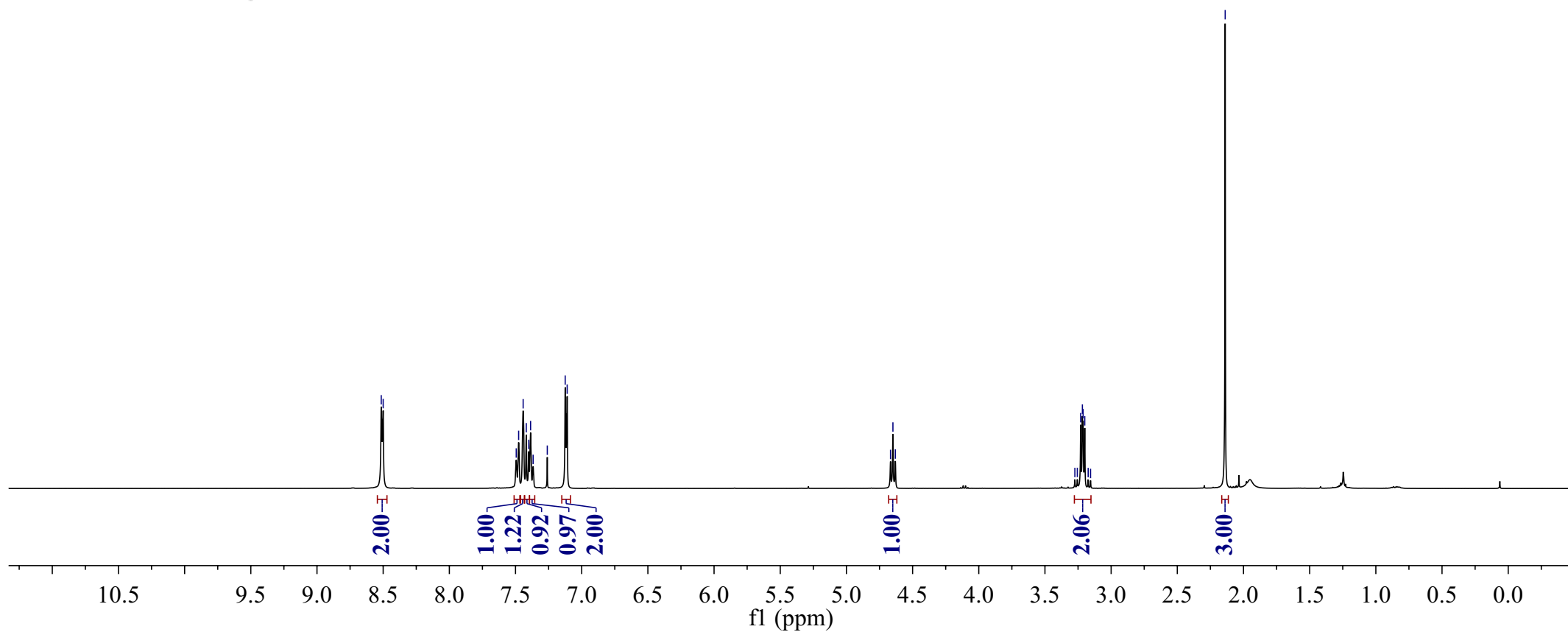


8.515
8.500
7.495
7.476
7.442
7.419
7.400
7.386
7.367
7.260
7.125
7.110

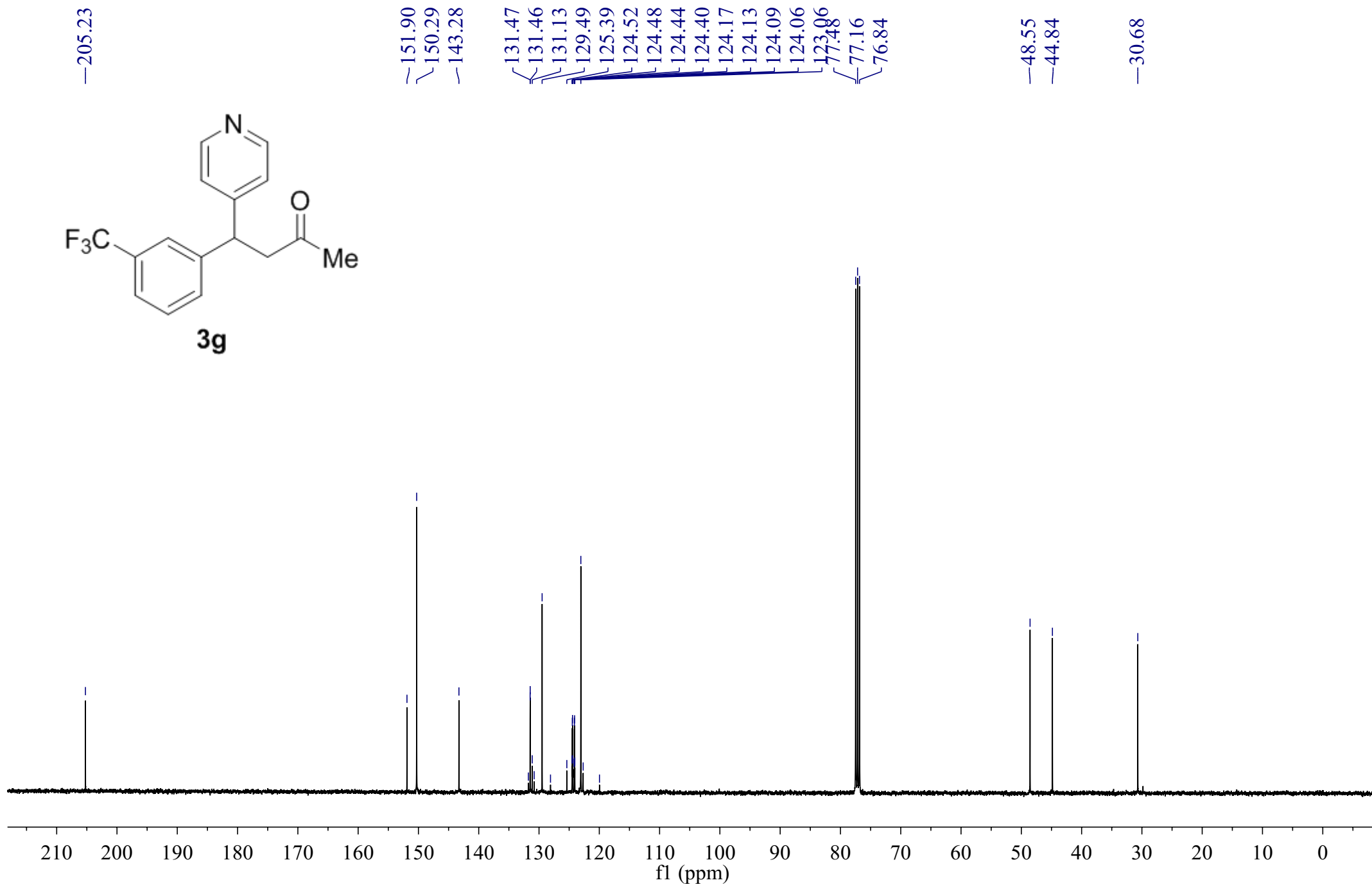
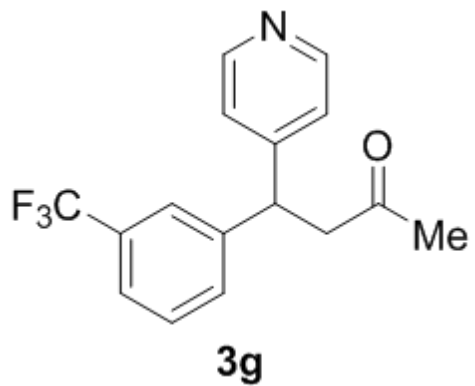
4.667
4.649
4.630

3.274
3.255
3.230
3.217
3.212
3.199
3.173
3.155

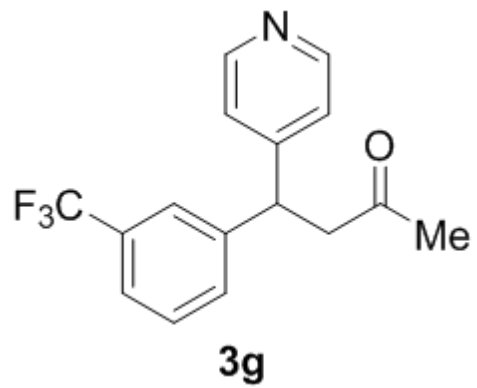
— 2.138



ty-4-71 C13 CDCl3 101 M Hz



ty-4-71 F19 CDCl3 376 M Hz

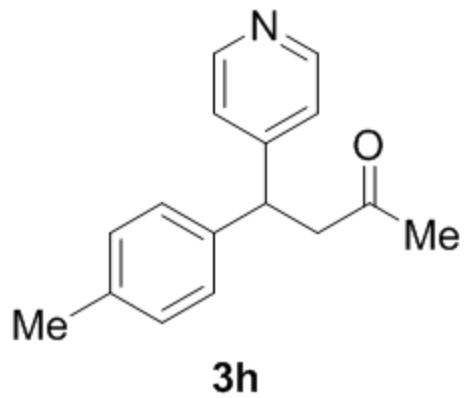


---62.58



10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)

ty-4-64 H1 CDCl3 400 M Hz



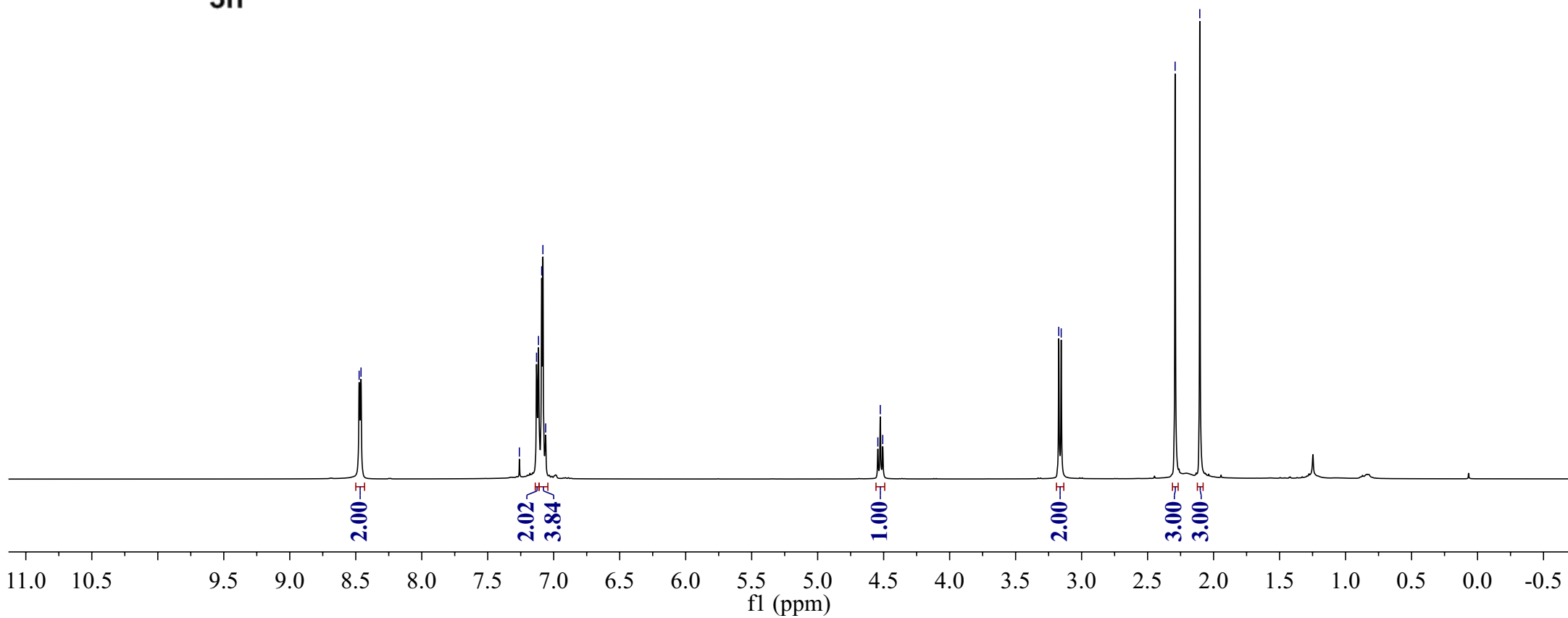
8.474
8.460

7.260
7.130
7.115
7.091
7.082
7.061

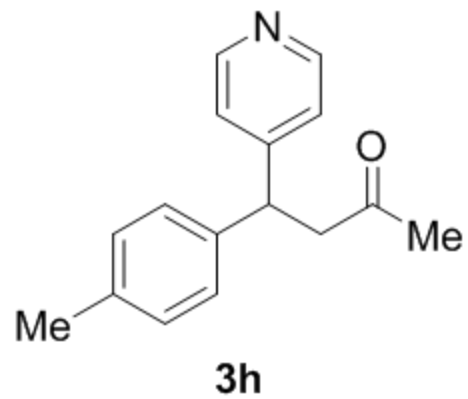
4.544
4.525
4.507

3.173
3.155

2.292
2.105



ty-4-64 C13 CDCl3 101 M Hz



—206.09

—153.10

—150.02

—139.17

—136.78

—129.62

—127.68

—123.06

—77.48

—77.16

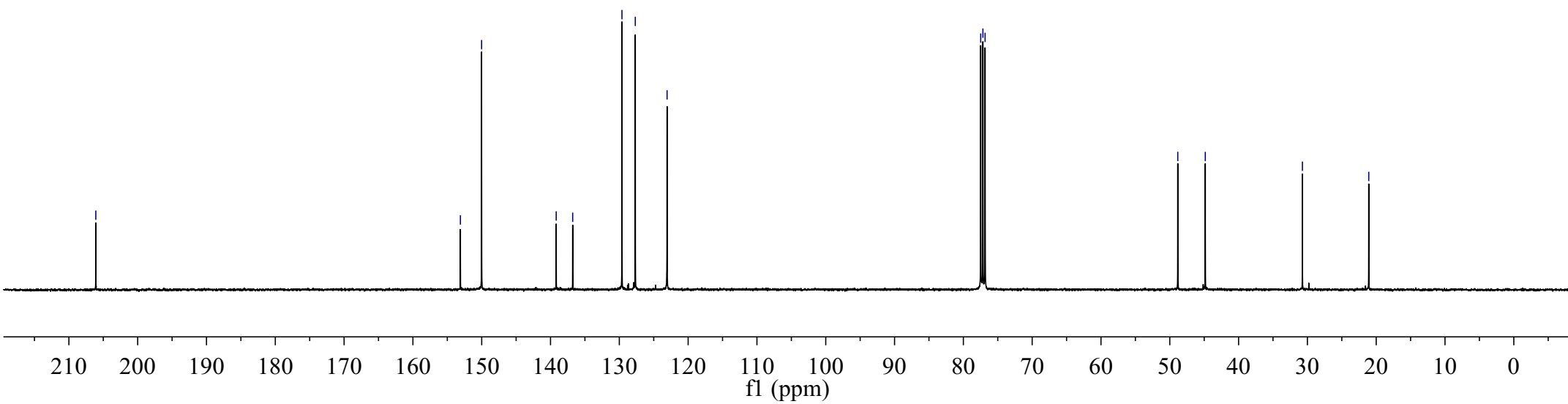
—76.84

—48.84

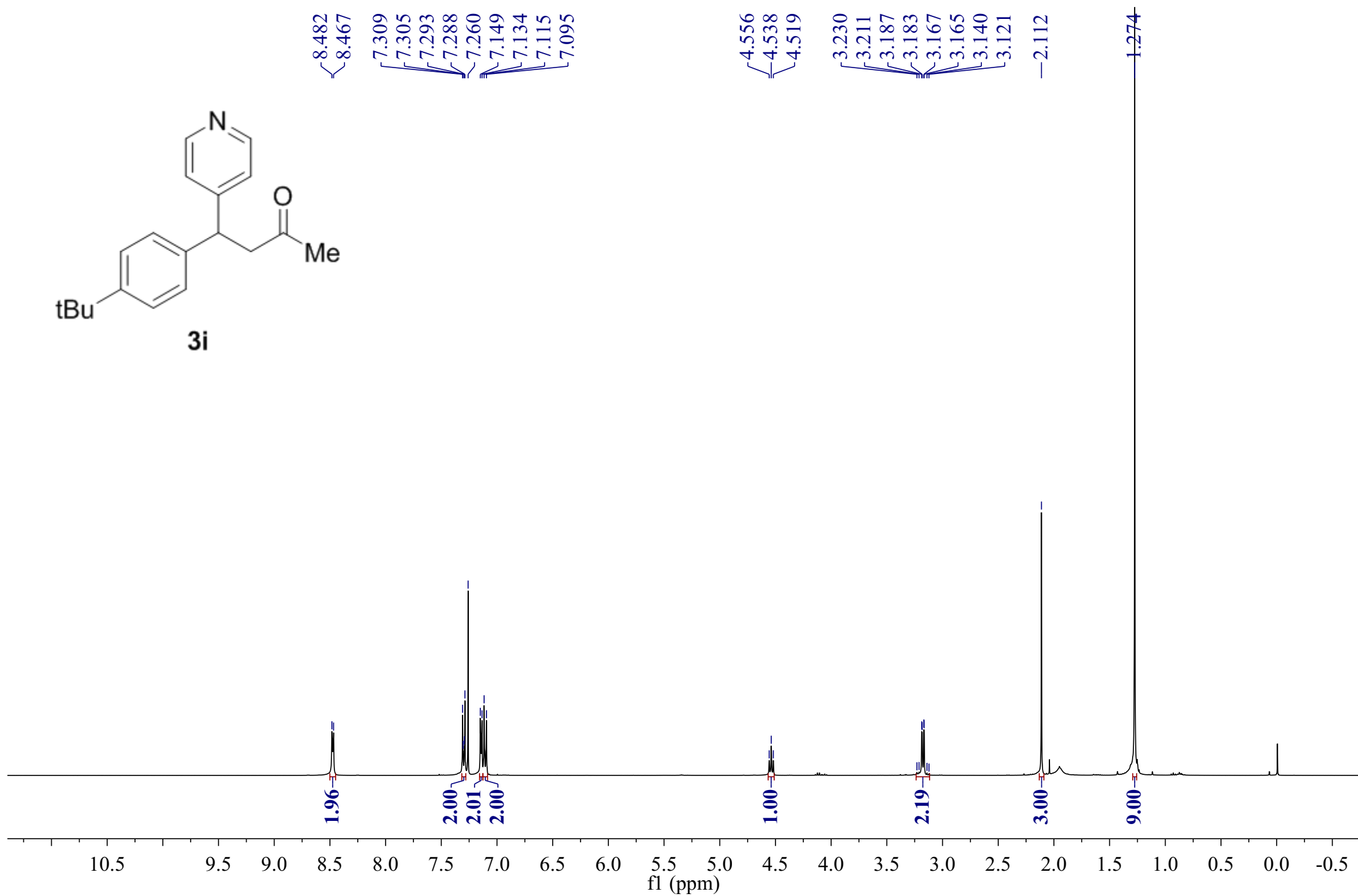
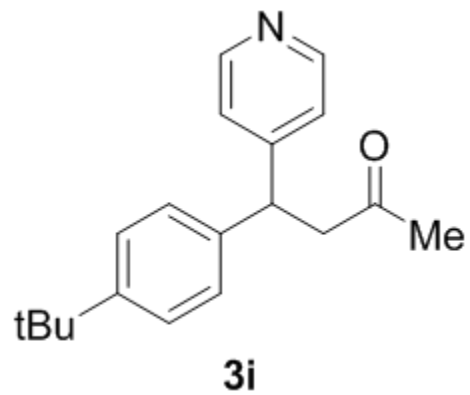
—44.84

—30.72

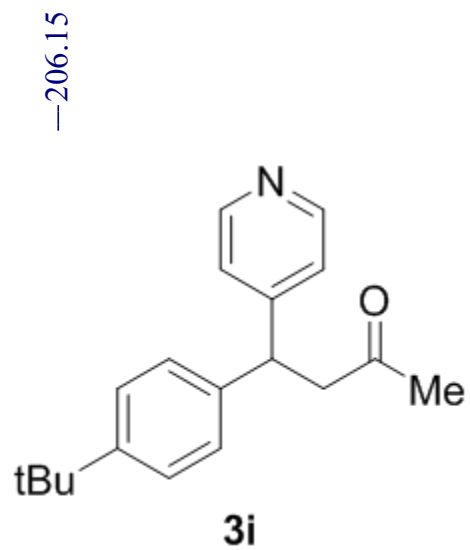
—21.08



ty-3-64 H1 CDCl3 400 M Hz



ty-3-64 C13 CDCl3 101 M Hz



—206.15

~153.13

~149.99

—139.08

~127.43

~125.86

~123.20

~77.48

~77.16

~76.84

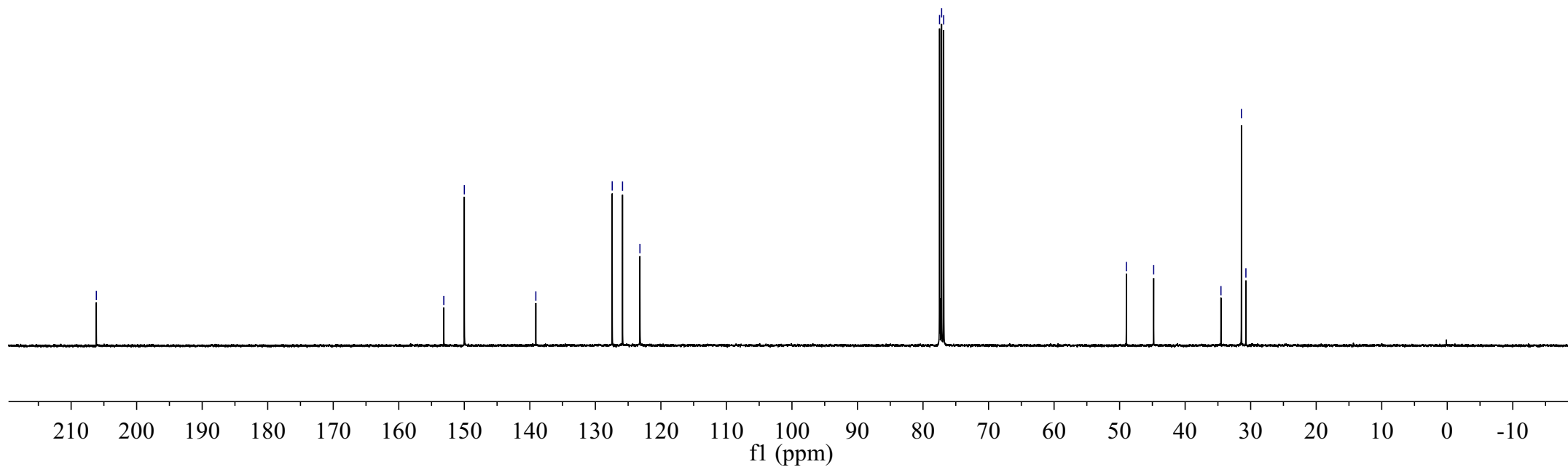
—48.97

—44.80

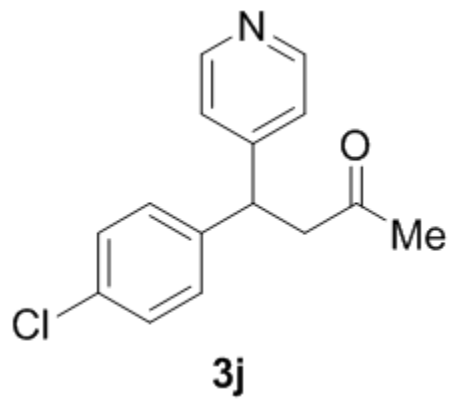
~34.53

~31.41

~30.73



ty-3-68-2 H1 CDCl3 400 M Hz



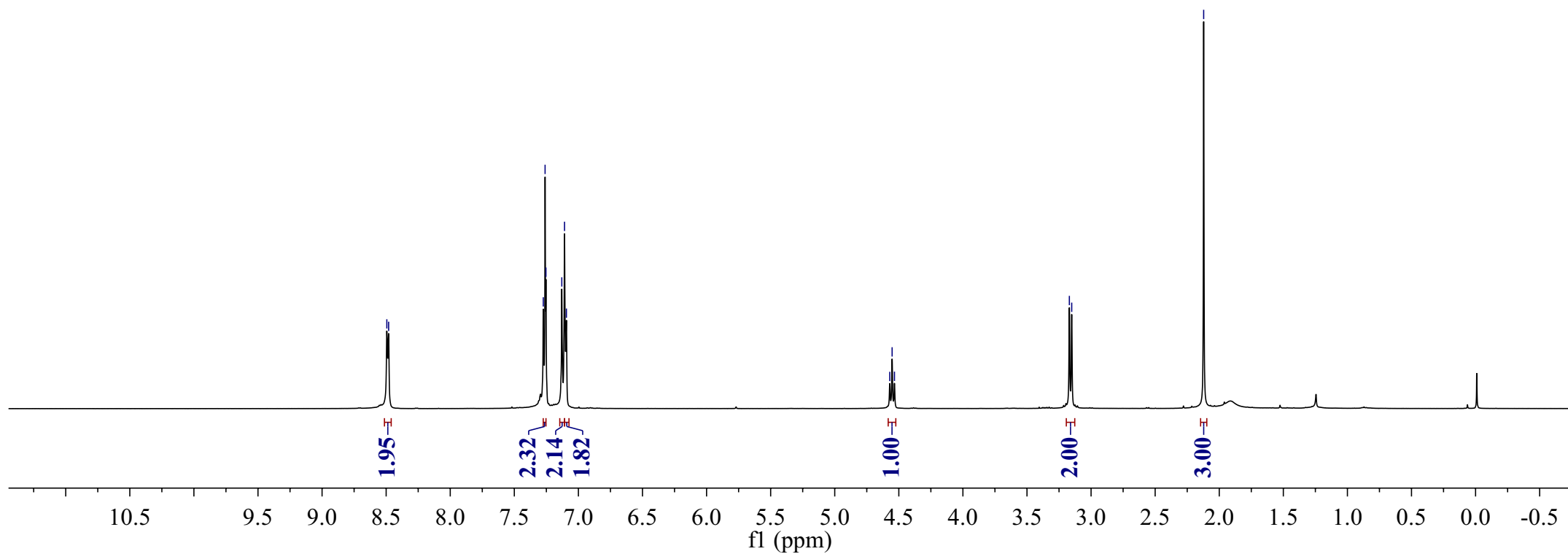
8.495
8.481

7.274
7.260
7.253
7.130
7.108
7.094

4.571
4.552
4.534

3.169
3.151

-2.121



ty-3-68-2 C13 CDCl3 101 M Hz

—205.53

~152.42
~150.16

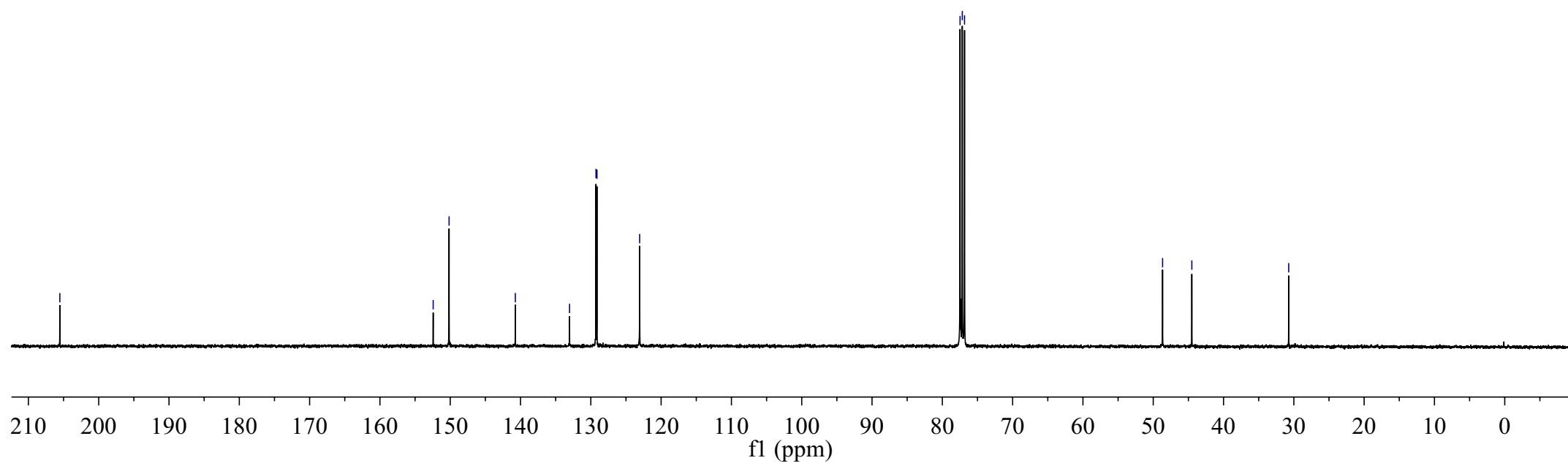
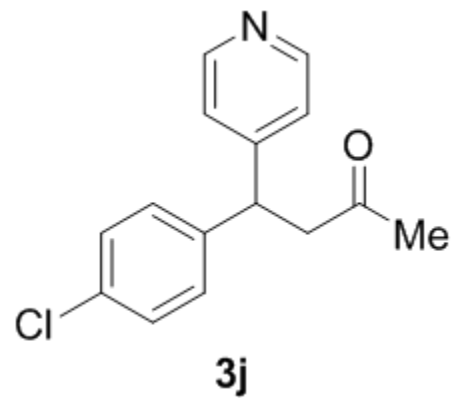
—140.74

~133.03
~129.27
~129.13
~123.05

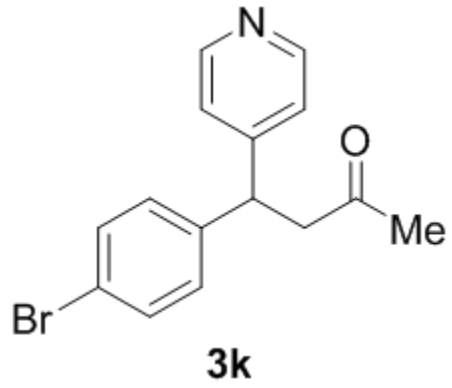
{77.48
77.16
76.84

—48.67
—44.51

—30.73



ty-4-73 H1 CDCl3 400 M Hz

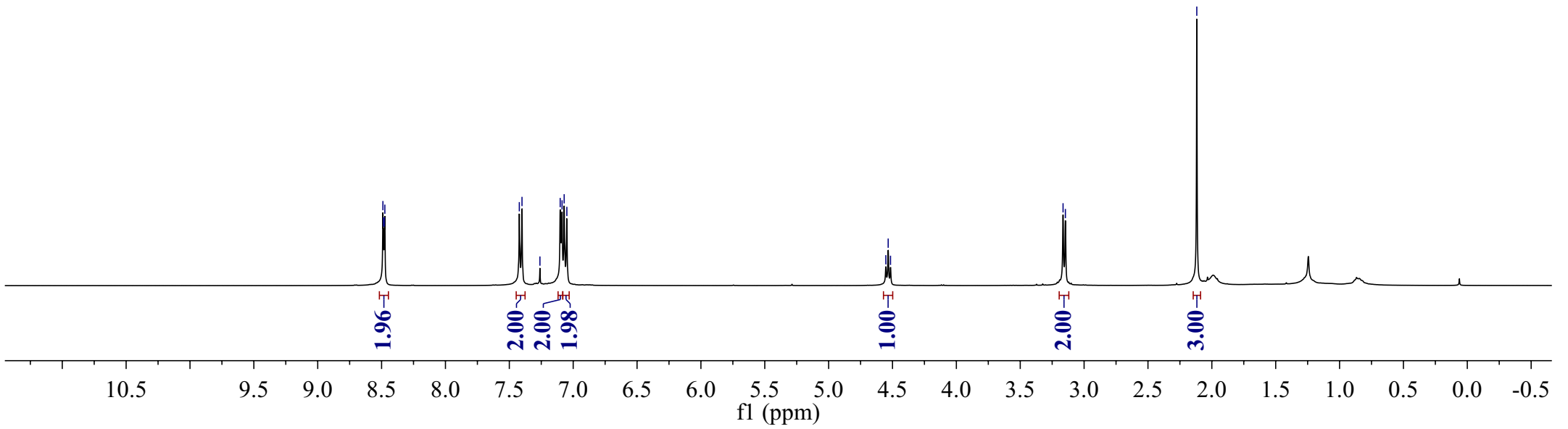


8.490
8.486
8.478
8.475
7.422
7.401
7.260
7.102
7.087
7.070
7.050

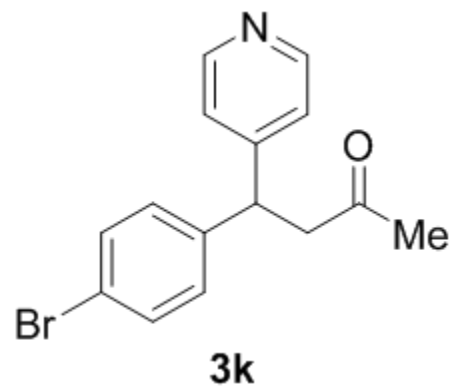
4.552
4.534
4.516

3.165
3.147

-2.118



ty-4-73 C13 CDCl3 101 M Hz



—205.50

~152.28

~150.16

—141.26

~132.05

~129.62

~123.02

~121.07

77.48

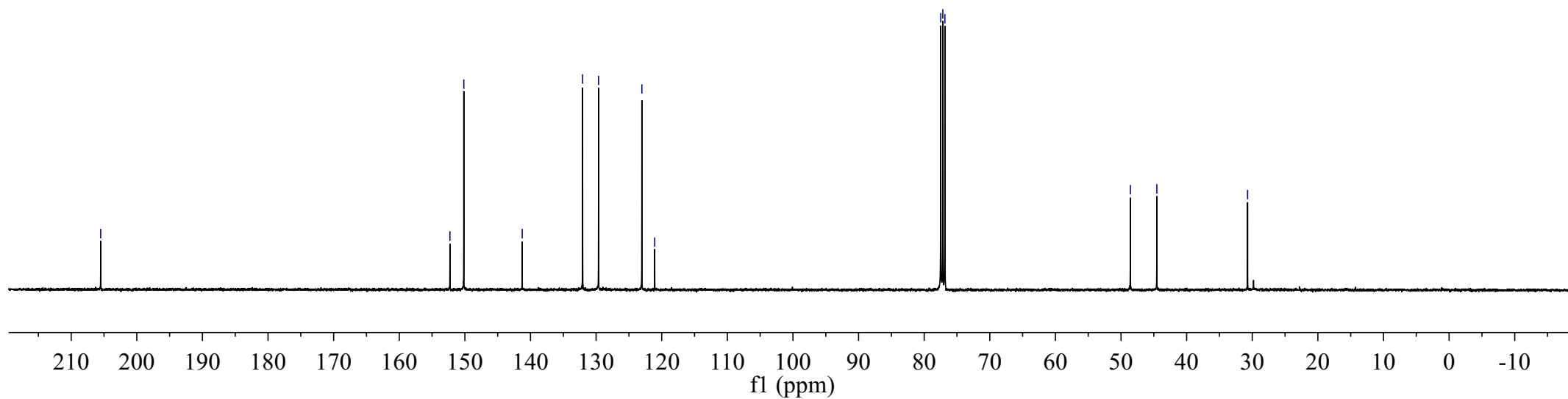
77.16

76.84

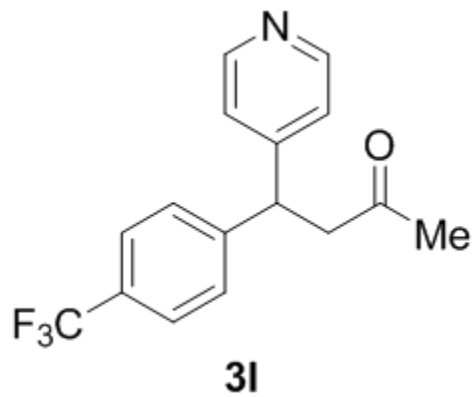
—48.58

—44.54

—30.71



ty-4-14 H1 CDCl3 400 M Hz



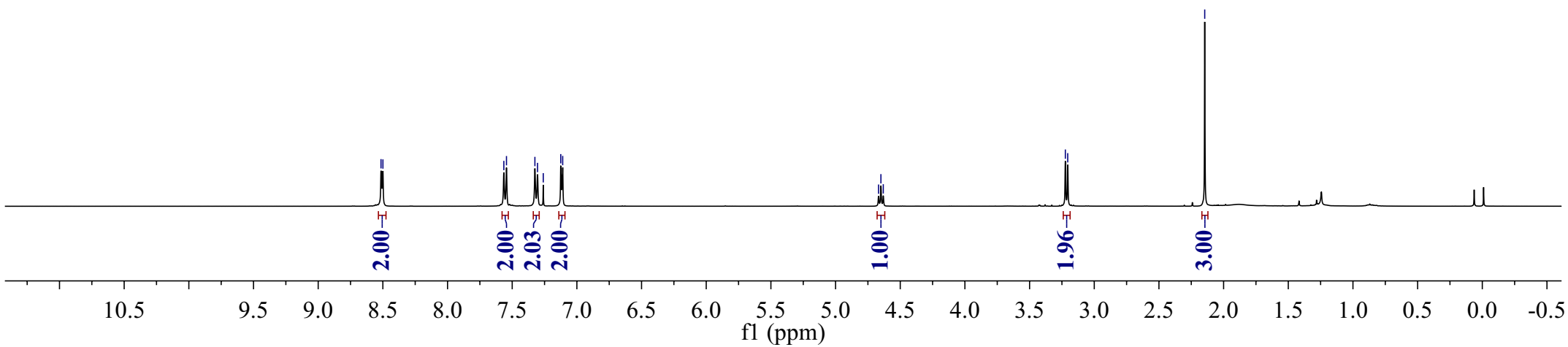
8.514
8.500

7.565
7.544
7.325
7.304
7.260
7.125
7.110

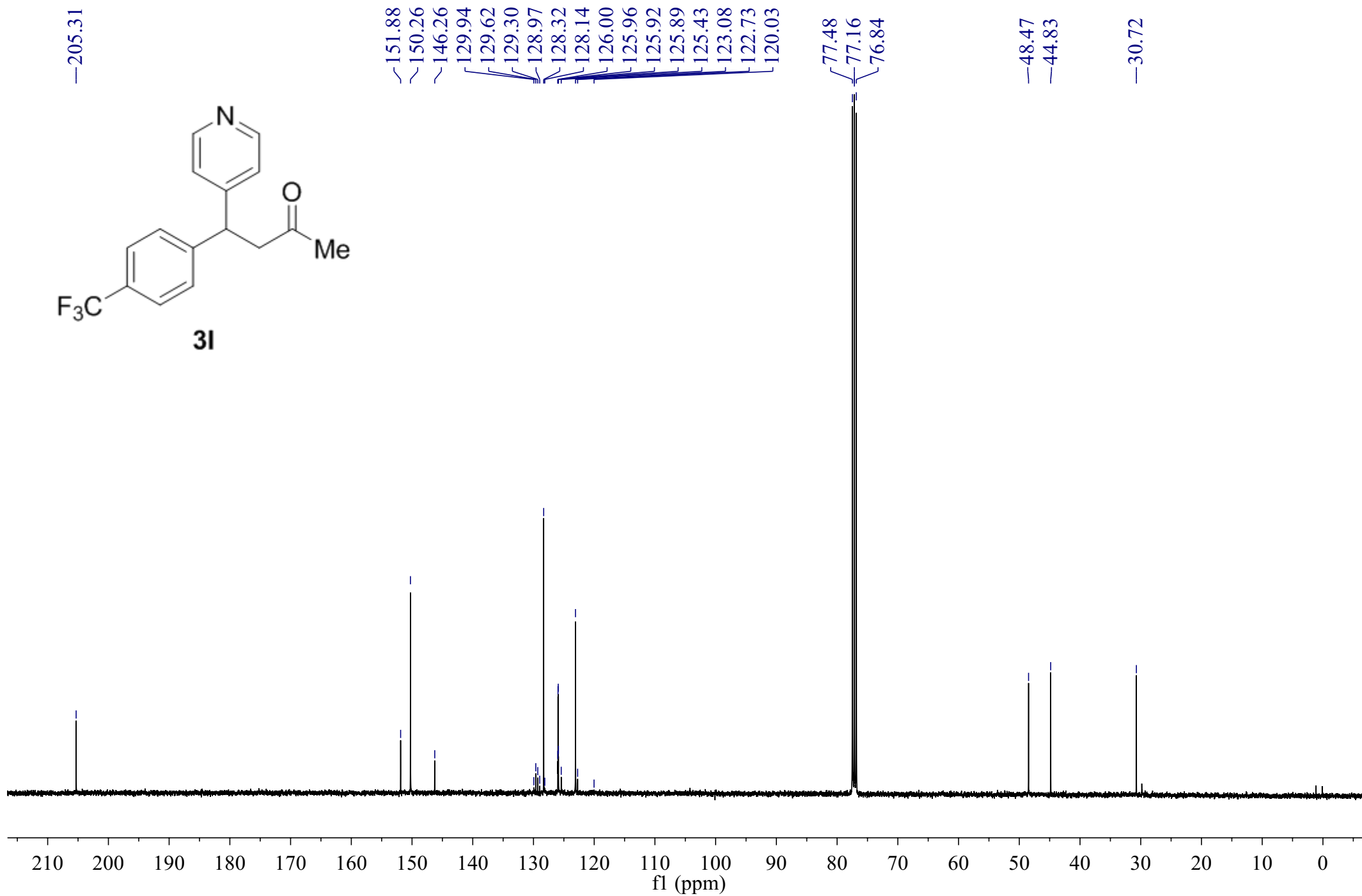
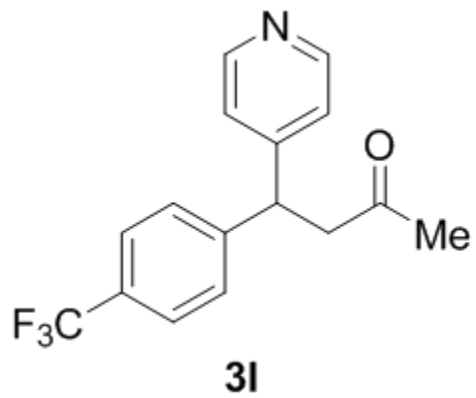
4.668
4.649
4.631

3.224
3.205

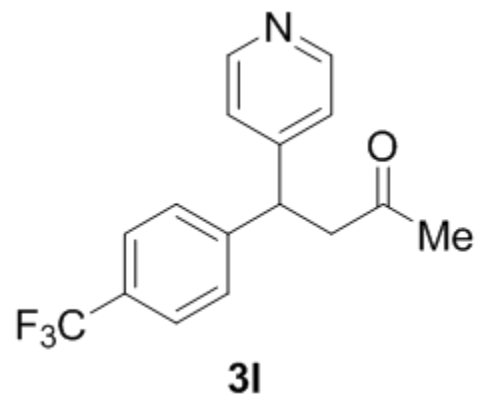
2.146



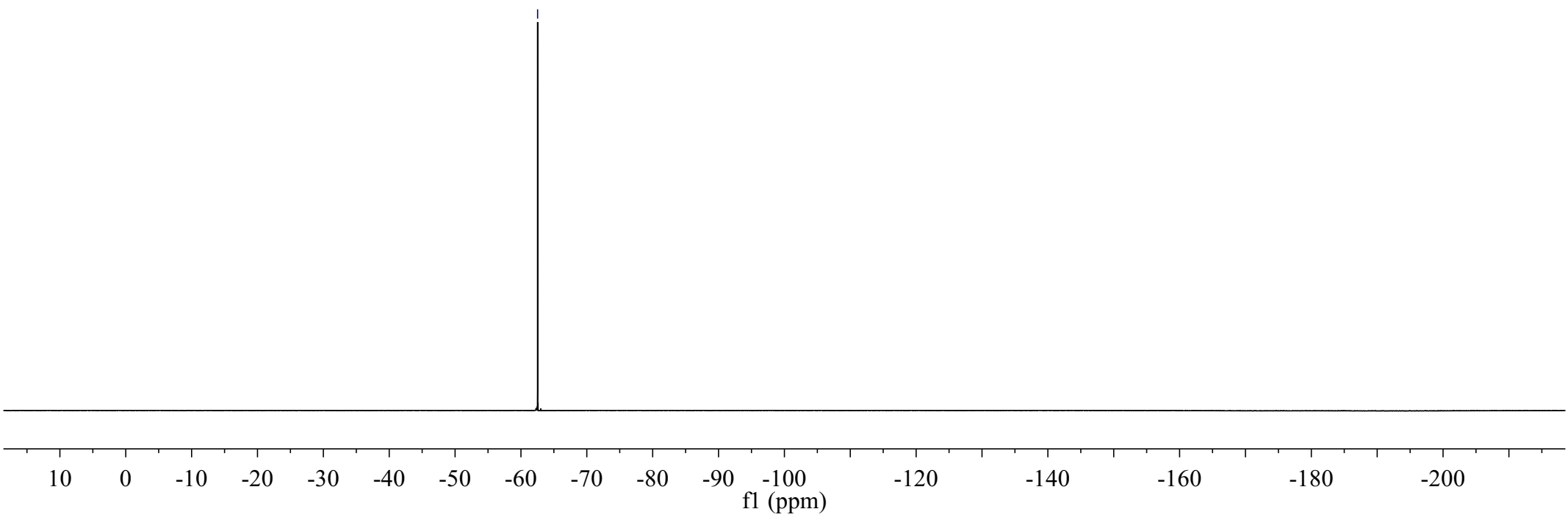
ty-4-14 C13 CDCl3 101 M Hz



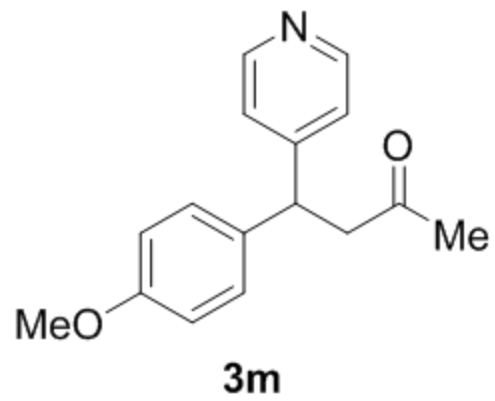
ty-4-14 F19 CDCl3 376 M Hz



---62.53



ty-4-10 H1 CDCl3 400 M Hz



8.477
8.462

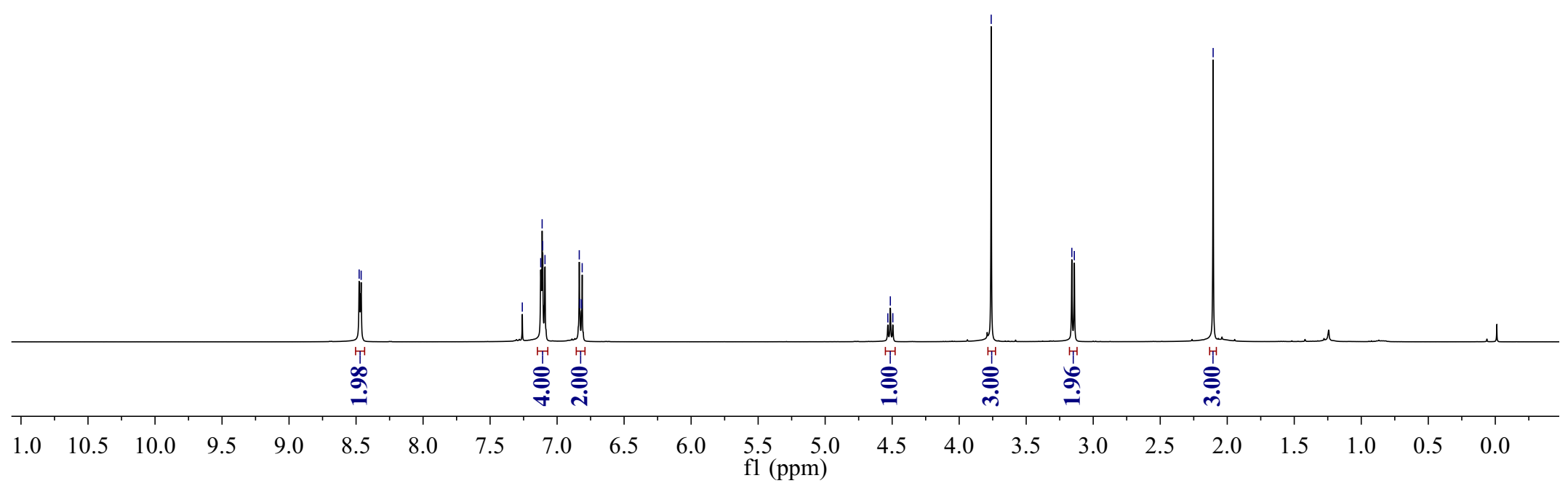
7.260
7.122
7.112
7.108
7.090
6.835
6.830
6.817
6.813

4.532
4.514
4.495

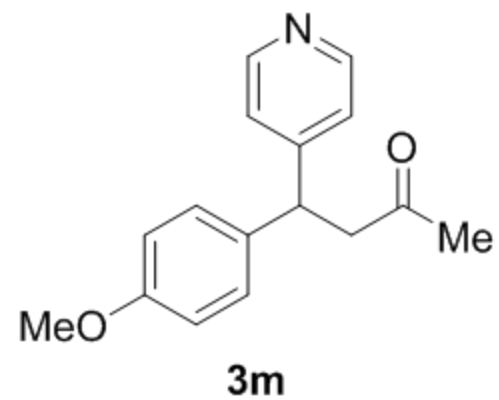
3.761

3.159
3.141

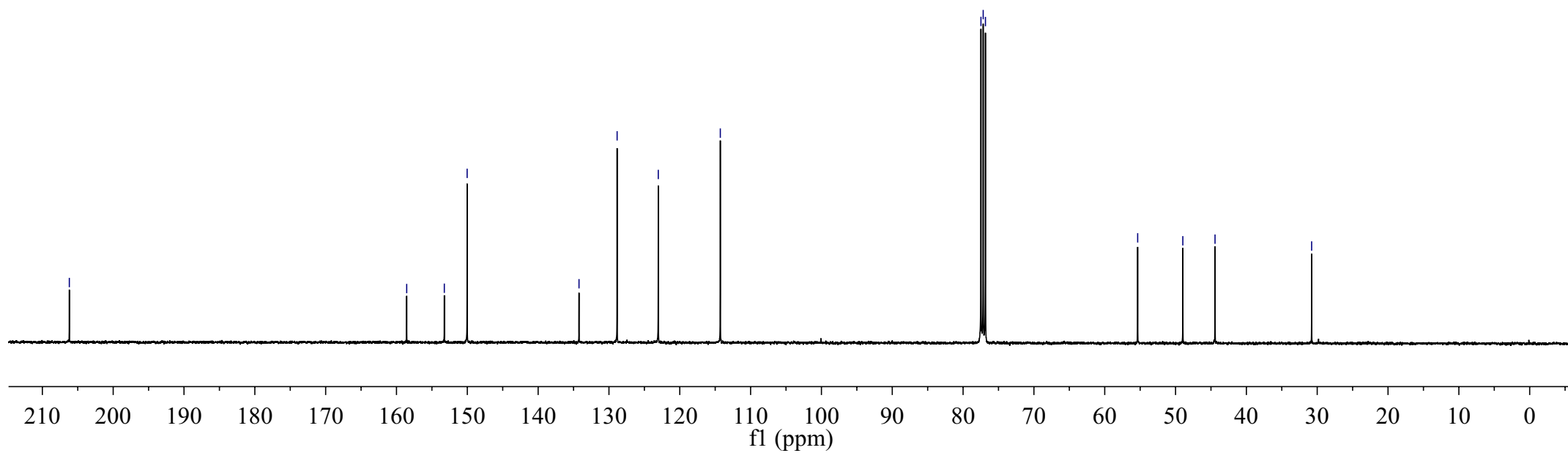
2.105



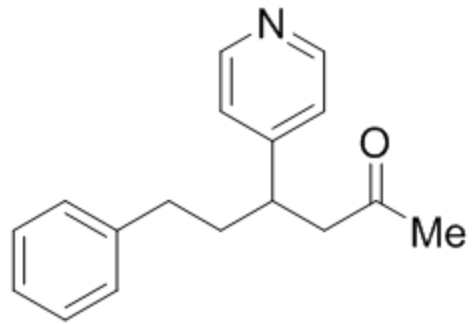
ty-4-10 C13 CDCl3 101 M Hz



—206.19 ~158.56 ~153.25 ~150.02 ~134.23 ~128.85 ~123.04 —114.28 {77.48 {77.16 {76.84 ~55.35 ~48.97 ~44.43 —30.79



ty-4-34 H1 CDCl3 400 M Hz

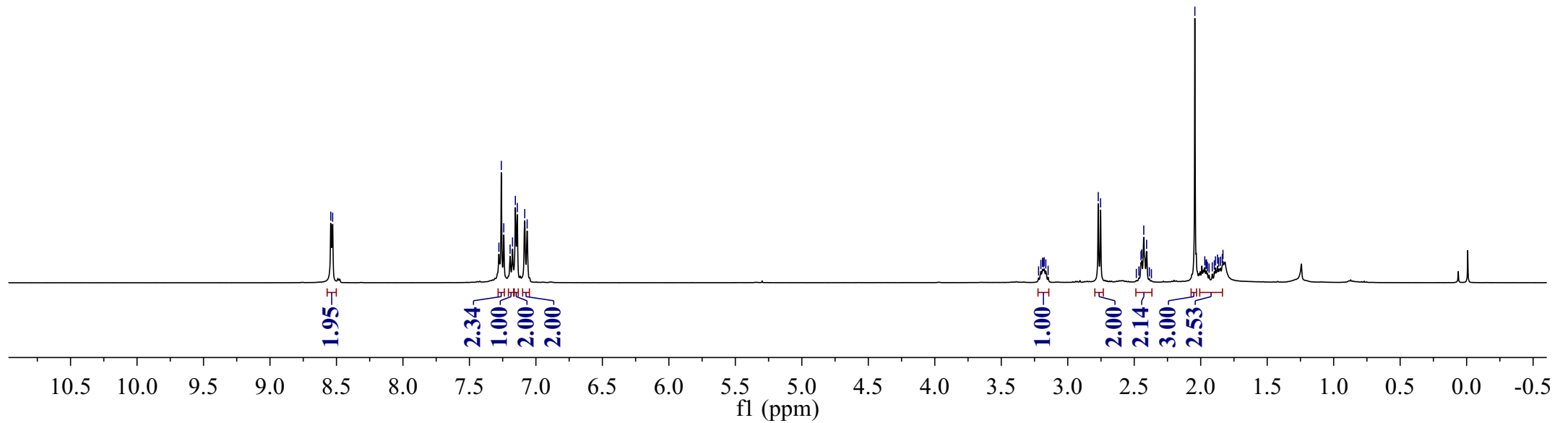


3n

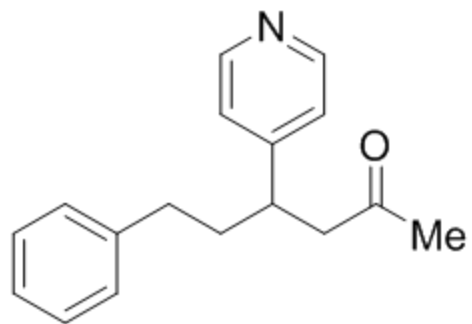
8.543
8.529

7.278
7.260
7.242
7.194
7.176
7.155
7.140
7.084
7.066

3.219
3.202
3.189
3.184
3.177
3.165
3.147
2.771
2.753
2.484
2.465
2.449
2.444
2.428
2.407
2.386
2.371
2.044
1.969
1.960
1.956
1.950
1.937
1.913
1.898
1.889
1.874
1.864
1.851
1.838
1.832



ty-4-34 C13 CDCl3 101 M Hz



3n

—206.69

—153.41

—150.14

—141.38

—128.56

—128.39

—126.15

—123.26

—77.48

—77.16

—76.84

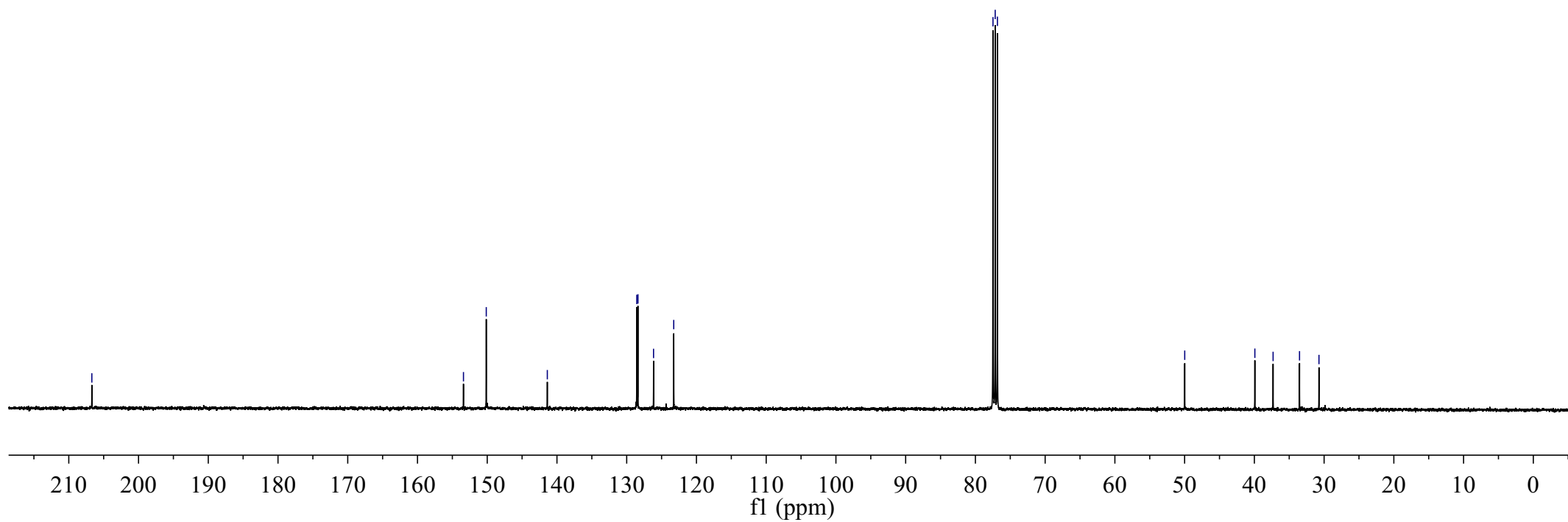
—49.98

—39.93

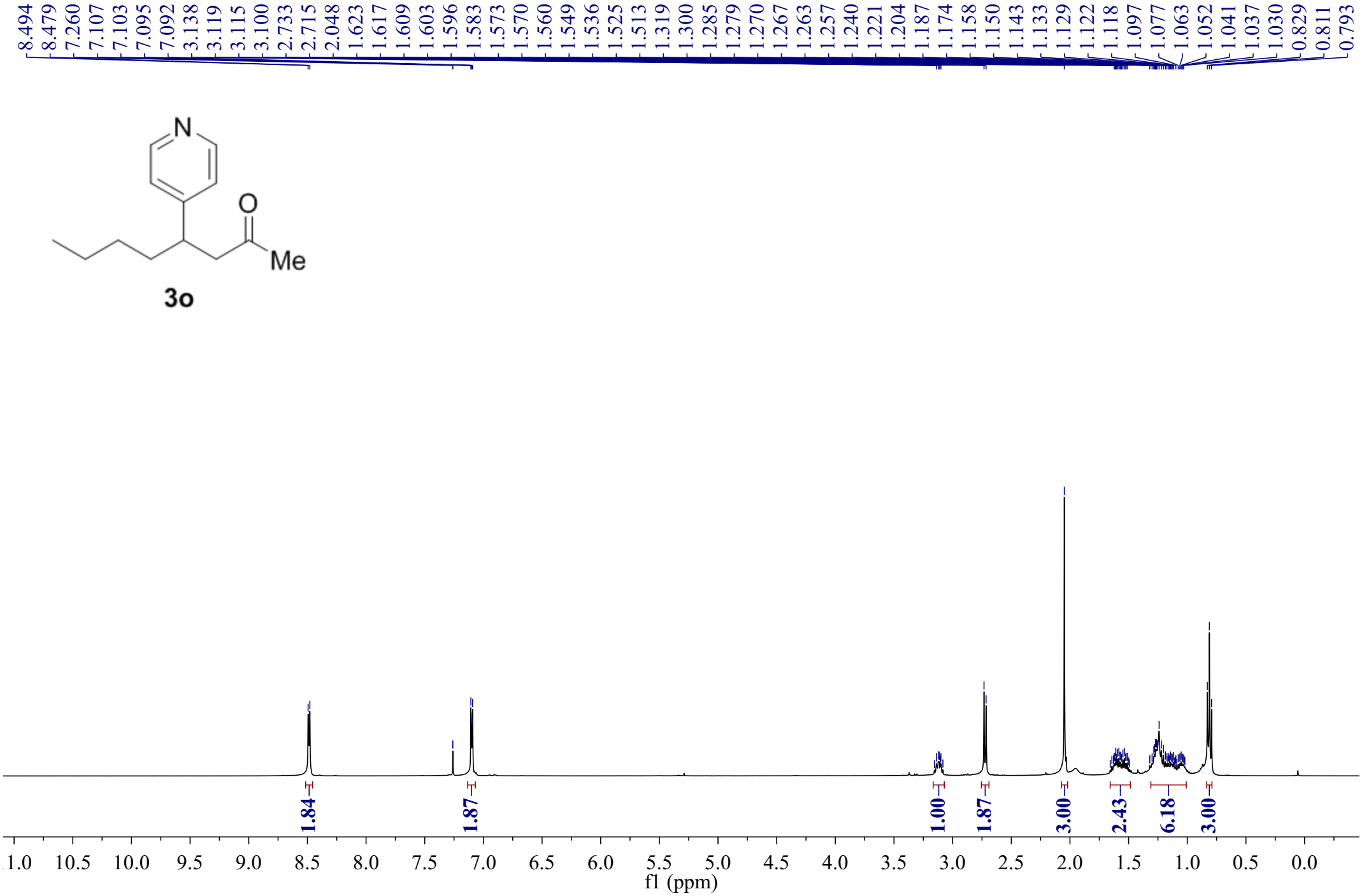
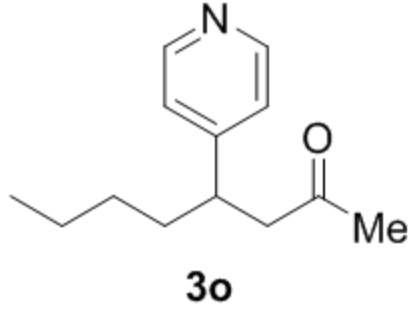
—37.31

—33.52

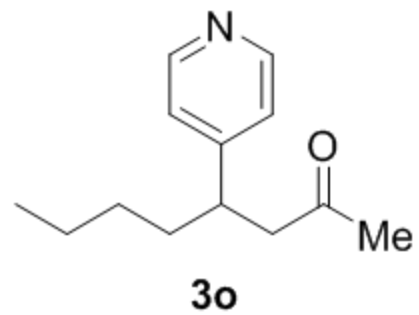
—30.74



ty-4-56 H1 CDCl3 400 M Hz



ty-4-56 C13 CDCI3 101 M Hz



—206.92

—153.99

—149.98

—123.15

77.48

77.16

76.84

—49.94

~40.36

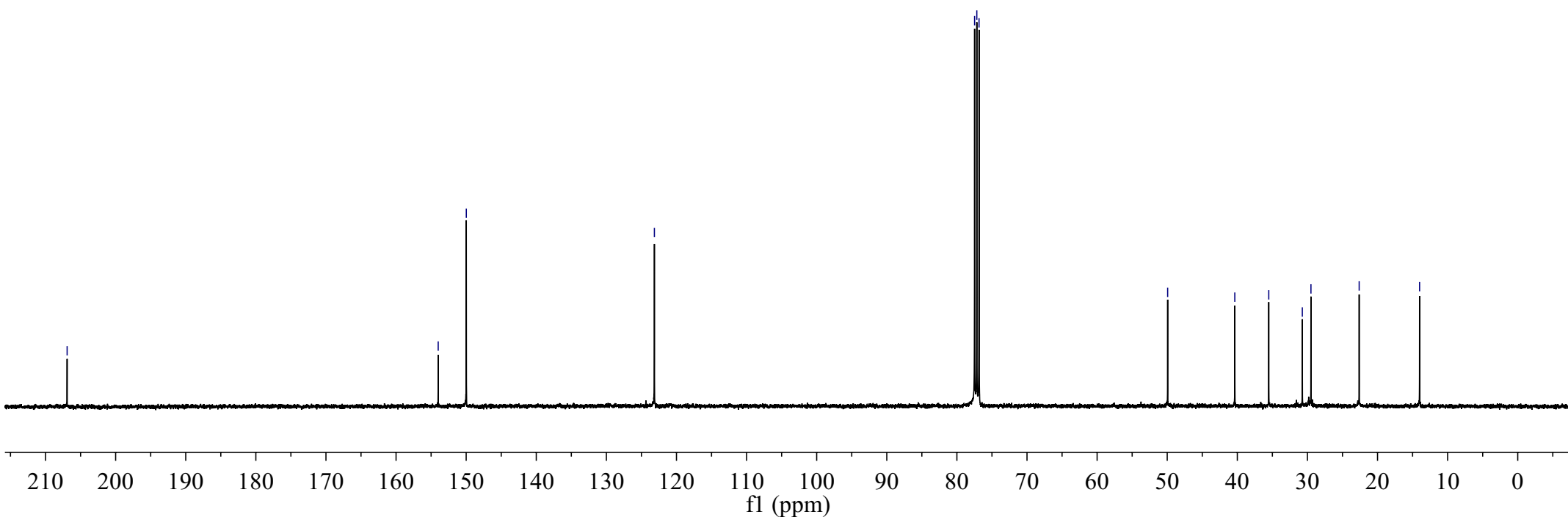
~35.51

~30.73

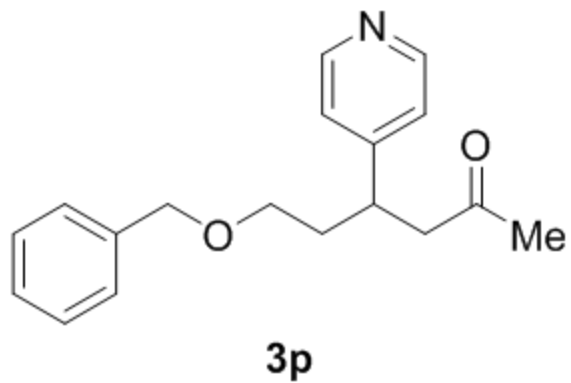
~29.50

~22.62

—14.00



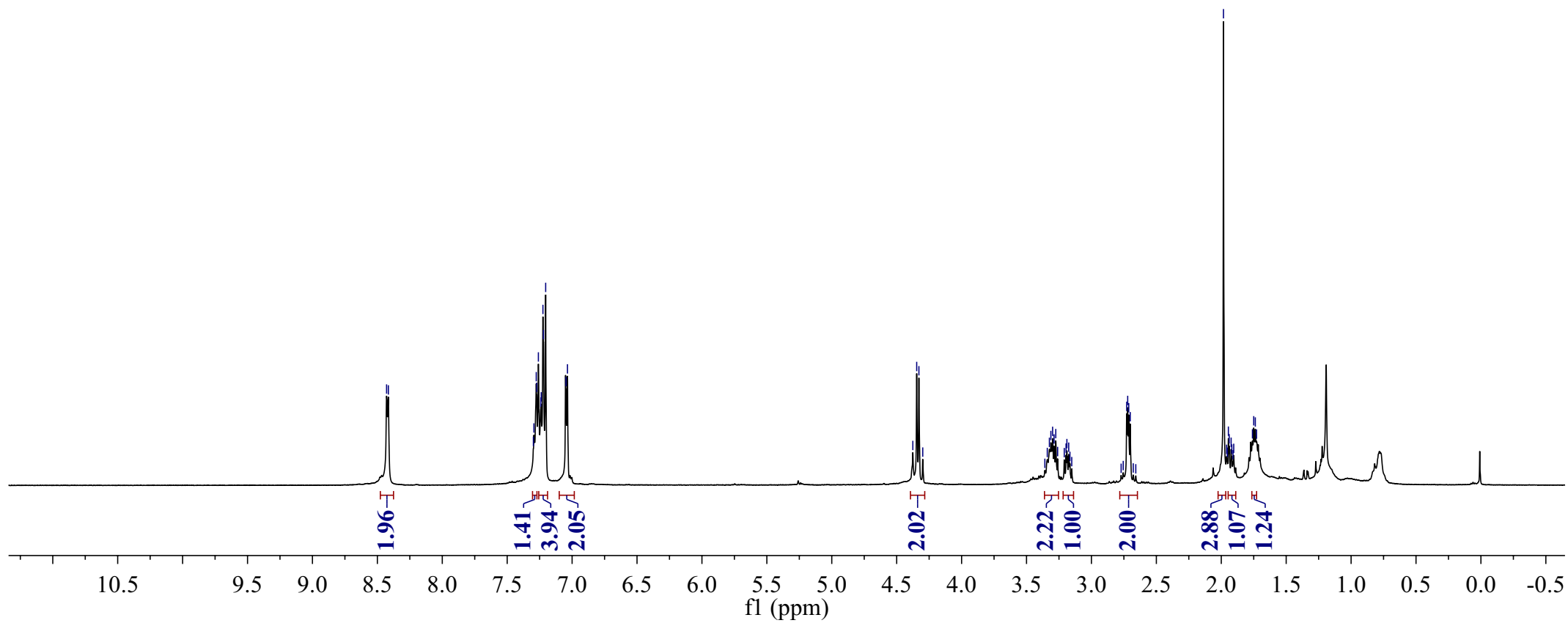
ty-4-90 H1 CDCl3 400 M Hz



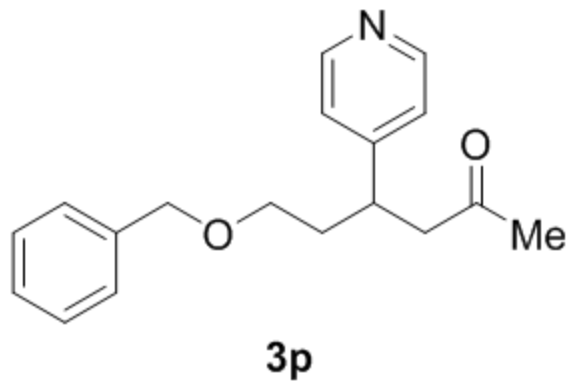
8.429
8.415
7.298
7.294
7.276
7.273
7.260
7.241
7.238
7.225
7.221
7.204
7.047
7.036

4.376
4.346
4.329
4.299

3.312
3.299
3.275
2.728
2.721
2.713
2.701
2.683
1.959
1.954
1.945
1.939
1.924
1.919
1.910
1.904
1.760
1.750
1.738
1.728



ty-4-90 C13 CDCl3 101 M Hz



—206.54

—153.35

—149.99

—138.24

—128.54

—127.87

—127.82

—123.19

—77.48

—77.16

—76.84

—73.10

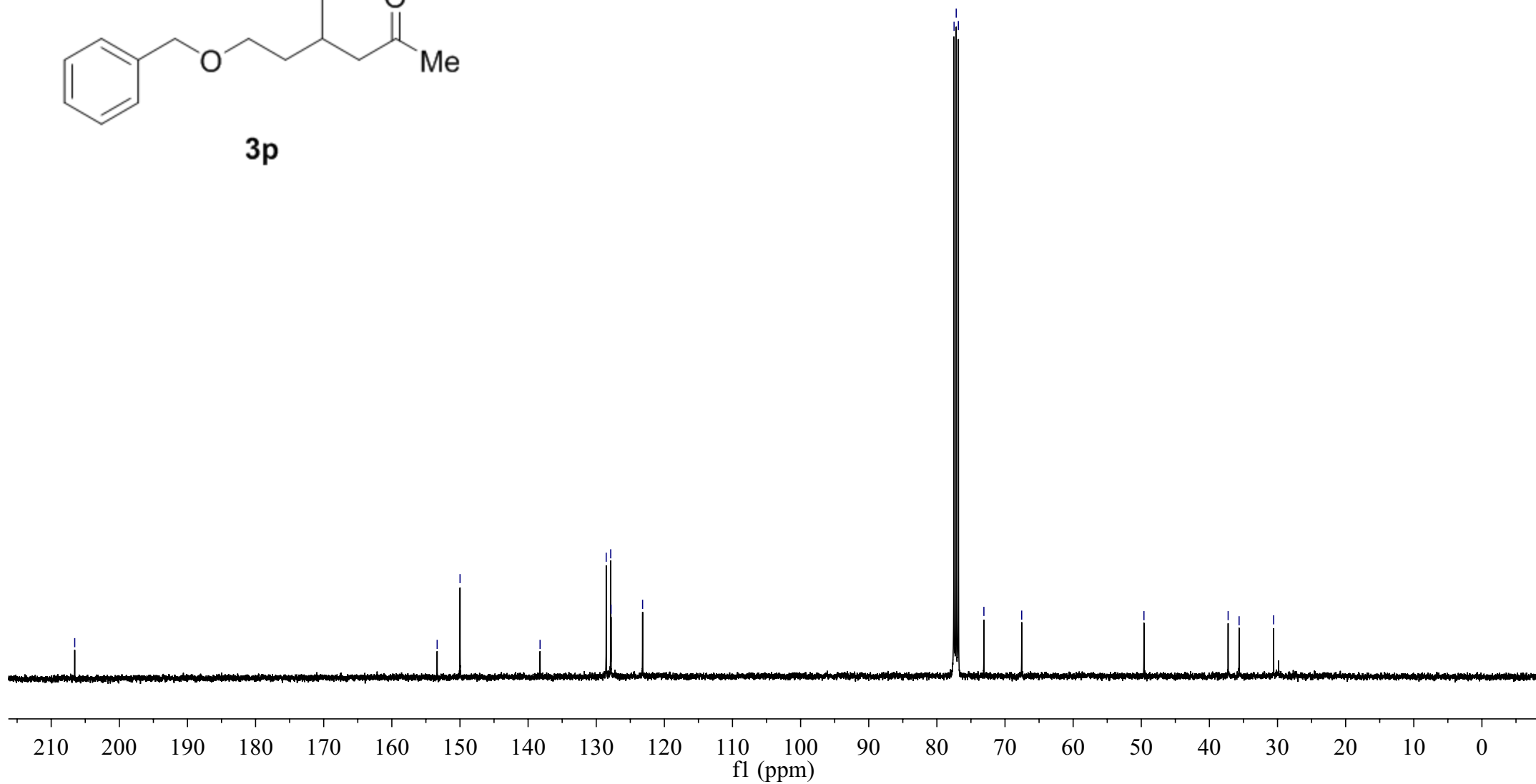
—67.55

—49.61

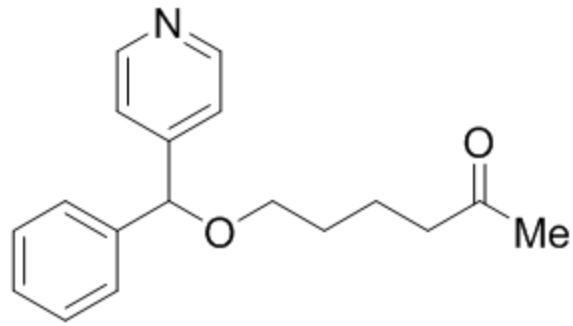
—37.25

—35.64

—30.57



ty-4-45 H1 CDCl3 400 M Hz



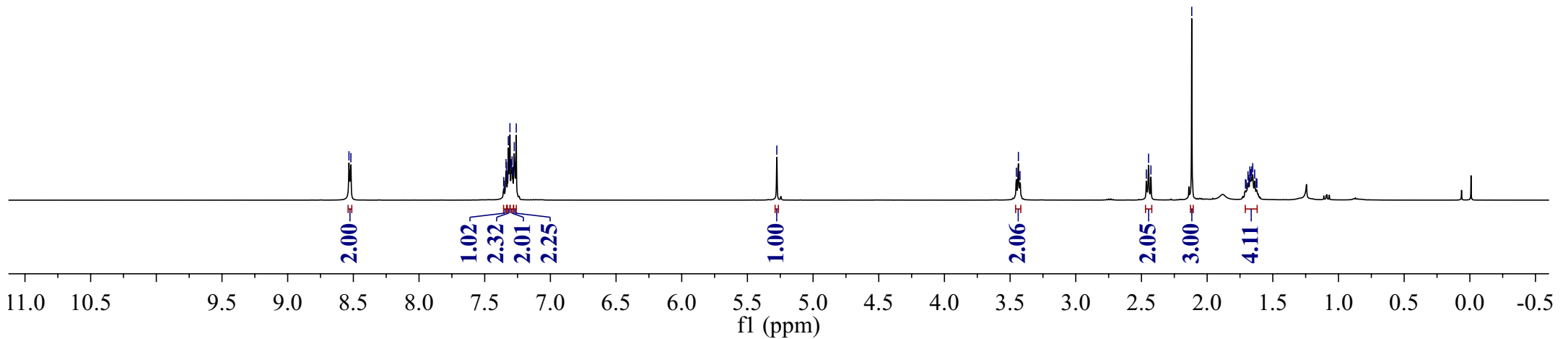
3p'

8.533
8.519
7.356
7.352
7.338
7.334
7.327
7.320
7.308
7.299
7.296
7.291
7.286
7.275
7.260

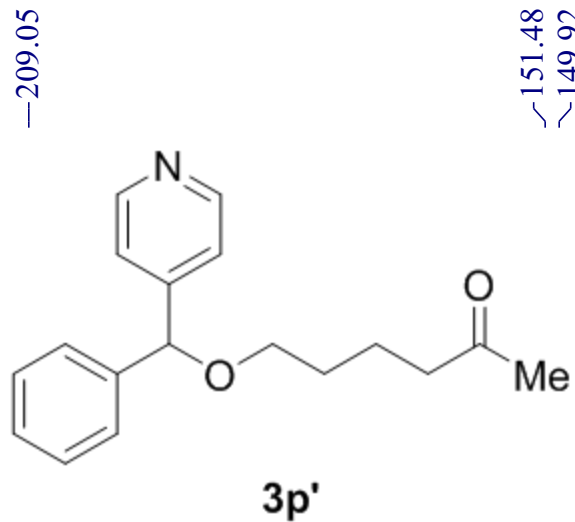
5.276

3.452
3.437
3.425

2.463
2.446
2.428
2.117
1.708
1.703
1.689
1.682
1.675
1.670
1.666
1.661
1.653
1.638
1.626
1.621



ty-4-45 C13 CDC13 101 M Hz



—209.05

~151.48
~149.92

—140.91

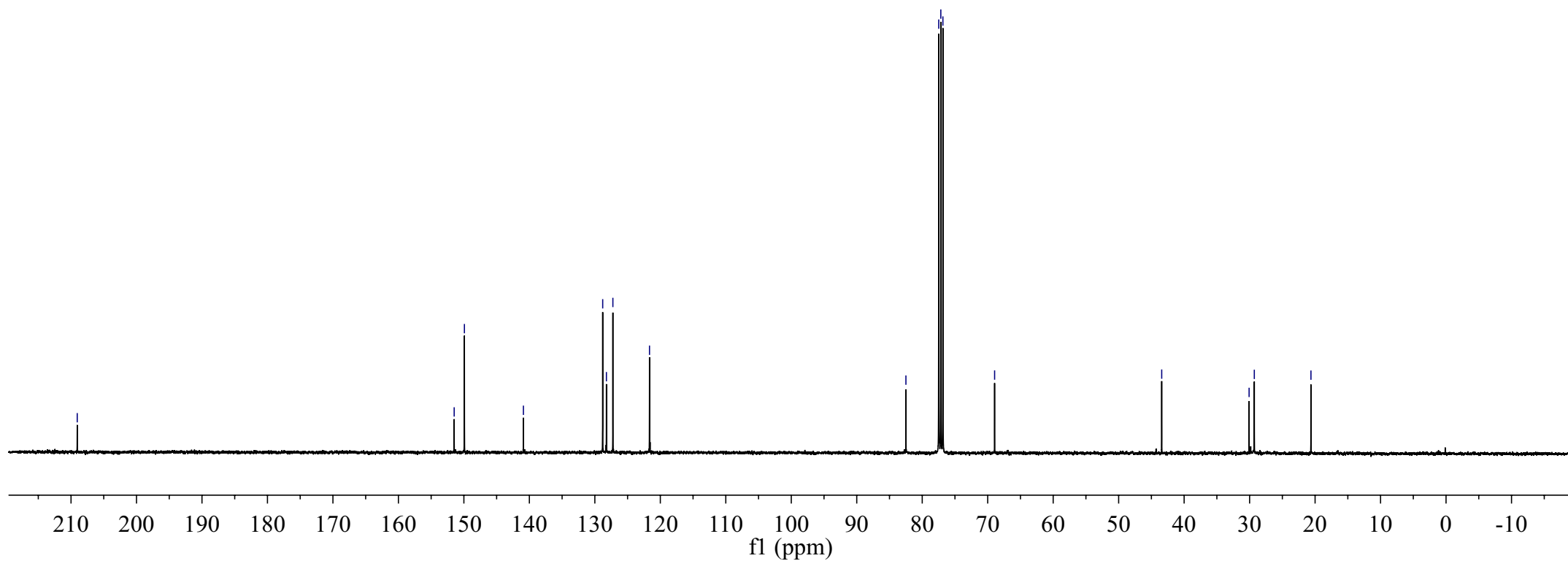
~128.80
~128.23
~127.24
~121.65

~82.49
~77.48
~77.16
~76.84
~68.95

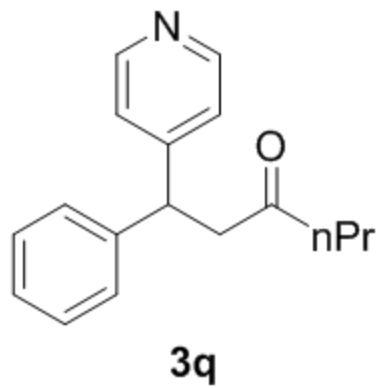
—43.42

~30.08
~29.28

—20.63



ty-4-46 H1 CDCl3 400 M Hz



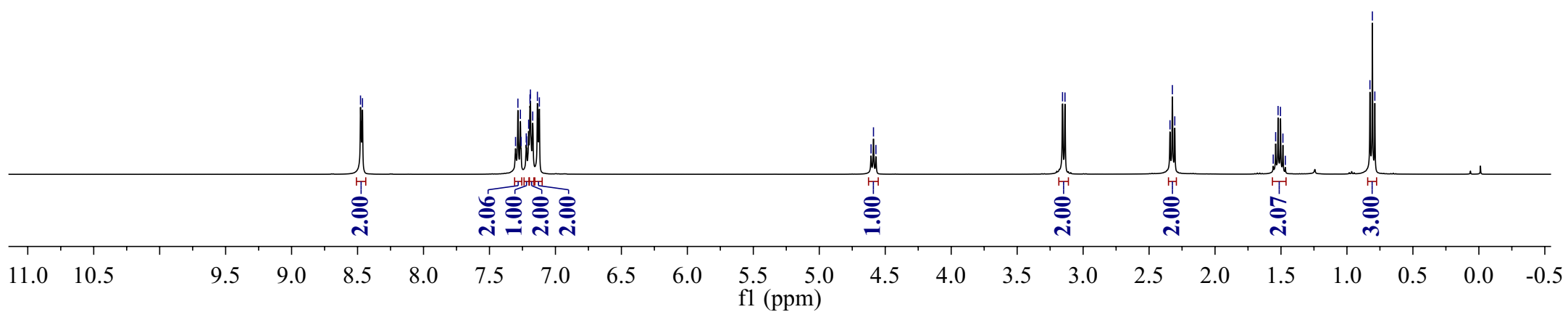
8.478
8.463
7.302
7.285
7.266
7.260
7.221
7.219
7.203
7.193
7.190
7.172
7.137
7.122

4.608
4.589
4.571

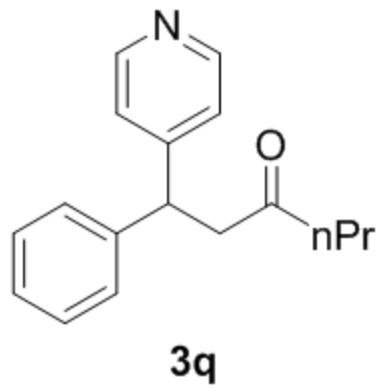
3.156
3.137

2.341
2.323
2.305

1.540
1.522
1.504
1.485
0.826
0.807
0.789



ty-4-46 C13 CDCl3 101 M Hz



208.28

152.99

149.98

142.29

128.90

127.86

127.08

123.15

77.48

77.16

76.84

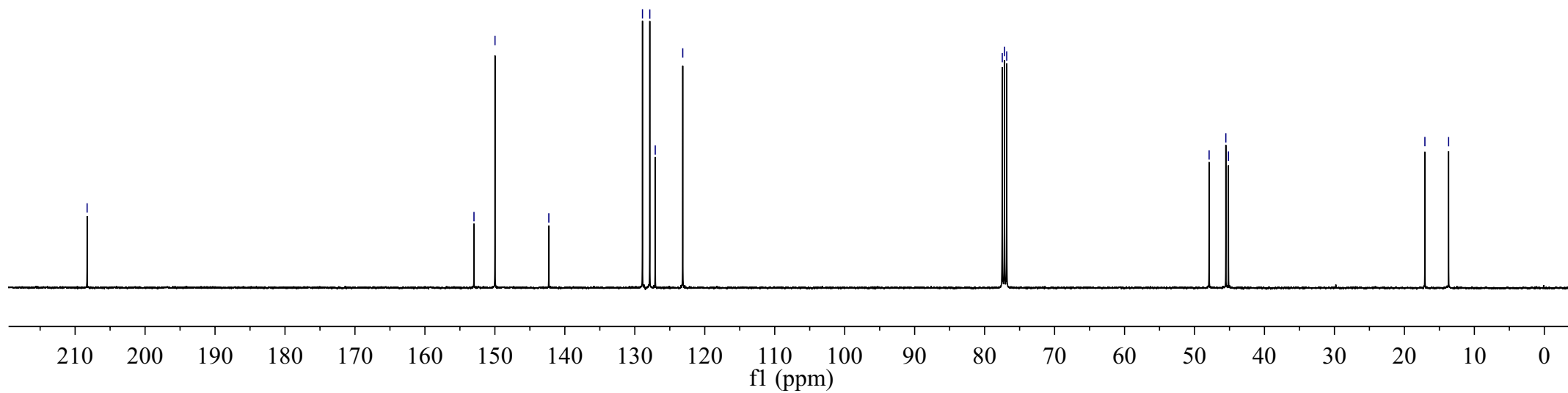
47.91

45.52

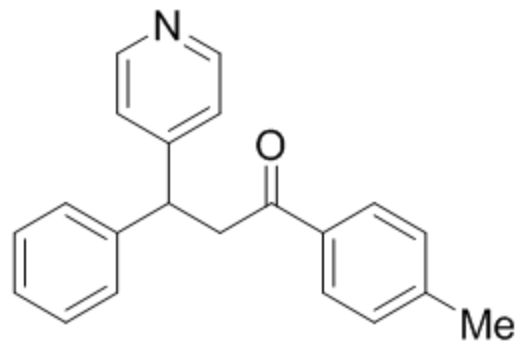
45.15

17.07

13.68



ty-5-48 H1 CDCl3 400 M Hz

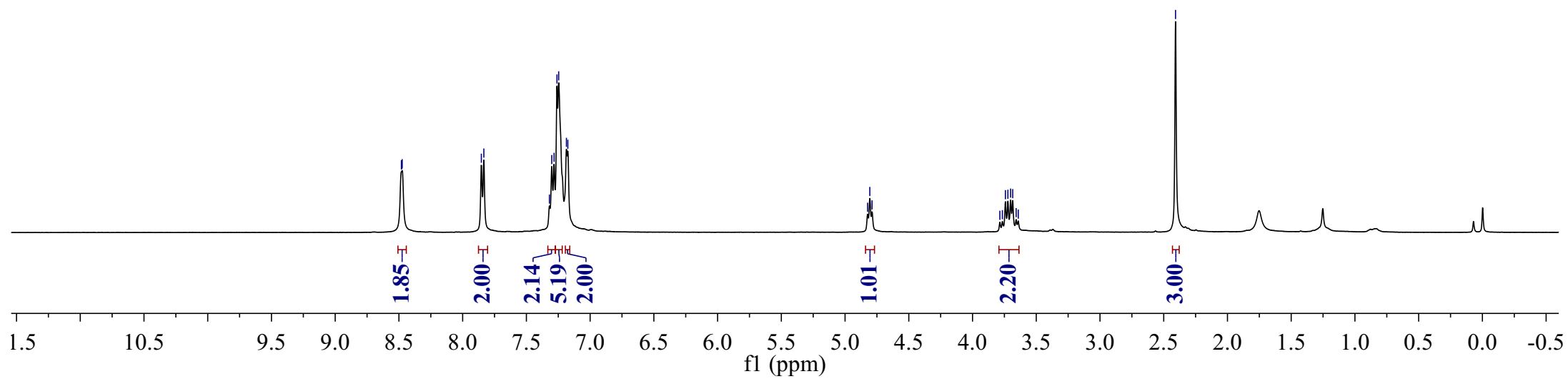


3r

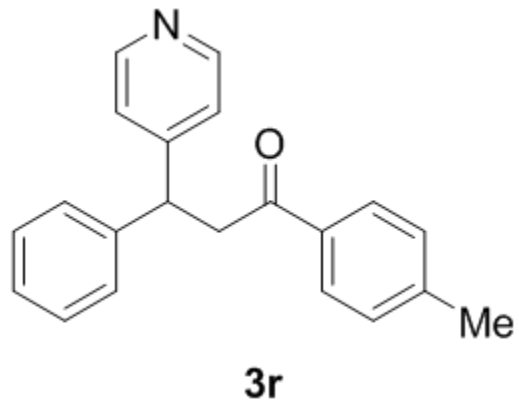
8.481
8.479
8.474
7.853
7.834
7.319
7.301
7.283
7.260
7.247
7.186
7.175

4.823
4.806
4.788
3.786
3.766
3.742
3.723
3.701
3.685
3.658
3.641

—2.407



ty-5-48 C13 CDCl3 101 M Hz



—196.93

~153.16

~150.04

~144.44

~142.69

134.32

129.53

128.96

128.29

128.00

127.08

123.32

77.48

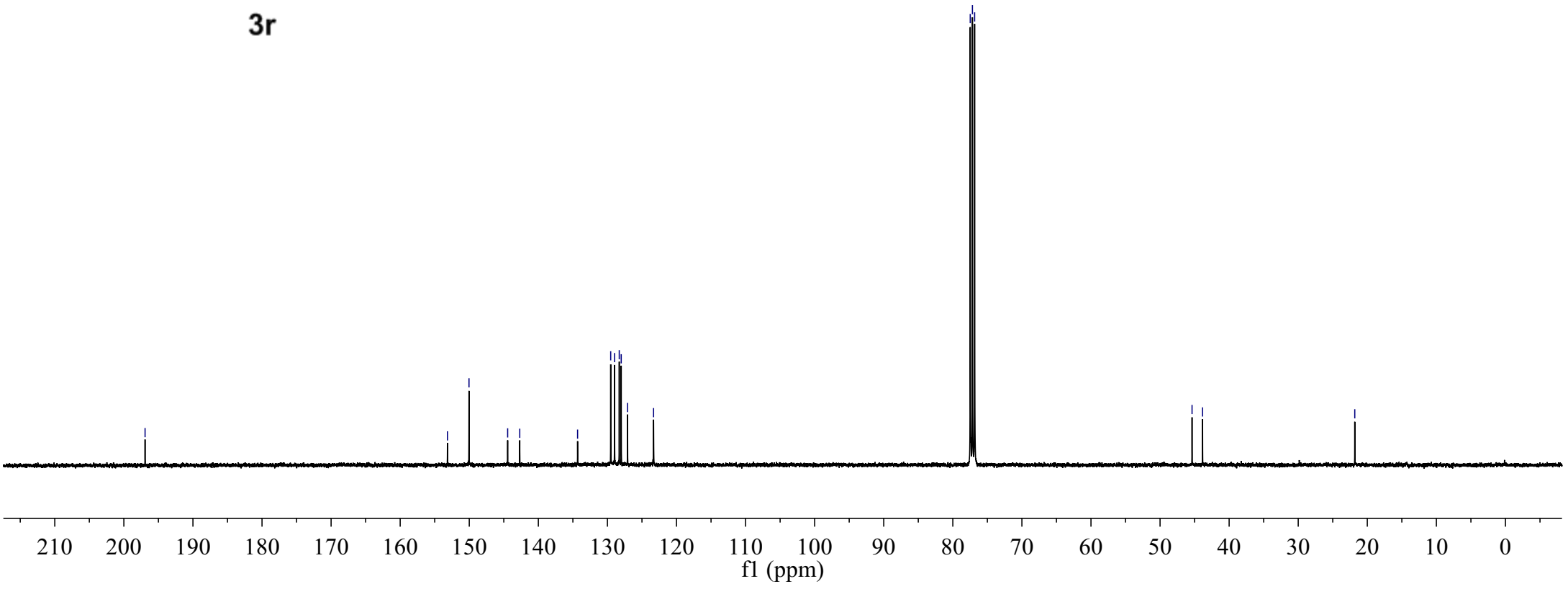
77.16

76.84

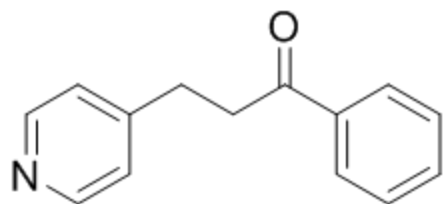
~45.37

~43.85

—21.81



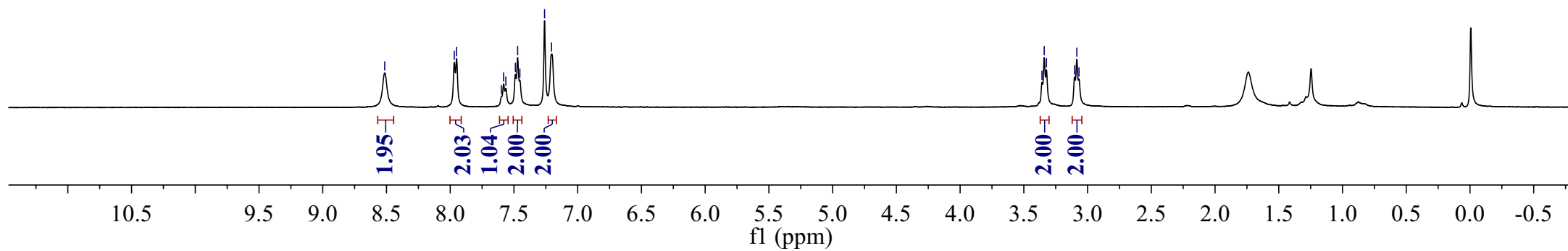
ty-5-30 H1 CDCl3 400 M Hz



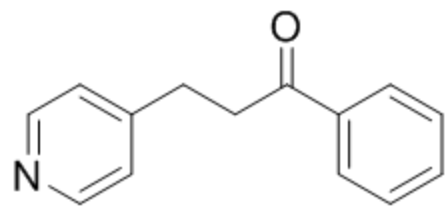
3s

8.514
7.968
7.950
7.599
7.581
7.564
7.489
7.471
7.454
7.260
7.205

3.358
3.340
3.322
3.102
3.085
3.067



ty-5-30 C13 CDCl3 101 M Hz



3s

—198.36

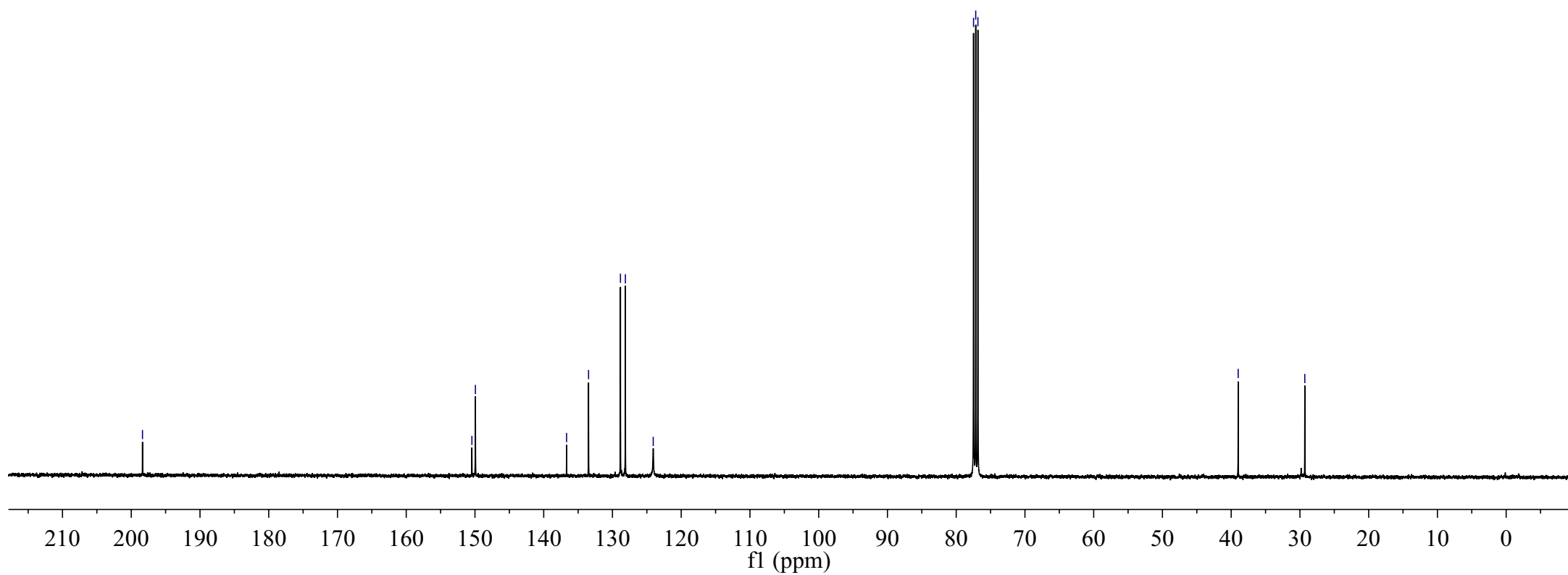
150.45
149.94

136.68
133.48
128.84
128.12
124.07

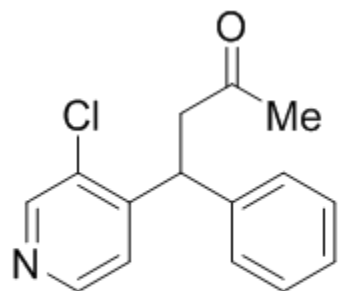
77.48
77.16
76.84

—38.98

—29.29

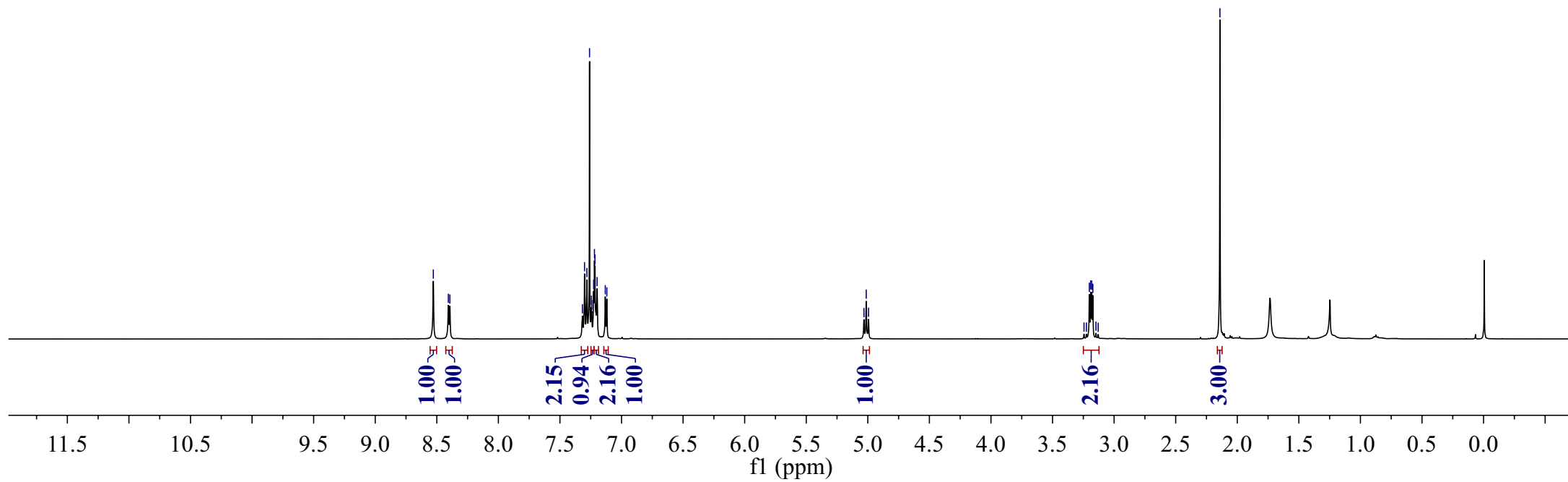


ty-3-54-3 H1 CDCl3 400 M Hz

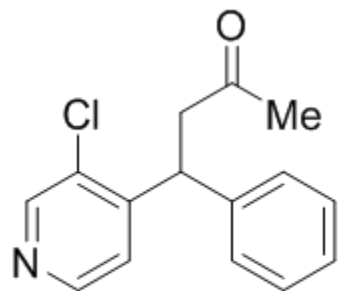


3aa

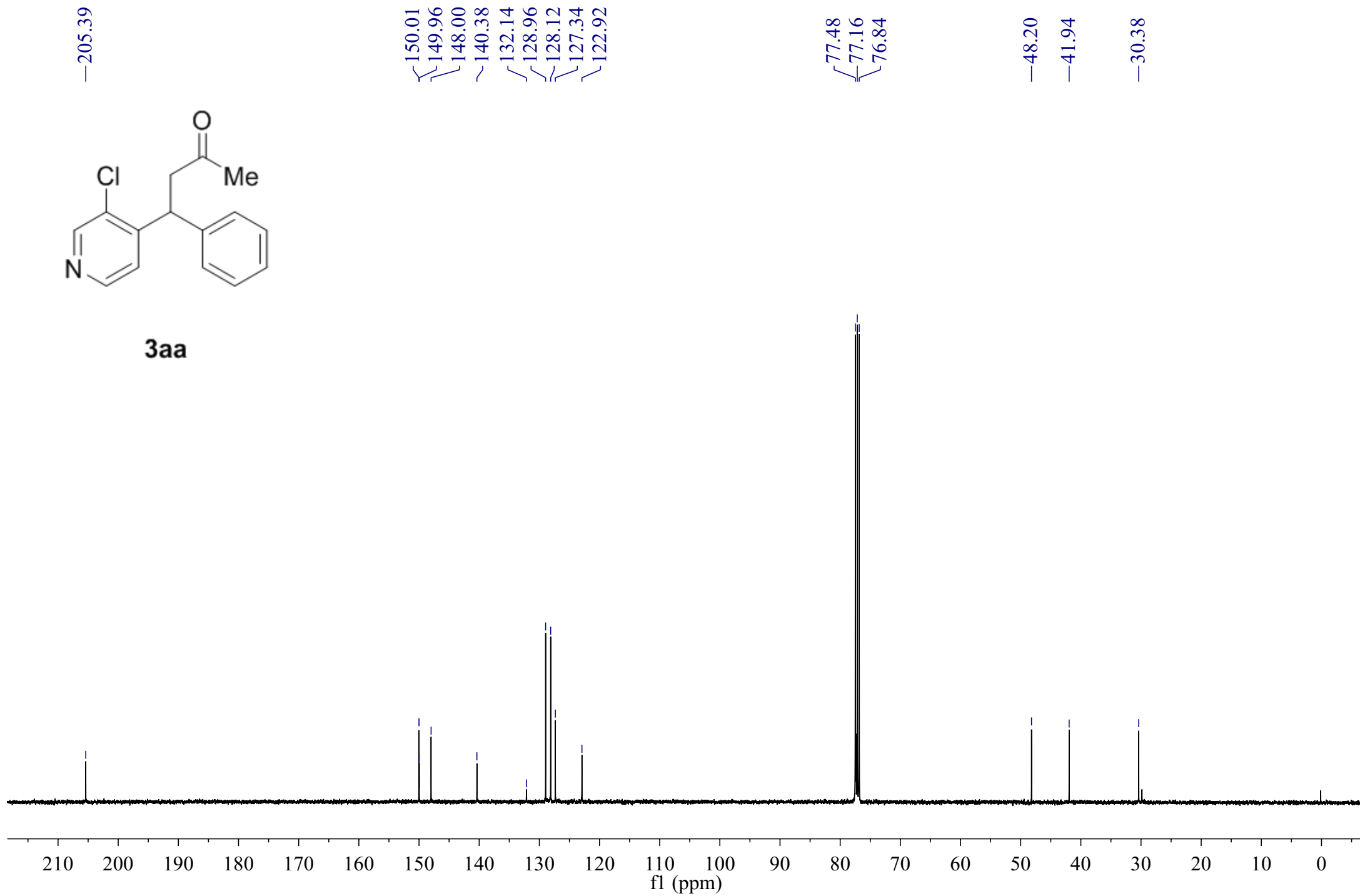
8.528
8.406
8.394
7.318
7.300
7.281
7.260
7.244
7.241
7.226
7.220
7.216
7.199
7.132
7.119
5.032
5.013
4.994
3.245
3.225
3.201
3.191
3.182
3.173
3.148
3.129
-2.141



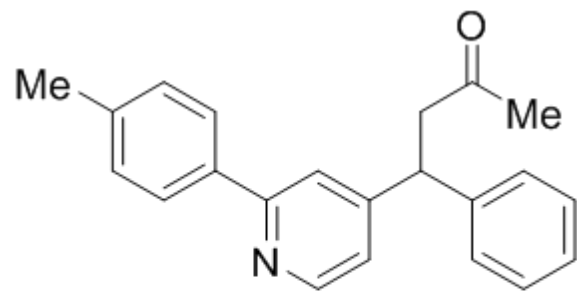
ty-3-54-3 C13 CDCl3 101 M Hz



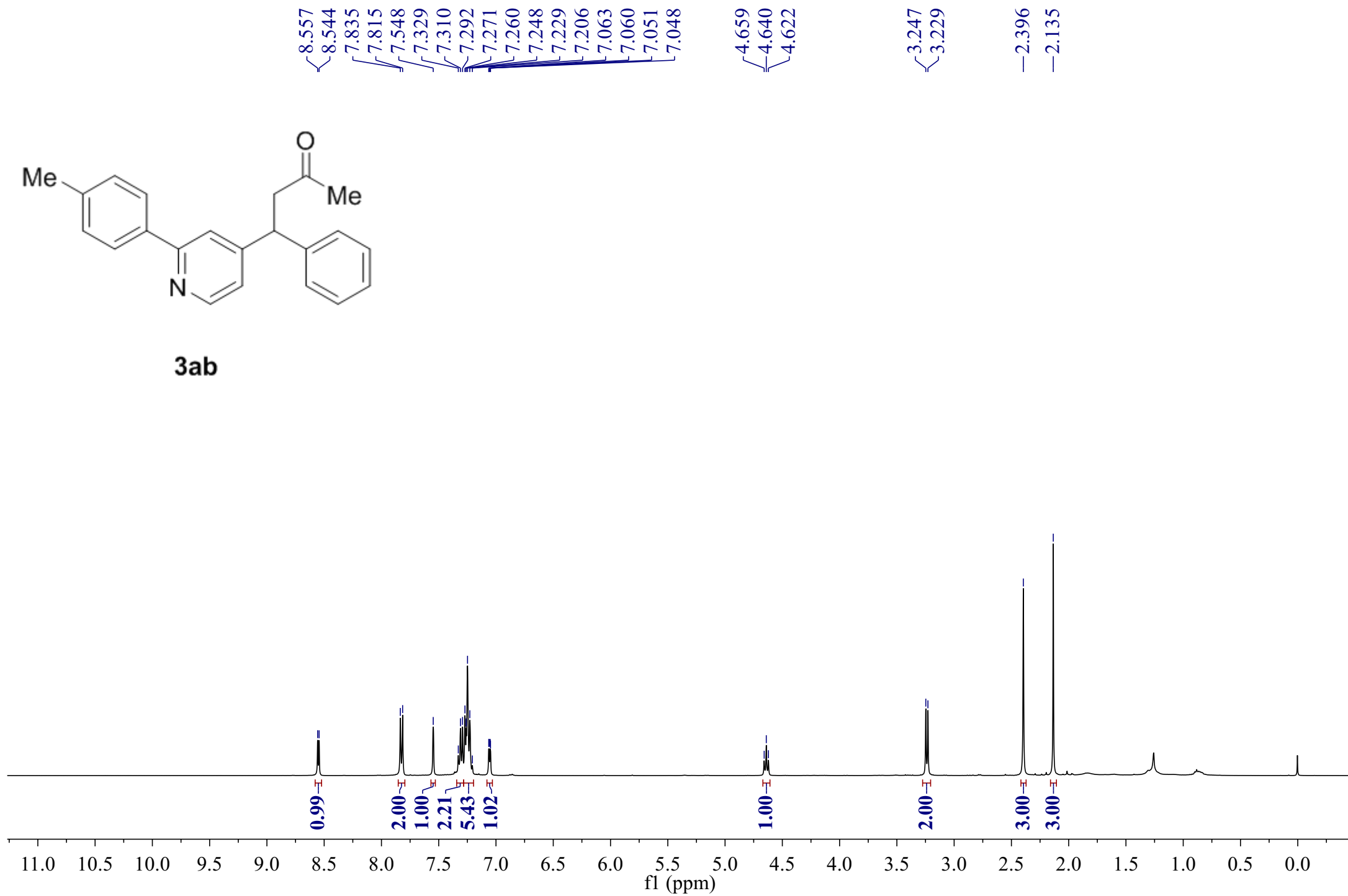
3aa



ty-4-41 H1 CDCl3 400 M Hz

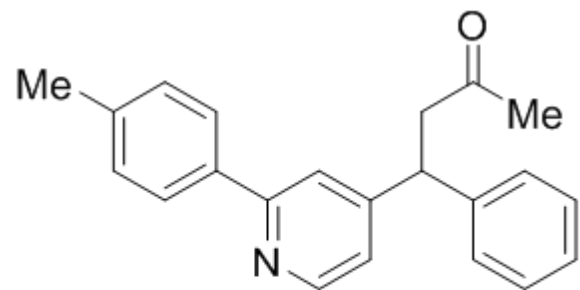


3ab

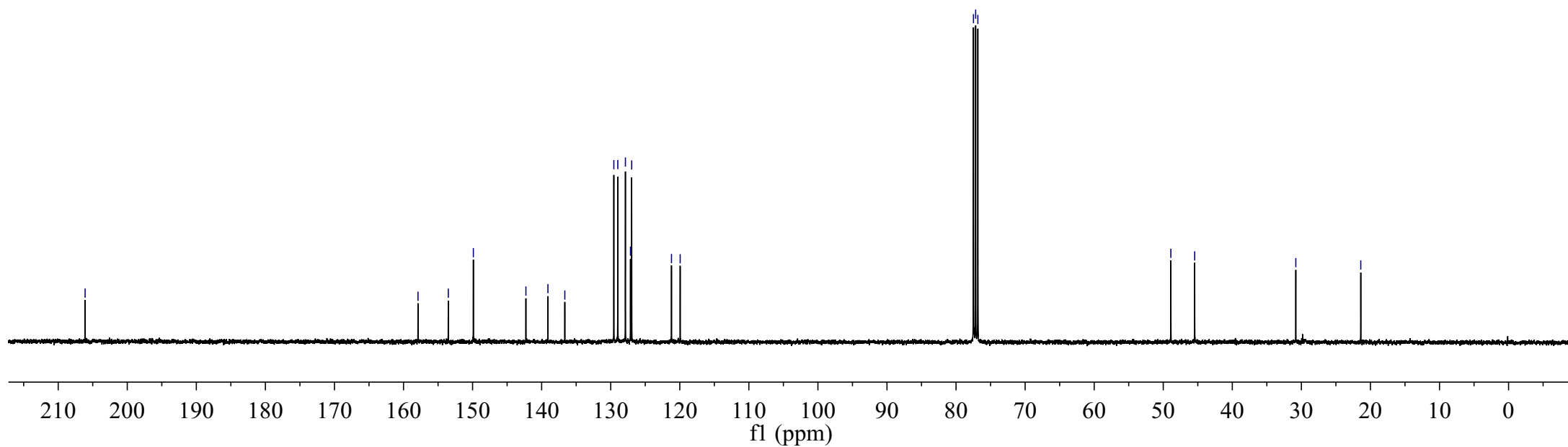


ty-4-41 C13 CDCl3 101 M Hz

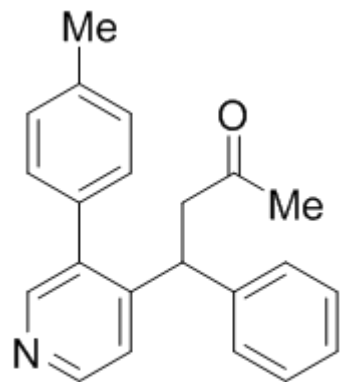
206.10
157.91
153.52
149.89
142.28
139.09
136.64
129.55
128.98
127.87
127.14
126.96
121.20
119.94
77.48
77.16
76.84
48.90
45.45
30.80
21.40



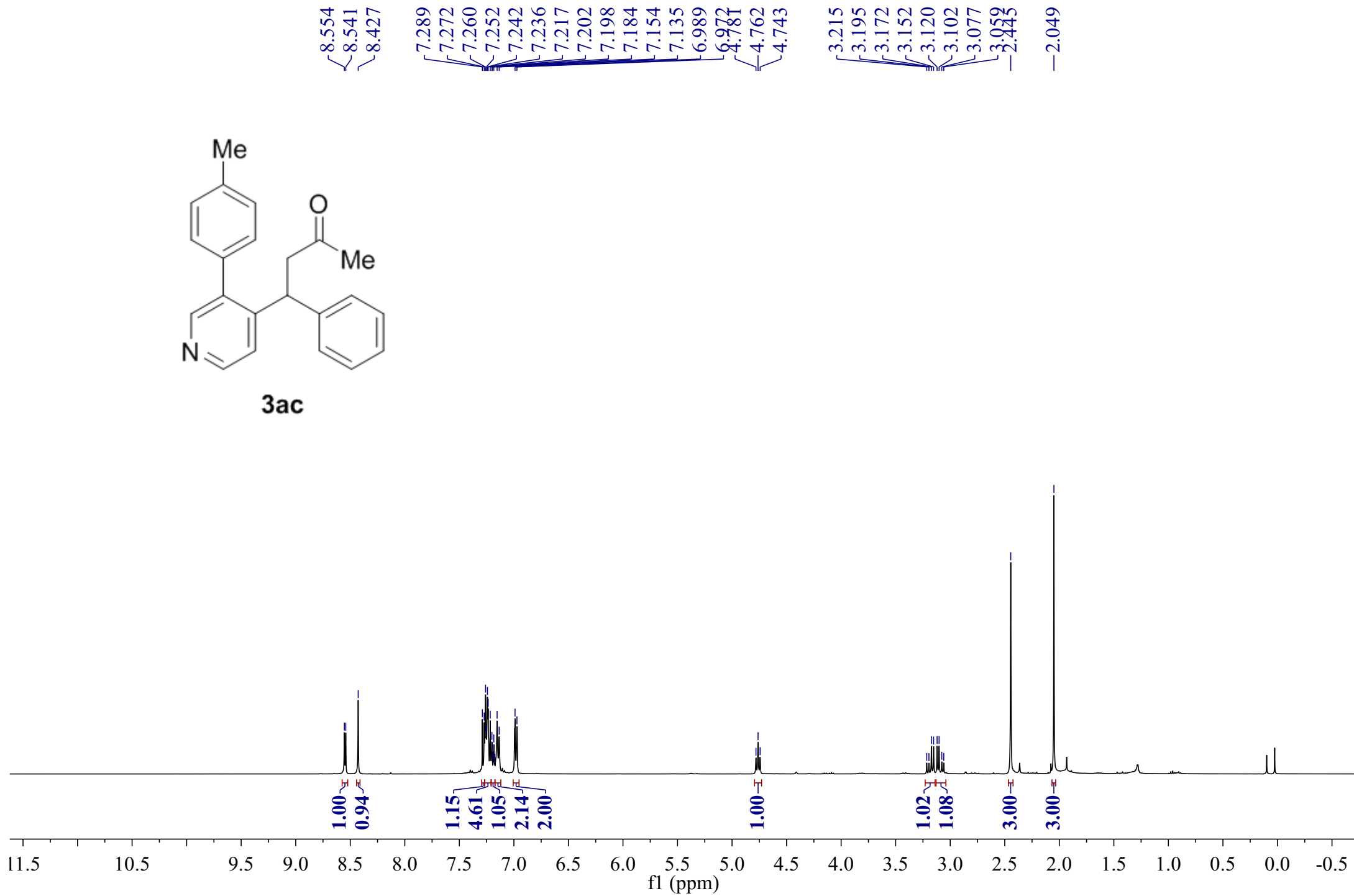
3ab



ty-4-38 H1 CDCl3 400 M Hz



3ac



ty-4-38 C13 CDCl3 101 M Hz

—205.94

150.94
149.93
148.75
142.14
137.95
137.70
134.51
129.54
129.18
128.71
127.78
126.82
121.42

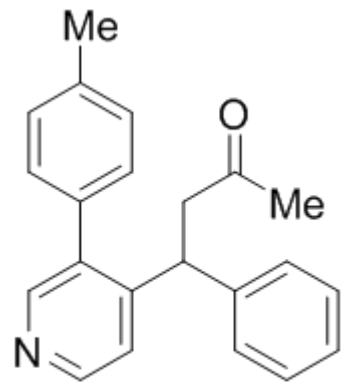
77.48
77.16
76.84

—49.53

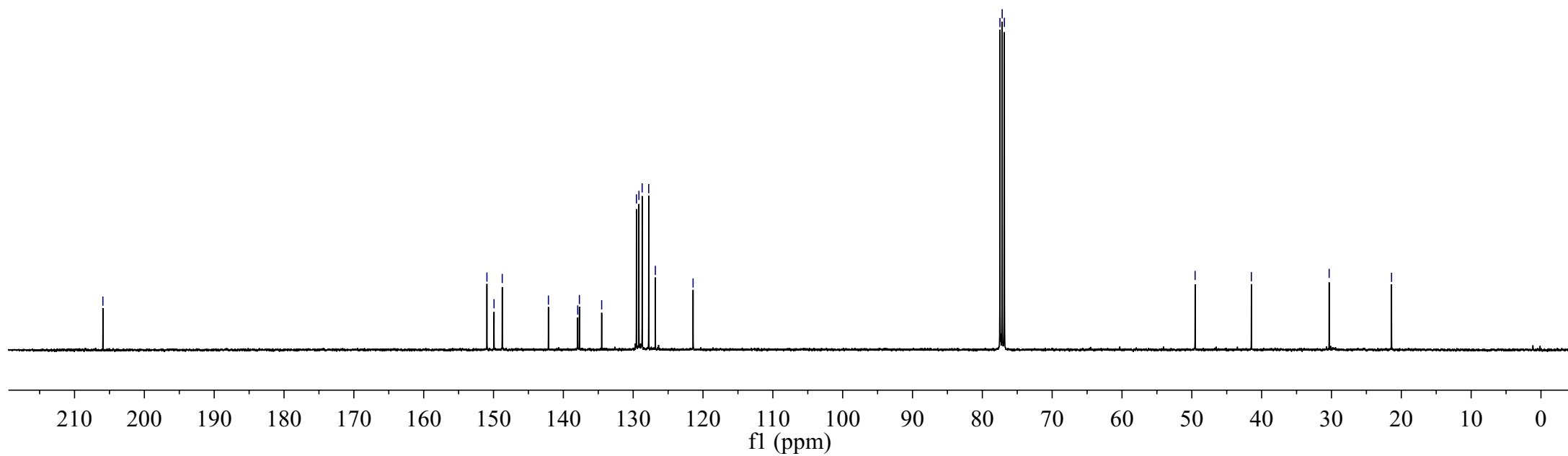
—41.47

—30.33

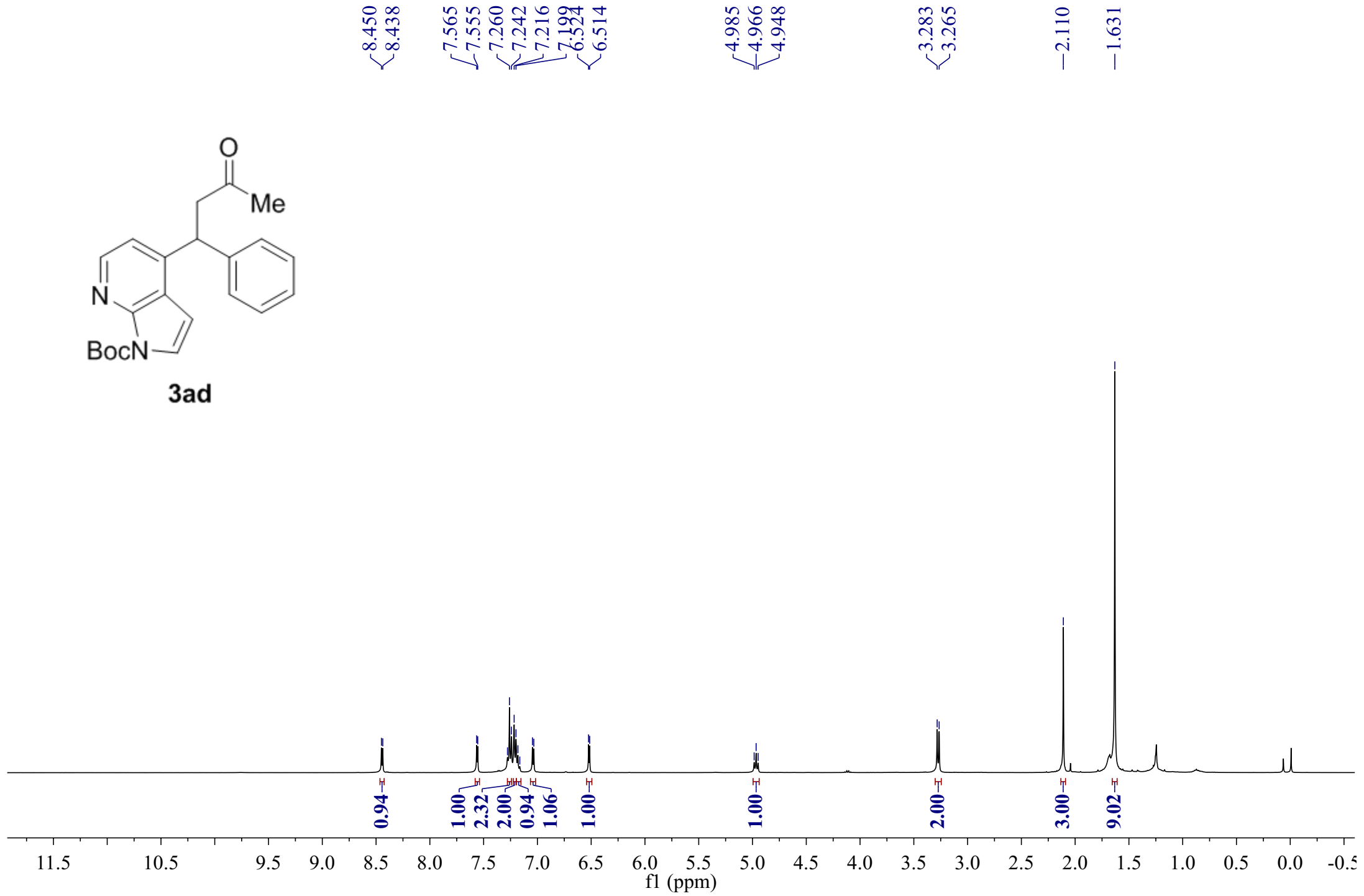
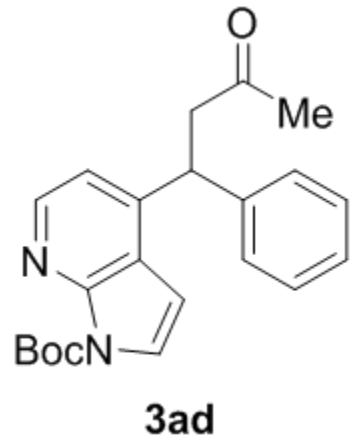
—21.40



3ac



ty-4-42 H1 CDCl3 400 M Hz



ty-4-42 C13 CDCI3 101 M Hz

—206.22

148.63

147.91

145.56

145.50

142.19

128.86

127.84

127.02

126.34

122.30

116.35

—103.11

84.12

77.48

77.16

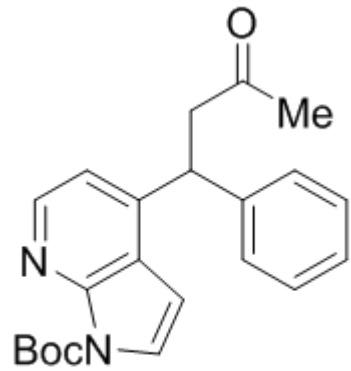
76.84

—48.61

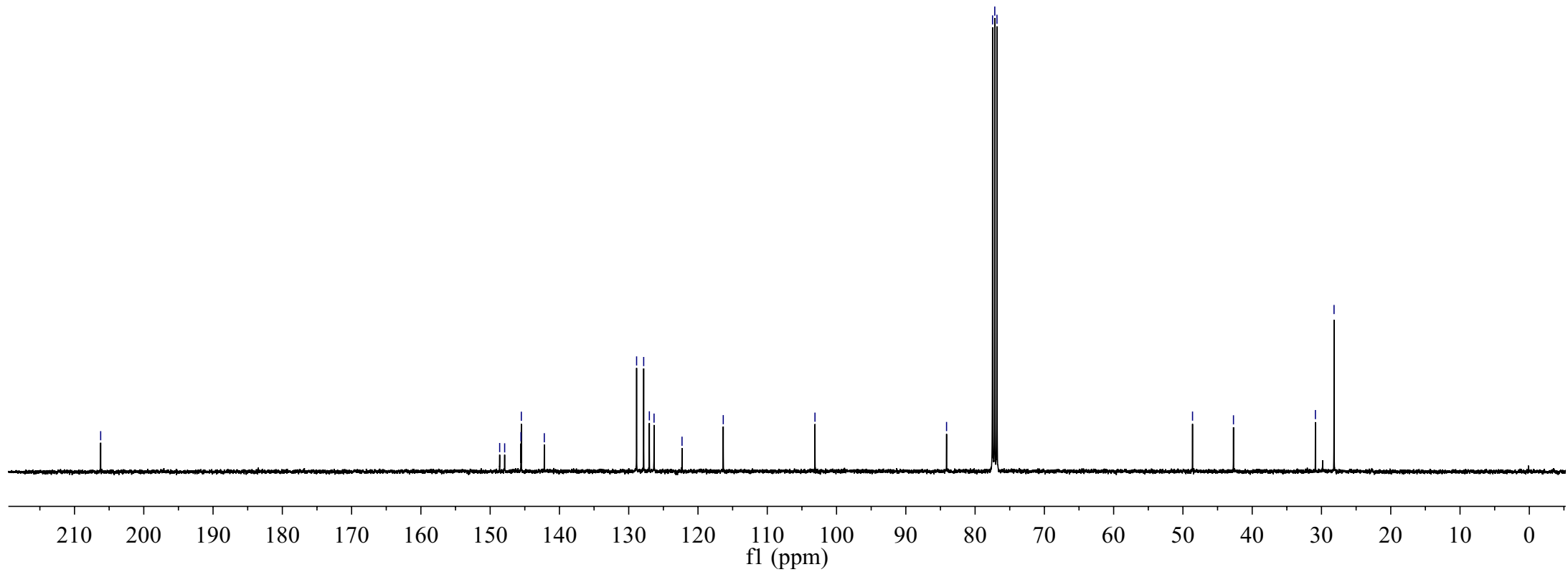
—42.70

~30.88

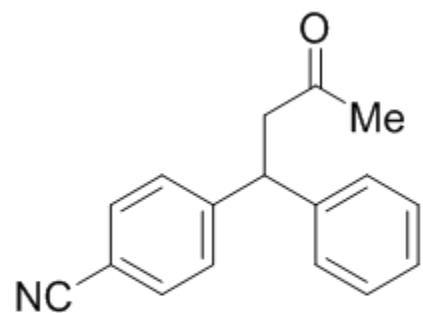
~28.19



3ad



ty-3-48 H1 CDCl3 400 M Hz



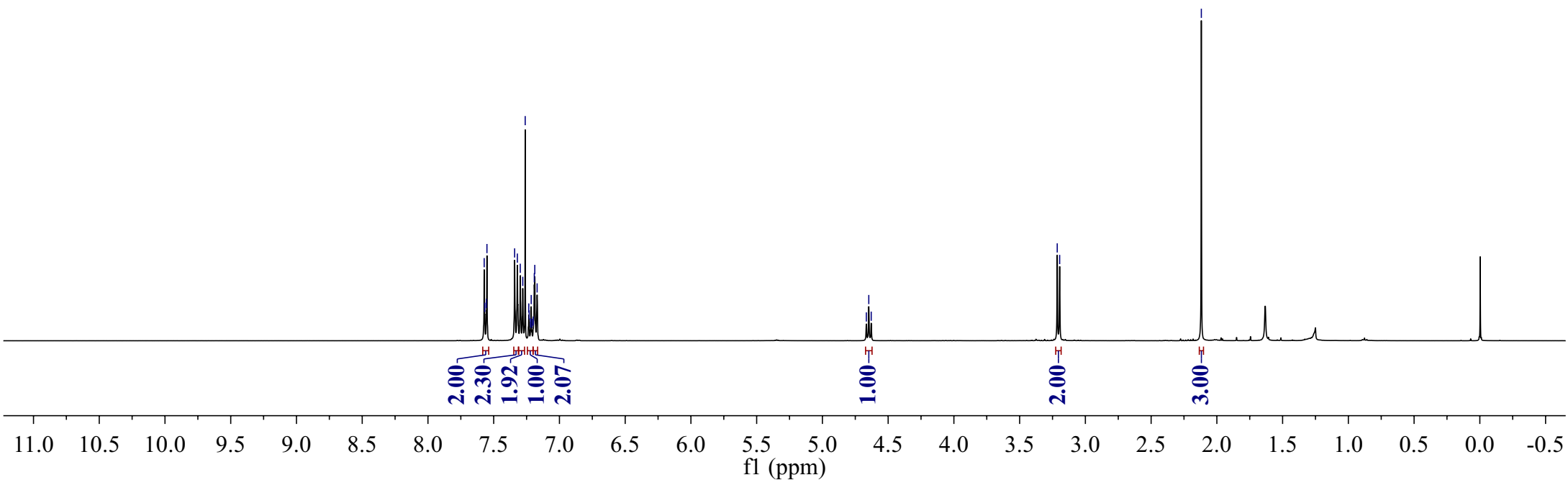
3ae

7.572
7.568
7.556
7.551
7.341
7.320
7.298
7.279
7.260
7.233
7.230
7.220
7.215
7.209
7.199
7.191
7.187
7.170

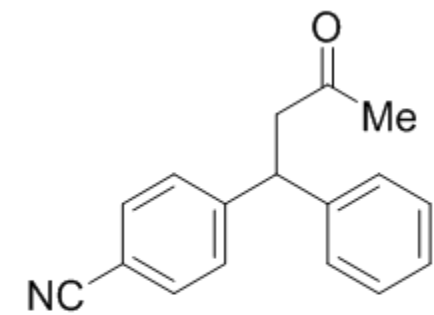
4.666
4.647
4.629

3.214
3.196

-2.118

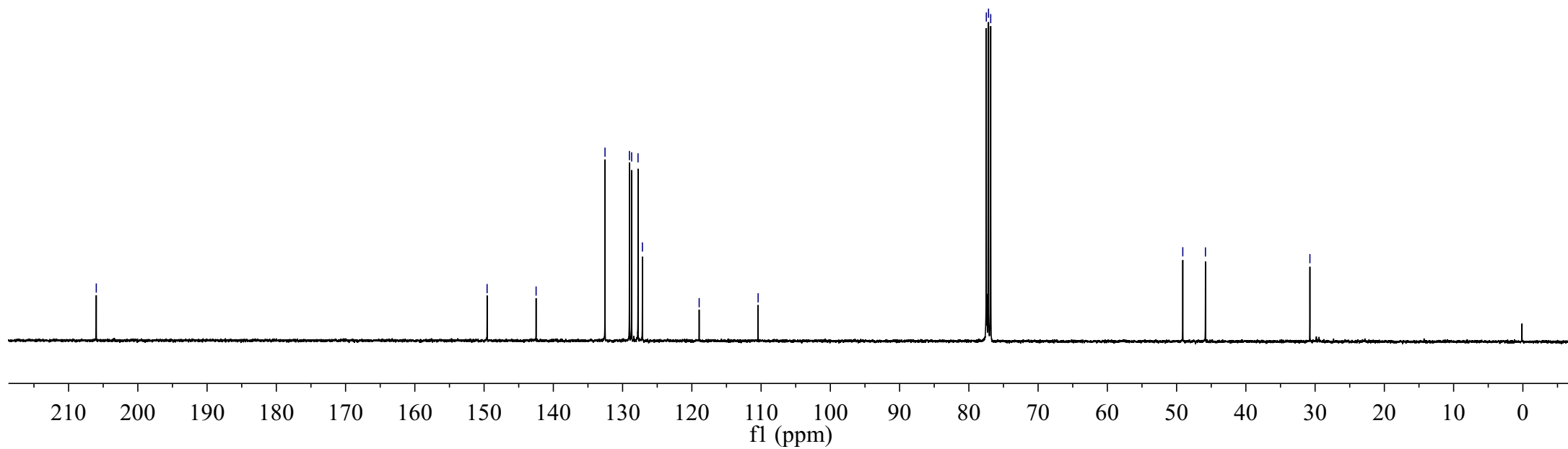


ty-3-48 C13 CDCl3 101 M Hz

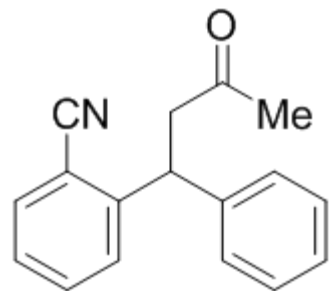


3ae

—206.00
—149.57
—142.49
132.54
129.01
128.69
127.77
127.14
—118.94
—110.43
77.48
77.16
76.84
—49.11
—45.84
—30.75

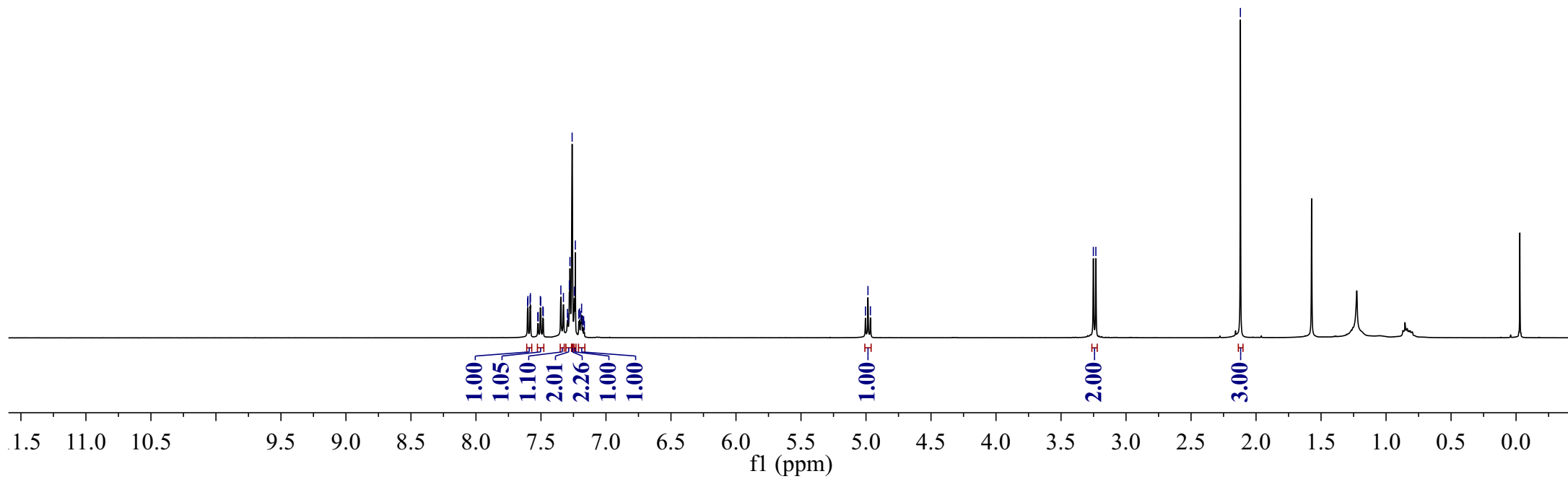


ty-3-54-7 H1 CDCl3 400 M Hz



3af

7.603
7.600
7.584
7.581
7.524
7.521
7.505
7.502
7.486
7.483
7.347
7.327
7.296
7.292
7.282
7.277
7.260
7.243
7.236
7.209
7.204
7.194
7.187
7.179
7.172
7.166
5.004
4.985
4.966
3.251
3.232
-2.120



ty-3-54-7 C13 CDCl3 101 M Hz

—205.61

—147.45

—141.56

133.61

133.13

128.95

127.93

128.77

—112.79

77.48

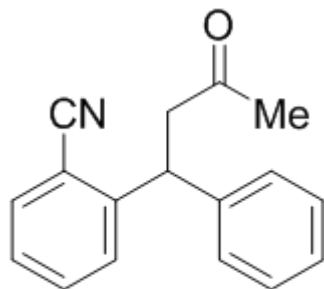
77.16

76.84

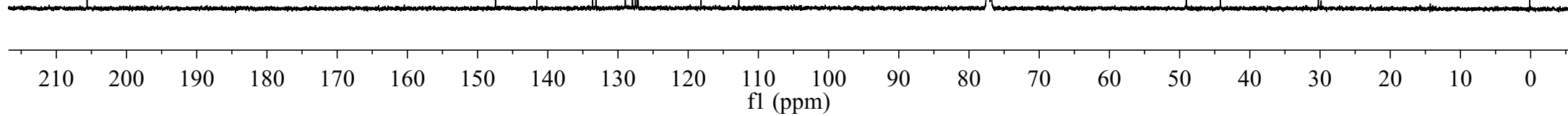
—49.05

—44.19

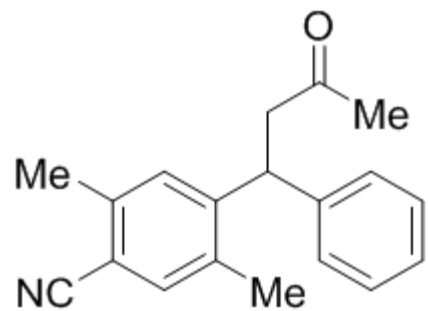
—30.24



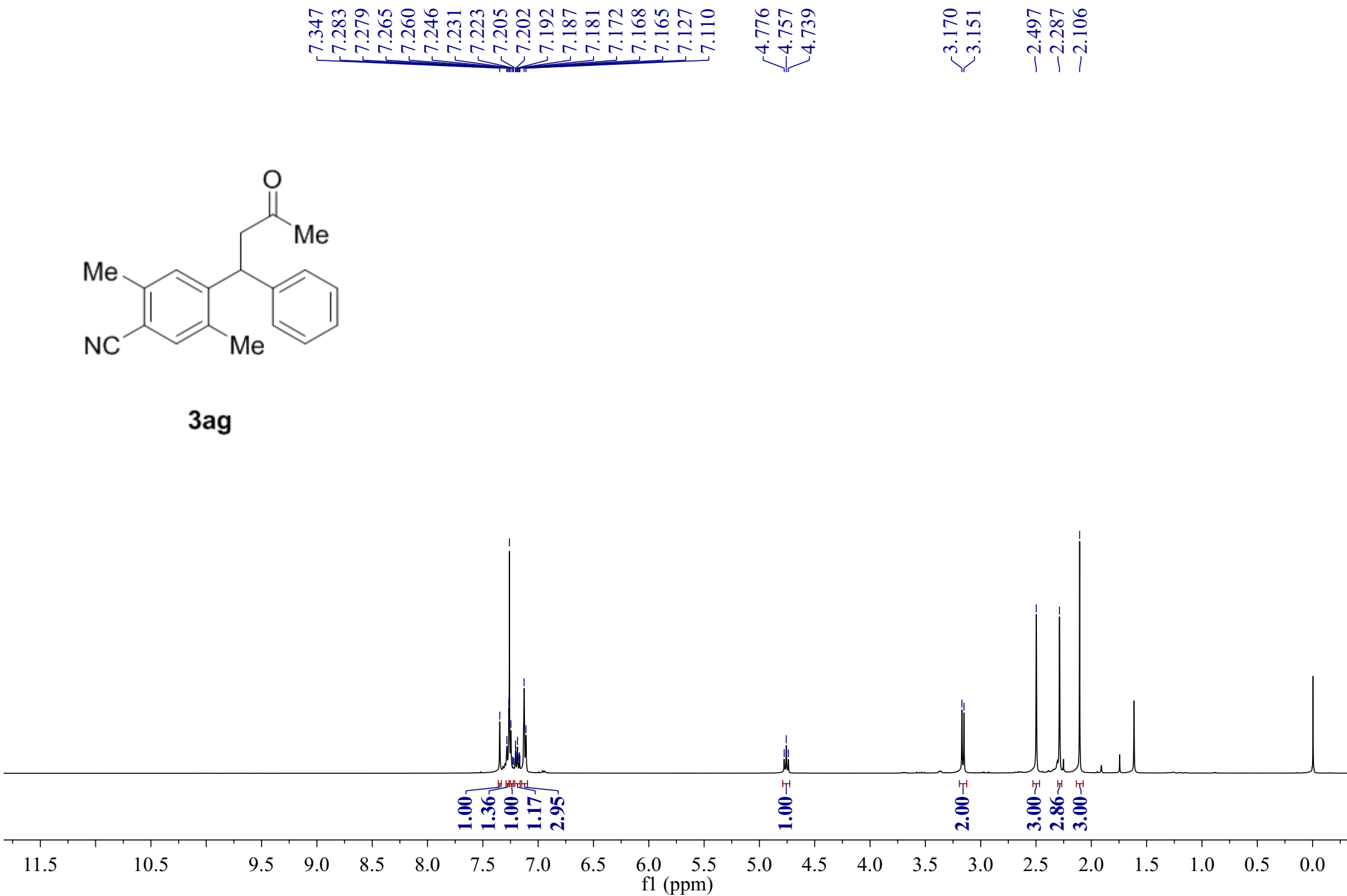
3af



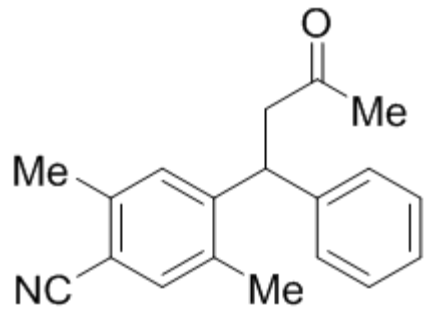
ty-3-54-5 H1 CDCl3 400 M Hz



3ag



ty-3-54-5 C13 CDCI3 101 M Hz



3ag

—206.23

147.17

142.20

139.56

135.05

134.46

128.87

128.22

127.96

126.89

—118.41

—110.70

77.48

77.16

76.84

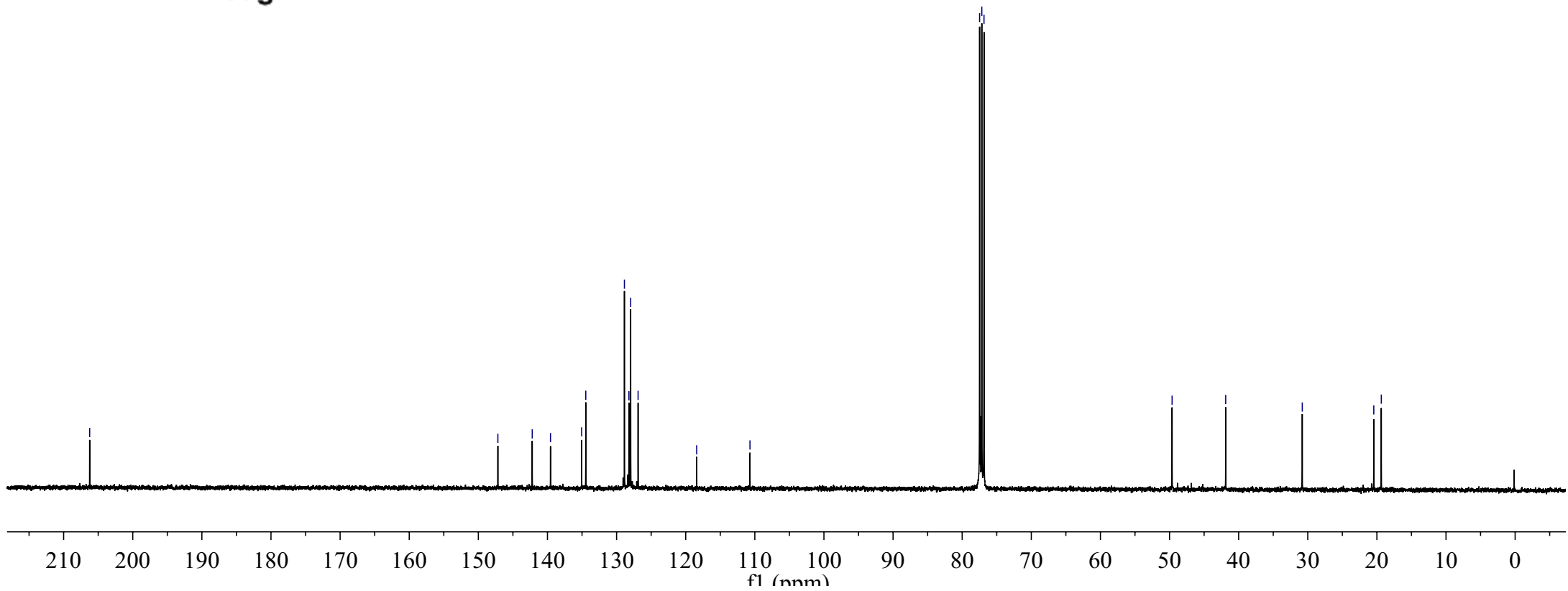
—49.63

—41.87

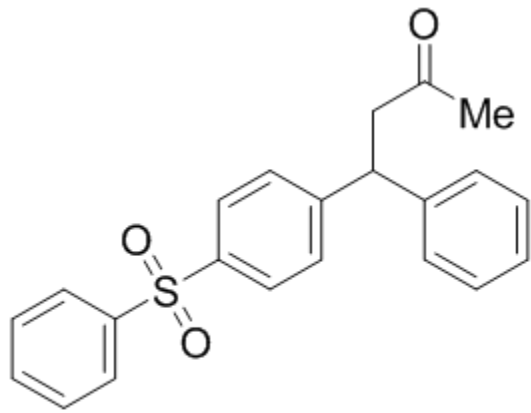
—30.80

20.45

19.36

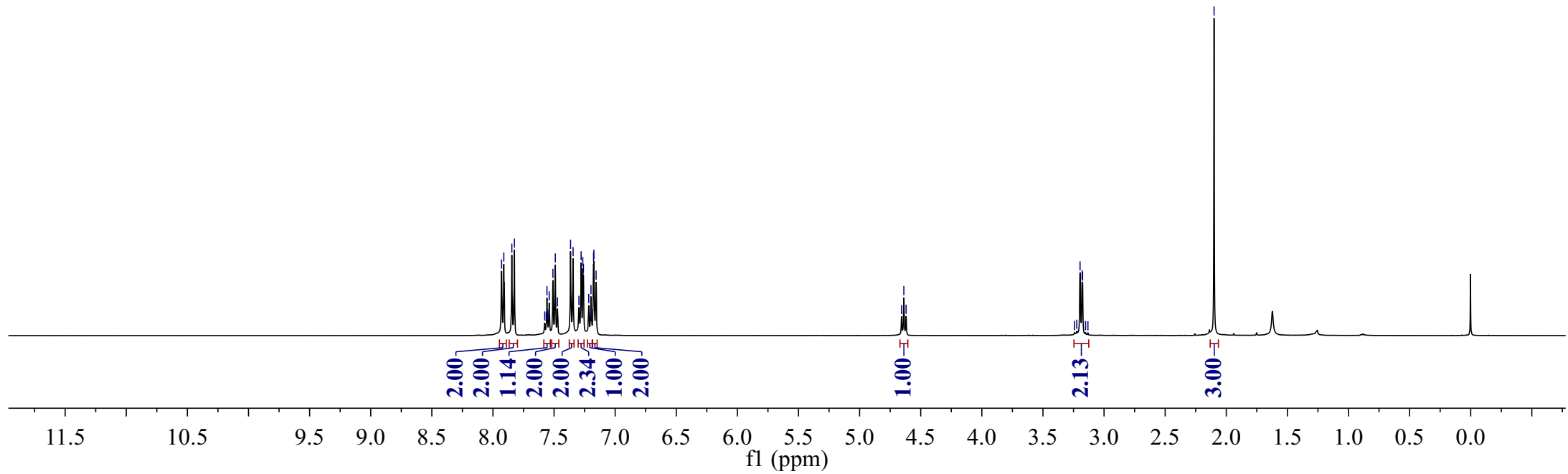


ty-3-54-6 H1 CDCl3 400 M Hz

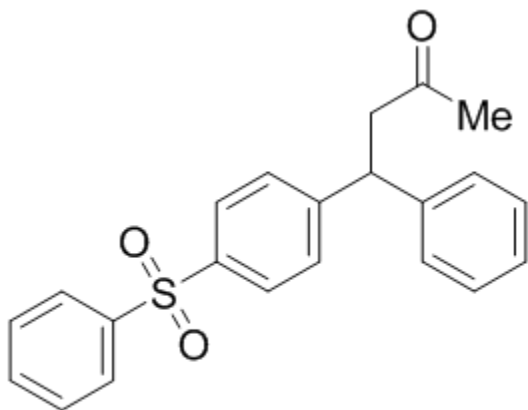


3ah

7.929
7.911
7.845
7.825
7.576
7.564
7.558
7.553
7.540
7.509
7.490
7.472
7.365
7.344
7.296
7.279
7.265
7.260
7.216
7.198
7.193
7.177
7.174
7.156
4.656
4.638
4.620
3.241
3.223
3.196
3.179
3.176
3.151
3.132
-2.100



ty-3-54-6 C13 CDCl3 101 M Hz



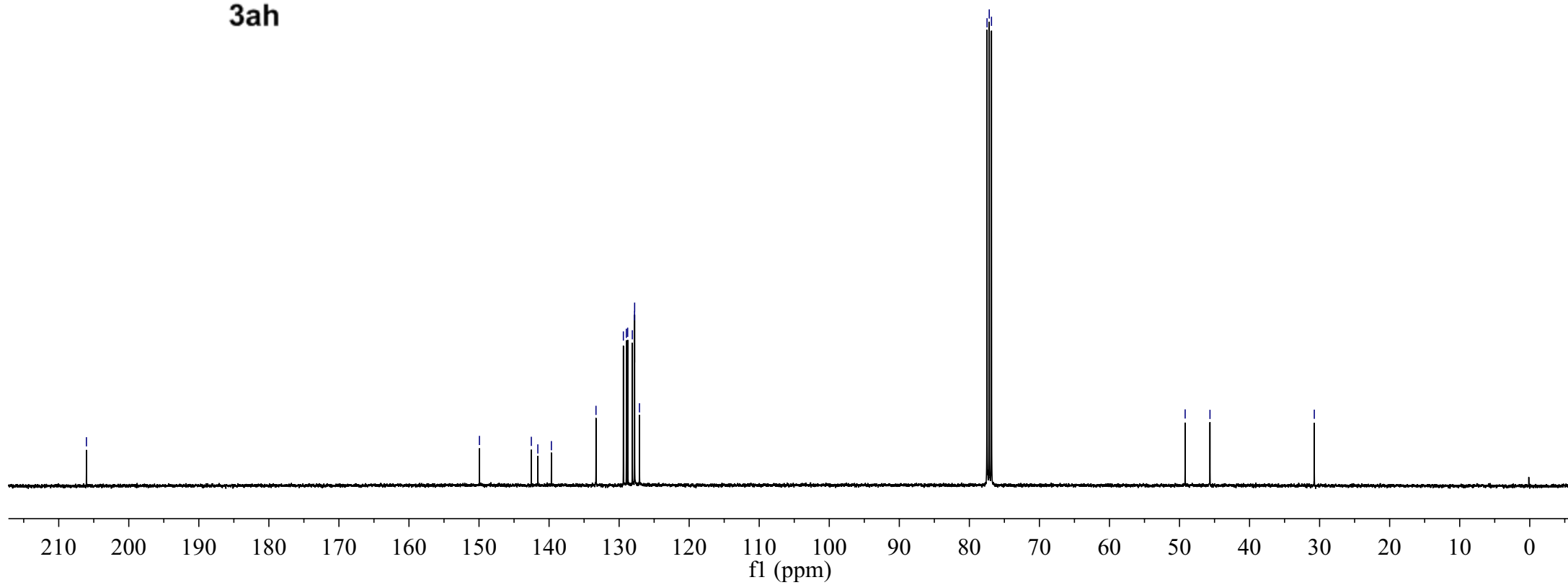
3ah

206.05
149.94
142.53
141.60
139.67
133.30
129.39
128.97
128.78
128.11
127.80
127.78
127.09

77.48
77.16
76.84

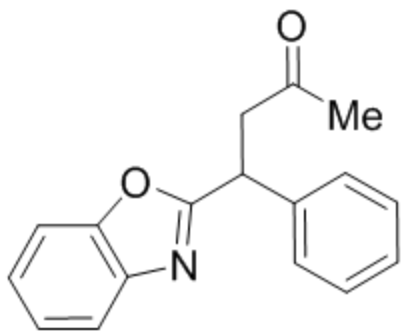
49.19
45.65

30.76

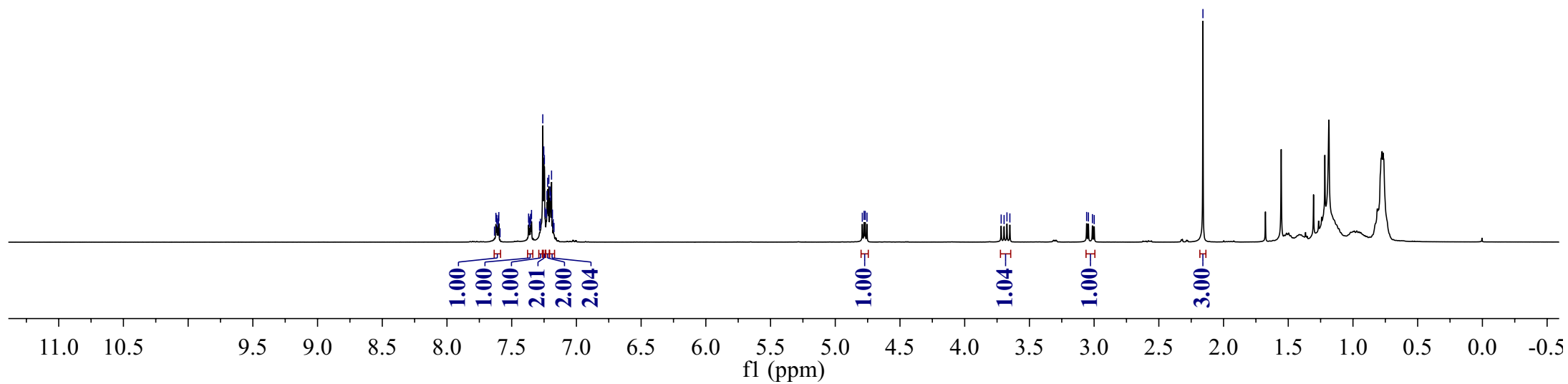


ty-4-89 H1 CDCl3 400 M Hz

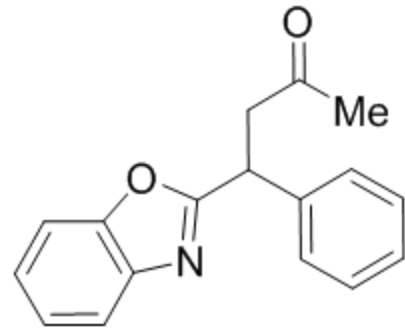
7.633
7.622
7.616
7.609
7.603
7.600
7.590
7.370
7.366
7.360
7.354
7.352
7.347
7.285
7.278
7.260
7.252
7.247
7.241
7.232
7.227
7.222
7.213
7.204
7.199
7.192
7.185
7.179
7.173
4.791
4.777
4.769
4.755
3.718
3.696
3.673
3.651
3.058
3.044
3.013
2.999
-2.159



3ai



ty-4-89 C13 CDCI3 101 M Hz



3ai

—205.75 —167.47 —151.08 —141.14 —139.22 —129.11 —127.98 —127.75 —124.89 —124.29 —119.89 —110.77 —77.48 —77.16 —76.84 —48.02 —40.60 —30.47

