Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic Supplementary Information

for

Synthesis of α-Functionalized α-Indol-3-yl Carbonyls through Direct S_N Reactions of Indol-3-yl α-Acyloins

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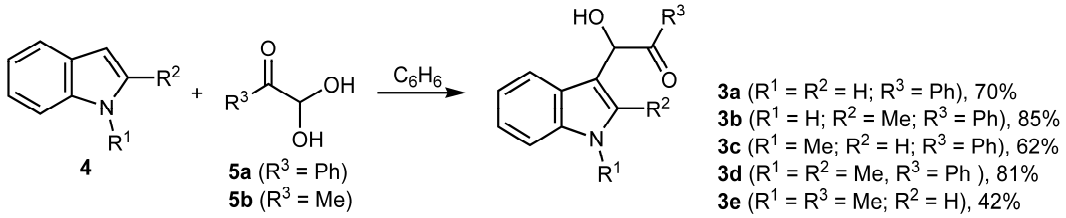
General considerations:

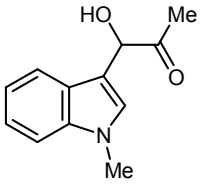
All reactions involving air sensitive compounds were carried out under a N_2 atmosphere (99.99%). All glassware was oven-dried (120 °C), evacuated and purged with nitrogen. All common reagents and solvents were obtained from commercial suppliers and used without any further purification. Solvents were dried by standard methods. Hexane and ethyl acetate were purchased as extra pure grade reagents and used as received. TLC was performed on aluminum-backed plates coated with silica gel 60 with F_{254} indicator; the chromatograms were visualized under ultraviolet light and/or by staining with a Ce/Mo reagent and subsequent heating. R_f values are reported on silica gel. Flash column chromatography was carried out on silica gel 60, 230-240 mesh. Deactivated silica gel was obtained by stirring with an aqueous K_2HPO_4 solution for 3 h and subsequent filtration and drying at 140 ºC for 3 days. ^{1}H NMR spectra were recorded at 300 or 400 MHz. Chemical shifts are reported in ppm using the residual solvent peak as reference. Data are reported as follows: chemical shift, multiplicity (s: singlet, bs: broad singlet, d: doublet, t: triplet, at: apparent triplet, dd: doublet of doublets, dt: doublet of triplets, ddd: doublet of doublet of doublets, m: multiplet), coupling constant (*J* in Hz), and integration. ^{13}C NMR spectra were recorded at 75.4 MHz or 100.6 MHz using broadband proton decoupling and chemical shifts are reported in ppm using residual solvent peaks as reference and the multiplicities were determined by DEPT experiments. High resolution mass spectra (HRMS) were recorded on a Micromass Autospec spectrometer equipped with a magnetic sector ion analyzer using EI at 70eV. Melting points were measured on a Gallenkamp apparatous using open capillary tubes and are uncorrected. GC-MS and low resolution mass spectra (LRMS) measurements were recorded on an Agilent 6890N/5973 Network GC System, equipped with a HP-5MS column.

Synthesis of α-acyloins 3:



Acyloins **3a-d** were prepared by reaction of phenyl glyoxal (5 mmol) with the corresponding indole (5 mmol) in benzene following a reported procedure.[1] Acyloin **3e** was prepared in the same way from pyruvic aldehyde (**5b**) (1.5 mL of a 40% w/w aqueous solution, 10 mmol) and *N*-methylindole (**4c**) (1.31 g, 10 mmol) in benzene (20 mL) at r.t .for 16 h. Characterization data for acyloins **3a-d** have been previously reported.[1,2]

Spectroscopic and characterization data for new α-acyloin 3e:



1-Hydroxy-1-(1-methyl-1*H*-indol-3-yl)propan-2-one (3e): White foam; yield = 42% (0.85 g); R_f = 0.20 (hexane/EtOAc, 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.08 (s, 3H), 3.67 (s, 3H), 4.40 (bs, 1H), 5.35 (s, 1H), 7.07 (s, 1H), 7.12–7.20 (m, 1H), 7.22–7.36 (m, 2H), 7.52–7.60 (m, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 25.0 (CH_3), 32.5 (CH_3), 73.2 (CH), 109.5 (CH), 110.9 (C), 118.9 (CH), 119.6 (CH), 122.9 (CH), 125.6 (C), 128.6 (CH), 137.1 (C), 208.2 (C); LRMS (70 eV, EI): *m/z* (%) 203 (M^+, 13), 158 (100); HRMS (EI^+) calcd for $C_{12}H_{13}NO_2$: 203.0946, found: 203.0945.

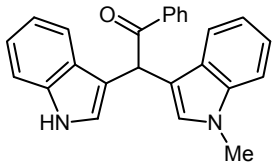
General procedure for the synthesis of α-(indol-3-yl) carbonyl compounds 6-9:

PTSA (5 mol%, 9 mg) was added to a solution of the corresponding α-acyloin **3** (1 mmol) and nucleophile (1 mmol for the synthesis of **6-8**, 1.1 mmol of *p*-nitroaniline for the synthesis of **9**) in MeCN (2 mL). The resulting reaction mixture was stirred until the final product precipitates or the starting acyloin was consumed as determined by TLC (0.25–16 h). In the first case, the precipitated product was isolated in pure form by simple filtration, whereas in the last case, the crude mixture was quenched with aqueous NaOH (0.5 M) and extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated at reduced

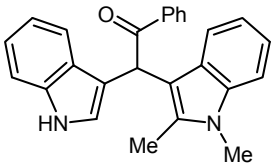
[1] S. P. Ivonin, A. V. Lapandin, A. A. Anishchenko, V. G. Shtamburg, *Synth. Commun.,* 2004, **34**, 451.
[2] L. Guanghui, C. Xu, Z. Yang, L. Weijian, H. Li, W. Yong, *Chem. Res. Chin. Univ.,* 2016, **32**, 212.

pressure. The residue was purified by flash chromatography on silica gel (deactivated in the case of **7f,g**) using mixtures of hexane and EtOAc as eluents to obtain the corresponding α-(indol-3-yl) carbonyl compounds derivatives **6-9** in the yields reported in Tables 1-2 or Schemes 3-4.

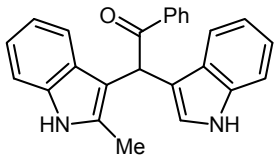
Spectroscopic and characterization data for compounds 6–9:



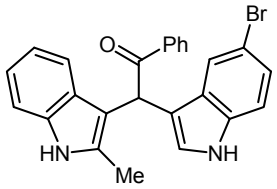
2-(1*H*-Indol-3-yl)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (6ac): Brown solid; yield = 92% (335 mg); mp = 204–206 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 3.71 (s, 3H), 6.57 (s, 1H), 6.89 (s, 1H), 6.96–7.02 (m, 1H), 7.09–7.17 (m, 2H), 7.19–7.24 (m, 1H), 7.25–7.28 (m, 1H), 7.28–7.33 (m, 1H), 7.34–7.39 (m, 1H), 7.42–7.48 (m, 2H), 7.52–7.57 (m, 1H), 7.59–7.64 (m, 2H), 8.12 (s, 1H), 8.14–8.20 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 32.9 (CH_3), 42.0, (CH), 109.5 (CH), 111.4 (CH), 112.7 (C), 114.6 (C), 119.14 (CH), 119.29 (CH), 119.3 (CH), 119.8 (CH), 121.9 (CH), 122.3 (CH), 124.0 (CH), 126.7 (C), 127.2 (C), 128.7, (2 × CH), 128.9 (2 × CH), 133.0 (CH), 136.6 (C), 137.1 (C), 137.4 (C), 198.8 (C) one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 364 (M^+, 3), 259 (100); HRMS (EI^+) calcd for $C_{25}H_{20}N_2O$: 364.1576, found: 364.1577.



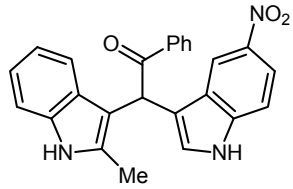
2-(1,2-Dimethyl-1*H*-indol-3-yl)-2-(1*H*-indol-3-yl)-1-phenylethanone (6ad): Violet solid; yield = 86% (325 mg); mp = 105–107 ºC; ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ (ppm) = 2.40 (s, 3H), 3.63 (s, 3H), 6.43 (d, *J* = 1.1 Hz, 1H), 6.85 (dd, *J* = 2.5, 1.1 Hz, 1H), 7.00–7.10 (m, 2H), 7.12–7.19 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.28–7.43 (m, 4H), 7.44–7.51 (m, 1H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.97 (s, 1H), 8.04–8.10 (m, 2H); ^{13}C NMR (75.4 MHz, $(CD_3)_2CO$): δ (ppm) = 11.0 (CH_3), 29.7 (CH_3), 42.6 (CH), 107.5 (C), 108.8 (CH), 111.4 (CH), 114.8 (C), 119.05 (CH), 119.1 (CH), 119.4 (CH), 119.6 (CH), 120.8 (CH), 122.1 (CH), 127.1 (C), 127.3 (C), 128.6 (2 × CH), 128.7 (2 × CH), 132.7 (CH), 134.6 (C), 136.6 (C), 136.9 (C), 137.4 (C), 198.1 (C); LRMS (70 eV, EI): *m/z* (%) 378 (M^+, 3), 273 (100); HRMS (EI^+) calcd for $C_{26}H_{22}N_2O$: 378.1732, found: 378.1730.



2-(1*H*-Indol-3-yl)-2-(2-methyl-1*H*-indol-3-yl)-1-phenylethanone (6ba)*:* Yellow solid; yield = 99% (361 mg); mp = 220–222 ºC; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 2.24 (s, 3H), 6.38 (s, 1H), 6.71 (s, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 7.05–7.19 (m, 3H), 7.21–7.24 (m, 1H), 7.33–7.41 (m, 4H), 7.44–7.50 (m, 1H), 7.60–7.65 (m, 1H), 7.83 (s, 1H), 7.95 (s, 1H), 8.04–8.09 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.4 (CH_3), 42.4 (CH), 108.2 (C), 110.5 (CH), 111.5 (CH), 114.3 (C), 118.9 (CH), 119.0 (CH), 119.6 (CH), 119.7 (CH), 121.2 (C), 122.1 (CH), 124.3 (CH), 127.0 (C), 128.2 (C), 128.6 (2 × CH), 128.7 (2 × CH), 132.8 (CH), 132.9 (CH), 135.3 (C), 136.6 (C), 137.3 (C), 198.4 (C); LRMS (70 eV, EI): *m/z* (%) 364 (M^+, 2), 259 (100); HRMS (EI^+) calcd for $C_{25}H_{20}N_2O$: 364.1576, found: 364.1581.

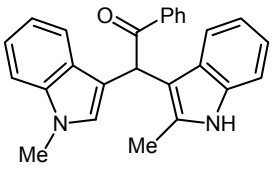


2-(5-Bromo-1*H*-indol-3-yl)-2-(2-methyl-1*H*-indol-3-yl)-1-phenylethanone (6be): White solid; yield = 93% (412 mg); mp = 152–154 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.30 (s, 3H), 6.28 (s, 1H), 6.65 (s, 1H), 7.00–7.12 (m, 3H), 7.14–7.27 (m, 2H), 7.33–7.40 (m, 2H), 7.44–7.52 (m, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.91 (s, 1H), 8.02–8.10 (m, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.4 (CH_3), 42.3 (CH), 108.0 (C), 110.5 (CH), 112.9 (CH), 113.0 (CH), 114.0 (C), 118.9 (CH), 119.8 (CH), 121.4 (CH), 121.5 (CH), 124.9 (CH), 125.7 (CH), 127.9 (C), 128.7 (4 × CH), 132.7 (C), 133.0 (C), 135.26 (C), 135.35 (C), 136.9 (C), 198.1 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 444 [$(M+2)^+$, 3], 442 (M^+, 2); 339 (99) 337 (100); HRMS (EI^+) calcd for $C_{18}H_{14}BrN_2$ $(M–C_7H_5O)^+$: 337.0340, found, 337.0339.

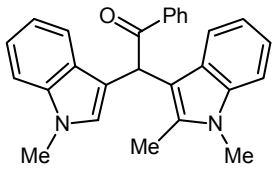


2-(2-Methyl-1*H*-indol-3-yl)-2-(5-nitro-1*H*-indol-3-yl)-1-phenylethanone (6bf): Yellow solid; yield = 91% (373 mg); mp = 145–147 °C; ^{1}H NMR (300 MHz, $(CD_3)_2SO$): δ (ppm) = 2.40 (s, 3H), 6.69 (s, 1H), 6.85–6.98 (m, 2H), 7.10 (s, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.42 (at, *J* = 7.4 Hz, 2H), 7.46–7.56 (m, 3H), 7.97 (dd, *J* = 9.0, 1.0 Hz, 1H), 8.07 (d, *J* = 8.1 Hz, 2H), 8.42 (s, 1H), 10.98 (s, 1H), 11.57 (s, 1H); ^{13}C NMR (75.4 MHz, $(CD_3)_2SO$): δ (ppm) = 11.9 (CH_3), 41.5 (CH), 106.8 (C), 110.7 (CH), 112.0 (CH), 116.5 (CH), 116.6 (CH), 116.7 (C), 118.3 (CH), 118.7 (CH), 120.3 (CH), 126.3 (C), 127.3 (C), 128.2 (CH), 128.4 (2 × CH), 128.6 (2 × CH), 132.8 (CH), 133.4 (C), 135.4 (C), 136.8 (C),

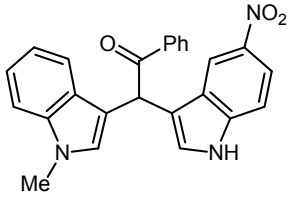
139.7 (C), 140.2 (C), 198.0 (C); LRMS (70 eV, EI): *m/z* (%) 409 (M^+, 2), 304 (100); HRMS (EI^+) calcd for $C_{25}H_{19}N_3O_3$: 409.1426, found: 409.1429.



2-(1-Methyl-1*H*-indol-3-yl)-2-(2-methyl-1*H*-indol-3-yl)-1-phenylethanone (6cb): Yellow solid; yield = 90% (340 mg); mp = 201–203 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.40 (s, 3H), 3.69 (s, 3H), 6.44 (s, 1H), 6.80 (s, 1H), 7.05–7.19 (m, 3H), 7.21–7.47 (m, 3H), 7.48–7.55 (m, 3H), 7.48–7.58 (m, 1H), 7.66–7.73 (m, 1H), 7.92 (s, 1H), 8.09–8.16 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ (ppm) = 12.4 (CH_3), 32.8 (CH_3), 42.3 (CH), 108.3 (C), 109.5 (CH), 110.4 (CH), 112.8 (C), 118.9 (CH), 119.1 (CH), 119.7 (CH), 121.2 (CH), 121.7 (CH), 127.4 (CH), 128.1 (CH), 128.6 (2 × CH), 128.7 (2 × CH), 128.8 (CH), 132.75 (C), 132.77 (C), 135.3 (C), 137.2 (C), 137.4 (C), 198.3 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 378 (M^+, 4), 260 (100); HRMS (EI^+) calcd for $C_{26}H_{22}N_2O$: 378.1732, found: 378.1733.

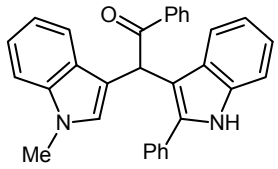


2-(1,2-Dimethyl-1*H*-indol-3-yl)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (6cd): Yellow solid; yield = 98% (384 mg); mp = 197–199 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 2.42 (s, 3H), 3.64 (s, 3H), 3.67 (s, 3H), 6.43 (s, 1H), 6.77 (s, 1H), 7.01–7.10 (m, 2H), 7.12–7.30 (m, 4H), 7.34–7.42 (m, 3H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 8.05–8.09 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) = 11.0 (CH_3), 29.7 (CH_3), 32.9 (CH_3), 42.6 (CH), 107.7 (C), 108.8 (CH), 109.5 (CH), 113.2 (C), 119.07 (CH), 119.09 (CH), 119.2 (CH), 119.4 (CH), 120.8 (CH), 121.7 (CH), 127.2 (C), 127.5 (C), 128.6 (2 × CH), 128.7 (2 × CH), 128.9 (CH), 132.7 (CH), 134.5 (C), 136.9 (C), 137.4 (C), 198.1 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 392 (M^+, 3), 287 (100); HRMS (EI^+) calcd for $C_{27}H_{24}N_2O$: 392.1889, found: 392.1889.

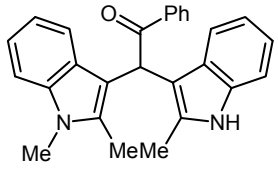


2-(1-Methyl-1*H*-indol-3-yl)-2-(5-nitro-1*H*-indol-3-yl)-1-phenylethanone (6cf): Yellow solid; yield = 90% (368 mg); mp = 170–172 °C; ^{1}H NMR (300 MHz, $(CD_3)_2SO$) δ (ppm) = 3.68 (s, 3H), 6.88 (s, 1H), 6.96–7.04 (m, 1H), 7.08–7.14 (m, 1H), 7.17 (s, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.44–7.60 (m,

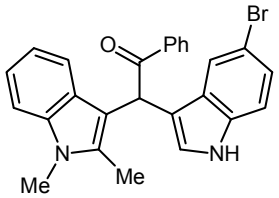
5H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.98 (dd, *J* = 9.0, 2.3 Hz, 1H), 8.18–8.26 (m, 2H), 8.63 (d, *J* = 2.2 Hz, 1H), 11.73 (s, 1H); ^{13}C NMR (75.4 MHz, $(CD_3)_2SO$) δ (ppm) = 32.4 (CH_3) 41.1 (CH), 109.9 (CH), 111.7 (C), 112.1 (CH), 116.1 (C), 116.6 (2 × CH), 118.9 (CH), 119.2 (CH), 121.4 (CH), 125.9 (C), 126.6 (C), 128.5 (CH), 128.6 (CH), 128.8 (2 × CH), 133.2 (CH), 136.2 (C), 136.8 (C), 139.6 (C), 140.4 (C), 197.8 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 409 (M^+, 3), 304 (100); HRMS (EI^+) calcd for $C_{25}H_{19}N_3O_3$: 409.1426, found: 409.1428.



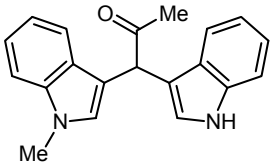
2-(1*H*-Indol-3-yl)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (6cg): White solid; yield = 95% (418 mg); mp = 240–242 °C; ^{1}H NMR (300 MHz, $(CD_3)_2SO$): δ (ppm) = 3.69 (s, 3H), 6.40 (s, 1H), 6.86 (s, 1H), 6.89–6.98 (m, 2H), 7.05 (at, *J* = 7.5 Hz, 1H), 7.10–7.18 (m, 2H), 7.24 (t, *J* = 7.3 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.39–7.51 (m, 8H), 7.61 (ad, *J* = 7.6 Hz, 2H), 11.54 (s, 1H); ^{13}C NMR (75.4 MHz, $(CD_3)_2SO$): δ (ppm) = 32.4 (CH_3), 42.6 (CH), 107.7 (C), 109.8 (CH), 111.5 (CH), 112.6 (C), 118.7 (2 × CH), 119.2 (CH), 120.3 (CH), 121.2 (CH), 121.5 (CH), 126.8 (CH), 127.4 (CH), 127.9 (2 × CH), 128.2 (2 × CH), 128.5 (2 × CH), 129.0 (2 × CH), 132.3 (C), 132.8 (C), 136.0 (C), 136.2 (C), 136.3 (C), 136.9 (C), 196.8 (C), two aromatic carbon peaks were misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 440 (M^+, 2), 335 (100); HRMS (EI^+) calcd for $C_{31}H_{24}N_2O$: 440.1889, found: 440.1889.



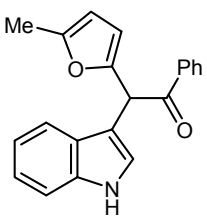
2-(1,2-Dimethyl-1*H*-indol-3-yl)-2-(2-methyl-1*H*-indol-3-yl)-1-phenylethanone (6db): Yellow foam; yield = 89% (352 mg); R_f = 0.25 (hexane/EtOAc, 5:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.05 (s, 3H), 2.24 (s, 3H), 3.59 (s, 3H), 6.47 (s, 1H), 6.94–7.04 (m, 2H), 7.07 (d, *J* = 6.9 Hz, 1H), 7.10–7.17 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.34–7.41 (m, 4H), 7.43–7.52 (m, 1H), 7.88 (s, 1H), 8.05–8.16 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 10.9 (CH_3), 12.6 (CH_3), 29.6 (CH_3), 43.3 (CH), 108.8 (CH), 108.9 (C), 110.4 (CH), 118.5 (CH), 118.6 (CH), 118.7 (CH), 119.2 (CH), 119.4 (CH), 120.6 (CH), 120.9 (CH), 127.7 (C), 128.6 (2 × CH), 128.7 (2 × CH), 132.6 (C), 132.7 (C), 132.8 (C), 134.4 (C), 135.1 (C), 136.6 (C), 137.2 (C), 199.3 (C); LRMS (70 eV, EI): *m/z* (%) 392 (M^+, 3), 287 (100); HRMS (EI^+) calcd for $C_{27}H_{24}N_2O$: 392.1889, found: 392.1890.



2-(5-Bromo-1*H*-indol-3-yl)-2-(1,2-dimethyl-1*H*-indol-3-yl)-1-phenylethanone (6de): White solid; yield = 85% (388 mg); mp = 231–233 °C; ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ (ppm) = 2.41 (s, 3H), 3.59 (s, 3H), 6.55 (s, 1H), 6.89 (s, 1H), 6.92 (d, *J* = 7.9 Hz, 1H), 7.00 (at, *J* = 7.5 Hz, 1H), 7.14 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.30 (ad, *J* = 8.5 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.47–7.54 (m, 3H), 8.02–8.07 (m, 2H), 11.01 (s, 1H); ^{13}C NMR (100.6 MHz, $(CD_3)_2SO$) δ (ppm) = 10.4 (CH_3), 29.4 (CH_3), 41.6 (CH), 106.9 (C), 109.2 (CH), 110.9 (C), 113.3 (C), 113.4 (CH), 118.5 (CH), 118.8 (CH), 120.2 (CH), 121.3 (CH), 123.3 (CH), 126.0 (CH), 126.4 (C), 128.3 (2 × CH), 128.5 (2 × CH), 128.7 (C), 132.7 (CH), 134.8 (C), 135.0 (C), 136.3 (C), 136.9 (C), 197.9 (C); LRMS (70 eV, EI): *m/z* (%) 458 [$(M+2)^+$, 5], 456 (M^+, 5), 353 (100), 351 (100); HRMS (EI^+) calcd for $C_{26}H_{21}BrN_2O$: 456.0837, found: 456.0836.

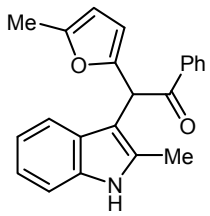


1-(1*H*-indol-3-yl)-1-(1-methyl-1*H*-indol-3-yl)propan-2-one (6ea): White foam; yield = 70% (211 mg); R_f = 0.25 (hexane/EtOAc, 4:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.33 (s, 3H), 3.71 (s, 3H), 5.56 (s, 1H), 6.93 (s, 1H), 7.03-7.06 (m, 1H), 7.08–7.14 (m, 2H), 7.16–7.27 (m, 2H), 7.28–7.37 (m, 2H), 7.58 (d, *J* = 7.9 Hz, 2H), 8.13 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ (ppm) = 29.0 (CH_3), 32.8 (CH_3), 48.1 (CH), 109.5 (CH), 111.5 (CH), 111.9 (C), 113.4 (C), 119.2 (CH), 119.2 (2 × CH), 119.7 (CH), 121.9 (CH), 122.3 (CH), 123.5 (CH), 126.8 (C), 127.3 (C), 128.2 (CH), 136.5 (C), 137.2 (C), 207.6 (C); LRMS (70 eV, EI): *m/z* (%) 302 (M^+, 2), 259 (100); HRMS (EI^+) calcd for $C_{20}H_{18}N_2O$: 302.1419, found: 302.1412.

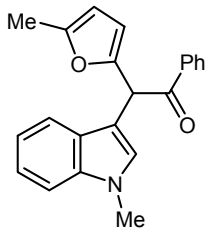


2-(1*H*-Indol-3-yl)-2-(5-methylfuran-2-yl)-1-phenylethanone (7a): Yellow solid; yield = 73% (230 mg); mp = 146–148 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.55 (s, 3H), 5.88 (dd, *J* = 2.9, 0.9 Hz, 1H), 5.97 (d, *J* = 3.0 Hz, 1H), 6.27 (s, 1H), 7.07 (d, *J* = 2.5 Hz, 1H), 7.15 (ddd, *J* = 7.6, 7.1, 1.3 Hz, 1H), 7.18–7.24 (m, 1H), 7.32–7.44 (m, 3H), 7.48–7.54 (m, 1H), 7.64–7.67 (m, 1H), 8.03–8.09 (m, 2H), 8.24 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 13.8 (CH_3), 44.8 (CH), 106.5 (CH), 109.5 (CH), 111.3 (C), 111.5 (CH), 118.9 (CH), 120.0 (CH), 122.5 (CH), 124.1 (CH), 126.5 (C), 128.7 (2 × CH), 129.0 (2 ×

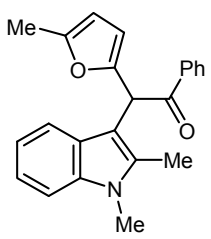
CH), 133.1 (CH), 136.4 (C), 150.8 (C), 151.8 (C), 196.4 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 315 (M^+, 3), 210 (100); HRMS (EI^+) calcd for $C_{21}H_{17}NO_2$: 315.1259, found: 315.1259.



2-(2-Methyl-1*H*-indol-3-yl)-2-(5-methylfuran-2-yl)-1-phenylethanone (7b): Yellow solid; yield = 69% (227 mg); mp = 80–82 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.30 (s, 3H), 2.42 (s, 3H), 5.88–5.96 (m, 2H), 6.15 (s, 1H), 7.09–7.18 (m, 2H), 7.29–7.31 (m, 1H), 7.33–7.41 (m, 2H), 7.45–7.50 (m, 1H), 7.63–7.70 (m, 1H), 7.95–8.03 (m, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.4 (CH_3), 13.7 (CH_3), 45.0 (CH), 106.2 (C), 106.3 (CH), 109.6 (CH), 110.5 (CH), 118.6 (CH), 119.9 (CH), 121.4 (CH), 127.8 (C), 128.5 (2 × CH), 128.6 (2 × CH), 132.9 (CH), 133.2 (C), 135.3 (C), 136.6 (C), 150.6 (C), 151.7 (C), 196.4 (C); LRMS (70 eV, EI): *m/z* (%) 329 (M^+, 2), 224 (100); HRMS (EI^+) calcd for $C_{22}H_{19}NO_2$: 329.1416, found: 329.1414.

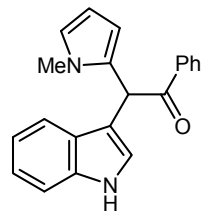


2-(1-Methyl-1*H*-indol-3-yl)-2-(5-methylfuran-2-yl)-1-phenylethanone (7c): Yellow solid; yield = 81% (266 mg); mp = 154–156 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.29 (s, 3H), 3.72 (s, 3H), 5.89–5.92 (m, 1H), 6.02 (d, *J* = 2.1 Hz, 1H), 6.29 (s, 1H), 7.04 (s, 1H), 7.13–7.20 (m, 1H), 7.23–7.34 (m, 2H), 7.41 (ddd, *J* = 8.3, 2.3, 0.9 Hz, 2H), 7.49–7.55 (m, 1H), 7.65–7.70 (m, 1H), 8.06–8.11 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 13.8 (CH_3), 32.9 (CH_3), 44.6 (CH), 106.5 (CH), 109.4 (CH), 109.5 (CH), 109.7 (C), 119.0 (CH), 119.5 (CH), 122.0 (CH), 126.9 (C), 128.5 (CH), 128.6 (2 × CH), 128.9 (2 × CH), 133.1 (CH), 136.4 (C), 137.2 (C), 151.1 (C), 151.7 (C), 196.2 (C); LRMS (70 eV, EI): *m/z* (%) 329 (M^+, 3), 224 (100); HRMS (EI^+) calcd for $C_{22}H_{19}NO_2$: 329.1416, found: 329.1417.

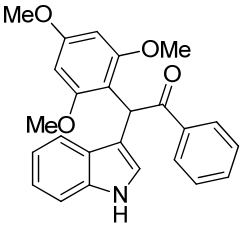


2-(1,2-Dimethyl-1H-indol-3-yl)-2-(5-methylfuran-2-yl)-1-phenylethanone (7d): Yellow foam; yield = 65% (223 mg); mp = 112–114 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.29 (s, 3H), 2.42 (s, 3H), 3.61 (s, 3H), 5.89–5.90 (m, 1H), 5.93 (d, *J* = 2.4 Hz, 1H), 6.17 (s, 1H), 7.07–7.26 (m, 3H), 7.31–7.35 (m, 2H), 7.41–7.47 (m, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.95–8.03 (m, 2H); ^{13}C NMR (75.4

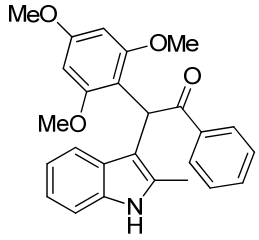
MHz, $CDCl_3$): δ (ppm) = 10.9 (CH_3), 13.8 (CH_3), 29.7 (CH_3), 45.2 (CH), 105.6 (C), 106.3 (CH), 108.8 (CH), 109.6 (CH), 118.7 (CH), 119.6 (CH), 121.0 (CH), 126.8 (C), 128.5 (2 × CH), 128.6 (2 × CH), 132.8 (CH), 134.9 (C), 136.6 (C), 136.8 (C), 150.9 (C), 151.6 (C), 196.2 (C); LRMS (70 eV, EI): *m/z* (%) 343 (M^+, 2), 238 (100); HRMS (EI^+) calcd for $C_{23}H_{21}NO_2$: 343.1572, found: 343.1568.



2-(1*H*-Indol-3-yl)-2-(1-methyl-1*H*-pyrrol-2-yl)-1-phenylethanone (7e): Yellow foam; yield = 50% (157 mg); mp = 144–146 °C; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.51 (s, 3H), 5.91–5.94 (m, 1H), 6.07 (dd, *J* = 3.6, 2.8 Hz, 1H), 6.21 (s, 1H), 6.63–6.67 (m, 1H), 6.83 (d, *J* = 2.1 Hz, 1H), 7.10 (ddd, *J* = 8.0, 7.1, 1.1 Hz, 1H), 7.15–7.22 (m, 1H), 7.32 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.38–7.46 (m, 2H), 7.49–7.57 (m, 2H), 8.01–8.08 (m, 2H), 8.23 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 34.2 (CH_3), 43.8 (CH), 107.0 (CH), 109.5 (CH), 111.5 (CH), 112.5 (C), 118.8 (CH), 119.8 (CH), 122.3 (CH), 122.9 (CH), 124.5 (CH), 126.5 (C), 128.7 (2 × CH), 128.8 (2 × CH), 129.7 (C), 133.1 (CH), 136.5 (C), 136.7 (C), 197.2 (C); LRMS (70 eV, EI): *m/z* (%) 314 (M^+, 3), 209 (100); HRMS (EI^+) calcd for $C_{21}H_{18}N_2O$: 314.1419, found: 314.1417.

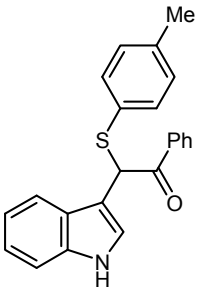


2-(1*H*-Indol-3-yl)-1-phenyl-2-(2,4, 6-trimethoxyphenyl)ethanone (7f): White foam; yield = 51% (205 mg); ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.71 (s, 6H), 3.74 (s, 3H), 6.05 (s, 2H), 6.27 (s, 1H), 6.95 (s, 1H), 7.05–7.18 (m, 2H), 7.24–7.33 (m, 3H), 7.36–7.43 (m, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.81–7.90 (m, 2H), 8.07 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 41.7 (CH), 55.2 (CH_3), 55.6 (2 × CH_3), 91.0 (2 × CH), 111.0 (C), 111.3 (CH), 113.1 (C), 118.9 (CH), 119.2 (CH), 121.2 (CH), 124.3 (CH), 127.6 (C), 127.9 (2 × CH), 128.0 (2 × CH), 131.7 (CH), 136.1 (C), 137.6 (C), 158.0 (2 x C), 160.3 (C), 199.7 (C); LRMS (70 eV, EI): *m/z* (%) 401 (M^+, 2), 296 (100); HRMS (EI^+) calcd for $C_{25}H_{23}NO_4$: 401.1627, found, 401.1622.

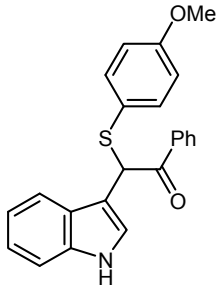


2-(2-Methyl-1*H*-indol-3-yl)-1-phenyl-2-(2,4,6-trimethoxyphenyl)ethanone (7g): White foam; yield = 38% (158 mg); ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.24 (s, 3H), 3.65 (s, 6H), 3.74 (s, 3H), 6.07 (s, 2H), 6.21 (s, 1H), 6.98–7.04 (m, 2H), 7.12–7.20 (m, 1H), 7.24–7.34 (m, 2H), 7.35–7.42 (m, 1H), 7.52 (d, *J*

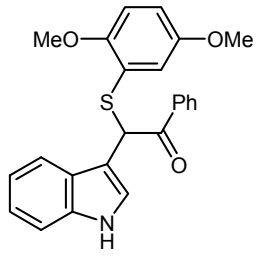
= 7.5 Hz, 1H), 7.77 (s, 1H), 7.86–7.81 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): 12.6 (CH_3), 42.3 (CH), 55.3 (CH_3), 55.6 (2 × CH_3), 91.1 (2 × CH), 109.5 (C), 110.0 (C), 110.4 (CH), 119.1 (CH), 119.5 (CH), 128.08 (2 × CH), 128.12 (2 × CH), 129.1 (C), 131.8 (CH), 132.7 (C), 135.2 (C), 137.6 (C), 158.3 (2 × C), 160.3 (C), 198.7 (C); LRMS (70 eV, EI): *m/z* (%) 415 (M^+, 9), 310 (100); HRMS (EI^+) calcd for $C_{26}H_{25}NO_4$: 415.1784, found, 415.1779.



2-(1*H*-Indol-3-yl)-1-phenyl-2-(*p*-tolylthio)ethanone (8a): White solid; yield = 87% (311 mg); mp = 113–115 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.29 (s, 3H), 6.22 (s, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 2.5 Hz, 1H), 7.18–7.27 (m, 4H), 7.32–7.42 (m, 3H), 7.51 (at, *J* = 7.3 Hz, 1H), 7.82–7.86 (m, 1H), 8.02 (ad, *J* = 7.7 Hz, 2H), 8.39 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 21.2 (CH_3), 51.4 (CH), 110.0 (C), 111.7 (CH), 119.0 (CH), 120.1 (CH), 122.5 (CH), 125.0 (CH), 126.0 (C), 128.6 (2 × CH), 128.8 (2 × CH), 129.6 (2 × CH), 130.4 (C), 133.2 (CH), 134.0 (2 × CH), 136.1 (C), 136.3 (C), 138.3 (C), 194.9 (C); LRMS (70 eV, EI): *m/z* (%) 357 (M^+, 4), 234 (100); HRMS (EI^+) calcd for $C_{23}H_{19}NOS$: 357.1187, found: 357.1185.

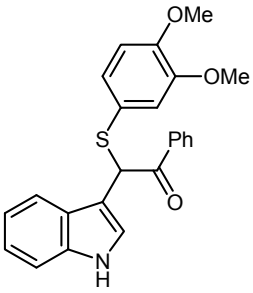


2-(1*H*-Indol-3-yl)-2-((4-methoxyphenyl)thio)-1-phenylethanone (8b): Brown solid; yield = 83% (310 mg); R_f = 0.25 (hexane/EtOAc, 6:1); ^{1}H NMR (300 MHz, $(CD_3)_2CO$): δ (ppm) = 3.73 (s, 3H), 6.45 (s, 1H), 6.73□6.81 (m, 2H), 7.06–7.26 (m, 4H), 7.29 (d, *J* = 2.6 Hz, 1H), 7.37–7.56 (m, 4H), 7.90 (d, *J* = 7.6 Hz, 1H), 8.08–8.12 (m, 1H), 10.27 (s, 1H); ^{13}C NMR (75.4 MHz, $(CD_3)_2CO$): δ (ppm) = 52.9 (CH_3), 55.5 (CH), 110.4 (C), 112.4 (CH), 114.9 (2 × CH), 120.1 (CH), 120.2 (CH), 122.6 (CH), 125.3 (C), 126.4 (CH), 127.0 (C), 129.3 (2 × CH), 129.5 (2 × CH), 133.7 (CH), 137.0 (2 × CH), 137.1 (C), 137.5 (C), 160.8 (C), 195.1 (C); LRMS (70 eV, EI): *m/z* (%) 373 (M^+, 3), 234 (100); HRMS (EI^+) calcd for $C_{23}H_{19}NO_2S$: 373.1136, found: 373.1136.

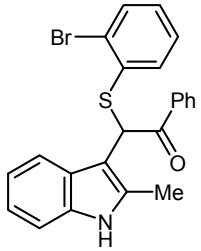


2-((2,5-Dimethoxyphenyl)thio)-2-(1*H*-indol-3-yl)-1-phenylethanone (8c): White foam; yield = 76% (307 mg); R_f = 0.25 (hexane/EtOAc, 4:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.52 (s, 3H), 3.67 (s, 3H), 6.47 (s, 1H), 6.71–6.74 (m, 2H), 6.82 (t, *J* = 1.7 Hz, 1H), 7.11 (d, *J* = 2.5 Hz, 1H),

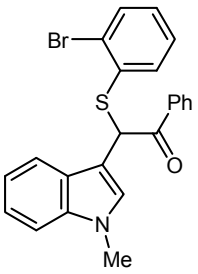
7.14–7.21 (m, 2H), 7.26–7.39 (m, 3H), 7.43–7.50 (m, 1H), 7.79–7.85 (m, 1H), 7.96–8.01 (m, 2H), 8.61 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 49.2 (CH), 55.6 (CH_3), 56.2 (CH_3), 109.9 (C), 111.7 (CH), 111.8 (CH), 114.6 (CH), 118.9 (CH), 119.1 (CH), 120.0 (CH), 122.4 (CH), 123.6 (C), 124.7 (CH), 126.1 (C), 128.5 (2 × CH), 128.7 (2 × CH), 133.1 (CH), 136.1 (C), 136.4 (C), 153.1 (C), 153.3(C), 195.5 (C); LRMS (70 eV, EI): *m/z* (%) 387 [(M–O)$^+$, 25], 282 (100); HRMS (EI$^+$) calcd for $C_{24}H_{21}NO_2S$ (M–O)$^+$: 387.1293, found: 387.1295.



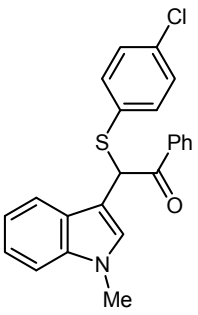
2-((3,4-Dimethoxyphenyl)thio)-2-(1*H*-indol-3-yl)-1-phenylethanone (8d): Orange oil; yield = 75% (303 mg); R_f = 0.34 (hexane/EtOAc, 5:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.48 (s, 3H), 3.81 (s, 3H), 6.14 (s, 1H), 6.54 (d, *J* = 1.8 Hz, 1H), 6.70 (d, *J* = 8.3 Hz, 1H), 6.94 (dd, *J* = 8.3, 2.0 Hz, 1H), 7.09 (d, *J* = 2.5 Hz, 1H), 7.17–7.28 (m, 2H), 7.31–7.44 (m, 3H), 7.51 (at, *J* = 7.3 Hz, 1H), 7.78–7.83 (m, 1H), 8.00 (d, *J* = 7.6 Hz, 2H), 8.43 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 51.3 (CH_3), 55.6 (CH_3), 55.9 (CH_3), 109.9 (C), 111.1 (CH), 111.5 (CH), 118.3 (CH), 119.1 (CH), 120.1 (CH), 122.6 (CH), 124.2 (C), 125.2 (CH), 126.2 (C), 128.4 (CH), 128.7 (2 × CH), 128.8 (2 × CH), 133.2 (CH), 136.1 (C), 136.2 (C), 148.3 (C), 149.6 (C), 194.9 (C); LRMS (70 eV, EI): *m/z* (%) 387 [(M–O)$^+$, 19], 282 (100); HRMS (EI$^+$) calcd for $C_{24}H_{21}NO_2S$ (M–O)$^+$: 387.1293, found: 387.1294.



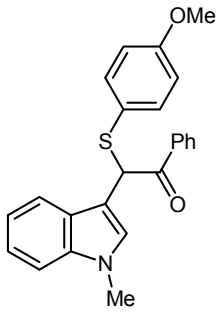
2-((2-Bromophenyl)thio)-2-(2-methyl-1*H*-indol-3-yl)-1-phenylethanone (8e): Black solid; yield = 78% (340 mg); mp = 99–101 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.21 (s, 3H), 6.38 (s, 1H), 6.95–7.05 (m, 2H), 7.06–7.13 (m, 3H), 7.16–7.21 (m, 1H), 7.31 (at, *J* = 7.5 Hz, 2H), 7.43 (dd, *J* = 8.3, 6.4 Hz, 1H), 7.56 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.71 (dd, *J* = 5.9, 3.2 Hz, 1H), 7.86 (s, 1H), 7.90–7.94 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.0 (CH_3), 52.8 (CH), 105.7 (C), 110.5 (CH), 119.0 (CH), 120.3 (CH), 121.7 (CH), 127.1 (C), 127.6 (CH), 128.66 (2 × CH), 128.70 (2 × CH), 128.9 (C), 129.2 (CH), 133.0 (CH), 133.2 (CH), 134.1 (C), 135.3 (C), 135.6 (C), 135.7 (CH), 135.9 (C), 194.4 (C); LRMS (70 eV, EI): *m/z* (%) 435 [(M+2)$^+$, 3], 437 (M$^+$, 3), 248 (100); HRMS (EI$^+$) calcd for $C_{23}H_{18}BrNOS$: 435.0292, found: 435.0291.



2-((2-Bromophenyl)thio)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (8f): Orange solid; yield = 86% (375 mg); mp = 129–131 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.67 (s, 3H), 6.51 (s, 1H), 7.00–7.09 (m, 2H), 7.10 (s, 1H), 7.21 (ddd, *J* = 7.8, 6.6, 3.8 Hz, 1H), 7.26–7.31 (m, 3H), 7.37 (at, *J* = 7.8 Hz, 2H), 7.49 (at, *J* = 7.4 Hz, 1H), 7.55–7.59 (m, 1H), 7.80–7.86 (m, 1H), 7.98–8.04 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 33.0 (CH_3), 50.1 (CH), 107.7 (C), 109.7 (CH), 119.1 (CH), 120.0 (CH), 122.3 (CH), 126.6 (C), 126.8 (C), 127.8 (CH), 128.6 (CH), 128.7 (2 × CH), 128.8 (2 × CH), 129.3 (CH), 133.1 (CH), 133.3 (CH), 135.9 (C), 136.2 (C), 137.2 (C), 194.4 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 435 [(M+2)$^+$, 1], 437 (M$^+$, 1), 248 (100); HRMS (EI$^+$) calcd for $C_{23}H_{18}BrNOS$: 435.0292, found: 435.0293.

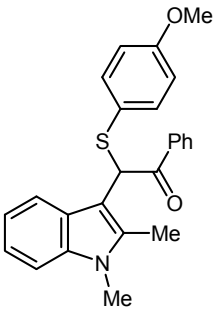


2-((4-Chlorophenyl)thio)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (8g): White solid; yield = 89% (349 mg); mp = 114–116 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.67 (s, 3H), 6.25 (s, 1H), 7.04 (s, 1H), 7.14–7.28 (m, 5H), 7.28–7.34 (m, 2H), 7.36–7.44 (m, 2H), 7.48–7.55 (m, 1H), 7.77–7.83 (m, 1H), 7.98–8.03 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 32.9 (CH_3), 51.1 (CH), 108.0 (C), 109.7 (CH), 119.0 (CH), 119.9 (CH), 122.3 (CH), 126.4 (C), 128.7 (2 × CH), 128.8 (2 × CH), 128.9 (2 × CH), 129.4 (CH), 132.7 (C), 133.3 (CH), 134.2 (C), 135.0 (2 × CH), 135.9 (C), 137.1 (C), 194.3 (C); LRMS (70 eV, EI): *m/z* (%) 393 [(M+2)$^+$, 1], 391 (M$^+$, 3), 248 (100); HRMS (EI$^+$) calcd for $C_{23}H_{18}ClNOS$: 391.0798, found: 391.0799.

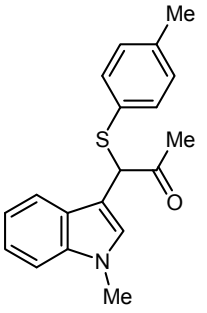


2-((4-Methoxyphenyl)thio)-2-(1-methyl-1*H*-indol-3-yl)-1-phenylethanone (8h): Yellow solid; yield = 87% (337 mg); mp = 145–147 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 3.67 (s, 3H), 3.76 (s, 3H), 6.17 (s, 1H), 6.72–6.78 (m, 2H). 7.06 (s, 1H), 7.20–7.27 (m, 3H), 7.28–7.33 (m, 2H), 7.40 (at, *J* = 7.7 Hz, 2H), 7.51 (at, *J* = 7.0 Hz, 1H), 7.80–7.84 (m, 1H), 8.02 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 32.8 (CH_3), 51.3 (CH), 55.3 (CH_3), 108.4 (C), 109.5 (CH), 114.2 (2 × CH), 119.0 (CH), 119.7 (CH), 122.1 (CH), 124.2 (C), 126.6 (CH), 128.6 (2 × CH), 128.7 (2 × CH), 129.4 (C), 133.0 (CH), 136.2 (C), 136.8 (2 × CH), 136.9 (C), 160.1 (C), 194.6 (C); LRMS

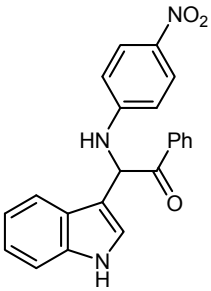
(70 eV, EI): *m/z* (%) 387 (M^+, 1), 139 (100); HRMS (EI^+) calcd for $C_{17}H_{16}NOS$: $(M–C_7H_5O)^+$, 282.0953, found: 282.0951.



2-(1,2-Dimethyl-1*H*-indol-3-yl)-2-((4-methoxyphenyl)thio)-1-phenylethanone (8i): White solid; yield = 75% (301 mg); mp = 213–215 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.11 (s, 3H), 3.54 (s, 3H), 3.75 (s, 3H), 6.03 (s, 1H), 6.68–6.74 (m, 2H), 7.08–7.17 (m, 2H), 7.18–7.23 (m, 3H), 7.25–7.31 (m, 2H), 7.37–7.43 (m, 1H), 7.69–7.74 (m, 1H), 7.85–7.90 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 10.2 (CH_3), 29.6 (CH_3), 55.3 (CH_3), 56.1 (CH), 105.7 (C), 108.8 (CH), 114.1 (2 × CH), 119.1 (CH), 119.7 (CH), 121.1 (CH), 125.2 (C), 126.0 (C), 128.4 (2 × CH), 128.5 (2 × CH), 132.9 (CH), 135.5 (C), 136.1 (C), 136.8 (2 × CH), 159.9 (C), 195.2 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 401 (M^+, 1), 262 (100); HRMS (EI^+) calcd for $C_{18}H_{18}NOS$ $(M–C_7H_5O)^+$: 296.1109, found: 296.1108.

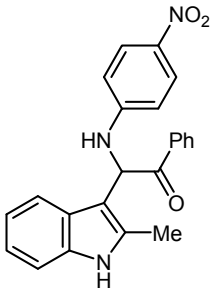


1-(1-Methyl-1*H*-indol-3-yl)-1-(*p*-tolylthio)propan-2-one (8j): Yellow foam; yield = 73% (225 mg); R_f = 0.30 (hexane/EtOAc, 5:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.28 (s, 3H), 2.35 (s, 3H), 3.74 (s, 3H), 5.29 (s, 1H), 7.10 (s, 1H), 7.12–7.15 (m, 2H), 7.21 (ddd, *J* = 8.0, 6.5, 1.6 Hz, 1H), 7.27–7.37 (m, 4H), 7.71–7.75 (m, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 21.1 (CH_3), 26.8 (CH_3), 32.8 (CH_3), 56.0 (CH), 107.9 (C), 109.5 (CH), 119.1 (CH), 119.7 (CH), 122.2 (CH), 126.6 (C), 128.4 (CH), 129.7 (2 × CH), 130.2 (C), 133.0 (2 × CH), 137.0 (C), 138.0 (C), 203.3 (C); LRMS (70 eV, EI): *m/z* (%) 309 (M^+, 2), 186 (100); HRMS (EI^+) calcd for $C_{19}H_{19}NOS$: 309.1187, found: 309.1187.

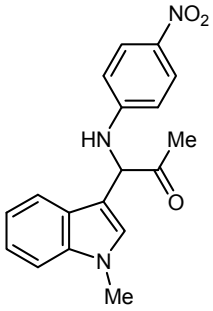


2-(1*H*-Indol-3-yl)-2-((4-nitrophenyl)amino)-1-phenylethanone (9a): Yellow foam; yield = 65% (241 mg); R_f = 0.25 (hexane/EtOAc, 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 6.05 (d, *J* = 6.3 Hz, 1H), 6.40 (d, *J* = 6.3 Hz, 1H), 6.56–6.67 (m, 2H), 7.15–7.28 (m, 3H), 7.31–7.44 (m, 3H), 7.47–7.56 (m, 1H), 7.73–7.81 (m, 1H), 7.95–8.09 (m, 4H), 8.44 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) =

55.1 (CH), 111.0 (CH), 111.96 (CH), 112.03 (CH), 113.5 (C), 118.8 (CH), 120.9 (CH), 123.1 (CH), 124.7 (CH), 125.4 (C), 126.4 (CH), 126.5 (CH), 128.8 (2 × CH), 128.9 (2 × CH), 133.9 (CH), 134.5 (C), 136.5 (C), 138.4 (C), 151.8 (C), 195.3 (C); LRMS (70 eV, EI): *m/z* (%) 266 [$(M-C_7H_5O)^+$, 100]; HRMS (EI^+) calcd for $C_{15}H_{12}N_3O_2$ $(M-C_7H_5O)^+$: 266.0930, found: 266.0930.



2-(2-Methyl-1*H*-indol-3-yl)-2-((4-nitrophenyl)amino)-1-phenylethanone (9b): Yellow solid; yield = 88% (339 mg); mp = 95–97 °C; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.46 (s, 3H), 6.21–6.33 (m, 2H), 6.56 (d, *J* = 9.1 Hz, 2H), 7.09–7.26 (m, 3H), 7.35 (at, *J* = 7.4 Hz, 2H), 7.47 (at, *J* = 7.3 Hz, 1H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.92–8.01 (m, 4H), 8.18 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.5 (CH_3), 54.9 (CH), 105.7 (C), 111.1 (CH), 112.0 (2 × CH), 117.7 (CH), 120.6 (CH), 121.9 (CH), 126.4 (2 × CH), 126.7 (C), 128.4 (2 × CH), 128.7 (2 × CH), 133.7 (CH), 134.1 (C), 134.8 (C), 135.3 (C), 138.1 (C), 151.7 (C), 194.6 (C); LRMS (70 eV, EI): *m/z* (%) 280 [$(M-C_7H_5O)^+$, 100]; HRMS (EI^+) calcd for $C_{16}H_{14}N_3O_2$ $(M-C_7H_5O)^+$: 280.1086, found: 280.1081.



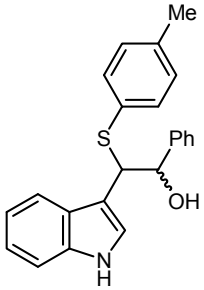
1-(1-Methyl-1*H*-indol-3-yl)-1-((4-nitrophenyl)amino)propan-2-one (9c): Slightly contaminated with *p*-nitroaniline. Yellow foam; yield = 67% (217 mg); R_f = 0.25 (hexane/EtOAc, 4:1); ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.20 (s, 3H), 3.78 (s, 3H), 5.40 (d, *J* = 4.5 Hz, 1H), 6.22 (d, *J* = 4.5 Hz, 1H), 6.49–6.56 (m, 2H), 7.13 (s, 1H), 7.17–7.38 (m, 3H), 7.67 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.94–7.98 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 26.7 (CH_3), 33.2 (CH_3), 59.5 (CH), 109.0 (C), 110.2 (CH), 112.1 (2 × CH), 118.7 (CH), 120.4 (CH), 122.7 (CH), 126.1 (C), 126.3 (2 × CH), 128.4 (CH), 137.5 (C), 138.4 (C), 151.4 (C), 203.1 (C); LRMS (70 eV, EI): *m/z* (%) 323 (M^+, 5), 280 (100); HRMS (EI^+) calcd for $C_{18}H_{17}N_3O_3$: 323.1270, found: 323.1271.

General procedure for the synthesis of tryptophol derivatives 10:

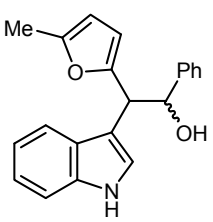
To a stirred solution of the corresponding α-(indol-3-yl) carbonyl compound derivative **7-9** (0.5 mmol) in MeOH (5 mL), $NaBH_4$ (0.6 mmol) was added portionwise at 0 ºC. After 1 h at room temperature the crude mixture was quenched with a saturated solution of NH_4Cl (5 mL) and

extracted with DCM (3 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated at reduced pressure. The residue was purified by flash chromatography using mixtures of hexane and EtOAc as eluents to obtain the corresponding tryptophol derivatives **10** in the yields reported in Scheme 5.

Spectroscopic and characterization data for compounds 10

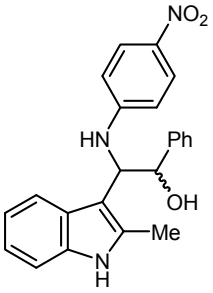


2-(1*H*-Indol-3-yl)-1-phenyl-2-(*p*-tolylthio)ethanol (10a): Generated and isolated as a ca. 2:1 mixture of diastereoisomers. Yellow solid; yield = 78% (140 mg); mp = 151–153 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.29 (s, 3H, one diast), 2.32 (s, 3H, one diast), 3.02 (bs, 1H, one diast), 3.64 (bs, 1H, one diast), 4.71 (d, *J* = 8.3 Hz, 1H, one diast), 4.84 (d, *J* = 4.8 Hz, 1H, one diast), 5.08 (d, *J* = 8.4 Hz, 1H, one diast), 5.12 (d, *J* = 4.8 Hz, 1H, one diast), 6.63 (d, *J* = 2.4 Hz, 1H, one diast), 6.99 (d, *J* = 8.3 Hz, 1H, one diast), 7.06–7.12 (m, 7H), 7.13–7.23 (m, 10H), 7.23–7.29 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 1H, one diast), 7.69 (d, *J* = 7.6 Hz, 1H, one diast), 7.87 (s, 1H, one diast), 8.07 (s, 1H, one diast); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 21.2 (CH_3), 21.3 (CH_3), 54.2 (CH), 56.4 (CH), 74.4 (CH), 75.1 (CH), 111.29 (CH), 111.32 (CH), 111.4 (C), 113.63 (C), 119.3 (CH), 119.5 (CH), 119.76 (CH), 119.79 (CH), 122.3 (CH), 123.5 (CH), 124.5 (CH), 126.3 (C), 126.6 (2 × CH), 126.9 (C), 127.0 (CH), 127.6 (CH), 127.7 (CH), 128.0 (2 × CH), 128.1 (2 × CH), 129.6 (2 × CH), 129.9 (2 × CH), 131.2 (C), 133.1 (2 × CH), 133.7 (2 × CH), 136.0 (C), 136.1 (C), 137.79 (C), 137.82 (C), 140.9 (C), 141.2 (C); LRMS (70 eV, EI): *m/z* (%) 252 [$(M–C_7H_7O)^+$, 100]; HRMS (EI^+) calcd for $C_{16}H_{14}NS$ $(M–C_7H_7O)^+$: 252.0847, found: 252.0847.



2-(2-Methyl-1*H*-indol-3-yl)-2-(5-methylfuran-2-yl)-1-phenylethanol (10b): Generated as ca. 4:1 mixture of diastereoisomers. The major one could be isolated and characterized. Yellow solid; yield = 80% (132 mg); mp = 165–167 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 2.13 (s, 3H), 2.19 (s, 3H), 2.32 (bs, 1H), 4.40 (d, *J* = 7.2 Hz, 1H), 5.60 (d, *J* = 7.2 Hz, 1H), 5.80 (dd, *J* = 3.0, 1.0 Hz, 1H), 5.96 (d, *J* = 2.9 Hz, 1H), 7.07–7.28 (m, 8H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.91 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 11.9 (CH_3), 13.7 (CH_3), 46.3 (CH), 75.2 (CH), 106.0 (CH), 107.3 (C), 107.8 (CH), 110.5

(CH), 119.6 (CH), 120.1 (CH), 121.3 (CH), 126.6 (2 × CH), 127.5 (CH), 127.9 (C), 128.1 (2 × CH), 134.0 (C), 135.5 (C), 142.9 (C), 150.5 (C), 152.8 (C); LRMS (70 eV, EI): *m/z* (%) 224 [$(M-C_7H_7O)^+$, 100]; HRMS (EI^+) calcd for $C_{15}H_{14}NO$ $(M-C_7H_7O)^+$: 224.1075, found: 224.1072.

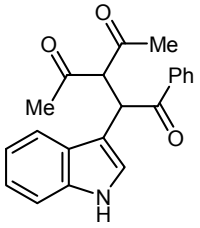


2-(2-Methyl-1*H*-indol-3-yl)-2-((4-nitrophenyl)amino)-1-phenylethanol (10c): Generated as ca. 2:1 mixture of diastereoisomers. The major one could be isolated and characterized. Yellow solid; yield = 81% (157 mg); mp = 184–186 °C; ^1H NMR (300 MHz, $CDCl_3$): δ (ppm) = 1.90 (s, 3H), 2.35 (d, *J* = 5.4 Hz, 1H), 4.85 (dd, *J* = 6.1, 4.7 Hz, 1H), 5.28 (at, *J* = 4.7 Hz, 1H), 5.51 (d, *J* = 6.1 Hz, 1H), 6.42 (ad, *J* = 9.2 Hz, 2H), 6.98–7.17 (m, 4H), 7.22–7.35 (m, 4H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.87–7.96 (m, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 11.8 (CH_3), 57.7 (CH), 77.3 (CH), 105.8 (C), 110.8 (CH), 111.8 (2 × CH), 119.0 (CH), 120.1 (CH), 121.6 (CH), 126.2 (2 × CH), 126.5 (2 × CH), 127.4 (C), 128.3 (CH), 128.5 (2 × CH), 134.2 (C), 135.4 (C), 138.1 (C), 140.2 (C), 152.6 (C); LRMS (70 eV, EI): *m/z* (%) 280 [$(M-C_7H_7O)^+$, 100]; HRMS (EI^+) calcd for $C_{16}H_{14}N_3O_2$ $(M-C_7H_7O)^+$: 280.1086, found: 280.1088.

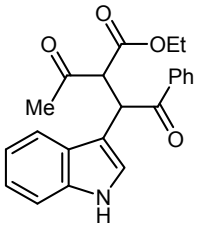
General procedure for the synthesis of tricarbonyl compounds 11:

$Cu(OTf)_2$ (10 mol%, 36 mg) was added to a solution of the corresponding α-acyloin **3** (1 mmol) and the corresponding 1,3-dicarbonyl compound (1 mmol) in toluene (4 mL) at room temperature**.** The resulting mixture was stirred until the alcohol was consumed as determined by TLC. The crude reaction mixture was quenched with aqueous NaOH (0.5M) and extracted with EtOAc (3 × 10 mL), and the combined organic layers were dried over anhydrous Na_2SO_4 and concentrated at reduced pressure. The residue was purified by flash chromatography on deactivated silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding tricarbonyl compounds **11** in the yields reported in Table 3.

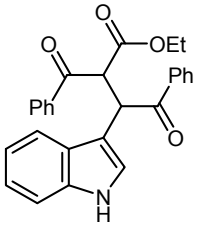
Spectroscopic and characterization data for compounds 11:



3-Acetyl-2-(1*H*-indol-3-yl)-1-phenylpentane-1,4-dione (11a): Yellow solid; yield = 90% (300 mg); mp = 159–161 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.88 (s, 3H), 2.29 (s, 3H), 5.04 (d, *J* = 11.1 Hz, 1H), 5.67 (d, *J* = 11.1 Hz, 1H), 7.04 (d, *J* = 2.6 Hz, 1H), 7.12–7.19 (m, 2H), 7.24–7.32 (m, 3H), 7.39 (at, *J* = 7.4 Hz, 1H), 7.71–7.75 (m, 1H), 7.93–7.96 (m, 2H), 8.28 (s, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) = 30.4 (CH_3), 31.6 (CH_3), 45.5 (CH), 70.3 (CH), 109.3 (C), 111.7 (CH), 119.0 (CH), 120.5 (CH), 122.7 (CH), 124.2 (C), 125.8 (C), 128.5 (2 × CH), 128.8 (2 × CH), 133.1 (CH), 135.9 (CH), 136.5 (C), 197.8 (C), 202.3 (C), 204.0 (C); LRMS (70 eV, EI): *m/z* (%) 333 (M^+, 6), 186 (100); HRMS (EI^+) calcd for $C_{21}H_{19}NO_3$: 333.1365, found: 333.1360.

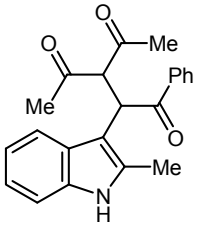


Ethyl 2-acetyl-3-(1*H*-indol-3-yl)-4-oxo-4-phenylbutanoate (11b): Isolated as a ca. 1.1:1 mixture of diastereoisomers. Yellow foam; yield = 68% (247 mg); R_f = 0.25 (hexane/EtOAc, 2:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 0.92 (t, *J* = 7.1 Hz, 3H, one diast), 1.23 (t, *J* = 7.1 Hz, 3H), 1.93 (s, 3H, one diast), 2.41 (s, 3H, one diast), 3.88 (m, 2H, one diast), 4.19 (q, *J* = 7.1 Hz, one diast), 4.79 (d, *J* = 11.1 Hz, 1H, one diast), 4.91 (d, *J* = 11.2 Hz, 1H, one diast), 5.66–5.79(m, 1H, both diast), 7.01 (s, 1H, one diast), 7.03–7.06 (m, 2H, both diast), 7.16–7.21 (m, 4H, both diast), 7.28–7.35 (m, 6H, both diast), 7.39–7.46 (m, 2H, both diast), 7.78–7.85 (m, 2H), 7.98–8.06 (m, 4H), 8.50–8.58 (m, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 13.6 (CH_3), 14.0 (CH_3), 29.7 (CH_2), 32.1 (CH_2), 44.3 (CH), 44.6 (CH), 61.3 (CH), 61.6 (CH_2), 61.8 (CH_2), 63.7 (CH), 108.9 (C), 109.5 (C), 111.5 (CH), 111.6 (CH), 119.1 (CH), 119.2 (CH), 120.1 (CH), 120.4 (CH), 122.4 (CH), 122.6 (CH), 124.1 (CH), 124.4 (CH), 125.8 (C), 126.1 (C), 128.47 (2 × CH), 128.50 (2 × CH), 128.8 (4 × CH), 133.0 (2 × CH), 135.9 (C), 136.37 (C), 136.42 (C), 168.2 (C), 168.6 (C), 197.8 (C), 197.9 (C), 202.1 (C), 203.9 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 363 (M^+, 10), 170 (100); HRMS (EI^+) calcd for $C_{22}H_{21}NO_4$: 363.1471, found: 363.1470.

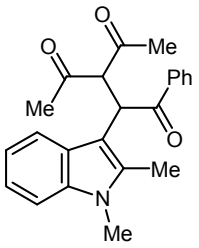


Ethyl 2-benzoyl-3-(1*H*-indol-3-yl)-4-oxo-4-phenylbutanoate (11c): Isolated as a ca. 1:1 mixture of diastereoisomers. White solid; yield = 80% (340 mg); mp = 149–151 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 0.76 (t, *J* = 7.1 Hz, 3H, one diast), 1.12 (t, *J* = 7.1 Hz, 3H, one diast), 3.67–3.80 (m, 2H, one diast), 4.13 (q, *J*

= 7.1 Hz, 2H, one diast), 5.48 (d, *J* = 8.8 Hz, 1H, one diast), 5.69 (d, *J* = 9.1 Hz, 1H, one diast), 5.92 (d, *J* = 11.0 Hz, 1H, one diast), 5.99 (d, *J* = 10.9 Hz, 1H, one diast), 6.95 (s, 1H, one diast), 7.07–7.10 (m, 3H), 7.16–7.20 (m, 3H), 7.26–7.33 (m, 5H), 7.38–7.45 (m, 2H), 7.48 (d, *J* = 7.7 Hz, 1H), 7.58 (at, *J* = 7.3 Hz, 2H), 7.71 (d, *J* = 7.3 Hz, 2H), 7.83 (t, *J* = 7.1 Hz, 2H), 8.01–8.05 (m, 4H), 8.14 (d, *J* = 7.5 Hz, 2H), 8.45 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 13.6 (CH_3), 14.0 (CH_3), 44.9 (CH), 45.4 (CH), 56.2 (CH), 59.1 (CH), 61.6 (CH_2), 61.8 (CH_2), 109.4 (C), 109.7 (C), 111.2 (CH), 111.5 (CH), 119.1 (CH), 119.4 (CH), 120.2 (CH), 120.3 (CH), 122.3 (CH), 122.5 (CH), 124.2 (CH), 126.0 (C), 126.3 (C), 128.2 (CH), 128.5 (2 × CH), 128.7 (CH), 128.8 (CH), 128.9 (2 × CH), 129.0 (2 × CH), 133.0 (2 × CH), 133.2 (CH), 133.8 (CH), 136.0 (C), 136.04 (C), 136.1 (C), 136.2 (C), 136.5 (C), 136.9 (C), 168.7 (C), 168.9 (C), 193.9 (C), 196.0 (C), 197.7 (C), 198.2 (C); LRMS (70 eV, EI): *m/z* (%) 425 (M^+, 13), 105 (100); HRMS (EI^+) calcd for $C_{27}H_{23}NO_4$: 425.1627, found: 425.1626.



3-Acetyl-2-(2-methyl-1*H*-indol-3-yl)-1-phenylpentane-1,4-dione (11d): White solid; yield = 93% (323 mg); mp = 143–145 °C; ^{1}H and ^{13}C NMR were consistent with the formation of rotamers; ^{1}H NMR (400 MHz, $(CD_3)_2SO$): δ (ppm) = 1.77 (s, 3H), 2.24 (s, 3H), 2,35 (bs, 3H), 5.13 (bs, 1H), 5.42 (bs, 1H), 6.89–6.96 (m, 2H), 7.08–7.23 (m, 1H), 7.34–747 (m, 4H), 7.85 (d, *J* = 7.5 Hz, 2H), 10.97 (s, 1H); ^{13}C NMR (100.6 MHz, $(CD_3)_2SO$): δ (ppm) = 11.1 (CH_3), 29.7 (CH_3), 31.0 (bs, CH_3), 44.1 (bs, CH), 66.0 (bs, CH), 102.1 (CH), 110.4 (CH), 117.4 (bs, C), 118.7 (CH), 120.1 (CH), 126.0 (bs, C), 127.6 (2 × CH), 127.8 (C), 128.2 (2 × CH), 128.5 (C), 132.5 (CH), 133.5 (bs, C), 134.9 (bs, C), 135.3 (C), 135.4 (CH), 201.6 (C), 203.3 (C), one aromatic carbon peak was misssing due to overlapping; LRMS (70 eV, EI): *m/z* (%) 347 (M^+, 9), 200 (100); HRMS (EI^+) calcd for $C_{22}H_{21}NO_3$: 347.1521, found: 347.1520.



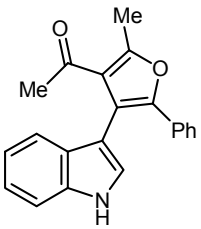
3-Acetyl-2-(1,2-dimethyl-1*H*-indol-3-yl)-1-phenylpentane-1,4-dione (11e): White solid; yield = 76% (274 mg); mp = 147–149 °C; ^{1}H and ^{13}C NMR were consistent with the formation of rotamers; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 1.82 (bs, 3H), 2.33 (s, 3H), 2.47 (bs, 3H), 3.53 (bs, 3H), 5.29 (bs, 1H), 5.58 (bs, 1H), 7.04–7.17 (m, 3H), 7.24–7.32 (m, 2H), 7.35–7.42 (m, 1H), 7.64 (bs, 1H),

7.90 (ad, *J* = 6.2 Hz, 2H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 10.7 (CH_3), 29.8 (CH_3), 30.6 (bs, CH_3), 32.6 (bs, CH_3), 46.4 (bs, CH), 67.2 (bs, CH), 103.5 (CH), 109.0 (CH), 118.8 (bs, C), 119.9 (CH), 121.1 (CH), 126.1 (bs, C), 128.4 (2 × CH), 128.5 (2 × CH), 132.8 (CH), 134.9 (bs, C), 136.3 (bs, C), 136.9 (bs, C), 198.0 (bs, C), 201.4 (C), 203.4 (C); LRMS (70 eV, EI): *m/z* (%) 361 (M^+, 20), 214 (100); HRMS (EI^+) calcd for $C_{23}H_{23}NO_3$: 361.1678, found: 361.1680.

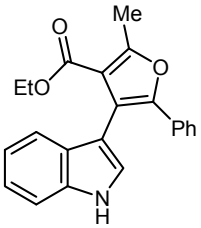
General procedure for the synthesis of furanylindoles 12 and 13:

$Cu(OTf)_2$ (10 mol%, 36 mg) was added to a solution of the corresponding α-acyloin **3** (1 mmol) and dicarbonyl compound (1 mmol) in toluene (4 mL) at room temperature. The resulting mixture was stirred for 2 h. Then, PTSA (10 mol%, 9 mg) was added and the reaction was heated at 50 ºC until the corresponding intermediate tricarbonyl derivative **11** was consumed as determined by TLC. The crude reaction mixture was quenched with aqueous NaOH (0.5M) and extracted with DCM (3 × 15 mL), and the combined organic layers were dried over anhydrous Na_2SO_4 and concentrated at reduced pressure. The residue was purified by flash chromatography on deactivated silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding furanylindoles **12** and **13** in the yields reported in Schemes 7 and 8.

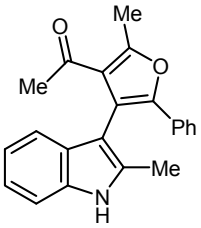
Spectroscopic and characterization data for compounds 12 and 13:



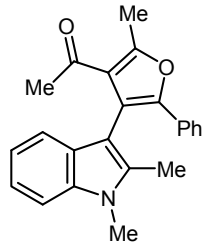
1-(4-(1*H*-Indol-3-yl)-2-methyl-5-phenylfuran-3-yl)ethanone (12a): Yellow solid; yield = 80% (253 mg); mp = 151–153 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 1.85 (s, 3H), 2.70 (s, 3H), 7.09–7.19 (m, 5H), 7.24–7.30 (m, 1H), 7.37–7.47 (m, 4H), 8.43 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ (ppm) = 14.9 (CH_3), 30.1 (CH_3), 108.5 (C), 111.5 (CH), 113.3 (C), 119.8 (CH), 120.5 (CH), 122.7 (CH), 123.8 (CH), 125.2 (2 × CH), 125.5 (C), 127.3 (CH), 127.9 (C), 128.3 (2 × CH), 130.6 (C), 136.3 (C), 148.6 (C), 157.8 (C), 197.0 (C); LRMS (70 eV, EI): *m/z* (%) 315 (M^+, 100); HRMS (EI^+) calcd for $C_{21}H_{17}NO_2$: 315.1259, found: 315.1259.



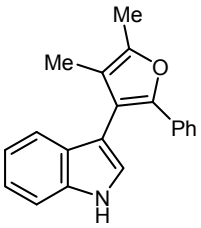
Ethyl 4-(1*H*-indol-3-yl)-2-methyl-5-phenylfuran-3-carboxylate (12b): Brown solid; yield = 67% (231 mg); mp = 179–181 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 0.85 (t, *J* = 7.1 Hz, 3H), 2.72 (s, 3H), 4.01 (q, *J* = 7.1 Hz, 2H), 7.04 (at, *J* = 7.5 Hz, 1H), 7.11–7.23 (m, 5H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.38–7.48 (m, 3H), 8.27 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 13.7 (CH_3), 14.5 (CH_3), 59.9 (CH_2), 108.5 (C), 111.1 (CH), 114.4 (C), 116.6 (C), 119.8 (CH), 120.3 (CH), 122.1 (CH), 123.9 (CH), 125.5 (2 × CH), 127.3 (CH), 127.9 (C), 128.3 (2 × CH), 130.8 (C), 136.2 (C), 148.6 (C), 158.4 (C), 164.4 (C); LRMS (70 eV, EI): *m/z* (%) 345 (M^+, 100); HRMS (EI^+) calcd for $C_{22}H_{19}NO_3$: 345.1365, found: 345.1368.



1-(2-Methyl-4-(2-methyl-1*H*-indol-3-yl)-5-phenylfuran-3-yl)ethanone (12c): Yellow solid; yield = 90% (296 mg); mp = 128–130 °C; ^{1}H NMR (300 MHz,($CDCl_3$): δ (ppm) = 1.84 (s, 3H), 2.20 (s, 3H), 2.72 (s, 3H), 7.07 (ddd, *J* = 7.9, 7.2, 0.9 Hz, 1H), 7.12–7.23 (m, 4H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.35–7.42 (m, 3H), 8.29 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 12.2 (CH_3), 14.9 (CH_3), 29.7 (CH_3), 105.5 (C), 110.6 (CH), 113.1 (C), 119.1 (CH), 120.4 (CH), 121.9 (CH), 124.8 (2 × CH), 125.2 (C), 127.2 (CH), 128.5 (2 × CH), 129.0 (C), 130.8 (C), 133.0 (C), 135.8 (C), 148.5 (C), 158.1 (C), 196.9 (C); LRMS (70 eV, EI): *m/z* (%) 329 (M^+, 100); HRMS (EI^+) calcd for $C_{22}H_{19}NO_2$: 329.1416, found: 329.1417.

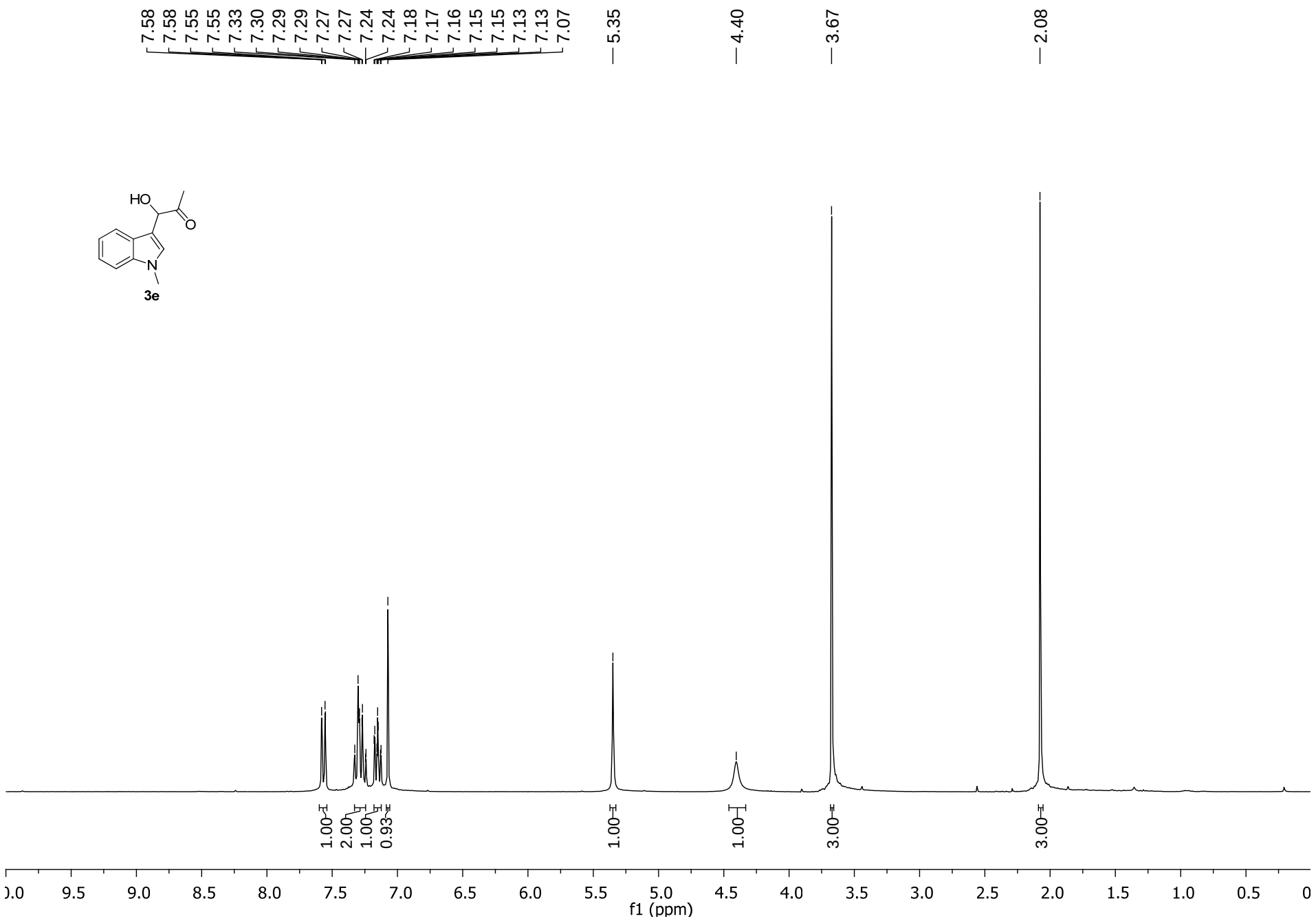


1-(4-(1,2-Dimethyl-1*H*-indol-3-yl)-2-methyl-5-phenylfuran-3-yl)ethanone (12d): Yellow solid; yield = 84% (288 mg); mp = 181–183 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 1.78 (s, 3H), 2.19 (s, 3H), 2.71 (s, 3H), 3.77 (s, 3H), 7.02–7.10 (m, 1H), 7.12–7.21 (m, 3H), 7.22–7.26 (m, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.34–7.41 (m, 3H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 11.0 (CH_3), 14.9 (CH_3), 29.8 (CH_3), 30.0 (CH_3), 104.8 (C), 109.0 (CH), 113.6 (C), 119.2 (CH), 120.1 (CH), 121.5 (CH), 124.8 (2 × CH), 125.4 (C), 127.2 (CH), 128.1 (C), 128.5 (2 × CH), 131.0 (C), 134.9 (C), 137.3 (C), 148.5 (C), 158.0 (C), 196.8 (C); LRMS (70 eV, EI): *m/z* (%) 343 (M^+, 100); HRMS (EI^+) calcd for $C_{23}H_{21}NO_2$: 343.1572, found: 343.1574.



3-(4,5-Dimethyl-2-phenylfuran-3-yl)-1*H*-indole (13): Yellow solid; yield = 58% (166 mg); mp = 116–118 °C; ^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 1.86 (s, 3H), 2.40 (s, 3H), 7.06–7.21 (m, 5H), 7.26 (at, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 8.1 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 2H), 8.21 (s, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) = 9.1 (CH_3), 12.0 (CH_3), 109.5 (C), 111.2 (CH), 116.5 (C), 118.1 (C), 119.9 (CH), 120.6 (CH), 122.3 (CH), 123.3 (CH), 124.8 (2 × CH), 126.3 (CH), 127.1 (C), 128.2 (2 × CH), 131.9 (C), 136.3 (C), 146.6 (C), 147.1 (C); LRMS (70 eV, EI): *m/z* (%) 287 (M^+, 100); HRMS (EI^+) calcd for $C_{20}H_{17}NO$: 287.1310, found: 287.1310.

^{1}H and ^{13}C NMR spectra of characterized compounds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7.16
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7.13
7.13
7.07
5.35
4.40
3.67
2.08
HO
O
N
3e
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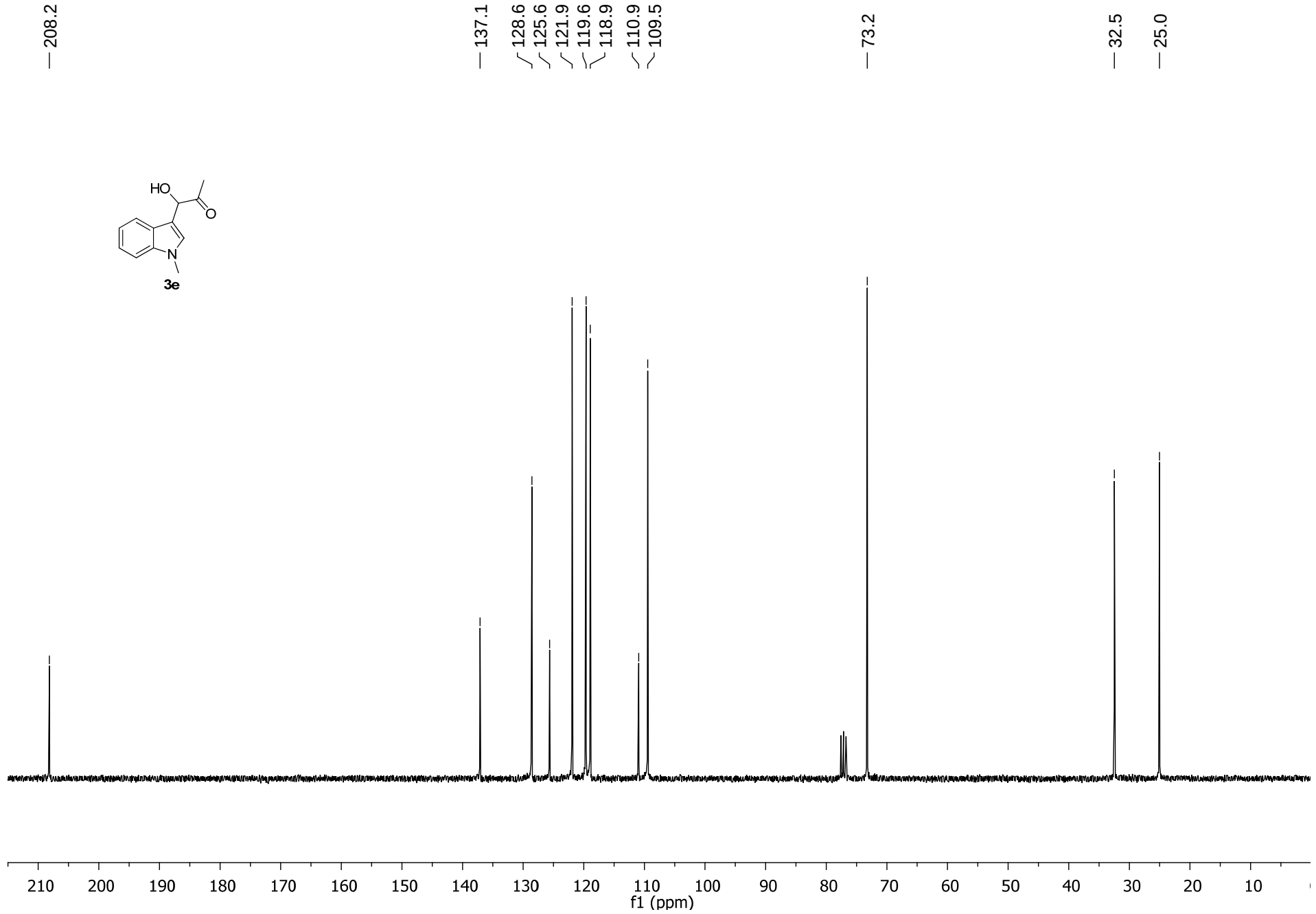
2.00
1.00
0.93
1.00
1.00
3.00
3.00
f1 (ppm)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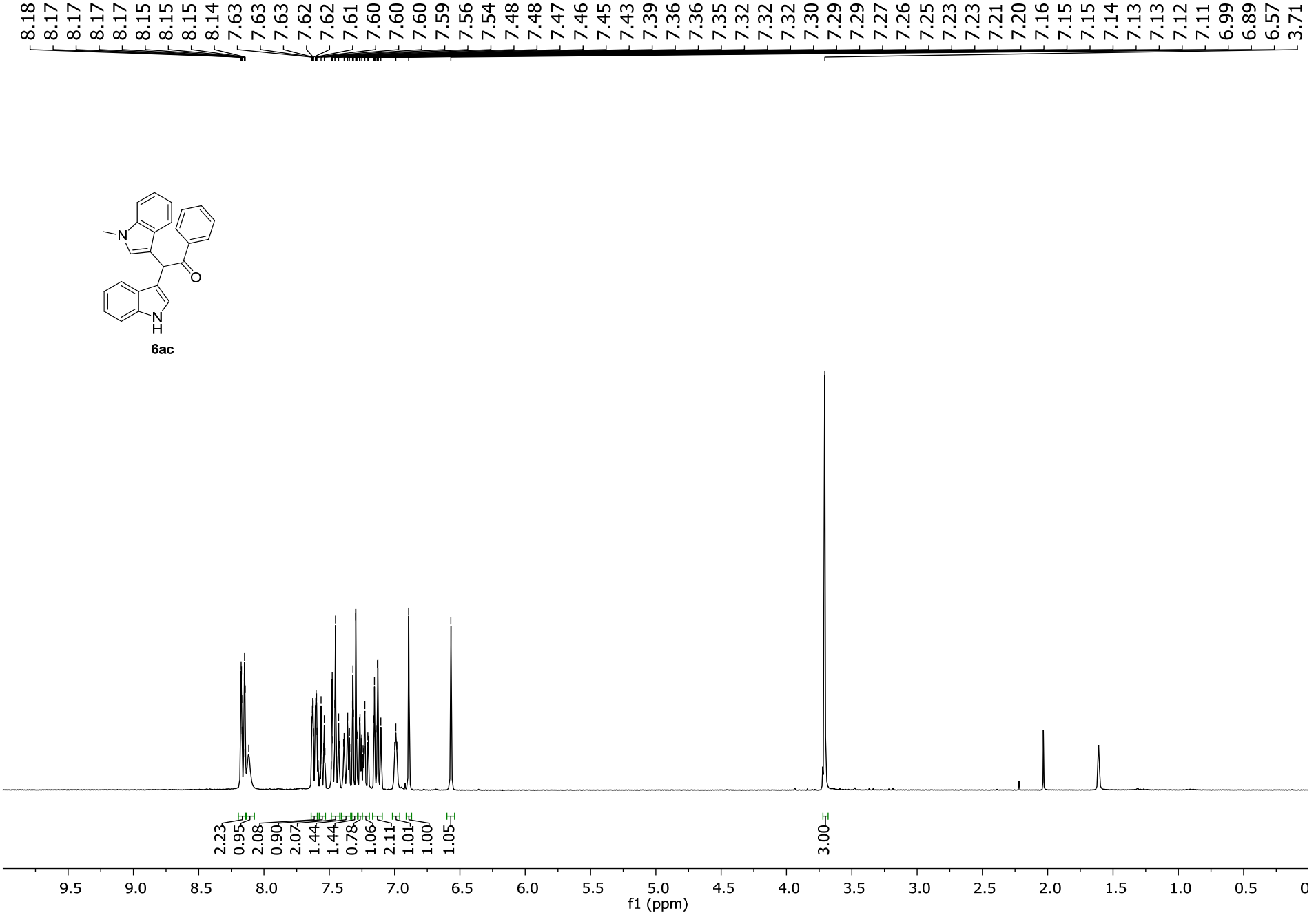
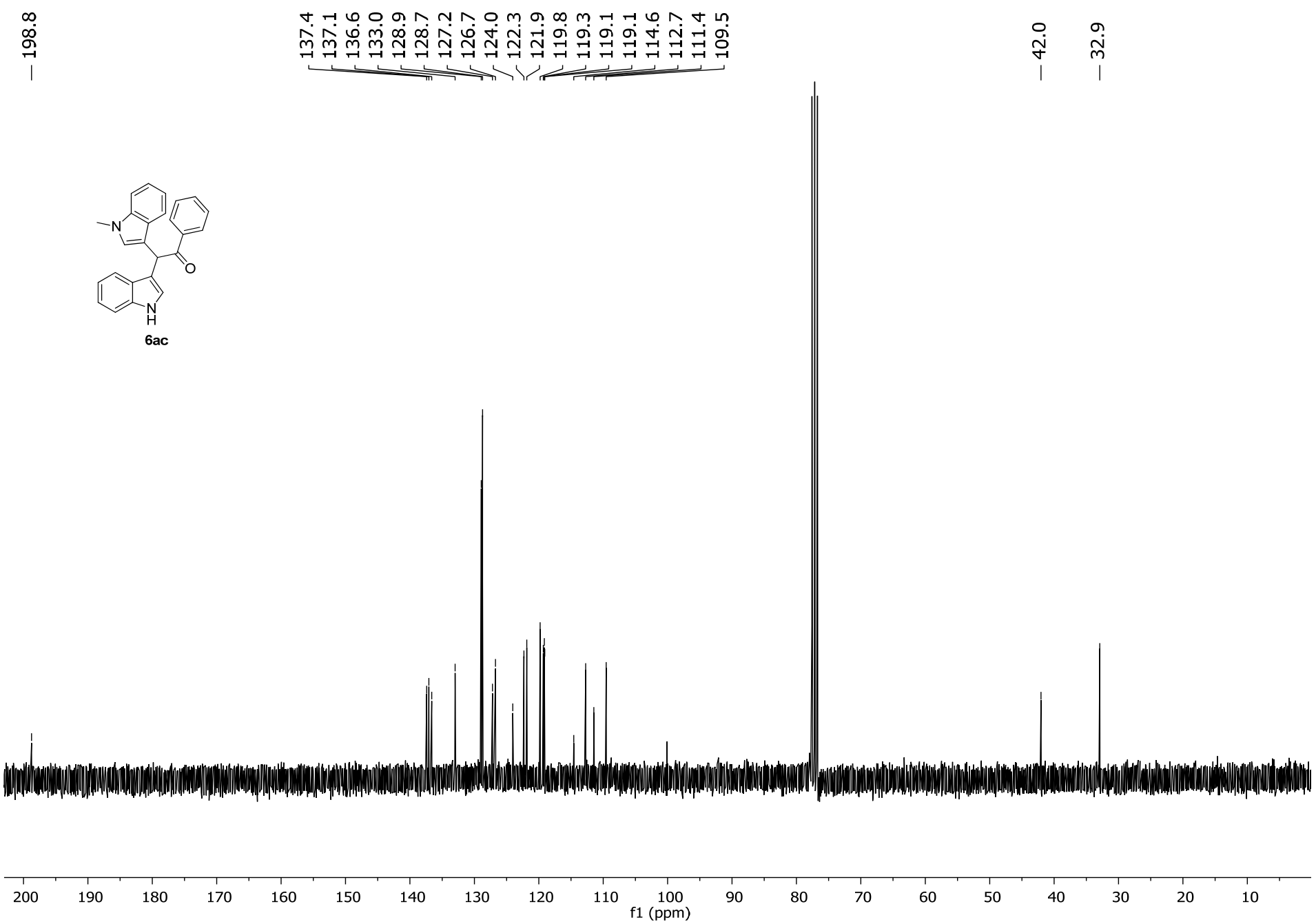
128.6
125.6
121.9
119.6
118.9
110.9
109.5
73.2
32.5
25.0
HO
O
N
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.18 8.17 8.17 8.17 8.17 8.15 8.15 8.15 8.14 7.63 7.63 7.63 7.62 7.62 7.61 7.60 7.60 7.60 7.59 7.56 7.54 7.48 7.48 7.47 7.46 7.45 7.43 7.39 7.36 7.36 7.35 7.32 7.32 7.32 7.30 7.29 7.29 7.27 7.26 7.25 7.23 7.23 7.21 7.20 7.16 7.15 7.15 7.14 7.13 7.13 7.12 7.11 6.99 6.89 6.57 3.71
N
O
N
H
6ac
2.23 0.95 2.08 0.90 2.07 1.44 1.44 0.78 1.06 2.11 1.01 1.00 1.05
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
f1 (ppm)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128.7
127.2
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124.0
122.3
121.9
119.8
119.3
119.1
119.1
114.6
112.7
111.4
109.5
42.0
32.9
N
O
N
H
6ac
200
190
180
170
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150
140
130
120
110
100
90
80
70
60
50
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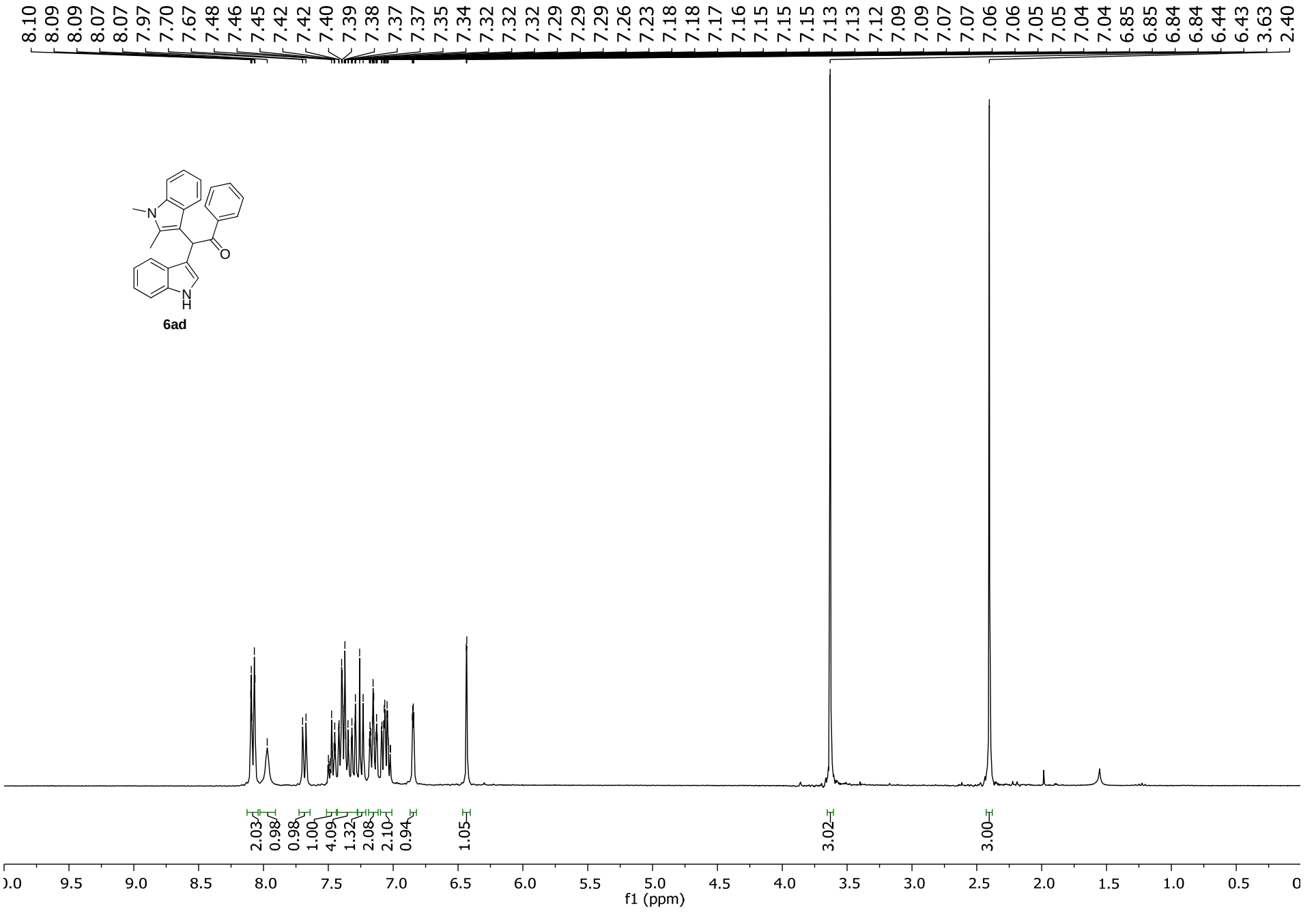
30
20
10
f1 (ppm)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N
O
N
H
6ad
2.03 0.98 0.98 1.00 4.09 1.32 2.08 2.10 0.94 1.05 3.02 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
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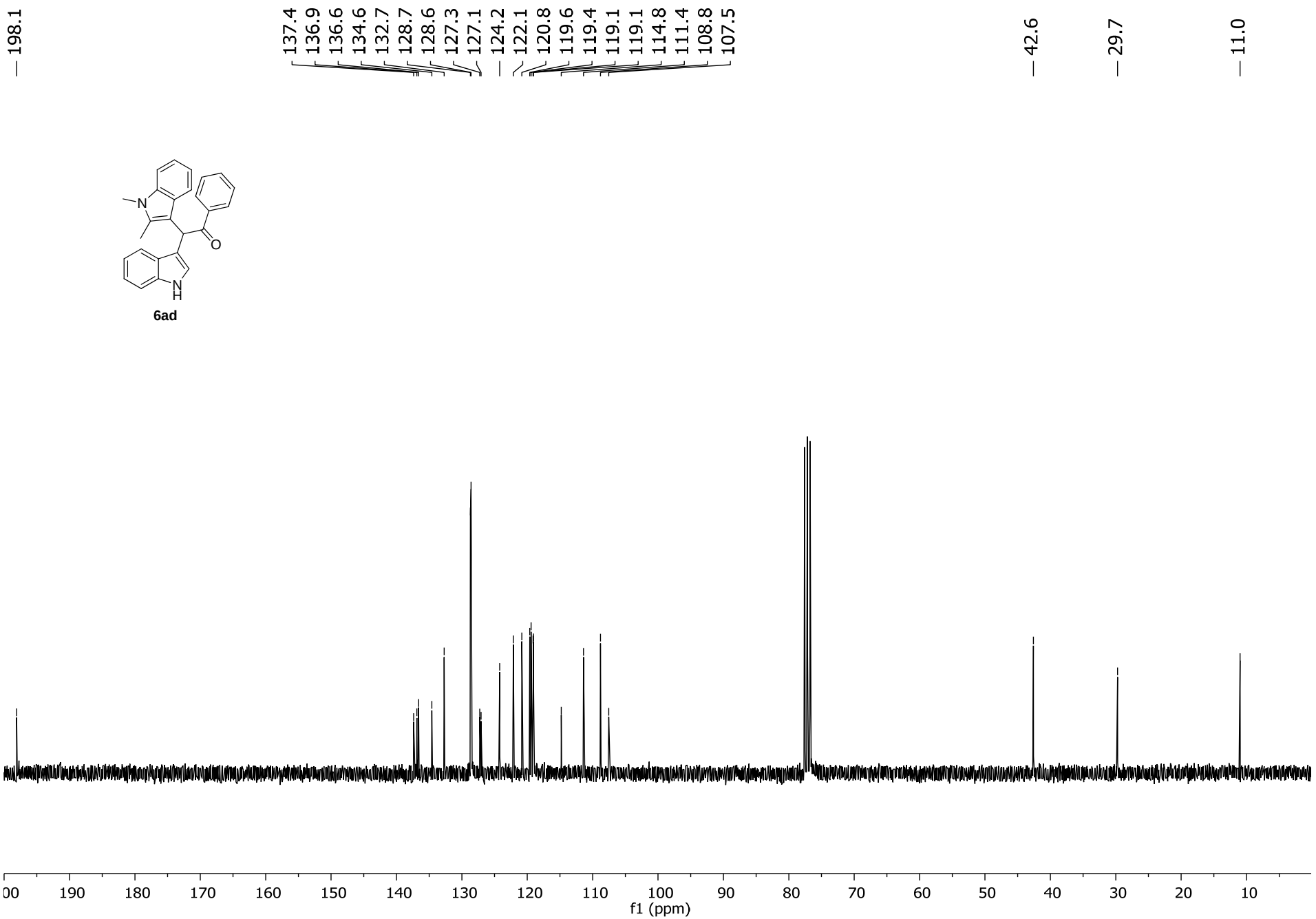
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119.4
119.1
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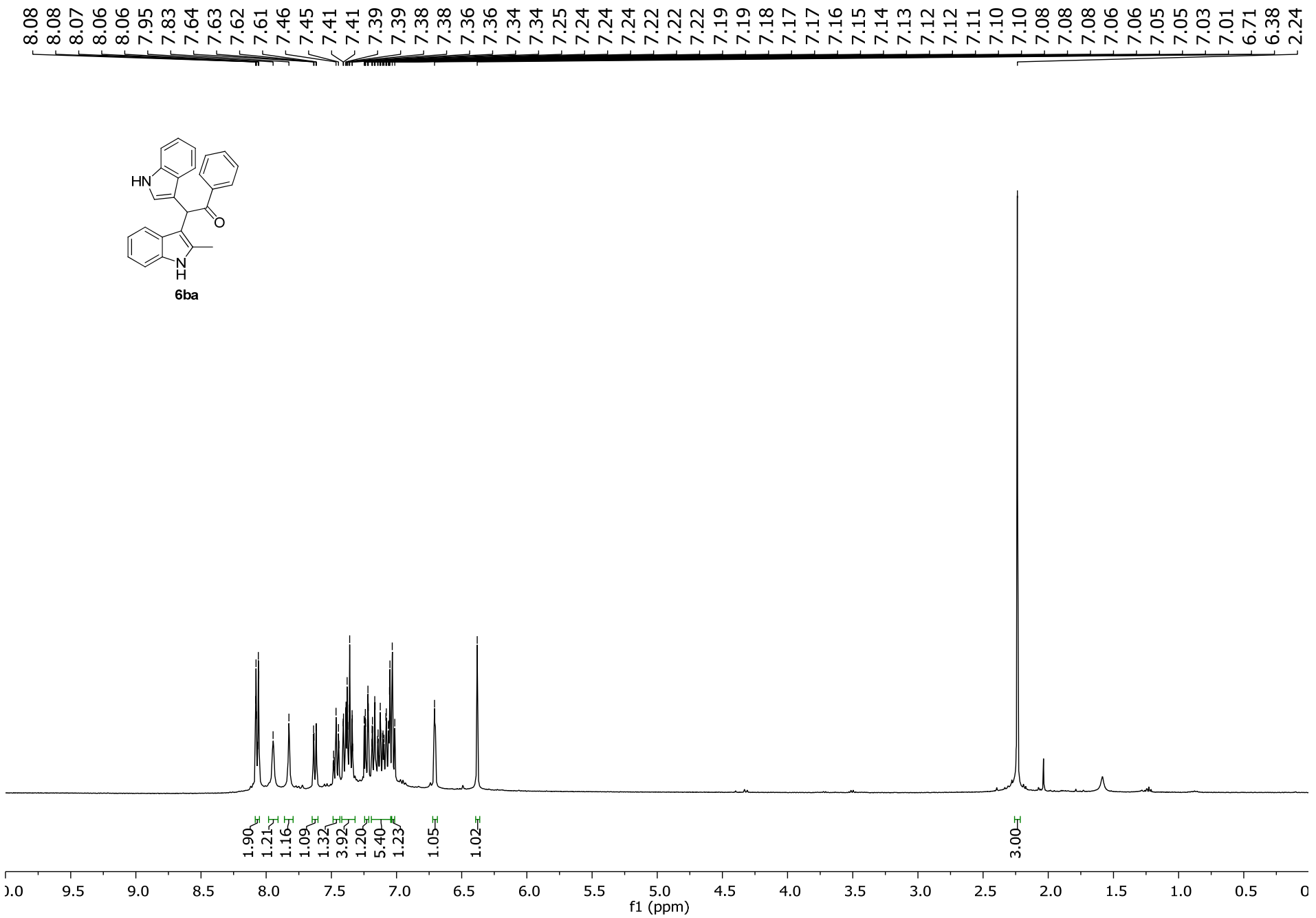
29.7
11.0
N
O
N
H
6ad
f1 (ppm)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HN
O
N
H
6ba
1.90 1.21 1.16 1.09 1.32 3.92 1.20 5.40 1.23 1.05 1.02 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
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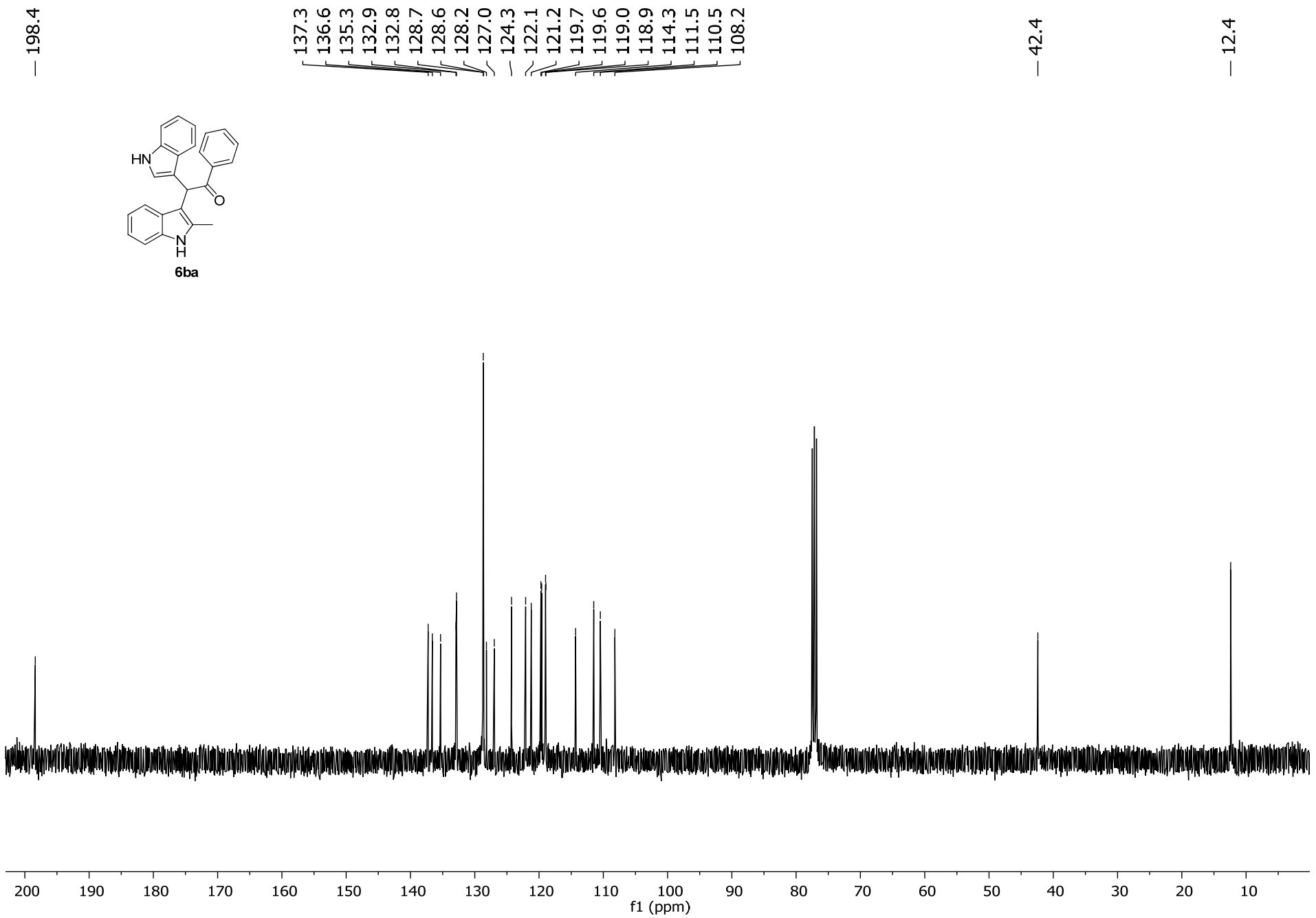
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119.0
118.9
114.3
111.5
110.5
108.2
42.4
12.4
HN
O
N
H
6ba
200
190
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140
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120
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100
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80
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60
50
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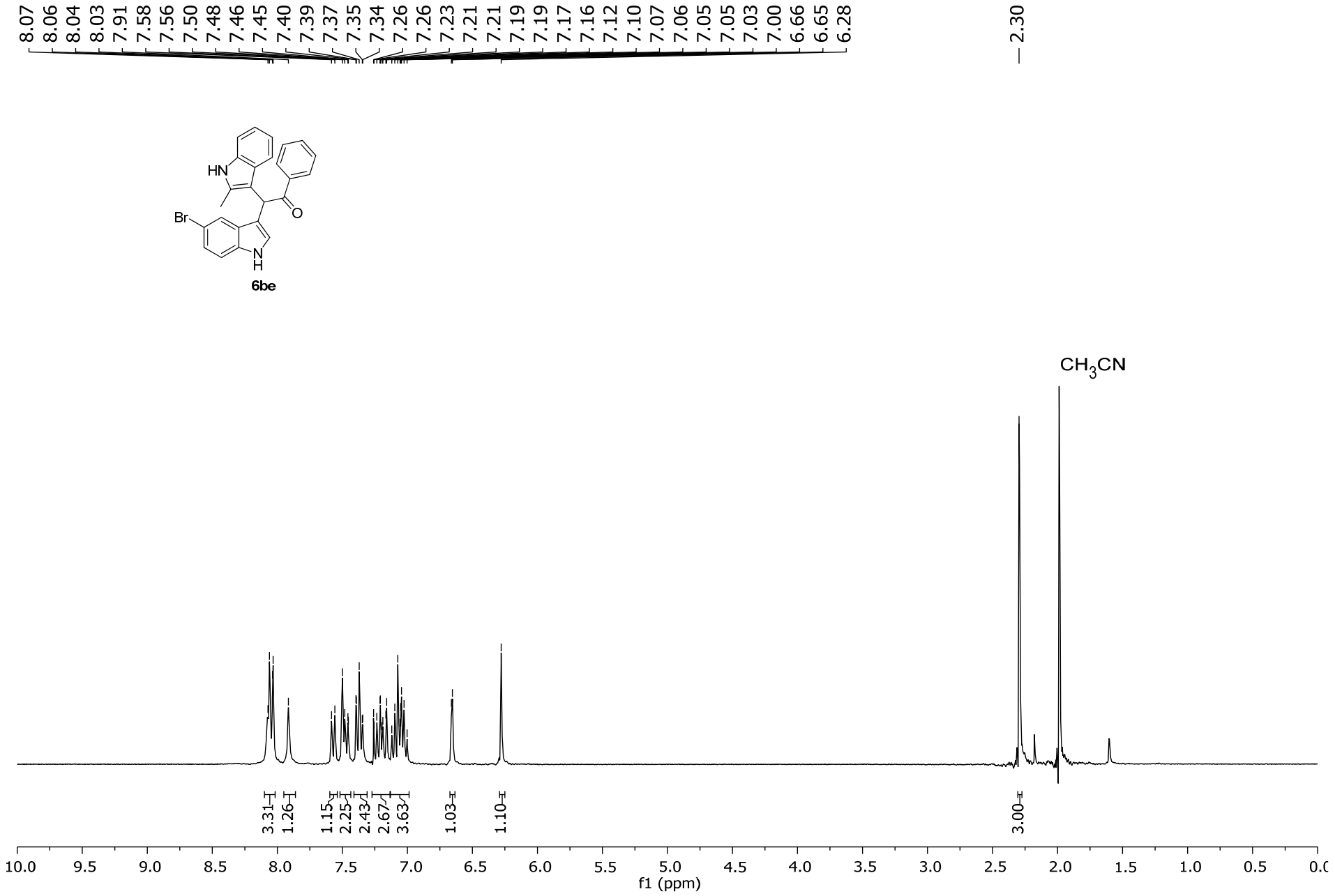
20
10
f1 (ppm)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7.34
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7.23
7.21
7.21
7.19
7.19
7.17
7.16
7.12
7.10
7.07
7.06
7.05
7.05
7.03
7.00
6.66
6.65
6.28
2.30
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Br
O
H
N
6be
CH3CN
3.31
1.26
1.15
2.25
2.43
2.67
3.63
1.03
1.10
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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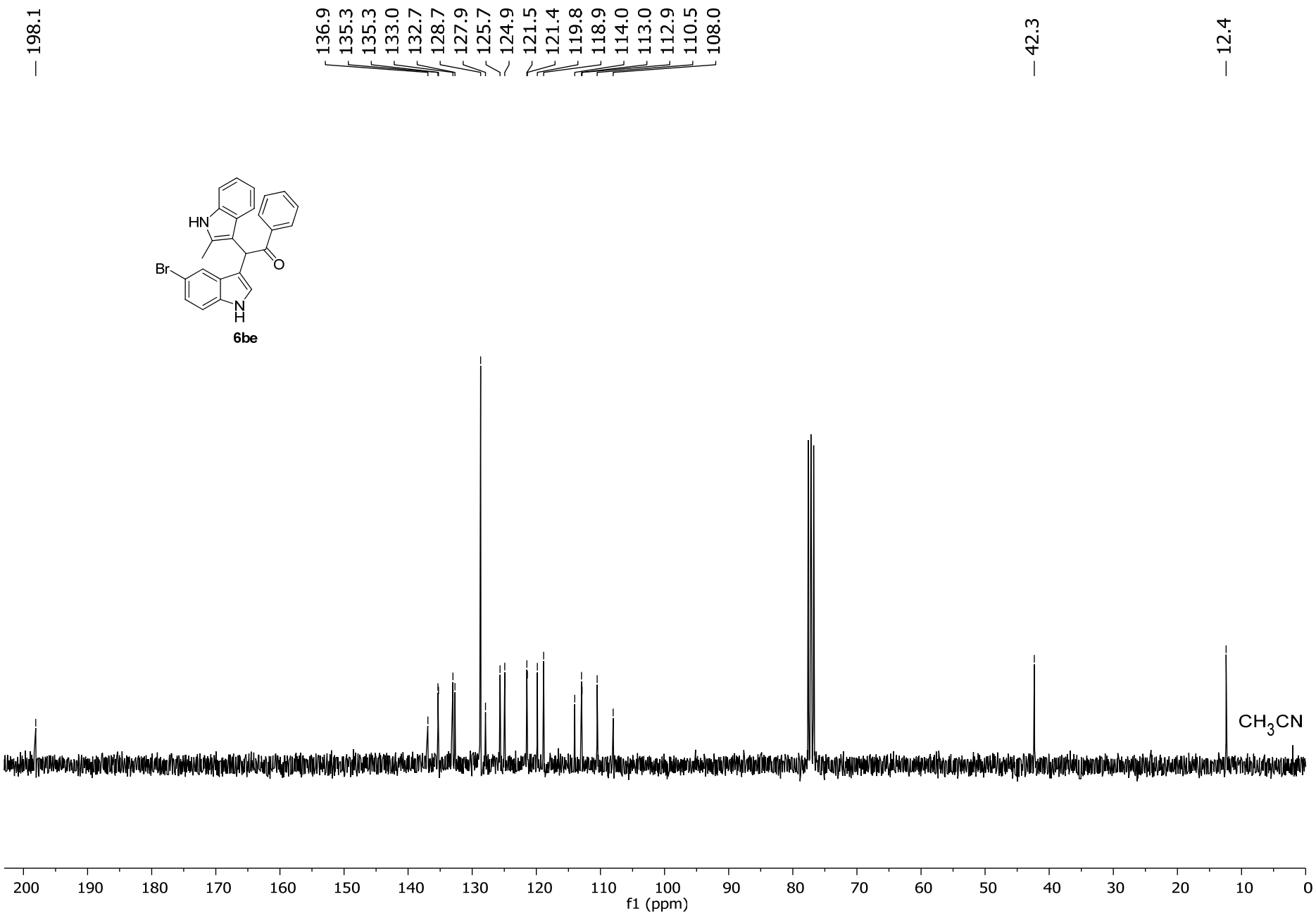
f1 (ppm)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121.4
119.8
118.9
114.0
113.0
112.9
110.5
108.0
42.3
12.4
HN
Br
O
N
H
6be
CH3CN
200
190
180
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130
120
110
100
90
80
70
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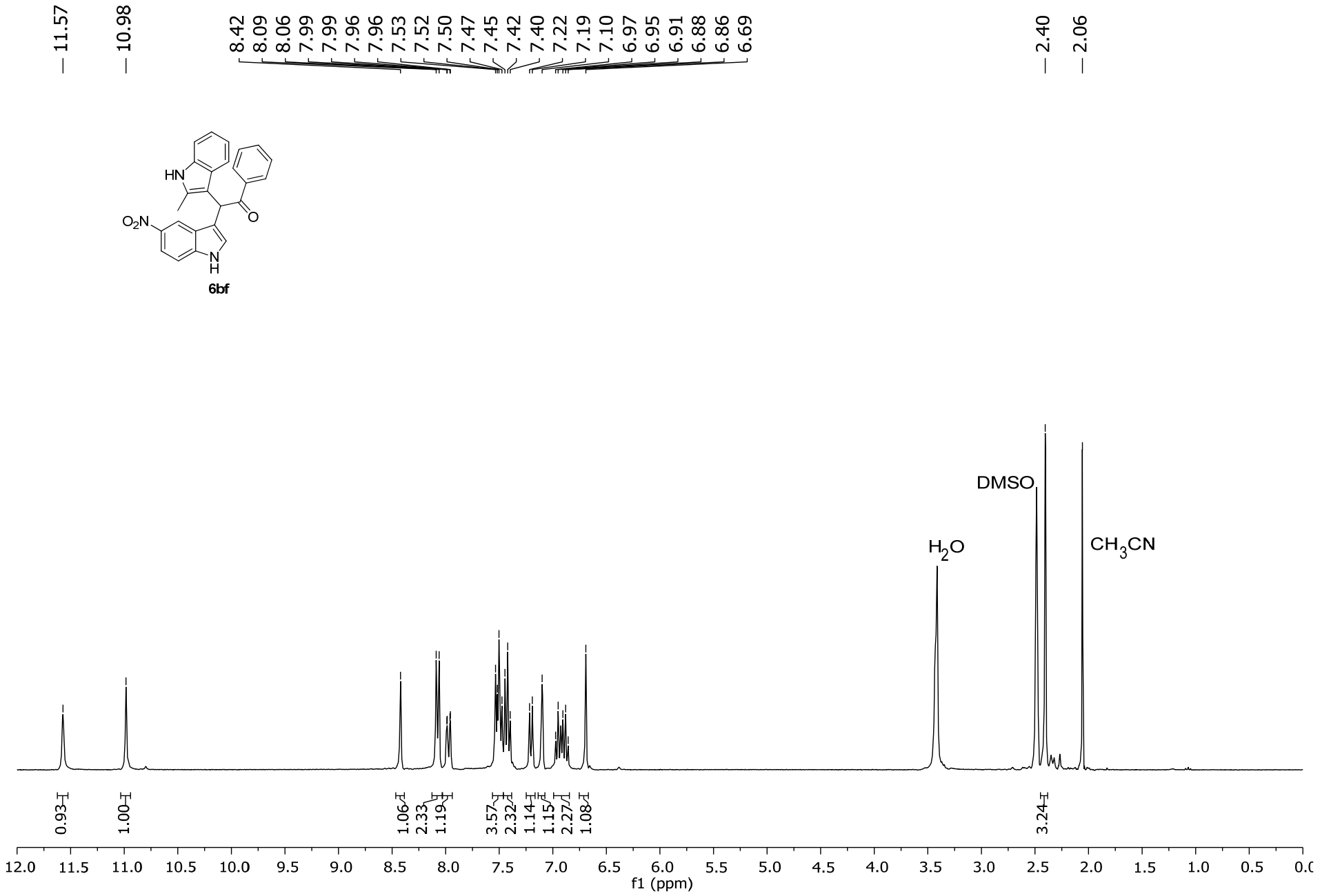
50
40
30
20
10
0
f1 (ppm)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7.53
7.52
7.50
7.47
7.45
7.42
7.40
7.22
7.19
7.10
6.97
6.95
6.91
6.88
6.86
6.69
2.40
2.06
HN
O2N
O
N
H
6bf
DMSO
H2O
CH3CN
0.93
1.00
1.06
2.33
1.19
3.57
2.32
1.14
1.15
2.27
1.08
3.24
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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4.0
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3.0
2.5
2.0
1.5
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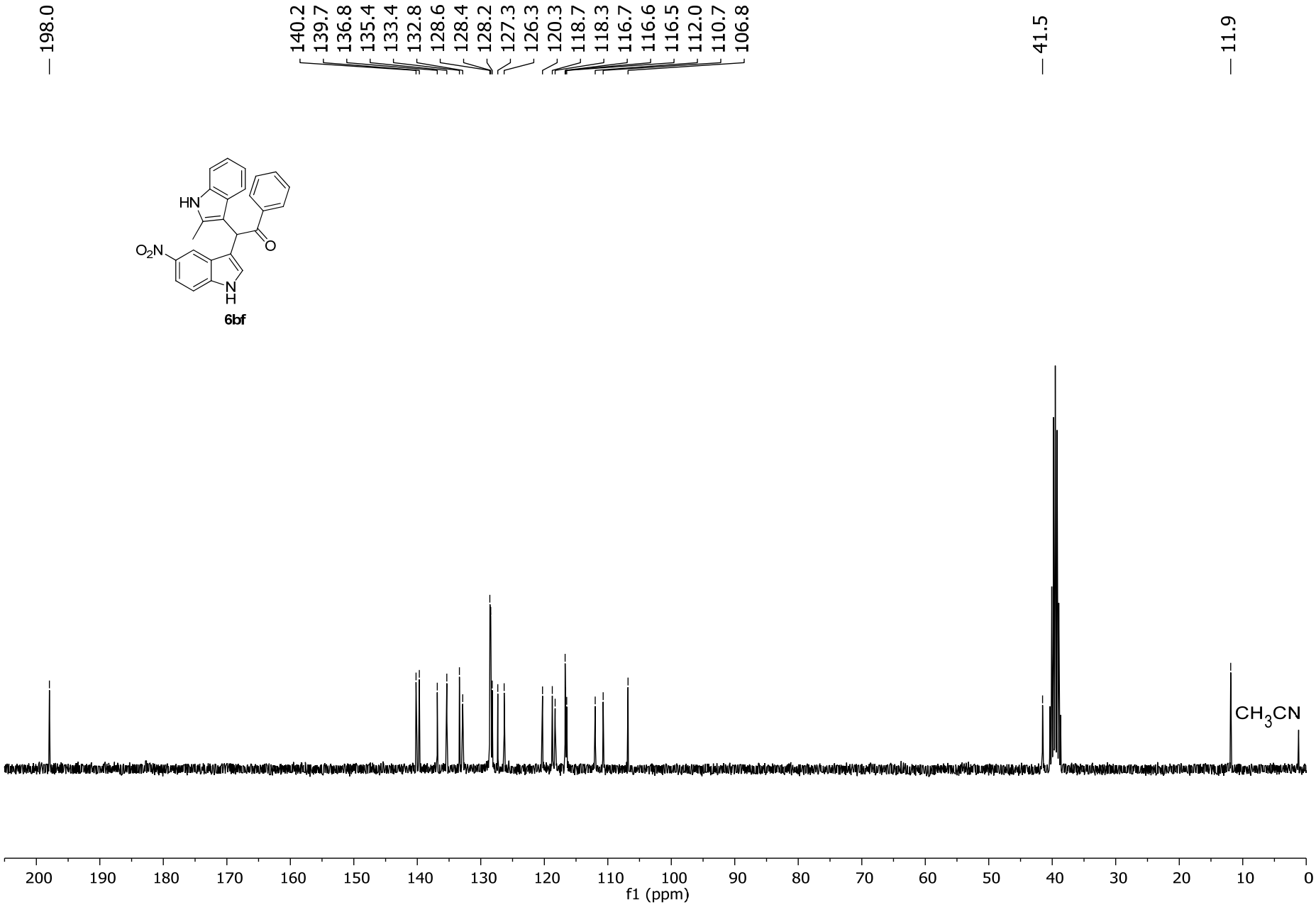
0.5
f1 (ppm)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132.8
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128.4
128.2
127.3
126.3
120.3
118.7
118.3
116.7
116.6
116.5
112.0
110.7
106.8
41.5
11.9
HN
O2N
O
N
H
6bf
CH3CN
200
190
180
170
160
150
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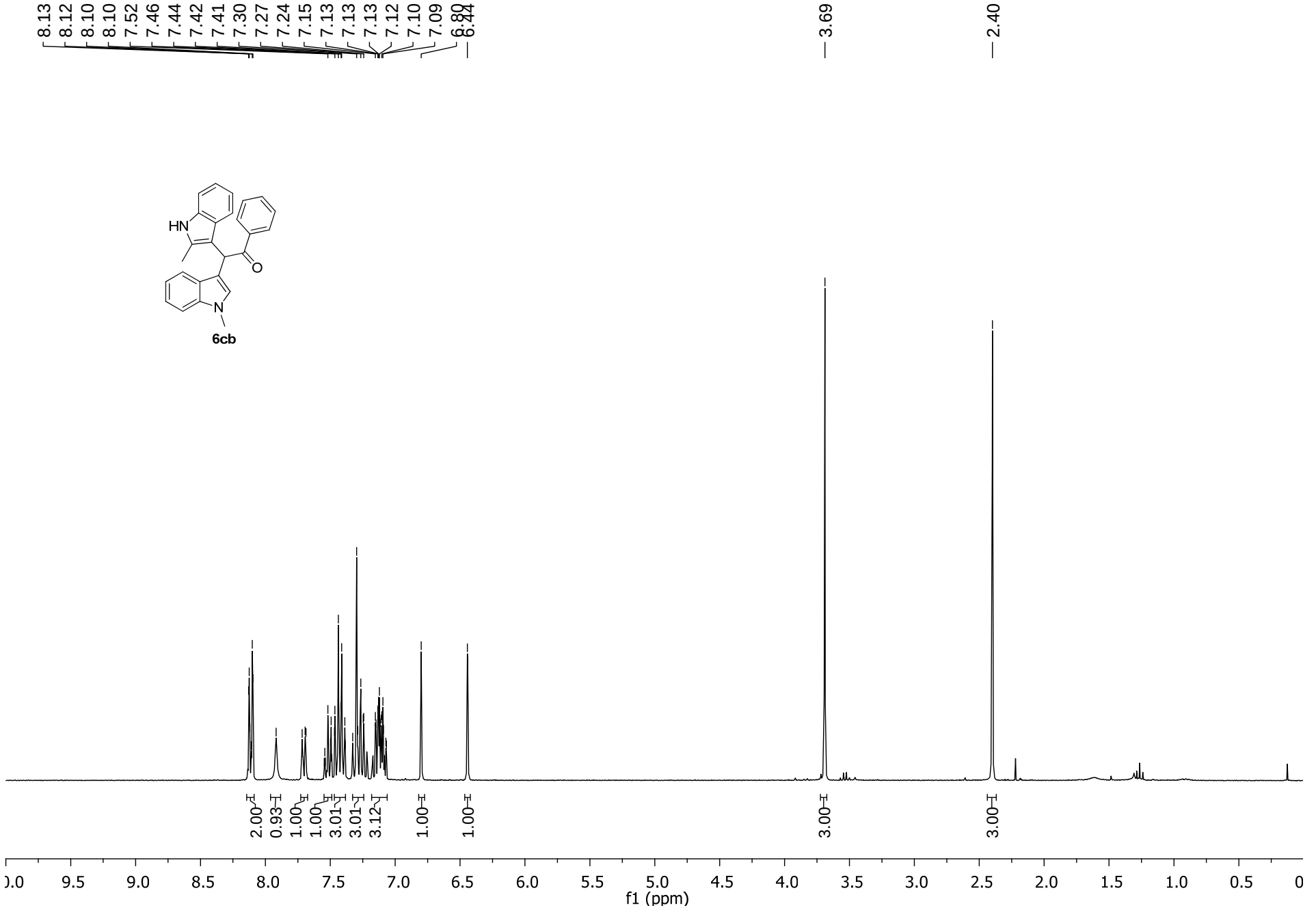
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.30
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7.15
7.13
7.13
7.13
7.12
7.10
7.09
6.80
6.44
3.69
2.40
HN
O
N
6cb
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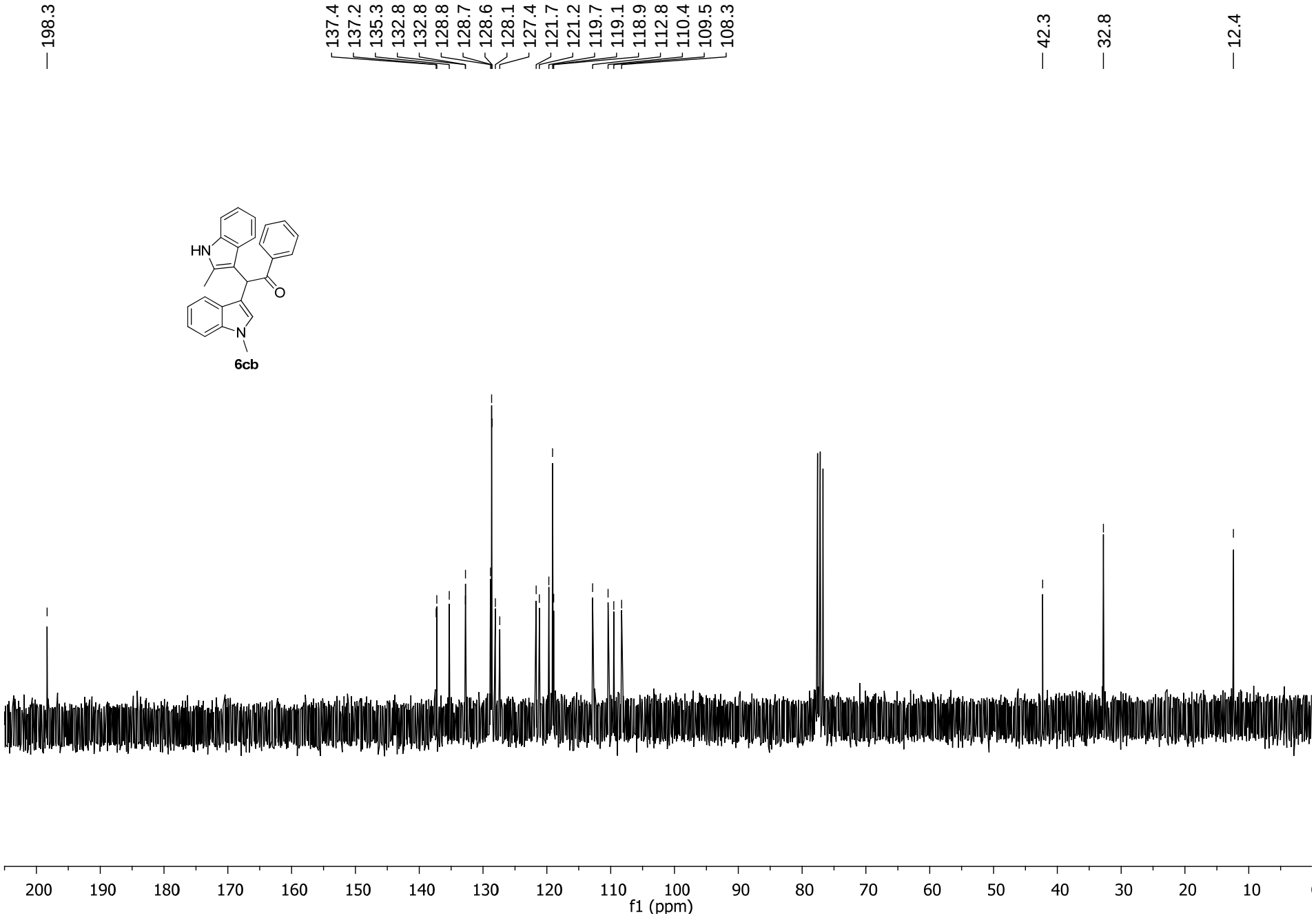
1.00
3.01
3.01
3.12
1.00
1.00
3.00
3.00
f1 (ppm)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127.4
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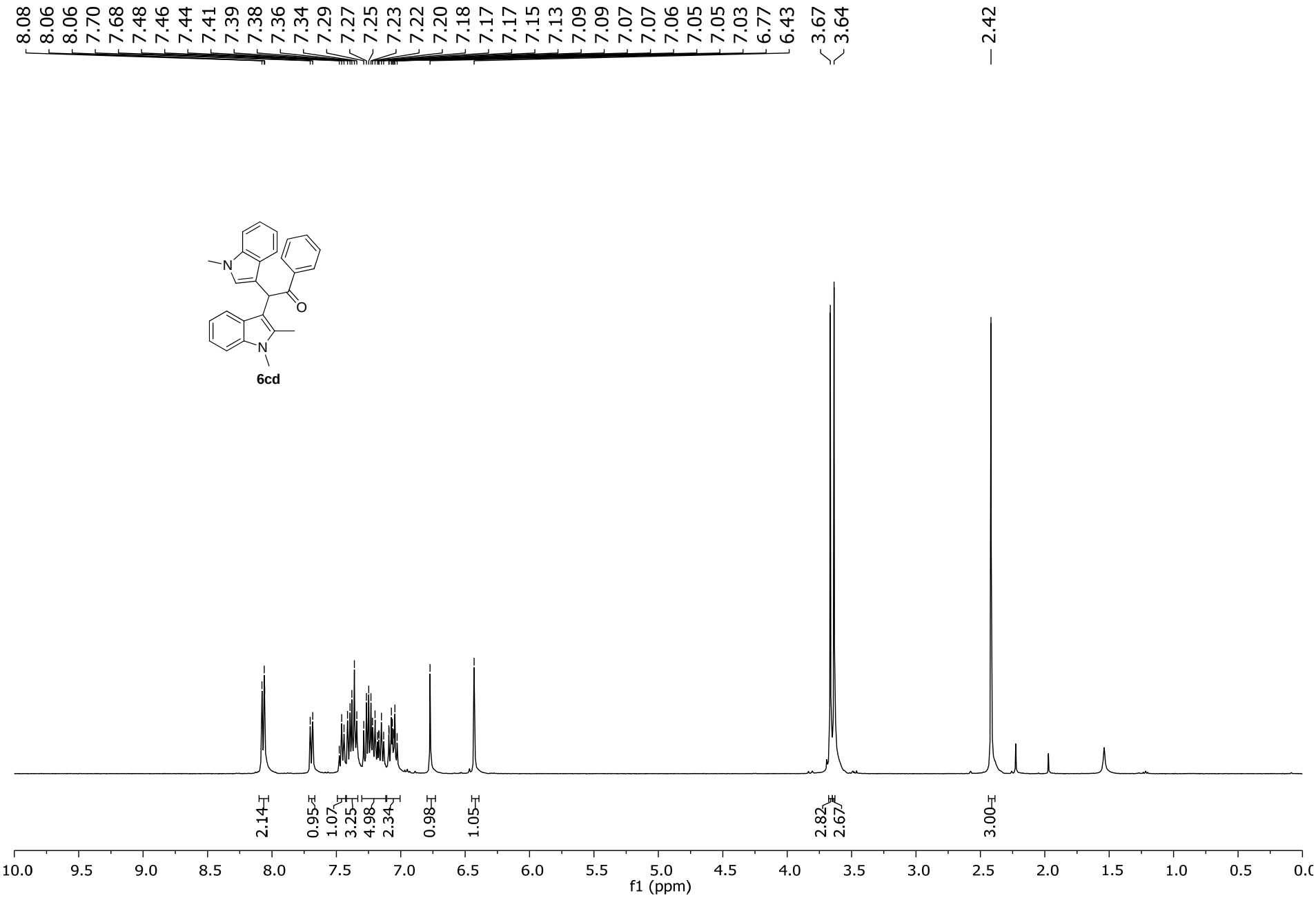
121.2
119.7
119.1
118.9
112.8
110.4
109.5
108.3
42.3
32.8
12.4
HN
O
N
6cb
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.36
7.34
7.29
7.27
7.25
7.23
7.22
7.20
7.18
7.17
7.17
7.15
7.13
7.09
7.09
7.07
7.07
7.06
7.05
7.05
7.03
6.77
6.43
3.67
3.64
2.42
6cd
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0.98
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2.82
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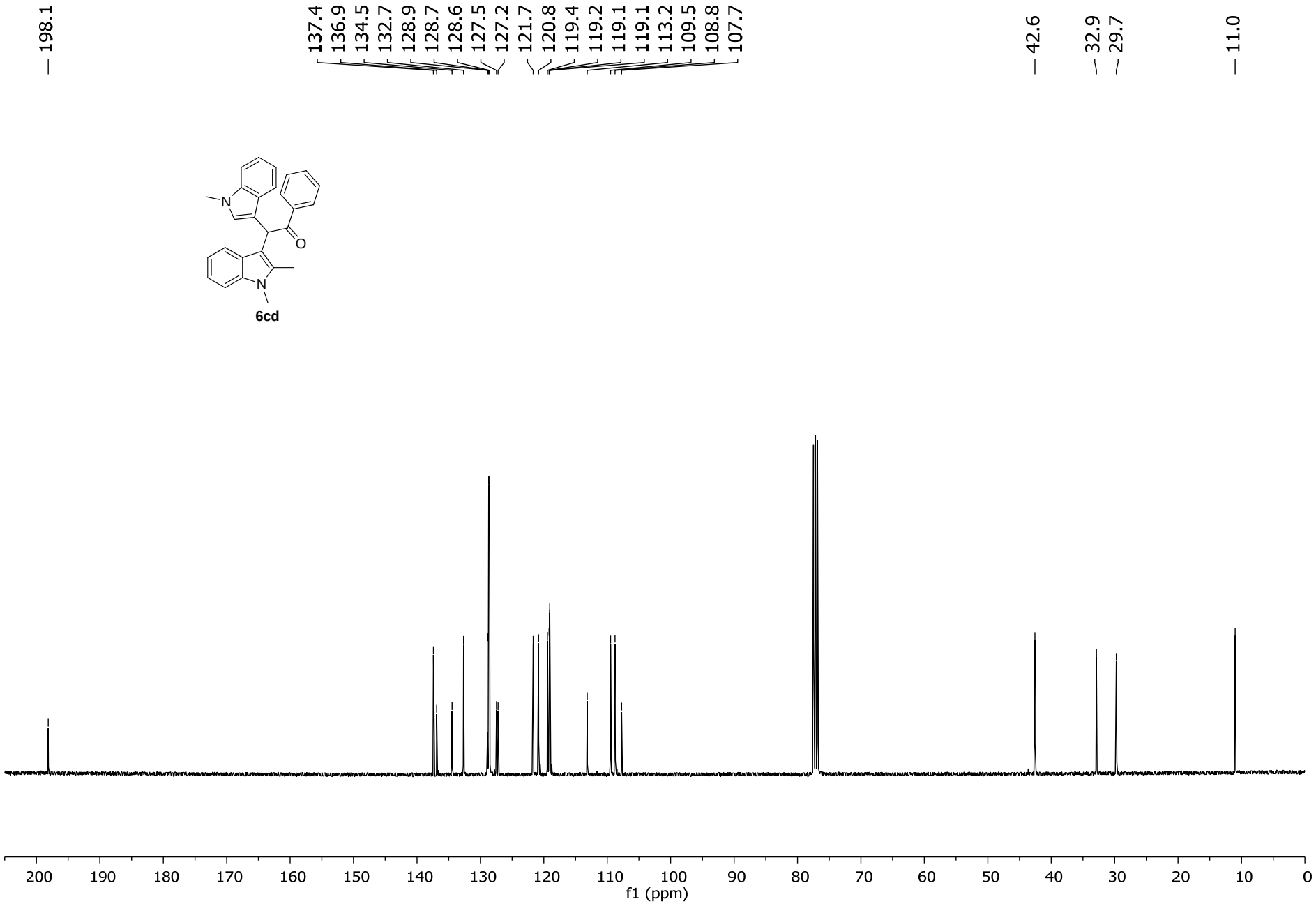
3.00
f1 (ppm)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119.1
119.1
113.2
109.5
108.8
107.7
42.6
32.9
29.7
11.0
N
O
N
6cd
200
190
180
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150
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130
120
110
100
90
80
70
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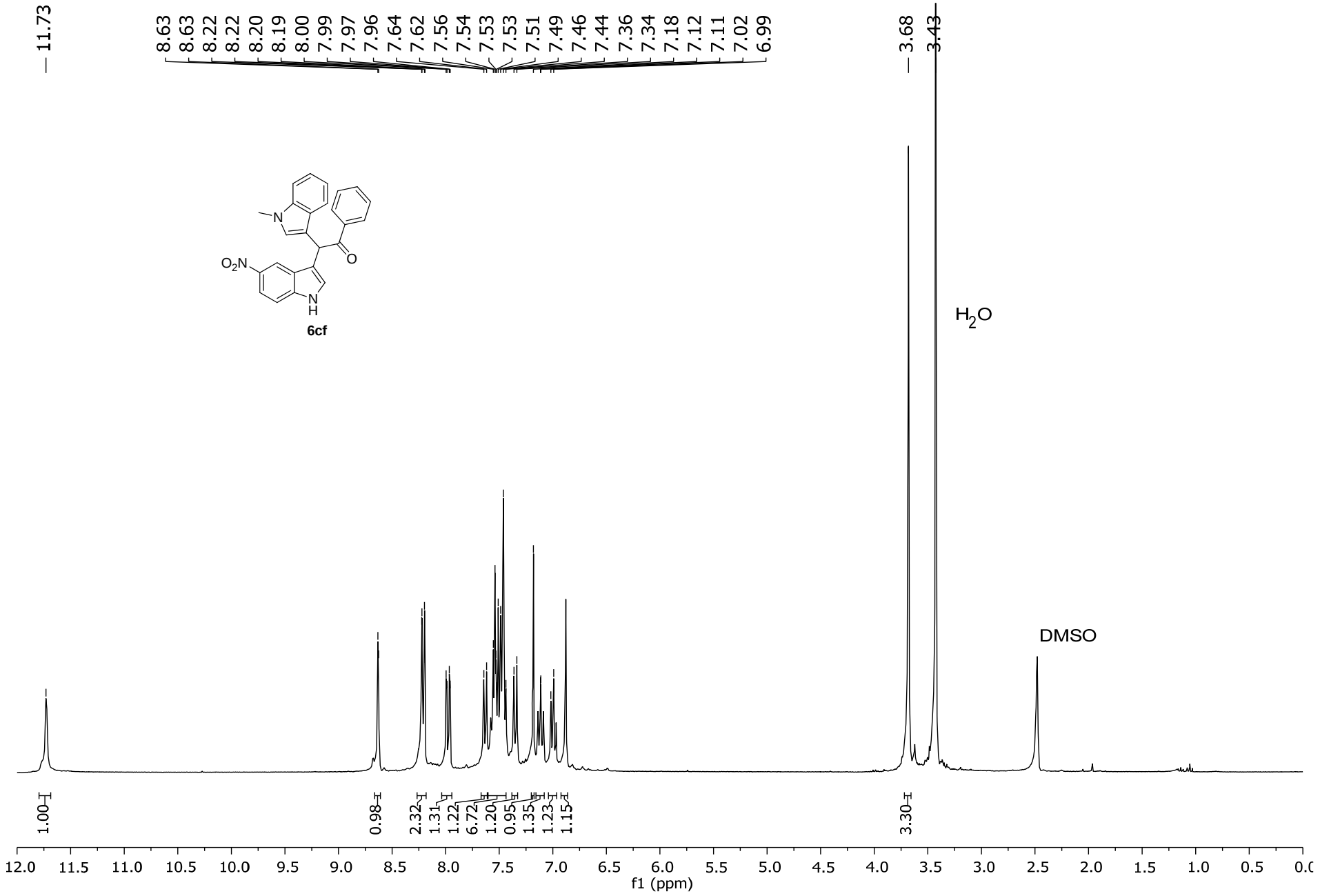
50
40
30
20
10
0
f1 (ppm)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7.99
7.97
7.96
7.64
7.62
7.56
7.54
7.53
7.53
7.51
7.49
7.46
7.44
7.36
7.34
7.18
7.12
7.11
7.02
6.99
3.68
3.43
H2O
DMSO
6cf
1.00
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1.22
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1.23
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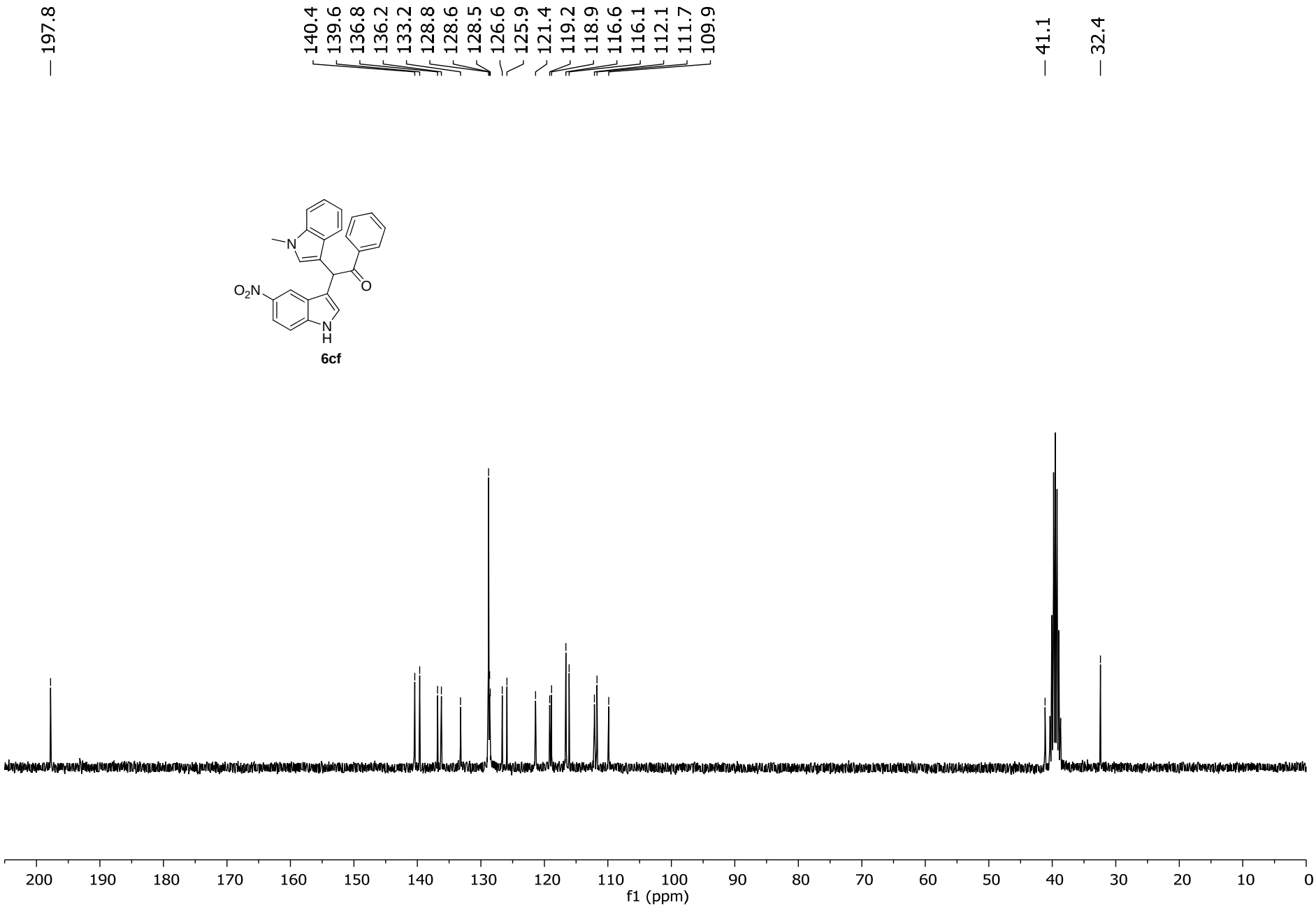
3.30
f1 (ppm)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121.4
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118.9
116.6
116.1
112.1
111.7
109.9
41.1
32.4
O2N
N
O
N
H
6cf
200
190
180
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130
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110
100
90
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70
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50
40
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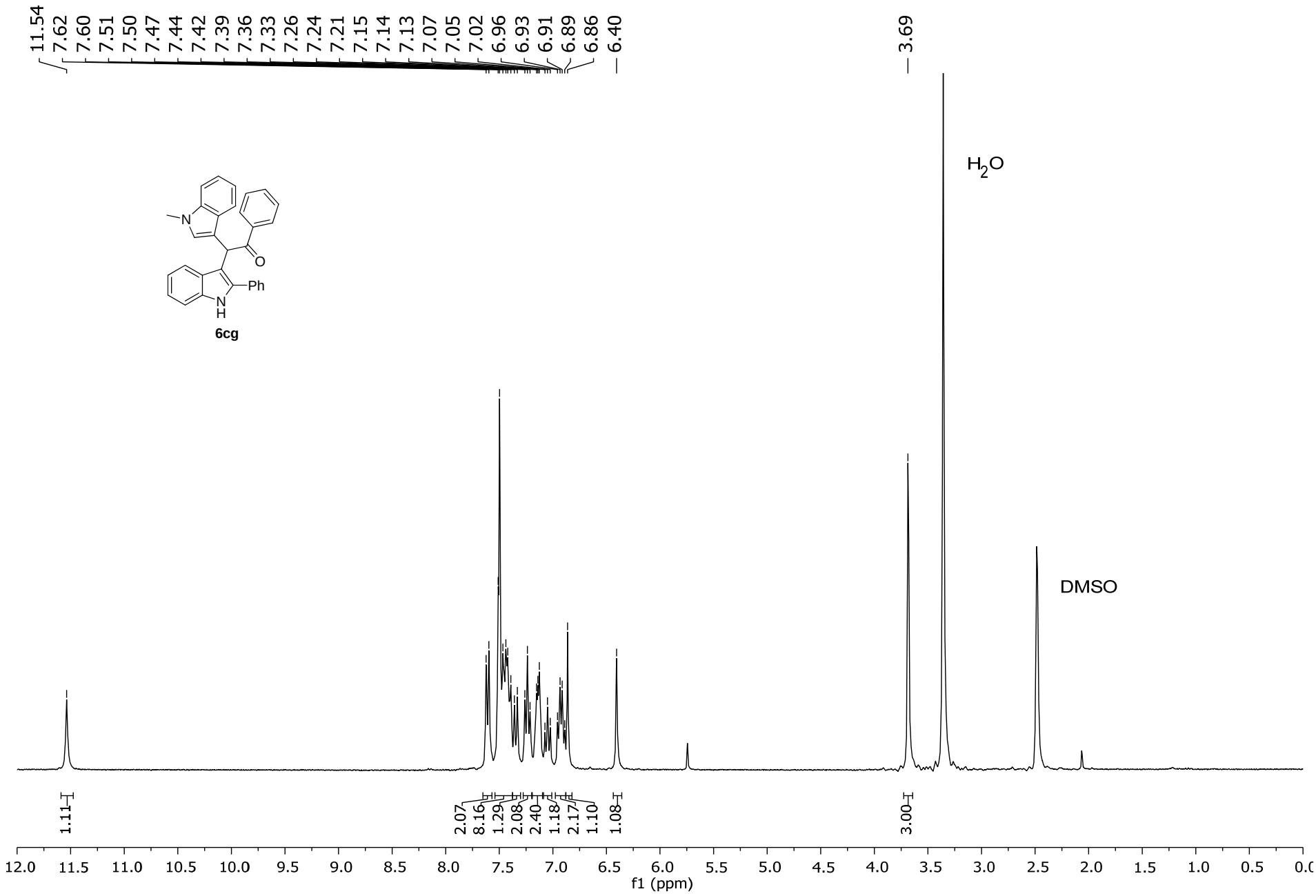
f1 (ppm)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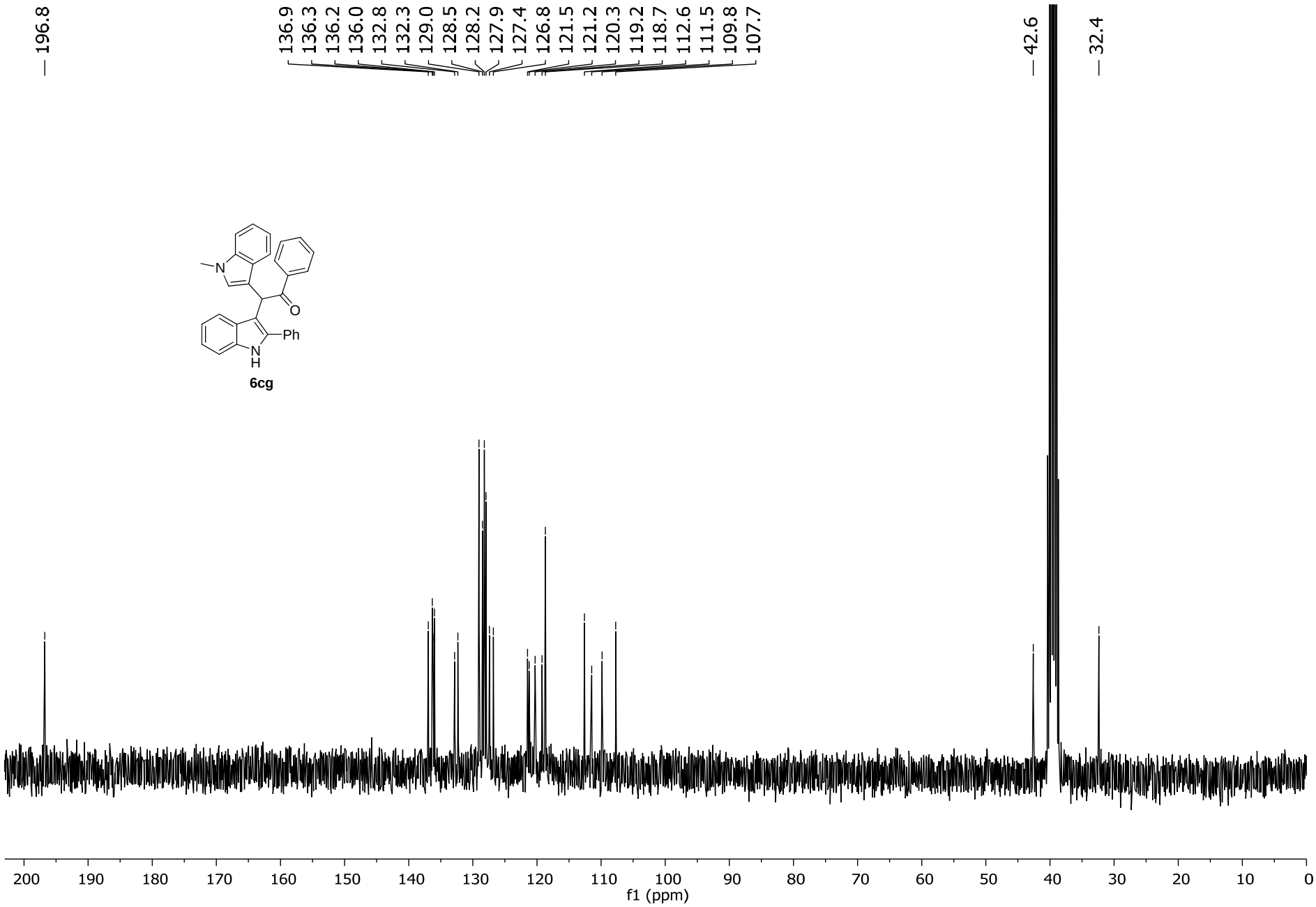
7.36
7.33
7.26
7.24
7.21
7.15
7.14
7.13
7.07
7.05
7.02
6.96
6.93
6.91
6.89
6.86
6.40
3.69
H2O
DMSO
N
O
Ph
N
H
6cg
1.11
2.07
8.16
1.29
2.08
2.40
1.18
2.17
1.10
1.08
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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121.5
121.2
120.3
119.2
118.7
112.6
111.5
109.8
107.7
42.6
32.4
N
O
Ph
N
H
6cg
200
190
180
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130
120
110
100
90
80
70
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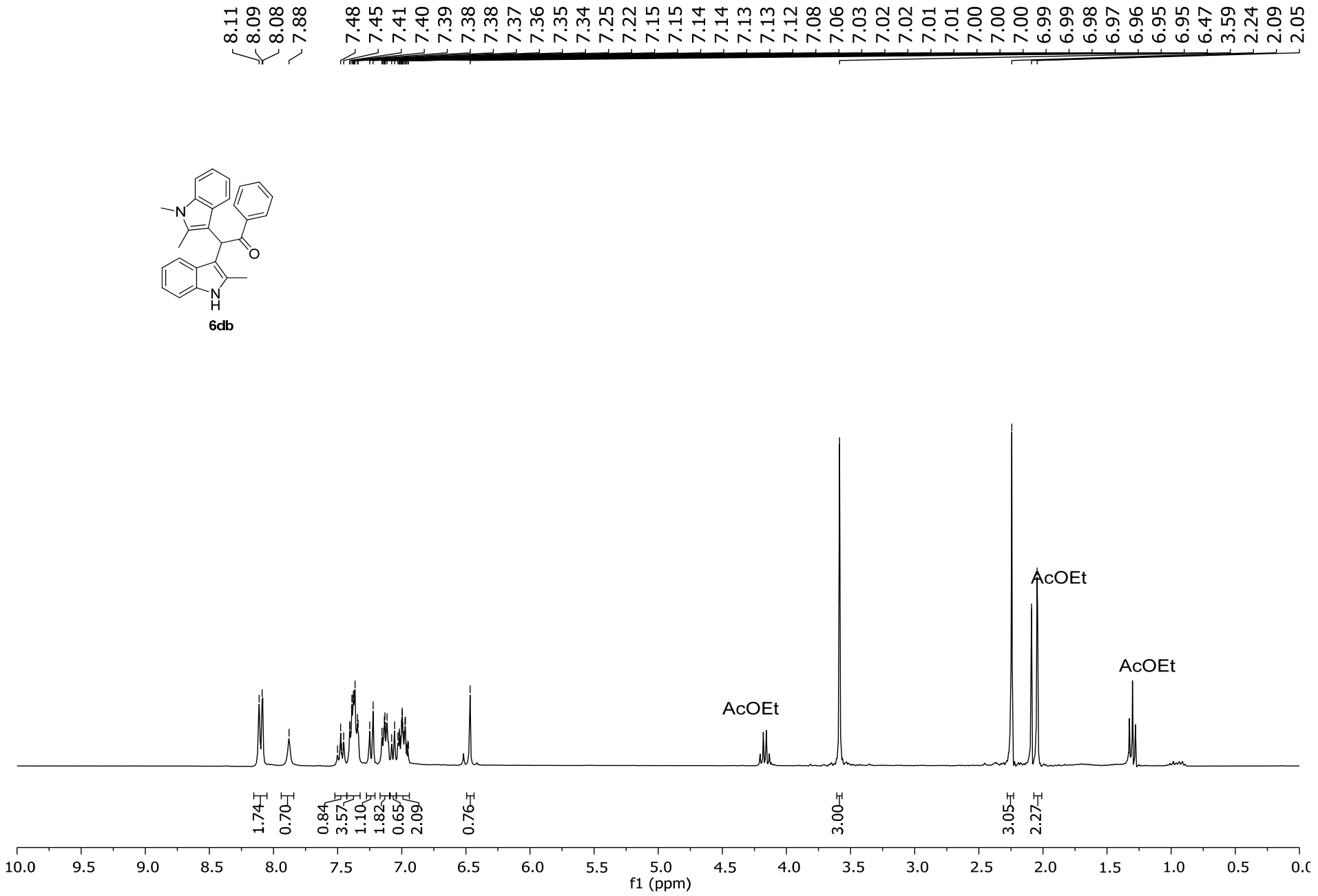
50
40
30
20
10
0
f1 (ppm)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7.36
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7.34
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7.15
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7.14
7.14
7.13
7.13
7.12
7.08
7.06
7.03
7.02
7.02
7.01
7.01
7.00
7.00
7.00
6.99
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6.98
6.97
6.96
6.95
6.95
6.47
3.59
2.24
2.09
2.05
6db
AcOEt
AcOEt
AcOEt
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0.70
0.84
3.57
1.10
1.82
0.65
2.09
0.76
3.00
3.05
2.27
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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3.0
2.5
2.0
1.5
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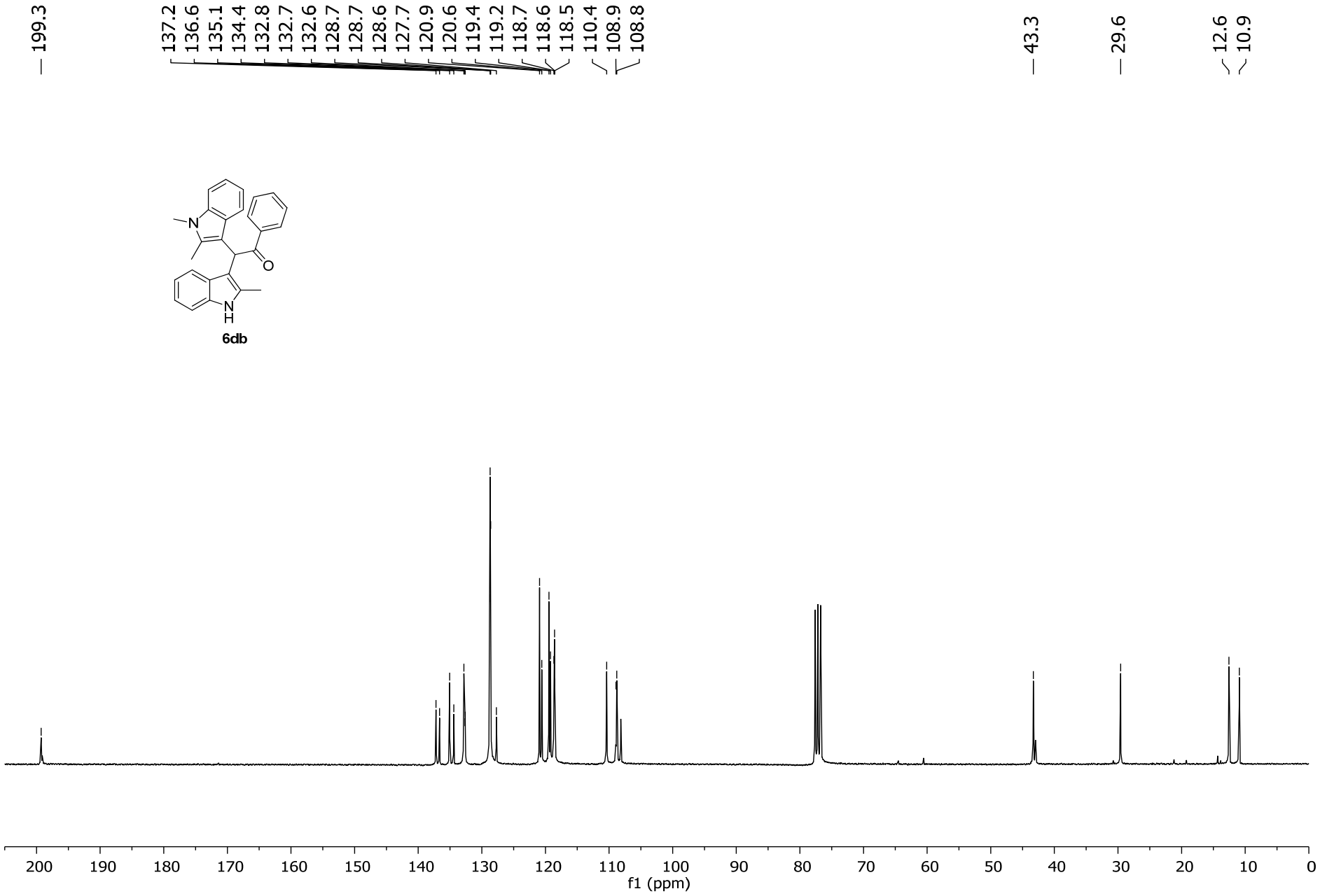
0.5
f1 (ppm)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119.4
119.2
118.7
118.6
118.5
110.4
108.9
108.8
43.3
29.6
12.6
10.9
6db
200
190
180
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130
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110
100
90
80
70
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50
40
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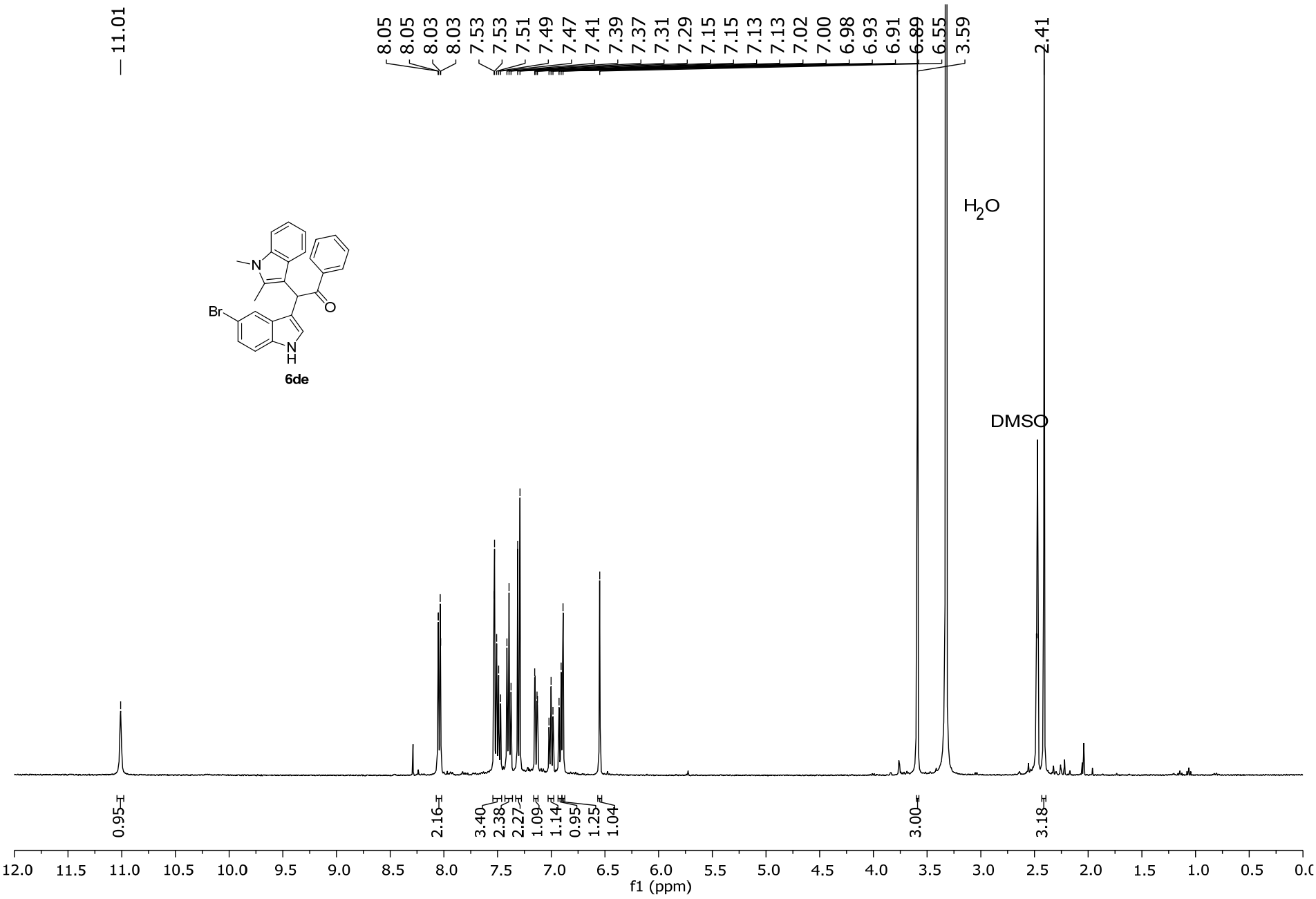
10
0
f1 (ppm)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7.37
7.31
7.29
7.15
7.15
7.13
7.13
7.02
7.00
6.98
6.93
6.91
6.89
6.55
3.59
2.41
H2O
DMSO
Br
N
O
N
H
6de
0.95
2.16
3.40
2.38
2.27
1.09
1.14
0.95
1.25
1.04
3.00
3.18
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
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6.5
6.0
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5.0
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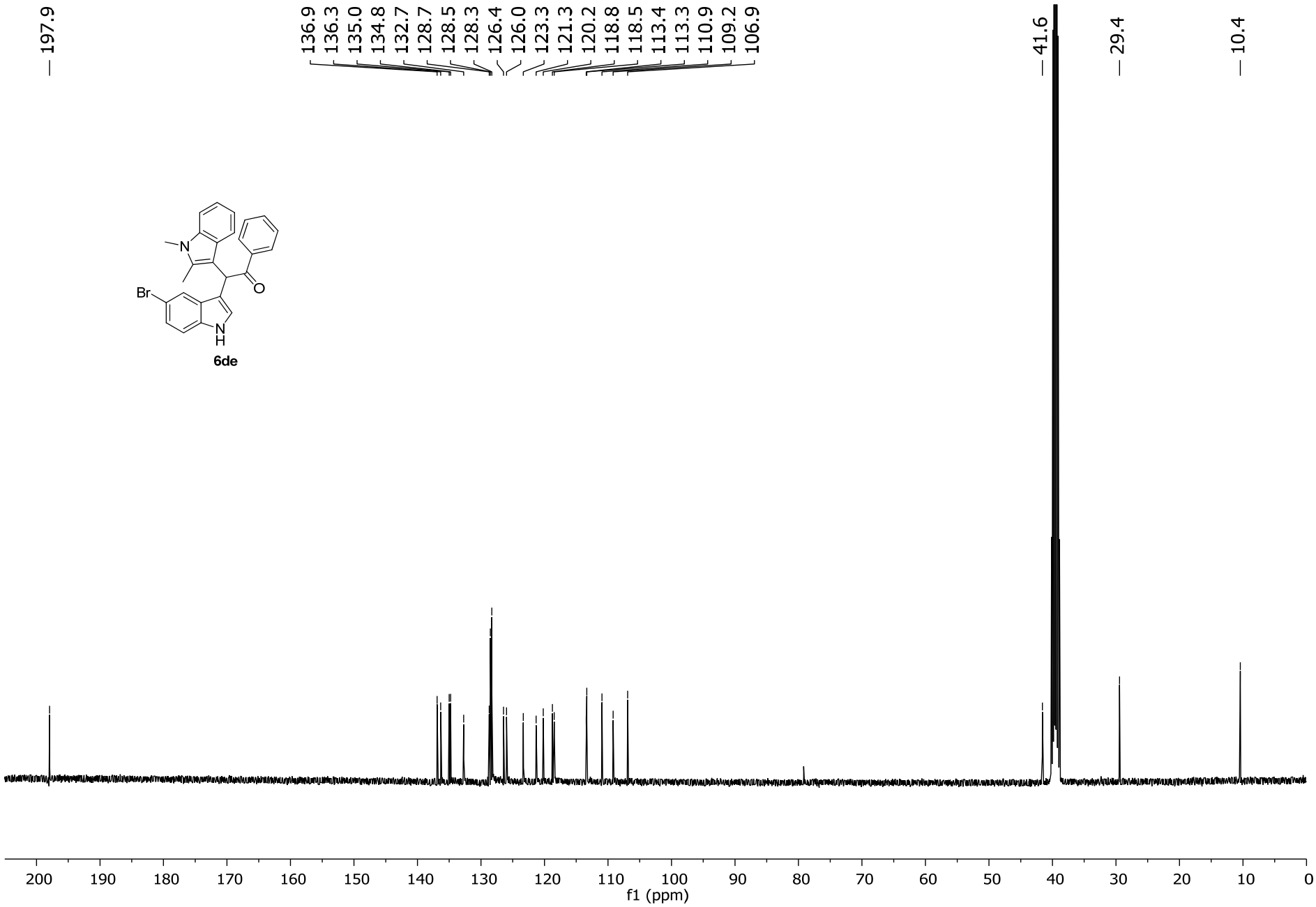
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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126.4
126.0
123.3
121.3
120.2
118.8
118.5
113.4
113.3
110.9
109.2
106.9
41.6
29.4
10.4
Br
N
O
N
H
6de
200
190
180
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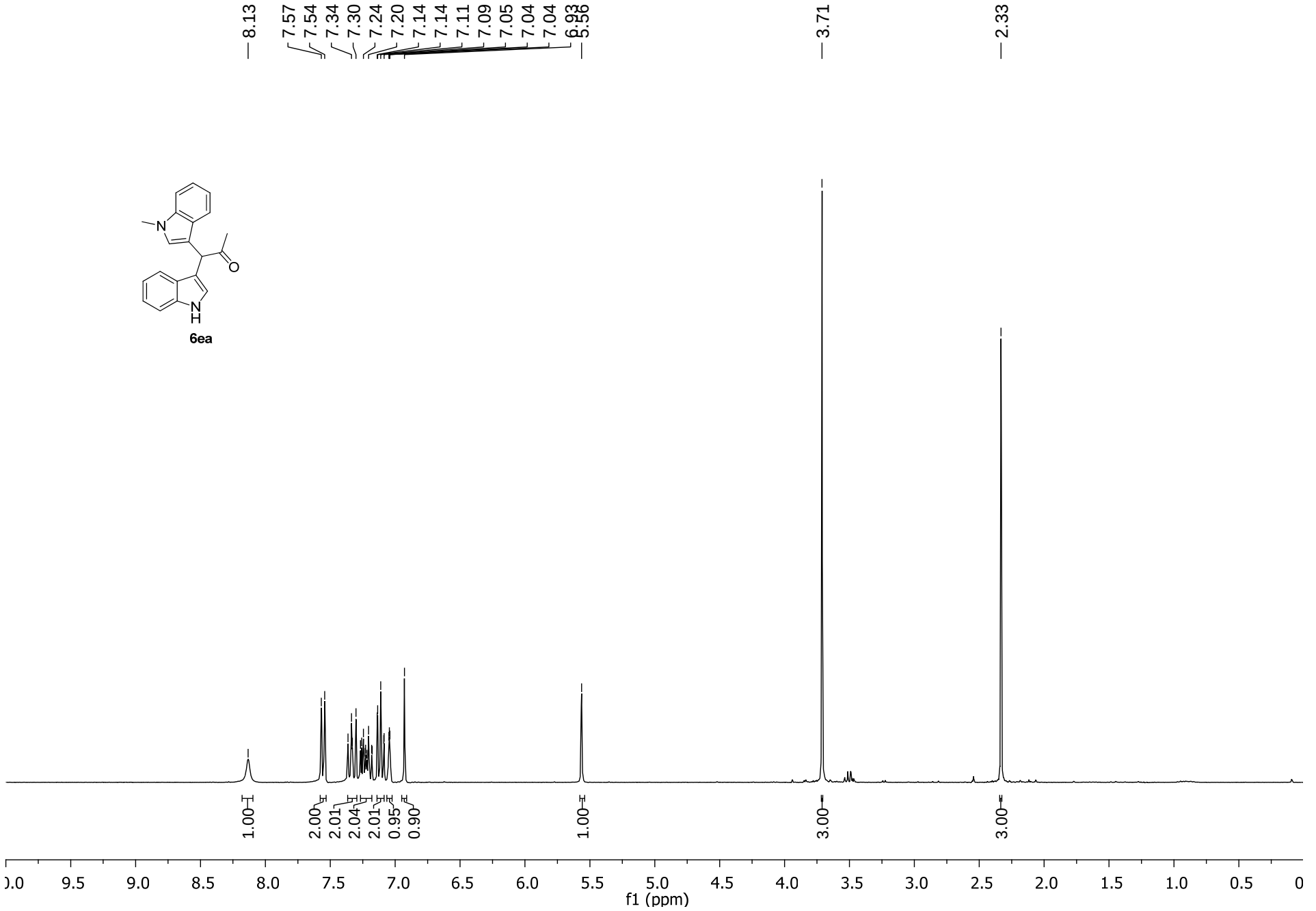
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.14
7.14
7.11
7.09
7.05
7.04
7.04
6.93
5.56
3.71
2.33
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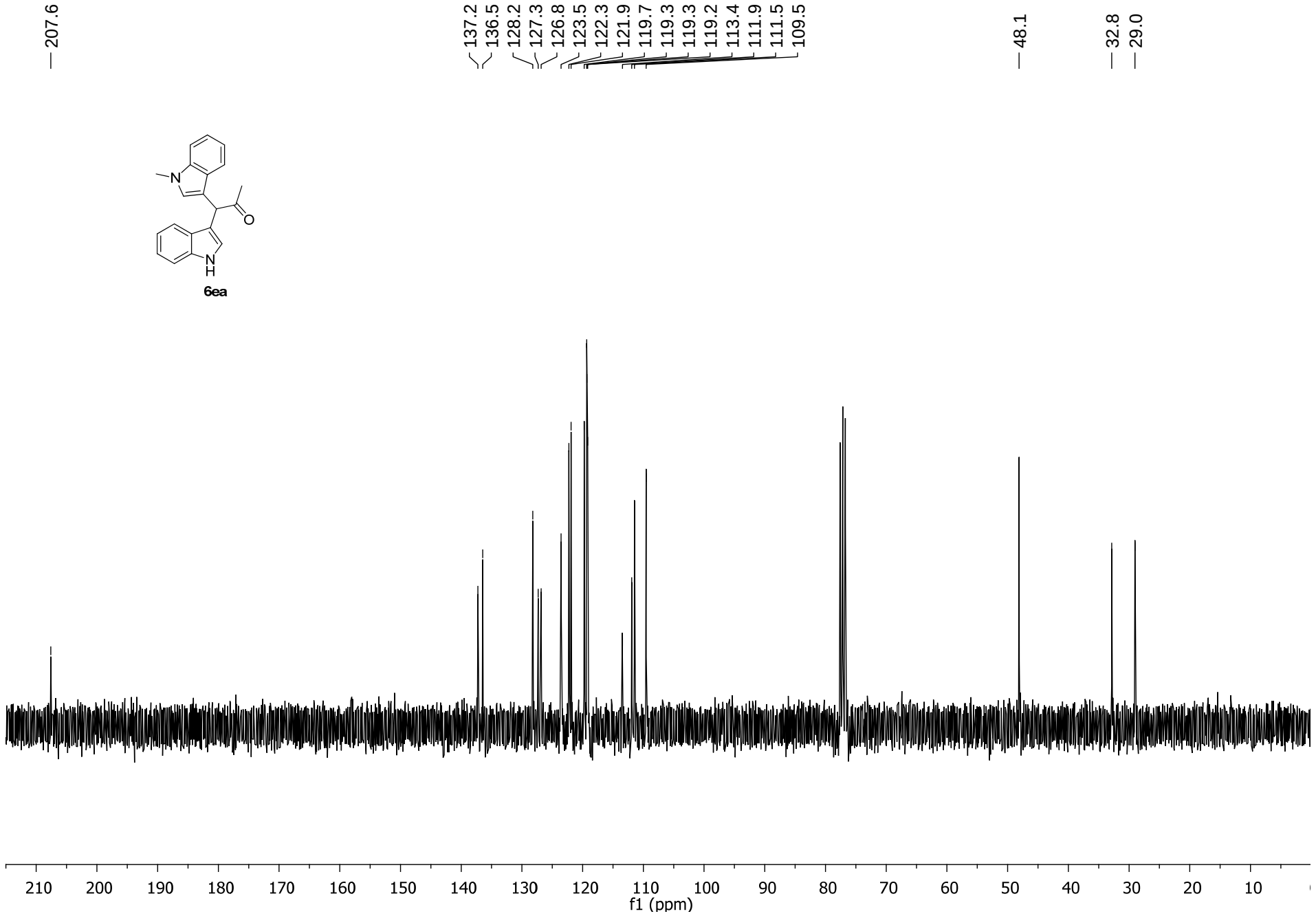
2.04
2.01
0.95
0.90
1.00
3.00
3.00
f1 (ppm)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111.9
111.5
109.5
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32.8
29.0
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O
N
H
6ea
210
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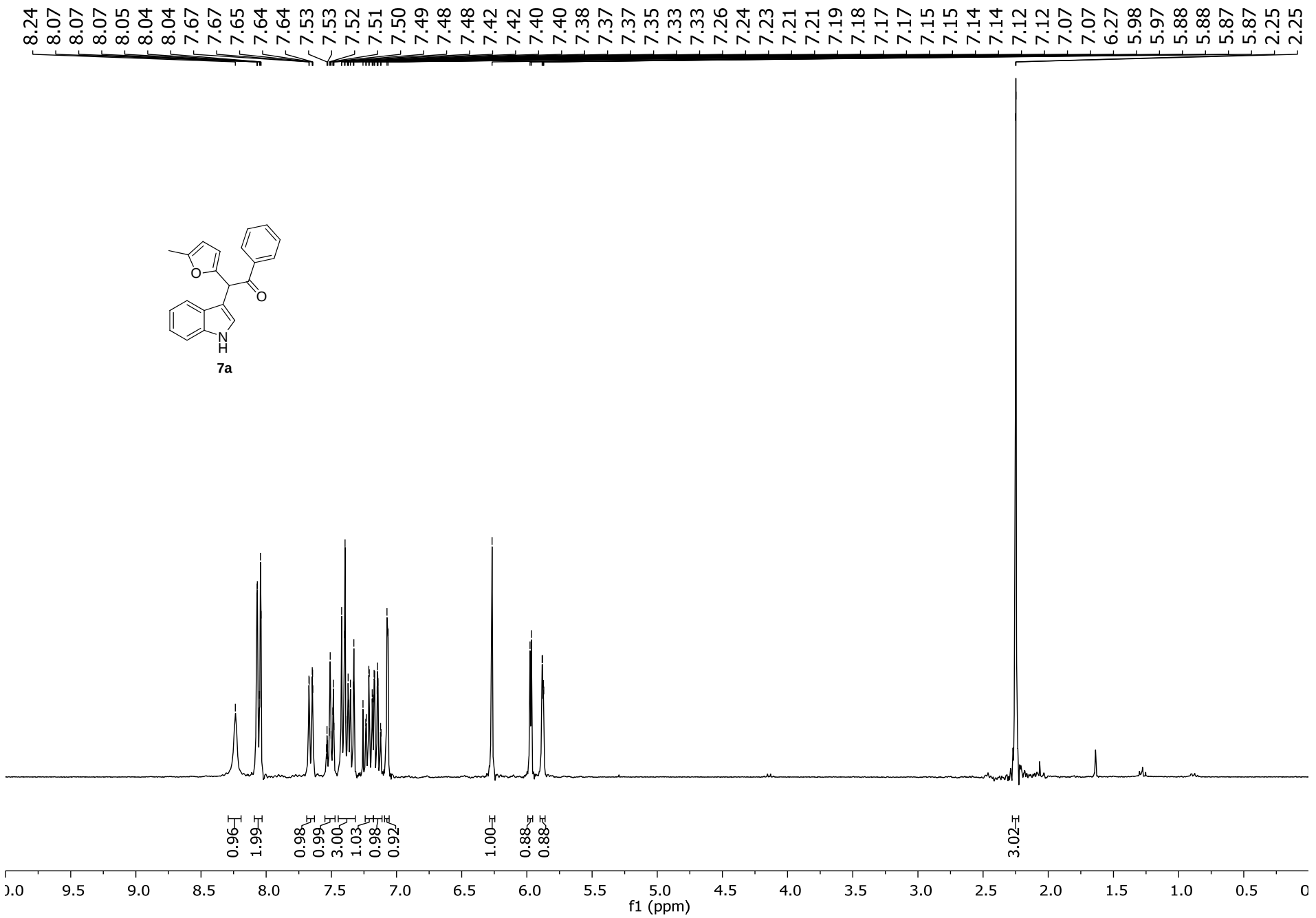
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7.52
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7.42
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7.33
7.33
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7.23
7.21
7.21
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7.18
7.17
7.17
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7.14
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7.12
7.07
7.07
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N
H
7a
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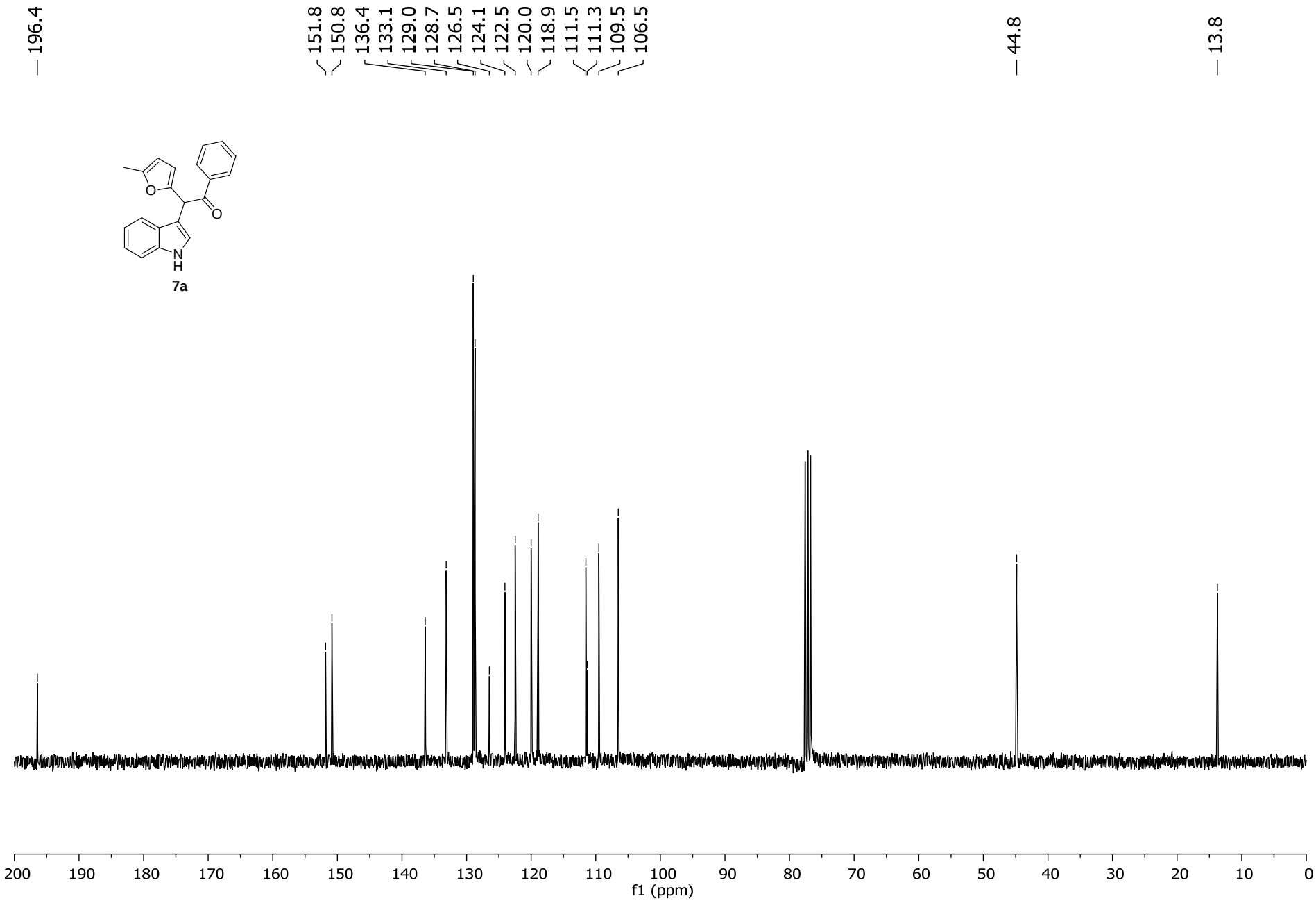
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111.3
109.5
106.5
44.8
13.8
O
O
N
H
7a
200
190
180
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50
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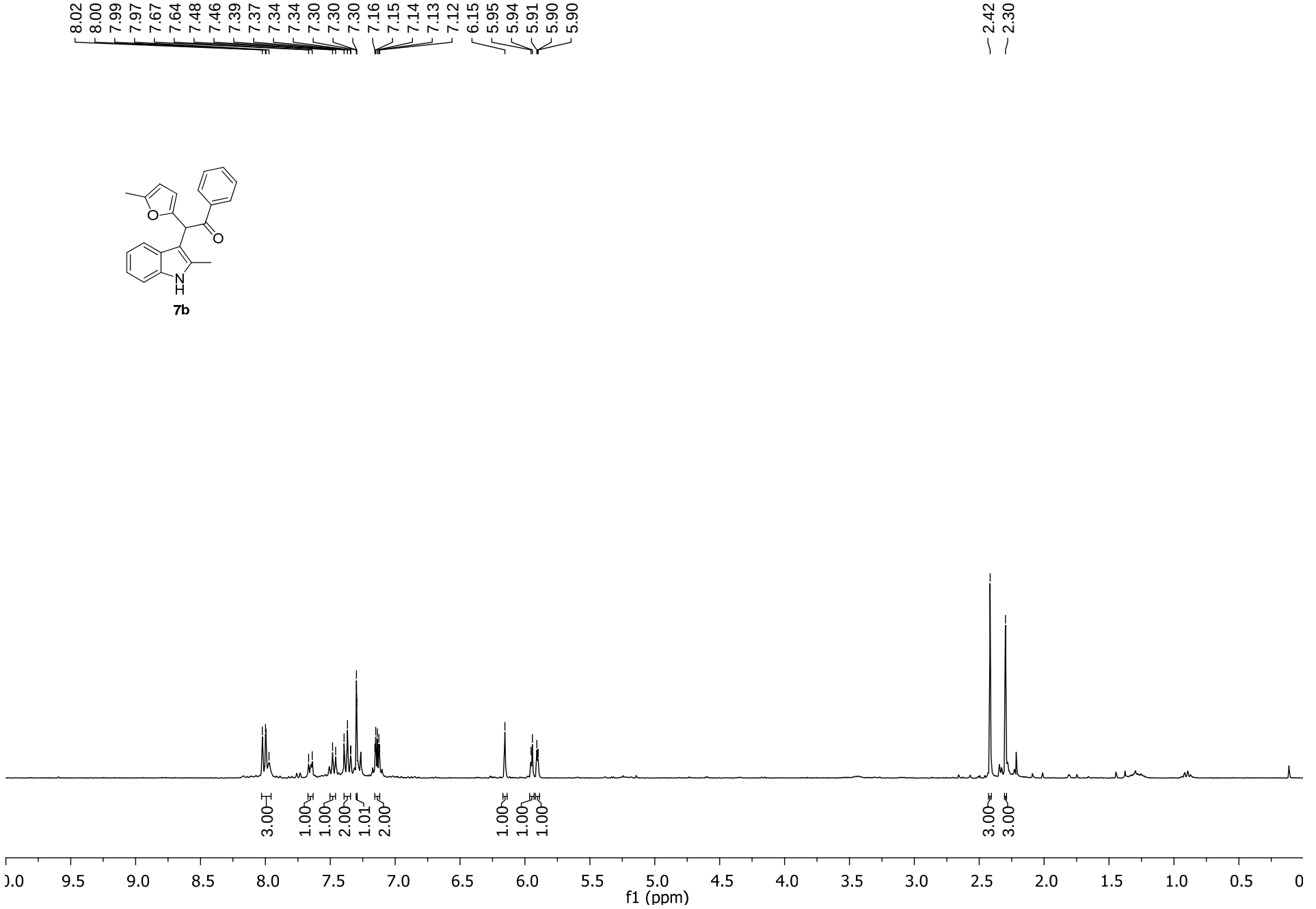
f1 (ppm)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7.15
7.14
7.13
7.12
6.15
5.95
5.94
5.91
5.90
5.90
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2.30
O
O
N
H
7b
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1.00
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3.00
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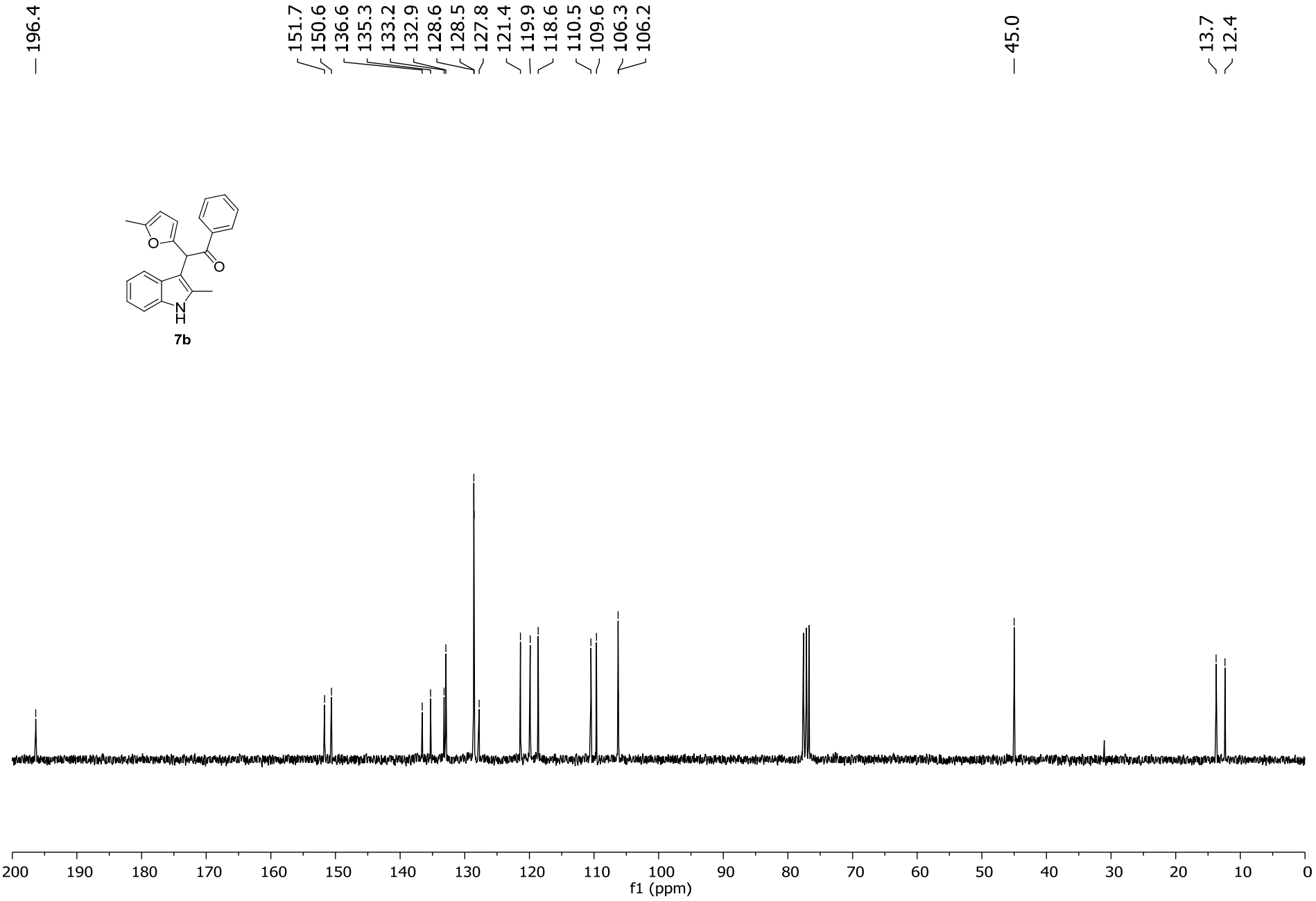
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118.6
110.5
109.6
106.3
106.2
45.0
13.7
12.4
O
O
N
H
7b
200
190
180
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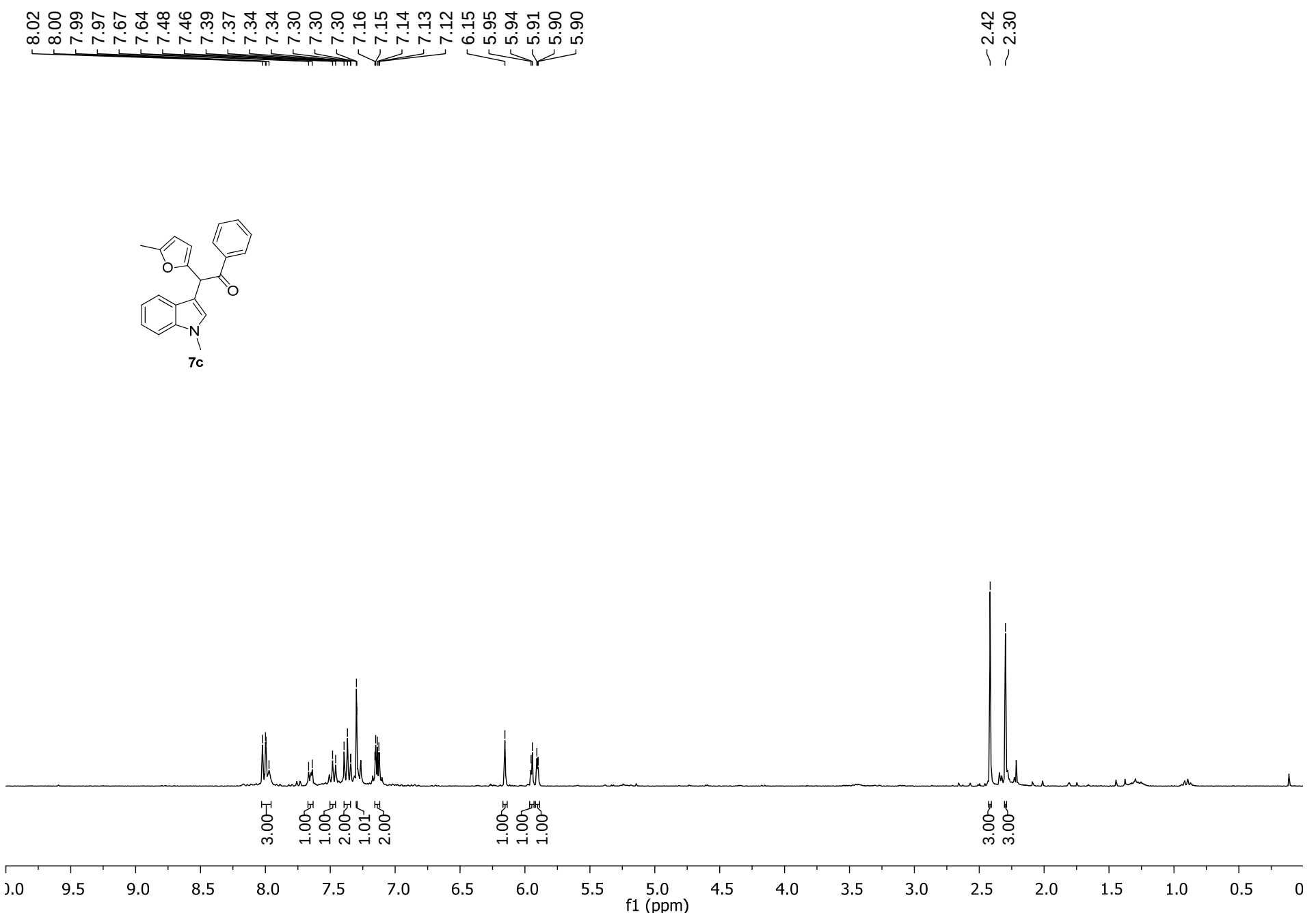
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7.14
7.13
7.12
6.15
5.95
5.94
5.91
5.90
5.90
2.42
2.30
O
O
N
7c
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2.00
1.00
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1.00
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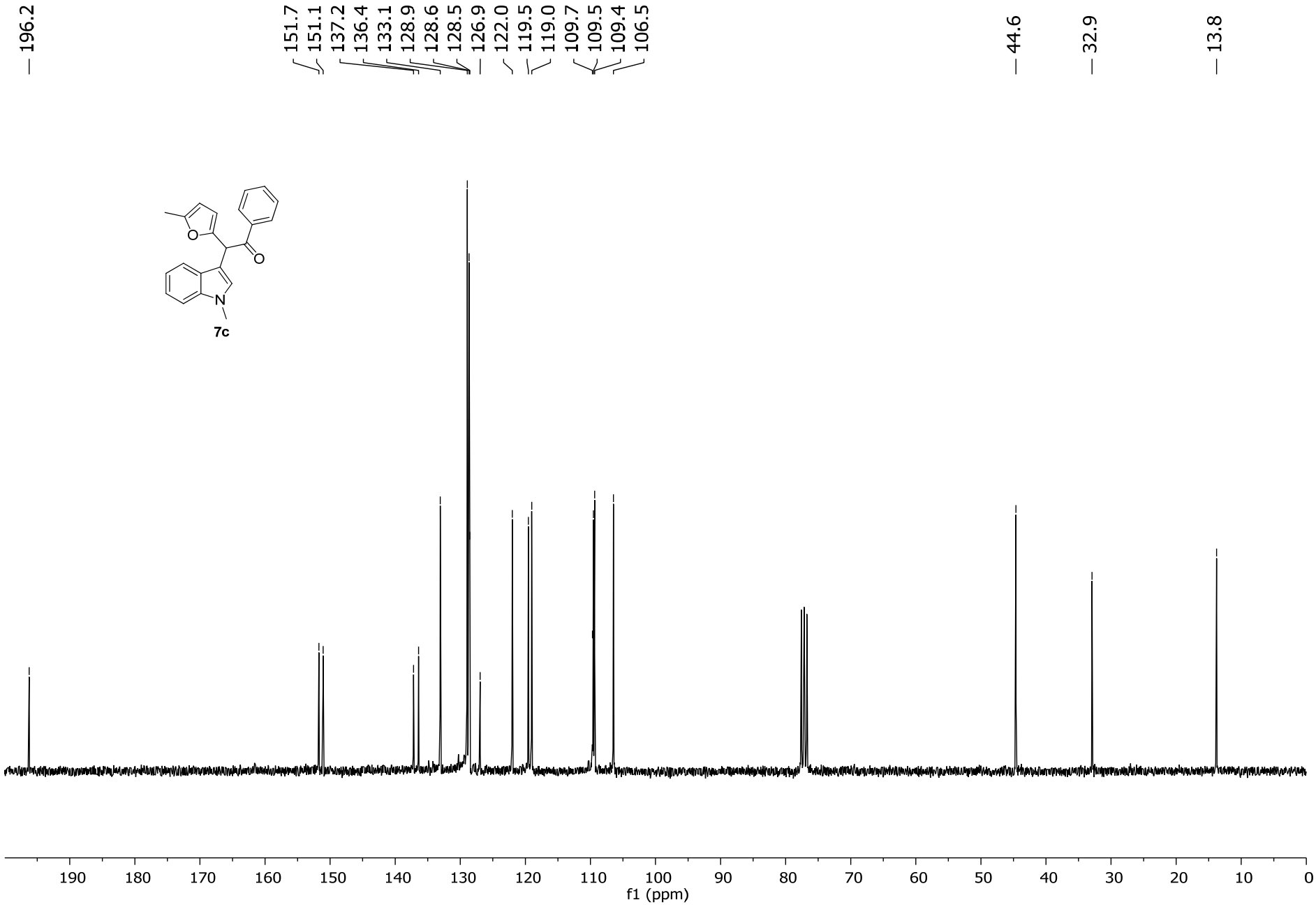
3.00
f1 (ppm)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119.0
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109.5
109.4
106.5
44.6
32.9
13.8
O
O
N
7c
190
180
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130
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30
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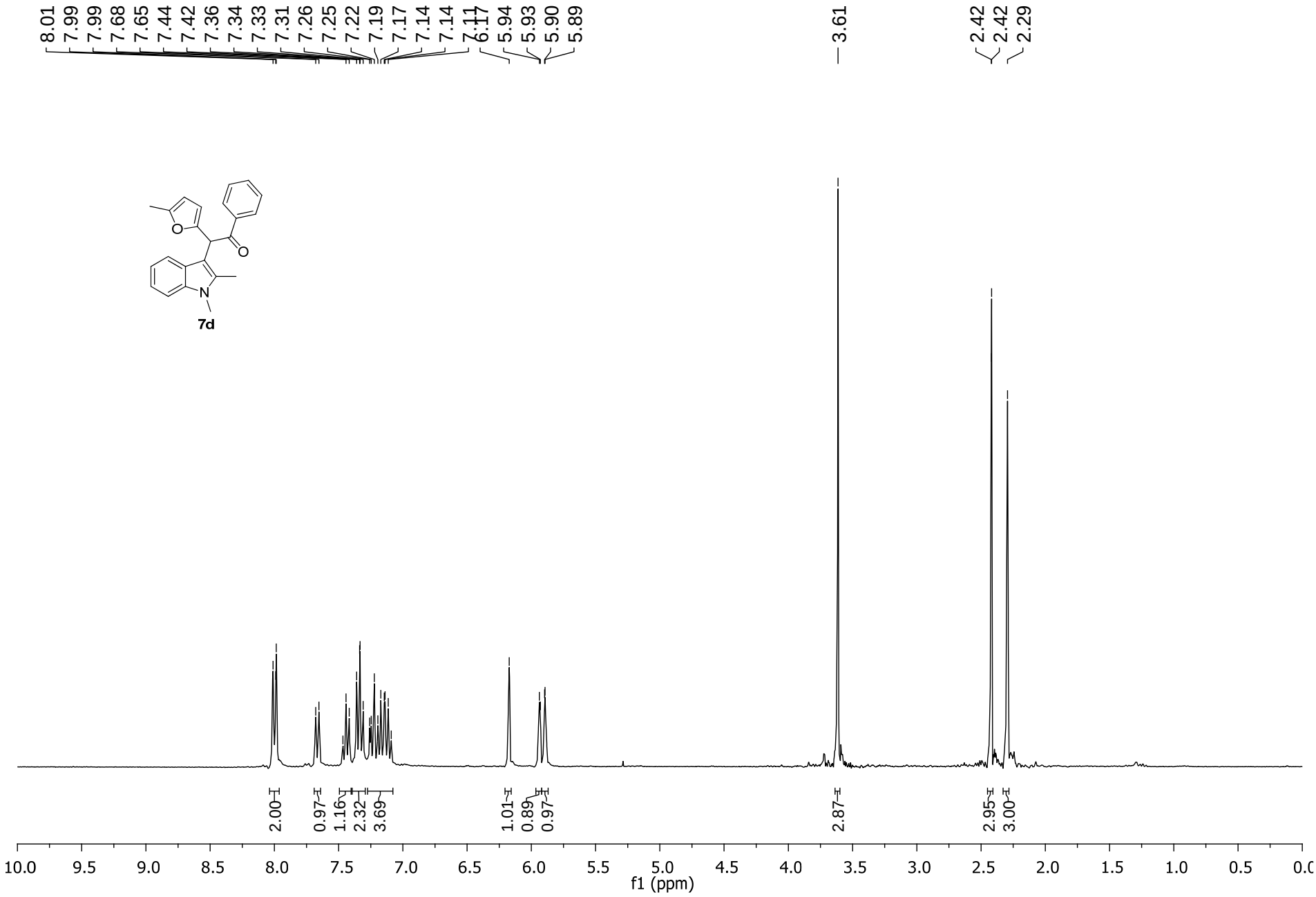
f1 (ppm)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7.25
7.22
7.19
7.17
7.14
7.14
7.11
6.17
5.94
5.93
5.90
5.89
3.61
2.42
2.42
2.29
O
O
N
7d
2.00
0.97
1.16
2.32
3.69
1.01
0.89
0.97
2.87
2.95
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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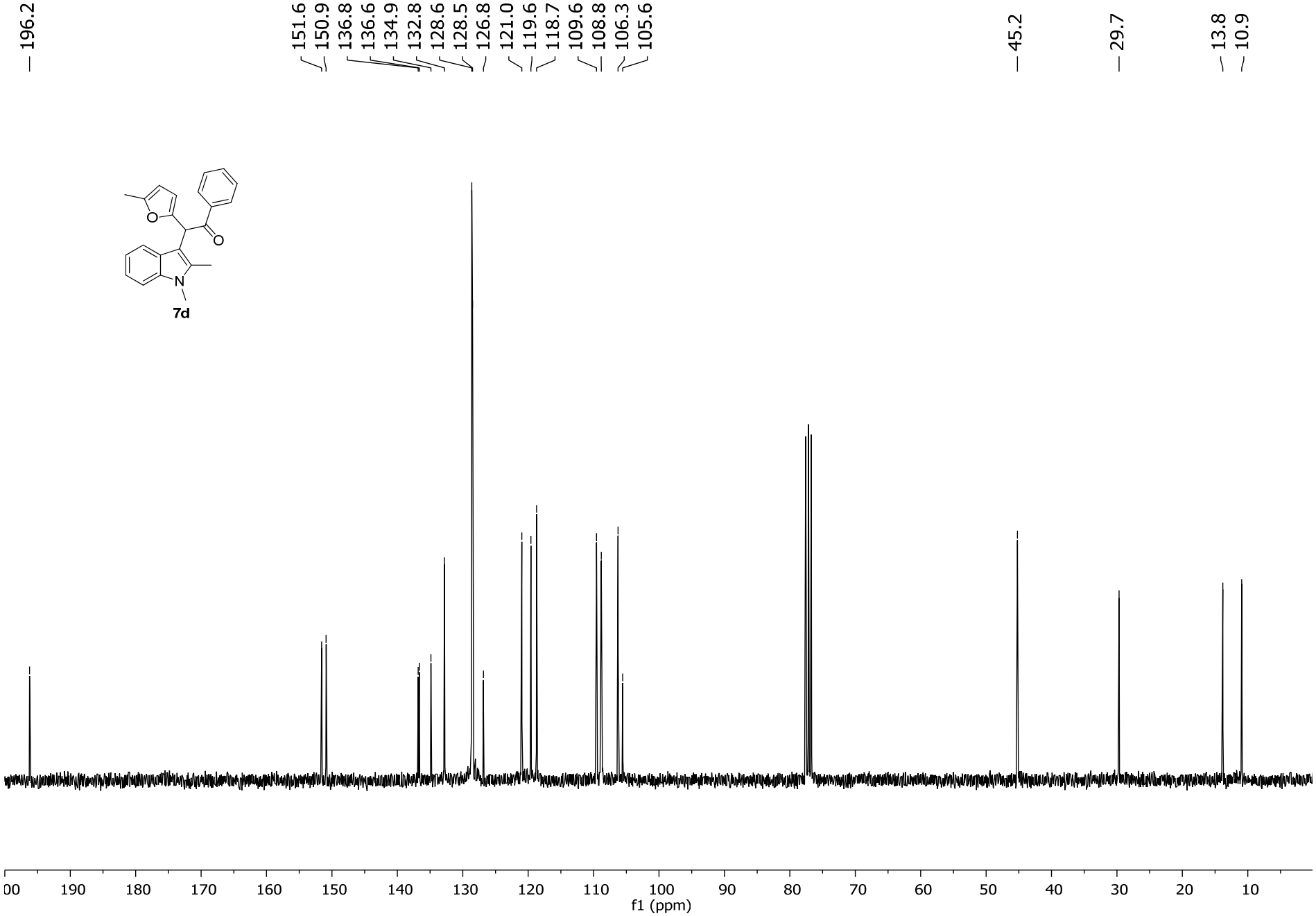
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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134.9
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128.5
126.8
121.0
119.6
118.7
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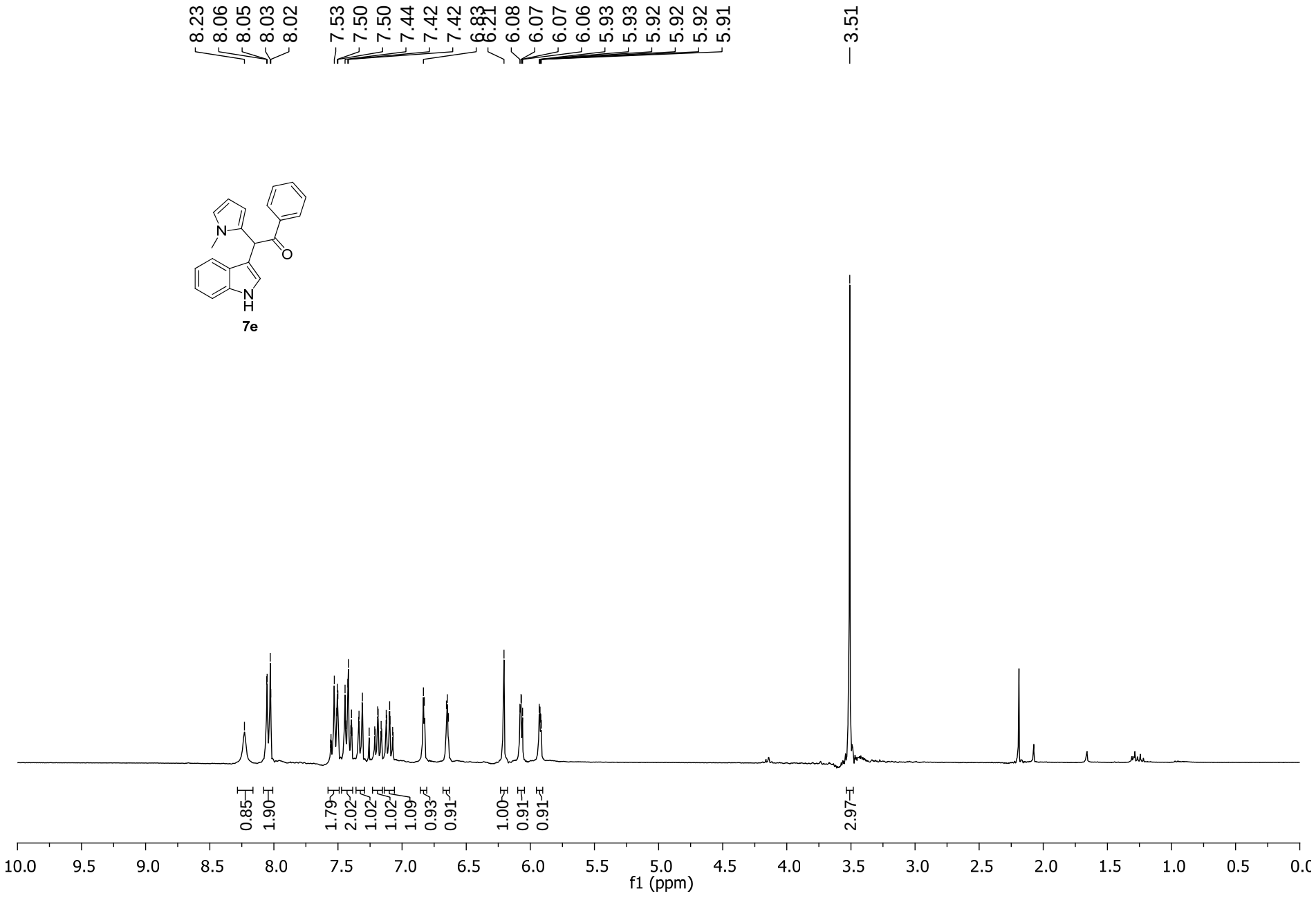
105.6
45.2
29.7
13.8
10.9
O
O
N
7d
f1 (ppm)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7.42
7.42
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6.08
6.07
6.07
6.06
5.93
5.93
5.92
5.92
5.92
5.91
3.51
N
O
N
H
7e
0.85
1.90
1.79
2.02
1.02
1.02
1.09
0.93
0.91
1.00
0.91
0.91
2.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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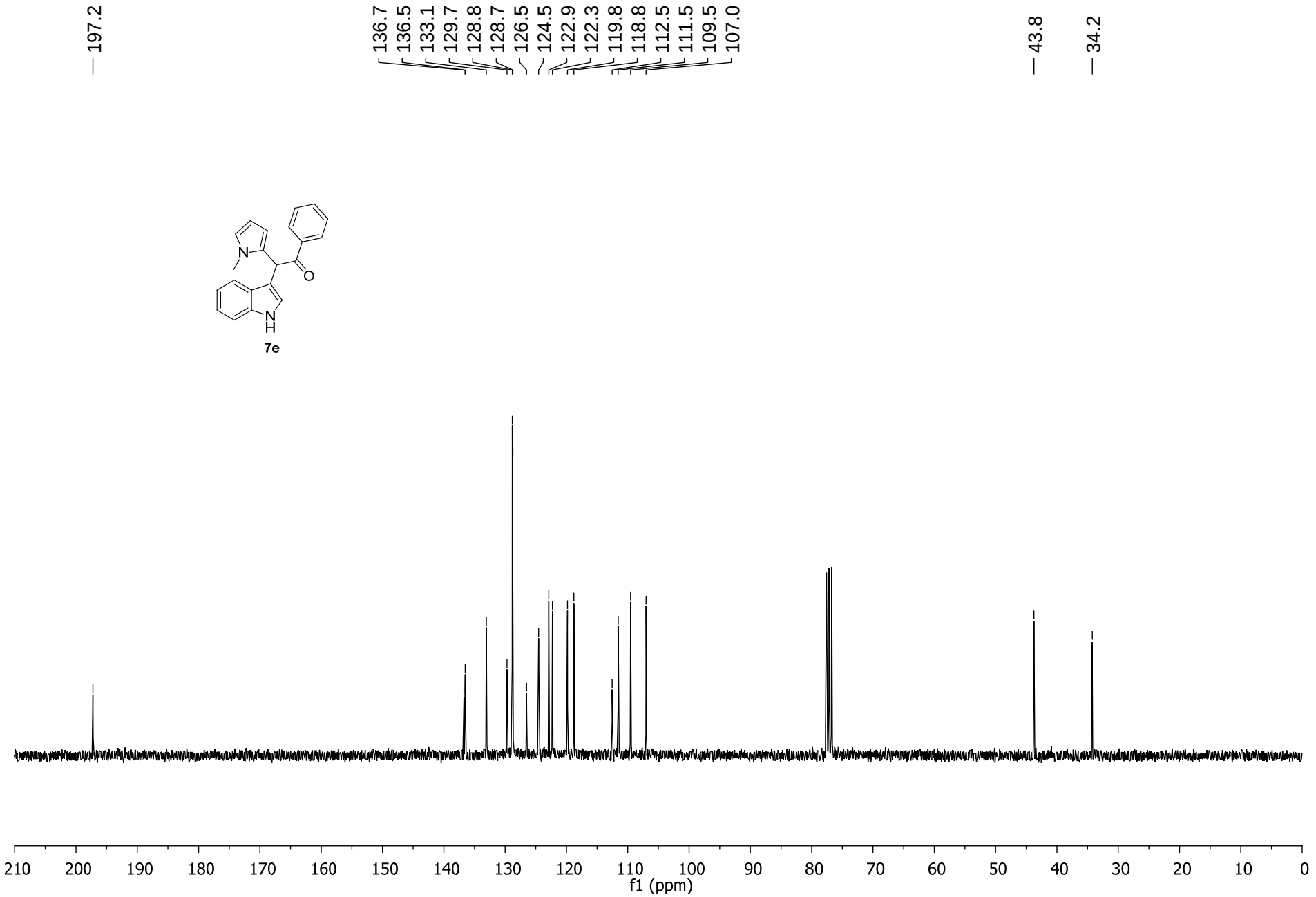
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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126.5
124.5
122.9
122.3
119.8
118.8
112.5
111.5
109.5
107.0
43.8
34.2
N
O
N
H
7e
210
200
190
180
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150
140
130
120
110
100
90
80
70
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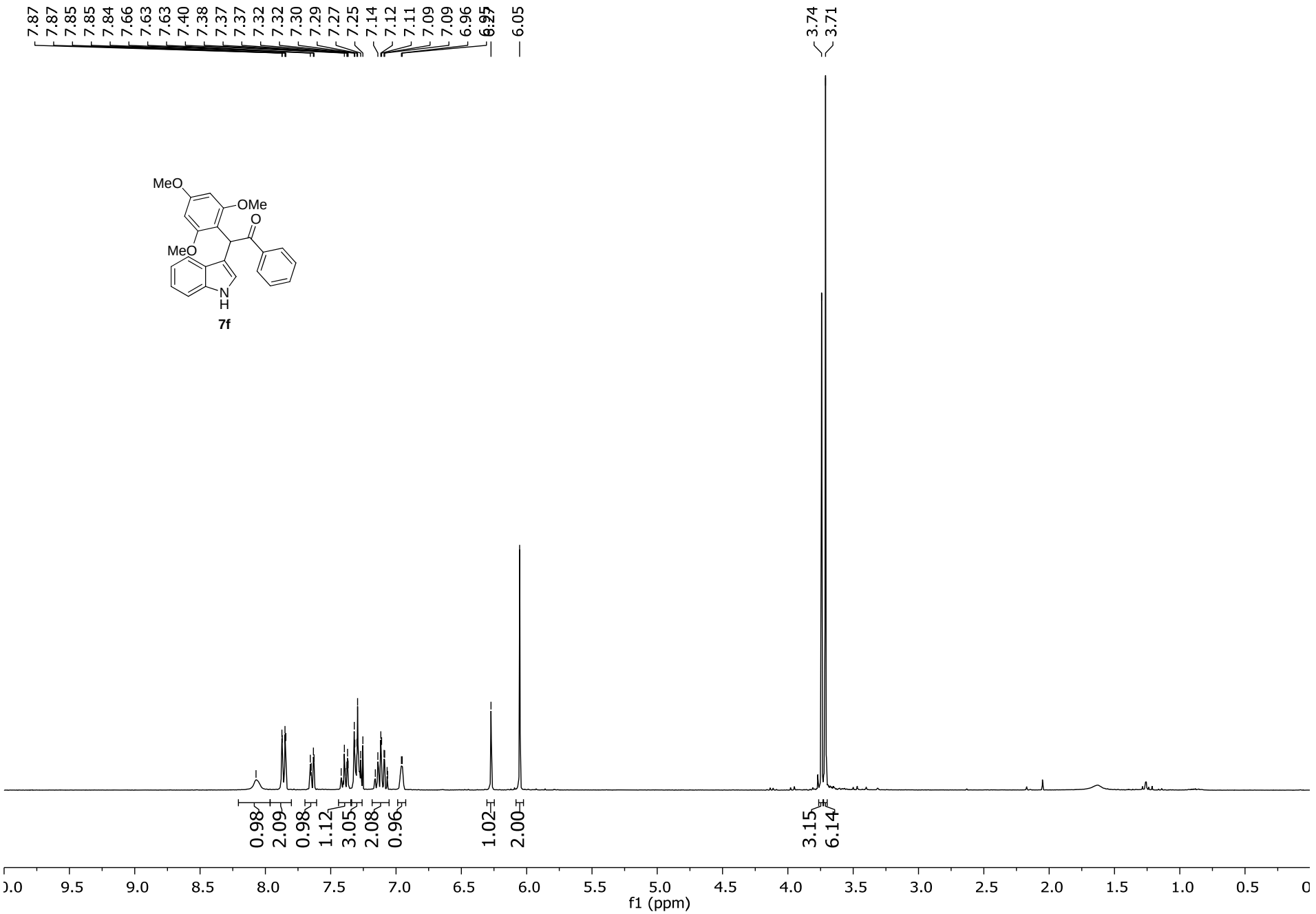
50
40
30
20
10
0
f1 (ppm)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7.37
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7.32
7.30
7.29
7.27
7.25
7.14
7.12
7.11
7.09
7.09
6.96
6.95
6.27
6.05
3.74
3.71
MeO
OMe
O
MeO
N
H
7f
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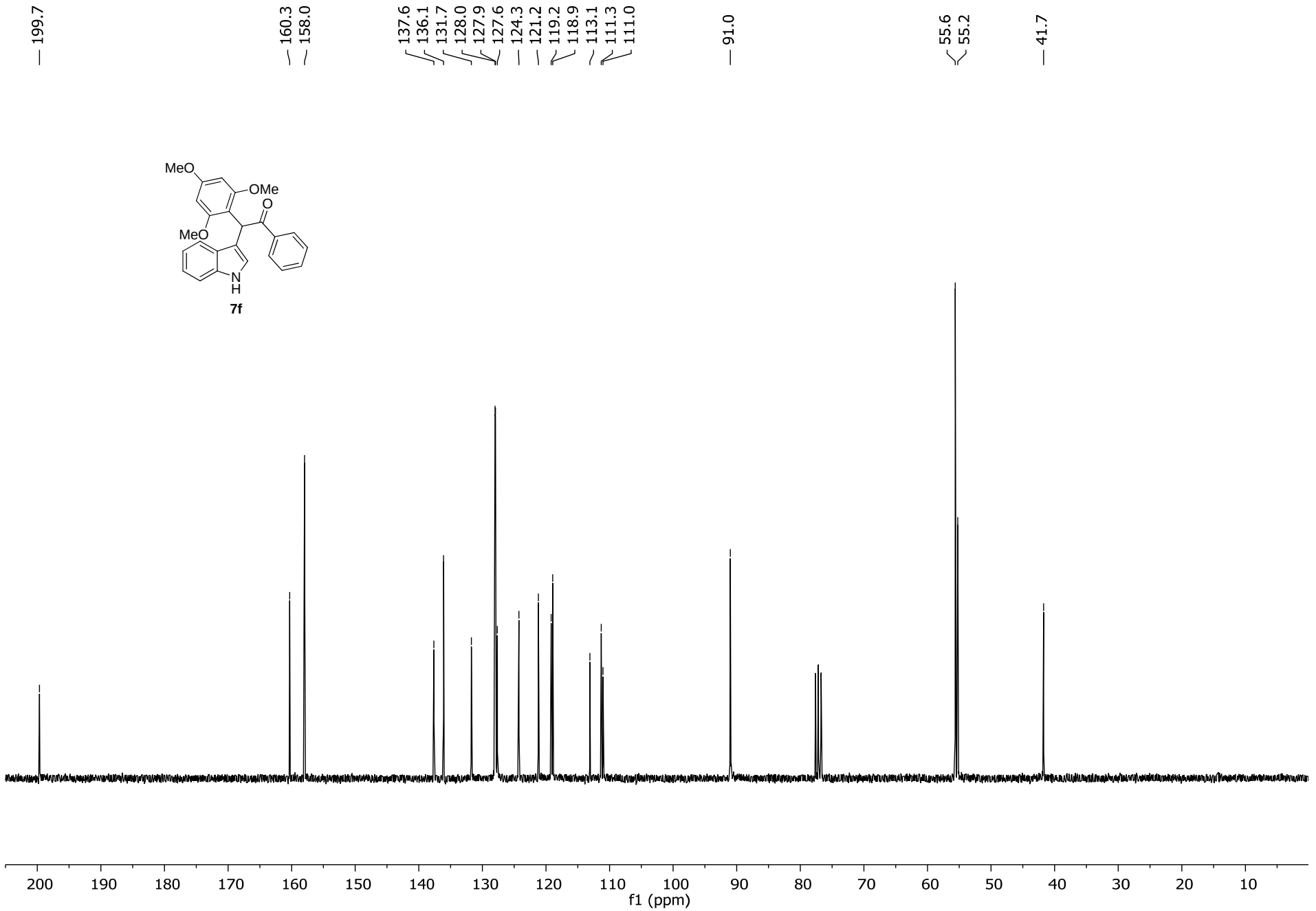
1.12
3.05
2.08
0.96
1.02
2.00
3.15
6.14
f1 (ppm)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124.3
121.2
119.2
118.9
113.1
111.3
111.0
91.0
55.6
55.2
41.7
MeO
OMe
O
MeO
N
H
7f
200
190
180
170
160
150
140
130
120
110
100
90
80
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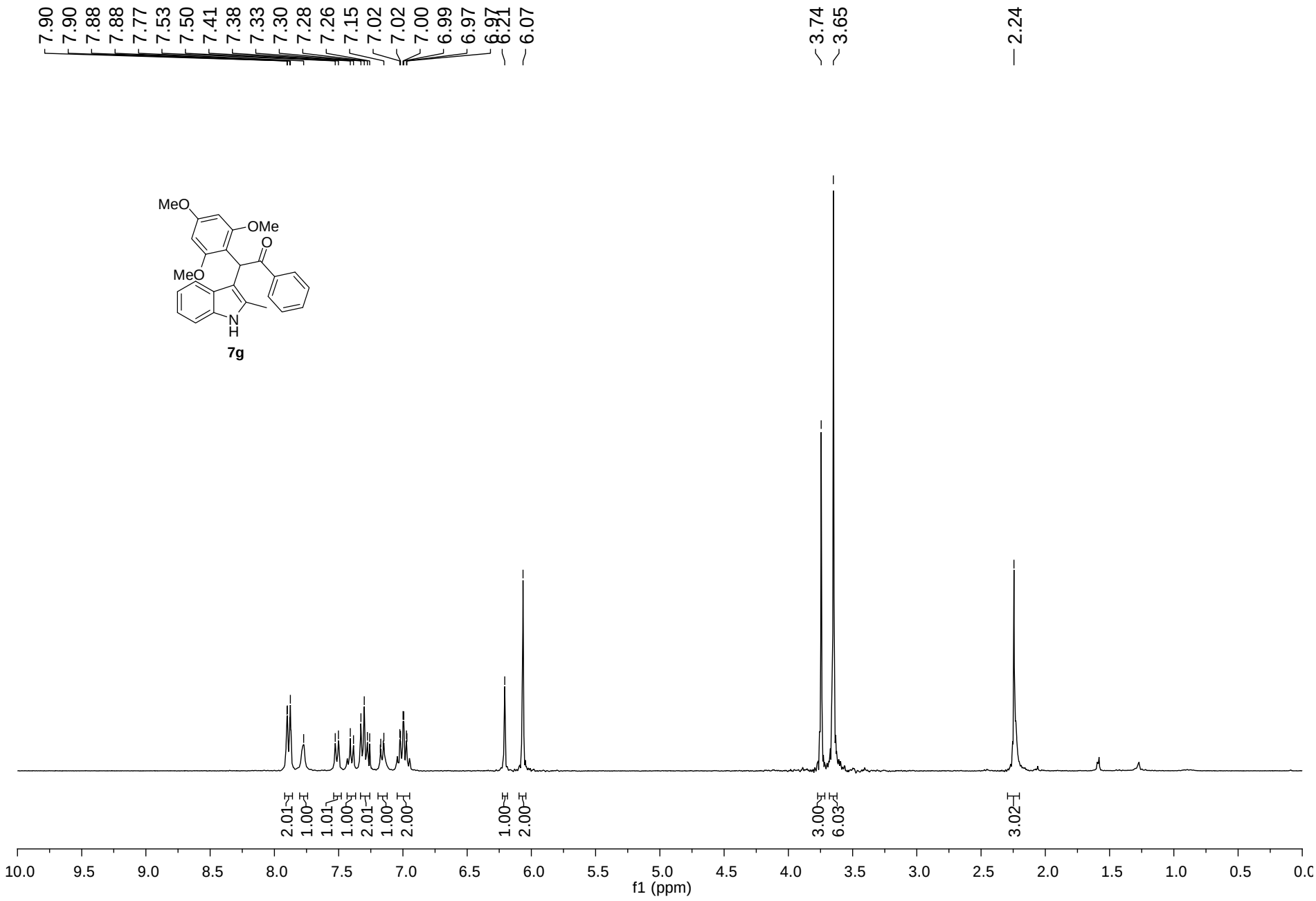
60
50
40
30
20
10
f1 (ppm)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7.26
7.15
7.02
7.02
7.00
6.99
6.97
6.97
6.21
6.07
3.74
3.65
2.24
MeO
OMe
O
MeO
N
H
7g
2.01
1.00
1.01
1.00
2.01
1.00
2.00
1.00
2.00
3.00
6.03
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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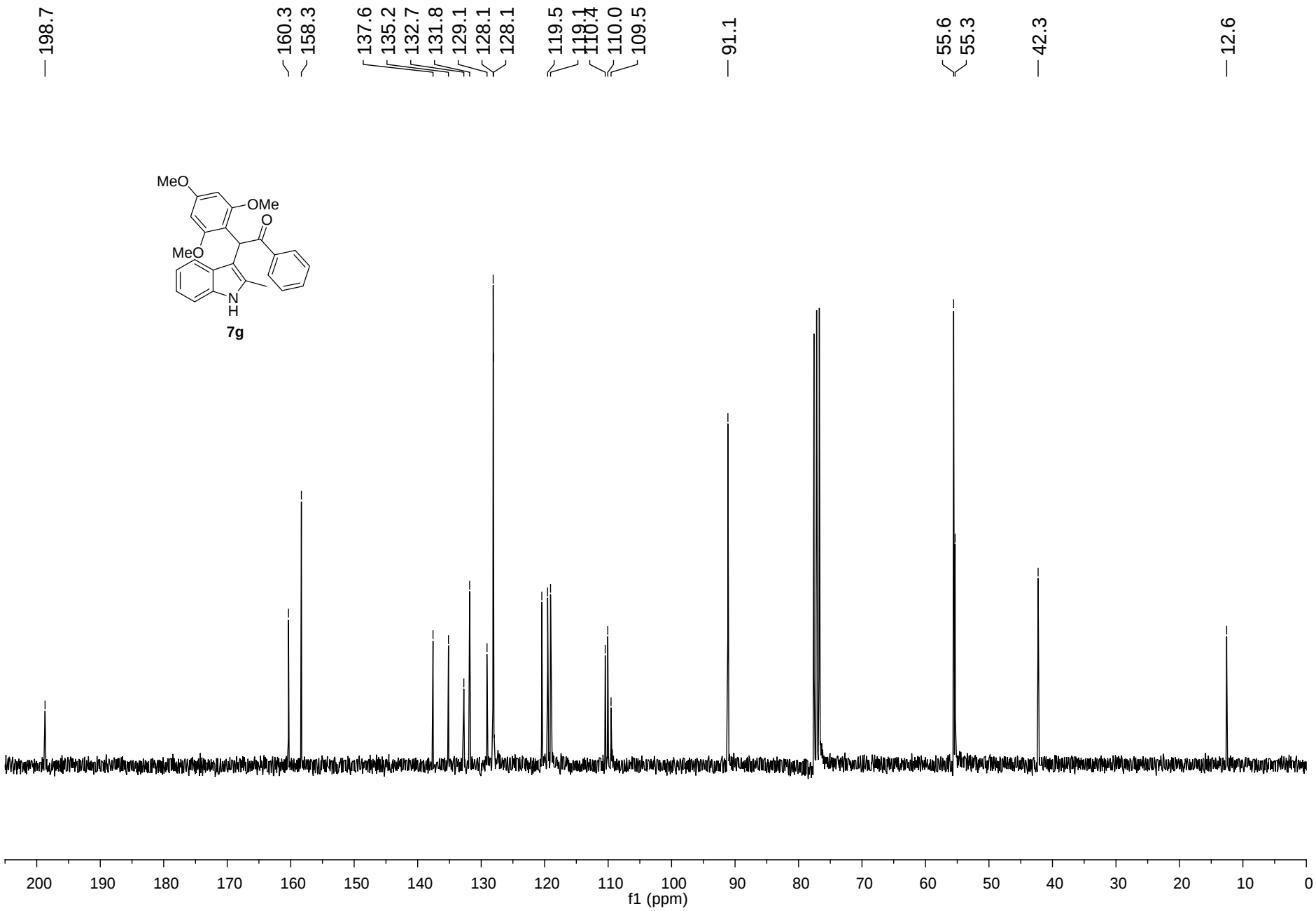
1.0
0.5
0.0
f1 (ppm)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129.1
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128.1
119.5
119.1
110.4
110.0
109.5
91.1
55.6
55.3
42.3
12.6
MeO
OMe
O
MeO
N
H
7g
200
190
180
170
160
150
140
130
120
110
100
90
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70
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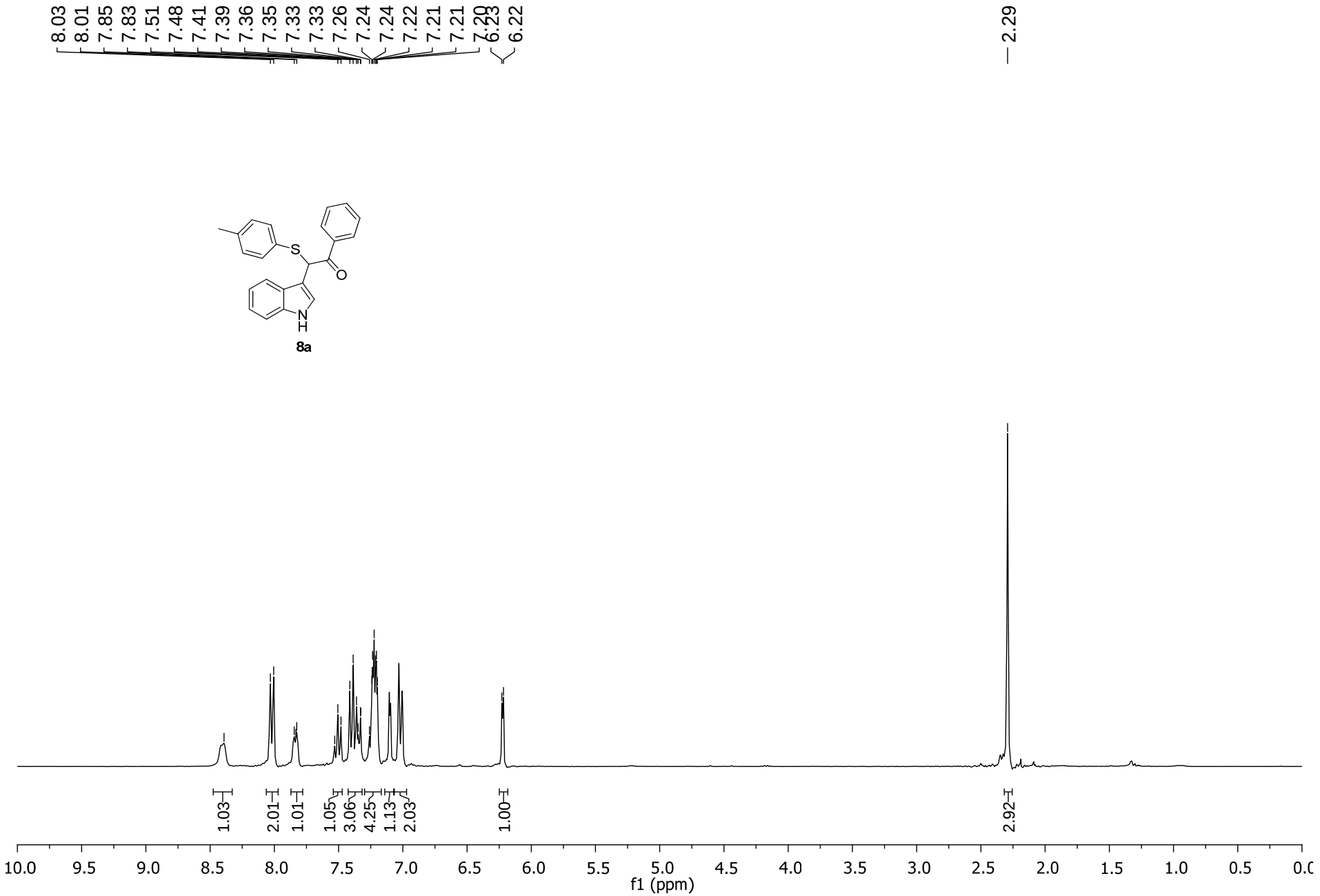
50
40
30
20
10
0
f1 (ppm)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7.26
7.24
7.24
7.22
7.21
7.21
7.20
6.23
6.22
2.29
S
O
N
H
8a
1.03
2.01
1.01
1.05
3.06
4.25
1.13
2.03
1.00
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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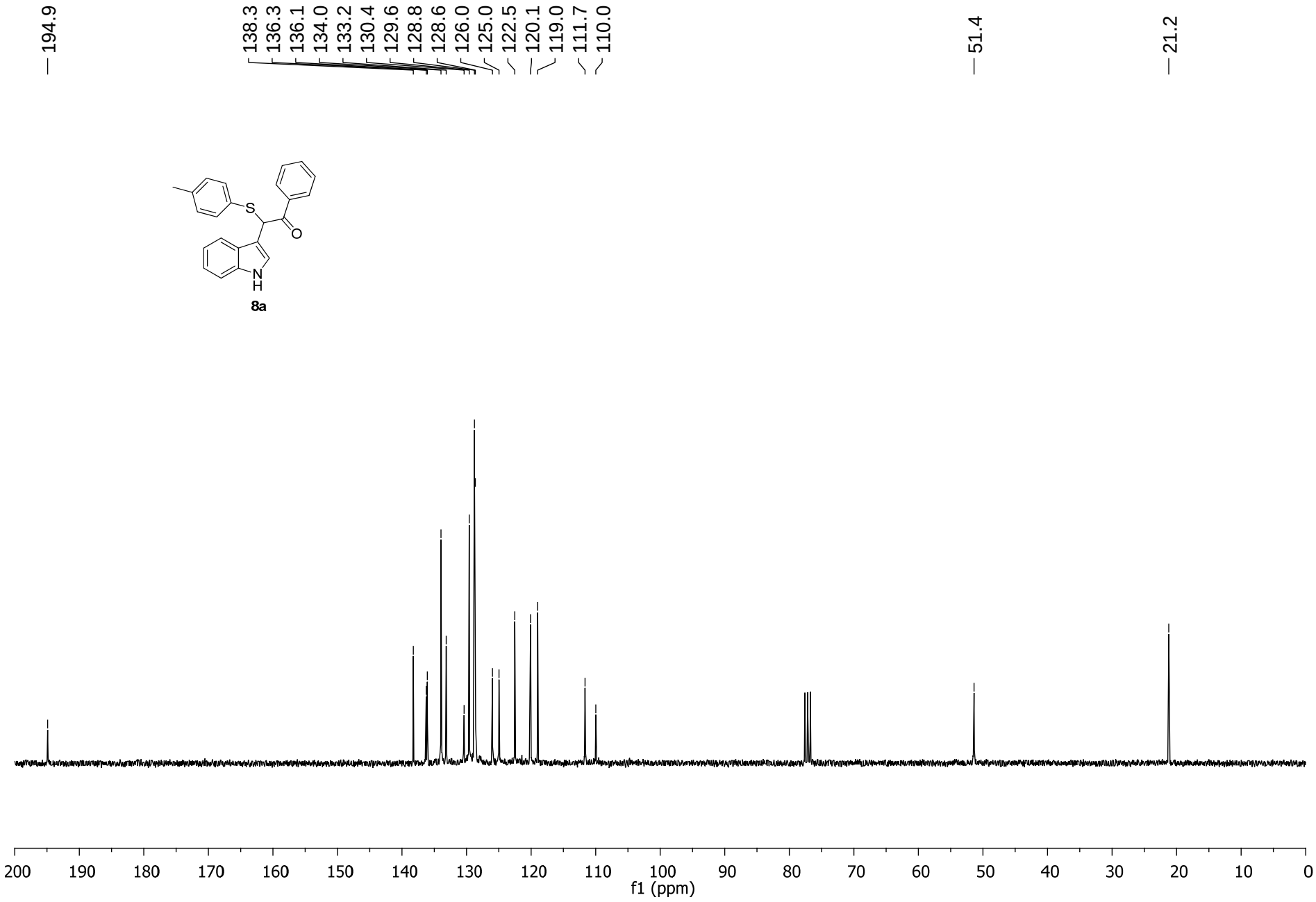
0.0
f1 (ppm)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126.0
125.0
122.5
120.1
119.0
111.7
110.0
51.4
21.2
S
O
N
H
8a
200
190
180
170
160
150
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130
120
110
100
90
80
70
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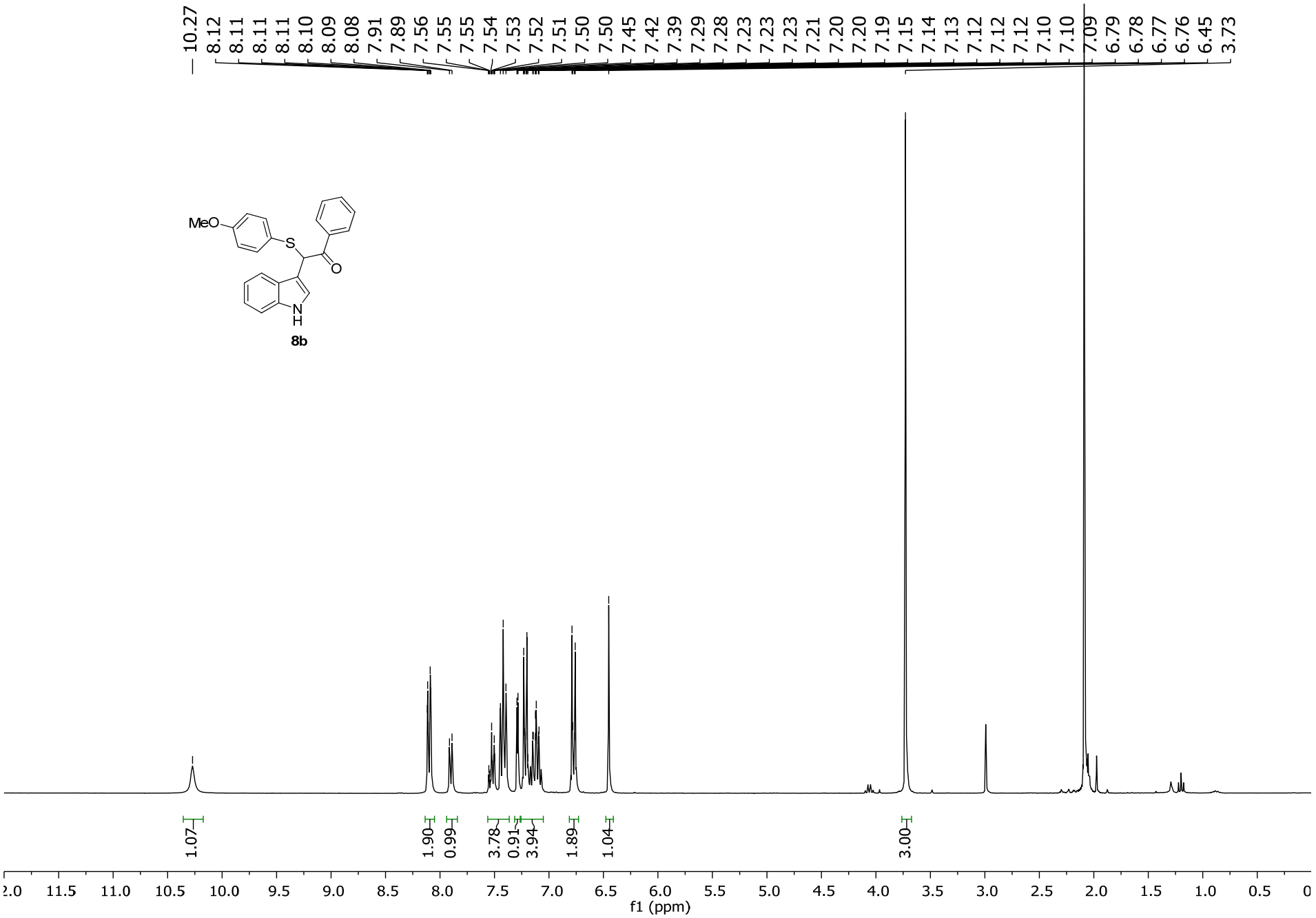
50
40
30
20
10
0
f1 (ppm)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7.55
7.54
7.53
7.52
7.51
7.50
7.50
7.45
7.42
7.39
7.29
7.28
7.23
7.23
7.23
7.21
7.20
7.20
7.19
7.15
7.14
7.13
7.12
7.12
7.12
7.10
7.10
7.09
6.79
6.78
6.77
6.76
6.45
3.73
MeO
S
O
N
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0.91
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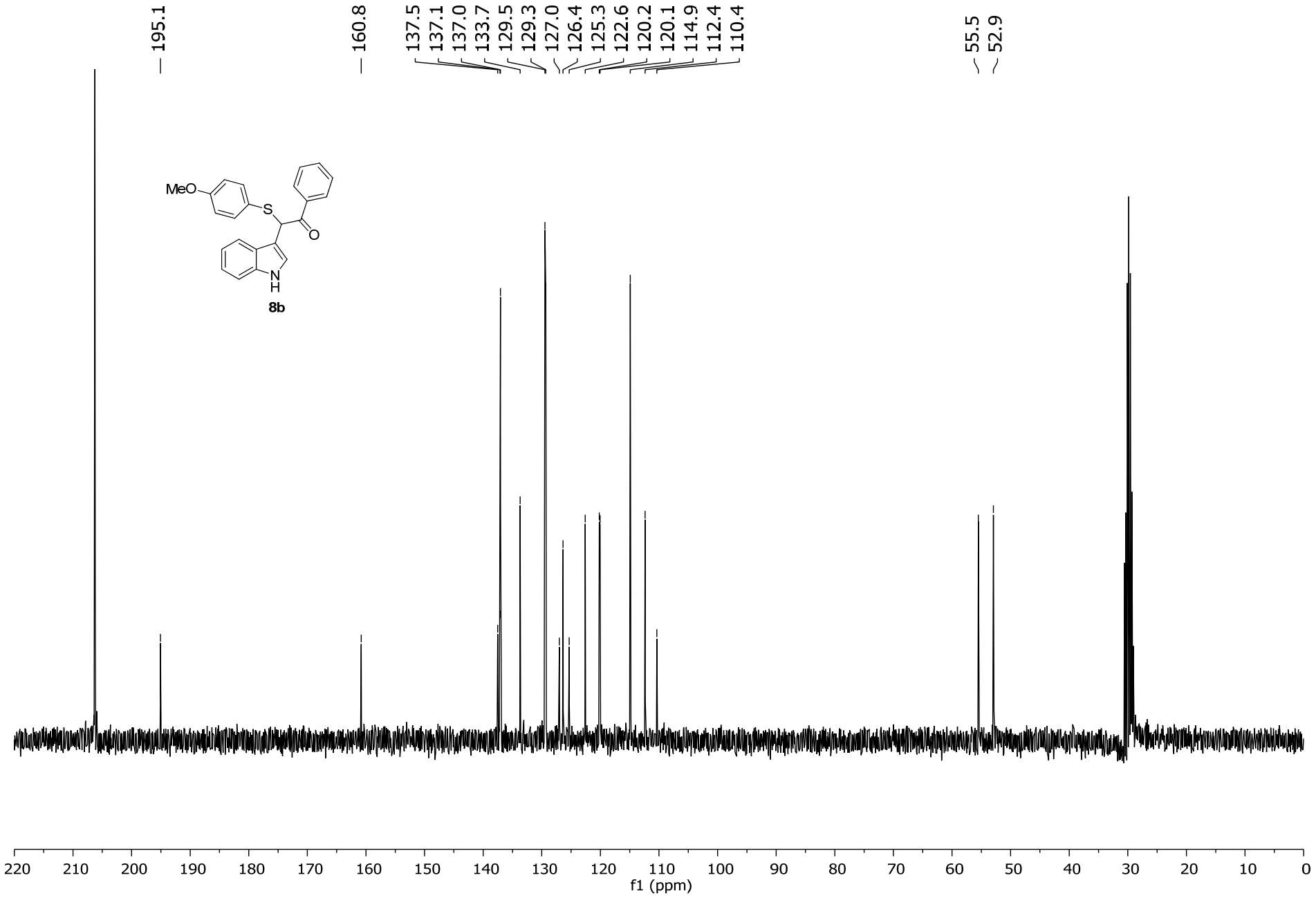
1.89
1.04
3.00
f1 (ppm)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129.3
127.0
126.4
125.3
122.6
120.2
120.1
114.9
112.4
110.4
55.5
52.9
MeO
S
O
N
H
8b
220
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
60
50
40
30
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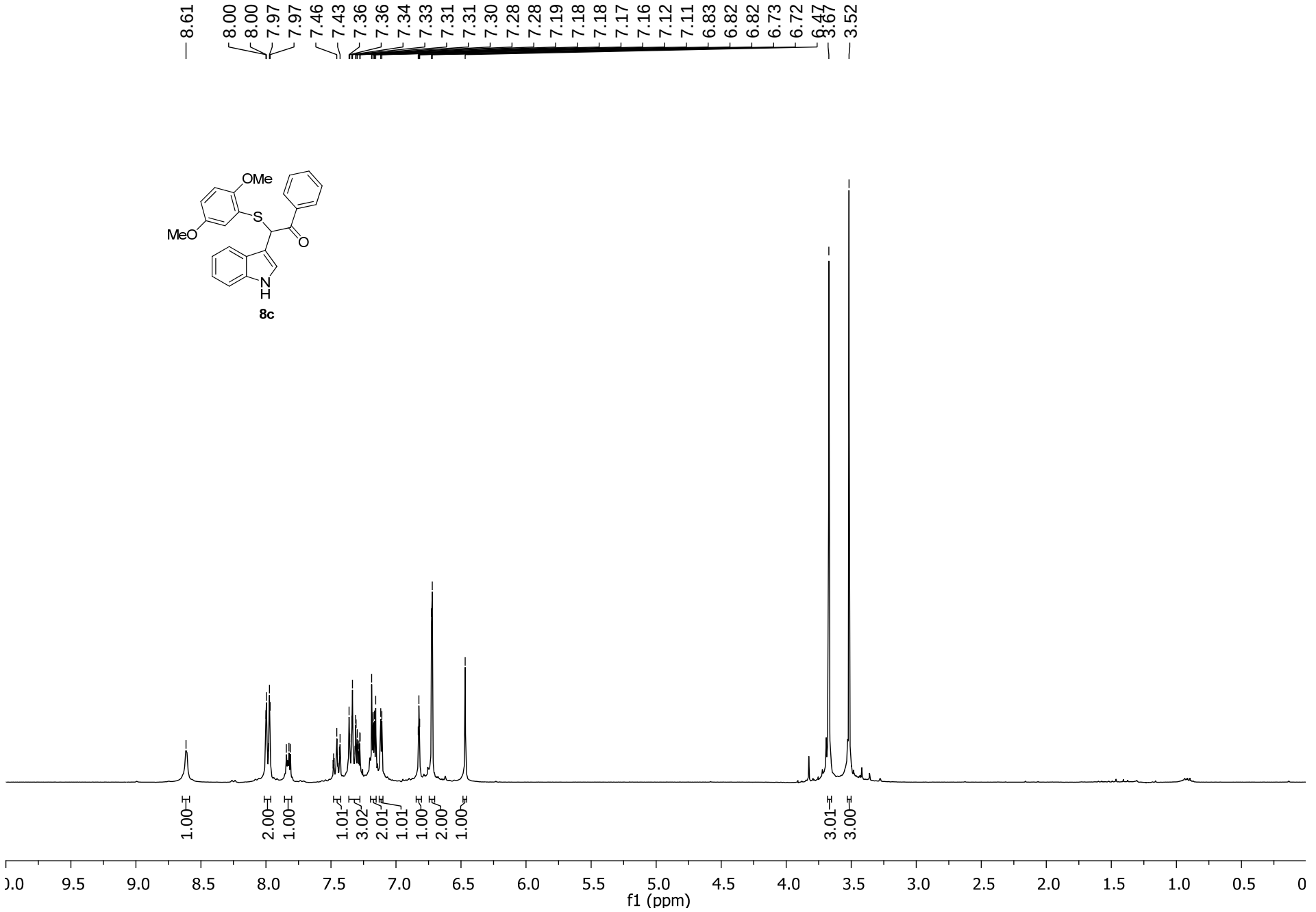
10
0
f1 (ppm)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7.30
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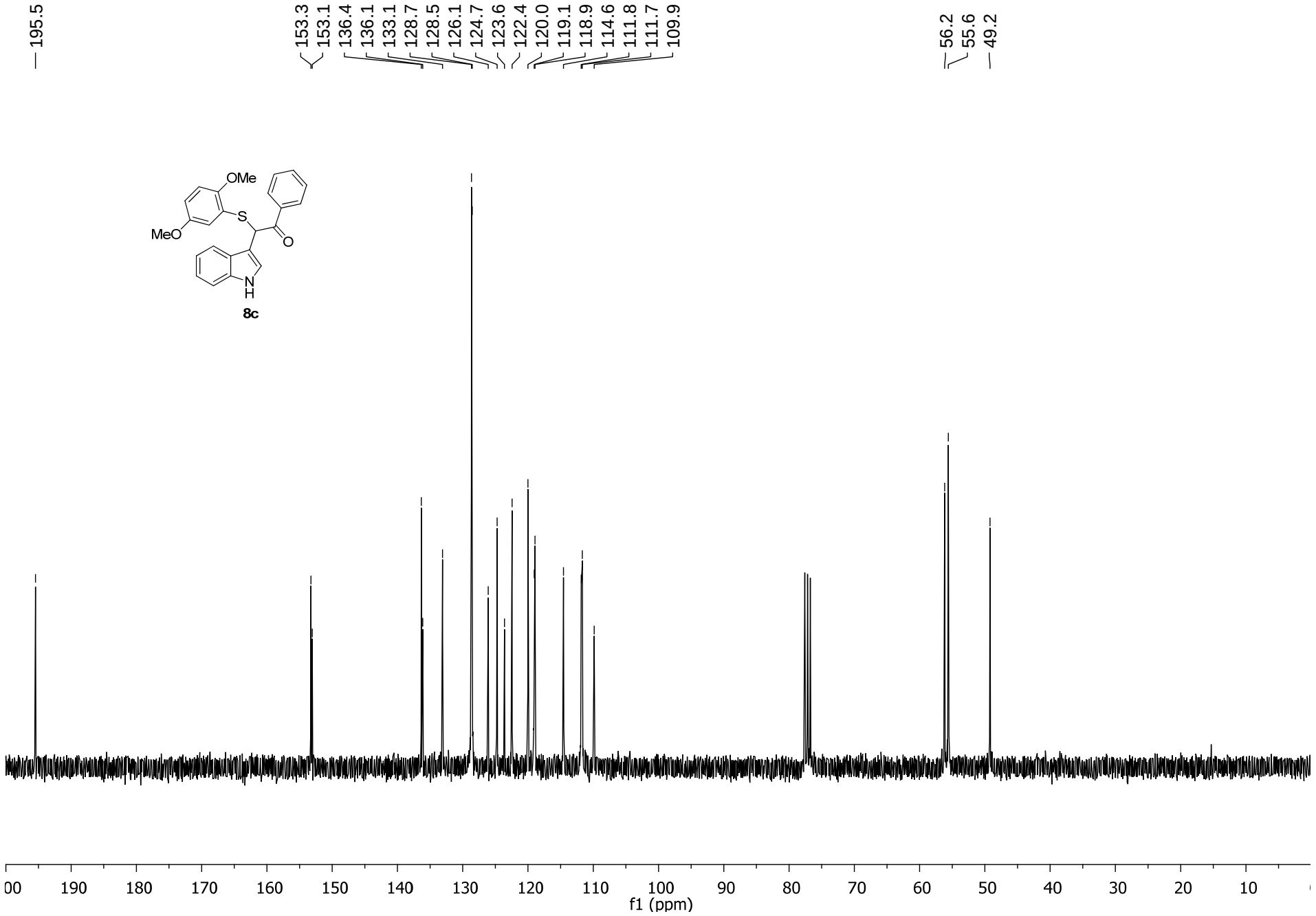
7.28
7.19
7.18
7.18
7.17
7.16
7.12
7.11
6.83
6.82
6.82
6.73
6.72
6.47
3.67
3.52
OMe
MeO
S
O
N
H
8c
1.00
2.00
1.00
1.01
3.02
2.01
1.01
1.00
2.00
1.00
3.01
3.00
f1 (ppm)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128.5
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124.7
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122.4
120.0
119.1
118.9
114.6
111.8
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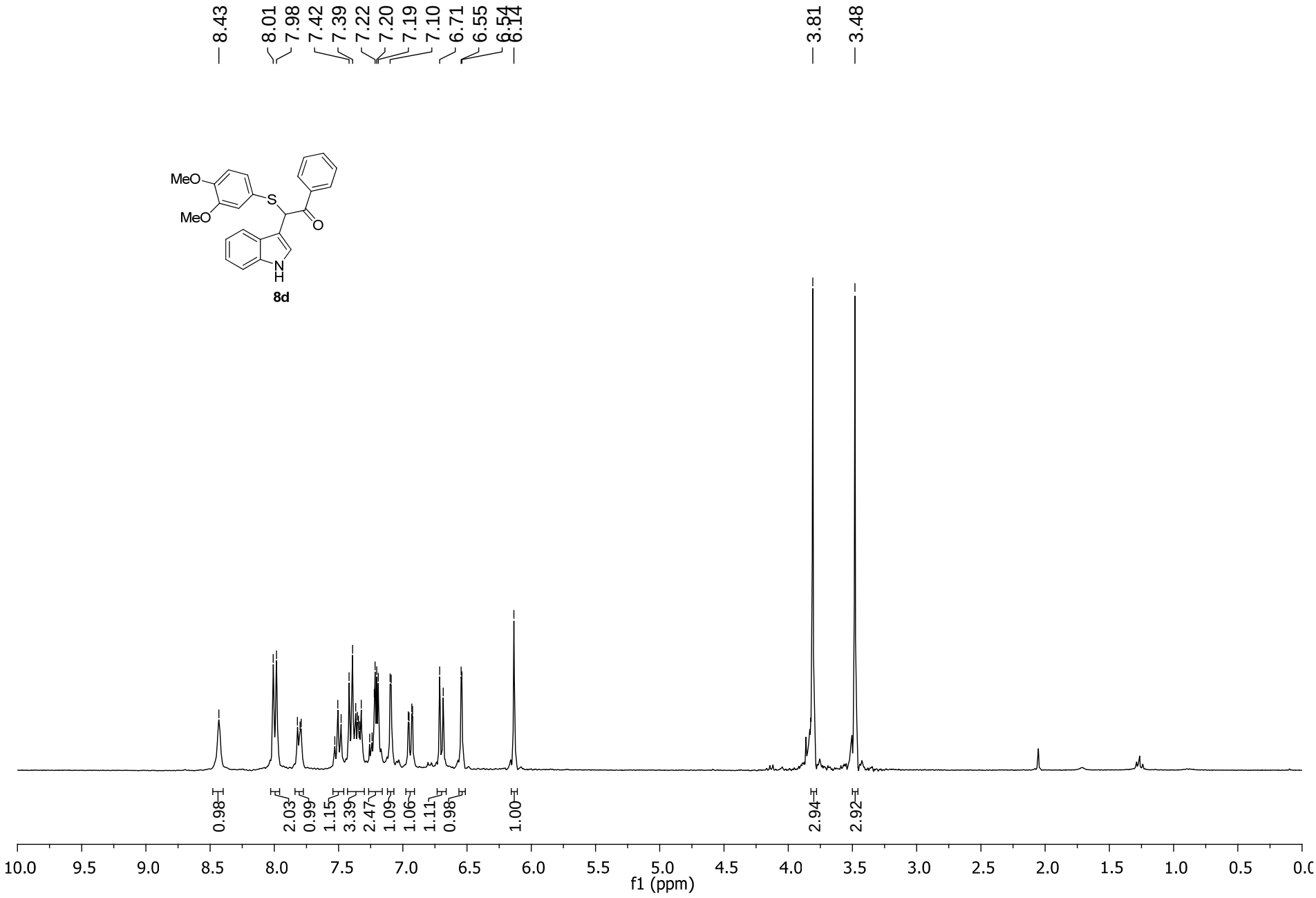
56.2
55.6
49.2
OMe
MeO
S
O
N
H
8c
f1 (ppm)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7.10
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6.55
6.54
6.14
3.81
3.48
MeO
MeO
S
O
N
H
8d
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2.03
0.99
1.15
3.39
2.47
1.09
1.06
1.11
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1.00
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2.92
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9.5
9.0
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8.0
7.5
7.0
6.5
6.0
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2.0
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1.0
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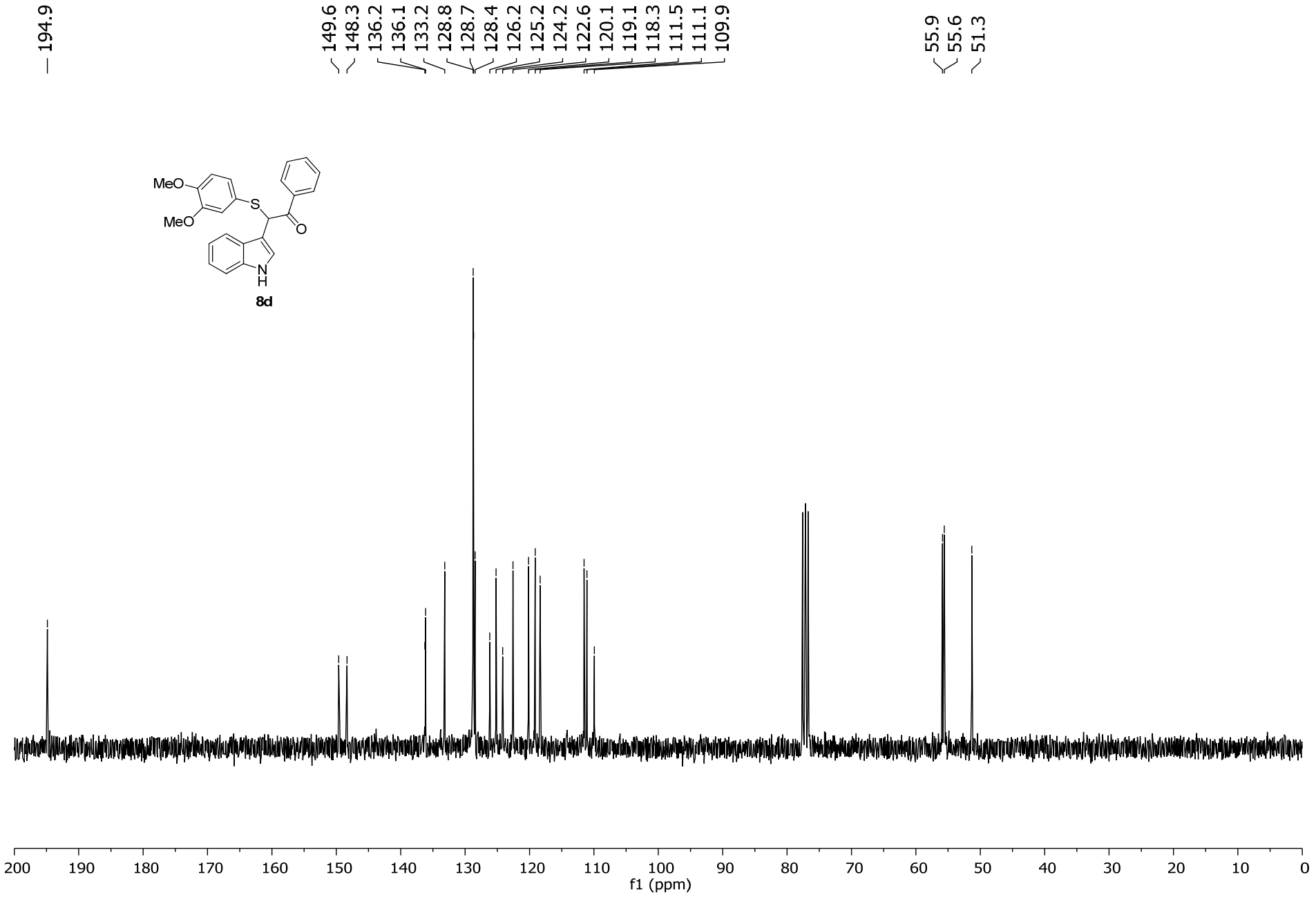
f1 (ppm)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136.2
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133.2
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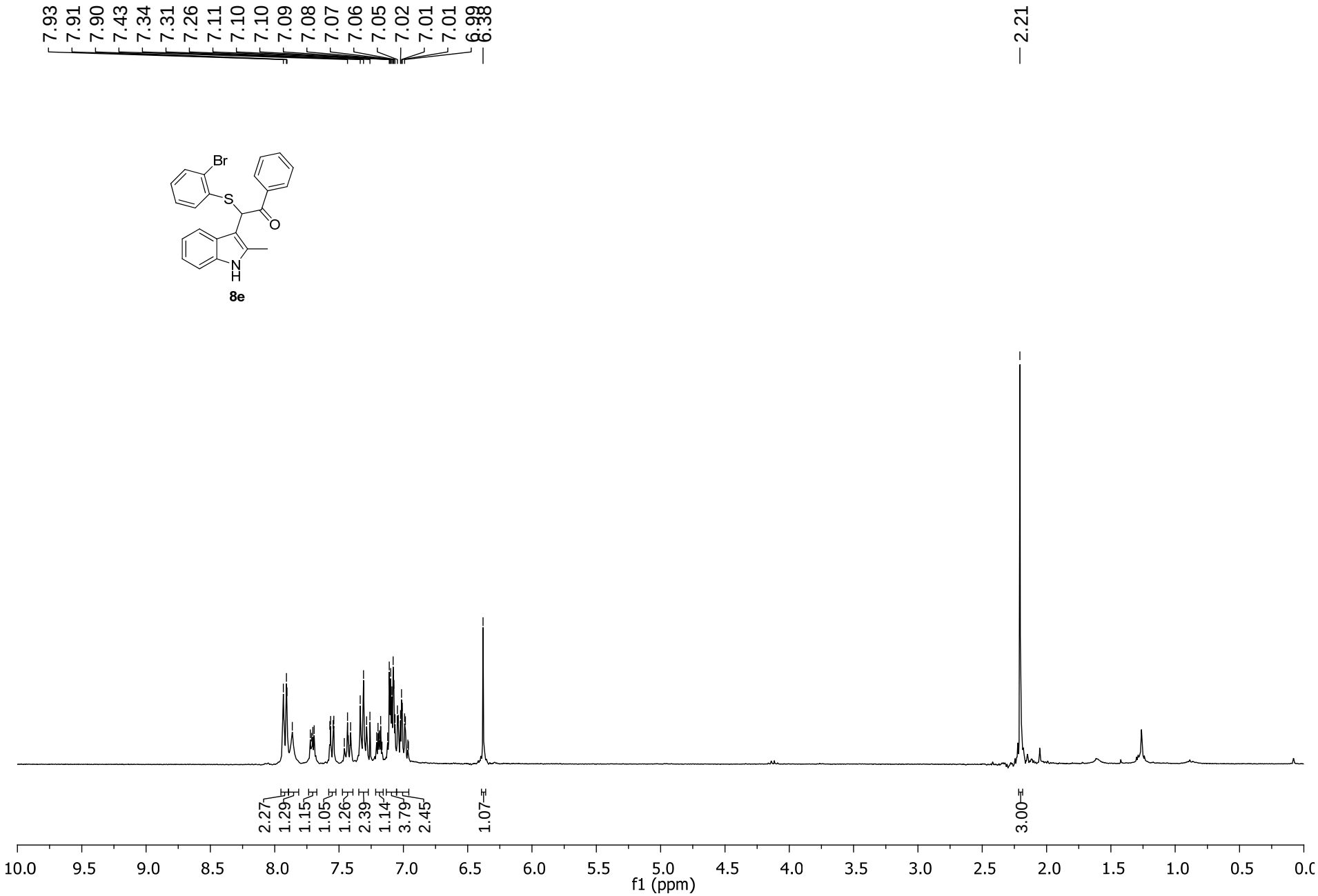
128.4
126.2
125.2
124.2
122.6
120.1
119.1
118.3
111.5
111.1
109.9
55.9
55.6
51.3
MeO
MeO
S
O
N
H
8d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.34
7.31
7.26
7.11
7.10
7.10
7.09
7.08
7.07
7.06
7.05
7.02
7.01
7.01
6.99
6.38
2.21
Br
S
O
N
H
8e
2.27
1.29
1.15
1.05
1.26
2.39
1.14
3.79
2.45
1.07
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
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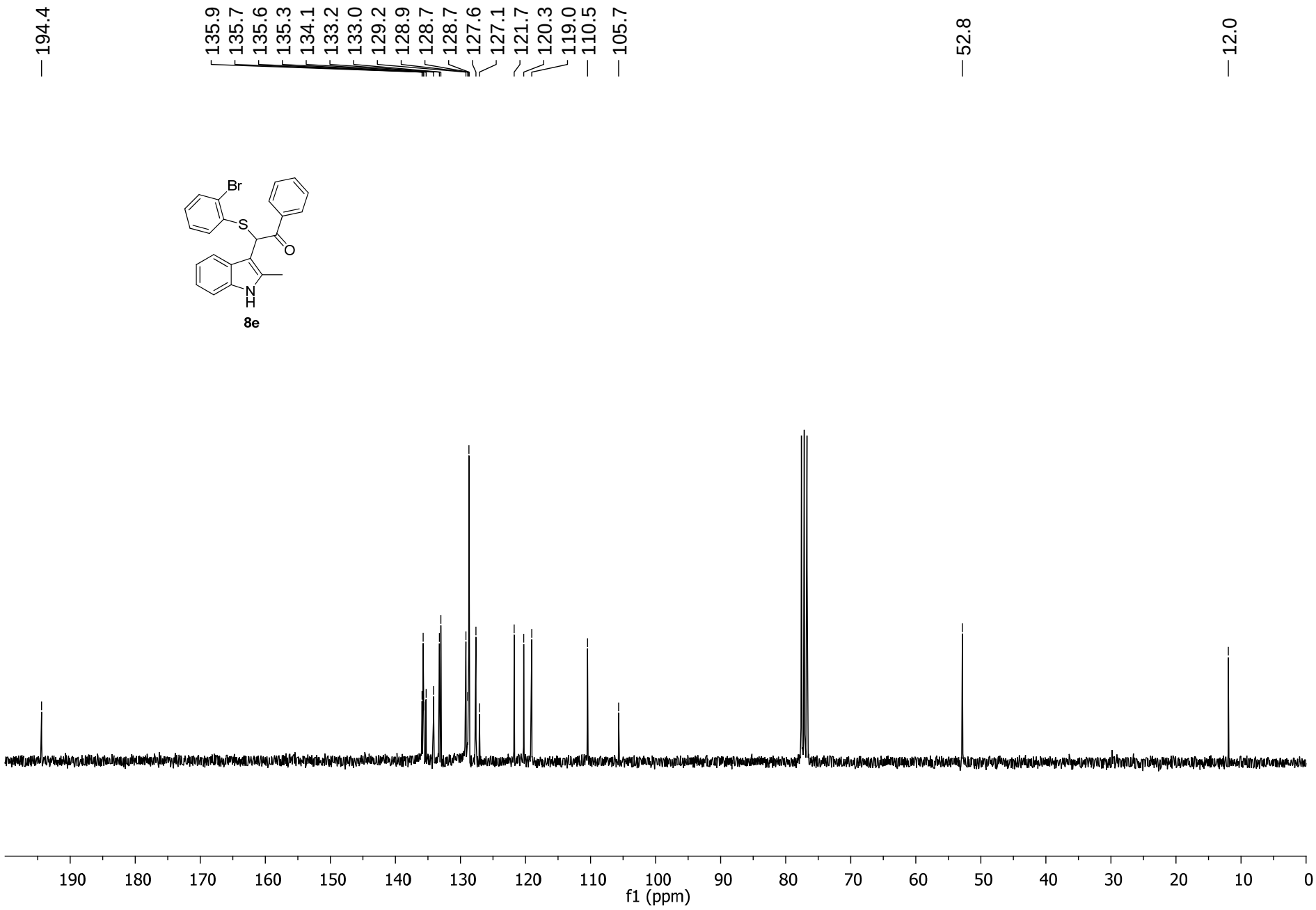
1.5
1.0
0.5
f1 (ppm)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135.9
135.7
135.6
135.3
134.1
133.2
133.0
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128.9
128.7
128.7
127.6
127.1
121.7
120.3
119.0
110.5
105.7
52.8
12.0
Br
S
O
N
H
8e
190
180
170
160
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130
120
110
100
90
80
70
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50
40
30
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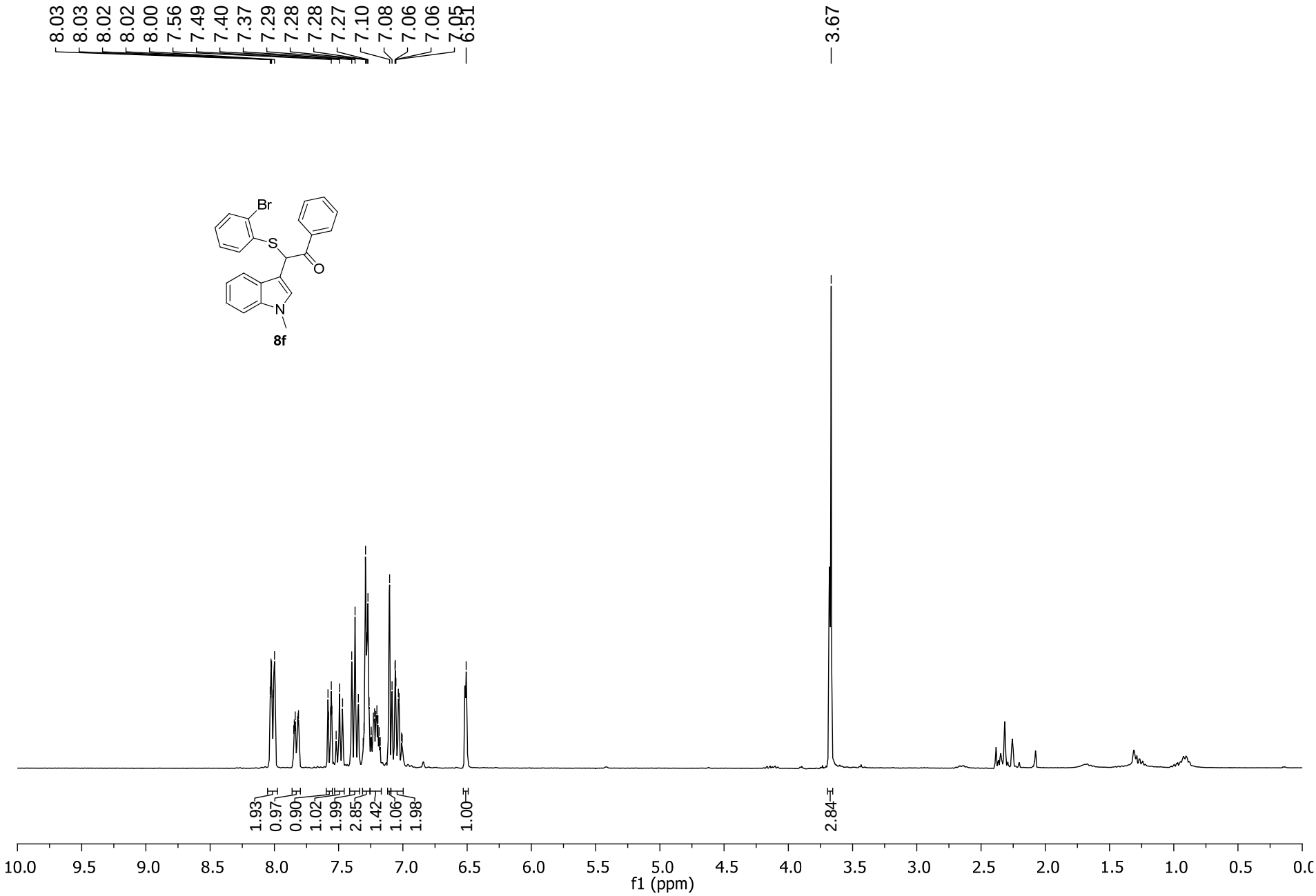
10
0
f1 (ppm)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8.03
8.02
8.02
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7.40
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7.29
7.28
7.28
7.27
7.10
7.08
7.06
7.06
7.05
6.51
3.67
Br
S
O
N
8f
1.93
0.97
0.90
1.02
1.99
2.85
1.42
1.06
1.98
1.00
2.84
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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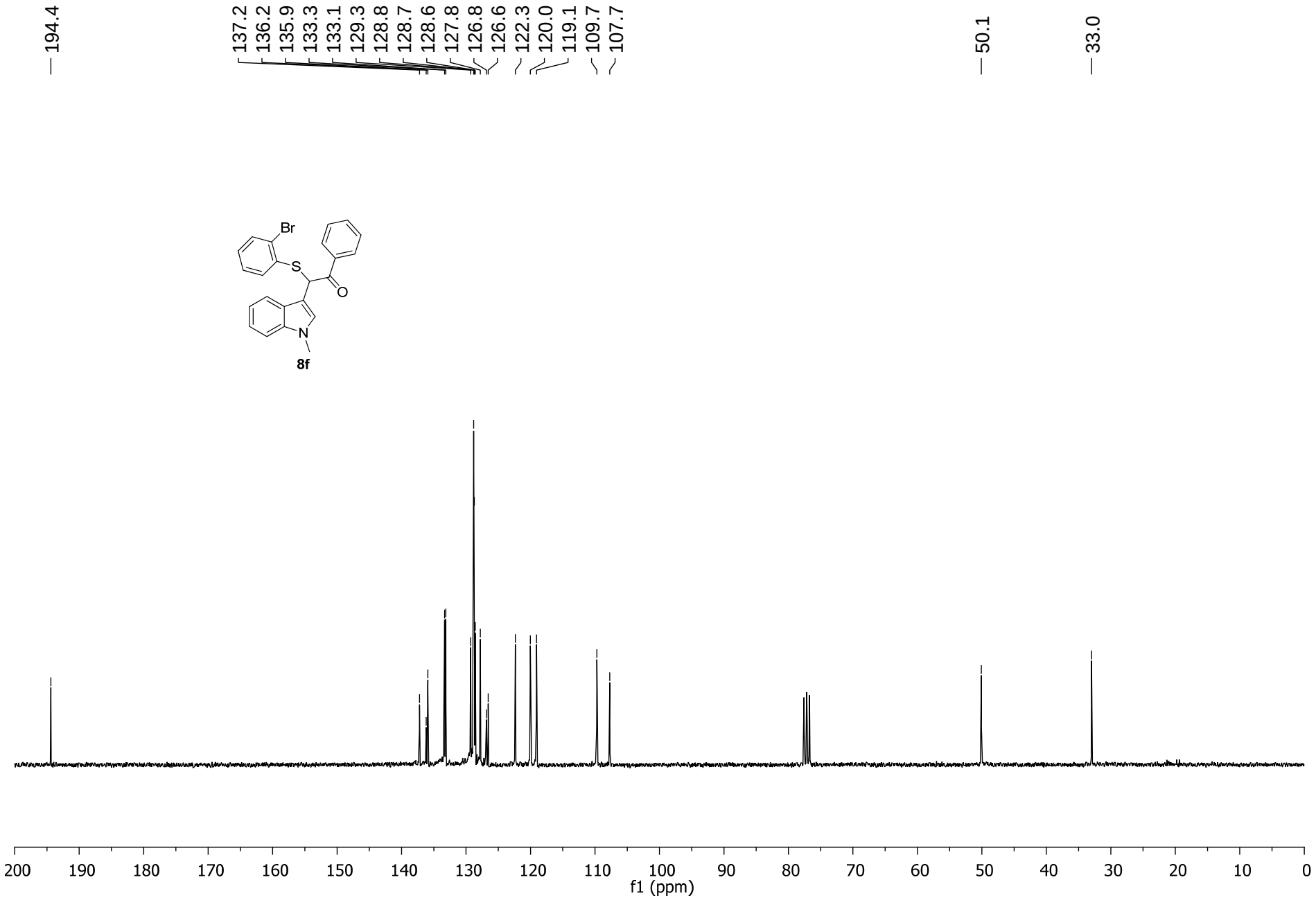
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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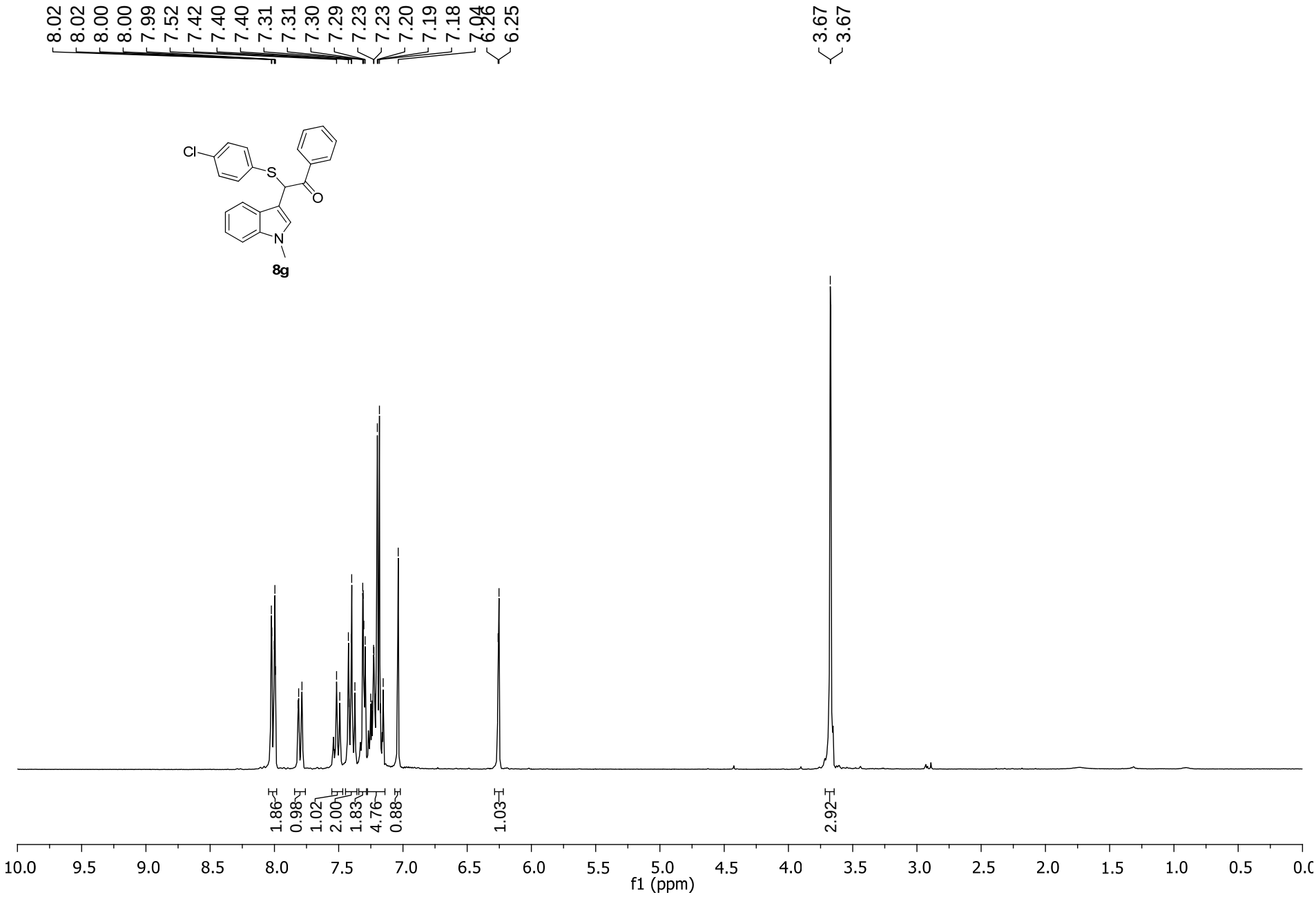
133.1
129.3
128.8
128.7
128.6
127.8
126.8
126.6
122.3
120.0
119.1
109.7
107.7
50.1
33.0
Br
S
O
N
8f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.02
8.00
8.00
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7.31
7.31
7.30
7.29
7.23
7.23
7.20
7.19
7.18
7.04
6.26
6.25
3.67
3.67
Cl
S
O
N
8g
1.86
0.98
1.02
2.00
1.83
4.76
0.88
1.03
2.92
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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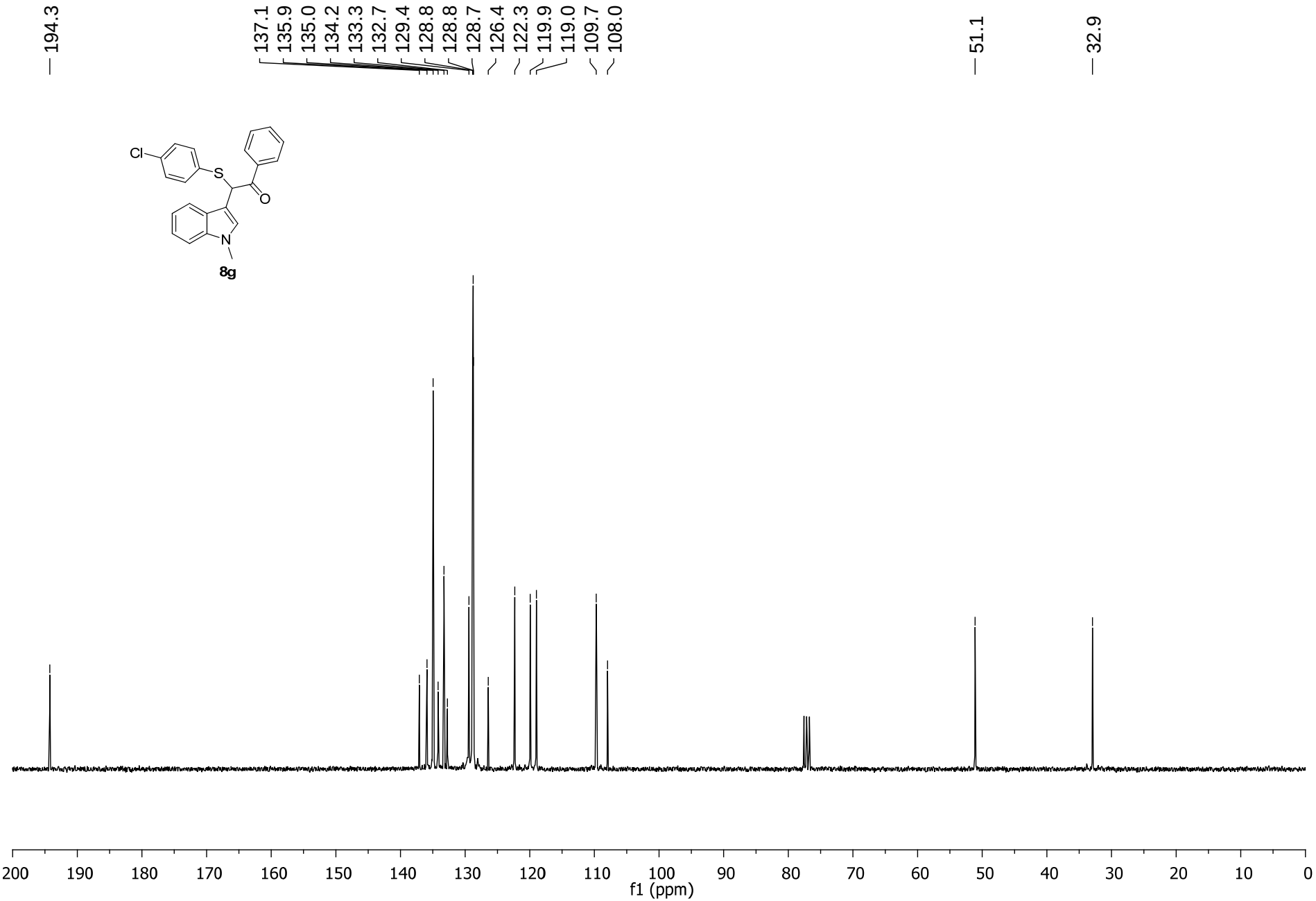
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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137.1
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132.7
129.4
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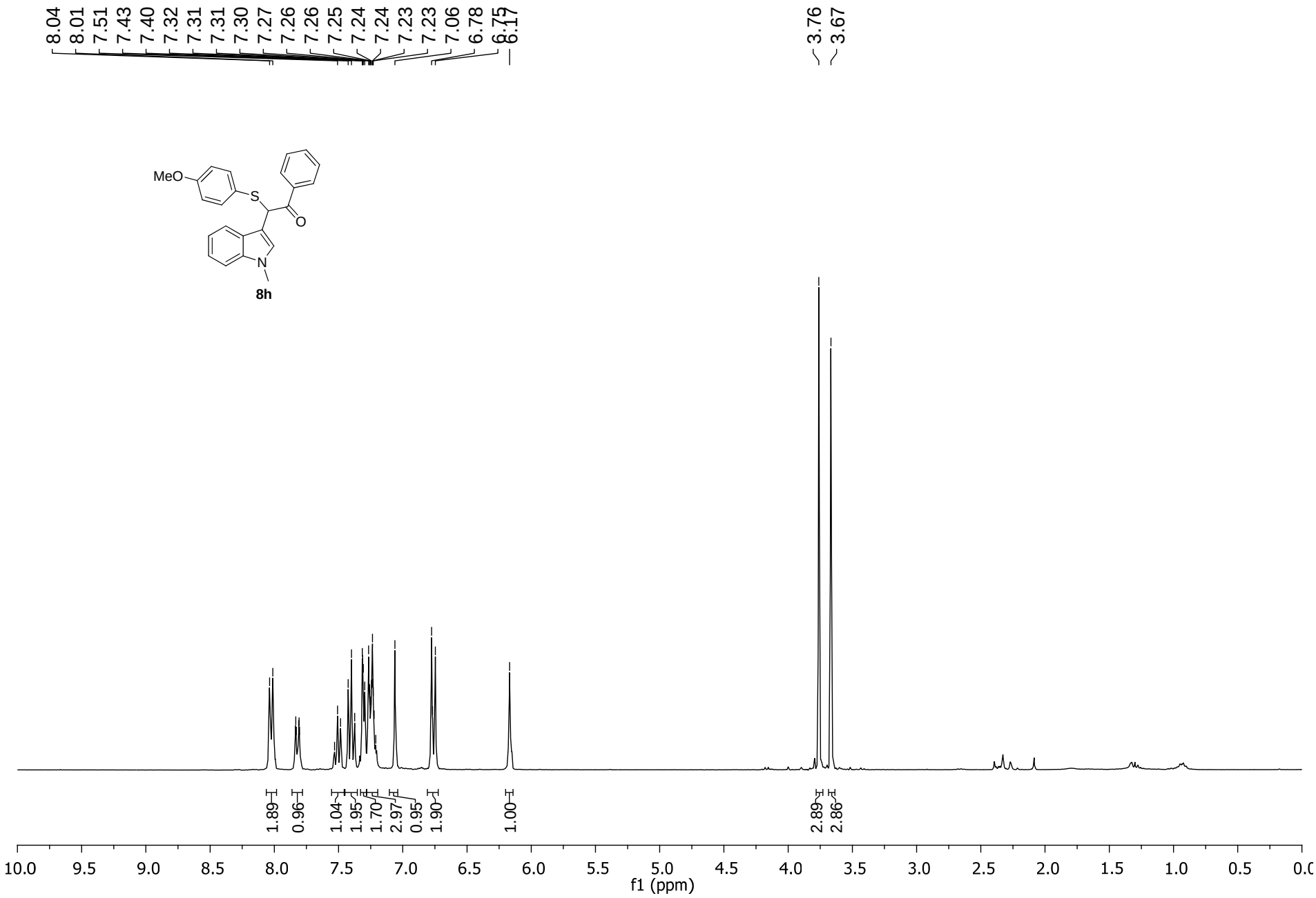
128.8
128.7
126.4
122.3
119.9
119.0
109.7
108.0
51.1
32.9
Cl
S
O
N
8g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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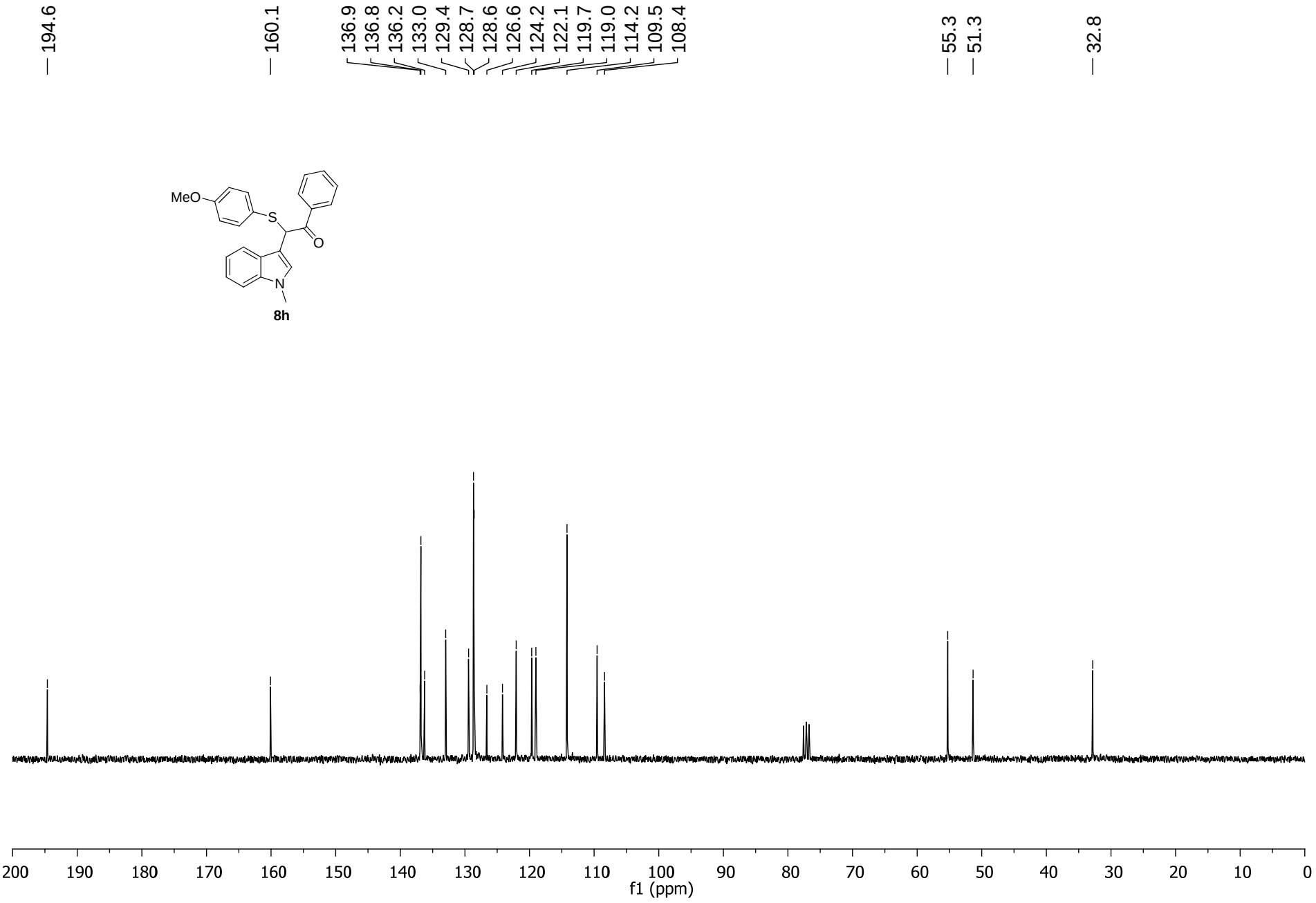
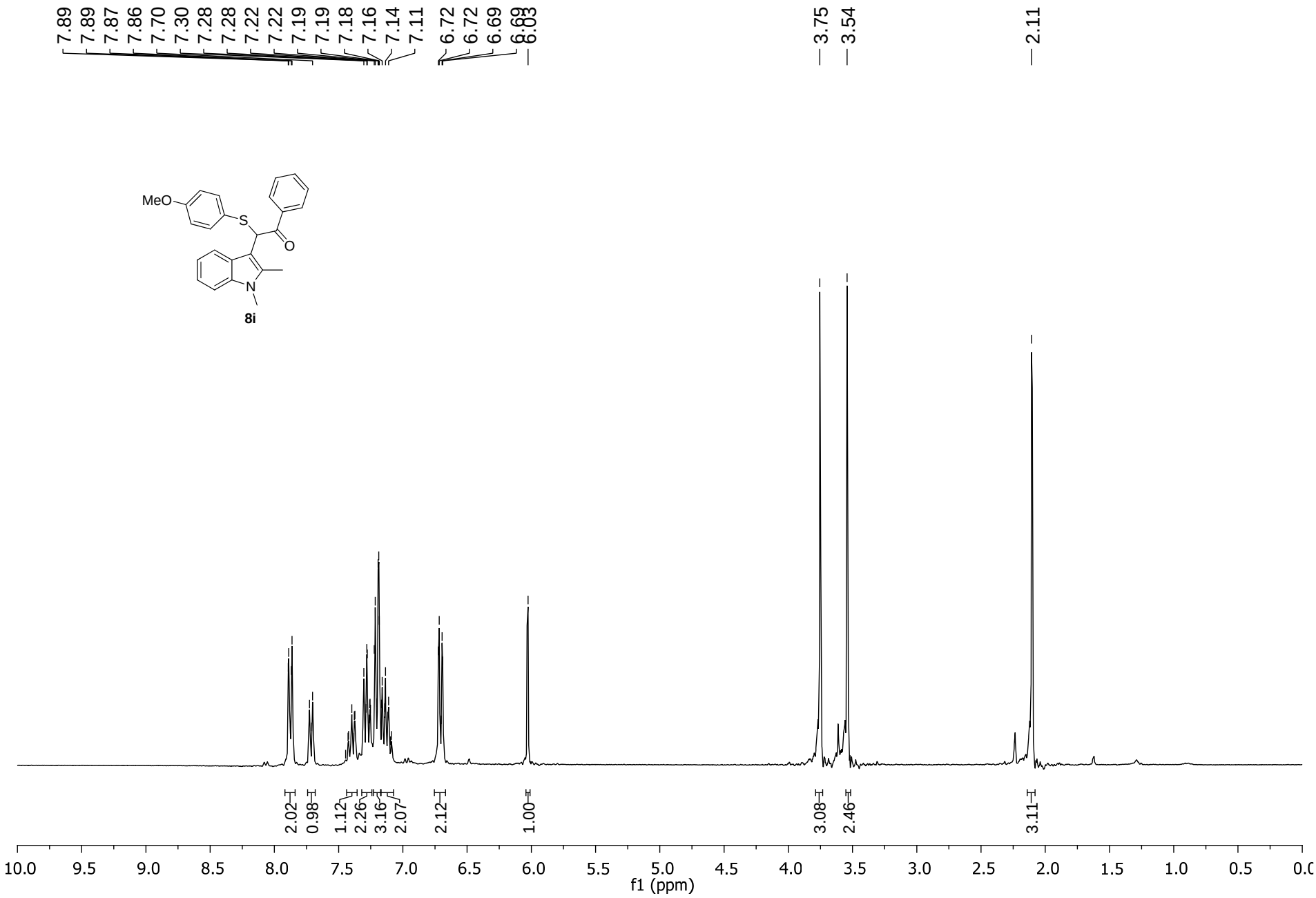
7.31
7.31
7.30
7.27
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.06
6.78
6.75
6.17
3.76
3.67
MeO
S
O
N
8h
1.89
0.96
1.04
1.95
1.70
2.97
0.95
1.90
1.00
2.89
2.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


194.6
160.1
136.9
136.8
136.2
133.0
129.4
128.7
128.6
126.6
124.2
122.1
119.7
119.0
114.2
109.5
108.4
55.3
51.3
32.8
MeO
S
O
N
8h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.89
7.89
7.87
7.86
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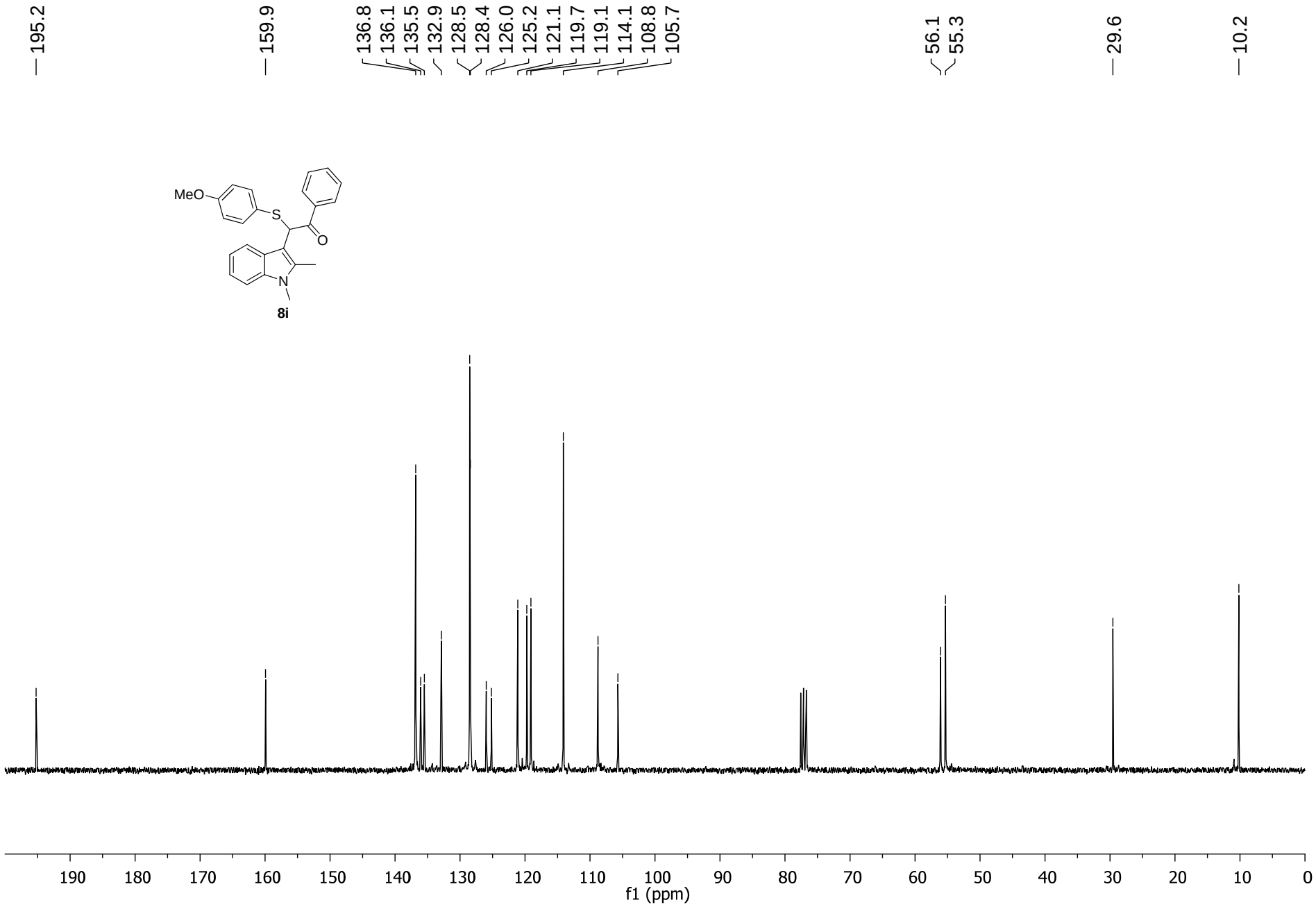
7.30
7.28
7.28
7.22
7.22
7.19
7.19
7.18
7.16
7.14
7.11
6.72
6.72
6.69
6.69
6.03
3.75
3.54
2.11
MeO
S
O
N
8i
2.02
0.98
1.12
2.26
3.16
2.07
2.12
1.00
3.08
2.46
3.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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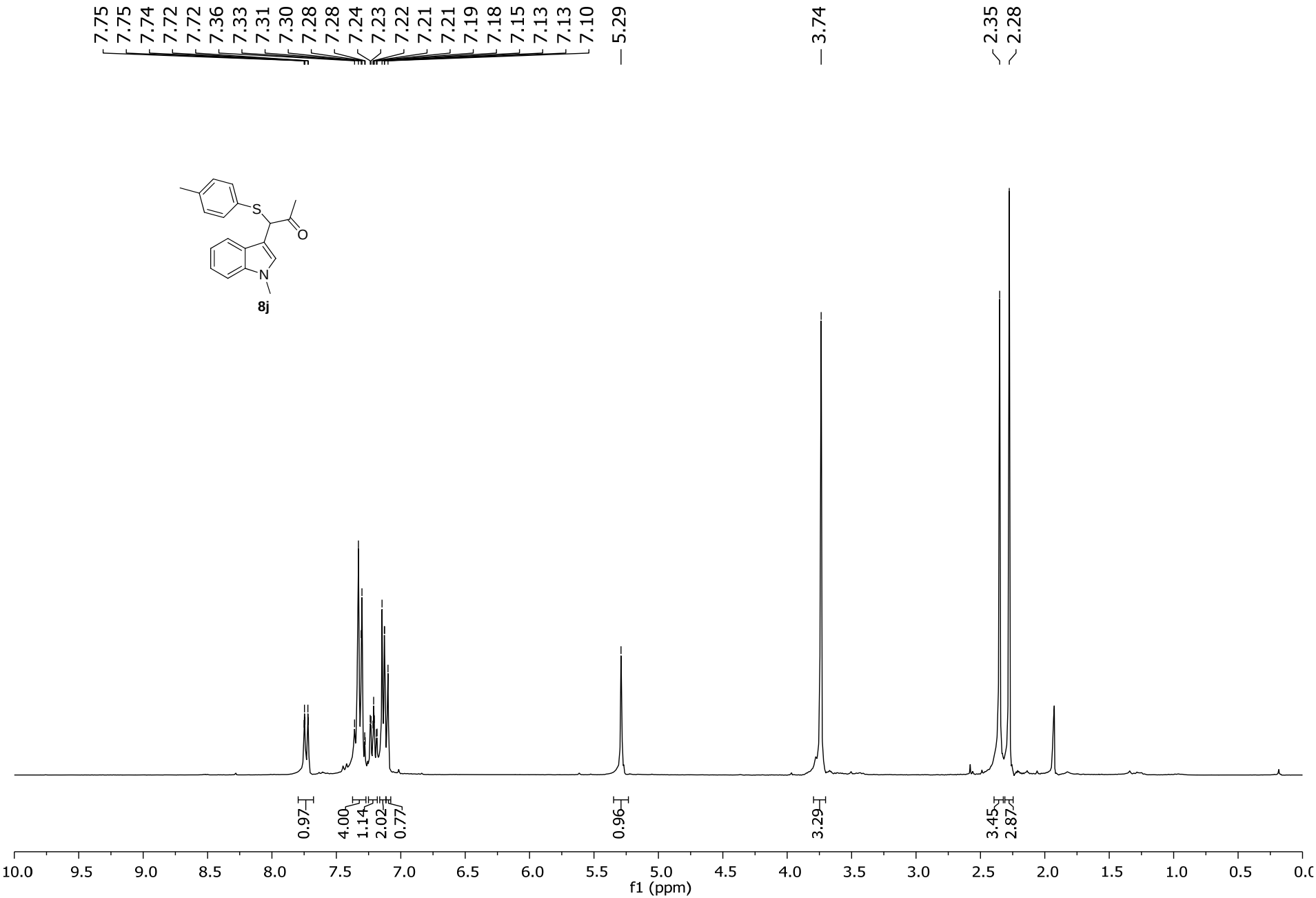
159.9
136.8
136.1
135.5
132.9
128.5
128.4
126.0
125.2
121.1
119.7
119.1
114.1
108.8
105.7
56.1
55.3
29.6
10.2
MeO
S
O
N
8i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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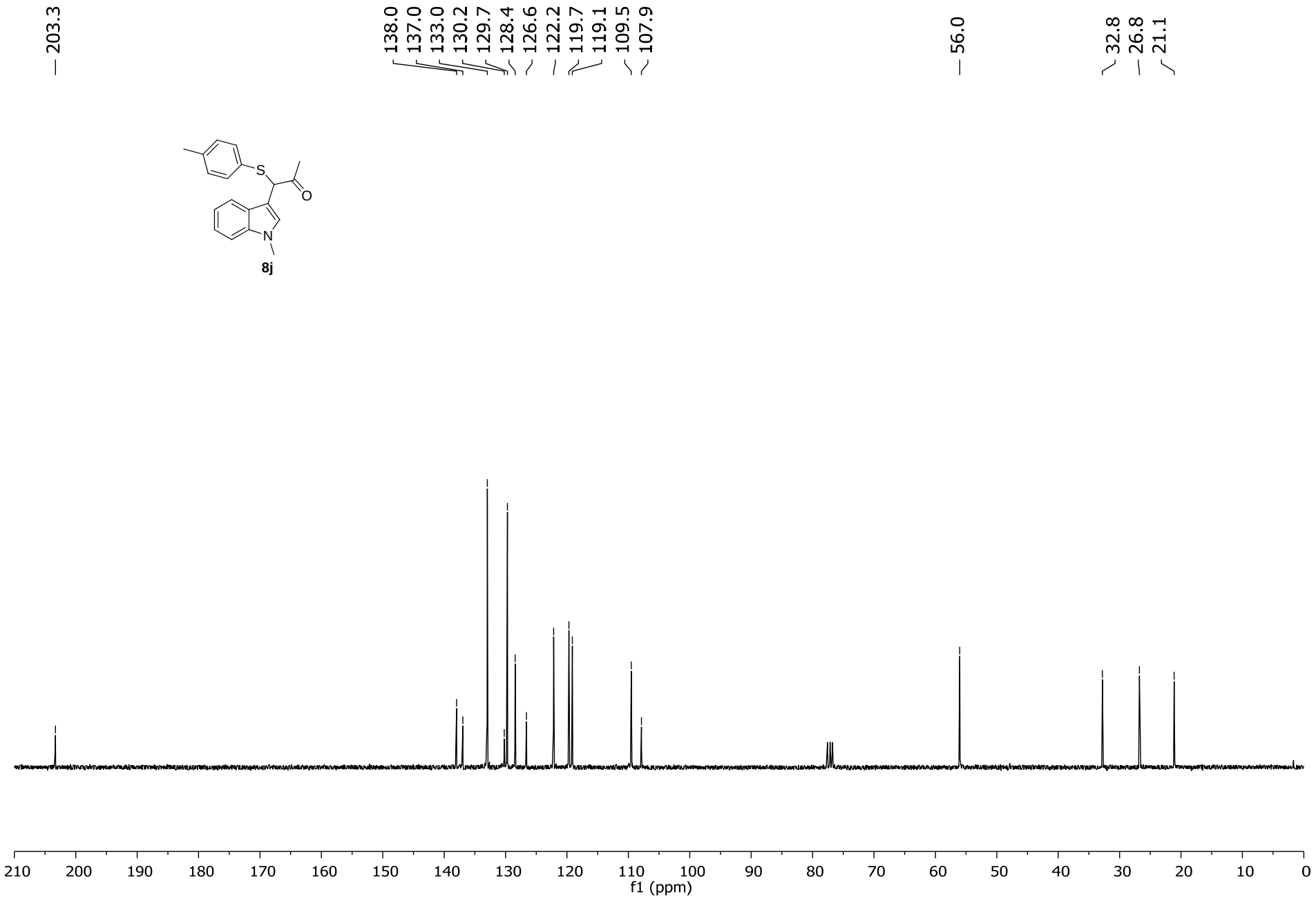
7.75
7.74
7.72
7.72
7.36
7.33
7.31
7.30
7.28
7.28
7.24
7.23
7.22
7.21
7.21
7.19
7.18
7.15
7.13
7.13
7.10
5.29
3.74
2.35
2.28
S
O
N
8j
0.97
4.00
1.14
2.02
0.77
0.96
3.29
3.45
2.87
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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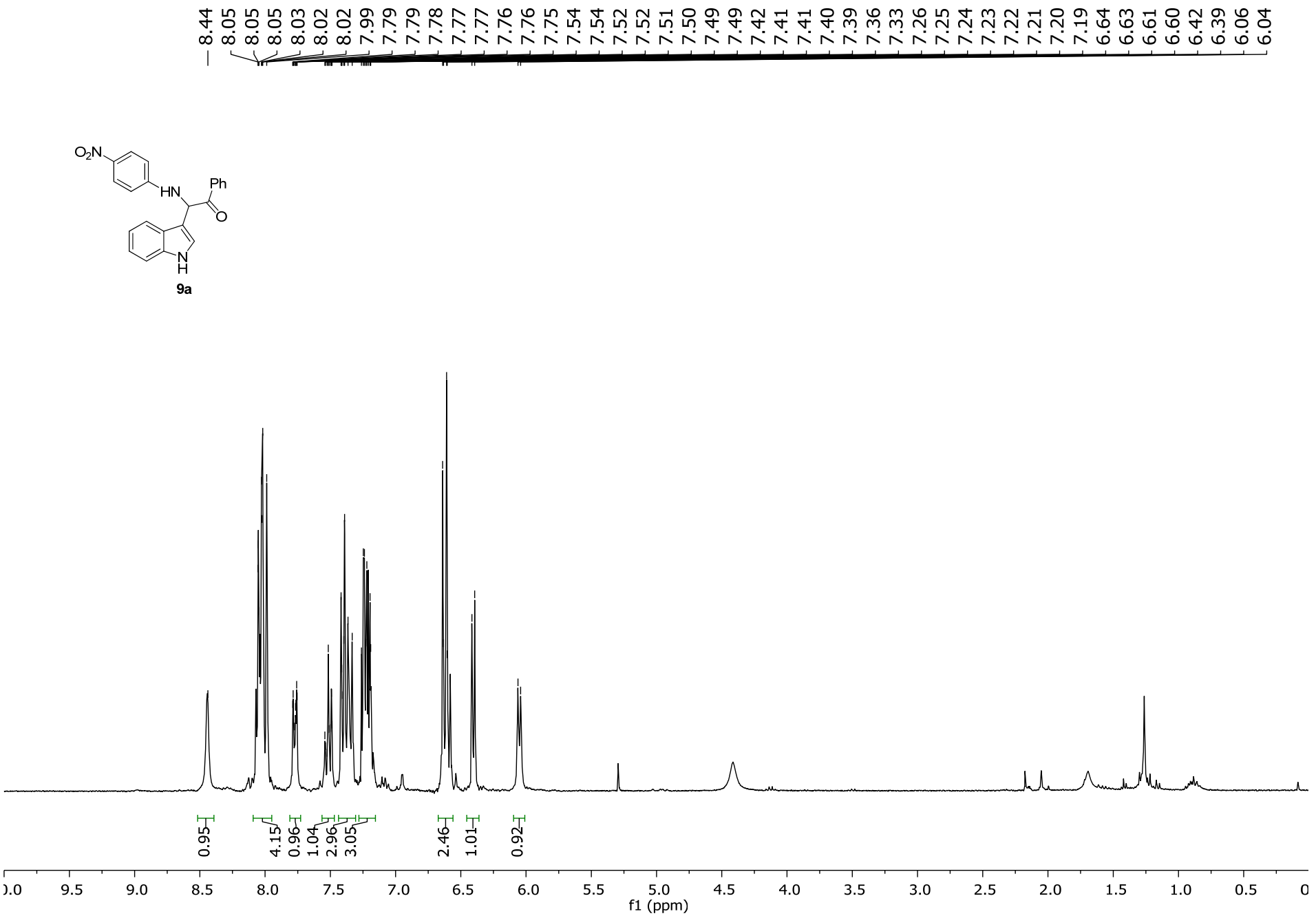
130.2
129.7
128.4
126.6
122.2
119.7
119.1
109.5
107.9
56.0
32.8
26.8
21.1
S
O
N
8j
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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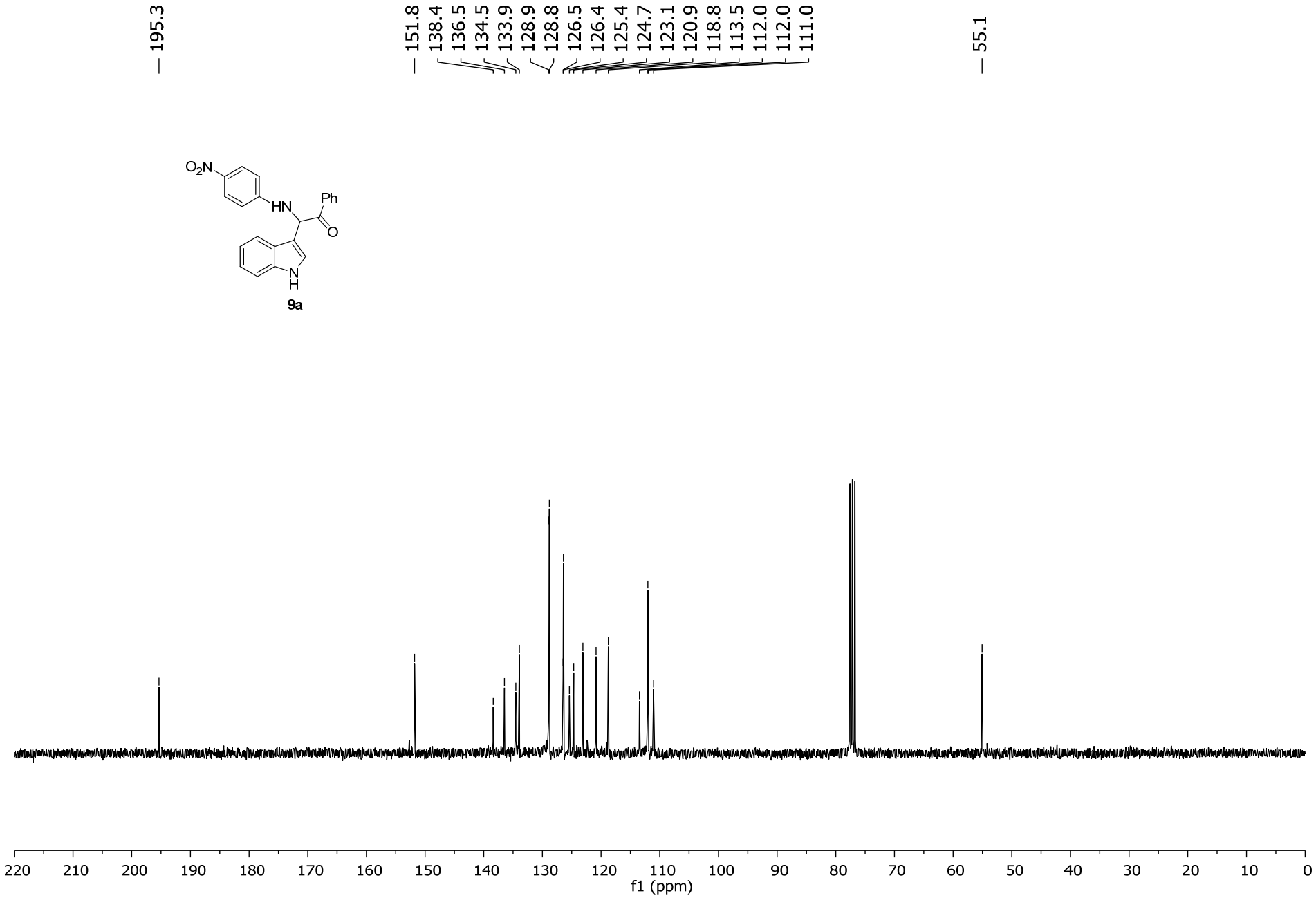
8.05
8.05
8.03
8.02
8.02
7.99
7.79
7.79
7.78
7.77
7.77
7.76
7.76
7.75
7.54
7.54
7.52
7.52
7.51
7.50
7.49
7.49
7.42
7.41
7.41
7.40
7.39
7.36
7.33
7.26
7.25
7.24
7.23
7.22
7.21
7.20
7.19
6.64
6.63
6.61
6.60
6.42
6.39
6.06
6.04
O2N
HN
Ph
O
N
H
9a
0.95
4.15
0.96
1.04
2.96
3.05
2.46
1.01
0.92
9.5
9.0
8.5
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
f1 (ppm)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133.9
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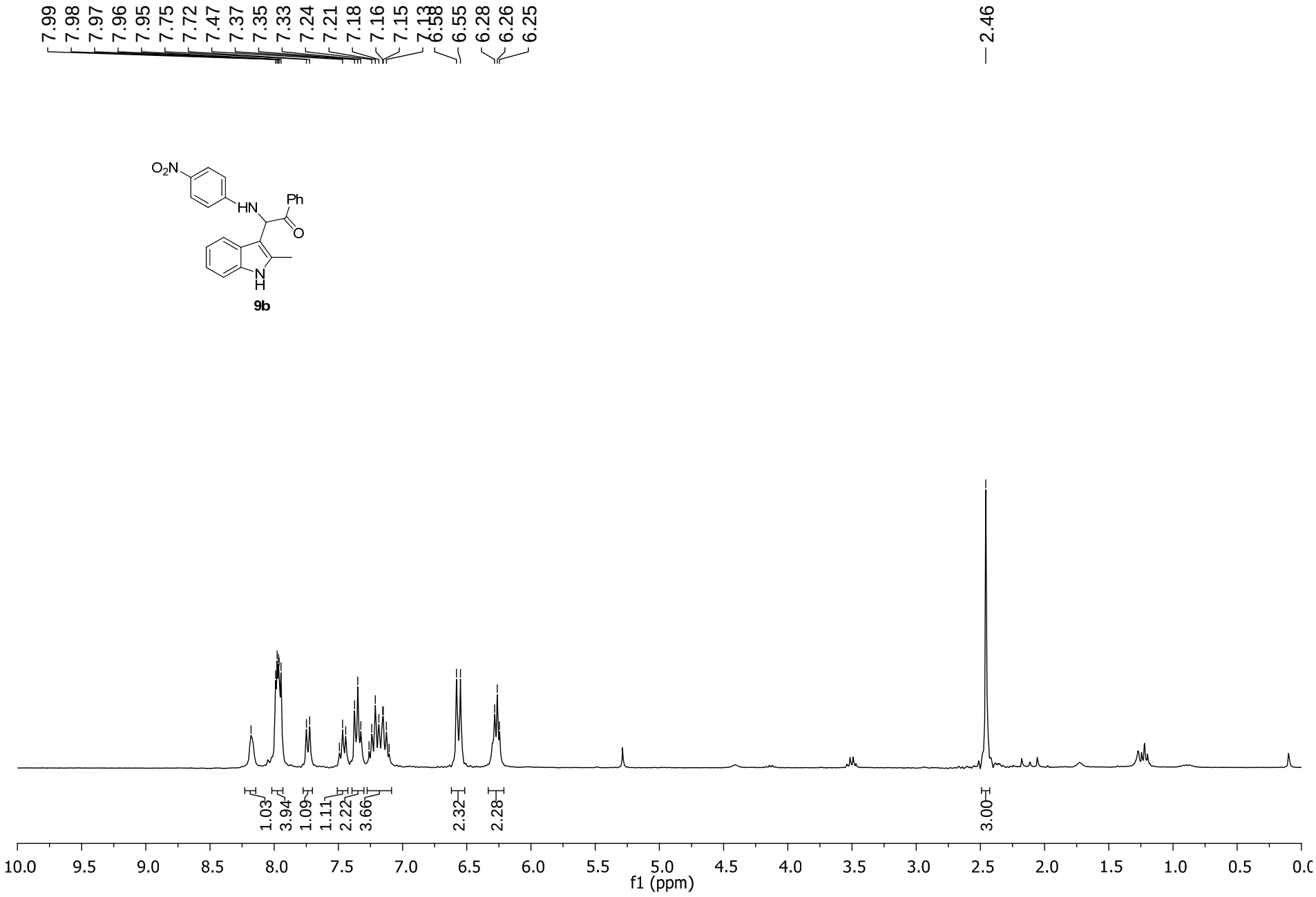
128.8
126.5
126.4
125.4
124.7
123.1
120.9
118.8
113.5
112.0
112.0
111.0
55.1
O2N
HN
Ph
O
N
H
9a
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.75
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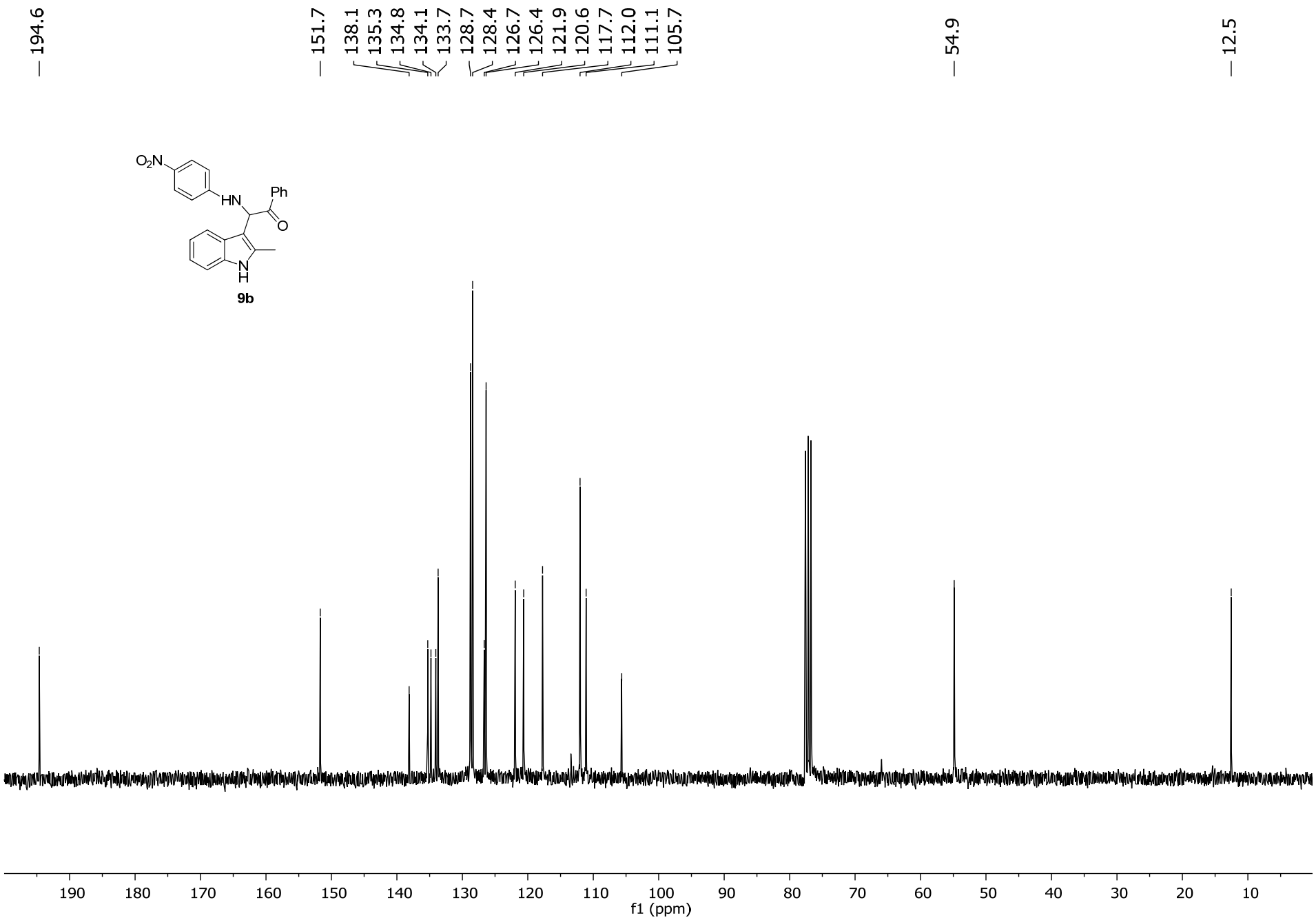
7.33
7.24
7.21
7.18
7.16
7.15
7.13
6.58
6.55
6.28
6.26
6.25
2.46
O2N
HN
Ph
O
N
H
9b
1.03
3.94
1.09
1.11
2.22
3.66
2.32
2.28
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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138.1
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134.8
134.1
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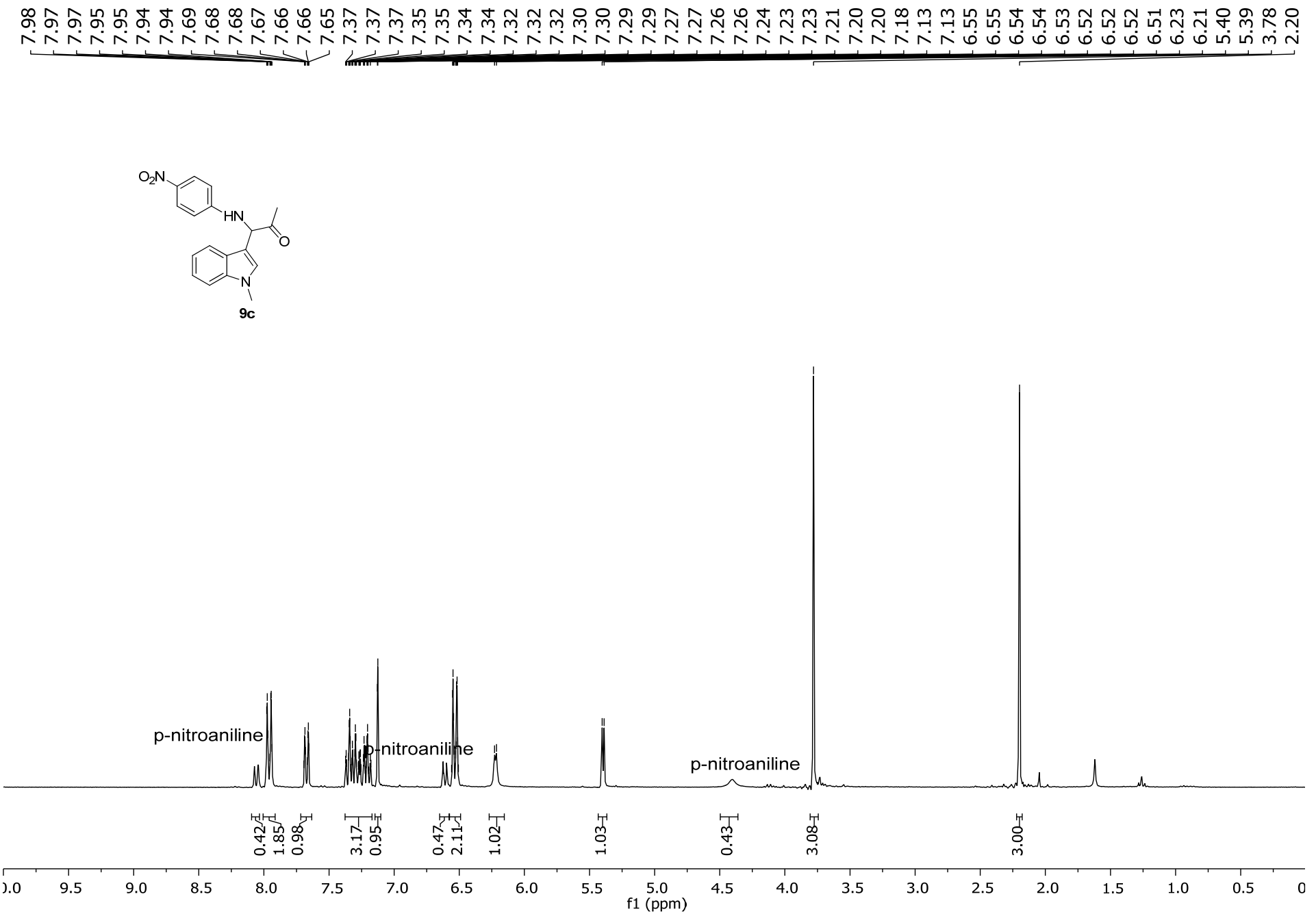
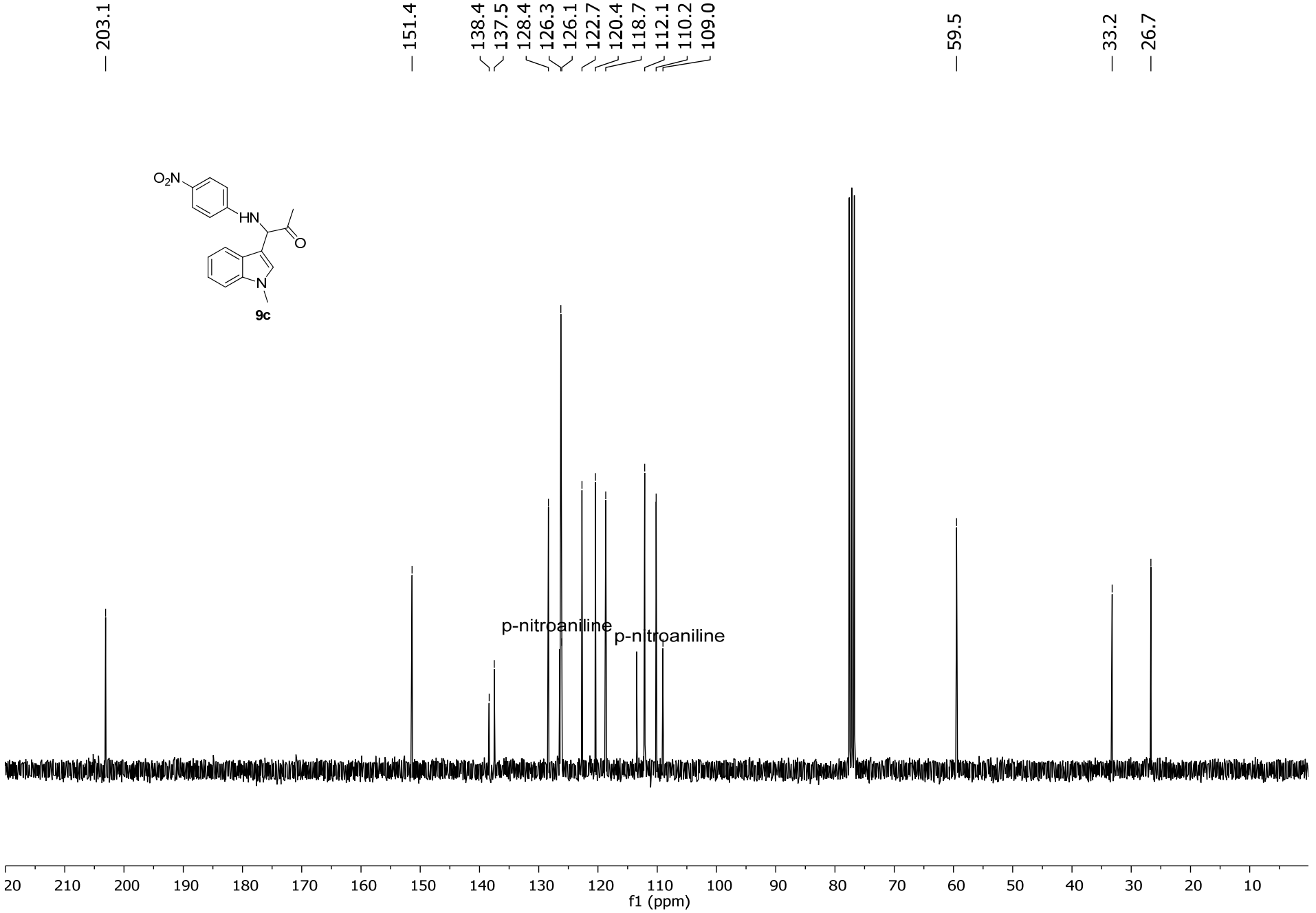
128.7
128.4
126.7
126.4
121.9
120.6
117.7
112.0
111.1
105.7
54.9
12.5
O2N
HN
Ph
O
N
H
9b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.98 7.97 7.97 7.95 7.95 7.94 7.94 7.69 7.68 7.68 7.67 7.66 7.66 7.65 7.37 7.37 7.37 7.35 7.35 7.34 7.34 7.32 7.32 7.32 7.30 7.30 7.29 7.29 7.27 7.27 7.26 7.26 7.24 7.23 7.23 7.21 7.20 7.20 7.18 7.13 7.13 6.55 6.55 6.54 6.54 6.53 6.52 6.52 6.52 6.51 6.23 6.21 5.40 5.39 3.78 2.20
O2N
HN
O
N
9c
p-nitroaniline
p-nitroaniline
p-nitroaniline
0.42 1.85 0.98 3.17 0.95 0.47 2.11 1.02 1.03 0.43 3.08 3.00
f1 (ppm)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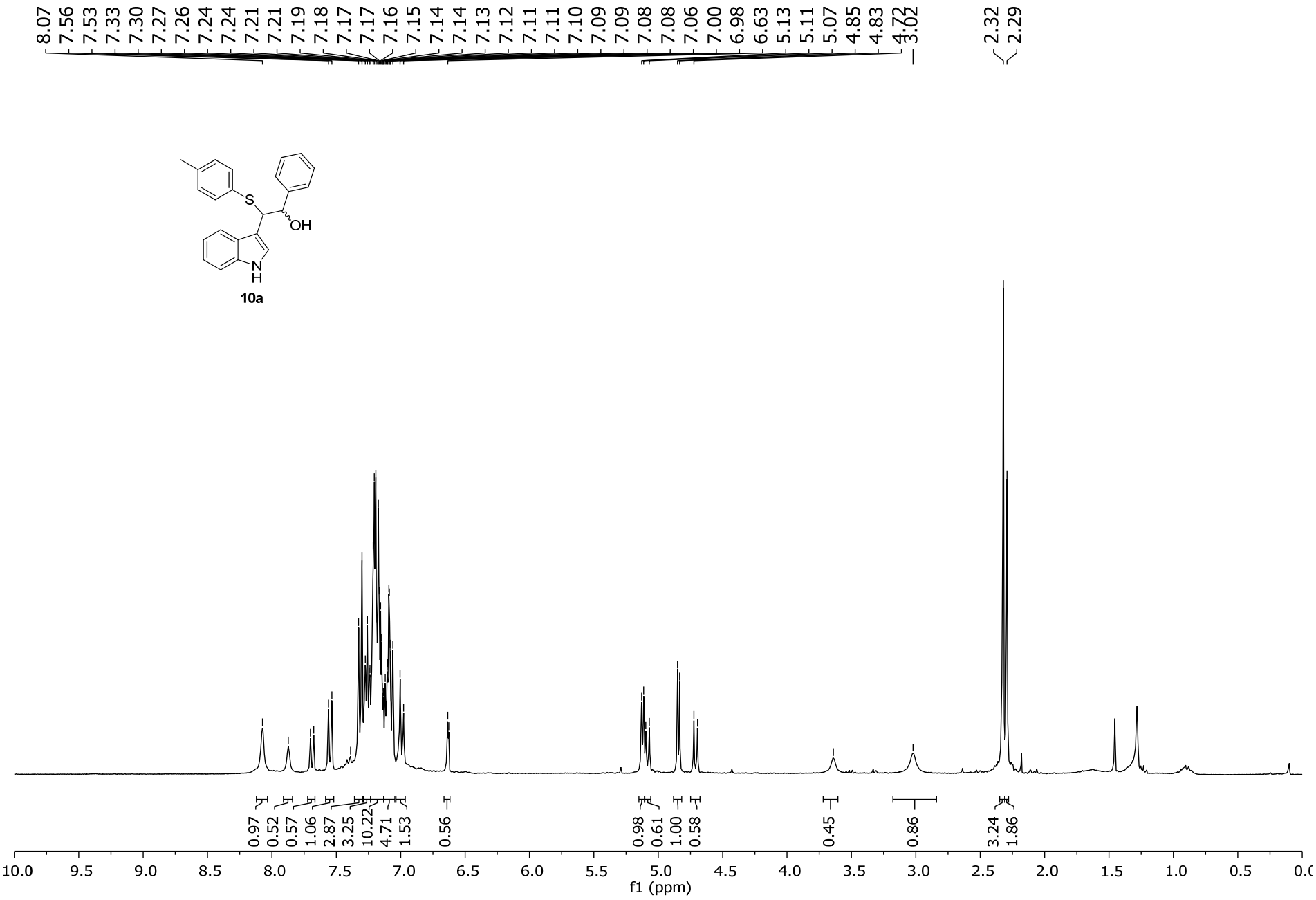
137.5
128.4
126.3
126.1
122.7
120.4
118.7
112.1
110.2
109.0
59.5
33.2
26.7
O2N
HN
O
N
9c
p-nitroaniline
p-nitroaniline
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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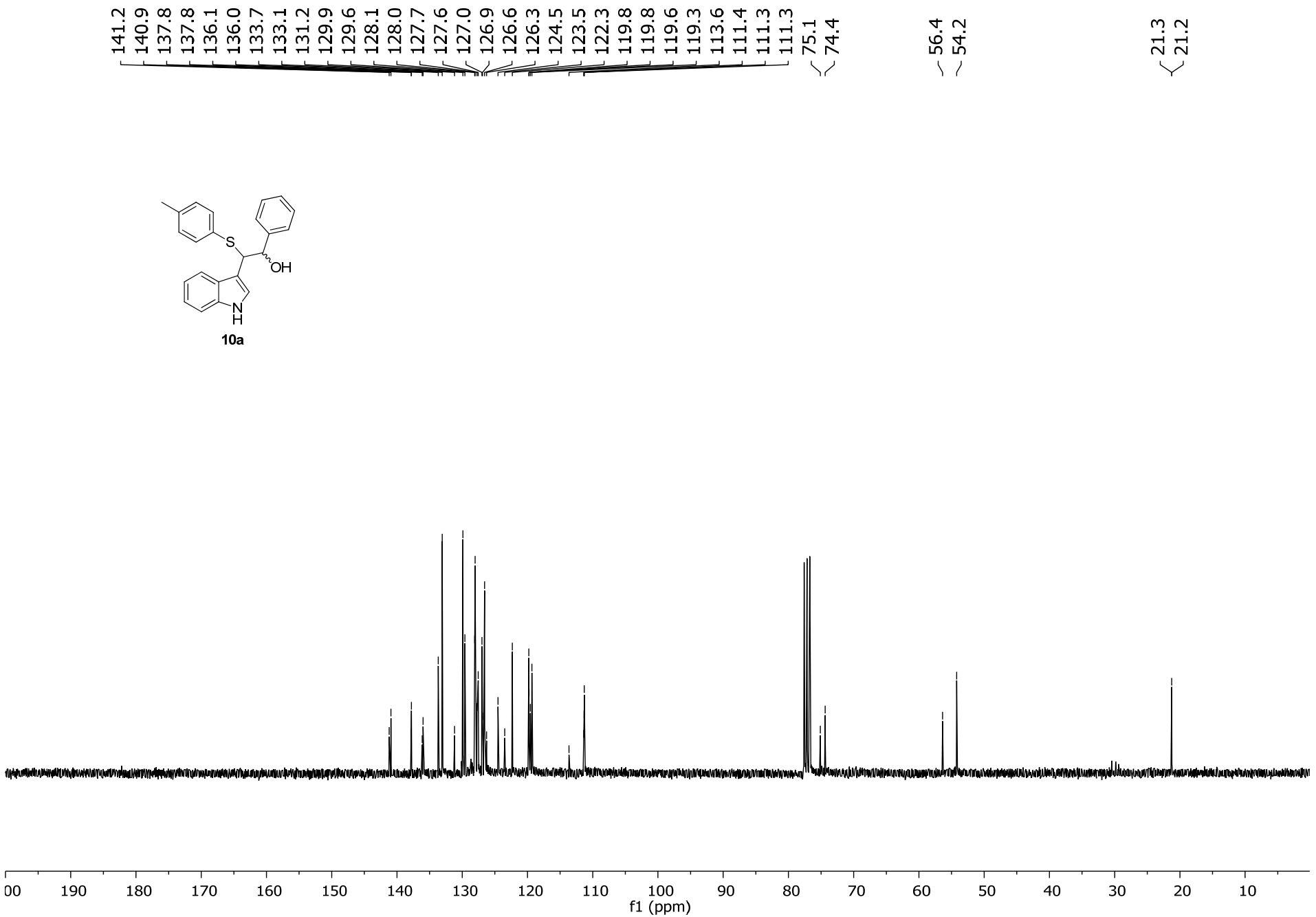
7.17
7.17
7.16
7.15
7.14
7.14
7.13
7.12
7.11
7.11
7.10
7.09
7.09
7.08
7.08
7.06
7.00
6.98
6.63
5.13
5.11
5.07
4.85
4.83
4.72
3.02
2.32
2.29
S
OH
N
H
10a
0.97
0.52
0.57
1.06
2.87
3.25
10.22
4.71
1.53
0.56
0.98
0.61
1.00
0.58
0.45
0.86
3.24
1.86
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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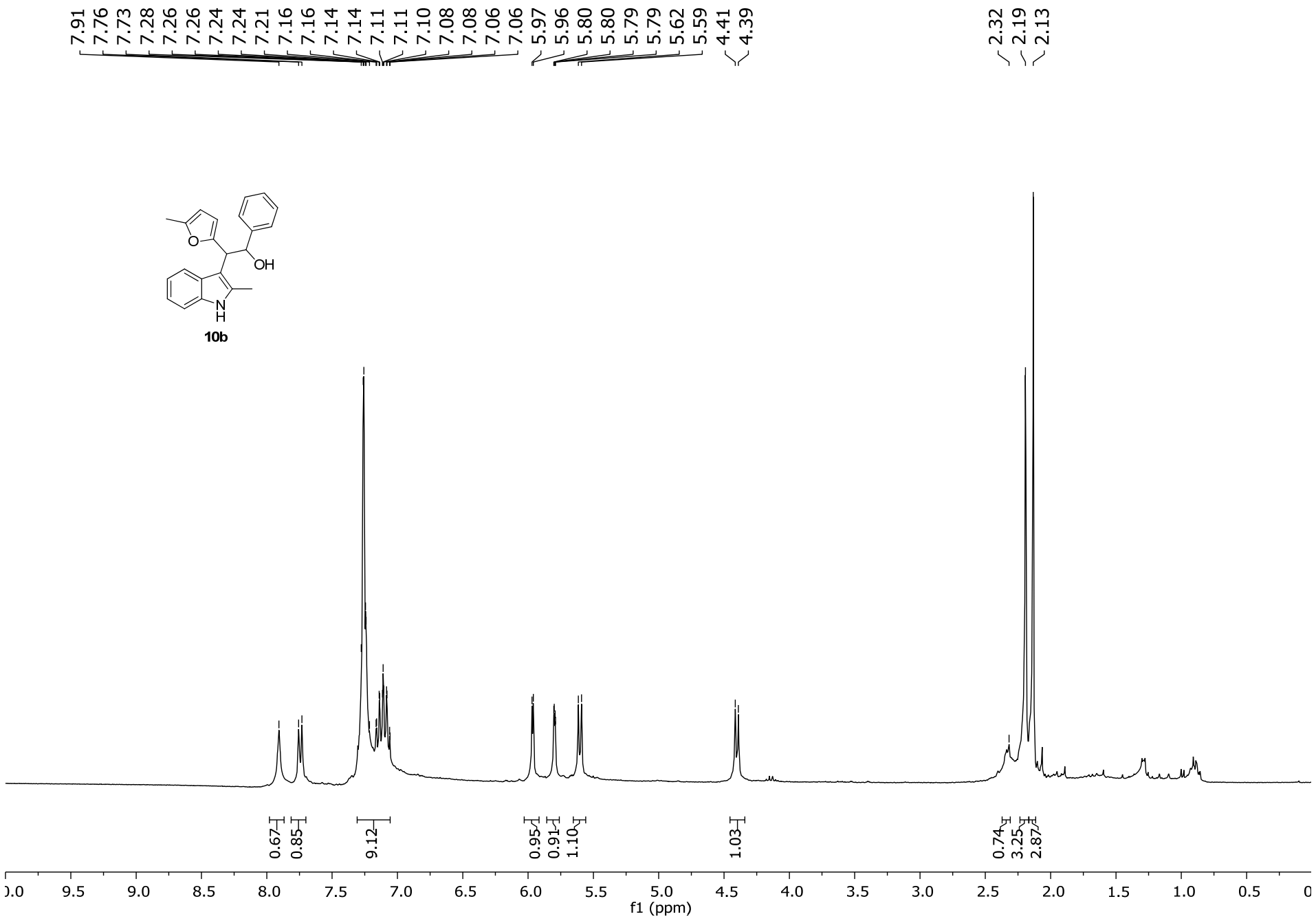
133.1
131.2
129.9
129.6
128.1
128.0
127.7
127.6
127.0
126.9
126.6
126.3
124.5
123.5
122.3
119.8
119.8
119.6
119.3
113.6
111.4
111.3
111.3
75.1
74.4
56.4
54.2
21.3
21.2
S
OH
N
H
10a
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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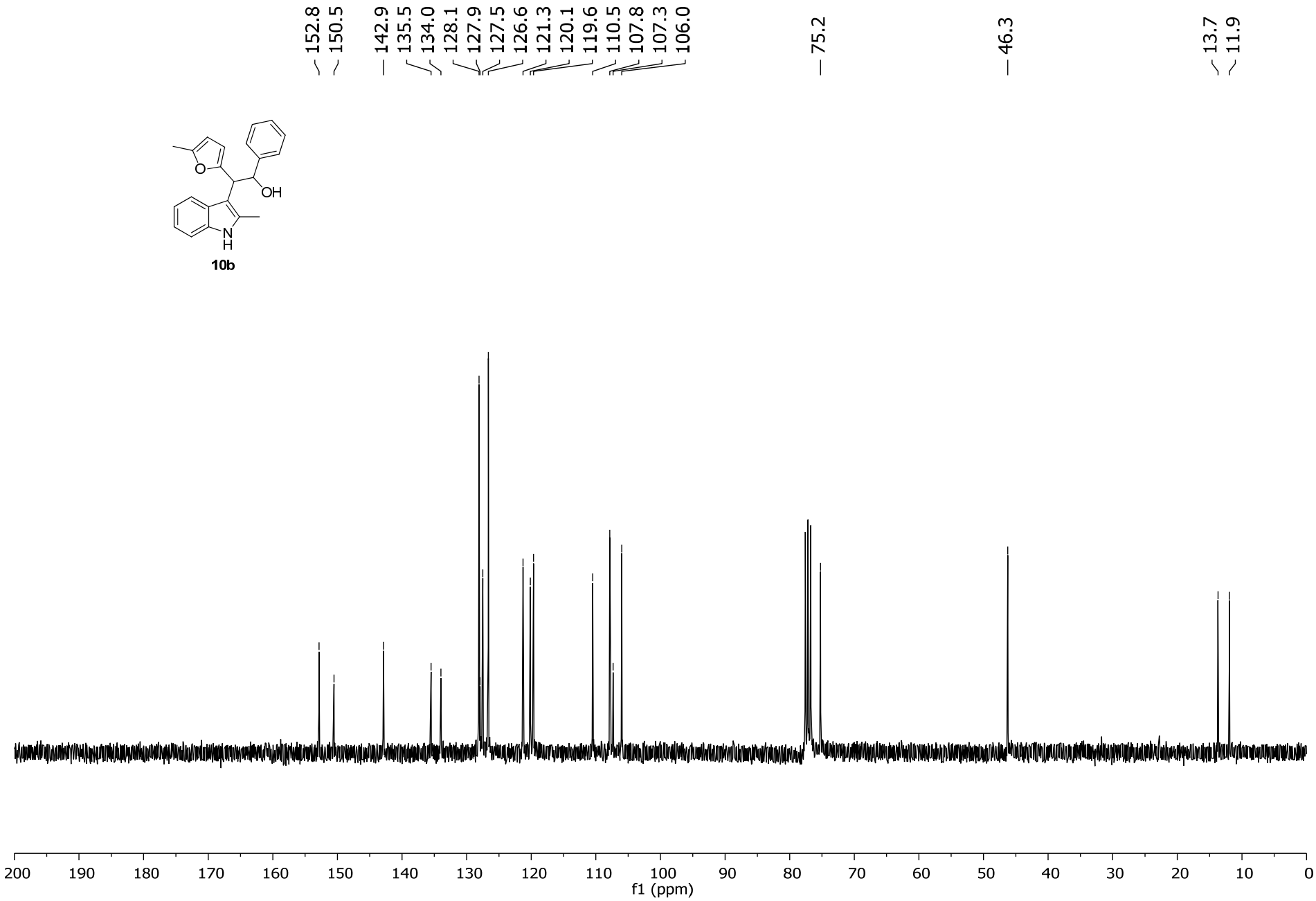
7.24
7.21
7.16
7.16
7.14
7.14
7.11
7.11
7.10
7.08
7.08
7.06
7.06
5.97
5.96
5.80
5.80
5.79
5.79
5.62
5.59
4.41
4.39
2.32
2.19
2.13
O
OH
N
H
10b
0.67
0.85
9.12
0.95
0.91
1.10
1.03
0.74
3.25
2.87
f1 (ppm)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135.5
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127.5
126.6
121.3
120.1
119.6
110.5
107.8
107.3
106.0
75.2
46.3
13.7
11.9
O
OH
N
H
10b
200
190
180
170
160
150
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130
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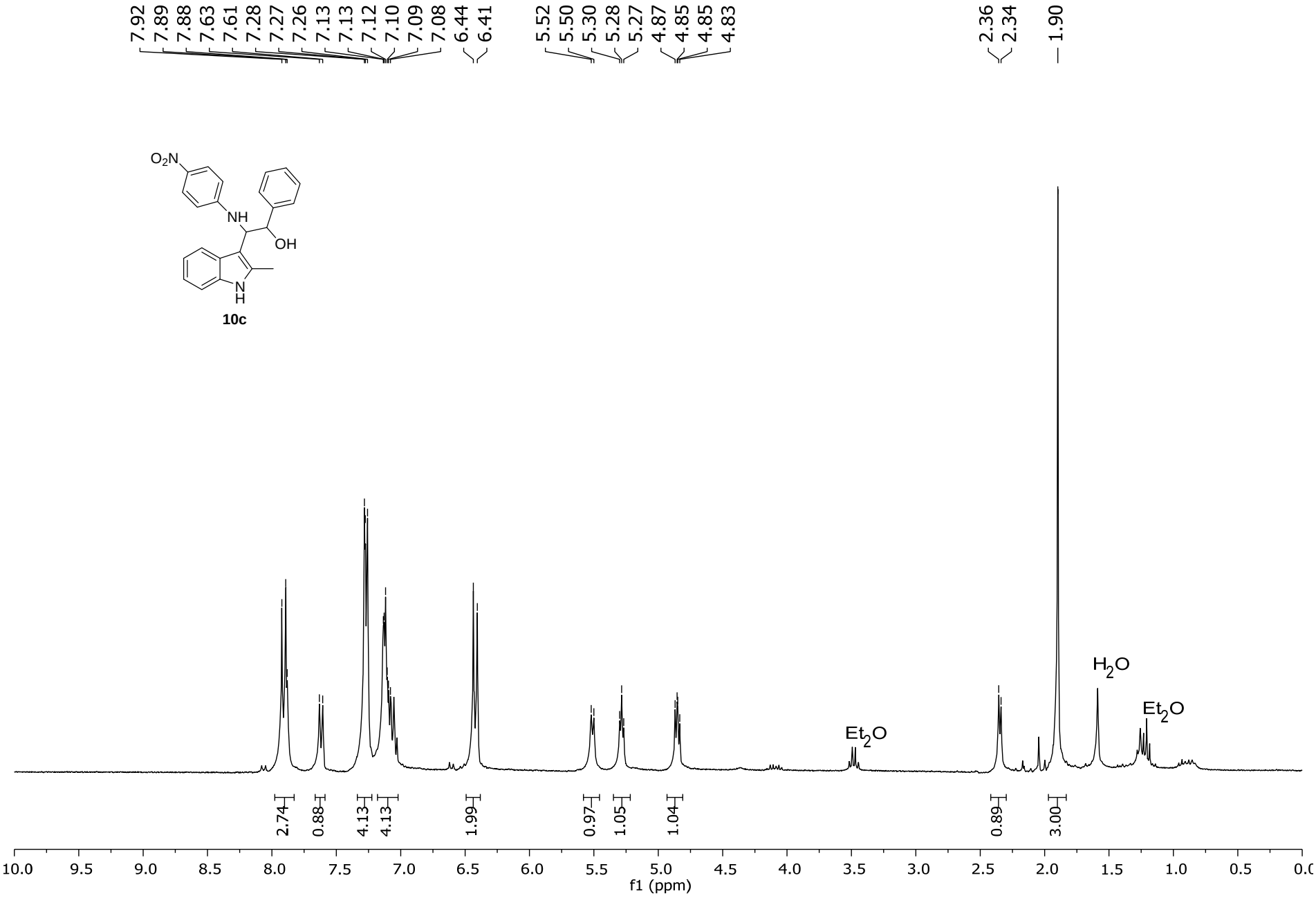
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7.08
6.44
6.41
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5.28
5.27
4.87
4.85
4.85
4.83
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2.34
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O2N
NH
OH
N
H
10c
Et2O
H2O
Et2O
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0.88
4.13
4.13
1.99
0.97
1.05
1.04
0.89
3.00
10.0
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9.0
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8.0
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7.0
6.5
6.0
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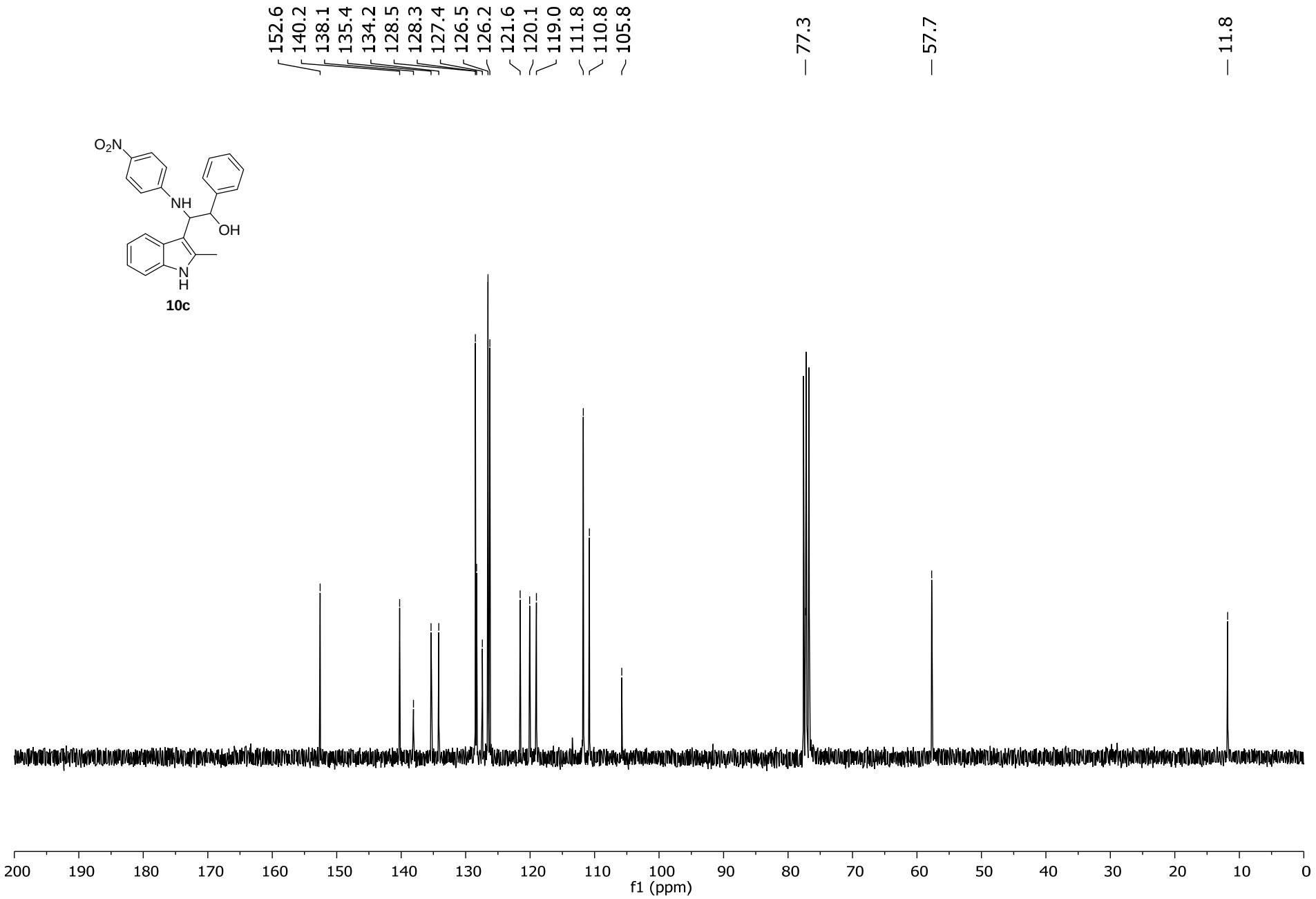
f1 (ppm)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119.0
111.8
110.8
105.8
77.3
57.7
11.8
O2N
NH
OH
N
H
10c
200
190
180
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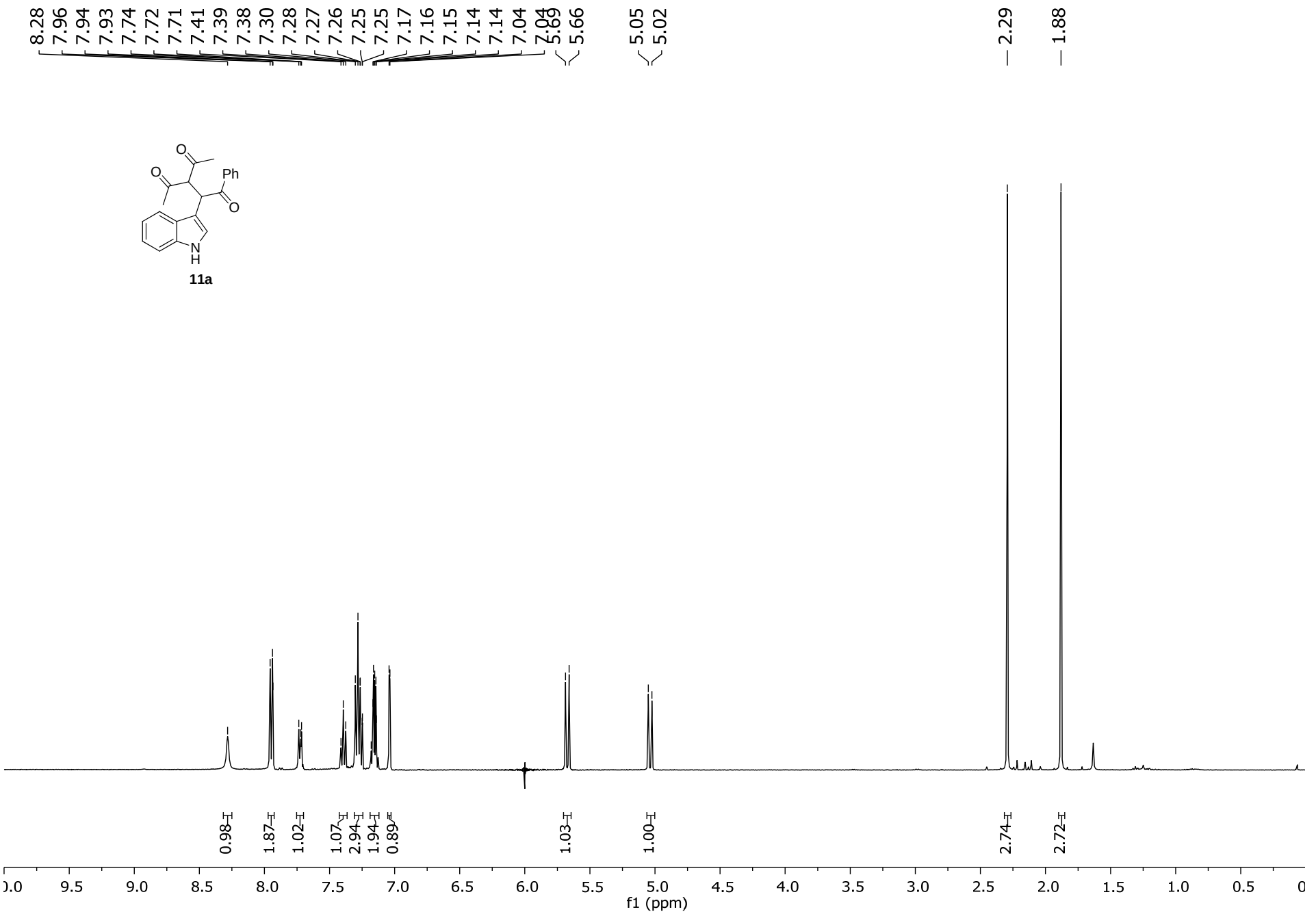
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7.38
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7.28
7.27
7.26
7.25
7.25
7.17
7.16
7.15
7.14
7.14
7.04
7.04
5.69
5.66
5.05
5.02
2.29
1.88
O
O
Ph
O
N
H
11a
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1.07
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1.94
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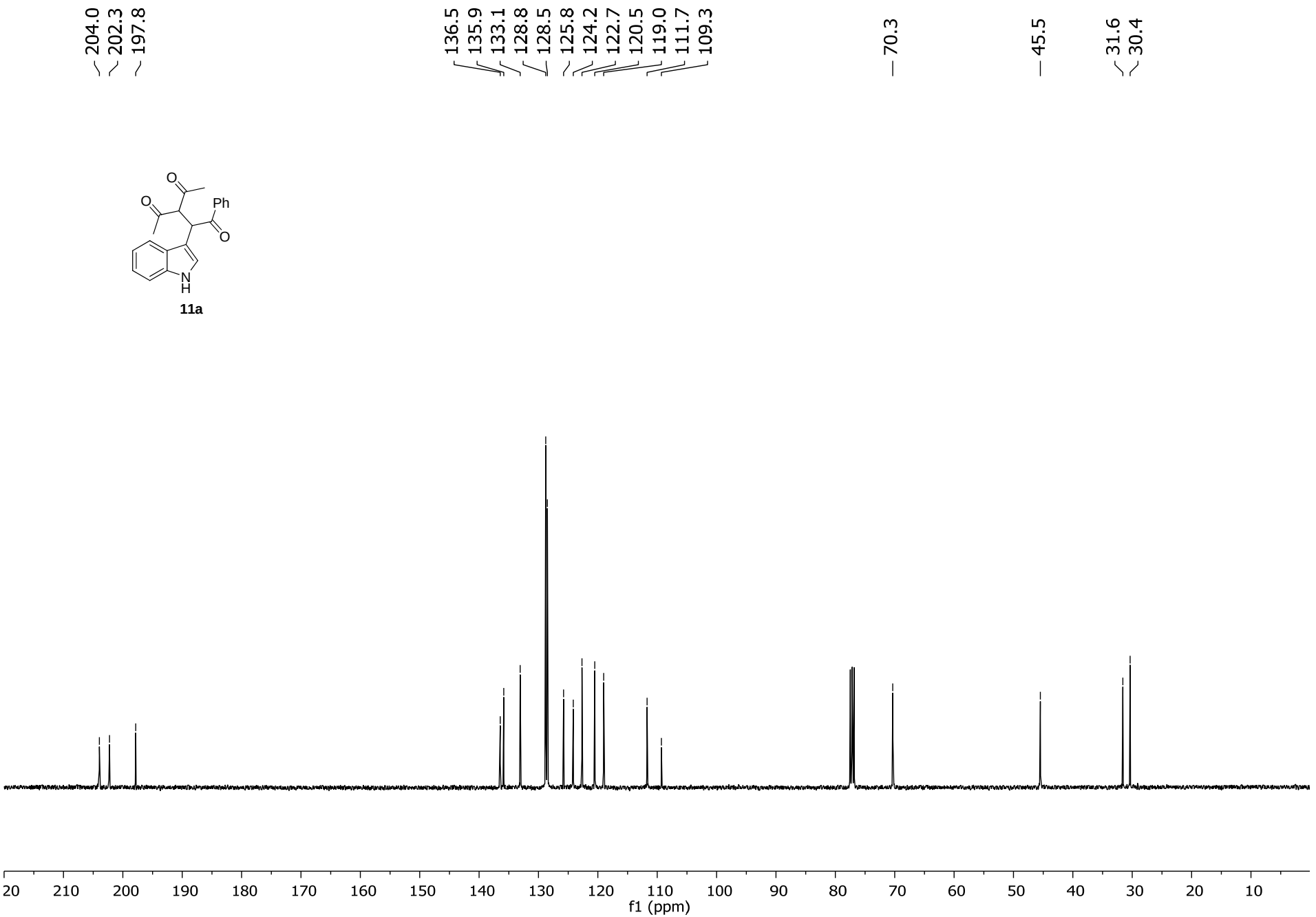
1.00
2.74
2.72
f1 (ppm)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128.5
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124.2
122.7
120.5
119.0
111.7
109.3
70.3
45.5
31.6
30.4
O
O
Ph
O
N
H
11a
20
210
200
190
180
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160
150
140
130
120
110
100
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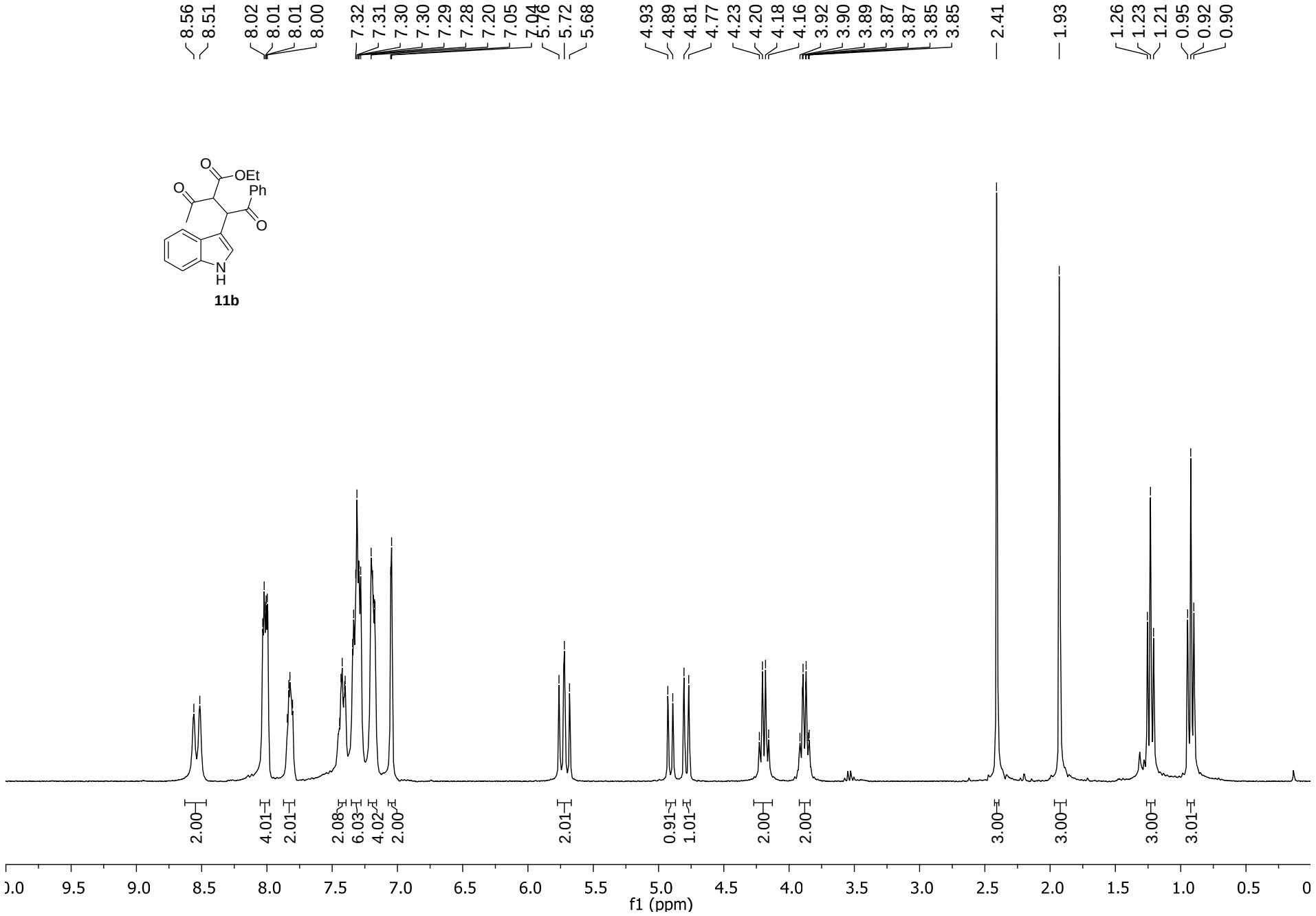
80
70
60
50
40
30
20
10
f1 (ppm)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7.05
7.04
5.76
5.72
5.68
4.93
4.89
4.81
4.77
4.23
4.20
4.18
4.16
3.92
3.90
3.89
3.87
3.87
3.85
3.85
2.41
1.93
1.26
1.23
1.21
0.95
0.92
0.90
O
OEt
O
Ph
O
N
H
11b
2.00
4.01
2.01
2.08
6.03
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2.00
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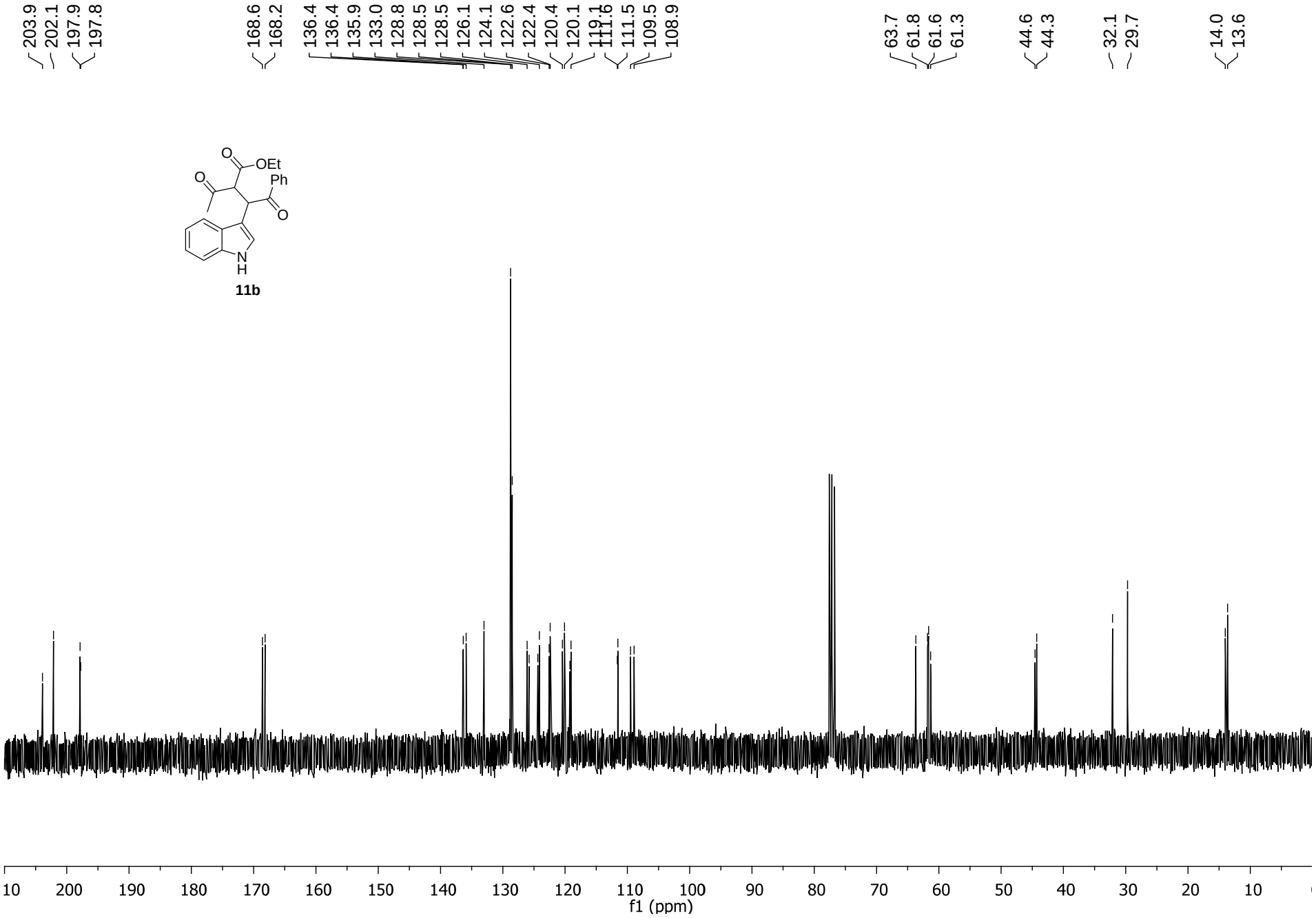
3.00
3.00
3.01
f1 (ppm)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135.9
133.0
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128.5
128.5
126.1
124.1
122.6
122.4
120.4
120.1
119.1
111.6
111.5
109.5
108.9
63.7
61.8
61.6
61.3
44.6
44.3
32.1
29.7
14.0
13.6
O
OEt
O
Ph
O
N
H
11b
10
200
190
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130
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100
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80
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60
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20
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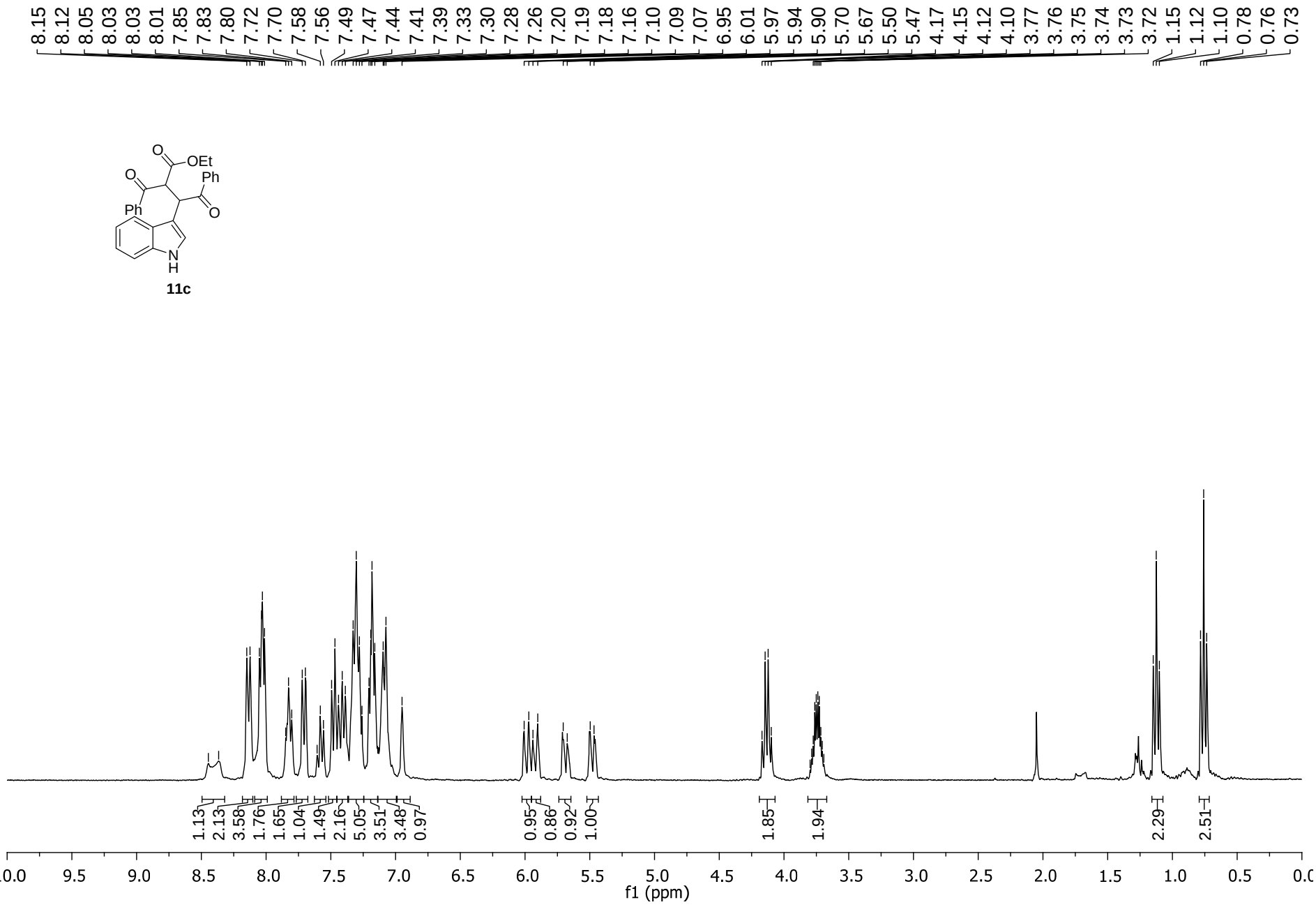
f1 (ppm)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7.56
7.49
7.47
7.44
7.41
7.39
7.33
7.30
7.28
7.26
7.20
7.19
7.18
7.16
7.10
7.09
7.07
6.95
6.01
5.97
5.94
5.90
5.70
5.67
5.50
5.47
4.17
4.15
4.12
4.10
3.77
3.76
3.75
3.74
3.73
3.72
1.15
1.12
1.10
0.78
0.76
0.73
O
OEt
O
Ph
Ph
O
N
H
11c
1.13
2.13
3.58
1.76
1.65
1.04
1.49
2.16
5.05
3.51
3.48
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0.95
0.86
0.92
1.00
1.85
1.94
2.29
2.51
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
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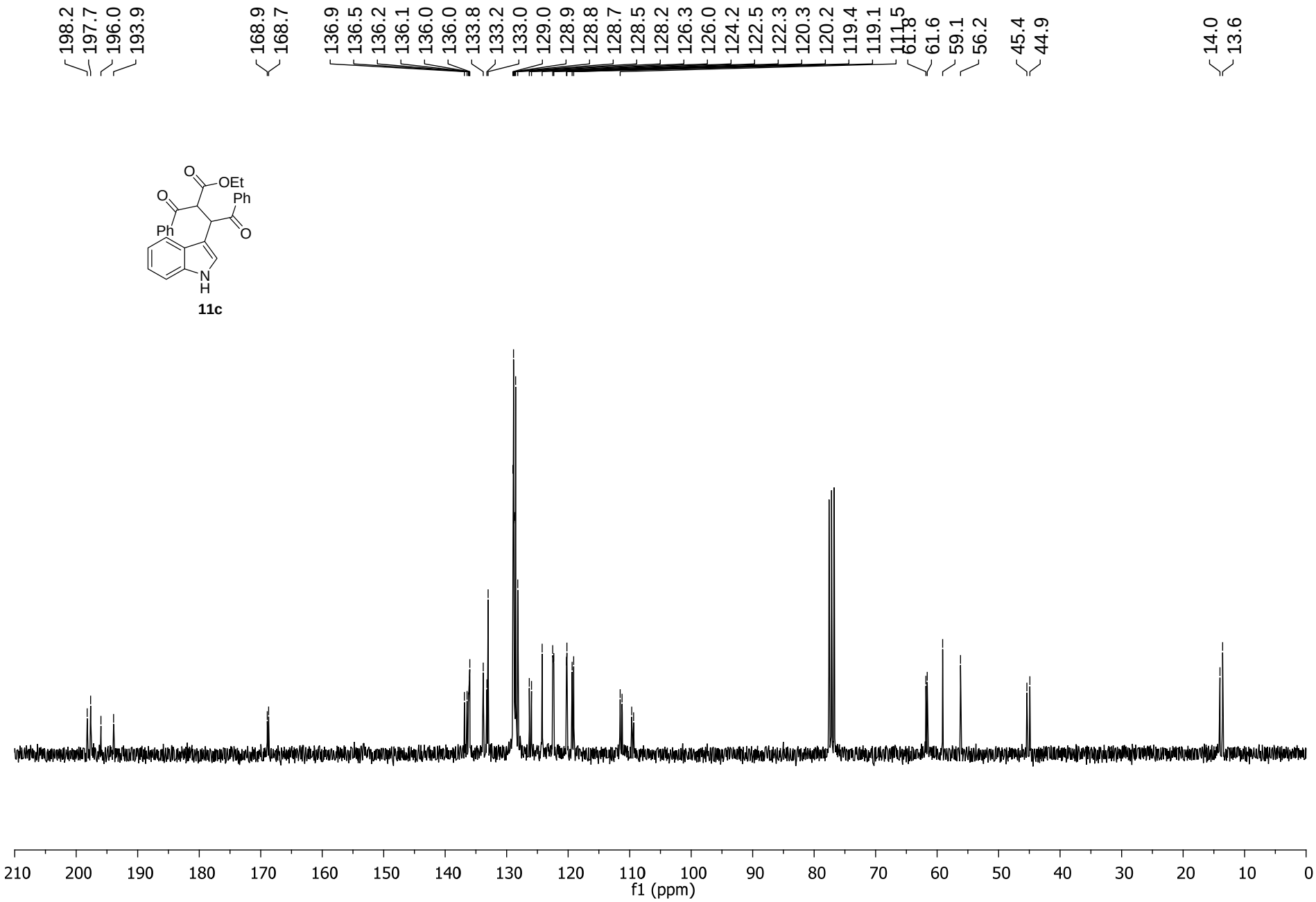
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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197.7
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168.7
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136.5
136.2
136.1
136.0
136.0
133.8
133.2
133.0
129.0
128.9
128.8
128.7
128.5
128.2
126.3
126.0
124.2
122.5
122.3
120.3
120.2
119.4
119.1
111.5
61.8
61.6
59.1
56.2
45.4
44.9
14.0
13.6
O
OEt
O
Ph
Ph
O
N
H
11c
210
200
190
180
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130
120
110
100
90
80
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50
40
30
20
10
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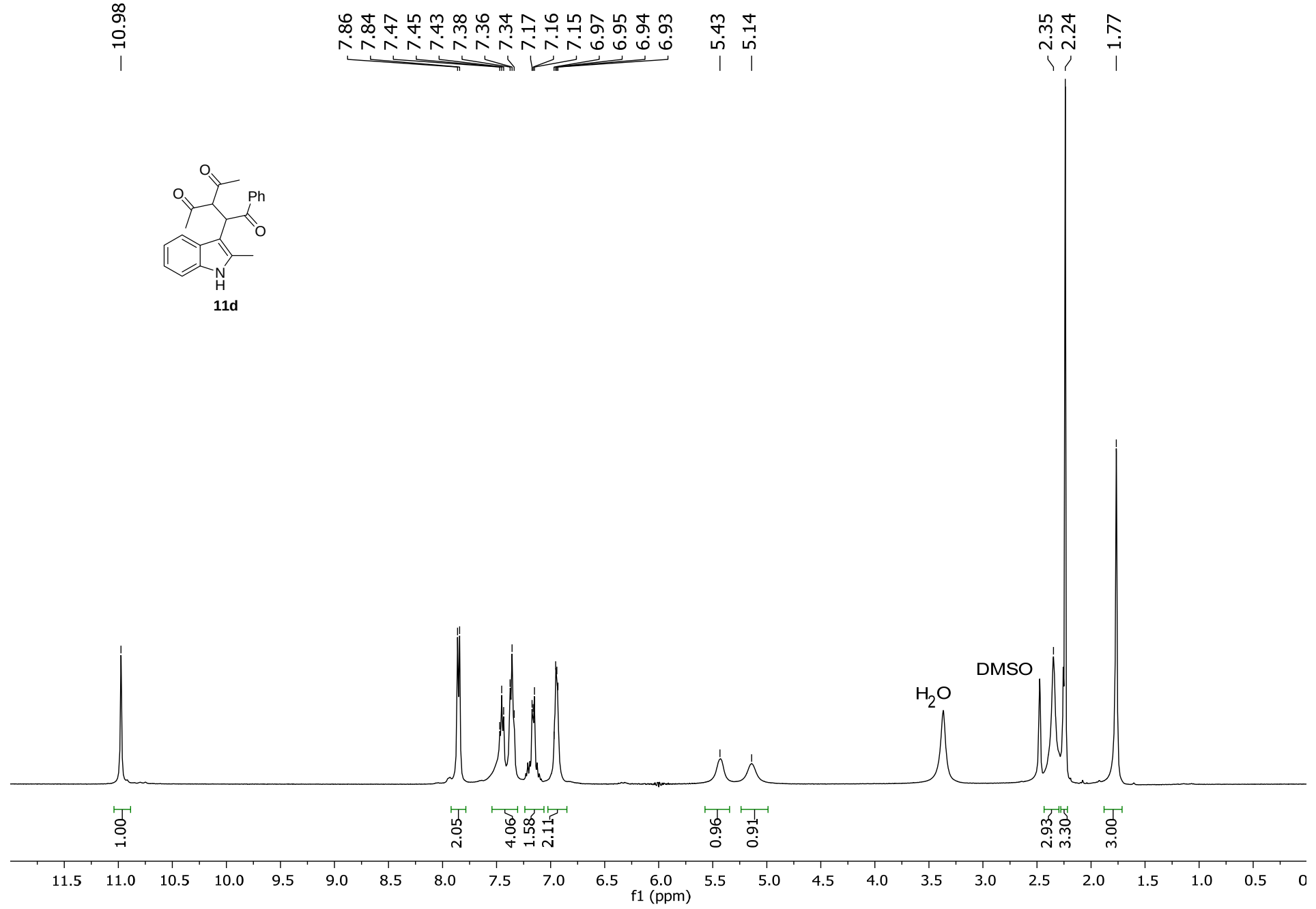
f1 (ppm)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6.95
6.94
6.93
5.43
5.14
2.35
2.24
1.77
O
O
Ph
O
N
H
11d
DMSO
H2O
1.00
2.05
4.06
1.58
2.11
0.96
0.91
2.93
3.30
3.00
11.5
11.0
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10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
3.5
3.0
2.5
2.0
1.5
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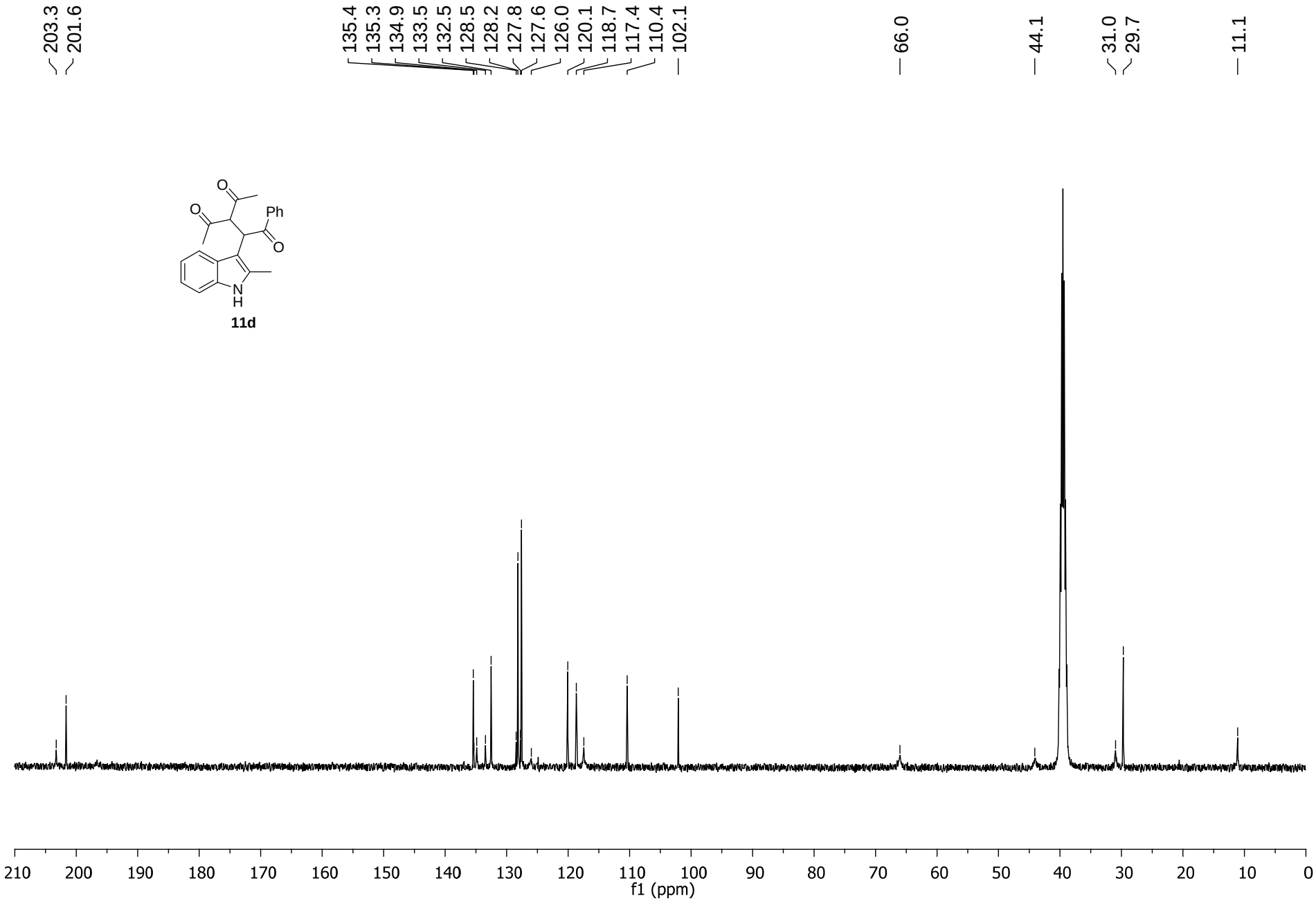
f1 (ppm)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127.8
127.6
126.0
120.1
118.7
117.4
110.4
102.1
66.0
44.1
31.0
29.7
11.1
O
O
Ph
O
N
H
11d
210
200
190
180
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130
120
110
100
90
80
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50
40
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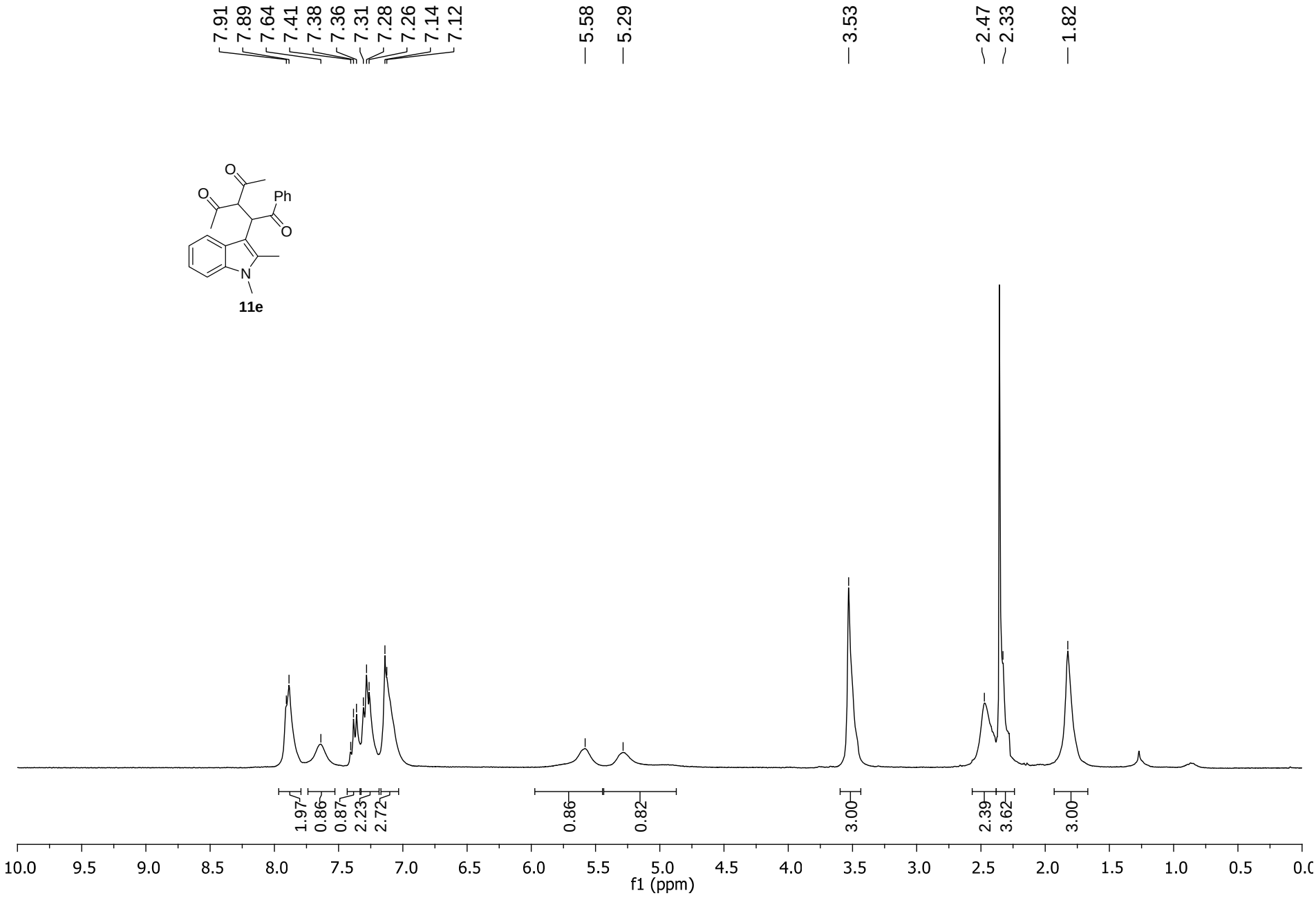
10
0
f1 (ppm)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5.58
5.29
3.53
2.47
2.33
1.82
O
O
Ph
O
N
11e
1.97
0.86
0.87
2.23
2.72
0.86
0.82
3.00
2.39
3.62
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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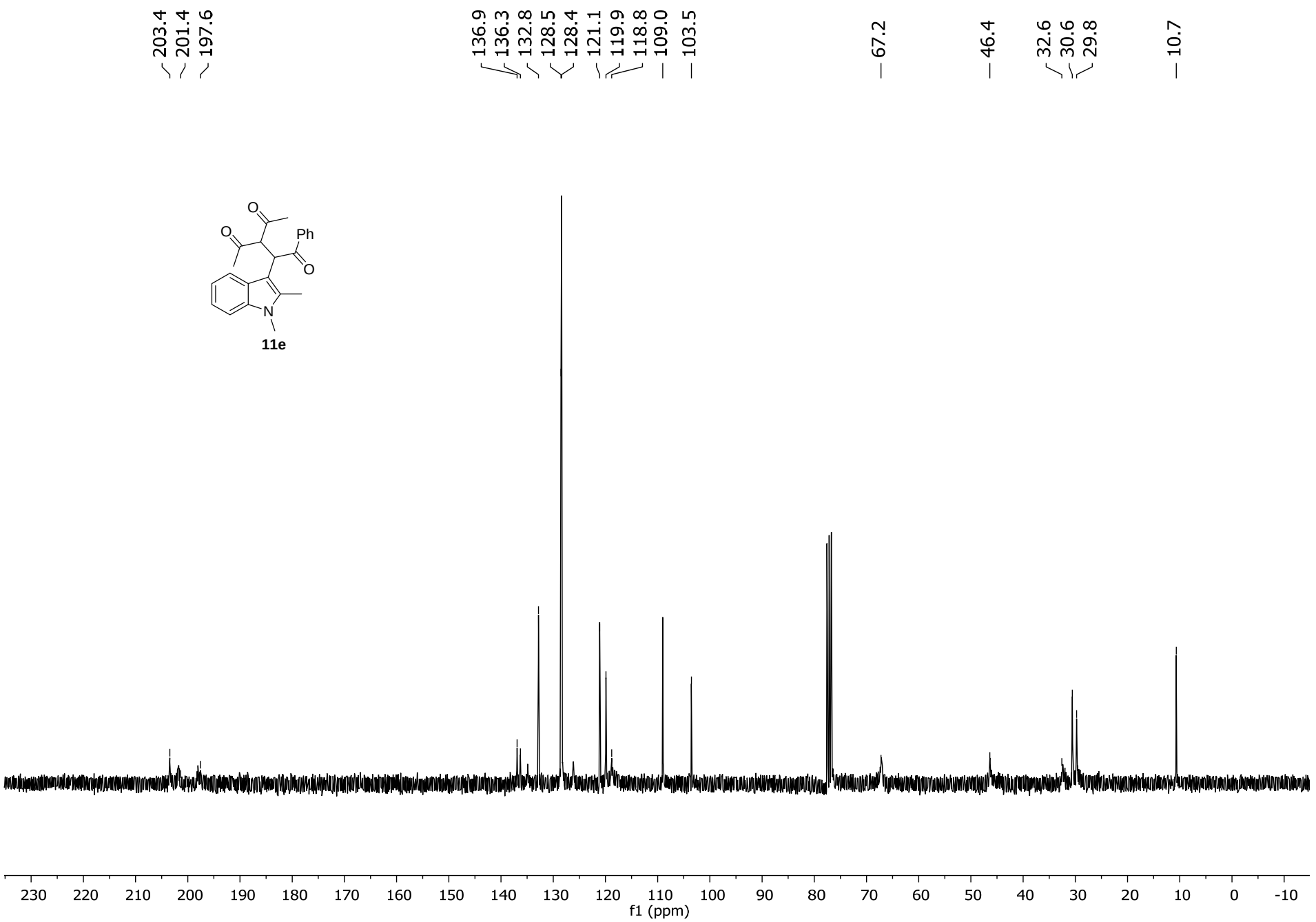
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.4
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119.9
118.8
109.0
103.5
67.2
46.4
32.6
30.6
29.8
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O
Ph
O
N
11e
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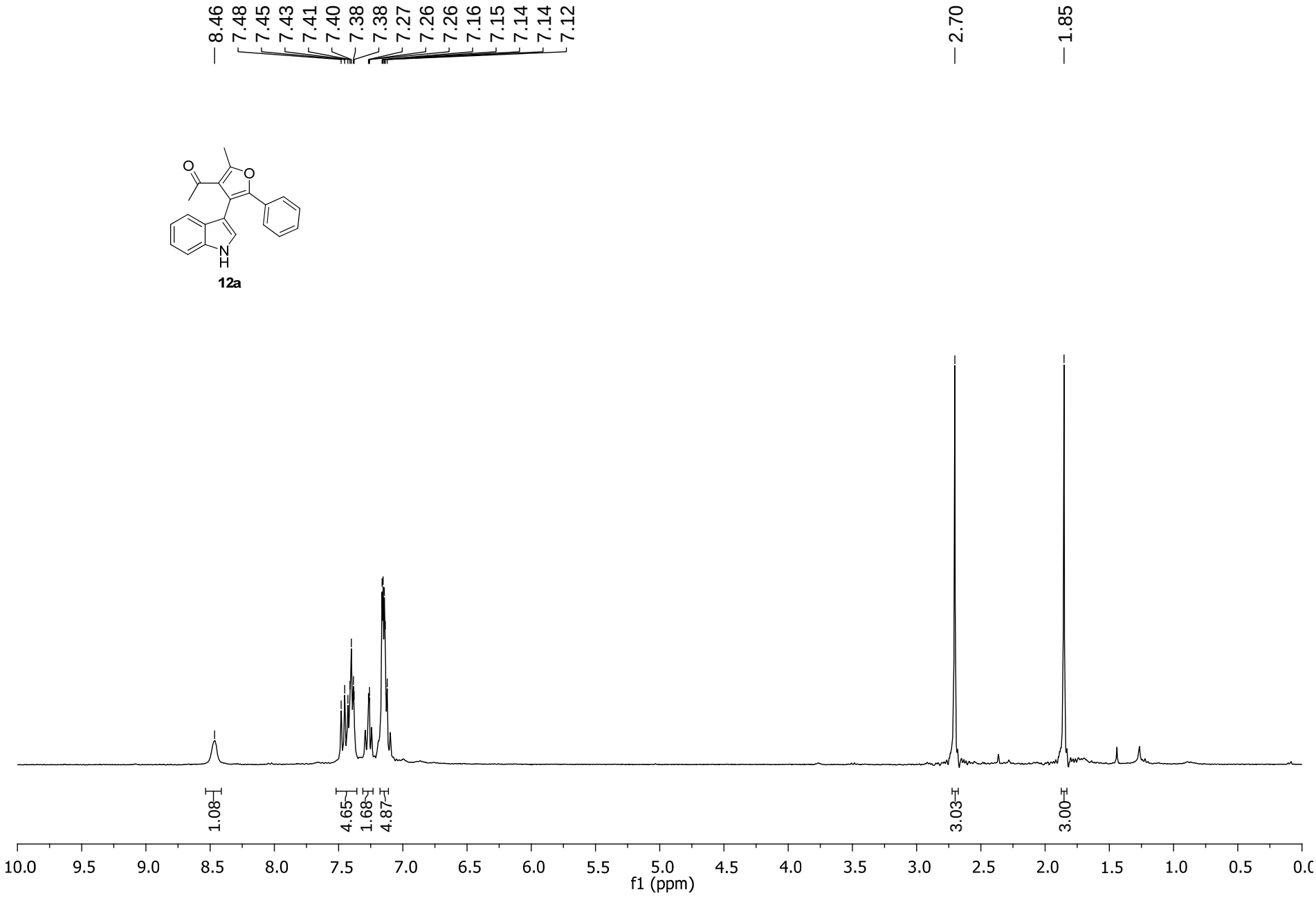
f1 (ppm)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7.14
7.14
7.12
2.70
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12a
1.08
4.65
1.68
4.87
3.03
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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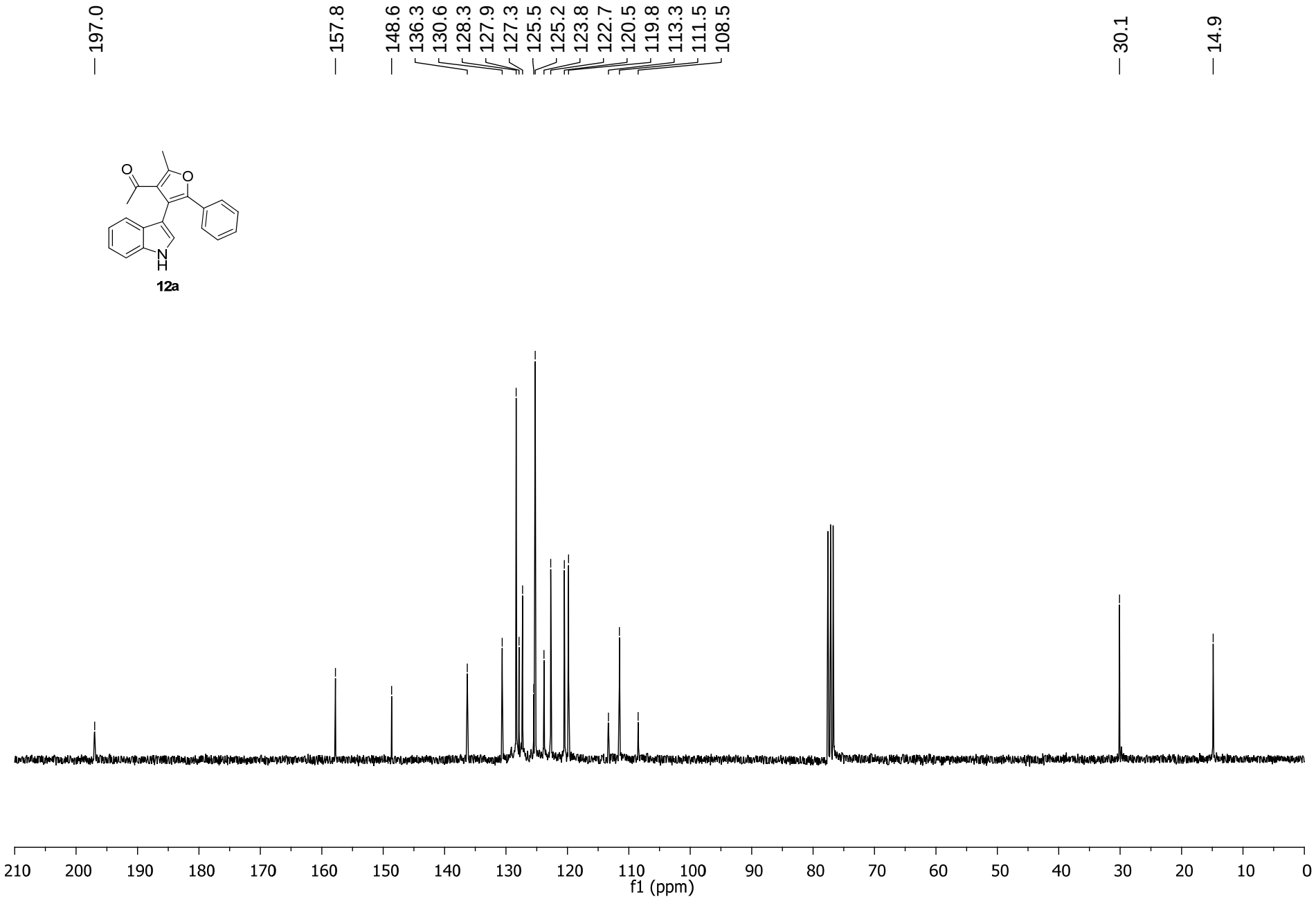
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.3
125.5
125.2
123.8
122.7
120.5
119.8
113.3
111.5
108.5
30.1
14.9
O
O
N
H
12a
210
200
190
180
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160
150
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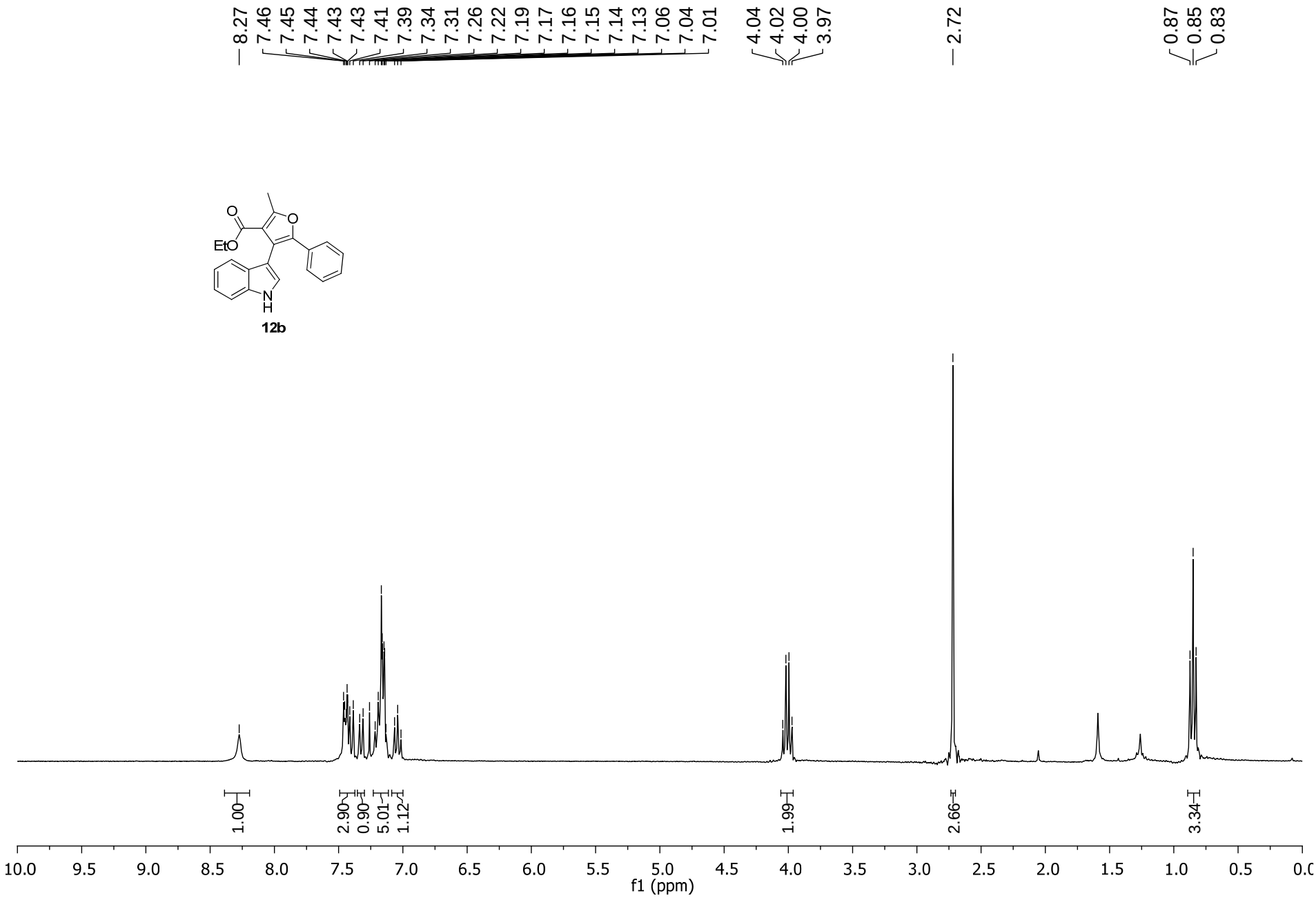
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.17
7.16
7.15
7.14
7.13
7.06
7.04
7.01
4.04
4.02
4.00
3.97
2.72
0.87
0.85
0.83
O
O
EtO
N
H
12b
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2.90
0.90
5.01
1.12
1.99
2.66
3.34
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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4.0
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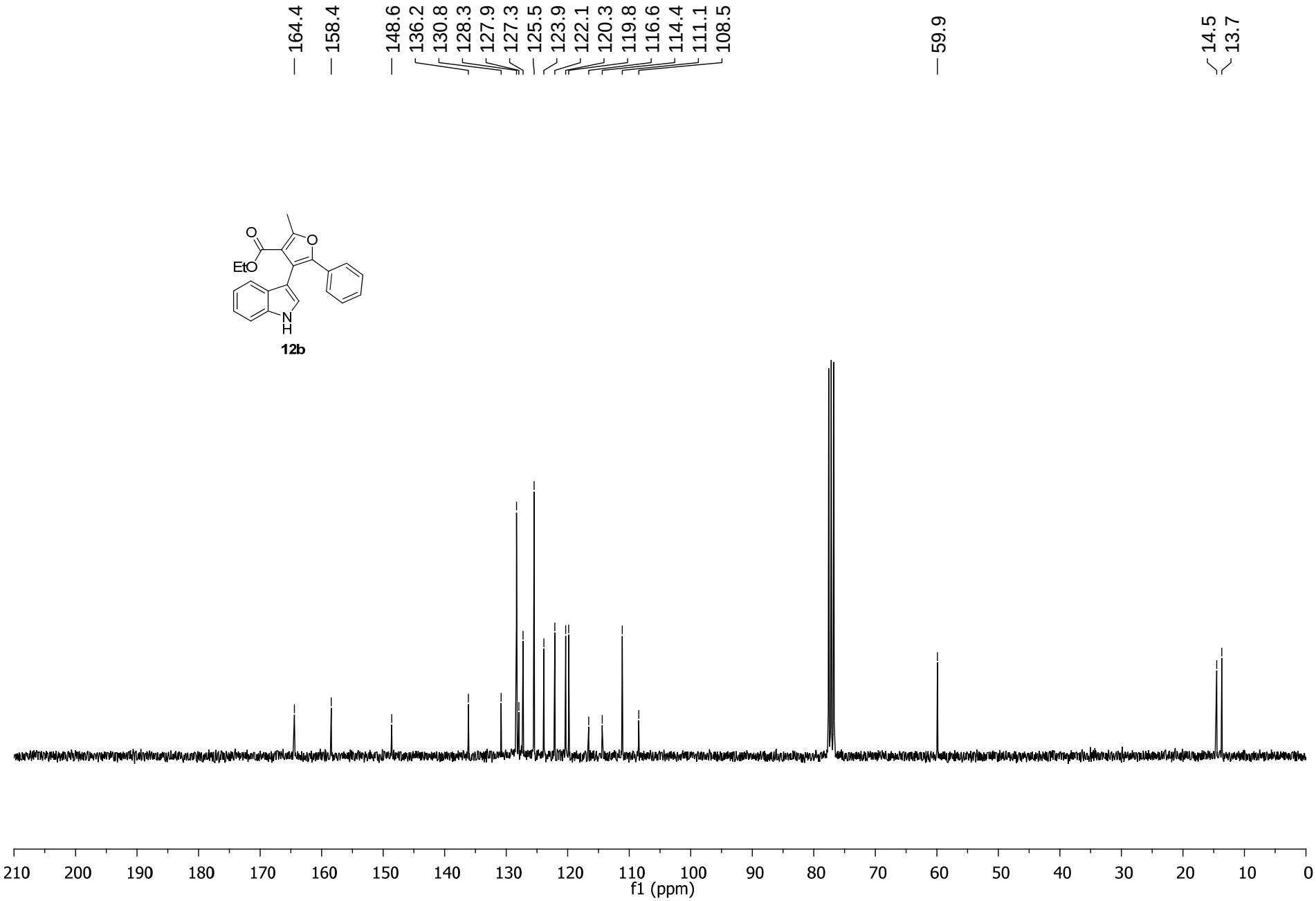
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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123.9
122.1
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119.8
116.6
114.4
111.1
108.5
59.9
14.5
13.7
O
O
EtO
N
H
12b
210
200
190
180
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130
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110
100
90
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70
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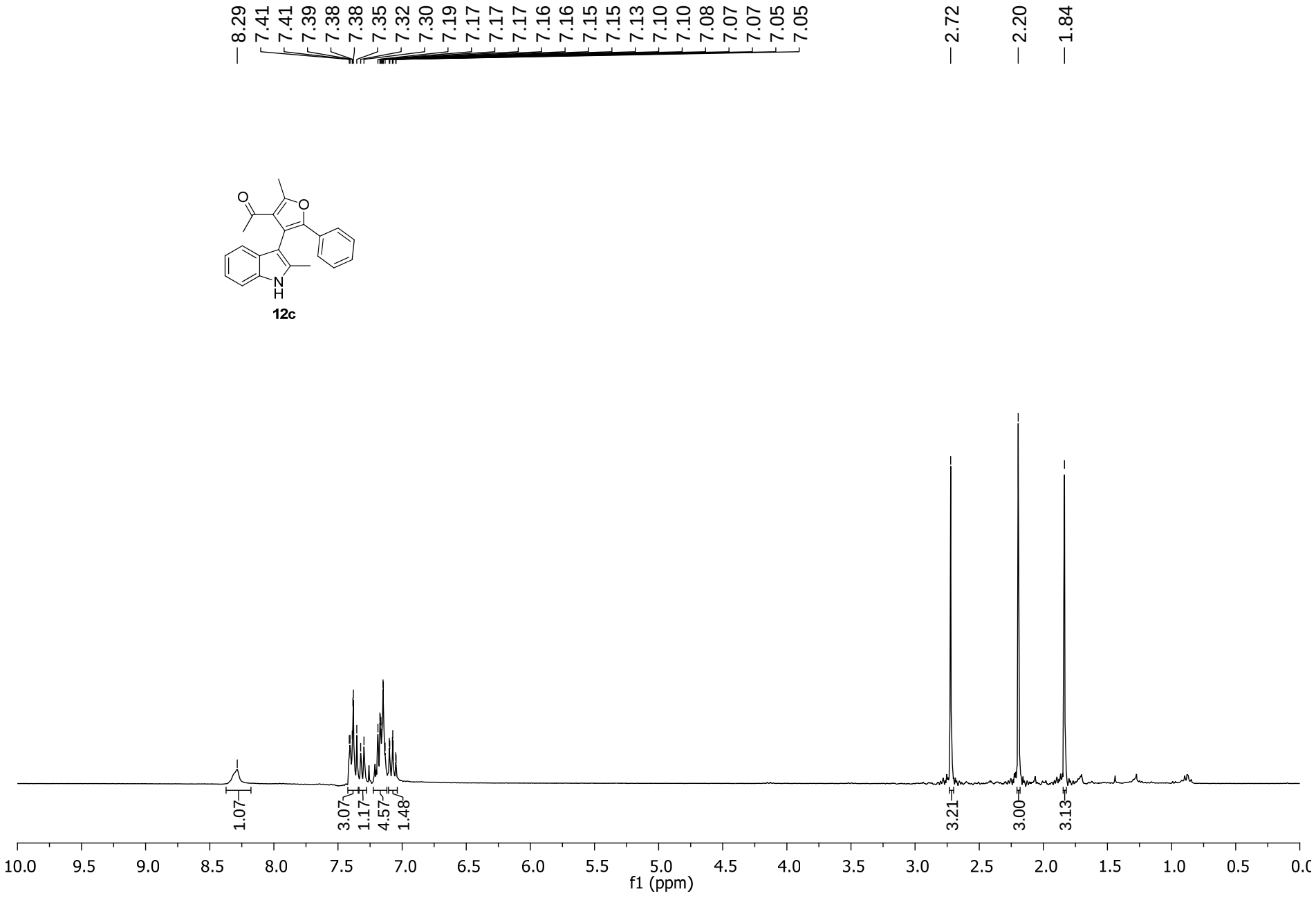
50
40
30
20
10
0
f1 (ppm)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7.16
7.15
7.15
7.13
7.10
7.10
7.08
7.07
7.07
7.05
7.05
2.72
2.20
1.84
O
O
N
H
12c
1.07
3.07
1.17
4.57
1.48
3.21
3.00
3.13
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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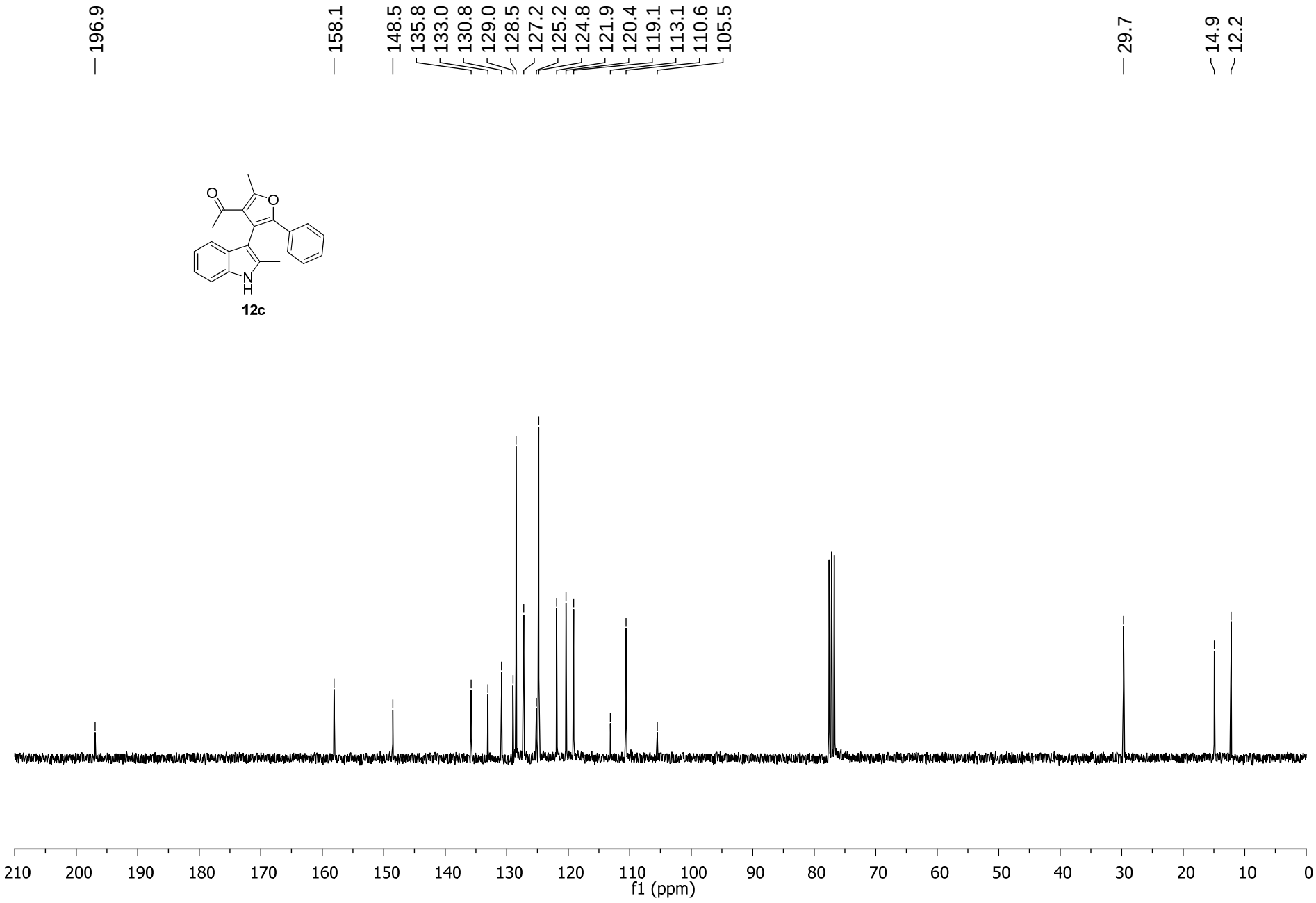
0.0
f1 (ppm)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130.8
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127.2
125.2
124.8
121.9
120.4
119.1
113.1
110.6
105.5
29.7
14.9
12.2
O
O
N
H
12c
210
200
190
180
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160
150
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130
120
110
100
90
80
70
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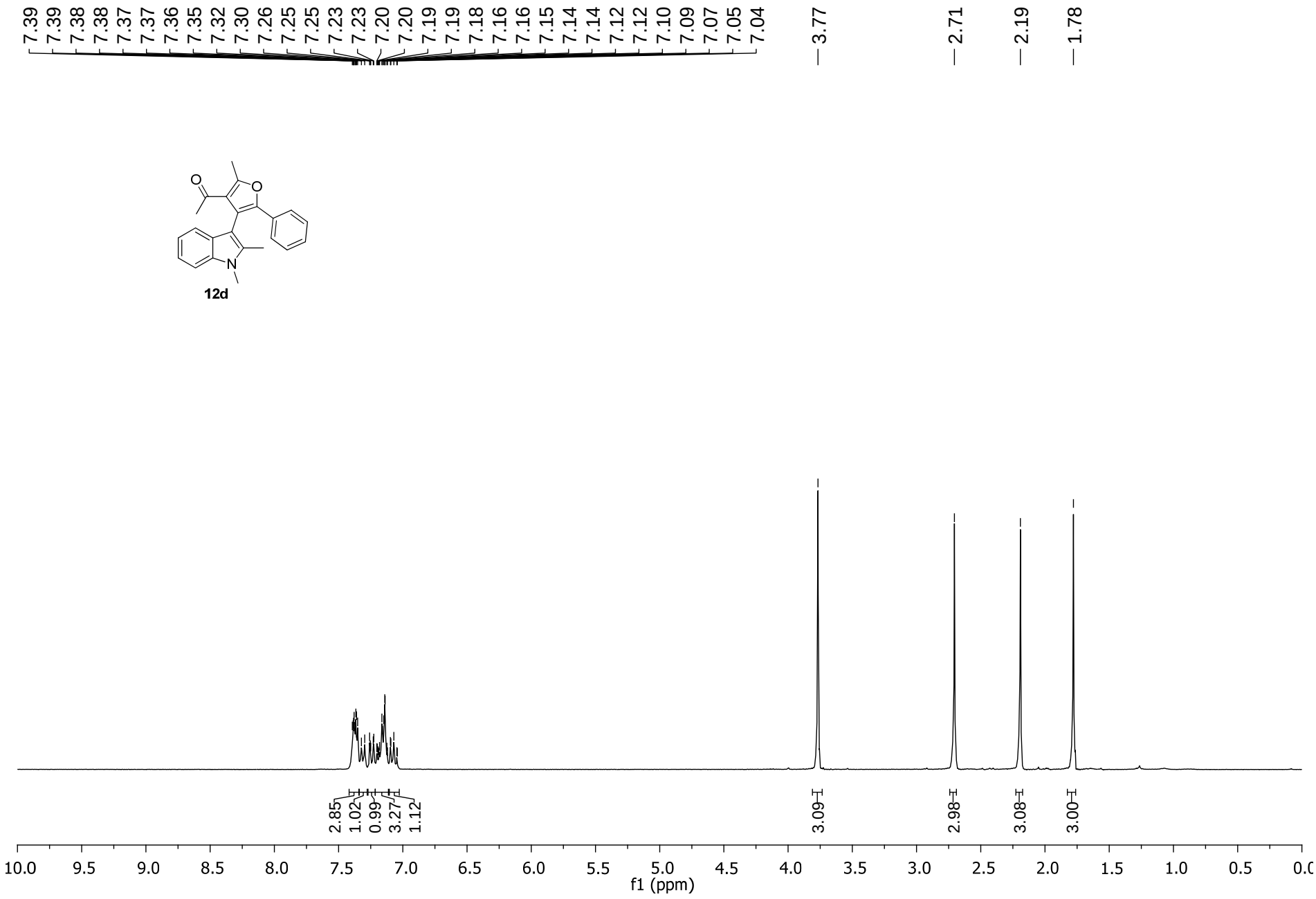
50
40
30
20
10
0
f1 (ppm)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7.19
7.18
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7.16
7.15
7.14
7.14
7.12
7.12
7.10
7.09
7.07
7.05
7.04
3.77
2.71
2.19
1.78
O
O
N
12d
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1.02
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1.12
3.09
2.98
3.08
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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6.0
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2.5
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1.0
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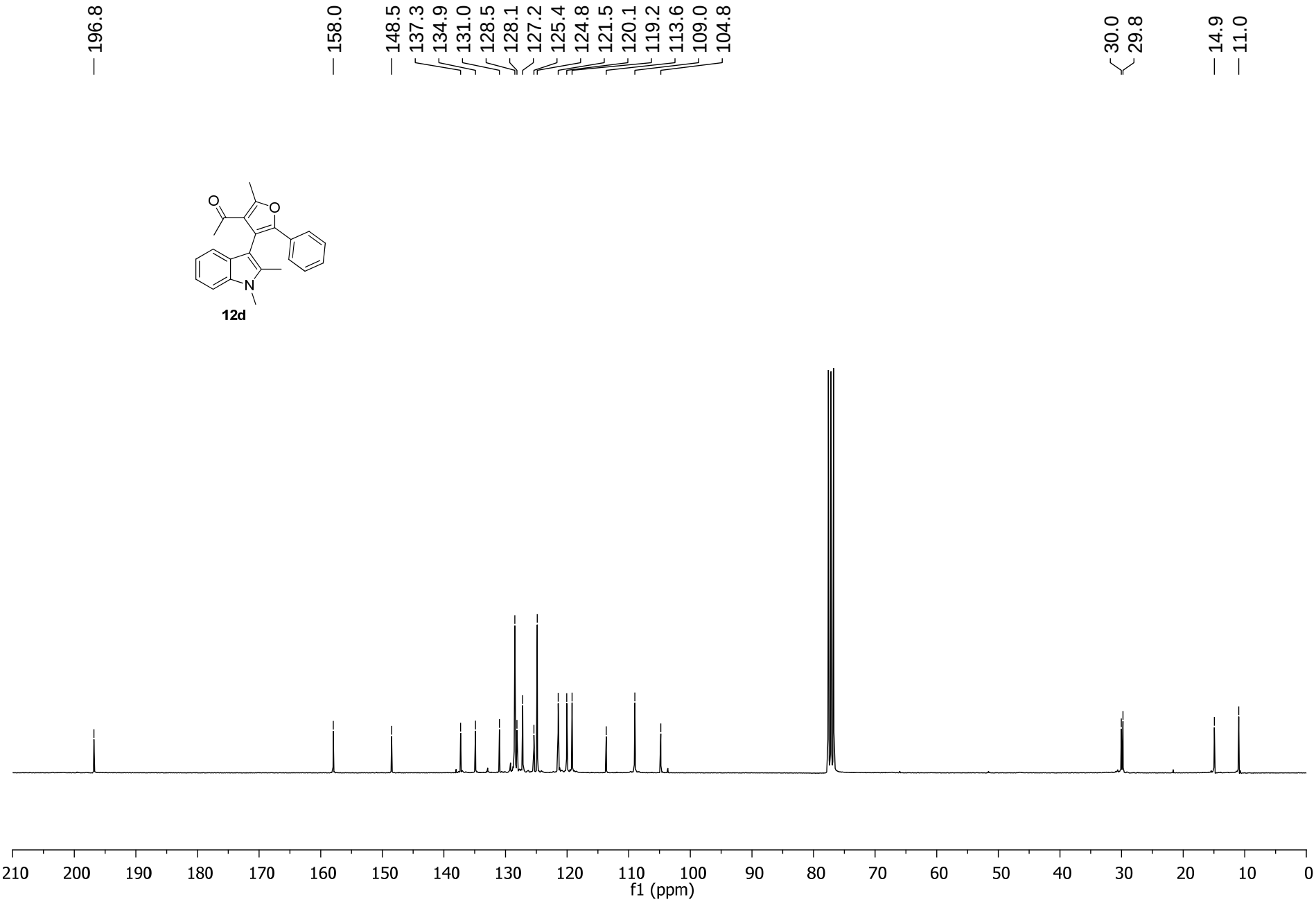
0.0
f1 (ppm)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128.1
127.2
125.4
124.8
121.5
120.1
119.2
113.6
109.0
104.8
30.0
29.8
14.9
11.0
O
O
N
12d
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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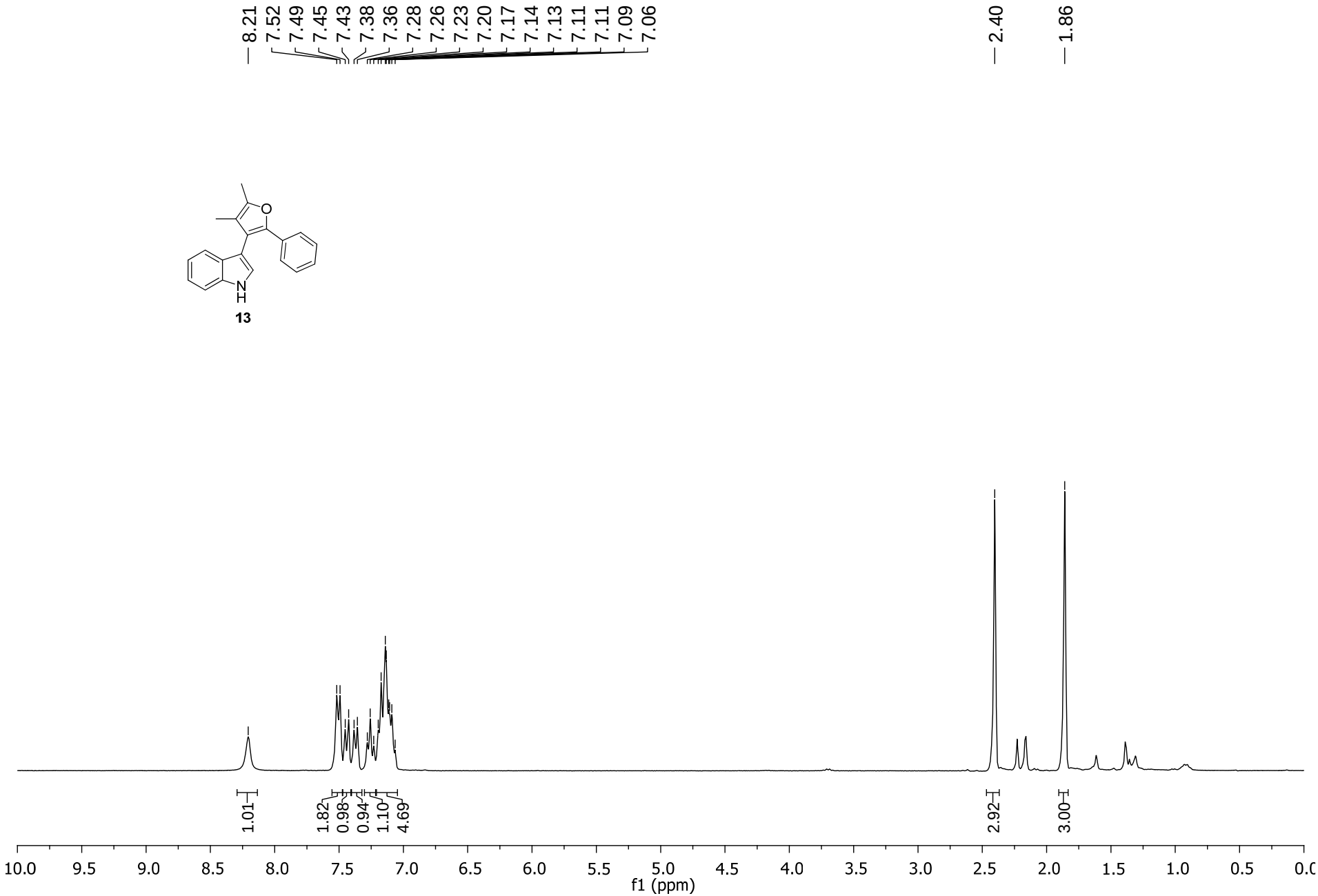
50
40
30
20
10
0
f1 (ppm)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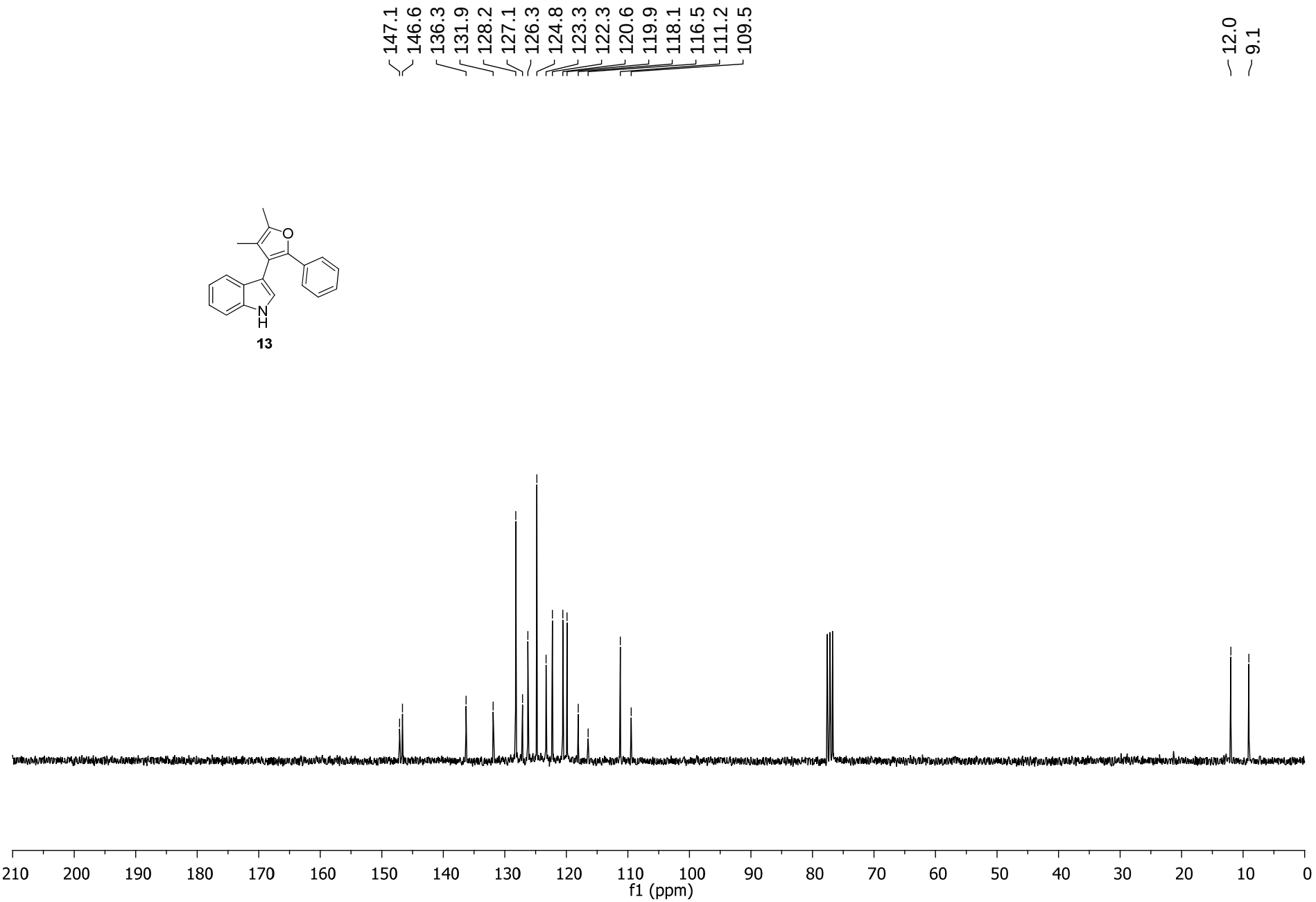
7.11
7.11
7.09
7.06
2.40
1.86
13
1.01
1.82
0.98
0.94
1.10
4.69
2.92
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


147.1
146.6
136.3
131.9
128.2
127.1
126.3
124.8
123.3
122.3
120.6
119.9
118.1
116.5
111.2
109.5
12.0
9.1
O
N
H
13
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)