Supporting information

$AlCl_3$-mediated Ring-opening Reactions of Indoline-2-thiones with Acyl Cyclopropanes, Bi-cyclopropanes and Spirocyclic Cyclopropanes

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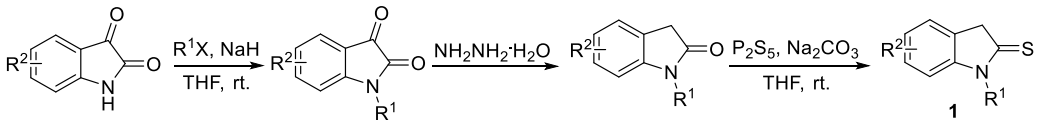
General Information

All starting materials and solvents were of the highest commercially available grade and used without further purification. Reactions were monitored by thin layer chromatography using silica gel HSGF254 plates. Silica gel column chromatography was performed using the silica gel of particle size 200-300 mesh. ^{1}H NMR spectra were recorded on 600 MHz in $CDCl_3$ or DMSO-d_6 and ^{13}C NMR spectra were recorded on 150 MHz in $CDCl_3$ or DMSO-d_6. ^{1}H NMR chemical shifts are reported in ppm (δ) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$, δ = 7.26 ppm or DMSO-d_6, δ = 2.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$, δ = 77.16 ppm or DMSO-d_6, δ = 39.52 ppm). ESI HRMS spectra were recorded on Bio TOF Q.

General Procedure for the Preparation of Indoline-2-thiones 1[1]



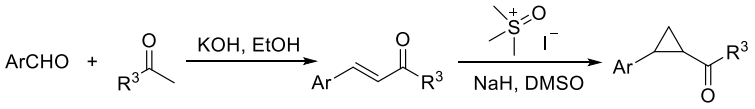
NaH (1.92 g, 48 mmol) (60% in mineral oil) was added by portion to a solution of indoline-2,3-dione derivative (40 mmol) in THF (50 mL) at 0 ºC under nitrogen atmosphere. The result reaction mixture was stirred at 0 ºC for 15 min under nitrogen atmosphere. Then the alkyl halide (40 mmol) was added to the reaction mixture dropwise. The resulting mixture was warmed to room temperature and stirred until the reaction finished. After the completion of reaction (monitoring by TLC), the reaction mixture was poured into ice cooled water to get a precipitation of the product. The precipitate was filtered and dried under vacuum desiccator to get the desired *N*-alkylated product.

N-alkylated indoline-2,3-dione derivative (20 mmol), hydrazine hydrate (30 mL) was added in a 100 mL round-bottom flask. The resulting mixture was refluxed until the reaction finished. The reaction mixture was neutralization with aqueous HCl and extracted with DCM three times. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered and concentrated to afford the crude product 2-oxindole derivative, which was used in the next step

without further purification.

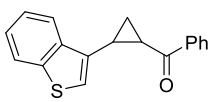
P_2S_5 (18 mmol, 1.8 equiv.), Na_2CO_3 (18 mmol, 1.8 equiv.) and THF (20 mL) was added to a 100 mL round-bottom flask. The mixture was stirred at room temperature for 20 min, then 2-oxindole derivative (10 mmol) in THF (10 mL) was added dropwise and the resulting mixture was stirred at 30 °C overnight. The reaction mixture was poured into stirred ice-cold water and solid precipitated, filtered, dried to get pure indoline-2-thiones **1**.

General Procedure for the Preparation of Acyl Cyclopropanes 2[2]



To a solution of aromatic aldehyde (20 mmol) and methyl ketones (20 mmol) in EtOH (30 mL), 5 mL KOH aqueous solution (40% wt) was added dropwise, then the reaction was carried out at room temperature until the disappearance of starting materials. The solution was poured into cold water and the mixture neutralized with 2 M HCl to a pH in the range of 2–3. After the resulting precipitate was collected and washed with water, the precipitate was recrystallized from EtOH to give the chalcones.

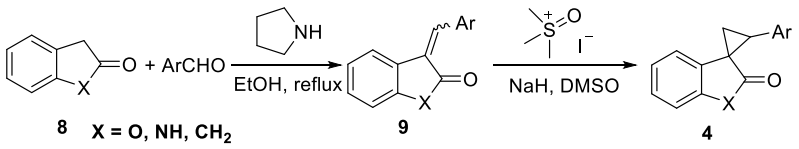
To a stirred suspension of NaH (5.85 mmol, 60% dispersion in mineral oil) in dry DMSO (15 mL) under a nitrogen atmosphere, trimethylsulfoxonium iodide (5.5 mmol, 1.21 g) was added in one portion at 0 °C, and the solution stirred at this temperature for 10 min. Then a solution of the appropriate chalcones (5 mmol) in anhydrous DMSO (5 mL) was added dropwise at 0 °C, and the reaction mixture allowed to stir at room temperature until the disappearance of starting materials. The solution was quenched by saturated NH_4Cl and extracted with EtOAc (3 × 15 mL). The combined organic phase was washed with water and brine, dried over anhydrous Na_2SO_4, filtered and concentrated *in vacuo* and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 20:1) to give acyl cyclopropanes **2**.



(2-(benzo[b]thiophen-3-yl)cyclopropyl)(phenyl)methanone (2l): white solid, mp 87.1-87.7 °C, two steps with 40% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (dd, J = 8.3, 1.1 Hz, 2H), 7.82 – 7.79 (m, 1H), 7.78 – 7.74 (m, 1H), 7.55 – 7.50 (m, 1H), 7.41 (dd, J = 10.8, 4.8 Hz, 2H), 7.34 – 7.28 (m, 2H), 7.06 (d,

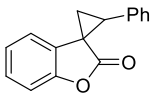
J = 0.9 Hz, 1H), 2.93 – 2.86 (m, 1H), 2.83 (dt, J = 8.2, 4.6 Hz, 1H), 1.93 – 1.90 (m, 1H), 1.61 – 1.58 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.7, 140.4, 139.3, 137.6, 135.8, 133.1, 128.7, 128.2, 124.7, 124.3, 122.9, 121.9, 121.2, 26.9, 23.6, 17.6. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{18}H_{15}OS^+$, 279.0838; Found, 279.0849.

General Procedure for the Preparation of Spirocyclic Cyclopropanes 4[3]



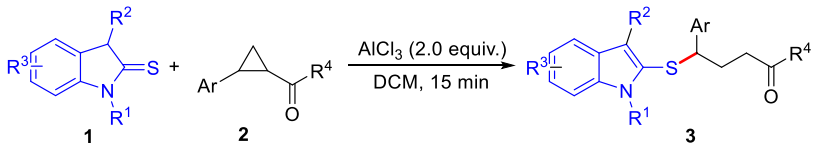
8 (20 mmol), pyrrolidine (2 mmol), aromatic aldehyde (20 mmol) were reflux in EtOH (40 mL) for 5-12 h. The resulting mixture was poured into stirred ice-cold water and solid precipitated, filtered, dried to get pure **9**.

To a stirred suspension of NaH (5.85 mmol, 60% dispersion in mineral oil) in dry DMSO (15 mL) under a nitrogen atmosphere, trimethylsulfoxonium iodide (5.5 mmol, 1.21 g) was added in one portion at 0 ℃, and the solution stirred at this temperature for 10 min. Then a solution of **9** (5 mmol) in anhydrous DMSO (5 mL) was added dropwise at 0 ℃, and the reaction mixture allowed to stir at room temperature until the disappearance of starting materials. The solution was quenched by saturated NH_4Cl and extracted with EtOAc (3 × 15 mL). The combined organic phase was washed with water and brine, dried over anhydrous Na_2SO_4, filtered and concentrated *in vacuo* and the residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 4:1 or 15:1) to give spirocyclic cyclopropanes **4**.



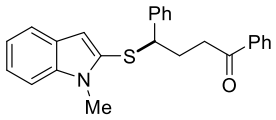
2'-phenyl-2H-spiro[benzofuran-3,1'-cyclopropan]-2-one (4a): light yellow solid, mp 128.6-129.8 ℃, two steps with 83% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 3H), 7.22 – 7.12 (m, 4H), 6.78 (td, J = 7.5, 1.2 Hz, 1H), 5.95 (dd, J = 7.6, 0.8 Hz, 1H), 3.44 (t, J = 8.7 Hz, 1H), 2.33 (dd, J = 9.2, 4.9 Hz, 1H), 2.12 (dd, J = 8.2, 4.9 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.3, 153.9, 133.8, 129.9, 128.7, 128.1, 127.6, 126.1, 123.5, 121.1, 110.5, 37.7, 31.1, 24.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{16}H_{12}O_2Na^+$, 259.0730; Found, 259.0736.

General Procedure for the $AlCl_3$ Mediated Ring-opening Reaction of Acyl Cyclopropanes 2

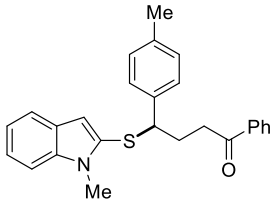


To the mixture of indoline-2-thiones **1** (0.2 mmol, 1.0 equiv.), acyl cyclopropanes **2** (0.2 mmol, 1.0 equiv.), and $AlCl_3$ (0.4 mmol, 53.3 mg, 2.0 equiv.), 2 mL DCM was added at room temperature. The reaction was stirred at room temperature for 15 min. Then the resulting mixture was firstly quenched by brine (10 mL), and extracted with DCM three times (5 mL×3). The combined organic phase was washed with brine, concentrated in vacuo and then column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 20:1) to afford the desired compounds **3**.

Experiment Data for the Indolylthio-substituted Ketones 3

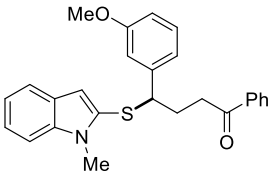


4-((1-methyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3aa): white solid, mp 120.6-121.3 ℃, 61.0 mg, 79% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91-7.83 (m, 2H), 7.54 (dd, J = 15.8, 7.7 Hz, 2H), 7.42 (t, J = 7.8 Hz, 2H), 7.25-7.16 (m, 5H), 7.09 (dt, J = 5.4, 3.1 Hz, 3H), 6.70 (s, 1H), 4.05 (dd, J = 8.3, 7.2 Hz, 1H), 3.36 (s, 3H), 3.13-3.00 (m, 2H), 2.51 (td, J = 14.6, 6.7 Hz, 1H), 2.46-2.36 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.3, 141.3, 138.4, 136.9, 133.2, 128.9, 128.7, 128.7, 128.1, 127.7, 127.7, 127.4, 122.6, 120.7, 119.8, 111.4, 109.9, 54.8, 36.5, 29.5, 29.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{23}NOSNa^+$, 408.1393; Found, 408.1404.

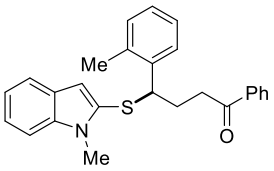


4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenyl-4-(p-tolyl)butan-1-one (3ab): white solid, mp 147-148 ℃, 52.6 mg, 66% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 8.1 Hz, 2H), 7.52 (d, J = 7.9 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.37 (t, J = 7.5 Hz, 2H), 7.21 – 7.12 (m, 2H), 7.09 – 7.03 (m, 1H),

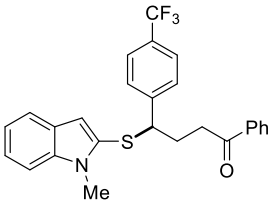
7.00 (d, J = 7.8 Hz, 2H), 6.96 (d, J = 7.8 Hz, 2H), 6.67 (s, 1H), 4.05 – 3.94 (m, 1H), 3.38 (s, 3H), 2.99 (dd, J = 14.5, 7.5 Hz, 2H), 2.44 (dd, J = 14.2, 7.2 Hz, 1H), 2.35 (dt, J = 14.4, 7.3 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.4, 138.4, 138.1, 137.4, 136.9, 133.2, 129.4, 129.2, 128.7, 128.1, 127.5, 127.4, 122.5, 120.6, 119.7, 111.2, 109.9, 54.5, 36.5, 29.6, 29.5, 21.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{25}NOSNa^+$, 422.1549; Found, 422.1548.



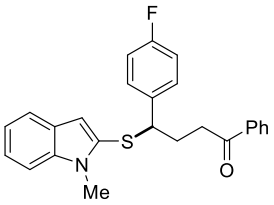
4-(3-methoxyphenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3ac): white solid, mp 61-62 °C, 71.5 mg, 86% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.87 – 7.81 (m, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.35 (d, J = 8.3 Hz, 1H), 7.20 – 7.15 (m, 2H), 7.03 (dd, J = 11.1, 3.8 Hz, 1H), 6.83 – 6.77 (m, 2H), 6.71 (s, 1H), 6.67 – 6.64 (m, 1H), 4.21 (dd, J = 8.5, 6.9 Hz, 1H), 3.53 (s, 3H), 3.45 (s, 3H), 3.12 – 3.07 (m, 1H), 3.03 – 2.97 (m, 1H), 2.37 – 2.31 (m, 1H), 2.30 – 2.23 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 199.0, 159.2, 142.5, 137.9, 136.4, 133.1, 129.5, 128.7, 128.6, 127.7, 126.7, 122.3, 120.1, 119.6, 119.5, 113.2, 112.7, 110.3, 110.2, 54.8, 53.2, 35.9, 29.4, 29.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{25}NO_2SNa^+$, 438.1498; Found, 438.1498.



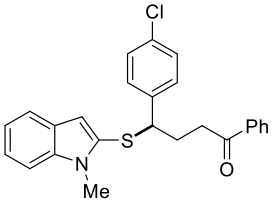
4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenyl-4-(o-tolyl)butan-1-one (3ad): orange oil, 59.0 mg, 74% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.89 – 7.80 (m, 2H), 7.61 – 7.55 (m, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.33 (d, J = 8.3 Hz, 1H), 7.19 – 7.10 (m, 3H), 7.09 – 6.98 (m, 3H), 6.71 (s, 1H), 4.44 (t, J = 7.6 Hz, 1H), 3.35 (s, 3H), 3.13 – 3.08 (m, 1H), 3.05 – 3.00 (m, 1H), 2.36 (td, J = 14.1, 6.7 Hz, 1H), 2.31 – 2.26 (m, 1H), 2.25 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 199.3, 138.6, 138.0, 136.5, 135.9, 133.2, 130.3, 128.7, 128.2, 127.8, 127.2, 126.6, 126.2, 126.0, 122.3, 120.1, 119.6, 110.8, 110.2, 48.5, 35.8, 29.2, 28.6, 18.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{25}NOSNa^+$, 422.1549; Found, 422.1548.



4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenyl-4-(4-(trifluoromethyl)phenyl)butan-1-one (3ae): white solid, mp 119-120 ℃, 51.8 mg, 57% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, J = 7.8 Hz, 2H), 7.58 – 7.50 (m, 2H), 7.45 (d, J = 7.1 Hz, 2H), 7.41 (t, J = 7.0 Hz, 2H), 7.27 – 7.13 (m, 4H), 7.07 (t, J = 7.3 Hz, 1H), 6.63 (d, J = 1.7 Hz, 1H), 4.07 (dd, J = 10.6, 4.6 Hz, 1H), 3.35 (d, J = 2.1 Hz, 3H), 3.16 – 3.01 (m, 2H), 2.58 – 2.45 (m, 1H), 2.38 (dt, J = 13.0, 6.4 Hz, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.9, 145.9, 138.0, 136.4, 133.2, 128.7, 128.4, 128.0, 127.8, 126.6, 125.3 (q, J = 3.0 Hz), 124.2 (q, J = 271.8 Hz), 122.4, 120.2, 119.6, 110.5, 110.3, 52.7, 35.8, 29.5, 28.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.49. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{22}F_3NOSNa^+$, 476.1266; Found, 476.1270.

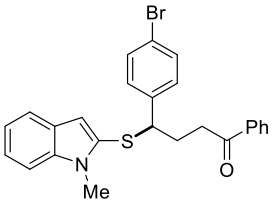


4-(4-fluorophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3af): white solid, mp 115.3-117 ℃, 58.3 mg, 72% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (d, J = 7.8 Hz, 2H), 7.55 (t, J = 8.2 Hz, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.26 – 7.16 (m, 2H), 7.10 (t, J = 7.1 Hz, 1H), 7.05 (dd, J = 8.4, 5.4 Hz, 2H), 6.91 (t, J = 8.6 Hz, 2H), 6.67 (s, 1H), 4.05 (t, J = 7.7 Hz, 1H), 3.40 (s, 3H), 3.07 (dd, J = 13.7, 6.3 Hz, 2H), 2.50 (td, J = 14.3, 7.2 Hz, 1H), 2.36 (td, J = 14.4, 8.0 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.2, 162.2 (d, J = 247.6 Hz), 138.4, 137.2 (d, J = 3.0 Hz), 136.9, 133.3, 129.2 (d, J = 7.6 Hz), 128.8, 128.5, 128.1, 127.3, 122.7, 120.7, 119.9, 115.5 (d, J = 22.7 Hz), 111.5, 109.9, 54.0, 36.3, 29.6, 29.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.60. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}FNOSNa^+$, 426.1298; Found, 426.1303.

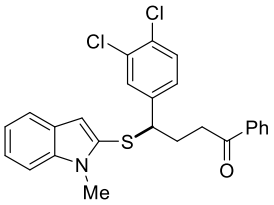


4-(4-chlorophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3ag): white solid, mp 142.7-143.9 ℃, 61.6 mg, 73% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 – 7.84 (m, 2H), 7.55 (t,

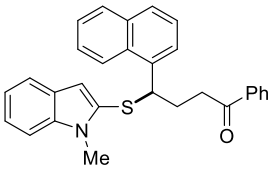
J = 8.0 Hz, 2H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.23 – 7.18 (m, 4H), 7.11 – 7.09 (m, 1H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.67 (s, 1H), 4.03 (t, *J* = 7.8 Hz, 1H), 3.40 (s, 3H), 3.07 (td, *J* = 7.4, 3.2 Hz, 2H), 2.49 (td, *J* = 14.4, 7.2 Hz, 1H), 2.38 – 2.32 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.1, 140.0, 138.4, 137.8, 133.4, 133.3, 129.0, 128.8, 128.8, 128.3, 128.1, 127.3, 122.7, 120.7, 119.9, 111.6, 110.0, 54.0, 36.3, 29.6, 29.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}ClNOSNa^+$, 442.1003; Found, 442.1002.



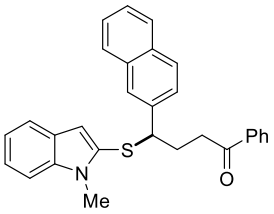
4-(4-bromophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3ah): white solid, mp 143.3-144.2 ℃, 65.7 mg, 71% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.91 – 7.80 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.55 – 7.42 (m, 5H), 7.38 (d, *J* = 8.3 Hz, 1H), 7.22 – 7.11 (m, 3H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.63 (s, 1H), 4.25 (dd, *J* = 8.3, 7.0 Hz, 1H), 3.51 (s, 3H), 3.13 – 3.08 (m, 1H), 3.04 – 2.98 (m, 1H), 2.31 (td, *J* = 14.3, 6.5 Hz, 1H), 2.26 – 2.19 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.9, 140.5, 138.0, 136.4, 133.2, 131.4, 129.8, 128.7, 128.3, 127.8, 126.6, 122.4, 120.5, 120.2, 119.6, 110.4, 110.3, 52.5, 35.8, 29.5, 28.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}BrNOSNa^+$, 486.0498; Found, 486.0497.



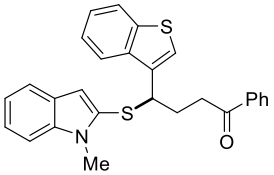
4-(3,4-dichlorophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3ai): white solid, mp 81-83 ℃, 66.9 mg, 74% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.86 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.46 (dd, *J* = 14.8, 7.9 Hz, 3H), 7.41 (d, *J* = 2.1 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 1H), 7.19 – 7.14 (m, 2H), 7.06 – 7.00 (m, 1H), 6.68 – 6.58 (m, 1H), 4.27 (dd, *J* = 8.3, 7.1 Hz, 1H), 3.52 (s, 3H), 3.14 – 3.08 (m, 1H), 3.06 – 3.00 (m, 1H), 2.32 (td, *J* = 14.3, 6.5 Hz, 1H), 2.28 – 2.22 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.8, 142.3, 138.0, 136.4, 133.1, 131.1, 130.5, 129.9, 129.5, 128.6, 127.8, 127.8, 127.8, 126.6, 122.4, 120.2, 119.6, 110.6, 110.2, 52.0, 35.7, 29.5, 28.7. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{21}Cl_2NOSNa^+$, 476.0613; Found, 476.0614.



4-((1-methyl-1*H*-indol-2-yl)thio)-4-(naphthalen-1-yl)-1-phenylbutan-1-one (3aj): white solid, mp 93.7-94.0 ℃, 60.0 mg, 69% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.30 (s, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.82 (dd, J = 13.1, 7.8 Hz, 3H), 7.58 – 7.51 (m, 4H), 7.41 (t, J = 7.7 Hz, 2H), 7.33 – 7.22 (m, 2H), 7.18 – 7.11 (m, 2H), 7.03 (t, J = 7.4 Hz, 1H), 6.76 (s, 1H), 5.15 (s, 1H), 3.20 (s, 2H), 3.10 (s, 3H), 2.52 (s, 1H), 2.45 (s, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 199.2, 138.0, 136.5, 136.3, 133.5, 133.1, 130.8, 128.9, 128.6, 127.9, 127.7, 126.6, 126.4, 125.8, 125.3, 123.8, 123.0, 122.3, 120.1, 119.5, 110.9, 110.1, 47.0, 36.0, 29.1, 28.7. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{29}H_{25}NOSNa^+$, 458.1549; Found, 458.1547.

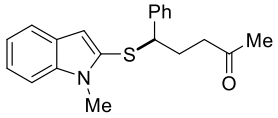


4-((1-methyl-1*H*-indol-2-yl)thio)-4-(naphthalen-2-yl)-1-phenylbutan-1-one (3ak): white solid, mp 111.1-111.3 ℃, 53.8 mg, 62% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.85 (dd, J = 8.1, 4.3 Hz, 2H), 7.83 – 7.79 (m, 2H), 7.71 (d, J = 7.7 Hz, 1H), 7.62 (s, 1H), 7.55 (t, J = 7.4 Hz, 1H), 7.51 – 7.37 (m, 6H), 7.30 (d, J = 8.2 Hz, 1H), 7.18 – 7.10 (m, 1H), 7.01 (dd, J = 11.0, 3.9 Hz, 1H), 6.67 (s, 1H), 4.41 (dd, J = 8.6, 6.8 Hz, 1H), 3.45 (s, 3H), 3.13 – 3.09 (m, 1H), 3.03 – 2.99 (m, 1H), 2.47 – 2.31 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 199.0, 138.4, 138.0, 136.4, 133.2, 132.8, 132.4, 128.7, 128.7, 128.3, 127.8, 127.7, 127.6, 126.7, 126.3, 126.2, 126.1, 125.7, 122.3, 120.1, 119.6, 110.3, 110.2, 53.6, 35.9, 29.5, 29.1. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{29}H_{25}NOSNa^+$, 458.1549; Found, 458.1547.

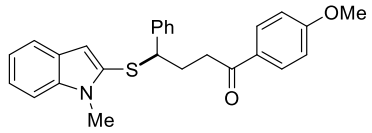


4-(benzo[b]thiophen-3-yl)-4-((1-methyl-1*H*-indol-2-yl)thio)-1-phenylbutan-1-one (3al): yellow solid, mp 52-53 ℃, 47.4 mg, 54% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.03 (d, J = 7.9 Hz, 1H),

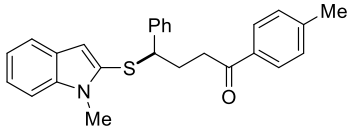
7.98 (d, J = 7.9 Hz, 1H), 7.93 – 7.85 (m, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.47 – 7.39 (m, 4H), 7.30 (d, J = 8.3 Hz, 1H), 7.23 (s, 1H), 7.18 – 7.12 (m, 1H), 7.03 (t, J = 7.4 Hz, 1H), 6.71 (s, 1H), 4.69 (t, J = 7.5 Hz, 1H), 3.24 (td, J = 7.0, 2.7 Hz, 2H), 3.20 (s, 3H), 2.49 – 2.35 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 199.2, 139.7, 138.0, 137.6, 136.5, 135.1, 133.2, 128.7, 127.8, 127.7, 126.7, 124.7, 124.2, 123.8, 123.1, 122.4, 122.2, 120.2, 119.6, 111.2, 110.2, 46.4, 36.0, 29.1, 28.1. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{27}H_{23}NOS_2Na^+$, 464.1113; Found, 464.1123.



5-((1-methyl-1*H*-indol-2-yl)thio)-5-phenylpentan-2-one (3am): brown solid, mp 85.5-88 ℃, 44.0 mg, 68% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.51 (d, J = 7.9 Hz, 1H), 7.35 (d, J = 8.3 Hz, 1H), 7.31 – 7.21 (m, 3H), 7.21 – 7.11 (m, 3H), 7.03 (t, J = 7.4 Hz, 1H), 6.65 (s, 1H), 4.10 (dd, J = 8.8, 6.6 Hz, 1H), 3.45 (s, 3H), 2.50 – 2.44 (m, 1H), 2.42 – 2.36 (m, 1H), 2.19 – 2.05 (m, 2H), 1.99 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 207.5, 140.9, 137.9, 128.7, 128.5, 127.4, 126.7, 122.2, 120.1, 119.5, 110.2, 53.2, 40.5, 29.8, 29.4, 28.6. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{20}H_{21}NOSNa^+$, 346.1236; Found, 346.1238.

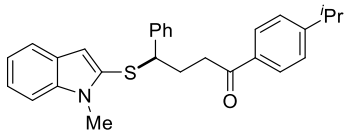


1-(4-methoxyphenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3an): white solid, mp 113.6-114.5 ℃, 40.0 mg, 48% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 7.7 Hz, 1H), 7.27 – 7.14 (m, 5H), 7.13 – 6.99 (m, 3H), 6.85 (d, J = 8.0 Hz, 2H), 6.67 (s, 1H), 4.01 (t, J = 7.7 Hz, 1H), 3.82 (t, J = 7.2 Hz, 3H), 3.32 (d, J = 0.8 Hz, 3H), 3.08 – 2.87 (m, 2H), 2.46 (td, J = 14.2, 7.1 Hz, 1H), 2.36 (dt, J = 14.5, 7.3 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 163.6, 141.4, 138.4, 130.4, 130.0, 128.9, 128.7, 127.7, 127.6, 127.3, 122.5, 120.6, 119.7, 113.8, 111.4, 109.9, 55.6, 54.8, 36.1, 29.6, 29.5. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{26}H_{25}NO_2SNa^+$, 438.1498; Found, 438.1498.

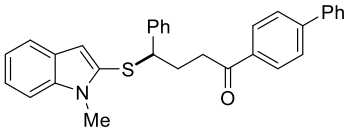


4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenyl-1-(p-tolyl)butan-1-one (3ao): white solid, mp 127.7-

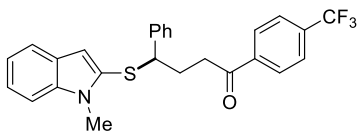
129.0 ℃, 39.0 mg, 49% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.28 – 7.13 (m, 7H), 7.12 – 7.00 (m, 3H), 6.68 (s, 1H), 4.07 – 3.97 (m, 1H), 3.33 (s, 3H), 3.01 (td, J = 8.5, 6.4 Hz, 2H), 2.48 (dd, J = 14.5, 7.6 Hz, 1H), 2.43 – 2.31 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.0, 144.0, 141.3, 138.4, 134.4, 129.4, 128.9, 128.7, 128.2, 127.6, 127.3, 122.5, 120.6, 119.7, 111.4, 109.9, 54.8, 36.3, 29.5, 29.4, 21.8. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{25}NOSNa^+$, 422.1549; Found, 422.1548.



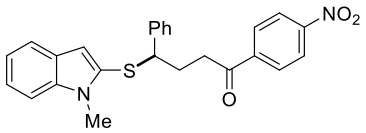
1-(4-isopropylphenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3ap): white solid, mp 105.1-105.9 ℃, 39.5 mg, 46% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (t, J = 8.1 Hz, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.28 – 7.12 (m, 7H), 7.12 – 6.96 (m, 3H), 6.68 (s, 1H), 4.03 (t, J = 7.7 Hz, 1H), 3.33 (s, 3H), 3.08 – 2.96 (m, 2H), 2.96 – 2.86 (m, 1H), 2.48 (td, J = 14.3, 7.2 Hz, 1H), 2.37 (td, J = 14.5, 8.1 Hz, 1H), 1.22 (dd, J = 16.4, 6.8 Hz, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.0, 154.7, 141.3, 138.4, 134.8, 128.9, 128.7, 128.4, 127.6, 127.3, 126.8, 122.5, 120.6, 119.7, 111.4, 109.9, 54.8, 36.4, 34.4, 29.5, 29.4, 23.8. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{28}H_{29}NOSNa^+$, 450.1862; Found, 450.1868.



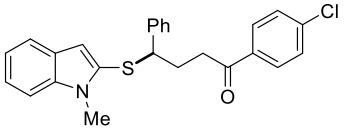
1-([1,1'-biphenyl]-4-yl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3aq): white solid, mp 124.1-124.7 ℃, 40.6 mg, 44% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, J = 8.2 Hz, 2H), 7.63 (dd, J = 16.9, 7.9 Hz, 4H), 7.57 (d, J = 7.9 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.41 (t, J = 7.3 Hz, 1H), 7.32 – 7.16 (m, 5H), 7.10 (dd, J = 11.2, 7.4 Hz, 3H), 6.73 (s, 1H), 4.08 (t, J = 7.7 Hz, 1H), 3.37 (s, 3H), 3.18 – 3.01 (m, 2H), 2.54 (td, J = 14.3, 7.0 Hz, 1H), 2.44 (td, J = 14.4, 8.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.9, 145.9, 141.3, 140.0, 138.4, 135.6, 129.1, 128.9, 128.7, 128.4, 127.7, 127.6, 127.4, 127.3, 122.6, 120.7, 119.8, 111.4, 109.9, 54.8, 36.5, 29.5, 29.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{31}H_{27}NOSNa^+$, 484.1706; Found, 484.1715.



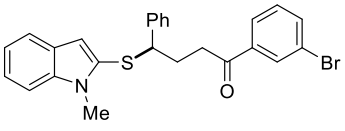
4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenyl-1-(4-(trifluoromethyl)phenyl)butan-1-one (3ar): white solid, mp 118.6-119.3 ℃, 35.3 mg, 39% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 7.7 Hz, 2H), 7.58 – 7.51 (m, 2H), 7.49 – 7.40 (m, 4H), 7.23 – 7.15 (m, 4H), 7.09 (t, J = 7.3 Hz, 1H), 6.65 (s, 1H), 4.08 (t, J = 7.7 Hz, 1H), 3.35 (s, 3H), 3.09 (t, J = 7.1 Hz, 2H), 2.51 (td, J = 14.3, 7.2 Hz, 1H), 2.38 (td, J = 14.6, 7.3 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.0, 145.6, 138.5, 136.8, 133.4, 129.8 (q, J = 33.2 Hz), 128.8, 128.1, 128.0, 128.0, 127.3, 125.6 (q, J = 4.5 Hz), 124.2 (q, J = 273.3 Hz), 122.9, 120.8, 120.0, 111.8, 110.0, 54.2, 36.2, 29.6, 29.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.49. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{22}F_3NOSNa^+$, 476.1266; Found, 476.1270.



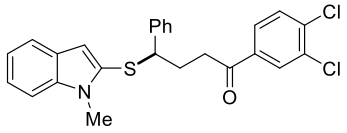
4-((1-methyl-1*H*-indol-2-yl)thio)-1-(4-nitrophenyl)-4-phenylbutan-1-one (3as): yellow solid, mp 116.6-117.3 ℃, 45.5 mg, 53% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 – 8.14 (m, 2H), 7.96 (dd, J = 9.0, 2.0 Hz, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.26 – 7.14 (m, 5H), 7.13 – 7.02 (m, 3H), 6.70 (s, 1H), 4.06 – 3.98 (m, 1H), 3.35 (s, 3H), 3.12 – 2.98 (m, 2H), 2.51 (td, J = 14.3, 7.1 Hz, 1H), 2.42 (dt, J = 14.5, 6.6 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.7, 150.4, 141.2, 140.9, 138.4, 129.1, 128.8, 128.6, 127.9, 127.6, 127.3, 123.9, 122.7, 120.7, 119.9, 111.4, 109.9, 54.4, 37.0, 29.5, 29.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}N_2O_3SNa^+$, 453.1243; Found, 453.1242.



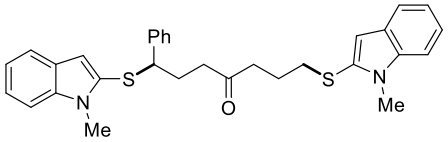
1-(4-chlorophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3at): white solid, mp 129.7-130.6 ℃, 50.5 mg, 60% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.97 – 7.71 (m, 2H), 7.59 – 7.43 (m, 3H), 7.36 (d, J = 8.0 Hz, 1H), 7.29 – 7.22 (m, 3H), 7.21 – 7.12 (m, 3H), 7.07 – 6.96 (m, 1H), 6.66 (d, J = 0.4 Hz, 1H), 4.22 (dd, J = 8.5, 6.9 Hz, 1H), 3.46 (s, 3H), 3.11 – 3.06 (m, 1H), 3.01 – 2.96 (m, 1H), 2.38 – 2.17 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.0, 140.9, 138.0, 137.9, 135.1, 129.7, 128.8, 128.6, 128.5, 127.5, 127.5, 126.7, 122.2, 120.1, 119.5, 110.2, 53.2, 35.9, 29.4, 28.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}ClNOSNa^+$, 442.1003; Found, 442.1002.



1-(3-bromophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3au): white solid, mp 108-109 °C, 50.0 mg, 54% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.76 (d, J = 7.8 Hz, 1H), 7.64 (dd, J = 7.9, 0.8 Hz, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.27 (d, J = 7.9 Hz, 1H), 7.24 – 7.17 (m, 5H), 7.07 (dt, J = 7.0, 5.9 Hz, 3H), 6.70 (s, 1H), 4.02 (t, J = 7.7 Hz, 1H), 3.34 (s, 3H), 3.09 – 2.92 (m, 2H), 2.48 (td, J = 14.4, 7.1 Hz, 1H), 2.38 (td, J = 14.4, 8.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 197.9, 141.1, 138.6, 138.4, 136.1, 131.2, 130.3, 128.8, 128.7, 127.8, 127.6, 127.3, 126.6, 123.1, 122.6, 120.7, 119.8, 111.5, 109.9, 54.6, 36.5, 29.5, 29.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}BrNOSNa^+$, 486.0498; Found, 486.0497.

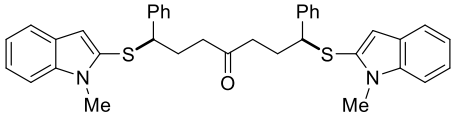


1-(3,4-dichlorophenyl)-4-((1-methyl-1*H*-indol-2-yl)thio)-4-phenylbutan-1-one (3av): yellow solid, mp 88.9-89.7 °C, 69.0 mg, 76% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.96 (d, J = 2.0 Hz, 1H), 7.74 (dd, J = 8.4, 2.0 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.48 (d, J = 7.9 Hz, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.28 – 7.20 (m, 3H), 7.20 – 7.11 (m, 3H), 7.04 – 6.99 (m, 1H), 6.66 (d, J = 0.6 Hz, 1H), 4.21 (dd, J = 8.3, 7.0 Hz, 1H), 3.44 (s, 3H), 3.12 – 3.07 (m, 1H), 3.02 – 2.97 (m, 1H), 2.36 – 2.18 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 197.2, 140.8, 137.9, 136.5, 135.9, 131.7, 130.9, 129.6, 128.6, 128.5, 127.7, 127.5, 127.4, 126.6, 122.2, 120.0, 119.5, 110.2, 110.1, 53.1, 36.0, 29.4, 28.9. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{21}Cl_2NOSNa^+$, 476.0613; Found, 476.0614.

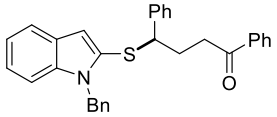


1,7-bis((1-methyl-1*H*-indol-2-yl)thio)-1-phenylheptan-4-one (3aw): green oil, 48.0 mg, 47% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.53 – 7.44 (m, 2H), 7.40 (dd, J = 8.3, 0.6 Hz, 1H), 7.35 (dd, J = 8.3, 0.6 Hz, 1H), 7.29 – 7.19 (m, 3H), 7.19 – 7.10 (m, 4H), 7.06 – 6.99 (m, 2H), 6.63 (d, J = 0.5 Hz, 1H), 6.61 (d, J = 0.6 Hz, 1H), 4.07 (dd, J = 8.8, 6.6 Hz, 1H), 3.72 (s, 3H), 3.45 (s, 3H), 2.72 (t, J = 7.3 Hz, 2H), 2.48 – 2.39 (m, 3H), 2.38 – 2.32 (m, 1H), 2.18 – 2.00 (m, 2H), 1.68 – 1.56 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 209.0, 140.8, 137.9, 130.7, 128.7, 128.5, 127.5, 126.9, 126.6, 122.2, 121.7, 120.1, 119.6, 119.5, 110.2, 110.1, 110.0, 107.1, 53.2, 40.3, 39.7, 34.4, 29.8, 29.4, 28.6, 22.9. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{31}H_{33}N_2OS_2^+$, 513.2029; Found,

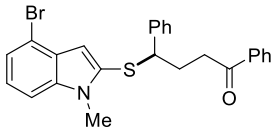
513.2032.



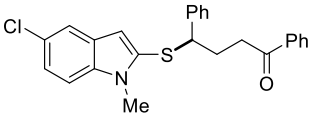
1,7-bis((1-methyl-1*H*-indol-2-yl)thio)-1,7-diphenylheptan-4-one (3ax): brown solid, mp 132.7-134.1 ℃, 63.6 mg, 54% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.50 (d, J = 7.9 Hz, 1H), 7.35 (d, J = 8.3 Hz, 1H), 7.26 – 7.19 (m, 3H), 7.19 – 7.14 (m, 1H), 7.13 – 7.06 (m, 2H), 7.05 – 7.01 (m, 1H), 6.61 (s, 1H), 4.04 (dt, J = 8.8, 6.5 Hz, 1H), 3.44 (s, 3H), 2.42 – 2.32 (m, 1H), 2.32 – 2.24 (m, 1H), 2.13 – 1.97 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 208.7, 140.7, 137.9, 128.7, 128.4, 127.4, 126.6, 122.2, 120.1, 119.5, 110.2, 110.1, 53.1, 29.4, 28.5, 28.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{37}H_{37}N_2OS_2^+$, 589.2342; Found, 589.2346.



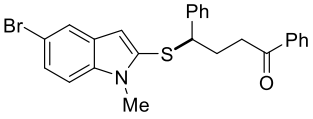
4-((1-benzyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3ba): red liquid, 47.8 mg, 52% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.80 (dd, J = 8.3, 1.1 Hz, 2H), 7.59 – 7.54 (m, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.32 (d, J = 8.2 Hz, 1H), 7.29 – 7.15 (m, 8H), 7.12 – 7.09 (m, 1H), 7.05 – 7.01 (m, 1H), 6.95 (d, J = 7.3 Hz, 2H), 6.73 (s, 1H), 5.30 (s, 2H), 4.11 (dd, J = 8.8, 6.6 Hz, 1H), 2.95 – 2.90 (m, 2H), 2.37 – 2.30 (m, 1H), 2.28 – 2.22 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.8, 140.8, 138.2, 137.5, 136.4, 133.1, 129.1, 128.7, 128.5, 128.5, 127.7, 127.6, 127.5, 127.1, 127.0, 126.2, 122.5, 120.2, 119.8, 110.6, 110.6, 53.4, 45.9, 35.8, 29.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{31}H_{27}NOSNa^+$, 484.1706; Found, 484.1711.



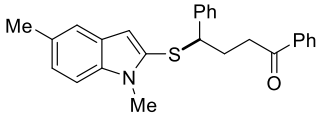
4-((4-bromo-1-methyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3ca): white solid, mp 119.3-120 ℃, 47.5 mg, 51% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 7.6 Hz, 2H), 7.53 (t, J = 7.3 Hz, 1H), 7.42 (t, J = 7.7 Hz, 2H), 7.32 – 7.19 (m, 4H), 7.16 – 6.98 (m, 4H), 6.74 (s, 1H), 4.10 (t, J = 7.7 Hz, 1H), 3.31 (s, 3H), 3.15 – 2.99 (m, 2H), 2.51 (dt, J = 14.3, 7.1 Hz, 1H), 2.42 (dt, J = 14.3, 7.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.3, 141.1, 138.6, 136.9, 133.3, 130.3, 128.8, 128.7, 128.1, 127.8, 127.6, 123.3, 122.7, 114.5, 111.2, 109.1, 55.0, 36.4, 30.0, 29.4. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}BrNOSNa^+$, 486.0498; Found, 486.0497.



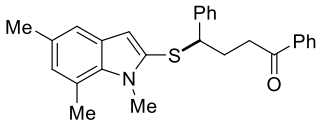
4-((5-chloro-1-methyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3da): white solid, mp 119.3-120.9 ℃, 39.5 mg, 47% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 – 7.82 (m, 2H), 7.57 – 7.52 (m, 1H), 7.50 (d, J = 1.9 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.25 – 7.17 (m, 3H), 7.14 (dd, J = 8.7, 2.0 Hz, 1H), 7.10 – 7.04 (m, 3H), 6.61 (s, 1H), 4.07 (dd, J = 8.3, 7.2 Hz, 1H), 3.31 (s, 3H), 3.10 – 3.02 (m, 2H), 2.50 (td, J = 14.4, 7.0 Hz, 1H), 2.43 – 2.37 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.2, 141.0, 136.8, 136.7, 133.3, 130.6, 128.7, 128.1, 127.8, 127.6, 125.5, 122.8, 119.9, 110.9, 110.6, 54.7, 36.4, 29.7, 29.3. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}ClNOSNa^+$, 442.1003; Found, 442.1002.



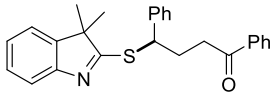
4-((5-bromo-1-methyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3ea): white solid, mp 123.7-124.9 ℃, 47.2 mg, 51% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.3, 1.2 Hz, 2H), 7.66 (d, J = 1.8 Hz, 1H), 7.59 – 7.49 (m, 1H), 7.41 (dd, J = 10.7, 4.8 Hz, 2H), 7.27 (dd, J = 8.9, 2.1 Hz, 1H), 7.24 – 7.15 (m, 3H), 7.07 – 7.03 (m, 3H), 6.61 (d, J = 0.5 Hz, 1H), 4.07 (dd, J = 8.4, 7.2 Hz, 1H), 3.31 (s, 3H), 3.08 – 3.04 (m, 2H), 2.50 (td, J = 14.4, 7.0 Hz, 1H), 2.43 – 2.37 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.2, 141.0, 136.9, 136.9, 133.3, 130.6, 128.8, 128.7, 128.1, 127.8, 127.6, 125.4, 123.0, 113.1, 111.3, 110.5, 54.8, 36.4, 29.7, 29.3. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}BrNOSNa^+$, 486.0498; Found, 486.0497.



4-((1,5-dimethyl-1*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3fa): white solid, mp 137.3-138.3 ℃, 38.2 mg, 48% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 7.3 Hz, 2H), 7.53 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.8 Hz, 2H), 7.33 (s, 1H), 7.25 – 7.14 (m, 3H), 7.15 – 6.98 (m, 4H), 6.61 (s, 1H), 4.02 (t, J = 7.7 Hz, 1H), 3.31 (s, 3H), 3.12 – 2.99 (m, 2H), 2.55 – 2.46 (m, 1H), 2.43 (s, 3H), 2.42 – 2.33 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.3, 141.4, 136.9, 136.9, 133.2, 129.0, 128.7, 128.6, 128.1, 127.6, 127.5, 124.3, 120.2, 110.9, 109.6, 54.8, 36.5, 29.5, 29.3, 21.5. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{26}H_{25}NOSNa^+$, 422.1549; Found, 422.1548.

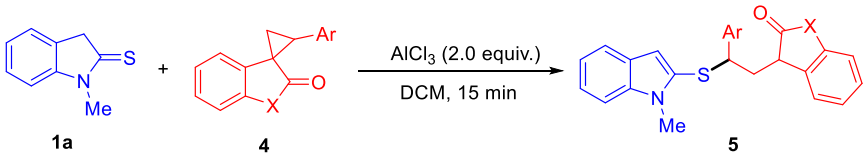


1,4-diphenyl-4-((1,5,7-trimethyl-1*H*-indol-2-yl)thio)butan-1-one (3ga): white solid, mp 134.6-136.7 °C, 47.2 mg, 57% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (dd, J = 8.3, 1.1 Hz, 2H), 7.56 (dd, J = 10.5, 4.2 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.26 (dd, J = 6.5, 3.7 Hz, 3H), 7.18 (s, 1H), 7.15 – 7.08 (m, 2H), 6.77 (s, 1H), 6.63 (s, 1H), 4.02 (dd, J = 8.2, 7.3 Hz, 1H), 3.65 (s, 3H), 3.10 – 3.05 (m, 2H), 2.67 (s, 3H), 2.51 (td, J = 14.5, 6.7 Hz, 1H), 2.44 – 2.40 (m, 1H), 2.39 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 199.4, 141.3, 136.9, 136.0, 133.2, 129.2, 129.0, 128.7, 128.7, 128.3, 128.1, 127.7, 127.6, 127.3, 121.1, 118.2, 111.7, 54.8, 36.5, 32.6, 29.3, 21.2, 20.0. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{27}H_{27}NOSNa^+$, 436.1706; Found, 436.1717.



4-((3,3-dimethyl-3*H*-indol-2-yl)thio)-1,4-diphenylbutan-1-one (3ha): colorless oil, 56.0 mg, 70% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.95 – 7.78 (m, 2H), 7.62 – 7.52 (m, 1H), 7.49 (d, J = 7.3 Hz, 2H), 7.44 (dd, J = 9.8, 4.3 Hz, 2H), 7.40 – 7.32 (m, 3H), 7.27 (dt, J = 15.9, 7.8 Hz, 2H), 7.22 (td, J = 7.6, 1.1 Hz, 1H), 7.10 (td, J = 7.4, 1.0 Hz, 1H), 5.18 (t, J = 7.4 Hz, 1H), 3.14 – 3.09 (m, 1H), 3.01 – 2.96 (m, 1H), 2.65 – 2.52 (m, 1H), 2.47 – 2.33 (m, 1H), 1.25 (s, 3H), 1.16 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 198.8, 186.9, 153.1, 145.6, 141.0, 136.4, 133.1, 128.7, 128.6, 127.8, 127.7, 127.6, 127.5, 124.1, 121.4, 118.3, 54.6, 47.9, 35.9, 30.6, 24.8, 24.6. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{26}H_{25}NOSNa^+$, 422.1549; Found, 422.1548.

General Procedure for the $AlCl_3$ Mediated Ring-opening Reaction of Spirocyclic Cyclopropanes 4

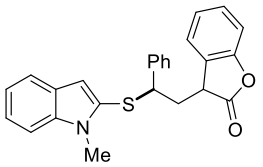


1a 4 5

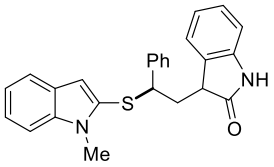
To the mixture of indoline-2-thiones **1** (0.2 mmol, 1.0 equiv.), spirocyclic cyclopropanes **4** (0.2 mmol, 1.0 equiv.), and $AlCl_3$ (0.4 mmol, 53.3 mg, 2.0 equiv.) 2 mL DCM was added at room temperature. The reaction was stirred at room temperature for 15 min. Then the resulting mixture

was firstly quenched by brine (10 mL), and extracted with DCM three times (5 mL × 3). The combined organic phase was washed with brine, concentrated in vacuo and then column chromatography on silica gel (eluent: petroleum ether/ethyl acetate = 3:1 or 20:1) to afford the desired compounds **5**.

Experiment Data for the product 5

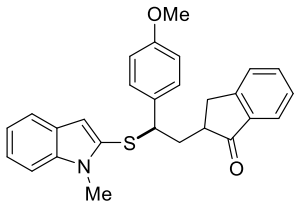


3-(2-((1-methyl-1*H*-indol-2-yl)thio)-2-phenylethyl)benzofuran-2(3*H*)-one (5a): white solid, mp 166.1-166.7 ℃, 50.1 mg, 63% yield, 1:1 dr. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.53 (d, J = 7.9 Hz, 1H), 7.47 (dd, J = 12.7, 7.7 Hz, 2H), 7.37 (d, J = 8.3 Hz, 1H), 7.35 – 7.27 (m, 4.2H), 7.27 – 7.21 (m, 5.5H), 7.21 – 7.12 (m, 7.3H), 7.13 – 7.08 (m, 1.5H), 7.08 – 6.97 (m, 2H), 6.70 (s, 1H), 6.53 (s, 1H), 4.40 (dd, J = 9.6, 6.2 Hz, 1H), 4.34 (t, J = 7.9 Hz, 1H), 4.08 (t, J = 6.5 Hz, 1H), 3.98 – 3.88 (m, 1H), 3.41 (s, 3H), 3.24 (s, 3H), 2.65 – 2.60 (m, 2H), 2.59 – 2.53 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 176.9, 176.4, 153.3, 153.2, 140.4, 139.5, 138.1, 138.0, 128.8, 128.8, 128.6, 128.0, 127.9, 127.8, 127.7, 127.7, 127.5, 127.2, 127.0, 126.6, 126.6, 124.8, 124.5, 124.1, 124.0, 122.5, 122.4, 120.3, 120.2, 119.7, 119.6, 110.7, 110.6, 110.4, 110.3, 110.3, 51.4, 50.9, 41.2, 40.9, 35.2, 35.0, 29.4, 29.2. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{25}H_{21}NO_2SNa^+$, 422.1185; Found, 422.1196.



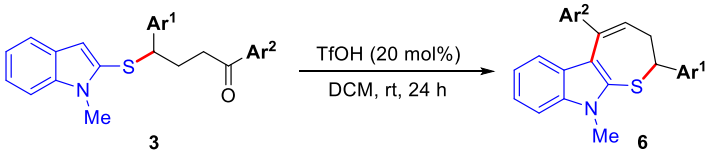
3-(2-((1-methyl-1*H*-indol-2-yl)thio)-2-phenylethyl)indolin-2-one (5b): white solid, mp 132.7-133.5 ℃, 64.5 mg, 81% yield, 1:0.8 dr. ^{1}H NMR (600 MHz, DMSO-d_6) δ 10.50 (s, 0.9H), 10.35 (s, 1H), 7.59 – 7.45 (m, 2.1H), 7.33 (dd, J = 23.7, 8.1 Hz, 3.4H), 7.29 – 7.10 (m, 13.7H), 7.07 – 6.98 (m, 2H), 6.93 (dd, J = 11.0, 4.1 Hz, 1H), 6.91 – 6.86 (m, 1H), 6.83 (d, J = 7.7 Hz, 0.9H), 6.77 (d, J = 7.5 Hz, 1H), 6.70 (s, 1H), 6.61 (s, 0.8H), 4.65 (dd, J = 9.5, 6.1 Hz, 1H), 4.58 (t, J = 7.9 Hz, 0.8H), 3.43 – 3.41 (m, 3.8H), 3.37 – 3.24 (m, 3.5H), 2.47 (dt, J = 14.5, 5.4 Hz, 2H), 2.42 – 2.31 (m, 1.8H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 178.5, 178.4, 142.6, 142.5, 140.7, 140.2, 138.0, 137.9, 129.1,

129.0, 128.5, 128.4, 128.0, 127.8, 127.7, 127.5, 127.5, 126.7, 126.6, 124.2, 123.9, 122.3, 121.3, 121.3, 120.2, 119.6, 119.5, 110.7, 110.4, 110.2, 109.4, 109.3, 51.1, 50.9, 43.1, 43.0, 35.8, 35.5, 29.4, 29.2. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{25}H_{22}N_2OSNa^+$, 421.1345; Found, 421.1352.



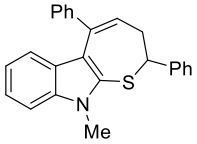
2-(2-(4-methoxyphenyl)-2-((1-methyl-1*H*-indol-2-yl)thio)ethyl)-2,3-dihydro-1*H*-inden-1-one (5c): yellow liquid, 43.6 mg, 51% yield, 1:1 dr. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.68 – 7.56 (m, 4H), 7.49 (td, J = 12.4, 7.7 Hz, 4H), 7.43 – 7.32 (m, 4H), 7.23 – 7.10 (m, 6H), 7.06 – 6.98 (m, 2H), 6.89 – 6.83 (m, 2H), 6.83 – 6.78 (m, 2H), 6.66 (dd, J = 3.9, 0.5 Hz, 2H), 4.42 (t, J = 7.7 Hz, 1H), 4.36 (dd, J = 10.5, 5.4 Hz, 1H), 3.71 – 3.70 (m, 6H), 3.52 (s, 3H), 3.48 (s, 3H), 3.20 – 3.10 (m, 2H), 2.87 – 2.84 (m, 1H), 2.78 (dd, J = 17.2, 4.2 Hz, 1H), 2.70 (dd, J = 17.1, 4.3 Hz, 1H), 2.49 – 2.43 (m, 1H), 2.41 – 2.33 (m, 1H), 2.03 – 1.89 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 207.4, 207.2, 158.6, 158.5, 153.6, 153.4, 137.9, 137.9, 135.9, 135.8, 134.9, 134.9, 133.3, 132.0, 129.0, 128.8, 128.8, 128.7, 127.4, 127.4, 126.8, 126.7, 126.7, 126.7, 123.2, 123.1, 122.2, 122.2, 120.1, 119.5, 119.5, 114.0, 113.7, 110.2, 110.2, 110.1, 110.1, 55.1, 52.3, 51.6, 45.5, 45.0, 36.7, 36.6, 32.8, 32.1, 29.5, 29.5. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ Calcd for $C_{27}H_{25}NO_2SNa^+$, 450.1498; Found, 450.1496.

General Procedure for the TfOH catalyzed intramolecular cyclization of the ring-opening products 3

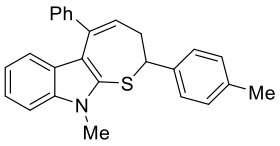


To the solvent of 4-indolylthiobutan-1-ones **3** (0.2 mmol, 1.0 equiv.) in 2 mL DCM, TfOH (0.04 mmol, 3.5 μL) was added at room temperature. The reaction was stirred at room temperature for 24 hours. The resulting mixture was directly purified by silica gel column chromatography (eluent: petroleum ether/ethyl acetate = 50:1) to afford the desired compounds **6**.

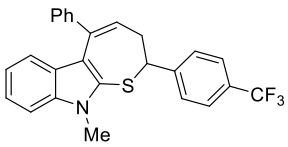
Experiment Data for the dihydro-2*H*-thiepino[2,3-b]indoles 6



10-methyl-2,5-diphenyl-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6a): white solid, mp 198.1-199.3 ℃, 72.7 mg, 99% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 – 7.35 (m, 3H), 7.35 – 7.28 (m, 7H), 7.28 – 7.24 (m, 1H), 7.22 (dd, J = 11.3, 3.9 Hz, 1H), 6.94 (t, J = 7.5 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.52 (t, J = 7.5 Hz, 1H), 5.14 (t, J = 7.8 Hz, 1H), 3.88 (s, 3H), 2.63 (t, J = 7.7 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.1, 140.6, 140.4, 138.2, 134.6, 128.8, 128.3, 127.9, 127.8, 127.6, 126.6, 126.3, 126.2, 122.3, 120.7, 119.8, 118.7, 109.8, 68.9, 37.4, 30.7. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{25}H_{22}NS^+$, 368.1467; Found, 368.1465.

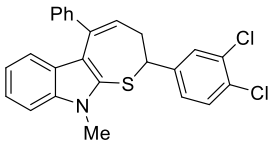


10-methyl-5-phenyl-2-(p-tolyl)-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6b): white solid, mp 139.3-140.2 ℃, 75.5 mg, 99% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.53 (d, J = 8.3 Hz, 1H), 7.37 – 7.26 (m, 5H), 7.23 (d, J = 8.1 Hz, 2H), 7.20 – 7.14 (m, 1H), 7.11 (d, J = 7.9 Hz, 2H), 6.91 – 6.83 (m, 1H), 6.67 (d, J = 8.0 Hz, 1H), 6.49 (t, J = 7.5 Hz, 1H), 5.26 (dd, J = 10.9, 4.4 Hz, 1H), 3.83 (s, 3H), 2.57 – 2.53 (m, 1H), 2.48 – 2.43 (m, 1H), 2.26 (s, 3H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 141.0, 139.9, 139.2, 137.8, 136.8, 134.1, 129.1, 128.3, 127.5, 127.3, 126.6, 126.3, 125.4, 121.9, 119.5, 119.5, 117.4, 110.5, 67.2, 36.9, 30.5, 20.7. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{26}H_{24}NS^+$, 382.1624; Found, 382.1624.

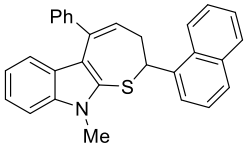


10-methyl-5-phenyl-2-(4-(trifluoromethyl)phenyl)-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6c): white solid, mp 205.5-206.5 ℃, 82.8 mg, 95% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.70 (d, J = 8.2 Hz, 2H), 7.59 – 7.55 (m, 3H), 7.35 – 7.31 (m, 5H), 7.23 – 7.15 (m, 1H), 6.89 (dd, J = 11.1, 3.9 Hz, 1H), 6.68 (d, J = 8.0 Hz, 1H), 6.53 (t, J = 7.5 Hz, 1H), 5.42 (dd, J = 11.3, 4.4 Hz, 1H), 3.85 (s, 3H), 2.64 – 2.60 (m, 1H), 2.49 – 2.45 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 148.4,

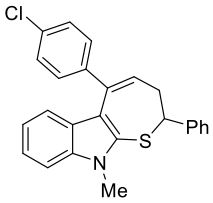
139.7, 139.5, 137.9, 133.4, 128.4, 128.0 (q, J = 31.7 Hz), 127.7, 127.3, 127.3, 126.3, 125.7 (q, J = 3.0 Hz), 125.4, 124.2 (q, J = 271.8 Hz), 122.1, 119.7, 119.5, 117.7, 110.7, 66.4, 36.5, 30.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.51. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{26}H_{21}F_3NS^+$, 436.1341; Found, 436.1353.



2-(3,4-dichlorophenyl)-10-methyl-5-phenyl-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6d): white solid, mp 171.5-172.1 ℃, 83.8 mg, 96% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 – 7.28 (m, 8H), 7.25 (dd, J = 11.2, 3.9 Hz, 1H), 7.17 (dd, J = 8.3, 2.1 Hz, 1H), 6.96 (t, J = 7.4 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.50 (t, J = 7.5 Hz, 1H), 5.06 (dd, J = 11.0, 4.6 Hz, 1H), 3.90 (s, 3H), 2.63 – 2.59 (m, 1H), 2.57 – 2.52 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 144.3, 141.1, 140.1, 138.3, 133.5, 132.7, 131.6, 130.7, 128.7, 128.4, 127.9, 127.8, 126.2, 125.9, 125.5, 122.6, 120.8, 120.0, 119.1, 109.9, 67.6, 37.0, 30.7. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{25}H_{20}Cl_2NS^+$, 436.0688; Found, 436.0692.



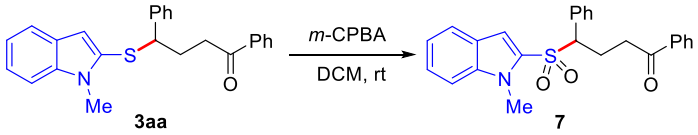
10-methyl-2-(naphthalen-1-yl)-5-phenyl-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6e): white solid, mp 164.1-165.1 ℃, 78.5 mg, 94% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.21 (d, J = 7.7 Hz, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.1 Hz, 1H), 7.68 (d, J = 7.1 Hz, 1H), 7.59 – 7.51 (m, 3H), 7.46 (t, J = 7.7 Hz, 1H), 7.34 (s, 5H), 7.17 (t, J = 7.6 Hz, 1H), 6.88 (t, J = 7.5 Hz, 1H), 6.69 (d, J = 7.9 Hz, 1H), 6.62 (t, J = 7.3 Hz, 1H), 6.14 (d, J = 7.2 Hz, 1H), 3.77 (s, 3H), 2.88 – 2.60 (m, 2H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 140.0, 139.0, 139.0, 137.8, 134.1, 133.5, 129.6, 128.8, 128.3, 128.0, 127.5, 127.3, 127.0, 126.4, 125.9, 125.6, 125.5, 123.8, 123.2, 122.0, 119.5, 117.5, 110.5, 35.4, 30.5. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ Calcd for $C_{29}H_{24}NS^+$, 418.1624; Found, 418.1621.



5-(4-chlorophenyl)-10-methyl-2-phenyl-3,10-dihydro-2*H*-thiepino[2,3-b]indole (6f): white solid, mp 181.7-182 ℃, 78.7 mg, 98% yield. ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.54 (d, J = 8.3 Hz,

1H), 7.38 (d, J = 8.5 Hz, 2H), 7.36 – 7.28 (m, 6H), 7.25 (t, J = 7.0 Hz, 1H), 7.18 (t, J = 7.5 Hz, 1H), 6.91 (t, J = 7.5 Hz, 1H), 6.69 (d, J = 8.0 Hz, 1H), 6.54 (t, J = 7.5 Hz, 1H), 5.30 (dd, J = 11.0, 4.4 Hz, 1H), 3.84 (s, 3H), 2.61 – 2.57 (m, 1H), 2.49 – 2.40 (m, 1H). ^{13}C NMR (150 MHz, DMSO-d_6) δ 143.8, 138.7, 138.0, 137.8, 134.2, 132.2, 129.0, 128.7, 128.4, 127.6, 127.4, 126.4, 125.3, 122.1, 119.8, 119.4, 116.9, 110.7, 67.2, 36.9, 30.6. HRMS (ESI-TOF) *m/z*: [M + H]$^+$ Calcd for $C_{25}H_{21}ClNS^+$, 402.1078; Found, 402.1077.

The Procedure for the Transformation to Sulfone 7 and the Experiment Data of 7



To the solution of **3aa** (0.2 mmol, 77.1 mg) in DCM (2 mL), *m*-CPBA (0.44 mmol, 89.3 mg, 85% wt) was added at 0 ℃. The resulting mixture was then allowed to warm to ambient temperature. Upon completion (as determined by TLC analysis), the reaction was diluted with CH_2Cl_2, washed with 5% aq. K_2CO_3 and 5% aq. $NaHCO_3$. The organic phase was dried over anhydrous Na_2SO_4, filtered, concentrated *in vacuo* and the residue was purified by flash column chromatography (petroleum ether/EtOAc = 5:1) to give sulfone **7** with 50% yield.

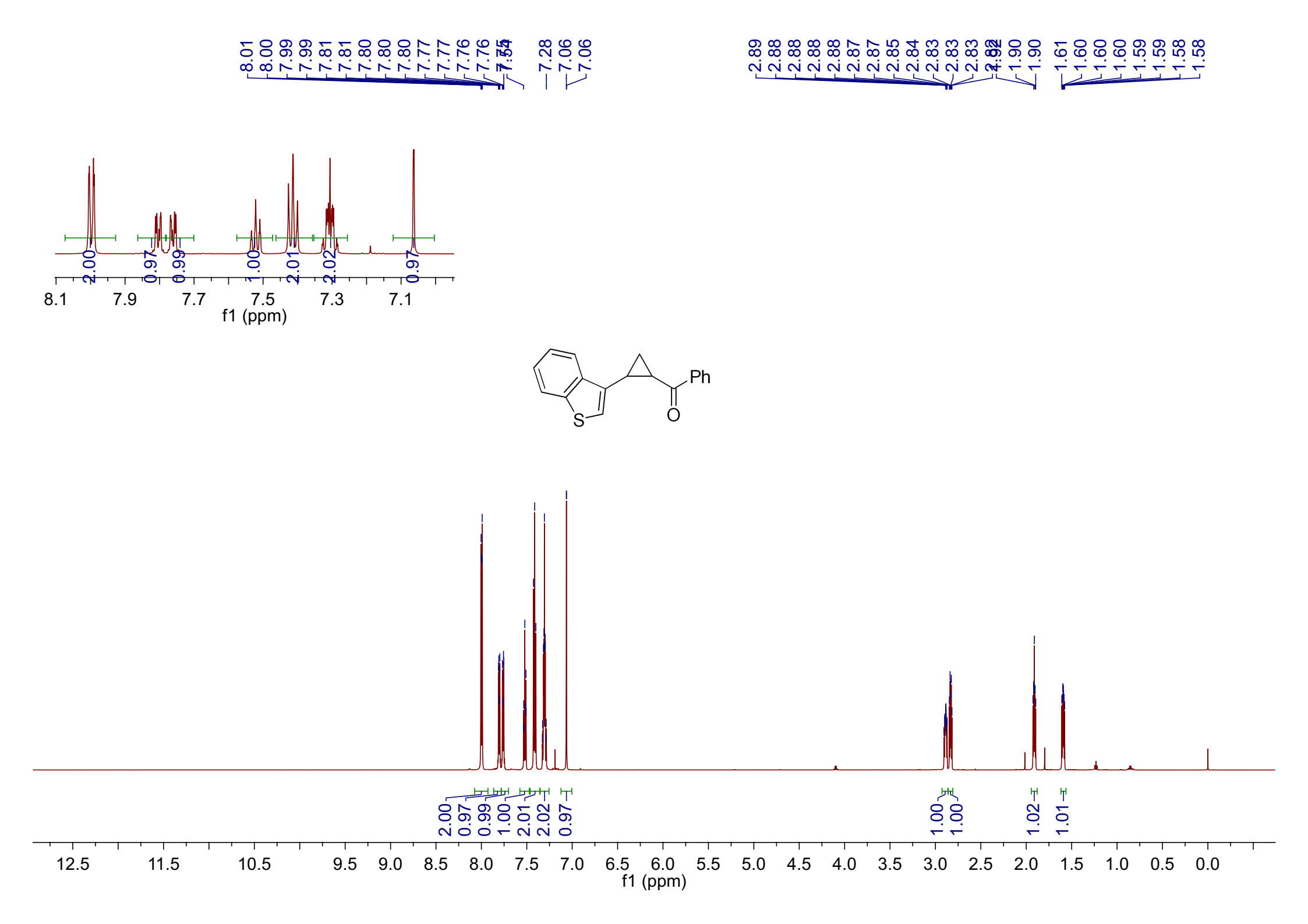
4-((1-methyl-1H-indol-2-yl)sulfonyl)-1,4-diphenylbutan-1-one (7): white solid, mp 154.2-155.3 ℃, 41.6 mg, 50% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 – 7.79 (m, 2H), 7.69 (d, J = 8.0 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.41 – 7.31 (m, 4H), 7.26 – 7.22 (m, 4H), 7.21 – 7.17 (m, 1H), 7.09 (d, J = 7.3 Hz, 2H), 4.46 (dd, J = 10.3, 5.0 Hz, 1H), 3.30 (s, 3H), 3.09 – 2.98 (m, 2H), 2.95 – 2.88 (m, 1H), 2.60 – 2.53 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 198.6, 139.3, 136.6, 133.4, 131.5, 131.3, 130.2, 129.5, 128.9, 128.7, 128.0, 125.9, 125.2, 122.9, 121.3, 112.9, 110.6, 77.4, 77.2, 76.9, 71.7, 35.4, 30.4, 22.8. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ Calcd for $C_{25}H_{23}NO_3SNa^+$, 440.1291; Found, 440.1297.

References

[1] a) M. S. C. Pedras, M. Jha, *J. Org. Chem*. 2005, **70**, 1828-1834; b) P. Thanigaimalai, K.-C. Lee, V. K. Sharma, N. Sharma, E. Roh, Y. Kim, S.-H. Jung, *Chem. Pharm. Bull*. 2011, **59**, 1285-1288.

[2] a) E. Richmond, V. D. Vuković, J. Moran, *Org. Lett*. 2018, **20**, 574-577; b) J. Liu, X.-P. Liu, H. Wu, Y. Wei, F.-D. Lu, K.-R. Guo, Y. Cheng, W.-J. Xiao, Chem. Commun. 2020, 56, 11508-11511.

[3] S. Kar, T. Sarkar, P. K. Maharana, A. K. Guha, T. Punniyamurthy, *Org. Lett.* 2022, **24**, 4965-4970.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1.90
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1.61
1.60
1.60
1.60
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1.58
1.58
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0.97
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1.00
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2.02
0.97
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7.9
7.7
7.5
7.3
7.1
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0.99
1.00
2.01
2.02
0.97
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1.00
1.02
1.01
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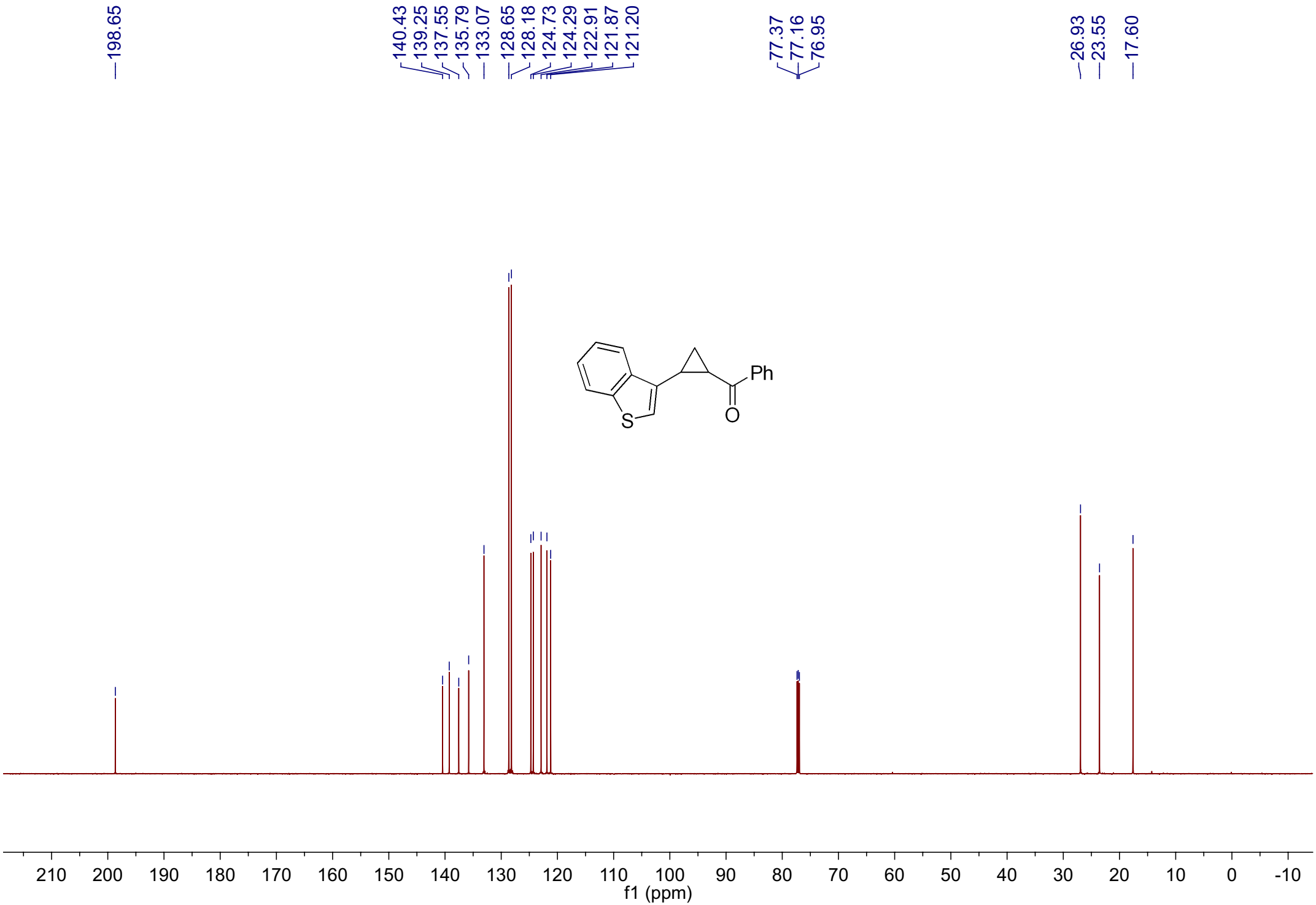
f1 (ppm)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Ph
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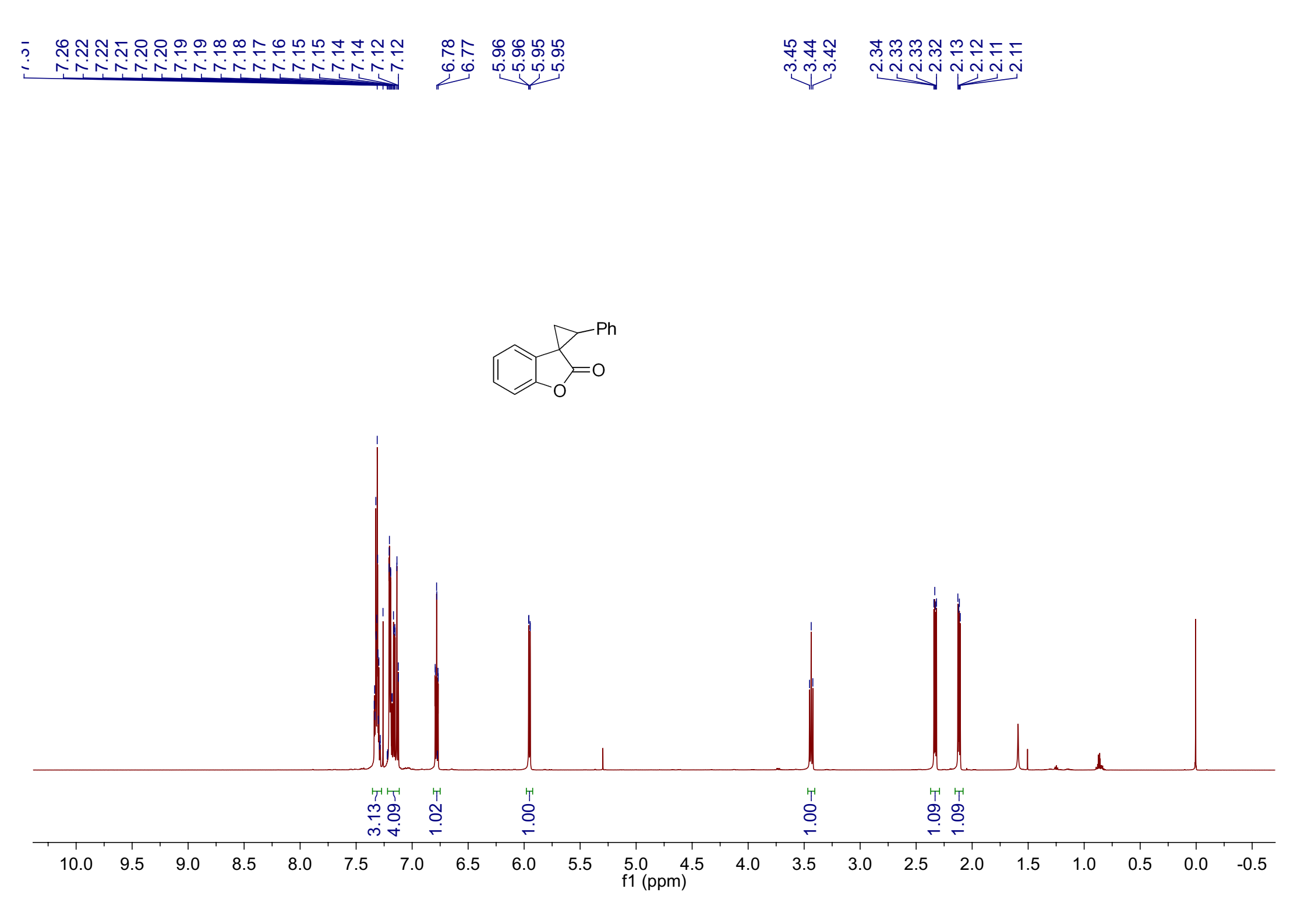
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2.12
2.11
2.11
Ph
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O
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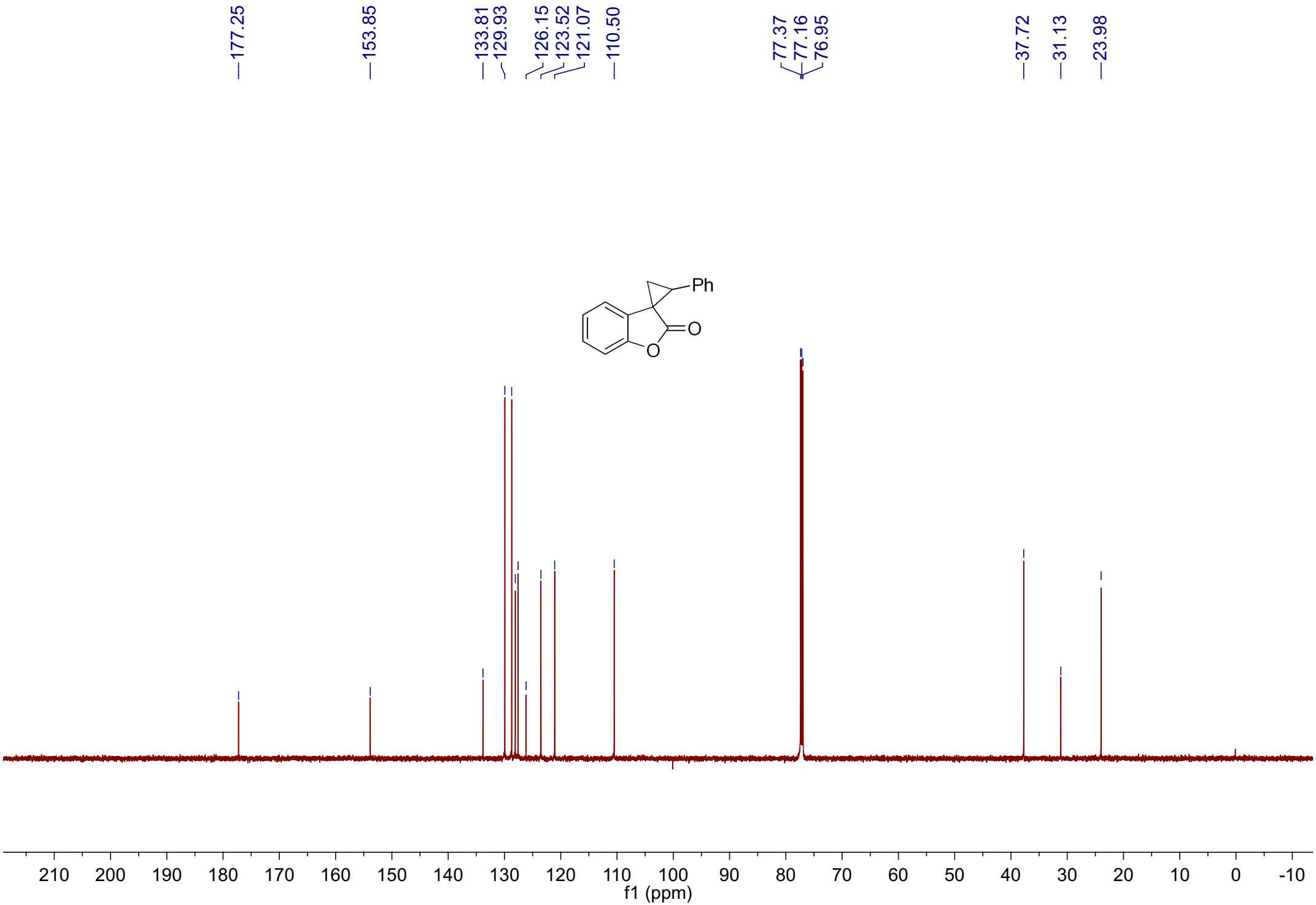
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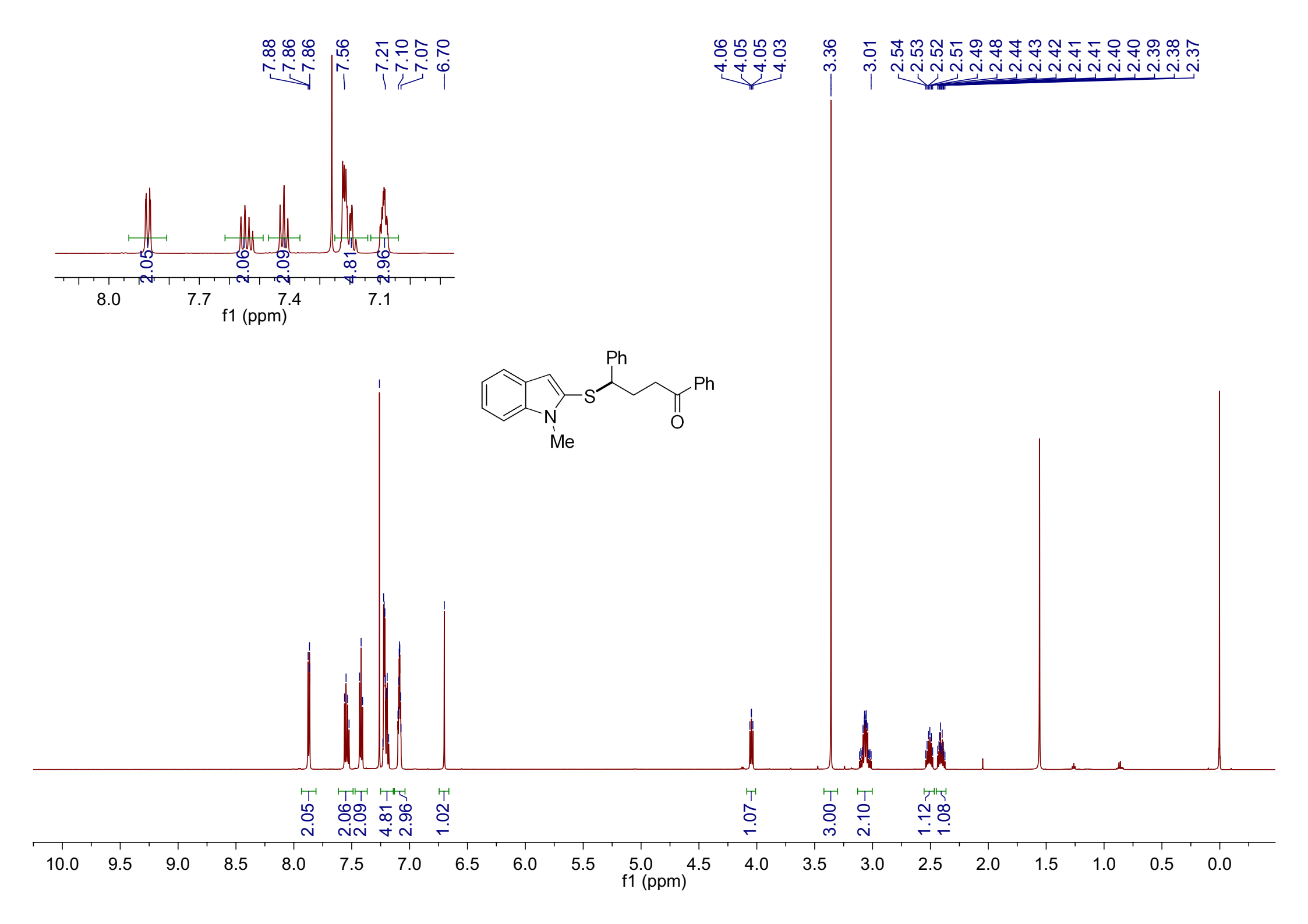
f1 (ppm)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Ph
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Me
O
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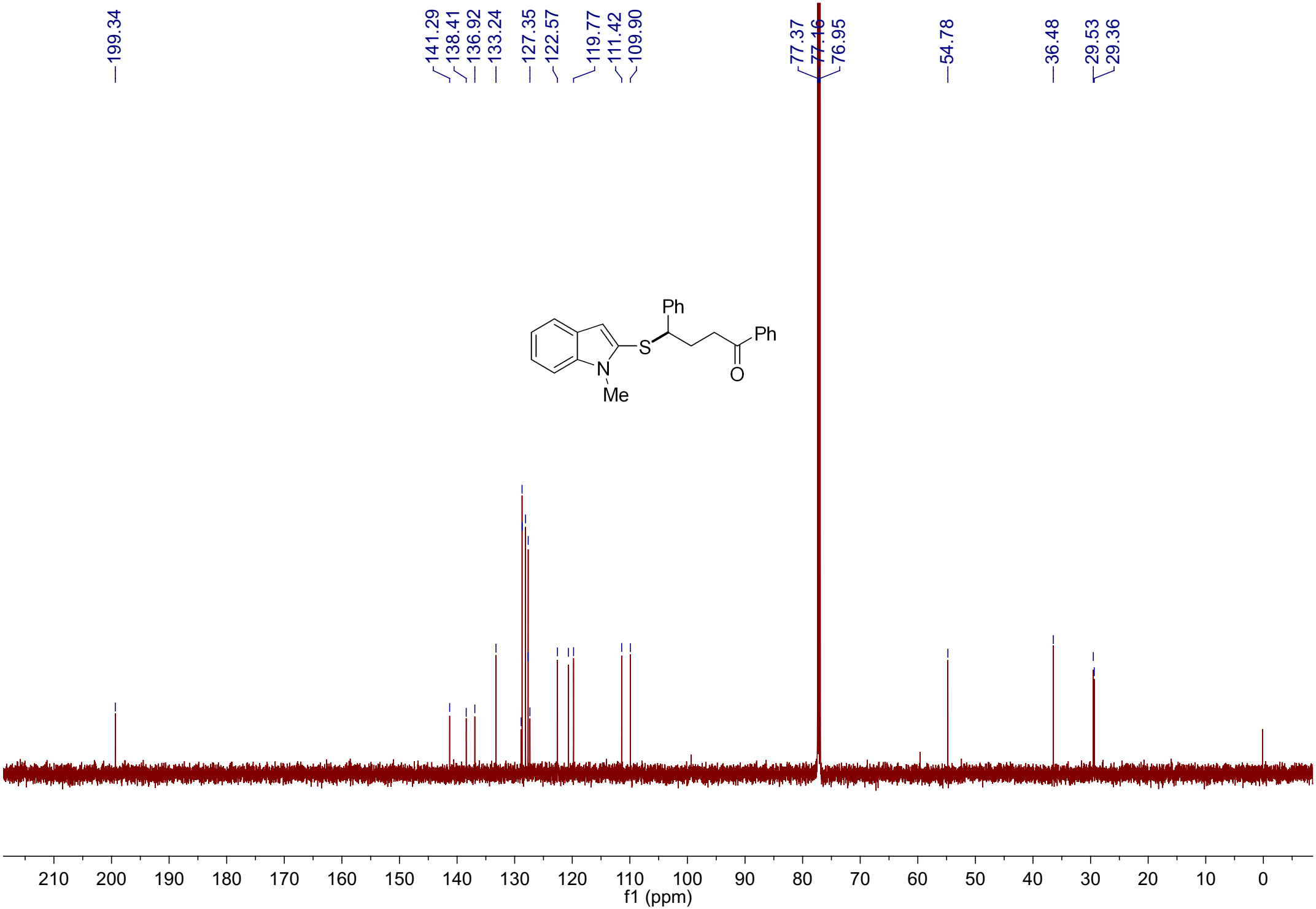
f1 (ppm)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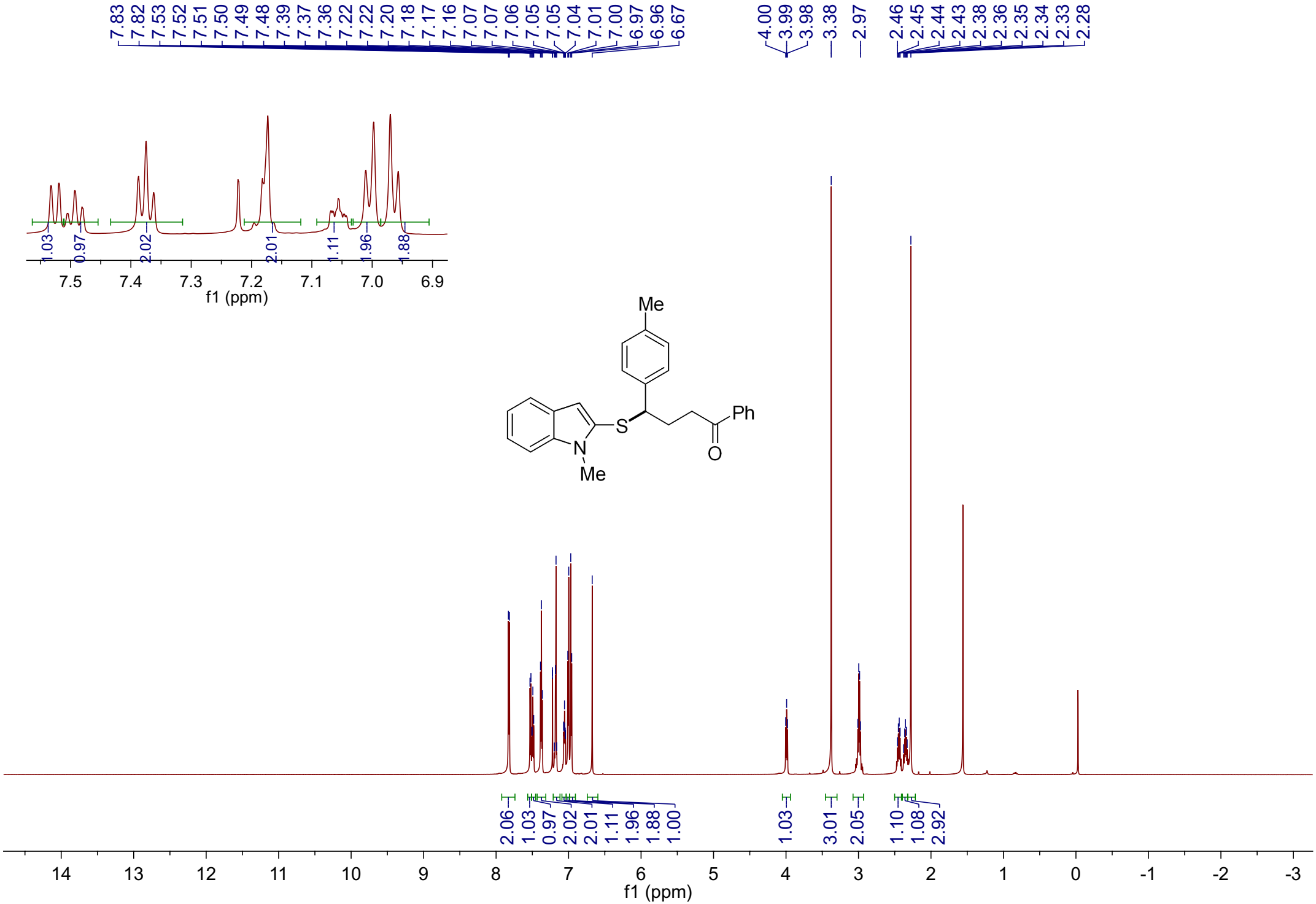
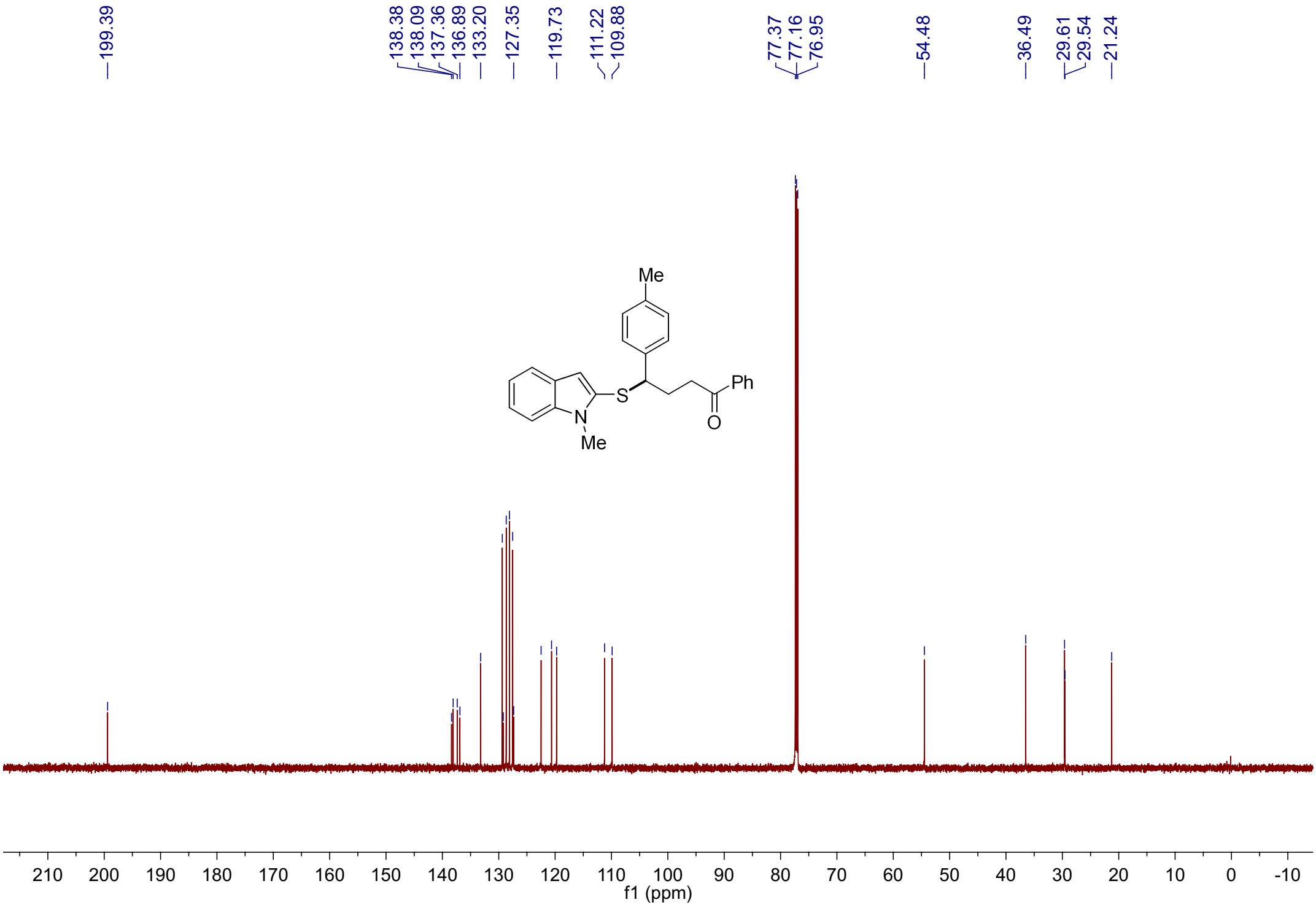
f1 (ppm)


7.83 7.82 7.53 7.52 7.51 7.50 7.49 7.48 7.39 7.37 7.36 7.22 7.22 7.20 7.18 7.17 7.16 7.07 7.07 7.06 7.05 7.05 7.04 7.01 7.00 6.97 6.96 6.67
4.00 3.99 3.98 3.38 2.97 2.46 2.45 2.44 2.43 2.38 2.36 2.35 2.34 2.33 2.28
1.03 0.97 2.02 2.01 1.11 1.96 1.88
7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
Me
Ph
S
N
Me
O
2.06 1.03 0.97 2.02 2.01 1.11 1.96 1.88 1.00 1.03 3.01 2.05 1.10 1.08 2.92
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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119.73
111.22
109.88
77.37
77.16
76.95
54.48
36.49
29.61
29.54
21.24
Me
S
Ph
O
N
Me
210
200
190
180
170
160
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140
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120
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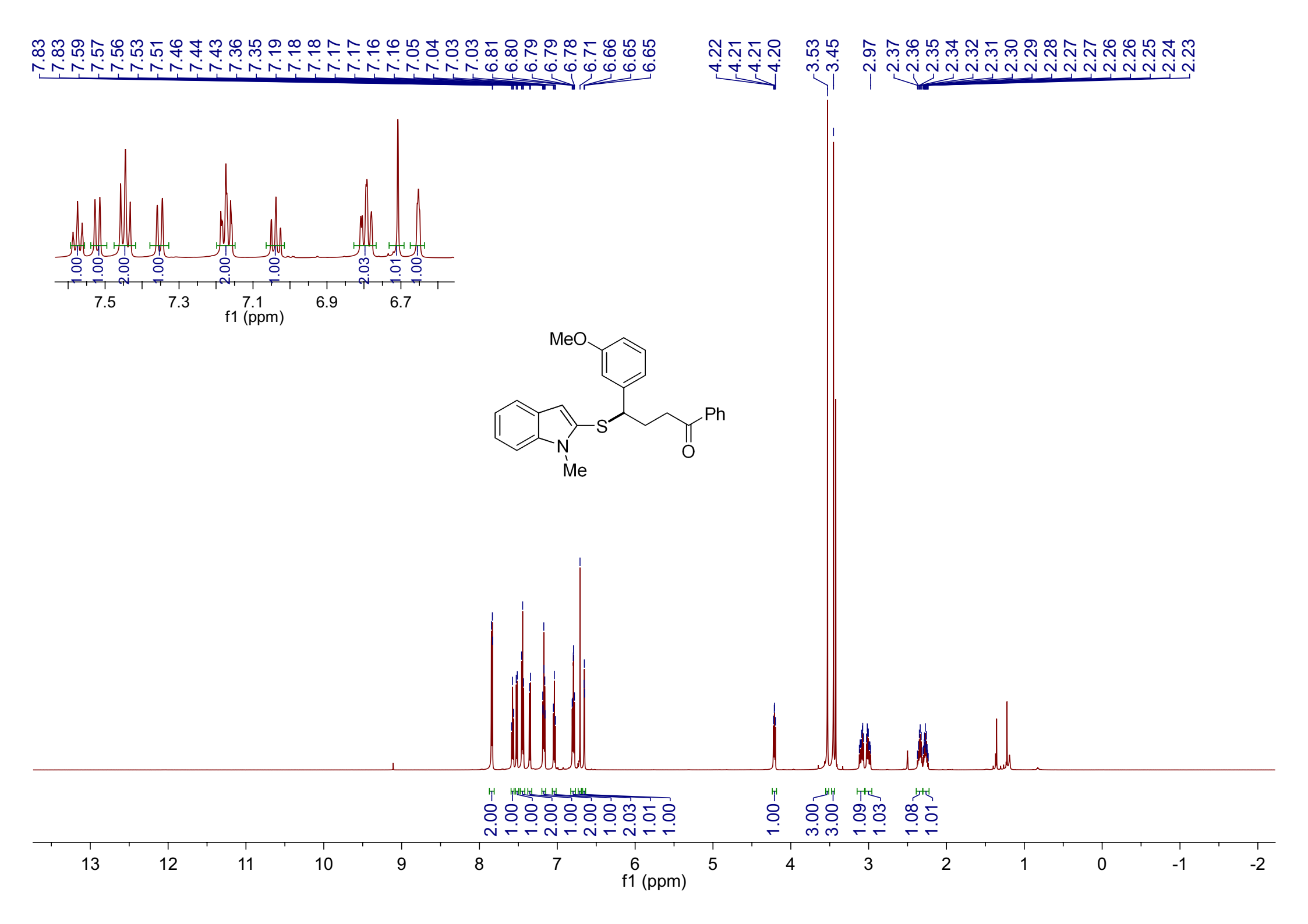
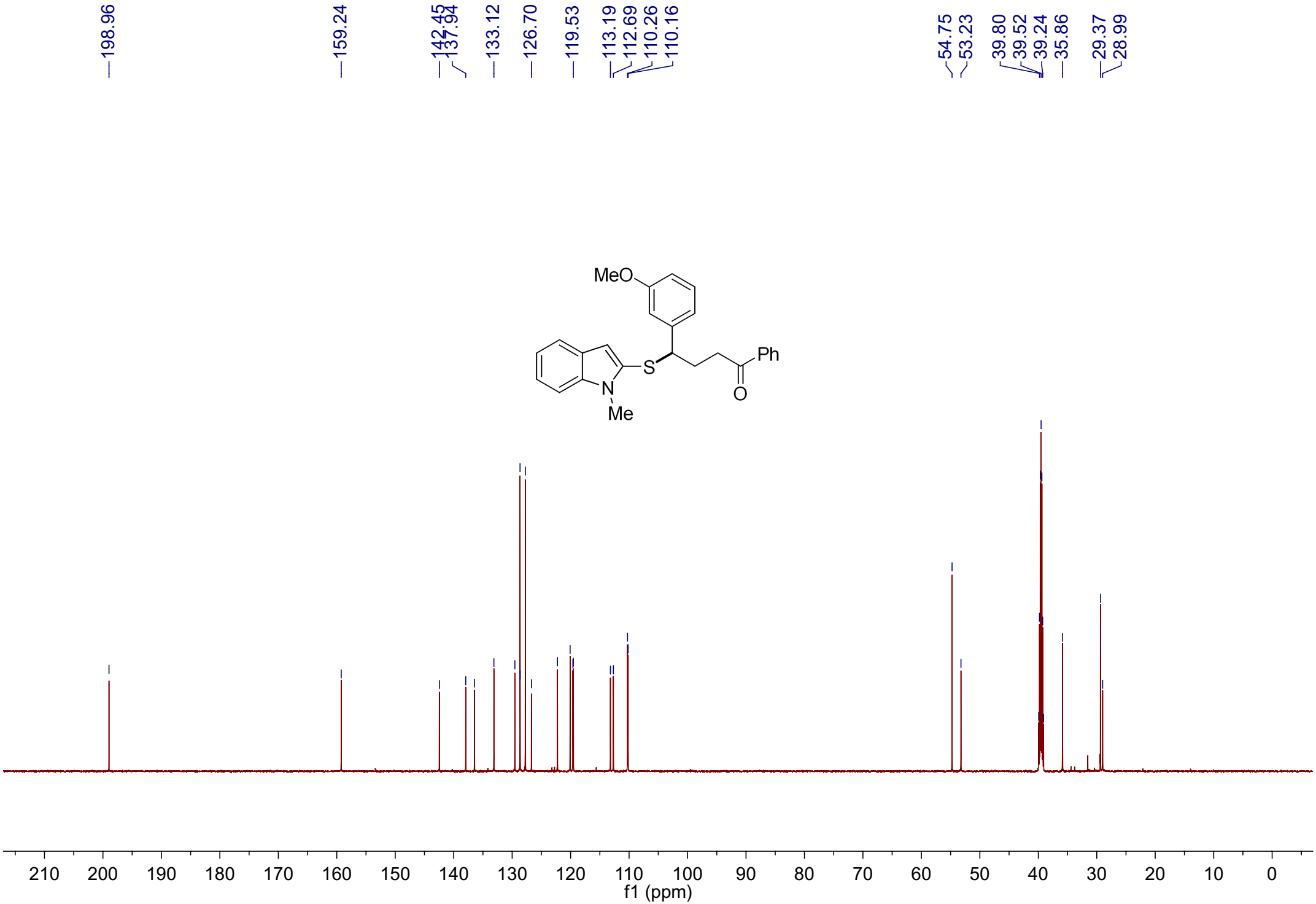
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.83 7.83 7.59 7.57 7.56 7.53 7.51 7.46 7.44 7.43 7.36 7.35 7.19 7.18 7.18 7.17 7.17 7.16 7.16 7.05 7.04 7.03 7.03 6.81 6.80 6.79 6.79 6.78 6.71 6.66 6.65 6.65
4.22 4.21 4.21 4.20
3.53 3.45
2.97
2.37 2.36 2.35 2.34 2.32 2.31 2.30 2.29 2.28 2.27 2.27 2.26 2.26 2.25 2.24 2.23
1.00 1.00 2.00 1.00 2.00 1.00 2.03 1.01 1.00
7.5 7.3 7.1 6.9 6.7
f1 (ppm)
MeO
Ph
S
N
Me
O
2.00 1.00 1.00 2.00 1.00 2.00 1.00 2.03 1.01 1.00
1.00
3.00 3.00
1.09 1.03
1.08 1.01
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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133.12
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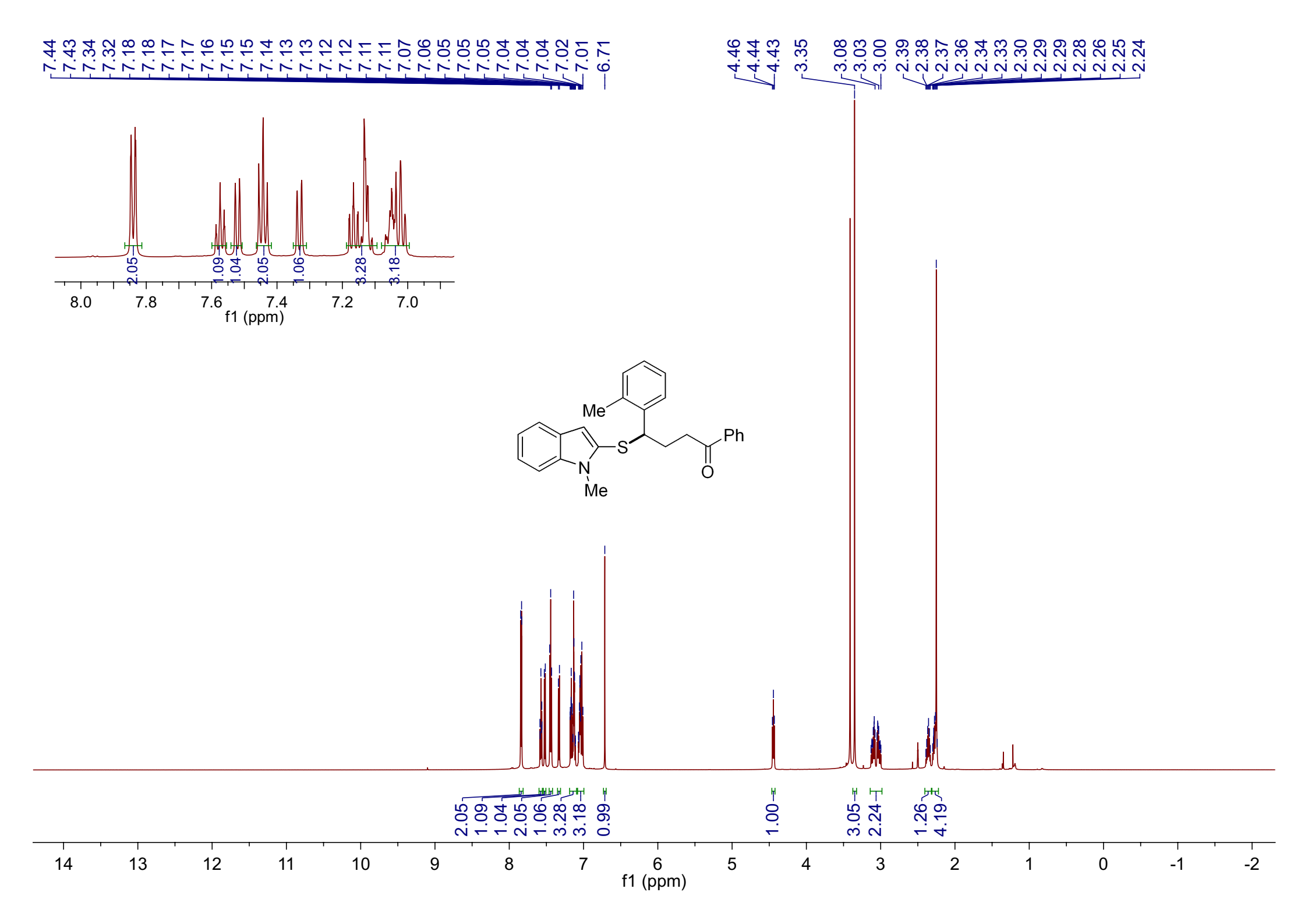
113.19
112.69
110.26
110.16
54.75
53.23
39.80
39.52
39.24
35.86
29.37
28.99
MeO
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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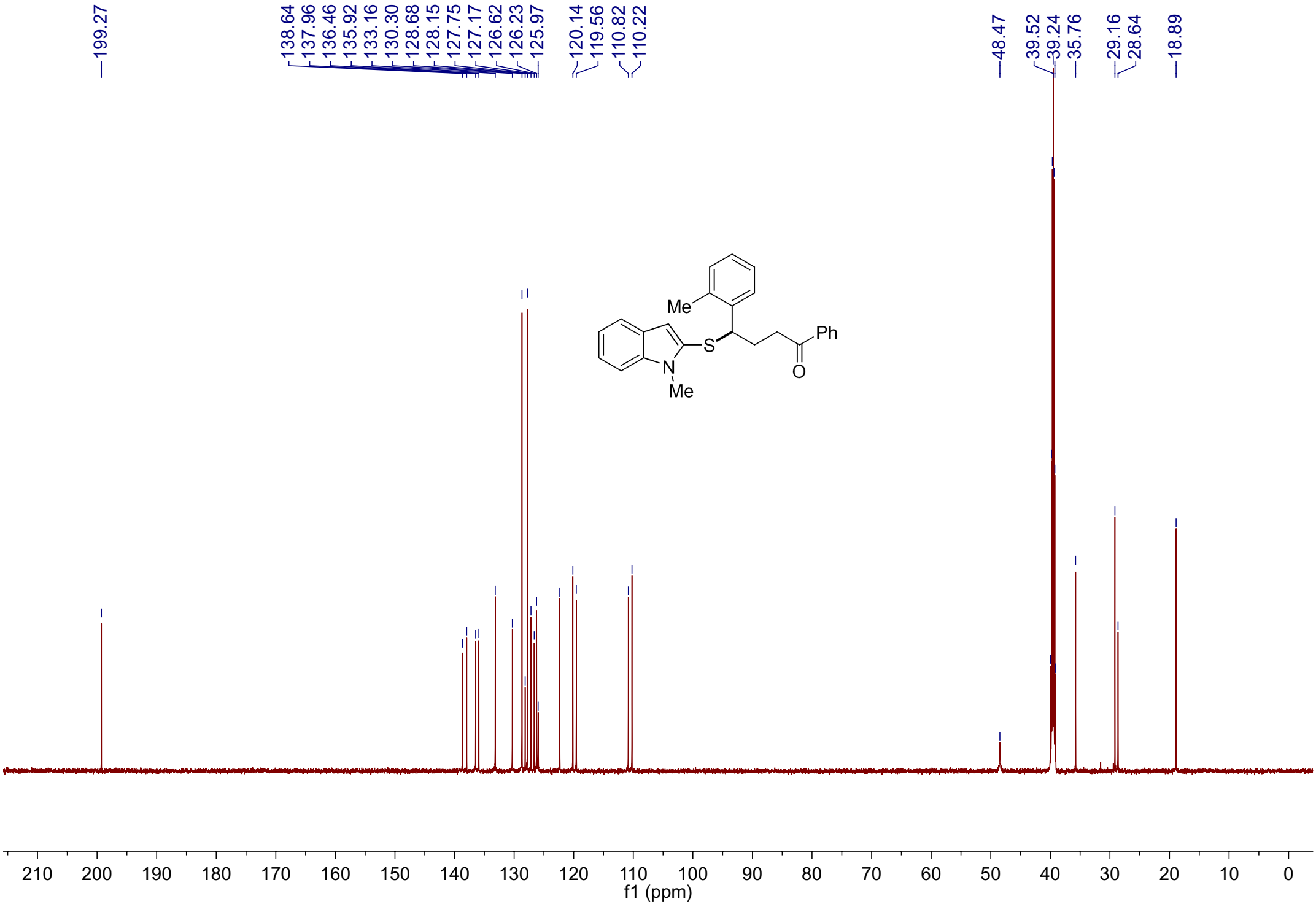
4.46 4.44 4.43 3.35 3.08 3.03 3.00 2.39 2.38 2.37 2.36 2.34 2.33 2.30 2.29 2.29 2.28 2.26 2.25 2.24
2.05 1.09 1.04 2.05 1.06 3.28 3.18
8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
Me
Ph
S
N
O
Me
2.05 1.09 1.04 2.05 1.06 3.28 3.18 0.99 1.00 3.05 2.24 1.26 4.19
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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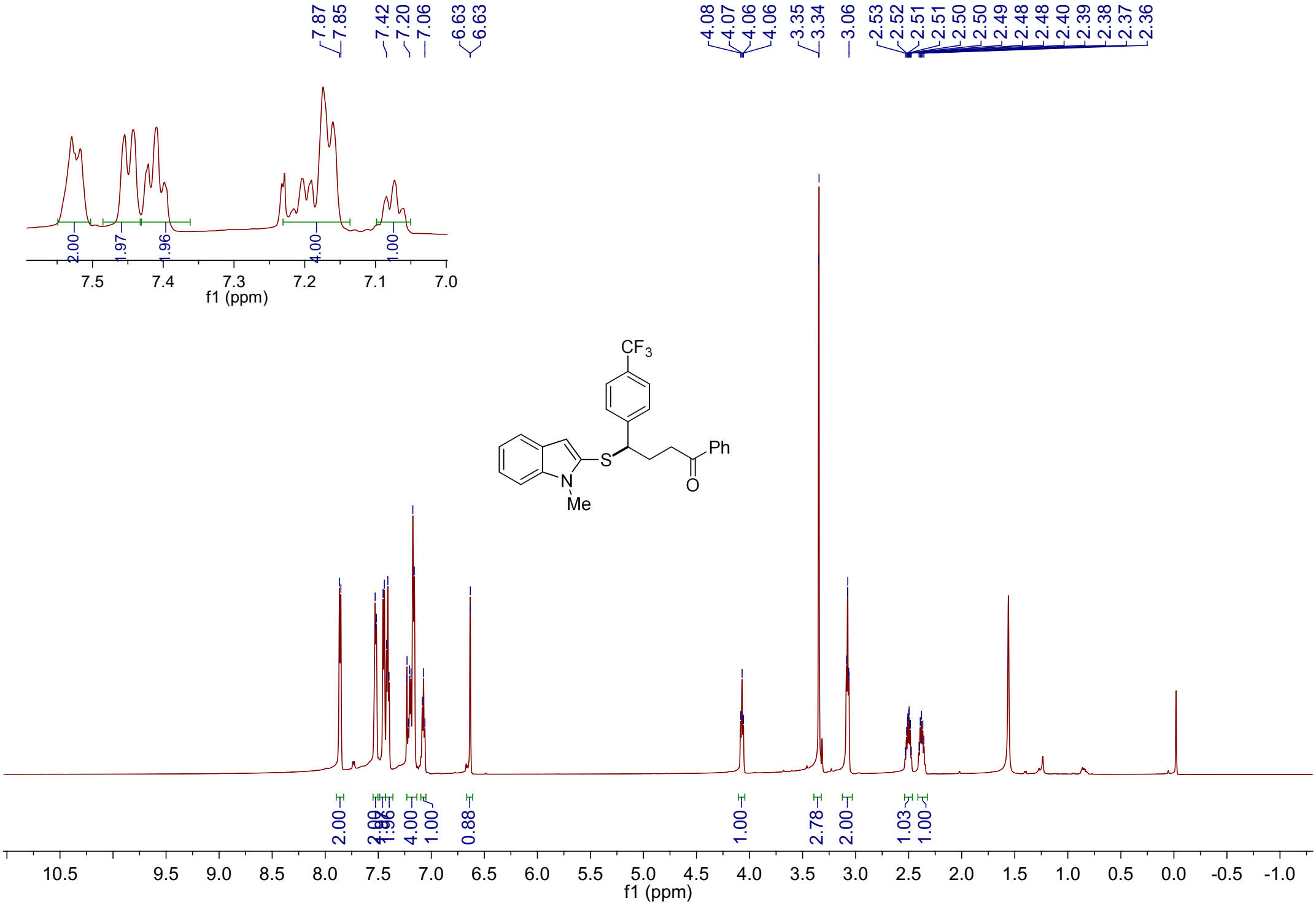
128.68
128.15
127.75
127.17
126.62
126.23
125.97
120.14
119.56
110.82
110.22
48.47
39.52
39.24
35.76
29.16
28.64
18.89
Me
S
Ph
O
N
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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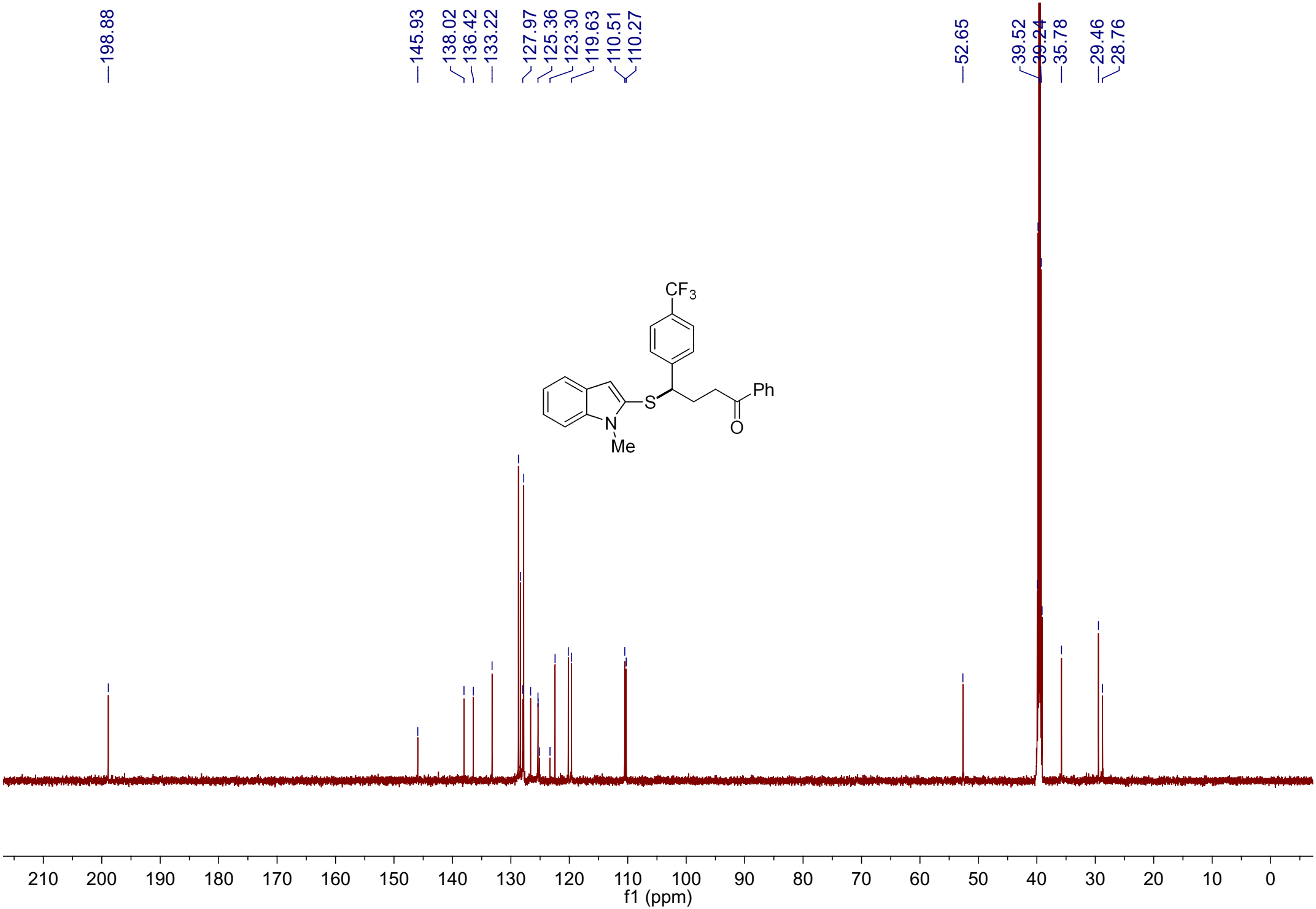
7.85
7.42
7.20
7.06
6.63
6.63
4.08
4.07
4.06
4.06
3.35
3.34
3.06
2.53
2.52
2.51
2.51
2.50
2.50
2.49
2.48
2.48
2.40
2.39
2.38
2.37
2.36
2.00
1.97
1.96
4.00
1.00
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
CF3
Ph
S
N
Me
O
2.00
2.00
1.96
4.00
1.00
0.88
1.00
2.78
2.00
1.03
1.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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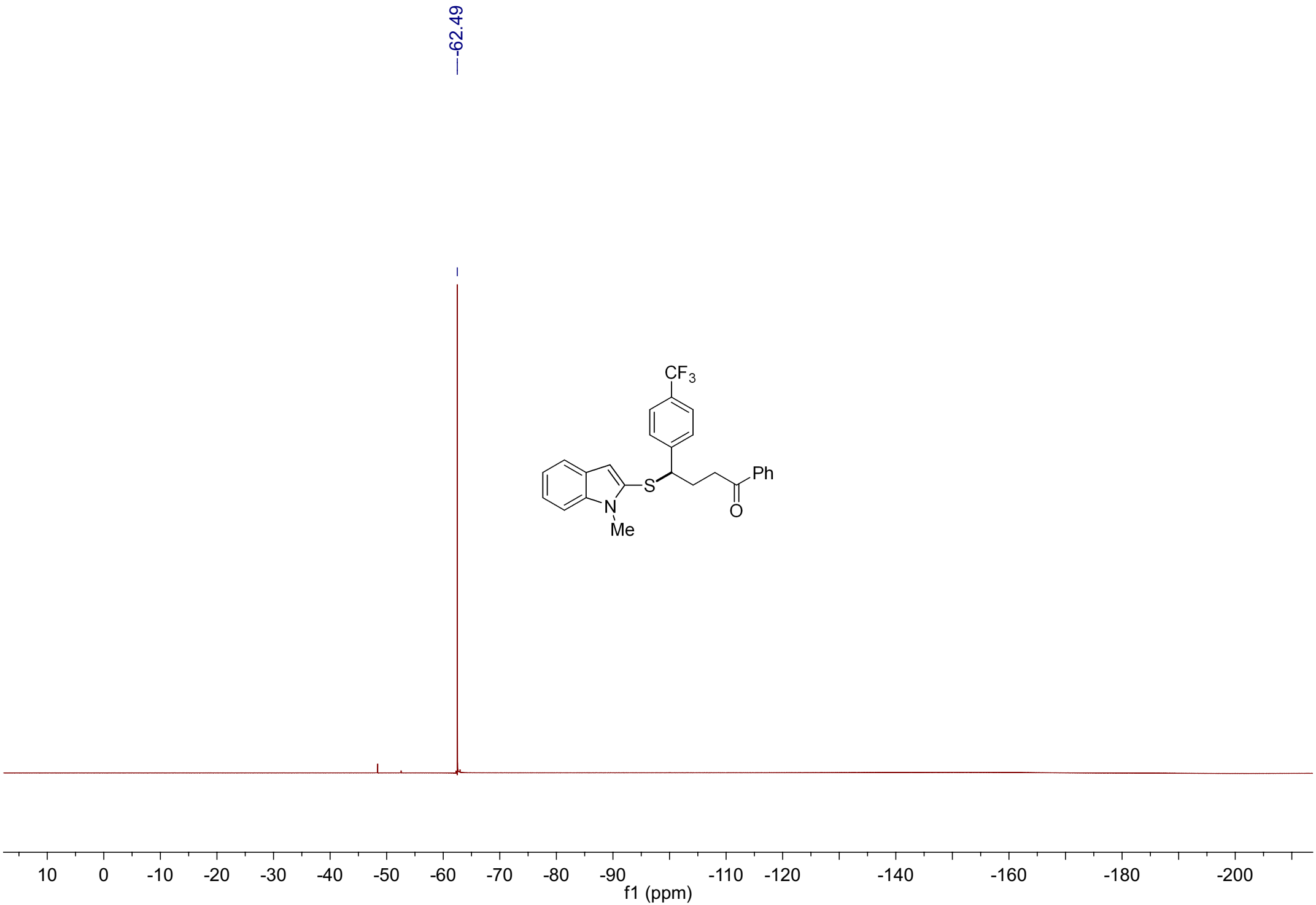
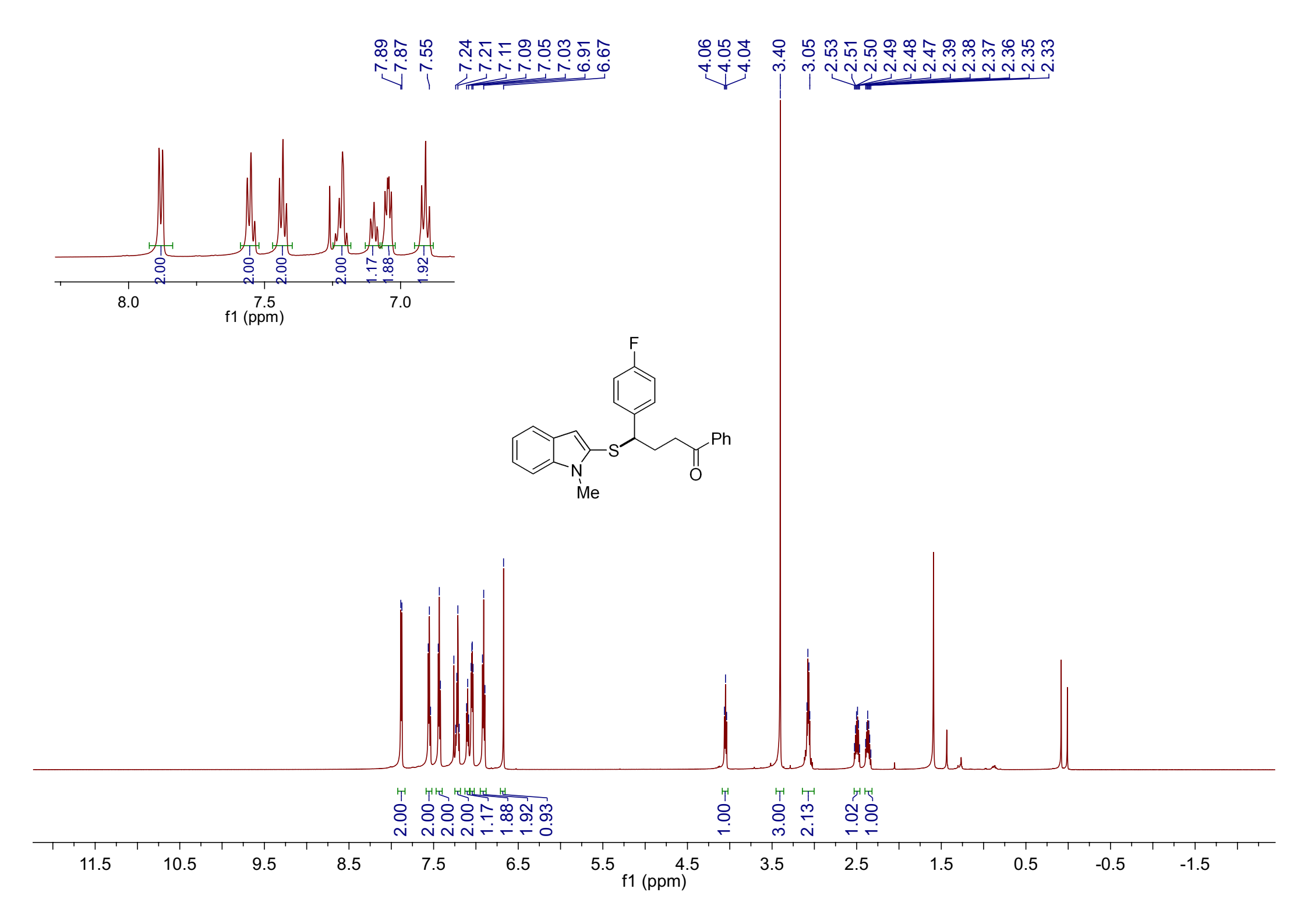
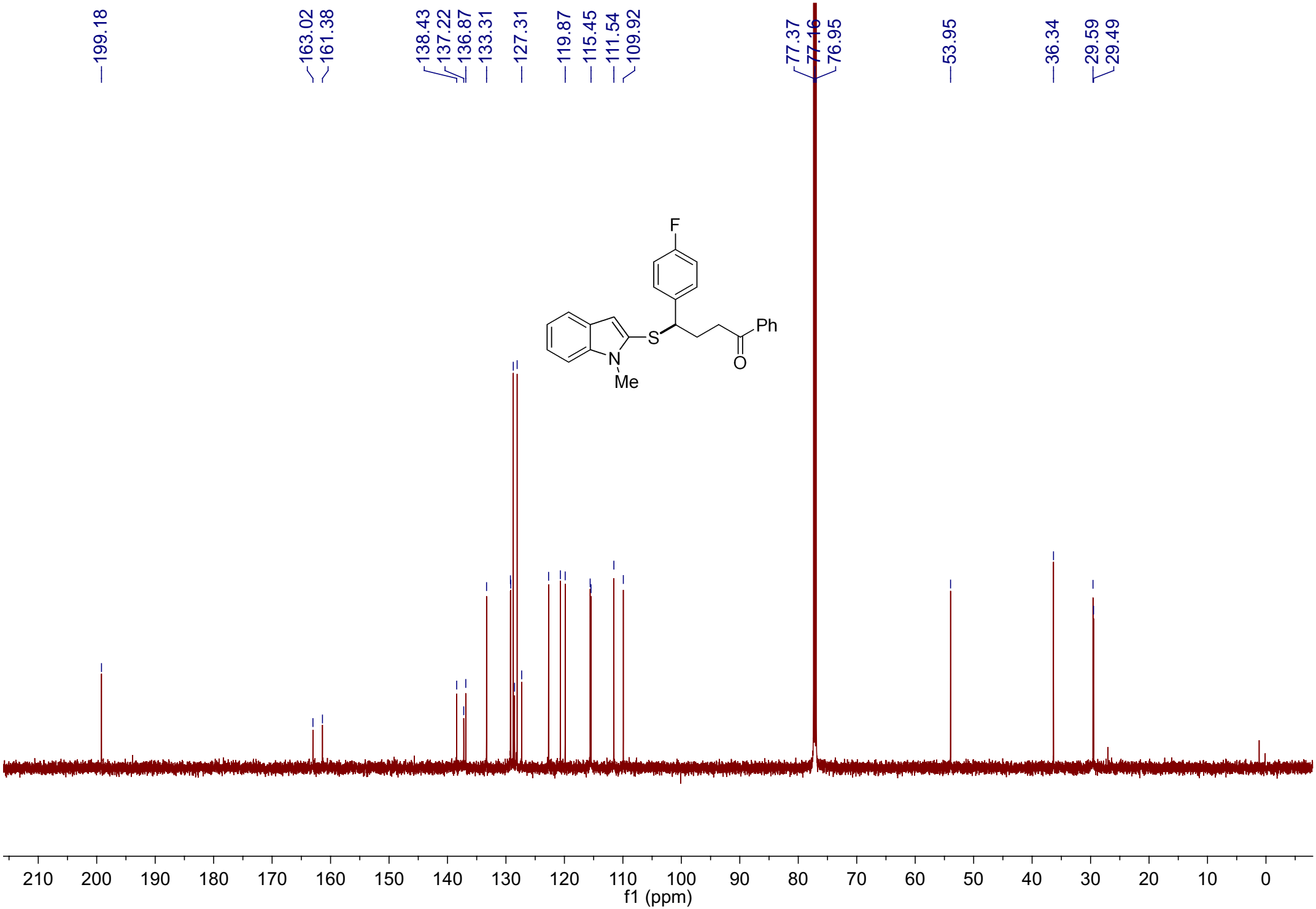
138.02
136.42
133.22
127.97
125.36
123.30
119.63
110.51
110.27
52.65
39.52
39.24
35.78
29.46
28.76
CF3
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.49
CF3
Ph
S
O
N
Me
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-120
-140
-160
-180
-200
f1 (ppm)


7.89
7.87
7.55
7.24
7.21
7.11
7.09
7.05
7.03
6.91
6.67
4.06
4.05
4.04
3.40
3.05
2.53
2.51
2.50
2.49
2.48
2.47
2.39
2.38
2.37
2.36
2.35
2.33
2.00
2.00
2.00
2.00
1.17
1.88
1.92
8.0
7.5
7.0
f1 (ppm)
F
S
N
Me
Ph
O
2.00
2.00
2.00
2.00
1.17
1.88
1.92
0.93
1.00
3.00
2.13
1.02
1.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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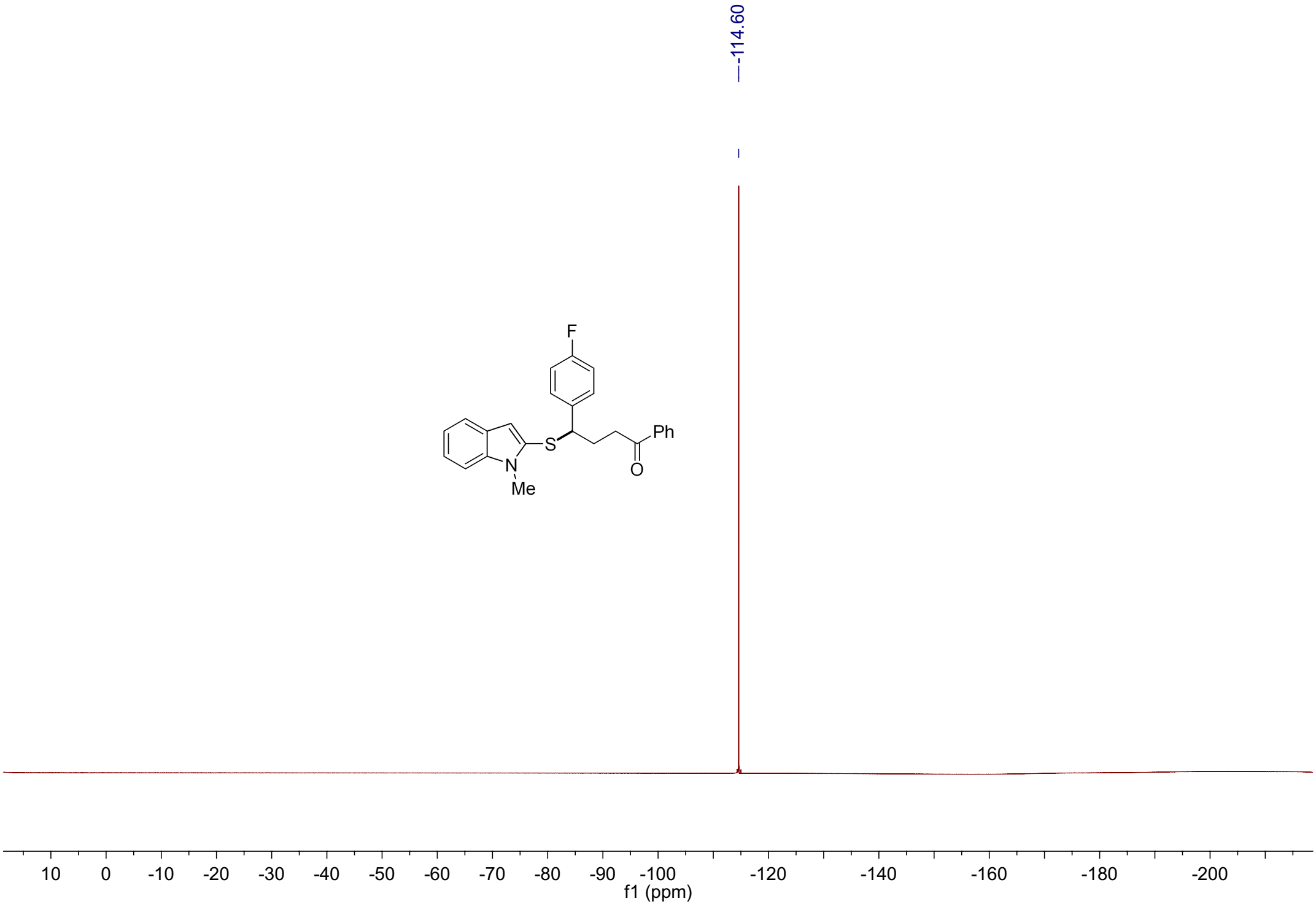
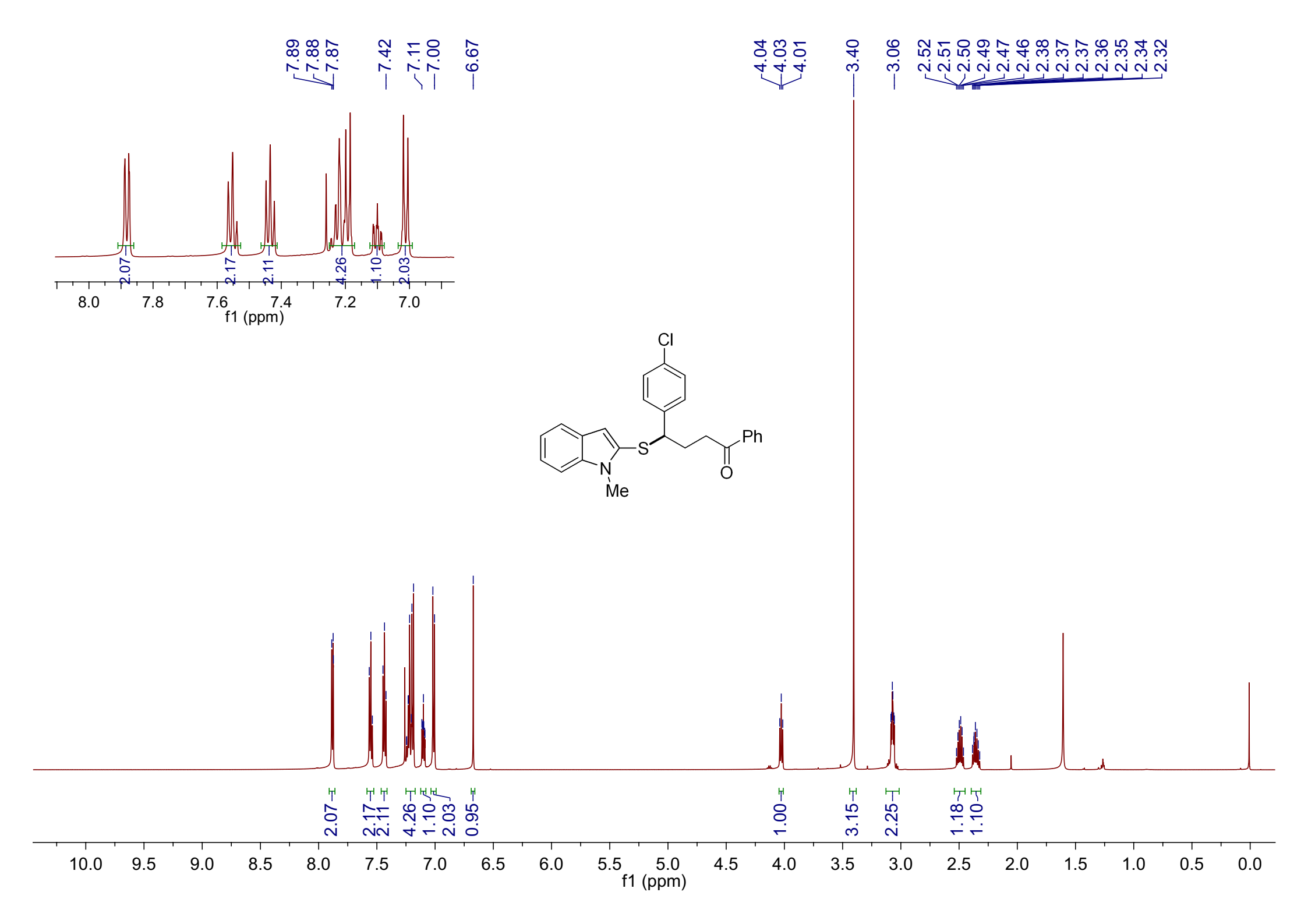
136.87
133.31
127.31
119.87
115.45
111.54
109.92
77.37
77.16
76.95
53.95
36.34
29.59
29.49
F
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-114.60
F
S
N
Me
Ph
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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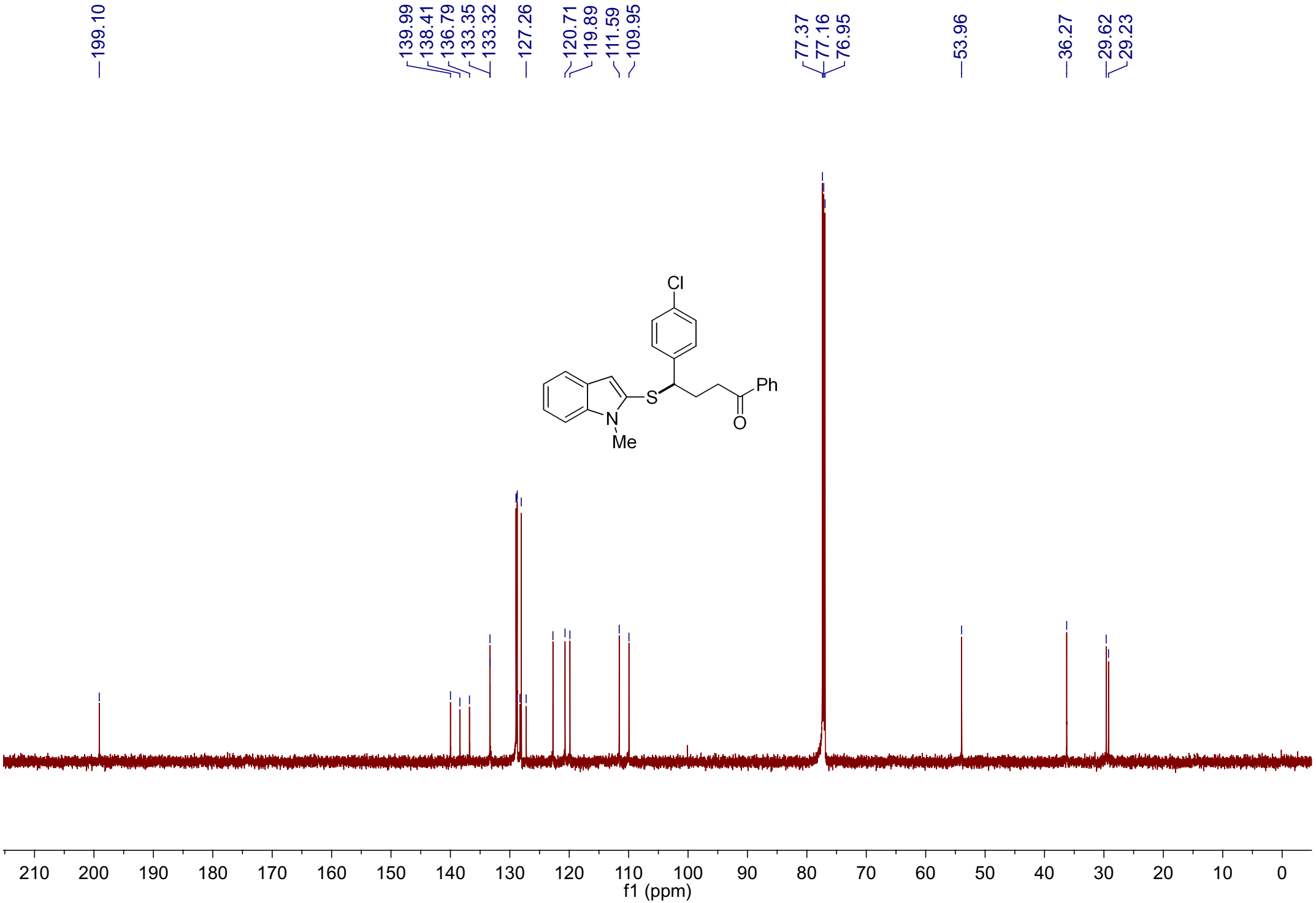
7.88
7.87
7.42
7.11
7.00
6.67
4.04
4.03
4.01
3.40
3.06
2.52
2.51
2.50
2.49
2.47
2.46
2.38
2.37
2.37
2.36
2.35
2.34
2.32
2.07
2.17
2.11
4.26
1.10
2.03
f1 (ppm)
Cl
Ph
S
N
Me
O
0.95
1.00
3.15
2.25
1.18
1.10
f1 (ppm)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120.71
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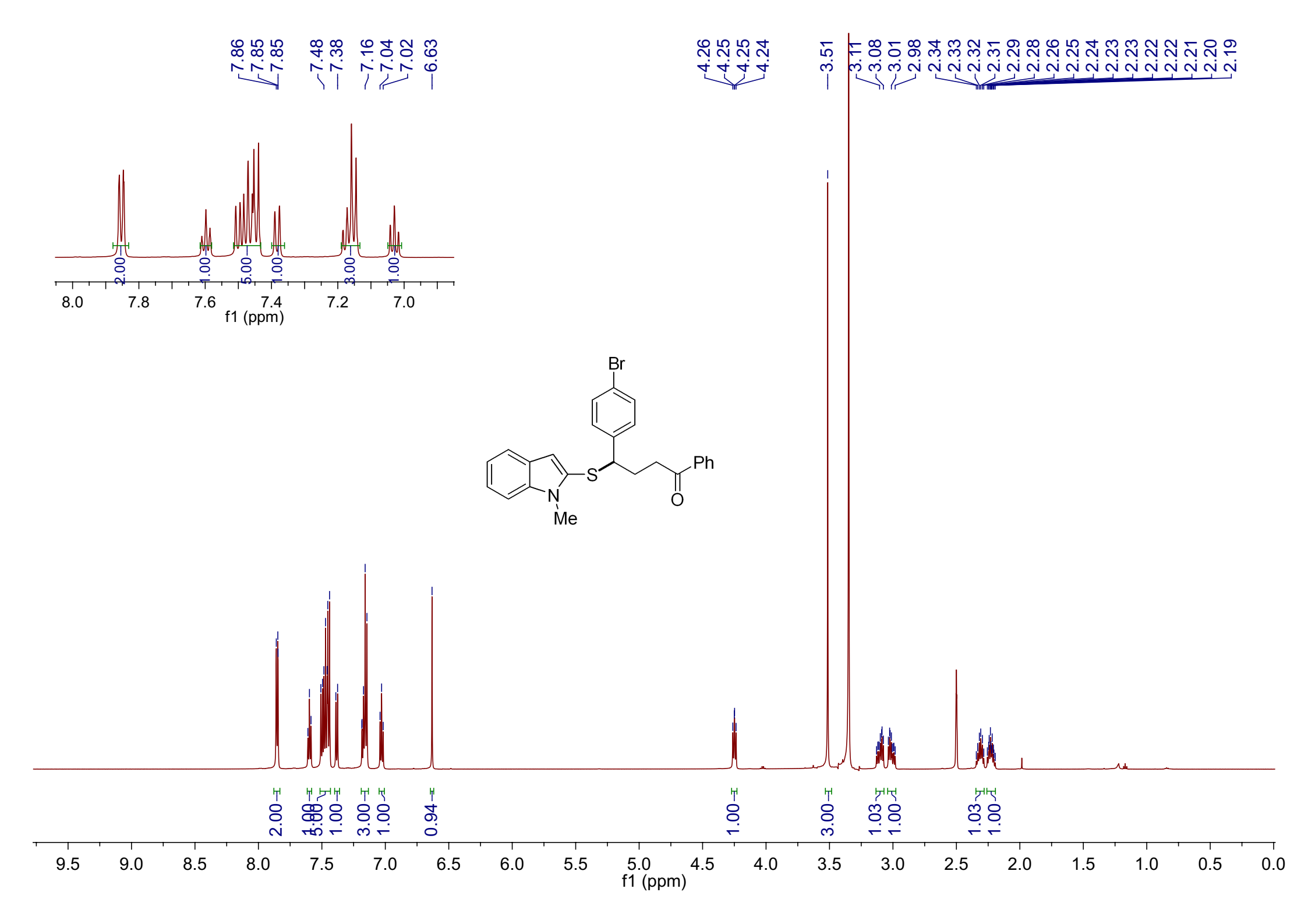
111.59
109.95
77.37
77.16
76.95
53.96
36.27
29.62
29.23
Cl
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.85
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7.04
7.02
6.63
4.26
4.25
4.25
4.24
3.51
3.11
3.08
3.01
2.98
2.34
2.33
2.32
2.31
2.29
2.28
2.26
2.25
2.24
2.23
2.23
2.22
2.22
2.21
2.20
2.19
2.00
1.00
5.00
1.00
3.00
1.00
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
Br
Ph
S
N
Me
O
2.00
1.00
3.00
1.00
0.94
1.00
3.00
1.03
1.00
1.03
1.00
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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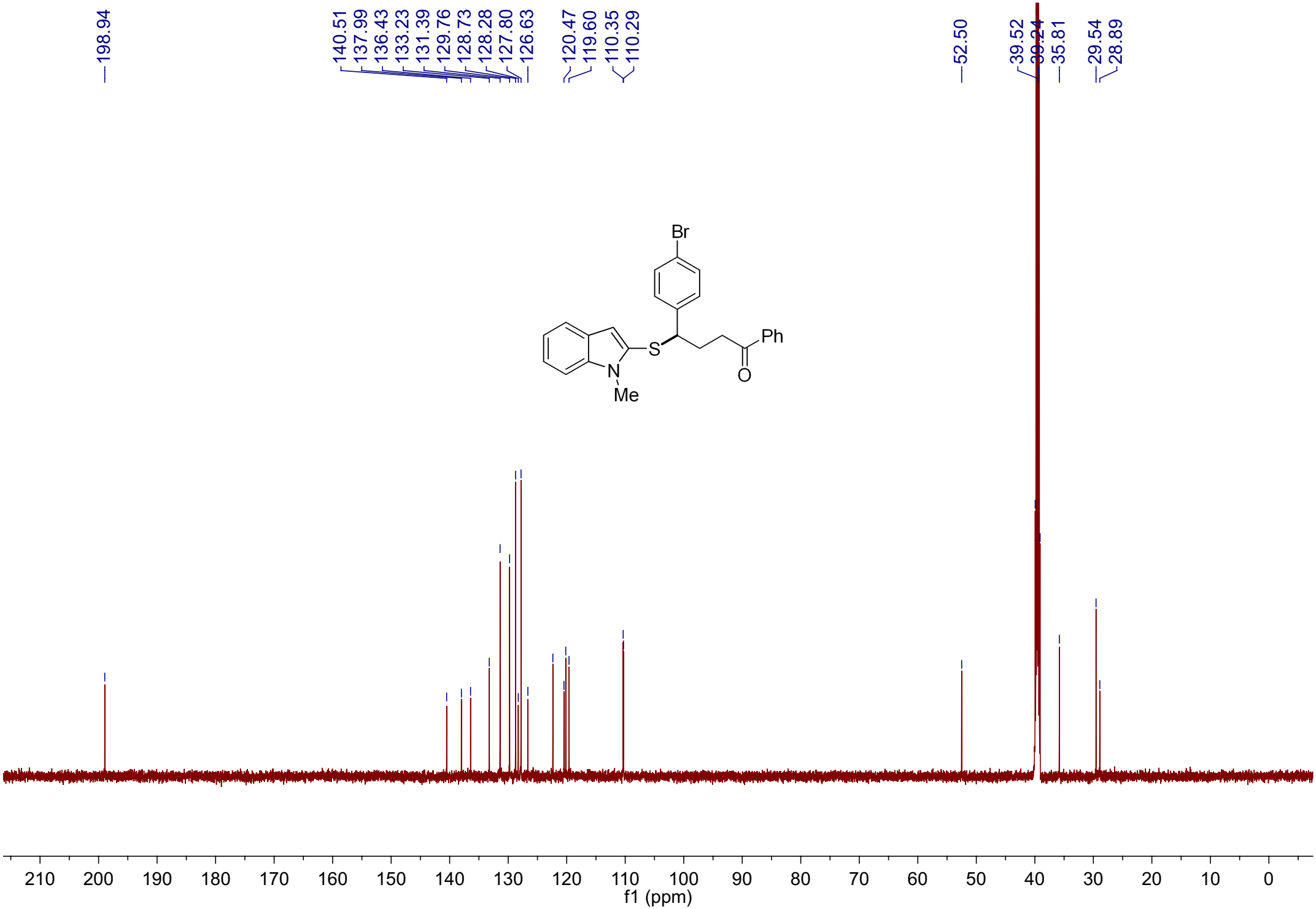
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.28
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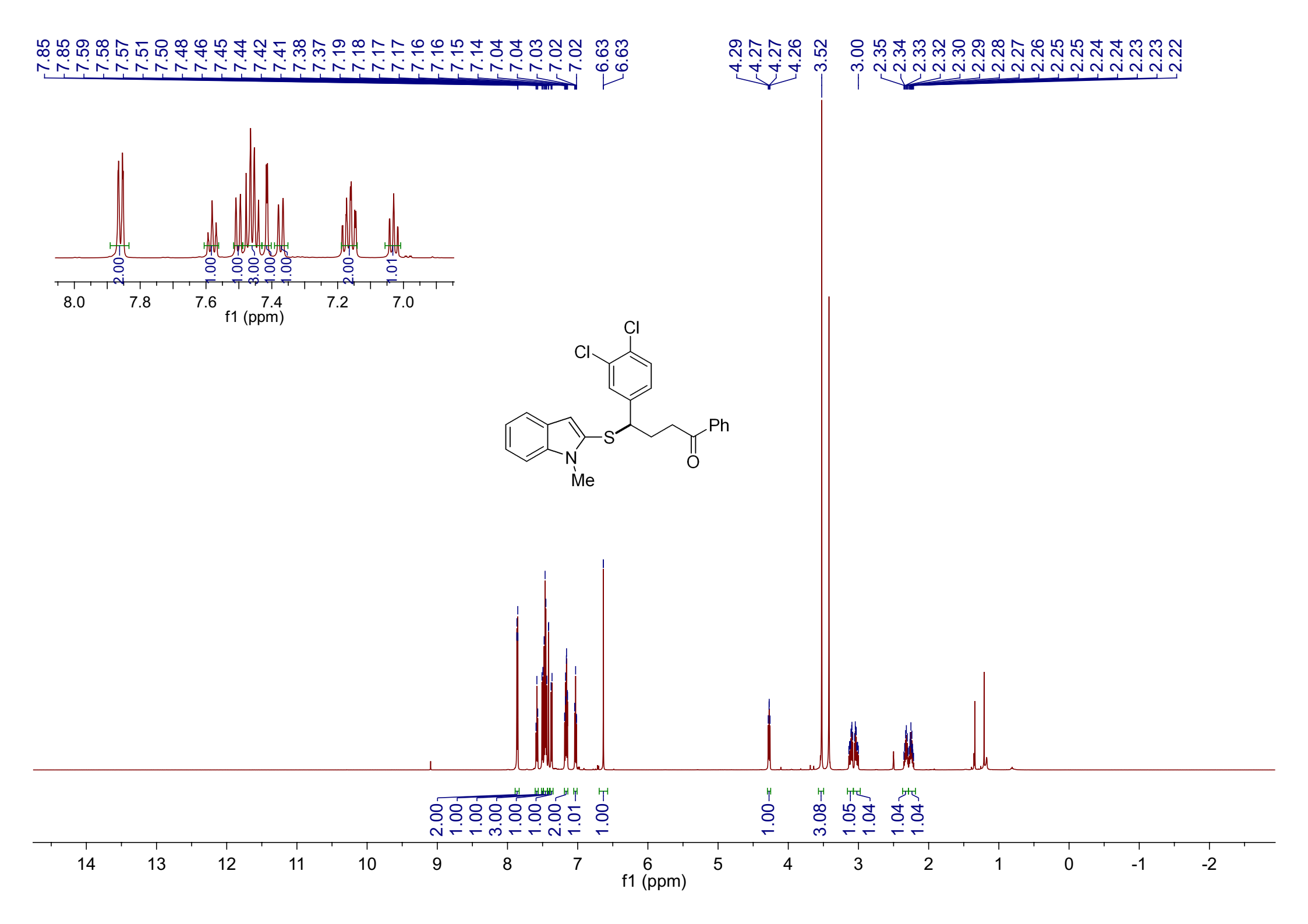
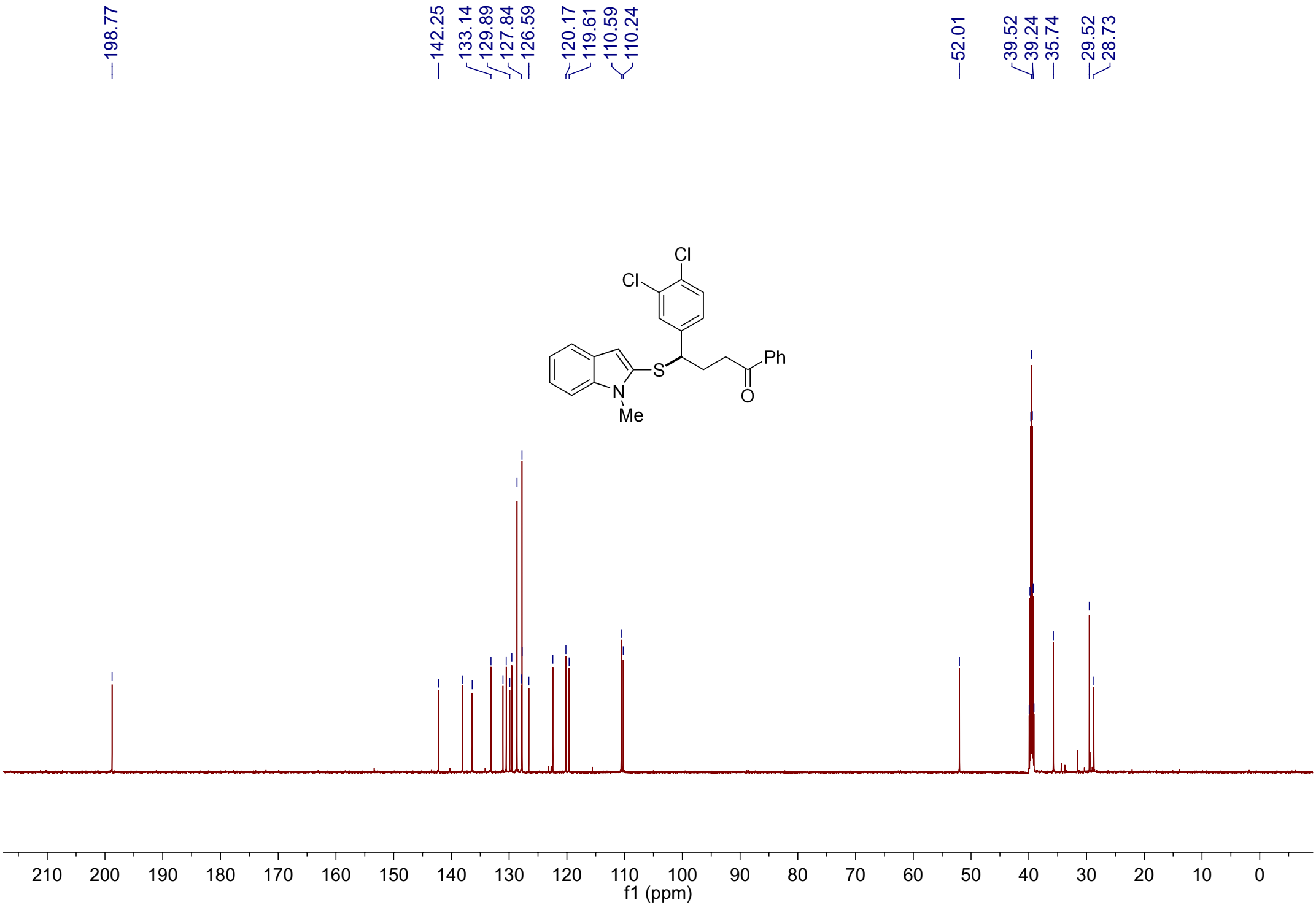
126.63
120.47
119.60
110.35
110.29
52.50
39.52
39.24
35.81
29.54
28.89
Br
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.85 7.85 7.59 7.58 7.57 7.51 7.50 7.48 7.46 7.45 7.44 7.42 7.41 7.38 7.37 7.19 7.18 7.17 7.17 7.16 7.16 7.15 7.14 7.04 7.04 7.03 7.02 7.02 6.63 6.63
4.29 4.27 4.27 4.26 3.52 3.00 2.35 2.34 2.33 2.32 2.30 2.29 2.28 2.27 2.26 2.25 2.25 2.24 2.24 2.23 2.23 2.22
2.00 1.00 1.00 3.00 1.00 1.00 2.00 1.01
8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
Cl
Cl
S
N
Me
Ph
O
2.00 1.00 1.00 3.00 1.00 1.00 2.00 1.01 1.00 1.00 3.08 1.05 1.04 1.04 1.04
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)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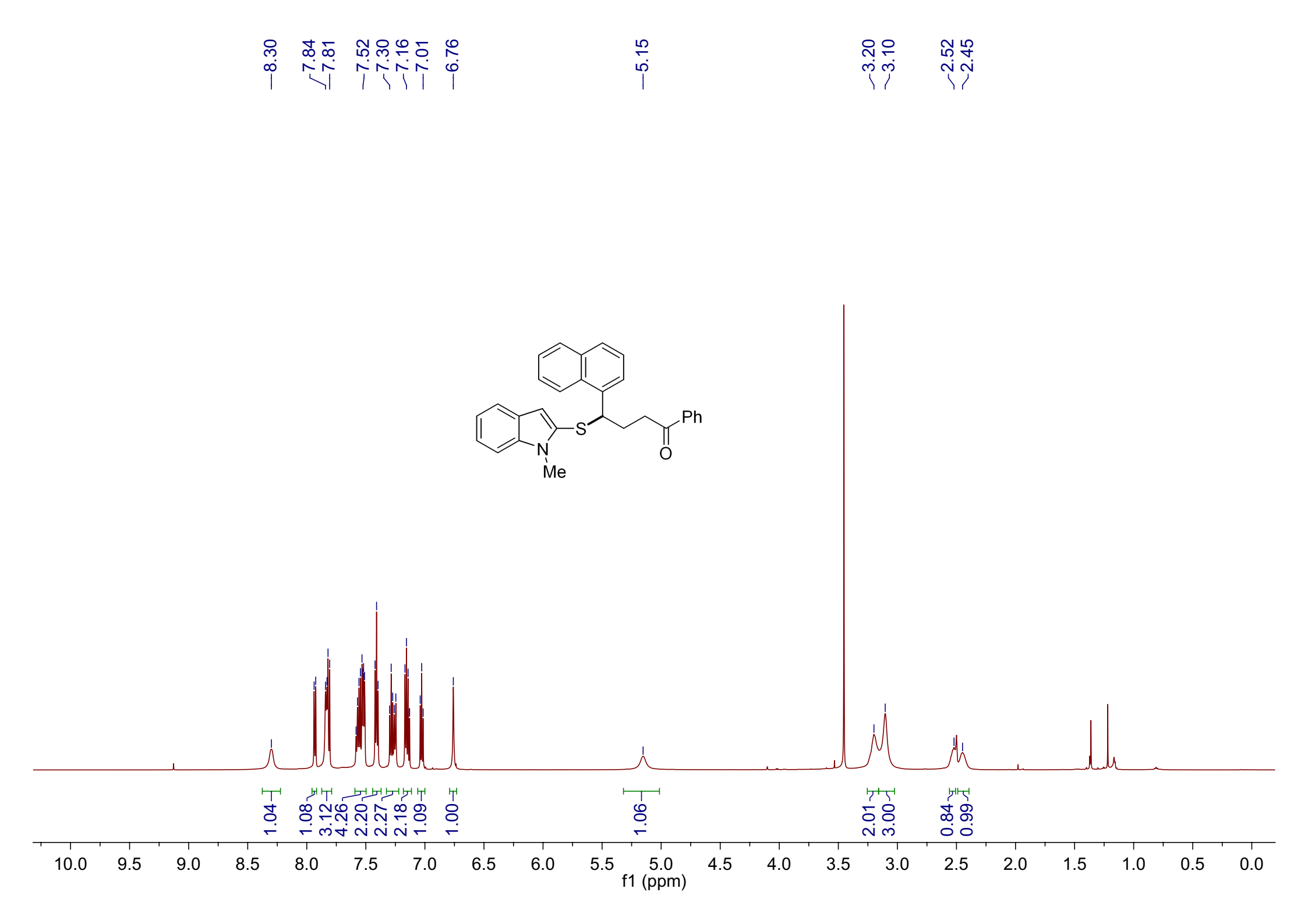
126.59
120.17
119.61
110.59
110.24
52.01
39.52
39.24
35.74
29.52
28.73
Cl
Cl
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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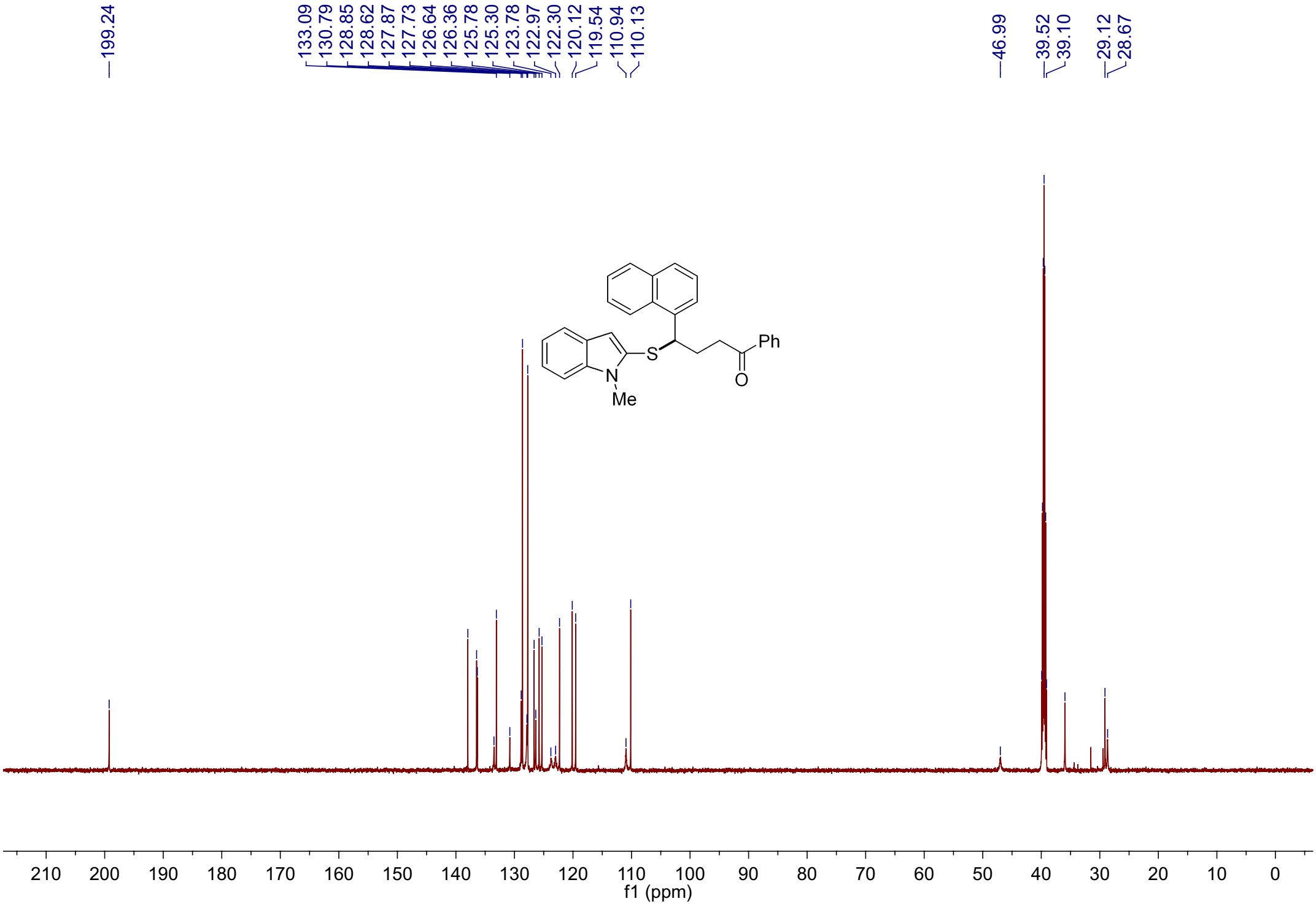
7.81
7.52
7.30
7.16
7.01
6.76
5.15
3.20
3.10
2.52
2.45
S
N
Me
Ph
O
1.04
1.08
3.12
4.26
2.20
2.27
2.18
1.09
1.00
1.06
2.01
3.00
0.84
0.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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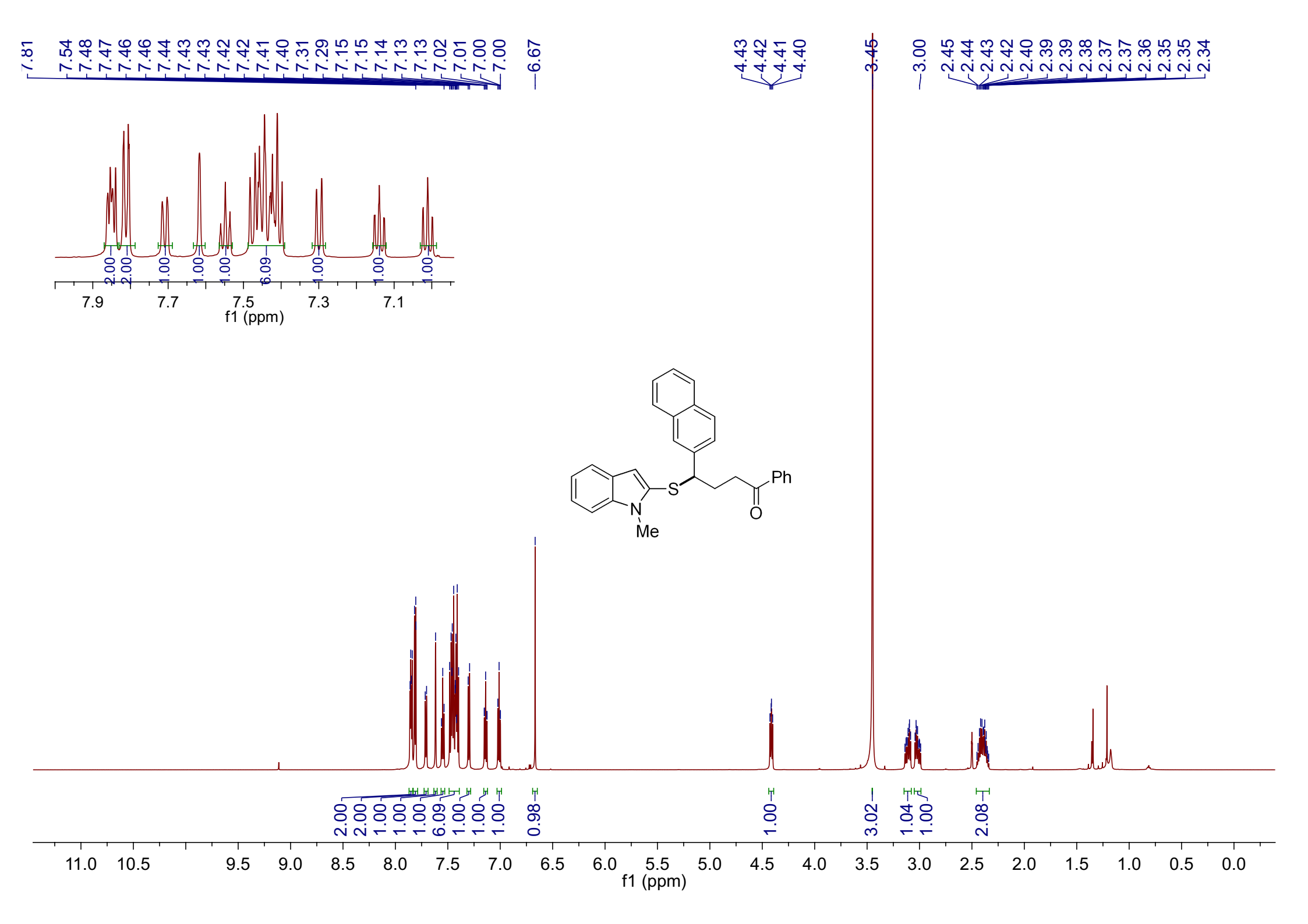
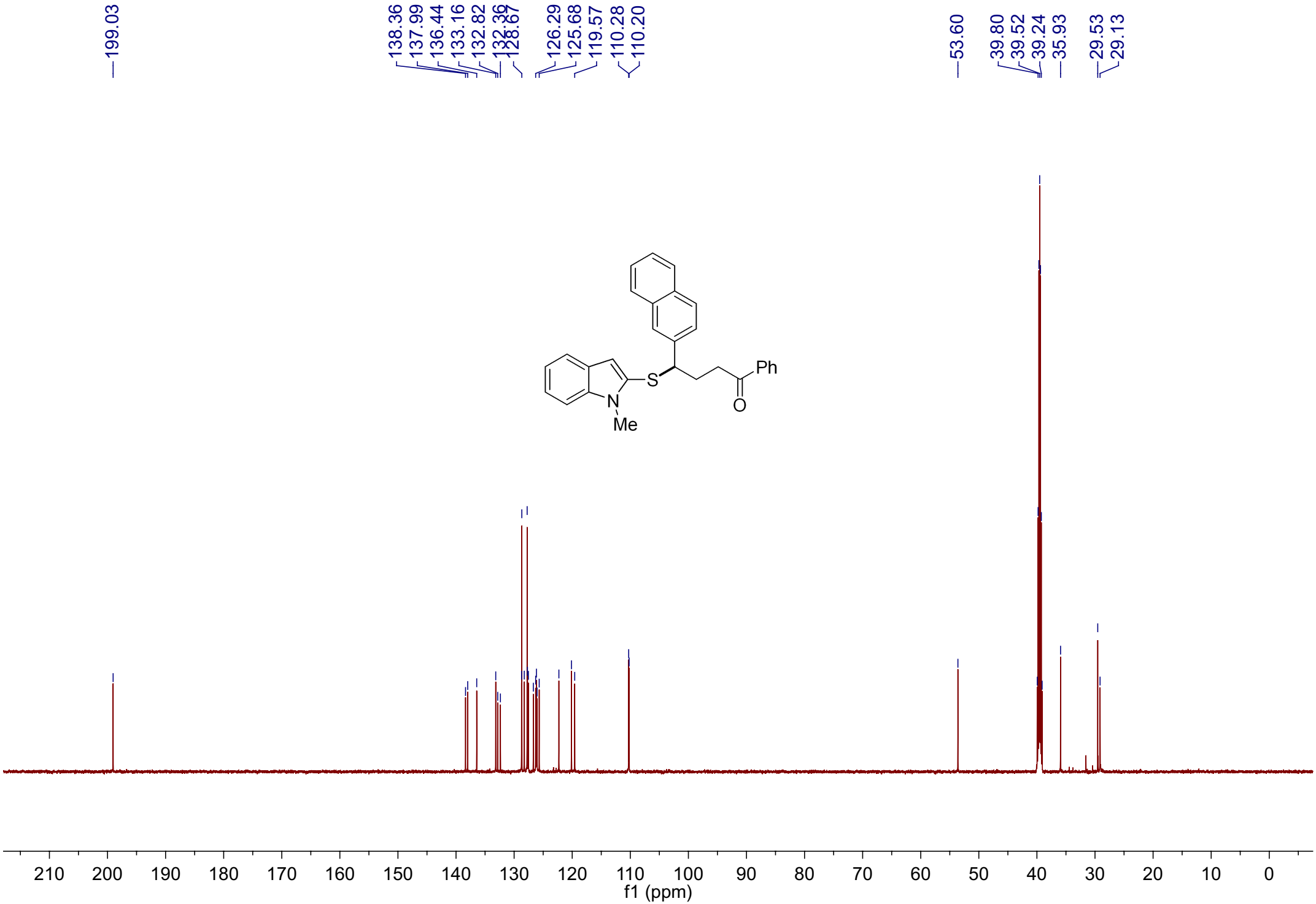
125.78
125.30
123.78
122.97
122.30
120.12
119.54
110.94
110.13
46.99
39.52
39.10
29.12
28.67
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.81 7.54 7.48 7.47 7.46 7.46 7.44 7.43 7.43 7.42 7.42 7.41 7.40 7.31 7.29 7.15 7.15 7.14 7.13 7.13 7.02 7.01 7.00 7.00 6.67
4.43 4.42 4.41 4.40 3.45 3.00 2.45 2.44 2.43 2.42 2.40 2.39 2.39 2.38 2.37 2.37 2.36 2.35 2.35 2.34
2.00 2.00 1.00 1.00 1.00 6.09 1.00 1.00 1.00
7.9 7.7 7.5 7.3 7.1
f1 (ppm)
Ph
S
N
Me
O
2.00 2.00 1.00 1.00 1.00 6.09 1.00 1.00 1.00 0.98 1.00 3.02 1.04 1.00 2.08
11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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136.44
133.16
132.82
132.36
128.67
126.29
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119.57
110.28
110.20
53.60
39.80
39.52
39.24
35.93
29.53
29.13
Ph
O
S
N
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
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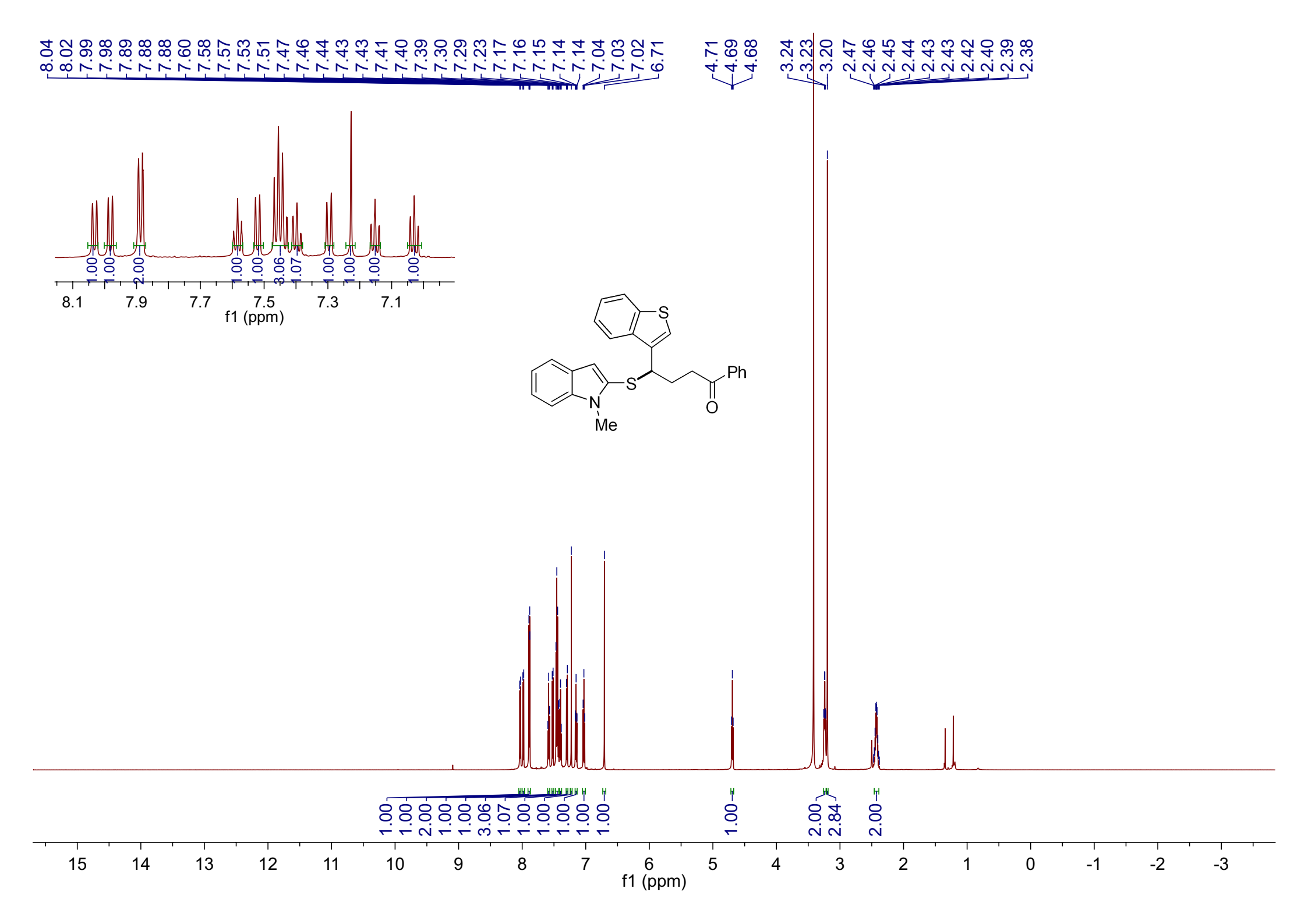
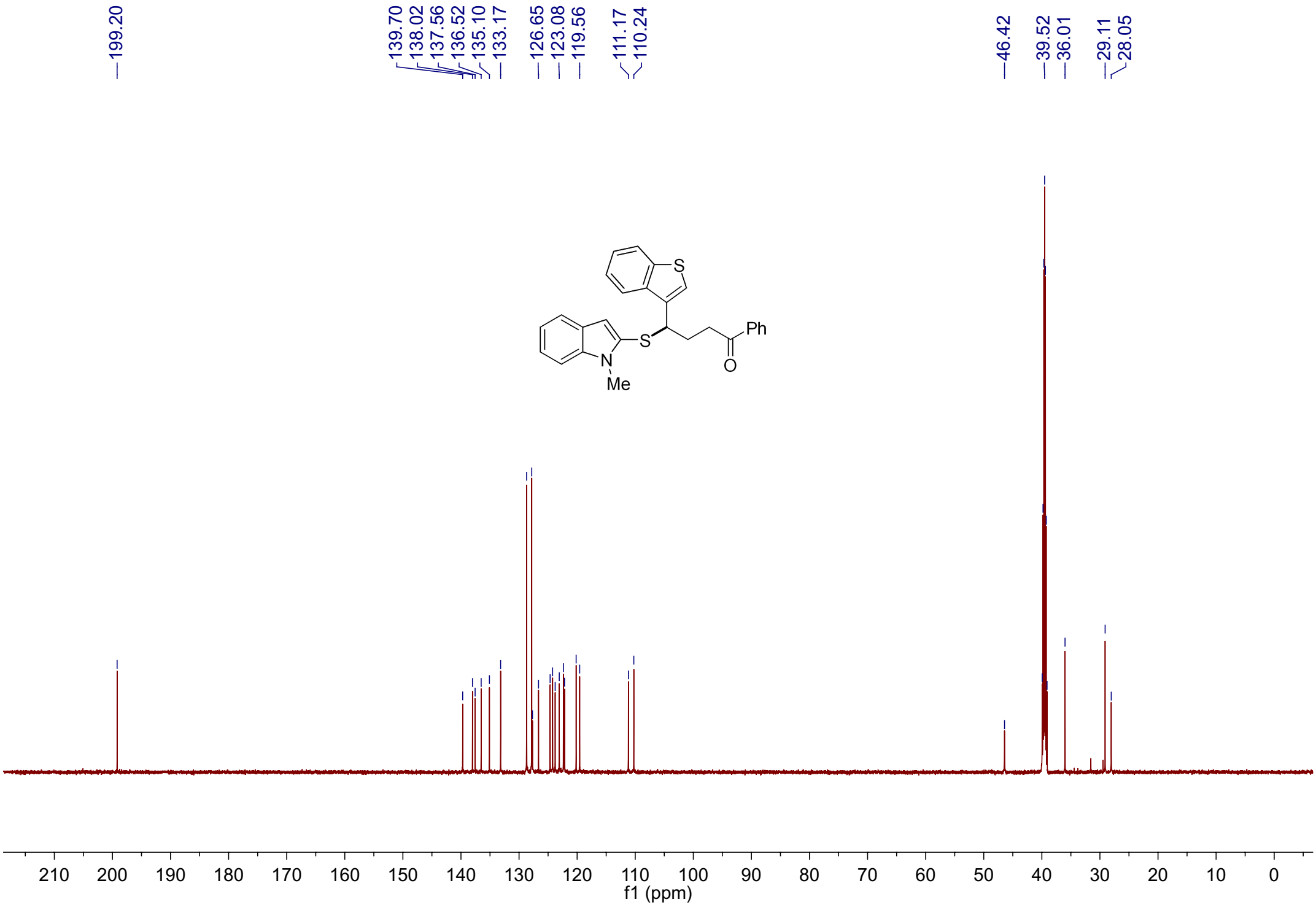
20
10
0
f1 (ppm)


8.04 8.02 7.99 7.98 7.89 7.88 7.88 7.60 7.58 7.57 7.53 7.51 7.47 7.46 7.44 7.43 7.43 7.41 7.40 7.39 7.30 7.29 7.23 7.17 7.16 7.15 7.14 7.14 7.04 7.03 7.02 6.71
4.71 4.69 4.68
3.24 3.23 3.20
2.47 2.46 2.45 2.44 2.43 2.43 2.42 2.40 2.39 2.38
1.00 1.00 2.00 1.00 1.00 3.06 1.07 1.00 1.00 1.00 1.00
8.1 7.9 7.7 7.5 7.3 7.1
f1 (ppm)
S
S
N
Me
Ph
O
1.00 1.00 2.00 1.00 1.00 3.06 1.07 1.00 1.00 1.00 1.00 1.00
1.00
2.00 2.84
2.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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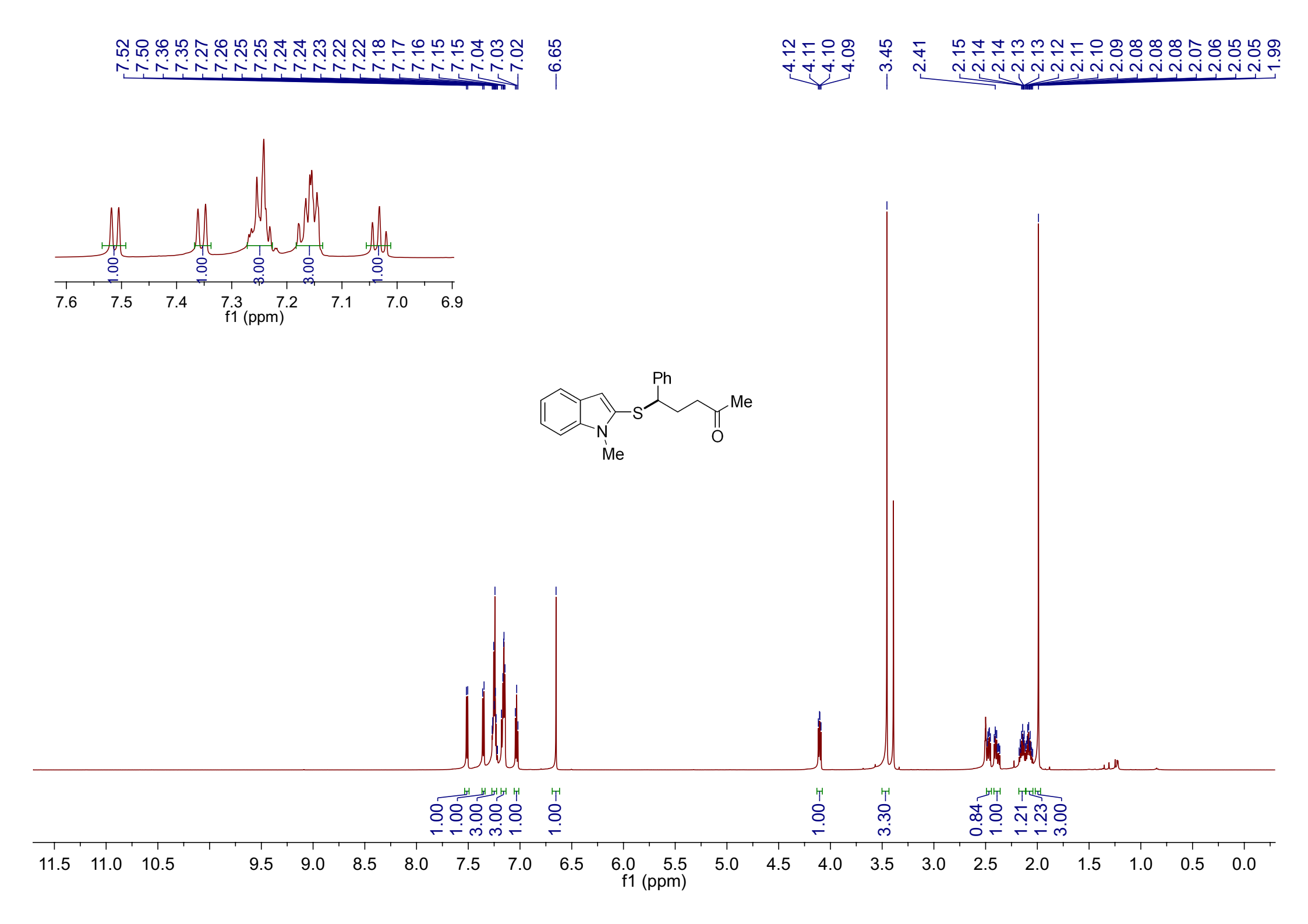
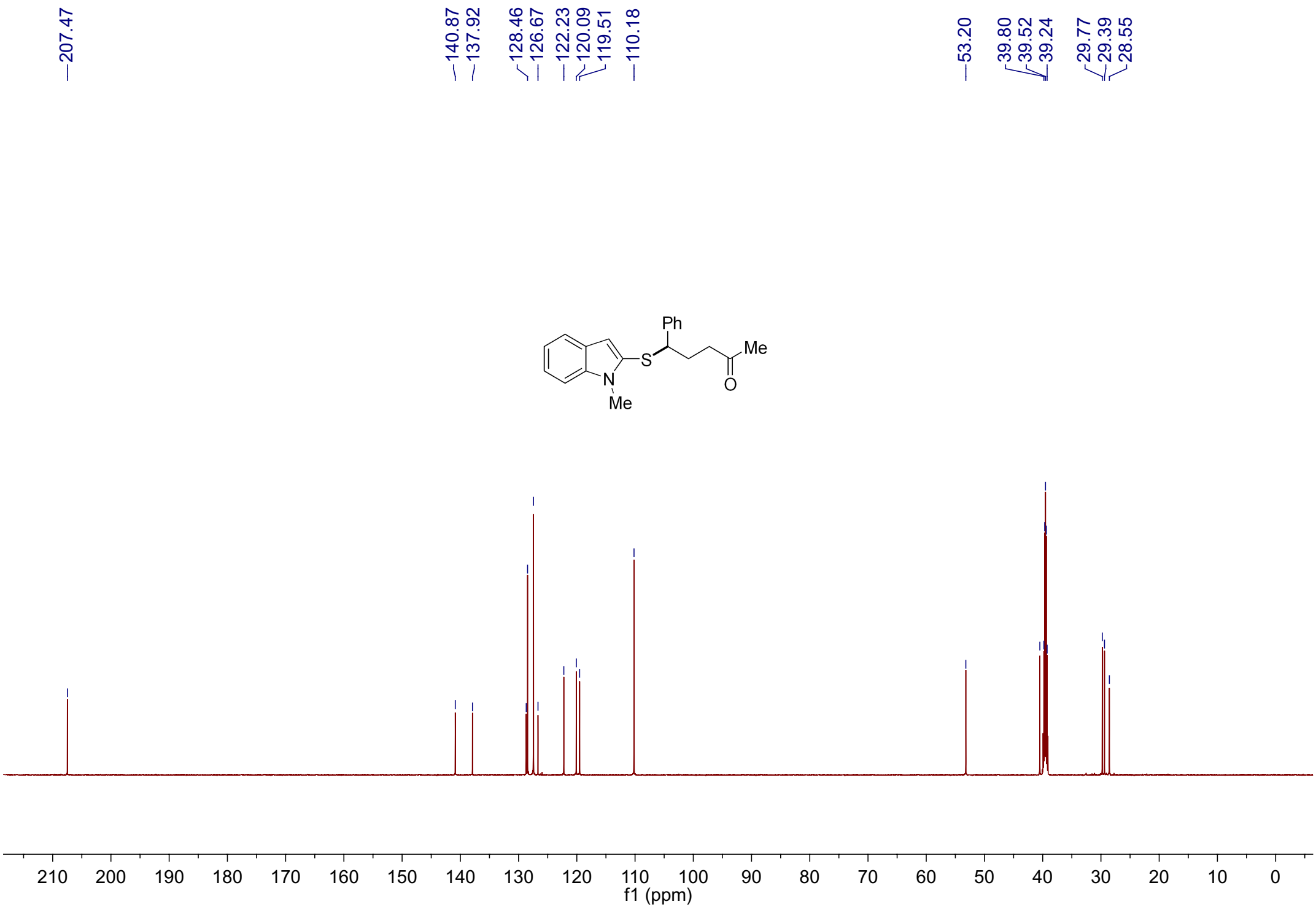
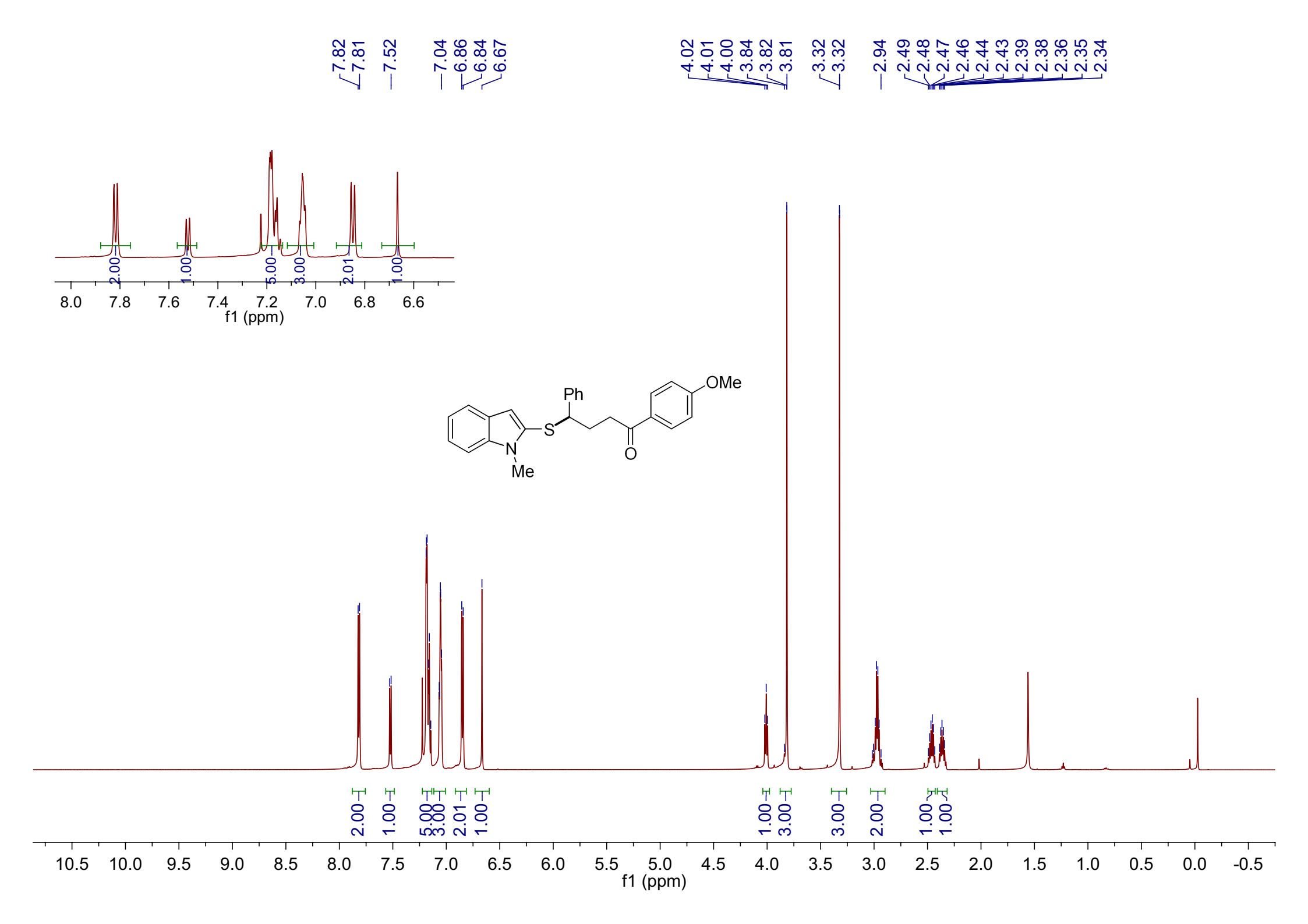
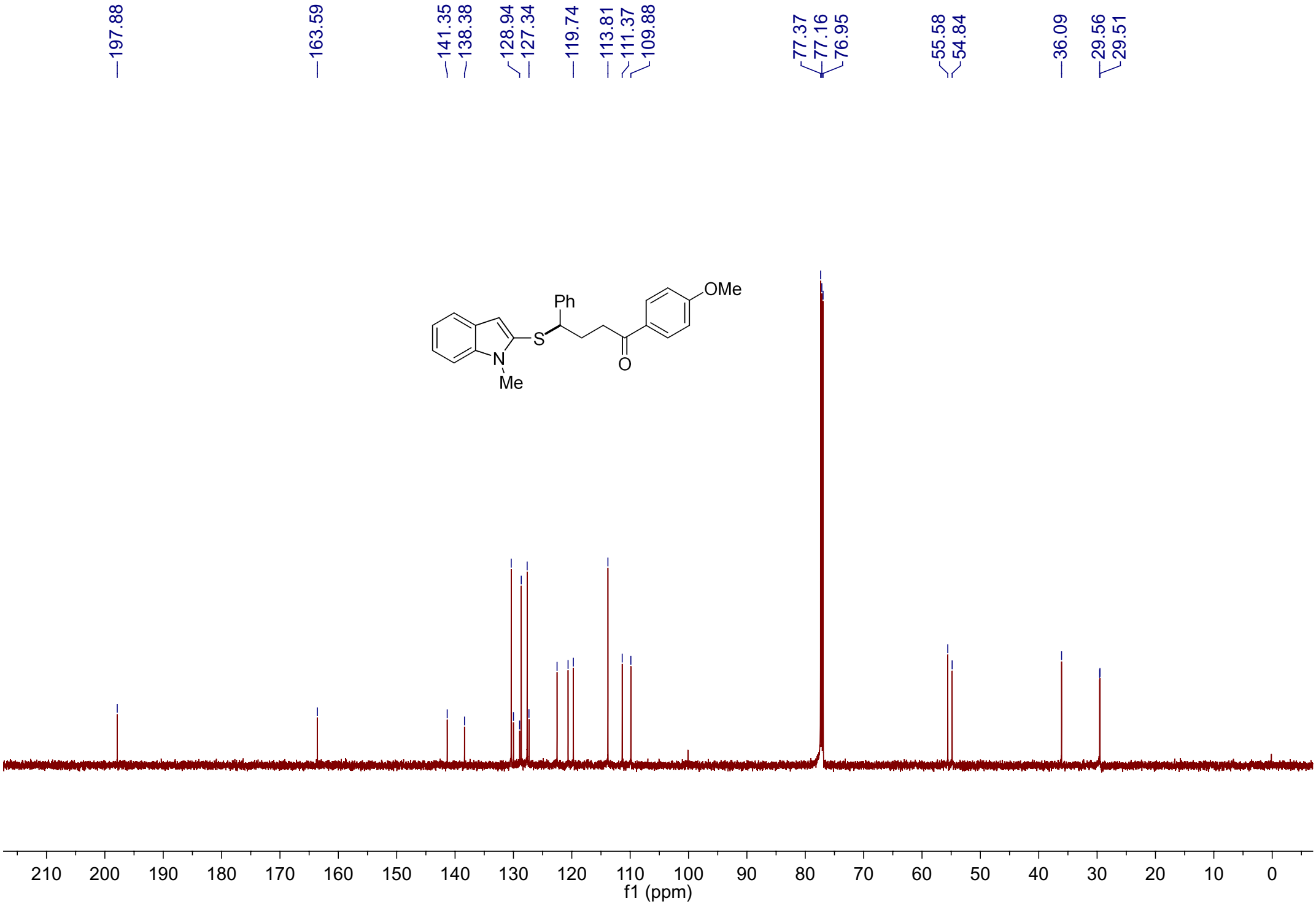
139.70
138.02
137.56
136.52
135.10
133.17
126.65
123.08
119.56
111.17
110.24
46.42
39.52
36.01
29.11
28.05
S
S
N
Me
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.52 7.50 7.36 7.35 7.27 7.26 7.25 7.25 7.24 7.24 7.23 7.22 7.22 7.18 7.17 7.16 7.15 7.15 7.04 7.03 7.02 6.65
4.12 4.11 4.10 4.09 3.45 2.41 2.15 2.14 2.14 2.13 2.13 2.12 2.11 2.10 2.09 2.08 2.08 2.08 2.07 2.06 2.05 2.05 1.99
1.00 1.00 3.00 3.00 1.00
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
Ph
S
Me
N
Me
O
1.00 1.00 3.00 3.00 1.00 1.00 1.00 3.30 0.84 1.00 1.21 1.23 3.00
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


207.47
140.87
137.92
128.46
126.67
122.23
120.09
119.51
110.18
53.20
39.80
39.52
39.24
29.77
29.39
28.55
Ph
S
Me
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.82
7.81
7.52
7.04
6.86
6.84
6.67
4.02
4.01
4.00
3.84
3.82
3.81
3.32
3.32
2.94
2.49
2.48
2.47
2.46
2.44
2.43
2.39
2.38
2.36
2.35
2.34
2.00
1.00
5.00
3.00
2.01
1.00
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
Ph
S
N
Me
OMe
O
2.00
1.00
5.00
3.00
2.01
1.00
1.00
3.00
3.00
2.00
1.00
1.00
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
-0.5
f1 (ppm)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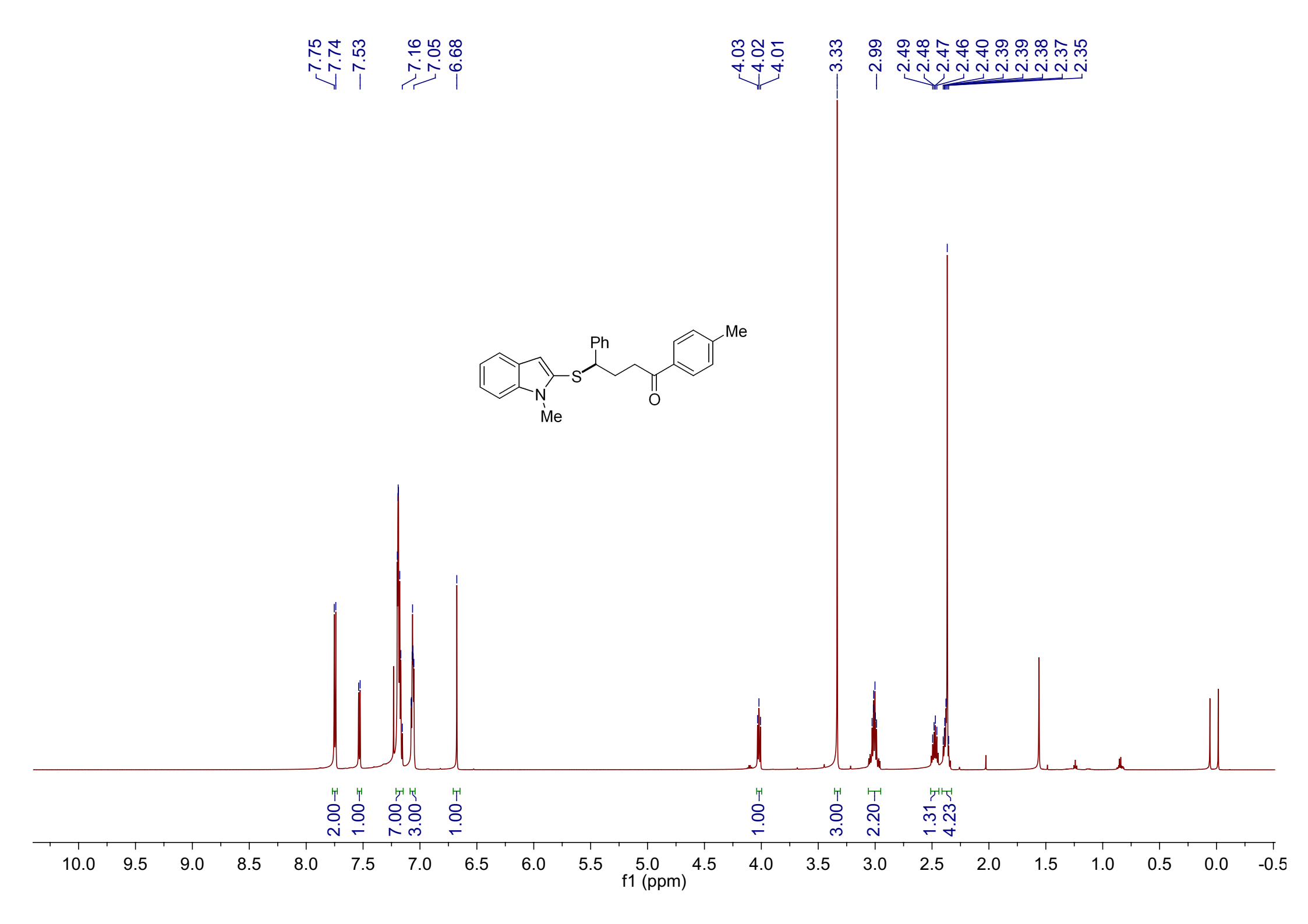
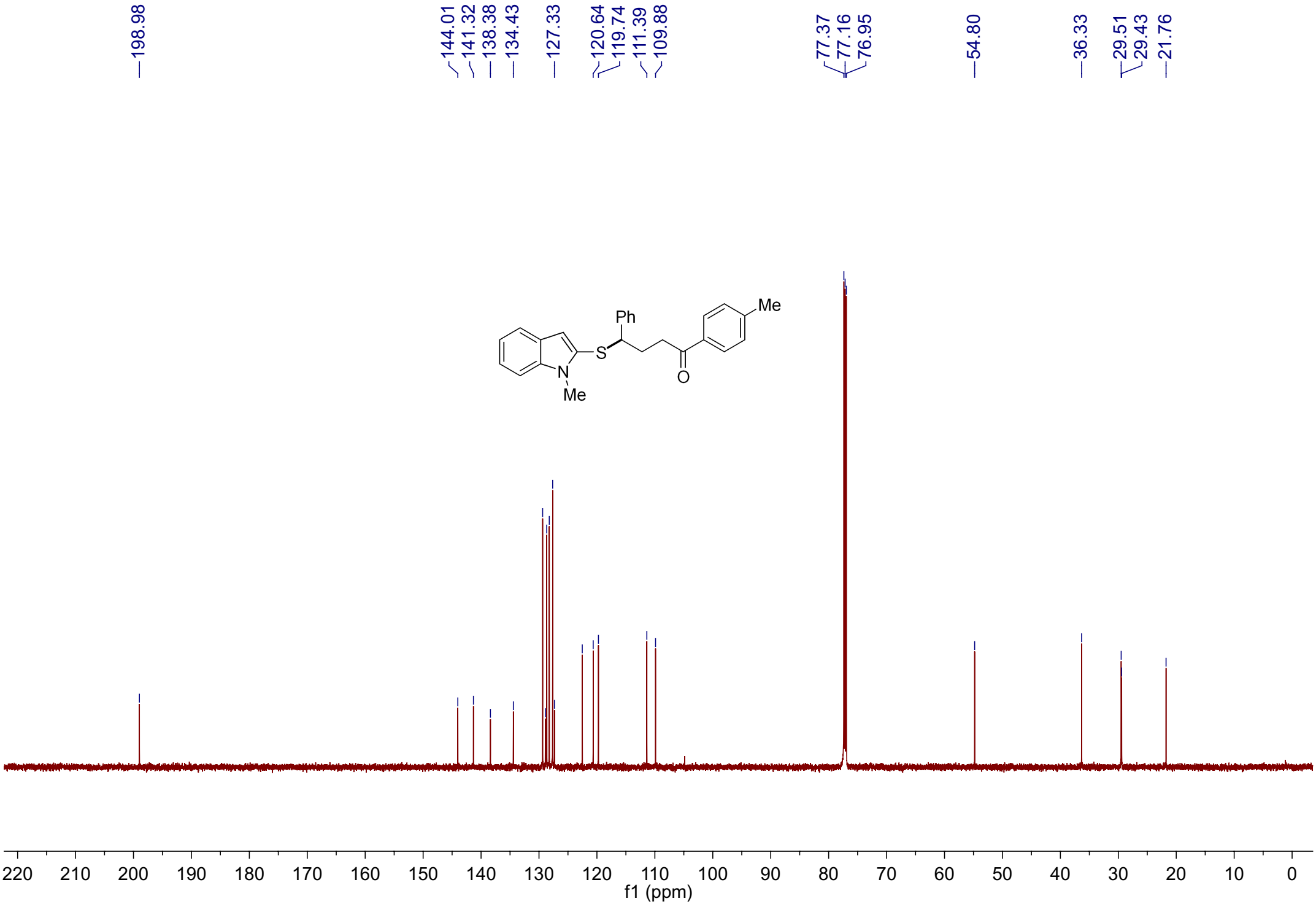
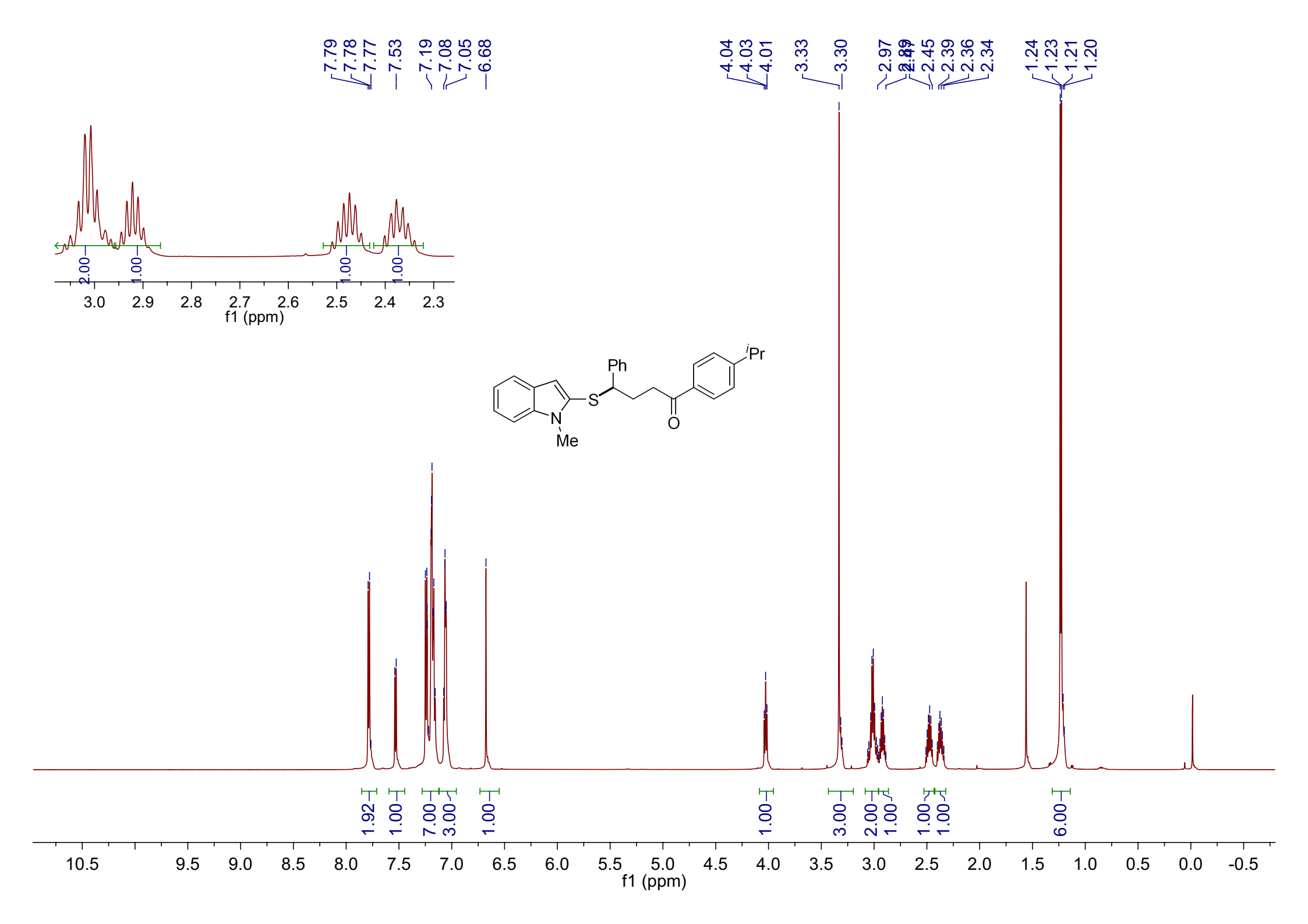
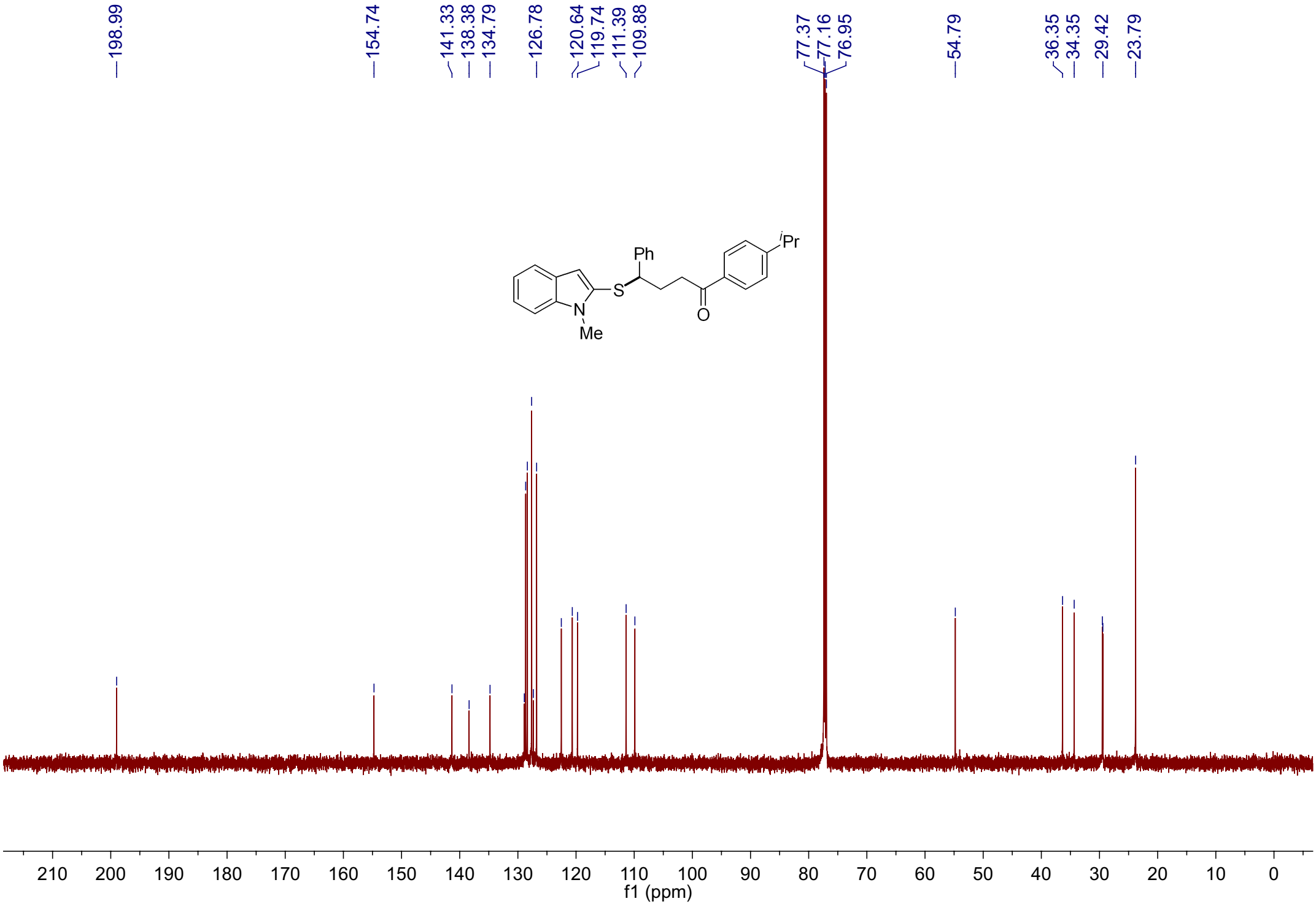
163.59
141.35
138.38
128.94
127.34
119.74
113.81
111.37
109.88
77.37
77.16
76.95
55.58
54.84
36.09
29.56
29.51
OMe
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.75
7.74
7.53
7.16
7.05
6.68
4.03
4.02
4.01
3.33
2.99
2.49
2.48
2.47
2.46
2.40
2.39
2.39
2.38
2.37
2.35
Me
Ph
S
N
Me
O
2.00
1.00
7.00
3.00
1.00
1.00
3.00
2.20
1.31
4.23
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
-0.5
f1 (ppm)


198.98
144.01
141.32
138.38
134.43
127.33
120.64
119.74
111.39
109.88
77.37
77.16
76.95
54.80
36.33
29.51
29.43
21.76
Ph
Me
S
N
Me
O
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)


7.79
7.78
7.77
7.53
7.19
7.08
7.05
6.68
4.04
4.03
4.01
3.33
3.30
2.97
2.45
2.39
2.36
2.34
1.24
1.23
1.21
1.20
Ph
S
N
Me
O
iPr
2.00
1.00
1.00
1.00
f1 (ppm)
1.92
1.00
7.00
3.00
1.00
1.00
3.00
2.00
1.00
1.00
1.00
6.00
f1 (ppm)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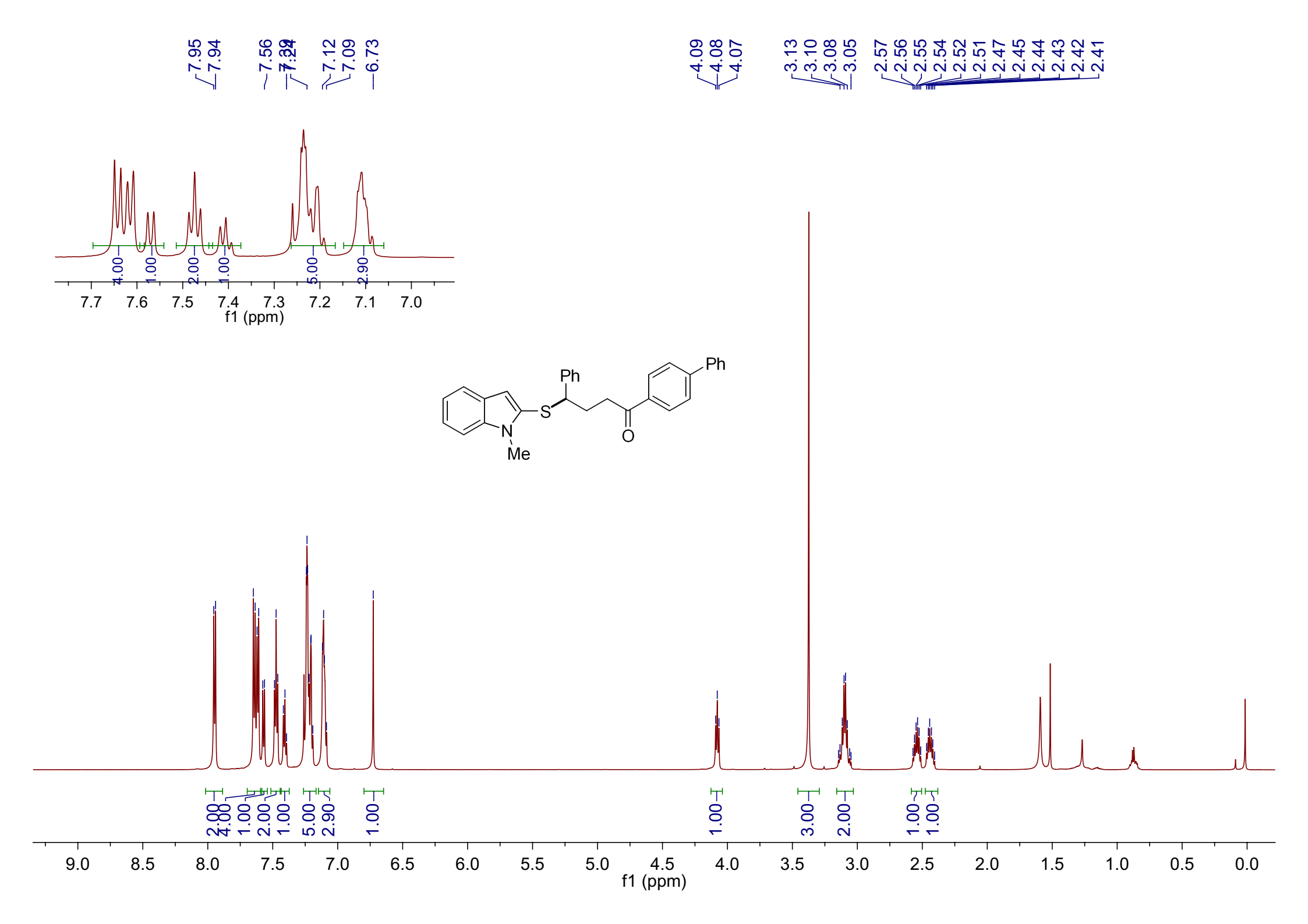
154.74
141.33
138.38
134.79
126.78
120.64
119.74
111.39
109.88
77.37
77.16
76.95
54.79
36.35
34.35
29.42
23.79
Ph
S
N
Me
O
iPr
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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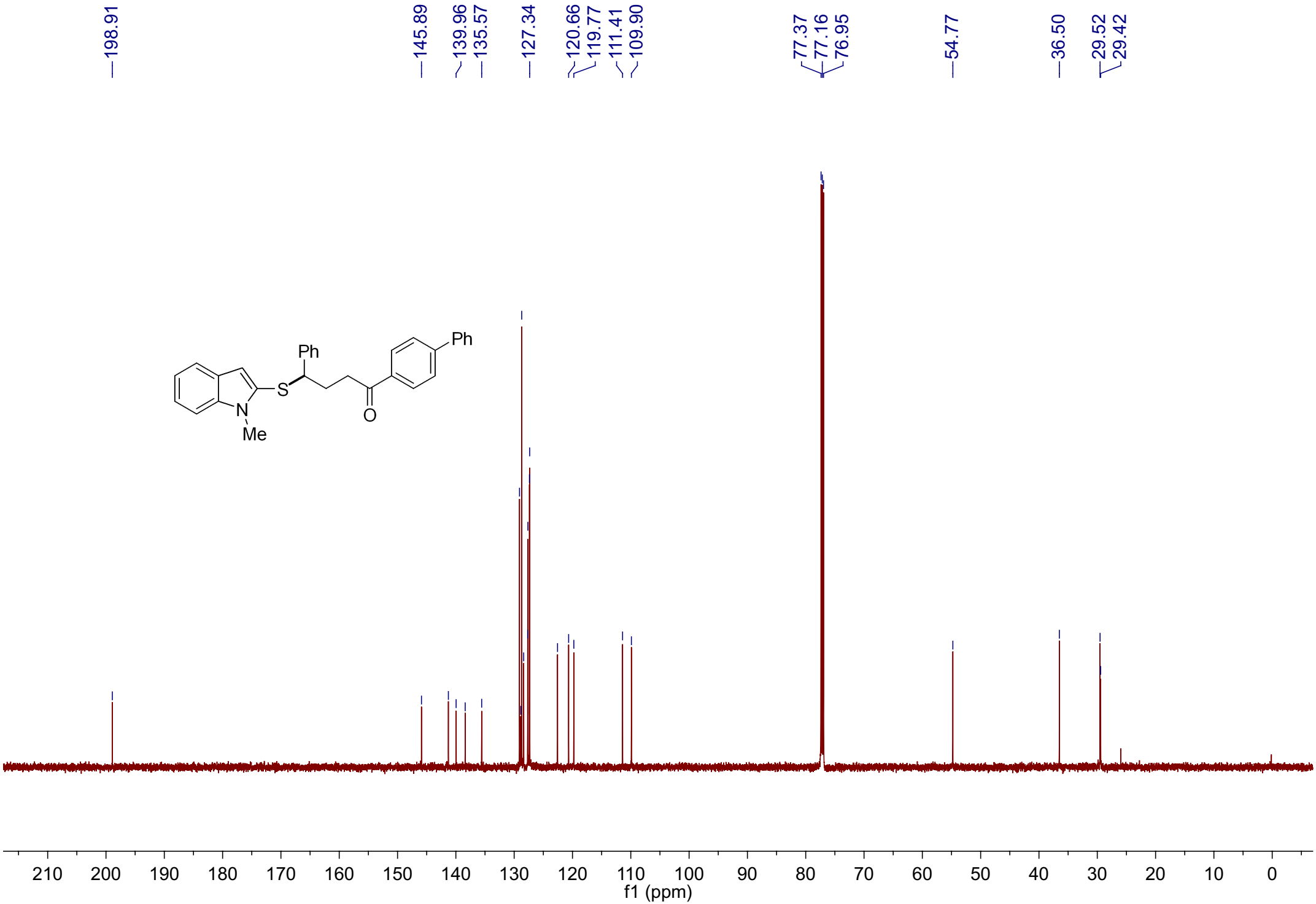
7.94
7.56
7.12
7.09
6.73
4.09
4.08
4.07
3.13
3.10
3.08
3.05
2.57
2.56
2.55
2.54
2.52
2.51
2.47
2.45
2.44
2.43
2.42
2.41
4.00
1.00
2.00
1.00
5.00
2.90
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
Ph
Ph
S
N
Me
O
2.00
4.00
1.00
2.00
1.00
5.00
2.90
1.00
1.00
3.00
2.00
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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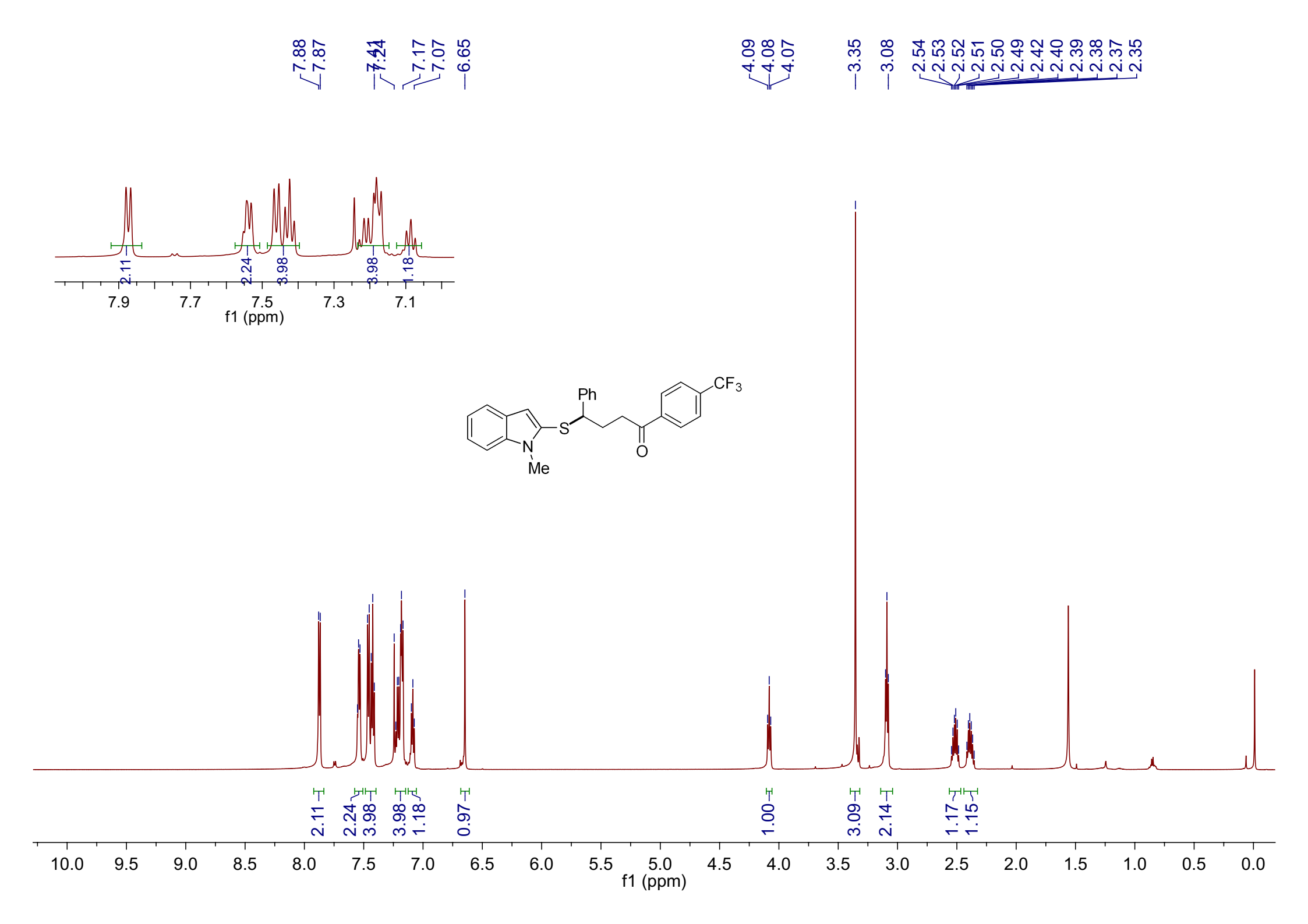
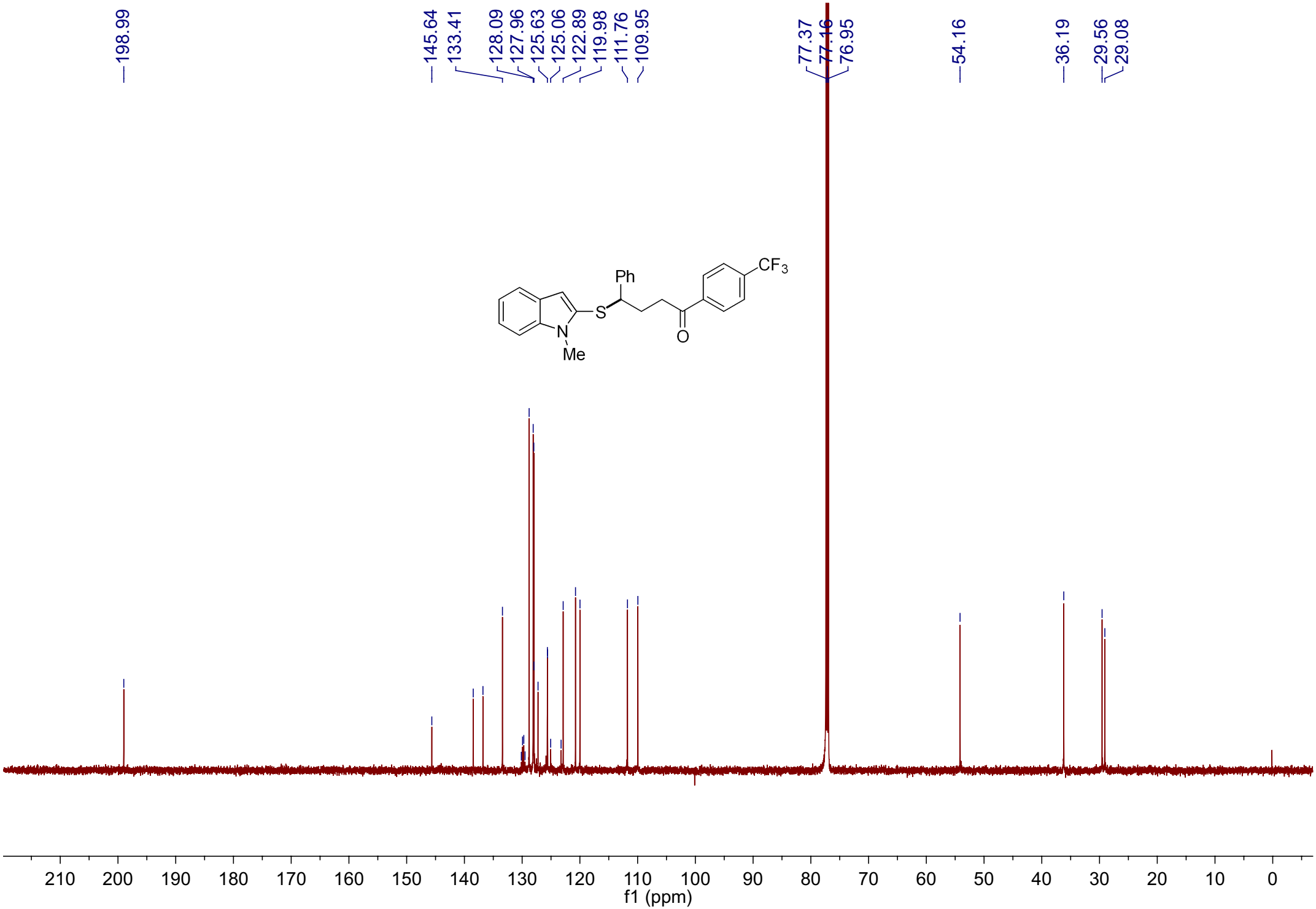
139.96
135.57
127.34
120.66
119.77
111.41
109.90
77.37
77.16
76.95
54.77
36.50
29.52
29.42
Ph
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.88
7.87
7.24
7.17
7.07
6.65
4.09
4.08
4.07
3.35
3.08
2.54
2.53
2.52
2.51
2.50
2.49
2.42
2.40
2.39
2.38
2.37
2.35
2.11
2.24
3.98
3.98
1.18
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
Ph
S
N
Me
O
CF3
2.11
2.24
3.98
3.98
1.18
0.97
1.00
3.09
2.14
1.17
1.15
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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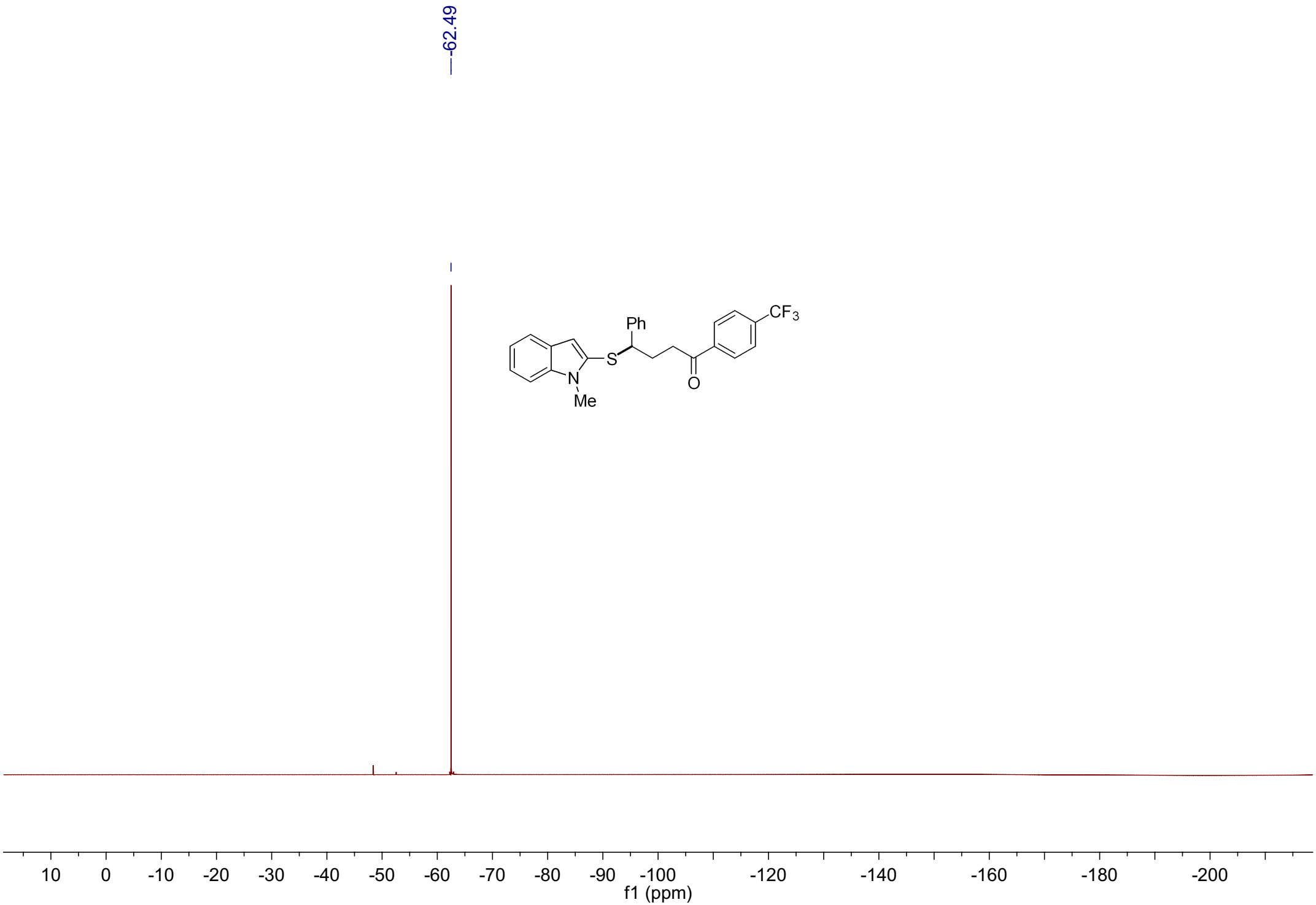
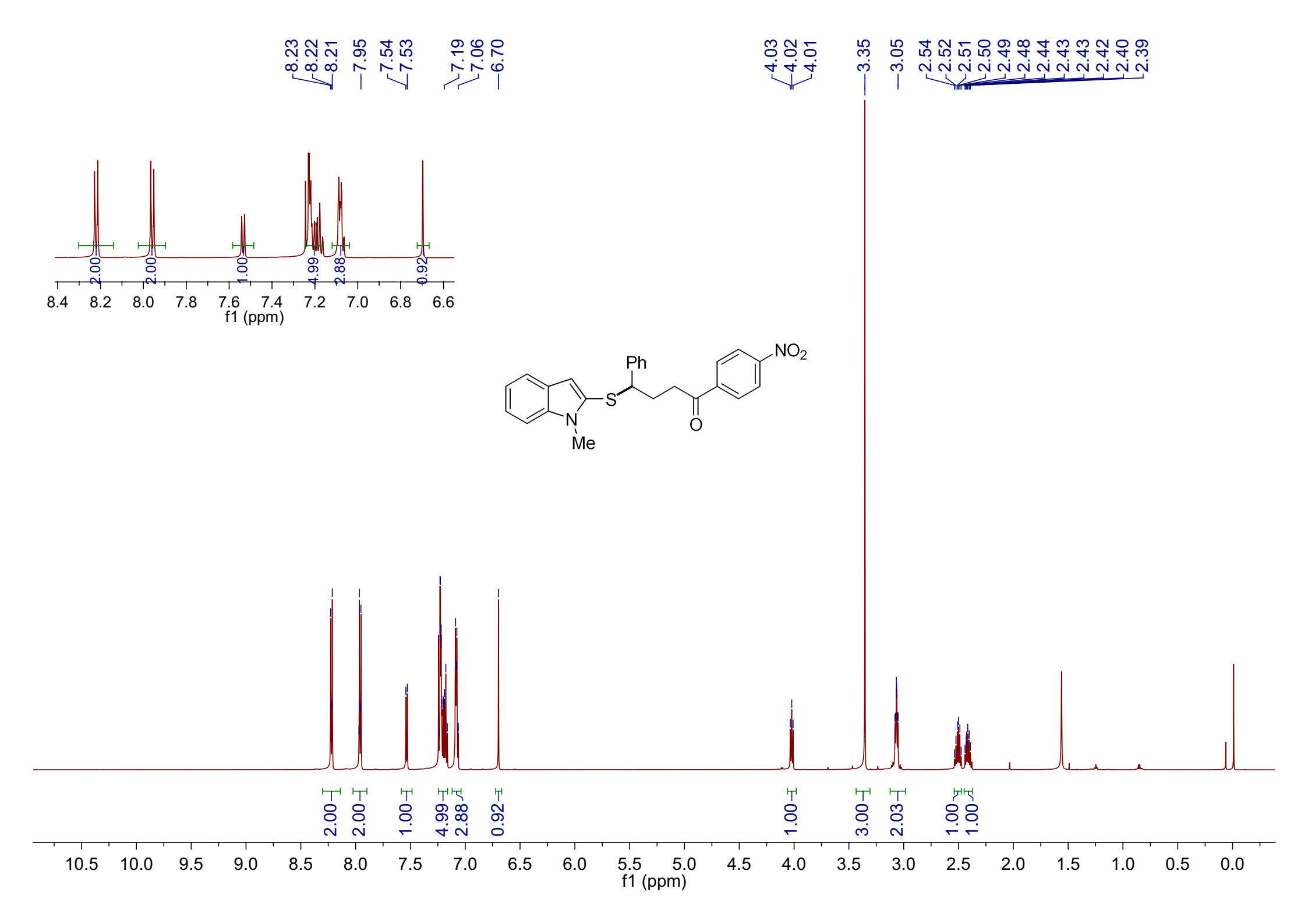
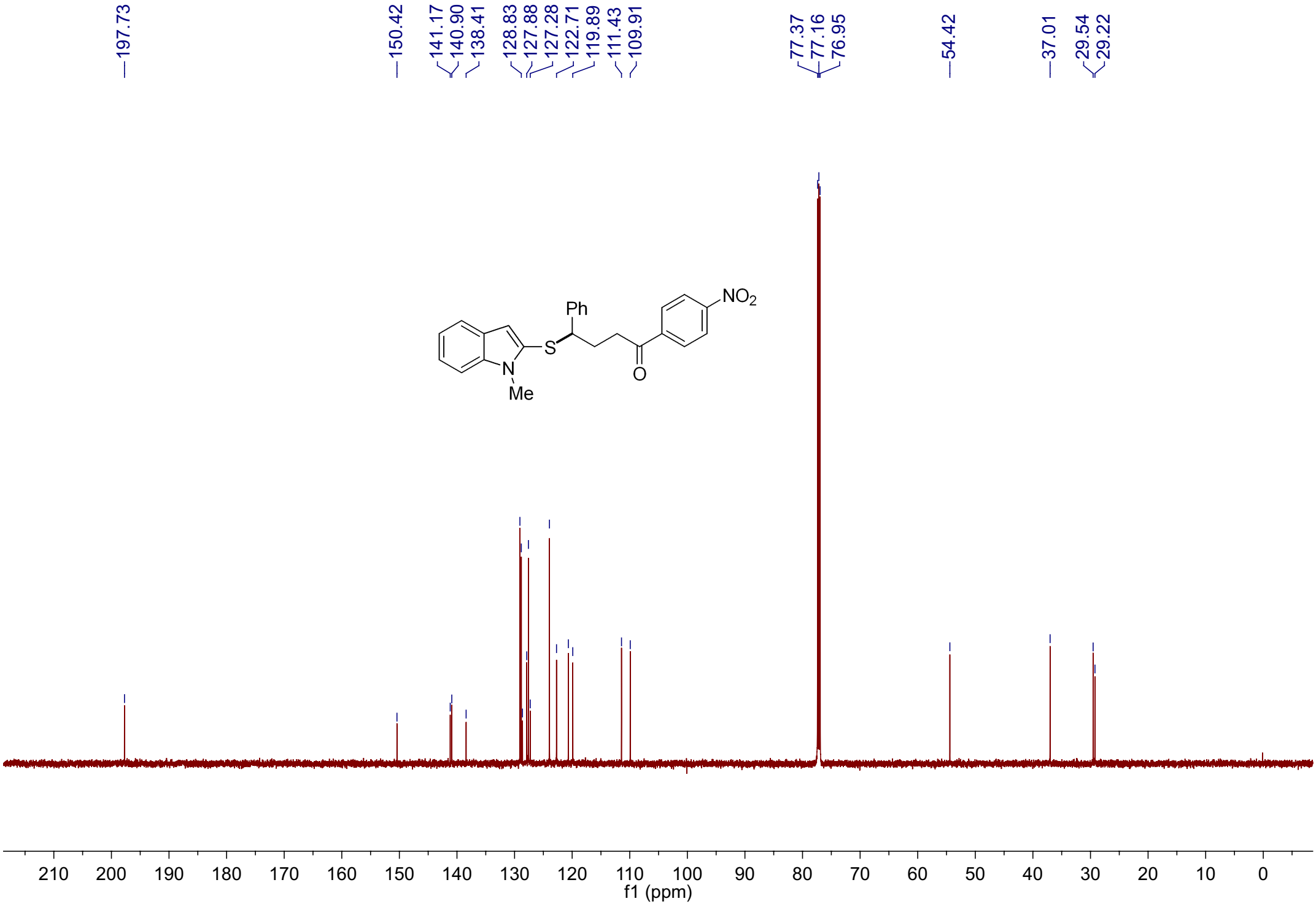
145.64
133.41
128.09
127.96
125.63
125.06
122.89
119.98
111.76
109.95
77.37
77.16
76.95
54.16
36.19
29.56
29.08
Ph
S
N
Me
O
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.49
Ph
S
N
Me
O
CF3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.23
8.22
8.21
7.95
7.54
7.53
7.19
7.06
6.70
4.03
4.02
4.01
3.35
3.05
2.54
2.52
2.51
2.50
2.49
2.48
2.44
2.43
2.43
2.42
2.40
2.39
2.00
2.00
1.00
4.99
2.88
0.92
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6
f1 (ppm)
Ph
NO2
S
N
Me
O
2.00
2.00
1.00
4.99
2.88
0.92
1.00
3.00
2.03
1.00
1.00
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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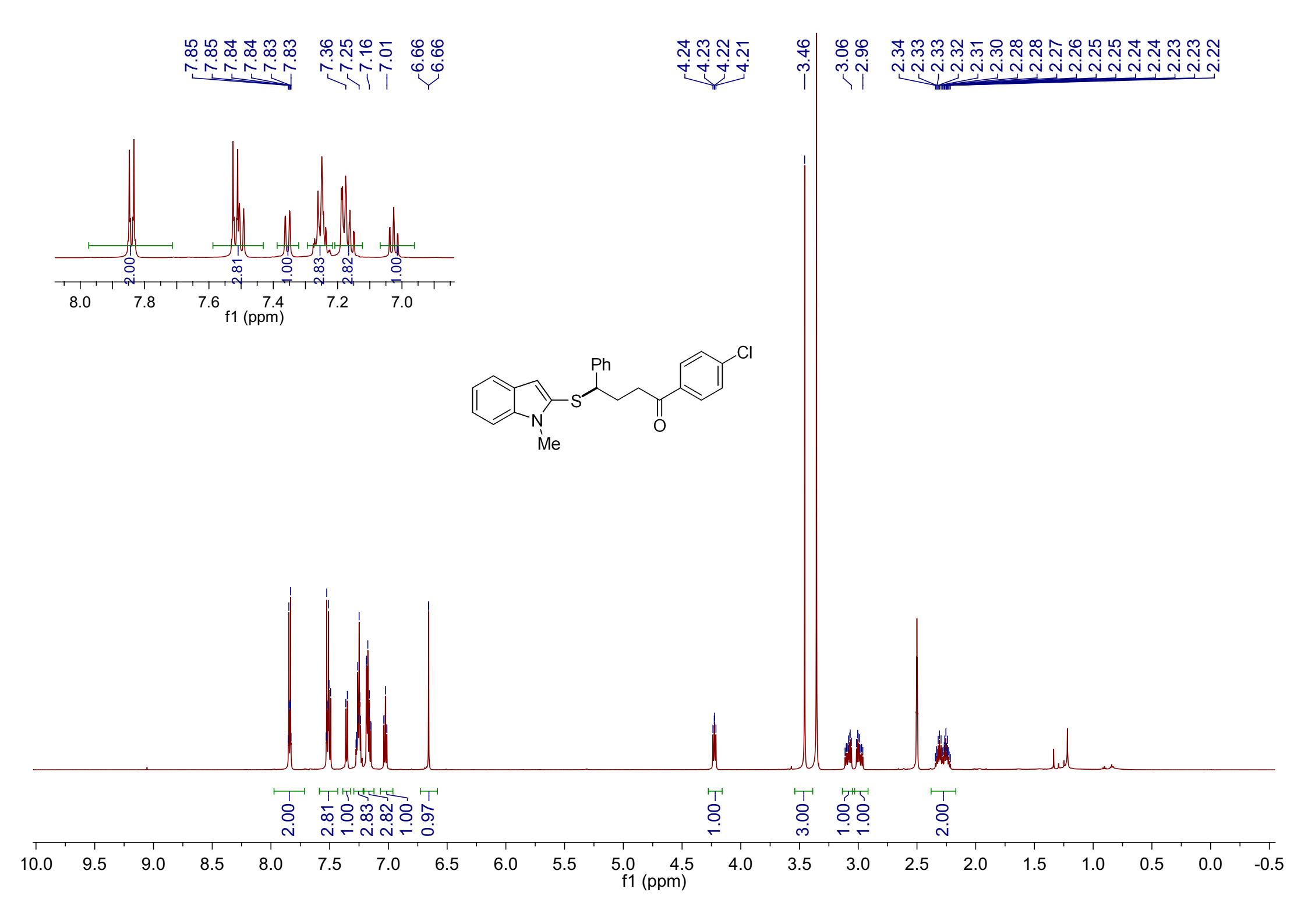
128.83
127.88
127.28
122.71
119.89
111.43
109.91
77.37
77.16
76.95
54.42
37.01
29.54
29.22
NO2
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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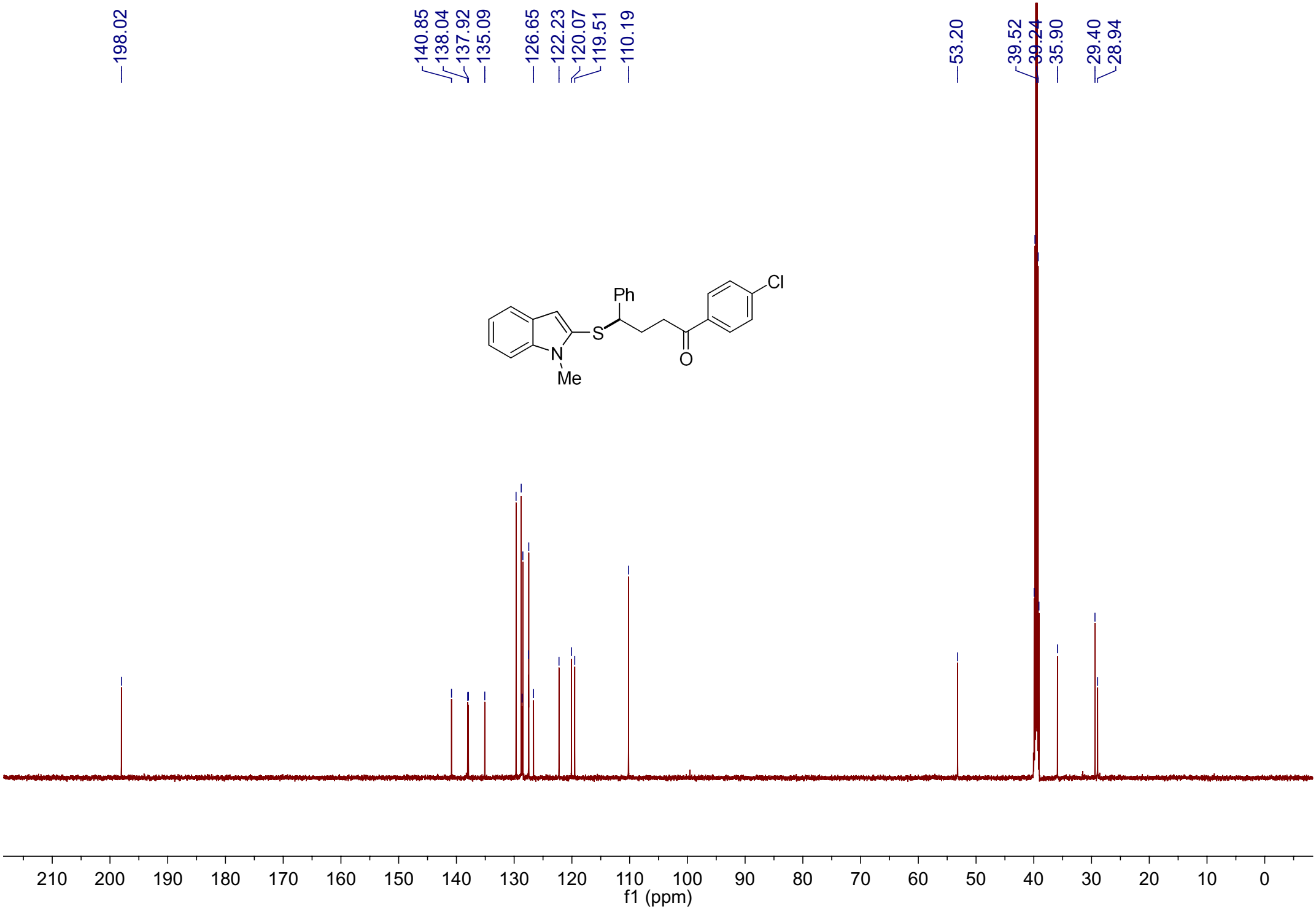
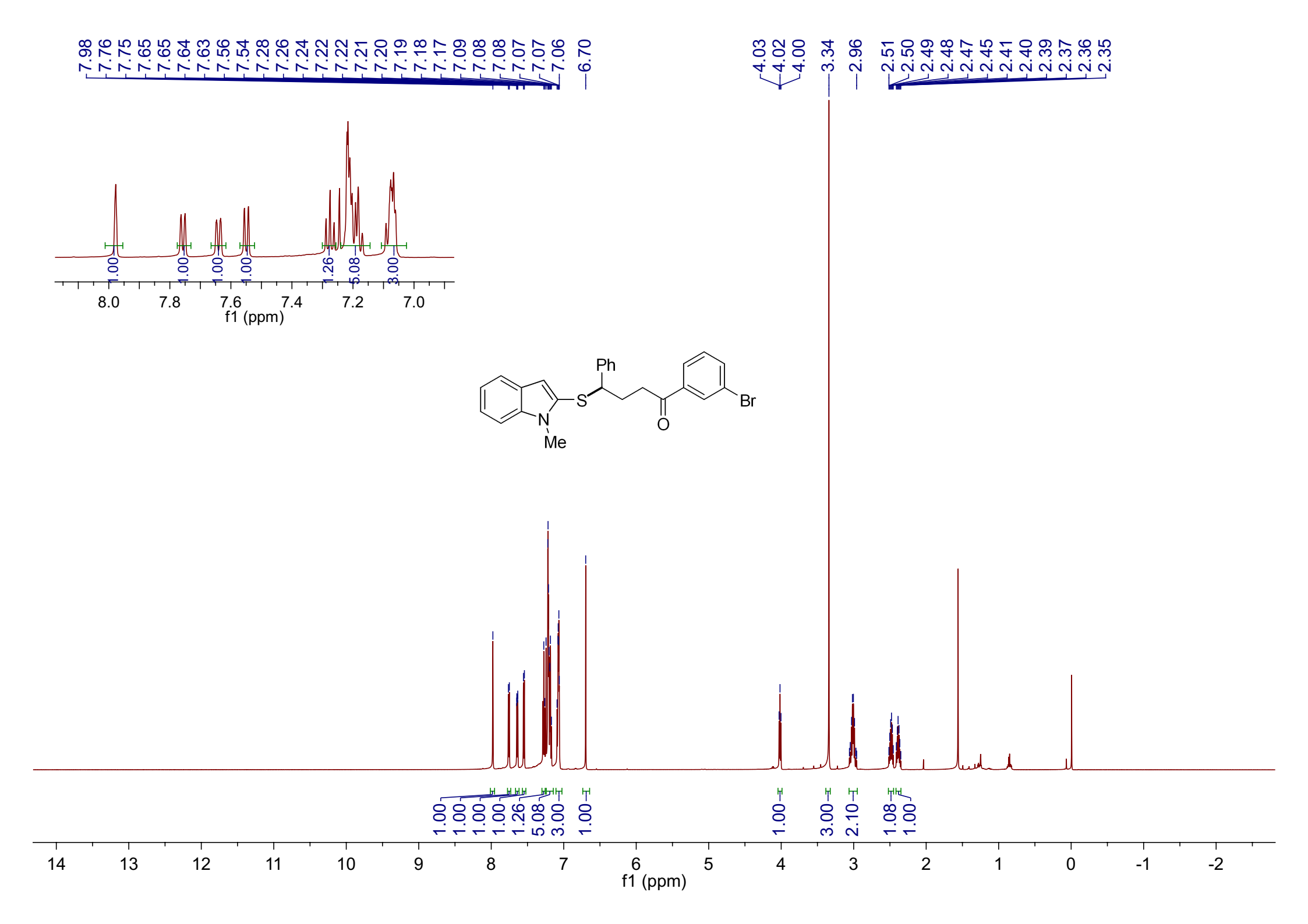
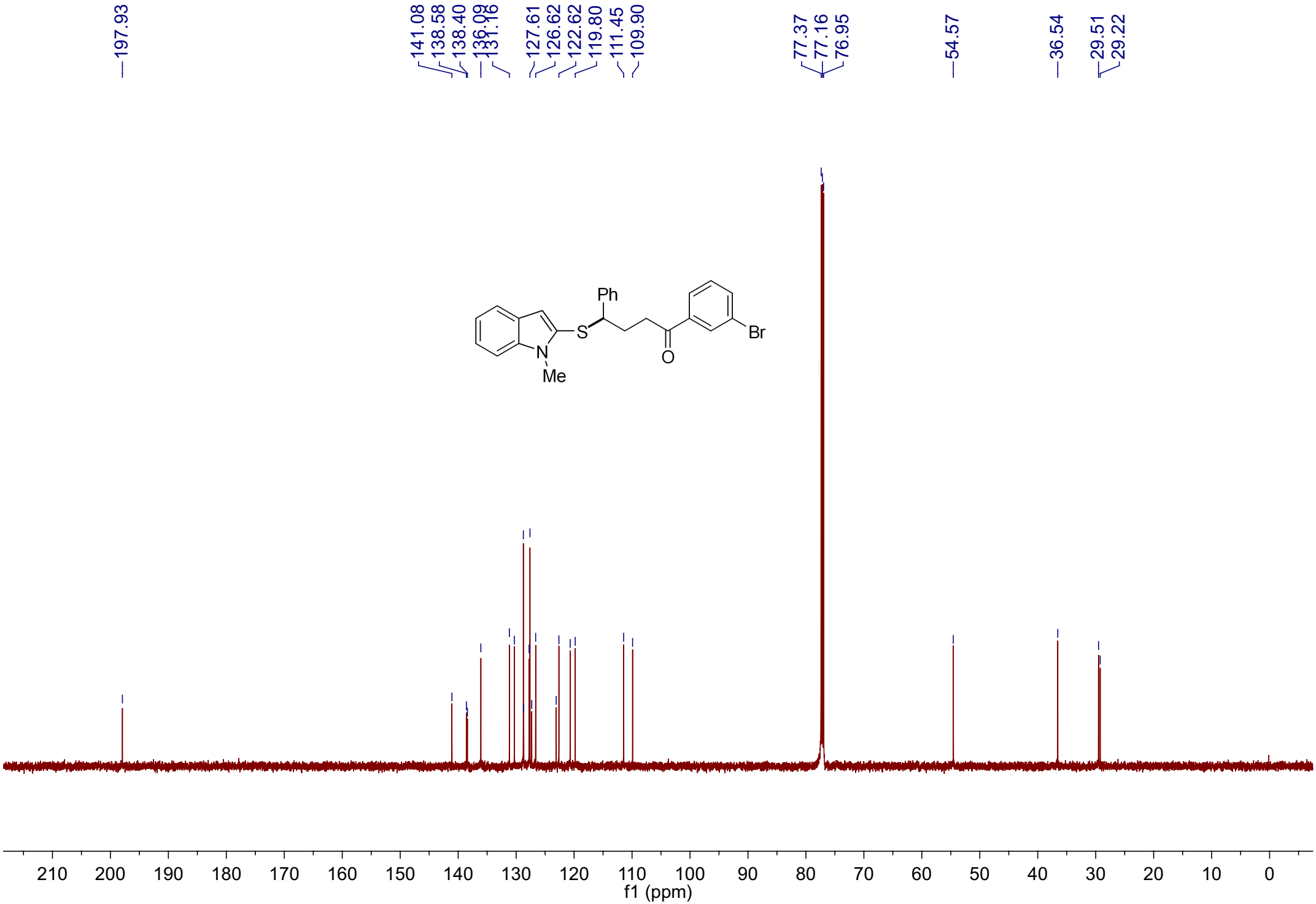
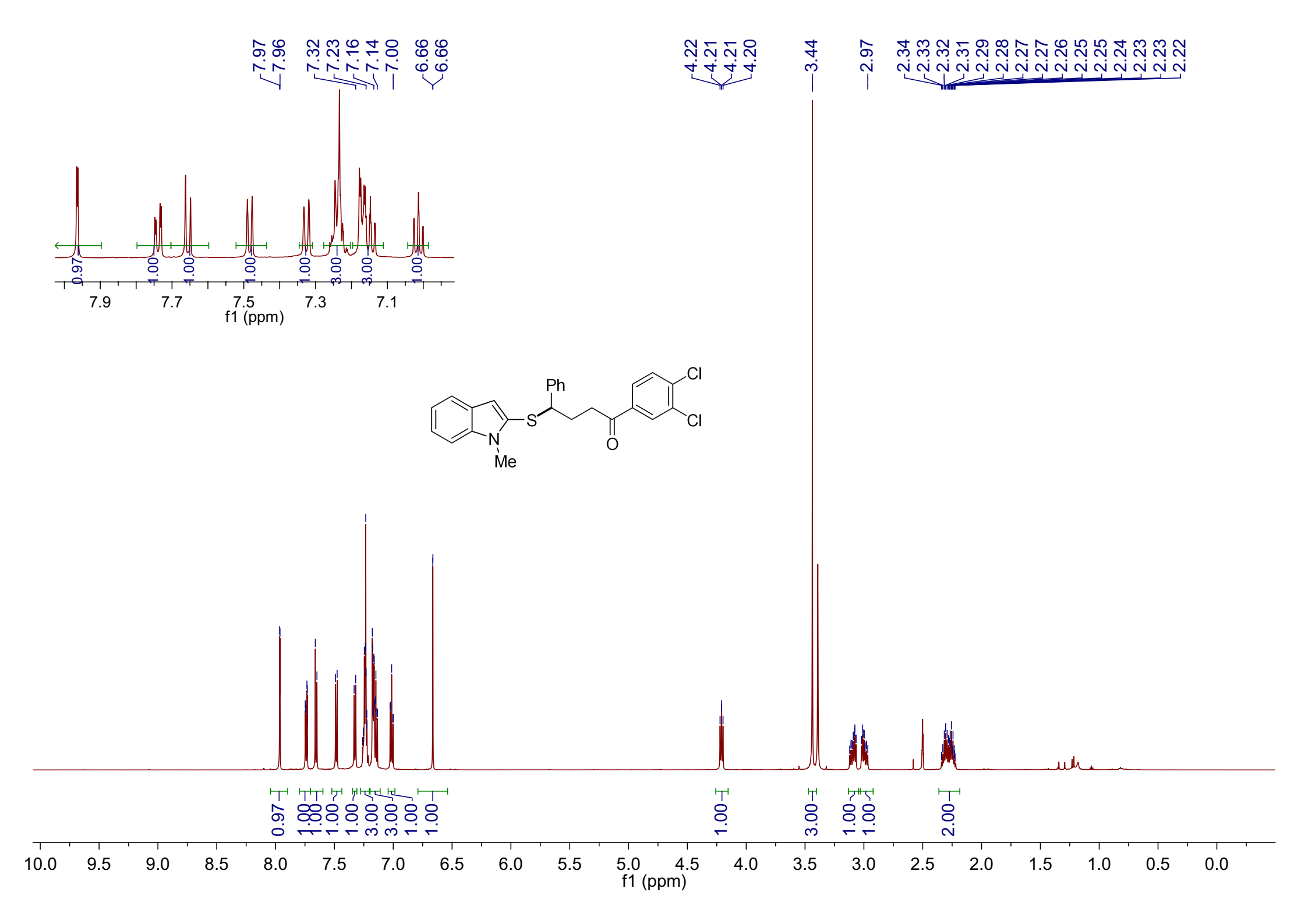
7.85
7.84
7.84
7.83
7.83
7.36
7.25
7.16
7.01
6.66
6.66
4.24
4.23
4.22
4.21
3.46
3.06
2.96
2.34
2.33
2.33
2.32
2.31
2.30
2.28
2.28
2.27
2.26
2.25
2.25
2.24
2.24
2.23
2.23
2.22
2.00
2.81
1.00
2.83
2.82
1.00
1.00
f1 (ppm)
Ph
Cl
S
N
Me
O
2.00
2.81
1.00
2.83
2.82
1.00
0.97
1.00
3.00
1.00
1.00
2.00
f1 (ppm)


198.02
140.85
138.04
137.92
135.09
126.65
122.23
120.07
119.51
110.19
53.20
39.52
39.24
35.90
29.40
28.94
Cl
Ph
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.98 7.76 7.75 7.65 7.65 7.64 7.63 7.56 7.54 7.28 7.26 7.24 7.22 7.22 7.21 7.20 7.19 7.18 7.17 7.09 7.08 7.08 7.07 7.07 7.06 6.70
4.03 4.02 4.00 3.34 2.96 2.51 2.50 2.49 2.48 2.47 2.45 2.41 2.40 2.39 2.37 2.36 2.35
1.00 1.00 1.00 1.00 1.26 5.08 3.00
8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
Ph
S
N
Me
O
Br
1.00 1.00 1.00 1.00 1.26 5.08 3.00 1.00
1.00 3.00 2.10 1.08 1.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


197.93
141.08
138.58
138.40
136.09
131.16
127.61
126.62
122.62
119.80
111.45
109.90
77.37
77.16
76.95
54.57
36.54
29.51
29.22
Ph
S
N
Me
O
Br
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.97
7.96
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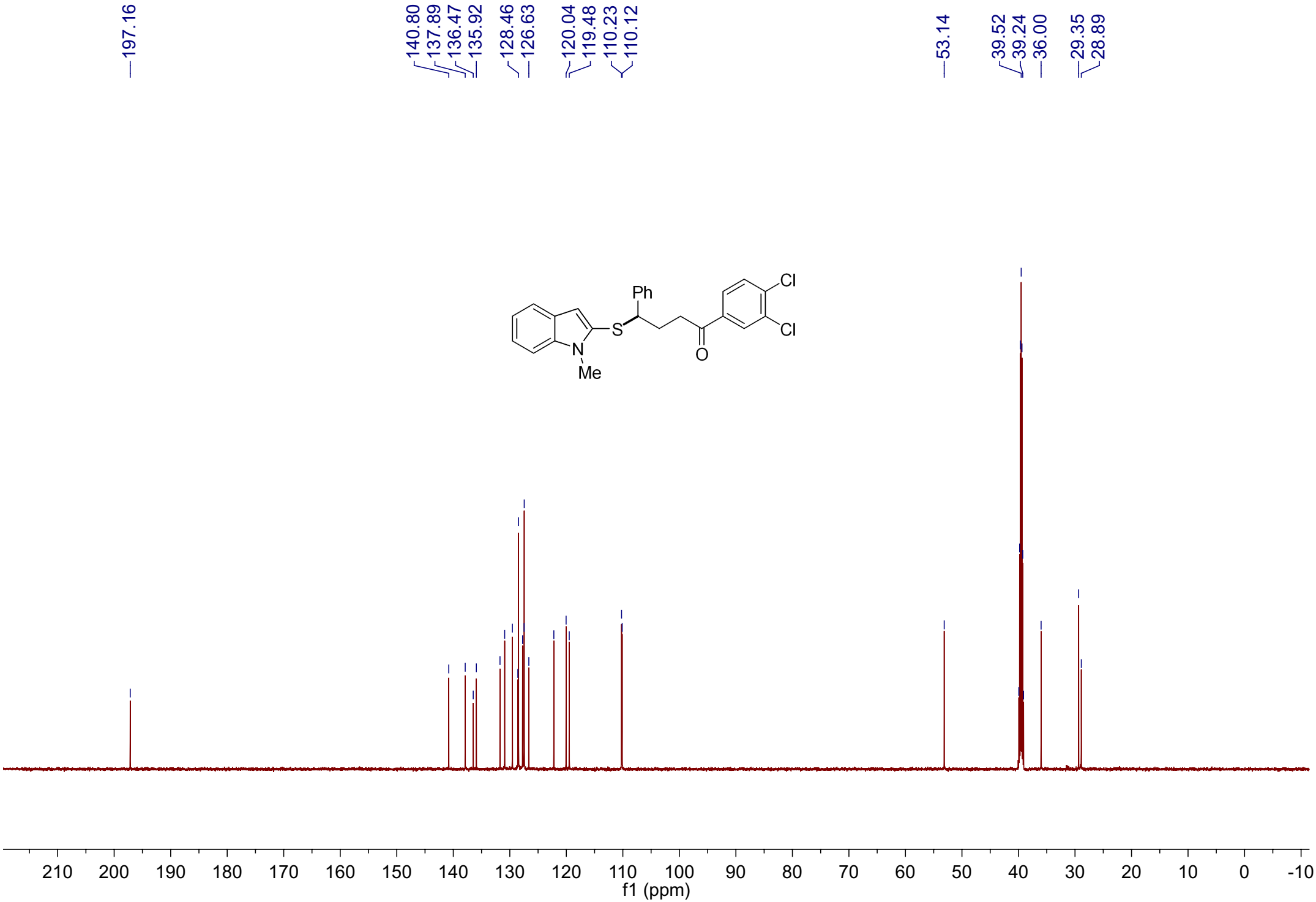
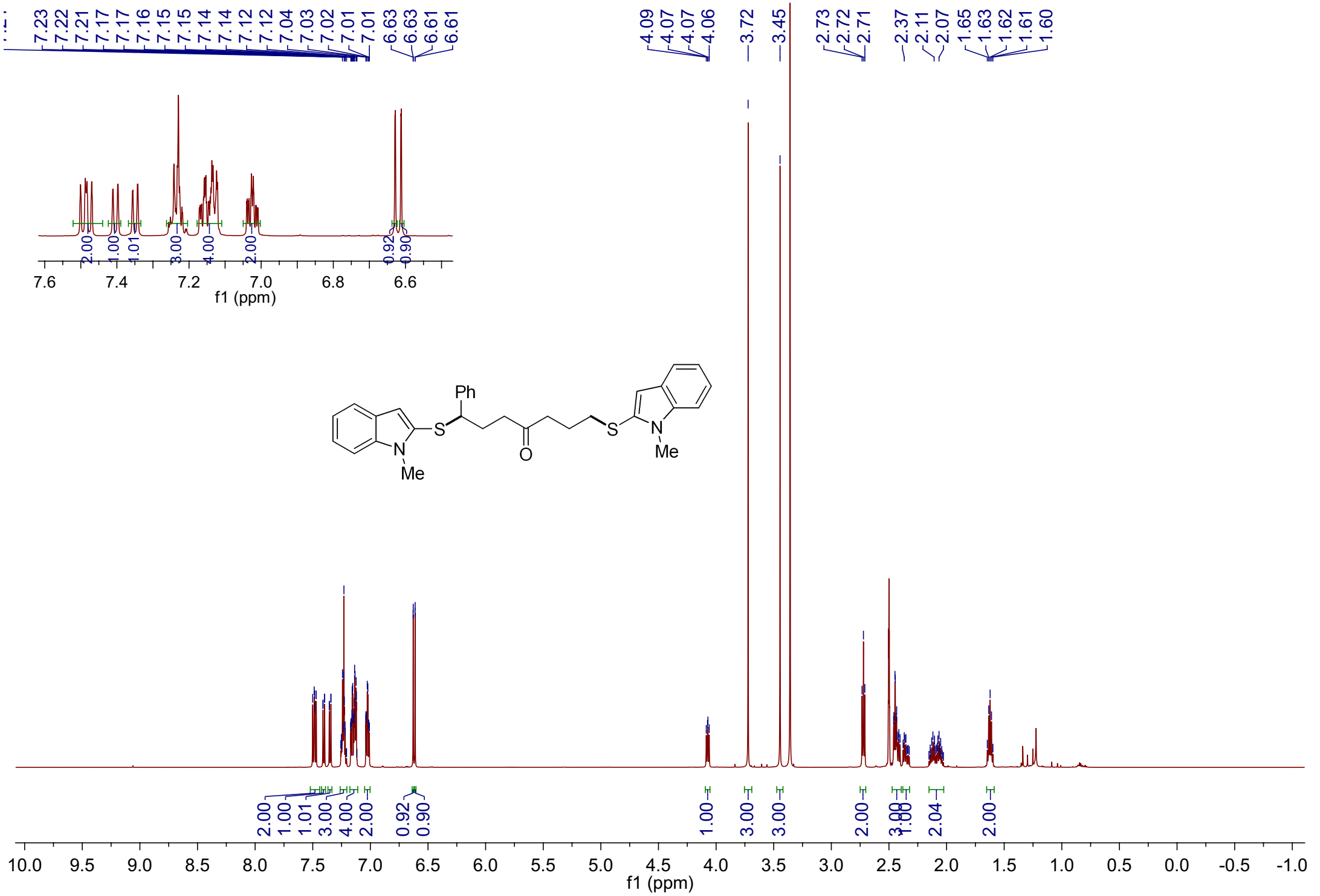
7.23
7.16
7.14
7.00
6.66
6.66
4.22
4.21
4.21
4.20
3.44
2.97
2.34
2.33
2.32
2.31
2.29
2.28
2.27
2.27
2.26
2.25
2.25
2.24
2.23
2.23
2.22
0.97
1.00
1.00
1.00
1.00
3.00
3.00
1.00
1.00
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
Ph
S
N
Me
O
Cl
Cl
1.00
3.00
1.00
1.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


197.16
140.80
137.89
136.47
135.92
128.46
126.63
120.04
119.48
110.23
110.12
53.14
39.52
39.24
36.00
29.35
28.89
Ph
S
N
Me
O
Cl
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.22
7.21
7.17
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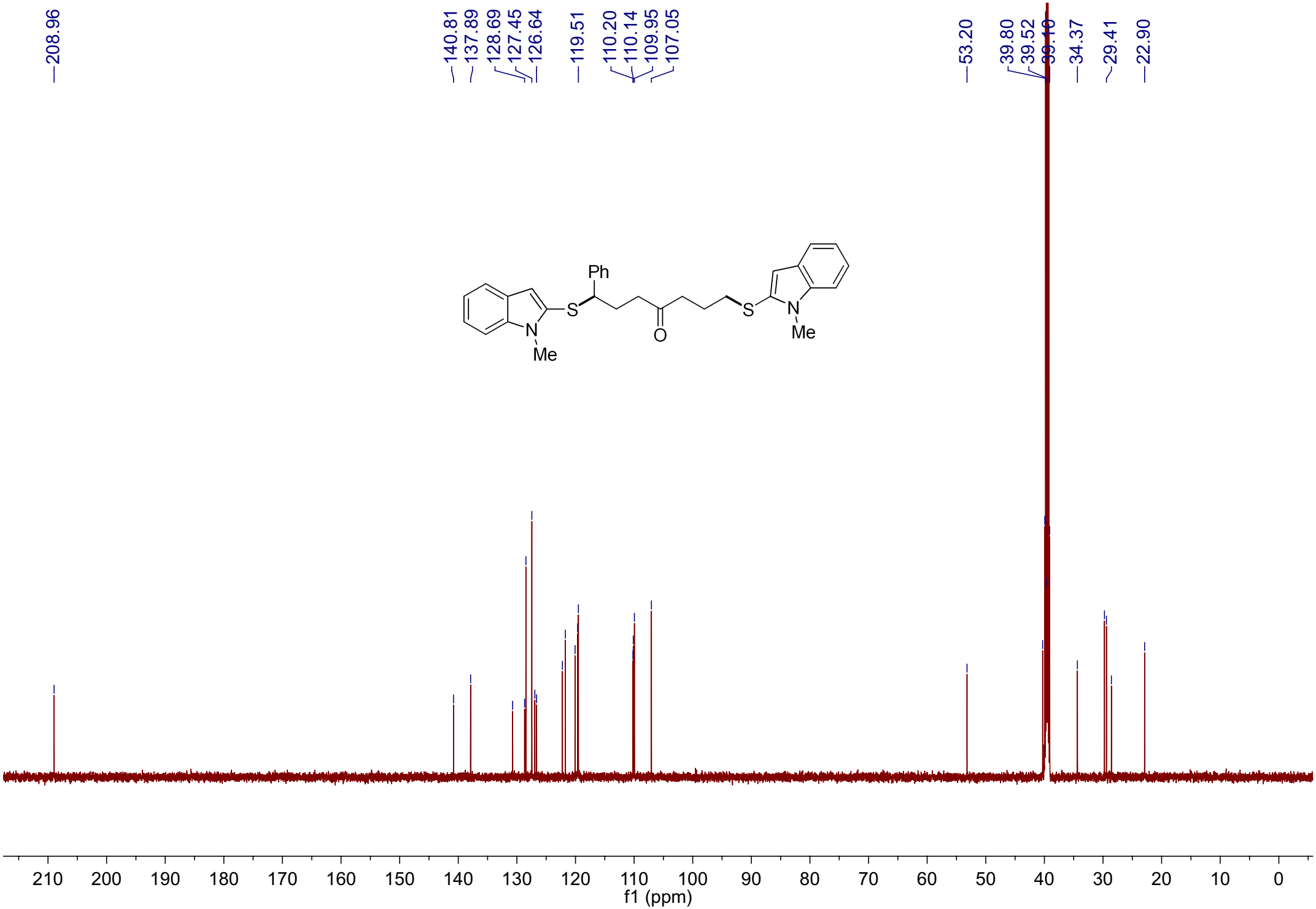
7.16
7.15
7.15
7.14
7.14
7.12
7.12
7.04
7.03
7.02
7.01
7.01
6.63
6.63
6.61
6.61
4.09
4.07
4.07
4.06
3.72
3.45
2.73
2.72
2.71
2.37
2.11
2.07
1.65
1.63
1.62
1.61
1.60
2.00
1.00
1.01
3.00
4.00
2.00
0.92
0.90
7.6
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
Ph
S
S
N
Me
N
Me
O
2.00
1.00
1.01
3.00
4.00
2.00
0.92
0.90
1.00
3.00
3.00
2.00
3.00
1.00
2.04
2.00
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
-0.5
-1.0
f1 (ppm)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140.81
137.89
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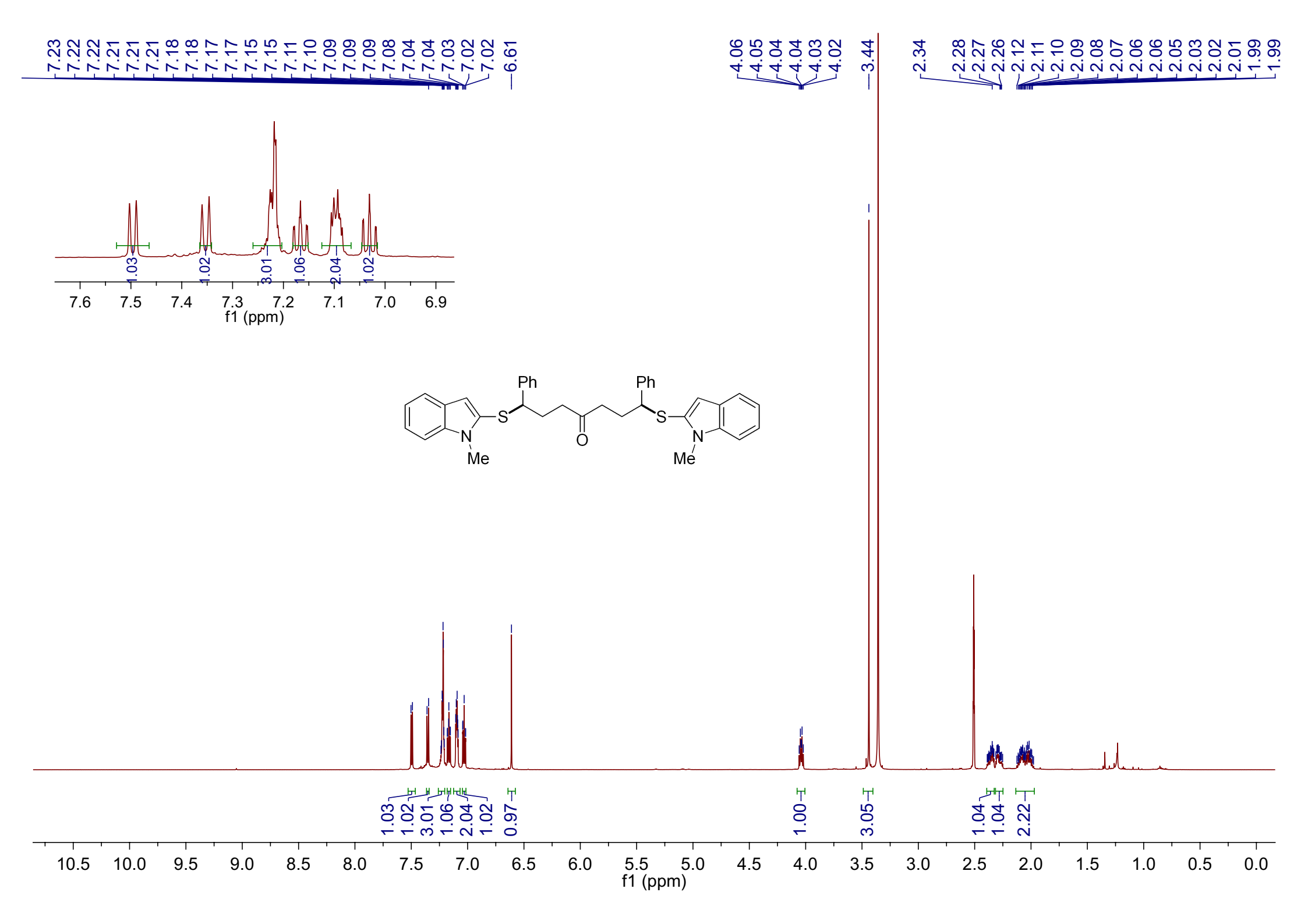
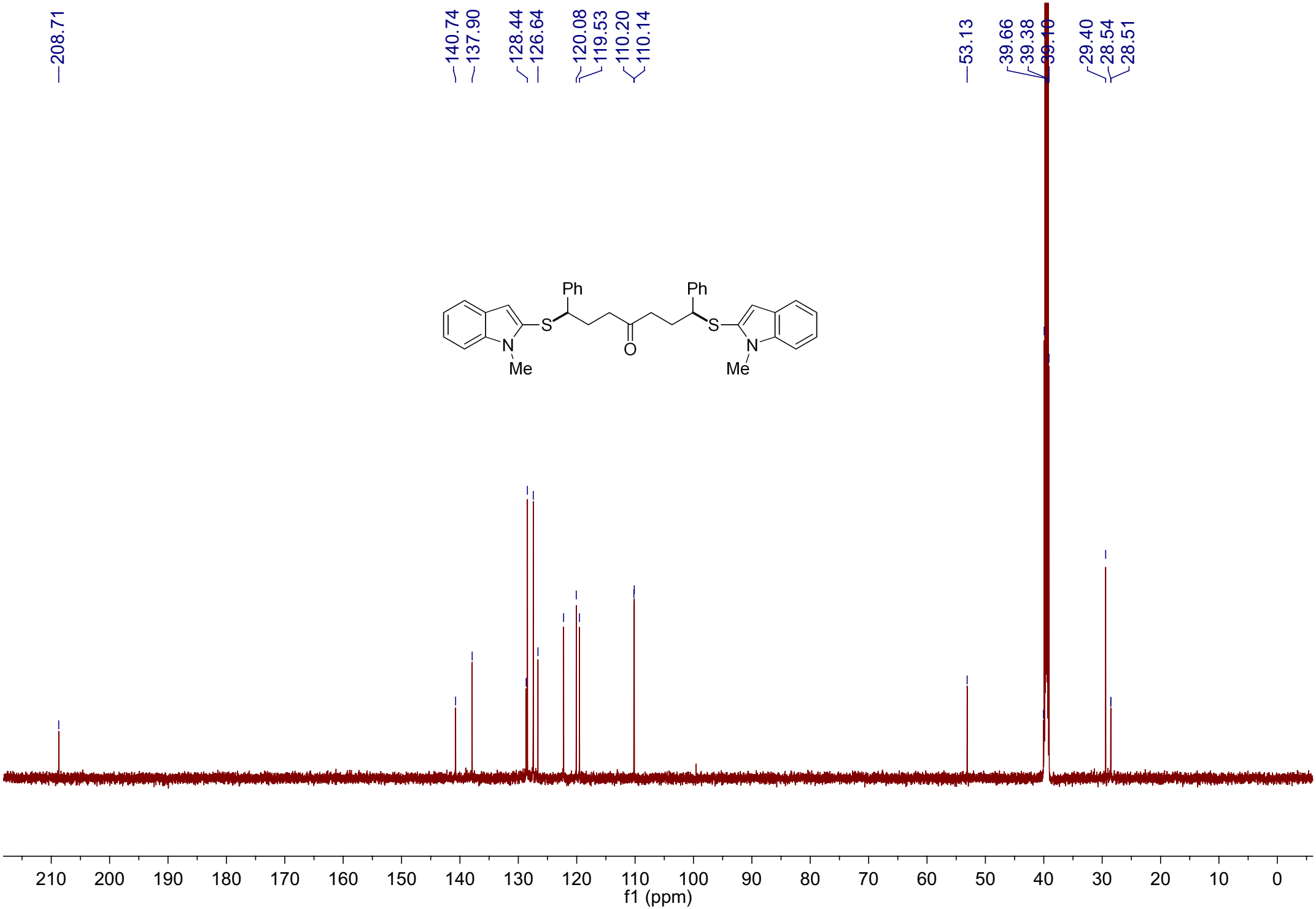
127.45
126.64
119.51
110.20
110.14
109.95
107.05
53.20
39.80
39.52
39.10
34.37
29.41
22.90
Ph
S
S
N
Me
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.23 7.22 7.22 7.21 7.21 7.21 7.18 7.18 7.17 7.17 7.15 7.15 7.11 7.10 7.09 7.09 7.09 7.08 7.04 7.04 7.03 7.02 7.02 6.61
4.06 4.05 4.04 4.04 4.03 4.02 3.44 2.34 2.28 2.27 2.26 2.12 2.11 2.10 2.09 2.08 2.07 2.06 2.06 2.05 2.03 2.02 2.01 1.99 1.99
1.03 1.02 3.01 1.06 2.04 1.02
7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
Ph
Ph
S
S
N
N
Me
Me
O
1.03 1.02 3.01 1.06 2.04 1.02 0.97 1.00 3.05 1.04 1.04 2.22
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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120.08
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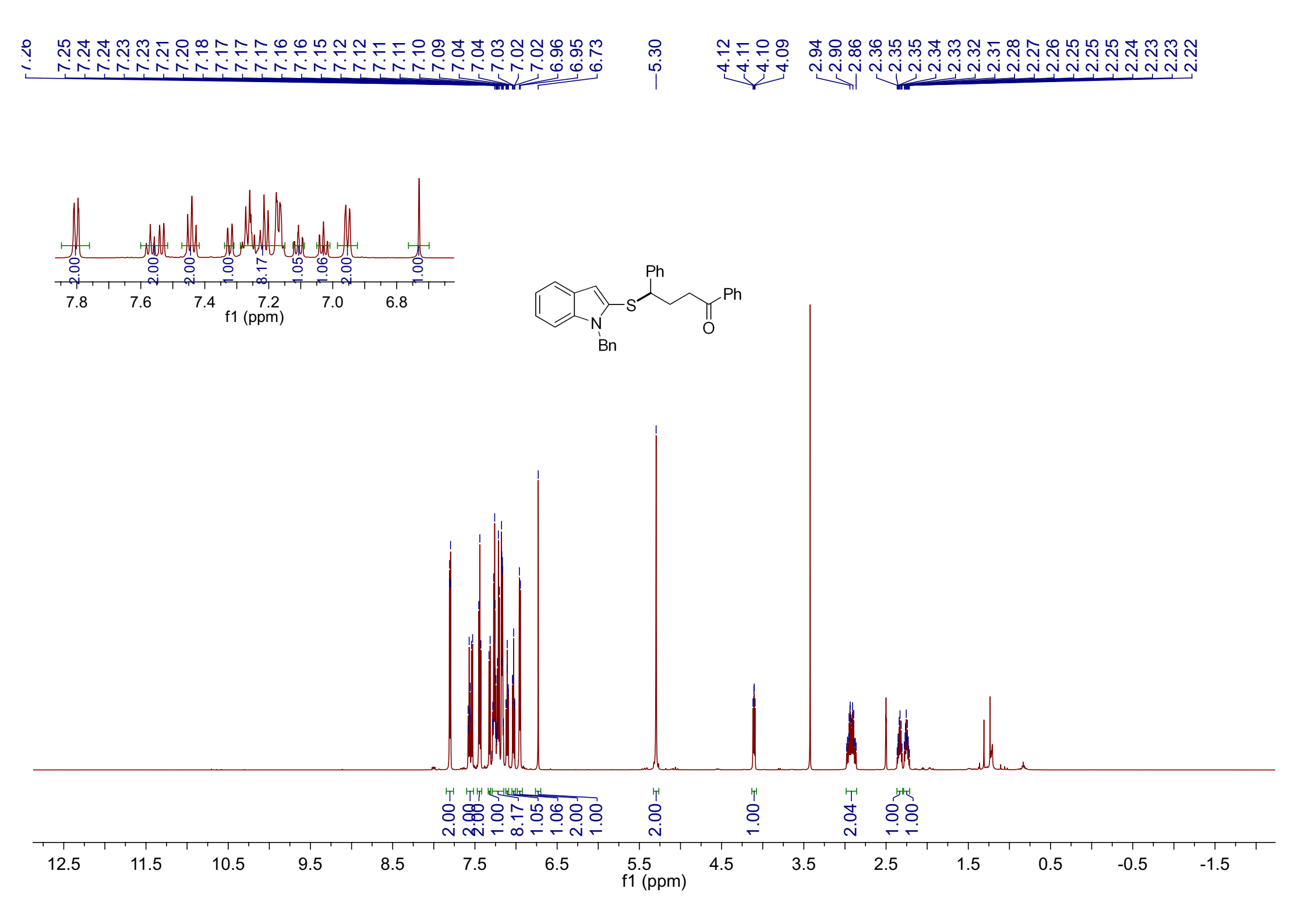
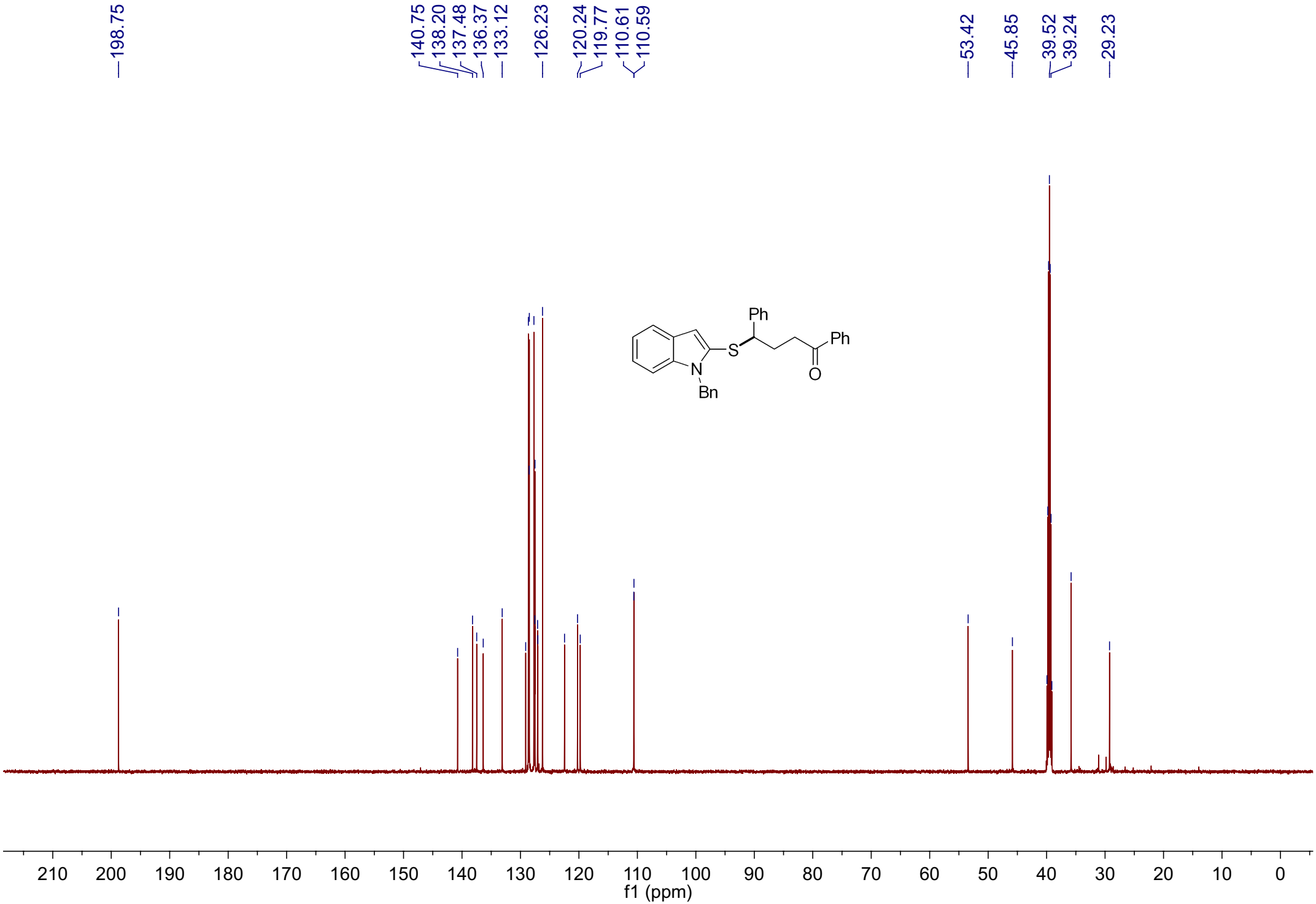
110.20
110.14
53.13
39.66
39.38
39.10
29.40
28.54
28.51
Ph
Ph
S
S
N
N
Me
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.25 7.24 7.24 7.23 7.23 7.21 7.20 7.18 7.17 7.17 7.17 7.16 7.16 7.15 7.12 7.12 7.11 7.11 7.10 7.09 7.04 7.04 7.03 7.02 7.02 6.96 6.95 6.73
5.30
4.12 4.11 4.10 4.09
2.94 2.90 2.86
2.36 2.35 2.35 2.34 2.33 2.32 2.31 2.28 2.27 2.26 2.25 2.25 2.25 2.24 2.23 2.23 2.22
2.00 2.00 2.00 1.00 8.17 1.05 1.06 2.00 1.00
7.8 7.6 7.4 7.2 7.0 6.8
f1 (ppm)
Ph
S
Ph
N
O
Bn
2.00 2.00 2.00 1.00 8.17 1.05 1.06 2.00 1.00 2.00 1.00 2.04 1.00 1.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)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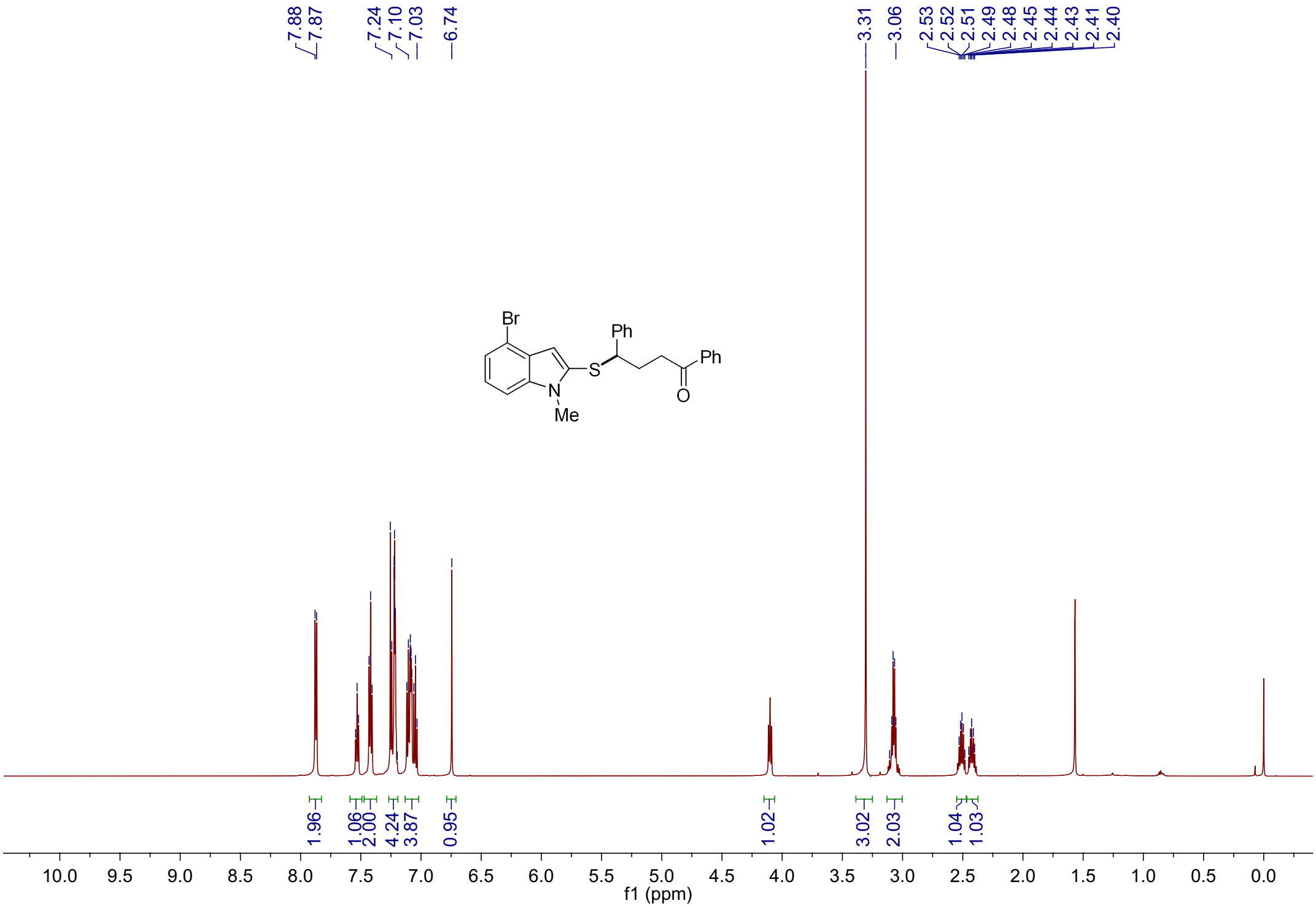
140.75
138.20
137.48
136.37
133.12
126.23
120.24
119.77
110.61
110.59
53.42
45.85
39.52
39.24
29.23
Ph
S
Ph
N
Bn
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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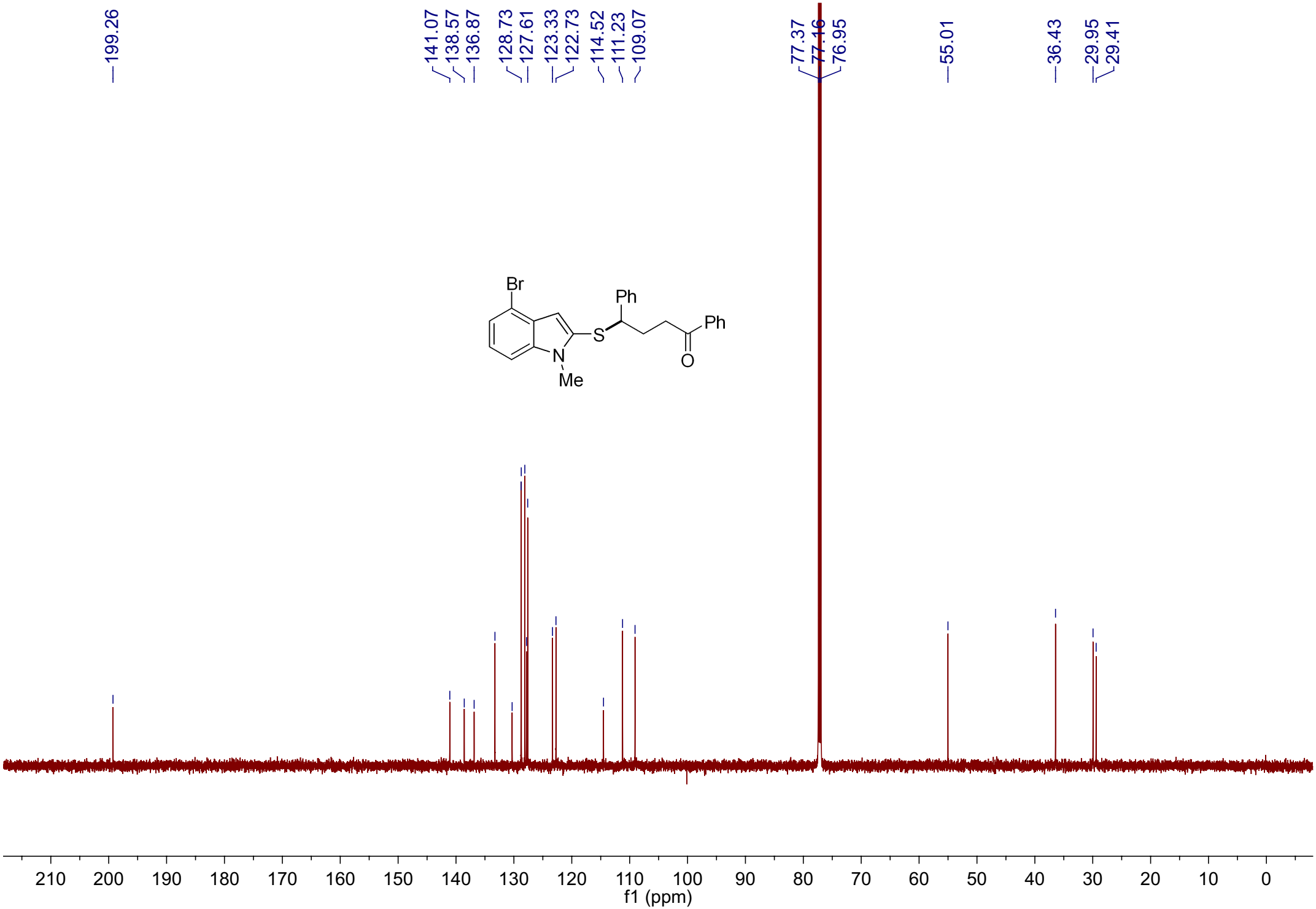
7.87
7.24
7.10
7.03
6.74
3.31
3.06
2.53
2.52
2.51
2.49
2.48
2.45
2.44
2.43
2.41
2.40
Br
Ph
Ph
S
N
Me
O
1.96
1.06
2.00
4.24
3.87
0.95
1.02
3.02
2.03
1.04
1.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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141.07
138.57
136.87
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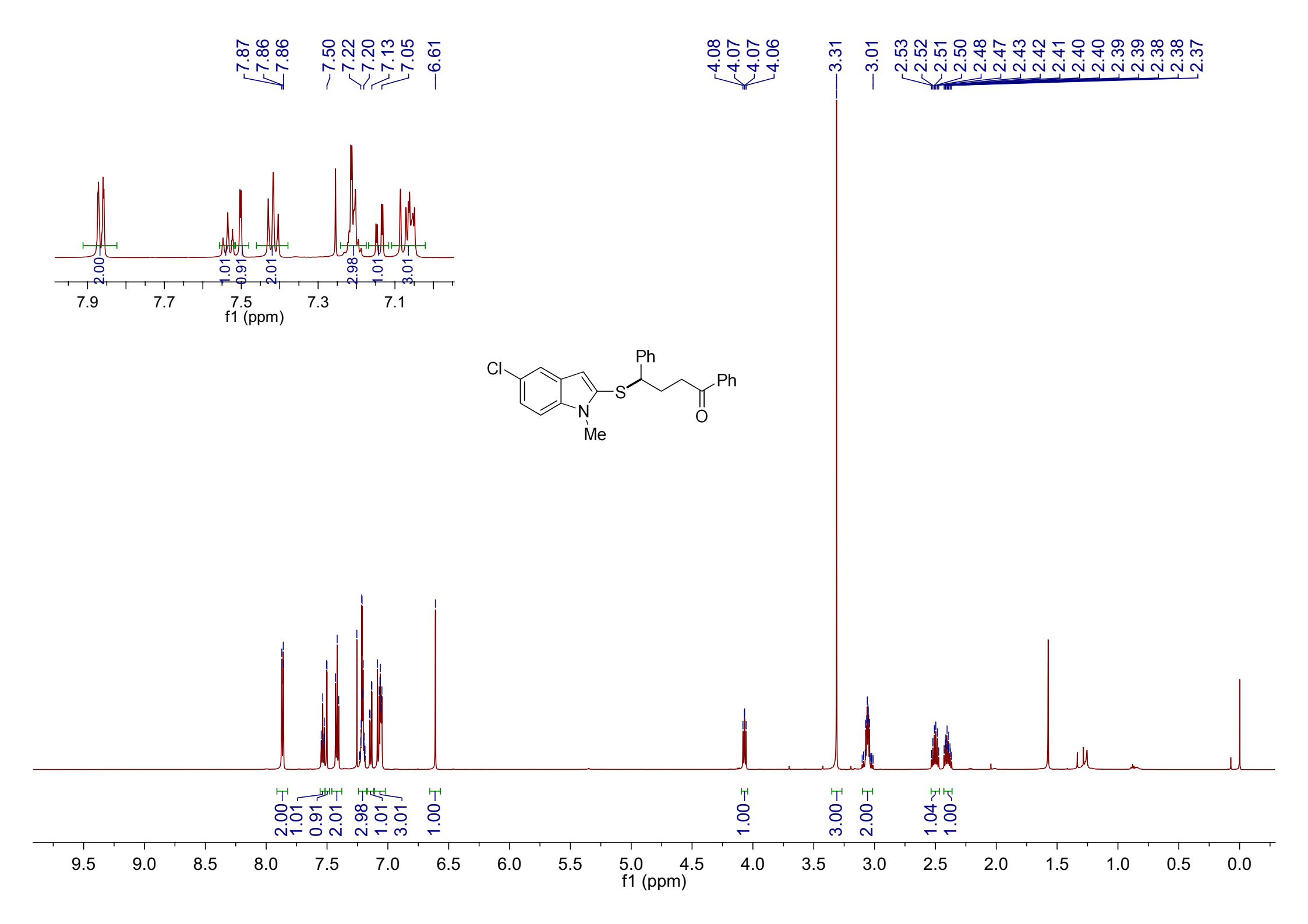
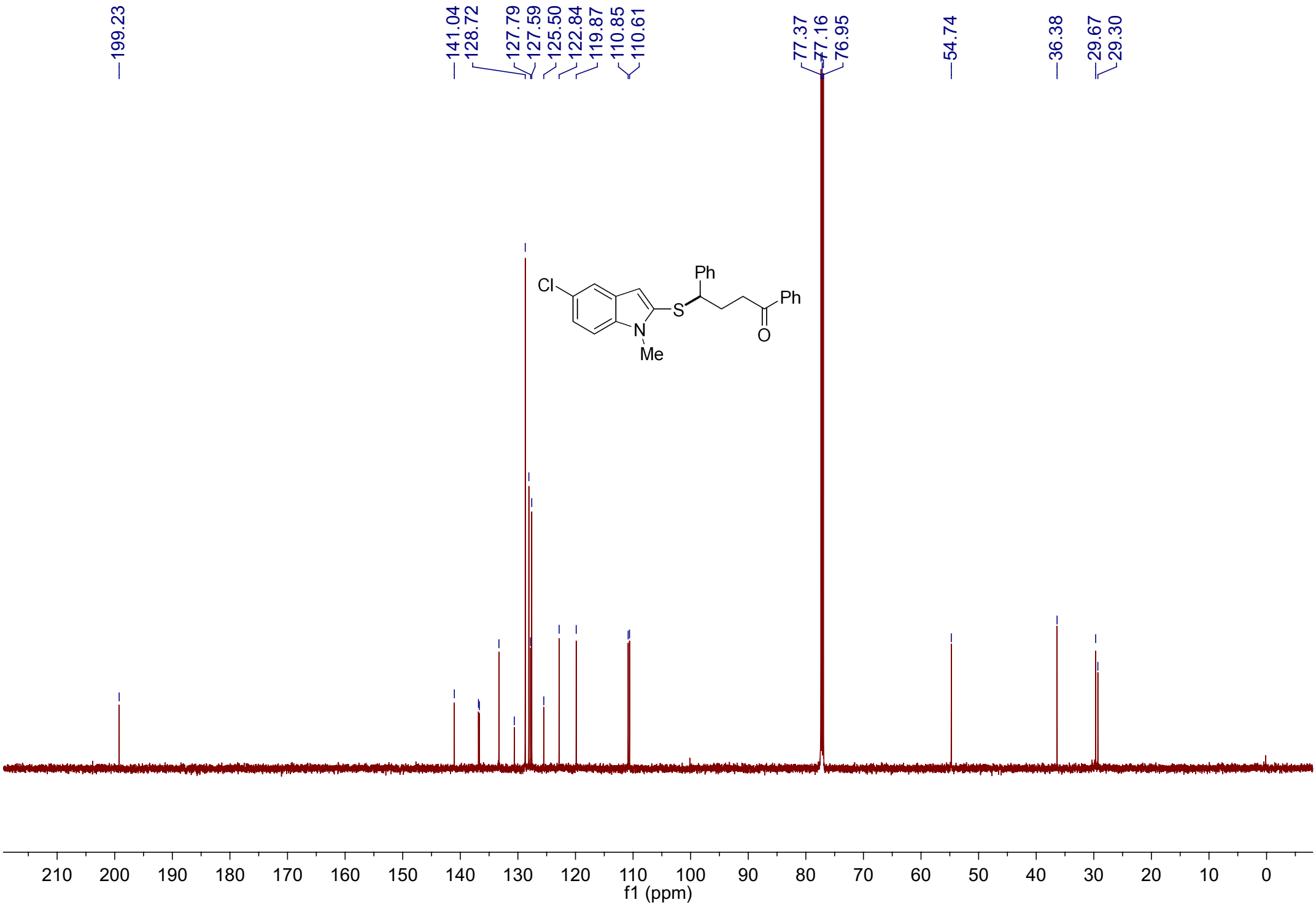
127.61
123.33
122.73
114.52
111.23
109.07
77.37
77.16
76.95
55.01
36.43
29.95
29.41
Br
Ph
S
Ph
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.87
7.86
7.86
7.50
7.22
7.20
7.13
7.05
6.61
4.08
4.07
4.07
4.06
3.31
3.01
2.53
2.52
2.51
2.50
2.48
2.47
2.43
2.42
2.41
2.40
2.40
2.39
2.39
2.38
2.38
2.37
2.00
1.01
0.91
2.01
2.98
1.01
3.01
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
Cl
Ph
S
Ph
N
Me
O
2.00
1.01
0.91
2.01
2.98
1.01
3.01
1.00
1.00
3.00
2.00
1.04
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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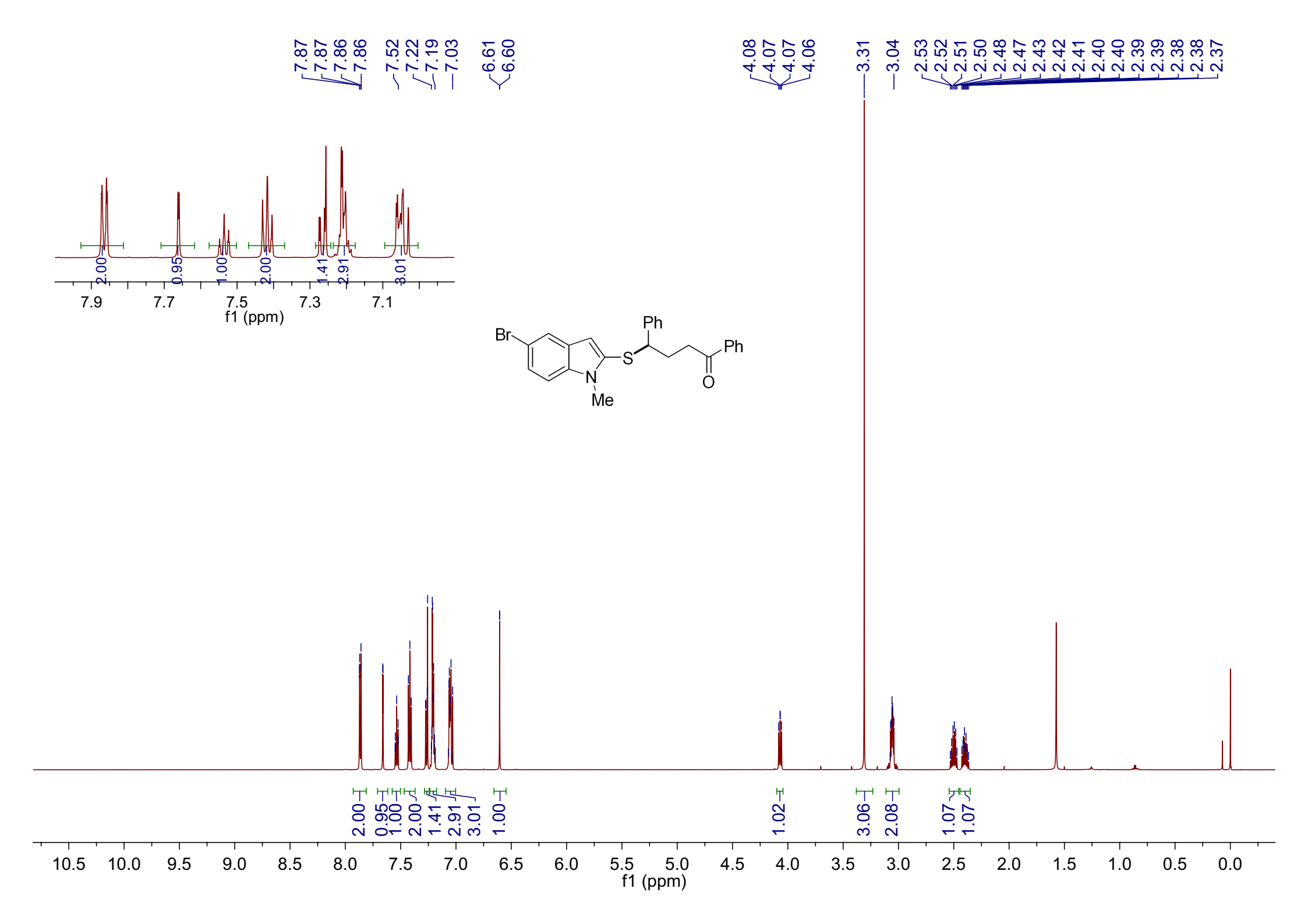
110.85
110.61
77.37
77.16
76.95
54.74
36.38
29.67
29.30
Cl
Ph
S
Ph
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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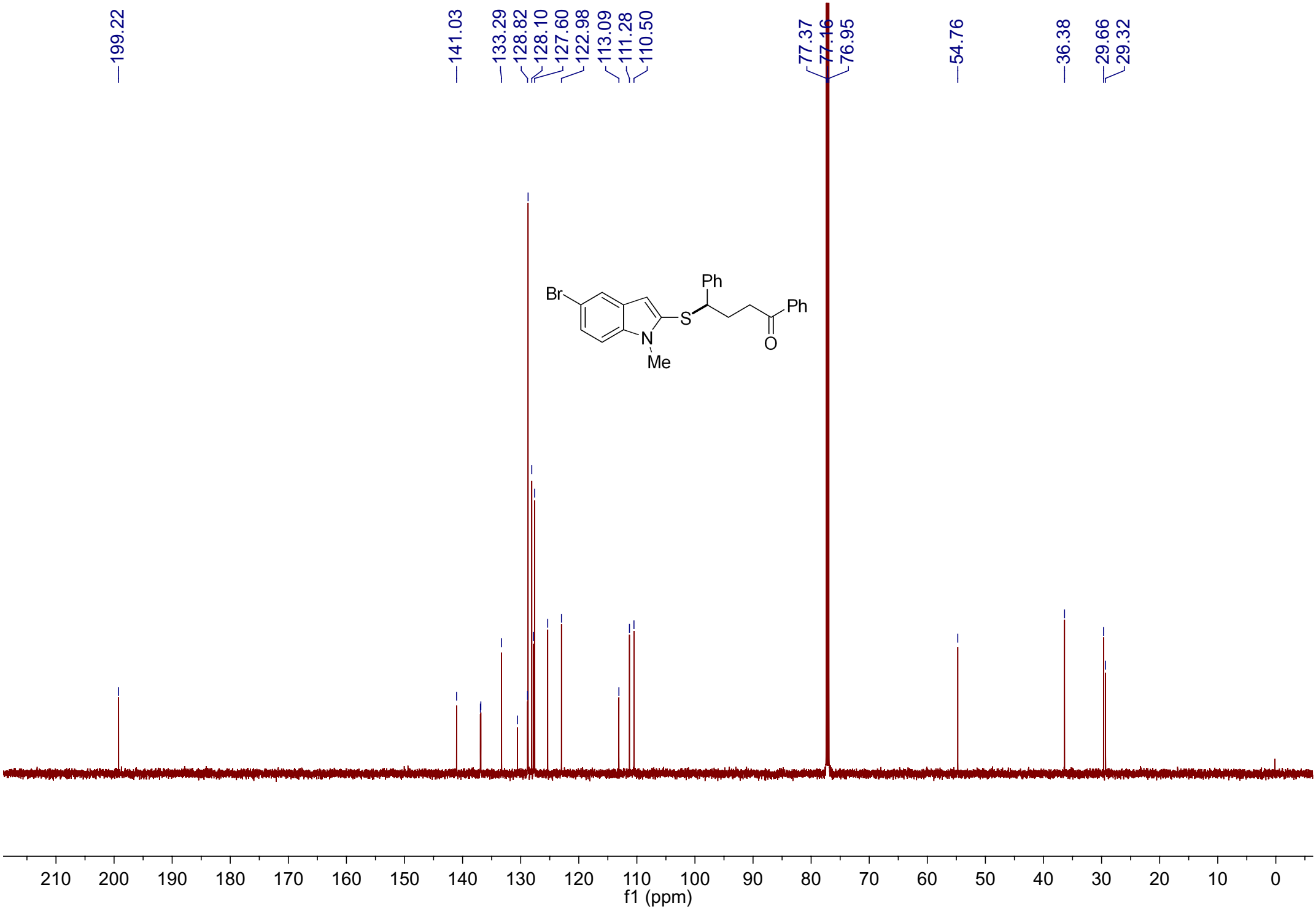
7.87
7.86
7.86
7.52
7.22
7.19
7.03
6.61
6.60
4.08
4.07
4.07
4.06
3.31
3.04
2.53
2.52
2.51
2.50
2.48
2.47
2.43
2.42
2.41
2.40
2.40
2.39
2.39
2.38
2.38
2.37
2.00
0.95
1.00
2.00
1.41
2.91
3.01
f1 (ppm)
Br
Ph
S
Ph
N
Me
O
1.02
3.06
2.08
1.07
1.07
f1 (ppm)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133.29
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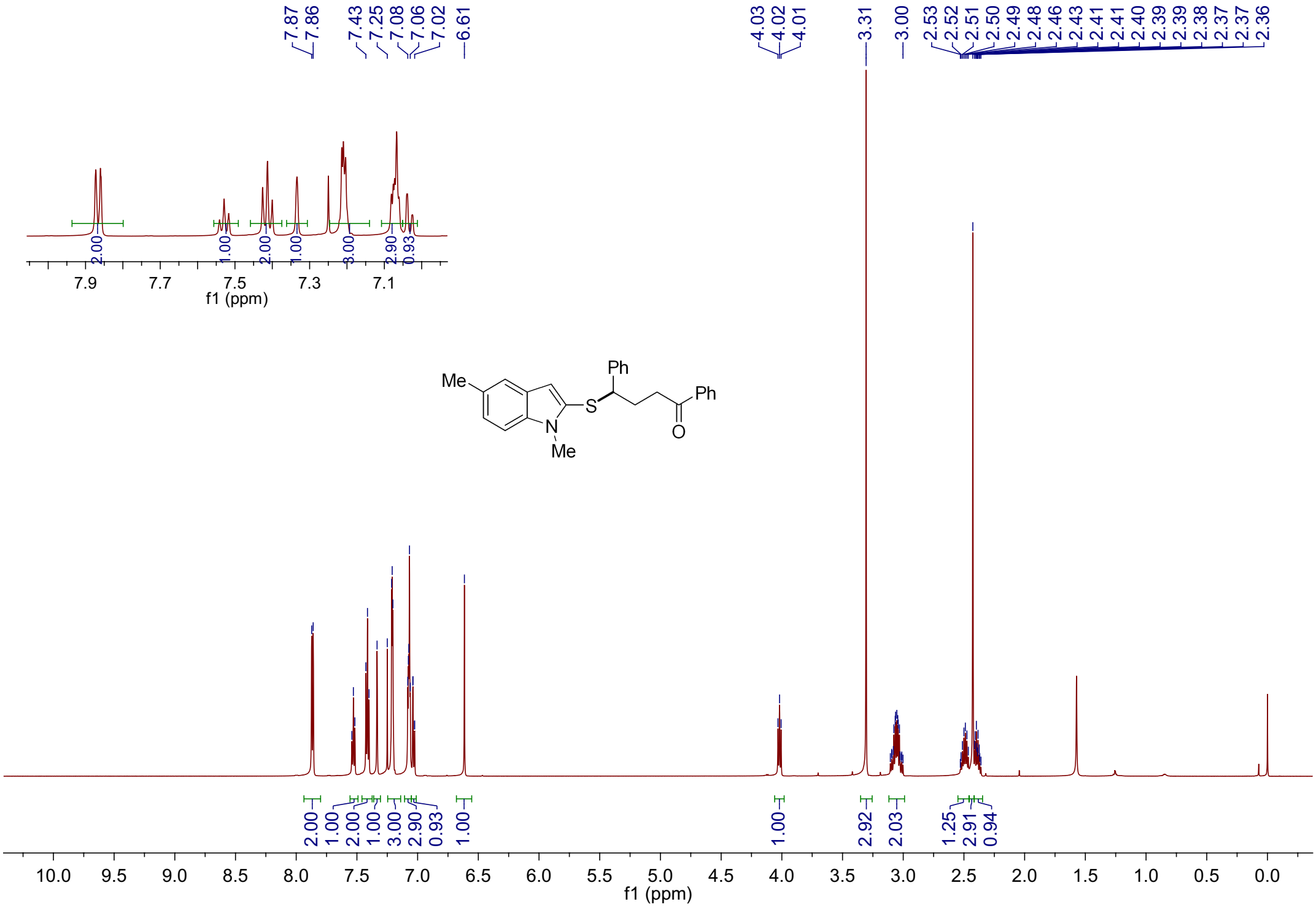
128.10
127.60
122.98
113.09
111.28
110.50
77.37
77.16
76.95
54.76
36.38
29.66
29.32
Br
Ph
S
Ph
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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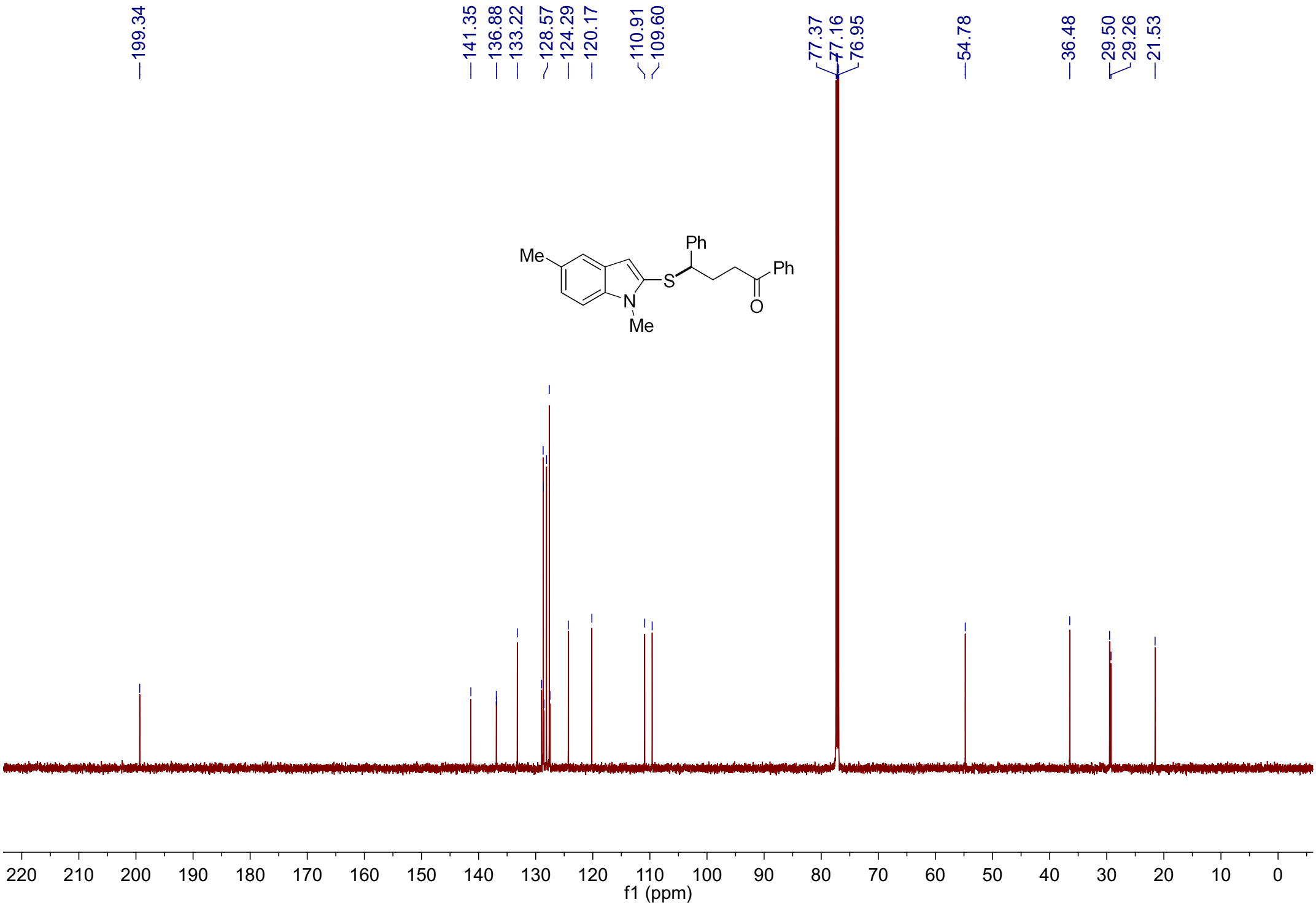
7.86
7.43
7.25
7.08
7.06
7.02
6.61
4.03
4.02
4.01
3.31
3.00
2.53
2.52
2.51
2.50
2.49
2.48
2.46
2.43
2.41
2.41
2.40
2.39
2.39
2.38
2.37
2.37
2.36
2.00
1.00
2.00
1.00
3.00
2.90
0.93
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
Me
Ph
S
Ph
N
O
Me
2.00
1.00
2.00
1.00
3.00
2.90
0.93
1.00
1.00
2.92
2.03
1.25
2.91
0.94
10.0
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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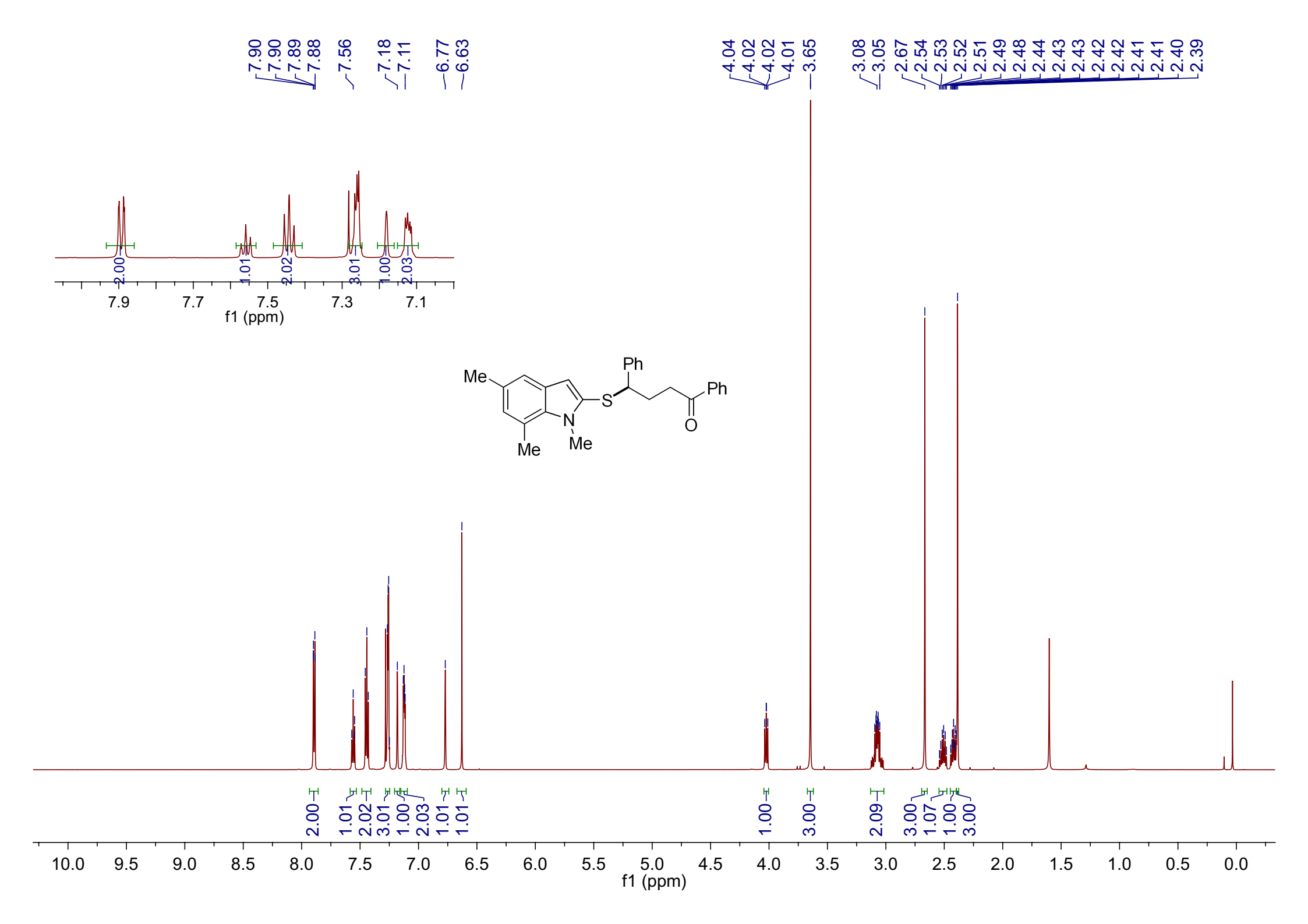
133.22
128.57
124.29
120.17
110.91
109.60
77.37
77.16
76.95
54.78
36.48
29.50
29.26
21.53
Me
Ph
S
Ph
N
Me
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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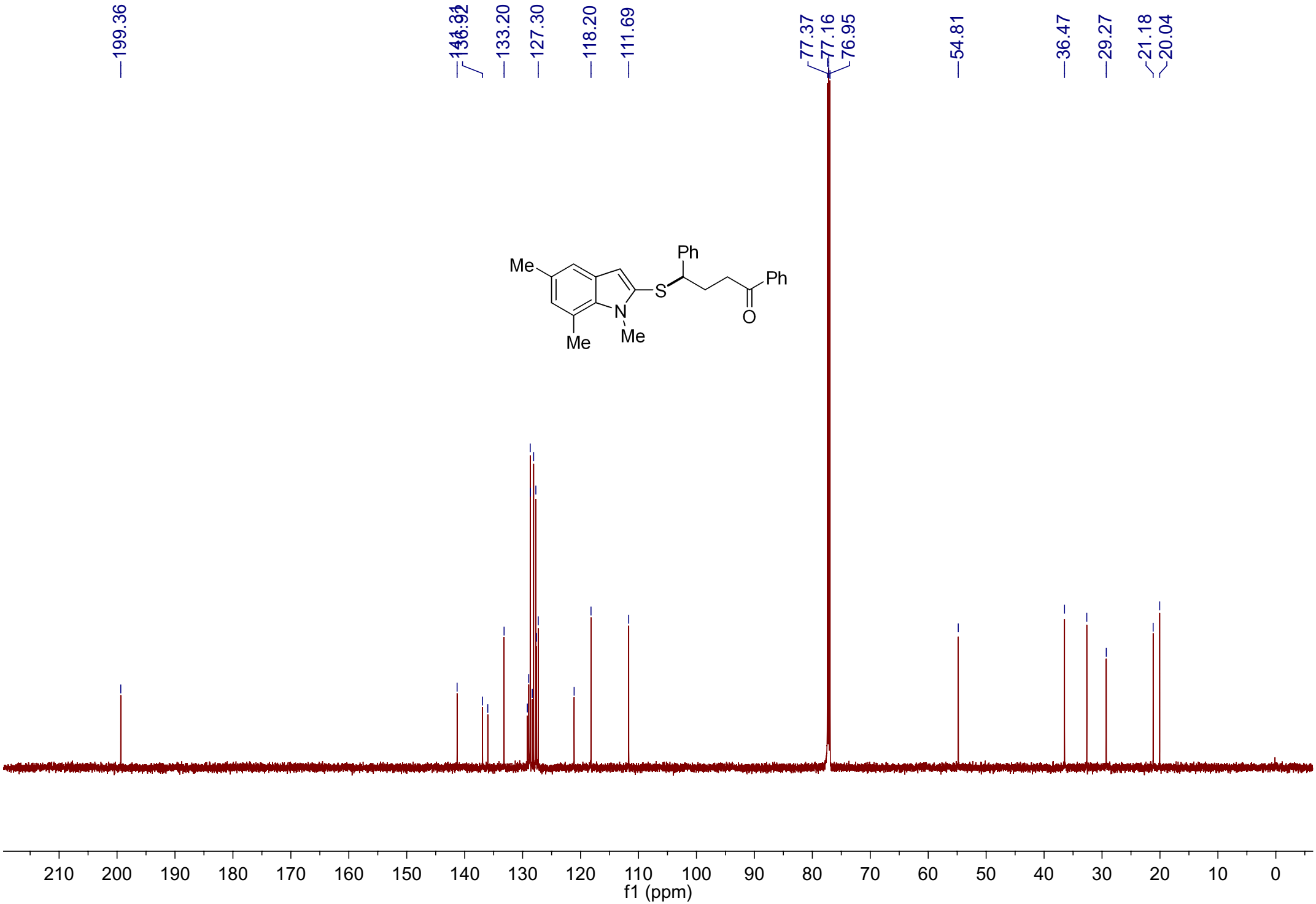
7.56
7.18
7.11
6.77
6.63
4.04
4.02
4.02
4.01
3.65
3.08
3.05
2.67
2.54
2.53
2.52
2.51
2.49
2.48
2.44
2.43
2.43
2.42
2.42
2.41
2.41
2.40
2.39
2.00
1.01
2.02
3.01
1.00
2.03
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
Me
Ph
S
Ph
N
O
Me
Me
2.00
1.01
2.02
3.01
1.00
2.03
1.01
1.01
1.00
3.00
2.09
3.00
1.07
1.00
3.00
10.0
9.5
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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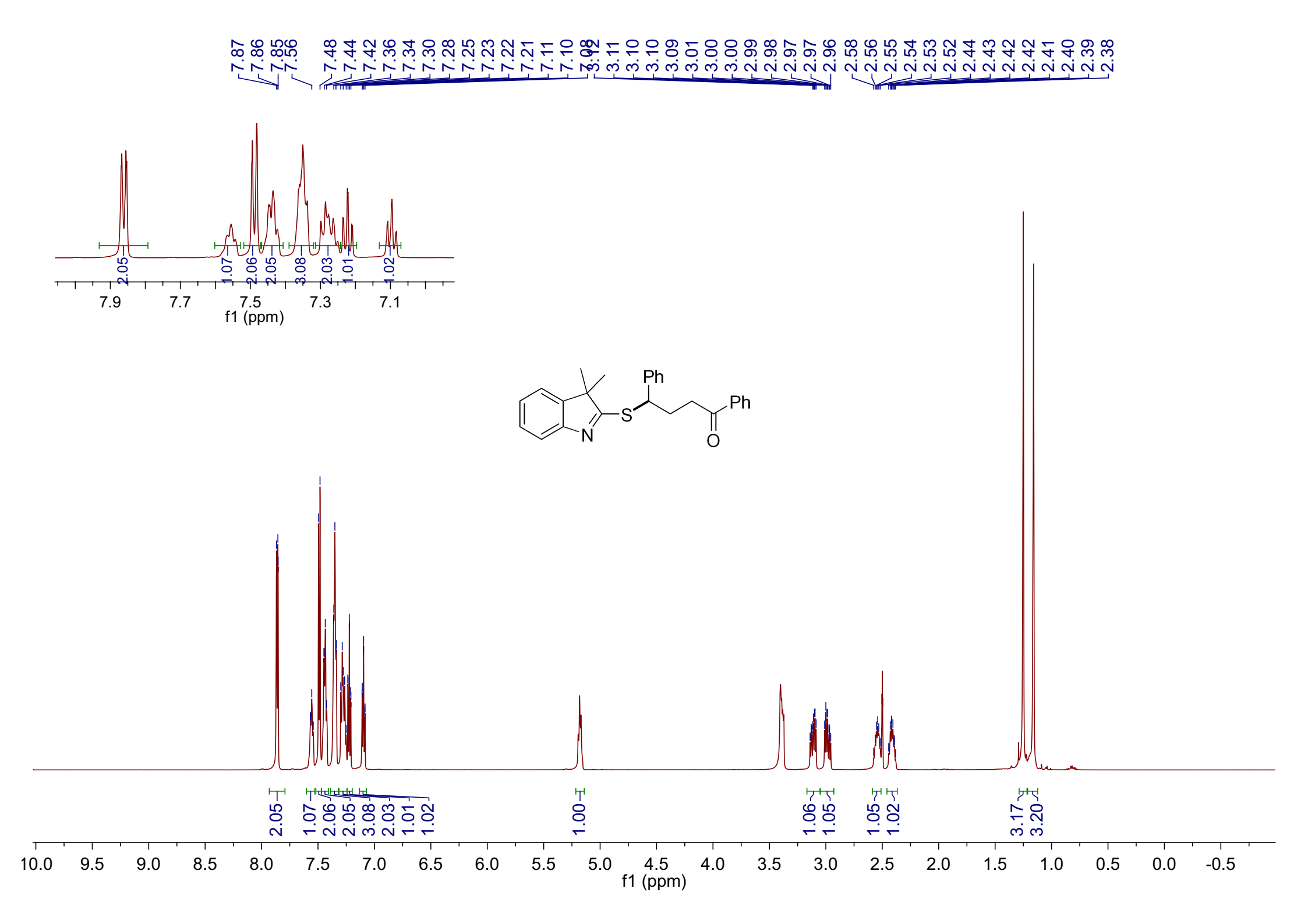
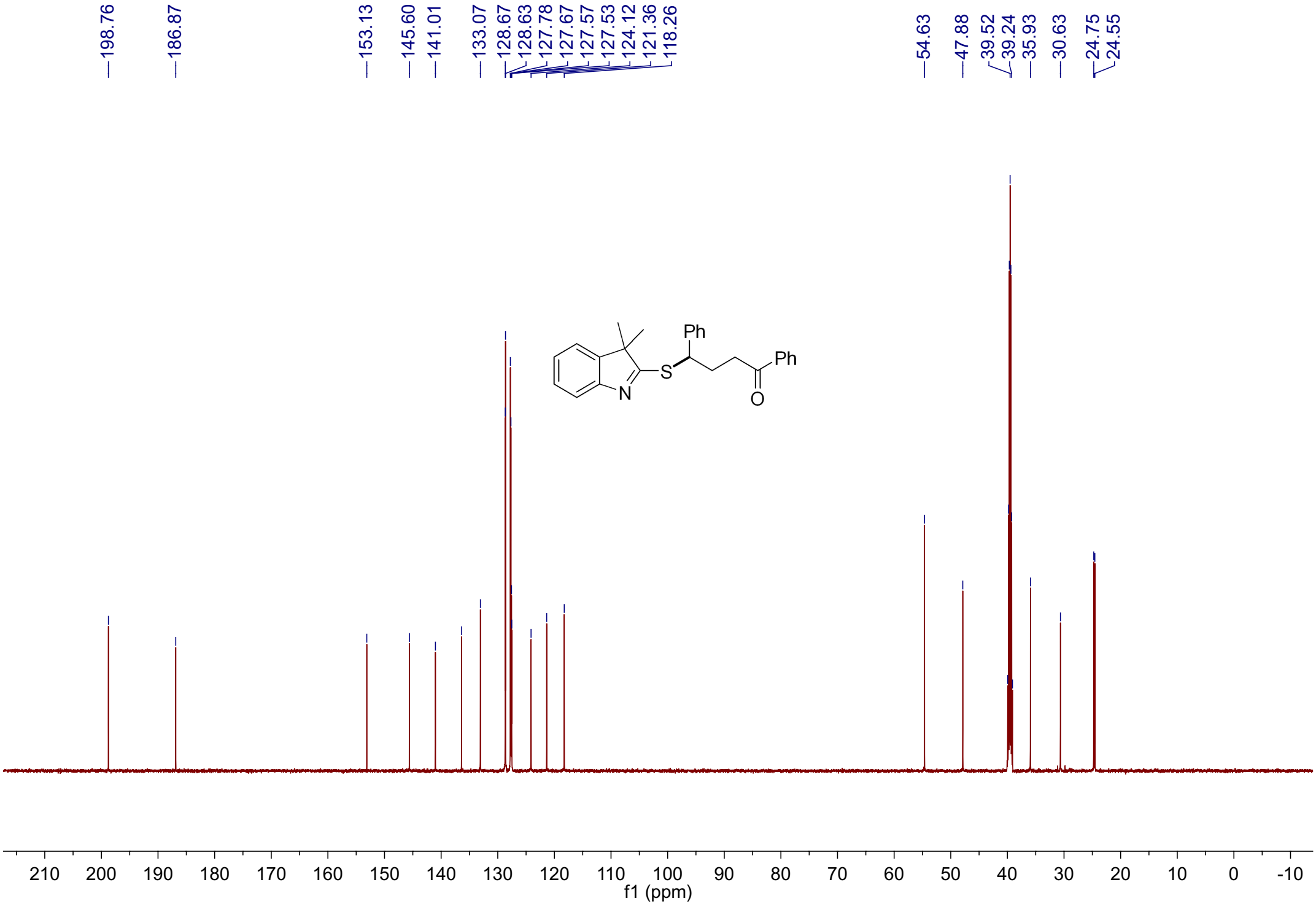
111.69
77.37
77.16
76.95
54.81
36.47
29.27
21.18
20.04
Me
Me
N
Me
S
Ph
Ph
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.87 7.86 7.85 7.56 7.48 7.44 7.42 7.36 7.34 7.30 7.28 7.25 7.23 7.22 7.21 7.11 7.10 3.11 3.10 3.10 3.09 3.01 3.00 3.00 2.99 2.98 2.97 2.97 2.96 2.58 2.56 2.55 2.54 2.53 2.52 2.44 2.43 2.42 2.42 2.41 2.40 2.39 2.38
2.05 1.07 2.06 2.05 3.08 2.03 1.01 1.02
7.9 7.7 7.5 7.3 7.1
f1 (ppm)
Ph
S
N
Ph
O
2.05 1.07 2.06 2.05 3.08 2.03 1.01 1.02 1.00 1.06 1.05 1.05 1.02 3.17 3.20
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 -0.5
f1 (ppm)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128.63
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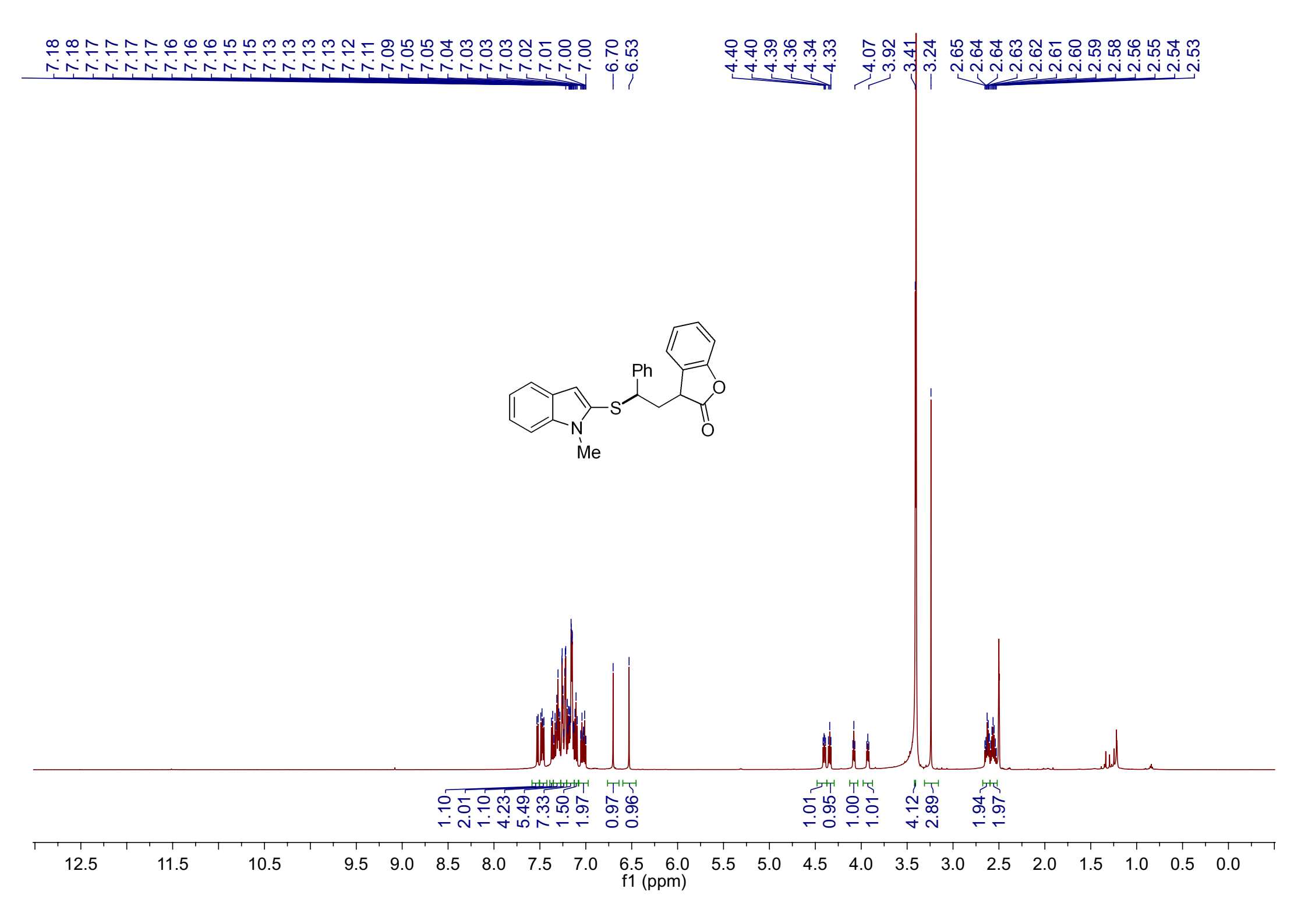
127.67
127.57
127.53
124.12
121.36
118.26
54.63
47.88
39.52
39.24
35.93
30.63
24.75
24.55
Ph
S
N
O
Ph
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.18 7.18 7.17 7.17 7.17 7.17 7.16 7.16 7.16 7.15 7.15 7.13 7.13 7.13 7.13 7.12 7.11 7.09 7.05 7.05 7.04 7.03 7.03 7.03 7.02 7.01 7.00 7.00 6.70 6.53
4.40 4.40 4.39 4.36 4.34 4.33 4.07 3.92 3.41 3.24 2.65 2.64 2.64 2.63 2.62 2.61 2.60 2.59 2.58 2.56 2.55 2.54 2.53
Ph
S
O
O
N
Me
1.10 2.01 1.10 4.23 5.49 7.33 1.50 1.97 0.97 0.96 1.01 0.95 1.00 1.01 4.12 2.89 1.94 1.97
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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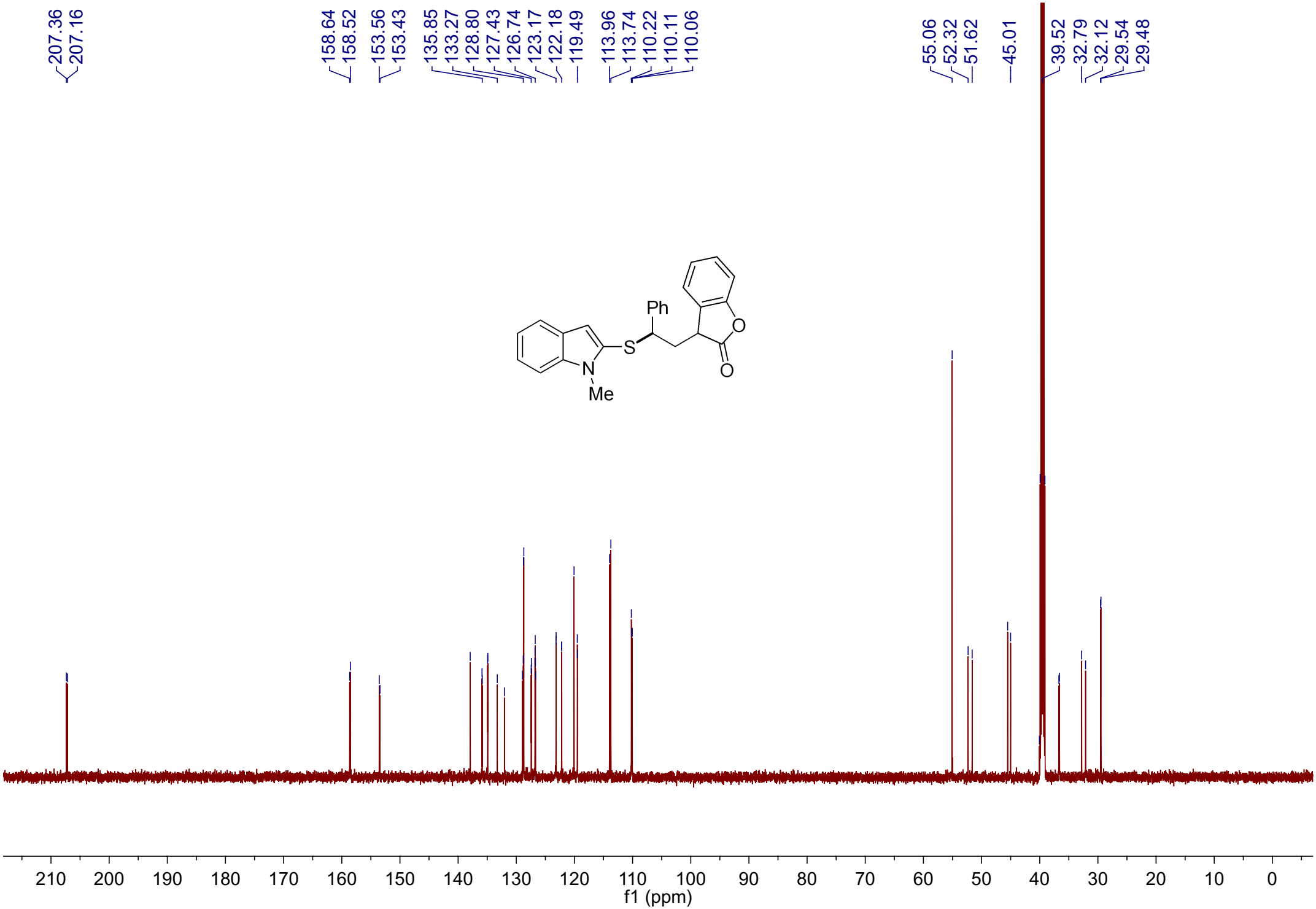
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127.43
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122.18
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113.96
113.74
110.22
110.11
110.06
55.06
52.32
51.62
45.01
39.52
32.79
32.12
29.54
29.48
Ph
S
N
Me
O
O
210
200
190
180
170
160
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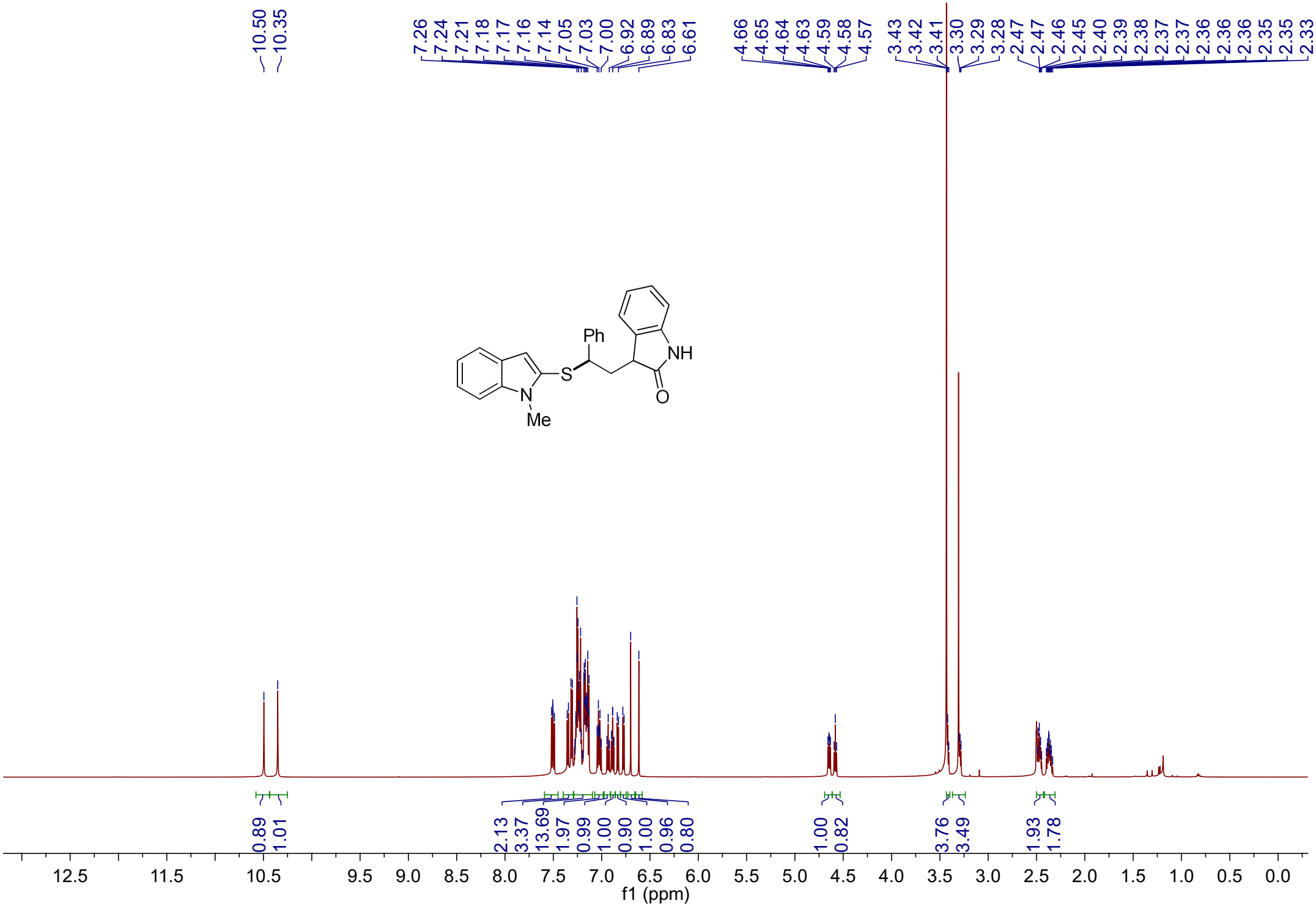
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.03
7.00
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6.89
6.83
6.61
4.66
4.65
4.64
4.63
4.59
4.58
4.57
3.43
3.42
3.41
3.30
3.29
3.28
2.47
2.47
2.46
2.45
2.40
2.39
2.38
2.37
2.37
2.36
2.36
2.36
2.35
2.35
2.33
Ph
NH
S
N
Me
O
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1.01
2.13
3.37
13.69
1.97
0.99
1.00
0.90
1.00
0.96
0.80
1.00
0.82
3.76
3.49
1.93
1.78
12.5
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9.5
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
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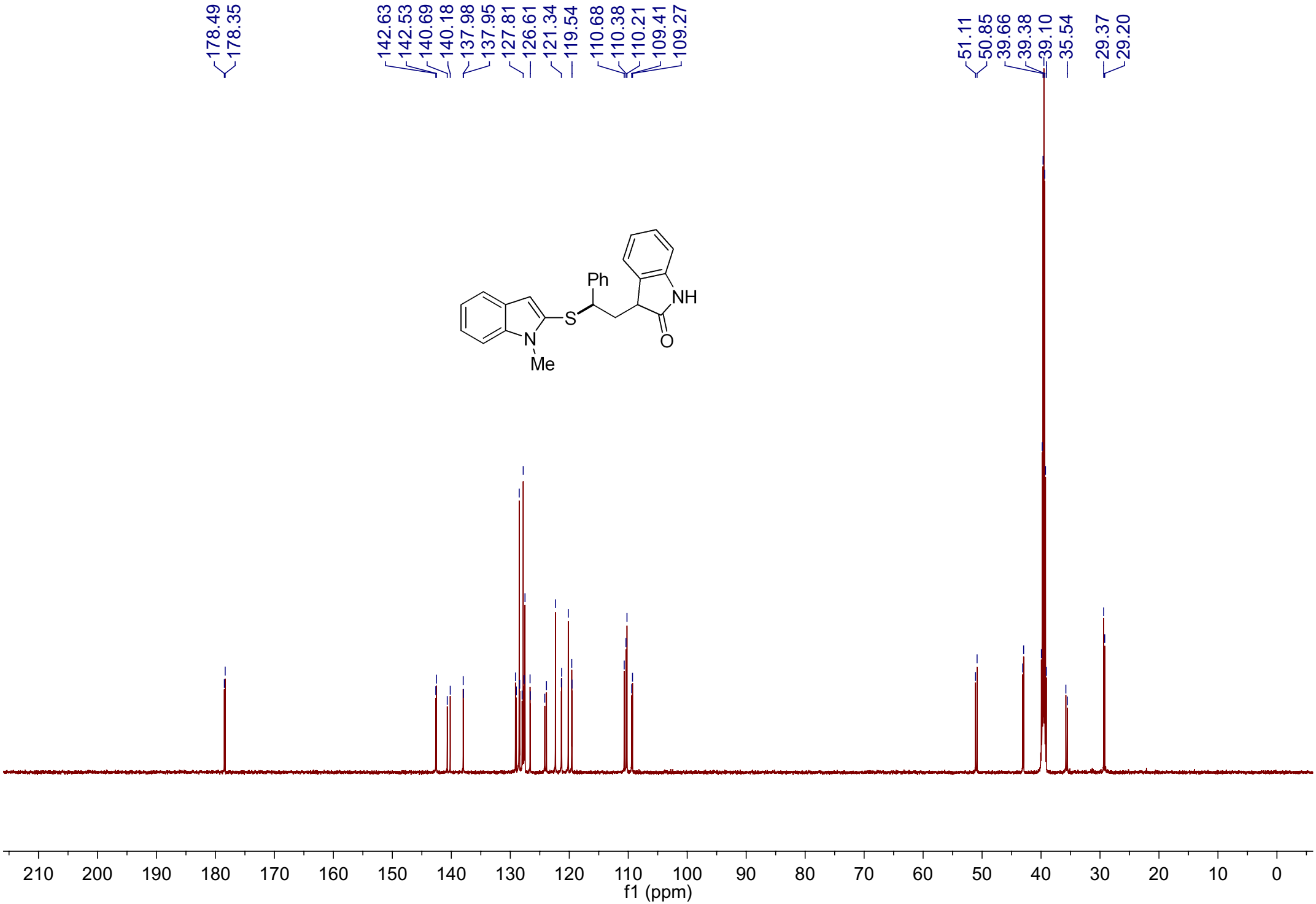
0.0
f1 (ppm)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110.38
110.21
109.41
109.27
51.11
50.85
39.66
39.38
39.10
35.54
29.37
29.20
Ph
NH
S
N
Me
O
210
200
190
180
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120
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50
40
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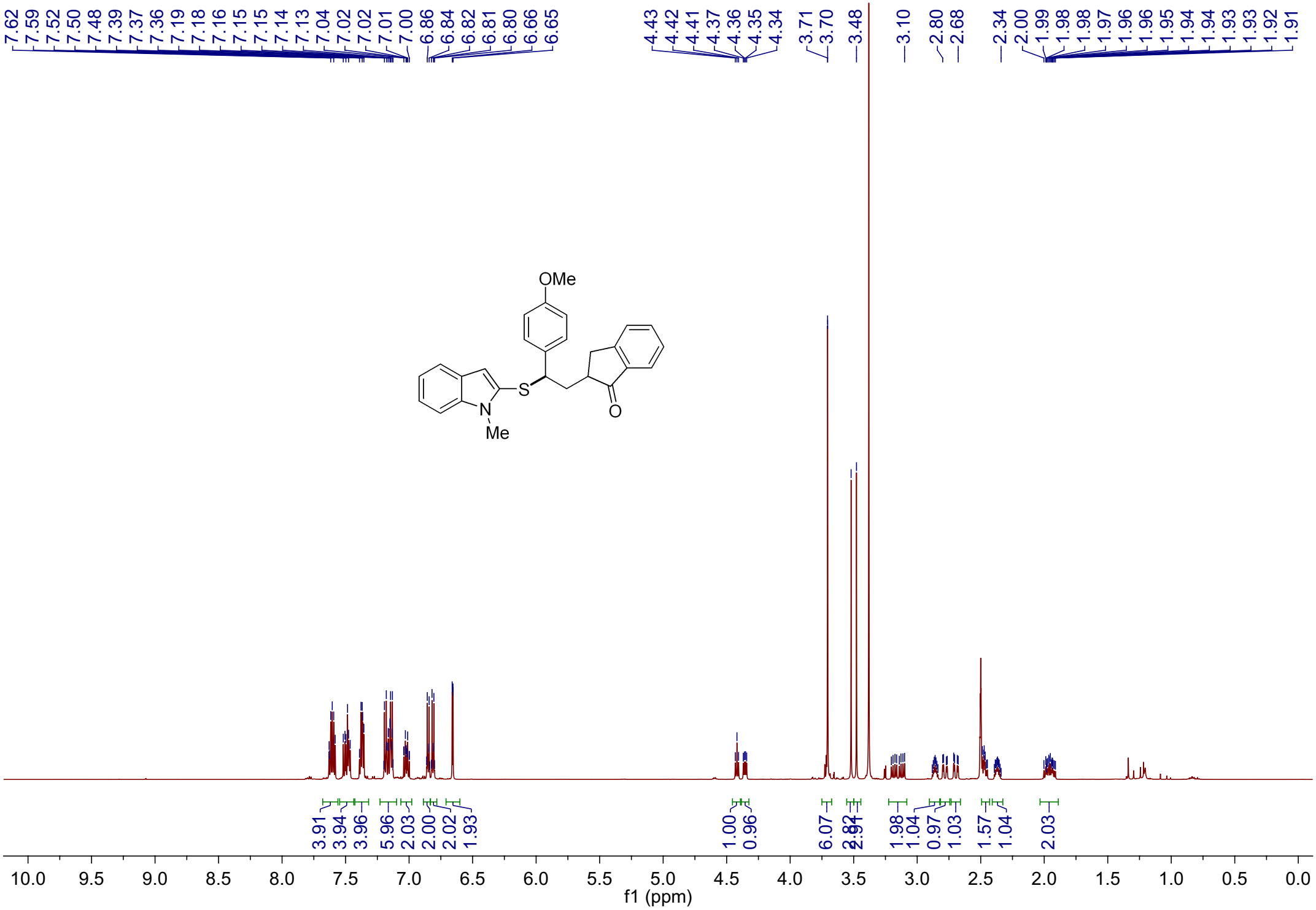
0
f1 (ppm)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7.36
7.19
7.18
7.16
7.15
7.15
7.14
7.13
7.04
7.02
7.02
7.01
7.00
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6.84
6.82
6.81
6.80
6.66
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4.43
4.42
4.41
4.37
4.36
4.35
4.34
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3.48
3.10
2.80
2.68
2.34
2.00
1.99
1.98
1.98
1.97
1.96
1.96
1.95
1.94
1.94
1.93
1.93
1.92
1.91
OMe
S
N
Me
O
3.91
3.94
3.96
5.96
2.03
2.00
2.02
1.93
1.00
0.96
6.07
1.98
1.04
0.97
1.03
1.57
1.04
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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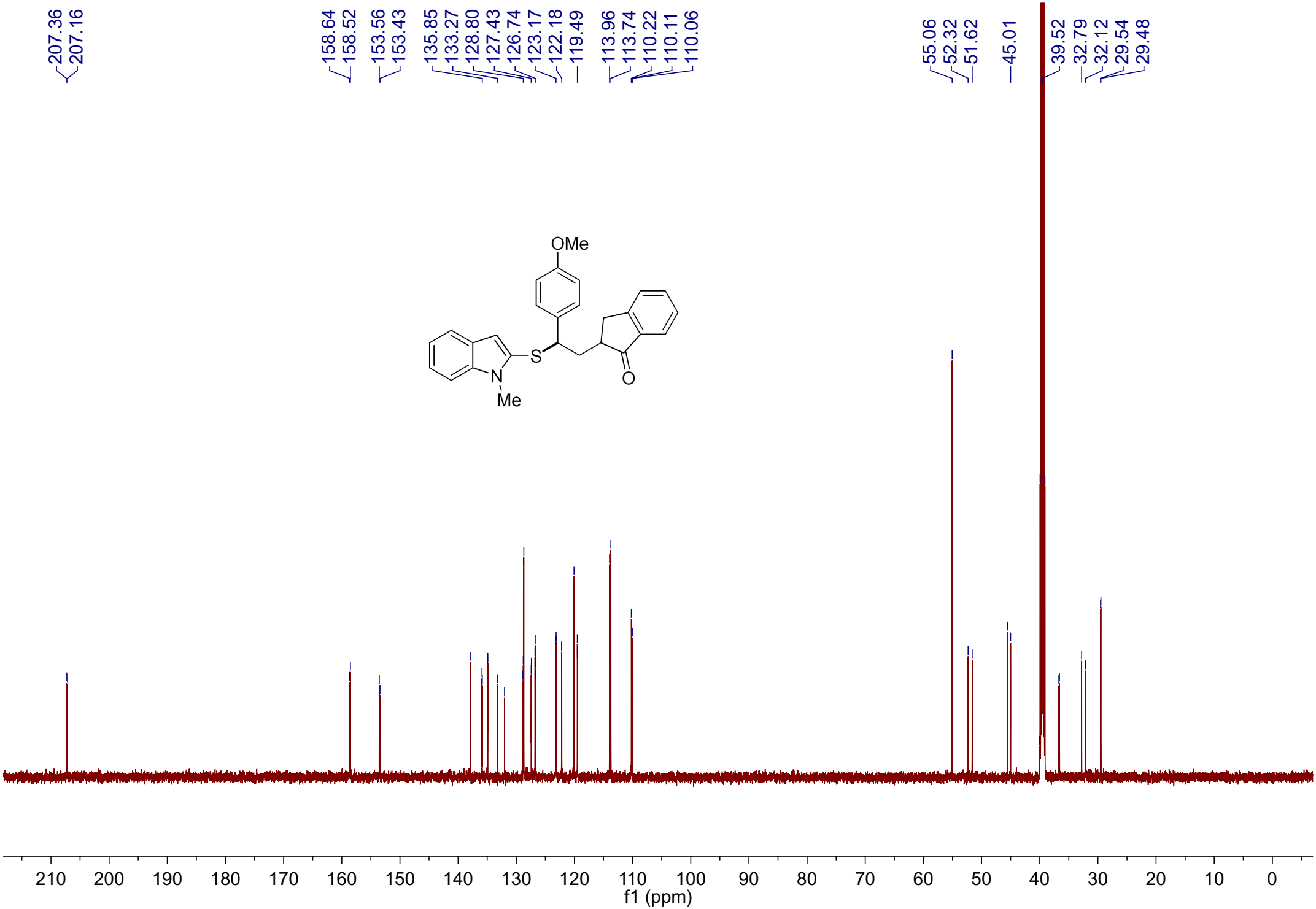
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.43
126.74
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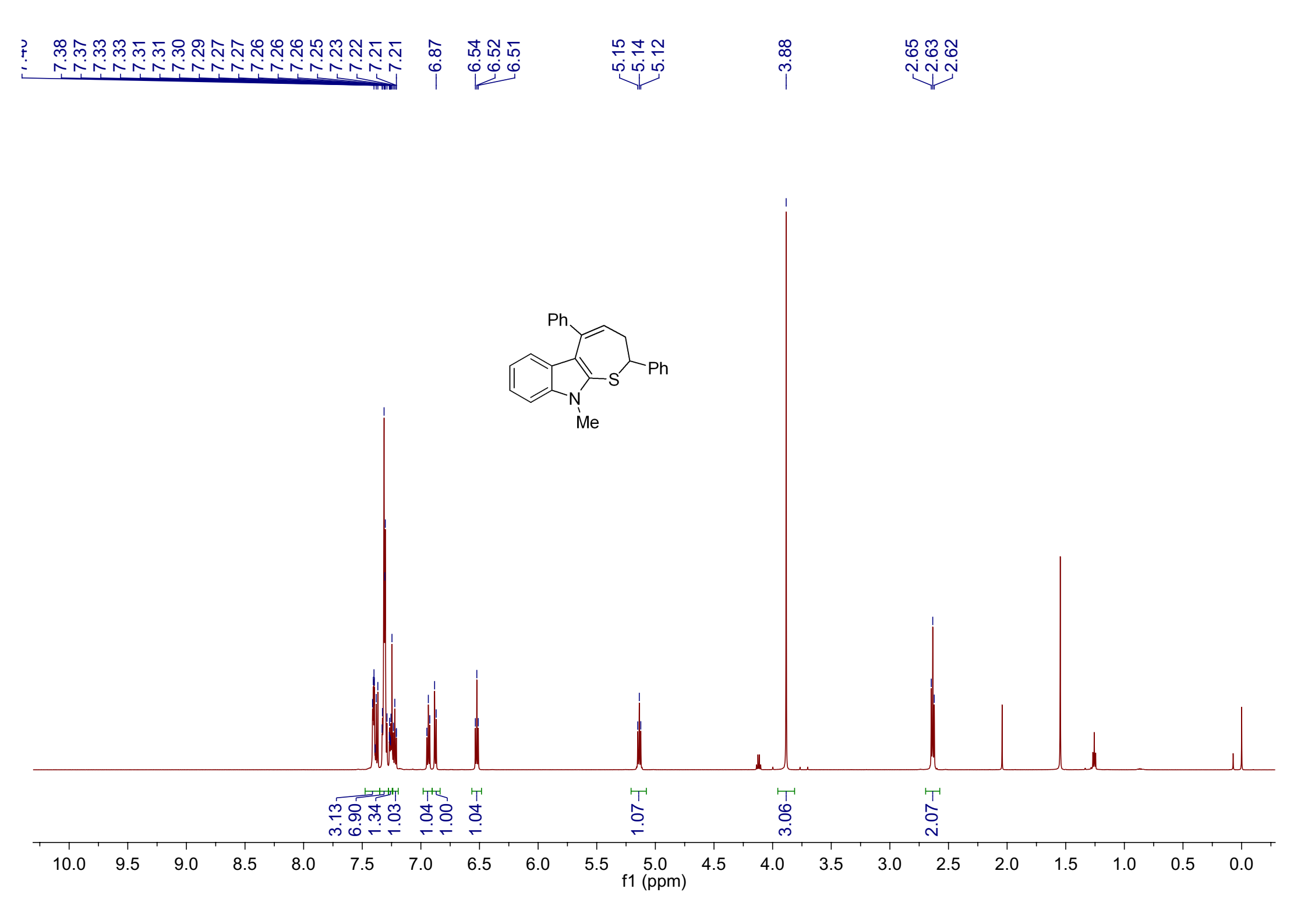
122.18
119.49
113.96
113.74
110.22
110.11
110.06
55.06
52.32
51.62
45.01
39.52
32.79
32.12
29.54
29.48
OMe
S
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.37
7.33
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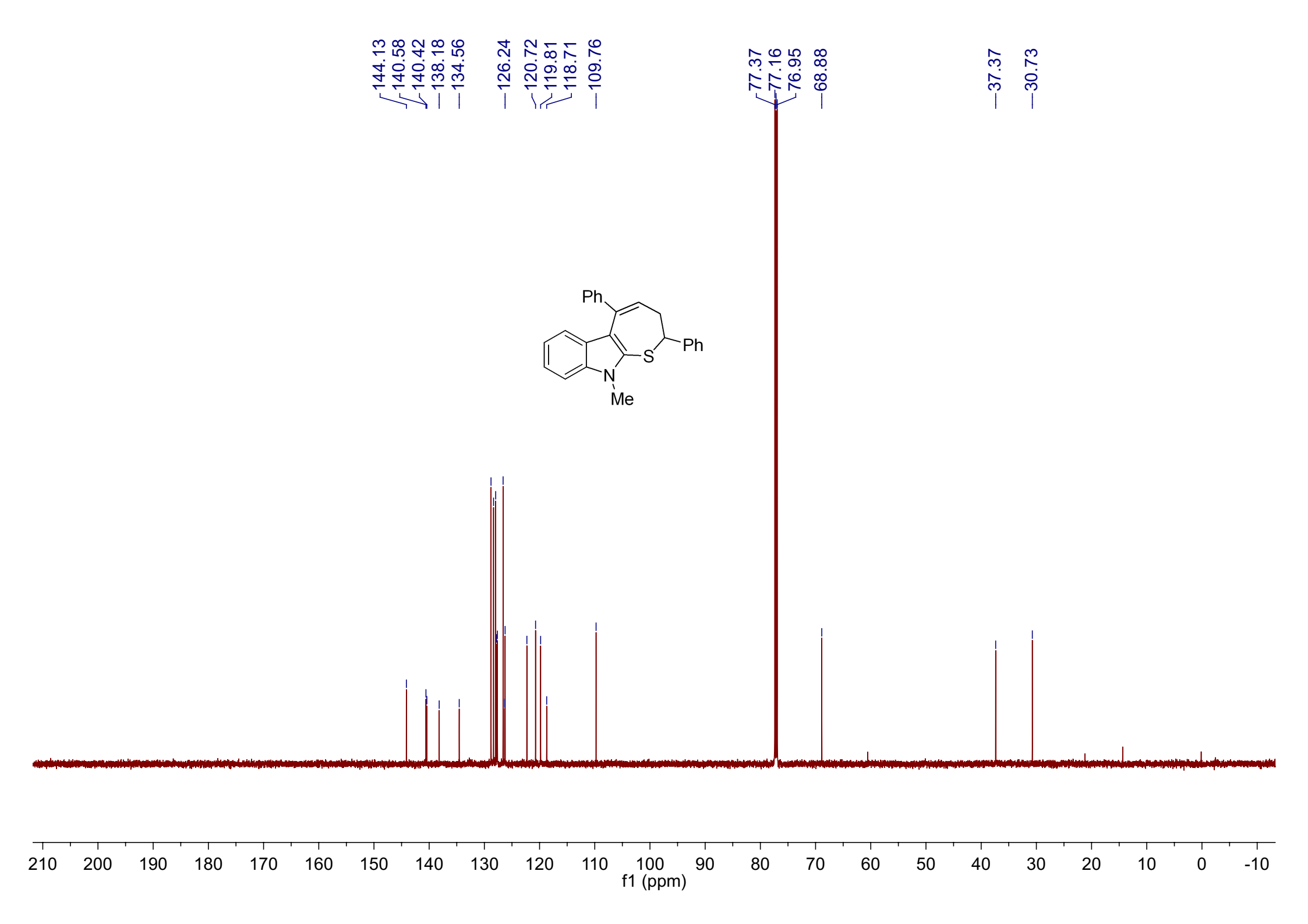
7.26
7.25
7.23
7.22
7.21
7.21
6.87
6.54
6.52
6.51
5.15
5.14
5.12
3.88
2.65
2.63
2.62
Ph
Ph
S
N
Me
3.13
6.90
1.34
1.03
1.04
1.00
1.04
1.07
3.06
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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134.56
126.24
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118.71
109.76
77.37
77.16
76.95
68.88
37.37
30.73
Ph
Ph
S
N
Me
210
200
190
180
170
160
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140
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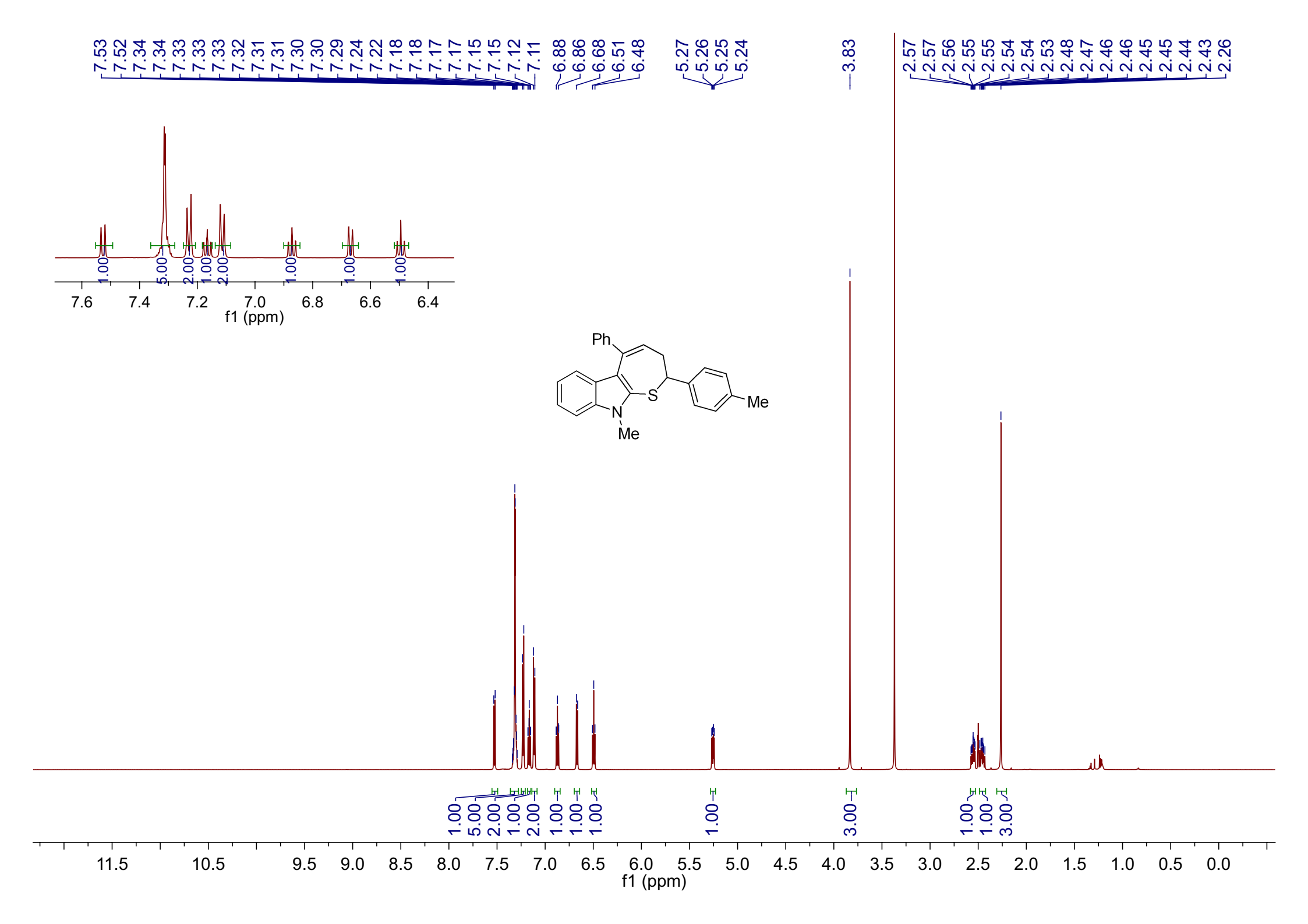
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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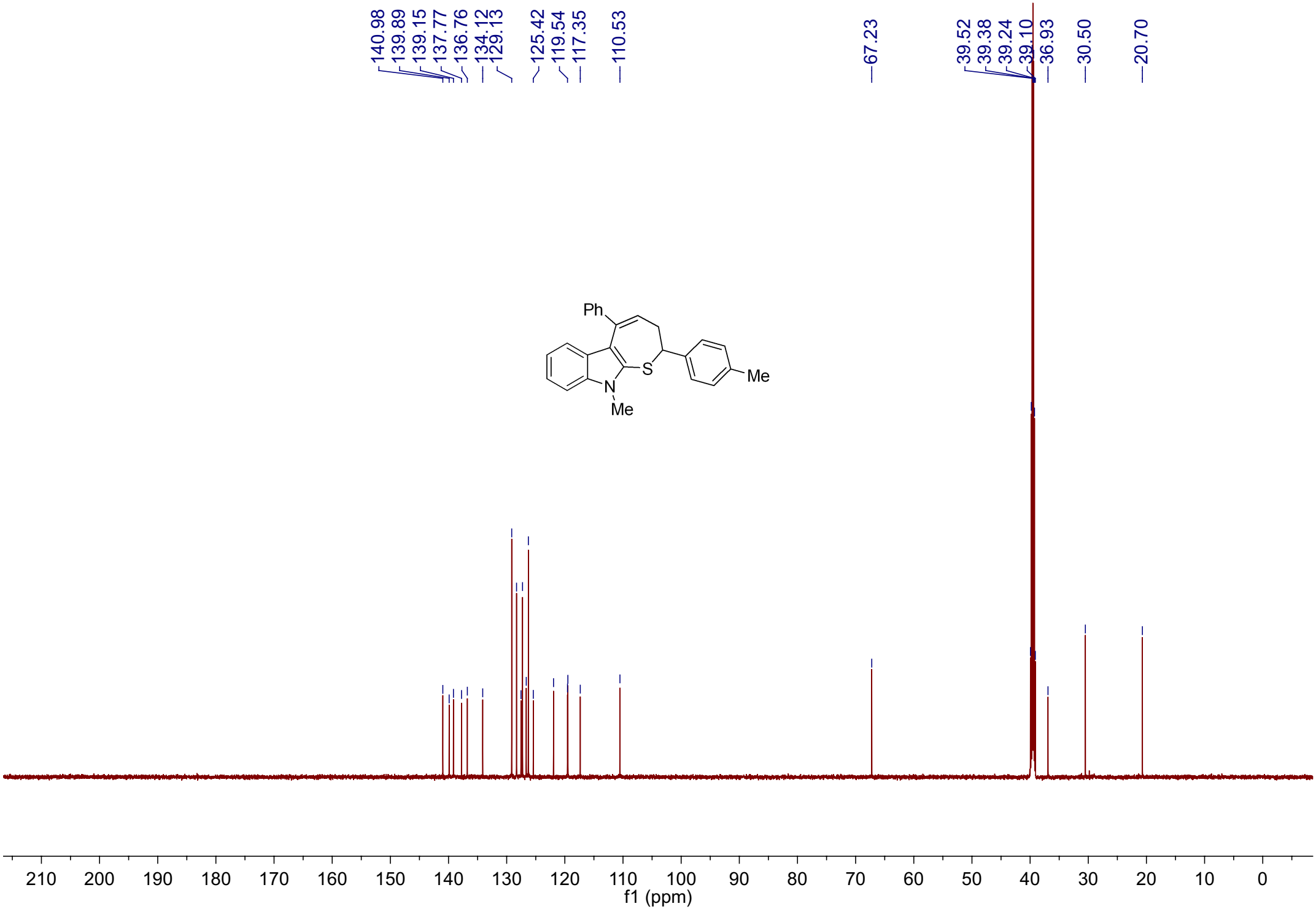
1.00 5.00 2.00 1.00 2.00 1.00 1.00 1.00
7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
Ph
S
N
Me
Me
1.00 5.00 2.00 1.00 2.00 1.00 1.00 1.00 1.00 3.00 1.00 1.00 3.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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110.53
67.23
39.52
39.38
39.24
39.10
36.93
30.50
20.70
Ph
S
N
Me
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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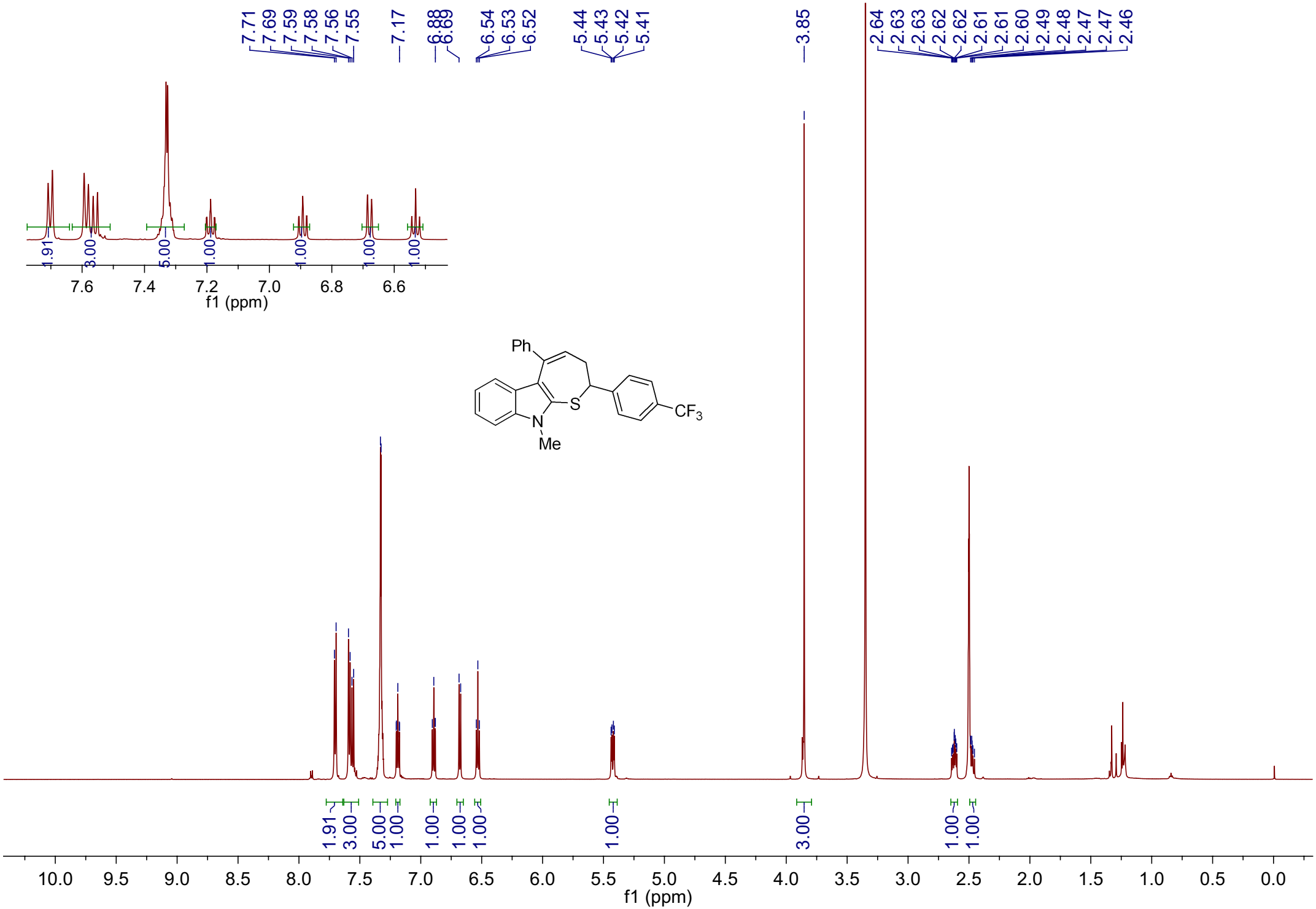
f1 (ppm)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5.43
5.42
5.41
3.85
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2.63
2.63
2.62
2.62
2.61
2.61
2.60
2.49
2.48
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2.47
2.46
1.91
3.00
5.00
1.00
1.00
1.00
1.00
7.6
7.4
7.2
7.0
6.8
6.6
f1 (ppm)
Ph
S
N
Me
CF3
1.91
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5.00
1.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
10.0
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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
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1.0
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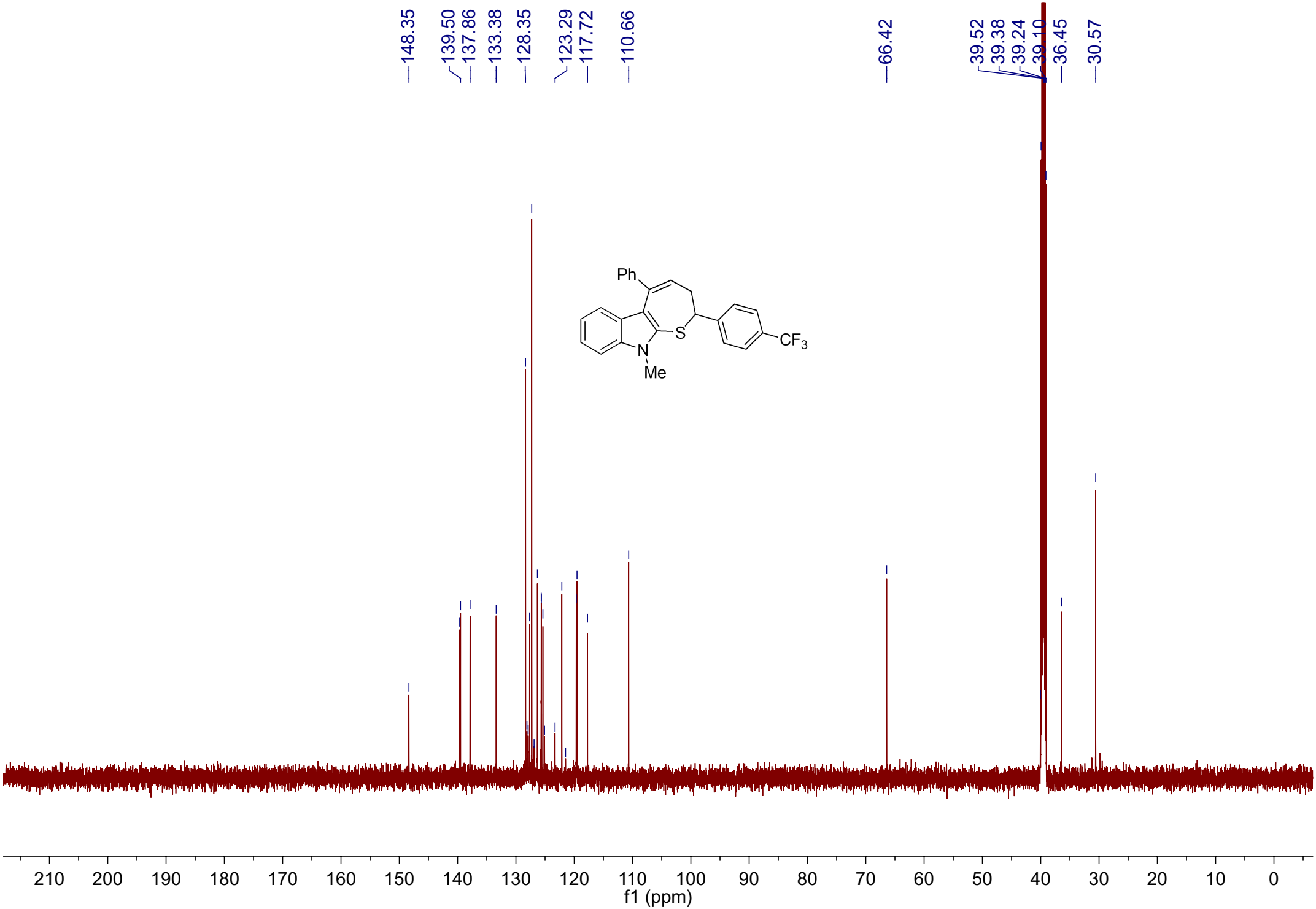
0.0
f1 (ppm)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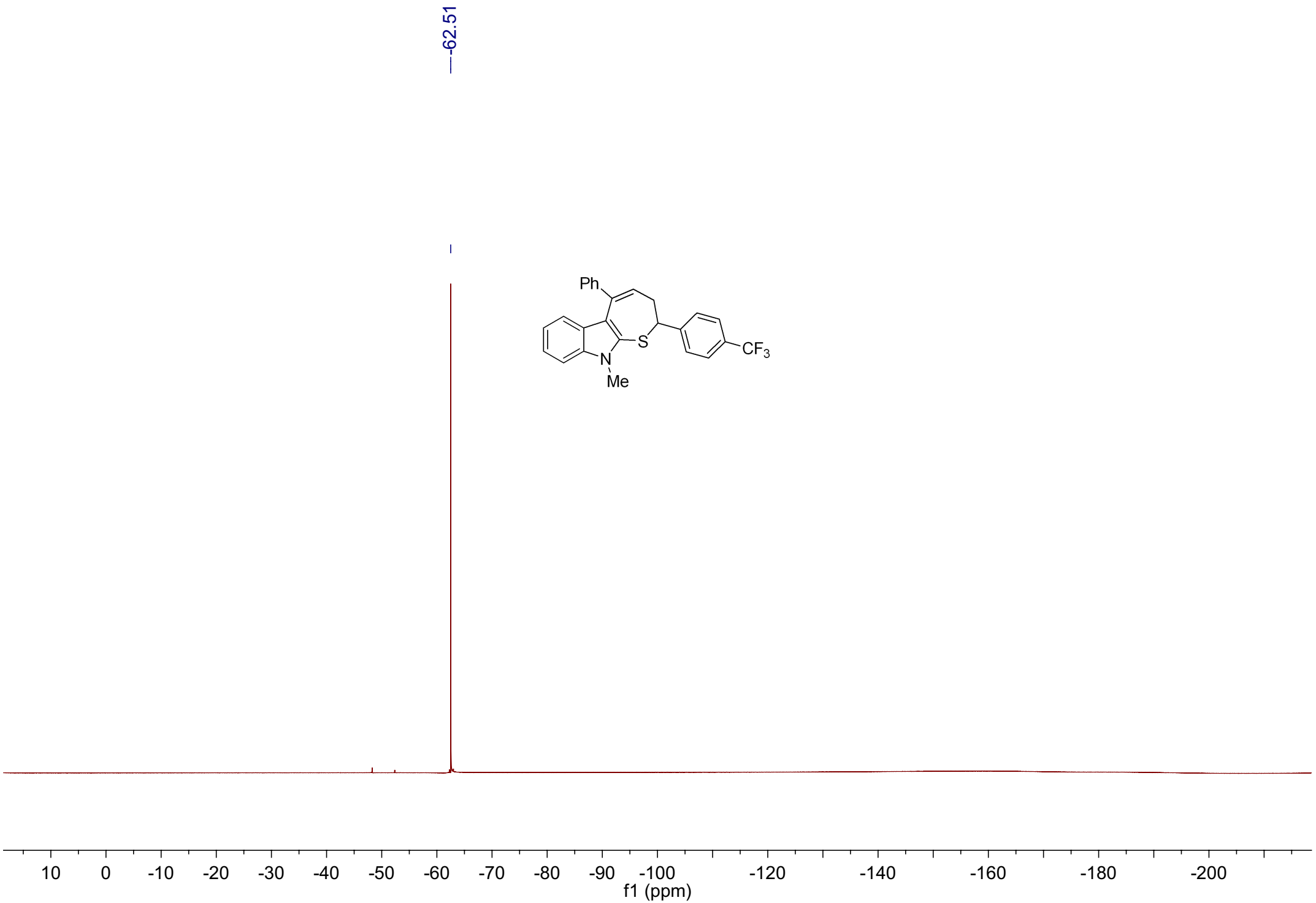
110.66
66.42
39.52
39.38
39.24
39.10
36.45
30.57
Ph
S
N
Me
CF3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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Me
CF3
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-50
-60
-70
-80
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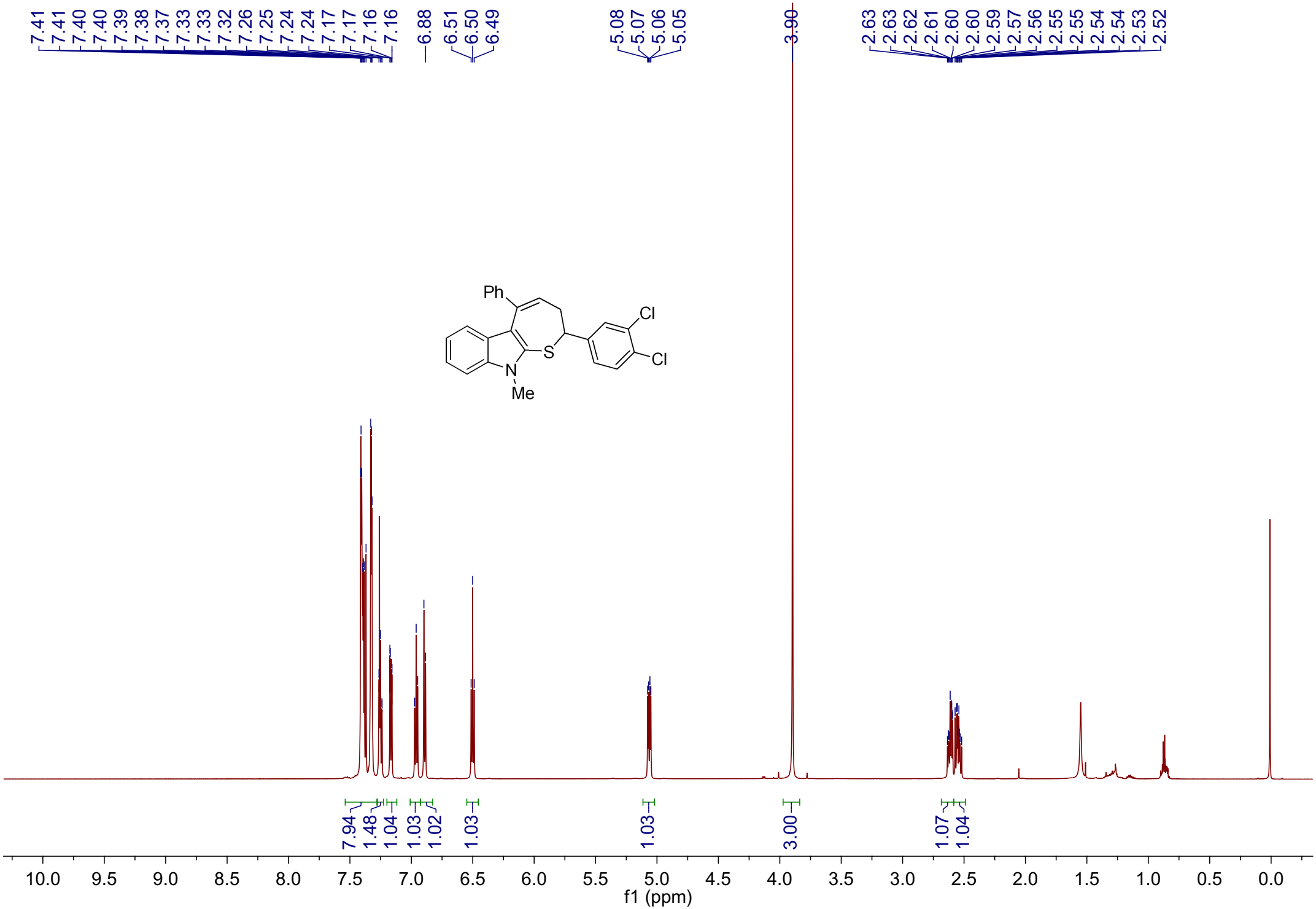
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.32
7.26
7.25
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2.62
2.61
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2.57
2.56
2.55
2.55
2.54
2.54
2.53
2.52
Ph
Cl
Cl
S
N
Me
7.94
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1.03
1.02
1.03
1.03
3.00
1.07
1.04
10.0
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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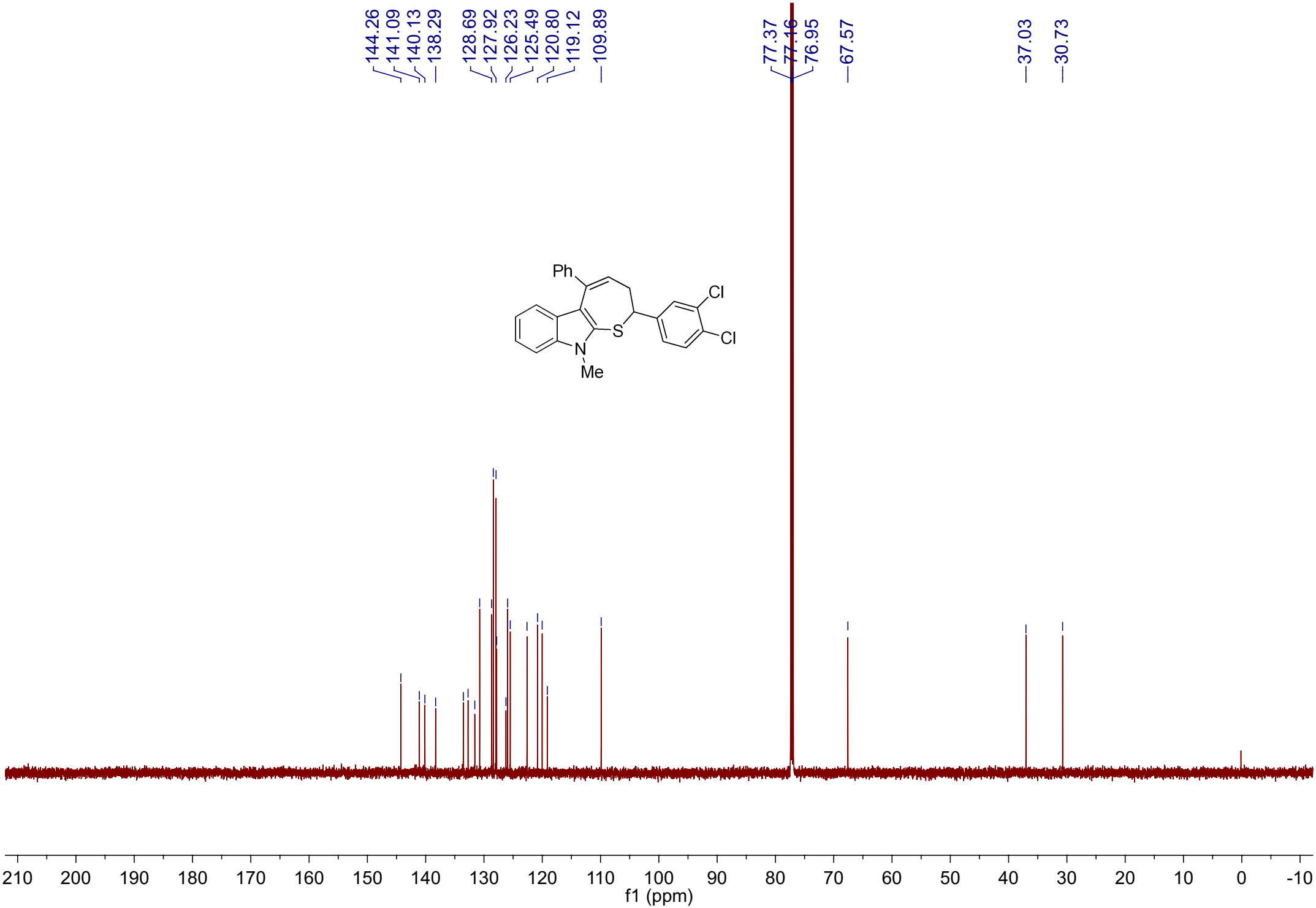
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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77.16
76.95
67.57
37.03
30.73
Ph
Cl
Cl
S
N
Me
210
200
190
180
170
160
150
140
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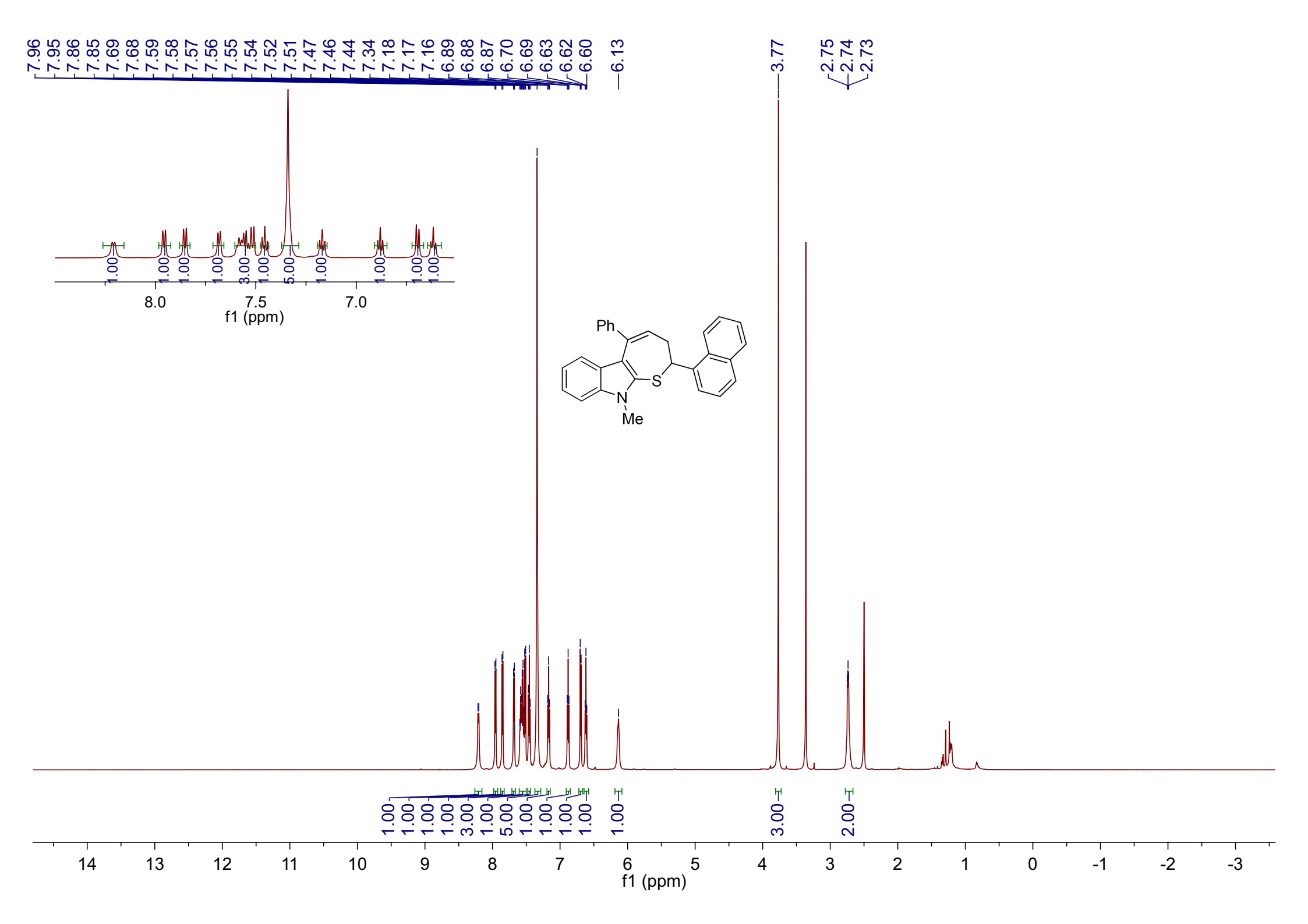
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.58
7.57
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7.54
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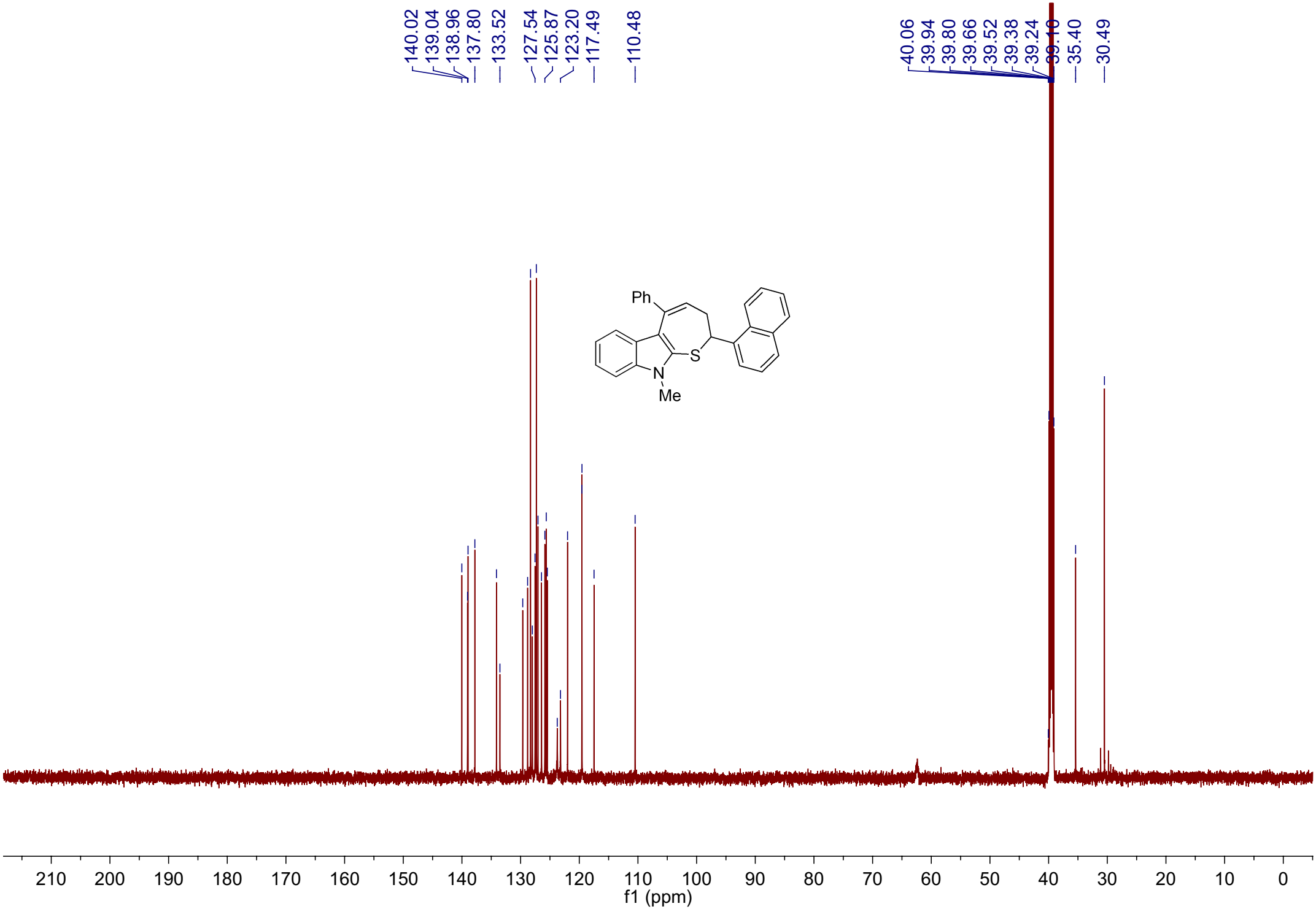
7.51
7.47
7.46
7.44
7.34
7.18
7.17
7.16
6.89
6.88
6.87
6.70
6.69
6.63
6.62
6.60
6.13
3.77
2.75
2.74
2.73
1.00
1.00
1.00
1.00
3.00
1.00
5.00
1.00
1.00
1.00
1.00
1.00
3.00
2.00
8.0
7.5
7.0
f1 (ppm)
Ph
S
N
Me
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)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Ph
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N
Me
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200
190
180
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10
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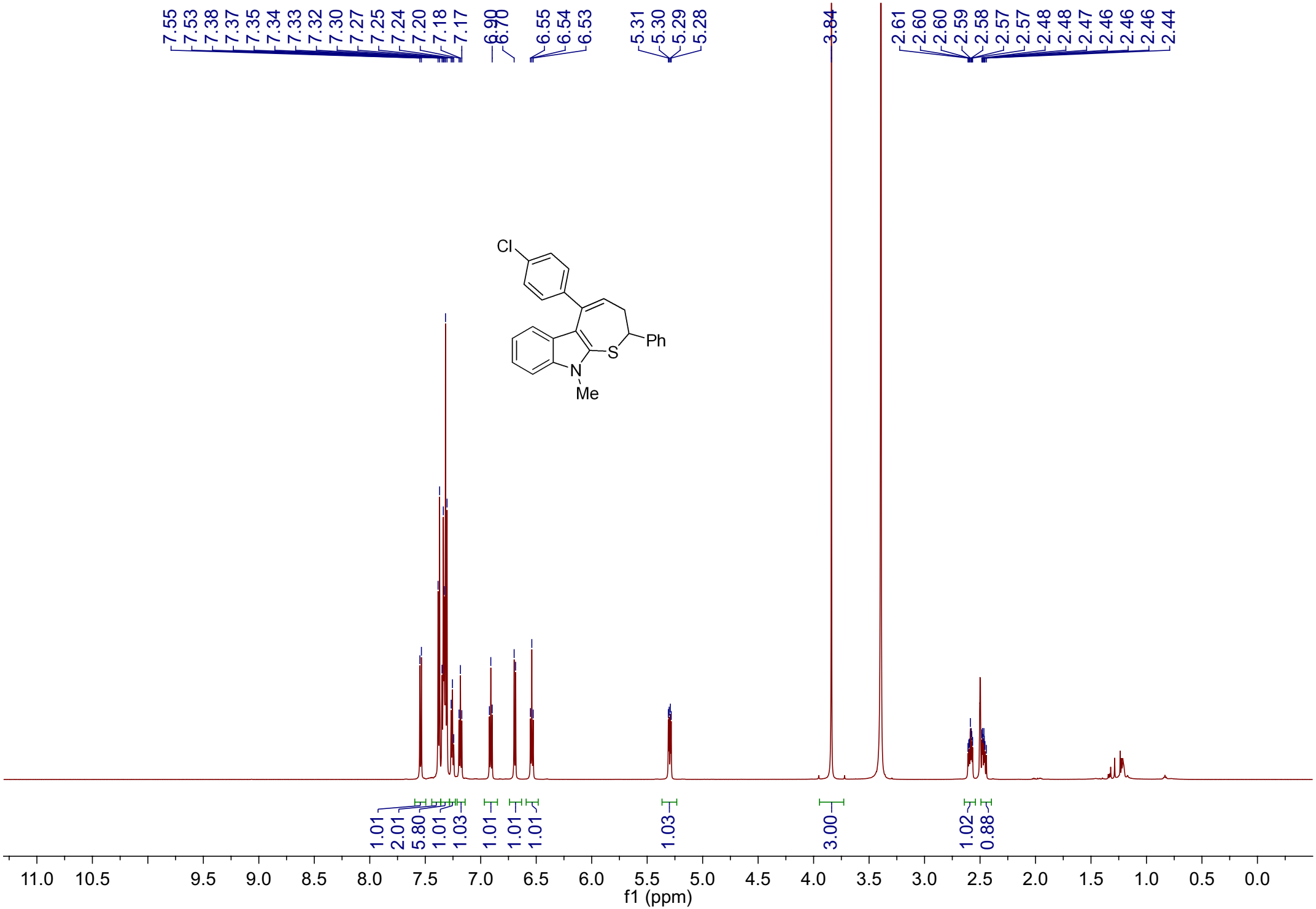
f1 (ppm)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7.17
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6.70
6.55
6.54
6.53
5.31
5.30
5.29
5.28
3.84
2.61
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2.58
2.57
2.57
2.48
2.48
2.47
2.46
2.46
2.46
2.44
Cl
Ph
S
N
Me
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2.01
5.80
1.01
1.03
1.01
1.01
1.01
1.03
3.00
1.02
0.88
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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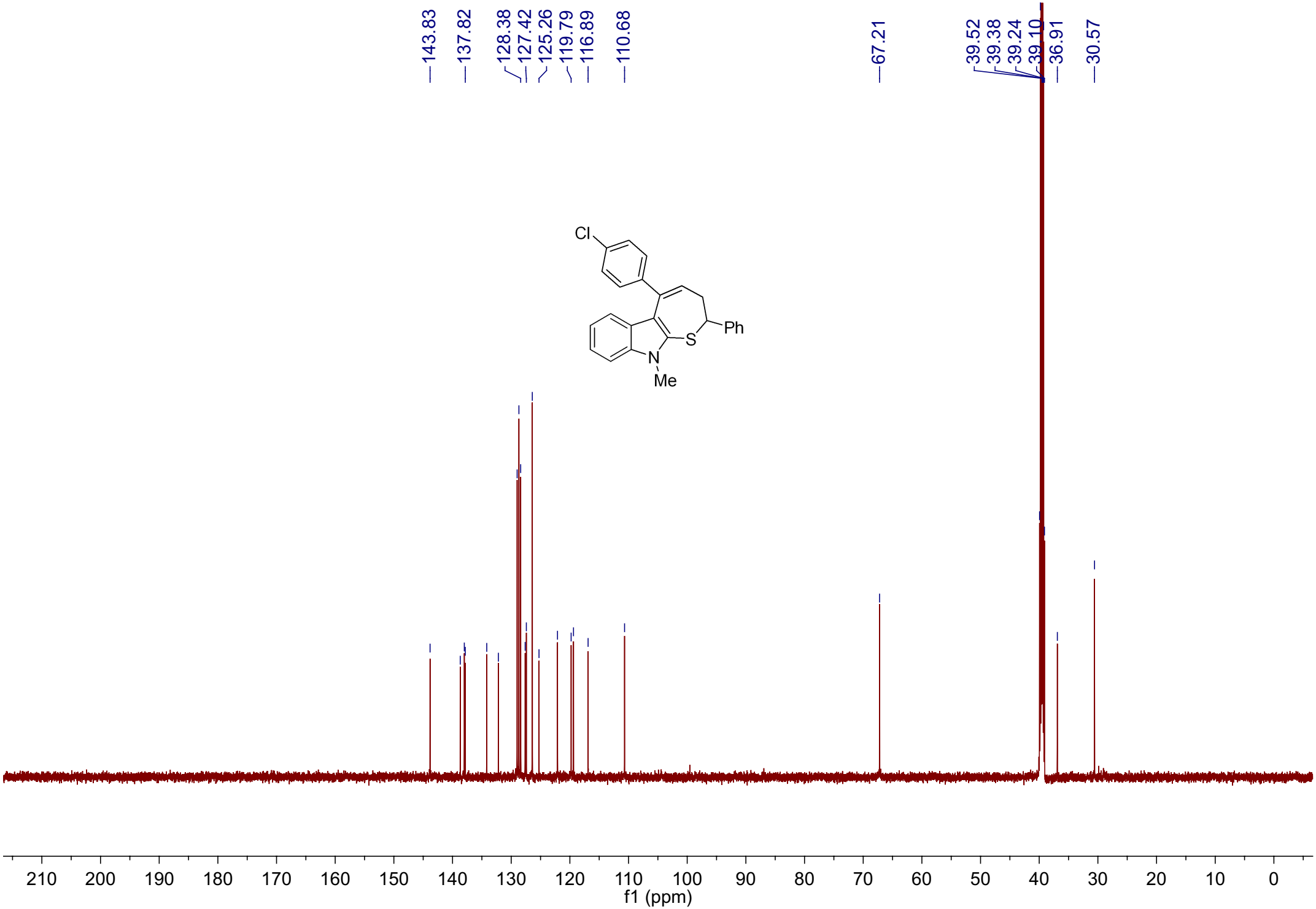
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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67.21
39.52
39.38
39.24
39.10
36.91
30.57
Cl
Ph
S
N
Me
210
200
190
180
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120
110
100
90
80
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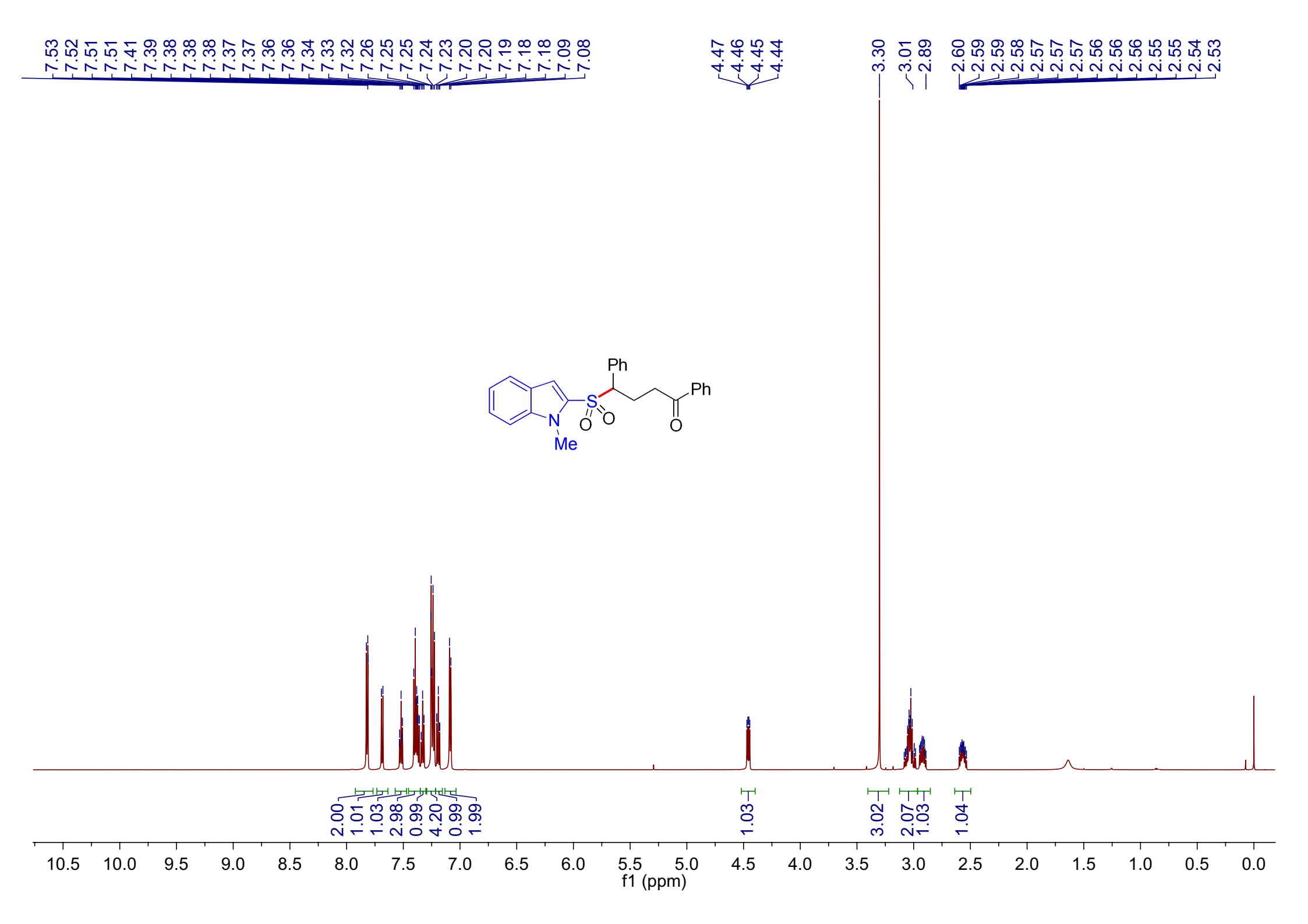
50
40
30
20
10
0
f1 (ppm)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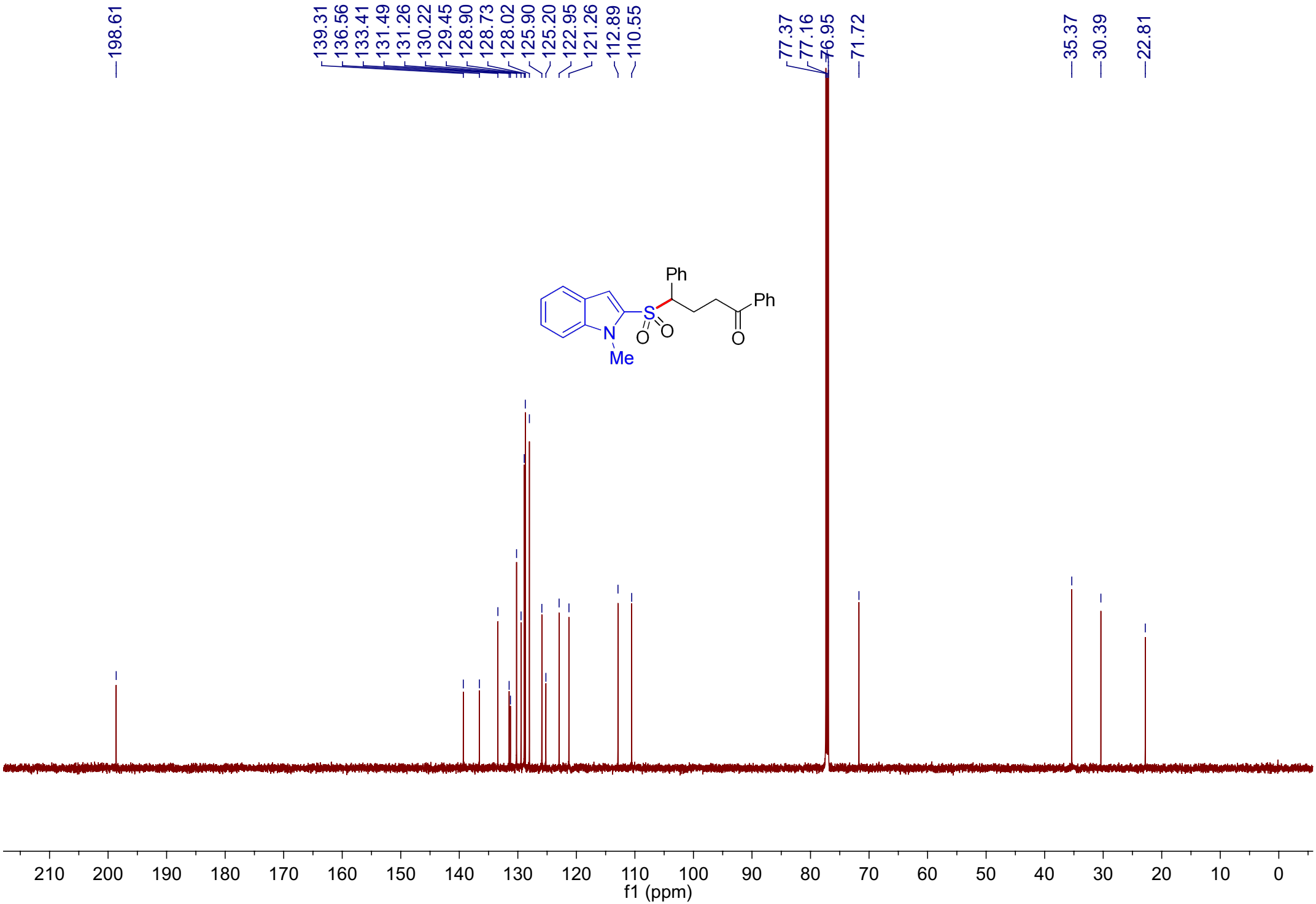
4.47 4.46 4.45 4.44
3.30 3.01 2.89
2.60 2.59 2.59 2.58 2.57 2.57 2.57 2.56 2.56 2.56 2.55 2.55 2.54 2.53
Ph
Ph
S
O
O
N
Me
O
2.00 1.01 1.03 2.98 0.99 4.20 0.99 1.99
1.03
3.02 2.07 1.03
1.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.73
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122.95
121.26
112.89
110.55
77.37
77.16
76.95
71.72
35.37
30.39
22.81
Ph
Ph
S
O
O
N
Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)