# Supporting Information

## Brønsted Acid-Catalyzed Two-component Tandem Condensation and Cycloisomerization to 6(2*H*)-Isoquinolinones

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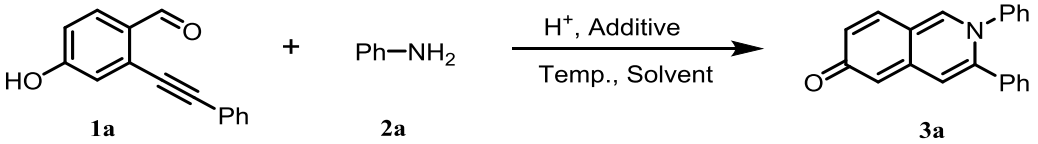
## S1. General Information

All commercial avialable chemicals were used without further purification. $Pd(PPh_3)_2Cl_2$, anhydrous 1,2-dicloroethane, anhydrous DMF were bought from Energy Chemical. Anhydrous tetrahydrofuran (THF) and toluene were heated over sodium under $N_2$ for at least four hours before distilled to use. Anhydrous DCM was heated over calcium hydride for two hours before distilled to use. Ethyl acetate (ACS grade), hexanes (ACS grade) were purchased from Fisher Scientific and used without further purification. The reactions that sensitive to the moisture were conducted in dry solvents.

Reactions were monitored by thin-layer chromatography (TLC) using Sorbent Technologies' precoated silica gel plates. The silica gel plates were first observed by ultraviolet (254 and 365 nm), then were stained with aqueous DNP, subsequently toasted by a heat gun. Flash column chromatography was performed over Sorbent Technologies' silica gel (230−400 mesh).

$^1$H NMR and $^{13}$C NMR spectra were recorded on a Bruker Advance spectrometer at 500 MHz, 125 MHz and 400 MHz, 100 MHz respectively. Chemical shift values are reported in $\delta$ (ppm) relative to $CDCl_3$ ($^1$H NMR, $\delta$ = 7.26; $^{13}$C NMR, $\delta$ = 77.16), $CD_3OD$ ($^1$H NMR, $\delta$ = 3.31; $^{13}$C NMR, $\delta$ = 49.0), $(CD_3)_2CO$ ($^1$H NMR, $\delta$ = 2.05; $^{13}$ C NMR, $\delta$ = 29.85), $(CD_3)_2SO$ ($^1$H NMR, $\delta$ = 2.50; $^{13}$C NMR, $\delta$ = 39.52). Signal shapes are shown as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), td (triplet double), m (multiplet). High resolution mass spectrometry (HRMS) was performed with a Thermo Scientific LTQ Orbitrap XL.

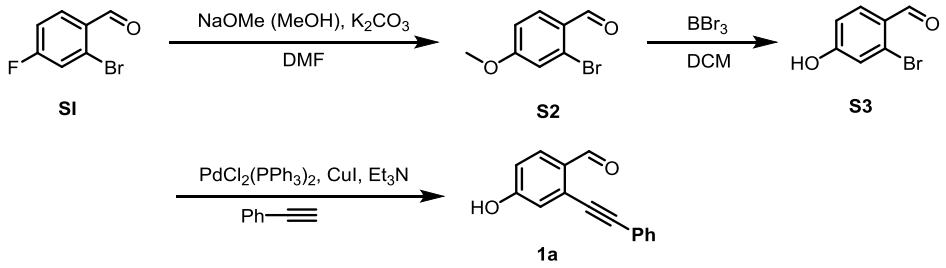
## Table S1. Optimization of Reaction Conditions[a]




| entry | amine (equiv) | $H^+$ (mol%) | additive | solvent | temp. (℃) | yield (%)[b] |
|---|---|---|---|---|---|---|
| 1 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | DCE | rt. | 47 |
| 2 | 1 | NIS (20) | $MgSO_4$ | DCE | rt. | ND |
| 3 | 1 | $I_2$ (20) | $MgSO_4$ | DCE | rt. | ND |
| 4 | 1 | $I_2$ (20)/$K_2CO_3$ (1 equiv.) | $MgSO_4$ | DCE | rt. | ND |
| 5 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | DCE | 60 | 76 |
| 6 | 1 | -- | $MgSO_4$ | DCE | 60 | ND |
| 7 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | DCE | 80 | 76 |
| 8 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | PhCl | 80 | 79 |
| 9 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | dioxane | 80 | 65 |
| 10 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | DMSO | 80 | 66 |
| 11 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | DMF | 80 | 73 |
| 12 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | toluene | 80 | 82 |
| 13 | 1 | $CH_3SO_3H$ (20) | $MgSO_4$ | toluene | 80 | 78 |
| 14 | 1 | $CH_3COOH$ (20) | $MgSO_4$ | toluene | 80 | 72 |
| 15 | 1 | HCOOH (20) | $MgSO_4$ | toluene | 80 | 70 |
| 16 | 1 | HCl-$Et_2O$ (20) | $MgSO_4$ | toluene | 80 | 71 |
| 17 | 1 | HOTf (20) | $MgSO_4$ | toluene | 80 | 64 |
| 18 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | toluene | 70 | 78 |
| 19 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | toluene | 90 (6 h) | 69 |
| 20 | 1 | $CF_3COOH$ (20) | $MgSO_4$ | toluene | 100 (4.5 h) | 54 |
| 21 | 1 | $CF_3COOH$ (10) | $MgSO_4$ | toluene | 80 | 83 |
| 22 | 1 | $CF_3COOH$ (5) | $MgSO_4$ | toluene | 80 | 79 |
| 23 | 1 | $CF_3COOH$ (2.5) | $MgSO_4$ | toluene | 80 | 76 |
| 24 | 1 | $CF_3COOH$ (40) | $MgSO_4$ | toluene | 80 | 82 |
| ***25*** | ***1.1*** | ***$CF_3COOH$ (10)*** | ***$MgSO_4$*** | ***toluene*** | ***80*** | ***92*** |
| 26 | 1.3 | $CF_3COOH$ (10) | $MgSO_4$ | toluene | 80 | 90 |
| 27 | 1.5 | $CF_3COOH$ (10) | $MgSO_4$ | toluene | 80 | 91 |
| 28 | 1.1 | $CF_3COOH$ (10) | $MgSO_4$ (3.0 eq) | toluene | 80 | 85 |
| 29 | 1.1 | $CF_3COOH$ (10) | $MgSO_4$ (4.0 eq) | toluene | 80 | 89 |
| 30 | 1.1 | $CF_3COOH$ (10) | $MgSO_4$ (4.5 eq) | toluene | 80 | 80 |
| 31 | 1.1 | $CF_3COOH$ (10) | 5Å-100mg | toluene | 80 | 55 |
| 32 | 1.1 | $CF_3COOH$ (10) | 5Å-200mg | toluene | 80 | 64 |
| 33 | 1.1 | $CF_3COOH$ (10) | 5Å-300mg | toluene | 80 | 75 |

[a] The reaction was performed on a 0.2 mmol scale; 2 mL of solvent was used; 3.4 eq. of $MgSO_4$ was added (80 mg); DCE = 1,2-dichloroethane; DMF = *N*, *N*-Dimethylformamide. [b] Isolated yields.

## S2. Synthesis of starting compounds




**General Procedure for the Synthesis of 1.**

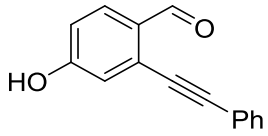
Example for the Synthesis of **1a**

MeONa in MeOH (2.3 mL, 12 mmol, 1.2 eq.) was dissolved in DMF (50 mL), $K_2CO_3$ (1.6585 g, 12 mmol, 1.2 eq.) was added and stirred for 15 minutes. 2-bromo-4-fluorobenzaldehyde (2.03 g, 10 mmol) was added to the solution and then stirred at 100 ℃ for 2 hours. After cooling to room temperature, EtOAc was added. Then the mixture washed with $NaHCO_3$ solution and saturated saline, dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel with hexane/ethyl acetate = 20:1 as the eluent to afford the product **S2** as white solid. (1.6344 g, yield: 76%).

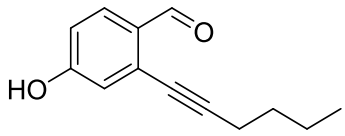
To a solution of **S2** (0.8602 g, 4 mmol) in 120 mL dry $CH_2Cl_2$ in -78 ℃, $BBr_3$ (1.2 mL, 12 mmol, 3 eq.) resolved in 10 mL $CH_2Cl_2$ was added over 15 minutes. The mixture was put in ice bath and allowed to warm up to room temperature and stirred for 24 hours. Then poured on ice and the product was extracted with $CH_2Cl_2$. The organic layer was washed with water and brine, dried over anhydrous $MgSO_4$, and then removed the solvent. After purification by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), afforded the desired product **S3** as slightly yellow solid (0.7793 g, yield: 91%).

To a dry round-bottom flask added 2-bromo-4-hydroxybenzaldehyde **S3** (804.08 mg, 4 mmol), $Pd(PPh_3)_2Cl_2$ (140.4 mg, 0.2 mmol, 0.05 eq.) and CuI (76.0 mg, 0.4 mmol, 0.1 eq.), then the mixture was degassed and flushed with $N_2$ for five times at room temperature. Then anhydrous DMF (10 mL), $Et_3N$ (1.3333 g, 13.2 mmol, 3.3 eq.) and Phenylacetylene (0.4903 g, 4.8 mmol, 1.2 eq.) were added. The mixture was

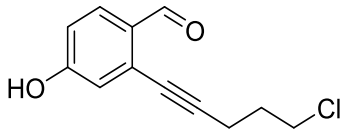
heated at 60 ℃ for 14 h, and then cooled to room temperature, diluted with water and neutralized with 0.1 N HCl. The mixture was extracted with EtOAc (3 × 50 mL) and the combined organic layers were washed with water (3 × 100 mL), brine (3 × 100 mL), and dried over $Na_2SO_4$, finally concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 6:1) to provide the desired product **1a** as yellow solid (0.7201 g, yield: 81%).



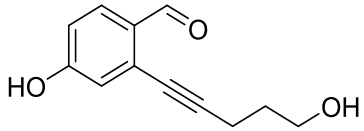

**4-hydroxy-2-(phenylethynyl)benzaldehyde** (**1a)**. Yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 6:1), 81% yield. m.p 151-155 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 10.34 (s, 1H), 7.79 (d, $J$ = 8.6 Hz, 1H), 7.54 (dd, $J$ = 6.7, 3.0 Hz, 2H), 7.38 (dd, $J$ = 5.0, 1.9 Hz, 3H), 6.99 (d, $J$ = 2.5 Hz, 1H), 6.88 (dd, $J$ = 8.6, 2.4 Hz, 1H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 191.39, 164.34, 132.66, 130.99, 130.18, 130.14, 129.66, 129.63, 123.62, 120.08, 117.63, 96.52, 85.75. HRMS (ESI) m/z: calcd for $C_{15}H_{11}O_2^+$ $(M+H)^+$ 223.0754, found 223.0756.



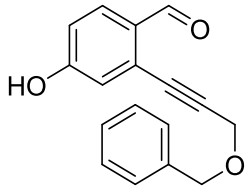

**2-(hex-1-yn-1-yl)-4-hydroxybenzaldehyde (1t)**. Orange oil, (purified by silica gel column chromatography by eluting with PE/EA = 8:1), 83% yield. $^1$H NMR (500 MHz, Chloroform-d): $\delta$ = 10.30 (s, 1H), 8,87 (br, 1H), 7.81 (d, $J$ = 8.7 Hz, 1H), 6.98 (d, $J$ = 2.4 Hz, 1H), 6.86 (dd, $J$ = 8.5, 2.4 Hz, 1H), 2.44 (t, $J$ = 7.1 Hz, 2H), 1.58 (p, $J$ = 7.1 Hz, 2H), 1.45 (h, $J$ = 7.3 Hz, 2H), 0.92 (t, $J$ = 7.3 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 192.37, 162.50, 131.11, 129.94, 128.74, 119.69, 116.23, 98.33, 76.18, 30.56, 22.13, 19.31, 13.62. HRMS (ESI) m/z: calcd for $C_{13}H_{15}O_2^+$ $(M+H)^+$ 203.1067, found 203.1067.



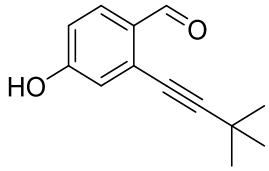
**2-(5-chloropent-1-yn-1-yl)-4-hydroxybenzaldehyde (1u)**. Red solid, (purified by silica gel column chromatography by eluting with PE/EA = 10:1 to 6:1), 55% yield. m.p 85.6-89.5 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 10.28 (s, 1H), 8.49 (br, 1H), 7.84 (d, *J* = 8.7 Hz, 1H), 7.00 (d, *J* = 2.4 Hz, 1H), 6.93 (dd, *J* = 8.7, 2.4 Hz, ik), 3.68 (t, *J* = 6.2 Hz, 2H), 2.66 (t, *J* = 6.9 Hz, 2H), 2.37 – 1.66 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 192.11, 162.27, 130.41, 130.31, 128.91, 119.87, 116.52, 96.03, 77.11, 43.72, 31.14, 17.13. HRMS (ESI) m/z: calcd for $C_{12}H_{11}ClO_2Na^+$ $(M+Na)^+$ 245.0340, found 245.0342.



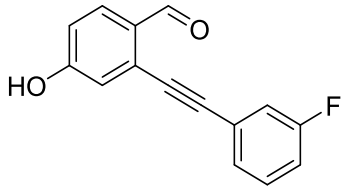

**4-hydroxy-2-(5-hydroxypent-1-yn-1-yl)benzaldehyde (1v)**. Light yellow oil, (purified by silica gel column chromatography by eluting with PE/EA = 4:1 to 2:1), 51% yield. $^{1}$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 10.25 (s, 1H), 7.73 (d, *J* = 8.6 Hz, 1H), 6.86 (d, *J* = 2.4 Hz, 1H), 6.82 (dd, *J* = 8.6, 2.0 Hz, 1H), 3.71 (t, *J* = 6.2 Hz, 2H), 2.59 (t, *J* = 7.1 Hz, 2H), 2.00 – 1.54 (m, 2H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 191.86, 164.40, 131.36, 130.56, 129.79, 120.19, 117.04, 97.75, 77.38, 61.55, 32.44, 16.64. HRMS (ESI) m/z: calcd for $C_{12}H_{12}O_3Na^+$ $(M+Na)^+$ 227.0679, found 227.0679.



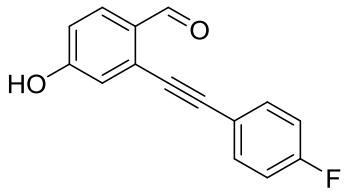

**2-(3-(benzyloxy)prop-1-yn-1-yl)-4-hydroxybenzaldehyde (1w)**. Yellow oil, (purified by silica gel column chromatography by eluting with PE/EA = 6:1 to 4:1), 43% yield. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 10.33 (s, 1H), 7.85 (d, *J* = 8.7 Hz, 1H), 7.42 – 7.34 (m, 4H), 7.32 (d, *J* = 5.4 Hz, 1H), 6.99 (s, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 4.69 (s, 2H), 4.45 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 190.99, 161.85, 136.99, 130.30, 128.70, 128.64, 128.36, 128.29, 128.20, 119.96, 117.11, 92.06, 82.28, 72.31, 57.93. HRMS (ESI) m/z: calcd for $C_{17}H_{14}O_3Na^+$ $(M+Na)^+$ 289.0835, found 289.0832.




**2-(3,3-dimethylbut-1-yn-1-yl)-4-hydroxybenzaldehyde (1x)**. Light yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 8:1), 80% yield. m.p 116.5-122.8 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 10.29 (s, 1H), 8.86 (br, 1H), 7.83 (d, *J* = 8.7 Hz, 1H), 6.98 (d, *J* = 2.5 Hz, 1H), 6.90 (dd, *J* = 8.6, 2.4 Hz, 1H), 1.32 (s, 9H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 192.59, 162.50, 131.20, 129.94, 128.59, 119.57, 116.25, 106.29, 74.70, 30.77, 28.36. HRMS (ESI) m/z: calcd for $C_{13}H_{14}O_2Na^+$ $(M+Na)^+$ 225.0886, found 225.0887.

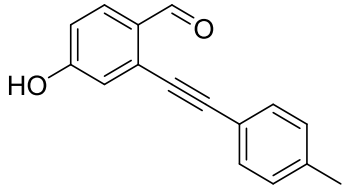



**2-((3-fluorophenyl)ethynyl)-4-hydroxybenzaldehyde (1y)**. Light yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 6:1), 86% yield. m.p 145.2-150.1 ℃. $^{1}$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 10.30 (s, 1H), 7.79 (d, *J* = 8.7 Hz, 1H), 7.45 – 7.33 (m, 2H), 7.29 (d, *J* = 9.4 Hz, 1H), 7.14 (t, *J* = 8.3 Hz, 1H), 6.99 (d, *J* = 2.4 Hz, 1H), 6.89 (dd, *J* = 8.7, 2.5 Hz, 1H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 191.21, 163.85 ($J_{CF}$ = 246.25 Hz), 164.79, 131.56 ($J_{CF}$ = 8.75Hz), 131.27, 129.59, 129.46, 128.78 ($J_{CF}$ = 3.75 Hz), 125.62 ($J_{CF}$ = 10 Hz), 120.43, 119.16 ($J_{CF}$ = 23.75 Hz),118.06, 117.29 ($J_{CF}$ = 21.25 Hz), 94.85 ($J_{CF}$ = 3.75 Hz), 86.80. HRMS (ESI) m/z: calcd for $C_{15}H_9FO_2Na^+$ $(M+Na)^+$ 263.0479, found 263.0480.

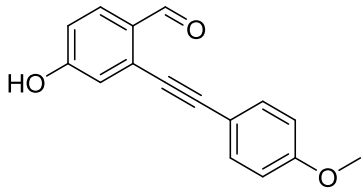



**2-((4-fluorophenyl)ethynyl)-4-hydroxybenzaldehyde (1z)**. Light yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 6:1), 70% yield. m.p 136.4-142.6 ℃. $^{1}$H NMR (400 MHz, Methanol-$d_4$): $\delta$ = 10.31 (s, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.58 (q, *J* = 8.6, 5.6 Hz, 2H), 7.13 (t, *J* = 8.8 Hz, 2H), 6.98 (d, *J* =

2.4 Hz, 1H), 6.88 (dd, $J$ = 8.6, 2.4 Hz, 1H); $^{13}$C NMR (100 MHz, MeOD): $\delta$ = 191.35, 164.35 ($J_{CF}$ = 247.8 Hz), 164.42, 134.92 ($J_{CF}$ = 8.6 Hz), 131.13, 129.96, 129.66, 120.12, 119.96 ($J_{CF}$ = 3.6 Hz), 117.69, 116.82 ($J_{CF}$ = 22.4 Hz), 95.36, 85.63. HRMS (ESI) m/z: calcd for $C_{15}H_9FO_2Na^+$ $(M+Na)^+$ 263.0479, found 263.0480.

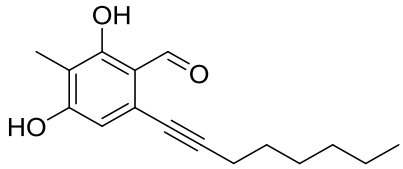



**4-hydroxy-2-(p-tolylethynyl)benzaldehyde (1aa)**. Yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 6:1), 83% yield. m.p 179.0-183.4 ℃ .$^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 10.34 (s, 1H), 7.79 (d, $J$ = 8.7 Hz, 1H), 7.44 (d, $J$ = 8.1 Hz, 2H), 7.21 (d, $J$ = 7.8 Hz, 2H), 6.98 (d, $J$ = 2.5 Hz, 1H), 6.88 (dd, $J$ = 8.6, 2.4 Hz, 1H), 2.36 (s, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 191.46, 164.41, 140.72, 132.63, 130.96, 130.51, 130.35, 129.62, 120.61, 119.98, 117.50, 96.86, 85.15, 21.55. HRMS (ESI) m/z: calcd for $C_{16}H_{12}O_2Na^+$ $(M+Na)^+$ 259.0730, found 259.0730.

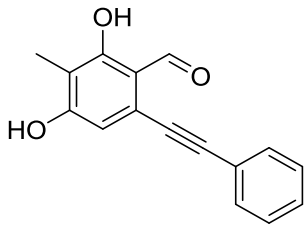



**4-hydroxy-2-((4-methoxyphenyl)ethynyl)benzaldehyde (1ab)**. Yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 6:1), 81% yield. m.p 140.6-145.3 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 10.33 (s, 1H), 7.78 (d, $J$ = 8.6 Hz, 1H), 7.48 (d, $J$ = 8.2 Hz, 2H), 6.96 (d, $J$ = 2.4 Hz, 1H), 6.93 (d, $J$ = 8.4 Hz, 2H), 6.86 (dd, $J$ = 8.6, 2.5 Hz, 1H), 3.81 (s, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 191.57, 164.37, 161.87, 134.26, 130.93, 130.78, 129.54, 119.85, 117.30, 115.58, 115.29, 96.95, 84.55, 55.83. HRMS (ESI) m/z: calcd for $C_{16}H_{12}NaO_3^+$ $(M+Na)^+$ 275.0679, found 275.0680.

**The synthesis of 1ac and 1ad refers to the reported literature.[1,2]**



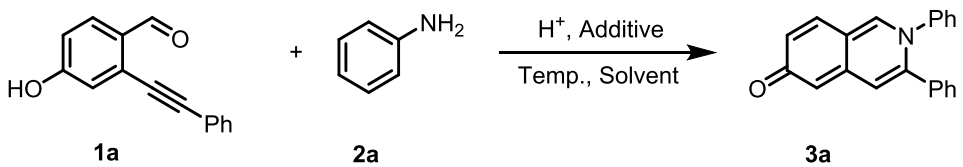

**2,4-dihydroxy-3-methyl-6-(oct-1-yn-1-yl)benzaldehyde (1ac)**. Known compound, Yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 10:1), 84% yield. m.p 81.5-83.4 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 12.25 (s, 1H), 10.18 (s, 1H), 6.88 (br, 1H), 6.51 (s, 1H), 2.43 (t, *J* = 7.2 Hz, 2H), 2.11 (s, 3H), 1.60 (m, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.7 Hz, 2H), 1.33 – 1.28 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 195.54, 163.21, 161.40, 127.74, 114.43, 112.62, 111.84, 97.67, 75.86, 31.41, 28.80, 28.58, 22.64, 19.66, 14.13, 7.28.




**2,4-dihydroxy-3-methyl-6-(phenylethynyl)benzaldehyde (1ad)**. Known compound, yellow solid, (purified by silica gel column chromatography by eluting with PE/EA = 8:1), 75% yield. mp 178 ℃ (decompose). $^{1}$H NMR (500 MHz, Acetone-$d_6$): $\delta$ = 12.45 (s, 1H), 10.31 (s, 1H), 9.76 (s, 1H), 7.75 – 7.56 (m, 2H), 7.52 – 7.33 (m, 3H), 6.77 (s, 1H), 2.08 (s, 3H). $^{13}$C NMR (125 MHz, Acetone): $\delta$ = 195.24, 163.92, 163.20, 132.51, 130.03, 129.52, 126.71, 123.10, 114.32, 113.49, 113.08, 95.76, 85.22, 7.58.

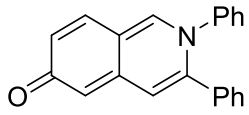
**S3. General Procedure for the Synthesis of 3.**

Example for the Synthesis of 3a

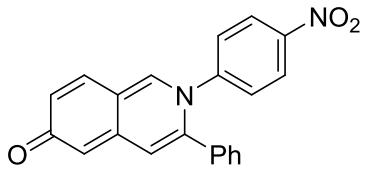



4-hydroxy-2-(phenylethynyl)benzaldehyde **1a** (66.6 mg, 0.3 mmol, 1.0 equiv), anhydrous $MgSO_4$ (120.0 mg, 3.4 equiv), aniline **2a** (30.7mg, 0.33 mmol, 1.1 equiv), 2mL dry toluene and 0.2 M solution of $CF_3COOH$ in toluene (150 μL, 0.1 equiv)

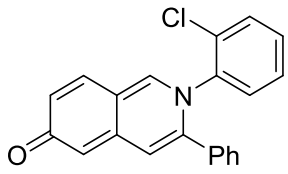
were added successively to a flame-dried vial. The resulting mixture was stirred at 80 ℃, and the process of the reaction was monitored by TLC. Upon completion, the reaction mixture was concentrated under vacuum. The crude product was purified by chromatography on silica gel (DCM/MeOH = 20:1 to 5:1) to afford the desired product **3a** in 92% yield.



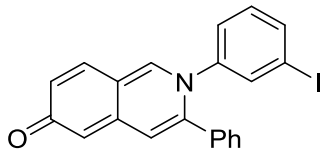

**2,3-diphenylisoquinolin-6(2H)-one (3a)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 92% yield. m.p 188.0-193.4 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.07 (s, 1H), 7.46 (d, *J* = 9.3 Hz, 1H), 7.31 – 7.27 (m, 3H), 7.23 – 7.04 (m, 7H), 6.97 (s, 1H), 6.92 (d, *J* = 8.5 Hz, 1H), 6.47 (s, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.93, 142.20, 142.04, 141.40, 140.23, 133.90, 132.82, 131.15, 129.58, 129.40, 128.99, 128.97, 128.36, 126.64, 118.63, 117.28, 111.43. HRMS (ESI) m/z: calcd for $C_{21}H_{16}NO^{+}$ $(M+H)^{+}$ 298.1226, found 298.1227.



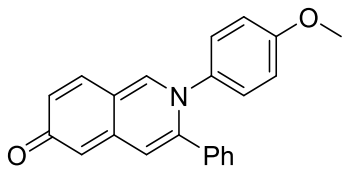

**2-(4-nitrophenyl)-3-phenylisoquinolin-6(2H)-one (3b)**. Red solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 85% yield. m.p 247.3-249.7 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.19 (s, 1H), 8.17 (s, 1H), 8.00 (s, 1H), 7.54 – 7.39 (m, 3H), 7.37 – 7.24 (m, 3H), 7.18 (s, 1H), 7.17 (s, 1H), 6.99 (s, 1H), 6.91 (dd, 1H), 6.44 (s, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 182.94, 147.27, 147.22, 141.49, 140.03, 139.90, 133.61, 133.40, 131.54, 129.67, 129.51, 129.01, 127.95, 125.07, 118.91, 117.76, 112.64. HRMS (ESI) m/z: calcd for $C_{21}H_{15}N_2O_3^{+}$ $(M+H)^{+}$ 343.1077, found 343.1074.



**2-(2-chlorophenyl)-3-phenylisoquinolin-6(2H)-one (3c)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 83% yield. m.p 149.0-155.5 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.85 (s, 1H), 7.46 (d, *J* = 9.3 Hz, 1H), 7.37 (d, *J* = 7.7 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.26 – 7.15 (m, 6H), 7.02 – 6.90 (m, 2H), 6.51 (s, 1H);$^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 182.66, 142.57, 140.90, 140.41, 139.29, 133.43, 133.11, 131.42, 131.30, 131.04, 130.65, 129.87, 129.33, 129.26, 128.29, 128.05, 118.01, 117.28, 112.02. HRMS (ESI) m/z: calcd for $C_{21}H_{15}ClNO^+$ $(M+H)^+$ 332.0837, found 332.0840.

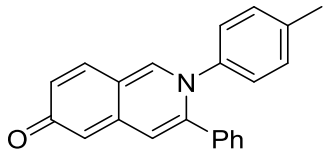



**2-(3-iodophenyl)-3-phenylisoquinolin-6(2H)-one (3d)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 78% yield. m.p 154.2-158.3 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.00 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.54 (s, 1H), 7.45 (d, 2H), 7.30 – 7.21 (m, 4H), 7.12 (d, *J* = 6.8 Hz, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.95 (s, 1H), 6.91 (d, *J* = 8.5 Hz, 1H), 6.45 (s, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 182.35, 142.80, 141.91, 141.05, 140.18, 138.08, 135.43, 133.51, 132.82, 131.33, 130.83, 129.41, 129.27, 128.56, 126.21, 118.68, 117.38, 111.69, 93.87. HRMS (ESI) m/z: calcd for $C_{21}H_{15}INO^+$ $(M+H)^+$ 424.0193, found 424.0193.

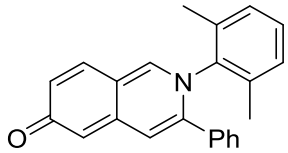



**2-(4-methoxyphenyl)-3-phenylisoquinolin-6(2H)-one (3e)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 71% yield. m.p 98.7-100.1 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.03 (s, 1H), 7.47 (d, *J* = 9.3 Hz, 1H), 7.25 – 7.19 (m, 3H), 7.13 (s, 1H), 7.11 (s, 1H), 7.07 (s, 1H), 7.05 (s, 1H), 7.00 (s, 1H), 6.97 (d, *J* = 9.2 Hz, 1H), 6.80 (s, 1H), 6.78 (s, 1H), 6.51 (s, 1H), 3.74 (s, 3H); $^{13}$C NMR (125 MHz, CDCl3): $\delta$ = 182.10, 159.67, 142.57, 141.66, 140.36, 135.05, 134.13, 133.02, 131.04, 129.55, 129.00, 128.45, 127.86, 118.67,

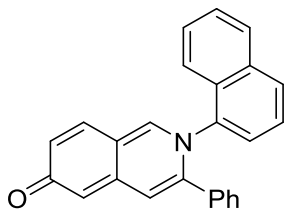
117.34, 114.67, 111.48, 55.63. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO_2^+$ $(M+H)^+$ 328.1332, found 328.1336.




**3-phenyl-2-(p-tolyl)isoquinolin-6(2H)-one (3f)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 87% yield. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.13 (s, 1H), 7.63 – 7.45 (m, 1H), 7.27 – 7.16 (m, 3H), 7.14 – 7.06 (m, 4H), 7.06 – 6.98 (m, 4H), 6.56 (s, 1H), 2.28 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.56, 142.49, 141.96, 140.42, 139.66, 139.35, 134.02, 132.68, 131.24, 130.19, 129.50, 129.04, 128.43, 126.37, 119.01, 117.52, 111.36, 21.11. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO^+$ $(M+H)^+$ 312.1383, found 312.1386.

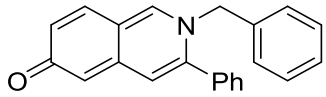



**2-(2,6-dimethylphenyl)-3-phenylisoquinolin-6(2H)-one (3g)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 94% yield. m.p 240.5-247.3 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.85 (s, 1H), 7.54 (d, *J* = 9.3 Hz, 1H), 7.27 – 7.22 (m, 1H), 7.22 – 7.12 (m, 3H), 7.14 – 7.08 (m, 3H), 7.07 – 6.99 (m, 3H), 6.61 (s, 1H), 2.03 (s, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.97, 142.71, 141.00, 140.64, 140.12, 134.63, 133.31, 133.11, 131.02, 129.90, 129.46, 129.05, 128.76, 128.21, 118.78, 117.82, 111.53, 18.15. HRMS (ESI) m/z: calcd for $C_{23}H_{20}NO^+$ $(M+H)^+$ 326.1539, found 326.1539.

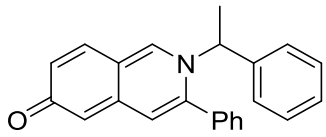



**2-(naphthalen-1-yl)-3-phenylisoquinolin-6(2H)-one (3h)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 94% yield. m.p 105.5-111.3 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.99 (s, 1H), 7.90

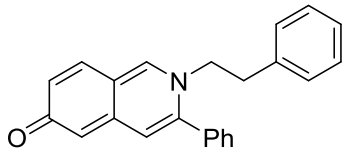
– 7.77 (m, 2H), 7.55 – 7.46 (m, 2H), 7.46 – 7.39 (m, 2H), 7.39 – 7.34 (m, 2H), 7.09 – 7.03 (m, 4H), 7.02 – 6.93 (m, 3H), 6.56 (d, 1H);$^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 182.39, 143.45, 141.70, 140.43, 137.97, 133.93, 133.67, 133.22, 131.05, 130.19, 129.34, 129.05, 128.88, 128.65, 128.23, 127.96, 127.20, 126.15, 124.97, 121.49, 118.09, 117.09, 111.77. HRMS (ESI) m/z: calcd for $C_{25}H_{18}NO^+$ $(M+H)^+$ 348.1383, found 348.1386



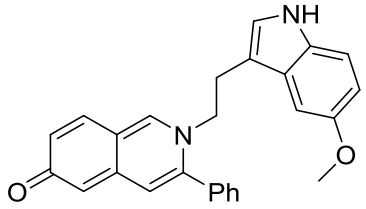

**2-benzyl-3-phenylisoquinolin-6(2H)-one (3i)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 65% yield. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.10 (s, 1H), 7.51 – 7.42 (m, 2H), 7.42 – 7.34 (m, 2H), 7.25 – 7.19 (m, 5H), 6.98 (dd, *J* = 9.3, 2.1 Hz, 1H), 6.91 (s, 1H), 6.83 (d, *J* = 5.8 Hz, 2H), 6.52 (s, 1H), 5.16 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.34, 143.01, 141.57, 140.38, 135.09, 133.57, 132.43, 131.04, 129.93, 129.46, 129.19, 128.91, 128.69, 127.05, 119.44, 118.03, 110.96, 58.31. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO^+$ $(M+H)^+$ 312.1383, found 312.1380.



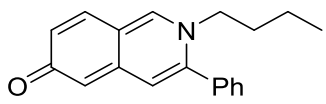

**3-phenyl-2-(1-phenylethyl)isoquinolin-6(2H)-one (3j)**. Brown solid, (purified by silica gel column chrmatography by eluting with DCM/MeOH = 20:1 to 10:1), 78% yield. m.p 223.7-230.1 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.02 (s, 1H), 7.59 – 7.45 (m, 5H), 7.38 – 7.30 (m, 4H), 7.10 (d, *J* = 6.3 Hz, 2H), 7.03 (dd, *J* = 9.4, 2.1 Hz, 1H), 6.99 (s, 1H), 6.60 (s, 1H), 5.55 (q, *J* = 7.0 Hz, 1H), 1.83 (d, *J* = 7.0 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.64, 142.98, 140.10, 139.09, 137.88, 133.94, 132.67, 131.01, 130.08, 129.42, 129.23, 128.93, 126.65, 119.15, 118.52, 111.00, 60.49, 20.98. HRMS (ESI) m/z: calcd for $C_{23}H_{20}NO^+$ $(M+H)^+$ 326.1539, found 326.1541.



**2-phenethyl-3-phenylisoquinolin-6(2H)-one (3k)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 73% yield. m.p 207.6-214.0 ℃. $^1$H NMR (500 MHz, Chloroform-d): $\delta$ = 7.86 (s, 1H), 7.57 – 7.46 (m, 3H), 7.39 (d, J = 9.3 Hz, 1H), 7.32 (s, 1H), 7.30 (s, 1H), 7.21 – 7.14 (m, 3H), 7.00 (dd, J = 9.3, 2.1 Hz, 1H), 6.92 (s, 1H), 6.80 – 6.74 (m, 2H), 6.53 (s, 1H), 4.21 (t, J = 7.3 Hz, 2H), 2.82 (t, J = 7.3 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.30, 142.43, 141.07, 140.21, 135.91, 133.64, 132.47, 130.77, 130.02, 129.50, 129.12, 129.06, 128.78, 127.49, 119.53, 117.89, 110.99, 56.50, 37.40. HRMS (ESI) m/z: calcd for $C_{23}H_{20}NO^+$ $(M+H)^+$ 326.1539, found 326.1539.

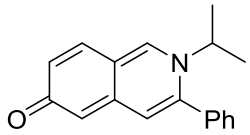



**2-(2-(5-methoxy-1H-indol-3-yl)ethyl)-3-phenylisoquinolin-6(2H)-one (3l)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 51% yield. m.p 178.4-184.1 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 8.47 (s, 1H), 7.63 (d, $J$ = 9.2 Hz, 1H), 7.52 – 7.46 (m, 1H), 7.44 – 7.39 (m, 2H), 7.21 – 7.15 (m, 3H), 7.14 (s, 1H), 7.01 (dd, $J$ = 9.3, 2.1 Hz, 1H), 6.68 (dd, $J$ = 8.8, 2.4 Hz, 1H), 6.65 (s, 1H), 6.61 (s, 1H), 6.40 (d, $J$ = 2.3 Hz, 1H), 4.42 (t, $J$ = 6.6 Hz, 2H), 3.57 (s, 3H), 3.00 (t, $J$ = 6.6 Hz, 2H);$^{13}$C NMR (125 MHz, MeOD): $\delta$ = 180.94, 155.23, 145.58, 145.21, 142.39, 134.79, 133.13, 132.58, 131.31, 130.80, 130.62, 129.81, 128.58, 125.17, 121.62, 119.72, 113.14, 113.12, 110.82, 110.05, 100.24, 57.58, 56.17, 27.97. HRMS (ESI) m/z: calcd for $C_{26}H_{23}N_2O_2^+$ $(M+H)^+$ 395.1754, found 395.1755.

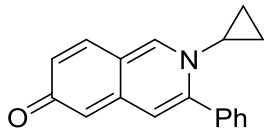



**2-butyl-3-phenylisoquinolin-6(2H)-one (3m)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 76% yield. $^1$H NMR (500 MHz, Chloroform-$d$): $\delta$ = 8.21 (s, 1H), 7.56 (d, $J$ = 9.3 Hz, 1H), 7.53 – 7.46 (m, 3H), 7.38 (m, $J$ = 7.5, 2.0 Hz, 2H), 7.05 (d, $J$ = 7.0 Hz, 1H), 6.97 (s, 1H), 6.58 (s, 1H), 4.01 (t, $J$ = 7.7 Hz, 2H), 1.65 – 1.50 (m, 2H), 1.20 – 1.03 (m, 2H), 0.73 (t,

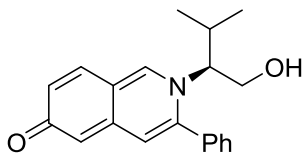
*J* = 7.4 Hz, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 180.46, 142.77, 141.63, 140.39, 133.66, 132.03, 130.94, 130.03, 129.44, 129.08, 119.91, 118.32, 110.59, 55.09, 33.23, 19.47, 13.40. HRMS (ESI) m/z: calcd for $C_{19}H_{20}NO^+$ $(M+H)^+$ 278.1539, found 278.1541.




**2-isopropyl-3-phenylisoquinolin-6(2H)-one (3n)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 83% yield. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 9.09 (s, 1H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.63 – 7.57 (m, 3H), 7.56 – 7.51 (m, 2H), 7.36 (s, 1H), 7.14 (dd, *J* = 9.2, 2.1 Hz, 1H), 6.74 (s, 1H), 4.72 – 4.60 (m, 1H), 1.54 (d, *J* = 6.8 Hz, 6H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ =179.86, 145.35, 142.29, 141.95, 135.11, 132.92, 131.17, 130.91, 130.49, 130.22, 122.04, 120.97, 110.58, 57.19, 22.99. HRMS (ESI) m/z: calcd for $C_{18}H_{18}NO^+$ $(M+H)^+$ 264.1383, found 264.1383.

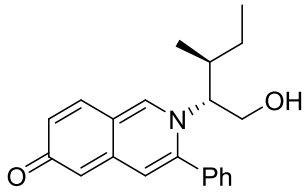



**2-cyclopropyl-3-phenylisoquinolin-6(2H)-one (3o)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1 to 10:1), 57% yield. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.18 (s, 1H), 7.60 – 7.38 (m, 6H), 7.01 – 6.93 (m, 1H), 6.91 (d, *J* = 2.6 Hz, 1H), 6.50 (s, 1H), 3.59 (tt, *J* = 7.1, 4.3 Hz, 1H), 0.84 (d, *J* = 8.5 Hz, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 180.77, 144.33, 142.12, 140.22, 134.26, 131.90, 131.07, 129.55, 129.25, 128.79, 119.14, 117.55, 110.92, 38.49, 9.56. HRMS (ESI) m/z: calcd for $C_{18}H_{16}NO^+$ $(M+H)^+$ 262.1226, found 262.1227.

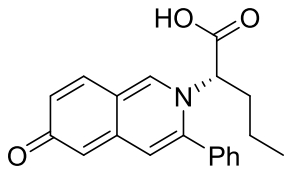



**(R)-2-(1-hydroxy-3-methylbutan-2-yl)-3-phenylisoquinolin-6(2H)-one (3p)**. Brown solid, (purified by silica gel column chromatography by eluting with

DCM/MeOH = 10:1), 41% yield. m.p 93.4-98.5 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 9.10 (s, 1H), 7.98 (d, $J$ = 9.2 Hz, 1H), 7.67 – 7.43 (m, 5H), 7.38 (s, 1H), 7.14 (dd, $J$ = 9.2, 2.1 Hz, 1H), 6.74 (s, 1H), 4.18 (ddd, $J$ = 10.6, 7.6, 3.4 Hz, 1H), 4.10 – 4.02 (m, 1H), 3.97 (dd, $J$ = 12.3, 3.5 Hz, 1H), 2.35 (dt, $J$ = 10.4, 6.6 Hz, 1H), 0.94 (d, $J$ = 6.5 Hz, 3H), 0.67 (d, $J$ = 6.7 Hz, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 179.59, 147.02, 142.97, 142.14, 135.20, 133.19, 131.41, 131.02, 130.81, 129.81, 121.90, 120.75, 110.52, 72.33, 62.76, 31.95, 20.00, 19.93. HRMS (ESI) m/z: calcd for $C_{20}H_{22}NO_2^+$ $(M+H)^+$ 308.1645, found 308.1642.

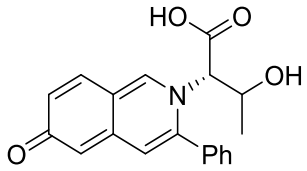



**2-((2R,3S)-1-hydroxy-3-methylpentan-2-yl)-3-phenylisoquinolin-6(2H)-one (3q)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 38% yield. m.p 82.1-89.5 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 9.09 (s, 1H), 7.97 (d, $J$ = 9.2 Hz, 1H), 7.57 (s, 5H), 7.35 (s, 1H), 7.12 (dd, $J$ = 9.2, 2.2 Hz, 1H), 6.71 (d, $J$ = 2.1 Hz, 1H), 4.27 (ddd, $J$ = 10.6, 7.8, 3.5 Hz, 1H), 4.08 (dd, $J$ = 12.3, 7.8 Hz, 1H), 3.98 (dd, $J$ = 12.3, 3.5 Hz, 1H), 2.10 (dtt, $J$ = 9.9, 6.6, 3.4 Hz, 1H), 1.08 (dtd, $J$ = 14.7, 7.4, 3.6 Hz, 1H), 0.91 (d, $J$ = 6.6 Hz, 3H), 0.87 – 0.75 (m, 1H), 0.71 (t, $J$ = 7.3 Hz, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 180.15, 146.93, 142.87, 142.15, 135.19, 133.15, 131.57, 131.05, 131.00, 130.14, 121.85, 120.54, 110.60, 70.87, 62.55, 38.42, 26.65, 15.75, 11.28. HRMS (ESI) m/z: calcd for $C_{21}H_{24}NO_2^+$ $(M+H)^+$ 322.1802, found 322.1805.

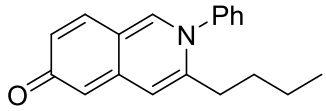



**(S)-2-(6-oxo-3-phenylisoquinolin-2(6H)-yl)pentanoic acid (3r)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 71% yield. m.p 154.7-161.2 ℃. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 9.55 (s, 1H), 8.32 (d, $J$ = 9.0 Hz, 1H), 7.85 (s, 1H), 7.67 – 7.47 (m, 5H), 7.43 (dd, 1H), 7.27 (s, 1H),

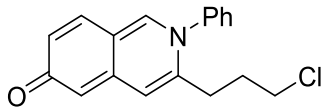
5.06 – 4.98 (m, 1H), 2.52 – 2.18 (m, 2H), 1.16 (hept, $J$ = 7.0 Hz, 2H), 0.80 (t, $J$ = 7.3 Hz, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 169.48, 148.16, 147.62, 141.91, 134.26, 134.16, 131.56, 130.71, 130.30, 125.95, 124.47, 122.71, 109.41, 36.55, 20.64, 13.60. HRMS (ESI) m/z: calcd for $C_{20}H_{20}NO_3^+$ $(M+H)^+$ 322.1438, found 322.1437.




**(2S)-3-hydroxy-2-(6-oxo-3-phenylisoquinolin-2(6H)-yl)butanoic acid (3s)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 51% yield. $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ = 9.73 (s, 1H), 8.34 (d, $J$ = 9.1 Hz, 1H), 7.85 (s, 1H), 7.57 (s, 5H), 7.47 (d, $J$ = 8.1 Hz, 1H), 7.25 (s, 1H), 4.89 (q, $J$ = 7.1 Hz, 1H), 3.17 (s, 1H), 1.83 (d, $J$ = 7.3 Hz, 3H); $^3$C NMR (125 MHz, DMSO): $\delta$ = 169.62, 168.11, 146.97, 144.95, 139.76, 133.05, 132.66, 129.99, 129.33, 128.88, 124.81, 122.39, 120.29, 108.02, 65.11, 48.54, 19.10. HRMS (ESI) m/z: calcd for $C_{19}H_{18}NO_4^+$ $(M+H)^+$ 324.1230, found 324.1231.

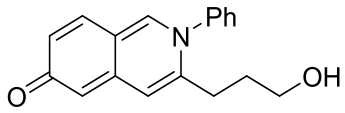



**3-butyl-2-phenylisoquinolin-6(2H)-one (3t)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1), 87% yield. $^1$H NMR (500 MHz, Chloroform-$d$): $\delta$ = 7.98 (s, 1H), 7.50 (s, 3H), 7.42 (d, $J$ = 9.7 Hz, 1H), 7.34 – 7.28 (m, 2H), 6.99 – 6.76 (m, 2H), 6.45 (s, 1H), 2.44 – 2.25 (m, 2H), 1.45 – 1.26 (m, 2H), 1.13 (dq, $J$ = 14.1, 6.9 Hz, 2H), 0.74 – 0.61 (m, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 180.80, 143.04, 141.70, 140.88, 131.90, 130.94, 130.15, 130.05, 126.72, 116.86, 116.01, 110.11, 110.08, 31.85, 30.49, 21.94, 13.44. HRMS (ESI) m/z: calcd for $C_{19}H_{20}NO^+$ $(M+H)^+$ 278.1539, found 278.1544.

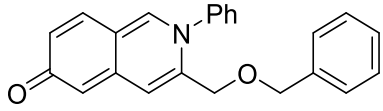



**3-(3-chloropropyl)-2-phenylisoquinolin-6(2H)-one (3u)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 15:1), 61% yield.

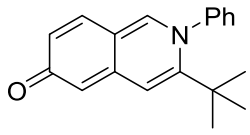
$^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.97 (s, 1H), 7.62 – 7.56 (m, 3H), 7.46 (d, *J* = 9.2 Hz, 1H), 7.39 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.03 – 6.90 (m, 2H), 6.52 (d, *J* = 6.9 Hz, 1H), 3.41 (tt, *J* = 5.3, 2.6 Hz, 2H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.96 – 1.85 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.23, 141.80, 141.40, 140.97, 140.80, 132.36, 131.13, 130.54, 130.43, 126.95, 117.15, 116.58, 110.75, 43.52, 31.12, 29.61. HRMS (ESI) m/z: calcd for $C_{18}H_{17}ClNO^+$ $(M+H)^+$ 298.0993, found 298.1000.



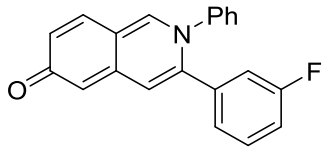

**3-(3-hydroxypropyl)-2-phenylisoquinolin-6(2H)-one (3v)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 84% yield. $^1$H NMR (500 MHz, Methanol-$d_4$): $\delta$ = 8.83 (s, 1H), 7.88 (d, *J* = 9.2 Hz, 1H), 7.72 – 7.65 (m, 3H), 7.64 – 7.55 (m, 2H), 7.50 (s, 1H), 7.10 (dd, *J* = 9.1, 2.2 Hz, 1H), 6.78 (d, *J* = 2.3 Hz, 1H), 3.47 (t, *J* = 6.1 Hz, 2H), 2.72 (t, 2H), 1.82 – 1.70 (m, 3H); $^{13}$C NMR (125 MHz, MeOD): $\delta$ = 179.08, 146.76, 146.02, 143.40, 142.54, 133.35, 131.67, 131.26, 130.29, 128.03, 119.48, 119.40, 110.18, 61.42, 32.19, 30.06. HRMS (ESI) m/z: calcd for $C_{18}H_{18}NO_2^+$ $(M+H)^+$ 280.1332, found 280.1333.



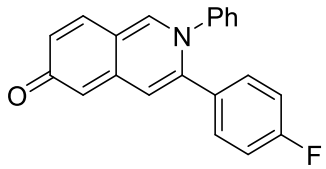

**3-((benzyloxy)methyl)-2-phenylisoquinolin-6(2H)-one (3w)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 69% yield. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.89 (s, 1H), 7.62 – 7.49 (m, 3H), 7.43 (d, *J* = 9.3 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.32 – 7.24 (m, 2H), 7.14 (d, *J* = 7.9 Hz, 2H), 7.11 – 7.06 (m, 1H), 7.00 – 6.93 (m, 1H), 6.51 (s, 2H), 4.29 (s, 1H), 4.19 (s, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.98, 141.40, 140.66, 140.10, 138.09, 136.77, 132.90, 131.17, 130.30, 129.97, 128.57, 128.13, 127.87, 126.96, 117.96, 117.07, 111.90, 73.02, 67.83. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO_2^+$ $(M+H)^+$ 342.1489, found 342.1488.



**3-(tert-butyl)-2-phenylisoquinolin-6(2H)-one (3x)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1), 55% yield. m.p 132.1-135.6 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 7.73 (s, 1H), 7.60 – 7.48 (m, 3H), 7.41 (d, *J* = 7.3 Hz, 2H), 7.37 (d, *J* = 9.2 Hz, 1H), 7.13 (s, 1H), 6.96 (dd, *J* = 9.2, 2.1 Hz, 1H), 6.52 (s, 1H), 1.20 (s, 9H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.93, 150.41, 144.27, 144.14, 140.83, 132.93, 130.54, 130.42, 129.48, 128.96, 116.09, 115.18, 111.11, 36.83, 31.72. HRMS (ESI) m/z: calcd for $C_{19}H_{20}NO^+$ $(M+H)^+$ 278.1539, found 278.1540.

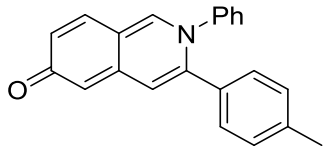



**3-(3-fluorophenyl)-2-phenylisoquinolin-6(2H)-one (3y)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1), 86% yield. m.p 228.9-236.1 ℃. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.17 (s, 1H), 7.55 (d, *J* = 9.3 Hz, 1H), 7.40 – 7.33 (m, 3H), 7.24 – 7.17 (m, 3H), 7.08 (s, 1H), 7.02 (d, *J* = 8.6 Hz, 1H), 7.00 – 6.92 (m, 2H), 6.87 (d, *J* = 9.3 Hz, 1H), 6.59 (s, 1H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 181.63, 162.28 ($J_{CF}$ = 247.50 Hz), 141.90, 141.87, 140.99 ($J_{CF}$ = 2.50 Hz), 140.16, 135.94 ($J_{CF}$ = 7.50 Hz), 132.82, 131.48, 130.28 ($J_{CF}$ = 7.50 Hz), 129.90, 129.44, 126.69, 125.51 ($J_{CF}$ = 2.50 Hz), 119.27, 117.67, 116.72 ($J_{CF}$ = 22.50 Hz), 116.30 ($J_{CF}$ = 20.00Hz), 111.86. HRMS (ESI) m/z: calcd for $C_{21}H_{15}FNO^+$ $(M+H)^+$ 316.1132, found 316.1133.

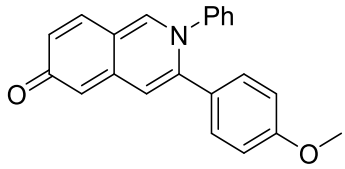



**3-(4-fluorophenyl)-2-phenylisoquinolin-6(2H)-one (3z)**. Brown solid (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1), 91% yield. m.p 235.1-238.8 ℃. $^{1}$H NMR (400 MHz, Methanol-$d_4$): $\delta$ = 8.86 (s, 1H), 7.87 (d, *J* = 9.2 Hz, 1H), 7.47 – 7.40 (m, 4H), 7.40 – 7.35 (m, 2H), 7.35 – 7.27 (m, 2H), 7.06 (dd, J = 9.2, 2.1 Hz, 1H), 7.04 – 6.98 (m, 2H), 6.71 (s, 1H); 13C NMR (100 MHz, MeOD): $\delta$ = 181.45, 164.33 ($J_{CF}$ = 247.7 Hz), 146.30, 143.66 ($J_{CF}$ = 35.3 Hz), 142.75, 133.59,

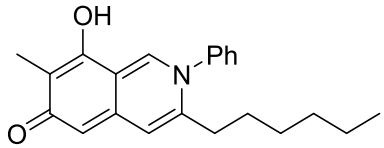
133.34 ($J_{CF}$ = 8.6 Hz), 131.58, 131.45 ($J_{CF}$ = 3.6 Hz), 130.68, 130.61, 128.26, 121.39, 119.36, 116.48, 116.26, 111.40. HRMS (ESI) m/z: calcd for $C_{21}H_{15}FNO^+$ $(M+H)^+$ 316.1132, found 316.1133.




**2-phenyl-3-(p-tolyl)isoquinolin-6(2H)-one (3aa)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 20:1), 85% yield. m.p 193.5-197.2 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.05 (s, 1H), 7.50 (d, *J* = 9.3 Hz, 1H), 7.39 – 7.31 (m, 3H), 7.20 – 7.11 (m, 2H), 7.02 (d, *J* = 9.6 Hz, 6H), 6.56 (s, 1H), 2.28 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 182.30, 142.41, 141.29, 140.48, 139.26, 133.20, 131.16, 131.09, 129.72, 129.42, 129.20, 129.08, 126.77, 118.71, 117.43, 111.67, 111.64, 21.32. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO^+$ $(M+H)^+$ 312.1383, found 312.1377.

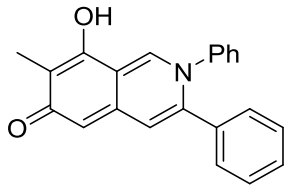



**3-(4-methoxyphenyl)-2-phenylisoquinolin-6(2H)-one (3ab)**. Brown solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 15:1), 96% yield. m.p 222.5-231.7 ℃. $^1$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.16 (s, 1H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.28 – 7.24 (m, 3H), 7.17 – 7.09 (m, 2H), 7.01 – 6.95 (m, 3H), 6.92 (d, *J* = 8.9 Hz, 1H), 6.67 (s, 1H), 6.65 (s, 1H), 6.49 (s, 1H), 3.66 (s, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 180.94, 159.92, 142.27, 142.10, 142.01, 140.50, 132.14, 131.28, 130.76, 129.58, 128.98, 126.58, 125.93, 118.69, 117.42, 113.78, 110.87, 55.21. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO_2^+$ $(M+H)^+$ 328.1332, found 328.1330.

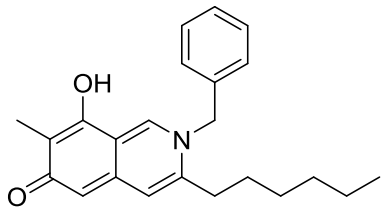



**3-hexyl-8-hydroxy-7-methyl-2-phenylisoquinolin-6(2H)-one (3ac)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1),

89% yield. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 9.08 (s, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.35 – 7.24 (m, 4H), 6.56 (s, 1H), 2.45 (t, *J* = 7.0 Hz, 2H), 2.20 (s, 3H), 1.72 – 1.56 (m, 2H), 1.52 – 1.41 (m, 2H), 1.36 – 1.30 (m, 4H), 0.91 (t, 3H); $^{13}$C NMR (125 MHz, $CDCl_3$): $\delta$ = 165.67, 160.00, 158.92, 146.43, 129.60, 126.58, 125.18, 120.75, 112.52, 112.49, 111.66, 96.15, 77.38, 31.51, 28.87, 28.78, 22.68, 19.71, 14.19, 7.87. HRMS (ESI) m/z: calcd for $C_{22}H_{26}NO_2^+$ $(M+H)^+$ 336.1958, found 336.1957.




**8-hydroxy-7-methyl-2,3-diphenylisoquinolin-6(2H)-one (3ad)**. Orange solid, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 90% yield. m.p 155.4-161.6 ℃. $^{1}$H NMR (500 MHz, Acetone-$d_6$): $\delta$ = 9.27 (s, 1H), 9.20 (s, 1H), 7.65 – 7.51 (m, 2H), 7.50 – 7.34 (m, 7H), 7.27 (t, *J* = 7.3 Hz, 1H), 6.78 (s, 1H), 2.17 (s, 3H); $^{13}$C NMR (125 MHz, Acetone): $\delta$ = 162.33, 160.97, 159.40, 148.56, 131.45, 129.51, 128.81, 128.62, 126.50, 123.62, 122.72, 121.08, 112.97, 112.08, 111.09, 94.09, 86.07, 29.46, 29.31, 29.16, 29.00, 28.85, 28.69, 28.54, 7.36. HRMS (ESI) m/z: calcd for $C_{22}H_{18}NO_2^+$ $(M+H)^+$ 328.1332, found 328.1333.




**2-benzyl-3-hexyl-8-hydroxy-7-methylisoquinolin-6(2H)-one (3ae)**. Brown oil, (purified by silica gel column chromatography by eluting with DCM/MeOH = 10:1), 66% yield. $^{1}$H NMR (500 MHz, Chloroform-*d*): $\delta$ = 8.68 (s, 1H), 7.45 – 7.27 (m, 6H), 6.47 (s, 1H), 4.75 (s, 2H), 2.40 (t, *J* = 7.1 Hz, 2H), 2.12 (s, 3H), 1.58 (p, *J* = 7.3 Hz, 2H), 1.44 (p, *J* = 7.0 Hz, 2H), 1.36 – 1.30 (m, 4H), 0.91 (t, *J* = 6.6 Hz, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$): $\delta$ = 168.30, 163.76, 159.28, 137.30, 128.88, 127.80, 127.80, 127.73, 124.38, 113.05, 111.21, 95.28, 77.36, 59.43, 31.46, 28.83, 28.77, 22.71, 19.63, 14.18, 7.94. HRMS (ESI) m/z: calcd for $C_{23}H_{28}NO_2^+$ $(M+H)^+$ 350.2115, found

350.2110.

## S4. Reference

(1) L. Lin, N. Mulholland, Q. Y. Wu, D. Beattie, S. W. Huang, D. Irwin, J. Clough, Y. C. Gu and G. F. Yang, *J. Agr. Food Chem.*, 2012, **60**, 4480-4491.

(2) J. Zhu, A. R. Germain and J. A. Porco, *Angew. Chem. Int. Ed.*, 2004, **43**, 1239-1243.

## S5. X-ray Data of 3a

The method of sample preparation: 1ml hexanes, 2 drops of dichloromethane were added in a 2ml vial which then was closed the lid with a needle on it. Put the sample on the room temperature (about 20 ℃) under a stable condition.

Figure S1. X-ray structure of **3a (**2081746**)**.

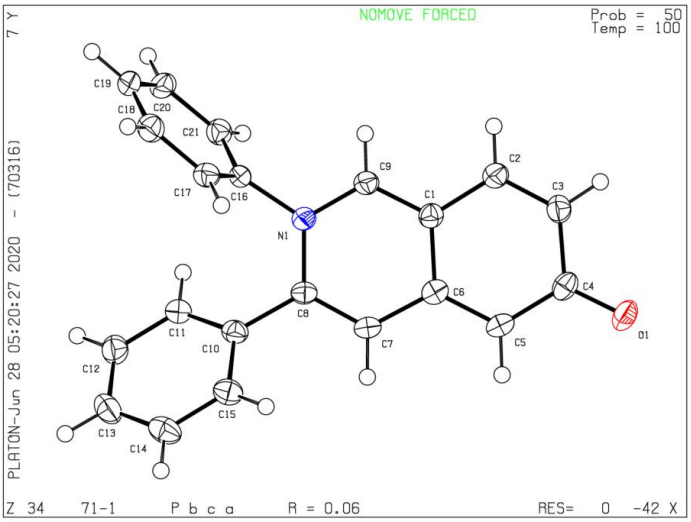



Table S2. Crystal data and structure refinement for **3a**

| **Table 1 Crystal data and structure refinement for 3a.** | |
|---|---|
| Identification code | 3a |
| Empirical formula | $C_{21}H_{15}NO$ |
| Formula weight | 297.34 |
| Temperature/K | 100.0(2) |
| Crystal system | orthorhombic |

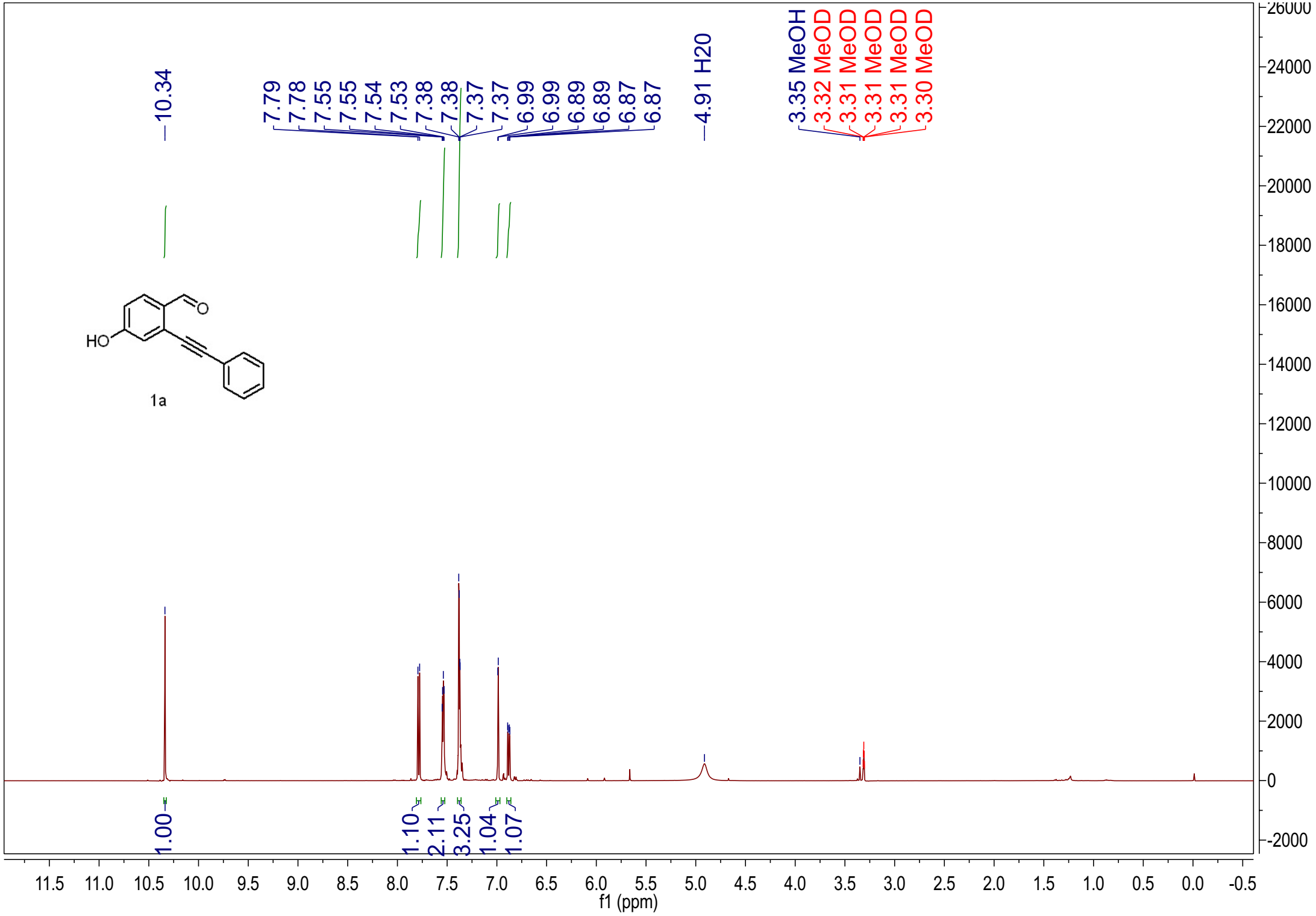
| | |
|---|---|
| Space group | Pbca |
| a/Å | 12.5288(5) |
| b/Å | 14.6591(5) |
| c/Å | 16.0719(6) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å$^3$ | 2951.78(19) |
| Z | 8 |
| $\rho_{calc}$g/cm$^3$ | 1.338 |
| μ/mm$^{-1}$ | 0.644 |
| F(000) | 1248.0 |
| Crystal size/mm$^3$ | 0.12 × 0.11 × 0.08 |
| Radiation | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 10.798 to 147.666 |
| Index ranges | -15 ≤ h ≤ 15, -18 ≤ k ≤ 17, -17 ≤ l ≤ 19 |
| Reflections collected | 11528 |
| Independent reflections | 2934 [$R_{int}$ = 0.0804, $R_{sigma}$ = 0.0562] |
| Data/restraints/parameters | 2934/0/208 |
| Goodness-of-fit on F$^2$ | 1.023 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0591, w$R_2$ = 0.1465 |
| Final R indexes [all data] | $R_1$ = 0.0752, w$R_2$ = 0.1607 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.24/-0.27 |

**Crystal structure determination of 3a**

**Crystal Data** for $C_{21}H_{15}NO$ (*M* =297.34 g/mol): orthorhombic, space group Pbca (no. 61), *a* = 12.5288(5) Å, *b* = 14.6591(5) Å, *c* = 16.0719(6) Å, *V* = 2951.78(19) Å$^3$, *Z* = 8, *T* = 100.0(2) K, μ(Cu Kα) = 0.644 mm$^{-1}$, *Dcalc* = 1.338 g/cm$^3$, 11528 reflections measured (10.798° ≤ 2Θ ≤ 147.666°), 2934 unique ($R_{int}$ = 0.0804, $R_{sigma}$ = 0.0562) which were used in all calculations.

The final $R_1$ was 0.0591 ($I > 2\sigma(I)$) and $wR_2$ was 0.1607 (all data)

## S6. $^{1}H$ and $^{13}C$ NMR spectrum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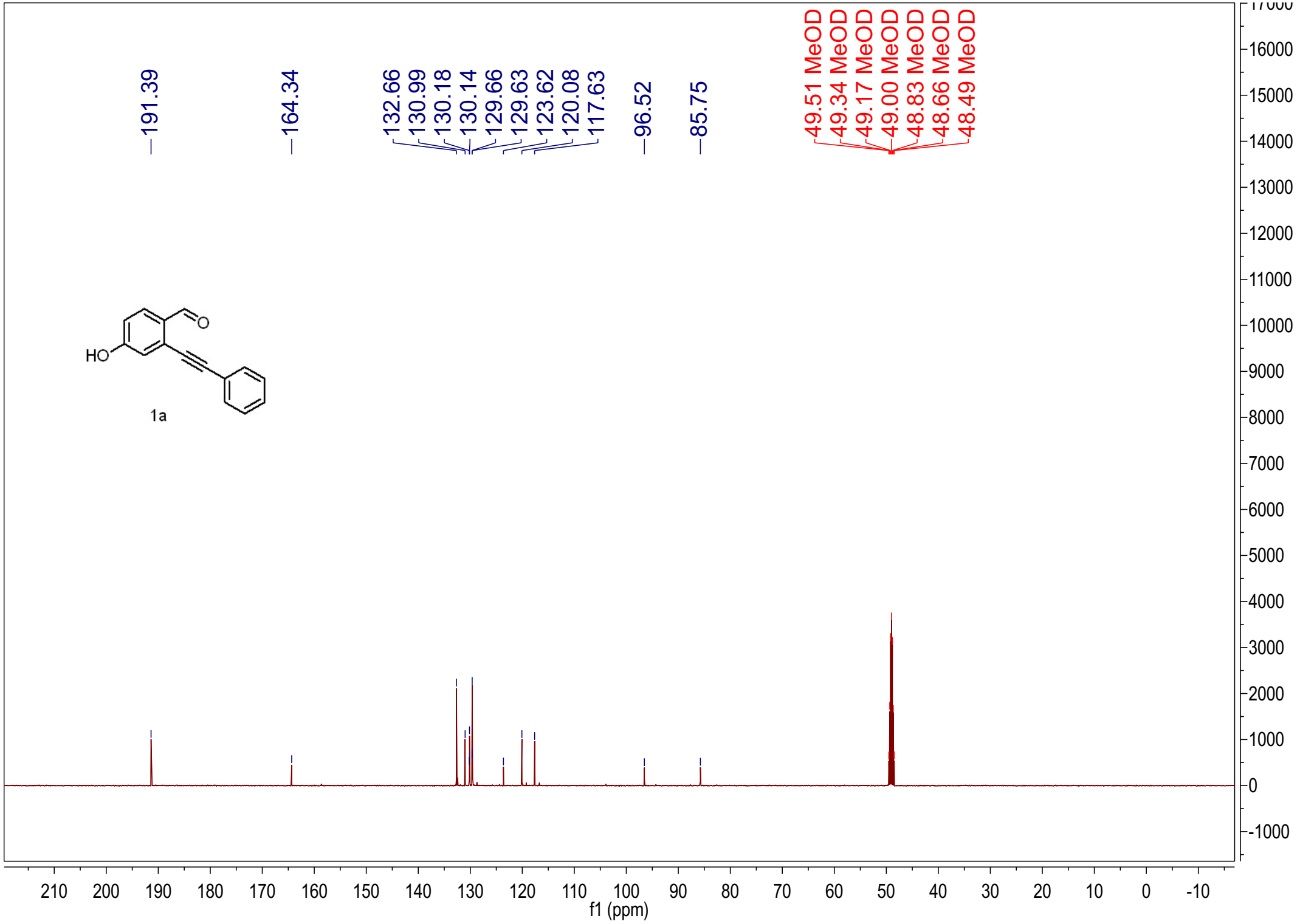
7.55
7.55
7.54
7.53
7.38
7.38
7.37
7.37
6.99
6.99
6.89
6.89
6.87
6.87
4.91 H20
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
HO
O
1a
1.00
1.10
2.11
3.25
1.04
1.07
f1 (ppm)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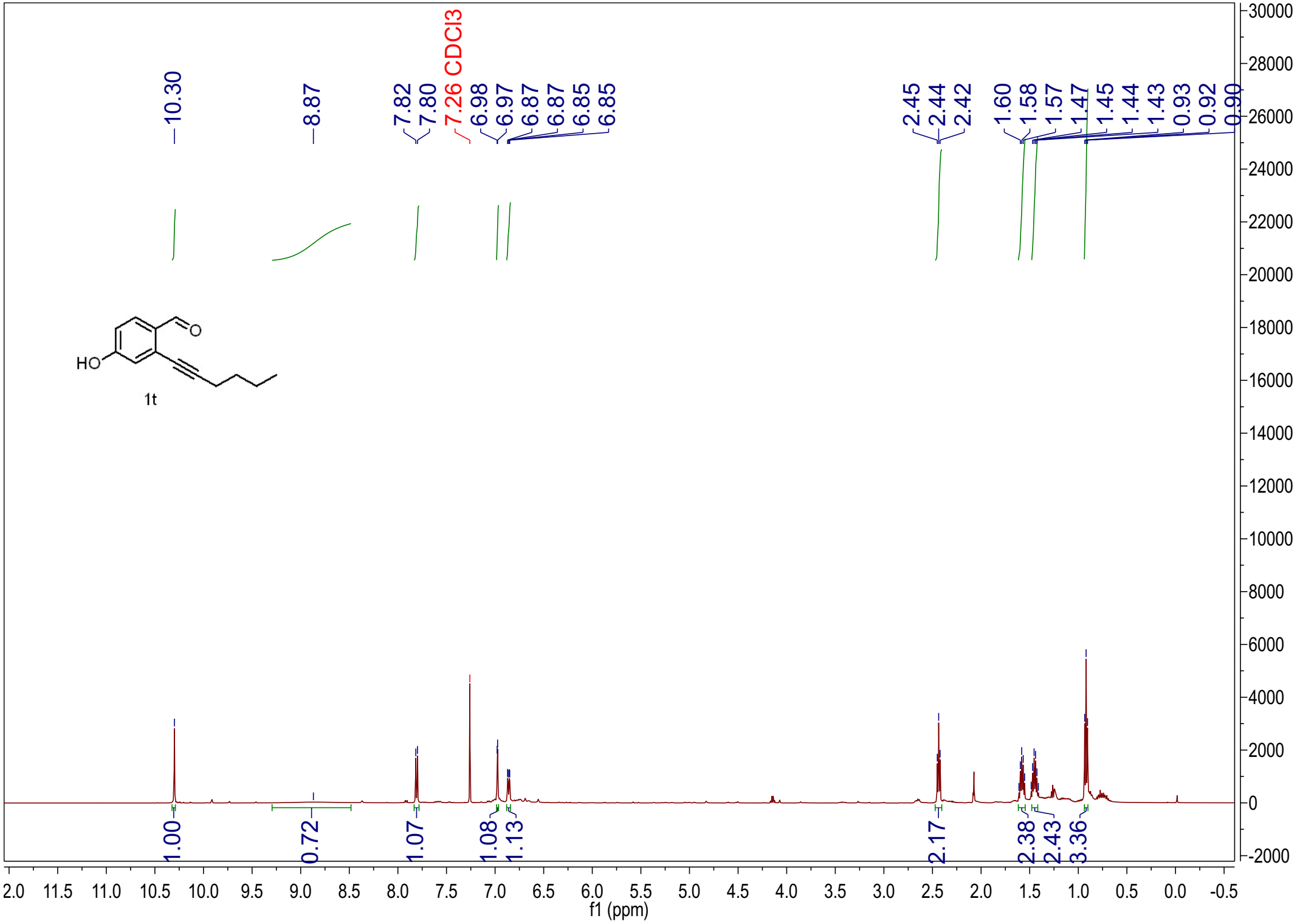
130.99
130.18
130.14
129.66
129.63
123.62
120.08
117.63
96.52
85.75
49.51 MeOD
49.34 MeOD
49.17 MeOD
49.00 MeOD
48.83 MeOD
48.66 MeOD
48.49 MeOD
HO
O
1a
f1 (ppm)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7.80
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6.87
6.85
6.85
2.45
2.44
2.42
1.60
1.58
1.57
1.47
1.45
1.44
1.43
0.93
0.92
0.90
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1.08
1.13
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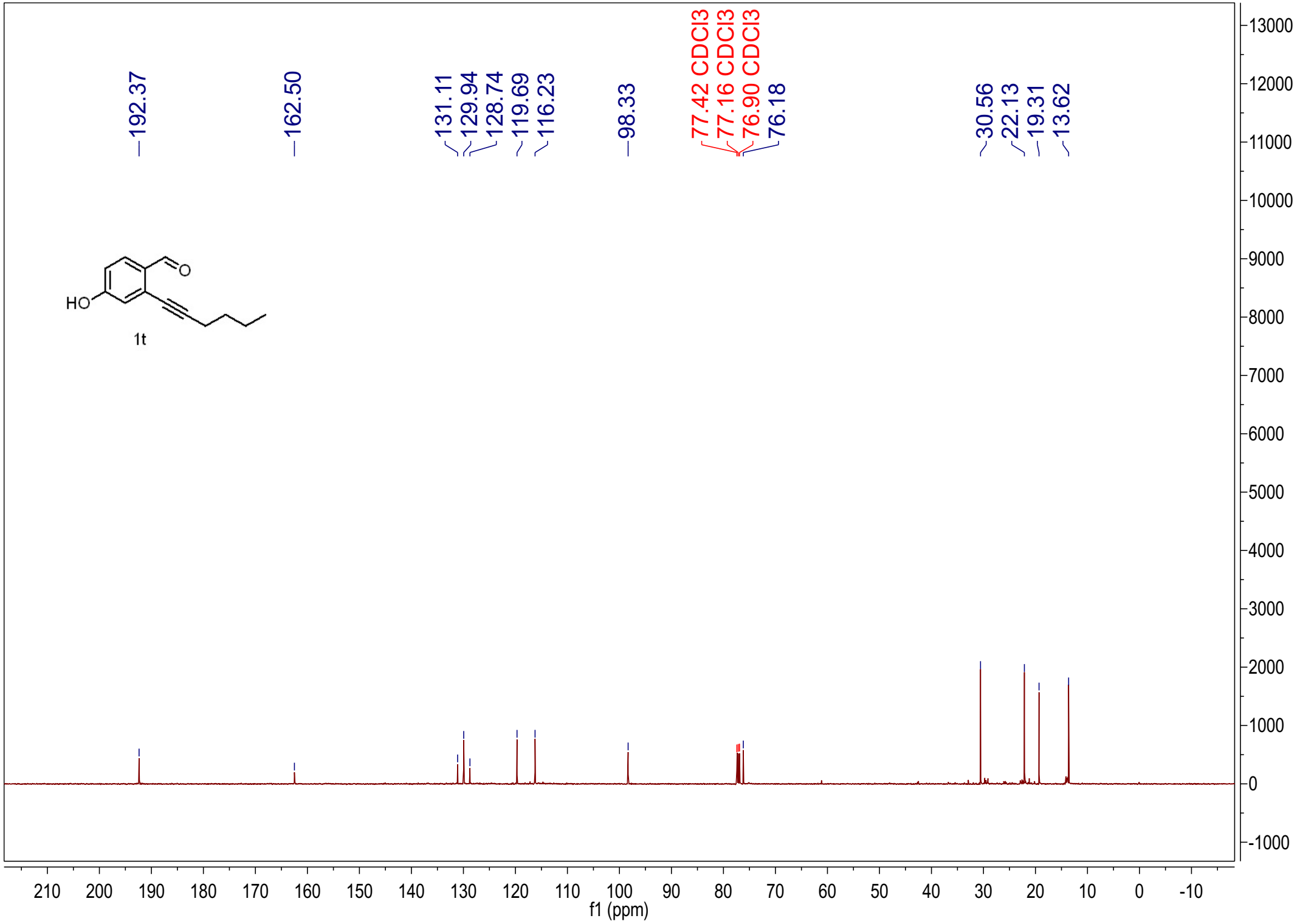
2.38
2.43
3.36
f1 (ppm)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119.69
116.23
98.33
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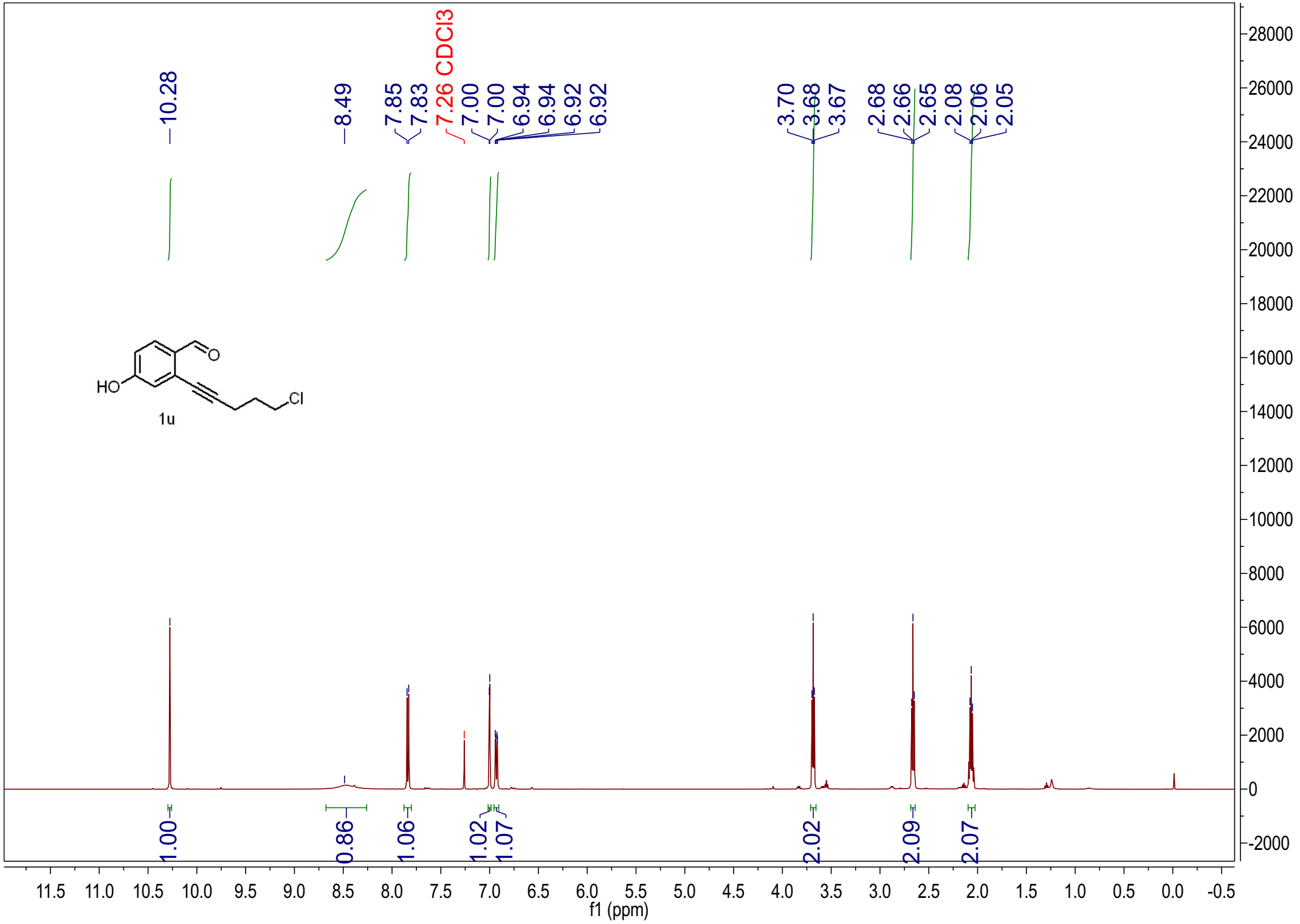
77.16 CDCl3
76.90 CDCl3
76.18
30.56
22.13
19.31
13.62
HO
O
1t
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.00
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6.94
6.92
6.92
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3.68
3.67
2.68
2.66
2.65
2.08
2.06
2.05
HO
O
Cl
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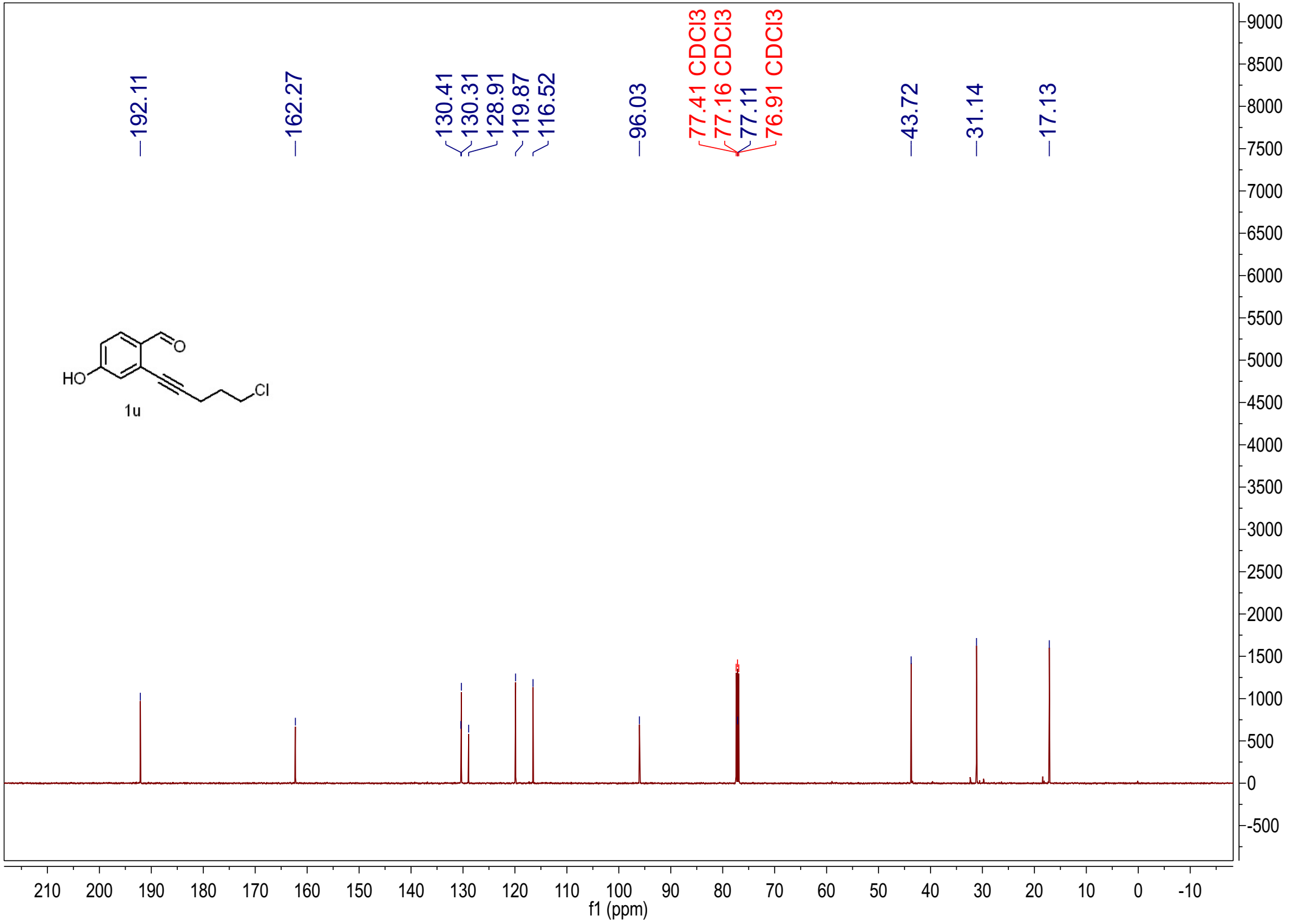
1.06
1.02
1.07
2.02
2.09
2.07
f1 (ppm)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119.87
116.52
96.03
77.41 CDCl3
77.16 CDCl3
77.11
76.91 CDCl3
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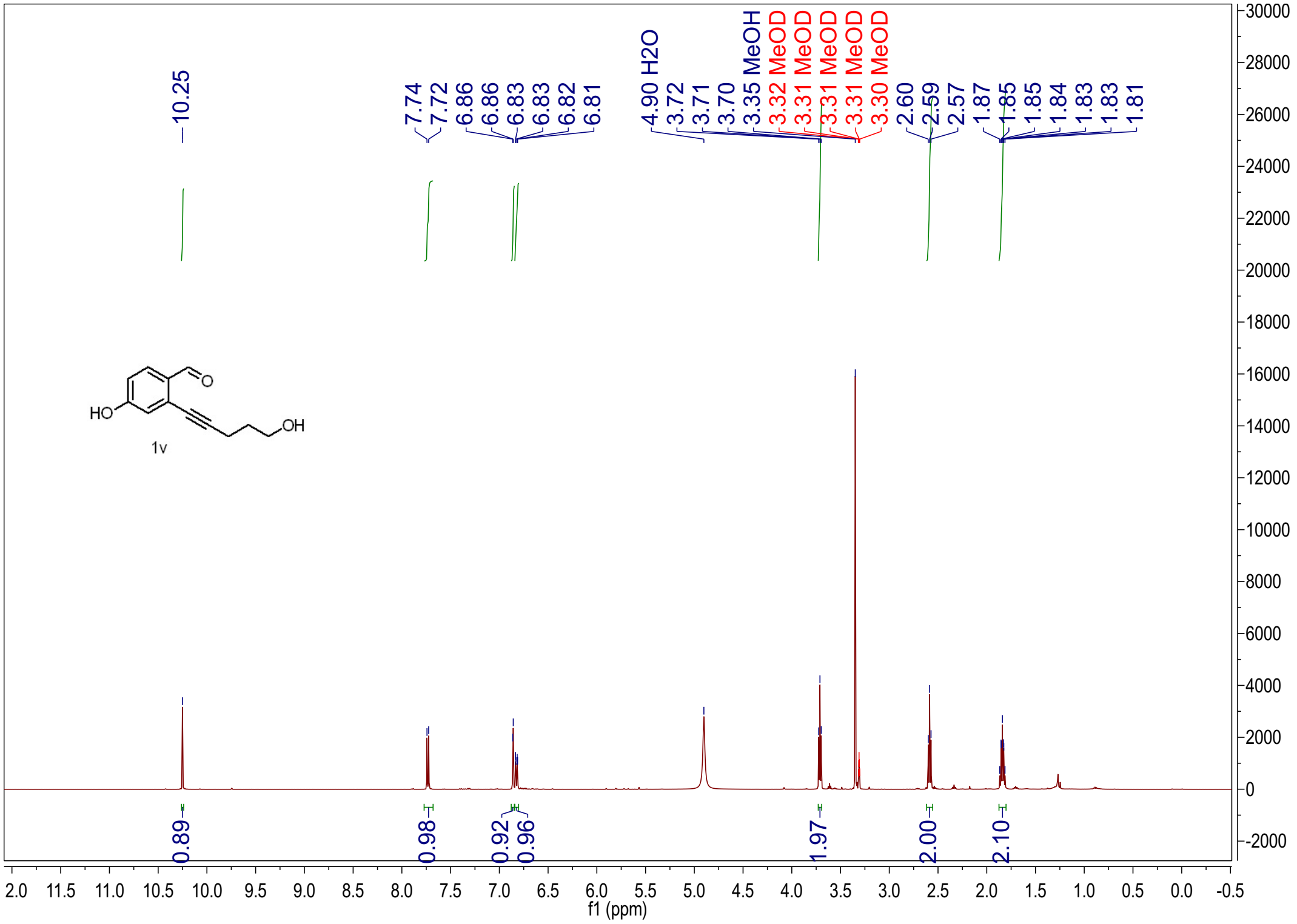
17.13
HO
O
Cl
1u
f1 (ppm)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6.81
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3.71
3.70
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
2.60
2.59
2.57
1.87
1.85
1.85
1.84
1.83
1.83
1.81
HO
O
OH
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0.98
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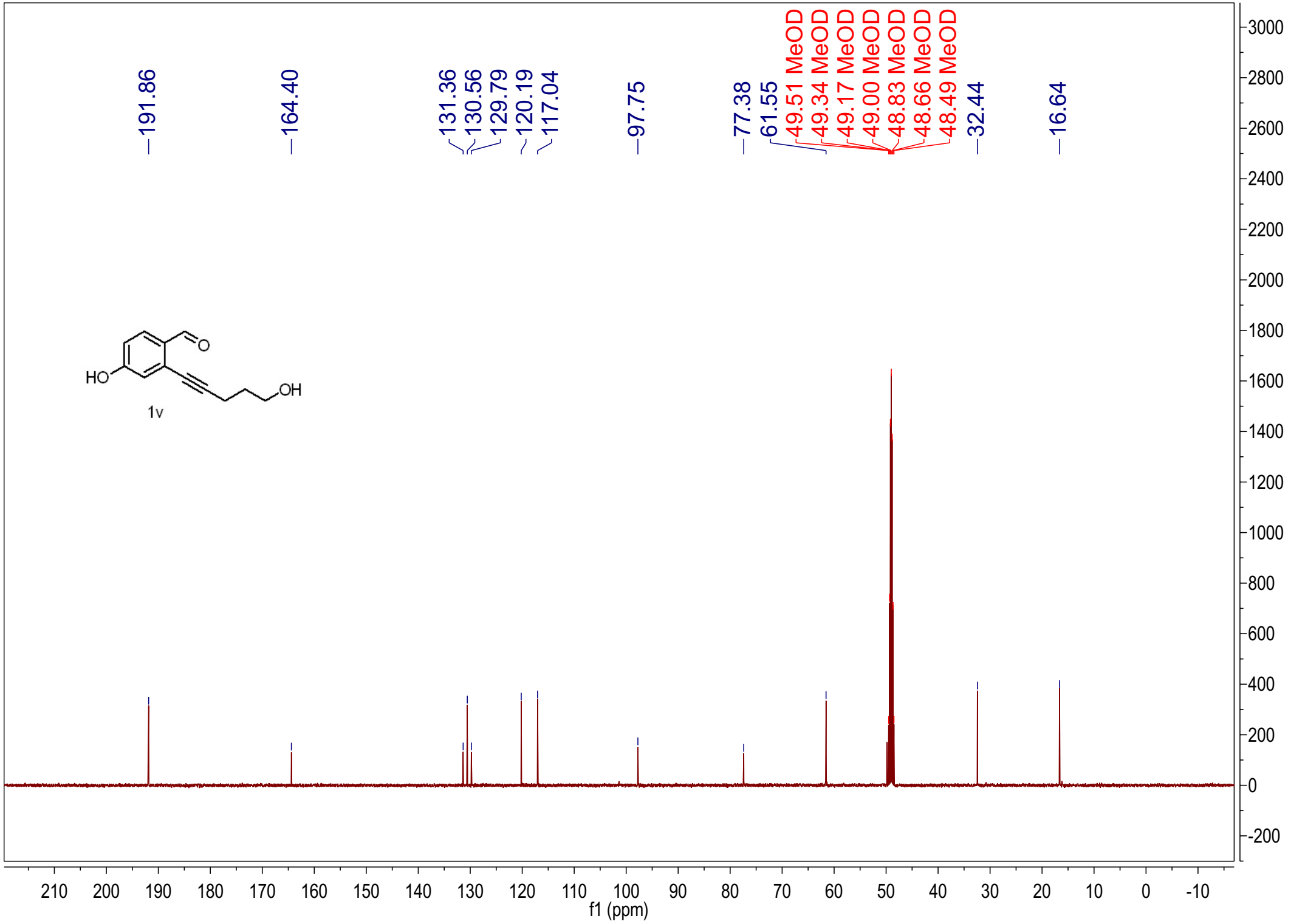
1.97
2.00
2.10
f1 (ppm)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49.17 MeOD
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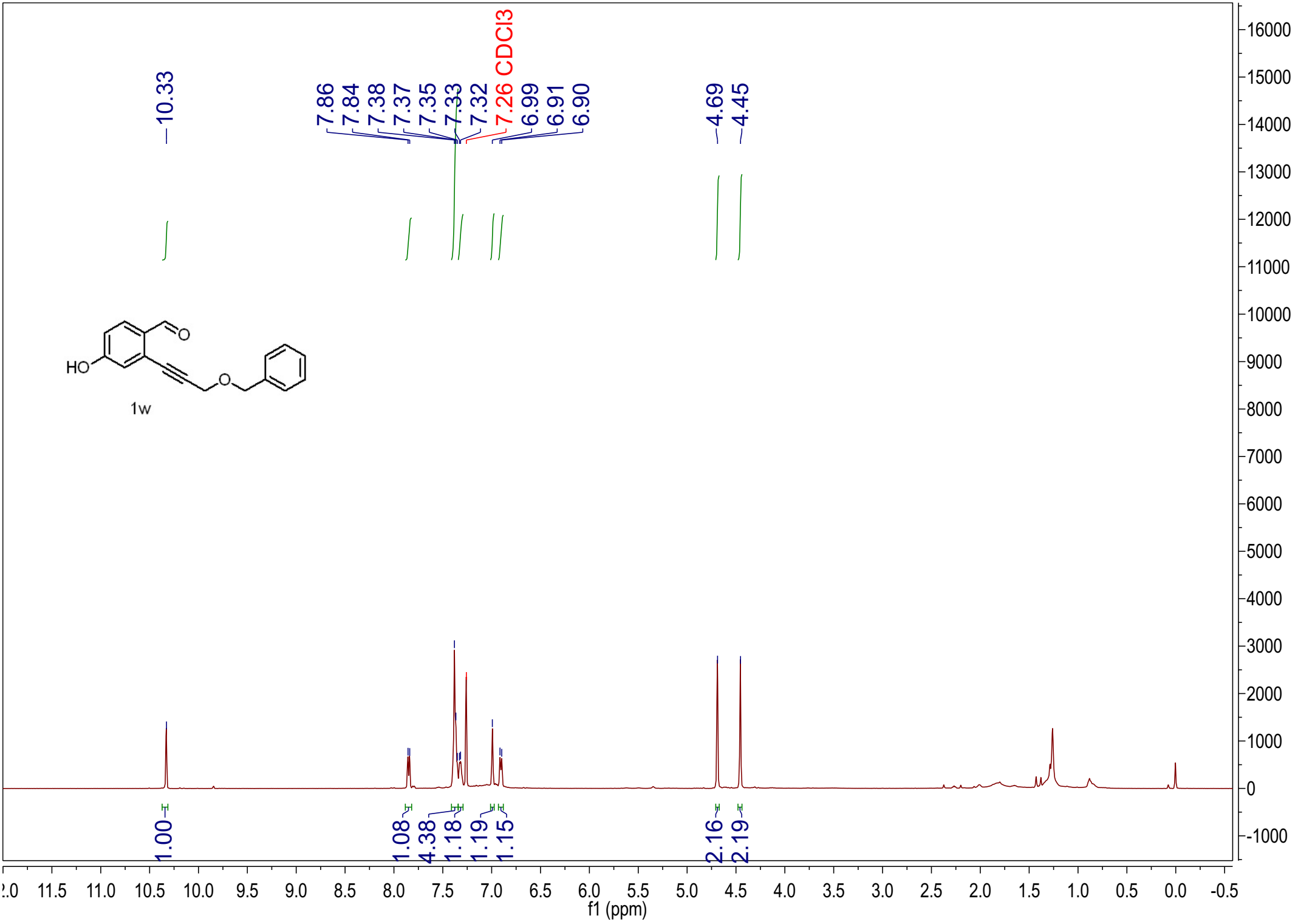
O
OH
1v
f1 (ppm)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6.90
4.69
4.45
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O
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4.38
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1.15
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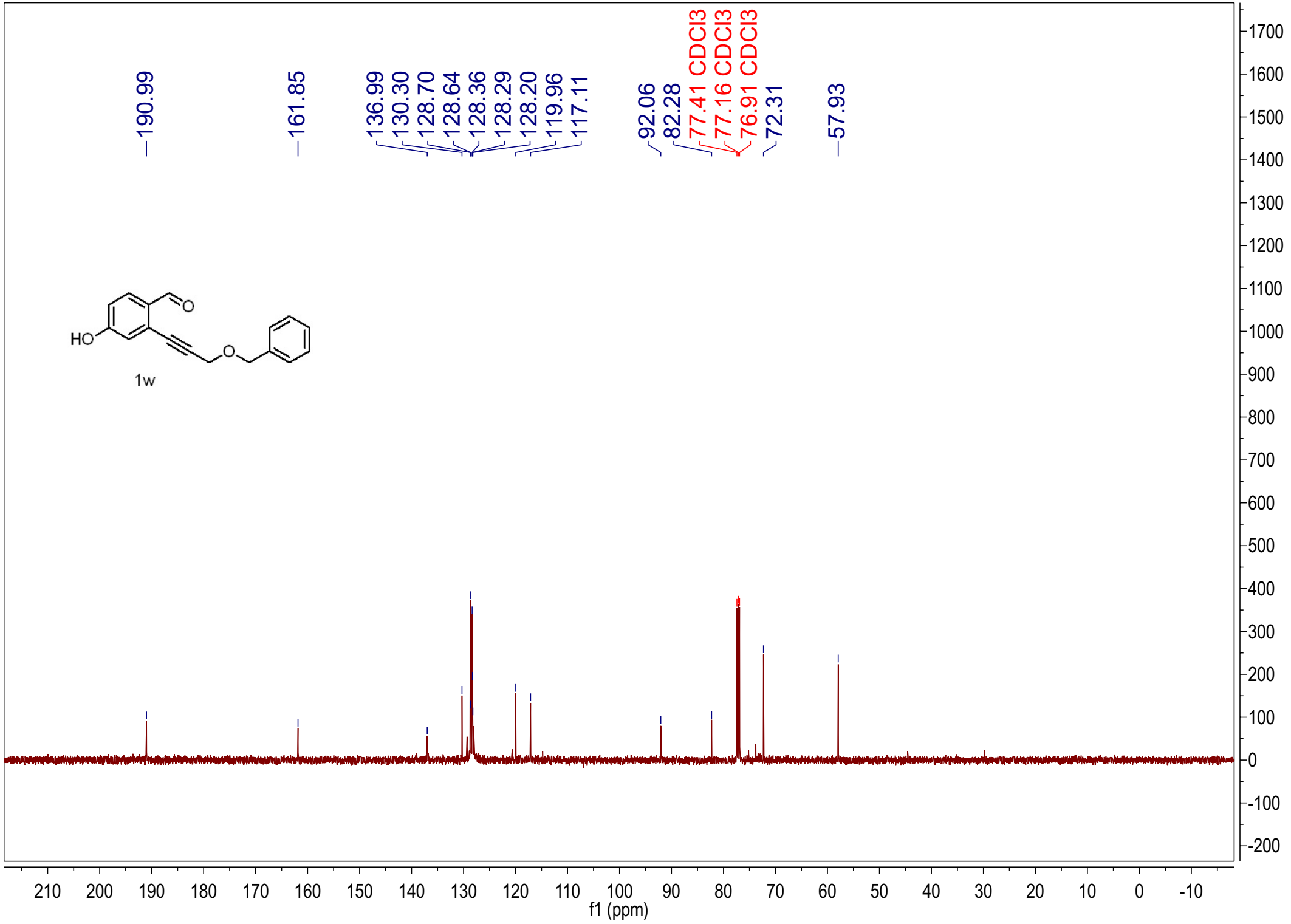
2.19
f1 (ppm)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117.11
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76.91 CDCl3
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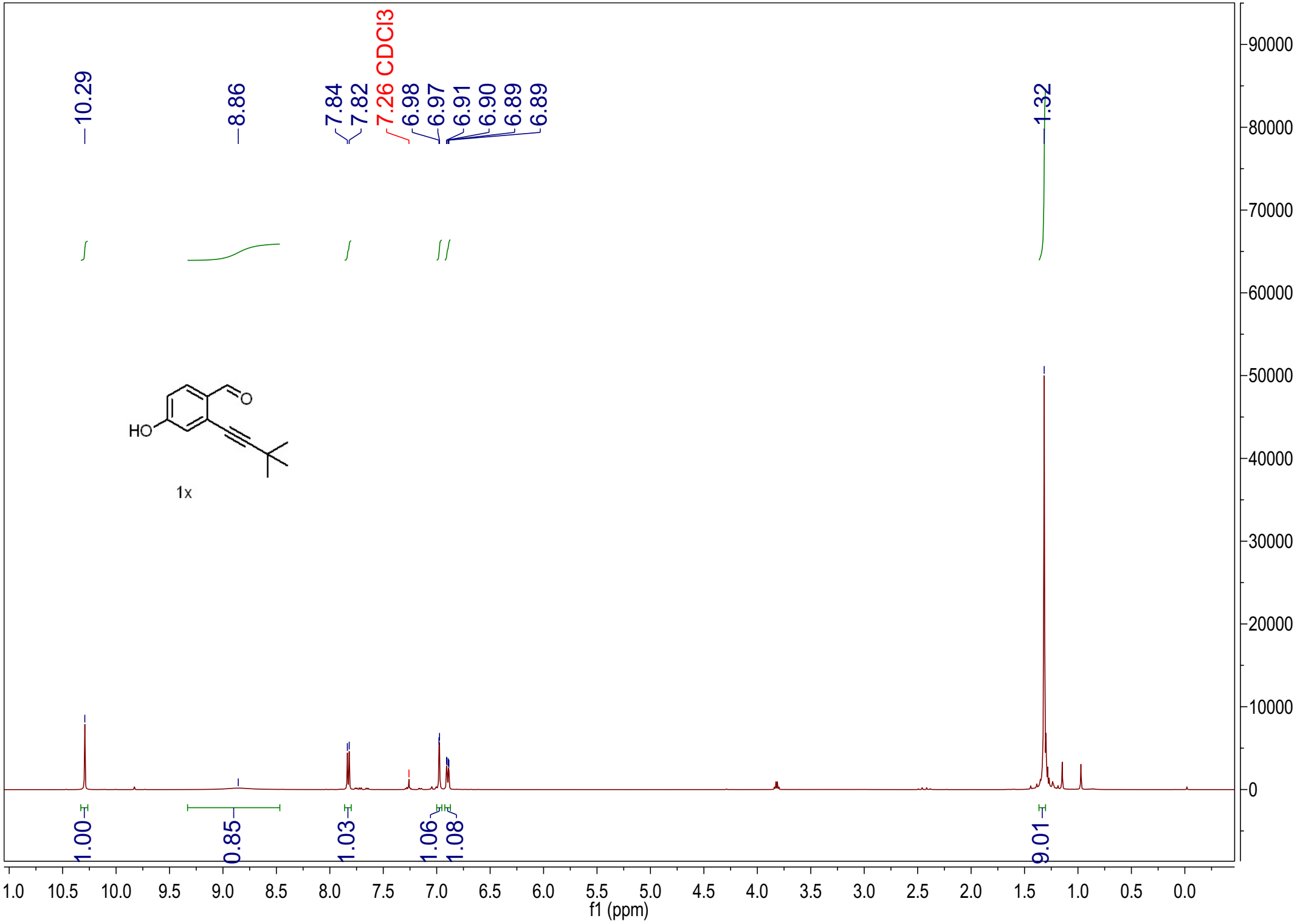
57.93
HO
O
O
1w
f1 (ppm)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7.84
7.82
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6.98
6.97
6.91
6.90
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6.89
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HO
O
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1.06
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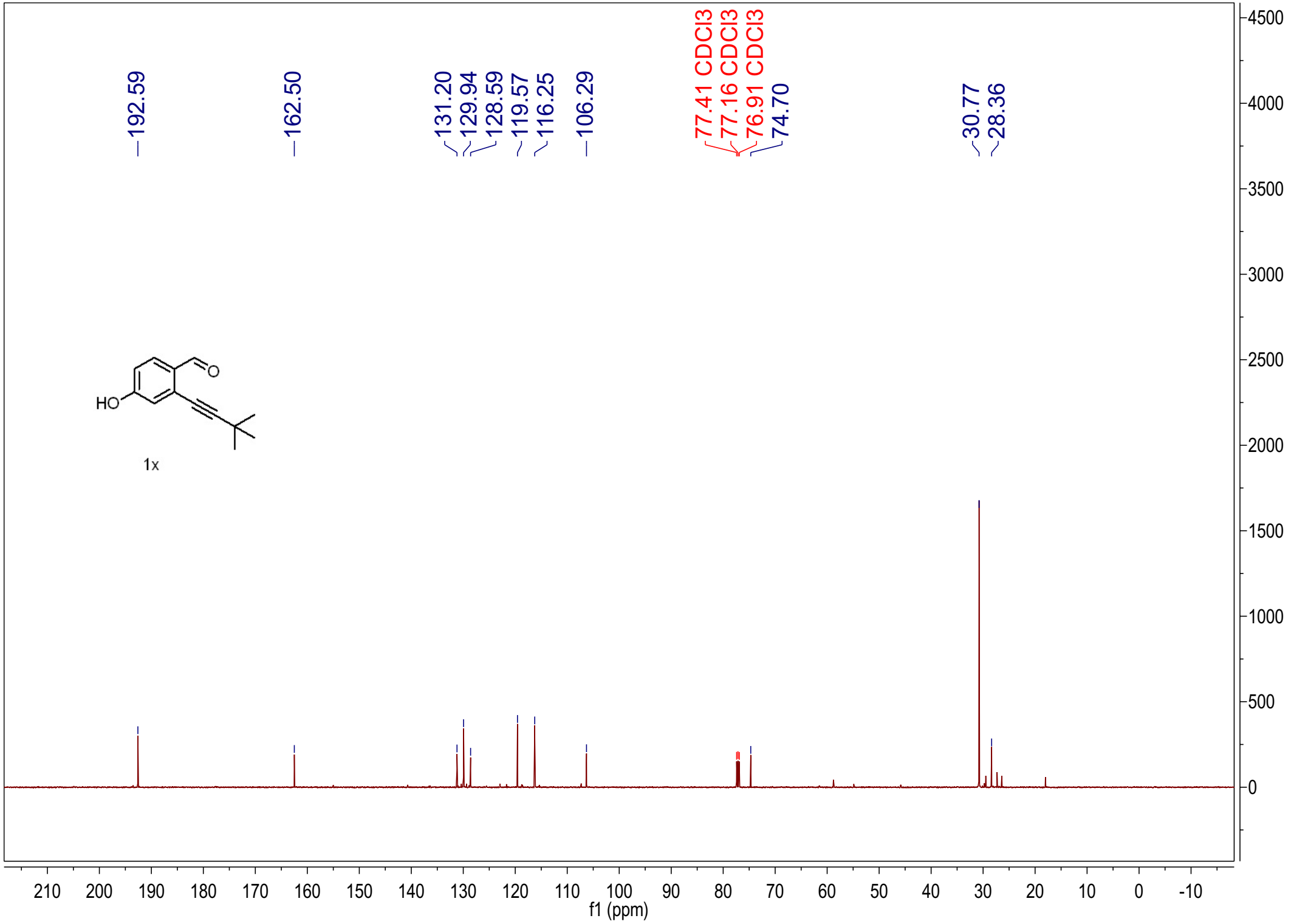
9.01
f1 (ppm)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76.91 CDCl3
74.70
30.77
28.36
HO
O
1x
4500
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2000
1500
1000
500
0
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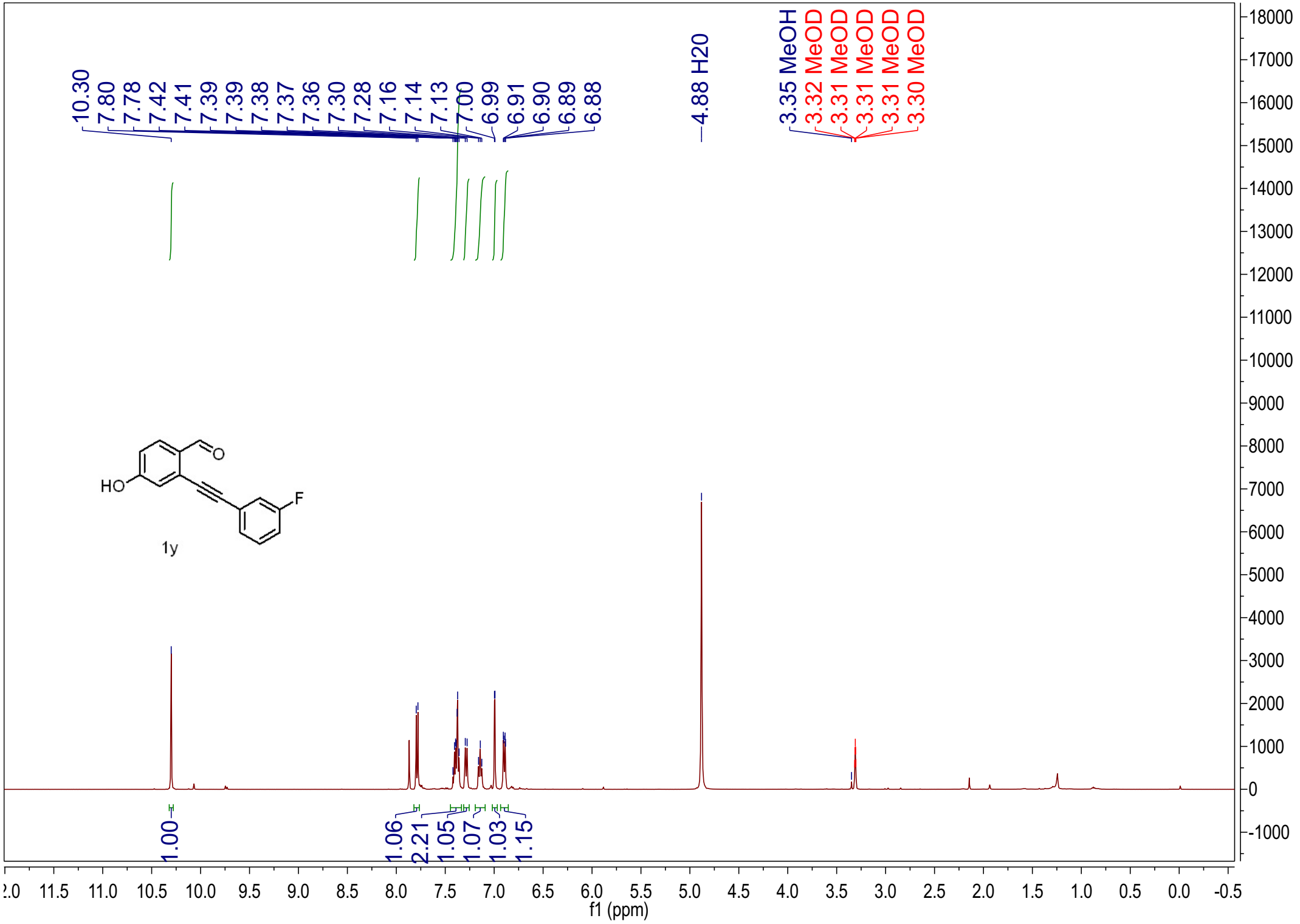
f1 (ppm)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6.90
6.89
6.88
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3.31 MeOD
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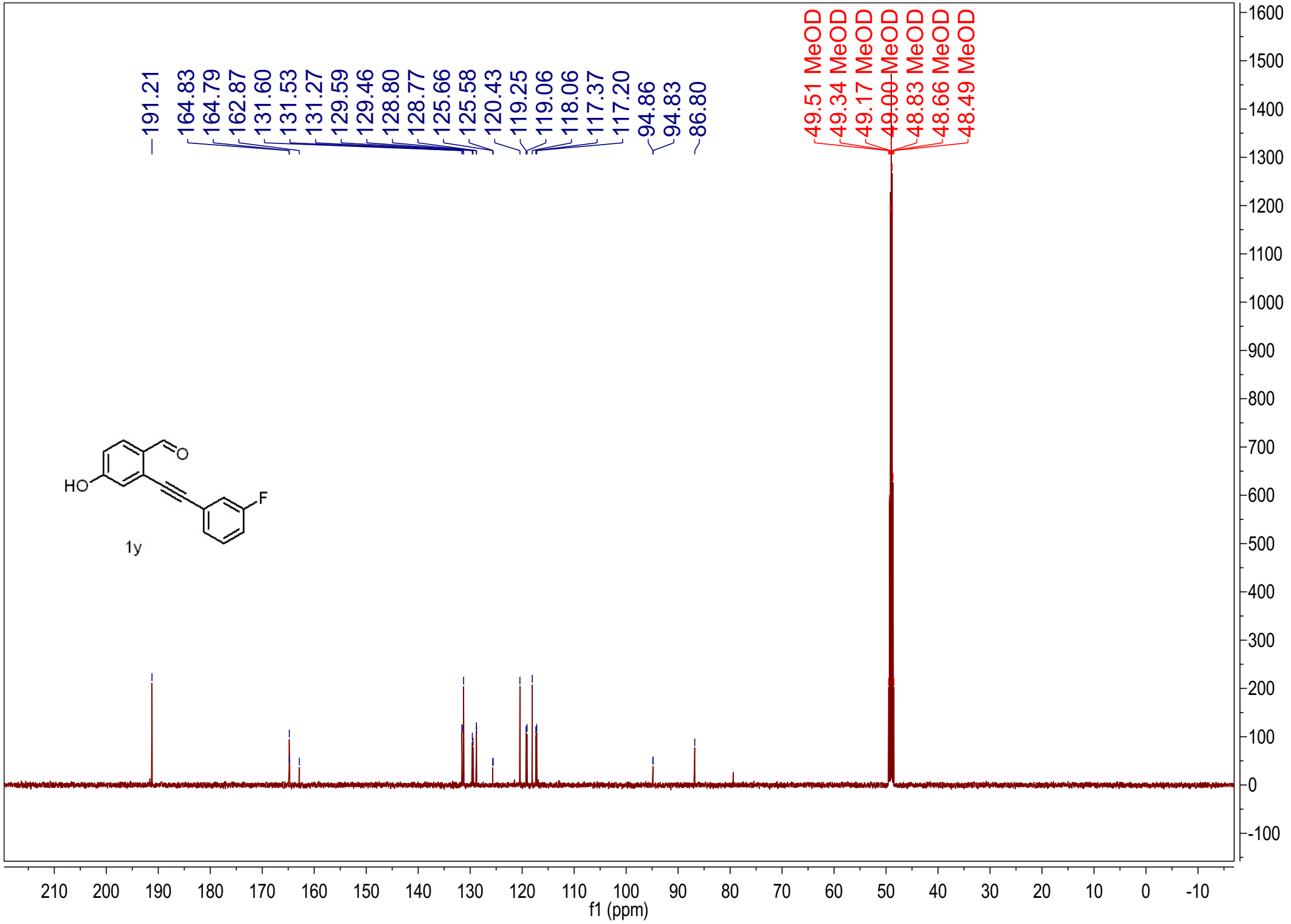
1.15
f1 (ppm)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120.43
119.25
119.06
118.06
117.37
117.20
94.86
94.83
86.80
49.51 MeOD
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HO
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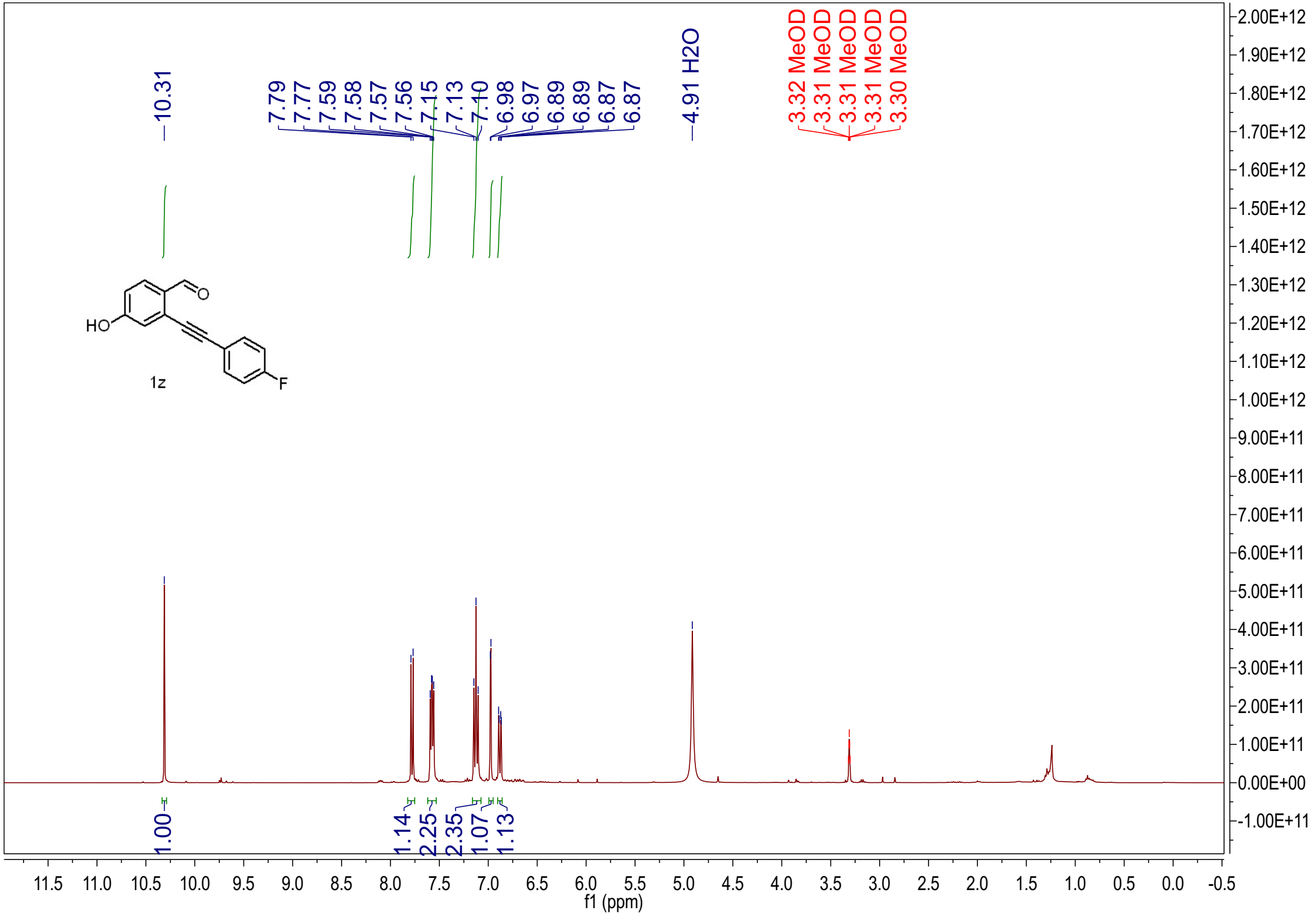
F
1y
f1 (ppm)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6.89
6.89
6.87
6.87
4.91 H2O
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
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O
F
1z
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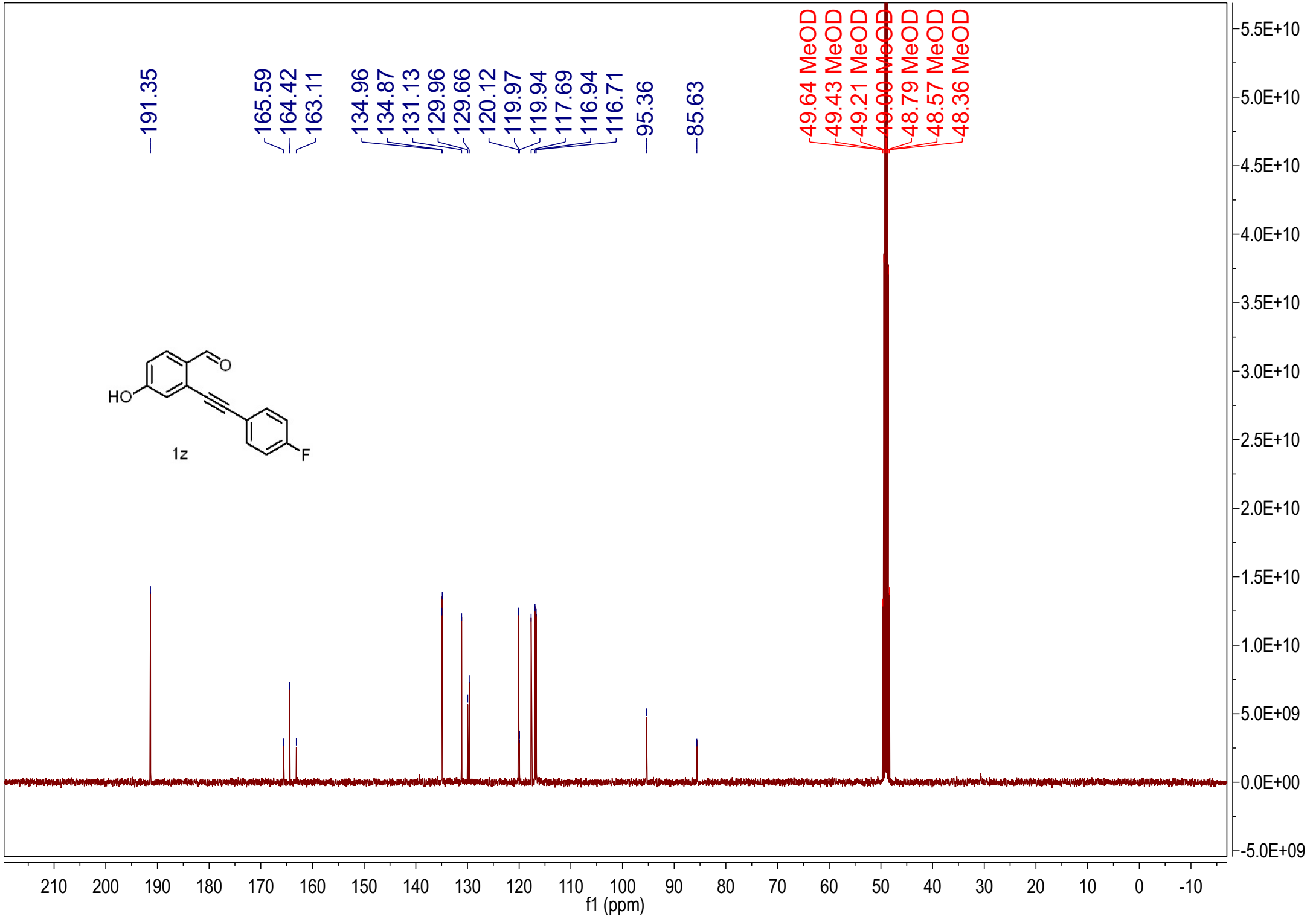
2.35
1.07
1.13
f1 (ppm)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117.69
116.94
116.71
95.36
85.63
49.64 MeOD
49.43 MeOD
49.21 MeOD
49.00 MeOD
48.79 MeOD
48.57 MeOD
48.36 MeOD
HO
O
F
1z
5.5E+10
5.0E+10
4.5E+10
4.0E+10
3.5E+10
3.0E+10
2.5E+10
2.0E+10
1.5E+10
1.0E+10
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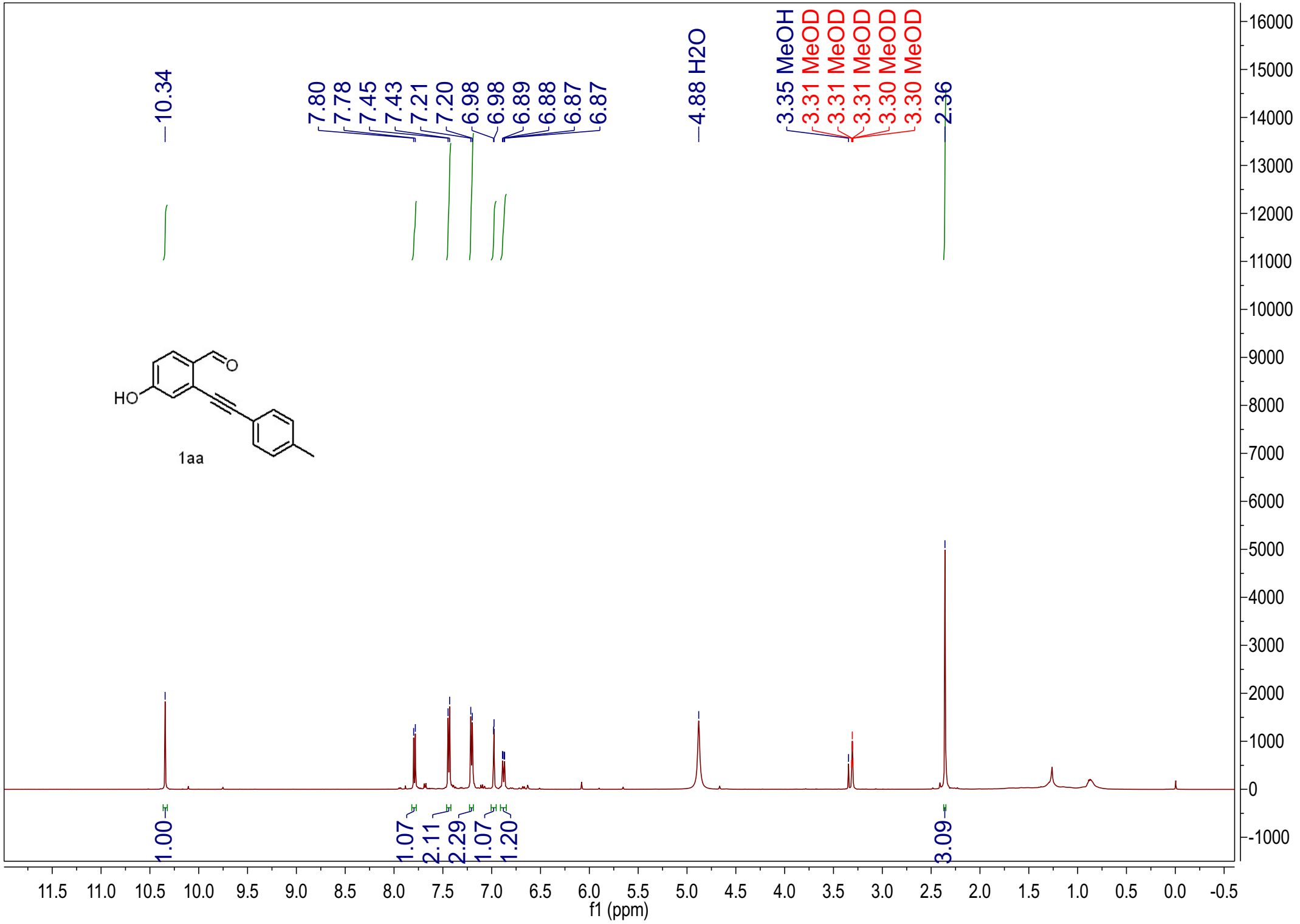
f1 (ppm)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6.88
6.87
6.87
4.88 H2O
3.35 MeOH
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.30 MeOD
2.36
HO
O
1aa
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1.07
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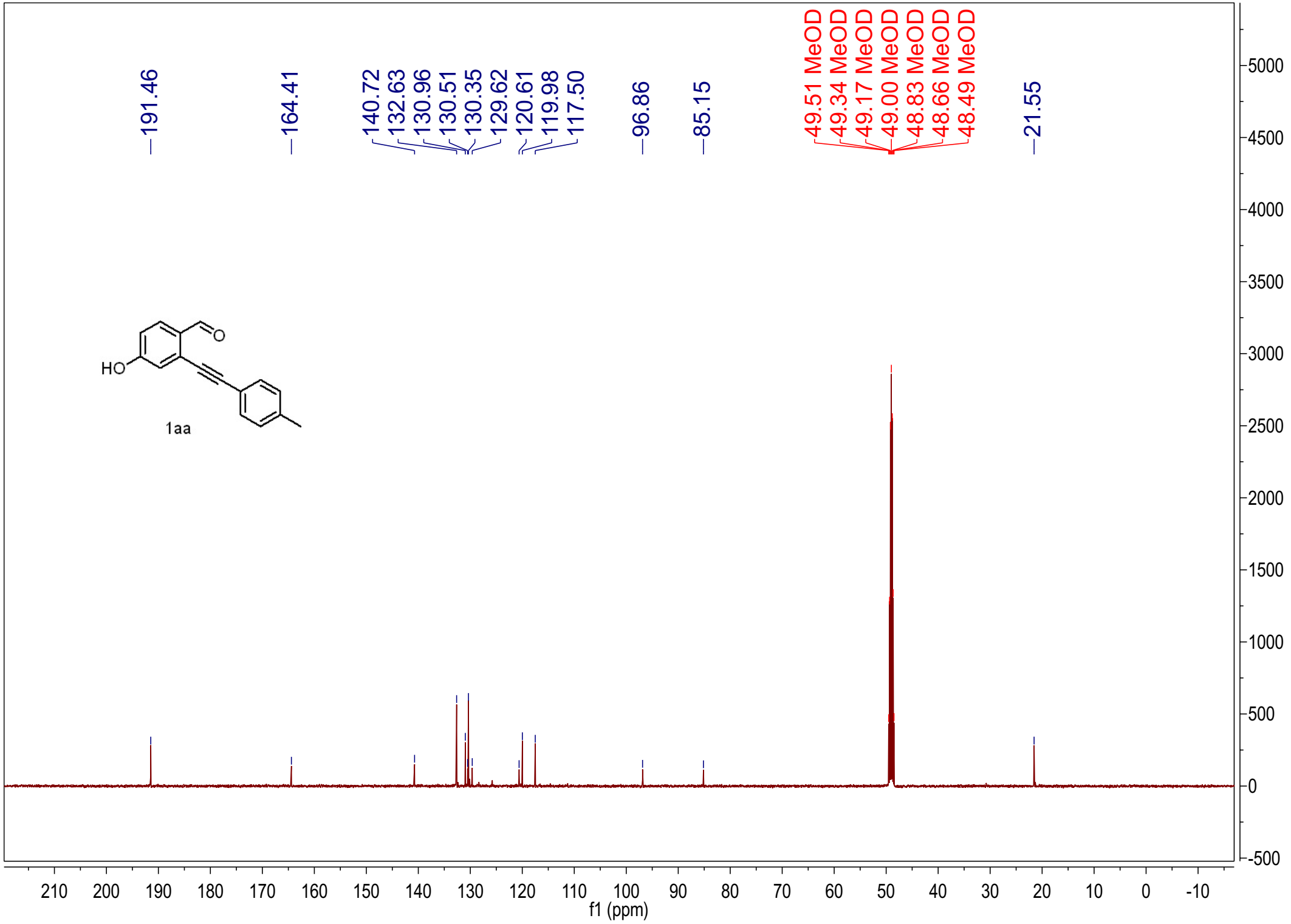
1.07
1.20
3.09
f1 (ppm)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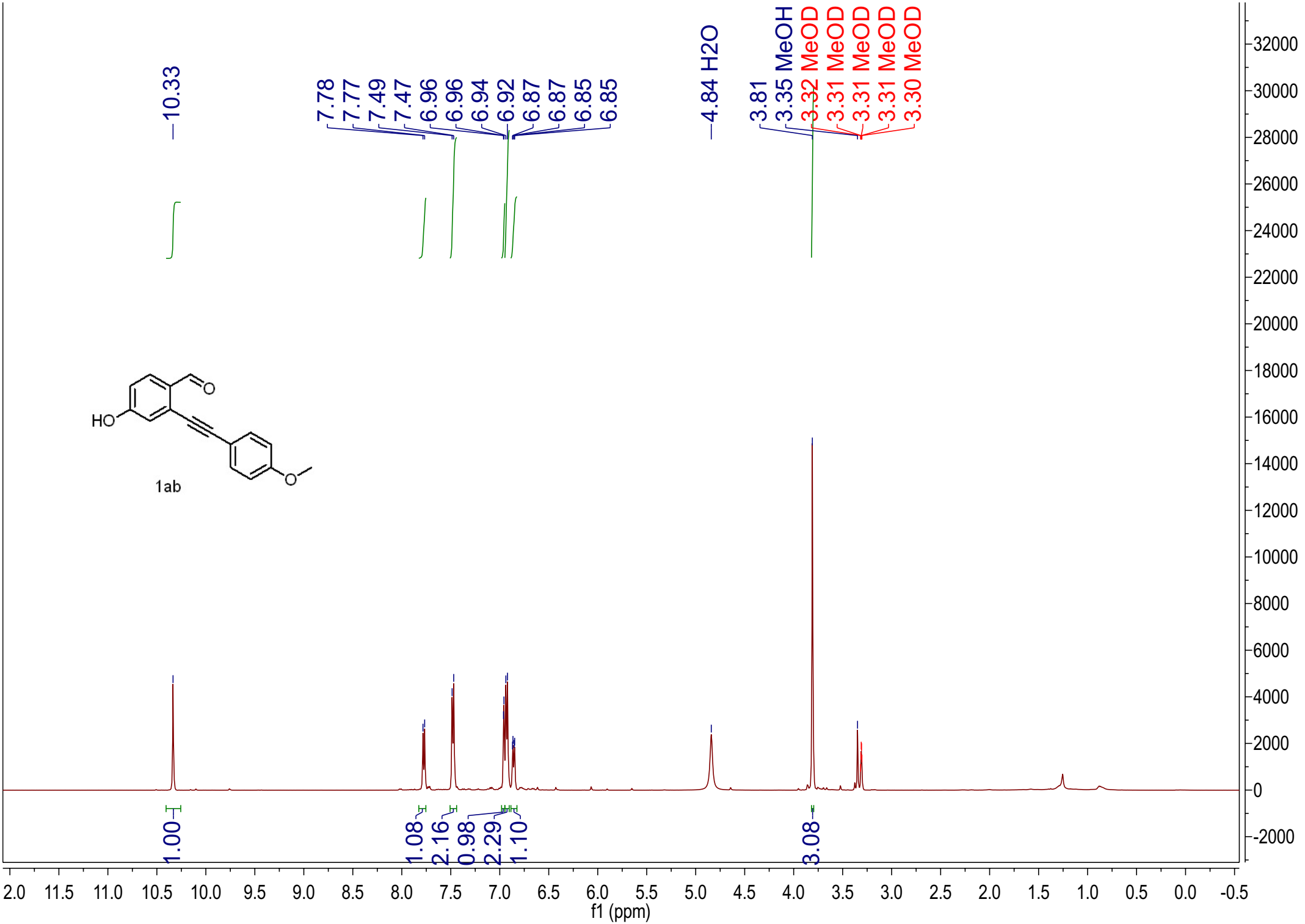
1aa
f1 (ppm)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6.85
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3.31 MeOD
3.31 MeOD
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O
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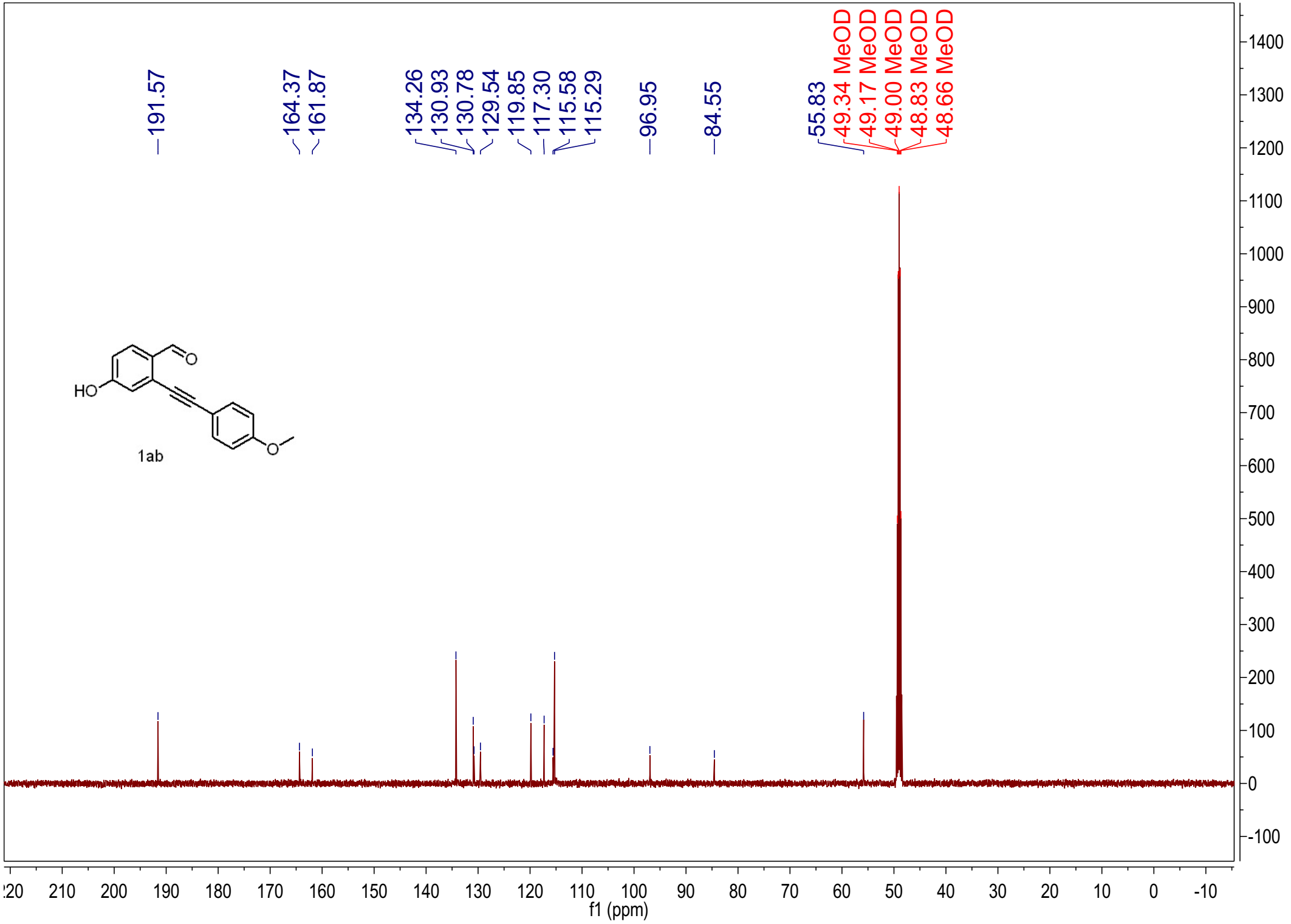
f1 (ppm)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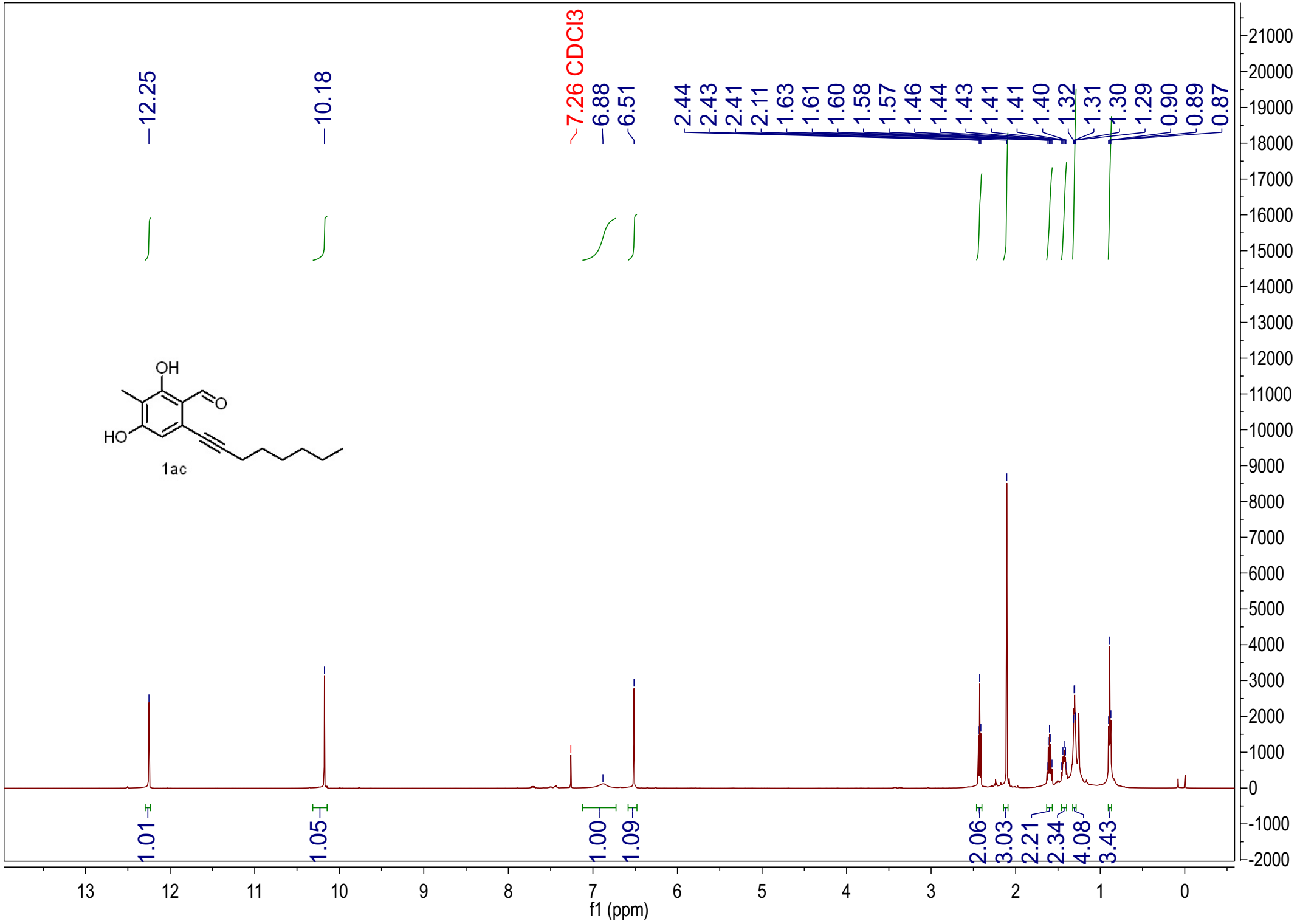
49.17 MeOD
49.00 MeOD
48.83 MeOD
48.66 MeOD
HO
O
O
1ab
f1 (ppm)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1.57
1.46
1.44
1.43
1.41
1.41
1.40
1.32
1.31
1.30
1.29
0.90
0.89
0.87
OH
HO
O
1ac
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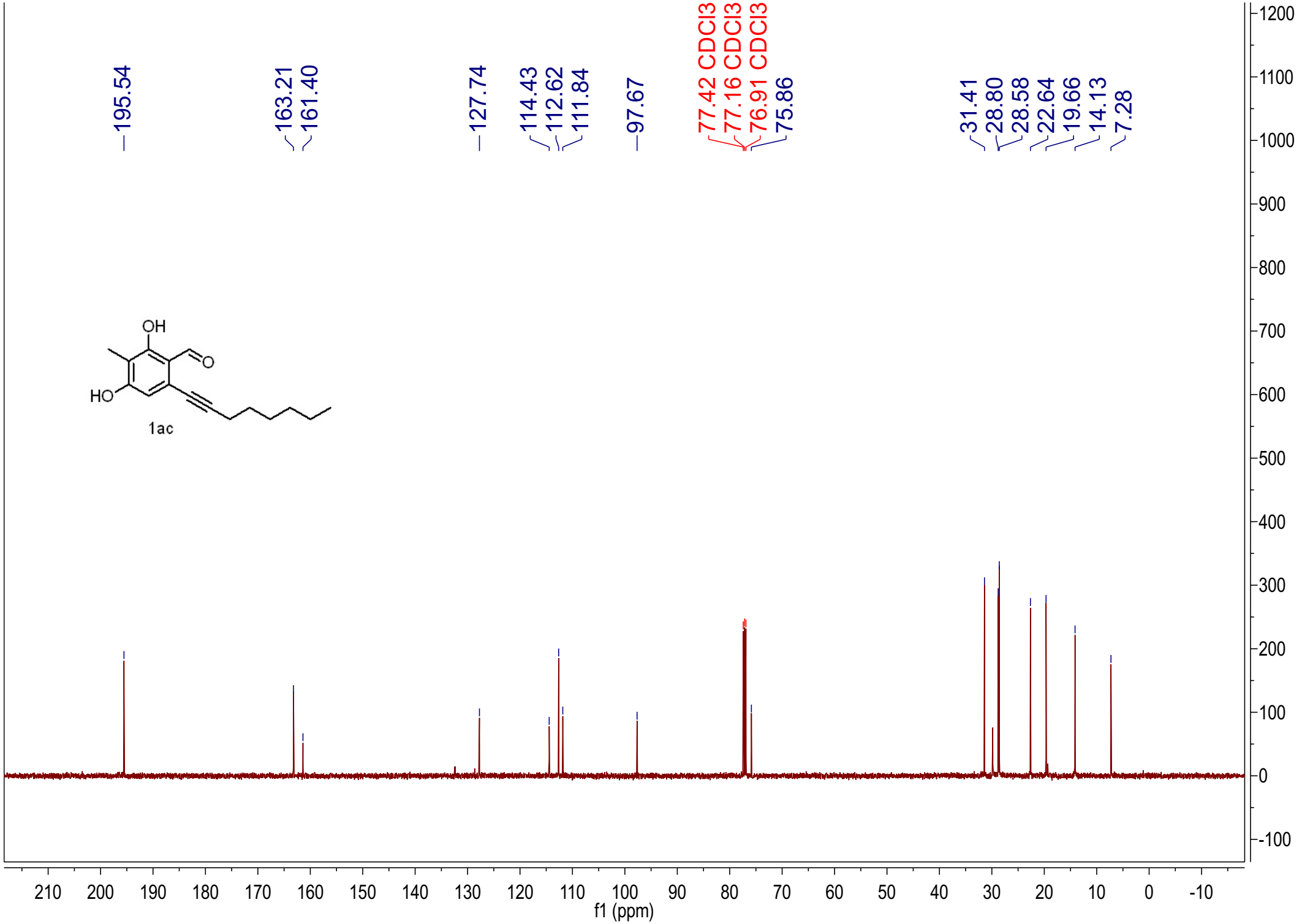
1.05
1.00
1.09
2.06
3.03
2.21
2.34
4.08
3.43
f1 (ppm)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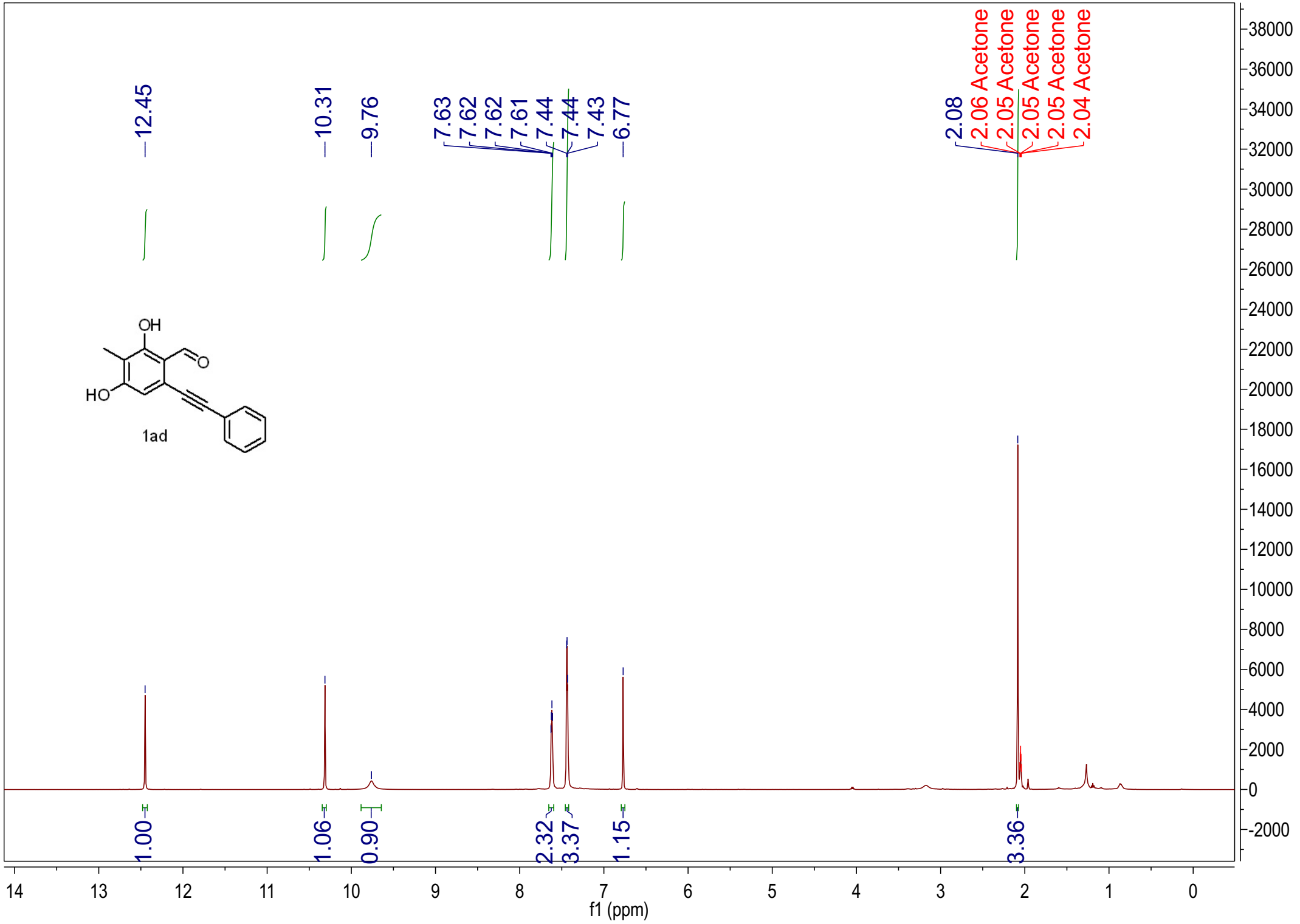
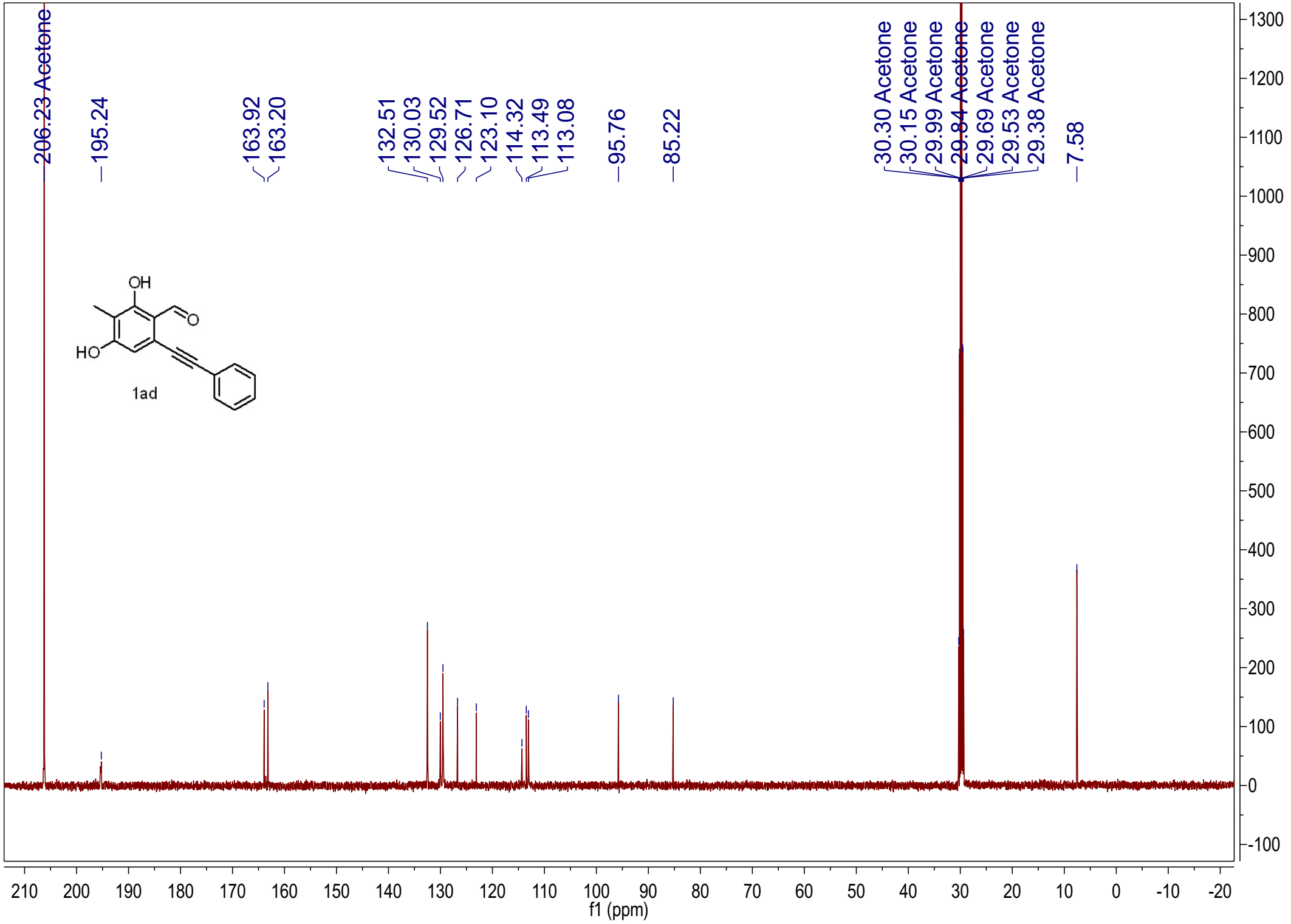
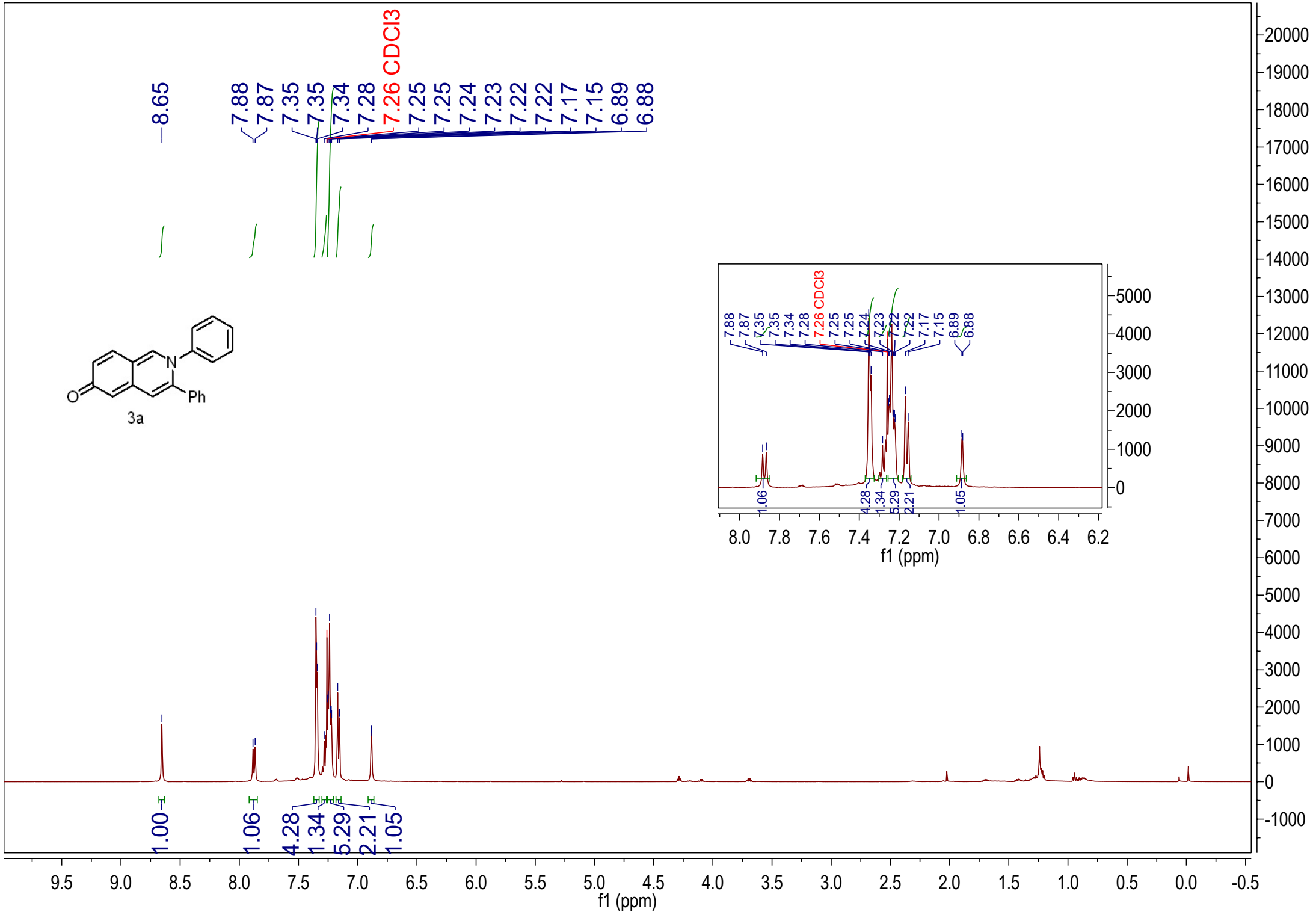
161.40
127.74
114.43
112.62
111.84
97.67
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3
75.86
31.41
28.80
28.58
22.64
19.66
14.13
7.28
OH
HO
O
1ac
f1 (ppm)


12.45
10.31
9.76
7.63
7.62
7.62
7.61
7.44
7.44
7.43
6.77
2.08
2.06 Acetone
2.05 Acetone
2.05 Acetone
2.05 Acetone
2.04 Acetone
OH
HO
O
1ad
1.00
1.06
0.90
2.32
3.37
1.15
3.36
f1 (ppm)


206.23 Acetone
195.24
163.92
163.20
132.51
130.03
129.52
126.71
123.10
114.32
113.49
113.08
95.76
85.22
30.30 Acetone
30.15 Acetone
29.99 Acetone
29.84 Acetone
29.69 Acetone
29.53 Acetone
29.38 Acetone
7.58
OH
HO
O
1ad
f1 (ppm)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7.34
7.28
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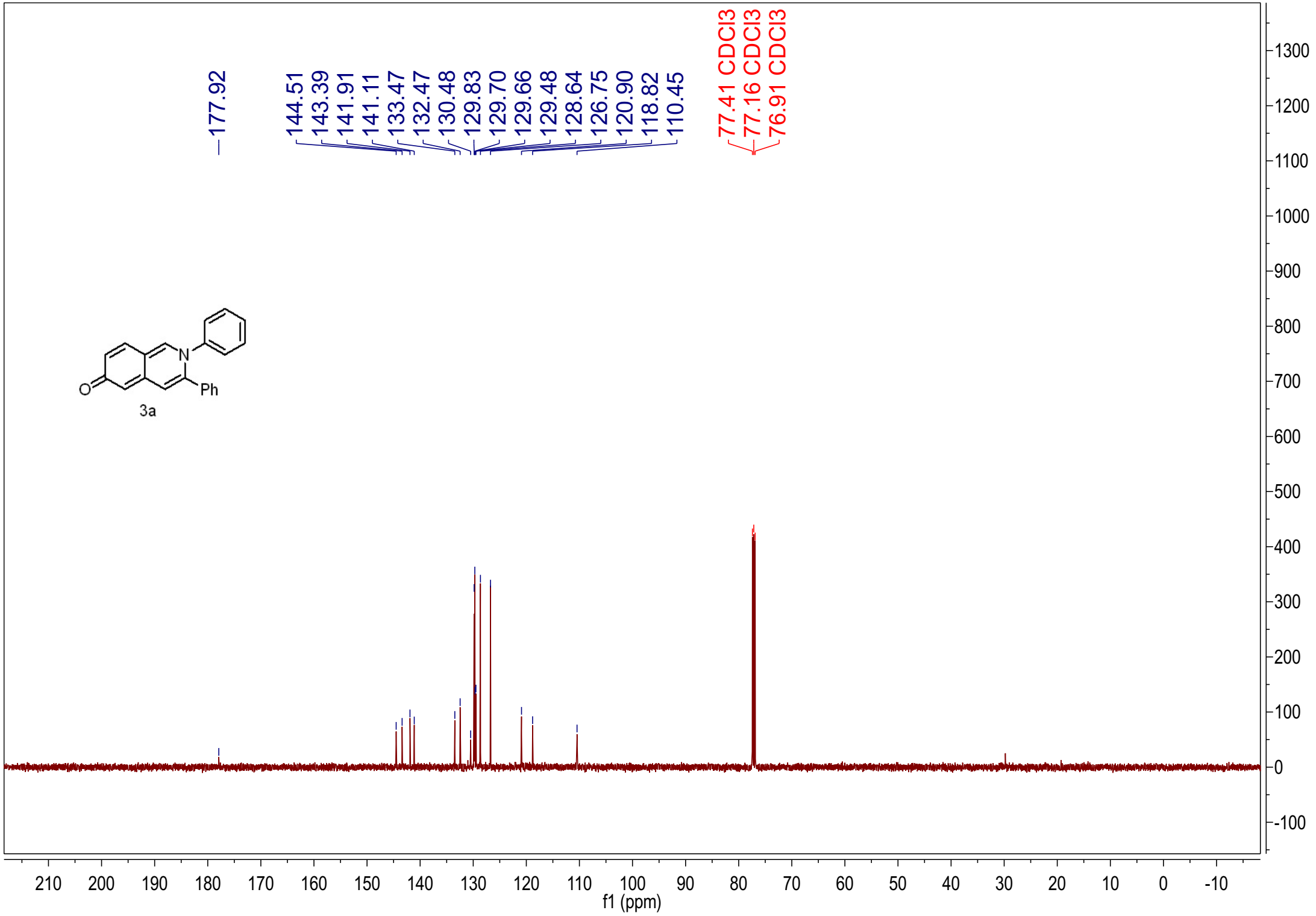
7.25
7.25
7.24
7.23
7.22
7.22
7.17
7.15
6.89
6.88
O
N
Ph
3a
1.00
1.06
4.28
1.34
5.29
2.21
1.05
f1 (ppm)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133.47
132.47
130.48
129.83
129.70
129.66
129.48
128.64
126.75
120.90
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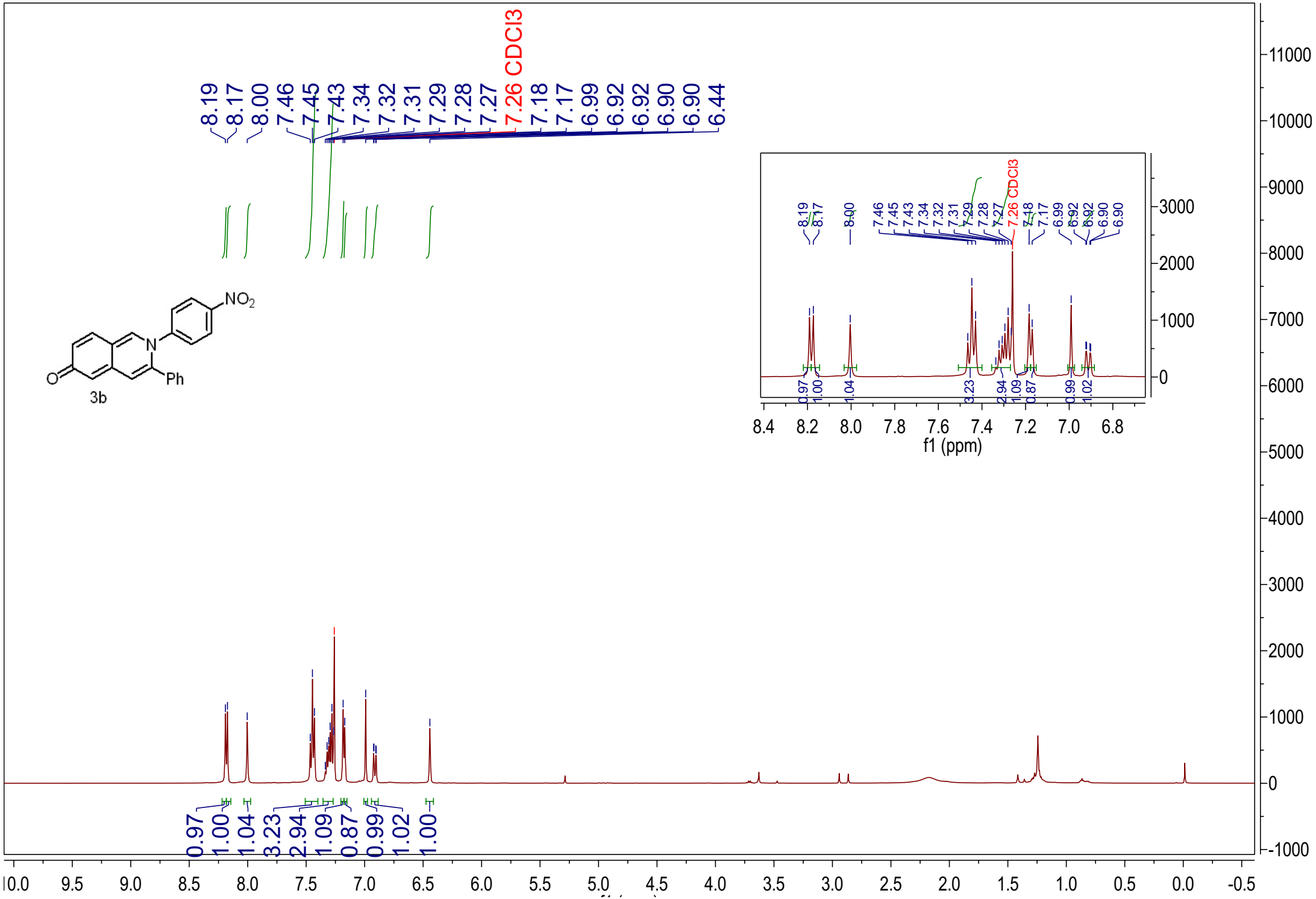
110.45
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
O
N
Ph
3a
f1 (ppm)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8.00
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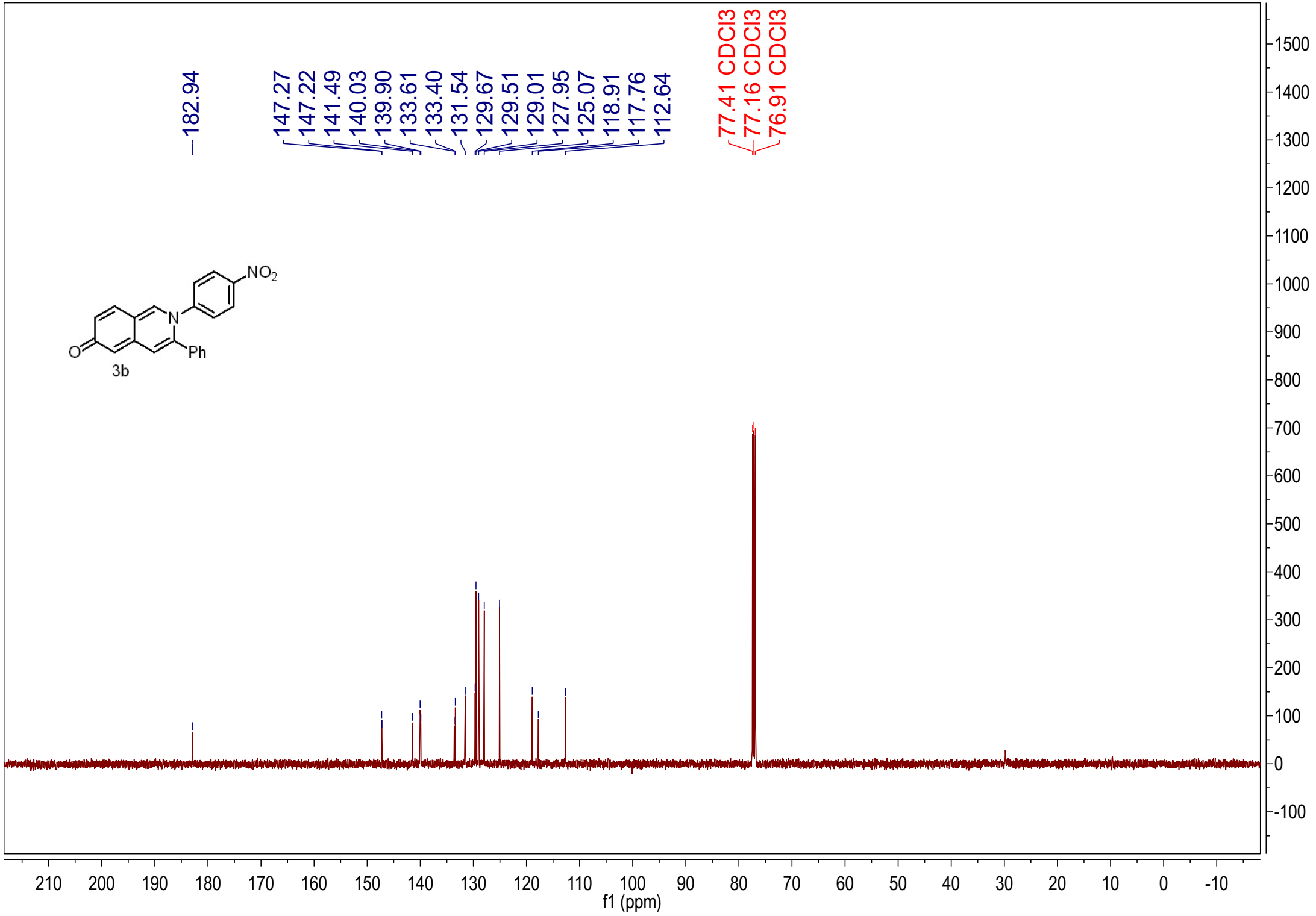
7.45
7.43
7.34
7.32
7.31
7.29
7.28
7.27
7.26 CDCl3
7.18
7.17
6.99
6.92
6.92
6.90
6.90
6.44
NO2
N
O
Ph
3b
0.97
1.00
1.04
3.23
2.94
1.09
0.87
0.99
1.02
1.00
f1 (ppm)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129.51
129.01
127.95
125.07
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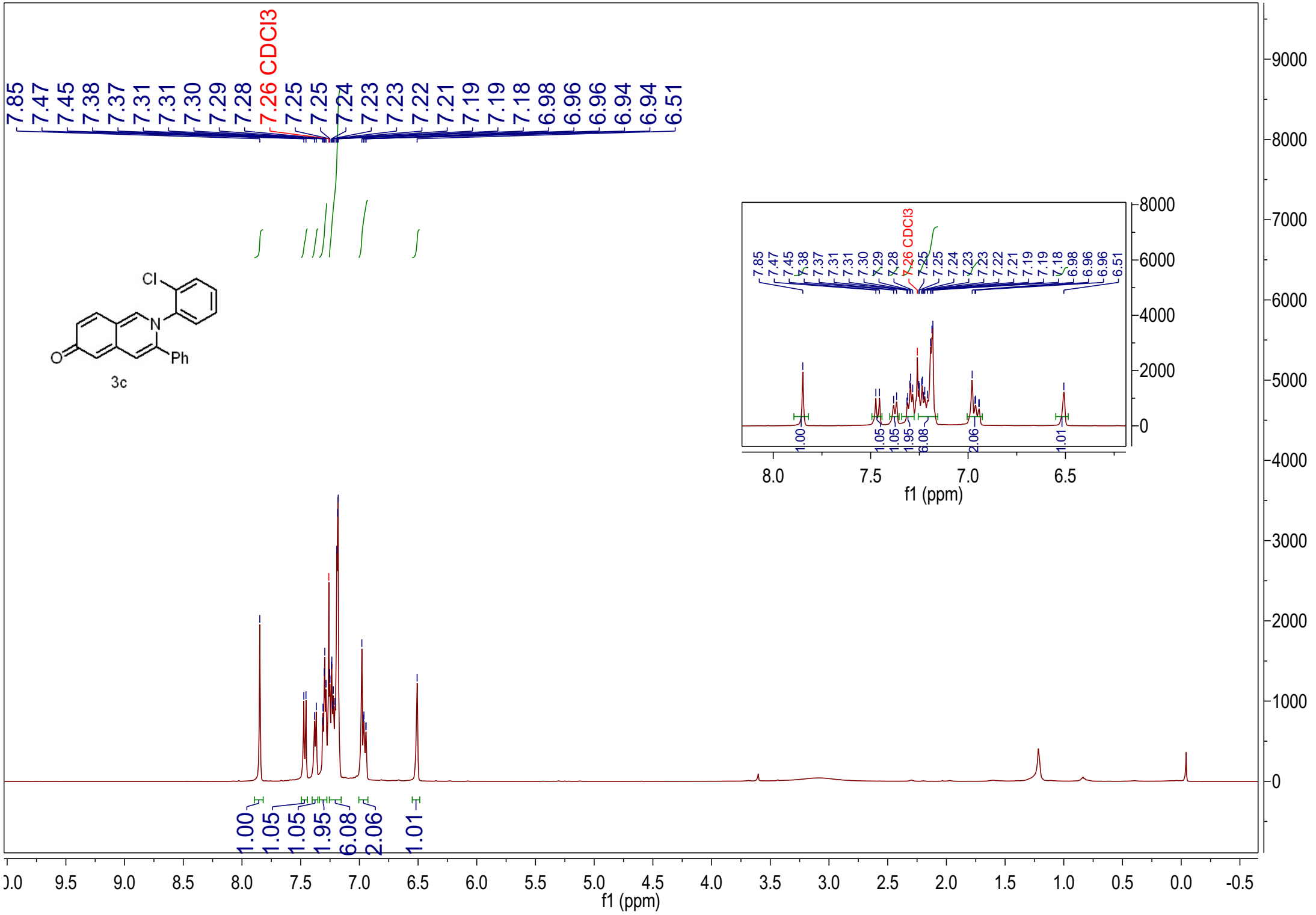
112.64
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
NO2
N
O
Ph
3b
f1 (ppm)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7.30
7.29
7.28
7.26 CDCl3
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.19
7.19
7.18
6.98
6.96
6.96
6.94
6.94
6.51
Cl
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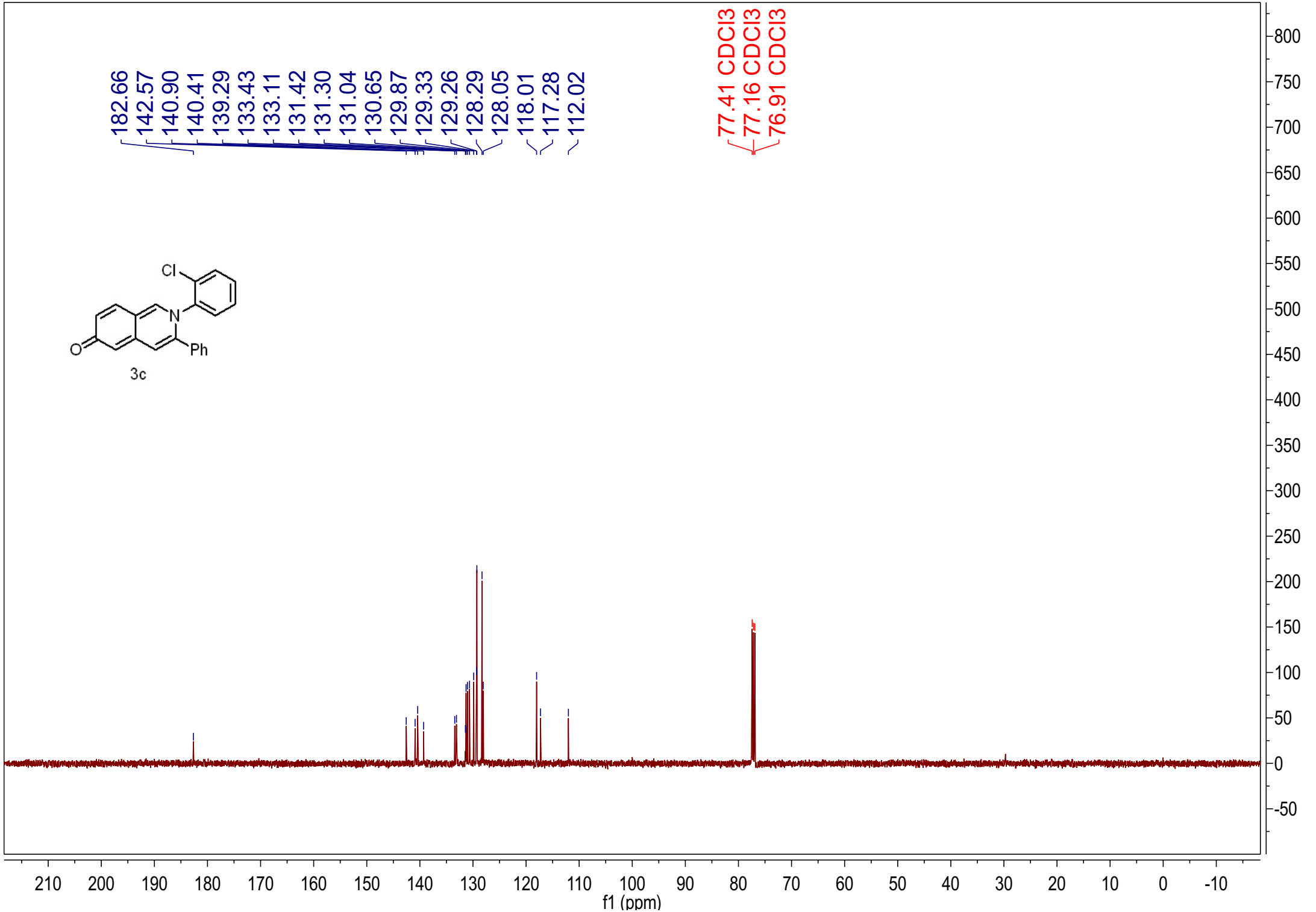
O
Ph
3c
1.00
1.05
1.05
1.95
6.08
2.06
1.01
f1 (ppm)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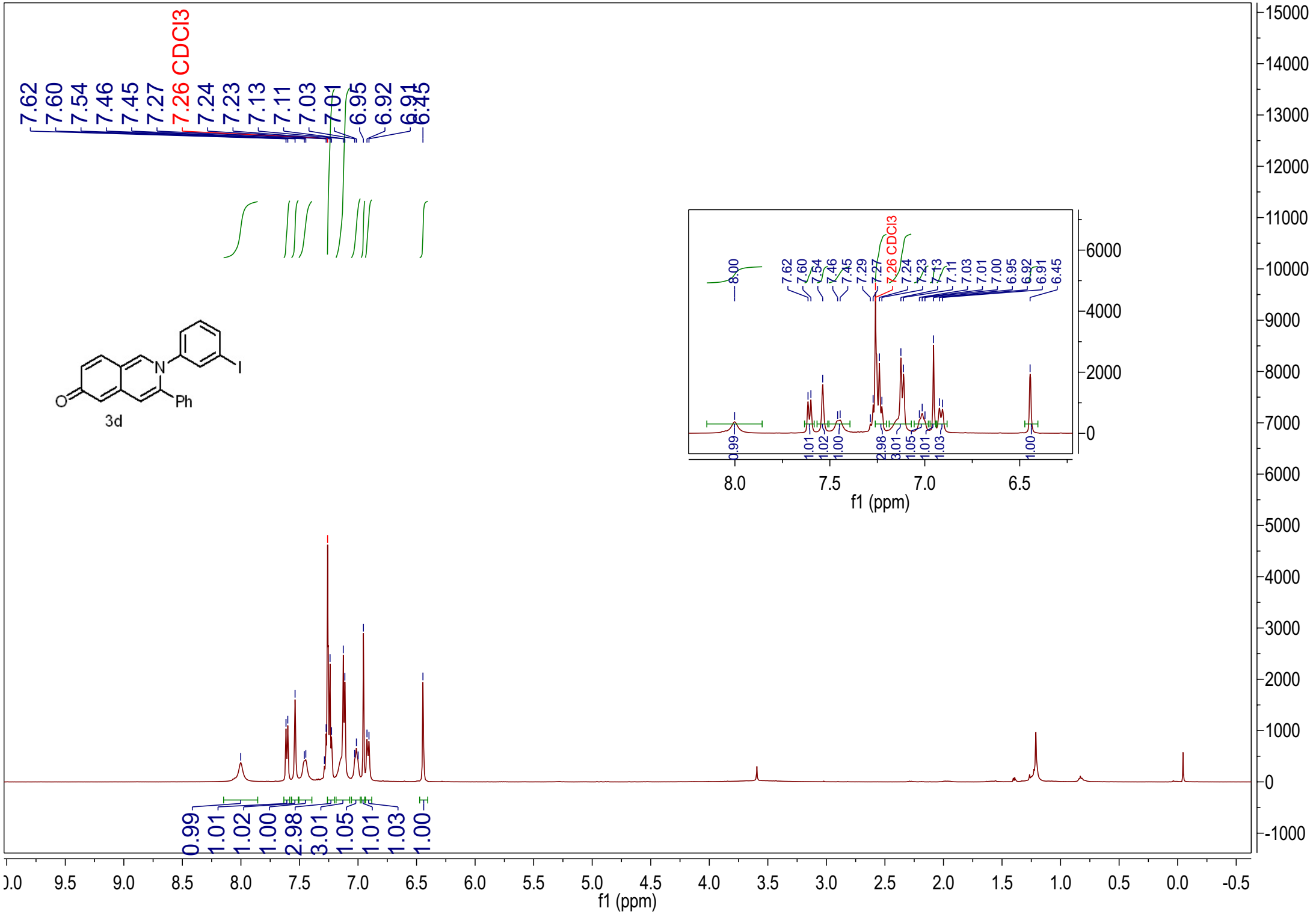
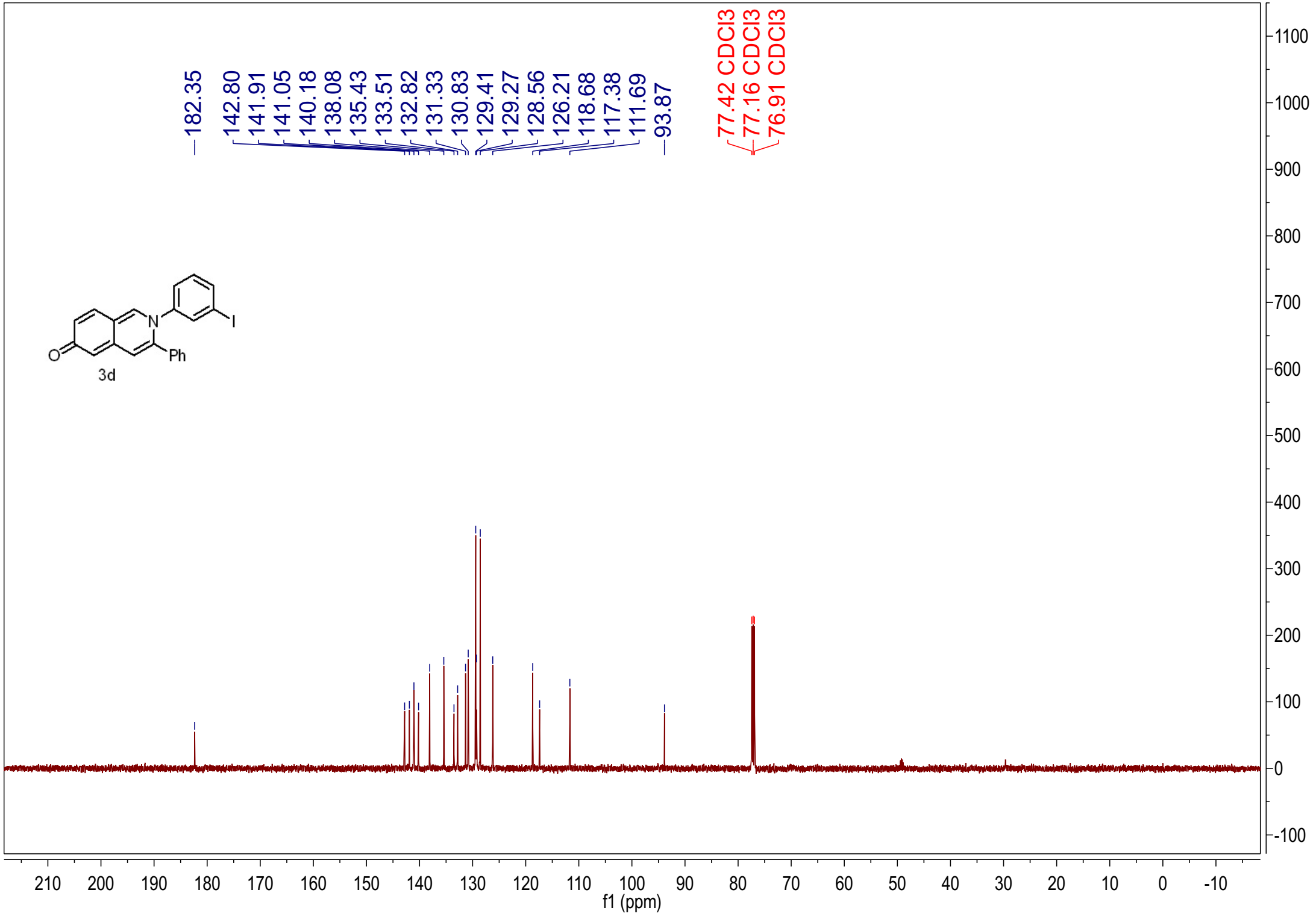
133.11
131.42
131.30
131.04
130.65
129.87
129.33
129.26
128.29
128.05
118.01
117.28
112.02
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
Cl
N
O
Ph
3c
800
750
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.62
7.60
7.54
7.46
7.45
7.27
7.26 CDCl3
7.24
7.23
7.13
7.11
7.03
7.01
6.95
6.92
6.91
6.45
N
I
O
Ph
3d
8.00
7.29
0.99
1.01
1.02
1.00
2.98
3.01
1.05
1.01
1.03
1.00
f1 (ppm)
0.99
1.01
1.02
1.00
2.98
3.01
1.05
1.01
1.03
1.00
f1 (ppm)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135.43
133.51
132.82
131.33
130.83
129.41
129.27
128.56
126.21
118.68
117.38
111.69
93.87
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3
O
N
I
Ph
3d
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
210
200
190
180
170
160
150
140
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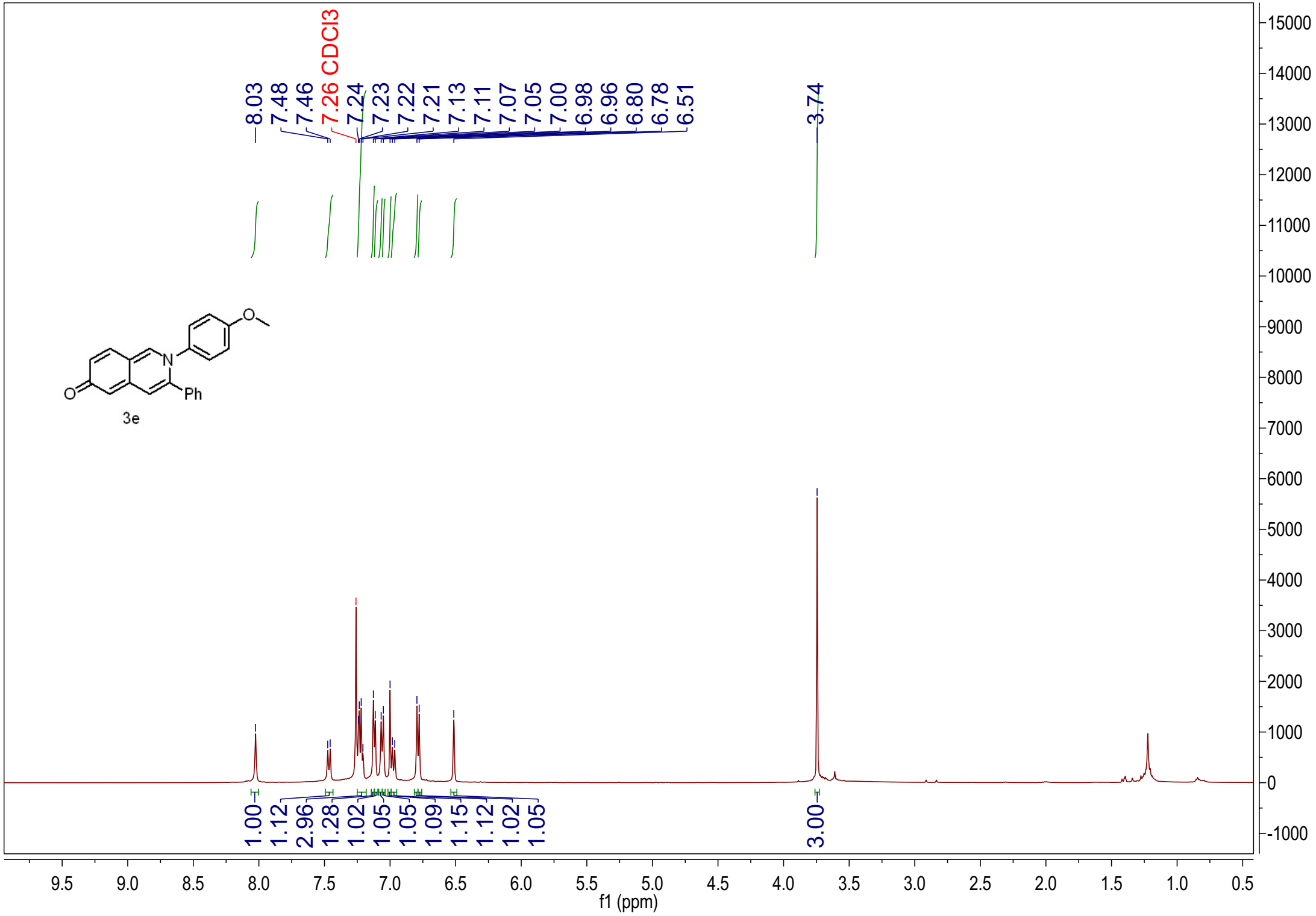
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.48
7.46
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7.24
7.23
7.22
7.21
7.13
7.11
7.07
7.05
7.00
6.98
6.96
6.80
6.78
6.51
3.74
O
N
Ph
O
3e
1.00
1.12
2.96
1.28
1.02
1.05
1.05
1.09
1.15
1.12
1.02
1.05
3.00
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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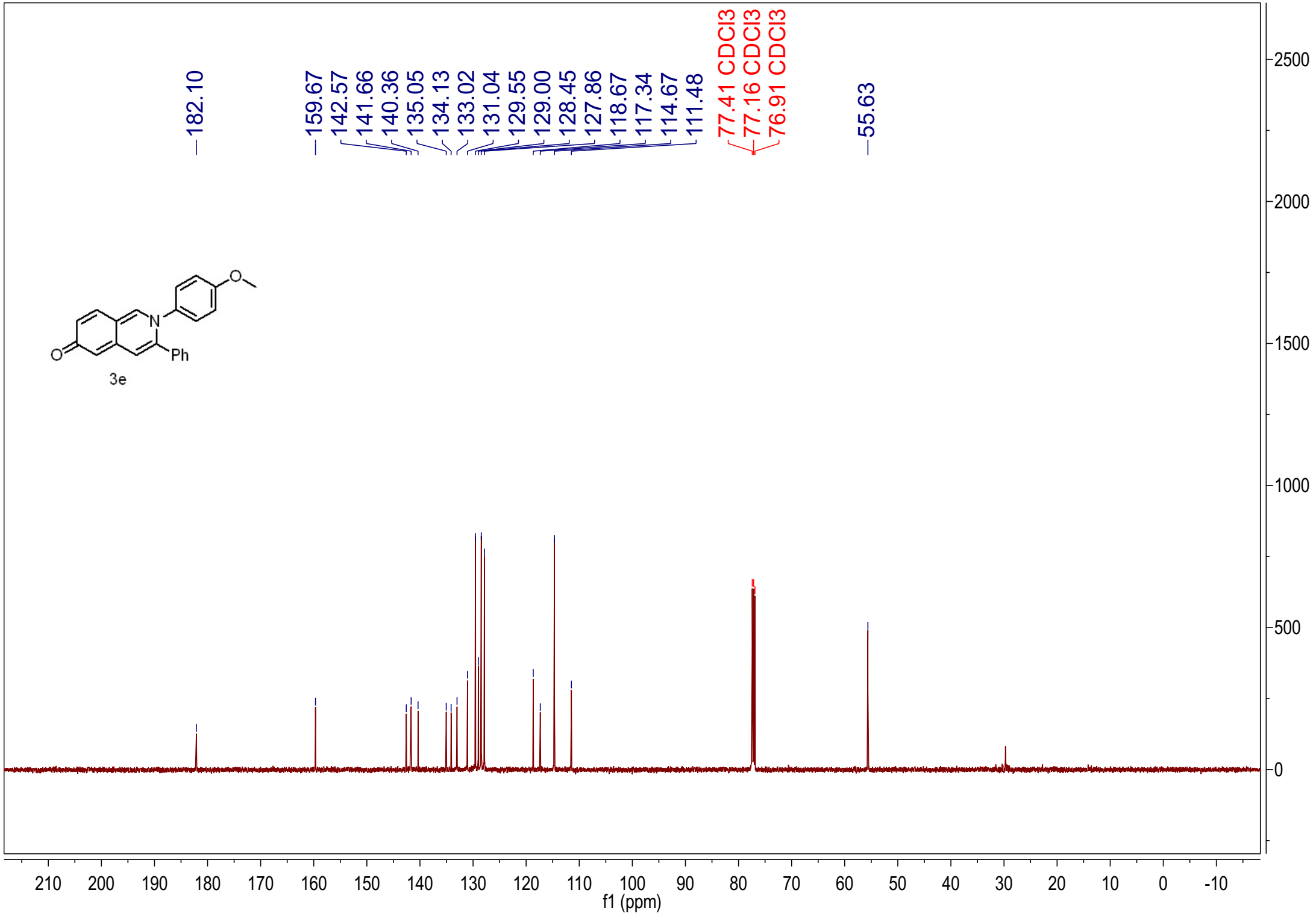
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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134.13
133.02
131.04
129.55
129.00
128.45
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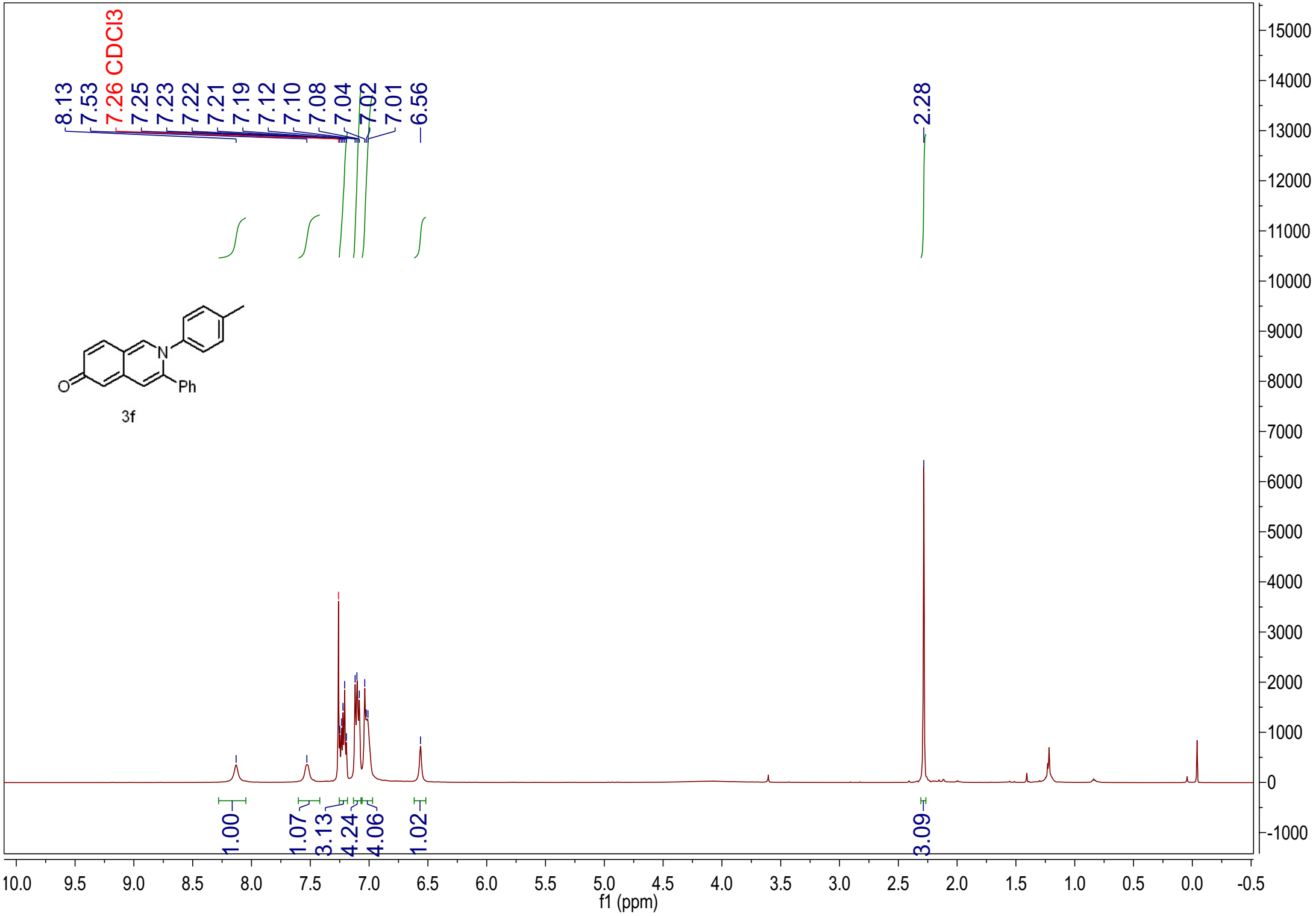
118.67
117.34
114.67
111.48
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
55.63
O
N
Ph
O
3e
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.53
7.26 CDCl3
7.25
7.23
7.22
7.21
7.19
7.12
7.10
7.08
7.04
7.02
7.01
6.56
2.28
O
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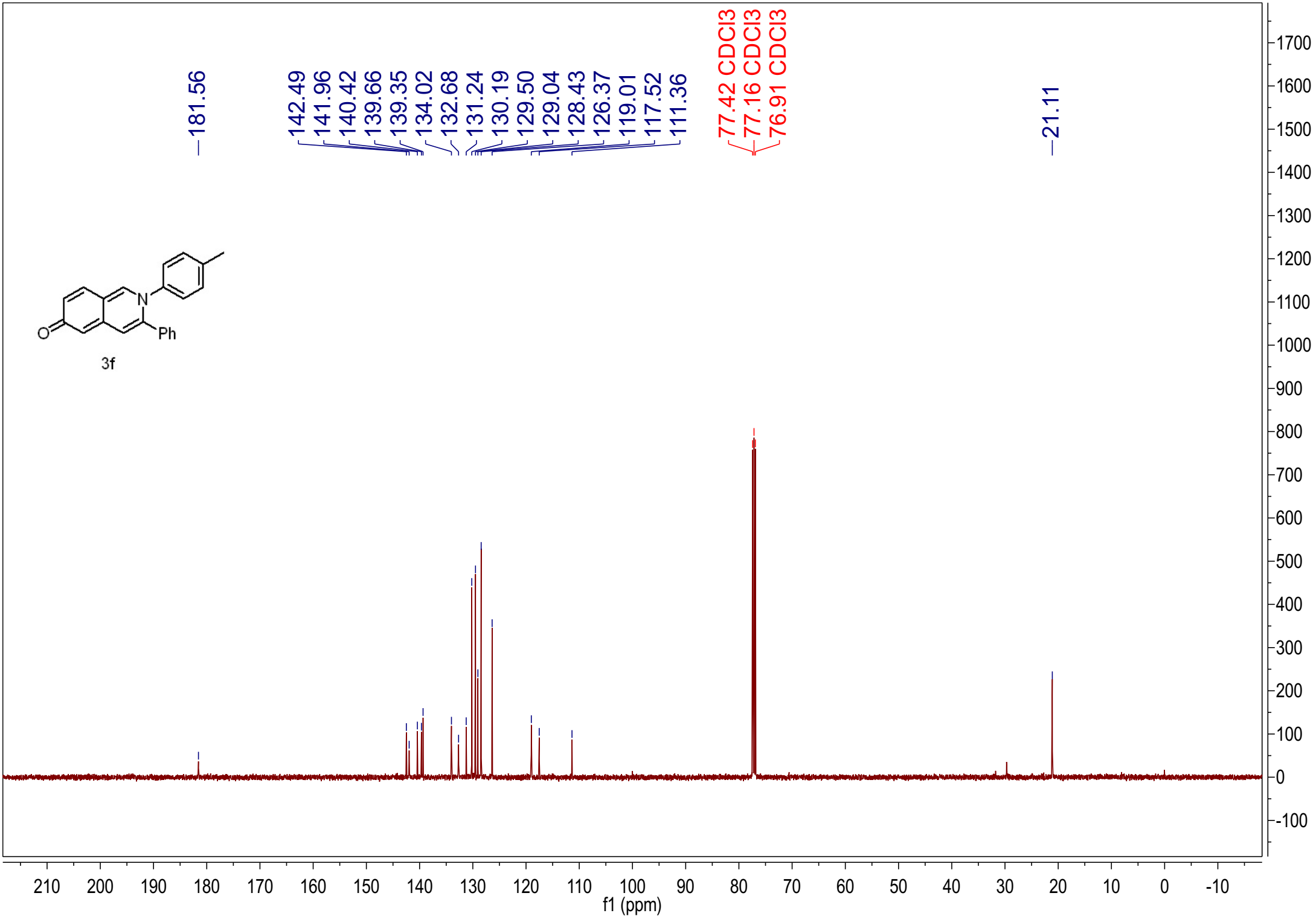
Ph
3f
1.00
1.07
3.13
4.24
4.06
1.02
3.09
f1 (ppm)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132.68
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130.19
129.50
129.04
128.43
126.37
119.01
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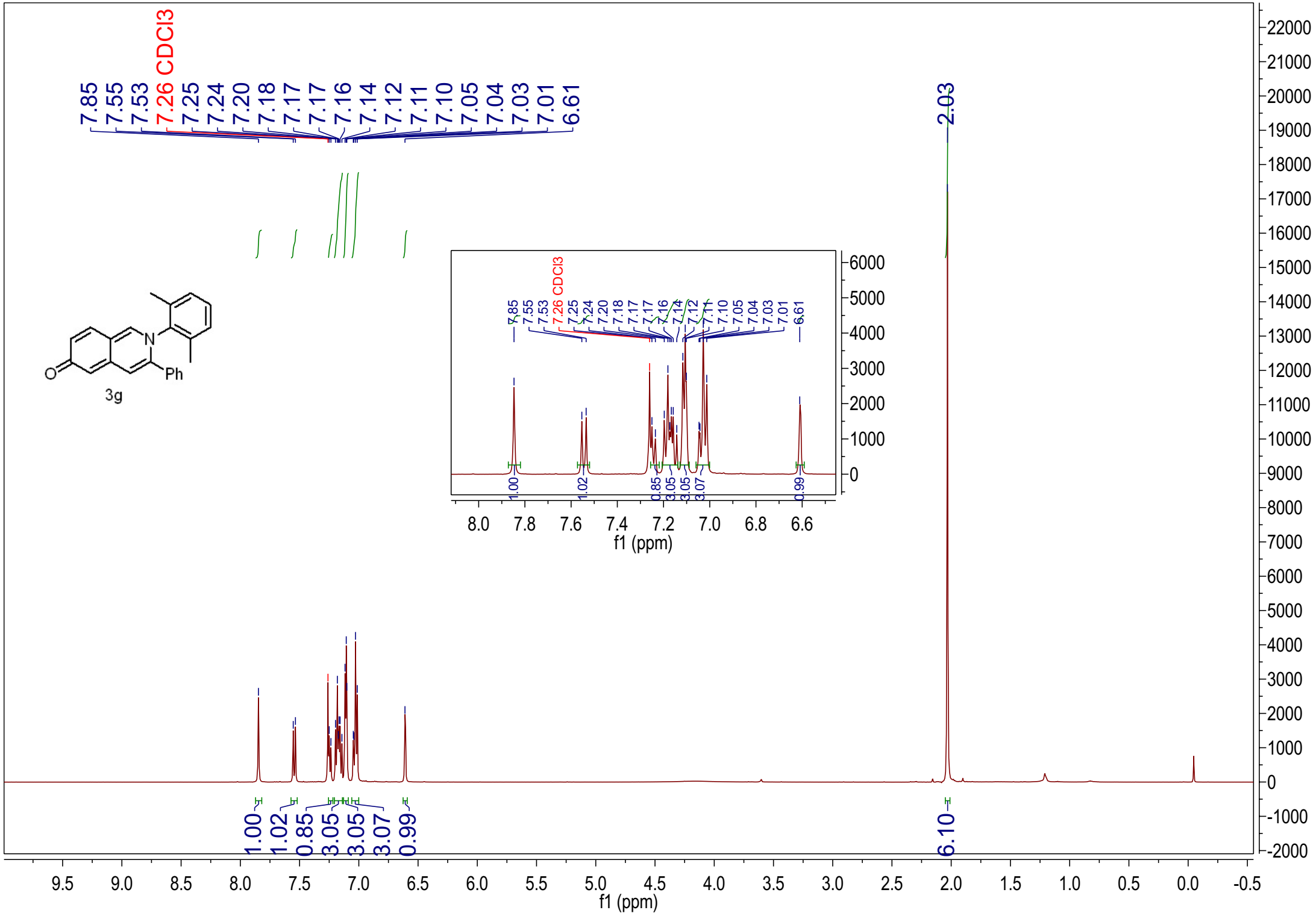
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3
21.11
O
N
Ph
3f
f1 (ppm)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7.25
7.24
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7.18
7.17
7.17
7.16
7.14
7.12
7.11
7.10
7.05
7.04
7.03
7.01
6.61
2.03
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O
Ph
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1.02
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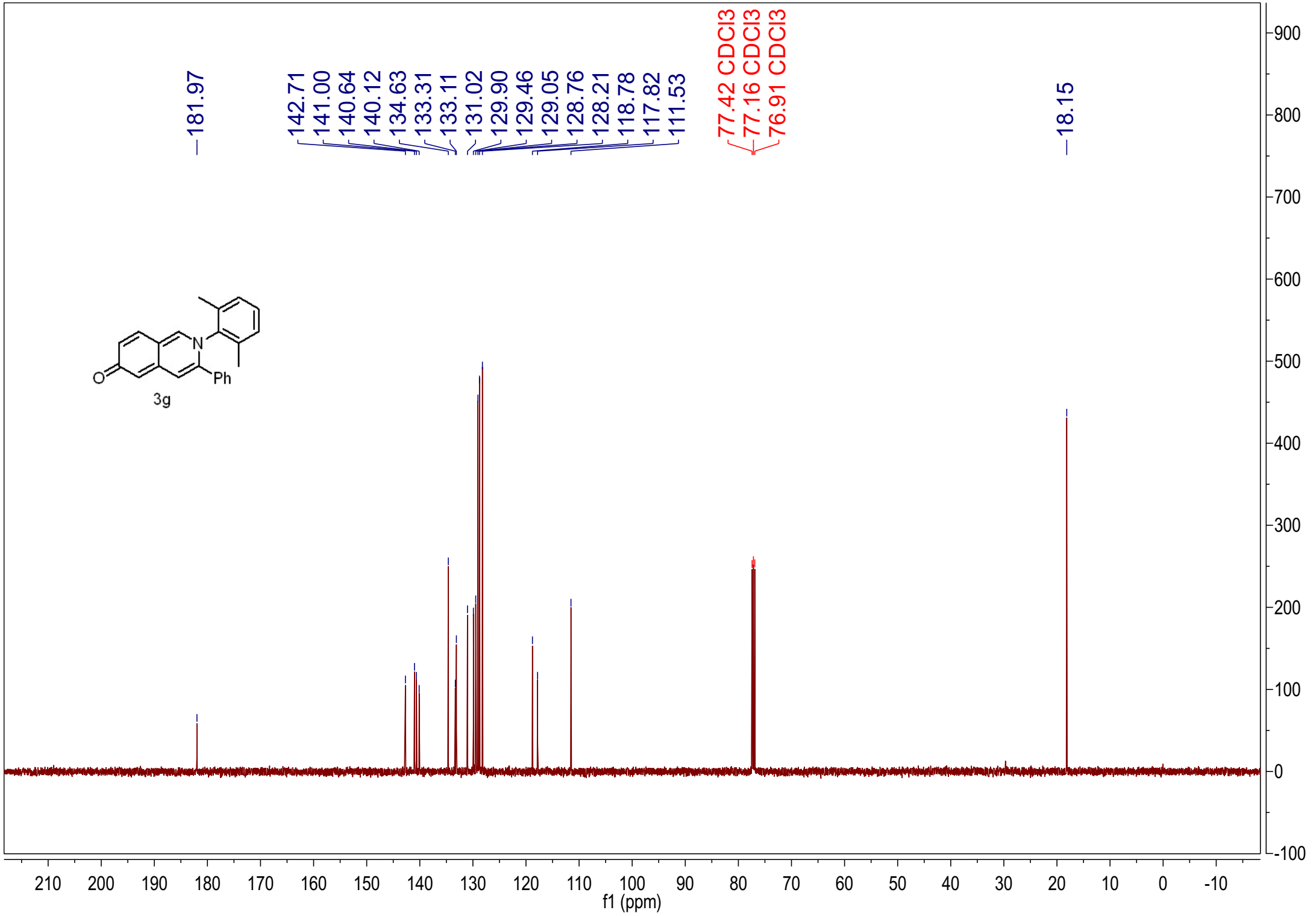
3.05
3.05
3.07
0.99
6.10
f1 (ppm)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129.05
128.76
128.21
118.78
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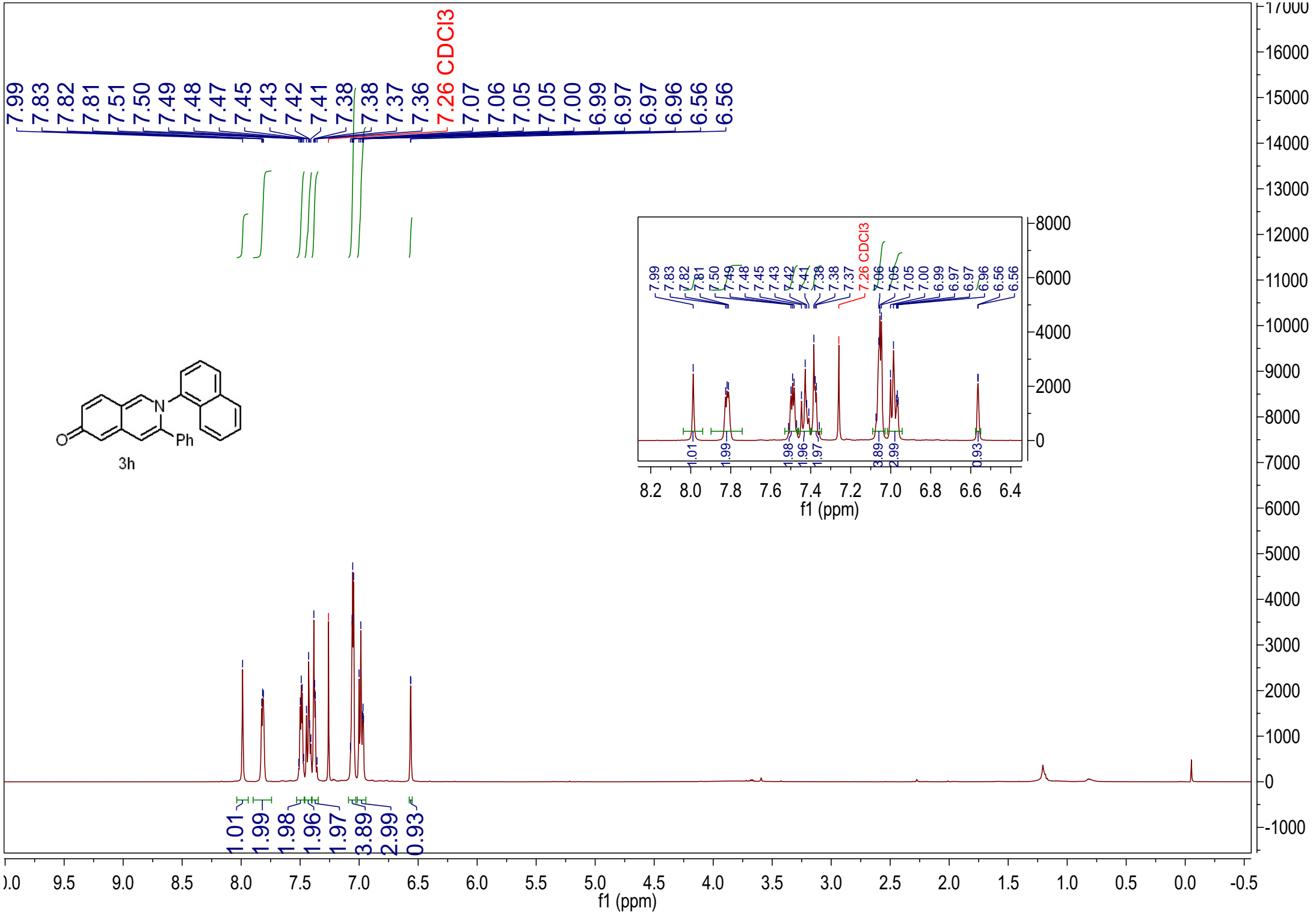
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3
18.15
O
N
Ph
3g
f1 (ppm)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7.48
7.47
7.45
7.43
7.42
7.41
7.38
7.38
7.37
7.36
7.26 CDCl3
7.07
7.06
7.05
7.05
7.00
6.99
6.97
6.97
6.96
6.56
6.56
O
N
Ph
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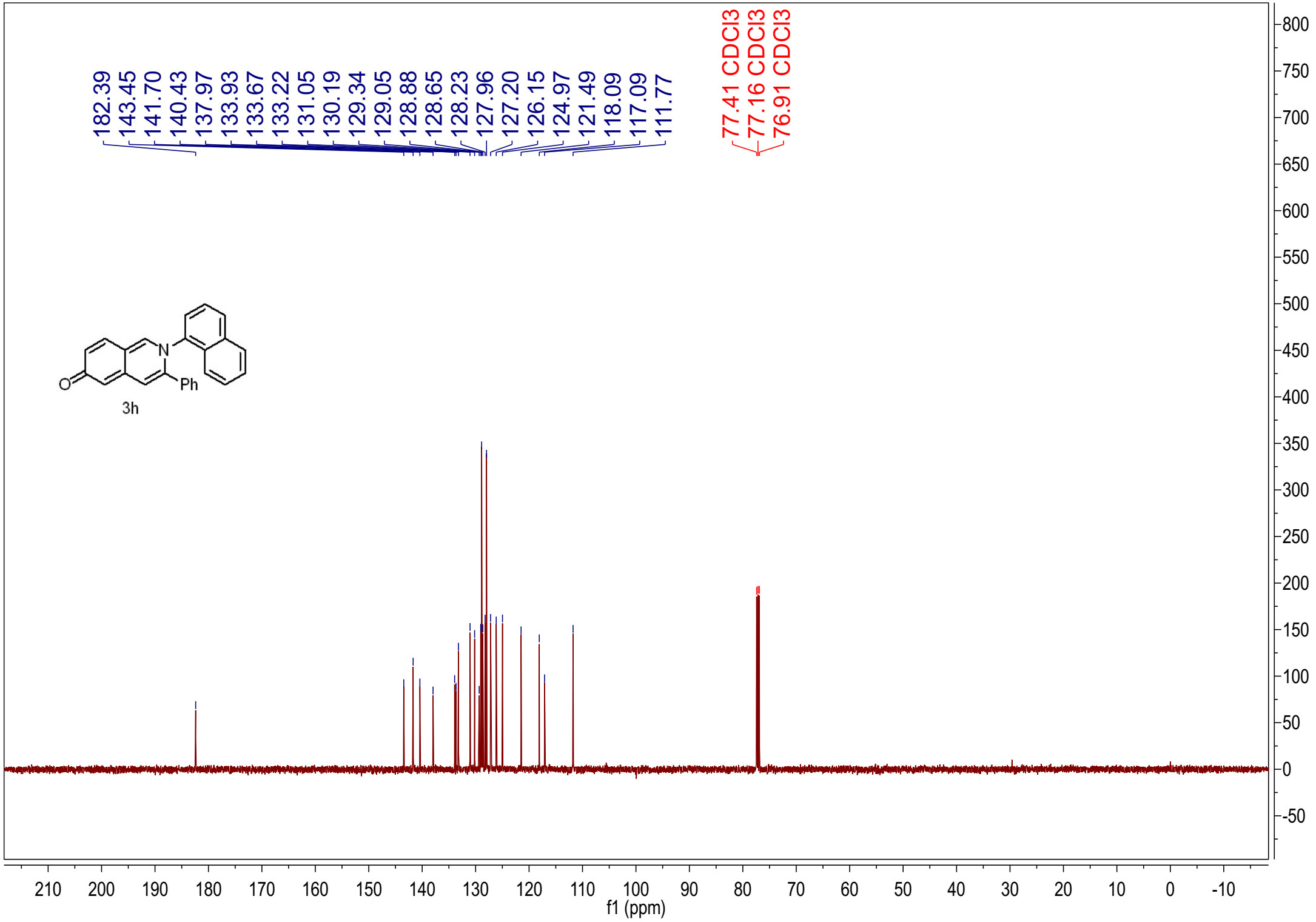
1.99
1.98
1.96
1.97
3.89
2.99
0.93
f1 (ppm)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133.22
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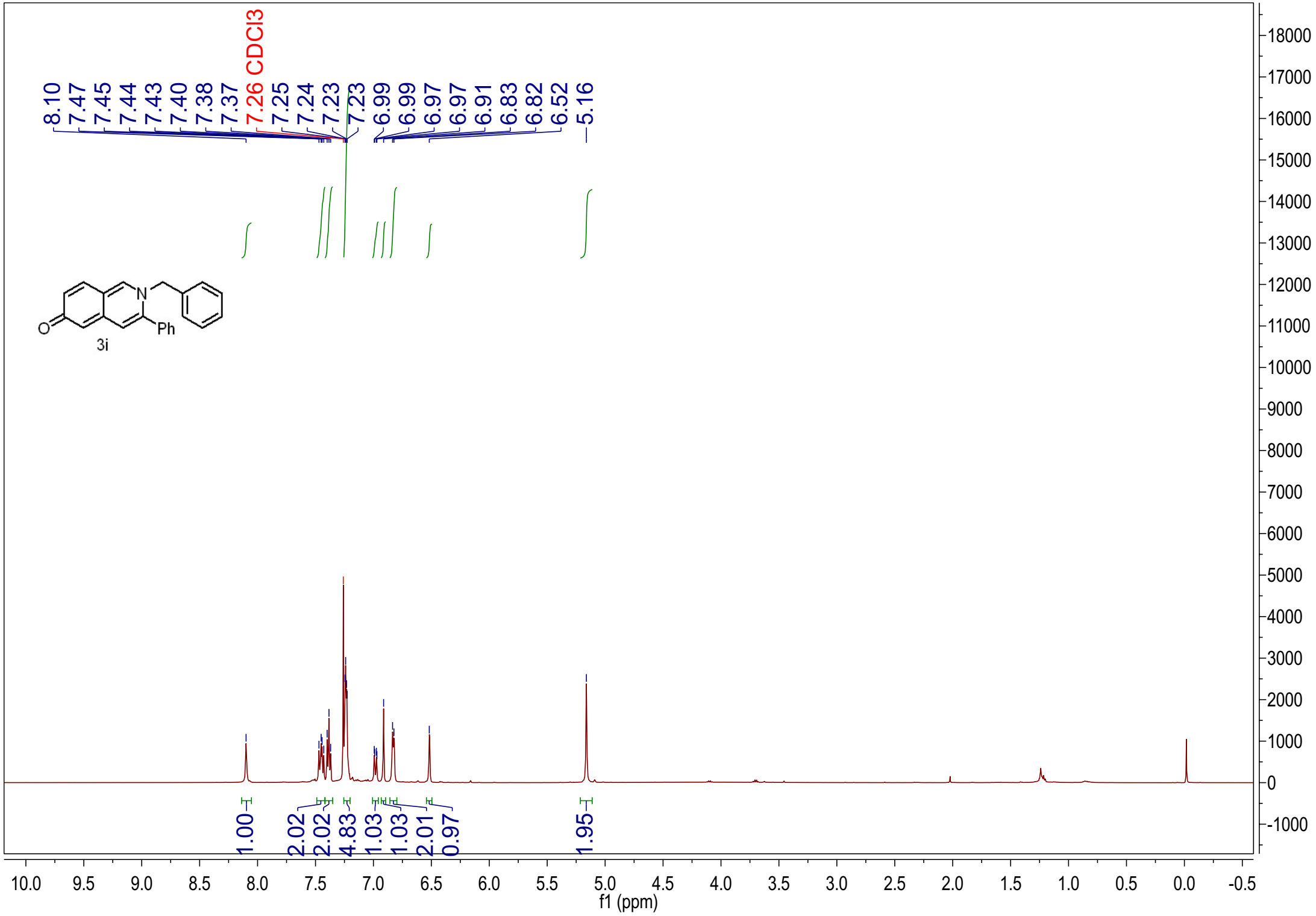
130.19
129.34
129.05
128.88
128.65
128.23
127.96
127.20
126.15
124.97
121.49
118.09
117.09
111.77
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
O
N
Ph
3h
f1 (ppm)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7.43
7.40
7.38
7.37
7.26 CDCl3
7.25
7.24
7.23
7.23
6.99
6.99
6.97
6.97
6.91
6.83
6.82
6.52
5.16
N
Ph
O
3i
1.00
2.02
2.02
4.83
1.03
1.03
2.01
0.97
1.95
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.5
2.0
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0.5
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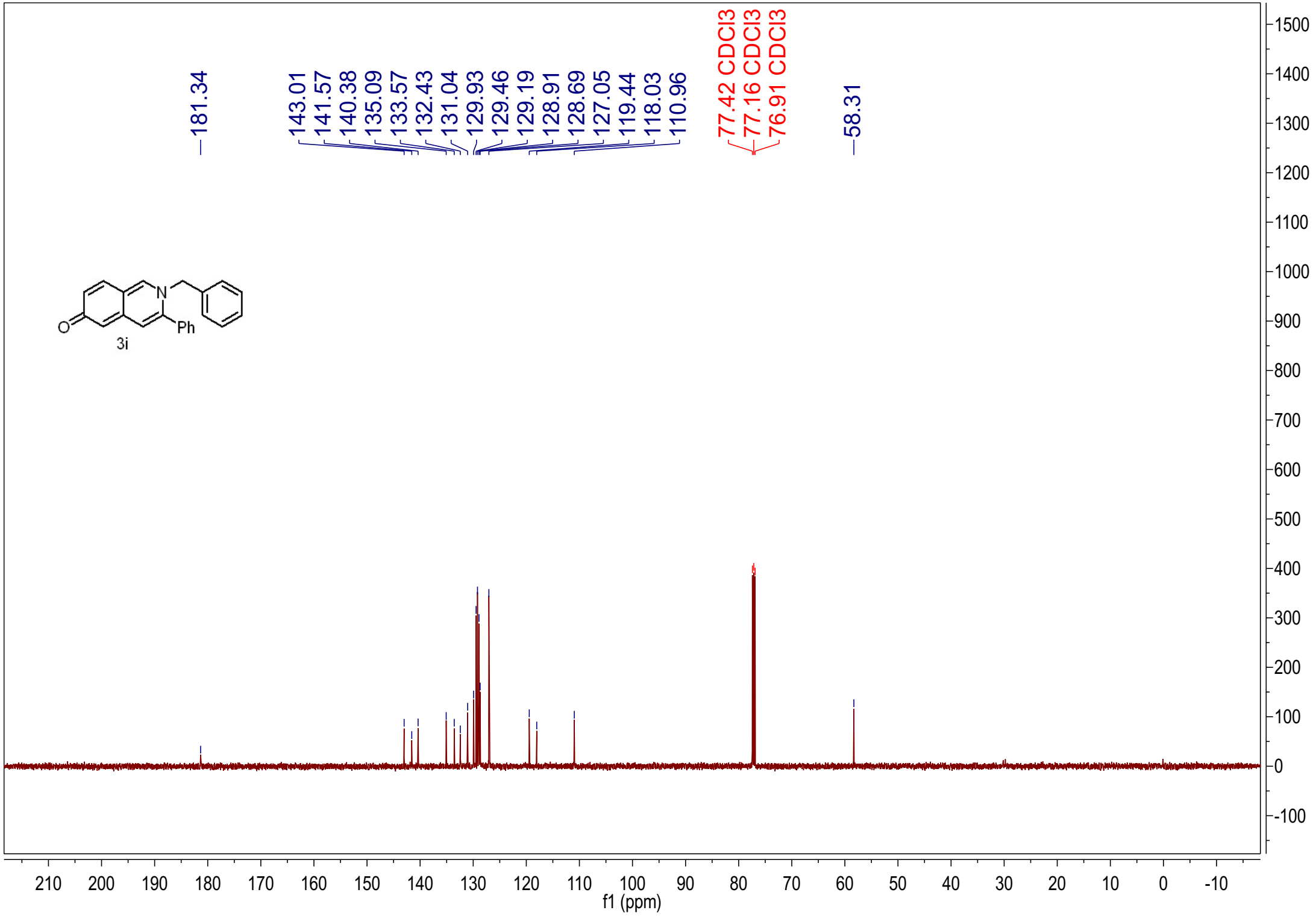
-0.5
f1 (ppm)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128.91
128.69
127.05
119.44
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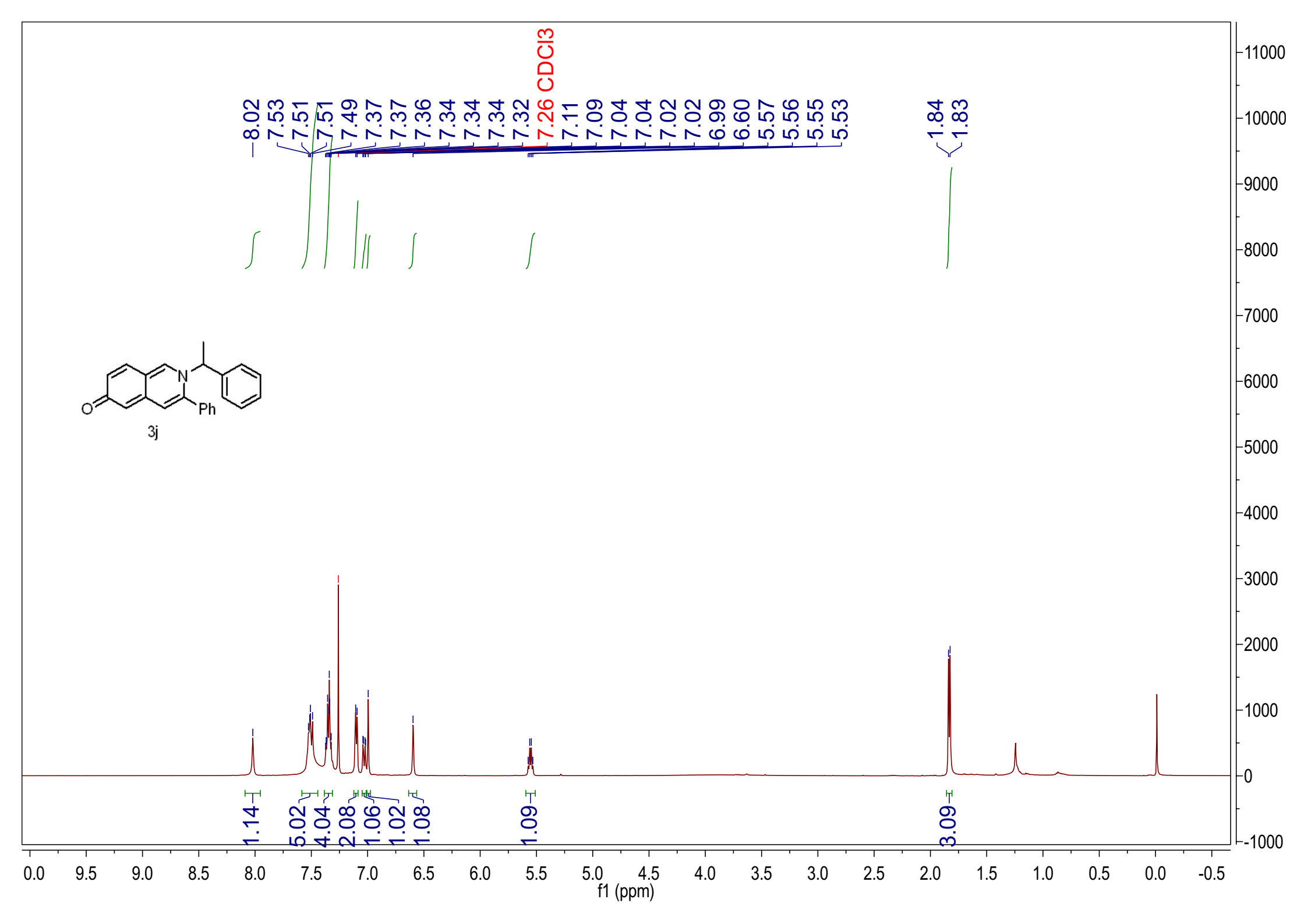
77.16 CDCl3
76.91 CDCl3
58.31
O
N
Ph
3i
f1 (ppm)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7.36
7.34
7.34
7.34
7.32
7.26 CDCl3
7.11
7.09
7.04
7.04
7.02
7.02
6.99
6.60
5.57
5.56
5.55
5.53
1.84
1.83
O
N
Ph
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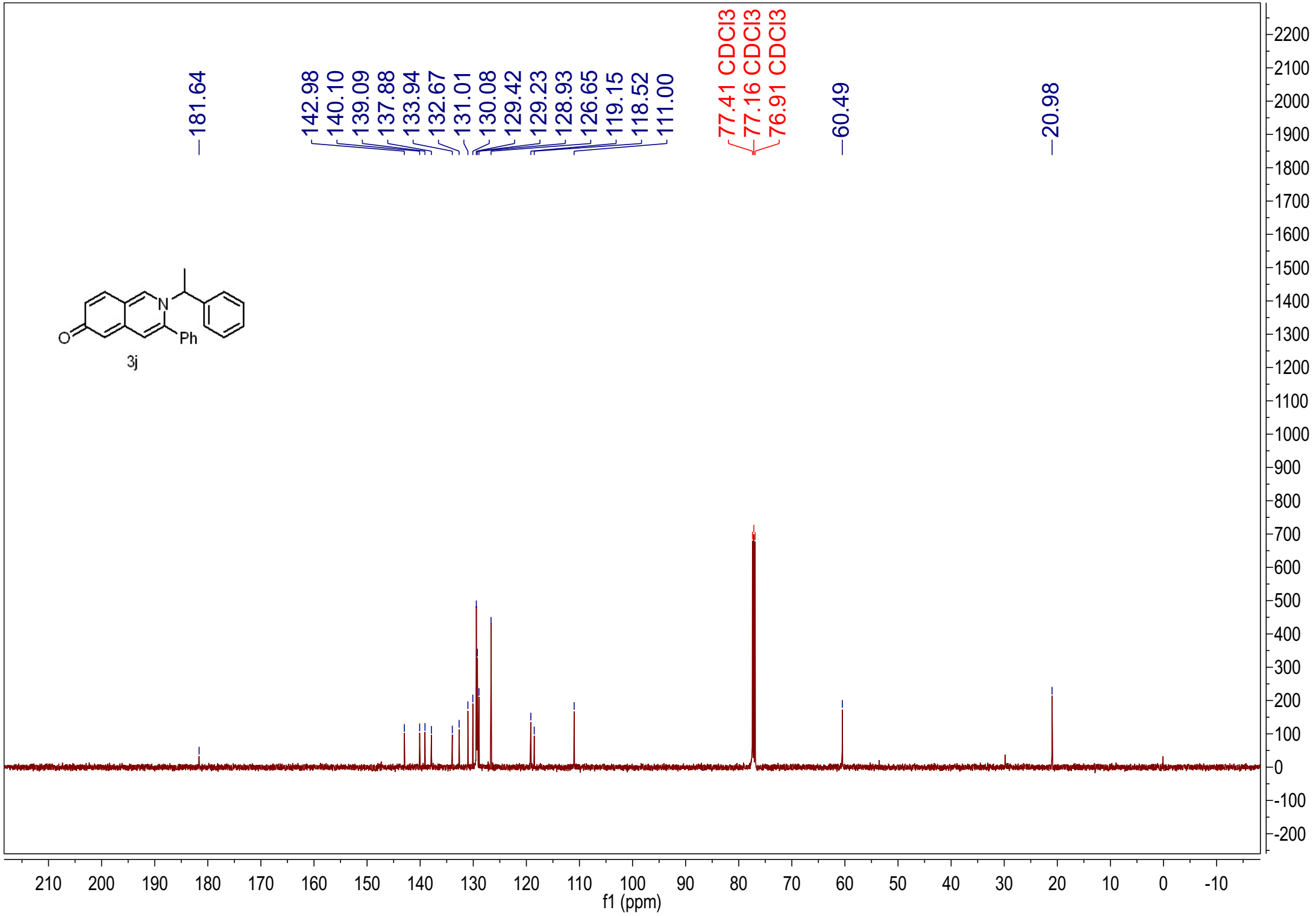
4.04
2.08
1.06
1.02
1.08
1.09
3.09
f1 (ppm)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129.23
128.93
126.65
119.15
118.52
111.00
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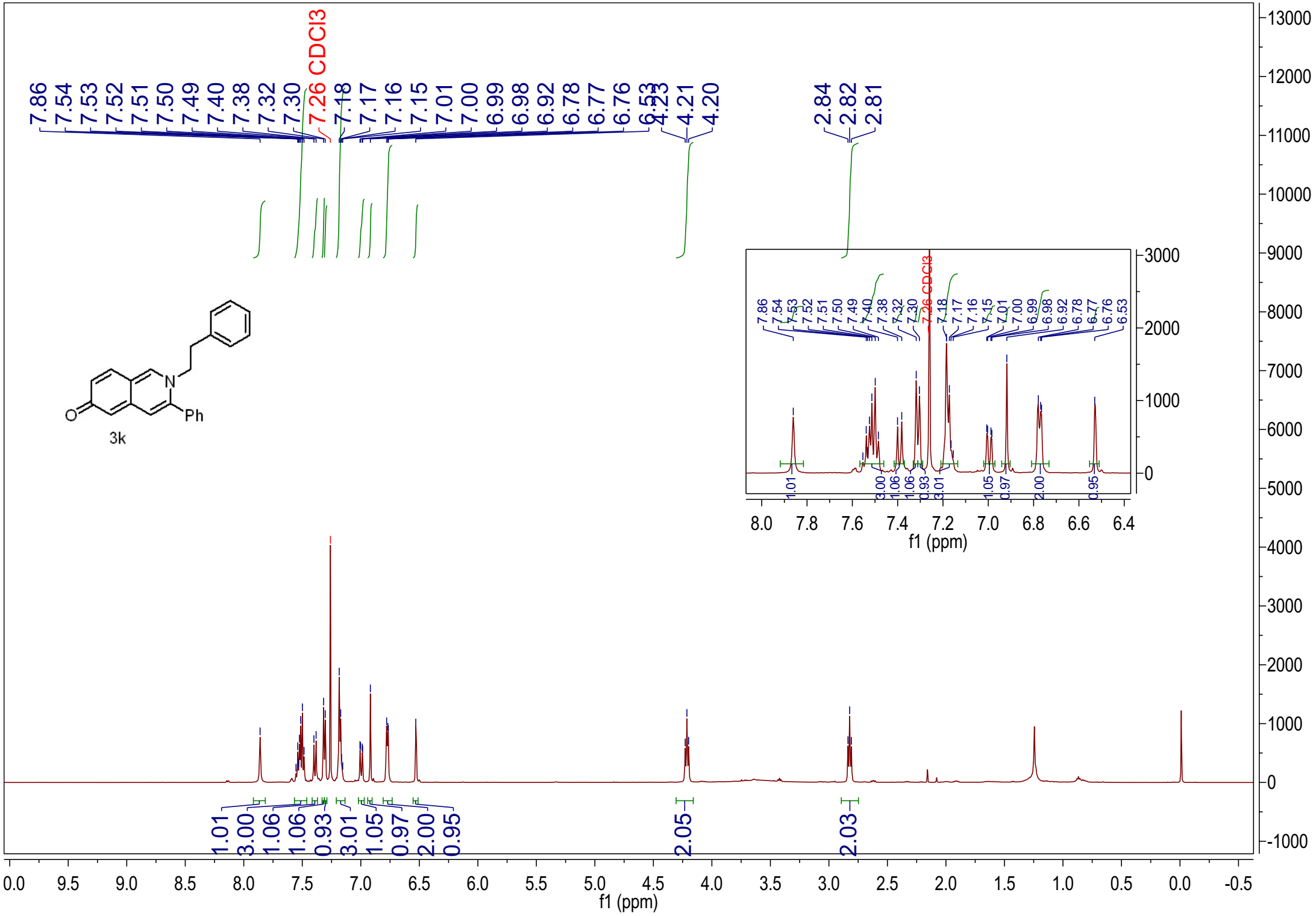
77.16 CDCl3
76.91 CDCl3
60.49
20.98
O
N
Ph
3j
f1 (ppm)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7.40
7.38
7.32
7.30
7.26 CDCl3
7.18
7.17
7.16
7.15
7.01
7.00
6.99
6.98
6.92
6.78
6.77
6.76
6.53
4.23
4.21
4.20
2.84
2.82
2.81
O
N
Ph
3k
1.01
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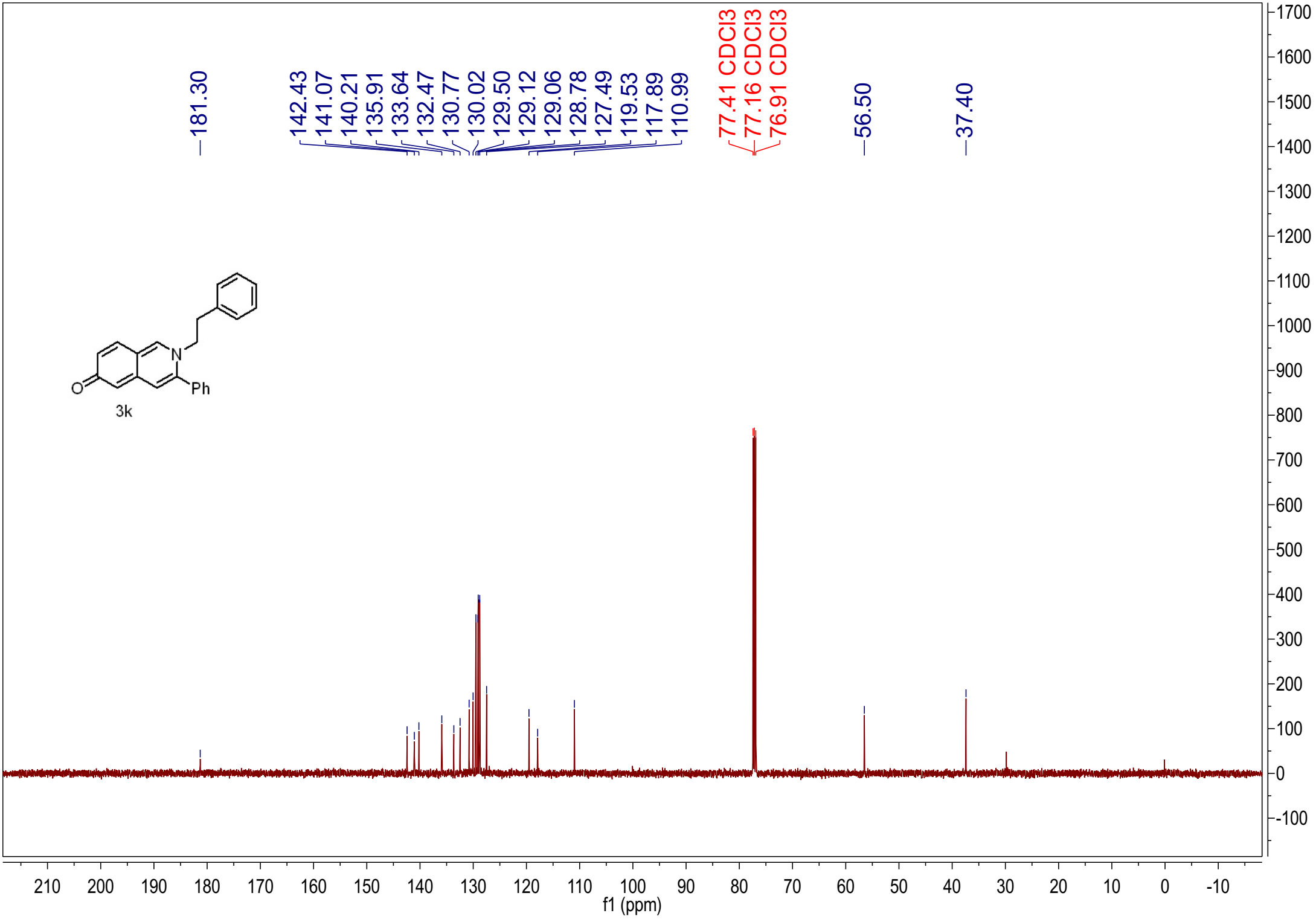
1.06
1.06
0.93
3.01
1.05
0.97
2.00
0.95
2.05
2.03
f1 (ppm)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133.64
132.47
130.77
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129.12
129.06
128.78
127.49
119.53
117.89
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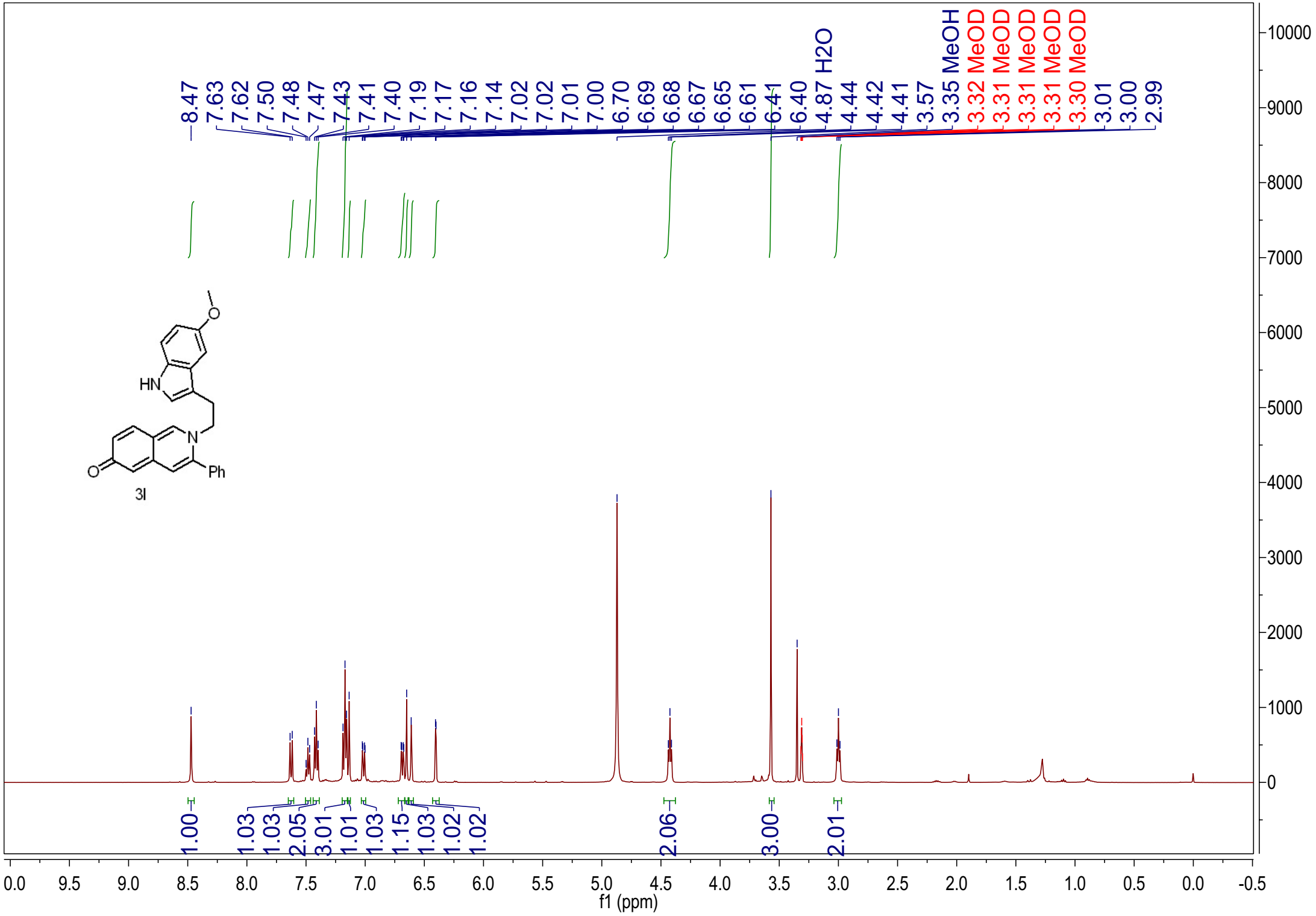
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
56.50
37.40
N
O
Ph
3k
f1 (ppm)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7.14
7.02
7.02
7.01
7.00
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6.69
6.68
6.67
6.65
6.61
6.41
6.40
4.87 H2O
4.44
4.42
4.41
3.57
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.01
3.00
2.99
HN
O
N
O
Ph
3l
1.00
1.03
1.03
2.05
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1.03
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1.03
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1.02
2.06
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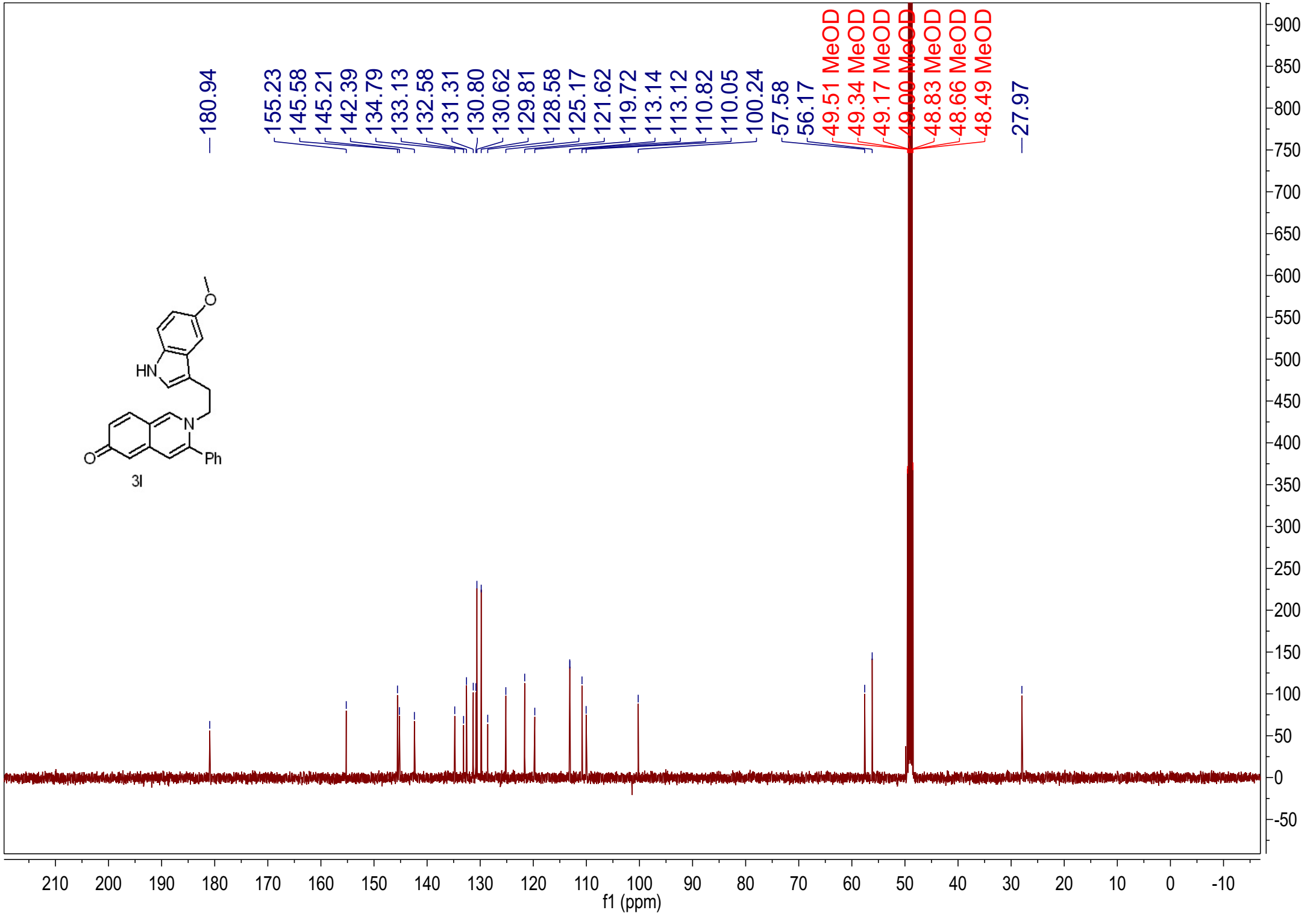
2.01
f1 (ppm)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125.17
121.62
119.72
113.14
113.12
110.82
110.05
100.24
57.58
56.17
49.51 MeOD
49.34 MeOD
49.17 MeOD
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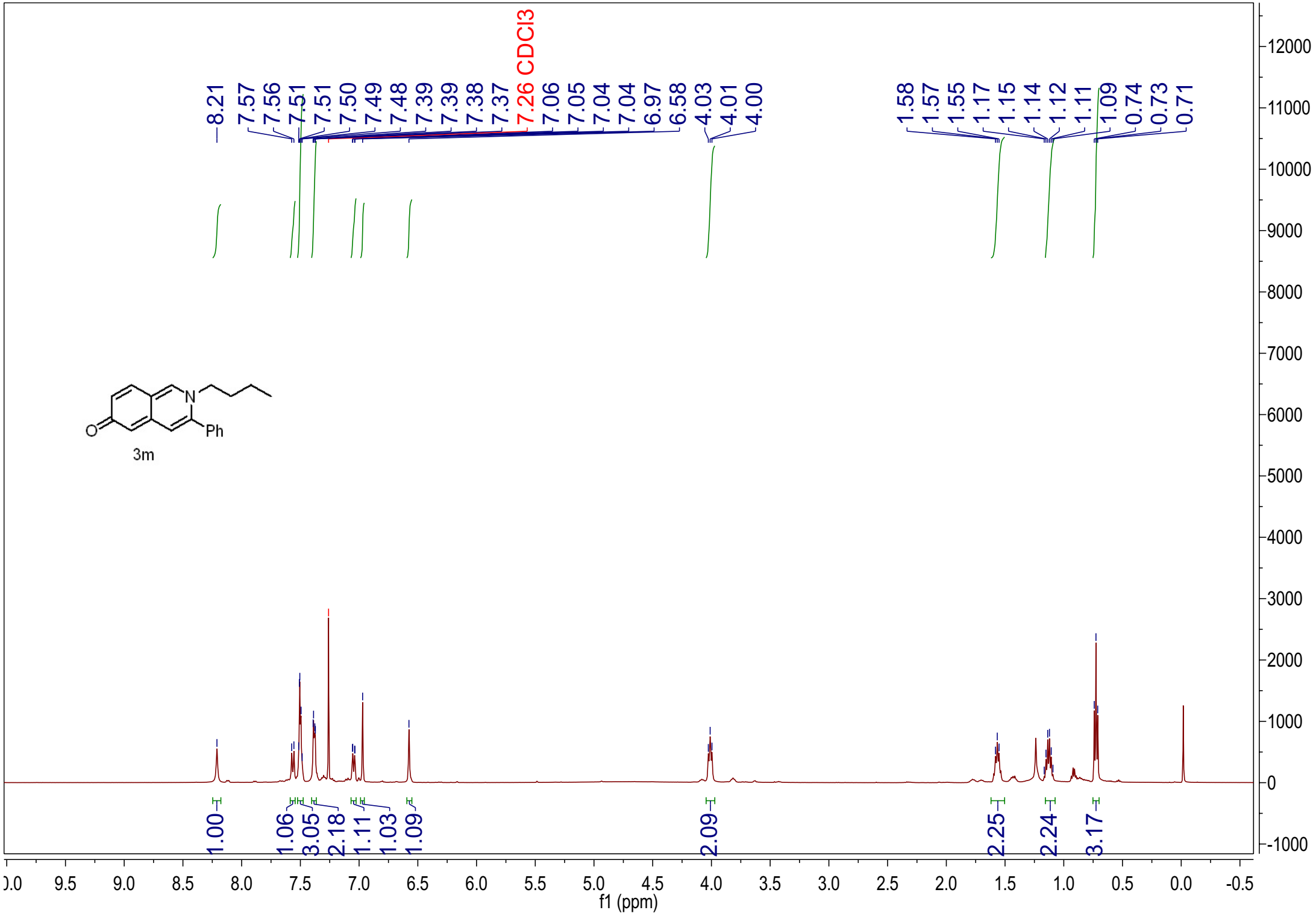
48.49 MeOD
27.97
HN
O
N
O
Ph
3l
f1 (ppm)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7.37
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7.06
7.05
7.04
7.04
6.97
6.58
4.03
4.01
4.00
1.58
1.57
1.55
1.17
1.15
1.14
1.12
1.11
1.09
0.74
0.73
0.71
N
O
Ph
3m
1.00
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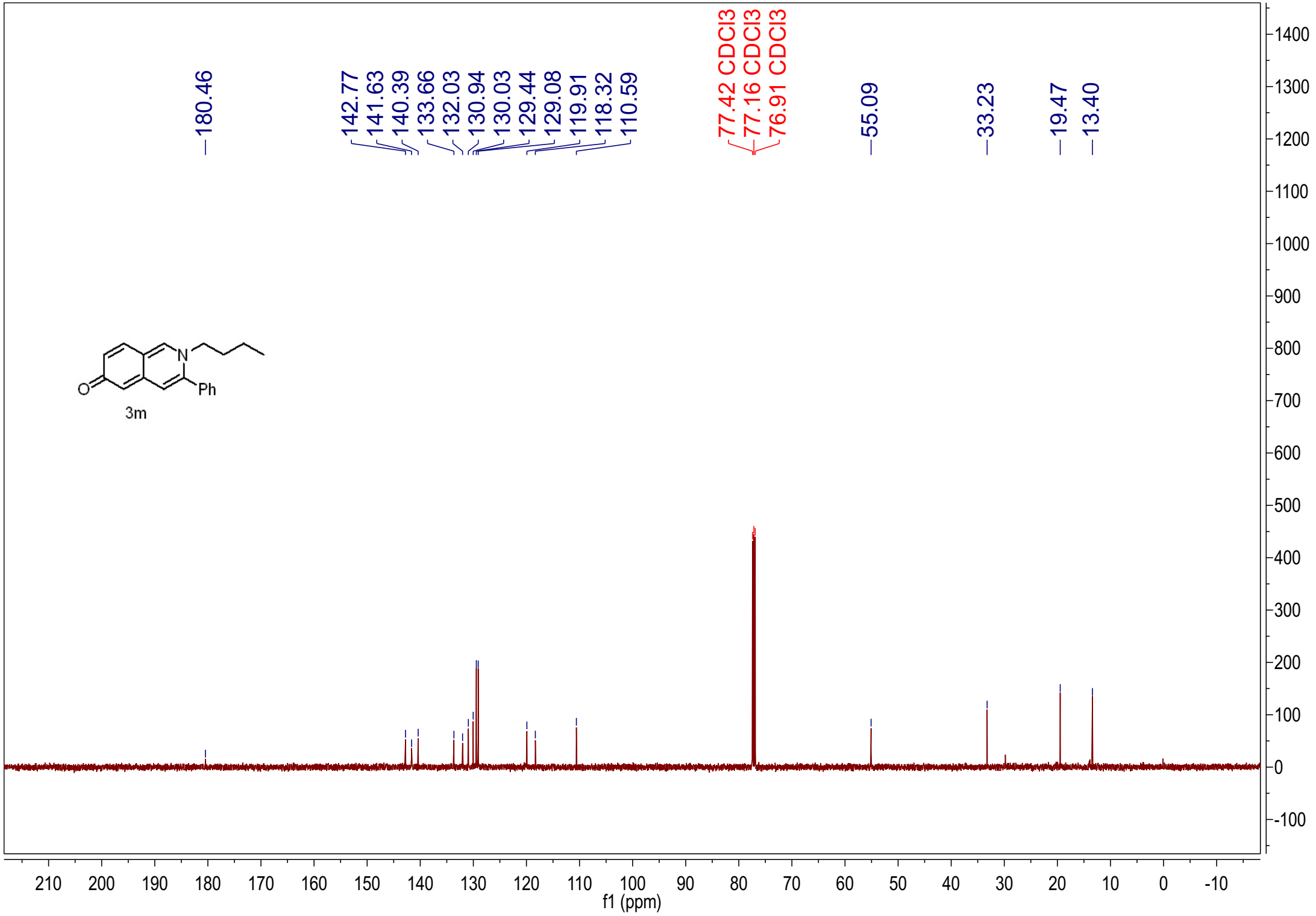
1.03
1.09
2.09
2.25
2.24
3.17
f1 (ppm)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110.59
77.42 CDCl3
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76.91 CDCl3
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13.40
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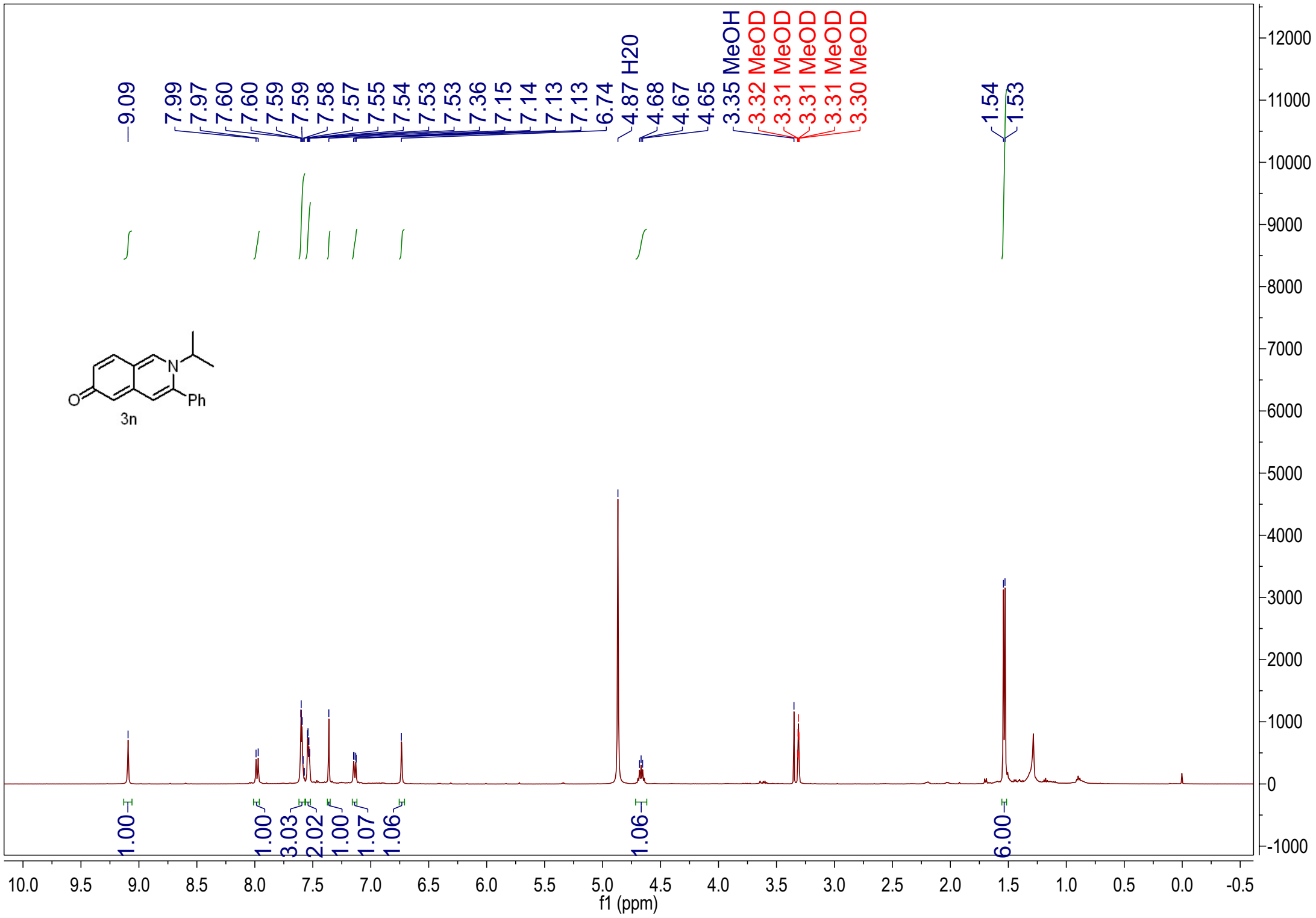
N
Ph
3m
f1 (ppm)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7.53
7.36
7.15
7.14
7.13
7.13
6.74
4.87 H20
4.68
4.67
4.65
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
1.54
1.53
N
O
Ph
3n
1.00
1.00
3.03
2.02
1.00
1.07
1.06
1.06
6.00
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
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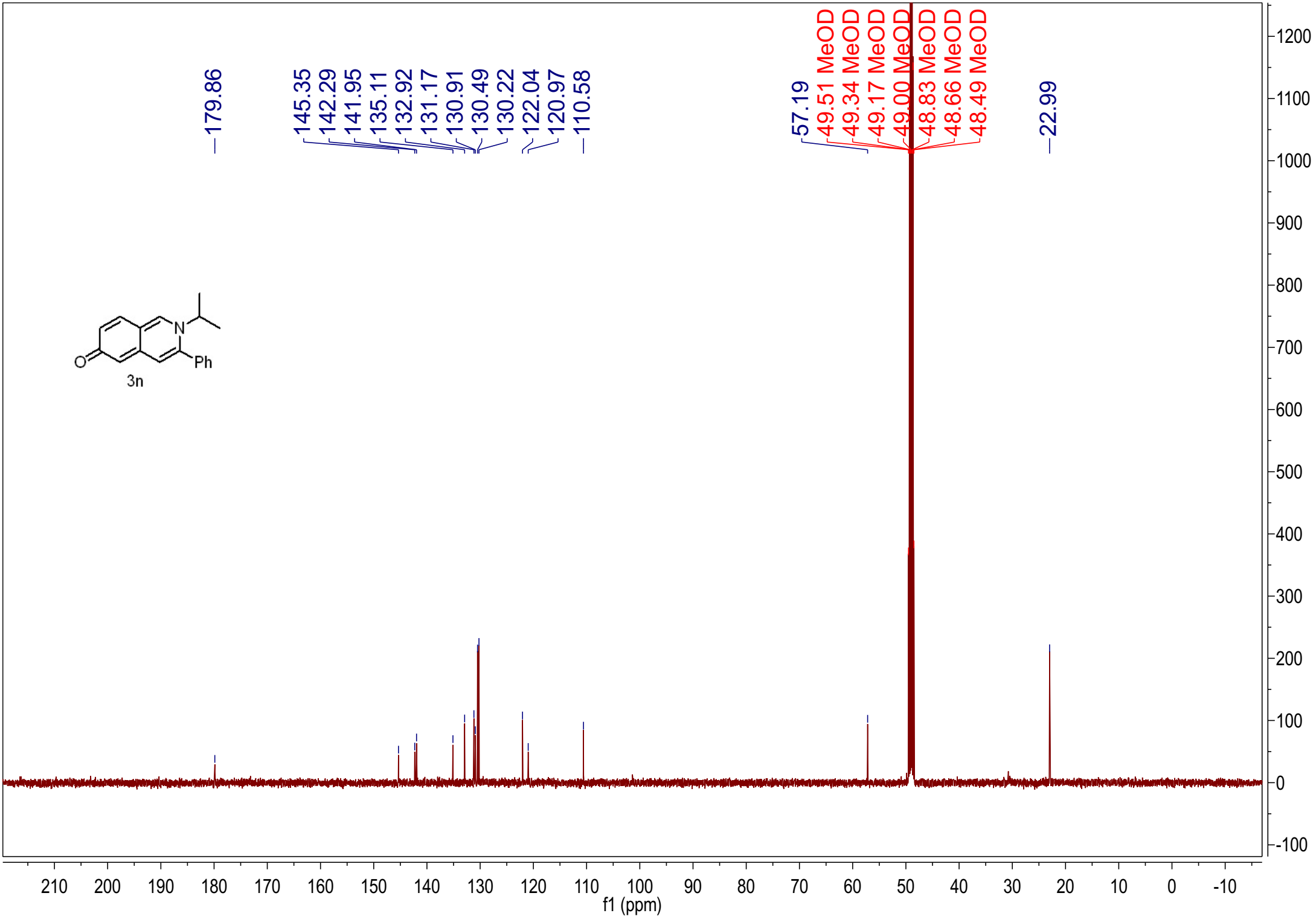
0.5
0.0
-0.5
f1 (ppm)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110.58
57.19
49.51 MeOD
49.34 MeOD
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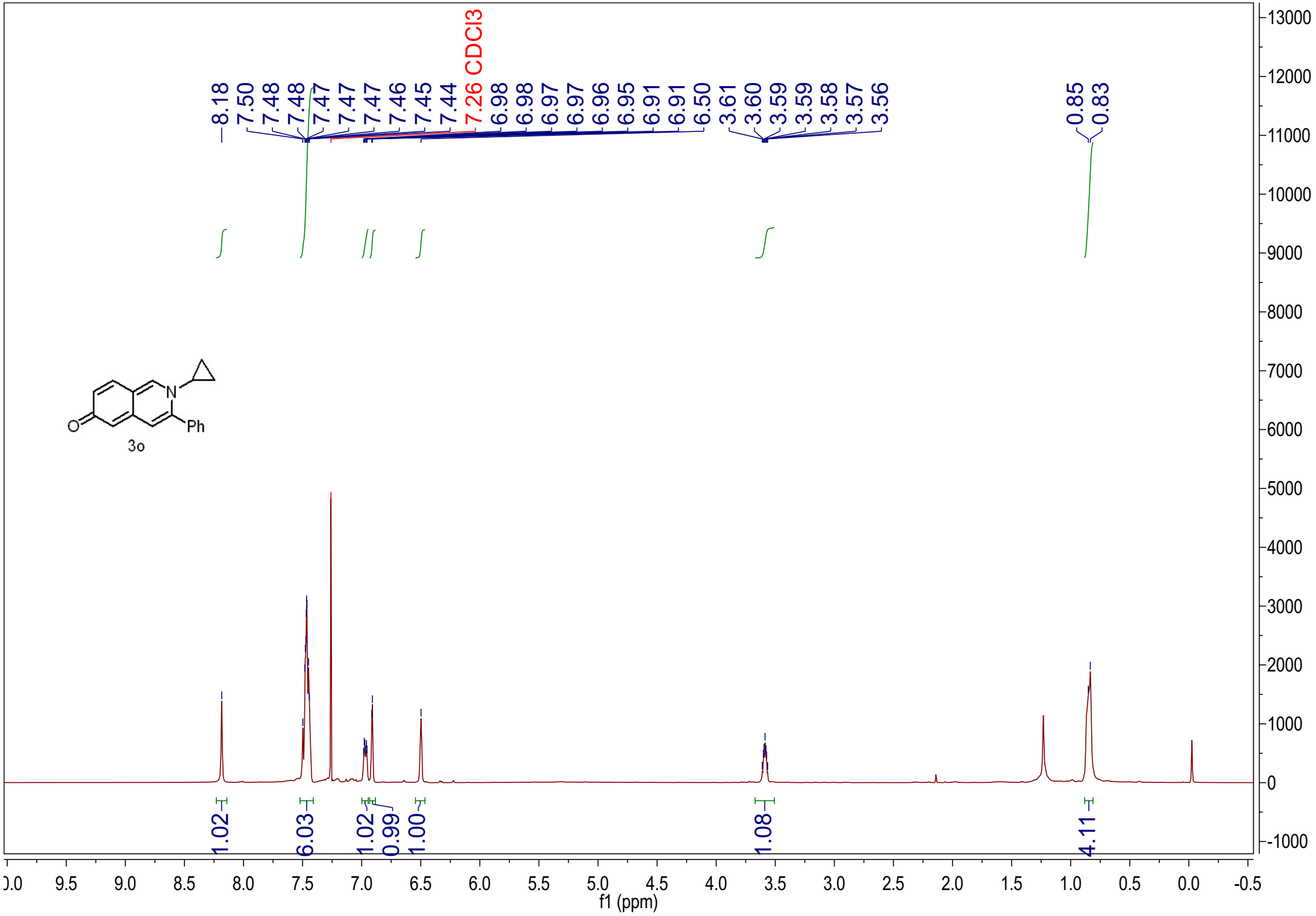
48.83 MeOD
48.66 MeOD
48.49 MeOD
22.99
O
N
Ph
3n
f1 (ppm)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7.44
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6.97
6.96
6.95
6.91
6.91
6.50
3.61
3.60
3.59
3.59
3.58
3.57
3.56
0.85
0.83
O
N
Ph
3o
1.02
6.03
1.02
0.99
1.00
1.08
4.11
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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2.0
1.5
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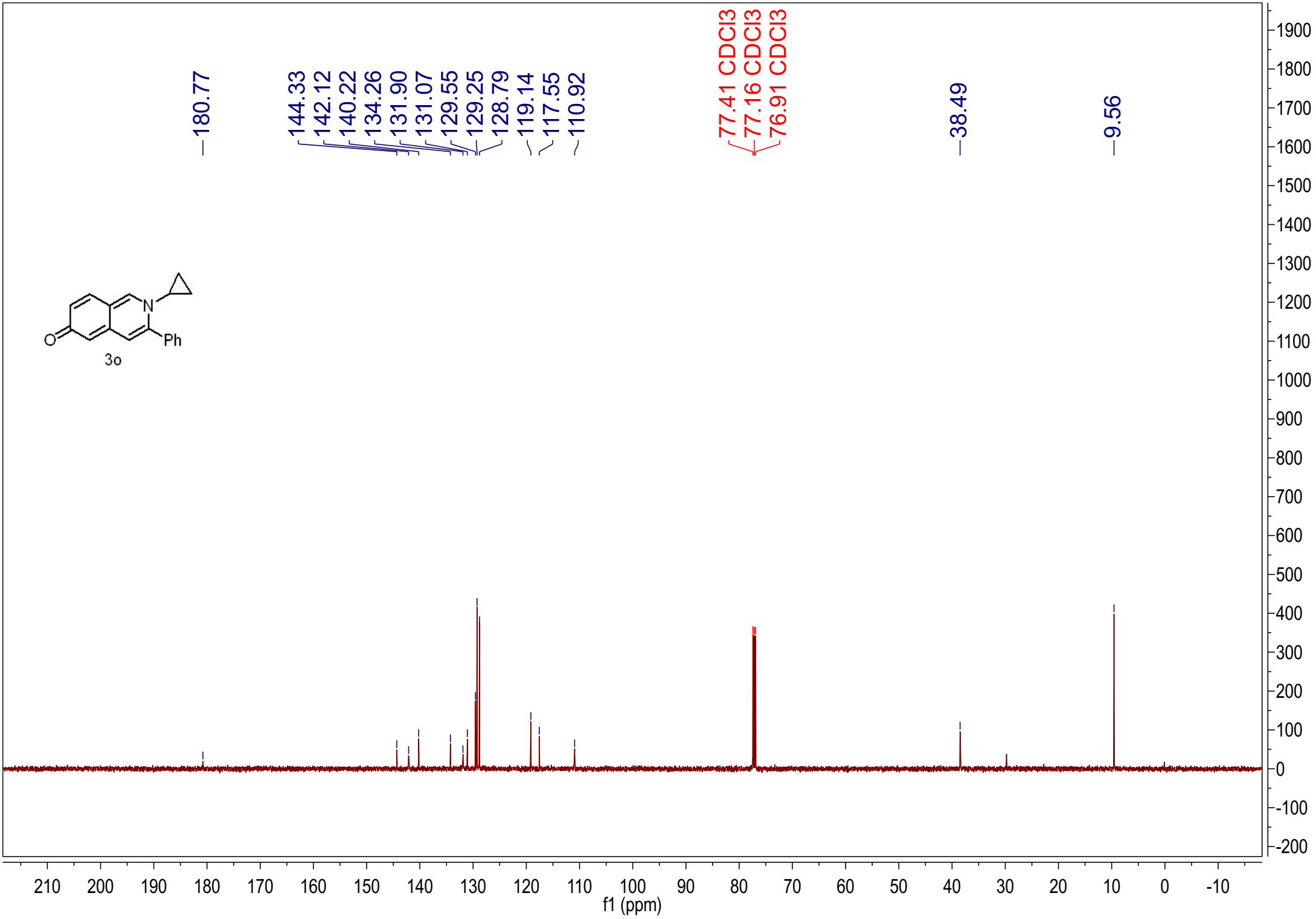
0.5
0.0
-0.5
f1 (ppm)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129.25
128.79
119.14
117.55
110.92
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
38.49
9.56
O
N
Ph
3o
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-200
210
200
190
180
170
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110
100
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80
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30
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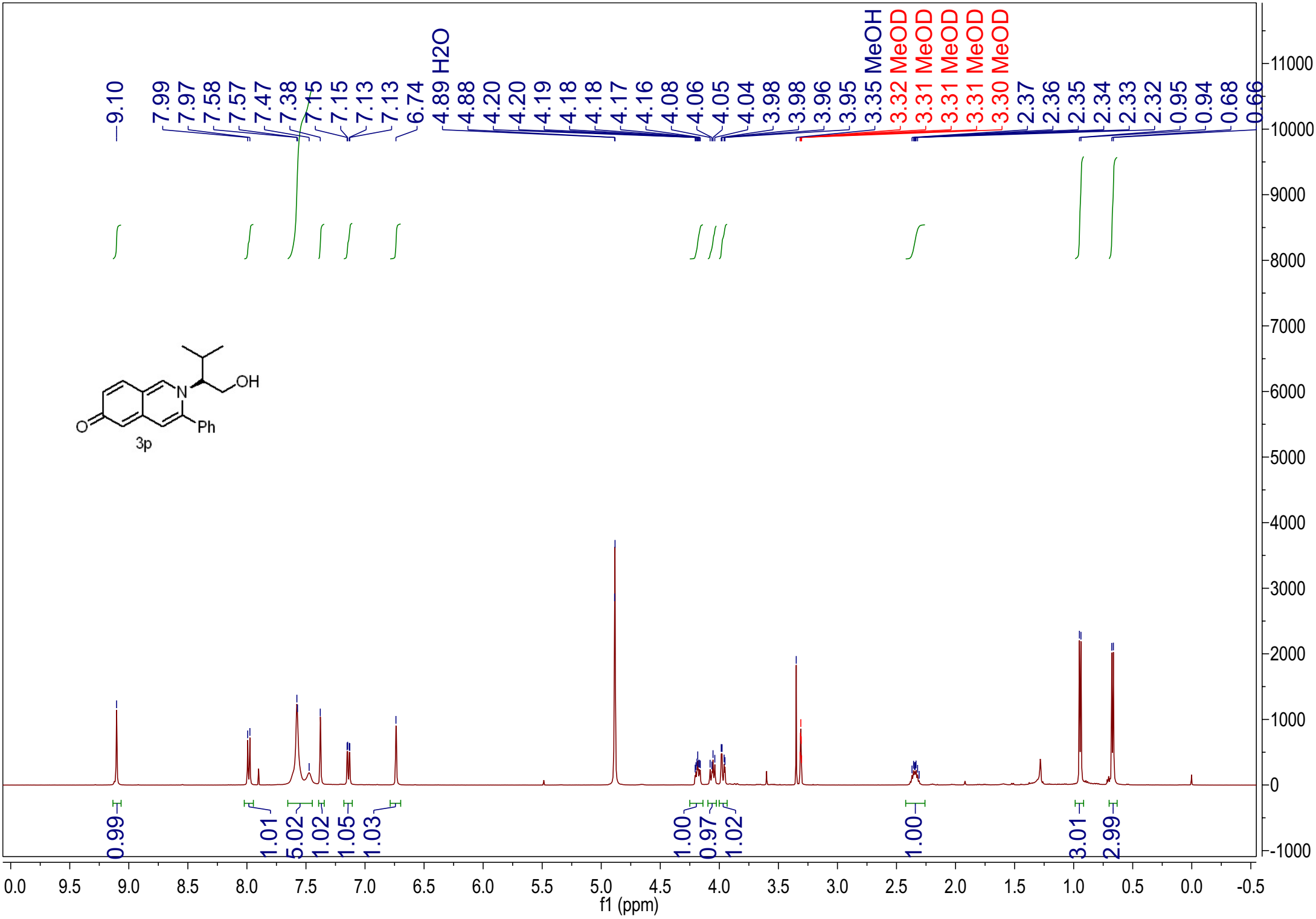
-10
f1 (ppm)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7.13
7.13
6.74
4.89 H2O
4.88
4.20
4.20
4.19
4.18
4.18
4.17
4.16
4.08
4.06
4.05
4.04
3.98
3.98
3.96
3.95
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
2.37
2.36
2.35
2.34
2.33
2.32
0.95
0.94
0.68
0.66
OH
N
O
Ph
3p
0.99
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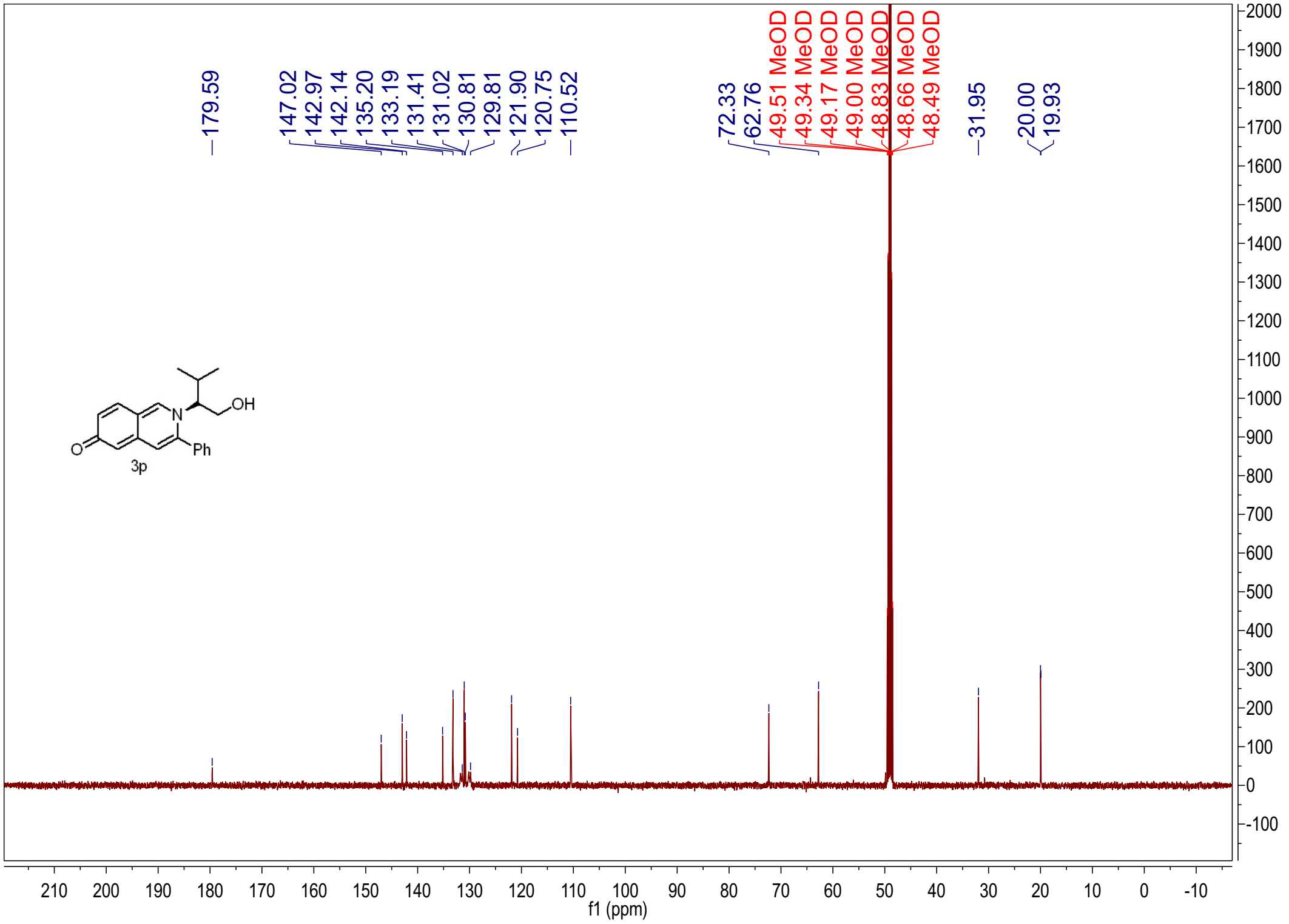
1.02
1.05
1.03
1.00
0.97
1.02
1.00
3.01
2.99
f1 (ppm)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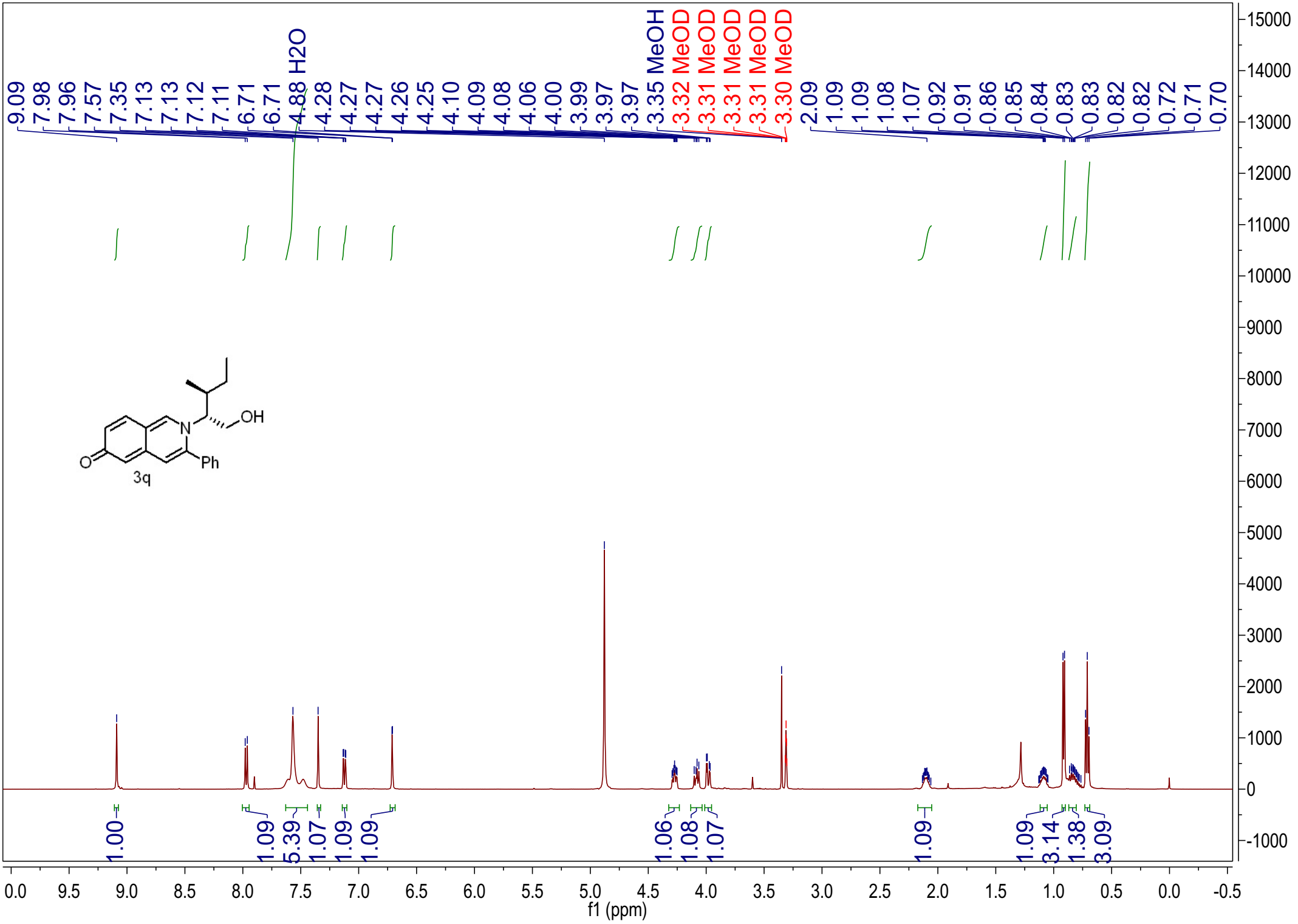
129.81
121.90
120.75
110.52
72.33
62.76
49.51 MeOD
49.34 MeOD
49.17 MeOD
49.00 MeOD
48.83 MeOD
48.66 MeOD
48.49 MeOD
31.95
20.00
19.93
OH
N
O
Ph
3p
f1 (ppm)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7.57
7.35
7.13
7.13
7.12
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6.71
6.71
4.88 H2O
4.28
4.27
4.27
4.26
4.25
4.10
4.09
4.08
4.06
4.00
3.99
3.97
3.97
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
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1.09
1.09
1.08
1.07
0.92
0.91
0.86
0.85
0.84
0.83
0.83
0.82
0.82
0.72
0.71
0.70
OH
N
O
Ph
3q
1.00
1.09
5.39
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1.06
1.08
1.07
1.09
1.09
3.14
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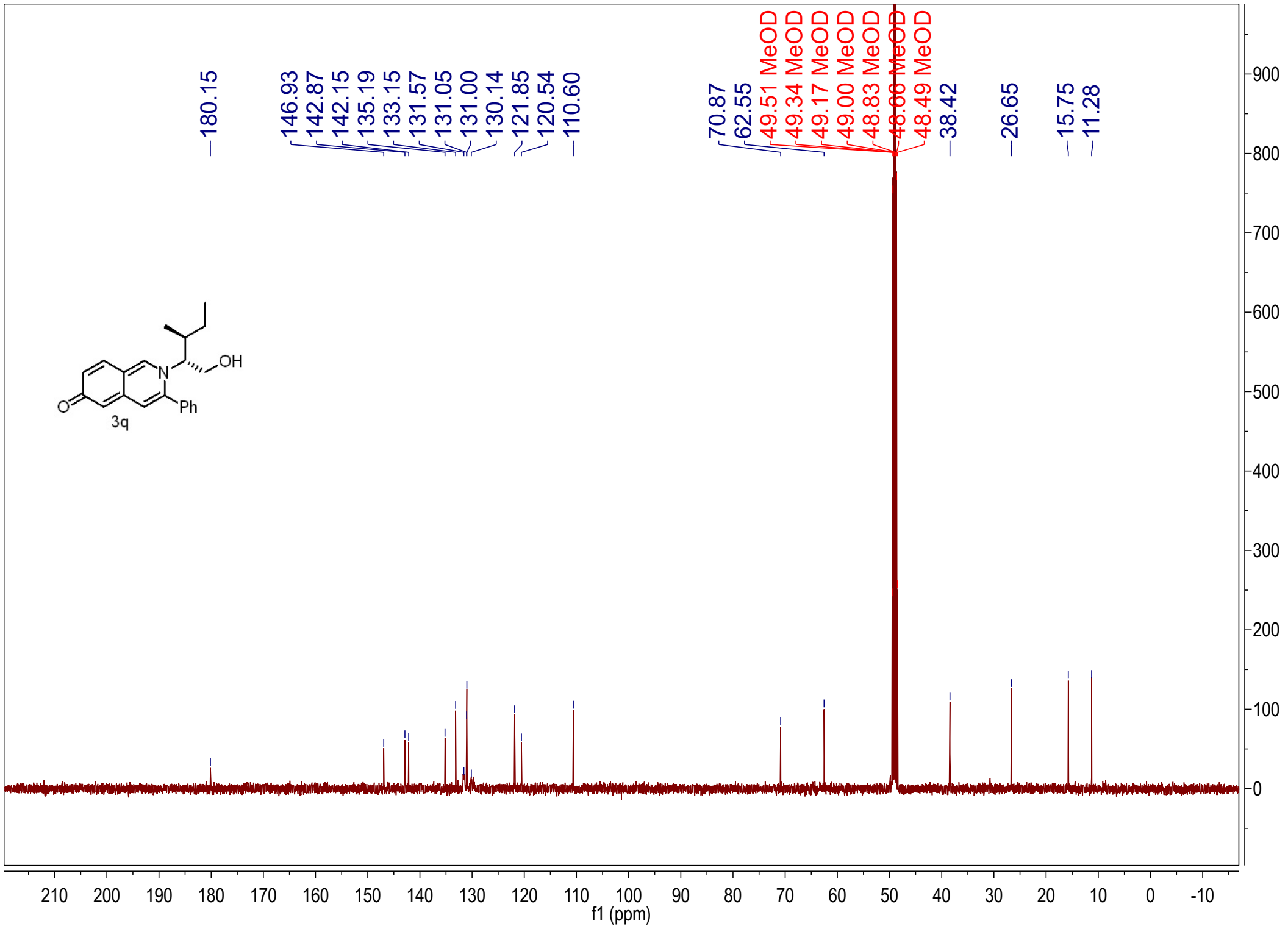
f1 (ppm)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70.87
62.55
49.51 MeOD
49.34 MeOD
49.17 MeOD
49.00 MeOD
48.83 MeOD
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38.42
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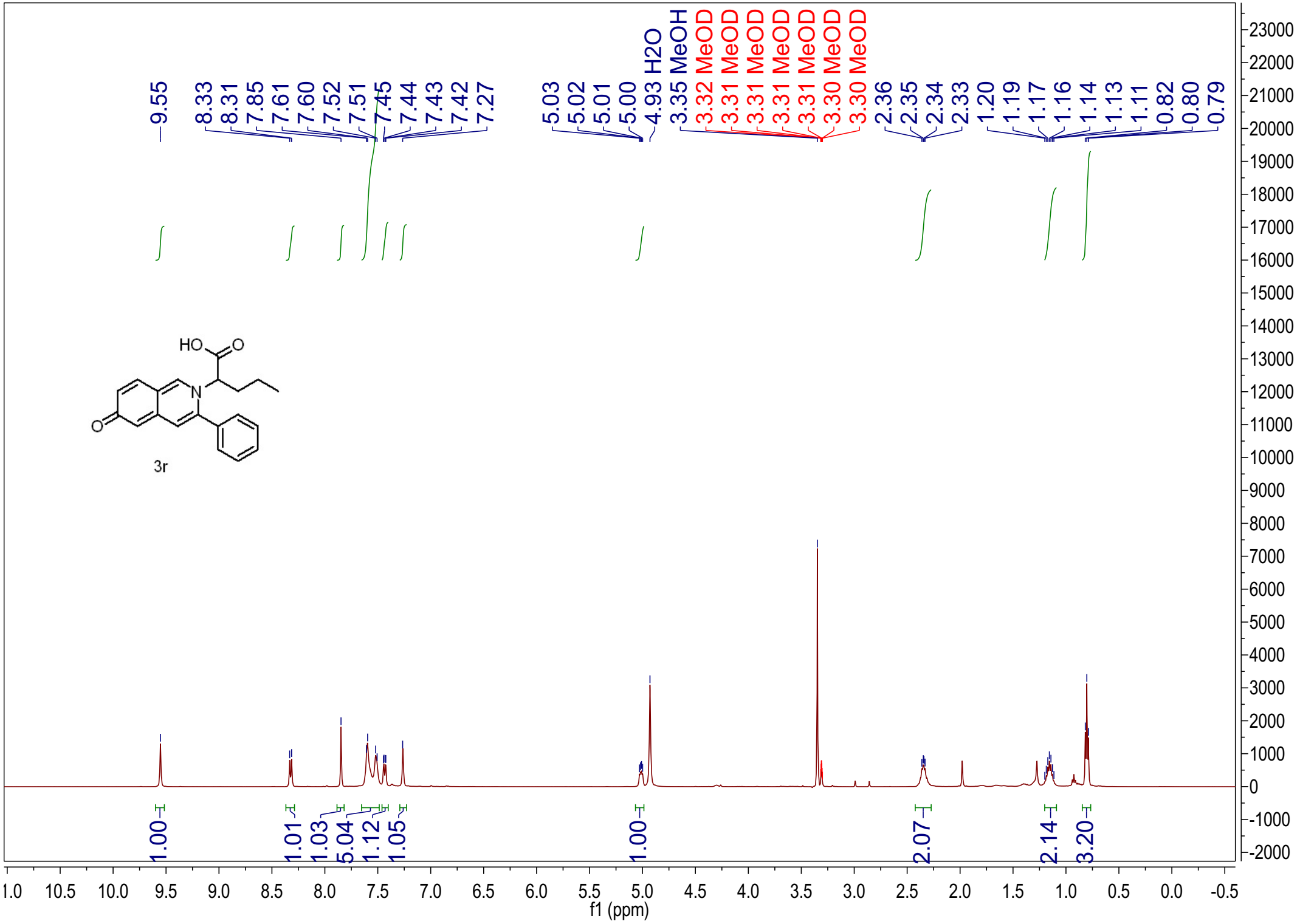
OH
N
O
Ph
3q
f1 (ppm)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5.03
5.02
5.01
5.00
4.93 H2O
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
3.30 MeOD
2.36
2.35
2.34
2.33
1.20
1.19
1.17
1.16
1.14
1.13
1.11
0.82
0.80
0.79
HO
O
N
O
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1.12
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2.07
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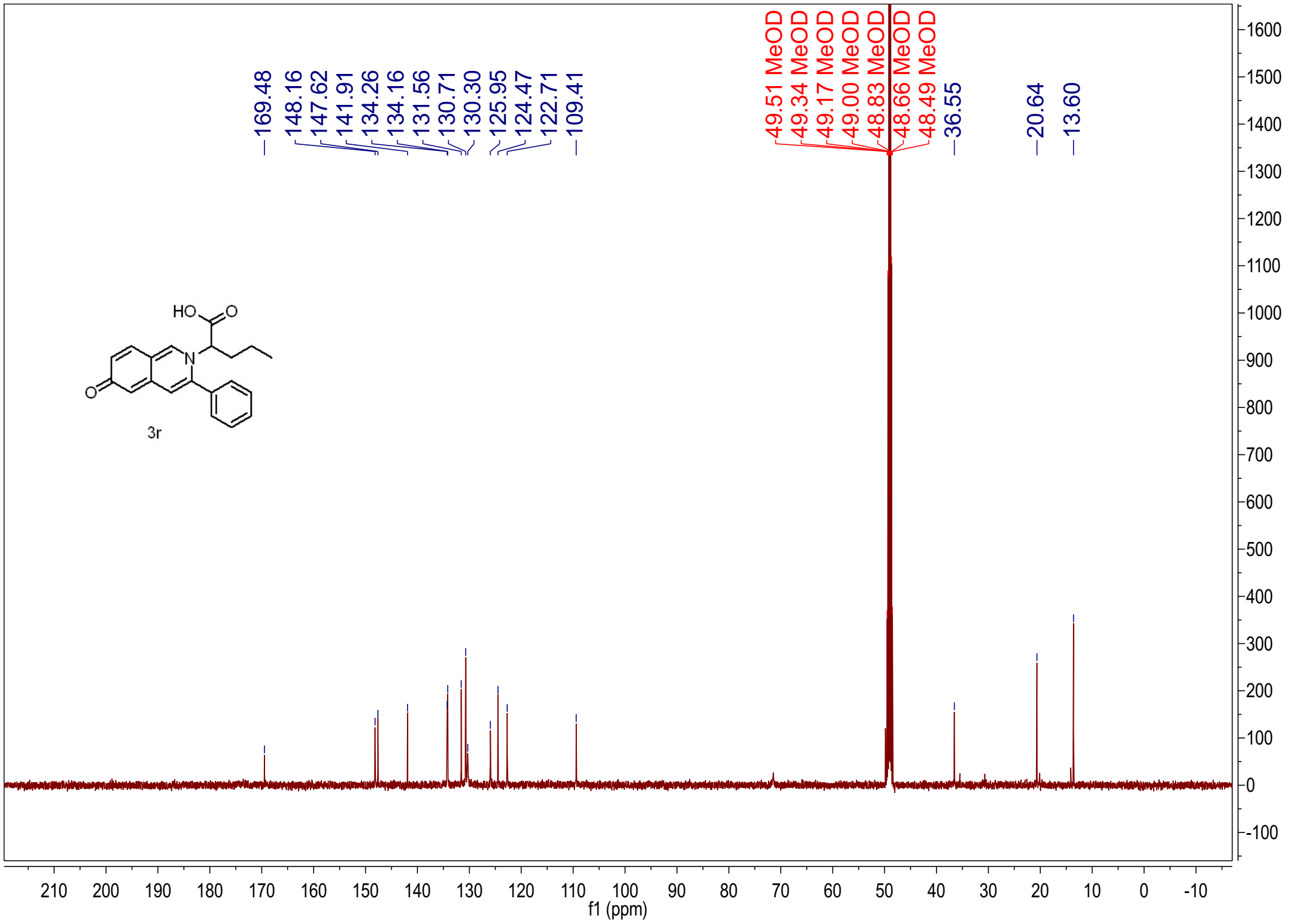
3.20
f1 (ppm)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49.34 MeOD
49.17 MeOD
49.00 MeOD
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48.49 MeOD
36.55
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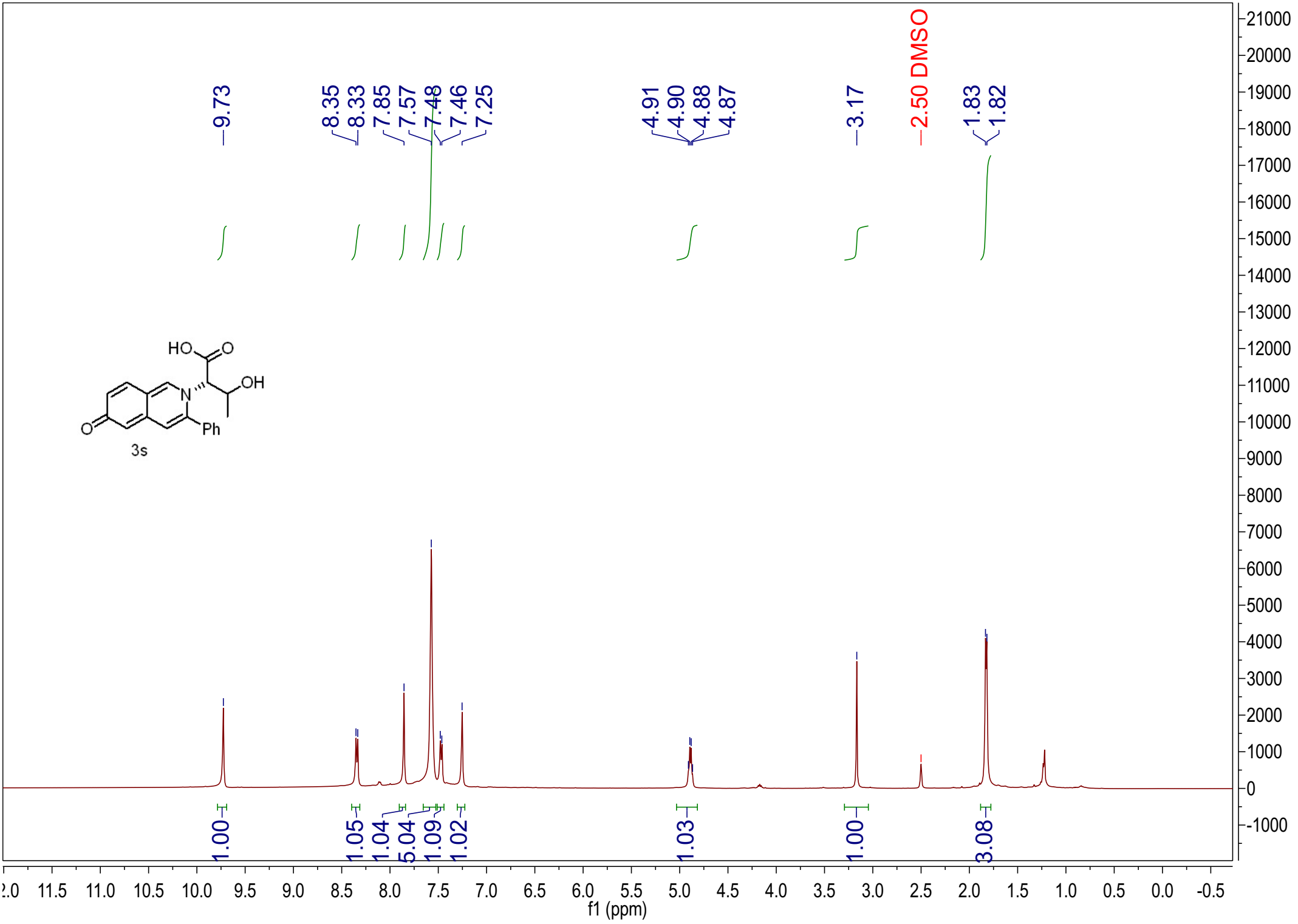
HO
O
N
O
3r
f1 (ppm)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4.88
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3.17
2.50 DMSO
1.83
1.82
HO
O
OH
N
Ph
O
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1.04
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1.03
1.00
3.08
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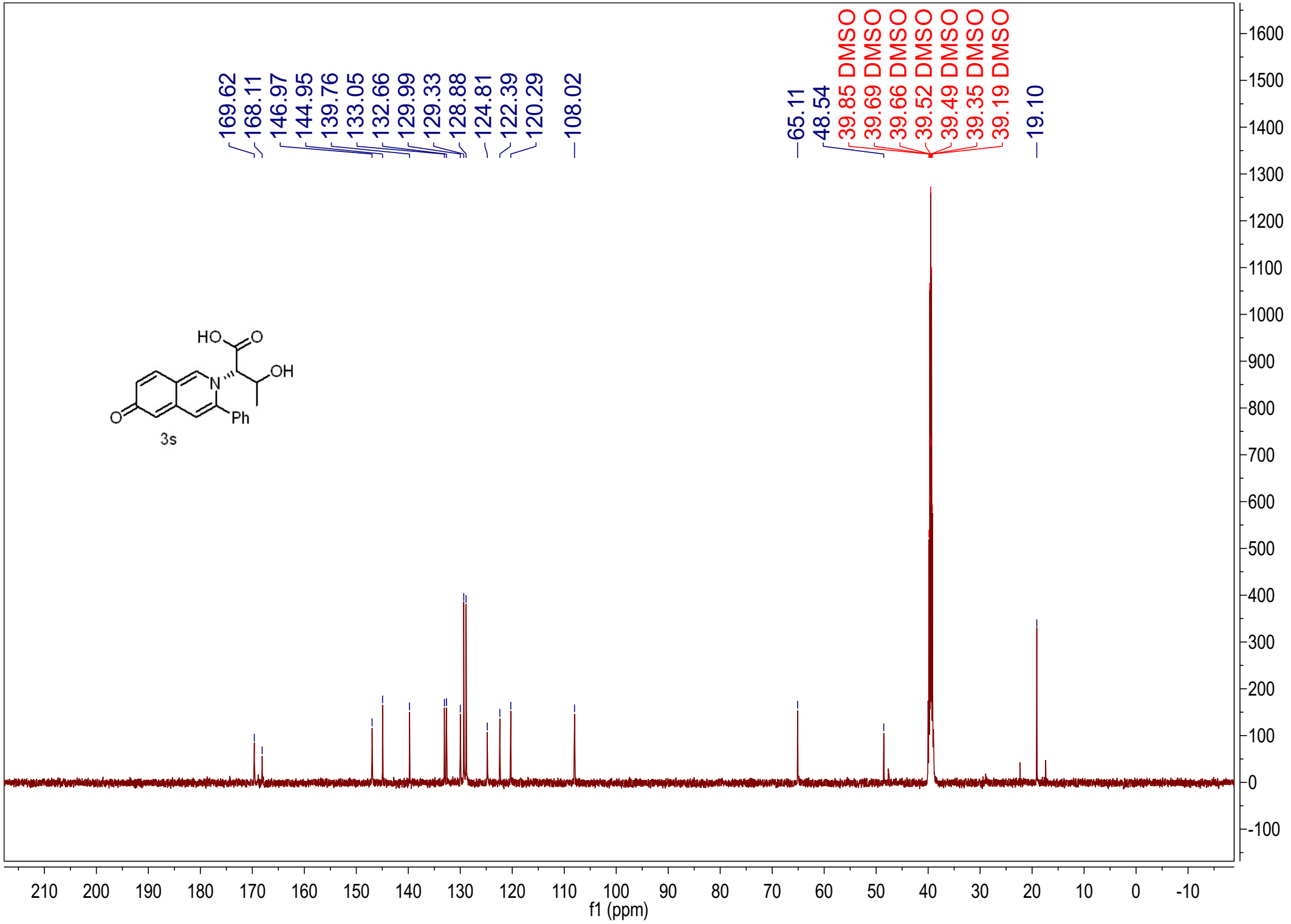
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108.02
65.11
48.54
39.85 DMSO
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39.66 DMSO
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39.35 DMSO
39.19 DMSO
19.10
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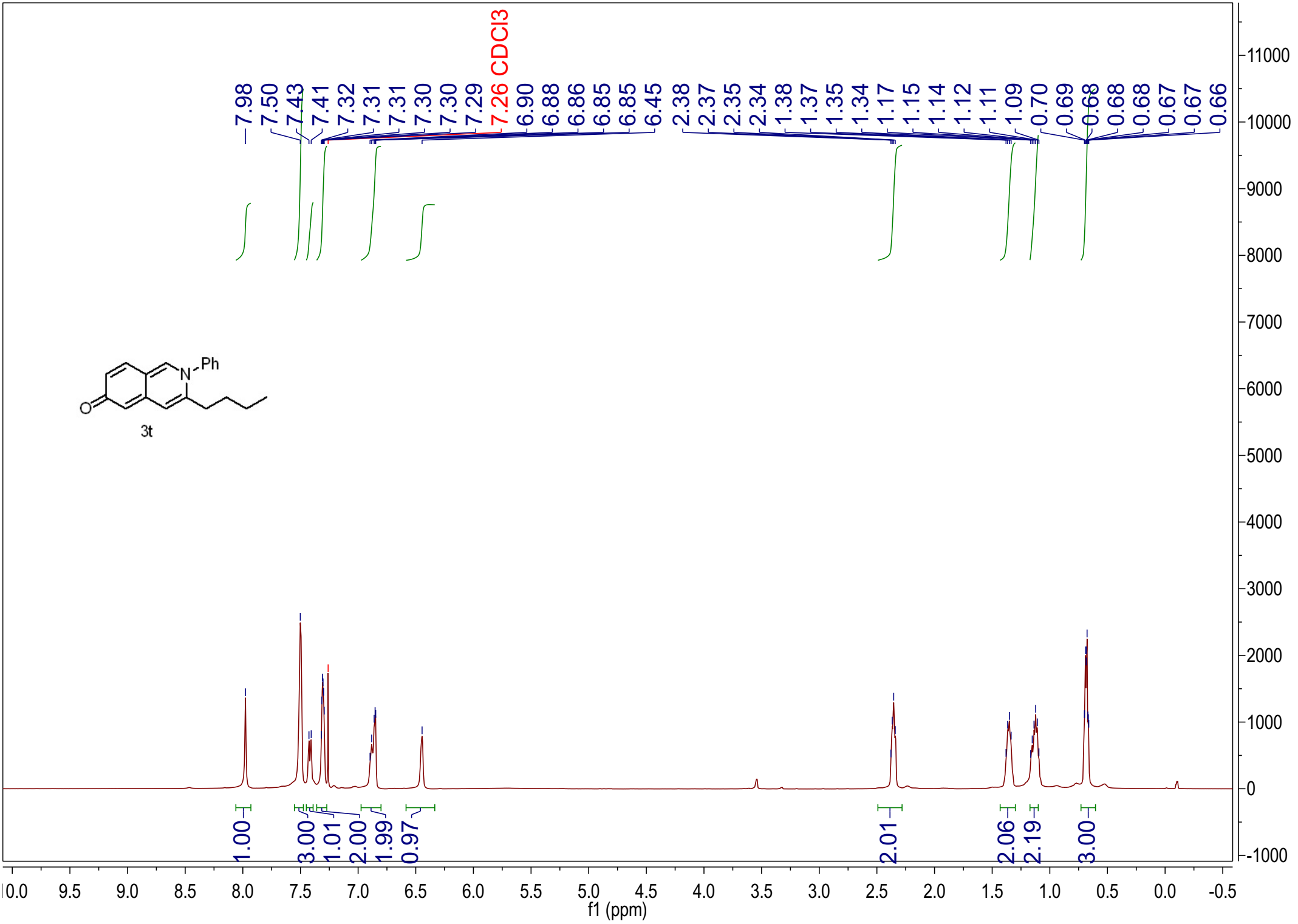
O
OH
N
Ph
O
3s
f1 (ppm)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6.86
6.85
6.85
6.45
2.38
2.37
2.35
2.34
1.38
1.37
1.35
1.34
1.17
1.15
1.14
1.12
1.11
1.09
0.70
0.69
0.68
0.68
0.68
0.67
0.67
0.66
Ph
N
O
3t
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1.01
2.00
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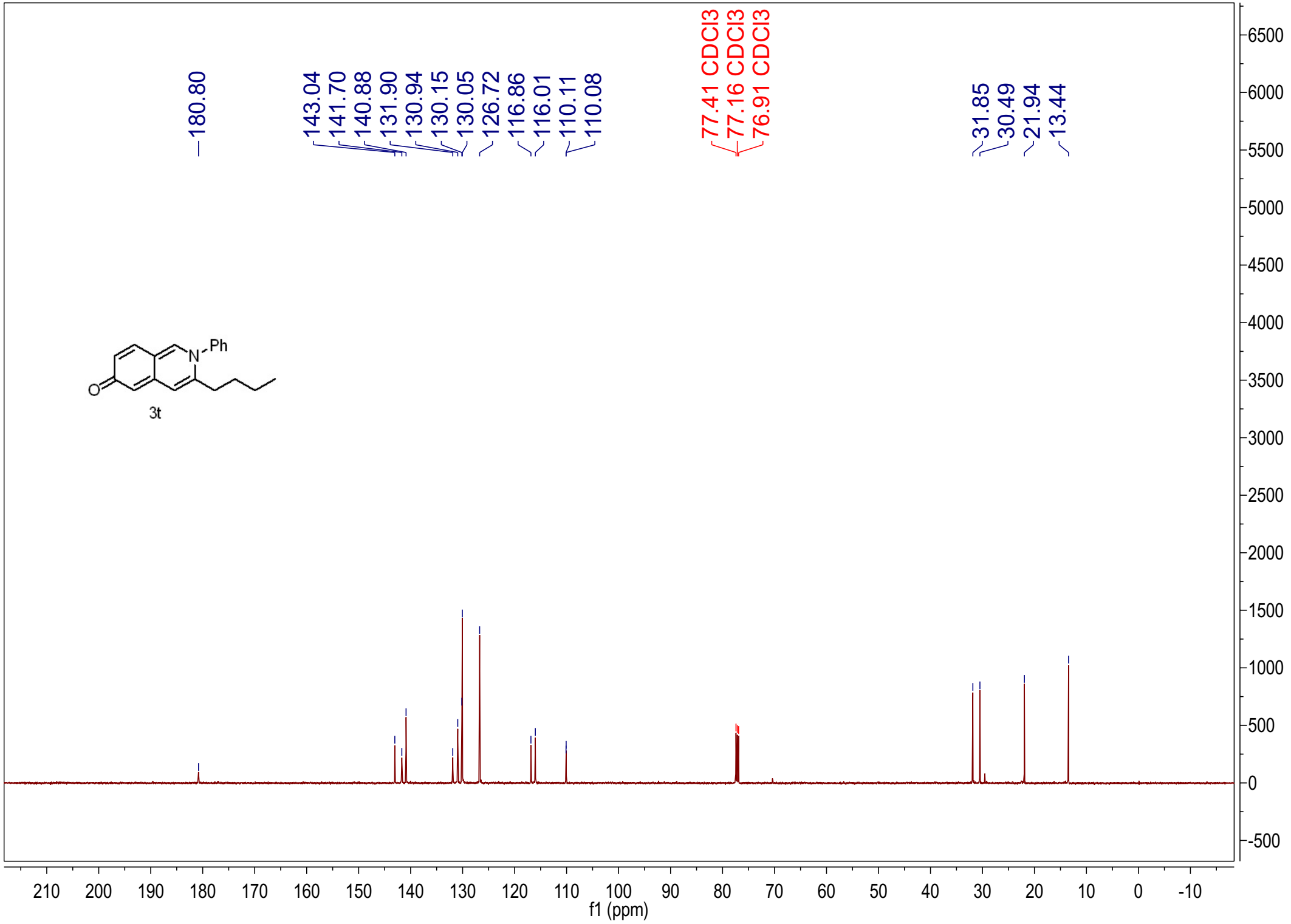
2.06
2.19
3.00
f1 (ppm)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130.05
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116.01
110.11
110.08
77.41 CDCl3
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76.91 CDCl3
31.85
30.49
21.94
13.44
Ph
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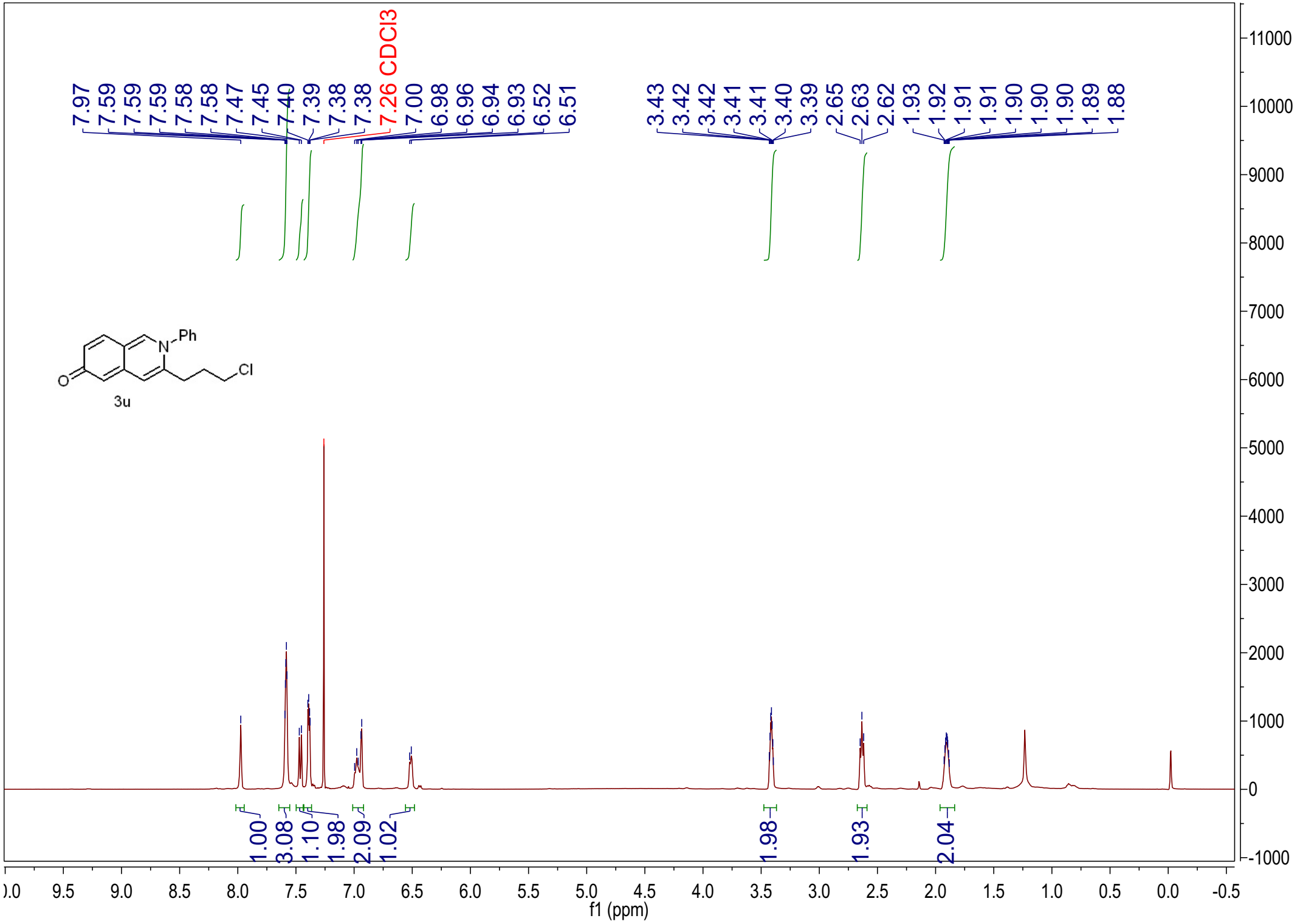
O
3t
f1 (ppm)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7.26 CDCl3
7.00
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6.96
6.94
6.93
6.52
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3.43
3.42
3.42
3.41
3.41
3.40
3.39
2.65
2.63
2.62
1.93
1.92
1.91
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1.90
1.90
1.90
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Ph
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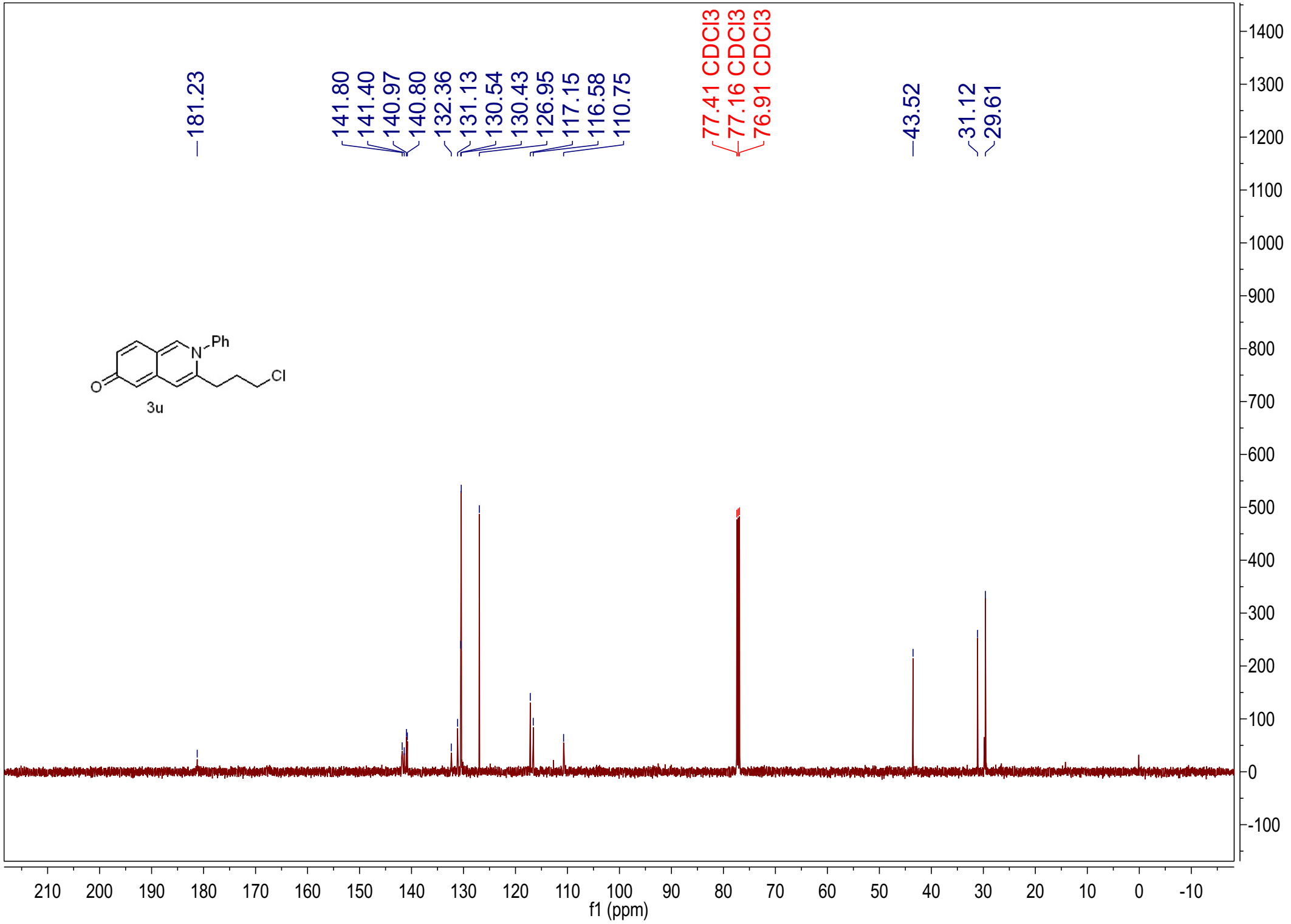
2.04
f1 (ppm)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117.15
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110.75
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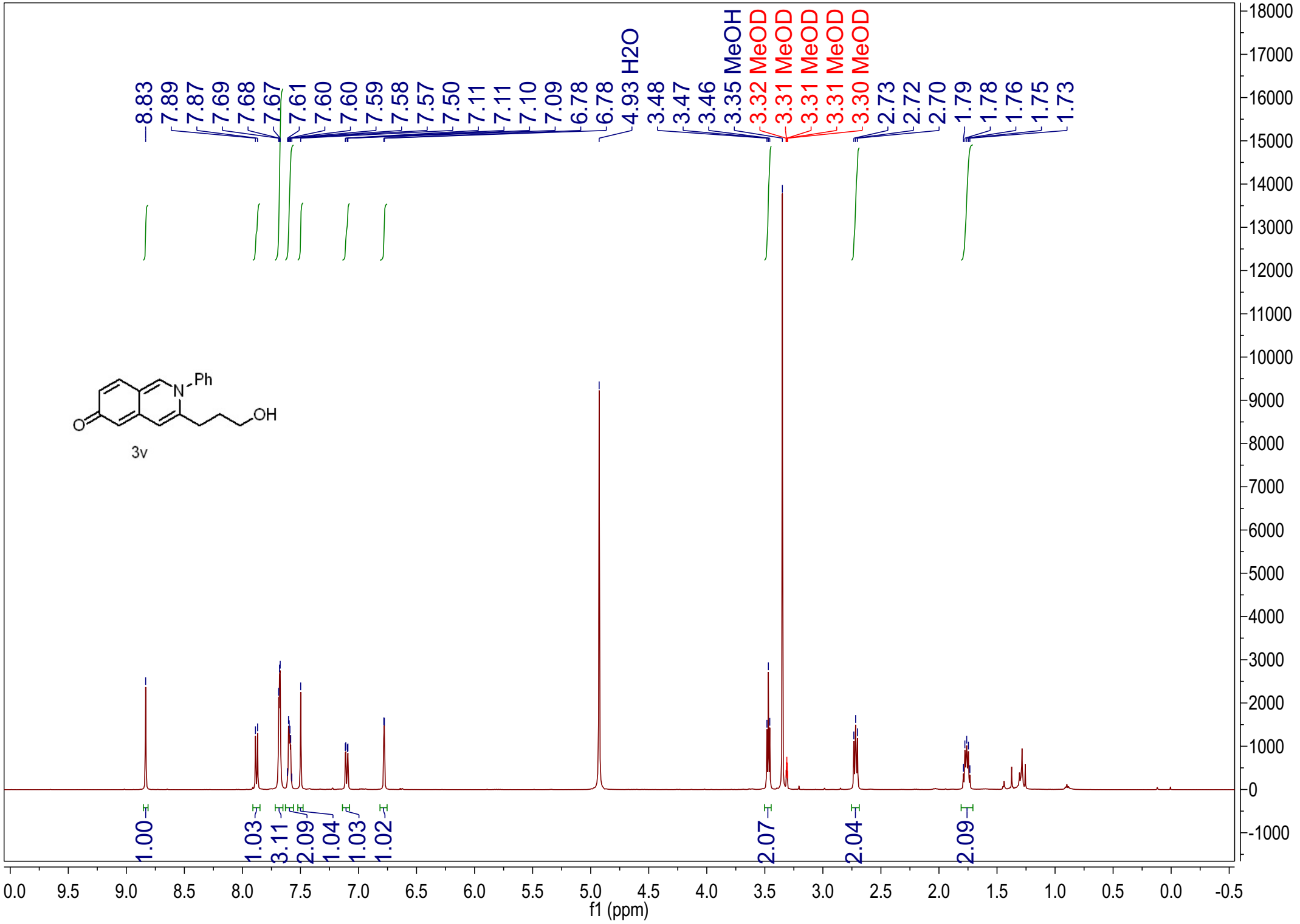
77.16 CDCl3
76.91 CDCl3
43.52
31.12
29.61
N
Ph
O
Cl
3u
f1 (ppm)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7.50
7.11
7.11
7.10
7.09
6.78
6.78
4.93 H2O
3.48
3.47
3.46
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3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
2.73
2.72
2.70
1.79
1.78
1.76
1.75
1.73
Ph
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OH
O
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1.04
1.03
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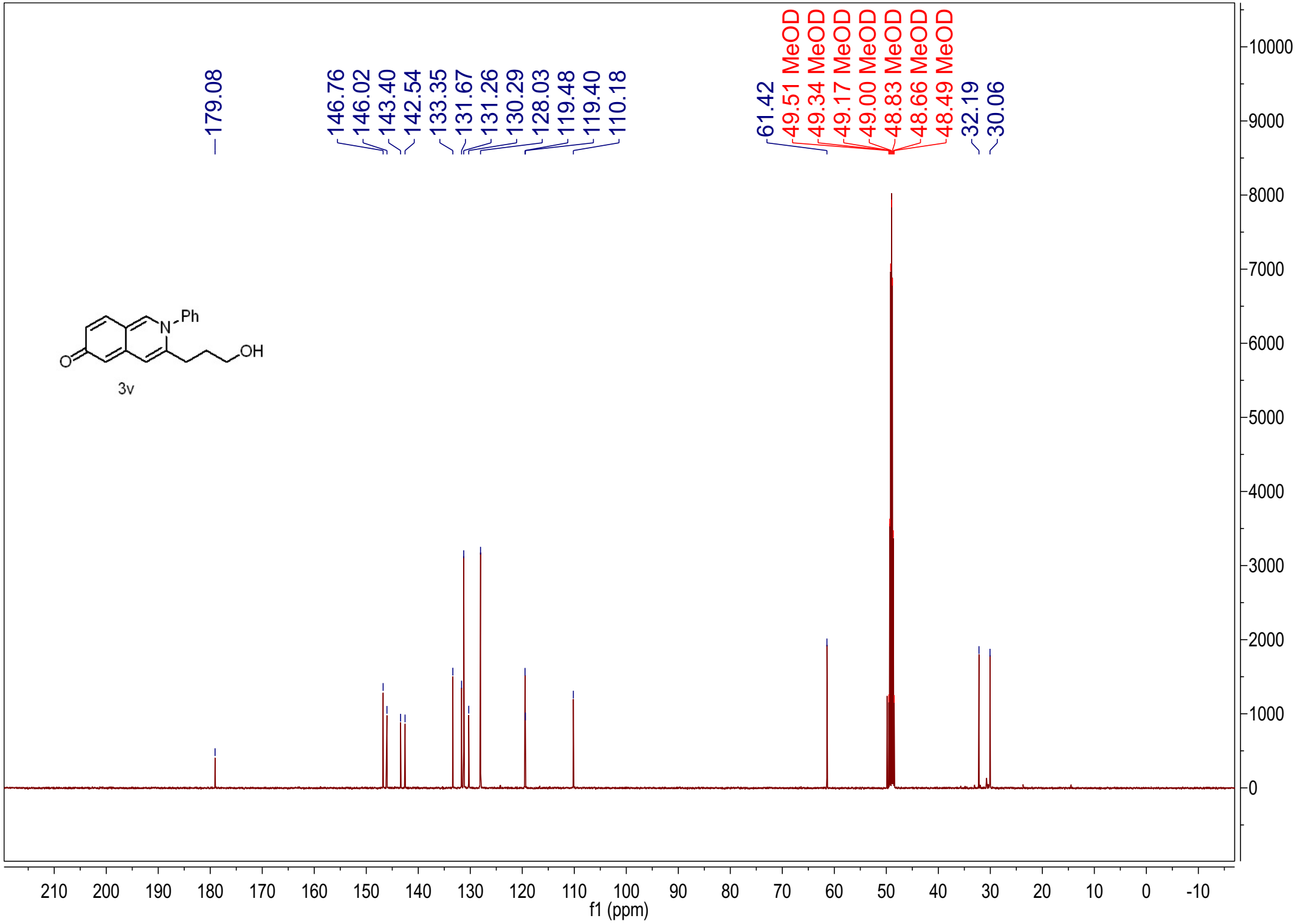
2.04
2.09
f1 (ppm)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128.03
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119.40
110.18
61.42
49.51 MeOD
49.34 MeOD
49.17 MeOD
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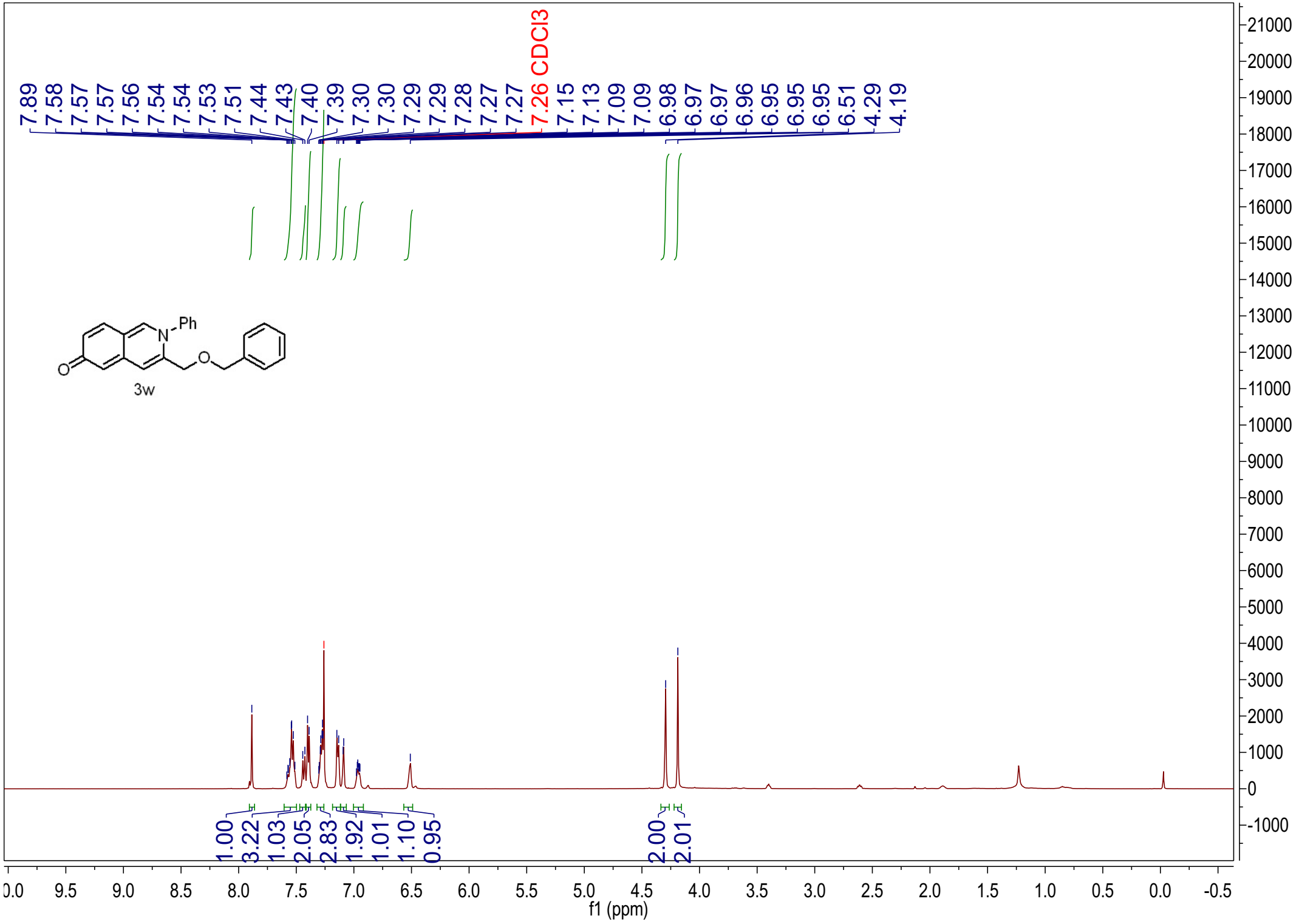
48.66 MeOD
48.49 MeOD
32.19
30.06
Ph
N
OH
O
3v
f1 (ppm)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7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.26 CDCl3
7.15
7.13
7.09
7.09
6.98
6.97
6.97
6.96
6.95
6.95
6.95
6.51
4.29
4.19
Ph
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O
O
3w
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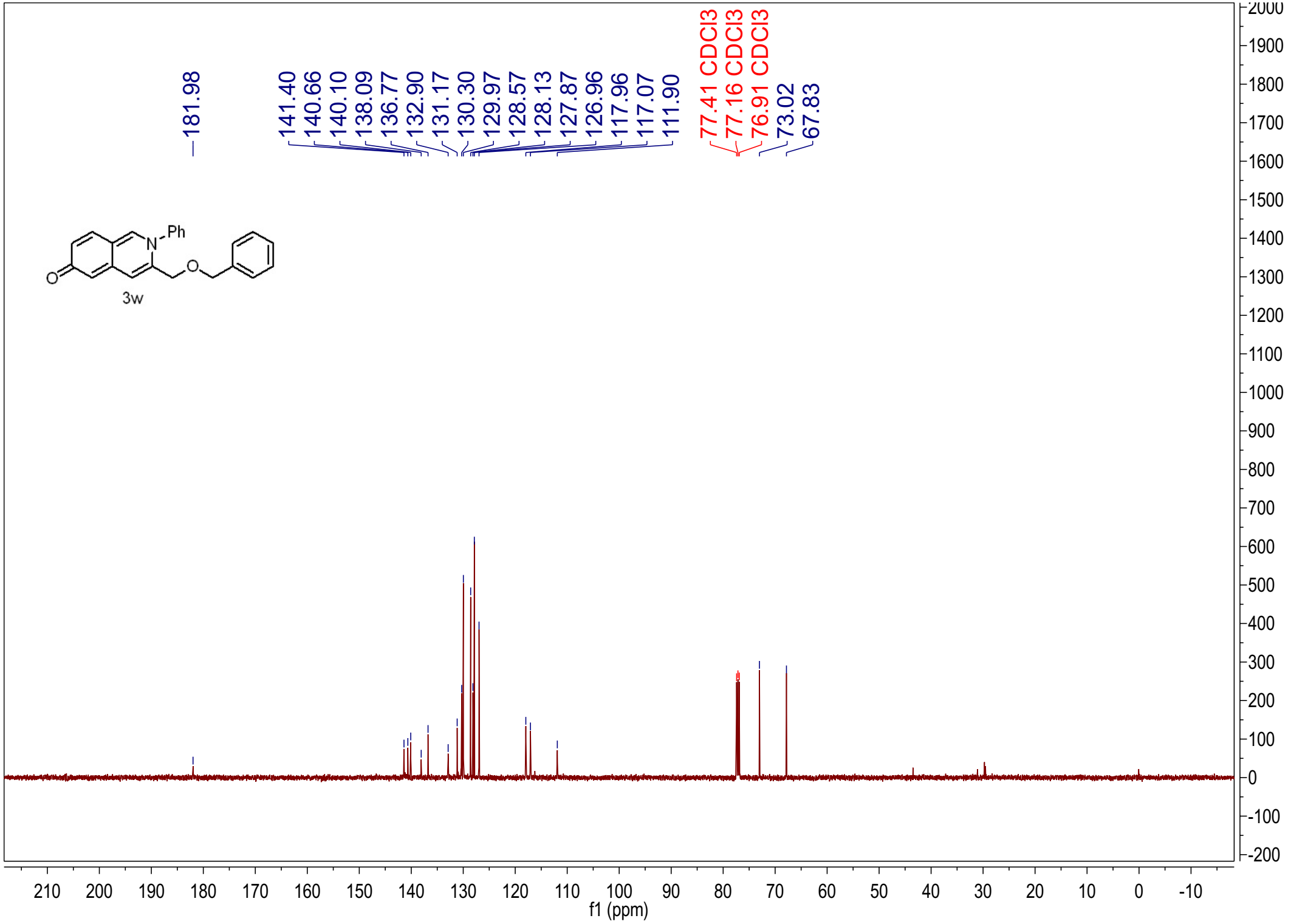
2.01
f1 (ppm)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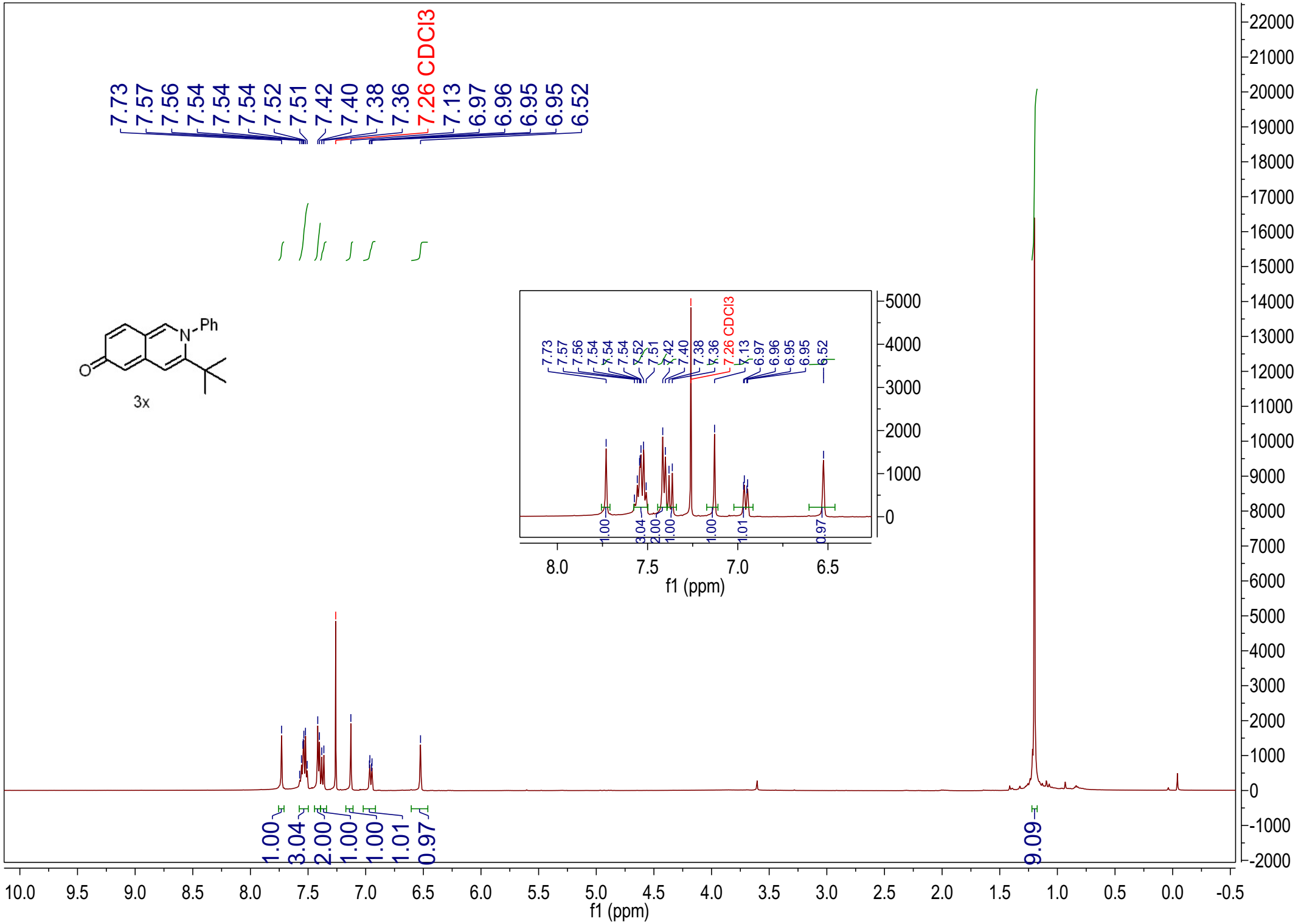
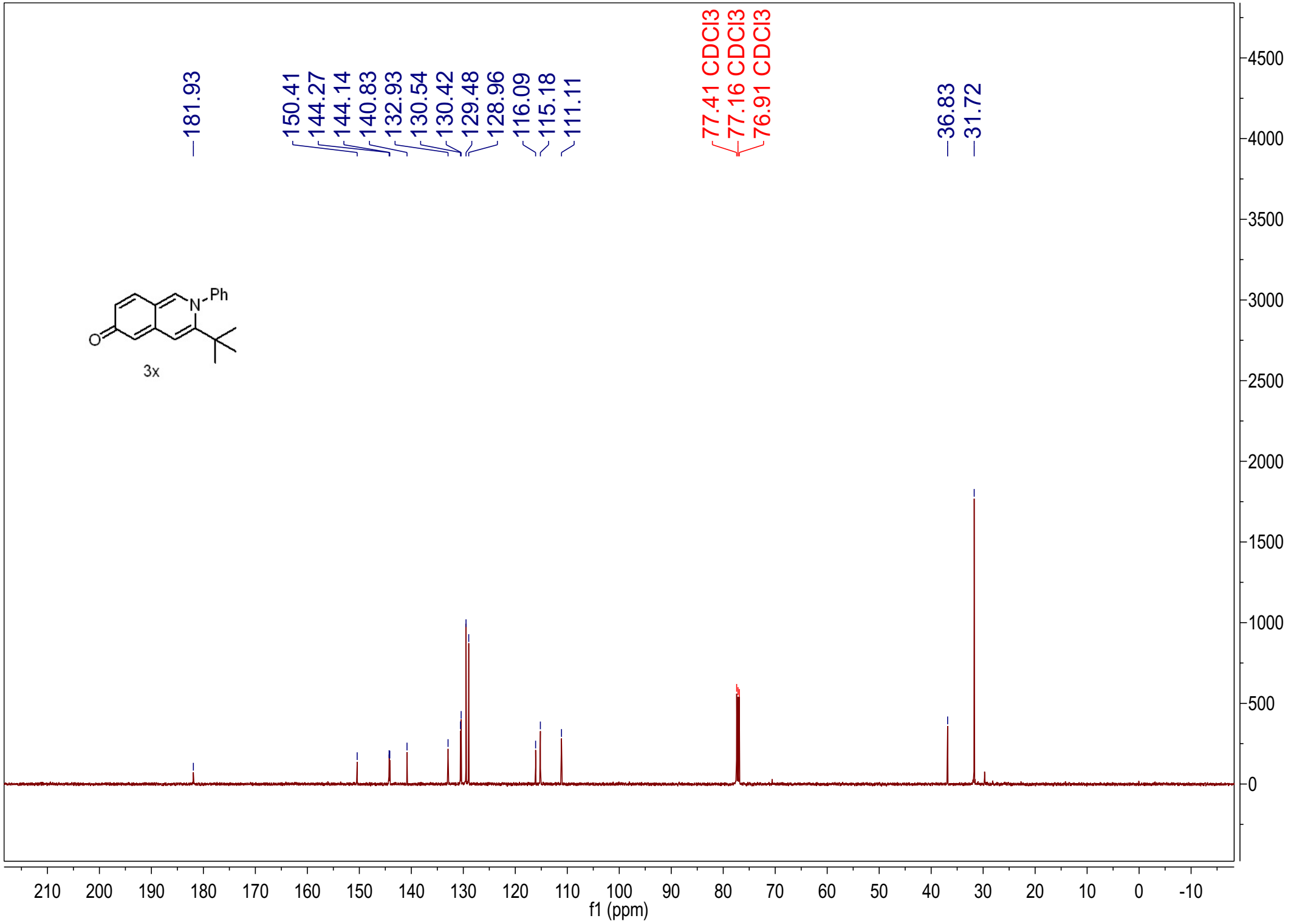
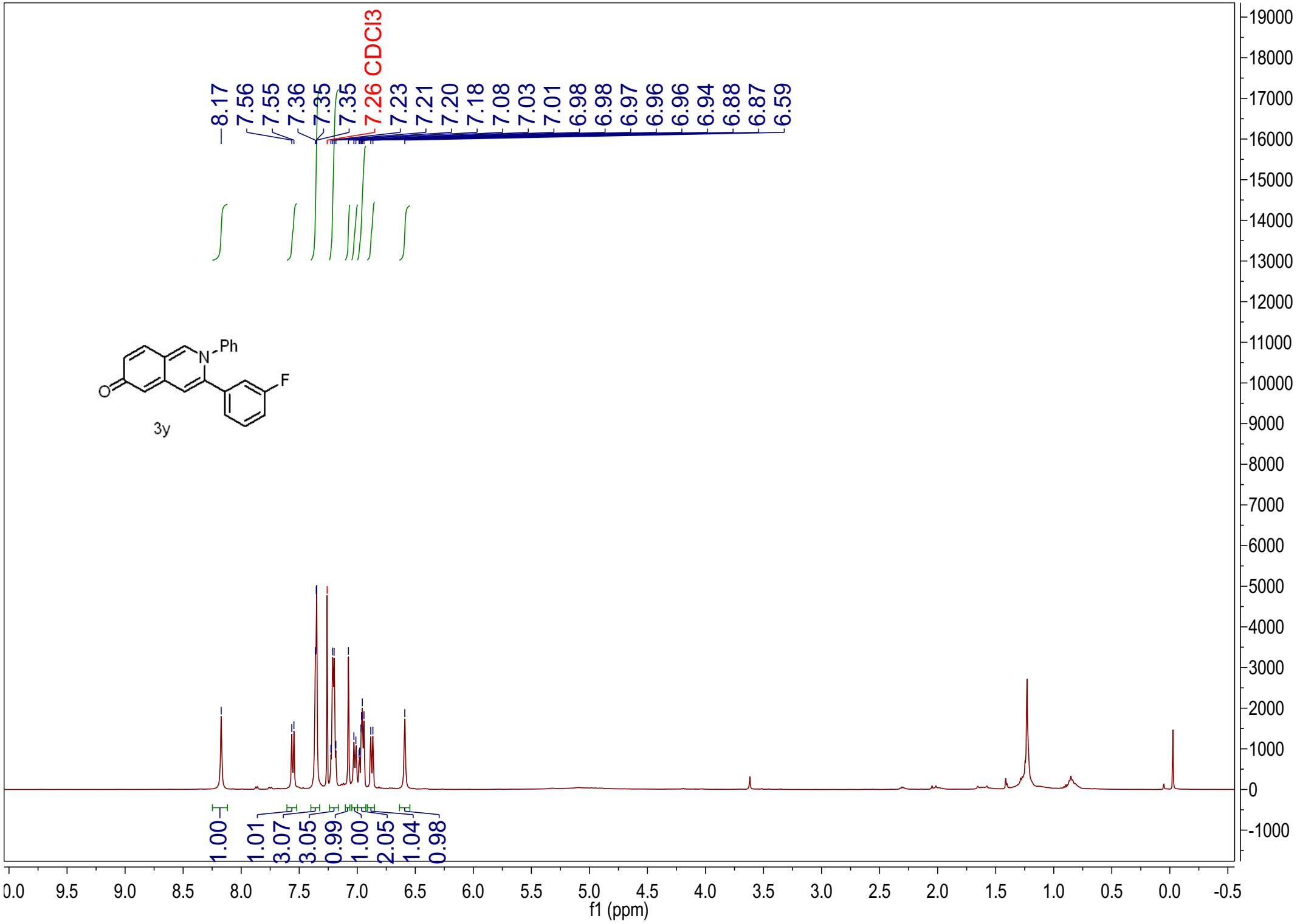
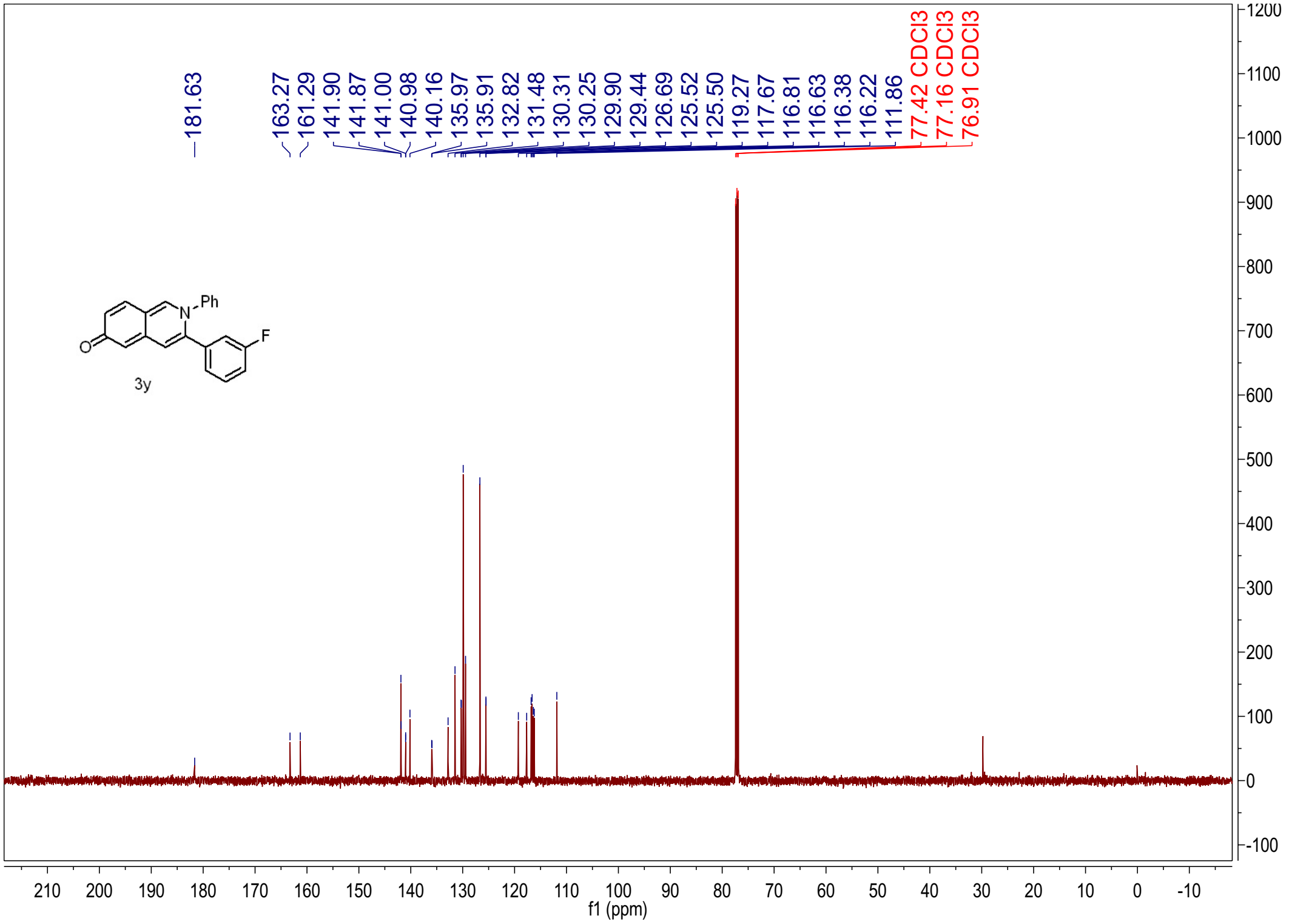
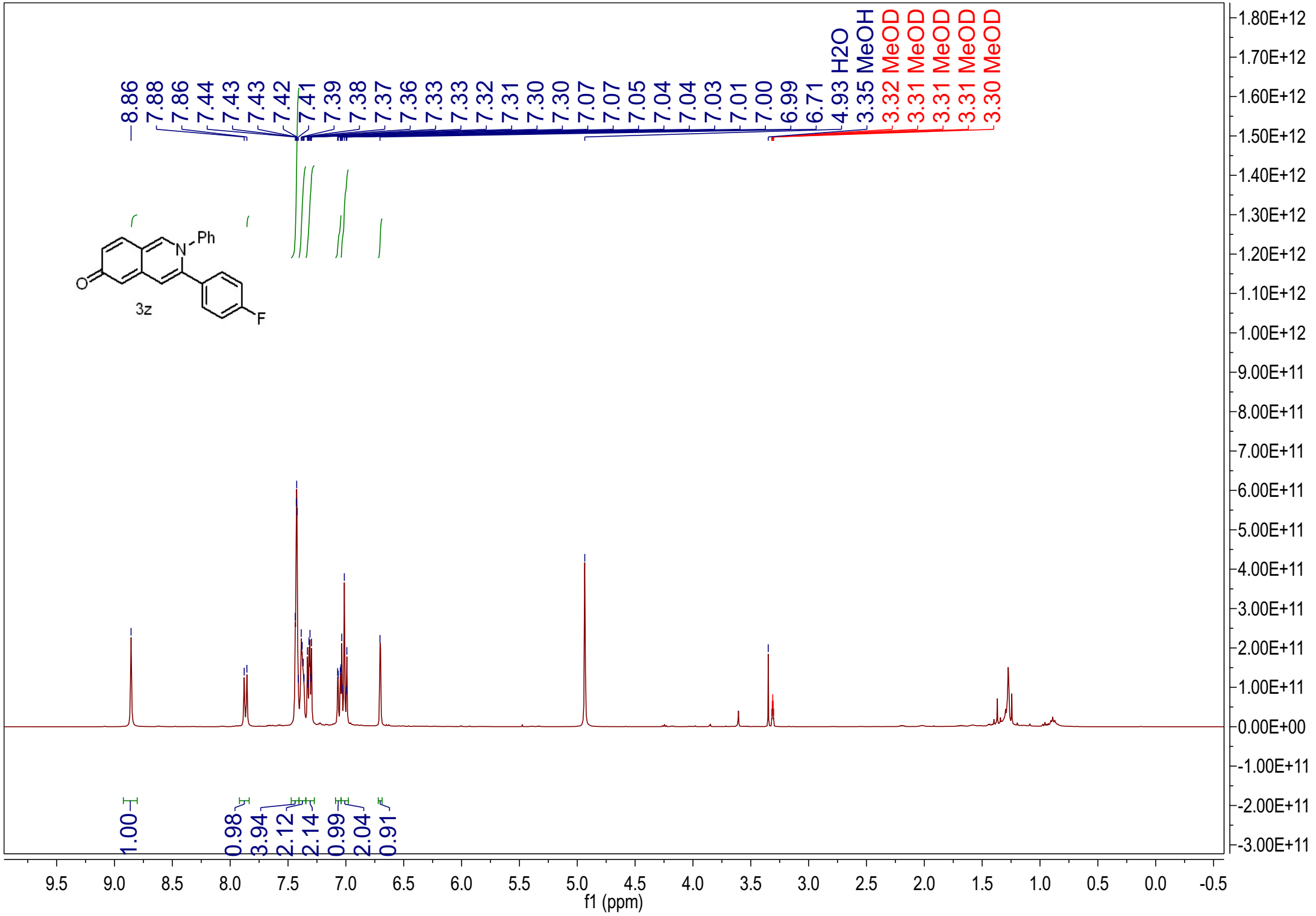
128.13
127.87
126.96
117.96
117.07
111.90
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
73.02
67.83
Ph
N
O
O
3w
f1 (ppm)

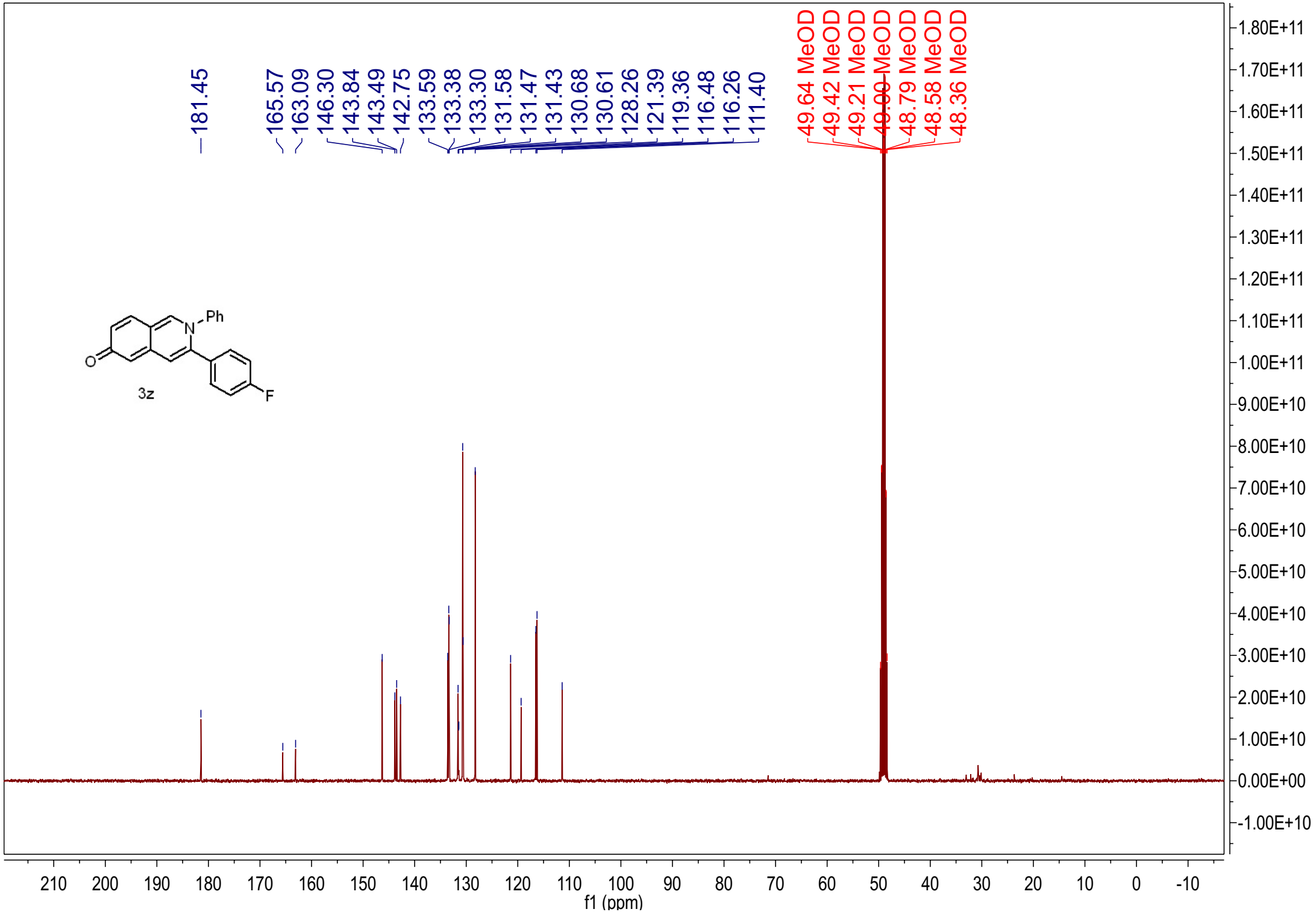

7.73
7.57
7.56
7.54
7.54
7.54
7.52
7.51
7.42
7.40
7.38
7.36
7.26 CDCl3
7.13
6.97
6.96
6.95
6.95
6.52
Ph
N
O
3x
1.00
3.04
2.00
1.00
1.00
1.01
0.97
9.09
f1 (ppm)

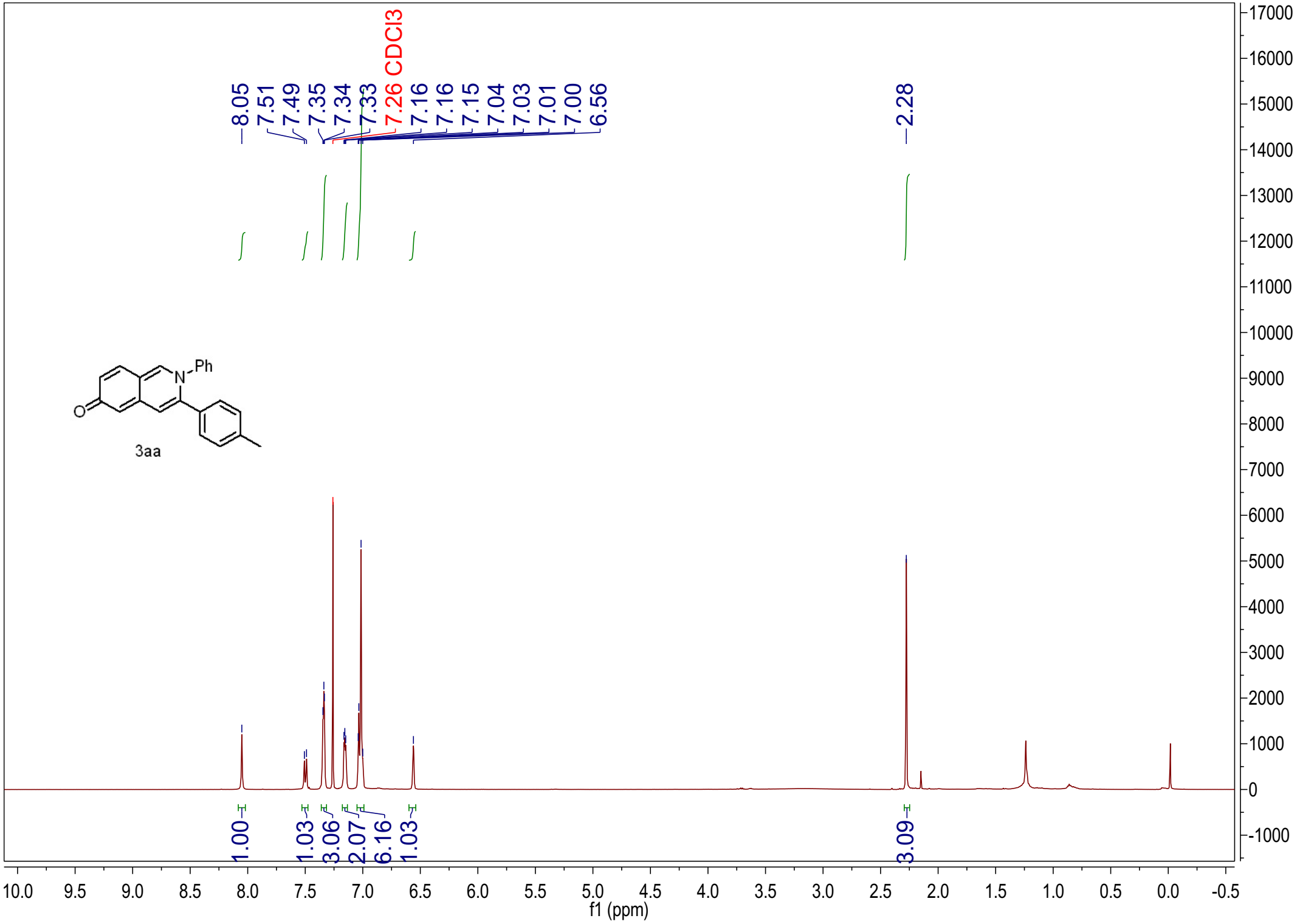

181.93
150.41
144.27
144.14
140.83
132.93
130.54
130.42
129.48
128.96
116.09
115.18
111.11
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
36.83
31.72
Ph
N
O
3x
4500
4000
3500
3000
2500
2000
1500
1000
500
0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

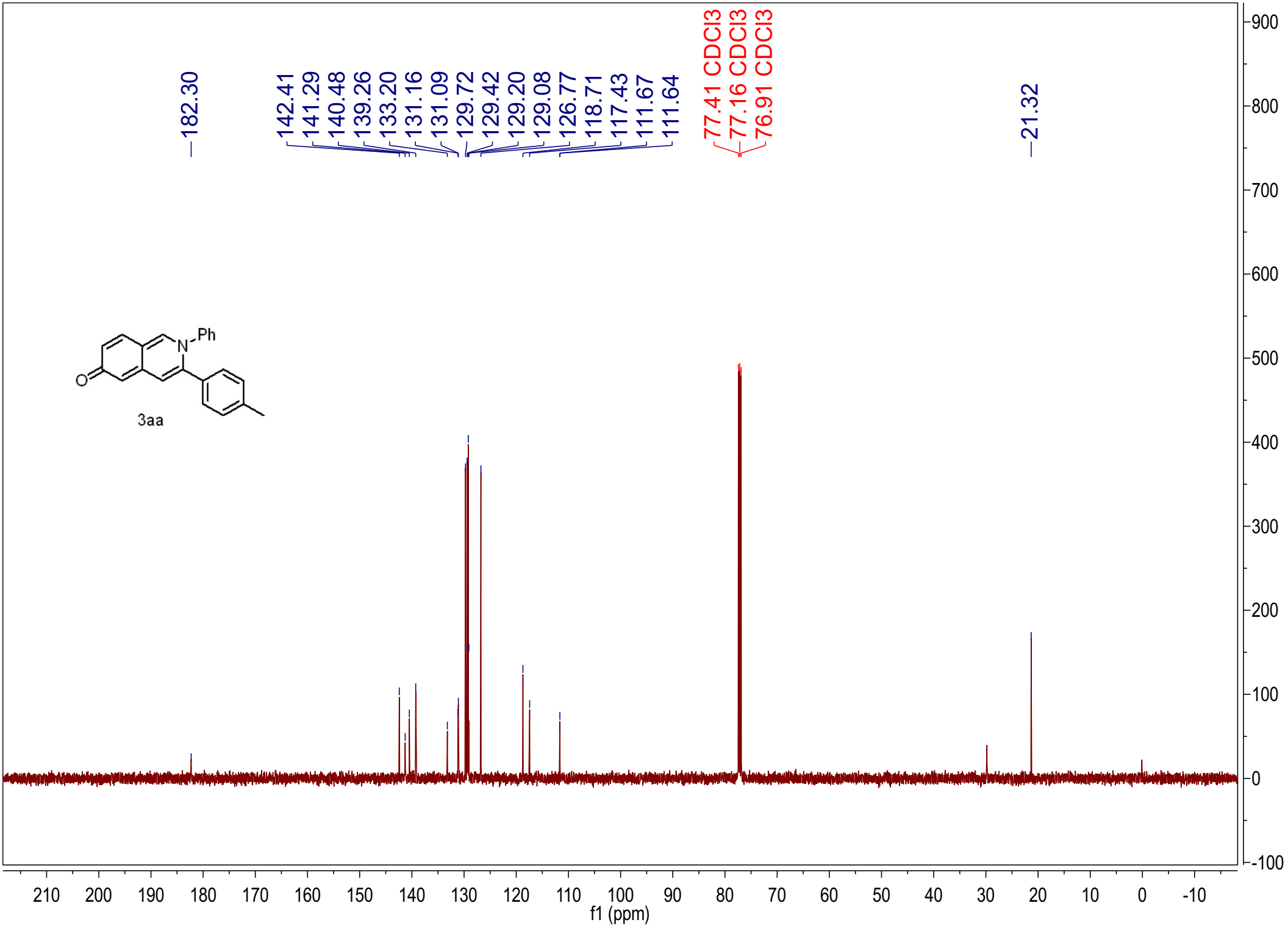

8.17
7.56
7.55
7.36
7.35
7.35
7.26 CDCl3
7.23
7.21
7.20
7.18
7.08
7.03
7.01
6.98
6.98
6.97
6.96
6.96
6.94
6.88
6.87
6.59
Ph
N
O
F
3y
1.00
1.01
3.07
3.05
0.99
1.00
2.05
1.04
0.98
f1 (ppm)

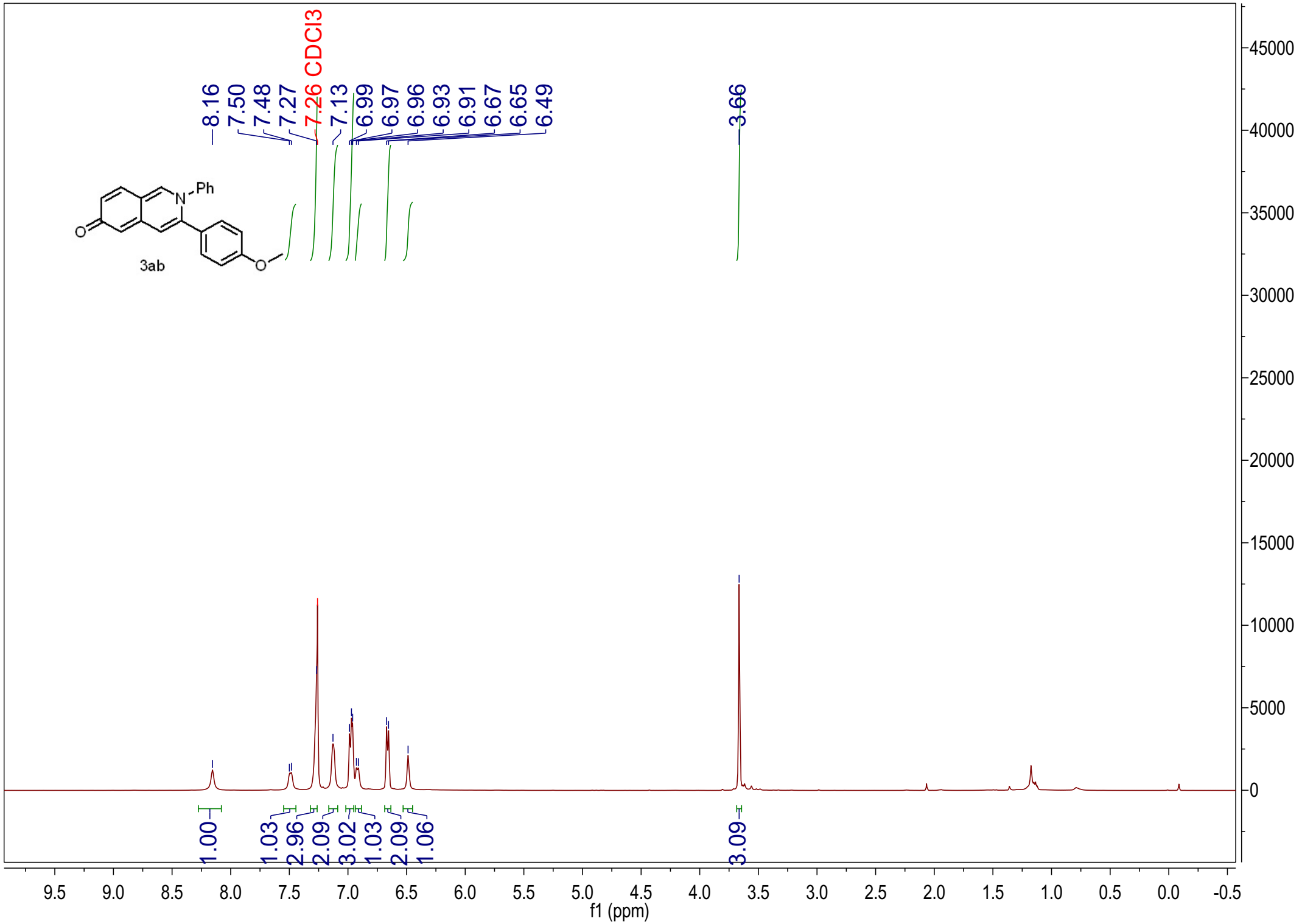

181.63
163.27
161.29
141.90
141.87
141.00
140.98
140.16
135.97
135.91
132.82
131.48
130.31
130.25
129.90
129.44
126.69
125.52
125.50
119.27
117.67
116.81
116.63
116.38
116.22
111.86
77.42 CDCl3
77.16 CDCl3
76.91 CDCl3
Ph
N
O
F
3y
f1 (ppm)

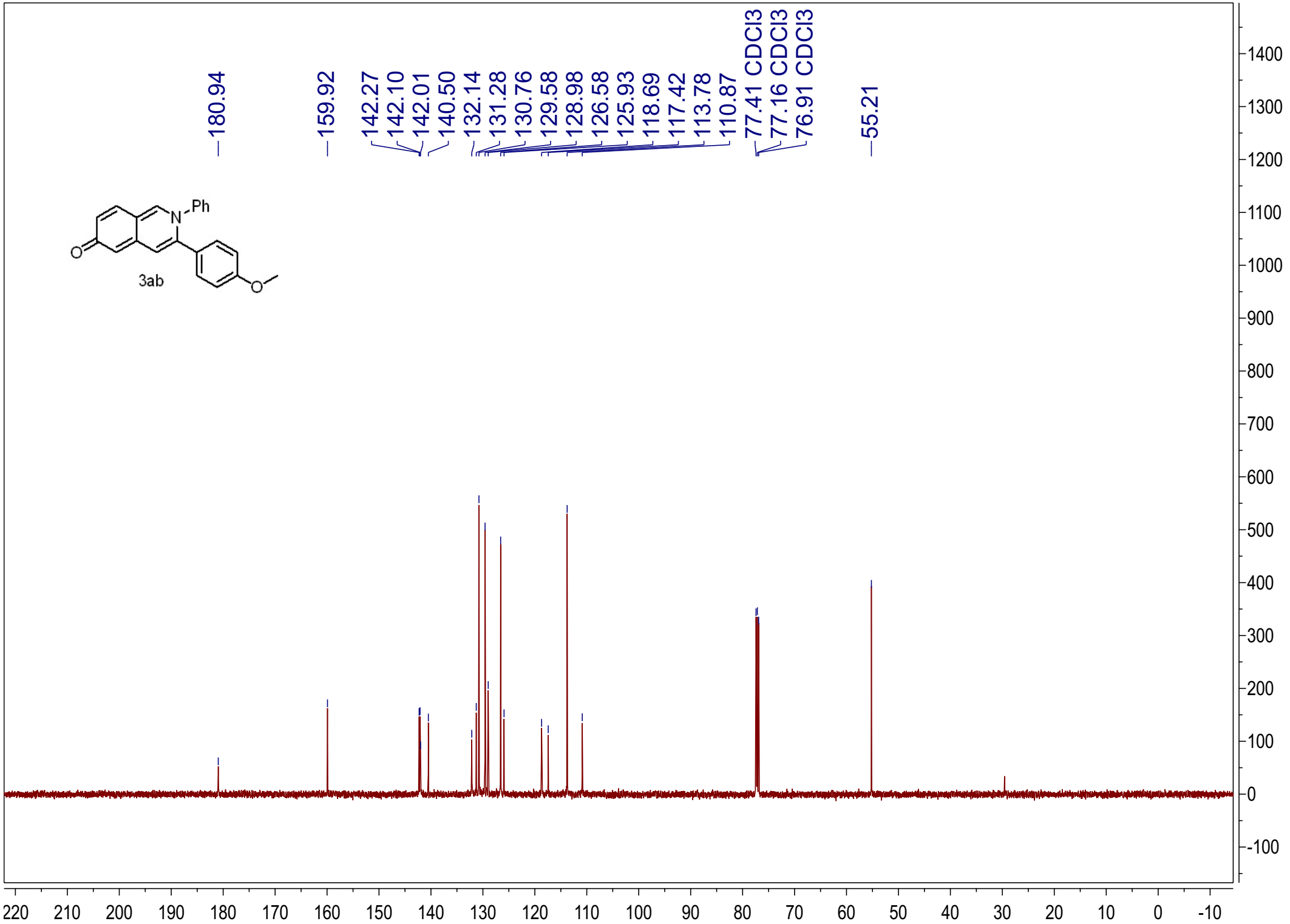

8.86
7.88
7.86
7.44
7.43
7.43
7.42
7.41
7.39
7.38
7.37
7.36
7.33
7.33
7.32
7.31
7.30
7.30
7.07
7.07
7.05
7.04
7.04
7.03
7.01
7.00
6.99
6.71
4.93 H2O
3.35 MeOH
3.32 MeOD
3.31 MeOD
3.31 MeOD
3.31 MeOD
3.30 MeOD
Ph
N
O
F
3z
1.00
0.98
3.94
2.12
2.14
0.99
2.04
0.91
f1 (ppm)

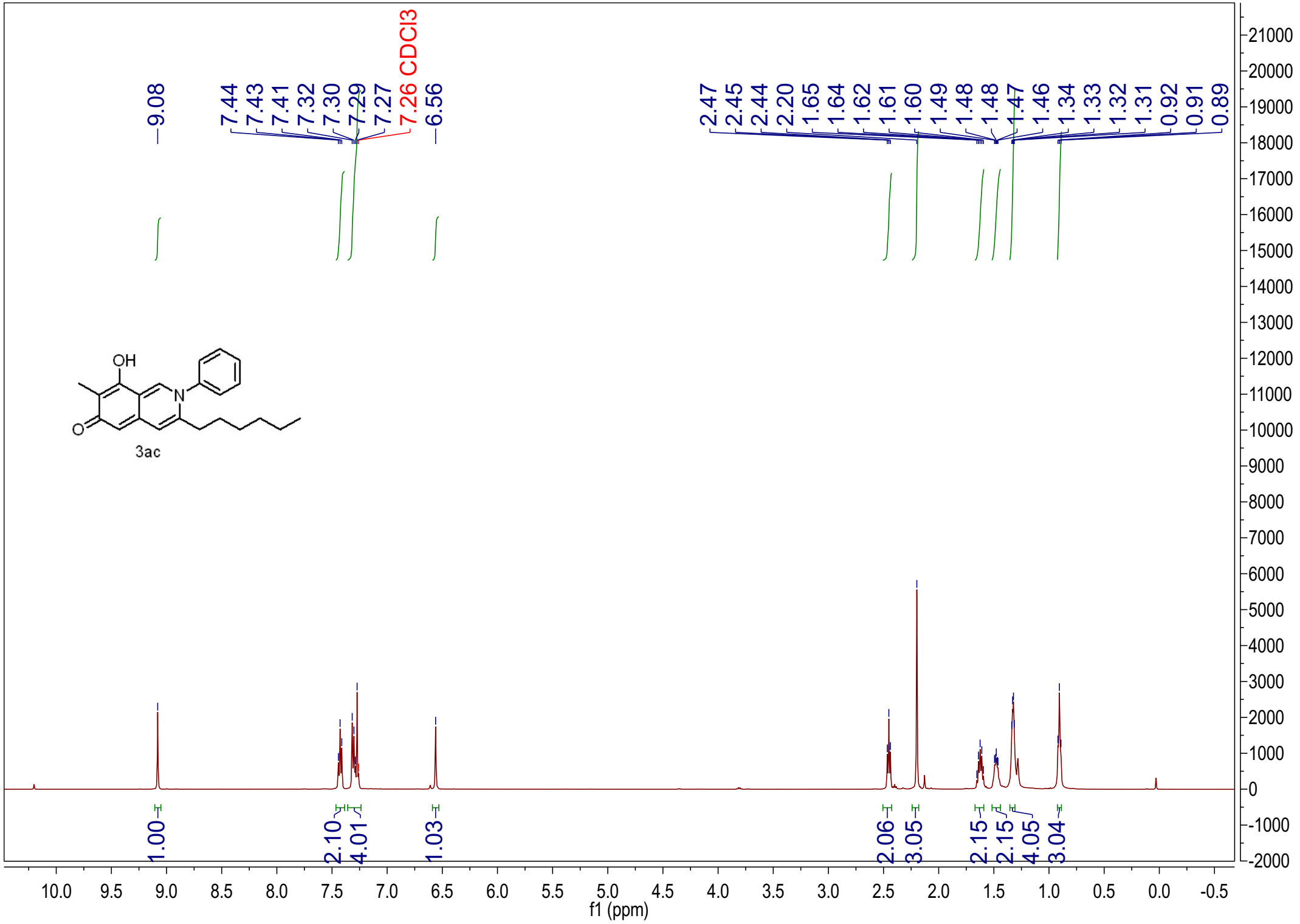

181.45
165.57
163.09
146.30
143.84
143.49
142.75
133.59
133.38
133.30
131.58
131.47
131.43
130.68
130.61
128.26
121.39
119.36
116.48
116.26
111.40
49.64 MeOD
49.42 MeOD
49.21 MeOD
49.00 MeOD
48.79 MeOD
48.58 MeOD
48.36 MeOD
Ph
N
O
F
3z
1.80E+11
1.70E+11
1.60E+11
1.50E+11
1.40E+11
1.30E+11
1.20E+11
1.10E+11
1.00E+11
9.00E+10
8.00E+10
7.00E+10
6.00E+10
5.00E+10
4.00E+10
3.00E+10
2.00E+10
1.00E+10
0.00E+00
-1.00E+10
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)

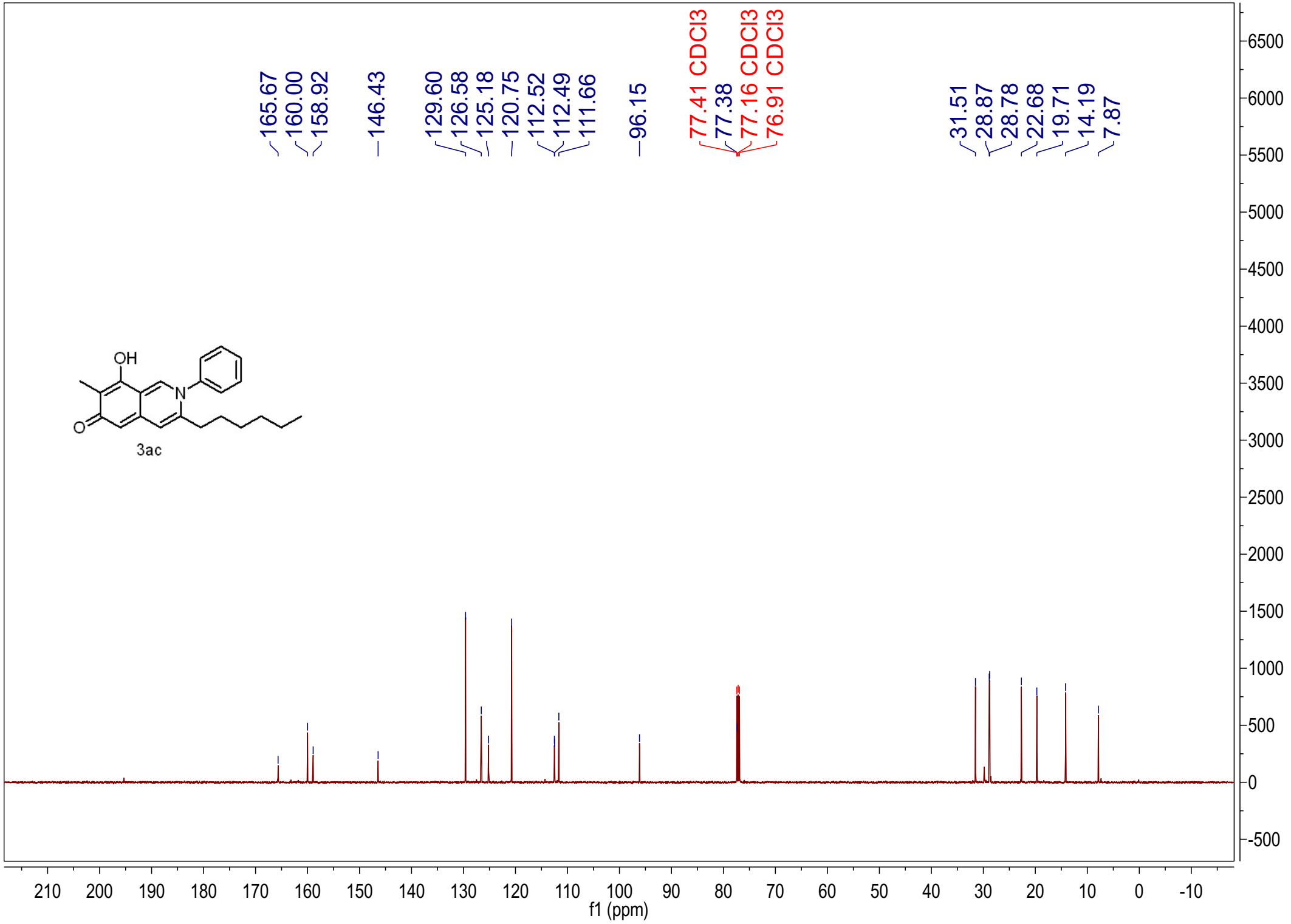

8.05
7.51
7.49
7.35
7.34
7.33
7.26 CDCl3
7.16
7.16
7.15
7.04
7.03
7.01
7.00
6.56
2.28
Ph
N
O
3aa
1.00
1.03
3.06
2.07
6.16
1.03
3.09
f1 (ppm)

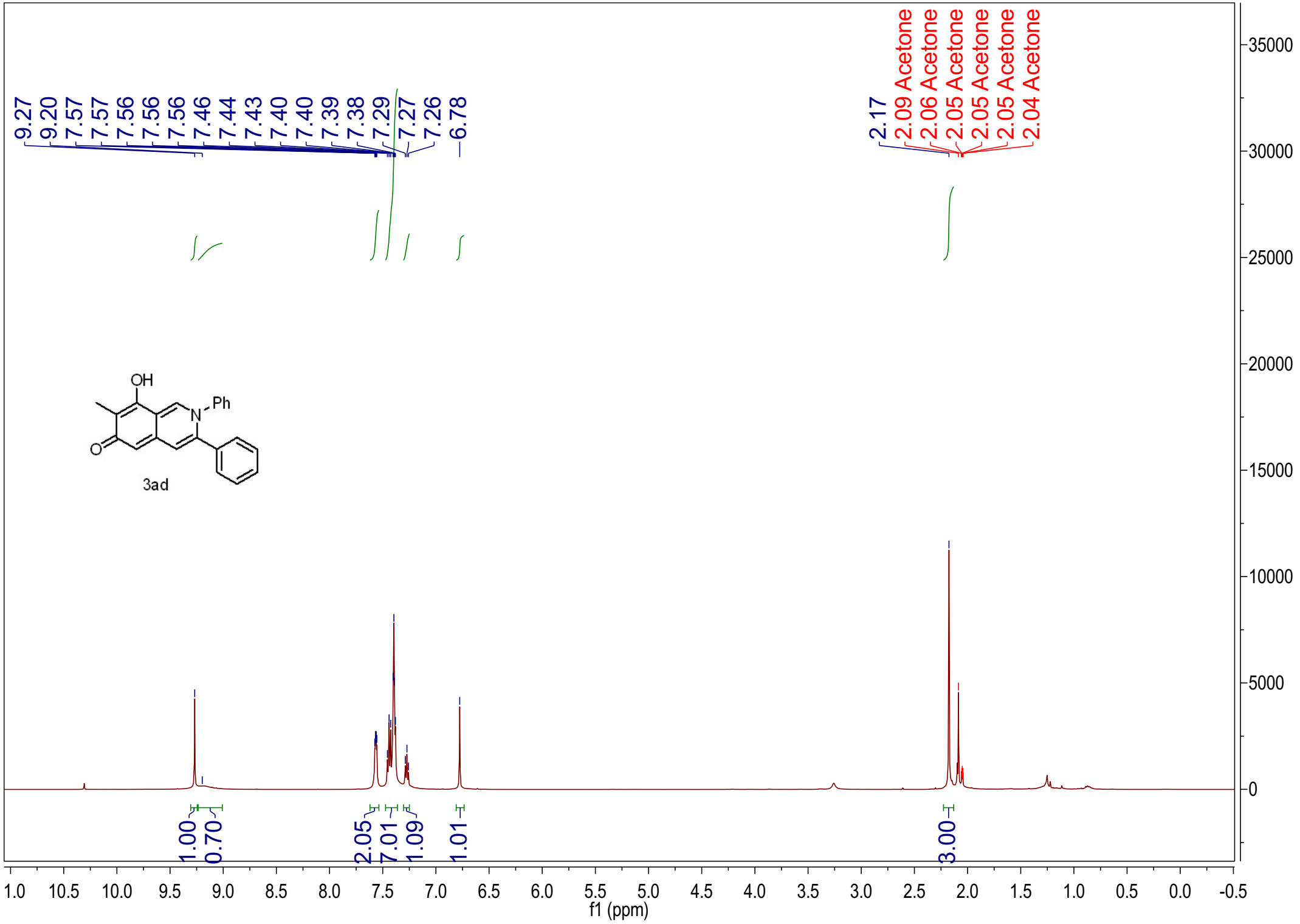

182.30
142.41
141.29
140.48
139.26
133.20
131.16
131.09
129.72
129.42
129.20
129.08
126.77
118.71
117.43
111.67
111.64
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
21.32
Ph
N
O
3aa
f1 (ppm)

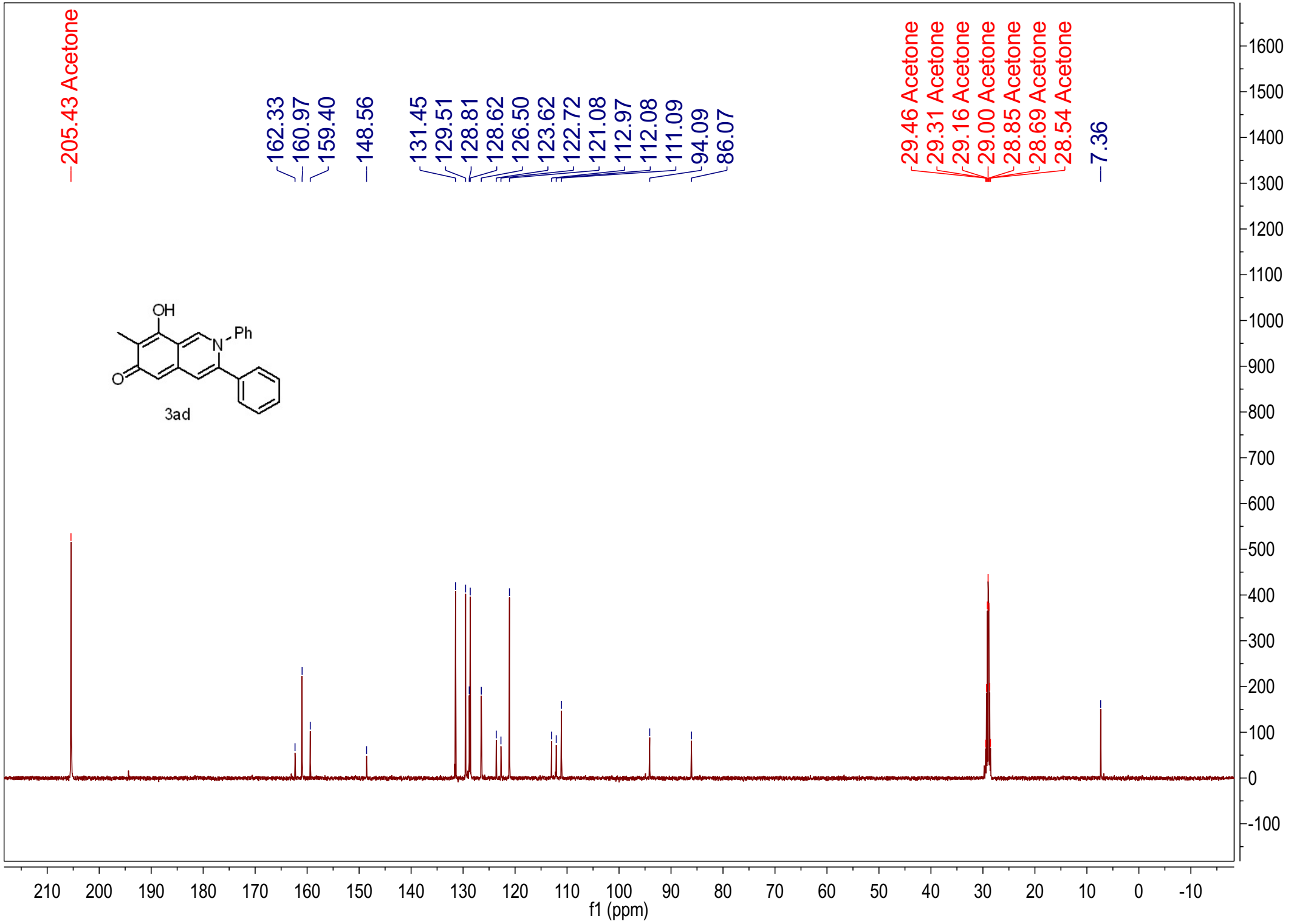

8.16
7.50
7.48
7.27
7.26 CDCl3
7.13
6.99
6.97
6.96
6.93
6.91
6.67
6.65
6.49
3.66
Ph
N
O
O
3ab
1.00
1.03
2.96
2.09
3.02
1.03
2.09
1.06
3.09
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

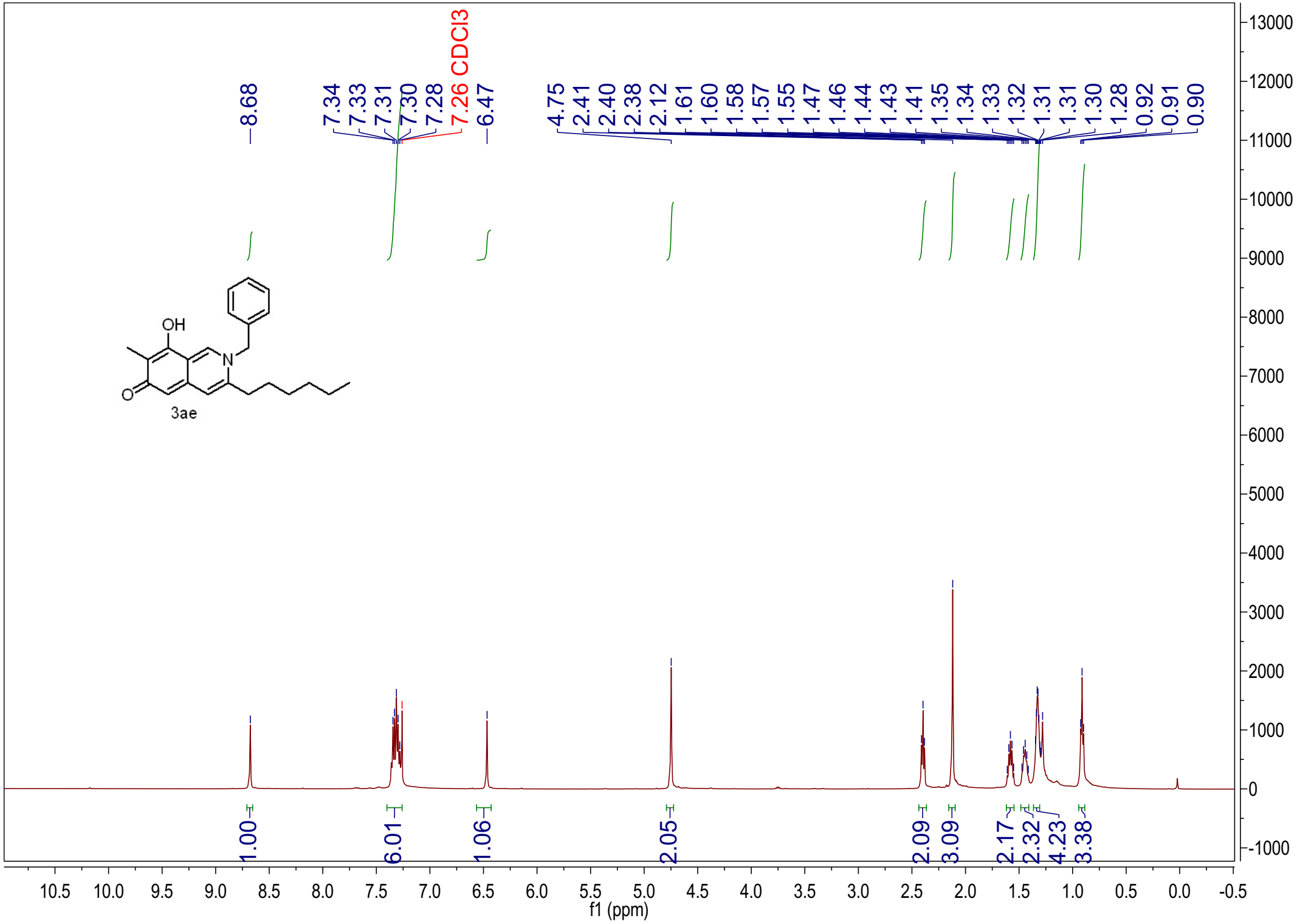

180.94
159.92
142.27
142.10
142.01
140.50
132.14
131.28
130.76
129.58
128.98
126.58
125.93
118.69
117.42
113.78
110.87
77.41 CDCl3
77.16 CDCl3
76.91 CDCl3
55.21
Ph
N
O
O
3ab
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

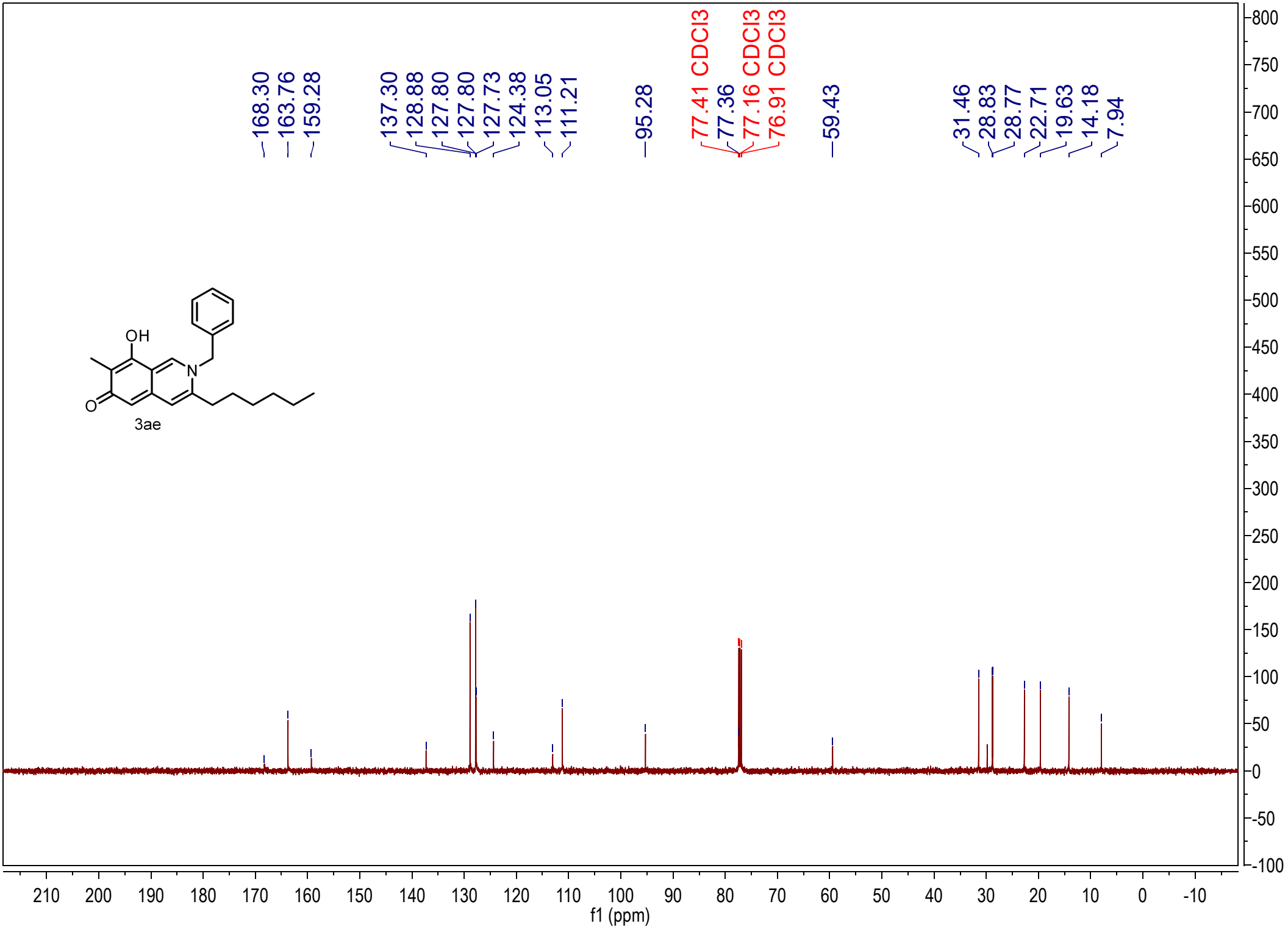

9.08
7.44
7.43
7.41
7.32
7.30
7.29
7.27
7.26 CDCl3
6.56
2.47
2.45
2.44
2.20
1.65
1.64
1.62
1.61
1.60
1.49
1.48
1.48
1.47
1.46
1.34
1.33
1.32
1.31
0.92
0.91
0.89
OH
N
O
3ac
1.00
2.10
4.01
1.03
2.06
3.05
2.15
2.15
4.05
3.04
f1 (ppm)


165.67
160.00
158.92
146.43
129.60
126.58
125.18
120.75
112.52
112.49
111.66
96.15
77.41 CDCl3
77.38
77.16 CDCl3
76.91 CDCl3
31.51
28.87
28.78
22.68
19.71
14.19
7.87
OH
N
O
3ac
f1 (ppm)


9.27
9.20
7.57
7.57
7.56
7.56
7.56
7.46
7.44
7.43
7.40
7.40
7.39
7.38
7.29
7.27
7.26
6.78
2.17
2.09 Acetone
2.06 Acetone
2.05 Acetone
2.05 Acetone
2.05 Acetone
2.04 Acetone
OH
Ph
N
O
3ad
1.00
0.70
2.05
7.01
1.09
1.01
3.00
35000
30000
25000
20000
15000
10000
5000
0
1.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


205.43 Acetone
162.33
160.97
159.40
148.56
131.45
129.51
128.81
128.62
126.50
123.62
122.72
121.08
112.97
112.08
111.09
94.09
86.07
29.46 Acetone
29.31 Acetone
29.16 Acetone
29.00 Acetone
28.85 Acetone
28.69 Acetone
28.54 Acetone
7.36
OH
Ph
N
O
3ad
f1 (ppm)


8.68
7.34
7.33
7.31
7.30
7.28
7.26 CDCl3
6.47
4.75
2.41
2.40
2.38
2.12
1.61
1.60
1.58
1.57
1.55
1.47
1.46
1.44
1.43
1.41
1.35
1.34
1.33
1.32
1.31
1.31
1.30
1.28
0.92
0.91
0.90
OH
N
O
3ae
1.00
6.01
1.06
2.05
2.09
3.09
2.17
2.32
4.23
3.38
f1 (ppm)


168.30
163.76
159.28
137.30
128.88
127.80
127.80
127.73
124.38
113.05
111.21
95.28
77.41 CDCl3
77.36
77.16 CDCl3
76.91 CDCl3
59.43
31.46
28.83
28.77
22.71
19.63
14.18
7.94
OH
N
O
3ae
f1 (ppm)