Supporting Information

Brønsted Acids Enable Three Molecular Rearrangements of One 3-Alkylidene-2*H*-1,2-oxazine Molecule into Distinct Heterocyles

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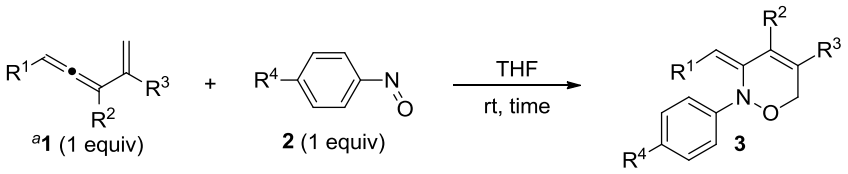
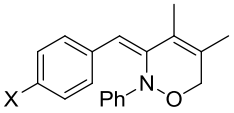
Contents:

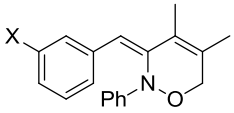
(1) a) Table S1. Regioselective [4+2]-cycloadditions of alkenylallenes with nitrosoarenes.



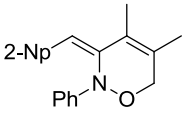
[a]**1** (1 equiv) **2** (1 equiv) **3**



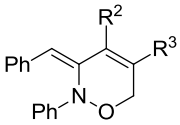
(1) X = H (**3a**, 10 min, 99%, **X-ray**)[b]
(2) X= OMe (**3b**, 10 min 99%)
(3) X = Me, (**3c**, 15 min, 99%)
(4) X = Cl, (**3d**, 0.5 h, 90%)
(5) X = CF_3, (**3e**, 1 h, 86%)



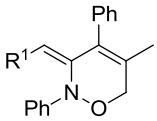
(6) X = OMe (**3f**, 0.5 h, 95%)
(7) X = Cl (**3g**, 1 h, 98%)



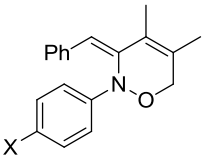
(8) **3h** (10 min, 85%)



(9) R^2 = Ph, R^3 = Me (**3i,** 15 min, 95%)
(10) R^2 = Me, R^3 = H (**3j**, 5 min, 99%)



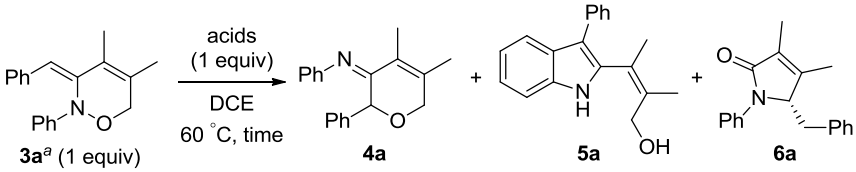
(11) R^1 = Me (**3l**, 0.5 h, 89%)
(12) R^1 = *i*-Pr (**3m**, 0.5 h, 95%)
(13) R^1 = Cy (**3n**, 1 h, 90%)



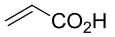
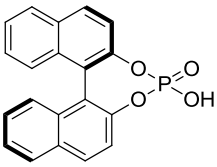
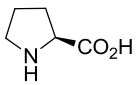
(14) X = Me (**3o**, 0.5 h, 86%)
(15) X = OMe (**3p**, 0.5 h, 88%)
(16) X = Cl (**3q**, 1 h, 82%)
(17) X = CO_2Et (**3r**, 1 h, 74%)

[a]**1** = 0.025 M. [b]Product yields are reported after THF evaporation to dryness, following by washing with hexane.

b) Table S2. Chemoselectivity using additional bronsted acids.



3a[a] (1 equiv) **4a** **5a** **6a**

entry	acids	time (h)	**3a**	**4a**	**5a**	**6a**
1	$PhCO_2H$	36 h	98%	--	--	--
2		16 h	95%	--	--	--
3	CH_3CO_2H	16 h	95%	--	--	--
4[b]		1.5 h	--	15%	--	50%
5		24 h	98%	--	--	--

[a]**3a** = 0.025 M. [b]Yields are reported after purification from a silica column.

(2) Representative Synthetic procedures

A) General Experimental:

Unless otherwise noted, all reactions were carried out under a N_2 atmosphere in reaction tube. Tetrahydrofuran was dried with sodium benzophenone and distilled before use. Dichloromethane were dried over CaH_2 and distilled before use. The triethylamine (Et_3N) were stored over 4 Å molecular sieves prior to use. Reagents were purchased from commercial sources and used without purification, unless otherwise stated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f- 254) using UV light as visualizing agents and/or potassium permanganate ($KMnO_4$). ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400, Varian 500 MHz and a Varian 600 MHz spectrometers using chloroform-*d* ($CDCl_3$) and *d*-benzene (C_6D_6) as the internal standard. Chemical shifts are reported in parts per million (ppm). Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). Coupling constants *J* are reported in Hertz (Hz). The vinylallene substrates **1a-1o** were prepared according to literature,[S1-S4] the nitrosoarene substrates **2a-2e** were prepared according to literature.[S5]

[S1] Bhunia, S.; Liu, R.-S. *J. Am. Chem. Soc.* **2008**, *130*, 16488-16489.

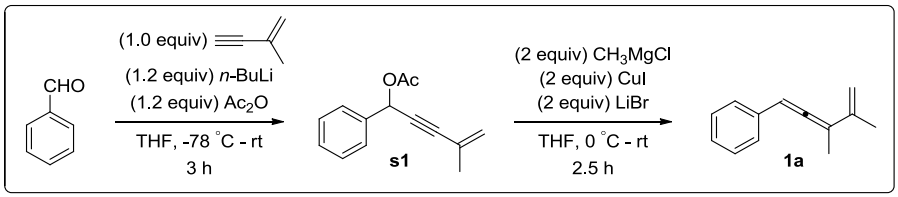
[S2] Macdonald, T. M.; Reagan, D. R. *J. Org. Chem.* **1980**, *45*, 4740-4747.

[S3] Chaudhari, R.; Liao, H.-Y.; Liu, R.-S. *Chem. Eur. J.* **2009**, *15*, 8895-8901.

[S4] Choe, J.; Yang, J.; Park, K.; Palani, T.; Lee, S. *Tetrahedron Lett.* **2012**, 6908-6912.

[S5] Kubitschke, J.; Näther, C.; Herges, R. *Eur. J. Org. Chem.* **2010**, 5041-5055.

B) Synthesis of the substrate (3,4-dimethylpenta-1,2,4-trien-1-yl)benzene (1a):



a) Synthesis of 4-methyl-1-phenylpent-4-en-2-yn-1-yl acetate (s1):

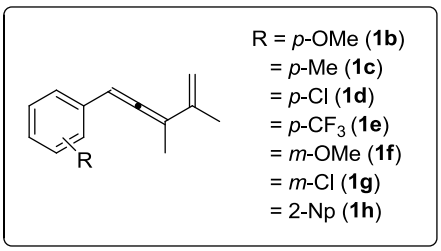
To a THF (10 mL) solution of 2-methylbut-1-en-3-yne (1.0 g, 15.13 mmol) was added *n*-BuLi (2.5 M in hexane, 7.3 mL, 18.15 mmol) at -78 °C and stirred at this temperature for 0.5

h. The THF (10 mL) solution of PhCHO (1.61 g, 15.13 mmol) was added and the reaction mixture was stirred at rt for additional 1.5 h. The resulting mixture was quenched by acetic anhydride (1.86 g, 18.15 mmol) and stirred for next 1 h. After completion of reaction, saturated NH_4Cl was added and extracted with diethyl ether (2 x 50 mL). The combined organic layer were dried over $MgSO_4$ and concentrated under reduced pressure. The cude reaction mass was purified by silica column eluting with hexane/ethyl acetate (5:1) to afford 4-methyl-1-phenylpent-4-en-2-yn-1-ol **s1** (3.1 g, 14.48 mmol, 95.7%) as pale yellow oil.

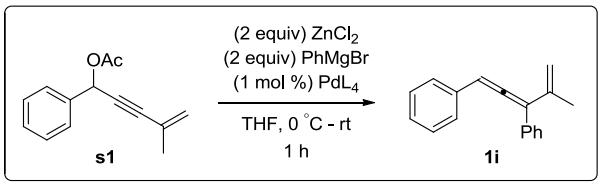
b) Synthesis of (3,4-dimethylpenta-1,2,4-trien-1-yl)benzene (1a):

To a dry 250-mL flask were added LiBr (0.81 g, 9.33 mmol) and CuI (1.78 g, 9.33 mmol), evacuated and backfilled with N_2 balloon before dried THF (25 mL) was added. The reaction mixture was cooled to 0 °C, CH_3MgCl (3.0 M in THF, 2.1 mL, 9.33 mmol) was added. The resulting solution was stirred reaction mixture at 0 °C for additional 0.5 h. To this solution was added propargylic acetate (**s1**) (1 g, 4.67 mmol), and the mixture was stirred for 2 h. The resulting mixture was quenched by a saturated NH_4Cl, filtrated, and extracted with diethyl ether (2 x 50 mL). The extract was dried over $MgSO_4$, concentrated in vacuo and purified by a silica column to afford (3,4-dimethylpenta-1,2,4-trien-1-yl)benzene **1a** (0.60 g, 3.52 mmol, 75.6%) as pale yellow oil.

Substrates **1b-1h** were synthesized using same as above procedure.



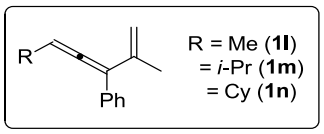
C) Synthesis of the substrate (4-methylpenta-1,2,4-triene-1,3-diyl)dibenzene (1i):



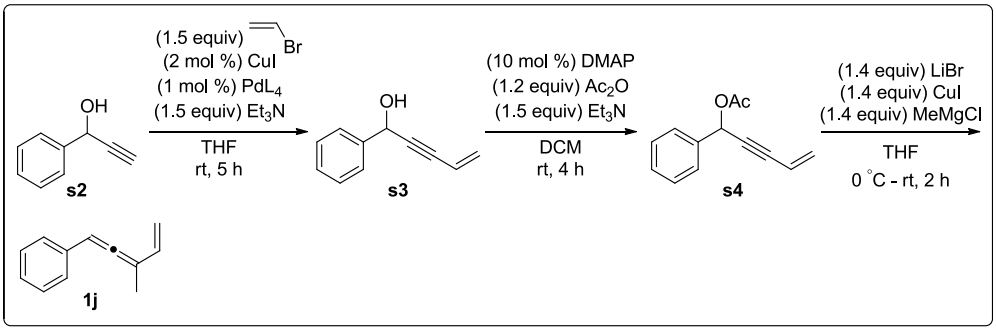
Synthesis of (4-methylpenta-1,2,4-triene-1,3-diyl)dibenzene (1i):

A dry 250-mL flask was added with $ZnCl_2$ (1.27 g, 9.93 mmol), dried in vacuo and refilled with N_2 balloon. To this flask was added dry THF (25 mL) and then PhMgBr (1.69 g, 9.93 mmol); the mixture was stirred at 25 °C for 0.5 h. After stirring for 20 min, $[Pd(PPh_3)_4]$ (54.0 mg, 0.047 mmol) and compound **s1** (1 g, 46.7 mmol) were added to this reaction mixture; the resulting solution was stirred for 1 h before quenching with water. The organic layer was extracted with diethyl ether (2 x 25 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The residue was eluted through a silica column to afford (4-methylpenta-1,2,4-triene-1,3-diyl)dibenzene **1i** (0.8 g, 3.44 mmol, 73.8%) as orange-yellow liquid.

Substrates **1l-1n** were synthesized using same as above procedure.



D) Synthesis of the substrate (3-methylpenta-1,2,4-trien-1-yl)benzene (1j):



a) Synthesis of 1-phenylpent-4-en-2-yn-1-ol (s3):

Copper (I) iodide (0.029 g, 0.15 mmol) and tetrakis(triphenylphosphin)palladium (0.087 g, 0.076 mmol) were dissolved in anhydrous and degassed Et_3N (3.2 mL, 22.7 mmol), and the mixture was cooled to 0 °C. To this solution was added alkyne **s2** (1 g, 7.57 mmol) and vinyl bromide (1 M in THF, 1.21 g, 11.35 mmol), and the mixture was stirred at room temperature until a complete consumption of starting material. The reaction solution was filtered through a celite pad, concentrated and eluted through a silica column to give 1-phenylpent-4-en-2-yn-1-ol **s3** (0.55 g, 2.75 mmol, 45.9%) as colorless oil.

b) Synthesis of 1-phenylpent-4-en-2-yn-1-yl acetate (s4):

To a DCM solution of 1-phenylpent-4-en-2-yn-1-ol (1.0 g, 6.33 mmol) were added

DMAP (77 mg, 0.63 mmol), Et_3N (0.96 g, 9.49 mmol) and the mixtures were stirred at 0 °C for 15 min. To this solution was added Ac_2O (0.78 g, 7.59 mmol), and the mixture was slowly warmed to room temperature for a stirring of 4 h. The solution was quenched by water and extracted with DCM (2 x 25 mL). The combined organic layer was dried over $MgSO_4$, concentrated in vacuo, and further purified by a silica column to afford 1-phenylpent-4-en-2-yn-1-yl acetate **s4** (1.19 g, 7.52 mmol, 93.7%) as pale yellow oil.

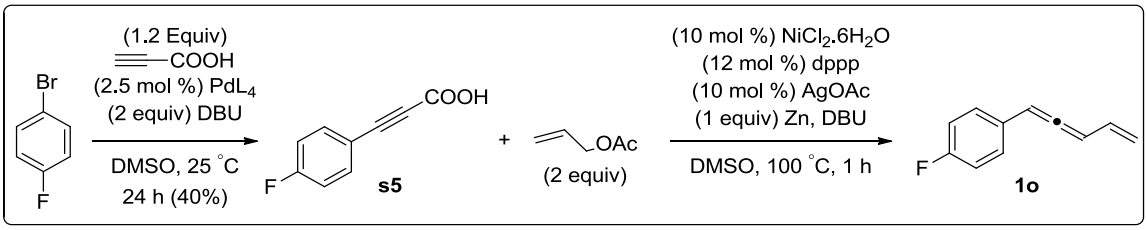
c) Synthesis of (3-methylpenta-1,2,4-trien-1-yl)benzene (1j):

The substarte **1j** was synthesized using similar synthetic procedure of substrate **1a** from **s1**.

E) Synthesis of the substrate penta-1,2,4-trien-1-ylbenzene (1k):

The substarte **1k** was synthesized according to literature procedure.[S4]

F) Synthesis of the substrate 1-fluoro-4-(penta-1,2,4-trien-1-yl)benzene (1o):



a) Synthesis of 3-(4-fluorophenyl)propiolic acid (s5):

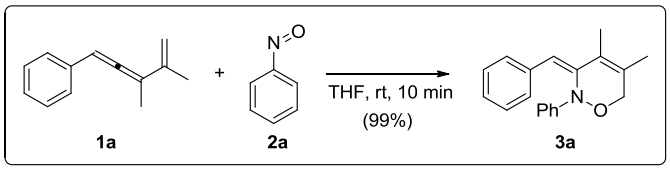
To a DMSO (20 mL) solution of 1-bromo-4-fluorobenzene (2 g, 11.42 mmol) was added propiolic acid (0.96 g, 13.71 mmol), DBU (3.48 g, 22.84 mmol) and $Pd(PPh_3)_4$ (0.33 g, 0.3 mmol); the mixture was stirred at 25 °C for 24 h. The reaction solution was poured into ethyl acetate (50 mL) and extracted with a saturated aqueous $NaHCO_3$ solution. The aqueous layer was separated, acidified to pH 2.0 with cold HCl (1 N), and extracted with DCM (3 x 25 mL). The combined organic layers were dried with $MgSO_4$, and the solvent was removed under reduced pressure. Crude product was purified by flash chromatography on silica gel using ethyl acetate/hexane, 1:4 with HOAc (1 %, v/v) to afford 3-(4-fluorophenyl)propiolic acid **s5** (0.76 g, 4.63 mmol, 40.4%) as pale yellow solid.

b) Synthesis of 1-fluoro-4-(penta-1,2,4-trien-1-yl)benzene (1o):

To a DMSO (10 mL) solution of 3-(4-fluorophenyl)propiolic acid (1 g, 6.09 mmol) was

added $Ni(OAc)_2 \cdot 4H_2O$ (0.145 g, 0.61 mmol), 1,3-bis(diphenylphosphino)propane (0.302 g, 0.73 mmol), allyl acetate (1.22 g, 12.2 mmol), AgOAc (0.102 g, 0.61 mmol), zinc (0.4 g, 6.09 mmol) and DBU (0.93 g, 6.09 mmol) in a 100-mL round-bottomed flask, and the resulting mixture was stirred at 100 °C for 1 h. The reaction mixture was poured into water and extracted with EtOAc (2 x 20 mL). The solution was removed under vacuum and the resulting crude product was purified by flash chromatography on silica gel to give desired 1-fluoro-4-(penta-1,2,4-trien-1-yl)benzene **1o** (0.62 g, 3.87 mmol, 60.5%) as pale yellow oil.

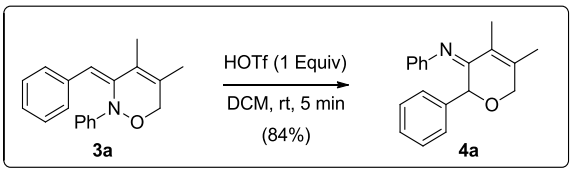
G) Preparation of the (*Z*)-3-benzylidene-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3a):



A 25-mL flask was charged with nitrosobenzene **2a** (107.1 mg, 1.0 mmol), then evacuated and backfilled with a N_2 balloon. To this solid was added anhydrous THF (4 mL), and the resulting mixture was stirred at room temperature until the solid was dissolved. A THF solution (4.3 mL) of **1a** (170.5 mg, 1.0 mmol) was added; the mixture was stirred at room temperature for additional 10 min. The resulting solution was concentrated under reduced pressure to romove solvent, affording compound **3a** (323.0 mg, 1.18 mmol, 99%) as yellow solid. This yellow solid was recrystallized in hexane/chloroform for X-ray analysis.

(3) Standard procedures for Brønsted acids enable reactions

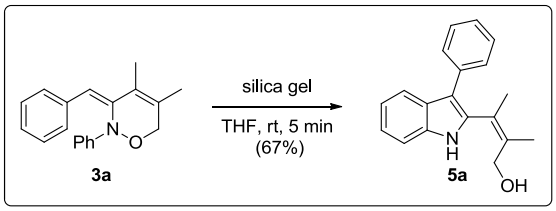
a) Typical procedure for the preparation of (*Z*)-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4a):



To a DCM (7 mL) solution of compound **3a** (277.4 mg, 1.0 mmol) was added HOTf (150.1 mg, 1.0 mmol) under N_2 atmosphere and stirred at 25 °C for 5 min. The resulting

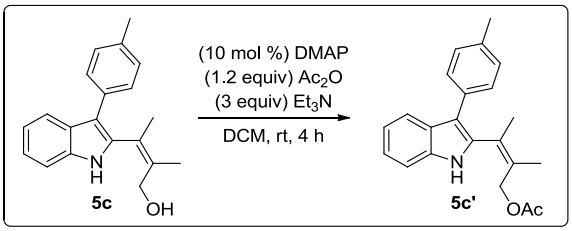
solution was quenched with saturated $NaHCO_3$ and extracted with DCM (2 x 14 mL). The combined organic layers were dried over $MgSO_4$, concentrated in vacuo and further purification by silica column to afford compound **4a** (230 mg, 0.83 mmol, 83%) as colorless oil.

b) i) Typical procedure for the preparation of (*Z*)-2-methyl-3-(3-phenyl-1*H*-indol-2-yl)but-2-en-1-ol (5a):



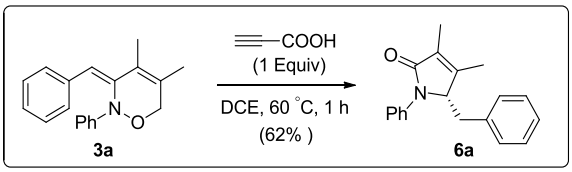
To a THF (5.6 mL) solution of compound **3a** (277.4 mg, 1.0 mmol) was added silica gel (600.9 mg, 10.0 mmol) under N_2 atmosphere and the mixture was stirred at 25 °C for 1 h. The resulting suspension was concentrated under reduced pressure, and further purifed by a silica column to afford compound **5a** (185.8 mg, 0.67 mmol, 67%) as colorless oil.

ii) Synthesis of (*Z*)-2-methyl-3-(3-(*p*-tolyl)-1*H*-indol-2-yl)but-2-en-1-yl acetate (5c'):



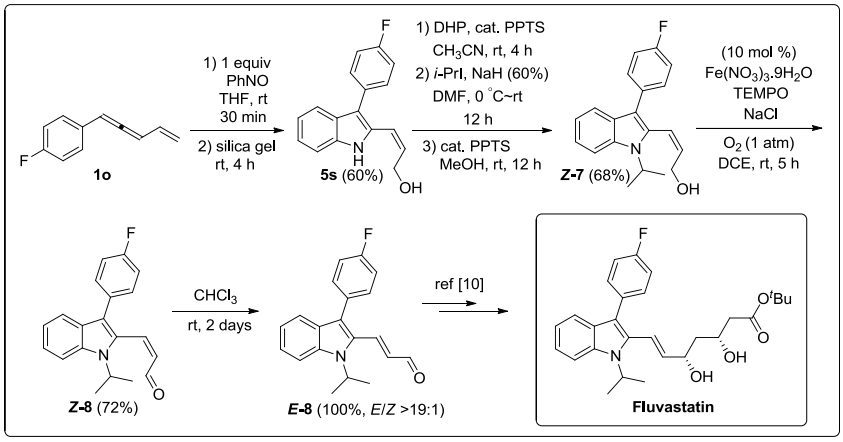
Compound **5c'** (171 mg, 0.51 mmol, 95%) was synthesized using similar procedure to that of compound **s4**. This solid was recrystallized in hexane/dichloromethane for X-ray analysis.

c) Typical procedure for the preparation of (*S*)-5-benzyl-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6a):



To a DCE (7 mL) solution of compound **3a** (277.4 mg, 1.0 mmol) was added propiolic acid (14.0 mg, 0.2 mmol) under N_2 atmosphere and stirred at 60 °C for 1 h. The resulting solution was concentrated under reduced pressure, and further purified by a silica column to afford compound **6a** (169 mg, 0.61 mmol, 61%) as pale yellow solid.

(4) Formal Synthesis of Fluvastatin



a) Synthesis of (*Z*)-3-(3-(4-fluorophenyl)-1*H*-indol-2-yl)prop-2-en-1-ol (5s):

To a THF (25 mL) solution of nitrosobenzene **2a** (0.67 g, 6.24 mmol) was added compound **1o** (1 g, 6.24 mmol) under N_2 atmosphere, and the reaction mixture was stirred at rt for additional 30 min. The solution was concentrated under reduced pressure, further purified on an acidic silica column to afford compound **5s** (1 g, 3.74 mmol, 60%) as yellow oil.

b) Synthesis of (*Z*)-3-(3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl)prop-2-en-1-ol (*Z*-7):

1) To a CH_3CN (5 mL) solution of Indole **5s** (160.0 mg, 0.6 mmol) were added pyridinium *p*-toluenesulfonate (15.0 mg, 0.06 mmol) and dihydropyran (0.27 mL, 3.0 mmol), and the mixtures were stirred at rt for 4 h. The mixture was concentrated in vacuo, added with water (10 mL) and extracted with diethyl ether (10 mL). The organic layer was dried over $MgSO_4$, concentrated to form crude product **int-A** (179.0 mg, 0.51 mmol, 85%). This species was directly used in the next step without purification.

2) To a DMF (5 mL) suspension of NaH (60%, 36 mg, 0.9 mmol) was added **int-A** (263.0 mg, 0.75 mmol) at 0 °C under N_2, and the mixture was stirred for additional 15 min. To this

mixture was added *i*-PrI (0.3 mL, 3.0 mmol); the mixture was warmed to rt for 12 h. The resulting solution was quenched with saturated NH_4Cl and extracted with EtOAc (10 mL). The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure to afford **int-B** (220.0 mg, 0.56 mmol, 75%). This crude product was used in the next step without purification.

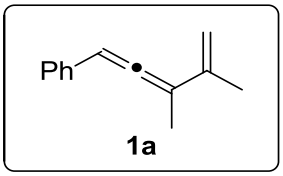
3) To a MeOH (5 mL) solution of **int-B** (234.0 mg, 0.59 mmol) was added pyridinium *p*-toluenesulfonate (15.0 mg, 0.06 mmol) and the reaction mixture was stirred at rt for 12 h. The resulting mixture was concentrated in vacuo and further purified by a silica column to afford compound ***Z*-7** (125 mg, 0.41 mmol, 68%).

c) Synthesis of (*E*)-3-(3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl)acrylaldehyde (*E*-8):

A DCE (2 mL) solution of ***Z*-7** (125.0 mg, 0.4 mmol) were charged with $Fe(NO_3)_3 \cdot 9H_2O$ (16.0 mg, 0.04 mmol), TEMPO (6.3 mg, 0.04 mmol), NaCl (2.5 mg, 0.04 mmol) under O_2, and the solution was stirred at rt for 5 h. The mixture was concentrated in vacuo, and purified by a silica column to afford ***Z*-8** (88.5 mg, 0.28 mmol, 72%) as colorless oil. ***Z*-8** was easily transformed to ***E*-8** (50.0 mg, 0.16 mmol, 100%) in *d*-chloroform ($CdCl_3$) for 2 days.

(5) Spectral Data of Key Compounds

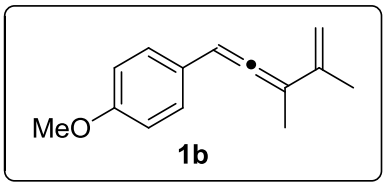
Spectral data for (3,4-dimethylpenta-1,2,4-trien-1-yl)benzene (1a):



1a

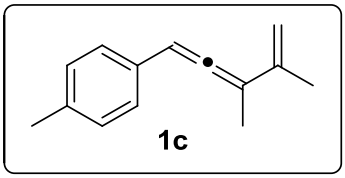
Pale yellow oil (0.600 g, 3.52 mmol, 75.6%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.30 ~ 7.24 (m, 4H), 7.19 ~ 7.16 (m, 1H), 6.28 (s, 1H), 5.00 (s, 1H), 4.96 (d, *J* = 1.4 Hz, 1H), 1.97 (d, *J* = 2.6 Hz, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.6, 140.5, 134.9, 128.6, 126.8, 126.7, 111.5, 106.5, 95.4, 21.5, 16.3; HRMS (EI+, m/z) calcd for $C_{13}H_{14}[M^+]$: 170.1096, found : 170.1091.

Spectral data for 1-(3,4-dimethylpenta-1,2,4-trien-1-yl)-4-methoxybenzene (1b):



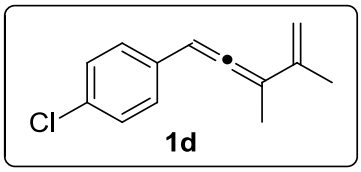
Pale yellow oil (0.260 g, 1.30 mmol, 63.4%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.20 ~ 7.17 (m, 2H), 6.84 ~ 6.82 (m, 2H), 6.24 (s, 1H), 4.98 (s, 1H), 4.95 (d, *J* = 1.3 Hz, 1H), 3.78 (s, 3H), 1.95 (d, *J* = 2.7 Hz, 3H), 1.84 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.0, 158.7, 140.9, 127.8, 127.2, 114.1, 111.2, 106.4, 94.7, 55.3, 21.5, 16.5; HRMS (ESI, m/z) calcd for $C_{14}H_{17}O$[M+H] : 201.1279, found : 201.1271.

Spectral data for 1-(3,4-dimethylpenta-1,2,4-trien-1-yl)-4-methylbenzene (1c):



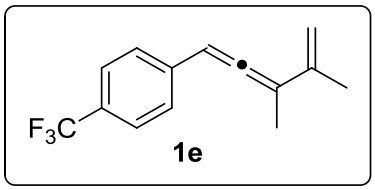
Pale yellow oil (0.282 g, 1.53 mmol, 70.0%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.16 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.25 (s, 1H), 4.99 (s, 1H), 4.95 (d, *J* = 1.4 Hz, 1H), 2.31 (s, 3H), 1.96 (d, *J* = 2.6 Hz, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.3, 140.7, 136.5, 131.9, 129.3, 126.6, 111.3, 106.4, 95.2, 21.4, 21.1, 16.3; HRMS (EI+, m/z) calcd for $C_{14}H_{16}$[M^+] : 184.1253, found : 184.1253.

Spectral data for 1-chloro-4-(3,4-dimethylpenta-1,2,4-trien-1-yl)benzene (1d):



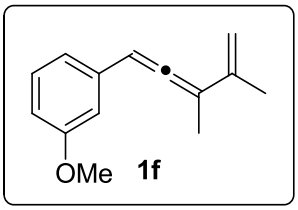
Pale yellow oil (0.340 g, 1.66 mmol, 82.5%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.26 ~ 7.25 (m, 2H), 7.20 ~ 7.18 (m, 2H), 6.25 (s, 1H), 5.03 (s, 1H), 4.99 (d, *J* = 1.4 Hz, 1H), 1.98 (d, *J* = 2.6 Hz, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.7, 140.2, 133.5, 132.4, 128.7, 127.9, 111.9, 107.0, 94.5, 21.4, 16.2; HRMS (EI+, m/z) calcd for $C_{13}H_{13}Cl$[M^+] : 204.0706, found : 204.0705.

Spectral data for 1-(3,4-dimethylpenta-1,2,4-trien-1-yl)-4-(trifluoromethyl)benzene (1e):



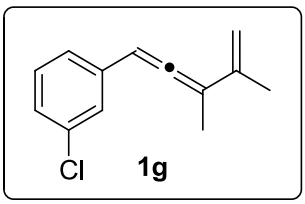
Pale yellow oil (0.360 g, 1.51 mmol, 85.3%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.3 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 2H), 6.31 (s, 1H), 5.05 (s, 1H), 5.00 (d, *J* = 1.3 Hz, 1H), 1.99 (d, *J* = 2.6 Hz, 3H), 1.89 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 208.6, 139.9, 139.0, 129.9 ($J_{C\text{-}F}$ = 283.8), 128.2 ($J_{C\text{-}F}$ = 32.0), 126.8, 125.6, 125.5, 112.3, 107.2, 94.7, 29.7, 21.4, 16.1; HRMS (EI+, m/z) calcd for $C_{14}H_{13}F_3[M^+]$: 238.0969, found : 238.0966.

Spectral data for 1-(3,4-dimethylpenta-1,2,4-trien-1-yl)-3-methoxybenzene (1f):



Pale yellow oil (0.295 g, 1.47 mmol, 72.0%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.22 (t, *J* = 7.9 Hz, 1H), 6.89 (dd, *J* = 7.6, 1.0 Hz, 1H), 6.84 ~ 6.83 (m, 1H), 6.76 (dt, *J* = 8.3, 1.5 Hz, 1H), 6.27 (s, 1H), 5.03 (s, 1H), 4.99 (d, *J* = 1.3 Hz, 1H), 3.80 (s, 3H), 1.99 (d, *J* = 2.6 Hz, 3H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.7, 159.9, 140.5, 136.5, 129.5, 119.4, 112.3, 112.2, 111.5, 106.6, 95.3, 55.1, 21.5, 16.3; HRMS (EI+, m/z) calcd for $C_{14}H_{16}O[M^+]$: 200.1201, found : 200.1203.

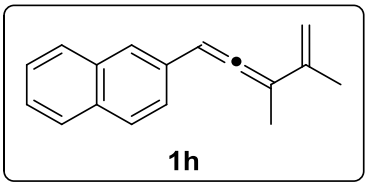
Spectral data for 1-chloro-3-(3,4-dimethylpenta-1,2,4-trien-1-yl)benzene (1g):



Pale yellow oil (0.330 g, 1.33 mmol, 80.1%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.26 (s, 1H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.17 ~ 7.13 (m, 2H), 6.24 (s, 1H), 5.05 (s, 1H), 5.01 (s, 1H), 1.99 (d, *J* = 2.7 Hz, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.9, 140.1, 137.0, 134.6,

129.8, 126.8, 126.5, 124.9, 112.1, 107.1, 94.5, 21.4, 16.2; HRMS (EI+, m/z) calcd for $C_{13}H_{13}Cl[M^+]$: 204.0706, found : 204.0703.

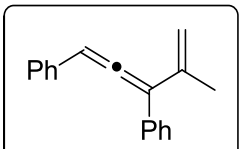
Spectral data for 2-(3,4-dimethylpenta-1,2,4-trien-1-yl)naphthalene (1h):



1h

Pale yellow solid (0.650 g, 2.95 mmol, 78.0%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.79 ~ 7.75 (m, 3H), 7.66 (s, 1H), 7.47 ~ 7.41 (m, 3H), 6.49 (s, 1H), 5.07 (s, 1H), 5.02 (s, 1H), 2.05 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 208.2, 140.6, 133.7, 132.6, 132.5, 128.2, 127.7, 127.6, 126.2, 125.5, 125.4, 124.7, 111.6, 106.7, 95.8, 21.5, 16.4; HRMS (ESI, m/z) calcd for $C_{17}H_{17}[M+H]$: 221.1330, found : 221.1324.

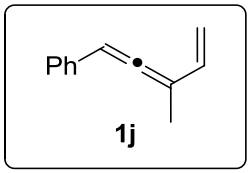
Spectral data for (4-methylpenta-1,2,4-triene-1,3-diyl)dibenzene (1i):



1i

Orange yellow oil (0.800 g, 3.44 mmol, 73.8%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.44 ~ 7.42 (m, 2H), 7.40 ~ 7.33 (m, 6H), 7.31 ~ 7.30 (m, 1H), 7.25 ~ 7.22 (m, 1H), 6.56 (s, 1H), 5.17 ~ 5.16 (m, 1H), 5.00 ~ 5.00 (m, 1H), 2.04 (t, J = 0.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 207.7, 139.8, 136.2, 134.3, 129.0, 128.7, 128.3, 127.3, 127.2, 126.8, 115.5, 96.9, 22.0; HRMS (EI+, m/z) calcd for $C_{18}H_{16}[M^+]$: 232.1252, found : 232.1253.

Spectral data for (3-methylpenta-1,2,4-trien-1-yl)benzene (1j):

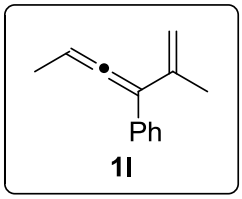


1j

Pale yellow oil (0.450 g, 2.88 mmol, 57.7%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 ~ 7.34 (m, 4H), 7.28 ~ 7.24 (m, 1H), 6.50 (dd, J = 17.6, 10.8 Hz, 1H), 6.33 (s, 1H), 5.30 (dd, J = 17.6,

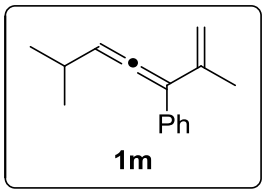
1.2 Hz, 1H), 5.19 (dd, *J* = 10.4, 0.8 Hz, 1H), 2.03 (d, *J* = 2.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 209.1, 134.8, 134.6, 128.6, 126.9, 126.9, 113.4, 104.1, 94.2, 14.5.

Spectral data for (2-methylhexa-1,3,4-trien-3-yl)benzene (1l):



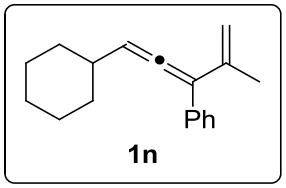
Pale yellow oil (0.700 g, 4.11 mmol, 62.5%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.32 ~ 7.31 (m, 4H), 7.25 ~ 7.23 (m, 1H), 5.48 (q, *J* = 7.1 Hz, 1H), 5.03 ~ 5.02 (m, 1H), 4.82 (d, *J* = 0.6 Hz, 1H), 1.95 (s, 3H), 1.76 (dd, *J* = 7.1, 0.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 206.2, 140.5, 137.3, 129.1, 128.1, 126.8, 114.2, 110.8, 88.0, 22.1, 14.5; HRMS (EI+, m/z) calcd for $C_{13}H_{14}[M^+]$: 170.1096, found : 170.1089.

Spectral data for (2,6-dimethylhepta-1,3,4-trien-3-yl)benzene (1m):



Pale yellow oil (0.725 g, 3.66 mmol, 65.9%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 ~ 7.30 (m, 4H), 7.25 ~ 7.21 (m, 1H), 5.52 (d, *J* = 5.6 Hz, 1H), 5.02 ~ 5.00 (m, 1H), 4.80 (d, *J* = 0.4 Hz, 1H), 2.43 ~ 2.38 (m, 1H), 1.96 (s, 3H), 1.08 (d, *J* = 3.2, 3H), 1.06 (d, *J* = 3.2, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 203.8, 140.5, 137.4, 129.0, 128.1, 126.8, 114.1, 112.4, 100.7, 28.5, 22.5, 22.4, 22.1; HRMS (EI+, m/z) calcd for $C_{15}H_{18}[M^+]$: 198.1409, found : 198.1407.

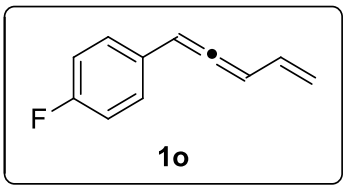
Spectral data for (1-cyclohexyl-4-methylpenta-1,2,4-trien-3-yl)benzene (1n):



Pale yellow oil (0.350 g, 1.47 mmol, 64.8%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 ~ 7.30 (m,

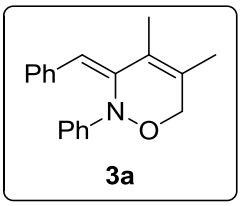
4H), 7.28 ~ 7.22 (m, 1H), 5.51 (d, J = 5.6 Hz, 1H), 5.03 ~ 5.01 (m, 1H), 4.82 (s, 1H), 2.18 ~ 2.05 (m, 1H), 1.97 (s, 3H), 1.83 (d, J = 12.0 Hz, 2H), 1.75 ~ 1.72 (m, 2H), 1.68 ~ 1.63 (m, 1H), 1.35 ~ 1.12 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 204.2, 140.5, 137.4, 129.0, 128.0, 126.7, 114.0, 99.3, 37.8, 33.2, 33.0, 26.1, 22.2; HRMS (EI+, m/z) calcd for $C_{18}H_{22}[M^+]$: 238.1722, found : 238.1725.

Spectral data for 1-fluoro-4-(penta-1,2,4-trien-1-yl)benzene (1o):



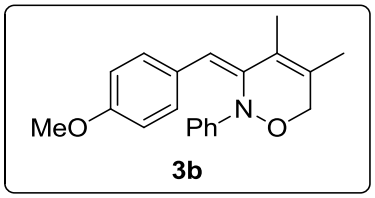
Pale yellow oil (0.620 g, 3.87 mmol, 60.5%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.27 ~ 7.24 (m, 2H), 7.02 ~ 6.99 (m, 2H), 6.33 ~ 6.23 (m, 3H), 5.35 ~ 5.30 (m, 1H), 5.12 ~ 5.10 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 209.1, 162.8, 161.2, 131.9, 129.7 (d, $J_{C\text{-}F}$ = 3.1), 128.4 (d, $J_{C\text{-}F}$ = 8.0), 117.1, 115.6 (d, $J_{C\text{-}F}$ = 21.7), 98.5, 95.0.

Spectral data for (*Z*)-3-benzylidene-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3a):



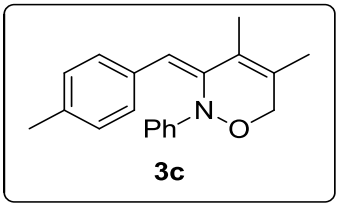
Pale yellow solid (0.323 g, 1.18 mmol, 99%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.54 (d, J = 7.7 Hz, 2H), 7.23 (t, J = 7.7 Hz, 2H), 7.17 (t, J = 7.6 Hz, 2H), 7.10 (t, J = 7.6 Hz, 1H), 7.01 (d, J = 8.3 Hz, 2H), 6.92 (td, J = 3.7, 1.0 Hz, 1H), 6.39 (s, 1H), 4.19 (s, 2H), 2.04 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.1, 137.2, 135.1, 129.7, 129.1, 128.2, 127.1, 122.3, 121.9, 118.5, 117.1, 66.0, 15.5, 13.3; HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO[M+H]$: 278.1545, found : 278.1548.

Spectral data for (*Z*)-3-(4-methoxybenzylidene)-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3b):



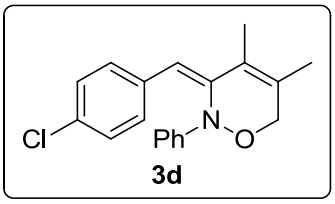
Pale green oil (0.304 g, 0.99 mmol, 99%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.9 Hz, 2H), 7.22 (t, *J* = 8.2 Hz, 2H), 6.99 (d, *J* = 8.1 Hz, 2H), 6.91 (td, *J* = 3.7, 1.0 Hz, 1H), 6.71 (d, *J* = 9.0 Hz, 2H), 6.34 (s, 1H), 4.18 (s, 2H), 3.71 (s, 3H), 2.01 (s, 3H), 1.64 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.7, 144.2, 135.4, 131.1, 129.1, 127.9, 127.9, 122.3, 121.7, 118.2, 116.9, 113.7, 66.0, 55.1, 15.5, 13.3; HRMS (ESI, m/z) calcd for $C_{22}H_{22}NO_2$[M+H] : 308.1651, found : 308.1647.

Spectral data for (*Z*)-4,5-dimethyl-3-(4-methylbenzylidene)-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3c):



Greenish oil (0.312 g, 1.07 mmol, 99%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 8.2 Hz, 2H), 7.24 (t, *J* = 7.6 Hz, 2H), 7.03 ~ 6.99 (m, 4H), 6.93 (td, *J* = 3.7, 1.0 Hz, 1H), 6.39 (s, 1H), 4.21 (s, 2H), 2.25 (s, 3H), 2.04 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.1, 137.0, 136.4, 132.3, 129.6, 129.0, 129.0, 128.5, 122.3, 121.7, 118.5, 117.0, 66.0, 21.1, 15.5, 13.3; HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO$[M+H] : 292.1696 ; found : 292.1697.

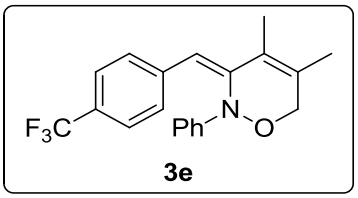
Spectral data for (*Z*)-3-(4-chlorobenzylidene)-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3d):



Pale yellow solid (0.275 g, 0.88 mmol, 90%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.48 ~ 7.46 (m, 2H), 7.14 (dd, *J* = 10.5, 1.3 Hz, 2H), 7.10 (t, *J* = 8.0 Hz, 2H), 6.92 ~ 6.89 (m, 2H), 6.80 ~

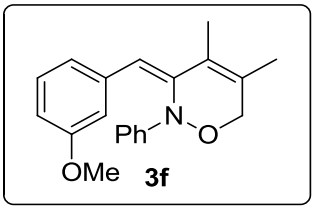
6.77 (m, 1H), 6.16 (s, 1H), 3.93 (s, 2H), 1.72 (d, J = 0.8 Hz, 3H), 1.09 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 144.4, 138.3, 134.1, 133.1, 131.3, 130.0, 129.6, 128.7, 122.4, 122.3, 117.3, 117.0, 66.0, 15.1, 13.0; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1080.

Spectral data for (*Z*)-4,5-dimethyl-2-phenyl-3-(4-(trifluoromethyl)benzylidene)-3,6-dihydro-2*H*-1,2-oxazine (3e):



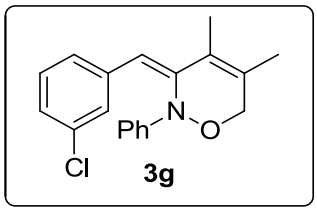
Light brown oil (0.248 g, 0.72 mmol, 86%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.51 (d, J = 8.3 Hz, 2H), 7.14 (dd, J = 12.1, 3.1 Hz, 4H), 7.09 (t, J = 7.7 Hz, 2H), 6.78 (td, J = 7.7, 0.9 Hz, 1H), 6.16 (s, 1H), 3.90 (s, 2H), 1.70 (s, 3H), 1.08 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 144.3, 139.7, 139.0, 131.1, 130.1, 129.6, 128.8 ($J_{C\text{-}F}$ = 32.3), 125.4 ($J_{C\text{-}F}$ = 3.4), 122.7, 122.2, 117.4, 116.7, 66.0, 15.1, 13.0; HRMS (EI+, m/z) calcd for $C_{20}H_{18}F_3NO[M^+]$: 345.1340, found : 345.1346.

Spectral data for (*Z*)-3-(3-methoxybenzylidene)-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3f):



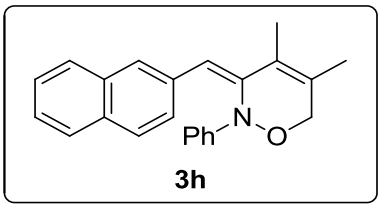
Off white solid (0.248 g, 0.95 mmol, 95%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.52 (s, 1H), 7.27 (dd, J = 7.7, 0.5 Hz, 1H), 7.20 (d, J = 8.3 Hz, 2H), 7.08 (t, J = 8.0 Hz, 2H), 6.97 (t, J = 8.9 Hz, 1H), 6.77 ~ 6.75 (m, 1H), 6.63 (dd, J = 8.2, 2.6 Hz, 1H), 6.38 (s, 1H), 3.95 (s, 2H), 3.21 (s, 3H), 1.74 (t, J = 0.9, 0.6 Hz, 3H), 1.11 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 160.1, 144.7, 137.8, 137.0, 129.5, 129.5, 129.4, 123.1, 122.5, 122.2, 118.4, 117.5, 114.7, 114.2, 66.2, 54.4, 15.1, 13.1; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1575.

Spectral data for (*Z*)-3-(3-chlorobenzylidene)-4,5-dimethyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3g):



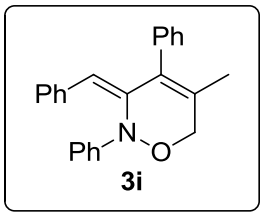
Off white solid (0.299 g, 0.96 mmol, 98%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.60 ~ 7.59 (m, 2H), 7.14 (d, *J* = 8.2, Hz, 2H), 7.08 (t, *J* = 7.9 Hz, 2H), 6.83 (d, *J* = 7.4 Hz, 1H), 6.76 (td, *J* = 7.4, 0.8 Hz, 1H), 6.65 (t, *J* = 8.0 Hz, 1H), 6.10 (s, 1H), 3.89 (s, 2H), 1.69 (s, 3H), 1.08 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 144.3, 138.9, 137.6, 134.3, 130.5, 130.1, 129.8, 129.6, 127.7, 127.3, 122.6, 122.2, 117.5, 116.7, 66.0, 15.1, 13.0; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1076.

Spectral data for (*Z*)-4,5-dimethyl-3-(naphthalen-2-ylmethylene)-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3h):



Pale yellow solid (0.253 g, 0.77 mmol, 85%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.96 (s, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.72 ~ 7.67 (m, 2H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.41 ~ 7.35 (m, 2H), 7.24 (t, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.58 (s, 1H), 4.25 (s, 2H), 2.21 (s, 3H), 1.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 144.0, 137.5, 133.3, 132.9, 132.5, 129.3, 129.2, 129.1, 128.2, 127.6, 127.3, 127.3, 125.8, 125.7, 122.3, 121.9, 118.2, 117.1, 66.0, 15.6, 13.3; HRMS (EI+, m/z) calcd for $C_{23}H_{21}NO[M^+]$: 327.1623, found : 327.1626.

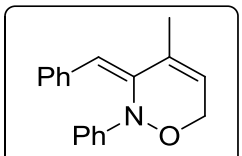
Spectral data for (*Z*)-3-benzylidene-5-methyl-2,4-diphenyl-3,6-dihydro-2*H*-1,2-oxazine (3i):



3i

Light brown oil (0.278 g, 0.82 mmol, 95%); ^{1}H NMR (500 MHz, C_6D_6): δ 7.52 (d, *J* = 7.5 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 2H), 6.99 (dd, *J* = 8.6, 1.7 Hz, 2H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.85 ~ 6.78 (m, 4H), 6.73 (s, 5H), 4.22 (s, 2H), 1.11 (s, 3H); ^{13}C NMR (125 MHz, C_6D_6): δ 147.8, 137.5, 136.7, 135.5, 134.3, 130.8, 129.7, 129.4, 129.4, 127.6, 127.1, 126.7, 126.6, 126.3, 122.4, 117.3, 67.3, 15.5; HRMS (EI+, m/z) calcd for $C_{24}H_{21}NO[M^+]$: 339.1623, found : 339.1625.

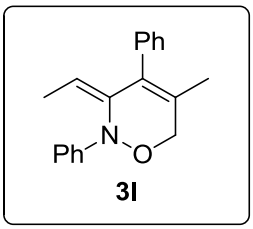
Spectral data for (*Z*)-3-benzylidene-4-methyl-2-phenyl-3,6-dihydro-2*H*-1,2-oxazine (3j):



3j

Light brown oil (0.295 g, 0.91 mmol, 99%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.07 (t, *J* = 7.8 Hz, 2H), 6.97 (t, *J* = 7.6 Hz, 2H), 6.87 (t, *J* = 7.2 Hz, 1H), 6.77 (td, *J* = 7.2, 0.8 Hz, 1H), 6.27 (s, 1H), 5.15 (s, 1H), 4.03 (s, 2H), 1.75 (d, *J* = 1.2 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 144.6, 137.7, 135.2, 130.3, 129.5, 128.7, 128.6, 127.8, 123.6, 122.3, 120.3, 117.5, 62.7, 18.9; HRMS (EI+, m/z) calcd for $C_{18}H_{17}NO[M^+]$: 263.1310, found : 263.1308.

Spectral data for (*Z*)-3-ethylidene-5-methyl-2,4-diphenyl-3,6-dihydro-2*H*-1,2-oxazine (3l):

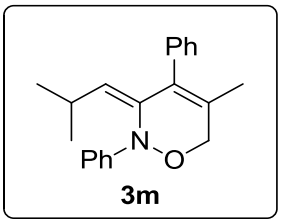


3l

Light brown oil (0.290 g, 1.0 mmol, 89%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.34 ~ 7.32 (m, 2H),

7.29 ~ 7.26 (m, 3H), 7.24 ~ 7.22 (m, 3H), 7.21 ~ 7.18 (m, 1H), 6.99 ~ 6.96 (m, 1H), 5.19 (q, *J* = 7.1 Hz, 1H), 4.11 (s, 2H), 1.59 (d, *J* = 7.7 Hz, 3H), 1.12 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 146.0, 139.1, 138.2, 130.4, 130.3, 129.7, 128.6, 128.6, 127.3, 121.8, 119.9, 116.8, 65.7, 15.7, 12.8; HRMS (EI+, m/z) calcd for $C_{19}H_{19}NO[M^+]$: 277.1467, found : 277.1469.

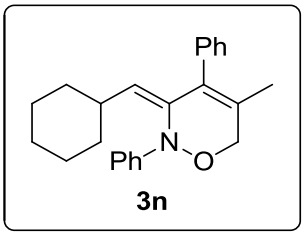
Spectral data for (*Z*)-5-methyl-3-(2-methylpropylidene)-2,4-diphenyl-3,6-dihydro-2*H*-1,2-oxazine (3m):



3m

Light brown oil (0.293 g, 0.96 mmol, 95%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.37 (d, *J* = 8.8 Hz, 2H), 7.27 (t, *J* = 7.8 Hz, 2H), 7.24 ~ 7.18 (m, 4H), 7.13 ~ 7.09 (m, 1H), 6.93 ~ 6.89 (m, 1H), 5.09 (d, *J* = 10.0 Hz, 1H), 4.03 (s, 2H), 2.93 ~ 2.84 (m, 1H), 1.04 (s, 3H), 0.78 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, C_6D_6): δ 146.9, 138.3, 136.1, 133.2, 130.4, 130.3, 129.5, 129.2, 128.6, 127.4, 122.1, 117.2, 65.5, 26.7, 22.4, 15.7; HRMS (EI+, m/z) calcd for $C_{21}H_{23}NO[M^+]$: 305.1780, found : 305.1775.

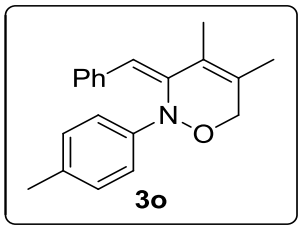
Spectral data for (*Z*)-3-(cyclohexylmethylene)-5-methyl-2,4-diphenyl-3,6-dihydro-2*H*-1,2-oxazine (3n):



3n

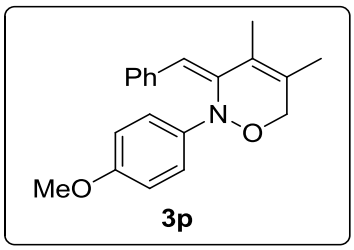
Light brown oil (0.261 g, 0.76 mmol, 90%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.41 (q, *J* = 8.3 Hz, 2H), 7.28 ~ 7.21 (m, 6H), 7.16 ~ 7.11 (m, 1H), 6.92 ~ 6.88 (m, 1H), 5.14 (d, *J* = 9.8 Hz, 1H), 4.05 (s, 2H), 2.69 ~ 2.63 (m, 1H), 1.70 (d, *J* = 12.7 Hz, 2H), 1.41 ~ 1.37 (m, 2H), 1.33 ~ 1.31 (m, 1H), 1.03 (s, 3H), 0.97 ~ 0.77 (m, 5H); ^{13}C NMR (150 MHz, C_6D_6): δ 147.1, 138.4, 136.3, 132.1, 130.5, 130.4, 129.6, 129.1, 128.6, 127.4, 122.1, 117.1, 65.4, 36.2, 32.5, 26.1, 25.7, 15.7; HRMS (EI+, m/z) calcd for $C_{24}H_{27}NO[M^+]$: 345.2093, found : 345.2096.

Spectral data for (*Z*)-3-benzylidene-4,5-dimethyl-2-(p-tolyl)-3,6-dihydro-2*H*-1,2-oxazine (3o):



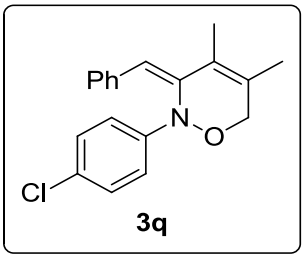
Pale yellow solid (0.295 g, 1.01 mmol, 86%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.71 (d, *J* = 7.8 Hz, 2H), 7.13 (d, *J* = 6.0 Hz, 2H), 7.02 ~ 6.99 (m, 2H), 6.91 ~ 6.86 (m, 3H), 6.35 (s, 1H), 3.98 (s, 2H), 2.01 (s, 3H), 1.78 (s, 3H), 1.16 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 142.4, 138.3, 135.9, 131.5, 130.2, 130.1, 129.6, 128.5, 127.3, 122.5, 118.3, 117.7, 65.8, 20.6, 15.1, 13.1; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO[M^+]$: 291.1623, found : 291.1624.

Spectral data for (*Z*)-3-benzylidene-2-(4-methoxyphenyl)-4,5-dimethyl-3,6-dihydro-2*H*-1,2-oxazine (3p):



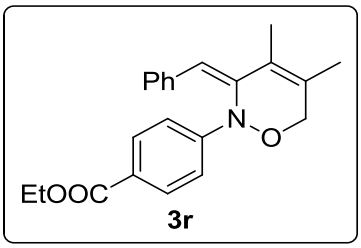
Pale yellow oil (0.319 g, 1.04 mmol, 88%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.29 (d, *J* = 9.6 Hz, 2H), 7.15 ~ 7.13 (m, 2H), 7.07 ~ 6.99 (m, 3H), 6.79 (d, *J* = 9.0 Hz, 2H), 6.54 (s, 1H), 4.11 (s, 2H), 3.31 (s, 3H), 1.57 (s, 3H), 1.13 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 156.5, 141.9, 141.3, 137.5, 132.7, 129.8, 128.1, 127.1, 122.8, 121.2, 119.8, 114.5, 68.0, 55.0, 16.9, 14.4; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1571.

Spectral data for (*Z*)-3-benzylidene-2-(4-chlorophenyl)-4,5-dimethyl-3,6-dihydro-2*H*-1,2-oxazine (3q):



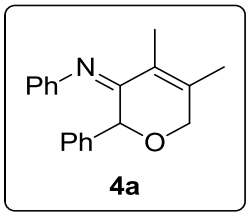
Pale yellow solid (0.300 g, 0.96 mmol, 82%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.64 (d, *J* = 7.2 Hz, 2H), 7.04 ~ 7.00 (m, 4H), 6.94 ~ 6.88 (m, 3H), 6.28 (s, 1H), 3.86 (s, 2H), 1.69 (d, *J* = 0.8 Hz, 3H), 1.18 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 143.3, 137.3, 135.5, 130.0, 129.5, 129.3, 128.7, 127.7, 127.1, 122.4, 118.8, 118.5, 66.1, 15.0, 13.0; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1070.

Spectral data for (*Z*)-ethyl 4-(3-benzylidene-4,5-dimethyl-3,6-dihydro-2*H*-1,2-oxazin-2-yl)benzoate (3r):



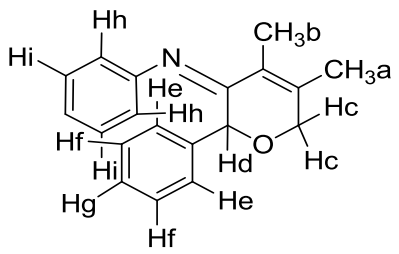
Off white solid (0.305 g, 0.87 mmol, 74%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 9.1 Hz, 2H), 7.48 (d, *J* = 7.7 Hz, 2H), 7.18 ~ 7.15 (m, 2H), 7.12 ~ 7.09 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.42 (s, 1H), 4.29 (q, *J* = 7.2 Hz, 2H), 4.27 (s, 2H), 2.03 (s, 3H), 1.66 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.4, 147.7, 136.1, 134.7, 131.0, 129.5, 128.9, 128.4, 127.5, 123.1, 122.5, 119.0, 115.2, 67.1, 60.5, 15.4, 14.3, 13.3; HRMS (EI+, m/z) calcd for $C_{22}H_{23}NO_3[M^+]$: 349.1678, found : 349.1676.

Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4a):



Pale yellow oil (0.230 g, 0.83 mmol, 83%); ^{1}H NMR (400 MHz, C6D6): δ 7.24 (d, *J* = 7.2 Hz, 2H), 7.08 ~ 7.01 (m, 3H), 6.93 (t, *J* = 7.9 Hz, 2H), 6.76 ~ 6.71 (m, 3H), 5.75 (s, 1H), 3.72 (s, 2H), 2.17 (s, 3H), 1.15 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 162.9, 151.4, 141.9, 137.1, 129.5, 128.9, 128.7, 128.5, 128.4, 123.3, 119.3, 73.2, 64.5, 15.3, 11.8; HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO[M+H]$: 278.1545, found : 278.1537.

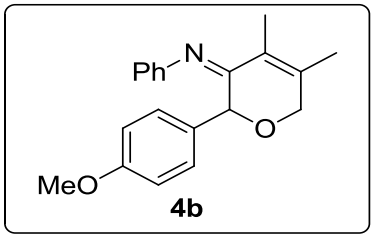
^{1}H NOE of Compound (*Z*)-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4a):



4a

Sr. No.	Irradiation	Intensity Increase % (Key peaks)
1	H_b (δ 2.17)	H_a (δ 1.15, 1.98%), H_e (δ 7.24, 0.46%)
2	H_d (δ 5.75)	H_e (δ 7.24, 5.96%), H_h (δ 6.72, 5.47%)
3	H_h (δ 6.72)	H_d (δ 5.75, 1.06%), H_i (δ 6.93, 11.05%), H_e (δ 7.24, 2.93%), H_f (δ 7.08 ~ 7.01, 1.83%)
4	H_e (δ 7.24)	H_c (δ 3.72, 0.73%), H_d (δ 5.75, 3.05%), H_h (δ 6.72, 1.54%), H_{fg} (δ 7.08 ~ 7.01, 1.51%)

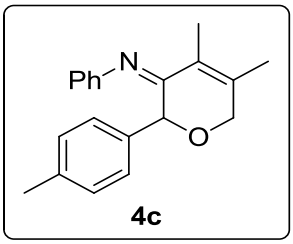
Spectral data for (*Z*)-*N*-(2-(4-methoxyphenyl)-4,5-dimethyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4b):



4b

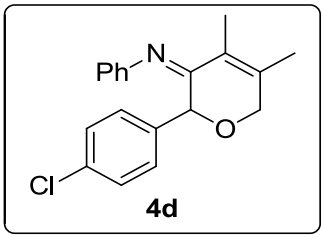
Light brown oil (0.085 g, 0.28 mmol, 85%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.12 ~ 7.06 (m, 4H), 6.92 (t, *J* = 7.4 Hz, 1H), 6.82 ~ 6.80 (m, 2H), 6.55 (dd, *J* = 7.4, 1.0 Hz, 2H), 5.33 (s, 1H), 3.93 (d, *J* = 17.5 Hz, 1H), 3.84 (d, *J* = 17.6 Hz, 1H), 3.78 (s, 3H), 2.10 (s, 3H), 1.75 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.0, 159.4, 150.4, 141.9, 129.5, 128.4, 128.0, 127.6, 122.9, 119.0, 113.5, 72.5, 64.1, 55.0, 15.8, 11.6; HRMS (ESI+, m/z) calcd for $C_{20}H_{22}NO_2$[M+H] : 308.1651, found : 308.1647.

Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-(*p*-tolyl)-2*H*-pyran-3(6*H*)-ylidene)aniline (4c):



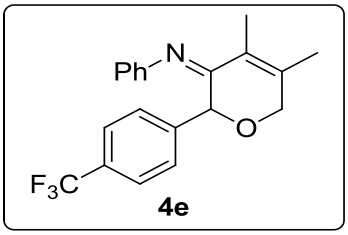
Pale yellow oil (0.085 g, 0.29 mmol, 85%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.12 ~ 7.04 (m, 6H), 6.91 (t, *J* = 7.4 Hz, 1H), 6.57 (d, *J* = 7.9 Hz, 2H), 5.37 (s, 1H), 3.93 (d, *J* = 17.5 Hz, 1H), 3.85 (d, *J* = 17.5 Hz, 1H), 2.33 (s, 3H), 2.10 (s, 3H), 1.74 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.1, 150.3, 142.1, 138.0, 133.0, 128.9, 128.5, 128.2, 127.7, 123.1, 119.1, 72.7, 64.3, 21.2, 15.9, 11.7; HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO$[M+H] : 292.1701, found : 292.1709.

Spectral data for (*Z*)-*N*-(2-(4-chlorophenyl)-4,5-dimethyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4d):



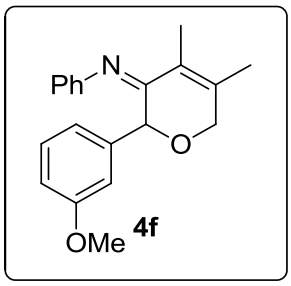
Light brown oil (0.088 g, 0.28 mmol, 88%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.00 ~ 6.93 (m, 6H), 6.77 ~ 6.75 (m, 1H), 6.65 (d, *J* = 8.4 Hz, 2H), 5.60 (s, 1H), 3.68 (d, *J* = 17.5 Hz, 1H), 3.59 (d, *J* = 17.6 Hz, 1H), 2.12 (s, 3H), 1.17 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 162.3, 151.2, 141.9, 135.4, 134.4, 130.0, 129.0, 128.7, 123.4, 119.2, 72.4, 64.4, 15.3, 11.8; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1080.

Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-(4-(trifluoromethyl)phenyl)-2*H*-pyran-3(6*H*)-ylidene)aniline (4e):



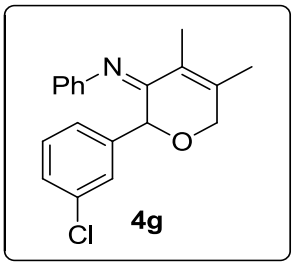
Light brown oil (0.082 g, 0.24 mmol, 82%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.22 (d, *J* = 8.2 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.93 (t, *J* = 7.8 Hz, 2H), 6.74 (t, *J* = 7.4 Hz, 1H), 6.64 (d, *J* = 7.7 Hz, 2H), 5.65 (s, 1H), 3.67 (d, *J* = 17.6 Hz, 1H), 3.51 (d, *J* = 17.6 Hz, 1H), 2.13 (s, 3H), 1.14 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 162.0, 151.1, 141.9, 140.8, 130.5 ($J_{C\text{-}F}$ = 32.5), 129.1, 128.8, 125.4 ($J_{C\text{-}F}$ = 2.8), 123.5, 119.1, 72.3, 64.5, 15.3, 11.8; HRMS (EI+, m/z) calcd for $C_{20}H_{18}F_3NO[M^+]$: 345.1340, found : 345.1343.

Spectral data for (*Z*)-*N*-(2-(3-methoxyphenyl)-4,5-dimethyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4f):



Light brown oil (0.092 g, 0.30 mmol, 92%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.02 (t, *J* = 7.9 Hz, 1H), 6.96 ~ 6.91 (m, 4H), 6.78 ~ 6.73 (m, 3H), 6.66 (dd, *J* = 8.2, 2.4 Hz, 1H), 5.76 (s, 1H), 3.84 ~ 3.73 (m, 2H), 3.23 (s, 3H), 2.16 (s, 3H), 1.17 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 162.8, 160.2, 151.4, 141.8, 138.6, 129.5, 128.9, 123.3, 120.8, 119.4, 114.4, 114.1, 73.1, 64.6, 54.6, 15.3, 11.8; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1574.

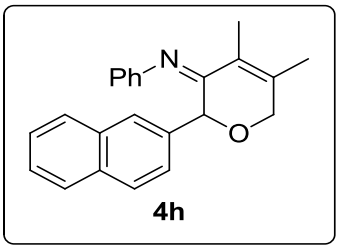
Spectral data for (*Z*)-*N*-(2-(3-chlorophenyl)-4,5-dimethyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4g):



Light brown oil (0.085 g, 0.27 mmol, 85%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.33 (s, 1H), 6.97 (td, *J* = 8.5, 1.4 Hz, 2H), 6.93 (t, *J* = 7.9 Hz, 2H), 6.76 ~ 6.72 (m, 2H), 6.69 (dd, *J* = 7.5, 1.0 Hz, 2H), 5.64 (s, 1H), 3.67 ~ 3.59 (m, 2H), 2.10 (s, 3H), 1.10 (s, 3H); ^{13}C NMR (150 MHz,

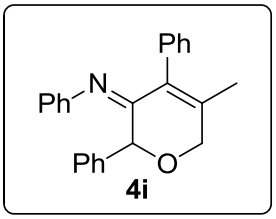
C_6D_6): δ 162.1, 151.2, 142.0, 139.2, 134.7, 129.8, 129.0, 128.7, 128.7, 126.6, 123.4, 119.1, 72.4, 64.5, 15.2, 11.8; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1076.

Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-(naphthalen-2-yl)-2*H*-pyran-3(6*H*)-ylidene)aniline (4h):



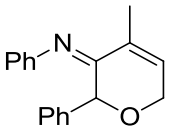
Light brown oil (0.080 g, 0.24 mmol, 80%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.84 ~ 7.79 (m, 2H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.59 (s, 1H), 7.51 ~ 7.47 (m, 2H), 7.36 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.07 (t, *J* = 7.9 Hz, 2H), 6.89 (t, *J* = 7.4 Hz, 1H), 6.61 (dd, *J* = 8.3, 1.0 Hz, 2H), 5.56 (s, 1H), 3.97 (d, *J* = 17.3 Hz, 1H), 3.83 (d, *J* = 17.4 Hz, 1H), 2.16 (s, 3H), 1.73 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.8, 150.4, 142.0, 133.6, 133.2, 132.8, 128.6, 128.2, 128.1, 127.6, 127.3, 126.4, 126.2, 126.0, 123.1, 119.0, 72.9, 64.6, 15.9, 11.8; HRMS (EI+, m/z) calcd for $C_{23}H_{21}NO[M^+]$: 327.1623, found : 327.1620.

Spectral data for (*Z*)-*N*-(5-methyl-2,4-diphenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4i):



Light brown oil (0.082 g, 0.24 mmol, 82%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.47 ~ 7.44 (m, 4H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.19 ~ 7.14 (m, 3H), 7.08 (t, *J* = 7.4 Hz, 1H), 6.88 (t, *J* = 7.9 Hz, 2H), 6.71 (t, *J* = 7.4 Hz, 1H), 6.65 (d, *J* = 7.7 Hz, 2H), 5.86 (s, 1H), 3.89 (q, *J* = 13.6 Hz, 2H), 1.19 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 162.2, 151.1, 144.0, 137.0, 136.9, 134.9, 130.8, 128.8, 128.7, 128.6, 128.6, 128.2, 127.3, 123.3, 119.1, 79.1, 64.5, 16.6; HRMS (EI+, m/z) calcd for $C_{24}H_{21}NO[M^+]$: 339.1623, found : 339.1624.

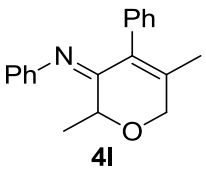
Spectral data for (*Z*)-*N*-(4-methyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4j):



4j

Pale yellow oil (0.090 g, 0.28 mmol, 90%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.30 ~ 7.23 (m, 2H), 7.15 ~ 7.08 (m, 3H), 7.01 ~ 6.97 (m, 2H), 6.84 ~ 6.81 (m, 1H), 6.80 ~ 6.75 (m, 2H), 5.79 (s, 1H), 5.71 ~ 5.69 (m, 1H), 3.90 ~ 3.74 (m, 2H), 2.23 (t, *J* = 1.8 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 163.2, 150.8, 136.8, 134.5, 133.4, 128.9, 128.6, 128.5 (1 CH-merged), 123.5, 119.2, 73.6, 60.5, 17.5; HRMS (EI+, m/z) calcd for $C_{18}H_{17}NO[M^+]$: 263.1310, found : 263.1313.

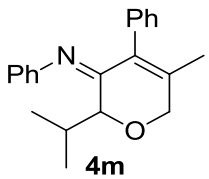
Spectral data for (*Z*)-*N*-(2,5-dimethyl-4-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4l):



4l

Pale yellow oil (0.080 g, 0.29 mmol, 80%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.27 ~ 7.22 (m, 4H), 7.14 ~ 7.11 (m, 1H), 7.02 (t, *J* = 7.9 Hz, 2H), 6.80 (t, *J* = 7.5 Hz, 1H), 6.59 (dd, *J* = 8.4, 1.1 Hz, 2H), 4.86 (q, *J* = 6.8 Hz, 1H), 4.11 (d, *J* = 17.9 Hz, 1H), 3.95 (d, *J* = 17.9 Hz, 1H), 1.28 (s, 3H), 1.14 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 165.1, 151.7, 147.7, 137.0, 133.2, 130.8, 129.1, 128.0, 127.1, 122.8, 118.8, 67.5, 63.9, 16.5, 16.1; HRMS (EI+, m/z) calcd for $C_{19}H_{19}NO[M^+]$: 277.1467, found : 277.1464.

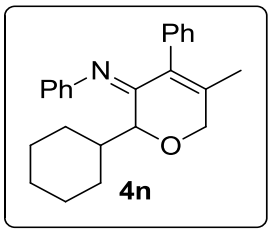
Spectral data for (*Z*)-*N*-(2-isopropyl-5-methyl-4-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4m):



4m

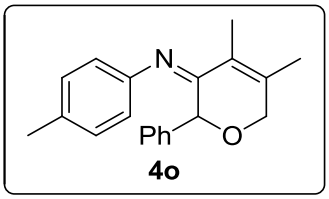
Pale yellow oil (0.085 g, 0.28 mmol, 85%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.26 (d, *J* = 4.4 Hz, 4H), 7.13 (s, 1H), 7.02 (t, *J* = 7.8 Hz, 2H), 6.78 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 2H), 4.55 (d, *J* = 9.6 Hz, 1H), 4.01 (dd, *J* = 18.0, 23.6 Hz, 2H), 2.03 ~ 1.97 (m, 1H), 1.28 (s, 3H), 0.87 (d, *J* = 6.4 Hz, 3H), 0.70 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 164.2, 151.5, 141.6, 137.5, 134.3, 130.7, 128.9, 128.1, 127.1, 122.9, 119.9, 75.1, 64.8, 27.7, 19.4, 18.9, 16.1; HRMS (EI+, m/z) calcd for $C_{21}H_{23}NO[M^+]$: 305.1780, found : 305.1776.

Spectral data for (*Z*)-*N*-(2-cyclohexyl-5-methyl-4-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4n):



Pale yellow oil (0.082 g, 0.24 mmol, 82%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.30 (d, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 7.0 Hz, 2H), 7.14 ~ 7.13 (m, 1H), 7.8 (t, *J* = 7.2 Hz, 2H), 6.79 (t, *J* = 7.4 Hz, 1H), 6.75 (d, *J* = 7.7 Hz, 2H), 4.71 (d, *J* = 9.9 Hz, 1H), 4.13 (d, *J* = 18.1 Hz, 1H), 4.03 (d, *J* = 18.1 Hz, 1H), 2.03 ~ 1.90 (m, 2H), 1.63 ~ 1.44 (m, 4H), 1.30 (s, 3H), 1.21 ~ 1.03 (m, 3H), 0.91 ~ 0.70 (m, 2H); ^{13}C NMR (150 MHz, C_6D_6): δ 163.9, 151.5, 141.7, 137.5, 134.4, 130.8, 128.9, 128.1, 127.1, 122.9, 119.9, 74.1, 64.8, 37.7, 30.1, 29.2, 26.3, 26.3, 26.0, 16.2; HRMS (EI+, m/z) calcd for $C_{24}H_{27}NO[M^+]$: 345.2093, found : 345.2089.

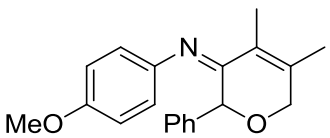
Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)-4-methylaniline (4o):



Light brown oil (0.085 g, 0.29 mmol, 85%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.29 ~ 7.28 (m, 2H), 7.09 ~ 7.06 (m, 2H), 7.04 ~ 7.02 (m, 1H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.69 ~ 6.67 (m, 2H), 5.81 (s, 1H), 3.73 (s, 2H), 2.19 (s, 3H), 1.97 (s, 3H), 1.16 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 162.9, 148.8, 141.5, 137.2, 132.4, 129.5, 128.7 (1-q merged), 128.5, 128.4, 119.4,

73.1, 64.5, 20.7, 15.3, 11.9; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO[M^+]$: 291.1623, found : 291.1625.

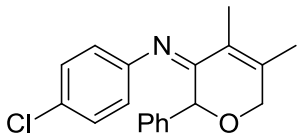
Spectral data for (*Z*)-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)-4-methoxyaniline (4p):



4p

Light brown oil (0.090 g, 0.29 mmol, 90%); ^{1}H NMR (500 MHz, C_6D_6): δ 7.30 (d, *J* = 7.5 Hz, 2H), 7.11 ~ 7.03 (m, 3H), 6.70 ~ 6.68 (m, 2H), 6.54 ~ 6.51 (m, 2H), 5.83 (s, 1H), 3.74 (s, 2H), 3.19 (s, 3H), 2.20 (s, 3H), 1.18 (s, 3H); ^{13}C NMR (125 MHz, C_6D_6): δ 163.0, 156.4, 144.3, 141.1, 137.4, 128.7, 128.6, 128.4, 128.3, 120.8, 114.3, 73.0, 64.5, 54.8, 15.3, 12.0; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1573.

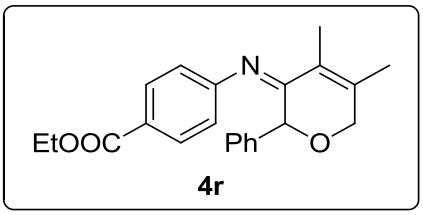
Spectral data for (*Z*)-4-chloro-*N*-(4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)aniline (4q):



4q

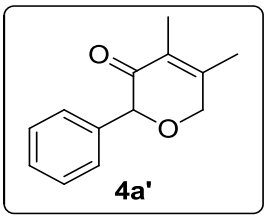
Pale yellow oil (0.092 g, 0.30 mmol, 92%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.18 (d, *J* = 7.6 Hz, 2H), 7.07 ~ 7.02 (m, 3H), 6.82 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.41 (dd, *J* = 8.4, 1.6 Hz, 2H), 5.58 (s, 1H), 3.70 (s, 2H), 2.12 (s, 3H), 1.15 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 163.5, 149.7, 142.6, 136.8, 128.9, 128.6, 128.6, 120.7, 73.2, 64.4, 15.3, 11.7; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1074.

Spectral data for (*Z*)-ethyl 4-((4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-ylidene)amino)benzoate (4r):



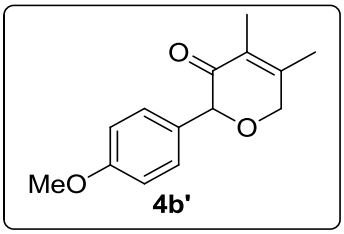
Pale yellow oil (0.081 g, 0.23 mmol, 81%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.19 ~ 7.15 (m, 2H), 7.04 ~ 7.02 (m, 3H), 6.59 (d, *J* = 8.0 Hz, 2H), 5.59 (s, 1H), 4.06 (q, *J* = 7.1 Hz, 2H), 3.70 (s, 2H), 2.11 (s, 3H), 1.15 (s, 3H), 0.96 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 166.0, 163.0, 155.5, 143.2, 136.6, 130.8, 128.6, 125.9, 119.0, 73.6, 64.4, 60.4, 15.4, 14.3, 11.7; HRMS (EI+, m/z) calcd for $C_{12}H_{23}NO_3[M^+]$: 349.1678, found : 349.1675.

Spectral data for 4,5-dimethyl-2-phenyl-2*H*-pyran-3(6*H*)-one (4a'):



Pale yellow oil (0.059 g, 0.29 mmol, 85%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 ~ 7.28 (m, 5H), 5.04 (s, 1H), 4.32 ~ 4.30 (m, 2H), 1.85 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.8, 152.5, 135.6, 129.3, 128.3, 128.2, 127.5, 81.2, 67.2, 16.2, 9.8; HRMS (ESI, m/z) calcd for $C_{13}H_{15}O_2[M+H]$: 203.1072, found : 203.1069.

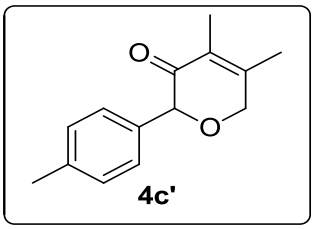
Spectral data for 2-(4-methoxyphenyl)-4,5-dimethyl-2*H*-pyran-3(6*H*)-one (4b'):



Pale yellow oil (0.042 g, 0.18 mmol, 56%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.22 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 4.99 (s, 1H), 4.33 ~ 4.23 (m, 2H), 3.78 (s, 3H), 1.85 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.2, 159.5, 152.5, 129.3, 128.9, 127.8, 113.8, 80.9, 67.1, 55.2, 16.2, 9.8; HRMS (EI+, m/z) calcd for $C_{14}H_{16}O_3[M^+]$: 232.1099,

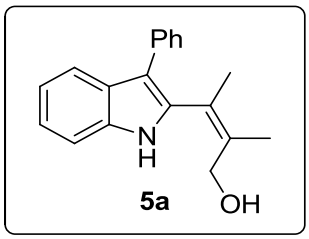
found : 232.1096.

Spectral data for 4,5-dimethyl-2-(*p*-tolyl)-2*H*-pyran-3(6*H*)-one (4c'):



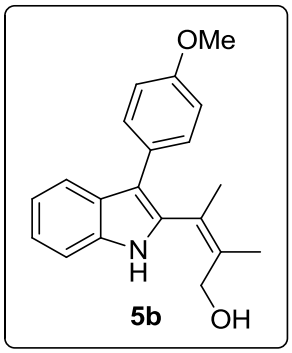
Pale yellow oil (0.037 g, 0.17 mmol, 50%); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.24 ~ 7.12 (m, 4H), 5.01 (s, 1H), 4.34 ~ 4.24 (m, 2H), 2.33 (s, 3H), 1.84 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.0, 152.4, 138.0, 132.5, 129.3, 129.0, 127.5, 81.0, 67.0, 21.1, 16.2, 9.8; HRMS (ESI, m/z) calcd for $C_{14}H_{17}O_2$[M+H] : 217.1229, found : 217.1234.

Spectral data for (*Z*)-2-methyl-3-(3-phenyl-1*H*-indol-2-yl)but-2-en-1-ol (5a):



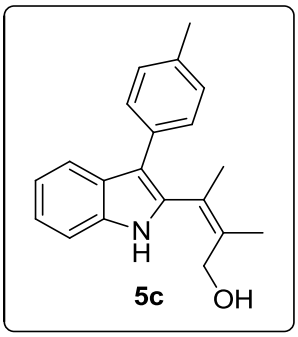
Light brown oil (0.186 g, 0.67 mmol, 67%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (bs, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.40 (t, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 1H), 7.20 (td, *J* = 7.0, 1.2 Hz, 1H), 7.13 (td, *J* = 7.0, 1.1 Hz, 1H), 3.89 (s, 2H), 1.95 (s, 3H), 1.87 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.0, 135.8, 135.5, 135.3, 129.1, 128.6, 127.2, 126.1, 125.8, 122.2, 120.1, 119.2, 114.6, 110.8, 65.4, 19.7, 16.9; HRMS (ESI, m/z) calcd for $C_{19}H_{20}NO$ [M+H] : 278.1545, found : 278.1549.

Spectral data for (*Z*)-3-(3-(4-methoxyphenyl)-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5b):



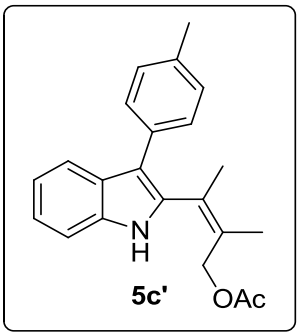
Pale yellow oil (0.068 g, 0.17 mmol, 68%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.48 (bs, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.19 (t, *J* = 7.1 Hz, 1H), 7.12 (t, *J* = 7.1 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 3.90 (s, 2H), 3.84 (s, 3H), 1.94 (s, 3H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 158.0, 135.6, 135.5, 135.2, 130.1, 127.8, 127.3, 126.0, 122.0, 119.9, 119.2, 114.1, 113.7, 110.8, 65.4, 55.2, 19.6, 16.9; HRMS: (ESI, m/z) calcd for $C_{20}H_{22}NO_2$ [M+H] : 308.1651, found : 308.1647.

Spectral data for (*Z*)-2-methyl-3-(3-(*p*-tolyl)-1*H*-indol-2-yl)but-2-en-1-ol (5c):



Pale yellow oil (0.052 g, 0.18 mmol, 52%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.40 (bs, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.18 (td, *J* = 7.6, 1.0 Hz, 1H), 7.11 (td, *J* = 7.0, 1.0 Hz, 1H), 3.88 (s, 2H), 2.37 (s, 3H), 1.96 (s, 3H), 1.87 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 135.7, 135.7, 135.7, 135.3, 132.4, 129.3, 129.0, 127.2, 125.8, 122.1, 112.0, 119.3, 114.5, 110.8, 65.5, 21.2, 19.7, 16.9; HRMS (ESI, m/z) calcd for $C_{20}H_{22}NO$ [M+H] : 292.1701, found : 292.1691.

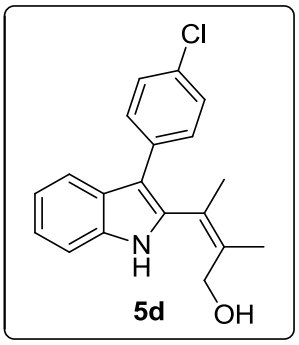
Spectral data for (*Z*)-2-methyl-3-(3-(*p*-tolyl)-1*H*-indol-2-yl)but-2-en-1-yl acetate (5c'):



5c'

Pale yellow solid (0.171 g, 0.51 mmol, 95%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.00 (bs, 1H), 7.77 (d, *J* = 7.9 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 3H), 7.24 ~ 7.21 (m, 3H), 7.15 (td, *J* = 7.4, 0.9 Hz, 1H), 4.57 (s, 2H), 2.42 (s, 3H), 2.07 (s, 3H), 1.91 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 171.5, 135.3, 135.2, 134.9, 132.4, 131.1, 129.1, 128.8, 128.0, 127.4, 122.0, 119.8, 119.2, 115.0, 110.9, 67.5, 21.2, 20.9, 19.7, 15.9; HRMS (ESI, m/z) calcd for $C_{22}H_{23}NNaO_2$[M+Na] : 356.1621, found : 356.1620.

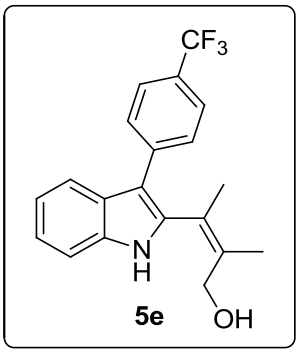
Spectral data for (*Z*)-3-(3-(4-chlorophenyl)-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5d):



5d

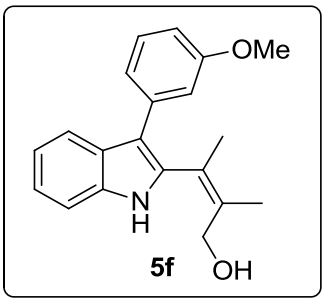
Light brown oil (0.095 g, 0.30 mmol, 95%); ^{1}H NMR (600 MHz, C_6D_6): δ 8.03 (bs, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.33 ~ 7.31 (m, 2H), 7.24 ~ 7.17 (m, 4H), 7.15 ~ 7.14 (m, 1H), 3.59 (s, 2H), 1.67 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 136.3, 136.1, 135.7, 134.7, 131.9, 130.5, 129.0, 128.3, 126.1, 122.6, 120.7, 119.5, 113.7, 111.3, 65.0, 19.4, 16.7; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1075.

Spectral data for (*Z*)-2-methyl-3-(3-(4-(trifluoromethyl)phenyl)-1*H*-indol-2-yl)but-2-en-1-ol (5e):



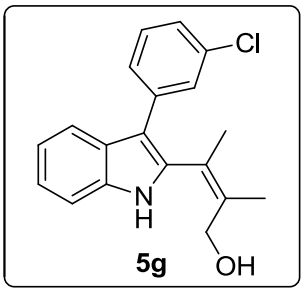
Light brown oil (0.062 g, 0.18 mmol, 62%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.89 (bs, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.46 ~ 7.45 (m, 4H), 7.26 ~ 7.23 (m, 1H), 7.21 ~ 7.18 (m, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 3.54 (s, 2H), 1.66 (s, 3H), 1.62 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 140.1, 136.9, 136.5, 135.7, 129.3, 128.3, 127.5, 126.0, 125.7 ($J_{C\text{-}F}$ = 3.0), 122.8, 120.9, 119.4, 113.4, 111.4, 64.9, 19.4, 16.8; HRMS (EI+, m/z) calcd for $C_{20}H_{18}F_3NO[M^+]$: 345.1340, found : 345.1343.

Spectral data for (*Z*)-3-(3-(3-methoxyphenyl)-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5f):



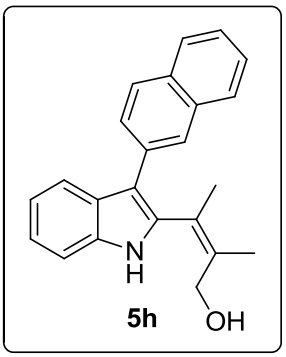
Light brown oil (0.088 g, 0.29 mmol, 88%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.94 (d, *J* = 7.9 Hz, 1H), 7.86 (bs, 1H), 7.28 ~ 7.27 (m, 1H), 7.25 ~ 7.16 (m, 5H), 6.76 ~ 6.75 (m, 1H), 3.68 (s, 2H), 3.37 (s, 3H), 1.75 (s, 3H), 1.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 160.4, 137.6, 136.2, 136.1, 135.8, 129.8, 128.3, 126.1, 122.4, 121.8, 120.6, 119.8, 115.1, 114.8, 111.9, 111.2, 65.2, 54.7, 19.6, 16.7; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1576.

Spectral data for (*Z*)-3-(3-(3-chlorophenyl)-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5g):



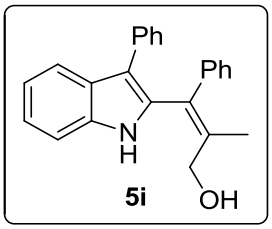
Light brown oil (0.084 g, 0.27 mmol, 84%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.99 (bs, 1H), 7.79 (d, *J* = 7.9 Hz, 1H), 7.66 (s, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.16 ~ 7.09 (m, 3H), 6.96 (t, *J* = 7.9 Hz, 1H), 3.56 (s, 2H), 1.66 (s, 3H), 1.65 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 138.3, 136.6, 136.3, 135.7, 134.7, 130.0, 129.2, 127.6, 127.3, 126.1, 126.0, 122.6, 120.8, 119.4, 113.4, 111.3, 64.9, 19.4, 16.7; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1080.

Spectral data for (*Z*)-2-methyl-3-(3-(naphthalen-2-yl)-1*H*-indol-2-yl)but-2-en-1-ol (5h):



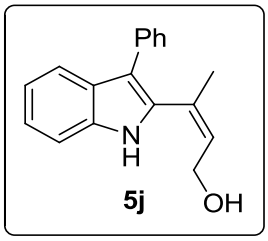
Light yellow solid (0.060 g, 0.18 mmol, 60%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.58 (bs, 1H), 7.96 (s, 1H), 7.88 ~ 7.80 (m, 4H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.50 ~ 7.43 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 7.9 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 3.96 (s, 2H), 1.94 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.3, 135.8, 135.2, 133.7, 133.0, 131.9, 127.9, 127.8, 127.7, 127.3, 127.2, 126.4, 126.0, 125.4, 122.2, 120.2, 119.2, 114.5, 110.9, 65.4, 19.7, 17.1; HRMS (EI+, m/z) calcd for $C_{23}H_{22}NO[M^+]$: 327.1623, found : 327.1625.

Spectral data for (*Z*)-2-methyl-3-phenyl-3-(3-phenyl-1*H*-indol-2-yl)prop-2-en-1-ol (5i):



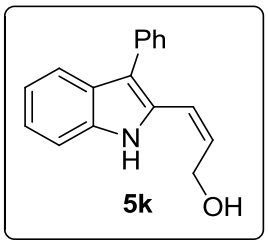
Light brown oil (0.085 g, 0.25 mmol, 85%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.99 (bs, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.7 Hz, 2H), 7.33 ~ 7.24 (m, 7H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 3.88 (s, 2H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 140.2, 138.5, 135.8, 135.2, 134.3, 129.8, 129.4, 129.3, 128.7, 128.2, 127.4, 126.9, 126.4, 122.5, 120.2, 119.4, 116.6, 110.8, 65.6, 18.0; HRMS (EI+, m/z) calcd for $C_{24}H_{21}NO[M^+]$: 339.1623, found : 277.1627.

Spectral data for (*Z*)-3-(3-phenyl-1*H*-indol-2-yl)but-2-en-1-ol (5j):



Pale yellow oil (0.096 g, 0.30 mmol, 96%); ^{1}H NMR (400 MHz, C_6D_6): δ 8.60 (bs, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.48 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.21 ~ 7.16 (m, 3H), 7.12 ~ 7.03 (m, 3H), 5.55 ~ 5.51 (m, 1H), 3.66 (d, *J* = 7.2 Hz, 2H), 1.73 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 136.2, 136.1, 133.6, 132.4, 132.4, 129.9, 129.7, 128.8, 126.3, 122.8, 120.6, 119.8, 116.1, 111.5, 60.1, 23.7; HRMS (EI+, m/z) calcd for $C_{18}H_{17}NO[M^+]$: 263.1310, found : 263.1312.

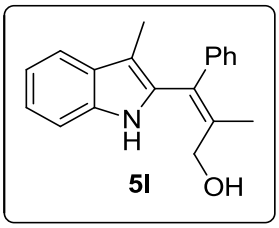
Spectral data for (*Z*)-3-(3-phenyl-1*H*-indol-2-yl)prop-2-en-1-ol (5k):



Pale yellow oil (0.080 g, 0.32 mmol, 80%); ^{1}H NMR (400 MHz, C_6D_6): δ 10.3 (bs, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.59 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.24 ~ 7.12 (m,

4H), 6.73 (d, J = 12.0 Hz, 1H), 5.41 ~ 5.35 (m, 1H), 3.75 (d, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, C_6D_6): δ 137.3, 135.6, 131.7, 130.6, 128.8, 128.2, 126.6, 125.7, 125.3, 123.6, 120.7, 120.3, 119.3, 111.6, 58.8; HRMS (ESI+, m/z) calcd for $C_{17}H_{16}NO$[M+H] : 250.1232, found : 250.1230.

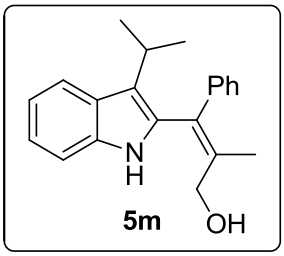
Spectral data for (*Z*)-2-methyl-3-(3-methyl-1*H*-indol-2-yl)-3-phenylprop-2-en-1-ol (5l):



5l

Pale yellow oil (0.084 g, 0.30 mmol, 84%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.85 (bs, 1H), 7.59 (dd, J = 7.6, 0.8 Hz, 1H), 7.24 ~ 7.18 (m, 2H), 7.10 (d, J = 4.5 Hz, 4H), 7.06 ~ 7.02 (m, 2H), 3.84 (s, 2H), 2.02 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 141.0, 137.1, 136.1, 130.4, 134.4, 132.0, 130.1, 129.7, 128.3, 127.2, 122.3, 119.6, 119.2, 111.0, 110.6, 65.3, 18.5, 9.4; HRMS (EI+, m/z) calcd for $C_{19}H_{19}NO[M^+]$: 277.1467, found : 277.1463.

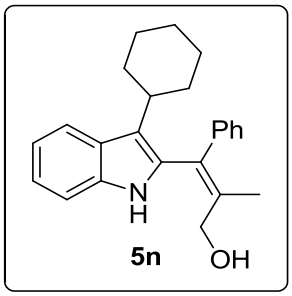
Spectral data for (*Z*)-3-(3-isopropyl-1*H*-indol-2-yl)-2-methyl-3-phenylprop-2-en-1-ol (5m):



5m

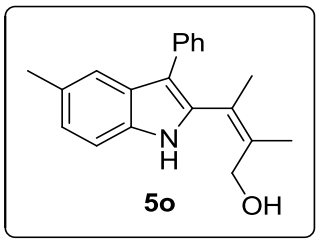
Pale yellow oil (0.082 g, 0.27 mmol, 82%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.81 (d, J = 8.0 Hz, 1H), 7.63 (bs, 1H), 7.20 ~ 7.17 (m, 1H), 7.14 ~ 7.01 (m, 7H), 3.83 (s, 2H), 3.00 (p, J = 7.2 Hz, 1H), 1.90 (s, 3H), 1.33 (s, 3H), 1.31 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 141.3, 138.1, 136.7, 133.0, 132.1, 129.9, 128.2, 127.3, 127.1, 121.9, 121.0, 120.5, 119.3, 111.4, 65.4, 26.7, 22.8, 18.1; HRMS (EI+, m/z) calcd for $C_{21}H_{23}NO[M^+]$: 305.1780, found : 305.1774.

Spectral data for (*Z*)-3-(3-cyclohexyl-1*H*-indol-2-yl)-2-methyl-3-phenylprop-2-en-1-ol (5n):



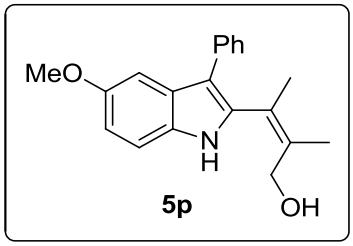
Pale yellow oil (0.086 g, 0.25 mmol, 86%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.87 (d, *J* = 7.8 Hz, 1H), 7.81 (bs, 1H), 7.21 ~ 7.15 (m, 4H), 7.11 ~ 7.08 (m, 3H), 7.04 ~ 7.01 (m, 1H), 3.86 (s, 2H), 2.65 ~ 2.61 (m, 1H), 1.98 ~ 1.95 (m, 2H), 1.90 (s, 3H), 1.71 ~ 1.69 (m, 4H), 1.64 ~ 1.62 (m, 1H), 1.24 ~ 1.11 (m, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 141.4, 137.8, 136.7, 133.3, 132.5, 130.0, 128.2, 127.7, 127.2, 121.8, 121.3, 120.0, 119.2, 111.4, 65.4, 37.3, 33.1, 27.6, 26.6, 18.2; HRMS (EI+, m/z) calcd for $C_{24}H_{27}NO[M^+]$: 345.2093, found : 345.2094.

Spectral data for (*Z*)-2-methyl-3-(5-methyl-3-phenyl-1*H*-indol-2-yl)but-2-en-1-ol (5o):



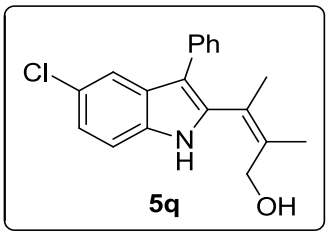
Pale yellow oil (0.061 g, 0.21 mmol, 61%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.34 (bs, 1H), 7.51 (s, 1H), 7.49 ~ 7.44 (m, 2H), 7.40 (t, *J* = 8.0 Hz, 2H), 7.28 ~ 7.22 (m, 2H), 7.02 (d, *J* = 8.2 Hz, 1H), 3.88 (s, 2H), 2.43 (s, 3H), 1.95 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 136.1, 135.6, 135.6, 133.6, 129.4, 129.2, 128.5, 127.4, 126.0, 125.8, 123.7, 118.8, 114.2, 110.5, 65.4, 21.5, 19.7, 16.9; HRMS (ESI+, m/z) calcd for $C_{20}H_{22}NO[M+H]$: 292.1701, found : 292.1698.

Spectral data for (*Z*)-3-(5-methoxy-3-phenyl-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5p):



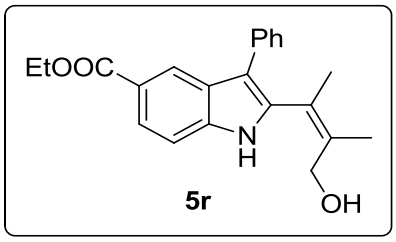
Yellow oil (0.045 g, 0.15 mmol, 45%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.33 (bs, 1H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.41 (t, *J* = 8.2 Hz, 2H), 7.29 ~ 7.23 (m, 2H), 7.18 (s, 1H), 6.87 ~ 6.84 (m, 1H), 3.89 (s, 2H), 3.81 (s, 3H), 1.93 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.6, 136.9, 135.7, 135.6, 130.4, 129.0, 128.6, 127.5, 126.0, 125.9, 114.5, 112.4, 111.6, 101.1, 65.5, 56.0, 19.7, 16.9; HRMS (ESI+, m/z) calcd for $C_{20}H_{22}NO_2$[M+H] : 308.1651, found : 308.1646.

Spectral data for (*Z*)-3-(5-chloro-3-phenyl-1*H*-indol-2-yl)-2-methylbut-2-en-1-ol (5q):



Light brown oil (0.082 g, 0.26 mmol, 82%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.93 (d, *J* = 1.2 Hz, 1H), 7.84 (bs, 1H), 7.42 ~ 7.40 (m, 2H), 7.24 ~ 7.17 (m, 3H), 7.09 ~ 7.05 (m, 1H), 6.85 (d, *J* = 8.8 Hz, 1H), 3.56 (s, 2H), 1.65 (s, 6H); ^{13}C NMR (100 MHz, C_6D_6): δ 137.5, 136.3, 135.4, 134.0, 129.3, 129.0, 128.9, 126.5, 126.4, 125.8, 122.7, 119.3, 114.8, 112.2, 65.1, 19.4, 16.8; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1073.

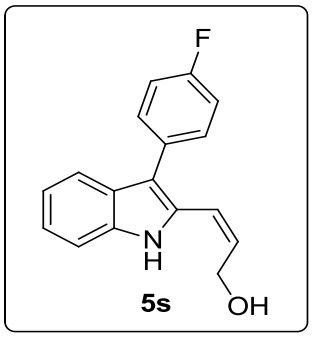
Spectral data for (*Z*)-ethyl 2-(4-hydroxy-3-methylbut-2-en-2-yl)-3-phenyl-1*H*-indole-5-carboxylate (5r):



Pale yellow oil (0.072 g, 0.21 mmol, 72%); ^{1}H NMR (600 MHz, C_6D_6): δ 9.00 (s, 1H), 8.36 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.18 (bs, 1H), 7.54 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.19 (t, *J* = 7.7 Hz, 2H), 7.09 (d, *J* = 8.6 Hz, 1H), 7.06 (t, *J* = 7.4 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 3.61 (s, 2H), 1.67 (s, 3H), 1.66 (s, 3H), 1.05 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 167.5, 138.2, 137.4, 136.4, 135.4, 139.5, 129.0, 127.6, 126.6, 125.8, 124.2, 123.5, 122.6, 116.2, 111.0, 65.1, 60.6, 19.4, 16.9, 14.4; HRMS (EI+, m/z) calcd for $C_{22}H_{23}NO_3[M^+]$: 349.1678,

found : 349.1673.

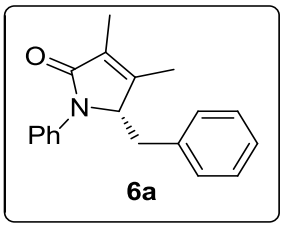
Spectral data for (*Z*)-3-(3-(4-fluorophenyl)-1*H*-indol-2-yl)prop-2-en-1-ol (5s):



5s

Light brown oil (1.0 g, 3.74 mmol, 60%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 10.26 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.46 ~ 7.40 (m, 3H), 7.23 ~ 7.21 (m, 1H), 7.16 ~ 7.09 (m, 3H), 6.72 (d, *J* = 11.9 Hz, 1H), 5.93 (dt, *J* = 11.8, 6.9 Hz, 1H), 4.42 (d, *J* = 6.9 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.5, 160.9, 136.6, 131.54, 131.49, 131.3, 130.7, 127.3, 125.6, 125.4, 123.3, 120.2, 119.6, 117.8, 115.4, 115.3, 111.4, 59.1; HRMS (ESI, m/z) calcd for $C_{17}H_{14}FNO$[M+H] : 268.1132, found : 268.1125.

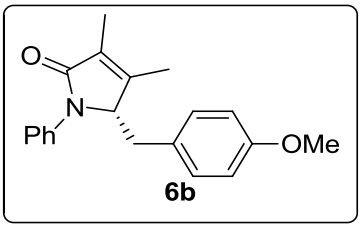
Spectral data for (*S*)-5-benzyl-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6a):



6a

Light yellow solid (0.169 g, 0.61 mmol, 61%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.71 (d, *J* = 8.6 Hz, 2H), 7.25 (t, *J* = 8.0 Hz, 2H), 6.98 ~ 6.95 (m, 4H), 6.71 (d, *J* = 7.6 Hz, 2H), 4.06 (s, 1H), 2.75 (dd, *J* = 14.5, 5.7 Hz, 1H), 2.51 (dd, *J* = 14.5, 3.1 Hz, 1H), 1.57 (d, *J* = 0.8 Hz, 3H), 1.39 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 170.2, 147.7, 138.6, 135.4, 130.4, 129.4, 129.2, 128.2, 126.9, 123.7, 121.2, 62.5, 34.9, 12.4, 8.6; HRMS (EI+, m/z) calcd for $C_{19}H_{19}NO[M^+]$: 277.1467, found : 277.1465.

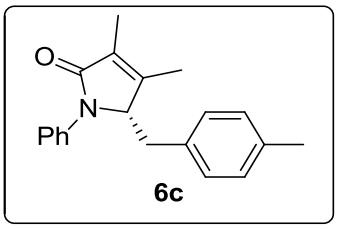
Spectral data for (*S*)-5-(4-methoxybenzyl)-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6b):



6b

Yellow oil (0.021 g, 0.07 mmol, 21%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.74 (dd, *J* = 2.8, 1.6 Hz, 2H), 7.29 ~ 7.25 (m, 2H), 7.00 ~ 6.95 (m, 1H), 6.65 (dd, *J* = 8.4, 1.2 Hz, 2H), 6.60 (dd, *J* = 8.8, 1.2 Hz, 2H), 4.06 (s, 1H), 3.20 (d, *J* = 1.2 Hz, 3H), 2.80 (dd, *J* = 16.8, 5.6 Hz, 1H), 2.50 (dd, *J* = 14.4, 3.2 Hz, 1H), 1.58 (s, 3H), 1.44 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.3, 159.0, 147.8, 138.7, 131.9, 130.5, 130.4, 129.2, 123.7, 121.2, 113.7, 62.7, 54.6, 33.9, 12.4, 8.6; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1570.

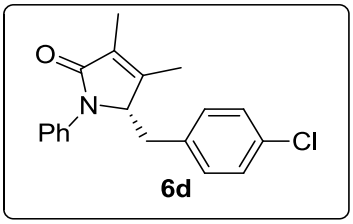
Spectral data for (*S*)-3,4-dimethyl-5-(4-methylbenzyl)-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6c):



6c

Yellow oil (0.038 g, 0.13 mmol, 38%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.26 (t, *J* = 7.8 Hz, 2H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.82 (d, *J* = 7.6 Hz, 2H), 6.67 (d, *J* = 8.0 Hz, 2H), 4.07 (s, 1H), 2.79 (dd, *J* = 14.4, 5.6 Hz, 1H), 2.54 (dd, *J* = 14.4, 3.2 Hz, 1H), 2.00 (s, 3H), 1.58 (s, 3H), 1.43 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.2, 147.8, 138.7, 136.3, 132.3, 130.5, 129.4, 129.2, 129.0, 123.7, 121.2, 62.6, 34.5, 21.0, 12.4, 8.6; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO[M^+]$: 291.1623, found : 291.1620.

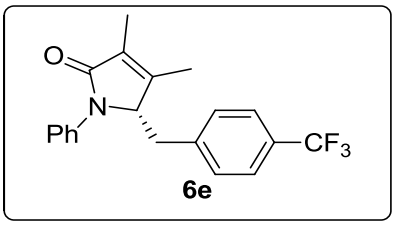
Spectral data for (*S*)-5-(4-chlorobenzyl)-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6d):



6d

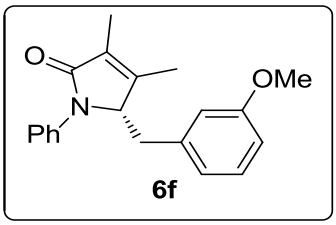
Light yellow oil (0.072 g, 0.23 mmol, 72%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 2H), 6.96 (t, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 8.2 Hz, 2H), 3.99 (s, 1H), 2.64 (dd, *J* = 14.4, 5.4 Hz, 1H), 2.33 (dd, *J* = 14.4, 3.0 Hz, 1H), 1.54 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.0, 147.4, 138.4, 133.8, 132.9, 130.7, 130.7, 129.2, 128.2, 123.9, 121.2, 62.2, 34.0, 12.3, 8.5; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1080.

Spectral data for (*S*)-3,4-dimethyl-1-phenyl-5-(4-(trifluoromethyl)benzyl)-1*H*-pyrrol-2(5*H*)-one (6e):



Off white solid (0.086 g, 0.25 mmol, 86%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.60 (dd, *J* = 8.8, 1.2 Hz, 2H), 7.23 (t, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.97 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.00 (s, 1H), 2.65 (dd, *J* = 14.4, 5.6 Hz, 1H), 2.33 (dd, *J* = 14.4, 3.2 Hz, 1H), 1.51 (d, *J* = 0.8 Hz, 3H), 1.32 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 169.9, 147.2, 139.7, 138.2, 130.7, 129.7, 129.2, 128.9, ($J_{C\text{-}F}$ = 268.1), 125.0 ($J_{C\text{-}F}$ = 5.5), 124.0, 121.2, 62.0, 34.5, 12.2, 8.5; HRMS (EI+, m/z) calcd for $C_{20}H_{18}F_3NO[M^+]$: 345.1340, found : 345.1347.

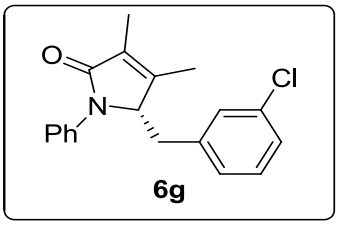
Spectral data for (*S*)-5-(3-methoxybenzyl)-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6f):



Sticky yellow solid (0.065 g, 0.21 mmol, 65%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.71 (d, *J* = 7.7 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 2H), 6.96 ~ 6.91 (m, 2H), 7.71 (dd, *J* = 8.2, 2.6 Hz, 1H), 6.43 (t, *J* = 1.9 Hz, 1H), 6.39 (d, *J* = 7.6 Hz, 1H), 4.08 (s, 1H), 3.28 (s, 3H), 2.78 (dd, *J* = 14.5, 5.6 Hz, 1H), 2.51 (dd, *J* = 14.5, 3.4 Hz, 1H), 1.57 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (150

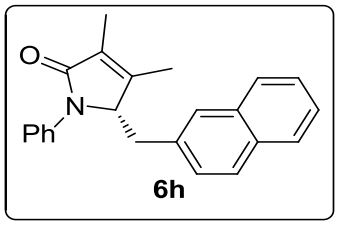
MHz, C_6D_6): δ 170.3, 159.8, 147.8, 138.6, 137.0, 130.4, 129.2, 129.1, 123.7, 121.7, 121.2, 115.2, 112.6, 62.5, 54.7, 34.8, 12.3, 8.6; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO_2[M^+]$: 307.1572, found : 307.1575.

Spectral data for (*S*)-5-(3-chlorobenzyl)-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6g):



Light yellow solid (0.078 g, 0.25 mmol, 78%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.8 Hz, 2H), 6.96 (t, *J* = 7.2 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.75 (s, 1H), 6.65 (t, *J* = 7.8 Hz, 1H), 6.44 (d, *J* = 8.0 Hz, 1H), 4.00 (s, 1H), 2.62 (dd, *J* = 14.4, 5.6 Hz, 1H), 2.34 (dd, *J* = 14.8, 3.2 Hz, 1H), 1.55 (s, 3H), 1.35 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.0, 147.4, 138.3, 137.5, 133.9, 130.7, 129.6, 129.4, 129.2, 127.5, 127.1, 123.9, 121.3, 62.1, 34.4, 12.2, 8.5; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1079.

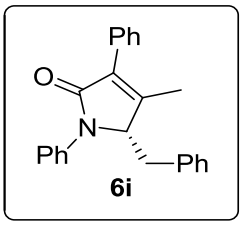
Spectral data for (*S*)-3,4-dimethyl-5-(naphthalen-2-ylmethyl)-1-phenyl-1*H*-pyrrol-2(5*H*)-one (6h):



Light yellow solid (0.052 g, 0.16 mmol, 52%); ^{1}H NMR (600 MHz, C_6D_6): δ 7.74 (d, *J* = 7.9 Hz, 2H), 7.54 (t, *J* = 7.5 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.27 (t, *J* = 8.0 Hz, 2H), 7.23 ~ 7.16 (m, 3H), 6.99 (t, *J* = 7.4 Hz, 1H), 6.89 (dd, *J* = 8.4, 1.6 Hz, 1H), 4.15 (s, 1H), 2.89 (dd, *J* = 14.5, 5.9 Hz, 1H), 2.69 (dd, *J* = 14.5, 3.4 Hz, 1H), 1.50 (s, 3H), 1.41 (s, 3H); ^{13}C NMR (150 MHz, C_6D_6): δ 170.1, 147.8, 138.6, 133.6, 133.2, 132.8, 130.5, 129.2, 128.3, 128.0, 127.9, 127.7, 127.5, 126.2, 125.8, 123.8, 121.4, 62.6, 35.2, 12.4, 8.5; HRMS (EI+, m/z) calcd

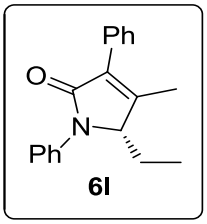
for $C_{23}H_{21}NO[M^+]$: 327.1623, found : 327.1625.

Spectral data for (*S*)-5-benzyl-4-methyl-1,3-diphenyl-1*H*-pyrrol-2(5*H*)-one (6i):



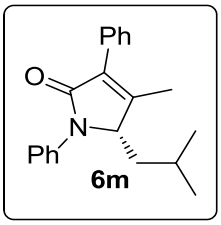
Sticky brown solid (0.070 g, 0.21 mmol, 70%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.79 (dd, *J* = 8.8, 0.8 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.19 ~ 7.12 (m, 2H), 7.06 ~ 7.01 (m, 4H), 6.93 ~ 6.90 (m, 3H), 6.54 (dd, *J* = 6.4, 1.6 Hz, 2H), 4.90 ~ 4.88 (m, 1H), 2.94 (dd, *J* = 14.0, 4.8 Hz, 1H), 2.53 (dd, *J* = 14.4, 3.2 Hz, 1H), 1.81 (d, *J* = 1.2 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.1, 149.2, 138.4, 134.7, 133.6, 131.4, 129.8, 129.2, 128.8, 128.7, 128.2, 127.7, 126.9, 124.1, 121.5, 60.6, 35.2, 10.1; HRMS (EI+, m/z) calcd for $C_{24}H_{21}NO[M^+]$: 339.1623, found : 339.1629.

Spectral data for (*S*)-5-ethyl-4-methyl-1,3-diphenyl-1*H*-pyrrol-2(5*H*)-one (6l):



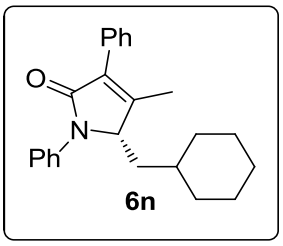
Pale yellow oil (0.088 g, 0.32 mmol, 88%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.68 (d, *J* = 11.5 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 2H), 7.17 ~ 7.04 (m, 5H), 6.96 (t, *J* = 7.4 Hz, 1H), 4.71 (t, *J* = 1.5 Hz, 1H), 2.01 (d, *J* = 1.6 Hz, 3H), 1.61 ~ 1.51 (m, 1H), 1.23 ~ 1.13 (m, 1H), 0.23 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.4, 150.1, 138.2, 133.6, 131.1, 129.1, 128.9, 128.7, 128.4, 124.3, 122.1, 61.2, 21.6, 10.2, 5.3; HRMS (EI+, m/z) calcd for $C_{19}H_{19}NO[M^+]$: 277.1467, found : 277.1469.

Spectral data for (*S*)-5-isobutyl-4-methyl-1,3-diphenyl-1*H*-pyrrol-2(5*H*)-one (6m):



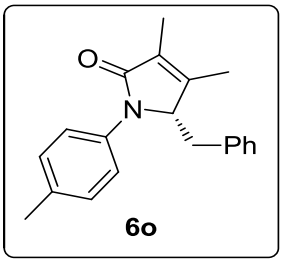
Pale yellow oil (0.090 g, 0.29 mmol, 90%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.22 ~ 7.19 (m, 2H), 7.15 ~ 7.11 (m, 3H), 7.03 ~ 6.99 (m, 1H), 4.89 (t, *J* = 1.6 Hz, 1H), 2.07 (s, 3H), 1.59 ~ 1.53 (m, 1H), 1.39 ~ 1.27 (m, 2H), 0.53 (d, *J* = 6.4 Hz, 3H), 0.49 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.2, 151.5, 138.5, 133.9, 130.5, 129.0, 128.8, 128.7, 128.5, 124.3, 122.2, 60.6, 38.5, 23.6, 23.4, 23.3, 10.3; HRMS (EI+, m/z) calcd for $C_{21}H_{23}NO[M^+]$: 305.1780, found : 305.1778.

Spectral data for (*S*)-5-(cyclohexylmethyl)-4-methyl-1,3-diphenyl-1*H*-pyrrol-2(5*H*)-one (6n):



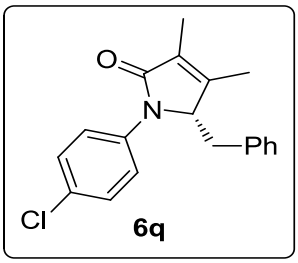
Pale yellow oil (0.082 g, 0.24 mmol, 82%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.83 (d, *J* = 8.4 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 ~ 7.20 (m, 2H), 7.18 ~ 7.13 (m, 3H), 7.05 (t, *J* = 7.4 Hz, 1H), 4.90 ~ 4.87 (m, 1H), 2.11 (s, 3H), 1.60 ~ 1.53 (m, 1H), 1.46 ~ 1.32 (m, 6H), 1.07 ~ 0.87 (m, 4H), 0.59 ~ 0.50 (m, 2H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.2, 151.6, 138.6, 134.1, 130.6, 129.1, 128.8, 128.6, 128.5, 124.3, 122.2, 60.2, 37.6, 34.0, 33.9, 32.9, 26.3, 10.3; HRMS (EI+, m/z) calcd for $C_{24}H_{27}NO[M^+]$: 345.2093, found : 345.2097.

Spectral data for (*S*)-5-benzyl-3,4-dimethyl-1-(*p*-tolyl)-1*H*-pyrrol-2(5*H*)-one (6o):



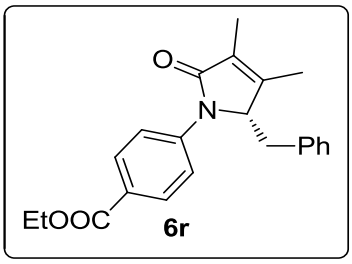
Pale yellow oil (0.045 g, 0.15 mmol, 45%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 7.01 ~ 6.95 (m, 3H), 6.75 (dd, *J* = 7.9, 1.8 Hz, 2H), 4.11 (s, 1H), 2.80 (dd, *J* = 14.4, 5.7 Hz, 1H), 2.56 (dd, *J* = 14.4, 3.3 Hz, 1H), 2.15 (s, 3H), 1.58 (s, 3H), 1.42 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.1, 147.6, 136.1, 135.6, 133.1, 130.5, 129.8, 129.4, 128.2, 126.9, 121.4, 62.7, 35.0, 20.8, 12.4, 8.6; HRMS (EI+, m/z) calcd for $C_{20}H_{21}NO[M^+]$: 291.1623, found : 291.1622.

Spectral data for (*S*)-5-benzyl-1-(4-chlorophenyl)-3,4-dimethyl-1*H*-pyrrol-2(5*H*)-one (6q):



Light brown oil (0.072 g, 0.23 mmol, 72%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.45 ~ 7.41 (m, 2H), 7.20 ~ 7.17 (m, 2H), 6.98 ~ 6.94 (m, 3H), 6.63 (dd, *J* = 7.3, 3.8 Hz, 2H), 3.89 (s, 1H), 2.63 (dd, *J* = 14.4, 5.6 Hz, 1H), 2.43 (dd, *J* = 14.4, 3.4 Hz, 1H), 1.53 (s, 3H), 1.39 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.1, 148.0, 137.0, 135.1, 130.4, 129.3, 129.2, 128.9, 128.2, 127.1, 122.3, 62.5, 34.8, 12.3, 8.5; HRMS (EI+, m/z) calcd for $C_{19}H_{18}ClNO[M^+]$: 311.1077, found : 311.1074.

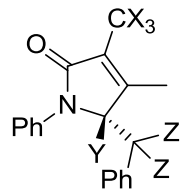
Spectral data for (*S*)-ethyl 4-(2-benzyl-3,4-dimethyl-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)benzoate (6r):



Pale yellow solid (0.074 g, 0.21 mmol, 74%); ^{1}H NMR (500 MHz, C_6D_6): δ 8.27 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 6.95 ~ 6.92 (m, 3H), 6.62 (dd, *J* = 7.5, 3.5 Hz, 2H), 4.19 (q, *J* = 7.0 Hz, 2H), 3.94 (s, 1H), 2.71 (dd, *J* = 15.0, 6.0 Hz, 1H), 2.58 (dd, *J* = 14.5, 3.0 Hz, 1H),

1.52 (s, 3H), 1.40 (s, 3H), 1.06 (t, J = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, C_6D_6): δ 170.3, 166.0, 148.5, 142.4, 134.9, 131.0, 130.4, 129.3, 128.2, 127.1, 125.7, 119.9, 62.3, 60.6, 34.7, 14.3, 12.4, 8.4; HRMS (EI+, m/z) calcd for $C_{22}H_{23}NO_3[M^+]$: 305.1780, found : 305.1778.

Spectral data for Deuterated (*S*)-5-benzyl-3,4-dimethyl-1-phenyl-1*H*-pyrrol-2(5*H*)-one (d-6a):

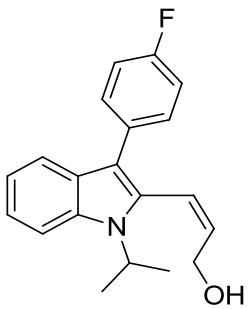


d-**6a**

X = (0.50 D, 0.50 H)
Y = (0.33 D, 0.67 H)
Z = (0.77 D, 0.23 H)

Light brown oil (0.055 g, 0.19 mmol, 54%); ^{1}H NMR (400 MHz, C_6D_6): δ 7.70 (d, J = 7.6 Hz, 2H), 7.25 (t, J = 7.4 Hz, 2H), 6.99 ~ 6.96 (m, 4H), 6.71 (d, J = 7.6 Hz, 2H), 4.08 (s, 0.67H, 0.33D), 2.76 (dd, J = 14.4, 5.6 Hz, 0.23H, 0.77D), 2.53 (d, J = 12.8 Hz, 0.23H, 0.77D), 1.56 (d, J = 7.2 Hz, 1.5H, 1.5D), 1.40 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6): δ 170.2, 147.7, 138.6, 135.4, 130.4, 129.4, 129.2, 128.2, 126.9, 123.7, 121.2, 62.5 (d, J = 9 Hz), 35.0 ~ 34.4 (m), 12.4, 8.5 ~ 8.2 (m); HRMS (ESI+, m/z) calcd for $C_{19}H_{13}D_6NO[M+H]$: 284.1921, found : 284.1895.

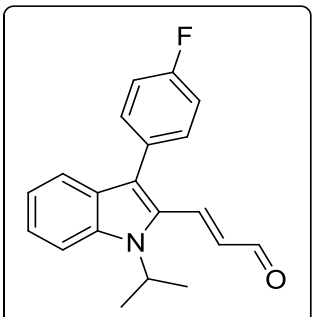
Spectral data for (*Z*)-3-(3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl)prop-2-en-1-ol (*Z*-7):



***Z*-7**

Light brown oil (0.125 g, 0.41 mmol, 68%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.65 (d, *J* = 7.9 Hz, 1H), 7.55 (d, *J* = 8.3 Hz, 1H), 7.44 ~ 7.42 (m, 2H), 7.23 (t, *J* = 7.1 Hz, 1H), 7.14 ~ 7.10 (m, 3H), 6.56 (d, *J* = 11.3 Hz, 1H), 5.93 (dt, *J* = 11.3, 6.5 Hz, 1H), 4.78 ~ 4.70 (m, 1H), 3.66 (dd, *J* = 6.5, 1.5 Hz, 2H), 1.64 (s, 3H), 1.63 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.0, 160.4, 135.8, 135.1, 131.8, 131.3, 131.2, 131.1, 127.5, 121.9, 119.8, 119.7, 119.3, 115.6, 115.2, 115.1, 111.4, 60.3, 48.0, 21.7.

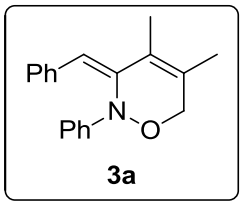
Spectral data for (*E*)-3-(3-(4-fluorophenyl)-1-isopropyl-1*H*-indol-2-yl)acrylaldehyde (*E*-8):



***E*-8**

Light yellow oil (0.050 g, 0.16 mmol, 100%); ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.55 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.55 (d, *J* = 16.3 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.38 ~ 7.35 (m, 2H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.17 (t, *J* = 8.7 Hz, 2H), 7.11 (t, *J* = 7.3 Hz, 1H), 6.30 (dd, *J* = 16.2, 7.6 Hz, 1H), 4.99 ~ 4.93 (m, 1H), 1.72 (s, 3H), 1.71 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 193.3, 163.1, 161.4, 141.0, 137.5, 131.9, 131.9, 130.4, 129.9, 129.5, 128.3, 124.6, 122.7, 121.0, 120.6, 116.0, 115.8, 112.5, 48.2, 21.8; HRMS (ESI+, m/z) calcd for $C_{20}H_{19}FNO$[M+H] : 308.1451, found : 308.1448.

(5) a) X-ray crystallographic structure and data for compound (3a)



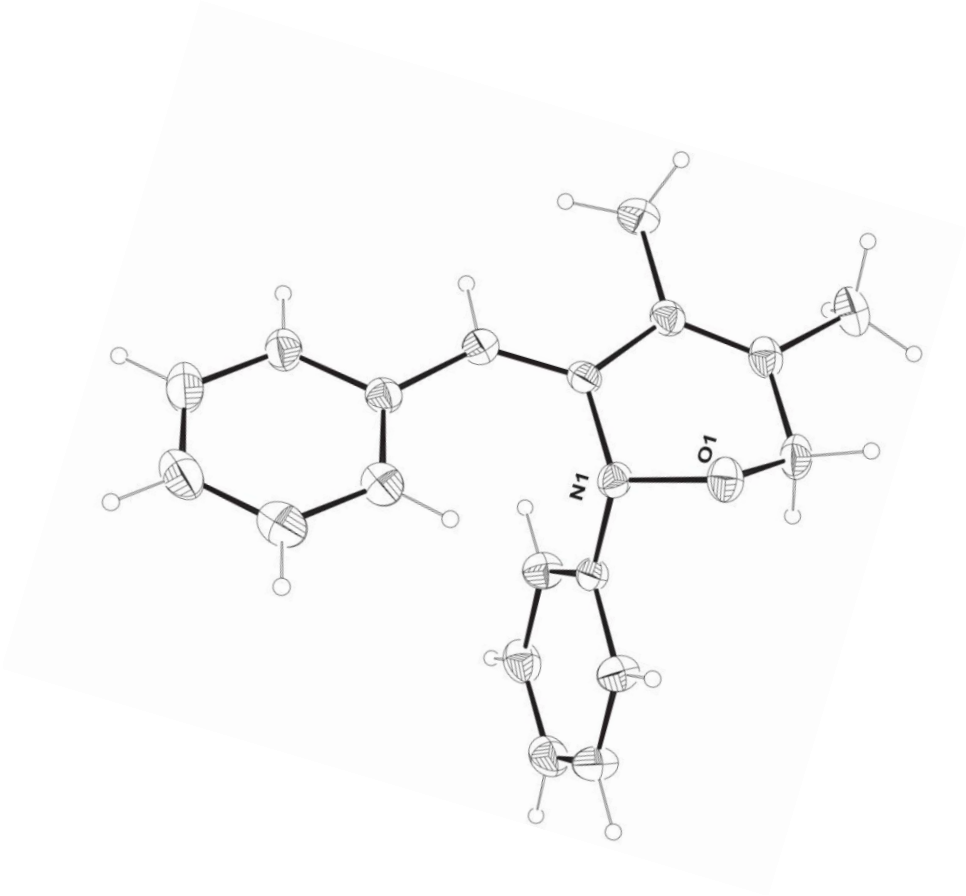


Table S3. Crystal data and structure refinement for a18320.

Identification code	a18320	
Empirical formula	C19 H19 N O	
Formula weight	277.35	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 5.913(3) Å	α= 90°.
	b = 15.050(8) Å	β= 90°.
	c = 17.042(9) Å	γ = 90°.
Volume	1516.7(14) $Å^3$	
Z	4	
Density (calculated)	1.215 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	592	
Crystal size	0.58 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.81 to 25.23°.	
Index ranges	-7<=h<=6, -18<=k<=12, -20<=l<=15	
Reflections collected	10993	
Independent reflections	2637 [R(int) = 0.0500]	
Completeness to theta = 25.23°	98.9 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9941 and 0.9581	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2637 / 0 / 190	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1189	
R indices (all data)	R1 = 0.1242, wR2 = 0.1456	
Absolute structure parameter	0(3)	
Largest diff. peak and hole	0.176 and -0.177 e.$Å^{-3}$	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for a18320. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	621(5)	8951(2)	2571(2)	43(1)
C(2)	2352(6)	8789(3)	3091(3)	60(1)
C(3)	2164(7)	9057(3)	3846(3)	74(1)
C(4)	305(8)	9489(3)	4103(3)	73(1)
C(5)	-1433(7)	9678(3)	3593(3)	68(1)
C(6)	-1256(5)	9404(3)	2814(2)	58(1)
C(7)	-705(5)	8874(2)	1203(2)	44(1)
C(8)	-785(5)	9696(3)	908(2)	52(1)
C(9)	663(5)	10474(2)	1022(2)	49(1)
C(10)	2750(6)	10480(3)	1396(2)	61(1)
C(11)	4032(7)	11236(4)	1442(2)	73(1)
C(12)	3223(9)	12015(3)	1127(3)	82(1)
C(13)	1179(8)	12029(3)	764(3)	76(1)
C(14)	-84(6)	11270(3)	709(2)	60(1)
C(15)	-2300(5)	8160(2)	1009(2)	50(1)
C(16)	-4109(6)	8343(3)	418(2)	71(1)
C(17)	-2094(6)	7373(3)	1359(2)	54(1)
C(18)	-3689(6)	6607(2)	1268(3)	75(1)
C(19)	-121(6)	7197(2)	1883(2)	63(1)
N(1)	958(4)	8681(2)	1783(2)	46(1)
O(1)	1725(4)	7787(2)	1733(1)	58(1)

Table S5. Bond lengths [Å] and angles [°] for a18320.

C(1)-C(6)	1.367(4)
C(1)-C(2)	1.375(5)
C(1)-N(1)	1.418(4)
C(2)-C(3)	1.353(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.350(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.376(6)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(5)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.336(4)
C(7)-N(1)	1.424(4)
C(7)-C(15)	1.468(4)
C(8)-C(9)	1.464(5)
C(8)-H(8)	0.9300
C(9)-C(14)	1.383(5)
C(9)-C(10)	1.389(5)
C(10)-C(11)	1.369(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.376(6)
C(11)-H(11)	0.9300
C(12)-C(13)	1.358(6)
C(12)-H(12)	0.9300
C(13)-C(14)	1.368(5)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(17)	1.332(4)
C(15)-C(16)	1.495(5)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(19)	1.492(5)

C(17)-C(18)	1.498(5)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-O(1)	1.430(4)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
N(1)-O(1)	1.422(4)

C(6)-C(1)-C(2)	119.8(4)
C(6)-C(1)-N(1)	123.0(3)
C(2)-C(1)-N(1)	117.0(3)
C(3)-C(2)-C(1)	119.9(4)
C(3)-C(2)-H(2)	120.1
C(1)-C(2)-H(2)	120.1
C(4)-C(3)-C(2)	121.3(4)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	120.1(4)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	119.0(4)
C(4)-C(5)-H(5)	120.5
C(6)-C(5)-H(5)	120.5
C(1)-C(6)-C(5)	119.8(4)
C(1)-C(6)-H(6)	120.1
C(5)-C(6)-H(6)	120.1
C(8)-C(7)-N(1)	118.4(3)
C(8)-C(7)-C(15)	124.7(3)
N(1)-C(7)-C(15)	116.8(3)
C(7)-C(8)-C(9)	132.0(3)
C(7)-C(8)-H(8)	114.0
C(9)-C(8)-H(8)	114.0
C(14)-C(9)-C(10)	117.1(3)
C(14)-C(9)-C(8)	117.0(3)
C(10)-C(9)-C(8)	125.8(3)

C(11)-C(10)-C(9)	121.5(4)
C(11)-C(10)-H(10)	119.2
C(9)-C(10)-H(10)	119.2
C(10)-C(11)-C(12)	119.6(4)
C(10)-C(11)-H(11)	120.2
C(12)-C(11)-H(11)	120.2
C(13)-C(12)-C(11)	120.0(4)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(12)-C(13)-C(14)	120.3(4)
C(12)-C(13)-H(13)	119.9
C(14)-C(13)-H(13)	119.9
C(13)-C(14)-C(9)	121.5(4)
C(13)-C(14)-H(14)	119.3
C(9)-C(14)-H(14)	119.3
C(17)-C(15)-C(7)	119.4(3)
C(17)-C(15)-C(16)	122.1(3)
C(7)-C(15)-C(16)	118.5(3)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-C(19)	119.8(3)
C(15)-C(17)-C(18)	125.5(4)
C(19)-C(17)-C(18)	114.7(3)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
O(1)-C(19)-C(17)	112.3(3)
O(1)-C(19)-H(19A)	109.1
C(17)-C(19)-H(19A)	109.1

O(1)-C(19)-H(19B)	109.1
C(17)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.9
C(1)-N(1)-O(1)	111.9(2)
C(1)-N(1)-C(7)	120.1(3)
O(1)-N(1)-C(7)	111.8(3)
N(1)-O(1)-C(19)	109.5(2)

Symmetry transformations used to generate equivalent atoms:

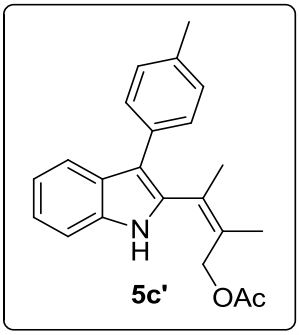
Table S6. Anisotropic displacement parameters (Å ^{2}x 10^3)for a18320. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(2)	41(2)	41(2)	2(2)	0(2)	-4(2)
C(2)	60(2)	69(3)	52(3)	3(2)	-7(2)	5(2)
C(3)	83(3)	84(3)	54(3)	1(3)	-19(2)	-4(2)
C(4)	104(3)	65(3)	51(3)	-5(2)	8(3)	-17(3)
C(5)	79(3)	57(3)	67(3)	-13(3)	16(3)	5(2)
C(6)	55(2)	67(3)	52(3)	-4(2)	4(2)	6(2)
C(7)	47(2)	44(2)	40(2)	-5(2)	-1(2)	-3(2)
C(8)	56(2)	52(2)	48(3)	2(2)	-1(2)	-1(2)
C(9)	57(2)	50(3)	41(2)	-3(2)	6(2)	-4(2)
C(10)	59(2)	64(3)	60(3)	-4(2)	11(2)	-7(2)
C(11)	67(2)	88(3)	65(3)	-11(3)	13(2)	-19(3)
C(12)	106(3)	71(3)	70(3)	-16(3)	23(3)	-31(3)
C(13)	104(3)	49(3)	76(3)	-1(3)	21(3)	-6(3)
C(14)	71(2)	48(3)	60(3)	-1(2)	8(2)	0(2)
C(15)	57(2)	47(2)	46(3)	-6(2)	6(2)	2(2)
C(16)	74(2)	74(3)	64(3)	-6(2)	-18(3)	-9(2)
C(17)	60(2)	45(3)	57(3)	-6(2)	16(2)	5(2)
C(18)	77(2)	48(2)	100(4)	-10(3)	6(3)	-8(2)
C(19)	80(2)	38(2)	71(3)	1(2)	8(2)	10(2)
N(1)	50(1)	43(2)	45(2)	0(2)	1(2)	9(1)
O(1)	56(1)	48(2)	69(2)	-5(2)	10(1)	15(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for a18320.

	x	y	z	U(eq)
H(2)	3649	8495	2924	73
H(3)	3338	8942	4194	88
H(4)	199	9660	4627	88
H(5)	-2706	9983	3765	82
H(6)	-2412	9529	2461	70
H(8)	-1984	9791	565	62
H(10)	3289	9958	1621	73
H(11)	5440	11222	1685	88
H(12)	4076	12532	1163	99
H(13)	636	12557	551	92
H(14)	-1475	11289	455	72
H(16A)	-3969	8943	232	106
H(16B)	-5565	8264	657	106
H(16C)	-3956	7939	-15	106
H(18A)	-3172	6117	1581	112
H(18B)	-3745	6431	727	112
H(18C)	-5172	6781	1438	112
H(19A)	-592	7261	2425	75
H(19B)	381	6590	1808	75

b) X-ray crystallographic structure and data for compound (5c')



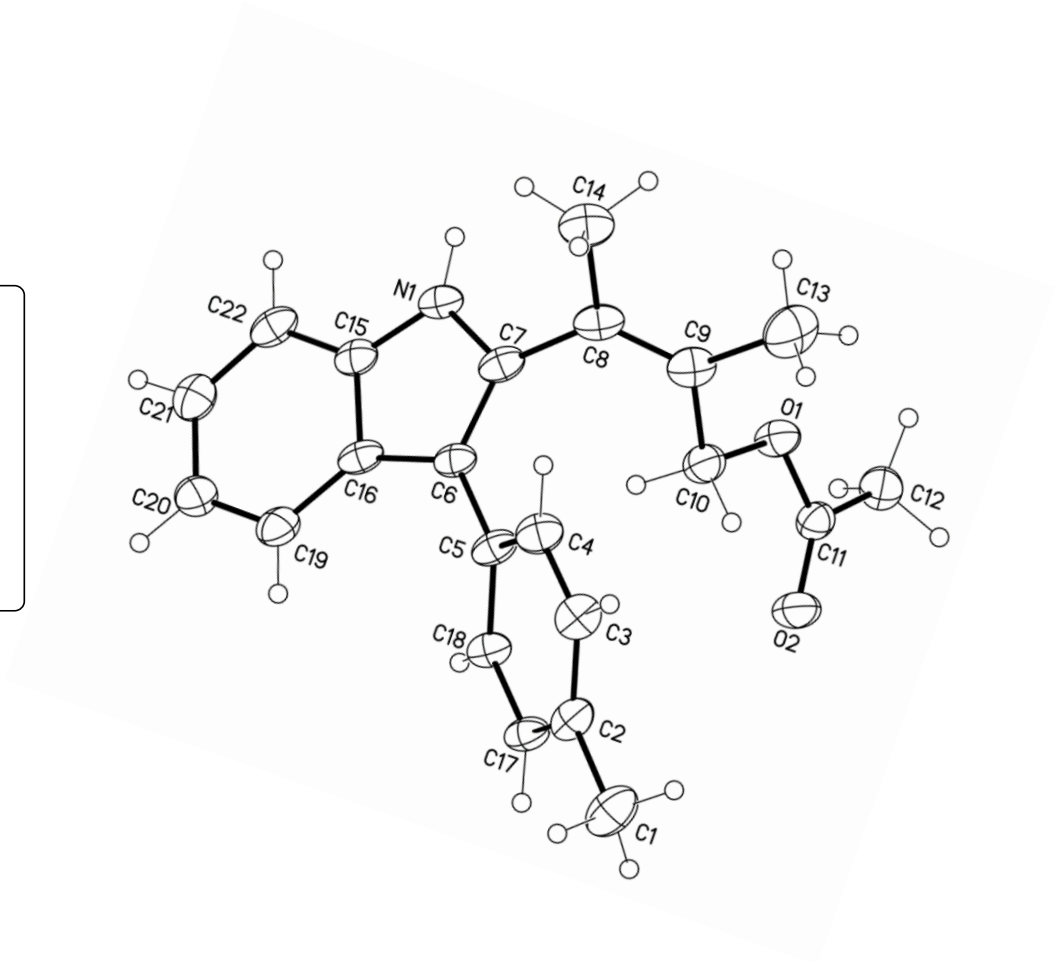


Table S8. Crystal data and structure refinement for 161032LT_PL.

Identification code	161032lt_pl	
Empirical formula	C22 H23 N O2	
Formula weight	333.41	
Temperature	99(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 7.345(4) Å	α= 90°.
	b = 14.462(8) Å	β= 92.936(12)°.
	c = 17.703(10) Å	γ = 90°.
Volume	1878.0(18) $Å^3$	
Z	4	
Density (calculated)	1.179 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	712	
Crystal size	0.22 x 0.20 x 0.15 mm^3	
Theta range for data collection	1.819 to 26.455°.	
Index ranges	-9<=h<=6, -17<=k<=17, -21<=l<=22	
Reflections collected	13355	
Independent reflections	3792 [R(int) = 0.0843]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9484 and 0.6665	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3792 / 0 / 230	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0638, wR2 = 0.1605	
R indices (all data)	R1 = 0.0910, wR2 = 0.1780	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.261 and -0.319 e.$Å^{-3}$	

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for 161032LT_PL. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9665(2)	2364(1)	4131(1)	29(1)
O(2)	12382(2)	2148(1)	3636(1)	34(1)
N(1)	4502(2)	2971(1)	2511(1)	26(1)
C(1)	13555(3)	5924(2)	1942(2)	38(1)
C(2)	11840(3)	5348(2)	1986(1)	28(1)
C(3)	10385(3)	5642(2)	2398(1)	30(1)
C(4)	8799(3)	5126(2)	2423(1)	29(1)
C(5)	8613(3)	4275(2)	2045(1)	24(1)
C(6)	6957(3)	3695(1)	2079(1)	24(1)
C(7)	5975(3)	3535(1)	2706(1)	24(1)
C(8)	6248(3)	3873(2)	3488(1)	27(1)
C(9)	7787(3)	3708(2)	3903(1)	28(1)
C(10)	9331(3)	3141(2)	3615(1)	29(1)
C(11)	11241(3)	1902(2)	4057(1)	26(1)
C(12)	11386(3)	1058(2)	4547(1)	32(1)
C(13)	8168(4)	4115(2)	4674(2)	44(1)
C(14)	4694(3)	4450(2)	3774(2)	36(1)
C(15)	4532(3)	2733(1)	1770(1)	24(1)
C(16)	6051(3)	3188(1)	1470(1)	24(1)
C(17)	11656(3)	4504(2)	1605(1)	27(1)
C(18)	10078(3)	3974(2)	1634(1)	25(1)
C(19)	6309(3)	3097(2)	697(1)	28(1)
C(20)	5115(3)	2559(2)	262(1)	32(1)
C(21)	3648(3)	2095(2)	575(1)	31(1)
C(22)	3341(3)	2178(2)	1330(1)	29(1)

Table S10. Bond lengths [Å] and angles [°] for 161032LT_PL.

O(1)-C(11)	1.349(3)
O(1)-C(10)	1.461(3)
O(2)-C(11)	1.204(3)
N(1)-C(15)	1.358(3)
N(1)-C(7)	1.384(3)
N(1)-H(20)	0.8791
C(1)-C(2)	1.515(3)
C(1)-H(1)	0.9800
C(1)-H(12)	0.9800
C(1)-H(13)	0.9800
C(2)-C(3)	1.392(3)
C(2)-C(17)	1.397(3)
C(3)-C(4)	1.385(3)
C(3)-H(14)	0.9500
C(4)-C(5)	1.404(3)
C(4)-H(15)	0.9500
C(5)-C(18)	1.399(3)
C(5)-C(6)	1.481(3)
C(6)-C(7)	1.374(3)
C(6)-C(16)	1.439(3)
C(7)-C(8)	1.471(3)
C(8)-C(9)	1.338(3)
C(8)-C(14)	1.522(3)
C(9)-C(13)	1.501(4)
C(9)-C(10)	1.509(3)
C(10)-H(21)	0.9900
C(10)-H(22)	0.9900
C(11)-C(12)	1.498(3)
C(12)-H(2)	0.9800
C(12)-H(3)	0.9800
C(12)-H(23)	0.9800
C(13)-H(4)	0.9800
C(13)-H(5)	0.9800
C(13)-H(6)	0.9800

C(14)-H(7)	0.9800
C(14)-H(8)	0.9800
C(14)-H(9)	0.9800
C(15)-C(22)	1.394(3)
C(15)-C(16)	1.421(3)
C(16)-C(19)	1.397(3)
C(17)-C(18)	1.393(3)
C(17)-H(11)	0.9500
C(18)-H(10)	0.9500
C(19)-C(20)	1.377(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.407(3)
C(20)-H(18)	0.9500
C(21)-C(22)	1.372(3)
C(21)-H(17)	0.9500
C(22)-H(16)	0.9500

C(11)-O(1)-C(10)	115.97(16)
C(15)-N(1)-C(7)	109.81(18)
C(15)-N(1)-H(20)	125.1
C(7)-N(1)-H(20)	125.1
C(2)-C(1)-H(1)	109.5
C(2)-C(1)-H(12)	109.5
H(1)-C(1)-H(12)	109.5
C(2)-C(1)-H(13)	109.5
H(1)-C(1)-H(13)	109.5
H(12)-C(1)-H(13)	109.5
C(3)-C(2)-C(17)	117.5(2)
C(3)-C(2)-C(1)	121.5(2)
C(17)-C(2)-C(1)	121.0(2)
C(4)-C(3)-C(2)	121.4(2)
C(4)-C(3)-H(14)	119.3
C(2)-C(3)-H(14)	119.3
C(3)-C(4)-C(5)	121.2(2)
C(3)-C(4)-H(15)	119.4
C(5)-C(4)-H(15)	119.4

C(18)-C(5)-C(4)	117.5(2)
C(18)-C(5)-C(6)	120.0(2)
C(4)-C(5)-C(6)	122.50(19)
C(7)-C(6)-C(16)	106.18(19)
C(7)-C(6)-C(5)	126.4(2)
C(16)-C(6)-C(5)	127.4(2)
C(6)-C(7)-N(1)	109.5(2)
C(6)-C(7)-C(8)	130.7(2)
N(1)-C(7)-C(8)	119.82(19)
C(9)-C(8)-C(7)	121.9(2)
C(9)-C(8)-C(14)	122.8(2)
C(7)-C(8)-C(14)	115.3(2)
C(8)-C(9)-C(13)	122.9(2)
C(8)-C(9)-C(10)	122.7(2)
C(13)-C(9)-C(10)	114.3(2)
O(1)-C(10)-C(9)	108.20(18)
O(1)-C(10)-H(21)	110.1
C(9)-C(10)-H(21)	110.1
O(1)-C(10)-H(22)	110.1
C(9)-C(10)-H(22)	110.1
H(21)-C(10)-H(22)	108.4
O(2)-C(11)-O(1)	122.8(2)
O(2)-C(11)-C(12)	124.7(2)
O(1)-C(11)-C(12)	112.51(18)
C(11)-C(12)-H(2)	109.5
C(11)-C(12)-H(3)	109.5
H(2)-C(12)-H(3)	109.5
C(11)-C(12)-H(23)	109.5
H(2)-C(12)-H(23)	109.5
H(3)-C(12)-H(23)	109.5
C(9)-C(13)-H(4)	109.5
C(9)-C(13)-H(5)	109.5
H(4)-C(13)-H(5)	109.5
C(9)-C(13)-H(6)	109.5
H(4)-C(13)-H(6)	109.5
H(5)-C(13)-H(6)	109.5

C(8)-C(14)-H(7)	109.5
C(8)-C(14)-H(8)	109.5
H(7)-C(14)-H(8)	109.5
C(8)-C(14)-H(9)	109.5
H(7)-C(14)-H(9)	109.5
H(8)-C(14)-H(9)	109.5
N(1)-C(15)-C(22)	130.1(2)
N(1)-C(15)-C(16)	107.2(2)
C(22)-C(15)-C(16)	122.7(2)
C(19)-C(16)-C(15)	118.1(2)
C(19)-C(16)-C(6)	134.6(2)
C(15)-C(16)-C(6)	107.3(2)
C(18)-C(17)-C(2)	121.5(2)
C(18)-C(17)-H(11)	119.2
C(2)-C(17)-H(11)	119.2
C(17)-C(18)-C(5)	120.8(2)
C(17)-C(18)-H(10)	119.6
C(5)-C(18)-H(10)	119.6
C(20)-C(19)-C(16)	119.1(2)
C(20)-C(19)-H(19)	120.5
C(16)-C(19)-H(19)	120.5
C(19)-C(20)-C(21)	121.9(2)
C(19)-C(20)-H(18)	119.1
C(21)-C(20)-H(18)	119.1
C(22)-C(21)-C(20)	120.6(2)
C(22)-C(21)-H(17)	119.7
C(20)-C(21)-H(17)	119.7
C(21)-C(22)-C(15)	117.6(2)
C(21)-C(22)-H(16)	121.2
C(15)-C(22)-H(16)	121.2

Symmetry transformations used to generate equivalent atoms:

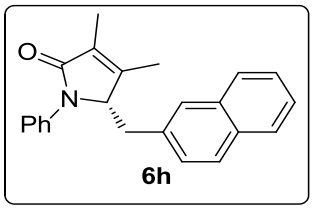
Table S11. Anisotropic displacement parameters (Å ^{2}x 10^3) for 161032LT_PL. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	25(1)	29(1)	34(1)	4(1)	6(1)	-2(1)
O(2)	26(1)	39(1)	37(1)	5(1)	9(1)	-3(1)
N(1)	21(1)	24(1)	34(1)	4(1)	7(1)	-1(1)
C(1)	29(1)	30(1)	55(2)	6(1)	-2(1)	-6(1)
C(2)	22(1)	24(1)	38(1)	11(1)	-3(1)	-3(1)
C(3)	33(1)	19(1)	38(1)	1(1)	0(1)	-2(1)
C(4)	27(1)	24(1)	35(1)	1(1)	6(1)	2(1)
C(5)	21(1)	20(1)	32(1)	5(1)	4(1)	0(1)
C(6)	21(1)	19(1)	31(1)	3(1)	6(1)	3(1)
C(7)	21(1)	18(1)	35(1)	2(1)	6(1)	3(1)
C(8)	25(1)	18(1)	39(1)	1(1)	10(1)	-2(1)
C(9)	29(1)	21(1)	36(1)	-2(1)	7(1)	-7(1)
C(10)	26(1)	29(1)	34(1)	6(1)	4(1)	-3(1)
C(11)	24(1)	27(1)	26(1)	-3(1)	2(1)	-4(1)
C(12)	32(1)	29(1)	34(1)	3(1)	3(1)	-3(1)
C(13)	42(2)	42(2)	48(2)	-13(1)	1(1)	-13(1)
C(14)	35(1)	26(1)	47(2)	-3(1)	12(1)	2(1)
C(15)	22(1)	21(1)	30(1)	5(1)	5(1)	5(1)
C(16)	18(1)	19(1)	35(1)	3(1)	4(1)	3(1)
C(17)	19(1)	26(1)	38(1)	8(1)	4(1)	3(1)
C(18)	24(1)	20(1)	32(1)	4(1)	4(1)	1(1)
C(19)	23(1)	29(1)	33(1)	3(1)	6(1)	3(1)
C(20)	30(1)	35(1)	30(1)	-1(1)	4(1)	4(1)
C(21)	29(1)	28(1)	36(1)	-2(1)	-2(1)	3(1)
C(22)	21(1)	23(1)	43(2)	4(1)	3(1)	2(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for 161032LT_PL.

	x	y	z	U(eq)
H(20)	3671	2794	2821	31
H(1)	13387	6378	1534	57
H(12)	14585	5520	1839	57
H(13)	13802	6246	2423	57
H(14)	10480	6208	2669	36
H(15)	7820	5352	2700	34
H(21)	9004	2911	3099	35
H(22)	10442	3525	3594	35
H(2)	10989	515	4252	47
H(3)	10608	1132	4977	47
H(23)	12654	975	4734	47
H(4)	7021	4315	4882	66
H(5)	8984	4648	4637	66
H(6)	8749	3648	5008	66
H(7)	5015	5107	3754	54
H(8)	4483	4277	4298	54
H(9)	3585	4338	3456	54
H(11)	12630	4287	1320	33
H(10)	9996	3401	1372	30
H(19)	7293	3403	474	34
H(18)	5289	2498	-263	38
H(17)	2861	1722	261	37
H(16)	2353	1868	1546	35

c) X-ray crystallographic structure and data for compound (6h)



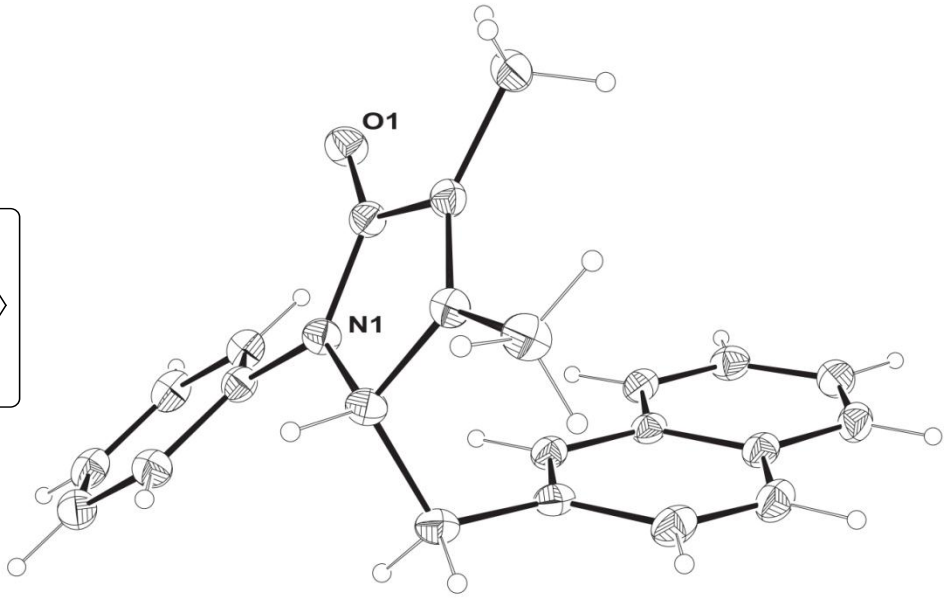


Table S13. Crystal data and structure refinement for d18946.

Identification code	d18946	
Empirical formula	C23 H21 N O	
Formula weight	327.41	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 24.6486(10) Å	α= 90°.
	b = 6.5021(3) Å	β= 90°.
	c = 10.8527(4) Å	γ = 90°.
Volume	1739.34(12) $Å^3$	
Z	4	
Density (calculated)	1.250 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	696	
Crystal size	0.15 x 0.13 x 0.03 mm^3	
Theta range for data collection	2.50 to 25.04°.	
Index ranges	-29<=h<=29, -7<=k<=7, -12<=l<=12	
Reflections collected	24731	
Independent reflections	3059 [R(int) = 0.0476]	
Completeness to theta = 25.04°	99.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9977 and 0.9887	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3059 / 1 / 229	
Goodness-of-fit on F^2	1.141	
Final R indices [I>2sigma(I)]	R1 = 0.0337, wR2 = 0.0835	
R indices (all data)	R1 = 0.0473, wR2 = 0.0951	
Absolute structure parameter	-0.7(17)	
Extinction coefficient	0.029(3)	
Largest diff. peak and hole	0.118 and -0.145 e.$Å^{-3}$	

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for d18946. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6828(1)	7172(3)	4114(2)	40(1)
C(2)	6691(1)	6838(3)	2807(2)	39(1)
C(3)	6795(1)	8462(3)	1873(2)	52(1)
C(4)	6494(1)	4940(3)	2679(2)	40(1)
C(5)	6310(1)	3921(3)	1517(2)	52(1)
C(6)	6487(1)	3834(3)	3892(2)	41(1)
C(7)	5920(1)	3099(3)	4294(2)	46(1)
C(8)	5483(1)	4711(3)	4209(2)	42(1)
C(9)	5460(1)	6335(3)	5015(2)	41(1)
C(10)	5058(1)	7884(3)	4915(2)	40(1)
C(11)	4667(1)	7746(4)	3965(2)	45(1)
C(12)	4688(1)	6041(4)	3160(2)	53(1)
C(13)	5080(1)	4592(4)	3275(2)	53(1)
C(14)	4275(1)	9334(4)	3847(2)	54(1)
C(15)	4272(1)	10959(4)	4626(2)	56(1)
C(16)	4650(1)	11067(4)	5597(2)	53(1)
C(17)	5032(1)	9575(3)	5736(2)	46(1)
C(18)	6823(1)	4979(3)	5994(2)	40(1)
C(19)	6964(1)	2996(3)	6361(2)	46(1)
C(20)	7079(1)	2610(4)	7596(2)	52(1)
C(21)	7054(1)	4164(4)	8451(2)	54(1)
C(22)	6915(1)	6122(4)	8082(2)	52(1)
C(23)	6794(1)	6539(4)	6862(2)	47(1)
N(1)	6709(1)	5384(2)	4735(2)	39(1)
O(1)	7025(1)	8735(2)	4565(2)	51(1)

Table S15. Bond lengths [Å] and angles [°] for d18946.

C(1)-O(1)	1.229(2)
C(1)-N(1)	1.375(3)
C(1)-C(2)	1.474(3)
C(2)-C(4)	1.334(3)
C(2)-C(3)	1.485(3)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(5)	1.494(3)
C(4)-C(6)	1.501(3)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-N(1)	1.468(3)
C(6)-C(7)	1.539(3)
C(6)-H(6)	1.0000
C(7)-C(8)	1.506(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.372(3)
C(8)-C(13)	1.421(3)
C(9)-C(10)	1.417(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.415(3)
C(10)-C(17)	1.417(3)
C(11)-C(12)	1.413(3)
C(11)-C(14)	1.420(3)
C(12)-C(13)	1.356(3)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(15)	1.353(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.408(4)
C(15)-H(15)	0.9500

C(16)-C(17)	1.361(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(23)	1.386(3)
C(18)-C(19)	1.394(3)
C(18)-N(1)	1.419(3)
C(19)-C(20)	1.393(3)
C(19)-H(19)	0.9500
C(20)-C(21)	1.374(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.378(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.384(3)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500

O(1)-C(1)-N(1)	125.99(18)
O(1)-C(1)-C(2)	126.6(2)
N(1)-C(1)-C(2)	107.41(16)
C(4)-C(2)-C(1)	108.66(18)
C(4)-C(2)-C(3)	130.48(19)
C(1)-C(2)-C(3)	120.84(17)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-C(5)	127.52(19)
C(2)-C(4)-C(6)	110.86(18)
C(5)-C(4)-C(6)	121.61(17)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5

H(5B)-C(5)-H(5C)	109.5
N(1)-C(6)-C(4)	102.33(15)
N(1)-C(6)-C(7)	112.10(16)
C(4)-C(6)-C(7)	114.05(17)
N(1)-C(6)-H(6)	109.4
C(4)-C(6)-H(6)	109.4
C(7)-C(6)-H(6)	109.4
C(8)-C(7)-C(6)	114.57(16)
C(8)-C(7)-H(7A)	108.6
C(6)-C(7)-H(7A)	108.6
C(8)-C(7)-H(7B)	108.6
C(6)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.6
C(9)-C(8)-C(13)	118.0(2)
C(9)-C(8)-C(7)	121.71(18)
C(13)-C(8)-C(7)	120.32(18)
C(8)-C(9)-C(10)	121.74(18)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-H(9)	119.1
C(11)-C(10)-C(17)	118.42(19)
C(11)-C(10)-C(9)	119.21(19)
C(17)-C(10)-C(9)	122.38(18)
C(12)-C(11)-C(10)	118.34(19)
C(12)-C(11)-C(14)	122.7(2)
C(10)-C(11)-C(14)	119.0(2)
C(13)-C(12)-C(11)	121.0(2)
C(13)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	119.5
C(12)-C(13)-C(8)	121.7(2)
C(12)-C(13)-H(13)	119.1
C(8)-C(13)-H(13)	119.1
C(15)-C(14)-C(11)	120.9(2)
C(15)-C(14)-H(14)	119.5
C(11)-C(14)-H(14)	119.5
C(14)-C(15)-C(16)	120.3(2)
C(14)-C(15)-H(15)	119.9

C(16)-C(15)-H(15)	119.9
C(17)-C(16)-C(15)	120.3(2)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(10)	121.0(2)
C(16)-C(17)-H(17)	119.5
C(10)-C(17)-H(17)	119.5
C(23)-C(18)-C(19)	119.72(19)
C(23)-C(18)-N(1)	120.58(19)
C(19)-C(18)-N(1)	119.70(18)
C(20)-C(19)-C(18)	119.5(2)
C(20)-C(19)-H(19)	120.2
C(18)-C(19)-H(19)	120.2
C(21)-C(20)-C(19)	120.5(2)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(22)	119.6(2)
C(20)-C(21)-H(21)	120.2
C(22)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	120.9(2)
C(21)-C(22)-H(22)	119.6
C(23)-C(22)-H(22)	119.6
C(22)-C(23)-C(18)	119.7(2)
C(22)-C(23)-H(23)	120.2
C(18)-C(23)-H(23)	120.2
C(1)-N(1)-C(18)	125.94(16)
C(1)-N(1)-C(6)	110.74(15)
C(18)-N(1)-C(6)	123.13(16)

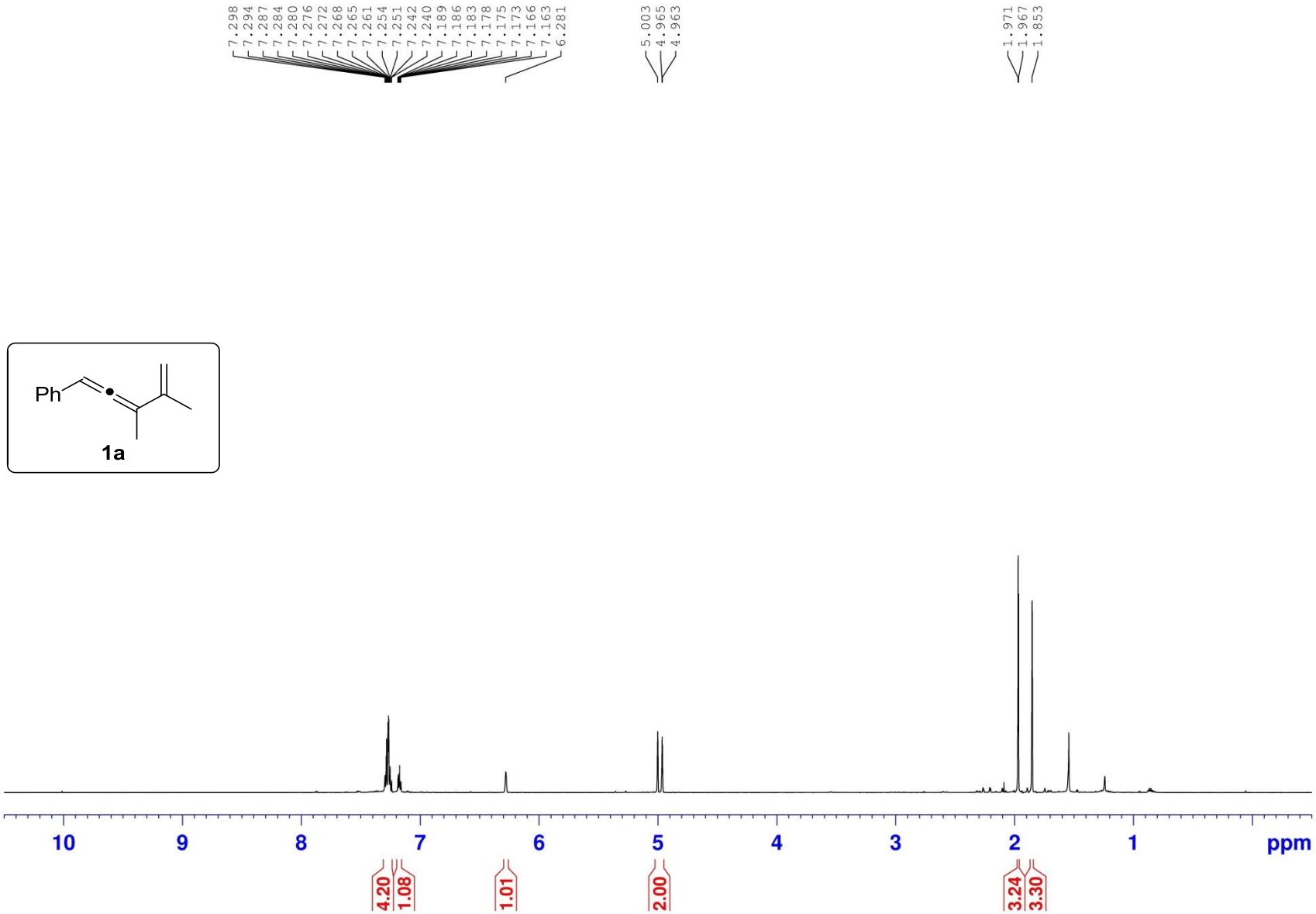
Symmetry transformations used to generate equivalent atoms:

Table S16. Anisotropic displacement parameters (Å ^{2}x 10^3)for d18946. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	39(1)	34(1)	47(1)	-2(1)	0(1)	0(1)
C(2)	37(1)	38(1)	42(1)	0(1)	-1(1)	2(1)
C(3)	55(1)	47(1)	54(1)	10(1)	-8(1)	-4(1)
C(4)	42(1)	40(1)	40(1)	-2(1)	3(1)	2(1)
C(5)	66(1)	48(1)	43(1)	-4(1)	-1(1)	-4(1)
C(6)	48(1)	33(1)	40(1)	-4(1)	3(1)	-2(1)
C(7)	53(1)	39(1)	47(1)	-1(1)	2(1)	-9(1)
C(8)	44(1)	42(1)	40(1)	1(1)	5(1)	-11(1)
C(9)	40(1)	49(1)	33(1)	1(1)	1(1)	-9(1)
C(10)	35(1)	48(1)	36(1)	3(1)	5(1)	-8(1)
C(11)	38(1)	60(1)	37(1)	3(1)	4(1)	-9(1)
C(12)	44(1)	72(2)	42(1)	-3(1)	-4(1)	-11(1)
C(13)	52(1)	63(2)	44(1)	-8(1)	0(1)	-16(1)
C(14)	38(1)	77(2)	47(1)	11(1)	0(1)	-1(1)
C(15)	45(1)	63(1)	59(1)	8(1)	9(1)	6(1)
C(16)	47(1)	53(1)	60(1)	-1(1)	11(1)	-2(1)
C(17)	41(1)	53(1)	43(1)	-2(1)	1(1)	-7(1)
C(18)	36(1)	45(1)	38(1)	-2(1)	3(1)	-1(1)
C(19)	47(1)	46(1)	44(1)	0(1)	5(1)	1(1)
C(20)	48(1)	59(1)	48(1)	7(1)	5(1)	2(1)
C(21)	41(1)	82(2)	39(1)	2(1)	1(1)	-5(1)
C(22)	44(1)	71(2)	42(1)	-14(1)	4(1)	-2(1)
C(23)	45(1)	50(1)	46(1)	-9(1)	2(1)	1(1)
N(1)	45(1)	35(1)	38(1)	-4(1)	0(1)	-3(1)
O(1)	62(1)	36(1)	55(1)	-6(1)	-5(1)	-6(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for d18946.

	x	y	z	U(eq)
H(3A)	7034	7920	1230	78
H(3B)	6968	9646	2270	78
H(3C)	6450	8892	1504	78
H(5A)	6287	4944	856	78
H(5B)	5952	3302	1647	78
H(5C)	6570	2847	1286	78
H(6)	6738	2629	3854	49
H(7A)	5814	1913	3774	56
H(7B)	5941	2609	5156	56
H(9)	5721	6423	5657	49
H(12)	4423	5907	2529	63
H(13)	5086	3468	2716	64
H(14)	4010	9254	3212	65
H(15)	4015	12031	4518	67
H(16)	4638	12188	6158	64
H(17)	5285	9668	6394	55
H(19)	6980	1915	5773	55
H(20)	7177	1261	7848	62
H(21)	7131	3890	9293	65
H(22)	6903	7200	8672	63
H(23)	6691	7888	6621	56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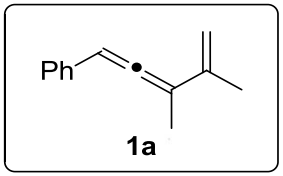
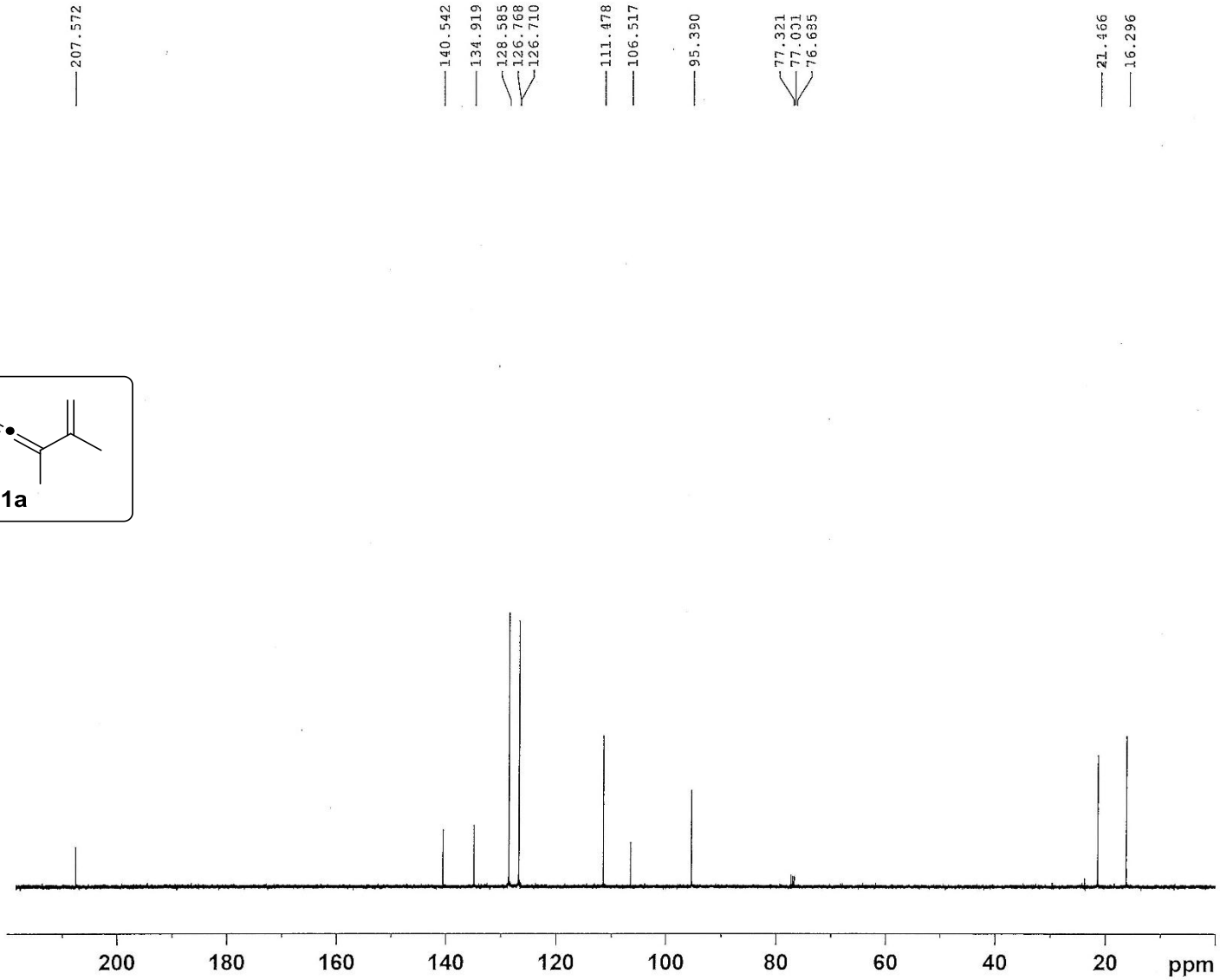
7.287
7.284
7.280
7.276
7.272
7.268
7.265
7.261
7.254
7.251
7.242
7.240
7.189
7.186
7.183
7.178
7.175
7.173
7.166
7.163
6.281
5.003
4.965
4.963
1.971
1.967
1.853
Ph
1a
10
9
8
7
6
5
4
3
2
1
ppm
4.20
1.08
1.01
2.00
3.24
3.30


Ph
1a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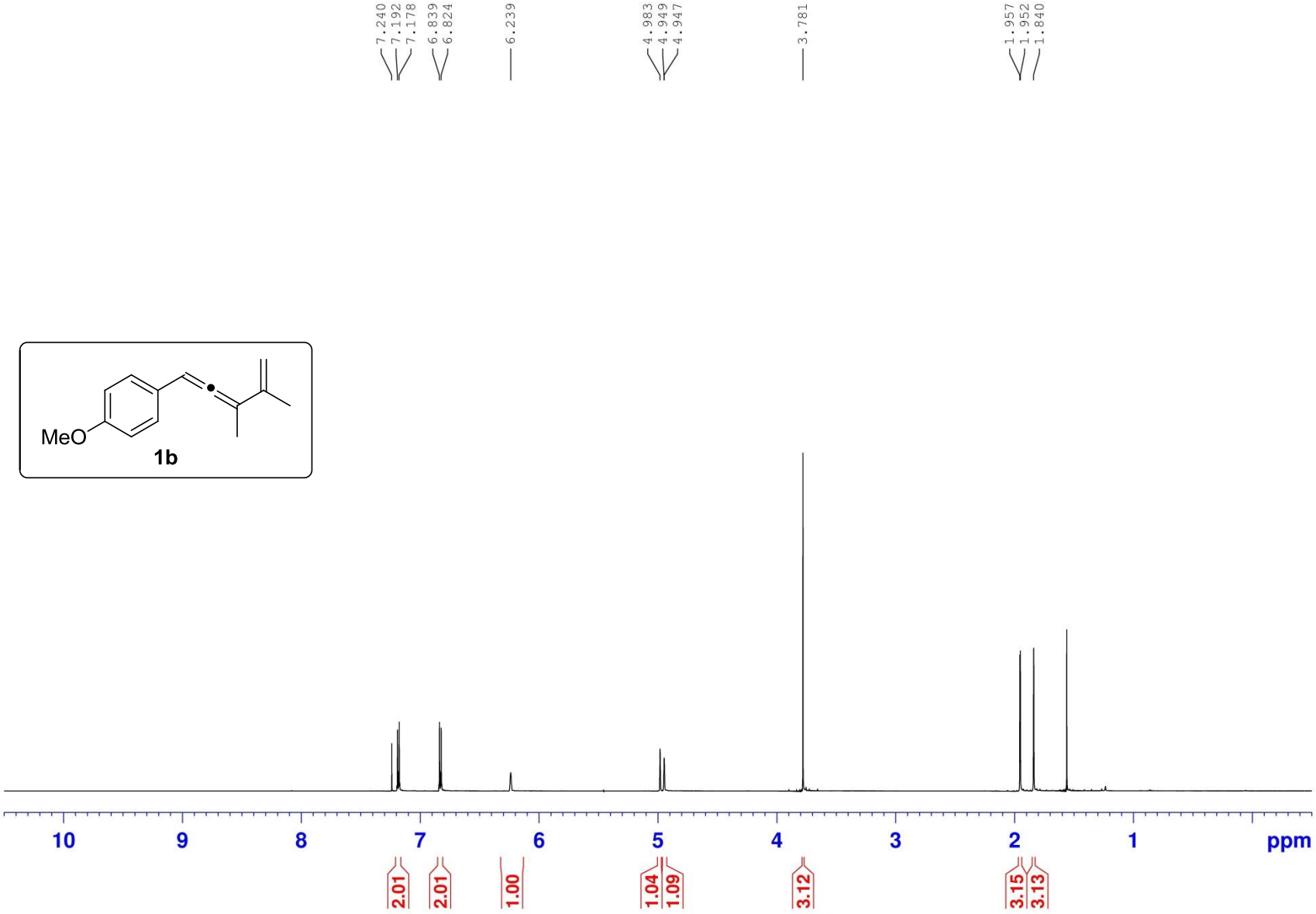
140.542
134.919
128.585
126.768
126.710
111.478
106.517
95.390
77.321
77.031
76.635
21.466
16.296
200
180
160
140
120
100
80
60
40
20
ppm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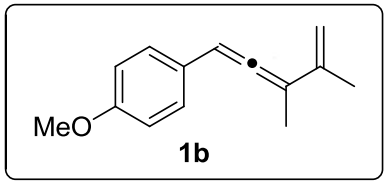
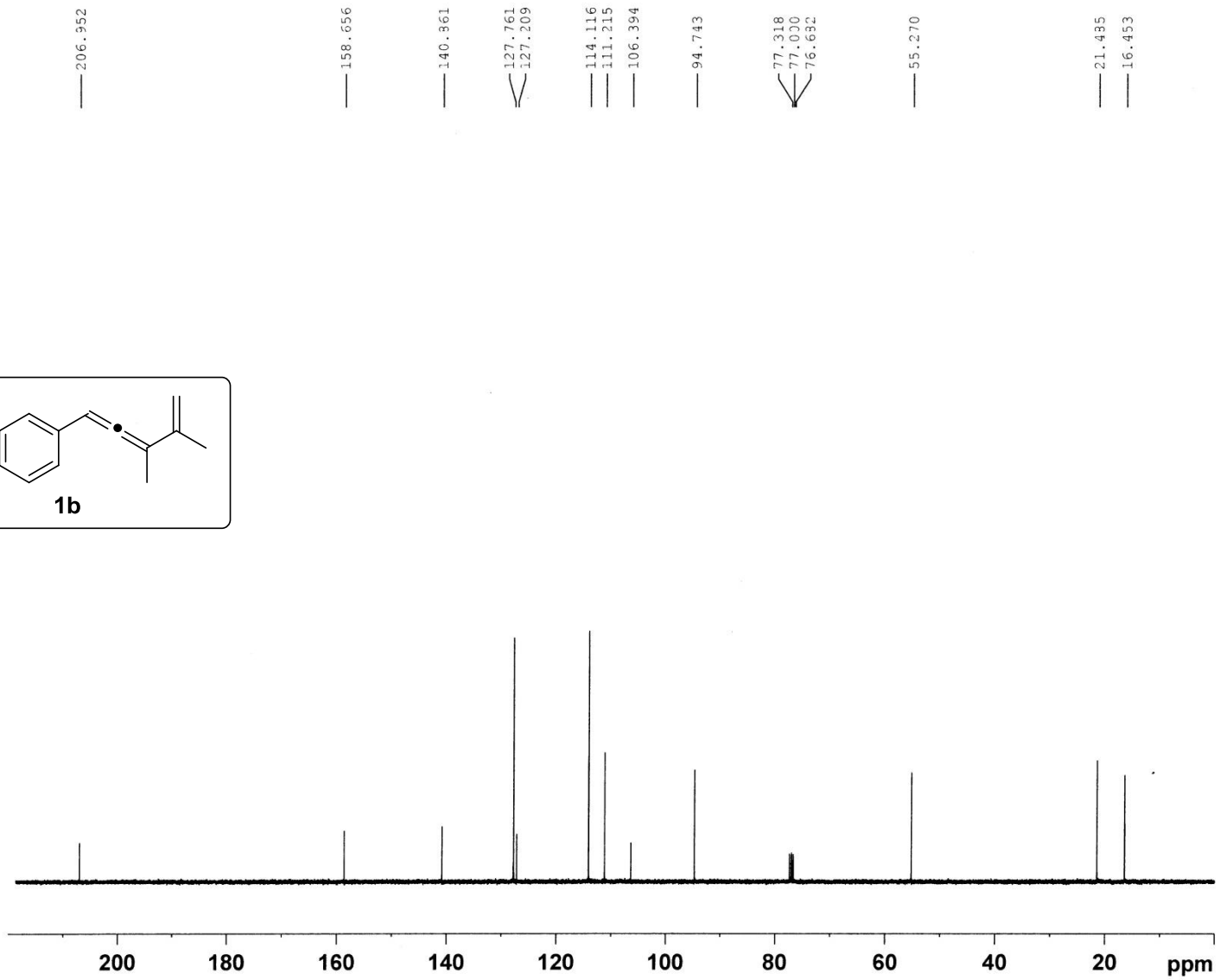
7.192
7.178
6.839
6.824
6.239
4.983
4.949
4.947
3.781
1.957
1.952
1.840
MeO
1b
10
9
8
7
6
5
4
3
2
1
ppm
2.01
2.01
1.00
1.04
1.09
3.12
3.15
3.13


MeO
1b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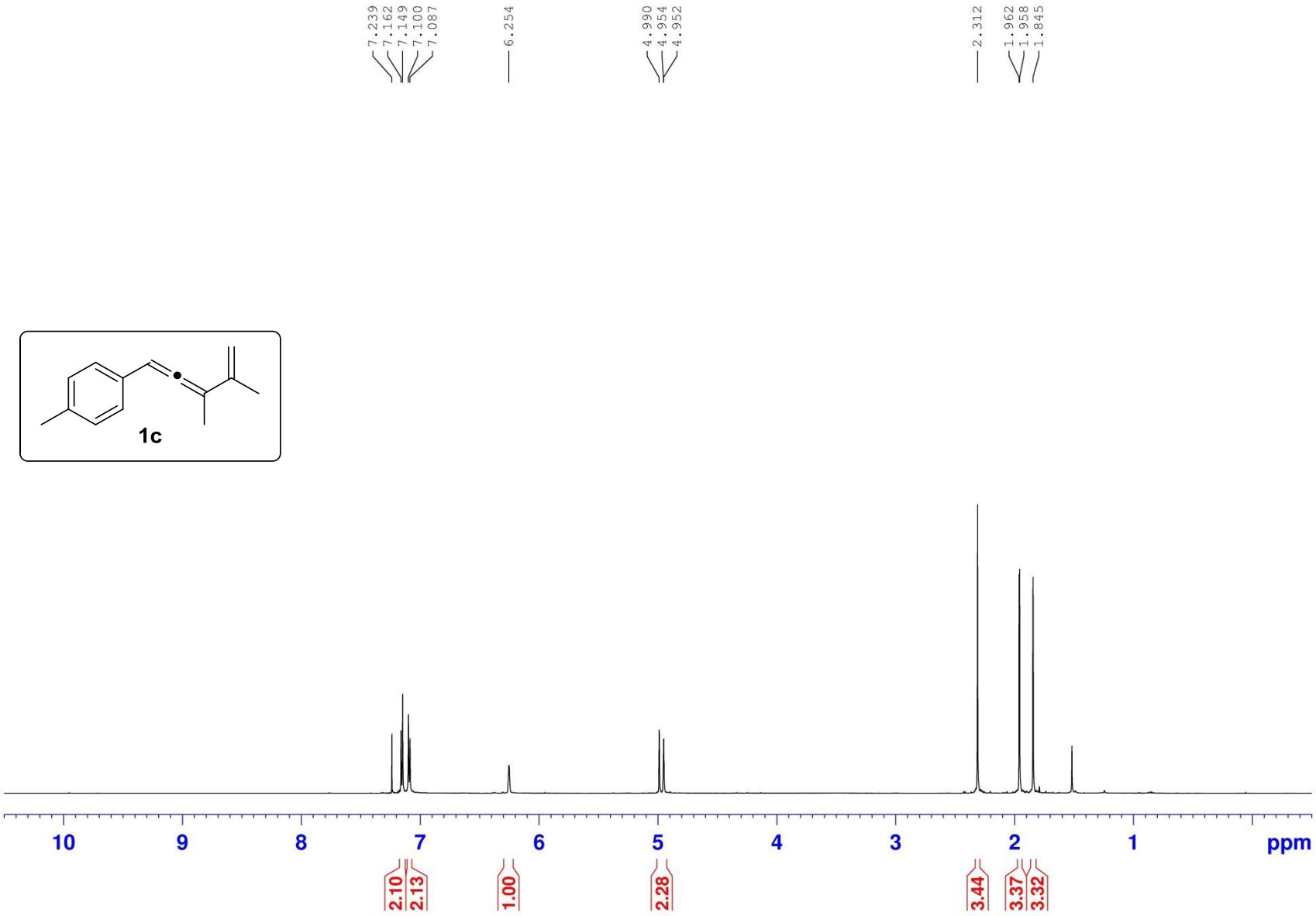
158.656
140.361
127.761
127.209
114.116
111.215
106.394
94.743
77.318
77.030
76.682
55.270
21.485
16.453
200
180
160
140
120
100
80
60
40
20
ppm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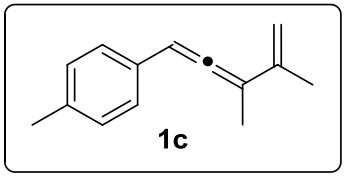
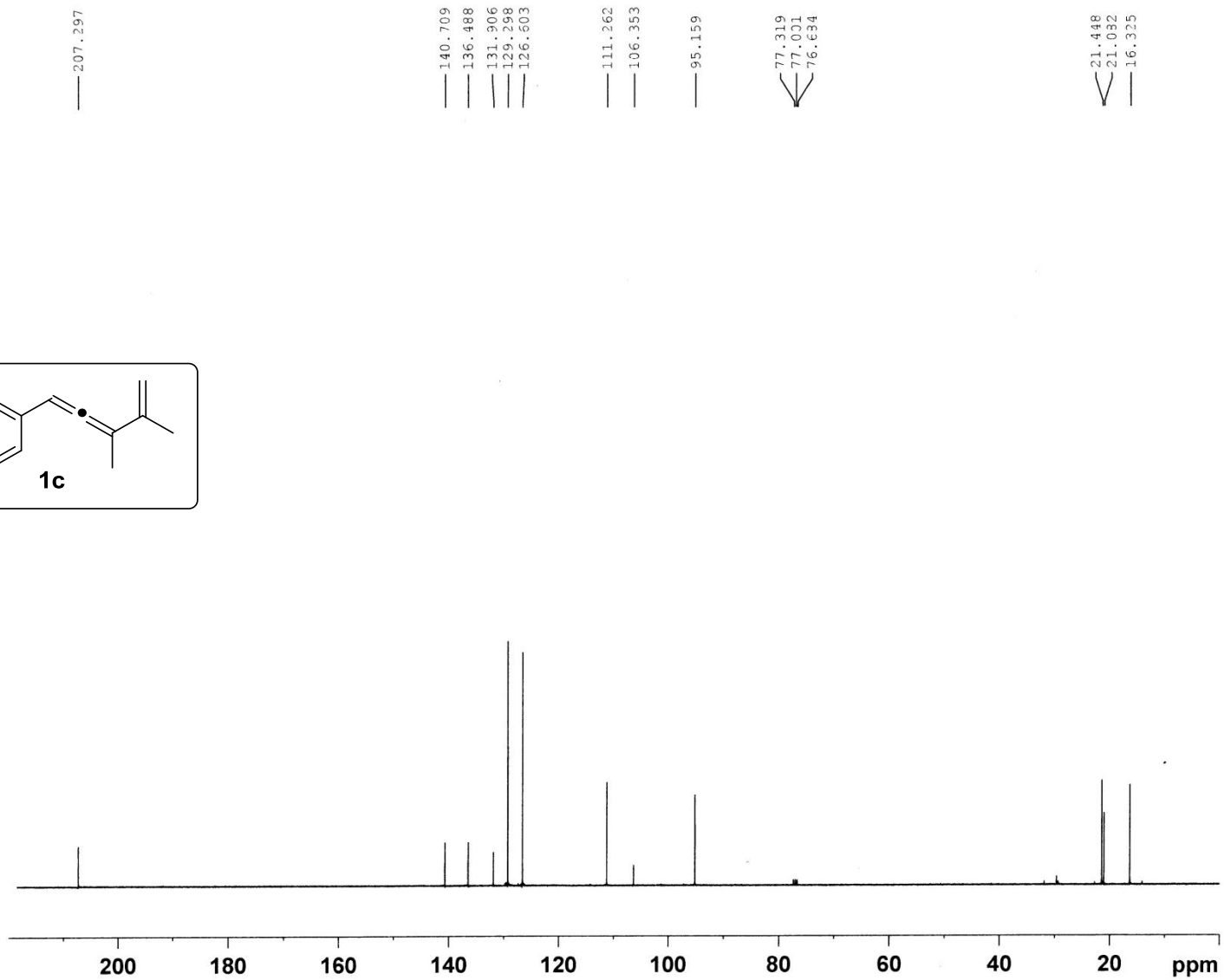
7.162
7.149
7.100
7.087
6.254
4.990
4.954
4.952
2.312
1.962
1.958
1.845
1c
10
9
8
7
6
5
4
3
2
1
ppm
2.10
2.13
1.00
2.28
3.44
3.37
3.32


1c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106.353
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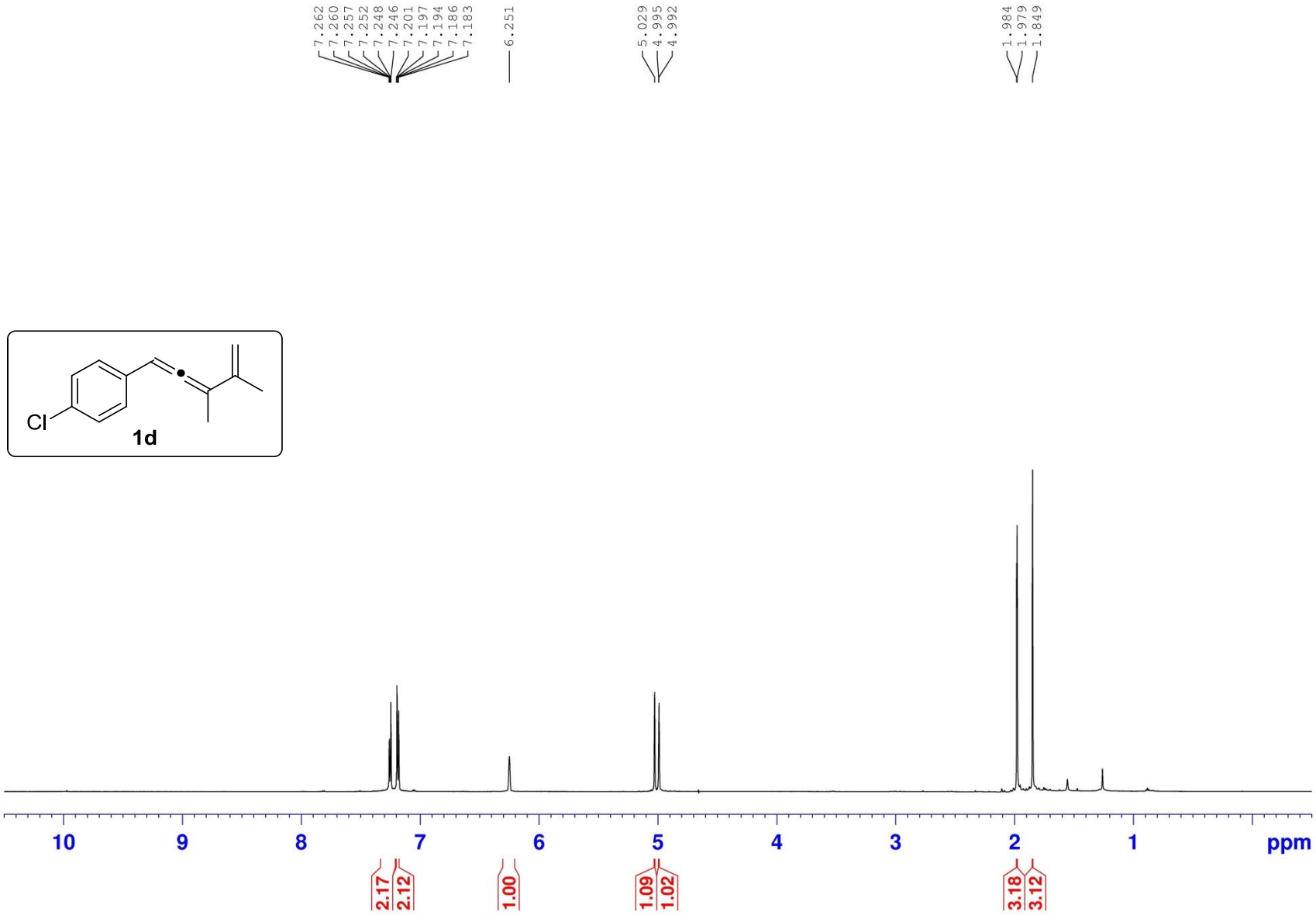
76.634
21.448
21.032
16.325
200
180
160
140
120
100
80
60
40
20
ppm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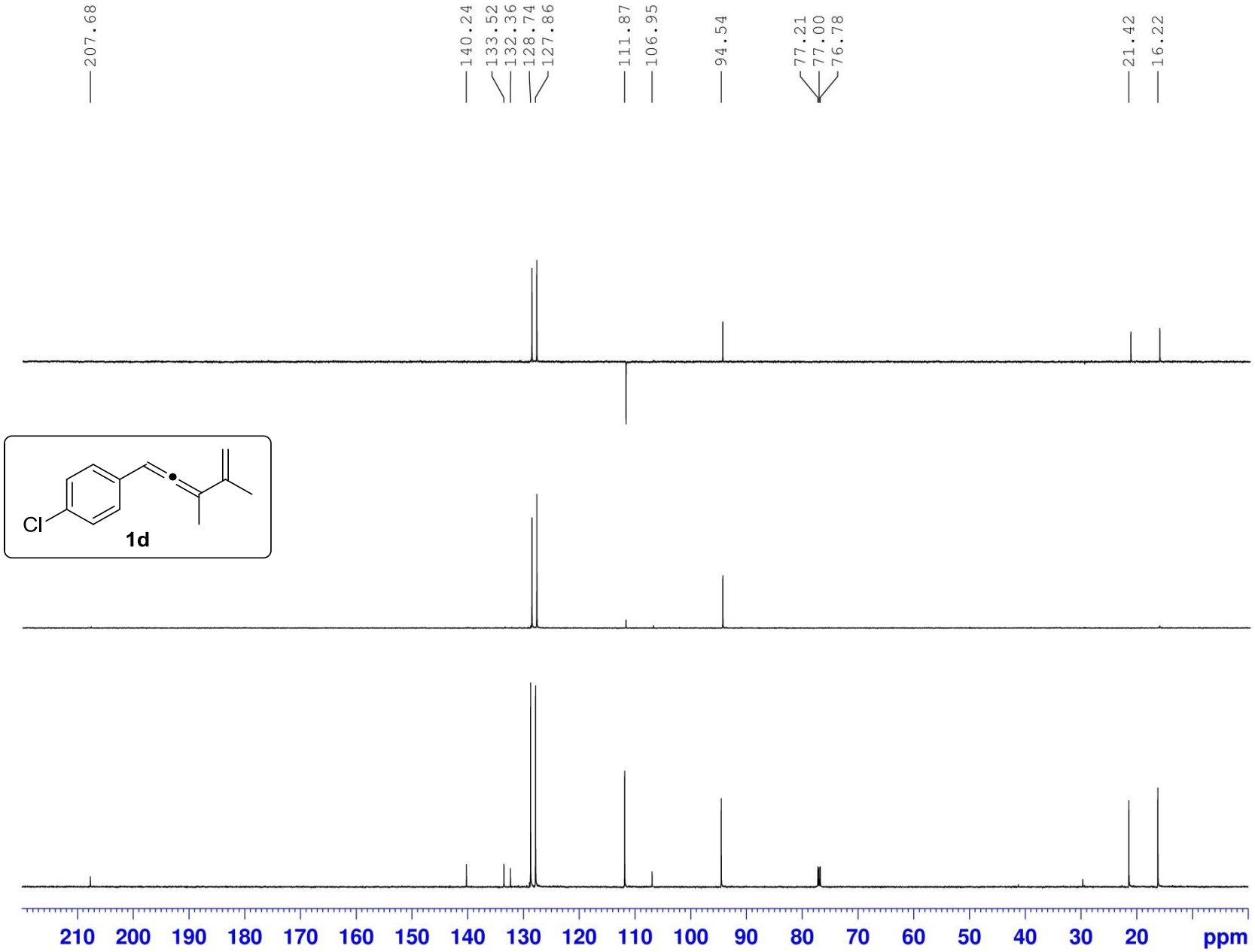
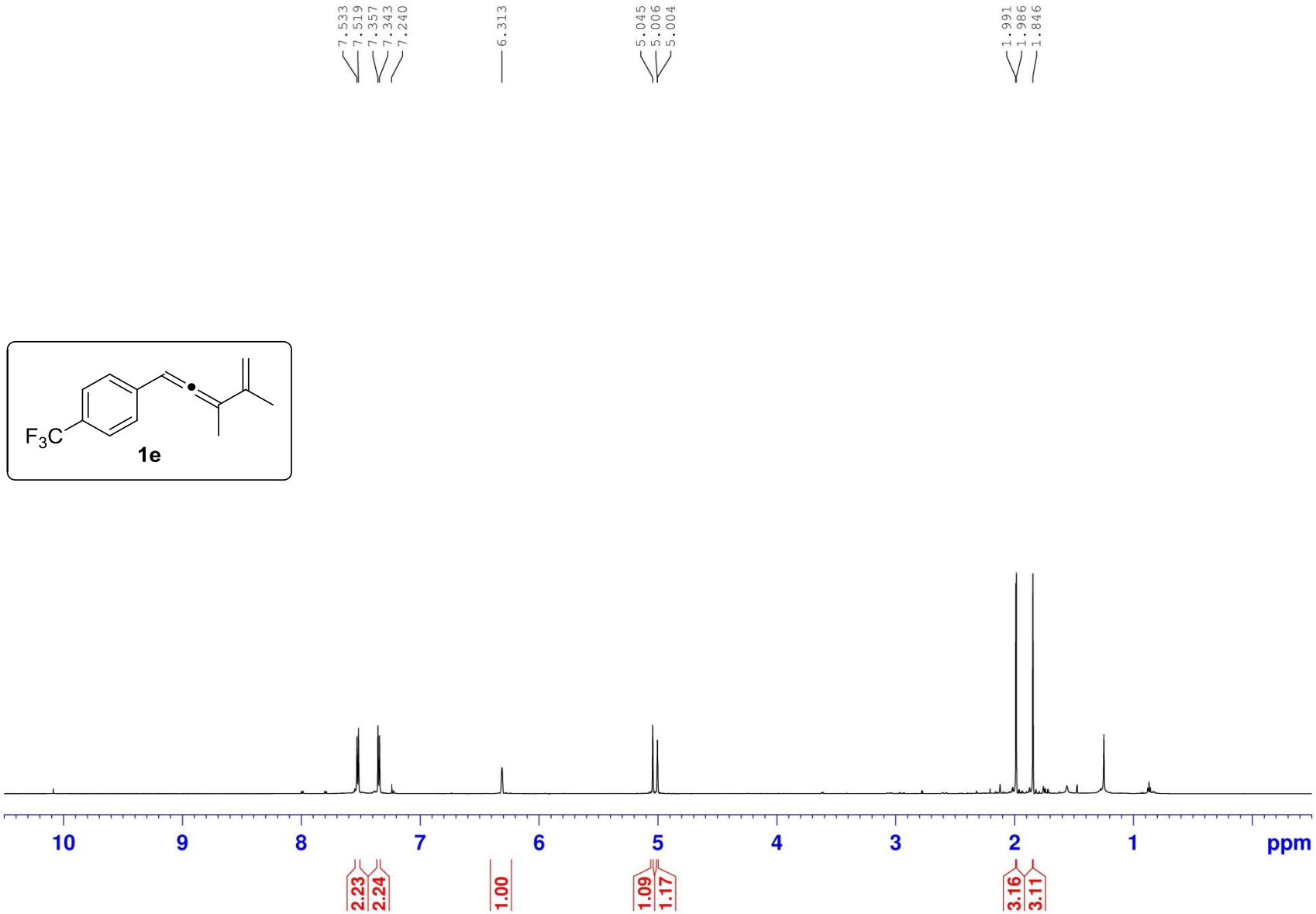
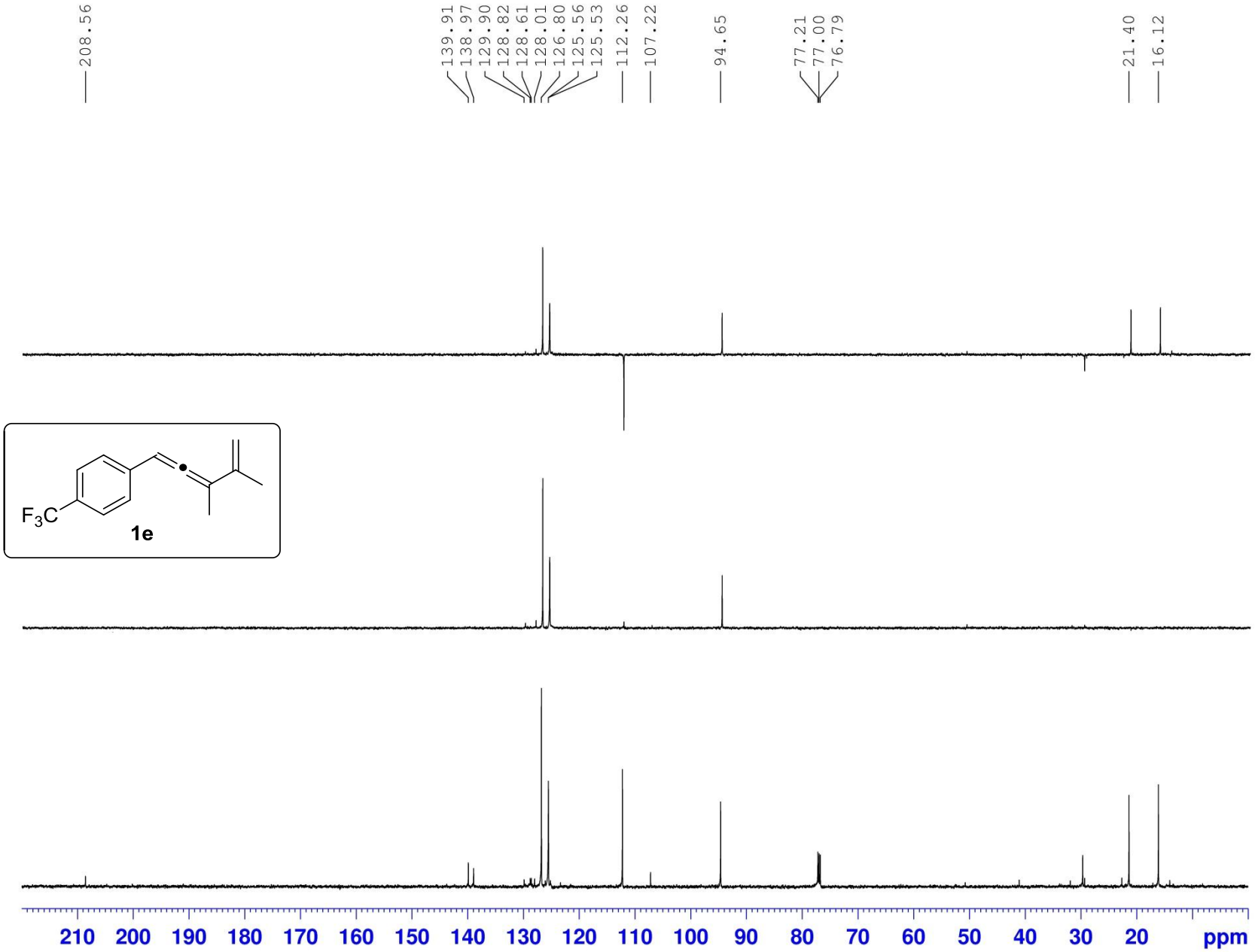
7.257
7.252
7.248
7.246
7.201
7.197
7.194
7.186
7.183
6.251
5.029
4.995
4.992
1.984
1.979
1.849
Cl
1d
10
9
8
7
6
5
4
3
2
1
ppm
2.17
2.12
1.00
1.09
1.02
3.18
3.12


207.68
140.24
133.52
132.36
128.74
127.86
111.87
106.95
94.54
77.21
77.00
76.78
21.42
16.22
Cl
1d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.533
7.519
7.357
7.343
7.240
6.313
5.045
5.006
5.004
1.991
1.986
1.846
F3C
1e
10
9
8
7
6
5
4
3
2
1
ppm
2.23
2.24
1.00
1.09
1.17
3.16
3.11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128.61
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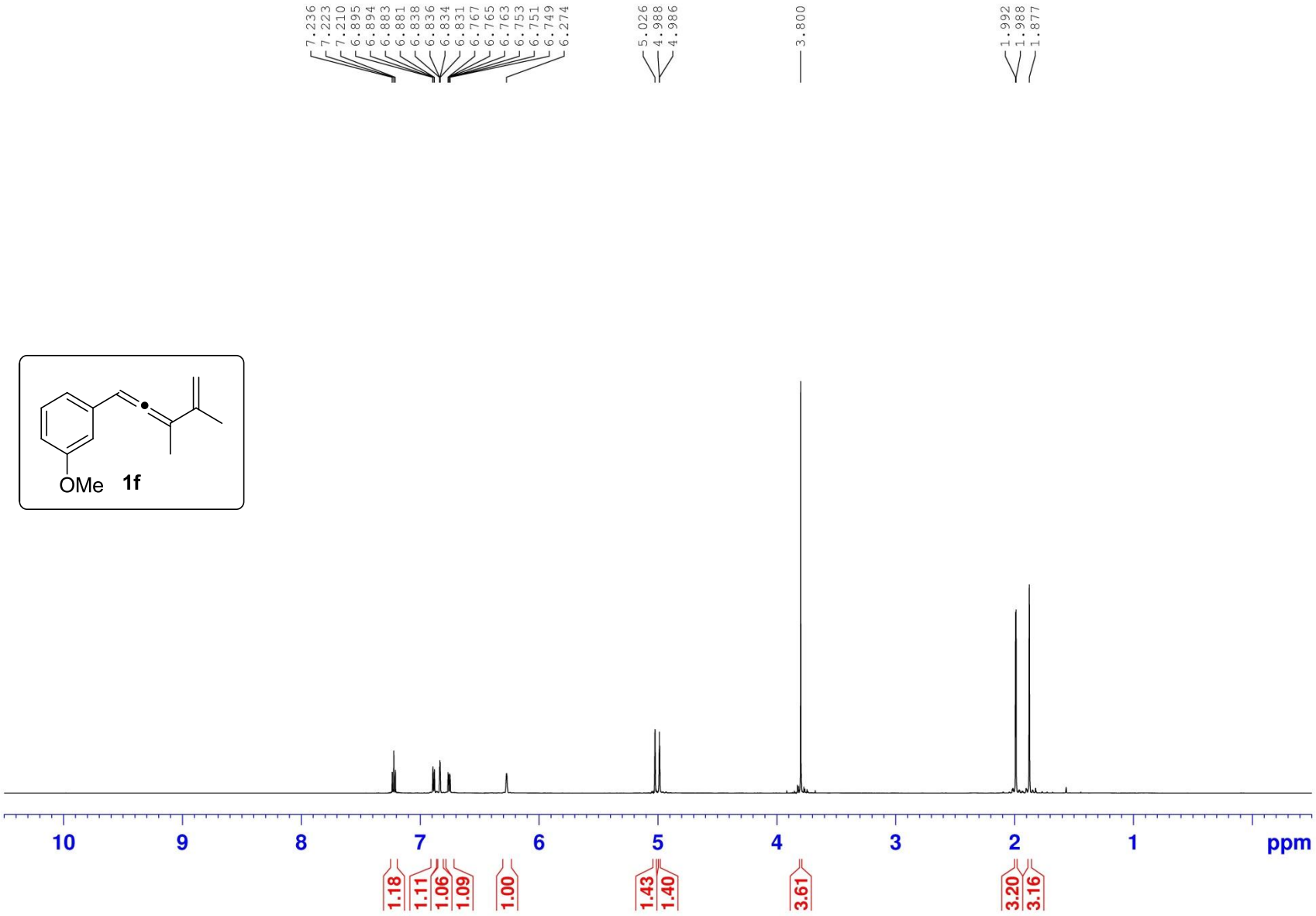
126.80
125.56
125.53
112.26
107.22
94.65
77.21
77.00
76.79
21.40
16.12
F3C
1e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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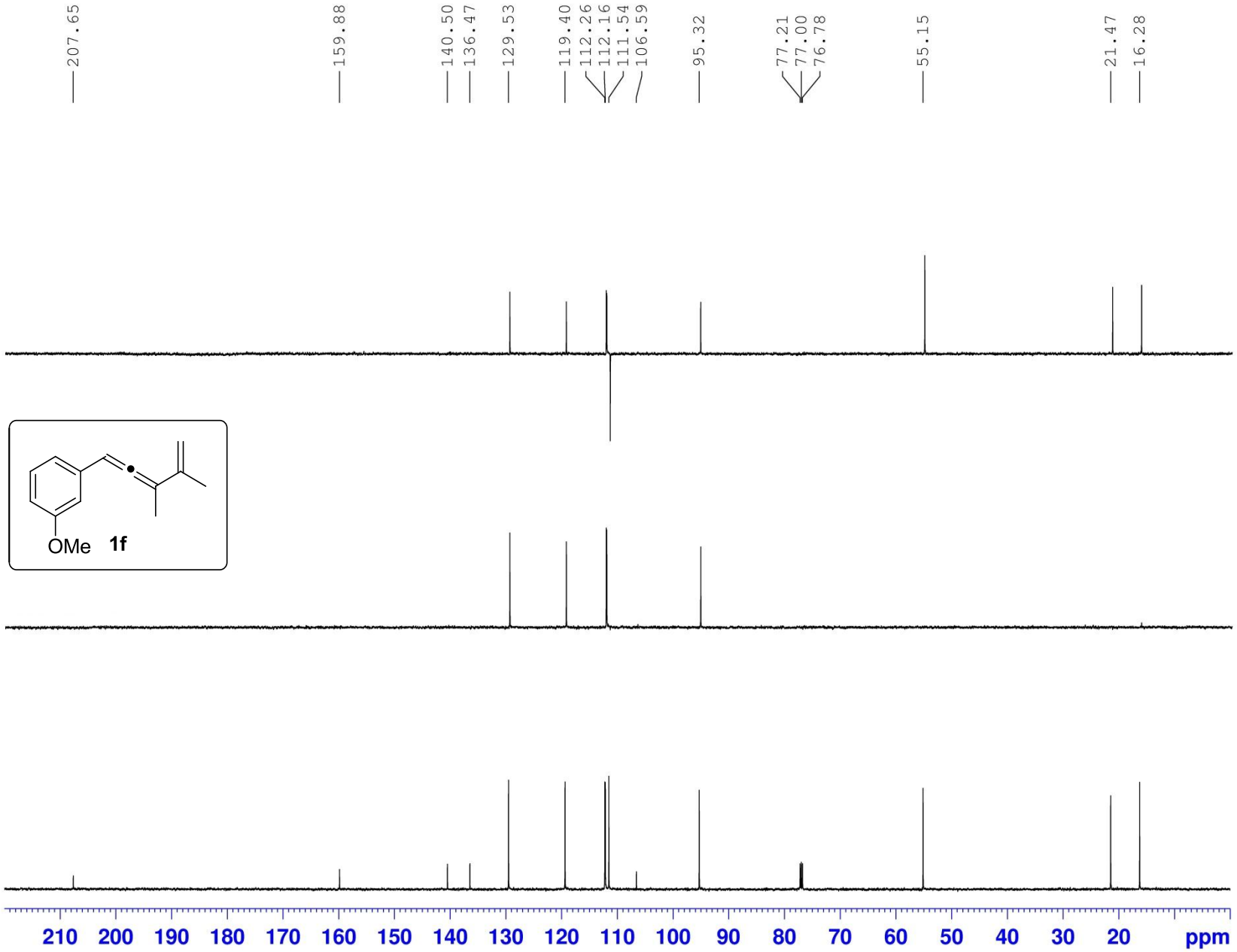
6.894
6.883
6.881
6.838
6.836
6.834
6.831
6.767
6.765
6.763
6.753
6.751
6.749
6.274
5.026
4.988
4.986
3.800
1.992
1.988
1.877
OMe
1f
10
9
8
7
6
5
4
3
2
1
ppm
1.18
1.11
1.06
1.09
1.00
1.43
1.40
3.61
3.20
3.16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112.16
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106.59
95.32
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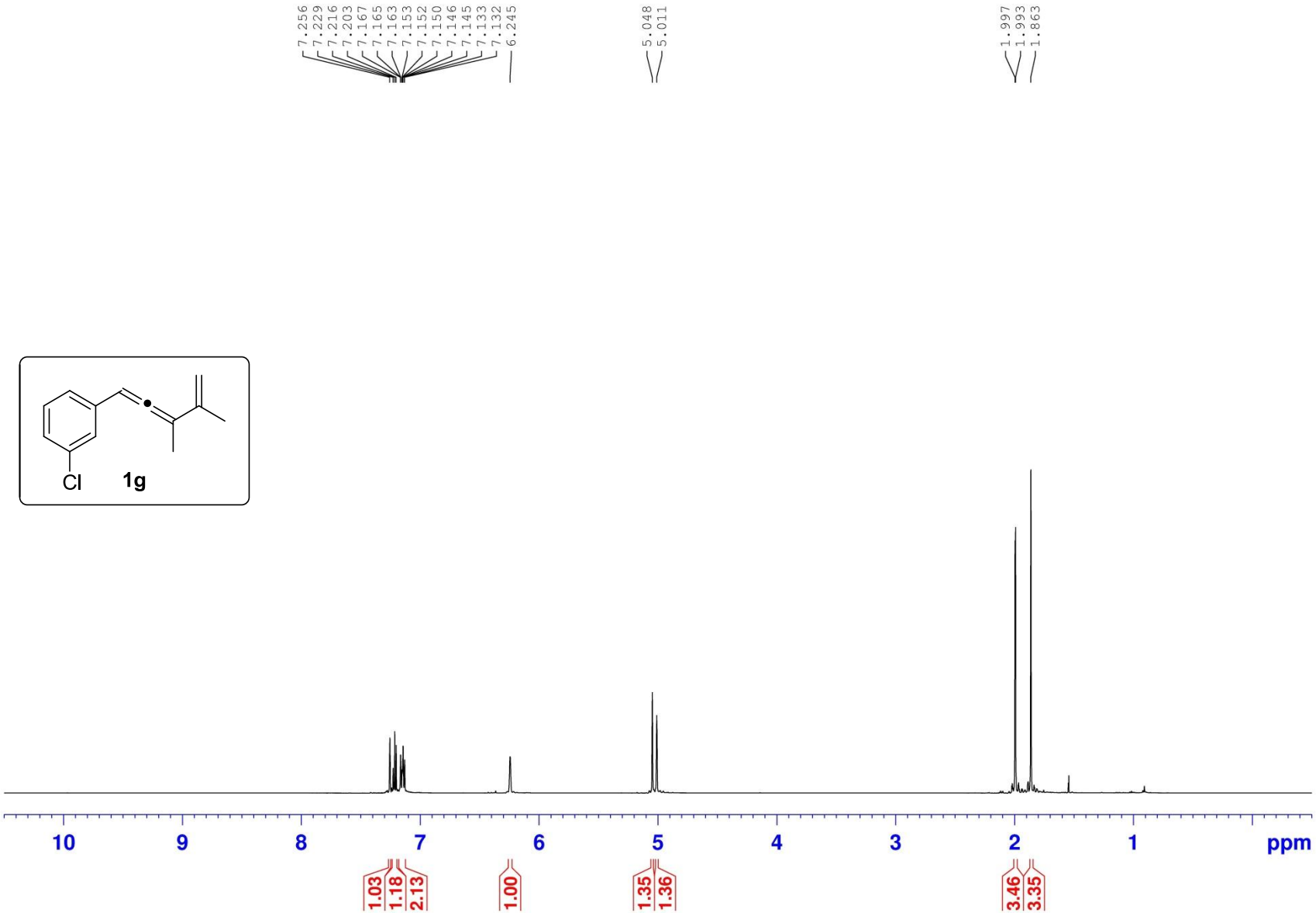
77.00
76.78
55.15
21.47
16.28
OMe
1f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.153
7.152
7.150
7.146
7.145
7.133
7.132
6.245
5.048
5.011
1.997
1.993
1.863
Cl
1g
10
9
8
7
6
5
4
3
2
1
ppm
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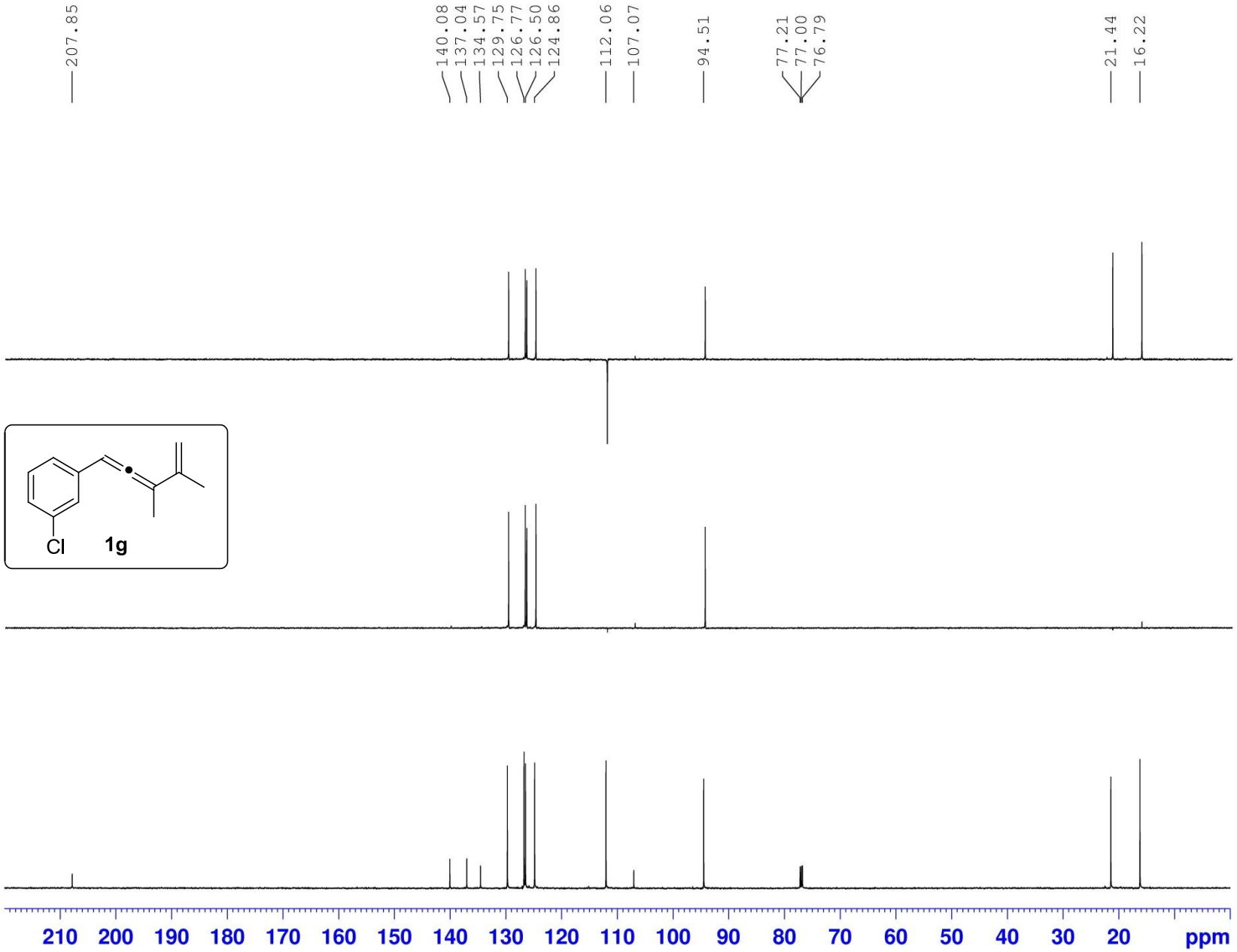
2.13
1.00
1.35
1.36
3.46
3.35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126.50
124.86
112.06
107.07
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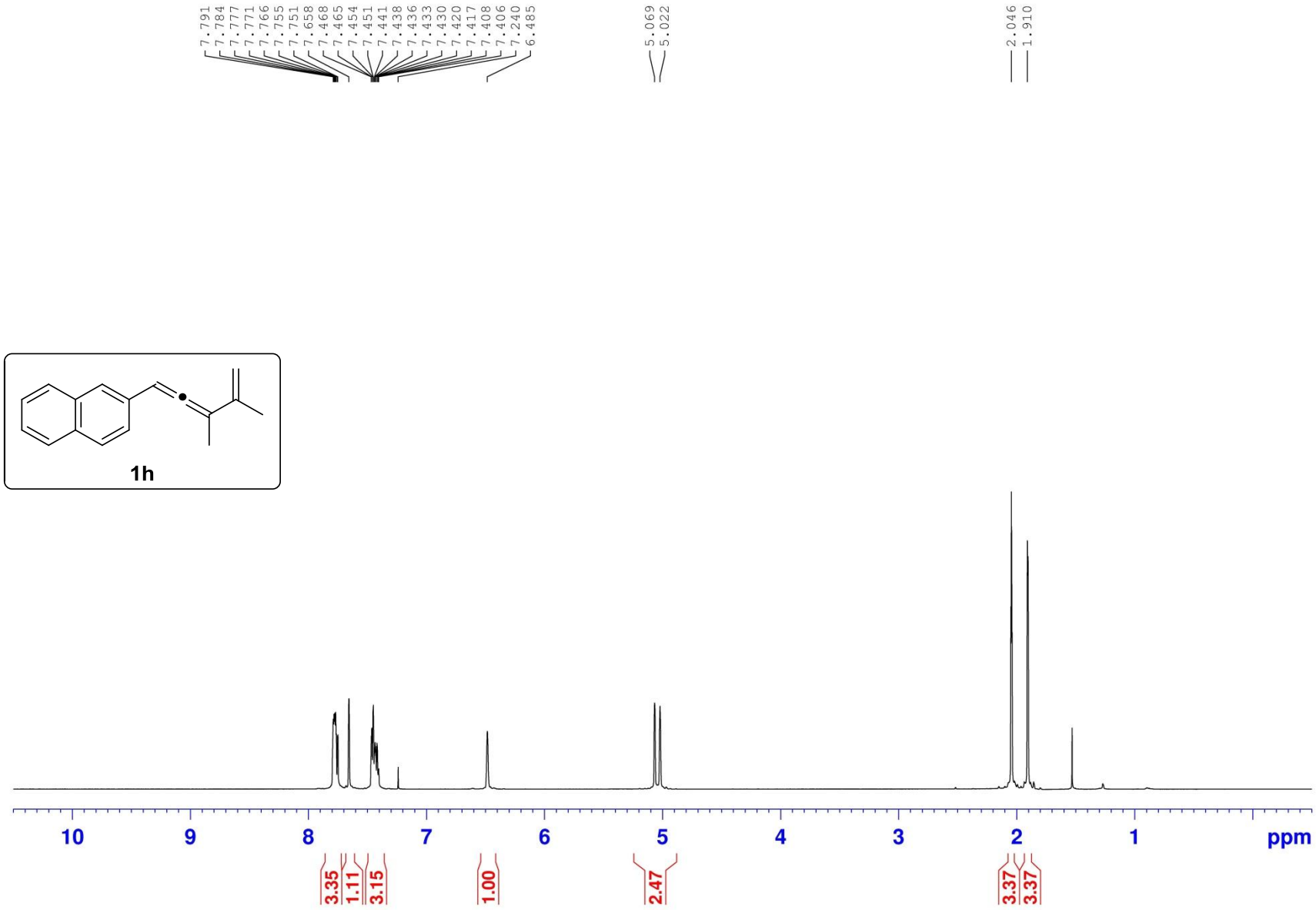
77.00
76.79
21.44
16.22
Cl
1g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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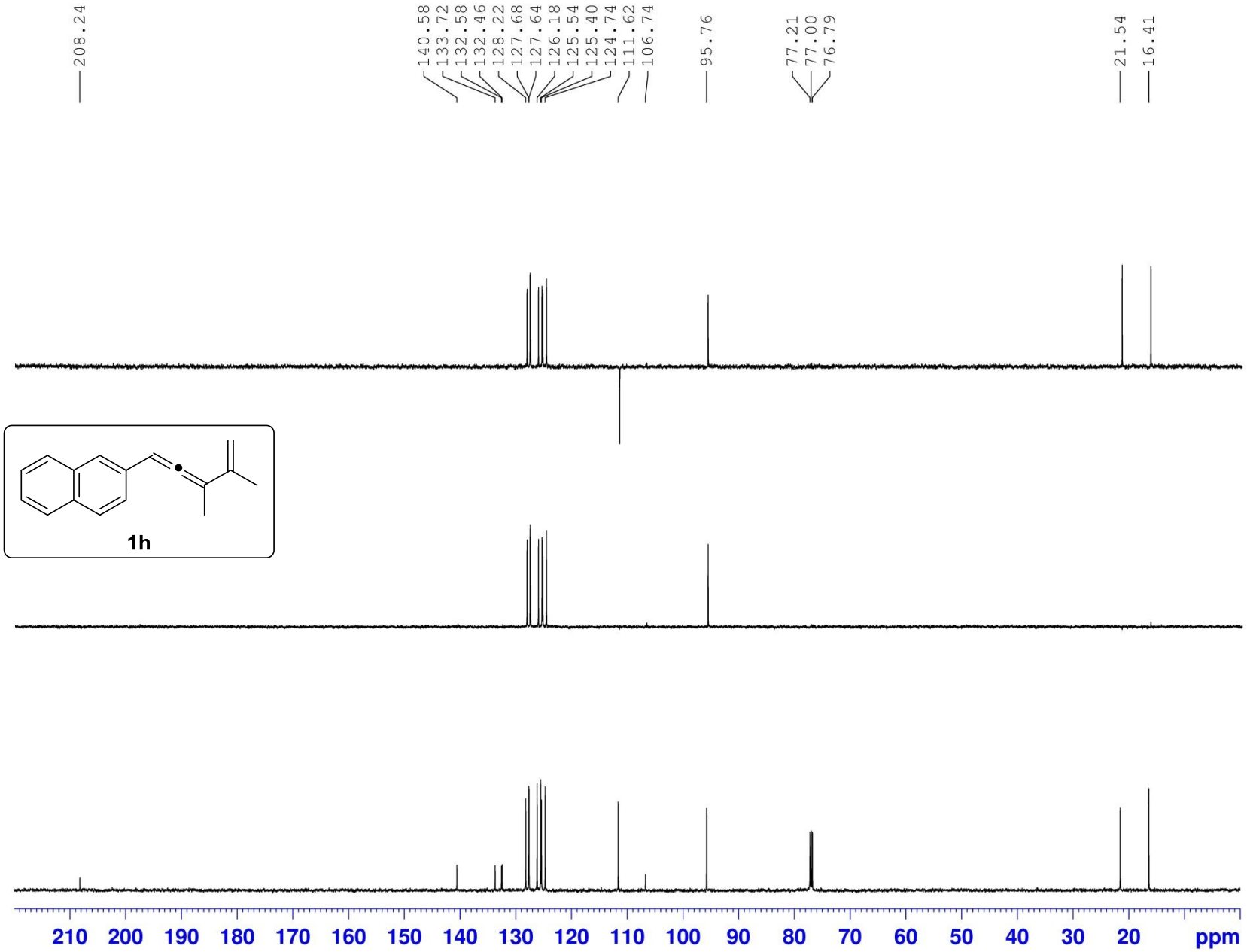
7.438
7.436
7.433
7.430
7.420
7.417
7.408
7.406
7.240
6.485
5.069
5.022
2.046
1.910
1h
10
9
8
7
6
5
4
3
2
1
ppm
3.35
1.11
3.15
1.00
2.47
3.37
3.37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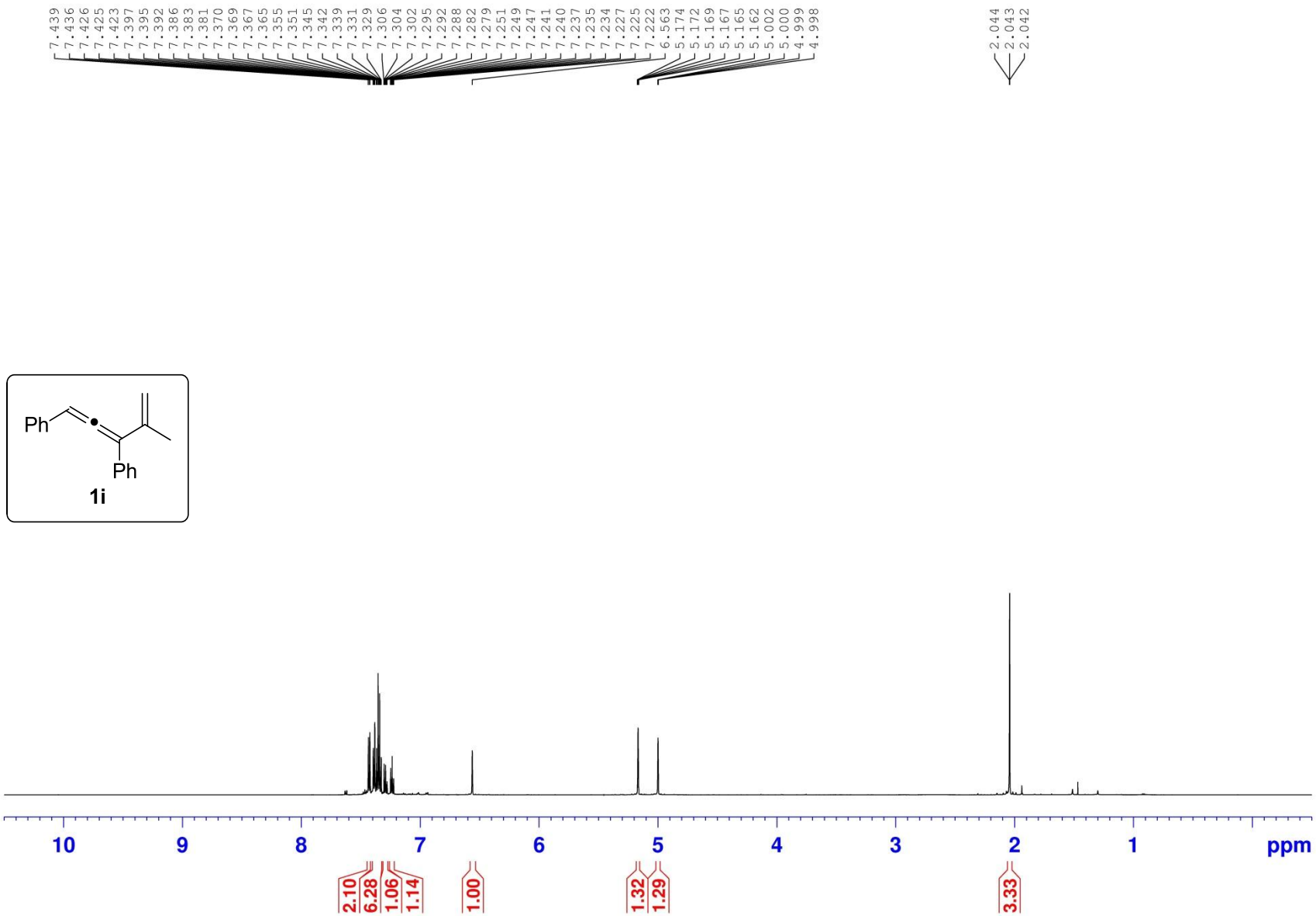
126.18
125.54
125.40
124.74
111.62
106.74
95.76
77.21
77.00
76.79
21.54
16.41
1h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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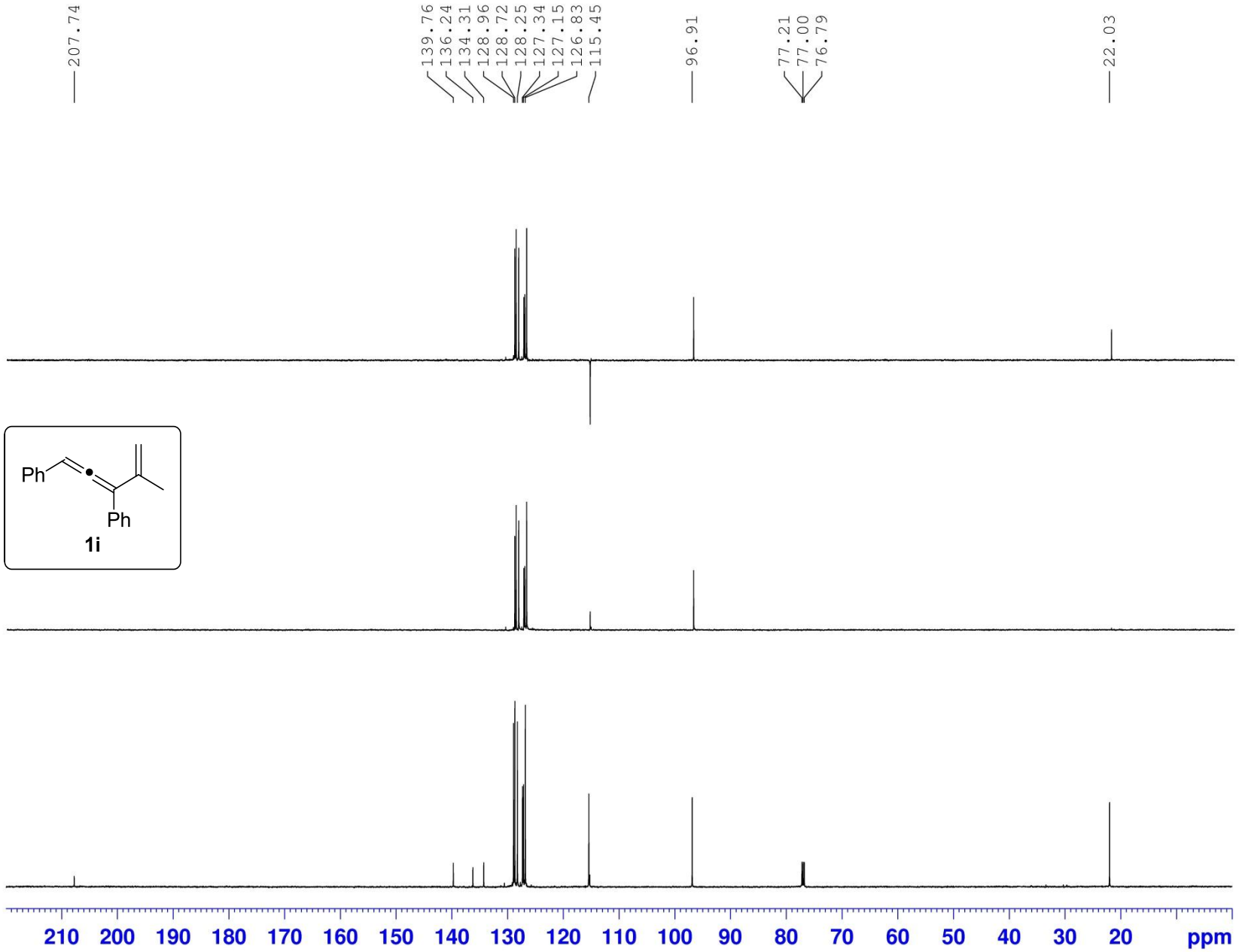
7.369
7.367
7.365
7.355
7.351
7.345
7.342
7.339
7.331
7.329
7.306
7.304
7.302
7.295
7.292
7.288
7.282
7.279
7.251
7.249
7.247
7.241
7.240
7.237
7.235
7.234
7.227
7.225
7.222
6.563
5.174
5.172
5.169
5.167
5.165
5.162
5.000
4.999
4.998
2.044
2.043
2.042
Ph
Ph
1i
10
9
8
7
6
5
4
3
2
1
ppm
2.10
6.28
1.06
1.14
1.00
1.32
1.29
3.33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127.34
127.15
126.83
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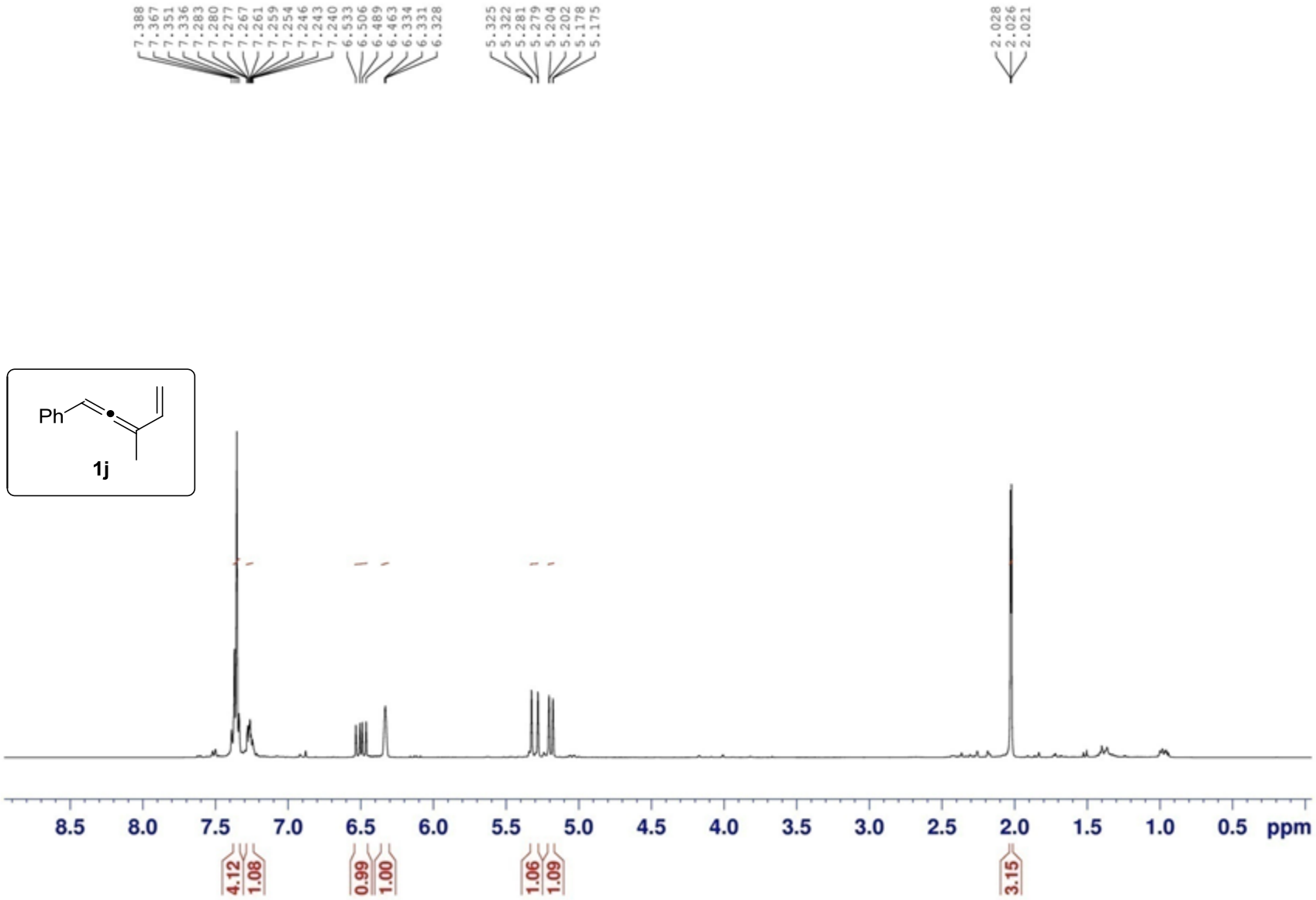
96.91
77.21
77.00
76.79
22.03
Ph
Ph
1i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.280
7.277
7.267
7.261
7.259
7.254
7.246
7.243
7.240
6.533
6.506
6.489
6.463
6.334
6.331
6.328
5.325
5.322
5.281
5.279
5.204
5.202
5.178
5.175
2.028
2.026
2.021
Ph
1j
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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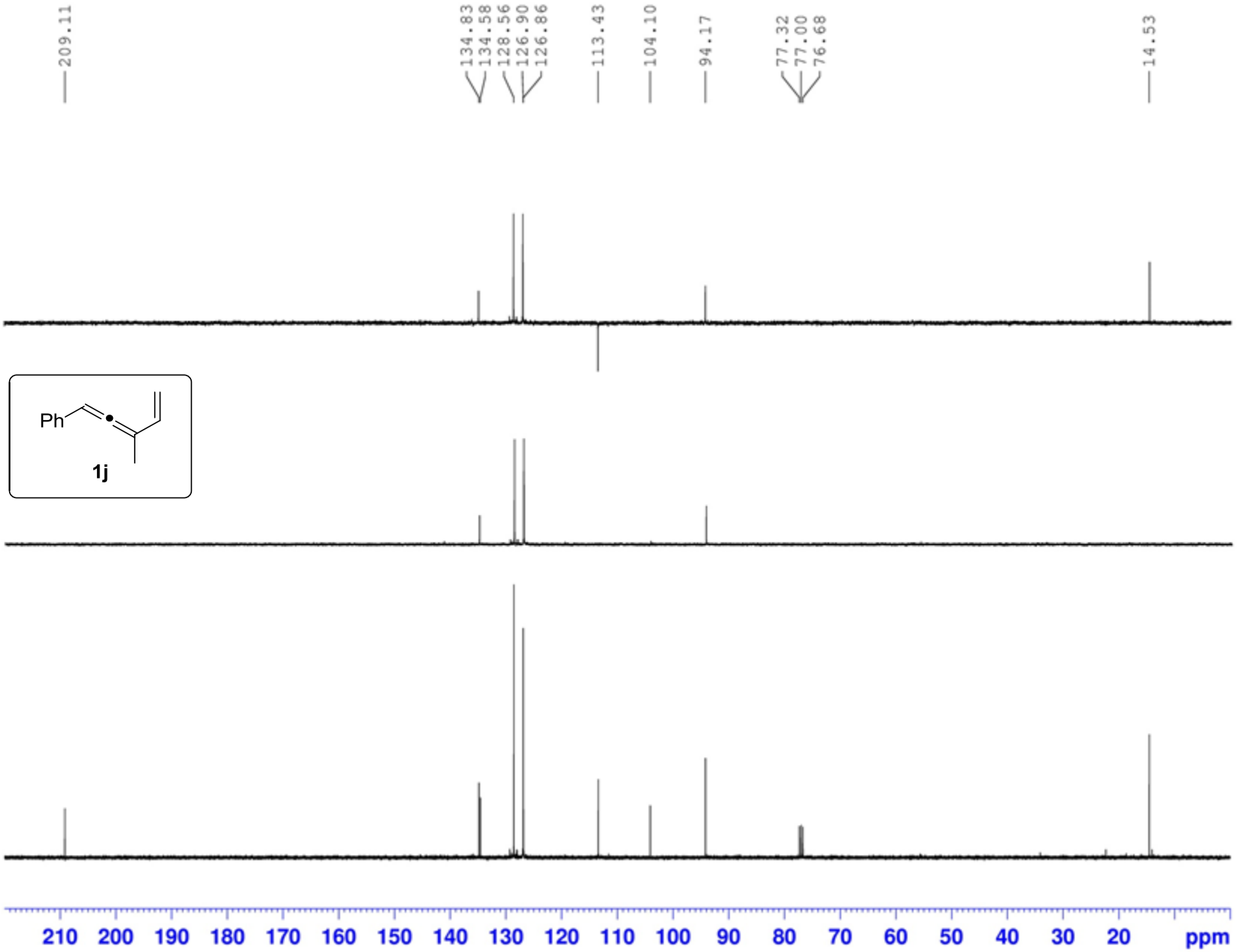
1.09
3.15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134.83
134.58
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113.43
104.10
94.17
77.32
77.00
76.68
14.53
Ph
1j
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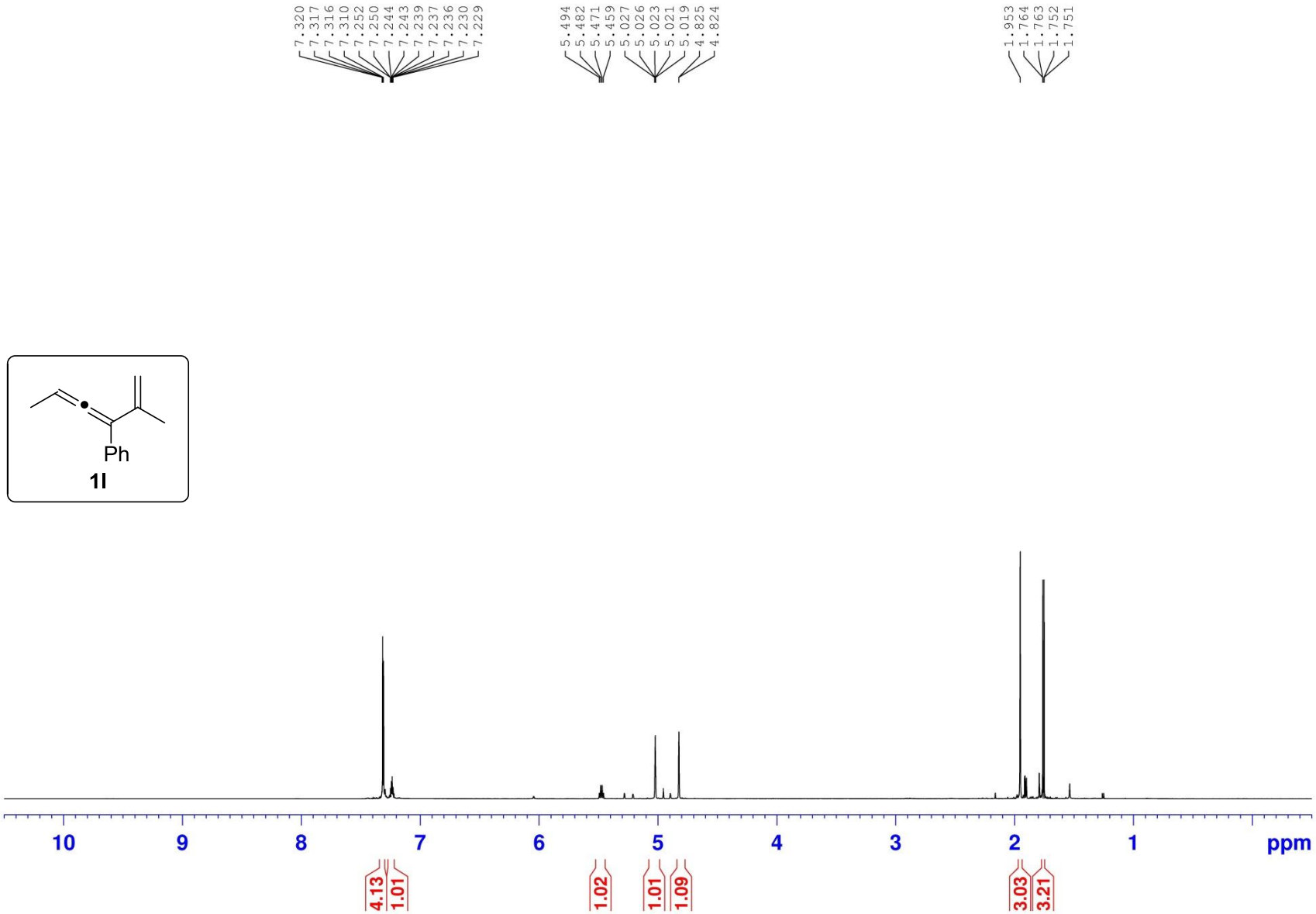
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7.229
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5.482
5.471
5.459
5.027
5.026
5.023
5.021
5.019
4.825
4.824
1.953
1.764
1.763
1.752
1.751
Ph
1l
10
9
8
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2
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ppm
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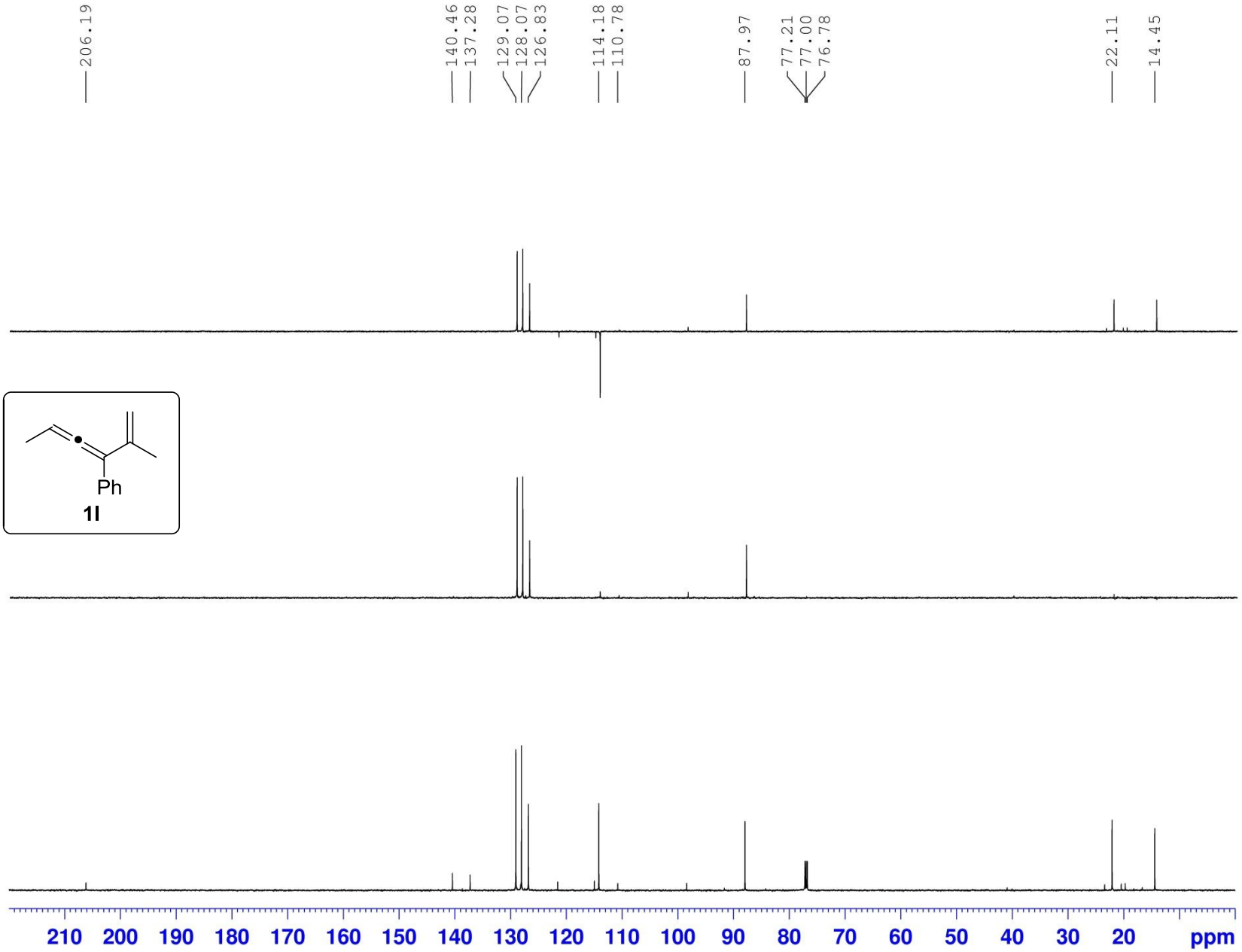
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114.18
110.78
87.97
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77.00
76.78
22.11
14.45
Ph
1l
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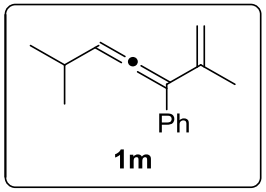
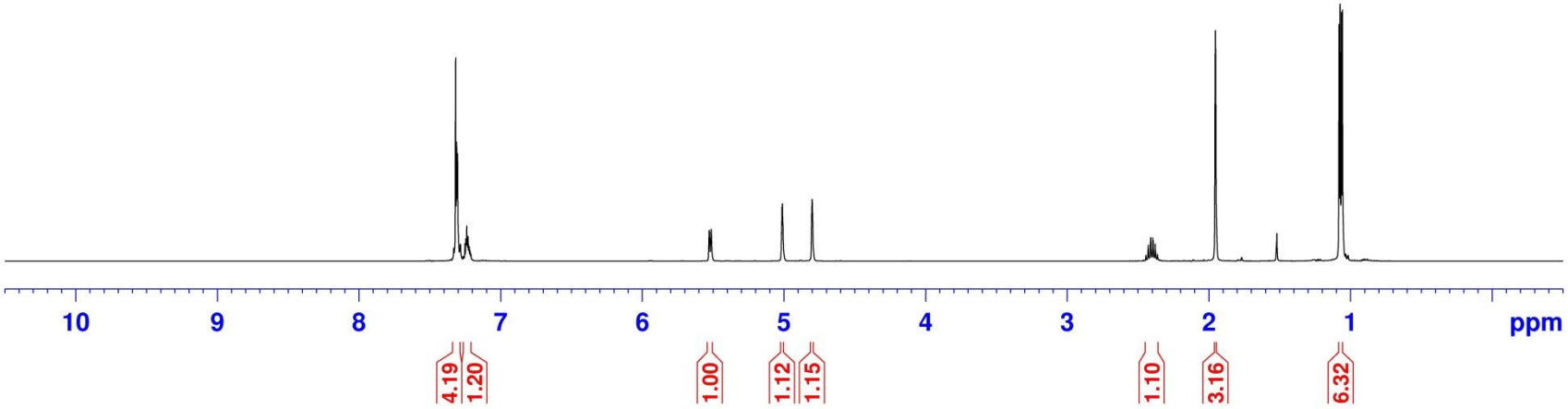

Ph
1m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7.231
7.226
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7.218
7.216
7.210
5.529
5.515
5.018
5.015
5.011
5.008
4.802
4.801
2.428
2.413
2.411
2.397
2.394
2.380
1.955
1.521
1.082
1.074
1.065
1.057
10
9
8
7
6
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2
1
ppm
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1.12
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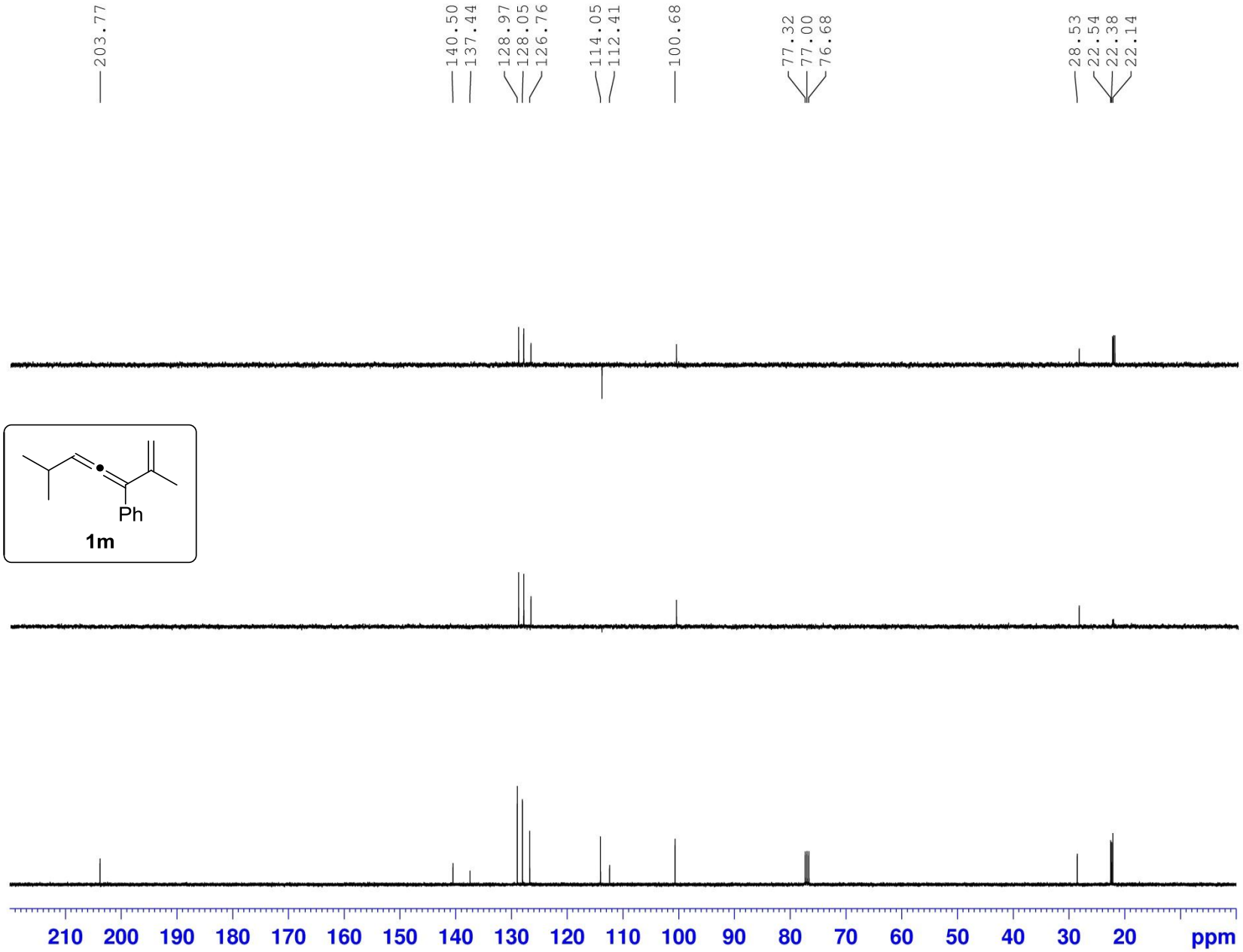
3.16
6.32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128.97
128.05
126.76
114.05
112.41
100.68
77.32
77.00
76.68
28.53
22.54
22.38
22.14
Ph
1m
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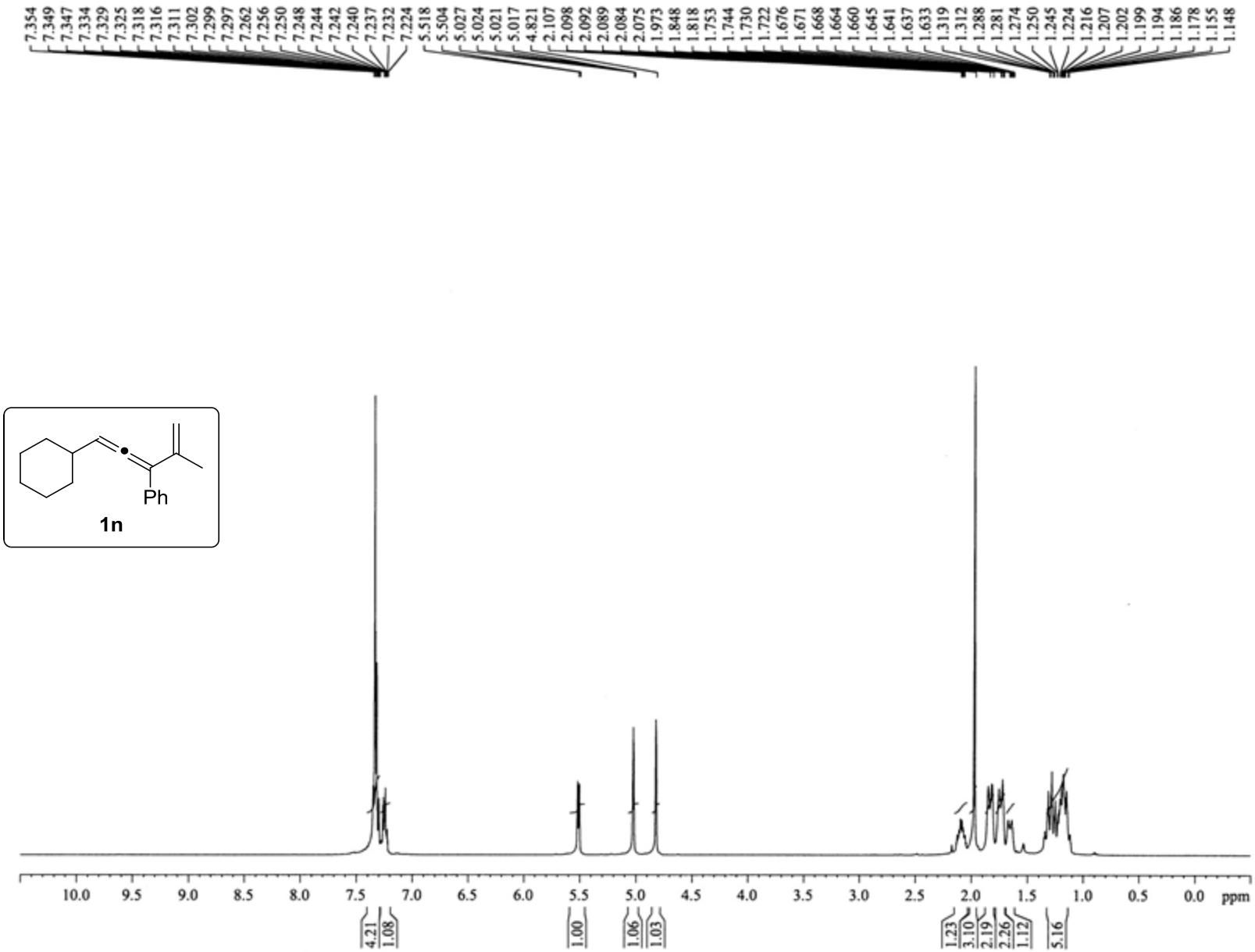
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5.518 5.504 5.027 5.024 5.021 5.017 4.821 2.107 2.098 2.092 2.089 2.084 2.075 1.973 1.848 1.818 1.753 1.744 1.730 1.722 1.676 1.671 1.668 1.664 1.660 1.645 1.641 1.637 1.633 1.319 1.312 1.288 1.281 1.274 1.250 1.245 1.224 1.216 1.207 1.202 1.199 1.194 1.186 1.178 1.155 1.148
Ph
1n
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 ppm
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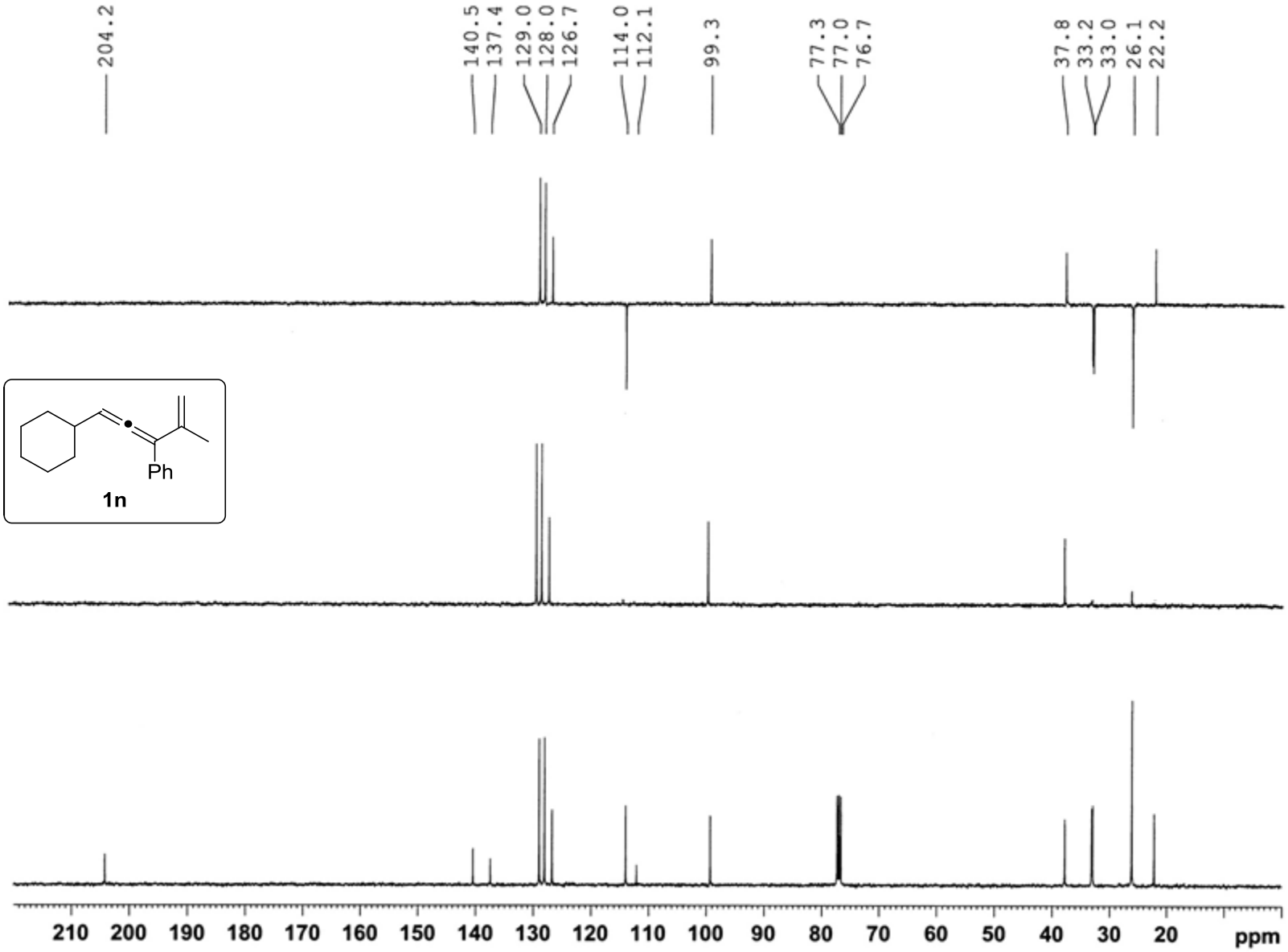
1.00
1.06 1.03
1.23 3.10 2.19 2.26 1.12 5.16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137.4
129.0
128.0
126.7
114.0
112.1
99.3
77.3
77.0
76.7
37.8
33.2
33.0
26.1
22.2
Ph
1n
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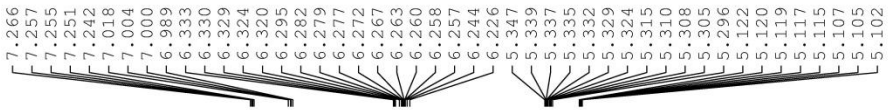
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7.255
7.251
7.242
7.018
7.004
7.000
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6.333
6.330
6.329
6.324
6.320
6.295
6.282
6.279
6.277
6.272
6.267
6.263
6.260
6.258
6.257
6.244
6.226
5.347
5.339
5.337
5.335
5.332
5.329
5.324
5.315
5.310
5.308
5.305
5.296
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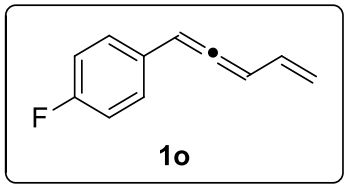
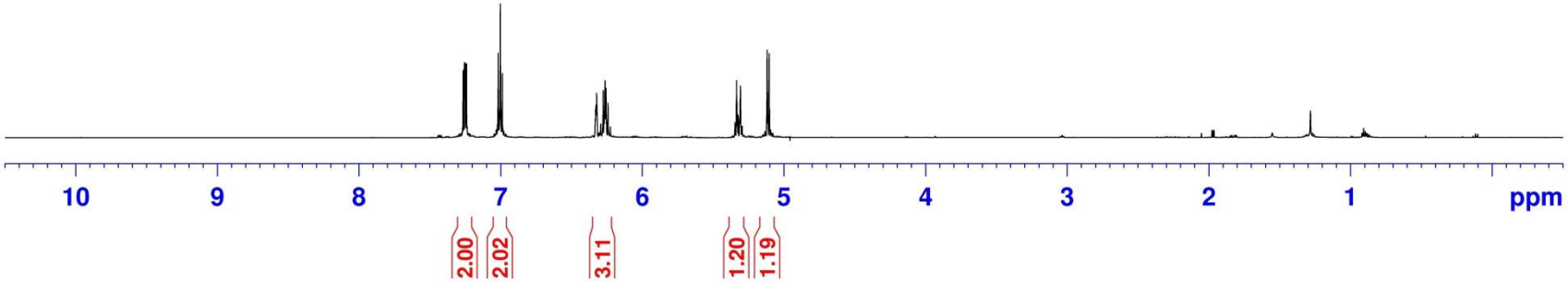
5.120
5.119
5.117
5.115
5.107
5.105
5.102


F
1o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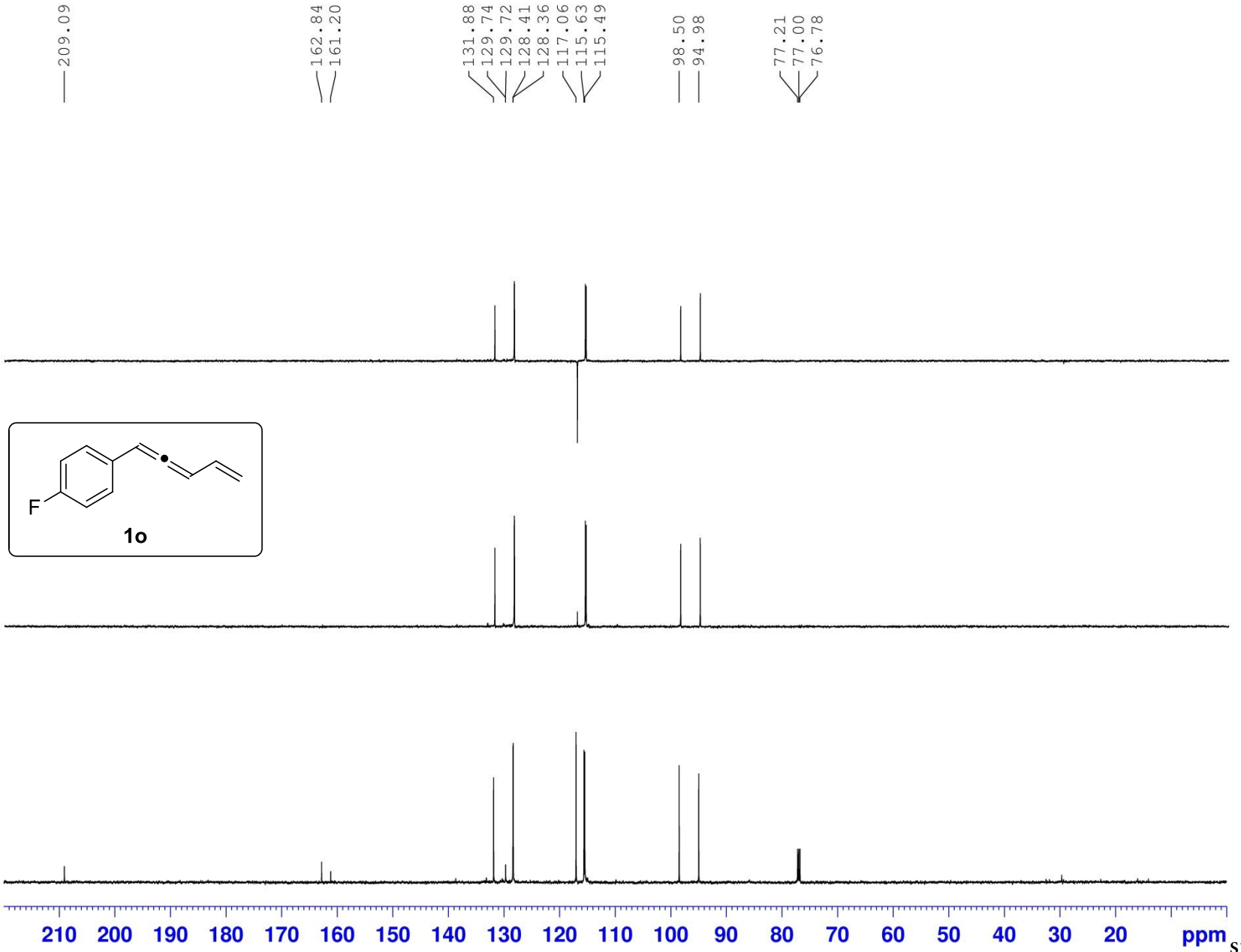
9
8
7
6
5
4
3
2
1
ppm
2.00
2.02
3.11
1.20
1.19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161.20
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129.72
128.41
128.36
117.06
115.63
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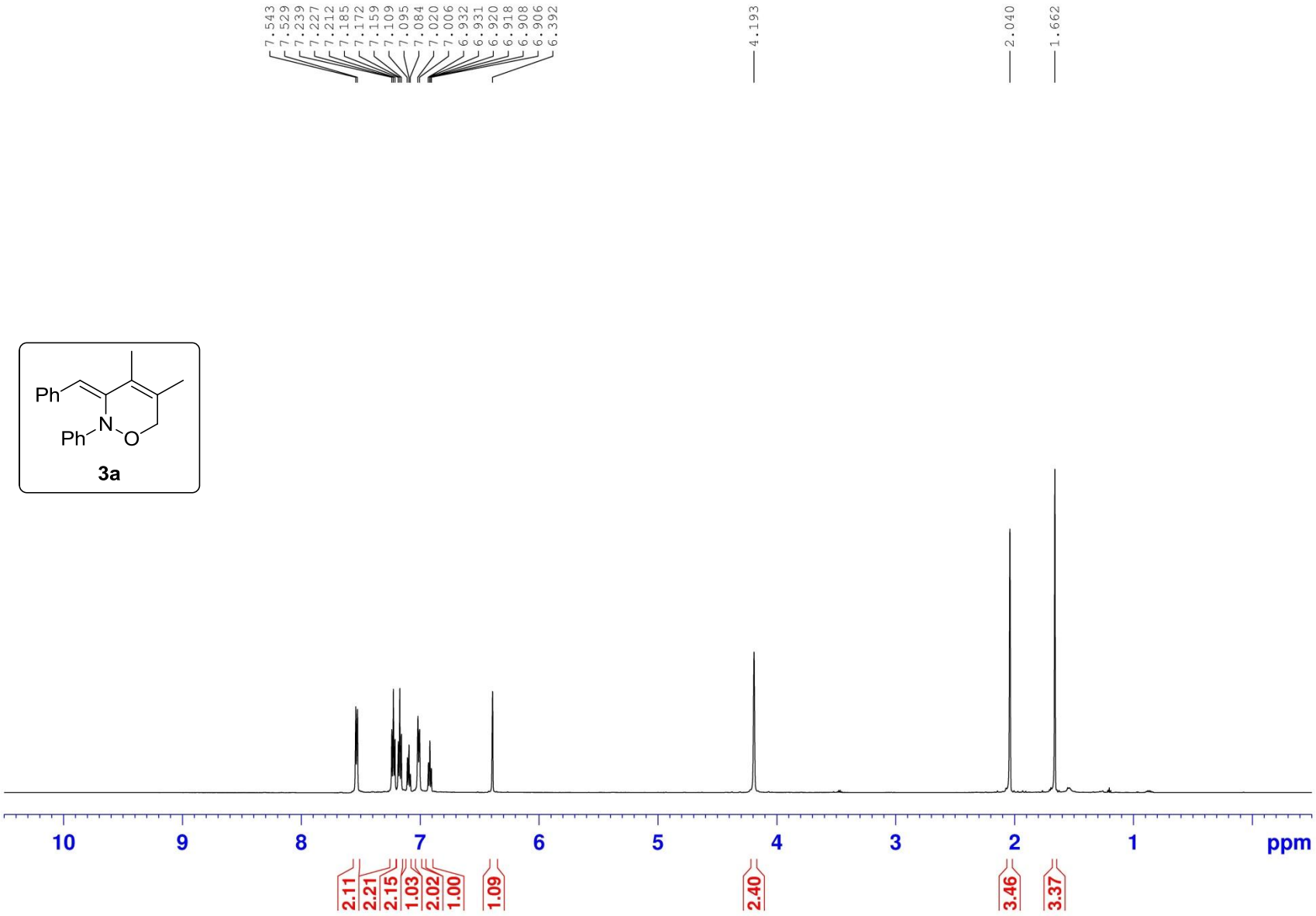
77.21
77.00
76.78
F
1o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.159
7.109
7.095
7.084
7.020
7.006
6.932
6.931
6.920
6.918
6.908
6.906
6.392
4.193
2.040
1.662
Ph
Ph
N
O
3a
10
9
8
7
6
5
4
3
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ppm
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2.21
2.15
1.03
2.02
1.00
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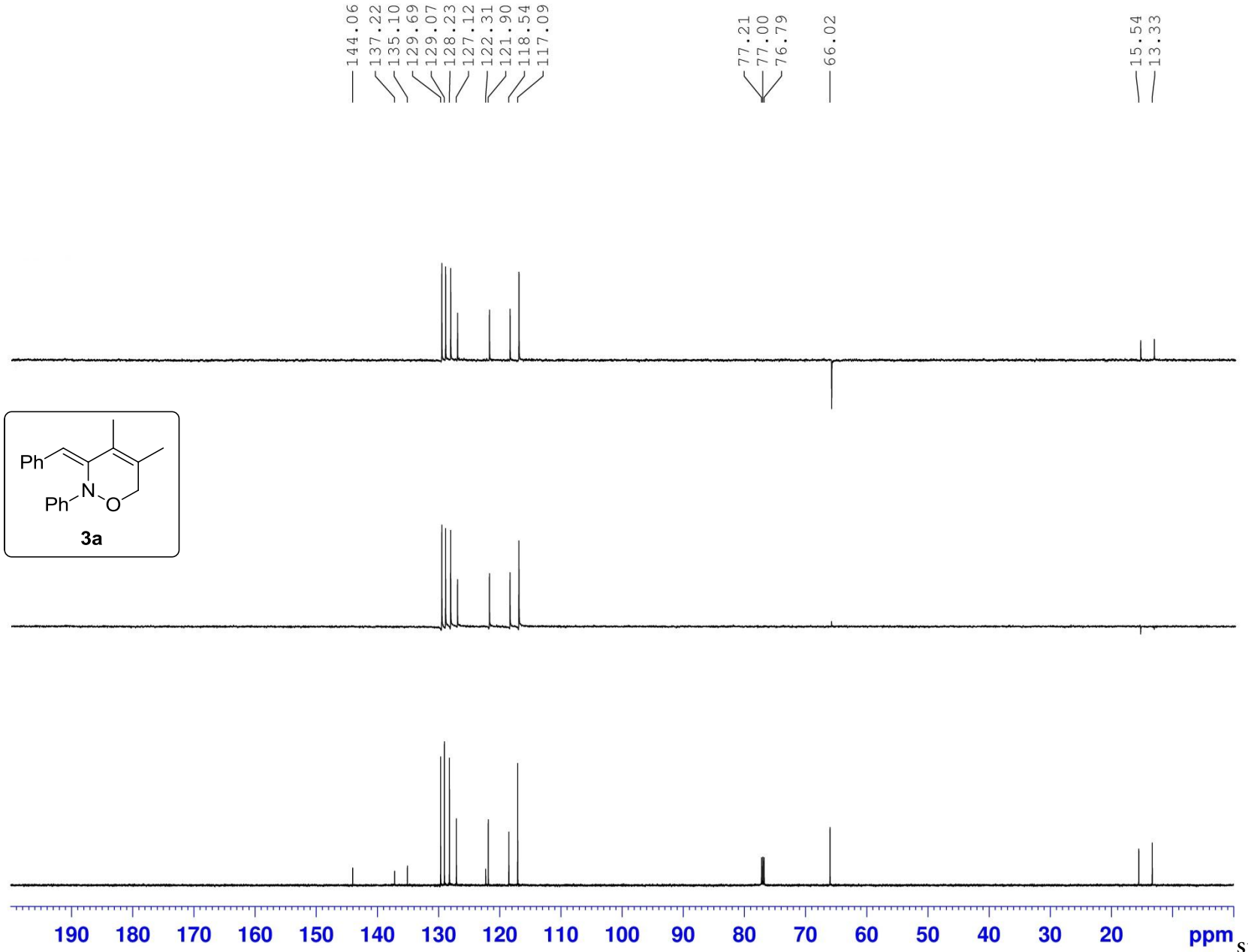
3.46
3.37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128.23
127.12
122.31
121.90
118.54
117.09
77.21
77.00
76.79
66.02
15.54
13.33
Ph
Ph
N
O
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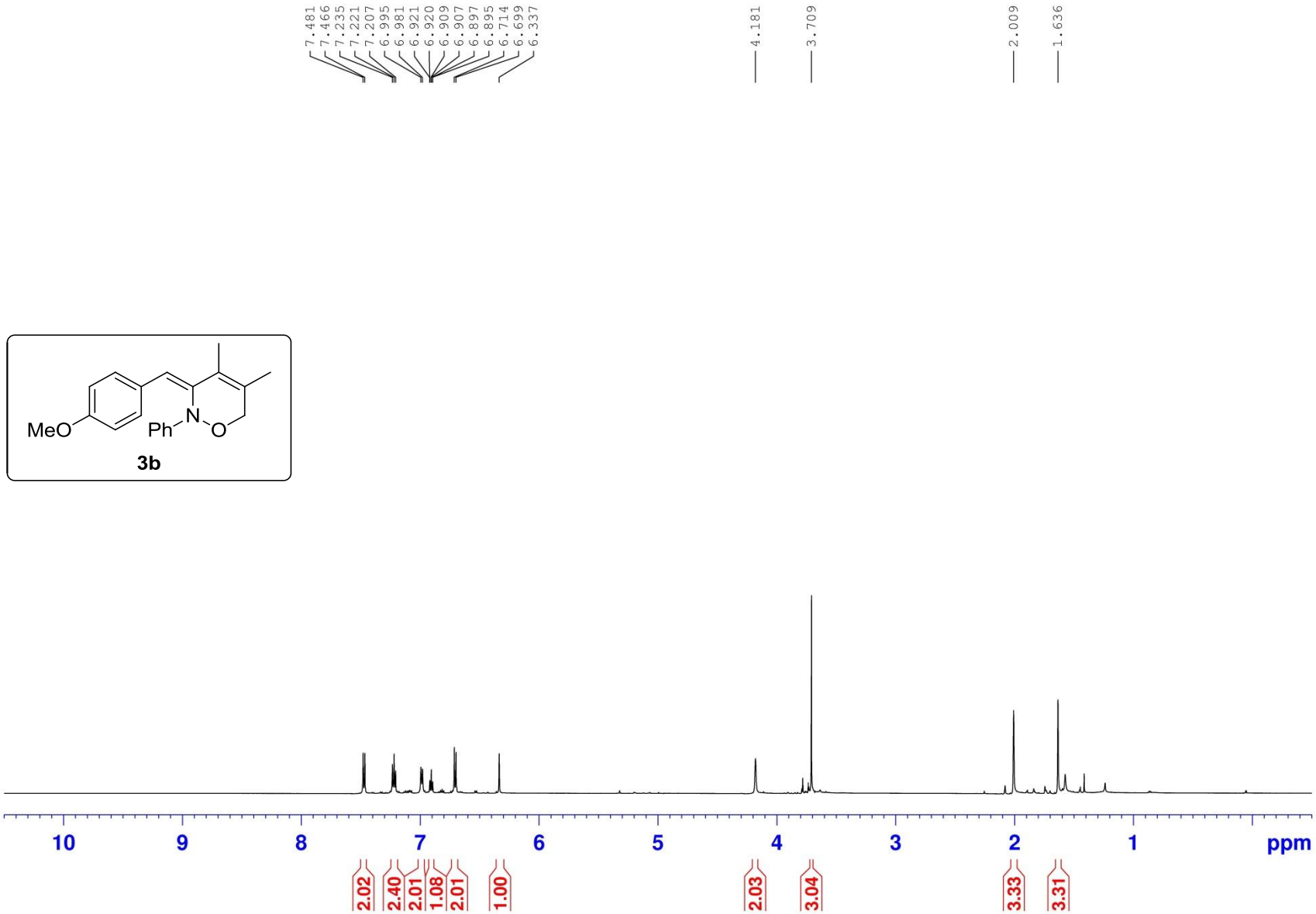
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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6.921
6.920
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6.907
6.897
6.895
6.714
6.699
6.337
4.181
3.709
2.009
1.636
MeO
Ph
N
O
3b
10
9
8
7
6
5
4
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2.40
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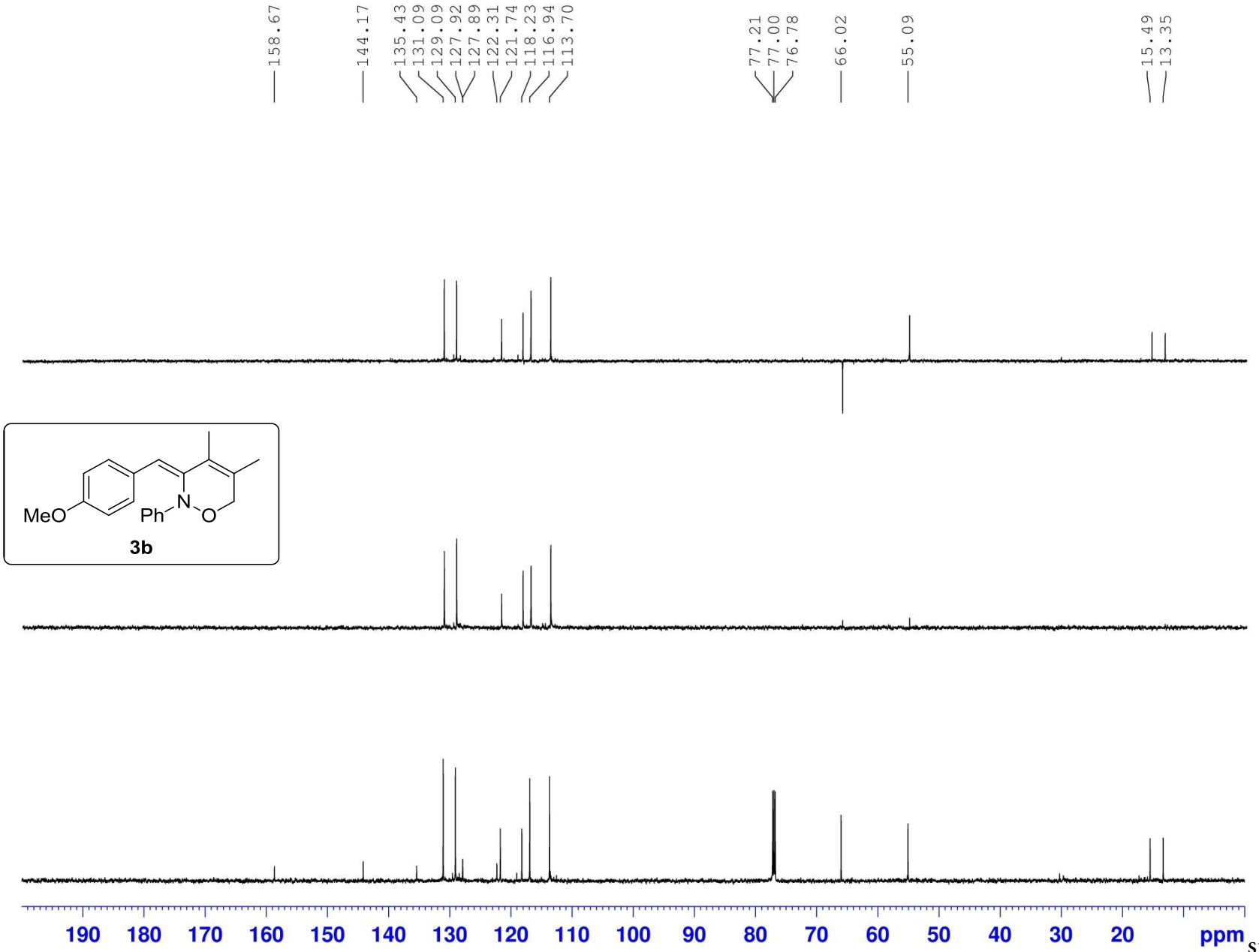
1.08
2.01
1.00
2.03
3.04
3.33
3.31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127.89
122.31
121.74
118.23
116.94
113.70
77.21
77.00
76.78
66.02
55.09
15.49
13.35
MeO
Ph
N
O
3b
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150
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80
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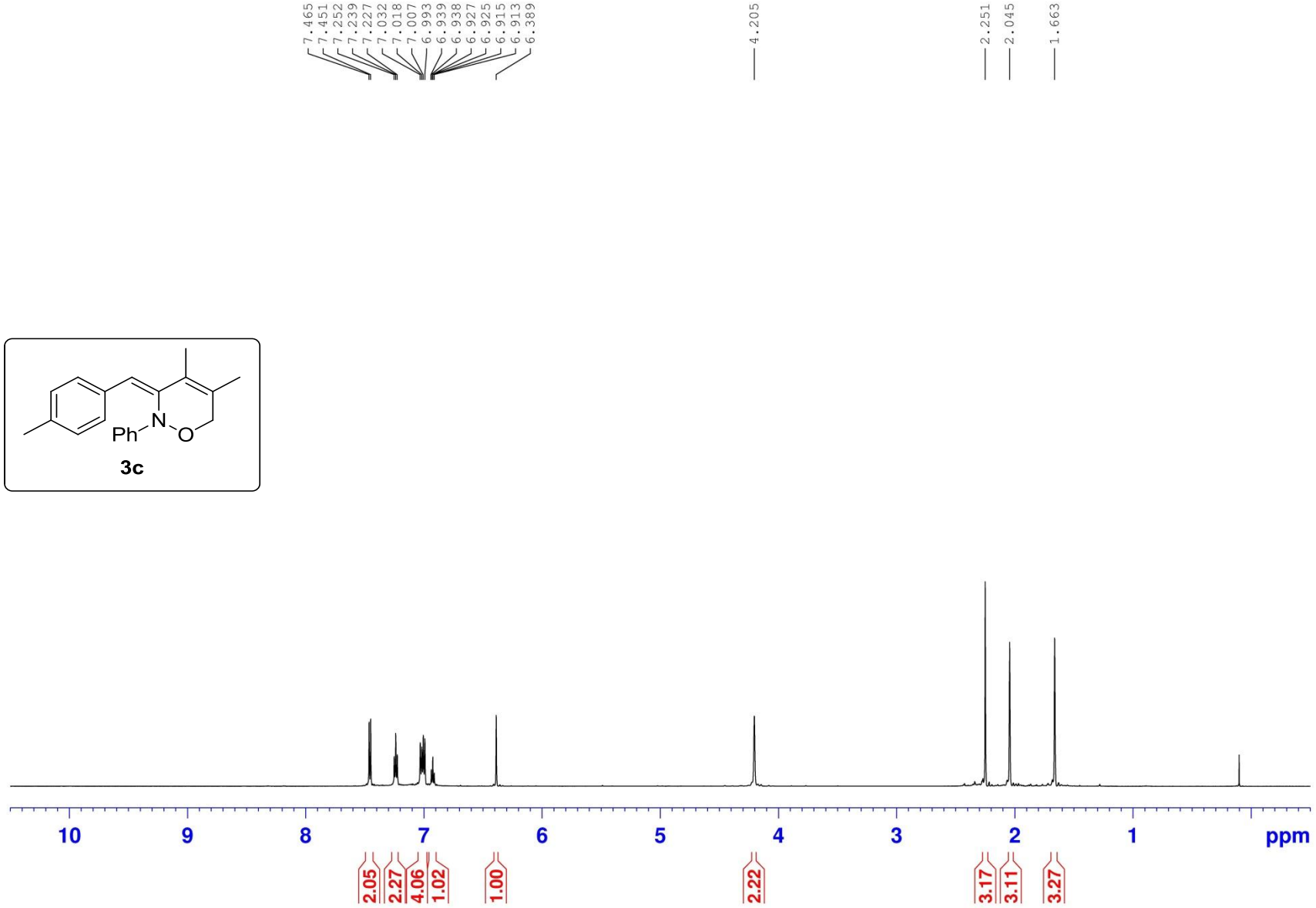
50
40
30
20
ppm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6.938
6.927
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6.915
6.913
6.389
4.205
2.251
2.045
1.663
Ph
N
O
3c
10
9
8
7
6
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ppm
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4.06
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1.00
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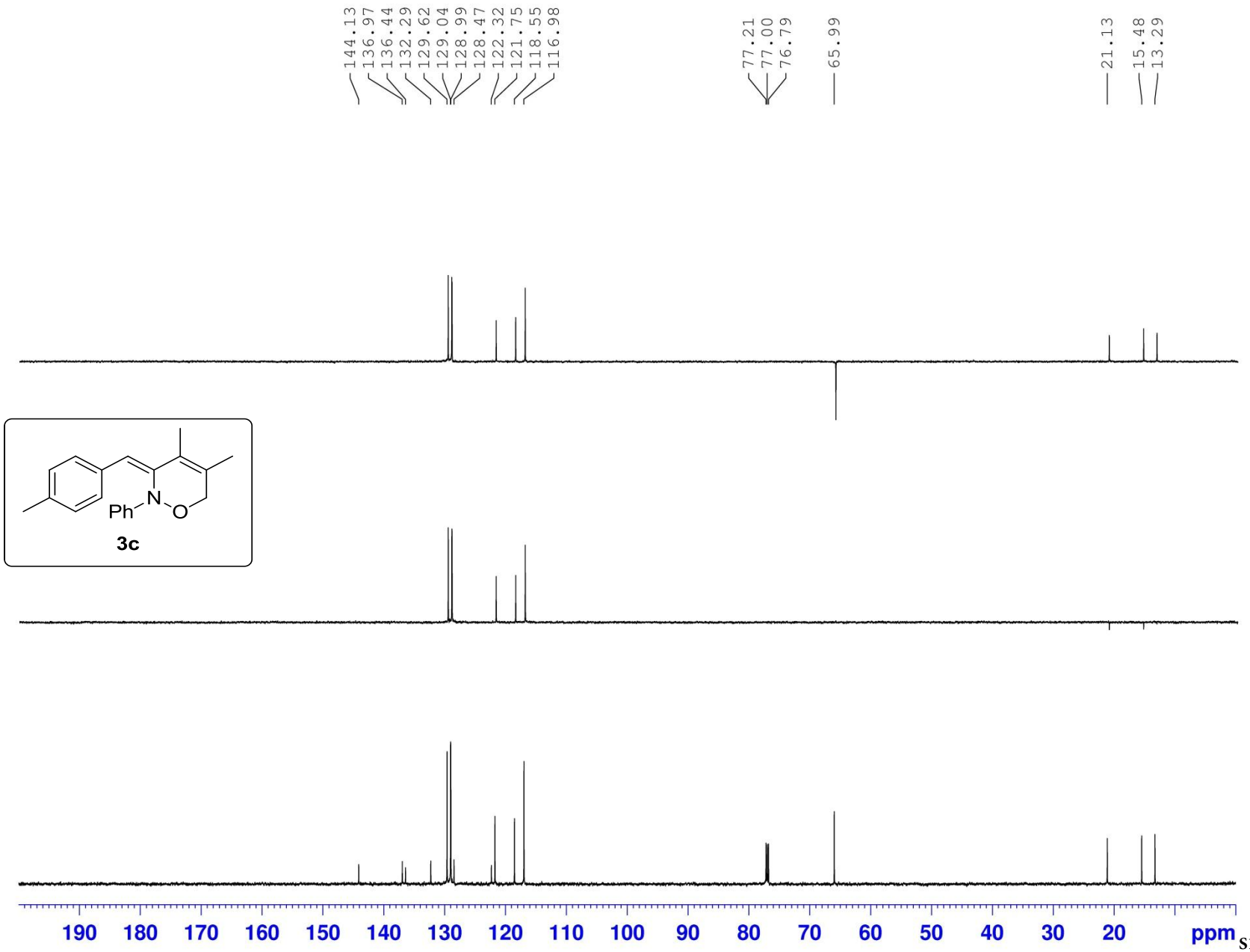
3.27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128.47
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121.75
118.55
116.98
77.21
77.00
76.79
65.99
21.13
15.48
13.29
Ph
N
O
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160
150
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120
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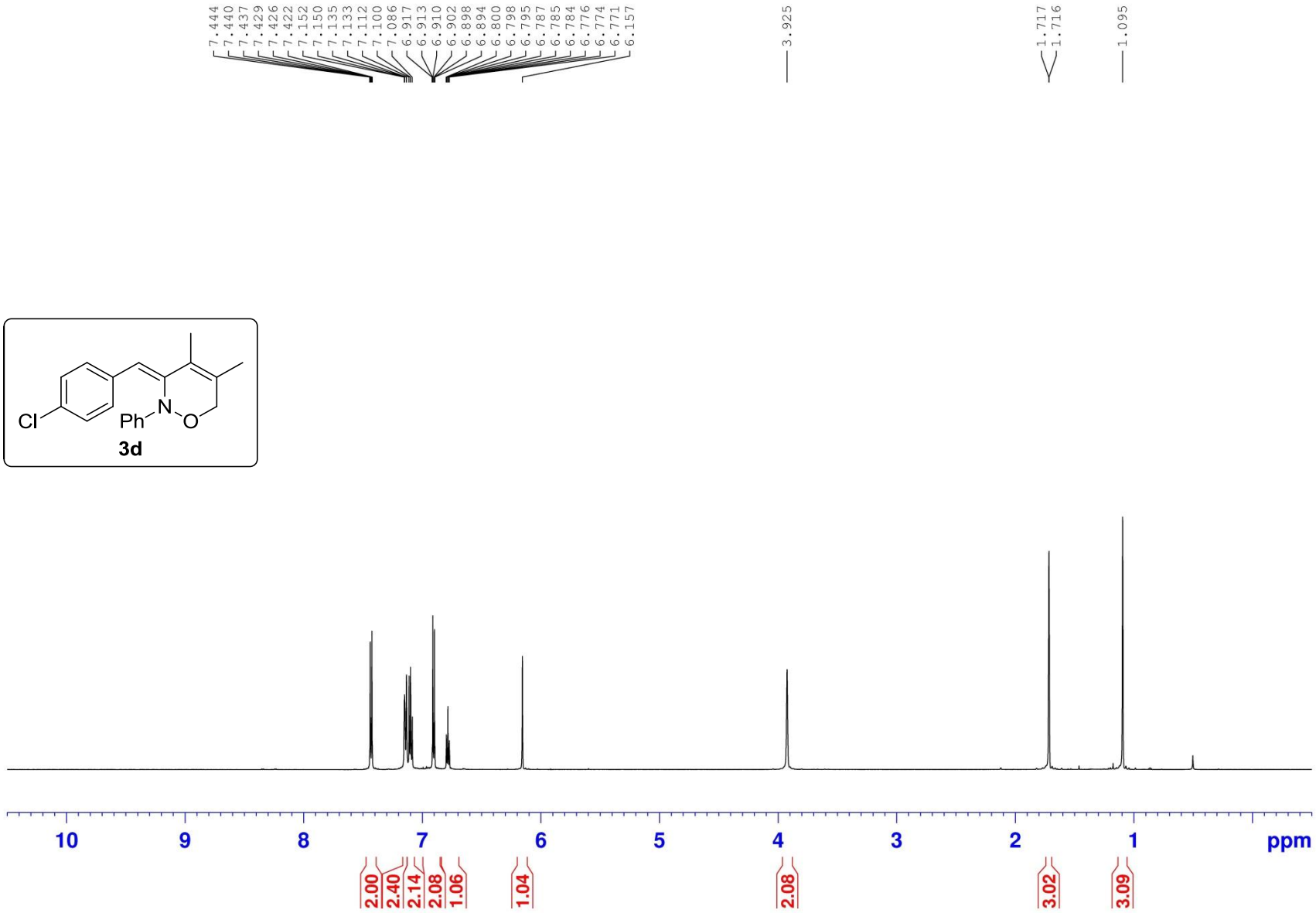
30
20
ppm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7.086
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6.913
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6.776
6.774
6.771
6.157
3.925
1.717
1.716
1.095
Cl
Ph
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O
3d
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7
6
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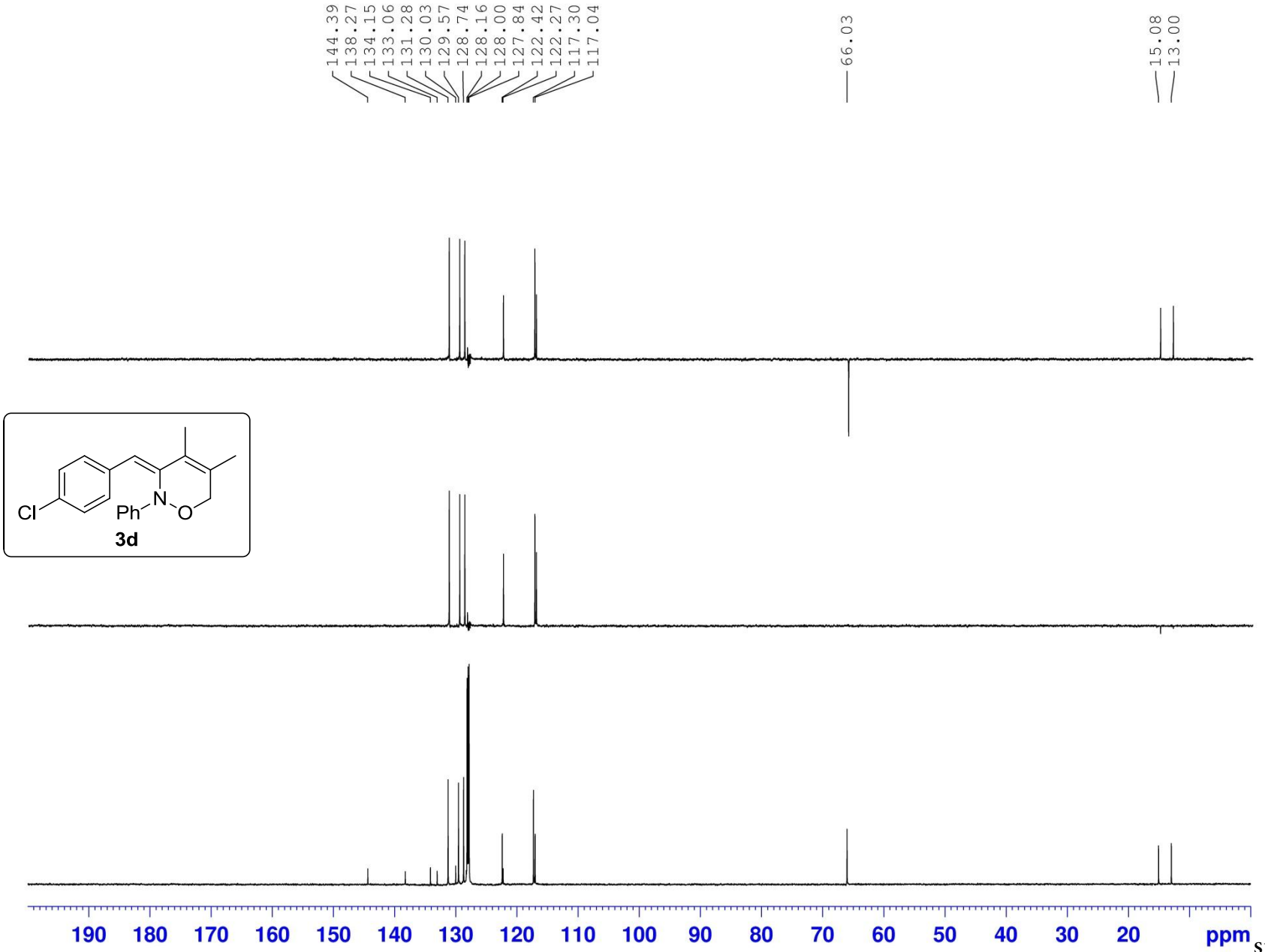
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13.00
Cl
Ph
N
O
3d
190
180
170
160
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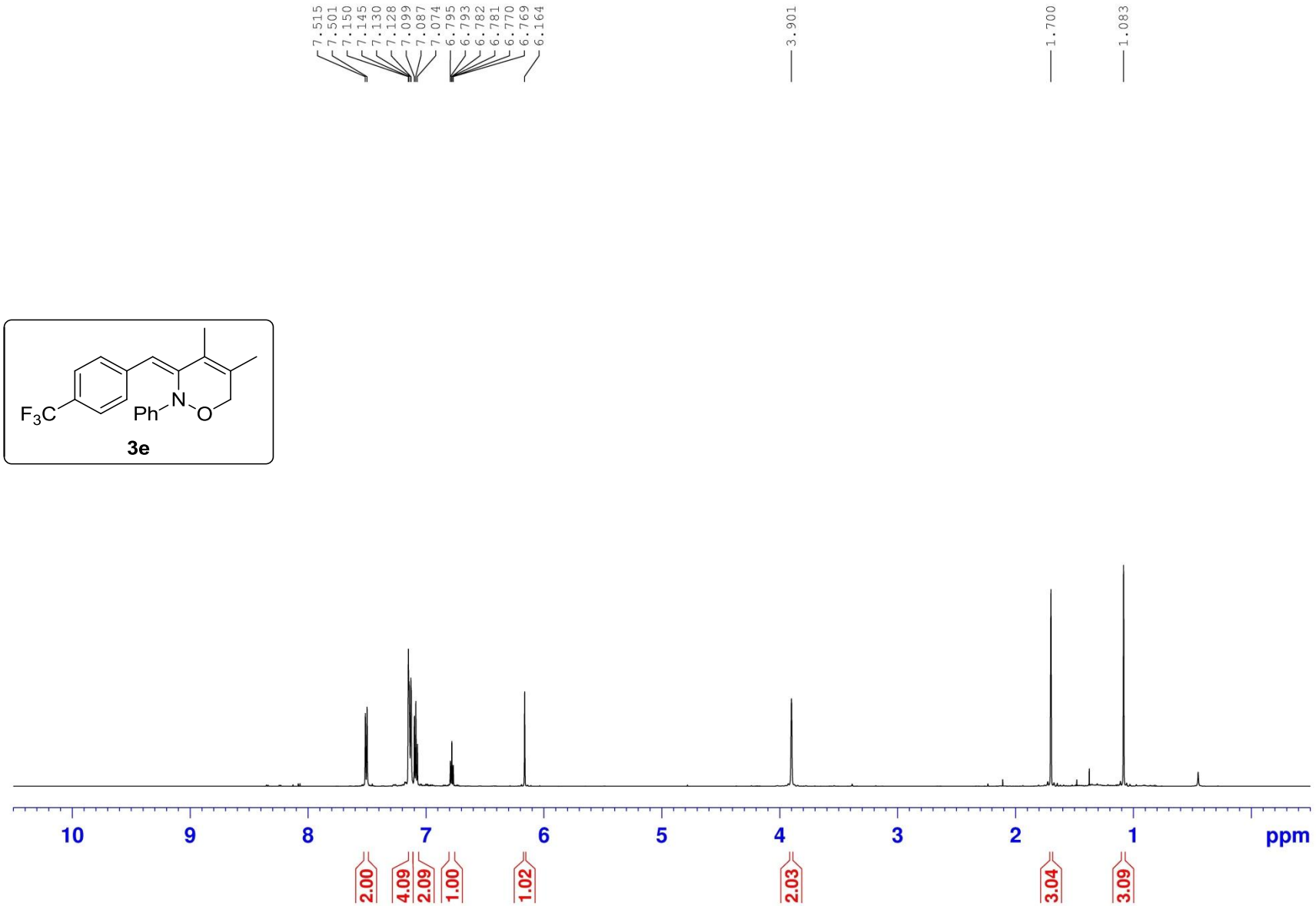
20
ppm

F3C
Ph
N
O
3e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6.781
6.770
6.769
6.164
3.901
1.700
1.083
10
9
8
7
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1.00
1.02
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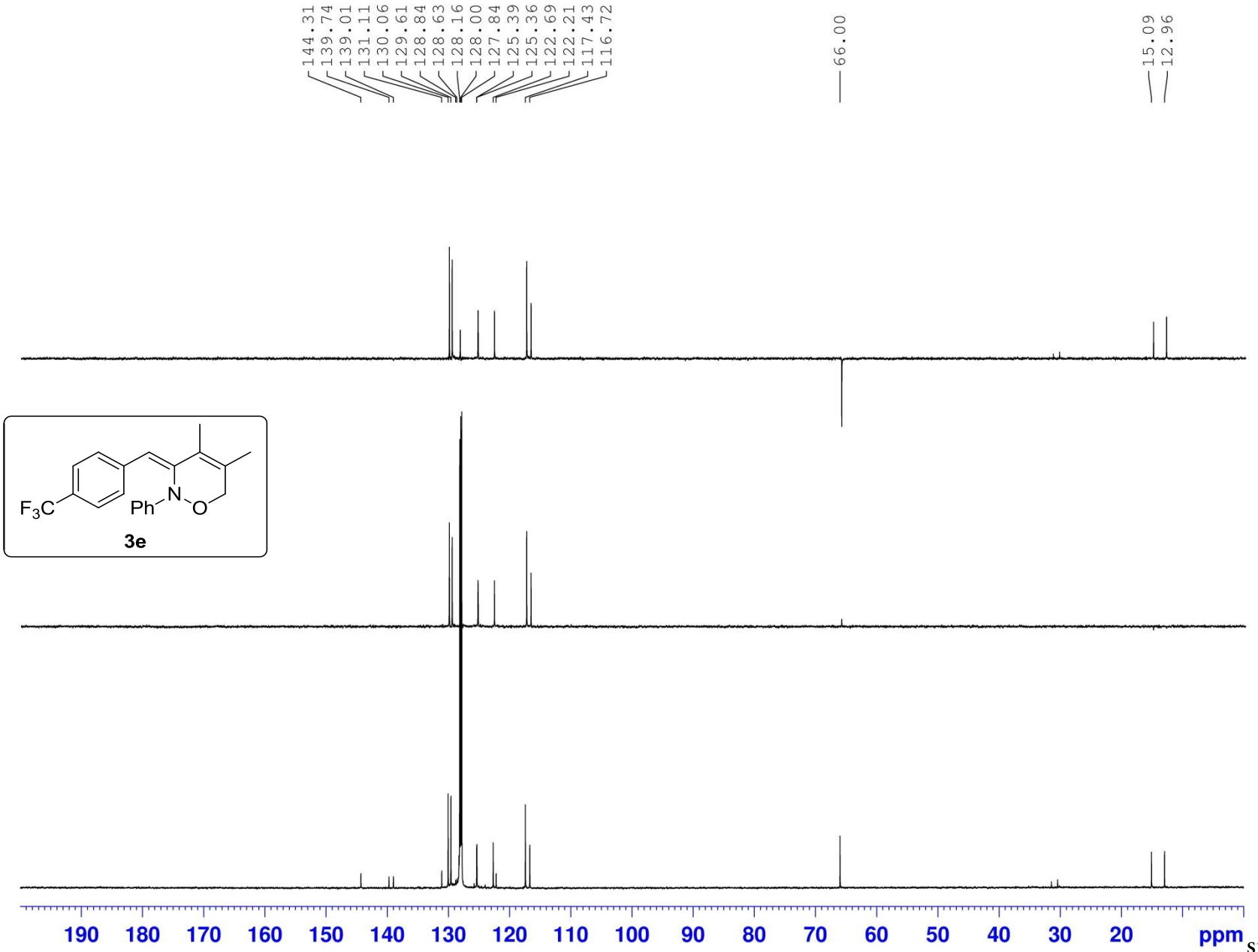
3.04
3.09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116.72
66.00
15.09
12.96
F3C
Ph
N
O
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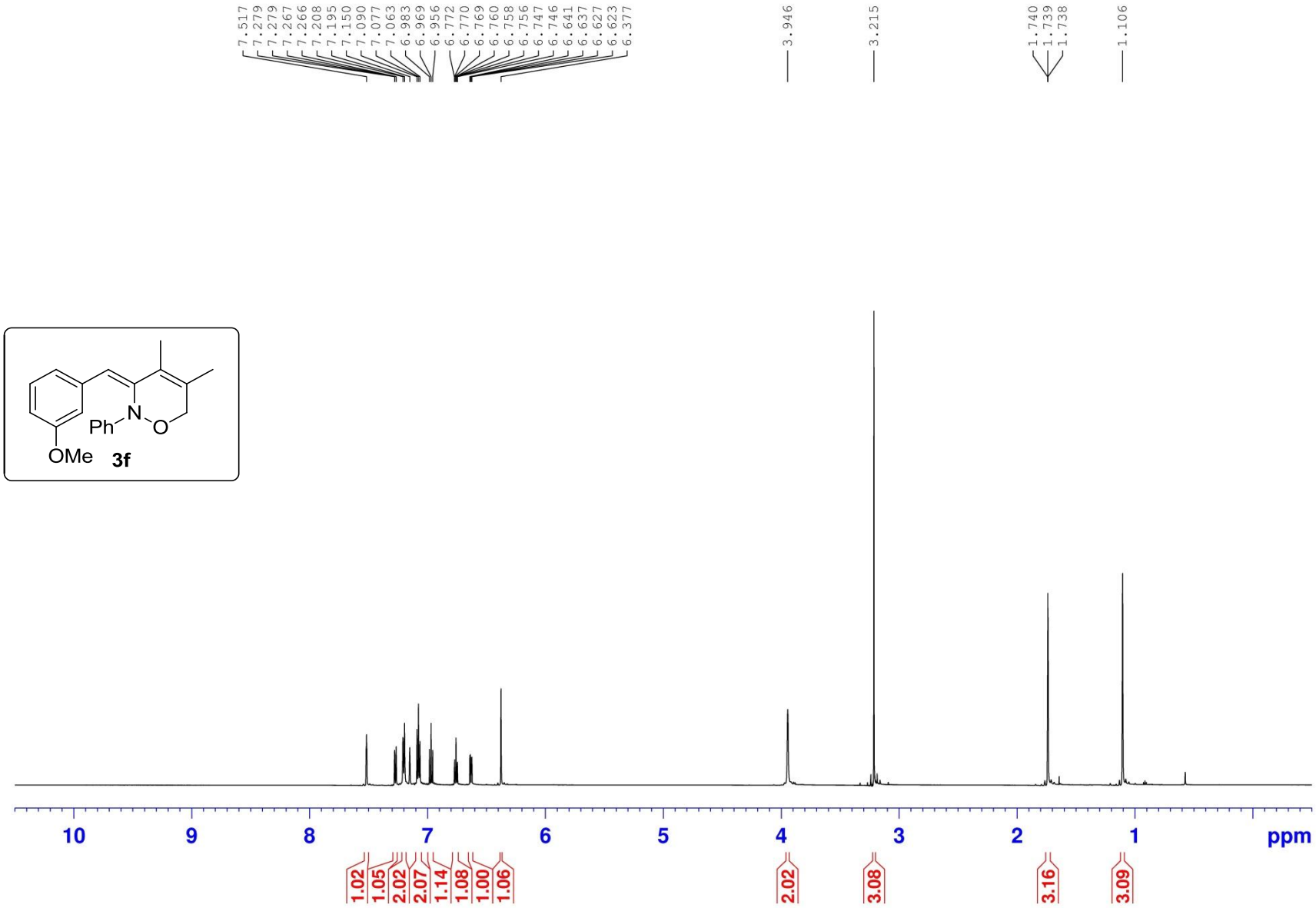
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6.956
6.772
6.770
6.769
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6.758
6.756
6.747
6.746
6.641
6.637
6.627
6.623
6.377
3.946
3.215
1.740
1.739
1.738
1.106
Ph
N
O
OMe
3f
10
9
8
7
6
5
4
3
2
1
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1.06
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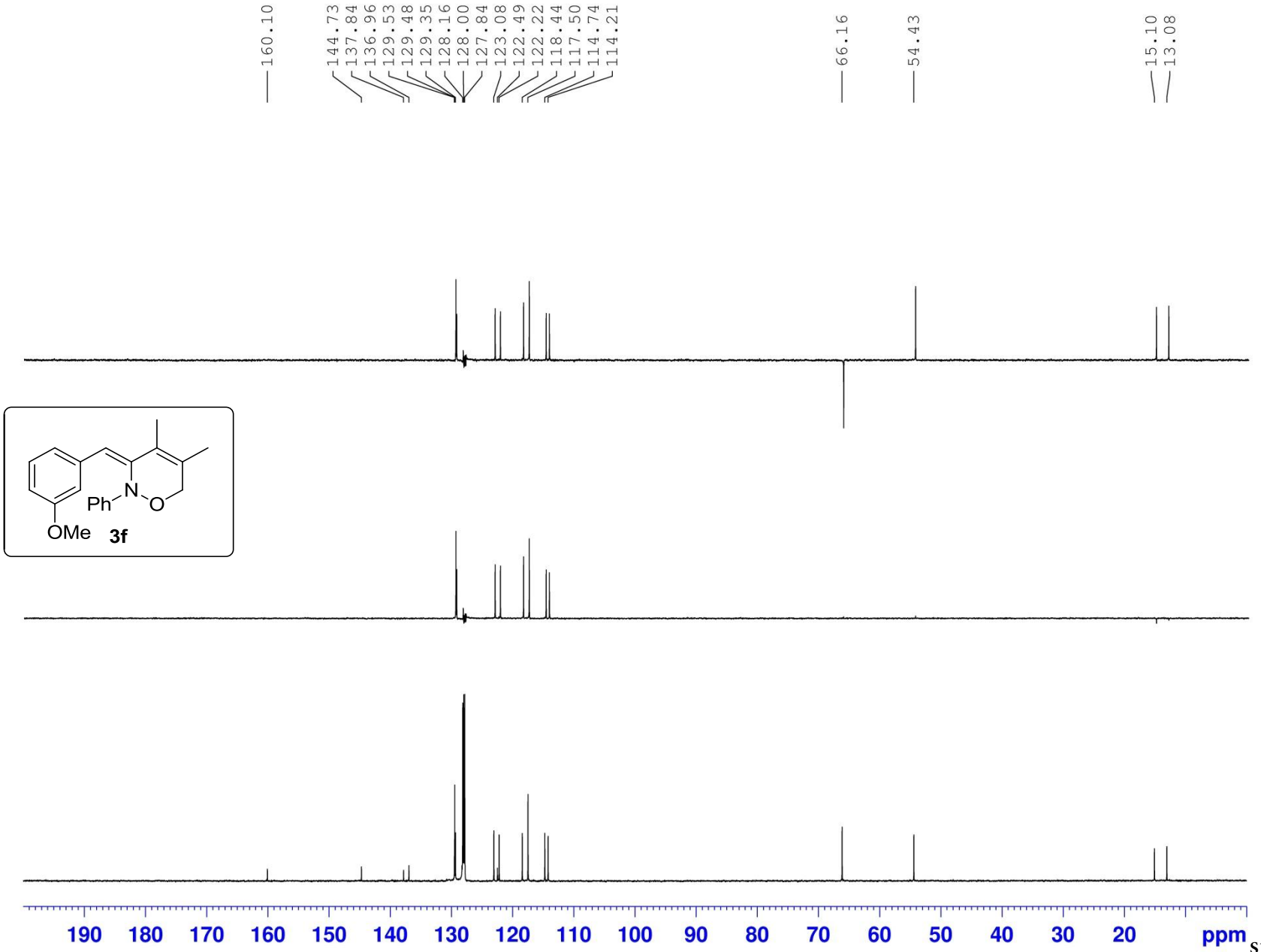
3.09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122.49
122.22
118.44
117.50
114.74
114.21
66.16
54.43
15.10
13.08
Ph
N
O
OMe
3f
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160
150
140
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120
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80
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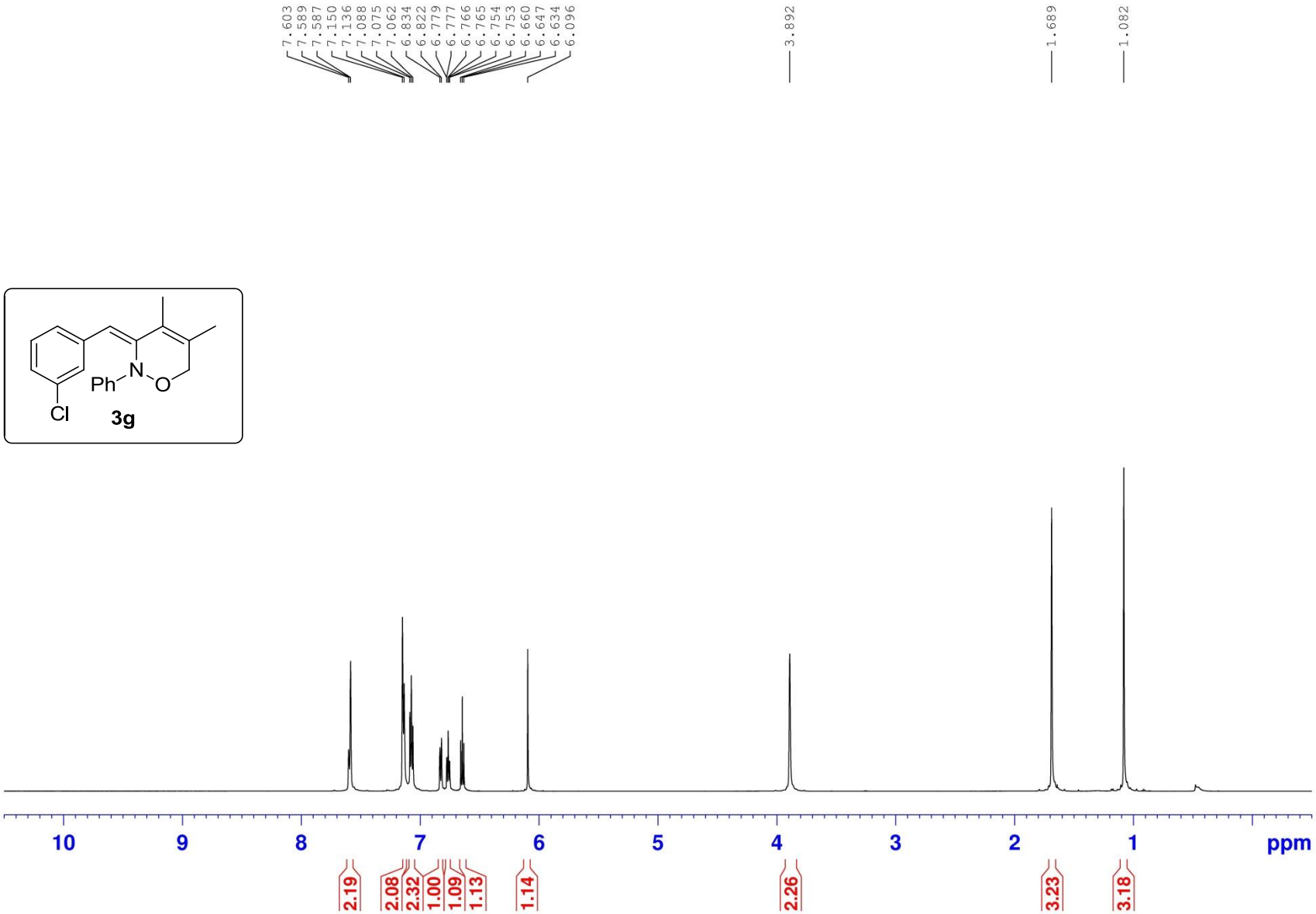
40
30
20
ppm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6.765
6.754
6.753
6.660
6.647
6.634
6.096
3.892
1.689
1.082
Ph
N
O
Cl
3g
10
9
8
7
6
5
4
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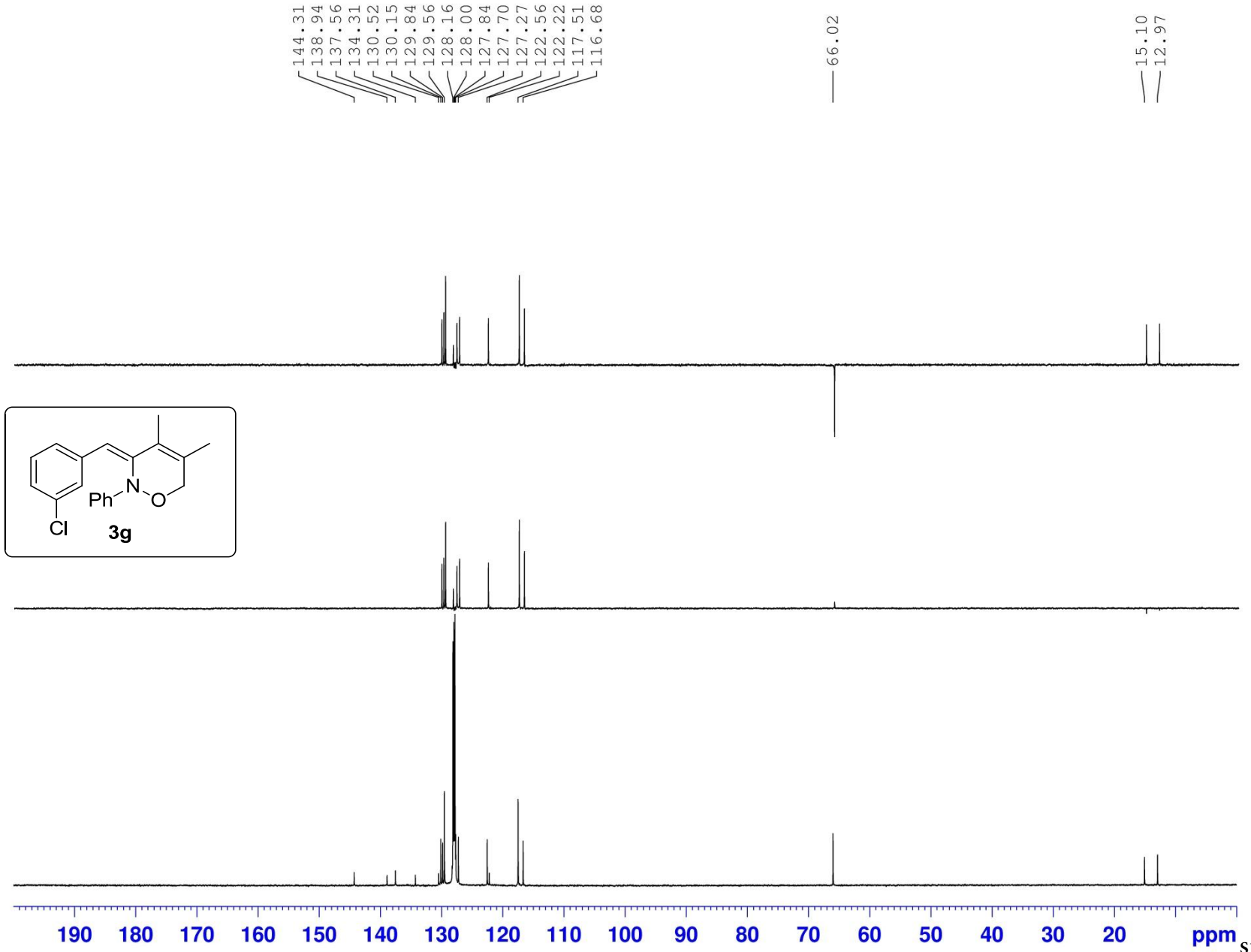
3.18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127.27
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122.22
117.51
116.68
66.02
15.10
12.97
Ph
N
O
Cl
3g
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160
150
140
130
120
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100
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80
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40
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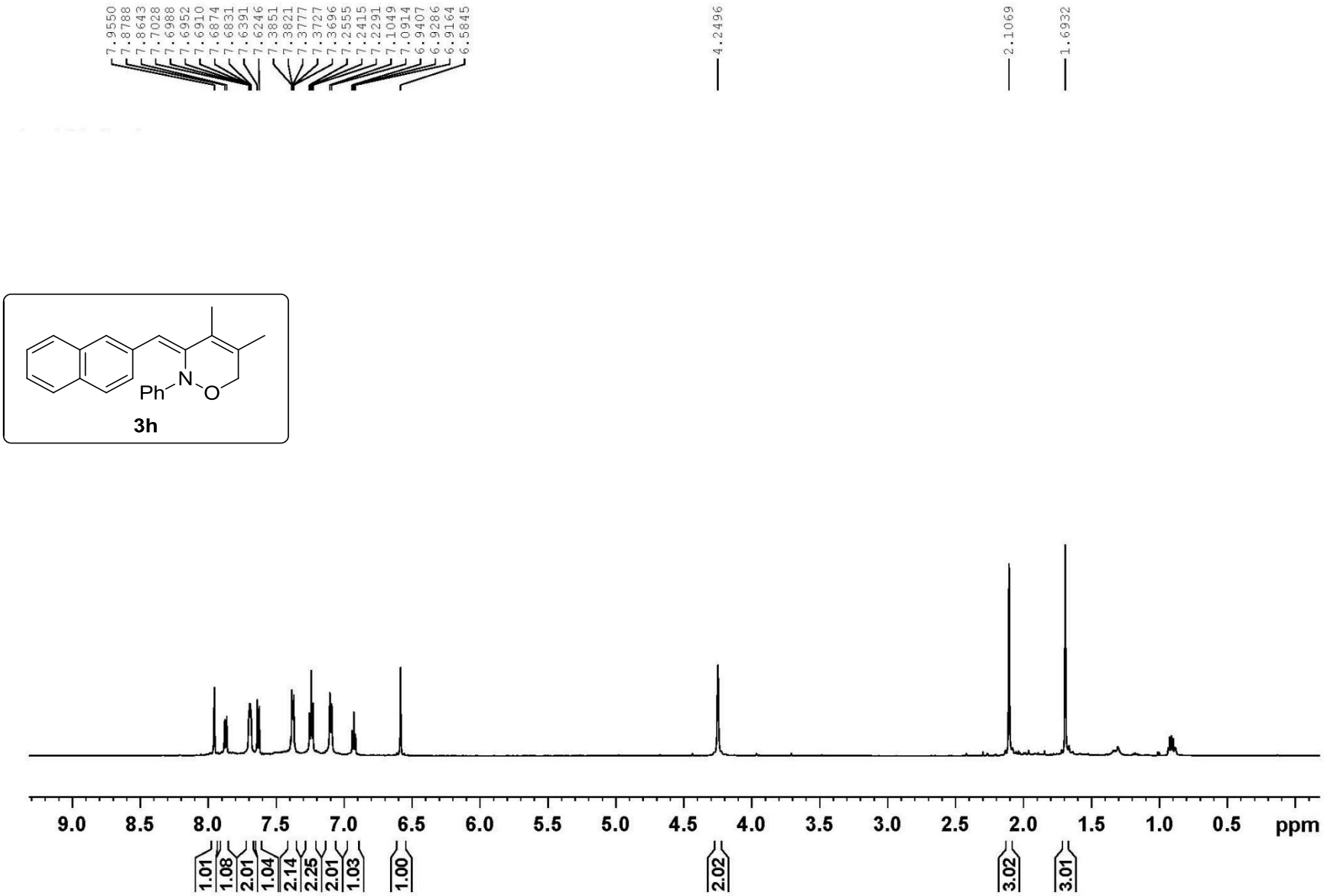
20
ppm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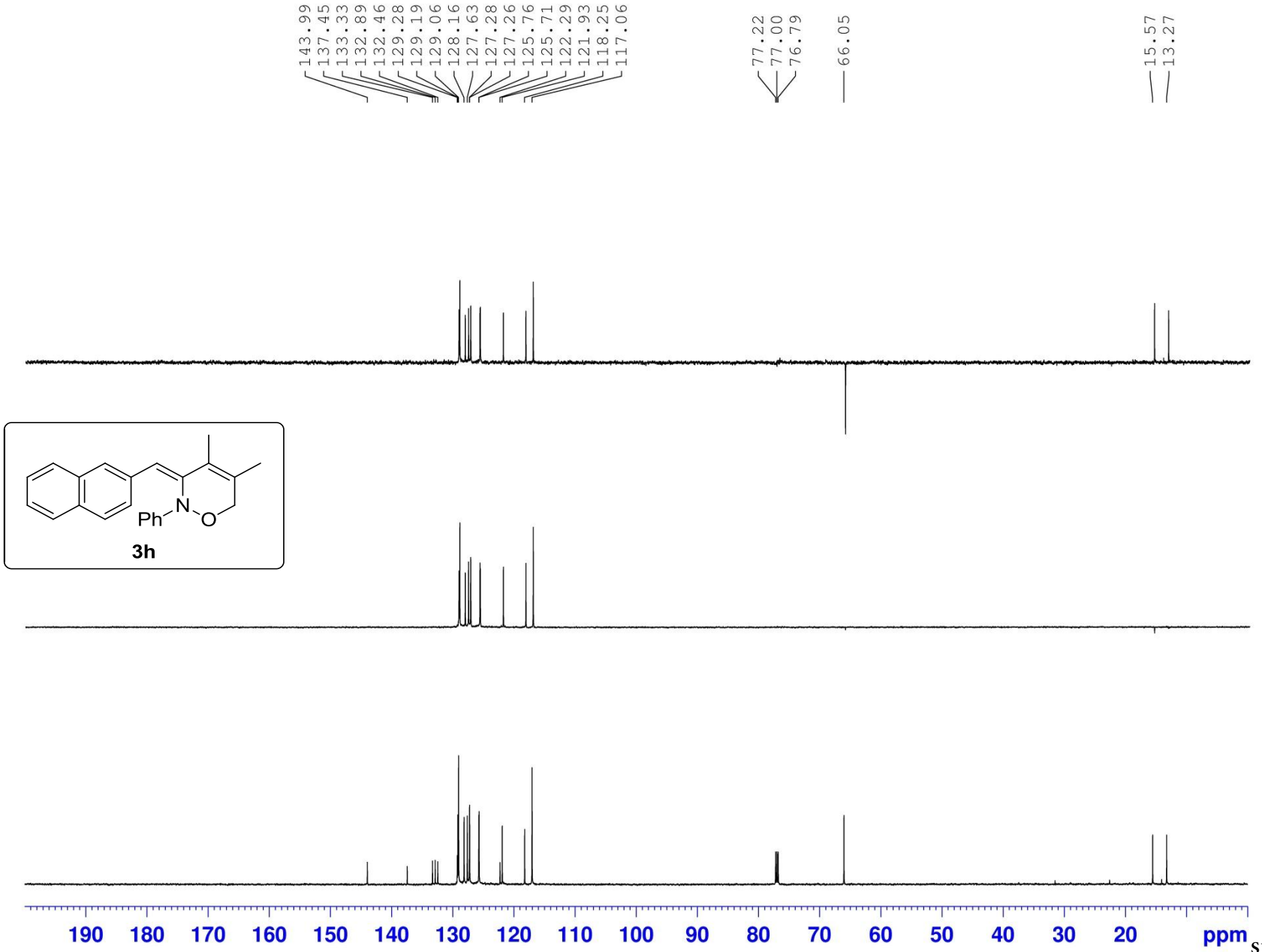
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O
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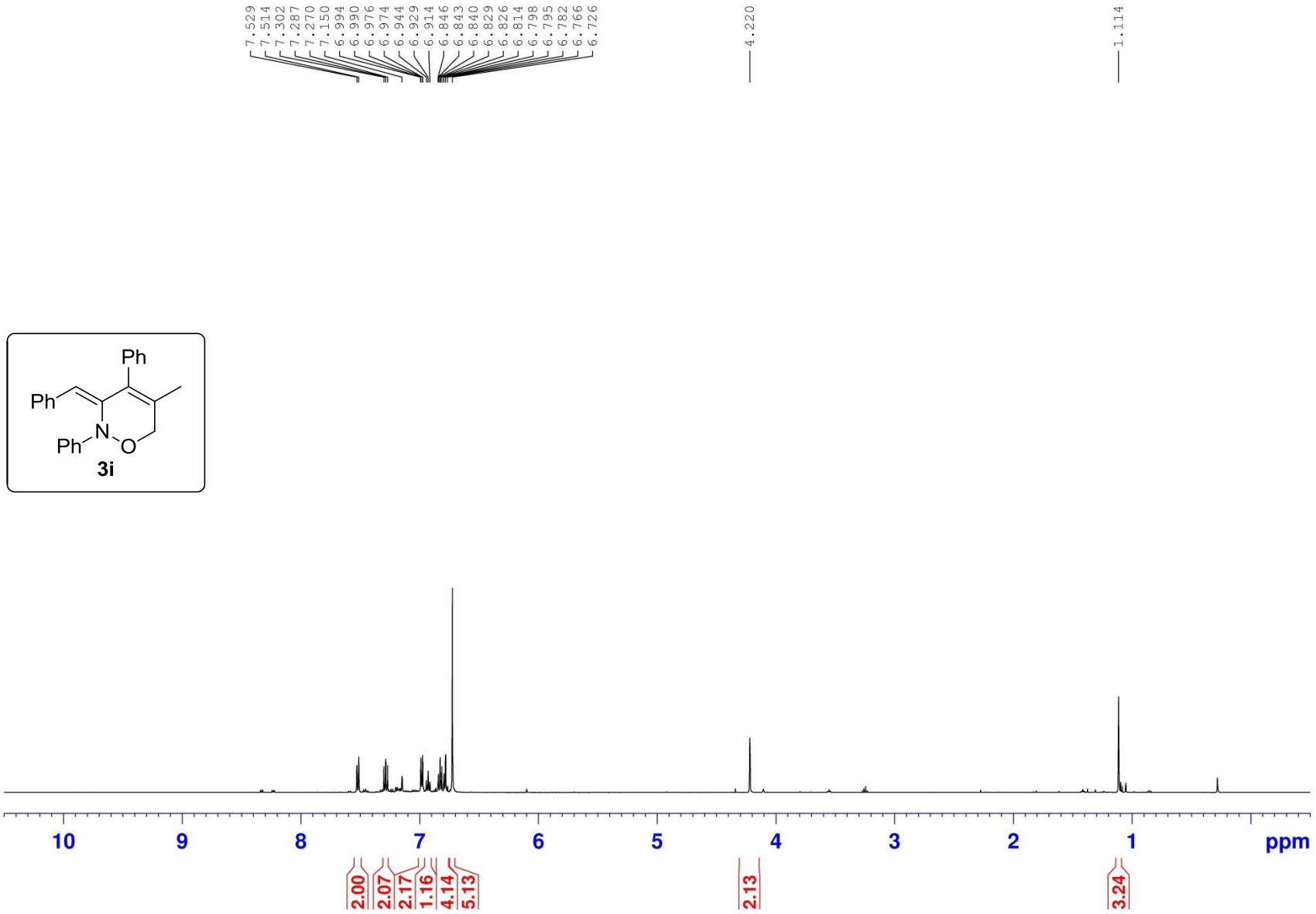
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Ph
Ph
Ph
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O
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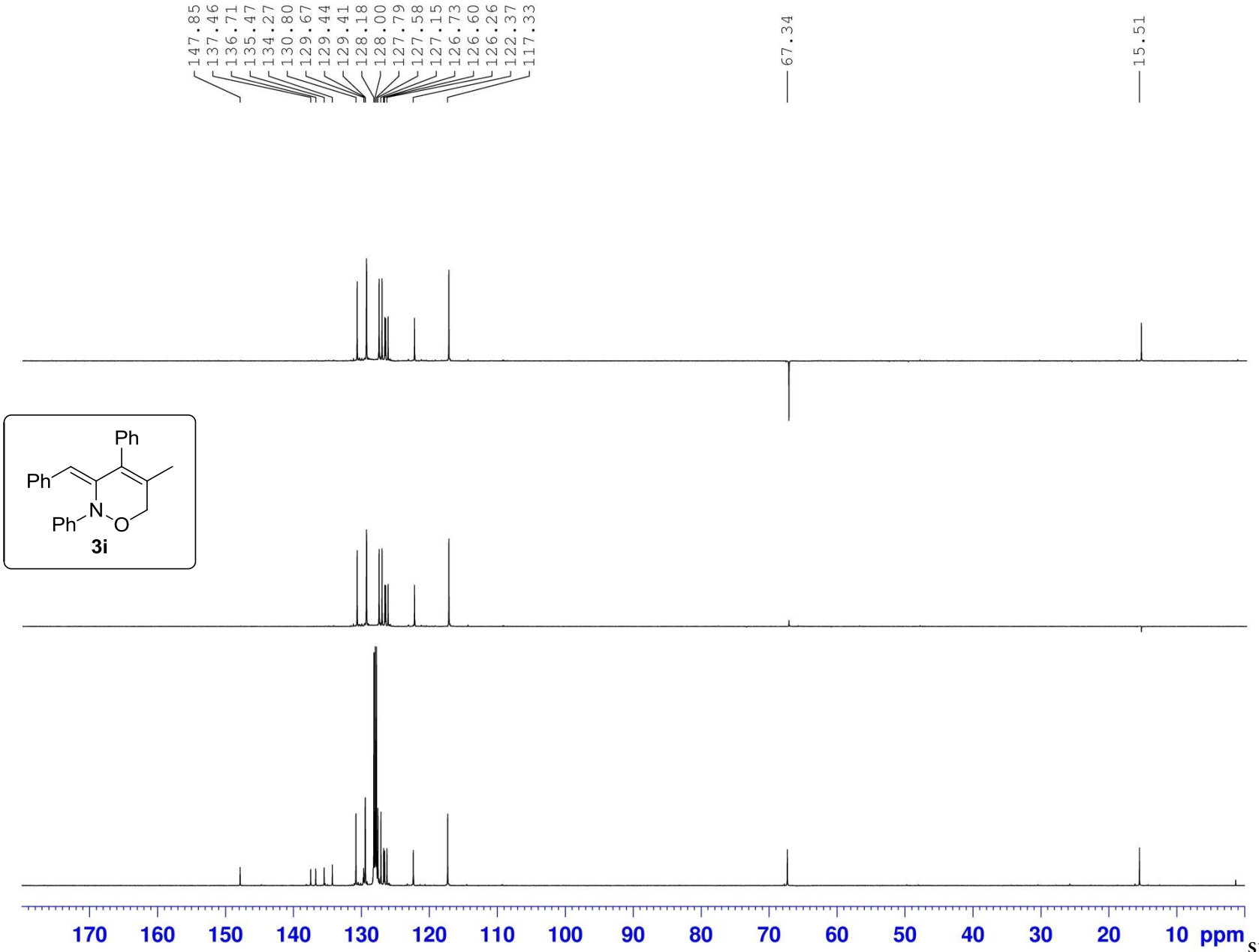
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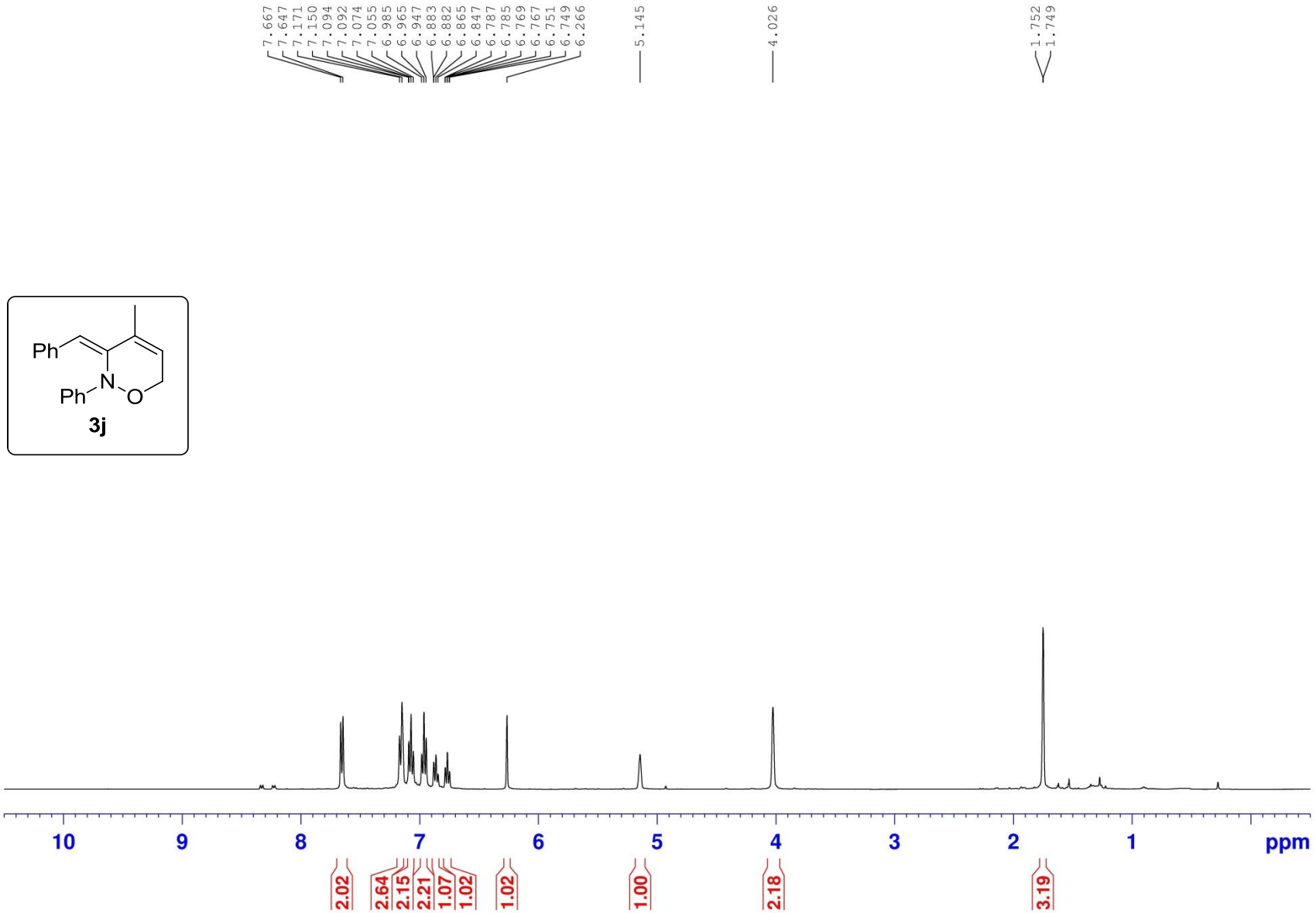
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Ph
N
O
3j
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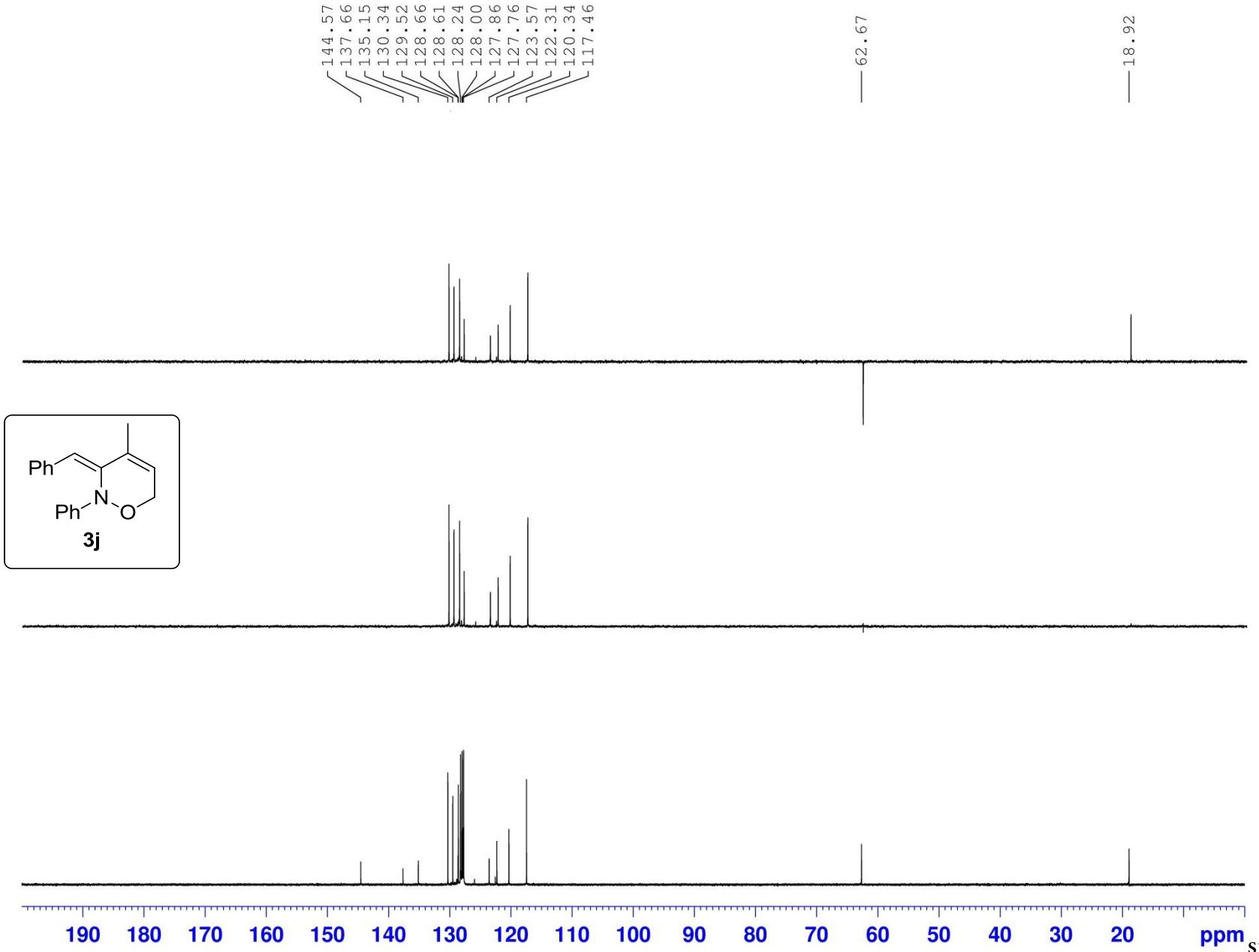
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Ph
Ph
N
O
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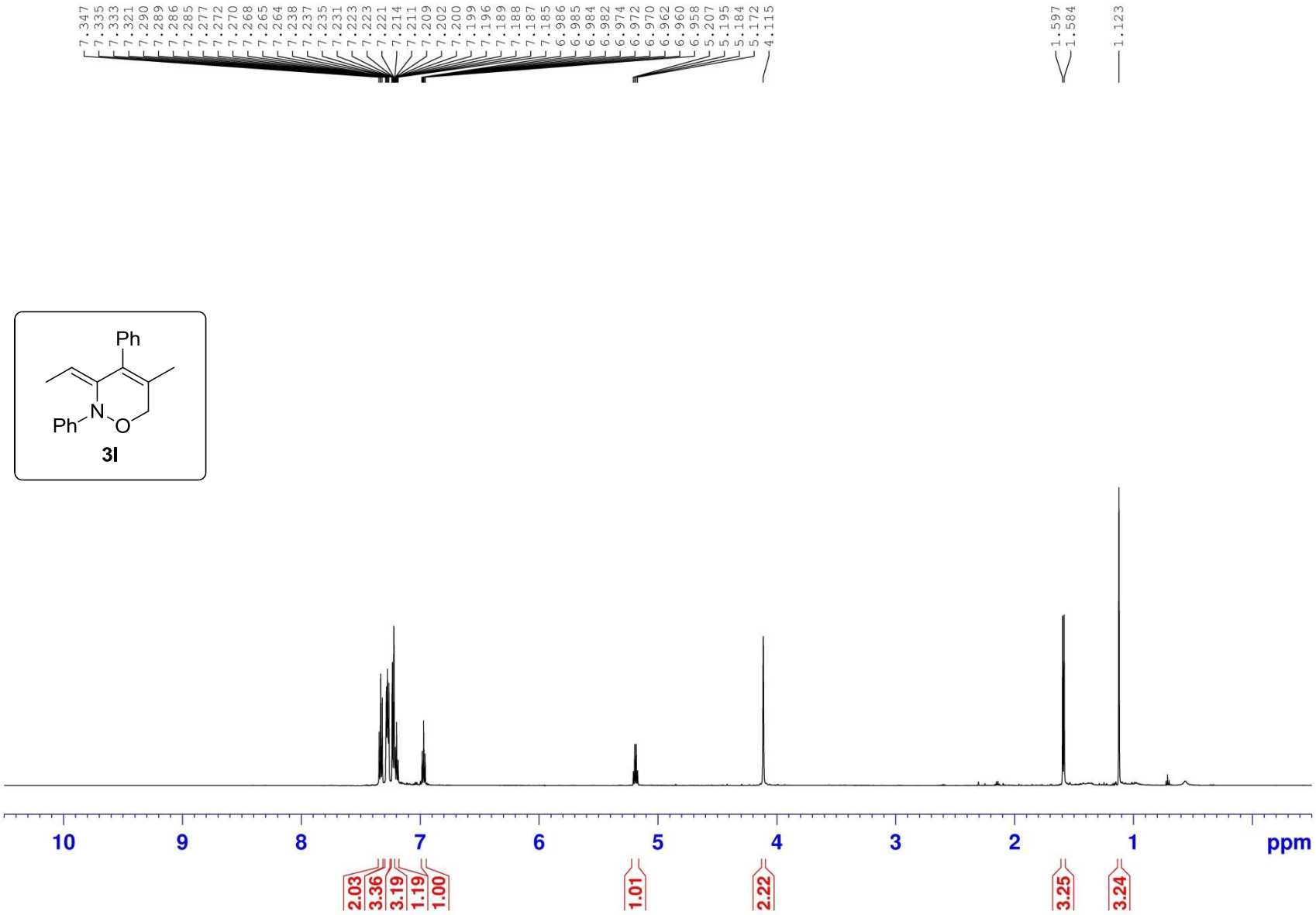
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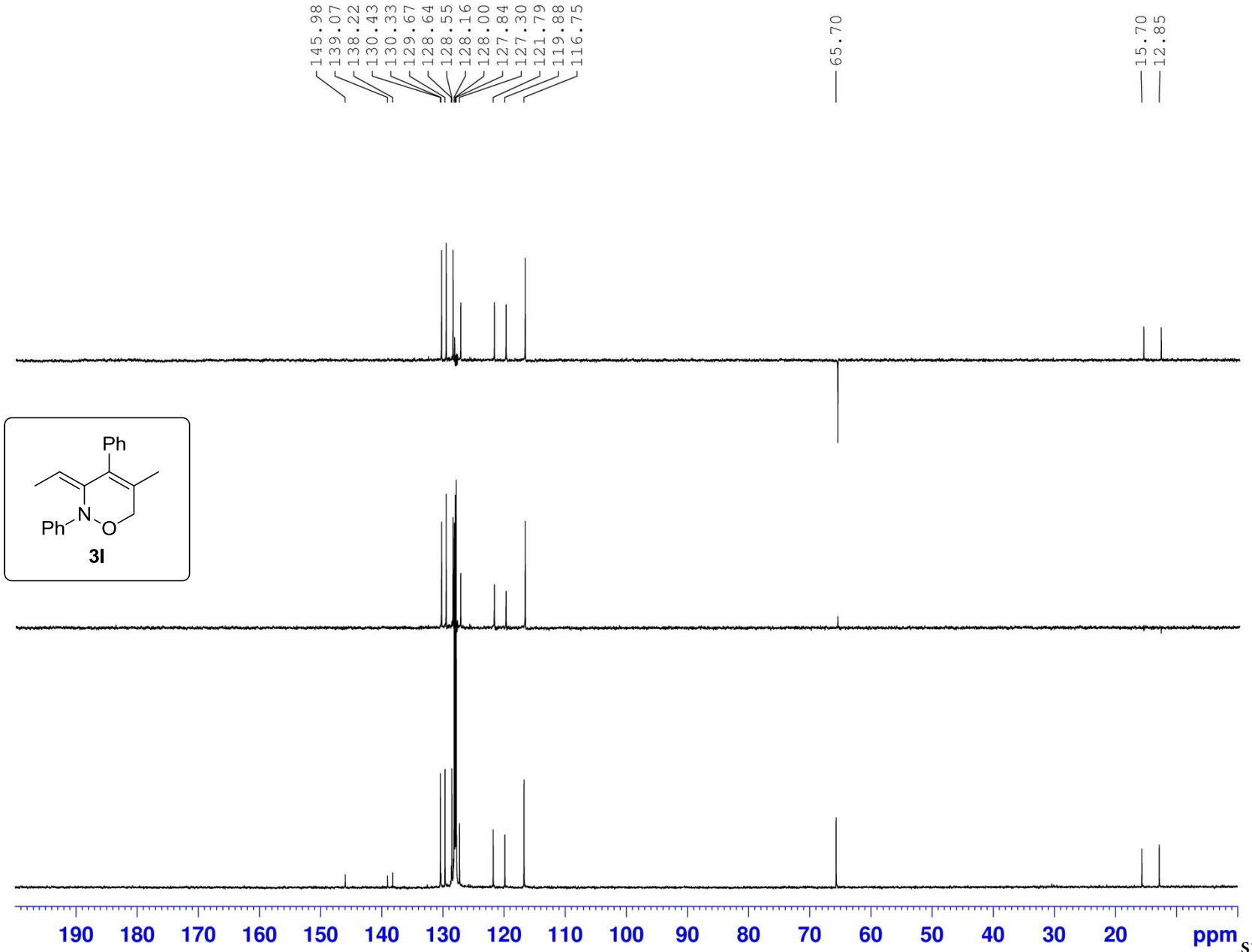
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116.75
65.70
15.70
12.85
Ph
Ph
N
O
3l
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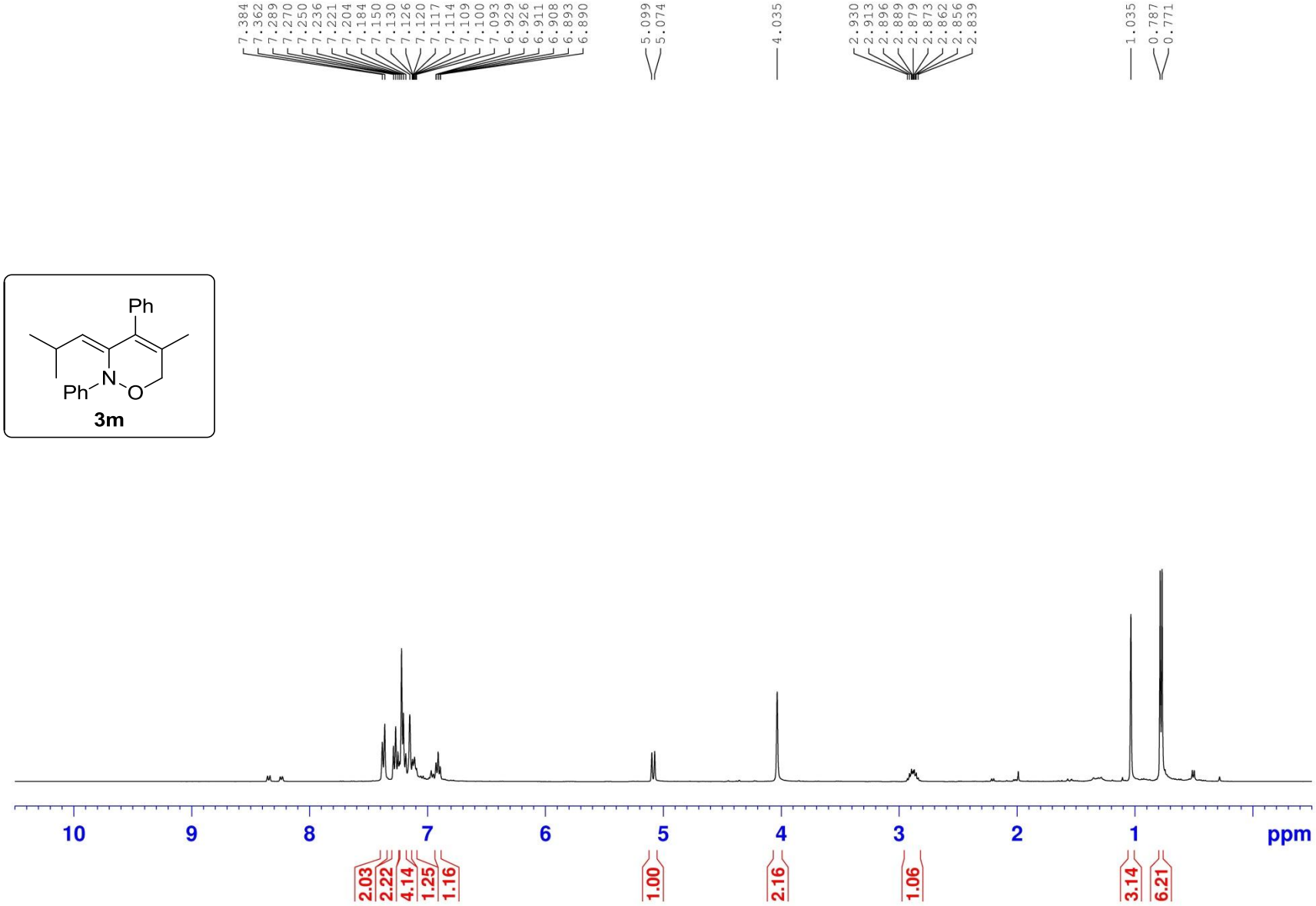
20
ppm

Ph
Ph
N
O
3m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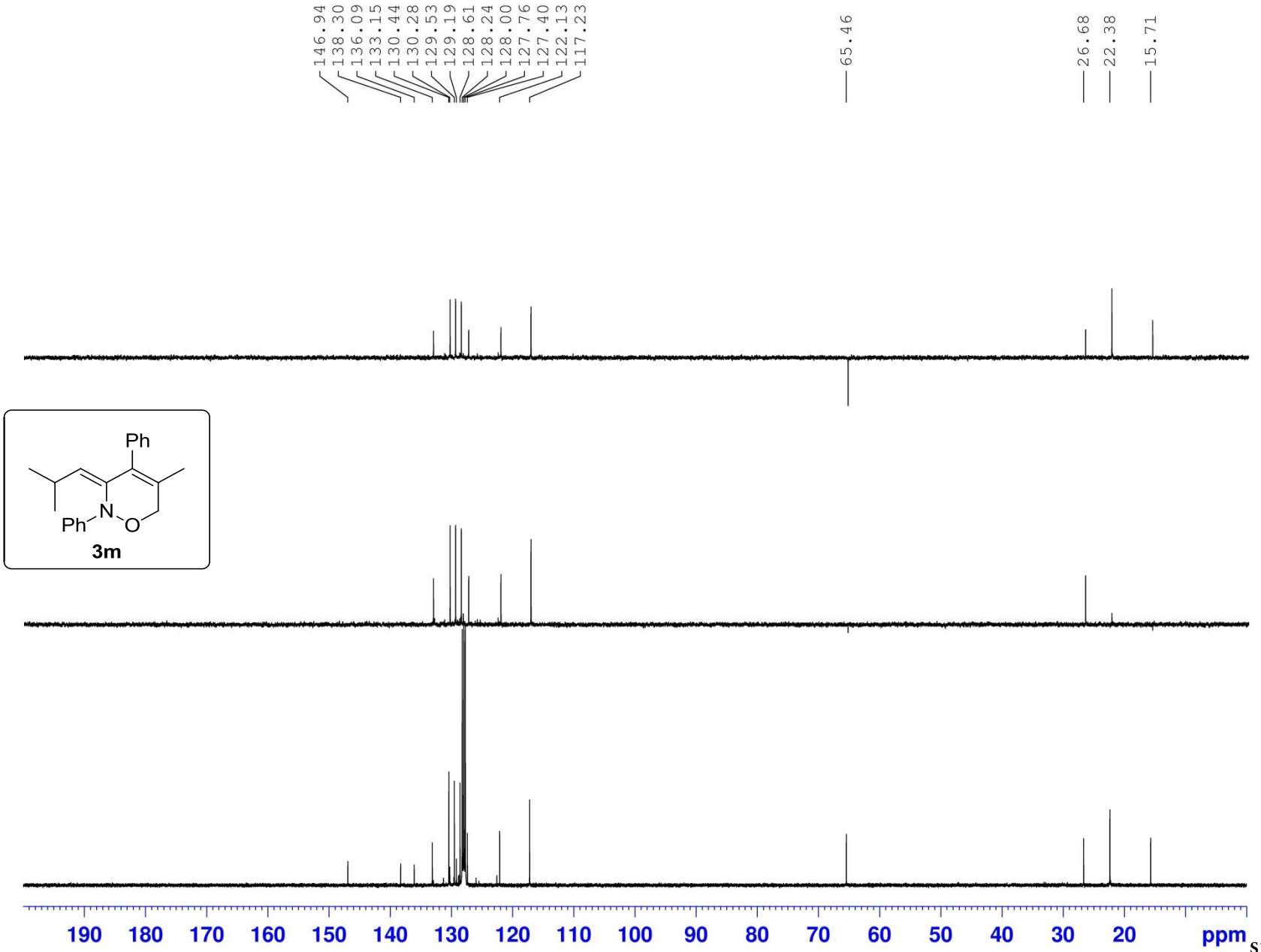
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26.68
22.38
15.71
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Ph
N
O
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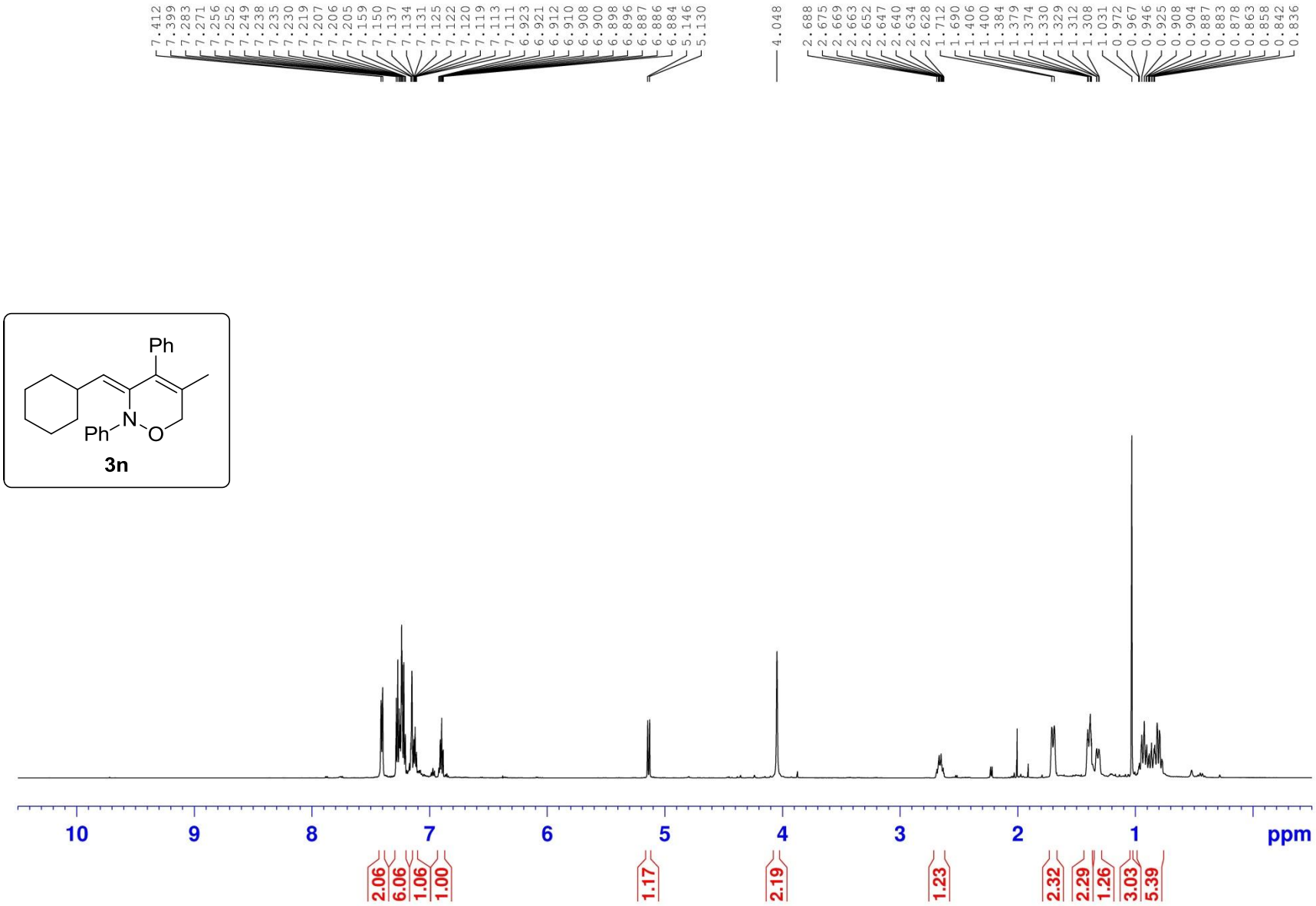
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O
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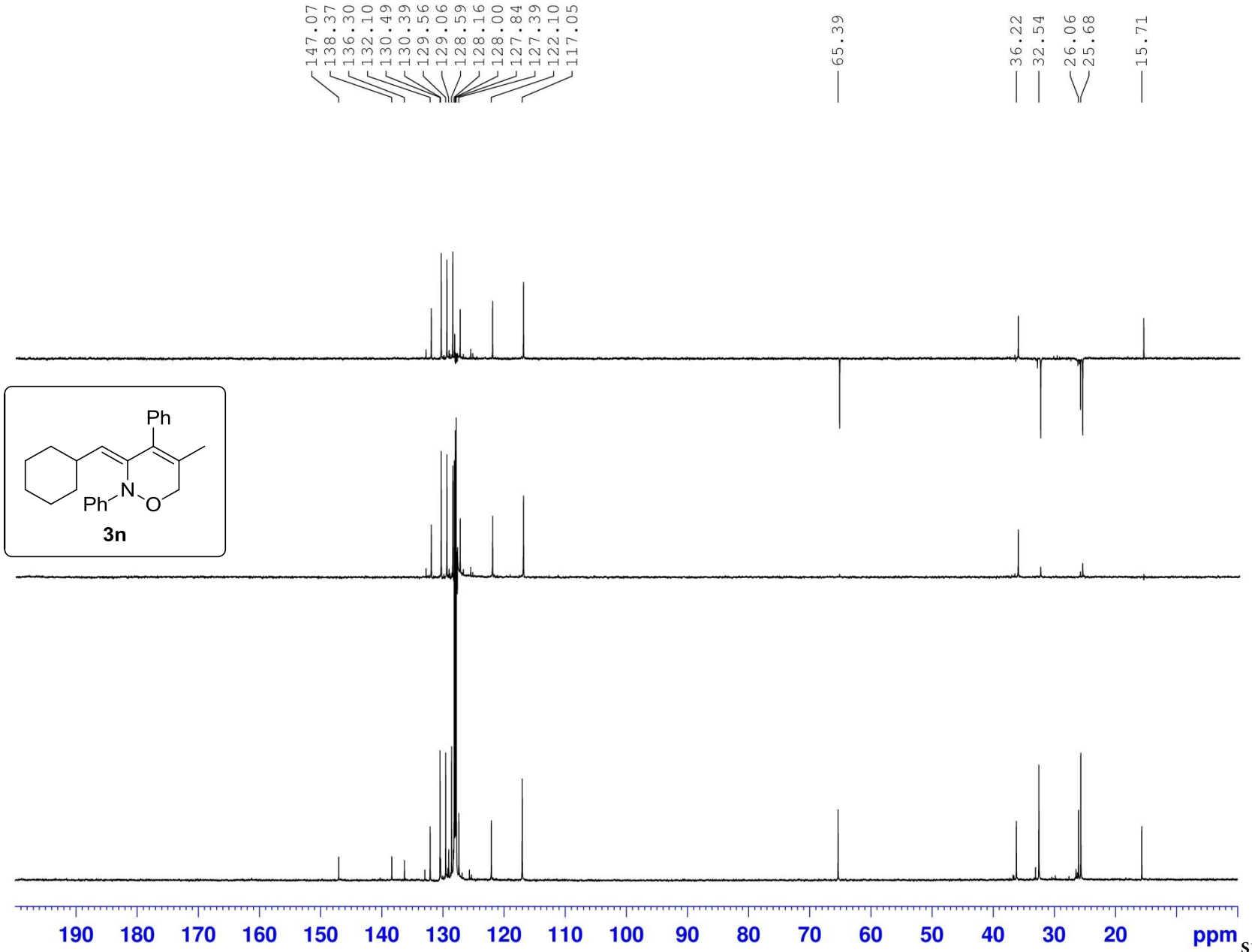
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O
Ph
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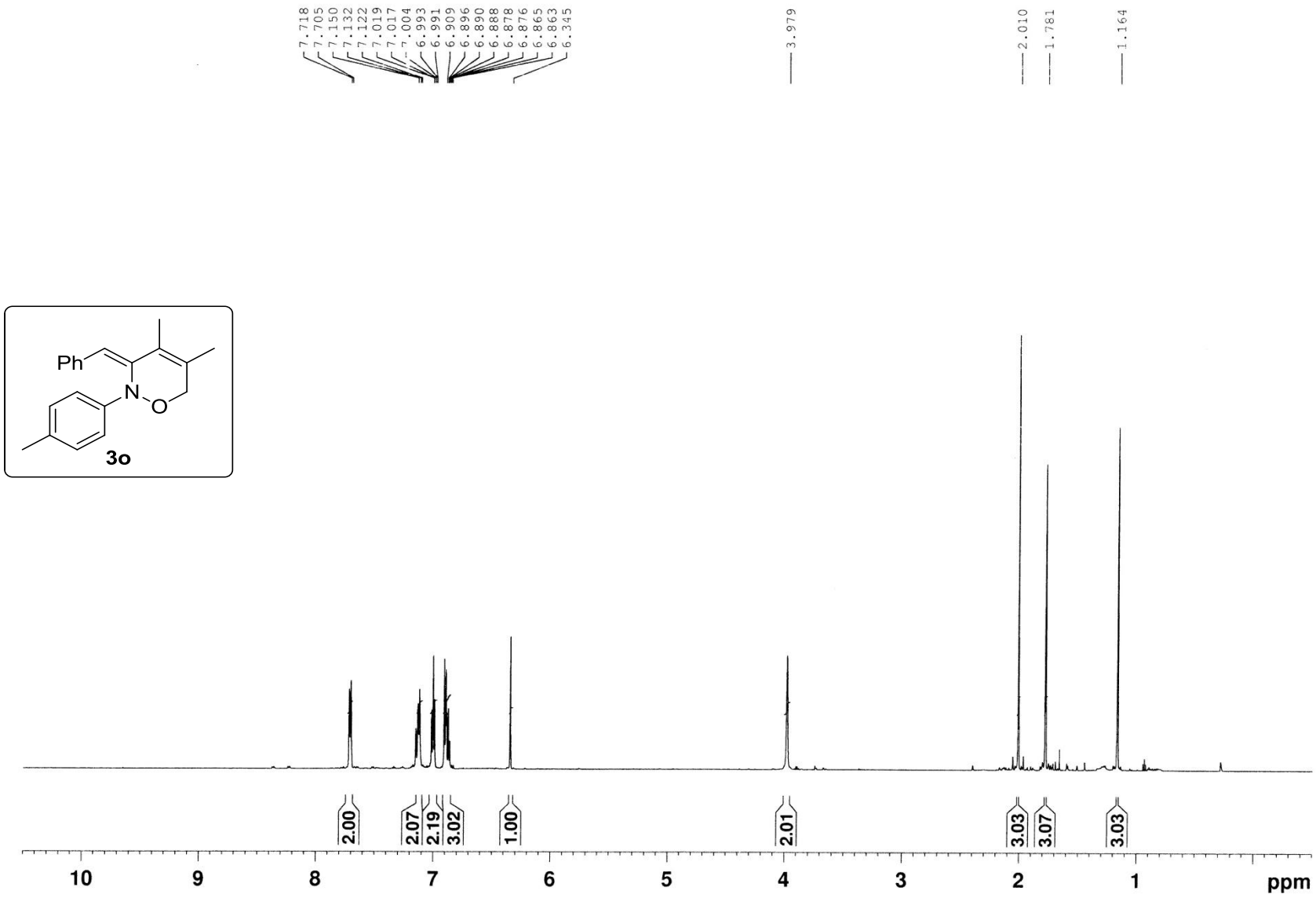
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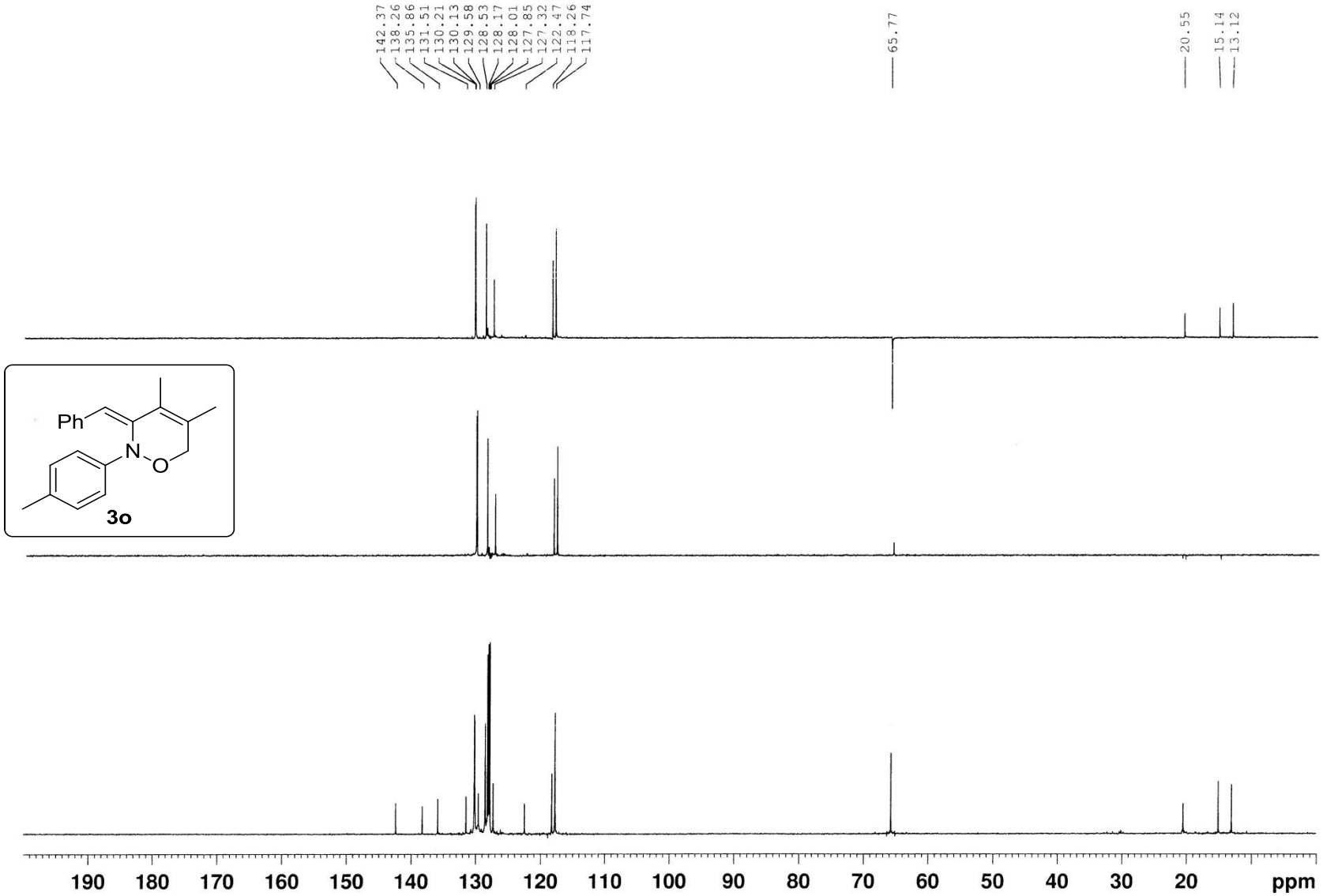
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O
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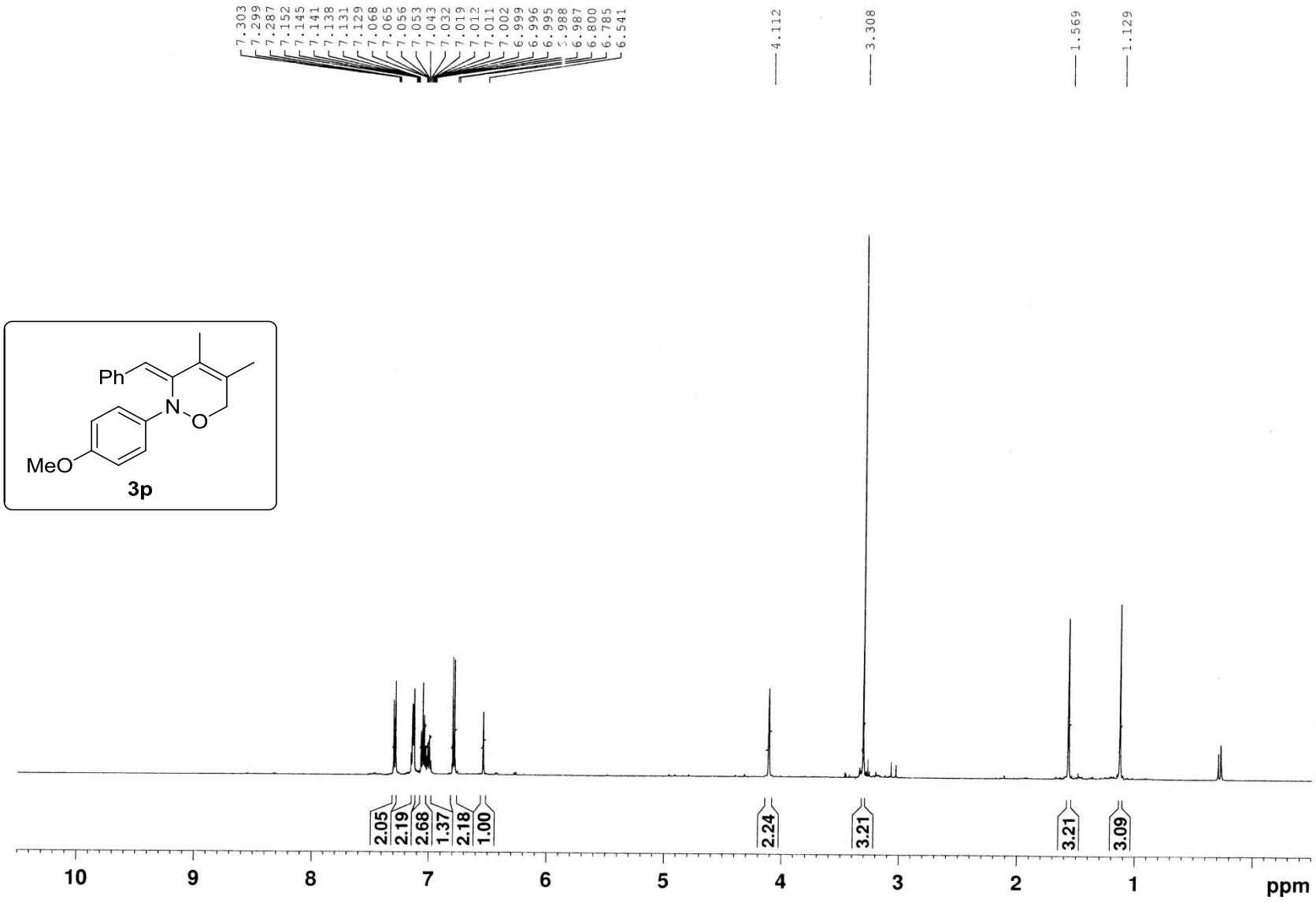
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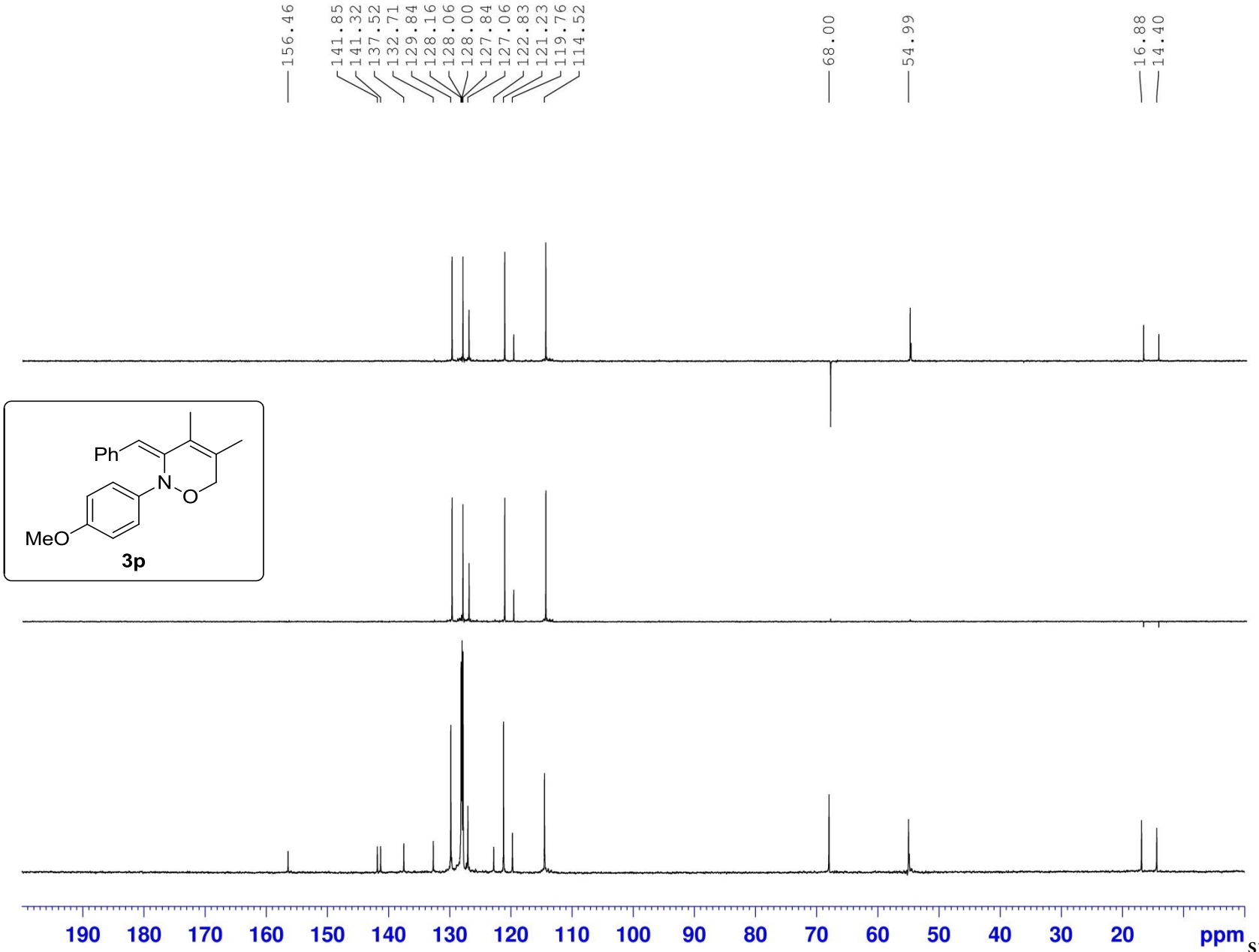
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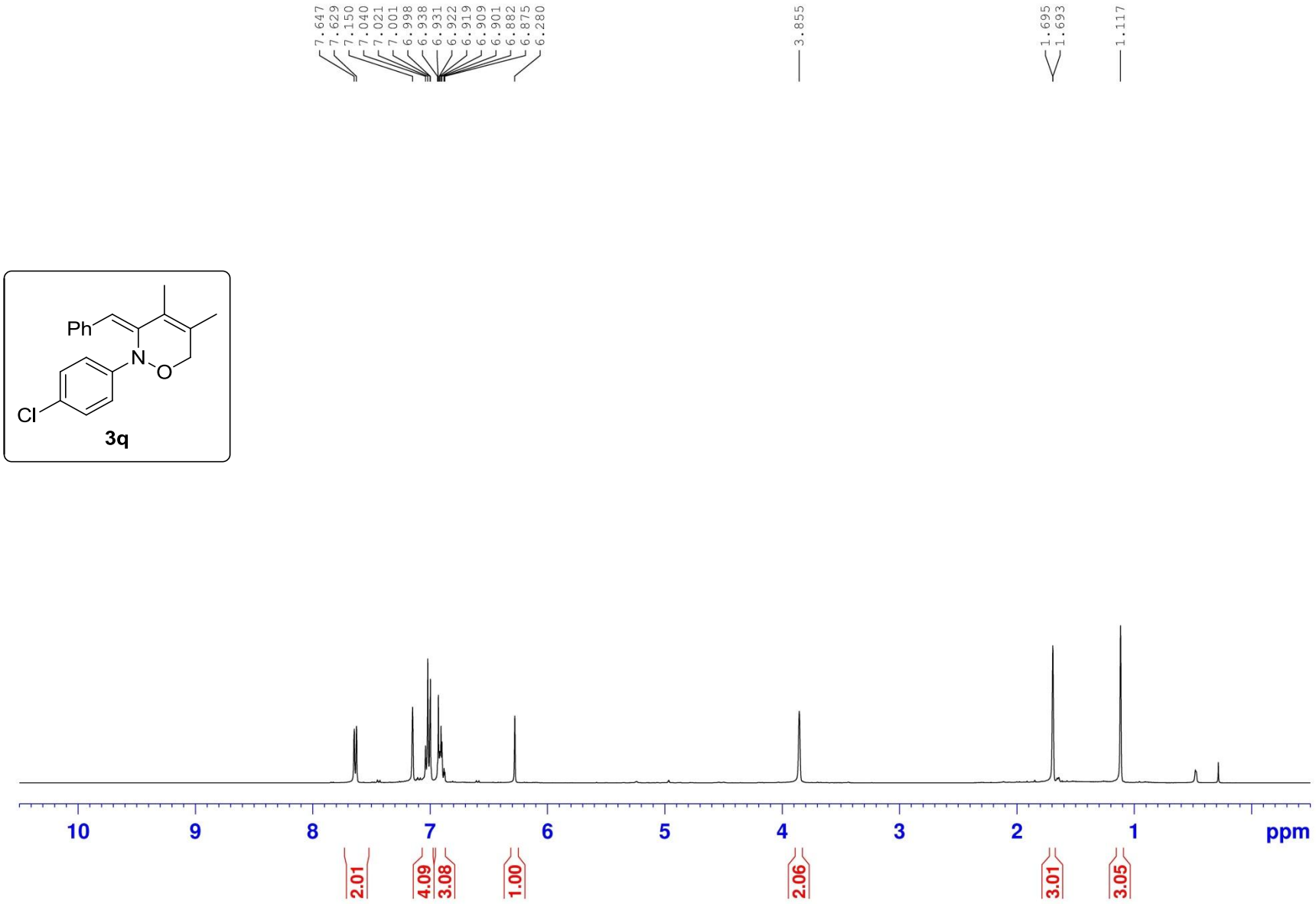
3q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1.693
1.117
10
9
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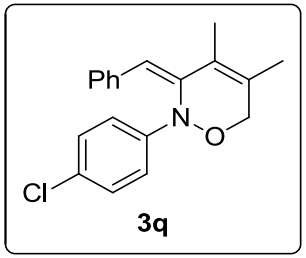
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Cl
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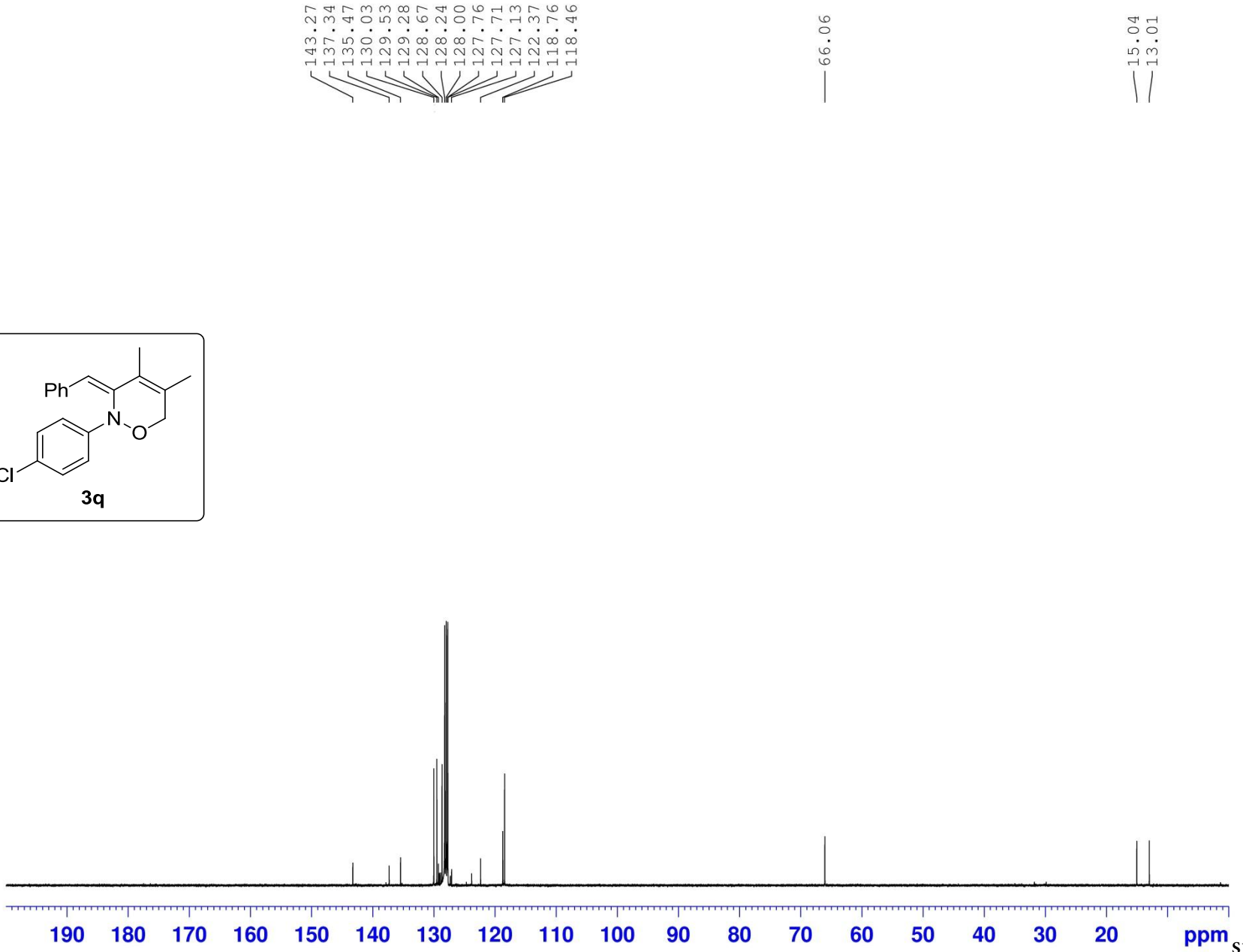
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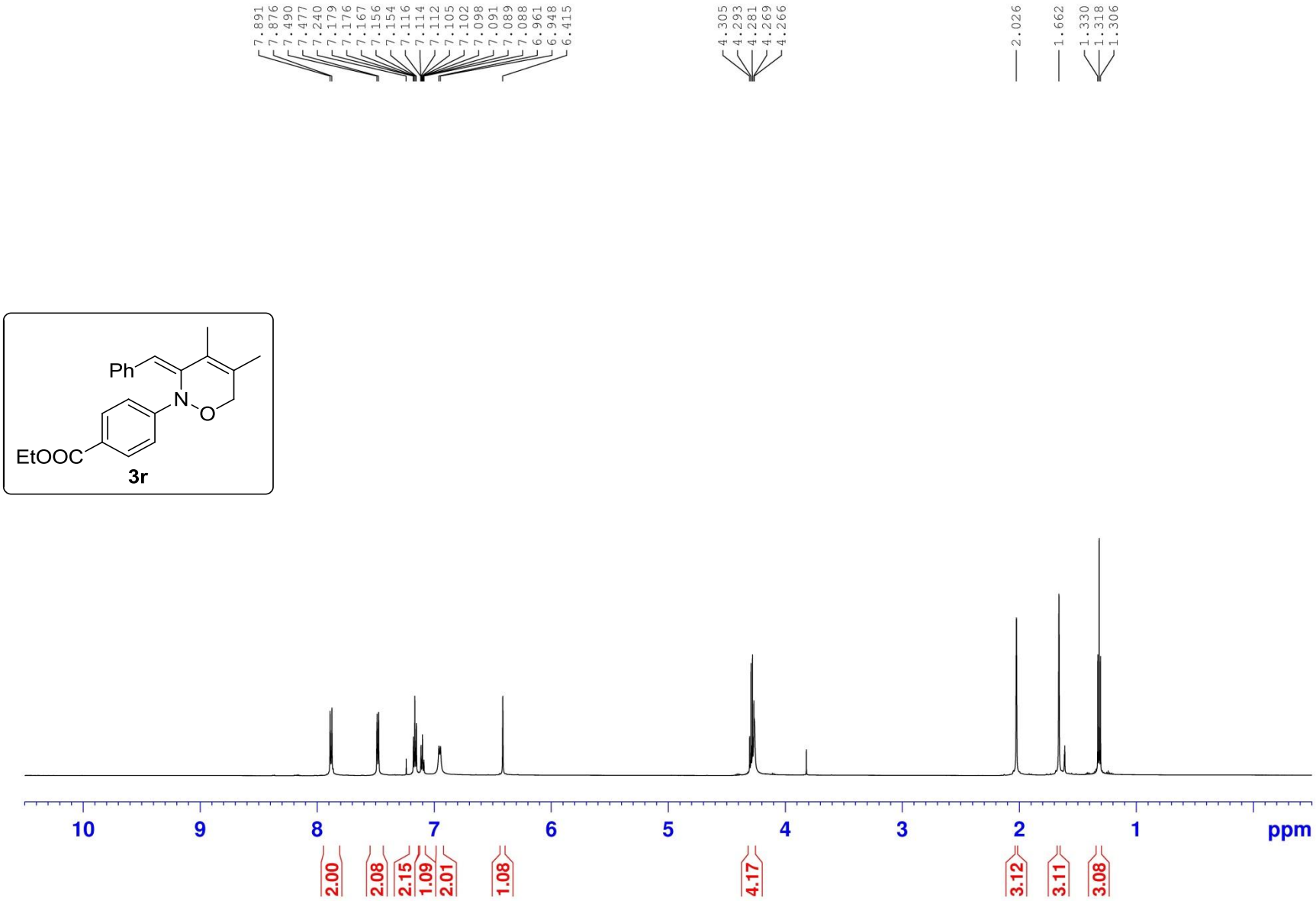
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O
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6
5
4
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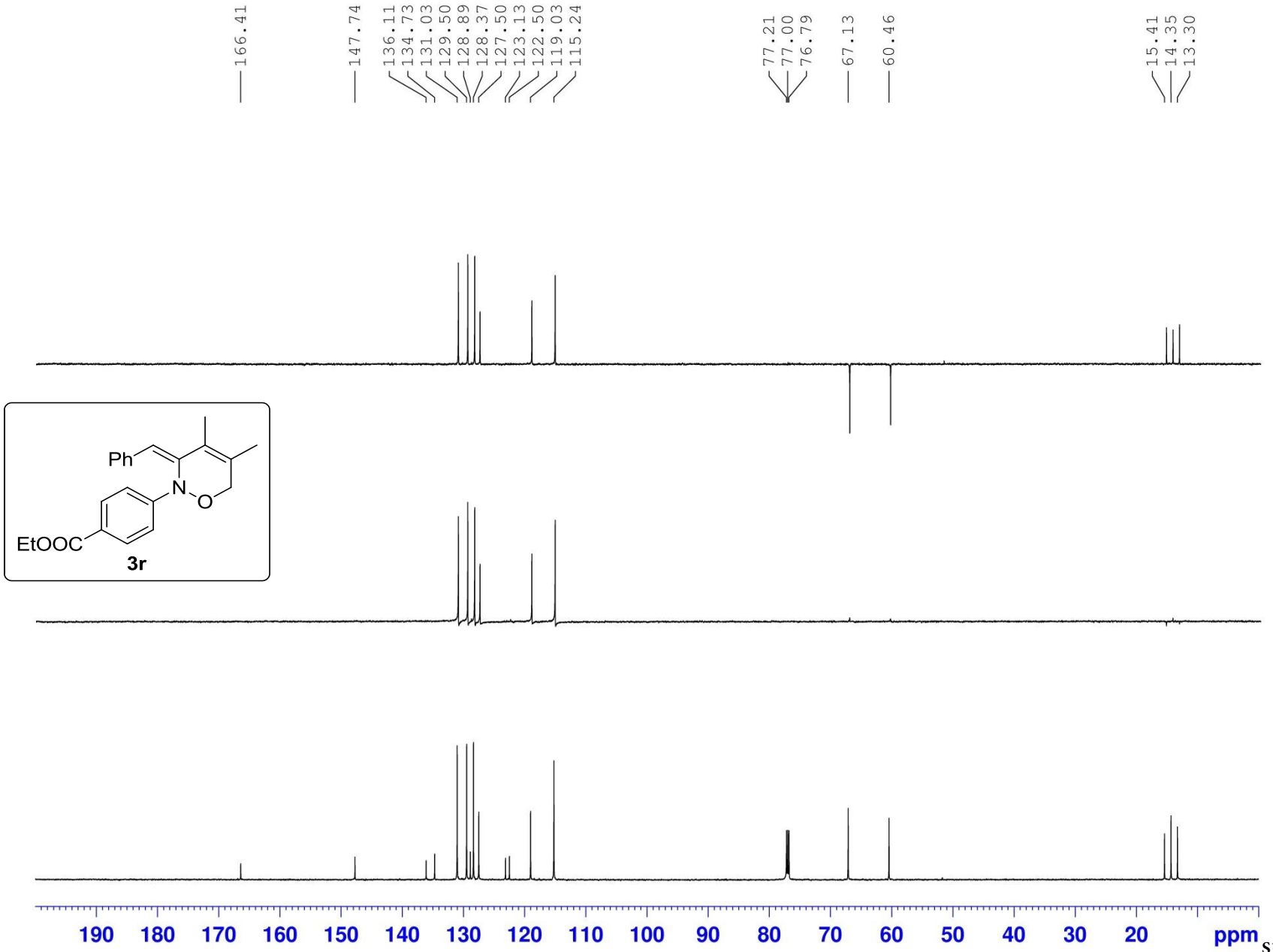
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EtOOC
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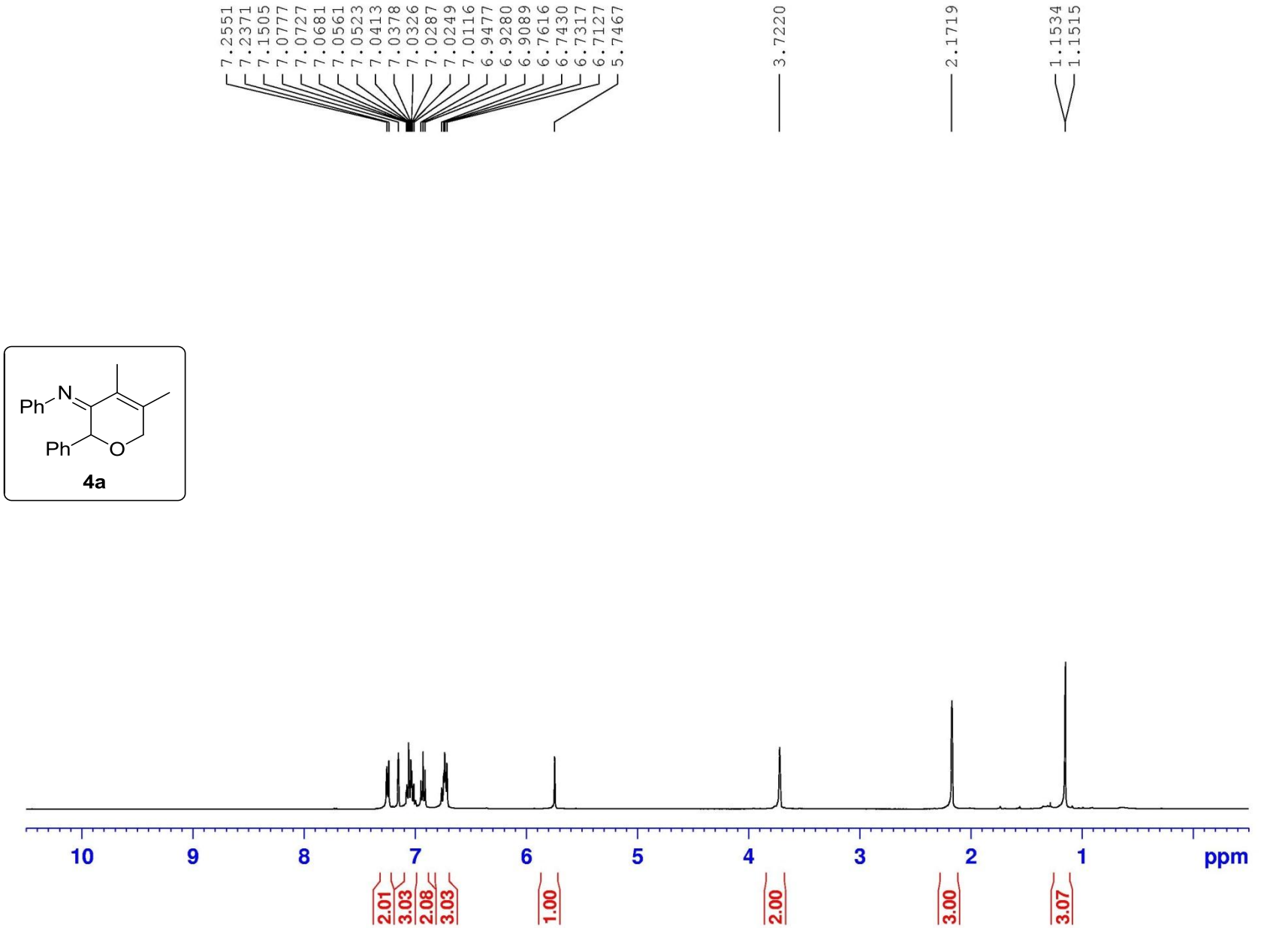
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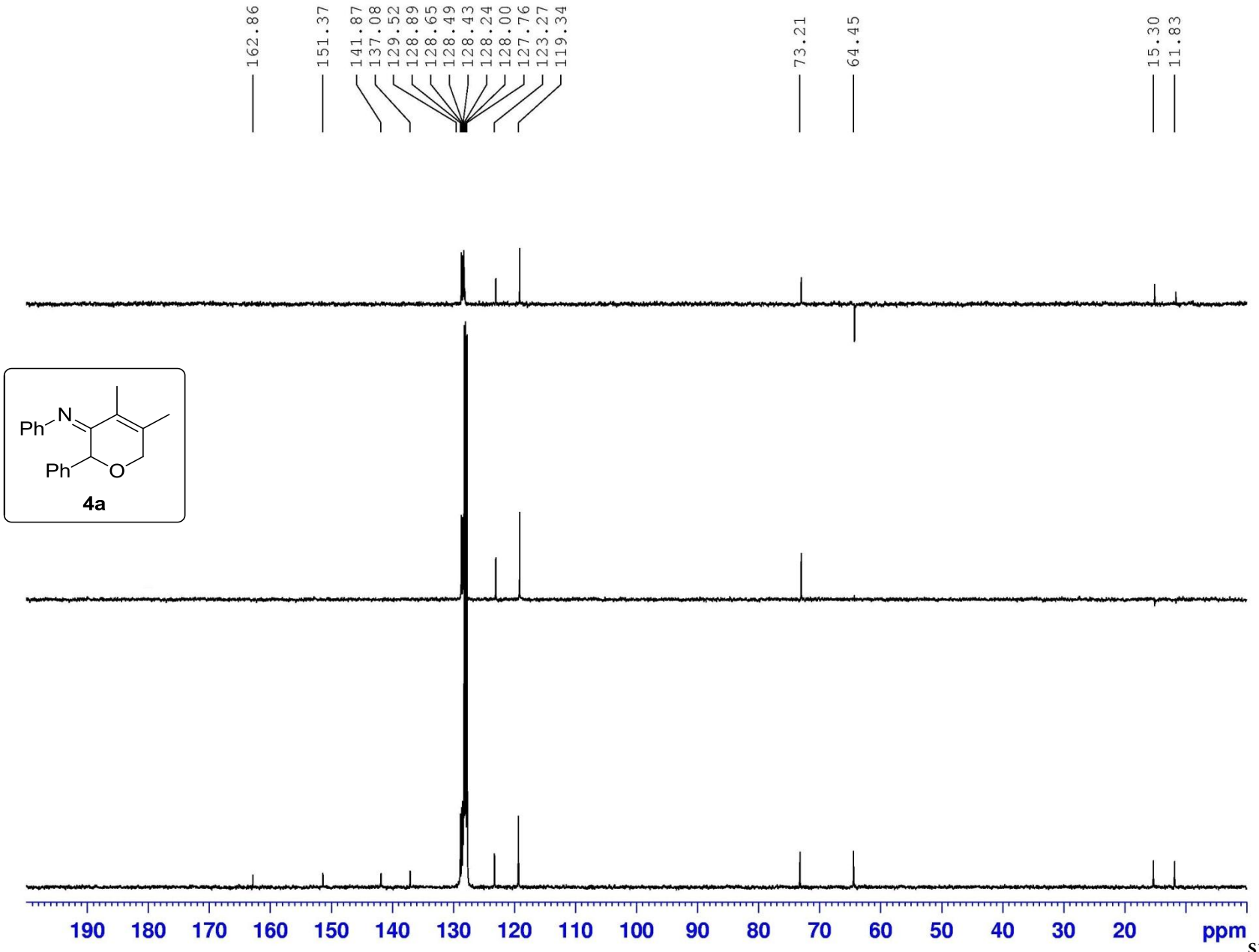
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Ph
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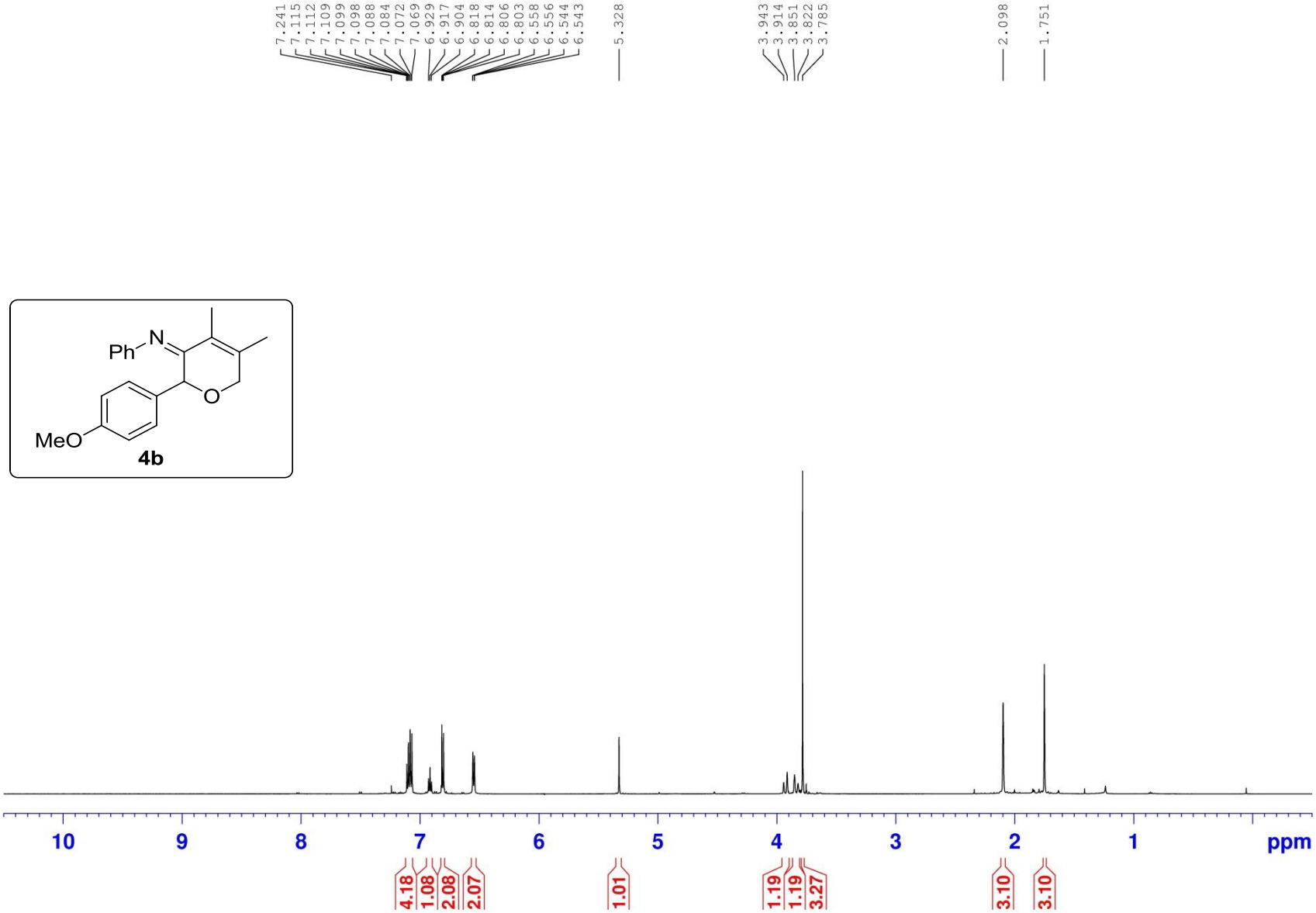
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MeO
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4
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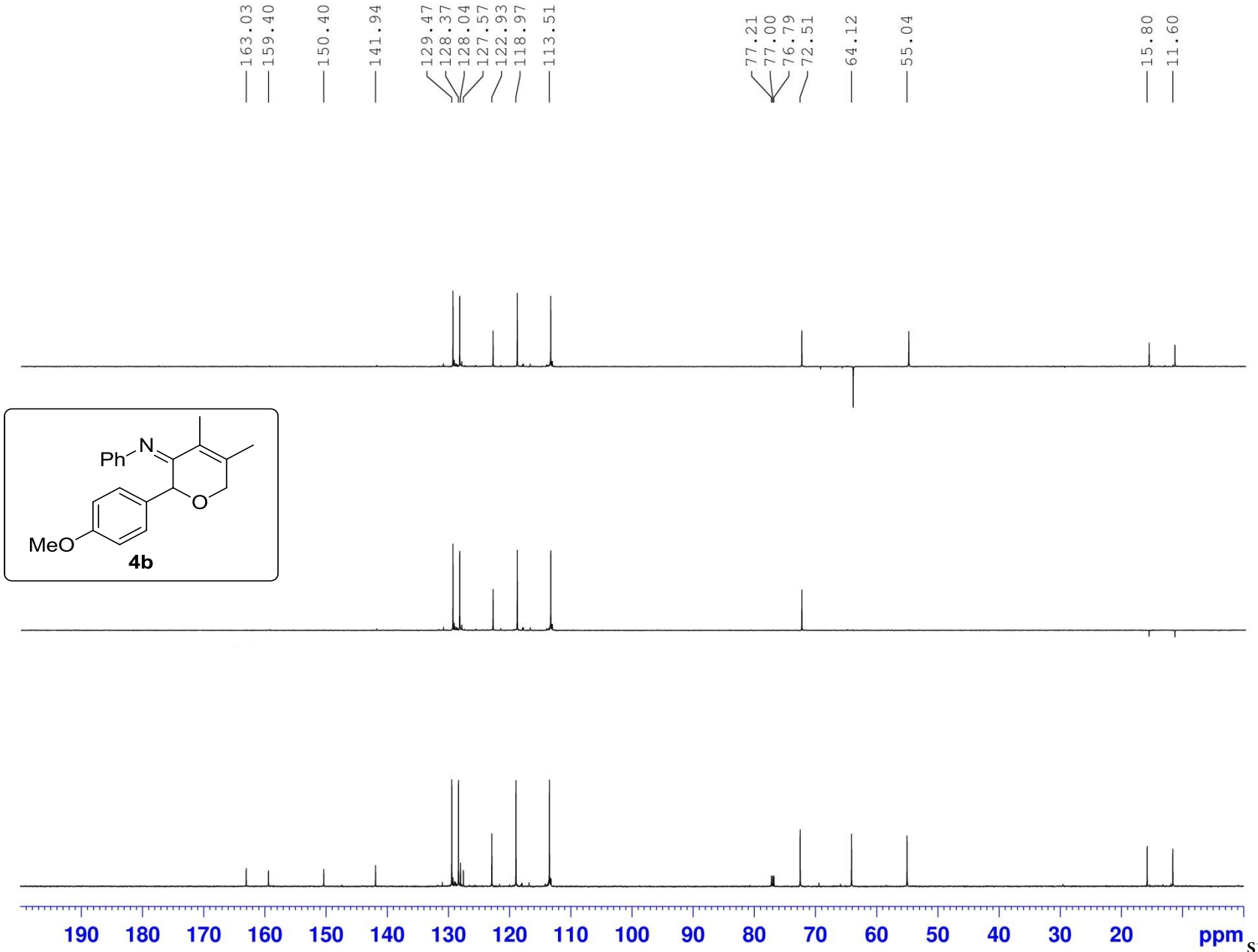
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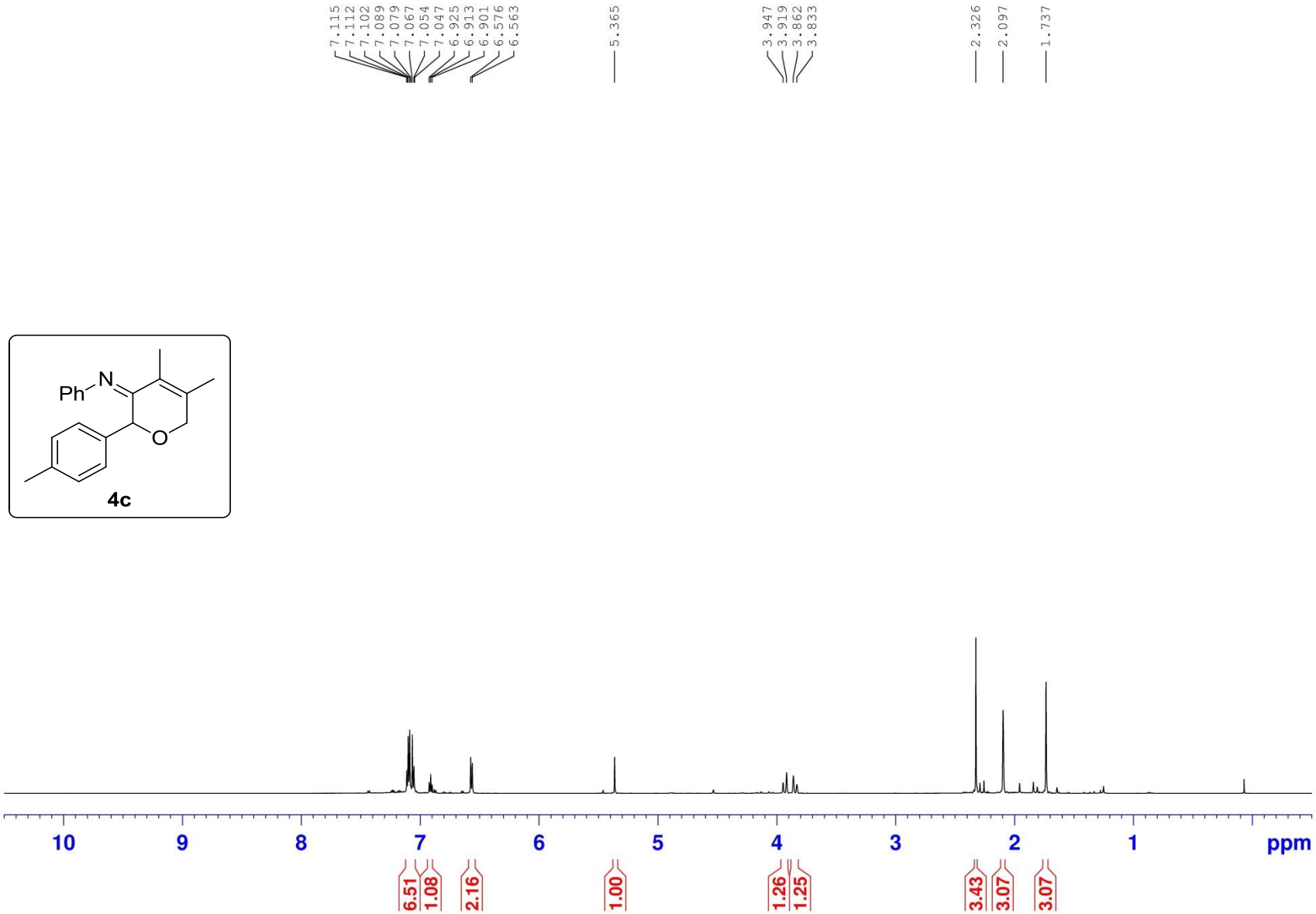
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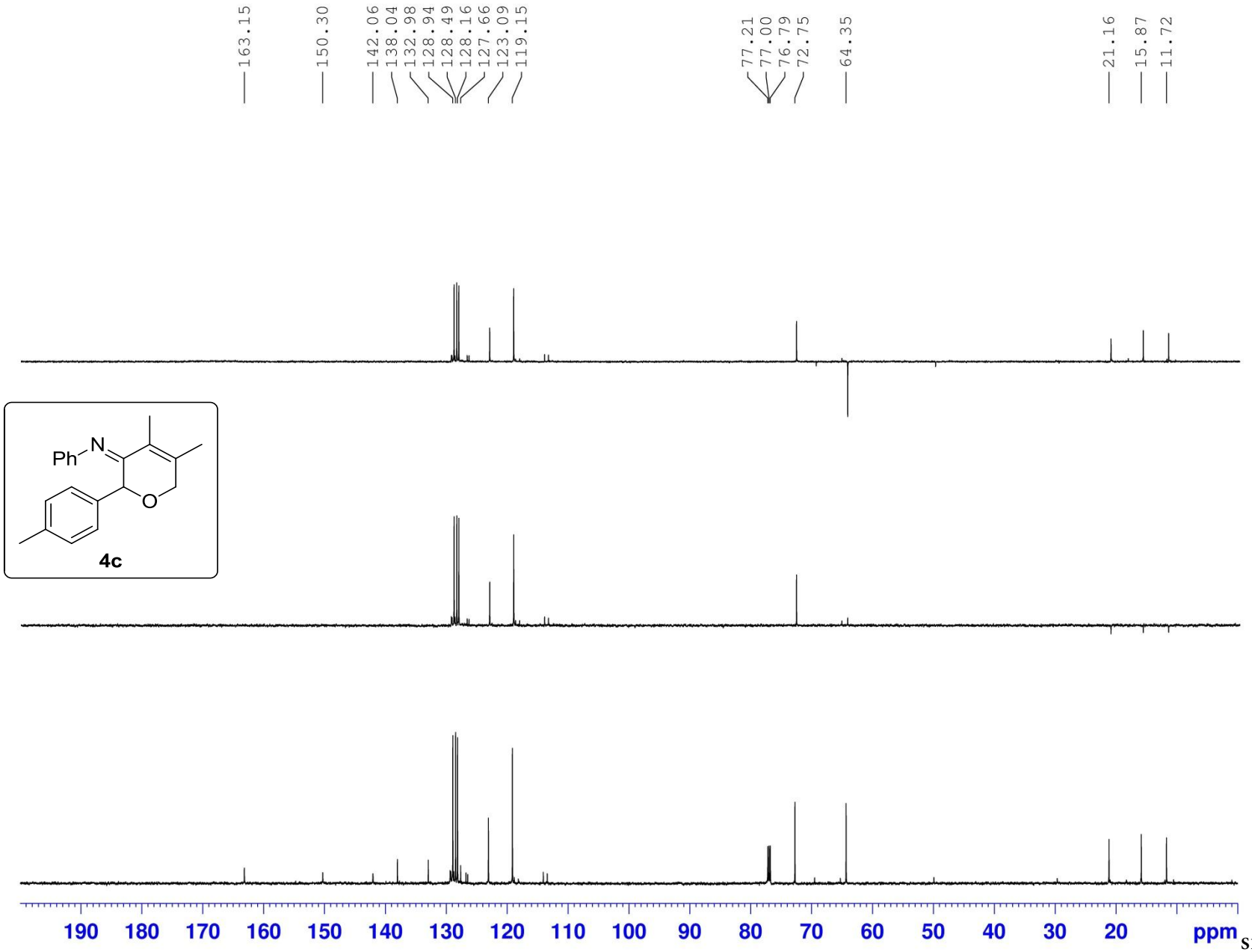
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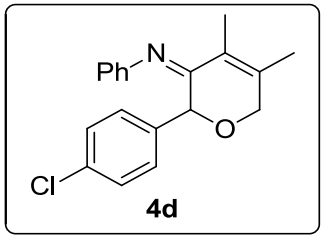
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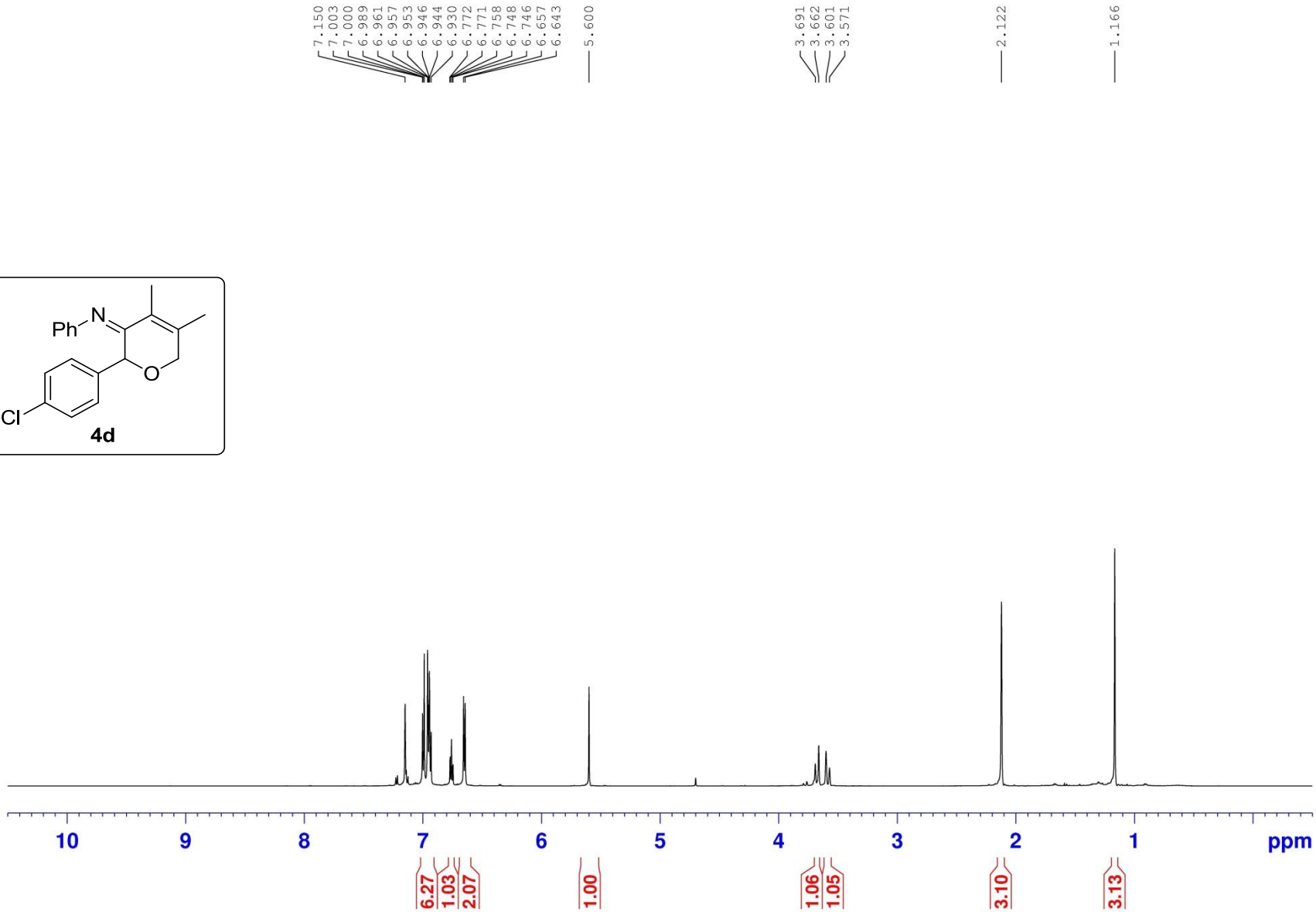
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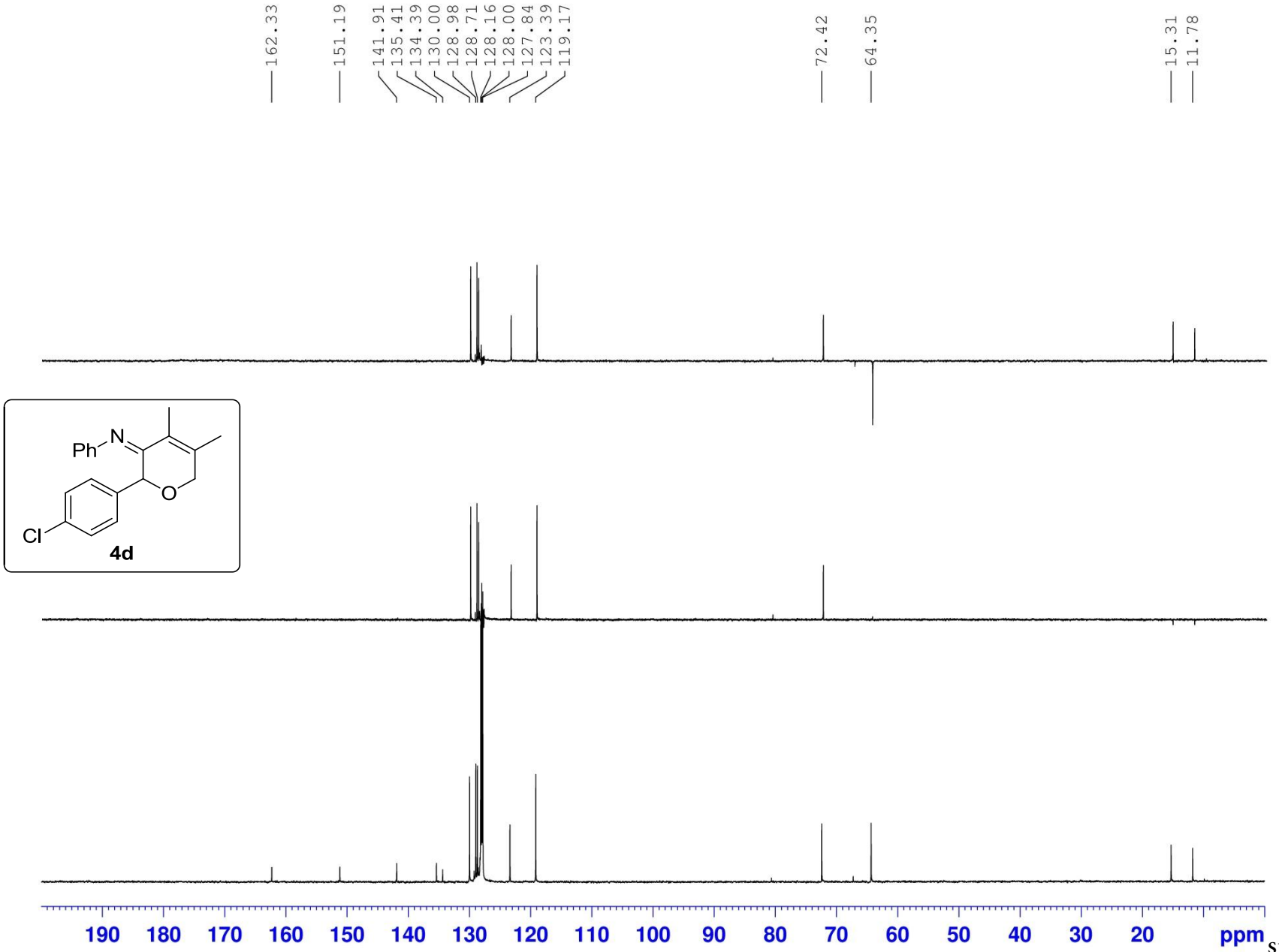
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N
O
Cl
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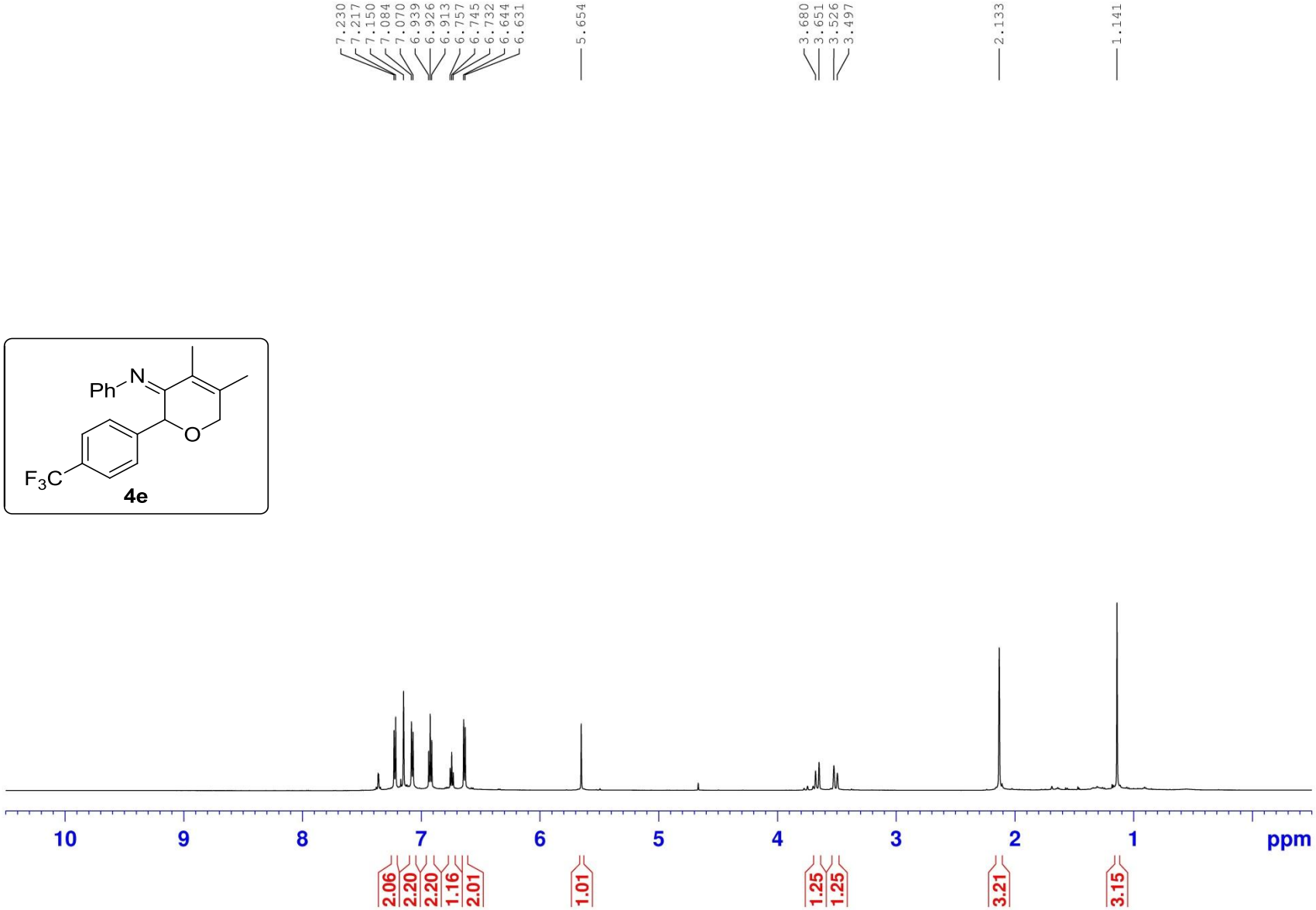
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3.651
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N
O
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4e
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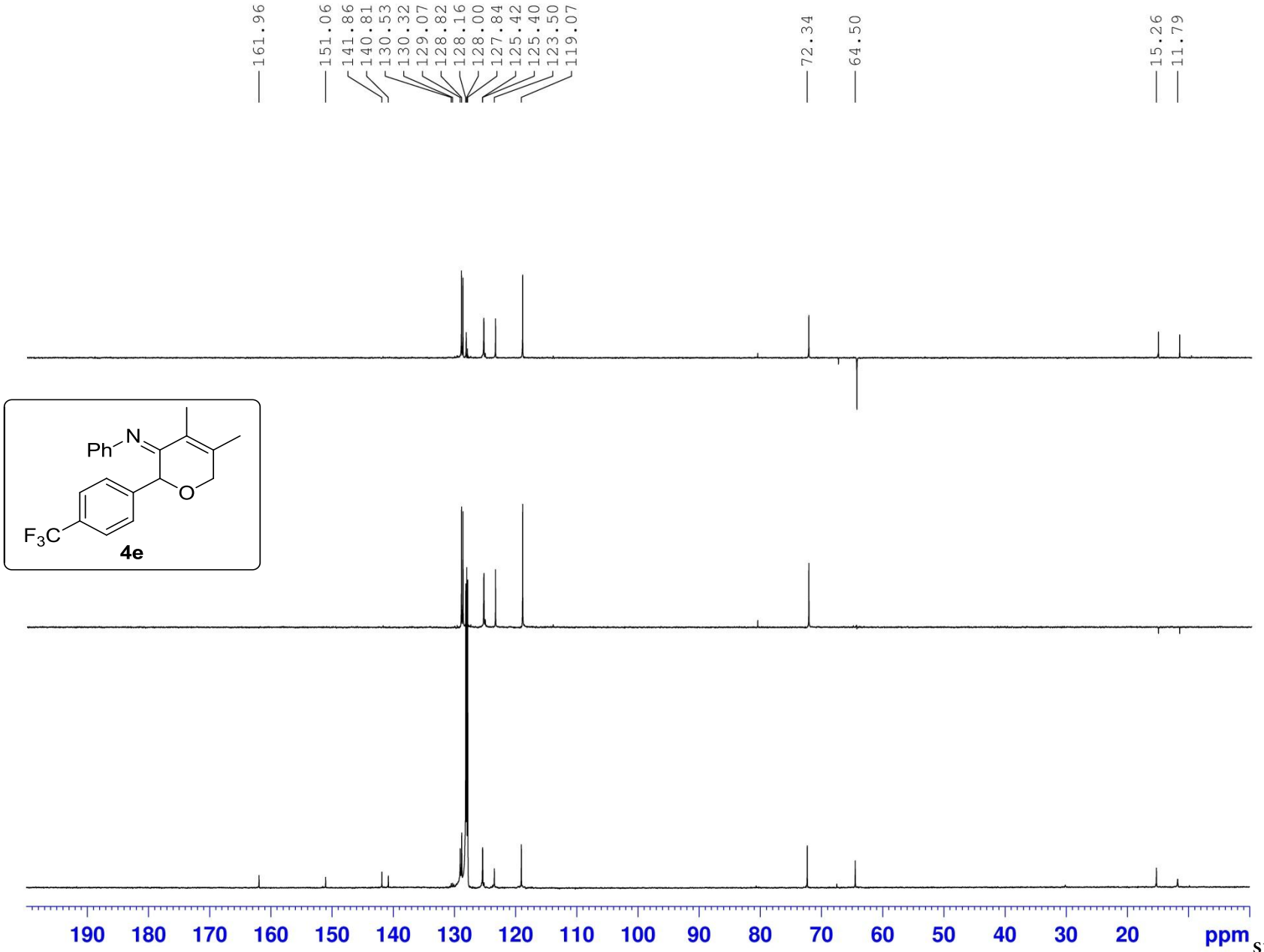
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O
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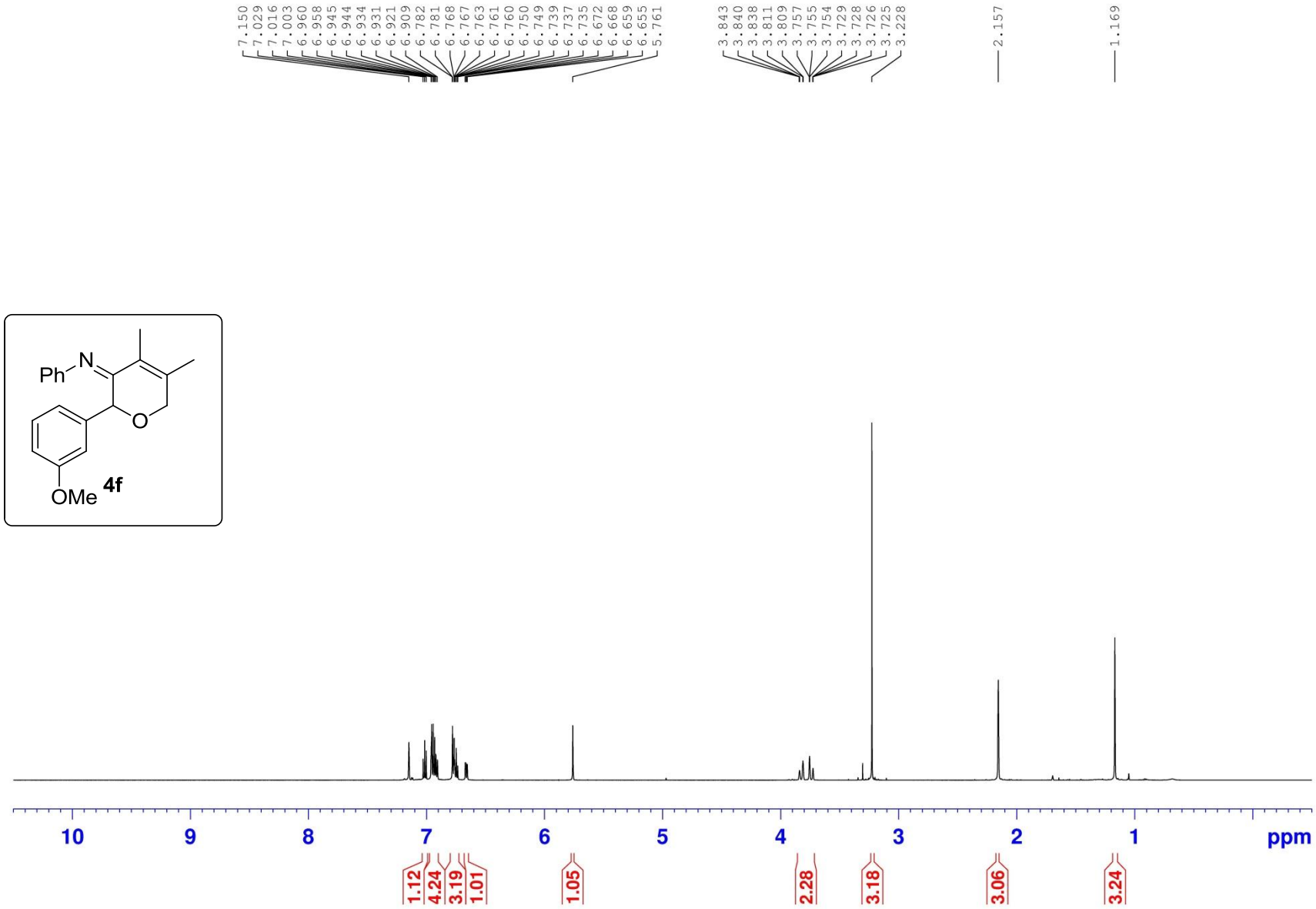
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6.763
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6.760
6.750
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6.659
6.655
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3.838
3.811
3.809
3.757
3.755
3.754
3.729
3.728
3.726
3.725
3.228
2.157
1.169
Ph
N
O
OMe
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7
6
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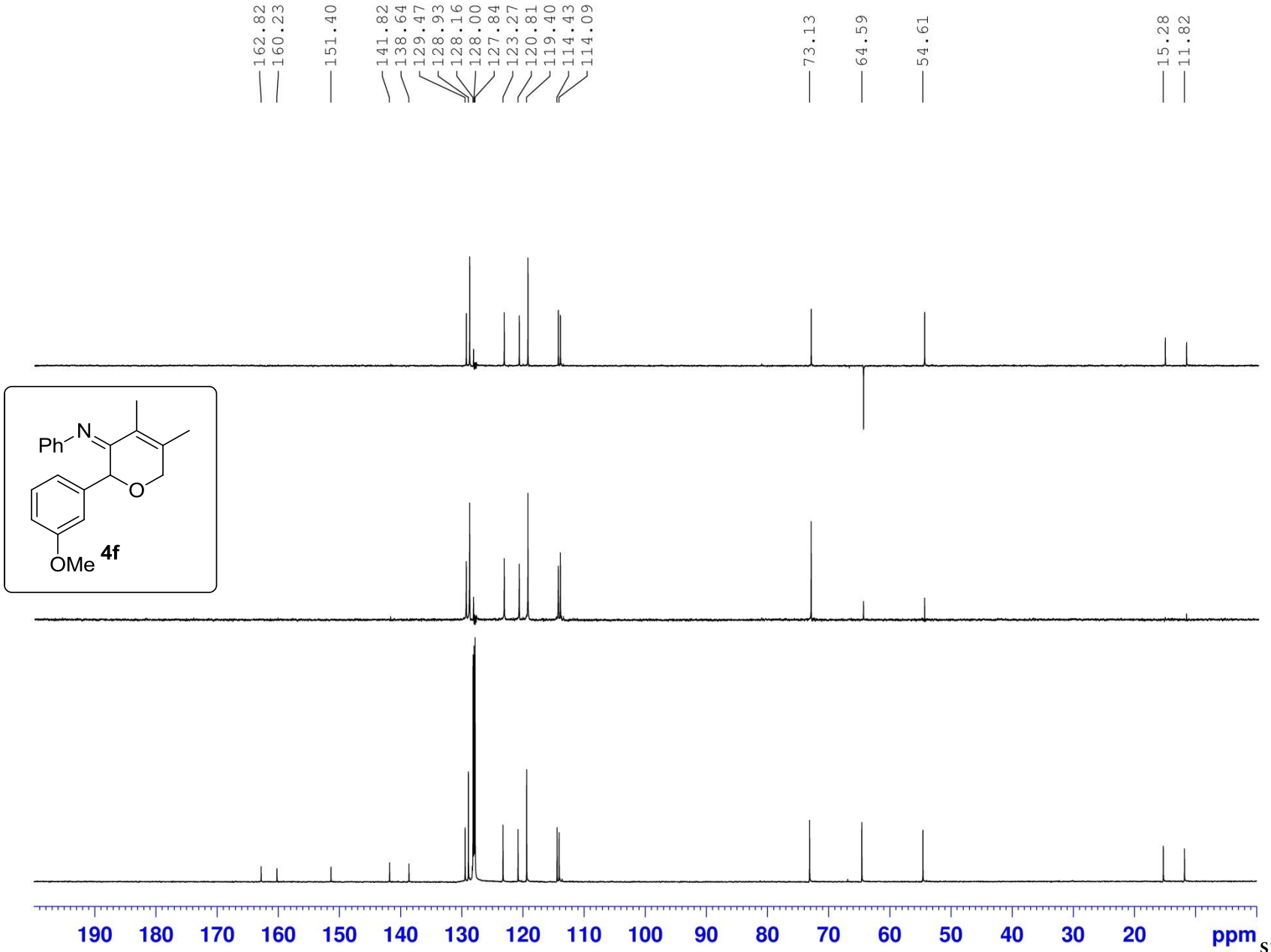
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114.09
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64.59
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15.28
11.82
Ph
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O
OMe
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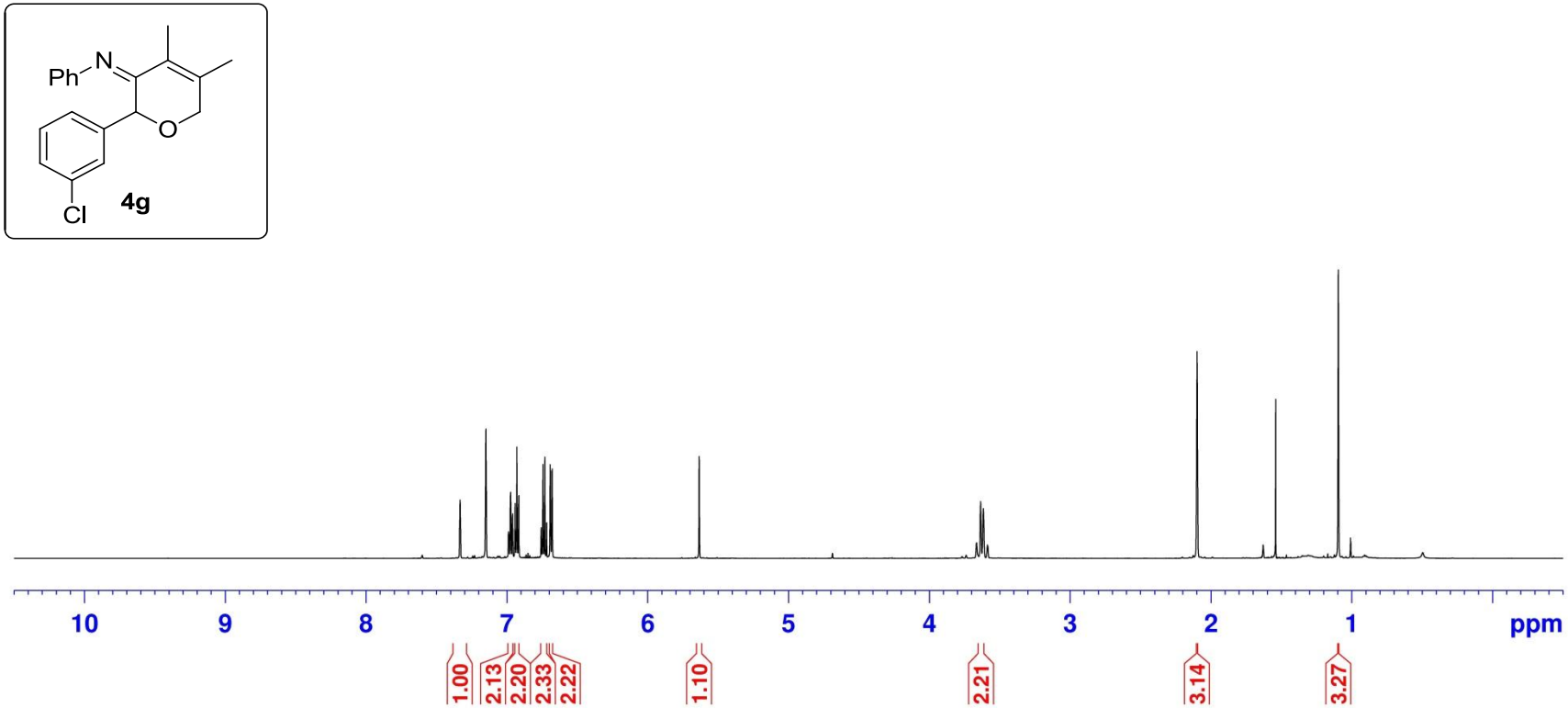
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3.617
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3.586
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Ph
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O
Cl
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7
6
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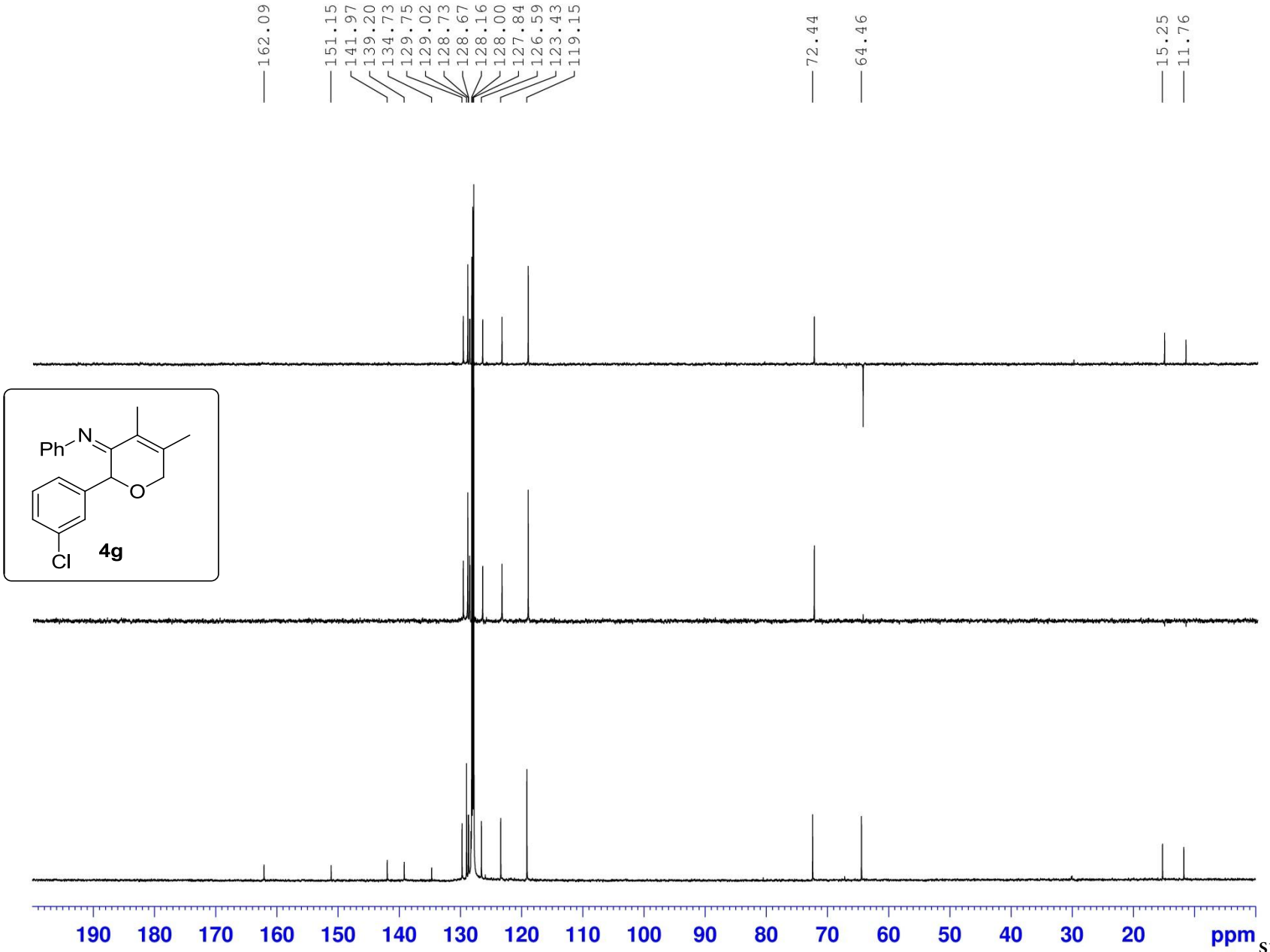
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O
Cl
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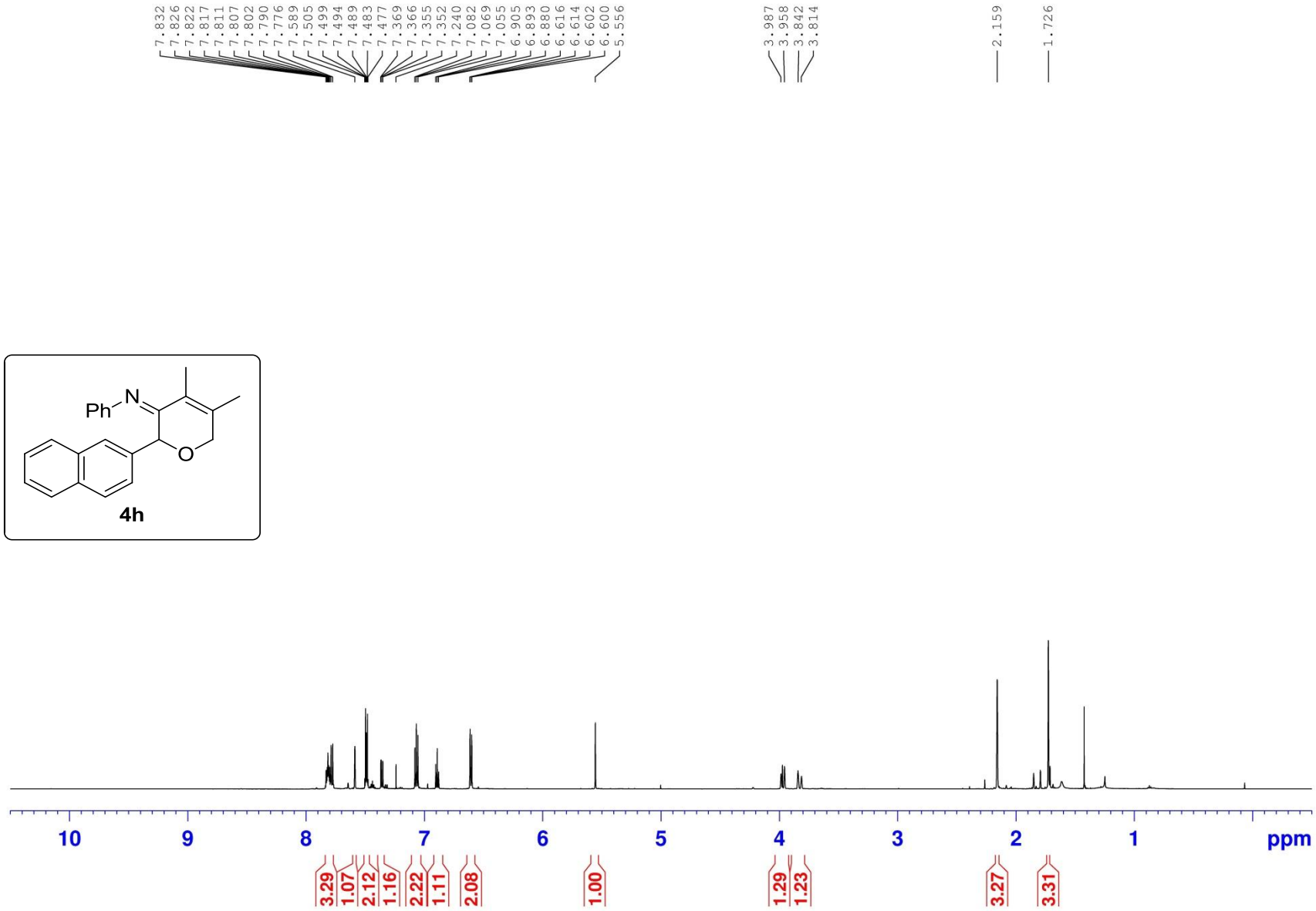
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O
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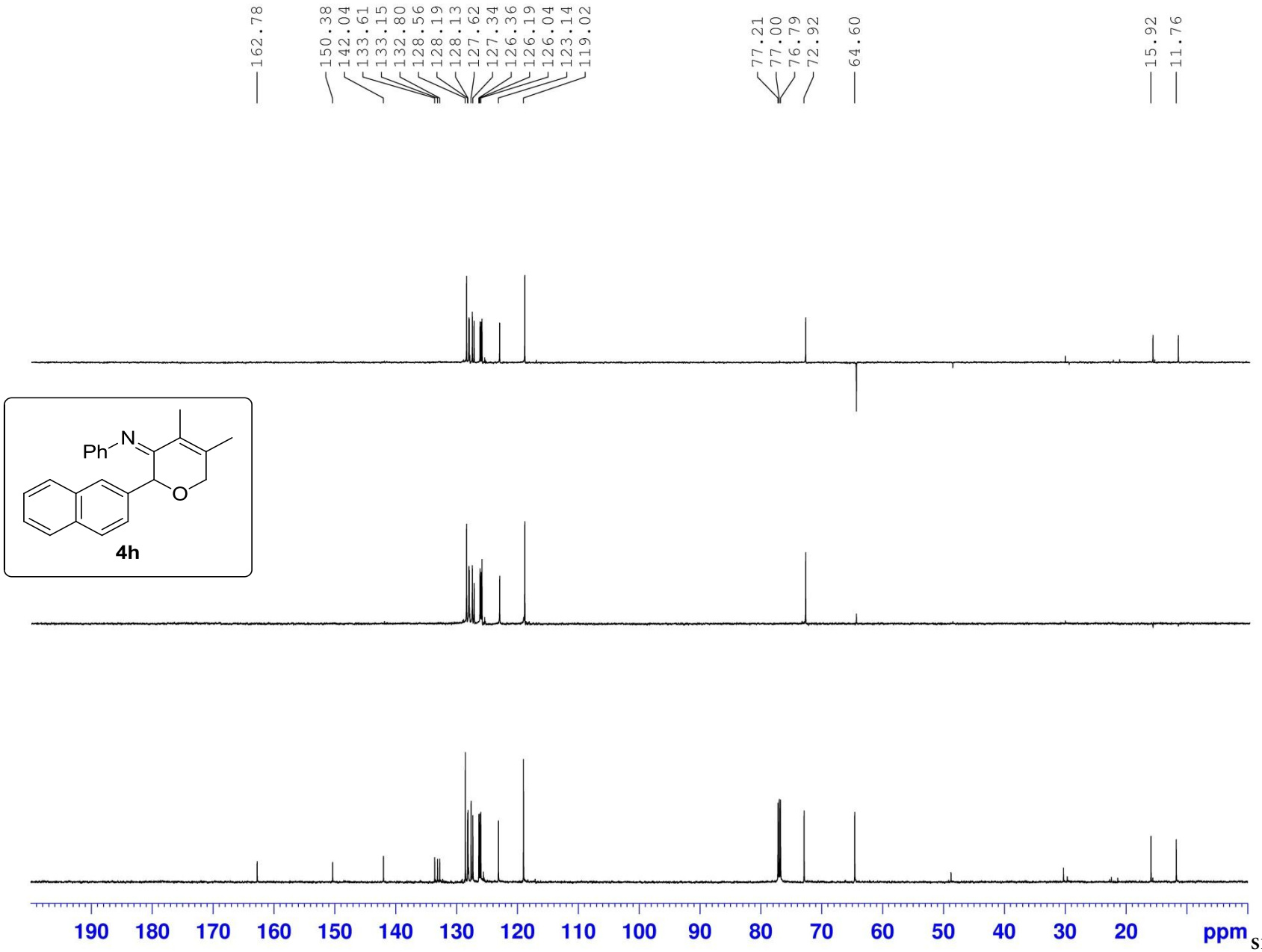
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Ph
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O
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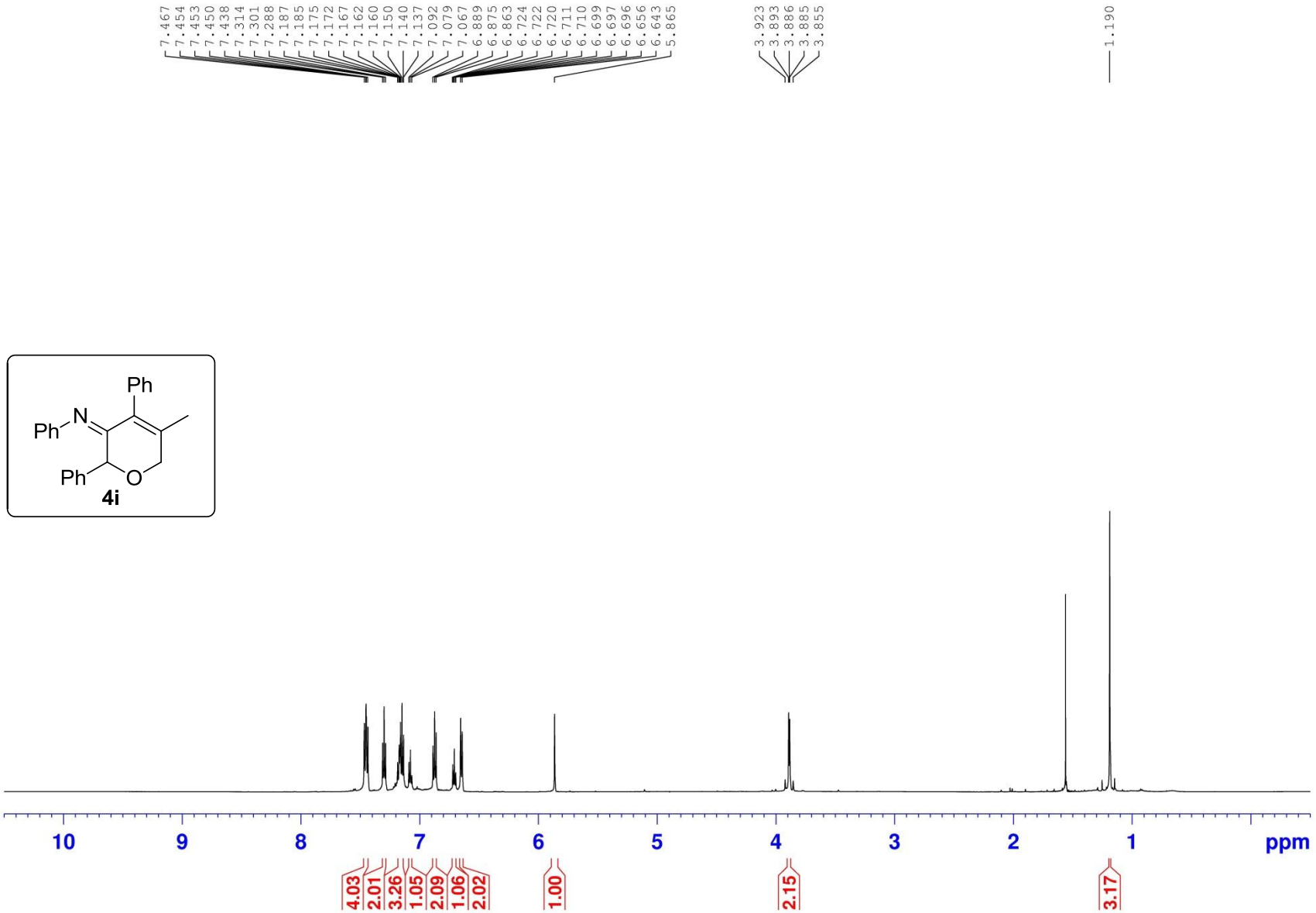
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Ph
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Ph
Ph
O
4i
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5
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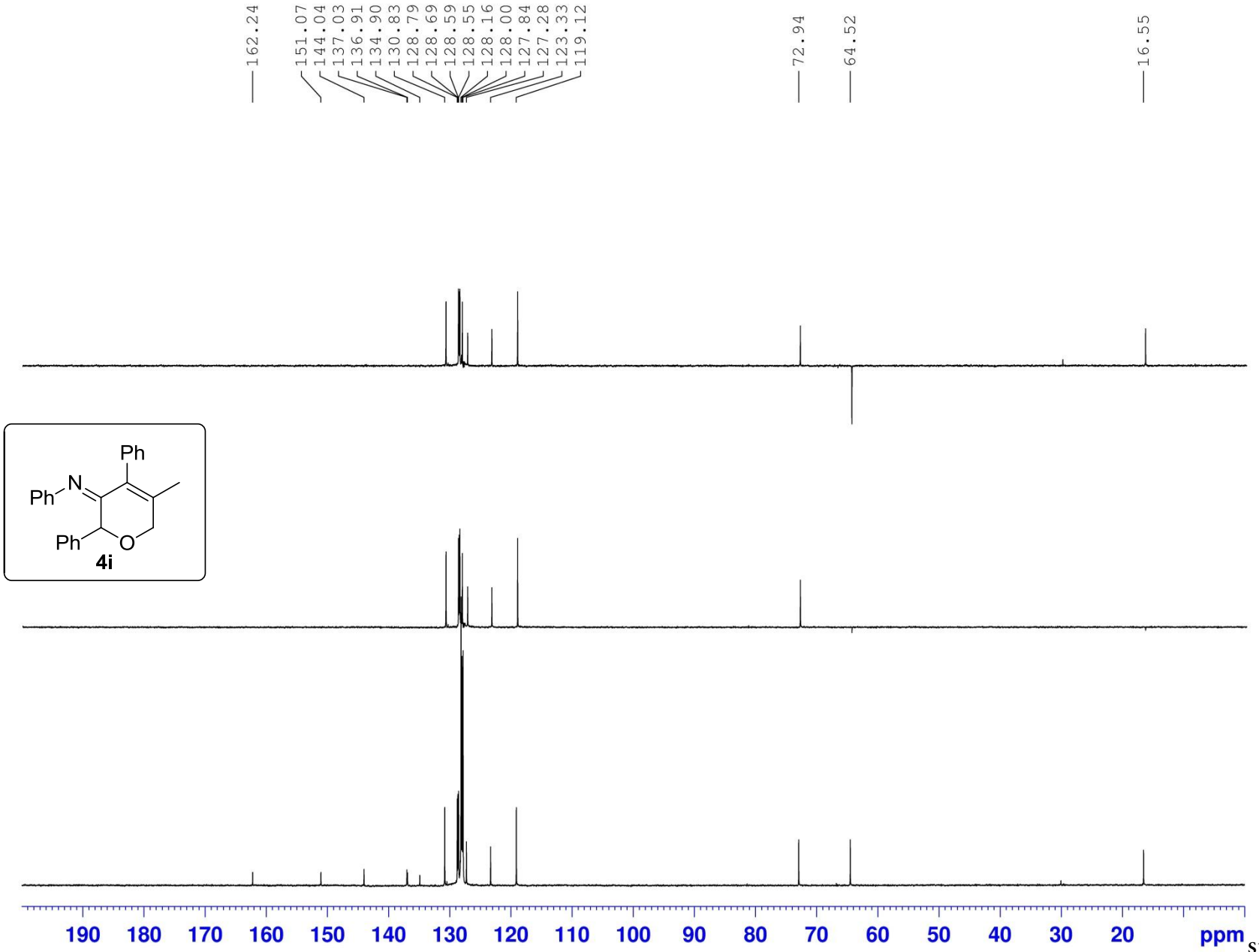
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127.28
123.33
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Ph
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Ph
O
4i
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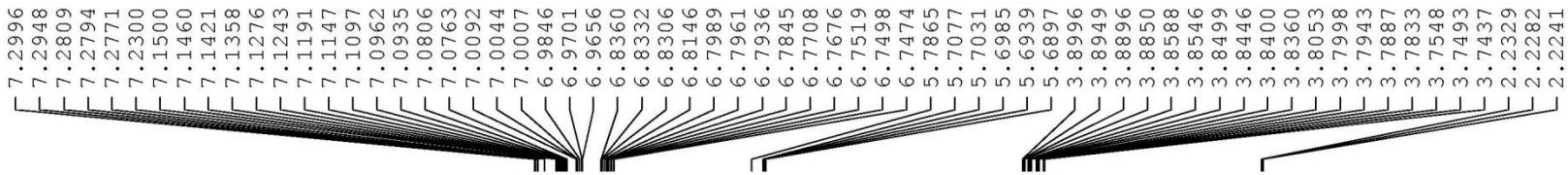
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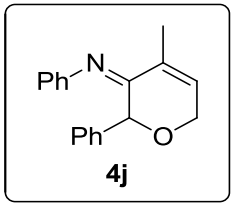
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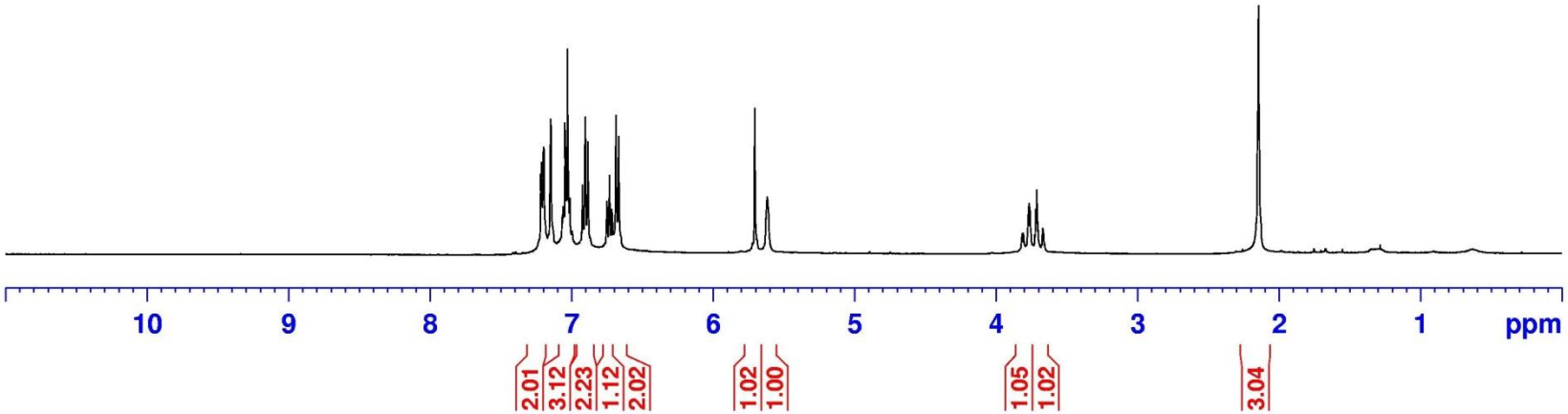
Ph
O
4j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1.02
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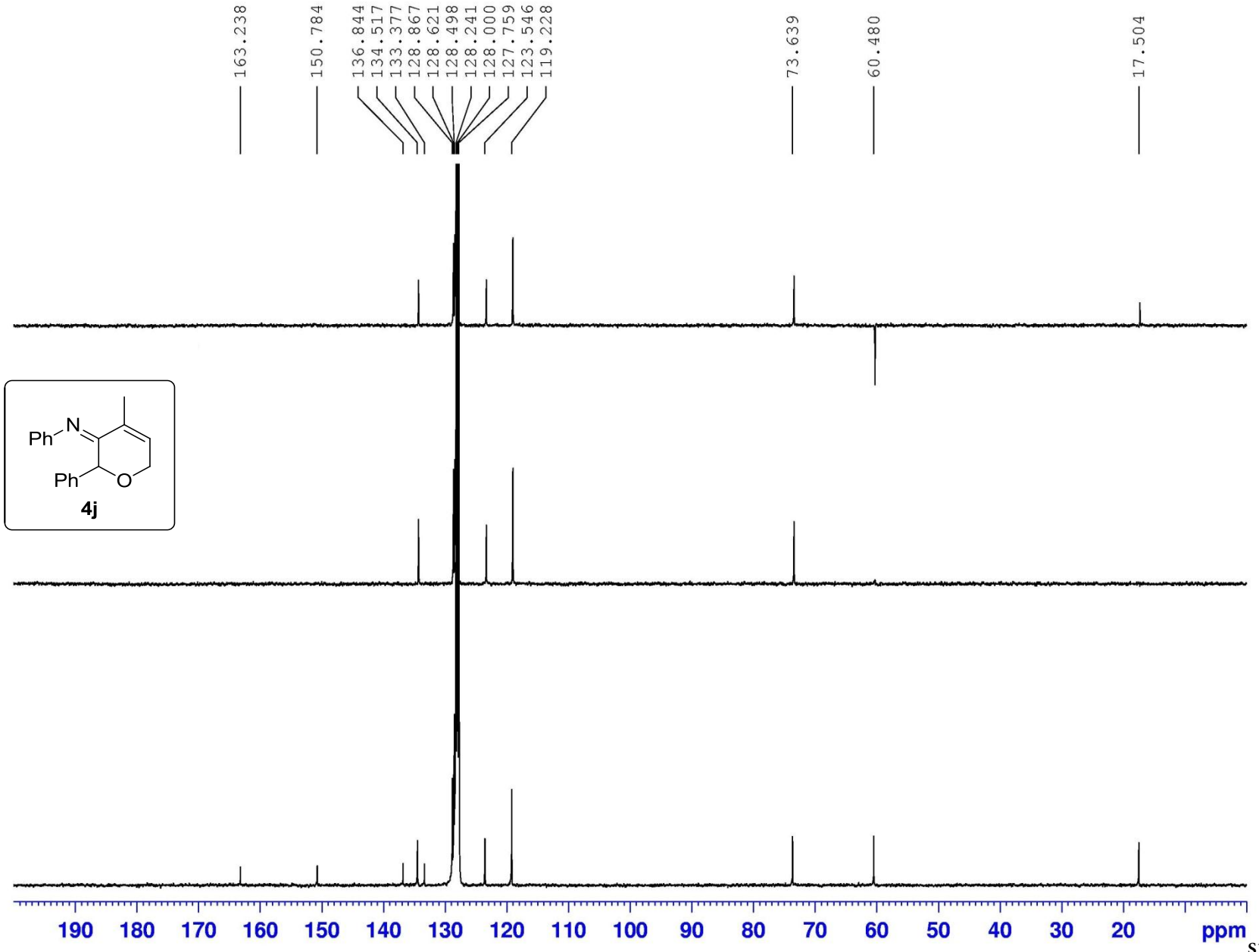
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Ph
O
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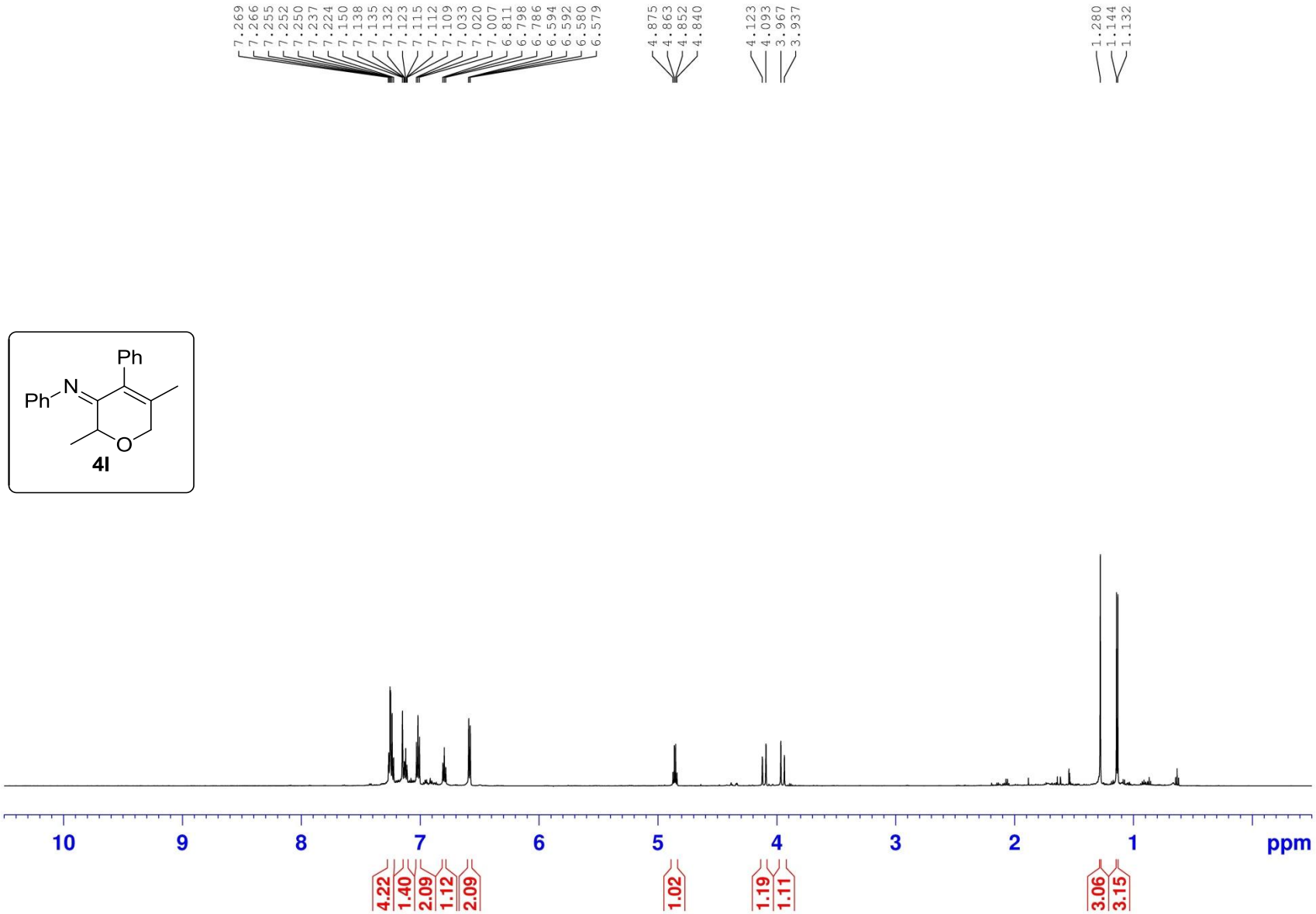
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6.580
6.579
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4.840
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1.144
1.132
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Ph
N
O
4l
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7
6
5
4
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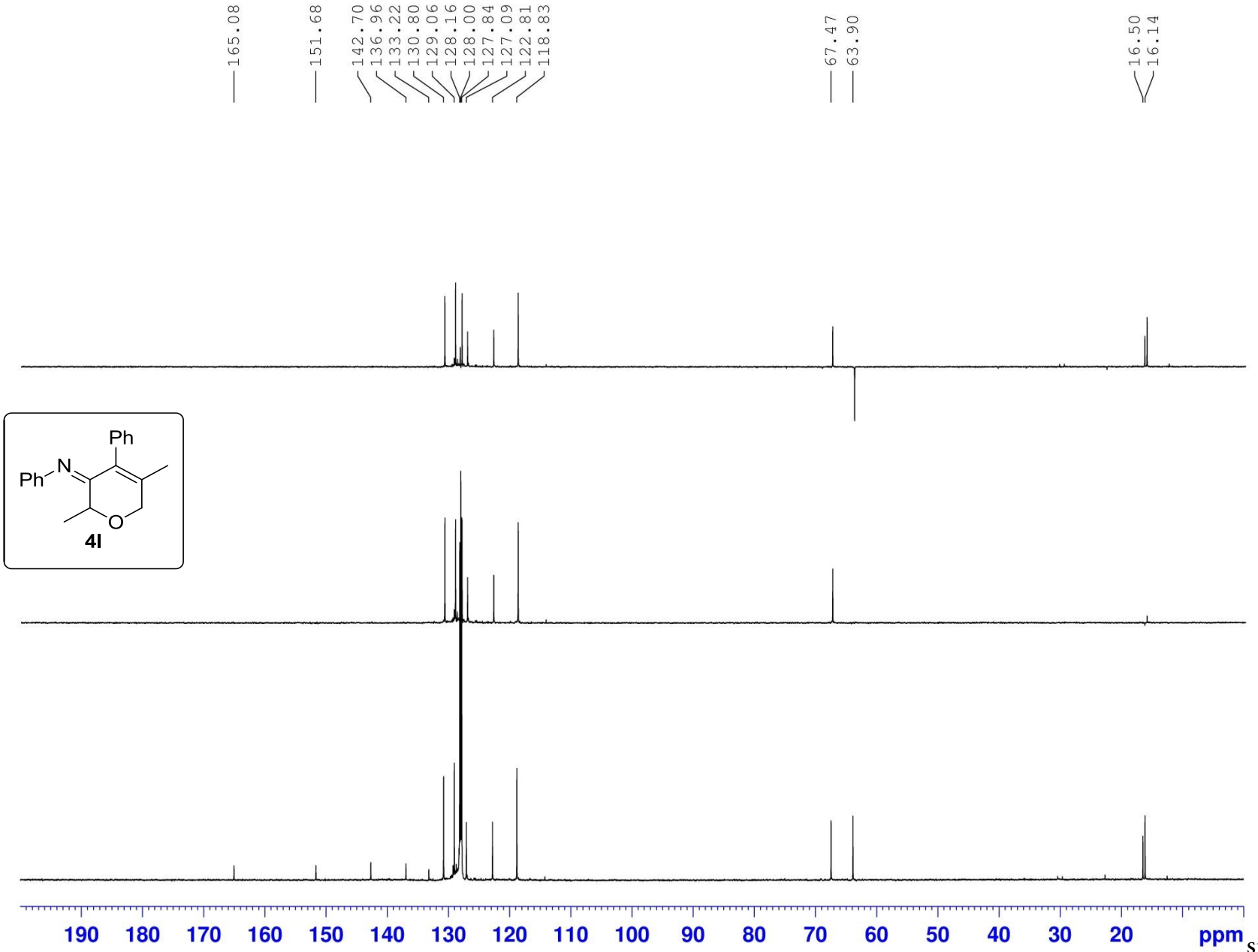
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67.47
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Ph
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Ph
O
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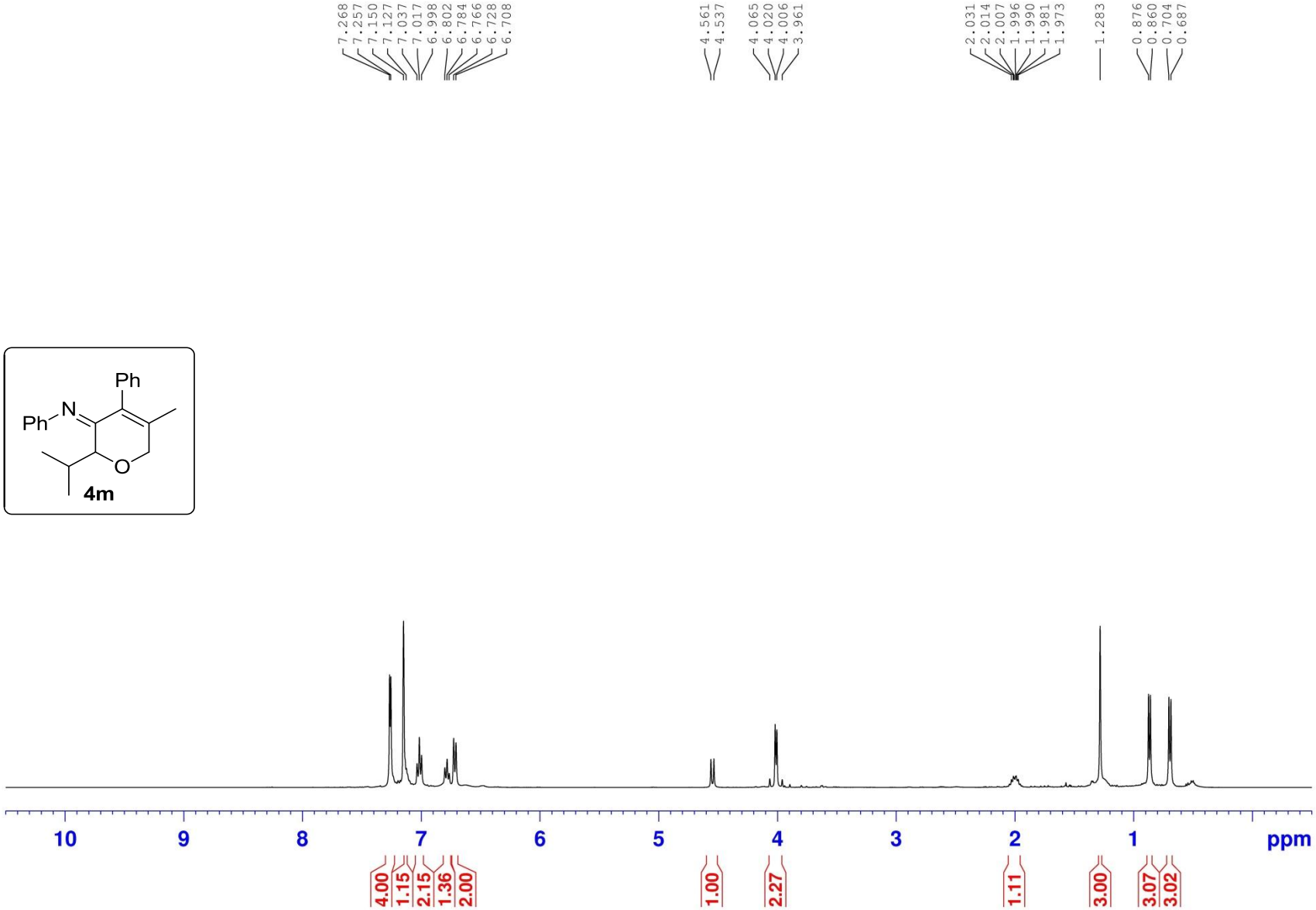
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1.990
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Ph
N
O
4m
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6
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2
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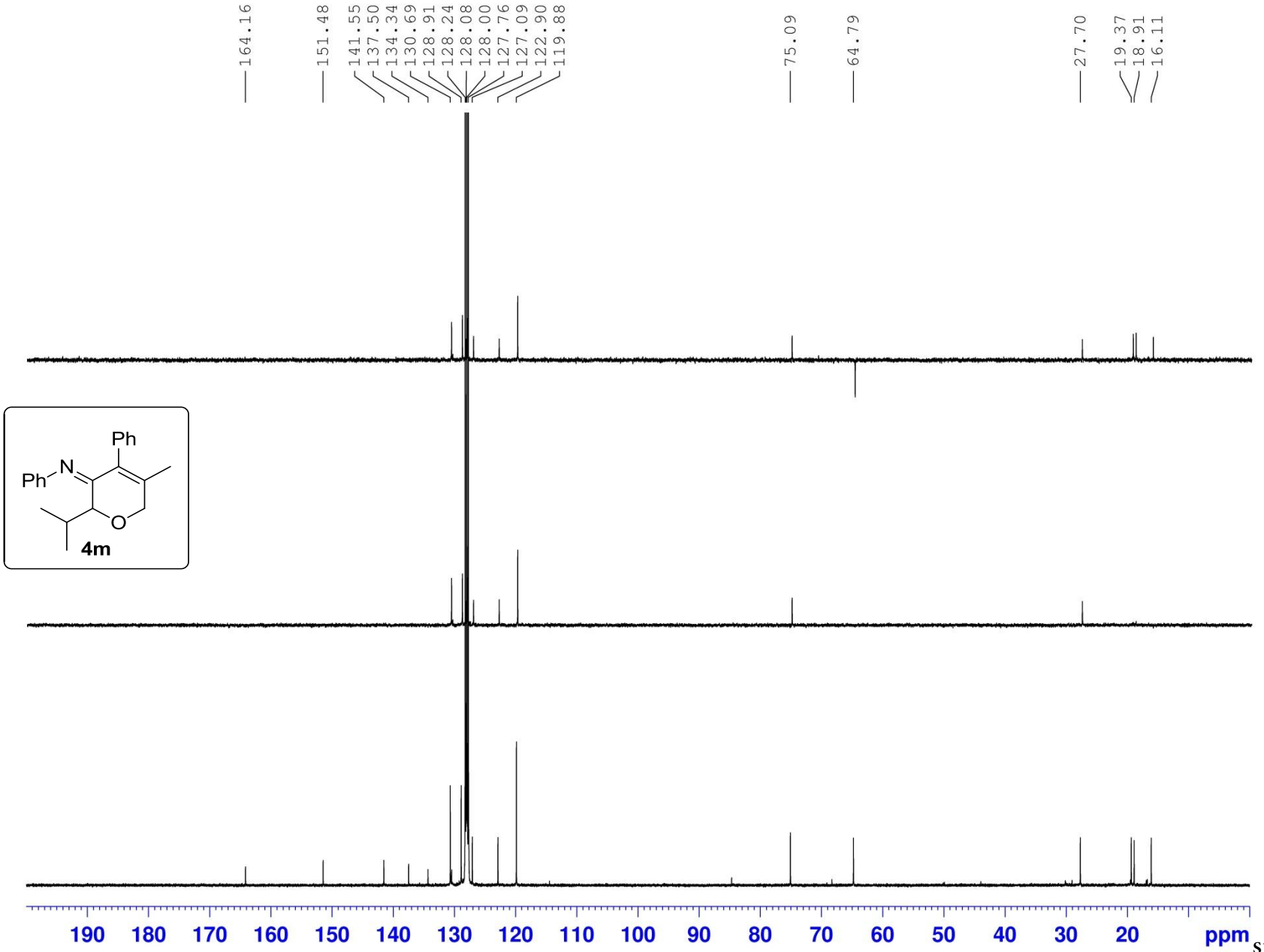
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Ph
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N
O
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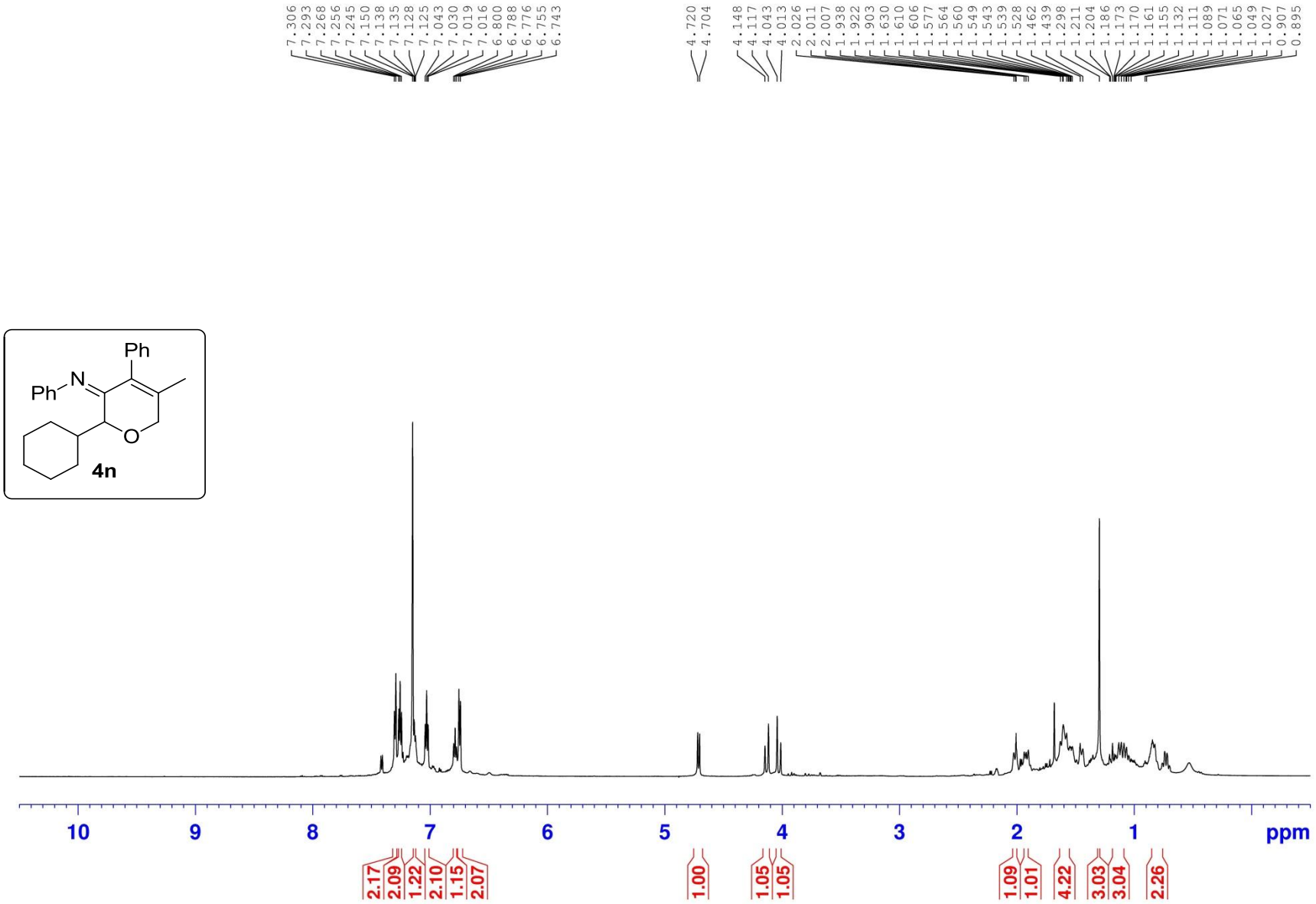
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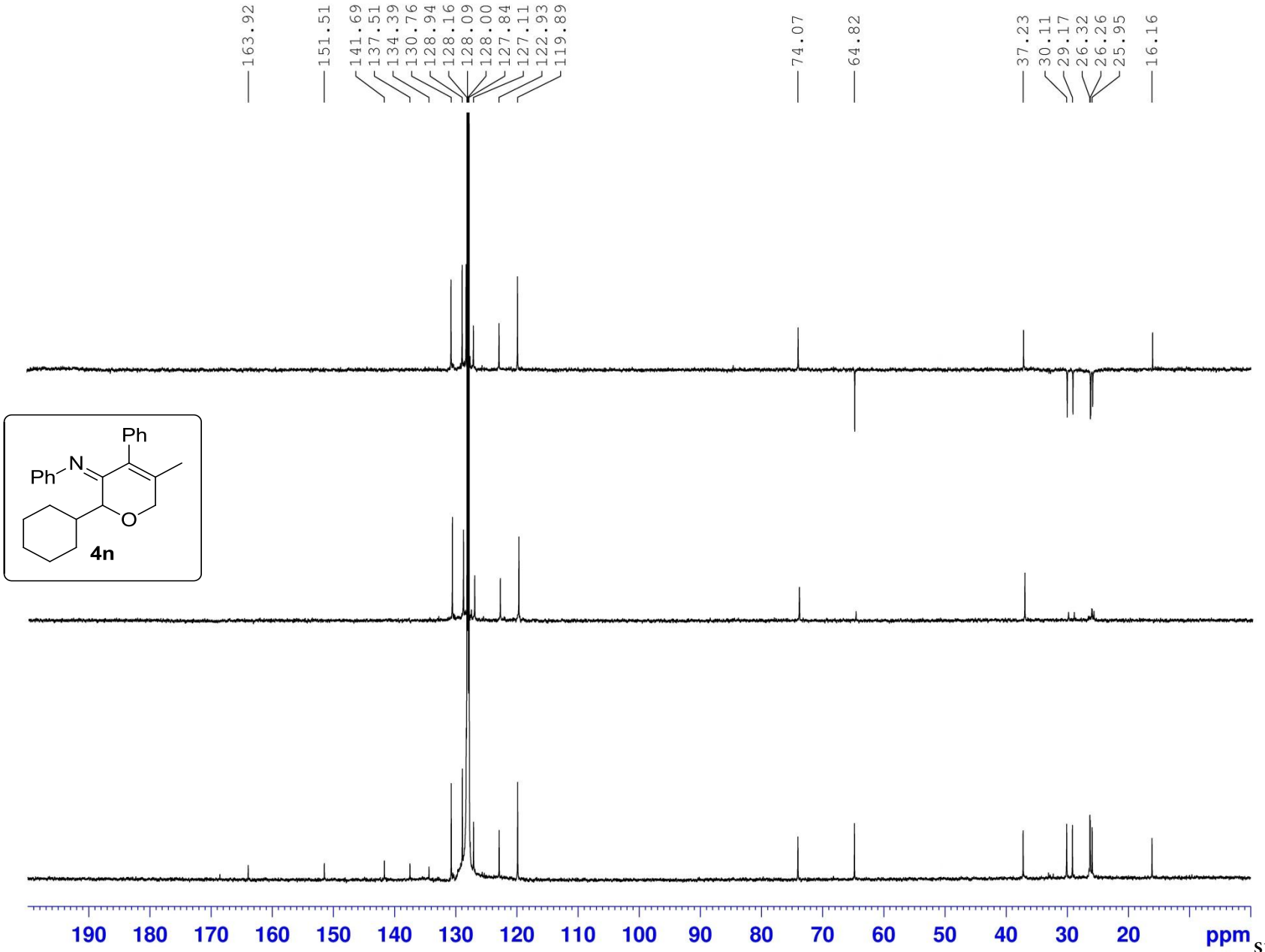
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127.11
122.93
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74.07
64.82
37.23
30.11
29.17
26.32
26.26
25.95
16.16
Ph
N
Ph
O
4n
190
180
170
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30
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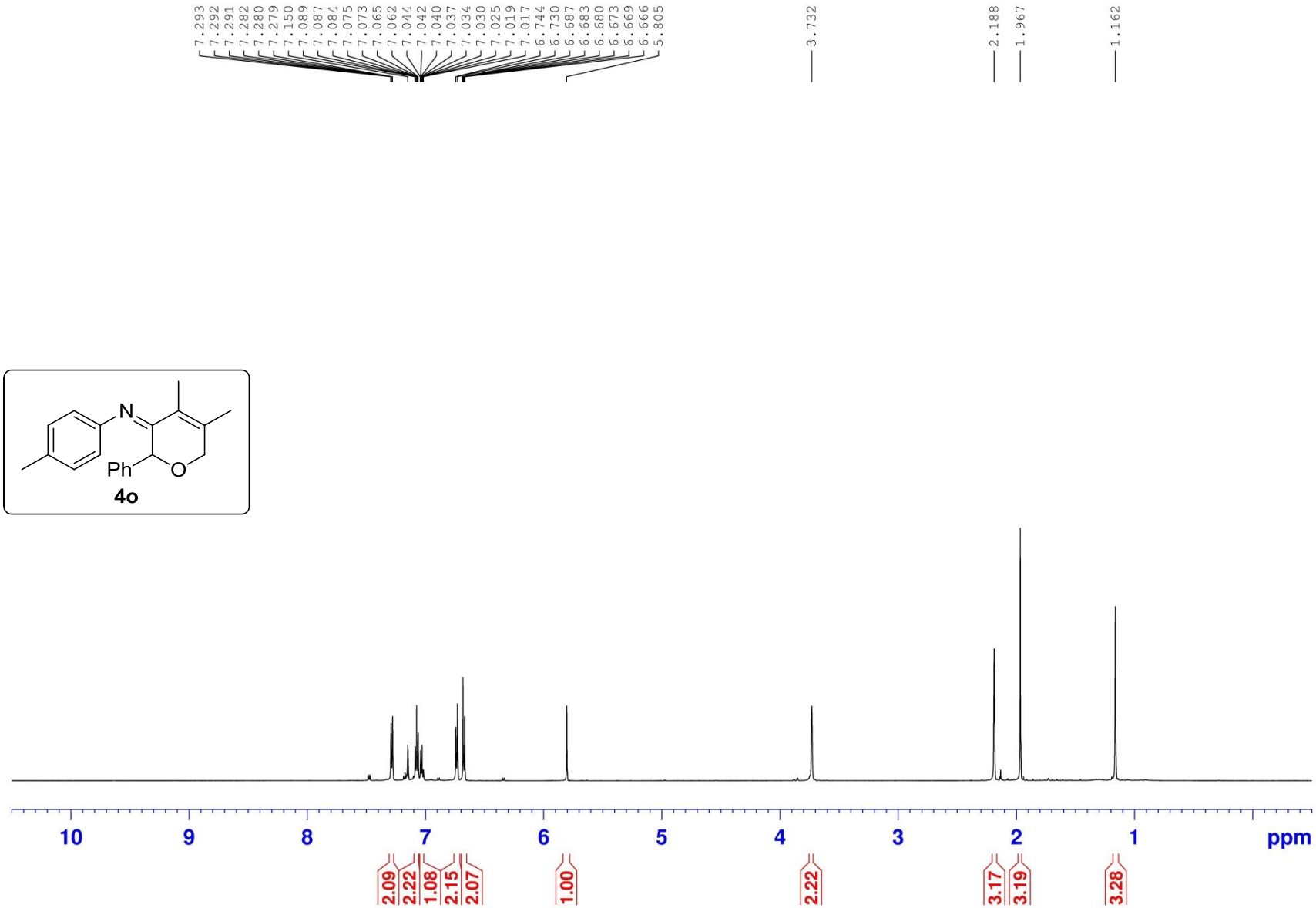
ppm

N
Ph
O
4o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7.044
7.042
7.040
7.037
7.034
7.030
7.025
7.019
7.017
6.744
6.730
6.687
6.683
6.680
6.673
6.669
6.666
5.805
3.732
2.188
1.967
1.162
10
9
8
7
6
5
4
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2.22
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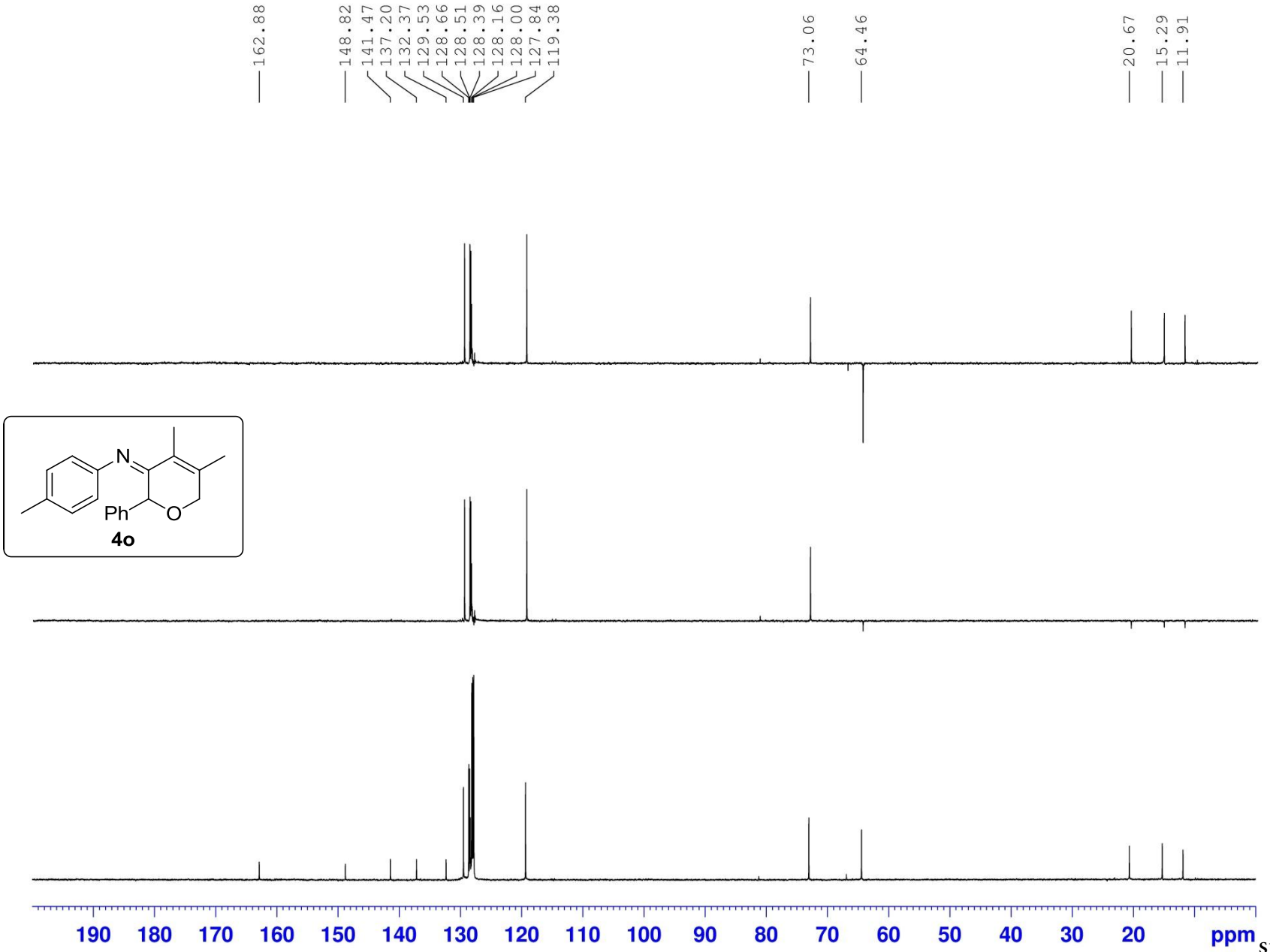
3.28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119.38
73.06
64.46
20.67
15.29
11.91
N
Ph
O
4o
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150
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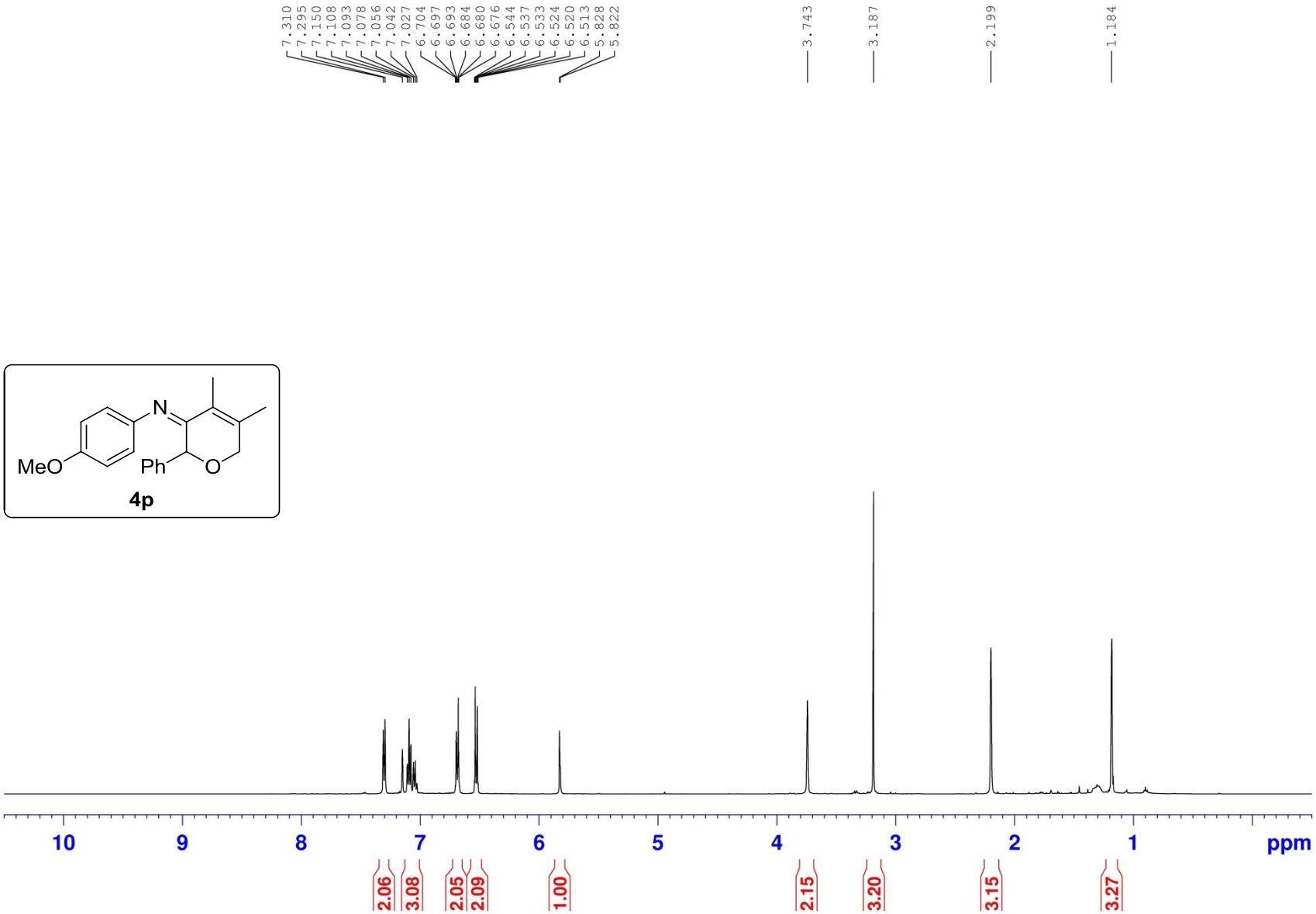
20
ppm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7.042
7.027
6.704
6.697
6.693
6.684
6.680
6.676
6.544
6.537
6.533
6.524
6.520
6.513
5.828
5.822
3.743
3.187
2.199
1.184
N
MeO
Ph
O
4p
10
9
8
7
6
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ppm
2.06
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2.05
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1.00
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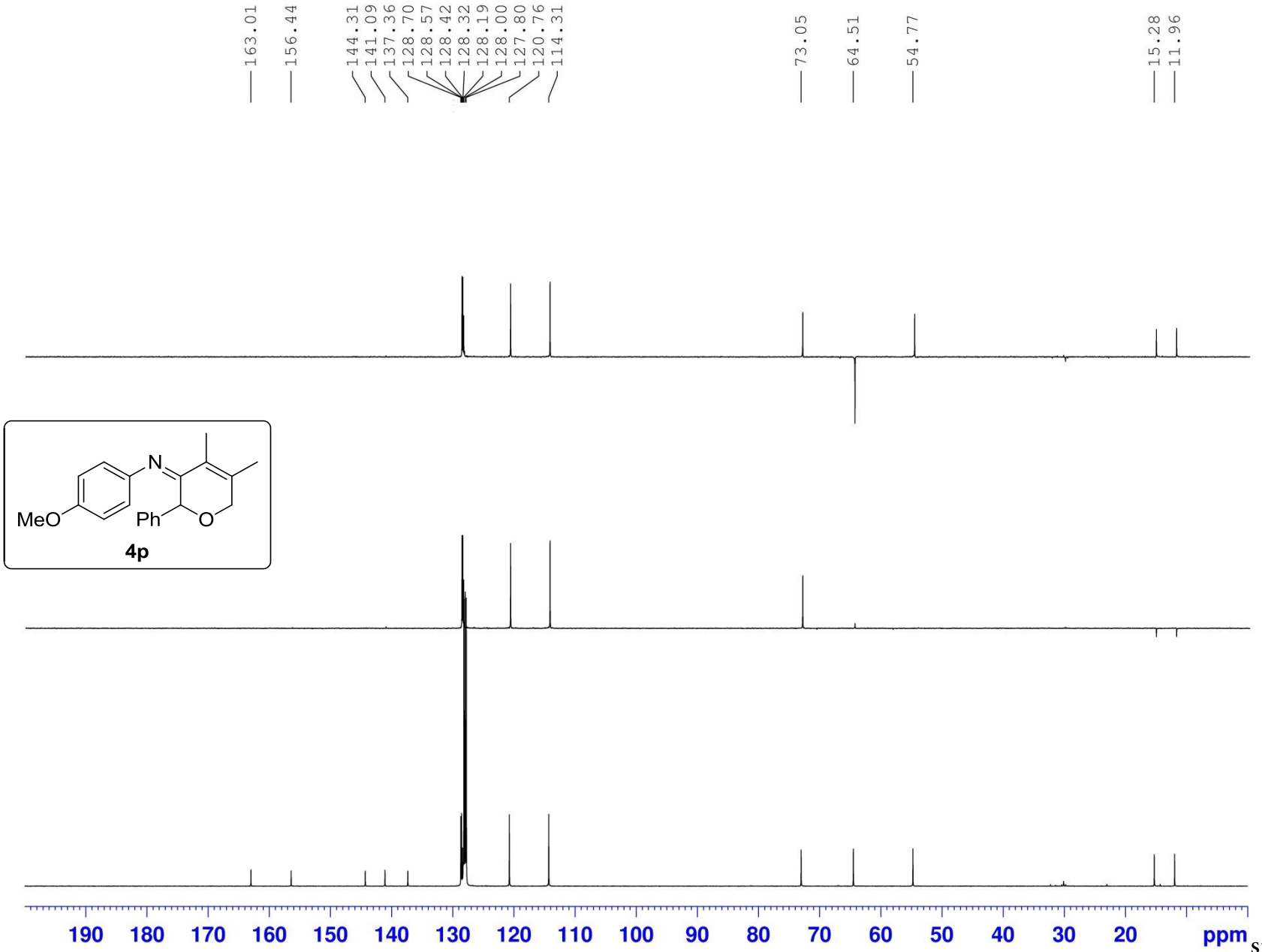
3.27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127.80
120.76
114.31
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11.96
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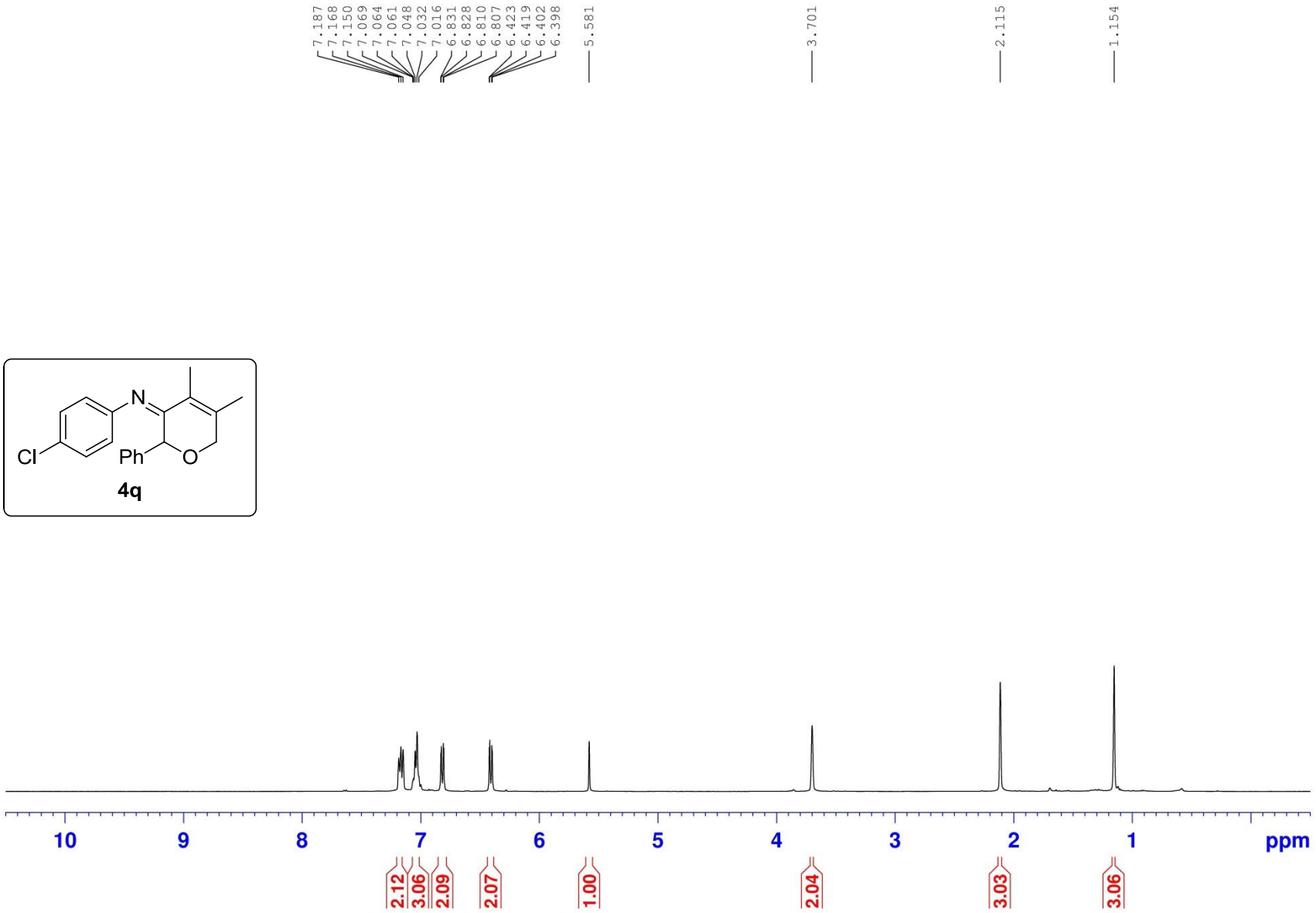
MeO
Ph
O
4p
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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7.069
7.064
7.061
7.048
7.032
7.016
6.831
6.828
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6.807
6.423
6.419
6.402
6.398
5.581
3.701
2.115
1.154
N
Cl
Ph
O
4q
10
9
8
7
6
5
4
3
2
1
ppm
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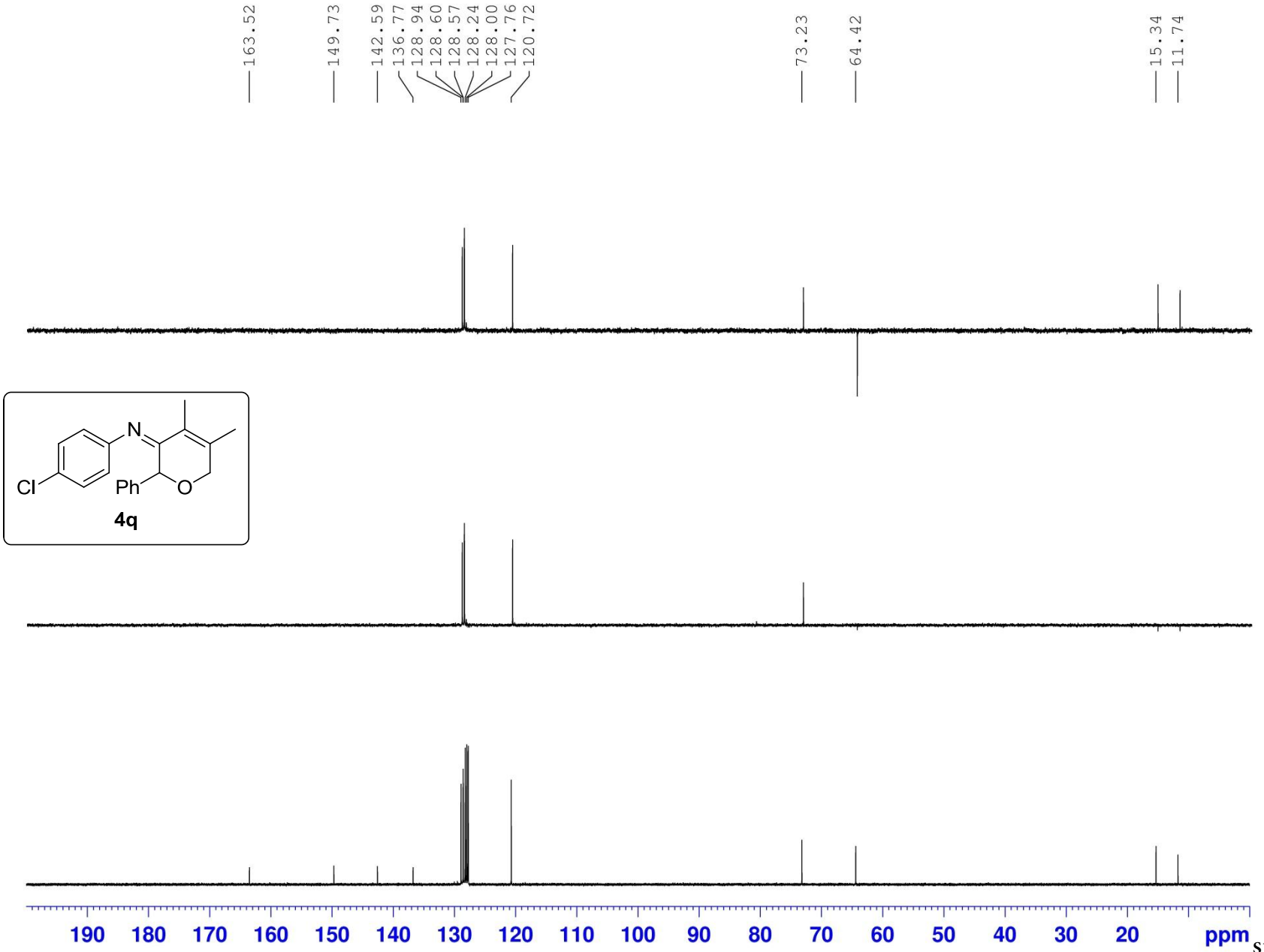
3.06
2.09
2.07
1.00
2.04
3.03
3.06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128.24
128.00
127.76
120.72
73.23
64.42
15.34
11.74
N
Cl
Ph
O
4q
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180
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160
150
140
130
120
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100
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80
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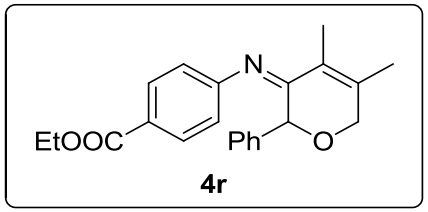
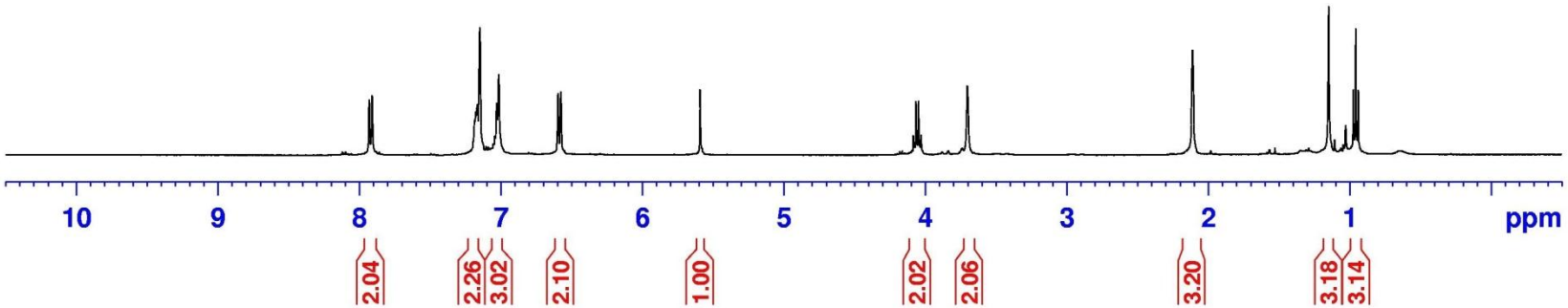
50
40
30
20
ppm


EtOOC
N
Ph
O
4r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7.1768
7.1663
7.1500
7.0421
7.0318
7.0273
7.0191
7.0157
6.5973
6.5773
5.5927
4.0840
4.0663
4.0485
4.0307
3.7032
2.1119
1.1501
0.9766
0.9753
0.9591
0.9576
0.9414
0.9401
10
9
8
7
6
5
4
3
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ppm
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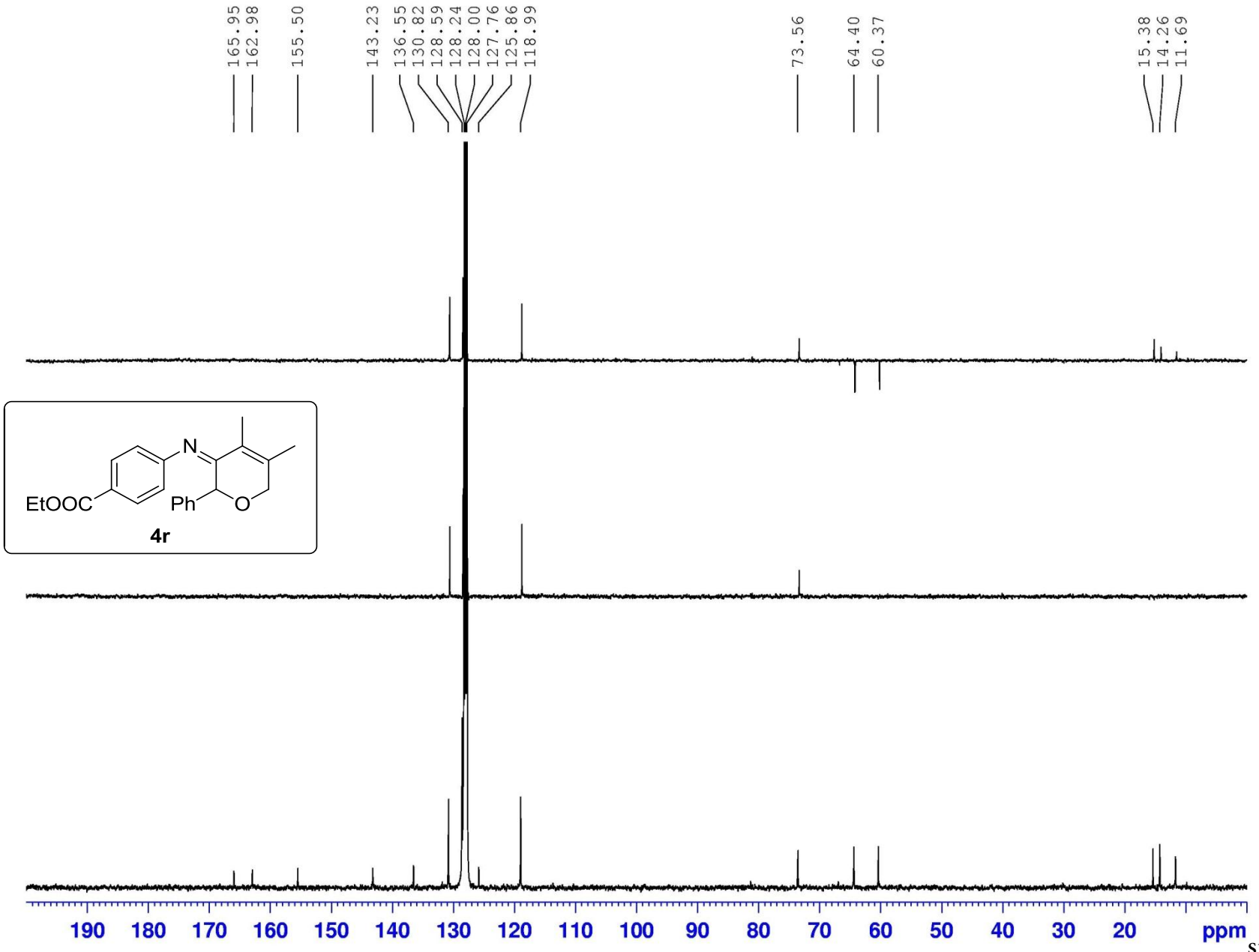
2.26
3.02
2.10
1.00
2.02
2.06
3.20
3.18
3.14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143.23
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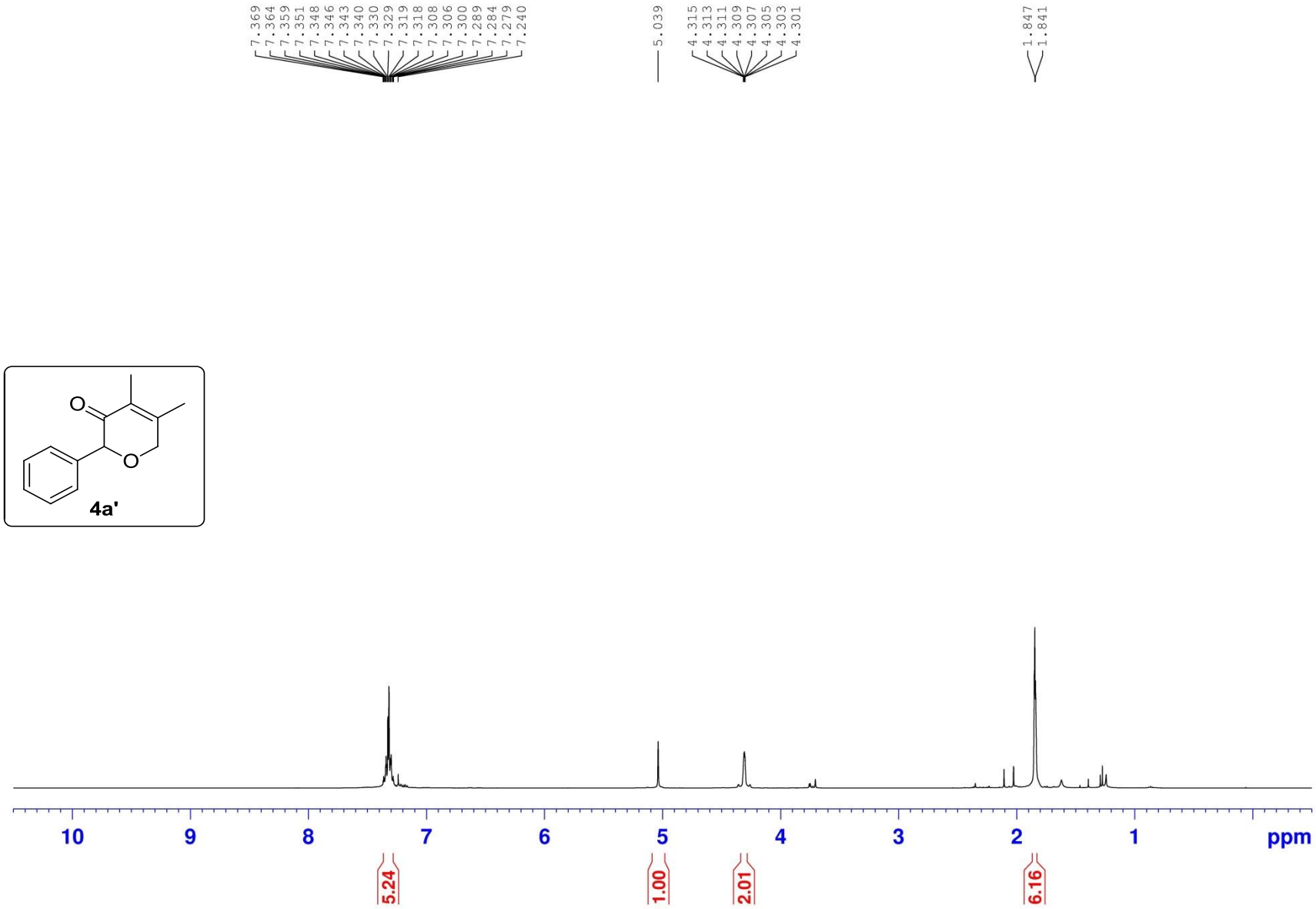
130.82
128.59
128.24
128.00
127.76
125.86
118.99
73.56
64.40
60.37
15.38
14.26
11.69
EtOOC
N
Ph
O
4r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

O
O
4a'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7.359
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7.348
7.346
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7.340
7.330
7.329
7.319
7.318
7.308
7.306
7.300
7.289
7.284
7.279
7.240
5.039
4.315
4.313
4.311
4.309
4.307
4.305
4.303
4.301
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1.841
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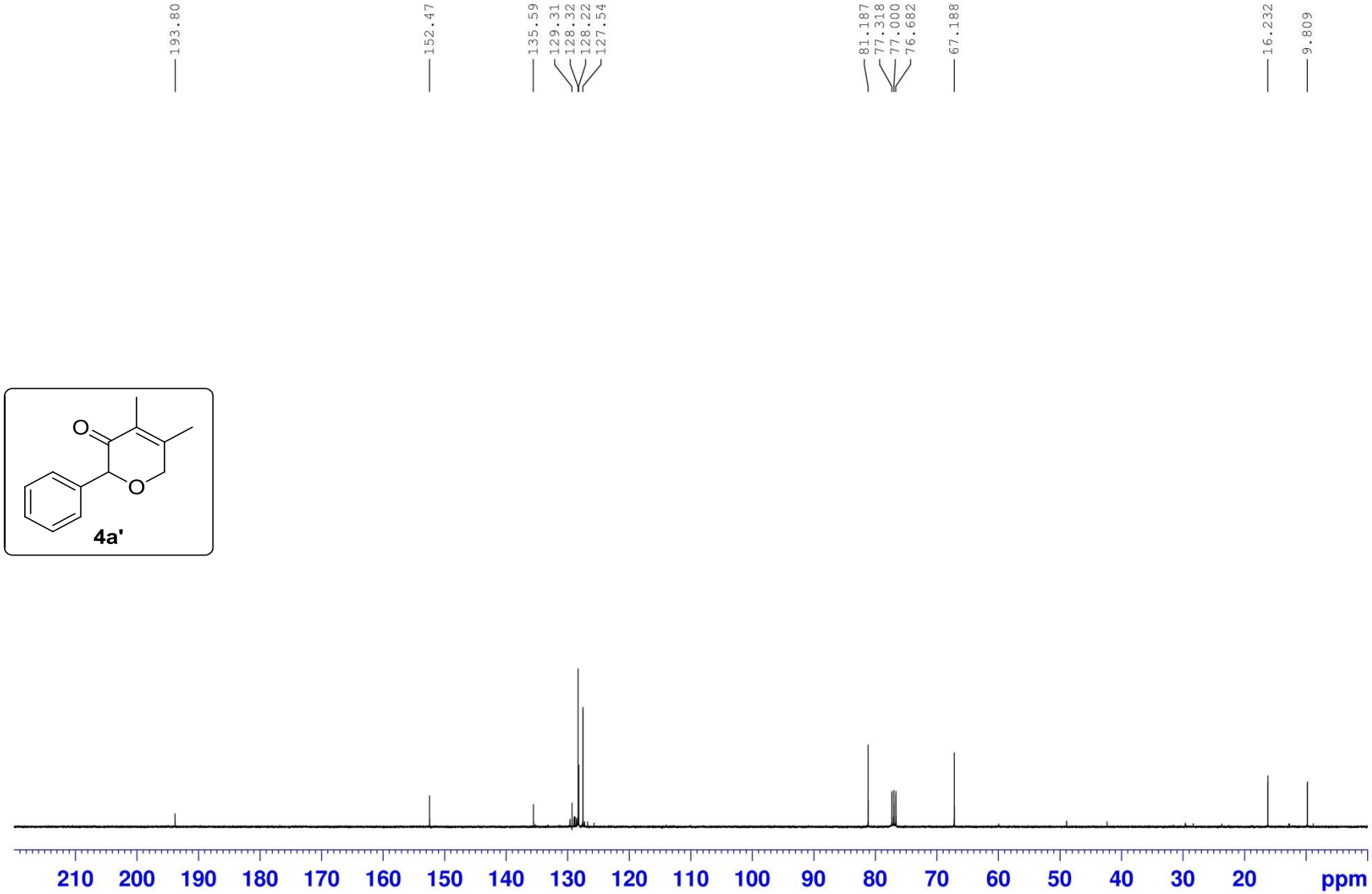
9
8
7
6
5
4
3
2
1
ppm
5.24
1.00
2.01
6.16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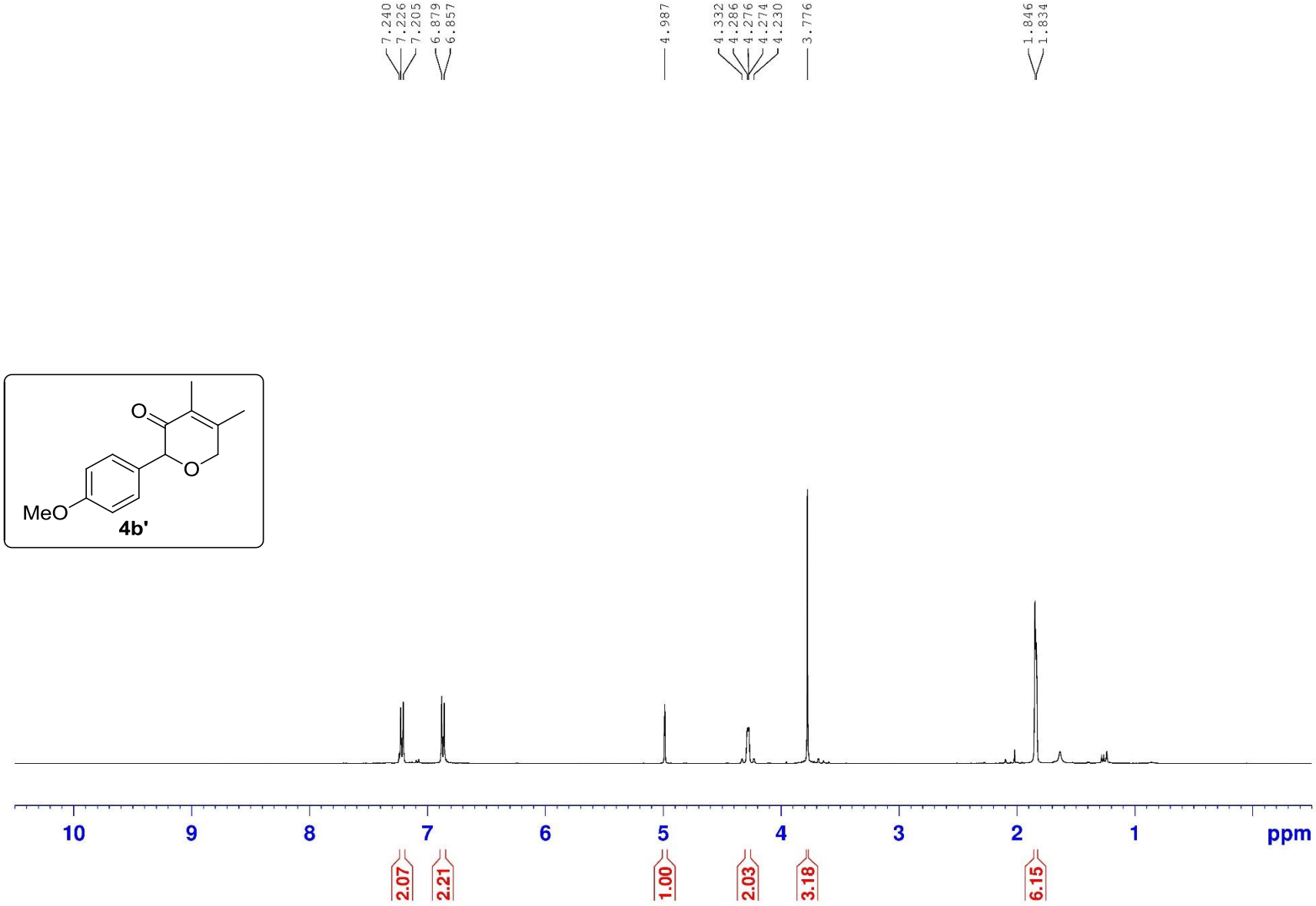
135.59
129.31
128.32
128.22
127.54
81.187
77.318
77.000
76.682
67.188
16.232
9.809
O
O
4a'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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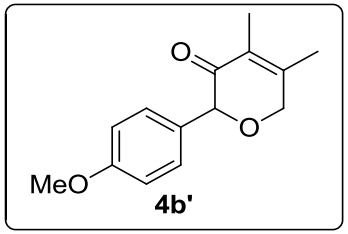
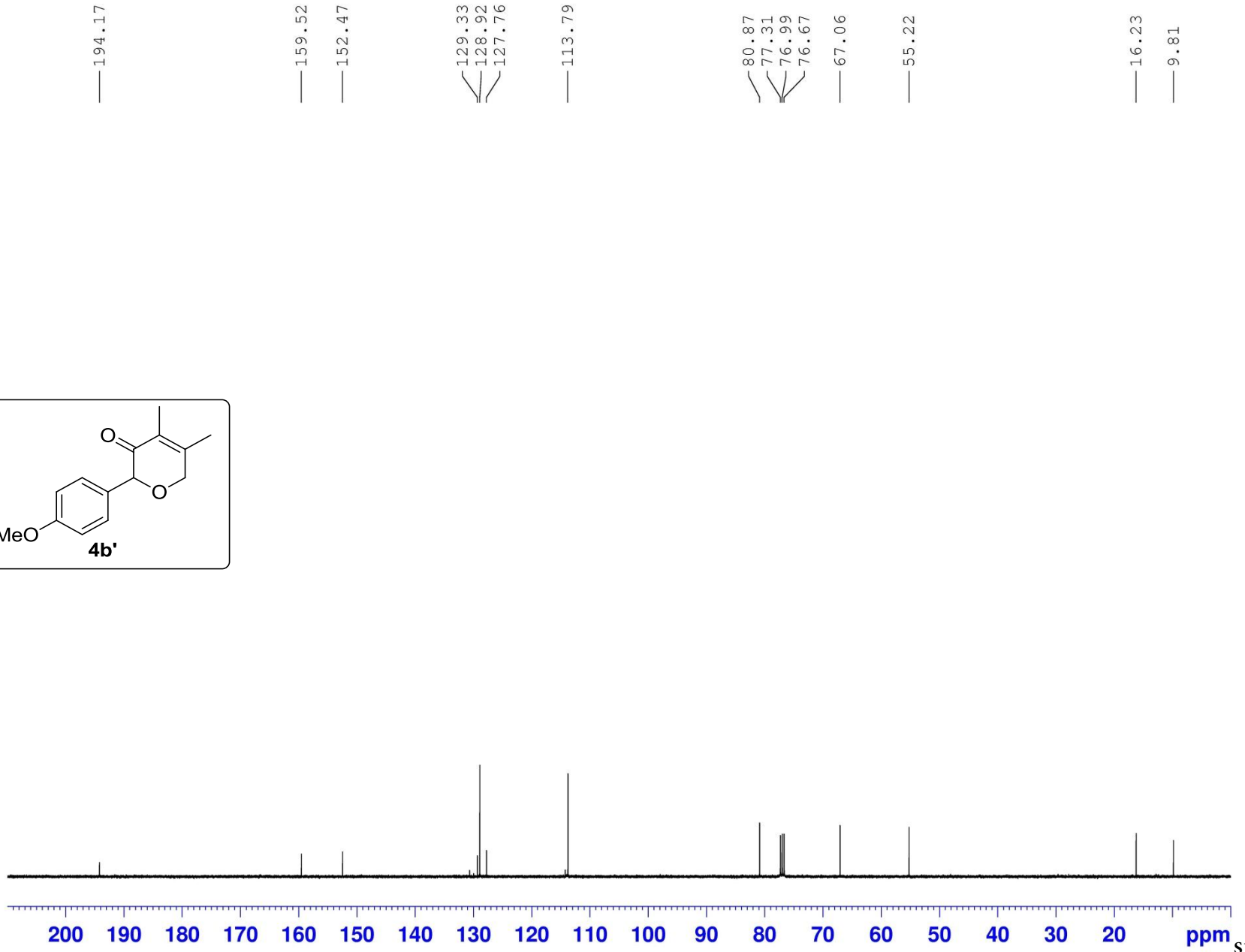
7.226
7.205
6.879
6.857
4.987
4.332
4.286
4.276
4.274
4.230
3.776
1.846
1.834
O
O
MeO
4b'
10
9
8
7
6
5
4
3
2
1
ppm
2.07
2.21
1.00
2.03
3.18
6.15


O
O
MeO
4b'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128.92
127.76
113.79
80.87
77.31
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76.67
67.06
55.22
16.23
9.81
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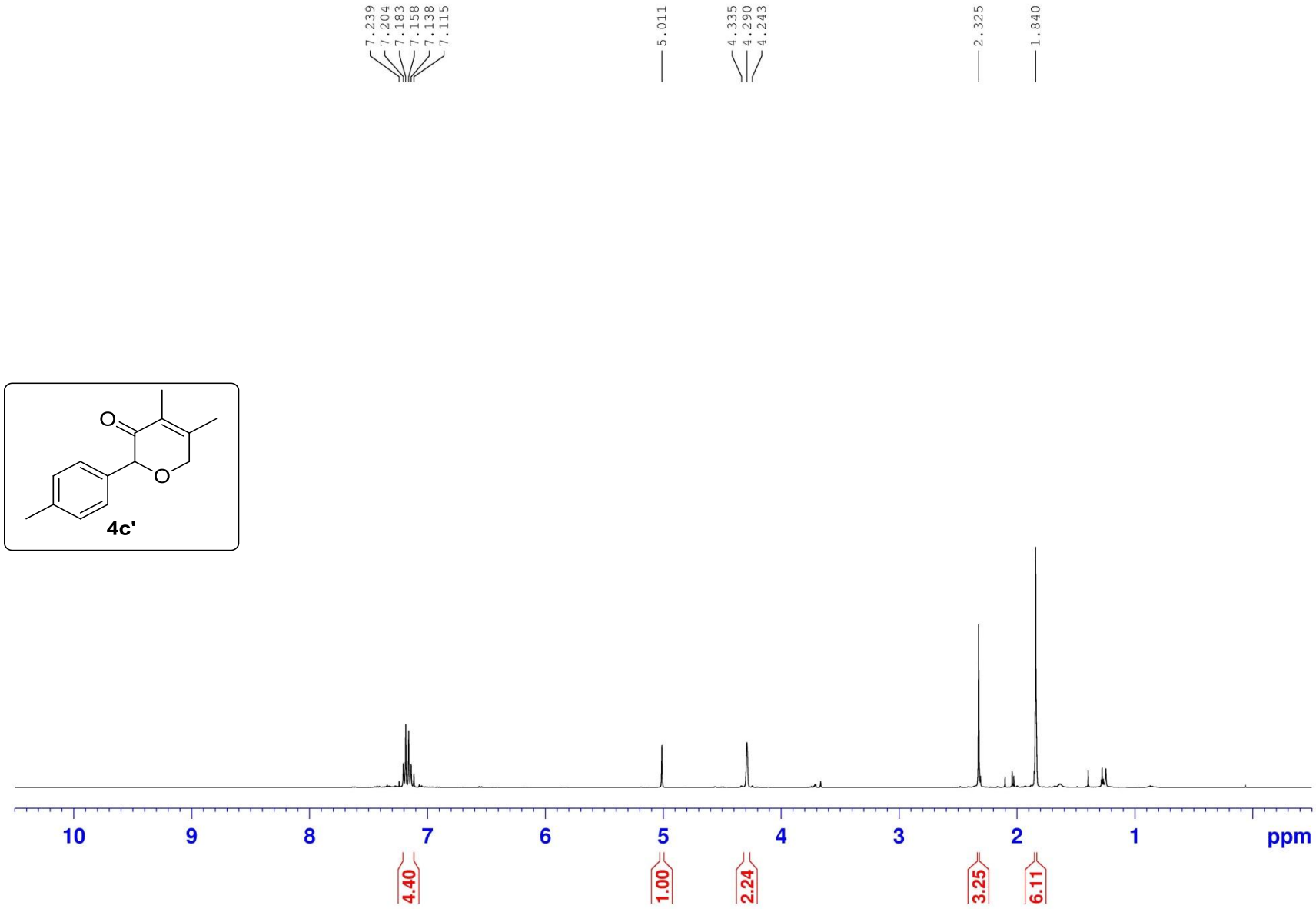
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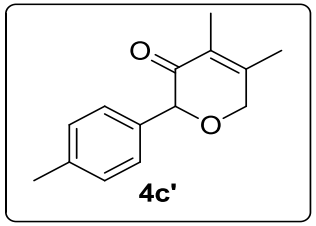
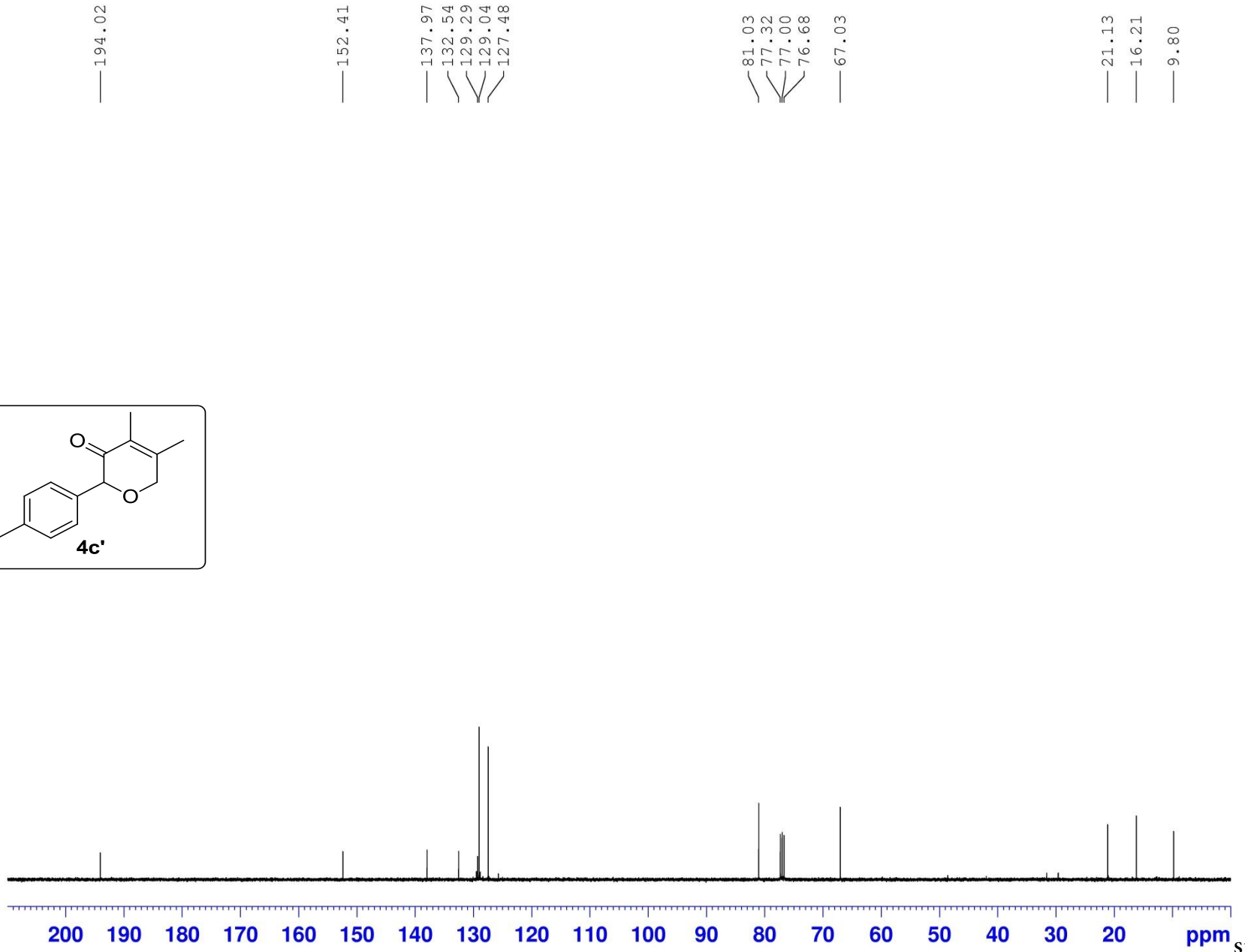
7.204
7.183
7.158
7.138
7.115
5.011
4.335
4.290
4.243
2.325
1.840
O
O
4c'
10
9
8
7
6
5
4
3
2
1
ppm
4.40
1.00
2.24
3.25
6.11


O
O
4c'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76.68
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21.13
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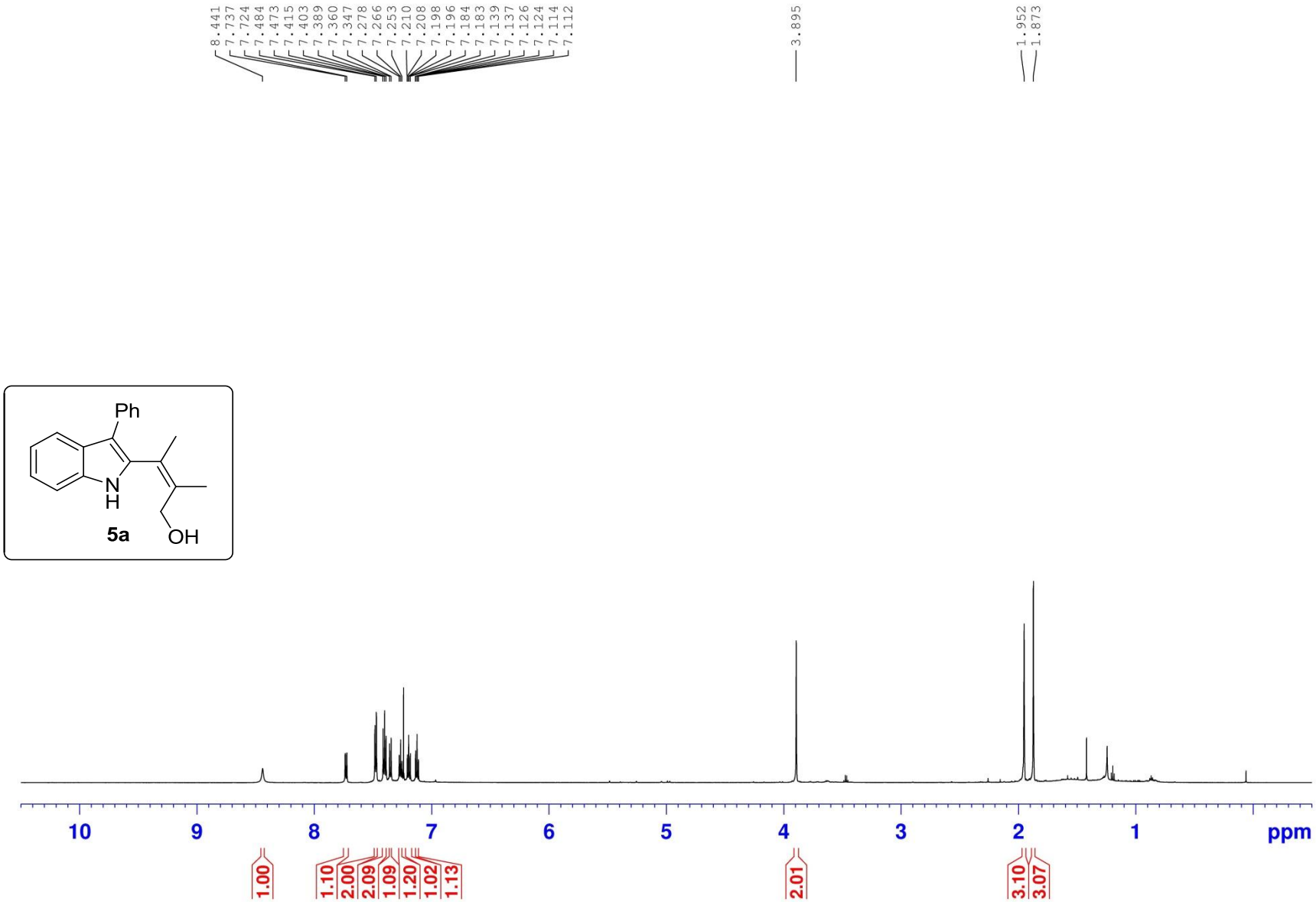
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7.266
7.253
7.210
7.208
7.198
7.196
7.184
7.183
7.139
7.137
7.126
7.124
7.114
7.112
3.895
1.952
1.873
Ph
N
H
OH
5a
10
9
8
7
6
5
4
3
2
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2.00
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1.09
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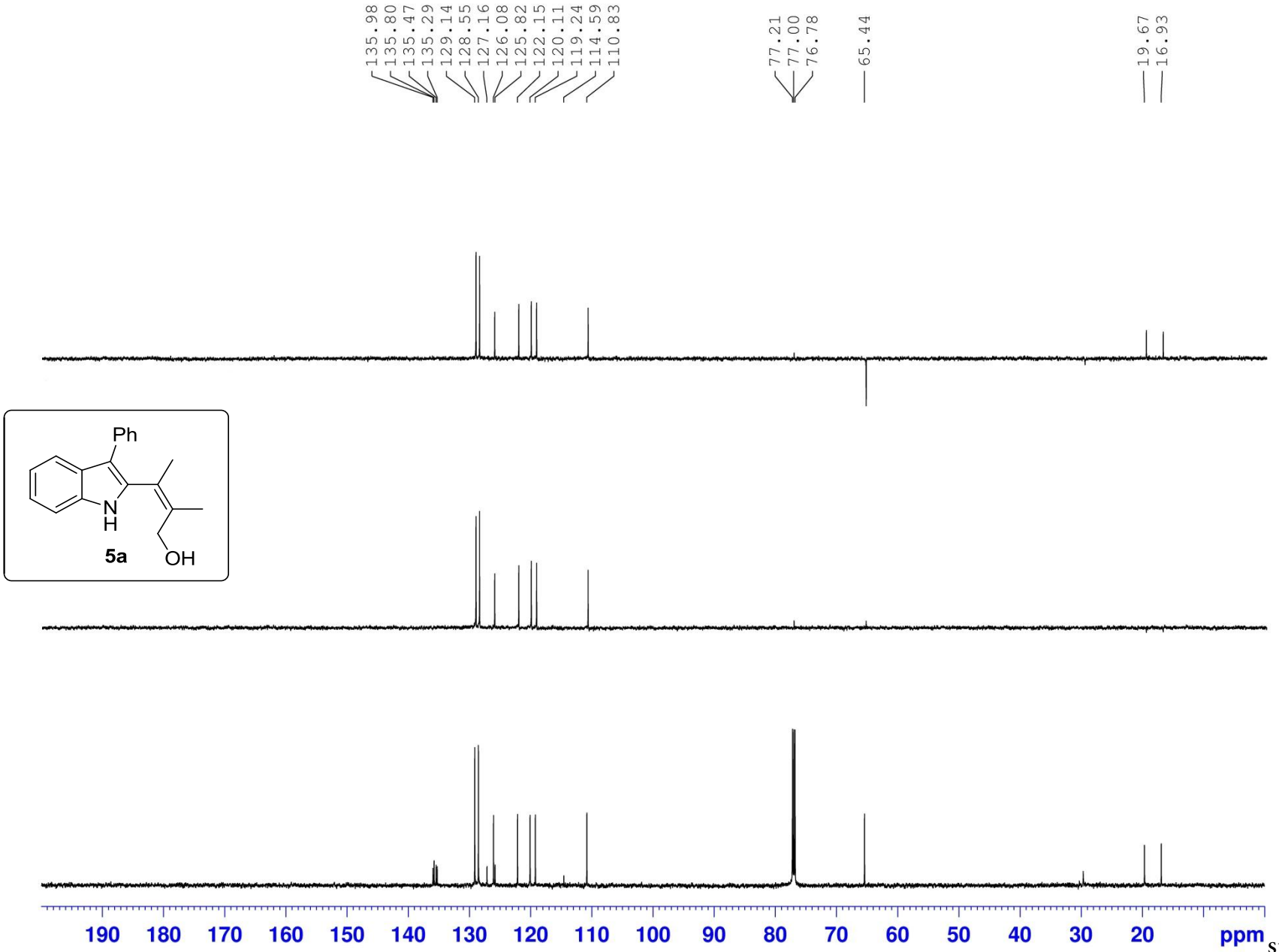
1.02
1.13
2.01
3.10
3.07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126.08
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122.15
120.11
119.24
114.59
110.83
77.21
77.00
76.78
65.44
19.67
16.93
Ph
N
H
5a
OH
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150
140
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120
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80
70
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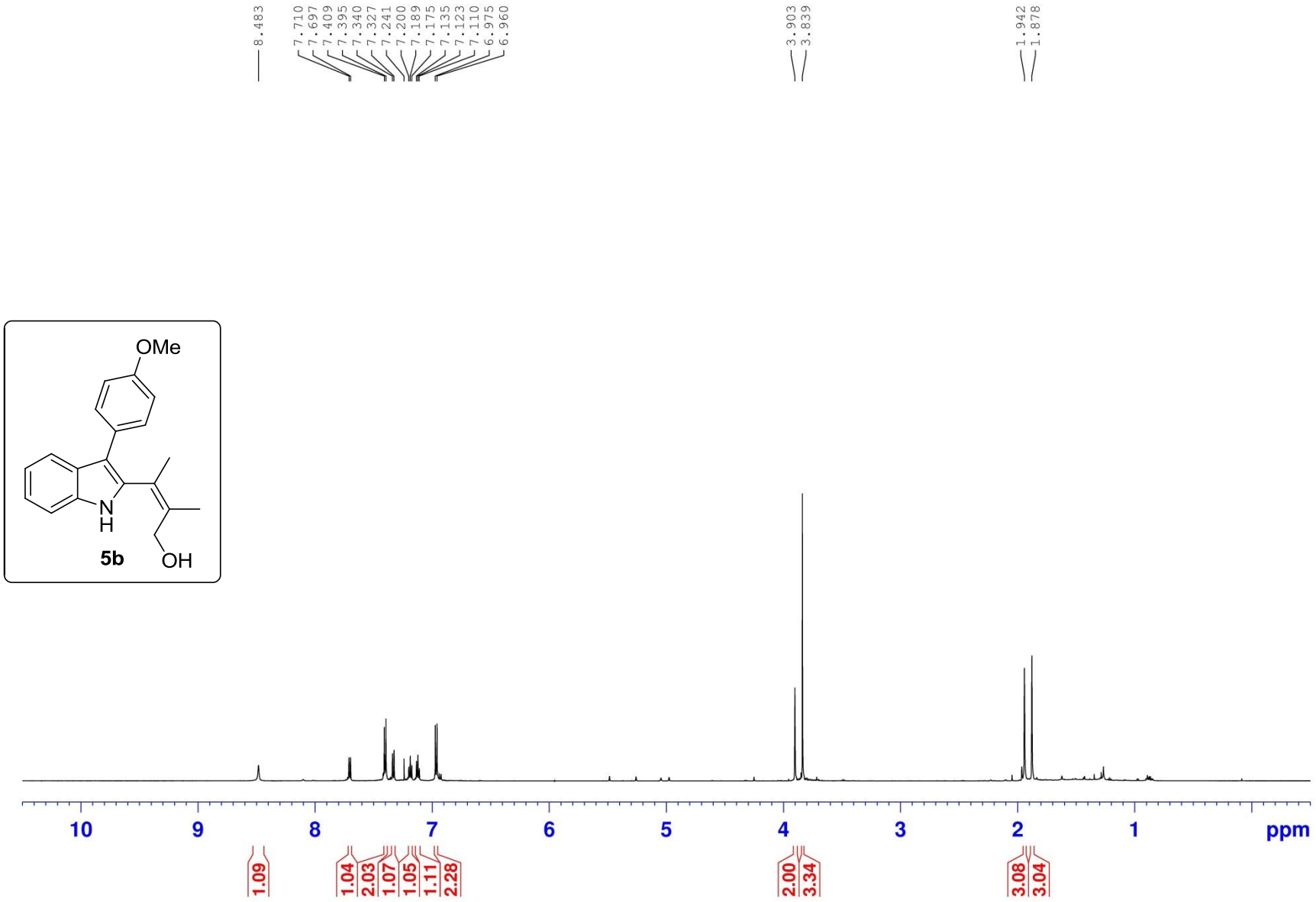
50
40
30
20
ppm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7.189
7.175
7.135
7.123
7.110
6.975
6.960
3.903
3.839
1.942
1.878
OMe
N
H
5b
OH
10
9
8
7
6
5
4
3
2
1
ppm
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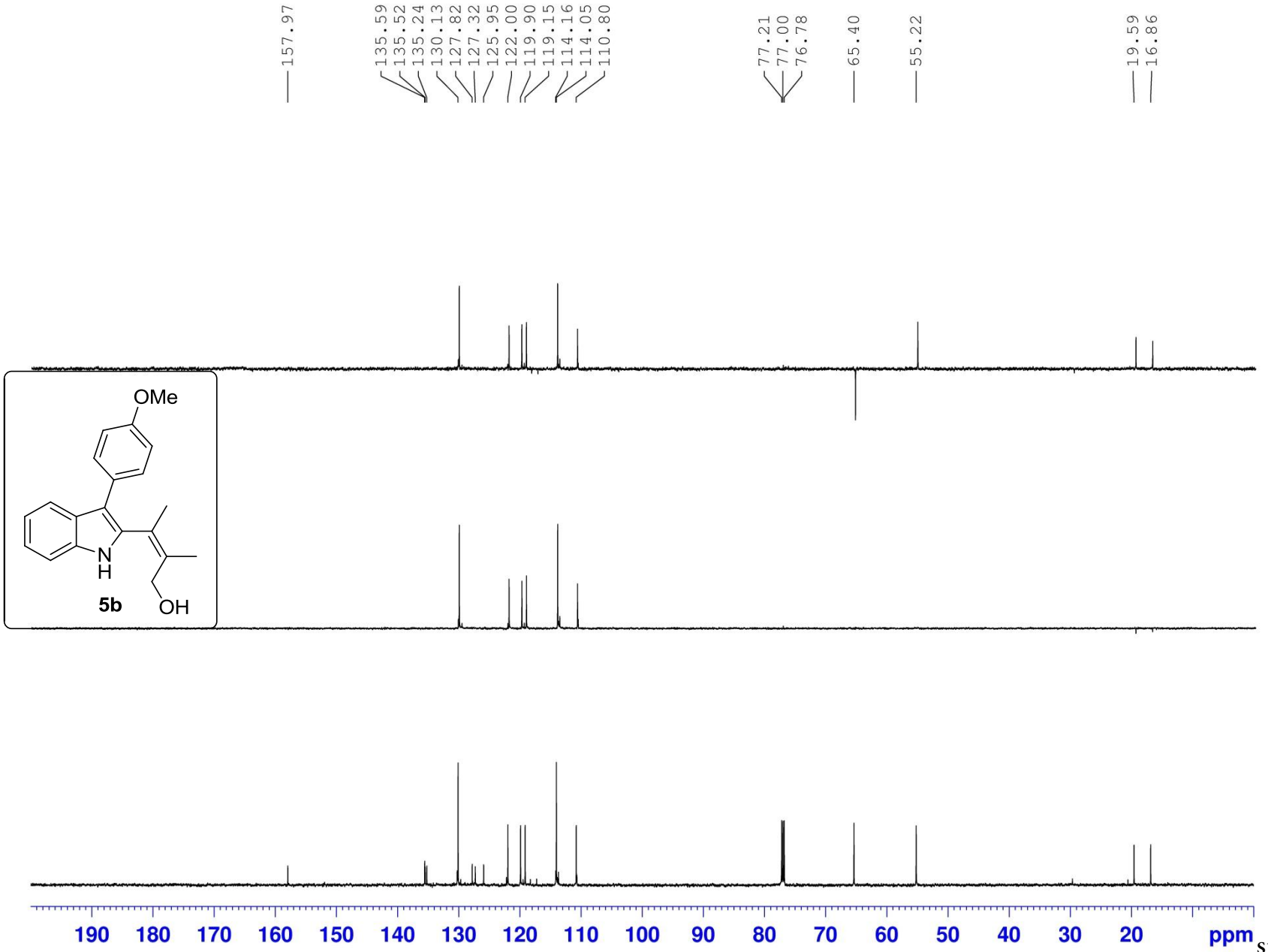
1.04
2.03
1.07
1.05
1.11
2.28
2.00
3.34
3.08
3.04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135.24
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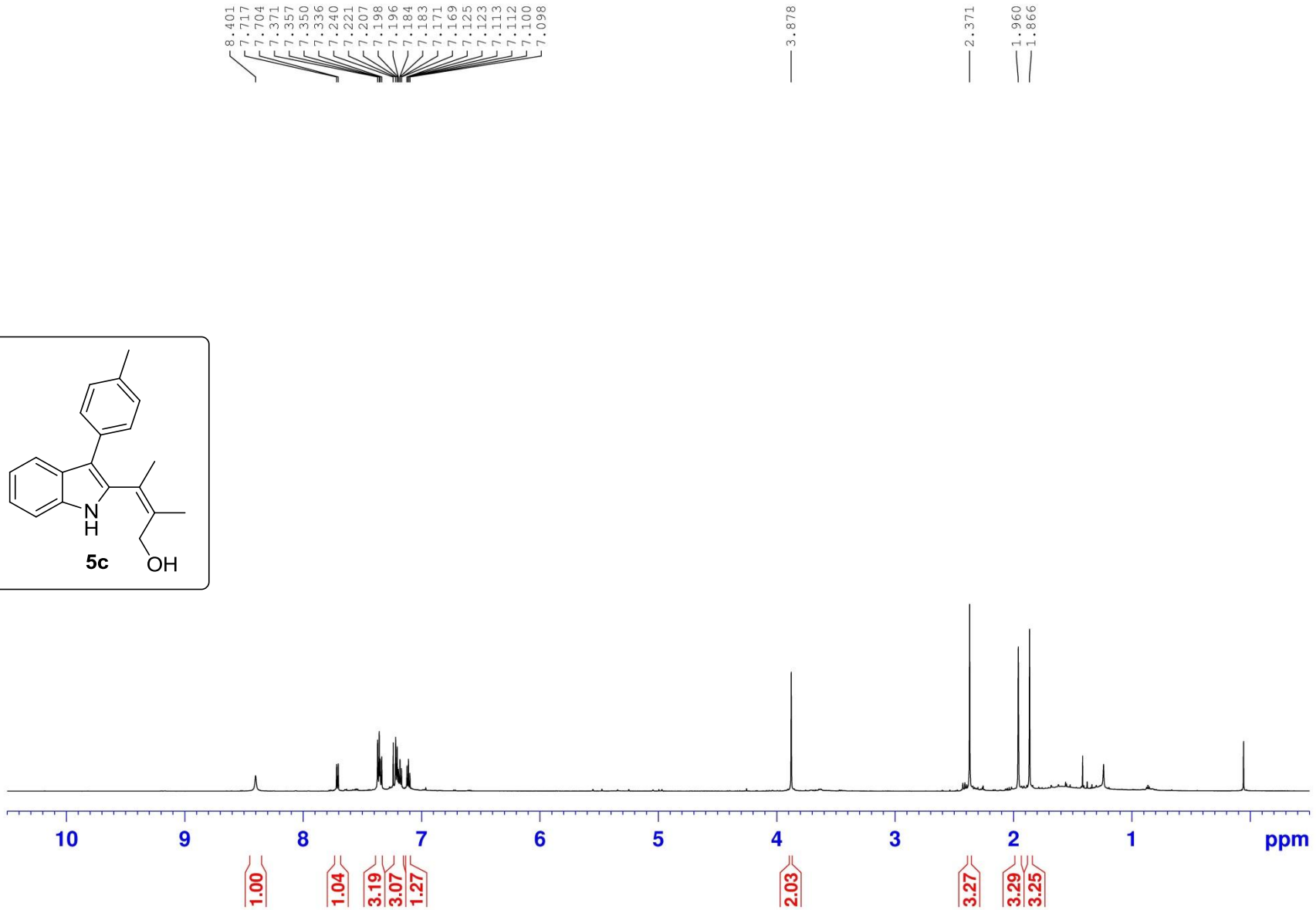
127.82
127.32
125.95
122.00
119.90
119.15
114.16
114.05
110.80
77.21
77.00
76.78
65.40
55.22
19.59
16.86
OMe
N
H
OH
5b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

N
H
OH
5c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7.196
7.184
7.183
7.171
7.169
7.125
7.123
7.113
7.112
7.100
7.098
3.878
2.371
1.960
1.866
10
9
8
7
6
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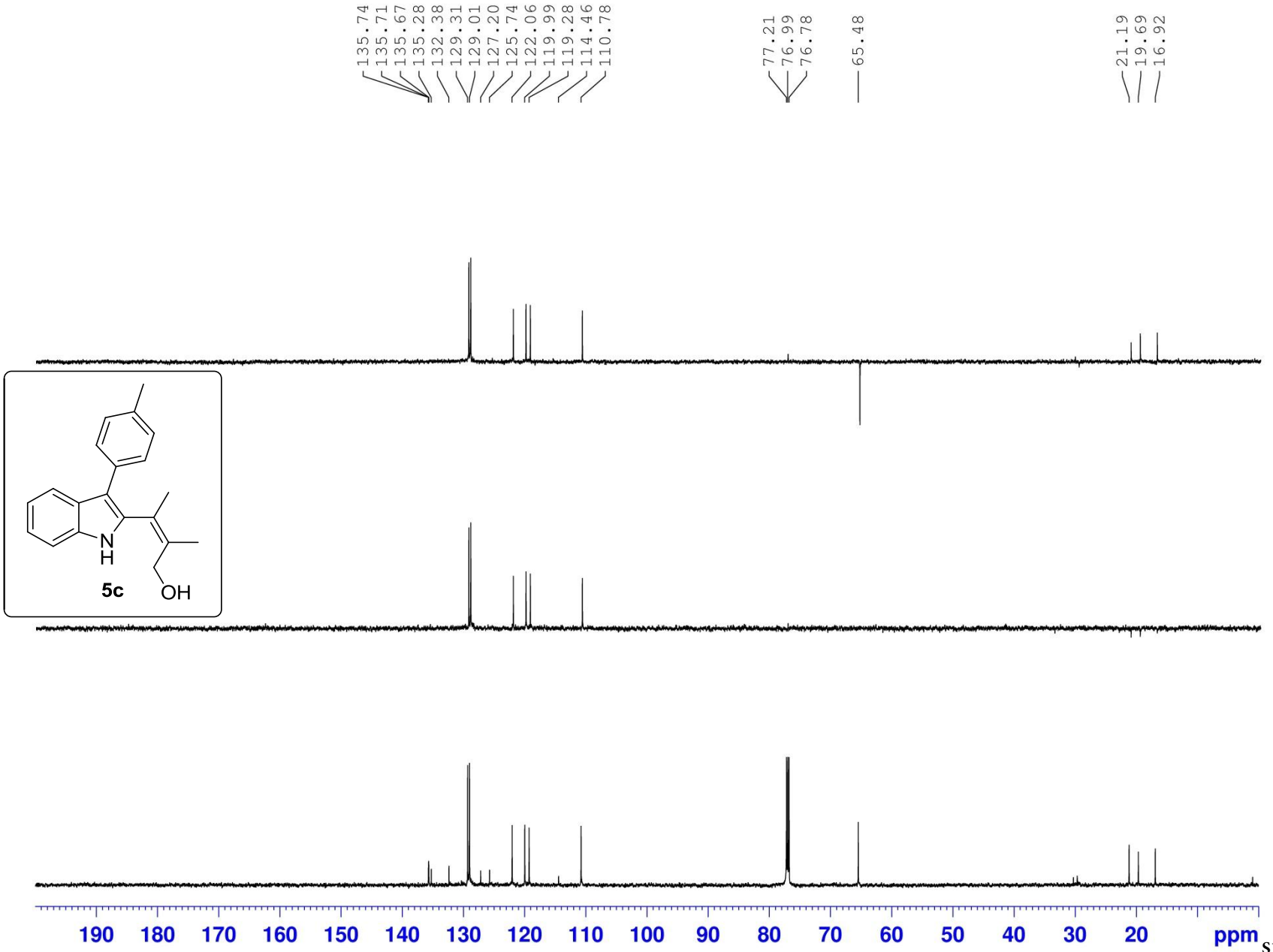
3.25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114.46
110.78
77.21
76.99
76.78
65.48
21.19
19.69
16.92
N
H
OH
5c
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160
150
140
130
120
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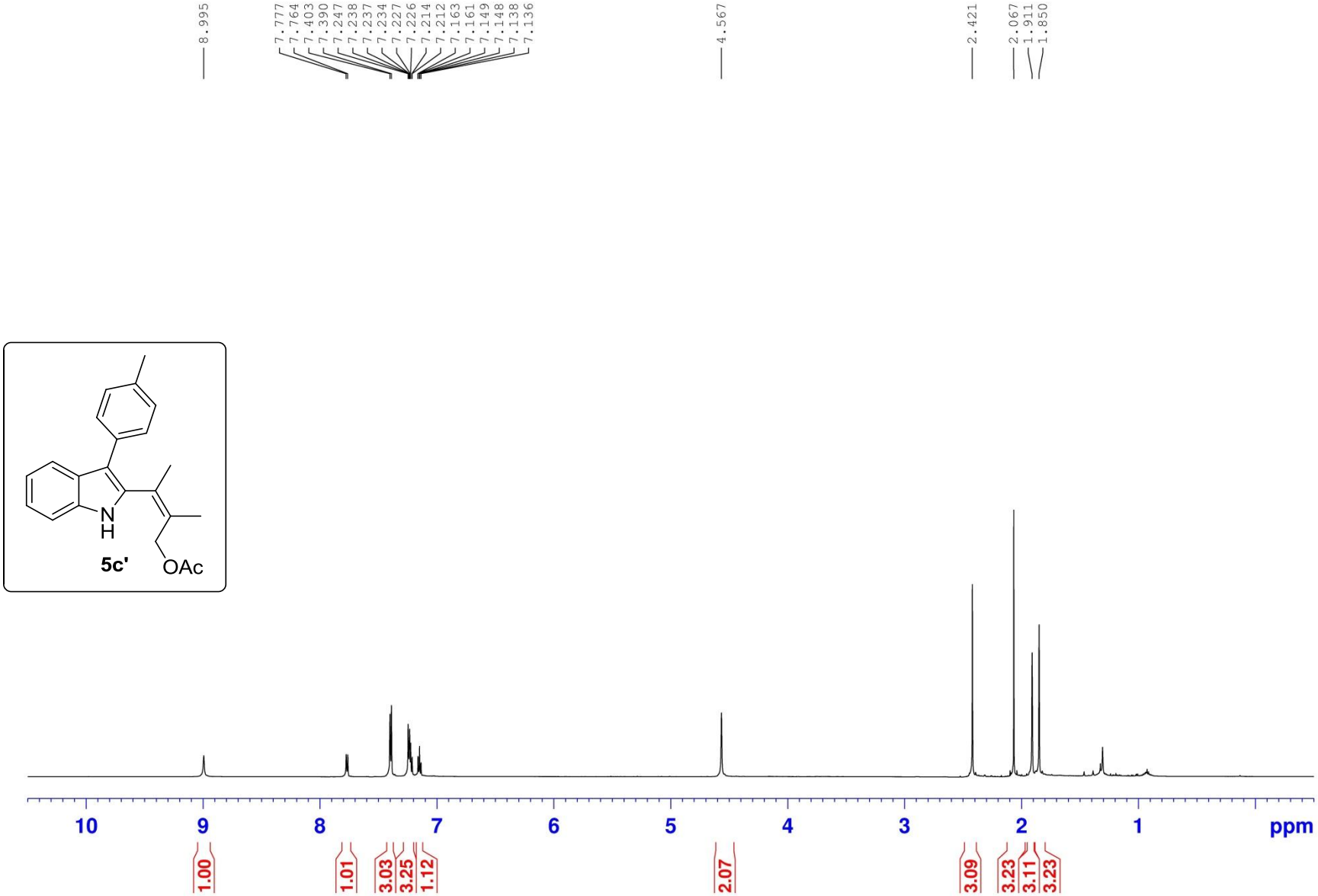
80
70
60
50
40
30
20
ppm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7.238
7.237
7.234
7.227
7.226
7.214
7.212
7.163
7.161
7.149
7.148
7.138
7.136
4.567
2.421
2.067
1.911
1.850
N
H
5c'
OAc
10
9
8
7
6
5
4
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1.01
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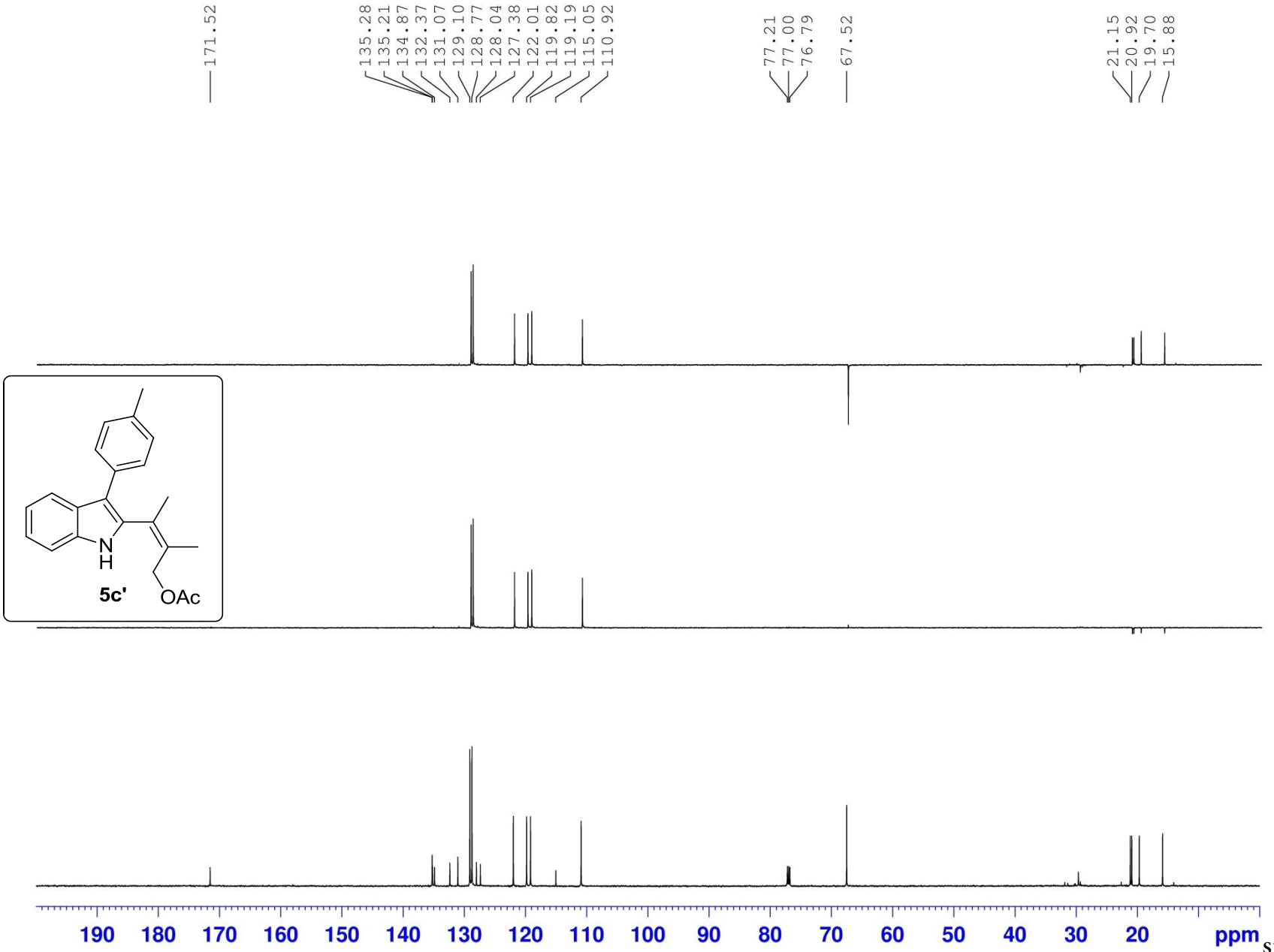
3.25
1.12
2.07
3.09
3.23
3.11
3.23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119.19
115.05
110.92
77.21
77.00
76.79
67.52
21.15
20.92
19.70
15.88
N
H
5c'
OAc
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180
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160
150
140
130
120
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100
90
80
70
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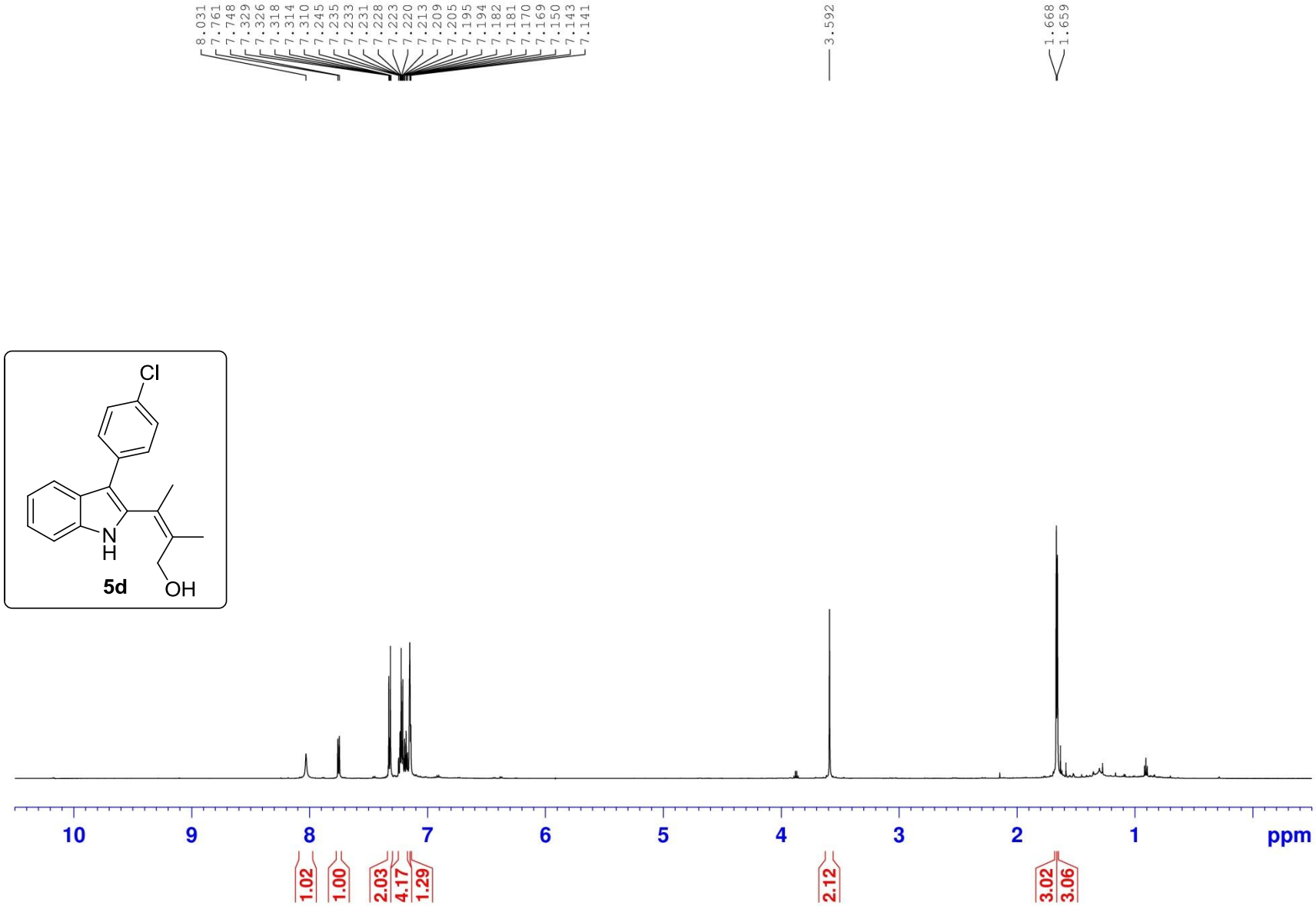
40
30
20
ppm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7.310
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7.235
7.233
7.231
7.228
7.223
7.220
7.213
7.209
7.205
7.195
7.194
7.182
7.181
7.170
7.169
7.150
7.143
7.141
3.592
1.668
1.659
Cl
N
H
OH
5d
10
9
8
7
6
5
4
3
2
1
ppm
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4.17
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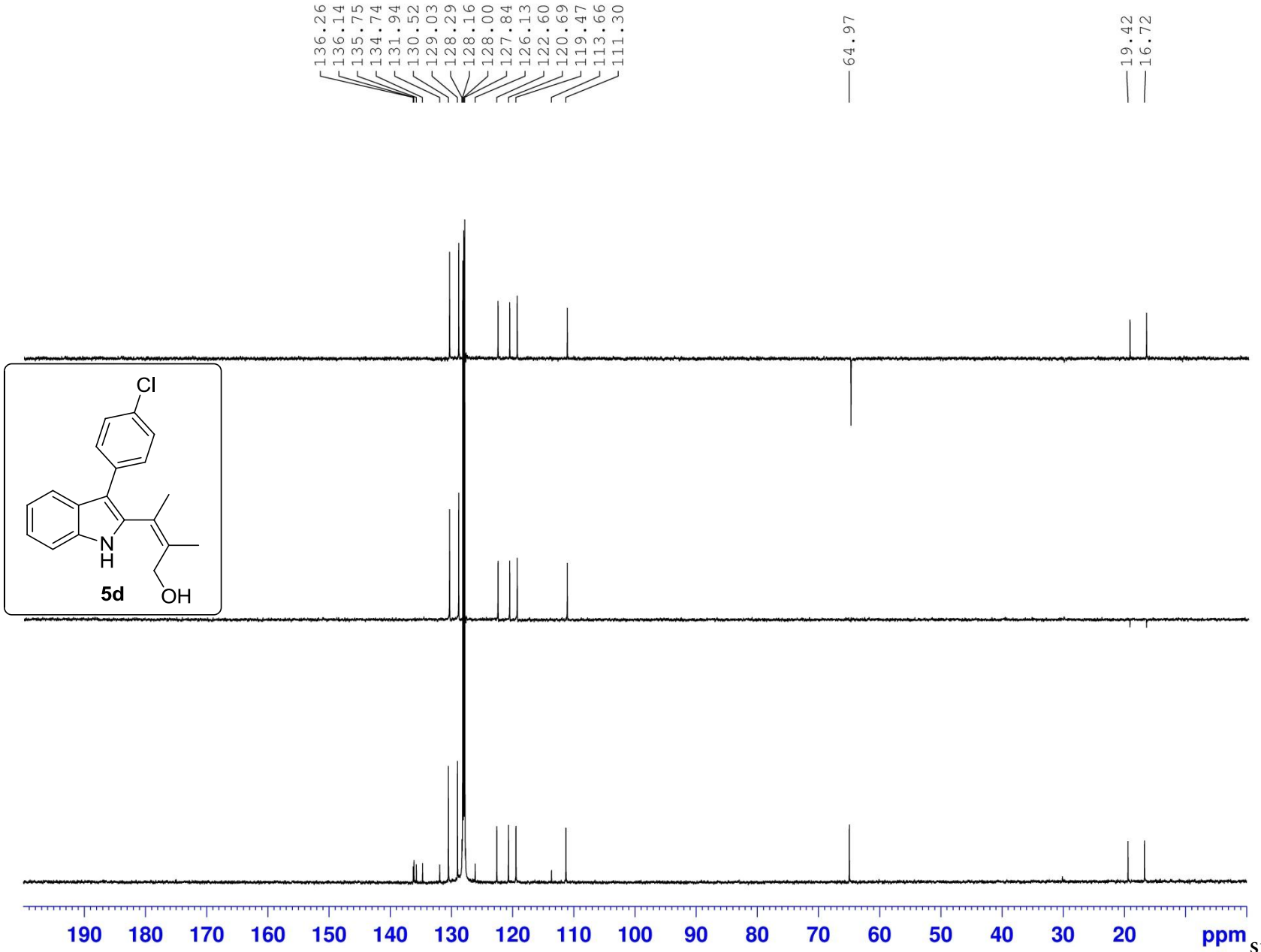
2.12
3.02
3.06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134.74
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126.13
122.60
120.69
119.47
113.66
111.30
64.97
19.42
16.72
Cl
N
H
OH
5d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
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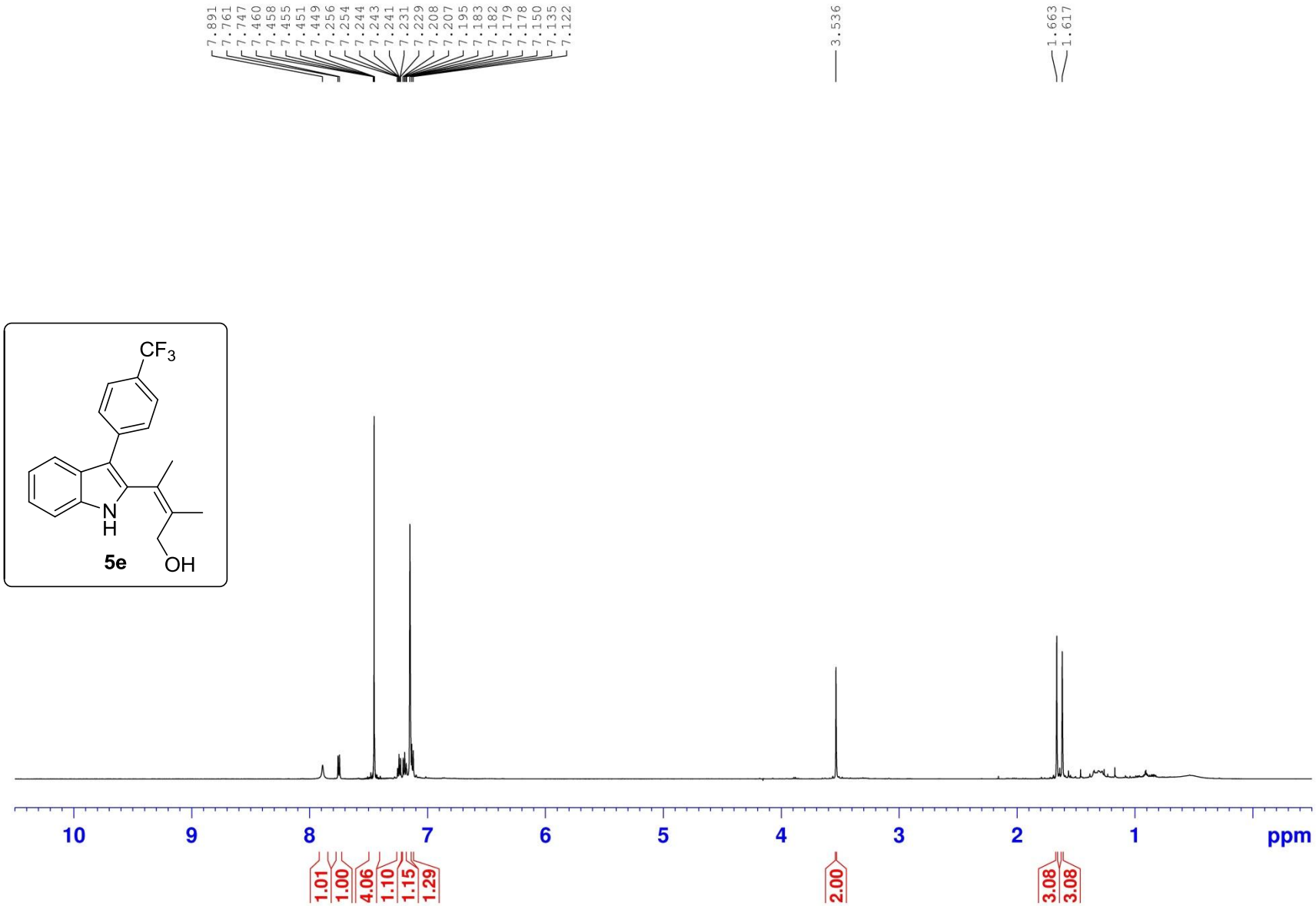
ppm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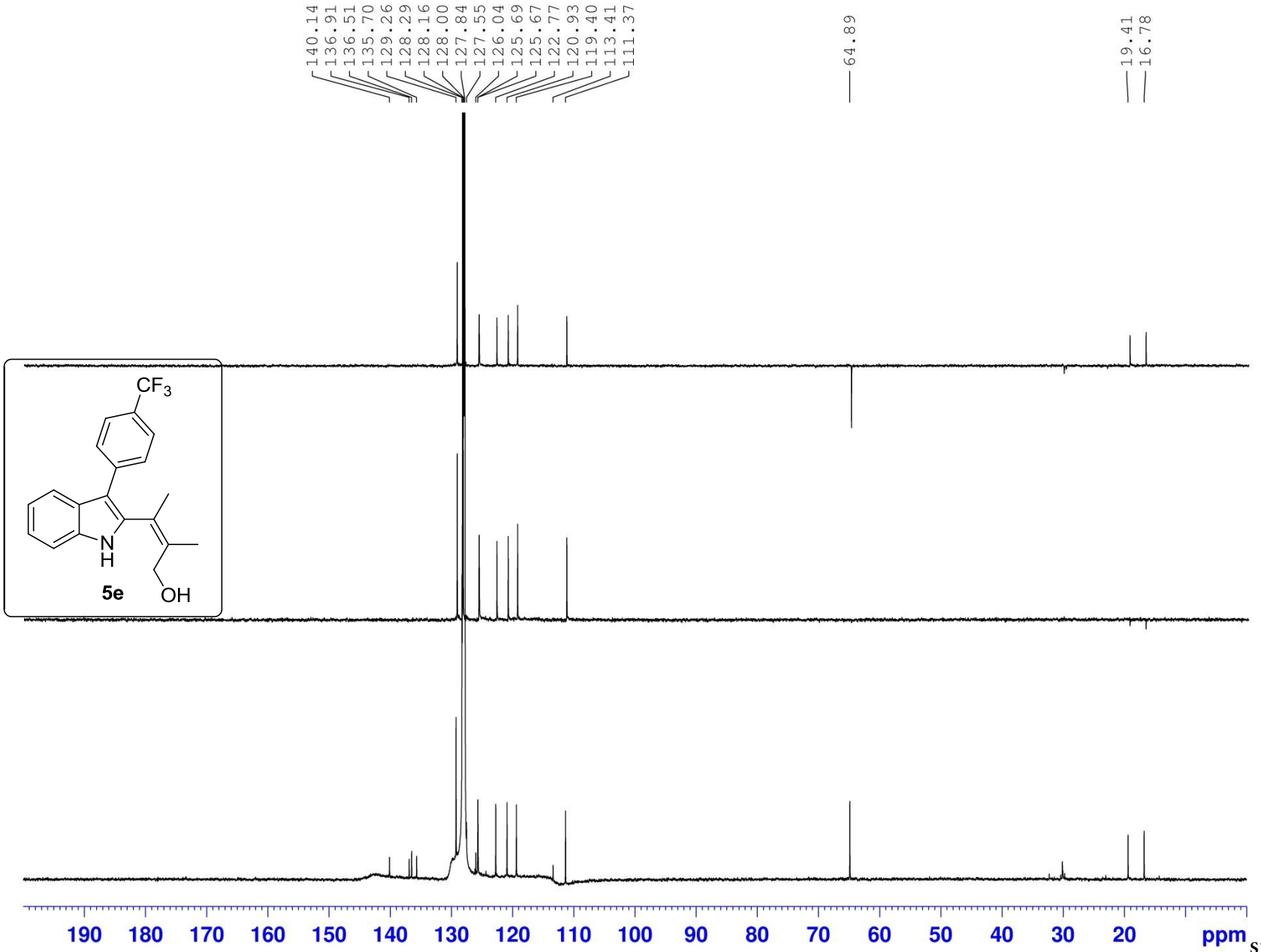
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CF3
N
H
OH
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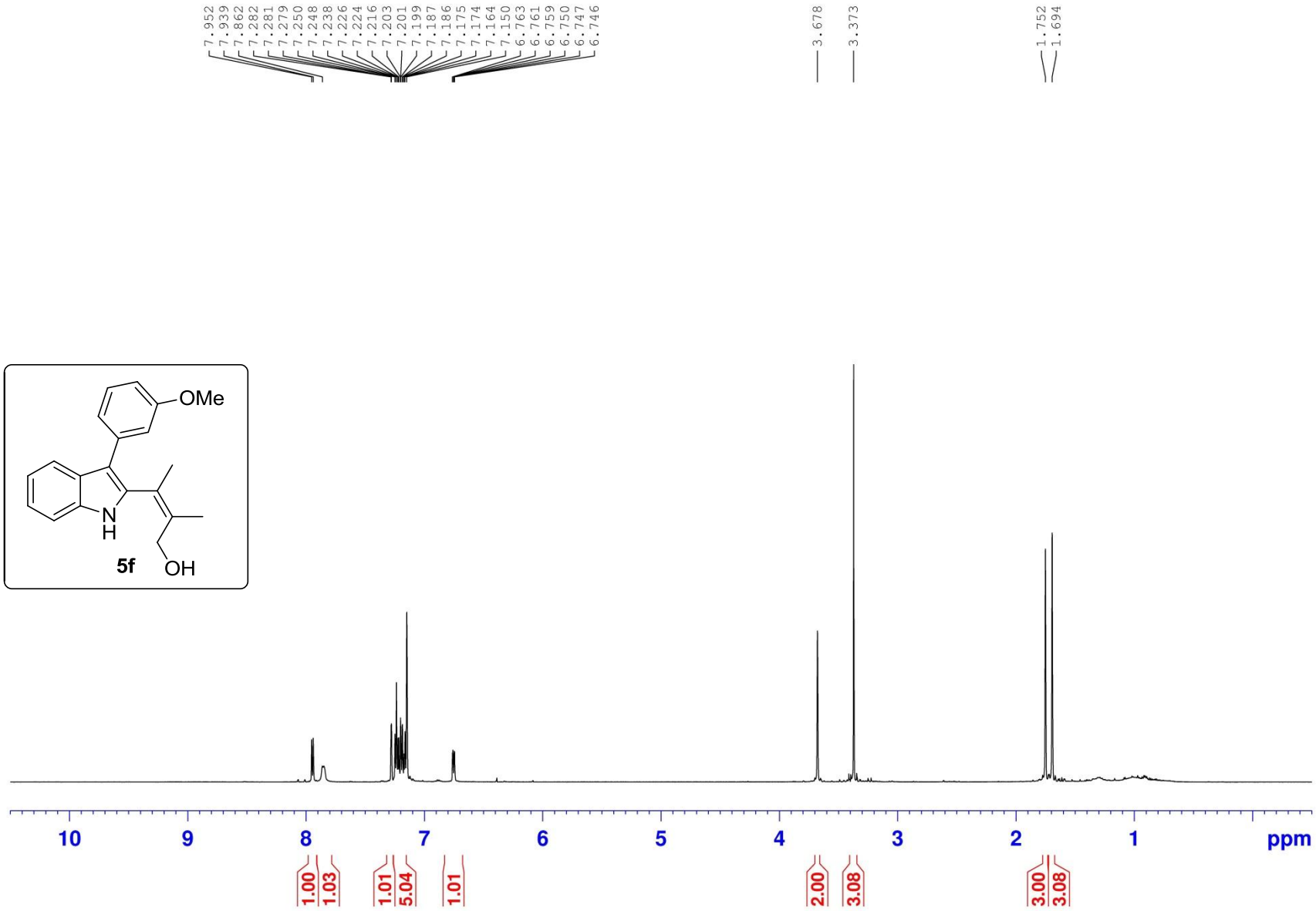
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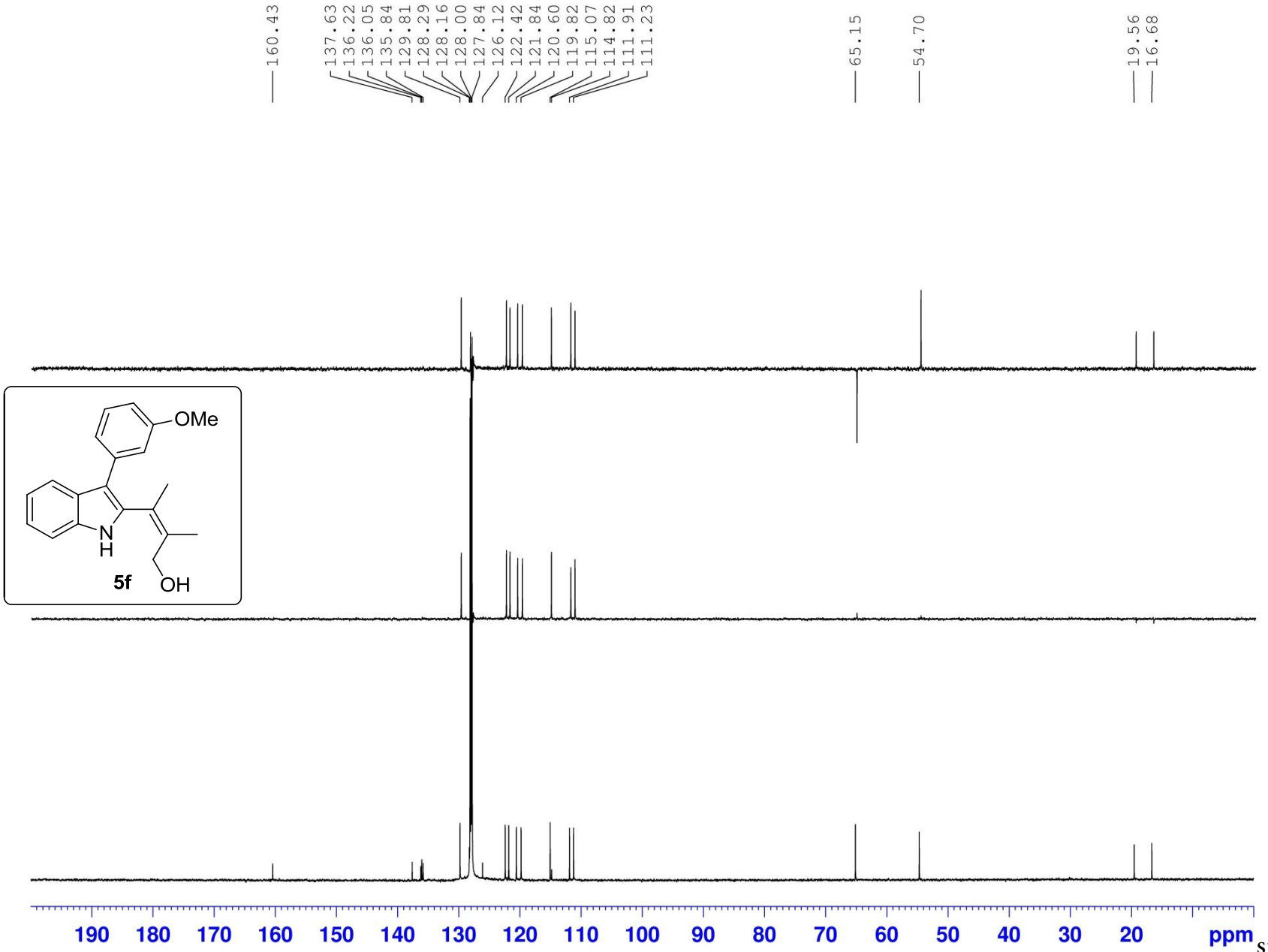
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H
5f
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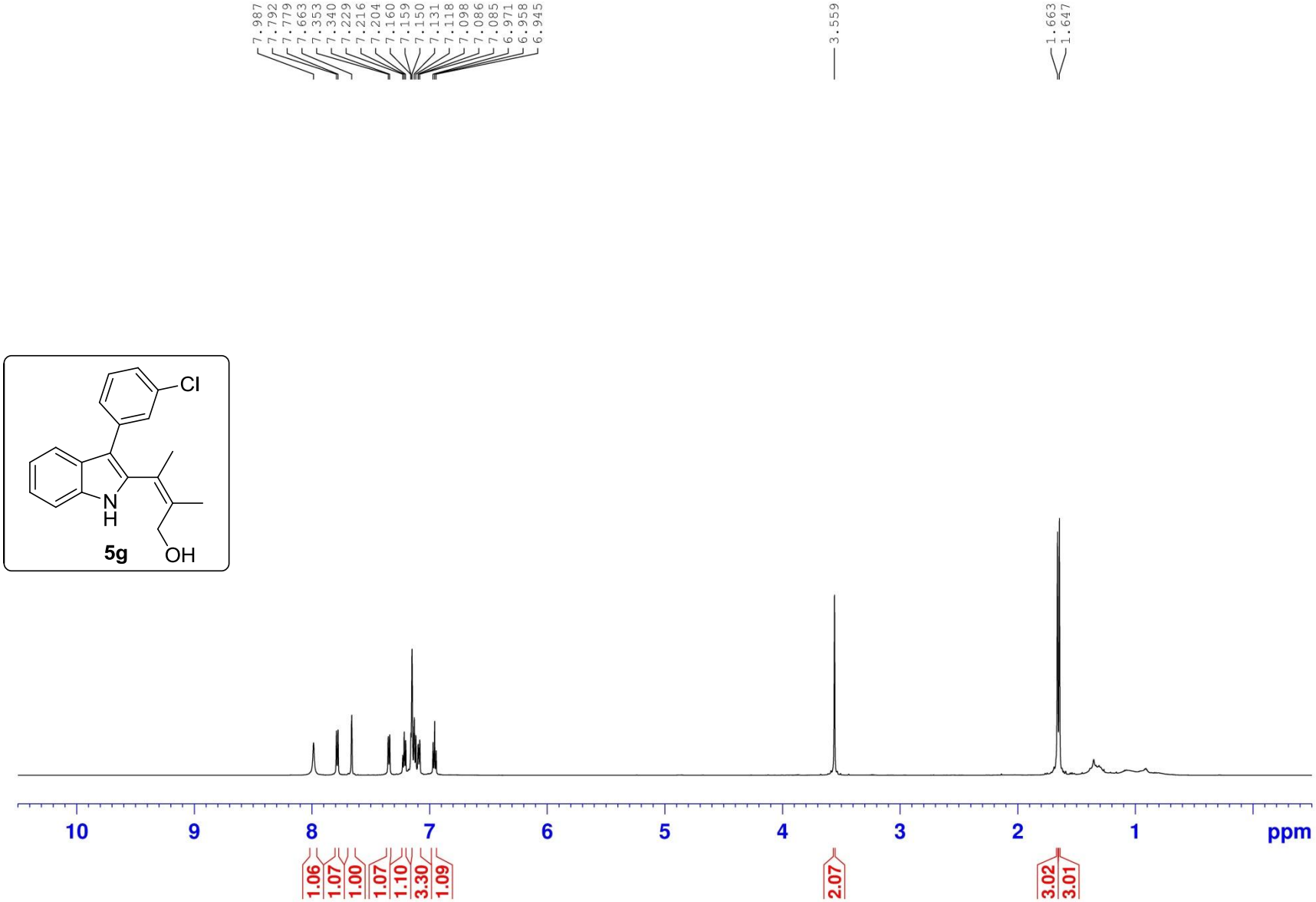
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Cl
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H
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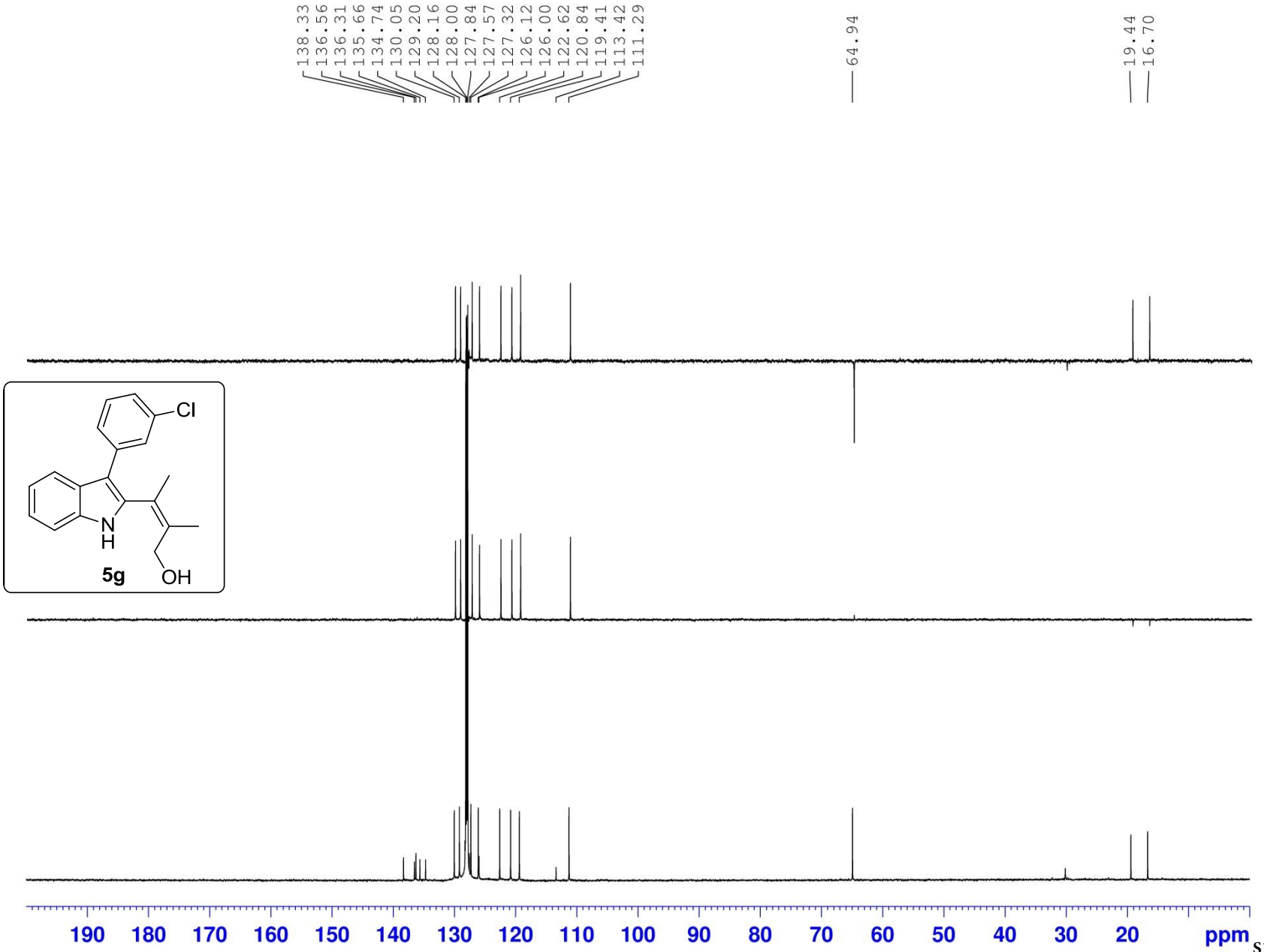
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H
5g
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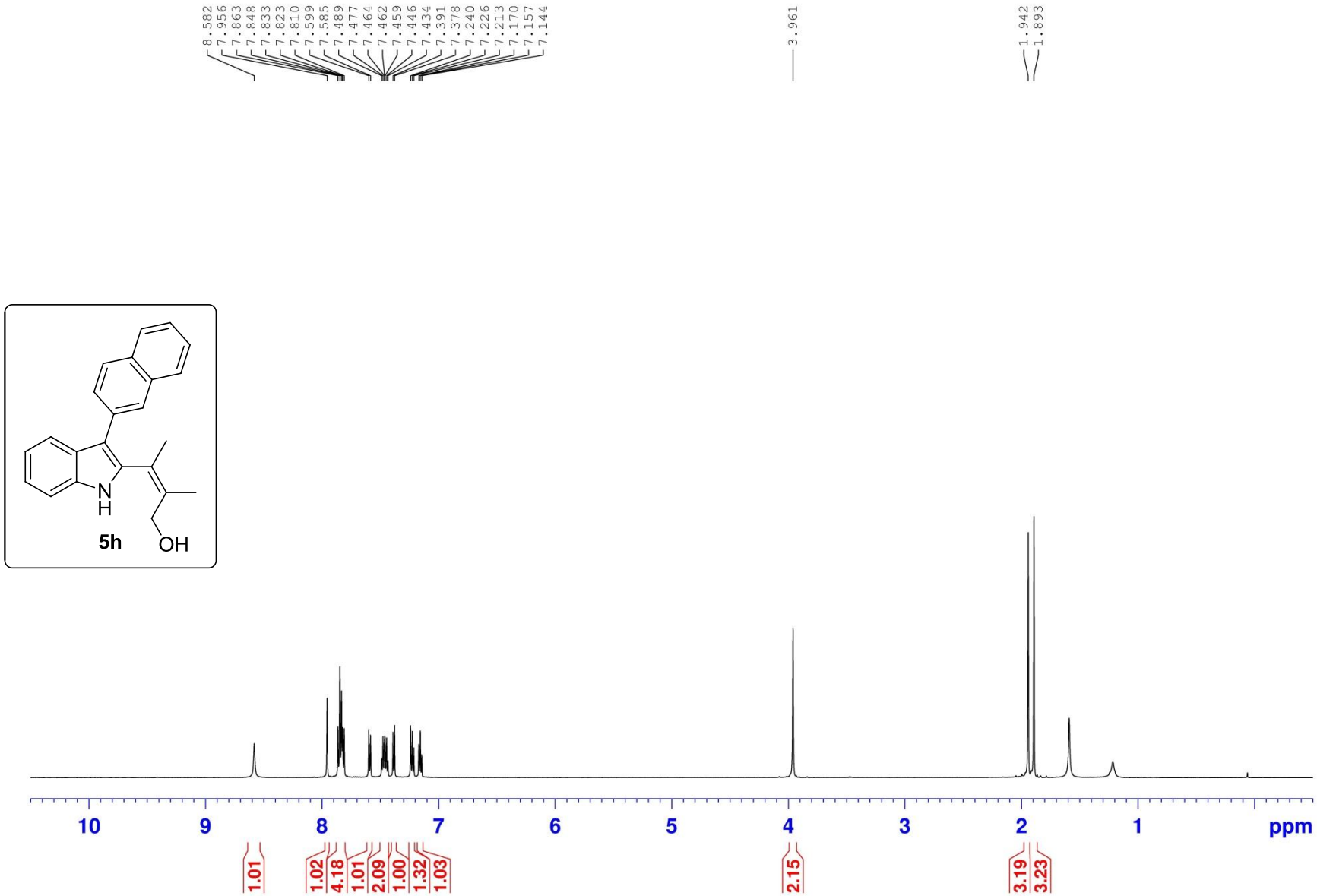
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7.459
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7.434
7.391
7.378
7.240
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7.213
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7.157
7.144
3.961
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1.893
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H
5h
OH
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9
8
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4
3
2
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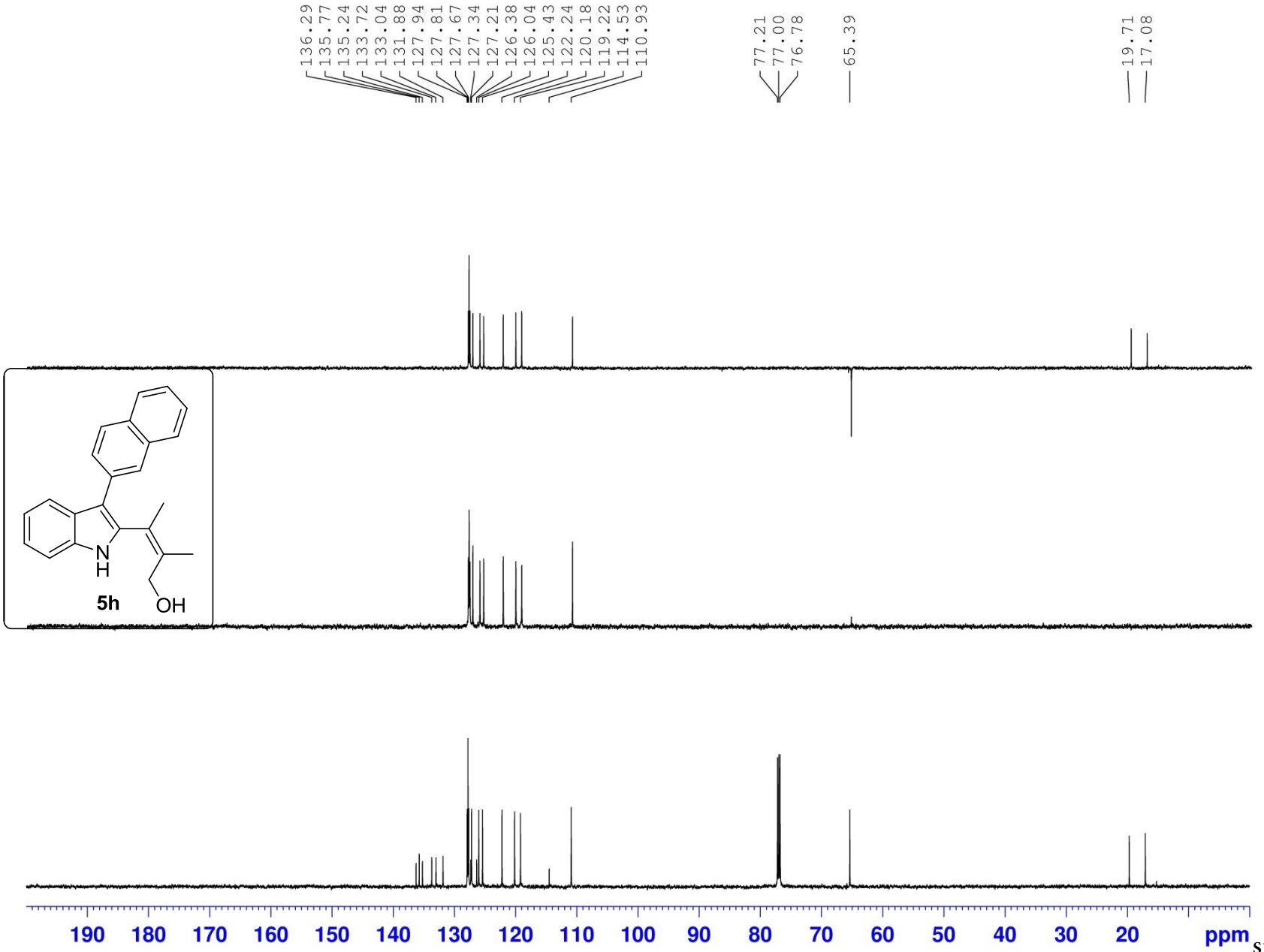
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125.43
122.24
120.18
119.22
114.53
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77.21
77.00
76.78
65.39
19.71
17.08
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H
OH
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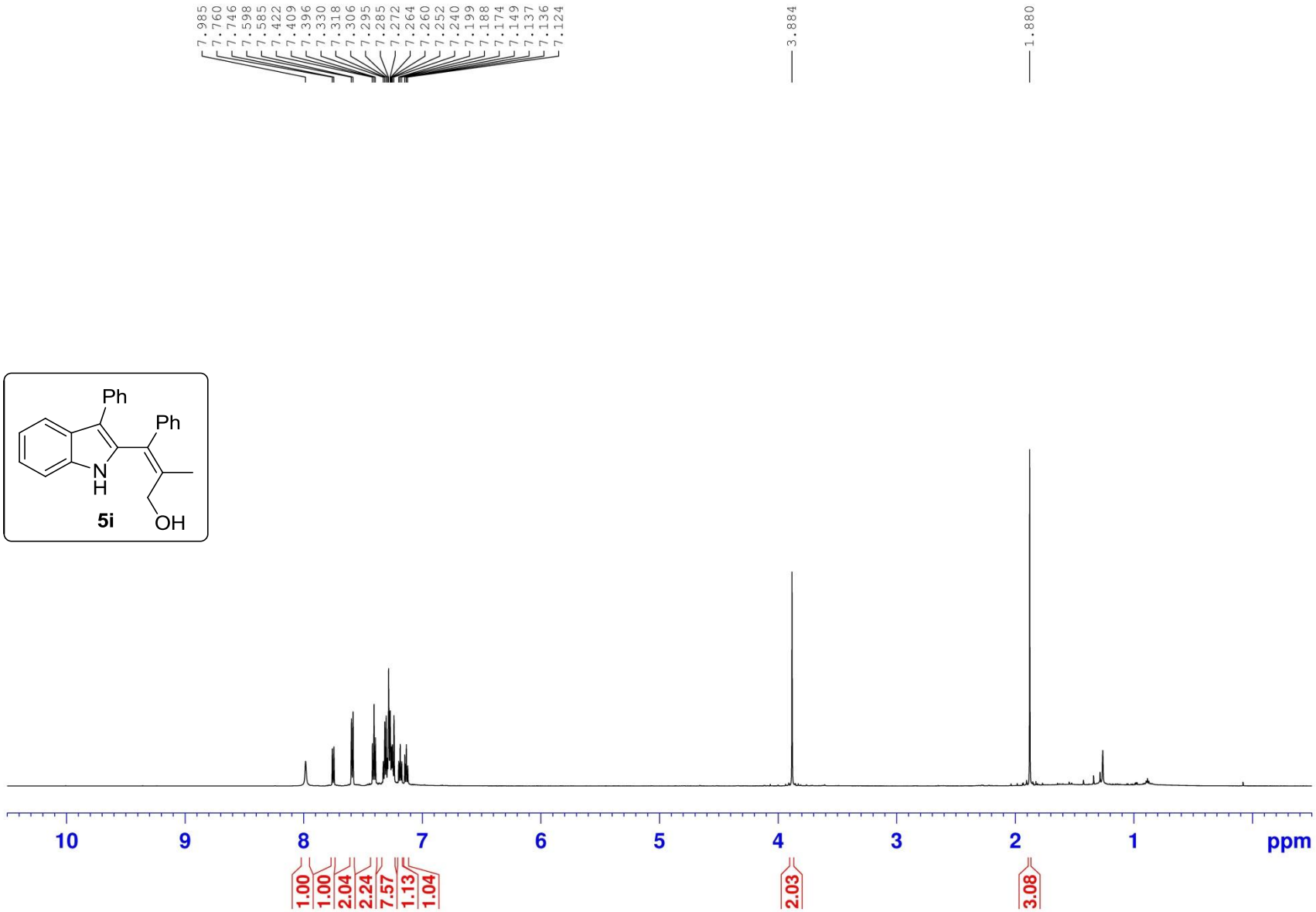
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7.272
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7.260
7.252
7.240
7.199
7.188
7.174
7.149
7.137
7.136
7.124
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1.880
Ph
Ph
N
H
5i
OH
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8
7
6
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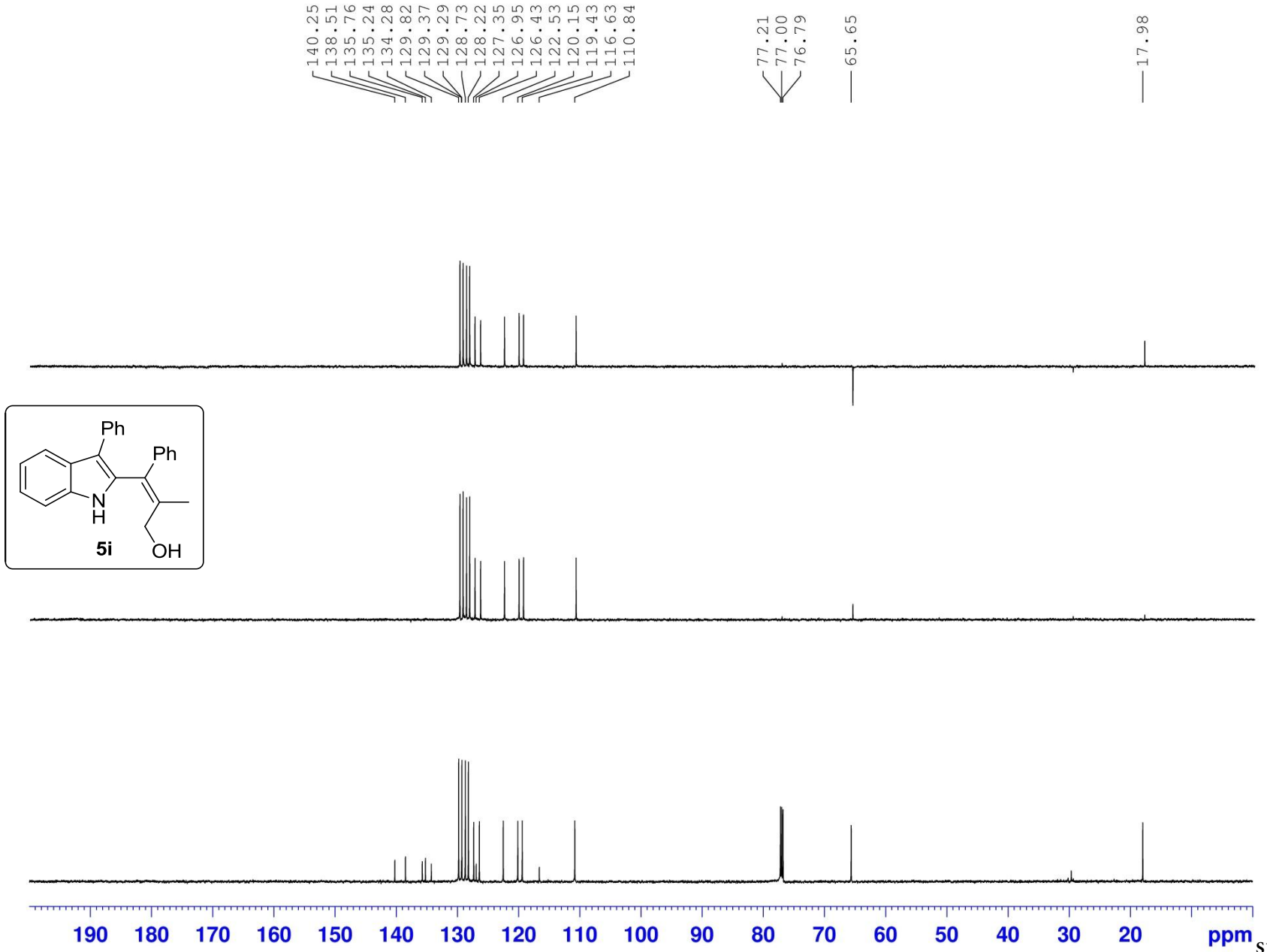
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116.63
110.84
77.21
77.00
76.79
65.65
17.98
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Ph
N
H
OH
5i
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180
170
160
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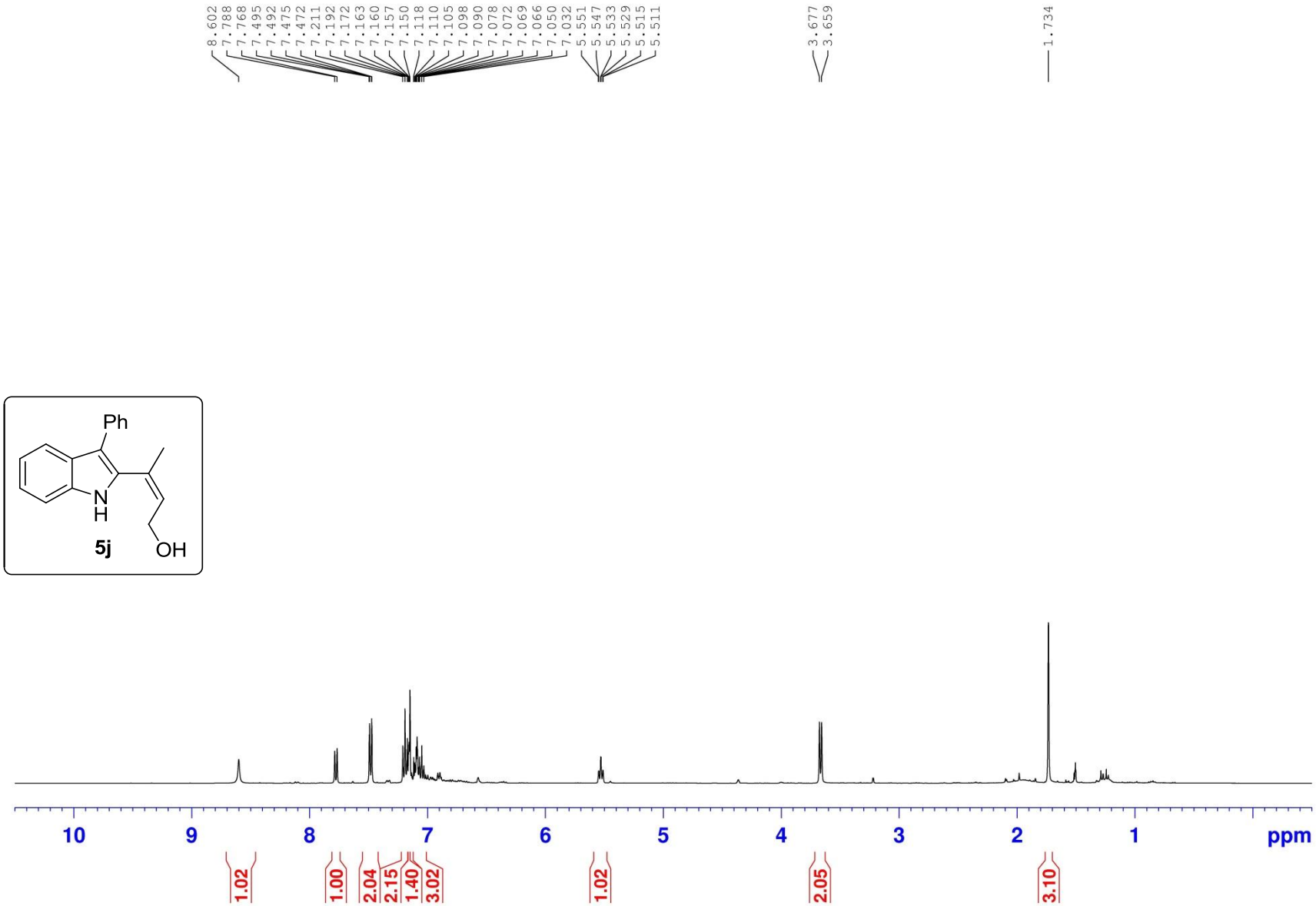
100
90
80
70
60
50
40
30
20
ppm

Ph
N
H
5j
OH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7.110
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7.066
7.050
7.032
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5.547
5.533
5.529
5.515
5.511
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3.659
1.734
10
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8
7
6
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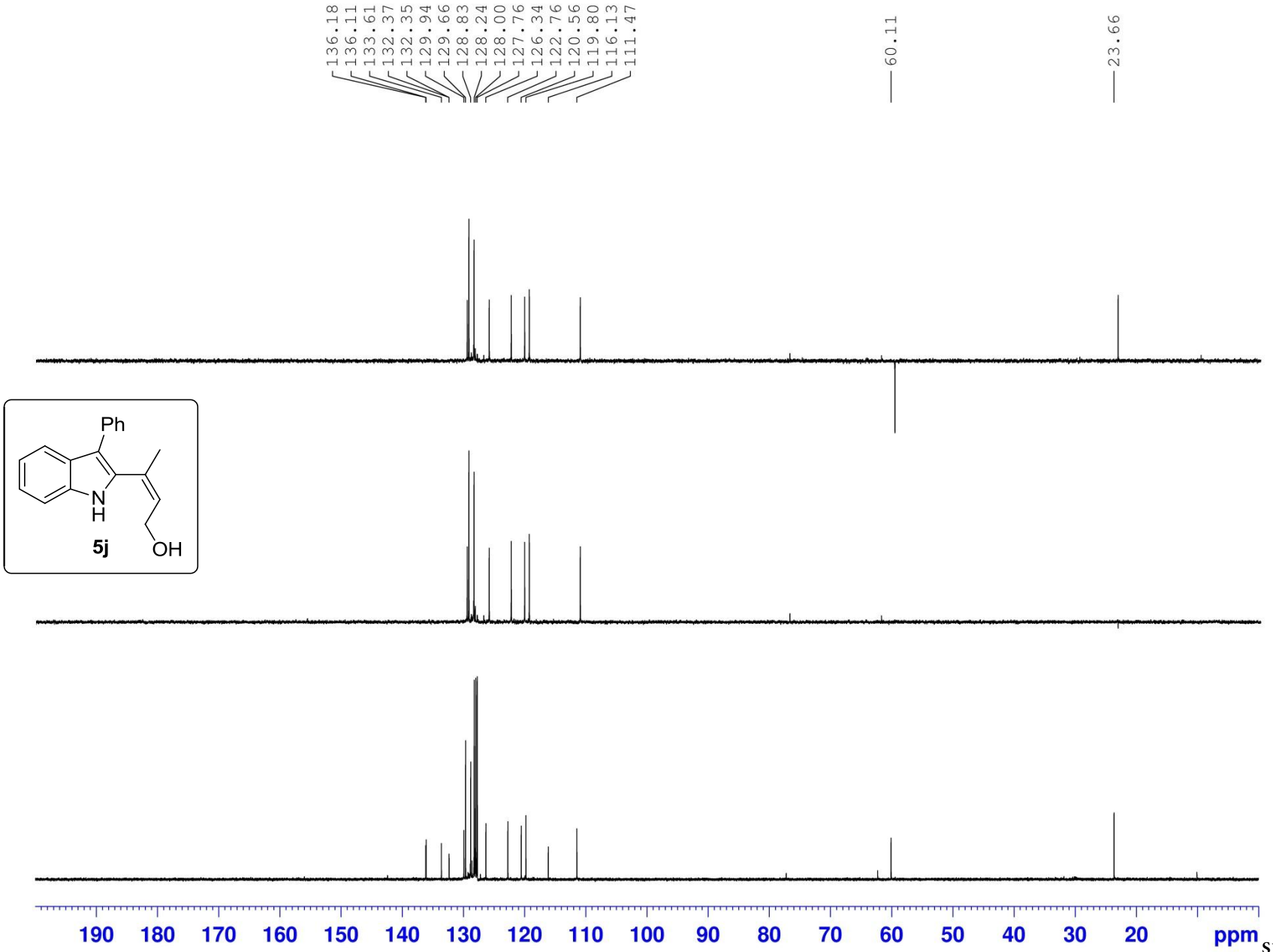
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120.56
119.80
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23.66
Ph
N
H
OH
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80
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40
30
20
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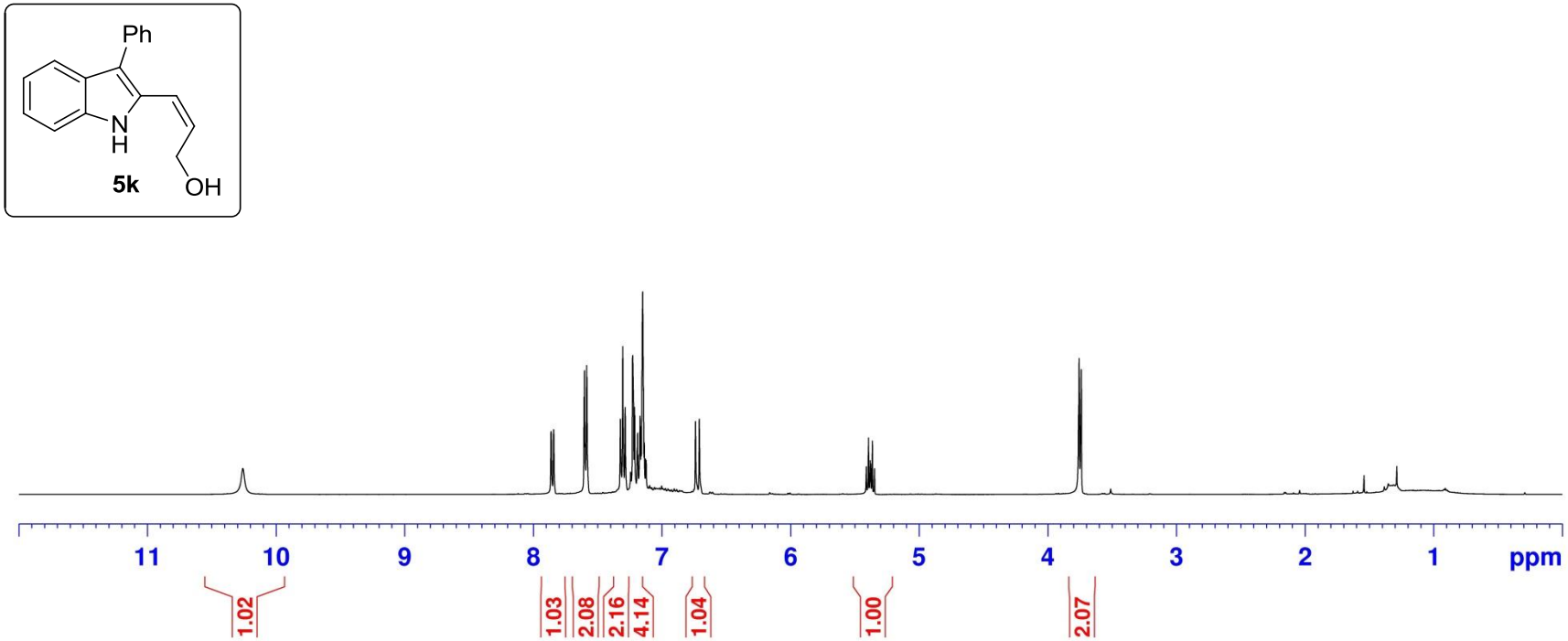
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7.229
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7.224
7.222
7.215
7.212
7.193
7.190
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7.176
7.172
7.167
7.163
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7.150
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OH
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9
8
7
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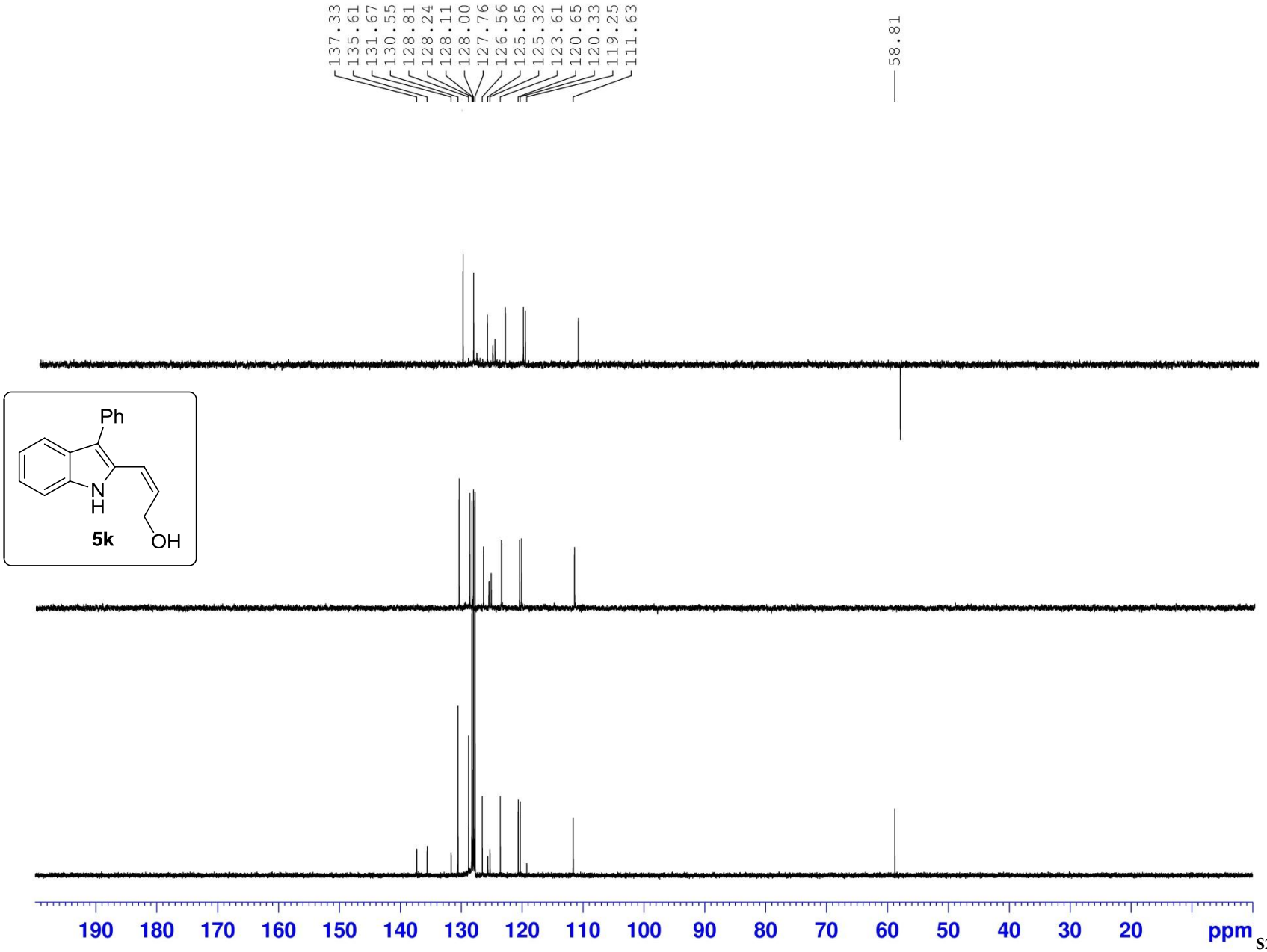
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125.32
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120.33
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111.63
58.81
Ph
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H
5k
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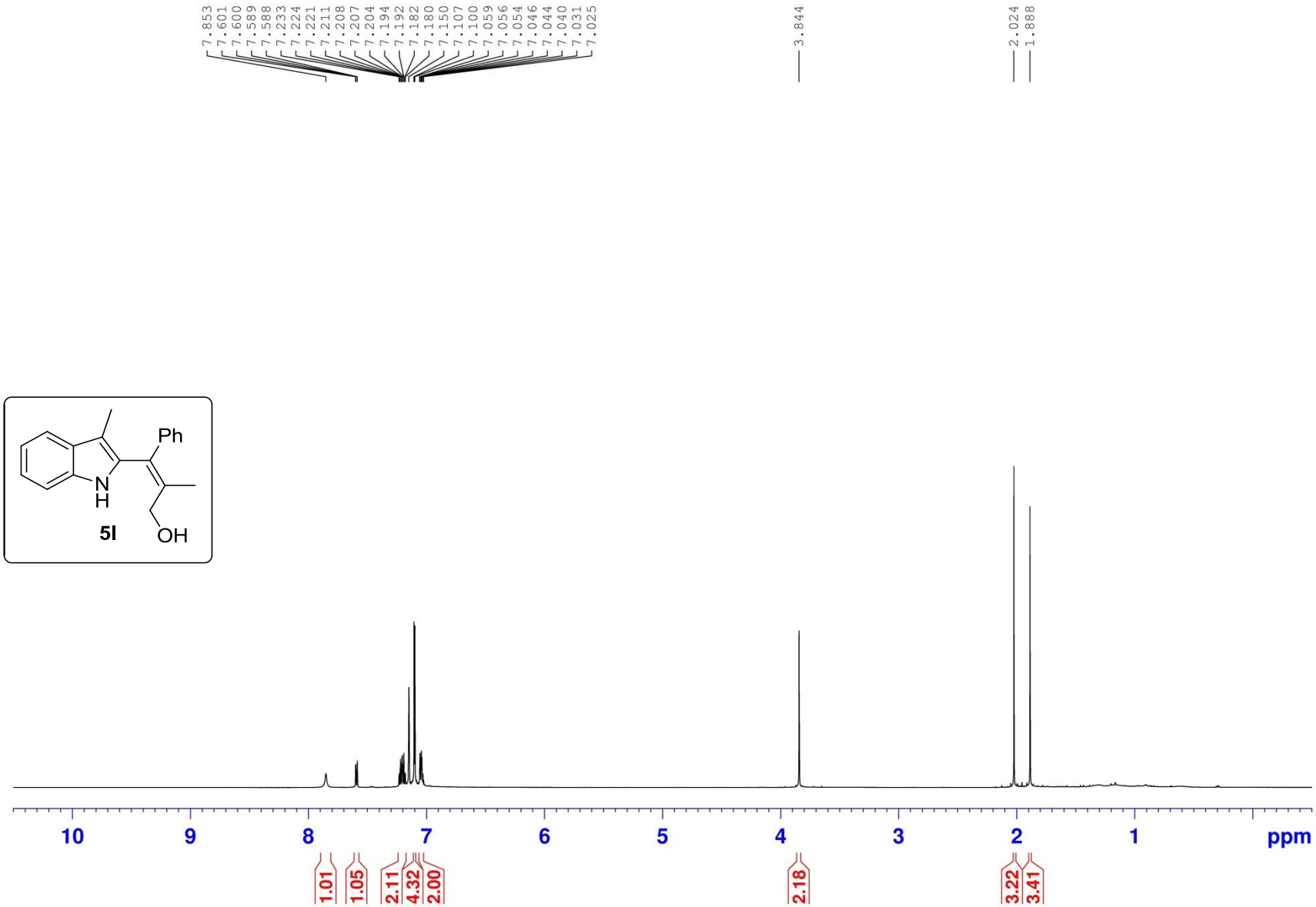
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7.056
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7.031
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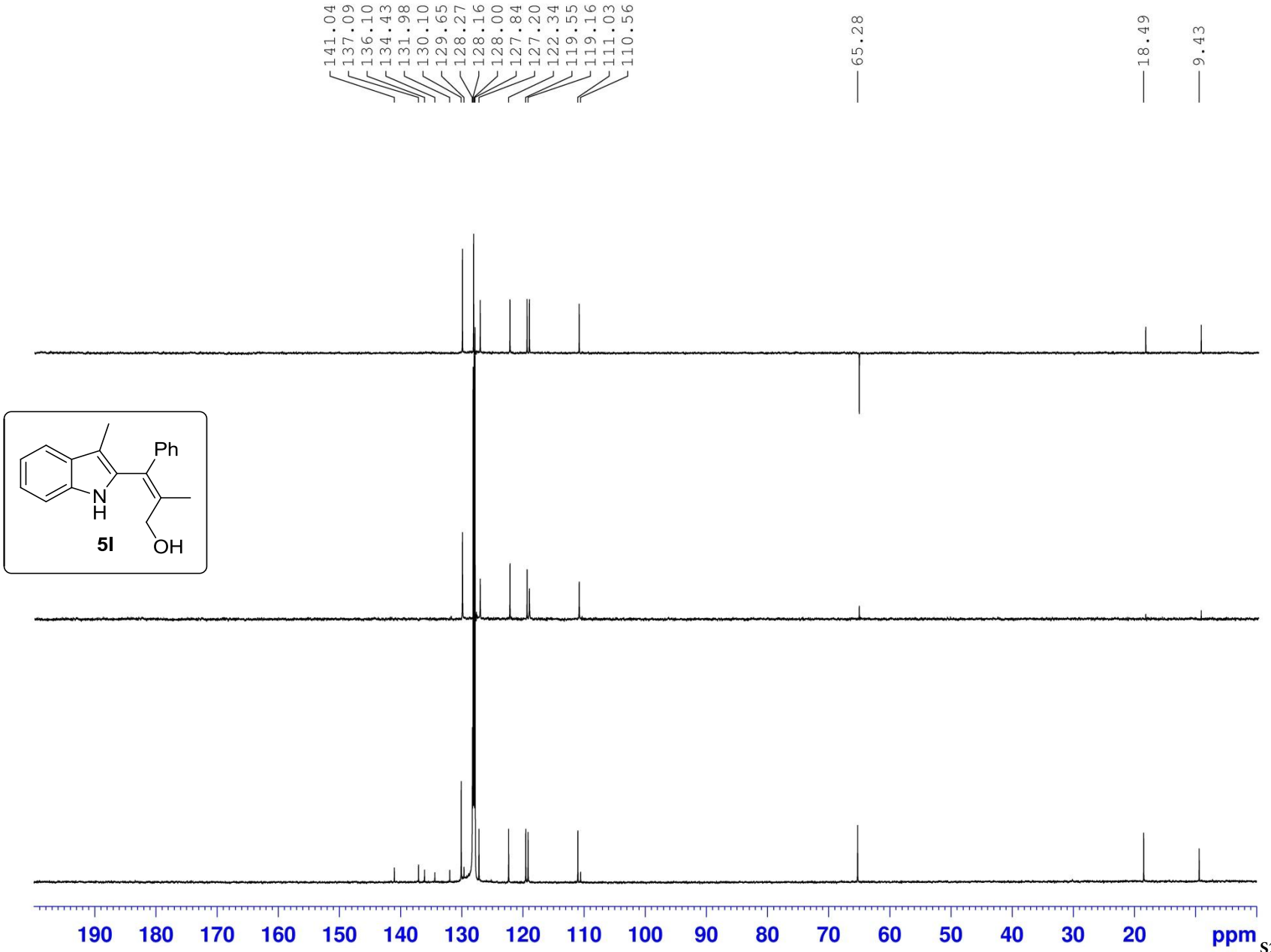
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111.03
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65.28
18.49
9.43
Ph
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H
5l
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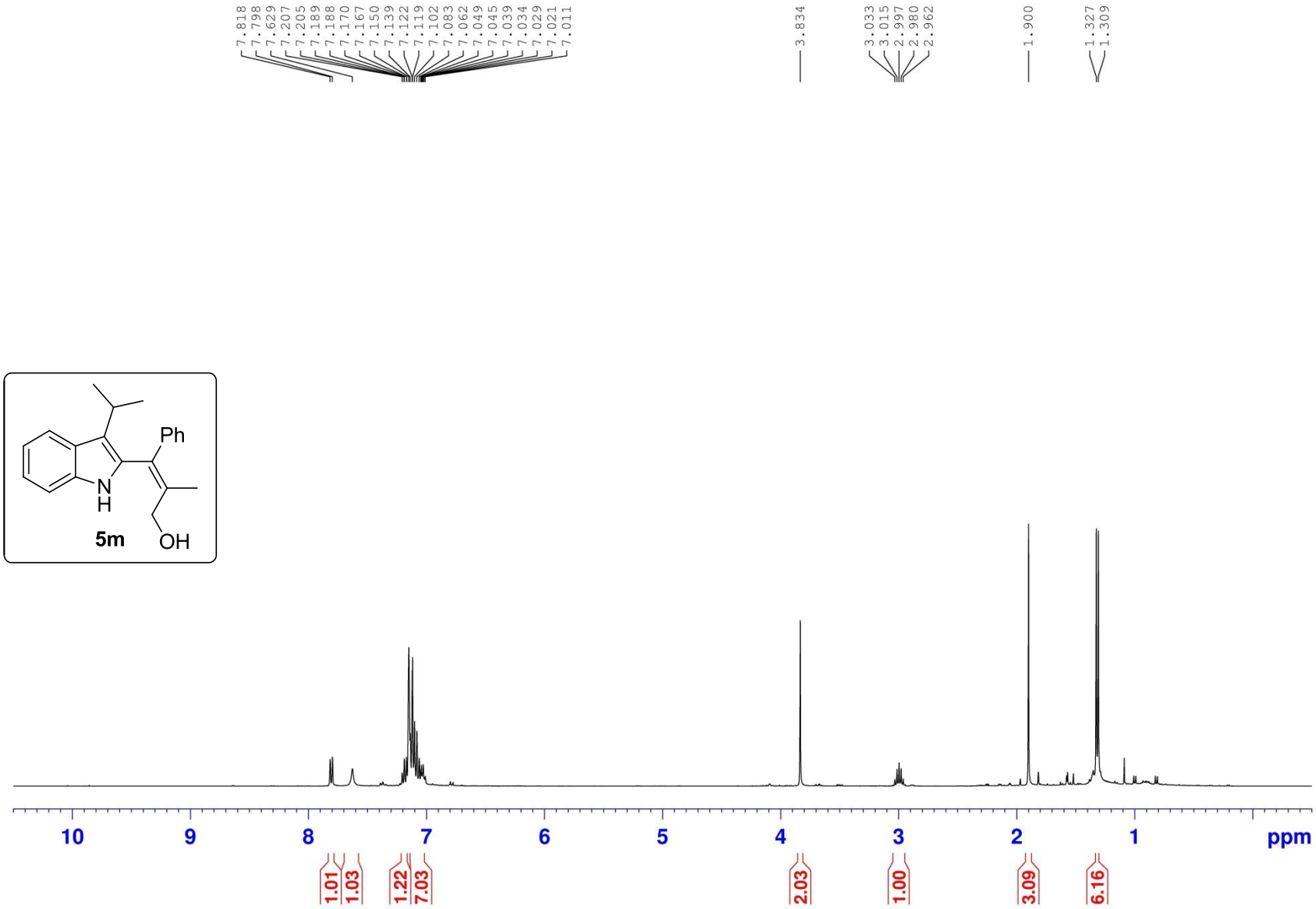
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7.083
7.062
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3.033
3.015
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1.327
1.309
Ph
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H
5m
OH
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9
8
7
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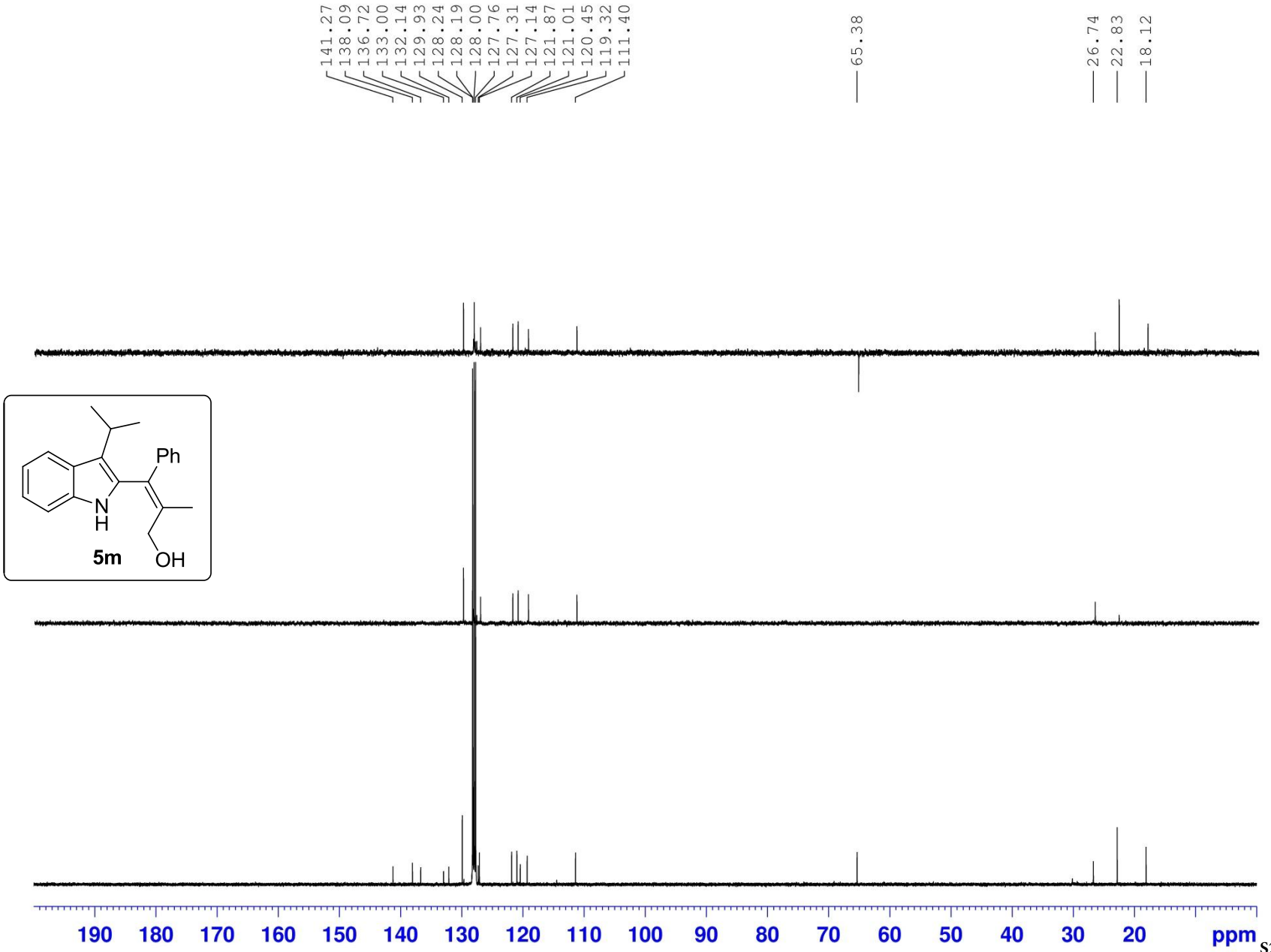
6.16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111.40
65.38
26.74
22.83
18.12
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H
5m
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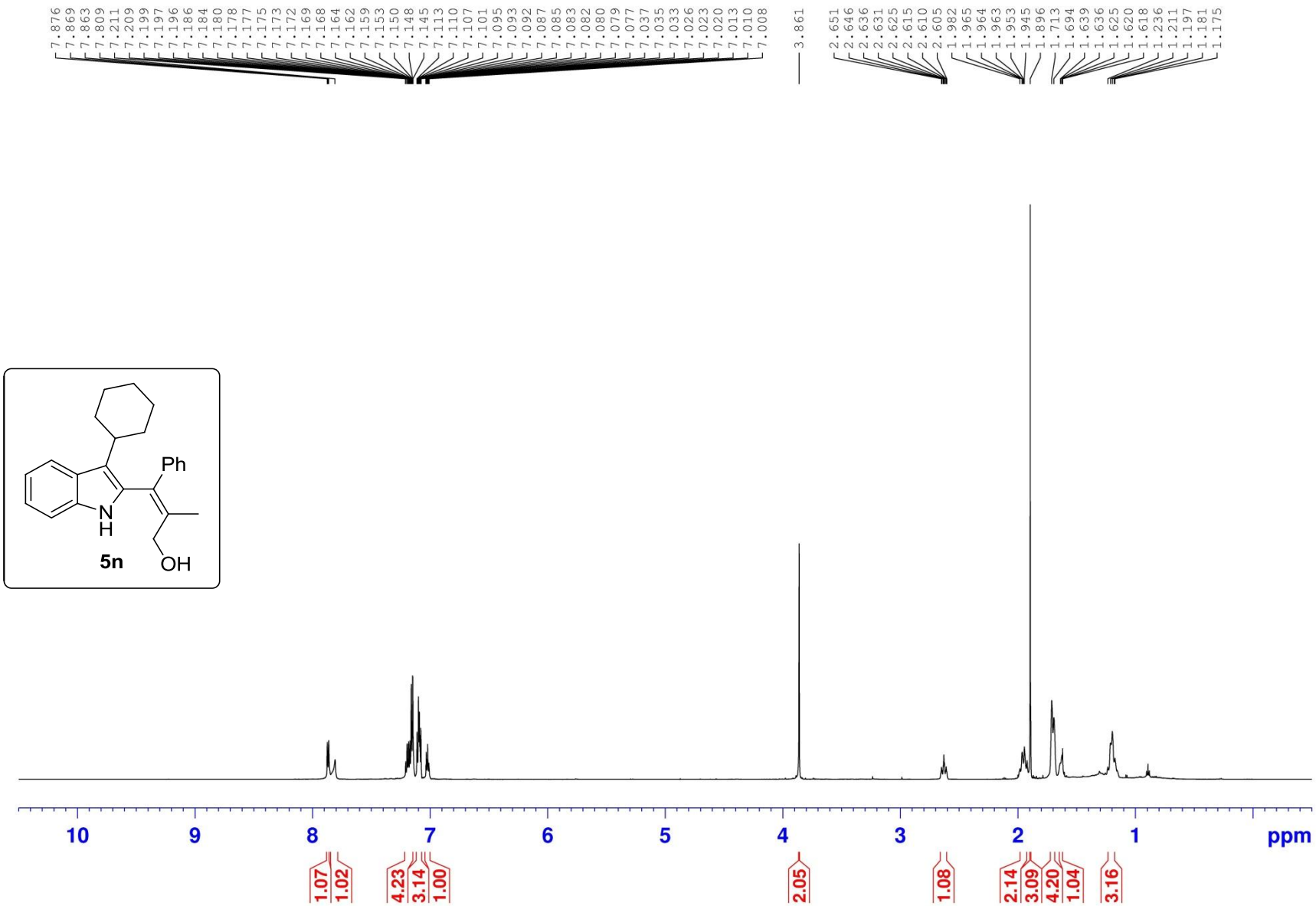
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3.861
2.651 2.646 2.636 2.631 2.625 2.615 2.610 2.605 1.982 1.965 1.964 1.963 1.953 1.945 1.896 1.713 1.694 1.639 1.636 1.625 1.620 1.618 1.236 1.211 1.197 1.181 1.175
Ph
N
H
5n
OH
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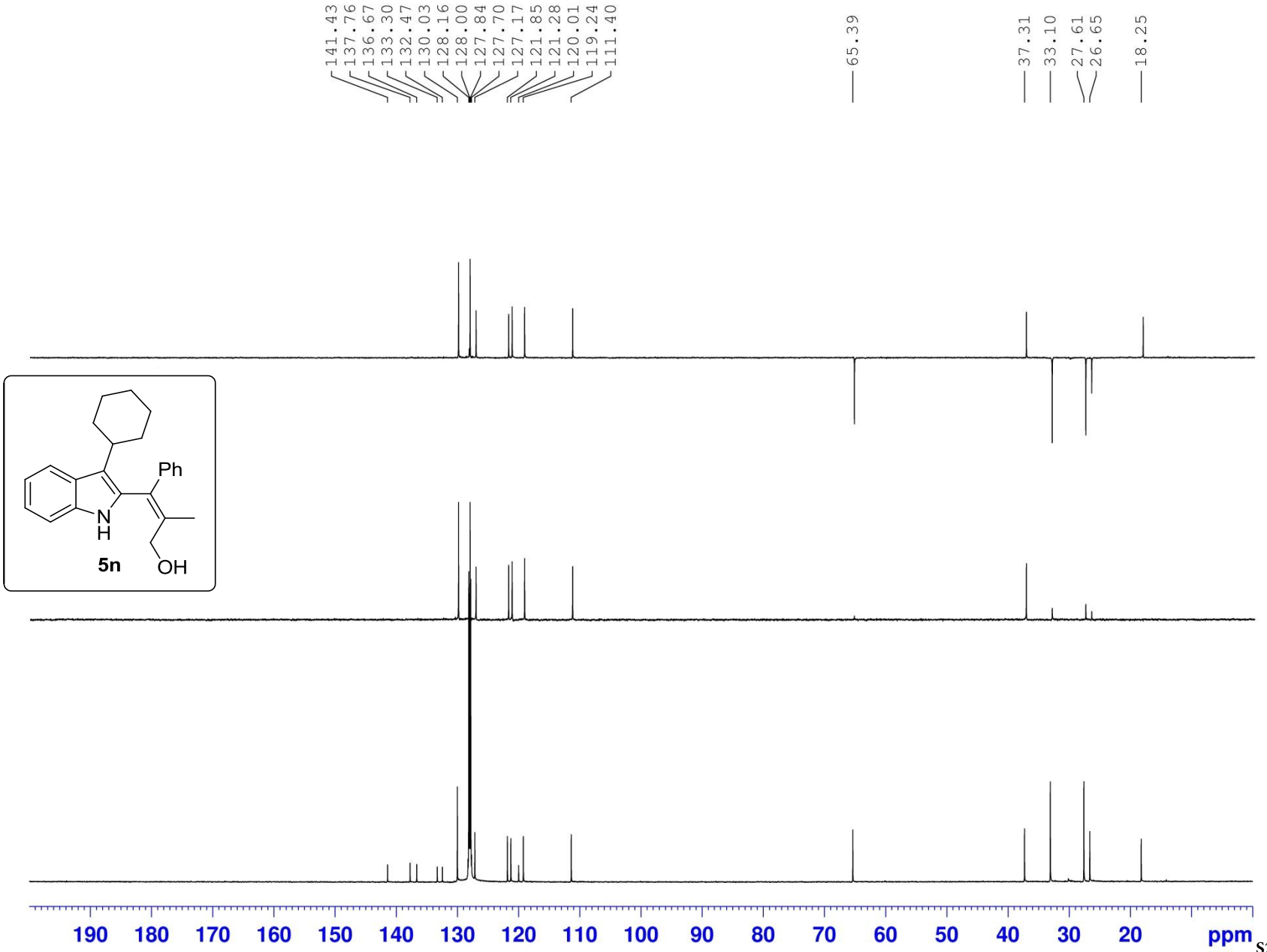
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121.28
120.01
119.24
111.40
65.39
37.31
33.10
27.61
26.65
18.25
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OH
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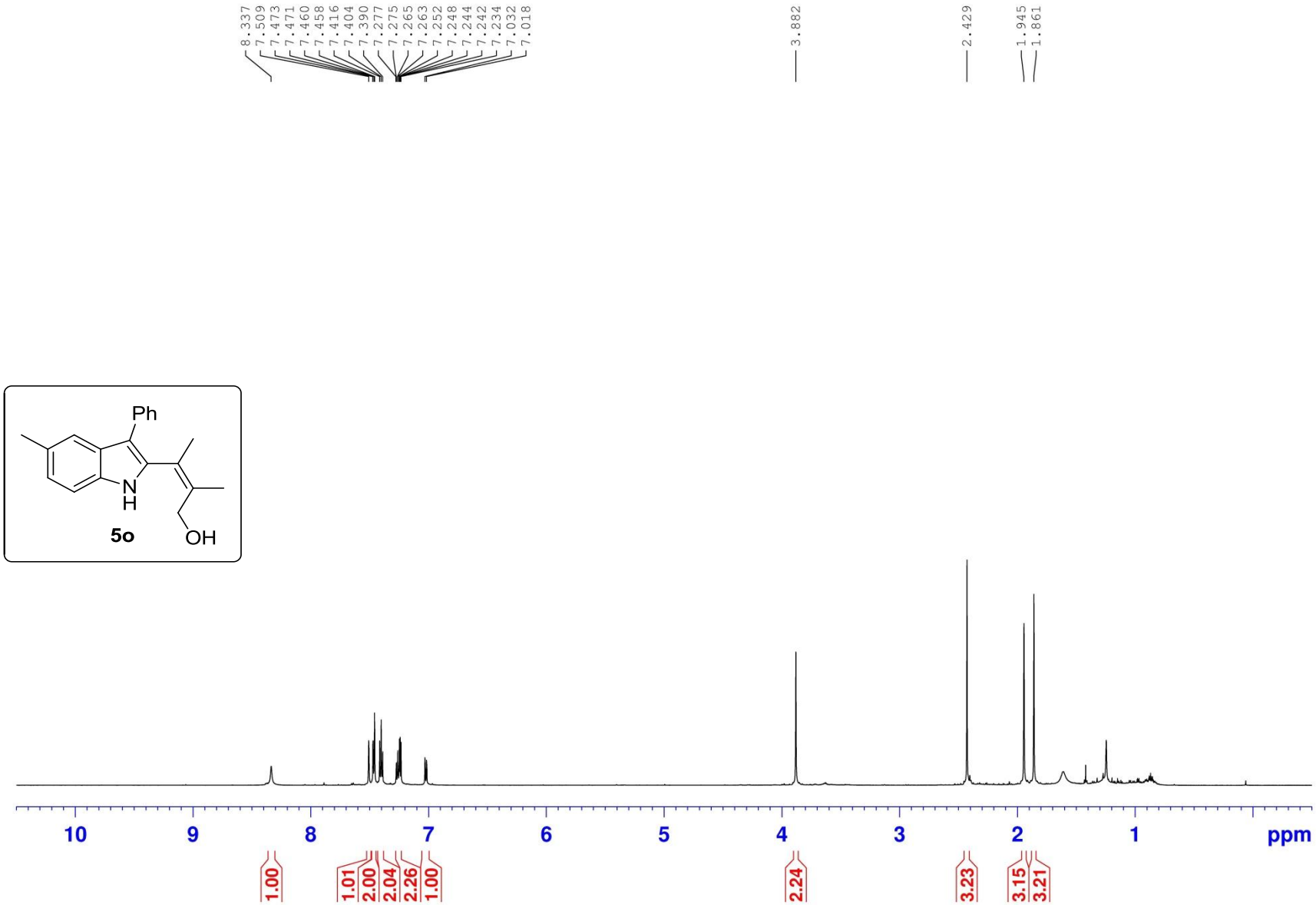
30
20
ppm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7.244
7.242
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1.861
Ph
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H
5o
OH
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8
7
6
5
4
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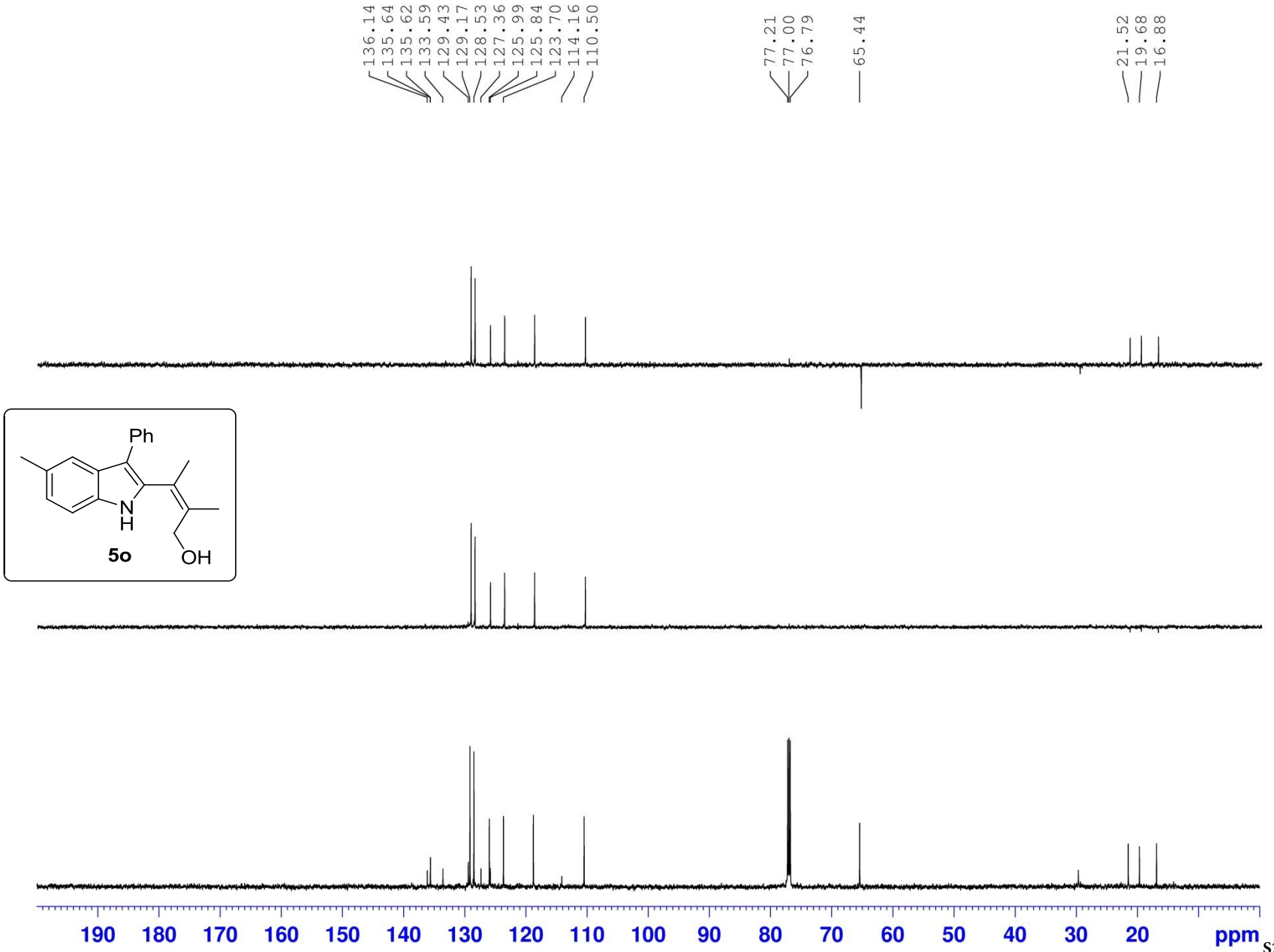
3.21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Ph
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H
5o
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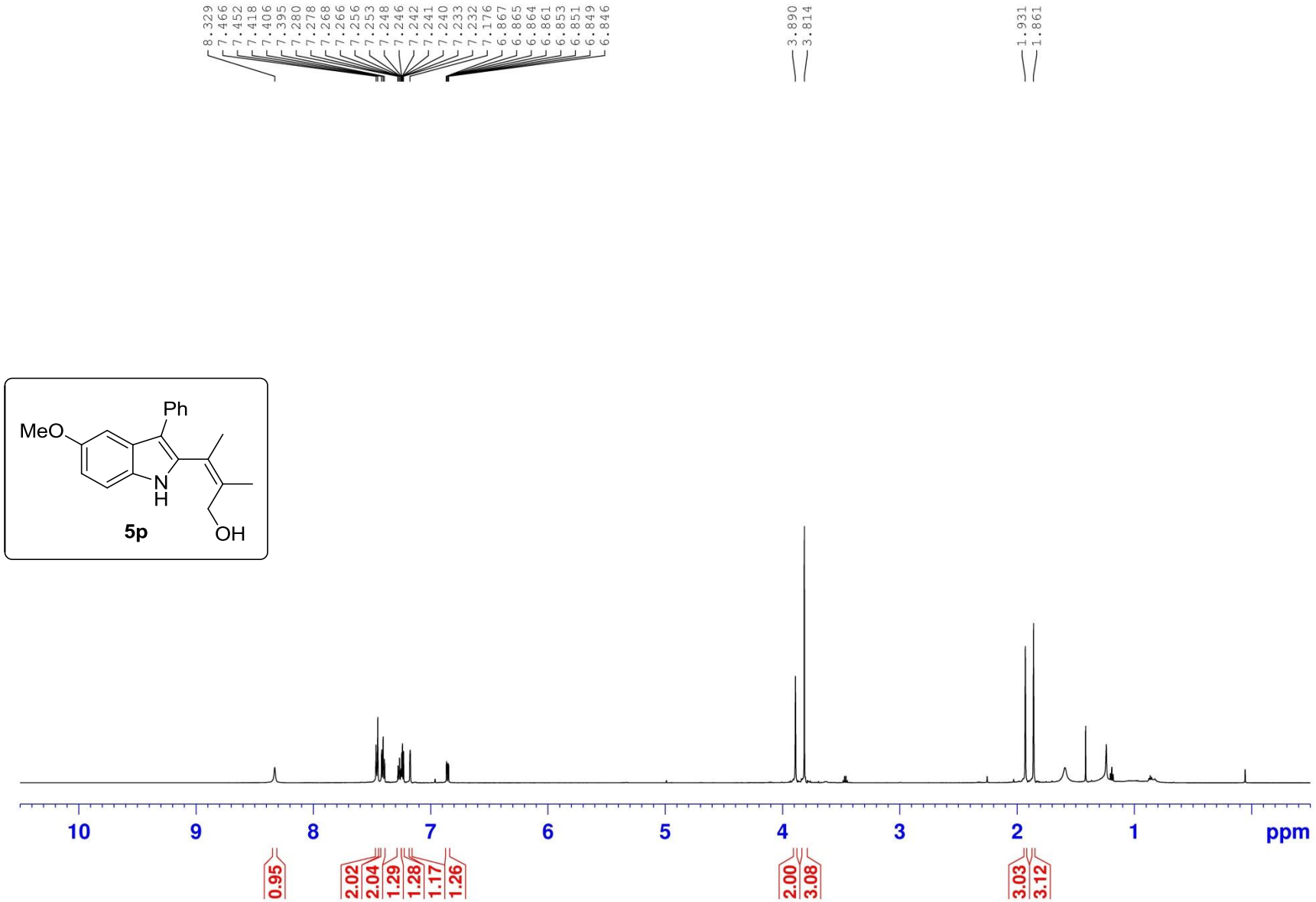
ppm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7.242
7.241
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Ph
MeO
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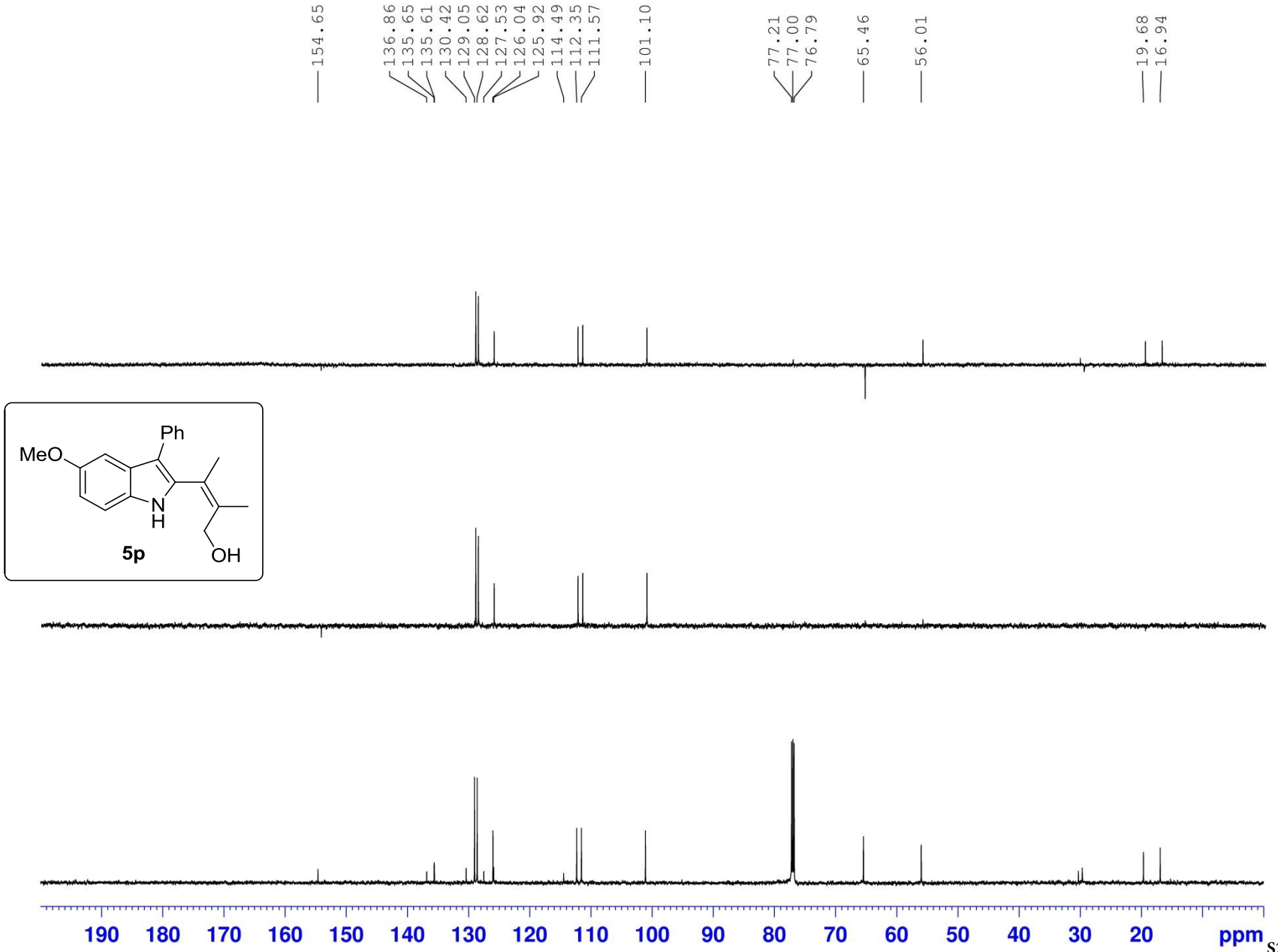
3.12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MeO
Ph
N
H
OH
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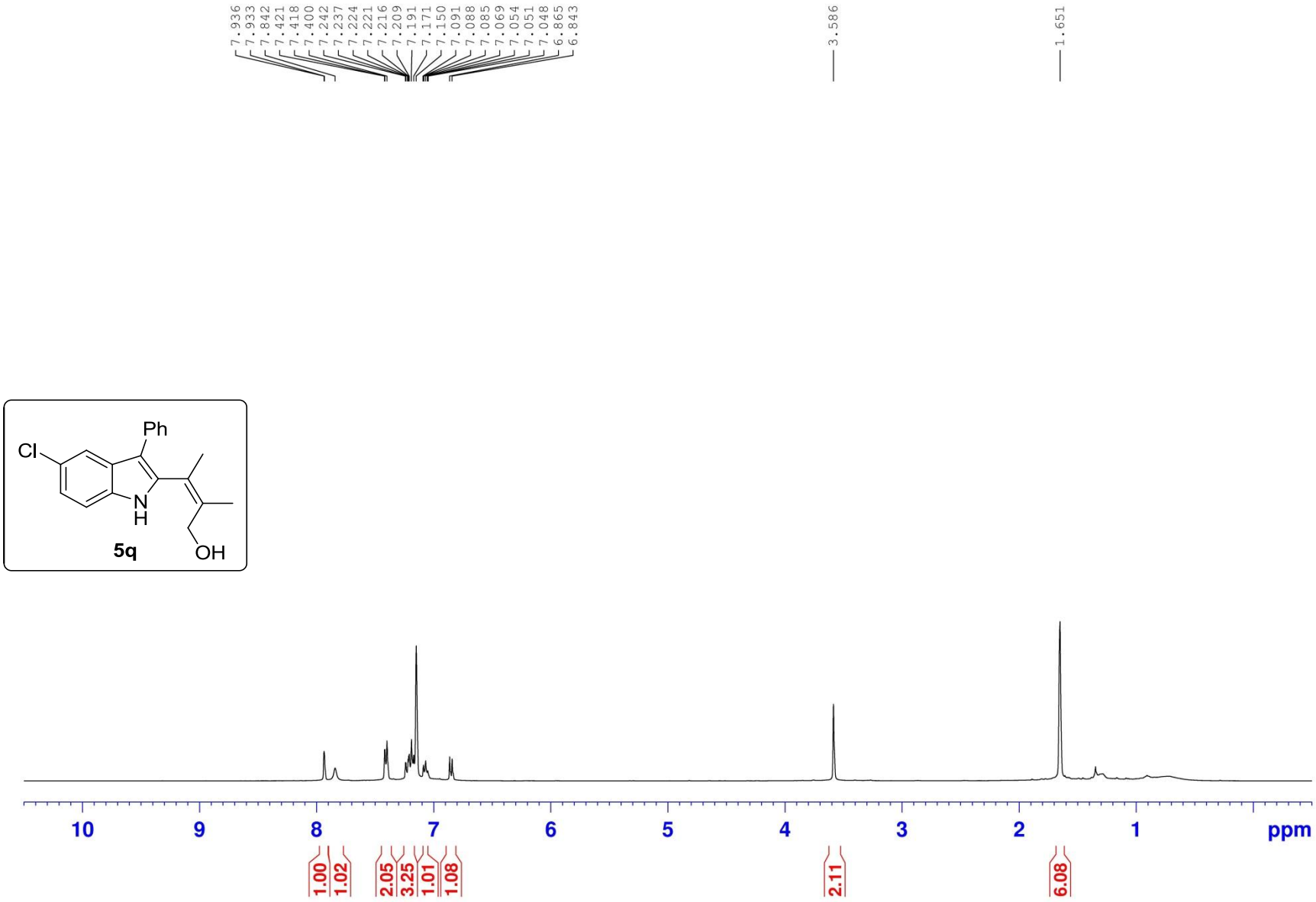
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Cl
Ph
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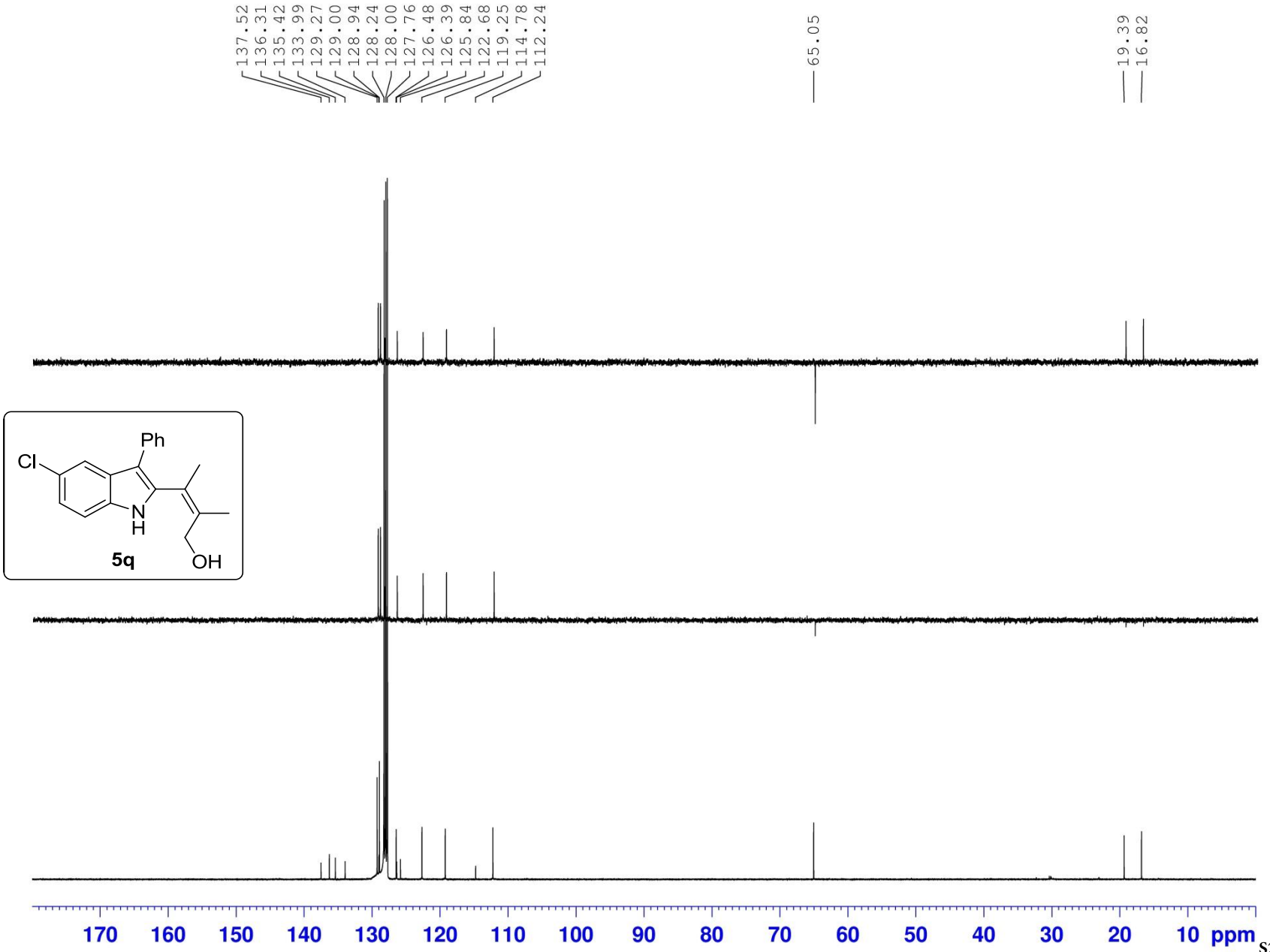
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H
5q
OH
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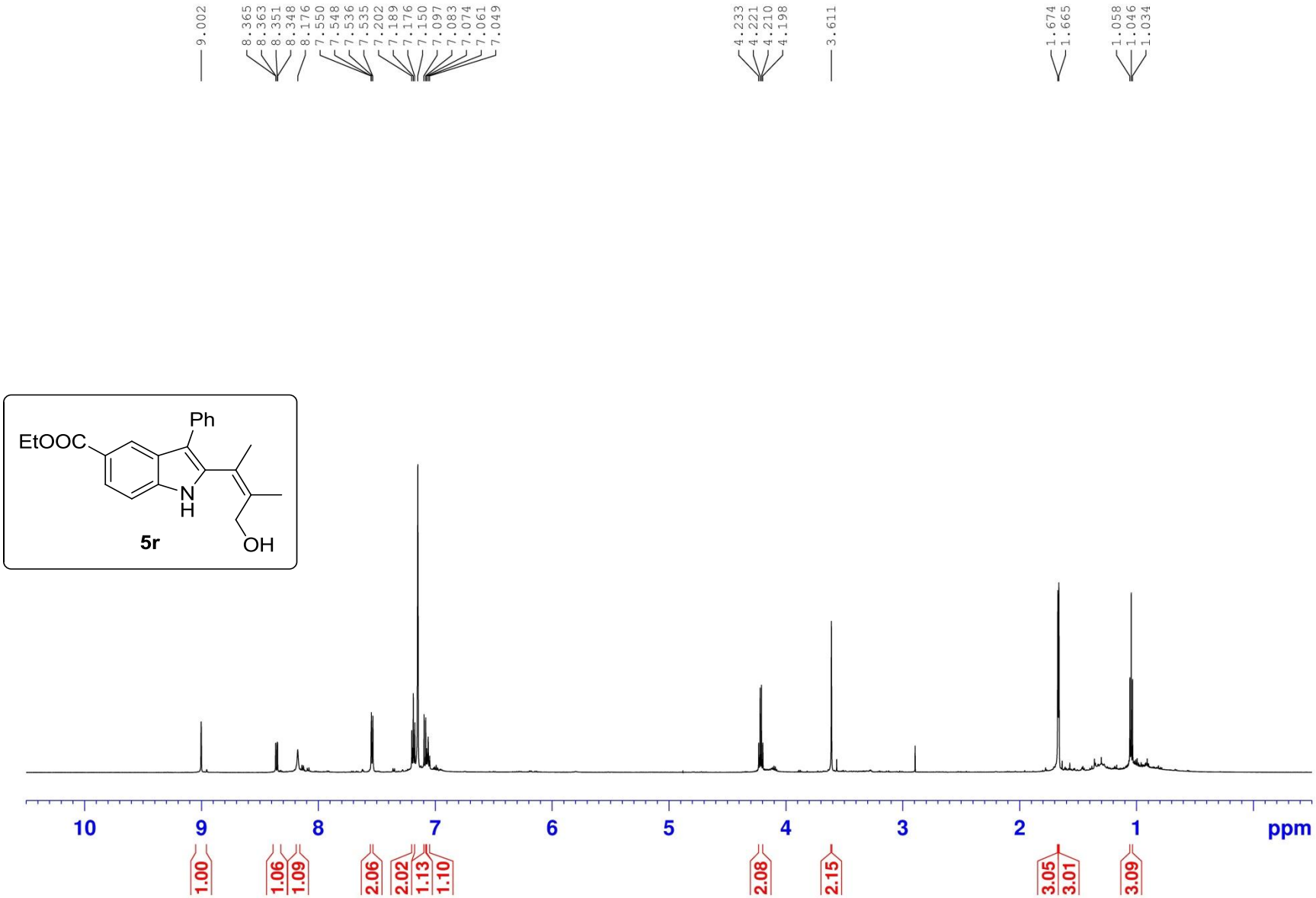
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7.150
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7.083
7.074
7.061
7.049
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EtOOC
Ph
N
H
OH
5r
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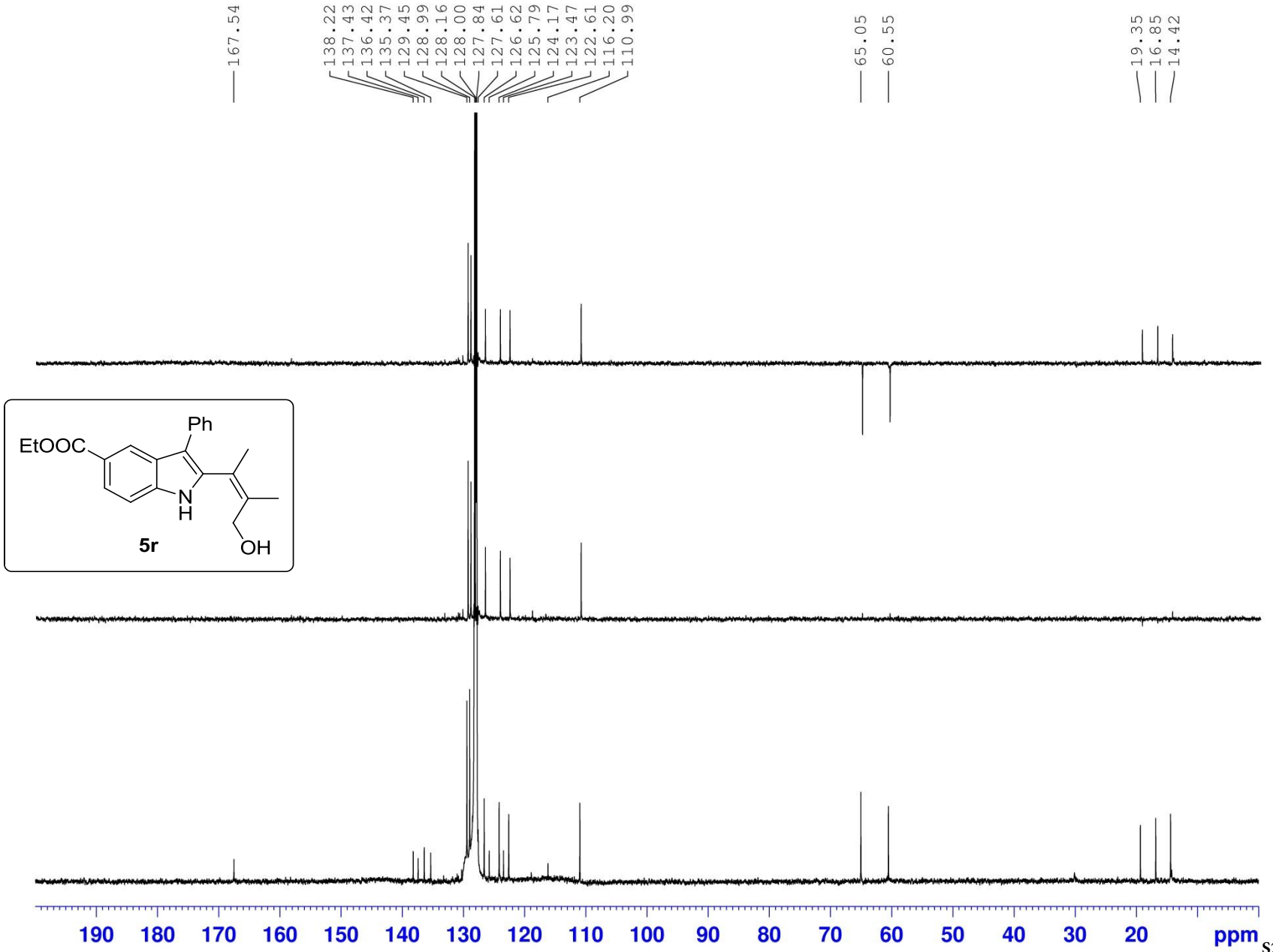
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Ph
N
H
OH
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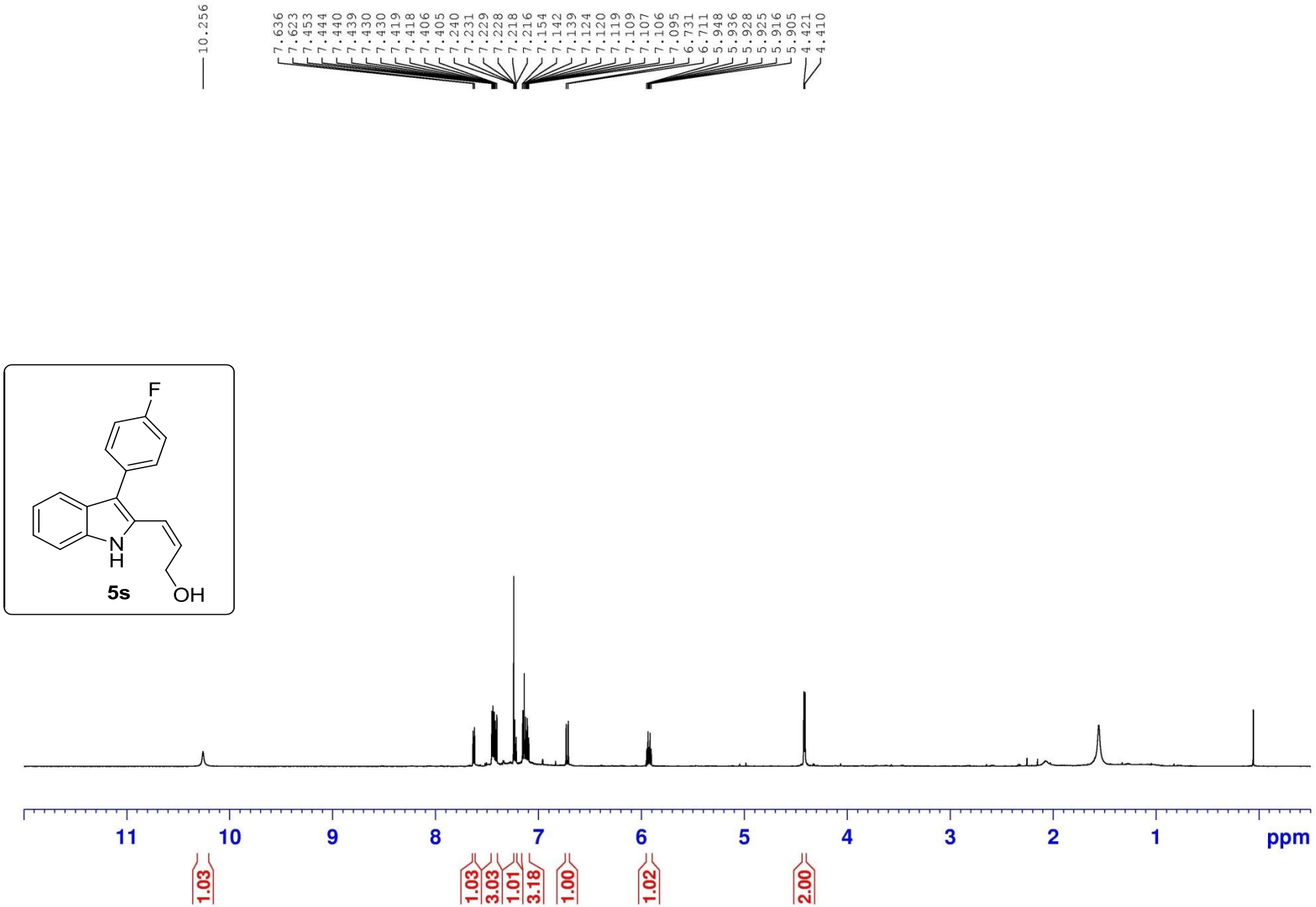
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7.405
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7.231
7.229
7.228
7.218
7.216
7.154
7.142
7.139
7.124
7.120
7.119
7.109
7.107
7.106
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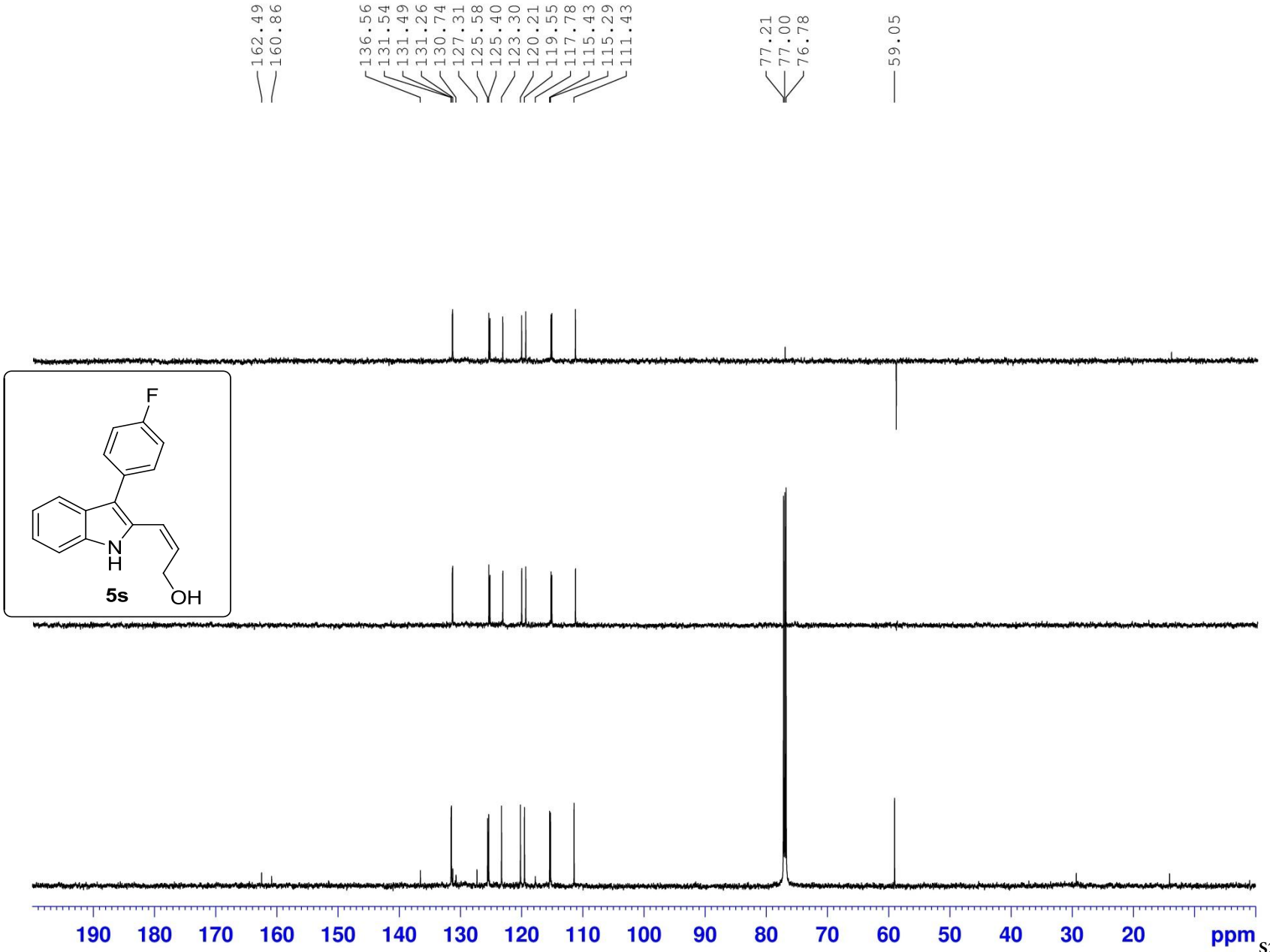
2.00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76.78
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F
N
H
OH
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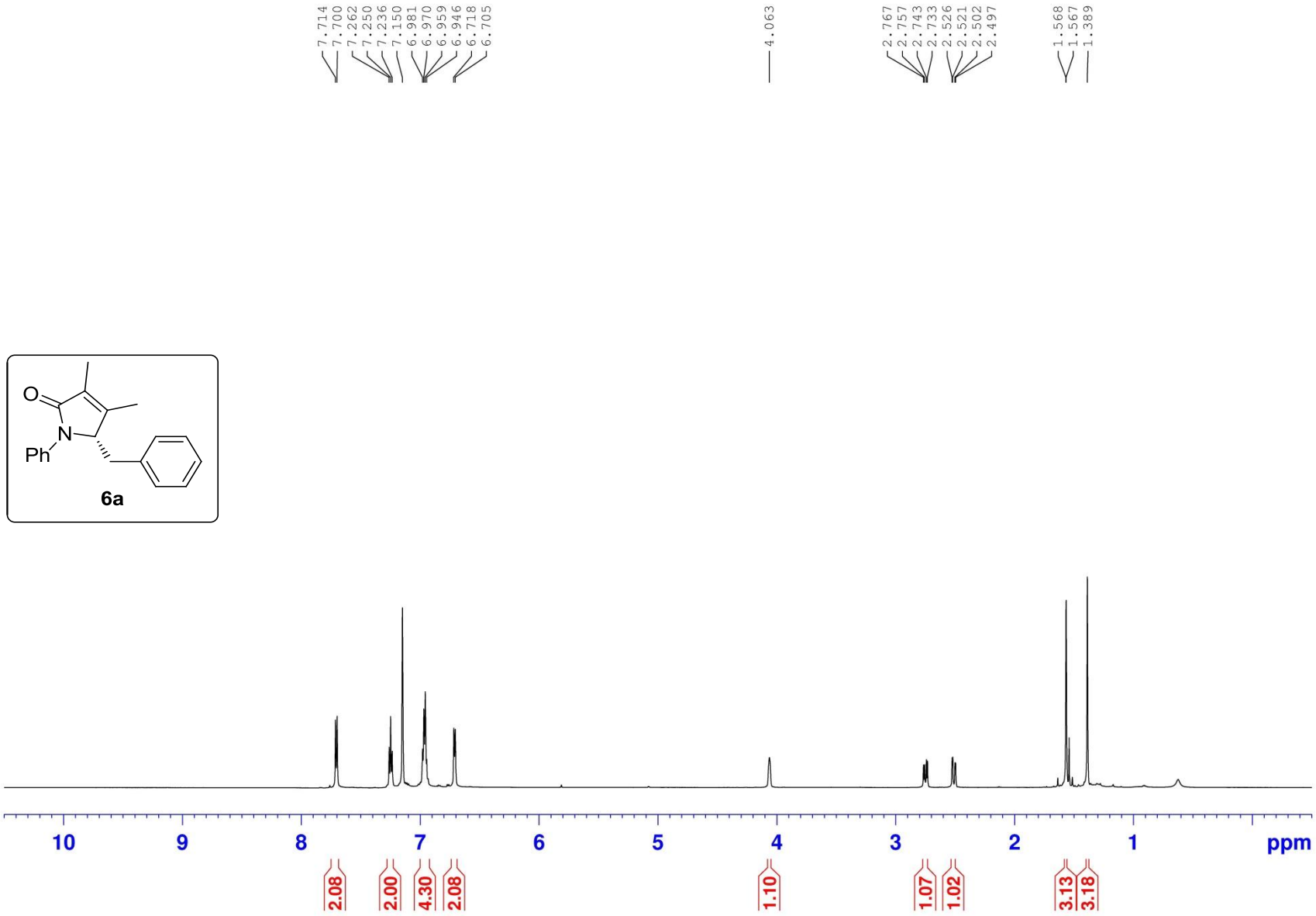
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6.705
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2.757
2.743
2.733
2.526
2.521
2.502
2.497
1.568
1.567
1.389
O
N
Ph
6a
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8
7
6
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ppm
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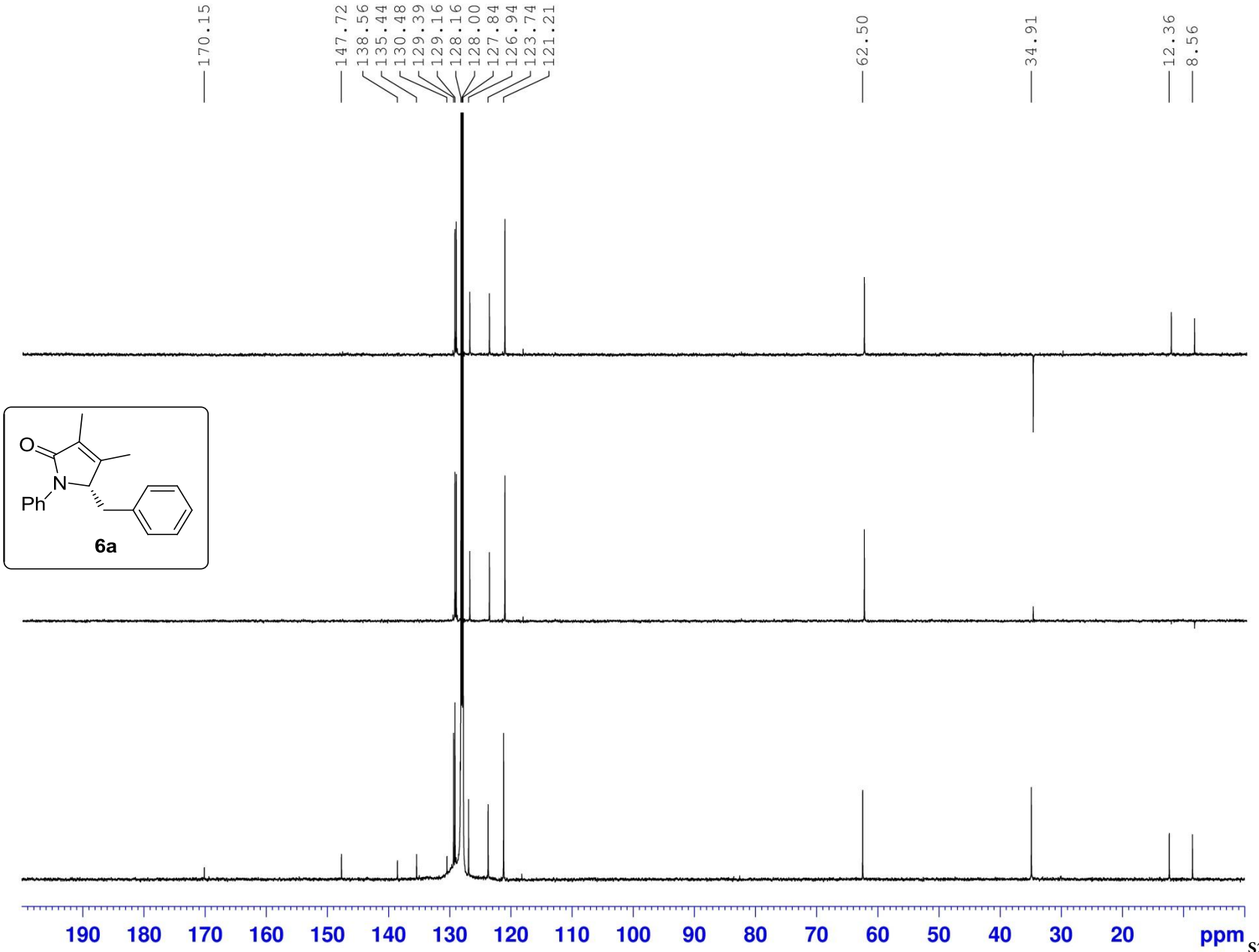
1.02
3.13
3.18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O
N
Ph
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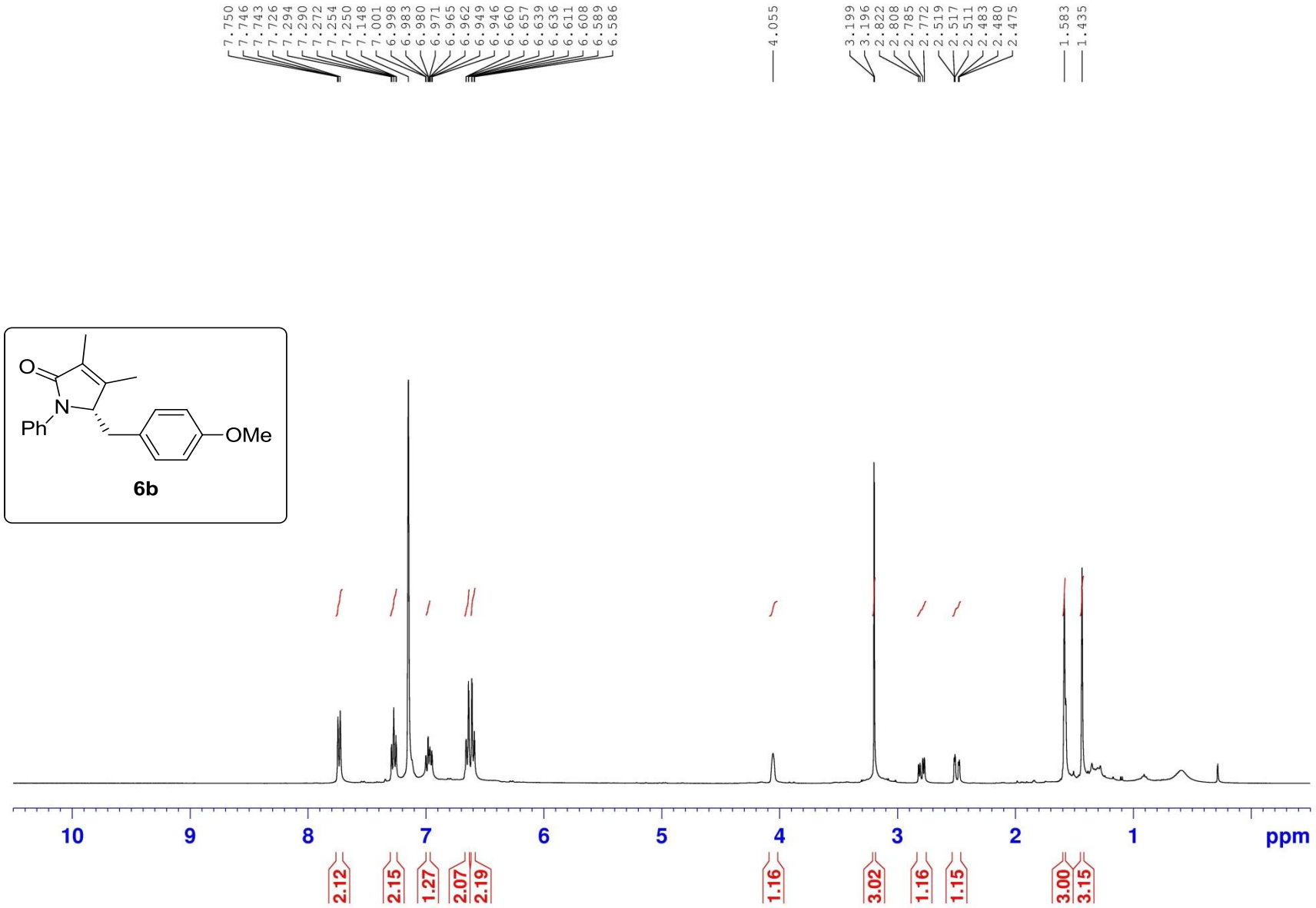
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6.949
6.946
6.660
6.657
6.639
6.636
6.611
6.608
6.589
6.586
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2.808
2.785
2.772
2.519
2.517
2.511
2.483
2.480
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1.435
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N
Ph
OMe
6b
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9
8
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4
3
2
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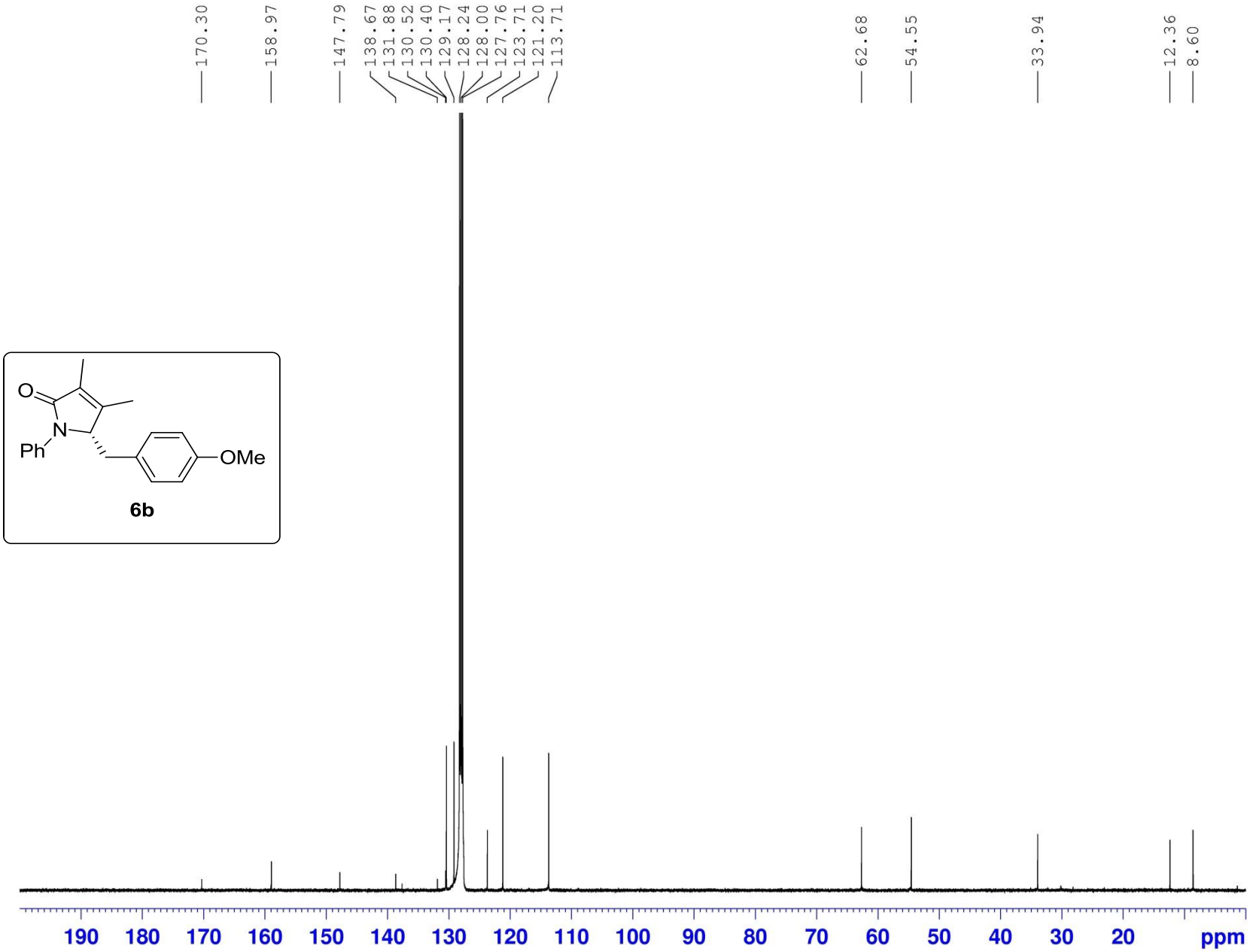
3.00
3.15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33.94
12.36
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N
Ph
OMe
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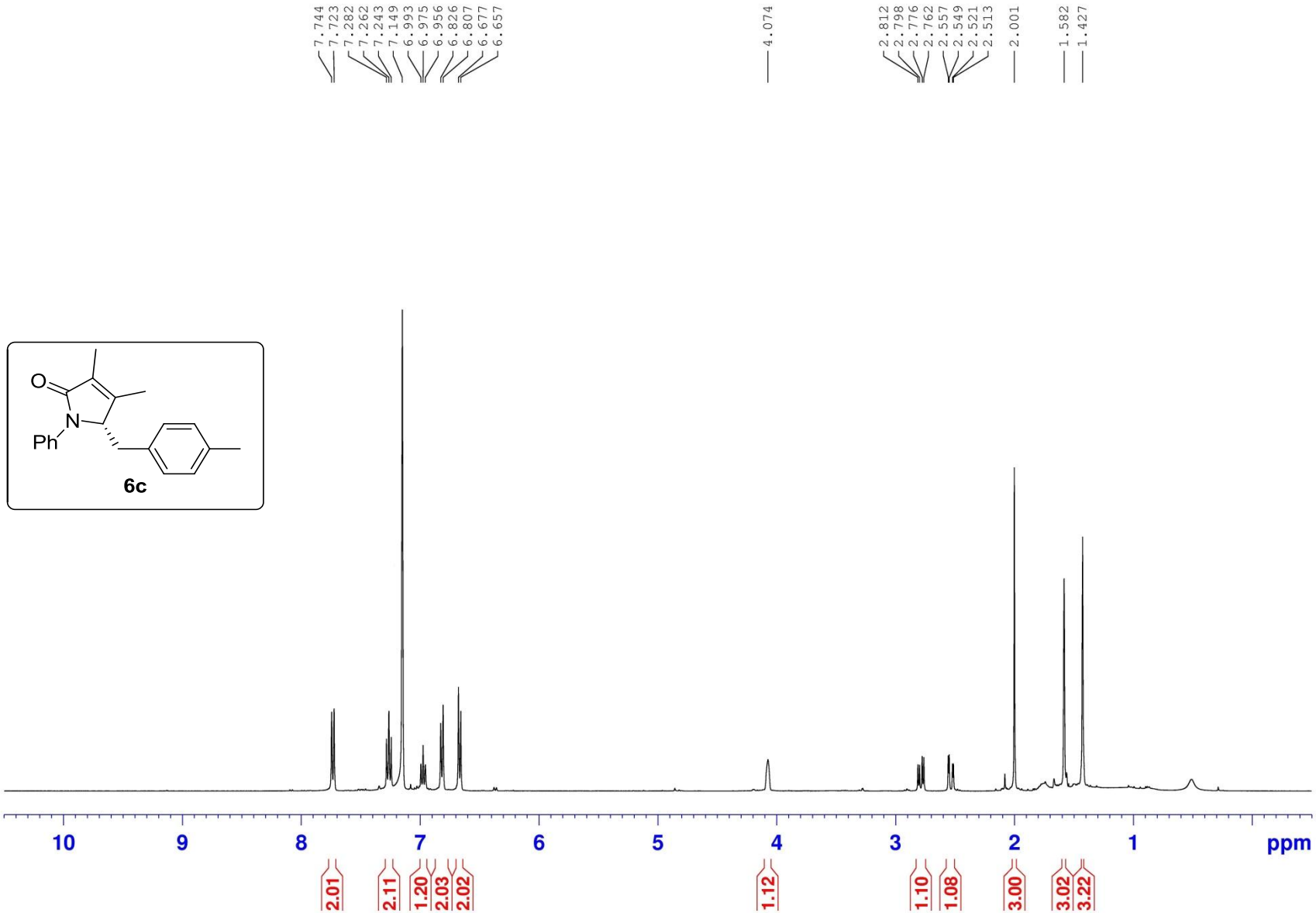
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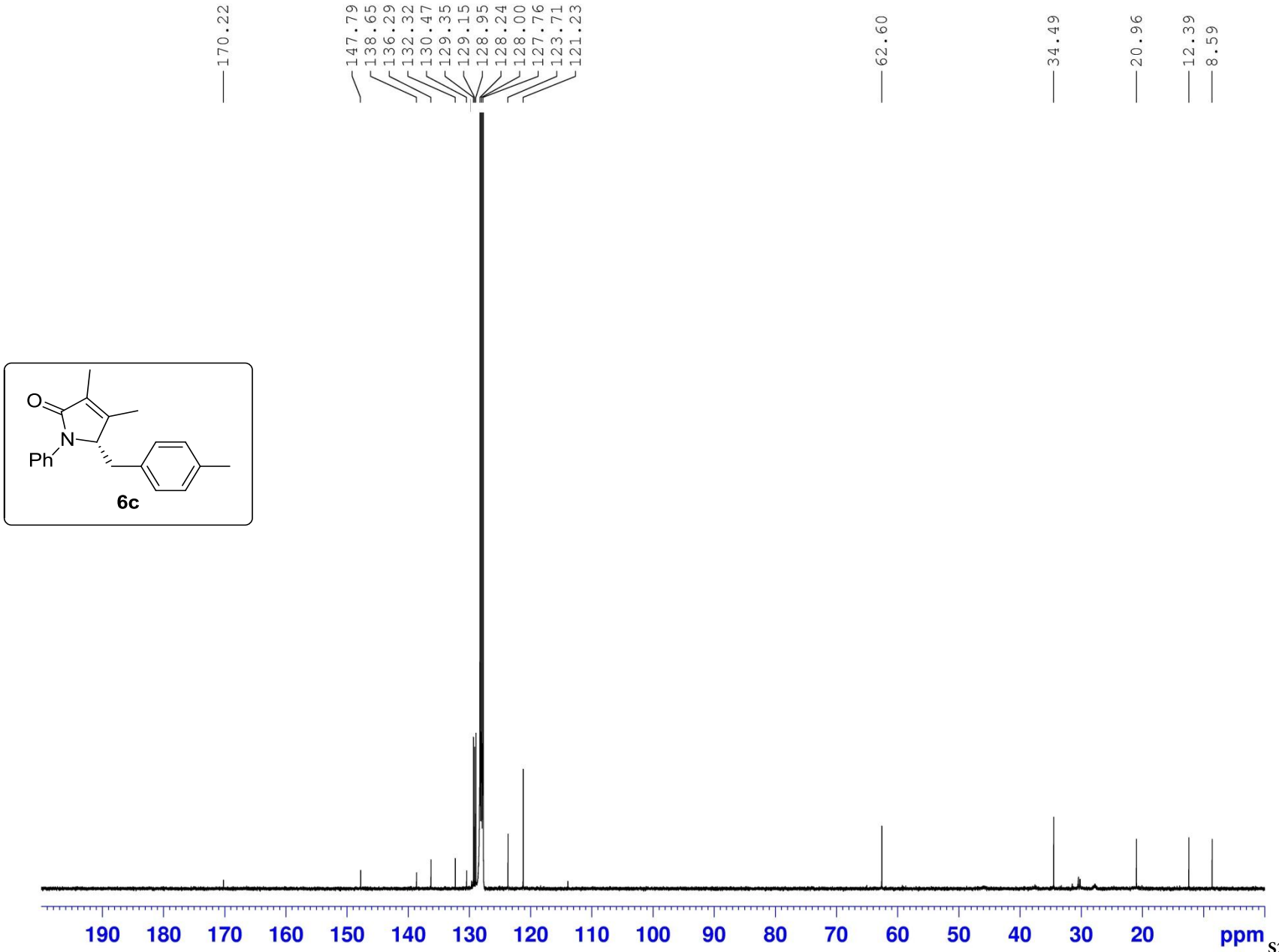
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8.59
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N
Ph
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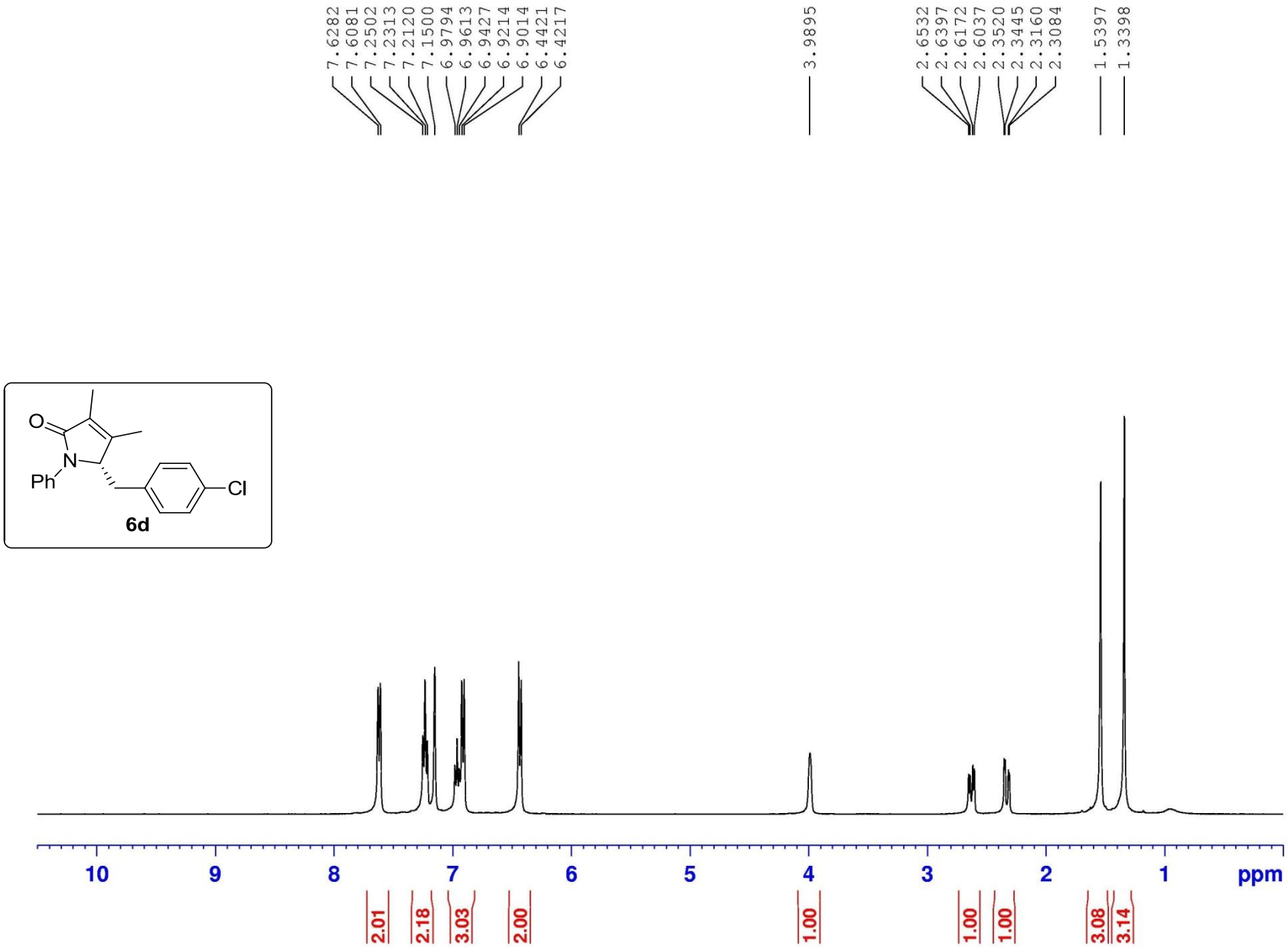
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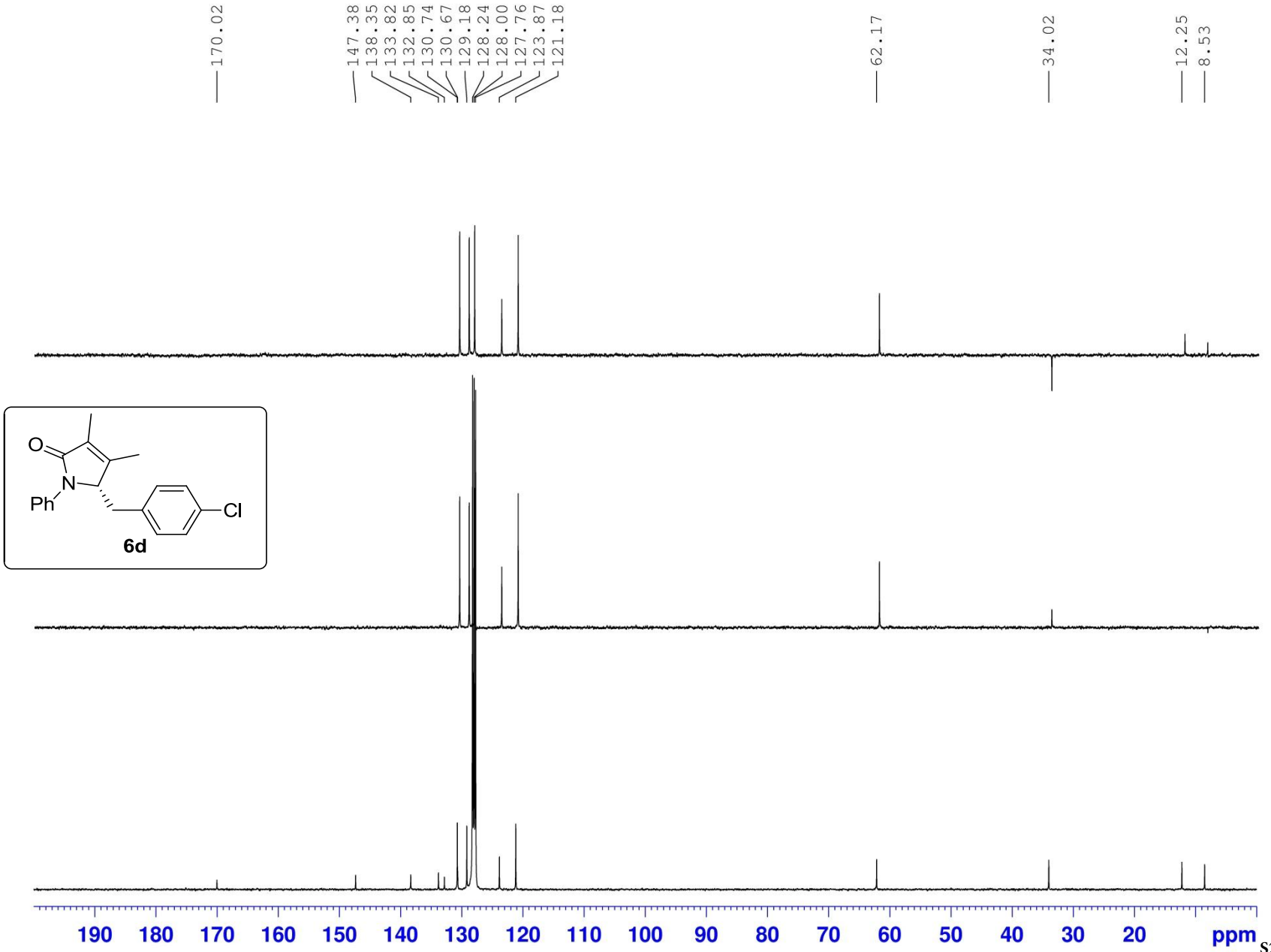
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N
Ph
Cl
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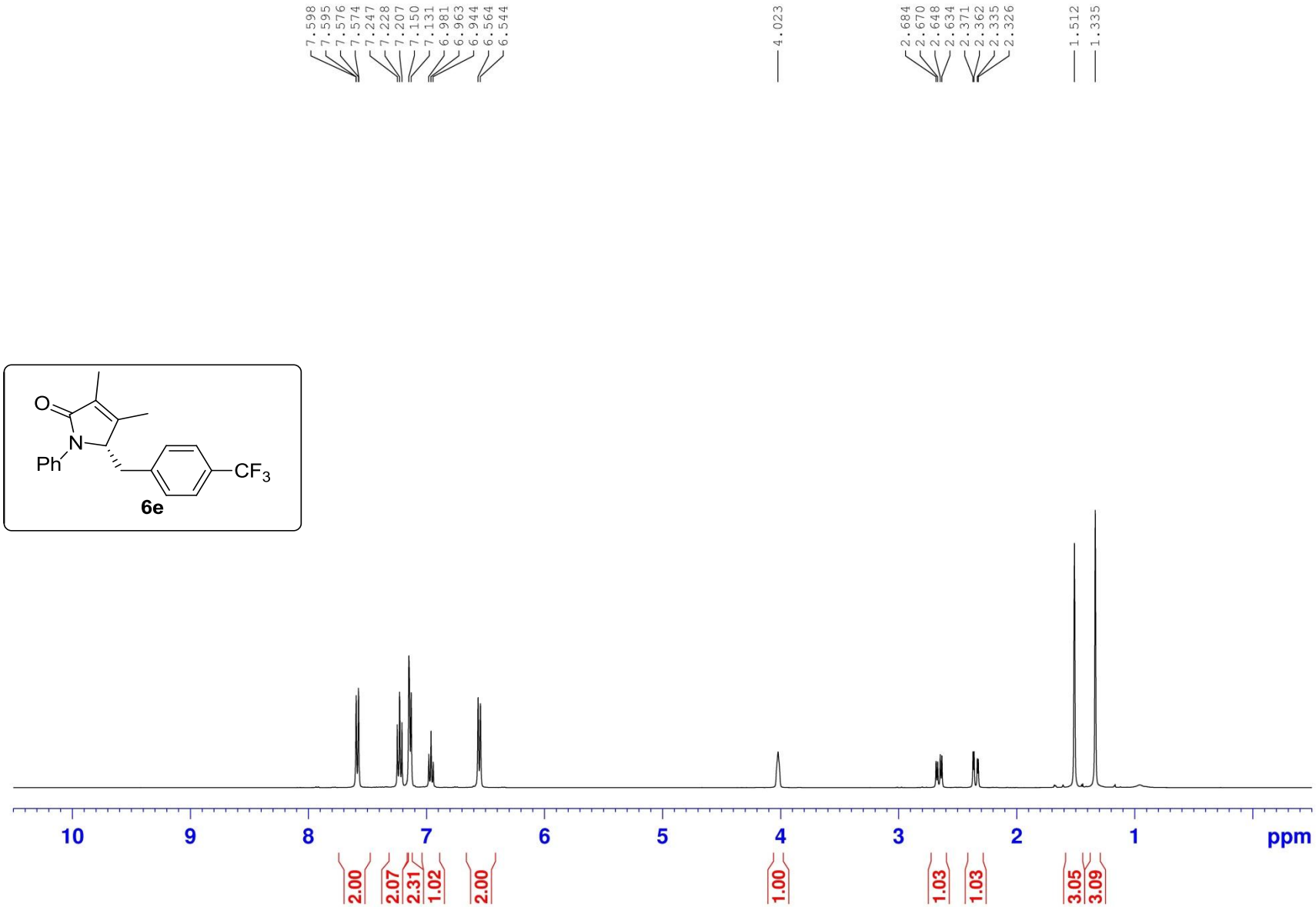
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4
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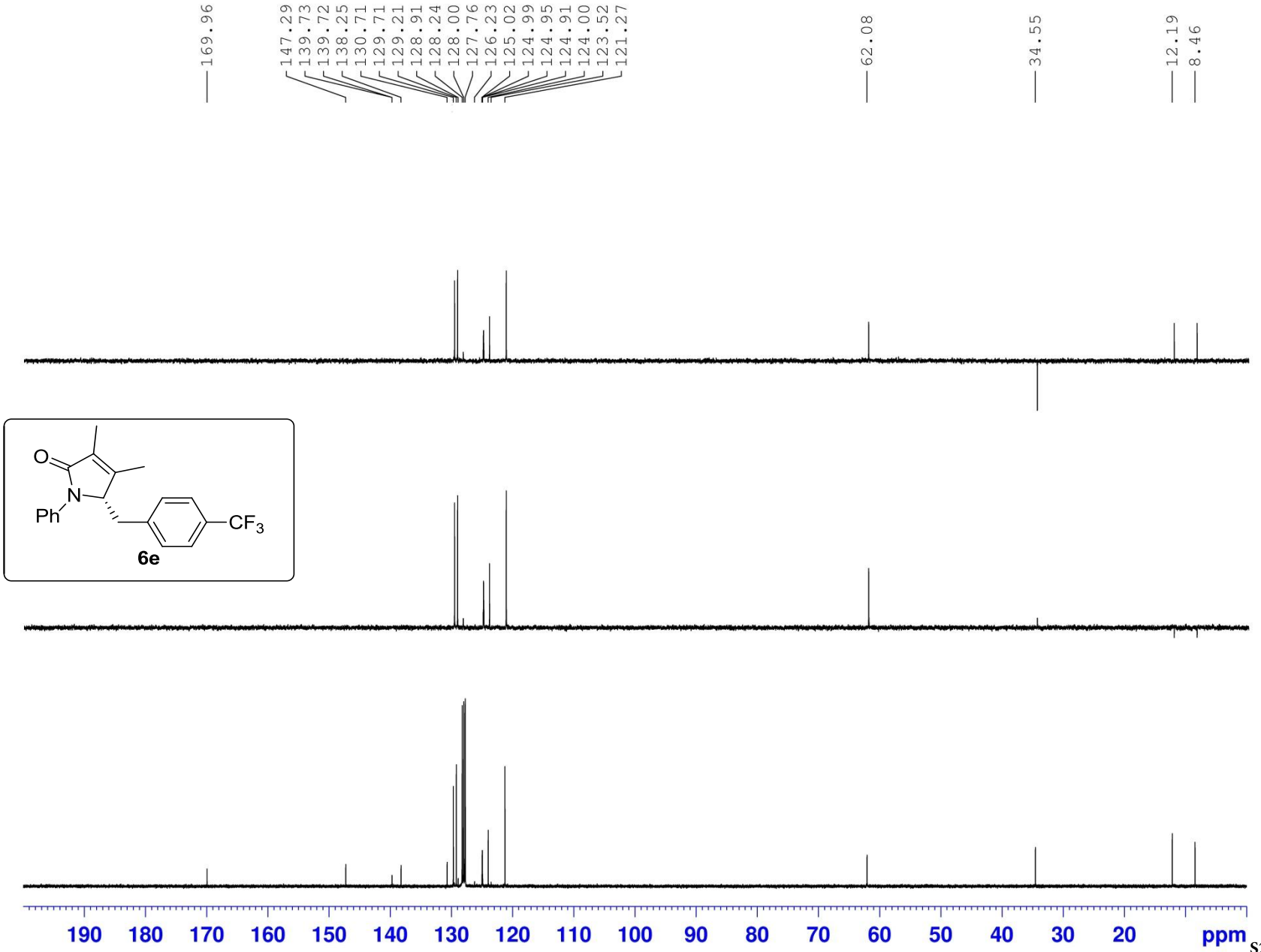
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124.00
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12.19
8.46
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N
Ph
CF3
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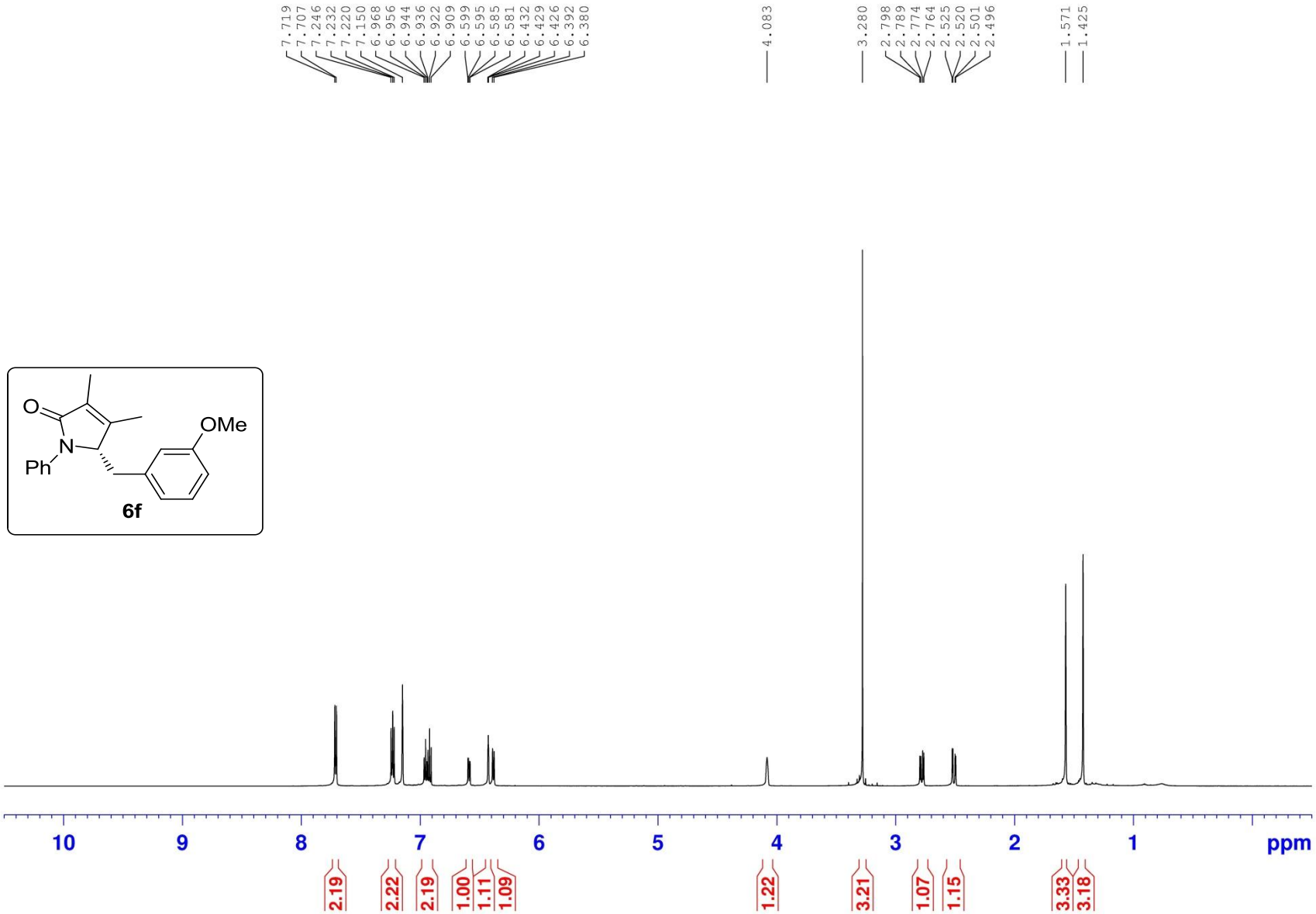
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Ph
OMe
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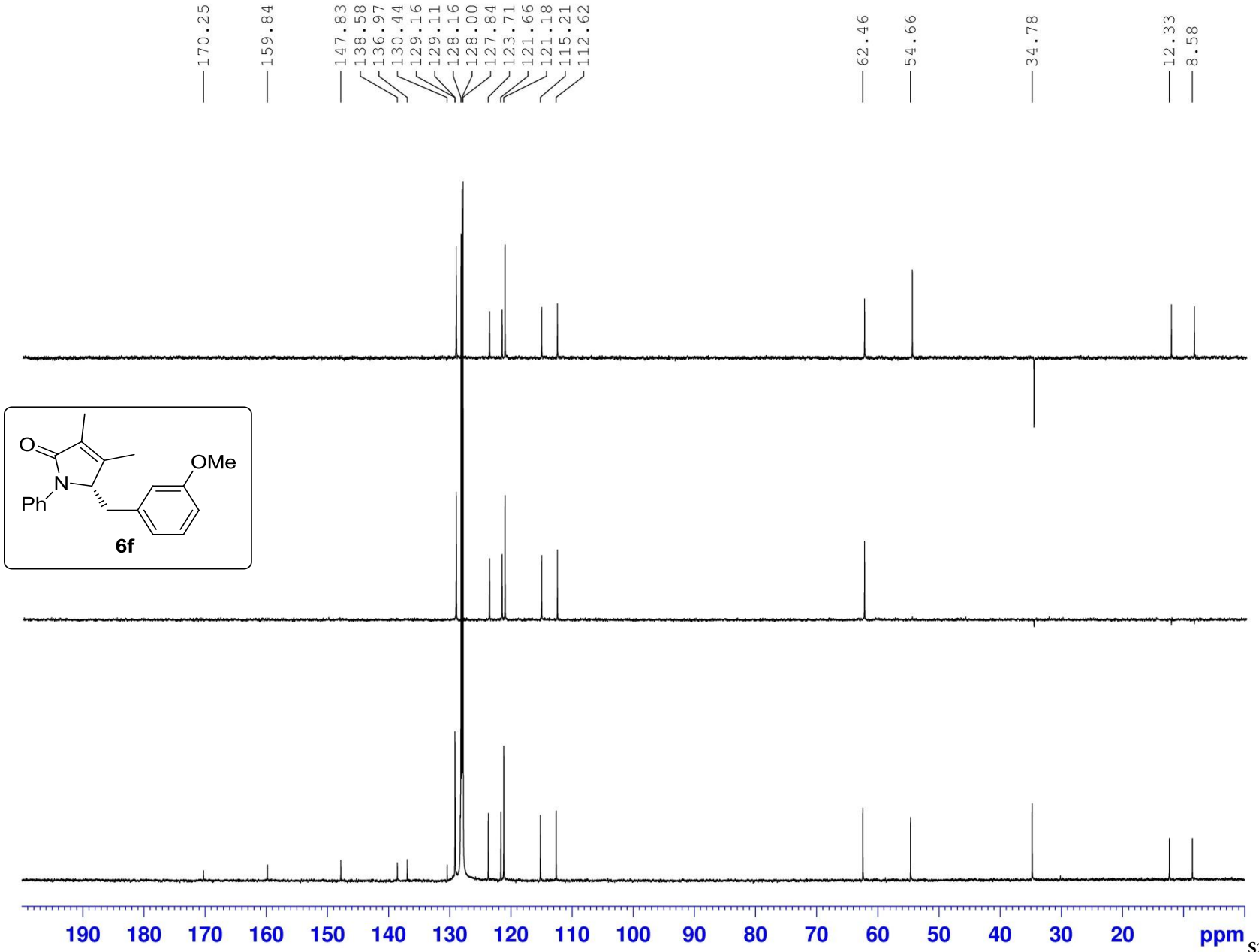
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Ph
OMe
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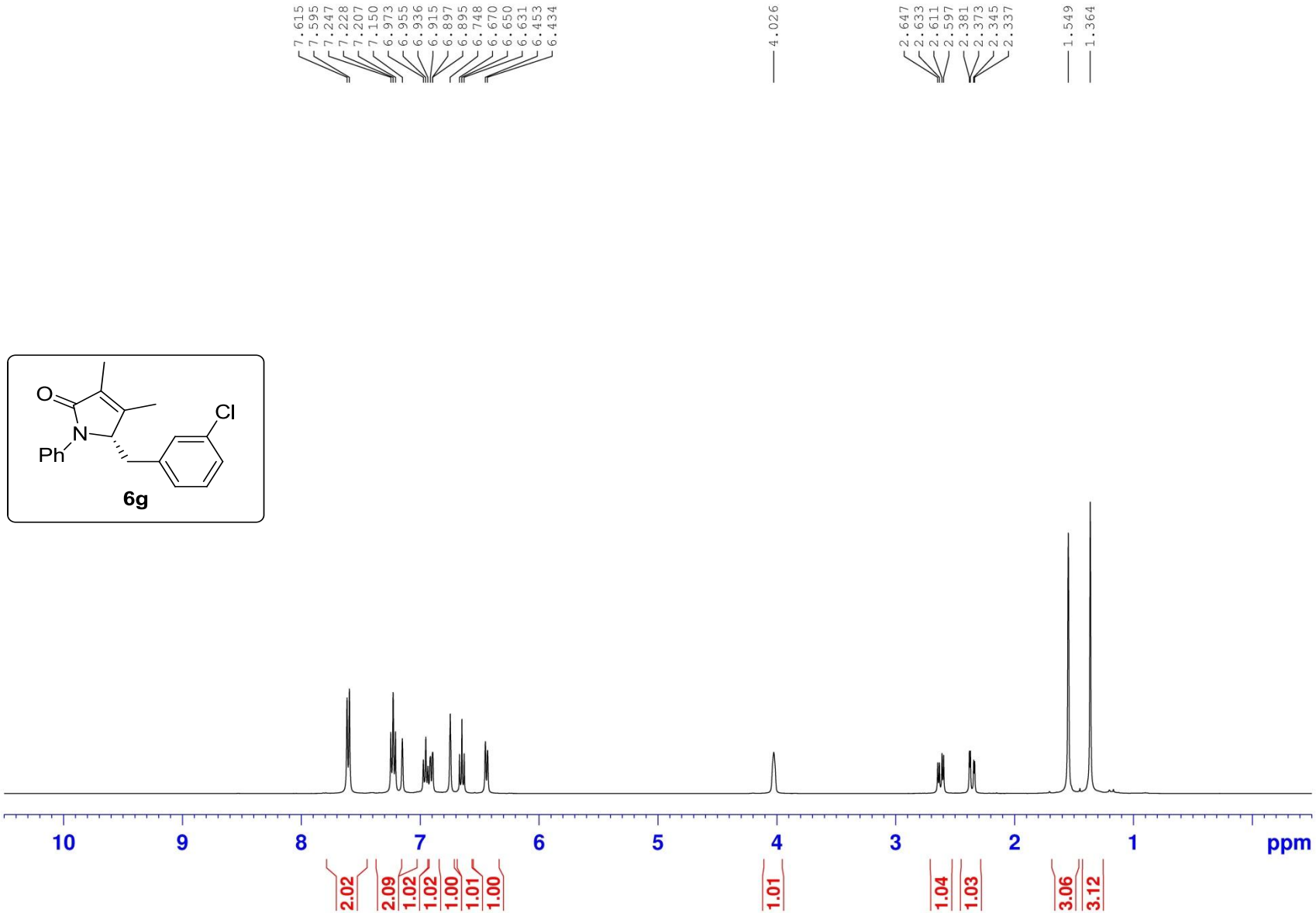
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Cl
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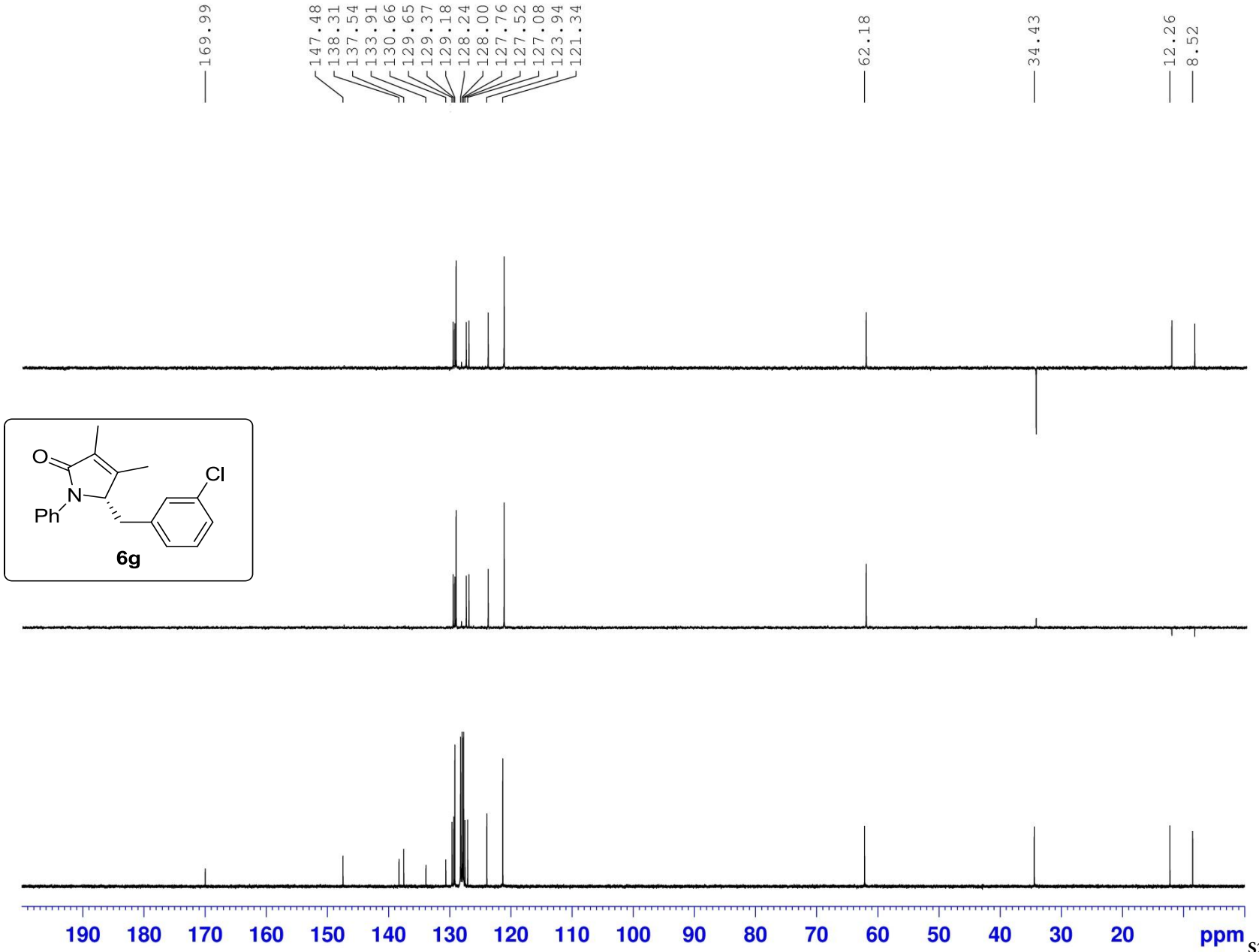
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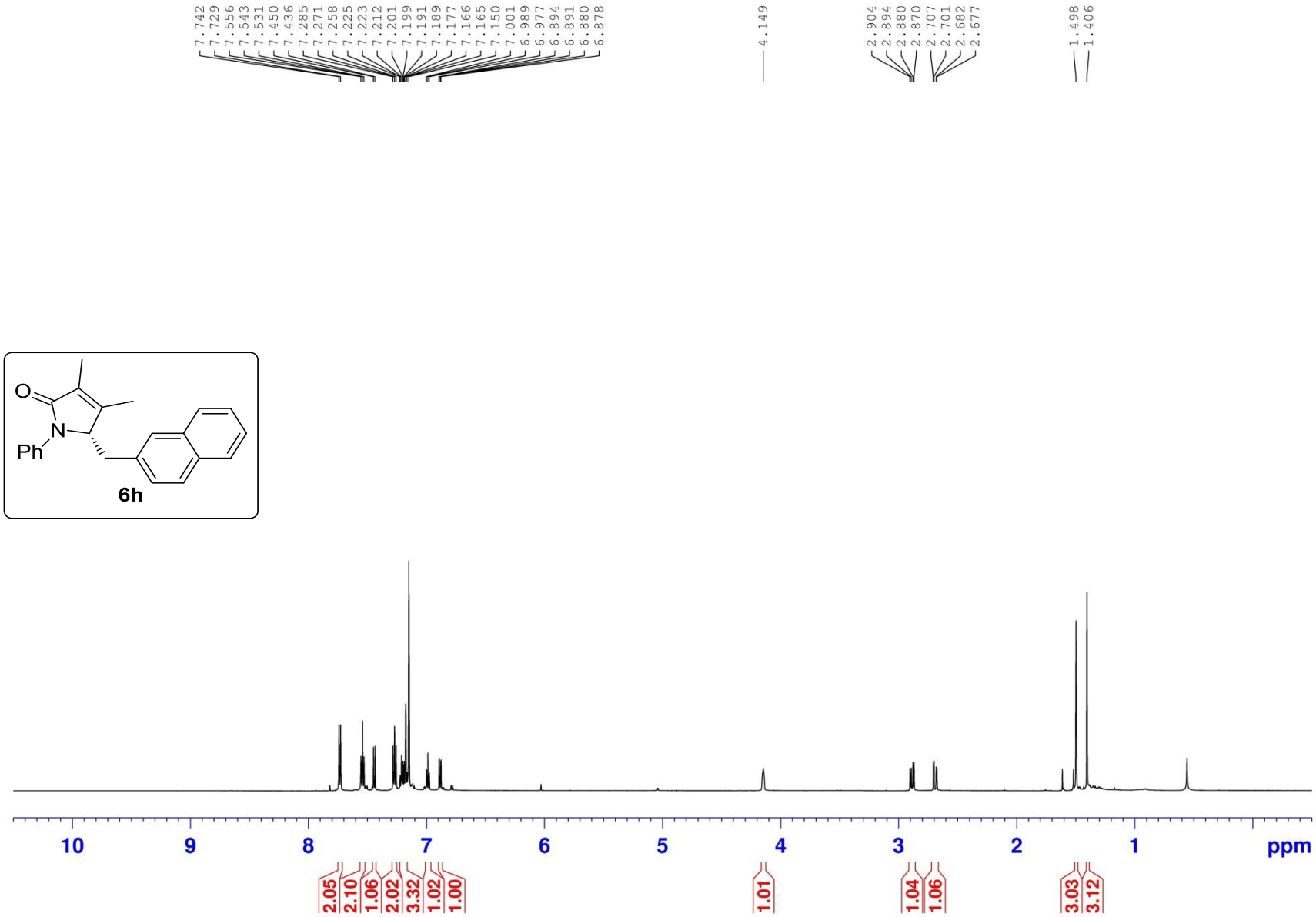
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7.165
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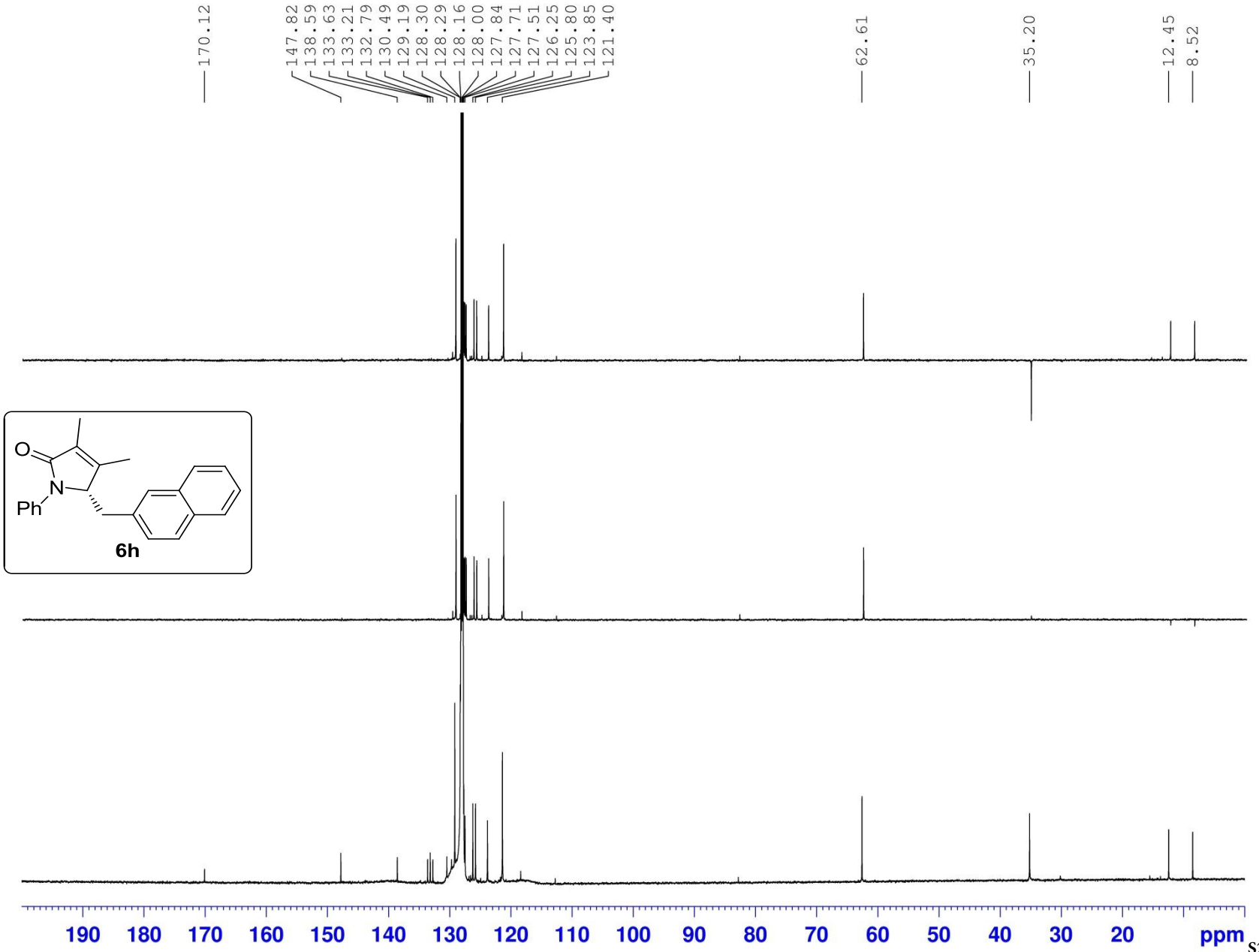
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8.52
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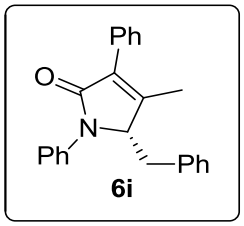
ppm


Ph
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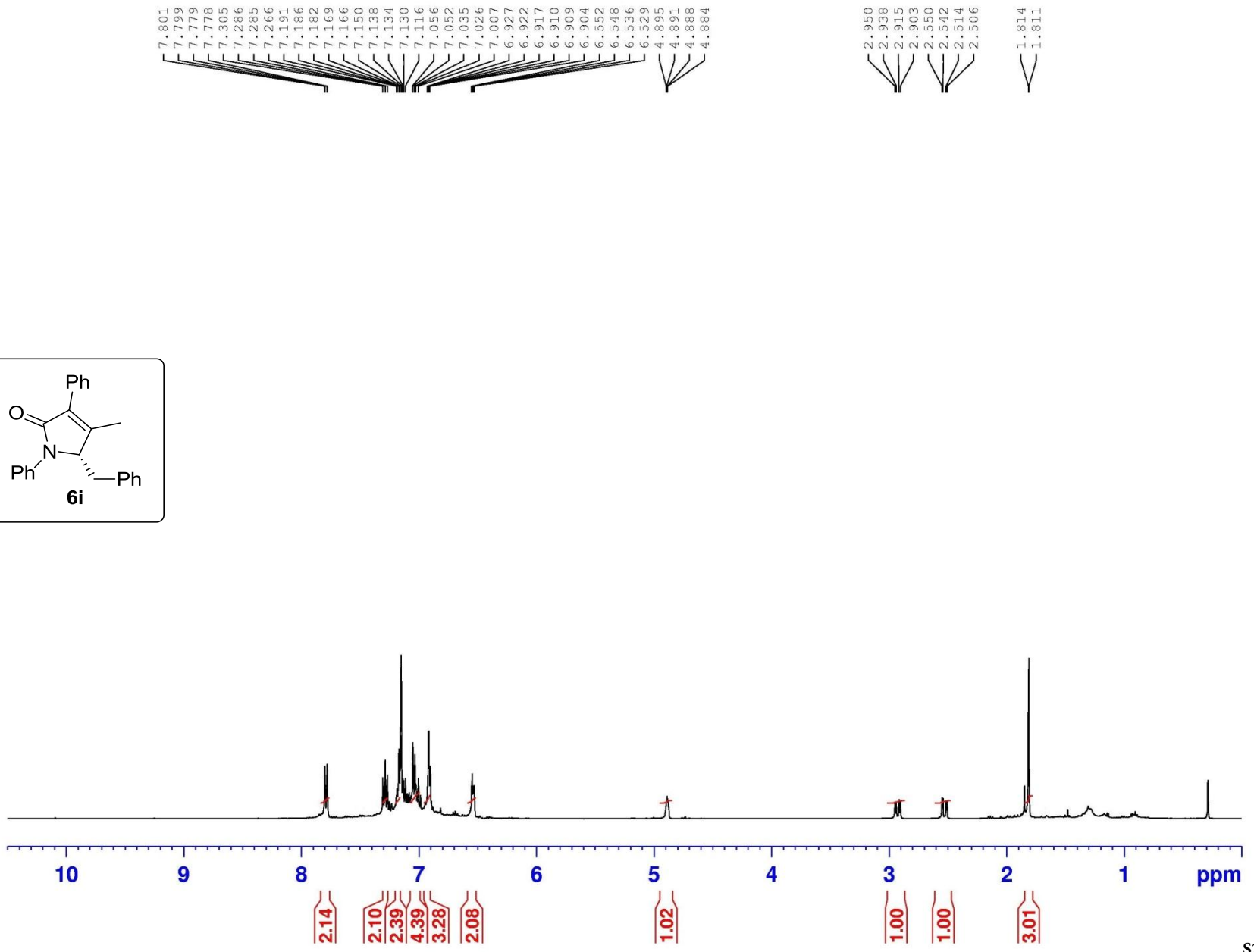
6i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6
5
4
3
2
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ppm
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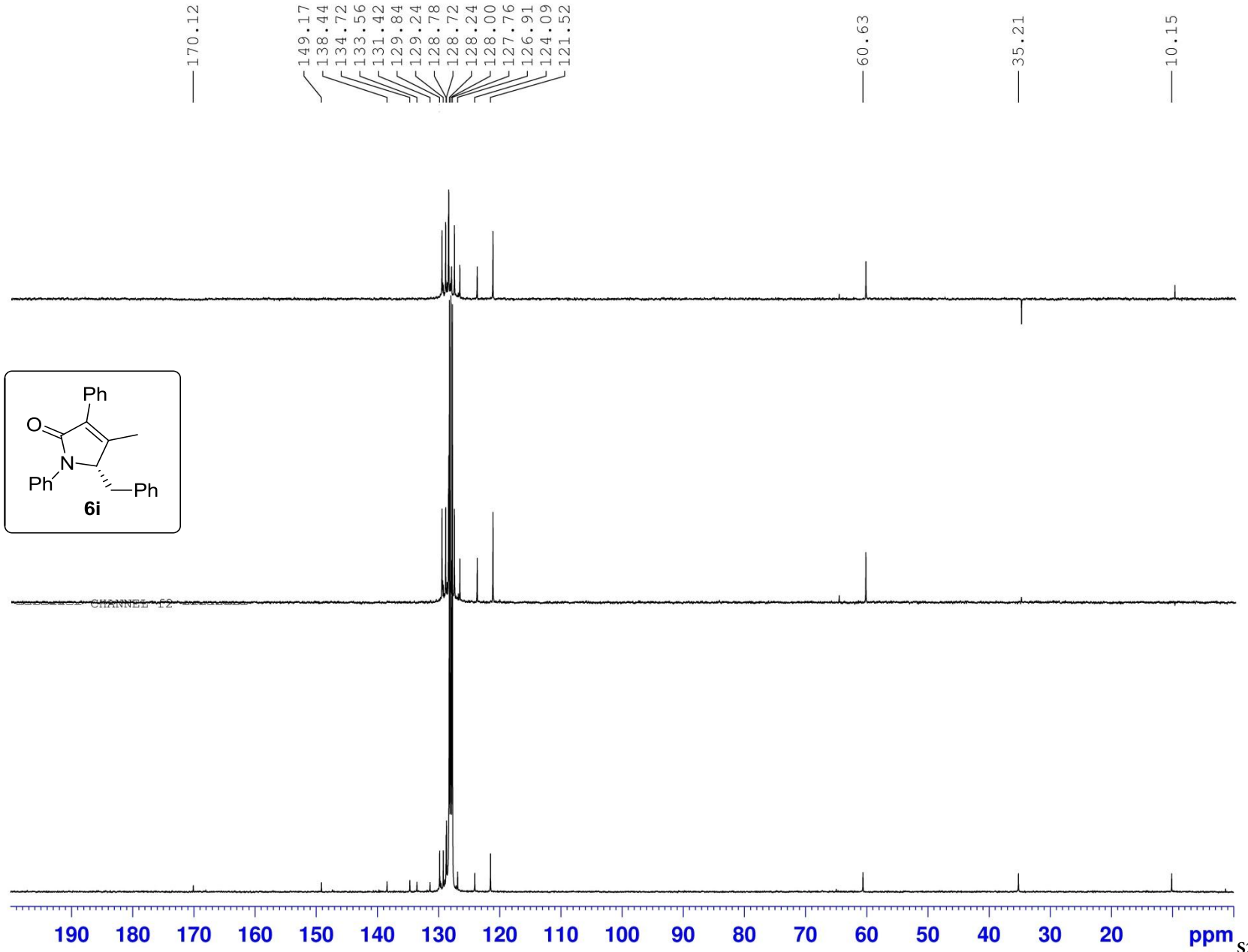
2.10
2.39
4.39
3.28
2.08
1.02
1.00
1.00
3.01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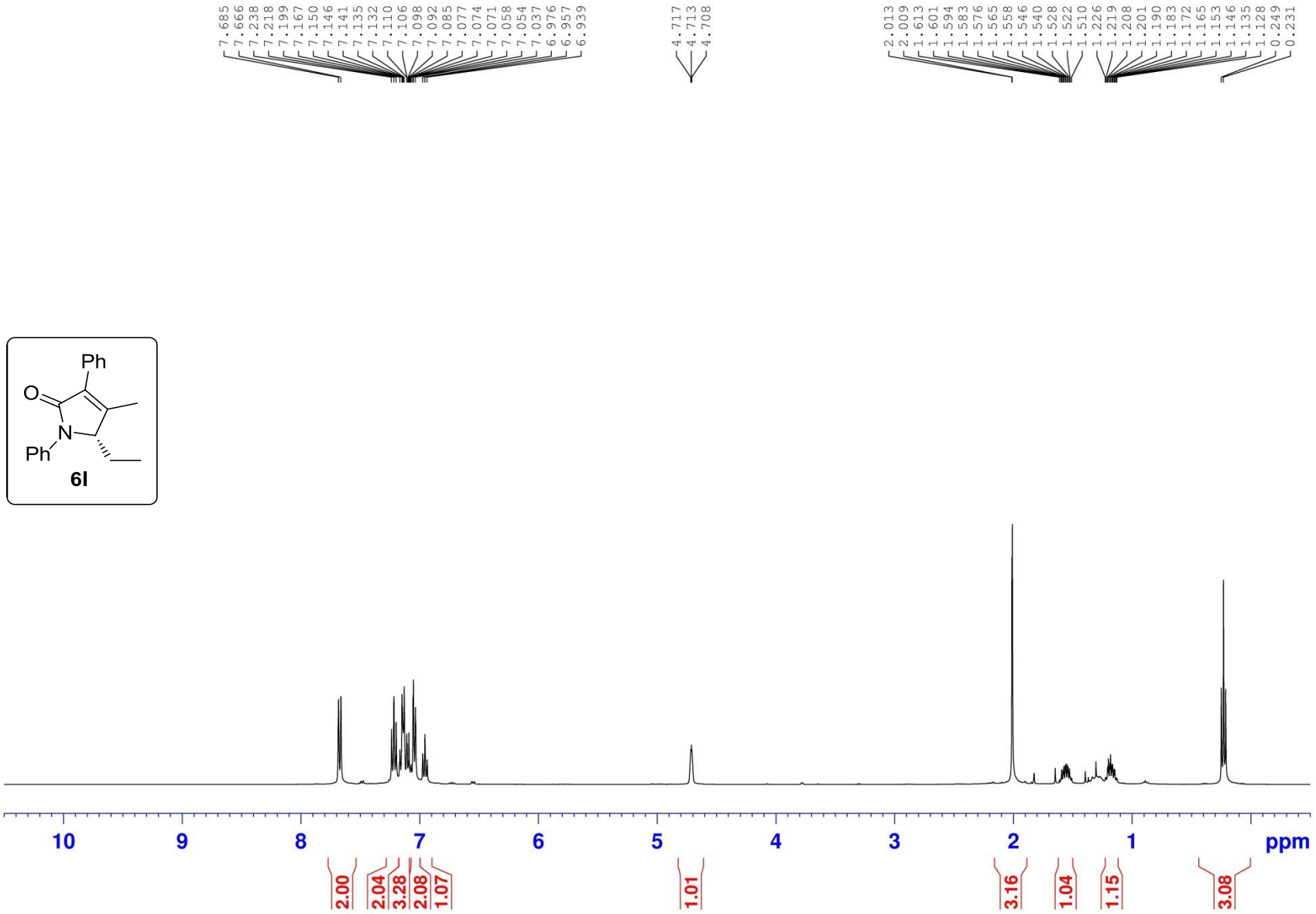
149.17
138.44
134.72
133.56
131.42
129.84
129.24
128.78
128.72
128.24
128.00
127.76
126.91
124.09
121.52
60.63
35.21
10.15
Ph
O
N
Ph
Ph
6i
CHANNEL f2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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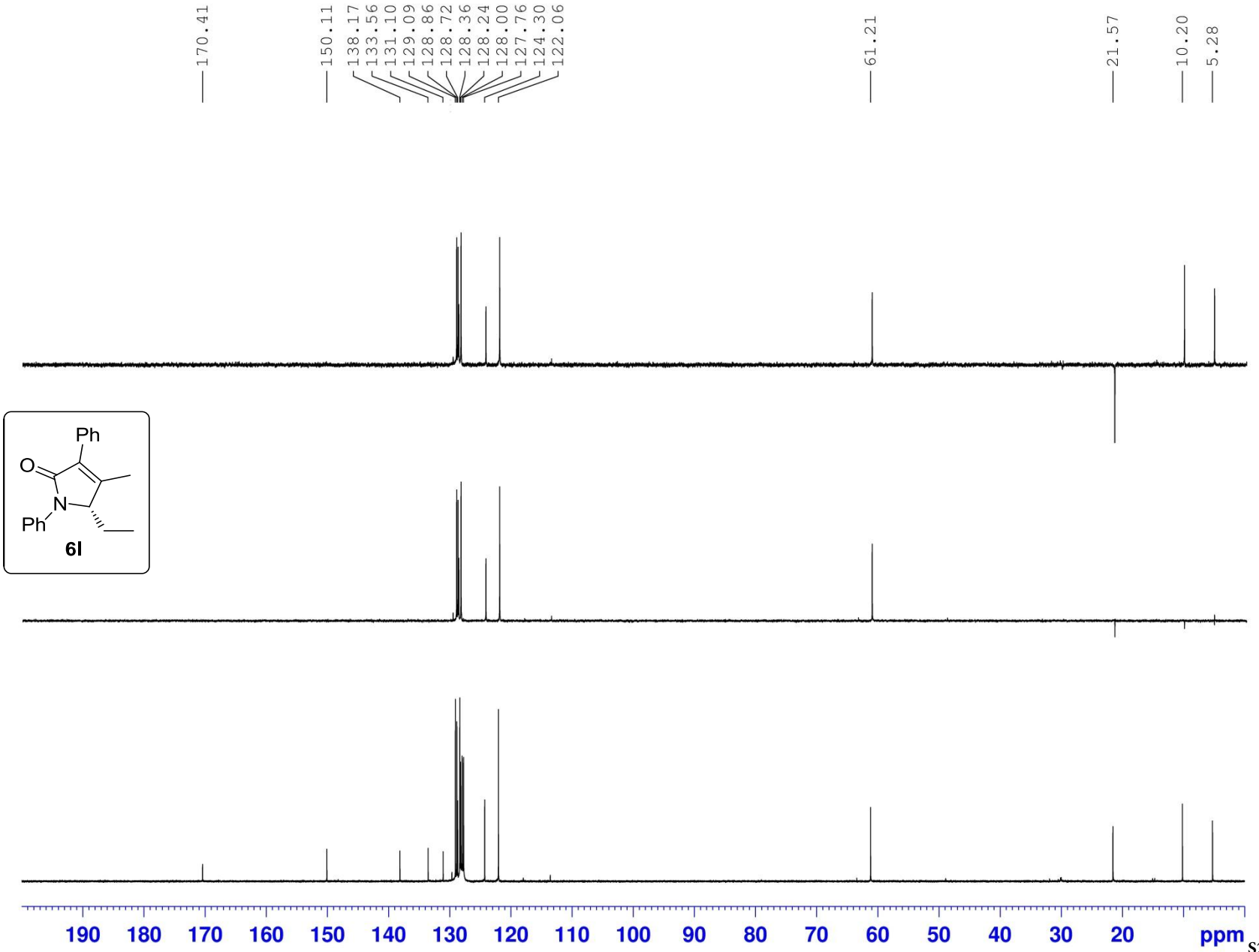
7.666
7.238
7.218
7.199
7.167
7.150
7.146
7.141
7.135
7.132
7.110
7.106
7.098
7.092
7.085
7.077
7.074
7.071
7.058
7.054
7.037
6.976
6.957
6.939
4.717
4.713
4.708
2.013
2.009
1.613
1.601
1.594
1.583
1.576
1.565
1.558
1.546
1.540
1.528
1.522
1.510
1.226
1.219
1.208
1.201
1.190
1.183
1.172
1.165
1.153
1.146
1.135
1.128
0.249
0.231
Ph
O
N
Ph
6l
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.04
3.28
2.08
1.07
1.01
3.16
1.04
1.15
3.08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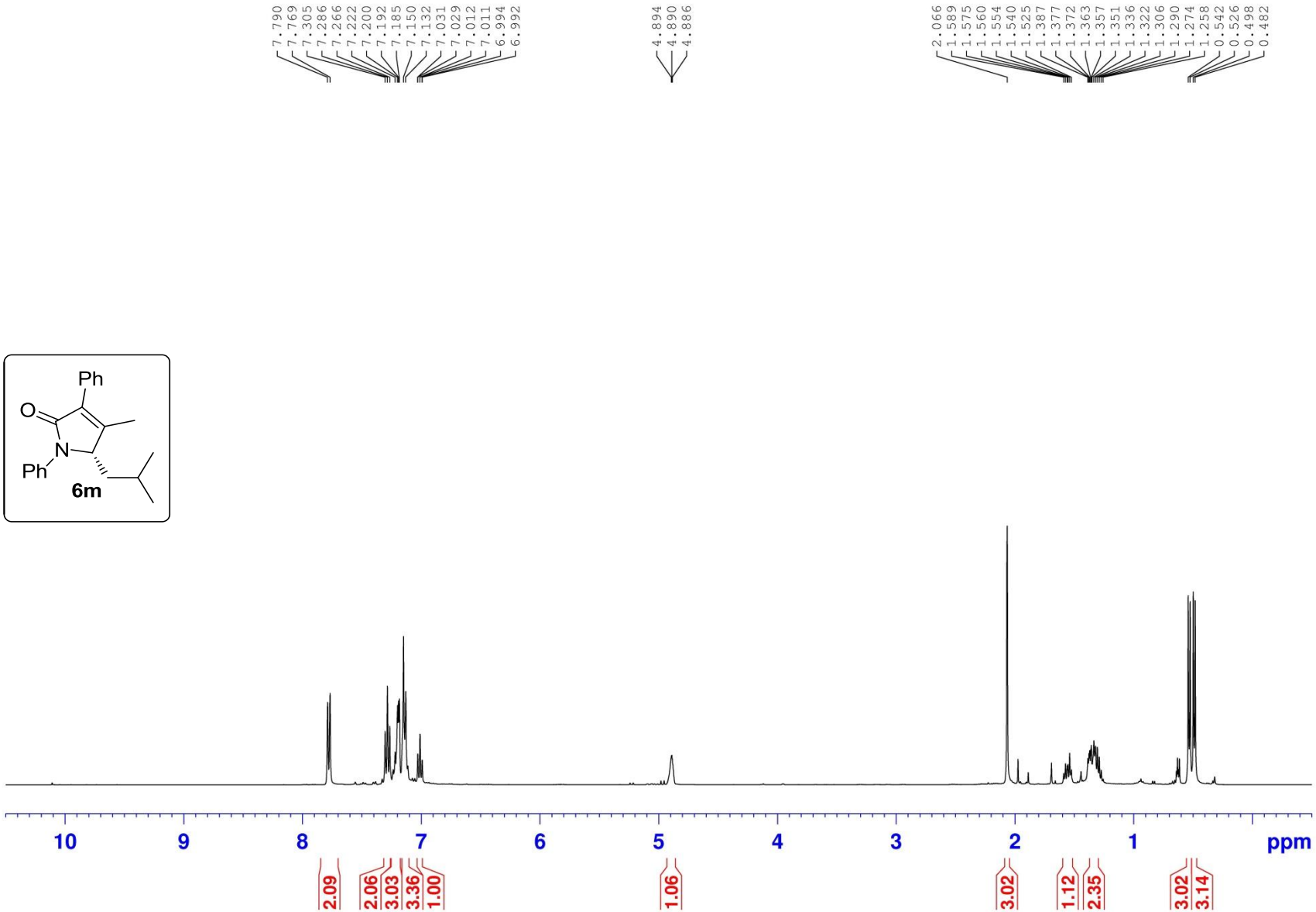
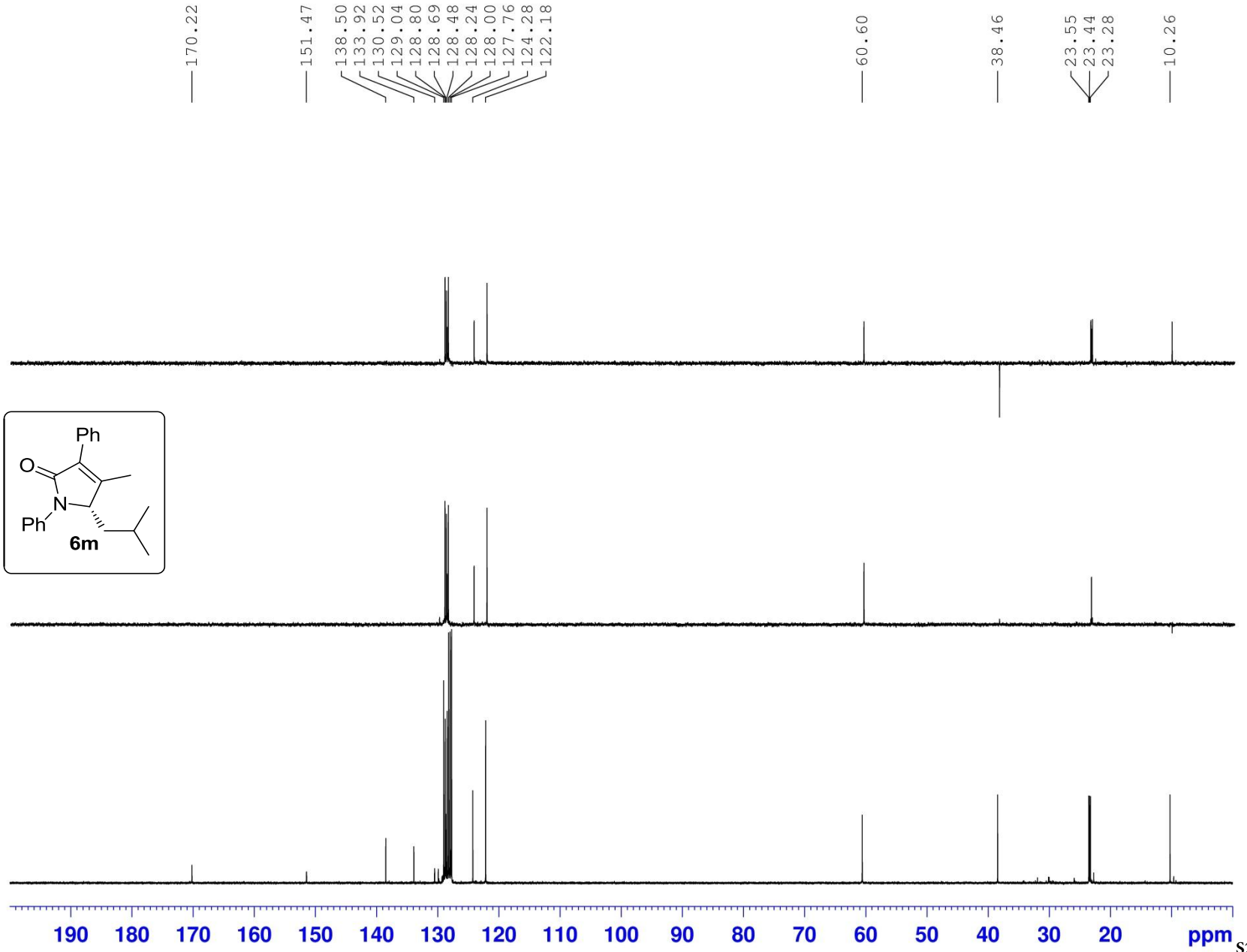
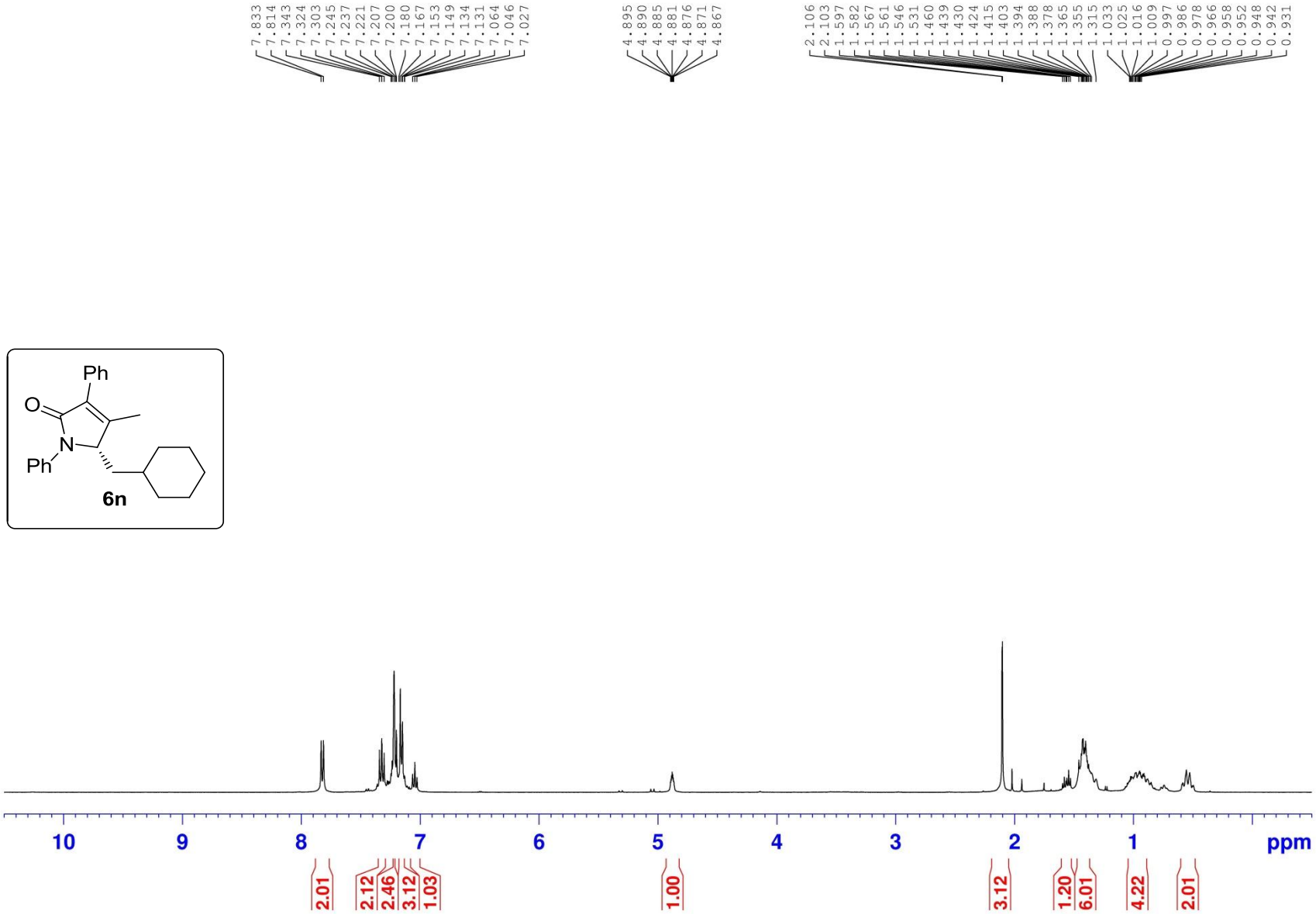
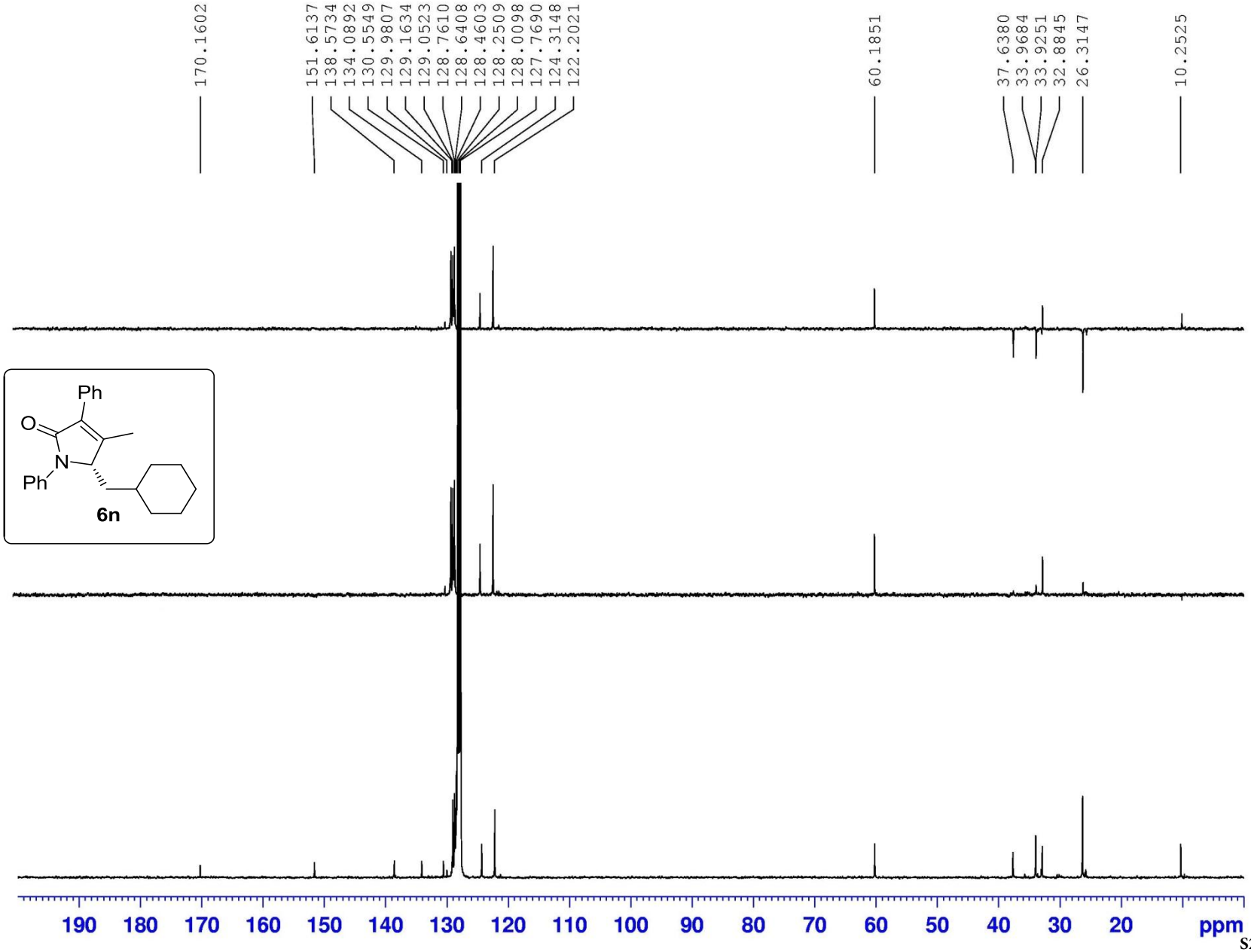
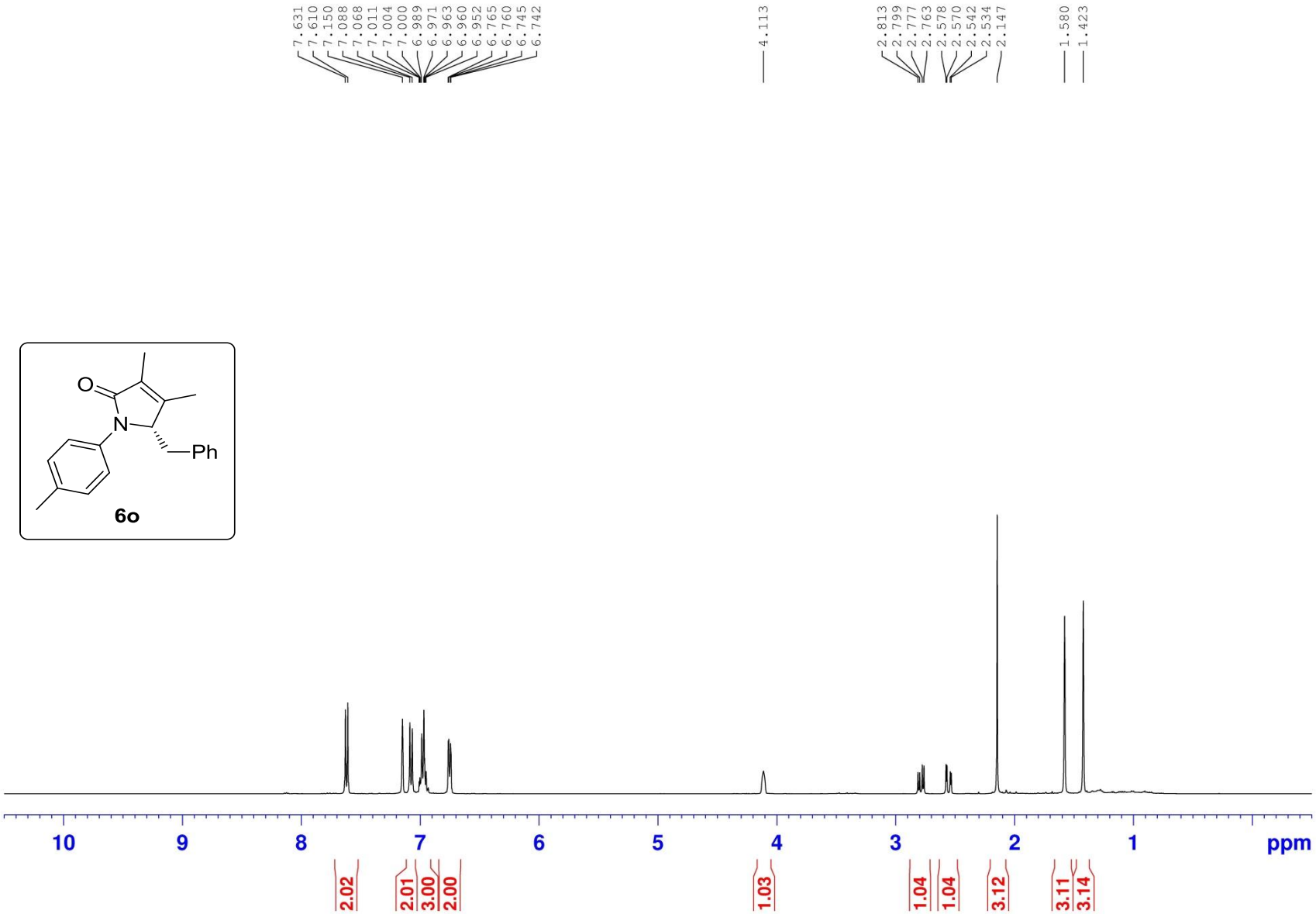
150.11
138.17
133.56
131.10
129.09
128.86
128.72
128.36
128.24
128.00
127.76
124.30
122.06
61.21
21.57
10.20
5.28
Ph
O
N
Ph
6l
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

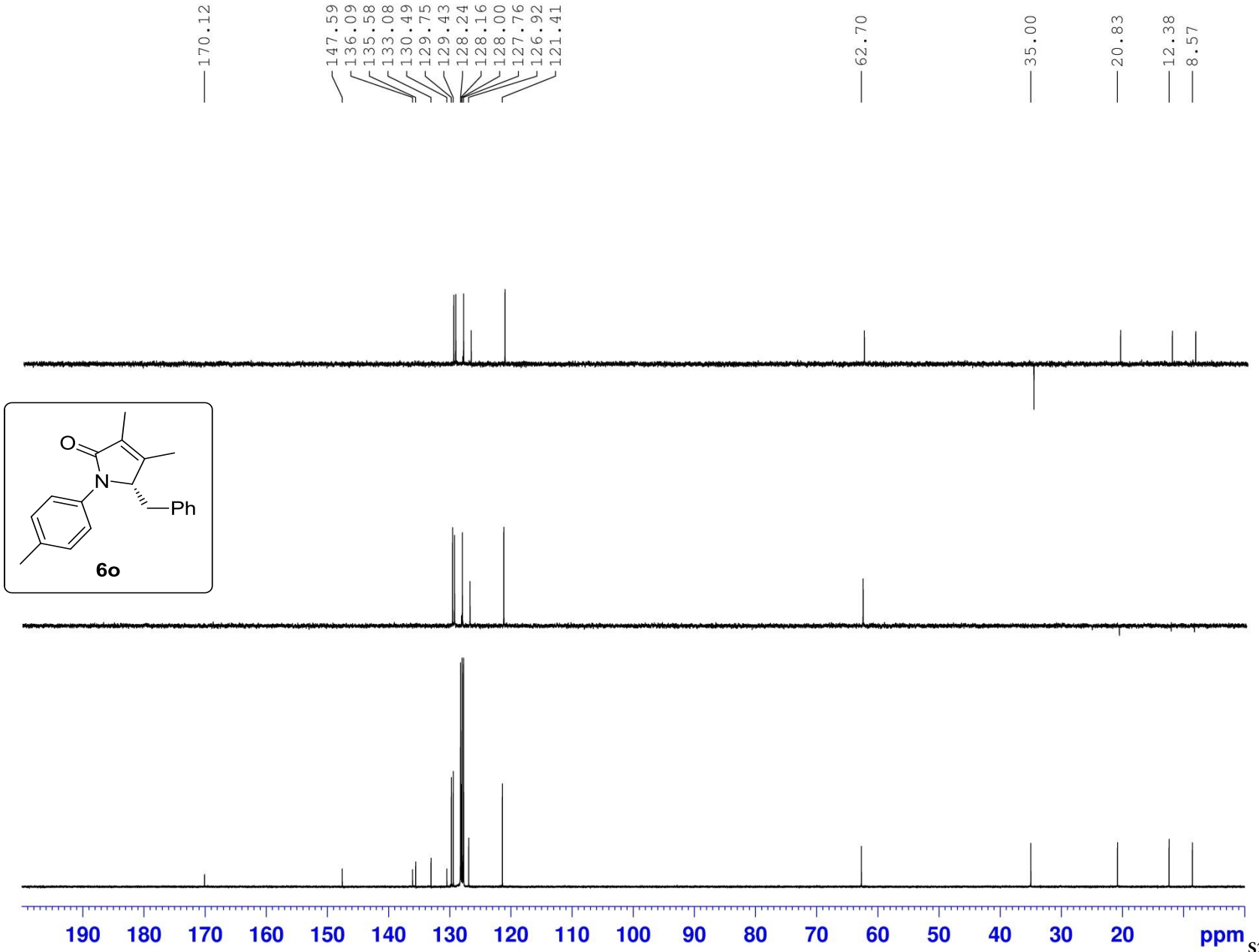

7.790
7.769
7.305
7.286
7.266
7.222
7.200
7.192
7.185
7.150
7.132
7.031
7.029
7.012
7.011
6.994
6.992
4.894
4.890
4.886
2.066
1.589
1.575
1.560
1.554
1.540
1.525
1.387
1.377
1.372
1.363
1.357
1.351
1.336
1.322
1.306
1.290
1.274
1.258
0.542
0.526
0.498
0.482
Ph
O
N
Ph
6m
10
9
8
7
6
5
4
3
2
1
ppm
2.09
2.06
3.03
3.36
1.00
1.06
3.02
1.12
2.35
3.02
3.14

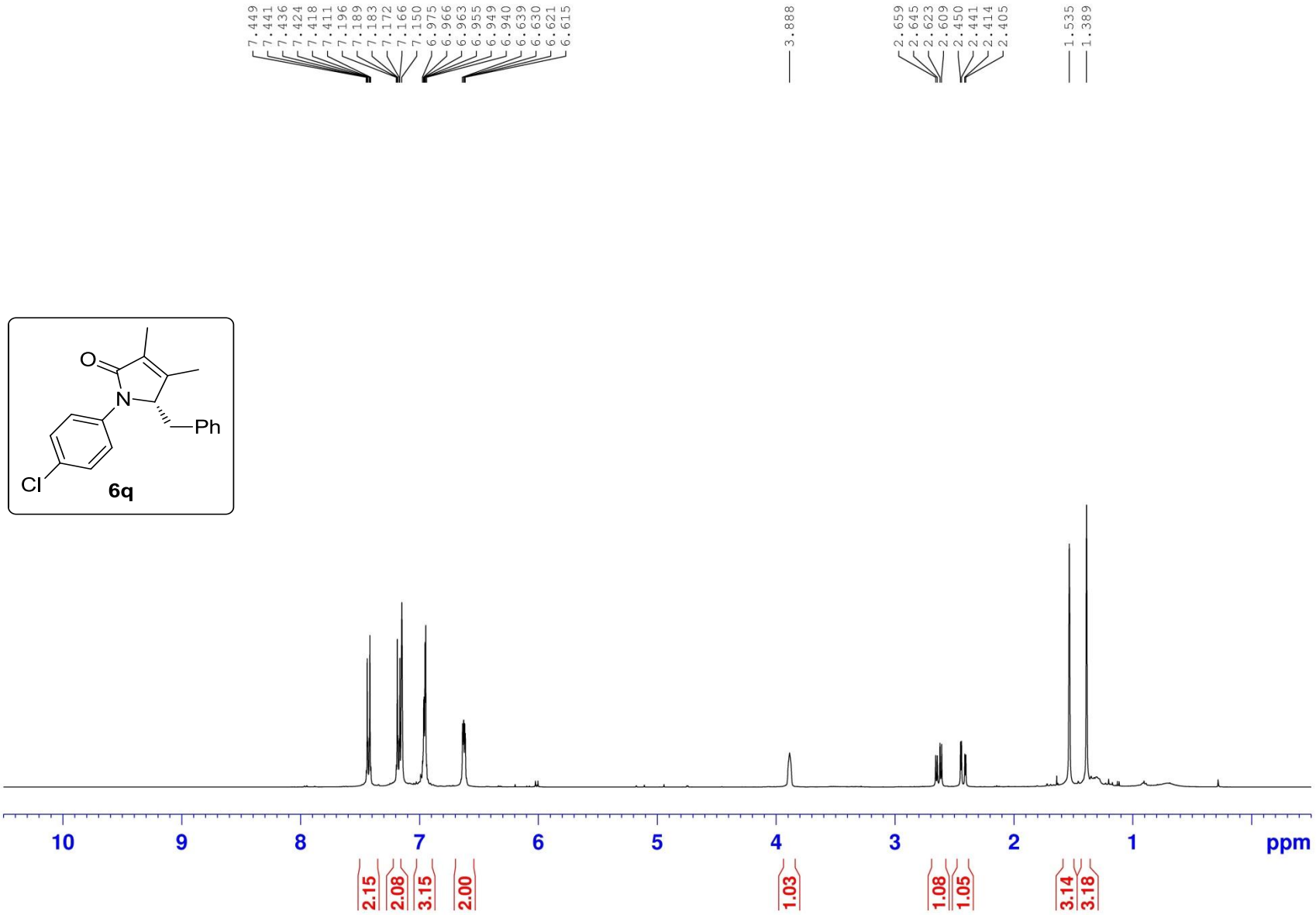

170.22
151.47
138.50
133.92
130.52
129.04
128.80
128.69
128.48
128.24
128.00
127.76
124.28
122.18
60.60
38.46
23.55
23.44
23.28
10.26
Ph
O
N
Ph
6m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

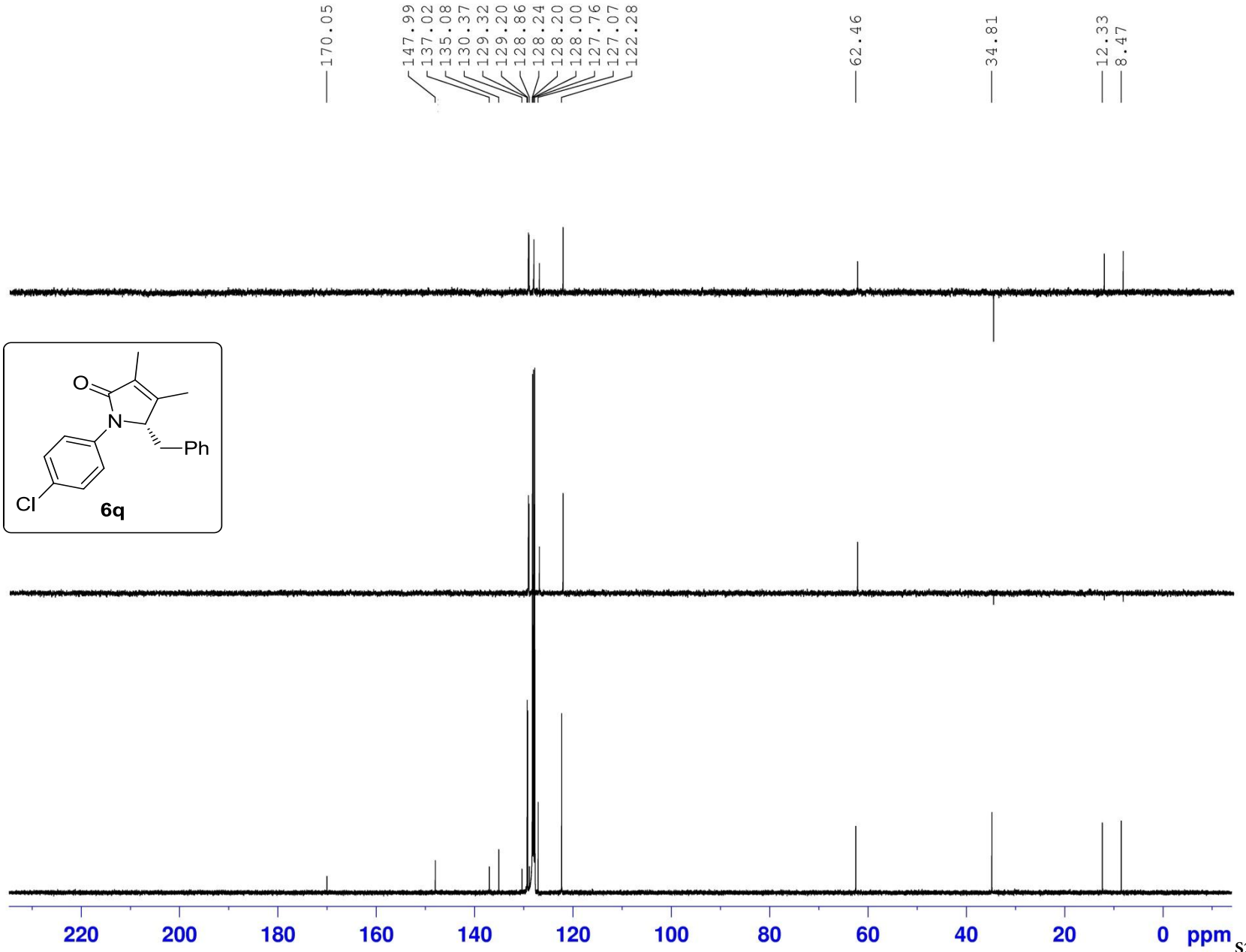

7.833
7.814
7.343
7.324
7.303
7.245
7.237
7.221
7.207
7.200
7.180
7.167
7.153
7.149
7.134
7.131
7.064
7.046
7.027
4.895
4.890
4.885
4.881
4.876
4.871
4.867
2.106
2.103
1.597
1.582
1.567
1.561
1.546
1.531
1.460
1.439
1.430
1.424
1.415
1.403
1.394
1.388
1.378
1.365
1.355
1.315
1.033
1.025
1.016
1.009
0.997
0.986
0.978
0.966
0.958
0.952
0.948
0.942
0.931
Ph
O
N
Ph
6n
10
9
8
7
6
5
4
3
2
1
ppm
2.01
2.12
2.46
3.12
1.03
1.00
3.12
1.20
6.01
4.22
2.01


170.1602
151.6137
138.5734
134.0892
130.5549
129.9807
129.1634
129.0523
128.7610
128.6408
128.4603
128.2509
128.0098
127.7690
124.3148
122.2021
60.1851
37.6380
33.9684
33.9251
32.8845
26.3147
10.2525
Ph
O
N
Ph
6n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

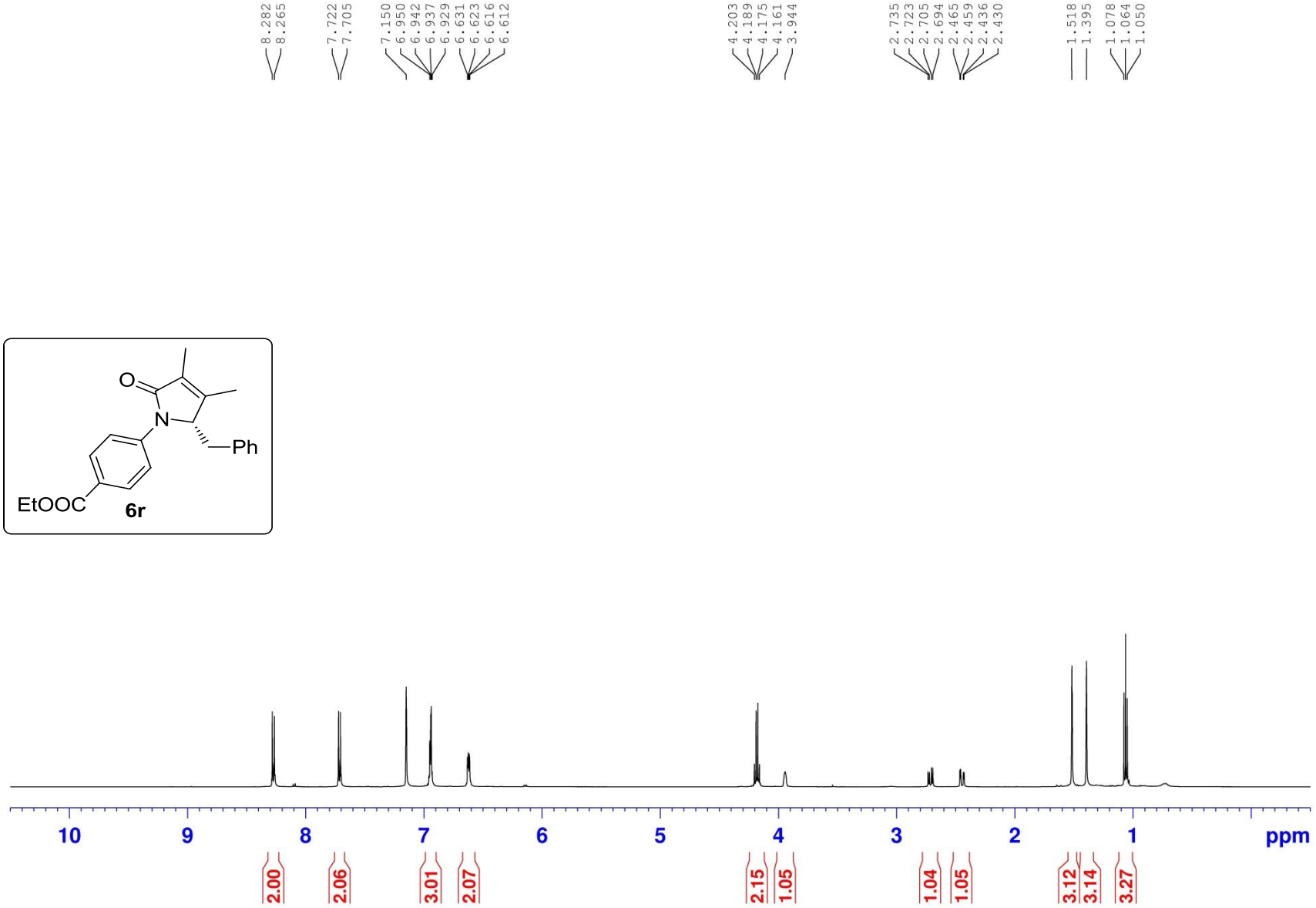

7.631
7.610
7.150
7.088
7.068
7.011
7.004
7.000
6.989
6.971
6.963
6.960
6.952
6.765
6.760
6.745
6.742
4.113
2.813
2.799
2.777
2.763
2.578
2.570
2.542
2.534
2.147
1.580
1.423
O
N
Ph
6o
10
9
8
7
6
5
4
3
2
1
ppm
2.02
2.01
3.00
2.00
1.03
1.04
1.04
3.12
3.11
3.14

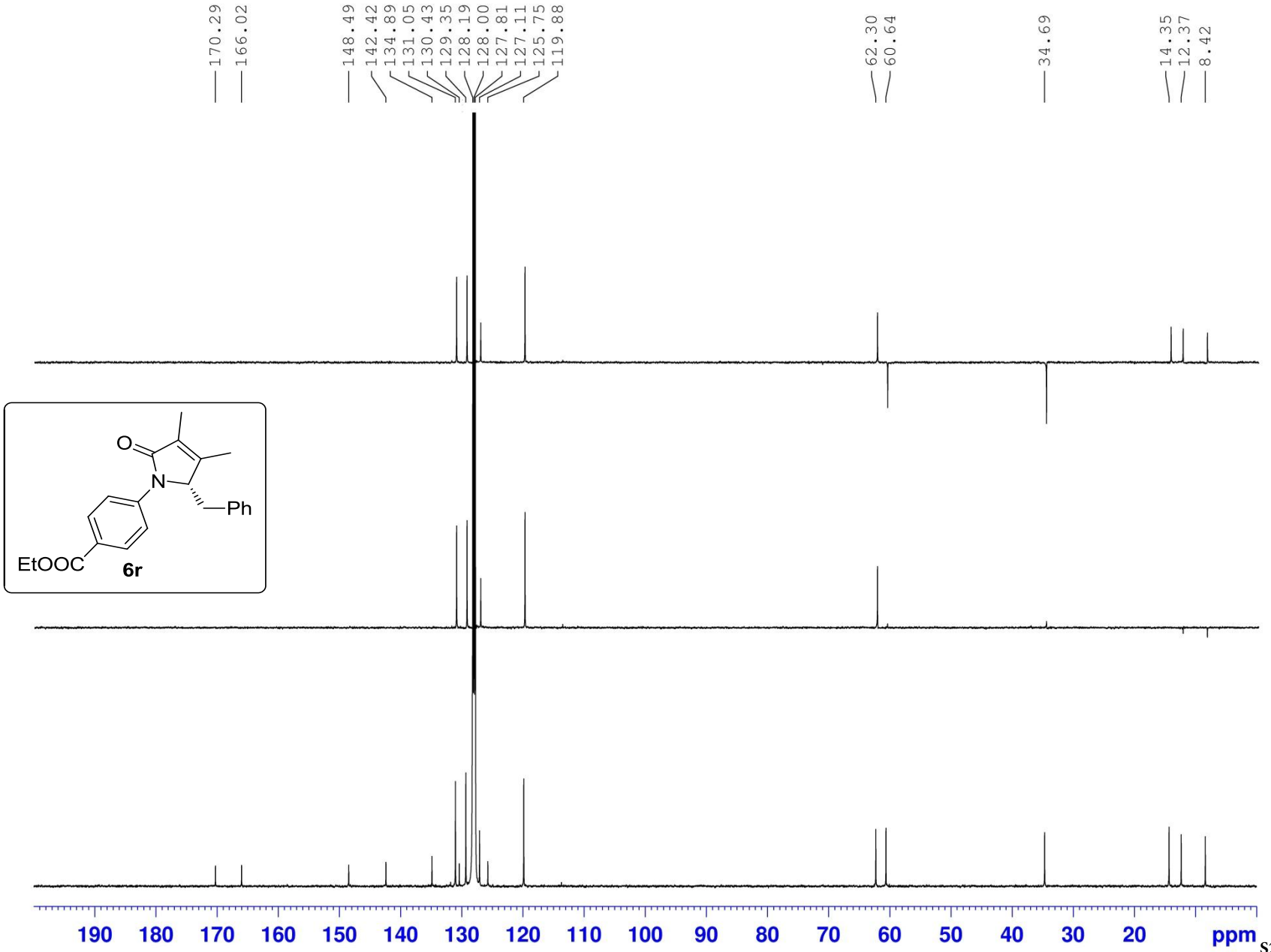

170.12
147.59
136.09
135.58
133.08
130.49
129.75
129.43
128.24
128.16
128.00
127.76
126.92
121.41
62.70
35.00
20.83
12.38
8.57
O
N
Ph
6o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

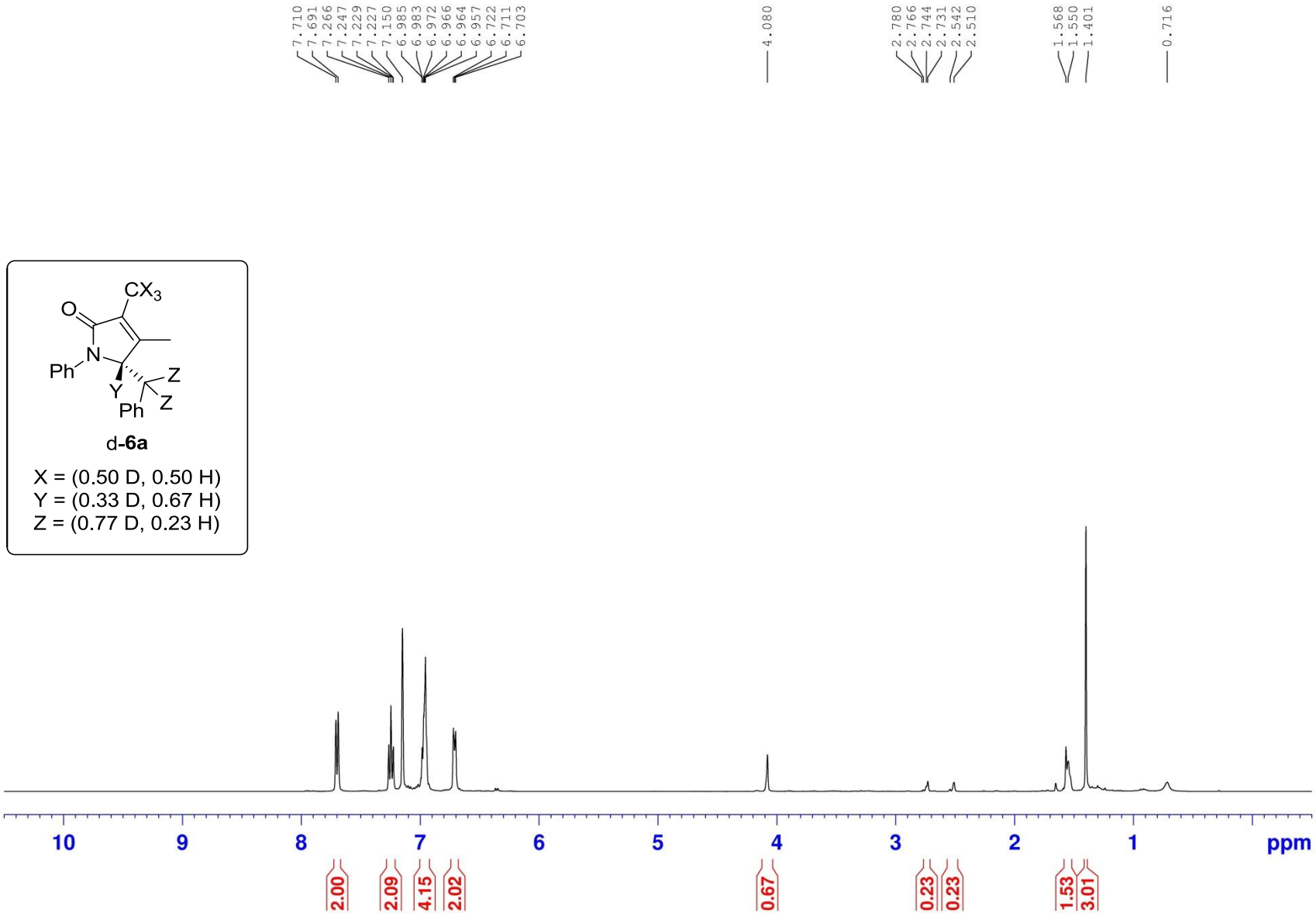

7.449
7.441
7.436
7.424
7.418
7.411
7.196
7.189
7.183
7.172
7.166
7.150
6.975
6.966
6.963
6.955
6.949
6.940
6.639
6.630
6.621
6.615
3.888
2.659
2.645
2.623
2.609
2.450
2.441
2.414
2.405
1.535
1.389
O
N
Ph
Cl
6q
10
9
8
7
6
5
4
3
2
1
ppm
2.15
2.08
3.15
2.00
1.03
1.08
1.05
3.14
3.18

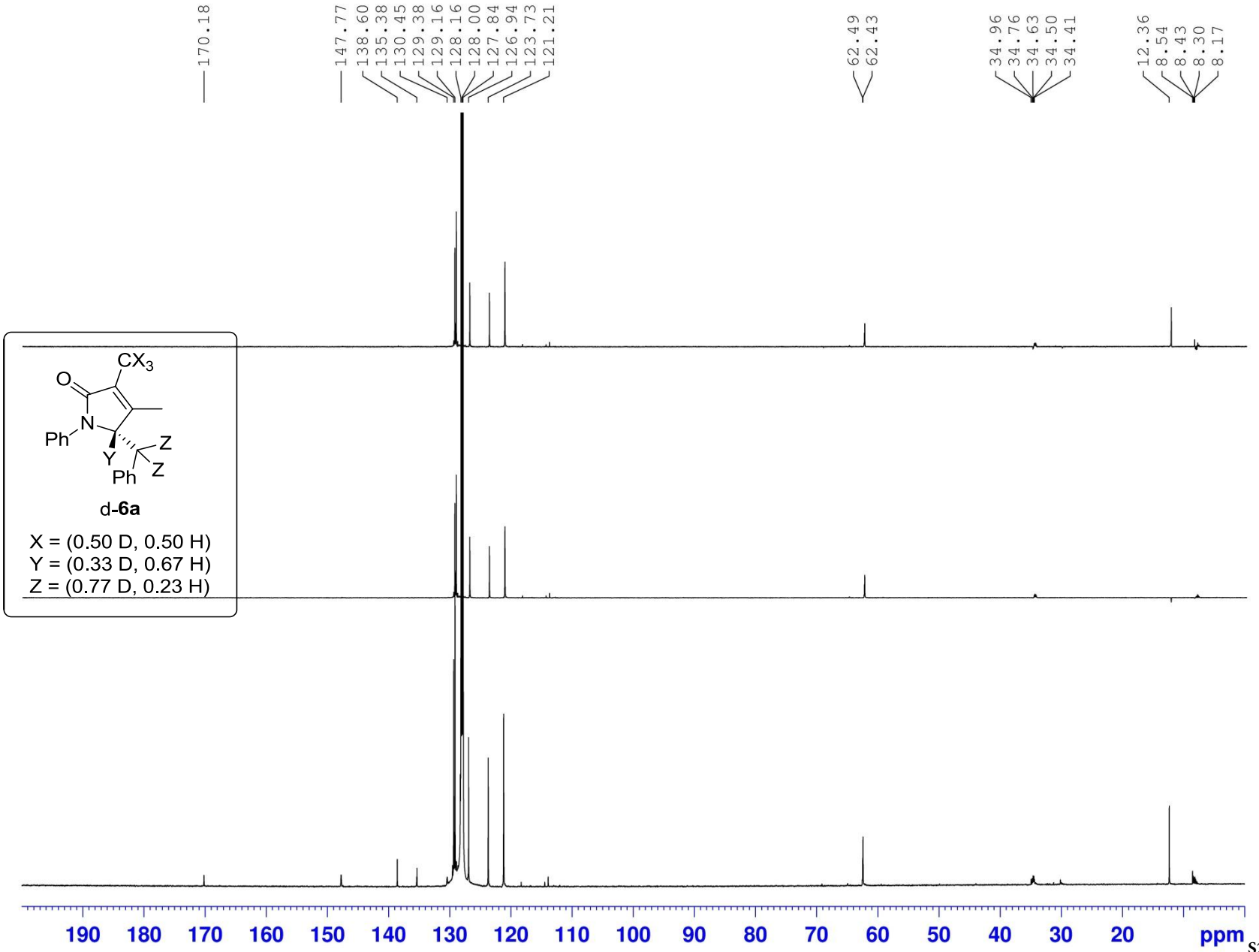

170.05
147.99
137.02
135.08
130.37
129.32
129.20
128.86
128.24
128.20
128.00
127.76
127.07
122.28
62.46
34.81
12.33
8.47
O
N
Ph
Cl
6q
220
200
180
160
140
120
100
80
60
40
20
0
ppm

O
N
Ph
EtOOC
6r


8.282
8.265
7.722
7.705
7.150
6.950
6.942
6.937
6.929
6.631
6.623
6.616
6.612
4.203
4.189
4.175
4.161
3.944
2.735
2.723
2.705
2.694
2.465
2.459
2.436
2.430
1.518
1.395
1.078
1.064
1.050
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.06
3.01
2.07
2.15
1.05
1.04
1.05
3.12
3.14
3.27


170.29
166.02
148.49
142.42
134.89
131.05
130.43
129.35
128.19
128.00
127.81
127.11
125.75
119.88
62.30
60.64
34.69
14.35
12.37
8.42
O
N
Ph
EtOOC
6r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.710
7.691
7.266
7.247
7.229
7.227
7.150
6.985
6.983
6.972
6.966
6.964
6.957
6.722
6.711
6.703
4.080
2.780
2.766
2.744
2.731
2.542
2.510
1.568
1.550
1.401
0.716
CX3
O
N
Ph
Y
Ph
Z
Z
d-6a
X = (0.50 D, 0.50 H)
Y = (0.33 D, 0.67 H)
Z = (0.77 D, 0.23 H)
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.09
4.15
2.02
0.67
0.23
0.23
1.53
3.01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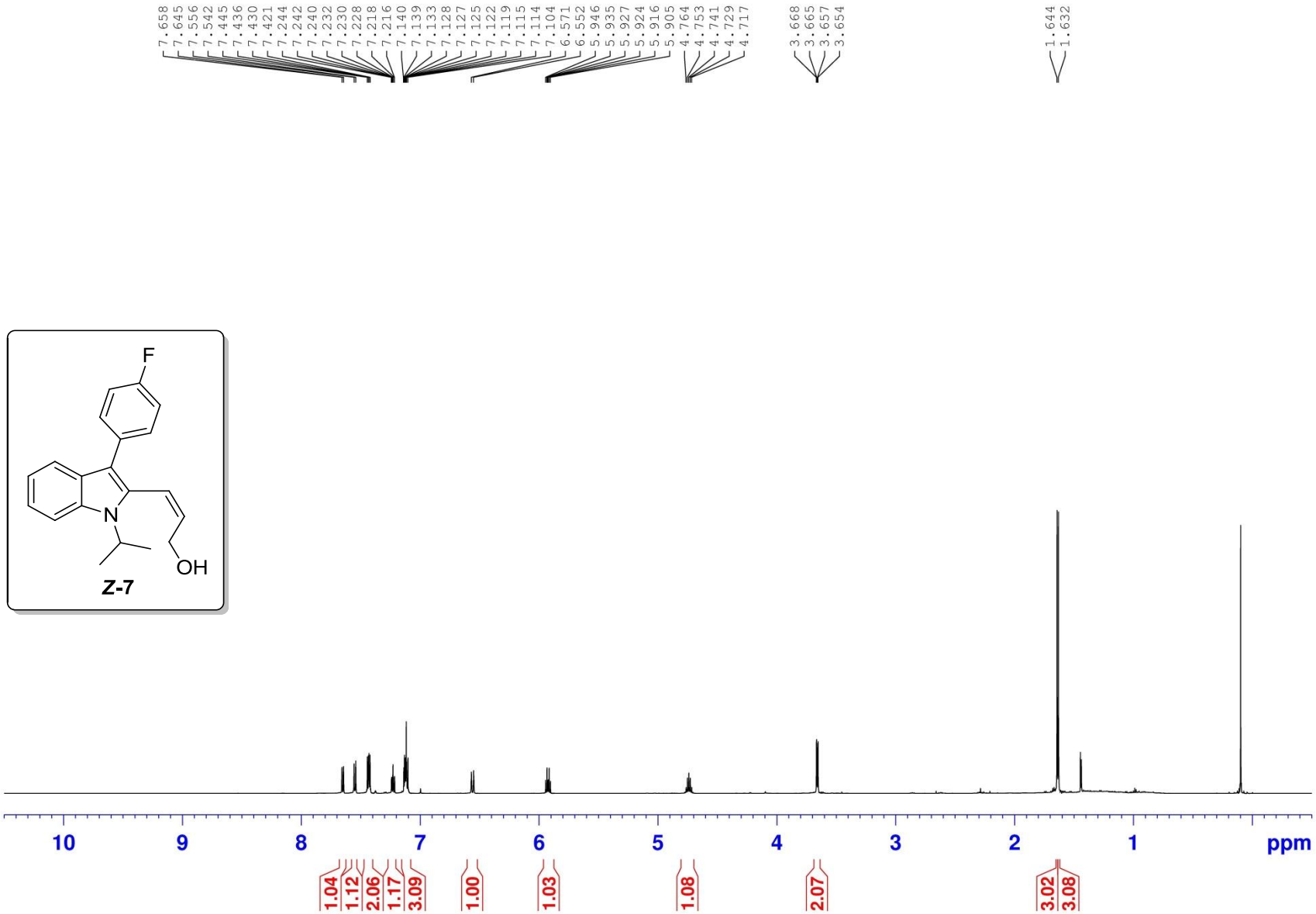
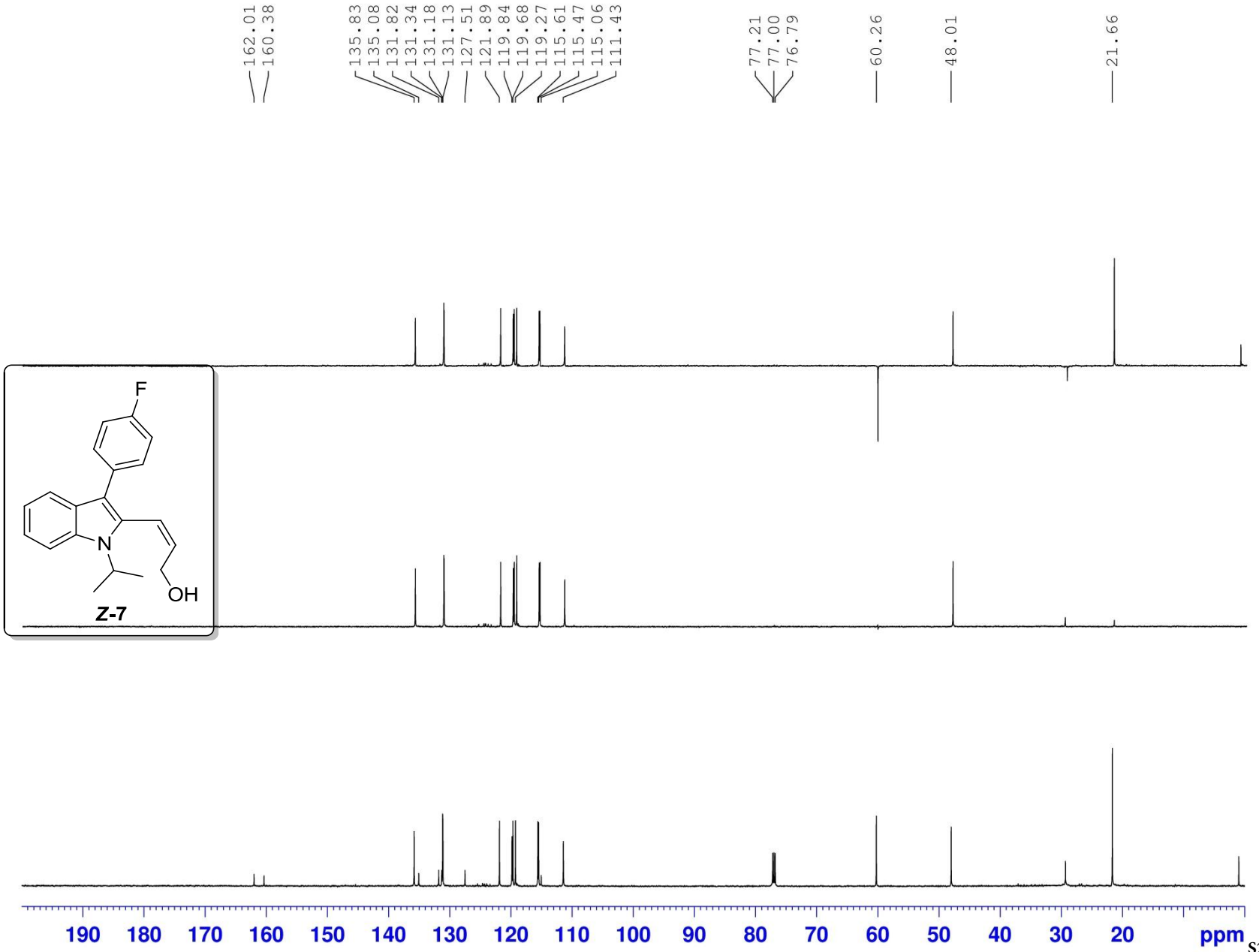
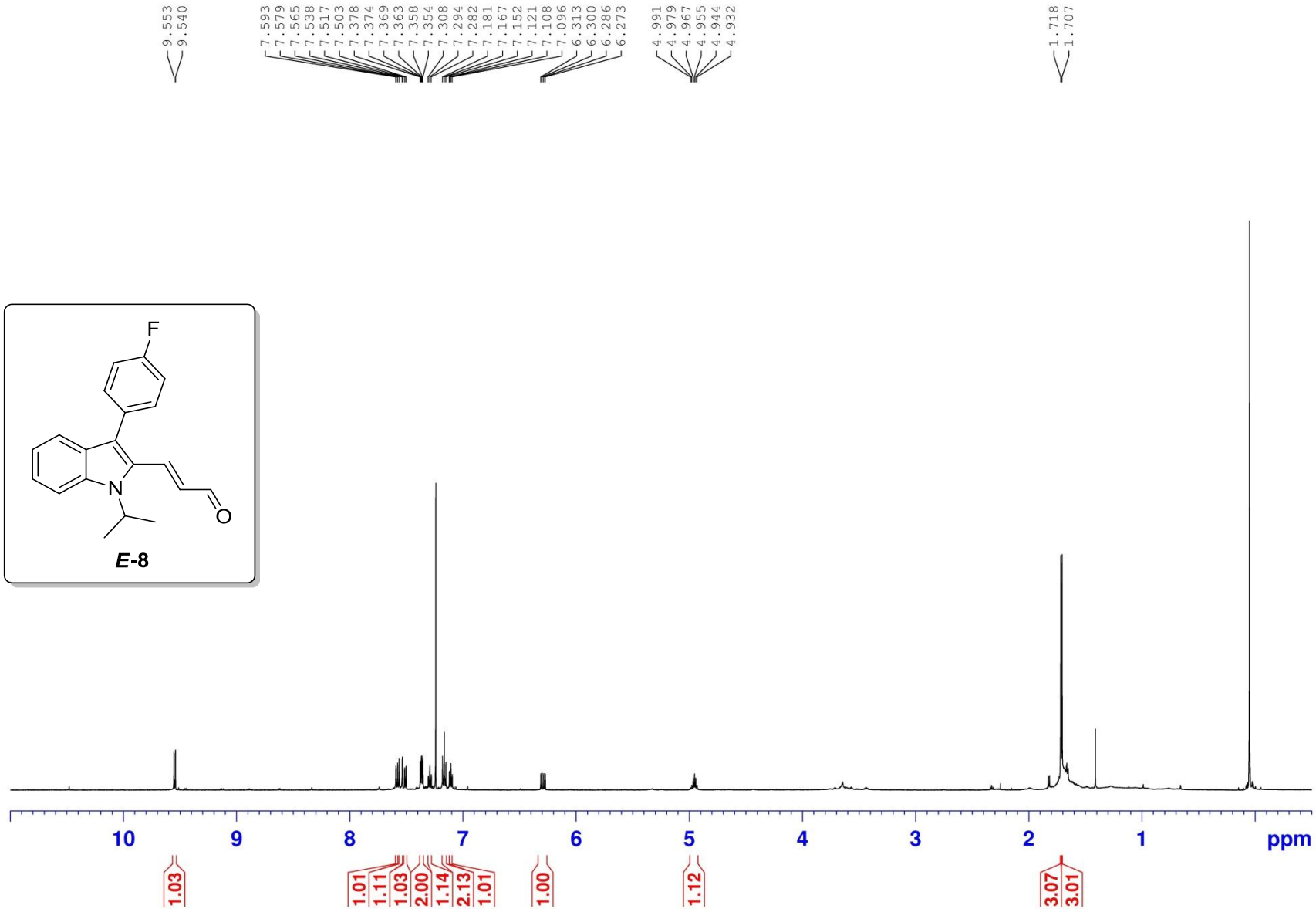
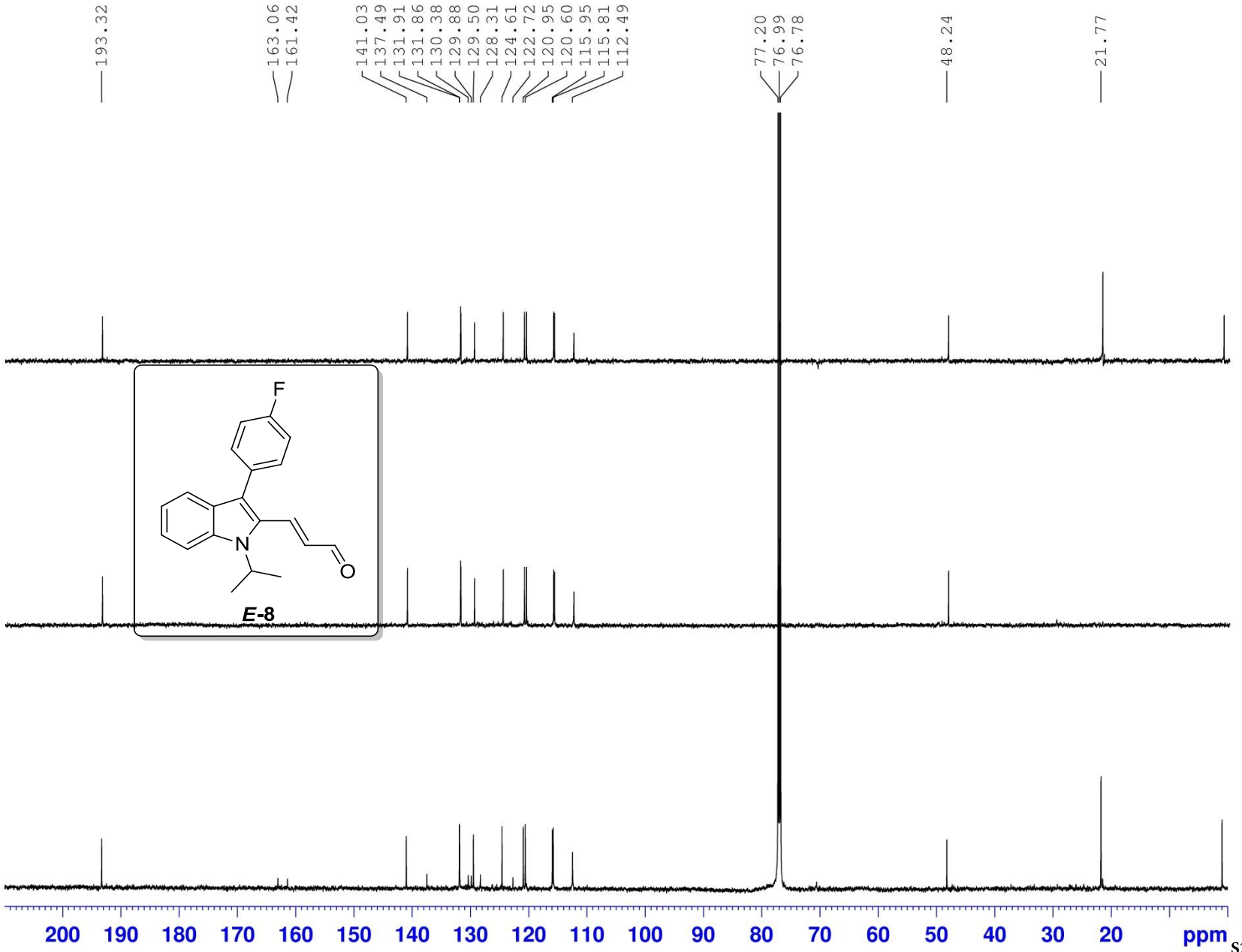
147.77
138.60
135.38
130.45
129.38
129.16
128.16
128.00
127.84
126.94
123.73
121.21
62.49
62.43
34.96
34.76
34.63
34.50
34.41
12.36
8.54
8.43
8.30
8.17
CX3
O
N
Ph
Y
Ph
Z
Z
d-6a
X = (0.50 D, 0.50 H)
Y = (0.33 D, 0.67 H)
Z = (0.77 D, 0.23 H)
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

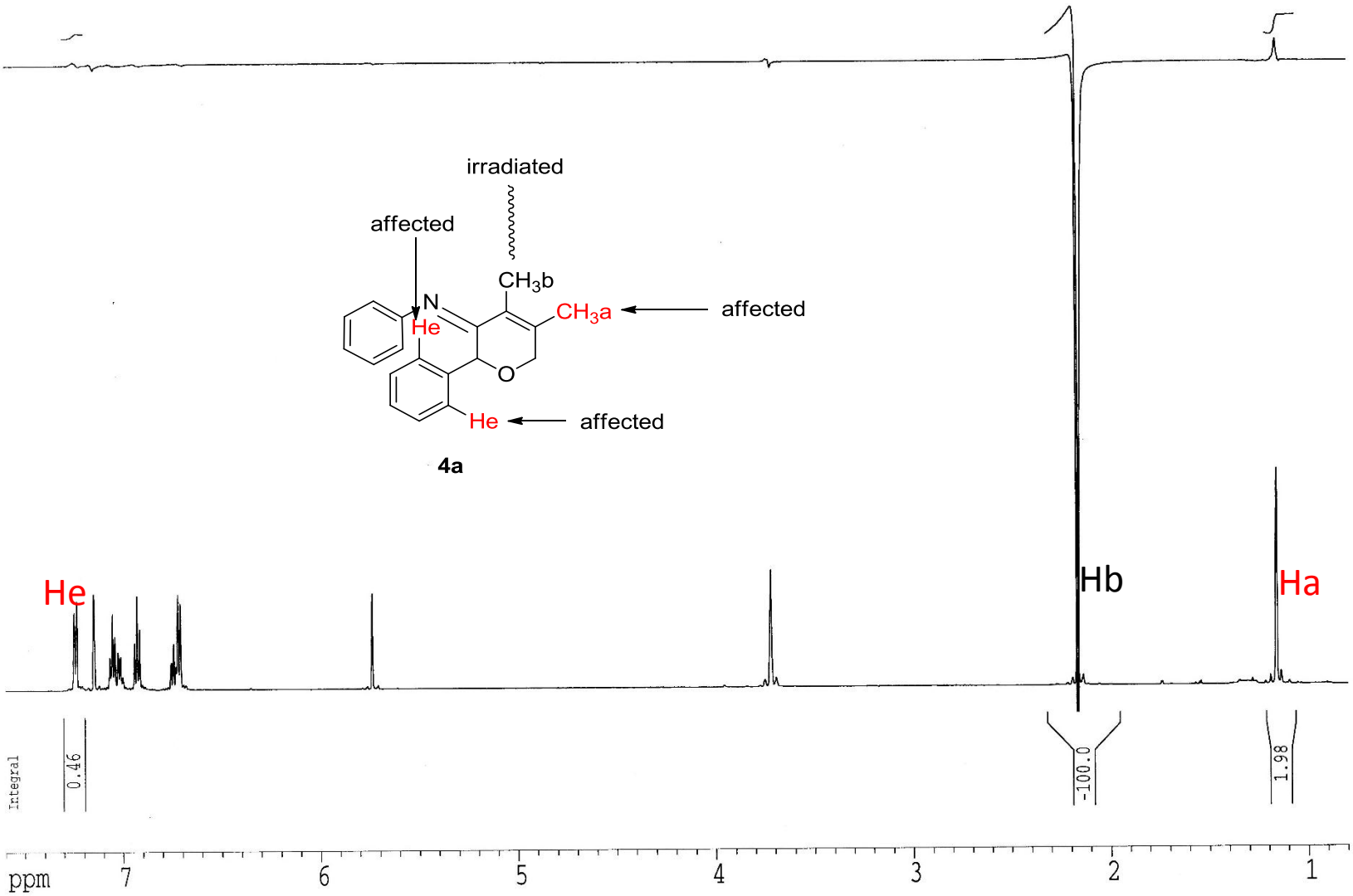

7.658
7.645
7.556
7.542
7.445
7.436
7.430
7.421
7.244
7.242
7.240
7.232
7.230
7.228
7.218
7.216
7.140
7.139
7.133
7.128
7.127
7.125
7.122
7.119
7.115
7.114
7.104
6.571
6.552
5.946
5.935
5.927
5.924
5.916
5.905
4.764
4.753
4.741
4.729
4.717
3.668
3.665
3.657
3.654
1.644
1.632
F
N
OH
Z-7
10
9
8
7
6
5
4
3
2
1
ppm
1.04
1.12
2.06
1.17
3.09
1.00
1.03
1.08
2.07
3.02
3.08


162.01
160.38
135.83
135.08
131.82
131.34
131.18
131.13
127.51
121.89
119.84
119.68
119.27
115.61
115.47
115.06
111.43
77.21
77.00
76.79
60.26
48.01
21.66
F
N
OH
Z-7
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

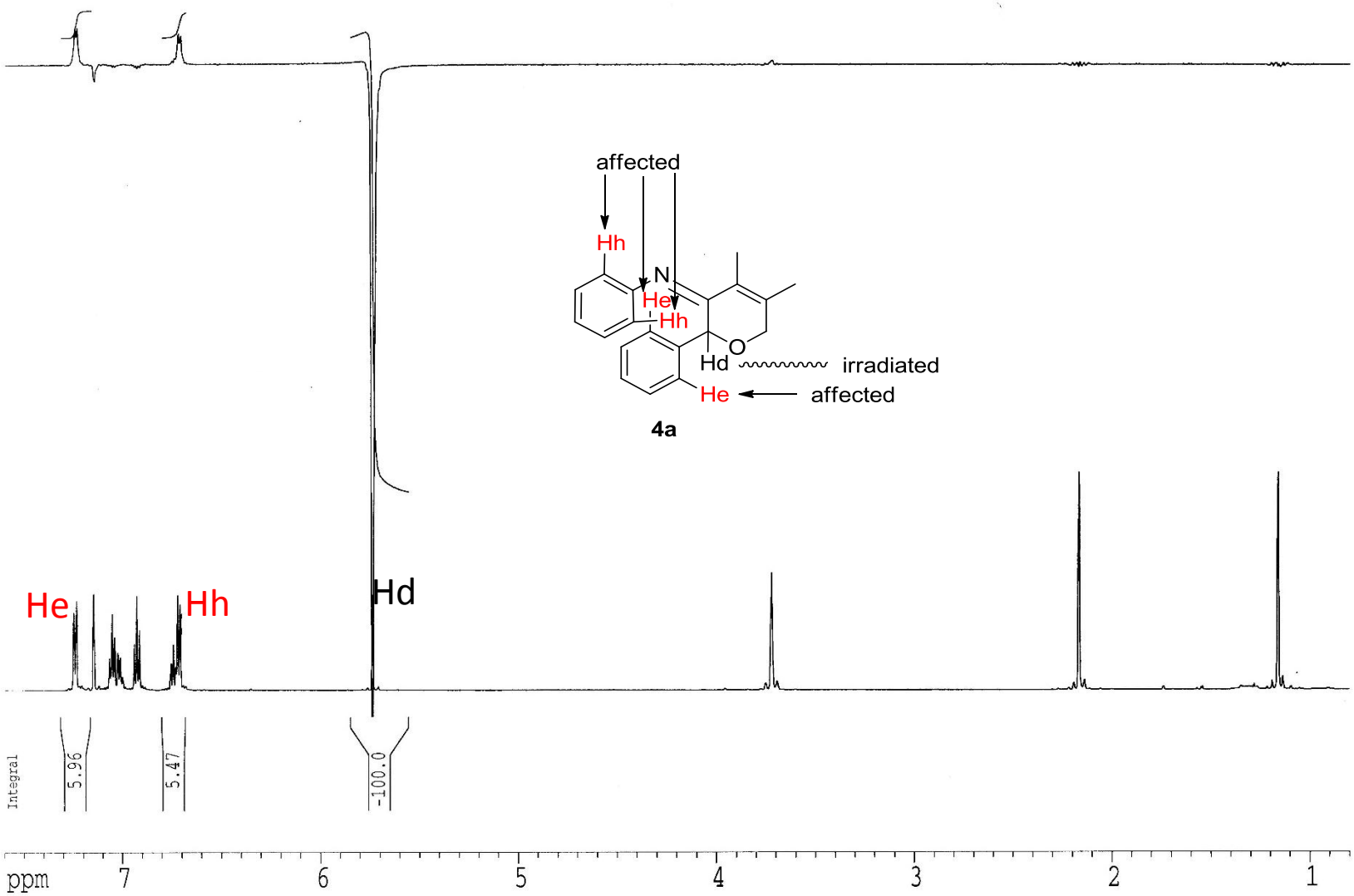

9.553
9.540
7.593
7.579
7.565
7.538
7.517
7.503
7.378
7.374
7.369
7.363
7.358
7.354
7.308
7.294
7.282
7.181
7.167
7.152
7.121
7.108
7.096
6.313
6.300
6.286
6.273
4.991
4.979
4.967
4.955
4.944
4.932
1.718
1.707
F
N
O
E-8
10
9
8
7
6
5
4
3
2
1
ppm
1.03
1.01
1.11
1.03
2.00
1.14
2.13
1.01
1.00
1.12
3.07
3.01


193.32
163.06
161.42
141.03
137.49
131.91
131.86
130.38
129.88
129.50
128.31
124.61
122.72
120.95
120.60
115.95
115.81
112.49
77.20
76.99
76.78
48.24
21.77
F
N
O
E-8
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

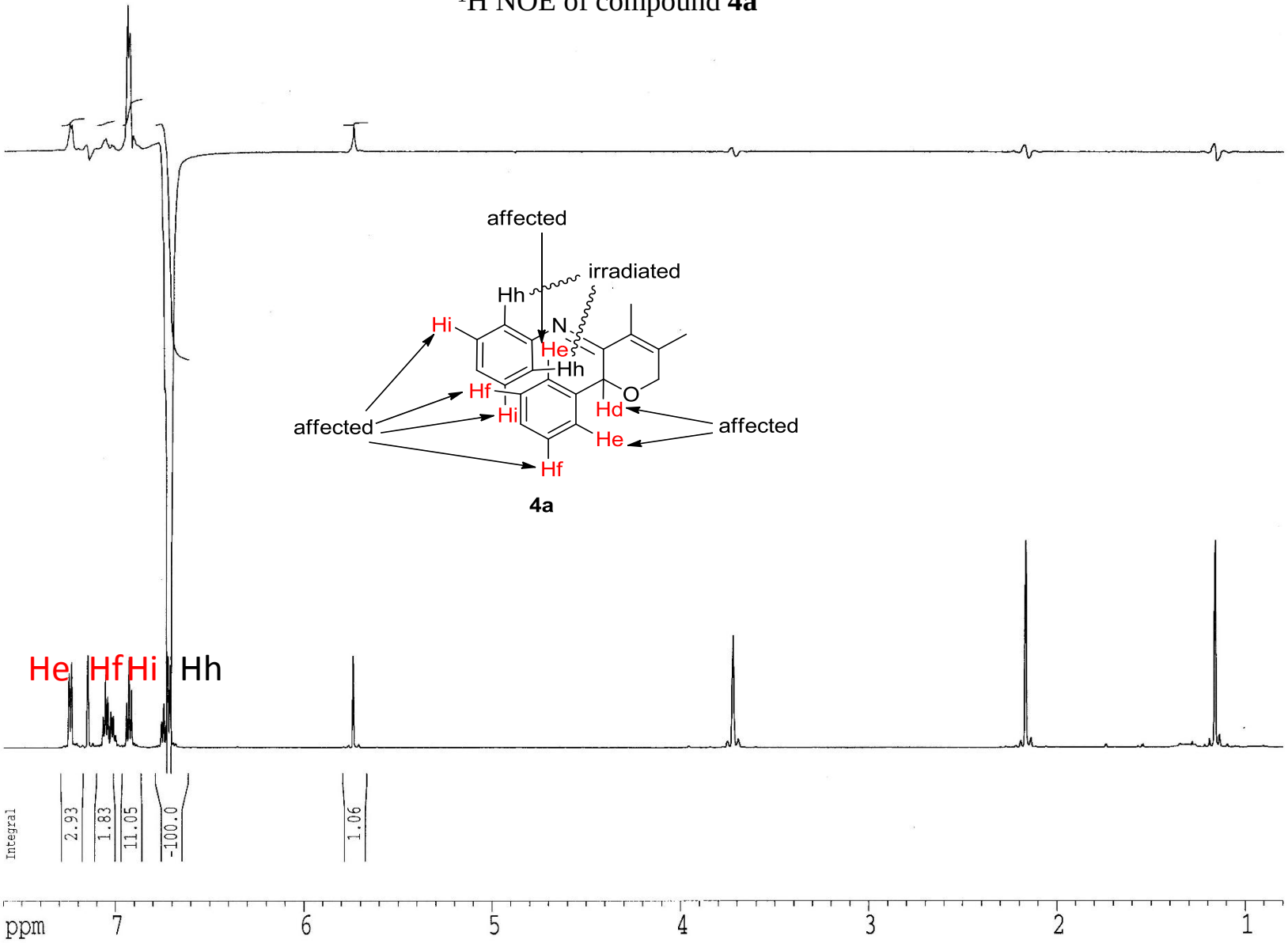
^{1}H NOE of compound **4a**



^{1}H NOE of compound **4a**



^{1}H NOE of compound **4a**



^{1}H NOE of compound **4a**