Supporting Information

Transition Metal-free Approach to Azafluoranthene Scaffolds by Aldol Condensation/[1 + 2 + 3] Cycloaddition Tandem Reaction of Isocyanoacetates with 8-(Alkynyl)-1-naphthaldehydes

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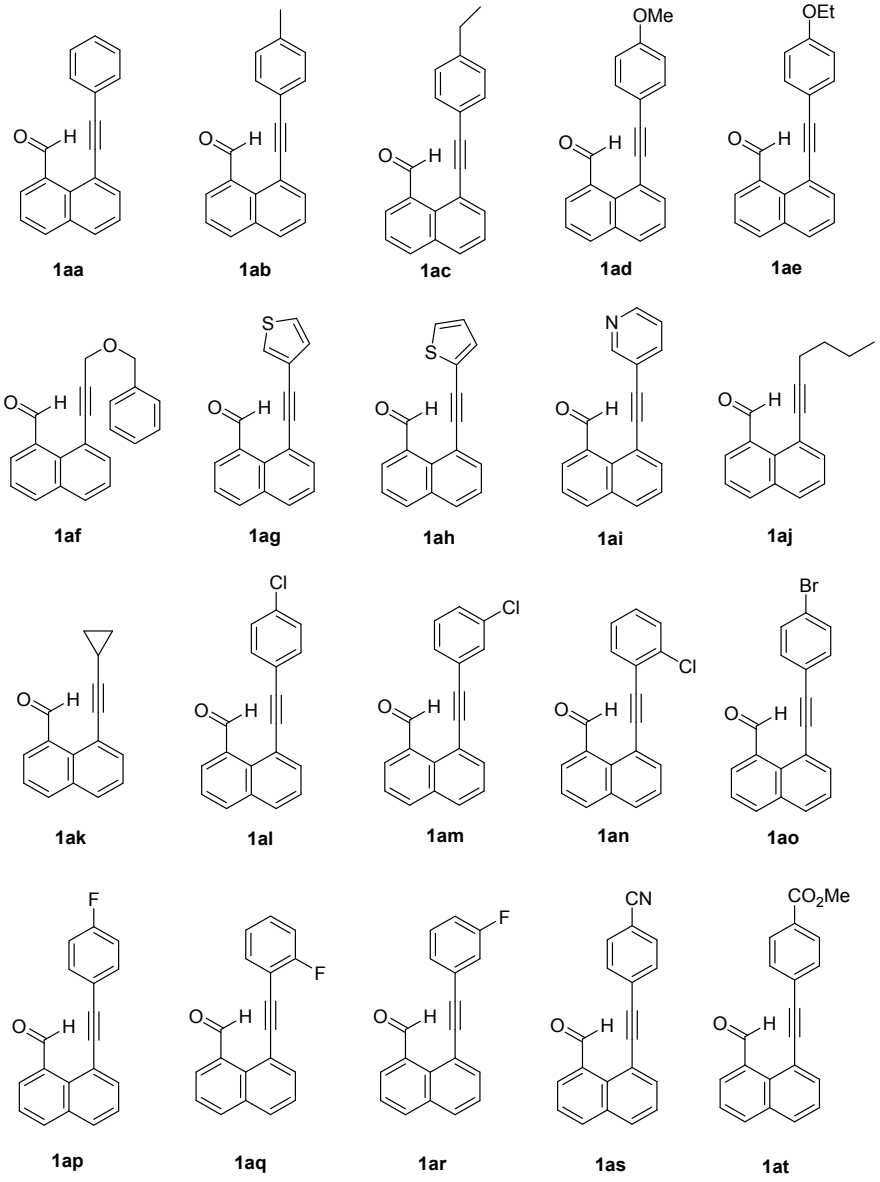
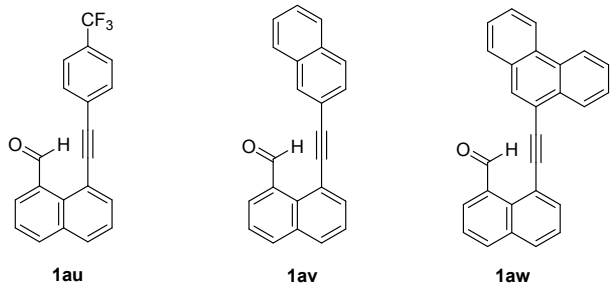
1. General Information

NMR spectra were prepared on a Bruker AV 400 MHz (^{1}H NMR at 400 MHz, ^{13}C NMR at 101 MHz), The ^{1}H NMR (400 MHz) chemical shifts and the ^{13}C NMR (101 MHz) chemical shifts were measured relative to $CDCl_3$ as the internal reference. Chemical shifts (δ) are reported in parts per million (ppm) and spin-spin coupling constants (*J*) are given in Hz. The following abbreviations are used to describe multiplicities: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), and multiplet (m). HRMS data were obtained on a Waters LCT Premierxe^{TM} (USA). Melting point (mp) was recorded on micro melting point instrument (SGWX-4A). Column chromatography were performed on silica gel 200-300 mesh.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. All the solvents were treated according to general methods.

2. List of Substrates

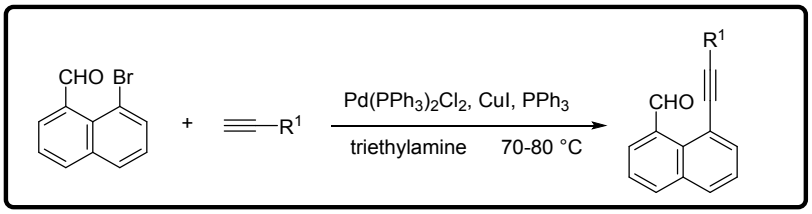




1au 1av 1aw

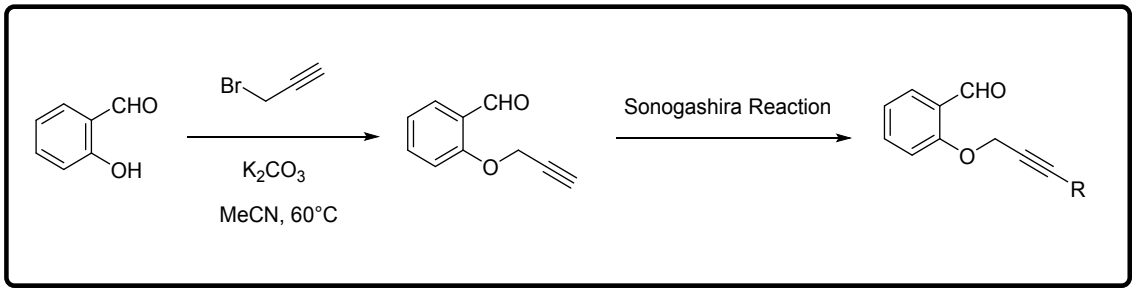
3. Synthesis of Substrates

3.1 General Procedure for the Synthesis of Substrates 1aa-1aw



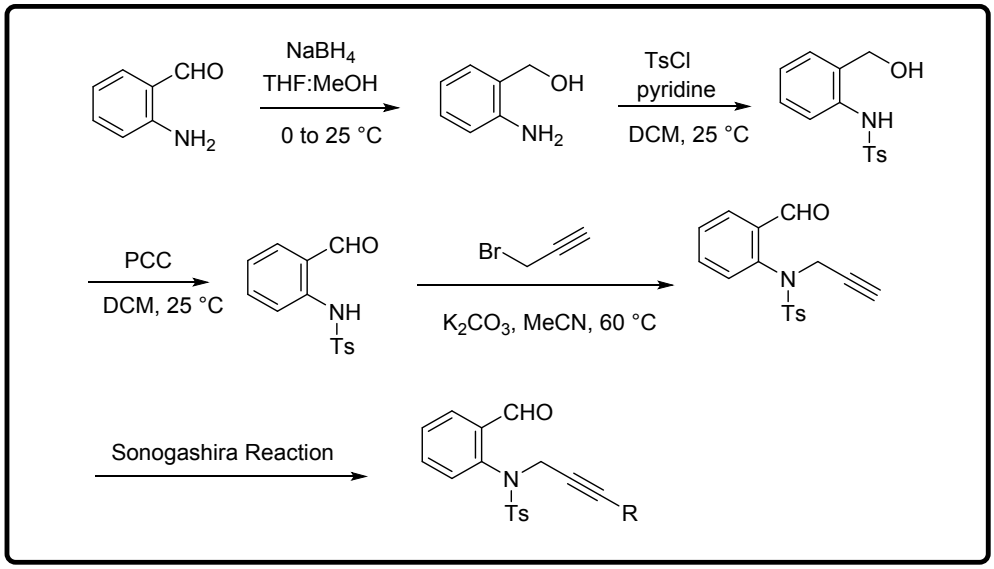
To a solution of the terminal alkyne (3.0 mmol, 1.2 equive) and 8-Bromo-1-naphthaldehyde (587.5 mg, 2.5 mmol, 1.0 equive) in NEt_3 (20 mL) in a screw-capped Pyrex bottle $Pd(PPh_3)_2Cl_2$ (87.7 mg, 5 mol %), CuI (47.6 mg, 10 mol %) and PPh_3 (65.5 mg, 10 mol %) are added at ambient temperature. The reaction mixture is purged with nitrogen for 5 min. The sealed bottle is heated at 70-80 °C overnight (ca. 10-12 h). After cooling to room temperature, the suspension is filtered through a thick layer of diatomaceous earth, and the diatomaceous earth is rinsed well with EA (40 mL). The solvent of the filtrate is removed under reduced pressure, and the residue is subjected to chromatography on silica gel. Elution with PE/EA affords the coupling product.

3.2 General Procedure for the Synthesis of Substrate 4aa-ad



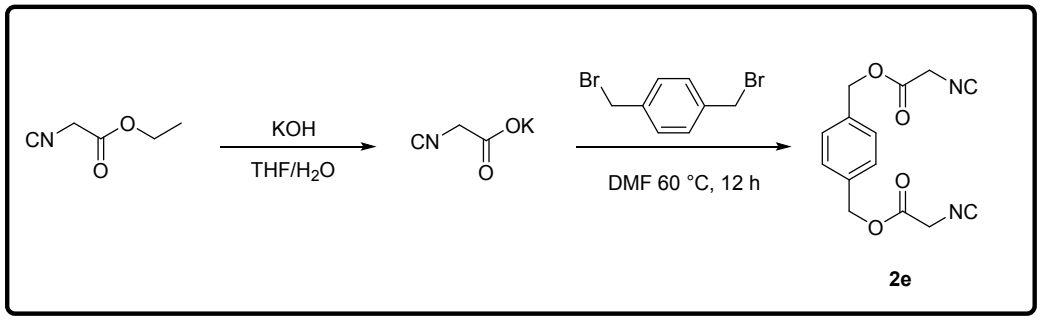
Substrate **4aa-ad** was synthesized using the procedure described in literature and the ^1H and ^{13}C NMR spectra of **4aa-ad** were consistent with literature[1]. (Muthu Karuppasamy, B. S. Vachan, Perumal Vinoth, Isravel Muthukrishnan, et al., *Org. Lett.* **2019,** *21* (15), 5784-5788).

3.3 General Procedure for the Synthesis of Substrate 4ba-bd



Substrate **4ba-bd** was synthesized using the procedure described in literature and the ^{1}H and ^{13}C NMR spectra of **4ba-bd** were consistent with literature[1] (Muthu Karuppasamy, B. S. Vachan, Perumal Vinoth, Isravel Muthukrishnan, et al., *Org. Lett.* **2019,** *21* (15), 5784-5788).

3.4 General Procedure for the Synthesis of 1,4-phenylenebis(methylene) bis(2-isocyanoacetate) 2e

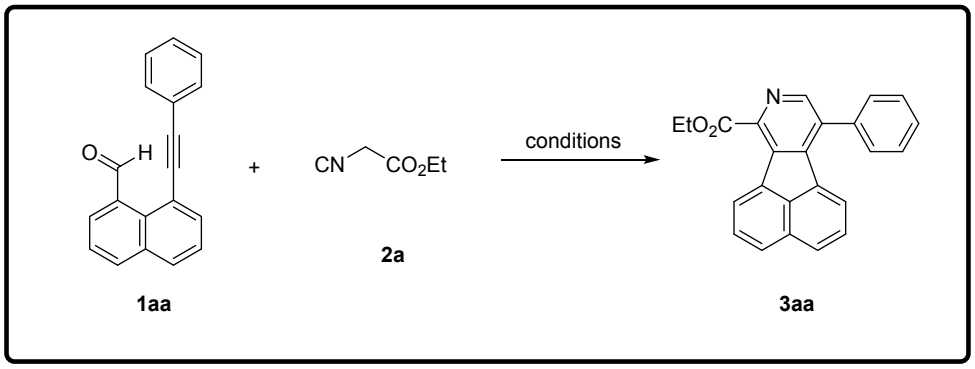


To a solution of the ethyl isocyanoacetate (1.131 g, 10 mmol, 1.0 equiv) in THF (20.0 mL) and water (5.0 mL) was added potassium hydroxide (560.0 mg, 10 mmol, 1.0 equiv), and the resultant mixture was stirred at room temperature for 5 h. The solvent was then removed in vacuum and the resultant salt was used without further purification.

To a 100 mL round-bottom flask were added potassium 2-isocyanoacetate (1.23 g, 10 mmol, 2.2 equiv), 1,4-bis(bromomethyl)benzene (1.18 g, 4.5 mmol, 1.0 equiv) and DMF (30 mL) under nitrogen. The solution was stirred at 60 °C for 12 h, and then the formed precipitates were removed by filtration and washed with ethyl acetate. The filtrate was extracted by EA/water in order to remove DMF. After the organic layer was dried with anhydrous magnesium sulfate, the solvent was removed by a rotary evaporator under reduced pressure, and the crude product was purified by a silica gel column chromatography using PE/EA (1:1 v/v) as eluent. Compounds were prepared by modification of a known procedure[2] (Tianyu Cheng, Yizhao Chen, Anjun Qin, and Ben Zhong Tang. *Macromolecules* **2018**, *51*, 5638−5645)

4. Optimization Results of the Reaction Conditions

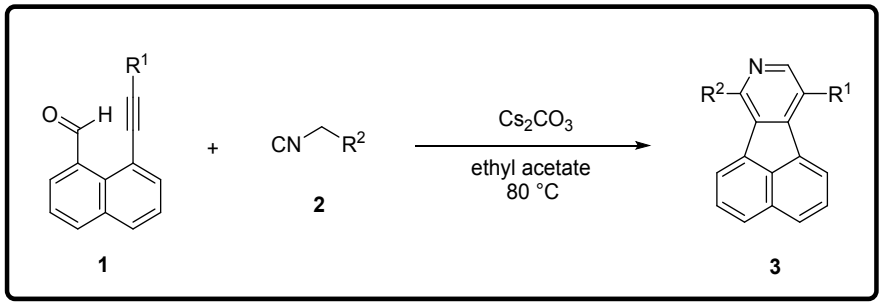
Table S1. Optimization of the Base, Solvent, Catalyst and Temperature[a]



Entry	Catalyst	Base	Solvent	*t*(℃)	Yield (%) [b]
1	-	DBU	MeCN	80	20
2	-	K_2CO_3	MeCN	80	31
3	-	K_3PO_4	MeCN	80	27
4	-	KOH	MeCN	80	25
5	-	*t*-BuOLi	MeCN	80	17
6	-	CsOH	MeCN	80	23
7	-	Cs_2CO_3	MeCN	80	39
8	-	Cs_2CO_3	1,4-dioxane	80	14
9	-	Cs_2CO_3	toluene	80	42
10	-	Cs_2CO_3	DMSO	80	ND [c]
11	-	Cs_2CO_3	DMF	80	ND [c]
12	-	Cs_2CO_3	diethyl ether	80	38
13	-	Cs_2CO_3	methyl acetate	80	62
14	-	Cs_2CO_3	ethanol	80	32
15	**-**	**Cs_2CO_3**	**ethyl acetate**	**80**	**67**
16	-	Cs_2CO_3	ethyl acetate	60	29
17	-	Cs_2CO_3	ethyl acetate	rt	ND [c]
18	-	Cs_2CO_3	ethyl acetate	100	60
19	AgOTf	Cs_2CO_3	ethyl acetate	80	50
20	Ag_2CO_3	Cs_2CO_3	ethyl acetate	80	57
21	AgOAc	Cs_2CO_3	ethyl acetate	80	61
22	$Zn(OTf)_2$	Cs_2CO_3	ethyl acetate	80	ND [c]
23	CuI	Cs_2CO_3	ethyl acetate	80	trace
24	Cu_2O	Cs_2CO_3	ethyl acetate	80	51
25	$PdCl_2$	Cs_2CO_3	ethyl acetate	80	trace
26	$Pd(OAc)_2$	Cs_2CO_3	ethyl acetate	80	trace
27	$Pd(PPh_3)_4$	Cs_2CO_3	ethyl acetate	80	59

[a] Reagents and reaction conditions: **1a** (0.2 mmol, 1.0 equiv), ethyl isocyanoacetate (0.3 mmol, 1.5 equiv), catalyst (10 mol %), base (0.4 mmol, 2 equiv), solvent (2 mL), 4-6 h. [b] Isolated yields. [c] No desired product was detected.

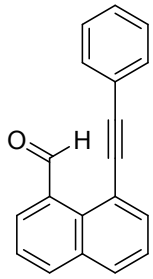
5. Synthesis of Products



A dry 10 mL Schlenk tube equipped with magnetic stirring bar are charged with substrate (0.2 mmol, 1.0 equiv), Cs_2CO_3(130.3 mg, 0.4 mmol, 2.0 equiv), isocyanide (0.3 mmol, 1.5 equiv) and Ethyl acetate (2 mL). The reaction mixture is stirred at 80 °C for 4-6 h. After cooling to room temperature, the mixture is filtered through a thick layer of diatomaceous earth, and the diatomaceous earth is rinsed well with EA (20 mL). The solvent of the filtrate is removed under reduced pressure, and the residue is subjected to chromatography on silica gel. Elution with PE/EA affords the product.

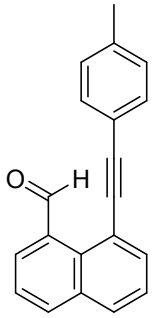
6. Characterization Data of Substrates and Products

8-phenylethynyl-1- naphthaldehyde(1aa)



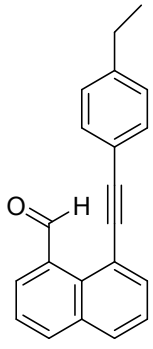
Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1aa** as a yellow solid (473.6 mg, 74% yield). mp:59-60 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.67 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.93-7.88 (m, 2H), 7.63-7.50 (m, 4H), 7.42-7.37 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 135.7, 134.1, 134.1, 134.0, 131.2, 131.1, 129.8, 128.8, 128.8, 128.5, 126.0, 125.8, 122.6, 118.6, 95.1, 90.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{13}O$ 257.0961; Found 257.0959.

8-(p-tolylethynyl)-1-naphthaldehyde (1ab)



Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1ab** as a yellow solid (560.5 mg, 83% yield). mp:85-86 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.67 (s, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.88 (d, *J* = 7.2 Hz, 2H), 7.59-7.47 (m, 4H), 7.20 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 139.1, 135.8, 134.1, 134.0, 133.9, 131.1, 131.1, 129.6, 129.3, 128.7, 126.0, 125.7, 119.6, 118.8, 95.4, 90.3, 21.6. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{14}ONa$ 293.0937; Found 293.0937.

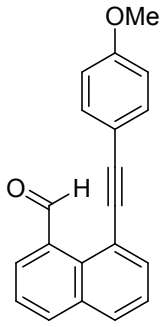
8-((4-ethylphenyl) ethynyl)-1-naphthaldehyde (1ac)



Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1ac** as a yellow oil (518.5 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.68 (s, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 2H),

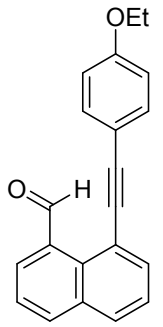
7.58 (t, J = 7.6 Hz, 1H), 7.53-7.50 (m, 3H), 7.23 (d, J = 8.0 Hz, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 145.4, 135.8, 134.1, 134.0, 133.9, 131.2, 131.1, 129.6, 128.7, 128.1, 125.9, 125.7, 119.8, 118.8, 95.4, 90.3, 28.9, 15.3. HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{21}H_{16}ONa$ 307.1093; Found 307.1090.

8-((4-methoxyphenyl) ethynyl)-1-naphthaldehyde (1ad)



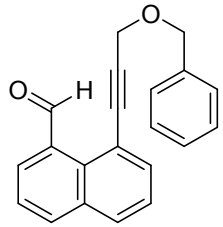
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1ad** as a white solid (343.3 mg, 48% yield). mp:101-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.66 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.96 (d, J = 7.2 Hz, 1H), 7.86 (d, J = 7.6 Hz, 2H), 7.57-7.48 (m, 4H), 6.91 (d, J = 8.4 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 160.1, 135.9, 134.1, 134.0, 133.6, 132.7, 131.1, 129.4, 128.6, 126.0, 125.7, 119.0, 114.7, 114.2, 95.3, 89.8, 55.3. HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{20}H_{14}O_2Na$ 309.0886; Found 309.0882.

8-((4-ethoxyphenyl)ethynyl)-1-naphthaldehyde (1ae)



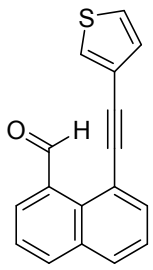
Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1ae** as a white solid (637.7 mg, 85% yield). mp:111-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.67 (s, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.87 (d, J = 6.4 Hz, 2H), 7.60-7.48 (m, 4H), 6.90 (d, J = 8.8 Hz, 2H), 4.06 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.7, 159.5, 135.8, 134.1, 134.0, 133.6, 132.7, 131.1, 129.4, 128.6, 126.0, 125.7, 119.0, 114.7, 114.5, 95.4, 89.7, 63.5, 14.7. HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{21}H_{16}O_2Na$ 323.1043; Found 323.1038.

8-(3-(benzyloxy)prop-1-yn-1-yl)-1-naphthaldehyde (1af)



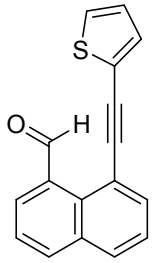
Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1af** as a brown oil (540.2 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.61 (s, 1H), 8.03-7.99 (m, 2H), 7.91 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 7.2 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.52-7.48 (m, 1H), 7.44 (d, J = 7.2 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.2 Hz, 1H), 4.71 (s, 2H), 4.50 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.2, 137.4, 135.4, 135.0, 134.3, 134.0, 131.2, 130.3, 129.0, 128.5, 128.2, 128.0, 125.9, 125.8, 117.8, 91.5, 87.7, 72.1, 58.1. HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{21}H_{16}O_2Na$ 323.1043; Found 323.1040.

8-(thiophen-3-ylethynyl)-1-naphthaldehyde (1ag)



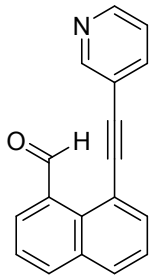
Purification by column chromatography on silica gel (PE/EA = 20/1, v/v) afforded **1ag** as a light brown solid (524.0 mg, 80% yield). mp:78-79 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.62 (s, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 7.2 Hz, 1H), 7.89 (t, J = 8.4 Hz, 2H), 7.64 (s, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.56-7.49 (m, 1H), 7.36-7.33 (m, 1H), 7.28 (d, J = 4.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 135.8, 134.1, 134.0, 133.7, 131.1, 129.7, 129.3, 129.2, 128.7, 126.0, 125.8, 125.7, 121.6, 118.6, 90.6, 90.4. HRMS (ESI) m/z: [M + Na]$^+$ Calcd for $C_{17}H_{10}OSNa$ 285.0345; Found 285.0343.

8-(thiophen-2-ylethynyl)-1-naphthaldehyde (1ah)



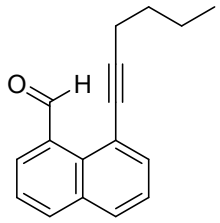
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1ah** as a light brown solid (478.2 mg, 73% yield). mp:88-89 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.58 (s, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.87 (d, *J* = 7.2 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.54-7.49 (m, 1H), 7.39 (d, *J* = 3.6 Hz, 1H), 7.36 (d, *J* = 6.0 Hz, 1H), 7.06 (dd, *J* = 5.2, 3.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 135.6, 134.2, 134.0, 133.8, 132.3, 130.83, 130.0, 128.8, 128.0, 127.3, 125.1, 125.8, 122.4, 118.2, 94.4, 88.6. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{10}OSNa$ 285.0345; Found 285.0341.

8-(pyridin-3-ylethynyl)-1-naphthaldehyde (1ai)



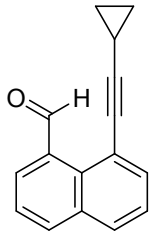
Purification by column chromatography on silica gel (PE/EA = 3/1, v/v) afforded **1ai** as a white solid (462.8 mg, 72% yield). mp:91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.56 (s, 1H), 8.79 (s, 1H), 8.56 (d, *J* = 4.4 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 6.0 Hz, 1H), 7.91-7.88 (m, 2H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.57-7.49 (m, 2H), 7.31-7.28 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.1, 151.7, 149.0, 138.0, 135.5, 134.4, 134.2, 133.9, 130.9, 130.4, 128.9, 125.9, 125.9, 123.2, 119.8, 117.7, 94.0, 91.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{18}H_{12}NO$ 258.0913; Found 258.0912.

8-(hex-1-yn-1-yl)-1-naphthaldehyde (1aj)



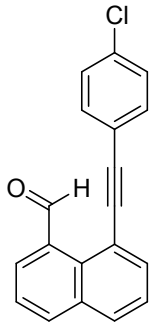
Purification by column chromatography on silica gel (PE/EA = 50/1, v/v) afforded **1j** as a yellowish liquid (265.6 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.59 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.2 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 2.50 (t, *J* = 7.2 Hz, 2H), 1.69-1.61 (m, 2H), 1.54-1.45 (m, 2H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 135.7, 134.1, 134.0, 133.9, 131.3, 129.0, 128.5, 125.9, 125.5, 119.4, 97.0, 82.2, 30.3, 22.2, 19.5, 13.6. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{17}H_{17}O$ 237.1274; Found 237.1271.

8-(cyclopropylethynyl)-1-naphthaldehyde (1ak)



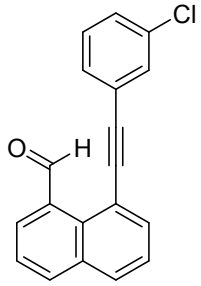
Purification by column chromatography on silica gel (PE/EA = 40/1, v/v) afforded **1k** as a yellow liquid (341.2 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.51 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 1.57-1.50 (m, 1H), 0.92-0.90 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 135.8, 134.0, 133.8, 131.3, 128.9, 128.4, 125.8, 125.5, 119.3, 99.7, 8.3, 0.6. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{16}H_{13}O$ 221.0961; Found 221.0957.

8-((4-chlorophenyl)ethynyl)-1-naphthaldehyde (1al)



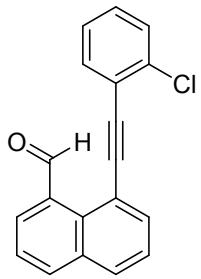
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1al** as a yellow solid (565.5 mg, 78% yield). mp:121-122 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.59 (s, 1H), 8.04-7.99 (m, 1H), 7.99-7.94 (m, 1H), 7.93-7.85 (m, 2H), 7.60-7.48 (m, 4H), 7.37-7.32 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 135.7, 134.9, 134.1, 134.1, 134.0, 132.4, 131.0, 130.1, 128.9, 128.8, 126.0, 125.8, 121.1, 118.2, 93.9, 91.8. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}ClO$ 291.0571; Found 291.0571.

8-((3-chlorophenyl)ethynyl)-1-naphthaldehyde (1am)



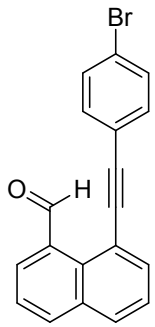
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1am** as a yellow solid (674.3 mg, 93% yield). mp:128-129 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.60 (s, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.99 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.95-7.89 (m, 2H), 7.62-7.52 (m, 3H), 7.47 (dt, *J* = 7.2, 1.6 Hz, 1H), 7.35-7.29 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 135.6, 134.4, 134.3, 134.2, 134.0, 131.1, 131.0, 130.3, 129.8, 129.4, 129.1, 128.9, 126.0, 125.9, 124.3, 118.1, 93.5, 91.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}ClO$ 291.0571; Found 291.0568.

8-((2-chlorophenyl)ethynyl)-1-naphthaldehyde (1an)



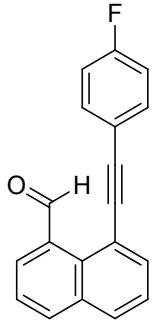
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1an** as a yellow solid (551.0 mg, 76% yield). mp:118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.74 (s, 1H), 8.06 (s, 1H), 8.04 (s, 1H), 7.98 (d, *J* = 7.2 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.64-7.61 (m, 1H), 7.59-7.53 (m, 2H), 7.47-7.43 (m, 1H), 7.31-7.27 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 135.9, 135.3, 135.0, 134.4, 134.1, 133.0, 130.9, 130.4, 129.8, 129.4, 129.0, 126.7, 125.9, 125.9, 122.7, 118.1, 95.5, 91.9. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{11}ClONa$ 313.0391; Found 313.0387.

8-((4-bromophenyl)ethynyl)-1-naphthaldehyde (1ao)



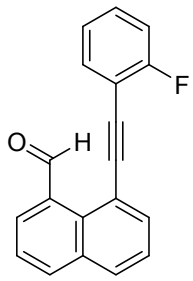
Purification by column chromatography on silica gel (PE/EA = 20/1, v/v) afforded **1ao** as a yellow solid (626.3 mg, 75% yield). mp:104-105 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.60 (s, 1H), 8.04 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.98 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.90 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.61-7.55 (m, 1H), 7.52 (dt, *J* = 8.8, 2.0 Hz, 3H), 7.45 (d, *J* = 2.0 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 135.7, 134.2, 134.1, 134.0, 132.6, 131.8, 131.0, 130.1, 128.9, 126.0, 125.9, 123.2, 121.5, 118.3, 93.9, 91.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}BrO$ 335.0066; Found 335.0067.

8-((4-fluorophenyl)ethynyl)-1-naphthaldehyde (1ap)



Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1ap** as a white solid (603.0 mg, 88% yield). mp:83-84 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.62 (s, 1H), 8.06-8.01 (m, 1H), 7.97 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.92-7.88 (m, 2H), 7.61-7.50 (m, 4H), 7.08 (t, *J* = 8.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 162.9 (C-F, $^1J_{C\text{-}F}$ = 251.5 Hz), 135.8, 134.1, 134.1, 134.0, 133.2 (C-F, $^3J_{C\text{-}F}$ = 8.1 Hz), 131.1, 129.9, 128.8, 126.0, 125.8, 118.8 (C-F, $^4J_{C\text{-}F}$ = 4.0 Hz), 118.5, 116.0 (C-F, $^2J_{C\text{-}F}$ = 22.2 Hz), 94.0, 90.6. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{11}FONa$ 297.0686; Found 297.0681.

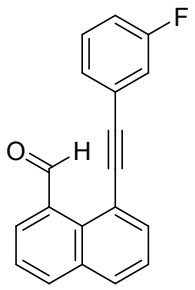
8-((2-fluorophenyl)ethynyl)-1-naphthaldehyde (1aq)



Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1aq** as a yellow solid (541.3 mg, 79% yield). mp:86-87 °C. ^{1}H NMR

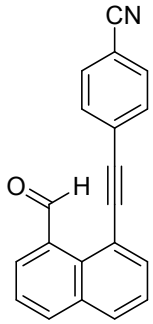
(400 MHz, $CDCl_3$) δ 11.70 (s, 1H), 8.03 (d, J = 7.6 Hz, 2H), 7.92 (t, J = 8.0 Hz, 2H), 7.60-7.55 (m, 3H), 7.35 (q, J = 7.2 Hz, 1H), 7.11-7.18 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 162.7 (C-F, $^1J_{C\text{-}F}$ = 252.5 Hz), 135.4, 134.7, 134.3, 134.0, 133.0, 130.9, 130.5 (C-F, $^3J_{C\text{-}F}$ = 7.1 Hz), 130.3, 129.0, 125.9 (C-F, $^3J_{C\text{-}F}$ = 6.1 Hz), 124.2 (C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 118.1, 115.6 (C-F, $^2J_{C\text{-}F}$ = 21.2 Hz), 111.3 (C-F, $^3J_{C\text{-}F}$ = 16.2 Hz), 95.6 (C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 88.6. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}FO$ 275.0867; Found 275.0866.

8-((3-fluorophenyl)ethynyl)-1-naphthaldehyde (1ar)



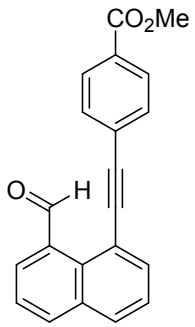
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1ar** as a yellow solid (603.0 mg, 88% yield). mp:82-83 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 11.58 (s, 1H), 8.03-7.93 (m, 2H), 7.84-7.88 (m, 2H), 7.59-7.46 (m, 2H), 7.35-7.31 (m, 2H), 7.26 (d, J = 9.2 Hz, 1H), 7.06 (t, J = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 162.4 (C-F, $^1J_{C\text{-}F}$ = 247.5 Hz), 135.6, 134.3, 134.1, 134.0, 131.0, 130.2, 130.2, 130.1, 128.8, 127.1 (C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 125.9 (C-F, $^3J_{C\text{-}F}$ = 9.1 Hz), 125.9 (C-F, $^3J_{C\text{-}F}$ = 9.1 Hz), 118.0 (C-F, $^2J_{C\text{-}F}$ = 22.2 Hz), 117.8, 116.1 (C-F, $^2J_{C\text{-}F}$ = 22.2 Hz), 93.6 (C-F, $^4J_{C\text{-}F}$ = 4.0 Hz), 91.7. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{19}H_{12}FO$ 275.0867; Found 275.0864.

4-((8-formylnaphthalen-1-yl)ethynyl)benzonitrile (1as)



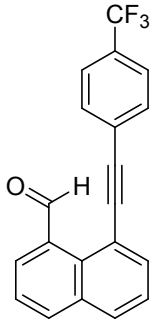
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **1as** as a yellow oil (597.3 mg, 85% yield). mp:148-149 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 11.55 (s, 1H), 8.06 (d, J = 8.4 Hz, 1H), 7.99-7.96 (m, 2H), 7.93 (d, J = 7.2 Hz, 1H), 7.65 (s, 4H), 7.62 (d, J = 8.0 Hz, 1H), 7.59-7.54 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.3, 135.6, 134.6, 134.3, 134.0, 132.2, 131.6, 131.0, 130.9, 129.1, 127.4, 126.0, 126.1, 118.4, 117.5, 112.0, 94.9, 93.1. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{20}H_{12}NO$ 282.0913; Found 282.0910.

methyl 4-((8-formylnaphthalen-1-yl)ethynyl)benzoate (1at)



Purification by column chromatography on silica gel (PE/EA/DCM = 10/1/1, v/v/v) afforded **1at** as a white solid (628.2 mg, 80% yield). mp:223-224 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 11.63 (s, 1H), 8.06 (d, J = 8.4 Hz, 3H), 8.00 (dd, J = 7.2, 1.2 Hz, 1H), 7.97-7.92 (m, 2H), 7.66-7.65 (m, 1H), 7.64-7.63 (m, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.56 (t, J = 6.8 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 166.5, 135.67, 134.5, 134.2, 134.0, 131.1, 131.1, 130.4, 130.0, 129.7, 129.0, 127.2, 126.0, 125.9, 118.0, 94.2, 93.6, 52.3. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{14}O_3Na$ 337.0835; Found 337.0827.

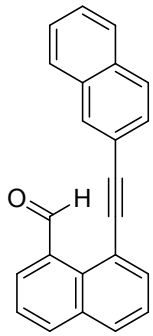
8-((4-(trifluoromethyl)phenyl)ethynyl)-1-naphthaldehyde (1au)



Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1au** as a white solid (380.8 mg, 47% yield). mp:82-83 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 11.60 (s, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 7.2 Hz, 1H), 7.94 (t, J = 8.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.61-7.53 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.4, 135.6, 134.5, 134.2, 134.0, 131.4, 131.1,

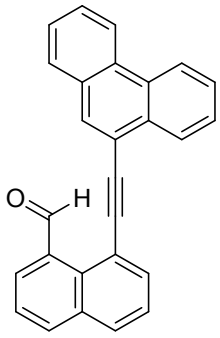
130.5, 130.2, 129.0, 126.4 (C-F, $^4J_{C\text{-}F}$ = 2.0 Hz), 126.0(C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 125.5 (C-F, $^4J_{C\text{-}F}$ = 4.0 Hz), 125.2, 122.5, 117.9, 93.4, 93.1. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{20}H_{12}F_3O$ 325.0835; Found 325.0833.

8-(naphthalen-2-ylethynyl)-1-naphthaldehyde (1av)



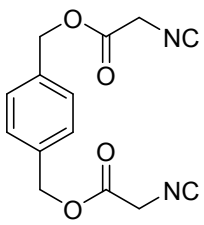
Purification by column chromatography on silica gel (PE/EA = 40/1, v/v) afforded **1av** as a yellow solid (329.1 mg, 43% yield). mp:102-103 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.75 (s, 1H), 8.12 (s, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.02 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.97 (d, *J* = 7.2 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.89-7.83 (m, 3H), 7.65 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.55-7.50 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.6, 135.8, 134.2, 134.1, 133.1, 133.0, 131.3, 131.1, 129.9, 128.8, 128.2, 128.0, 127.8, 127.7, 126.9, 126.6, 126.0, 125.8, 119.9, 118.7, 95.6, 91.2. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{14}ONa$ 329.0937; Found 329.0933.

8-(phenanthren-9-ylethynyl)-1-naphthaldehyde (1aw)



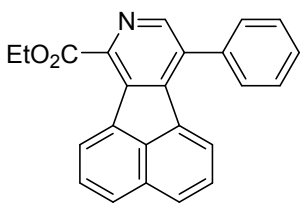
Purification by column chromatography on silica gel (PE/EA = 30/1, v/v) afforded **1aw** as a white solid (543.1 mg, 61% yield). mp:161-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.83 (s, 1H), 8.74-8.70 (m, 1H), 8.67 (d, *J* = 8.4 Hz, 1H), 8.53-8.50 (m, 1H), 8.16 (s, 1H), 8.11-8.05 (m, 3H), 7.95 (t, *J* = 8.0 Hz, 2H), 7.75-7.71 (m, 2H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.65-7.57 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.5, 135.7, 134.5, 134.3, 134.1, 132.1, 131.2, 131.1, 130.9, 130.4, 130.1, 130.0, 128.9, 128.9, 127.7, 127.2, 127.0, 126.7, 126.0, 125.9, 122.9, 122.6, 119.0, 118.7, 95.1, 93.7. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{27}H_{16}ONa$ 379.1093; Found 379.1091.

1,4-phenylenebis(methylene) bis(2-isocyanoacetate) (2e)



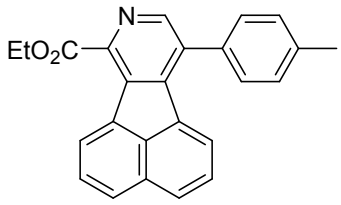
Purification by column chromatography on silica gel (PE/EA = 1/1, v/v) afforded **2e** as a white solid (517.0 mg, 38% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 4H), 5.24 (s, 4H), 4.26 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.8, 161.5, 135.1, 129.0, 77.4, 77.1, 76.8, 67.8, 43.5. HRMS (ESI) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{12}N_2O_4$ 295.0689; Found 295.0689.

ethyl 10-phenylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3aa)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3aa** as a white solid (47.1 mg, 67% yield). mp:115-116 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (d, *J* = 7.2 Hz, 1H), 8.60 (s, 1H), 7.94-7.88 (m, 2H), 7.74-7.70 (m, 1H), 7.62-7.54 (m, 5H), 7.42-7.40 (m, 2H), 4.67 (q, *J* = 7.2 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 148.2, 145.3, 142.4, 136.8, 135.7, 134.1, 133.0, 133.0, 132.8, 129.8, 129.5, 129.0, 128.9, 128.8, 128.6, 128.5, 128.0, 127.4, 125.1, 62.0, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}NO_2$ 352.1332; Found 352.1330.

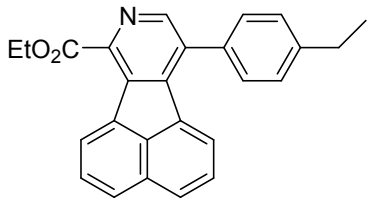
ethyl 10-(*p*-tolyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ab)



Purification by column chromatography on silica gel (PE/EA = 12/1, v/v) afforded **3ab** as a white solid (43.0 mg, 59% yield).

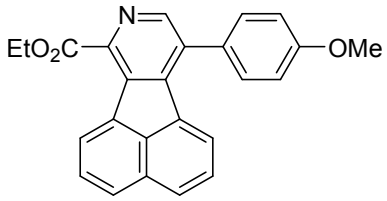
mp:119-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 7.2 Hz, 1H), 8.60 (s, 1H), 7.93 (t, *J* = 6.0 Hz, 2H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.50 (s, 1H), 7.49 (d, *J* = 7.6 Hz, 3H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 4.67 (q, *J* = 7.2 Hz, 2H), 2.51 (s, 3H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 148.4, 145.3, 142.1, 138.7, 135.8，134.2, 133.7, 133.2, 133.0, 132.8, 129.8, 129.6, 129.4, 128.9, 128.6, 128.5, 128.0, 127.4, 125.1, 62.1, 21.4, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{25}H_{20}NO_2$ 366.1489; Found 366.1484.

ethyl 10-(4-ethylphenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ac)



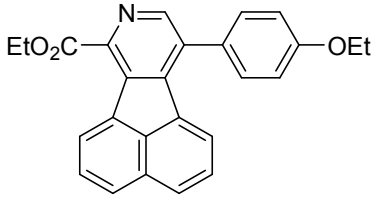
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ac** as a white solid (40.1 mg, 53% yield). mp:117-118 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 7.2 Hz, 1H), 8.61 (s, 1H), 7.97 (dd, *J* = 7.6, 5.2 Hz, 2H), 7.76 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 3H), 7.50-7.44 (m, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 4.67 (q, *J* = 7.2 Hz, 2H), 2.82 (q, *J* = 7.6 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H), 1.37 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 148.5, 145.3, 145.1, 142.1, 135.9, 134.2, 134.0, 133.2, 133.1, 132.9, 129.8, 129.5, 129.0, 128.6, 128.6, 128.4, 128.0, 127.4, 125.2, 62.1, 28.8, 15.5, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{25}H_{20}NO_2$ 380.1645; Found 380.1641.

ethyl 10-(4-methoxyphenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ad)



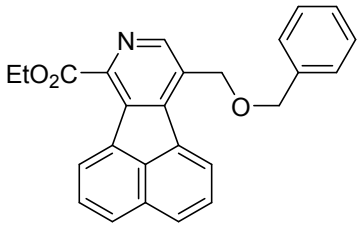
Purification by column chromatography on silica gel (PE/EA = 6/1, v/v) afforded **3ad** as a white solid (39.6 mg, 52% yield). mp:124-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (d, *J* = 7.2 Hz, 1H), 8.58 (s, 1H), 7.94-7.90 (m, 2H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.55-7.49 (m, 3H), 7.47-7.41 (m, 1H), 7.10 (d, *J* = 8.8 Hz, 2H), 4.66 (q, *J* = 7.1 Hz, 2H), 3.92 (s, 3H), 1.57 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 160.1, 148.5, 145.3, 142.0, 135.5, 134.2, 133.2, 133.0, 132.8, 130.3, 129.8, 129.4, 128.9, 128.6, 128.5, 128.0, 127.4, 125.0, 114.4, 62.0, 55.4, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{25}H_{20}NO_3$ 382.1438; Found 382.1432.

ethyl 10-(4-ethoxyphenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ae)



Purification by column chromatography on silica gel (PE/EA = 8/1, v/v) afforded **3ae** as a yellow solid (47.3 mg, 60% yield). mp:140-141 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, *J* = 7.2 Hz, 1H), 8.60 (s, 1H), 7.98-7.93 (m, 2H), 7.75 (td, *J* = 7.6, 3.2 Hz, 1H), 7.58-7.50 (m, 3H), 7.47 (td, *J* = 7.6, 3.2 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 2H), 4.66 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 6.8 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H), 1.51 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 159.5, 148.5, 145.3, 142.0, 135.6, 134.2, 133.2, 133.0, 132.8, 130.2, 129.8, 129.4, 128.7, 128.5, 128.5, 127.9, 127.4, 125.0, 114.9, 63.6, 62.0, 14.9, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{26}H_{22}NO_3$ 396.1594; Found 396.1575.

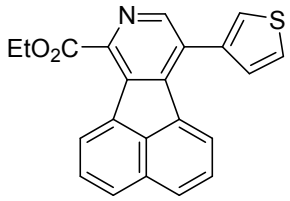
ethyl 10-((benzyloxy)methyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3af)



Purification by column chromatography on silica gel (PE/EA = 6/1, v/v) afforded **3af** as a yellow oil (37.9 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 7.2 Hz, 1H), 8.72 (s, 1H), 8.05 (d, *J* = 7.2 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 8.0

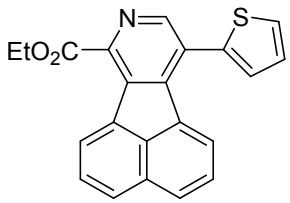
Hz, 1H), 7.70 (t, *J* = 8.0 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 7.39-7.29 (m, 5H), 5.03 (s, 2H), 4.65 (d, *J* = 6.8 Hz, 4H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 147.6, 146.4, 143.0, 137.4, 134.2, 132.8, 132.8, 132.7, 130.8, 129.7, 129.6, 128.6, 128.5, 128.5, 128.0, 127.9, 127.9, 127.8, 126.2, 72.4, 67.9, 62.1, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{26}H_{22}NO_3$ 396.1594; Found 396.1592.

ethyl 10-(thiophen-3-yl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ag)



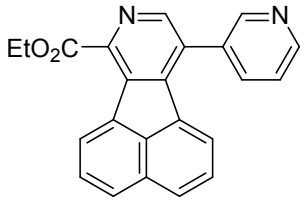
Purification by column chromatography on silica gel (PE/EA = 8/1, v/v) afforded **3ag** as a white solid (53.5 mg, 75% yield). mp:195-196 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 7.2 Hz, 1H), 8.63 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.62 (d, *J* = 7.2 Hz, 1H), 7.60-7.56 (m, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.37 (dd, *J* = 4.8, 1.2 Hz, 1H), 4.66 (q, *J* = 7.2 Hz, 2H), 1.56 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 148.3, 145.6, 142.4, 137.0, 134.2, 133.1, 133.0, 132.8, 130.8, 129.9, 129.6, 128.7, 128.6, 128.5, 128.1, 127.5, 126.7, 125.0, 124.5, 62.1, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{16}NO_2S$ 358.0896; Found 358.0874.

ethyl 10-(thiophen-3-yl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ah)



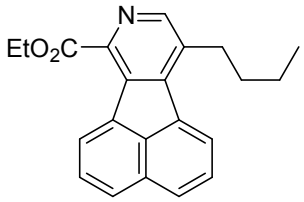
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ah** as a white solid (46.4 mg, 65% yield). mp:177-178 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 6.8 Hz, 1H), 8.67 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.77-7.67 (m, 2H), 7.58 (d, *J* = 4.8 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.39 (d, *J* = 2.4 Hz, 1H), 7.28 (d, *J* = 4.0 Hz, 1H), 4.66 (q, *J* = 7.2 Hz, 2H), 1.56 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 148.9, 146.4, 142.8, 137.1, 134.1, 133.0, 132.8, 132.5, 129.8, 128.7, 128.7, 128.6, 128.1, 128.10 127.8, 127.5, 127.2, 125.2, 62.1, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{16}NO_2S$ 358.0896; Found 358.0883.

ethyl 10-(pyridin-3-yl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ai)



Purification by column chromatography on silica gel (PE/EA = 1/1, v/v) afforded **3ai** as a white solid (40.1 mg, 57% yield). mp:144-145 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 7.2 Hz, 2H), 8.84 (d, *J* = 4.0 Hz, 1H), 8.57 (s, 1H), 7.98 (d, *J* = 8.4 Hz, 2H), 7.95 (dt, *J* = 7.6, 1.6 Hz, 1H), 7.76 (t, *J* = 7.7 Hz, 1H), 7.55 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 7.2 Hz, 1H), 4.66 (q, *J* = 7.2 Hz, 2H), 1.56 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 150.1, 149.7, 148.1, 145.7, 143.2, 136.7, 134.2, 133.0, 132.8, 132.7, 132.5, 131.9, 130.0, 129.9, 128.9, 128.8, 128.3, 127.5, 124.9, 123.8, 62.2, 14.4. HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{23}H_{16}N_2O_2$ 353.1285; Found 353.1284.

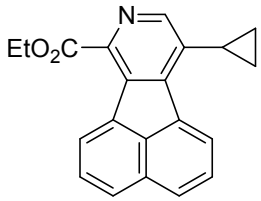
ethyl 10-butylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3aj)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3aj** as a white solid (31.1 mg, 47% yield). mp:110-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 7.2 Hz, 1H), 8.45 (s, 1H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 4.62 (q, *J* = 7.2 Hz, 2H), 3.05 (t, *J* = 7.6 Hz, 2H), 1.77-1.74 (m, 2H), 1.54 (t, *J* = 7.2 Hz, 3H), 1.49-1.45 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7,

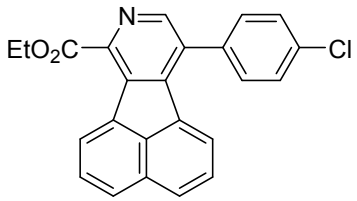
148.7, 145.2, 141.4, 136.2, 134.2, 133.5, 133.2, 132.8, 129.7, 129.0, 128.5, 128.3, 127.8, 127.5, 124.9, 61.9, 31.1, 31.1, 22.8, 14.5, 13.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{22}NO_2$ 332.1645; Found 332.1648.

ethyl 10-cyclopropylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3ak)



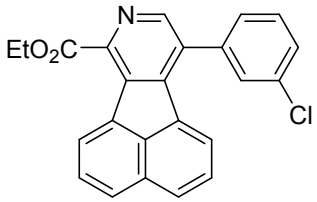
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ak** as a yellow solid (30.2 mg, 48% yield). mp:103-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, J = 7.2 Hz, 1H), 8.50 (s, 1H), 8.36 (d, J = 7.2 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 8.0 Hz, 1H), 7.72-7.66(m, 2H), 4.62 (q, J = 7.2 Hz, 2H), 2.42-2.35 (m, 1H), 1.54 (t, J = 7.2 Hz, 3H), 1.26-1.19 (m, 2H), 0.95-0.91 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 147.5, 146.9, 141.3, 135.9, 133.7, 133.7, 133.1, 132.9, 129.8, 129.3, 128.5, 128.5, 128.0, 127.6, 125.8, 62.0, 14.5, 12.3, 6.7. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{21}H_{18}NO_2$ 316.1332; Found 336.1331.

ethyl 10-(4-chlorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3al)



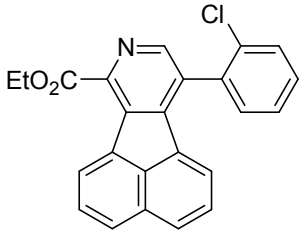
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3al** as a white solid (43.8 mg, 57% yield). mp:168-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 7.2 Hz, 1H), 8.57 (s, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.77 (t, J = 7.6 Hz, 1H), 7.61-7.53 (m, 4H), 7.48 (q, J = 7.2 Hz, 2H), 4.67 (q, J = 7.2 Hz, 2H), 1.57 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.9, 145.4, 142.5, 135.1, 135.1, 134.5, 134.2, 133.1, 132.8, 132.6, 130.4, 129.9, 129.8, 129.3, 128.8, 128.7, 128.2, 127.4, 125.1, 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}ClNO_2$ 386.0942; Found 386.0934.

ethyl 10-(3-chlorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3am)



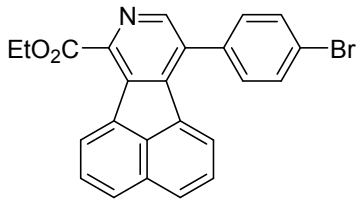
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3am** as a white solid (40.1 mg, 52% yield). mp:109-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 7.2 Hz, 1H), 8.59 (s, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.77 (t, J = 7.6 Hz, 1H), 7.61 (s, 1H), 7.59-7.48 (m, 4H), 7.44 (d, J = 7.2 Hz, 1H), 4.67 (q, J = 7.2 Hz, 2H), 1.58 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.7, 145.5, 142.6, 138.5, 135.0, 134.2, 133.1, 132.7, 132.5, 130.3, 129.9, 129.1, 129.1, 128.9, 128.7, 128.3, 127.5, 127.3, 125.2, 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}ClNO_2$ 386.0942; Found 386.0924.

ethyl 10-(2-chlorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3an)



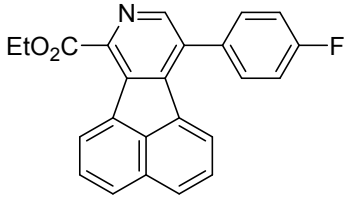
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3an** as a white solid (41.5 mg, 54% yield). mp:123-124 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.94 (d, J = 7.2 Hz, 1H), 8.61 (s, 1H), 7.99-7.93 (m, 2H), 7.76 (t, J = 7.6 Hz, 1H), 7.65 (d, J = 8.0 Hz, 1H), 7.56-7.50 (m, 1H), 7.49-7.43 (m, 3H), 7.08 (d, J = 7.2 Hz, 1H), 4.68 (q, J = 7.2 Hz, 2H), 1.58 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 148.1, 146.1, 142.7, 135.5, 134.1, 133.8, 133.1, 132.9, 132.8, 132.7, 131.0, 130.4, 130.1, 129.8, 129.7, 128.7, 128.6, 128.2, 127.6, 127.3, 124.6, 62.1, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}ClNO_2$ 386.0942; Found 386.0942.

ethyl 10-(4-bromophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ao)



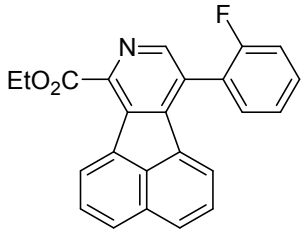
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ao** as a white solid (53.2 mg, 62% yield). mp:168-169 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (d, J = 7.2 Hz, 1H), 8.56 (s, 1H), 7.96 (d, J = 8.0 Hz, 2H), 7.76-7.71 (m, 3H), 7.48-7.43 (m, 4H), 4.66 (q, J = 7.2 Hz, 2H), 1.57 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.8, 145.3, 142.5, 135.6, 134.4, 134.2, 133.0, 132.8, 132.6, 132.2, 130.7, 129.9, 129.8, 128.8, 128.7, 128.2, 127.4, 125.1, 123.2, 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}BrNO_2$ 430.0437; Found 430.0421.

ethyl 10-(4-fluorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ap)



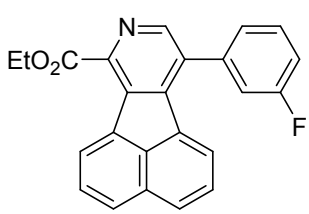
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ap** as a white solid (43.5 mg, 59% yield). mp:154-155 °C. ^{1}H NMR (400 MHz, $CDCl_3$ $CDCl_3$) δ 8.90 (d, J = 7.2 Hz, 1H), 8.57 (s, 1H), 7.96 (dd, J = 8.4, 2.8 Hz, 2H), 7.74 (t, J = 7.6 Hz, 1H), 7.58-7.55 (m, 2H), 7.46 (t, J = 7.6 Hz, 1H), 7.40 (d, J = 7.2 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 4.66 (q, J = 7.2 Hz, 2H), 1.57 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 163.2 (C-F, $^1J_{C\text{-}F}$ = 249.5 Hz), 148.1, 145.5, 142.4, 134.7, 134.2, 133.1, 132.9, 132.7, 132.7, 130.9, 130.8, 129.9, 129.7, 128.7 (C-F, $^3J_{C\text{-}F}$ = 10.1 Hz) 128.1, 127.4, 125.0, 116.1 (C-F, $^2J_{C\text{-}F}$ = 21.2 Hz), 62.1, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}FNO_2$ 370.1238; Found 370.1236.

ethyl 10-(2-fluorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3aq)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3aq** as a yellow solid (48.7 mg, 66% yield). mp:171-172 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, J = 7.2 Hz, 1H), 8.65 (s, 1H), 7.98 (d, J = 8.0 Hz, 2H), 7.76 (t, J = 7.2 Hz, 1H), 7.62-7.52 (m, 2H), 7.49 (t, J = 8.0 Hz 1H), 7.38 (td, J = 7.6, 1.2 Hz 1H), 7.33 (t, J = 8.4 Hz 2H), 4.68 (q, J = 7.1 Hz, 2H), 1.58 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 160.0 (C-F, $^1J_{C\text{-}F}$ = 250.5 Hz), 158.8, 148.4, 146.4, 142.6, 134.2, 133.1, 133.0, 132.7, 131.3 (C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 131.1 (C-F, $^3J_{C\text{-}F}$ = 8.1 Hz), 129.8, 129.2, 128.8, 128.6, 128.2, 127.6, 124.8 (C-F, $^4J_{C\text{-}F}$ = 4.0 Hz), 124.6, 124.3 (C-F, $^2J_{C\text{-}F}$ = 16.2 Hz), 116.3 (C-F, $^2J_{C\text{-}F}$ = 21.2 Hz), 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}FNO_2$ 370.1238; Found 370.1226.

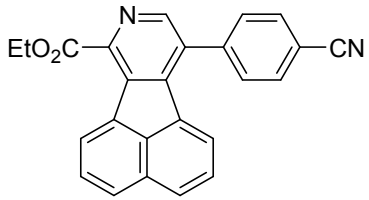
ethyl 10-(3-fluorophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3ar)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ar** as a yellow solid (40.6 mg, 55% yield). mp:146-147 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, J = 7.2 Hz, 1H), 8.59 (s, 1H), 7.99 (d, J = 8.0 Hz, 2H), 7.80-7.74 (m, 1H), 7.57 (td, J = 8.0, 6.0 Hz, 1H), 7.51-7.44 (m, 2H), 7.40 (d, J = 7.6 Hz, 1H), 7.35-7.27 (m, 2H), 4.67 (q, J = 7.2 Hz, 2H), 1.57 (t, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 163.0 (C-F, $^1J_{C\text{-}F}$ = 248.5 Hz), 147.8, 145.4, 142.6, 138.9 (C-F, $^3J_{C\text{-}F}$ = 7.1 Hz), 134.4, 134.2, 133.1, 132.7, 132.6, 130.7 (C-F, $^3J_{C\text{-}F}$ = 9.1 Hz), 129.9, 129.9, 128.8, 128.7, 128.2,

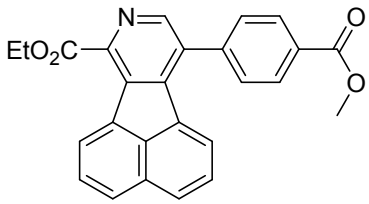
127.5, 125.2, 124.9 (C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 116.2 (C-F, $^2J_{C\text{-}F}$ = 22.2 Hz), 115.9 (C-F, $^2J_{C\text{-}F}$ = 20.0 Hz), 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{17}FNO_2$ 370.1238; Found 370.1223.

ethyl 10-(4-cyanophenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3as)



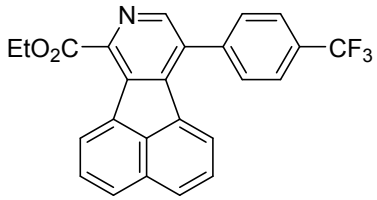
Purification by column chromatography on silica gel (PE/EA = 80/1, v/v) afforded **3as** as a white solid (48.8 mg, 65% yield). mp:185-186 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 7.2 Hz, 1H), 8.56 (s, 1H), 8.01 (d, *J* = 8.0 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 2H), 7.80-7.75 (m, 3H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 4.67 (q, *J* = 7.2 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.5, 145.2, 143.3, 141.7, 134.2, 133.6, 133.1, 132.8, 132.4, 132.4, 130.2, 130.0, 130.0, 129.0, 128.8, 128.4, 127.5, 124.9, 118.4, 112.9, 62.3, 14.4. HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{25}H_{16}N_2O_2$ 377.1285; Found 377.1275

ethyl 10-(4-(methoxycarbonyl)phenyl)acenaphtho[1,2-c]pyridine-7-carboxylate (3at)



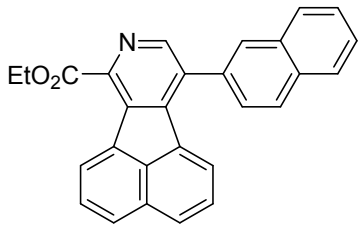
Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **3at** as a white solid (53.2 mg, 65% yield). mp:160-161 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (d, *J* = 7.2 Hz, 1H), 8.60 (s, 1H), 8.27 (d, *J* = 8.0 Hz, 2H), 7.99 (dd, *J* = 8.4, 3.6 Hz, 2H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 6.8 Hz, 1H), 4.67 (q, *J* = 7.2 Hz, 2H), 4.01 (s, 3H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 166.3, 147.5, 145.5, 142.6, 141.4, 134.7, 134.3, 133.1, 132.7, 132.5, 130.7, 130.3, 130.0, 129.9, 129.2, 128.9, 128.7, 128.3, 127.5, 125.2, 62.3, 52.4, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{26}H_{20}NO_4$ 410.1387; Found 410.1373.

ethyl 10-(4-(trifluoromethyl)phenyl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3au)



Purification by column chromatography on silica gel (PE/EA = 8/1, v/v) afforded **3au** as a white solid (58.6 mg, 70% yield). mp:150-151 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 7.2 Hz, 1H), 8.57 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.86 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 8.0 Hz, 3H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 4.67 (q, *J* = 7.2 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 147.8, 145.3, 142.9, 140.6, 134.2, 134.1, 133.0, 132.6, 132.5, 131.1(C-F, $^2J_{C\text{-}F}$ = 30.3 Hz), 130.0, 129.9, 129.6, 128.8(C-F, $^3J_{C\text{-}F}$ = 14.1 Hz), 128.3, 127.5, 126.0(C-F, $^4J_{C\text{-}F}$ = 3.0 Hz), 125.4, 125.0, 122.7, 62.2, 14.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{25}H_{17}F_3NO_2$ 420.1206; Found 420.1202.

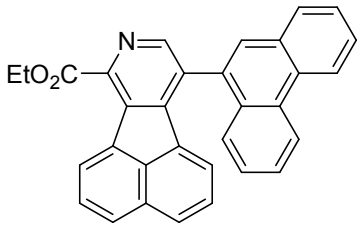
ethyl 10-(naphthalen-2-yl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3av)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3av** as a white solid (35.3 mg, 44% yield). mp:118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, *J* = 7.2 Hz, 1H), 8.71 (s, 1H), 8.09 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 8.02-7.92 (m, 4H), 7.77 (t, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 9.6 Hz, 1H), 7.61 (td, *J* = 6.8, 6.1, 3.6 Hz, 2H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 4.69 (q, *J* = 7.2 Hz, 2H), 1.59 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 148.4, 145.5, 142.3, 135.7, 134.2, 134.2, 133.4, 133.2, 133.1, 133.0, 132.8, 129.8, 129.6,

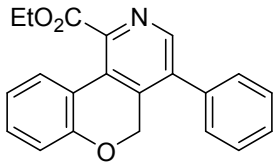
128.7, 128.6, 128.6, 128.3, 128.1, 128.1, 127.9, 127.4, 126.9, 126.8, 126.8, 125.2, 62.1, 14.5. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{28}H_{20}NO_2$ 402.1489; Found 402.1434.

ethyl 10-(phenanthren-9-yl)acenaphtho[1,2-*c*]pyridine-7-carboxylate (3aw)



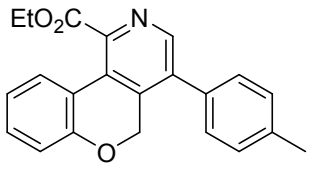
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3aw** as a white solid (35.2 mg, 39% yield). mp:209-210 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, *J* = 7.2 Hz, 1H), 8.86 (t, *J* = 8.4 Hz, 2H), 8.79 (s, 1H), 7.96 (dd, *J* = 8.0, 3.2 Hz, 2H), 7.93 (s, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.79 (t, *J* = 7.6 Hz, 2H), 7.69 (t, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.2 Hz, 1H), 4.73 (q, *J* = 7.2 Hz, 2H), 1.63 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 149.1, 147.0, 142.8, 142.8, 134.2, 133.9, 133.2, 133.1, 132.9, 132.9, 131.3, 130.7, 130.5, 130.5, 129.8, 129.5, 129.1, 128.8, 128.7, 128.3, 128.0, 127.6, 127.5, 127.2, 127.1, 126.5, 125.6, 123.2, 122.8, 62.2, 14.6. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{32}H_{22}NO_2$ 452.1645; Found 452.1642.

ethyl 4-phenyl-5H-chromeno[4,3-*c*]pyridine-1-carboxylate (5aa)



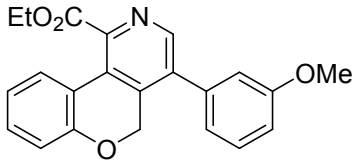
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **5aa** as a white solid (31.2 mg, 47% yield). mp:91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 7.55-7.45 (m, 4H), 7.36-7.28 (m, 3H), 7.07 (t, *J* = 8.4 Hz, 2H), 5.02 (s, 2H), 4.46 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 155.8, 148.0, 145.8, 141.0, 135.2, 135.2, 130.4, 129.1, 128.9, 128.8, 126.4, 124.4, 122.4, 120.2, 117.7, 65.6, 62.3, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{21}H_{18}NO_3$ 332.1281 ; Found 332.1279.

ethyl 4-(p-tolyl)-5H-chromeno[4,3-c]pyridine-1-carboxylate(5ab)



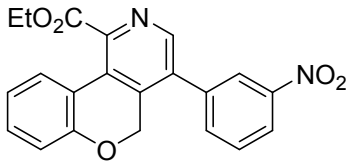
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **5ab** as a white solid (29.6 mg, 43% yield). mp:106-107 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 7.6 Hz, 2H), 5.03 (s, 2H), 4.46 (q, *J* = 7.2 Hz, 2H), 2.44 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 155.9, 148.0, 145.5, 141.0, 138.8, 135.2, 132.2, 130.8, 129.6, 129.0, 126.4, 124.4, 122.4, 120.22, 117.7, 65.7, 62.2, 21.3, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{20}NO_3$ 34601438 ; Found 346.1441.

ethyl 4-(3-methoxyphenyl)-5H-chromeno[4,3-c]pyridine-1-carboxylate(5ac)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **5ac** as a white solid (29.6 mg, 40% yield). mp:124-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.54 (d, *J* = 6.8 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.4 Hz, 1H), 7.06 (t, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 1H), 6.89-6.80 (m, 2H), 5.02 (s, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 159.8, 155.8, 147.8, 145.8, 141.0, 136.5, 135.1, 130.9, 130.0, 126.4, 124.4, 122.4, 121.4, 120.1, 117.7, 114.9, 114.0, 65.6, 62.2, 55.4, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{20}NO_4$ 362.1387 ; Found 362.1389.

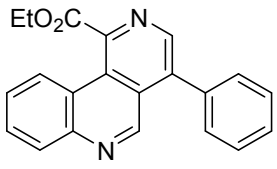
ethyl 4-(3-nitrophenyl)-5H-chromeno[4,3-c]pyridine-1-carboxylate(5ad)



Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **5ad** as a white solid (34.6 mg, 46% yield).

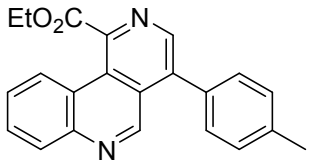
mp:134-135 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 8.33 (d, *J* = 9.2 Hz, 1H), 8.18 (s, 1H), 7.72 (t, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 7.11-7.00 (m, 2H), 4.99 (s, 2H), 4.45 (q, *J* = 7.2 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.7, 155.7, 148.4, 147.5, 146.8, 141.1, 136.8, 135.0, 132.8, 131.2, 130.2, 126.4, 124.6, 123.9, 123.7, 122.64, 119.7, 117.8, 65.3, 62.4, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{21}H_{17}N2O_5$ 377.1132 ; Found 377.1135.

ethyl 4-phenylbenzo[*c*][2,6]naphthyridine-1-carboxylate (5ba)



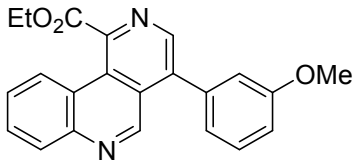
Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **5ba** as a white solid (26.5 mg, 52% yield). mp:131-132 °C . ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.41 (s, 1H), 8.82 (s, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 7.84 (t, *J* = 7.6 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.61-7.54 (m, 5H), 4.68 (q, *J* = 7.2 Hz, 2H), 1.50 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 150.5, 148.9, 145.3, 145.1, 135.8, 134.5, 130.7, 130.4, 130.0, 129.0, 129.0, 128.1, 128.1, 124.6, 123.6, 120.5, 62.9, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{21}H_{17}N_2O_2$ 329.1285 ; Found 329.1281

ethyl 4-(p-tolyl)benzo[c][2,6]naphthyridine-1-carboxylate(5bb)



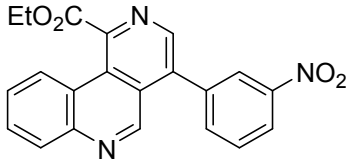
Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **5bb** as a white solid (26.5 mg, 47% yield). mp:139-140 °C . ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.80 (s, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 9.2 Hz, 1H), 7.83 (t, *J* = 7.2 Hz, 1H), 7.71 (t, *J* = 8.4 Hz, 1H), 7.46-7.36 (m, 4H), 4.67 (q, *J* = 7.2 Hz, 2H), 2.49 (s, 3H), 1.49 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 150.6, 148.7, 145.3, 145.2, 139.1, 135.9, 131.6, 130.7, 130.3, 130.0, 129.7, 128.1, 128.1, 124.6, 123.6, 120.6, 62.9, 21.34, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{19}N_2O_2$ 343.1441 ; Found 343.1441.

ethyl 4-(3-methoxyphenyl)benzo[c][2,6]naphthyridine-1-carboxylate(5bc)



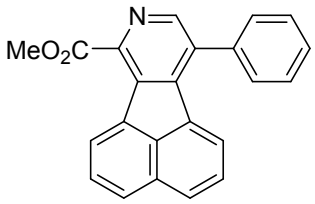
Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **5bc** as a white solid (27.2 mg, 38% yield). mp:147-148 °C .^{1}H NMR (400 MHz, $CDCl_3$) δ 9.42 (s, 1H), 8.81 (s, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.82 (t, *J* = 8.0 Hz, 1H), 7.70 (t, *J* = 8.4 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.15-7.04 (m, 3H), 4.66 (q, *J* = 7.2 Hz, 2H), 3.86 (s, 3H), 1.48 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 159.9, 150.5, 149.0, 145.3, 145.0, 135.9, 135.7, 130.7, 130.0, 128.1, 128.1, 124.6, 123.5, 122.9, 120.5, 116.1, 114.4, 62.9, 55.4, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{22}H_{19}N_2O_3$ 359.1390 ; Found 359.1392.

ethyl 4-(3-nitrophenyl)benzo[c][2,6]naphthyridine-1-carboxylate(5bd)



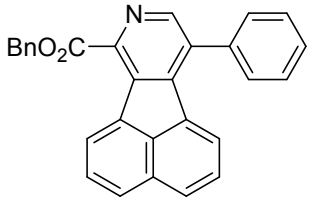
Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **5bd** as a yellow solid (29.8 mg, 40% yield). mp:161-162 °C .^{1}H NMR (400 MHz, $CDCl_3$) δ 9.27 (s, 1H), 8.80 (s, 1H), 8.45-8.39 (m, 2H), 8.36 (d, *J* = 9.2 Hz, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.85 (t, *J* = 7.6 Hz, 1H), 7.79 (t, *J* = 8.0 Hz, 1H), 7.76-7.71 (m, 1H), 4.67 (q, *J* = 7.2 Hz, 2H), 1.48 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.3, 150.2, 149.2, 148.6, 145.4, 144.9, 136.3, 136.3, 133.1, 130.9, 130.4, 130.2, 128.6, 127.8, 125.1, 124.5, 124.0, 123.7, 120.3, 63.1, 14.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{21}H_{16}N_3O_4$ 374.1135 ; Found 374.1137.

methyl 10-phenylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3ba)



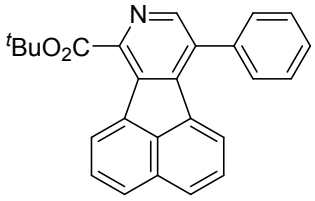
Purification by column chromatography on silica gel (PE/EA = 20/1, v/v) afforded **3ba** as a white solid (38.4 mg, 57% yield). mp:132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, *J* = 7.2 Hz, 1H), 8.59 (d, *J* = 2.8 Hz, 1H), 7.98-7.90 (m, 2H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.60-7.57 (m, 5H), 7.45-7.39 (m, 2H), 4.17 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9, 148.2, 145.4, 141.7, 136.7, 136.0, 134.5, 133.1, 133.0, 132.7, 129.83, 129.6, 129.1, 129.0, 128.9, 128.7, 128.6, 128.3, 127.4, 125.1, 53.0. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{23}H_{16}NO_2$ 338.1176; Found 338.1172.

benzyl 10-phenylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3ca)



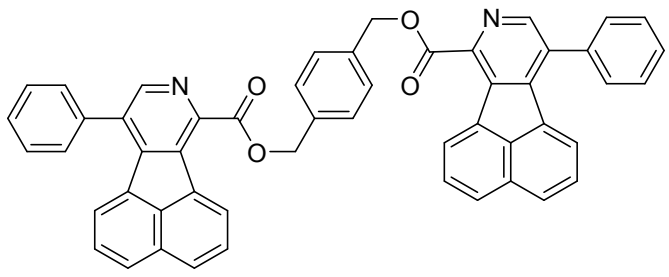
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3ca** as a white solid (43.7 mg, 53% yield). mp:136-137 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 7.2 Hz, 1H), 8.61 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.62-7.58 (m, 7H), 7.46-7.39 (m, 4H), 7.36 (t, *J* = 7.2 Hz, 1H), 5.66 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 148.3, 145.3, 142.2, 136.8, 135.8, 134.2, 133.1, 133.1, 132.7, 129.9, 129.6, 129.1, 129.0, 128.9, 128.7, 128.6, 128.4, 128.0, 127.4, 125.2, 67.6. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{29}H_{20}NO_2$ 414.1489; Found 414.1486.

tert-butyl 10-phenylacenaphtho[1,2-*c*]pyridine-7-carboxylate (3da)



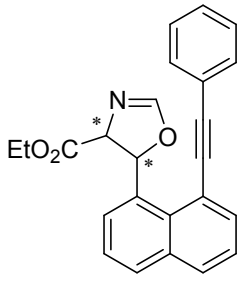
Purification by column chromatography on silica gel (PE/EA = 10/1, v/v) afforded **3da** as a white solid (38.6 mg, 51% yield). mp:124-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 7.2 Hz, 1H), 8.59 (s, 1H), 7.96-7.93 (m, 2H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.61-7.56 (m, 5H), 7.48-7.42 (m, 2H), 1.81 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 148.4, 145.0, 144.4, 136.9, 135.1, 133.3, 133.0, 132.9, 132.8, 129.9, 129.4, 129.1, 129.0, 128.8, 128.5, 128.4, 127.5, 126.9, 125.1, 82.8, 28.4. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{26}H_{22}NO_2$ 380.1645; Found 380.1648.

1,4-phenylenebis(methylene) bis(10-phenylacenaphtho[1,2-*c*]pyridine-7-carboxylate) (3ea)



Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **3ea** as a white solid (69.6 mg, 47% yield). mp:141-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 7.2 Hz, 2H), 8.61 (s, 2H), 7.92 (dd, *J* = 6.4, 2.4 Hz, 2H), 7.89 (s, 1H), 7.87 (s, 1H), 7.67 (t, *J* = 7.2 Hz, 6H), 7.59 (s, 10H), 7.45-7.40 (m, 4H), 5.67 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 148.3, 145.3, 142.0, 136.7, 136.1, 135.8, 134.3, 133.0, 133.0, 132.6, 129.8, 129.5, 129.0, 129.0, 128.9, 128.9, 128.6, 128.6, 128.0, 127.4, 125.1, 67.2. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{52}H_{33}N_2O_4$ 749.2435; Found 749.2446.

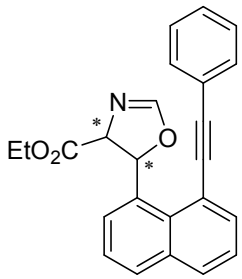
ethyl 5-(8-(phenylethynyl)naphthalen-1-yl)-4,5-dihydrooxazole-4-carboxylate (intermediate B1)



Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **B1** as a white solid (78.2 mg, 53% yield). ^{1}H NMR (400 MHz,

$CDCl_3$) δ 8.09 (d, *J* = 6.0 Hz, 1H), 7.93-7.84 (m, 3H), 7.63-7.57 (m, 3H), 7.53-7.45 (m, 2H), 7.43-7.33 (m, 3H), 7.26 (s, 1H), 4.67 (dd, *J* = 6.0, 2.0 Hz, 1H), 3.98-3.84 (m, 2H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.5, 157.0, 135.9, 135.9, 134.7, 131.5, 130.6, 130.5, 129.1, 128.7, 128.4, 125.9, 125.3, 123.0, 118.3, 95.9, 90.6, 78.6, 76.0, 61.6, 13.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{20}NO_3$ 370.1438; Found 370.1435.

ethyl 5-(8-(phenylethynyl)naphthalen-1-yl)-4,5-dihydrooxazole-4-carboxylate (intermediate B2)



Purification by column chromatography on silica gel (PE/EA = 5/1, v/v) afforded **B2** as a white solid (53.1 mg, 36% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90-7.83 (m, 2H), 7.83-7.79 (m, 2H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.58-7.53 (m, 2H), 7.50-7.45 (m, 2H), 7.43-7.39 (m, 3H), 7.47 (d, *J* = 1.6 Hz, 1H), 5.50 (dd, *J* = 10.8, 1.6 Hz, 1H), 3.47 (dq, *J* = 14.0, 6.8 Hz, 1H), 3.22 (dq, *J* = 14.0, 6.8 Hz, 1H), 0.30 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 157.4, 135.2, 134.2, 132.1, 131.1, 130.5, 130.1, 129.8, 128.8, 128.8, 125.6, 125.5, 125.0, 122.9, 118.5, 93.0, 90.9, 80.1, 72.8, 60.6, 12.9. HRMS (ESI) m/z: $[M + H]^+$ Calcd for $C_{24}H_{20}NO_3$ 370.1438; Found 370.1435.

7. X-ray Crystallography of 3aa

Compound **3aa** (40 mg) was dissolved in 10 mL of dichloromethane/n-hexane (v/v = 1:3), and it was crystallized to give crystal as a colorless block-shaped crystal after the solvent was slowly volatilized in 4 days at room temperature (~ 30 °C).

Data were measured using ϕ and ω scans using CuKα radiation. The maximum resolution that was achieved was Θ = 74.610° (0.80 Å). The unit cell was refined using **SAINT** (Bruker, V8.37A, after 2013) on 5629 reflections, 23% of the observed reflections. The final completeness is 99.70 % out to 74.610° in Θ. CCDC-2025268 (**3aa**) contain the supplementary crystallographic data. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre (http://www.ccdc.cam.ac.uk/). X-ray crystallographic data for **3aa** is available as Figure S1

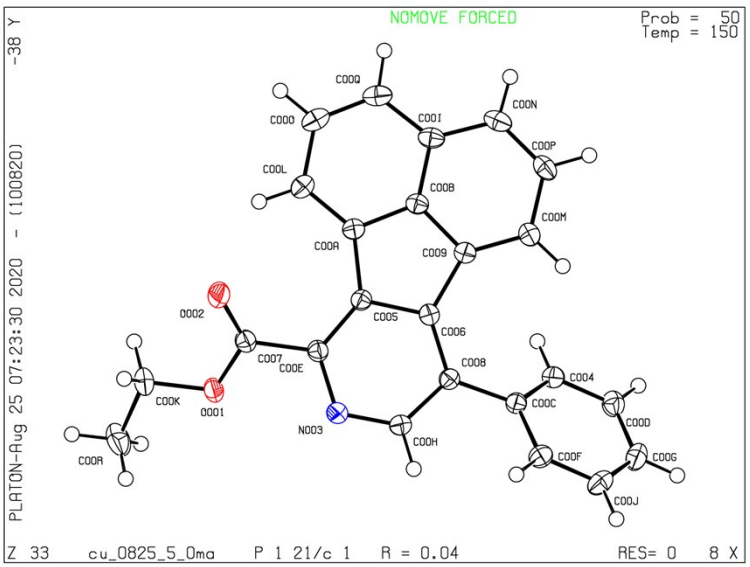


Figure S1. X-ray crystallographic for **3aa**

Table S2. Crystal Data and Structure Refinement for **3aa**.

Compound	**3aa**
Formula	$C_{24}H_{17}NO_2$
$D_{calc.}$/ g cm^{-3}	1.378
m/mm^{-1}	0.697
Formula Weight	351.38
Colour	colourless
Shape	block
Size/mm^3	0.20×0.15×0.10
T/K	150.0
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	11.9988(3)
b/Å	19.1984(5)
c/Å	7.6672(2)
a/°	90
b/°	106.467(2)
g/°	90
V/Å^3	1693.75(8)
Z	4
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK_a
Q_{min}/°	3.841
Q_{max}/°	74.610
Measured Refl's.	24320
Ind't Refl's	3446

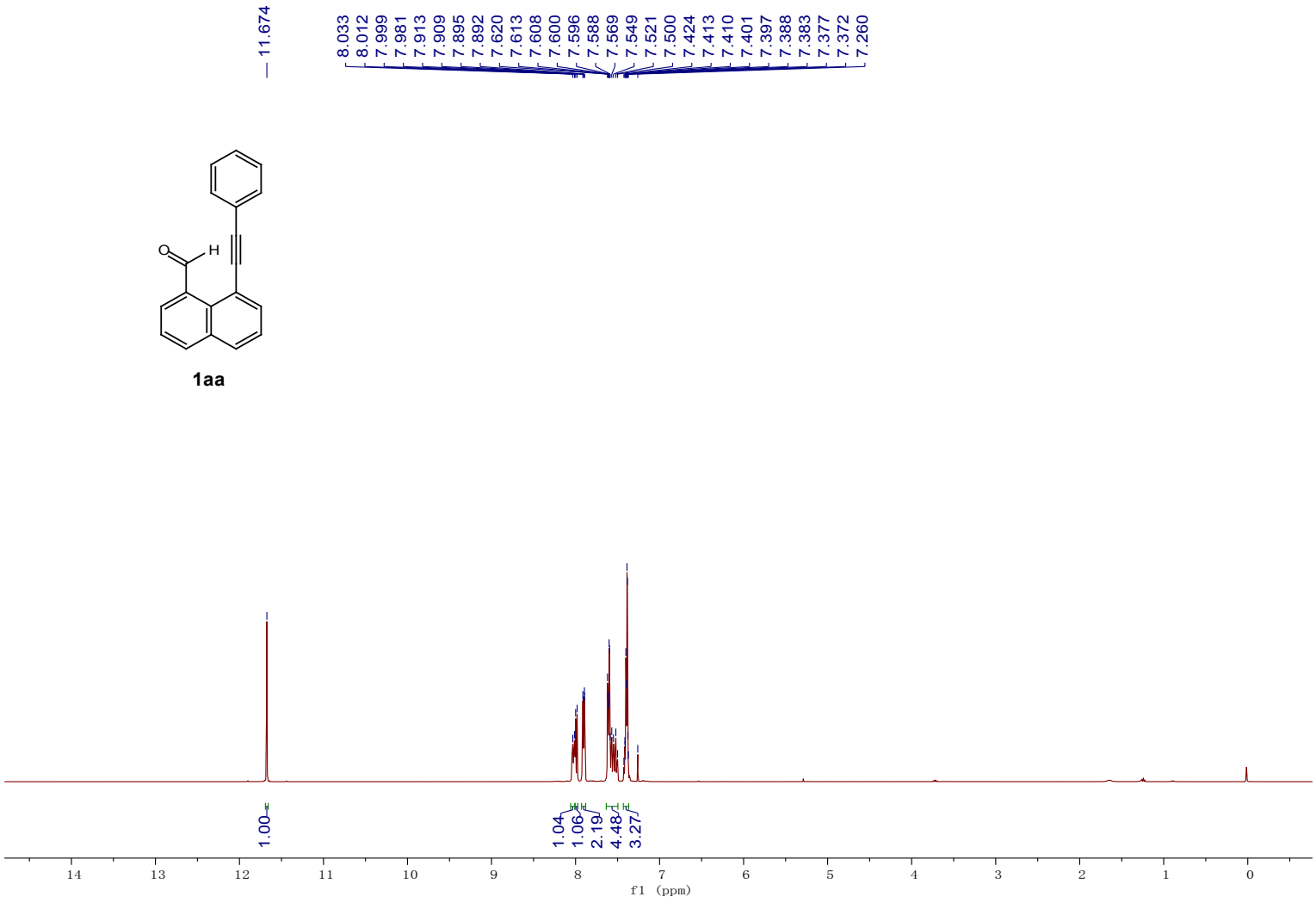
Refl's with I > 2(I)	2744
R_{int}	0.0650
Parameters	245
Restraints	0
Largest Peak	0.250
Deepest Hole	-0.307
GooF	1.095
wR_2 (all data)	0.1241
wR_2	0.1056
R_1 (all data)	0.0586
R_1	0.403

8. Reference：

(1) Muthu Karuppasamy, B. S. Vachan, Perumal Vinoth, Isravel Muthukrishnan, et al., *Org. Lett.* **2019,** *21* (15), 5784-5788.

(2) Tianyu Cheng, Yizhao Chen, Anjun Qin, and Ben Zhong Tang. *Macromolecules* **2018**, *51*, 5638−5645.

9. Copies of NMR Spectrum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8.012
7.999
7.981
7.913
7.909
7.895
7.892
7.620
7.613
7.608
7.600
7.596
7.588
7.569
7.549
7.521
7.500
7.424
7.413
7.410
7.401
7.397
7.388
7.383
7.377
7.372
7.260
O
H
1aa
1.00
1.04
1.06
2.19
4.48
3.27
14
13
12
11
10
9
8
7
6
5
4
3
2
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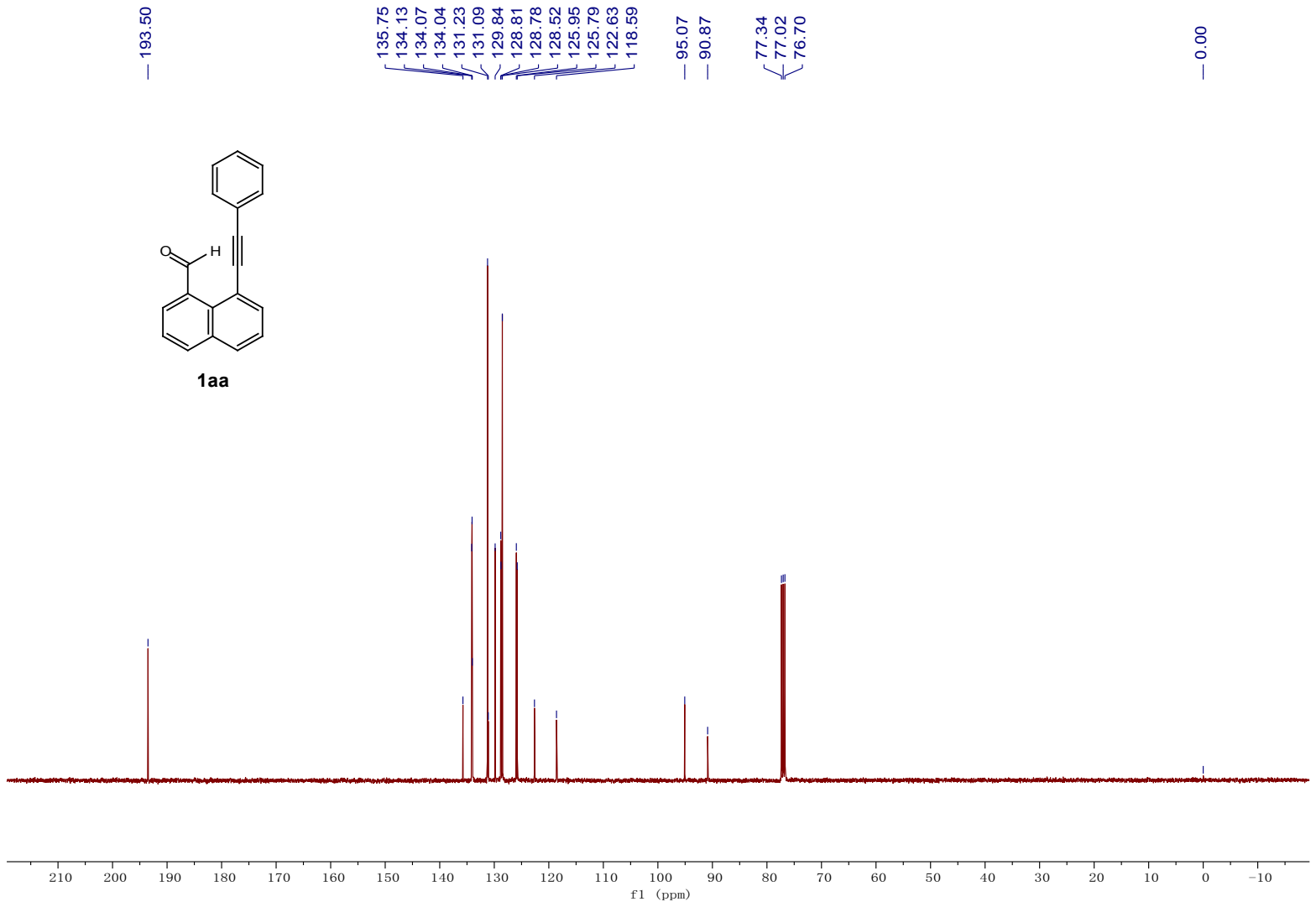
f1 (ppm)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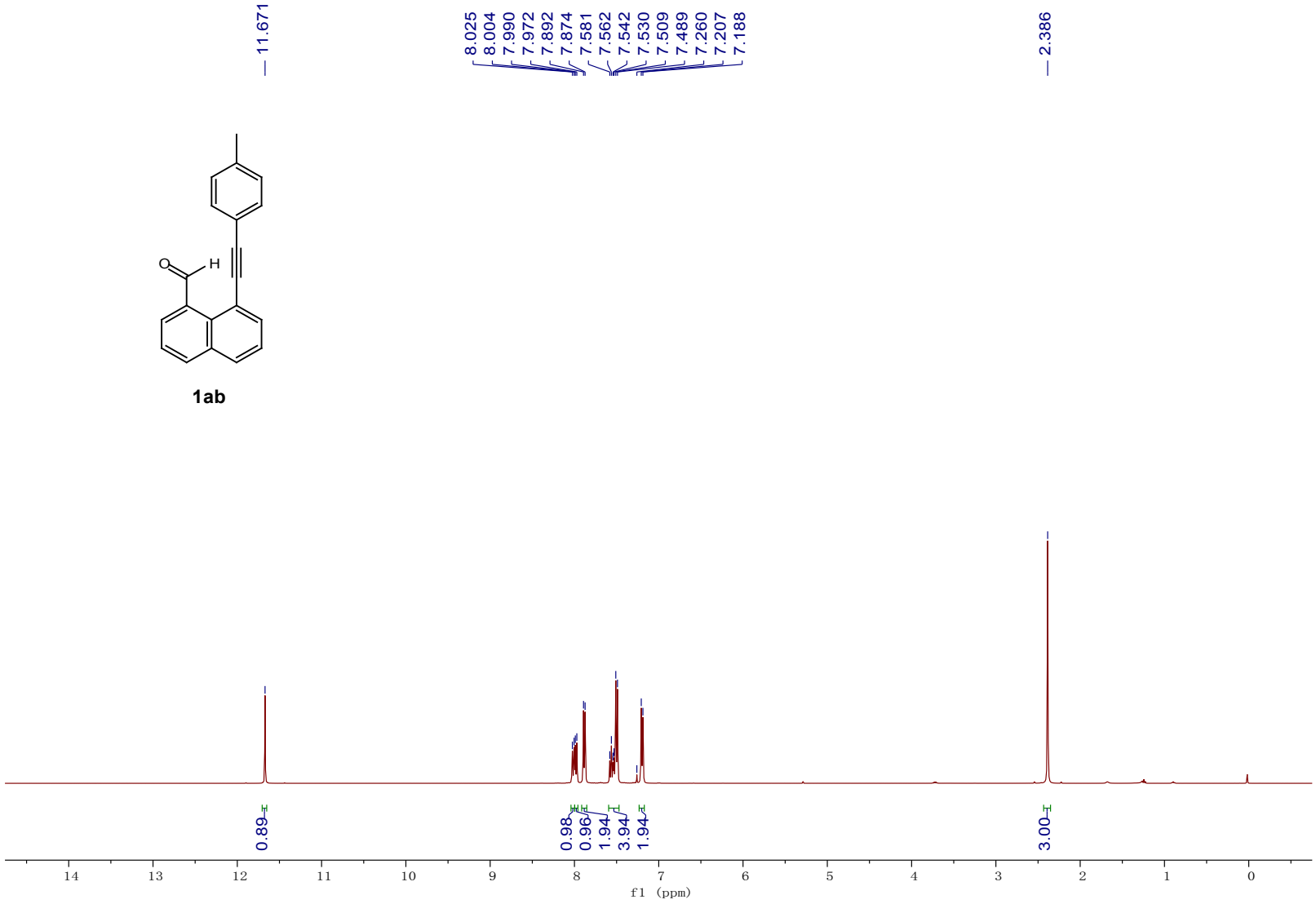
134.13
134.07
134.04
131.23
131.09
129.84
128.81
128.78
128.52
125.95
125.79
122.63
118.59
95.07
90.87
77.34
77.02
76.70
0.00
O
H
1aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.542
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7.489
7.260
7.207
7.188
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O
H
0.89
0.98
0.96
1.94
3.94
1.94
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f1 (ppm)

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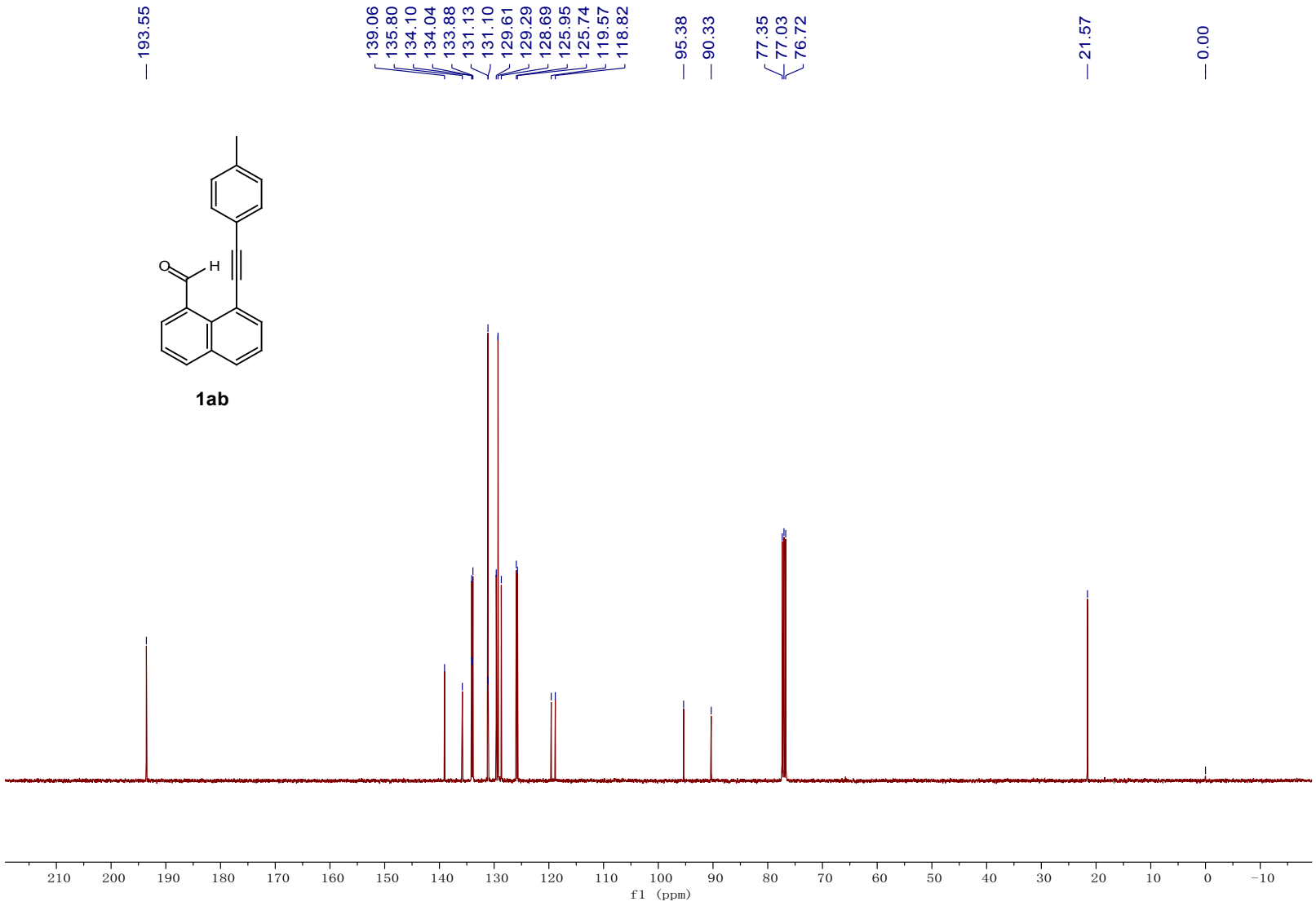
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131.10
129.61
129.29
128.69
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125.74
119.57
118.82
95.38
90.33
77.35
77.03
76.72
21.57
0.00
O
H
1ab
210
200
190
180
170
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150
140
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120
110
100
90
80
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30
20
10
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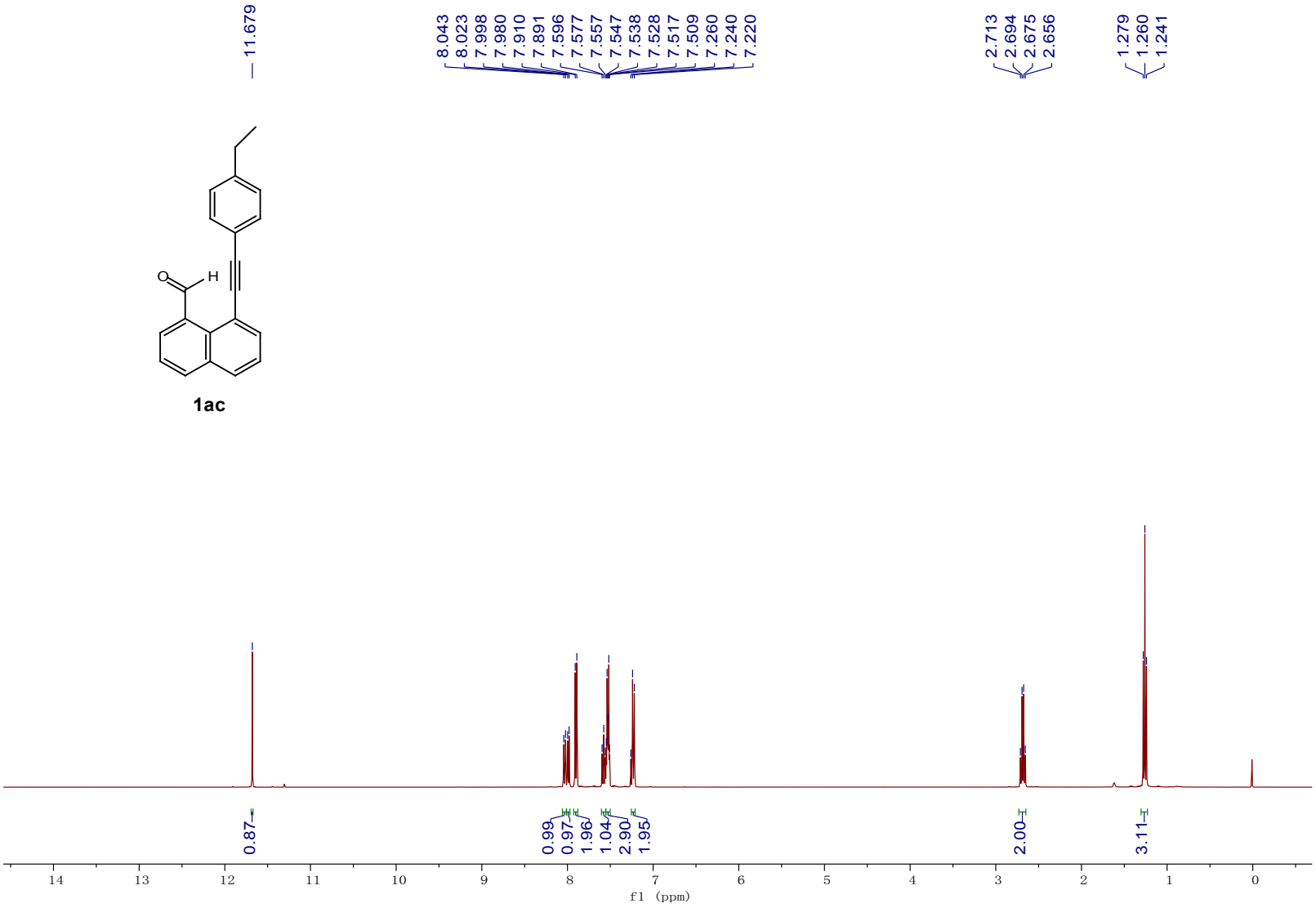
−10
f1 (ppm)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7.528
7.517
7.509
7.260
7.240
7.220
2.713
2.694
2.675
2.656
1.279
1.260
1.241
O
H
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0.99
0.97
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1.04
2.90
1.95
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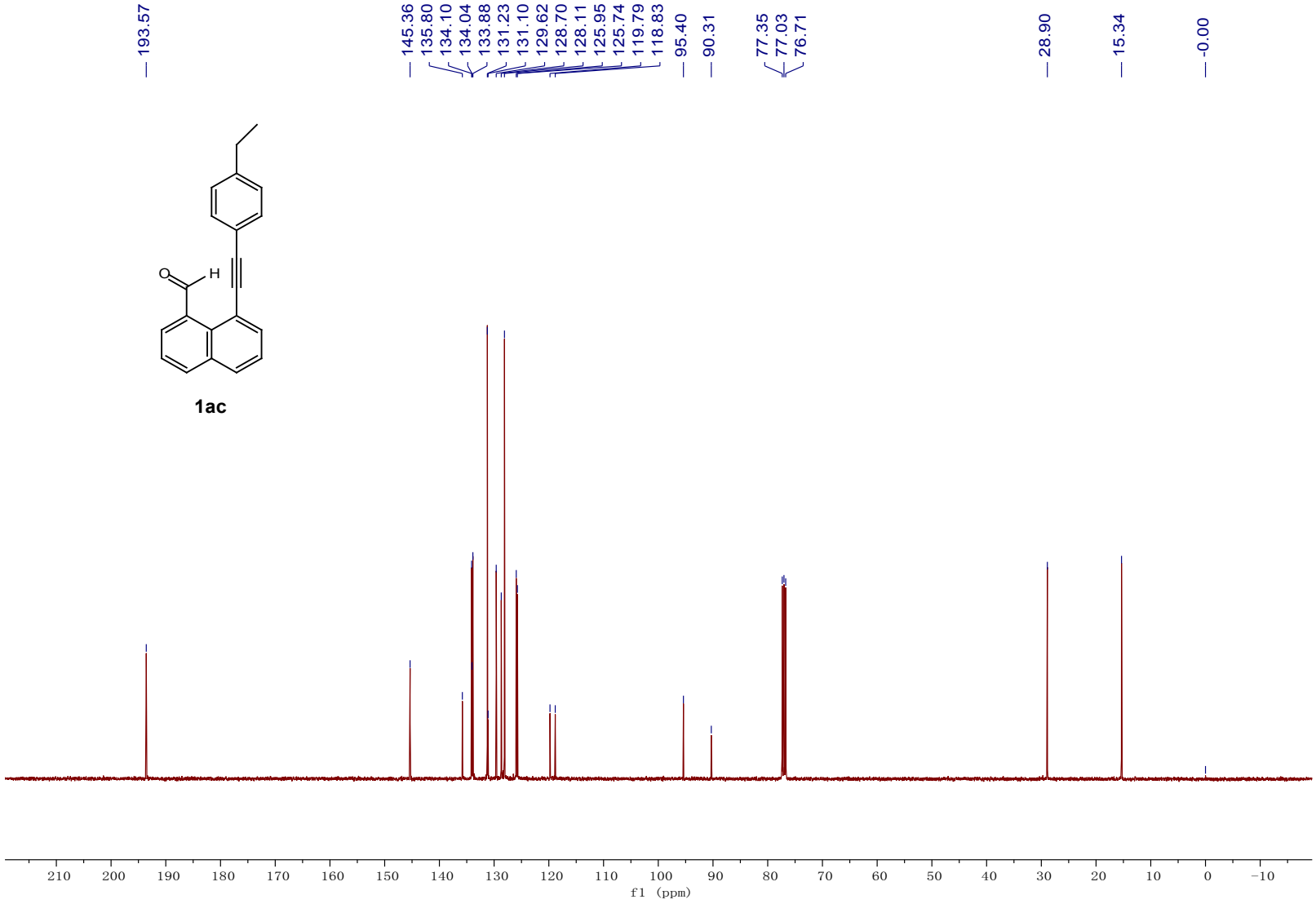
f1 (ppm)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131.10
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125.74
119.79
118.83
95.40
90.31
77.35
77.03
76.71
28.90
15.34
-0.00
O
H
1ac
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200
190
180
170
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120
110
100
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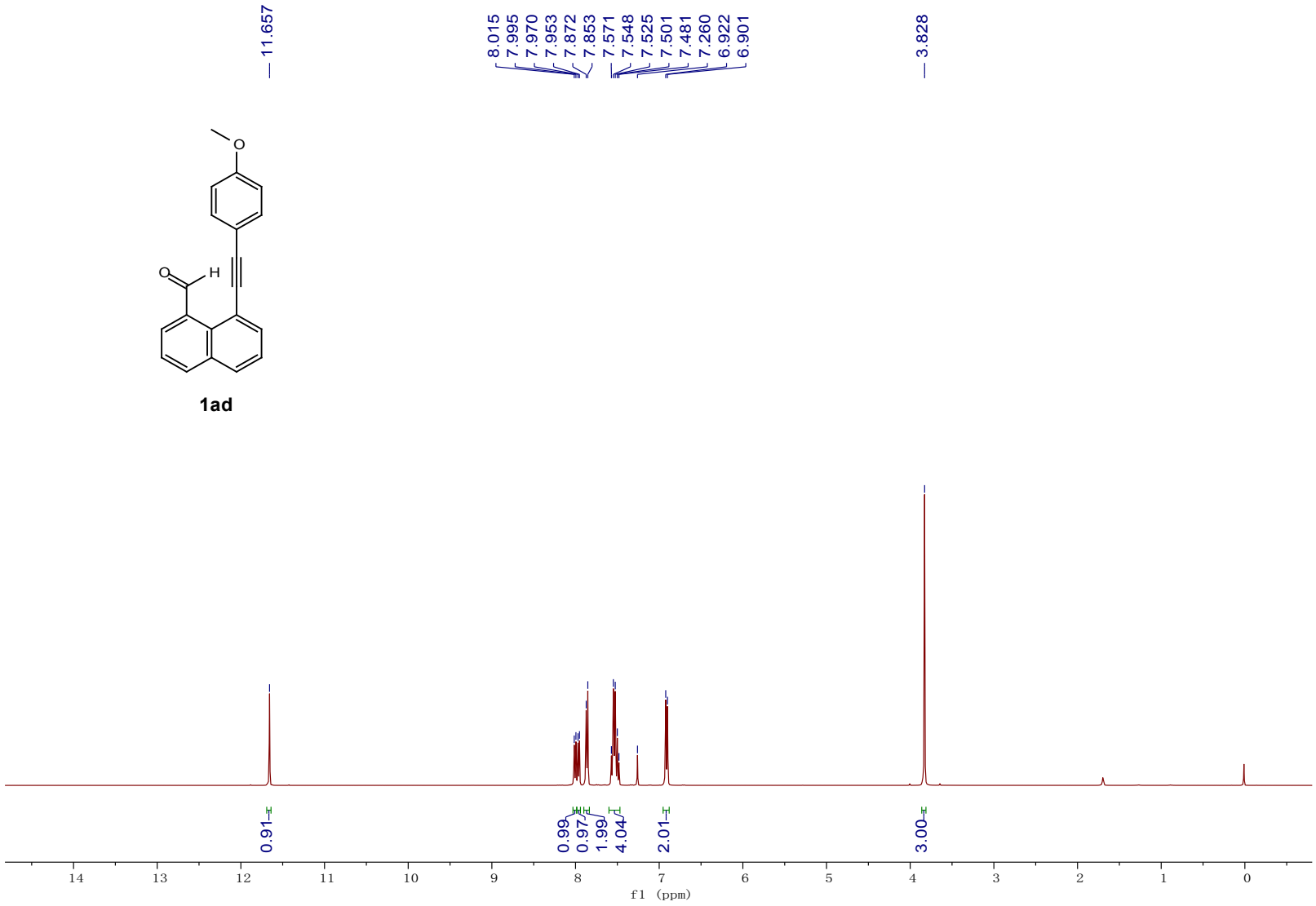
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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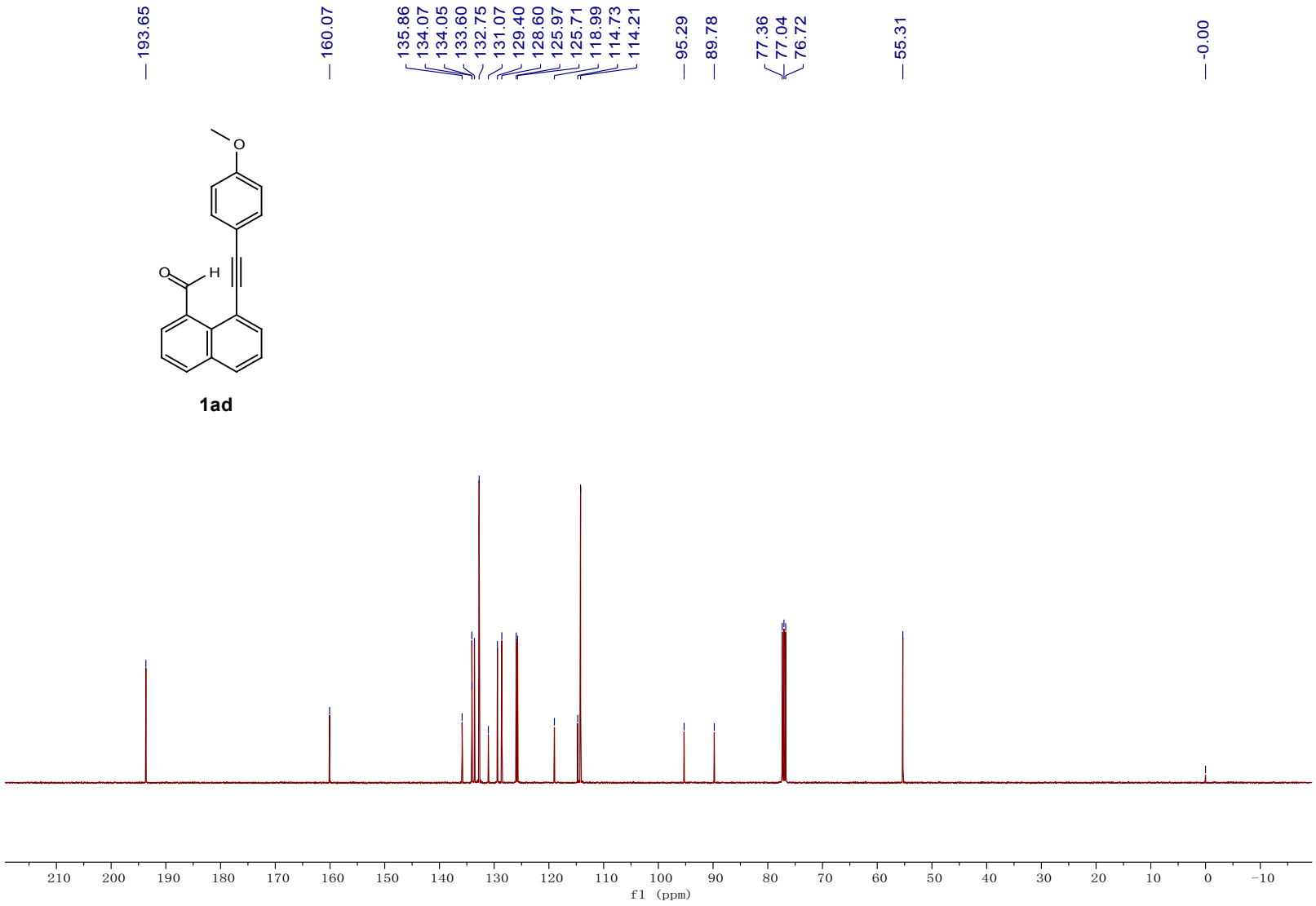
6.922
6.901
3.828
O
O
H
0.91
0.99
0.97
1.99
4.04
2.01
3.00
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1ad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134.07
134.05
133.60
132.75
131.07
129.40
128.60
125.97
125.71
118.99
114.73
114.21
95.29
89.78
77.36
77.04
76.72
55.31
-0.00
O
O
H
1ad
210
200
190
180
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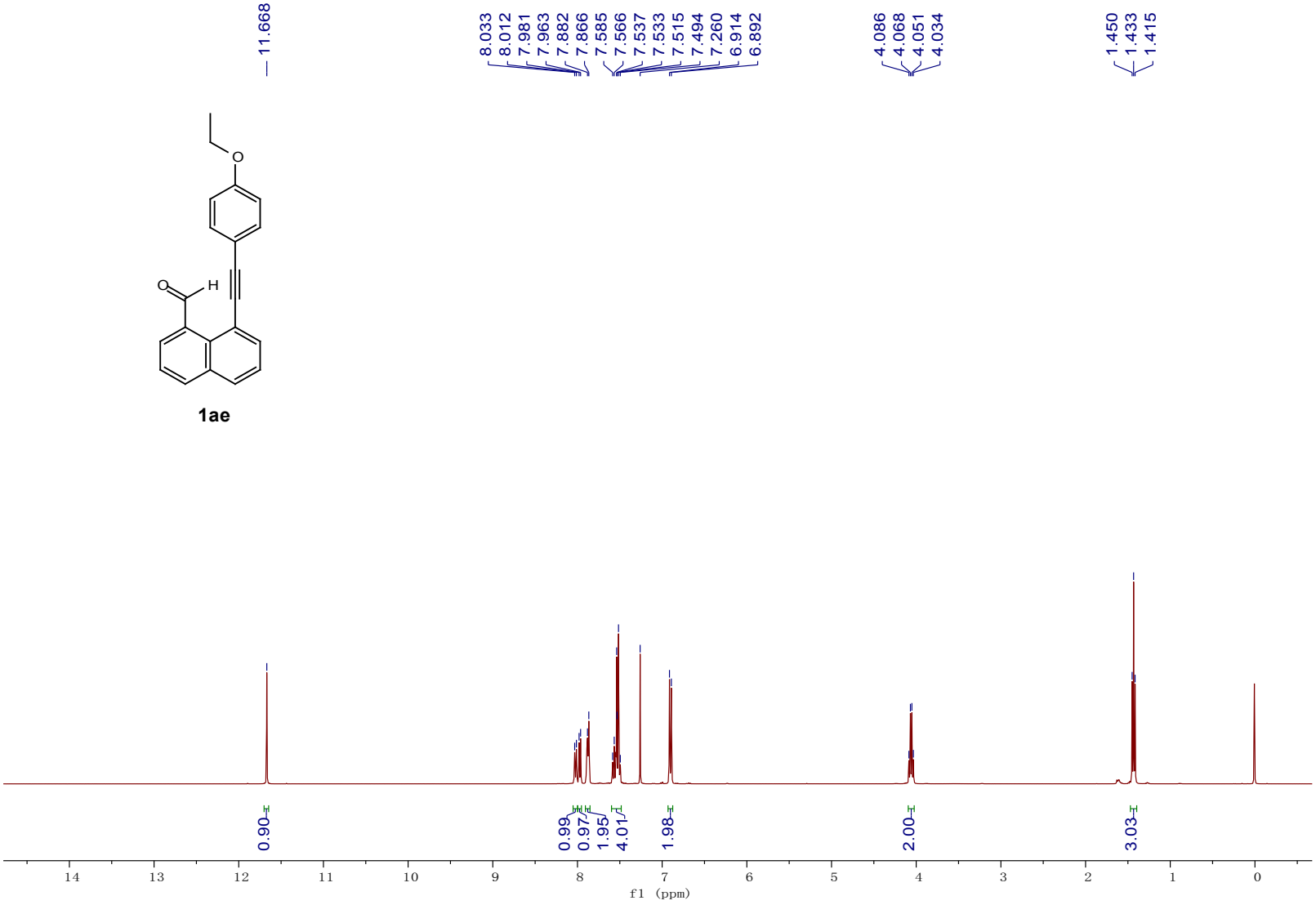
f1 (ppm)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4.068
4.051
4.034
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1.433
1.415
O
O
H
0.90
0.99
0.97
1.95
4.01
1.98
2.00
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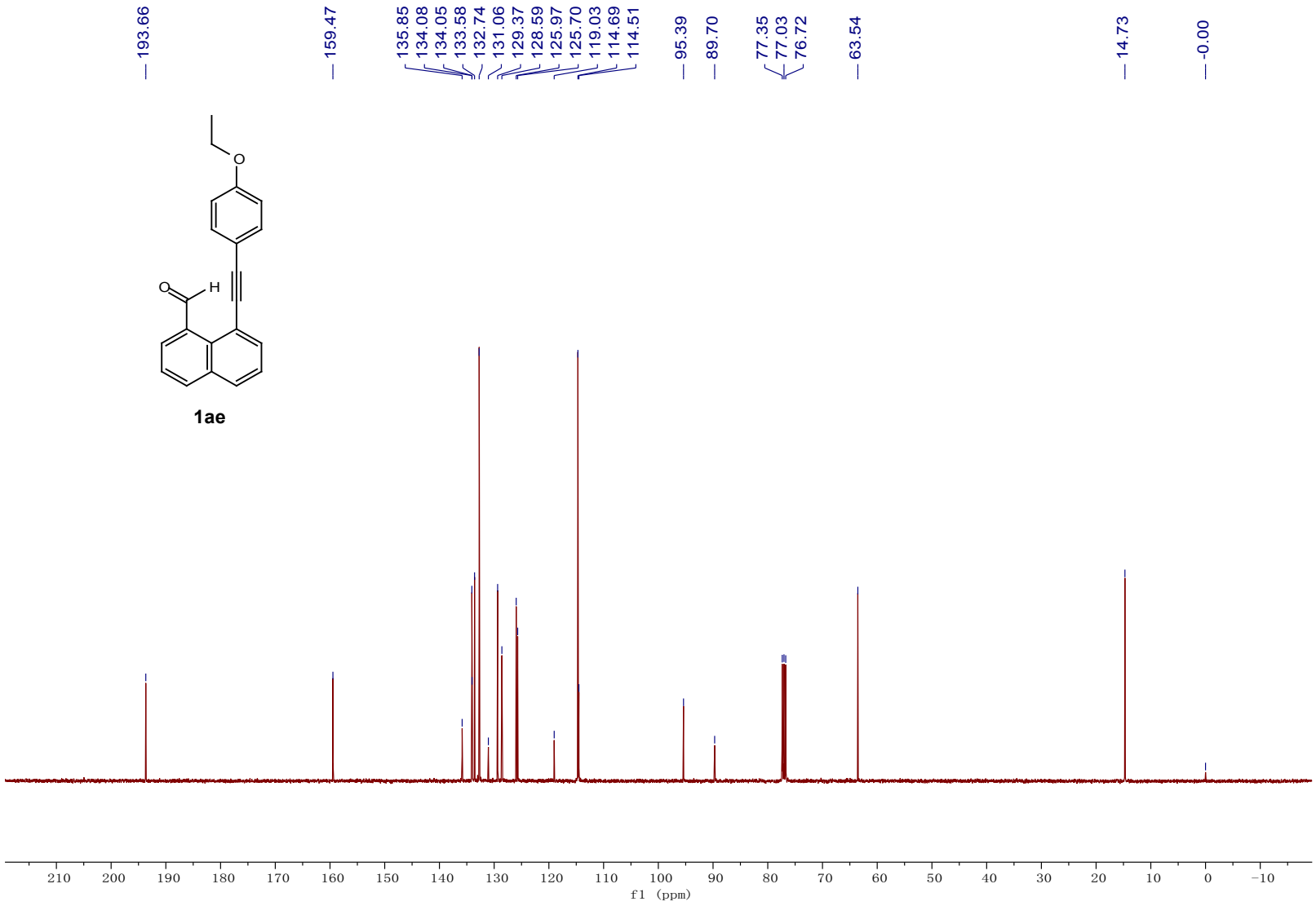
f1 (ppm)

1ae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200
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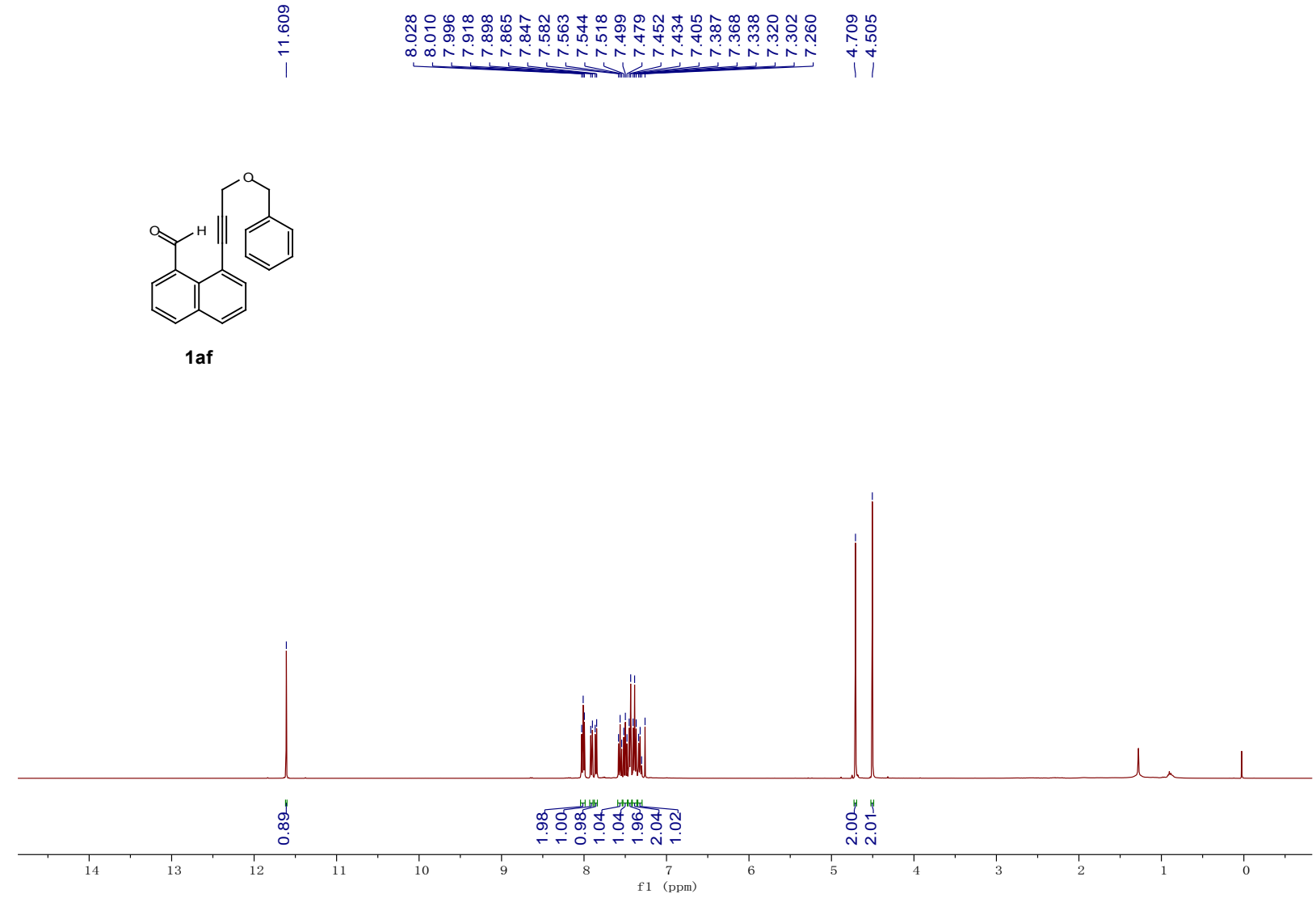
f1 (ppm)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7.434
7.405
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7.368
7.338
7.320
7.302
7.260
4.709
4.505
O
H
O
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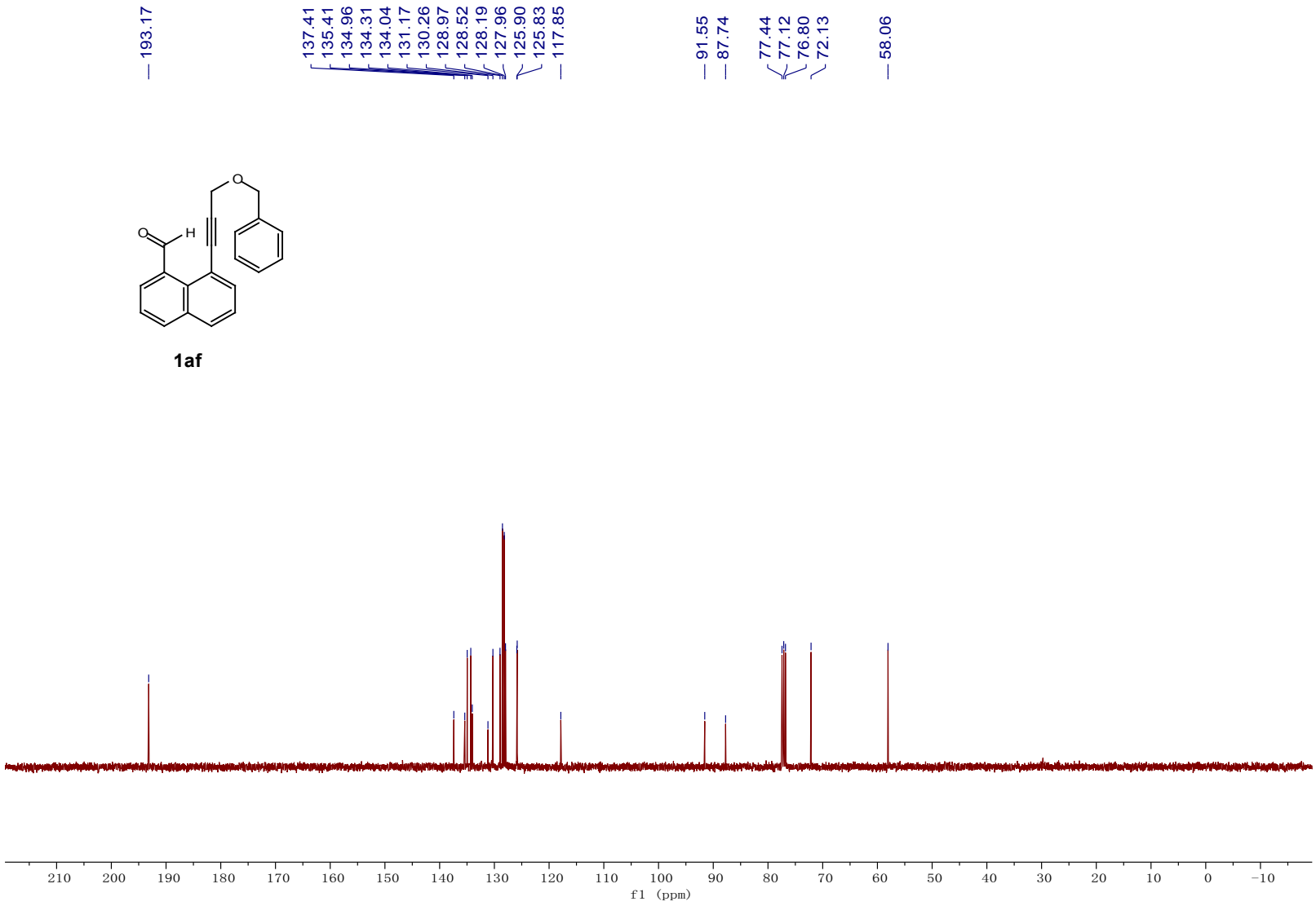
1.00
0.98
1.04
1.04
1.96
2.04
1.02
2.00
2.01
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1af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128.52
128.19
127.96
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125.83
117.85
91.55
87.74
77.44
77.12
76.80
72.13
58.06
O
H
O
210
200
190
180
170
160
150
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100
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80
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60
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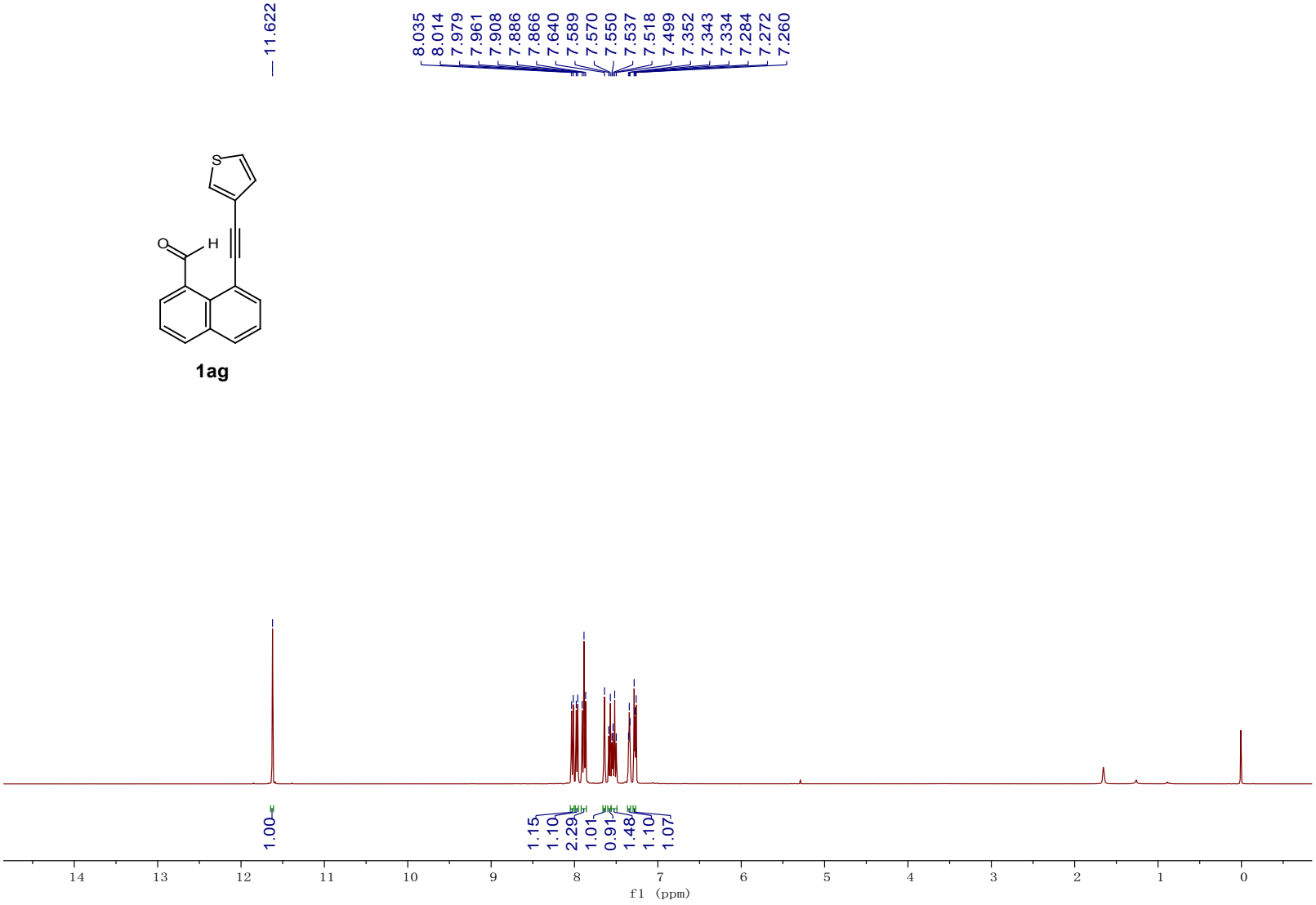
40
30
20
10
0
−10
f1 (ppm)

1af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7.866
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7.570
7.550
7.537
7.518
7.499
7.352
7.343
7.334
7.284
7.272
7.260
S
O
H
1ag
1.00
1.15
1.10
2.29
1.01
0.91
1.48
1.10
1.07
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13
12
11
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9
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7
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5
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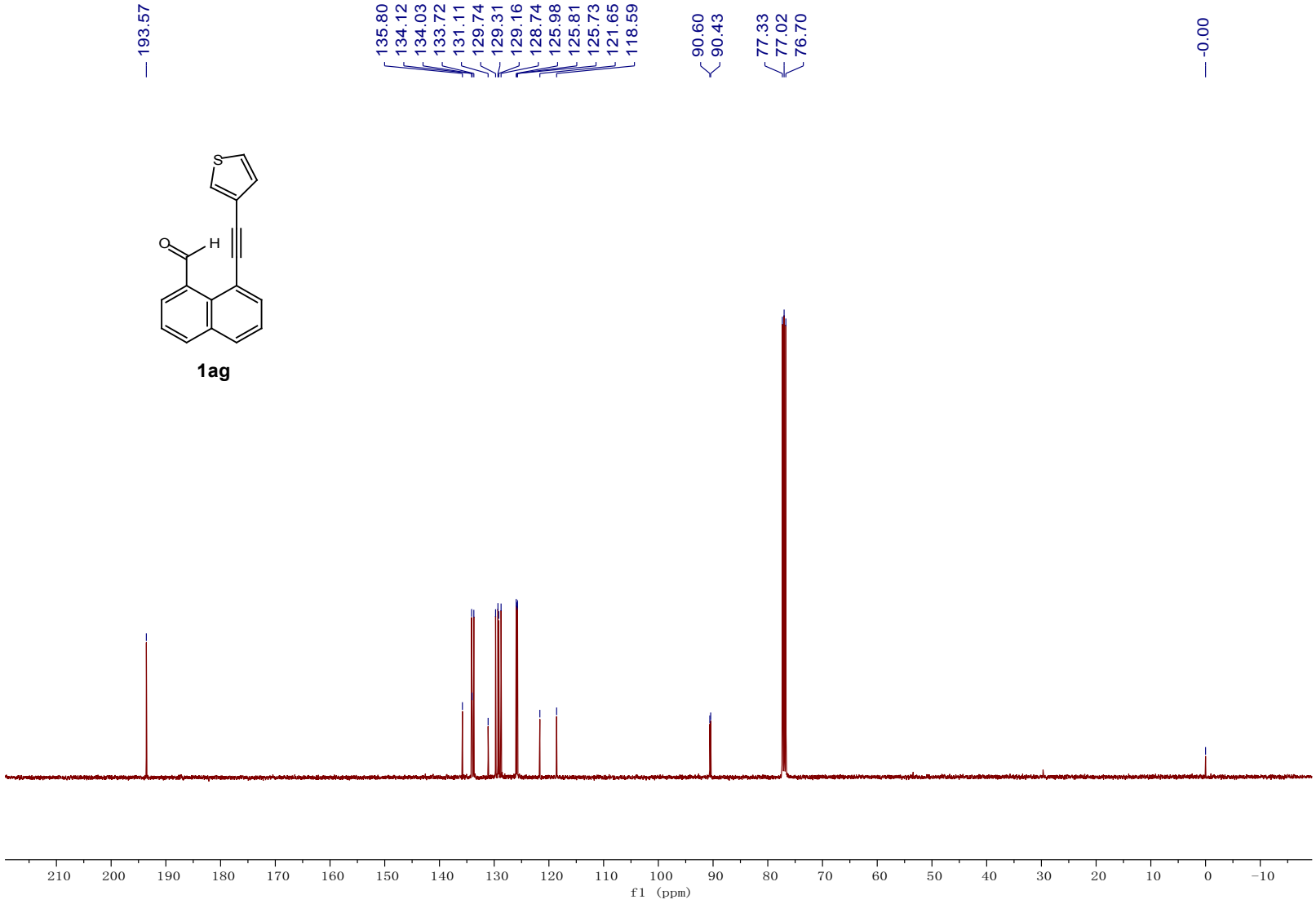
0
f1 (ppm)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125.73
121.65
118.59
90.60
90.43
77.33
77.02
76.70
-0.00
S
O
H
1ag
210
200
190
180
170
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80
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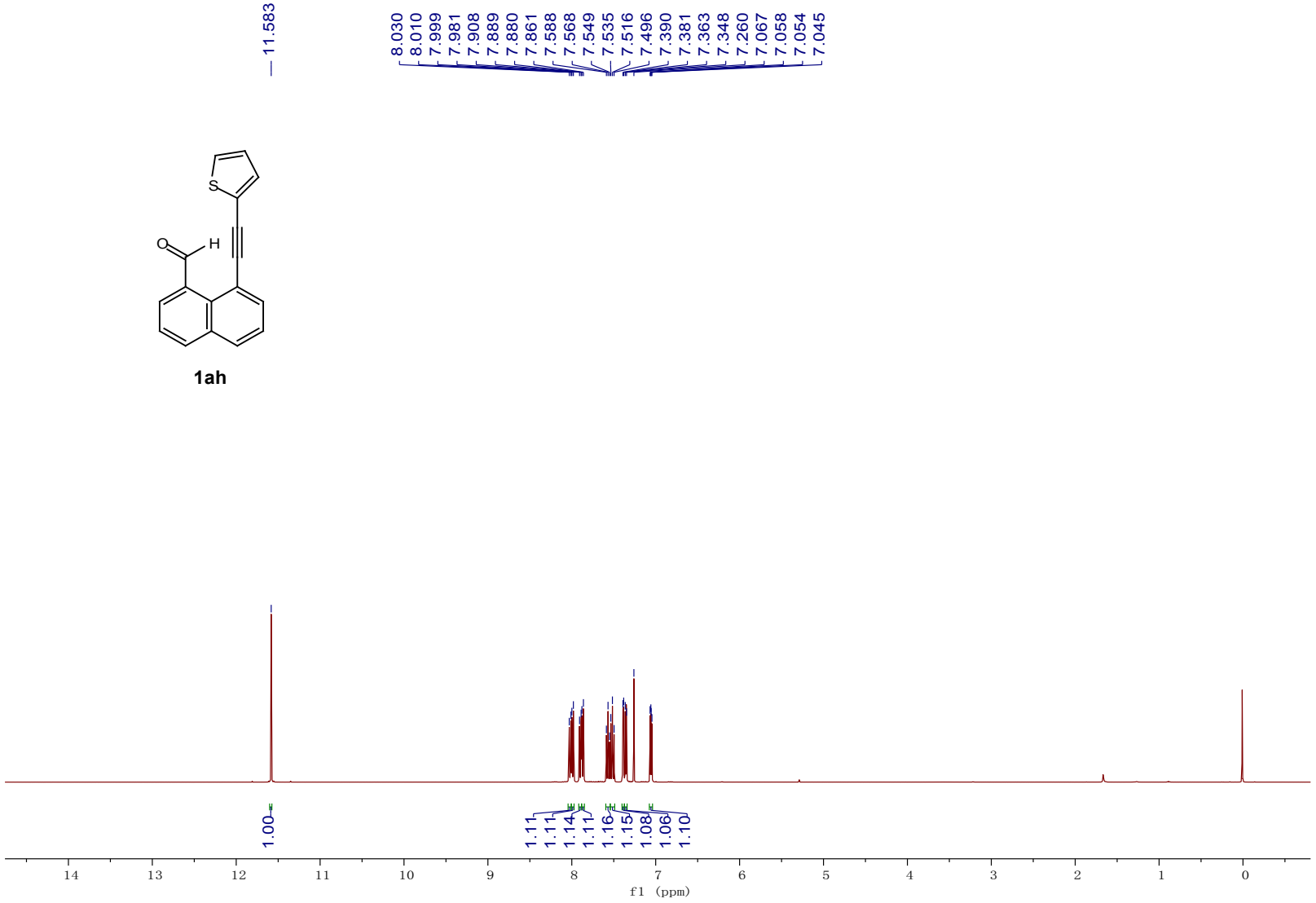
f1 (ppm)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7.549
7.535
7.516
7.496
7.390
7.381
7.363
7.348
7.260
7.067
7.058
7.054
7.045
S
O
H
1ah
1.00
1.11
1.11
1.14
1.11
1.16
1.15
1.08
1.06
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5
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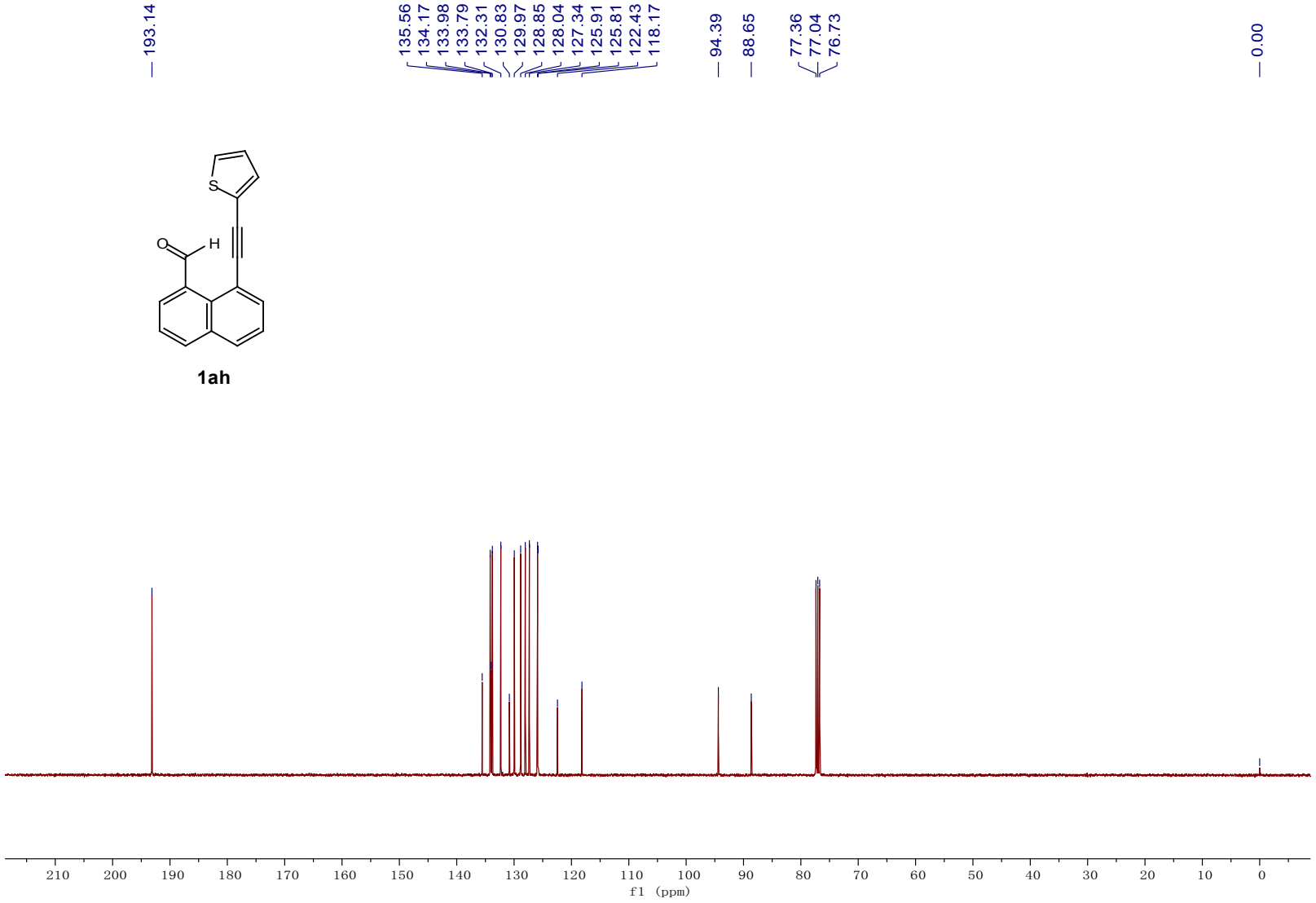
f1 (ppm)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132.31
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129.97
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128.04
127.34
125.91
125.81
122.43
118.17
94.39
88.65
77.36
77.04
76.73
0.00
S
O
H
210
200
190
180
170
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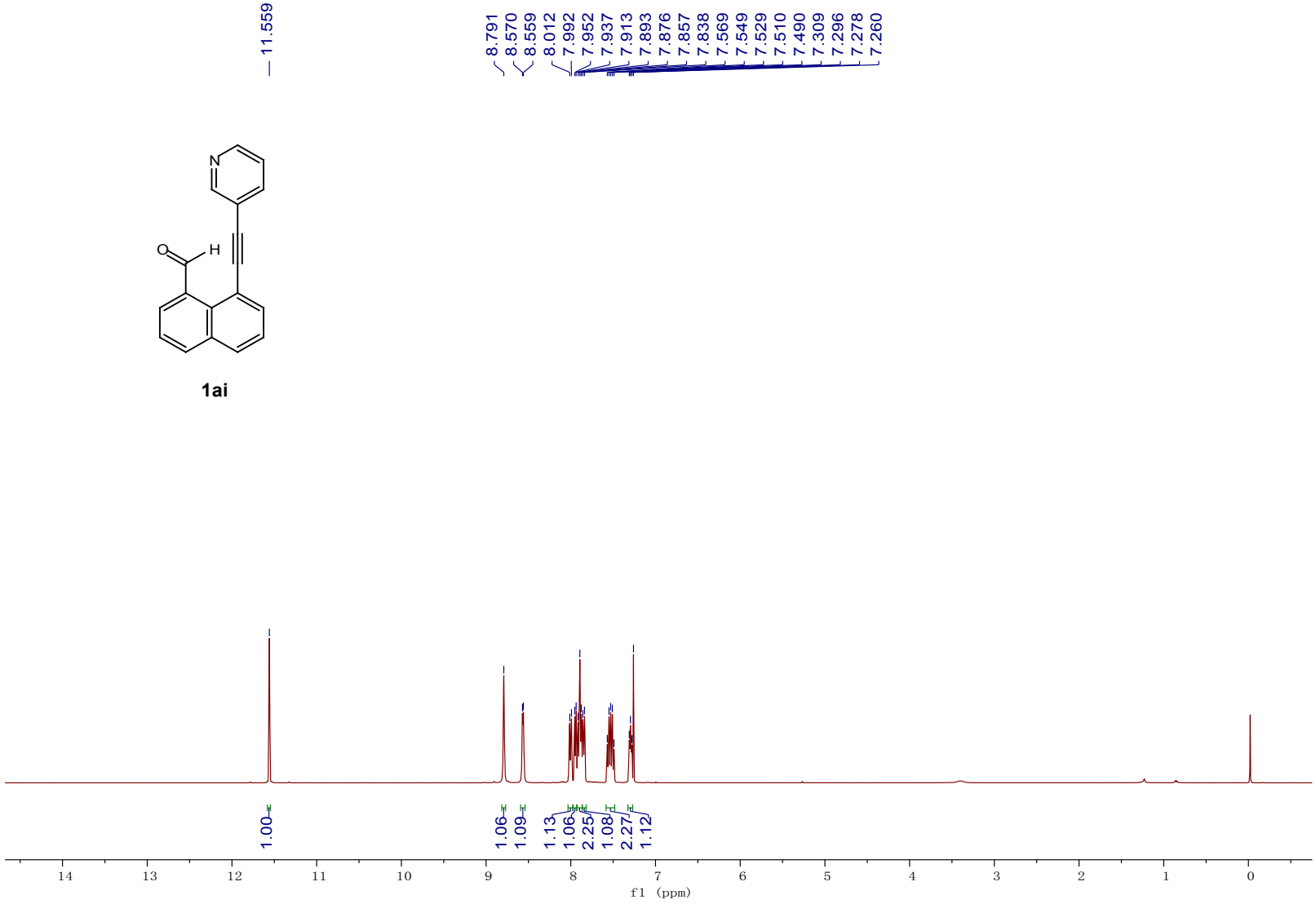
f1 (ppm)

1ah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7.937
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7.876
7.857
7.838
7.569
7.549
7.529
7.510
7.490
7.309
7.296
7.278
7.260
N
O
H
1.00
1.06
1.09
1.13
1.06
2.25
1.08
2.27
1.12
14
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12
11
10
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8
7
6
5
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3
2
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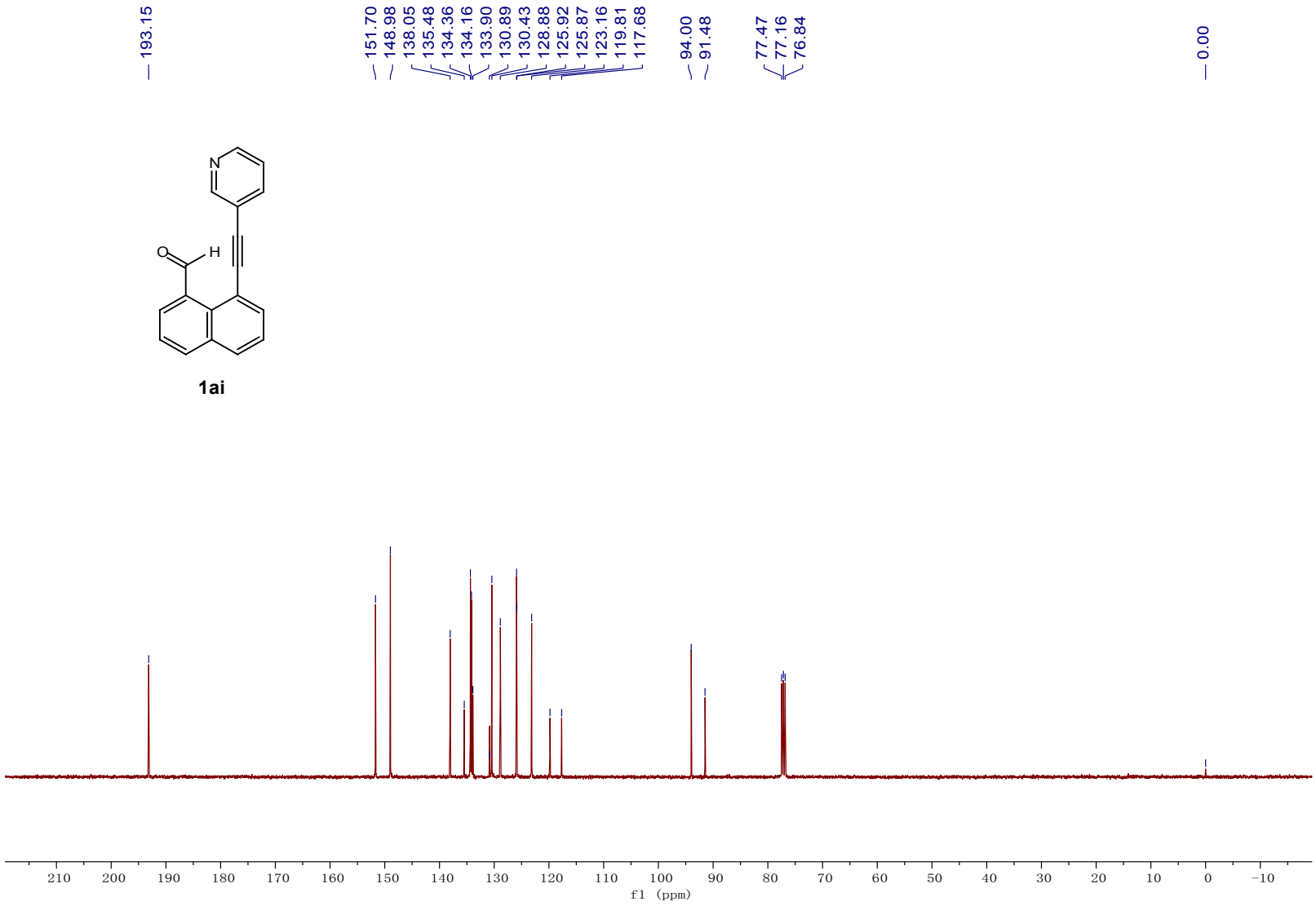
0
f1 (ppm)

1ai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134.36
134.16
133.90
130.89
130.43
128.88
125.92
125.87
123.16
119.81
117.68
94.00
91.48
77.47
77.16
76.84
0.00
N
O
H
210
200
190
180
170
160
150
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100
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60
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40
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20
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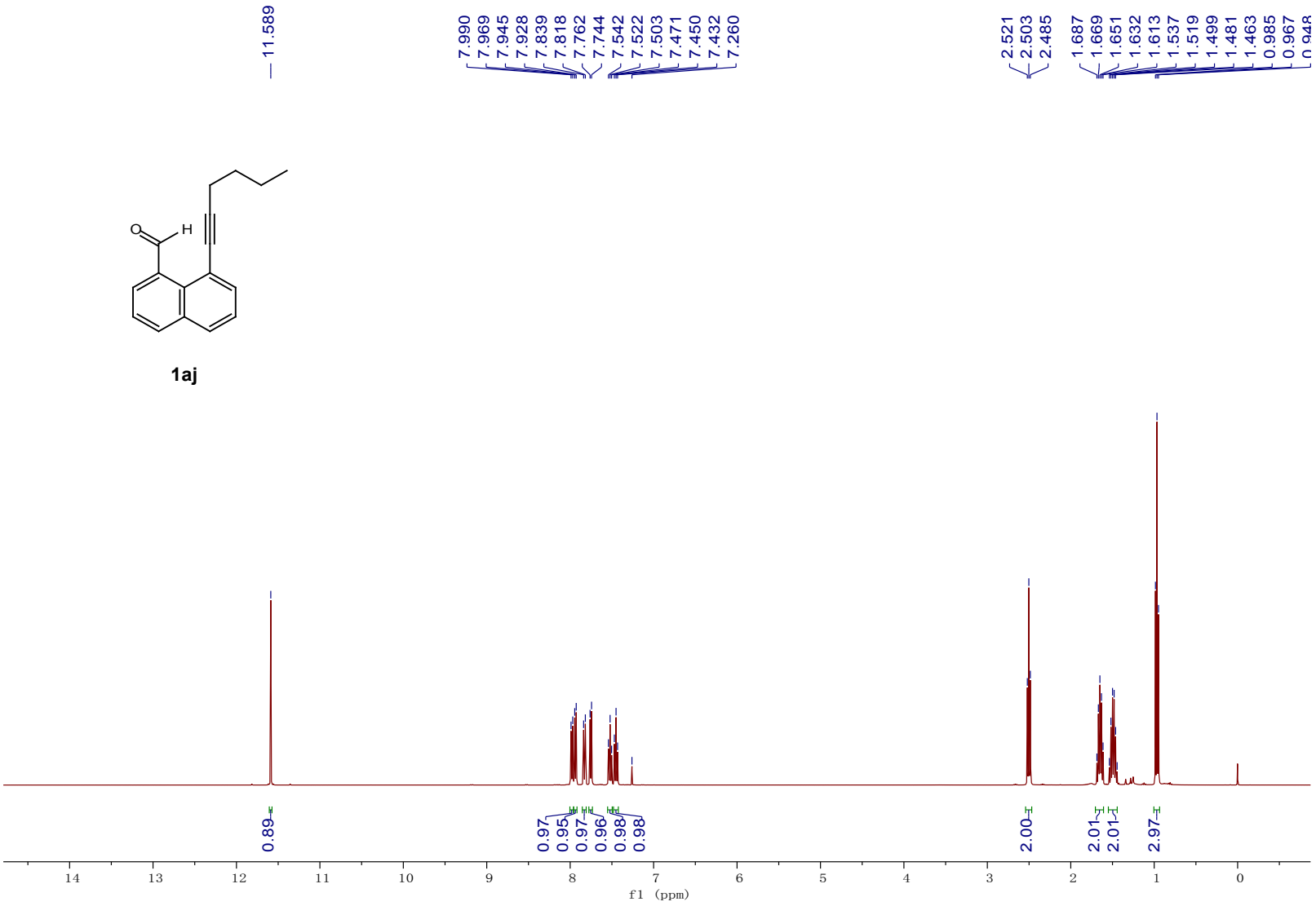
−10
f1 (ppm)

1ai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7.945
7.928
7.839
7.818
7.762
7.744
7.542
7.522
7.503
7.471
7.450
7.432
7.260
2.521
2.503
2.485
1.687
1.669
1.651
1.632
1.613
1.537
1.519
1.499
1.481
1.463
0.985
0.967
O
H
1aj
0.89
0.97
0.95
0.97
0.96
0.98
0.98
2.00
2.01
2.01
2.97
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13
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11
10
9
8
7
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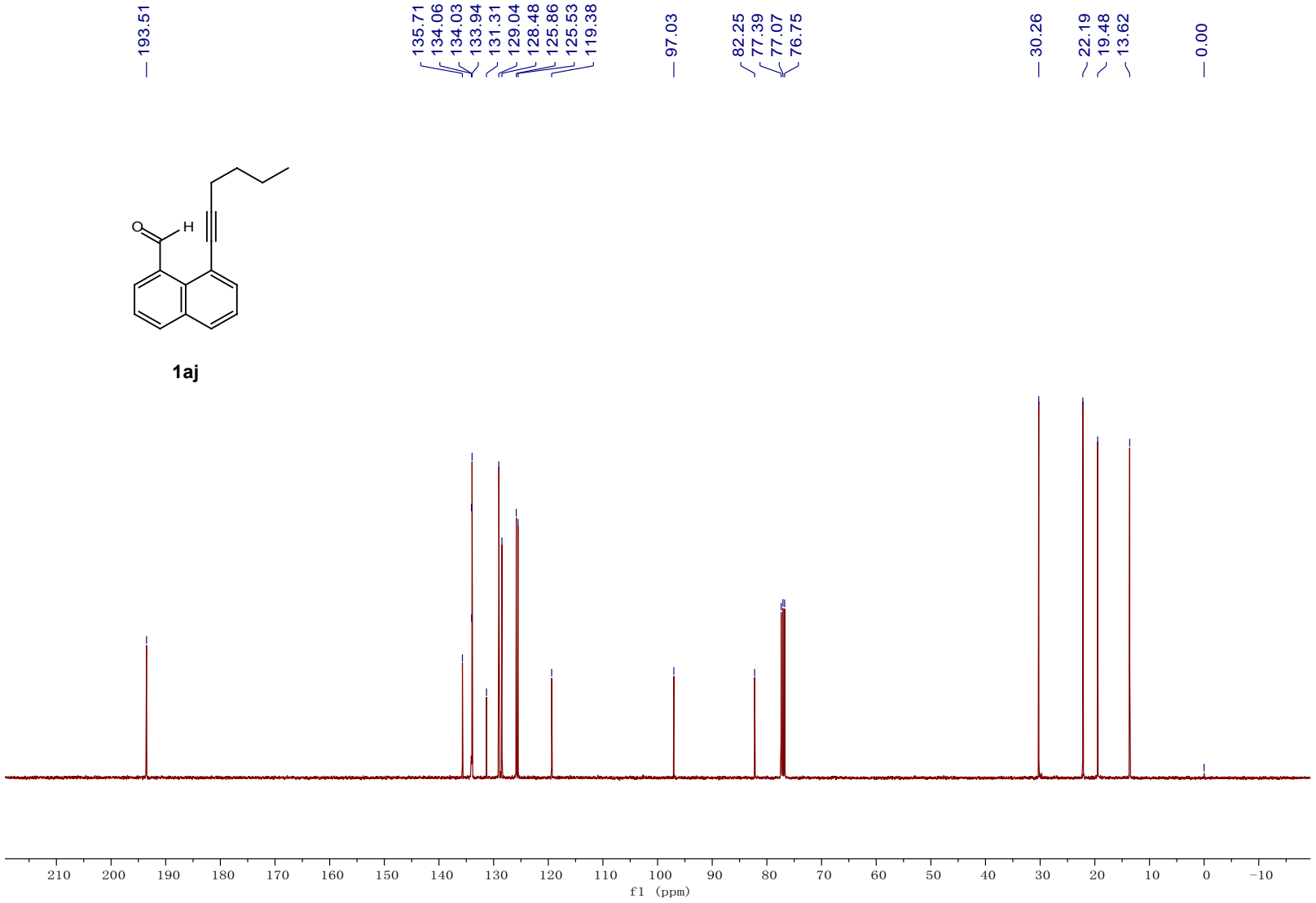
5
4
3
2
1
0
f1 (ppm)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133.94
131.31
129.04
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125.86
125.53
119.38
97.03
82.25
77.39
77.07
76.75
30.26
22.19
19.48
13.62
0.00
O
H
1aj
210
200
190
180
170
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150
140
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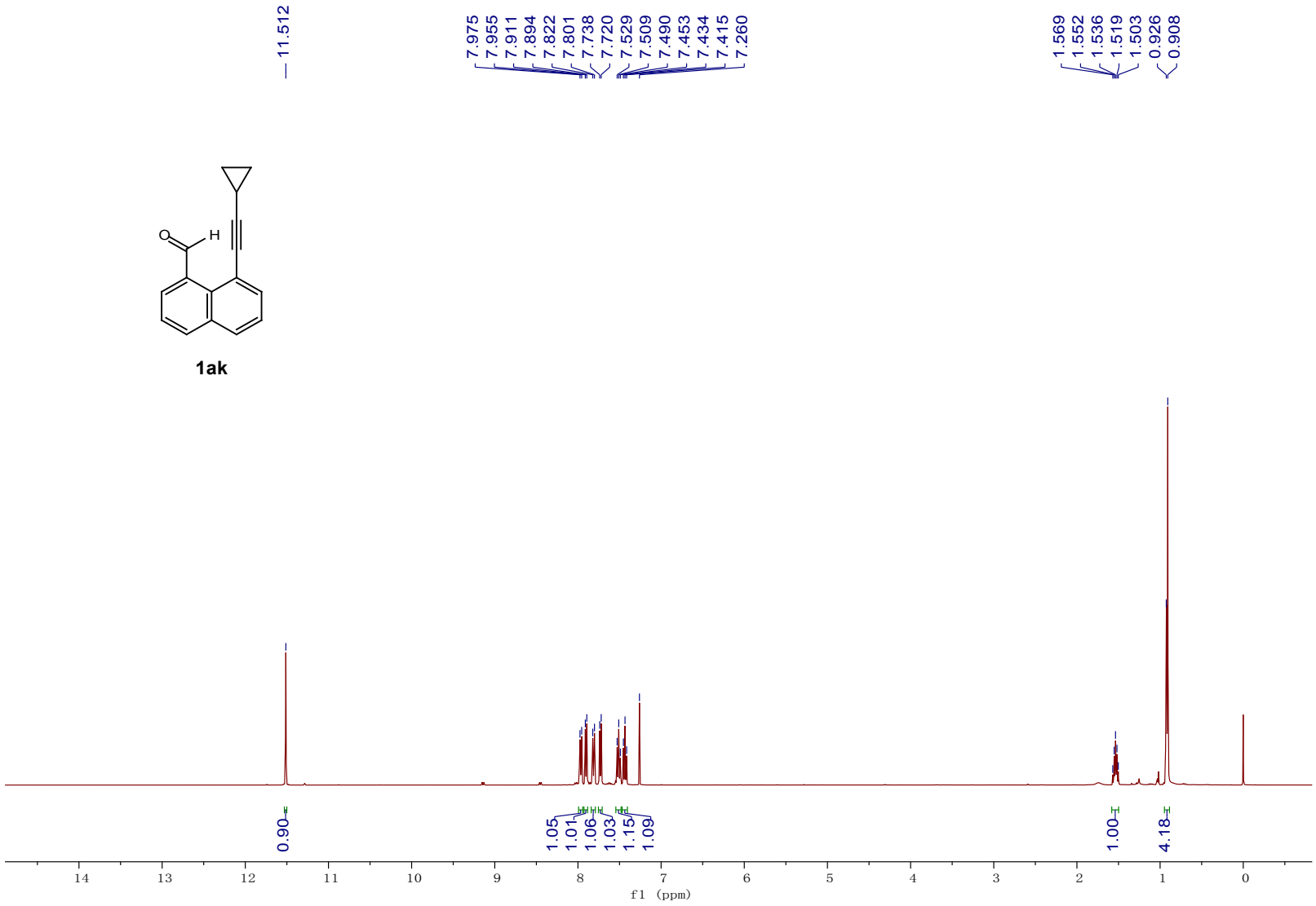
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.911
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7.822
7.801
7.738
7.720
7.529
7.509
7.490
7.453
7.434
7.415
7.260
1.569
1.552
1.536
1.519
1.503
0.926
0.908
O
H
1ak
0.90
1.05
1.01
1.06
1.03
1.15
1.09
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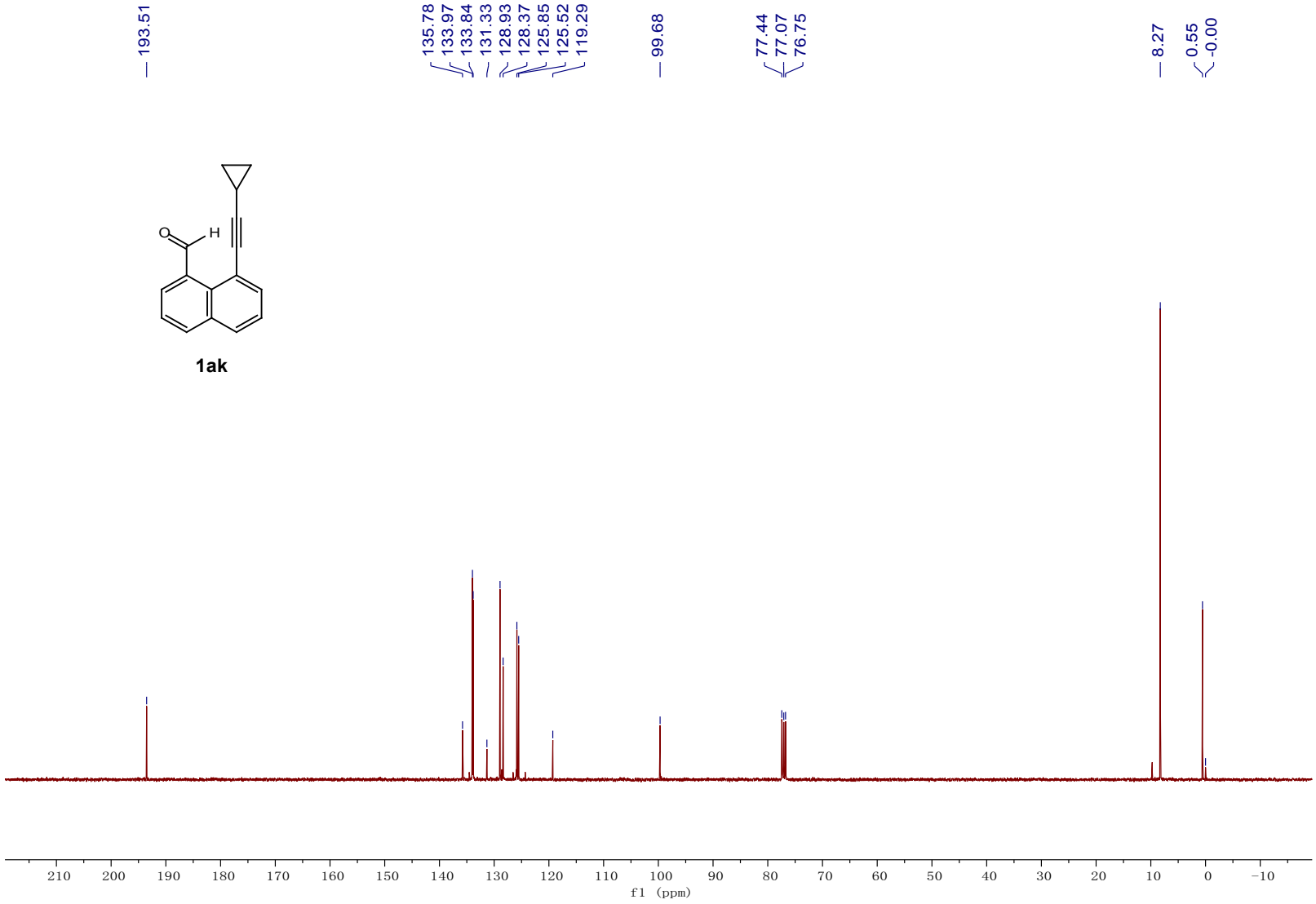
4.18
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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131.33
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128.37
125.85
125.52
119.29
99.68
77.44
77.07
76.75
8.27
0.55
-0.00
O
H
1ak
210
200
190
180
170
160
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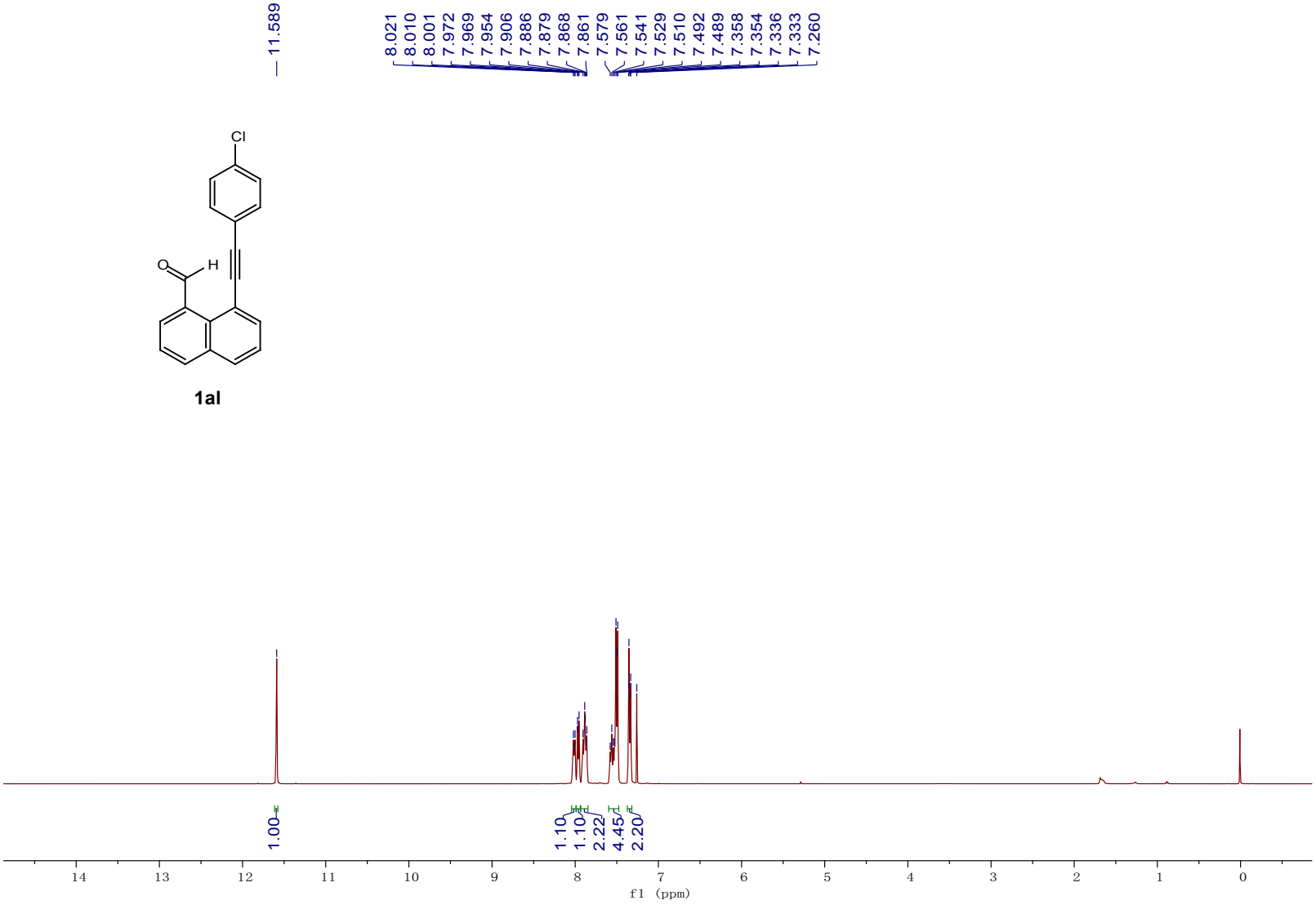
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.906
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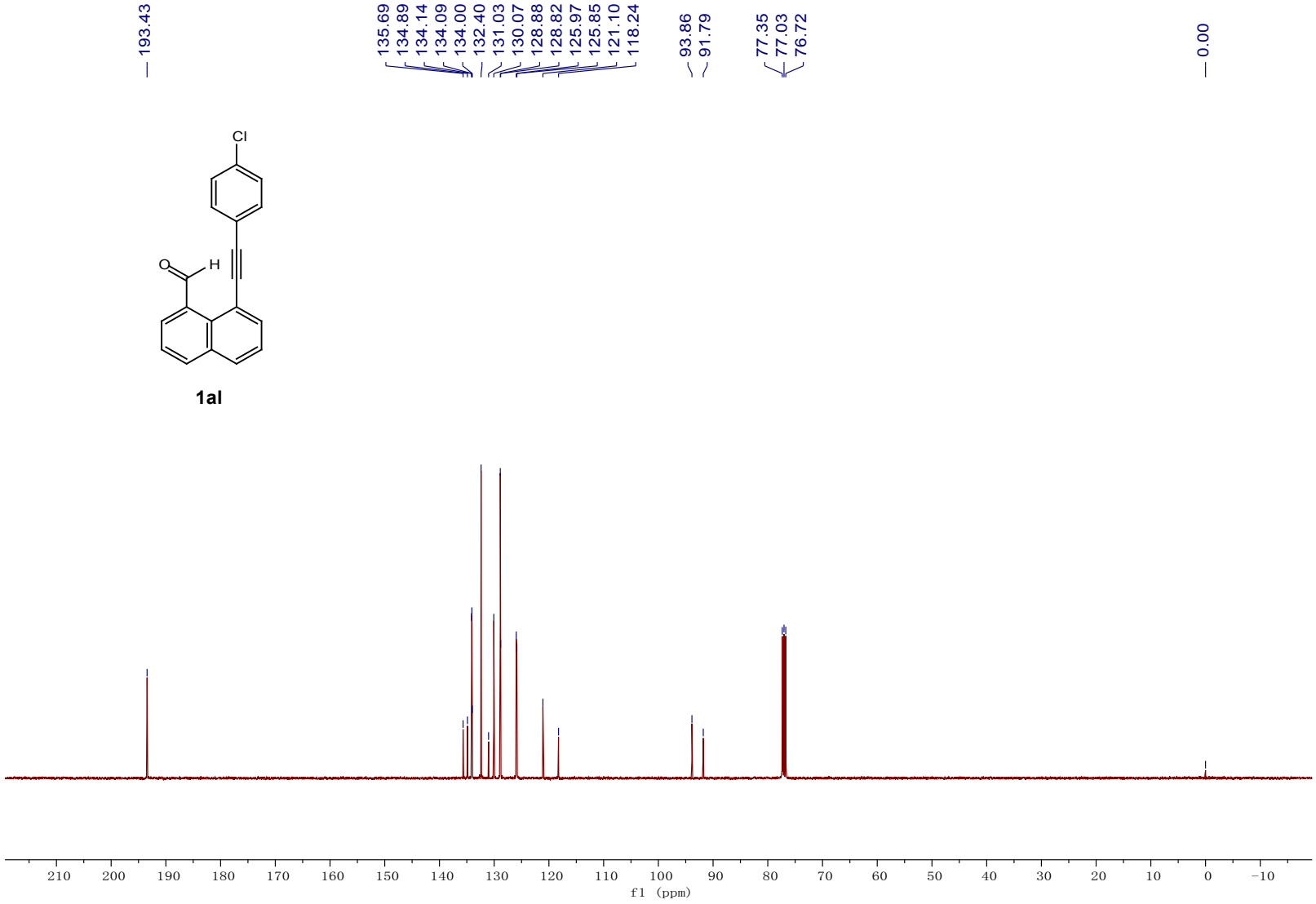
7.879
7.868
7.861
7.579
7.561
7.541
7.529
7.510
7.492
7.489
7.358
7.354
7.336
7.333
7.260
Cl
O
H
1.00
1.10
1.10
2.22
4.45
2.20
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1al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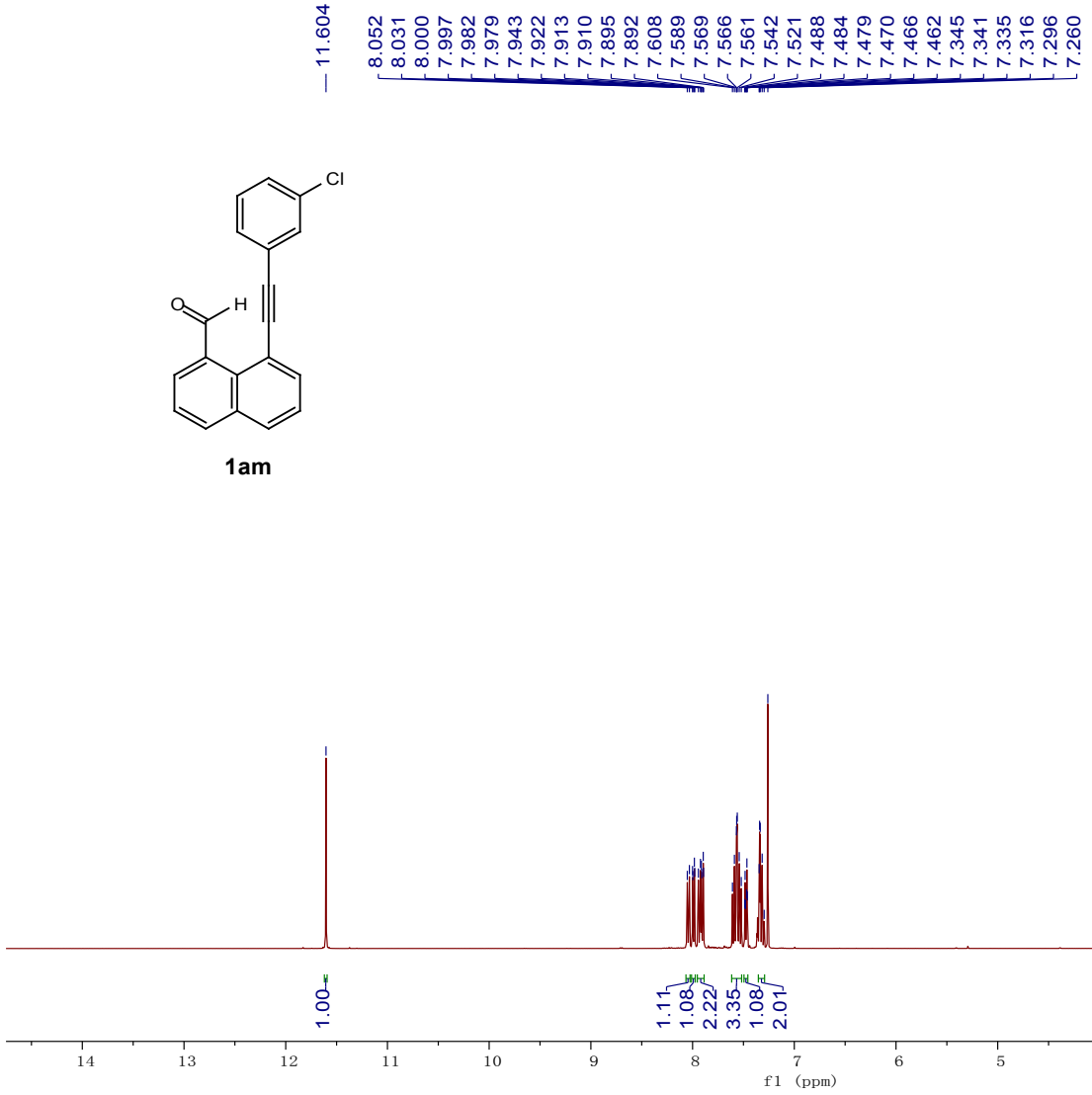
132.40
131.03
130.07
128.88
128.82
125.97
125.85
121.10
118.24
93.86
91.79
77.35
77.03
76.72
0.00
Cl
O
H
1al
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.982
7.979
7.943
7.922
7.913
7.910
7.895
7.892
7.608
7.589
7.569
7.566
7.561
7.542
7.521
7.488
7.484
7.479
7.470
7.466
7.462
7.345
7.341
7.335
7.316
7.296
7.260
Cl
O
H
1.00
1.11
1.08
2.22
3.35
1.08
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14
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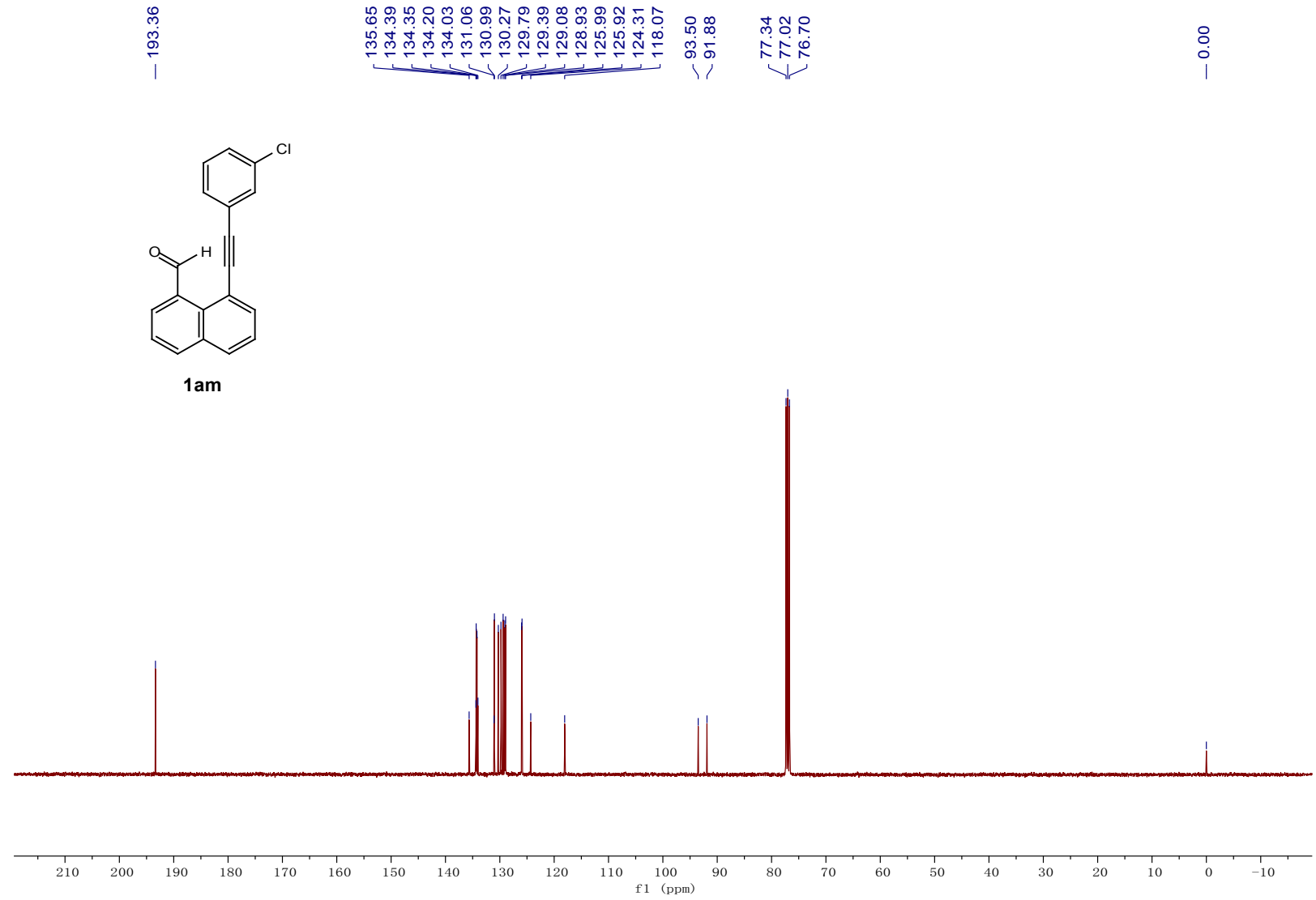
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1am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134.03
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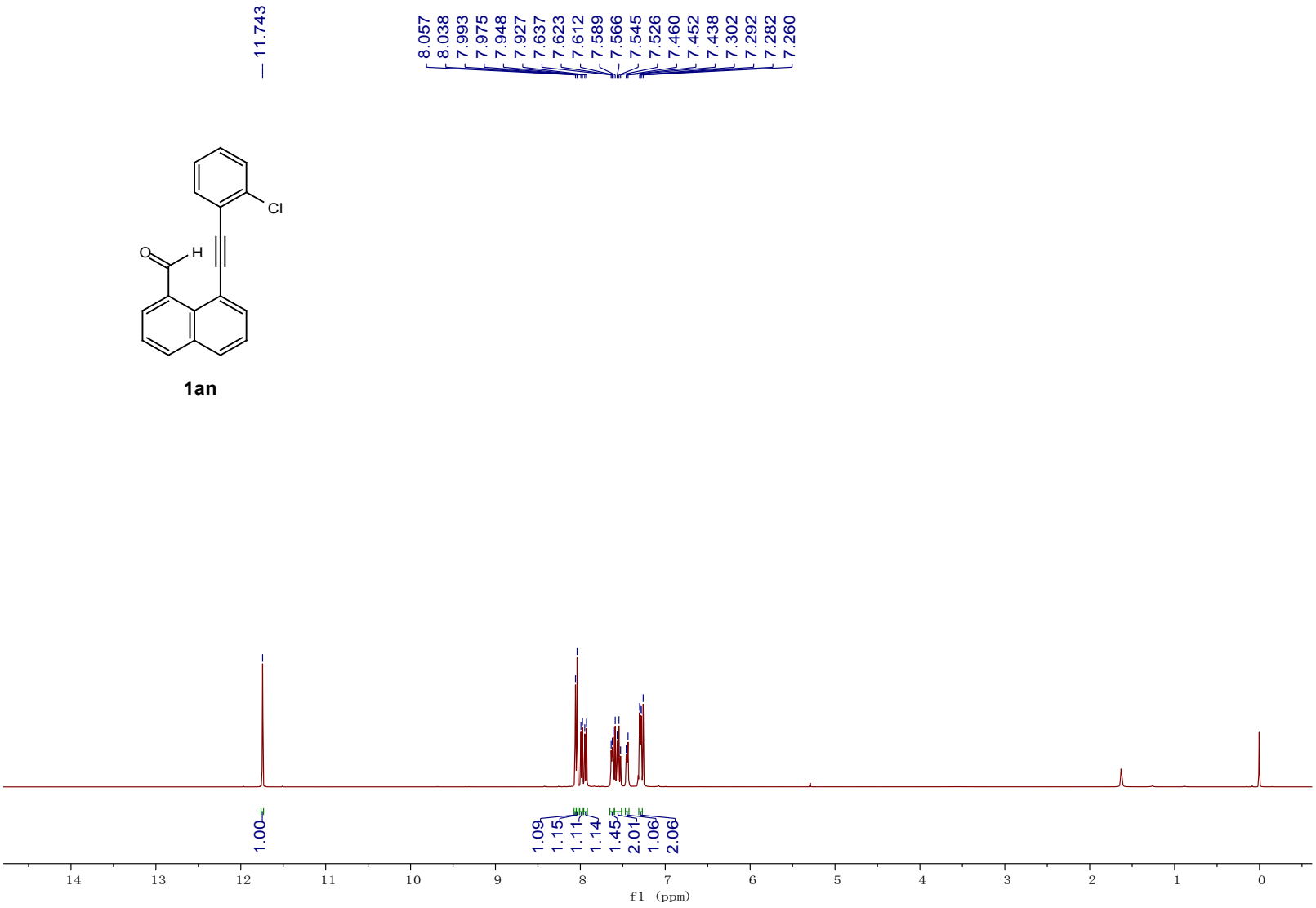
130.99
130.27
129.79
129.39
129.08
128.93
125.99
125.92
124.31
118.07
93.50
91.88
77.34
77.02
76.70
0.00
Cl
O
H
1am
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.637
7.623
7.612
7.589
7.566
7.545
7.526
7.460
7.452
7.438
7.302
7.292
7.282
7.260
Cl
O
H
1.00
1.09
1.15
1.11
1.14
1.45
2.01
1.06
2.06
14
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12
11
10
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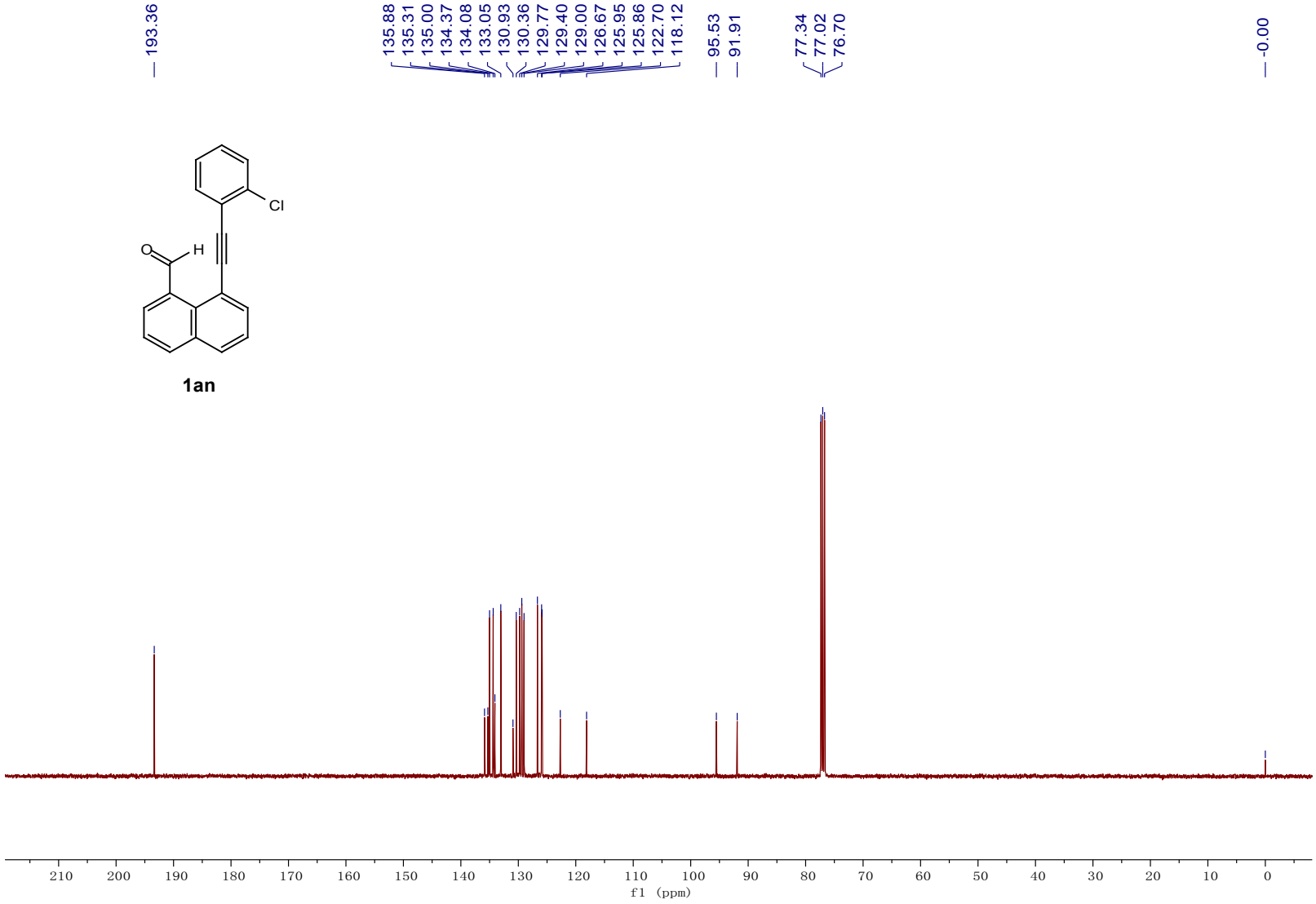
8
7
6
5
4
3
2
1
0
f1 (ppm)

1an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129.77
129.40
129.00
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125.95
125.86
122.70
118.12
95.53
91.91
77.34
77.02
76.70
-0.00
Cl
O
H
1an
210
200
190
180
170
160
150
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130
120
110
100
90
80
70
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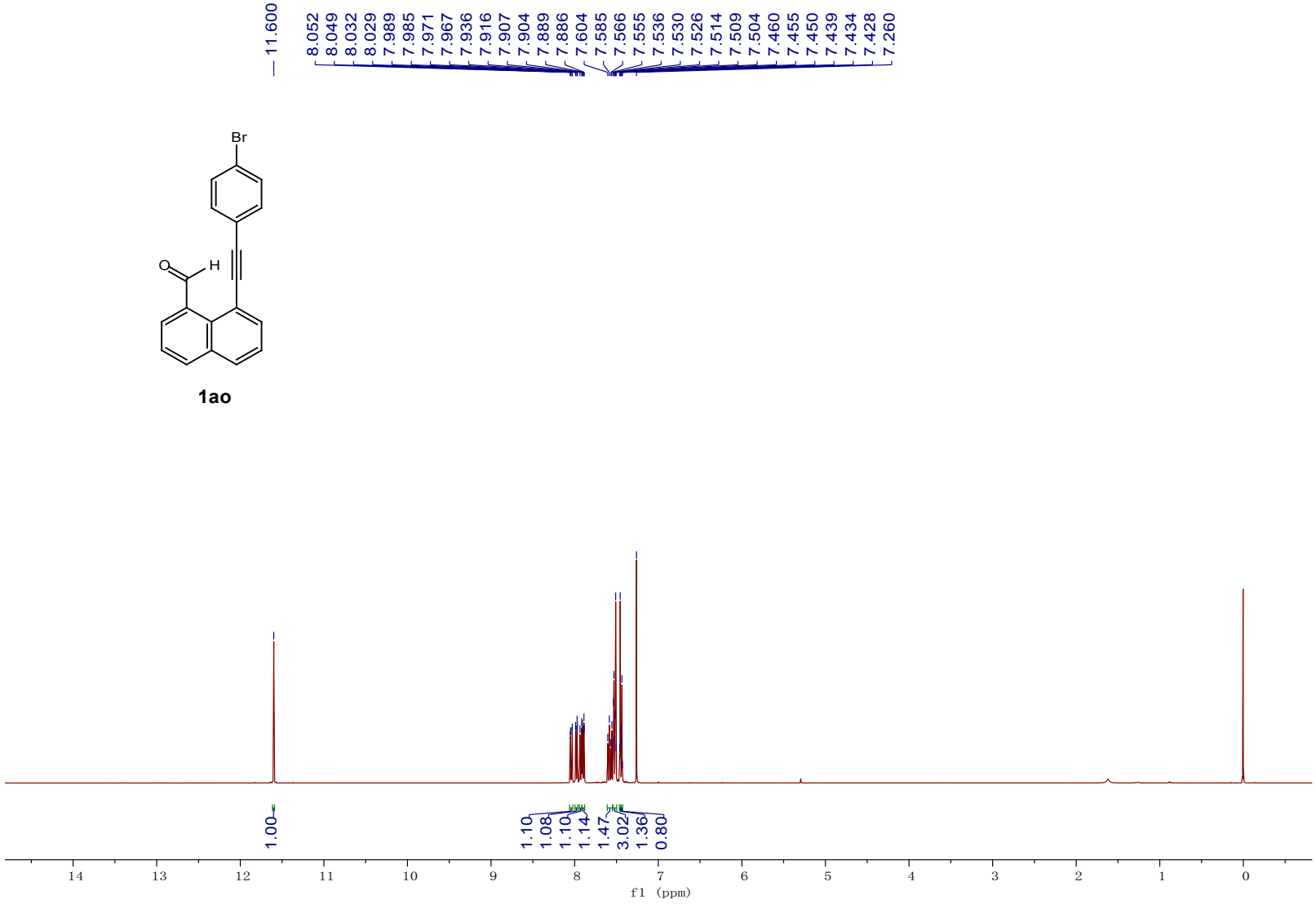
50
40
30
20
10
0
f1 (ppm)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7.907
7.904
7.889
7.886
7.604
7.585
7.566
7.555
7.536
7.530
7.526
7.514
7.509
7.504
7.460
7.455
7.450
7.439
7.434
7.428
7.260
Br
O
H
1.00
1.10
1.08
1.10
1.14
1.47
3.02
1.36
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14
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11
10
9
8
7
6
5
4
3
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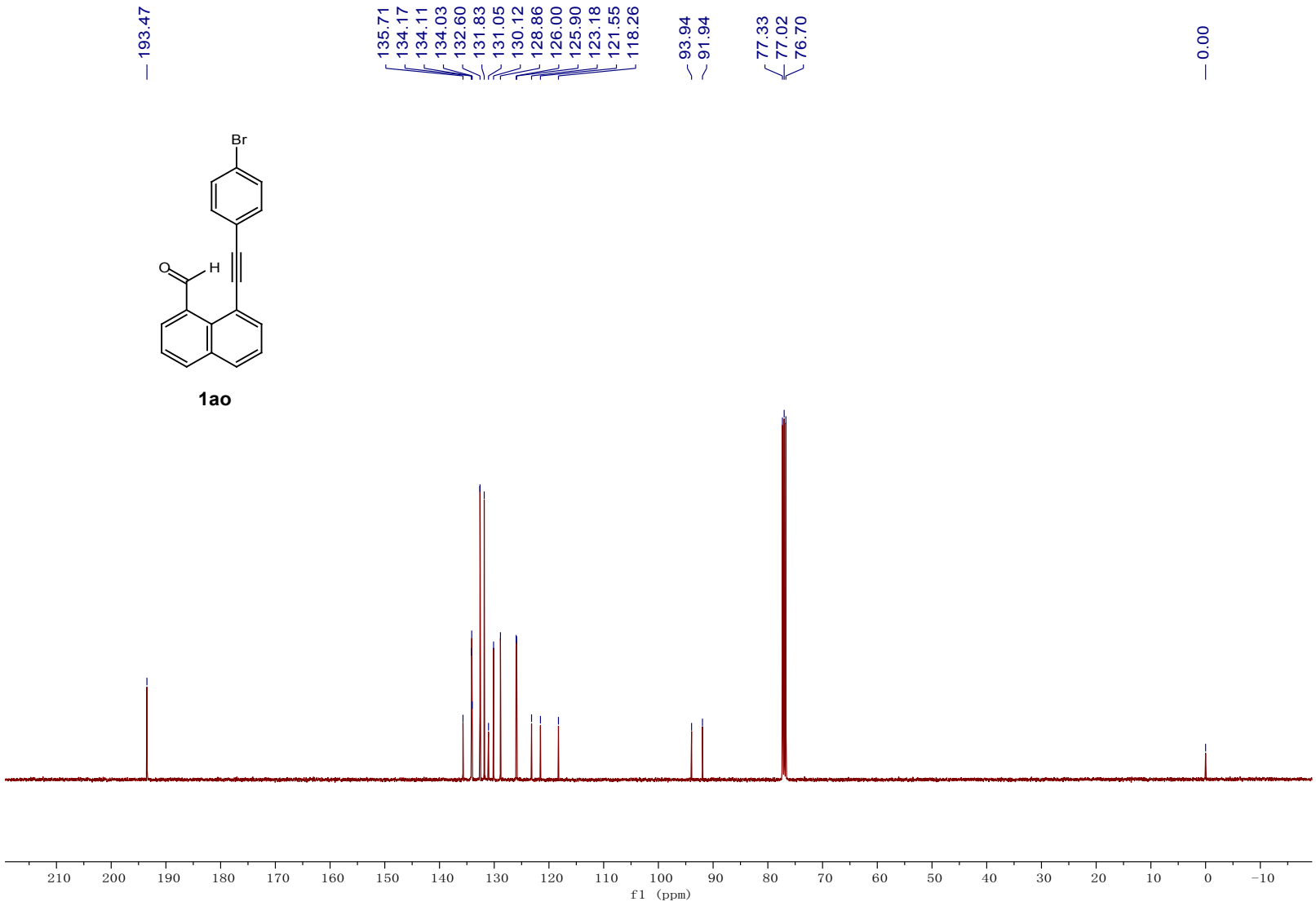
0
f1 (ppm)

1ao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128.86
126.00
125.90
123.18
121.55
118.26
93.94
91.94
77.33
77.02
76.70
0.00
Br
O
H
1ao
210
200
190
180
170
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110
100
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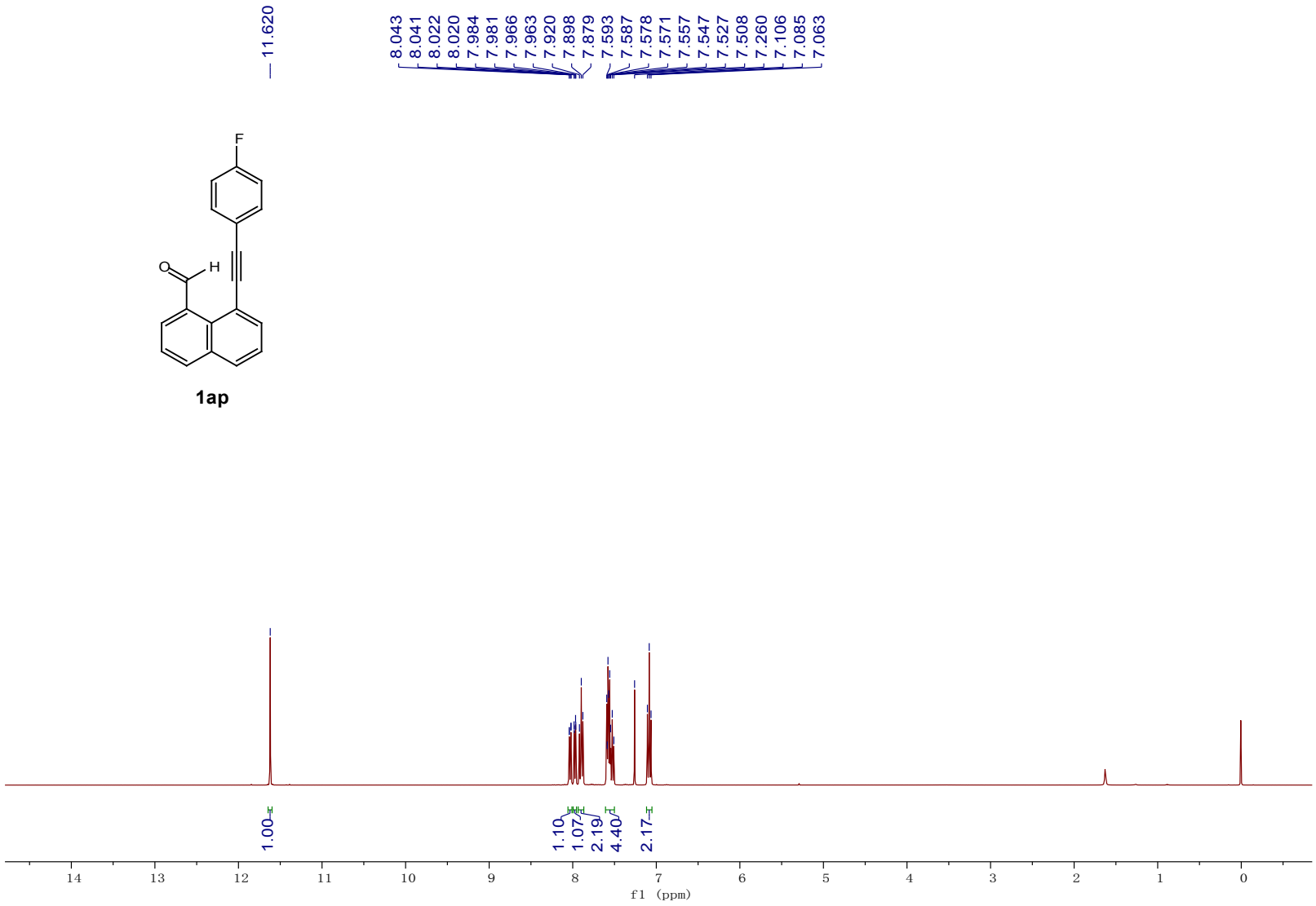
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.966
7.963
7.920
7.898
7.879
7.593
7.587
7.578
7.571
7.557
7.547
7.527
7.508
7.260
7.106
7.085
7.063
F
O
H
1ap
1.00
1.10
1.07
2.19
4.40
2.17
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13
12
11
10
9
8
7
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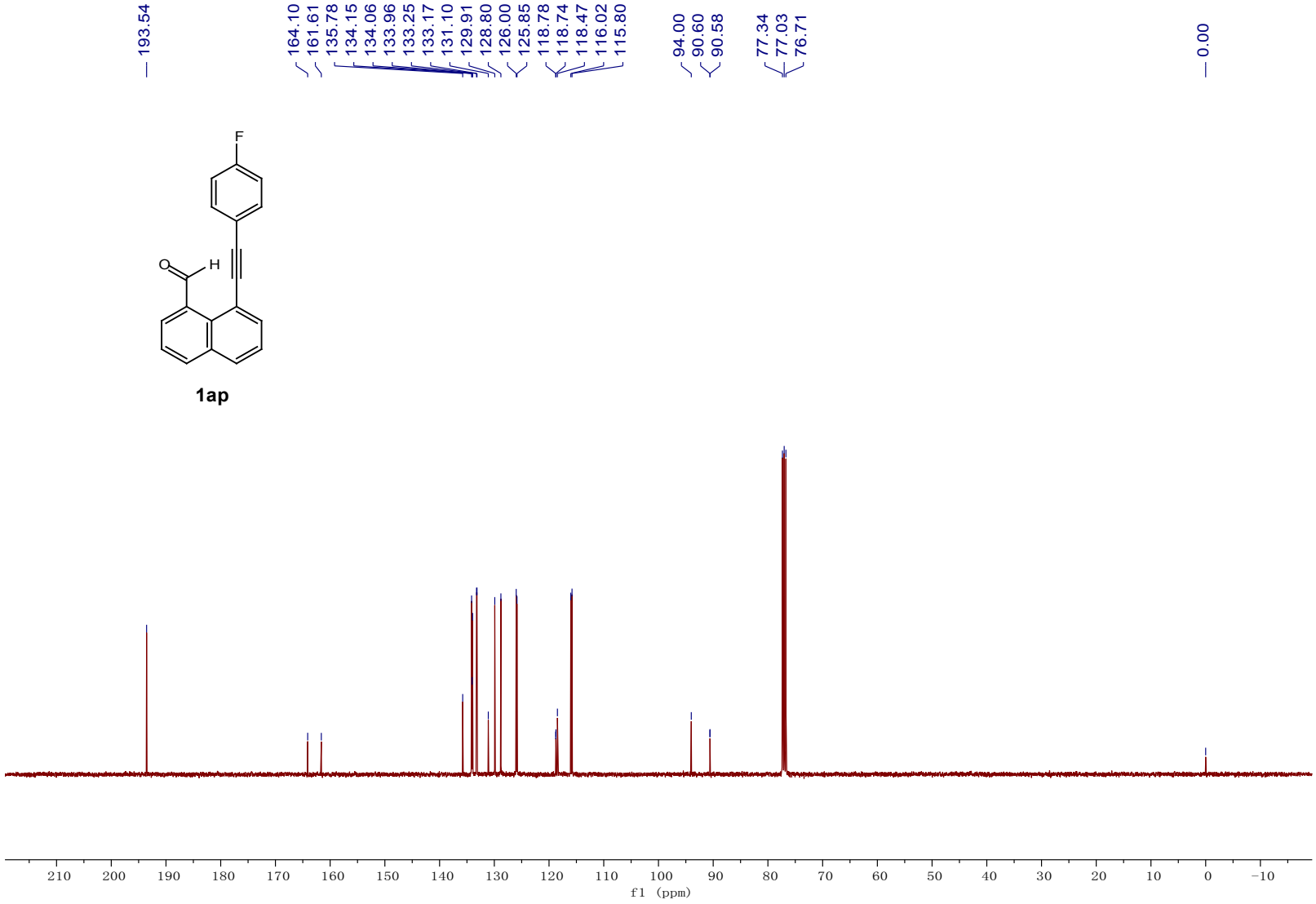
5
4
3
2
1
0
f1 (ppm)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134.06
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133.25
133.17
131.10
129.91
128.80
126.00
125.85
118.78
118.74
118.47
116.02
115.80
94.00
90.60
90.58
77.34
77.03
76.71
0.00
F
O
H
1ap
210
200
190
180
170
160
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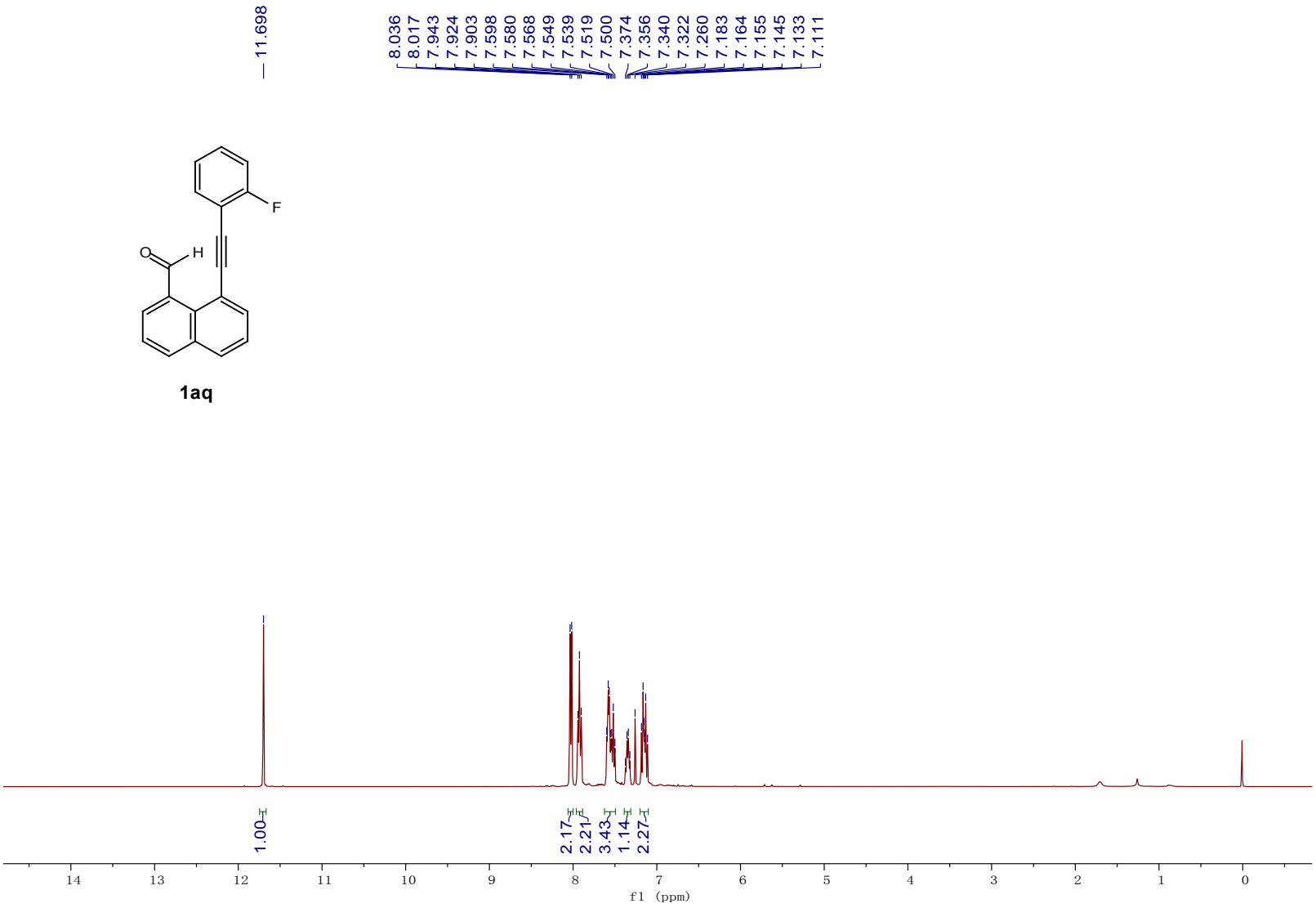
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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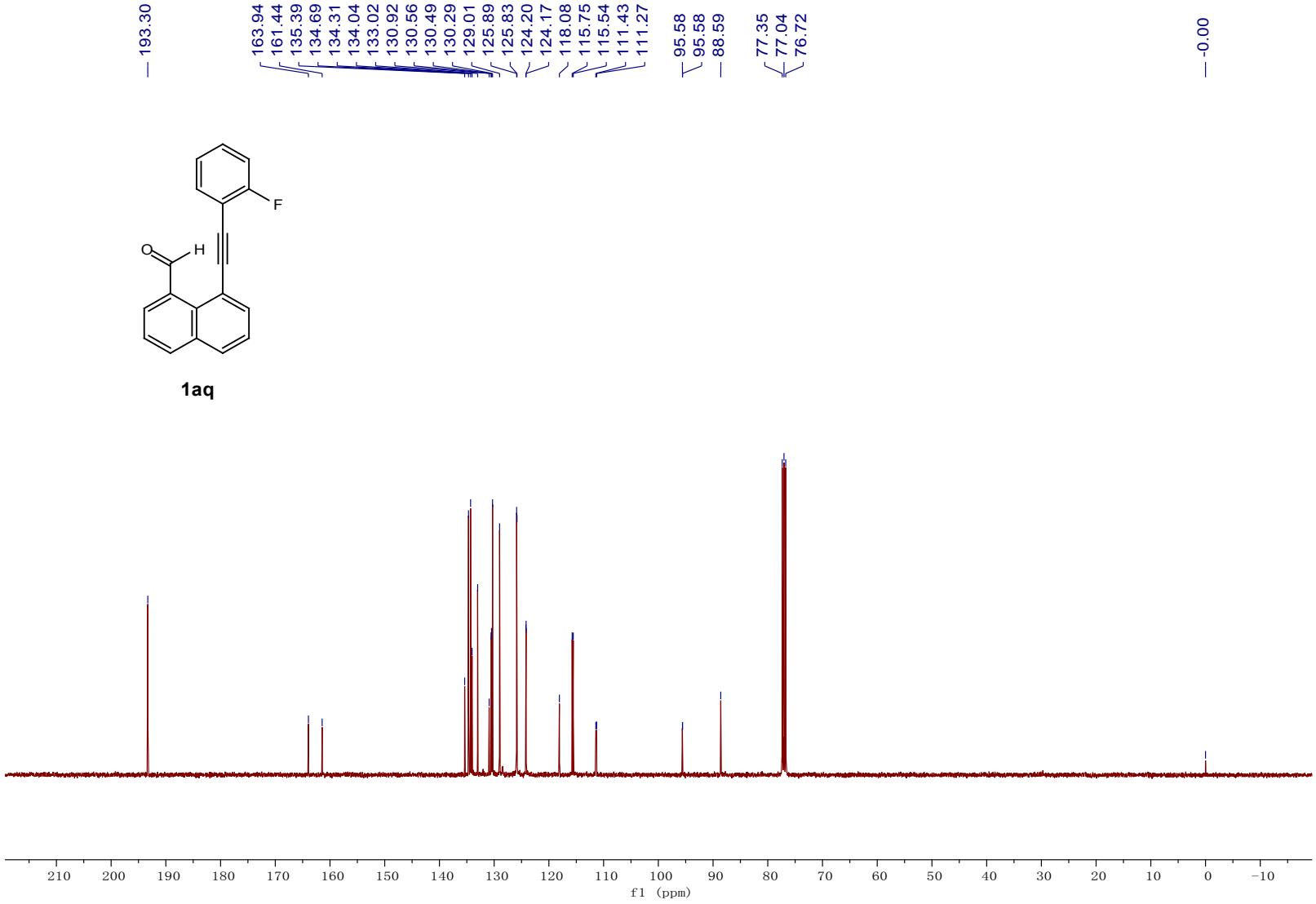
7.580
7.568
7.549
7.539
7.519
7.500
7.374
7.356
7.340
7.322
7.260
7.183
7.164
7.155
7.145
7.133
7.111
F
O
H
1.00
2.17
2.21
3.43
1.14
2.27
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1aq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134.04
133.02
130.92
130.56
130.49
130.29
129.01
125.89
125.83
124.20
124.17
118.08
115.75
115.54
111.43
111.27
95.58
95.58
88.59
77.35
77.04
76.72
-0.00
F
O
H
1aq
210
200
190
180
170
160
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140
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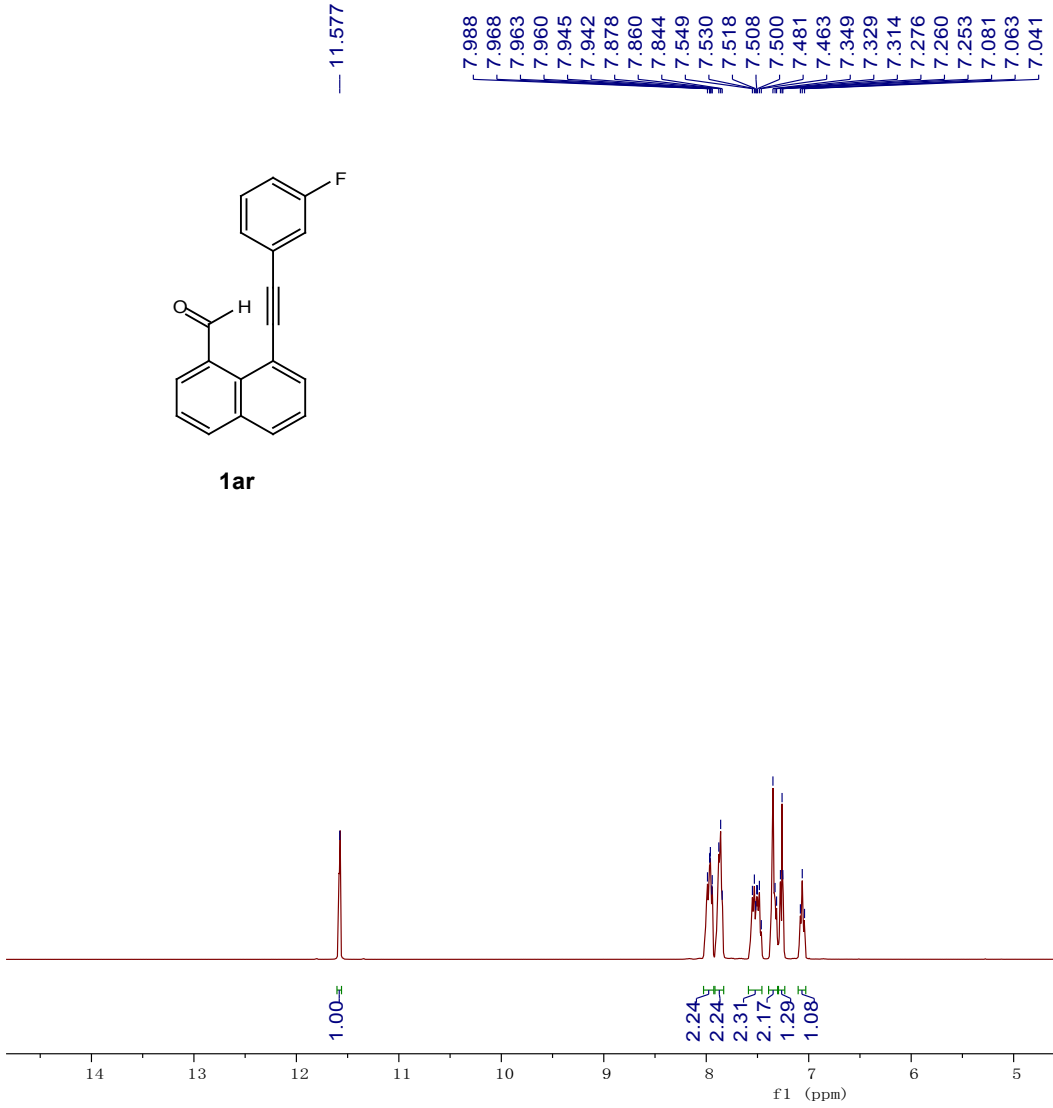
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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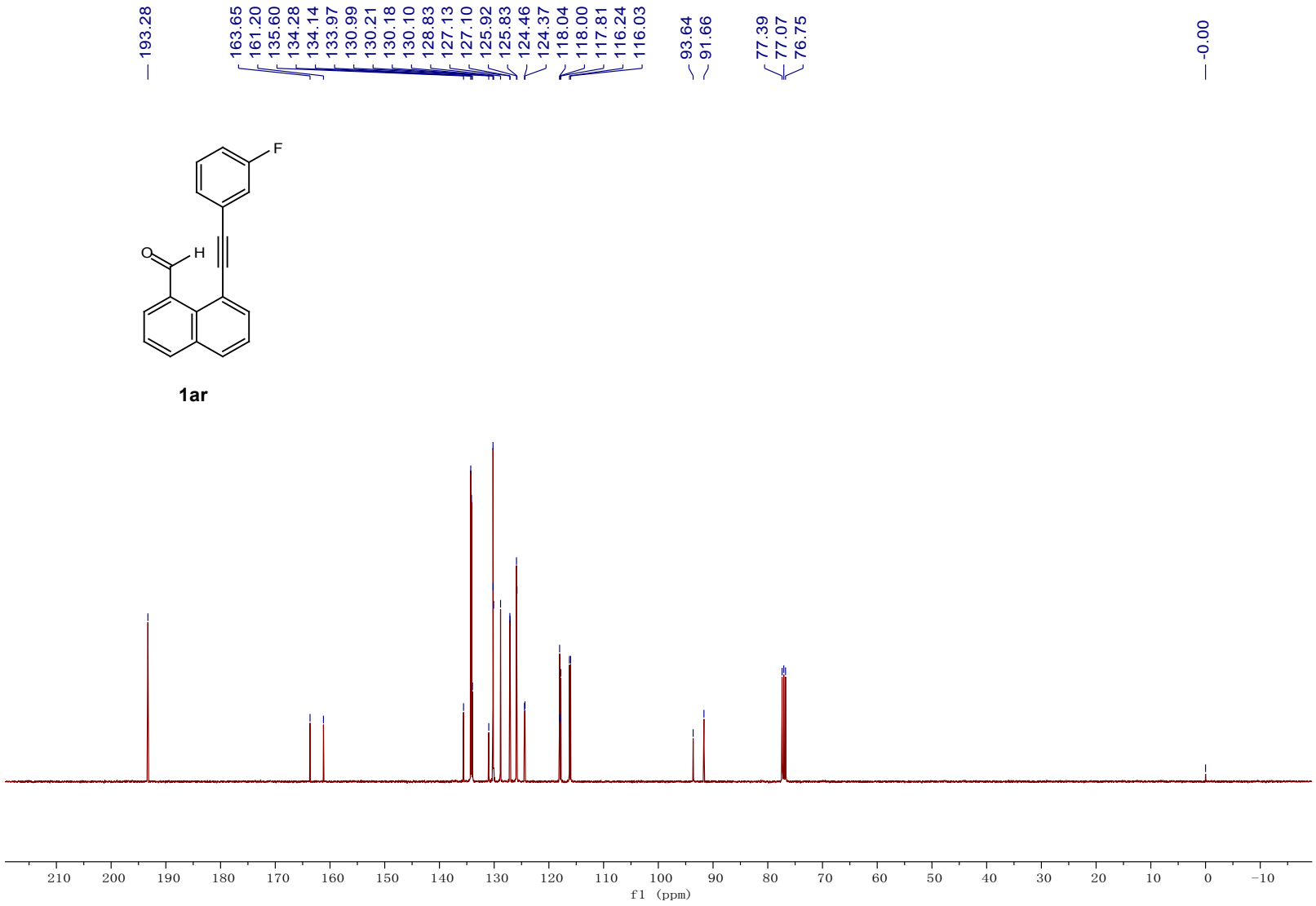
7.530
7.518
7.508
7.500
7.481
7.463
7.349
7.329
7.314
7.276
7.260
7.253
7.081
7.063
7.041
F
O
H
1.00
2.24
2.24
2.31
2.17
1.29
1.08
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1ar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134.14
133.97
130.99
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130.18
130.10
128.83
127.13
127.10
125.92
125.83
124.46
124.37
118.04
118.00
117.81
116.24
116.03
93.64
91.66
77.39
77.07
76.75
-0.00
F
O
H
1ar
210
200
190
180
170
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120
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100
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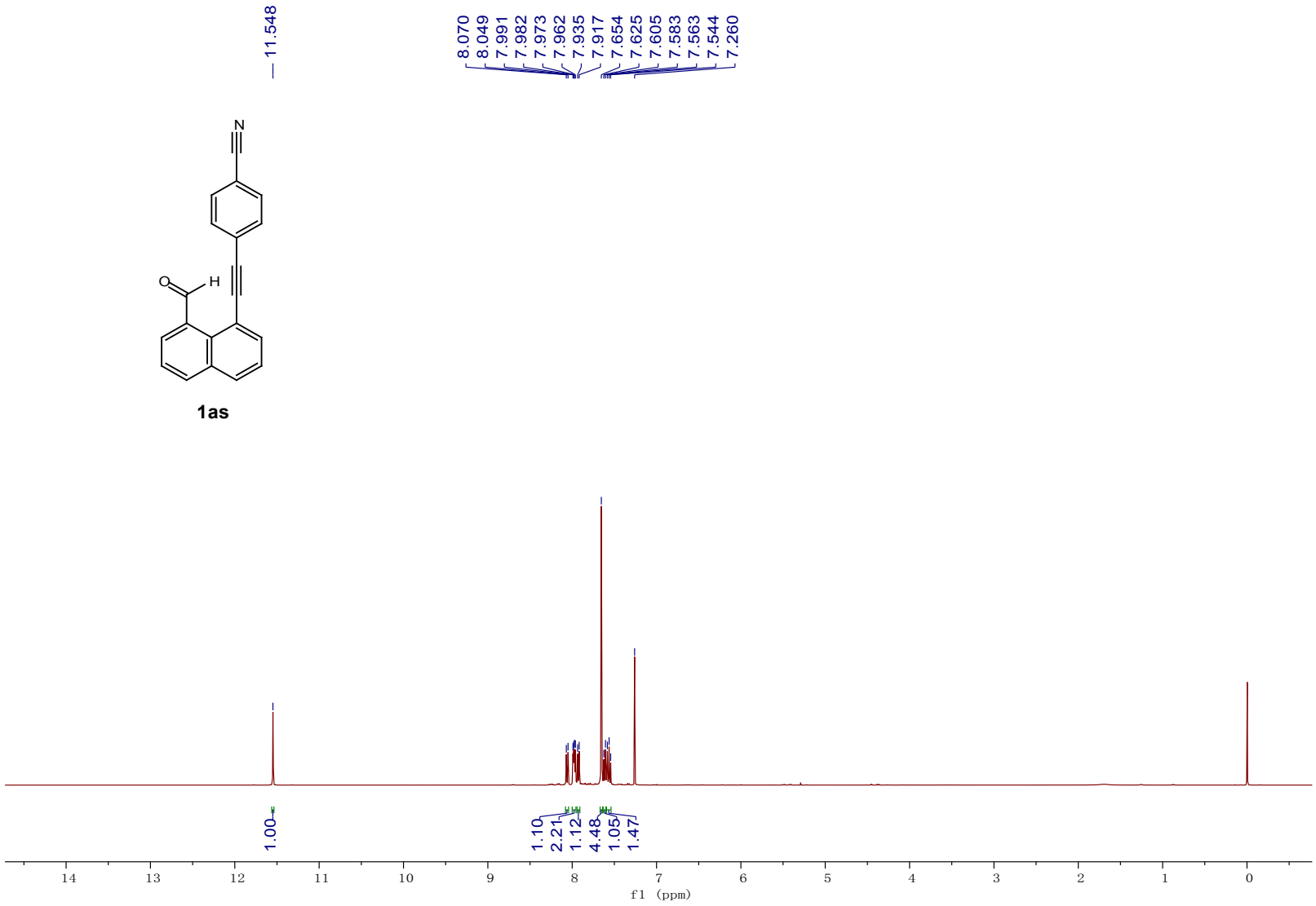
−10
f1 (ppm)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7.962
7.935
7.917
7.654
7.625
7.605
7.583
7.563
7.544
7.260
N
O
H
1as
1.00
1.10
2.21
1.12
4.48
1.05
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13
12
11
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9
8
7
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5
4
3
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1
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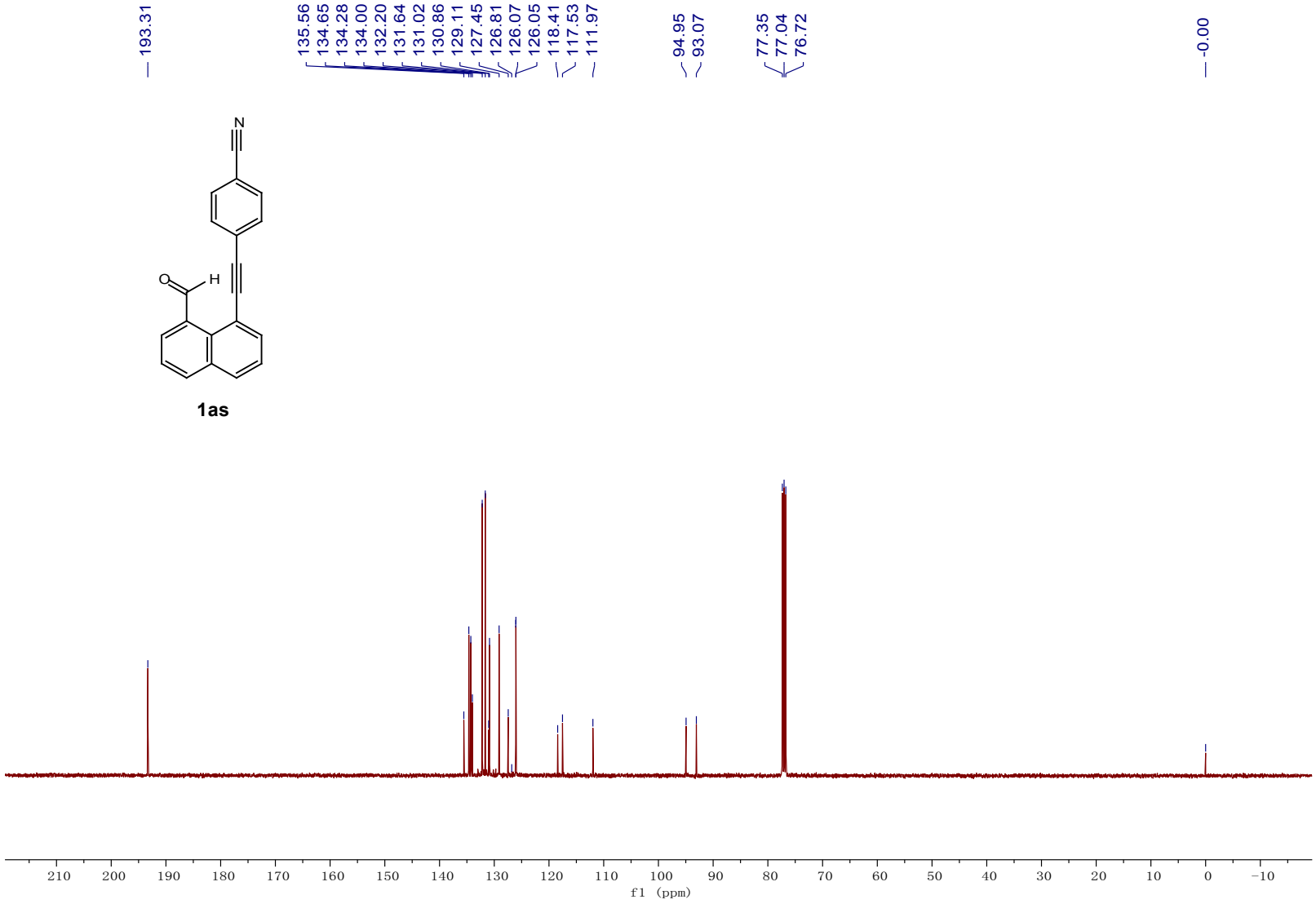
f1 (ppm)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132.20
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131.02
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129.11
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126.81
126.07
126.05
118.41
117.53
111.97
94.95
93.07
77.35
77.04
76.72
-0.00
N
O
H
1as
210
200
190
180
170
160
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140
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120
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100
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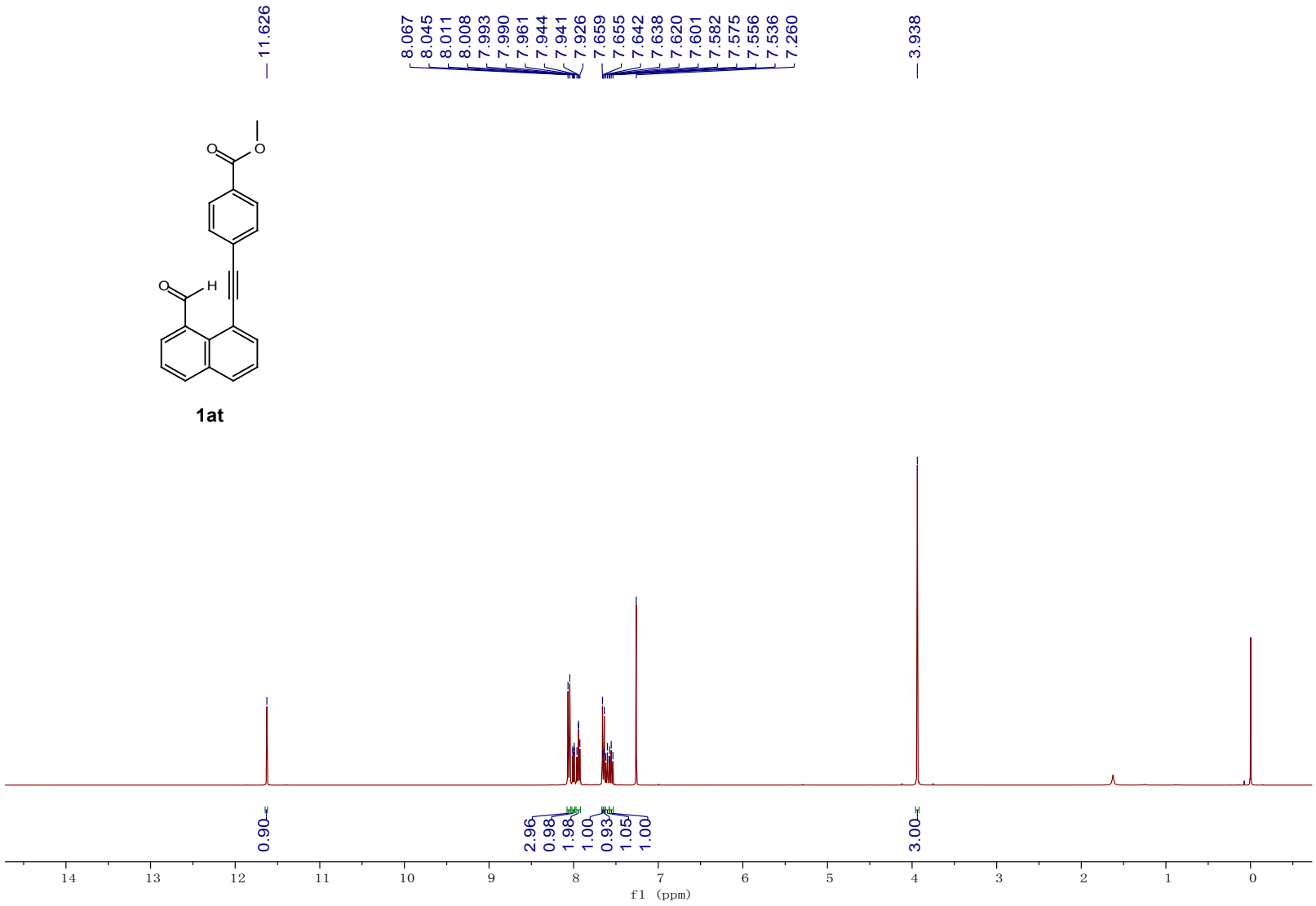
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.941
7.926
7.659
7.655
7.642
7.638
7.620
7.601
7.582
7.575
7.556
7.536
7.260
3.938
O
O
O
H
0.90
2.96
0.98
1.98
1.00
0.93
1.05
1.00
3.00
14
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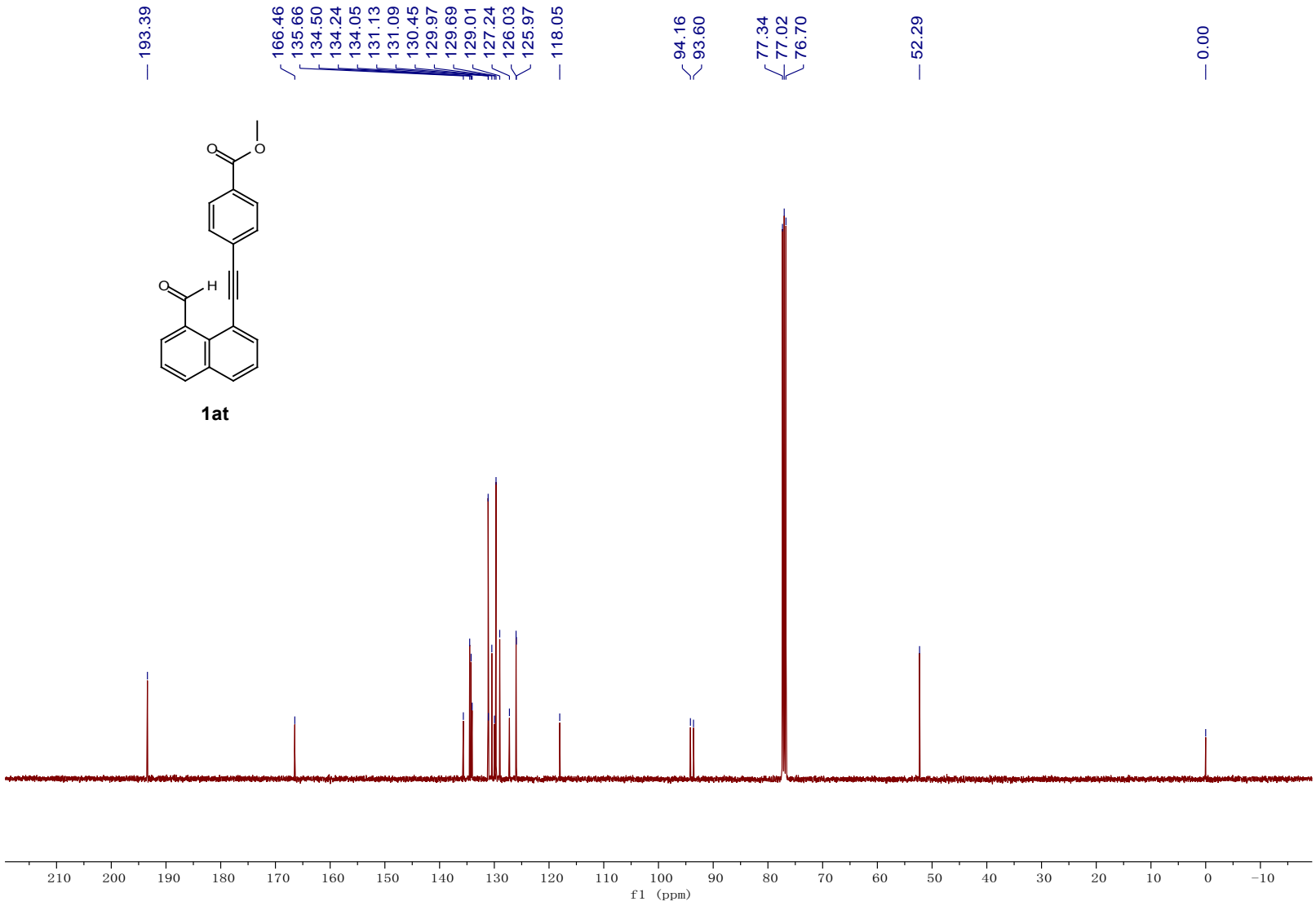
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1at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166.46
135.66
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134.24
134.05
131.13
131.09
130.45
129.97
129.69
129.01
127.24
126.03
125.97
118.05
94.16
93.60
77.34
77.02
76.70
52.29
0.00
O
O
O
H
1at
210
200
190
180
170
160
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140
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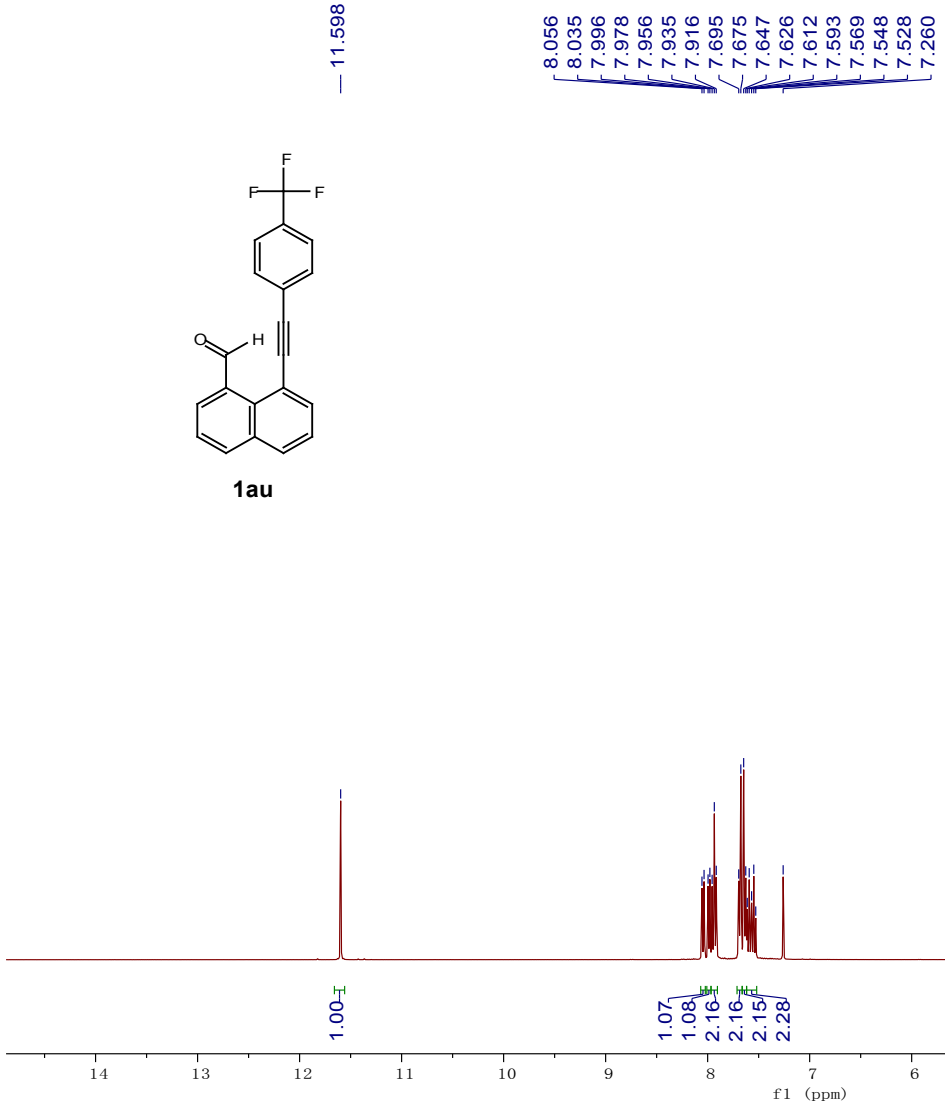
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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8.056
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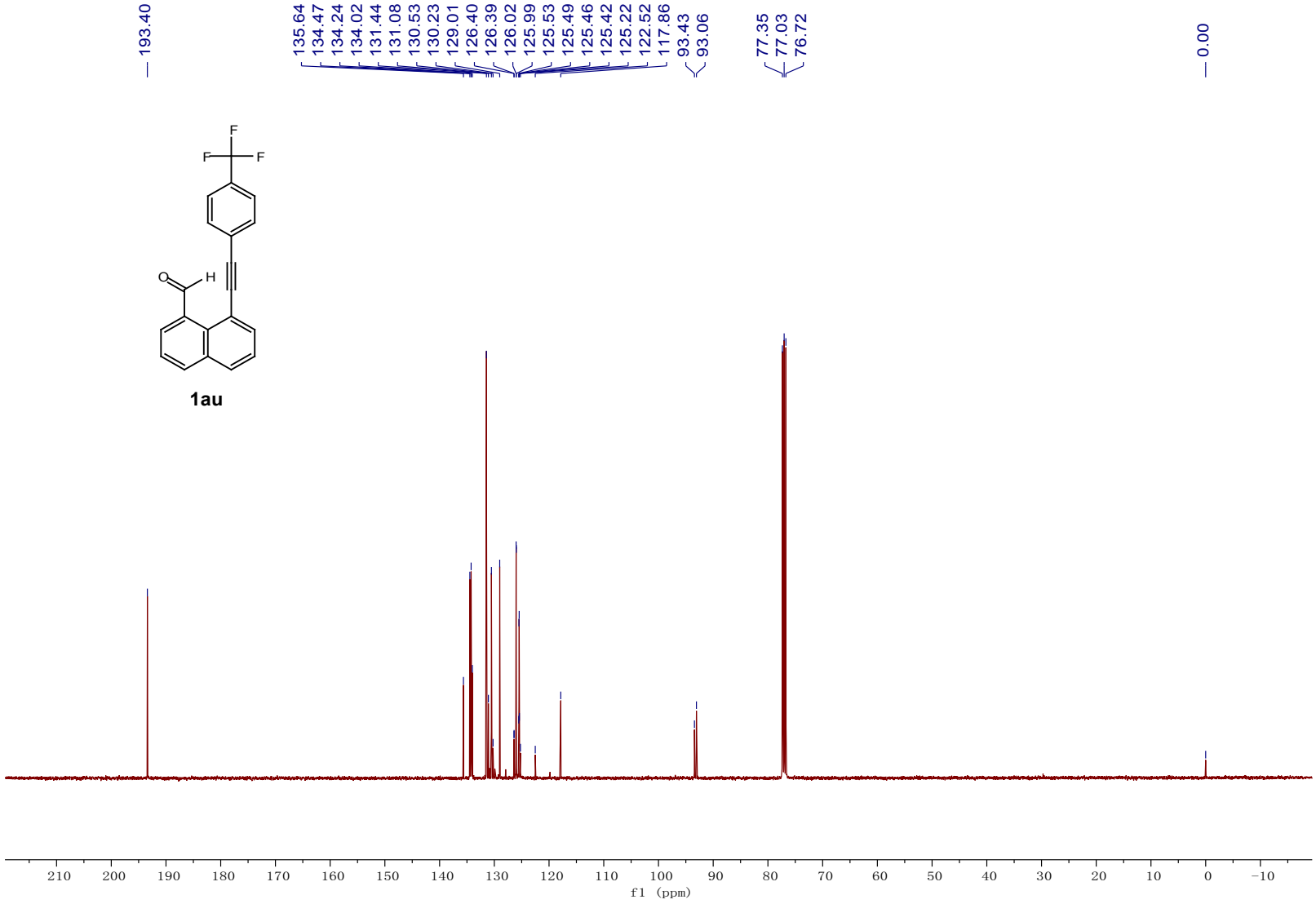
7.935
7.916
7.695
7.675
7.647
7.626
7.612
7.593
7.569
7.548
7.528
7.260
F
F
F
O
H
1.00
1.07
1.08
2.16
2.16
2.15
2.28
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

1au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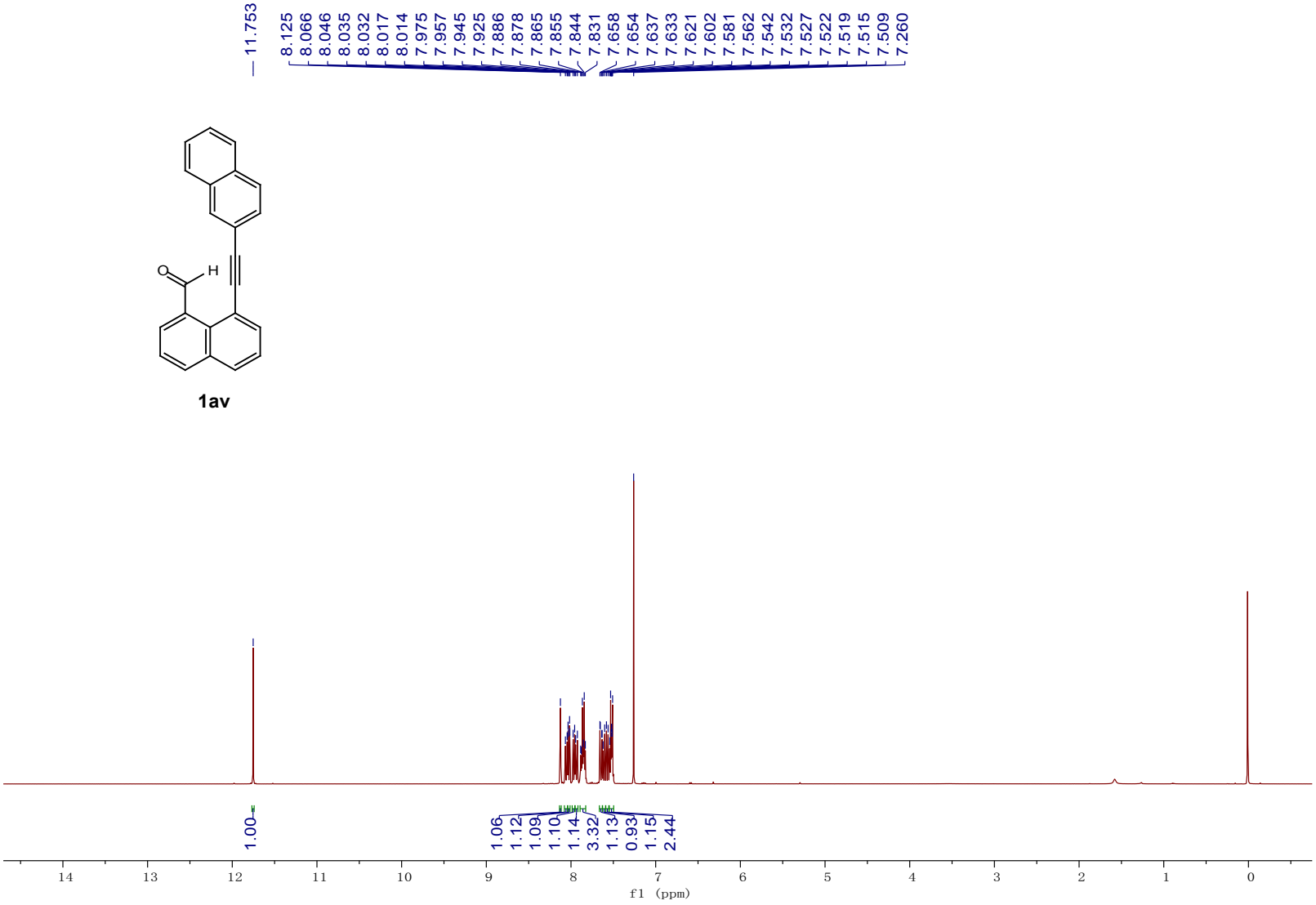
134.47
134.24
134.02
131.44
131.08
130.53
130.23
129.01
126.40
126.39
126.02
125.99
125.53
125.49
125.46
125.42
125.22
122.52
117.86
93.43
93.06
77.35
77.03
76.72
0.00
F
F
F
O
H
1au
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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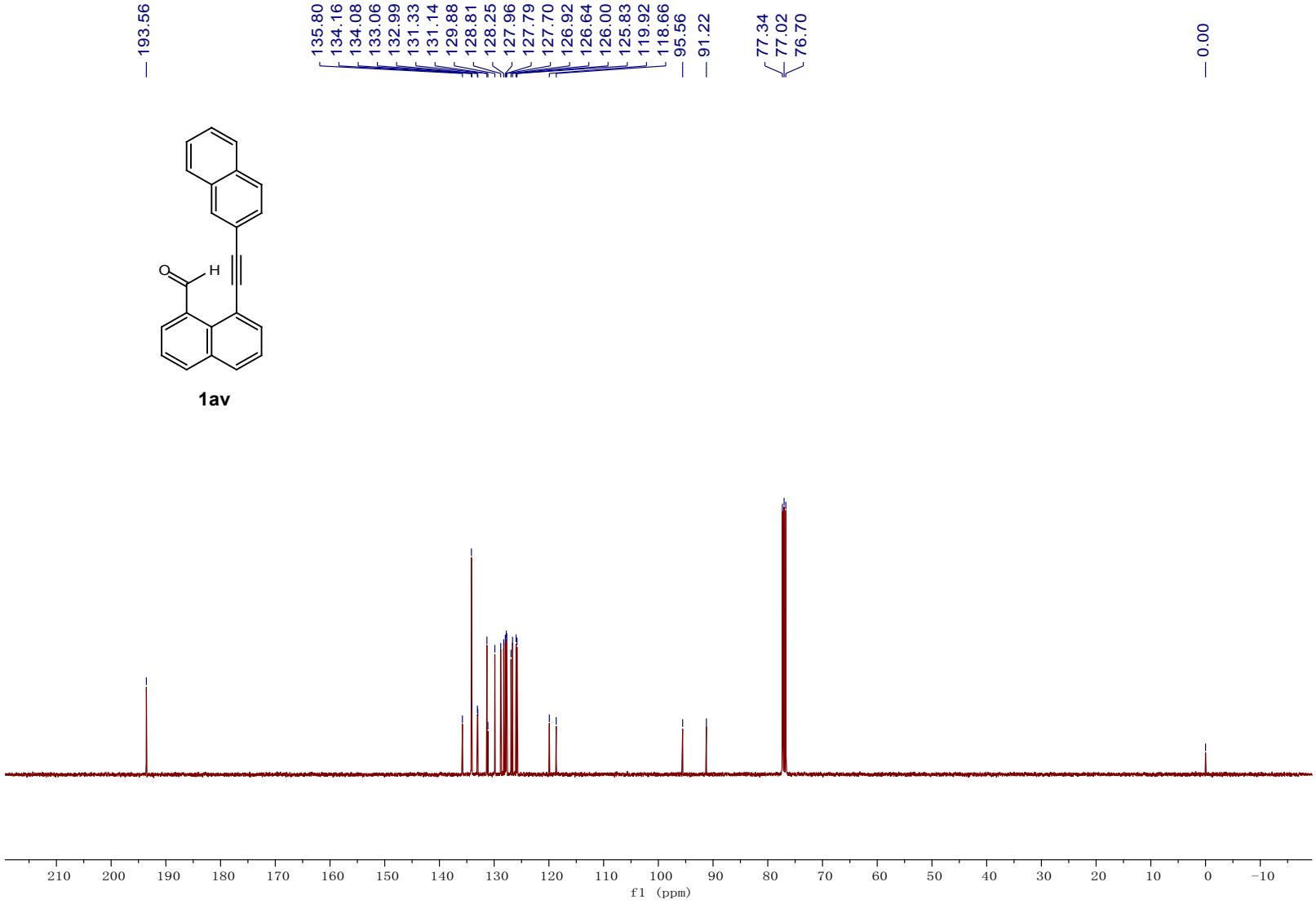
8.032
8.017
8.014
7.975
7.957
7.945
7.925
7.886
7.878
7.865
7.855
7.844
7.831
7.658
7.654
7.637
7.633
7.621
7.602
7.581
7.562
7.542
7.532
7.527
7.522
7.519
7.515
7.509
7.260
O
H
1av
1.00
1.06
1.12
1.09
1.10
1.14
3.32
1.13
0.93
1.15
2.44
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


193.56
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134.16
134.08
133.06
132.99
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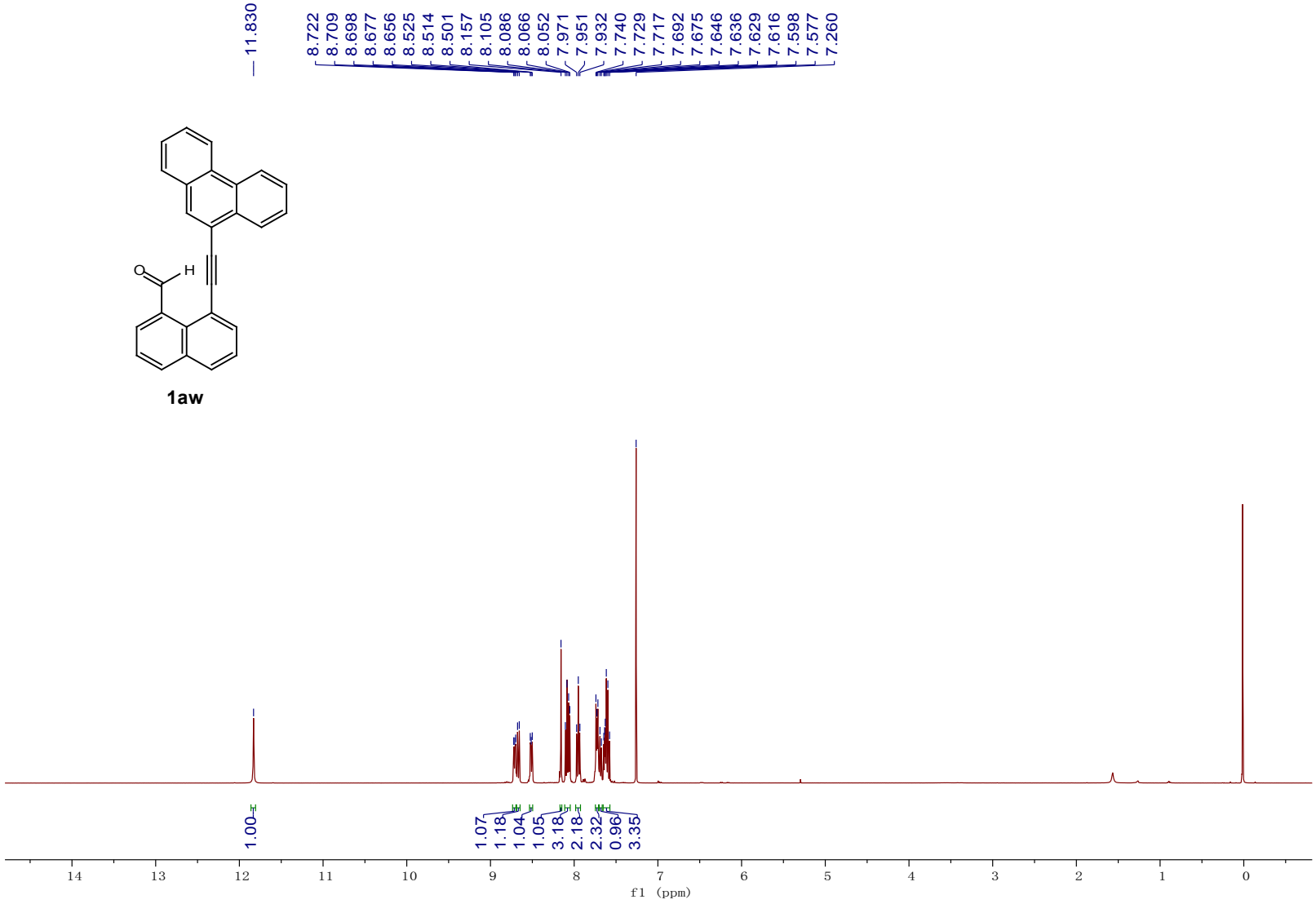
131.14
129.88
128.81
128.25
127.96
127.79
127.70
126.92
126.64
126.00
125.83
119.92
118.66
95.56
91.22
77.34
77.02
76.70
0.00
O
H
1av
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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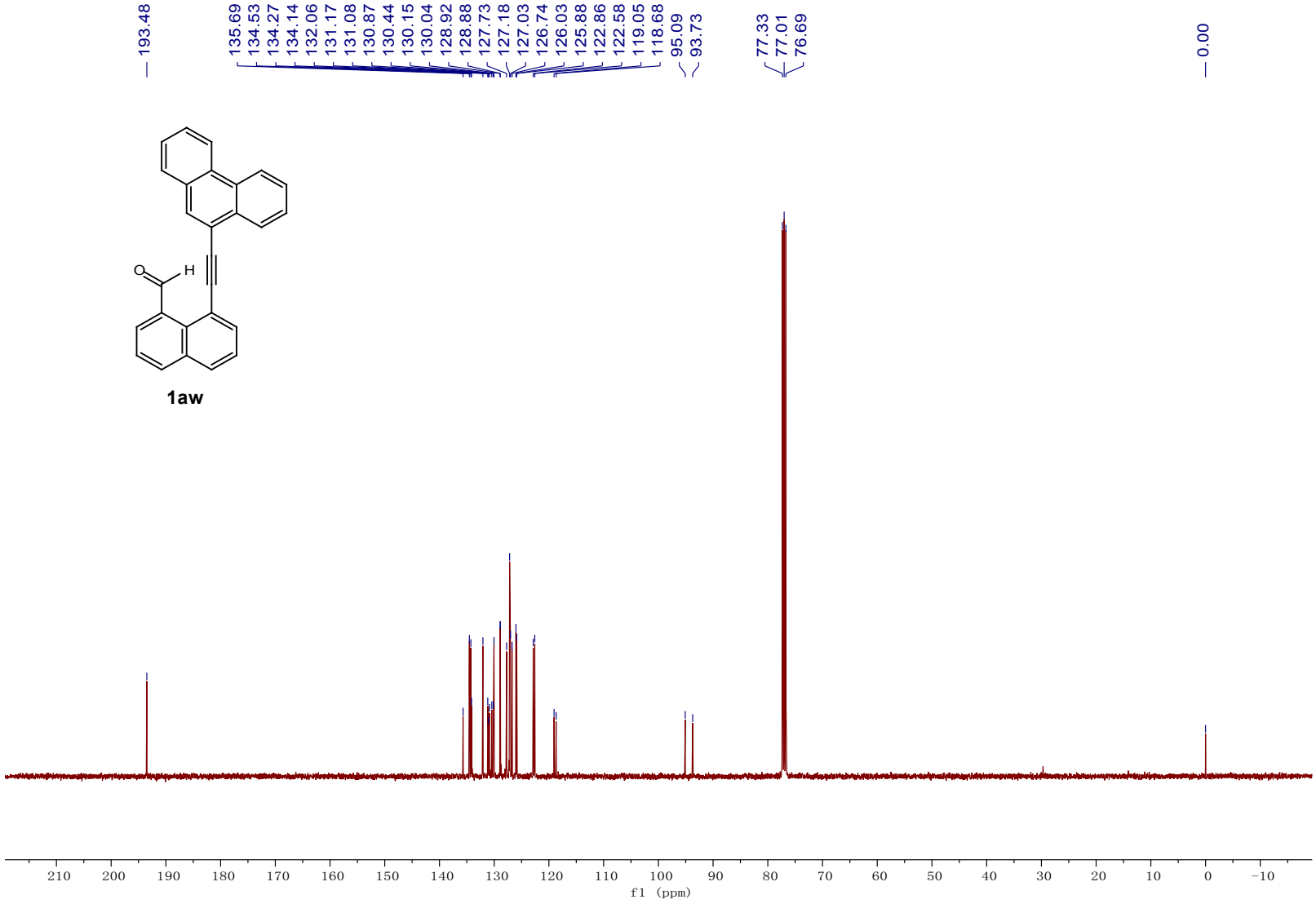
8.656
8.525
8.514
8.501
8.157
8.105
8.086
8.066
8.052
7.971
7.951
7.932
7.740
7.729
7.717
7.692
7.675
7.646
7.636
7.629
7.616
7.598
7.577
7.260
O
H
1aw
1.00
1.07
1.18
1.04
1.05
3.18
2.18
2.32
0.96
3.35
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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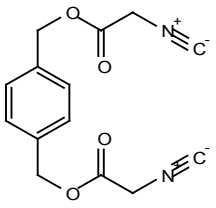
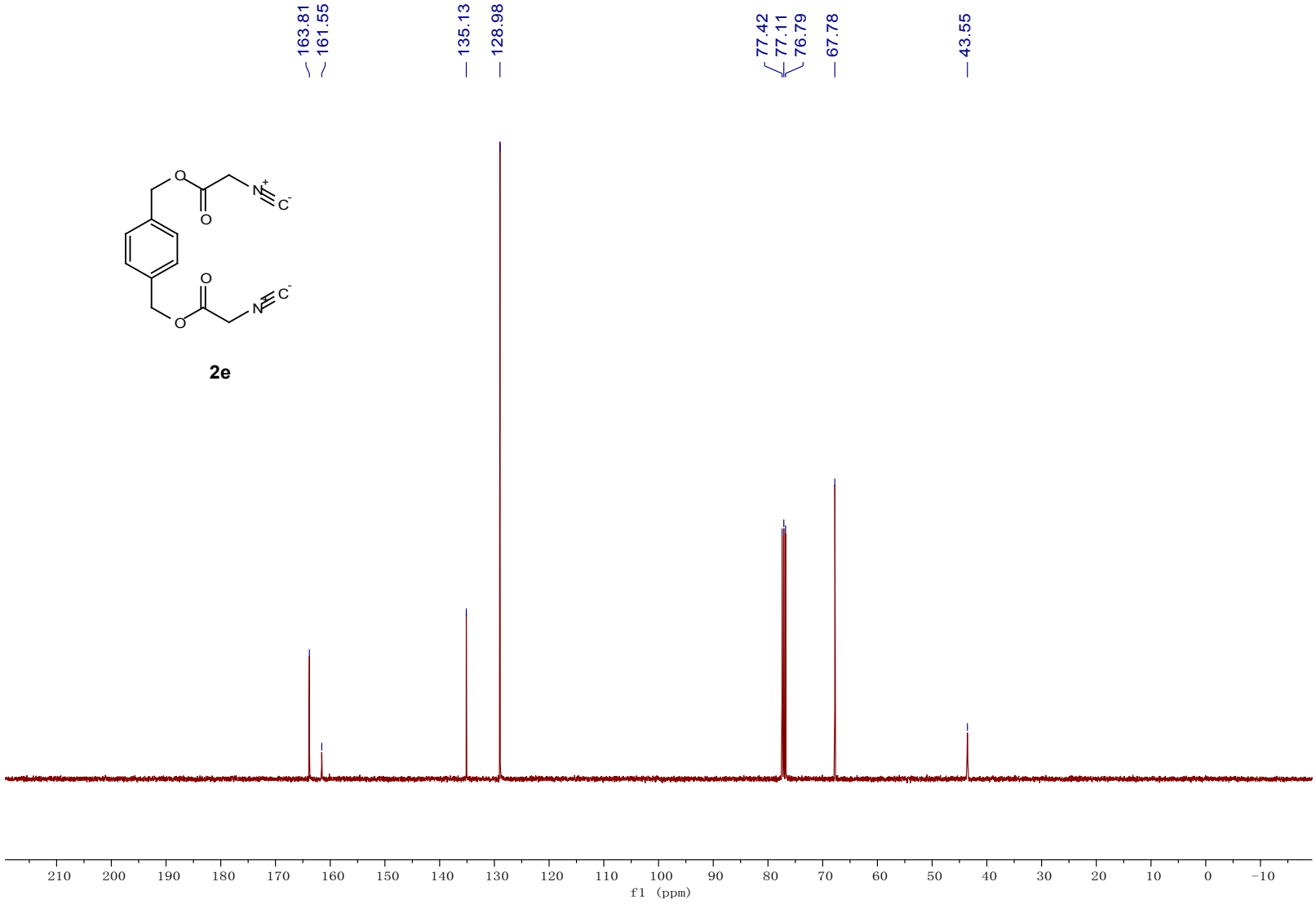
134.14
132.06
131.17
131.08
130.87
130.44
130.15
130.04
128.92
128.88
127.73
127.18
127.03
126.74
126.03
125.88
122.86
122.58
119.05
118.68
95.09
93.73
77.33
77.01
76.69
0.00
O
H
1aw
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



2e

7.392
7.260
5.239
4.263
4.05
4.11
4.00
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3
f1 (ppm)


163.81
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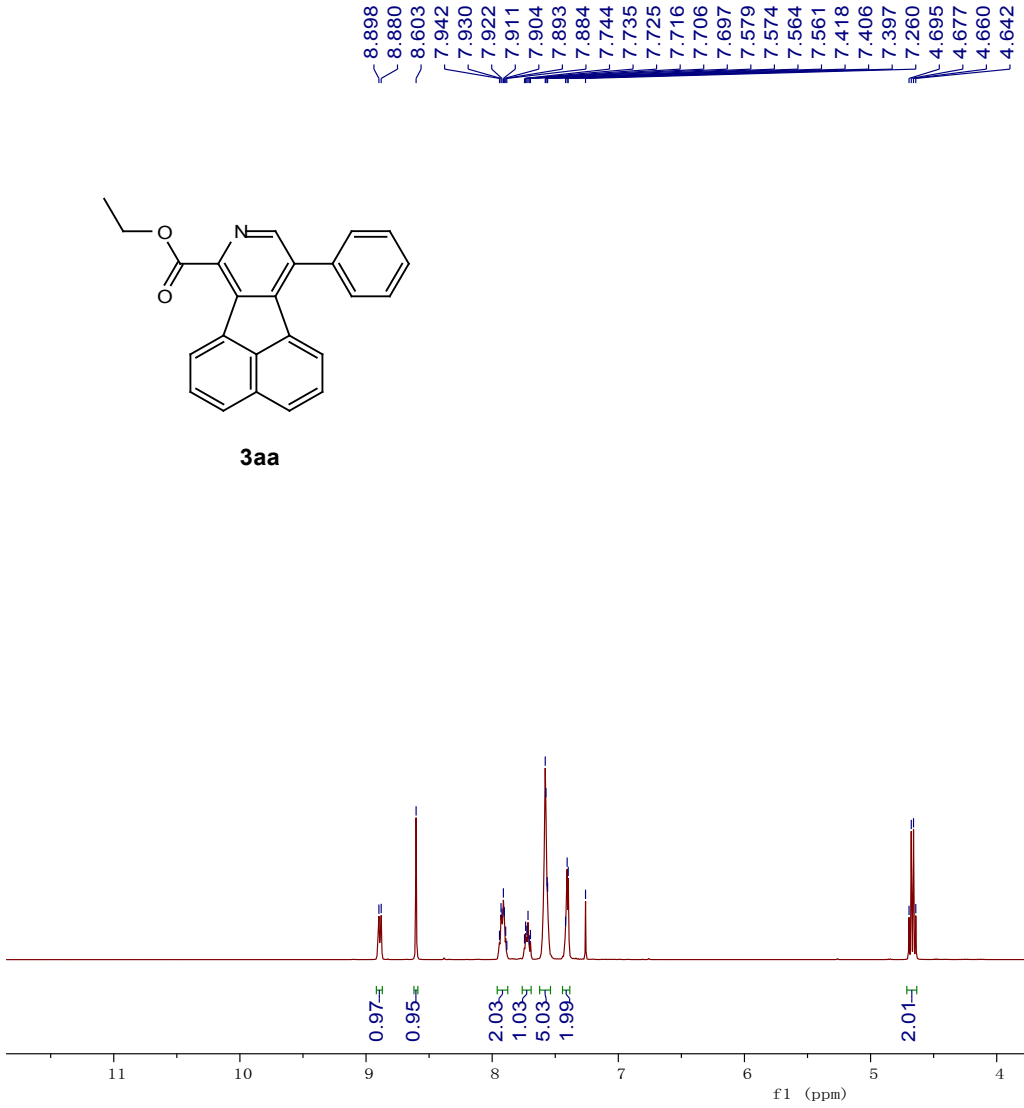
135.13
128.98
77.42
77.11
76.79
67.78
43.55
O
O
N+
C-
O
O
N
C-
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

2e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7.922
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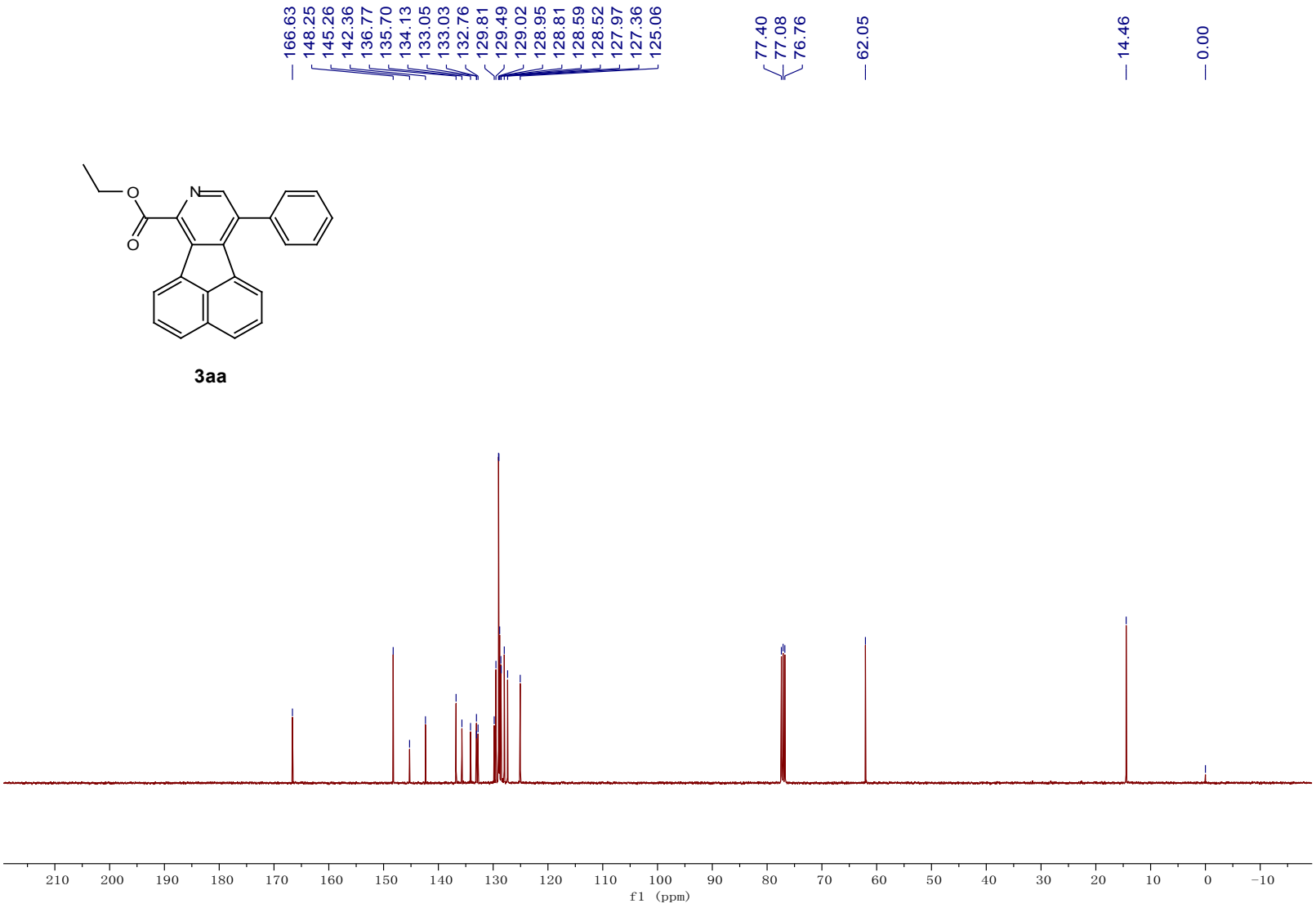
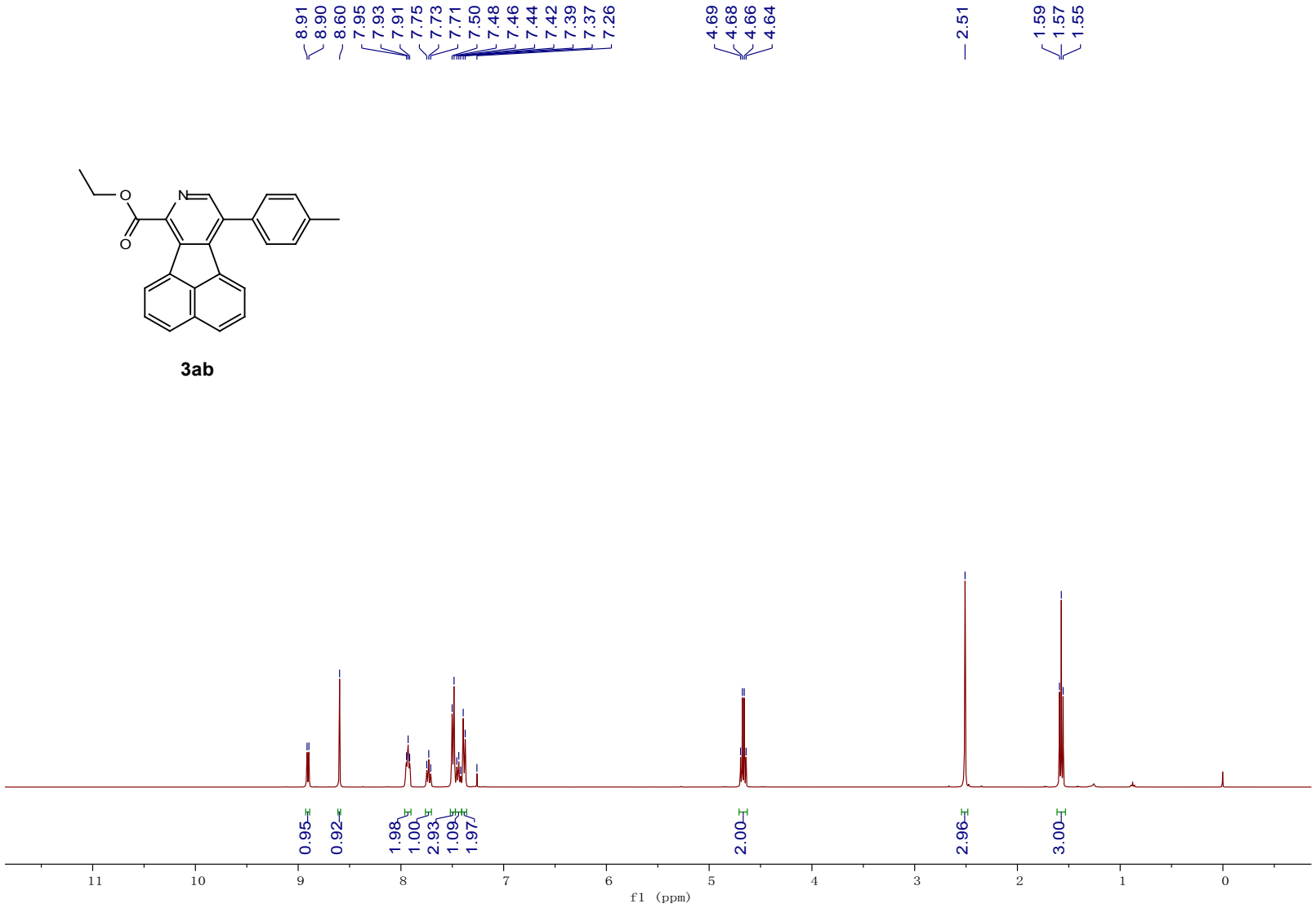
7.904
7.893
7.884
7.744
7.735
7.725
7.716
7.706
7.697
7.579
7.574
7.564
7.561
7.418
7.406
7.397
7.260
4.695
4.677
4.660
4.642
1.590
1.572
1.554
O
N
O
0.97
0.95
2.03
1.03
5.03
1.99
2.01
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3aa


166.63
148.25
145.26
142.36
136.77
135.70
134.13
133.05
133.03
132.76
129.81
129.49
129.02
128.95
128.81
128.59
128.52
127.97
127.36
125.06
77.40
77.08
76.76
62.05
14.46
0.00
O
O
N
3aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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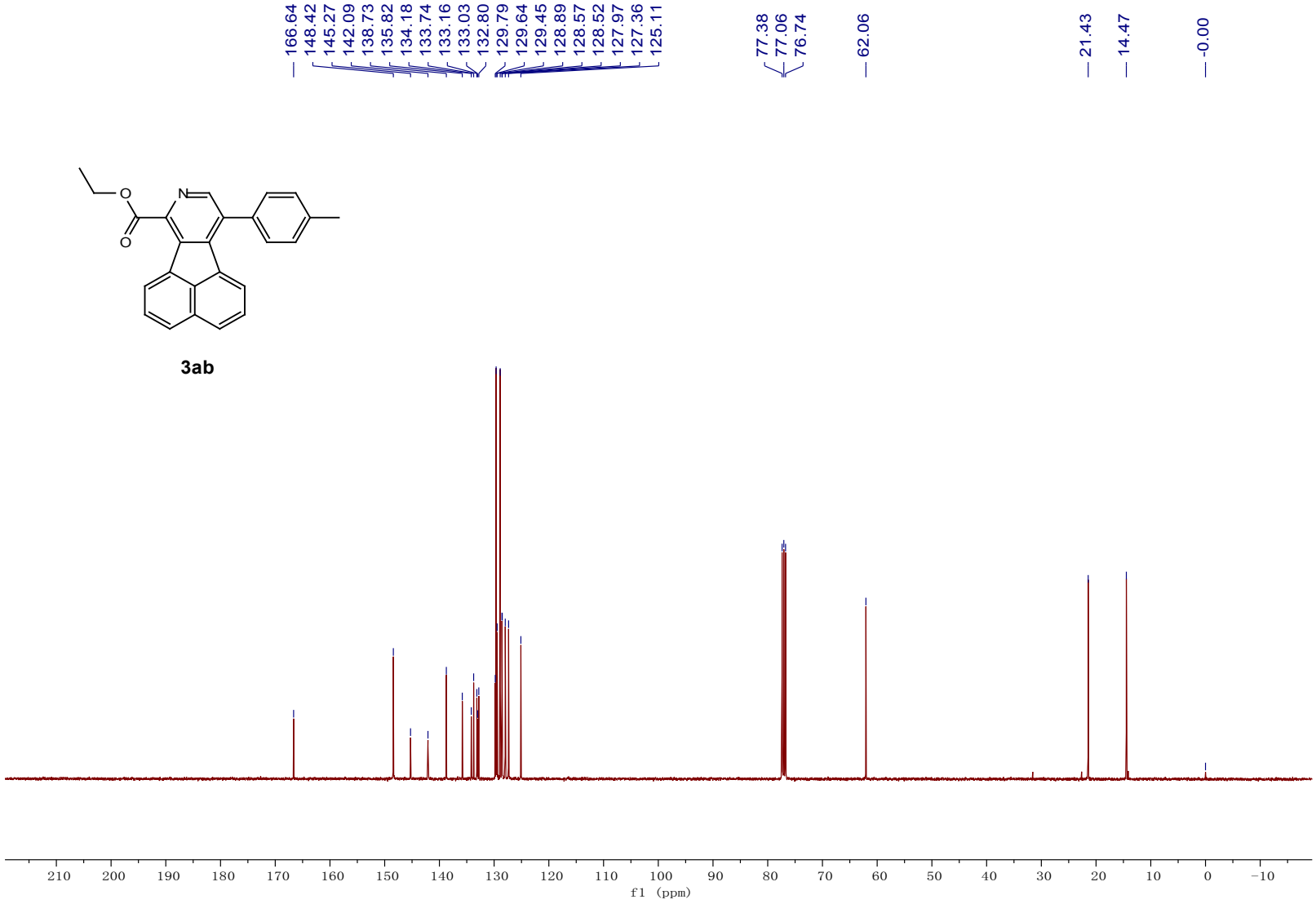
7.71
7.50
7.48
7.46
7.44
7.42
7.39
7.37
7.26
4.69
4.68
4.66
4.64
2.51
1.59
1.57
1.55
O
N
O
0.95
0.92
1.98
1.00
2.93
1.09
1.97
2.00
2.96
3.00
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ab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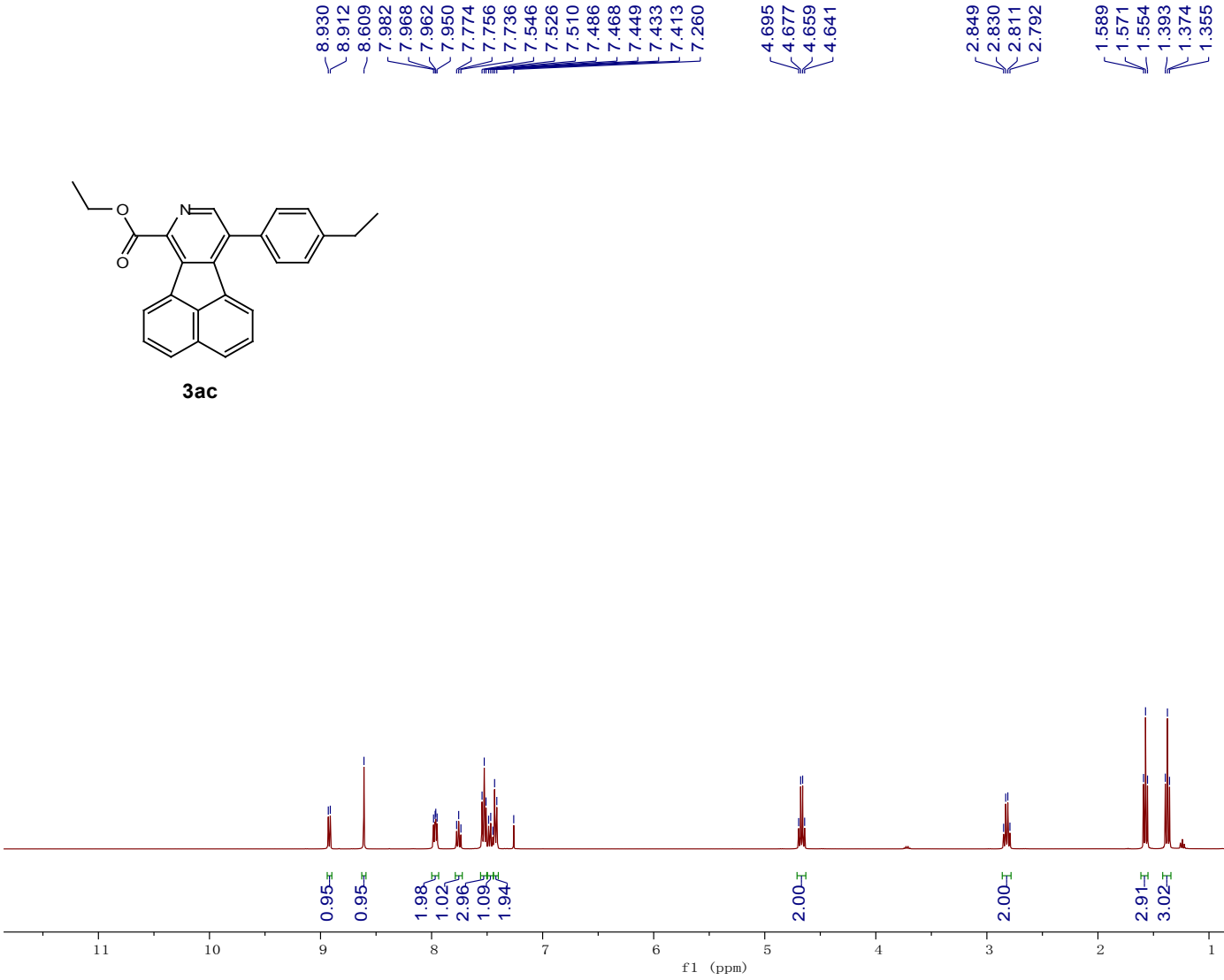
134.18
133.74
133.16
133.03
132.80
129.79
129.64
129.45
128.89
128.57
128.52
127.97
127.36
125.11
77.38
77.06
76.74
62.06
21.43
14.47
-0.00
O
N
O
3ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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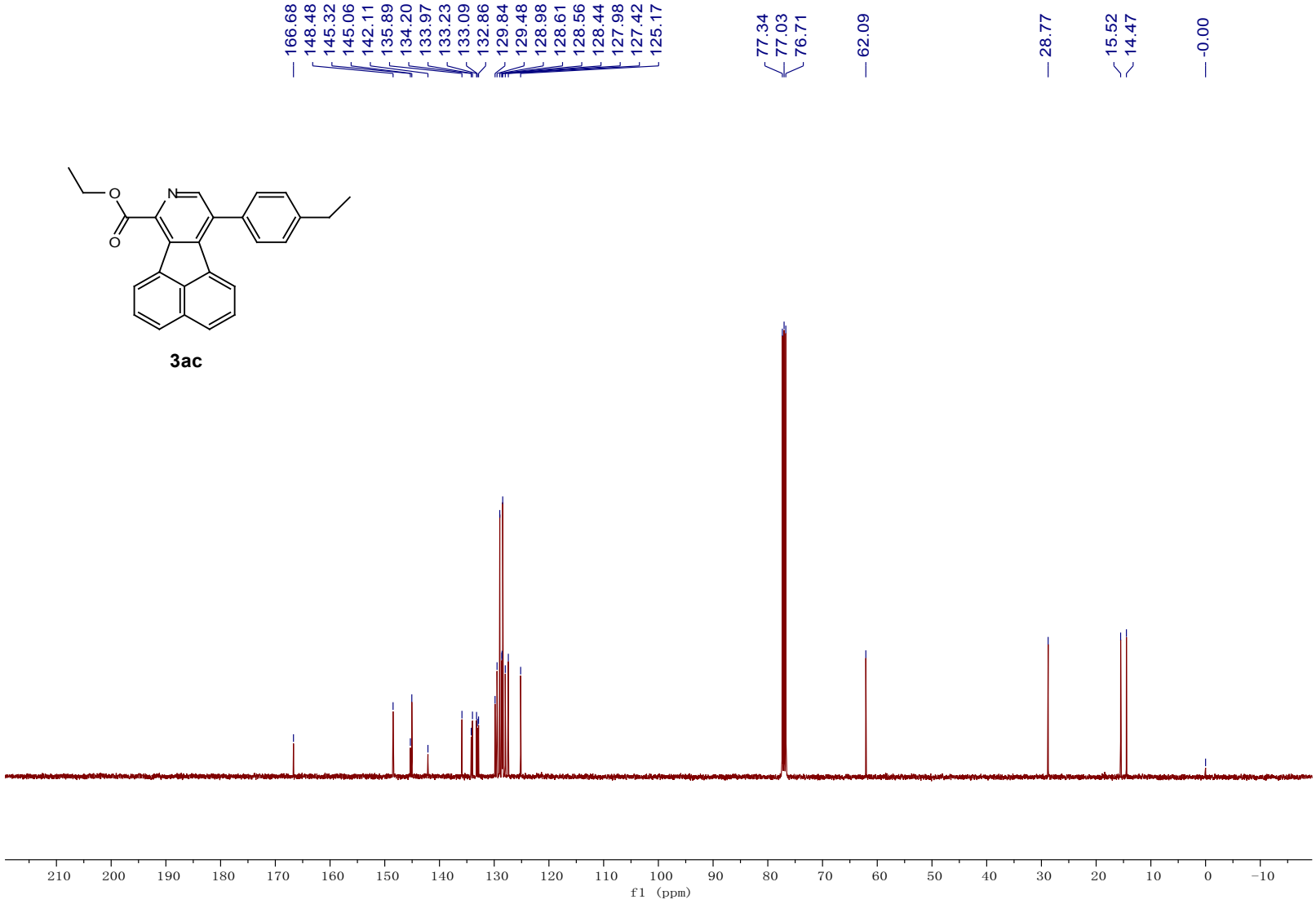
7.962
7.950
7.774
7.756
7.736
7.546
7.526
7.510
7.486
7.468
7.449
7.433
7.413
7.260
4.695
4.677
4.659
4.641
2.849
2.830
2.811
2.792
1.589
1.571
1.554
1.393
1.374
1.355
O
O
N
3ac
0.95
0.95
1.98
1.02
2.96
1.09
1.94
2.00
2.00
2.91
3.02
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


166.68
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133.97
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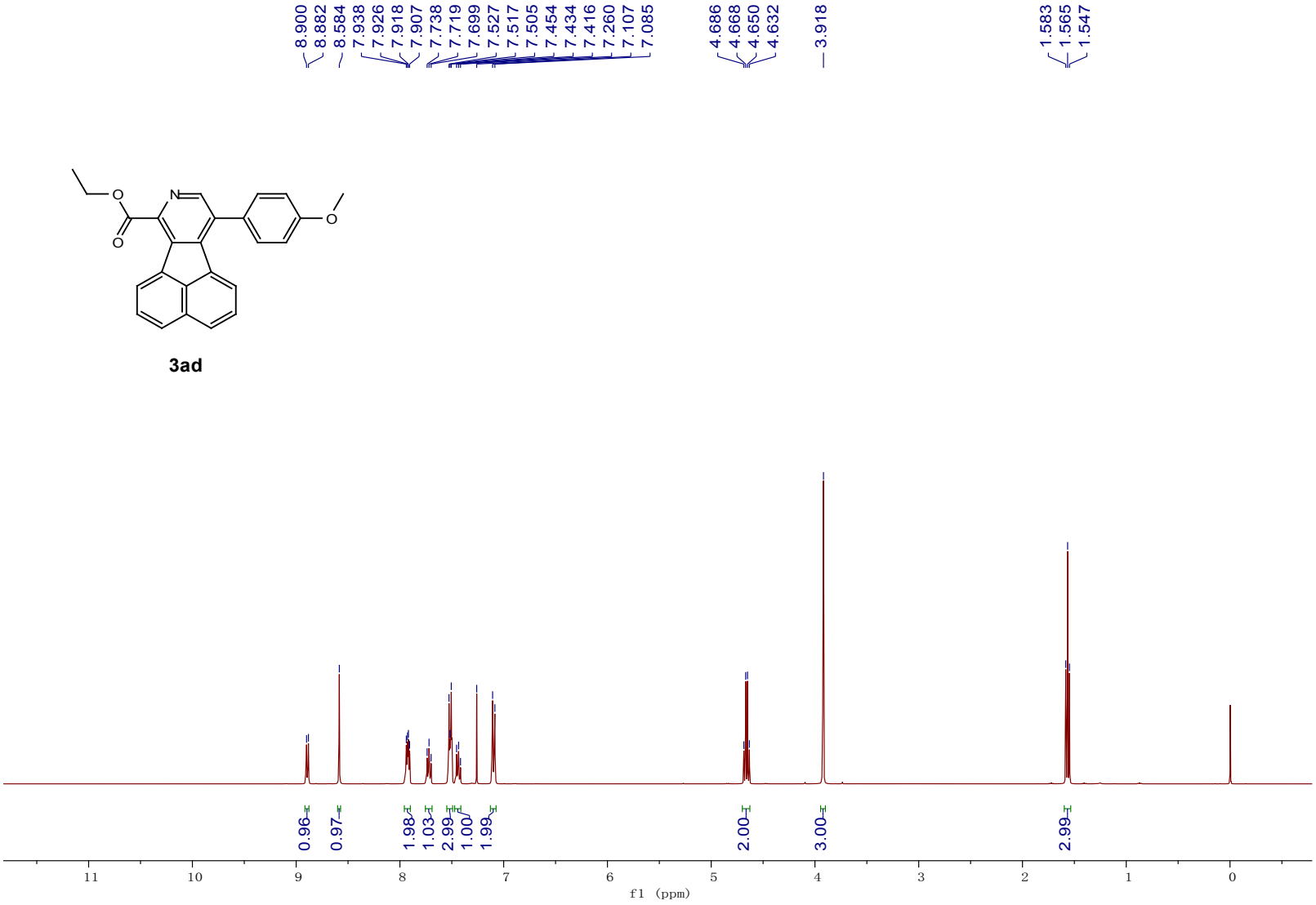
133.09
132.86
129.84
129.48
128.98
128.61
128.56
128.44
127.98
127.42
125.17
77.34
77.03
76.71
62.09
28.77
15.52
14.47
-0.00
O
N
O
O
3ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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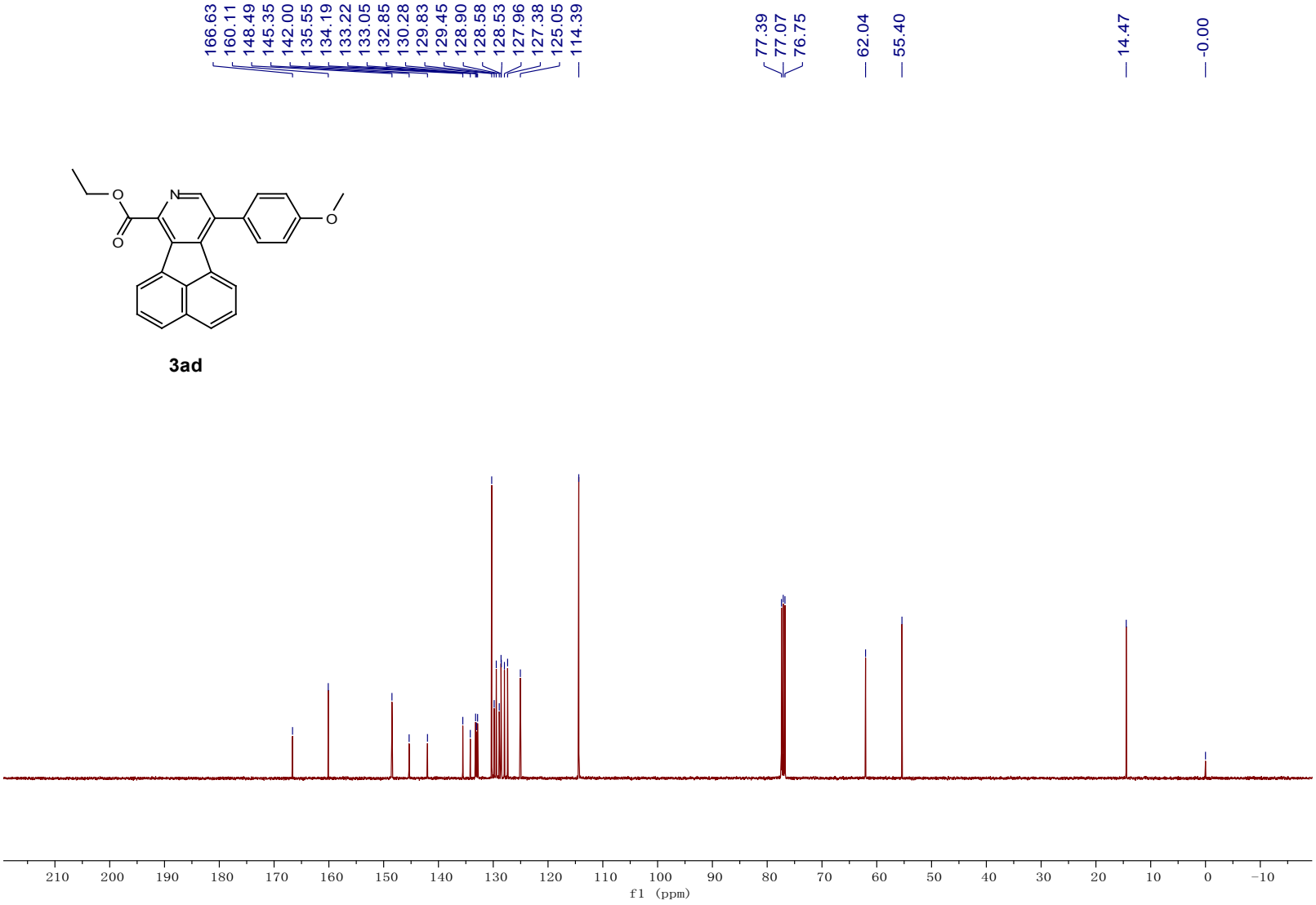
7.907
7.738
7.719
7.699
7.527
7.517
7.505
7.454
7.434
7.416
7.260
7.107
7.085
4.686
4.668
4.650
4.632
3.918
1.583
1.565
1.547
O
N
O
O
0.96
0.97
1.98
1.03
2.99
1.00
1.99
2.00
3.00
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ad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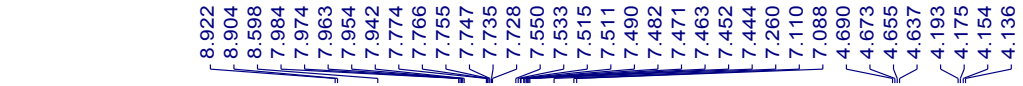
160.11
148.49
145.35
142.00
135.55
134.19
133.22
133.05
132.85
130.28
129.83
129.45
128.90
128.58
128.53
127.96
127.38
125.05
114.39
77.39
77.07
76.75
62.04
55.40
14.47
-0.00
O
N
O
O
3ad
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.954
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7.774
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7.747
7.735
7.728
7.550
7.533
7.515
7.511
7.490
7.482
7.471
7.463
7.452
7.444
7.260
7.110
7.088
4.690
4.673
4.655
4.637
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4.154
4.136
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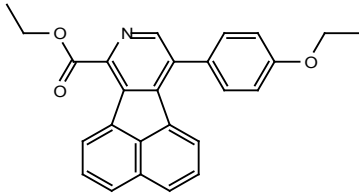
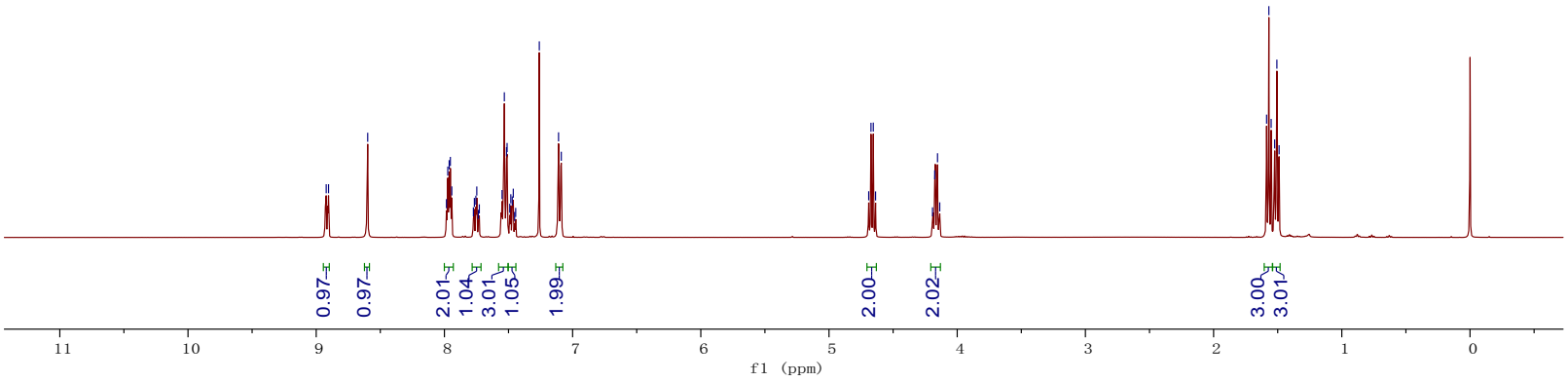
1.489


O
N
O
O

3ae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3.01
1.05
1.99
2.00
2.02
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3.01
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9
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4
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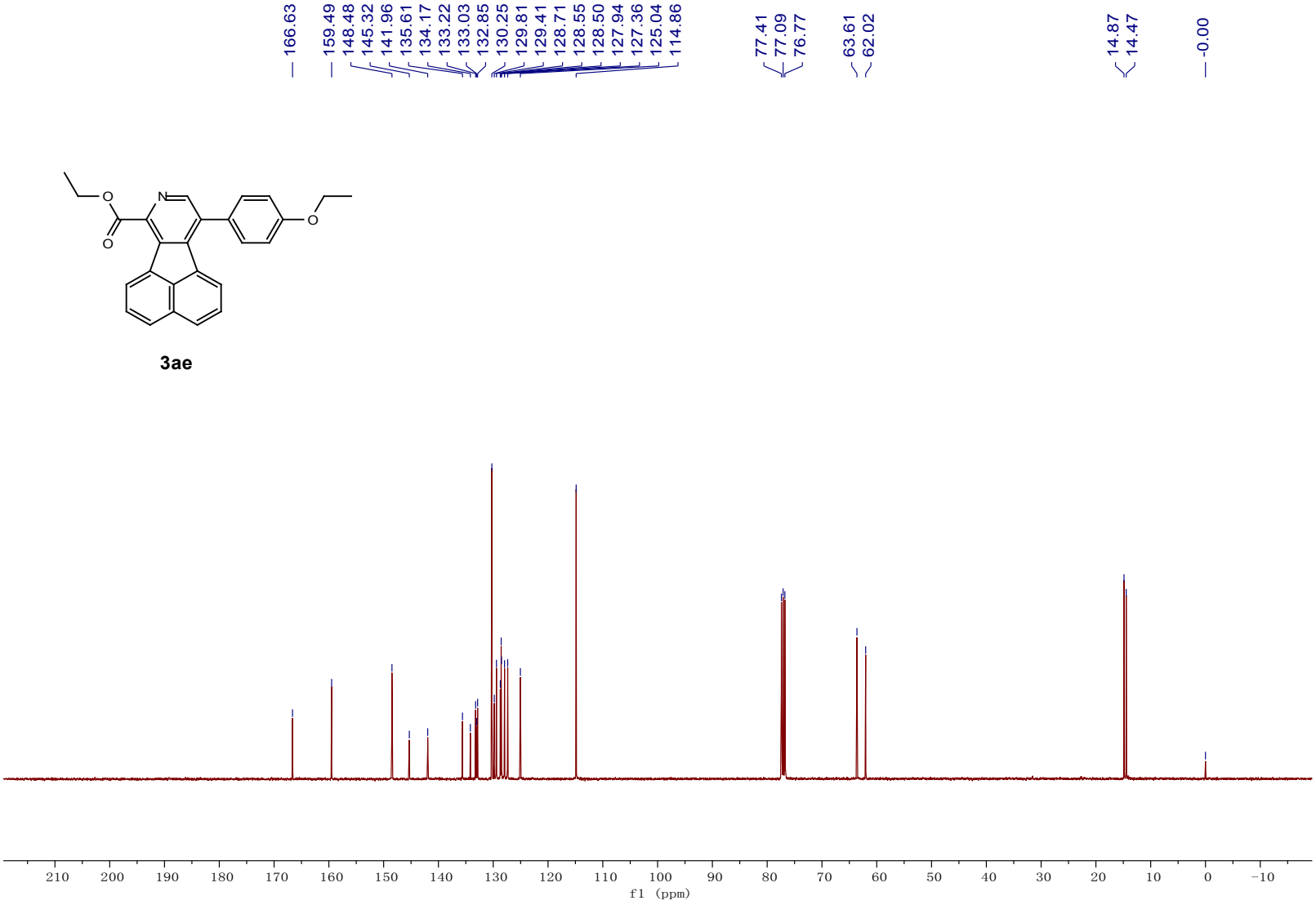
f1 (ppm)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133.22
133.03
132.85
130.25
129.81
129.41
128.71
128.55
128.50
127.94
127.36
125.04
114.86
77.41
77.09
76.77
63.61
62.02
14.87
14.47
-0.00
O
N
O
O
210
200
190
180
170
160
150
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120
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100
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60
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40
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20
10
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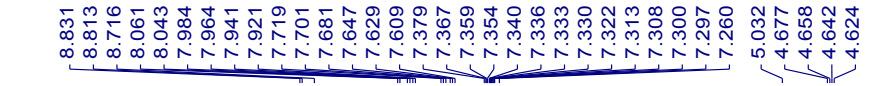
−10
f1 (ppm)

3ae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7.964
7.941
7.921
7.719
7.701
7.681
7.647
7.629
7.609
7.379
7.367
7.359
7.354
7.340
7.336
7.333
7.330
7.322
7.313
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7.297
7.260
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4.658
4.642
4.624
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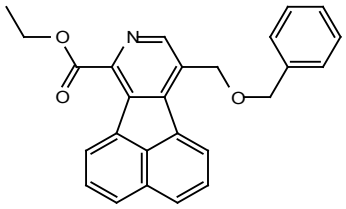
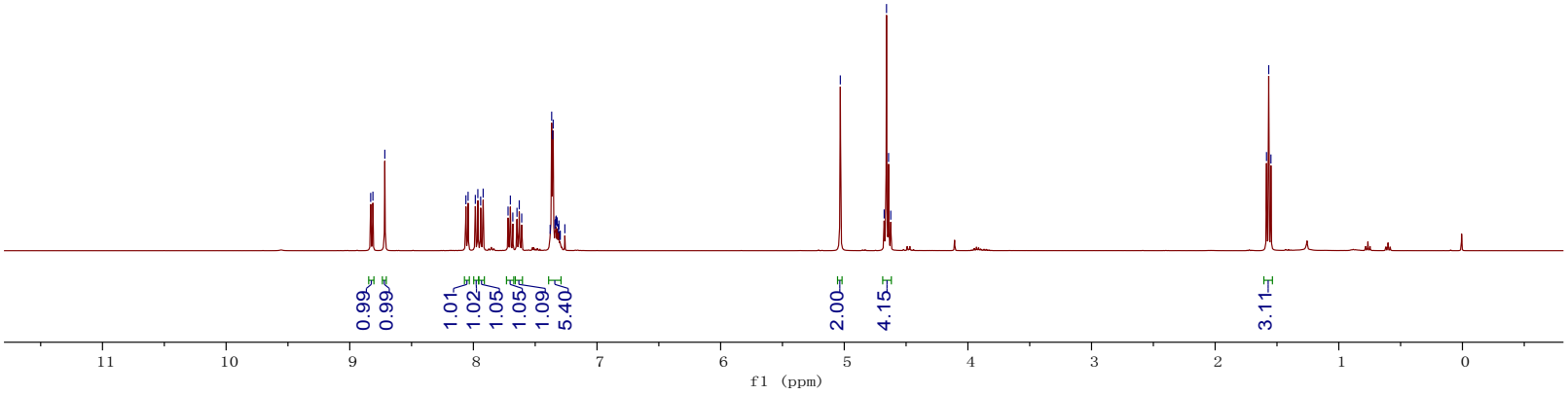
1.567
1.549


O
N
O
O

3af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1.05
1.09
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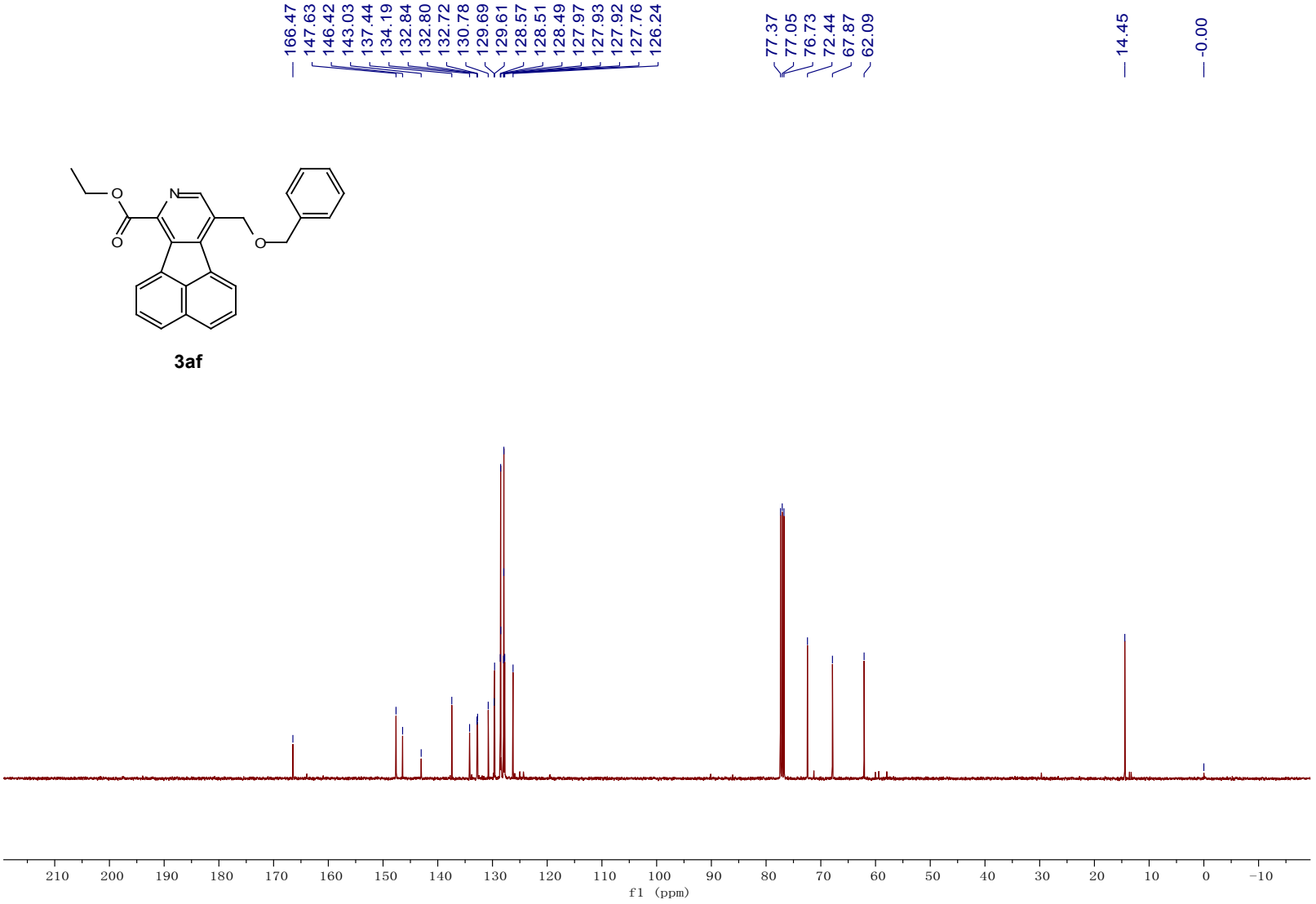
3.11
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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134.19
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132.80
132.72
130.78
129.69
129.61
128.57
128.51
128.49
127.97
127.93
127.92
127.76
126.24
77.37
77.05
76.73
72.44
67.87
62.09
14.45
-0.00
O
N
O
O
210
200
190
180
170
160
150
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120
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100
90
80
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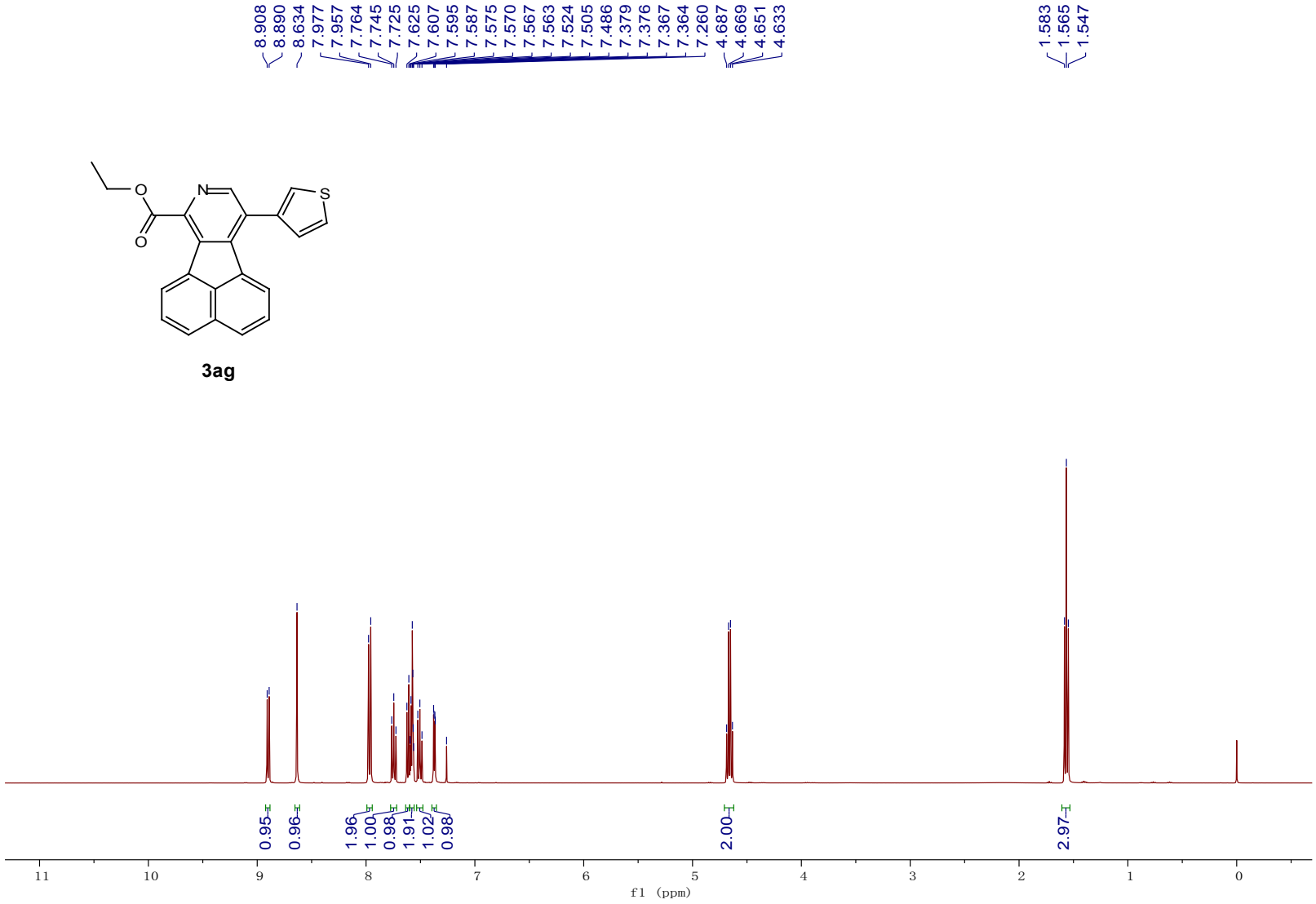
60
50
40
30
20
10
0
−10
f1 (ppm)

3af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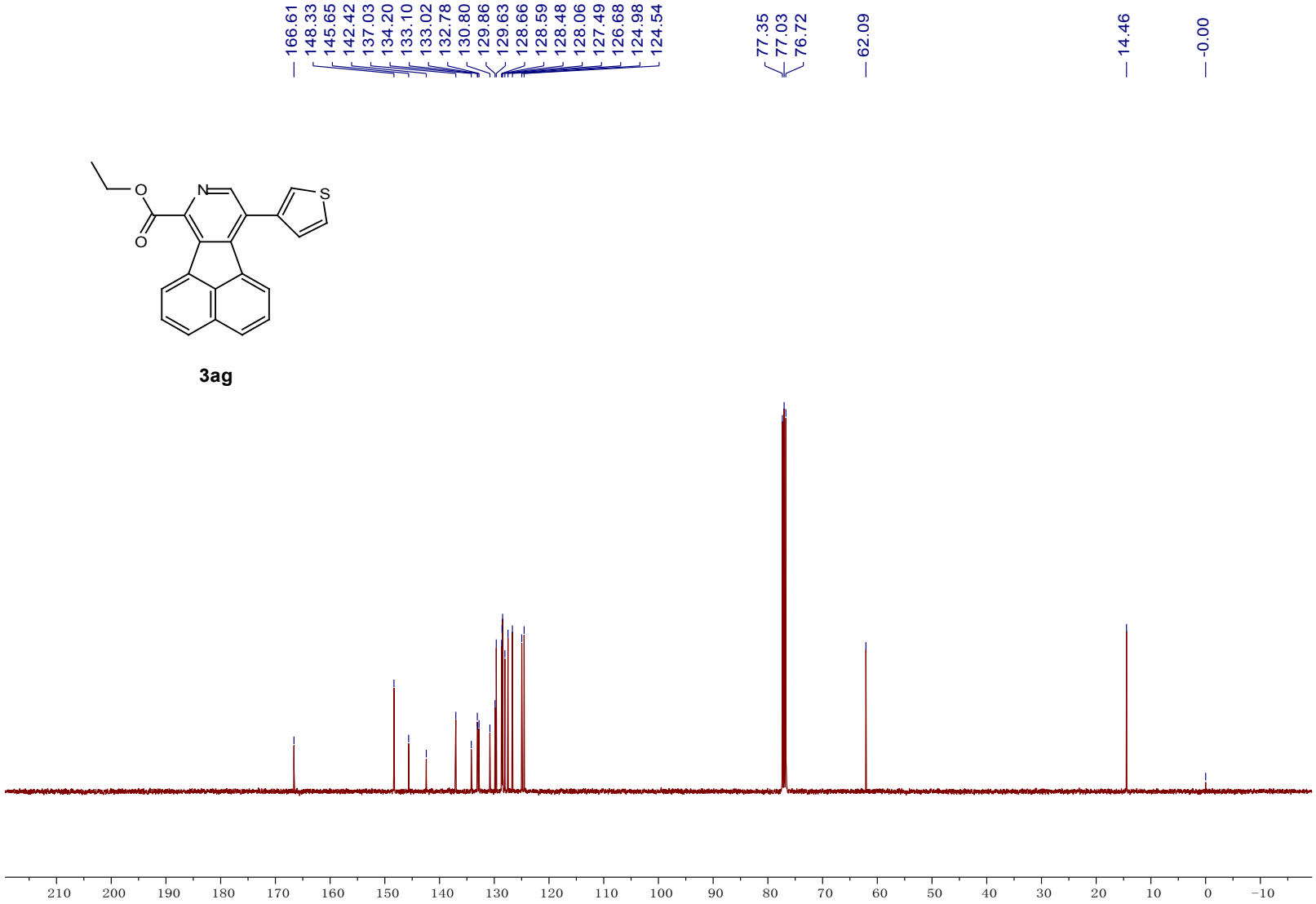
7.725
7.625
7.607
7.595
7.587
7.575
7.570
7.567
7.563
7.524
7.505
7.486
7.379
7.376
7.367
7.364
7.260
4.687
4.669
4.651
4.633
1.583
1.565
1.547
O
N
S
O
3ag
0.95
0.96
1.96
1.00
0.98
1.91
1.02
0.98
2.00
2.97
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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134.20
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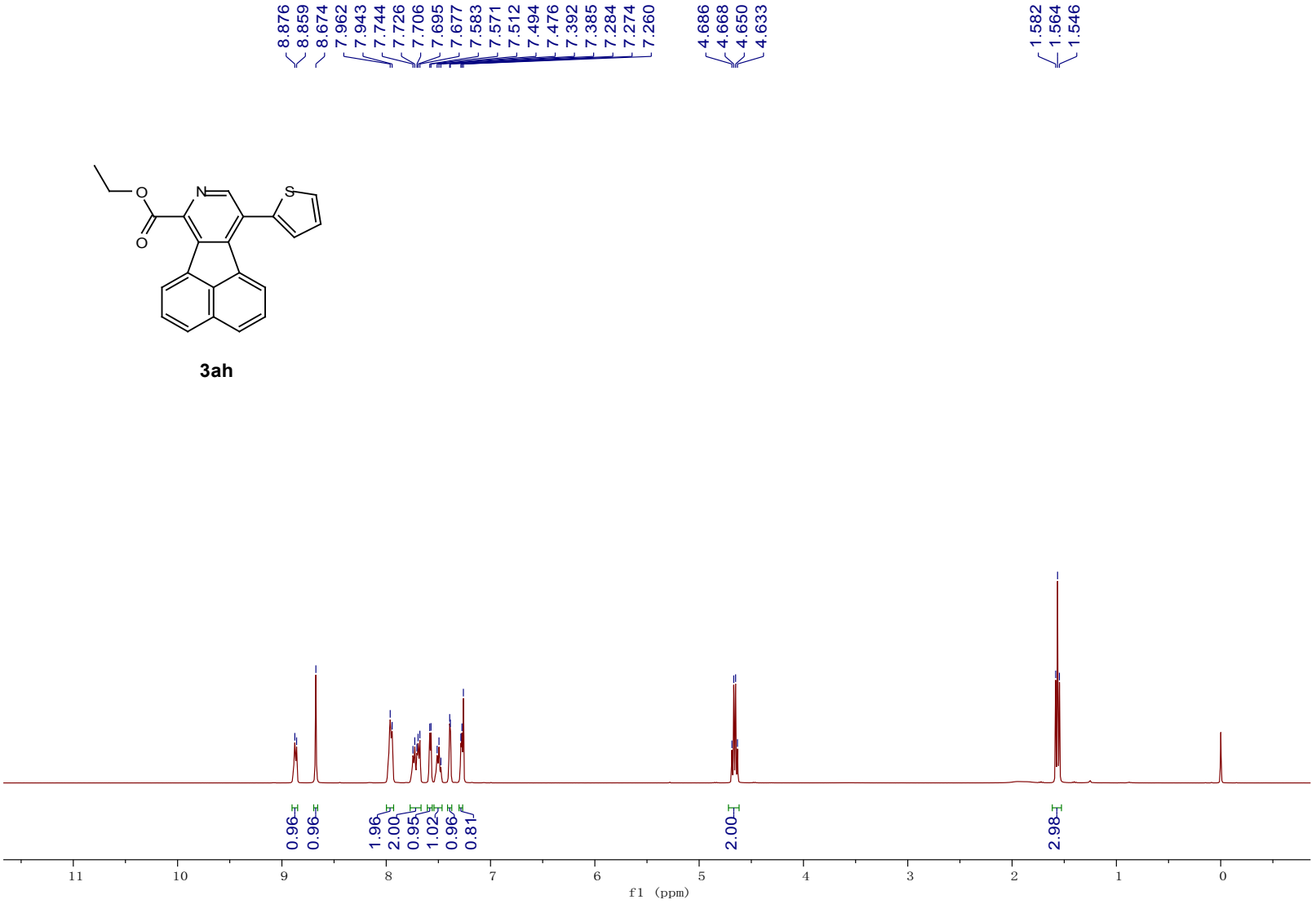
133.02
132.78
130.80
129.86
129.63
128.66
128.59
128.48
128.06
127.49
126.68
124.98
124.54
77.35
77.03
76.72
62.09
14.46
-0.00
O
N
S
O
O
3ag
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10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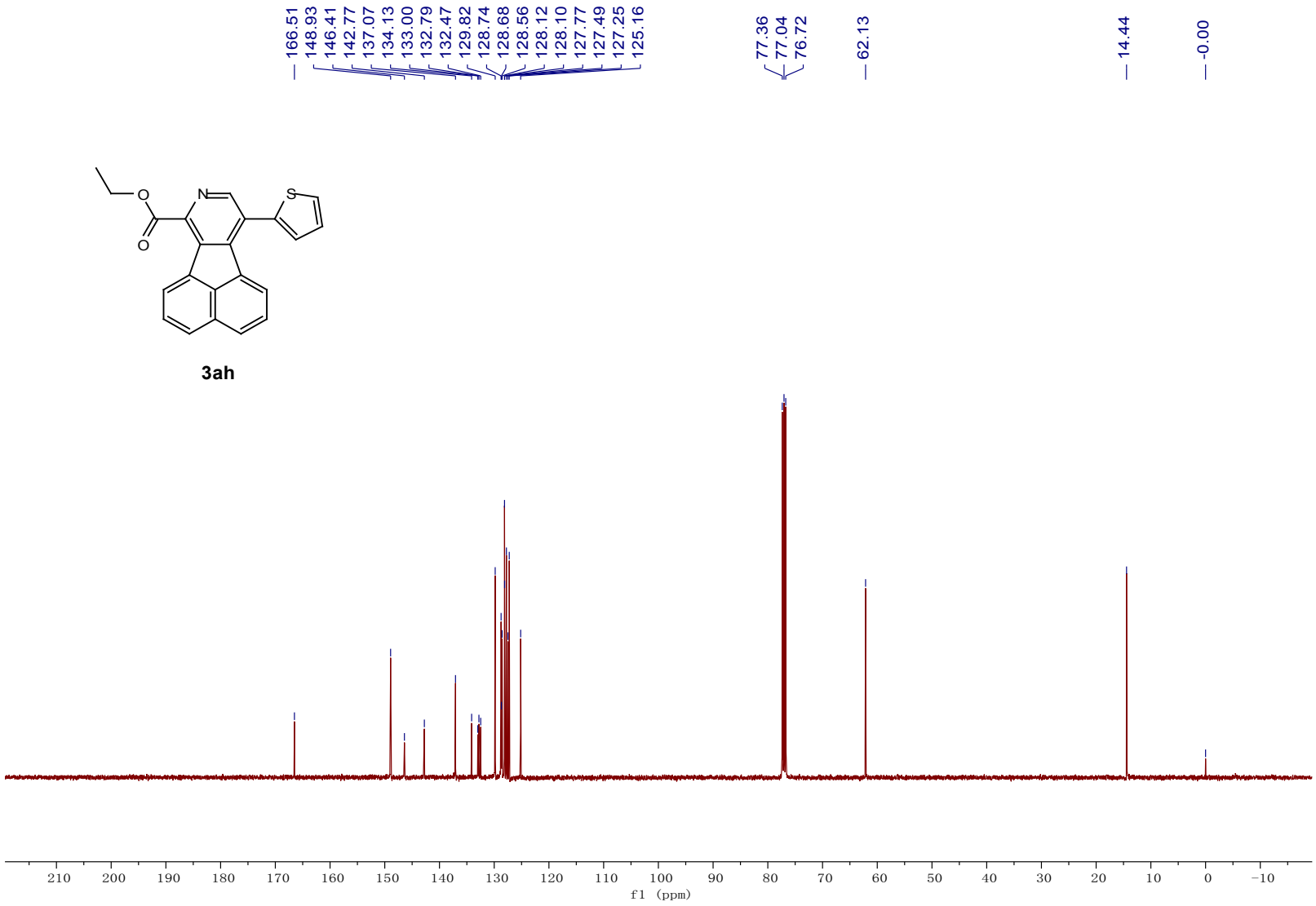
8.859
8.674
7.962
7.943
7.744
7.726
7.706
7.695
7.677
7.583
7.571
7.512
7.494
7.476
7.392
7.385
7.284
7.274
7.260
4.686
4.668
4.650
4.633
1.582
1.564
1.546
O
N
S
O
0.96
0.96
1.96
2.00
0.95
1.02
0.96
0.81
2.00
2.98
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ah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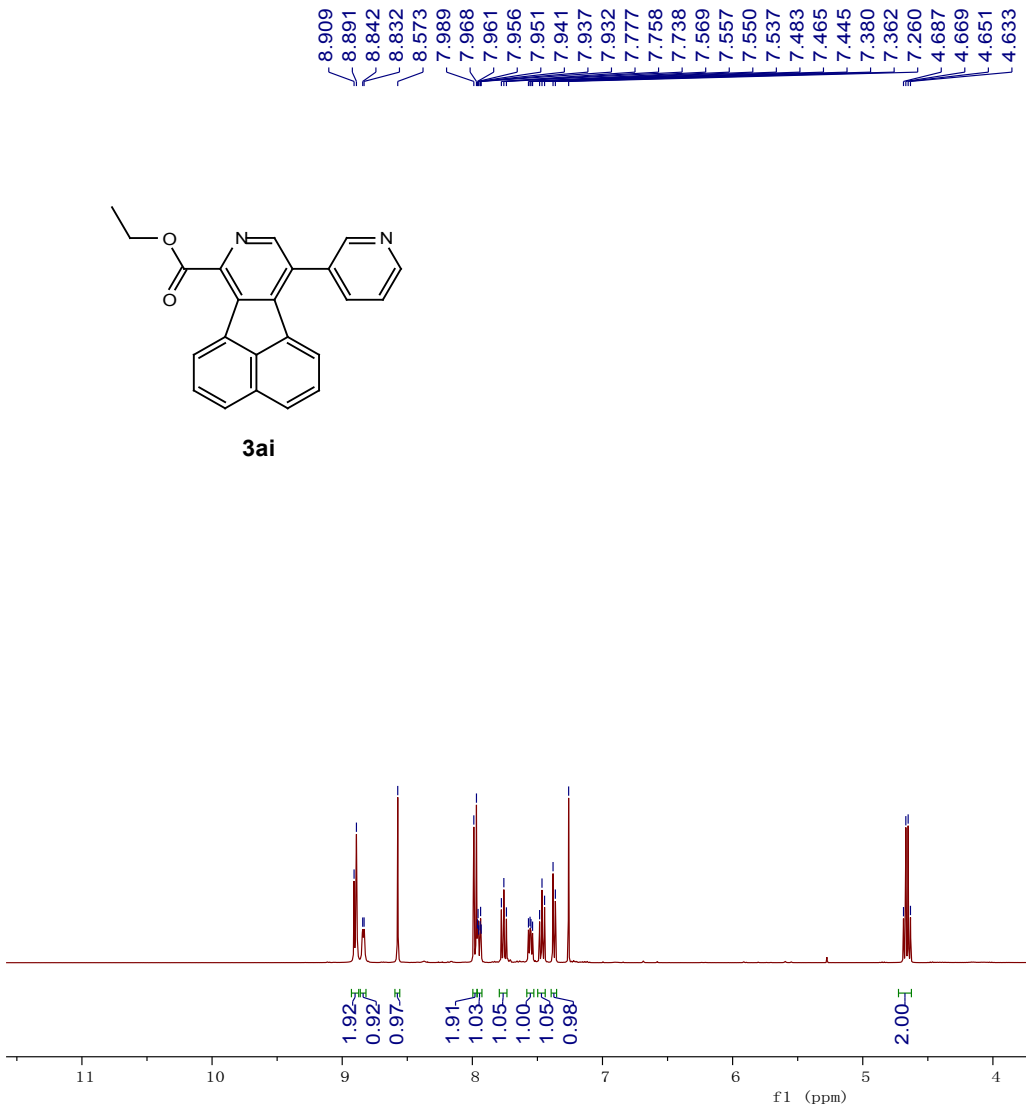
142.77
137.07
134.13
133.00
132.79
132.47
129.82
128.74
128.68
128.56
128.12
128.10
127.77
127.49
127.25
125.16
77.36
77.04
76.72
62.13
14.44
-0.00
O
N
S
O
3ah
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.961
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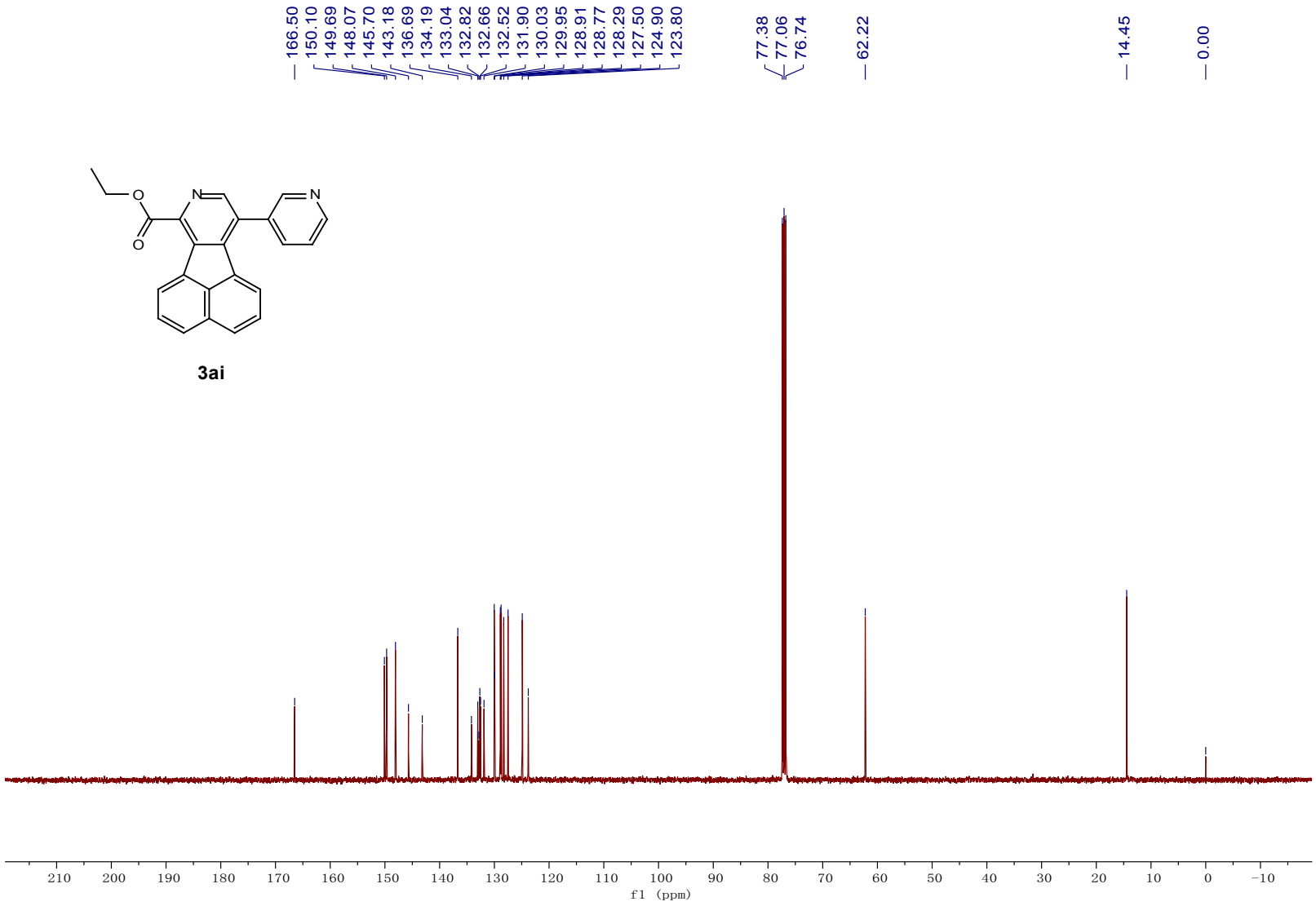
7.951
7.941
7.937
7.932
7.777
7.758
7.738
7.569
7.557
7.550
7.537
7.483
7.465
7.445
7.380
7.362
7.260
4.687
4.669
4.651
4.633
1.578
1.560
1.542
O
N
N
O
1.92
0.92
0.97
1.91
1.03
1.05
1.00
1.05
0.98
2.00
2.98
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ai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145.70
143.18
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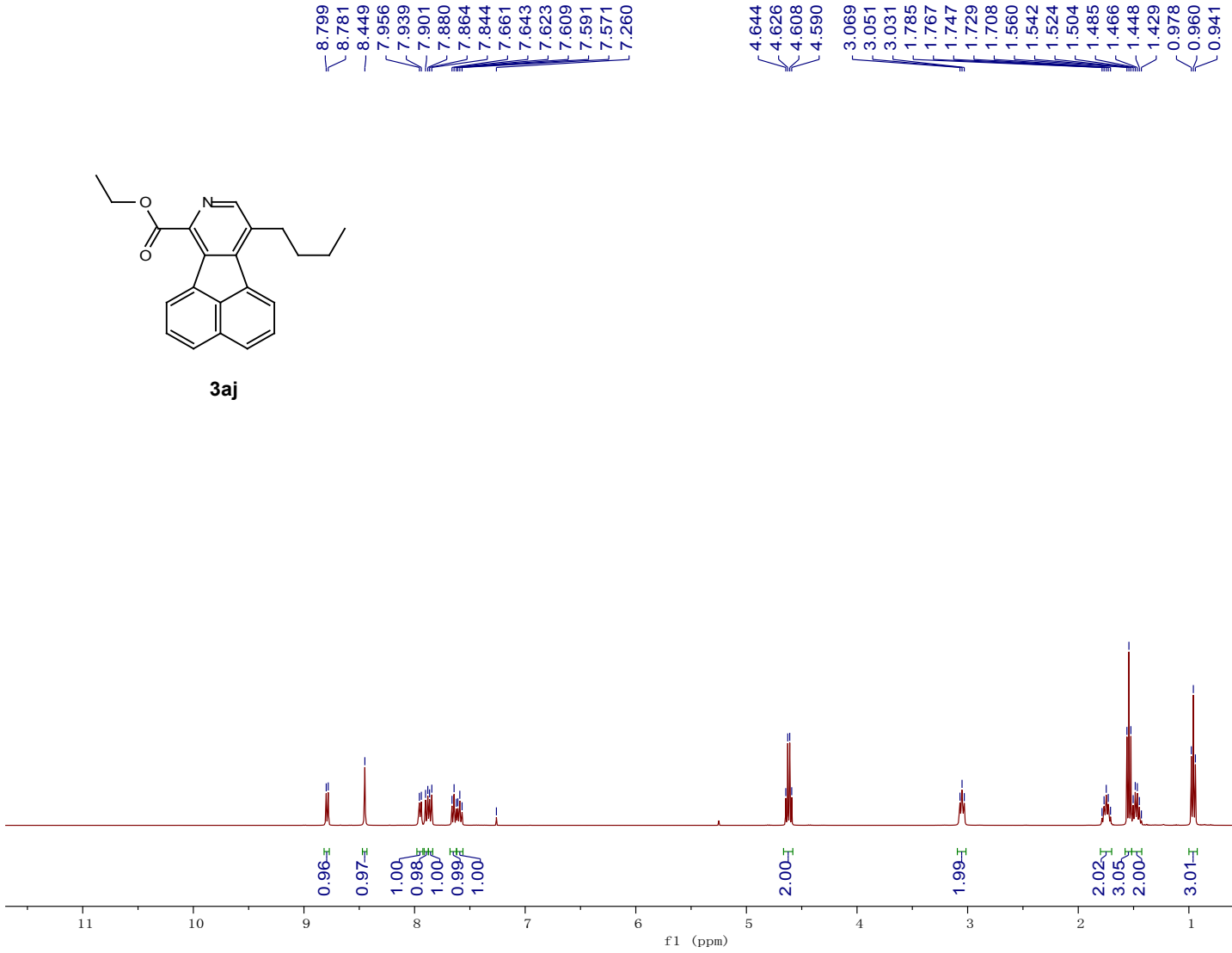
134.19
133.04
132.82
132.66
132.52
131.90
130.03
129.95
128.91
128.77
128.29
127.50
124.90
123.80
77.38
77.06
76.74
62.22
14.45
0.00
O
O
N
N
3ai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.939
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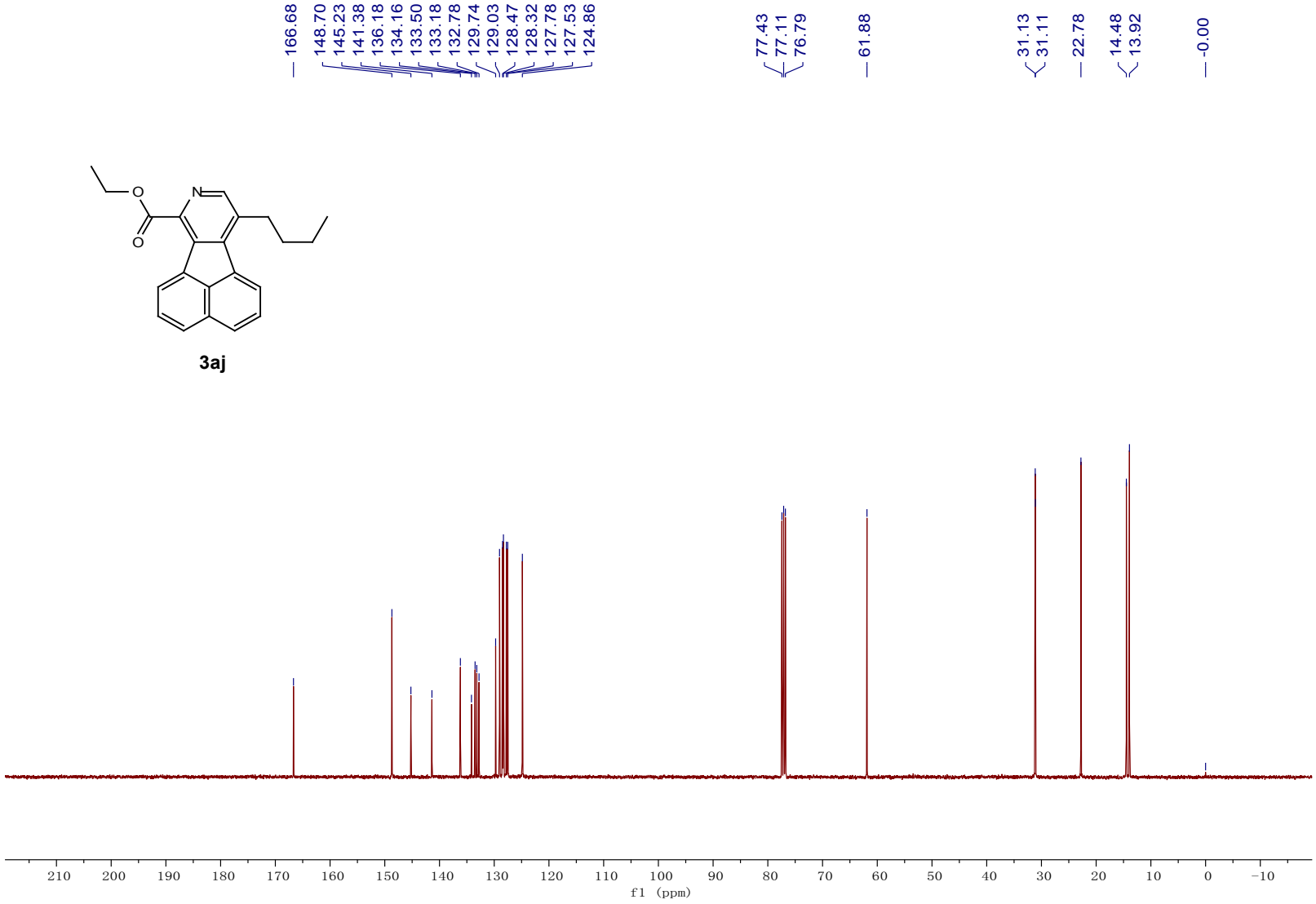
7.880
7.864
7.844
7.661
7.643
7.623
7.609
7.591
7.571
7.260
4.644
4.626
4.608
4.590
3.069
3.051
3.031
1.785
1.767
1.747
1.729
1.708
1.560
1.542
1.524
1.504
1.485
1.466
1.448
1.429
0.978
0.960
0.941
O
N
O
0.96
0.97
1.00
0.98
1.00
0.99
1.00
2.00
1.99
2.02
3.05
2.00
3.01
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3aj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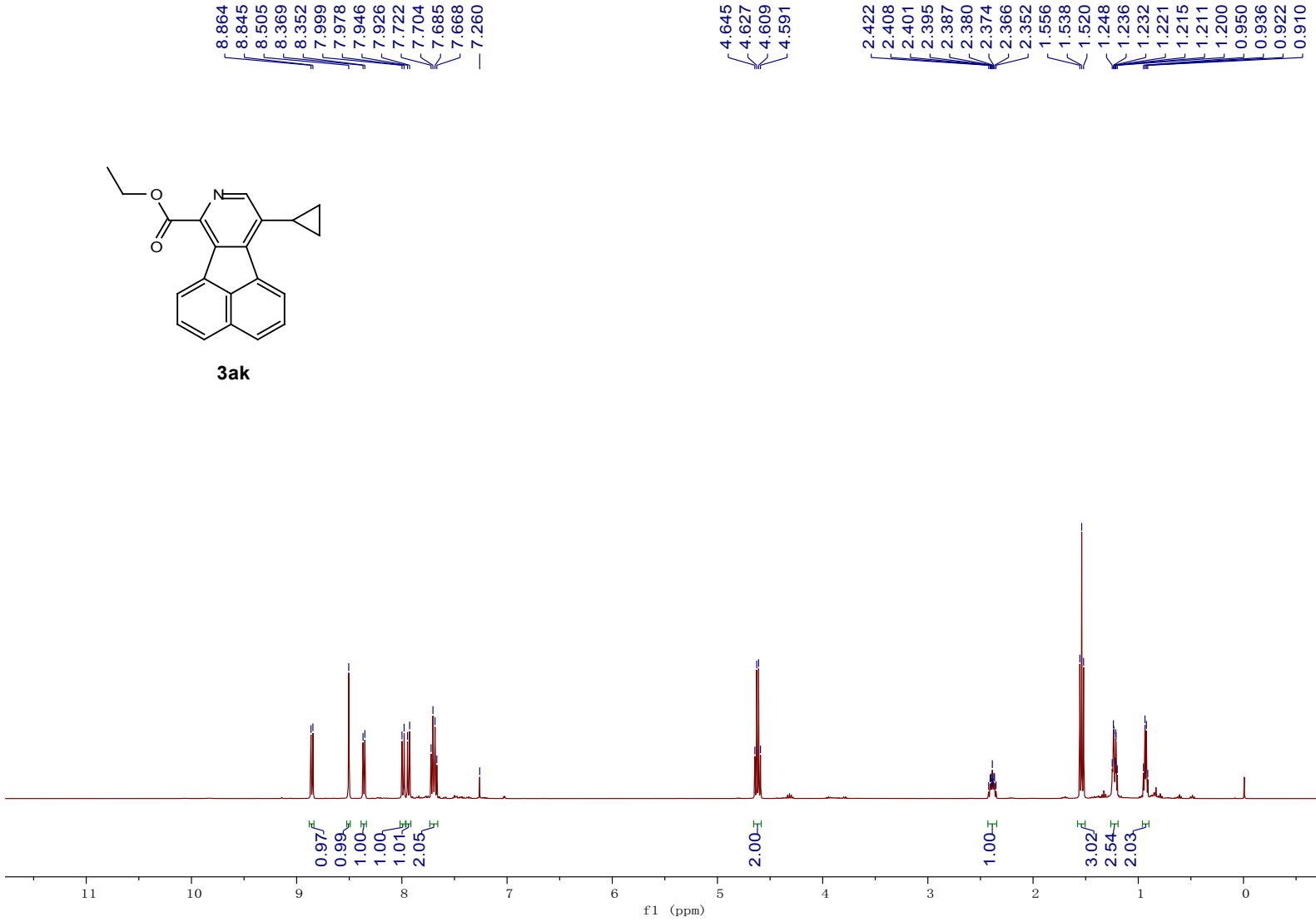
136.18
134.16
133.50
133.18
132.78
129.74
129.03
128.47
128.32
127.78
127.53
124.86
77.43
77.11
76.79
61.88
31.13
31.11
22.78
14.48
13.92
-0.00
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3aj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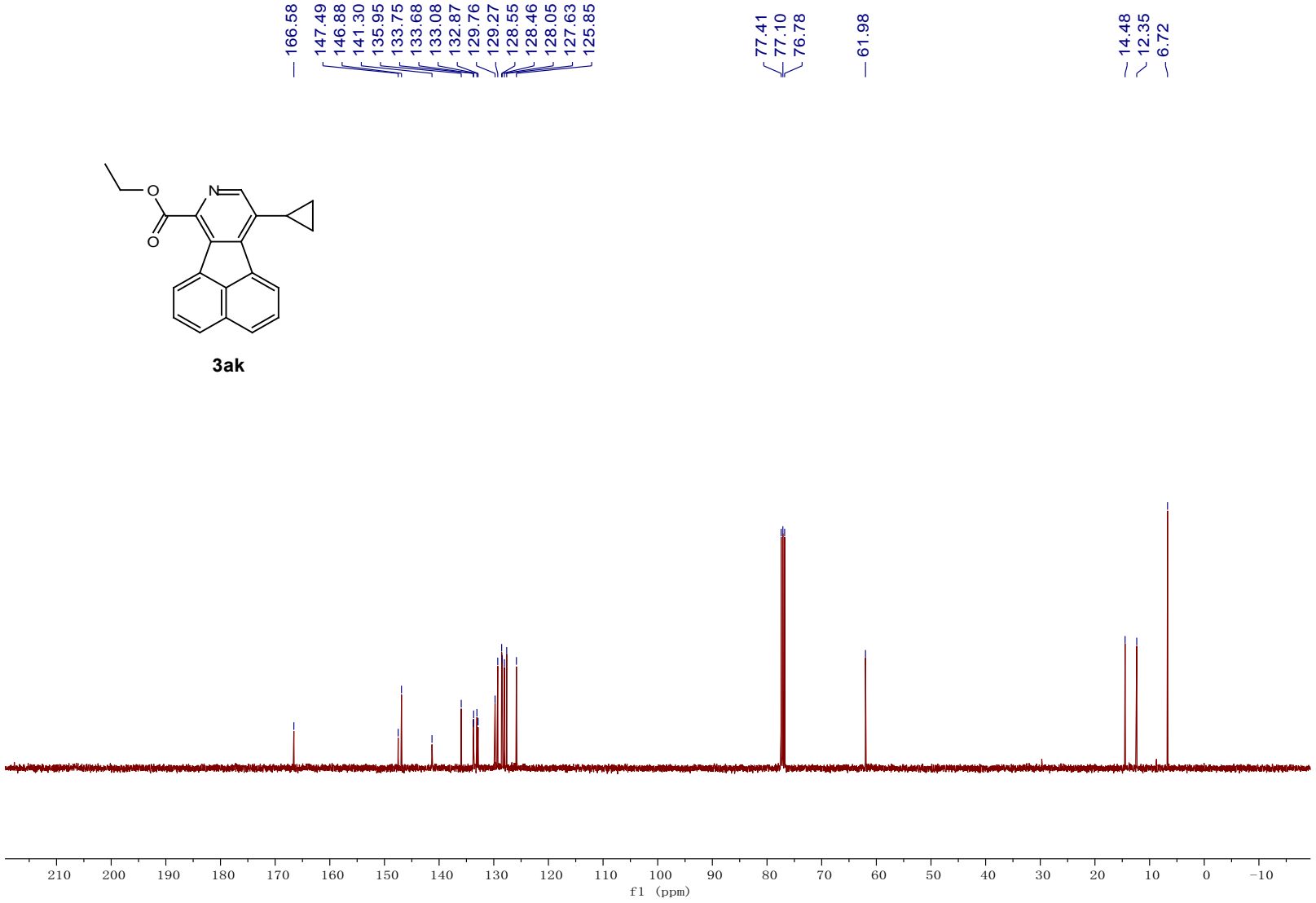
7.946
7.926
7.722
7.704
7.685
7.668
7.260
4.645
4.627
4.609
4.591
2.422
2.408
2.401
2.395
2.387
2.380
2.374
2.366
2.352
1.556
1.538
1.520
1.248
1.236
1.232
1.221
1.215
1.211
1.200
0.950
0.936
0.922
0.910
O
O
N
3ak
0.97
0.99
1.00
1.00
1.01
2.05
2.00
1.00
3.02
2.54
2.03
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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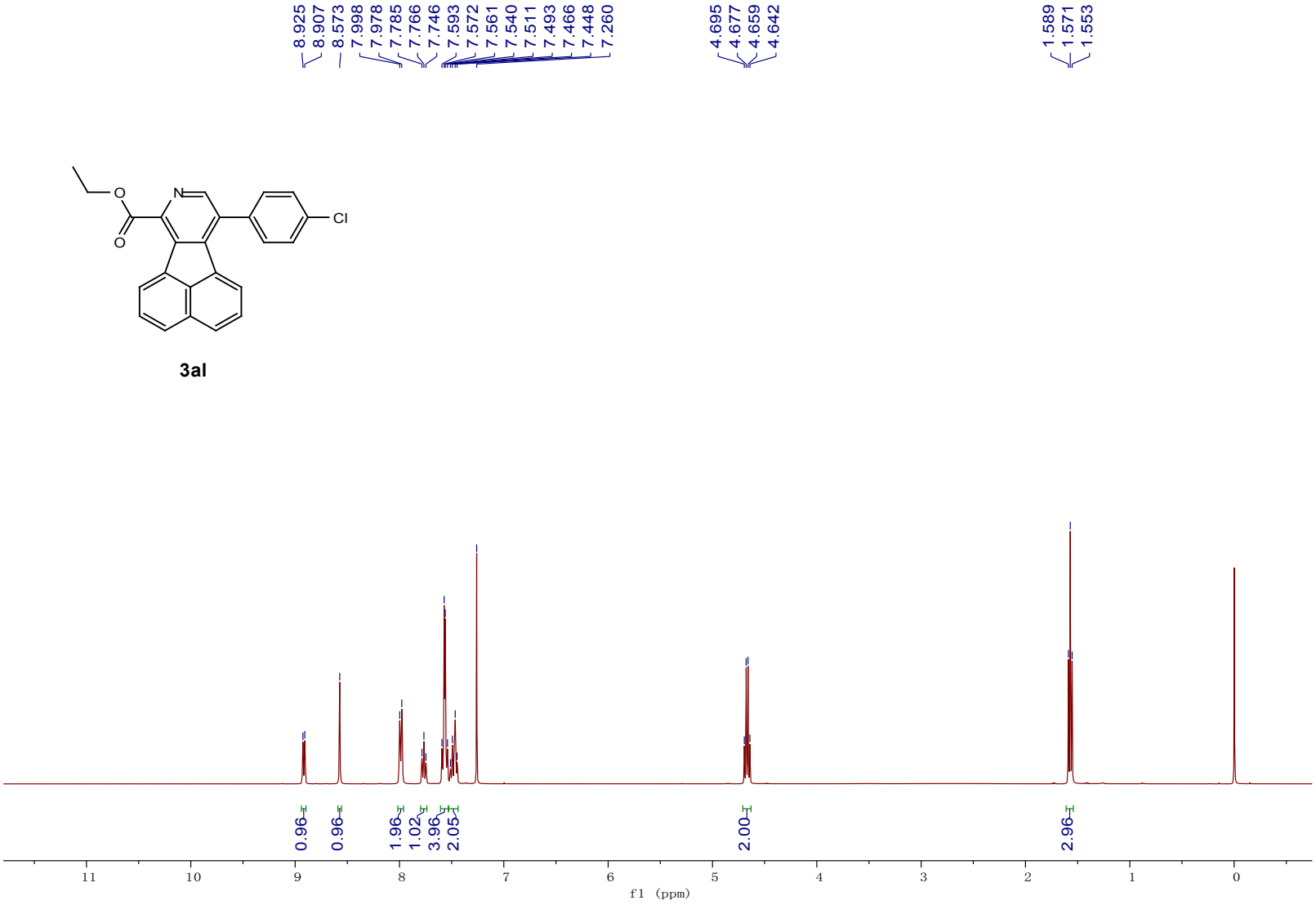
133.68
133.08
132.87
129.76
129.27
128.55
128.46
128.05
127.63
125.85
77.41
77.10
76.78
61.98
14.48
12.35
6.72
O
O
N
3ak
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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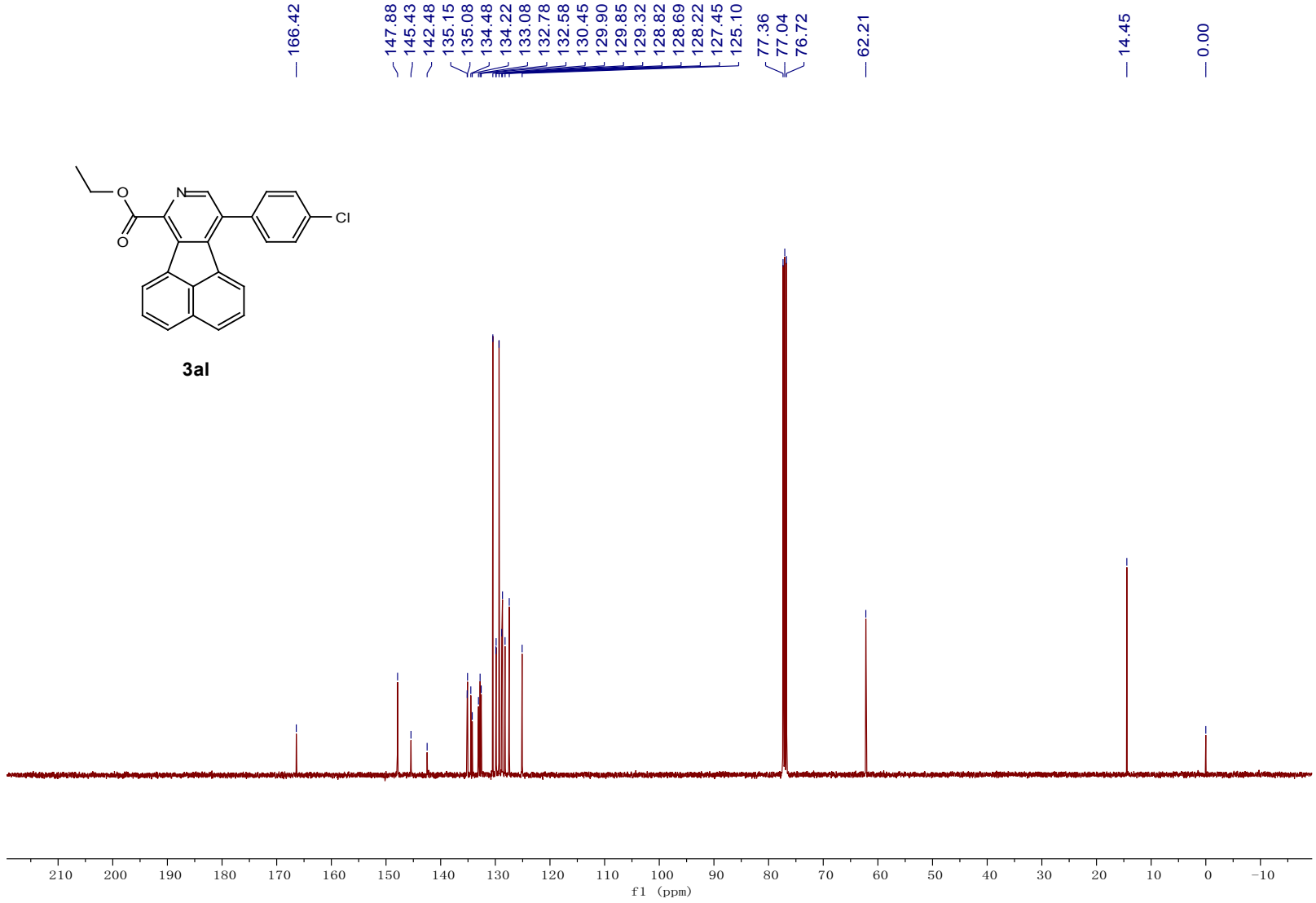
7.746
7.593
7.572
7.561
7.540
7.511
7.493
7.466
7.448
7.260
4.695
4.677
4.659
4.642
1.589
1.571
1.553
O
O
N
Cl
0.96
0.96
1.96
1.02
3.96
2.05
2.00
2.96
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3al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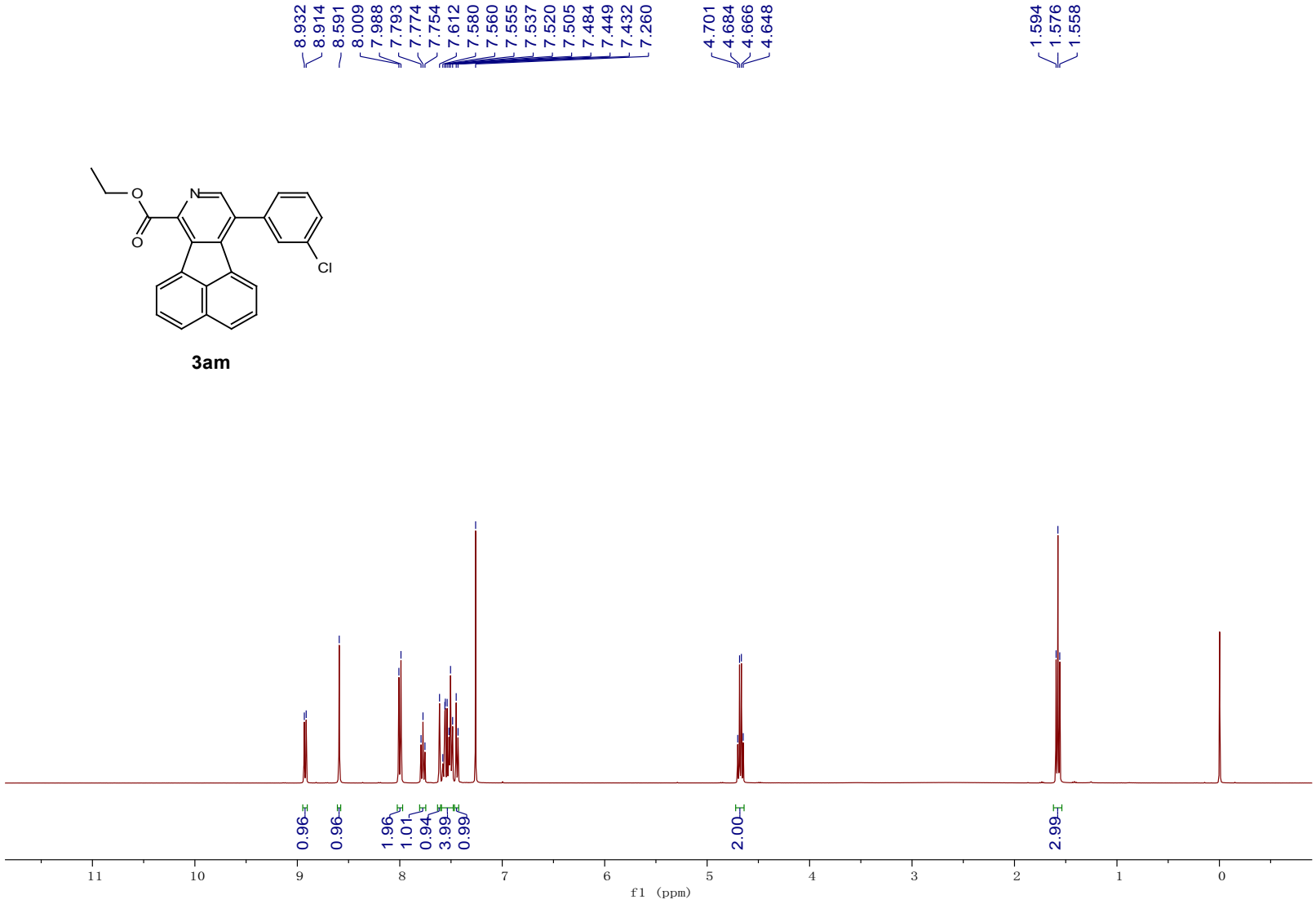
142.48
135.15
135.08
134.48
134.22
133.08
132.78
132.58
130.45
129.90
129.85
129.32
128.82
128.69
128.22
127.45
125.10
77.36
77.04
76.72
62.21
14.45
0.00
O
O
N
Cl
3al
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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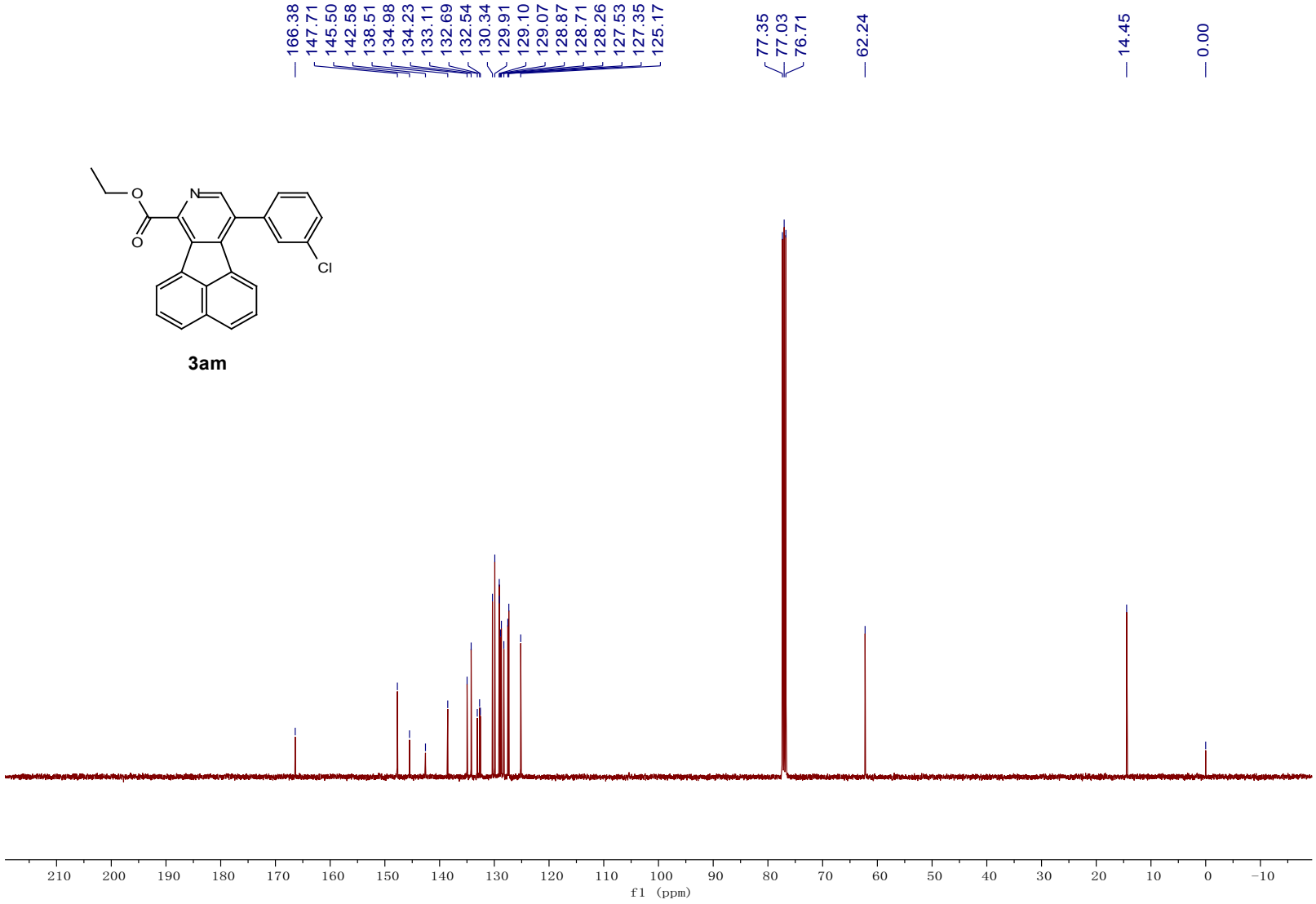
7.754
7.612
7.580
7.560
7.555
7.537
7.520
7.505
7.484
7.449
7.432
7.260
4.701
4.684
4.666
4.648
1.594
1.576
1.558
O
O
N
Cl
0.96
0.96
1.96
1.01
0.94
3.99
0.99
2.00
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3am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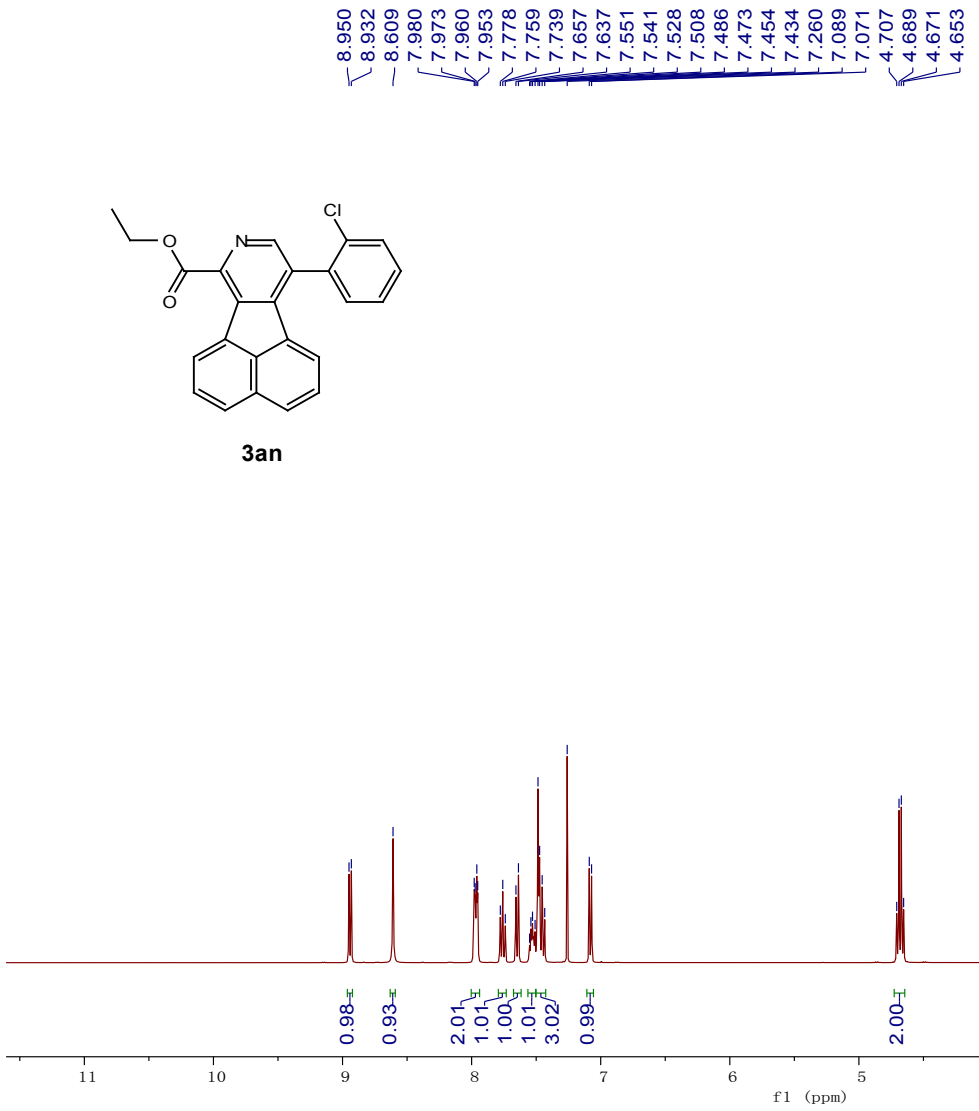
134.23
133.11
132.69
132.54
130.34
129.91
129.10
129.07
128.87
128.71
128.26
127.53
127.35
125.17
77.35
77.03
76.71
62.24
14.45
0.00
O
O
N
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3am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7.960
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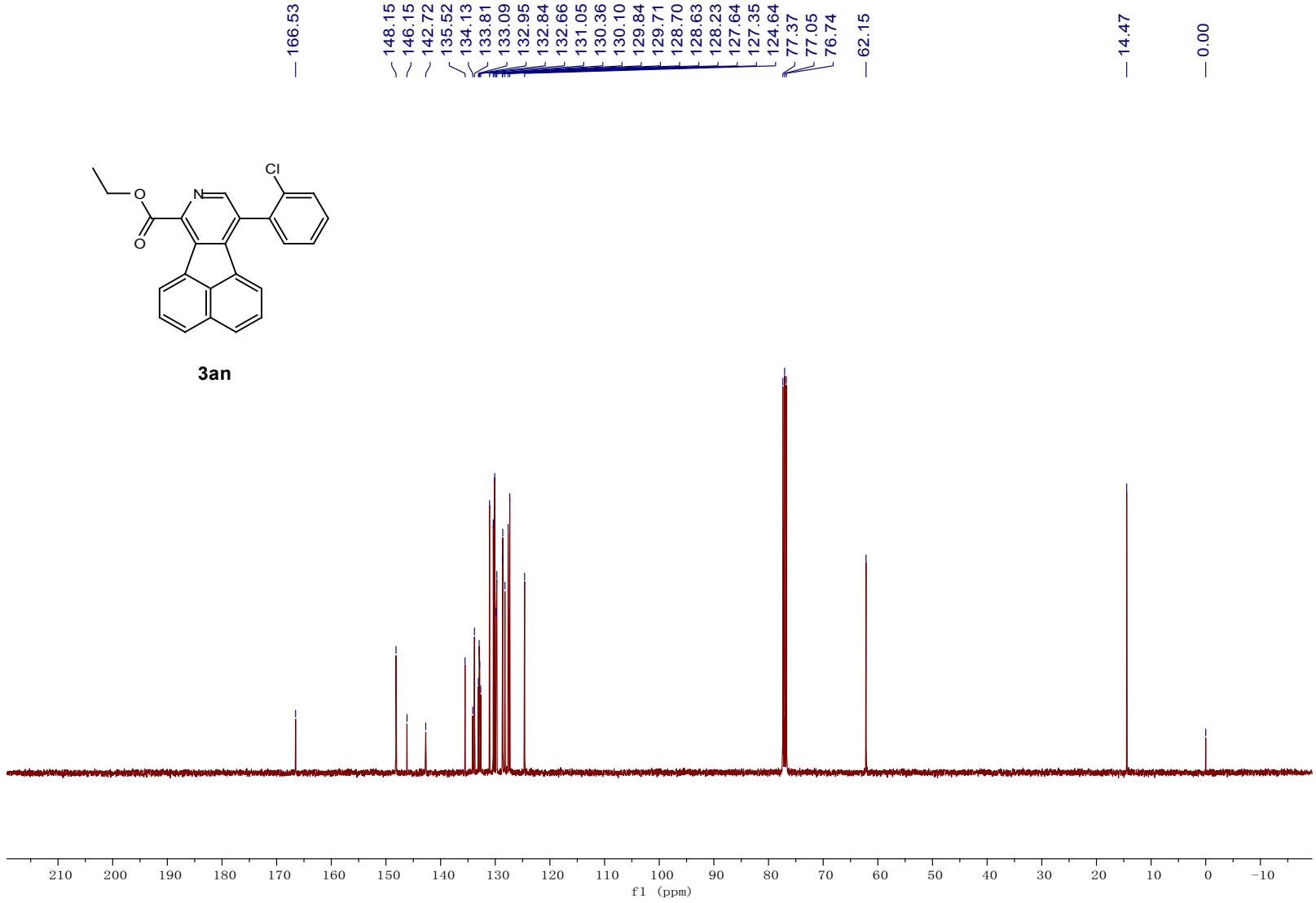
7.778
7.759
7.739
7.657
7.637
7.551
7.541
7.528
7.508
7.486
7.473
7.454
7.434
7.260
7.089
7.071
4.707
4.689
4.671
4.653
1.598
1.580
1.562
Cl
O
N
O
0.98
0.93
2.01
1.01
1.00
1.01
3.02
0.99
2.00
3.02
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3an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148.15
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142.72
135.52
134.13
133.81
133.09
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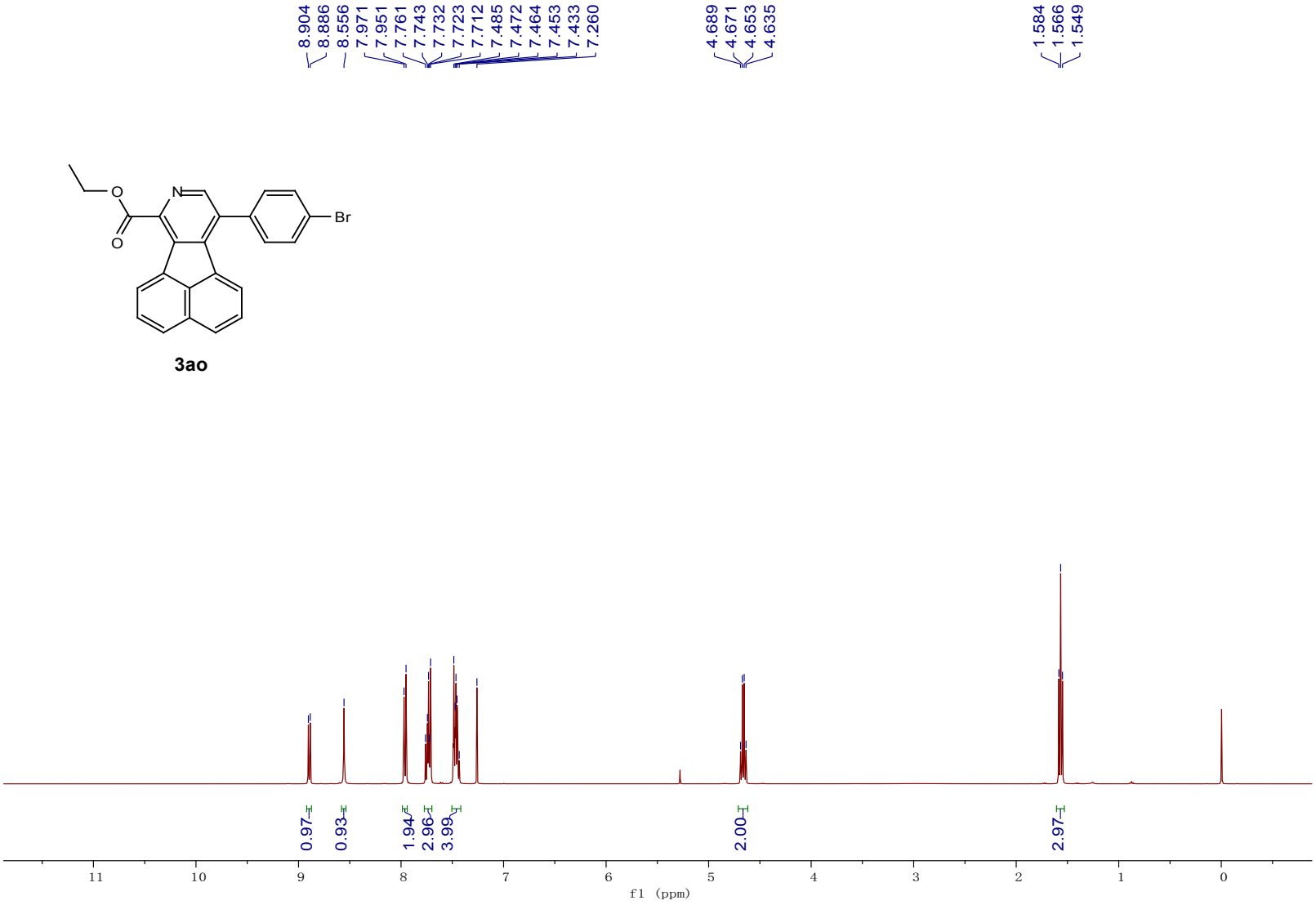
132.84
132.66
131.05
130.36
130.10
129.84
129.71
128.70
128.63
128.23
127.64
127.35
124.64
77.37
77.05
76.74
62.15
14.47
0.00
Cl
N
O
O
3an
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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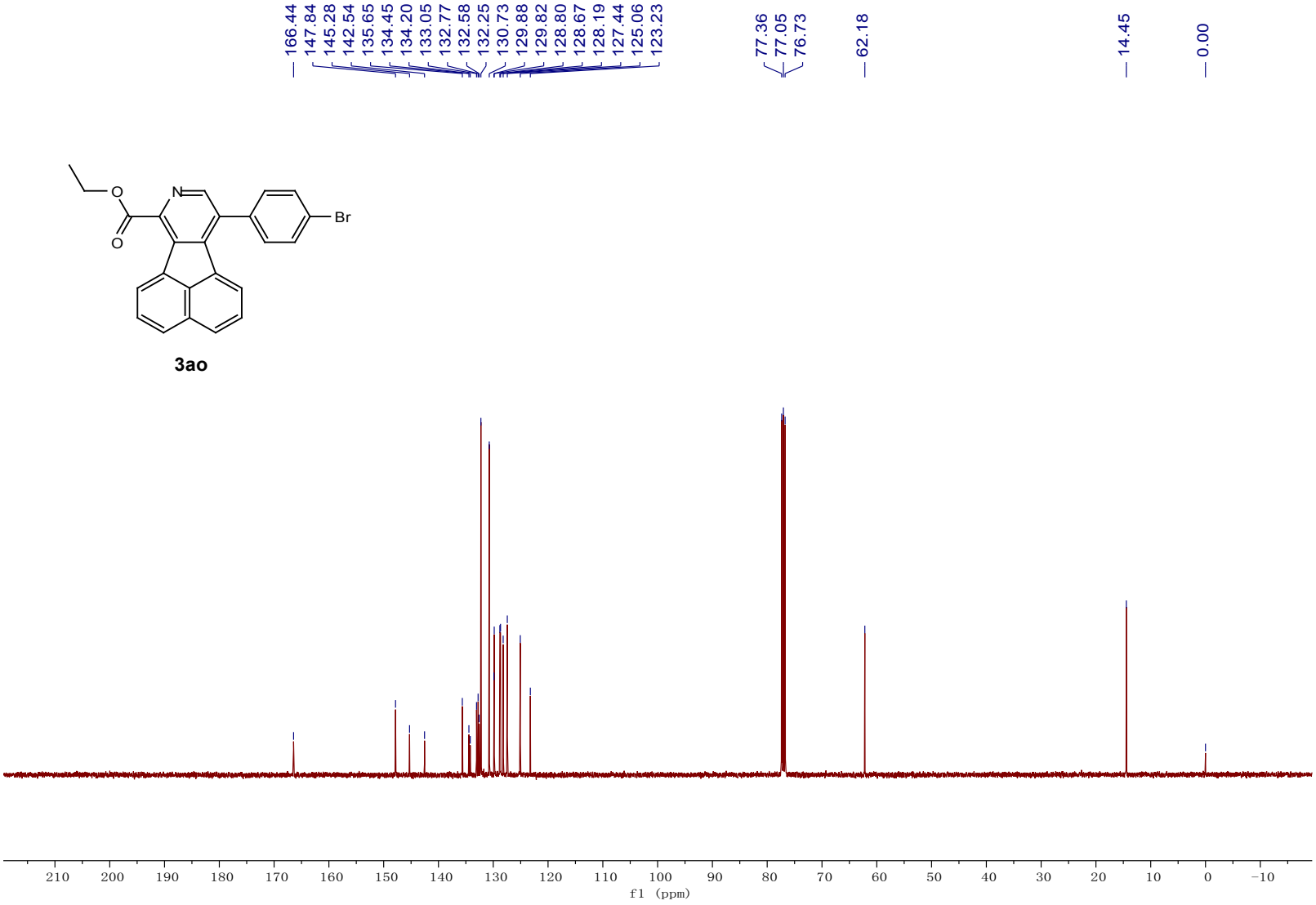
7.732
7.723
7.712
7.485
7.472
7.464
7.453
7.433
7.260
4.689
4.671
4.653
4.635
1.584
1.566
1.549
O
N
O
Br
0.97
0.93
1.94
2.96
3.99
2.00
2.97
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ao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134.45
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133.05
132.77
132.58
132.25
130.73
129.88
129.82
128.80
128.67
128.19
127.44
125.06
123.23
77.36
77.05
76.73
62.18
14.45
0.00
O
O
N
Br
3ao
210
200
190
180
170
160
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120
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100
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80
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60
50
40
30
20
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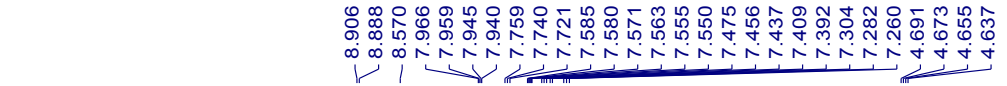
0
−10
f1 (ppm)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8.570
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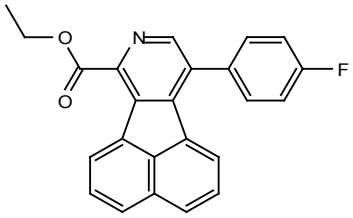
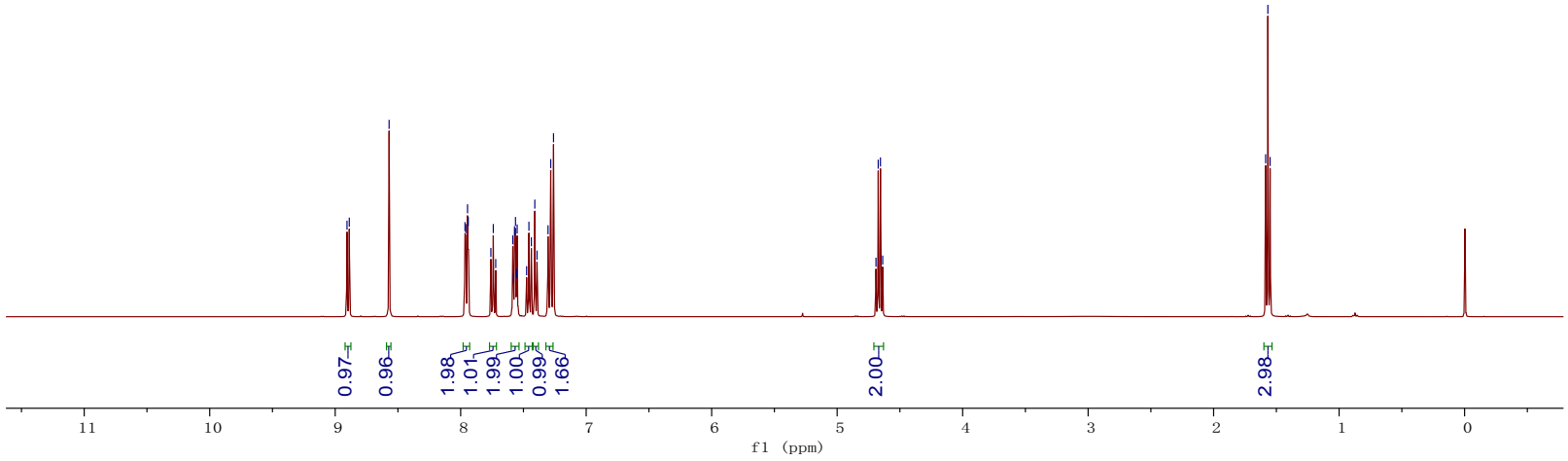
7.945
7.940
7.759
7.740
7.721
7.585
7.580
7.571
7.563
7.555
7.550
7.475
7.456
7.437
7.409
7.392
7.304
7.282
7.260
4.691
4.673
4.655
4.637
1.586
1.568
1.550


O
N
O
F

3ap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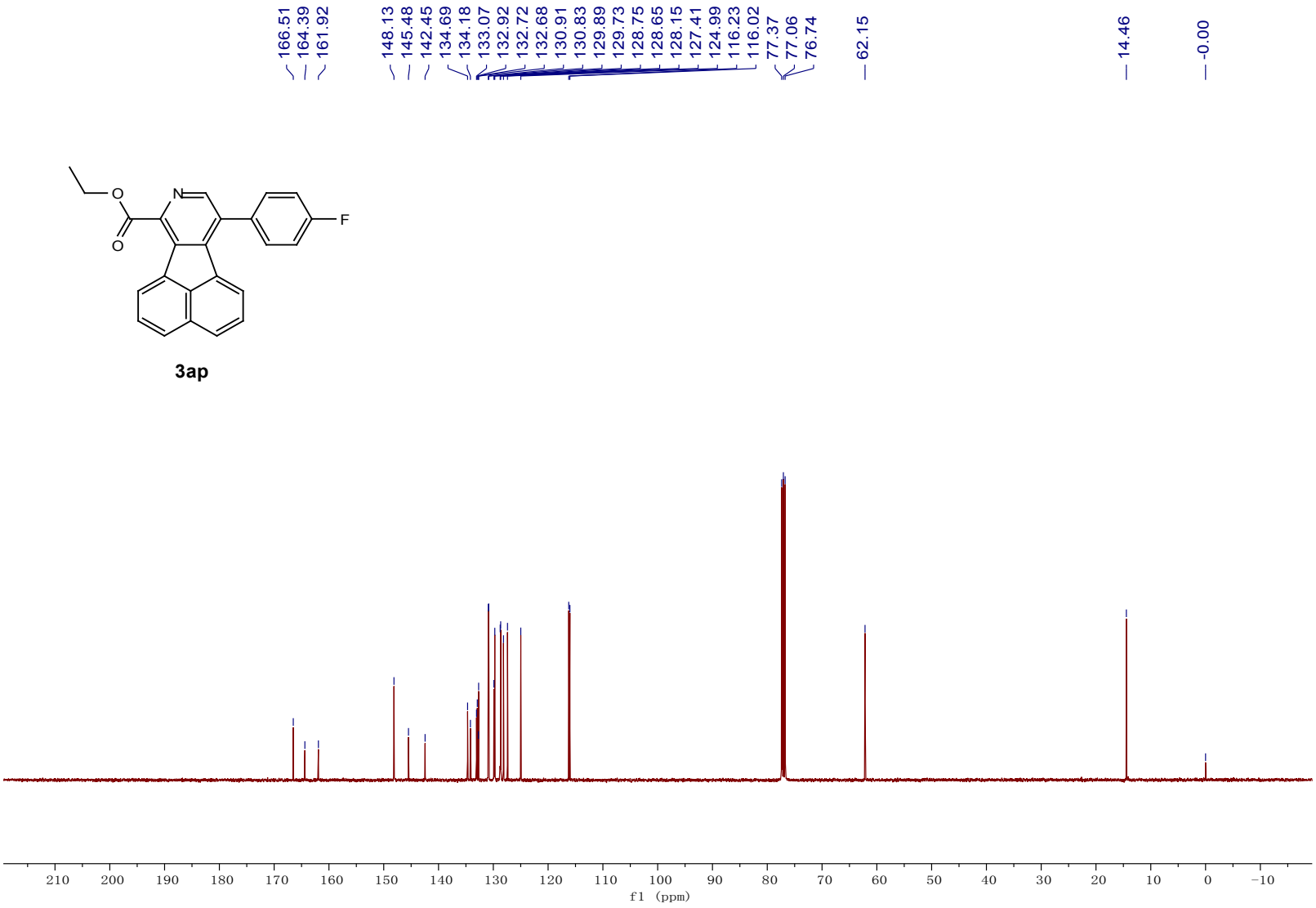
0.96
1.98
1.01
1.99
1.00
0.99
1.66
2.00
2.98
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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164.39
161.92
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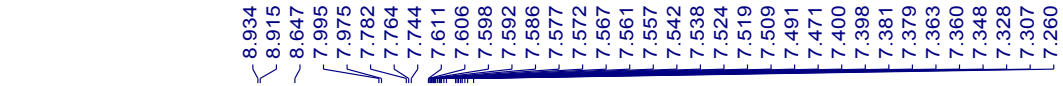
145.48
142.45
134.69
134.18
133.07
132.92
132.72
132.68
130.91
130.83
129.89
129.73
128.75
128.65
128.15
127.41
124.99
116.23
116.02
77.37
77.06
76.74
62.15
14.46
-0.00
O
O
N
F
3ap
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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8.915
8.647
7.995
7.975
7.782
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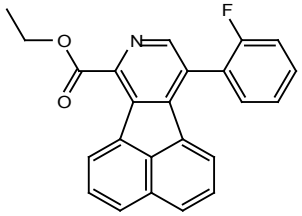
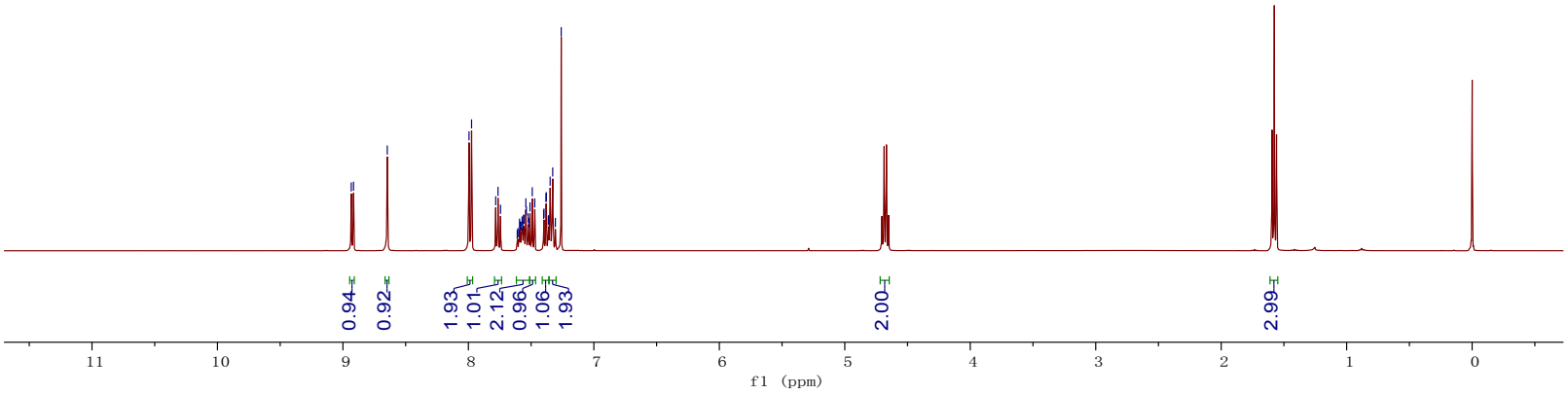
7.744
7.611
7.606
7.598
7.592
7.586
7.577
7.572
7.567
7.561
7.557
7.542
7.538
7.524
7.519
7.509
7.491
7.471
7.400
7.398
7.381
7.379
7.363
7.360
7.348
7.328
7.307
7.260


F
O
N
O

3aq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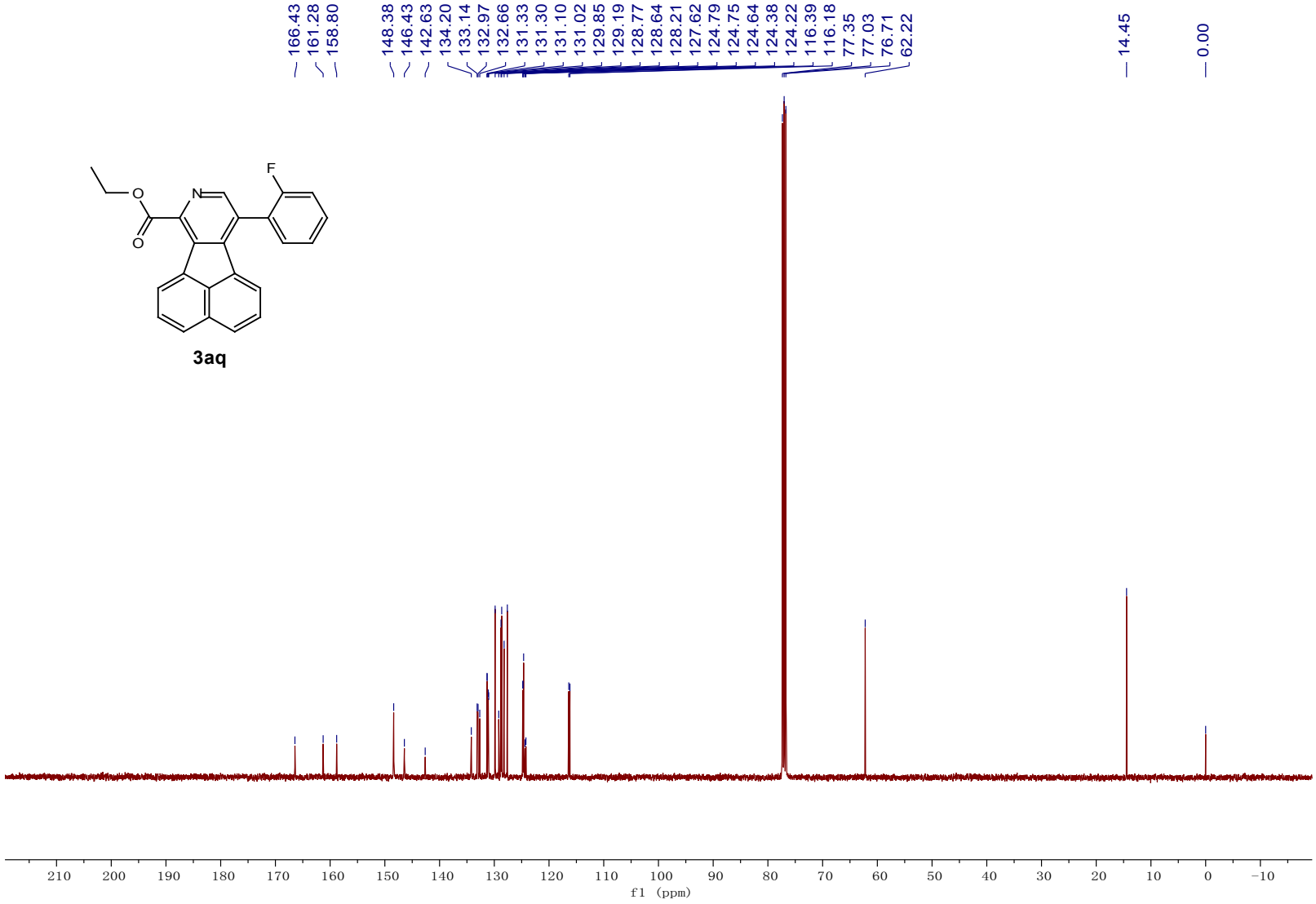
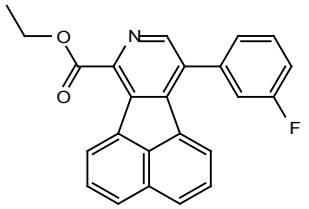
0.92
1.93
1.01
2.12
0.96
1.06
1.93
2.00
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

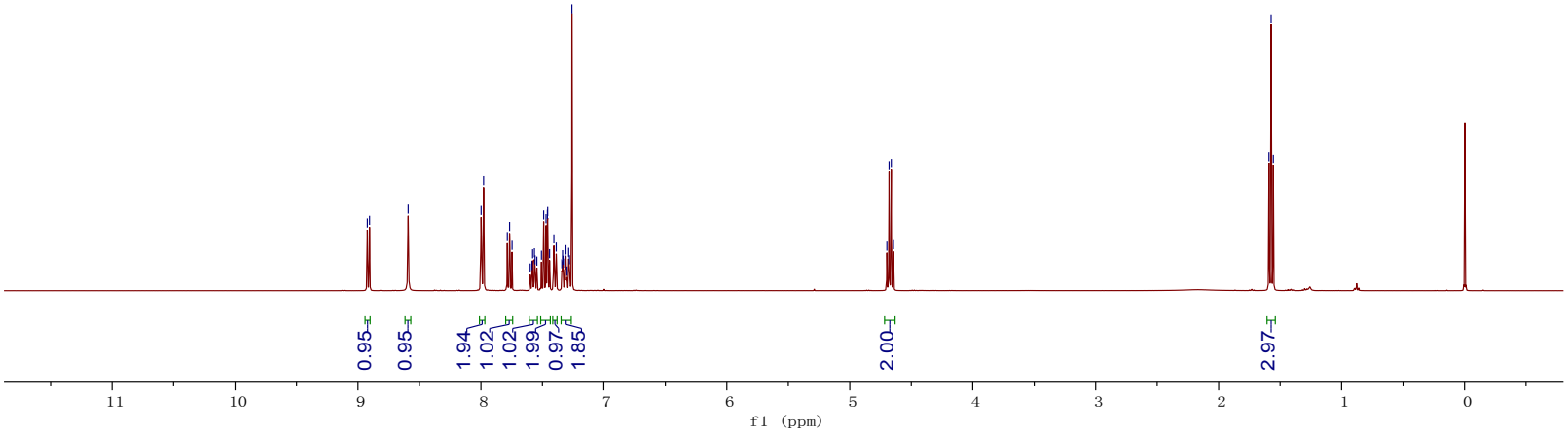

166.43
161.28
158.80
148.38
146.43
142.63
134.20
133.14
132.97
132.66
131.33
131.30
131.10
131.02
129.85
129.19
128.77
128.64
128.21
127.62
124.79
124.75
124.64
124.38
124.22
116.39
116.18
77.35
77.03
76.71
62.22
14.45
0.00
O
O
N
F
f1 (ppm)

3aq


8.924
8.906
8.592
7.999
7.978
7.785
7.767
7.747
7.599
7.585
7.580
7.565
7.560
7.545
7.508
7.490
7.471
7.460
7.457
7.442
7.407
7.388
7.342
7.336
7.332
7.319
7.313
7.309
7.299
7.286
7.280
7.260
4.698
4.680
4.663
4.645
1.591
1.573
1.555


O
N
O
F

3ar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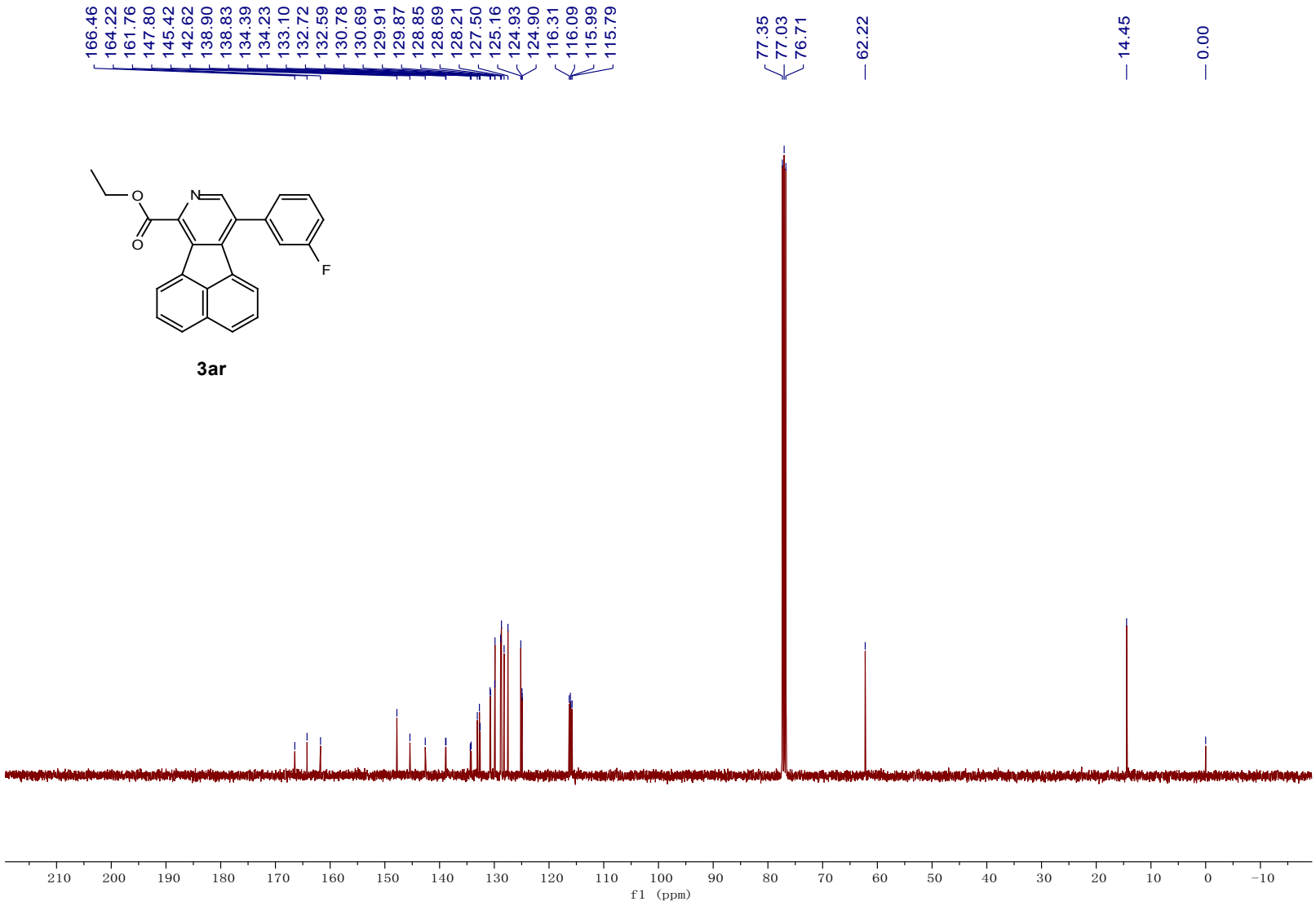
0.95
1.94
1.02
1.02
1.99
0.97
1.85
2.00
2.97
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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164.22
161.76
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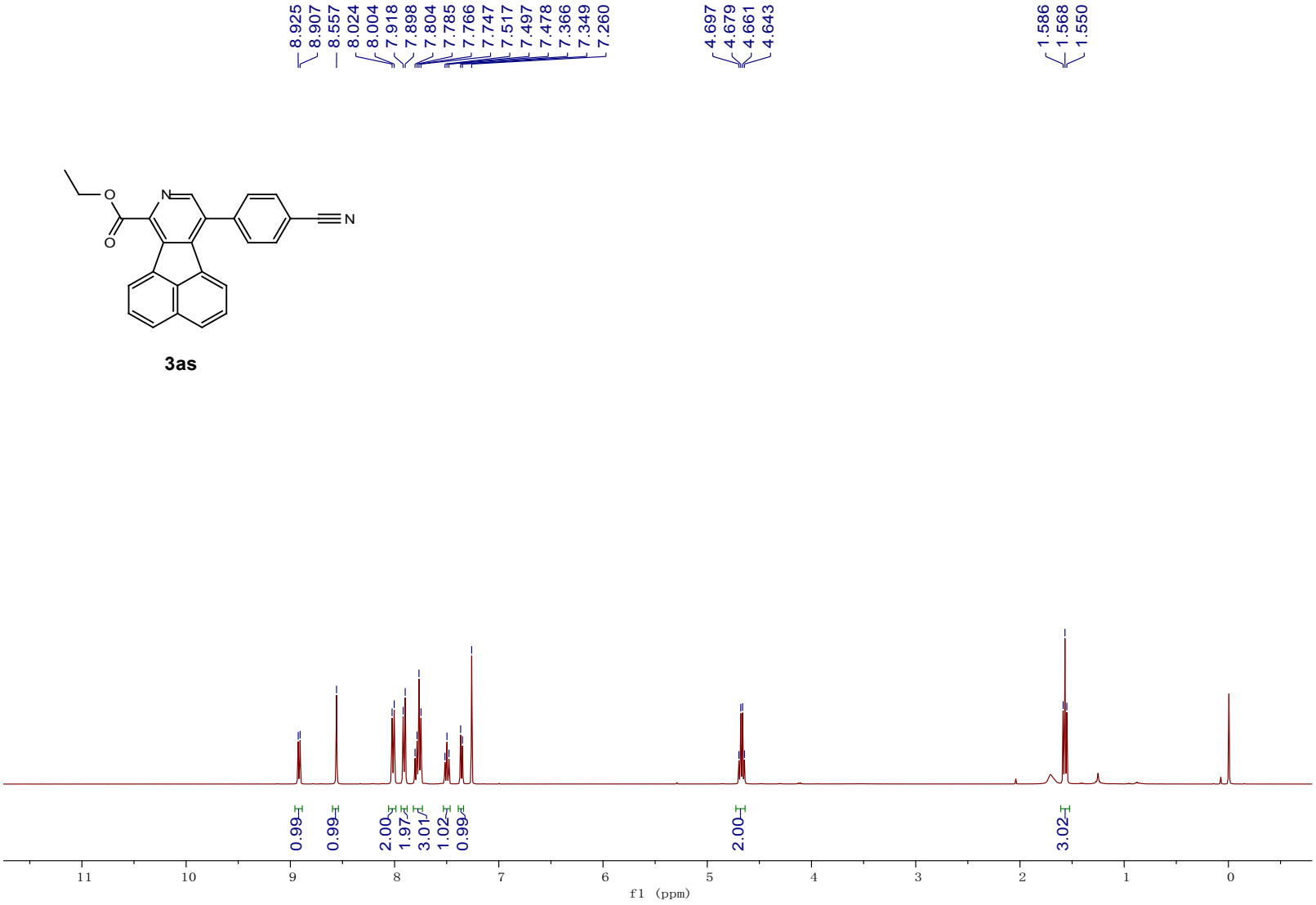
145.42
142.62
138.90
138.83
134.39
134.23
133.10
132.72
132.59
130.78
130.69
129.91
129.87
128.85
128.69
128.21
127.50
125.16
124.93
124.90
116.31
116.09
115.99
115.79
77.35
77.03
76.71
62.22
14.45
0.00
O
O
N
F
3ar
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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8.907
8.557
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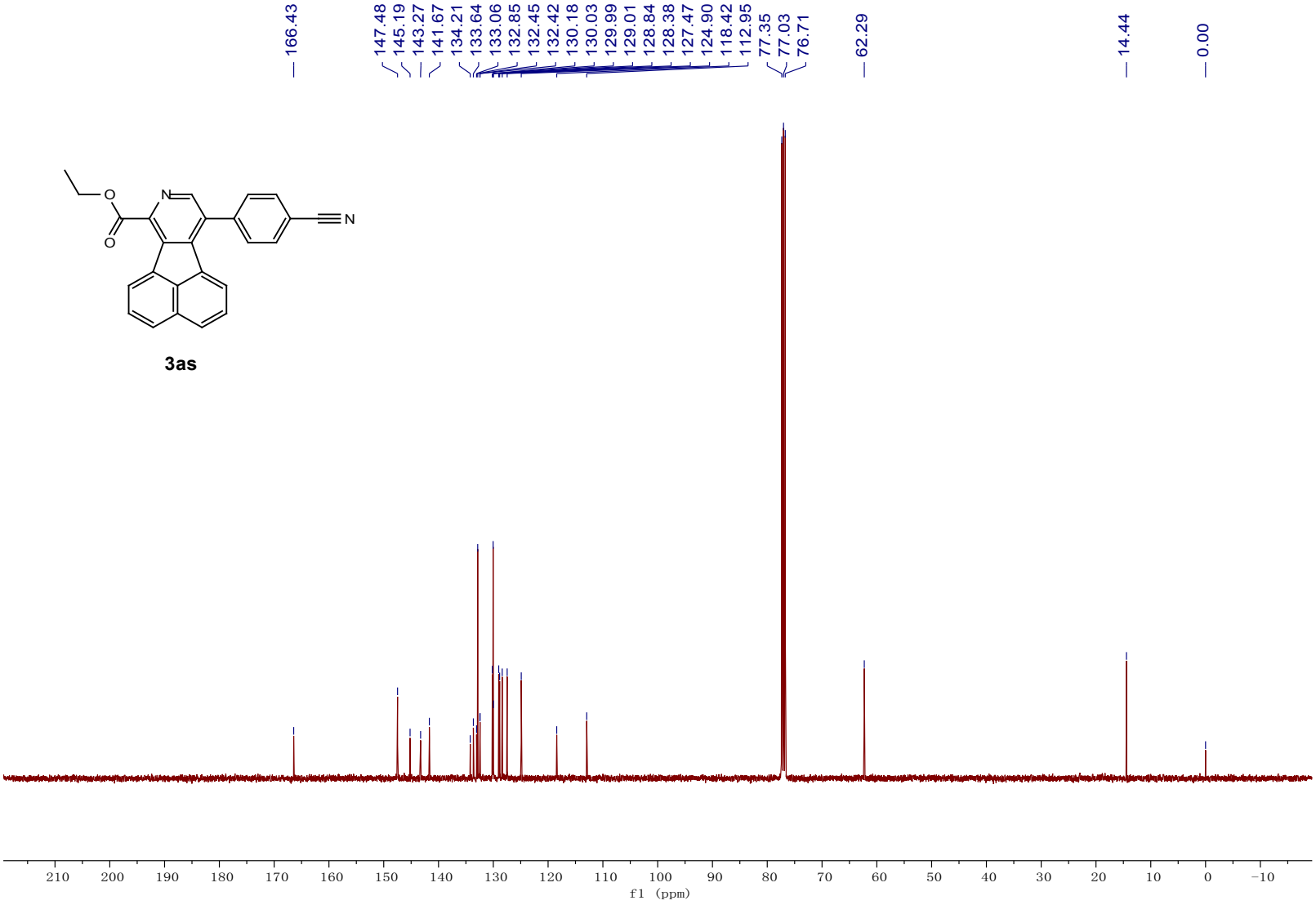
8.004
7.918
7.898
7.804
7.785
7.766
7.747
7.517
7.497
7.478
7.366
7.349
7.260
4.697
4.679
4.661
4.643
1.586
1.568
1.550
O
O
N
N
0.99
0.99
2.00
1.97
3.01
1.02
0.99
2.00
3.02
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3as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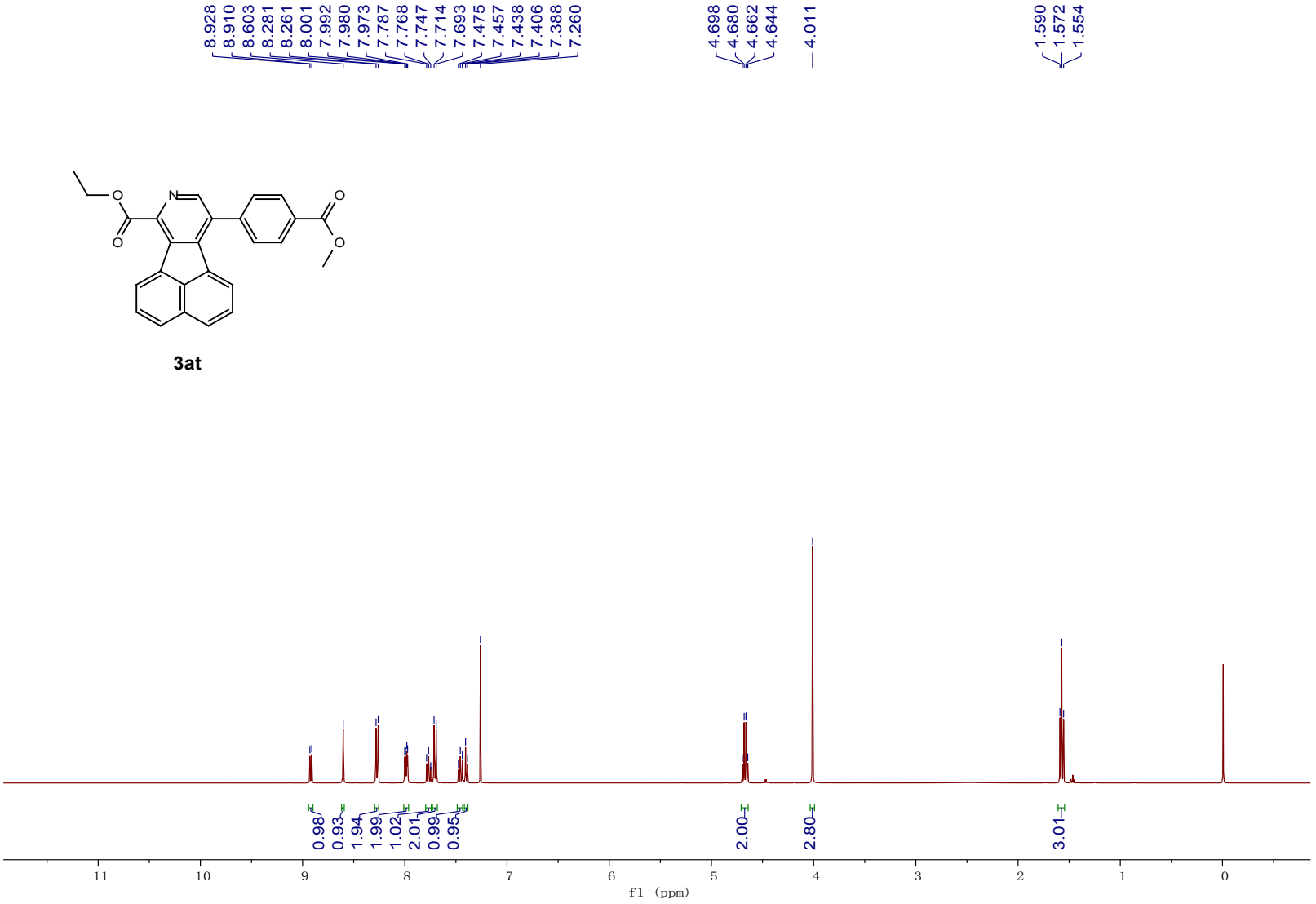
147.48
145.19
143.27
141.67
134.21
133.64
133.06
132.85
132.45
132.42
130.18
130.03
129.99
129.01
128.84
128.38
127.47
124.90
118.42
112.95
77.35
77.03
76.71
62.29
14.44
0.00
O
O
N
N
3as
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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8.261
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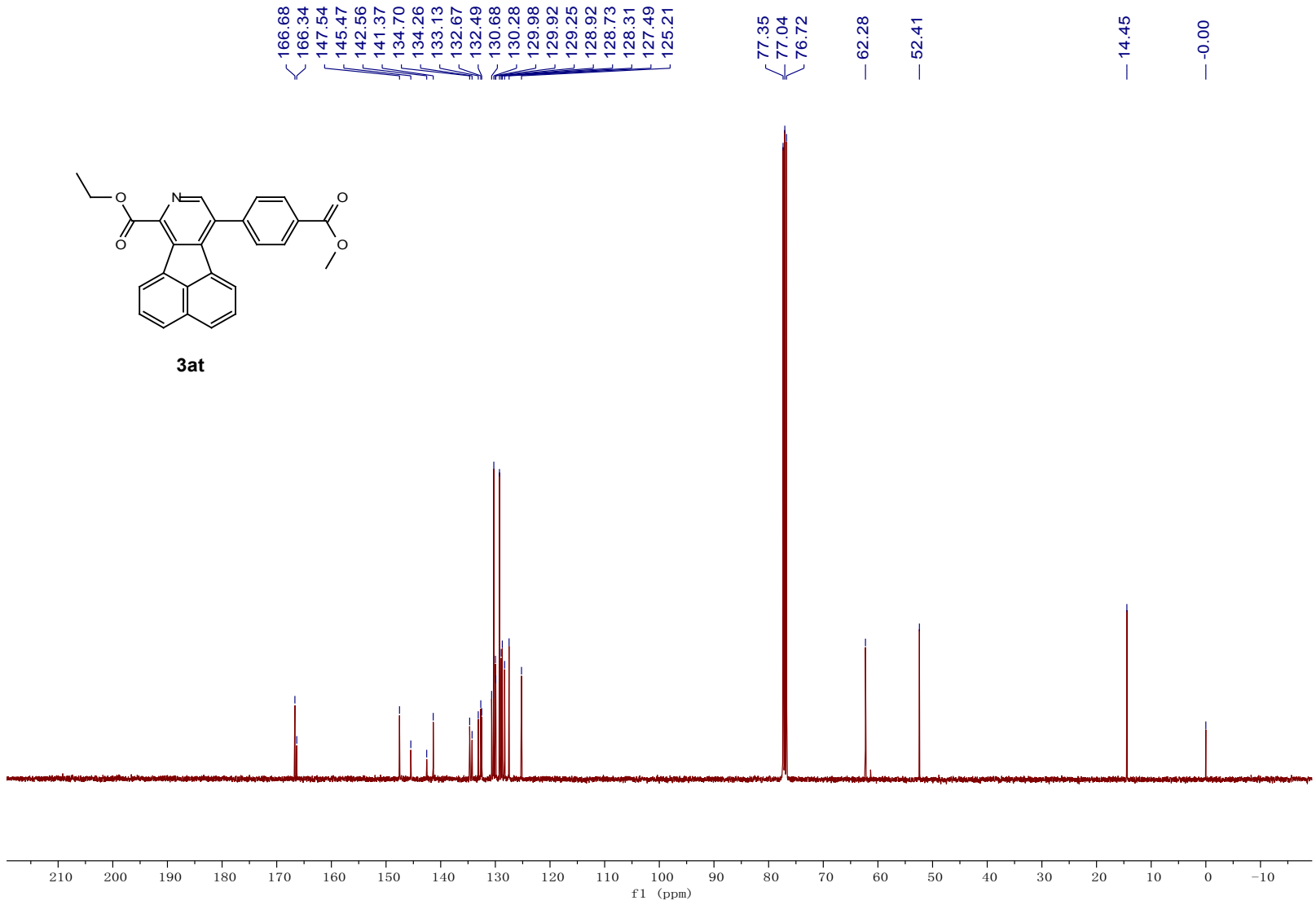
7.980
7.973
7.787
7.768
7.747
7.714
7.693
7.475
7.457
7.438
7.406
7.388
7.260
4.698
4.680
4.662
4.644
4.011
1.590
1.572
1.554
O
N
O
O
O
0.98
0.93
1.94
1.99
1.02
2.01
0.99
0.95
2.00
2.80
3.01
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3at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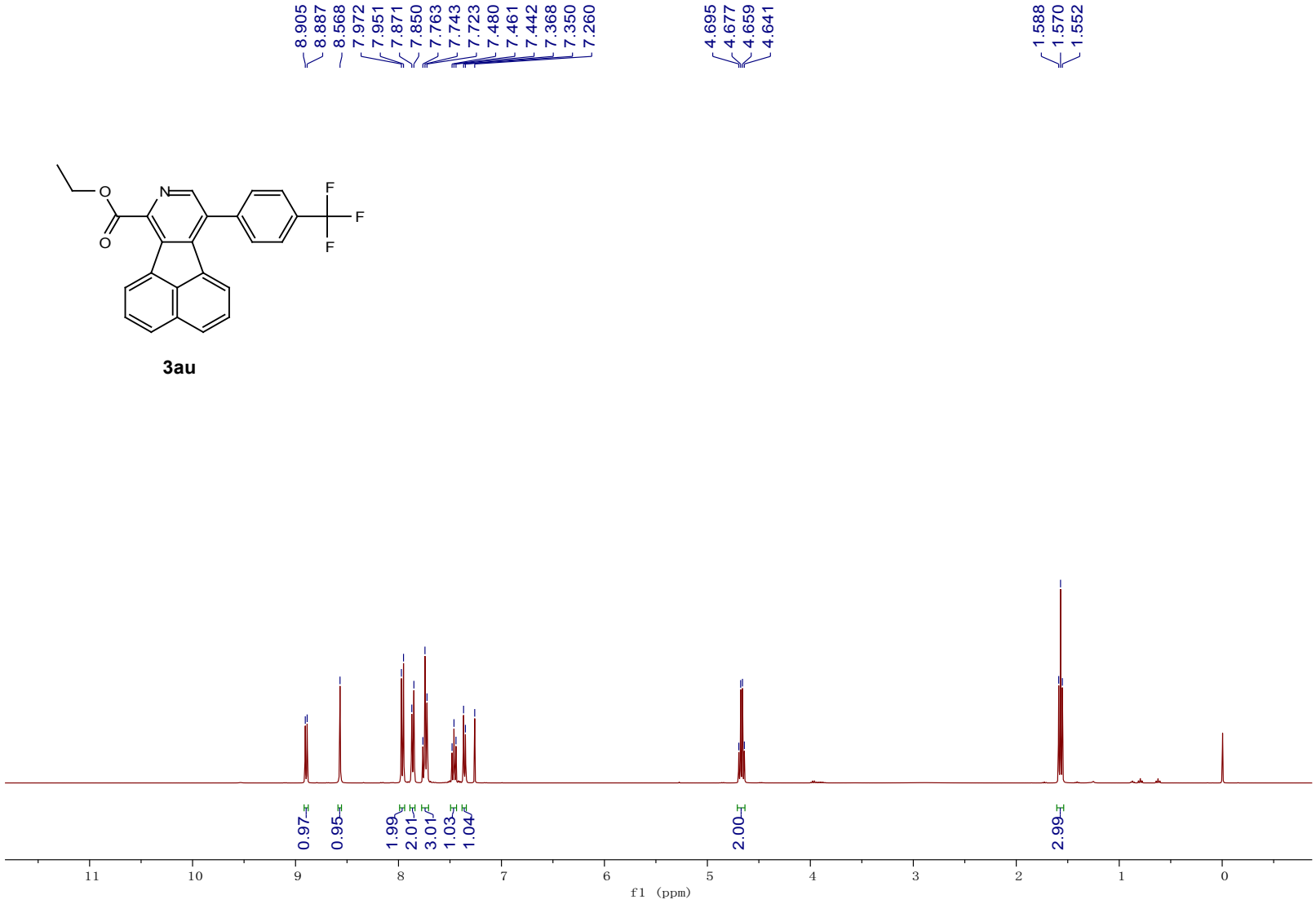
145.47
142.56
141.37
134.70
134.26
133.13
132.67
132.49
130.68
130.28
129.98
129.92
129.25
128.92
128.73
128.31
127.49
125.21
77.35
77.04
76.72
62.28
52.41
14.45
-0.00
O
N
O
O
O
O
3at
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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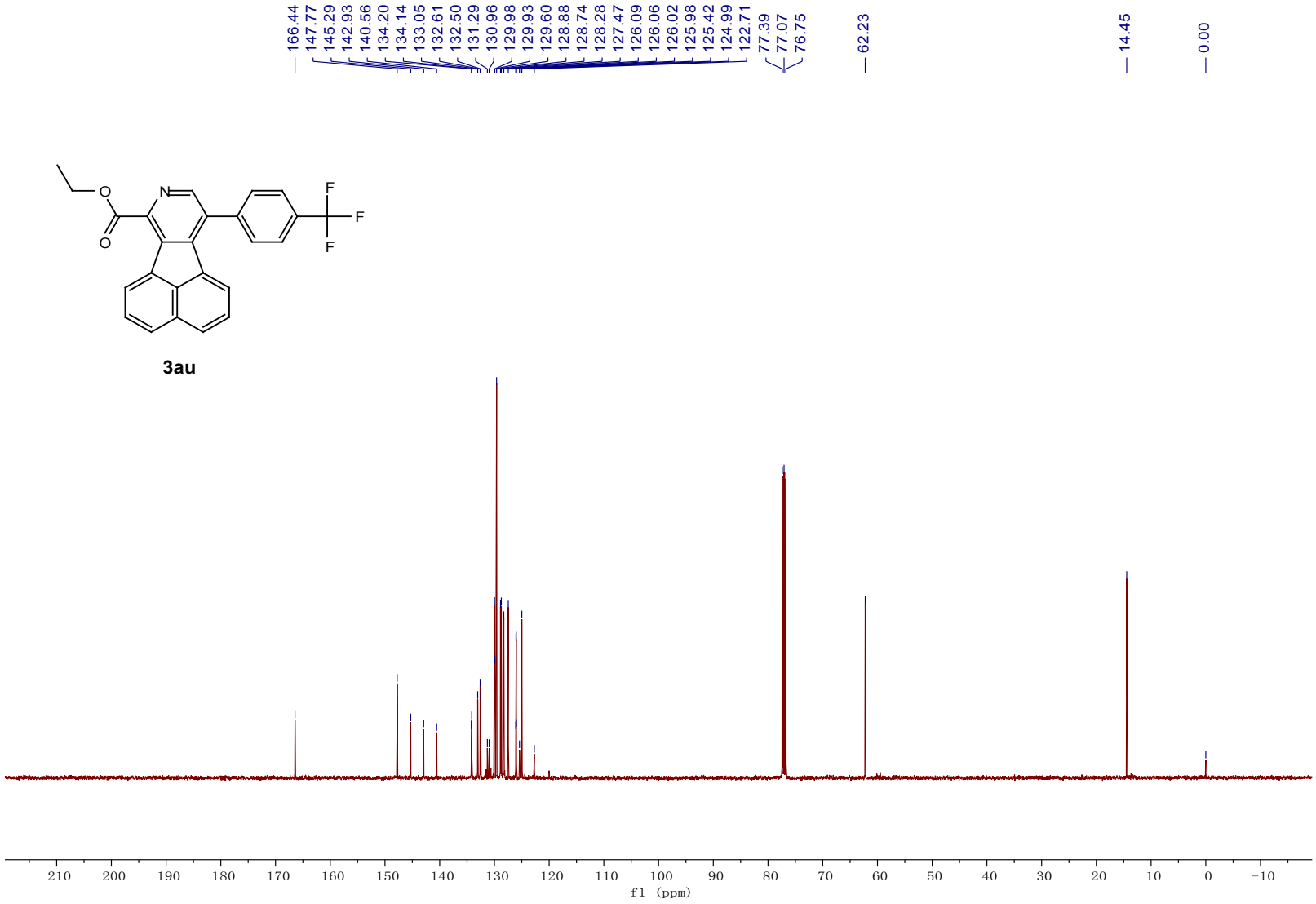
7.951
7.871
7.850
7.763
7.743
7.723
7.480
7.461
7.442
7.368
7.350
7.260
4.695
4.677
4.659
4.641
1.588
1.570
1.552
O
O
N
F
F
F
3au
0.97
0.95
1.99
2.01
3.01
1.03
1.04
2.00
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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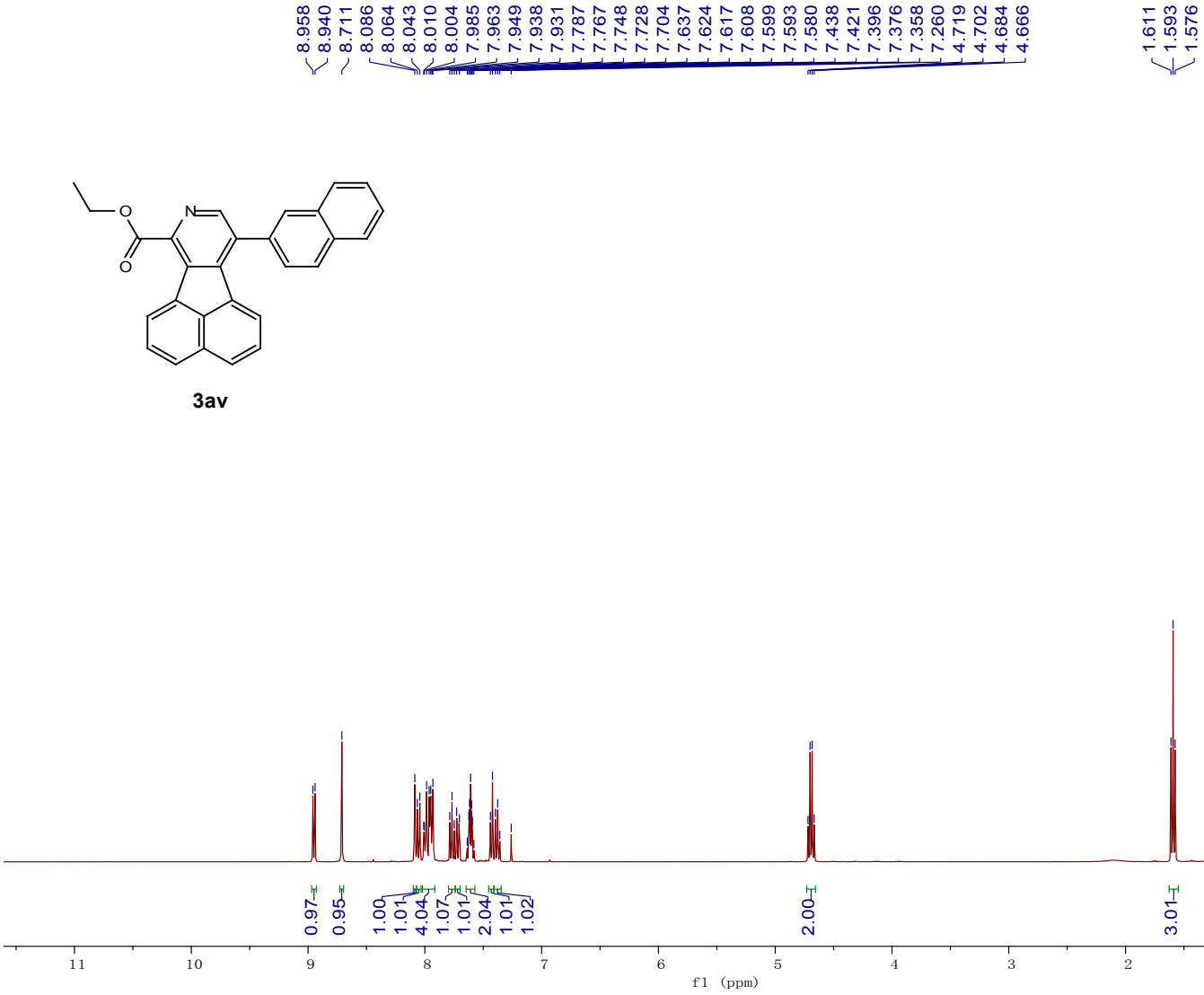
140.56
134.20
134.14
133.05
132.61
132.50
131.29
130.96
129.98
129.93
129.60
128.88
128.74
128.28
127.47
126.09
126.06
126.02
125.98
125.42
124.99
122.71
77.39
77.07
76.75
62.23
14.45
0.00
O
N
O
F
F
F
3au
f1 (ppm)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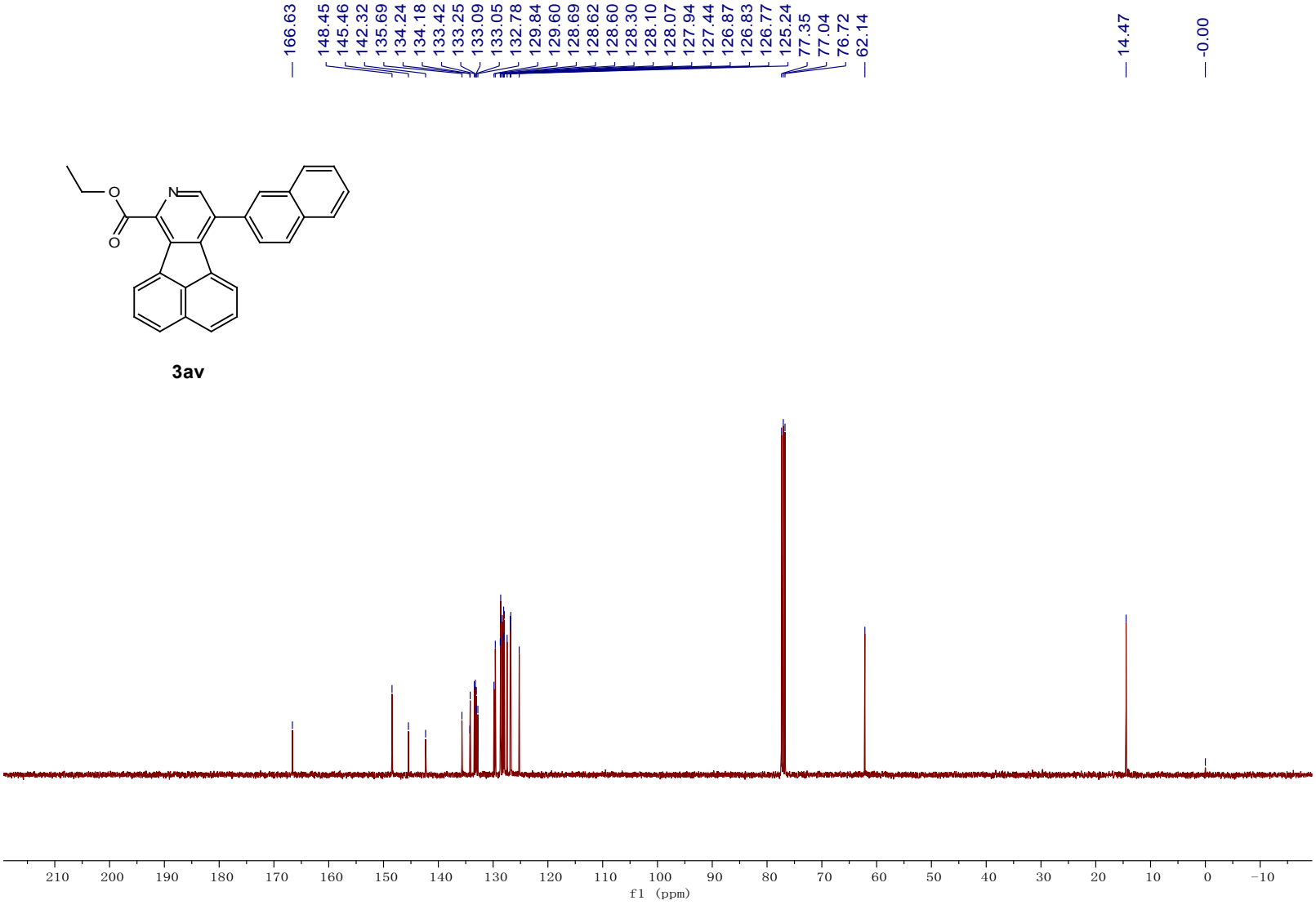
8.711
8.086
8.064
8.043
8.010
8.004
7.985
7.963
7.949
7.938
7.931
7.787
7.767
7.748
7.728
7.704
7.637
7.624
7.617
7.608
7.599
7.593
7.580
7.438
7.421
7.396
7.376
7.358
7.260
4.719
4.702
4.684
4.666
1.611
1.593
1.576
O
N
O
0.97
0.95
1.00
1.01
4.04
1.07
1.01
2.04
1.01
1.02
2.00
3.01
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3av


166.63
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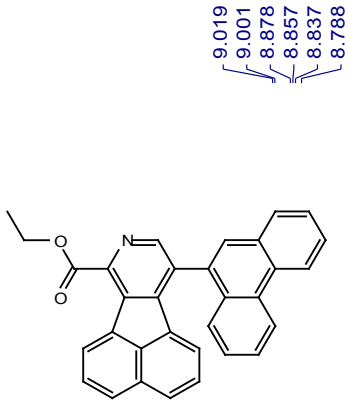
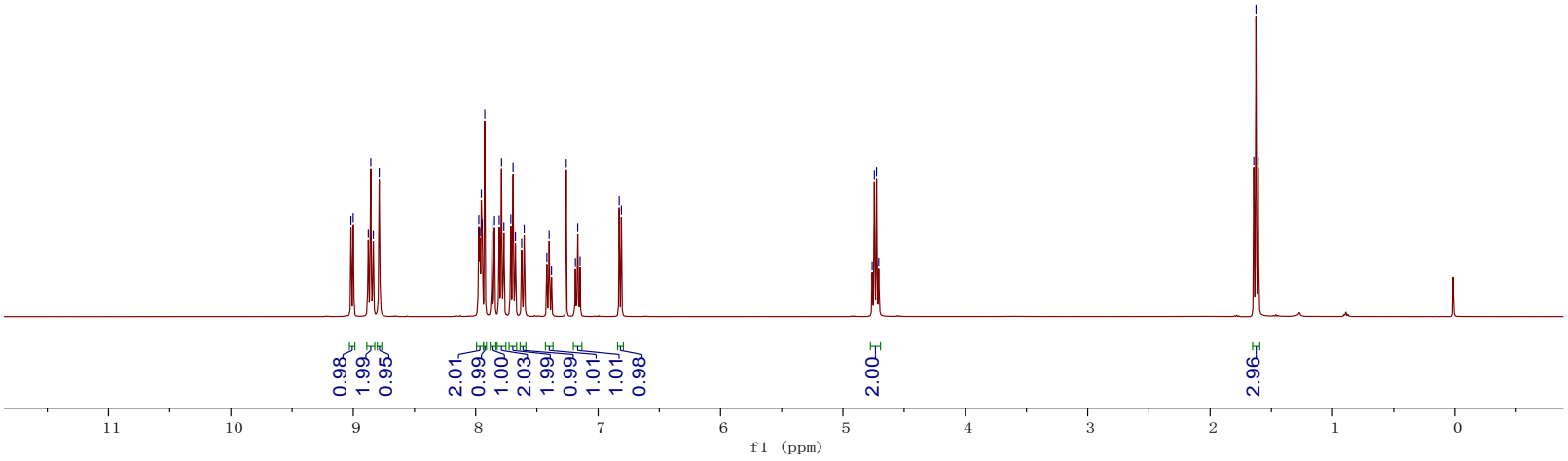
145.46
142.32
135.69
134.24
134.18
133.42
133.25
133.09
133.05
132.78
129.84
129.60
128.69
128.62
128.60
128.30
128.10
128.07
127.94
127.44
126.87
126.83
126.77
125.24
77.35
77.04
76.72
62.14
14.47
-0.00
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3av



3aw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8.788
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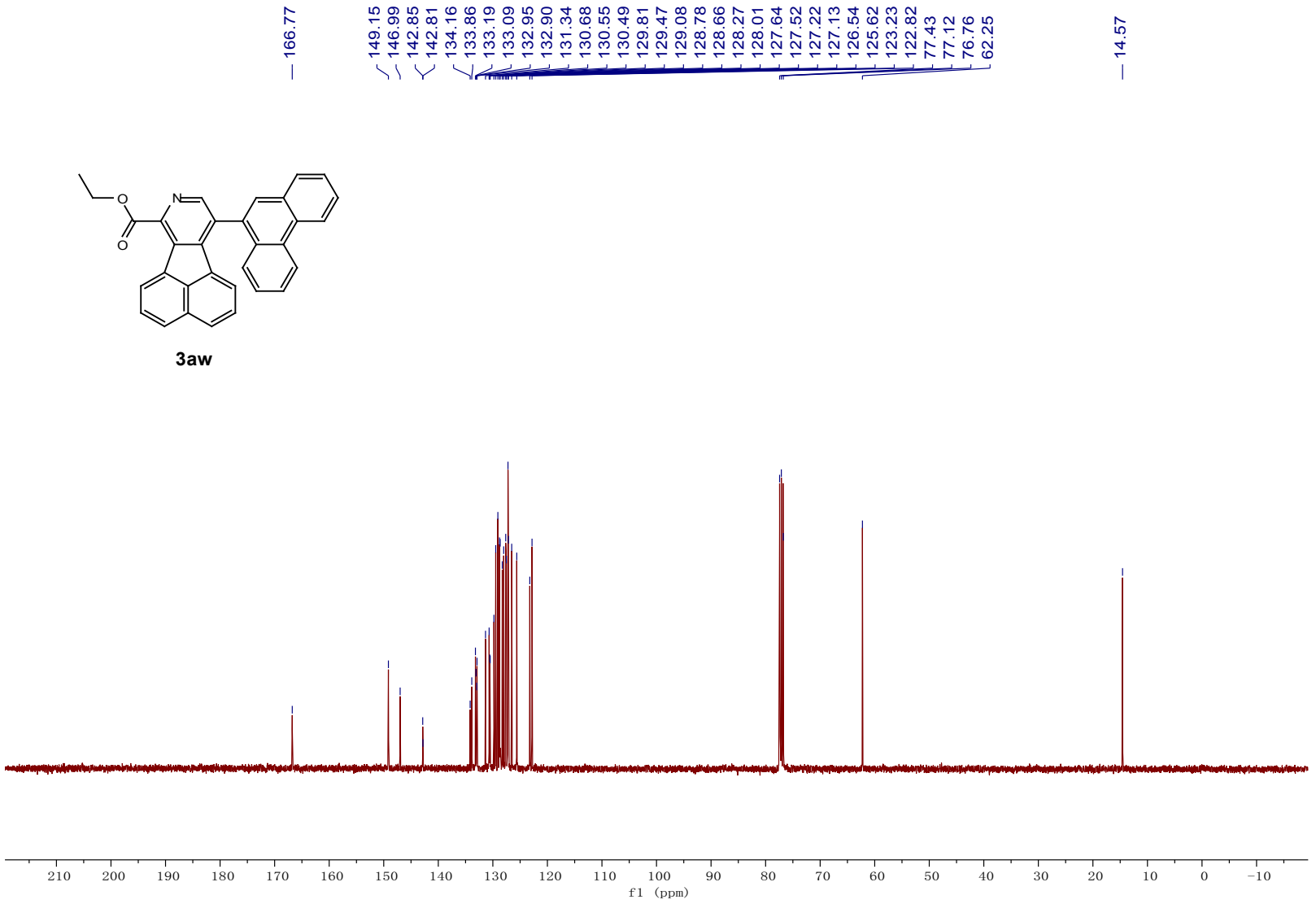
7.966
7.954
7.947
7.926
7.866
7.846
7.808
7.789
7.769
7.713
7.694
7.675
7.624
7.604
7.418
7.400
7.381
7.260
7.186
7.166
7.147
6.828
6.810
4.761
4.743
4.725
4.707
1.643
1.625
1.608
0.98
1.99
0.95
2.01
0.99
1.00
2.03
1.99
0.99
1.01
1.01
0.98
2.00
2.96
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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146.99
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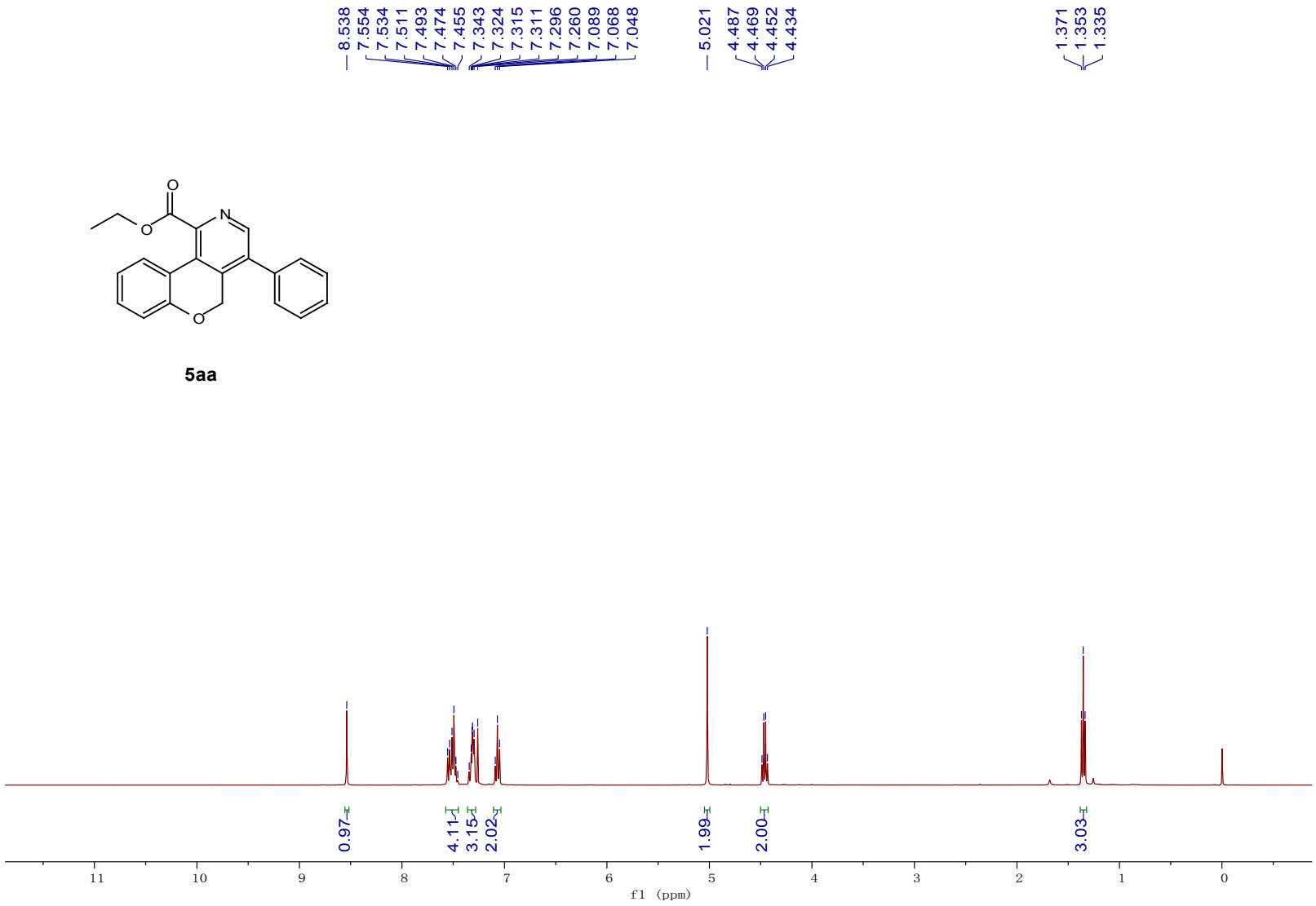
142.81
134.16
133.86
133.19
133.09
132.95
132.90
131.34
130.68
130.55
130.49
129.81
129.47
129.08
128.78
128.66
128.27
128.01
127.64
127.52
127.22
127.13
126.54
125.62
123.23
122.82
77.43
77.12
76.76
62.25
14.57
O
N
O
3aw
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.534
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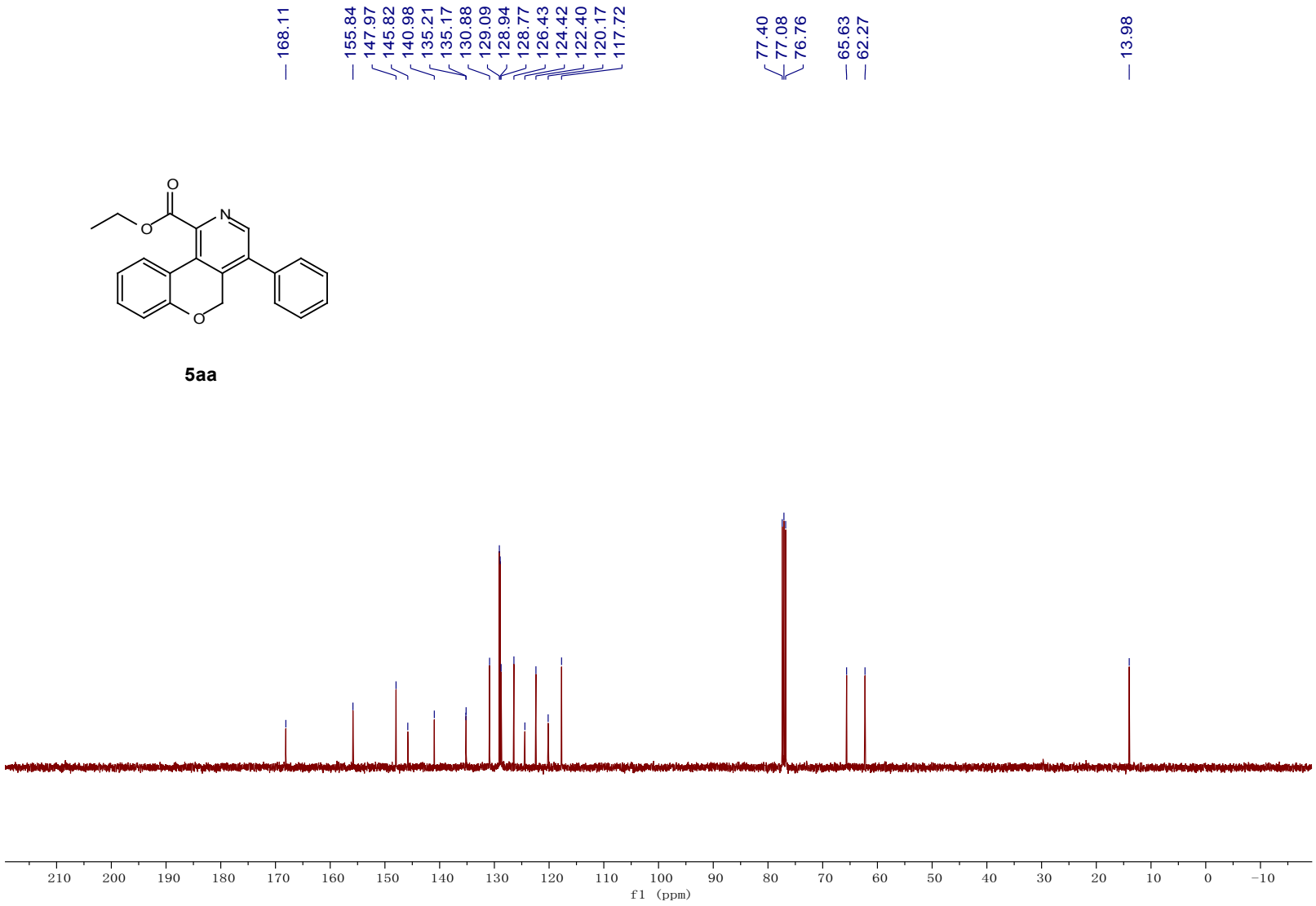
7.493
7.474
7.455
7.343
7.324
7.315
7.311
7.296
7.260
7.089
7.068
7.048
5.021
4.487
4.469
4.452
4.434
1.371
1.353
1.335
O
O
N
O
0.97
4.11
3.15
2.02
1.99
2.00
3.03
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

5aa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155.84
147.97
145.82
140.98
135.21
135.17
130.88
129.09
128.94
128.77
126.43
124.42
122.40
120.17
117.72
77.40
77.08
76.76
65.63
62.27
13.98
O
O
N
O
210
200
190
180
170
160
150
140
130
120
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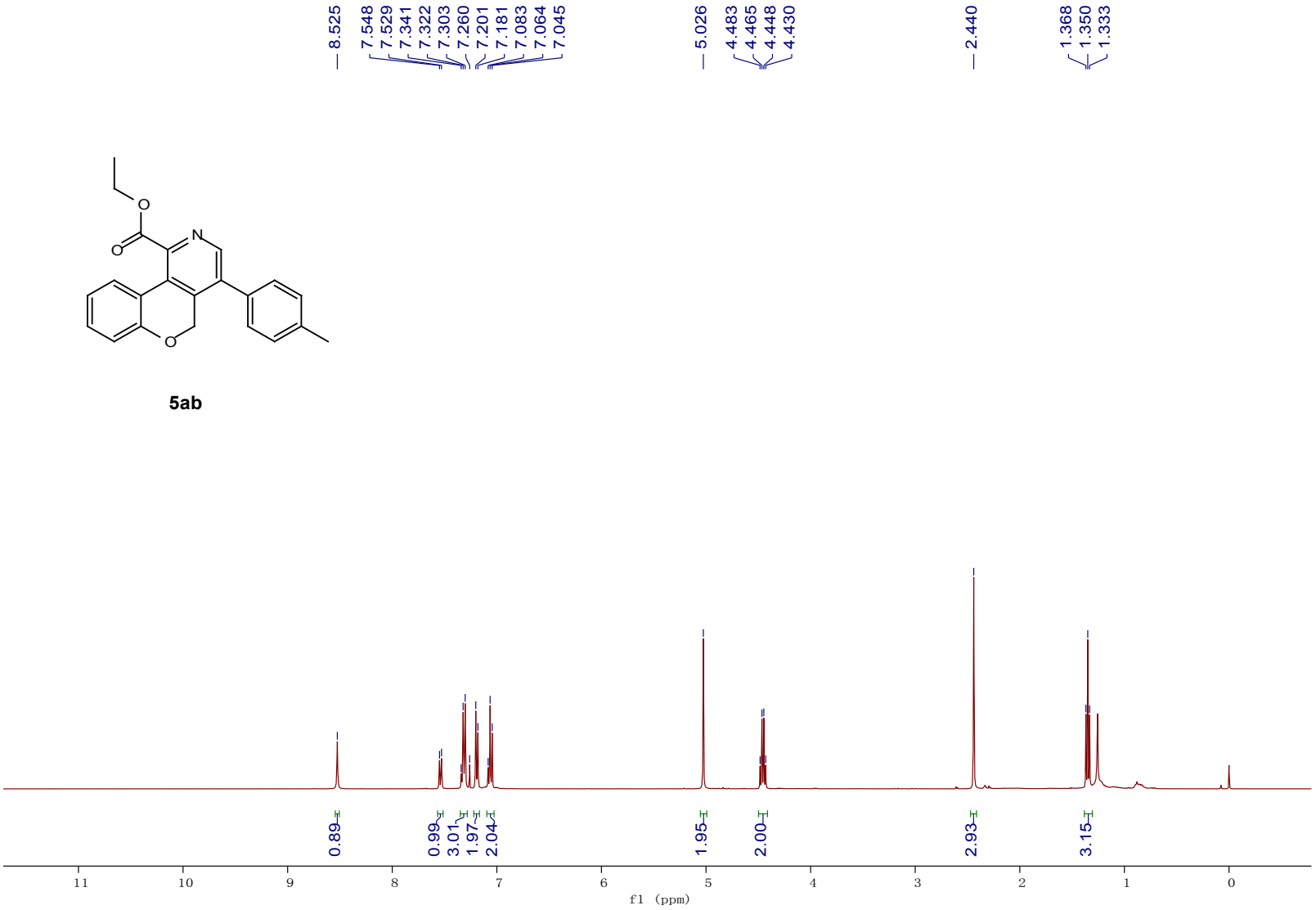
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

5aa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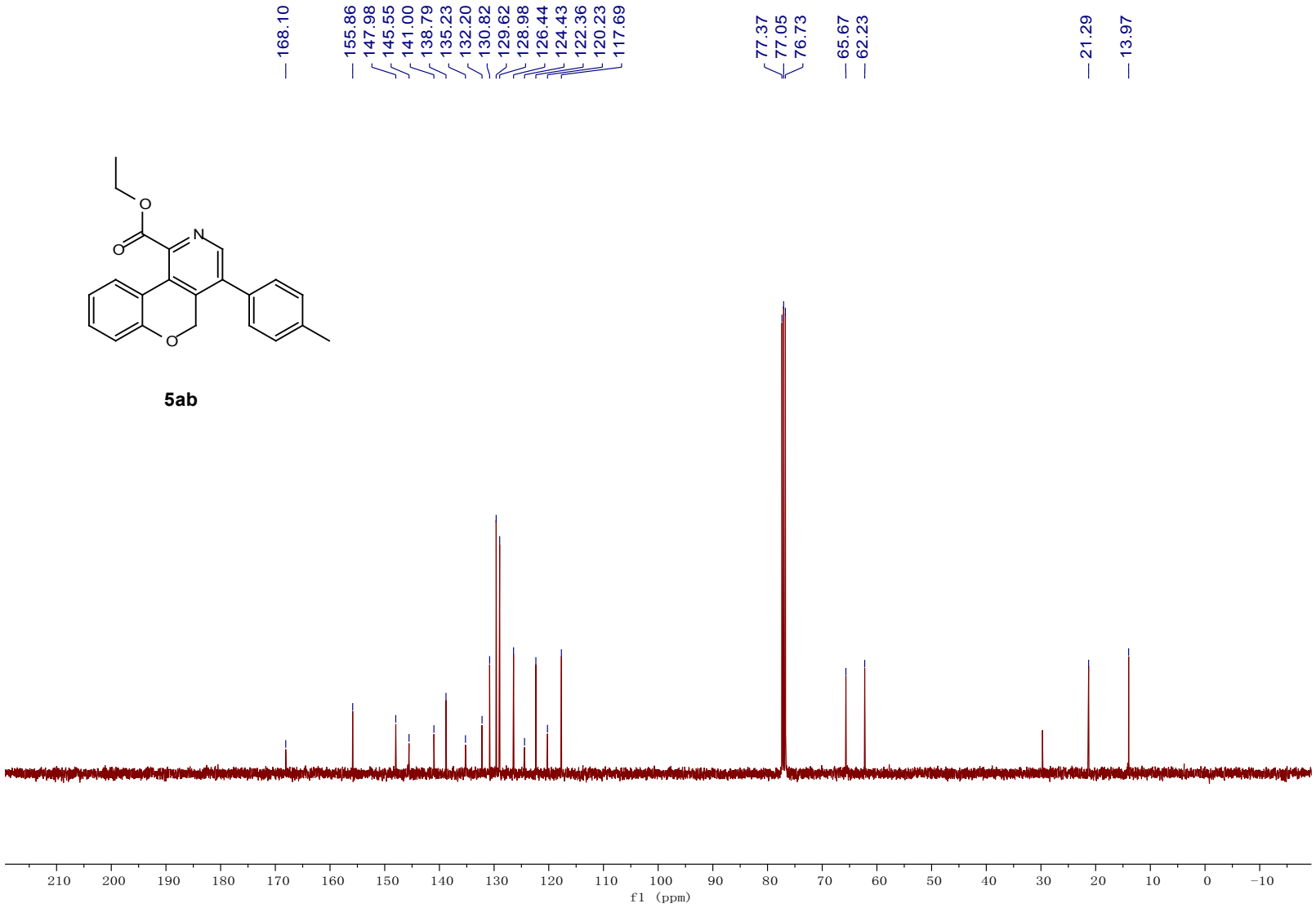
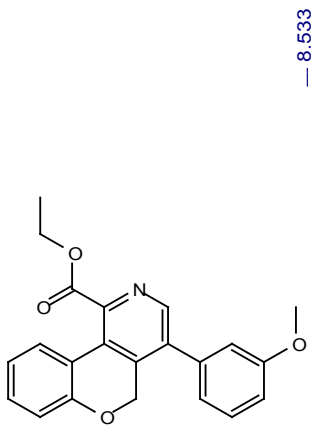
7.322
7.303
7.260
7.201
7.181
7.083
7.064
7.045
5.026
4.483
4.465
4.448
4.430
2.440
1.368
1.350
1.333
O
N
O
O
0.89
0.99
3.01
1.97
2.04
1.95
2.00
2.93
3.15
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

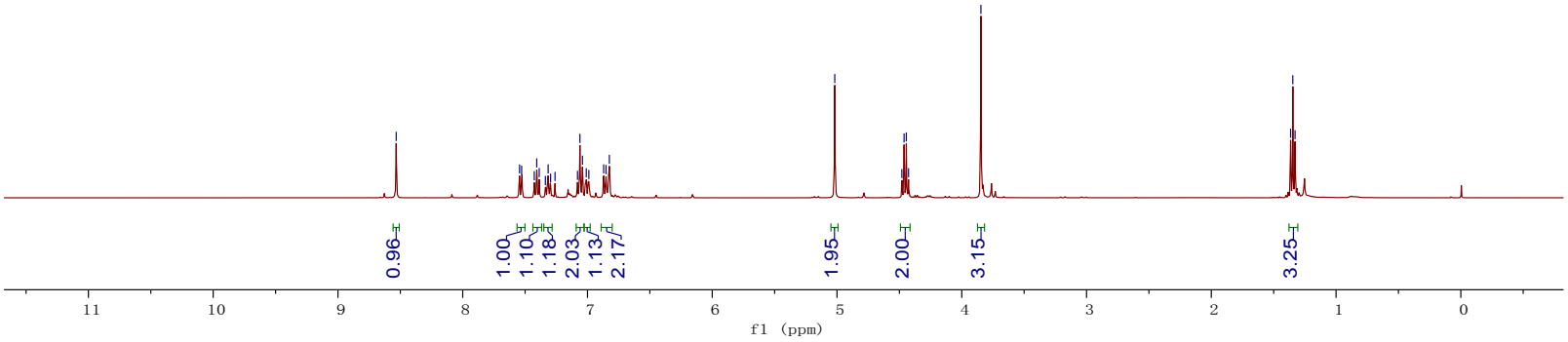
5ab

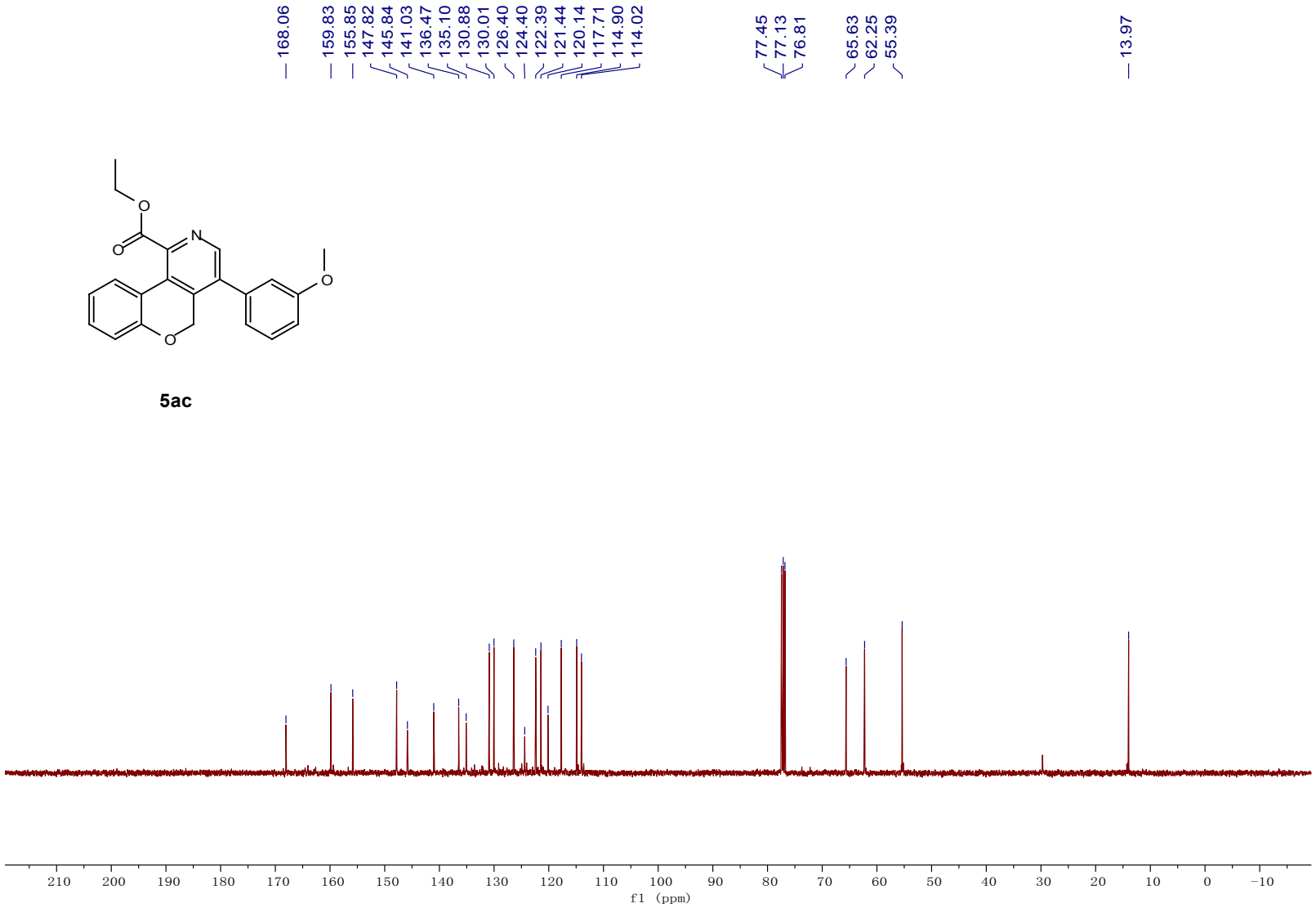

168.10
155.86
147.98
145.55
141.00
138.79
135.23
132.20
130.82
129.62
128.98
126.44
124.43
122.36
120.23
117.69
77.37
77.05
76.73
65.67
62.23
21.29
13.97
O
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

5ab

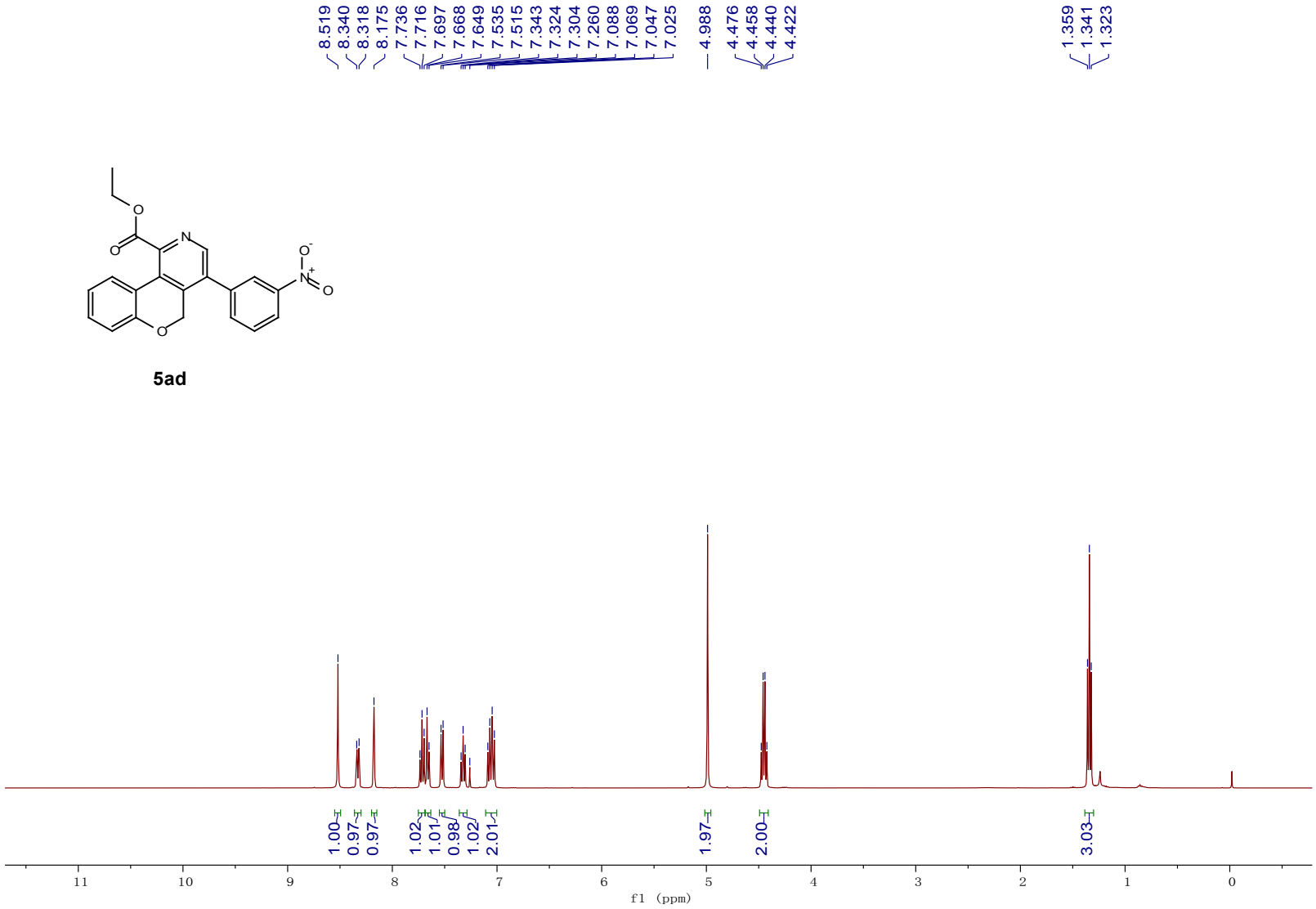


5ac

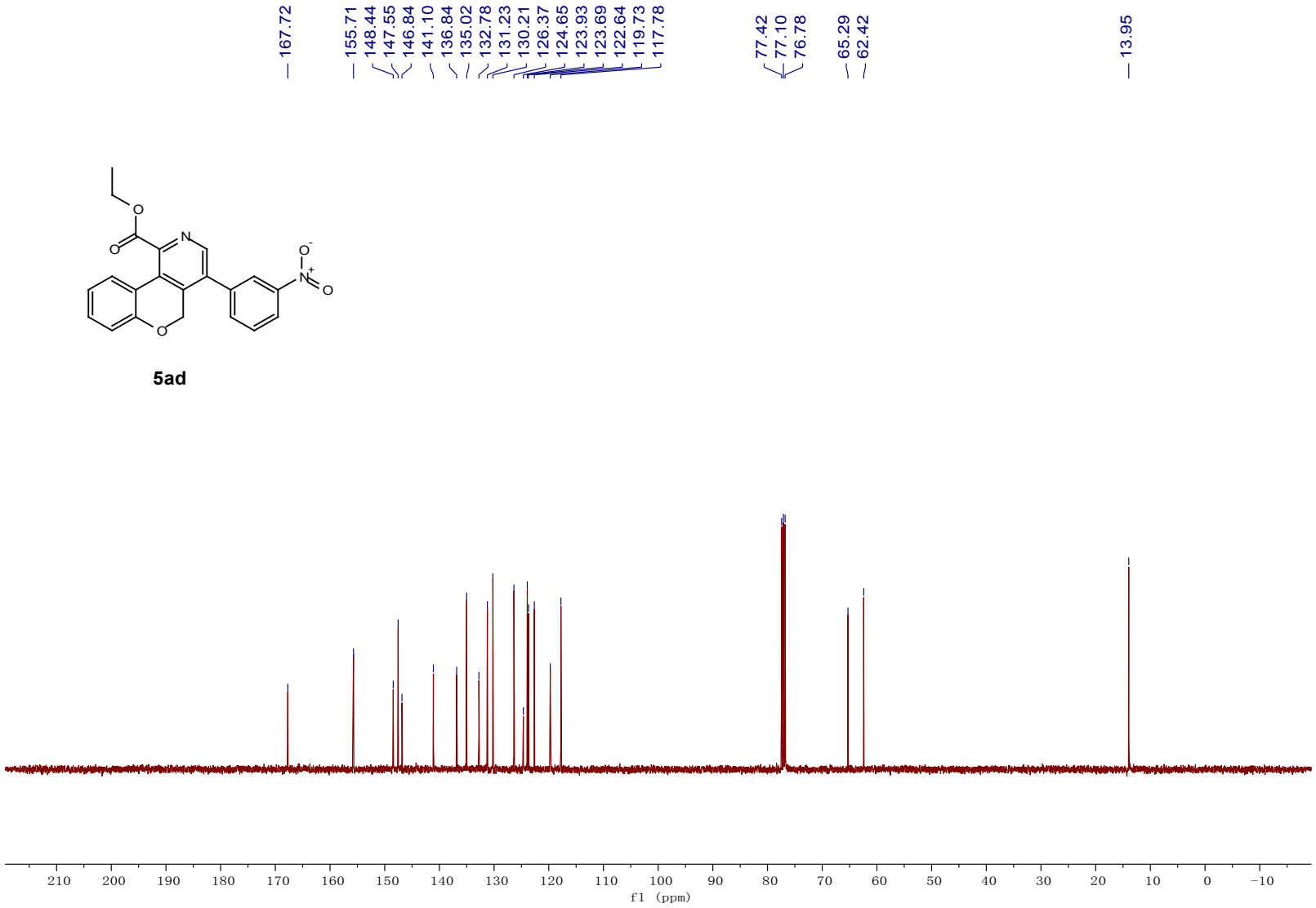

8.533
7.544
7.528
7.427
7.407
7.387
7.337
7.315
7.296
7.260
7.080
7.061
7.040
7.010
6.989
6.870
6.851
6.825
5.018
4.480
4.462
4.444
4.427
3.847
1.364
1.346
1.329
0.96
1.00
1.10
1.18
2.03
1.13
2.17
1.95
2.00
3.15
3.25
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


168.06
159.83
155.85
147.82
145.84
141.03
136.47
135.10
130.88
130.01
126.40
124.40
122.39
121.44
120.14
117.71
114.90
114.02
77.45
77.13
76.81
65.63
62.25
55.39
13.97
O
N
O
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

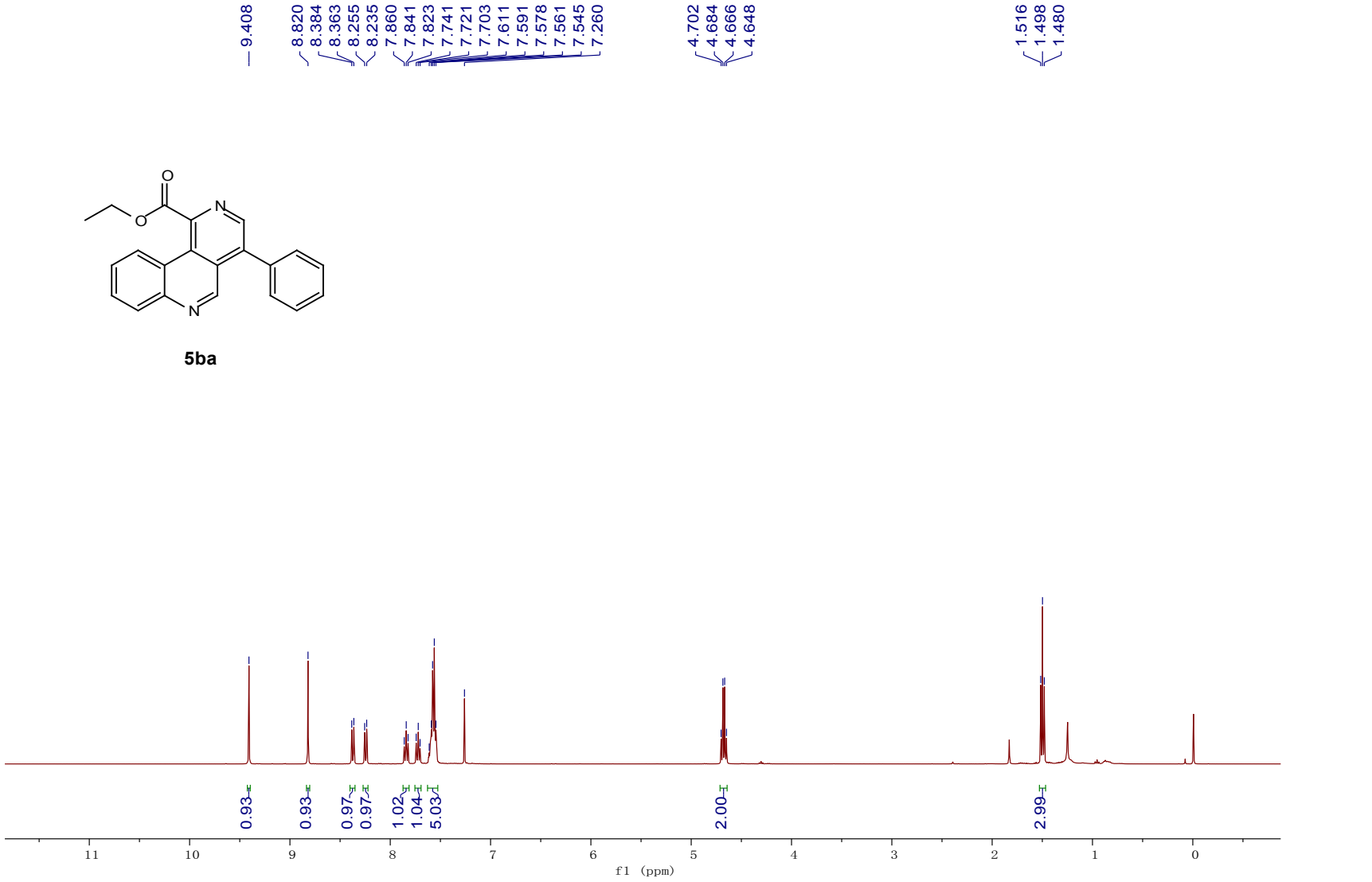
5ac


8.519
8.340
8.318
8.175
7.736
7.716
7.697
7.668
7.649
7.535
7.515
7.343
7.324
7.304
7.260
7.088
7.069
7.047
7.025
4.988
4.476
4.458
4.440
4.422
1.359
1.341
1.323
1.00
0.97
0.97
1.02
1.01
0.98
1.02
2.01
1.97
2.00
3.03
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

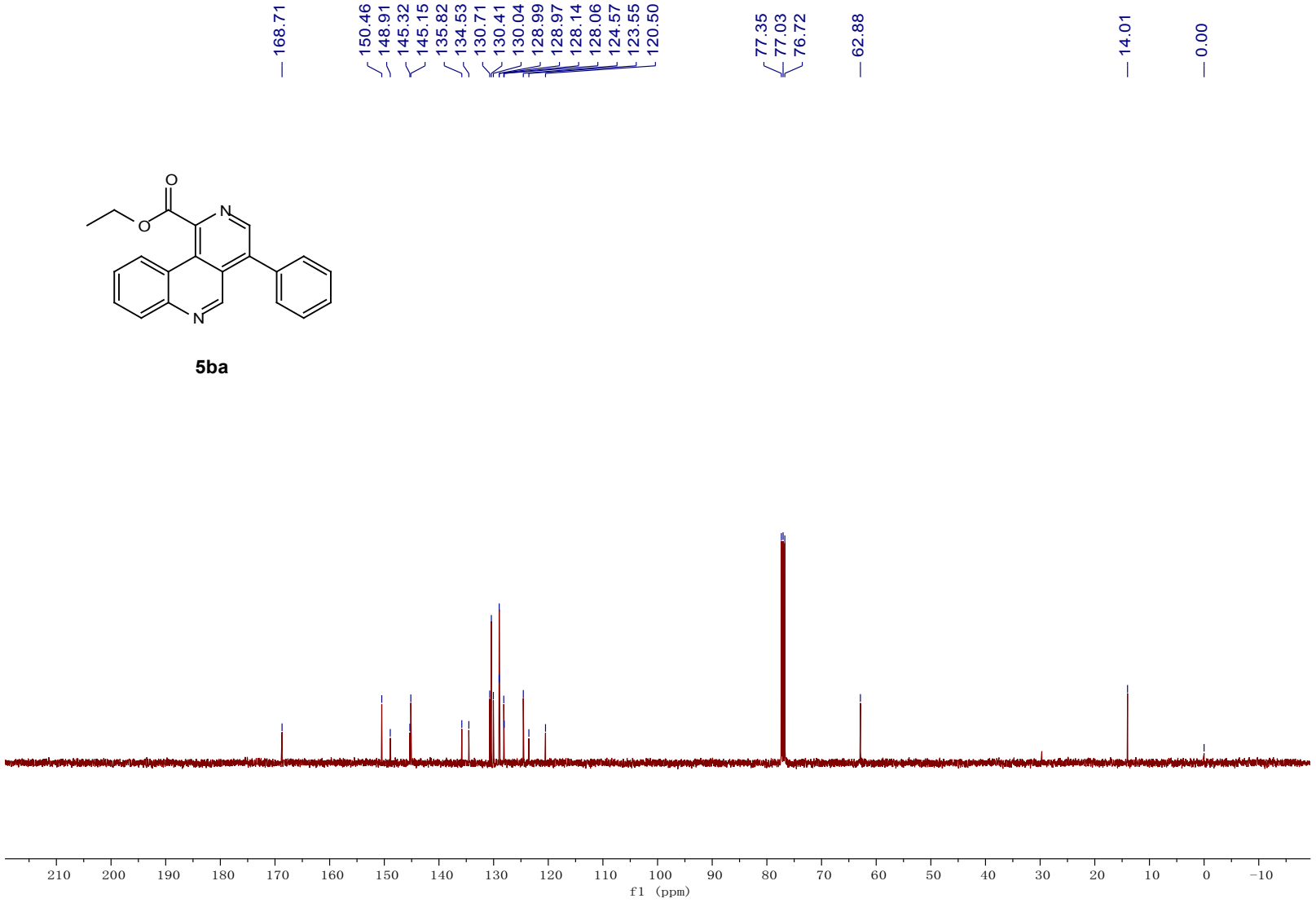
5ad

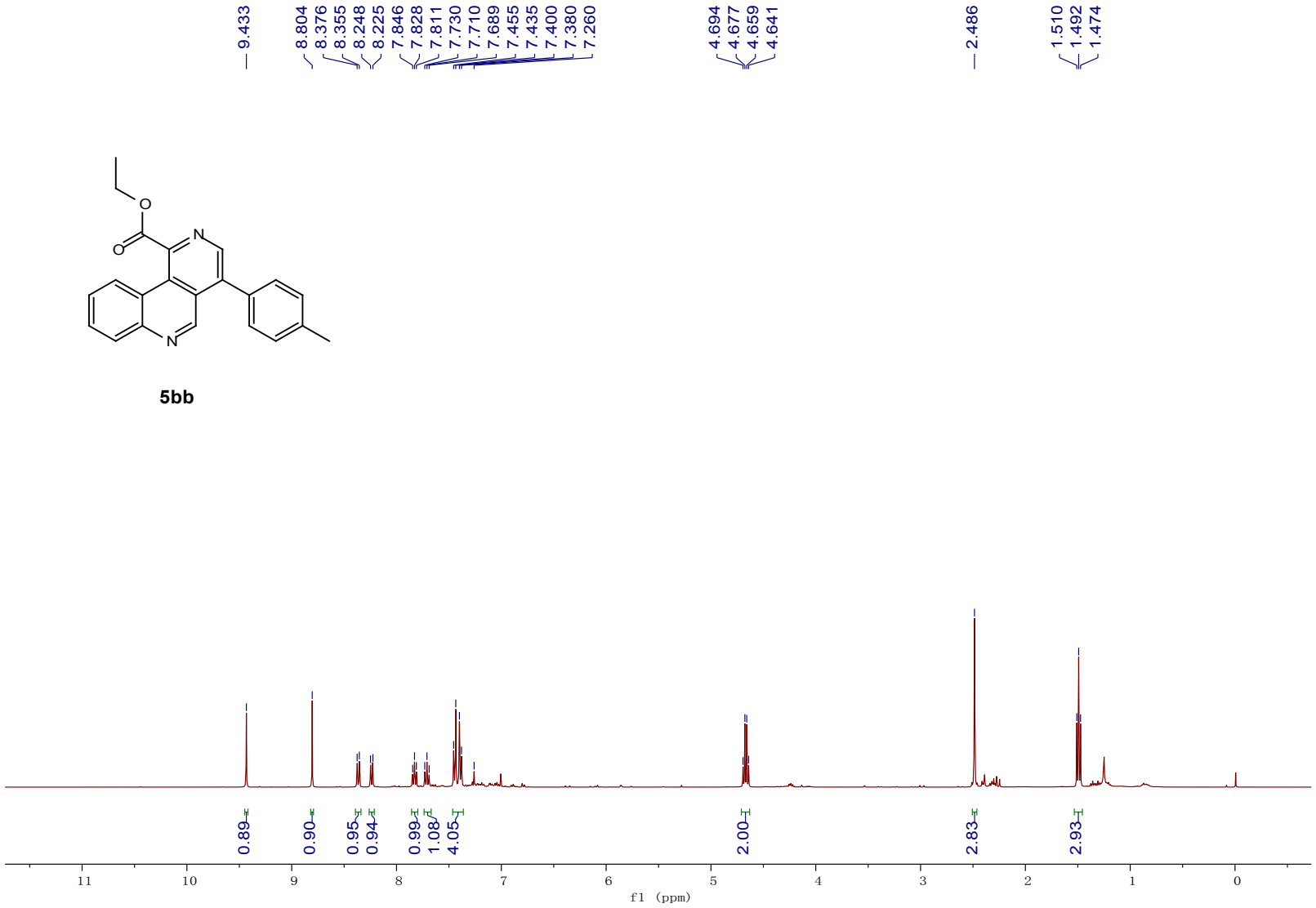

167.72
155.71
148.44
147.55
146.84
141.10
136.84
135.02
132.78
131.23
130.21
126.37
124.65
123.93
123.69
122.64
119.73
117.78
77.42
77.10
76.78
65.29
62.42
13.95
O
O
N
O
O
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

5ad

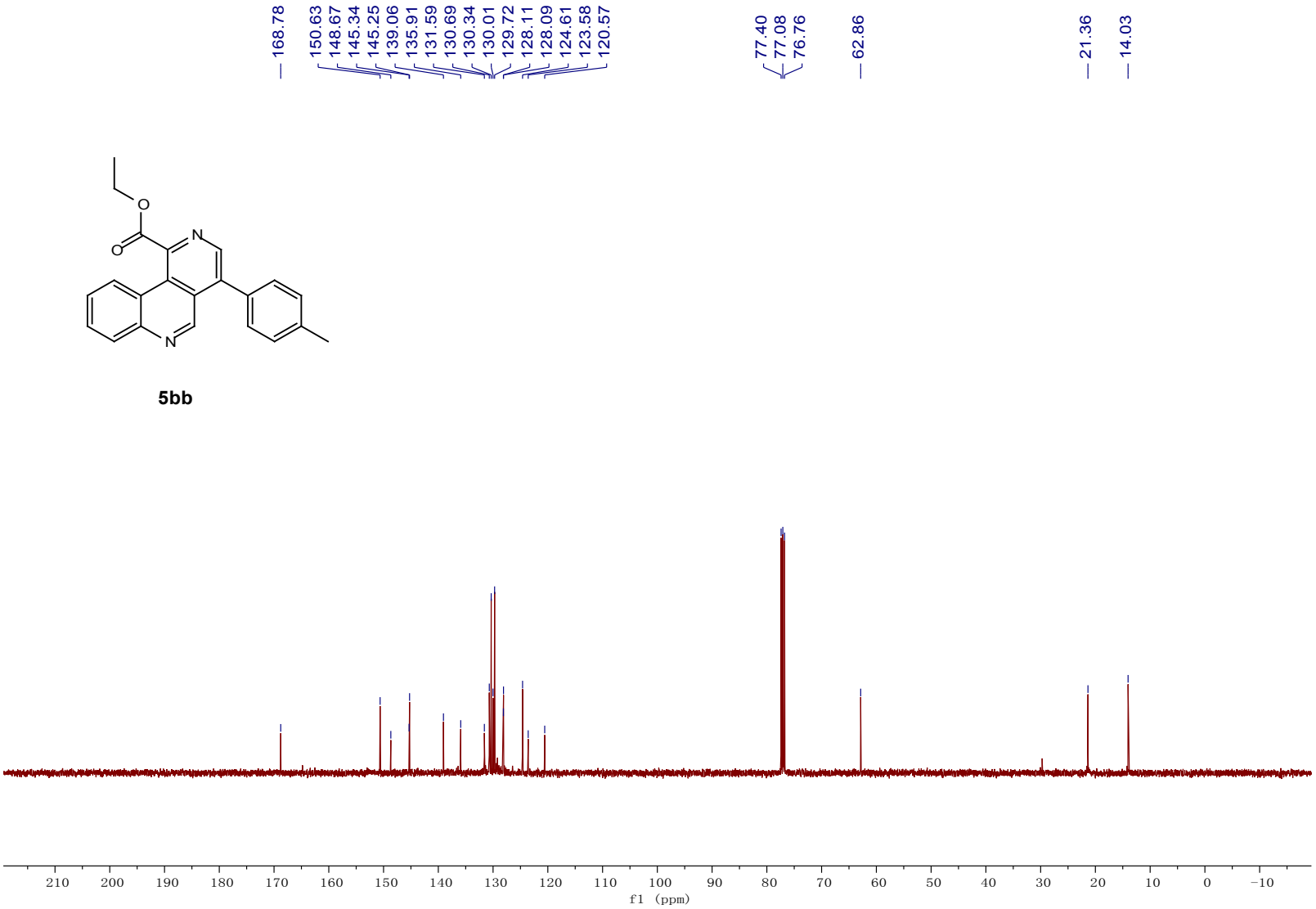

9.408
8.820
8.384
8.363
8.255
8.235
7.860
7.841
7.823
7.741
7.721
7.703
7.611
7.591
7.578
7.561
7.545
7.260
4.702
4.684
4.666
4.648
1.516
1.498
1.480
O
O
N
N
0.93
0.93
0.97
0.97
1.02
1.04
5.03
2.00
2.99
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

5ba

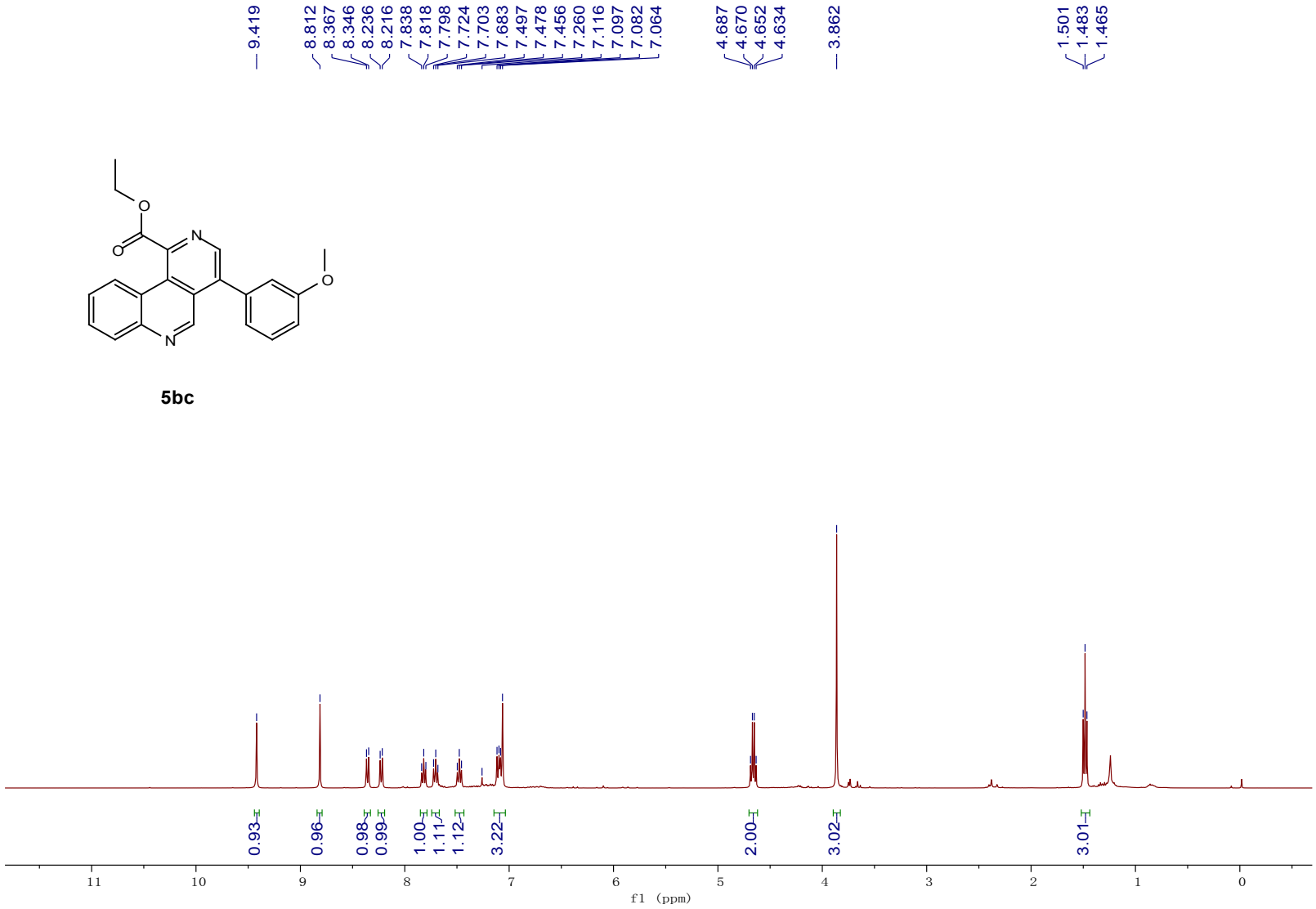

168.71
150.46
148.91
145.32
145.15
135.82
134.53
130.71
130.41
130.04
128.99
128.97
128.14
128.06
124.57
123.55
120.50
77.35
77.03
76.72
62.88
14.01
0.00
O
O
N
N
5ba
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


9.433
8.804
8.376
8.355
8.248
8.225
7.846
7.828
7.811
7.730
7.710
7.689
7.455
7.435
7.400
7.380
7.260
4.694
4.677
4.659
4.641
2.486
1.510
1.492
1.474
O
O
N
N
0.89
0.90
0.95
0.94
0.99
1.08
4.05
2.00
2.83
2.93
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

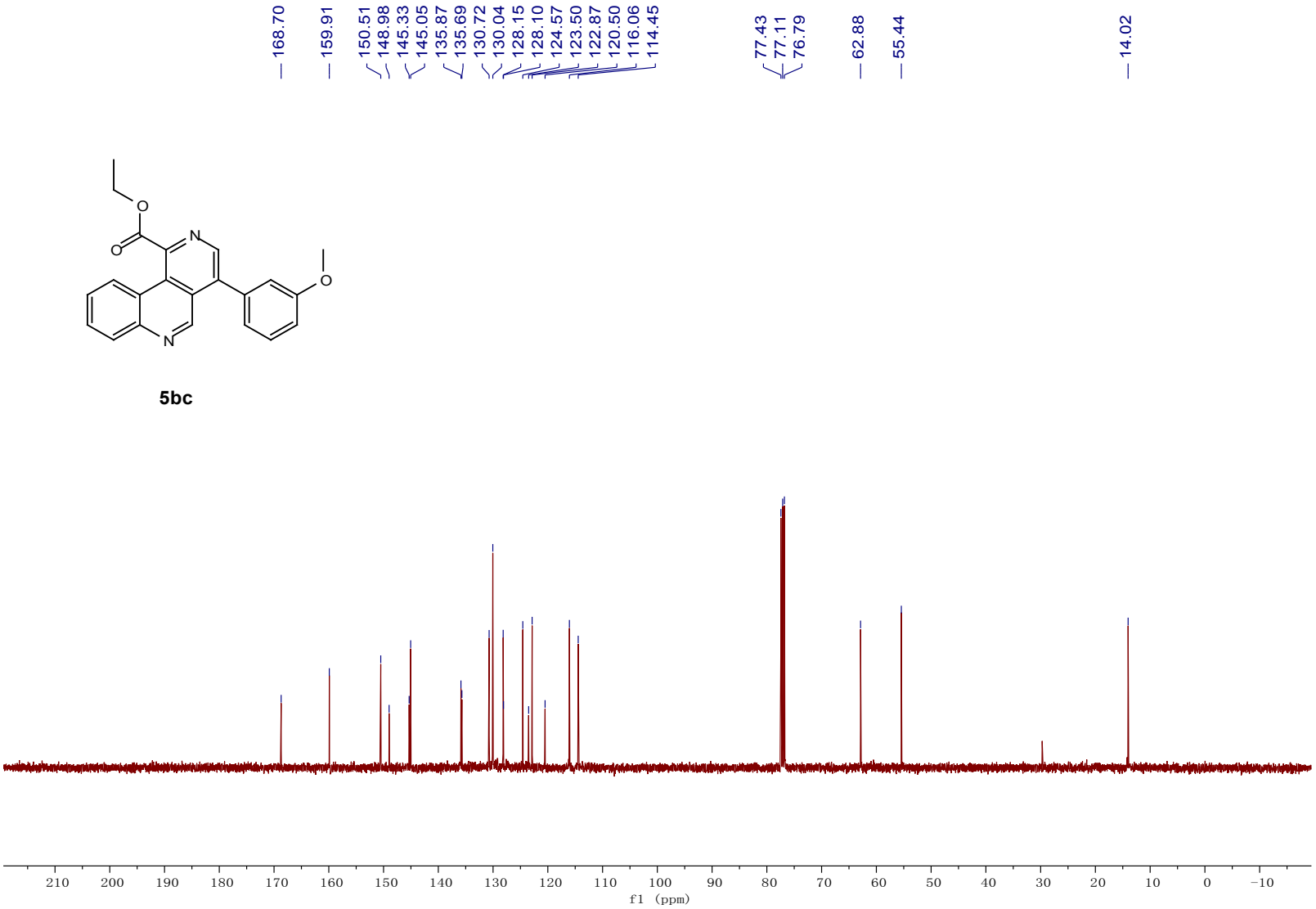
5bb


168.78
150.63
148.67
145.34
145.25
139.06
135.91
131.59
130.69
130.34
130.01
129.72
128.11
128.09
124.61
123.58
120.57
77.40
77.08
76.76
62.86
21.36
14.03
O
O
N
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

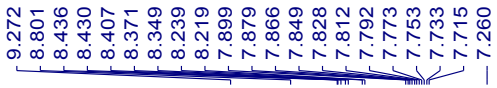
5bb

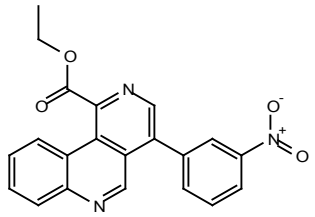

9.419
8.812
8.367
8.346
8.236
8.216
7.838
7.818
7.798
7.724
7.703
7.683
7.497
7.478
7.456
7.260
7.116
7.097
7.082
7.064
4.687
4.670
4.652
4.634
3.862
1.501
1.483
1.465
O
O
N
O
N
0.93
0.96
0.98
0.99
1.00
1.11
1.12
3.22
2.00
3.02
3.01
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

5bc

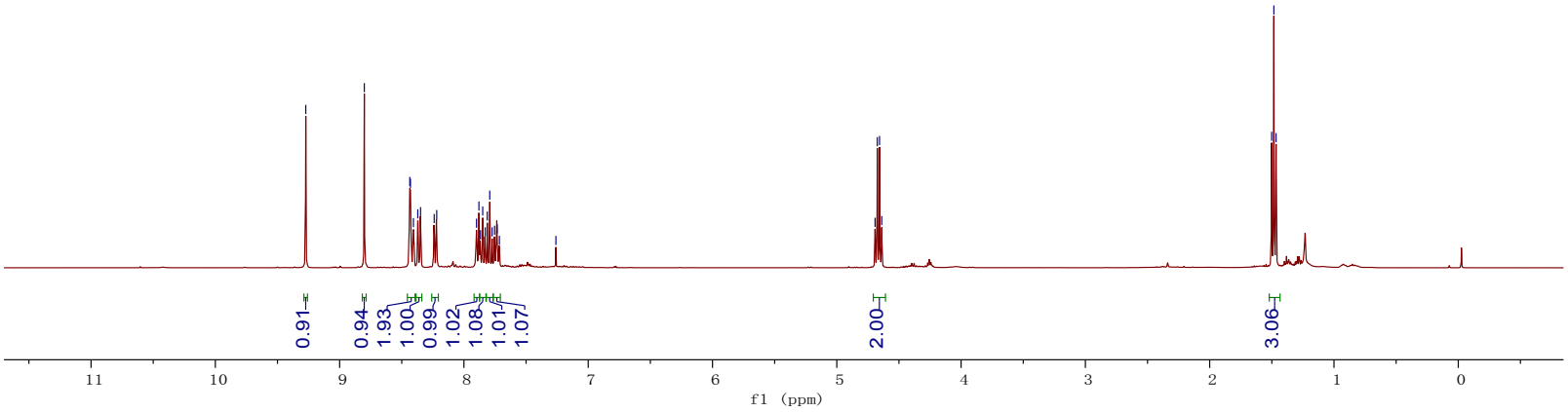

168.70
159.91
150.51
148.98
145.33
145.05
135.87
135.69
130.72
130.04
128.15
128.10
124.57
123.50
122.87
120.50
116.06
114.45
77.43
77.11
76.79
62.88
55.44
14.02
O
O
N
O
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

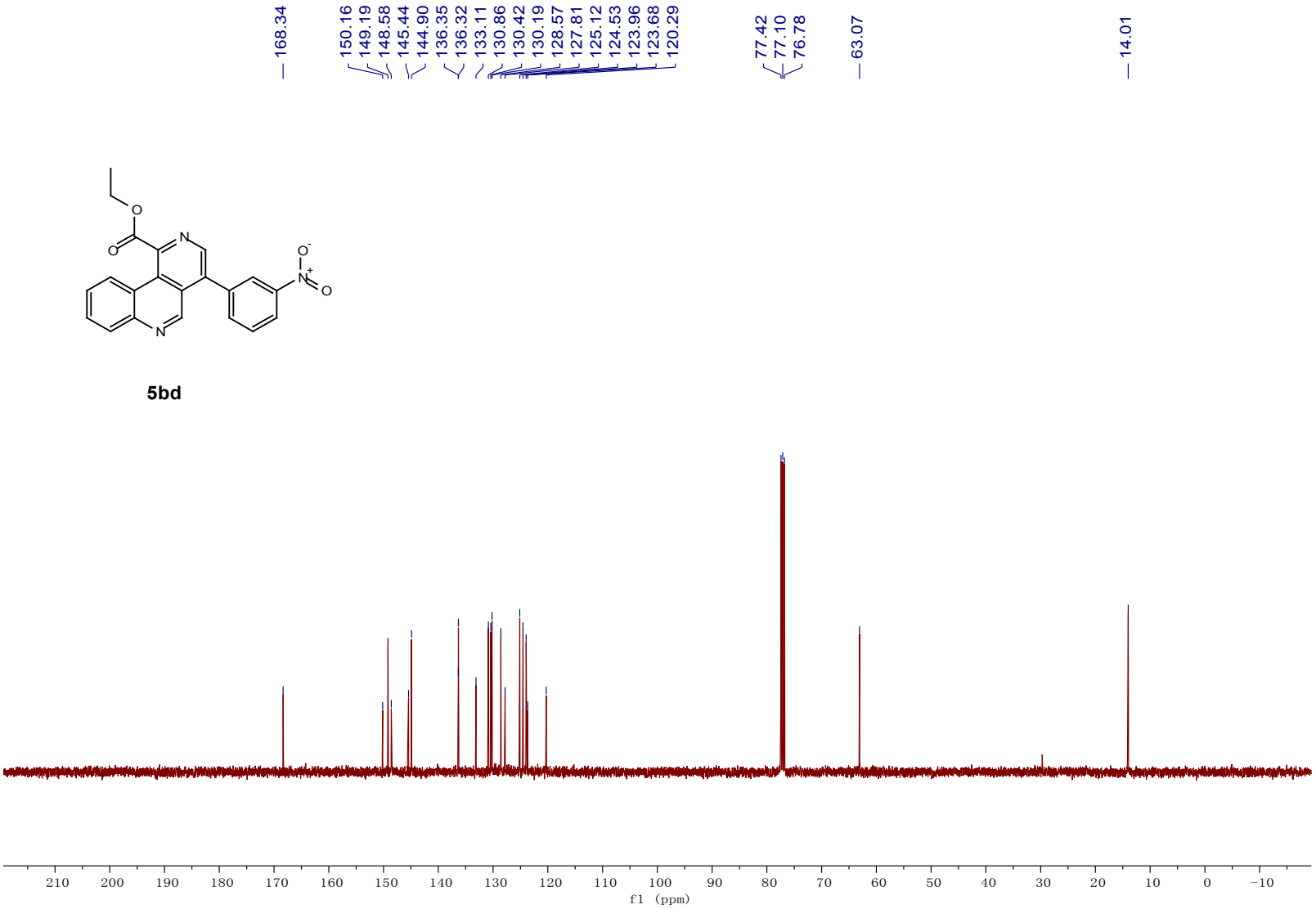
5bc


9.272
8.801
8.436
8.430
8.407
8.371
8.349
8.239
8.219
7.899
7.879
7.866
7.849
7.828
7.812
7.792
7.773
7.753
7.733
7.715
7.260
4.692
4.674
4.656
4.638
1.502
1.484
1.466

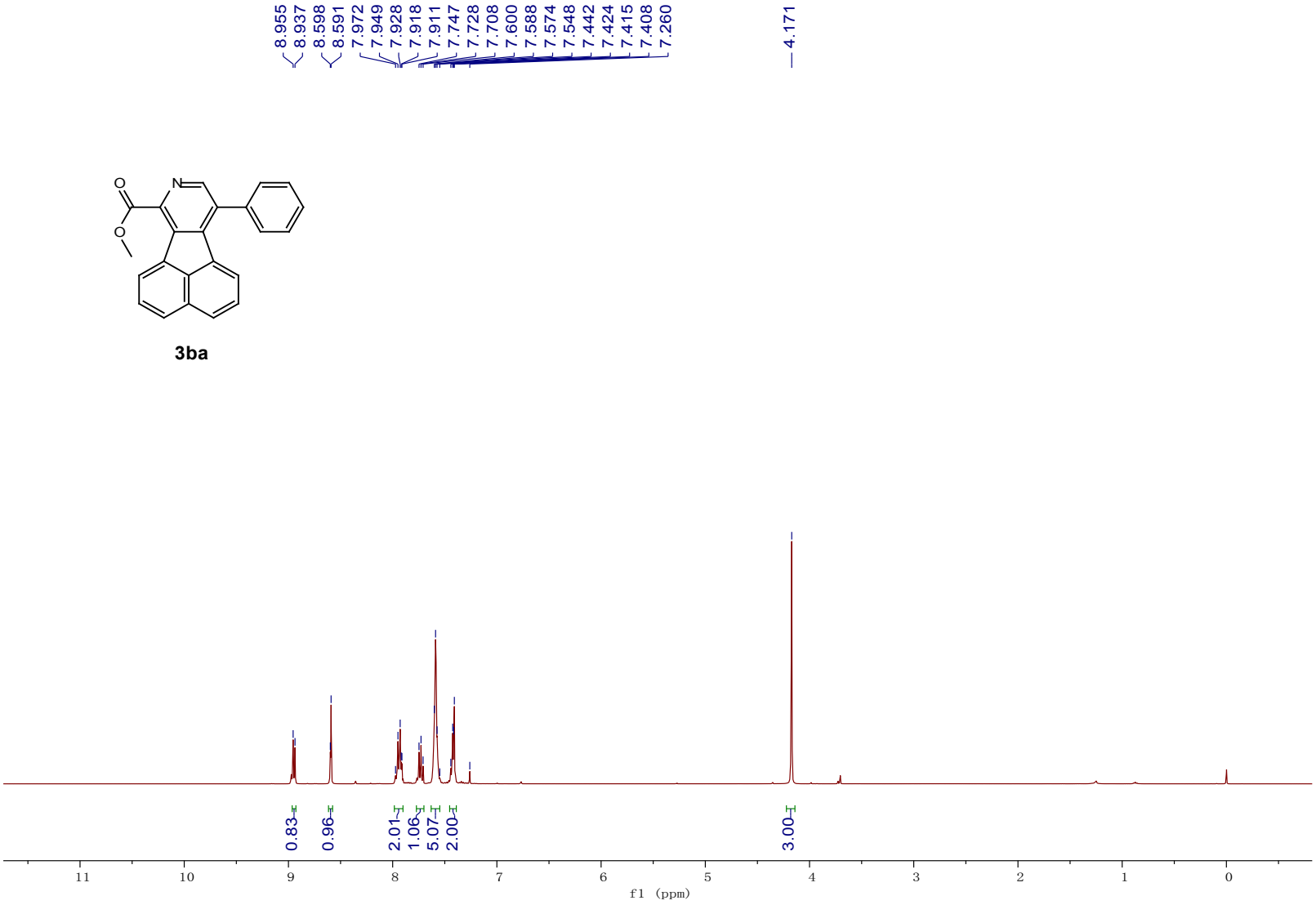


5bd

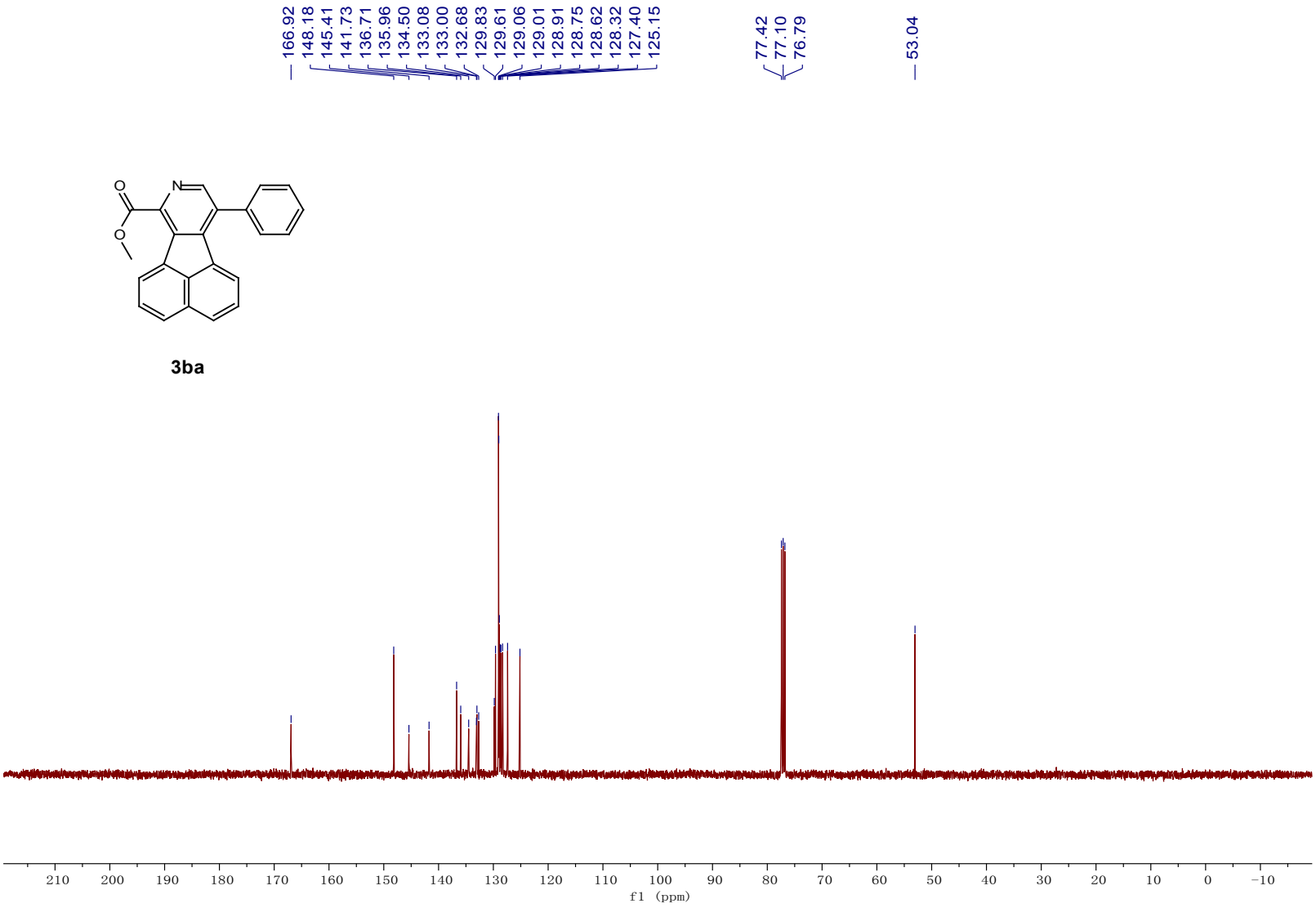

0.91
0.94
1.93
1.00
0.99
1.02
1.08
1.01
1.07
2.00
3.06
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


168.34
150.16
149.19
148.58
145.44
144.90
136.35
136.32
133.11
130.86
130.42
130.19
128.57
127.81
125.12
124.53
123.96
123.68
120.29
77.42
77.10
76.78
63.07
14.01
O
O
N
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

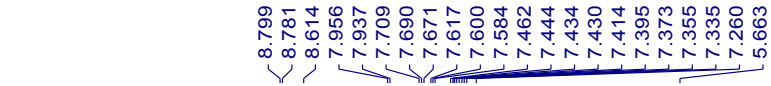
5bd

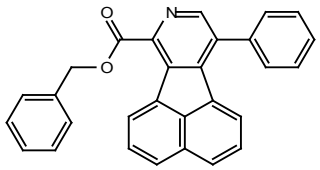

8.955
8.937
8.598
8.591
7.972
7.949
7.928
7.918
7.911
7.747
7.728
7.708
7.600
7.588
7.574
7.548
7.442
7.424
7.415
7.408
7.260
4.171
O
N
O
0.83
0.96
2.01
1.06
5.07
2.00
3.00
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

3ba

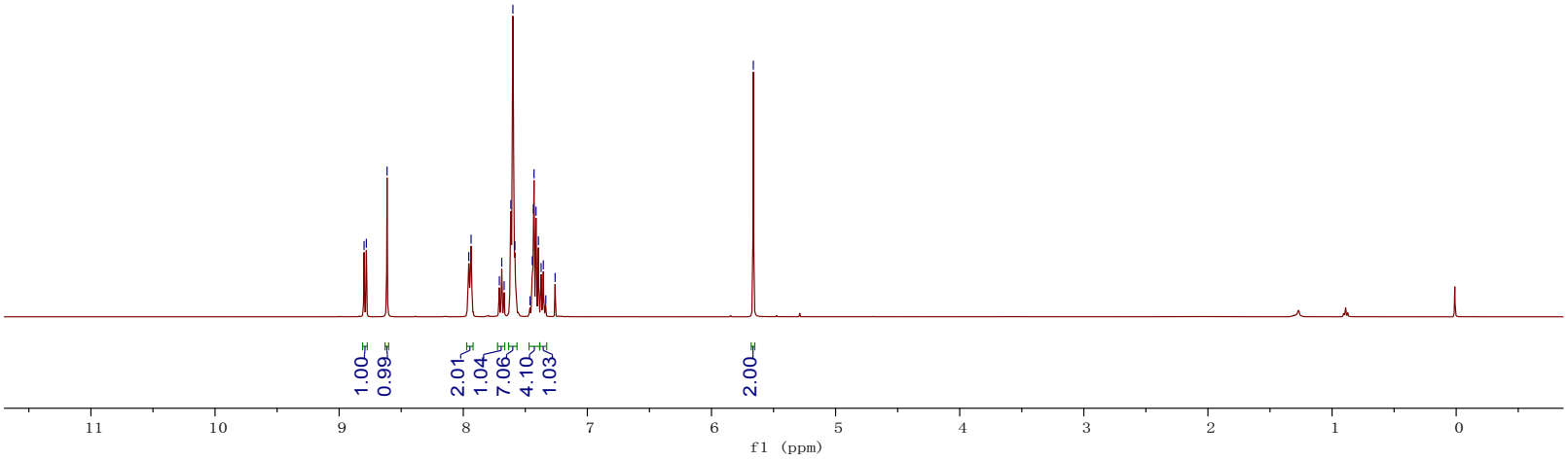

166.92
148.18
145.41
141.73
136.71
135.96
134.50
133.08
133.00
132.68
129.83
129.61
129.06
129.01
128.91
128.75
128.62
128.32
127.40
125.15
77.42
77.10
76.79
53.04
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

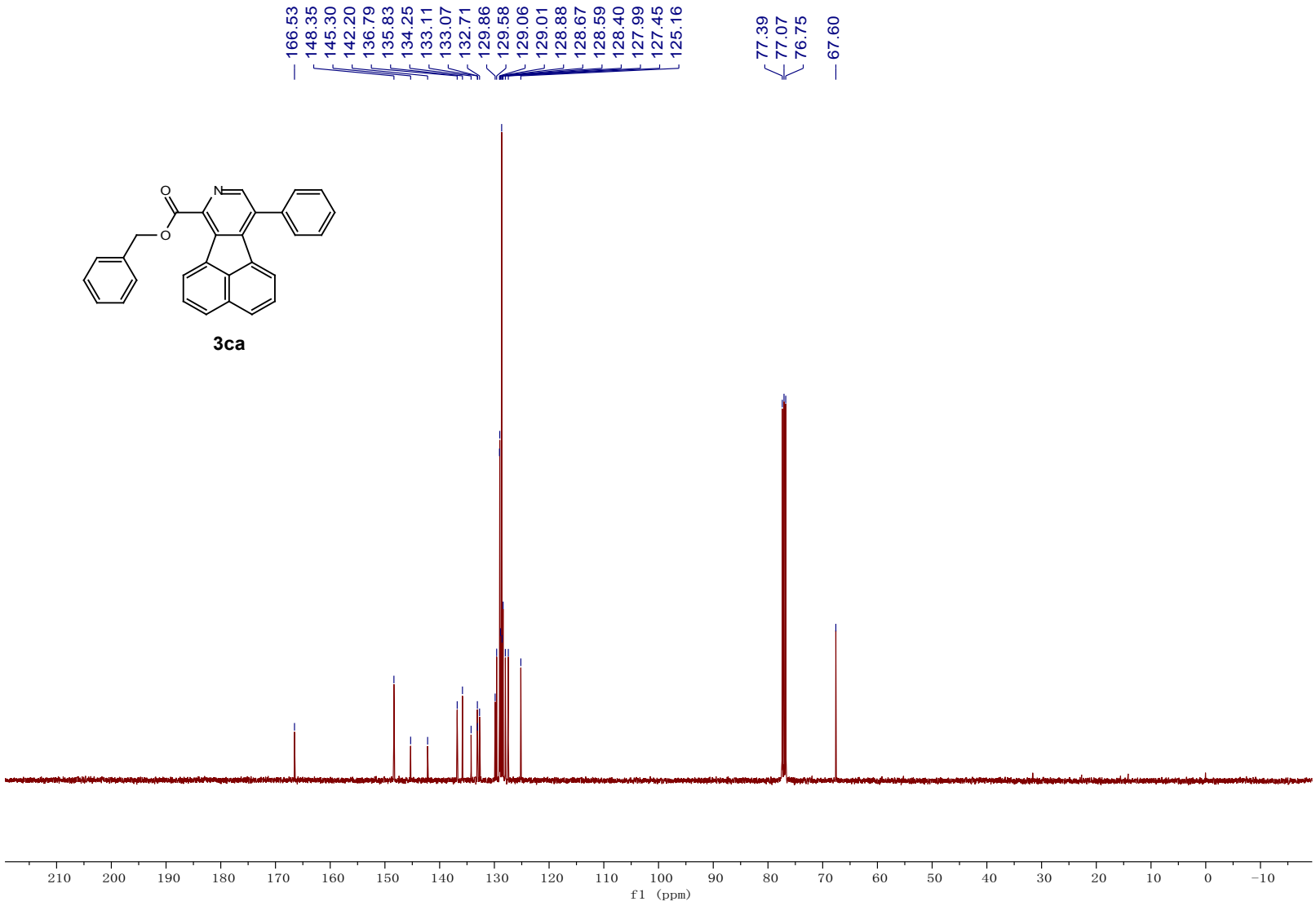
3ba

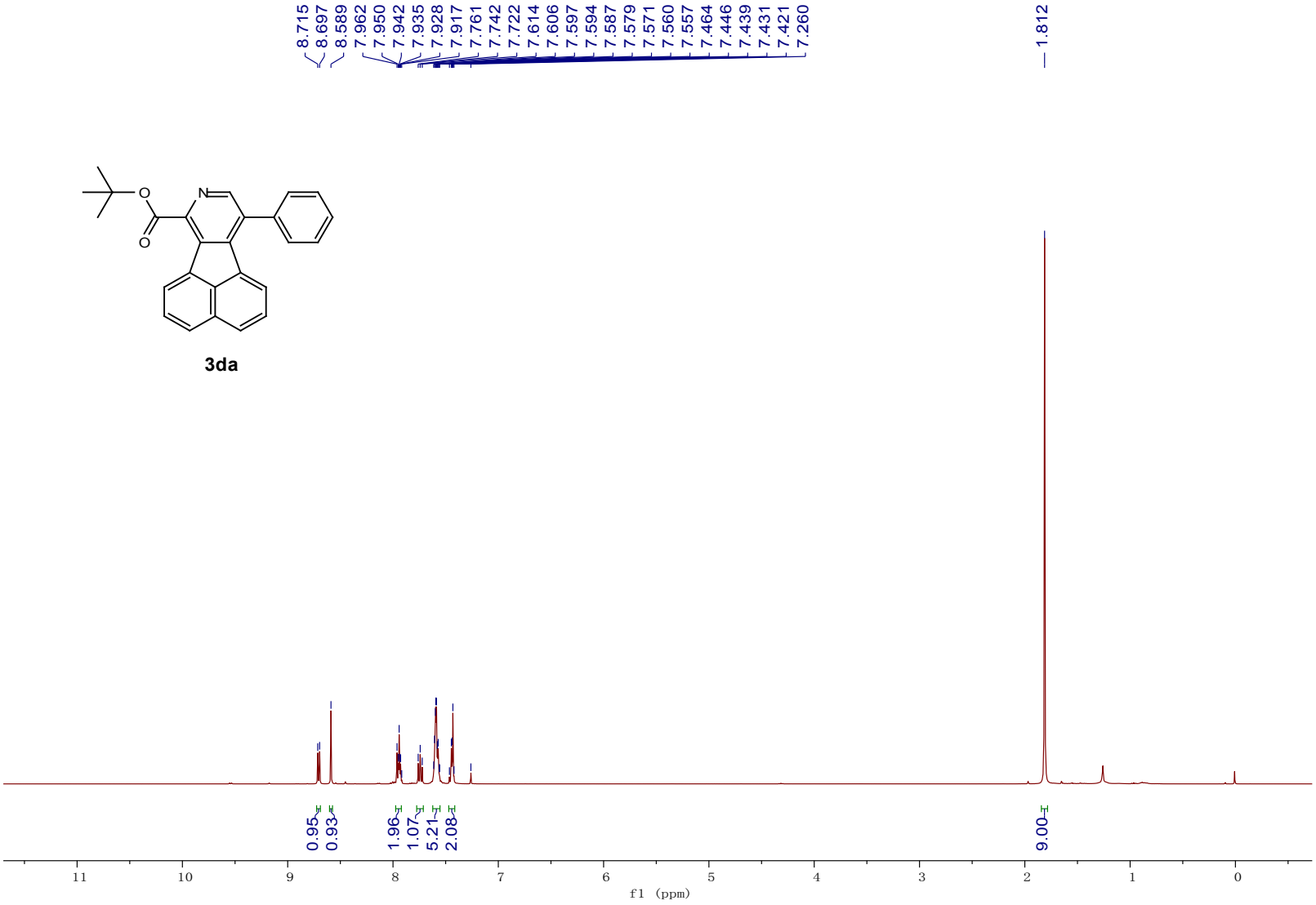

8.799
8.781
8.614
7.956
7.937
7.709
7.690
7.671
7.617
7.600
7.584
7.462
7.444
7.434
7.430
7.414
7.395
7.373
7.355
7.335
7.260
5.663

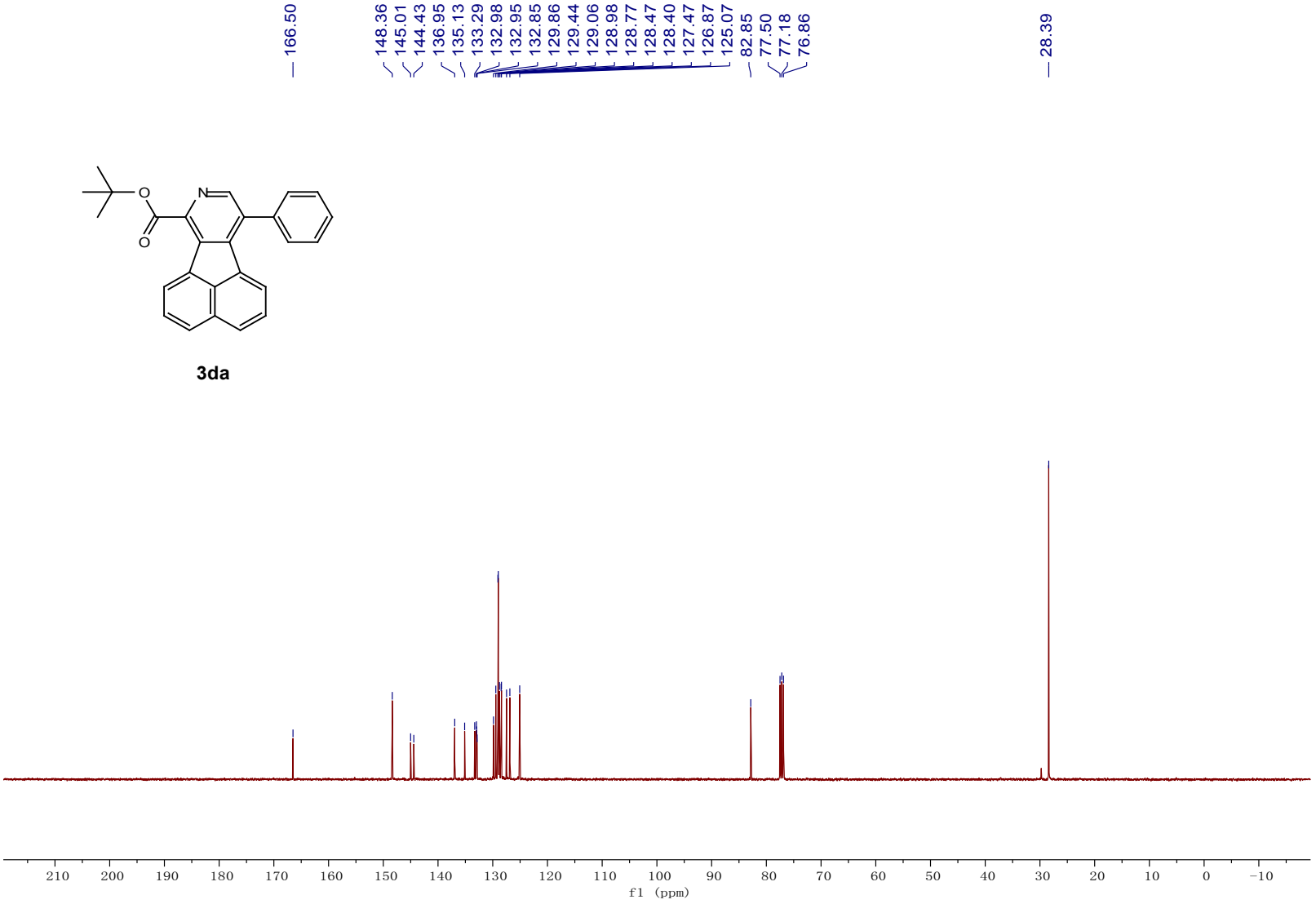

O
N
O

3ca

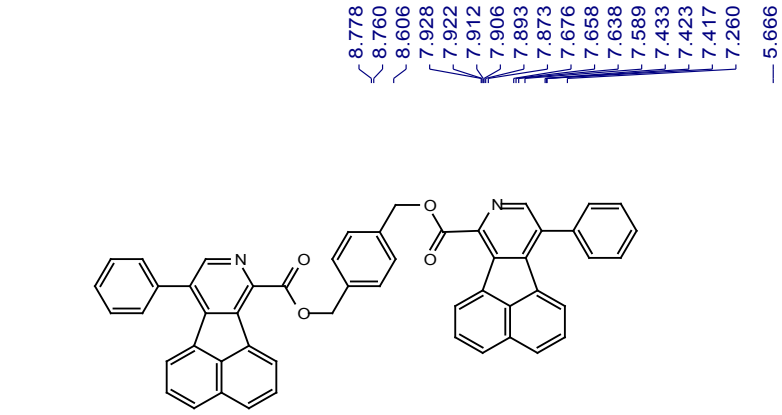

1.00
0.99
2.01
1.04
7.06
4.10
1.03
2.00
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


166.53
148.35
145.30
142.20
136.79
135.83
134.25
133.11
133.07
132.71
129.86
129.58
129.06
129.01
128.88
128.67
128.59
128.40
127.99
127.45
125.16
77.39
77.07
76.75
67.60
O
N
O
3ca
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

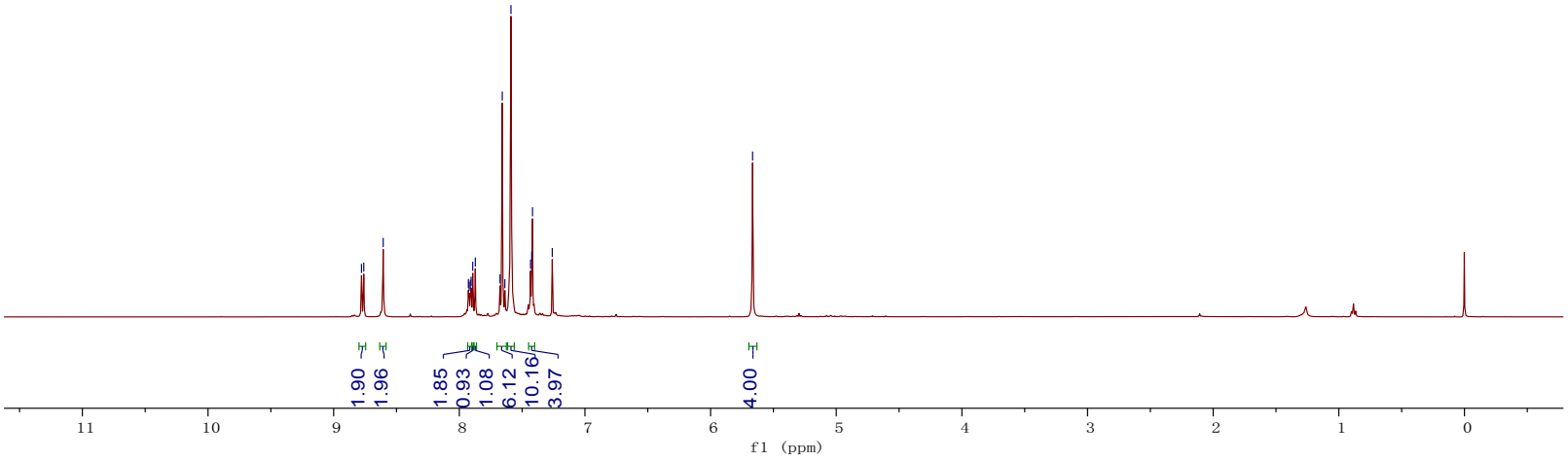

8.715
8.697
8.589
7.962
7.950
7.942
7.935
7.928
7.917
7.761
7.742
7.722
7.614
7.606
7.597
7.594
7.587
7.579
7.571
7.560
7.557
7.464
7.446
7.439
7.431
7.421
7.260
1.812
O
O
N
3da
0.95
0.93
1.96
1.07
5.21
2.08
9.00
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

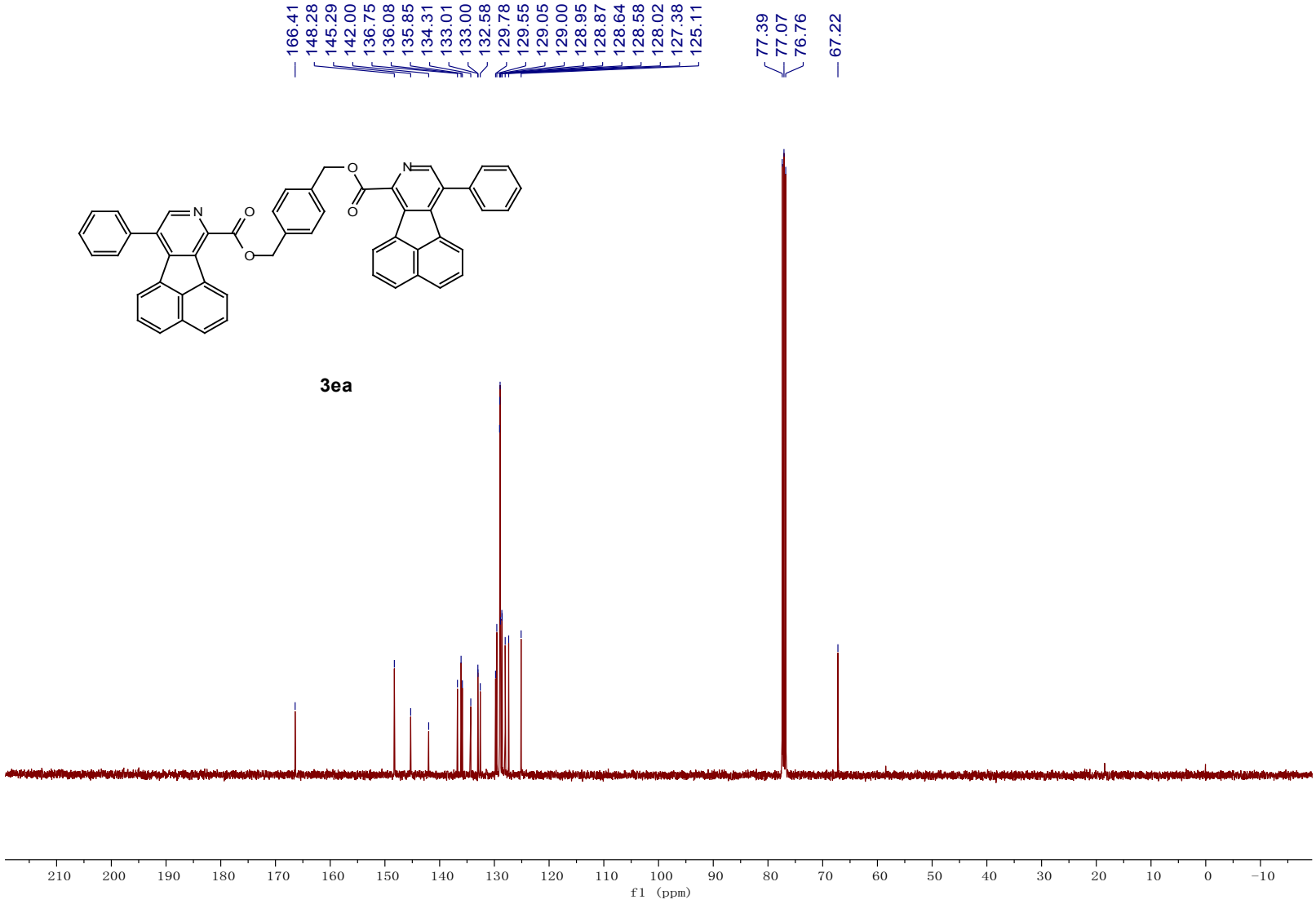

166.50
148.36
145.01
144.43
136.95
135.13
133.29
132.98
132.95
132.85
129.86
129.44
129.06
128.98
128.77
128.47
128.40
127.47
126.87
125.07
82.85
77.50
77.18
76.86
28.39
O
O
N
f1 (ppm)

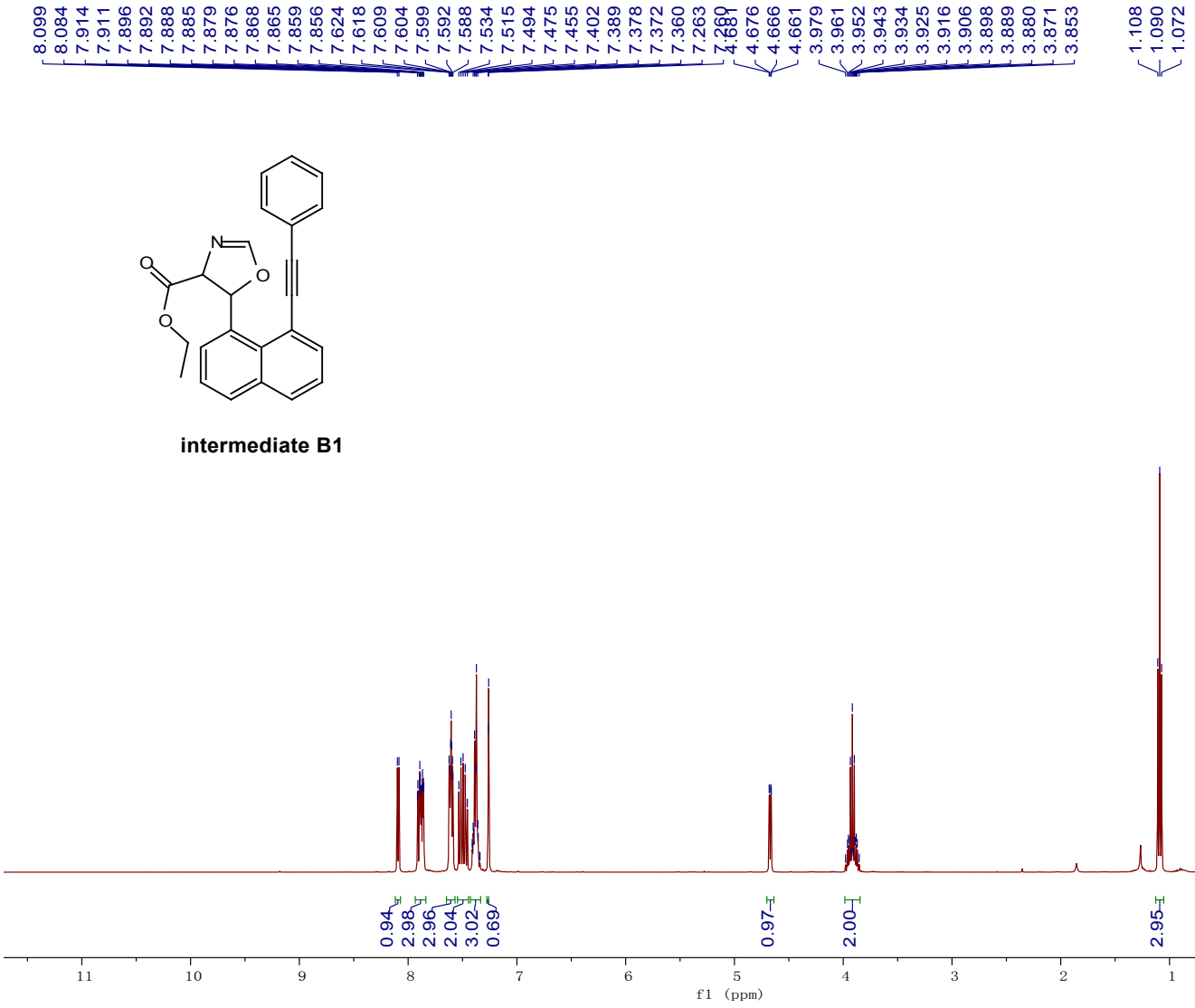
3da


8.778
8.760
8.606
7.928
7.922
7.912
7.906
7.893
7.873
7.676
7.658
7.638
7.589
7.433
7.423
7.417
7.260
5.666
N
O
O
O
O
N

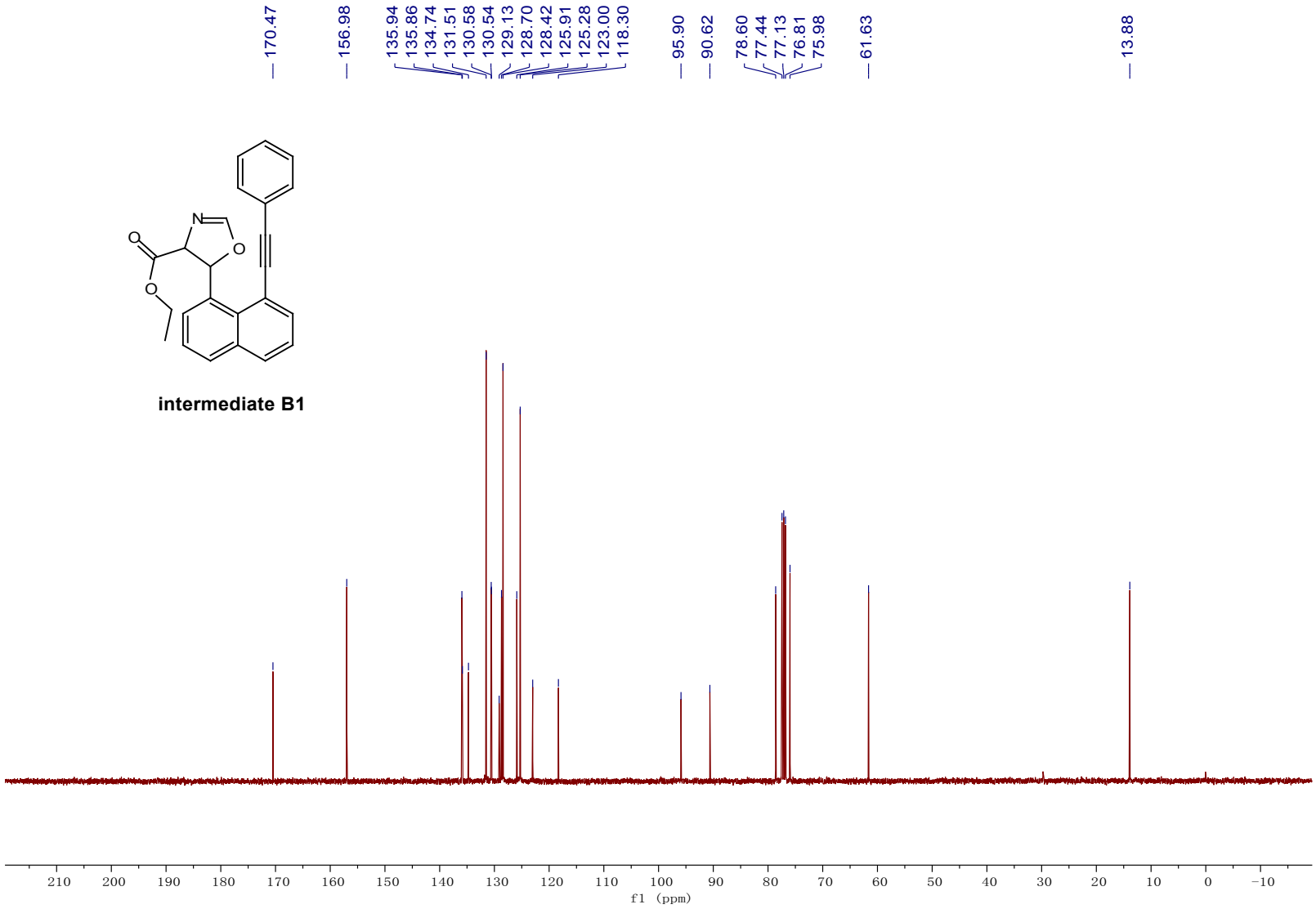
3ea

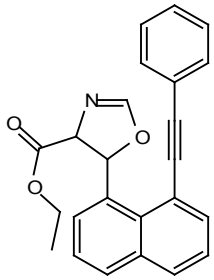

1.90
1.96
1.85
0.93
1.08
6.12
10.16
3.97
4.00
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


166.41
148.28
145.29
142.00
136.75
136.08
135.85
134.31
133.01
133.00
132.58
129.78
129.55
129.05
129.00
128.95
128.87
128.64
128.58
128.02
127.38
125.11
77.39
77.07
76.76
67.22
3ea
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

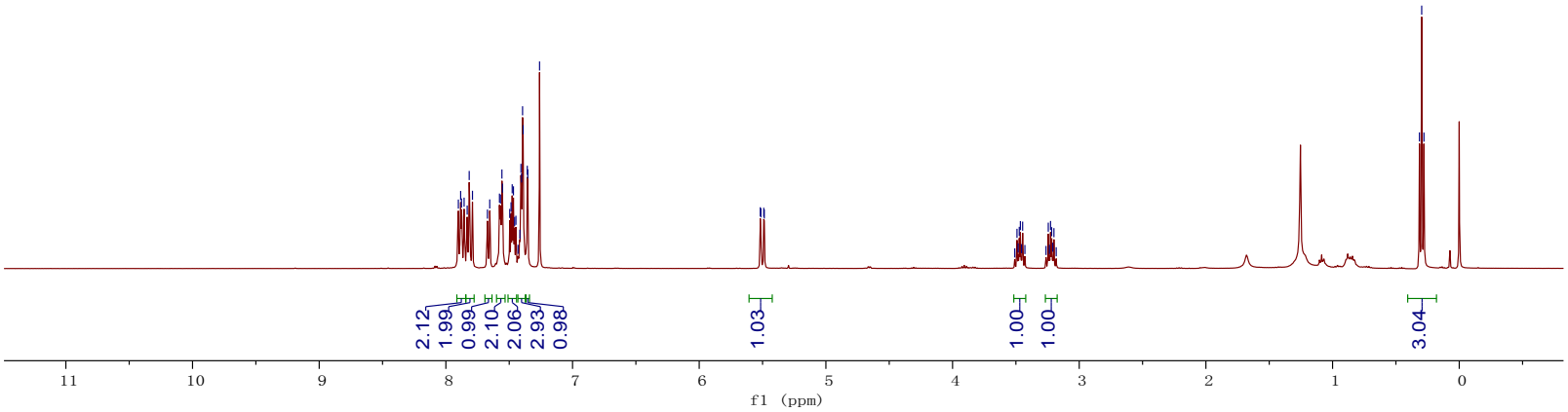


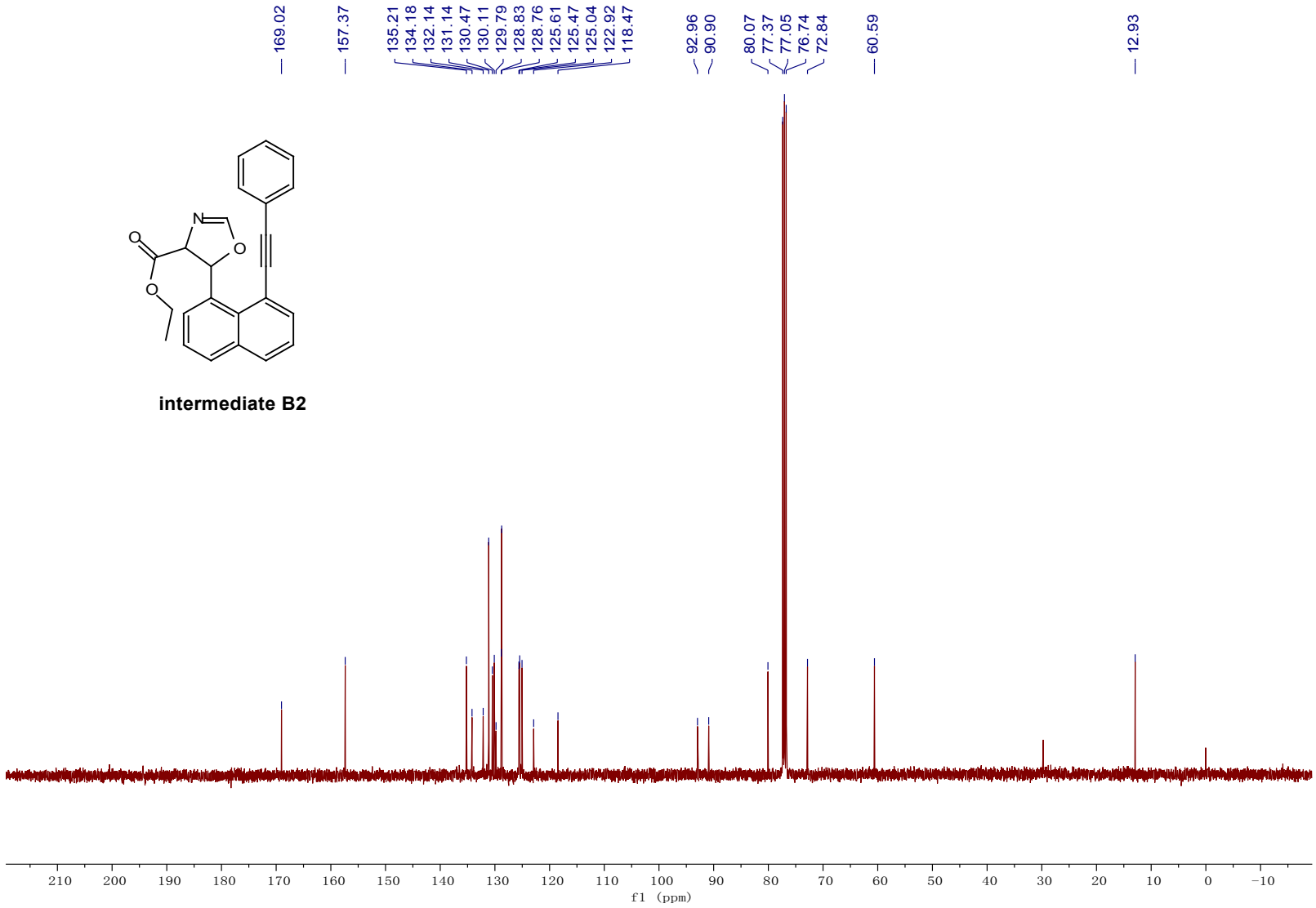
intermediate B1


170.47
156.98
135.94
135.86
134.74
131.51
130.58
130.54
129.13
128.70
128.42
125.91
125.28
123.00
118.30
95.90
90.62
78.60
77.44
77.13
76.81
75.98
61.63
13.88
O
N
O
O
O
intermediate B1
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)



intermediate B2





intermediate B2