Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Silver-Catalysed Tandem Hydroamination and Cyclization of 2-Trifluoromethyl-1,3- Enynes with Primary Amines: A Modular Entry to 4-Trifluoromethyl-3-Pyrrolines

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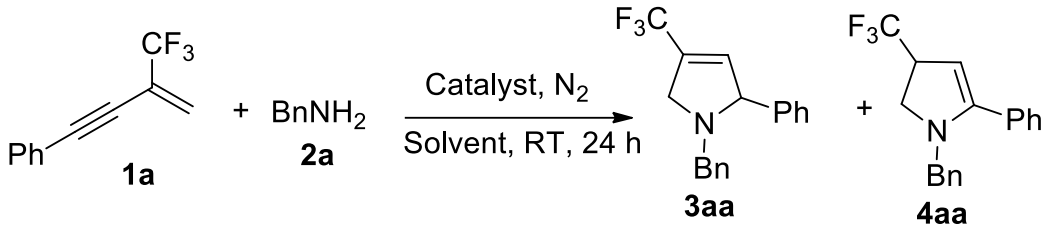
1. General information.

^{1}H NMR spectra, ^{13}C NMR spectra were recorded on a Bruker 400 MHz or 500 MHz spectrometer in chloroform-d3. All signals are reported in ppm with the internal TMS signal at 0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, br = broad signal, coupling constant(s) in Hz, integration). All reactions were carried out under an atmosphere of Argon in flame-dried glassware with magnetic stirring. $ClCH_2CH_2Cl$ (DCE), CH_2Cl_2 (DCM), CH_3CN, DMSO, DMF, Et_2O, chlorobenzene were freshly distilled from CaH_2; toluene and THF was freshly distilled from sodium metal prior to use. 2- trifluoromethyl 1,3-enynes **1** and 2-methyl 1,3-enynes **1z** were prepared in good yields according to the literature.[1] Enyne **1z'** were prepared in good yields according to the literature.[2]

[1] Q. Zeng, L. Zhang, J. Yang, B. Xu, Y. Xiao and J. Zhang, *Chem. Commun*., **2014**, *50*, 4203.

[2] H. Qian, X. Yu, J. Zhang, and J. Sun. *J. Am. Chem. Soc.*, **2013**, *135*, 18020.

2. Table S1. Screening results of reaction conditions.[a]



entry	Catalyst	Solvent	**2a**(equiv)/additive	**3aa** [%][b]	**4aa** [%][b]
1	$AgNO_3$	Et_2O	2.0/--	70(67)	21
2	$AgNO_3$	DCE	2.0/--	75	10
3	$FeCl_3$	DCE	2.0/--	--	--
4	$AuCl_3$	DCE	2.0/--	--	15
5	$PtCl_4$	DCE	2.0/--	--	12
6	$AgNO_3$	CH_3CN	2.0/--	57	27
7	$AgNO_3$	DMSO	2.0/--	29	60
8	$AgNO_3$	DMF	2.0/--	31	38
9	$AgNO_3$	Toluene	2.0/--	80	13
10	$CuBr_2$	Toluene	2.0/--	--	16
11	CuBr	Toluene	2.0/--	36	10
12	**$AgNO_3$**	**PhCl**	**2.0/--**	**90(85)**	**8**
13	**$AgSbF_6$**	**PhCl**	**2.0/--**	**91(85)**	**6**
14	AgOTf	PhCl	2.0/--	51	36
15	$AgNTf_2$	PhCl	2.0/--	72	25
16	$AgNO_3$	PhCl	1.5/--	50	4
17	$AgNO_3$	PhCl	1.5/Et_3N (1.0)	75	10
18	CF_3COOH	PhCl	2.0/--	-	-
19	CF_3SO_3H	PhCl	2.0/--	-	-

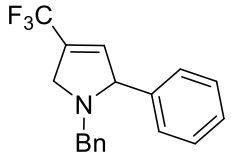
[a] Reactions were conducted on a 0.2 mmol scale, catalyst (10 mol%). [b] NMR yields using CH_2Br_2 as the internal reference, yields of isolated product are shown in parentheses.

To test our double hydroamination strategy for 4-trifluoromethyl-3-pyrrolines synthesis, 2-trifluoromethyl-4-phenyl- 1,3- enyne **1a** and benzylamine **2a** were used as model substrates for reaction screening. Initially, **1a** and **2a** (2.0 equiv) were subjected to the solution of 10 mol % of $AgNO_3$ in Et_2O under nitrogen at room temperature, to our pleased, the reaction indeed yielded desired 3-pyrroline **3aa** in 67% isolated yield, along with 2-pyrroline **4aa** in 21% NMR yield (Table S1, entry 1). The structure of **3aa** was unambiguously confirmed by x-ray crystallography analysis. The discovery of this reaction prompted us to optimized the reaction conditions towards maximizing the formation of double hydroamination product 3-pyrroline **3aa**. Our effort first turned to identify the most suitable solvent, which proved to be chlorobenzene (Table S1, entry 12), compared with other solvents (Table S1, entries 1-3, 7-9). The amount of primary amine used is critical for achieving high yield, with two equivalents being ideal (Table S1, compared entry 12 to entries 16-17). In addition, screening other silver catalysts revealed that $AgSbF_6$ was shown to be as effective as the $AgNO_3$ (Table S1, entries 12-15). While other metal catalyst such as $FeCl_3$, $AuCl_3$, $PtCl_4$, $CuBr_2$ and CuBr were ineffective catalysts (Table S1, entries 3-5, 10-11). Brönsted acid such as trifluoroacetic acid, methanesulfonic acid could not catalyzed the present transformation, no cyclization product **3aa** or **4aa** could be formed. (Table S1, entries 18-19). Considering the reaction economic efficiency, we

choose $AgNO_3$ as optimum catalyst for investigation the substrate scope.

3. General procedure for the synthesis of products 3

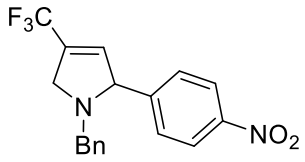
To the solution of 2-trifluoromethyl 1,3-conjugated enynes **1** (0.5 mmol), silver nitrate (10 mol %) in chlorobenzene (3.0 mL) under nitrogen at room temperature was added primary amine (1.0 mmol), the reaction was stirred at room temperature for 24 h. After **1** was completely consumed, which was determined by TLC analysis, the solvent was removed under reduced pressure and the crude reaction mixture was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 200:1~1:1) to give the desired 4-Trifluoromethyl-3-Pyrrolines **3**.



3aa

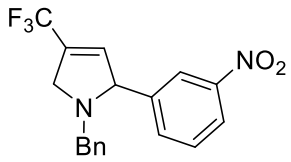
85% isolated yield. Colorless solid. Mp 53.4-54.6 ^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.2 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.31–7.24 (m, 5H), 7.23–7.18 (m, 1H), 6.19 (s, 1H), 4.71 (dd, *J* = 5.2, 2.7 Hz, 1H), 3.93 (d, *J* = 13.2 Hz, 1H), 3.85 (dd, *J* = 13.3, 5.2 Hz, 1H), 3.53 (d, *J* = 13.2 Hz, 1H), 3.46 (dd, *J* = 13.3, 6.3 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.30. ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.67, 138.73, 136.03 (q, *J* = 5.0 Hz), 130.48 (q, *J* = 34.6 Hz), 128.55 , 128.47 , 128.36 , 127.91 , 127.86 ,

127.13 , 121.85 (q, J = 269.0 Hz), 73.99 , 57.00 , 56.06 . HRMS(ESI) calcd for $C_{18}H_{17}F_3N$ [M+H$^+$]: 304.1308, found: 304.1317.



3ba

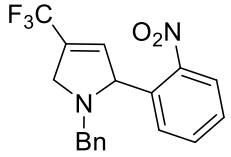
81% isolated yield .Yellow solid. Mp 63.7-66.8 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.8 Hz, 2H), 7.61 (d, J = 8.7 Hz, 2H), 7.36–7.19 (m, 5H), 6.17 (s, 1H), 4.92-4.84 (m, 1H), 3.96 (dd, J = 14.3, 6.2 Hz, 1H), 3.91 (d, J = 13.3 Hz, 1H), 3.66 (d, J = 13.3 Hz, 1H), 3.62–3.52 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.44. ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.32, 147.59, 137.91, 134.41 (q, J = 4.9 Hz), 131.62 (q, J = 35.0 Hz), 128.56, 128.46, 128.44, 127.44, 123.81, 121.47 (q, J = 269.2 Hz), 73.44, 57.44, 56.42. HRMS(ESI) calcd for $C_{18}H_{16}F_3N_2O_2$ [M+H$^+$]: 349.1165, found: 349.1158.



3ca

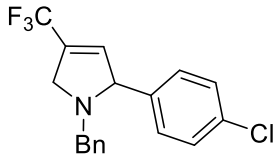
94% isolated yield. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (t, J = 1.9 Hz, 1H), 8.18-8.12 (m, 1H), 7.80–7.74 (m, 1H), 7.54 (t, J = 7.9 Hz, 1H), 7.34–7.18 (m, 5H), 6.20-6.16 (m, 1H), 4.90-4.84 (m, 1H), 3.97 (dd, J = 13.6, 6.7 Hz, 1H), 3.92 (d, J = 13.2 Hz, 1H), 3.67 (d, J = 13.2 Hz, 1H), 3.62-3.52 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.41. ^{13}C NMR (100

MHz, $CDCl_3$) δ 148.40, 143.31, 137.87, 134.54 (q, *J* = 4.9 Hz), 133.85, 131.58 (q, *J* = 35.0 Hz), 129.49, 128.47, 128.44, 127.38, 122.90, 122.73, 121.48 (q, *J* = 269.2 Hz), 73.35, 57.36, 56.35. HRMS(ESI) calcd for $C_{18}H_{16}F_3N_2O_2$ [M+H^+]: 349.1169, found: 349.1158.



3da

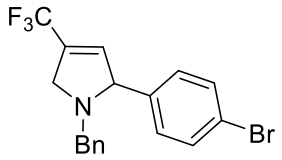
65% isolated yield. Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.93 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.69 (td, *J* = 7.9, 1.1 Hz, 1H), 7.47–7.39 (m, 1H), 7.35–7.17 (m, 5H), 6.41–6.37 (m, 1H), 5.34-5.28 (m, 1H), 3.97 (dd, *J* = 13.6, 5.5 Hz, 1H), 3.86 (d, *J* = 13.1 Hz, 1H), 3.63 (d, *J* = 13.1 Hz, 1H), 3.59–3.50 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.42. ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.87, 138.04, 136.54, 135.11 (q, *J* = 5.0 Hz), 133.66, 130.79 (q, *J* = 34.9 Hz), 130.24, 128.47, 128.43(2C), 127.36, 124.27, 121.58 (q, *J* = 269.2 Hz), 70.03, 58.05, 56.31. HRMS(ESI) calcd for $C_{18}H_{16}F_3N_2O_2$ [M+H^+]: 349.1169, found: 349.1158.



3ea

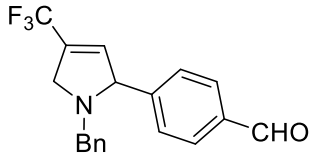
94% isolated yield. Colorless solid. Mp 39.9-41.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.31 (m, 4H), 7.31–7.21 (m, 5H), 6.16 (s, 1H), 4.73-4.67 (m, 1H), 3.91 (d, *J* = 13.2 Hz, 1H), 3.87 (dd, *J* = 13.5, 5.4 Hz, 1H), 3.55 (d,

J = 13.2 Hz, 1H), 3.51-3.43 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.38 . ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.28, 138.42, 135.47 (q, *J* = 5.0 Hz), 133.58, 130.85 (q, *J* = 34.8 Hz), 129.19, 128.70, 128.43, 128.40, 127.24, 121.69 (q, *J* = 269.1 Hz), 73.31, 56.97, 56.04. HRMS(ESI) calcd for $C_{18}H_{16}ClF_3N$ [M+H$^+$]: 338.0918, found: 338.0922.



3fa

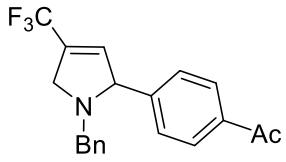
82% isolated yield. Colorless solid. Mp 66.5-68.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.3 Hz, 2H), 7.30 (d, *J* = 8.3 Hz, 2H), 7.22-7.34 (m, 5H), 6.16 (s, 1H), 4.69 (s, 1H), 3.91 (d, *J* = 13.2 Hz, 1H), 3.86 (dd, *J* = 13.5, 5.3 Hz, 1H), 3.55 (d, *J* = 13.2 Hz, 1H), 3.48 (dd, *J* = 13.4, 6.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.38. ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.81, 138.39, 135.38 (q, *J* = 5.0 Hz), 131.65, 130.88 (q, *J* = 34.8 Hz), 129.55, 128.42, 128.40, 127.24, 121.73, 121.67 (q, *J* = 269.1 Hz), 73.37, 56.98, 56.05. HRMS(ESI) calcd for $C_{18}H_{16}BrF_3N$ [M+H$^+$]: 382.0413, found: 382.0418.



3ga

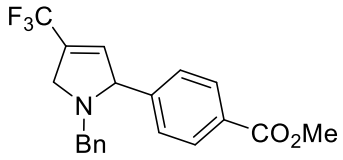
70% isolated yield. Colorless solid. Mp 50.2-51.5 °C. ^{1}H NMR (400 MHz,

$CDCl_3$) δ 10.03 (s, 1H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.34–7.20 (m, 5H), 6.21–6.17 (m, 1H), 4.87-4.80 (m, 1H), 3.93 (d, *J* = 13.2 Hz, 1H), 3.93 (dd, *J* = 13.3, 4.5 Hz, 1H), 3.62 (d, *J* = 13.2 Hz, 1H), 3.58-3.50 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.40. ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.94, 147.77, 138.19, 136.06, 134.89 (q, *J* = 4.9 Hz), 131.25 (q, *J* = 34.9 Hz), 130.07, 128.43, 127.33, 121.58 (q, *J* = 269.3 Hz), 73.87, 57.37, 56.36. HRMS(ESI) calcd for $C_{19}H_{17}F_3NO$ [M+H^+]: 332.1257, found: 332.1264.



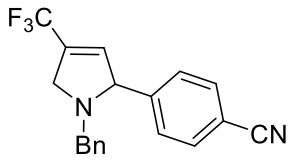
3ha

75% isolated yield. Colorless solid. Mp 80.3-82.2 °C. ^1H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.34–7.19 (m, 5H), 6.21–6.16 (m, 1H), 4.85–4.76 (m, 1H), 3.92 (d, *J* = 13.2 Hz, 1H), 3.91 (dd, *J* = 13.3, 7.3 Hz, 1H), 3.60 (d, *J* = 13.2 Hz, 1H), 3.57–3.47 (m, 1H), 2.61 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.39. ^{13}C NMR (125 MHz, $CDCl_3$) δ 197.72, 146.14, 138.31, 136.82, 135.10 (q, *J* = 4.9 Hz), 131.14 (q, *J* = 34.8 Hz), 128.67, 128.43, 128.41, 127.98, 127.28, 121.65 (q, *J* = 269.2 Hz), 73.73, 57.23, 56.25, 26.64. HRMS(ESI) calcd for $C_{20}H_{19}F_3NO$ [M+H^+]: 346.1413, found: 346.1419.



3ia

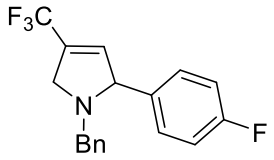
55% isolated yield. White solid. Mp 65.0-66.6 ºC. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 8.2 Hz, 2H), 7.34–7.16 (m, 5H), 6.19 (s, 1H), 4.85–4.75 (m, 1H), 3.92 (d, *J* = 13.2 Hz, 1H), 3.92 (s, 3H), 3.90 (dd, *J* = 13.3, 7.3 Hz, 1H), 3.59 (d, *J* = 13.2 Hz, 1H), 3.56–3.45 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.40. ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.86, 145.96, 138.34, 135.19 (q, *J* = 5.0 Hz), 131.09 (q, *J* = 34.8 Hz), 129.90, 129.79, 128.46, 128.40, 127.80, 127.27, 121.67 (q, *J* = 269.2 Hz), 73.77, 57.22, 56.24, 52.10. HRMS(ESI) calcd for $C_{20}H_{19}F_3NO_2$ [M+H$^+$]: 362.1362, found: 362.1373.



3ja

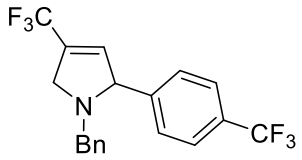
53% isolated yield. Colorless solid. Mp 51.0-52.0 ºC. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.33–7.18 (m, 5H), 6.16–6.11 (m, 1H), 4.84-4.74 (m, 1H), 3.92 (dd, *J* = 13.1, 6.0 Hz, 1H), 3.88 (d, *J* = 13.1 Hz, 1H), 3.62 (d, *J* = 13.1 Hz, 1H), 3.58–3.48 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.38. ^{13}C NMR (125 MHz, $CDCl_3$) δ 146.31, 137.96, 134.56 (q, *J* = 4.9 Hz), 132.33, 131.42 (q, *J* = 34.9 Hz), 128.43, 128.39(2C), 127.34, 121.49 (q, *J* = 269.3 Hz), 118.67, 111.64, 73.64, 57.34, 56.33. HRMS(ESI) calcd for $C_{19}H_{16}F_3N_2$ [M+H$^+$]: 329.1260,

found: 329.1262.



3ka

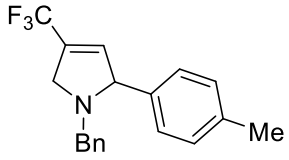
91% isolated yield. Colorless solid. Mp 45.3-46.0 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44–7.34 (m, 2H), 7.33–7.18 (m, 5H), 7.09–7.00 (m, 2H), 6.19–6.13 (m, 1H), 4.75-4.65 (m, 1H), 3.92 (d, *J* = 13.2 Hz, 1H), 3.88 (dd, *J* = 13.1, 6.0 Hz, 1H), 3.54 (d, *J* = 13.2 Hz, 1H), 3.51–3.42 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.38, -114.61. ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.44 (d, *J* = 245.9 Hz), 138.53, 136.46 (d, *J* = 2.6 Hz), 135.75 (q, *J* = 4.8 Hz), 130.67 (q, *J* = 34.8 Hz), 129.42 (d, *J* = 8.1 Hz), 128.43, 128.38, 127.20, 121.76 (q, *J* = 269.0 Hz), 115.37 (d, *J* = 21.5 Hz), 73.25, 56.91, 56.01. HRMS(ESI) calcd for $C_{18}H_{16}F_4N$ [M+H$^+$]: 322.1413, found: 322.1224.



3la

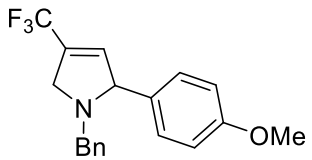
67% isolated yield. Colorless solid. Mp 61.7-62.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 2H), 7.34–7.20 (m, 5H), 6.20–6.14 (m, 1H), 4.85-4.75 (m, 1H), 3.91 (dd, *J* = 13.3, 6.1 Hz, 1H), 3.92 (d, *J* = 13.2 Hz, 1H), 3.60 (d, *J* = 13.2 Hz, 1H), 3.57–3.47 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.44, -65.45. ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.92, 138.25, 135.09 (q, *J* = 4.9 Hz), 131.24 (q, *J* = 34.8 Hz),

130.18 (q, *J* = 32.4 Hz), 128.46, 128.44, 128.14, 127.33, 125.54 (q, *J* = 3.8 Hz), 124.12 (q, *J* = 272.1 Hz), 121.65 (q, *J* = 269.2 Hz), 73.65, 57.25, 56.27. HRMS(ESI) calcd for $C_{19}H_{16}F_6N$ [M+H$^+$]: 372.1181, found: 372.1193.



3ma

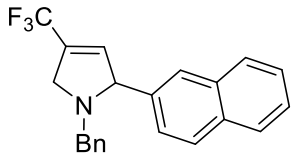
71% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.8 Hz, 2H), 7.28–7.19 (m, 5H), 7.17 (d, *J* = 7.8 Hz, 2H), 6.17 (s, 1H), 4.66 (s, 1H), 3.93 (d, *J* = 13.2 Hz, 1H), 3.87–3.79 (m, 1H), 3.50 (d, *J* = 13.2 Hz, 1H), 3.47–3.40 (m, 1H), 2.34 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.27. ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.82, 137.65, 137.62, 136.22 (q, *J* = 4.9 Hz), 130.36 (q, *J* = 34.6 Hz), 129.25, 128.48, 128.34, 127.82, 127.10, 121.89 (q, *J* = 268.9 Hz), 73.70, 56.90, 55.97, 21.11. HRMS(ESI) calcd for $C_{19}H_{19}F_3N$ [M+H$^+$]: 318.1464, found: 318.1475.



3na

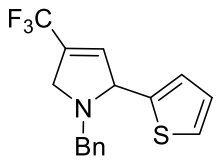
78% isolated yield. Colorless solid. Mp 56.2-58.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.6 Hz, 2H), 7.31–7.20 (m, 5H), 6.90 (d, *J* = 8.6 Hz, 2H), 6.20-6.16 (m, 1H), 4.63-4.69 (m, 1H), 3.93 (d, *J* = 13.2 Hz, 1H), 3.81 (s, 3H), 3.82 (dd, *J* = 13.3, 6.1 Hz, 1H), 3.51 (d, *J* = 13.2 Hz, 1H), 3.48–

3.40 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.35. ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.33, 138.81, 136.23 (q, *J* = 5.0 Hz), 132.70, 130.32 (q, *J* = 34.7 Hz), 129.01, 128.46, 128.33, 127.09, 121.87 (q, *J* = 268.9 Hz), 113.89, 73.33, 56.78, 55.89, 55.28. HRMS(ESI) calcd for $C_{19}H_{19}F_3NO$ [M+H$^+$]: 334.1413, found: 334.1418.



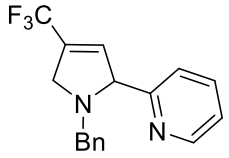
3oa

52% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 7.1 Hz, 1H), 7.96–7.92 (m, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.63–7.50 (m, 3H), 7.42–7.26 (m, 5H), 6.46 (s, 1H), 5.51 (s, 1H), 4.08 (d, *J* = 13.3 Hz, 1H), 4.04 (dd, *J* = 12.3, 6.0 Hz, 1H), 3.64 (d, *J* = 13.2 Hz, 1H), 3.64–3.54 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.38. ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.74, 135.85 (d, *J* = 5.0 Hz), 135.36, 134.03, 131.46, 130.45 (q, *J* = 34.8 Hz), 129.02, 128.48, 128.44, 128.34, 127.18, 126.14, 125.73, 125.60, 125.48, 122.81, 121.86 (q, *J* = 269.1 Hz), 71.18, 57.71, 56.04. HRMS(ESI) calcd for $C_{22}H_{19}F_3N$ [M+H$^+$]: 354.1464, found: 354.1474.



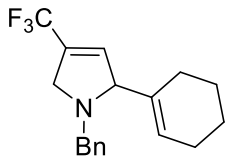
3pa

91% isolated yield. Colorless solid. Mp 60.6-62.7 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40–7.26 (m, 6H), 7.06–6.97 (m, 2H), 6.26 (s, 1H), 5.09 (s, 1H), 4.09 (d, *J* = 13.1 Hz, 1H), 3.83 (dd, *J* = 13.5, 4.8 Hz, 1H), 3.59 (d, *J* = 13.1 Hz, 1H), 3.51–3.40 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.44. ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.96, 138.47, 135.52 (q, *J* = 5.0 Hz), 130.65 (q, *J* = 34.9 Hz), 128.51, 128.41, 127.25, 126.80, 125.53, 124.67, 121.72 (q, *J* = 269.1 Hz), 69.14, 56.89, 55.56. HRMS(ESI) calcd for $C_{16}H_{15}F_3NS$ [M+H$^+$]: 310.0872, found: 310.0880.



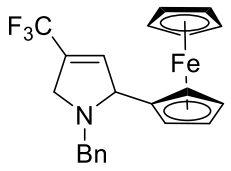
3qa

53% isolated yield. Colorless solid. Mp 56.2-58.4 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57-8.54 (m, 1H), 7.76-7.71 (m, 1H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.34–7.29 (m, 4H), 7.26–7.23 (m, 1H), 7.22-7.18 (m, 1H), 6.36-6.32 (m, 1H), 5.00-4.94 (m, 1H), 4.03 (d, *J* = 13.4 Hz, 1H), 3.95 (dd, *J* = 13.5, 5.6 Hz, 1H), 3.70 (d, *J* = 13.4 Hz, 1H), 3.59–3.52 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.37. ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.75, 149.09, 138.51, 137.00, 134.92 (q, *J* = 5.0 Hz), 130.93 (q, *J* = 34.7 Hz), 128.45, 128.43, 127.23, 122.58, 121.71 (q, *J* = 269.2 Hz), 121.67, 76.06, 57.88, 56.63. HRMS(ESI) calcd for $C_{17}H_{16}F_3N$ [M+H$^+$]: 305.1260, found: 305.1267.



3ra

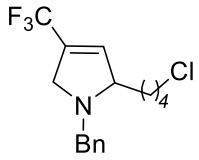
80% isolated yield. Colorless solid. Mp 51.2-52.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.21 (m, 5H), 6.16–6.11 (m, 1H), 5.71 (s, 1H), 4.04 (s, 1H), 3.98 (d, *J* = 13.4 Hz, 1H), 3.74 (dd, *J* = 13.2, 5.3 Hz, 1H), 3.44 (d, *J* = 13.4 Hz, 1H), 3.35–3.28 (m, 1H), 2.27–2.17 (m, 1H), 2.07-2.00 (m, 2H), 1.86-1.76 (m, 1H), 1.70–1.52 (m, 4H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.35. ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.45, 136.49, 135.46 (q, *J* = 5.0 Hz), 130.80 (q, *J* = 34.4 Hz), 128.37, 128.32, 126.94, 125.61, 121.84 (q, *J* = 268.9 Hz), 76.86, 56.97, 56.20, 25.20, 24.71, 22.70, 22.66. HRMS(ESI) calcd for $C_{18}H_{21}F_3N$ [M+H$^+$]: 308.1621, found: 308.1630.



3sa

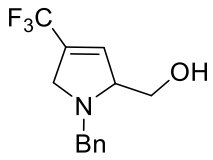
83% isolated yield. Red oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36–7.22 (m, 5H), 6.54 (s, 1H), 4.72–4.62 (m, 1H), 4.23–4.09 (m, 9H), 3.98 (d, *J* = 13.3 Hz, 1H), 3.73 (dd, *J* = 13.5, 4.3 Hz, 1H), 3.58 (d, *J* = 13.3 Hz, 1H), 3.54–3.45 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.14. ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.90, 135.46 (q, *J* = 5.0 Hz), 130.66 (q, *J* = 34.5 Hz), 128.49, 128.34, 127.06, 121.90 (q, *J* = 269.1 Hz), 86.80, 68.64, 68.47, 68.44, 67.88, 66.55, 57.26, 56.47. HRMS(ESI) calcd for $C_{22}H_{21}F_3FeN$

[M+H$^+$]: 412.0970, found: 412.0986.



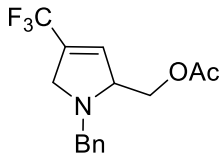
3ta

43% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.32 (m, 4H), 7.31–7.26 (m, 1H), 6.25 (s, 1H), 4.03 (d, *J* = 13.3 Hz, 1H), 3.85–3.75 (m, 2H), 3.59 (d, *J* = 13.3 Hz, 1H), 3.55 (t, *J* = 6.6 Hz, 2H), 3.38 (d, *J* = 10.1 Hz, 1H), 1.86–1.76 (m, 2H), 1.68–1.42 (m, 4H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.36. ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.12, 134.90 (q, *J* = 4.9 Hz), 130.46 (q, *J* = 34.4 Hz), 128.45, 128.42, 127.17, 121.82 (q, *J* = 268.9 Hz), 70.37, 58.77, 57.31, 44.80, 33.16, 32.69, 22.77. HRMS(ESI) calcd for $C_{16}H_{20}ClF_3N$ [M+H$^+$]: 318.1231, found: 318.1236.



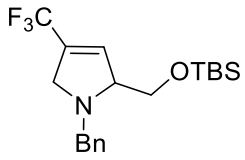
3ua

62% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40–7.27 (m, 5H), 6.27–6.20 (m, 1H), 4.04 (d, *J* = 13.1 Hz, 1H), 3.98-3.90 (m, 1H), 3.85 (dd, *J* = 13.6, 5.3 Hz, 1H), 3.67 (d, *J* = 13.1 Hz, 1H), 3.68 – 3.57 (m, 2H), 3.54-3.44 (m, 1H), 2.64 (brs, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.73. ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.18, 133.47 (q, *J* = 4.9 Hz), 131.60 (q, *J* = 34.8 Hz), 128.62, 128.47, 127.53, 121.42 (q, *J* = 269.1 Hz), 71.67, 61.17, 58.16, 57.33. HRMS(ESI) calcd for $C_{13}H_{15}F_3O$ [M+H$^+$]: 258.1100, found: 258.1104.



3va

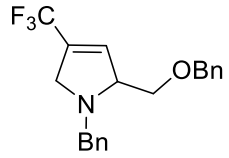
81% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37–7.24 (m, 5H), 6.29–6.24 (m, 1H), 4.26-4.16 (m, 1H), 4.10 (d, *J* = 13.3 Hz, 1H), 4.08–3.95 (m, 2H), 3.83 (dd, *J* = 15.2, 4.1 Hz, 1H), 3.69 (d, *J* = 13.3 Hz, 1H), 3.52–3.40 (m, 1H), 2.07 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -65.43. ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.74, 138.57, 132.23 (q, *J* = 4.9 Hz), 132.02 (q, *J* = 34.9 Hz), 128.47, 128.44, 127.32, 121.54 (q, *J* = 269.1 Hz), 69.22, 65.62, 59.00, 57.39, 20.77. HRMS(ESI) calcd for $C_{15}H_{17}F_3O_2N$ [M+H$^+$]: 300.1206, found: 300.1216.



3wa

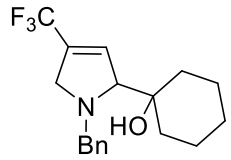
92% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36–7.29 (m, 4H), 7.28–7.23 (m, 1H), 6.33 (s, 1H), 4.08 (d, *J* = 13.3 Hz, 1H), 3.89–3.78 (m, 2H), 3.69 (d, *J* = 13.3 Hz, 1H), 3.66–3.61 (m, 1H), 3.57–3.51 (m, 1H), 3.44 (d, *J* = 12.7 Hz, 1H), 0.88 (d, *J* = 1.7 Hz, 9H), 0.04 (dd, *J* = 5.0, 1.3 Hz, 6H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.41. ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.12, 133.77 (q, *J* = 4.9 Hz), 130.88 (q, *J* = 34.4 Hz), 128.49, 128.42, 127.19, 121.82 (q, *J* = 269.1 Hz), 72.40, 66.01, 59.42, 57.81, 25.84, 18.22, -5.43, -5.47. HRMS(ESI) calcd for $C_{19}H_{29}F_3NOSi$

[M+H$^+$]: 372.1965, found: 372.1980.



3xa

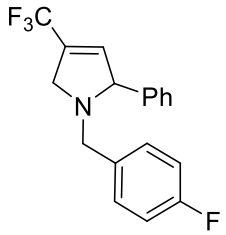
70% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.27 (m, 10H), 6.36 (s, 1H), 4.58 (d, *J* = 12.2 Hz, 1H), 4.55 (d, *J* = 12.2 Hz, 1H), 4.14 (d, *J* = 13.3 Hz, 1H), 4.01 (s, 1H), 3.84 (dd, *J* = 13.6, 4.4 Hz, 1H), 3.70 (d, *J* = 13.3 Hz, 1H), 3.61-3.55 (m, 1H), 3.53–3.48 (m, 1H), 3.46 (d, *J* = 13.7 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.41. ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.97, 138.05, 133.53 (q, *J* = 4.8 Hz), 131.06 (q, *J* = 34.5 Hz), 128.48, 128.41, 127.69, 127.61, 127.19, 121.73 (q, *J* = 269.1 Hz), 73.47, 72.93, 70.29, 59.29, 57.50. HRMS(ESI) calcd for $C_{20}H_{21}F_3NO$ [M+H$^+$]: 348.1570, found: 348.1580.



3ya

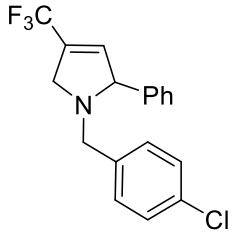
80% isolated yield. Colorless solid. Mp 49.9-51.7 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39–7.23 (m, 5H), 6.31 (s, 1H), 4.12 (d, *J* = 13.8 Hz, 1H), 3.96 –3.76 (m, 2H), 3.72 (d, *J* = 13.8 Hz, 1H), 3.40 (d, *J* = 14.8 Hz, 1H), 2.48 (s, 1H), 1.76–1.50 (m, 7H), 1.49 – 1.30 (m, 2H), 1.29 – 1.11 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.83. ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.99, 131.81 (q, *J* = 4.6 Hz), 131.20 (q, *J* = 34.0 Hz), 128.56, 127.97, 127.29, 121.61 (q, *J* = 269.3 Hz), 80.71, 73.52, 63.00, 59.08, 35.19, 33.63, 25.79,

21.69, 21.59. HRMS(ESI) calcd for $C_{18}H_{23}F_3NO$ [M+H$^+$]: 326.1726, found: 326.1738.



3ab

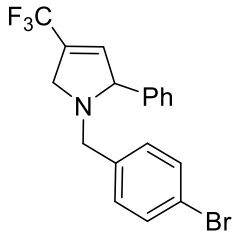
65% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.34 (m, 4H), 7.33–7.27 (m, 1H), 7.25–7.19 (m, 2H), 7.00–6.93 (m, 2H), 6.23–6.18 (m, 1H), 4.74-4.66 (m, 1H), 3.89 (d, *J* = 13.2 Hz, 1H), 3.84 (dd, *J* = 13.3, 5.3 Hz, 1H), 3.53 (d, *J* = 13.2 Hz, 1H), 3.49–3.41 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.36, -115.65. ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.98 (d, *J* = 245.0 Hz), 140.56, 136.01 (q, *J* = 5.0 Hz), 134.44 (d, *J* = 3.1 Hz), 130.43 (q, *J* = 34.7 Hz), 129.93 (d, *J* = 8.0 Hz), 128.58, 127.97, 127.85, 121.80 (q, *J* = 269.0 Hz), 115.14 (d, *J* = 21.3 Hz), 73.99, 56.30, 56.06. HRMS(ESI) calcd for $C_{18}H_{16}F_4N$ [M+H$^+$]: 322.1213, found: 322.1220.



3ac

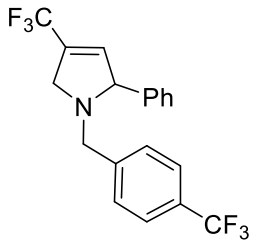
67% isolated yield. Colorless solid. Mp 49.1-50.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.33 (m, 4H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.33–7.23 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.23–6.18 (m, 1H), 4.74-4.67 (m, 1H), 3.89 (d, *J*

= 13.4 Hz, 1H), 3.85 (dd, *J* = 13.3, 5.3 Hz, 1H), 3.52 (d, *J* = 13.4 Hz, 1H), 3.48–3.40 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.35. ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.45, 137.26, 135.98 (q, *J* = 5.0 Hz), 132.80, 130.41 (q, *J* = 34.8 Hz), 129.74, 128.59, 128.49 , 128.01 , 127.85 , 121.77 (q, *J* = 269.0 Hz), 74.03, 56.33, 56.08 . HRMS(ESI) calcd for $C_{18}H_{16}ClF_3N$ [M+H$^+$]: 338.0918, found: 338.0927.



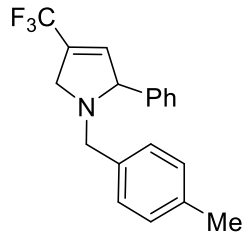
3ad

58% isolated yield. Colorless solid. Mp 64.6-66.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.2 Hz, 2H), 7.40–7.35 (m, 4H), 7.34–7.29 (m, 1H), 7.15 (d, *J* = 8.2 Hz, 2H), 6.22 (s, 1H), 4.72 (s, 1H), 3.88 (d, *J* = 13.4 Hz, 1H), 3.86 (dd, *J* = 13.2, 6.0 Hz, 1H), 3.53 (d, *J* = 13.4 Hz, 1H), 3.46 (dd, *J* = 13.2, 6.0 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.36 . ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.38, 137.74, 135.94 (q, *J* = 5.0 Hz), 131.46, 130.43 (q, *J* = 34.8 Hz), 130.12, 128.60, 128.03, 127.85, 121.76 (q, *J* = 269.1 Hz), 120.93, 74.04, 56.39, 56.09. HRMS(ESI) calcd for $C_{18}H_{16}BrF_3N$ [M+H$^+$]: 382.0413, found: 382.0423.



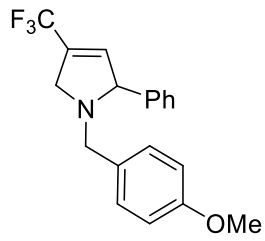
3ae

71% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.0 Hz, 2H), 7.45–7.37 (m, 4H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.36–7.31 (m, 1H), 6.25 (s, 1H), 4.80–4.73 (m, 1H), 4.00 (d, *J* = 13.7 Hz, 1H), 3.90 (dd, *J* = 13.2, 5.3 Hz, 1H), 3.66 (d, *J* = 13.7 Hz, 1H), 3.53-3.45 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.43, -65.39. ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.92, 140.35, 135.95 (q, *J* = 5.0 Hz), 130.43 (q, *J* = 34.7 Hz), 129.44 (q, *J* = 32.3 Hz), 128.64, 128.61, 128.10, 127.86, 125.30 (q, *J* = 3.8 Hz), 124.18 (q, *J* = 272.0 Hz), 121.75 (q, *J* = 269.0 Hz), 74.20, 56.64, 56.21. HRMS(ESI) calcd for $C_{19}H_{16}F_6N$ [M+H$^+$]: 372.1181, found: 372.1191.



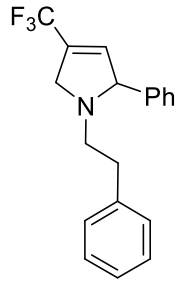
3af

91% isolated yield. Colorless solid. Mp 56.0-58.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.30 (m, 5H), 7.20 (d, J = 7.8 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 6.23 (s, 1H), 4.75 (s, 1H), 3.94 (d, *J* = 13.1 Hz, 1H), 3.89 (dd, *J* = 13.4, 5.0 Hz, 1H), 3.54 (d, *J* = 13.1 Hz, 1H), 3.50 (dd, *J* = 13.4, 5.0 Hz, 1H), 2.36 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.34. ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.72, 136.73, 136.04 (q, *J* = 5.0 Hz), 135.63, 130.47 (q, *J* = 34.6 Hz), 129.04, 128.54, 128.44, 127.85, 121.84 (q, *J* = 269.1 Hz), 73.87, 56.63, 55.96, 21.08. HRMS(ESI) calcd for $C_{19}H_{19}F_3N$ [M+H$^+$]: 318.1464, found: 318.1473.



3ag

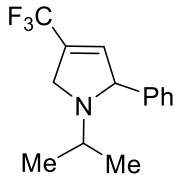
73% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50-7.30 (m, 5H), 7.23 (d, *J* = 8.3 Hz, 2H), 6.88 (d, *J* = 8.3 Hz, 2H), 6.24 (s, 1H), 4.74 (s, 1H), 3.92 (d, *J* = 13.1 Hz, 1H), 3.89 (dd, *J* = 13.4, 5.0 Hz, 1H), 3.82 (s, 3H), 3.53 (d, *J* = 13.1 Hz, 1H), 3.54–3.47 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.34. ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.75, 140.75, 136.06 (q, *J* = 4.7 Hz), 130.80, 130.49 (q, *J* = 34.6 Hz), 129.62, 128.53, 127.85(2C), 121.87 (q, *J* = 268.7 Hz), 113.72, 73.84, 56.31, 55.97, 55.19. HRMS(ESI) calcd for $C_{19}H_{19}F_3NO$ [M+H$^+$]: 334.1413, found: 334.1425.



3ah

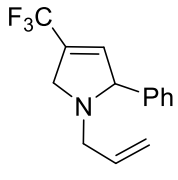
60% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34–7.13 (m, 8H), 7.09 (d, *J* = 7.0 Hz, 2H), 6.16 (s, 1H), 4.66–4.56 (m, 1H), 4.15 (dd, *J* = 13.0, 5.3 Hz, 1H), 3.61 (dd, *J* = 13.0, 6.2 Hz, 1H), 2.98–2.85 (m, 1H), 2.83–2.61 (m, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.21. ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.81, 139.87, 136.11 (q, *J* = 4.9 Hz), 130.11 (q, *J* = 34.6 Hz), 128.61, 128.47, 128.27, 127.73, 127.64, 126.03, 121.87 (q, *J* =

269.0 Hz), 74.50, 56.49, 54.92, 35.35. HRMS(ESI) calcd for $C_{21}H_{17}O_3F$ [M+H$^+$]: 318.1464, found: 318.1471.



3ai

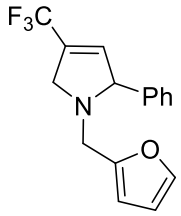
75% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32–7.15 (m, 5H), 6.06–6.03 (m, 1H), 4.84–4.63 (m, 1H), 3.91 (dd, *J* = 13.3, 5.9 Hz, 1H), 3.68 (dd, *J* = 13.3, 5.9 Hz, 1H), 2.89-2.77 (m, 1H), 0.94 (d, *J* = 6.9 Hz, 3H), 0.92 (d, *J* = 6.9 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.27. ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.46, 136.24 (q, *J* = 4.9 Hz), 129.58 (q, *J* = 34.4 Hz), 128.46, 127.49, 127.48, 122.02 (q, *J* = 269.0 Hz), 71.26, 51.98, 50.17, 22.07, 17.75. HRMS(ESI) calcd for $C_{14}H_{17}F_3N$ [M+H$^+$]: 256.1308, found: 256.1312.



3aj

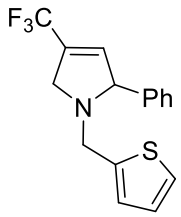
68% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42–7.27 (m, 5H), 6.25–6.18 (m, 1H), 5.90-5.74 (m, 1H), 5.22 (dd, *J* = 17.1, 1.2 Hz, 1H), 5.12 (d, *J* = 10.1 Hz, 1H), 4.71–4.62 (m, 1H), 4.06 (dd, *J* = 13.4, 5.4 Hz, 1H), 3.64–3.52 (m, 1H), 3.43–3.35 (m, 1H), 3.13 (dd, *J* = 13.7, 7.4 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.34. ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.73, 135.98 (q, *J* = 4.9 Hz), 135.27, 130.54 (q, *J* = 34.6

Hz), 128.53, 127.82, 127.76, 121.88 (q, J = 269.0 Hz), 117.23, 73.63, 56.17, 55.77. HRMS(ESI) calcd for $C_{14}H_{15}F_3N$ [M+H$^+$]: 254.1151, found: 254.1156.



3ak

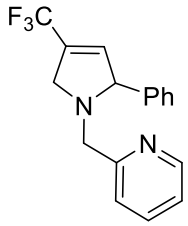
78% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45–7.35 (m, 5H), 7.35–7.29 (m, 1H), 6.32 (dd, J = 3.1, 1.9 Hz, 1H), 6.22-6.17 (m, 2H), 4.81-4.76 (m, 1H), 4.02 (dd, J = 13.2, 5.4 Hz, 1H), 3.84 (d, J = 14.7 Hz, 1H), 3.81–3.74 (m, 1H), 3.70 (d, J = 14.7 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.32. ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.06, 142.22, 140.21, 135.90 (q, J = 5.0 Hz), 130.46 (q, J = 34.7 Hz), 128.57, 127.90, 127.79, 121.79 (q, J = 269.0 Hz), 110.09, 108.38, 72.53, 55.66, 47.70. HRMS(ESI) calcd for $C_{16}H_{15}F_3NO$ [M+H$^+$]: 294.1100, found: 294.1107.



3al

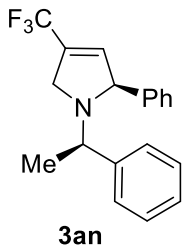
81% isolated yield. Colorless solid. Mp 42.4-43.8 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47–7.37 (m, 4H), 7.36–7.30 (m, 1H), 7.25 (dd, J = 5.1, 1.1 Hz, 1H), 6.96 (dd, J = 5.1, 3.4 Hz, 1H), 6.91 (d, J = 3.3 Hz, 1H), 6.23-6.19 (m,

1H), 4.83-4.77 (m, 1H), 4.05 (d, *J* = 14.2 Hz, 1H), 4.03 (dd, *J* = 13.2, 5.5 Hz, 1H), 3.89 (d, *J* = 14.2 Hz, 1H), 3.69–3.61 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.33. ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.73, 140.28, 135.88 (q, *J* = 5.0 Hz), 130.29 (q, *J* = 34.7 Hz), 128.61, 127.97, 127.76, 126.51, 125.53, 125.14, 121.77 (q, *J* = 269.1 Hz), 73.04, 55.78, 50.75. HRMS(ESI) calcd for $C_{16}H_{15}F_3NS$ [M+H$^+$]: 310.0872, found: 310.0880.



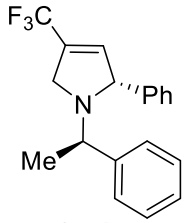
3am

63% isolated yield. Colorless solid. Mp 47.5-49.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.9 Hz, 1H), 7.56-7.49 (m, 1H), 7.34–7.17 (m, 6H), 7.04 (dd, *J* = 6.9, 5.2 Hz, 1H), 6.16–6.13 (m, 1H), 4.79-4.72 (m, 1H), 3.96 (d, *J* = 14.2 Hz, 1H), 3.90 (dd, *J* = 13.3, 5.4 Hz, 1H), 3.76 (d, *J* = 14.2 Hz, 1H), 3.60–3.53 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.33. ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.82, 148.94, 140.46, 136.50, 135.90 (q, *J* = 5.0 Hz), 130.52 (q, *J* = 34.7 Hz), 128.52, 127.91, 127.84, 122.74, 122.04, 121.77 (q, *J* = 269.1 Hz), 74.11, 58.72, 56.41. HRMS(ESI) calcd for $C_{17}H_{16}F_3N_2$ [M+H$^+$]: 305.1260, found: 305.1262.



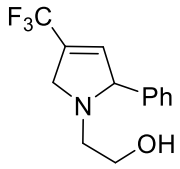
3an

47% isolated yield. Colorless solid. Mp 39.3-40.2 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44–7.23 (m, 10H), 6.11–6.08 (m, 1H), 4.91–4.86 (m, 1H), 3.90 (dd, *J* = 13.6, 5.9 Hz, 1H), 3.81 (q, *J* = 6.8 Hz, 1H), 3.64-3.58 (m, 1H), 1.19 (d, *J* = 6.8 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.30. ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.97, 142.62, 136.15 (q, *J* = 4.9 Hz), 129.15 (q, *J* = 34.5 Hz), 128.49, 128.47, 127.48, 127.42, 127.34, 127.09, 121.84 (q, *J* = 269.1 Hz), 72.09, 62.49, 55.60, 23.43. HRMS(ESI) calcd for $C_{19}H_{19}F_3N$ [M+H$^+$]: 318.1464, found: 318.1479.



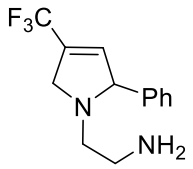
3an'

37% isolated yield. Colorless solid. Mp 39.5-40.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.24 (m, 10H), 6.28-6.25 (m, 1H), 5.03-4.97(m, 1H), 4.02 (q, *J* = 6.6 Hz, 1H), 3.97 (dd, *J* = 13.6, 6.0 Hz, 1H), 3.88-3.84 (m, 1H), 1.51 (d, *J* = 6.6 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.24. ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.07, 141.66, 136.03 (q, *J* = 4.9 Hz), 129.65 (q, *J* = 34.4 Hz), 128.22, 127.98, 127.72, 127.64, 127.35, 126.88, 121.91 (q, *J* = 269.0 Hz), 72.02, 58.80, 52.69, 16.66. HRMS(ESI) calcd for $C_{19}H_{19}F_3N$ [M+H$^+$]: 318.1464, found: 318.1475.



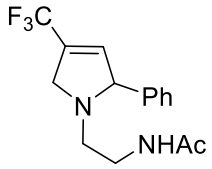
3ao

31% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.28 (m, 5H), 6.23-6.19 (m, 1H), 4.69-4.64 (m, 1H), 4.16 (dd, *J* = 13.2, 5.4 Hz, 1H), 3.65–3.52 (m, 2H), 3.50-3.44 (m, 1H), 2.93-2.86 (m, 1H), 2.81-2.75 (m, 1H), 2.09 (brs, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.32. ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.62, 135.80 (q, *J* = 5.0 Hz), 130.24 (q, *J* = 34.8 Hz), 128.78, 128.19, 127.62, 121.67 (q, *J* = 269.0 Hz), 74.70, 59.87, 56.72, 55.30. HRMS(ESI) calcd for $C_{13}H_{15}F_3NO$ [M+H$^+$]: 258.1100, found: 258.1106.



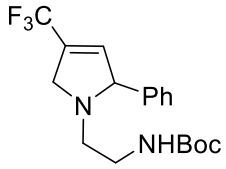
3ap

27% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.24 (m, 5H), 6.17 (s, 1H), 5.45 (brs, 2H), 4.69–4.63 (m, 1H), 4.16–4.07 (m, 1H), 3.64-3.57 (m, 1H), 2.90–2.65 (m, 4H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -65.26. ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.34, 135.76 (q, *J* = 4.8 Hz), 130.08 (q, *J* = 34.9 Hz), 128.79, 128.18, 127.67, 121.63 (q, *J* = 269.1 Hz), 74.63, 56.77, 52.72, 38.82. HRMS(ESI) calcd for $C_{13}H_{16}F_3N$ [M+H$^+$]: 257.1260, found: 257.1263.



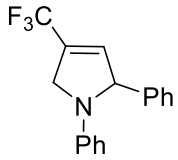
3aq

34% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40–7.27 (m, 5H), 6.20–6.15 (m, 1H), 5.59 (brs, 1H), 4.66-4.57 (m, 1H), 4.17–4.07 (m, 1H), 3.62–3.52 (m, 1H), 3.36-3.24 (m, 1H), 3.14–3.02 (m, 1H), 2.81–2.69 (m, 2H), 1.76 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.32. ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.97, 140.97, 135.59 (q, *J* = 4.9 Hz), 130.33 (q, *J* = 34.8 Hz), 128.74, 128.21, 127.69, 121.63 (q, *J* = 269.1 Hz), 74.64, 56.75, 52.45, 37.92, 22.99. HRMS(ESI) calcd for $C_{15}H_{18}F_3ON_2$ [M+H$^+$]: 299.1366, found: 299.1373.



3ar

73% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40–7.26 (m, 5H), 6.20–6.14 (m, 1H), 4.74–4.55 (m, 2H), 4.12 (dd, *J* = 13.0, 5.4 Hz, 1H), 3.56 (dd, *J* = 12.5, 5.2 Hz, 1H), 3.25–2.99 (m, 2H), 2.83–2.63 (m, 2H), 1.39 (s, 9H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.33. ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.88, 140.74, 135.87 (q, *J* = 4.9 Hz), 130.14 (q, *J* = 34.7 Hz), 128.65, 128.01, 127.65, 121.71 (q, *J* = 269.0 Hz), 79.03, 74.63, 56.55, 52.82, 39.13, 28.29. HRMS(ESI) calcd for $C_{18}H_{24}F_3O_2N_2$ [M+H$^+$]: 357.1784, found: 357.1792.

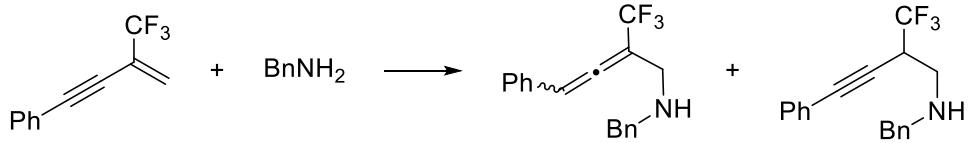


3as

78% isolated yield. Colorless solid. Mp 72.0-73.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31–7.18 (m, 5H), 7.13–7.07 (m, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 7.9 Hz, 2H), 6.33-6.28 (m, 1H), 5.51-5.45 (m, 1H), 4.58 (dd, *J* = 13.5, 6.7 Hz, 1H), 4.40-4.33 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.17. ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.60, 140.10, 135.58 (q, *J* = 4.8 Hz), 129.23, 129.10, 127.93, 127.85 (q, *J* = 35.4 Hz), 126.23, 121.61 (q, *J* = 268.9 Hz), 117.18, 112.26, 69.96, 53.65. MS (70 eV): m/z (%): 289 (M^+, 56.34), 212 (100). HRMS(EI) calcd for $C_{17}H_{14}F_3N$: 289.1078, found: 289.1081.

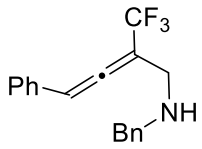
4. Control experiments

(1) Synthesis allenyl amine 4 and homo-propynylamine 5



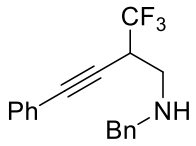
1a **2a** **4**, 41% **5**, 26%

To a solution of **1a** (0.5 mmol, 98 mg) in chlorobenzene (4.0 mL) was added **2a** (1.0 mmol, 107.2 mg) at room temperature. After stirring for 45 h, the reaction solvent was remove solvent under reduced pressure. Then the crude product was purified by column chromatography (silica gel, petroleum ether: dichloromethane = 1:2) to afford **4** (62.1 mg, 41%) as a Colorless oil and **5** (39.4 mg, 26%) as a colorless oil.



4

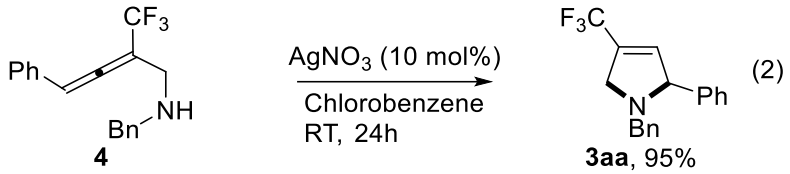
62.1 mg, 41% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.20 (m, 10H), 6.70 (d, J = 2.6 Hz, 1H), 3.82 (d, *J* = 13.0 Hz, 1H), 3.78 (d, *J* = 13.0 Hz, 1H), 3.59 (d, *J* = 16.0 Hz, 1H), 3.56 (d, *J* = 15.7 Hz, 1H), 1.59 (brs, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.53. ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.98 (q, *J* = 4.2 Hz), 139.49, 131.50, 128.95, 128.46, 128.42, 128.18, 127.49, 127.12, 123.25 (q, *J* = 274.7 Hz), 101.98, 101.33 (q, *J* = 32.7 Hz), 52.43, 45.76. HRMS(ESI) calcd for $C_{18}H_{17}F_3N$ [M+H$^+$]: 304.1308, found: 304.1316.



5

39.4 mg, 26% isolated yield. Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.45 (m, 2H), 7.41–7.27 (m, 8H), 3.93 (d, *J* = 13.3 Hz, 1H), 3.88 (d, *J* = 13.3 Hz, 1H), 3.71–3.60 (m, 1H), 3.15-3.03 (m, 2H), 1.79 (brs, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -69.52. ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.55, 131.90, 128.76, 128.50, 128.29, 128.01, 127.18, 124.83 (q, *J* = 279.9 Hz), 121.93, 85.51, 80.93 (q, *J* = 3.7 Hz), 53.20, 47.19 (q, J = 1.8 Hz), 39.04 (q, *J* = 29.4 Hz). HRMS(ESI) calcd for $C_{18}H_{17}F_3N$ [M+H$^+$]: 304.1308, found: 304.1318.

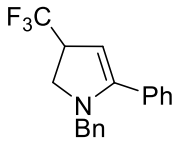
（2）Synthesis 3-pyrroline 3aa from allenyl amine 4



To a solution of allene **4** (30.3 mg, 0.1 mmol) in chlorobenzene (2.0 mL) at room temperature, silver nitrate (1.7 mg, 10 mol %) was added, the reaction was stirred at room temperature for 24 h. After **4** was completely consumed, which was determined by TLC analysis (hexanes : EA =5:1), the solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 100:1) to give the desired 3-pyrroline **3aa** (28.8 mg) in 95% isolated yield.

（3）Synthesis 2-pyrroline 4aa from homo-propynylamine 5

To a solution of homo-propynylamine **5** (30.3 mg, 0.1 mmol) with or without benzyl amine **2a** (10.7 mg, 0.1 mmol) in chlorobenzene (2.0 mL) at room temperature, silver nitrate (1.7 mg, 10 mol %) was added, the reaction was stirred at room temperature for 24 h. After **5** was completely consumed, which was determined by TLC analysis (hexanes : EA =5:1), the solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography on silica gel (petroleum ether: ethyl acetate = 200:1) to give the desired 2-pyrroline **4aa** as a colorless oil. **This compound was acid and air sensitive and easily decomposed after being purified via silica-gel chromatography.**

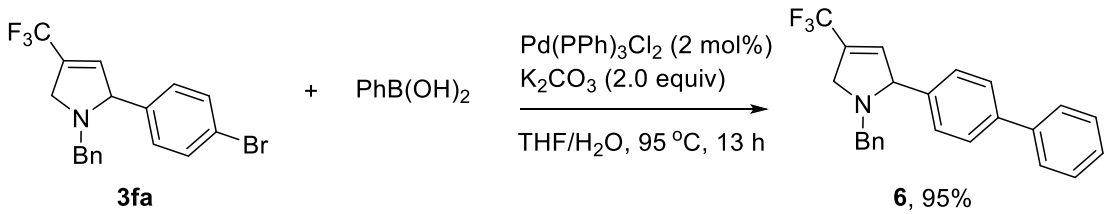


4aa

δ 7.48–7.16 (m, 10H), 4.71 (s, 1H), 4.02 (d, *J* = 15.0 Hz, 1H), 3.85 (d, *J* = 15.0 Hz, 1H), 3.57–3.39 (m, 2H), 3.30-3.19 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -72.60.

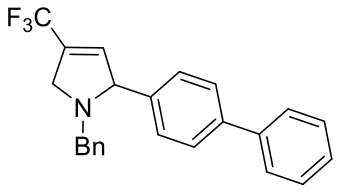
5. Derivatization of 4-Trifluoromethyl-3-Pyrrolines 3aa, 3fa and 3ua

(1) Synthesis of 3-pyrroline 6



3fa **6**, 95%

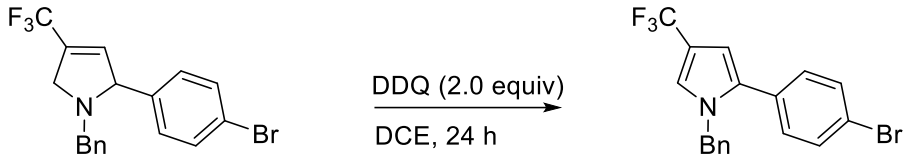
Under Ar, a mixture of phenylboronic acid (0.6 mmol, 73.2 mg), **3fa** (0.5 mmol, 191.1 mg), K_2CO_3 (1.0 mmol, 138.2 mg) and $Pd(PPh_3)_2Cl_2$ (0.01 mmol, 7.0 mg) in THF (2 mL) and H_2O (1 mL) was heated at 95 °C in a sealed tube for 13 h. The mixture was cooled to rt and the reaction was quenched with H_2O (5.0 mL), then extracted with ethyl acetate (3x5.0 mL). The organic layer was washed with brine, dried over $MgSO_4$ and concentrated, purified by column chromatography (silica gel, PE:EA = 10:1) to afford the desired product **6** (180 mg, 95%) as a Colorless solid.



6

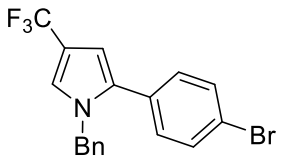
180 mg, 95% isolated yield. Colorless solid. Mp 101.1-102.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, J = 8.2 Hz, 4H), 7.58-7.44 (m, 4H), 7.43–7.27 (m, 6H), 6.28 (s, 1H), 4.82 (s, 1H), 4.04 (d, *J* = 13.2 Hz, 1H), 3.95 (dd, *J* = 13.2, 4.6 Hz, 1H), 3.62 (d, *J* = 13.2 Hz, 1H), 3.55 (dd, *J* = 13.1, 6.0 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -65.28. ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.89, 140.81, 139.73, 138.70, 135.95 (q, *J* = 4.9 Hz), 130.62 (q, *J* = 34.6 Hz), 128.77, 128.49, 128.38, 128.28, 127.32, 127.16, 127.10, 121.85 (q, *J* = 269.1 Hz), 73.71, 57.06, 56.10. HRMS(ESI) calcd for $C_{24}H_{21}F_3N$ [M+H$^+$]: 380.1621, found: 380.1637.

(2) **Synthesis of pyrrole 7**



3fa **7**, 92%

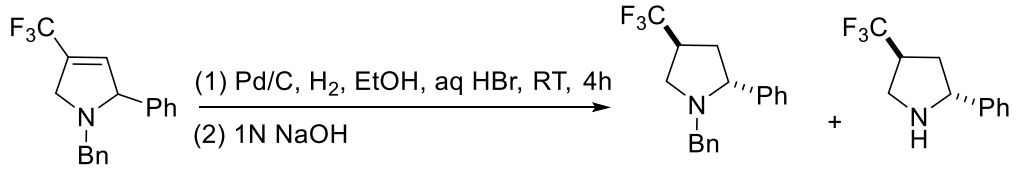
To a solution of **3fa** (0.3 mmol, 114.6 mg) in DCE (2.0 mL) was added DDQ (0.6 mmol, 136.2 mg) at room temperature. After stirring for 24 h, the reaction solvent was filtered through a celite plug and the filtrate was concentrated under reduced pressure. Then the crude product was purified by column chromatography (silica gel, petroleum ether: ethyl acetate = 100:1) to afford **7** (105 mg, 92%) as a Colorless oil.



7

105 mg, 92% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.5 Hz, 2H), 7.39–7.29 (m, 3H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.07 (s, 1H), 7.04–6.97 (m, 2H), 6.44 (s, 1H), 5.10 (s, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -57.23. ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.04, 134.61, 131.73, 130.69, 130.63, 128.94, 127.92, 126.49, 123.74 (q, *J* = 266.0 Hz), 122.23, 122.03 (q, *J* = 4.8 Hz), 114.87 (q, *J* = 37.2 Hz), 106.63 (d, J = 2.7 Hz), 51.05. MS (70 eV): m/z (%): 379 (M^+, 14.10), 381 (M^++2, 13.69), 91 (100). HRMS(EI) calcd for $C_{18}H_{13}BrF_3N$: 379.0183, found: 379.0180.

(3) Synthesis of *N*-Bn-pyrrolidine 8a



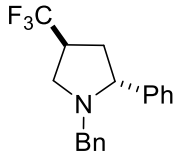
3aa

8a, 66%
d.r > 20:1

8b, 13%

A solution of compound 3aa (0.38 mmol 115 mg)，Pd/C (contain 10% Pd) (5 mol%) and aq HBr (47%, 0.5 mmol, 58uL) in EtOH (2 mL) was stirred under 1atm pressure of hydrogen at room temperature. After stirring for 4 h, **3aa** was consumed according to TLC analysis (hexanes). 1N NaOH (1.0 mL) was added to the reaction mixture and stirring for 15 min. The reaction mixture was filtered through a celite plug and then extracted with ethyl acetate (3x5.0 mL). The organic layer was combined

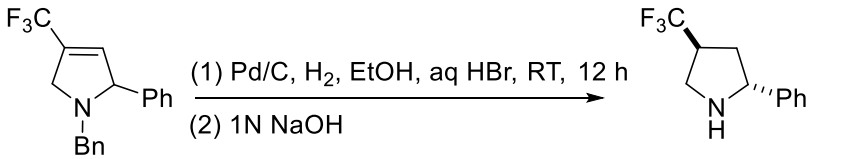
and washed with brine, dried over Na_2SO_4 and concentrated, purified by column chromatography (silica gel, PE:EA = 100:1) to afford the desired product **8a** (76 mg, 66%) as a colorless solid.



8a

76 mg, 66% isolated yield. Colorless solid. Mp 72.0-74.2 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.31-7.19 (m, 6H), 3.84 (d, *J* = 13.6 Hz, 1H), 3.45 (dd, *J* = 9.9, 6.6 Hz, 1H), 3.25 (dd, *J* = 10.6, 2.2 Hz, 1H), 3.00 (d, *J* = 13.6 Hz, 1H), 2.87–2.71 (m, 1H), 2.43–2.35 (m, 2H), 1.96-1.88 (m, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -71.58. ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.55, 138.82, 128.65, 128.25, 128.15, 127.87 (q, *J* = 277.4 Hz), 127.70, 127.54, 126.87, 69.05, 57.02, 52.33 (q, *J* = 2.6 Hz), 39.83 (q, J = 28.3 Hz), 35.66 (q, *J* = 1.7 Hz). HRMS(ESI) calcd for $C_{18}H_{19}F_3N$ [M+H$^+$]: 306.1464, found: 306.1474.

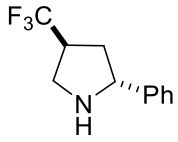
(4) Synthesis of pyrrolidine 8b



3aa **8b**, 74% (dr > 20 : 1)

A solution of compound 3aa (0.15 mmol 45.5 mg), Pd/C (contain 10% Pd) (5 mol%) and aq HBr (47%, 0.2 mmol, 23uL) in EtOH (2 mL) was stirred under 1atm pressure of hydrogen at room temperature. After

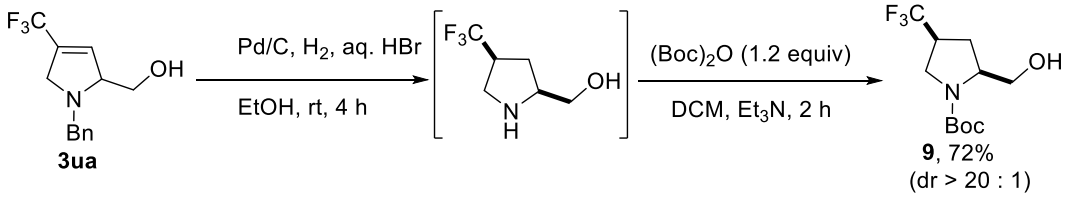
stirring for 12 h, 1N NaOH (1.0 mL) was added to the reaction mixture and stirring for 15 min. The reaction mixture was filtered through a celite plug and then extracted with ethyl acetate (3x5.0 mL). The organic layer was combined and washed with brine, dried over Na_2SO_4 and concentrated, purified by column chromatography (silica gel, PE:EA = 5:1) to afford the desired product **8b** (24 mg, 74%) as a colorless oil.



8b

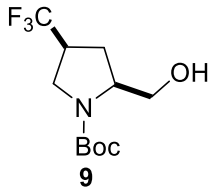
24 mg, 74% isolated yield. Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43–7.27 (m, 5H), 4.13 (dd, *J* = 10.2, 6.4 Hz, 1H), 3.39 (dd, *J* = 11.8, 4.2 Hz, 1H), 3.24–3.13 (m, 1H), 3.06–2.84 (m, 1H), 2.52-2.40 (m, 1H), 1.93 (brs, 1H), 1.88-1.76 (m, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -70.87. ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.68, 128.55, 128.00 (q, *J* = 277.2 Hz), 127.50, 126.50, 63.33, 47.00 (q, *J* = 2.6 Hz), 43.45 (q, *J* = 27.2 Hz), 34.78 (q, *J* = 1.4 Hz). HRMS(ESI) calcd for $C_{11}H_{13}F_3N$ [M+H$^+$]: 216.0995, found: 216.0995.

(5) Synthesis of *N*-Boc-*cis*-4-trifluoromethyl-prolinol 9



The solution of compound 3ua (0.55 mmol 140 mg) and Pd/C (contain 10% Pd) (5 mol%) and aq HBr (47%, 0.6 mmol, 70uL) in EtOH

(4 mL) under 1atm pressure of hydrogen at room temperature. After stirring for 4 h, the reactions were monitored through TLC (hexanes : EA =5:1). Then 1N NaOH (2.0 mL) was added to the reaction mixture and extracted with ethyl acetate (3x5.0 mL). The organic layer was combined and washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was used directly for next step without any purification. Then under N_2, to a solution of crude product in DCM (2.0 mL) was added trimethylamine (1.5 mmol, 205 uL) via syringe followed by di(tert-butyl)dicarbonate (0.6 mmol, 130 mg) in one portion. The reaction stirred for 2 h after which the resulting yellow solution was poured into 5.0 mL of water. The layers were separated, and the organic layer was washed with 2x2.0 mL of water. The organic layers were combined, dried with $MgSO_4$, filtered, and the solvent was removed in vacuo. The crude orange oil was purified by flash column chromatography (silica gel, PE : EA = 1:1) to afford *N*-Boc-*cis*-4-trifluoromethyl-prolinol **9** (106 mg, 72%) as a colorless oil.

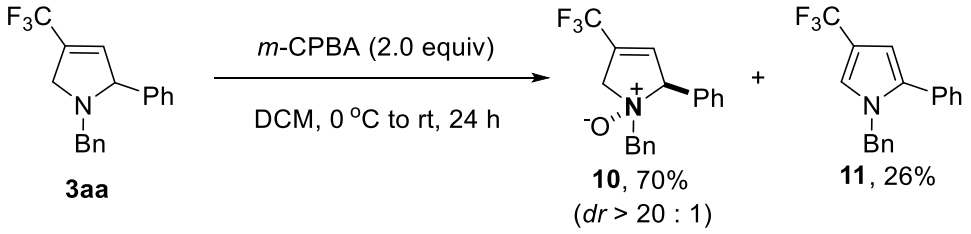


9

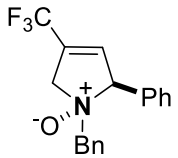
106 mg, 72% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.87 (s, 1H), 3.97 (d, *J* = 5.9 Hz, 1H), 3.78 (s, 1H), 3.72-3.60 (m, 2H), 3.31 (s, 1H), 2.90–2.75 (m, 1H), 2.31–2.23 (m, 1H), 1.67 (d, *J* = 7.4 Hz,

1H), 1.45 (s, 9H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -70.87. ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.15, 126.05 (q, *J* = 276.7 Hz), 81.19, 66.50, 60.52, 46.56, 40.90 (q, *J* = 29.1 Hz), 28.44 (q, *J* = 2.4 Hz), 28.29. HRMS(ESI) calcd for $C_{11}H_{18}F_3NNaO_3$ [M+Na$^+$]: 292.1131, found: 292.1132.

(6) Synthesis of pyrroline *N*-oxide 10 and pyrrole 11

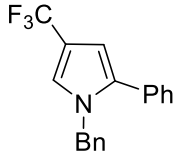


Under N_2, to a solution of **3aa** (0.3 mmol, 91 mg) in DCM (2.0 mL) was added *m*-CPBA (126.3 mg, 0.6 mmol; 85.0%) at 0 °C then stirring for 1 h, the reaction mixture was warmed to room temperature and was stirred for another 24 h, the reactions were monitored through TLC analysis (hexanes), After **3aa** was consumed, saturated $NaHCO_3$ solution (5 mL) was added to reaction mixture and extracted with ethyl acetate (3× 5 mL). Organic layers were combined, dried with anhydrous Na_2SO_4, filtered and evaporated to get crude residue which was purified through flash column chromatography (silica gel, PE:EA:DCM = 200:1:10) to afford pyrroline *N*-oxide **10** (67 mg, 70% yield) as a colorless oil and pyrrole **11** (24 mg, 26% yield) as a colorless oil.



10

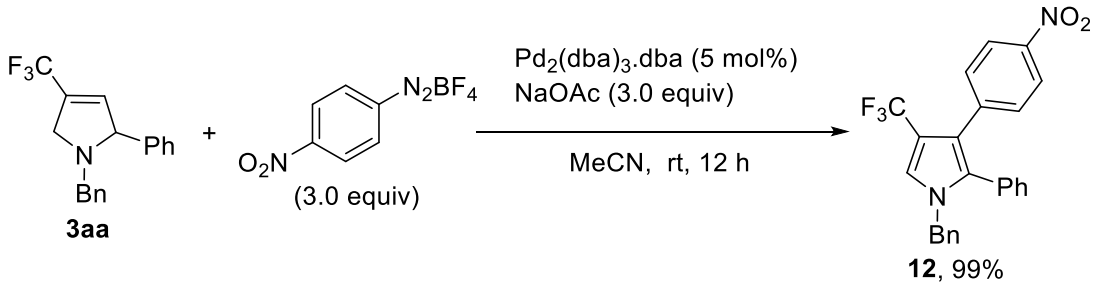
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.345-7.25 (m, 10H), 6.59 (s, 1H), 5.49 (s, 1H), 4.15 (d, *J* = 12.9 Hz, 1H), 3.96 (d, *J* = 12.9 Hz, 1H), 3.51 (s, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -68.12. ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.40, 136.06, 131.72, 128.94, 128.61, 128.53, 128.29, 127.96, 127.42, 127.02 (d, *J* = 31.9 Hz), 122.64 (q, *J* = 271.2 Hz), 78.15, 62.54, 51.14. MS (70 eV): m/z (%): 319 (M+, 6.84), 91 (100). HRMS(EI) calcd for $C_{18}H_{16}F_3NO$: 319.1184, found: 319.1186.



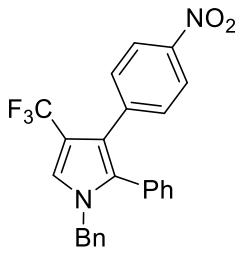
11

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.27 (m, 8H), 7.06-7.03 (m, 2H), 7.02 (s, 1H), 6.44 (s, 1H), 5.12 (s, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -57.19. ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.31, 135.95, 131.81, 129.18, 128.85, 128.55, 127.96, 127.80, 126.65, 123.88 (q, *J* = 265.8 Hz), 121.53 (q, *J* = 4.9 Hz), 114.69 (q, *J* = 36.9 Hz), 106.22 (q, *J* = 2.7 Hz), 50.98. MS (70 eV): m/z (%): 301 (M^+, 32.14), 91 (100). HRMS(EI) calcd for $C_{18}H_{14}F_3N$: 301.1078, found: 301.1077.

(7) Synthesis of pyrrole 12



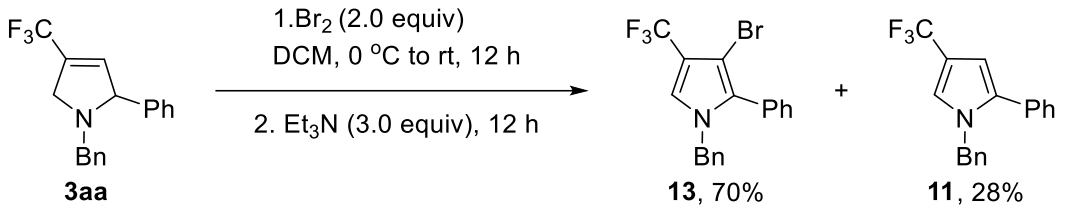
Under N_2, to a solution of **3aa** (0.2 mmol, 60.6 mg) in acetonitrile (2.0 mL) was added at once a mixture of *p*-NO_2-$C_6H_4N_2BF_4$ (0.6 mmol, 142.2 mg), $Pd_2(dba)_3$.dba (0.01 mmol, 11.5 mg) and anhydrous NaOAc (0.6 mmol, 50 mg). The mixture became dark almost immediately displaying intense nitrogen bubbling. Magnetic stirring continued for 12 h when TLC (hexanes) indicated complete consumption of the starting material **3aa**. The reaction solvent was removed under reduced pressure. Then the crude product was purified by column chromatography (silica gel, PE : DCM = 2: 1) to afford pyrrole **12** (84 mg, 99% yield) as a red solid.



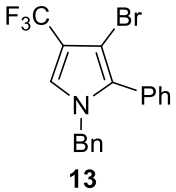
12

Red solid. Mp 115.2-116.9 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.6 Hz, 2H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.50-7.36 (m, 5H), 7.36–7.23 (m, 3H), 7.02 (d, *J* = 7.4 Hz, 2H), 6.83 (s, 1H), 5.68 (s, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -58.11. ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.58, 147.94, 141.50 (q, *J* = 2.7 Hz), 139.89, 137.67, 130.23, 129.31, 129.07, 128.92, 128.82, 127.53, 125.86, 124.64, 122.67 (q, *J* = 267.2 Hz), 122.65, 112.03 (q, *J* = 4.3 Hz), 111.33 (q, *J* = 38.9 Hz), 49.25. MS (70 eV): m/z (%): 422 (M^+, 7.88), 57 (100). HRMS(EI) calcd for $C_{24}H_{17}F_3N_2O_2$: 422.1242, found: 422.1250.

(8) Synthesis of 3-bromo pyrrole 13



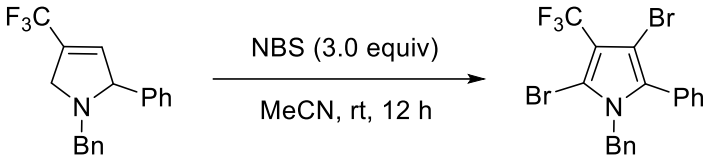
Under N_2, to a solution of **3aa** (0.3 mmol, 91 mg) in DCM (2.0 mL) was added Br_2 (0.6 mmol, 96 mg) at 0 °C then refluxed for 30 min, then the reaction mixture was stirred at room temperature for 12 h. Until the disappearance of substrate **3aa** as indicated by TLC (hexanes), then the reaction mixture was cooled to 0 °C. Et_3N (0.9 mmol, 0.124 mL) was added and the reaction mixture was stirred for 30 min and then warmed to room temperature. After being stirred at room temperature for 24 h, saturated $Na_2S_2O_3$ (2.0 mL) solution was added, extracted with ethyl acetate (3×5 mL). Organic layers were combined and evaporated to get crude residue which was purified through flash column chromatography (silica gel, PE : DCM = 20: 1) to afford 3-bromo pyrrole **13** (80 mg, 70% yield) as a colorless oil and pyrrole **11** (25 mg, 28% yield) as a colorless oil.



Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46–7.38 (m, 3H), 7.34–7.27 (m, 5H), 7.06 (q, *J* = 0.9 Hz, 1H), 6.98-6.94 (m, 2H), 4.98 (s, 2H). ^{19}F

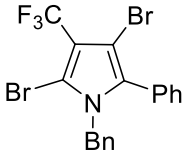
NMR (376 MHz, $CDCl_3$) δ -58.40. ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.36, 134.37, 130.77, 129.61, 128.92, 128.88, 128.56, 128.08, 126.96, 122.87 (q, *J* = 266.7 Hz), 121.64 (q, *J* = 5.0 Hz), 114.32 (q, *J* = 36.2 Hz), 93.09 (q, *J* = 2.2 Hz), 52.07. MS (70 eV): m/z (%): 379 (M^+, 16.44), 91 (100). HRMS(EI) calcd for $C_{18}H_{13}BrF_3N$: 379.0183, found: 379.0184.

(9) Synthesis of 2,4-dibromo pyrrole 14



3aa **14**, 87%

Under N_2, to a solution of **3aa** (0.2 mmol, 60.6 mg) in acetonitrile (2.0 mL) was added NBS (0.6 mmol, 108 mg) at room temperature. The reaction mixture was stirred for 12 h and monitored through TLC analysis (hexanes). The reaction solvent was removed under reduced pressure and residue was purified by column chromatography (silica gel, PE : DCM = 20: 1) to afford 2,4-dibromo pyrrole **14** (80 mg, 87% yield) as a colorless solid.

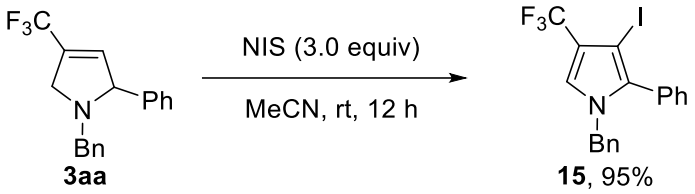


14

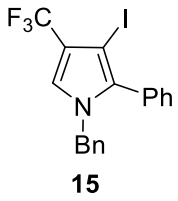
Colorless solid. Mp 89.5-90.8 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.42–7.32 (m, 3H), 7.30-7.23 (m, 3H), 7.22–7.17 (m, 2H), 6.86–6.81 (m, 2H), 5.12 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.41. ^{13}C NMR (125 MHz, $CDCl_3$) δ 136.12, 135.53, 130.77, 129.60, 129.29, 128.74, 128.57, 127.67,

125.95, 122.23 (q, J = 268.6 Hz), 113.12 (q, J = 35.6 Hz), 103.94 (q, J = 3.3 Hz), 94.51 (q, J = 1.6 Hz), 50.52. MS (70 eV): m/z (%): 459 (M^+, 9.64), 91 (100). HRMS(EI) calcd for $C_{18}H_{12}Br_2F_3N$: 456.9289, found: 456.9285.

(10) Synthesis of 3-iodo pyrrole 15



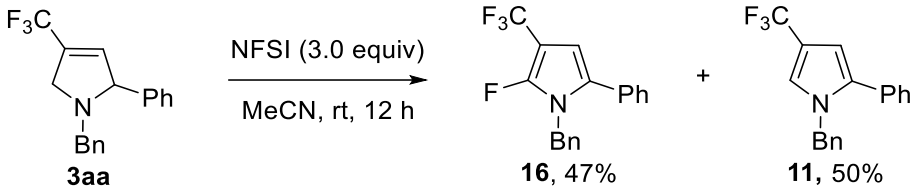
Under N_2, to a solution of **3aa** (0.2 mmol, 60.6 mg) in acetonitrile (2.0 mL) was added NIS (0.6 mmol, 135 mg) at room temperature. The reaction was monitored through TLC (hexanes). After stirring for 12 h, saturated $Na_2S_2O_3$ (2.0 mL) solution was added then stirring for 10 min until the reaction mixture turn to colorless, then extracted with ethyl acetate (3×5 mL). Organic layers were combined and evaporated to get crude residue which was purified through flash column chromatography (silica gel, PE : DCM = 20: 1) to afford 3-iodo pyrrole **15** (81 mg, 95% yield) as a colorless solid.



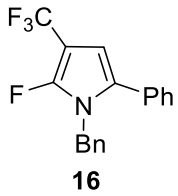
Colorless solid. Mp 62.9-64.6 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.37 (m, 3H), 7.30–7.22 (m, 5H), 7.12 (q, J = 0.9 Hz, 1H), 6.96–6.89 (m, 2H), 4.96 (s, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -58.23. ^{13}C NMR (125

MHz, $CDCl_3$) δ 138.36, 136.41, 131.04, 130.92, 129.00, 128.84, 128.51, 128.04, 126.96, 122.94 (q, *J* = 267.0 Hz), 122.92 (q, *J* = 5.3 Hz), 117.36 (q, *J* = 35.9 Hz), 59.79 (q, *J* = 2.0 Hz), 52.32. MS (70 eV): m/z (%): 427 (M^+, 35.56), 91 (100). HRMS(EI) calcd for $C_{18}H_{13}IF_3N$: 427.0045, found: 427.0047.

(11) Synthesis of 2-fluoro pyrrole 16



Under N_2, to a solution of **3aa** (0.2 mmol, 60.6 mg) in acetonitrile (2.0 mL) was added NFSI (0.6 mmol, 189.2 mg) at room temperature. The reaction mixture was stirred at room temperature for 12 h. After consumption of **3aa** according to TLC analysis (hexane), the reaction solvent was removed under reduced pressure. Then the crude product was purified by column chromatography (silica gel, PE : DCM = 20 : 1) to afford 2-fluoro pyrrole **16** (30 mg, 47% yield) as a colorless oil and pyrrole **12** (30 mg, 50% yield) as a colorless oil.



Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42–7.25 (m, 8H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.26 (d, *J* = 5.2 Hz, 1H), 5.10 (s, 2H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -56.31 (d, *J* = 9.6 Hz), -133.56 (q, *J* = 9.6 Hz). ^{13}C NMR (125

MHz, $CDCl_3$) δ 145.76–143.44 (m), 136.32, 131.13, 129.06, 128.88, 128.69, 128.11, 127.82, 126.60, 126.18, 125.54–119.31 (m), 103.03 (q, *J* = 2.5 Hz), 93.04-92.05 (m), 46.59. MS (70 eV): m/z (%): 319 (M^+, 9.72), 91 (100). HRMS(EI) calcd for $C_{18}H_{13}F_4N$: 319.0984, found: 319.0986.

6. **X-ray structures for pyrroline 3aa and 3-iodo pyrrole 15**

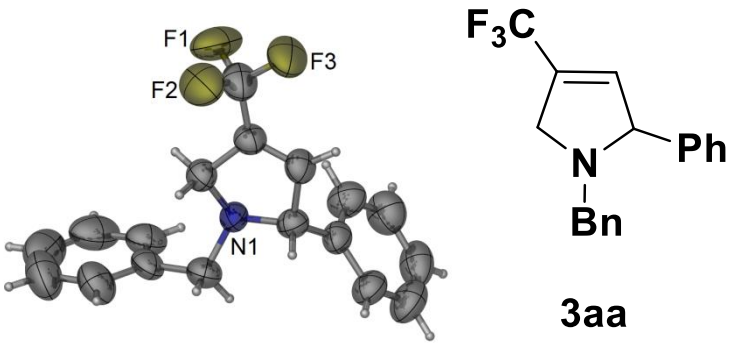


Figure 1. ORTEP depiction of compound **3aa**, CCDC1486638

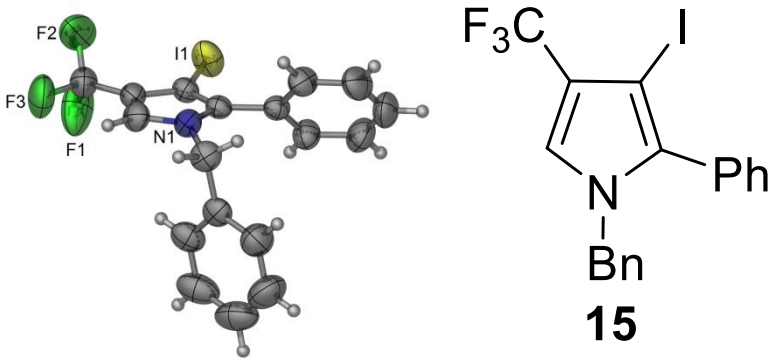
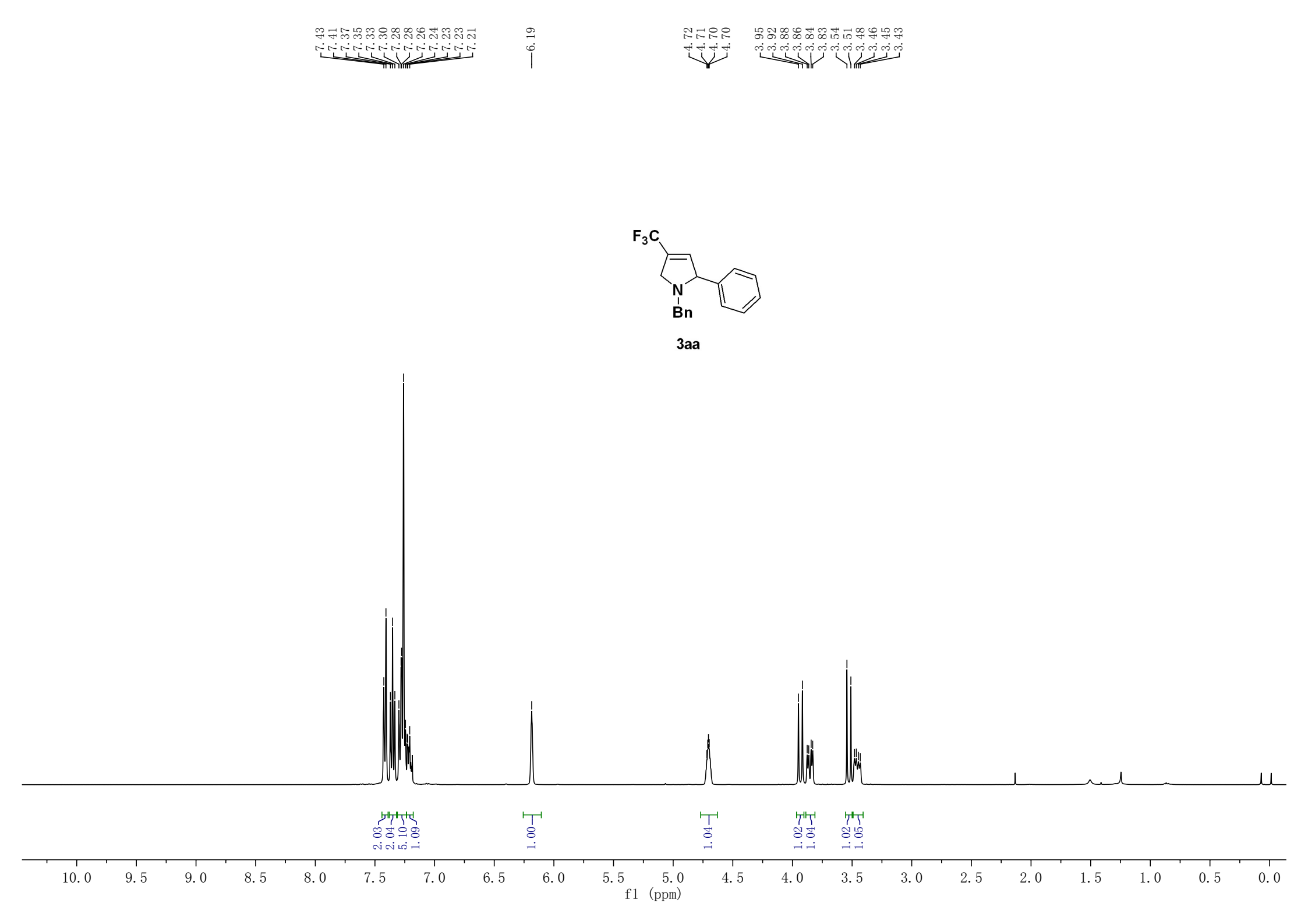


Figure 2. ORTEP depiction of 3-iodo pyrrole **15**, CCDC1498966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4.71
4.70
4.70
3.95
3.92
3.88
3.86
3.84
3.83
3.54
3.51
3.48
3.46
3.45
3.43
F3C
N
Bn
3aa
2.03
2.04
5.10
1.09
1.00
1.04
1.02
1.04
1.02
1.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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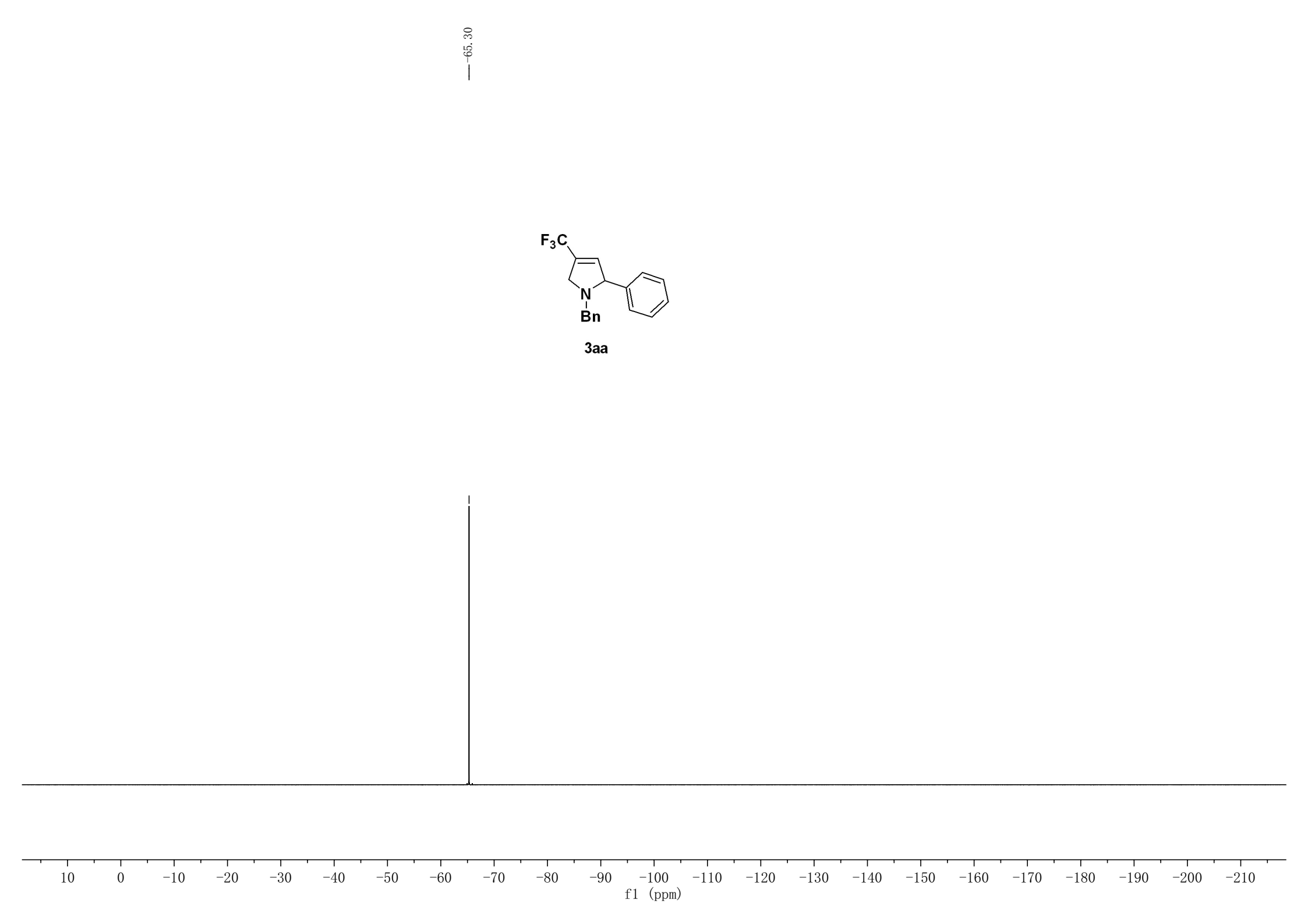
f1 (ppm)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-50
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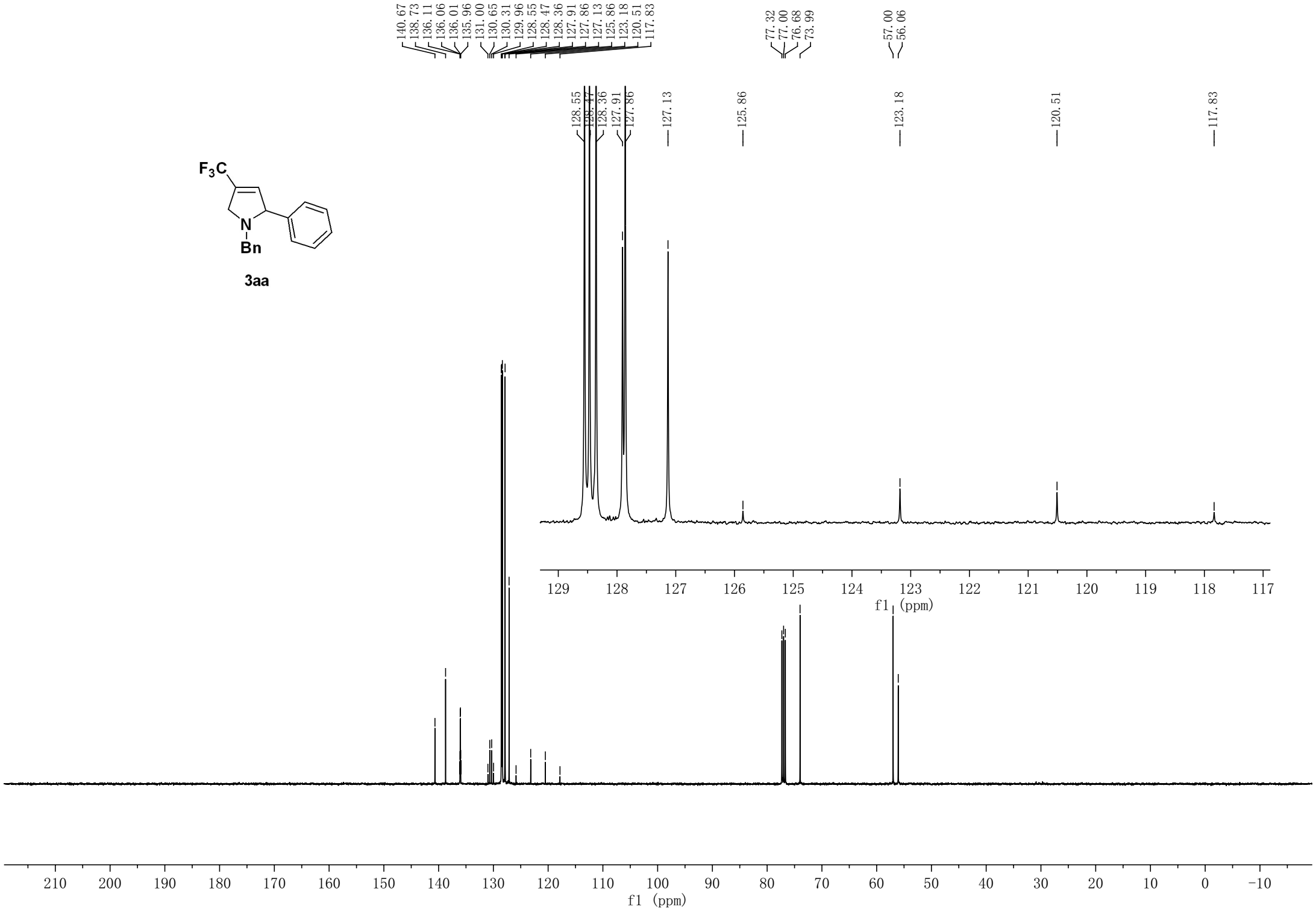
f1 (ppm)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127.13
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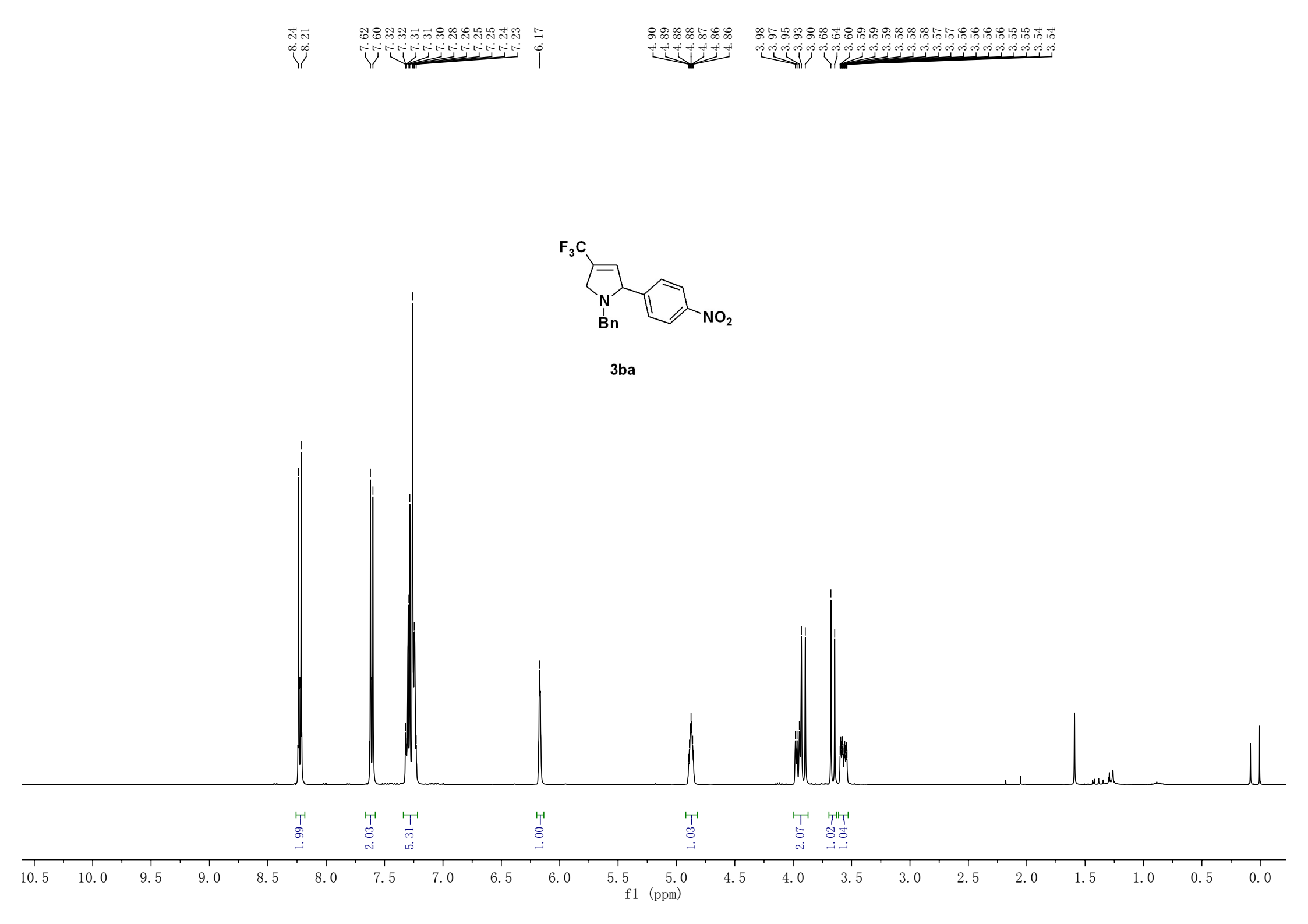
57.00
56.06
F3C
N
Bn
3aa
f1 (ppm)
f1 (ppm)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7.24
7.23
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1.02
1.04
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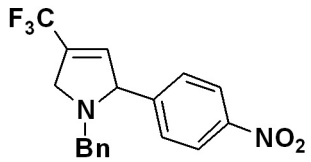
f1 (ppm)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Bn
NO2

3ba

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-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

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147.59
137.91
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134.34
132.14
131.79
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131.10
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128.44
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122.81
120.13
117.46

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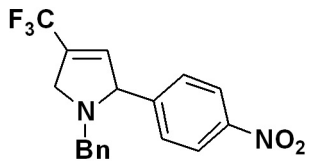
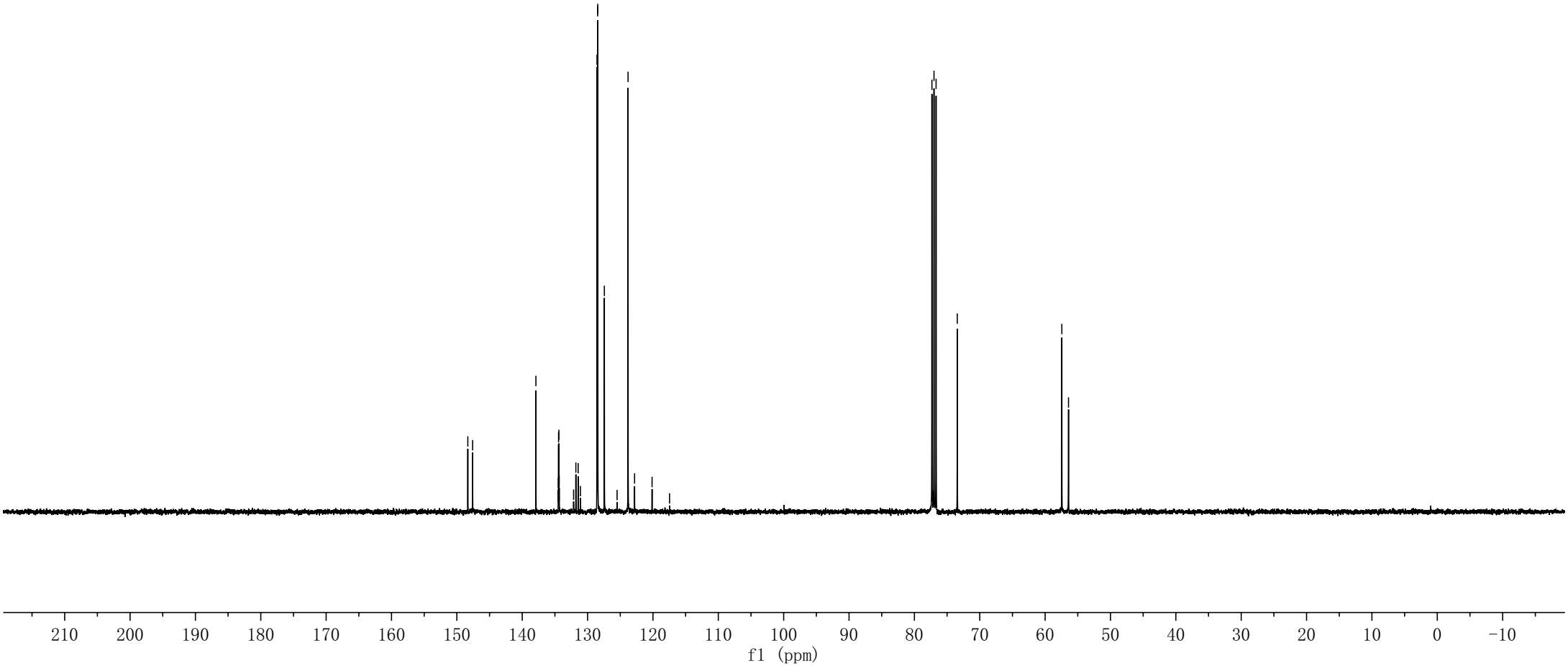
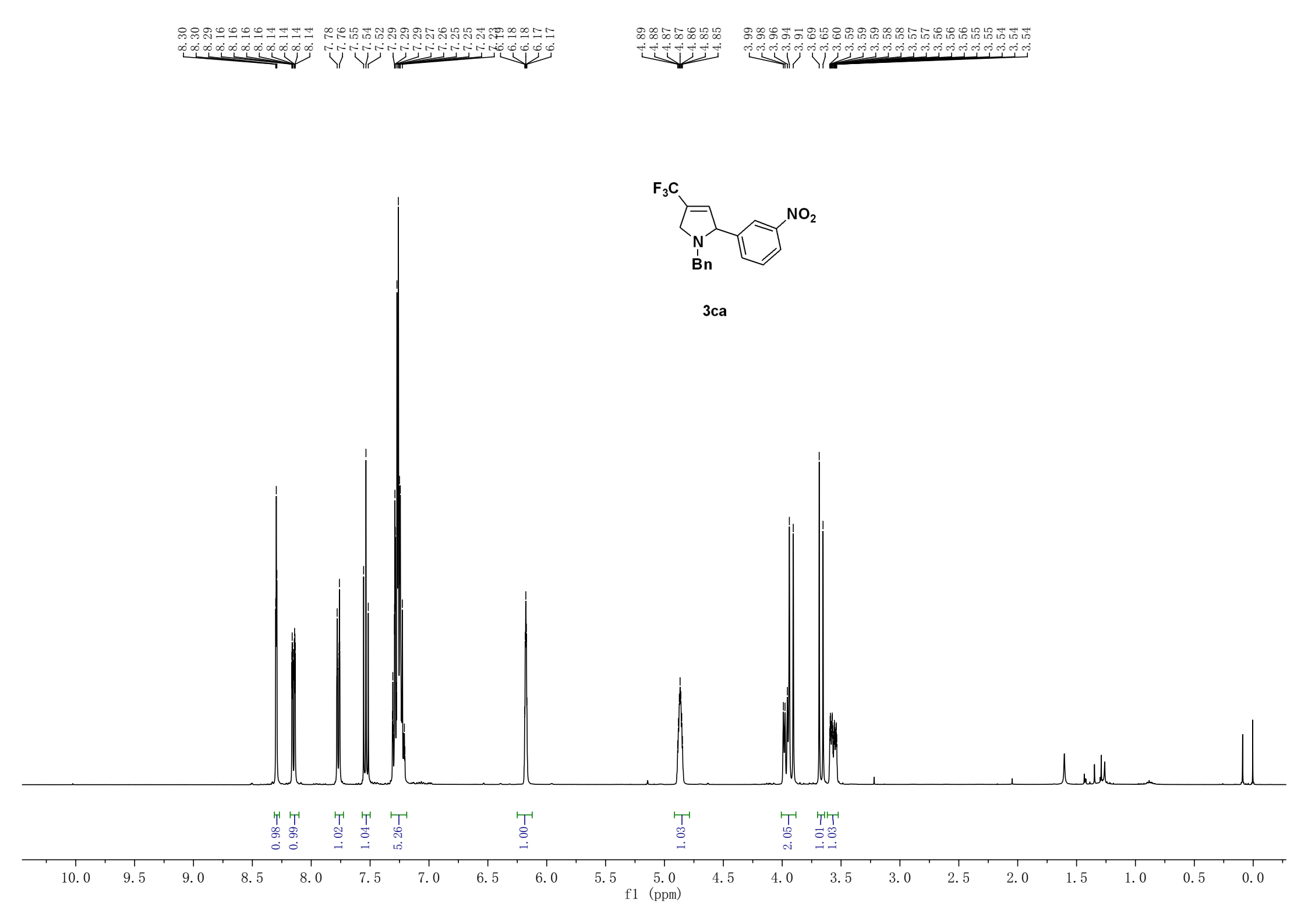
77.00
76.68
73.44

57.44
56.42



3ba

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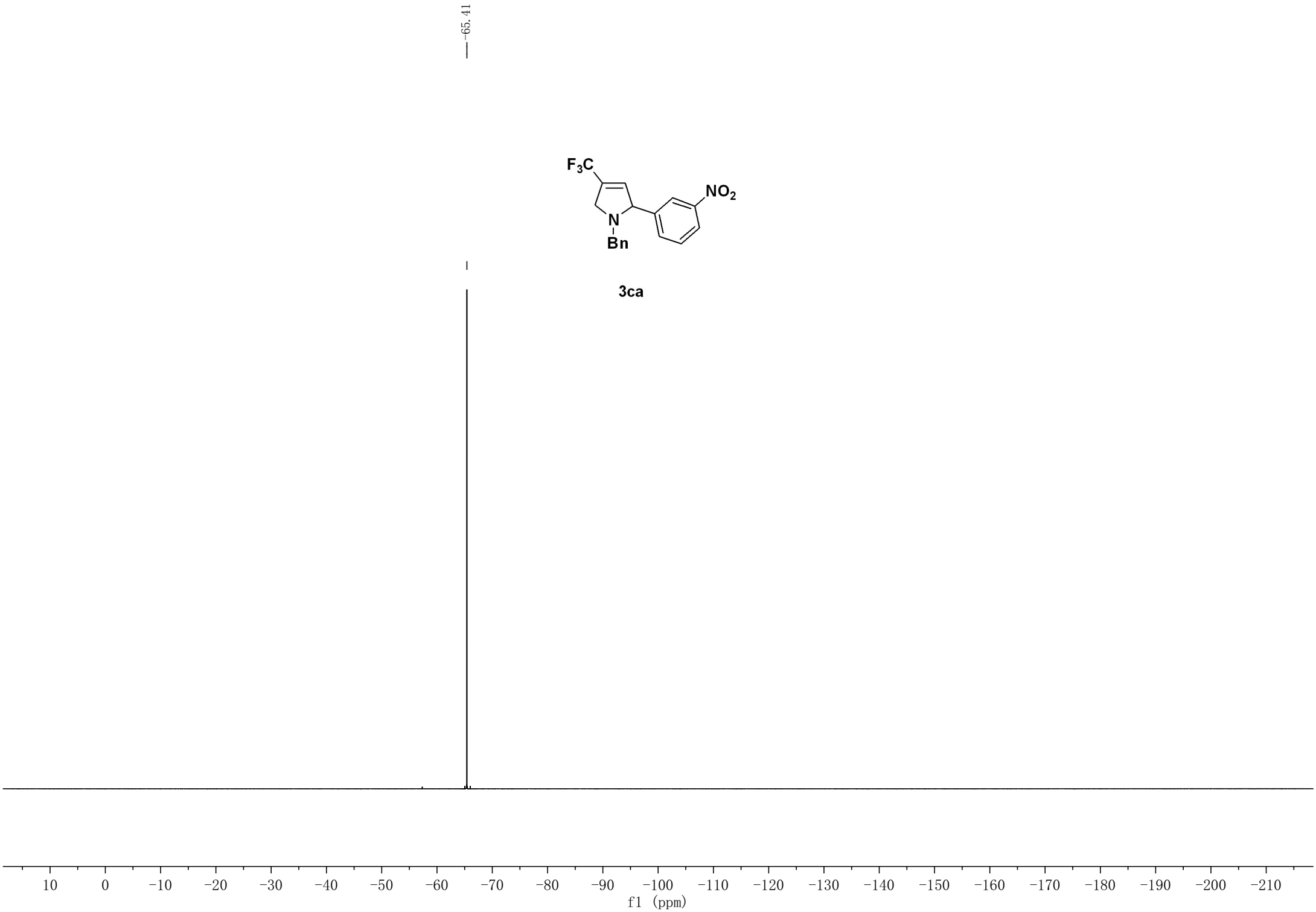
4.89 4.88 4.87 4.87 4.86 4.85 4.85
3.99 3.98 3.96 3.94 3.91 3.69 3.65 3.60 3.59 3.59 3.59 3.58 3.58 3.57 3.57 3.56 3.56 3.55 3.55 3.54 3.54
F3C
NO2
N
Bn
3ca
0.98 0.99 1.02 1.04 5.26 1.00 1.03 2.05 1.01 1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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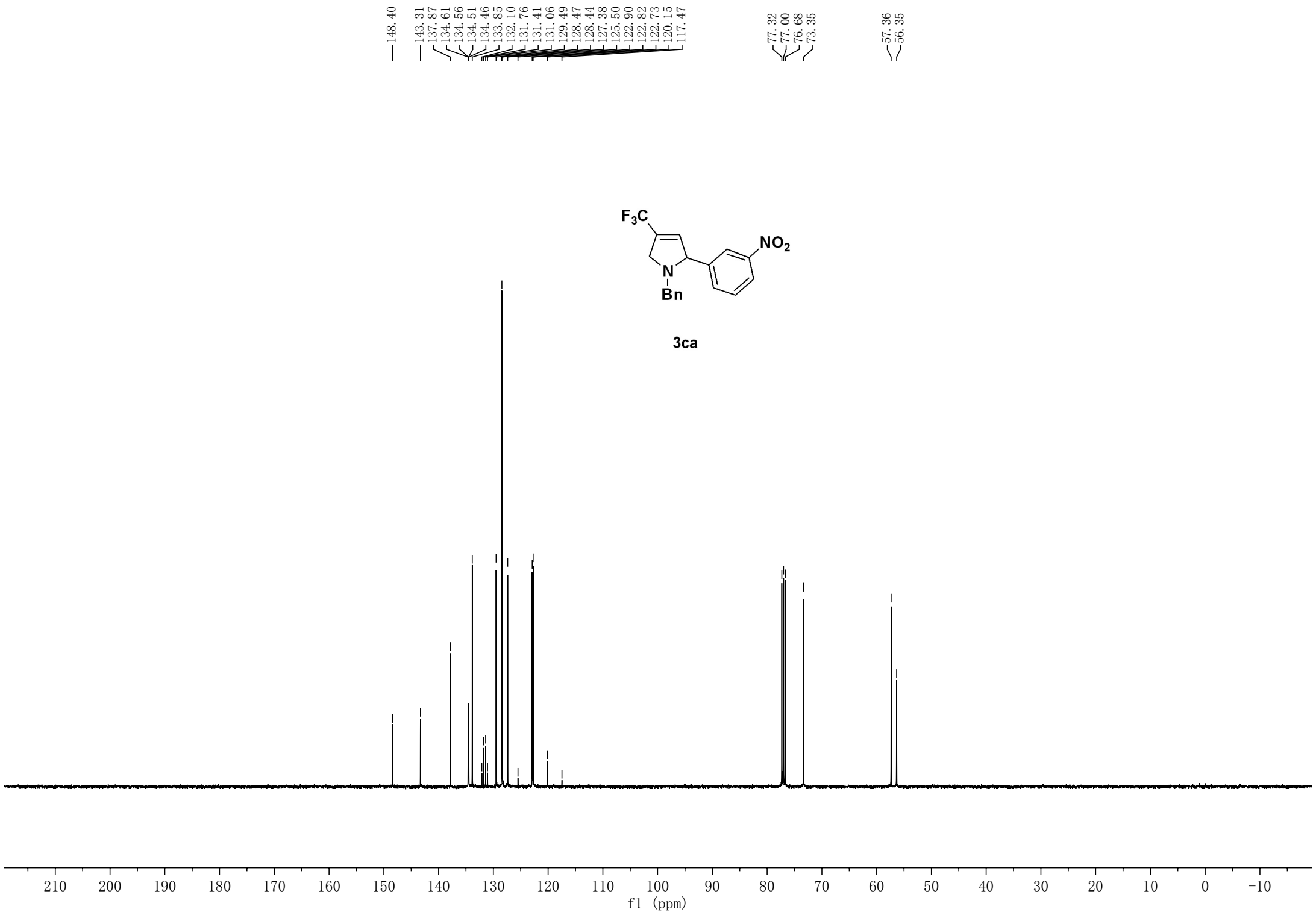
f1 (ppm)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N
Bn
3ca
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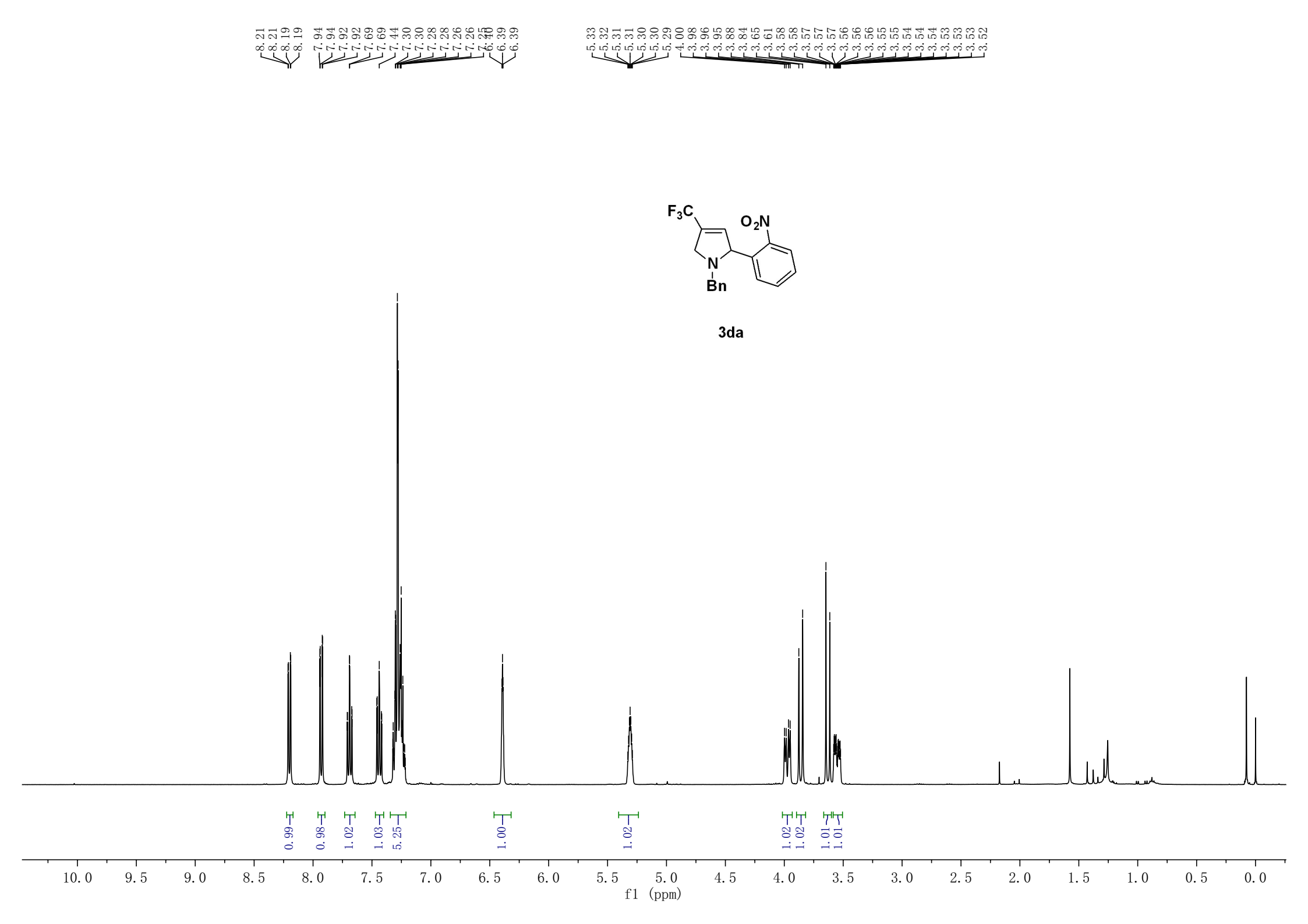
f1 (ppm)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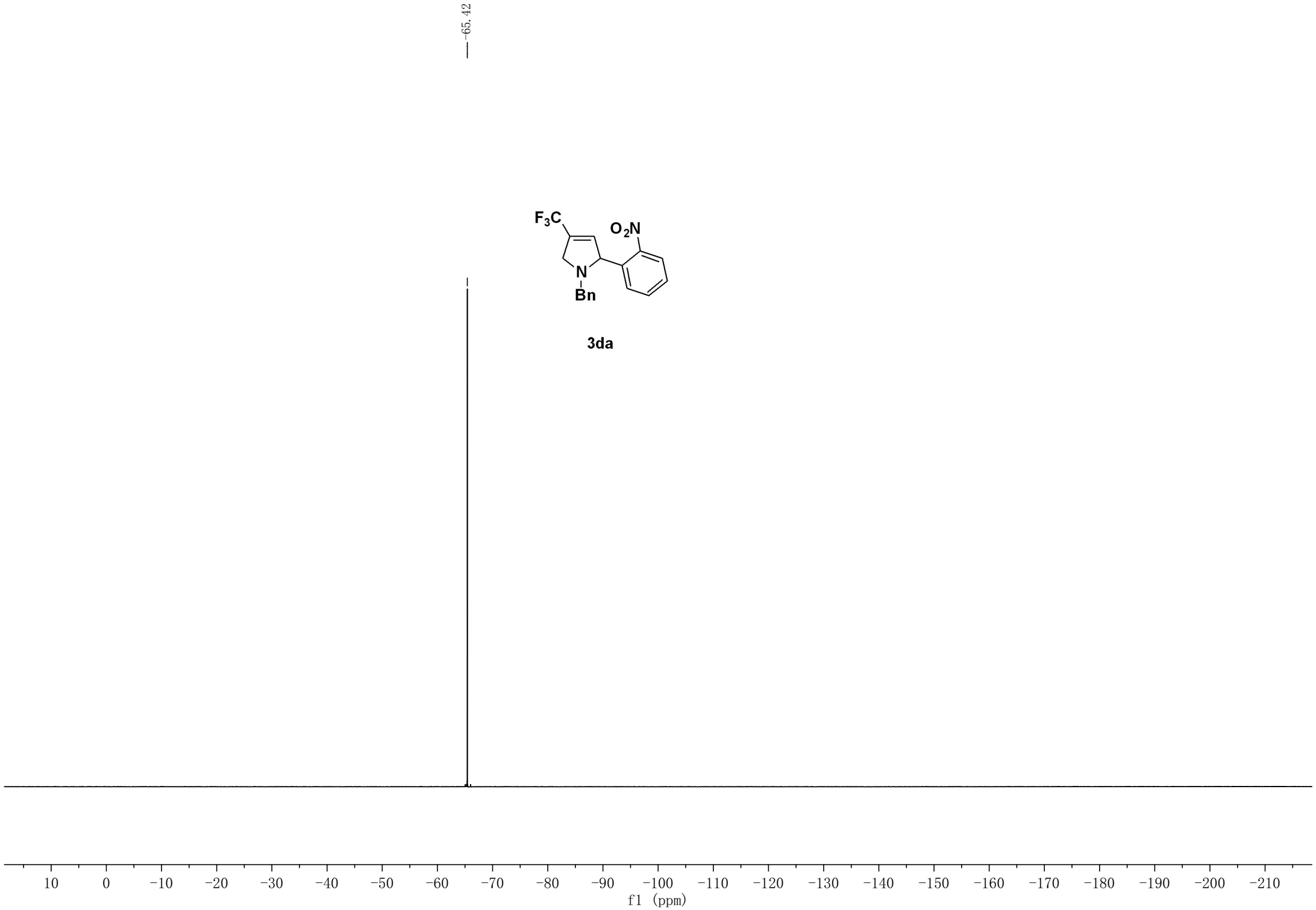
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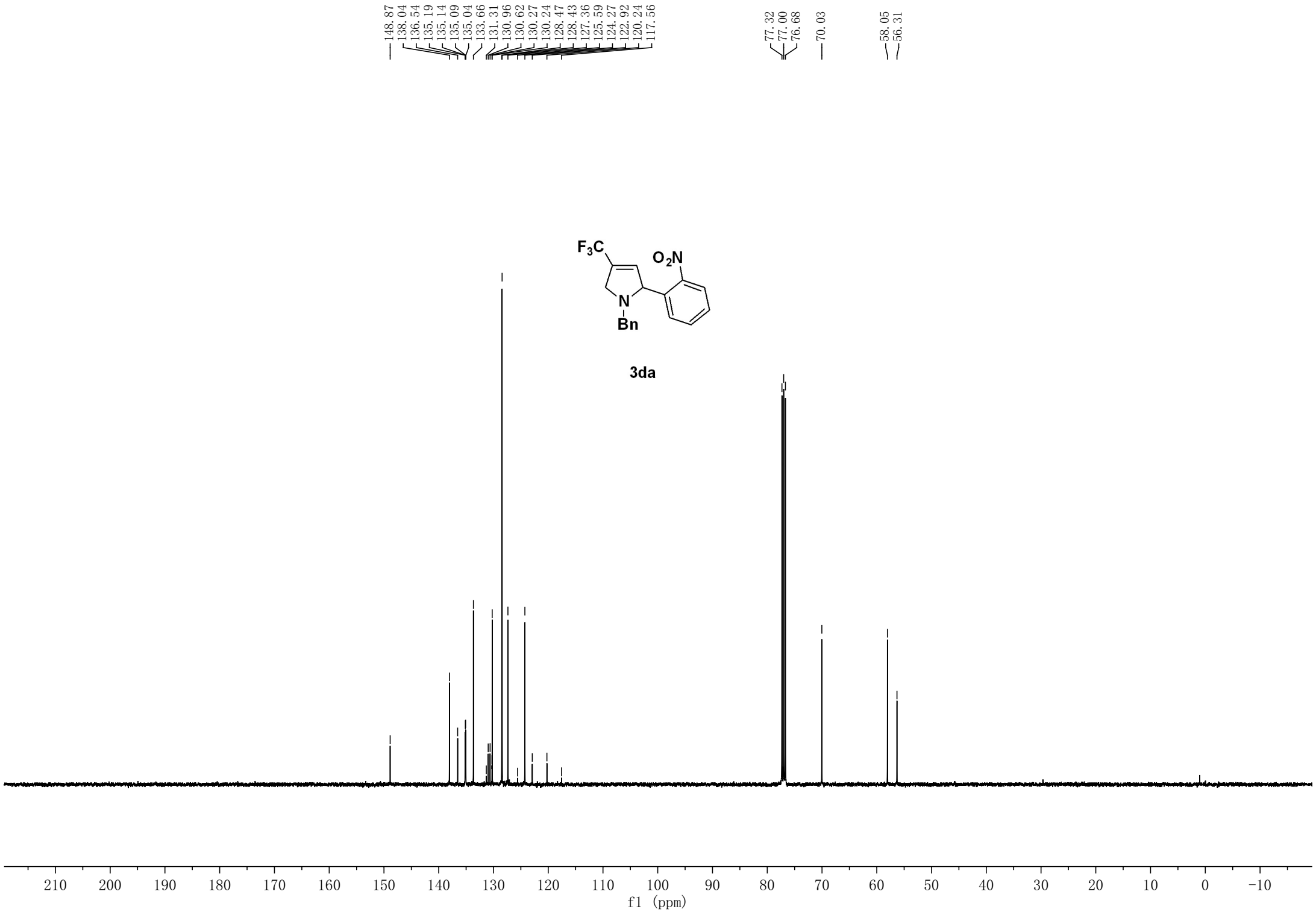
-200
-210
f1 (ppm)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70.03
58.05
56.31
F3C
O2N
N
Bn
3da
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200
190
180
170
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140
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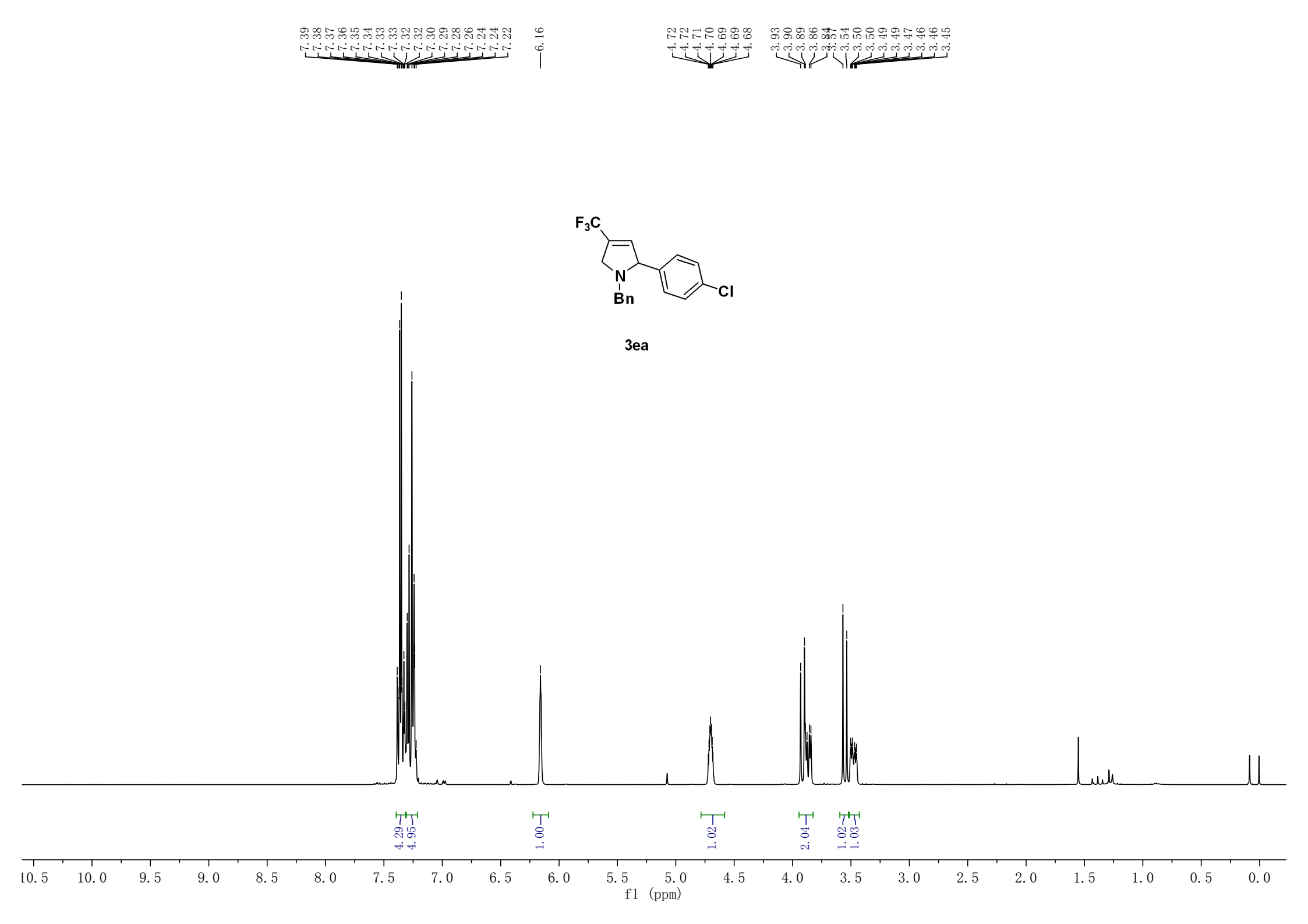
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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Cl
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7.0
6.5
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2.0
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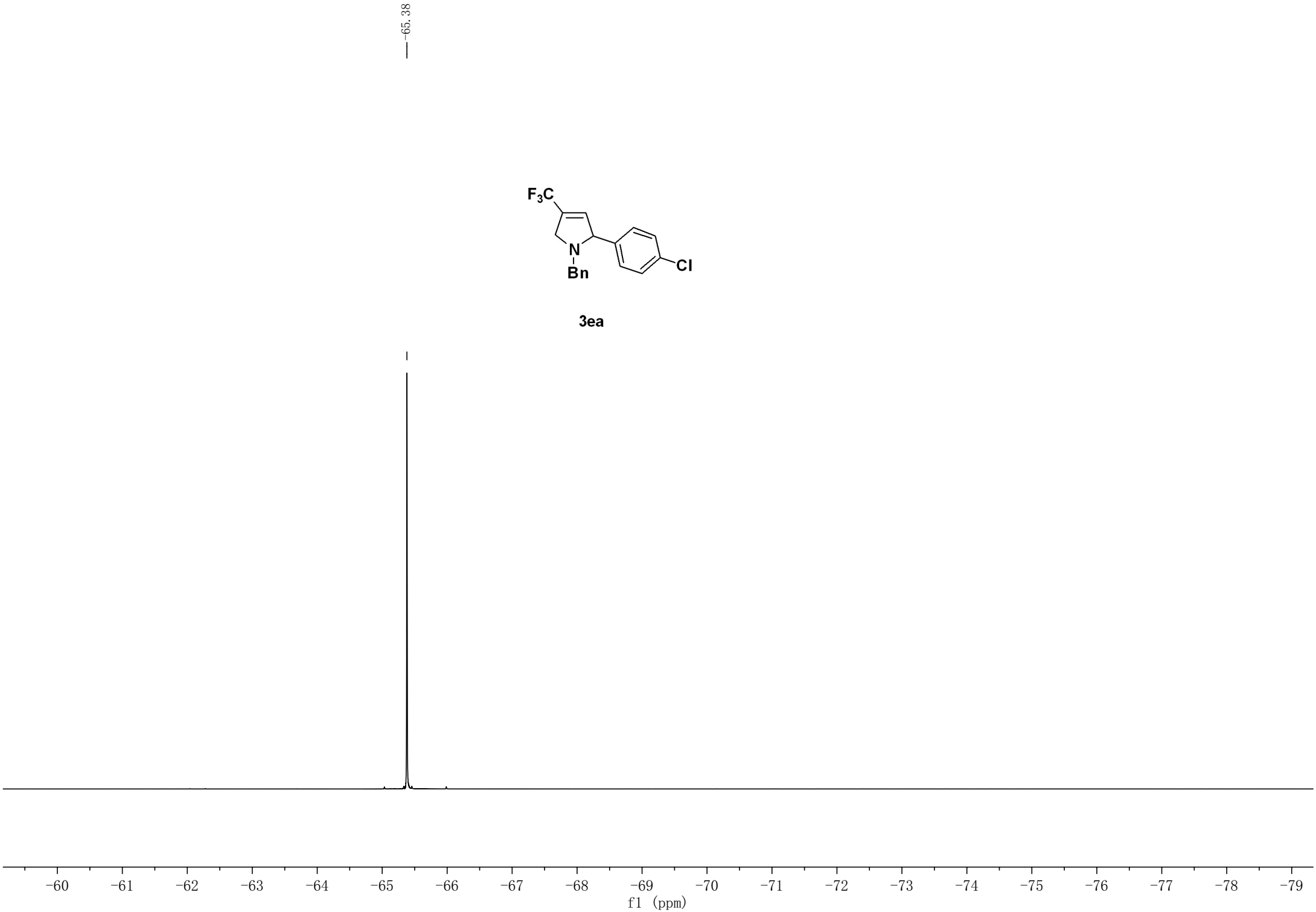
1.0
0.5
0.0
f1 (ppm)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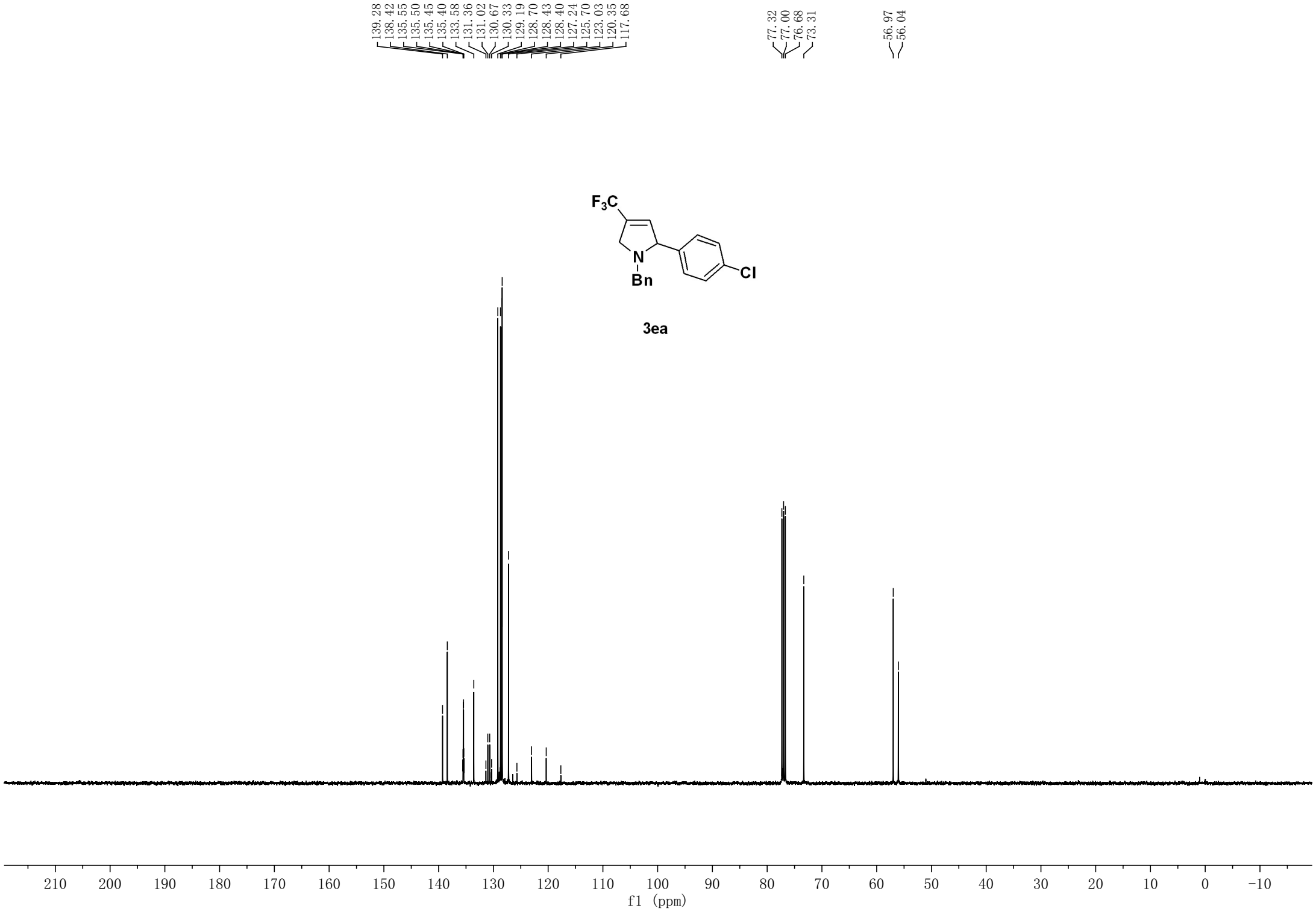
N
Bn
Cl
3ea
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
-73
-74
-75
-76
-77
-78
-79
f1 (ppm)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133.58
131.36
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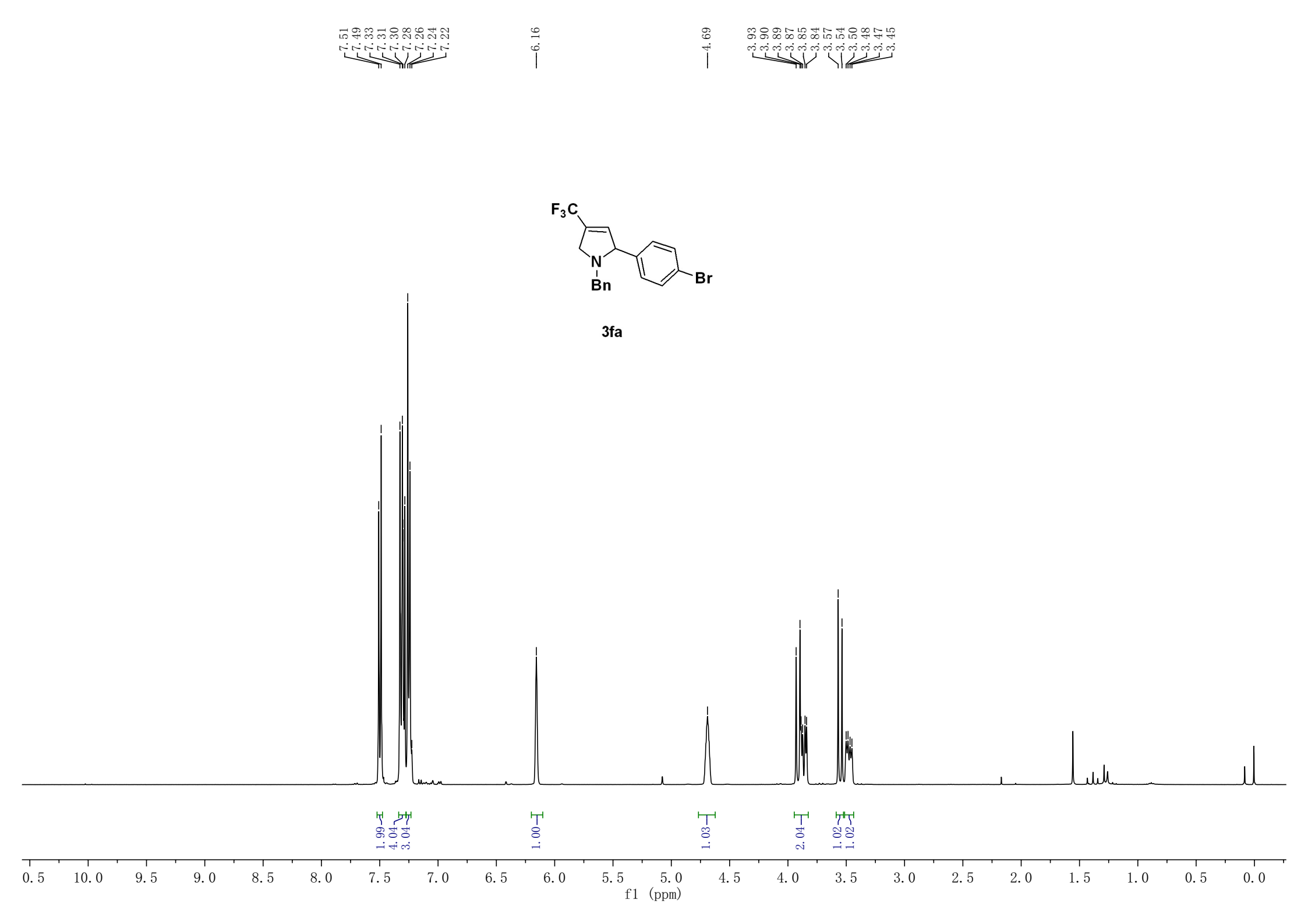
130.67
130.33
129.19
128.70
128.43
128.40
127.24
125.70
123.03
120.35
117.68
77.32
77.00
76.68
73.31
56.97
56.04
F3C
N
Bn
Cl
3ea
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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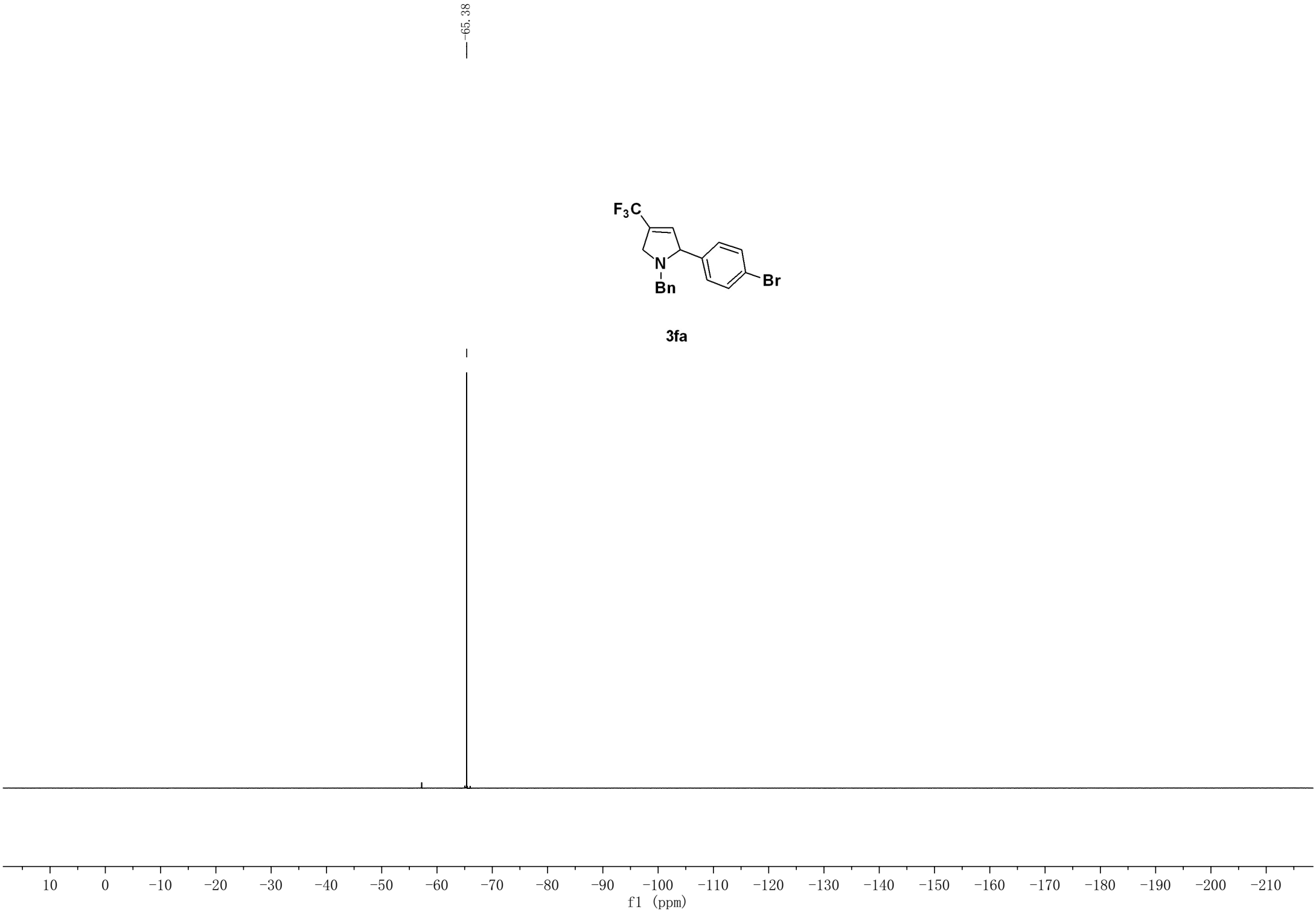
7.28
7.26
7.24
7.22
6.16
4.69
3.93
3.90
3.89
3.87
3.85
3.84
3.57
3.54
3.50
3.48
3.47
3.45
F3C
N
Bn
Br
3fa
1.99
4.04
3.04
1.00
1.03
2.04
1.02
1.02
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
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Bn
Br
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0
-10
-20
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-40
-50
-60
-70
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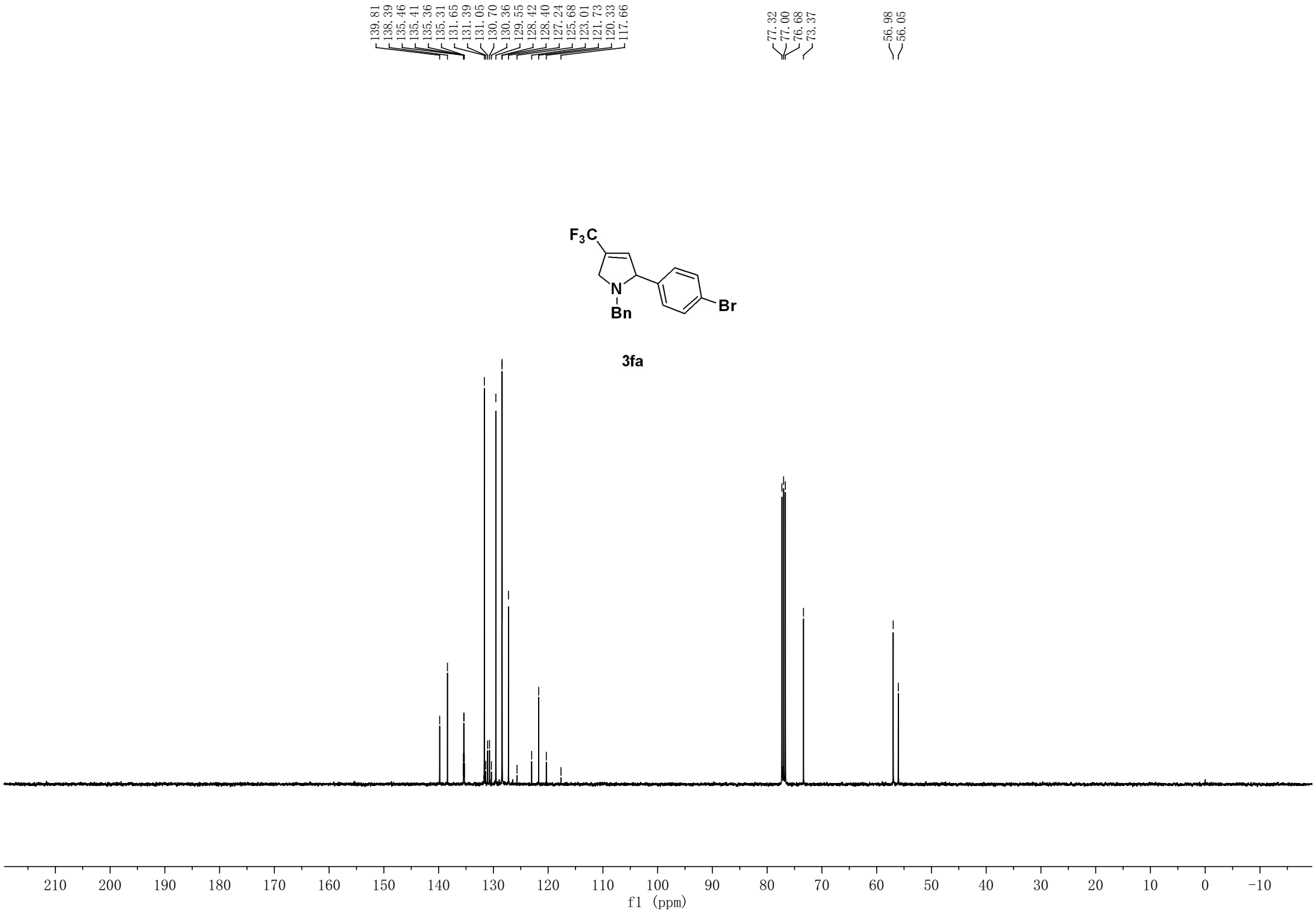
-160
-170
-180
-190
-200
-210
f1 (ppm)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131.39
131.05
130.70
130.36
129.55
128.42
128.40
127.24
125.68
123.01
121.73
120.33
117.66
77.32
77.00
76.68
73.37
56.98
56.05
F3C
N
Bn
Br
3fa
210
200
190
180
170
160
150
140
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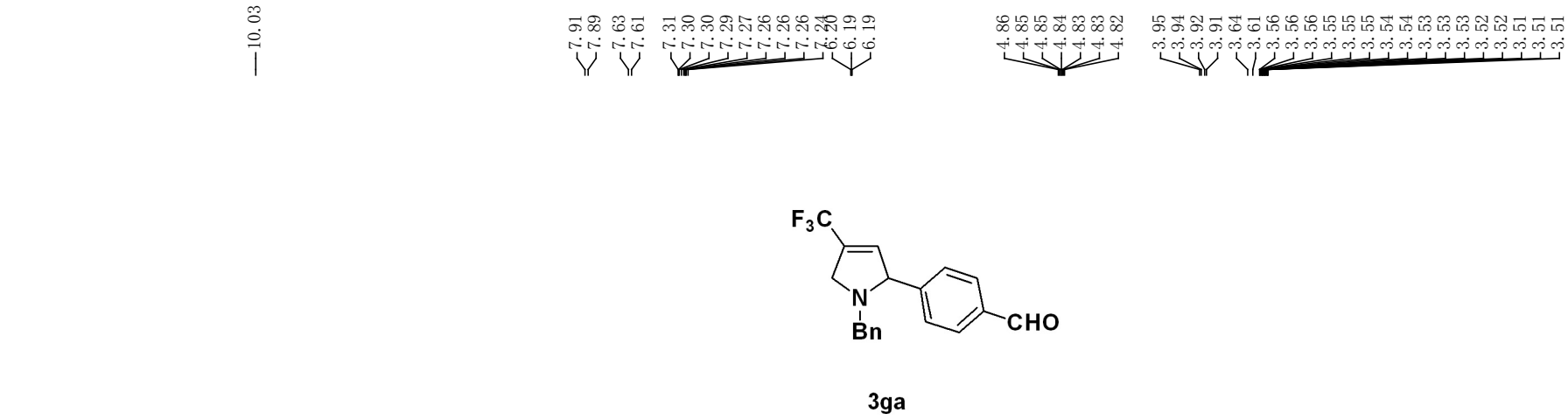
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.91
7.89
7.63
7.61
7.31
7.30
7.30
7.29
7.27
7.26
7.26
7.26
7.24
6.20
6.19
6.19
4.86
4.85
4.85
4.84
4.83
4.83
4.82
3.95
3.94
3.92
3.91
3.64
3.61
3.56
3.56
3.56
3.55
3.55
3.55
3.54
3.54
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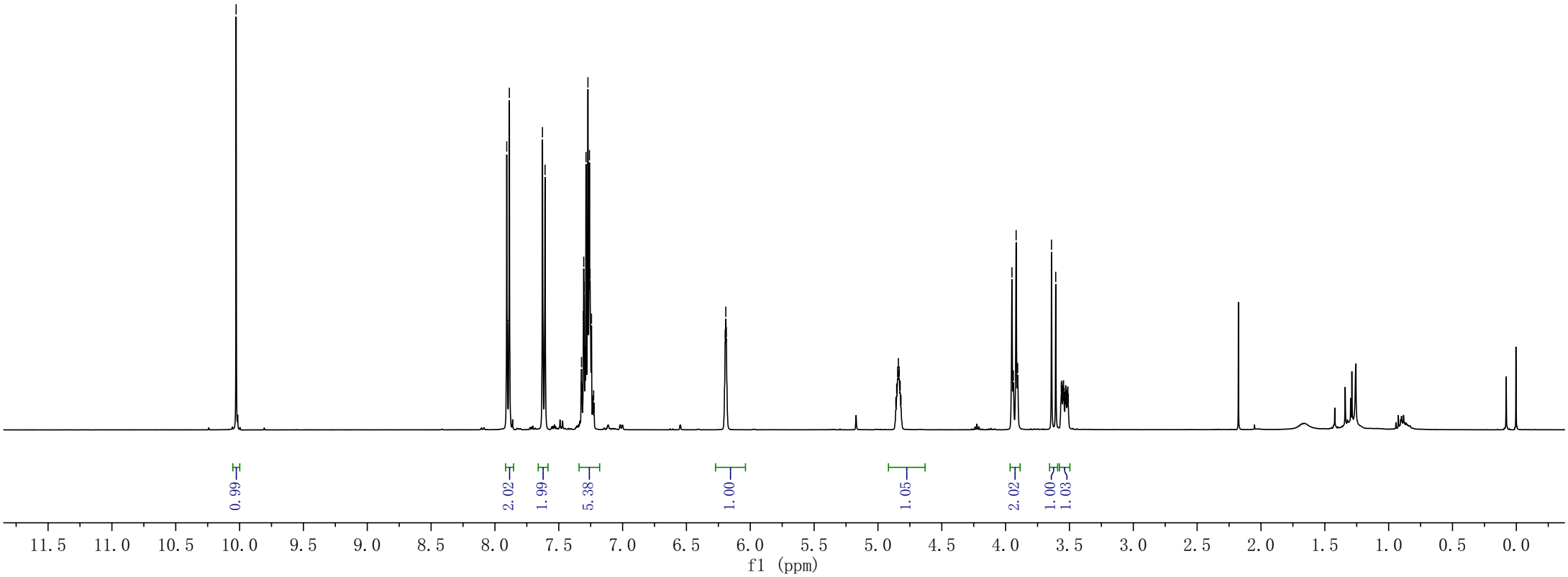
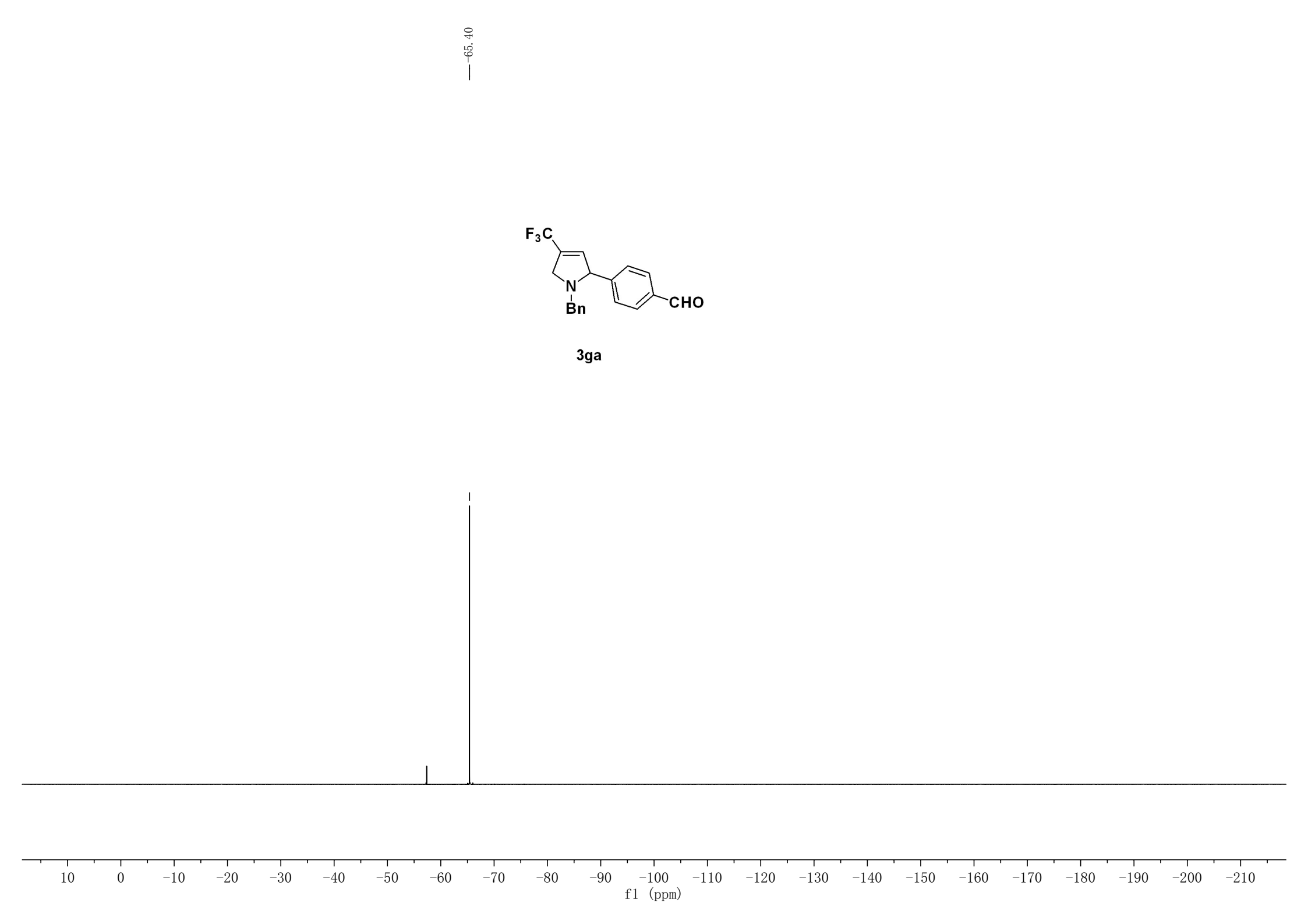
3.53
3.52
3.52
3.51
3.51
3.51
F3C
N
Bn
CHO
3ga


0.99
2.02
1.99
5.38
1.00
1.05
2.02
1.00
1.03
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
N
Bn
CHO
3ga
10
0
-10
-20
-30
-40
-50
-60
-70
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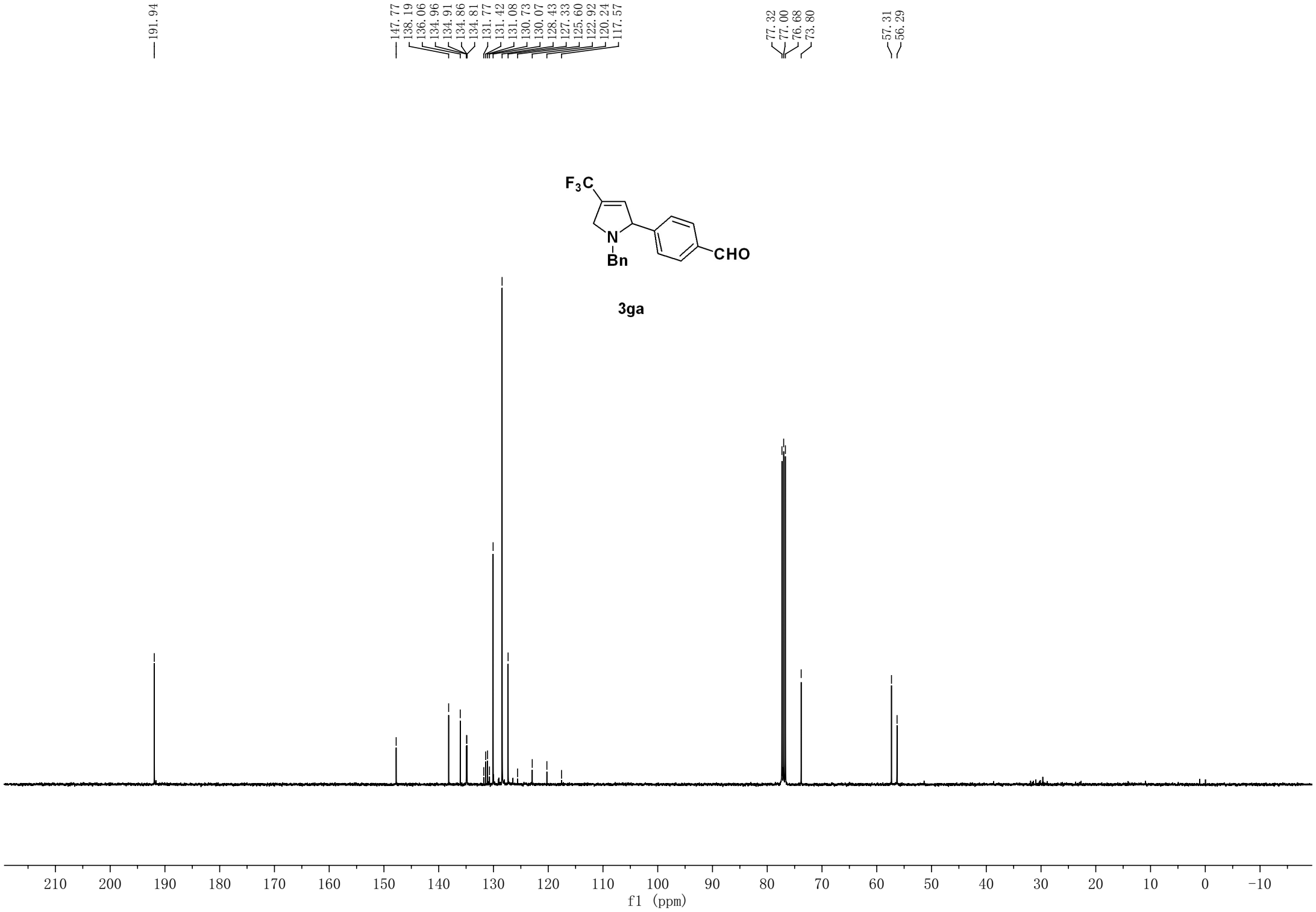
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


191.94
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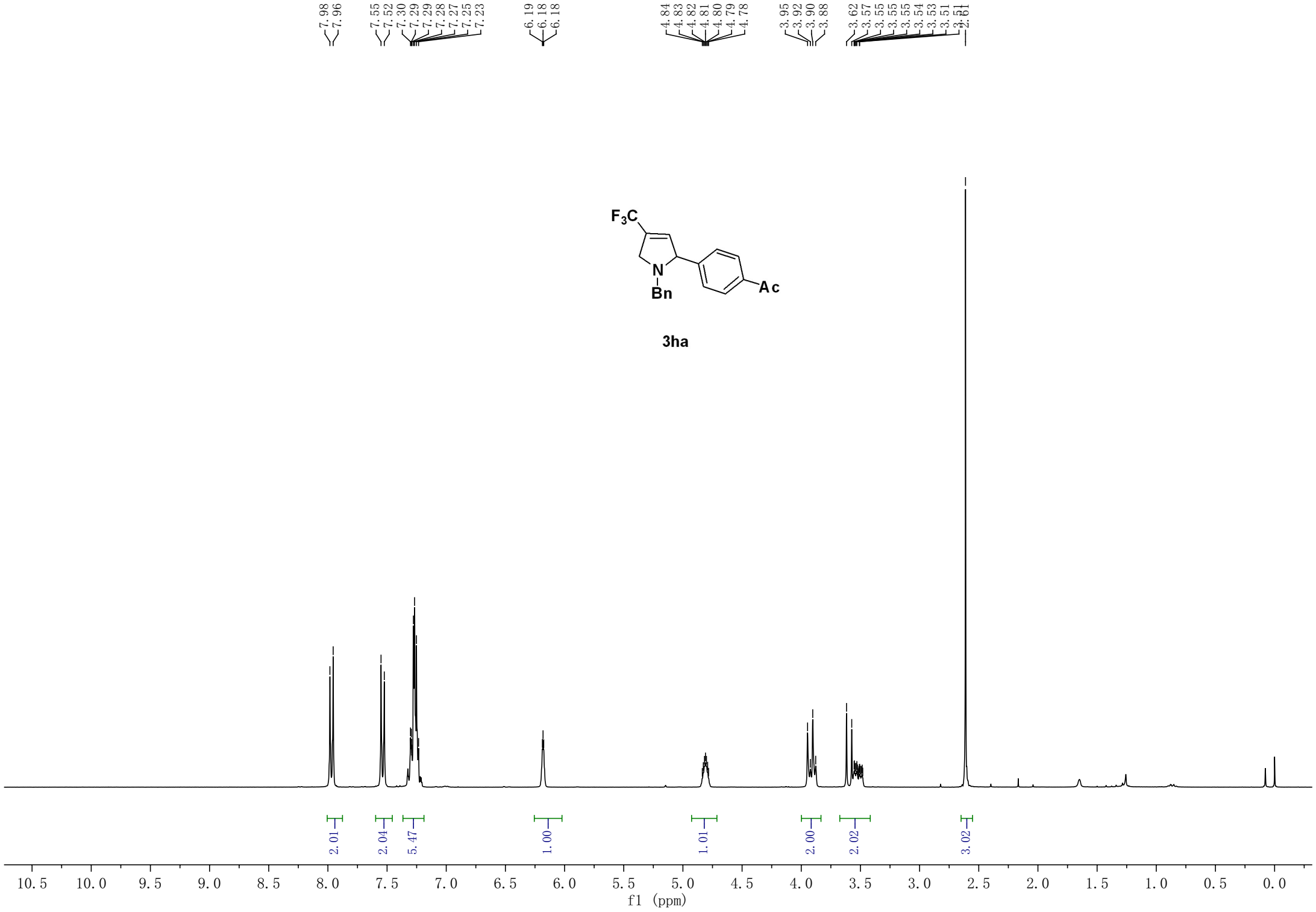
136.06
134.96
134.91
134.86
134.81
131.77
131.42
131.08
130.73
130.07
128.43
127.33
125.60
122.92
120.24
117.57
77.32
77.00
76.68
73.80
57.31
56.29
F3C
N
Bn
CHO
3ga
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.52
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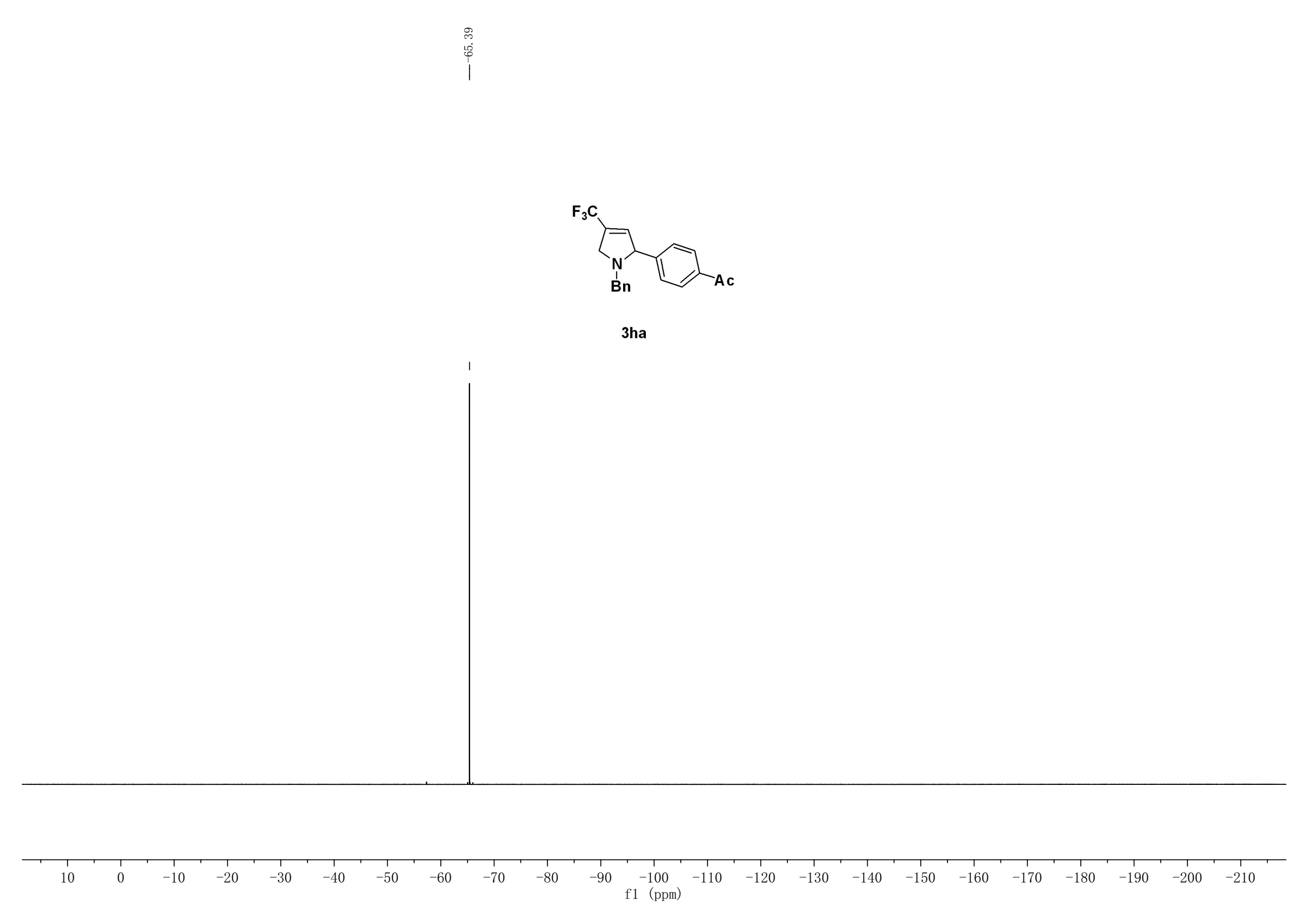
7.29
7.29
7.28
7.27
7.25
7.23
6.19
6.18
6.18
4.84
4.83
4.82
4.81
4.80
4.79
4.78
3.95
3.92
3.90
3.88
3.62
3.57
3.55
3.55
3.54
3.53
3.51
3.51
2.61
F3C
N
Bn
Ac
3ha
2.01
2.04
5.47
1.00
1.01
2.00
2.02
3.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
N
Bn
Ac
3ha
10
0
-10
-20
-30
-40
-50
-60
-70
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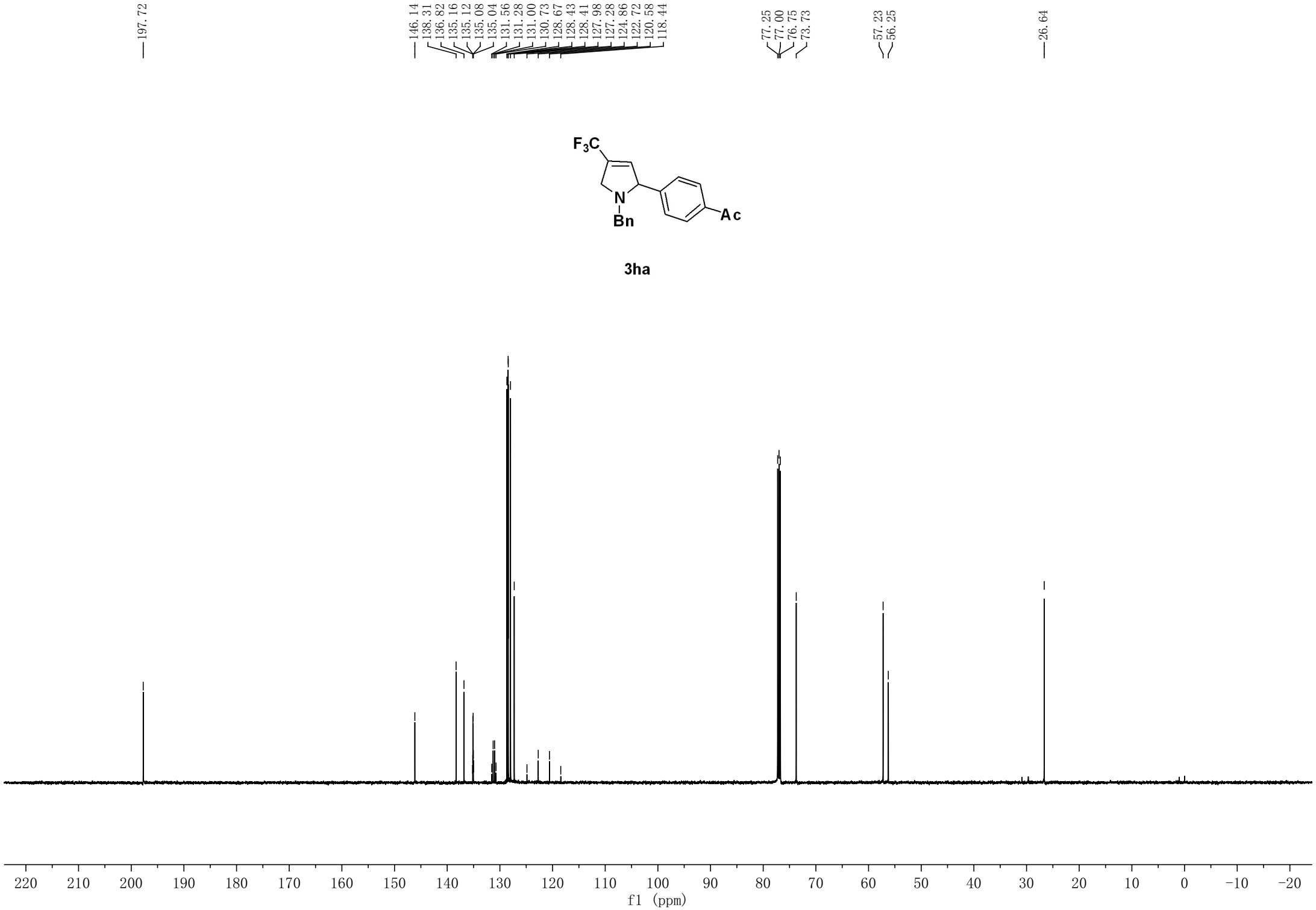
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


197.72
146.14
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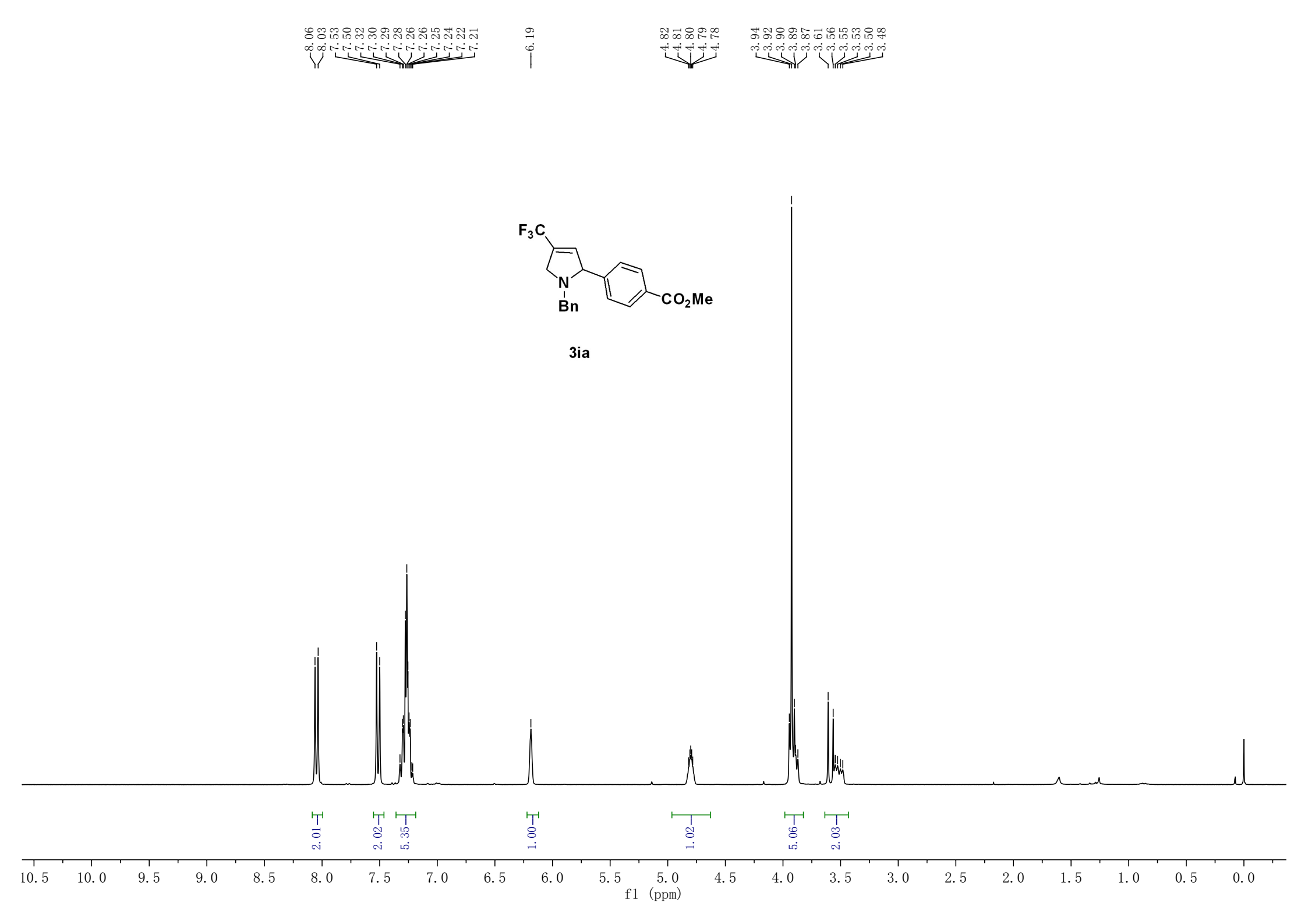
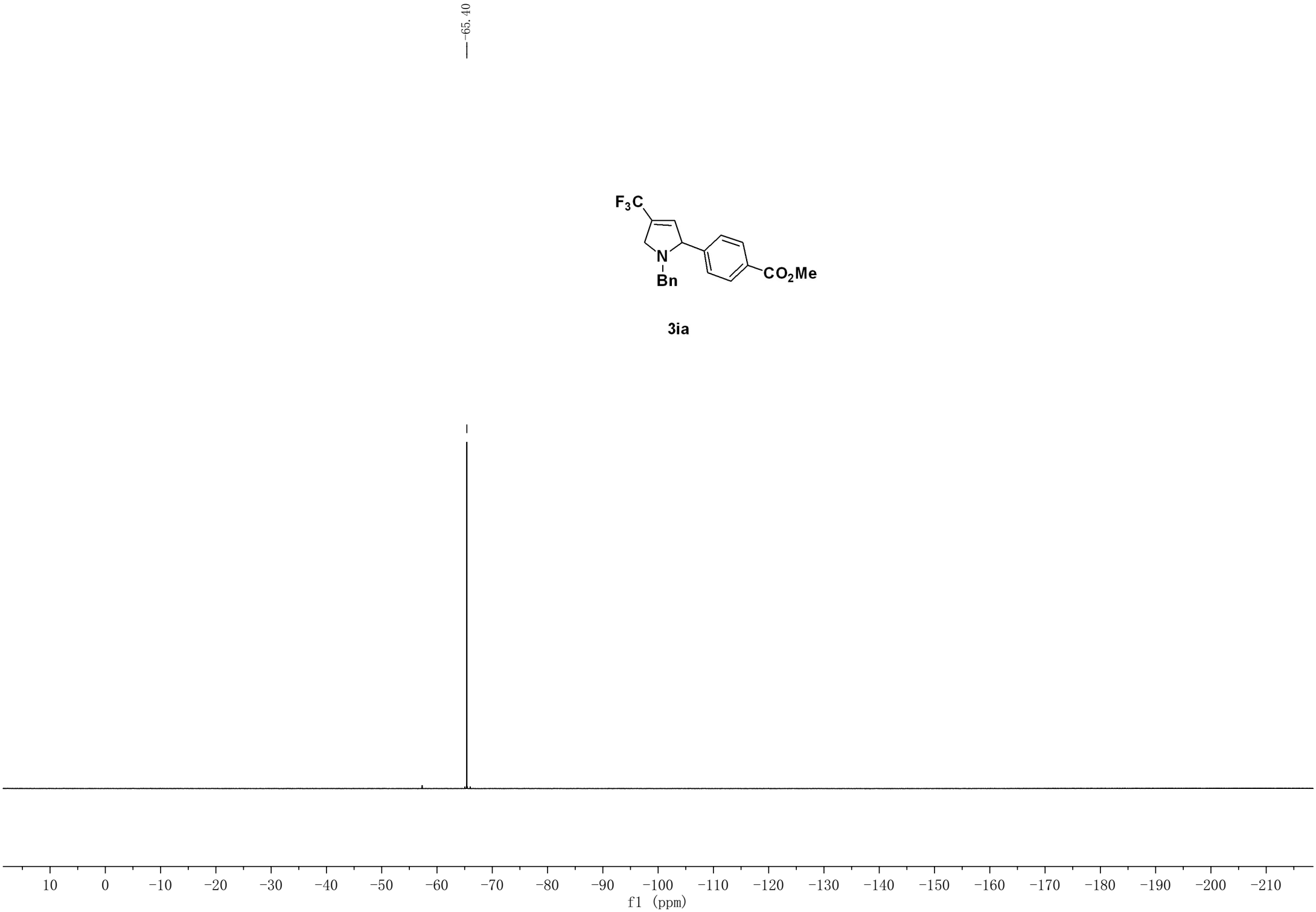
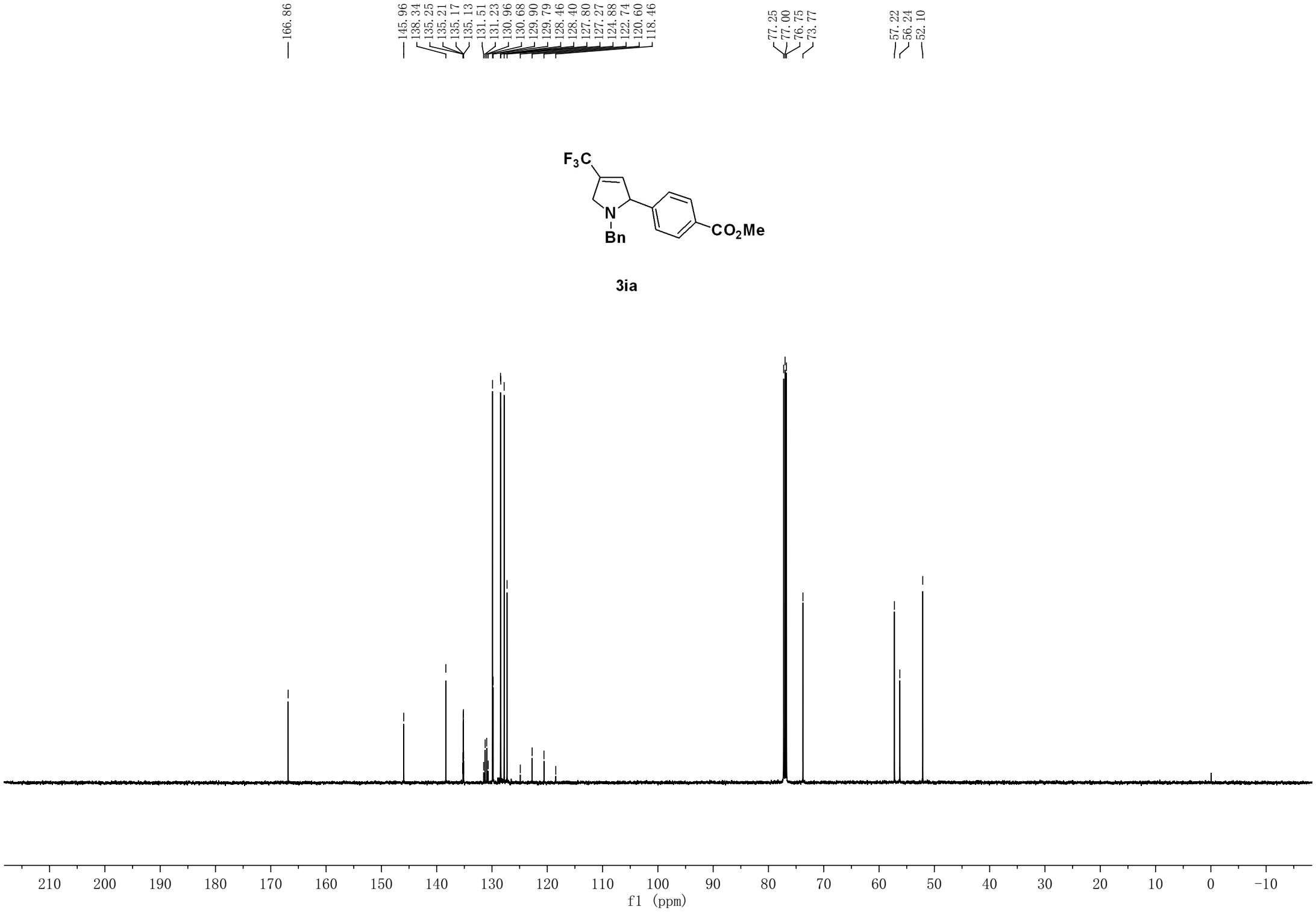
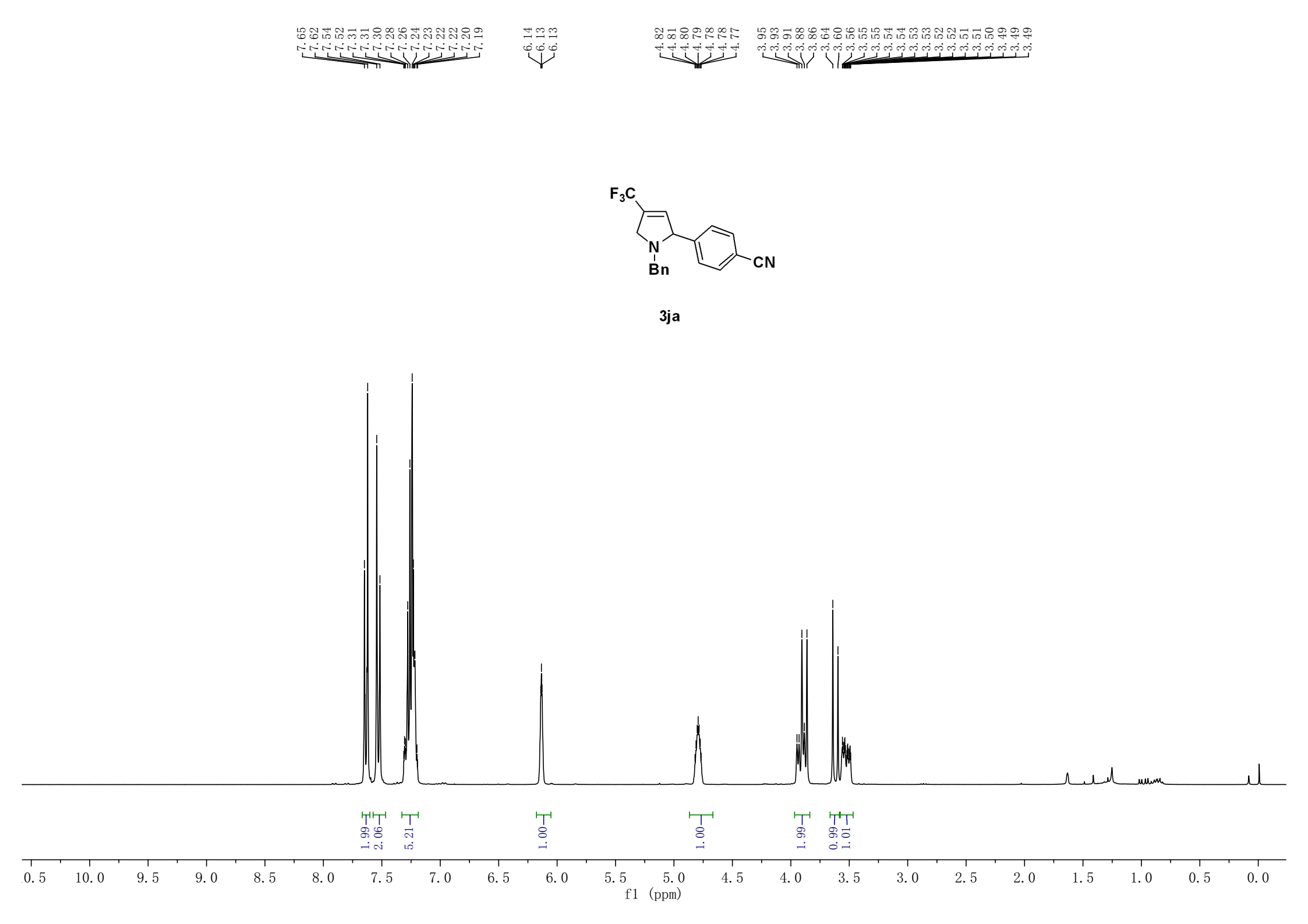
135.12
135.08
135.04
131.56
131.28
131.00
130.73
128.67
128.43
128.41
127.98
127.28
124.86
122.72
120.58
118.44
77.25
77.00
76.75
73.73
57.23
56.25
26.64
F3C
N
Bn
Ac
3ha
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


8.06
8.03
7.53
7.50
7.32
7.30
7.29
7.28
7.26
7.26
7.25
7.24
7.22
7.21
6.19
4.82
4.81
4.80
4.79
4.78
3.94
3.92
3.90
3.89
3.87
3.61
3.56
3.55
3.53
3.50
3.48
F3C
N
Bn
CO2Me
3ia
2.01
2.02
5.35
1.00
1.02
5.06
2.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.40
F3C
N
Bn
CO2Me
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

3ia


166.86
145.96
138.34
135.25
135.21
135.17
135.13
131.51
131.23
130.96
130.68
129.90
129.79
128.46
128.40
127.80
127.27
124.88
122.74
120.60
118.46
77.25
77.00
76.75
73.77
57.22
56.24
52.10
F3C
N
Bn
CO2Me
3ia
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.65
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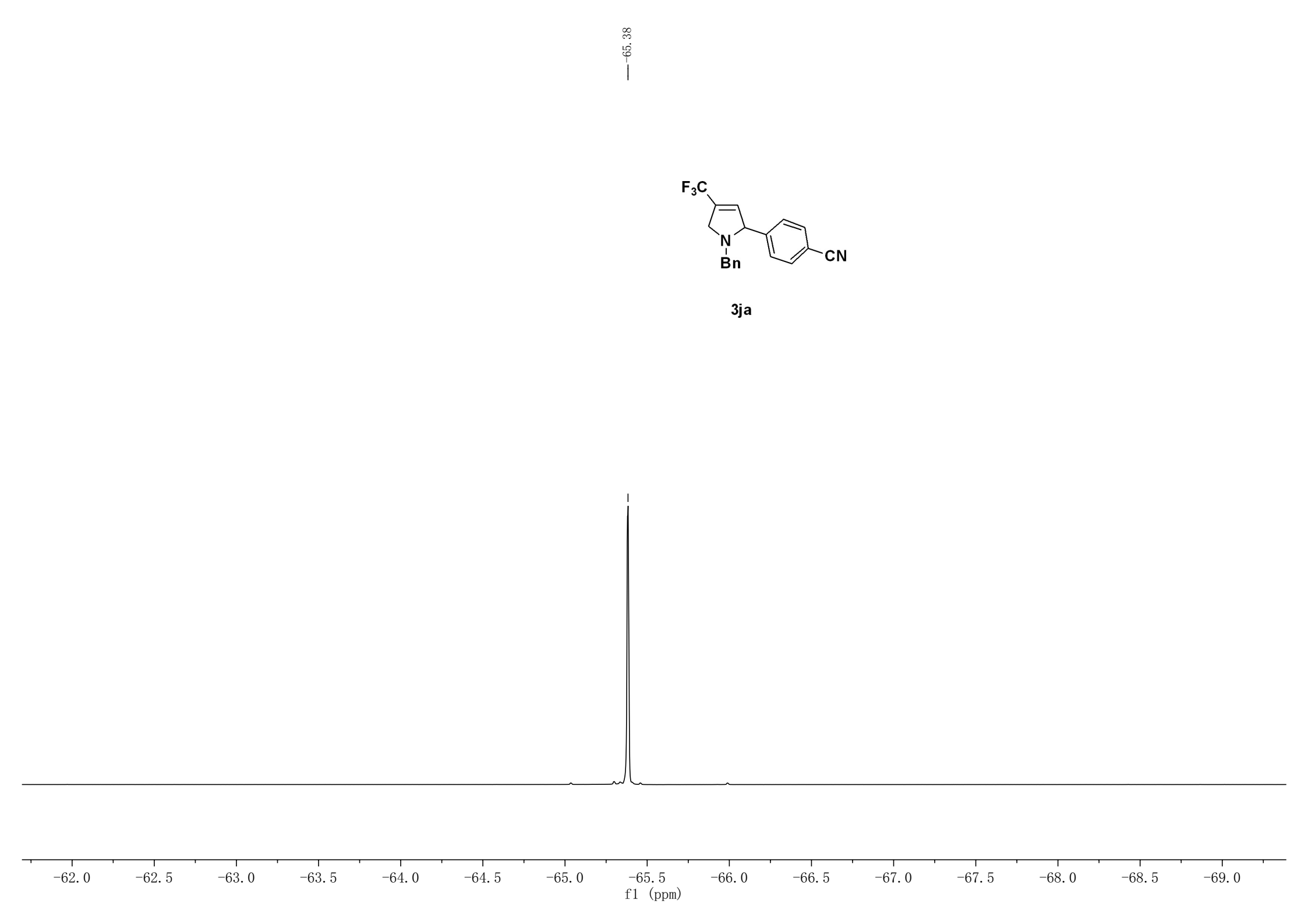
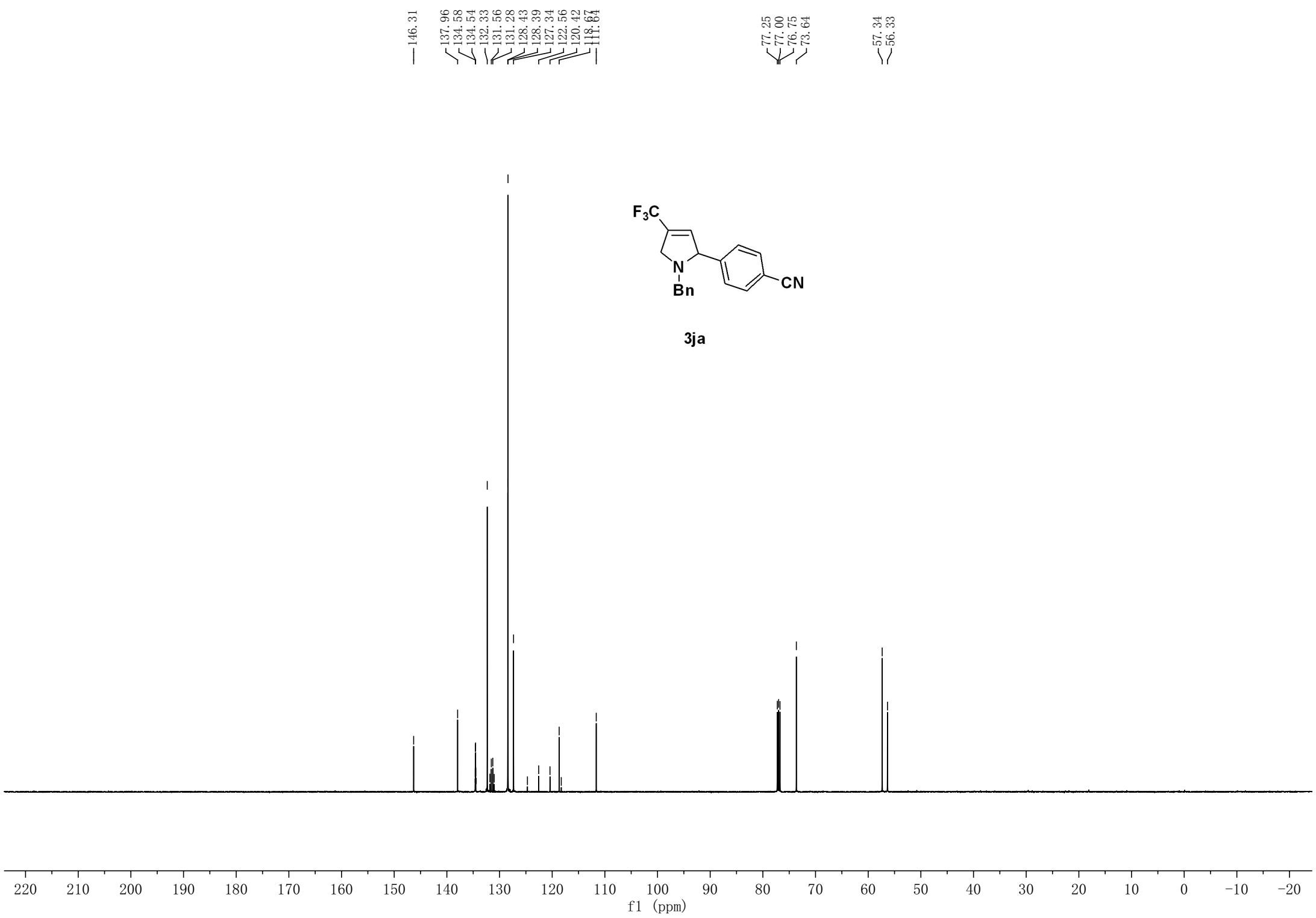
7.52
7.31
7.31
7.30
7.28
7.26
7.24
7.23
7.22
7.22
7.20
7.19
6.14
6.13
6.13
4.82
4.81
4.80
4.79
4.78
4.78
4.77
3.95
3.93
3.91
3.88
3.86
3.64
3.60
3.56
3.55
3.55
3.54
3.54
3.53
3.53
3.52
3.52
3.51
3.51
3.50
3.49
3.49
3.49
F3C
N
Bn
CN
3ja
1.99
2.06
5.21
1.00
1.00
1.99
0.99
1.01
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.38
F3C
N
Bn
CN
3ja
-62.0
-62.5
-63.0
-63.5
-64.0
-64.5
-65.0
-65.5
-66.0
-66.5
-67.0
-67.5
-68.0
-68.5
-69.0
f1 (ppm)


146.31
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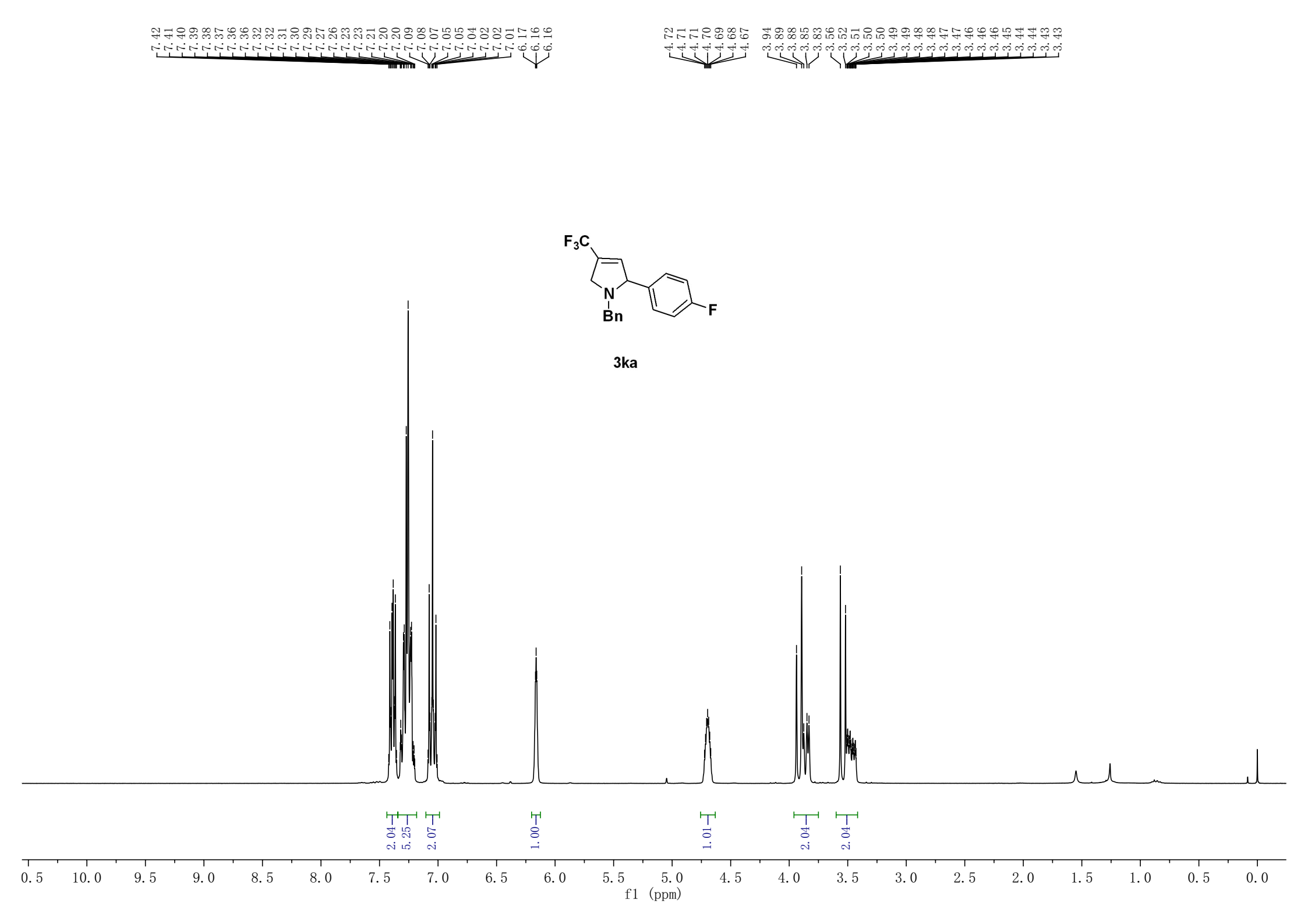
134.58
134.54
132.33
131.56
131.28
128.43
128.39
127.34
122.56
120.42
77.25
77.00
76.75
73.64
57.34
56.33
F3C
N
Bn
CN
3ja
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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7.36
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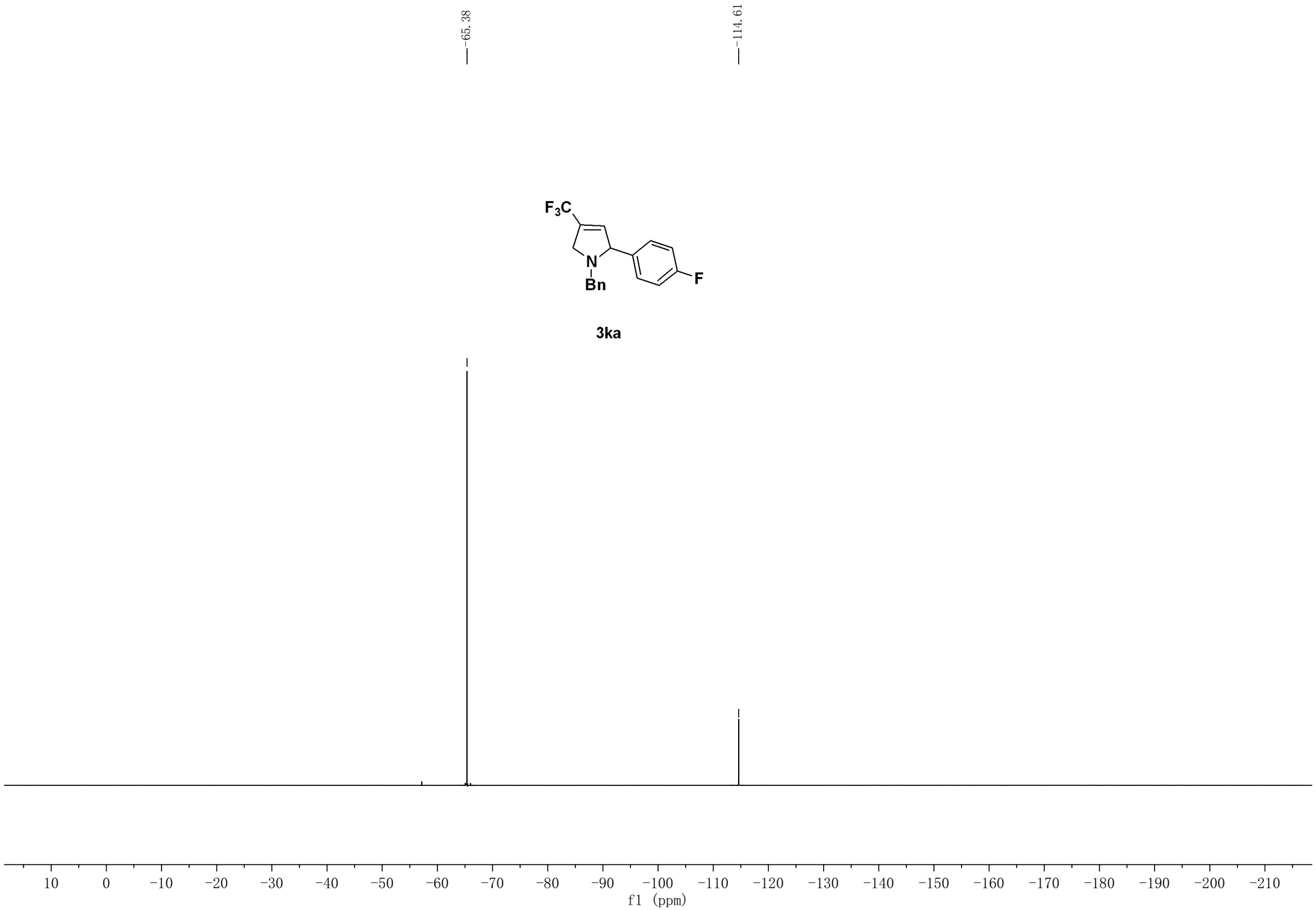
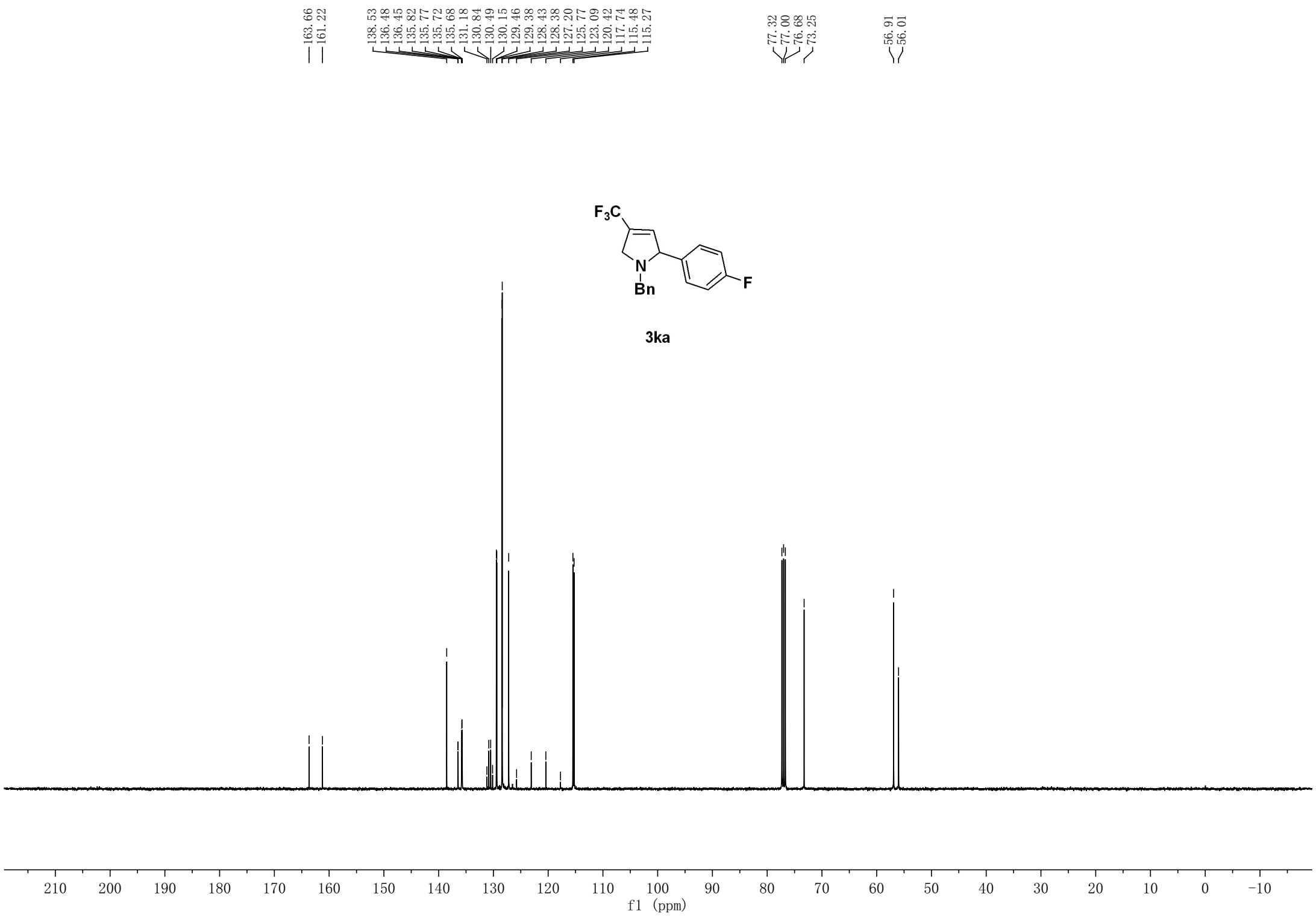
7.32
7.31
7.30
7.29
7.27
7.26
7.23
7.23
7.21
7.20
7.20
7.09
7.08
7.07
7.05
7.05
7.04
7.02
7.02
7.01
6.17
6.16
6.16
4.72
4.71
4.71
4.70
4.69
4.68
4.67
3.94
3.89
3.88
3.85
3.83
3.56
3.52
3.51
3.50
3.50
3.49
3.49
3.48
3.48
3.47
3.47
3.46
3.46
3.46
3.45
3.44
3.44
3.43
3.43
F3C
N
Bn
F
3ka
2.04
5.25
2.07
1.00
1.01
2.04
2.04
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


−65.38
−114.61
F3C
N
Bn
F
3ka
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)


163.66
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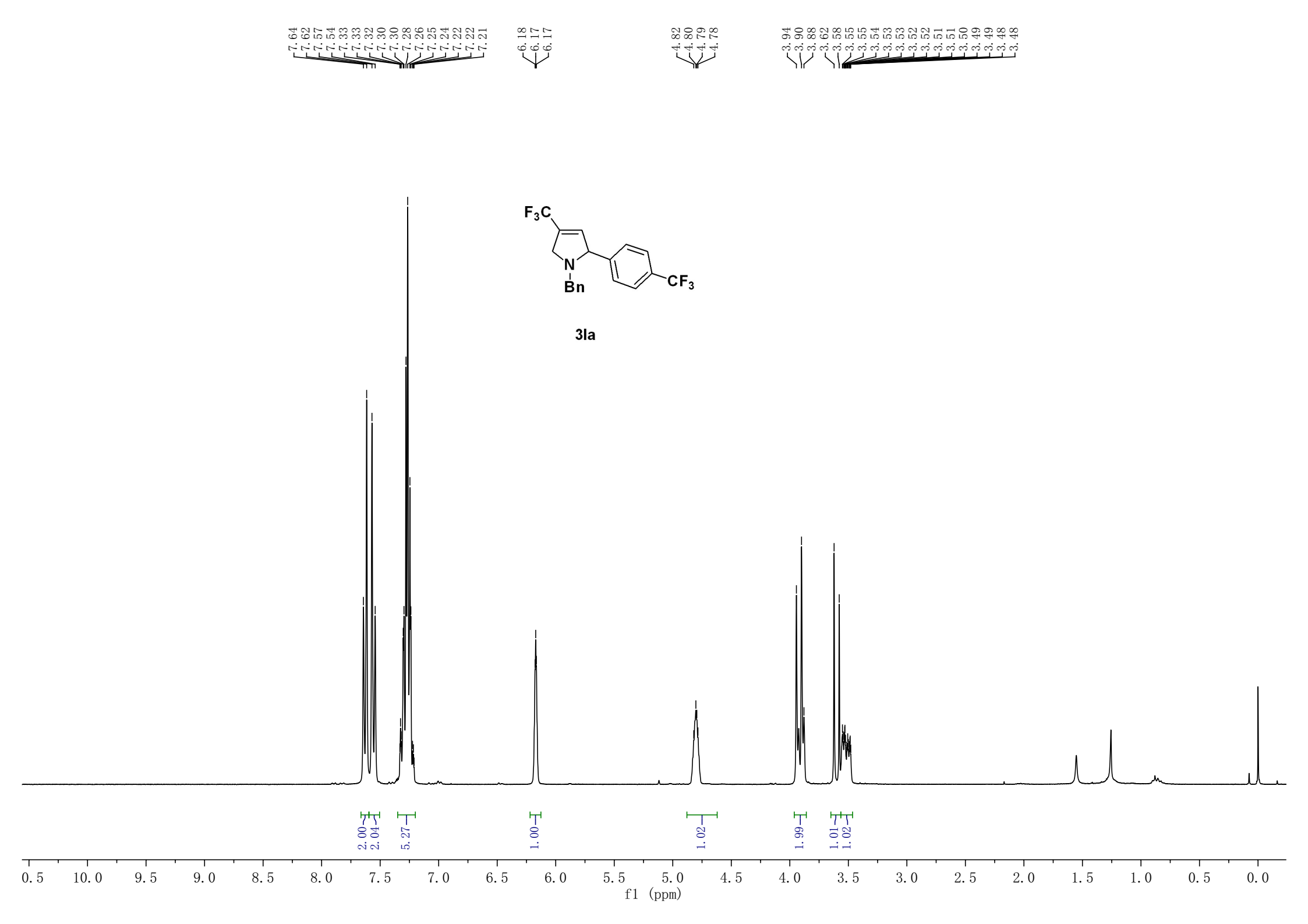
136.48
136.45
135.82
135.77
135.72
135.68
131.18
130.84
130.49
130.15
129.46
129.38
128.43
128.38
127.20
125.77
123.09
120.42
117.74
115.48
115.27
77.32
77.00
76.68
73.25
56.91
56.01
F3C
N
Bn
F
3ka
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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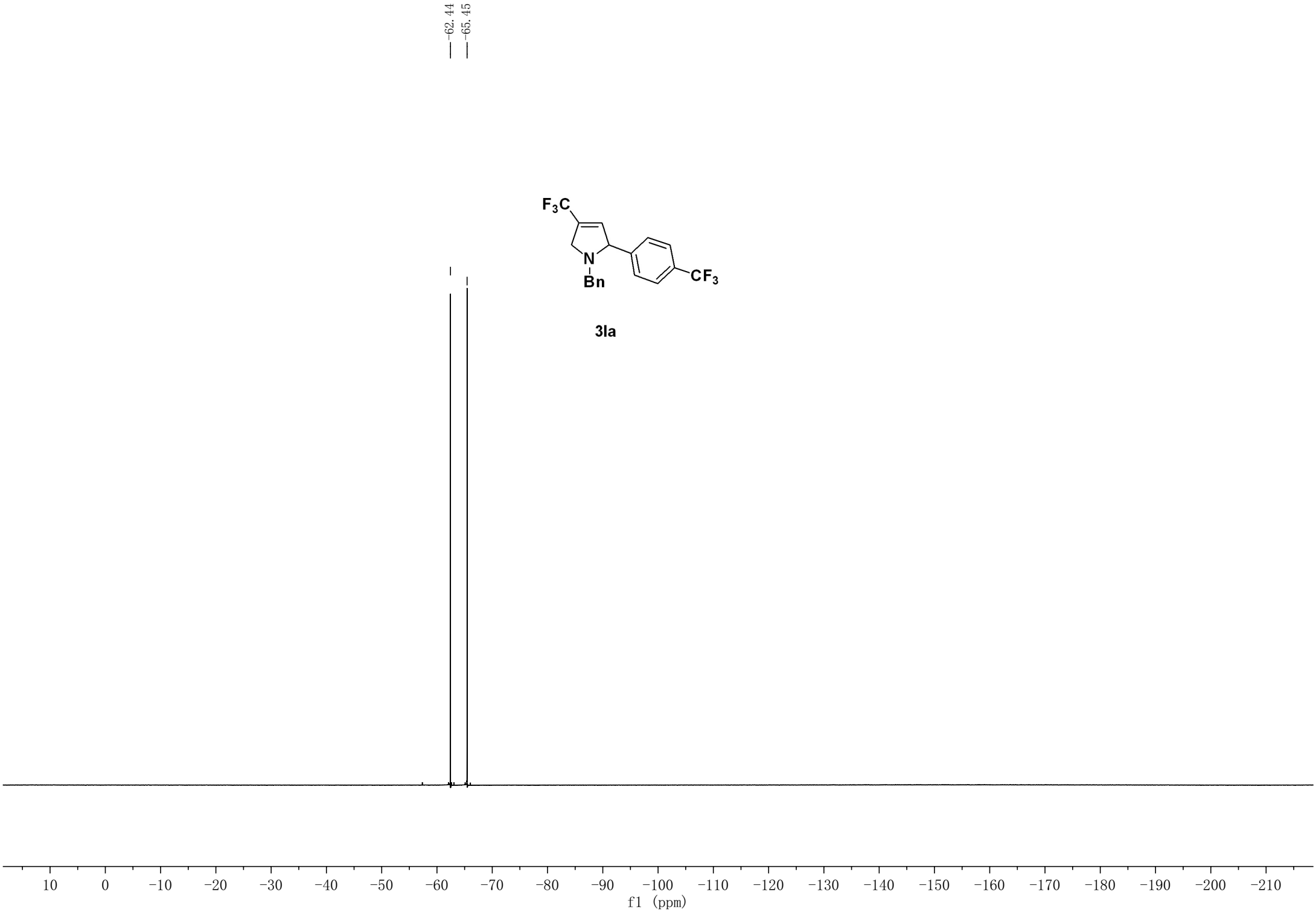
7.57
7.54
7.33
7.33
7.32
7.30
7.30
7.28
7.26
7.25
7.24
7.22
7.22
7.21
6.18
6.17
6.17
4.82
4.80
4.79
4.78
3.94
3.90
3.88
3.62
3.58
3.55
3.55
3.54
3.53
3.53
3.52
3.52
3.51
3.51
3.50
3.49
3.49
3.48
3.48
F3C
N
Bn
CF3
3Ia
2.00
2.04
5.27
1.00
1.02
1.99
1.01
1.02
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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-65.45
F3C
N
Bn
CF3
3la
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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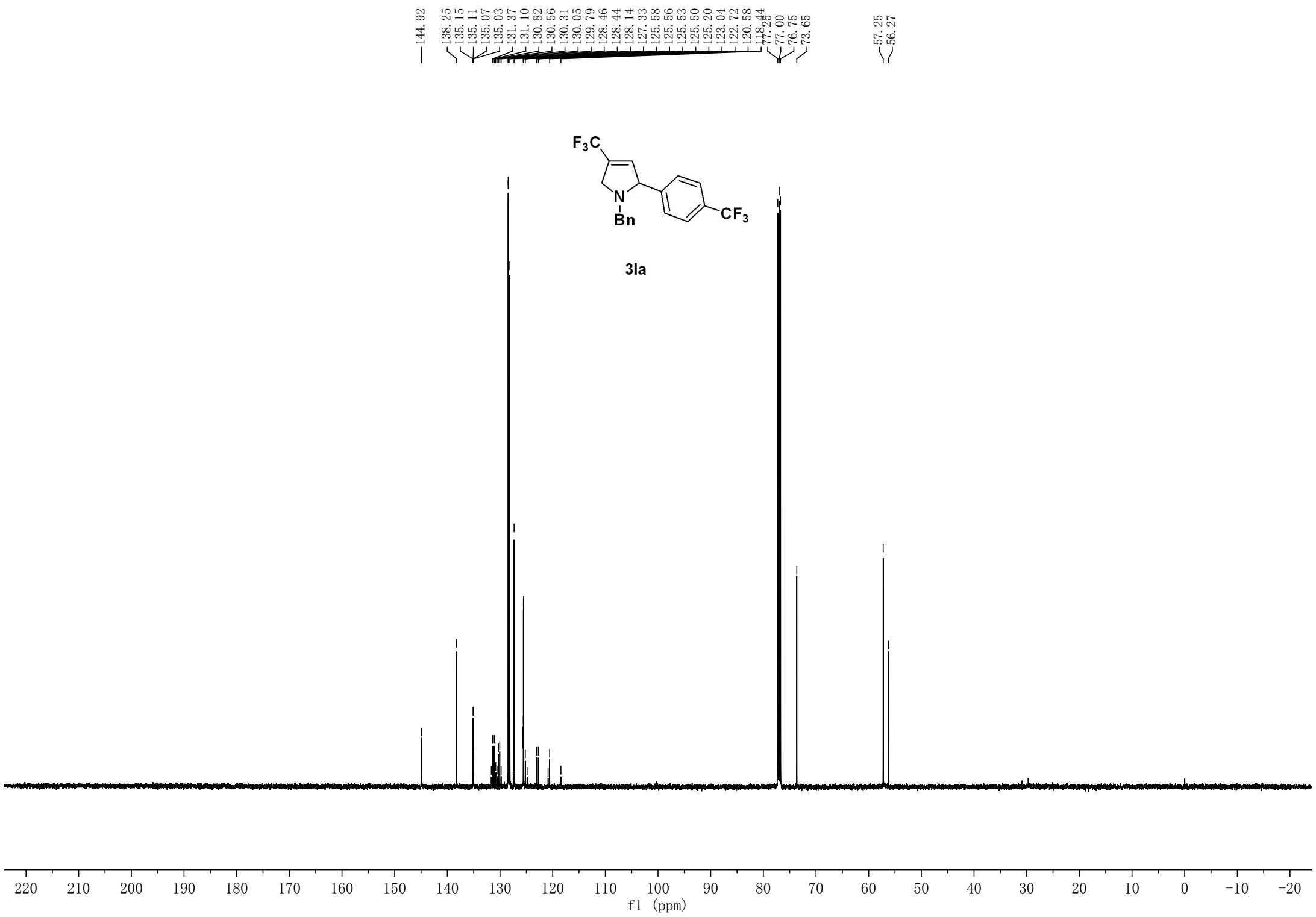
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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129.79
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128.44
128.14
127.33
125.58
125.56
125.53
125.50
125.20
123.04
122.72
120.58
118.44
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77.00
76.75
73.65
57.25
56.27
F3C
N
Bn
CF3
3la
220
210
200
190
180
170
160
150
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100
90
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60
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20
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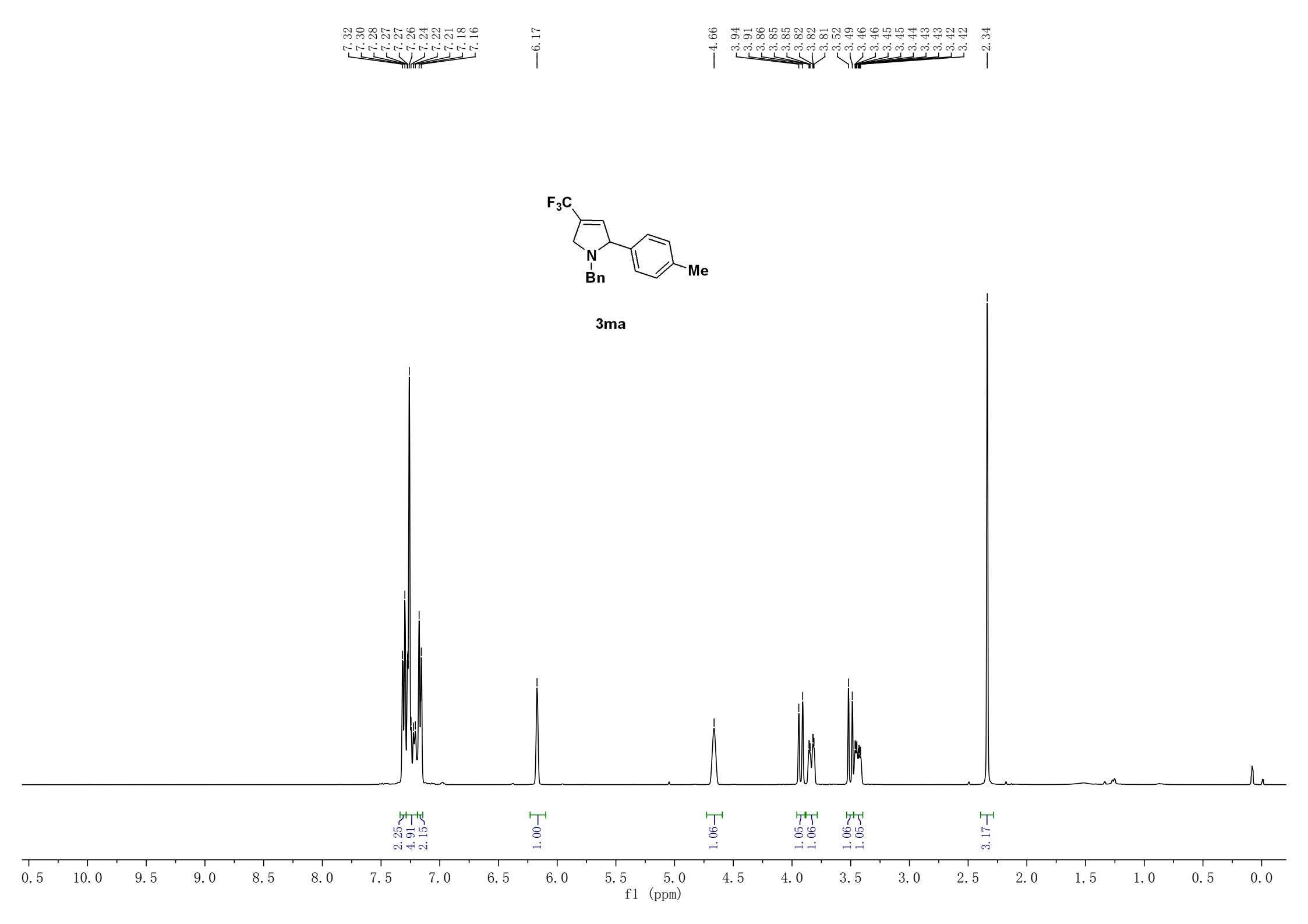
-10
-20
f1 (ppm)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7.18
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6.17
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3.94
3.91
3.86
3.85
3.85
3.82
3.82
3.81
3.52
3.49
3.46
3.46
3.45
3.45
3.44
3.43
3.43
3.42
3.42
2.34
F3C
N
Bn
Me
3ma
2.25
4.91
2.15
1.00
1.06
1.05
1.06
1.06
1.05
3.17
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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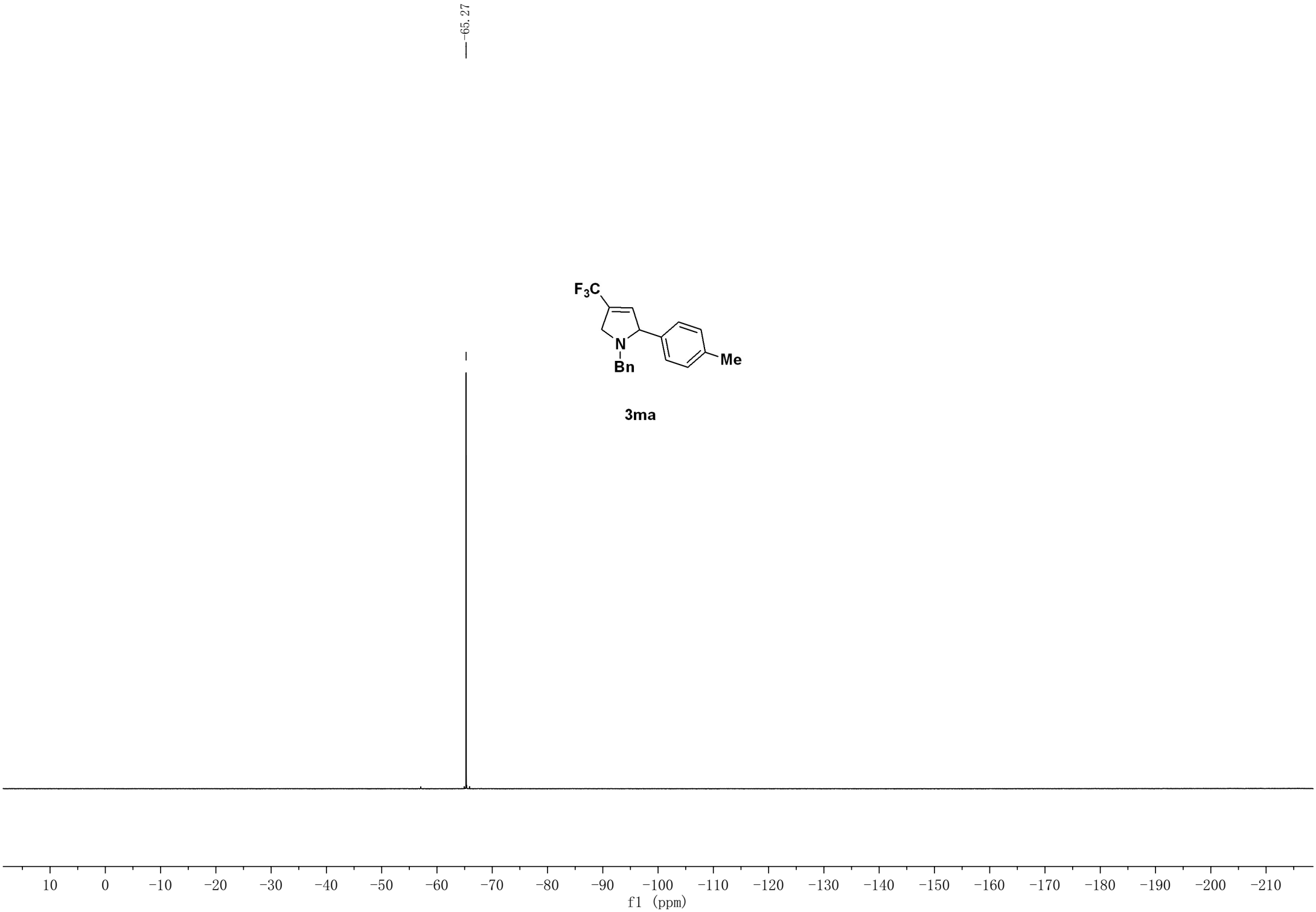
0.0
f1 (ppm)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Bn
Me
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0
-10
-20
-30
-40
-50
-60
-70
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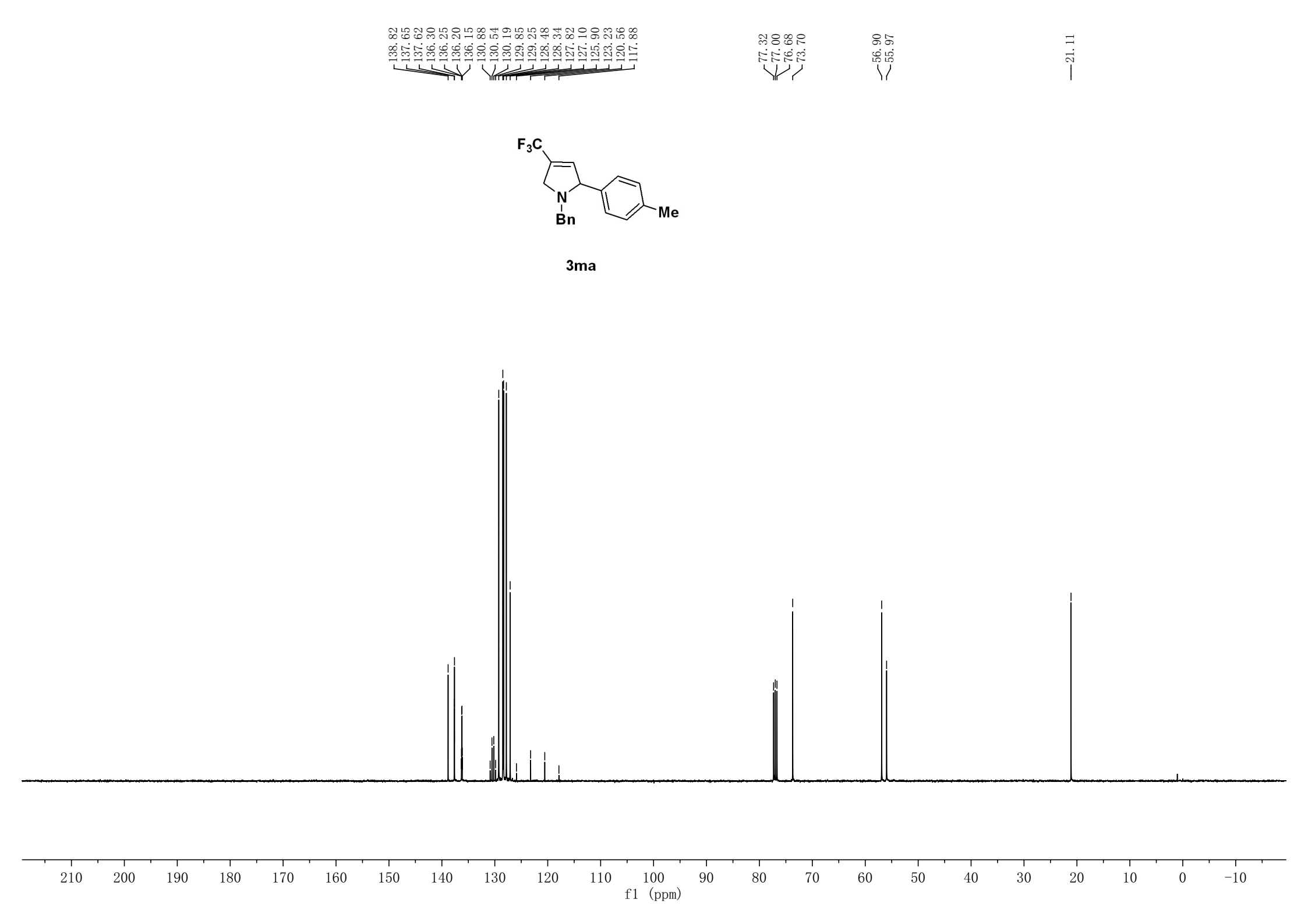
-170
-180
-190
-200
-210
f1 (ppm)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128.48
128.34
127.82
127.10
125.90
123.23
120.56
117.88
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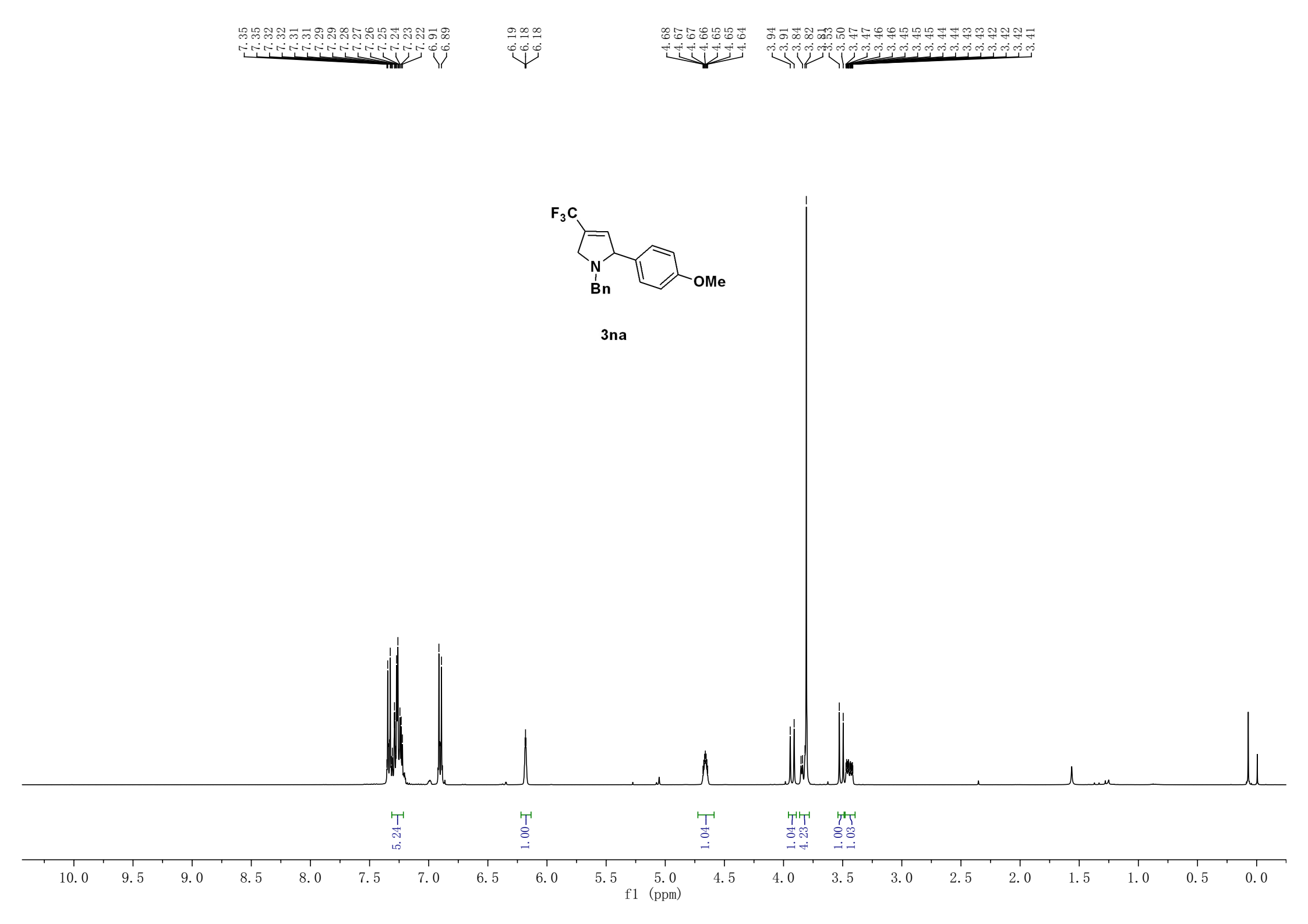
77.00
76.68
73.70
56.90
55.97
21.11
F3C
N
Bn
Me
3ma
f1 (ppm)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7.29
7.29
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7.26
7.25
7.24
7.23
7.22
6.91
6.89
6.19
6.18
6.18
4.68
4.67
4.67
4.66
4.65
4.65
4.64
3.94
3.91
3.84
3.82
3.81
3.53
3.50
3.47
3.47
3.46
3.46
3.45
3.45
3.45
3.44
3.44
3.43
3.42
3.42
3.42
3.41
F3C
N
Bn
OMe
3na
5.24
1.00
1.04
1.04
4.23
1.00
1.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
2.0
1.5
1.0
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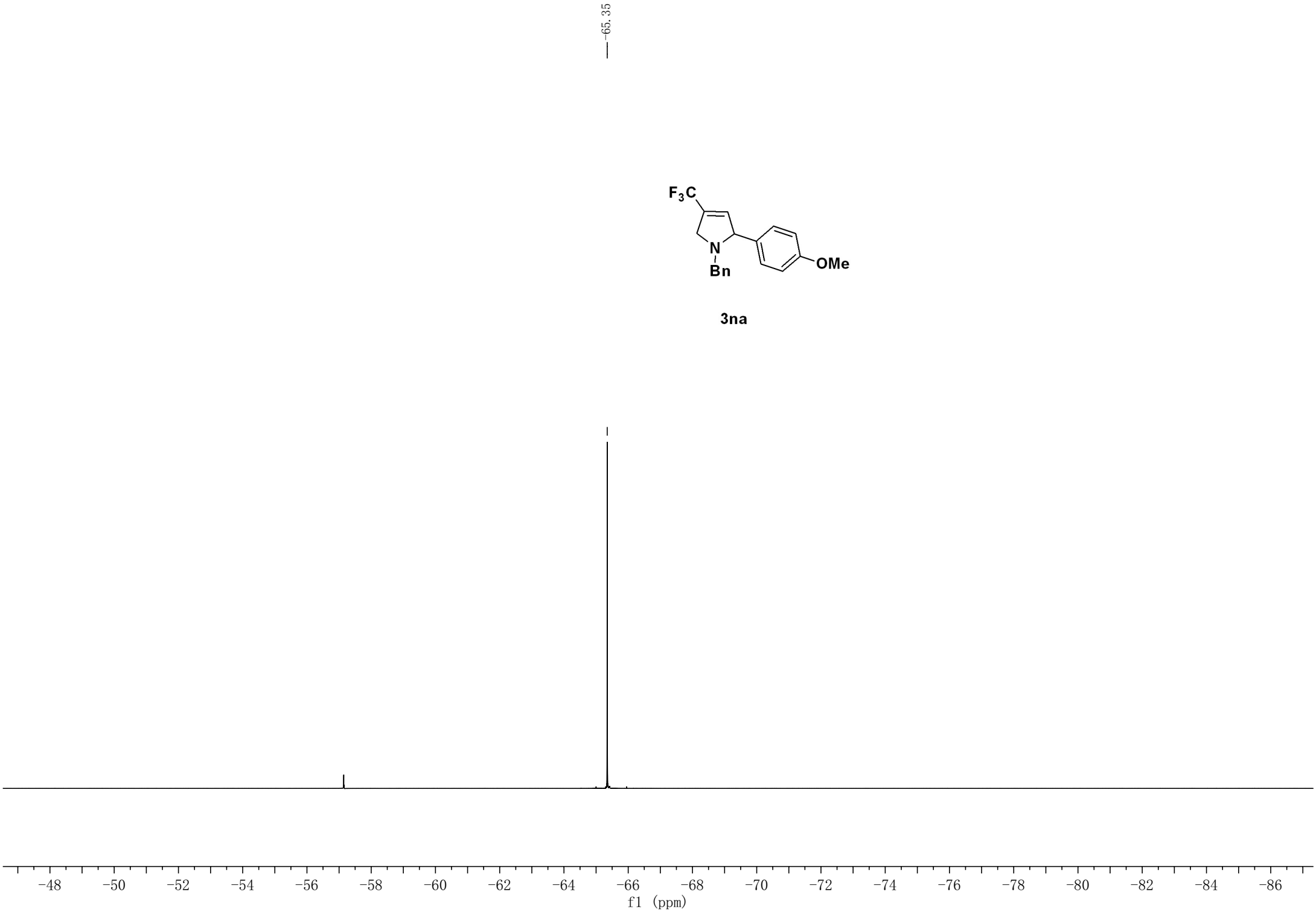
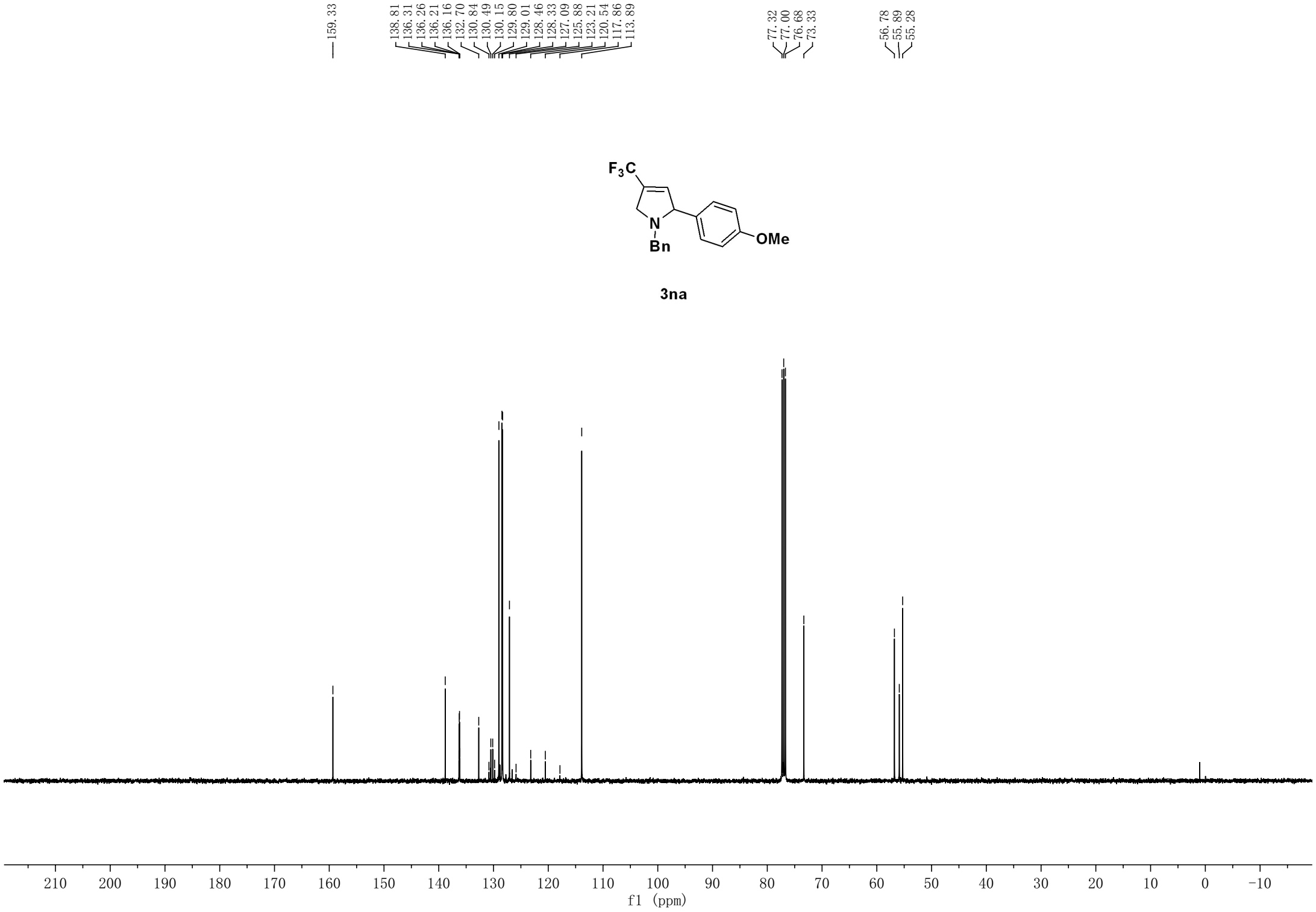
0.0
f1 (ppm)


-65.35
F3C
N
Bn
OMe
3na
-48
-50
-52
-54
-56
-58
-60
-62
-64
-66
-68
-70
-72
-74
-76
-78
-80
-82
-84
-86
f1 (ppm)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136.26
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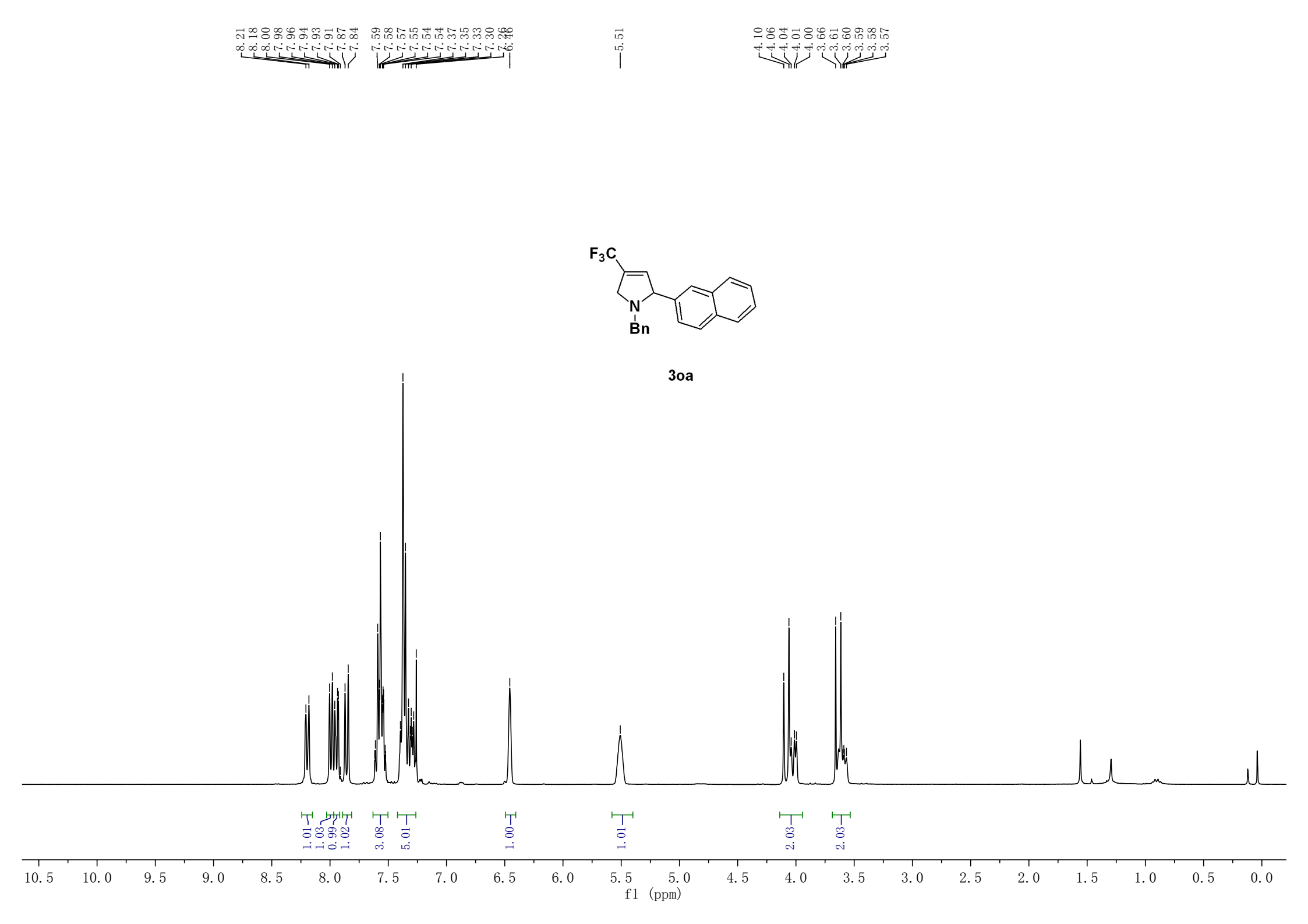
136.16
132.70
130.84
130.49
130.15
129.80
129.01
128.46
128.33
127.09
125.88
123.21
120.54
117.86
113.89
77.32
77.00
76.68
73.33
56.78
55.89
55.28
F3C
N
Bn
OMe
3na
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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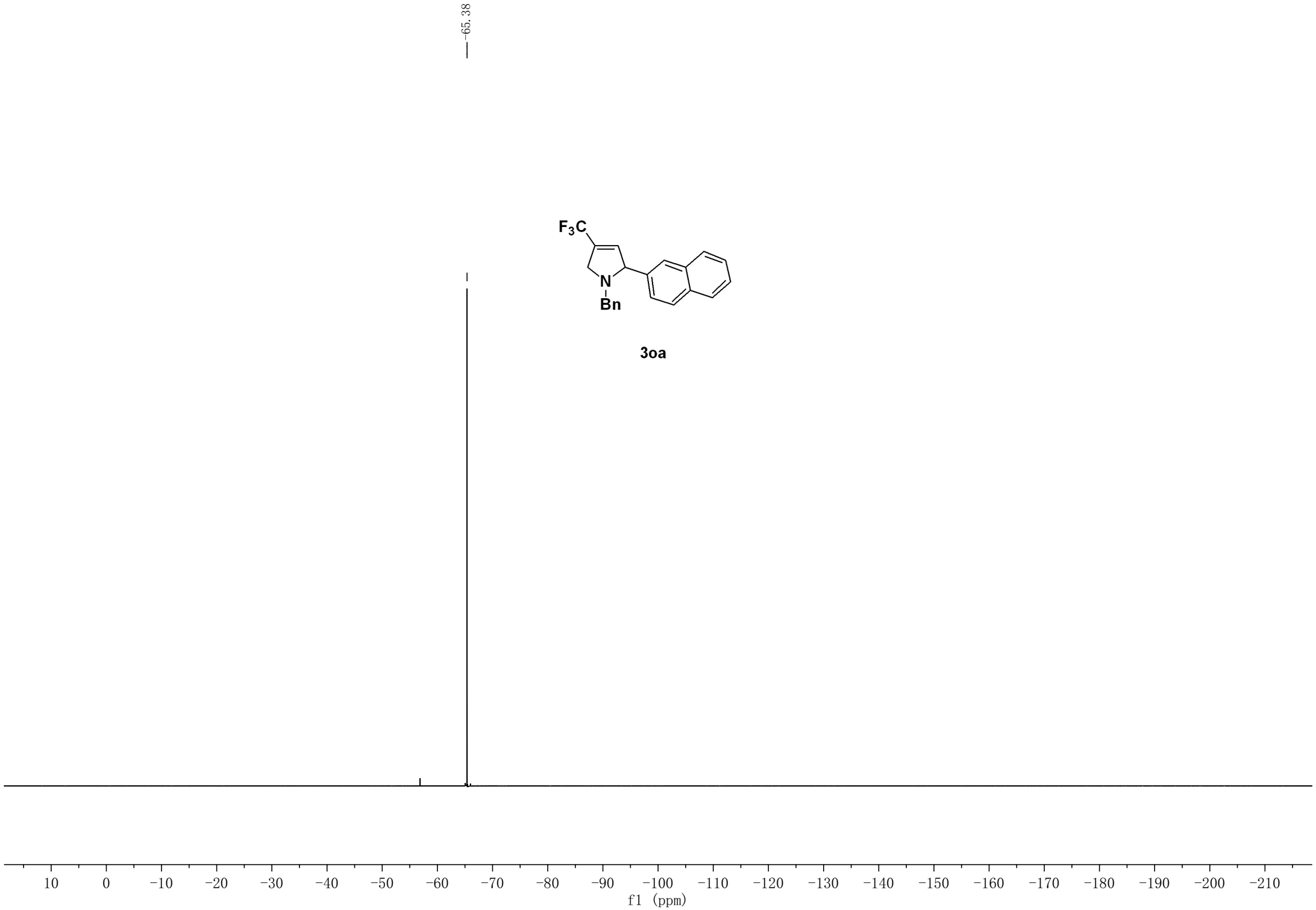
8.00
7.98
7.96
7.94
7.93
7.91
7.87
7.84
7.59
7.58
7.57
7.55
7.54
7.54
7.37
7.35
7.33
7.30
7.26
6.46
5.51
4.10
4.06
4.04
4.01
4.00
3.66
3.61
3.60
3.59
3.58
3.57
F3C
N
Bn
3oa
1.01
1.03
0.99
1.02
3.08
5.01
1.00
1.01
2.03
2.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
N
Bn
3oa
10
0
-10
-20
-30
-40
-50
-60
-70
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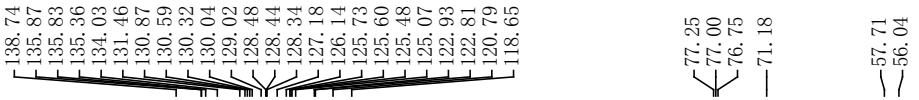
-170
-180
-190
-200
-210
f1 (ppm)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131.46
130.87
130.59
130.32
130.04
129.02
128.48
128.44
128.34
127.18
126.14
125.73
125.60
125.48
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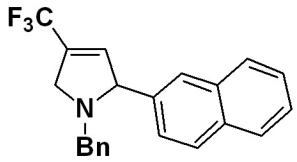
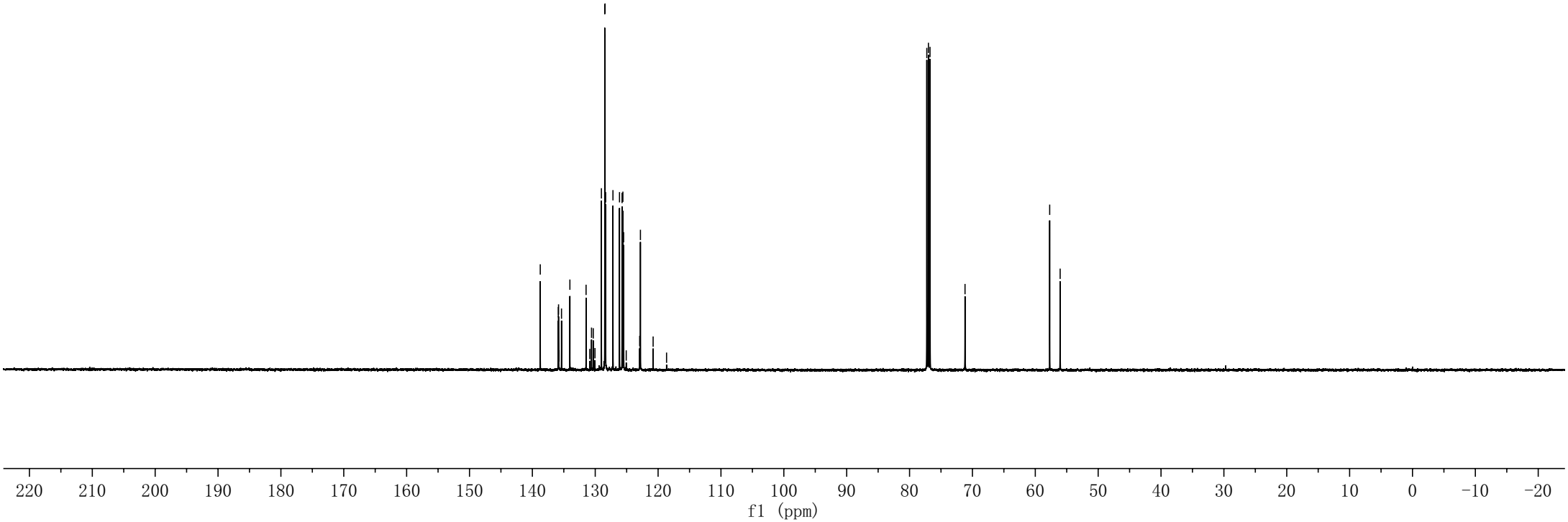
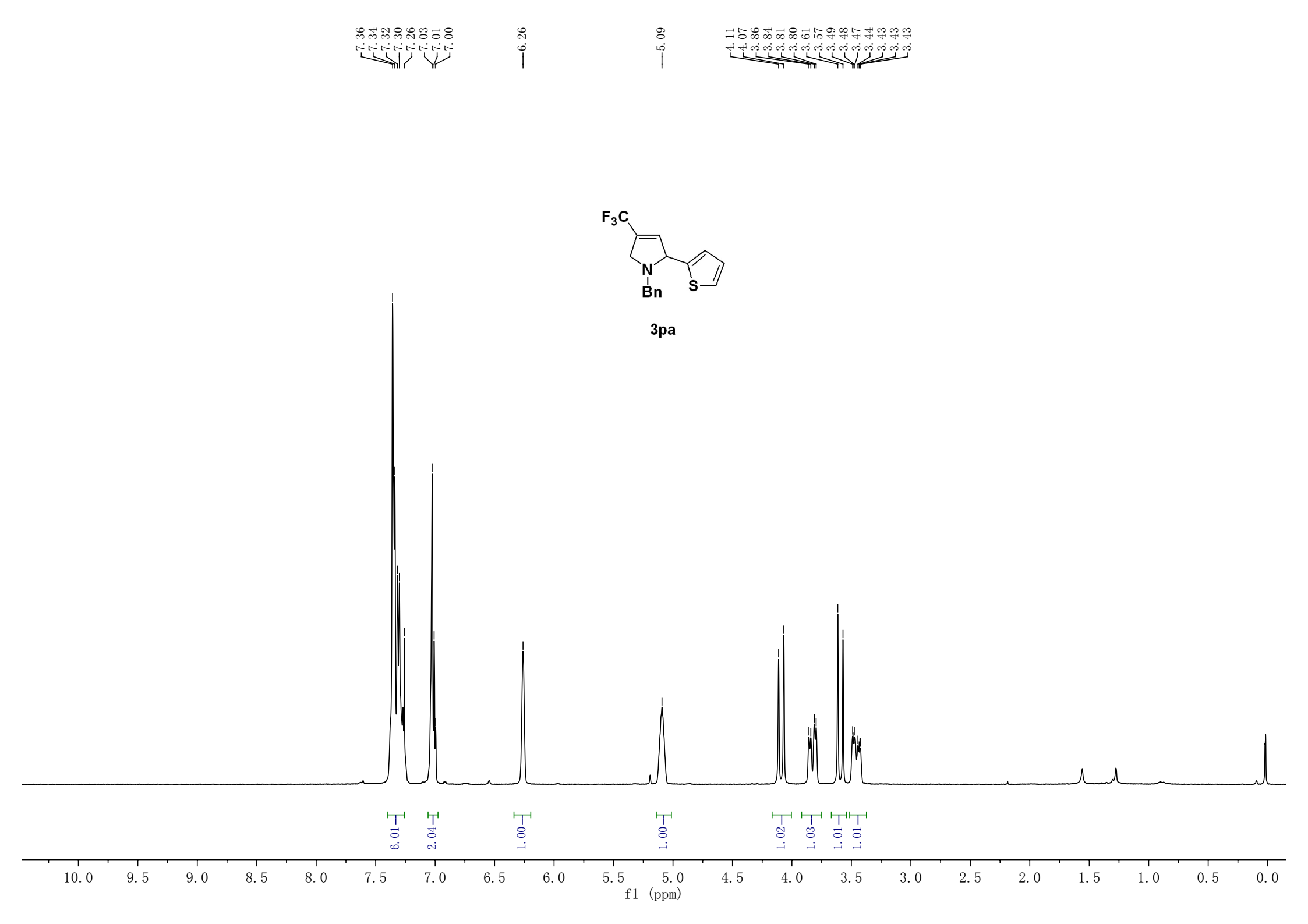
77.25
77.00
76.75
71.18
57.71
56.04


F3C
N
Bn

3oa


220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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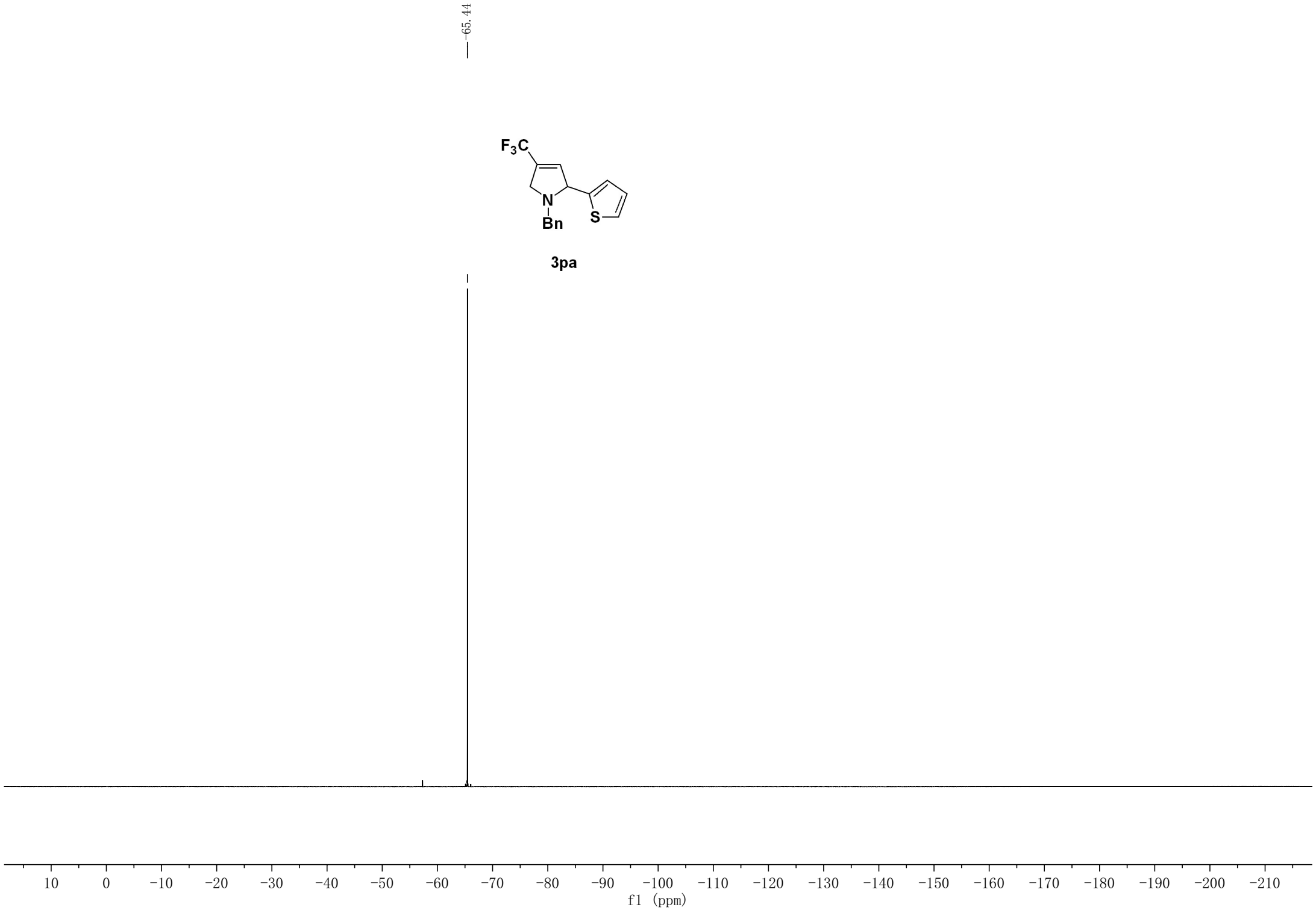
7.34
7.32
7.30
7.26
7.03
7.01
7.00
6.26
5.09
4.11
4.07
3.86
3.84
3.81
3.80
3.61
3.57
3.49
3.48
3.47
3.44
3.43
3.43
3.43
F3C
N
Bn
S
3pa
6.01
2.04
1.00
1.00
1.02
1.03
1.01
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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-60
-70
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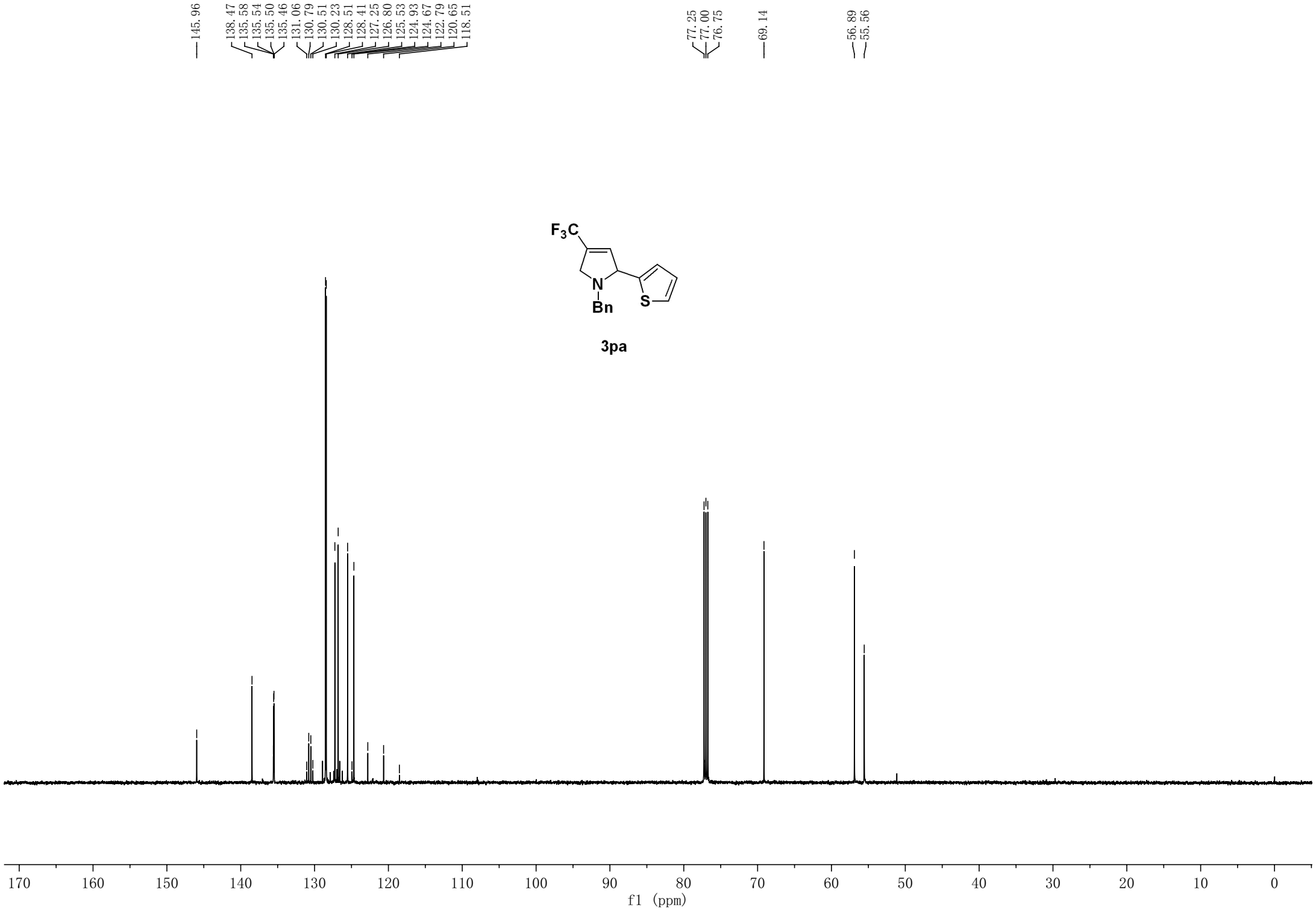
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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127.25
126.80
125.53
124.93
124.67
122.79
120.65
118.51
77.25
77.00
76.75
69.14
56.89
55.56
F3C
N
Bn
S
3pa
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150
140
130
120
110
100
90
80
70
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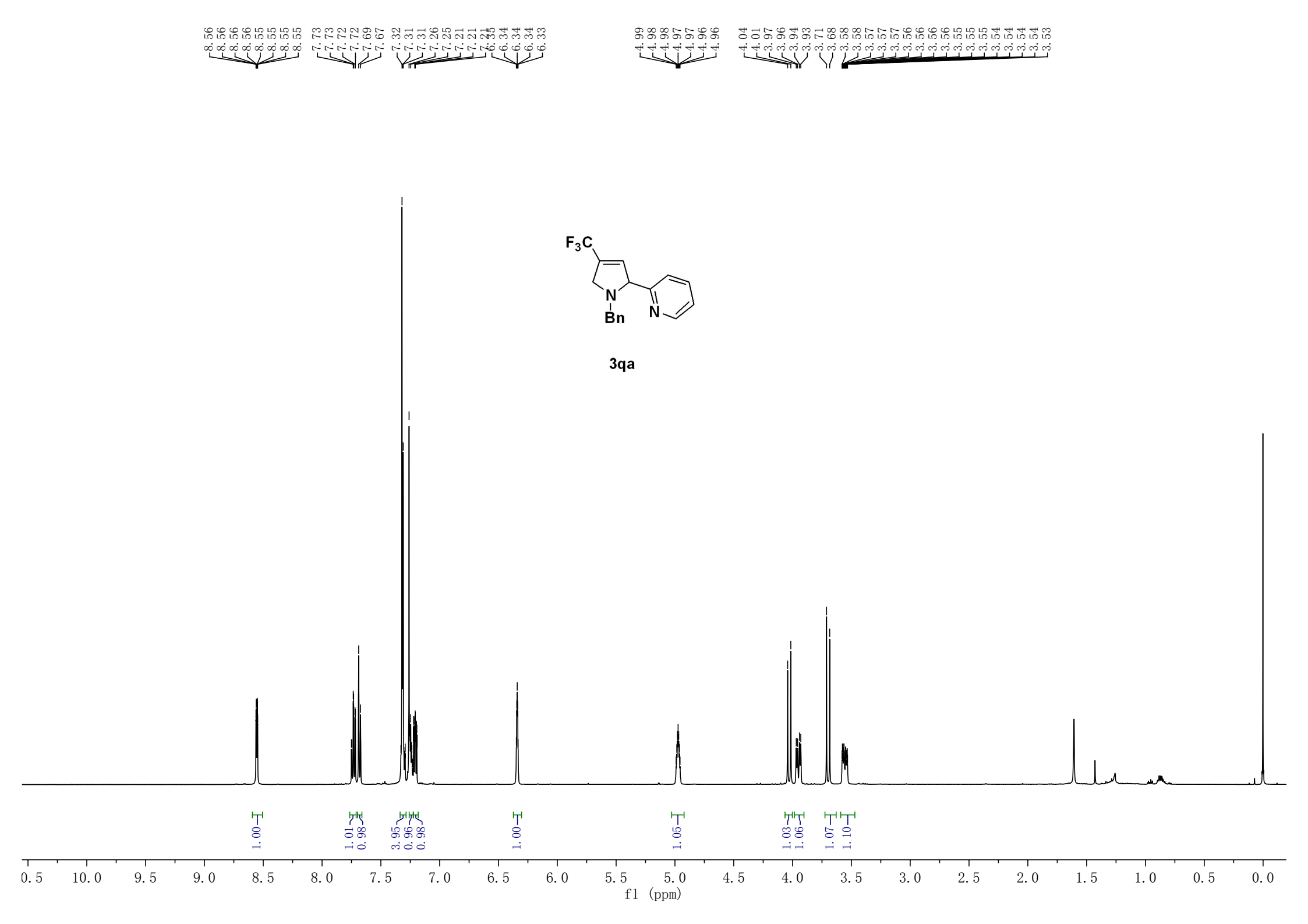
50
40
30
20
10
0
f1 (ppm)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8.56
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7.67
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7.21
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6.34
6.34
6.34
6.33
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4.98
4.98
4.97
4.97
4.96
4.96
4.04
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3.96
3.94
3.93
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3.55
3.54
3.54
3.54
3.54
3.53
F3C
N
Bn
N
3qa
1.00
1.01
0.98
3.95
0.96
0.98
1.00
1.05
1.03
1.06
1.07
1.10
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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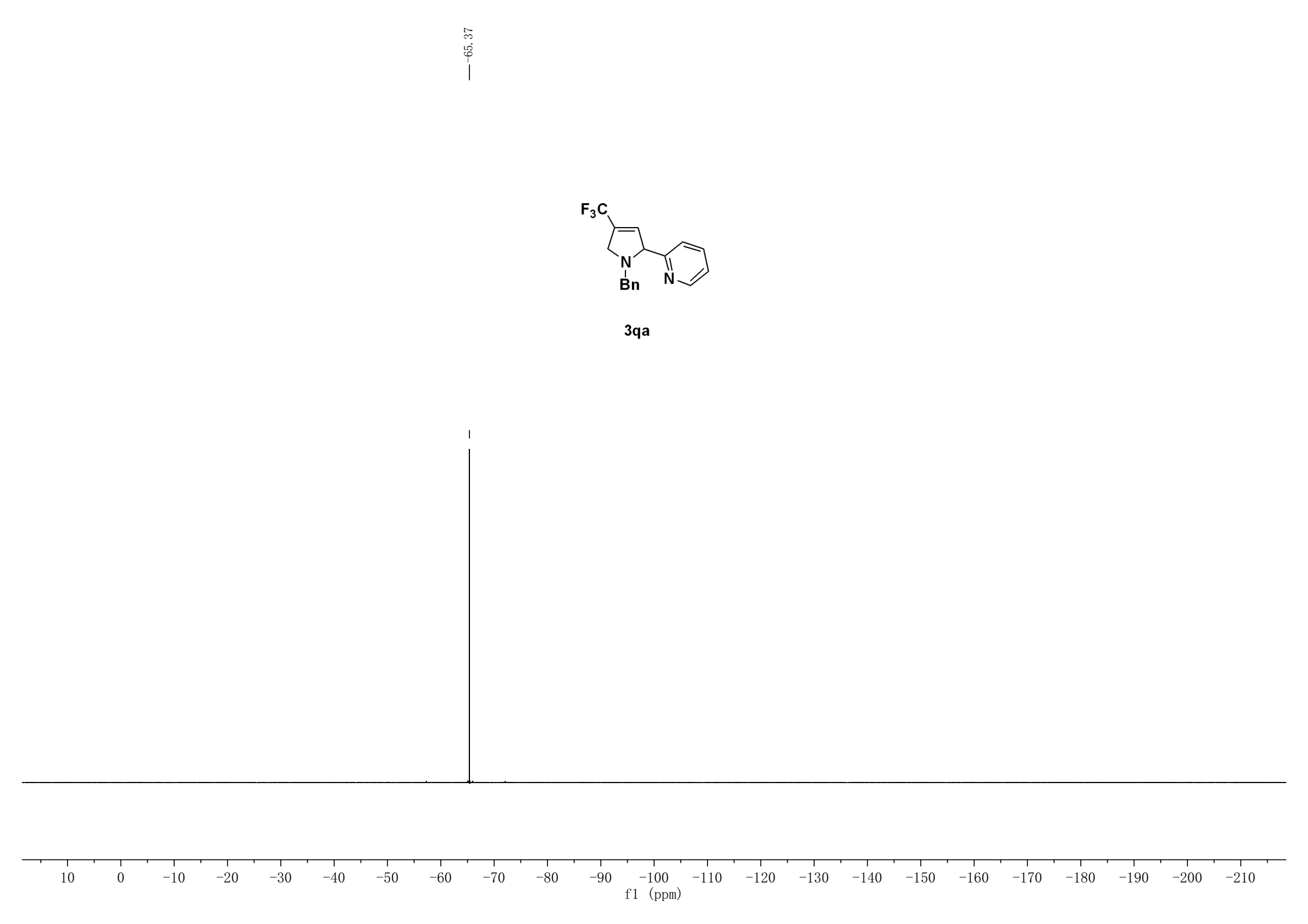
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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N
Bn
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10
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-10
-20
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-40
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-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

160.75
149.09
138.51
137.00
134.98
134.94
134.90
134.86
131.34
131.06
130.79
130.51
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128.43
127.23
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122.58
121.67
120.64
118.50
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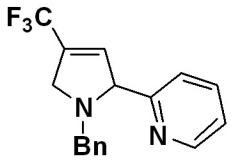
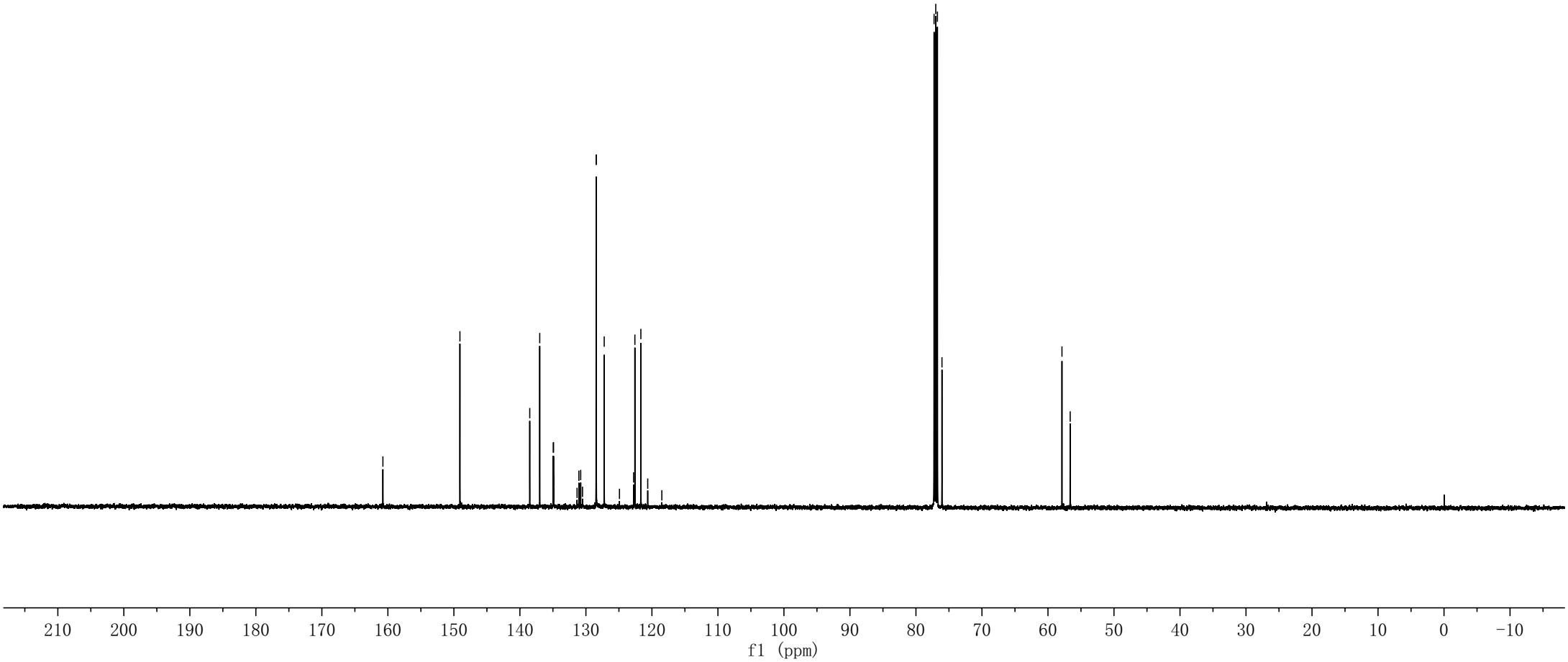
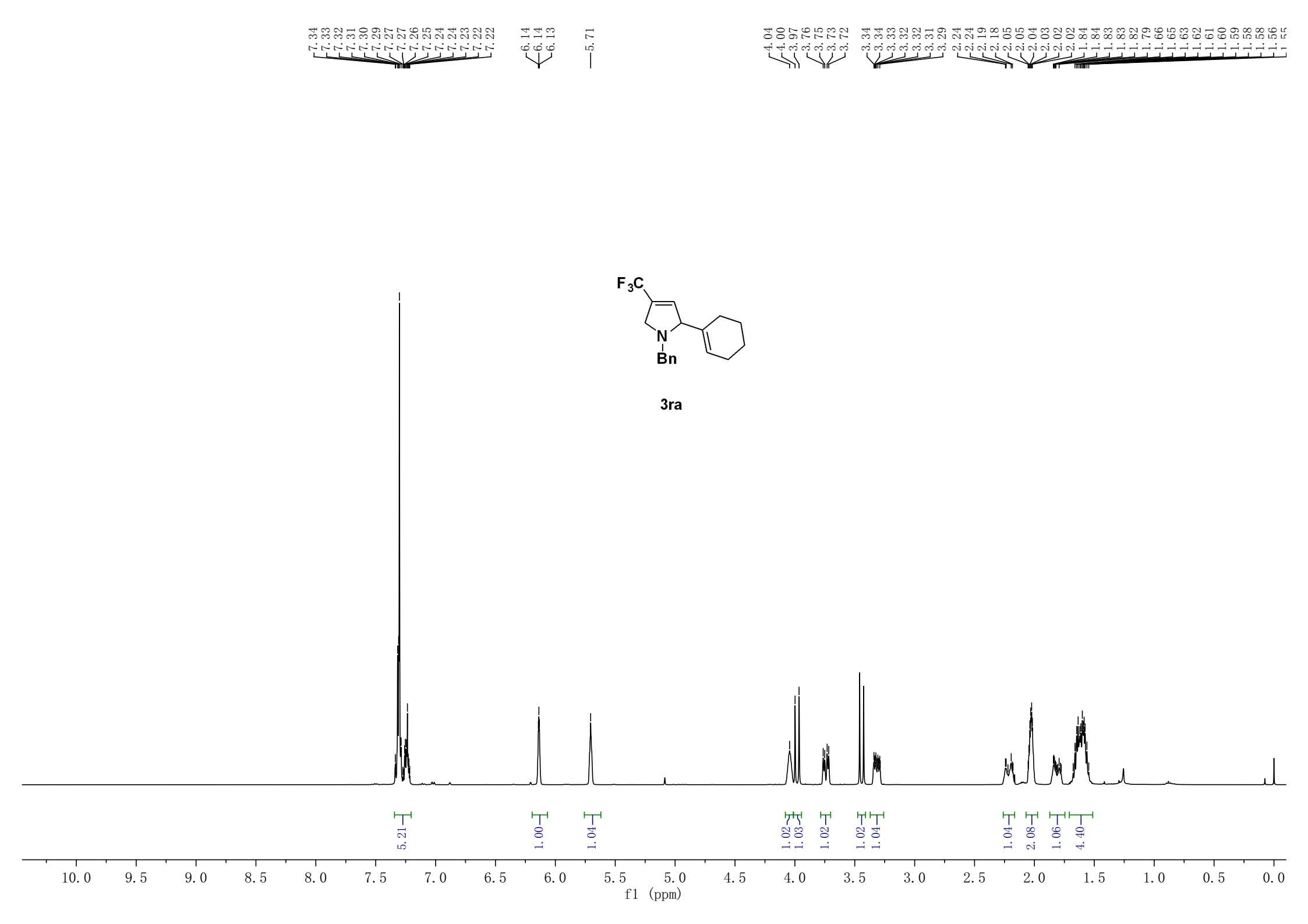
77.00
76.75
76.06
57.88
56.63



3qa

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7.25
7.24
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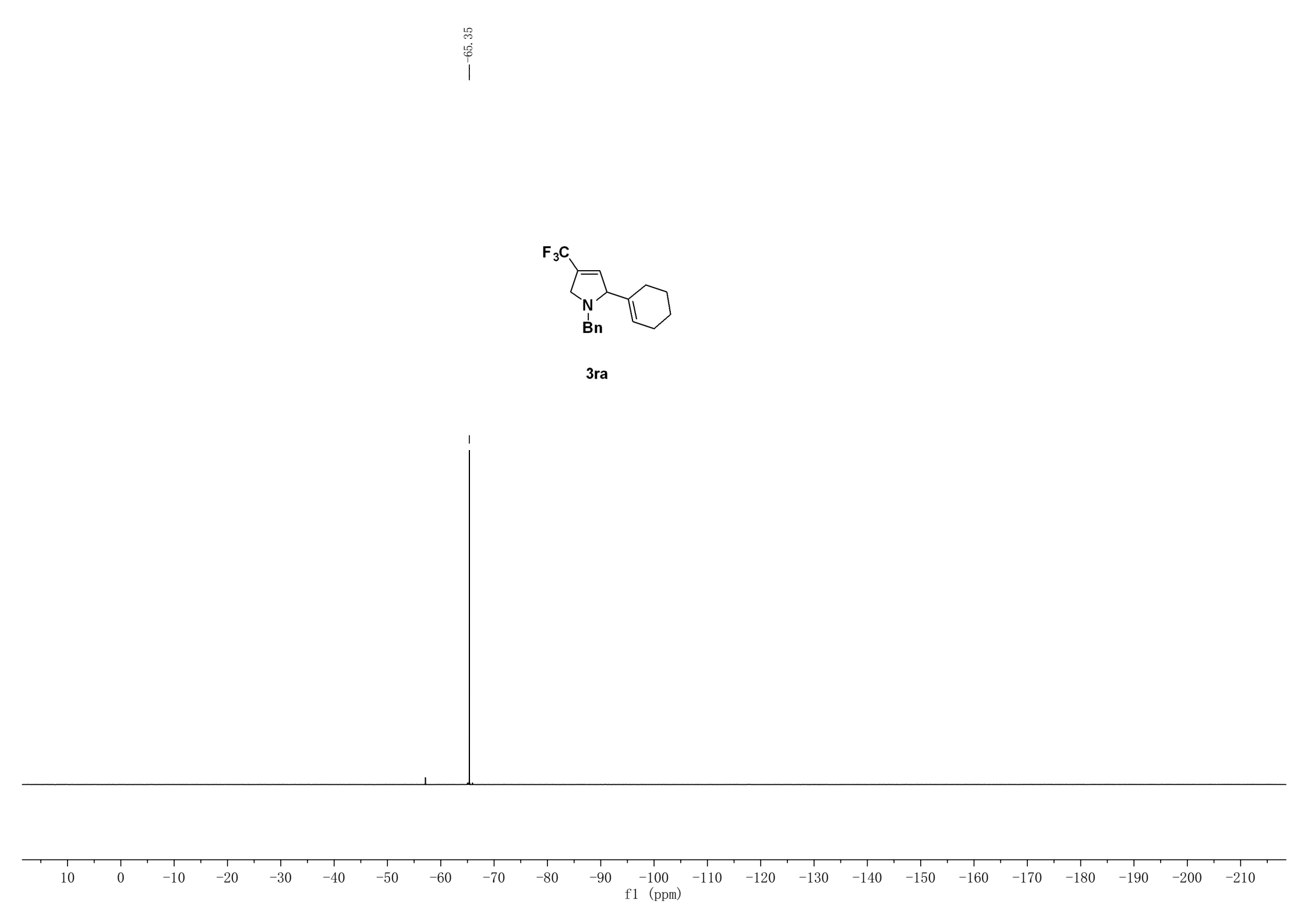
7.23
7.22
7.22
6.14
6.14
6.13
5.71
4.04
4.00
3.97
3.76
3.75
3.73
3.72
3.34
3.34
3.33
3.32
3.31
3.29
2.24
2.24
2.19
2.18
2.05
2.05
2.04
2.03
2.02
2.02
1.84
1.84
1.83
1.83
1.82
1.79
1.66
1.65
1.63
1.62
1.61
1.60
1.59
1.58
1.58
1.56
F3C
N
Bn
3ra
5.21
1.00
1.04
1.02
1.03
1.02
1.02
1.04
1.04
2.08
1.06
4.40
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
N
Bn
3ra
10
0
-10
-20
-30
-40
-50
-60
-70
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-130
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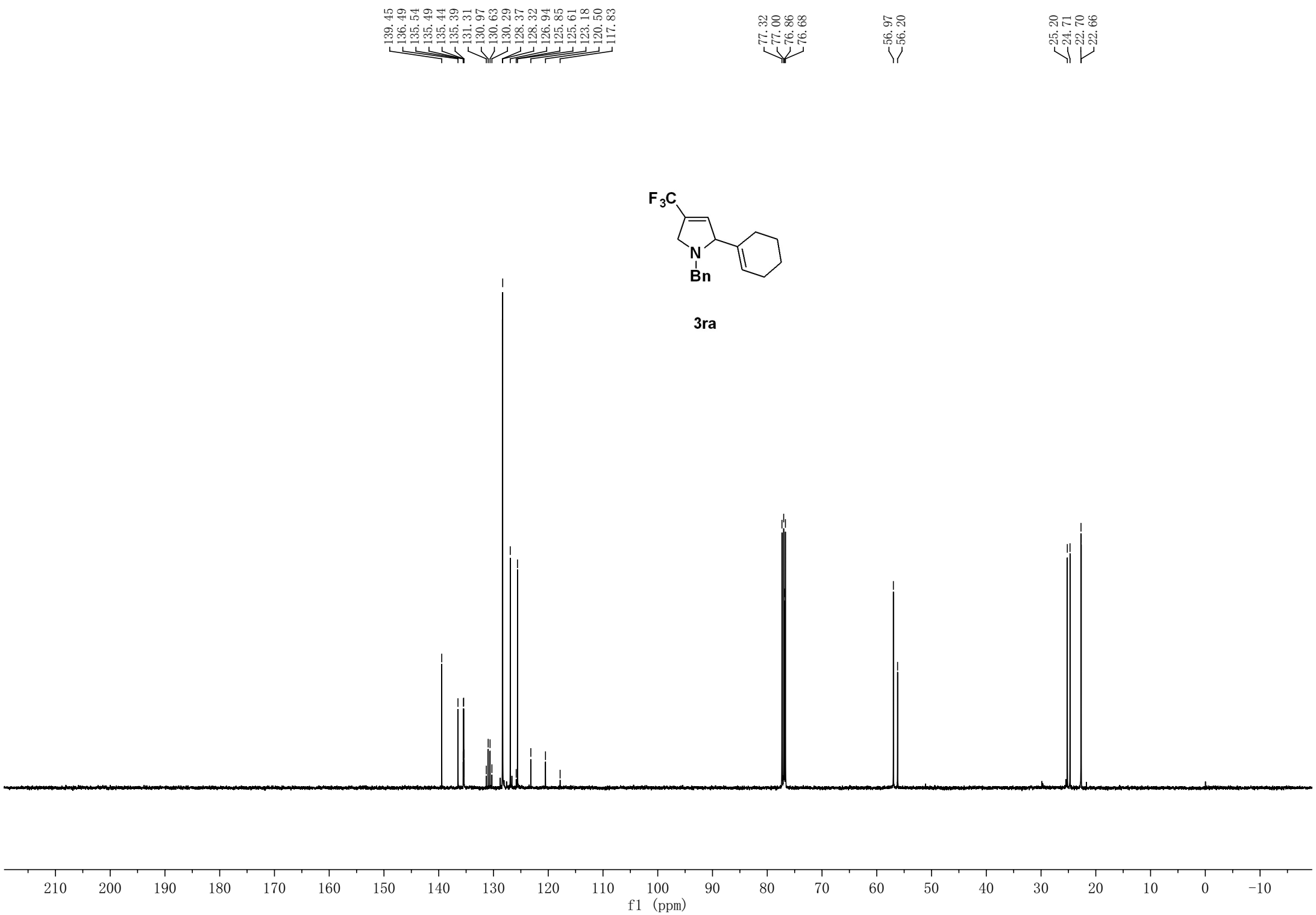
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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136.49
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135.49
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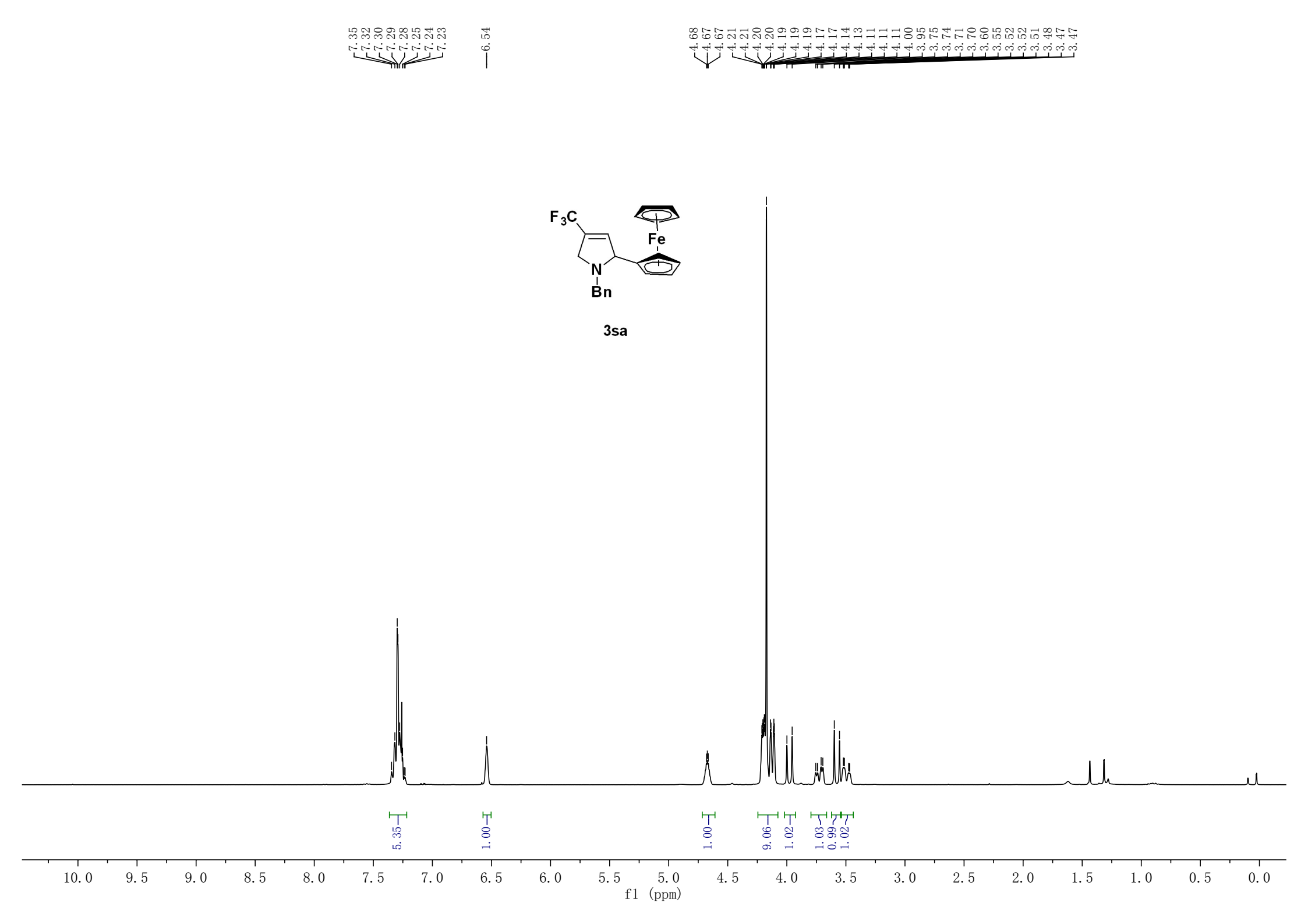
135.39
131.31
130.97
130.63
130.29
128.37
128.32
126.94
125.85
125.61
123.18
120.50
117.83
77.32
77.00
76.86
76.68
56.97
56.20
25.20
24.71
22.70
22.66
F3C
N
Bn
3ra
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.25
7.24
7.23
6.54
4.68
4.67
4.67
4.21
4.21
4.20
4.20
4.19
4.19
4.19
4.17
4.17
4.14
4.13
4.11
4.11
4.11
4.00
3.95
3.75
3.74
3.71
3.70
3.60
3.55
3.52
3.52
3.51
3.48
3.47
3.47
F3C
Fe
N
Bn
3sa
5.35
1.00
1.00
9.06
1.02
1.03
0.99
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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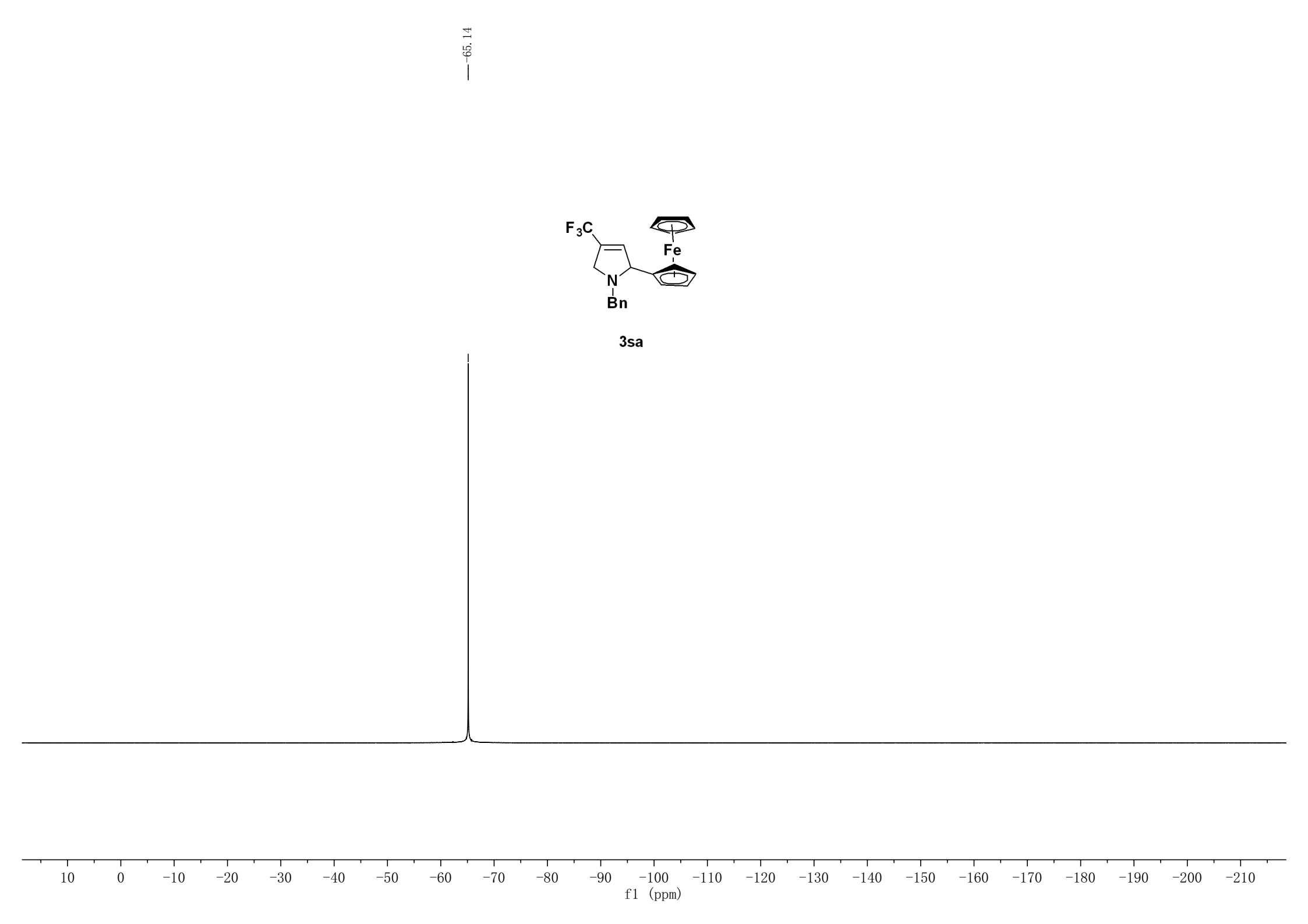
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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Fe
N
Bn
3sa
10
0
-10
-20
-30
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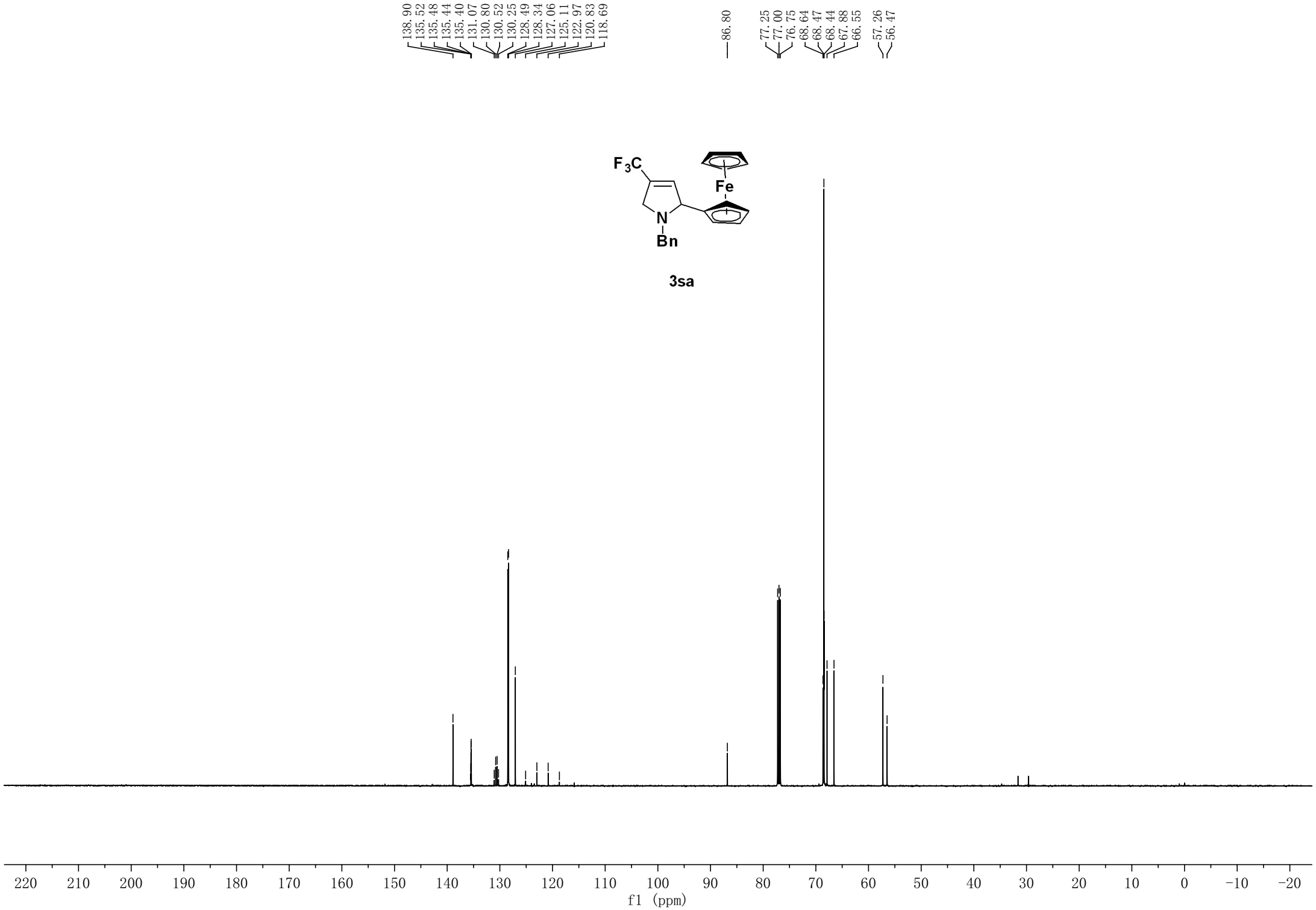
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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135.40
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130.52
130.25
128.49
128.34
127.06
125.11
122.97
120.83
118.69
86.80
77.25
77.00
76.75
68.64
68.47
68.44
67.88
66.55
57.26
56.47
F3C
Fe
N
Bn
3sa
220
210
200
190
180
170
160
150
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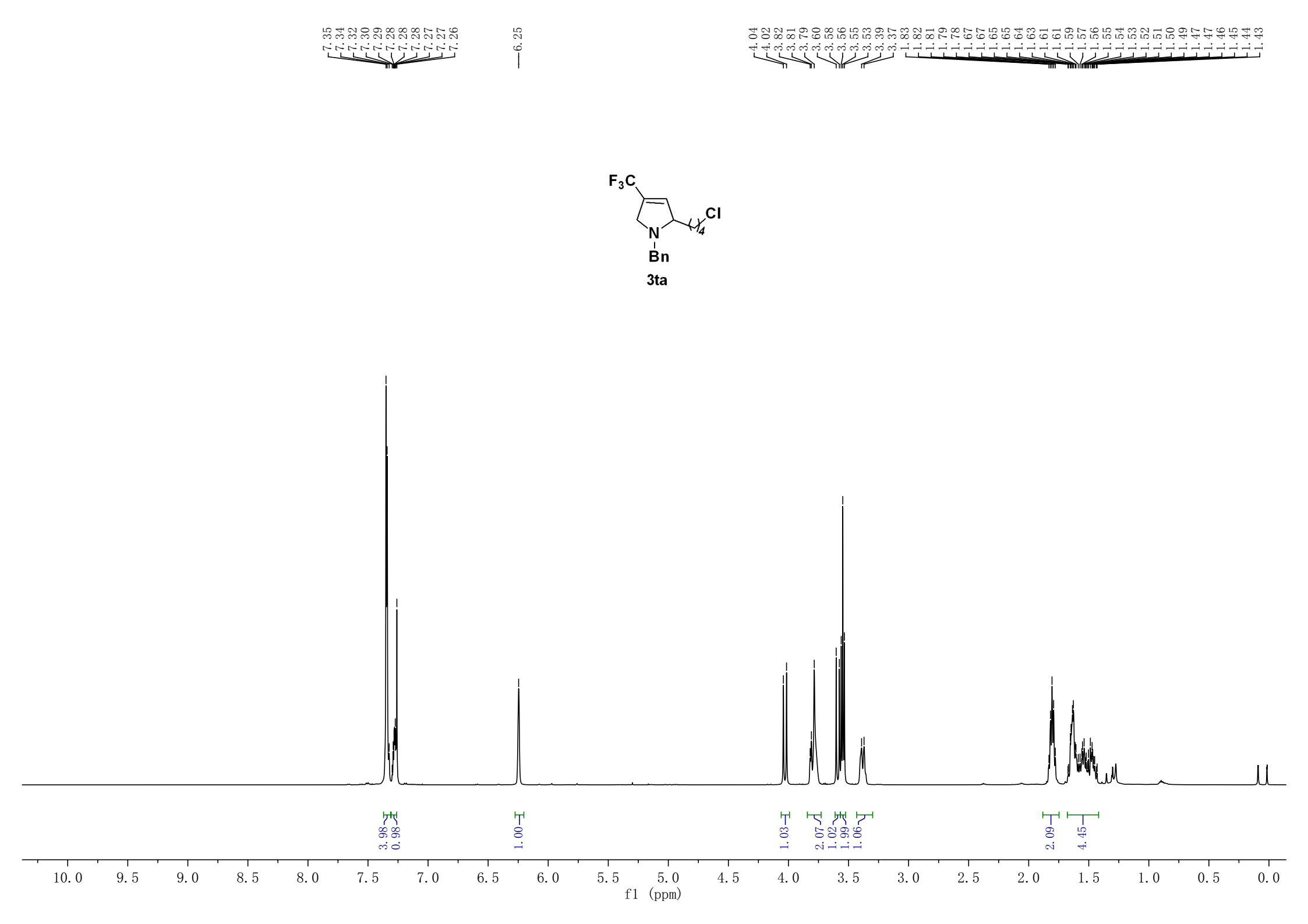
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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7.34
7.32
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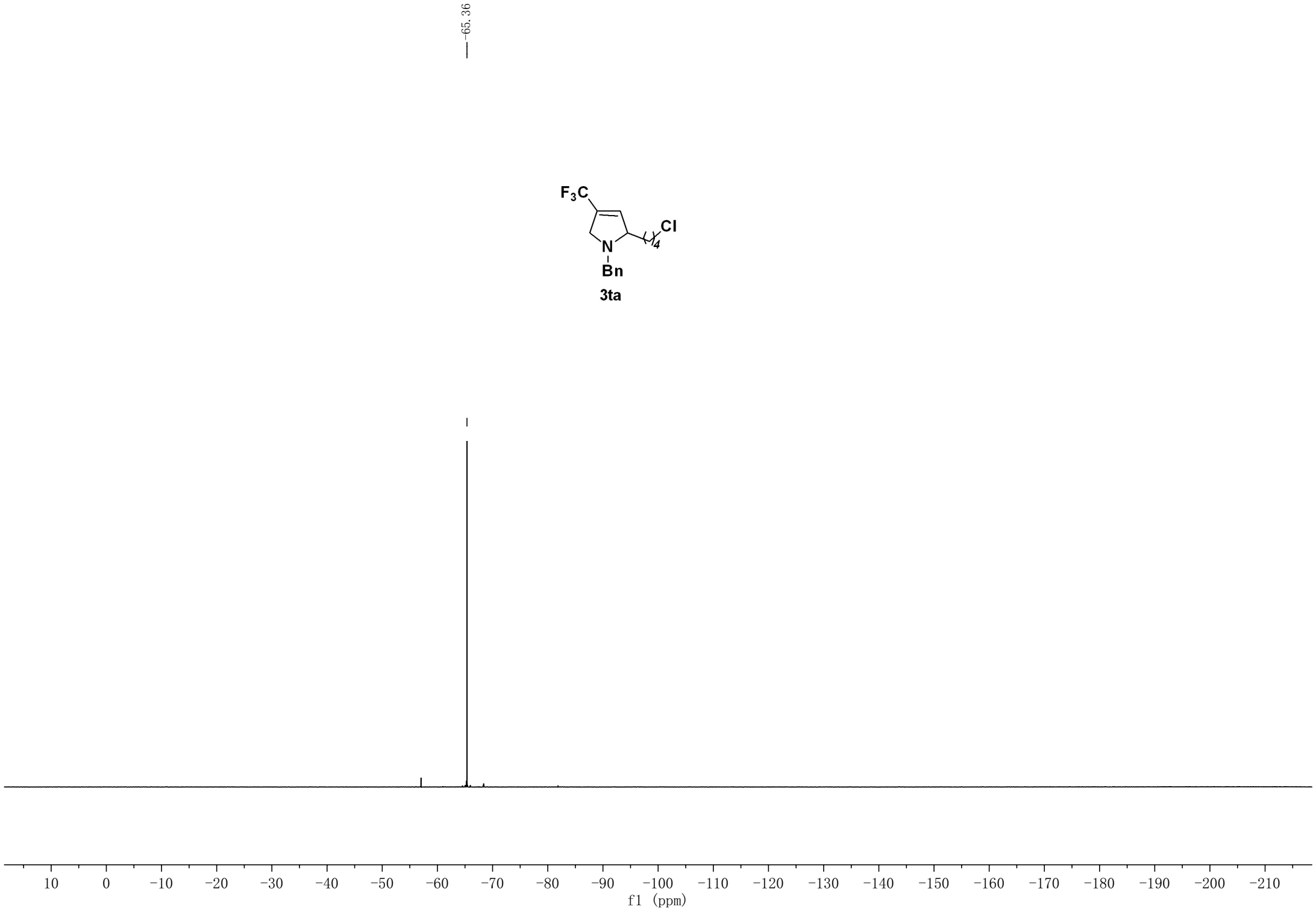
7.28
7.28
7.28
7.27
7.27
7.26
6.25
4.04
4.02
3.82
3.81
3.79
3.60
3.58
3.56
3.55
3.53
3.39
3.37
1.83
1.82
1.81
1.79
1.78
1.67
1.67
1.65
1.65
1.64
1.63
1.61
1.61
1.59
1.57
1.56
1.55
1.54
1.53
1.52
1.51
1.50
1.49
1.47
1.47
1.46
1.45
1.44
1.43
F3C
Cl
N
Bn
3ta
3.98
0.98
1.00
1.03
2.07
1.02
1.99
1.06
2.09
4.45
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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-10
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-40
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-60
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-80
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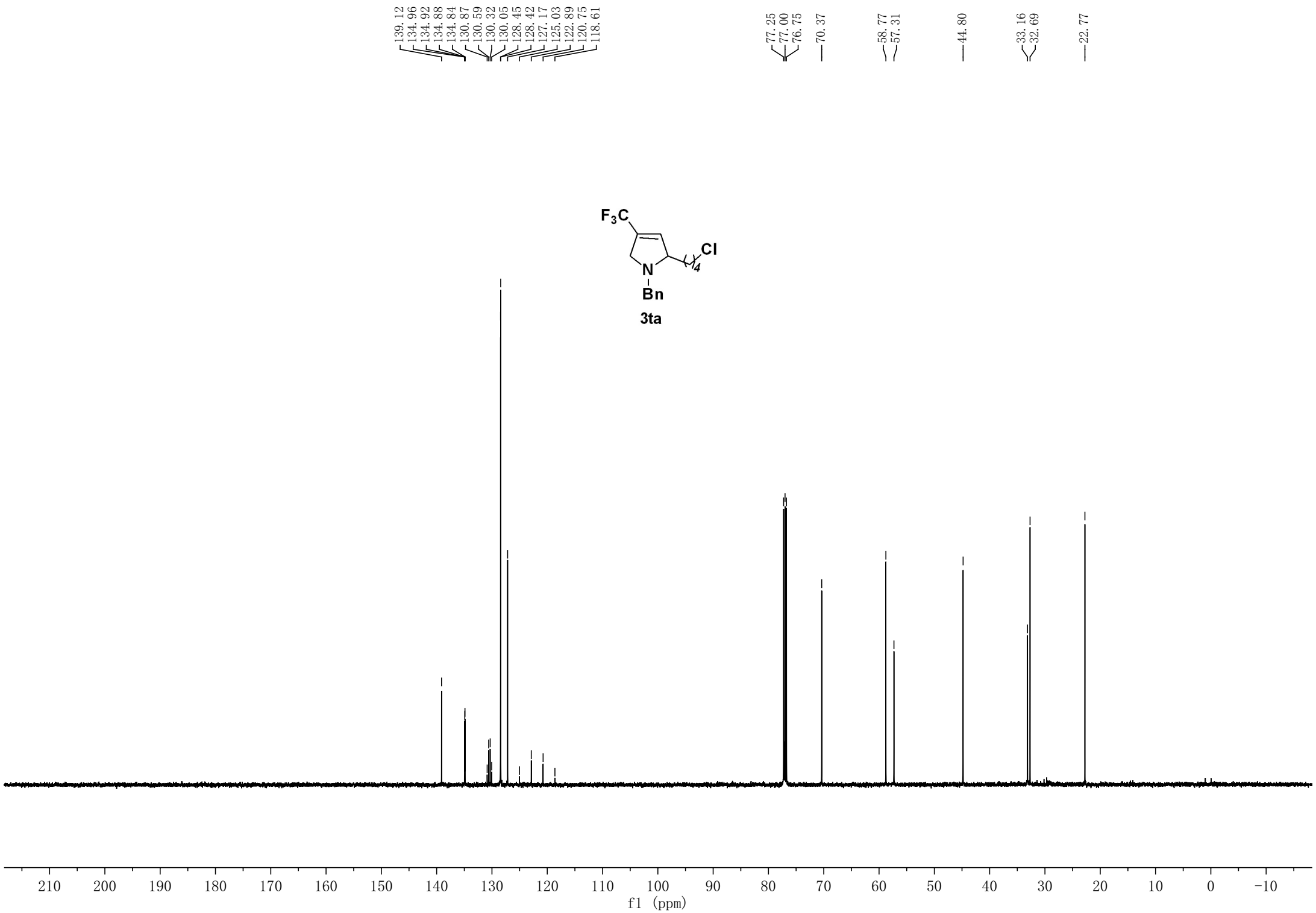
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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127.17
125.03
122.89
120.75
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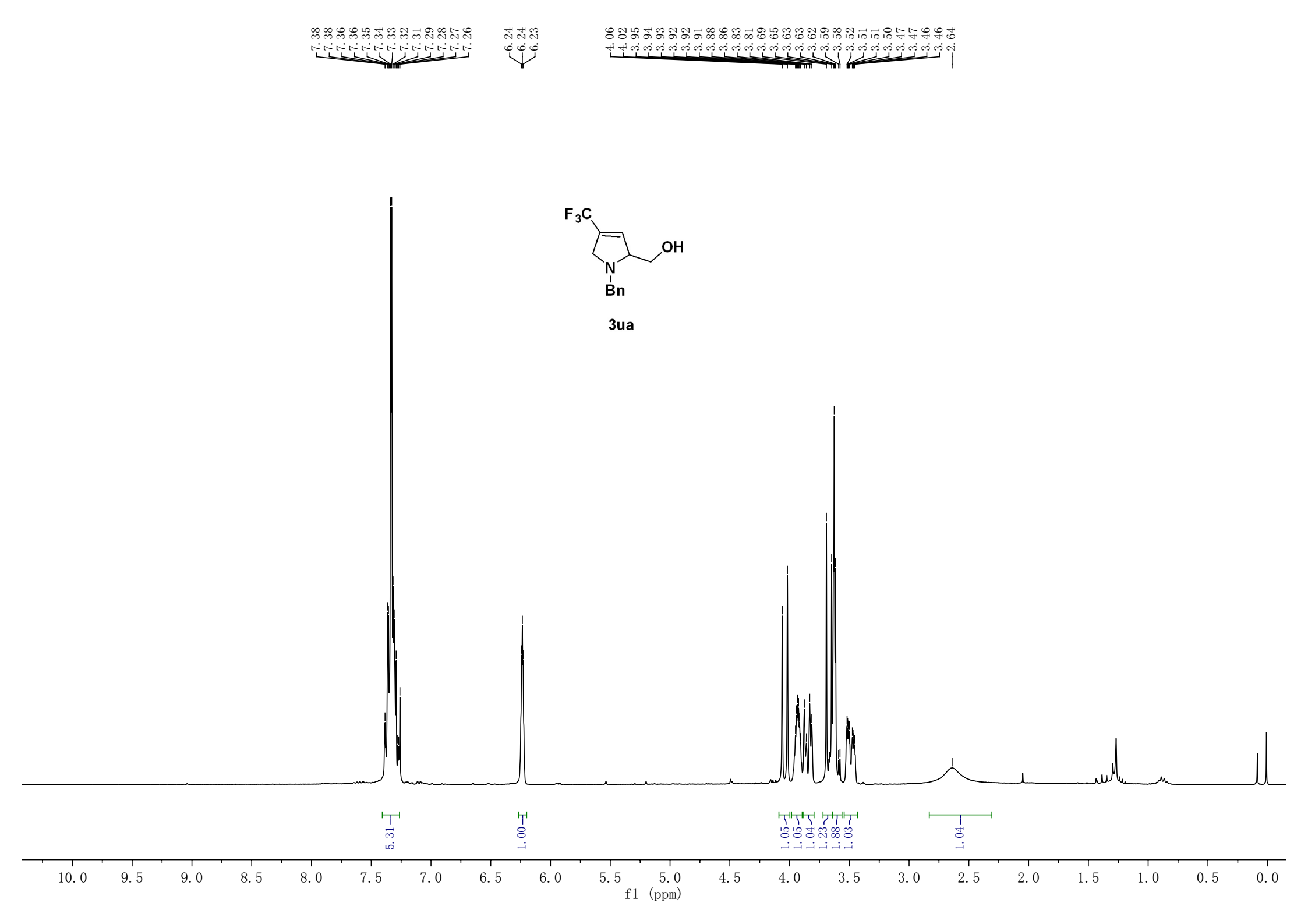
77.25
77.00
76.75
70.37
58.77
57.31
44.80
33.16
32.69
22.77
F3C
Cl
4
N
Bn
3ta
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.34
7.33
7.32
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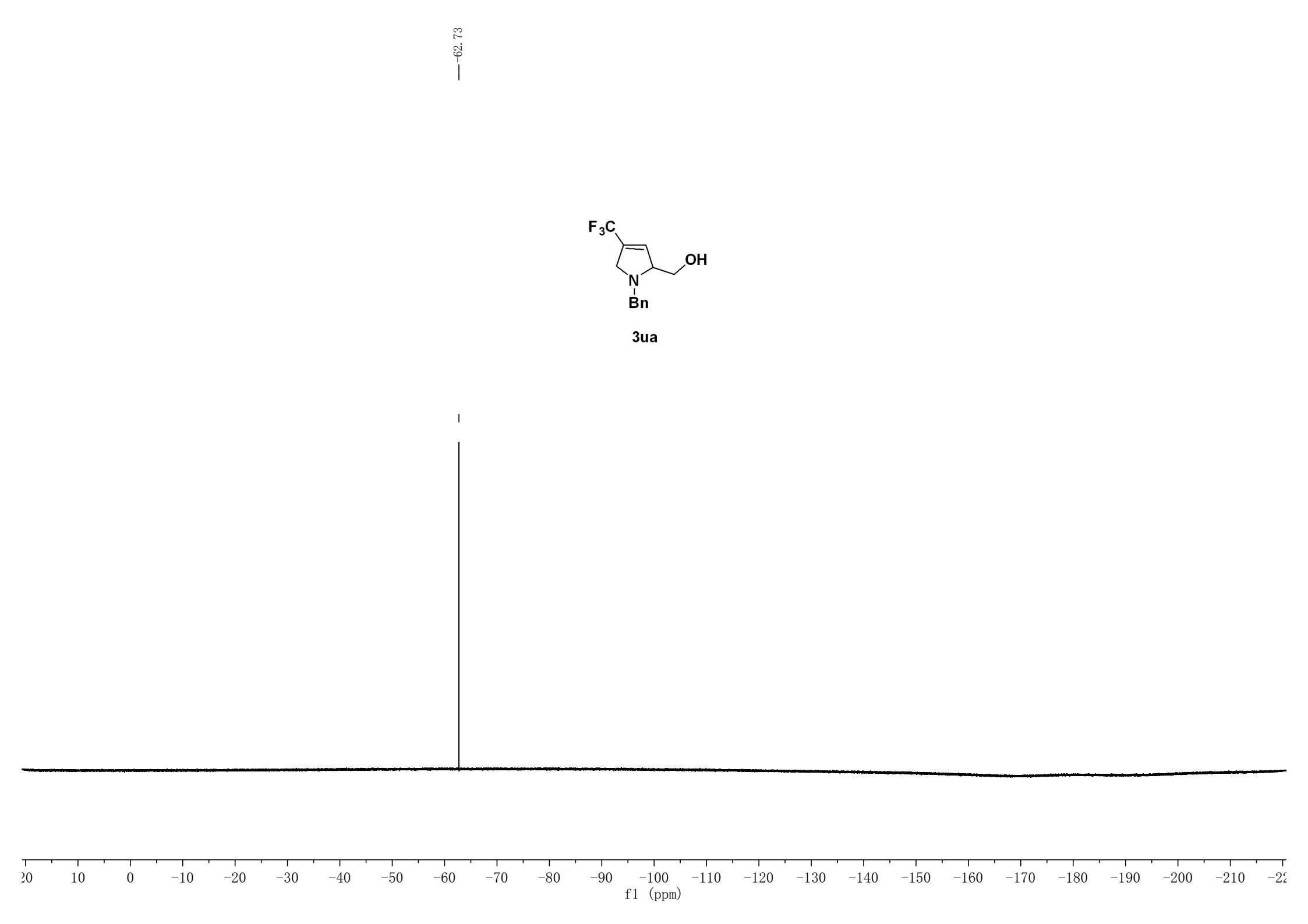
7.29
7.28
7.27
7.26
6.24
6.24
6.23
4.06
4.02
3.95
3.94
3.93
3.92
3.92
3.91
3.88
3.86
3.83
3.81
3.69
3.65
3.63
3.63
3.62
3.59
3.58
3.52
3.51
3.51
3.50
3.47
3.47
3.46
3.46
2.64
F3C
OH
N
Bn
3ua
5.31
1.00
1.05
1.05
1.04
1.23
1.88
1.03
1.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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OH
N
Bn
3ua
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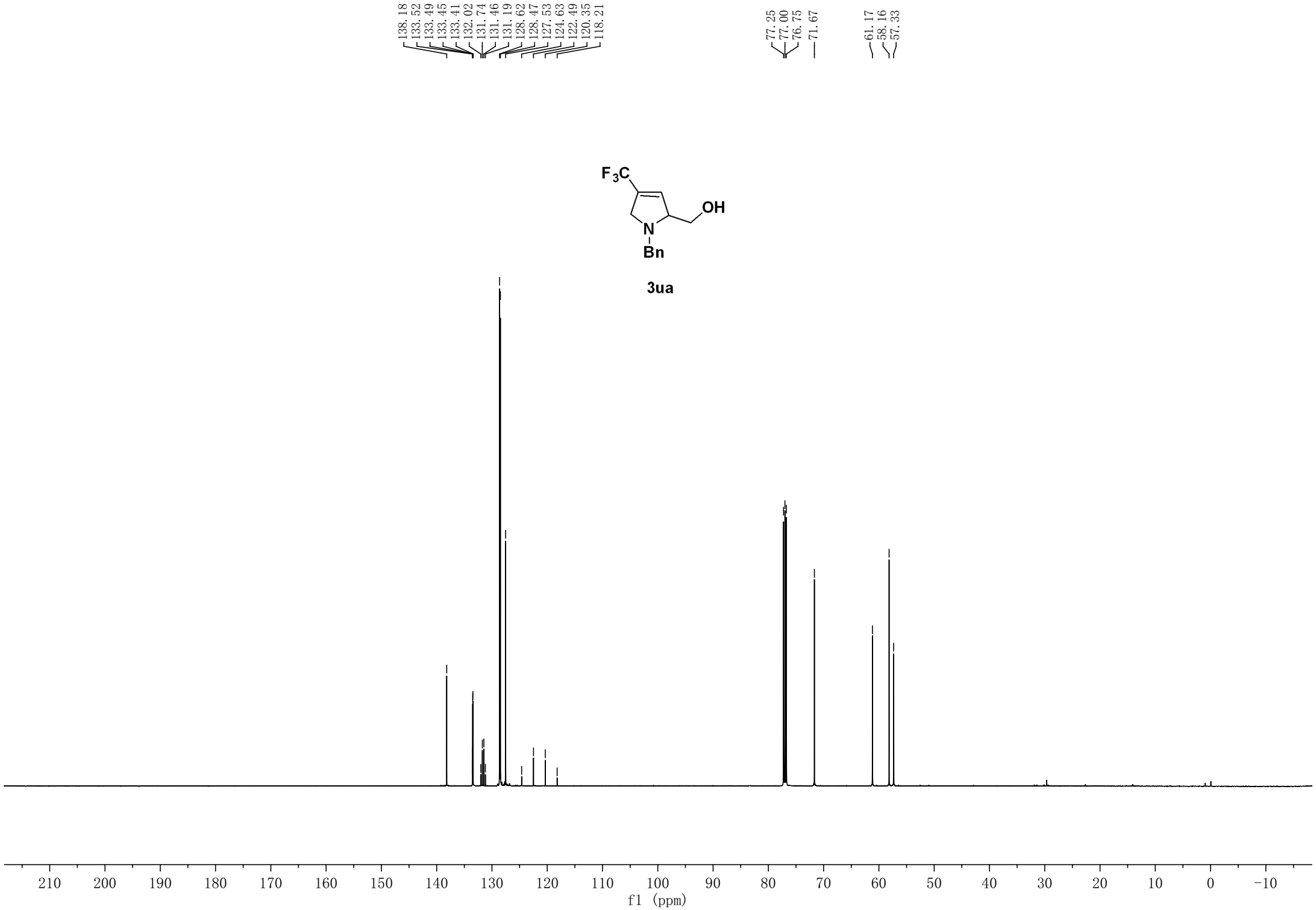
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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133.45
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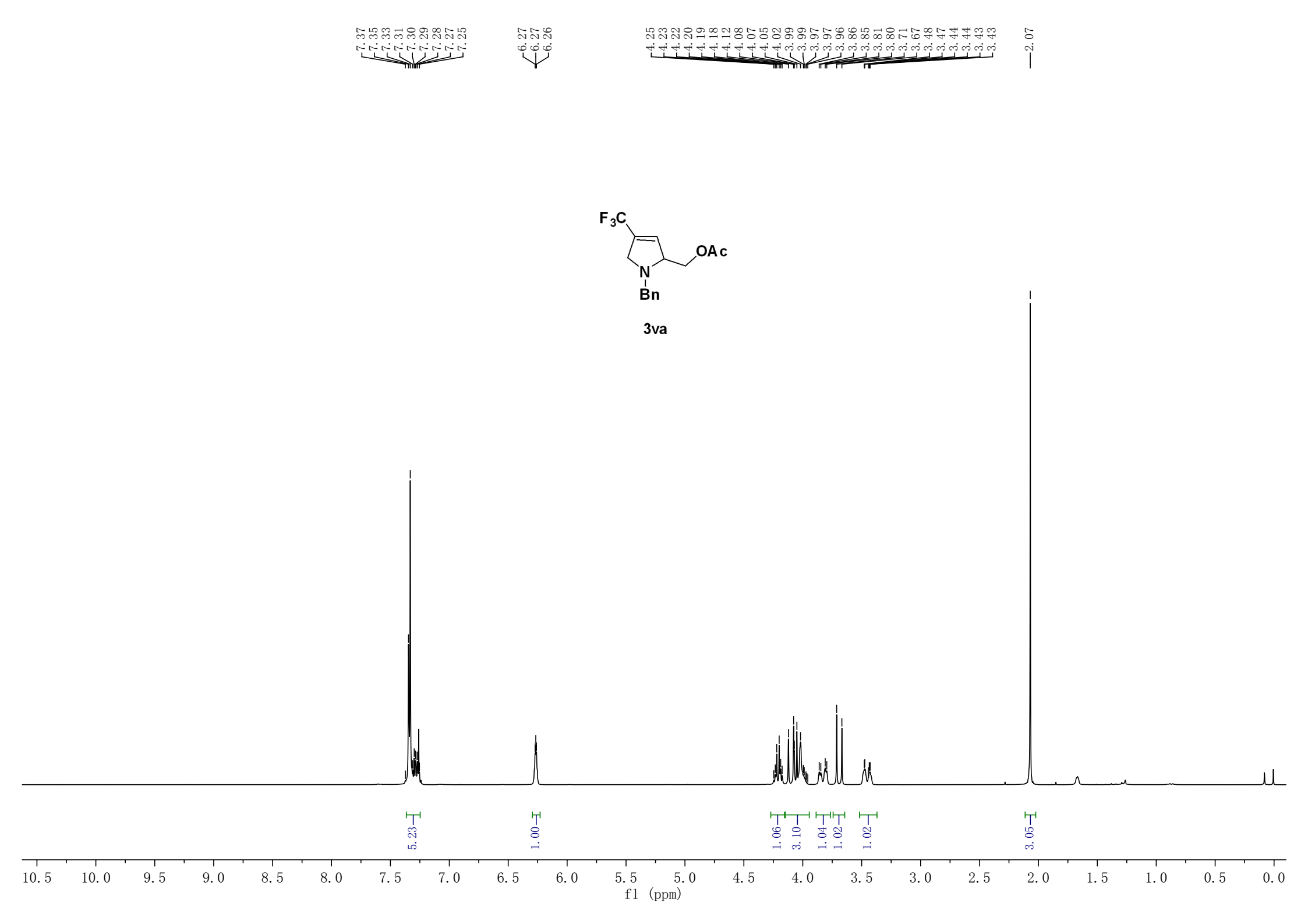
128.62
128.47
127.53
124.63
122.49
120.35
118.21
77.25
77.00
76.75
71.67
61.17
58.16
57.33
F3C
OH
N
Bn
3ua
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.33
7.31
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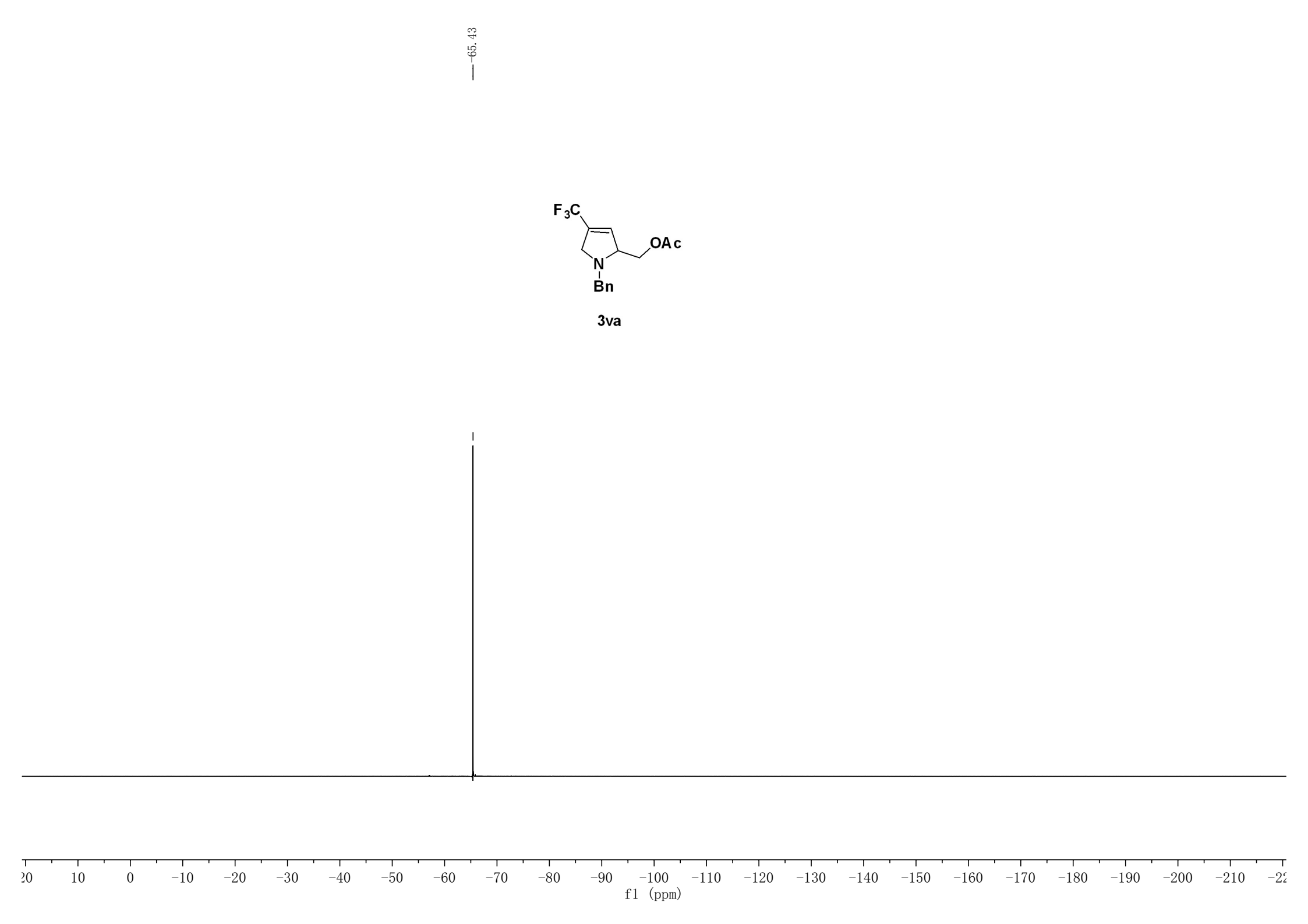
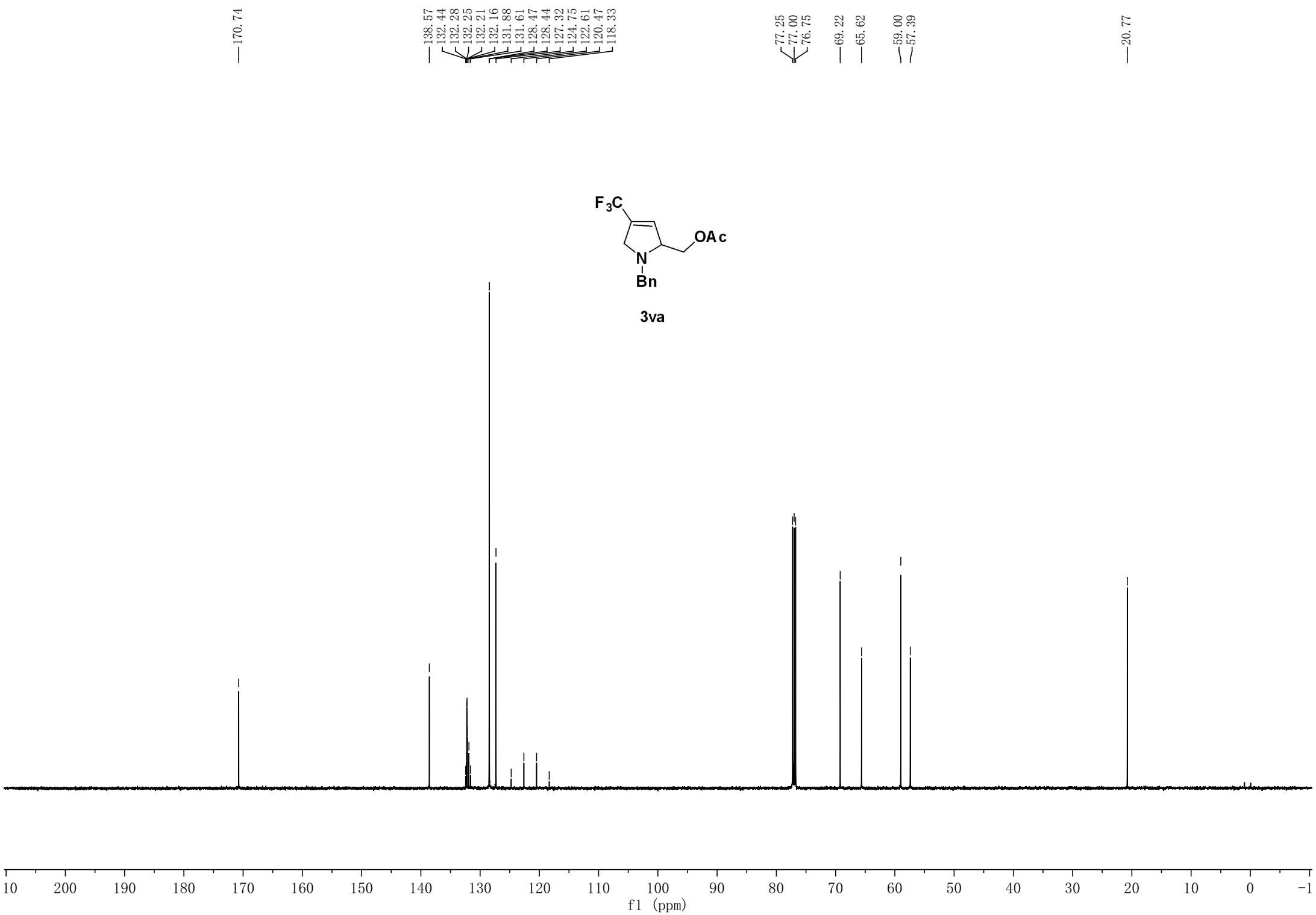
7.29
7.28
7.27
7.25
6.27
6.27
6.26
4.25
4.23
4.22
4.20
4.19
4.18
4.12
4.08
4.07
4.05
4.02
3.99
3.99
3.97
3.97
3.96
3.86
3.85
3.81
3.80
3.71
3.67
3.48
3.47
3.44
3.44
3.43
3.43
2.07
F3C
OAc
N
Bn
3va
5.23
1.00
1.06
3.10
1.04
1.02
1.02
3.05
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.43
F3C
OAc
N
Bn
3va
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


170.74
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132.16
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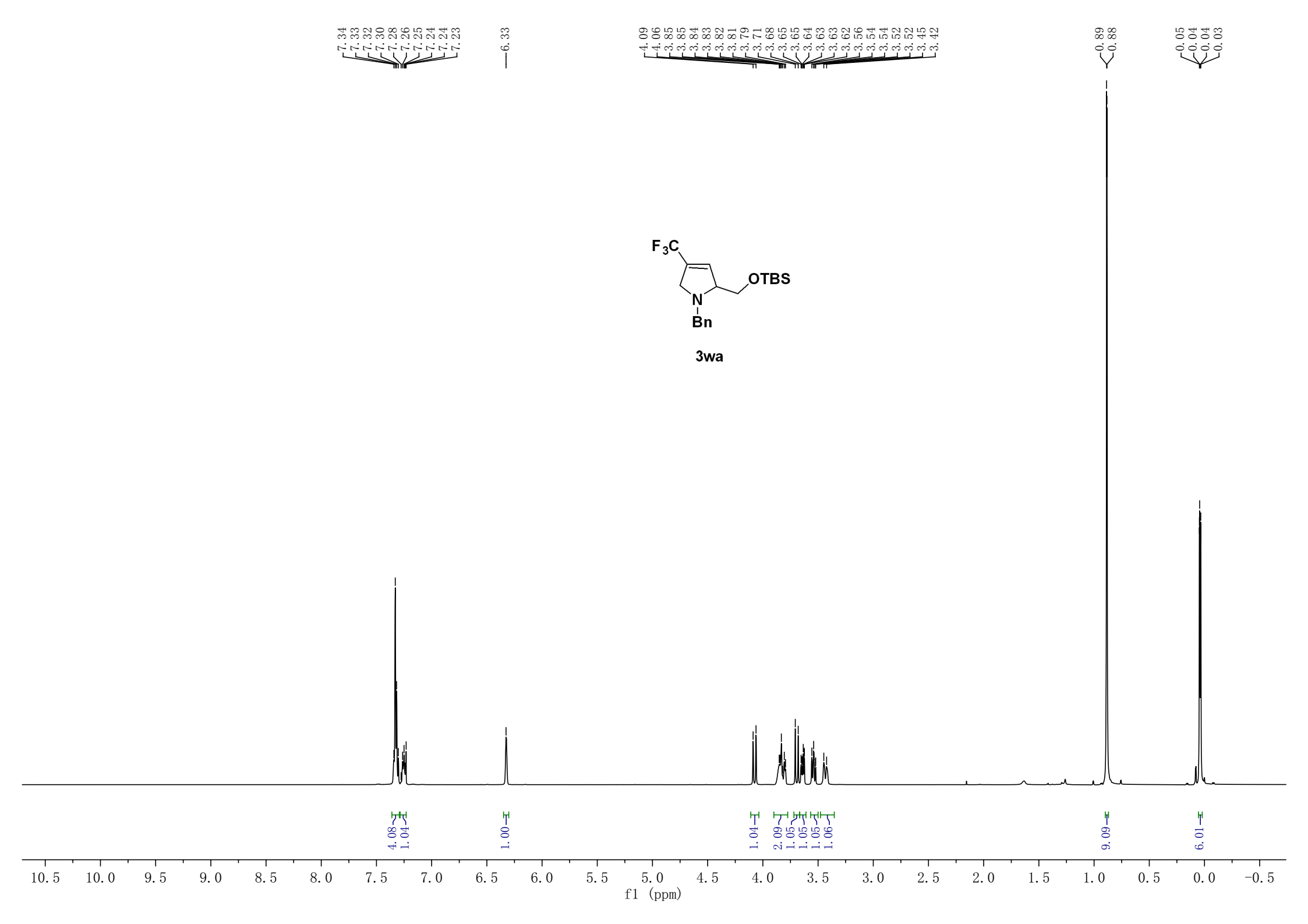
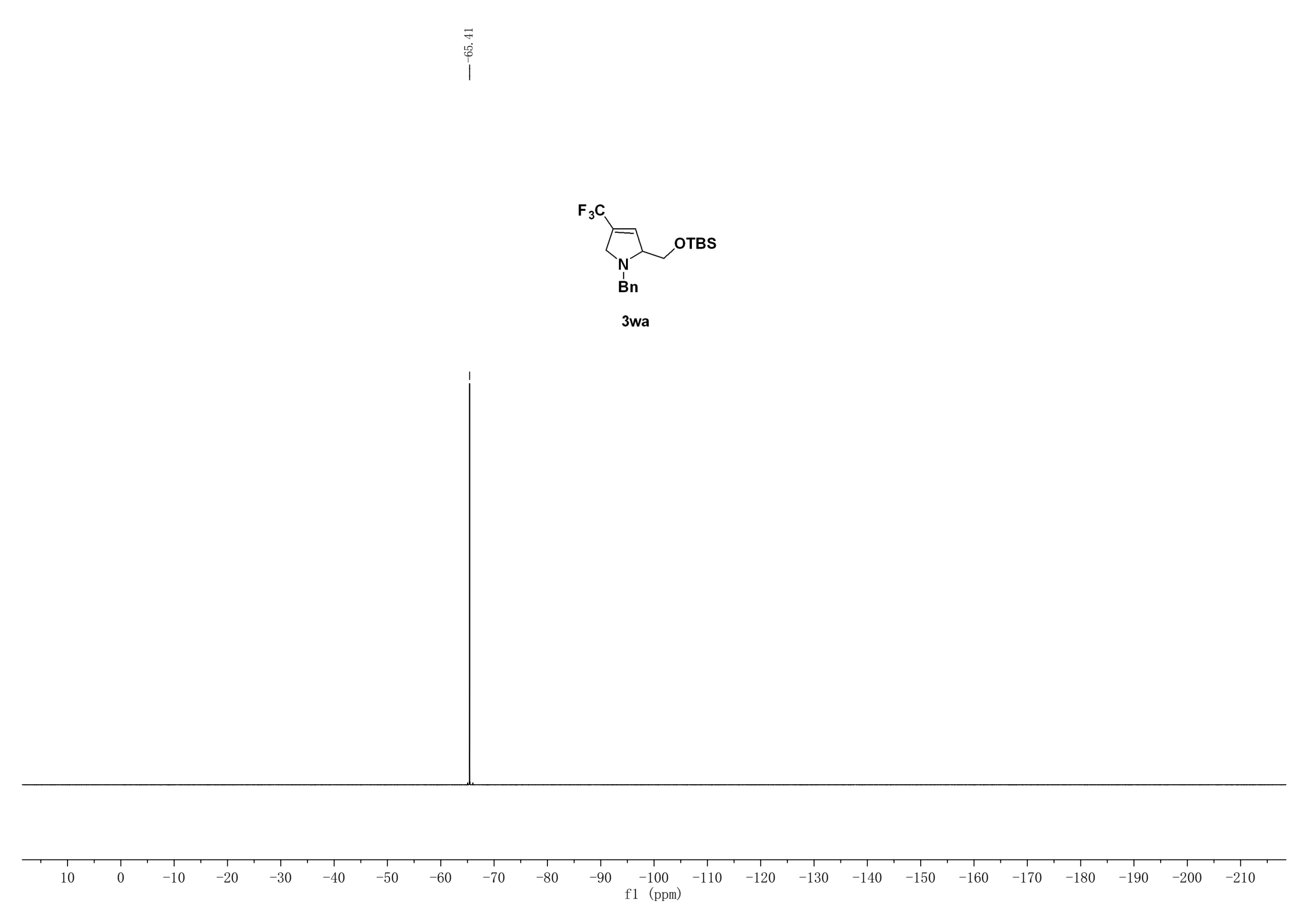
131.61
128.47
128.44
127.32
124.75
122.61
120.47
118.33
77.25
77.00
76.75
69.22
65.62
59.00
57.39
20.77
F3C
OAc
N
Bn
3va
f1 (ppm)


7.34
7.33
7.32
7.30
7.28
7.26
7.25
7.24
7.24
7.23
6.33
4.09
4.06
3.85
3.85
3.84
3.83
3.82
3.81
3.79
3.71
3.68
3.65
3.65
3.64
3.63
3.63
3.62
3.56
3.54
3.54
3.52
3.52
3.45
3.42
0.89
0.88
0.05
0.04
0.04
0.03
F3C
OTBS
N
Bn
3wa
4.08
1.04
1.00
1.04
2.09
1.05
1.05
1.05
1.06
9.09
6.01
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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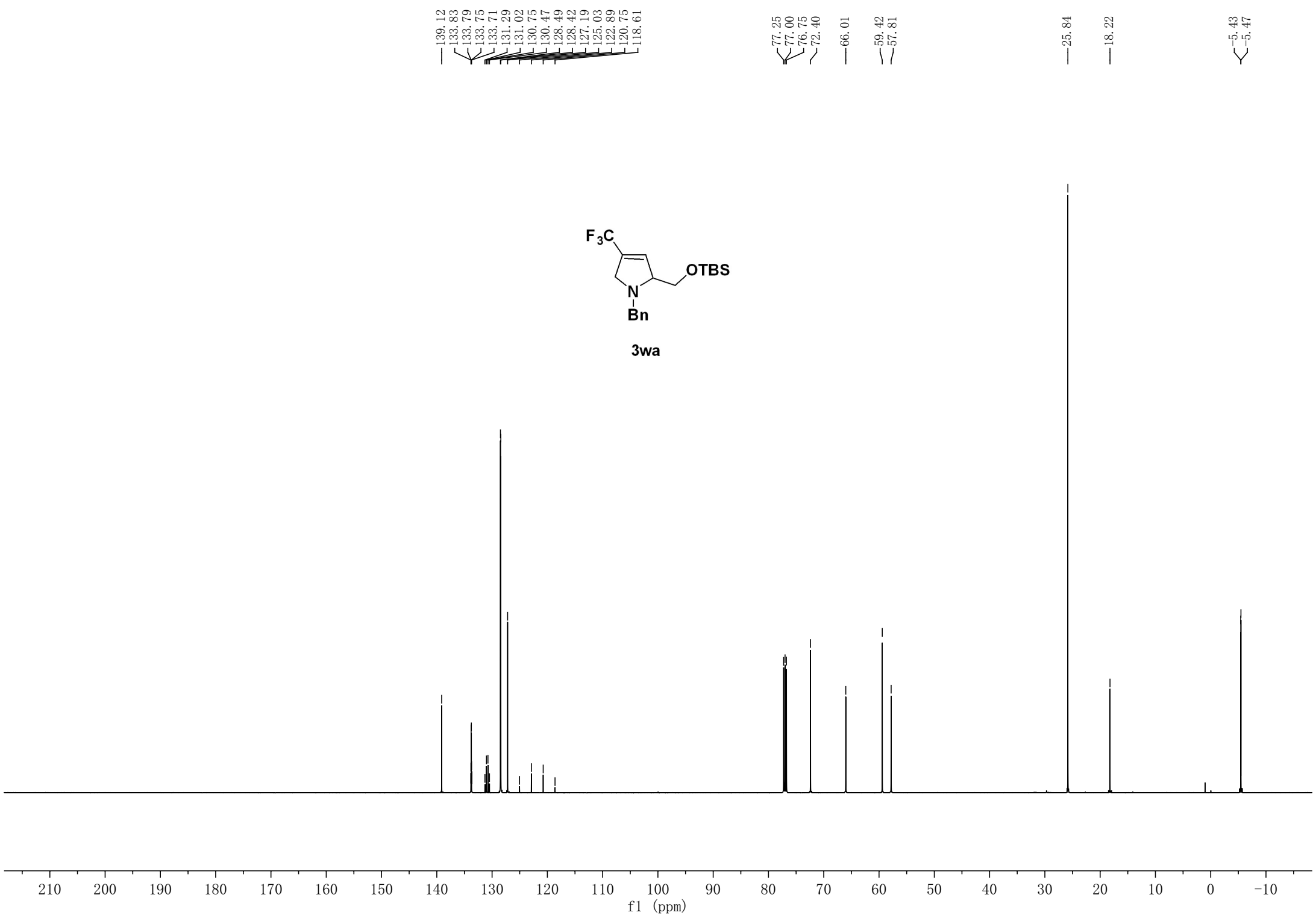
F3C
OTBS
N
Bn
3wa
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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133.83
133.79
133.75
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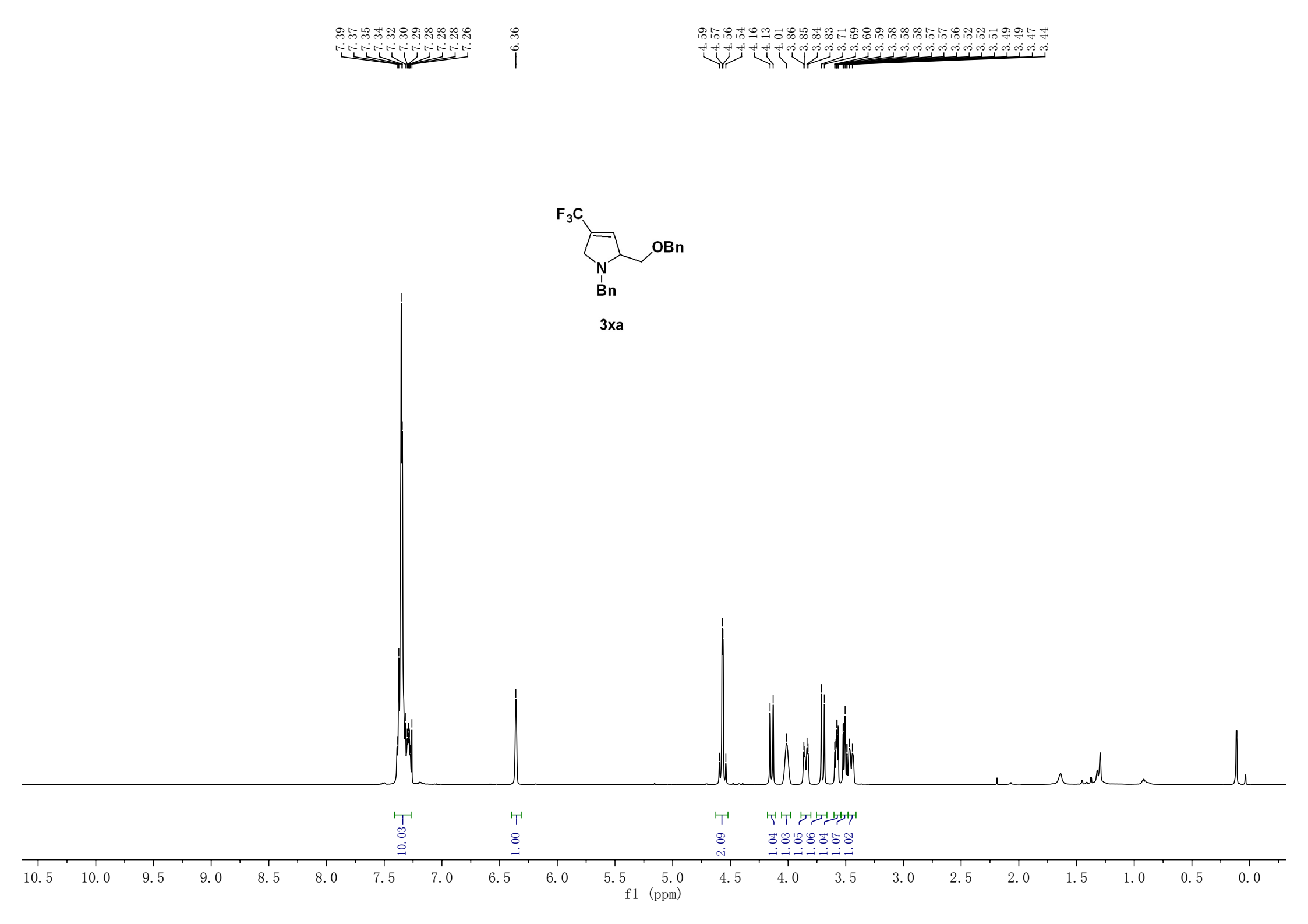
131.29
131.02
130.75
130.47
128.49
128.42
127.19
125.03
122.89
120.75
118.61
77.25
77.00
76.75
72.40
66.01
59.42
57.81
25.84
18.22
-5.43
-5.47
F3C
OTBS
N
Bn
3wa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.37
7.35
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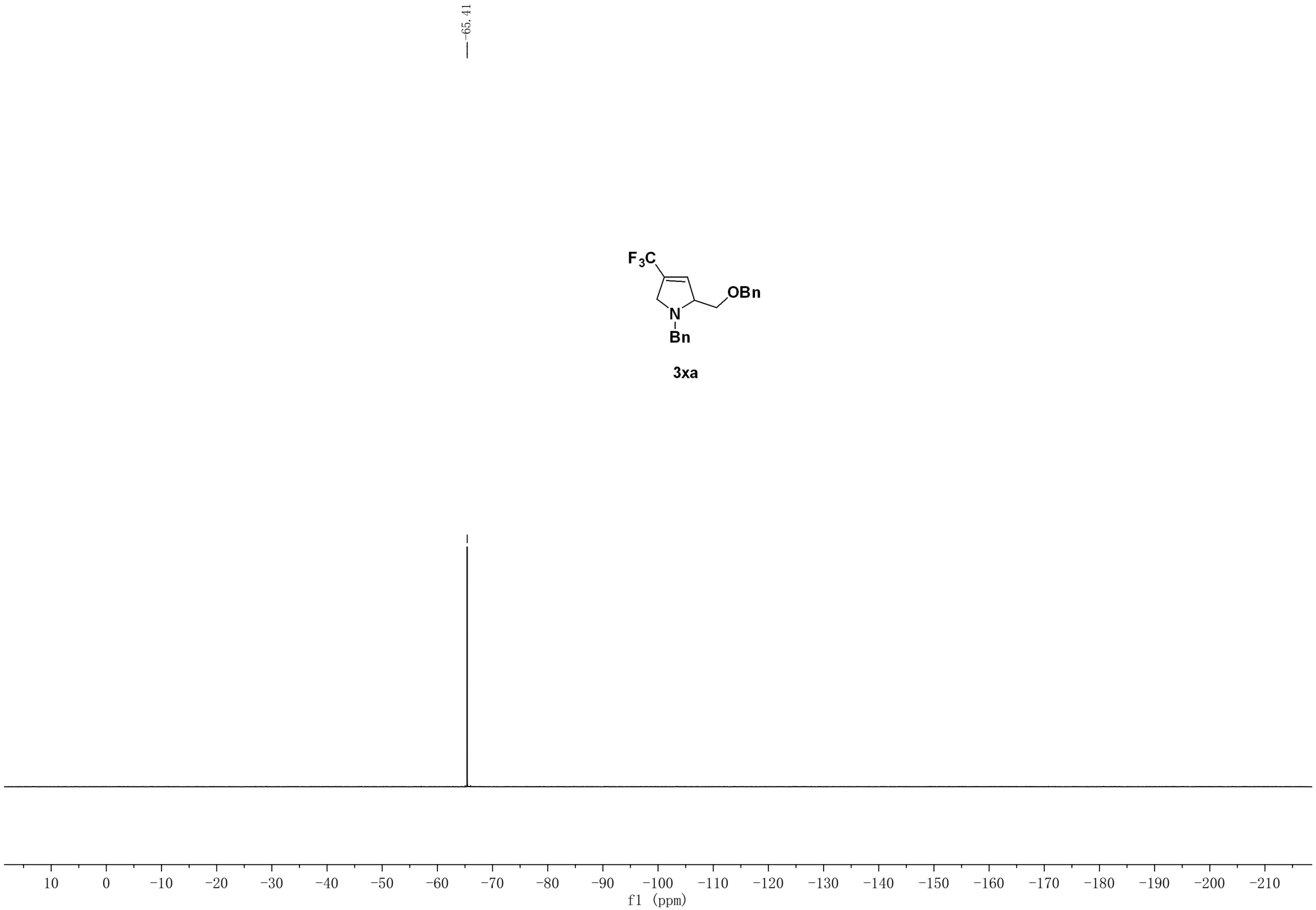
7.32
7.30
7.29
7.28
7.28
7.28
7.26
6.36
4.59
4.57
4.56
4.54
4.16
4.13
4.01
3.86
3.85
3.84
3.83
3.71
3.69
3.60
3.59
3.58
3.58
3.57
3.57
3.56
3.52
3.52
3.51
3.49
3.49
3.47
3.44
F3C
OBn
N
Bn
3xa
10.03
1.00
2.09
1.04
1.03
1.05
1.06
1.04
1.07
1.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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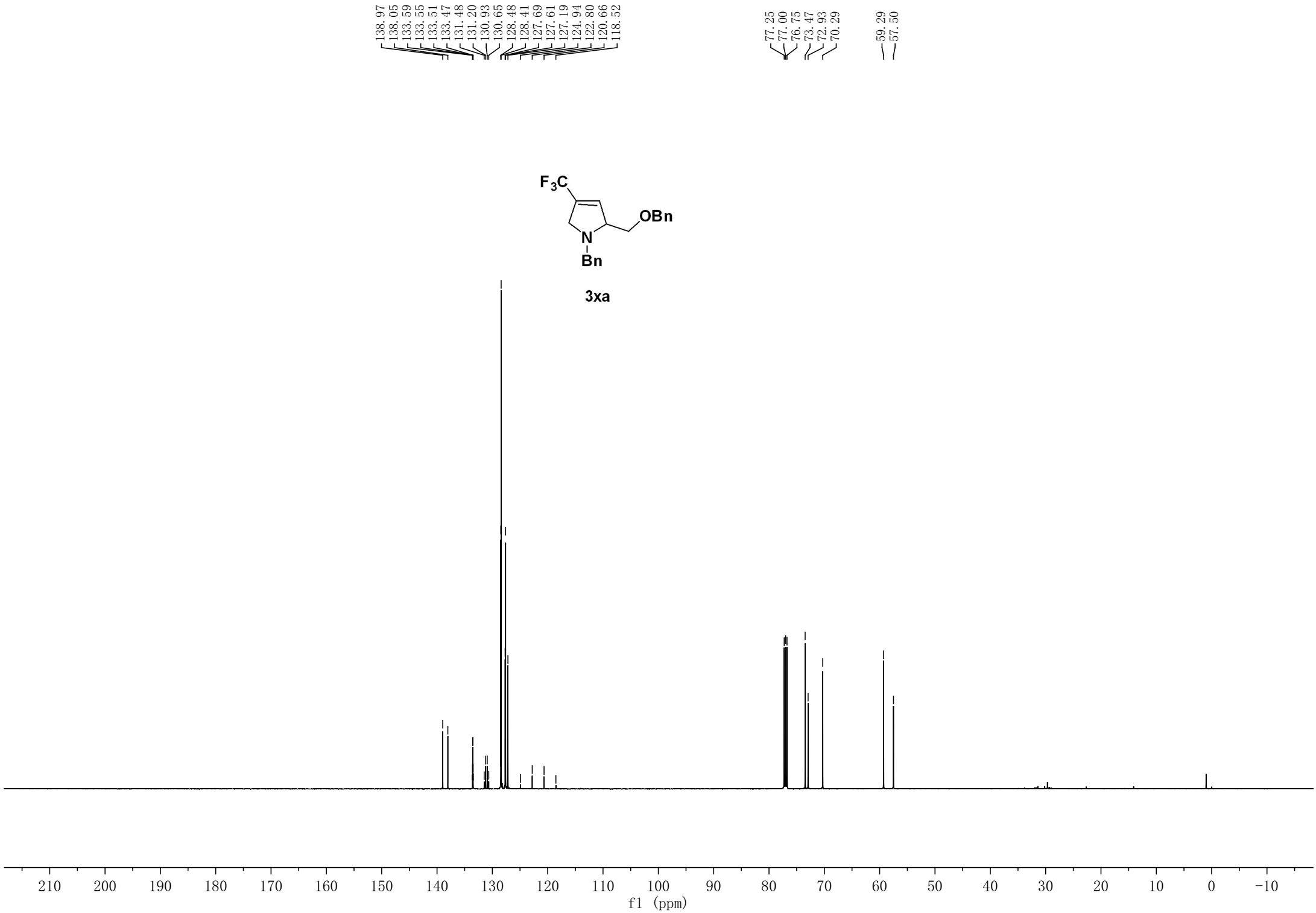
F3C
OBn
N
Bn
3xa
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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131.20
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130.65
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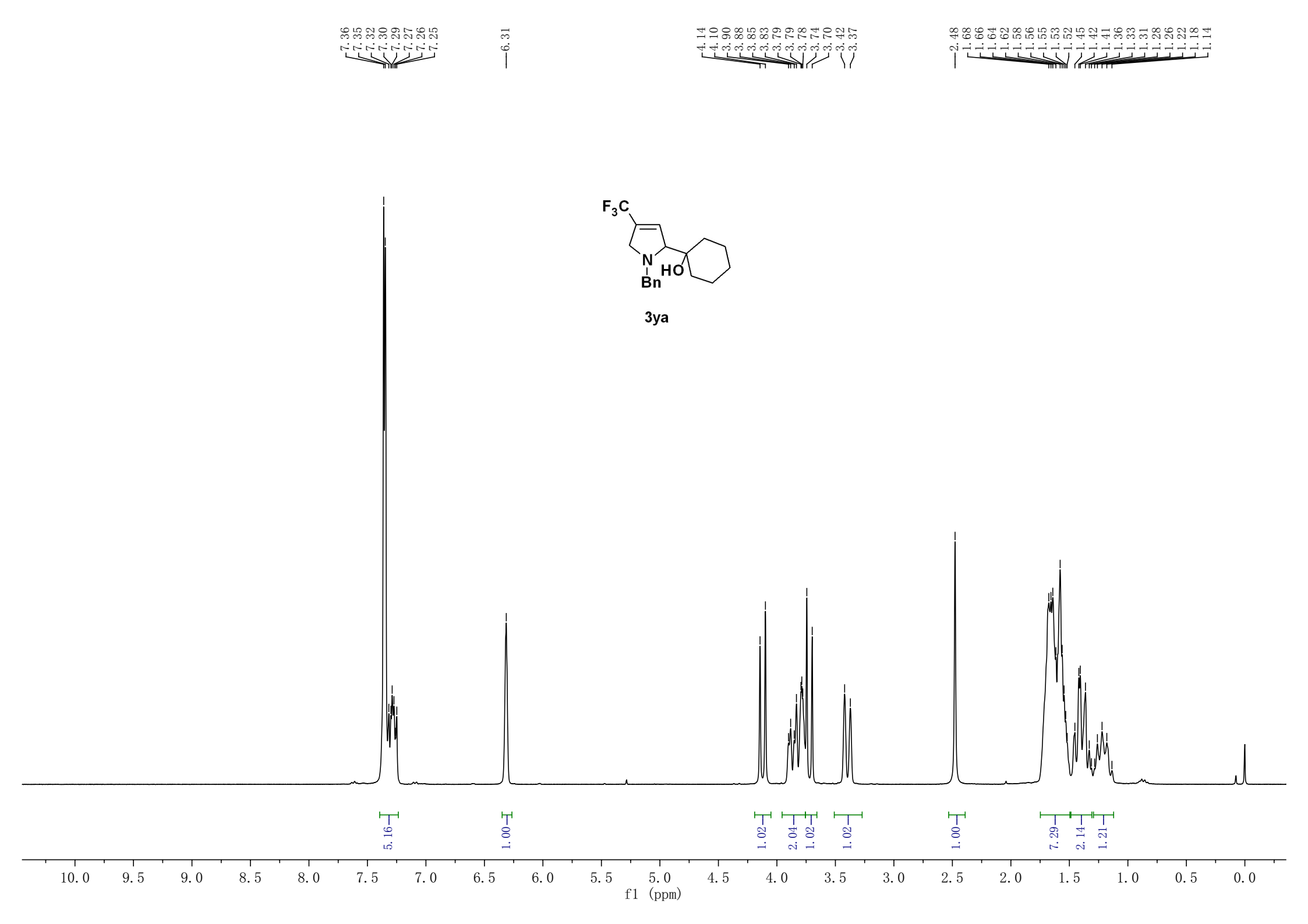
128.41
127.69
127.61
127.19
124.94
122.80
120.66
118.52
77.25
77.00
76.75
73.47
72.93
70.29
59.29
57.50
F3C
OBn
N
Bn
3xa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.35
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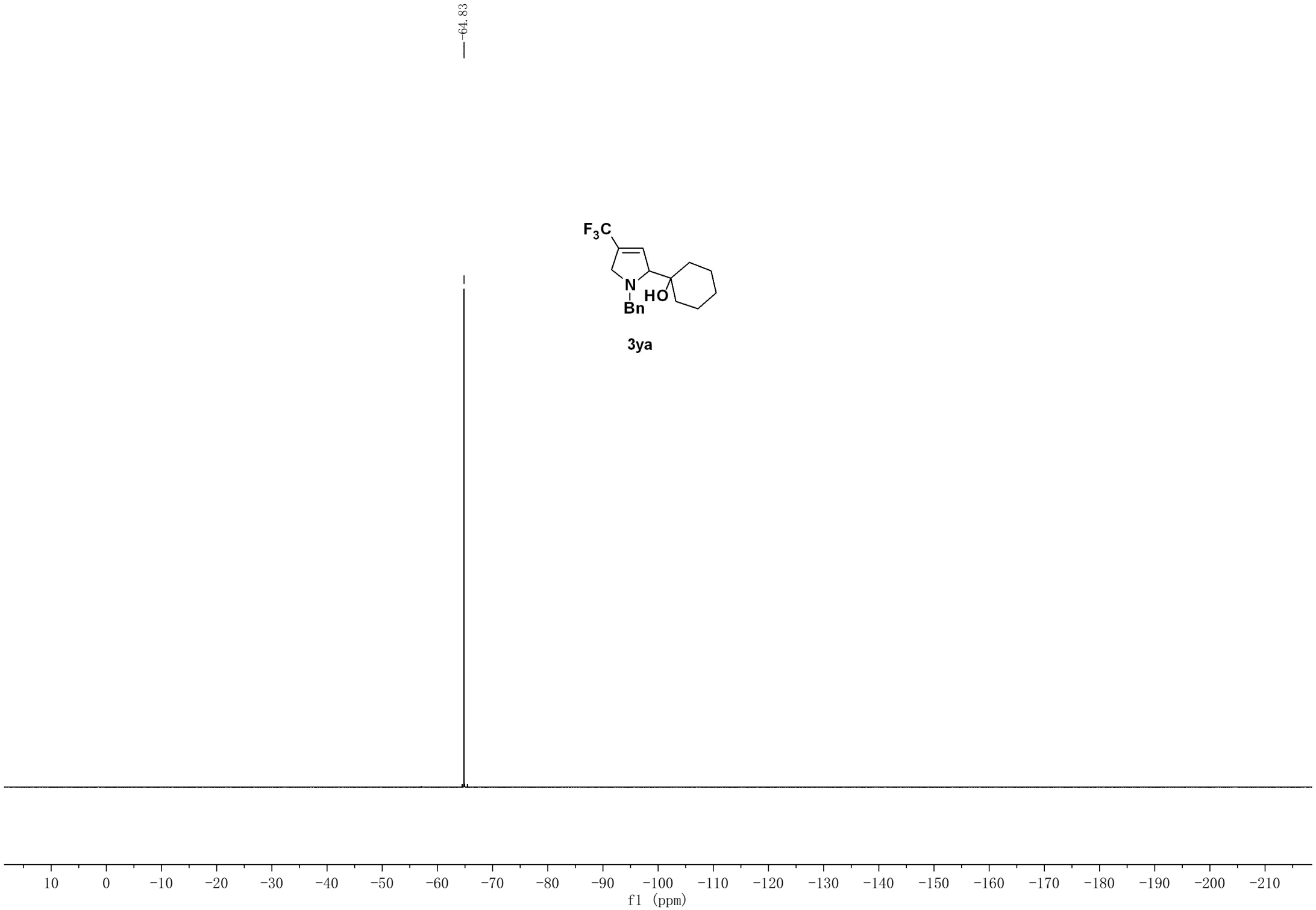
7.27
7.26
7.25
6.31
4.14
4.10
3.90
3.88
3.85
3.83
3.79
3.79
3.78
3.74
3.70
3.42
3.37
2.48
1.68
1.66
1.64
1.62
1.58
1.56
1.55
1.53
1.52
1.45
1.42
1.41
1.36
1.33
1.31
1.28
1.26
1.22
1.18
1.14
F3C
N
HO
Bn
3ya
5.16
1.00
1.02
2.04
1.02
1.02
1.00
7.29
2.14
1.21
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-64.83
F3C
N
Bn
HO
3ya
10
0
-10
-20
-30
-40
-50
-60
-70
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-120
-130
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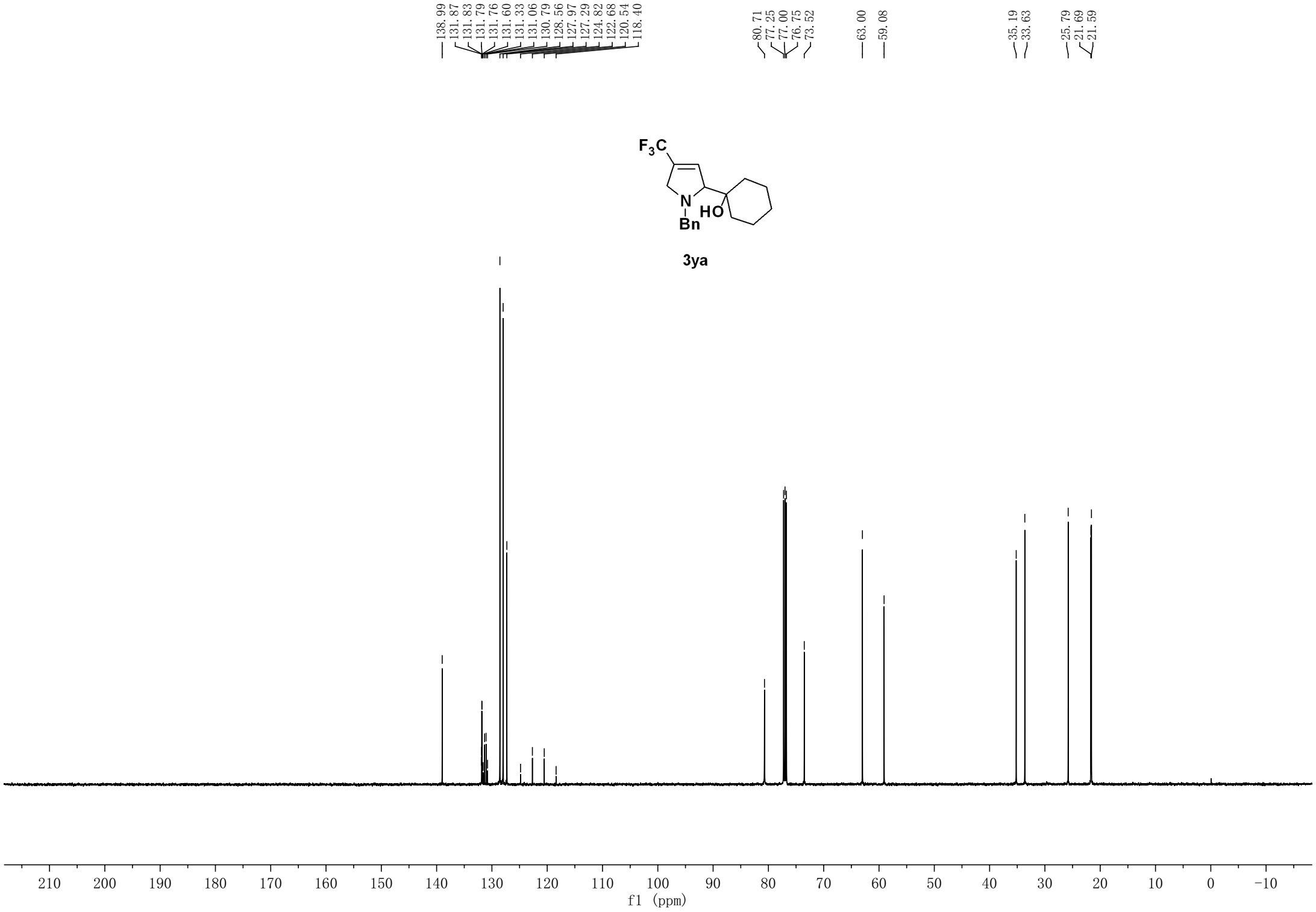
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


138.99
131.87
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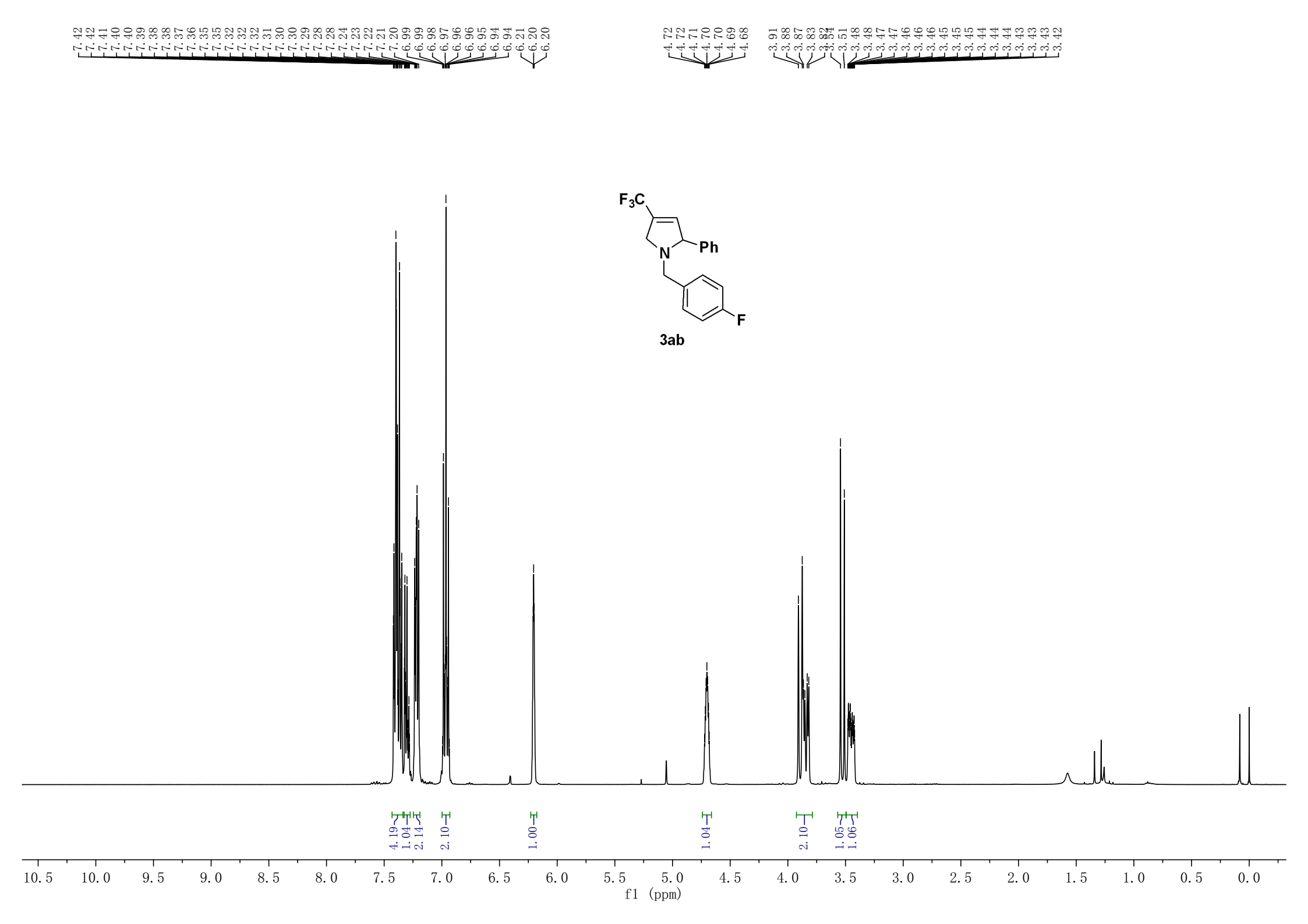
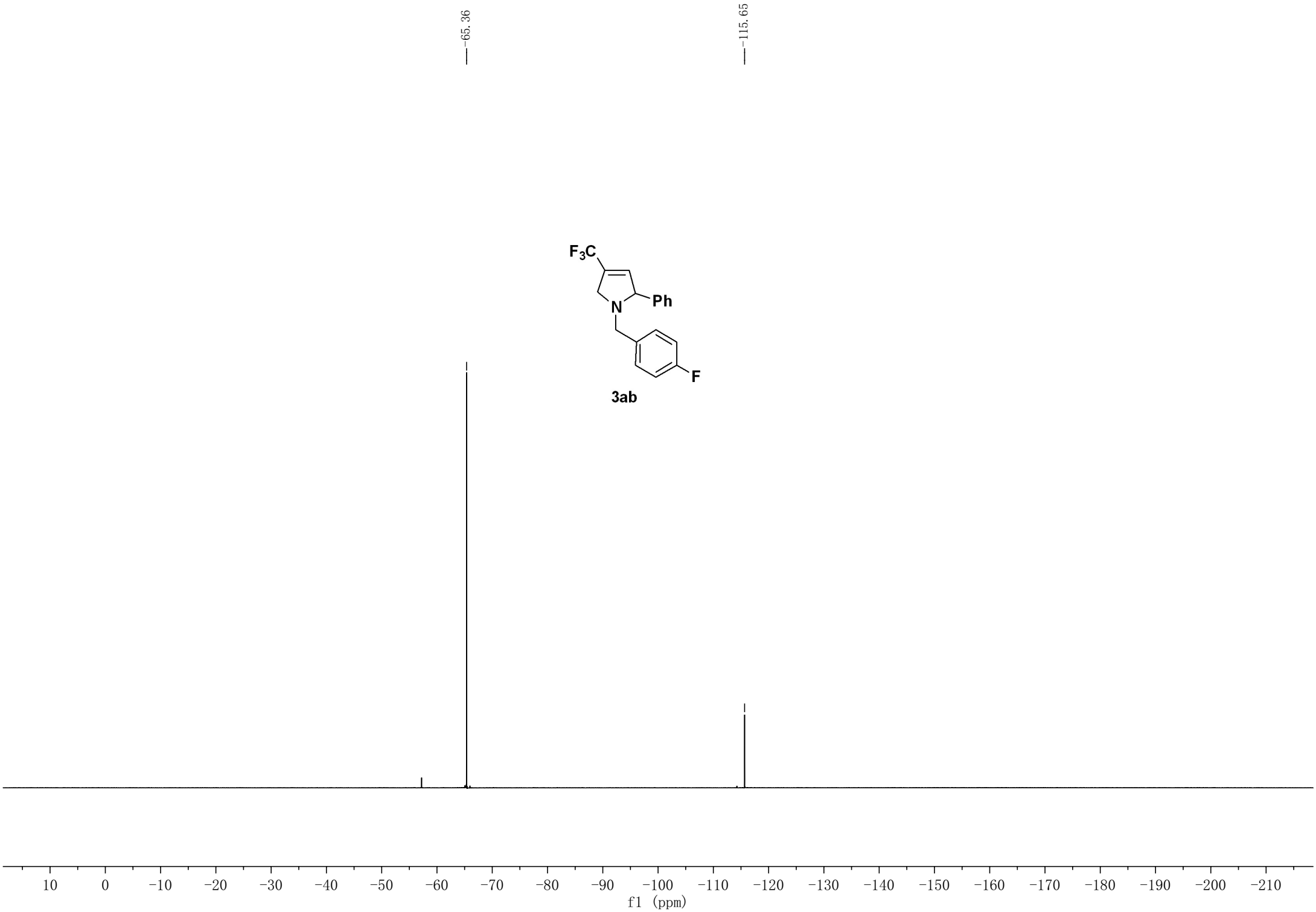
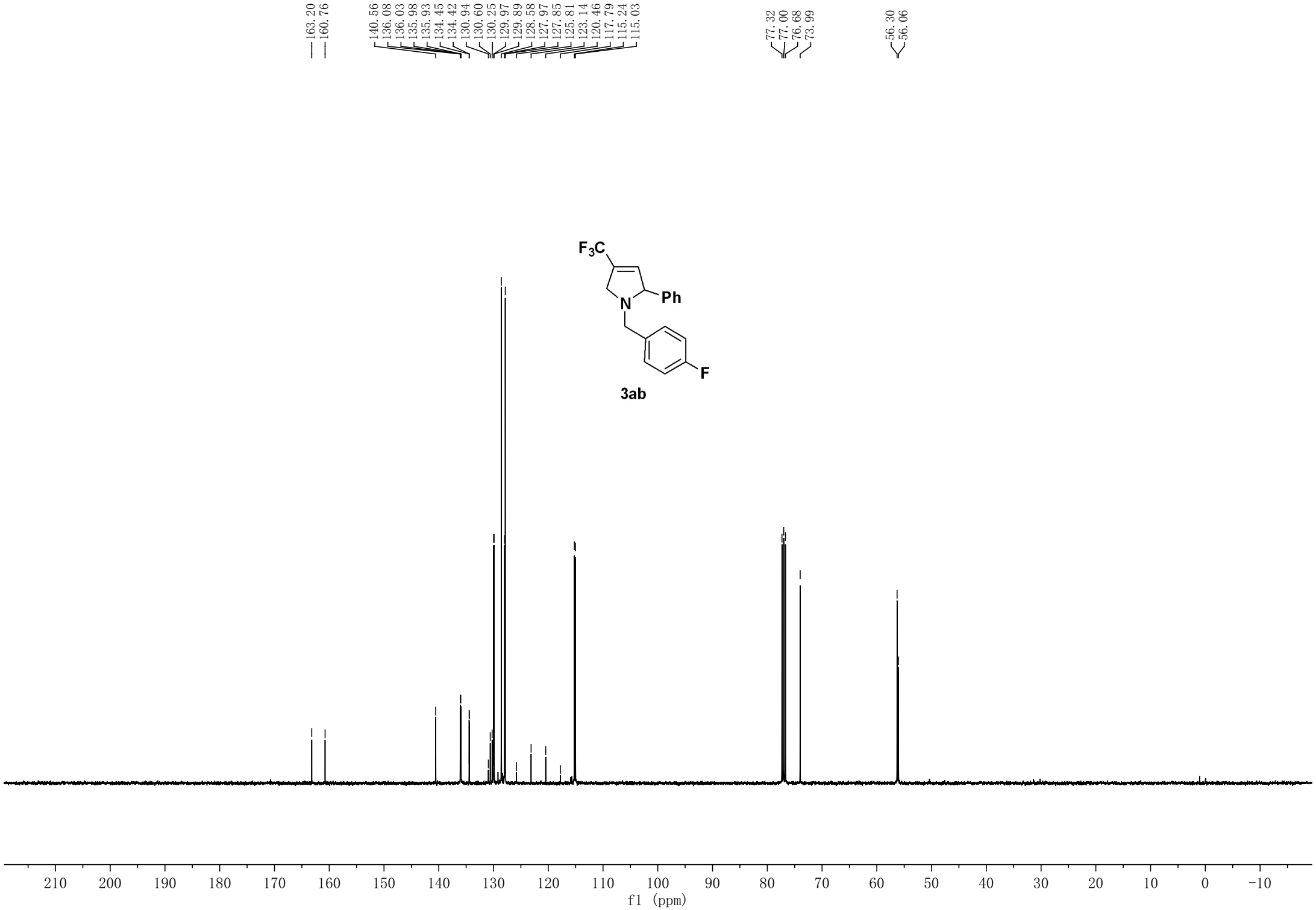
131.79
131.76
131.60
131.33
131.06
130.79
128.56
127.97
127.29
124.82
122.68
120.54
118.40
80.71
77.25
77.00
76.75
73.52
63.00
59.08
35.19
33.63
25.79
21.69
21.59
F3C
N
Bn
HO
3ya
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.42 7.42 7.41 7.40 7.40 7.39 7.38 7.38 7.37 7.36 7.35 7.35 7.32 7.32 7.32 7.31 7.30 7.30 7.29 7.28 7.28 7.24 7.23 7.22 7.21 7.20 6.99 6.99 6.98 6.97 6.96 6.96 6.95 6.94 6.94 6.21 6.20 6.20
4.72 4.72 4.71 4.70 4.70 4.69 4.68
3.91 3.88 3.87 3.83 3.82 3.51 3.48 3.47 3.47 3.46 3.46 3.45 3.45 3.45 3.44 3.44 3.44 3.43 3.43 3.42
F3C
Ph
N
F
3ab
4.19 1.04 2.14 2.10 1.00 1.04 2.10 1.05 1.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-65.36
-115.65
F3C
Ph
N
F
3ab
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


163.20
160.76
140.56
136.08
136.03
135.98
135.93
134.45
134.42
130.94
130.60
130.25
129.97
129.89
128.58
127.97
127.85
125.81
123.14
120.46
117.79
115.24
115.03
77.32
77.00
76.68
73.99
56.30
56.06
F3C
Ph
N
F
3ab
210
200
190
180
170
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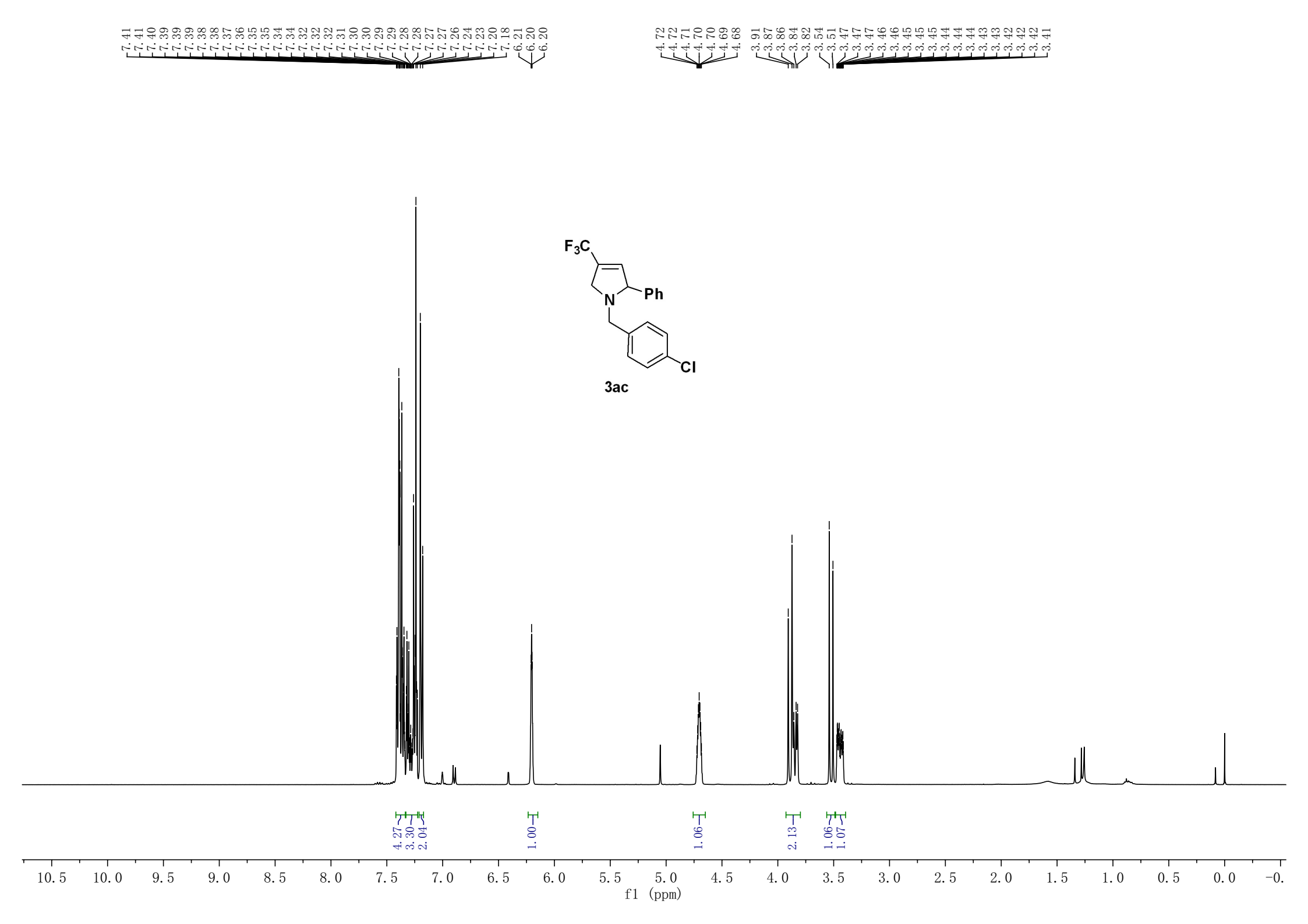
-10
f1 (ppm)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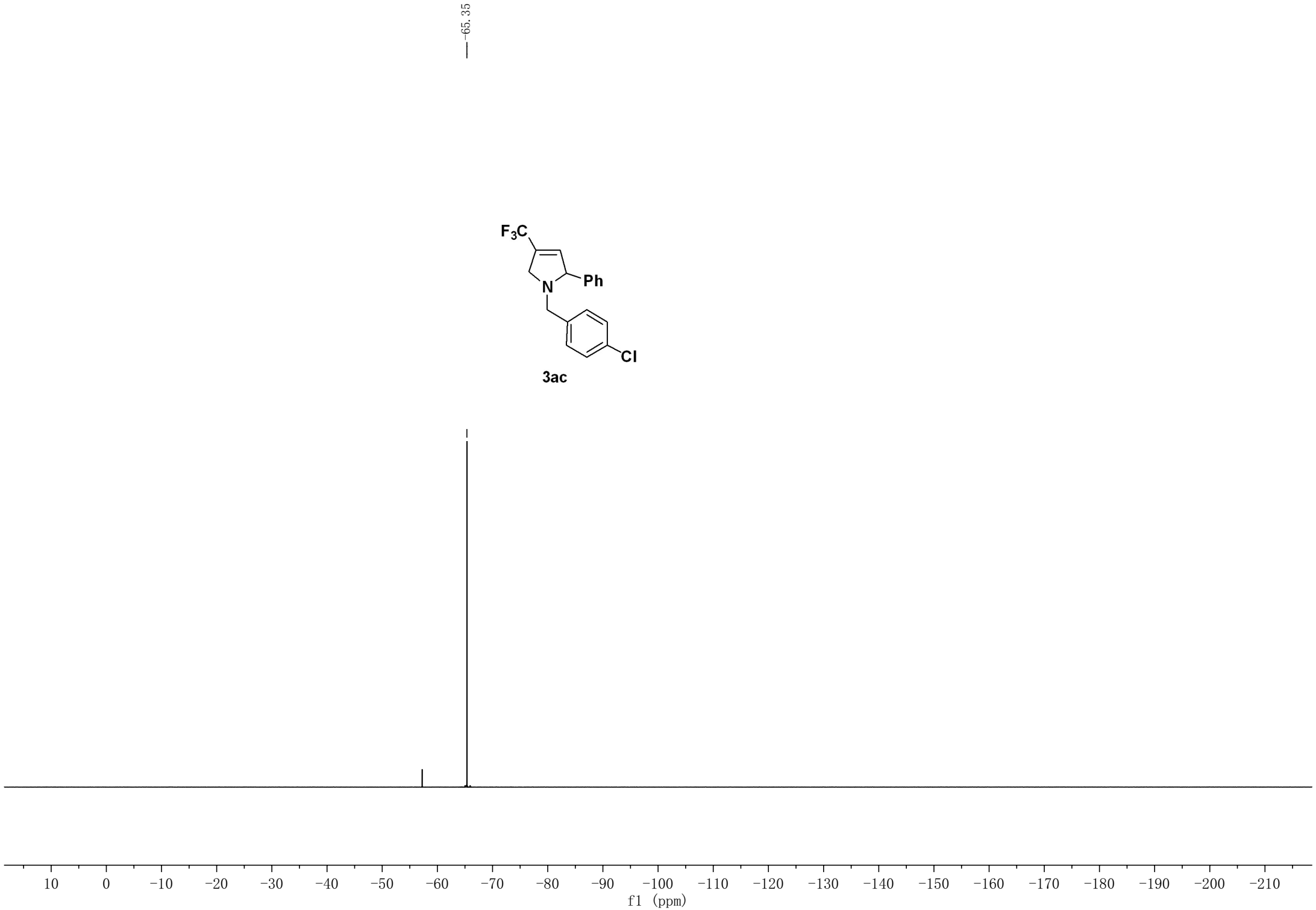
4.72 4.72 4.71 4.70 4.70 4.69 4.68
3.91 3.87 3.86 3.84 3.82 3.54 3.51 3.47 3.47 3.47 3.46 3.46 3.45 3.45 3.45 3.44 3.44 3.44 3.43 3.43 3.42 3.42 3.42 3.41
F3C
Ph
N
Cl
3ac
4.27
3.30
2.04
1.00
1.06
2.13
1.06
1.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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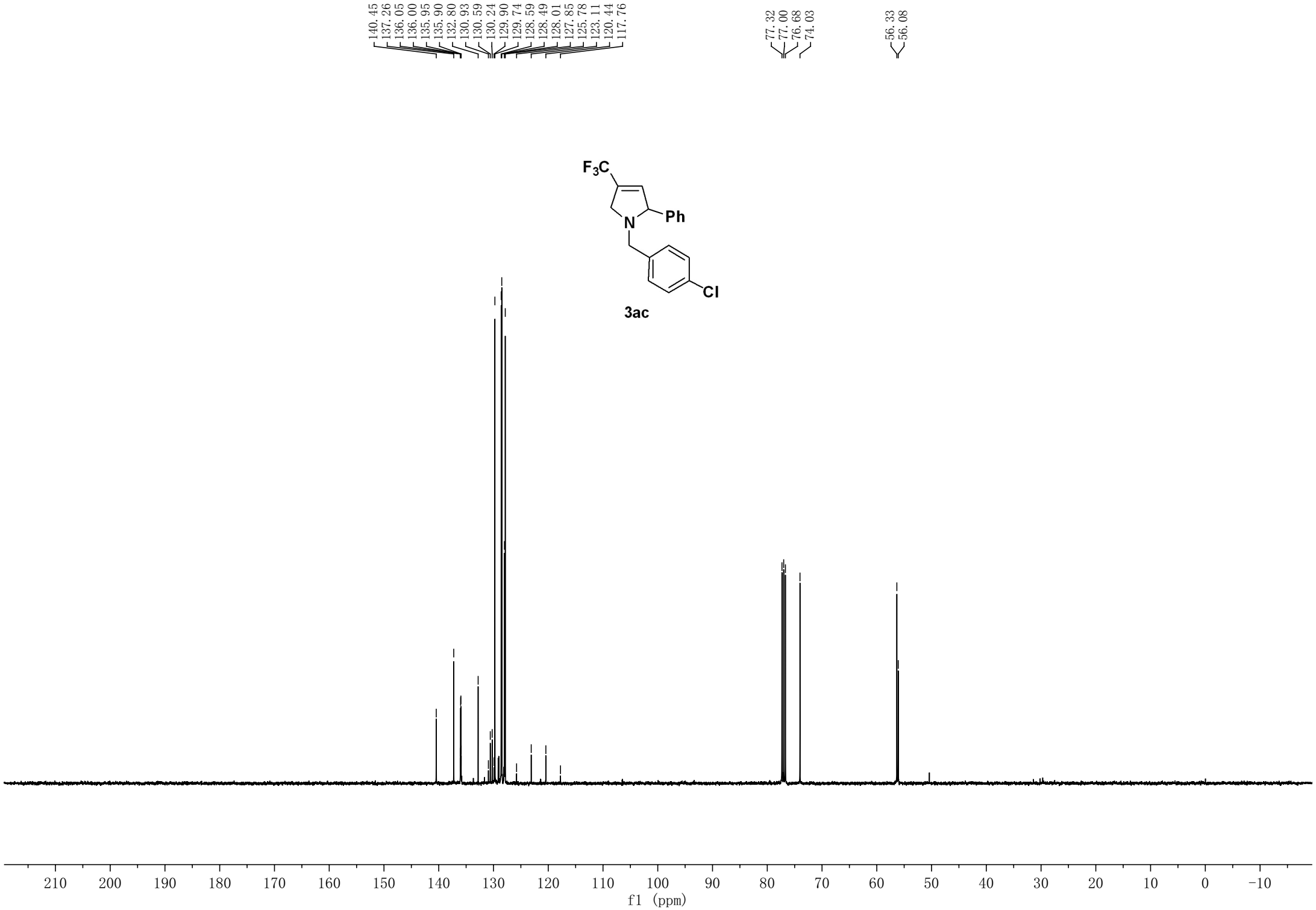
-170
-180
-190
-200
-210
f1 (ppm)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129.74
128.59
128.49
128.01
127.85
125.78
123.11
120.44
117.76
77.32
77.00
76.68
74.03
56.33
56.08
F3C
Ph
N
Cl
3ac
210
200
190
180
170
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120
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100
90
80
70
60
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40
30
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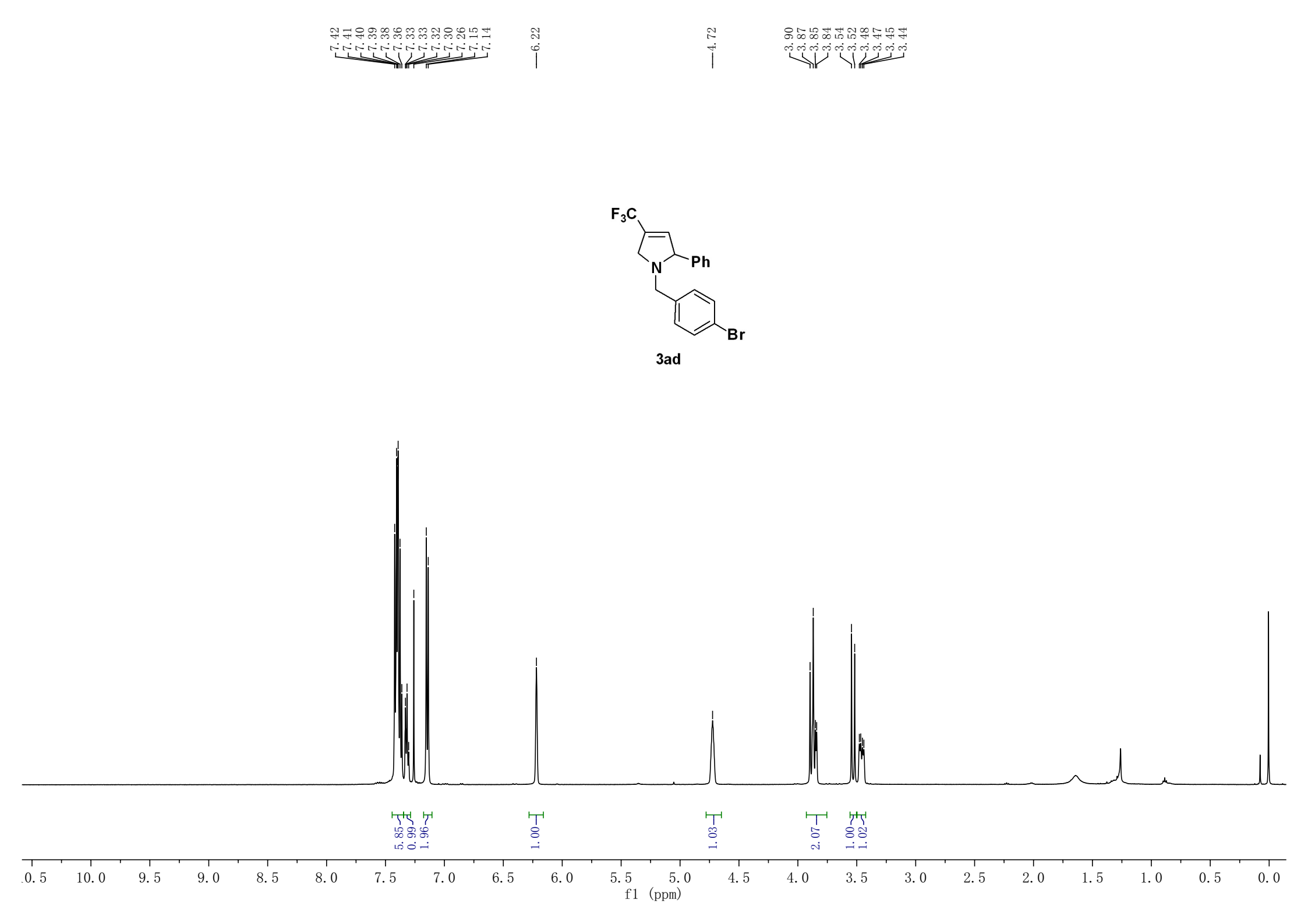
-10
f1 (ppm)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7.30
7.26
7.15
7.14
6.22
4.72
3.90
3.87
3.85
3.84
3.54
3.52
3.48
3.47
3.45
3.44
F3C
Ph
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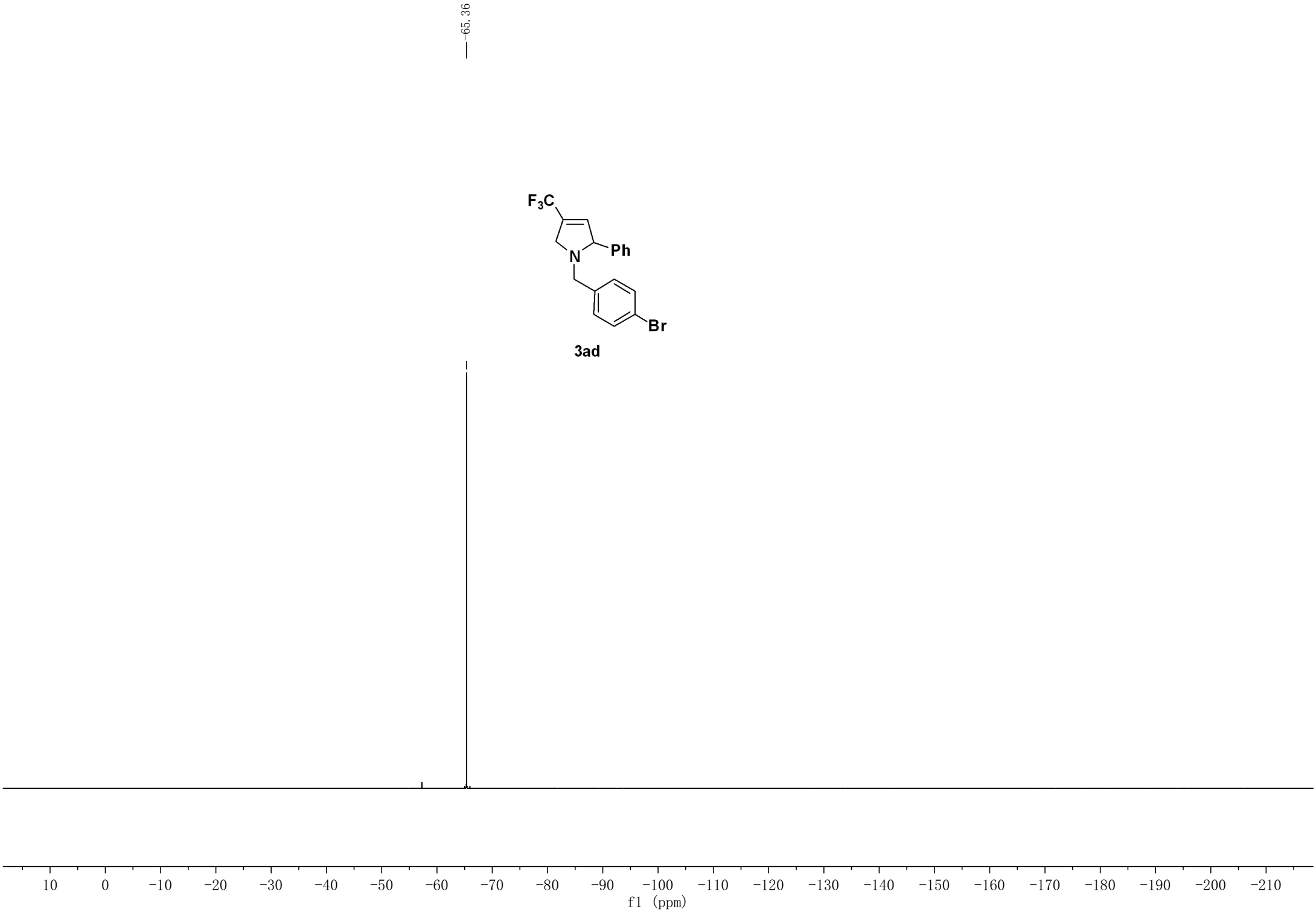
Br
3ad
5.85
0.99
1.96
1.00
1.03
2.07
1.00
1.02
f1 (ppm)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-30
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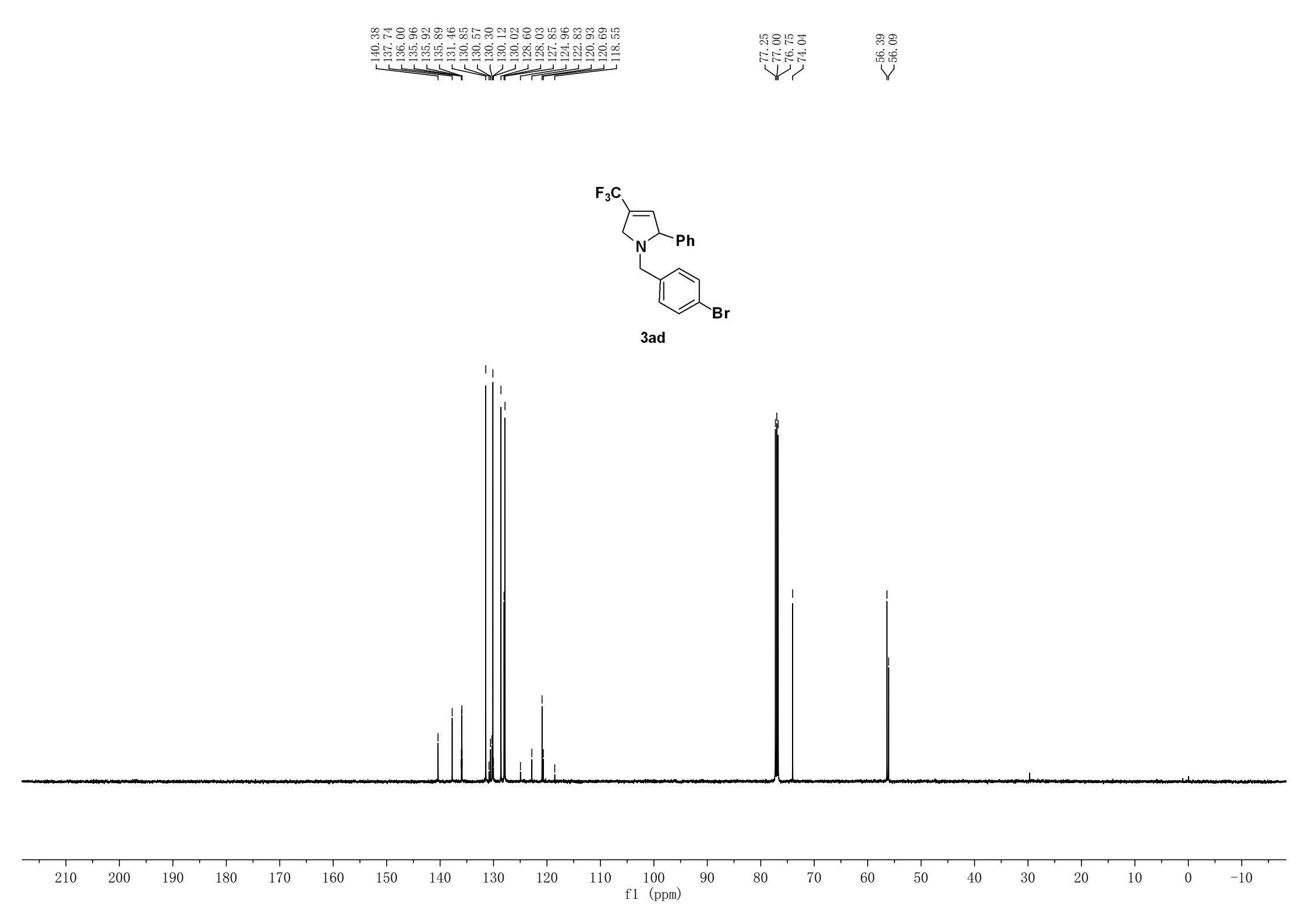
-170
-180
-190
-200
-210
f1 (ppm)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128.03
127.85
124.96
122.83
120.93
120.69
118.55
77.25
77.00
76.75
74.04
56.39
56.09
F3C
Ph
N
Br
3ad
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200
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180
170
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100
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80
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40
30
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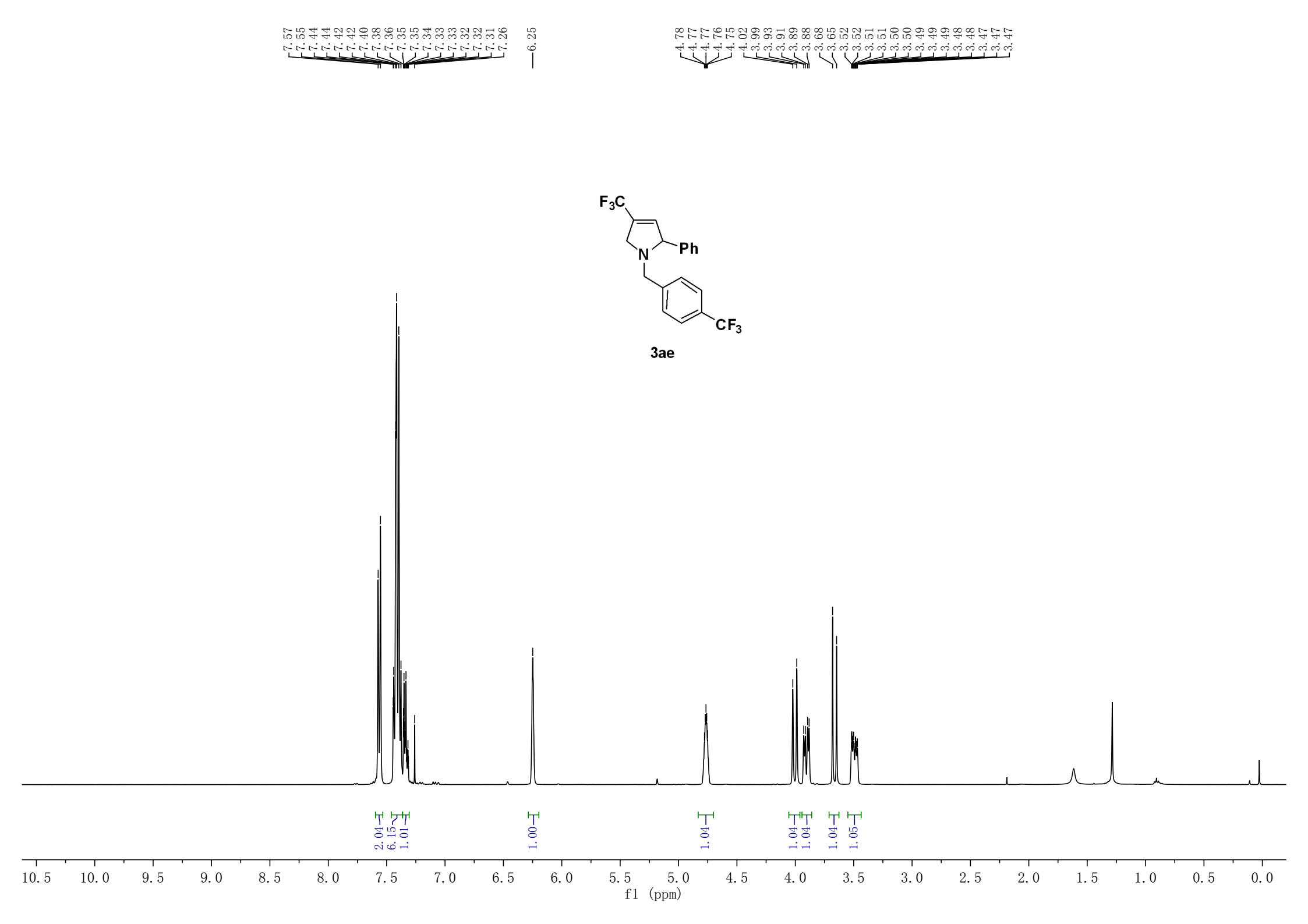
-10
f1 (ppm)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7.33
7.33
7.32
7.32
7.31
7.26
6.25
4.78
4.77
4.77
4.76
4.75
4.02
3.99
3.93
3.91
3.89
3.88
3.68
3.65
3.52
3.52
3.51
3.50
3.50
3.49
3.49
3.49
3.48
3.48
3.47
3.47
3.47
F3C
Ph
N
CF3
3ae
2.04
6.15
1.01
1.00
1.04
1.04
1.04
1.04
1.05
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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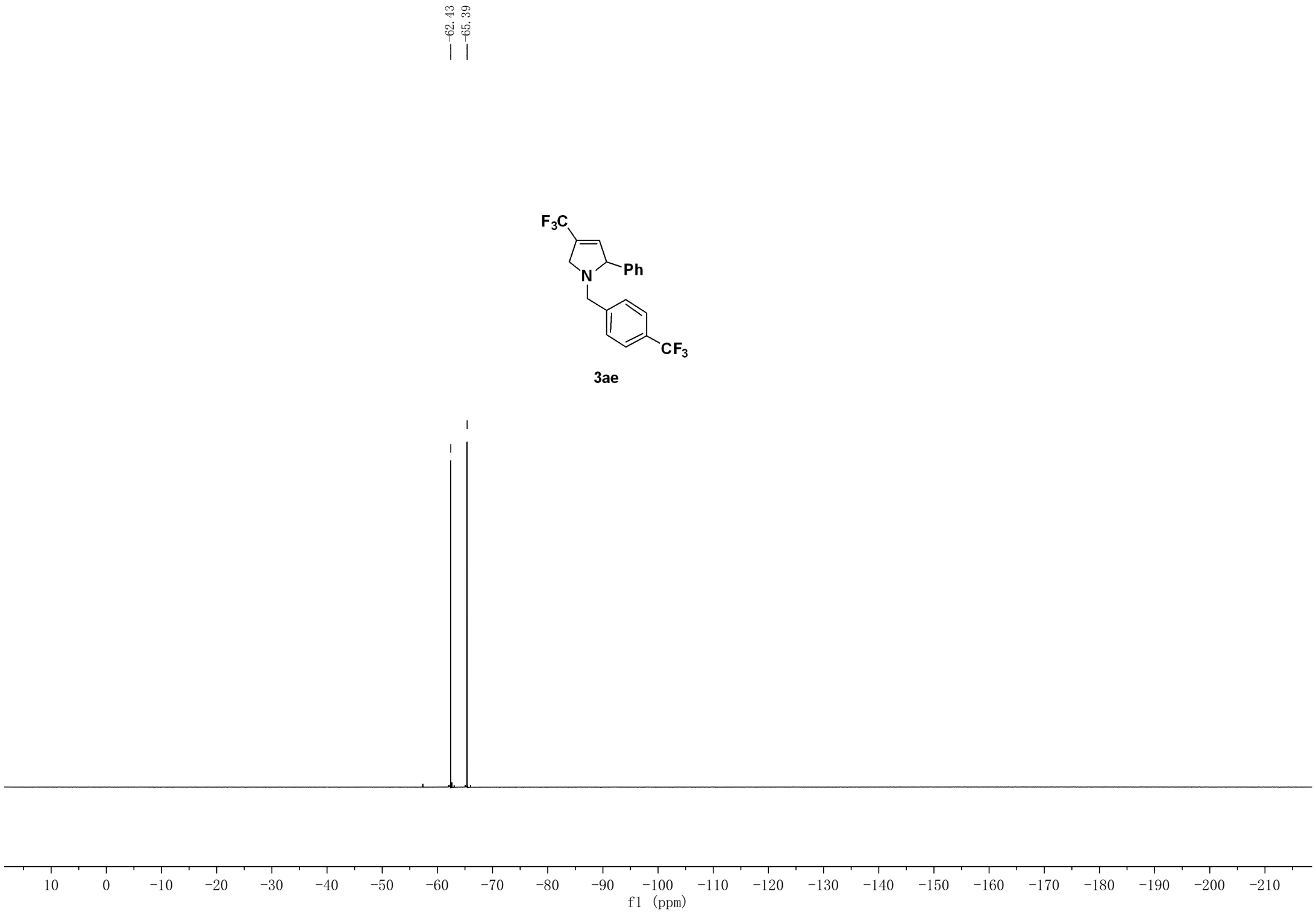
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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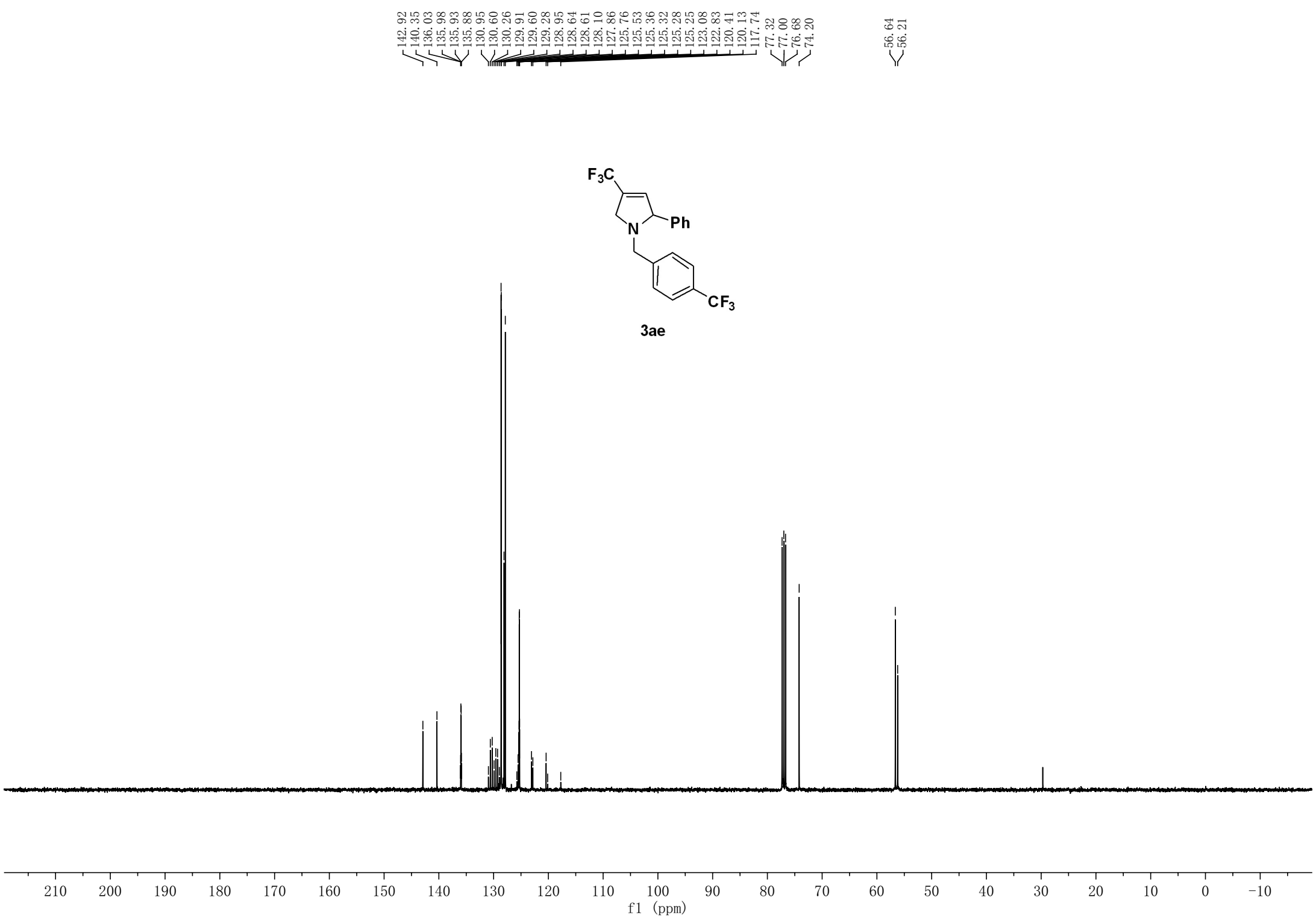
-65.39
F3C
Ph
N
CF3
3ae
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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129.91
129.60
129.28
128.95
128.64
128.61
128.10
127.86
125.76
125.53
125.36
125.32
125.28
125.25
123.08
122.83
120.41
120.13
117.74
77.32
77.00
76.68
74.20
56.64
56.21
F3C
Ph
N
CF3
3ae
210
200
190
180
170
160
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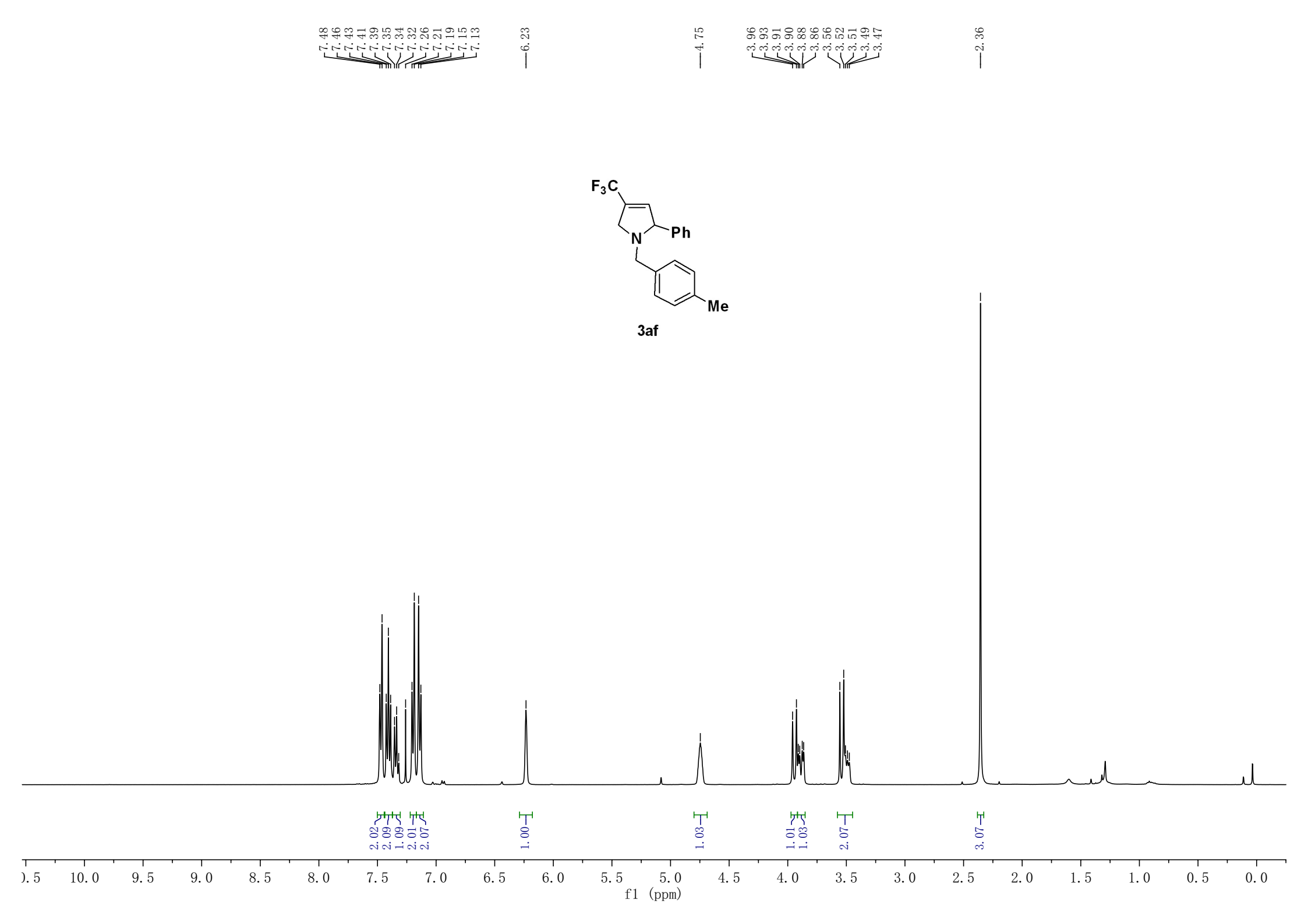
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.46
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7.35
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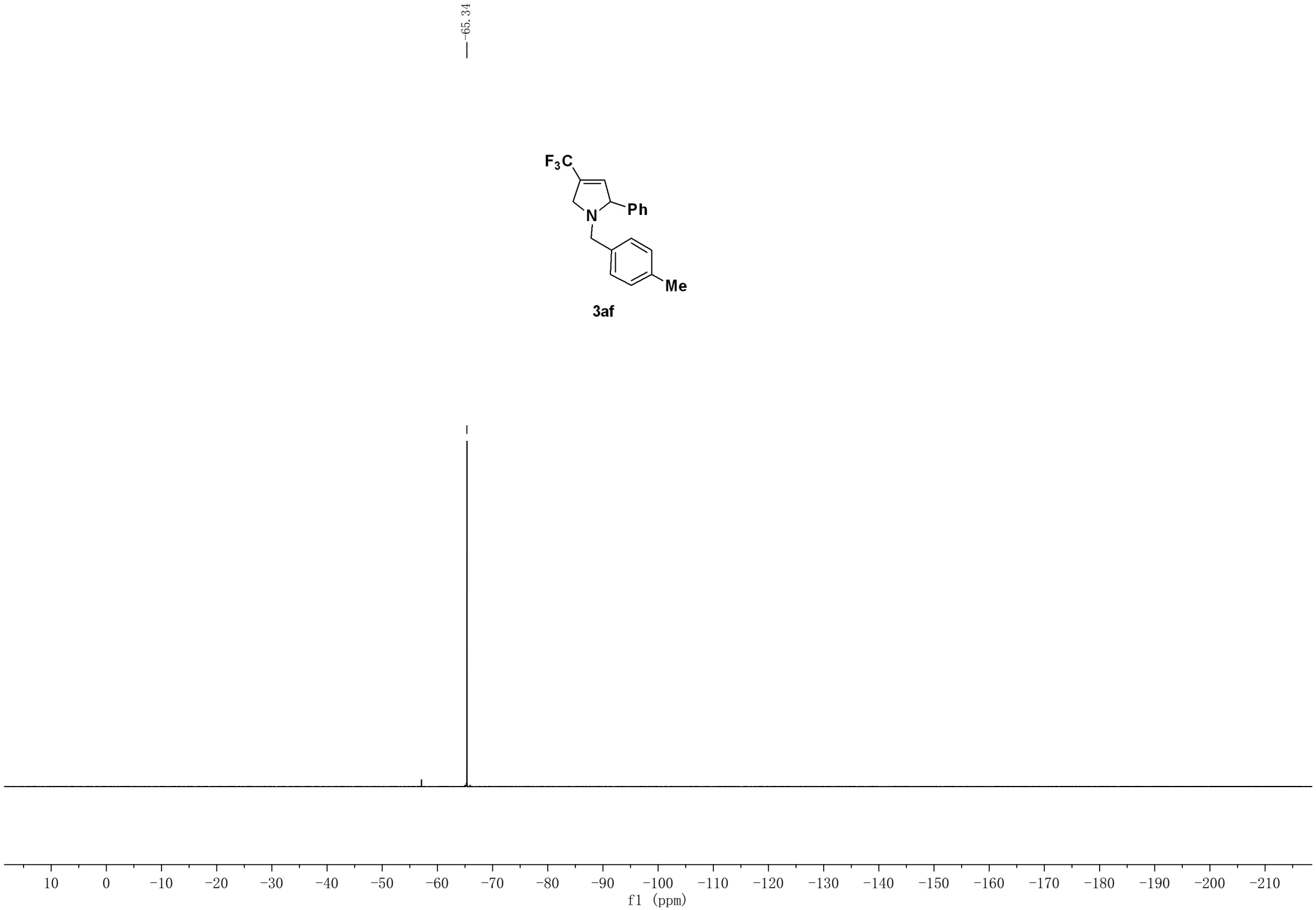
7.32
7.26
7.21
7.19
7.15
7.13
6.23
4.75
3.96
3.93
3.91
3.90
3.88
3.86
3.56
3.52
3.51
3.49
3.47
2.36
F3C
Ph
N
Me
3af
2.02
2.09
1.09
2.01
2.07
1.00
1.03
1.01
1.03
2.07
3.07
f1 (ppm)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F3C
Ph
N
Me
3af
10
0
-10
-20
-30
-40
-50
-60
-70
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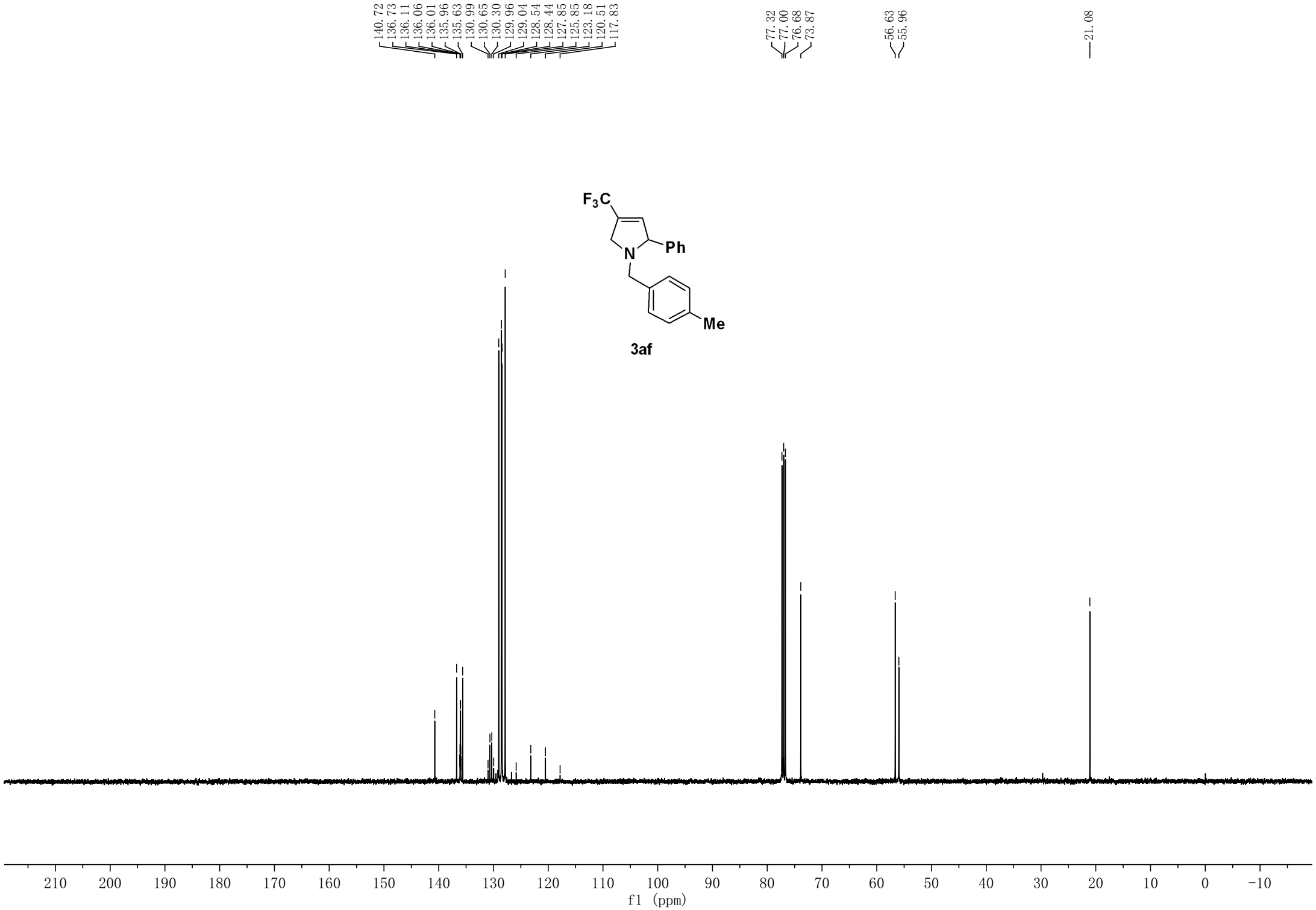
-170
-180
-190
-200
-210
f1 (ppm)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130.99
130.65
130.30
129.96
129.04
128.54
128.44
127.85
125.85
123.18
120.51
117.83
77.32
77.00
76.68
73.87
56.63
55.96
21.08
F3C
Ph
N
Me
3af
210
200
190
180
170
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140
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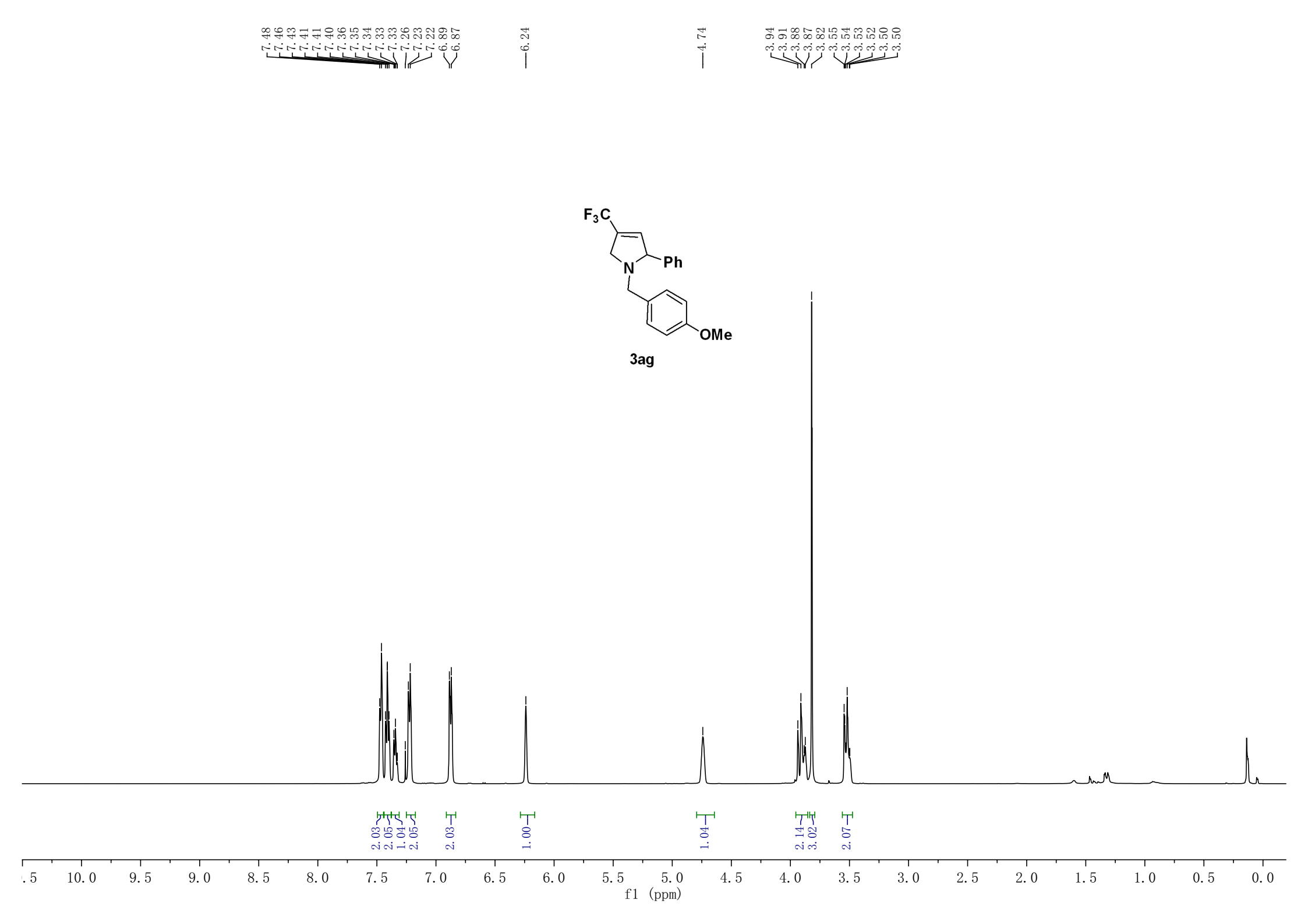
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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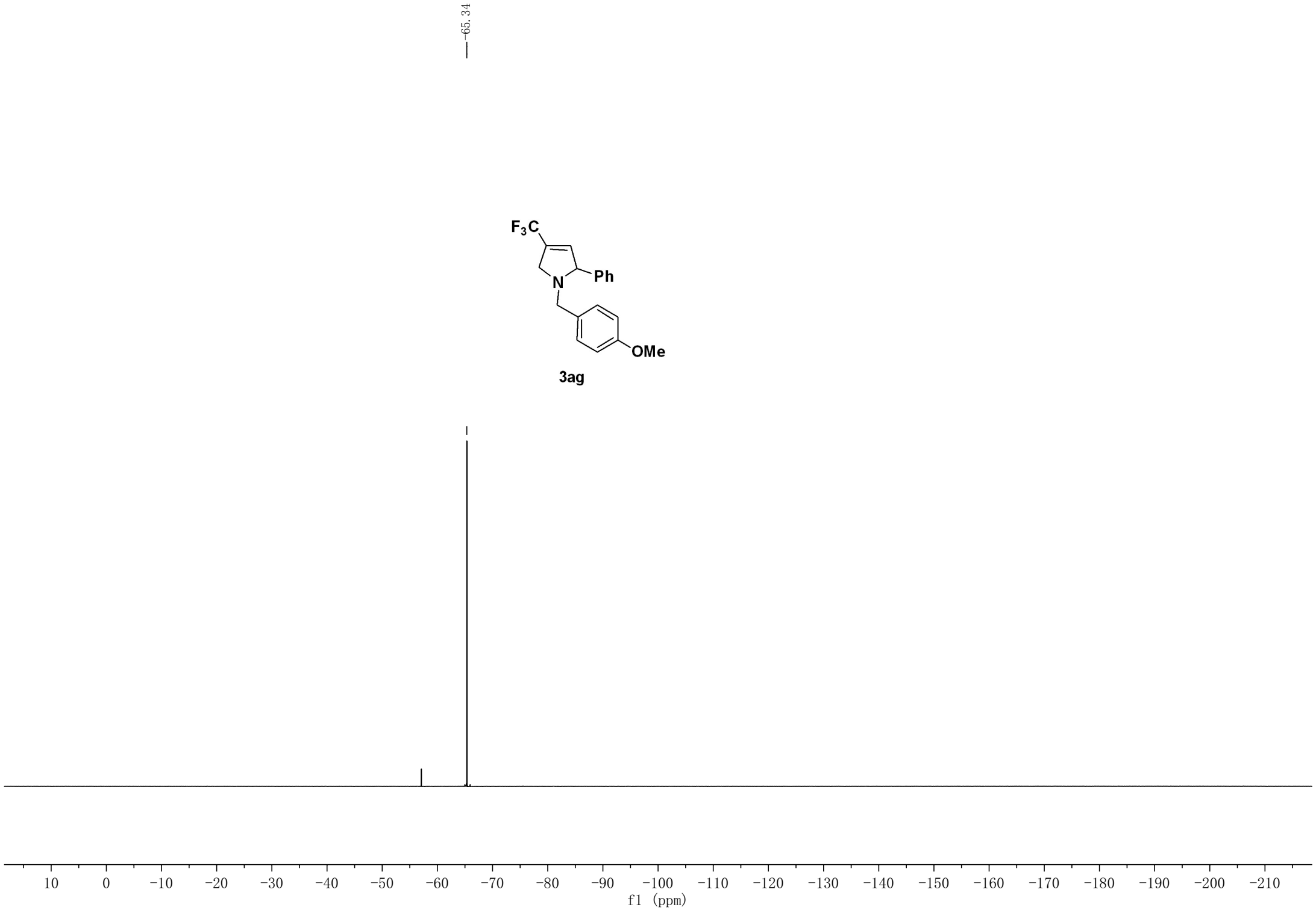
7.36
7.35
7.34
7.33
7.33
7.26
7.23
7.22
6.89
6.87
6.24
4.74
3.94
3.91
3.88
3.87
3.82
3.55
3.54
3.53
3.52
3.50
3.50
F3C
Ph
N
OMe
3ag
2.03
2.05
1.04
2.05
2.03
1.00
1.04
2.14
3.02
2.07
f1 (ppm)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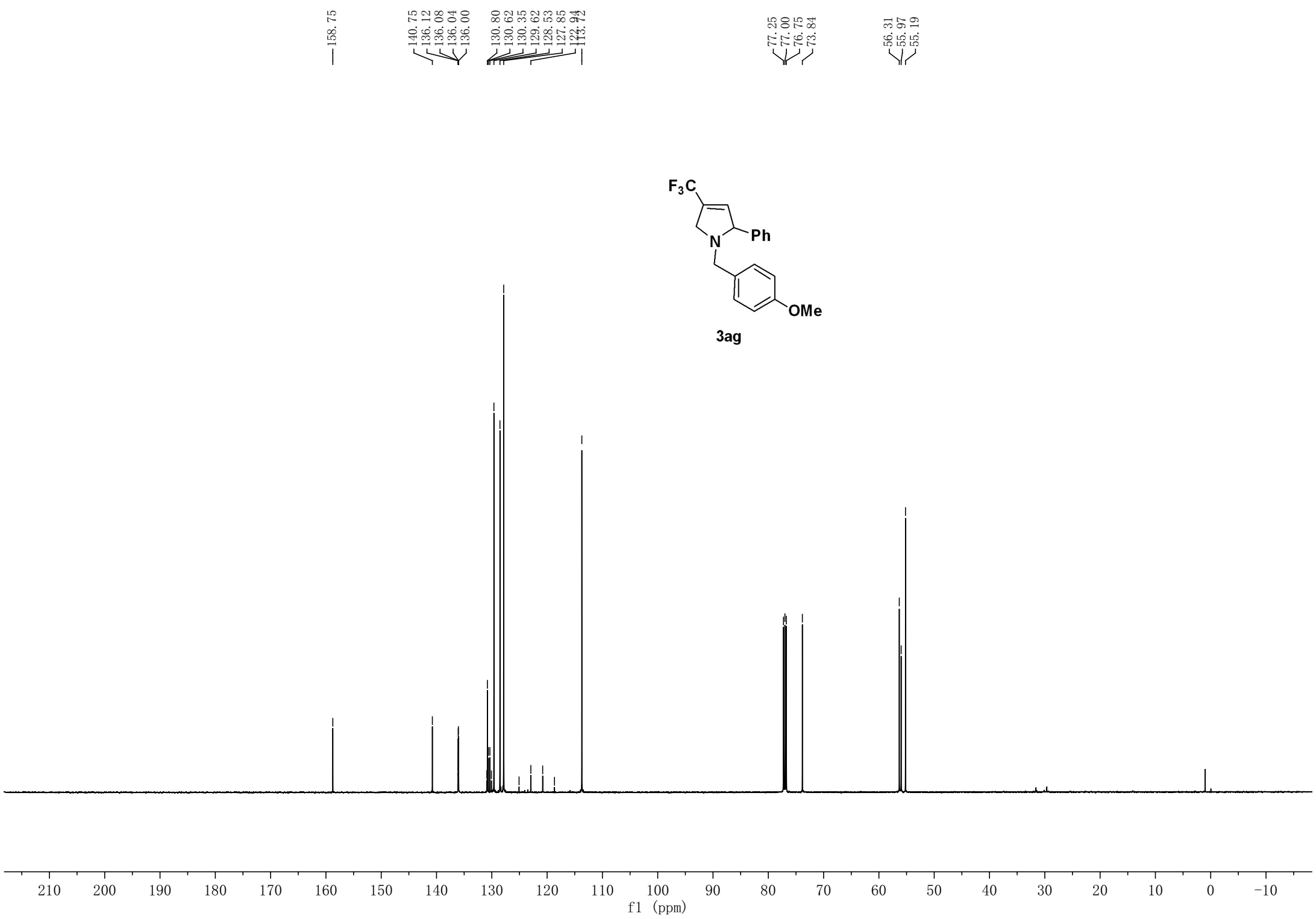
F3C
Ph
N
OMe
3ag
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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130.62
130.35
129.62
128.53
127.85
113.72
77.25
77.00
76.75
73.84
56.31
55.97
55.19
F3C
Ph
N
OMe
3ag
210
200
190
180
170
160
150
140
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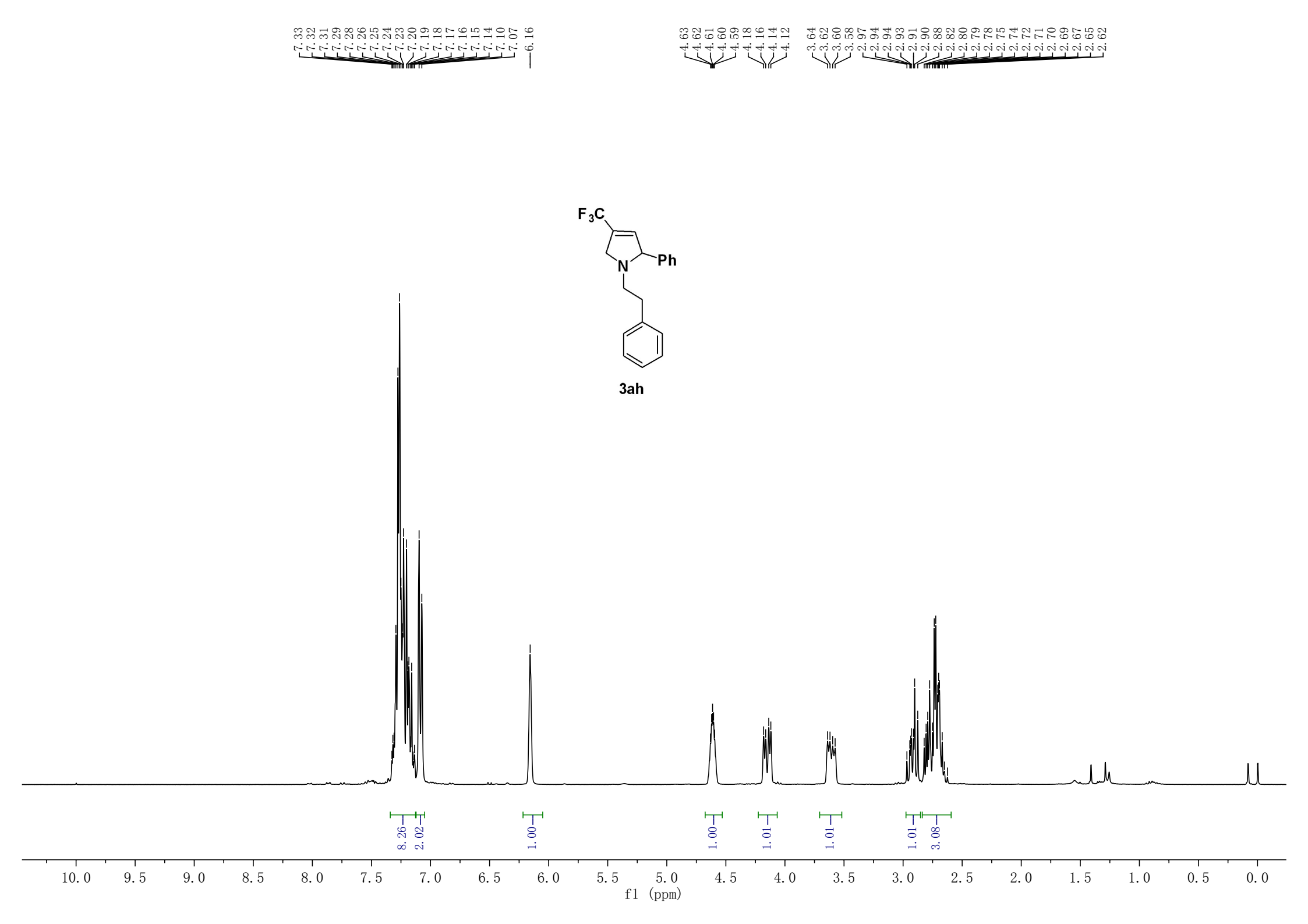
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.17
7.16
7.15
7.14
7.10
7.07
6.16
4.63
4.62
4.61
4.60
4.59
4.18
4.16
4.14
4.12
3.64
3.62
3.60
3.58
2.97
2.94
2.94
2.93
2.91
2.90
2.88
2.82
2.80
2.79
2.78
2.75
2.74
2.72
2.71
2.70
2.69
2.67
2.65
2.62
F3C
Ph
N
3ah
8.26
2.02
1.00
1.00
1.01
1.01
1.01
3.08
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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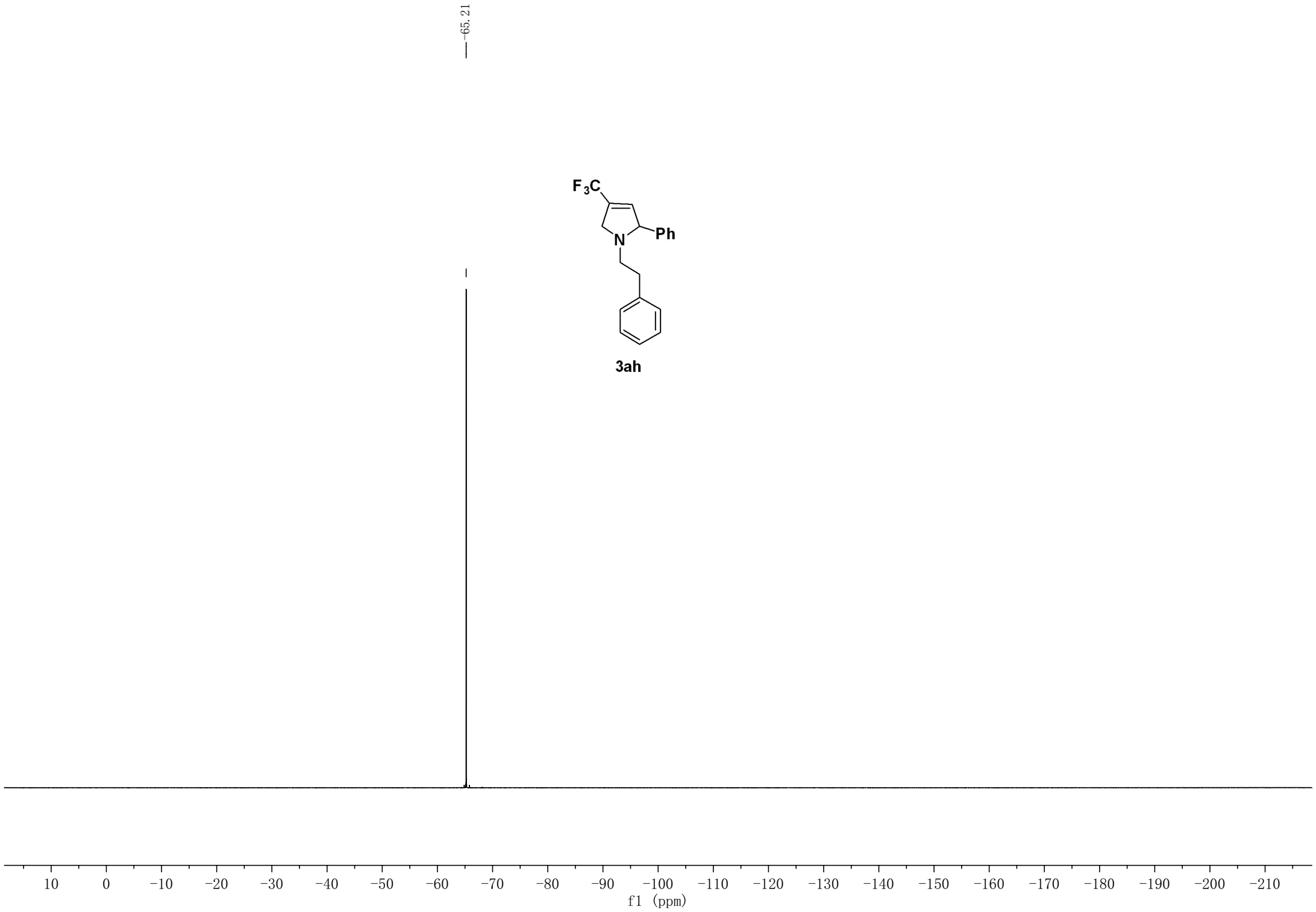
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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Ph
N
3ah
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-10
-20
-30
-40
-50
-60
-70
-80
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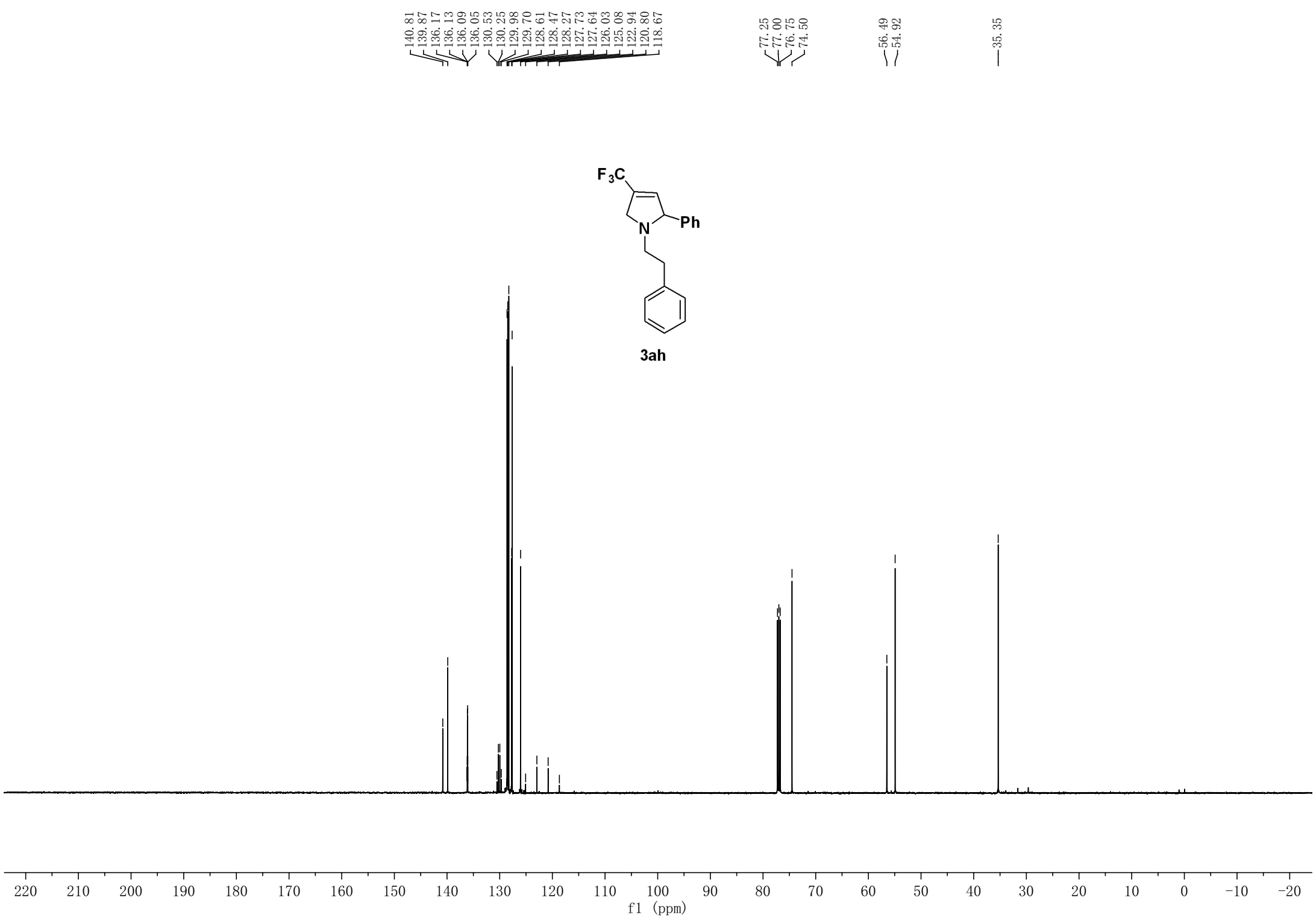
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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130.25
129.98
129.70
128.61
128.47
128.27
127.73
127.64
126.03
125.08
122.94
120.80
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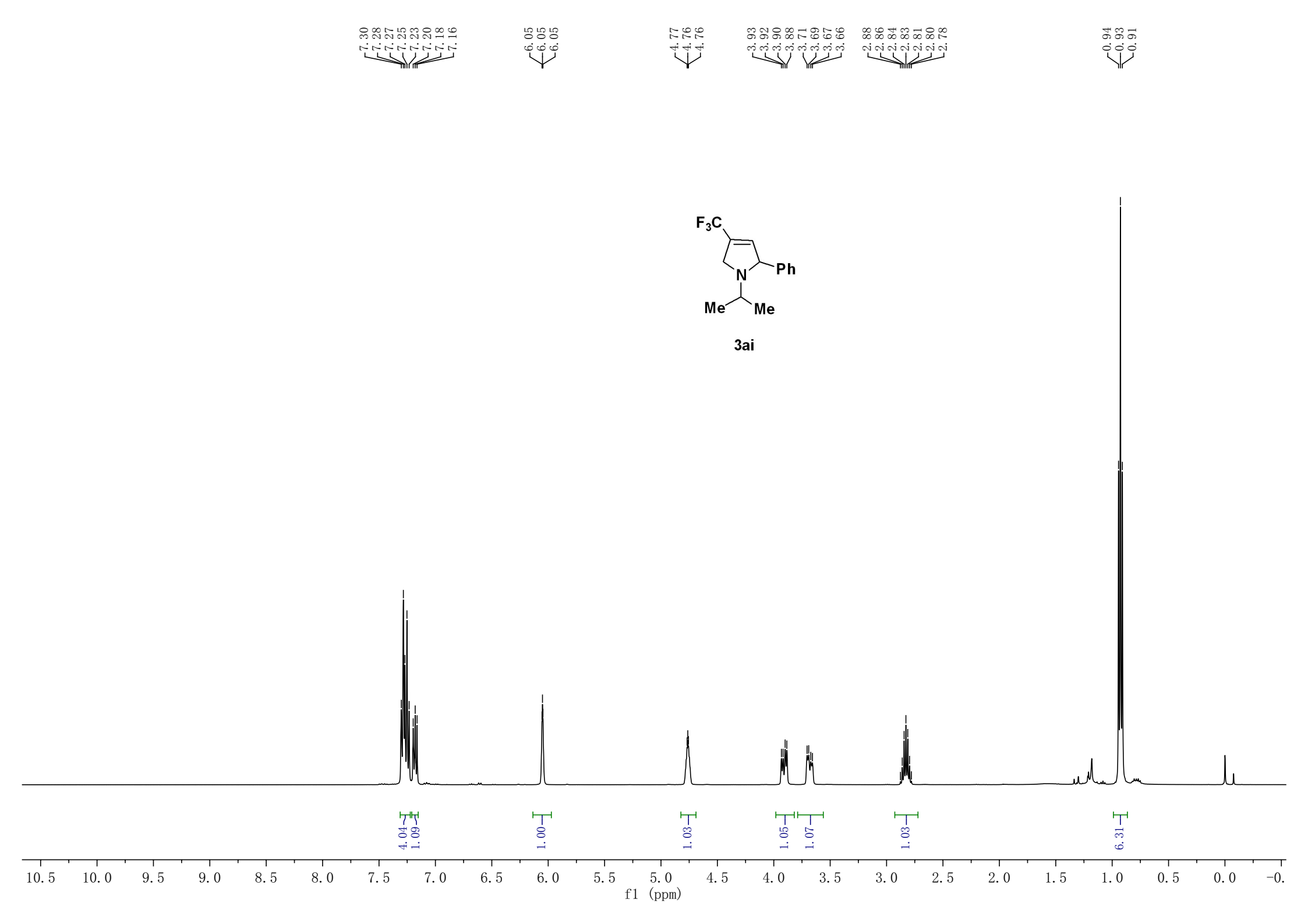
77.00
76.75
74.50
56.49
54.92
35.35
F3C
Ph
N
3ah
f1 (ppm)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7.20
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7.16
6.05
6.05
6.05
4.77
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4.76
3.93
3.92
3.90
3.88
3.71
3.69
3.67
3.66
2.88
2.86
2.84
2.83
2.81
2.80
2.78
0.94
0.93
0.91
F3C
Ph
N
Me
Me
3ai
4.04
1.09
1.00
1.03
1.05
1.07
1.03
6.31
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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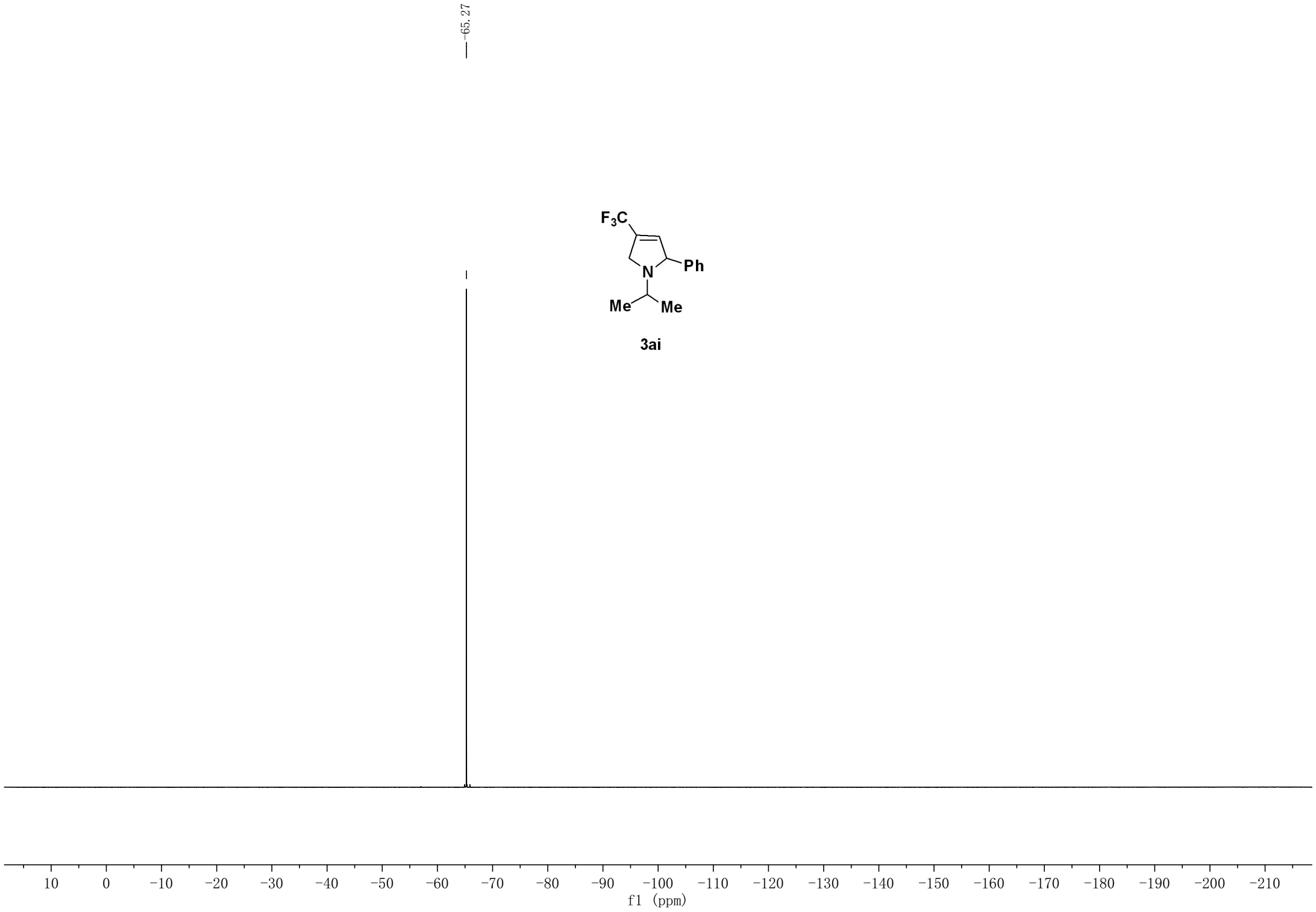
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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F3C
Ph
N
Me
Me
3ai
10
0
-10
-20
-30
-40
-50
-60
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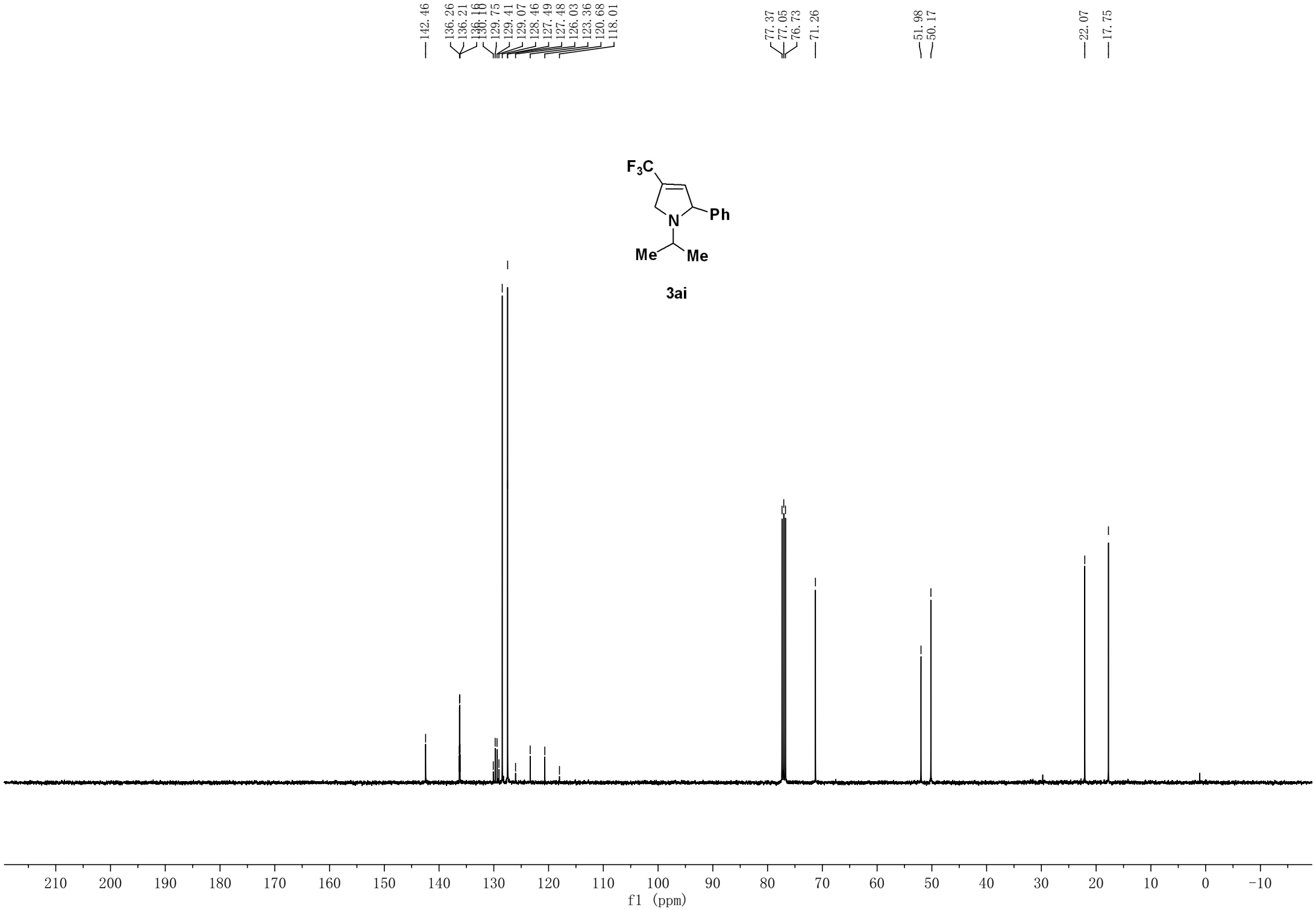
-170
-180
-190
-200
-210
f1 (ppm)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129.41
129.07
128.46
127.49
127.48
126.03
123.36
120.68
118.01
77.37
77.05
76.73
71.26
51.98
50.17
22.07
17.75
F3C
Ph
N
Me
Me
3ai
210
200
190
180
170
160
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140
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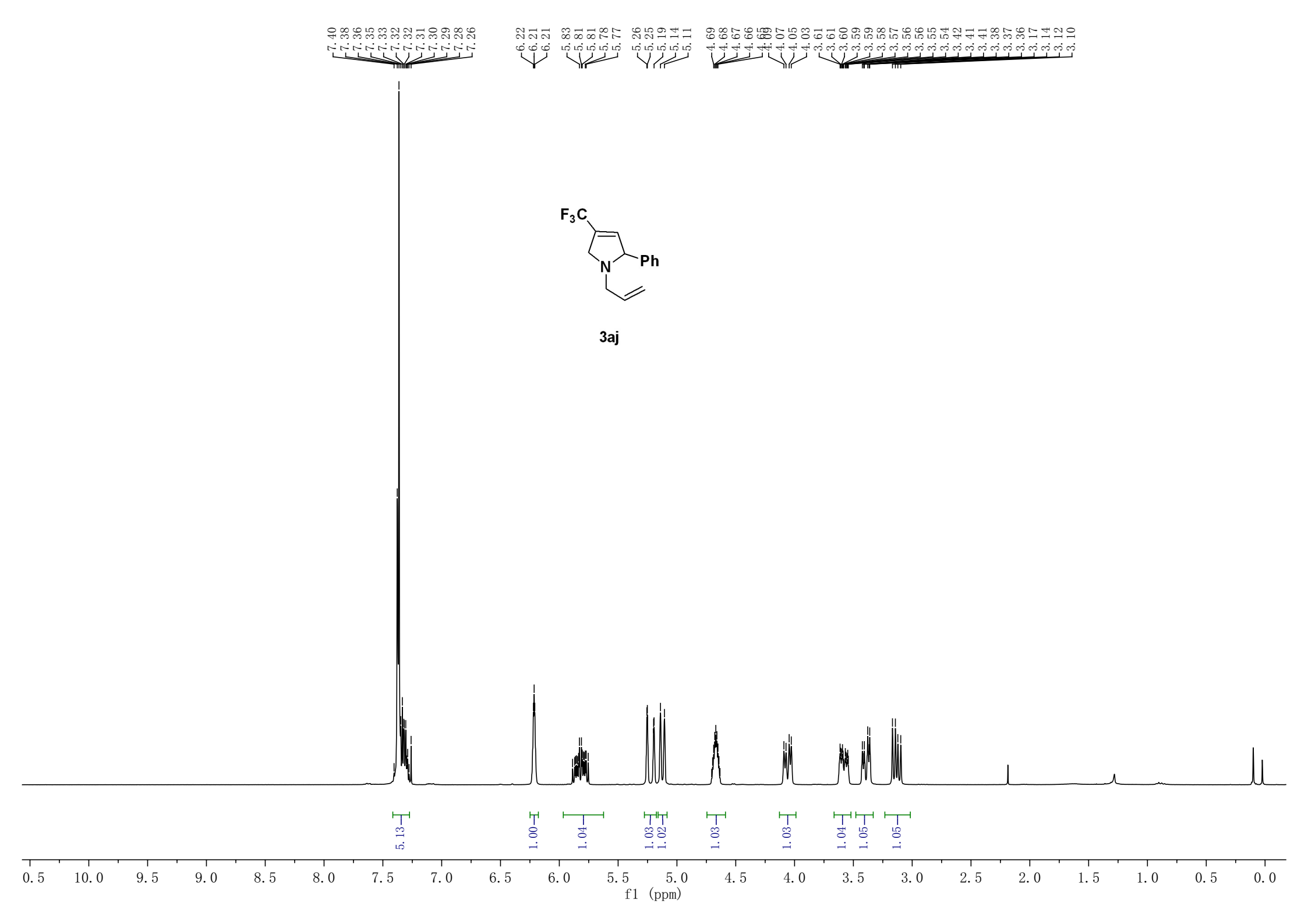
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.32
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7.31
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7.26
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6.21
6.21
5.83
5.81
5.81
5.78
5.77
5.26
5.25
5.19
5.14
5.11
4.69
4.68
4.67
4.66
4.07
4.05
4.03
3.61
3.61
3.60
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3.59
3.58
3.57
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3.56
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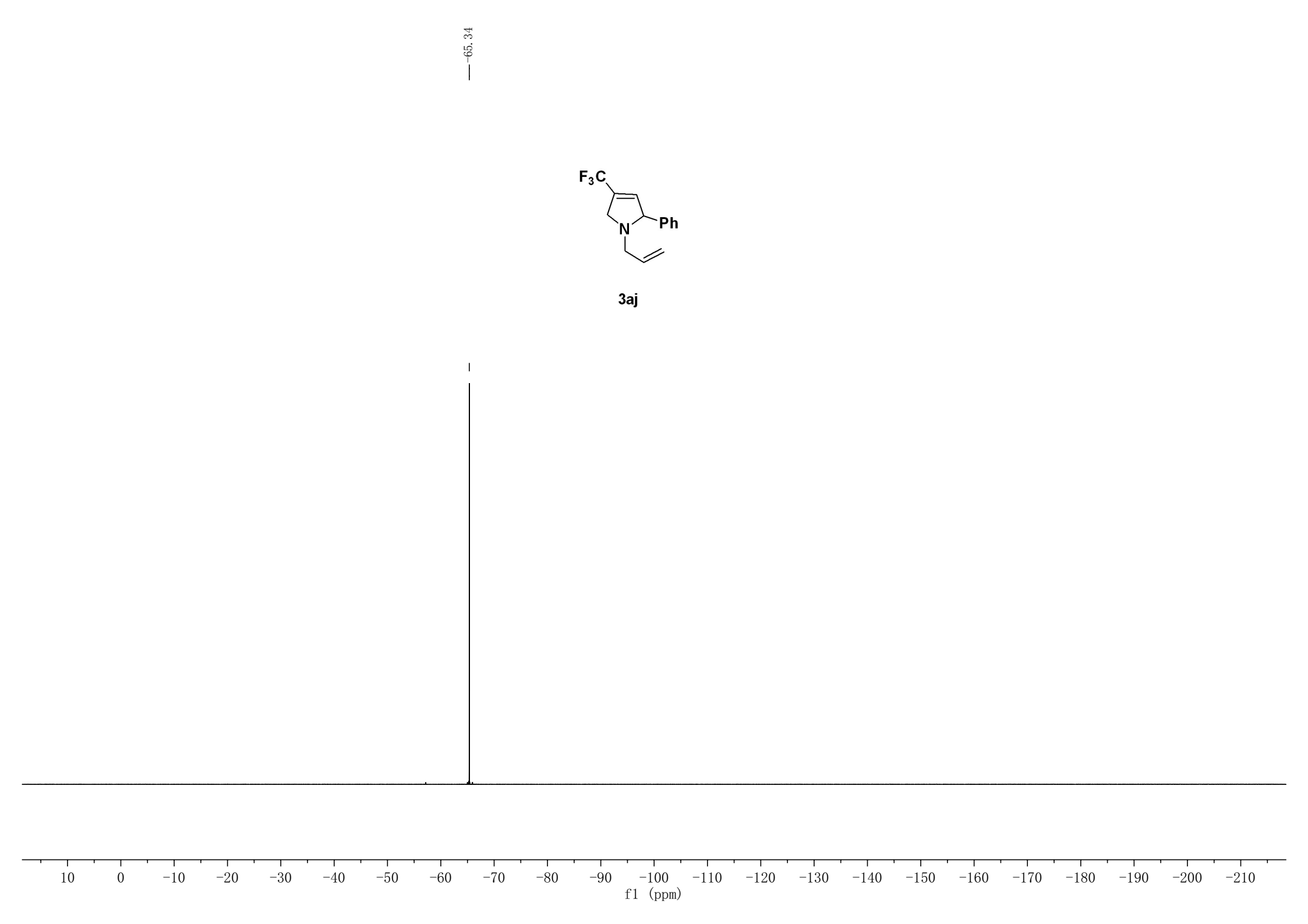
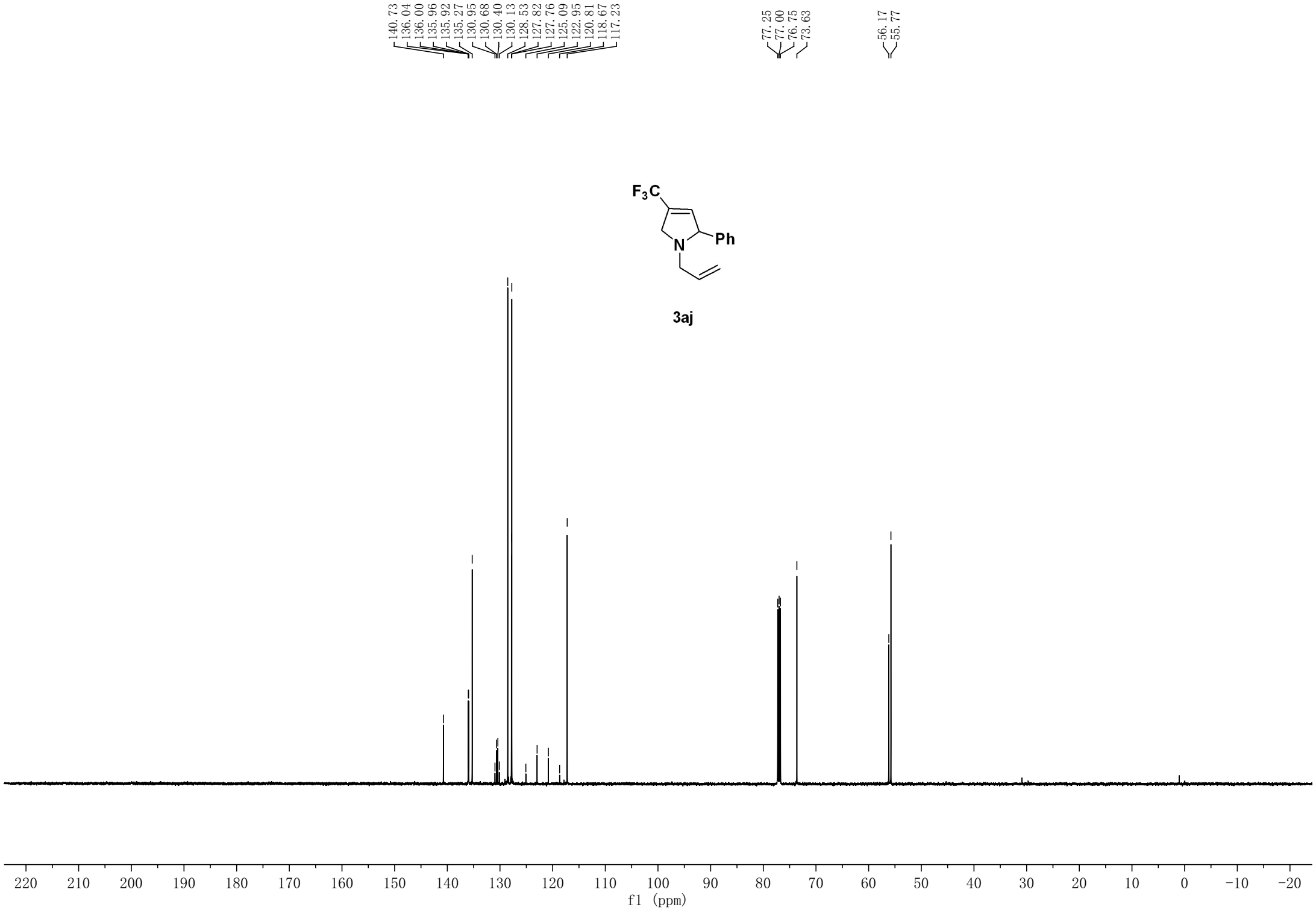
3.41
3.41
3.38
3.37
3.36
3.17
3.14
3.12
3.10
F3C
Ph
N
3aj
5.13
1.00
1.04
1.03
1.02
1.03
1.03
1.04
1.05
1.05
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.34
F3C
Ph
N
3aj
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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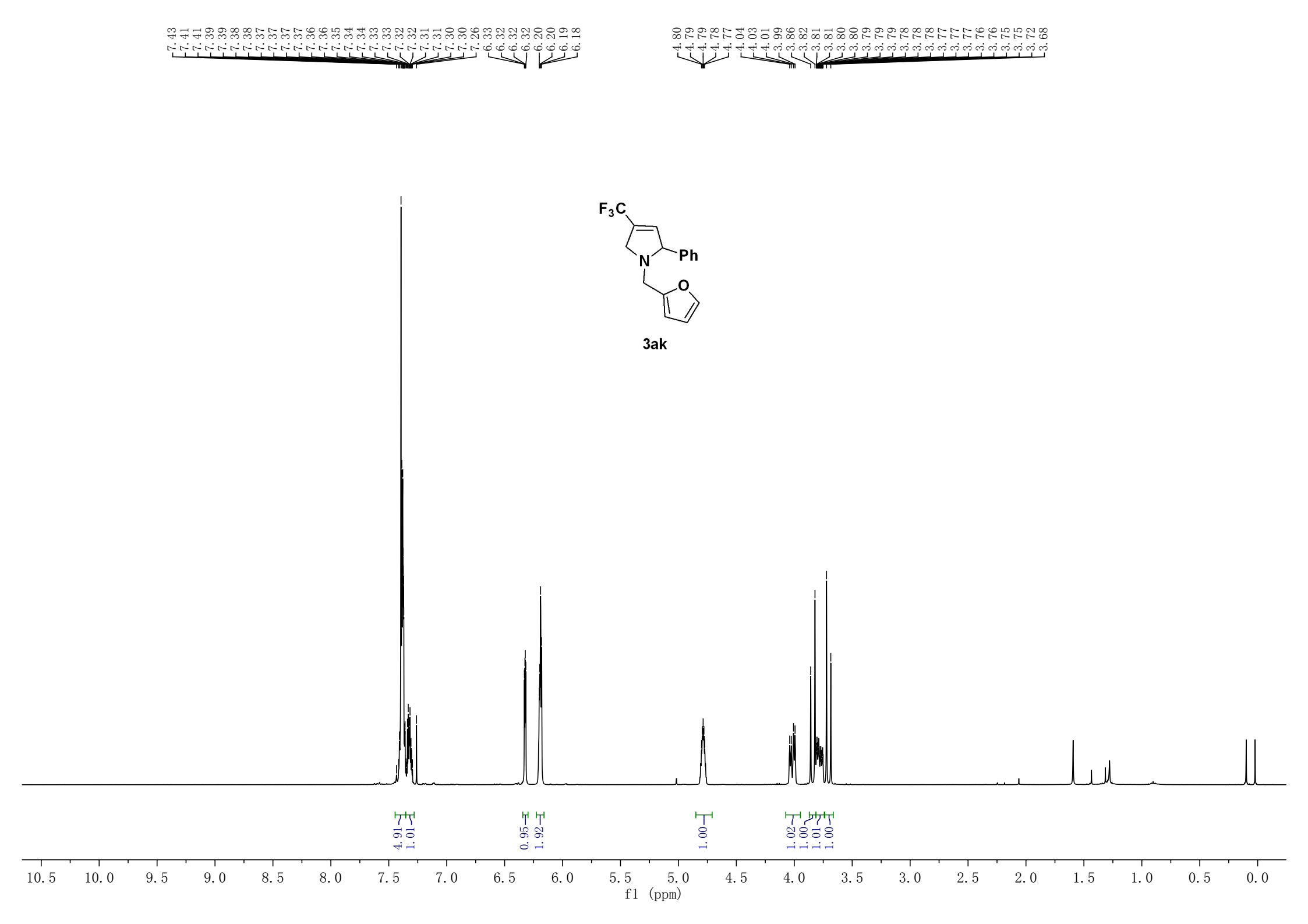
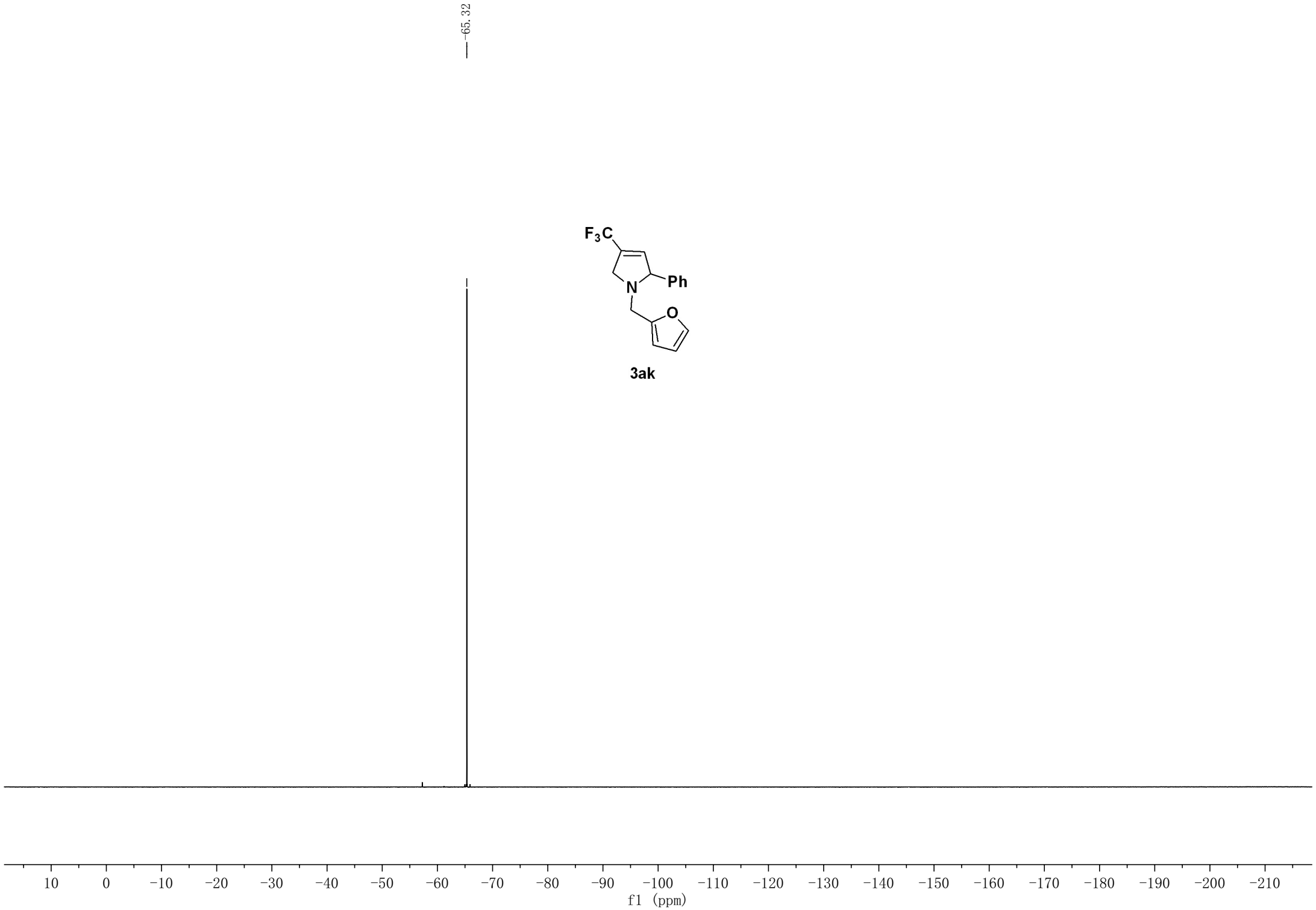
136.00
135.96
135.92
135.27
130.95
130.68
130.40
130.13
128.53
127.82
127.76
125.09
122.95
120.81
118.67
117.23
77.25
77.00
76.75
73.63
56.17
55.77
F3C
Ph
N
3aj
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


7.43 7.41 7.41 7.39 7.39 7.38 7.38 7.37 7.37 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.26 6.33 6.32 6.32 6.32 6.20 6.20 6.19 6.18
4.80 4.79 4.79 4.78 4.77 4.04 4.03 4.01 3.99 3.86 3.82 3.81 3.81 3.80 3.80 3.79 3.79 3.79 3.78 3.78 3.78 3.77 3.77 3.77 3.76 3.76 3.75 3.75 3.72 3.68
F3C
Ph
N
O
3ak
4.91 1.01 0.95 1.92 1.00 1.02 1.00 1.01 1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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Ph
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O
3ak
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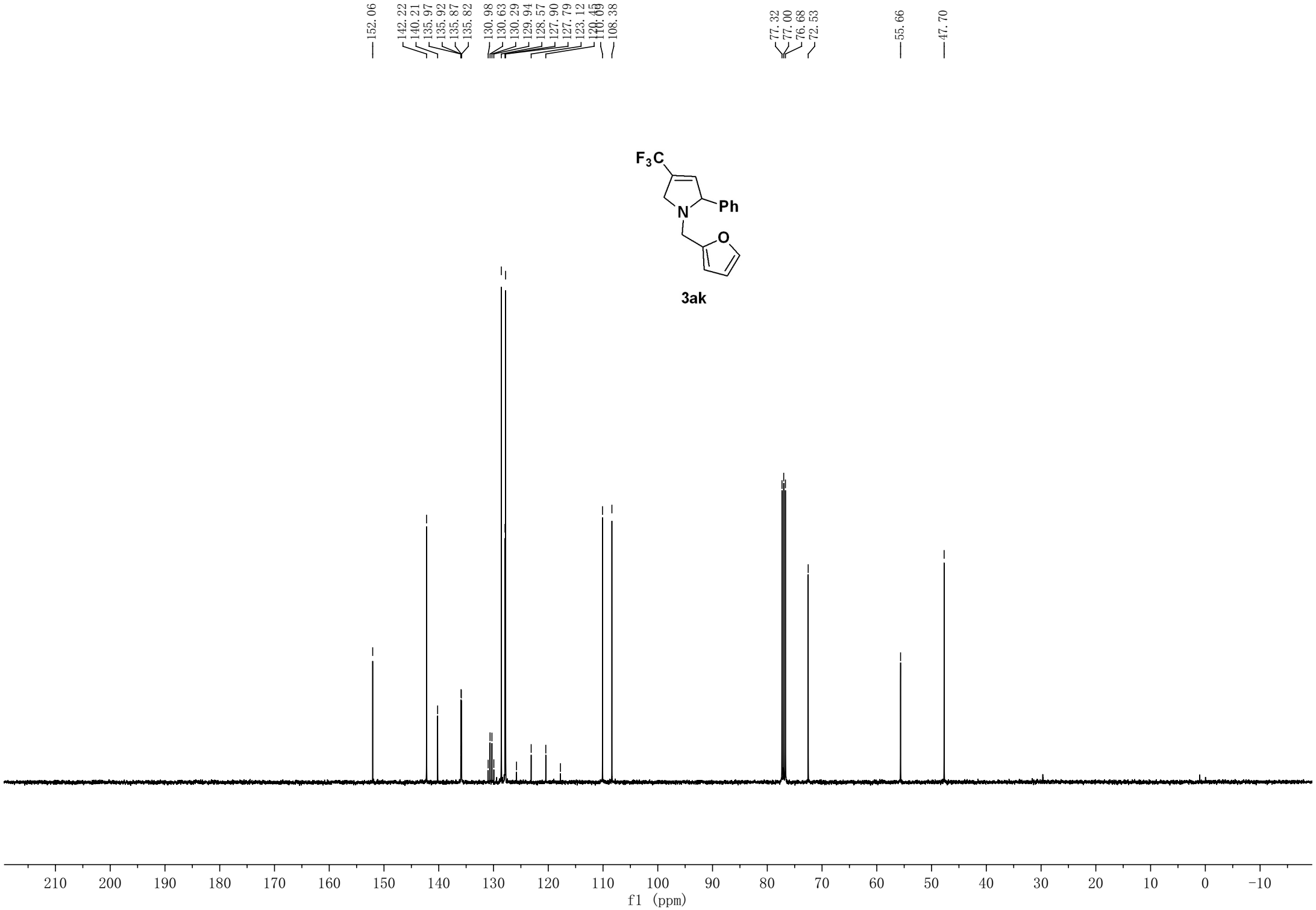
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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135.87
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130.98
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130.29
129.94
128.57
127.90
127.79
123.12
120.45
110.09
108.38
77.32
77.00
76.68
72.53
55.66
47.70
F3C
Ph
N
O
3ak
210
200
190
180
170
160
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140
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120
110
100
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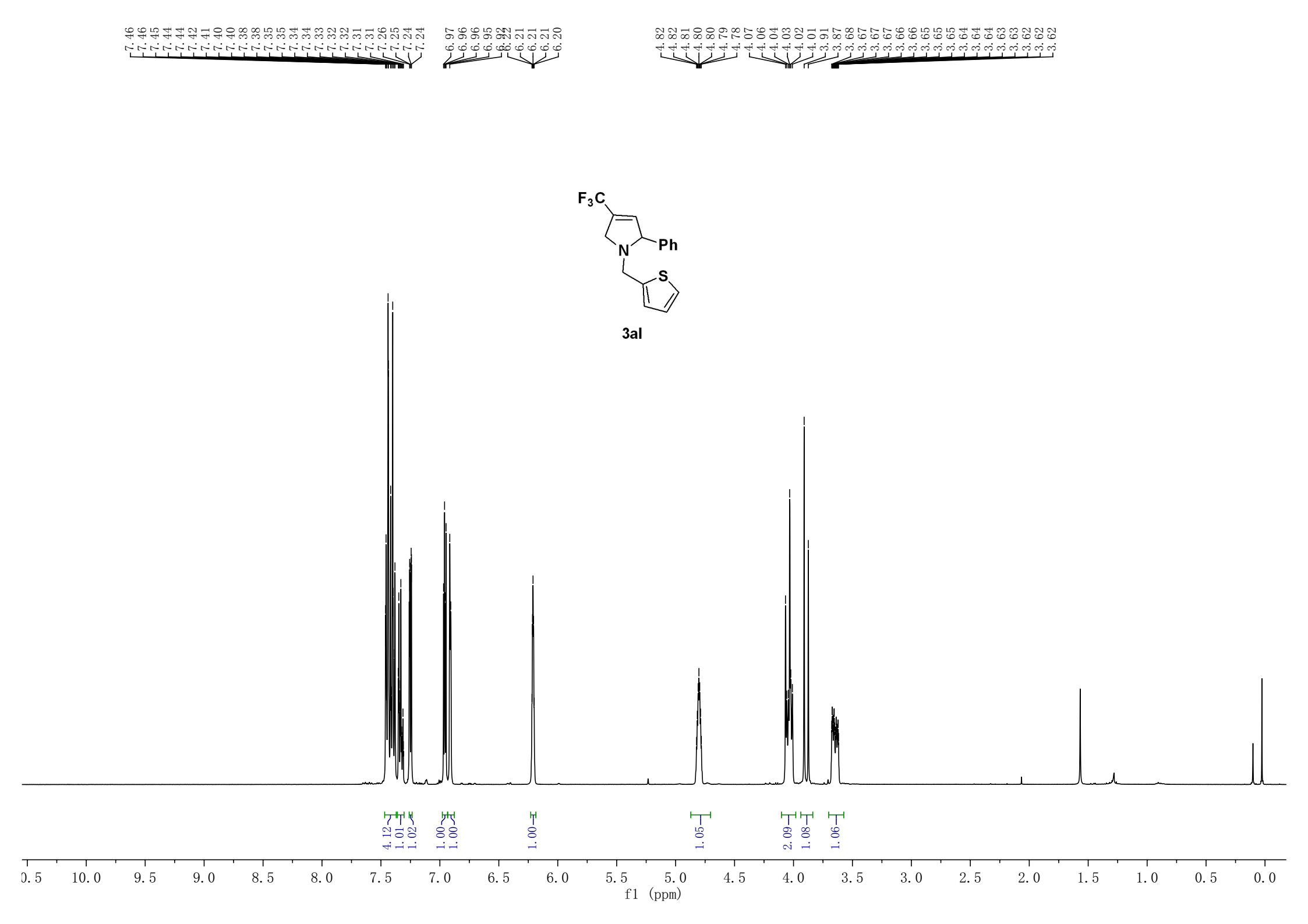
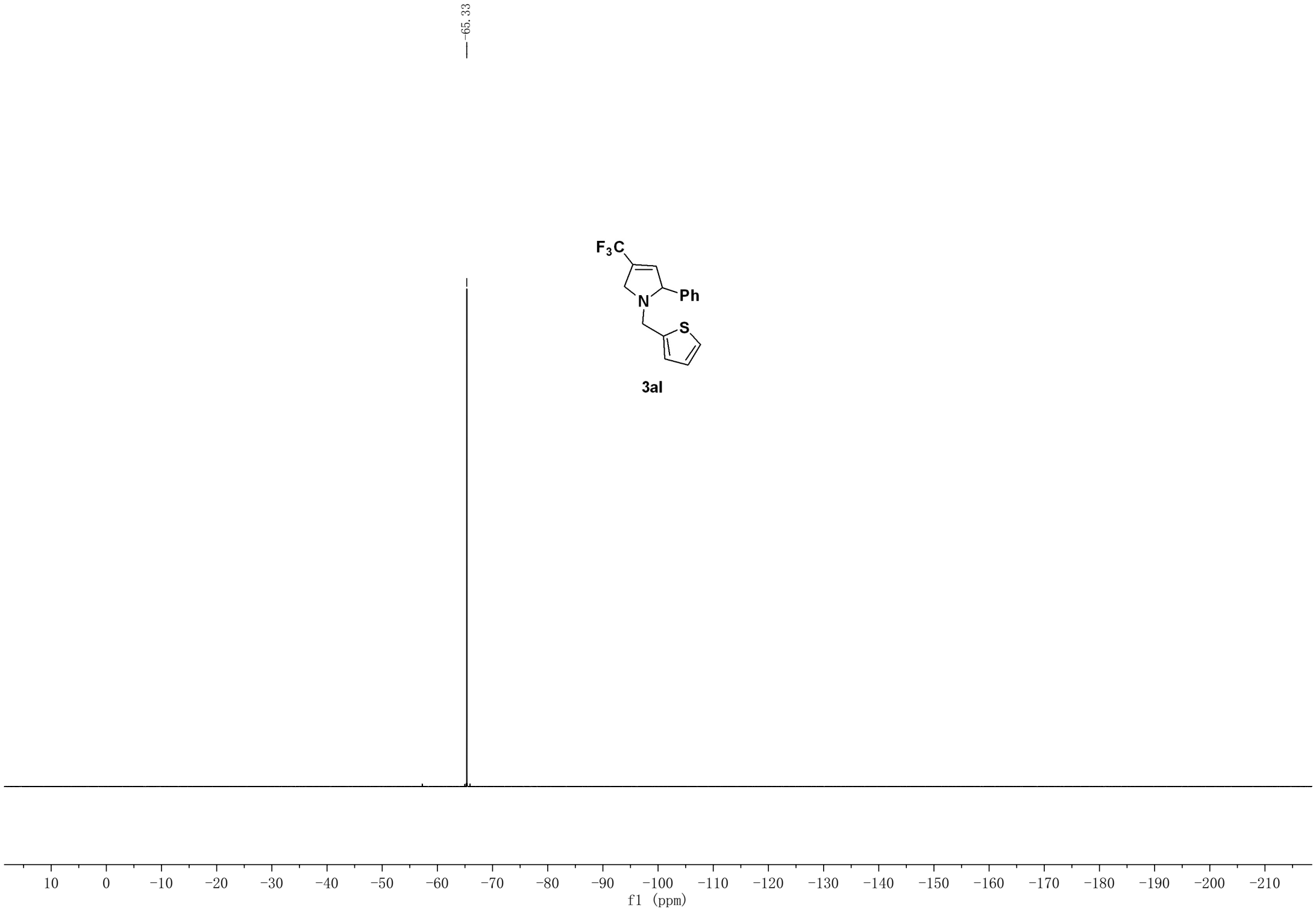
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.46 7.46 7.45 7.44 7.44 7.42 7.41 7.40 7.40 7.38 7.38 7.35 7.35 7.34 7.34 7.33 7.32 7.31 7.31 7.26 7.25 7.24 7.24
6.97 6.96 6.96 6.95 6.22 6.21 6.21 6.21 6.20
4.82 4.82 4.81 4.80 4.80 4.79 4.78 4.07 4.06 4.04 4.03 4.02 4.01 3.91 3.87 3.68 3.67 3.67 3.67 3.66 3.66 3.65 3.65 3.65 3.64 3.64 3.64 3.63 3.63 3.62 3.62 3.62
F3C
Ph
N
S
3al
4.12 1.01 1.02 1.00 1.00 1.00 1.05 2.09 1.08 1.06
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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F3C
Ph
N
S
3al
10
0
-10
-20
-30
-40
-50
-60
-70
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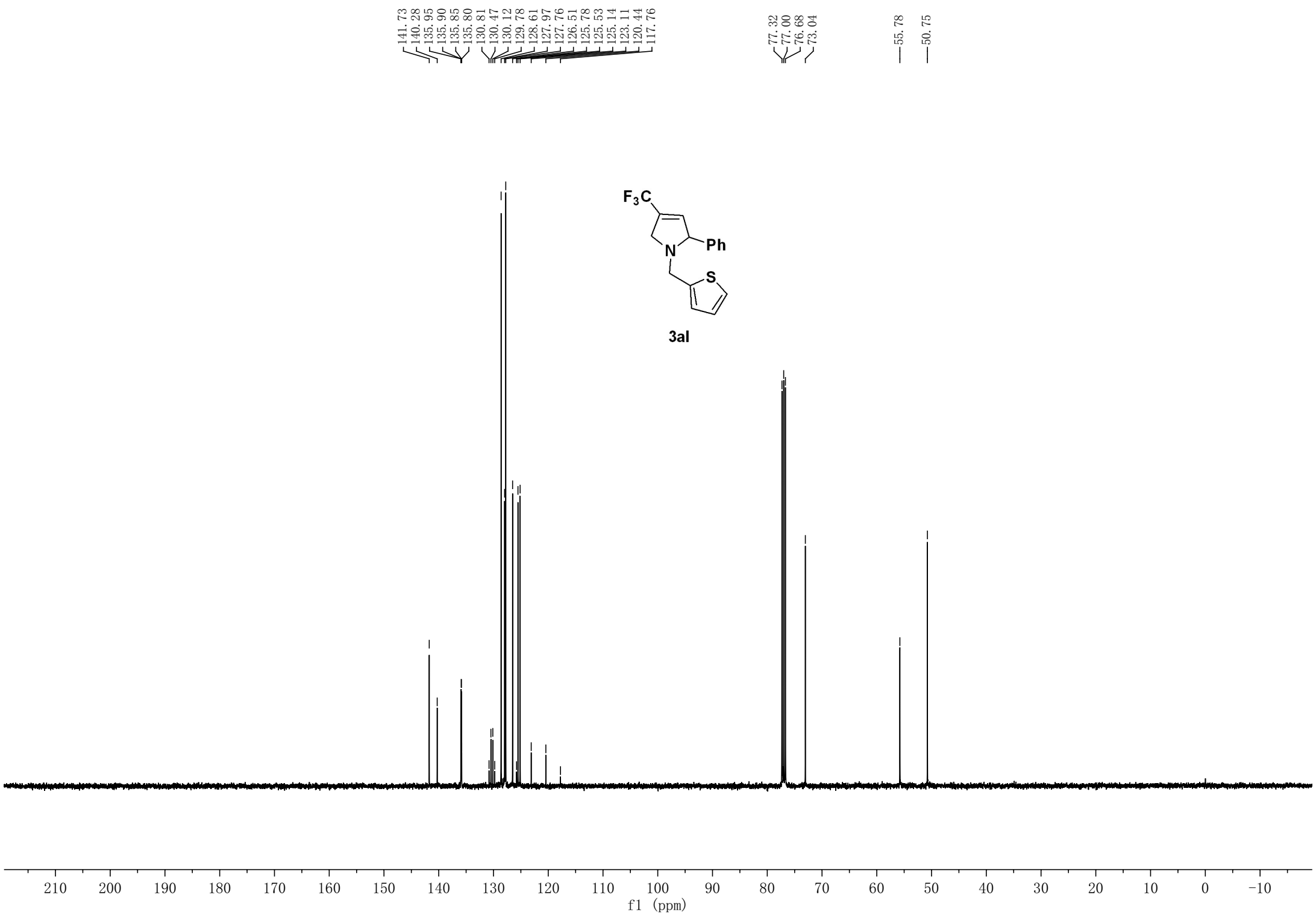
-170
-180
-190
-200
-210
f1 (ppm)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135.85
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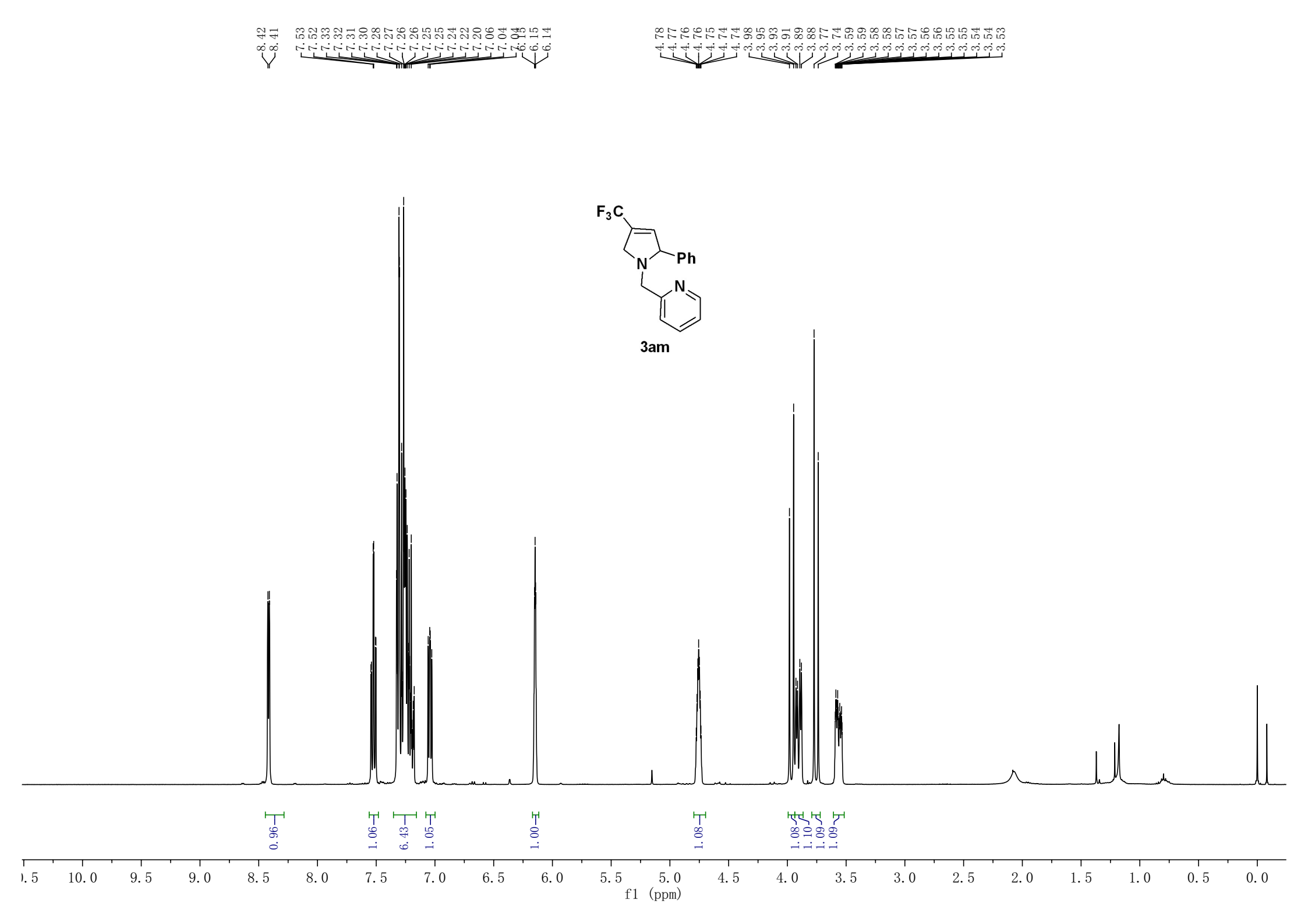
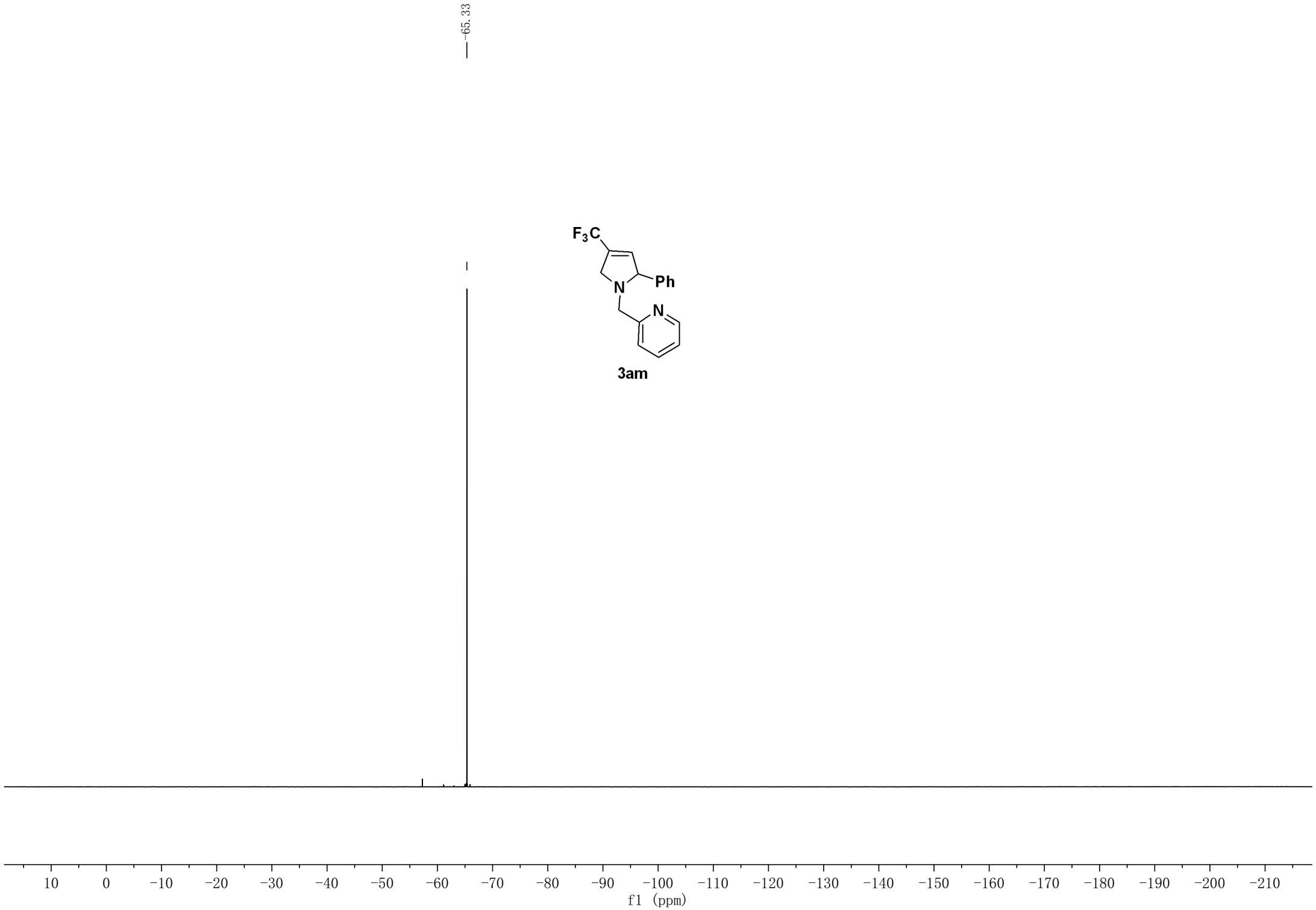
130.47
130.12
129.78
128.61
127.97
127.76
126.51
125.78
125.53
125.14
123.11
120.44
117.76
77.32
77.00
76.68
73.04
55.78
50.75
F3C
Ph
N
S
3al
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.42
8.41
7.53
7.52
7.33
7.32
7.31
7.30
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.22
7.20
7.06
7.04
6.15
6.14
4.78
4.77
4.76
4.76
4.75
4.74
4.74
3.98
3.95
3.93
3.91
3.89
3.88
3.77
3.74
3.59
3.59
3.58
3.58
3.57
3.57
3.56
3.56
3.55
3.55
3.54
3.54
3.53
F3C
Ph
N
N
3am
0.96
1.06
6.43
1.05
1.00
1.08
1.08
1.10
1.09
1.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.33
F3C
Ph
N
N
3am
10
0
-10
-20
-30
-40
-50
-60
-70
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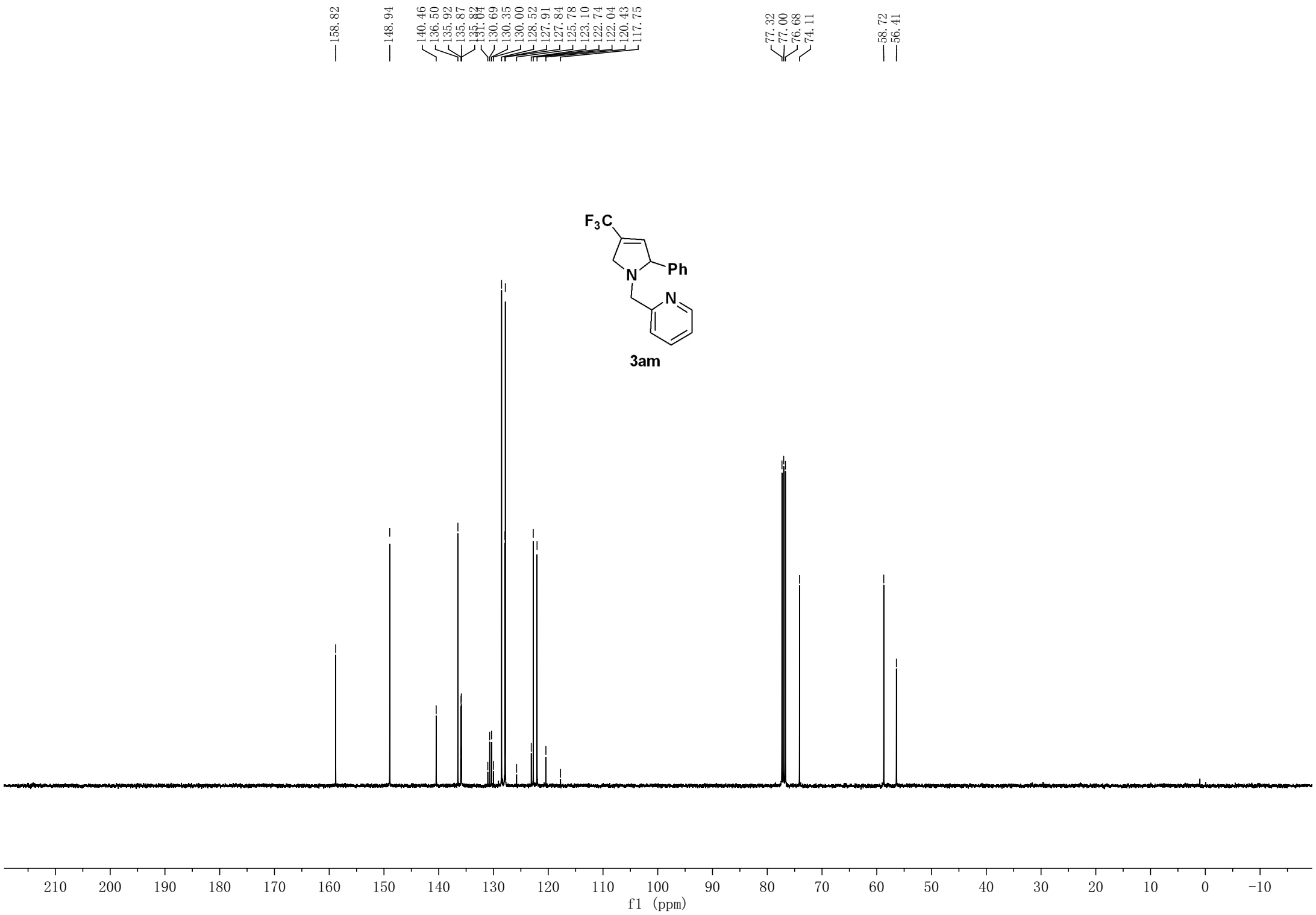
-170
-180
-190
-200
-210
f1 (ppm)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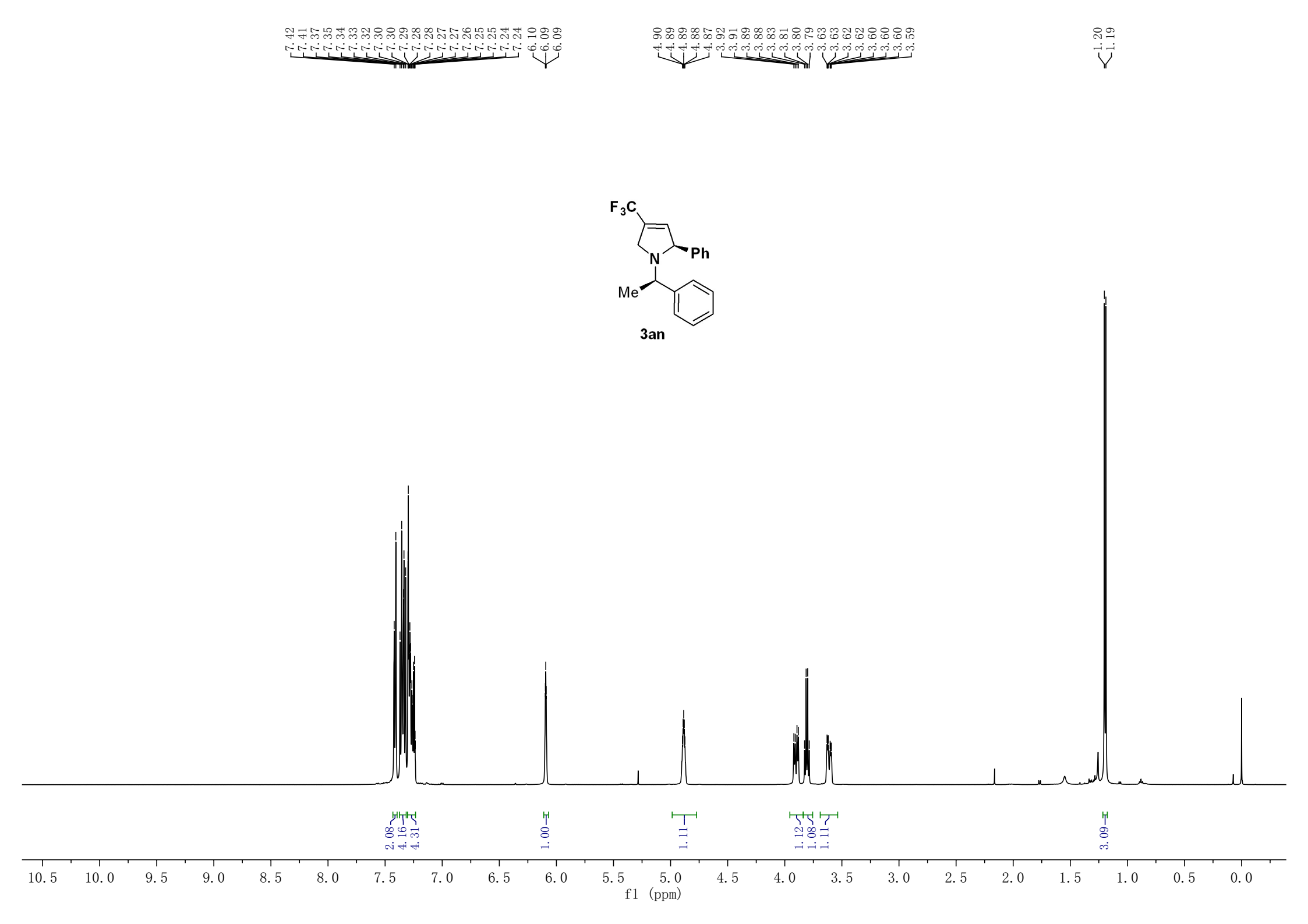
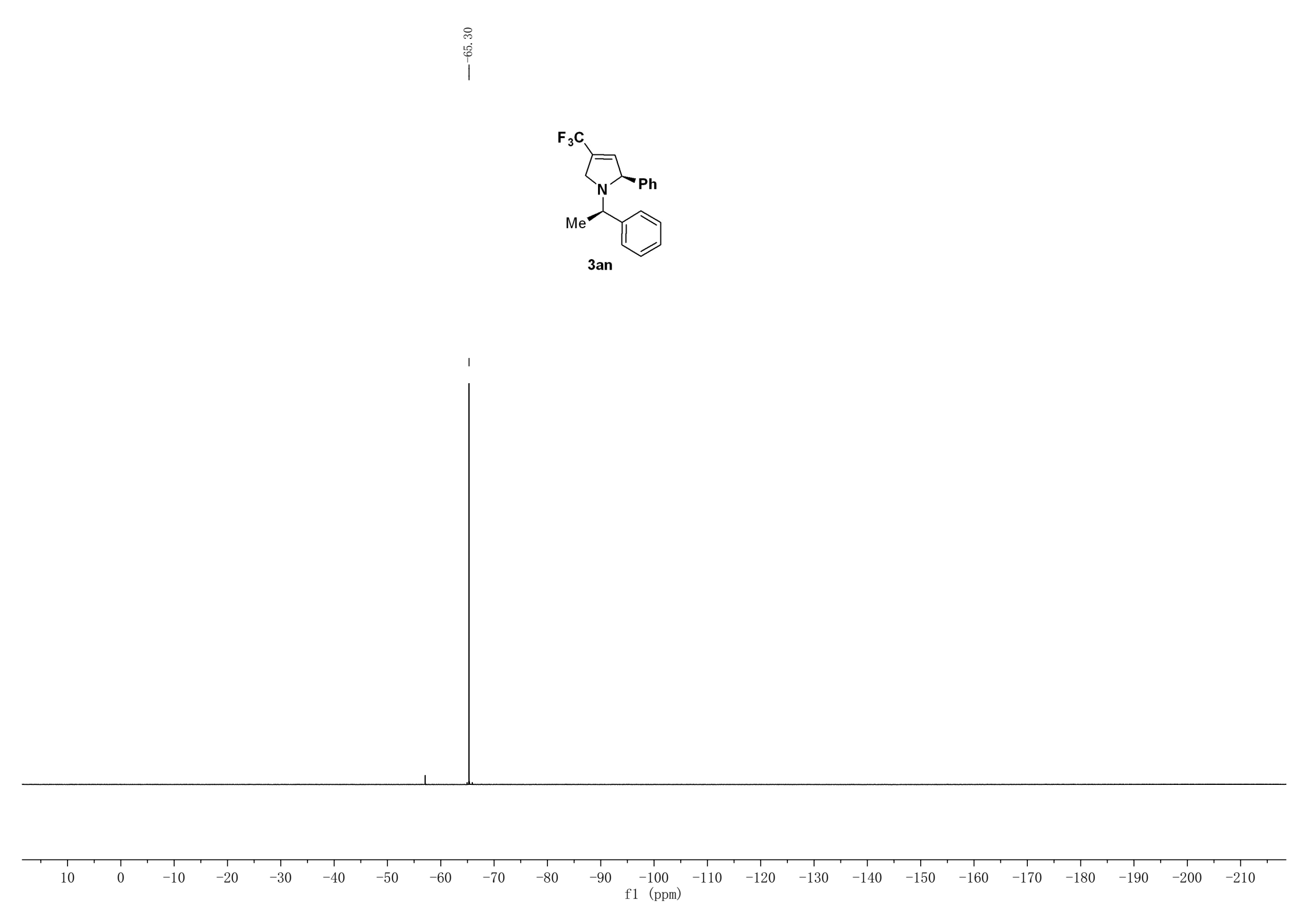
135.87
131.04
130.69
130.35
130.00
128.52
127.91
127.84
125.78
123.10
122.74
122.04
120.43
117.75
77.32
77.00
76.68
74.11
58.72
56.41
F3C
Ph
N
N
3am
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.42
7.41
7.37
7.35
7.34
7.33
7.32
7.30
7.30
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.24
6.10
6.09
6.09
4.90
4.89
4.89
4.88
4.87
3.92
3.91
3.89
3.88
3.83
3.81
3.80
3.79
3.63
3.63
3.62
3.62
3.60
3.60
3.60
3.59
1.20
1.19
F3C
Ph
N
Me
3an
2.08
4.16
4.31
1.00
1.11
1.12
1.08
1.11
3.09
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.30
F3C
N
Ph
Me
3an
10
0
-10
-20
-30
-40
-50
-60
-70
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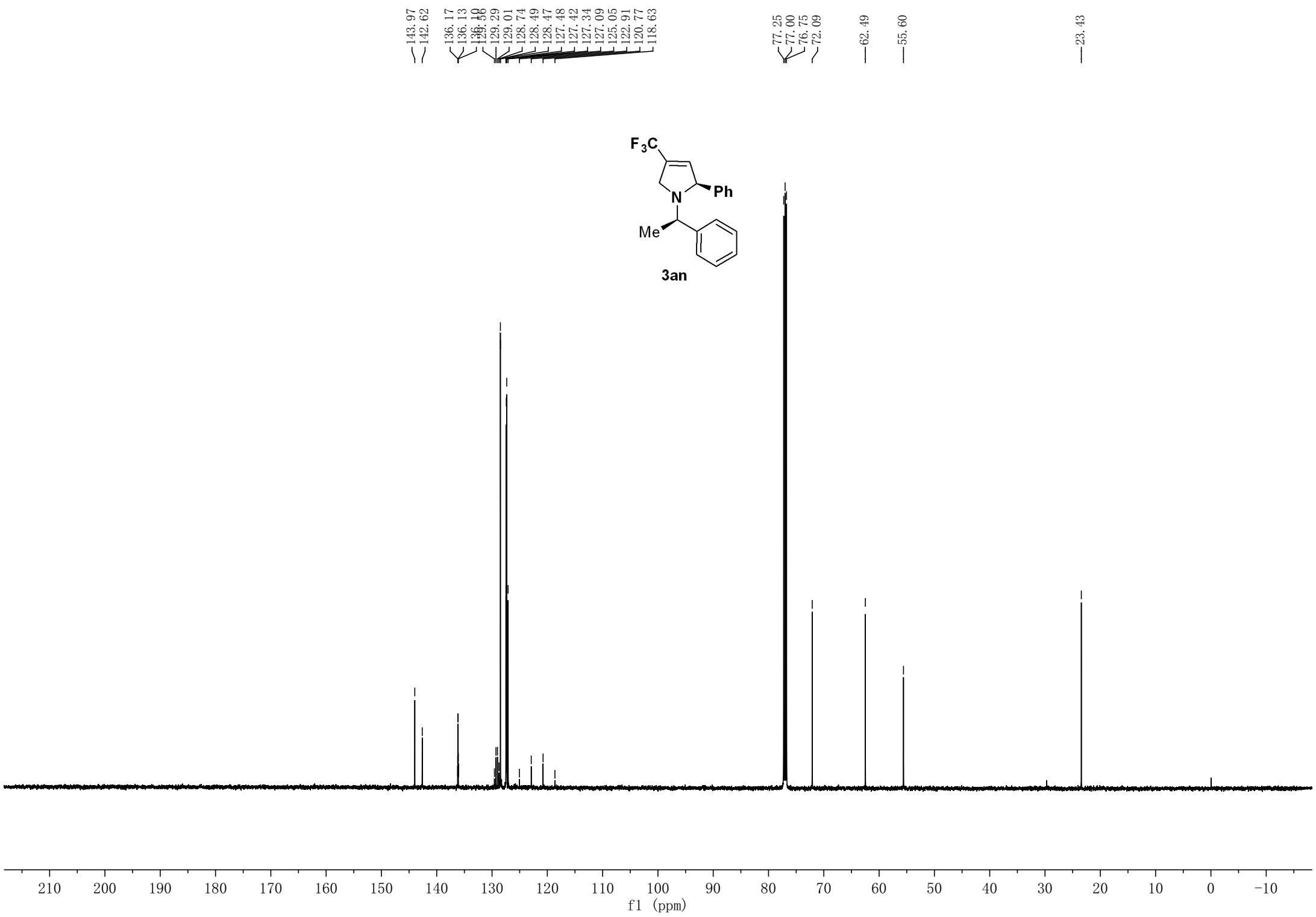
-170
-180
-190
-200
-210
f1 (ppm)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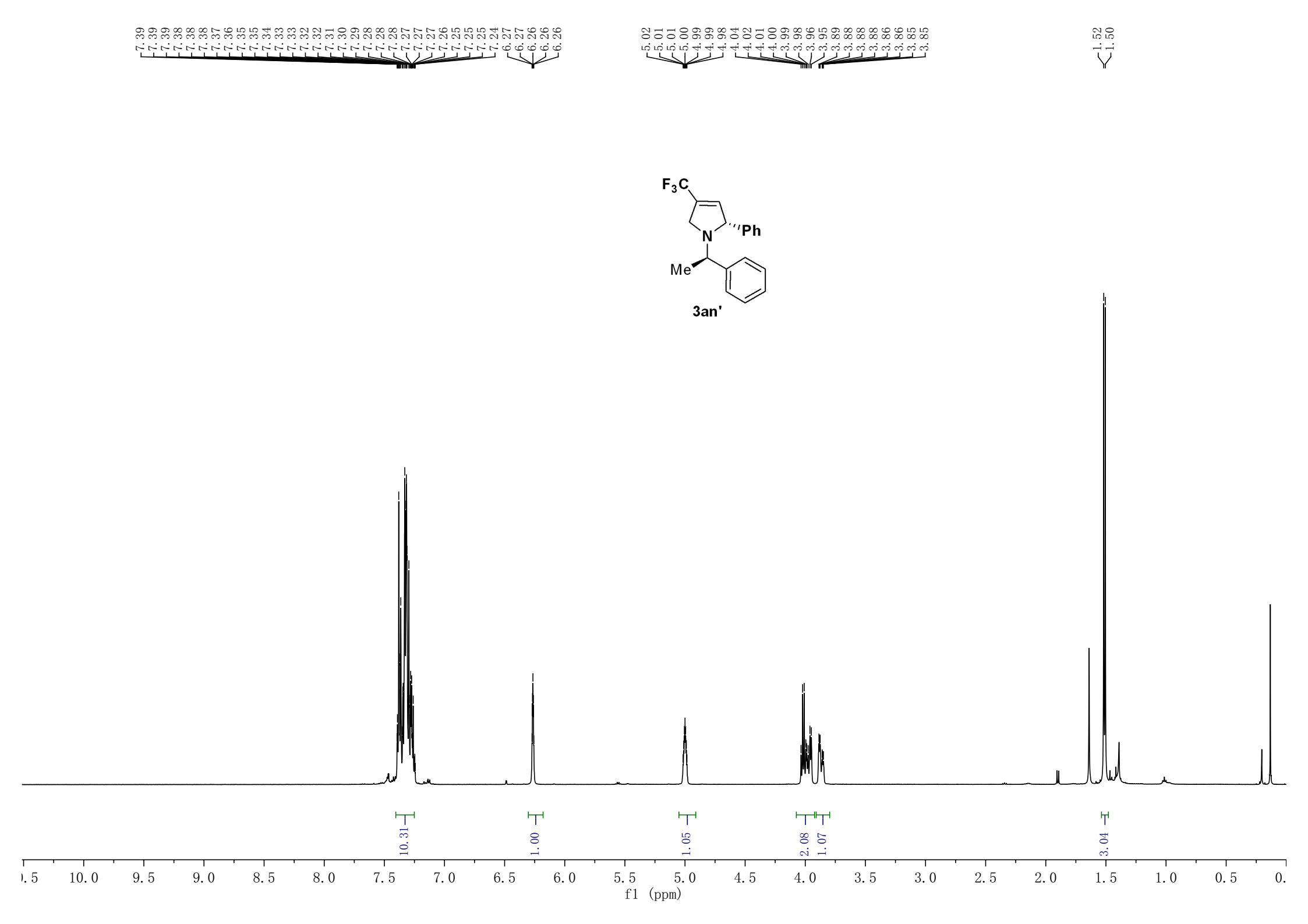
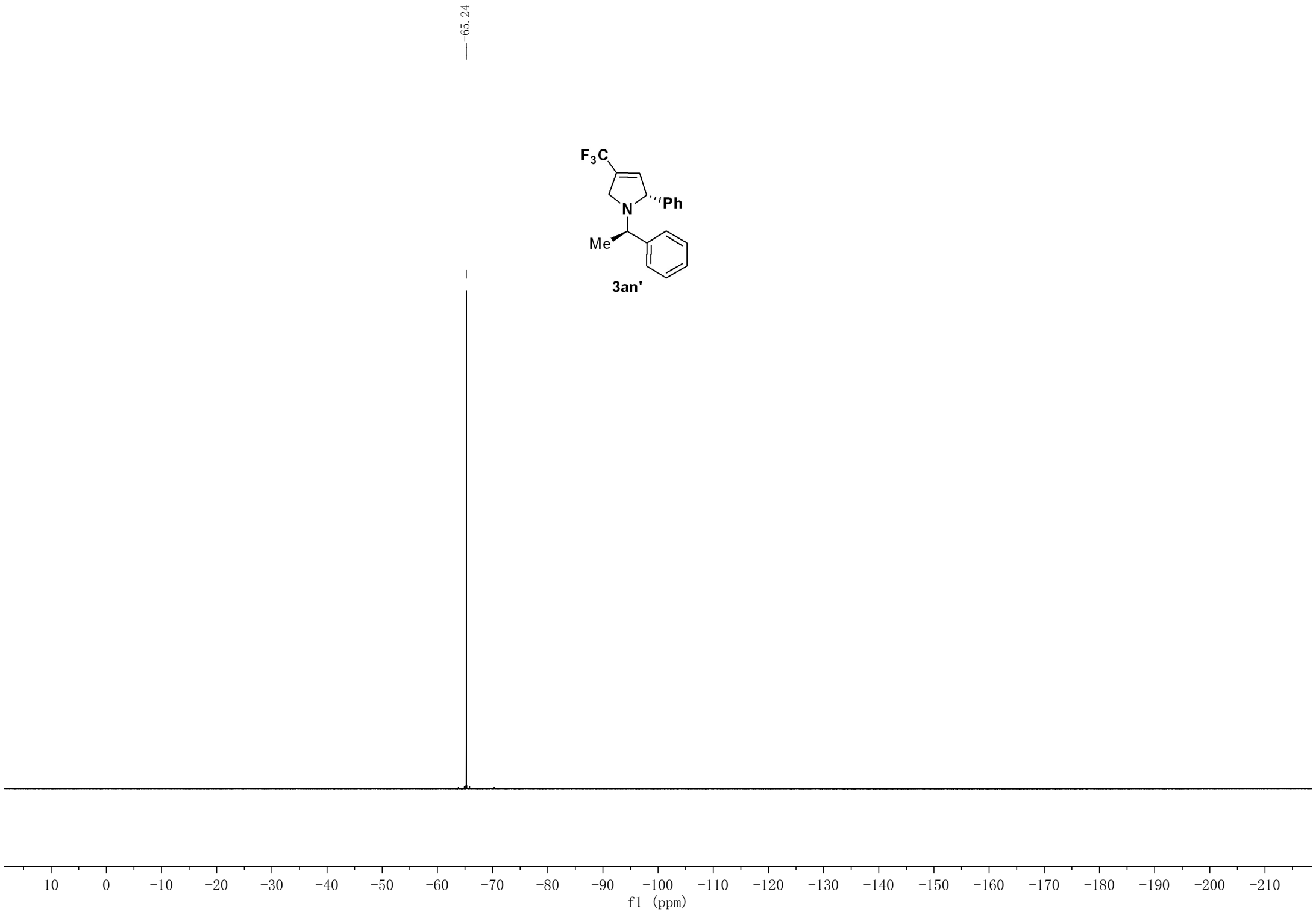
129.01
128.74
128.49
128.47
127.48
127.42
127.34
127.09
125.05
122.91
120.77
118.63
77.25
77.00
76.75
72.09
62.49
55.60
23.43
F3C
Ph
N
Me
3an
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.39 7.39 7.39 7.38 7.38 7.38 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.30 7.29 7.28 7.28 7.28 7.27 7.27 7.27 7.26 7.25 7.25 7.25 7.24 6.27 6.27 6.26 6.26 6.26
5.02 5.01 5.01 5.00 4.99 4.99 4.98 4.04 4.02 4.01 4.00 3.99 3.98 3.96 3.95 3.89 3.88 3.88 3.88 3.86 3.85 3.85
1.52 1.50
F3C
Ph
N
Me
3an'
10.31
1.00
1.05
2.08
1.07
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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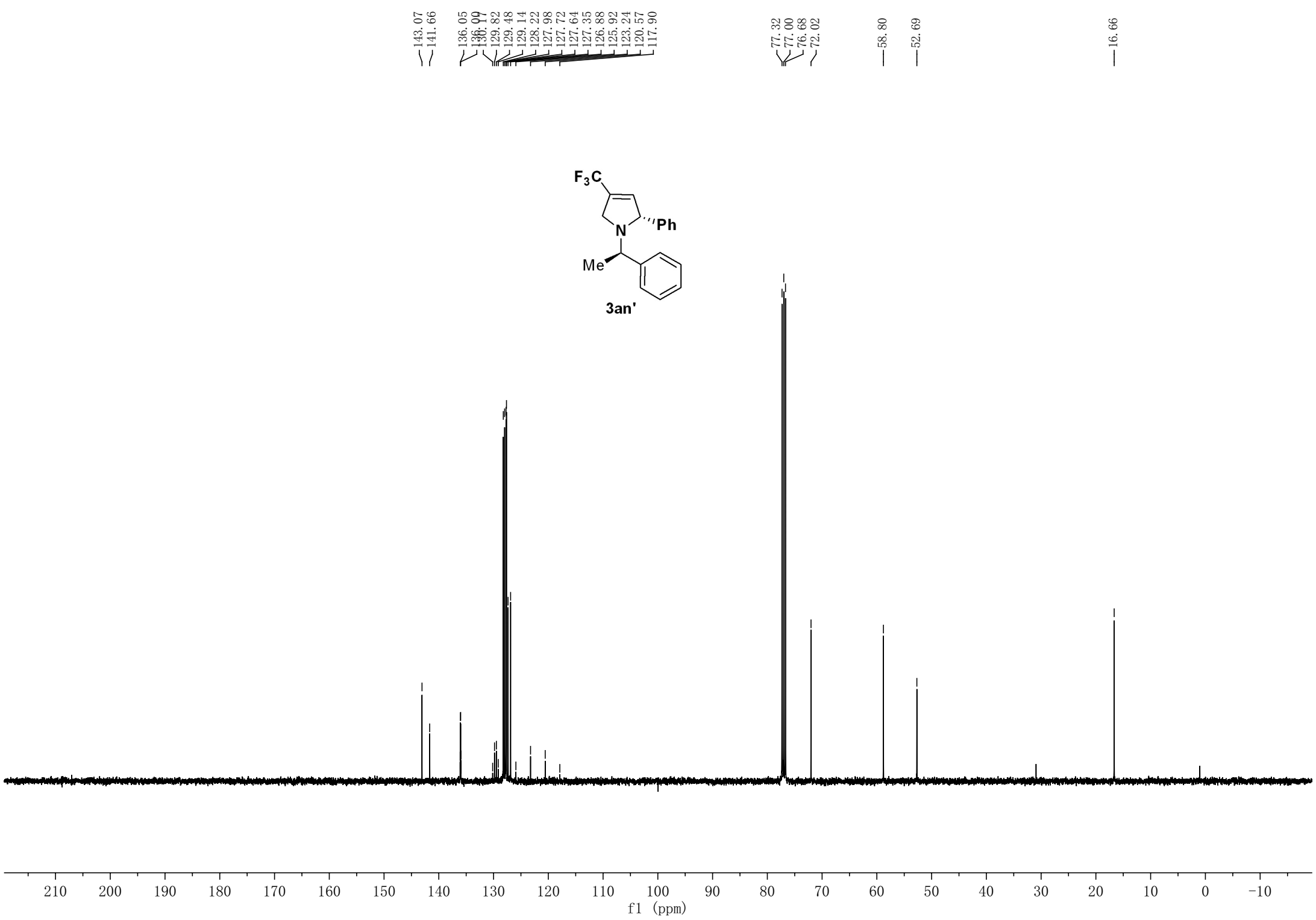
N
Ph
Me
3an'
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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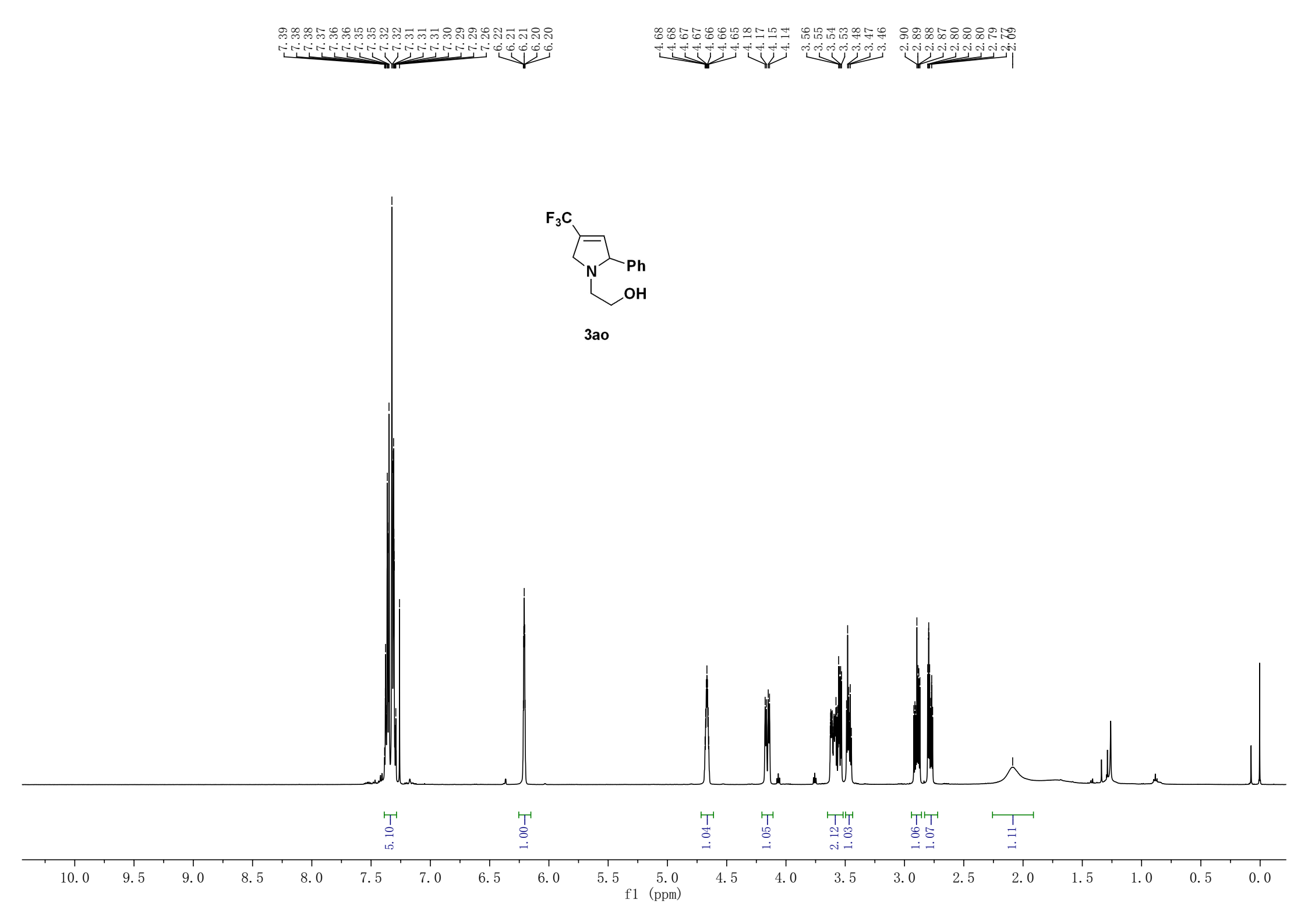
128.22
127.98
127.72
127.64
127.35
126.88
125.92
123.24
120.57
117.90
77.32
77.00
76.68
72.02
58.80
52.69
16.66
F3C
Ph
N
Me
3an'
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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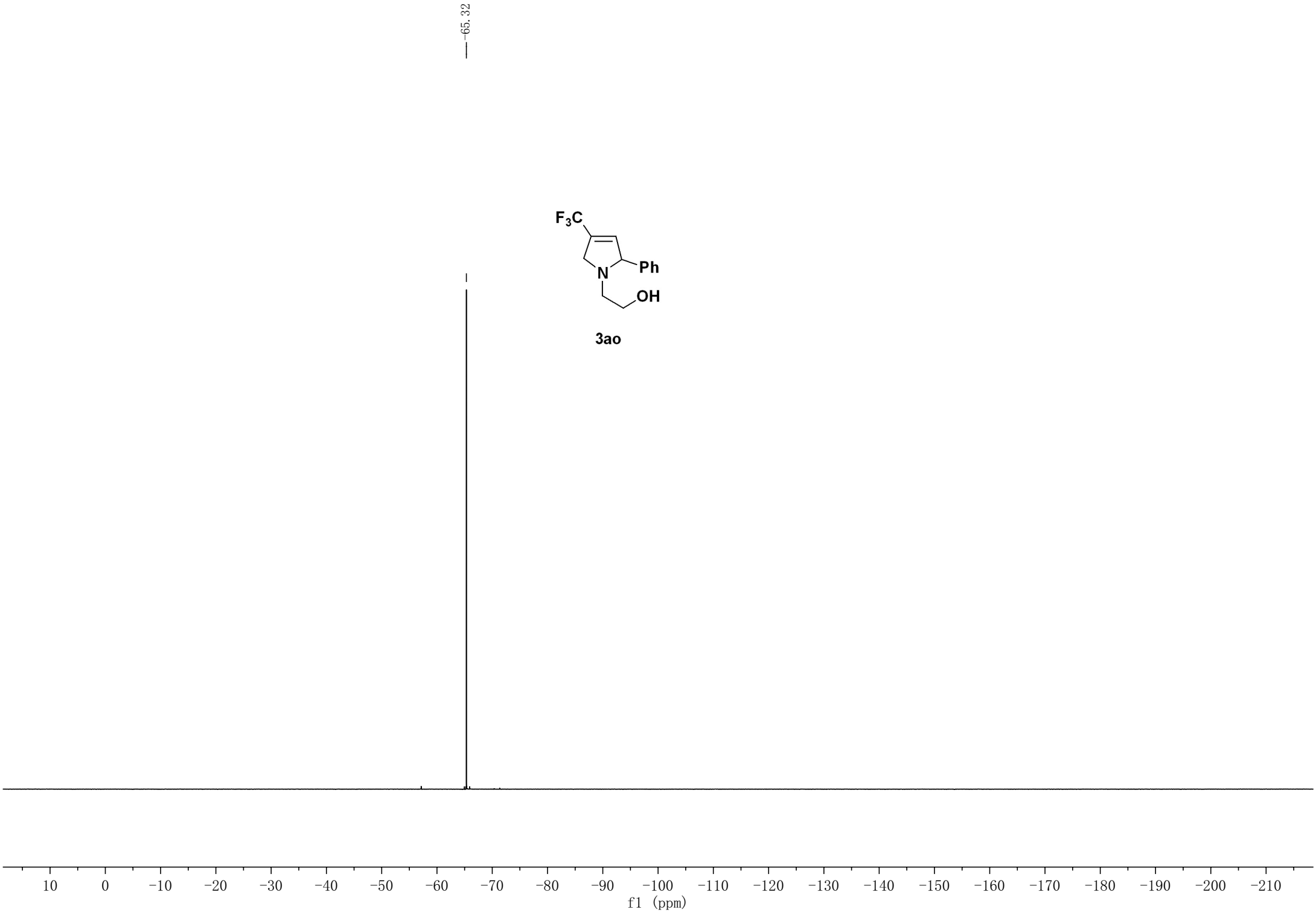
7.35
7.35
7.32
7.32
7.31
7.31
7.31
7.30
7.29
7.29
7.26
6.22
6.21
6.21
6.20
6.20
4.68
4.68
4.67
4.67
4.66
4.66
4.65
4.18
4.17
4.15
4.14
3.56
3.55
3.54
3.53
3.48
3.47
3.46
2.90
2.89
2.88
2.87
2.80
2.80
2.80
2.79
2.77
2.09
F3C
Ph
N
OH
3ao
5.10
1.00
1.04
1.05
2.12
1.03
1.06
1.07
1.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
Ph
N
OH
3ao
10
0
-10
-20
-30
-40
-50
-60
-70
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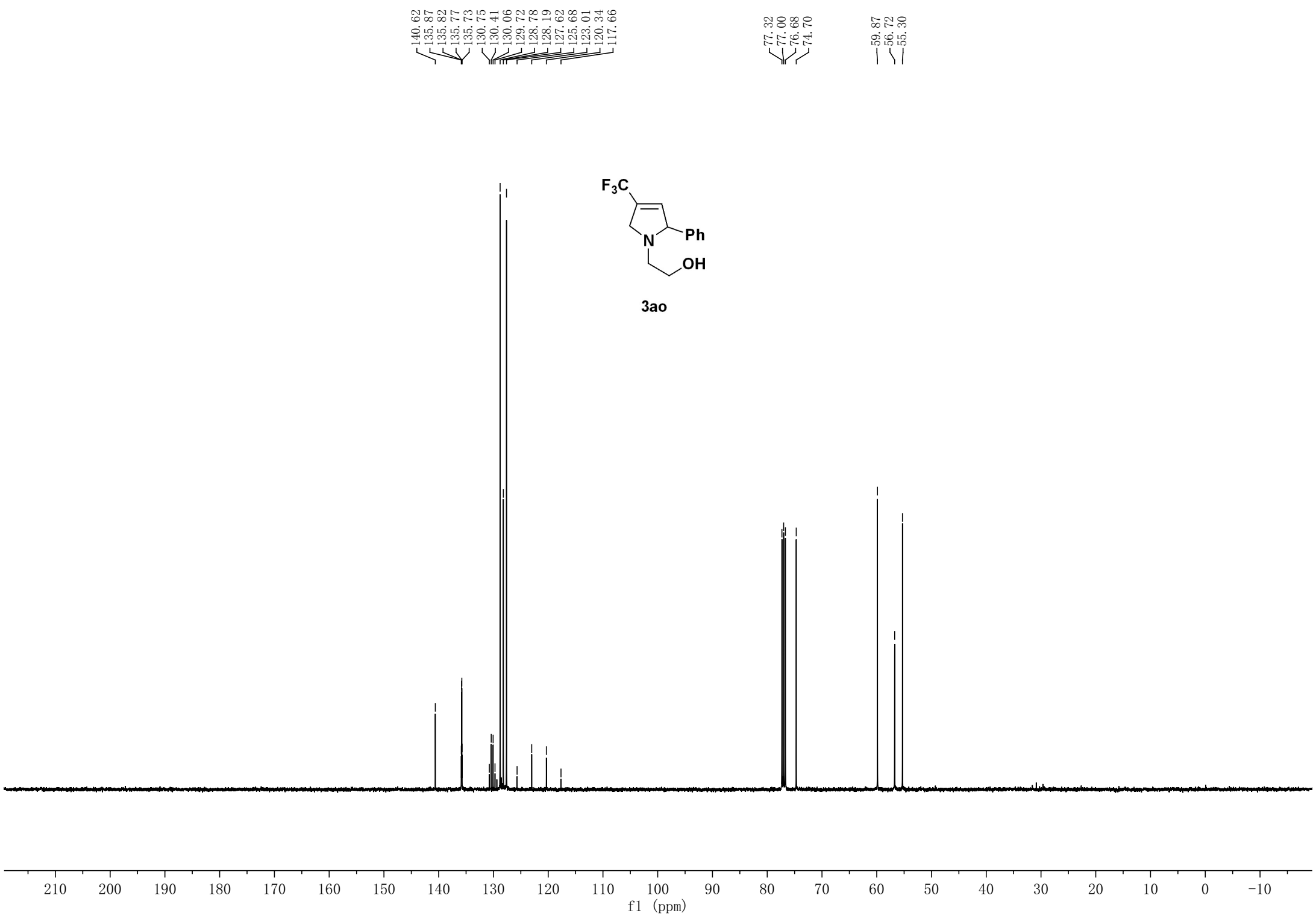
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)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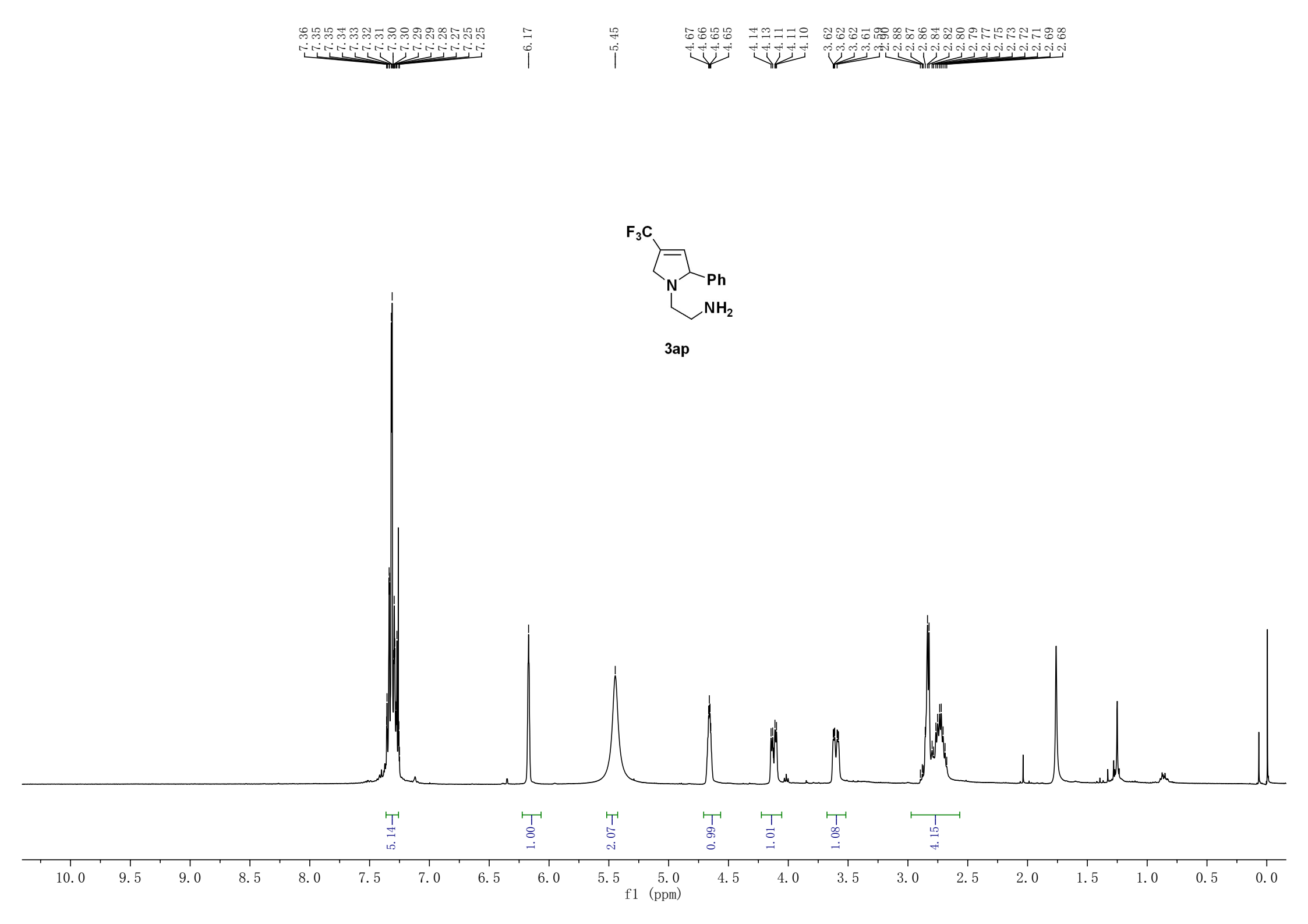
130.41
130.06
129.72
128.78
128.19
127.62
125.68
123.01
120.34
117.66
77.32
77.00
76.68
74.70
59.87
56.72
55.30
F3C
Ph
N
OH
3ao
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.35
7.35
7.34
7.33
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.25
7.25
6.17
5.45
4.67
4.66
4.65
4.65
4.14
4.13
4.11
4.11
4.10
3.62
3.62
3.62
3.61
2.88
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2.86
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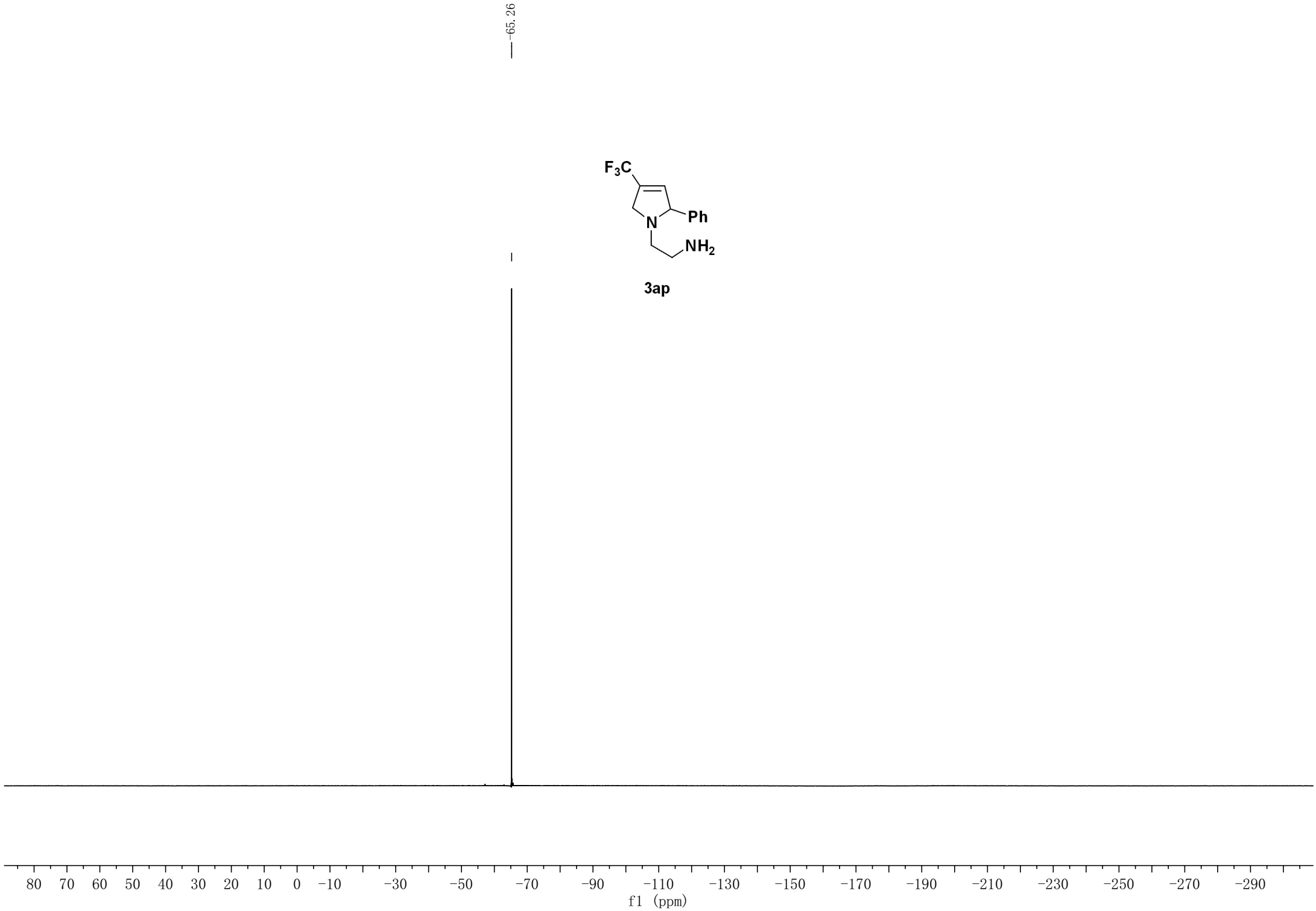
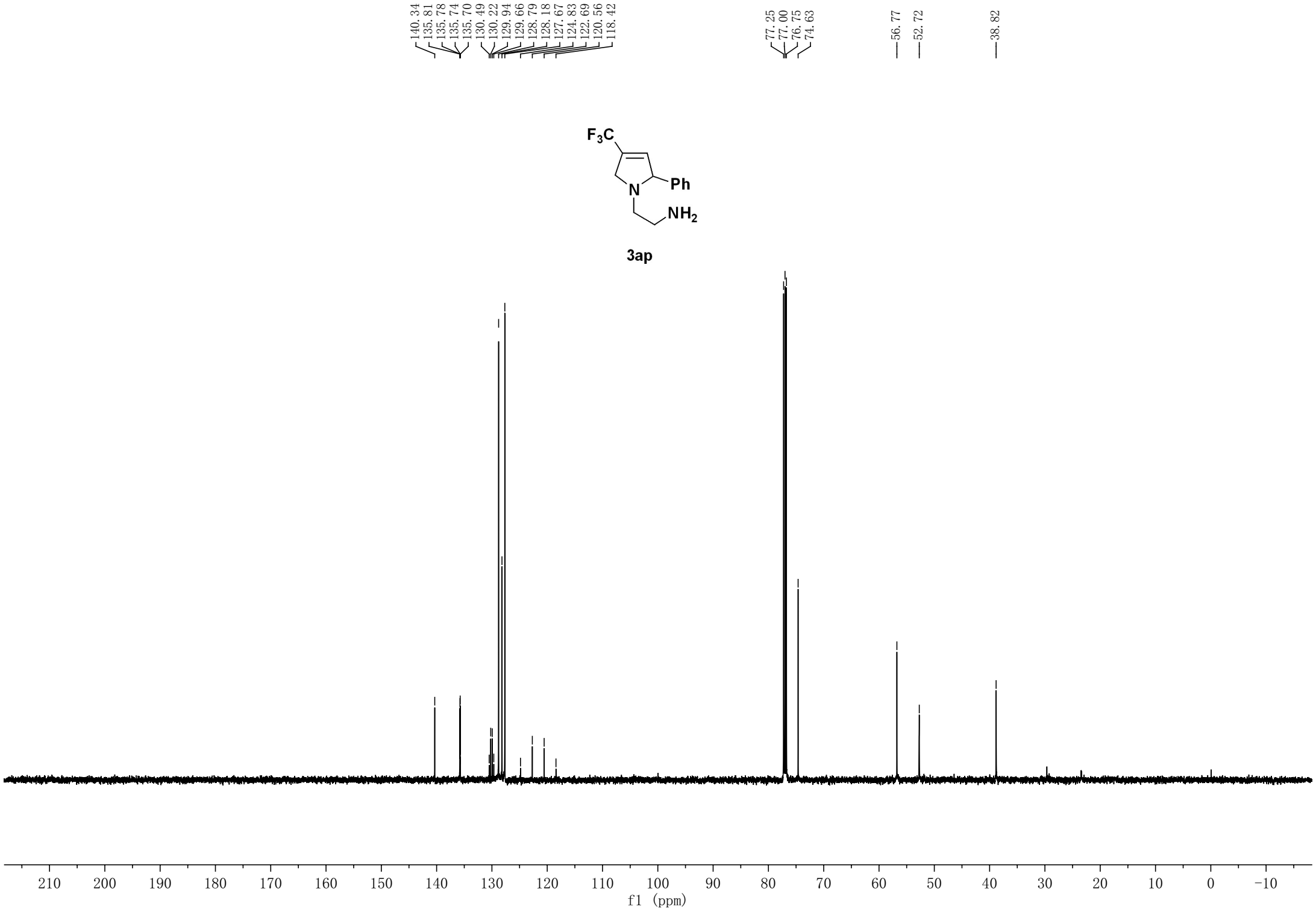
2.82
2.80
2.79
2.77
2.75
2.73
2.72
2.71
2.69
2.68
F3C
Ph
N
NH2
3ap
5.14
1.00
2.07
0.99
1.01
1.08
4.15
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.26
F3C
Ph
N
NH2
3ap
80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)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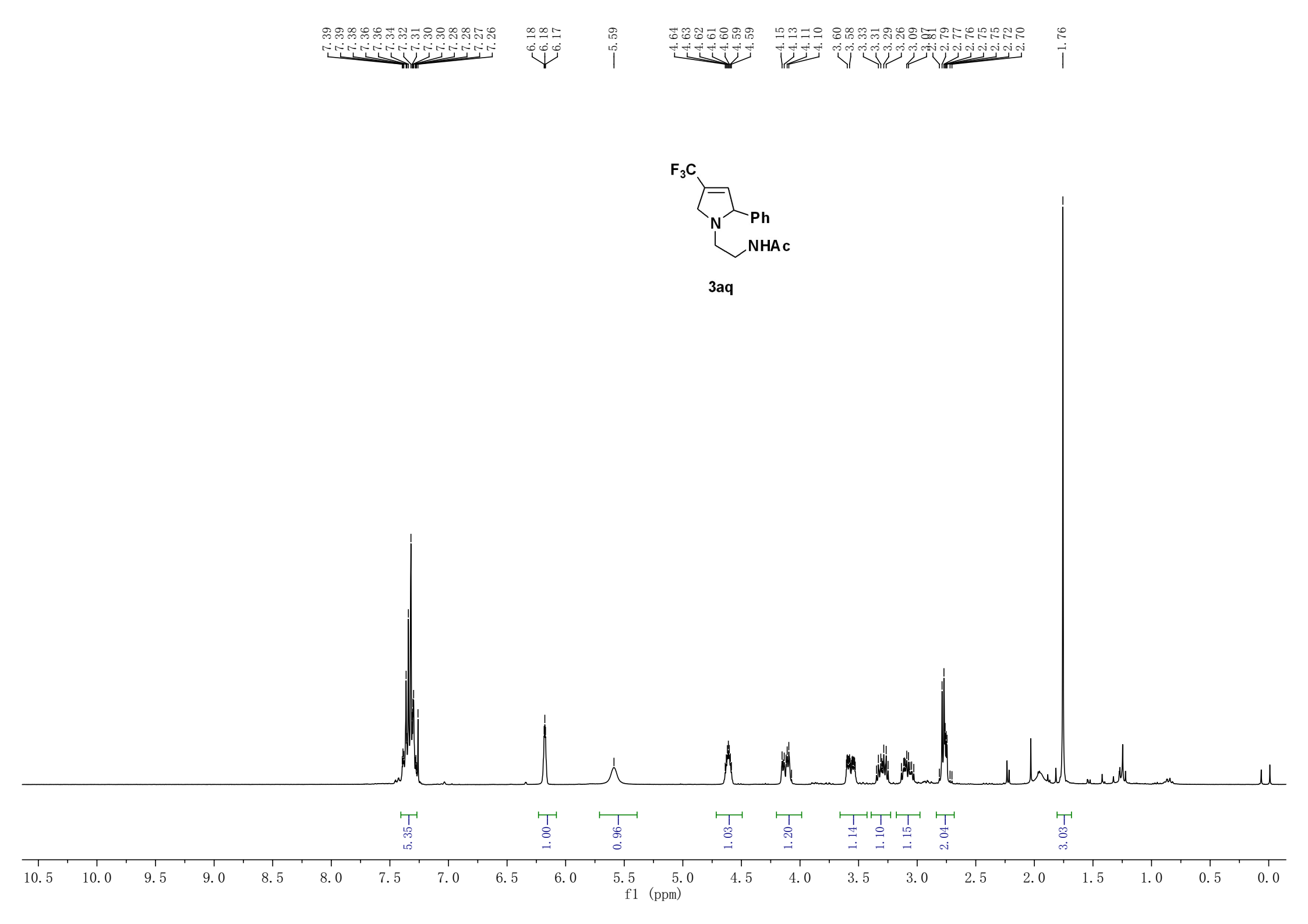
130.22
129.94
129.66
128.79
128.18
127.67
124.83
122.69
120.56
118.42
77.25
77.00
76.75
74.63
56.77
52.72
38.82
F3C
Ph
N
NH2
3ap
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.39
7.39
7.38
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7.36
7.34
7.32
7.31
7.30
7.30
7.28
7.28
7.27
7.26
6.18
6.18
6.17
5.59
4.64
4.63
4.62
4.61
4.60
4.59
4.59
4.15
4.13
4.11
4.10
3.60
3.58
3.33
3.31
3.29
3.26
3.09
2.81
2.79
2.77
2.76
2.75
2.75
2.72
2.70
1.76
F3C
Ph
N
NHAc
3aq
5.35
1.00
0.96
1.03
1.20
1.14
1.10
1.15
2.04
3.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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1.0
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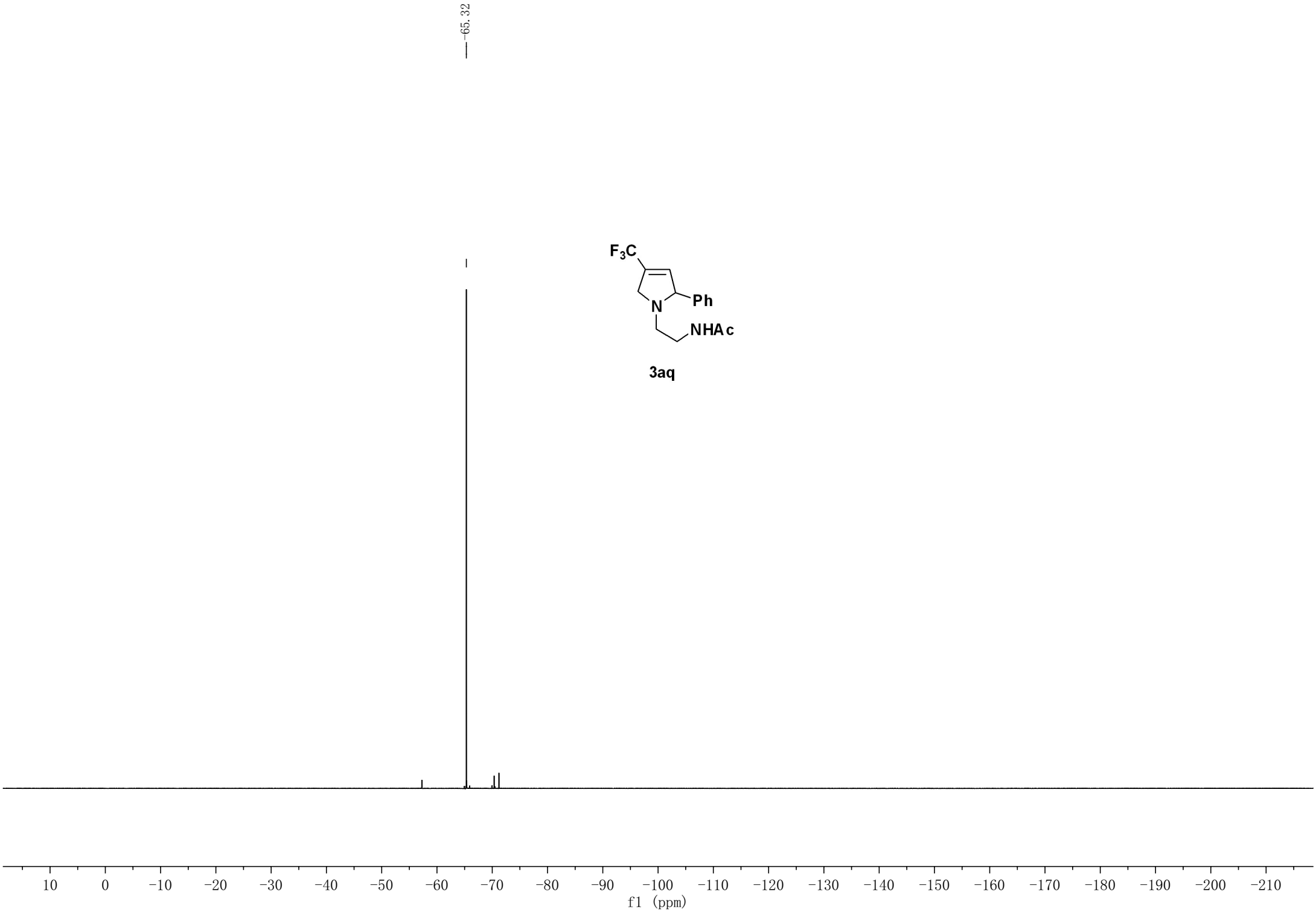
0.0
f1 (ppm)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F3C
N
Ph
NHAc
3aq
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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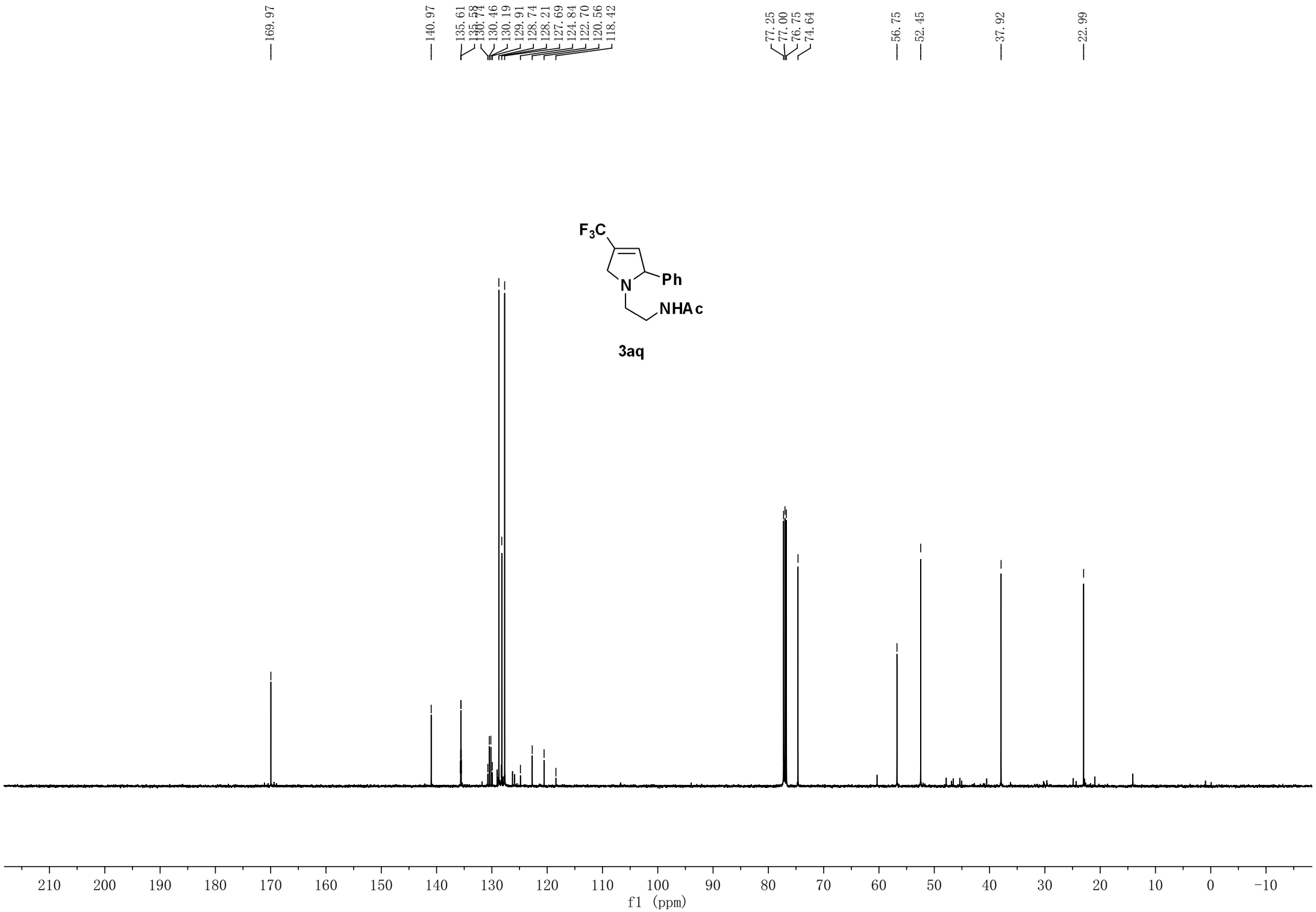
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


169.97
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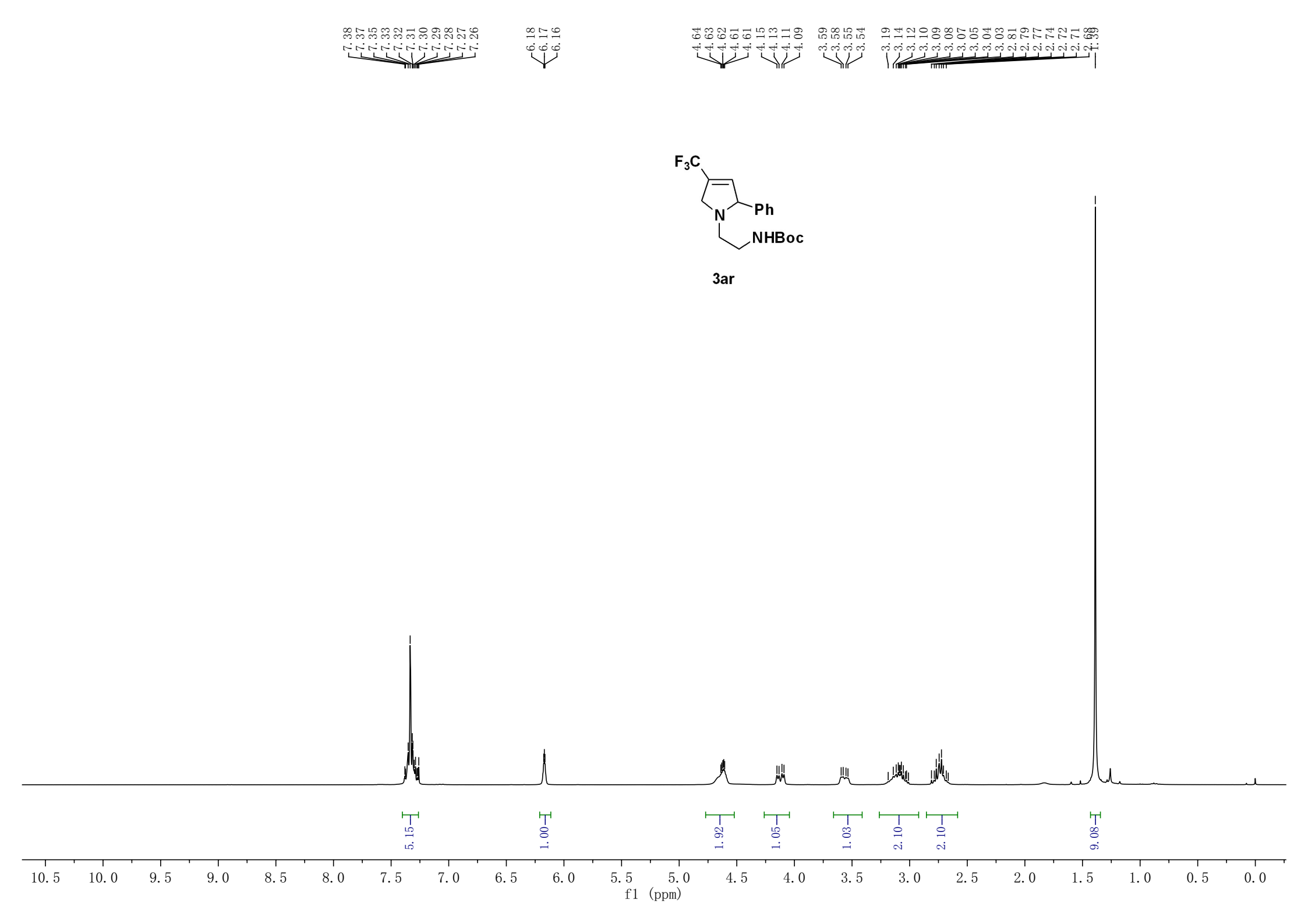
135.61
130.46
130.19
129.91
128.74
128.21
127.69
124.84
122.70
120.56
118.42
77.25
77.00
76.75
74.64
56.75
52.45
37.92
22.99
F3C
Ph
N
NHAc
3aq
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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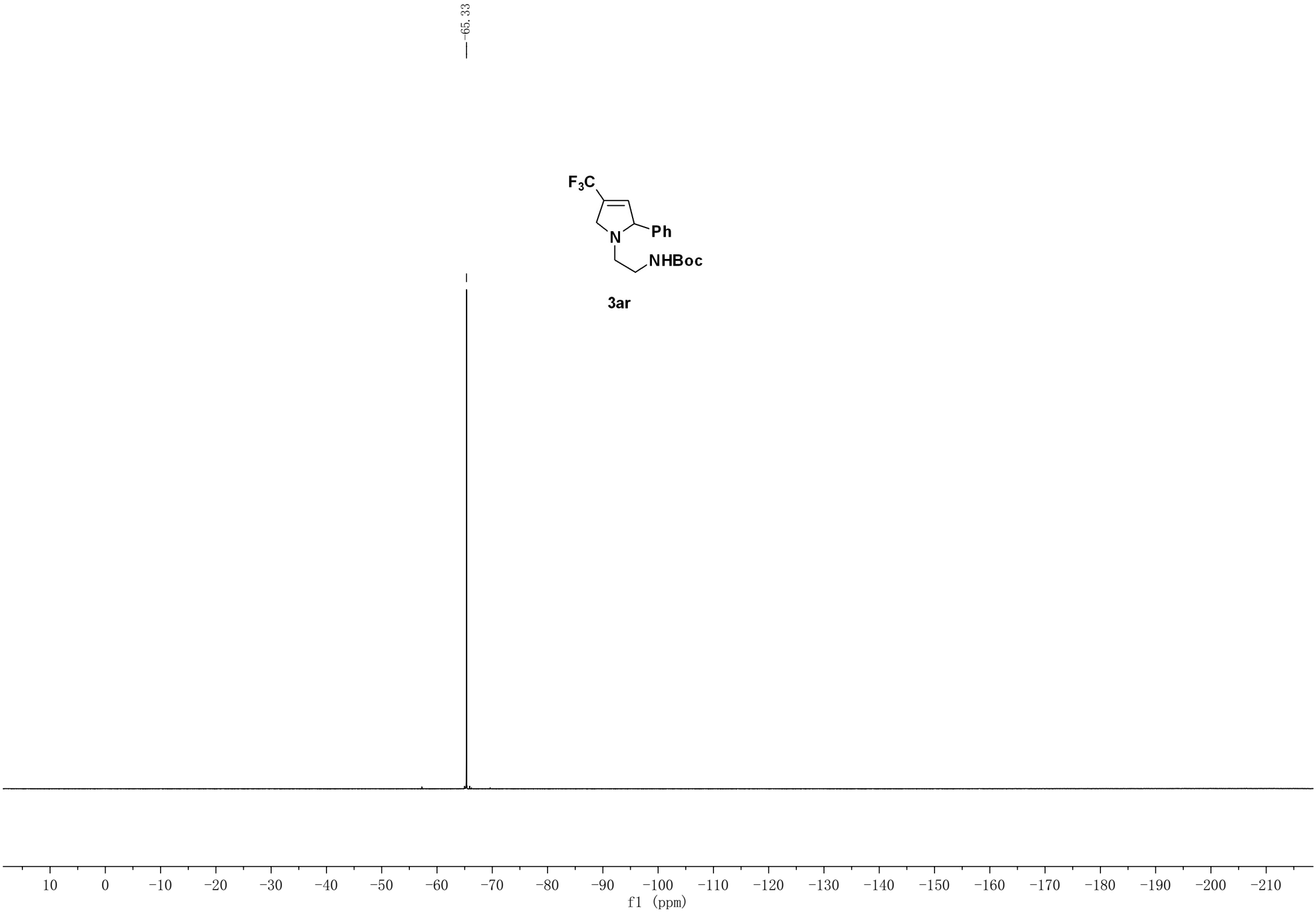
7.37
7.35
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.26
6.18
6.17
6.16
4.64
4.63
4.62
4.61
4.61
4.15
4.13
4.11
4.09
3.59
3.58
3.55
3.54
3.19
3.14
3.12
3.10
3.09
3.08
3.07
3.05
3.04
3.03
2.81
2.79
2.77
2.74
2.72
2.71
1.39
F3C
Ph
N
NHBoc
3ar
5.15
1.00
1.92
1.05
1.03
2.10
2.10
9.08
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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F3C
Ph
N
NHBoc
3ar
10
0
-10
-20
-30
-40
-50
-60
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-140
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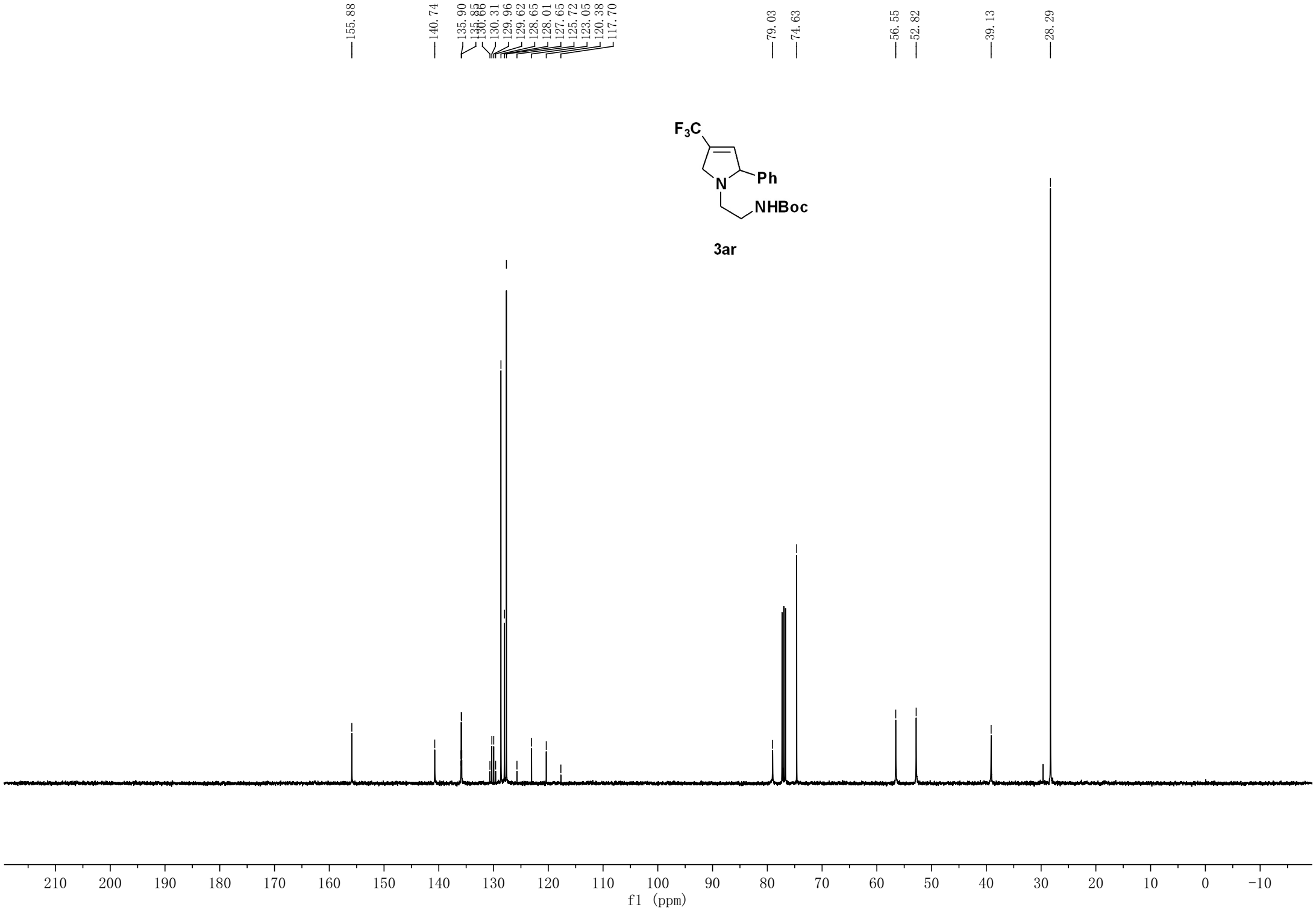
-160
-170
-180
-190
-200
-210
f1 (ppm)


155.88
140.74
135.90
130.31
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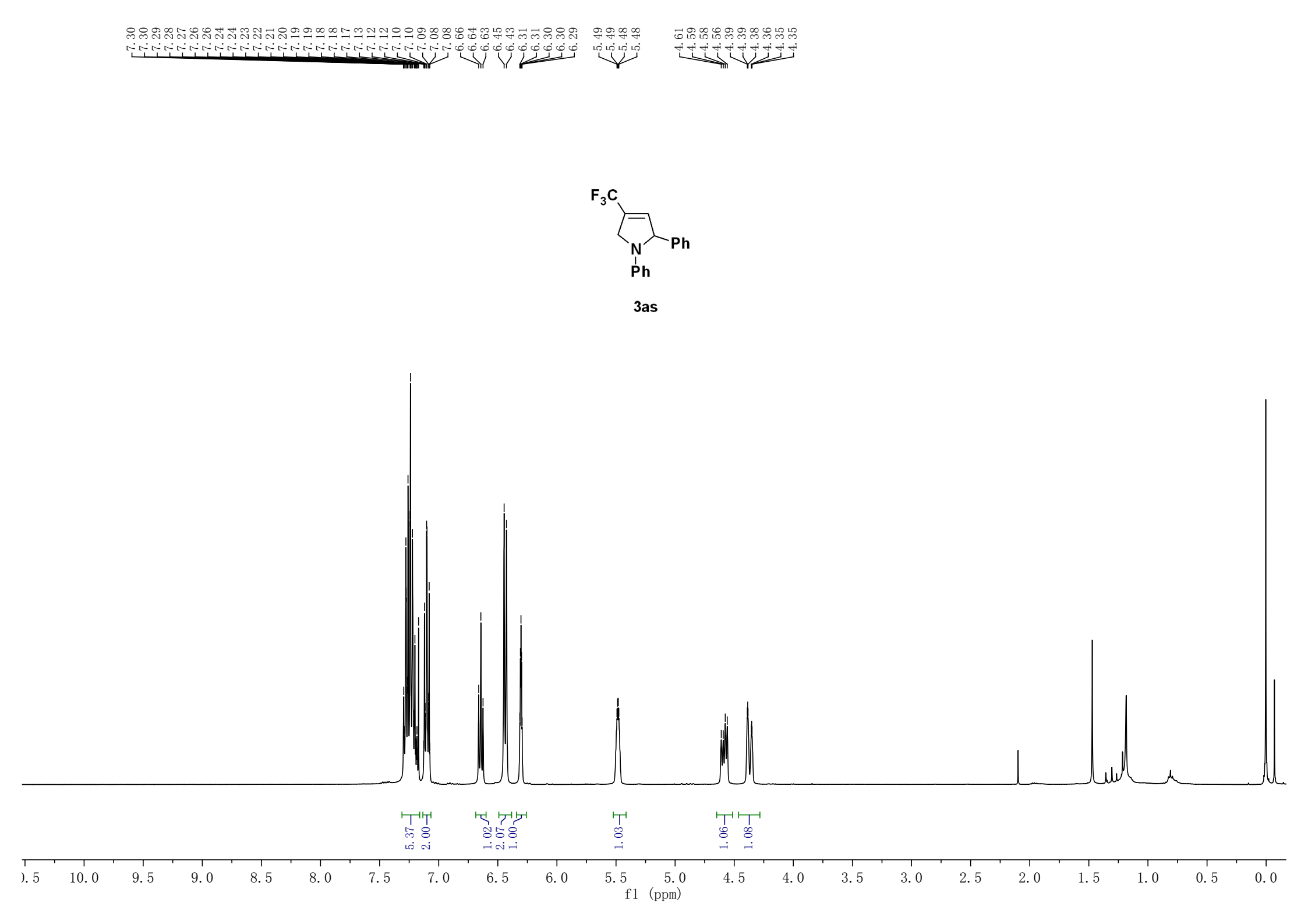
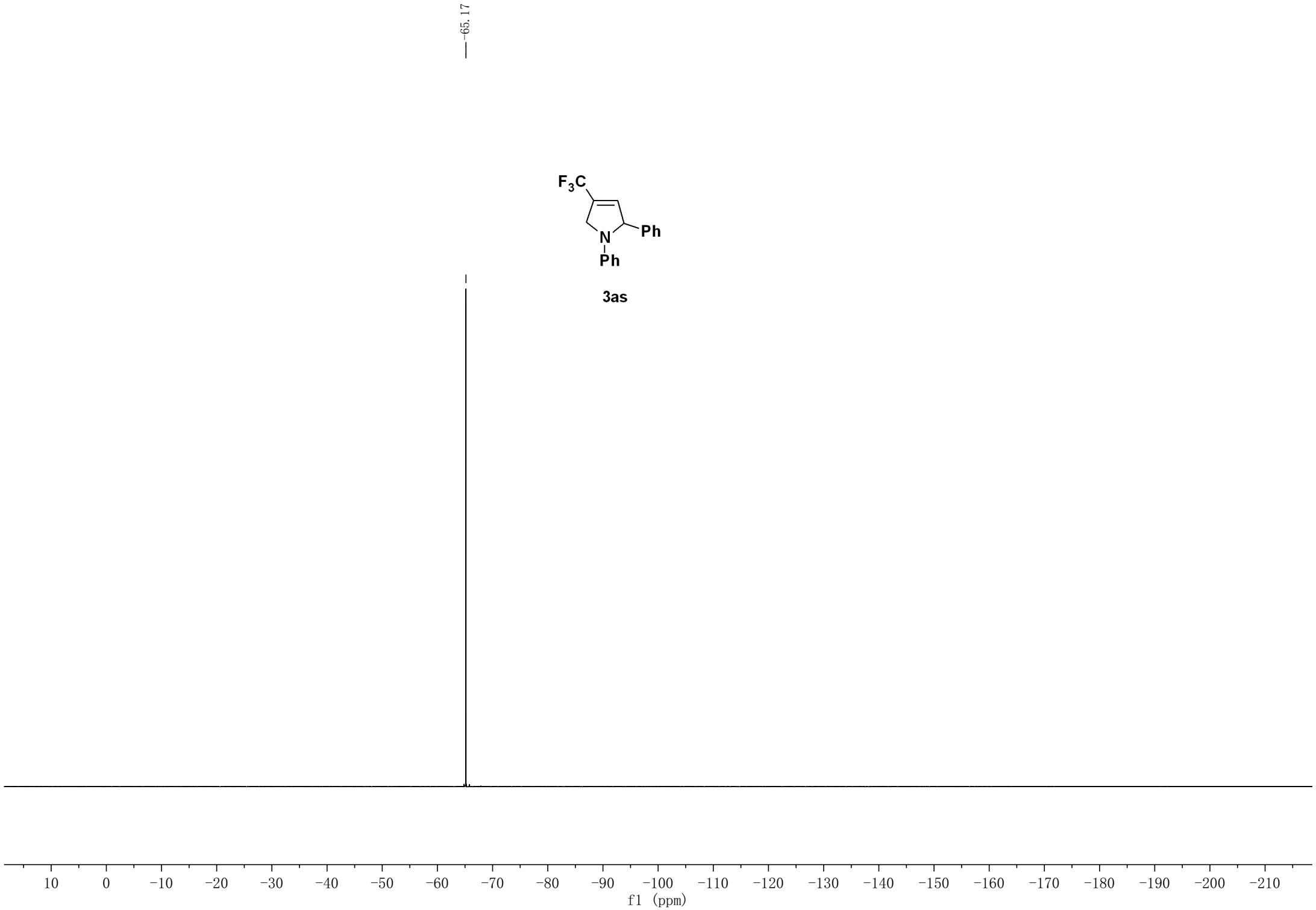
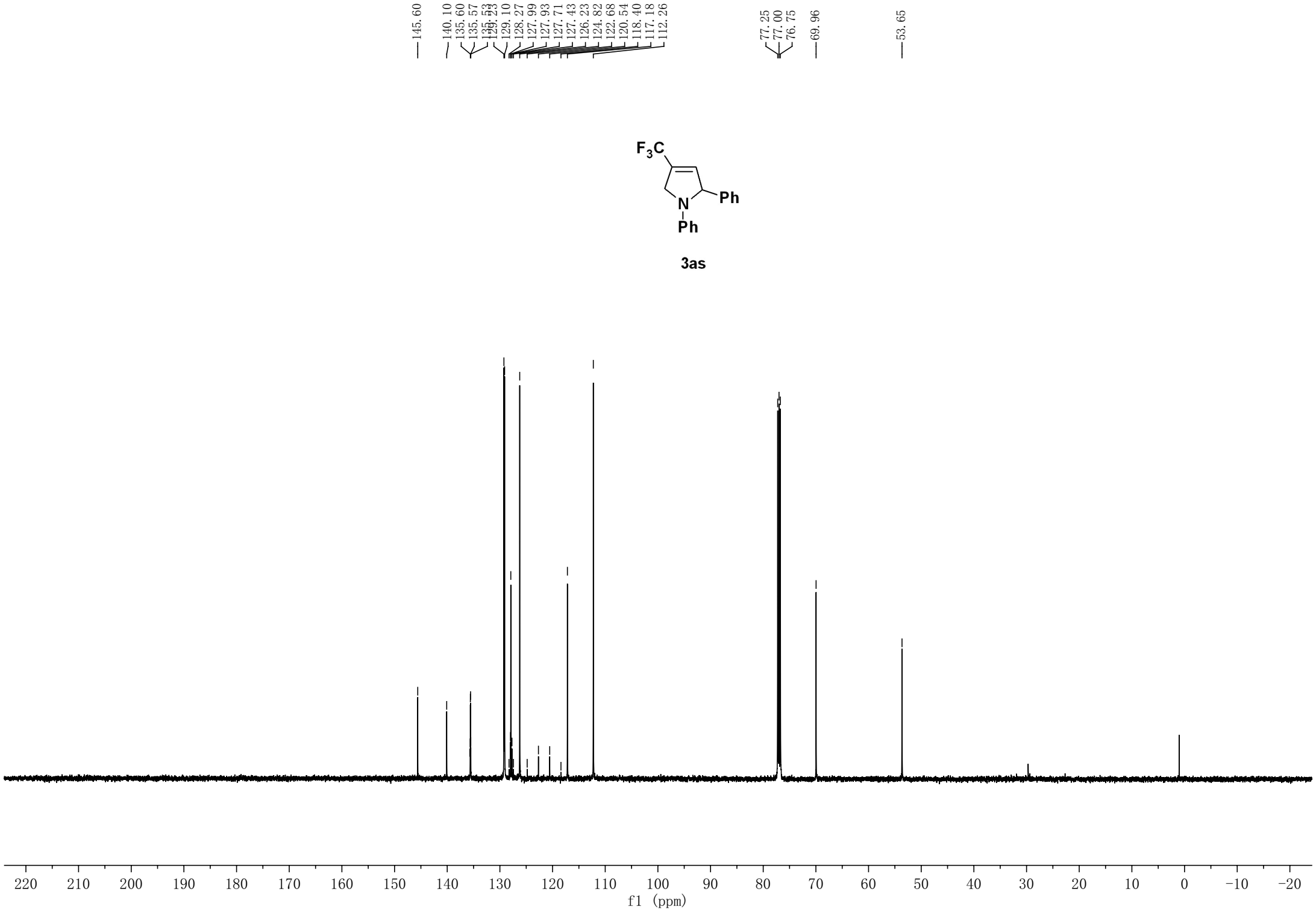
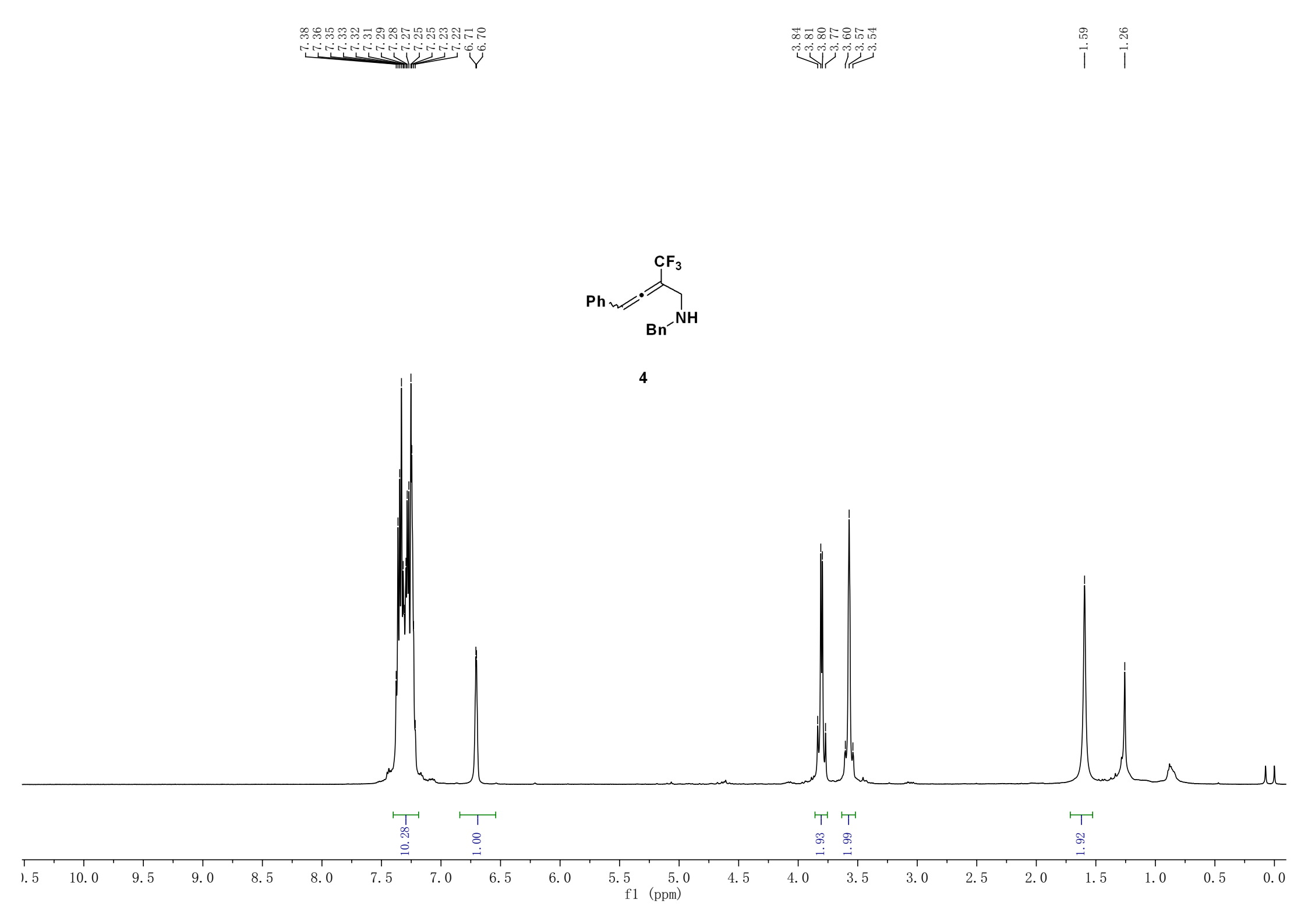
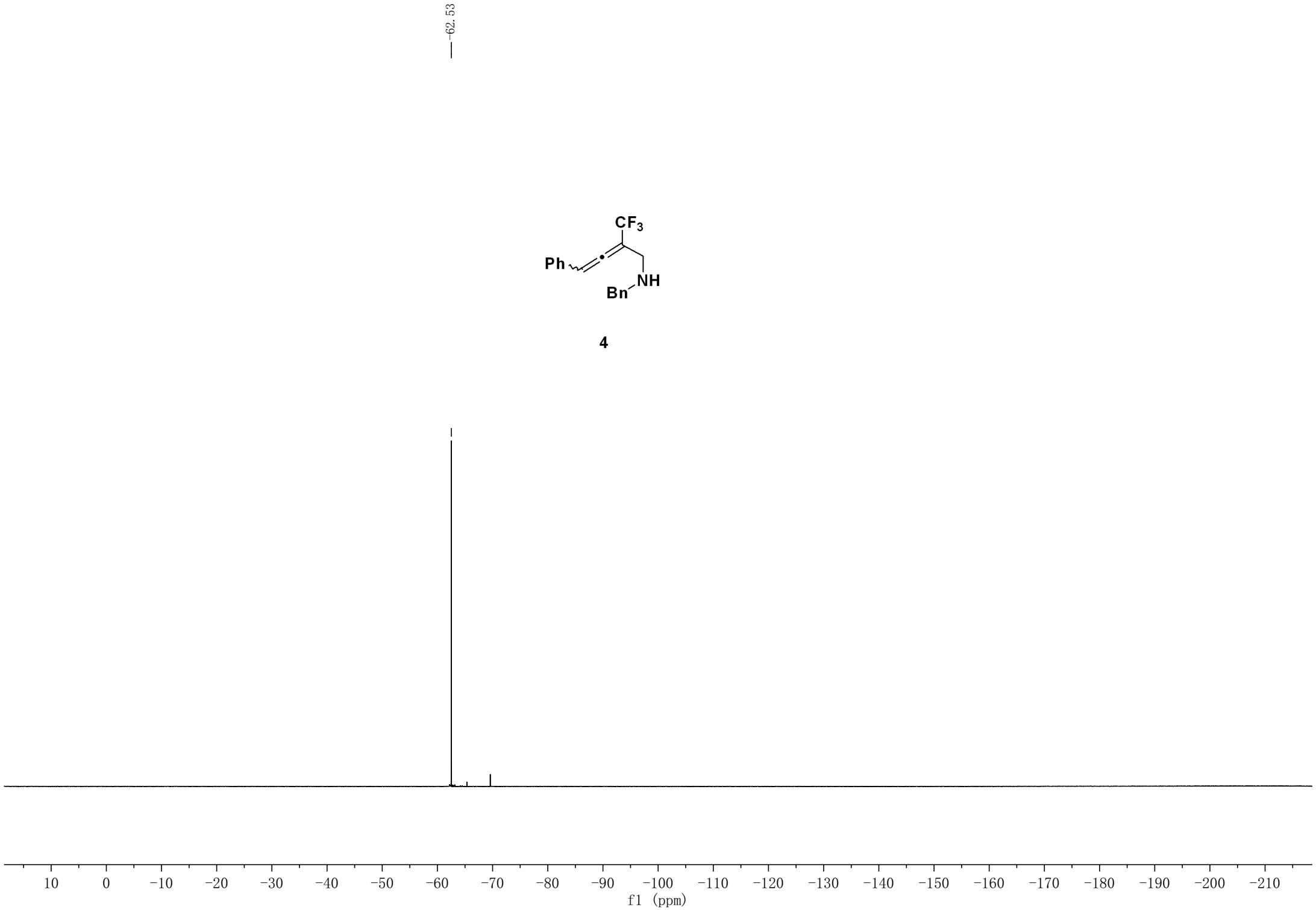
129.62
128.65
128.01
127.65
125.72
123.05
120.38
117.70
79.03
74.63
56.55
52.82
39.13
28.29
F3C
Ph
N
NHBoc
3ar
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.30
7.30
7.29
7.28
7.27
7.26
7.26
7.24
7.24
7.23
7.22
7.21
7.20
7.19
7.19
7.18
7.18
7.17
7.13
7.12
7.12
7.10
7.10
7.09
7.08
7.08
6.66
6.64
6.63
6.45
6.43
6.31
6.31
6.30
6.30
6.29
5.49
5.49
5.48
5.48
4.61
4.59
4.58
4.56
4.39
4.39
4.38
4.36
4.35
4.35
F3C
Ph
N
Ph
3as
5.37
2.00
1.02
2.07
1.00
1.03
1.06
1.08
f1 (ppm)


−65.17
F3C
Ph
N
Ph
3as
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)


145.60
140.10
135.60
135.57
129.10
128.27
127.99
127.93
127.71
127.43
126.23
124.82
122.68
120.54
118.40
117.18
112.26
77.25
77.00
76.75
69.96
53.65
F3C
Ph
N
Ph
3as
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


7.38
7.36
7.35
7.33
7.32
7.31
7.29
7.28
7.27
7.25
7.25
7.23
7.22
6.71
6.70
3.84
3.81
3.80
3.77
3.60
3.57
3.54
1.59
1.26
CF3
Ph
NH
Bn
4
10.28
1.00
1.93
1.99
1.92
f1 (ppm)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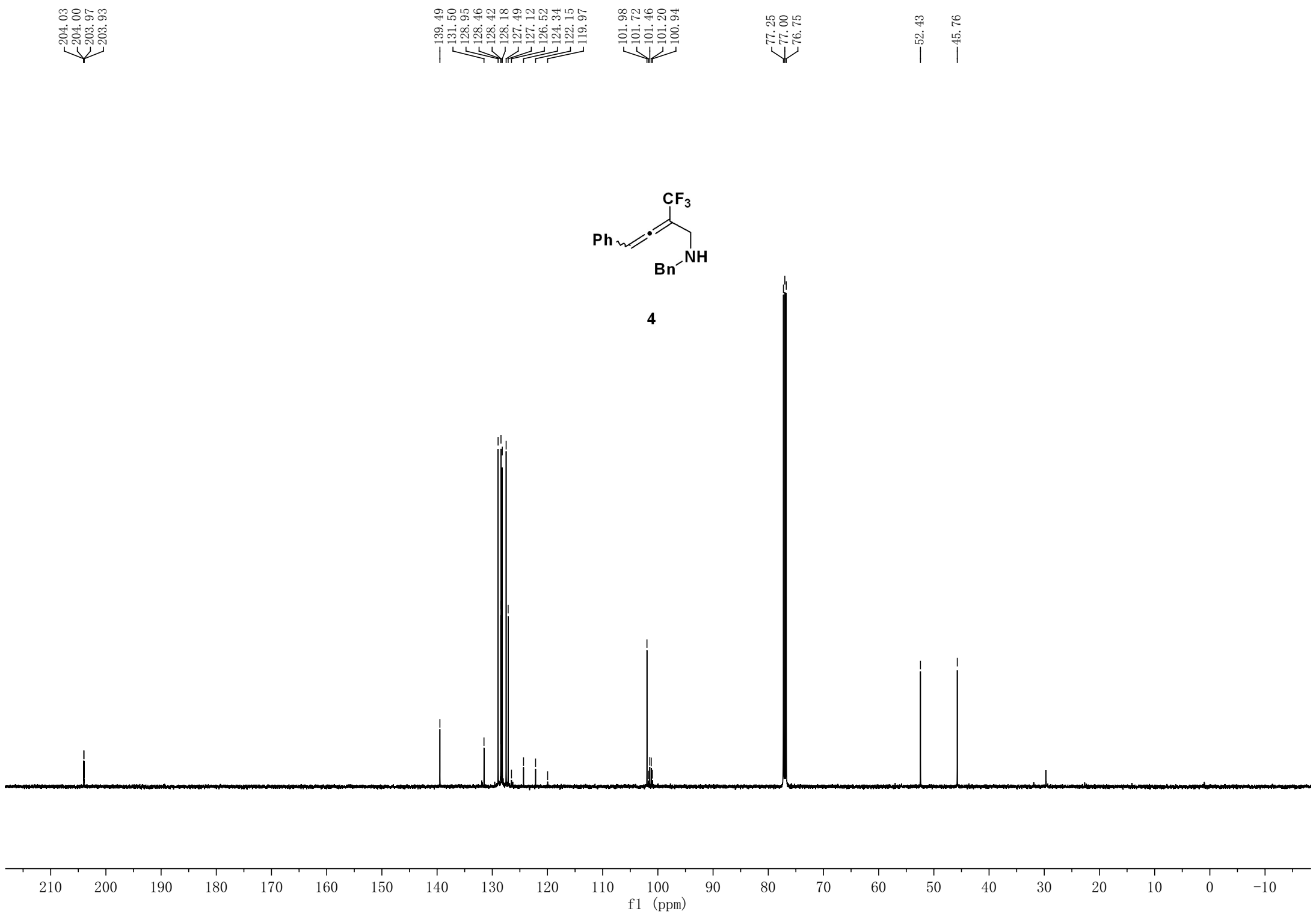
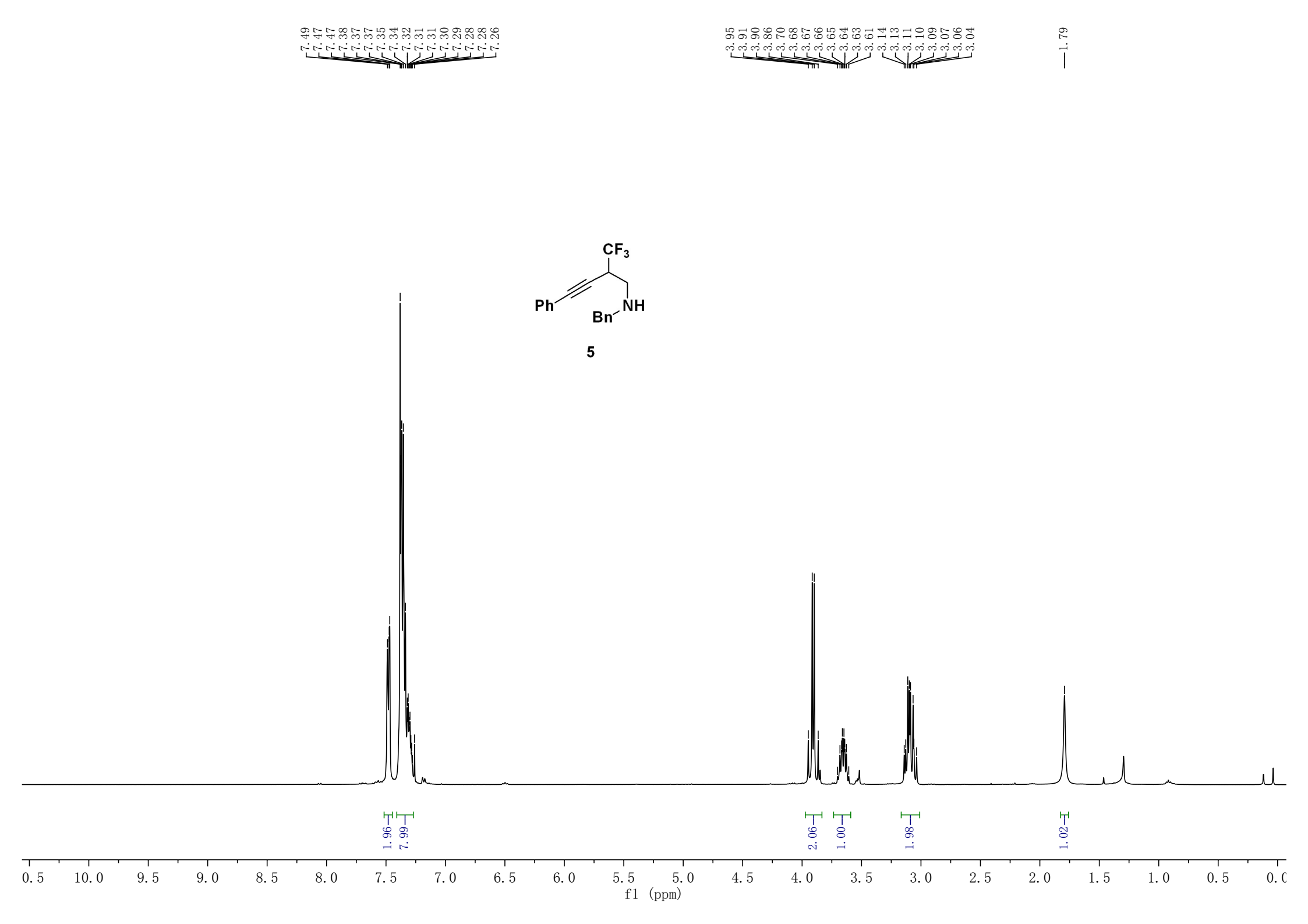
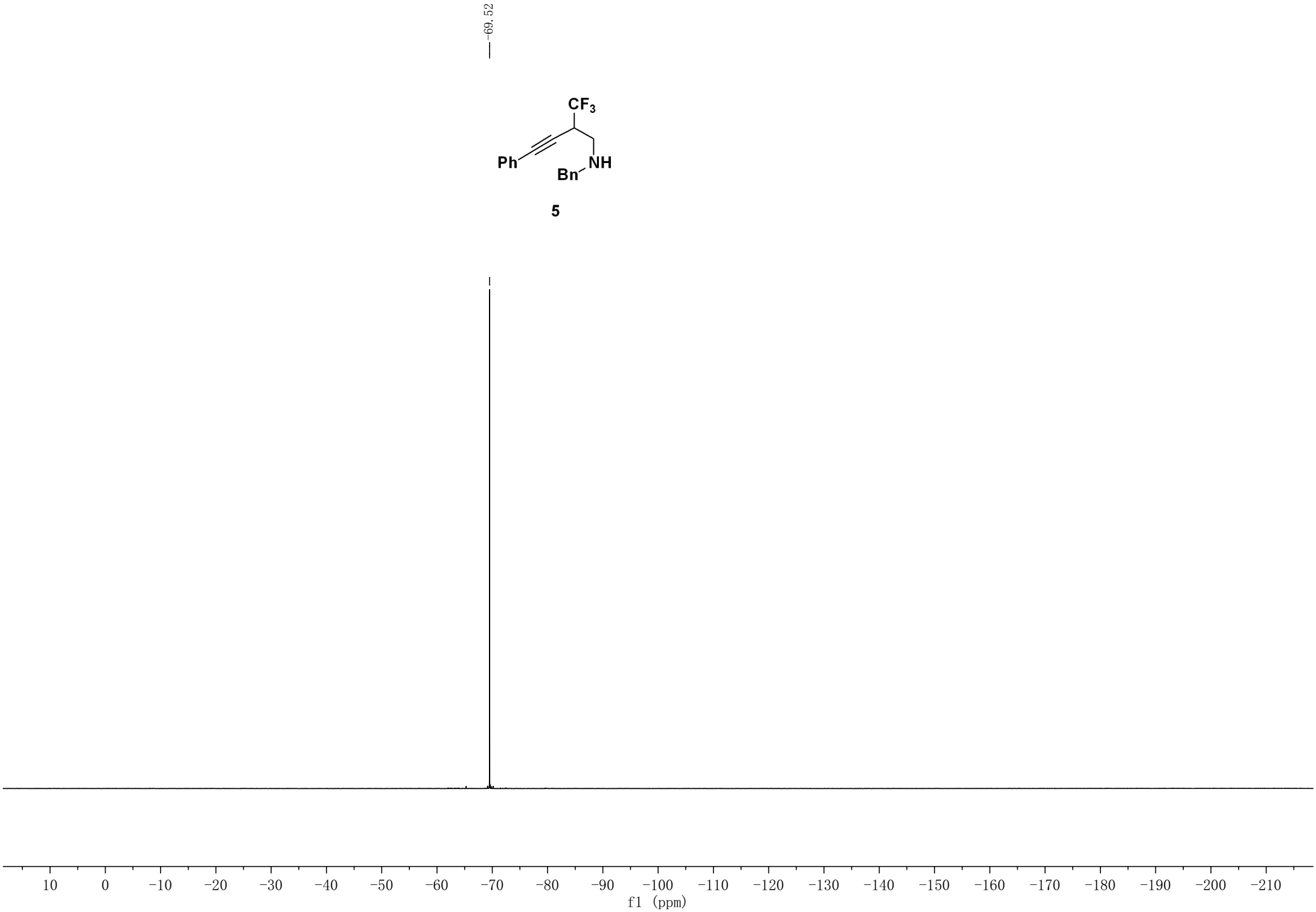
CF3
Ph
NH
Bn
4
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


204.03
204.00
203.97
203.93
139.49
131.50
128.95
128.46
128.42
128.18
127.49
127.12
126.52
124.34
122.15
119.97
101.98
101.72
101.46
101.20
100.94
77.25
77.00
76.75
52.43
45.76
CF3
Ph
NH
Bn
4
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.49
7.47
7.47
7.38
7.37
7.37
7.35
7.34
7.32
7.31
7.31
7.30
7.29
7.28
7.28
7.26
3.95
3.91
3.90
3.86
3.70
3.68
3.67
3.66
3.65
3.64
3.63
3.61
3.14
3.13
3.11
3.10
3.09
3.07
3.06
3.04
1.79
CF3
Ph
NH
Bn
5
1.96
7.99
2.06
1.00
1.98
1.02
f1 (ppm)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CF3
Ph
NH
Bn
5
10
0
-10
-20
-30
-40
-50
-60
-70
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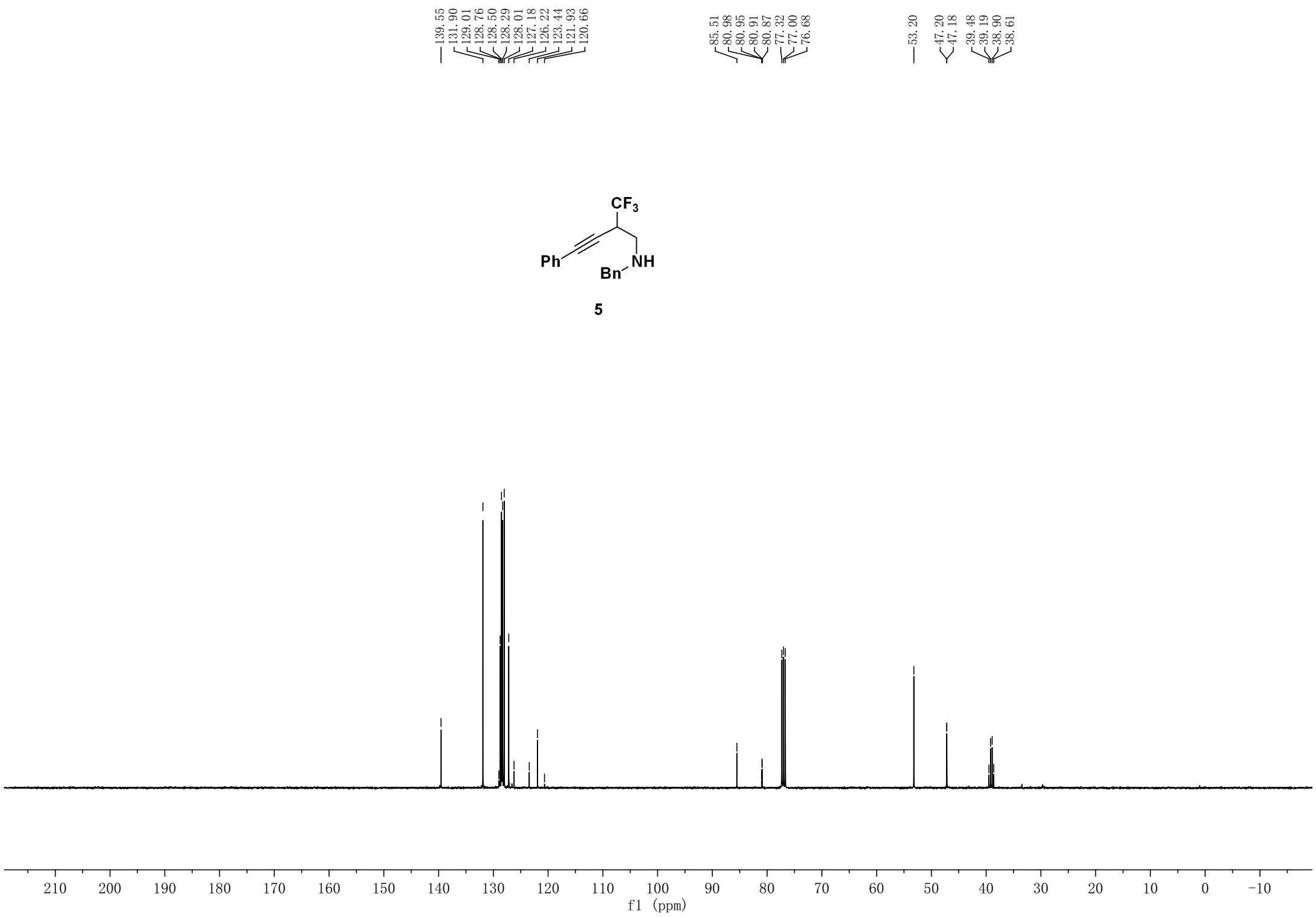
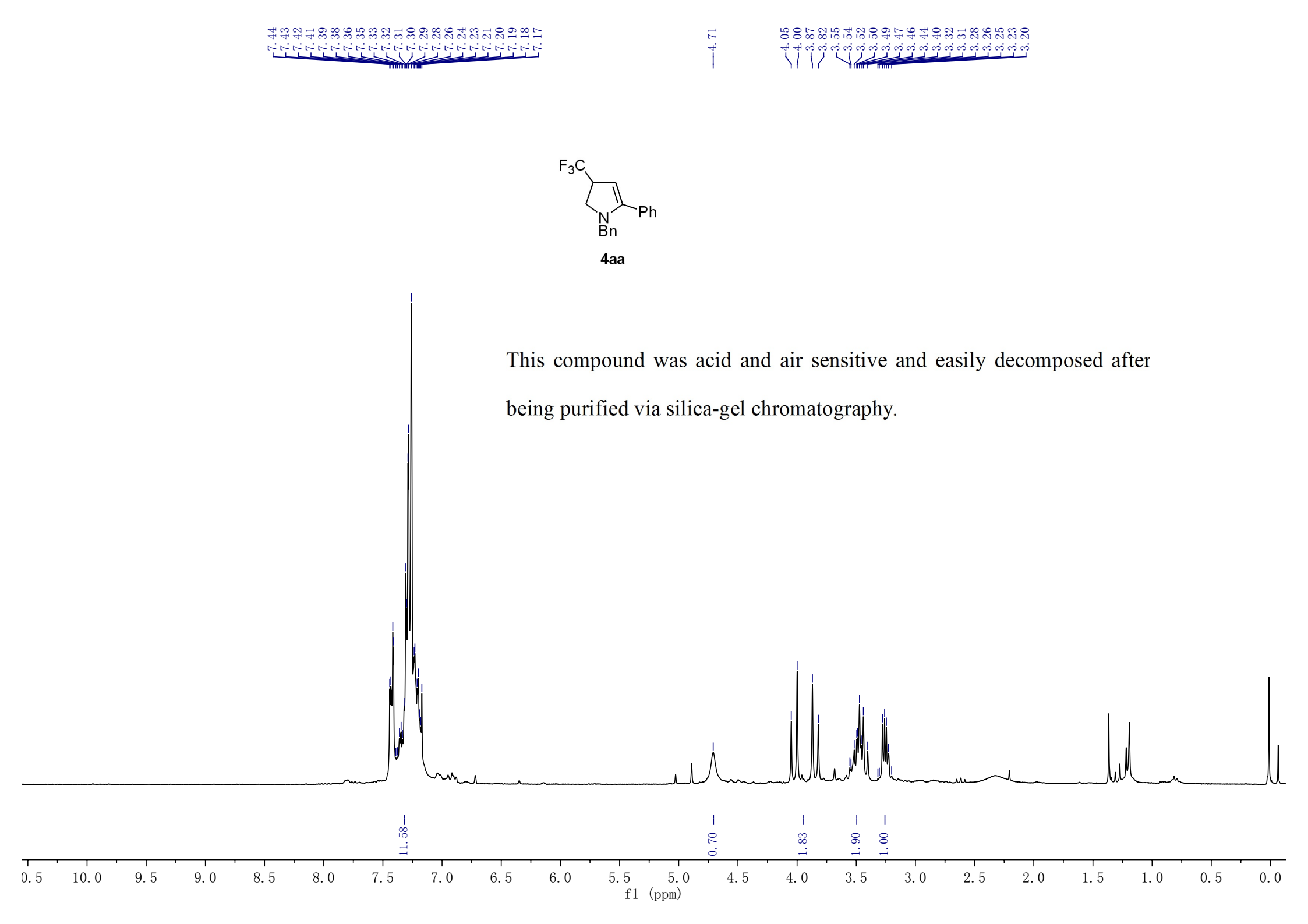
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


139.55
131.90
129.01
128.76
128.50
128.29
128.01
127.18
126.22
123.44
121.93
120.66
85.51
80.98
80.95
80.91
80.87
77.32
77.00
76.68
53.20
47.20
47.18
39.48
39.19
38.90
38.61
CF3
Ph
NH
Bn
5
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.44
7.43
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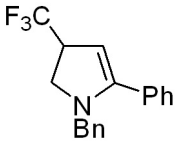
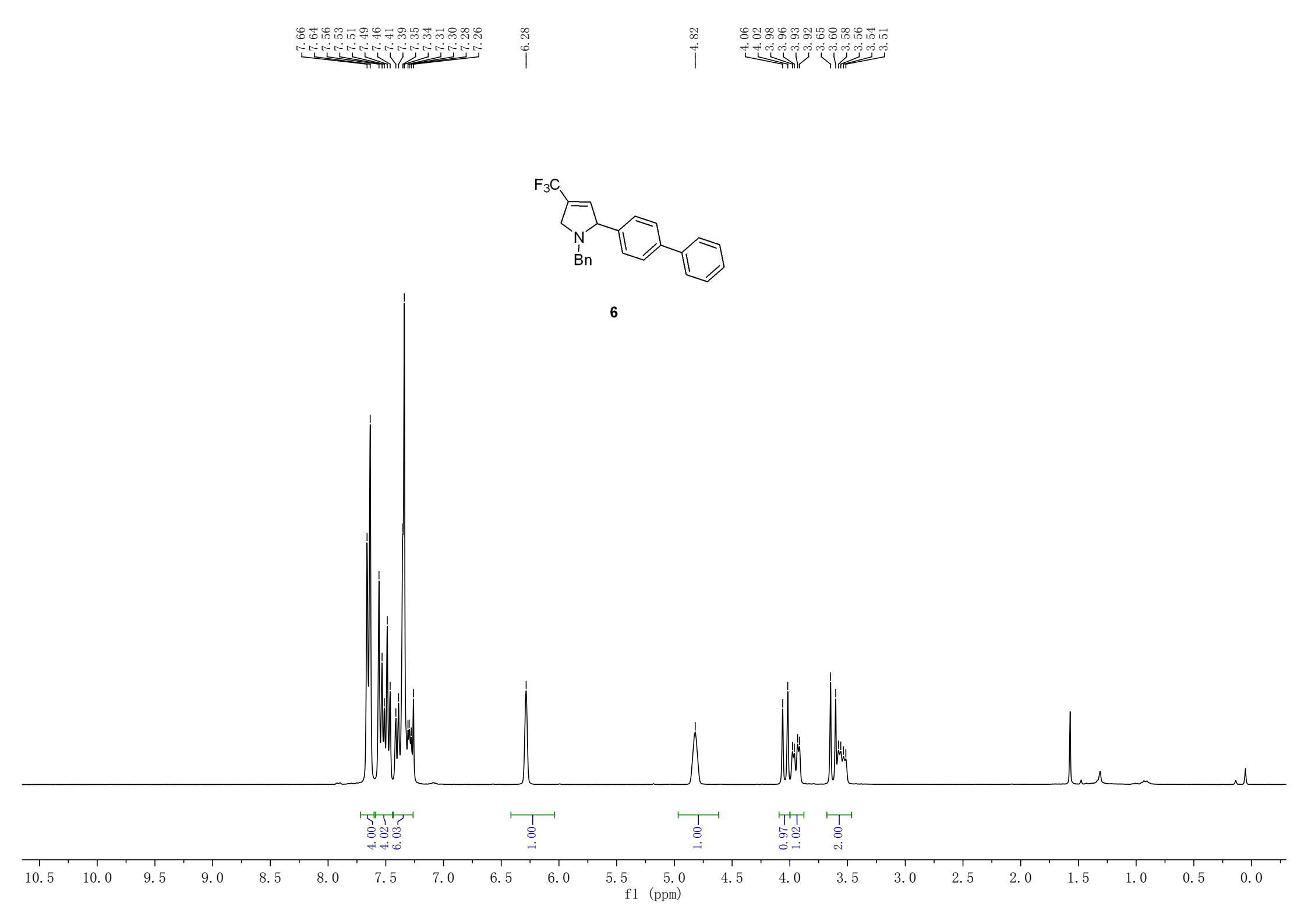
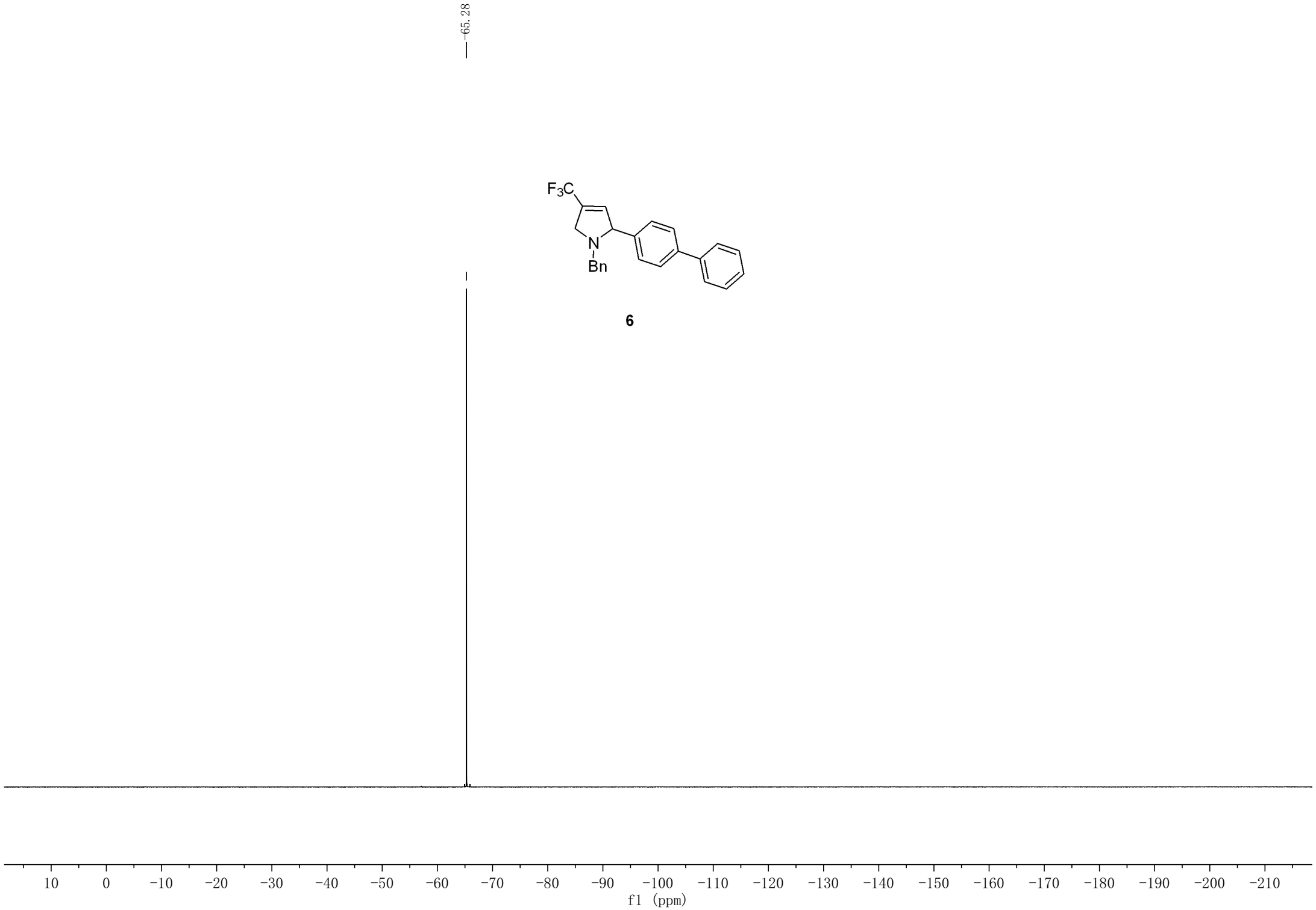
7.39
7.38
7.36
7.35
7.33
7.32
7.31
7.30
7.29
7.28
7.26
7.24
7.23
7.21
7.20
7.19
7.18
7.17
4.71
4.05
4.00
3.87
3.82
3.55
3.54
3.52
3.50
3.49
3.47
3.46
3.44
3.40
3.32
3.31
3.28
3.26
3.25
3.23
3.20
F3C
Ph
N
Bn
4aa
This compound was acid and air sensitive and easily decomposed after being purified via silica-gel chromatography.
11.58
0.70
1.83
1.90
1.00
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



4aa

This compound was acid and air sensitive and easily decomposed after being purified via silica-gel chromatography.


7.66
7.64
7.56
7.53
7.51
7.49
7.46
7.41
7.39
7.35
7.34
7.31
7.30
7.28
7.26
6.28
4.82
4.06
4.02
3.98
3.96
3.93
3.92
3.65
3.60
3.58
3.56
3.54
3.51
F3C
N
Bn
6
4.00
4.02
6.03
1.00
1.00
0.97
1.02
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-65.28
F3C
N
Bn
6
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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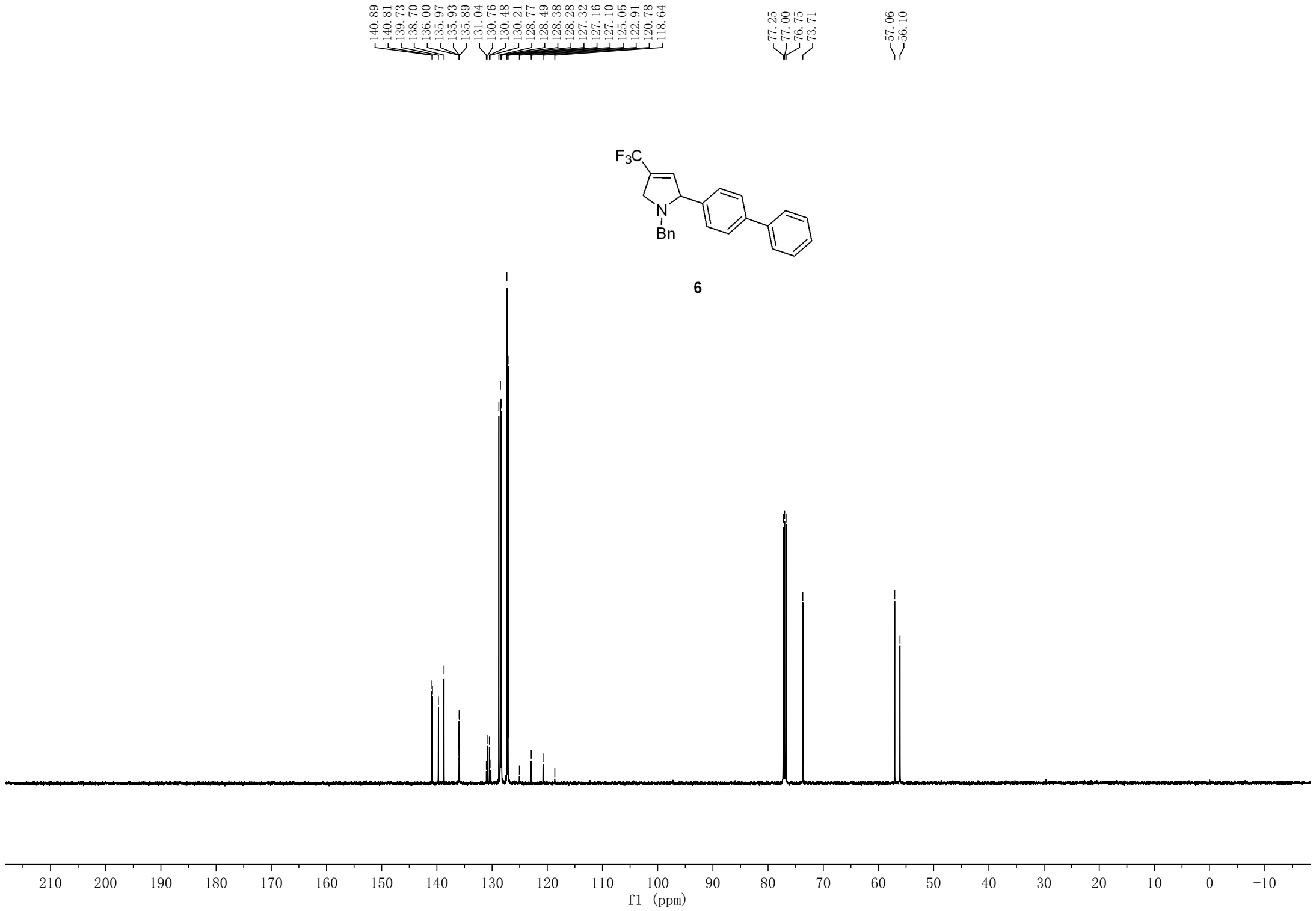
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


140.89
140.81
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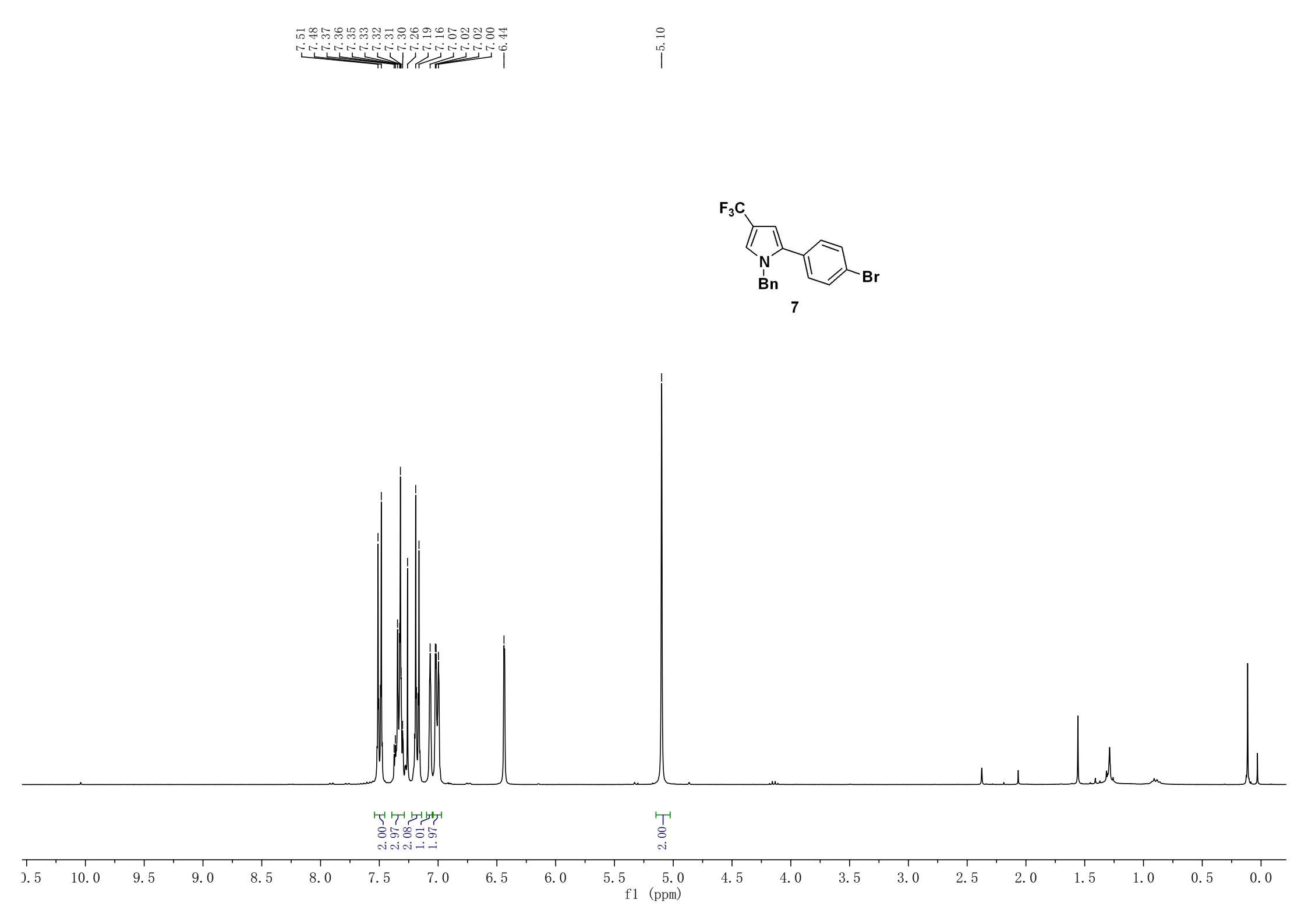
136.00
135.97
135.93
135.89
131.04
130.76
130.48
130.21
128.77
128.49
128.38
128.28
127.32
127.16
127.10
125.05
122.91
120.78
118.64
77.25
77.00
76.75
73.71
57.06
56.10
F3C
N
Bn
6
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.51
7.48
7.37
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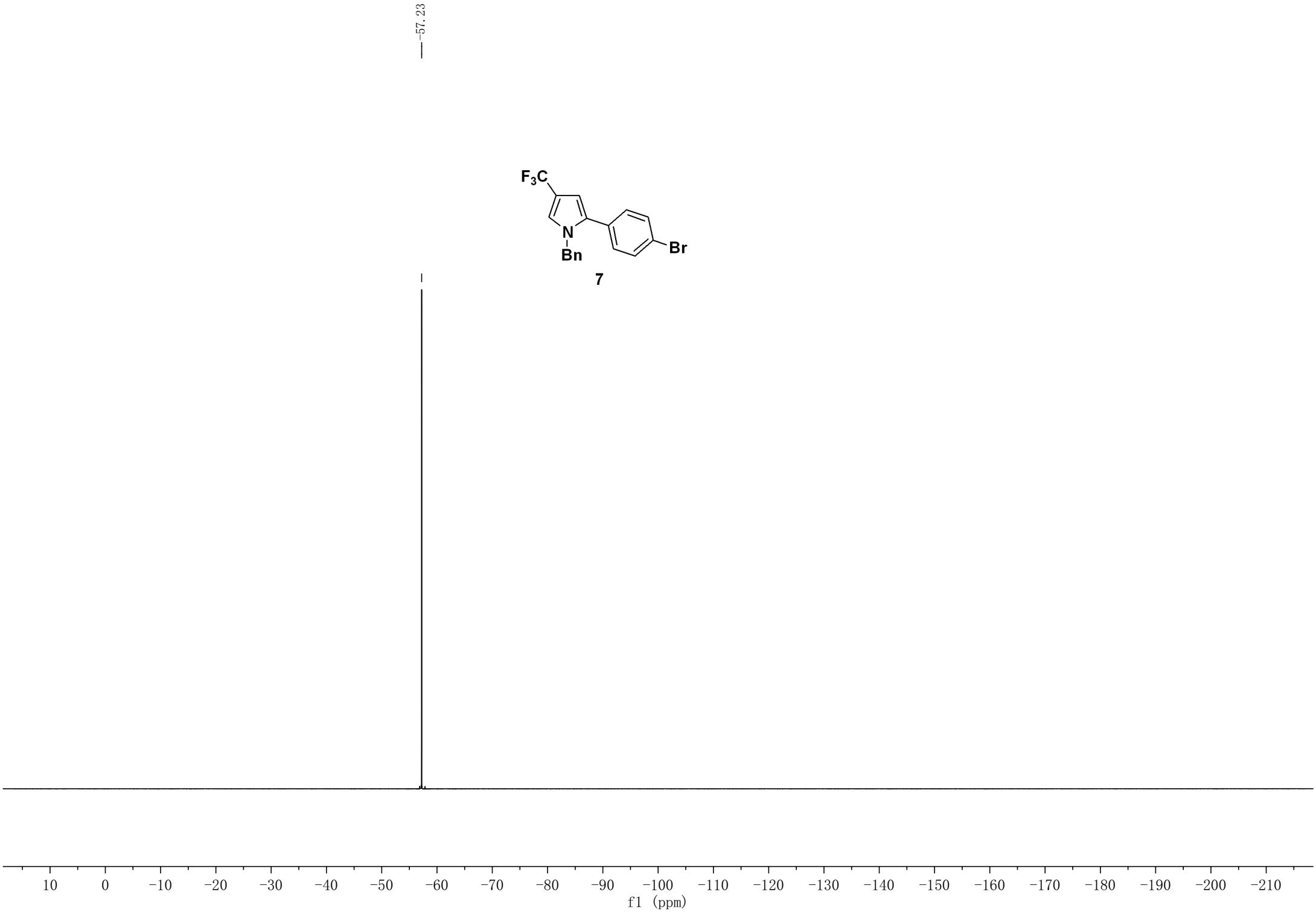
7.35
7.33
7.32
7.31
7.30
7.26
7.19
7.16
7.07
7.02
7.02
7.00
6.44
5.10
F3C
N
Bn
Br
7
2.00
2.97
2.08
1.01
1.97
2.00
f1 (ppm)


-57.23
F3C
N
Bn
Br
7
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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-100
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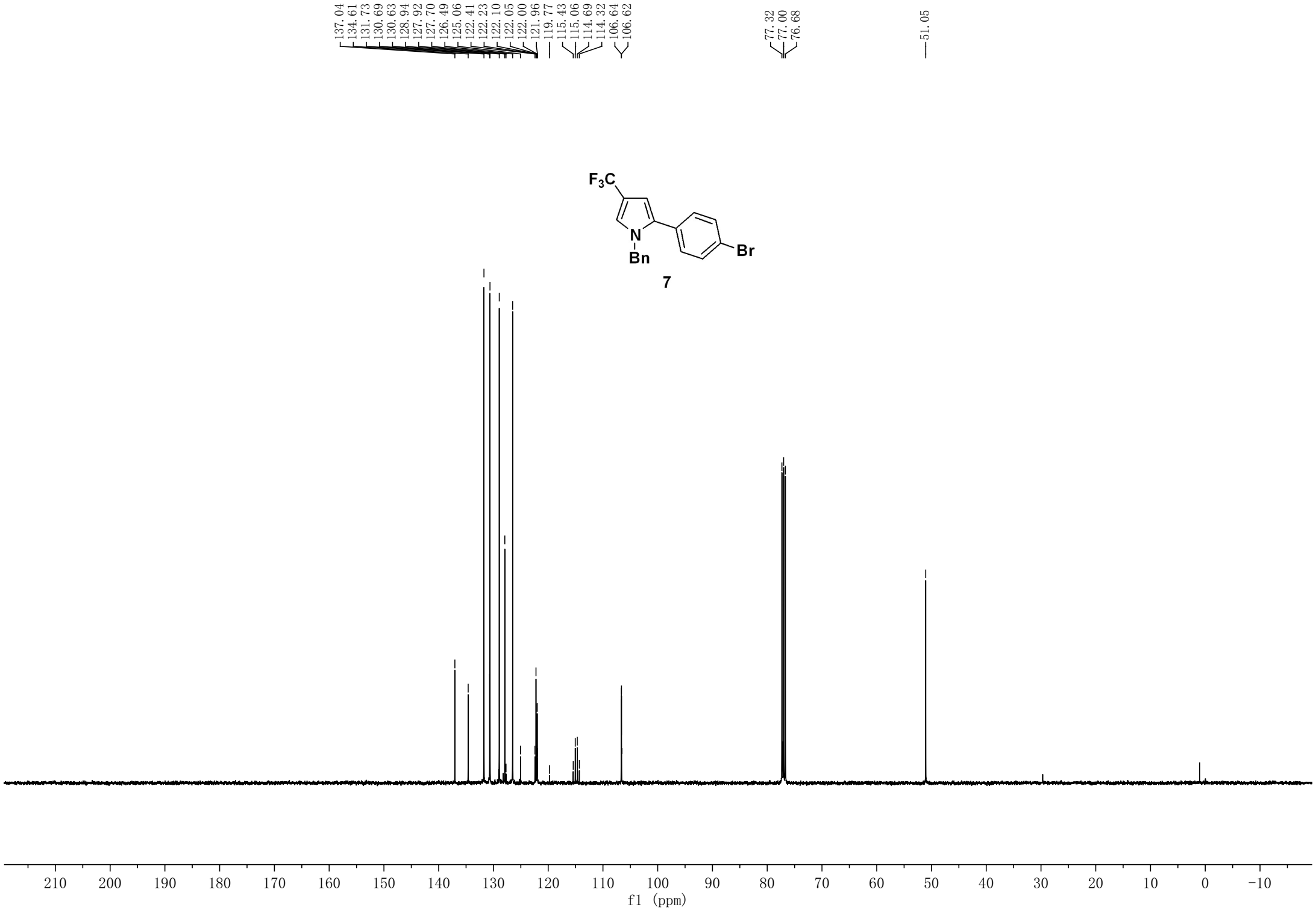
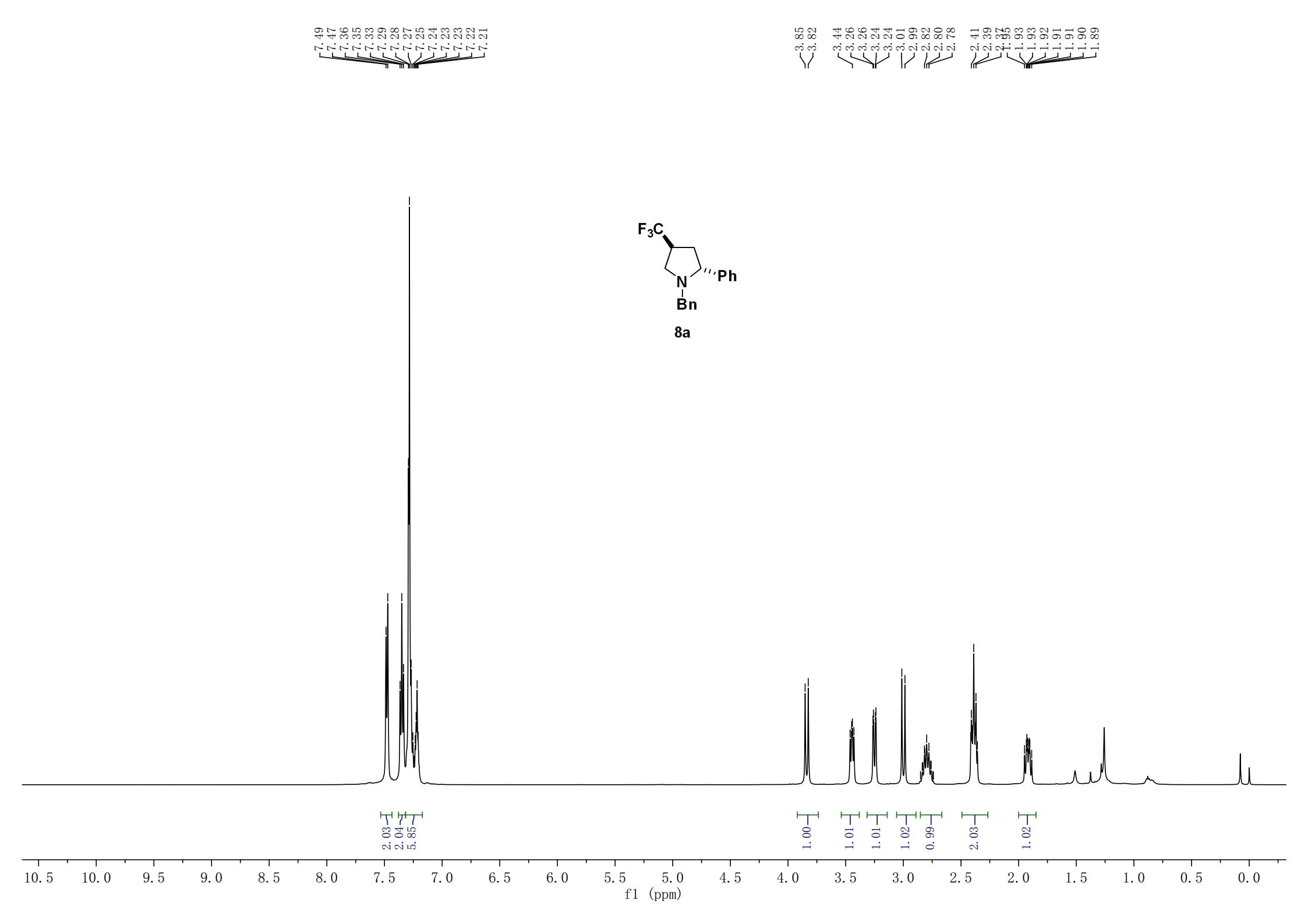
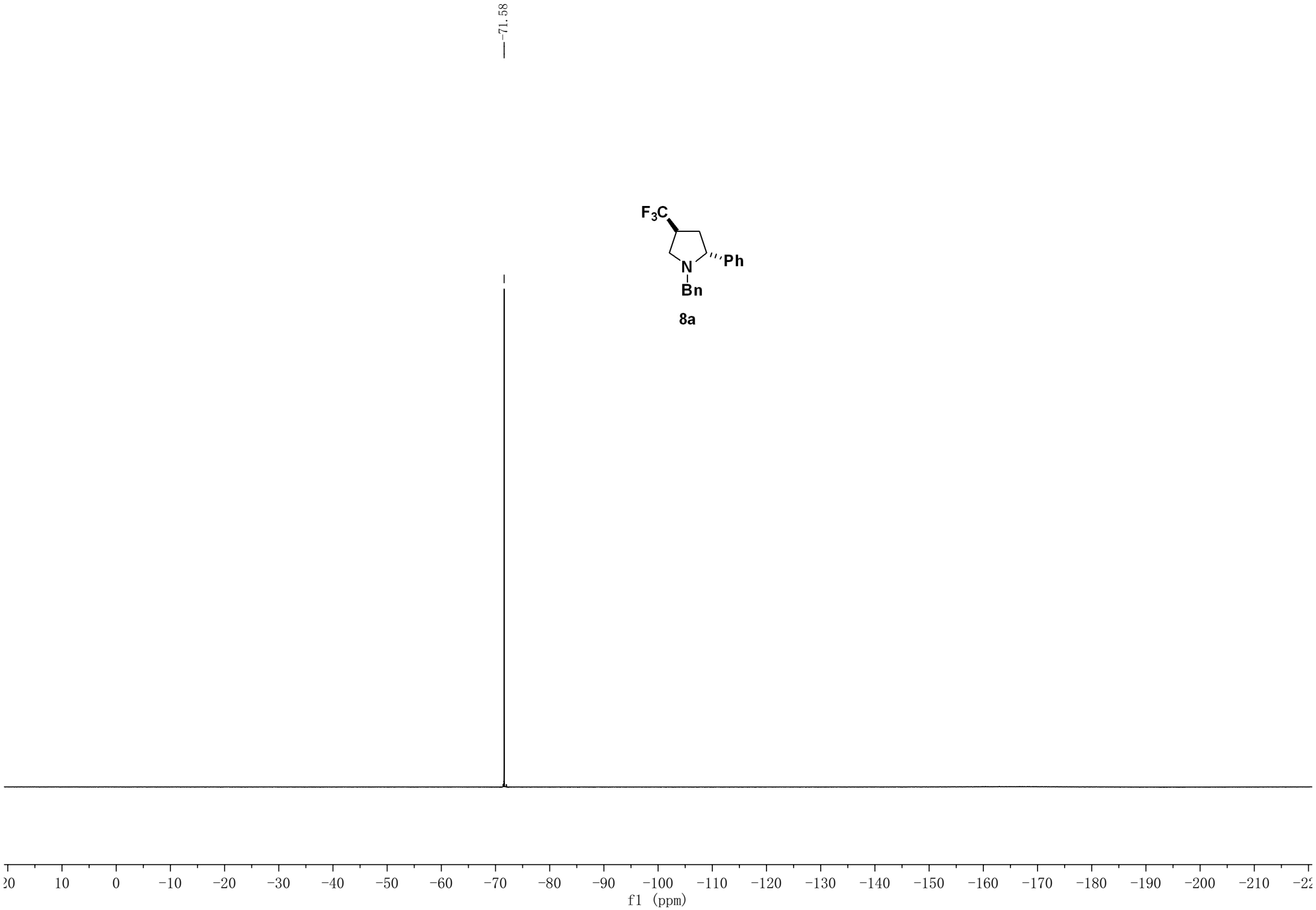
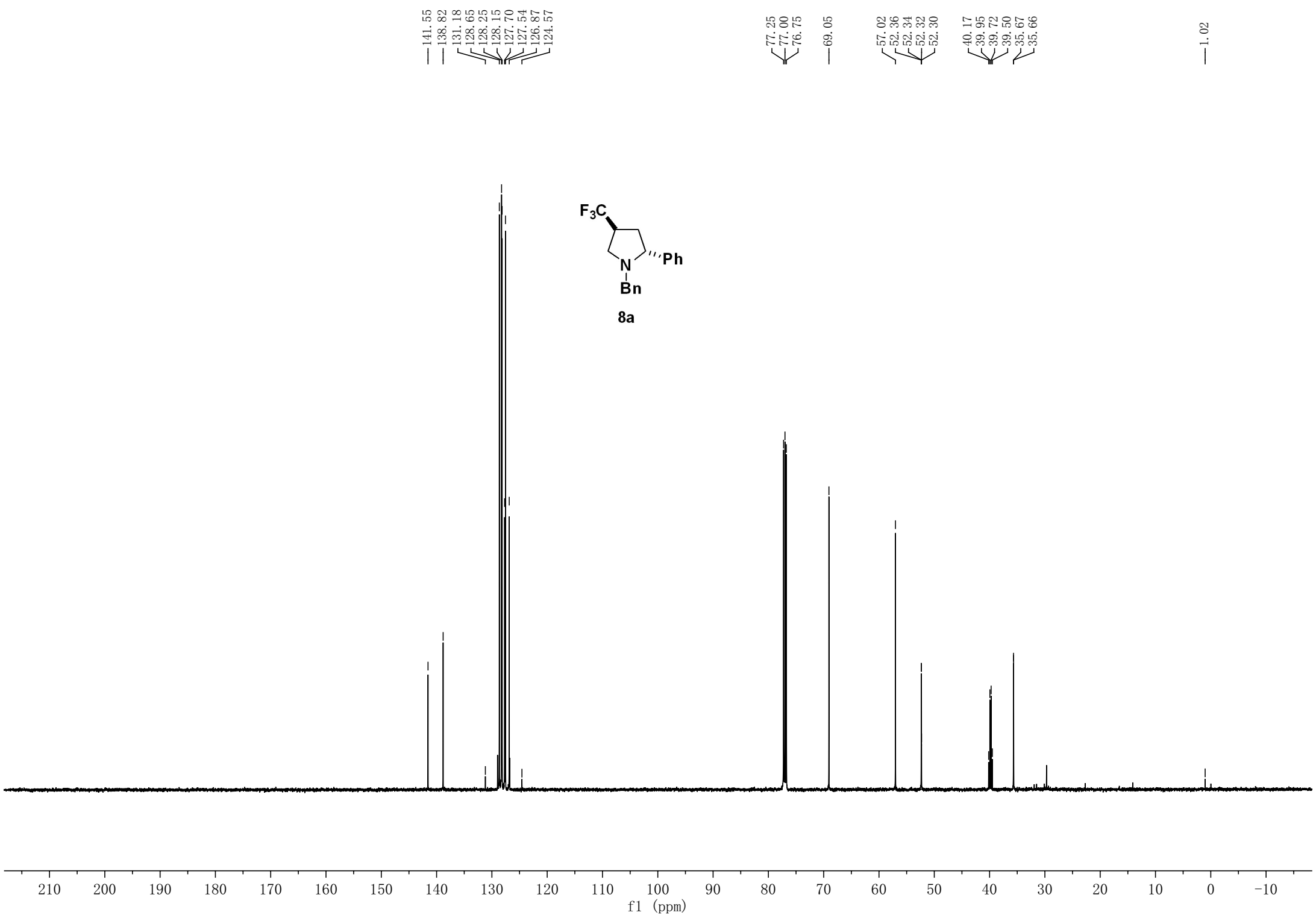
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


137.04
134.61
131.73
130.69
130.63
128.94
127.92
127.70
126.49
125.06
122.41
122.23
122.10
122.05
122.00
121.96
119.77
115.43
115.06
114.69
114.32
106.64
106.62
77.32
77.00
76.68
51.05
F3C
N
Bn
Br
7
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

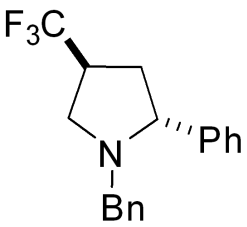

7.49
7.47
7.36
7.35
7.33
7.29
7.28
7.27
7.25
7.24
7.23
7.23
7.22
7.21
3.85
3.82
3.44
3.26
3.26
3.24
3.24
3.01
2.99
2.82
2.80
2.78
2.41
2.39
1.93
1.93
1.92
1.91
1.91
1.90
1.89
F3C
Ph
N
Bn
8a
2.03
2.04
5.85
1.00
1.01
1.01
1.02
0.99
2.03
1.02
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-71.58
F3C
Ph
N
Bn
8a
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

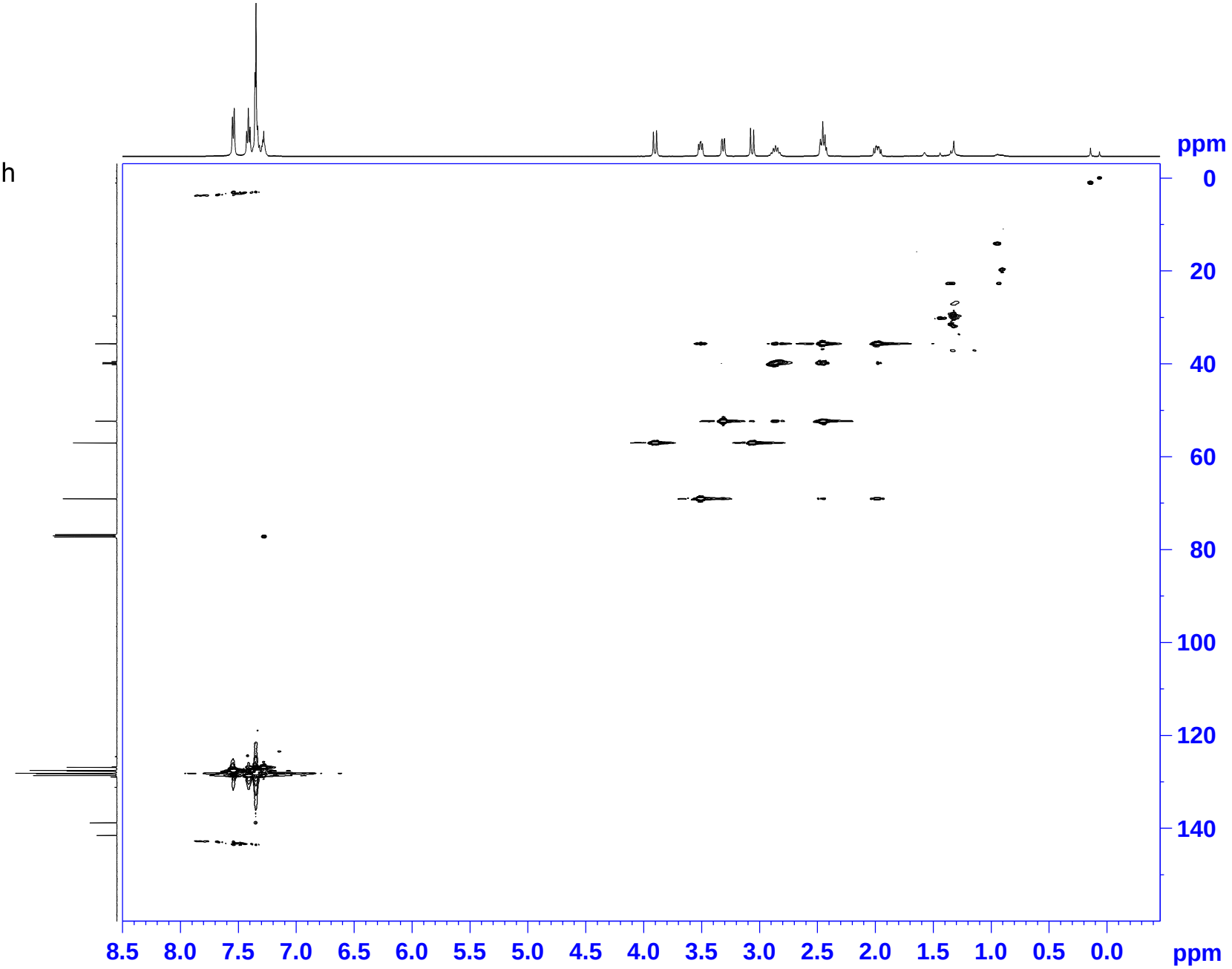

141.55
138.82
131.18
128.65
128.25
128.15
127.70
127.54
126.87
124.57
77.25
77.00
76.75
69.05
57.02
52.36
52.34
52.32
52.30
40.17
39.95
39.72
39.50
35.67
35.66
1.02
F3C
Ph
N
Bn
8a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

xml-6

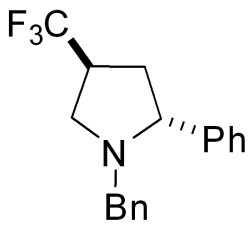
HSQC


F3C
Ph
N
Bn

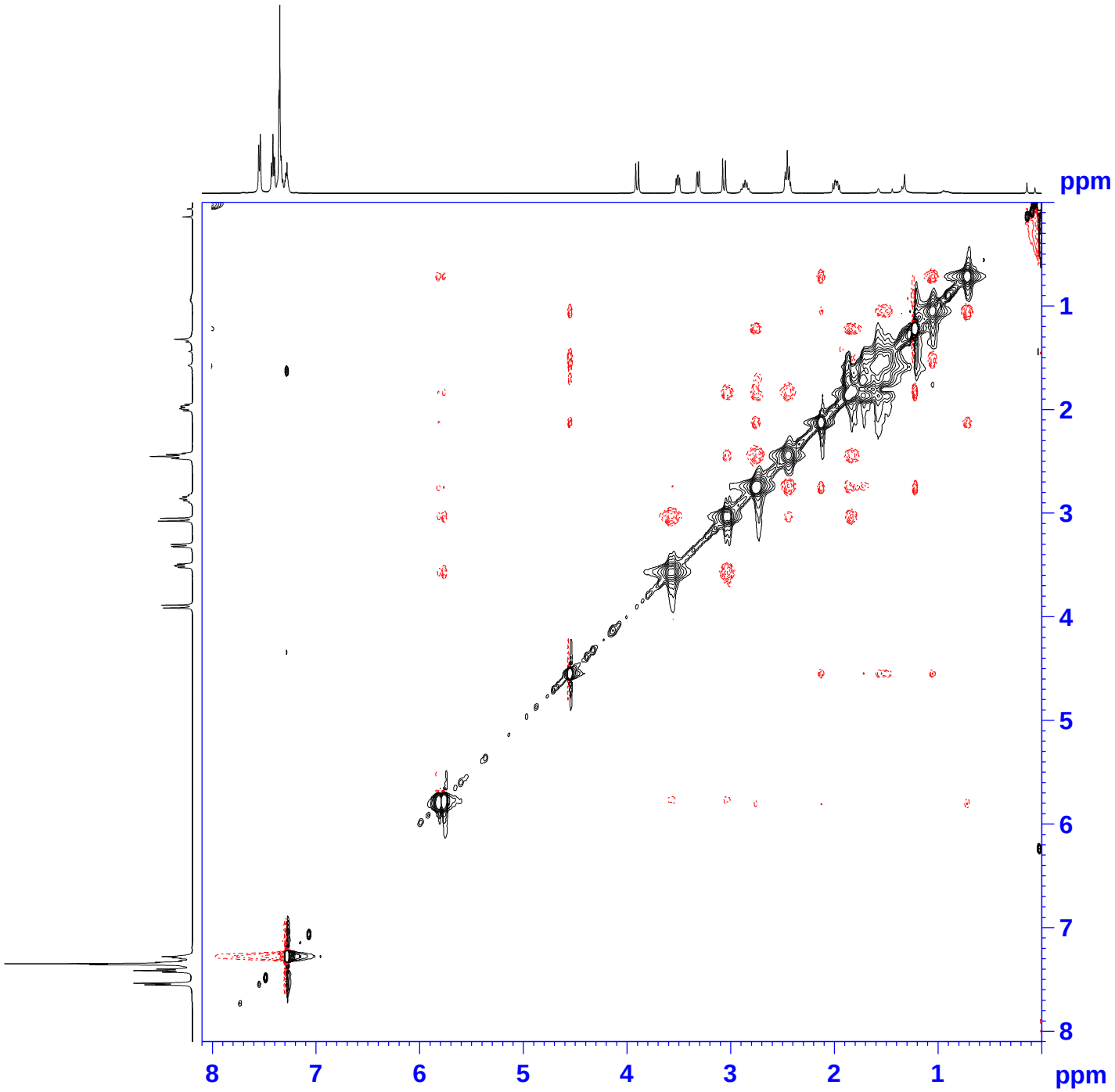
8a

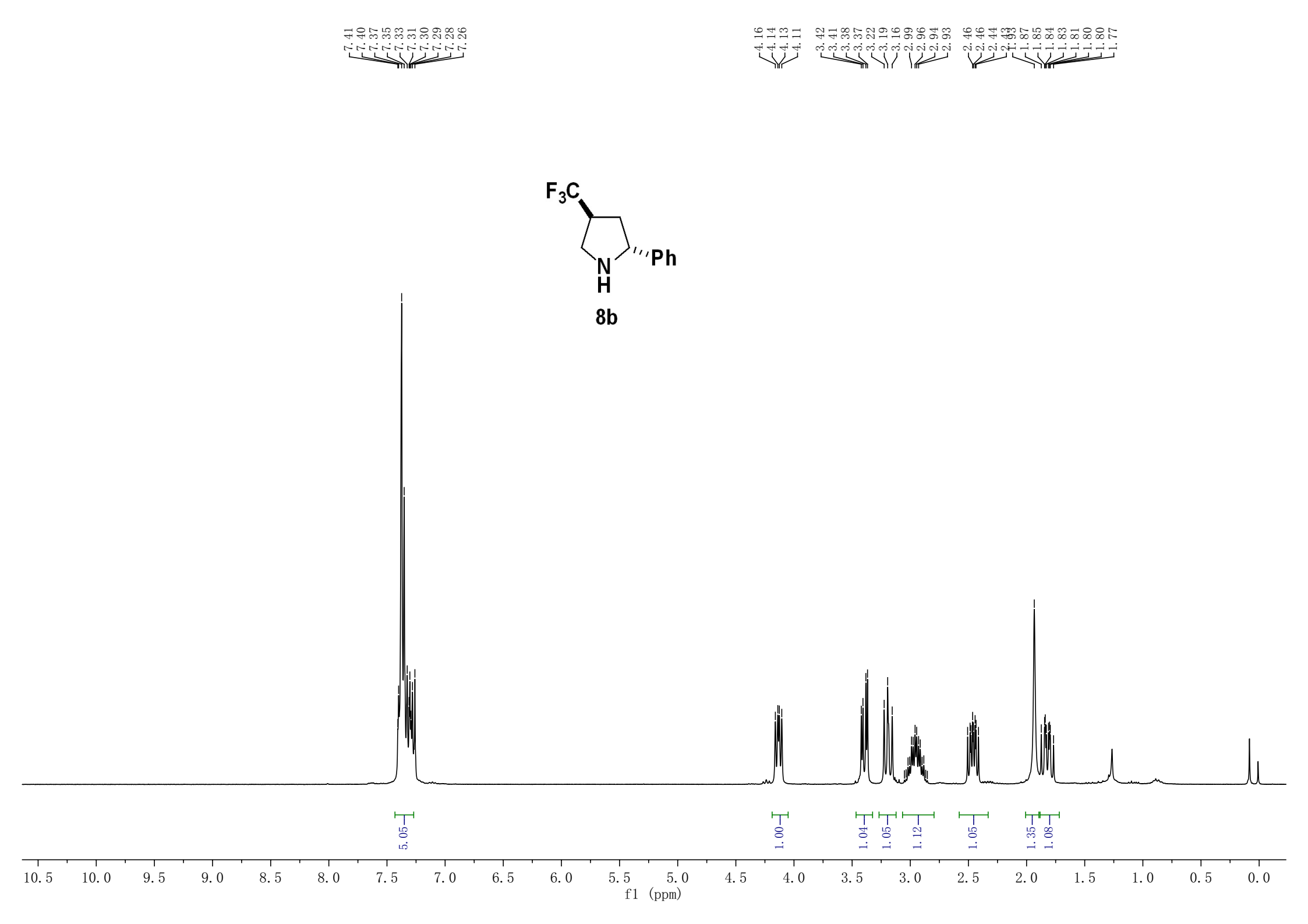

ppm
0
20
40
60
80
100
120
140
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

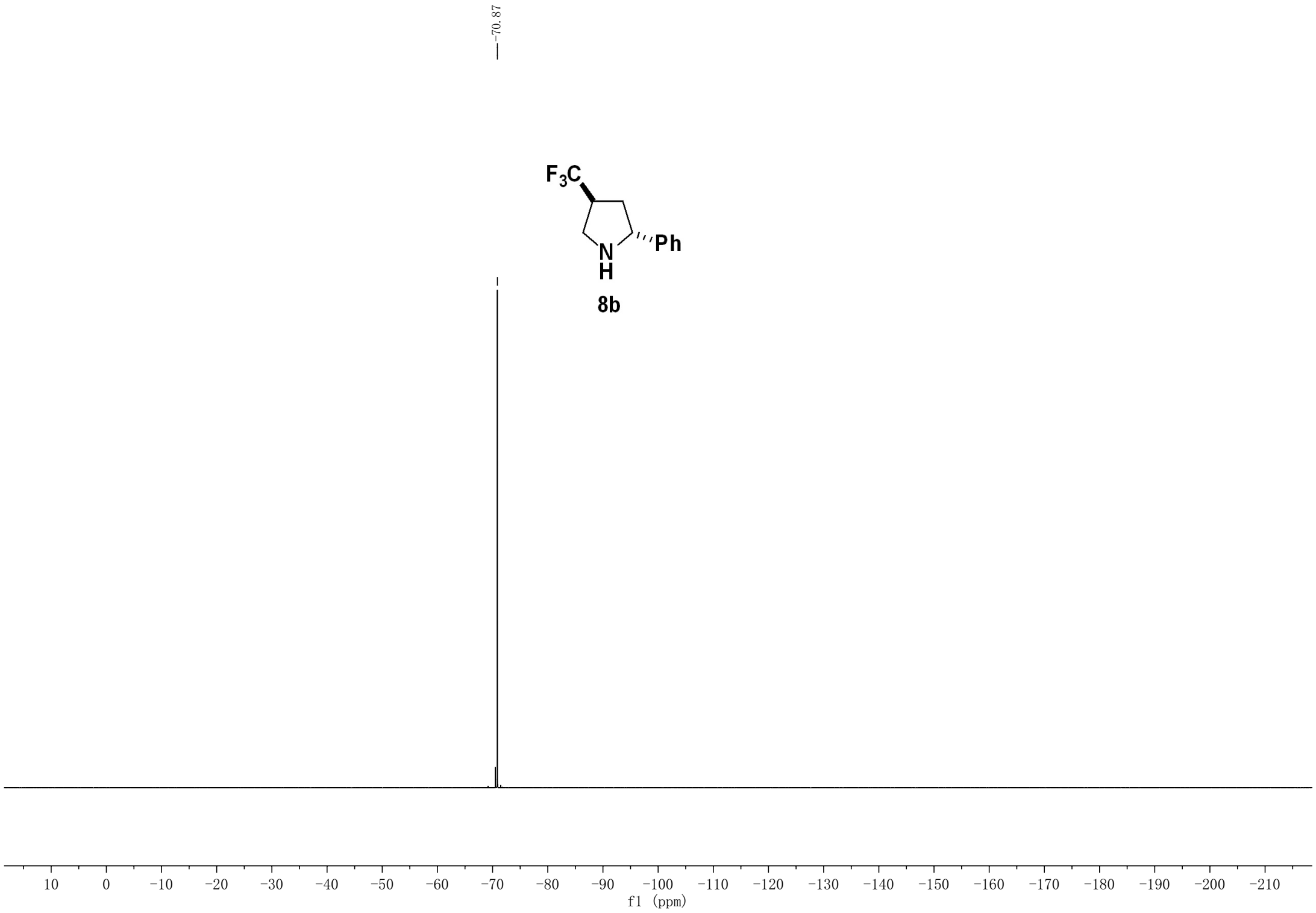
NOESY

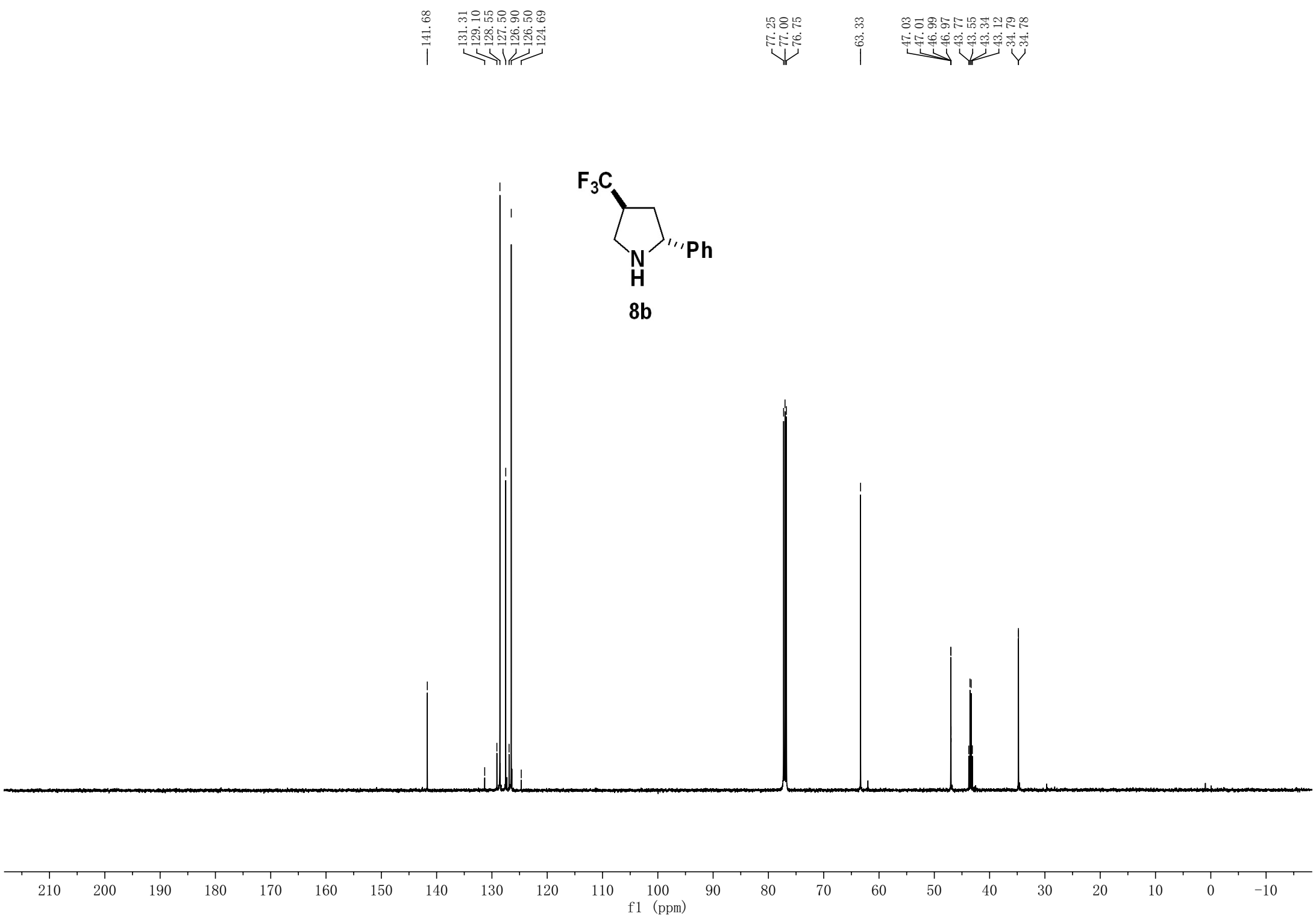


8a



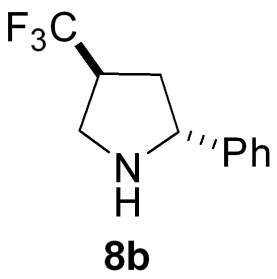

7.41
7.40
7.37
7.35
7.33
7.31
7.30
7.29
7.28
7.26
4.16
4.14
4.13
4.11
3.42
3.41
3.38
3.37
3.22
3.19
3.16
2.99
2.96
2.94
2.93
2.46
2.46
2.44
1.93
1.87
1.85
1.84
1.83
1.81
1.80
1.80
1.77
F3C
Ph
N
H
8b
5.05
1.00
1.04
1.05
1.12
1.05
1.35
1.08
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-70.87
F3C
Ph
N
H
8b
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

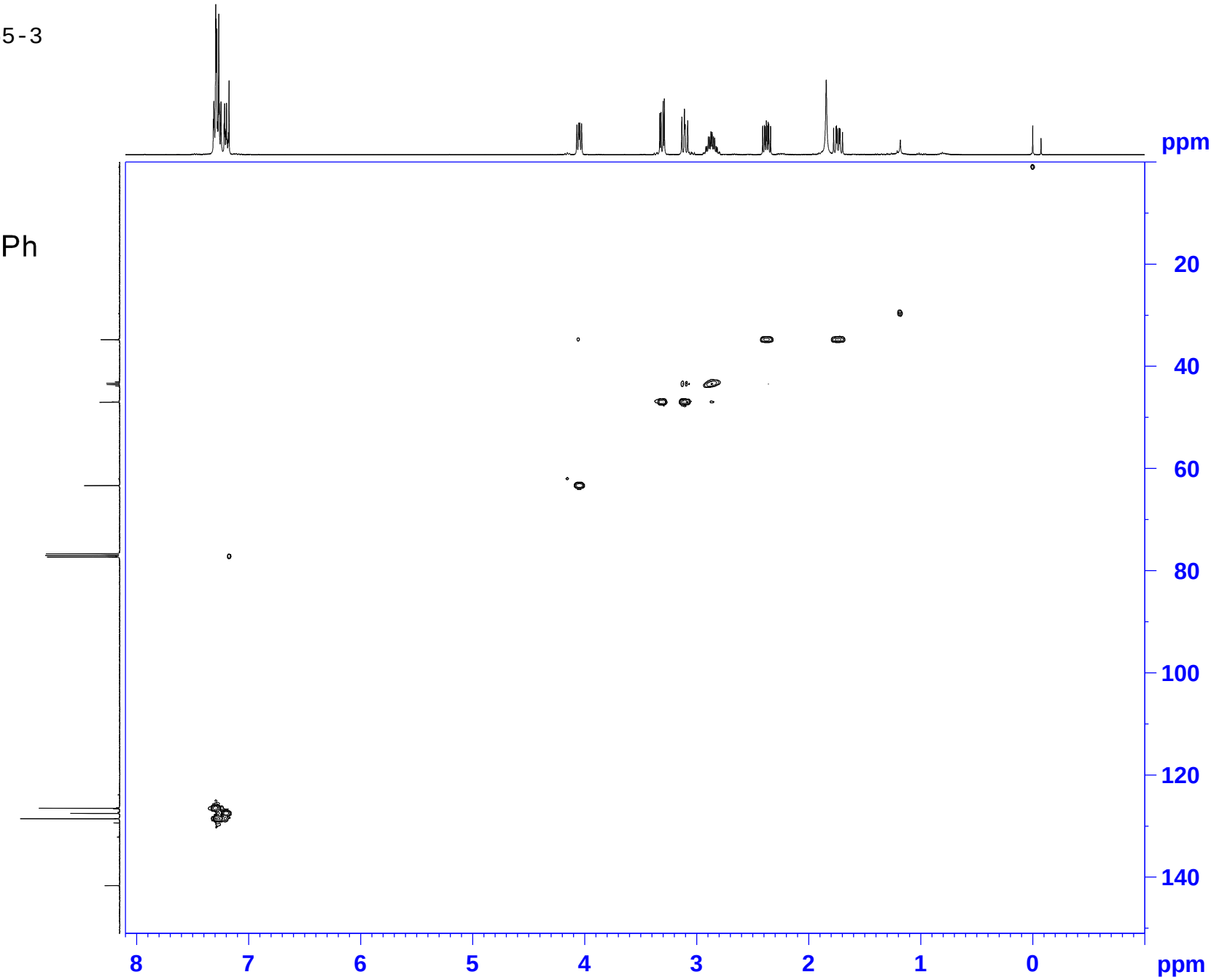

141.68
131.31
129.10
128.55
127.50
126.90
126.50
124.69
77.25
77.00
76.75
63.33
47.03
47.01
46.99
46.97
43.77
43.55
43.34
43.12
34.79
34.78
F3C
Ph
N
H
8b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

zxf-4-65-3

HSQC

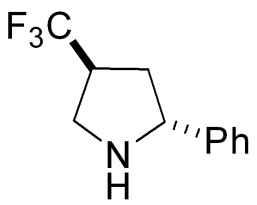


8b

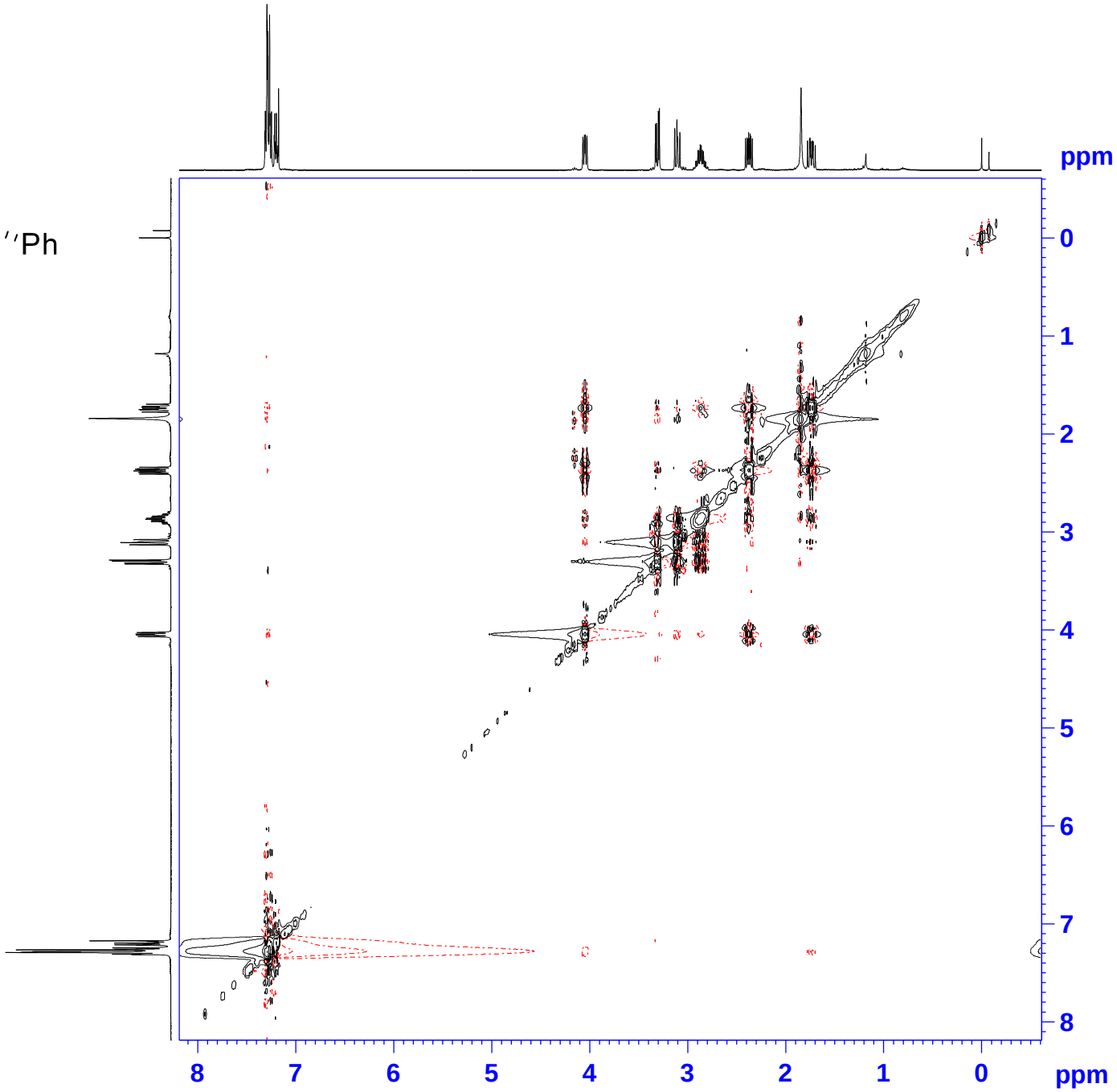


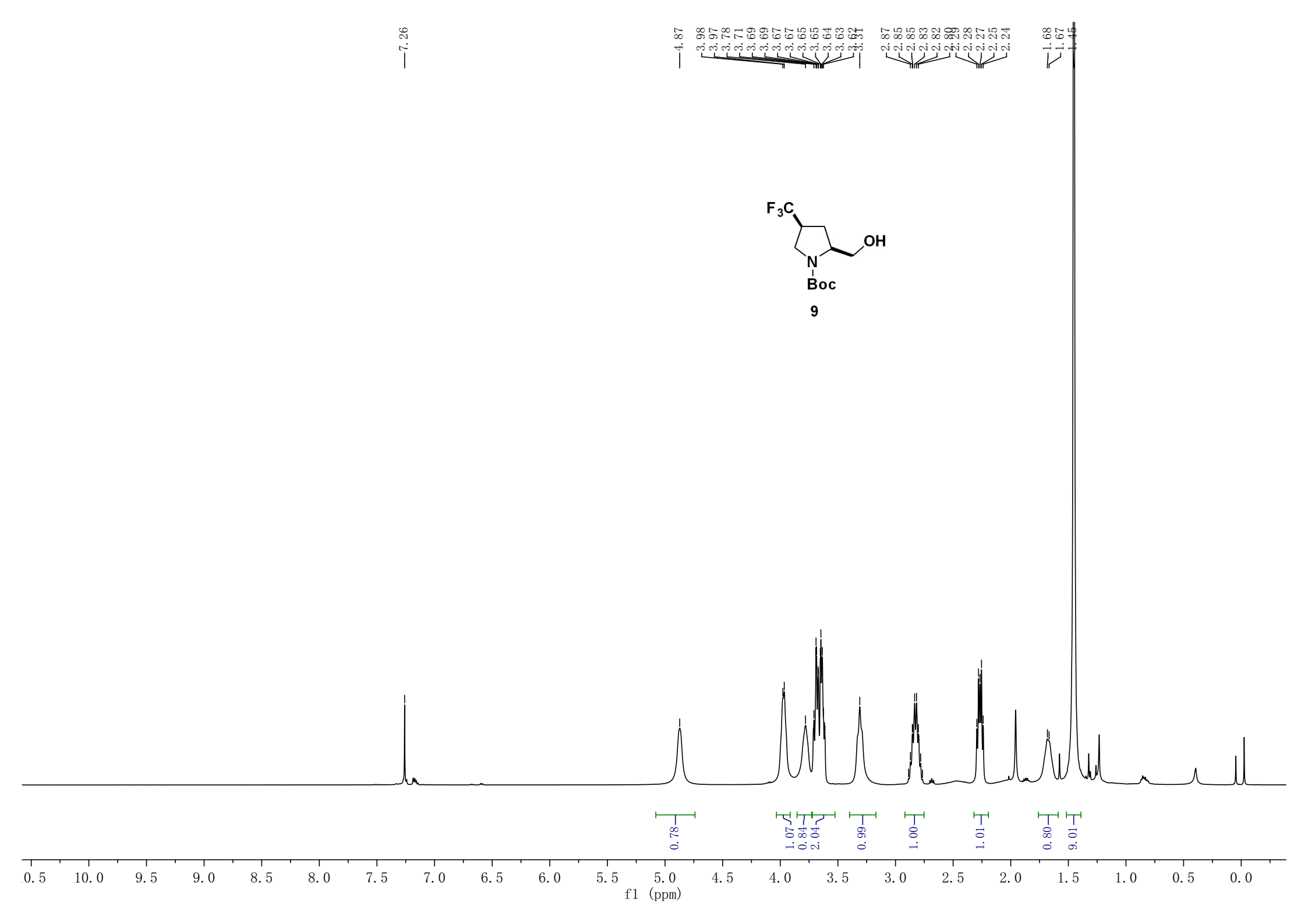
zxf-4-65-3

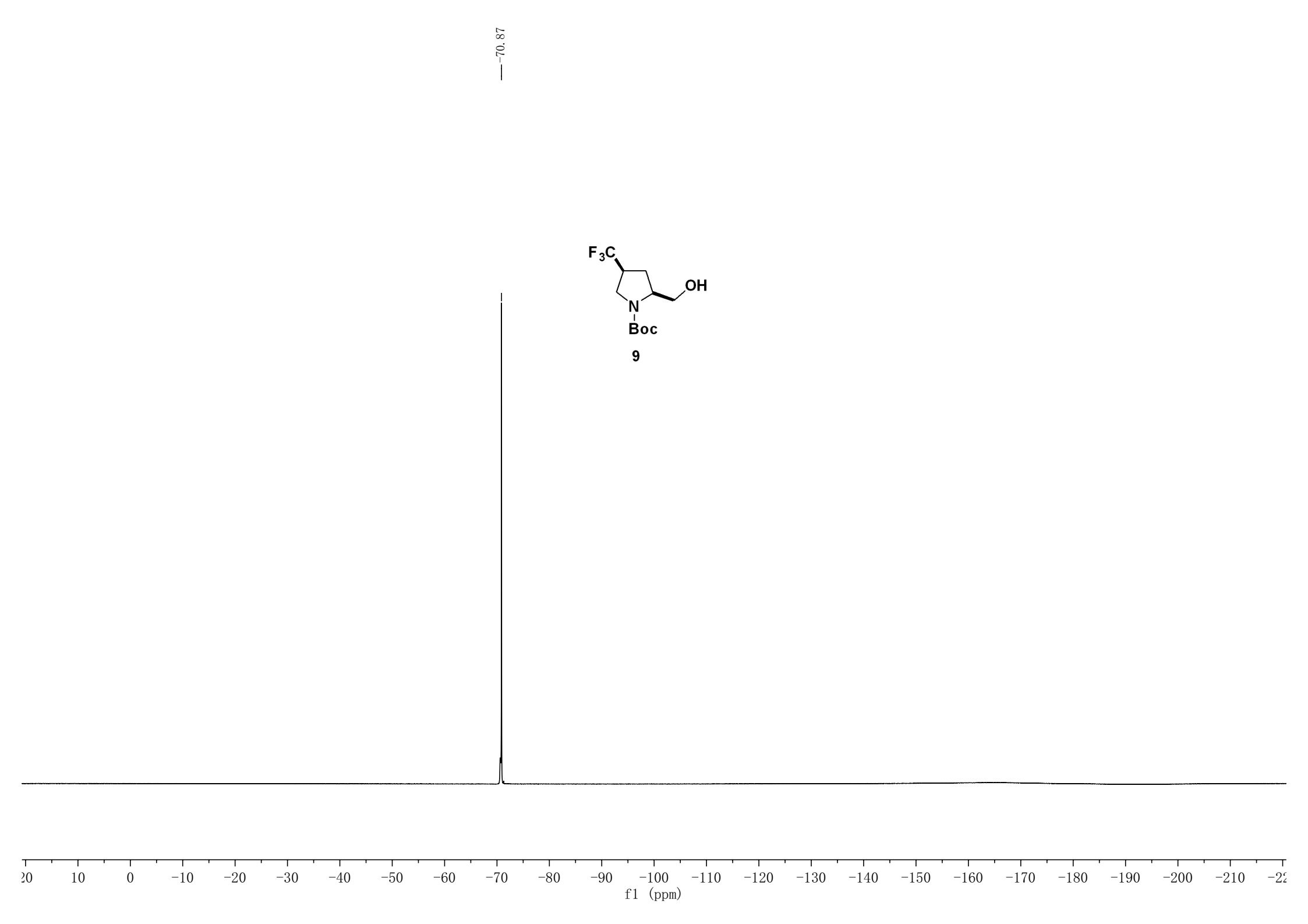
NOESY

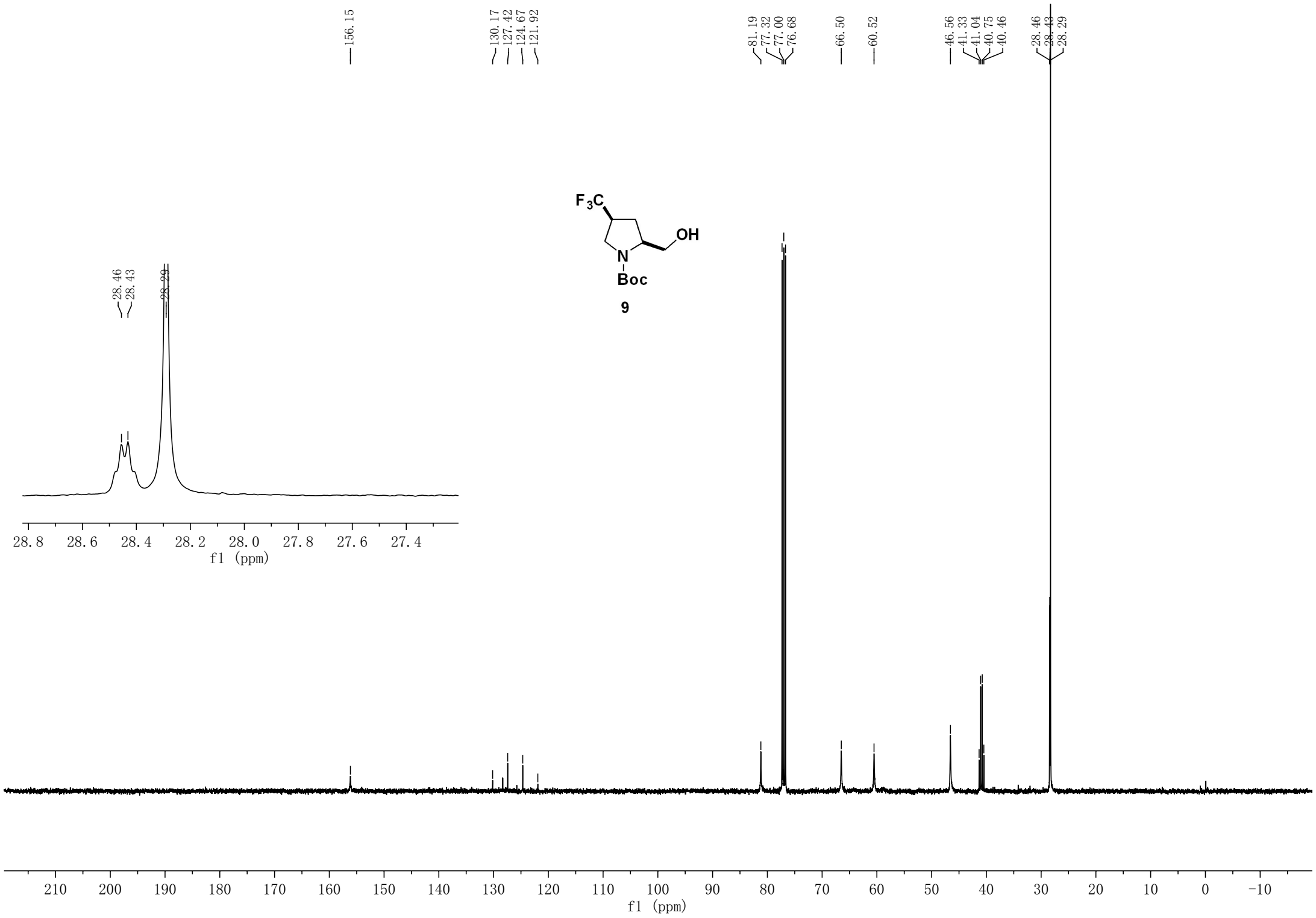


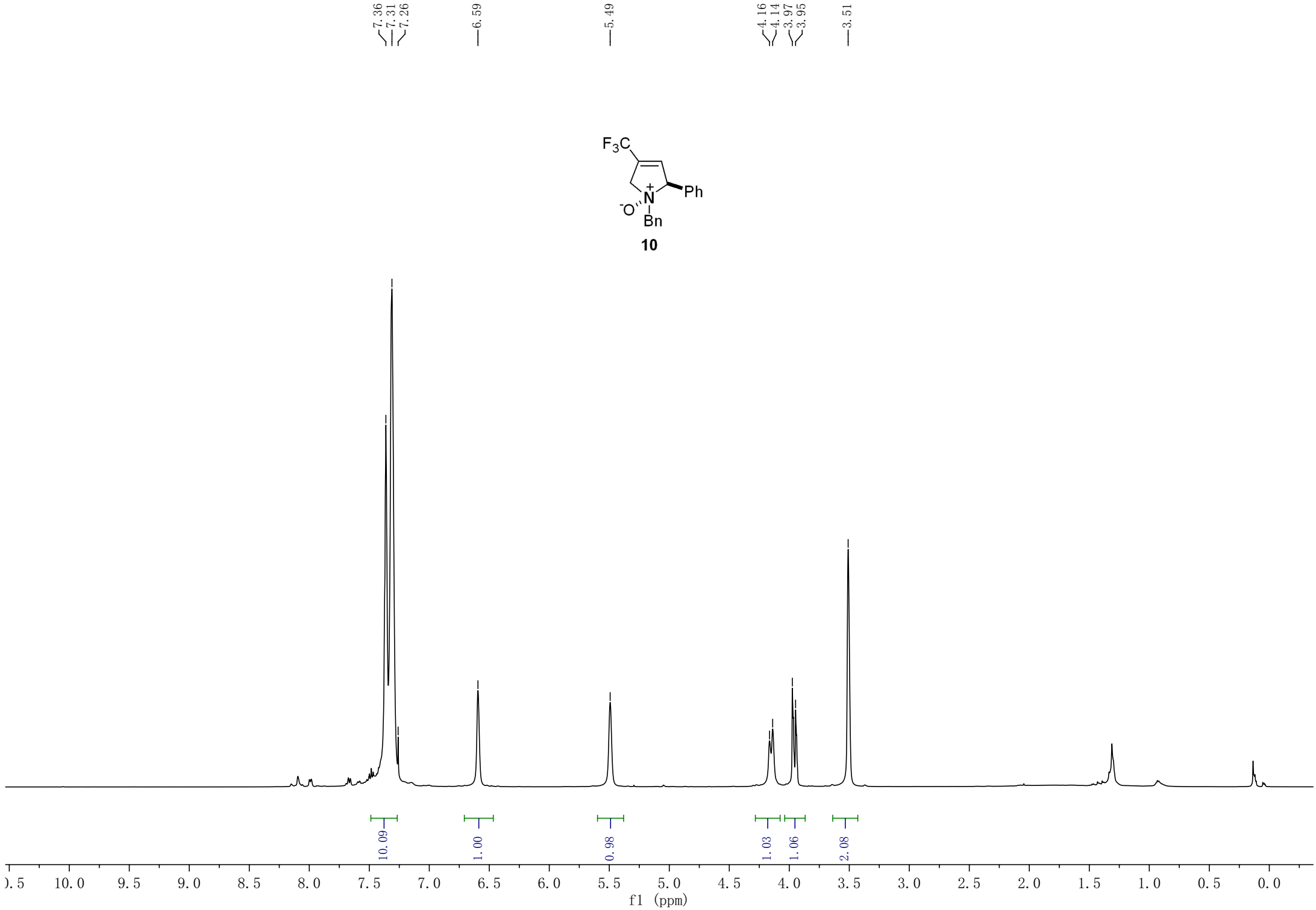
8b

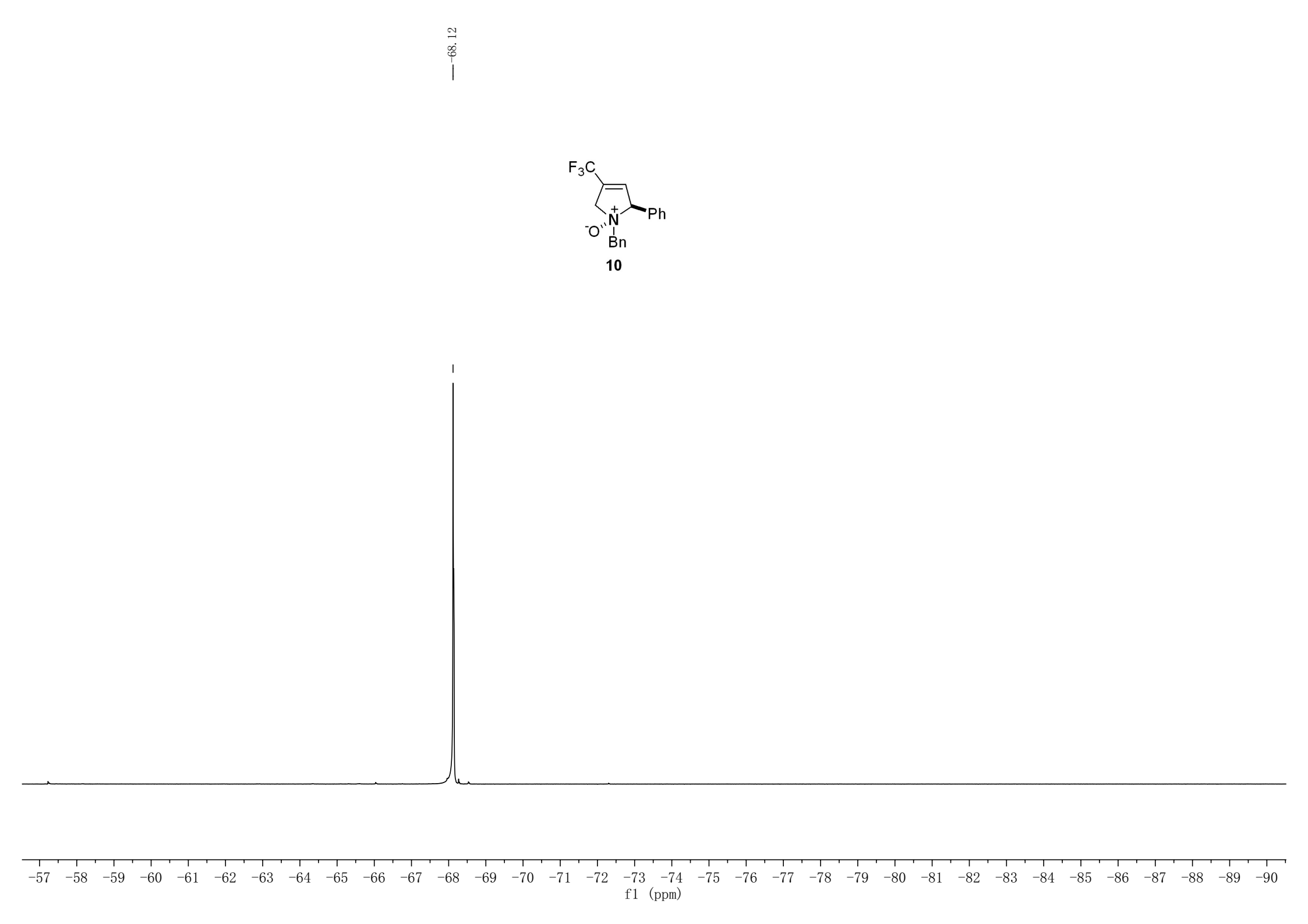


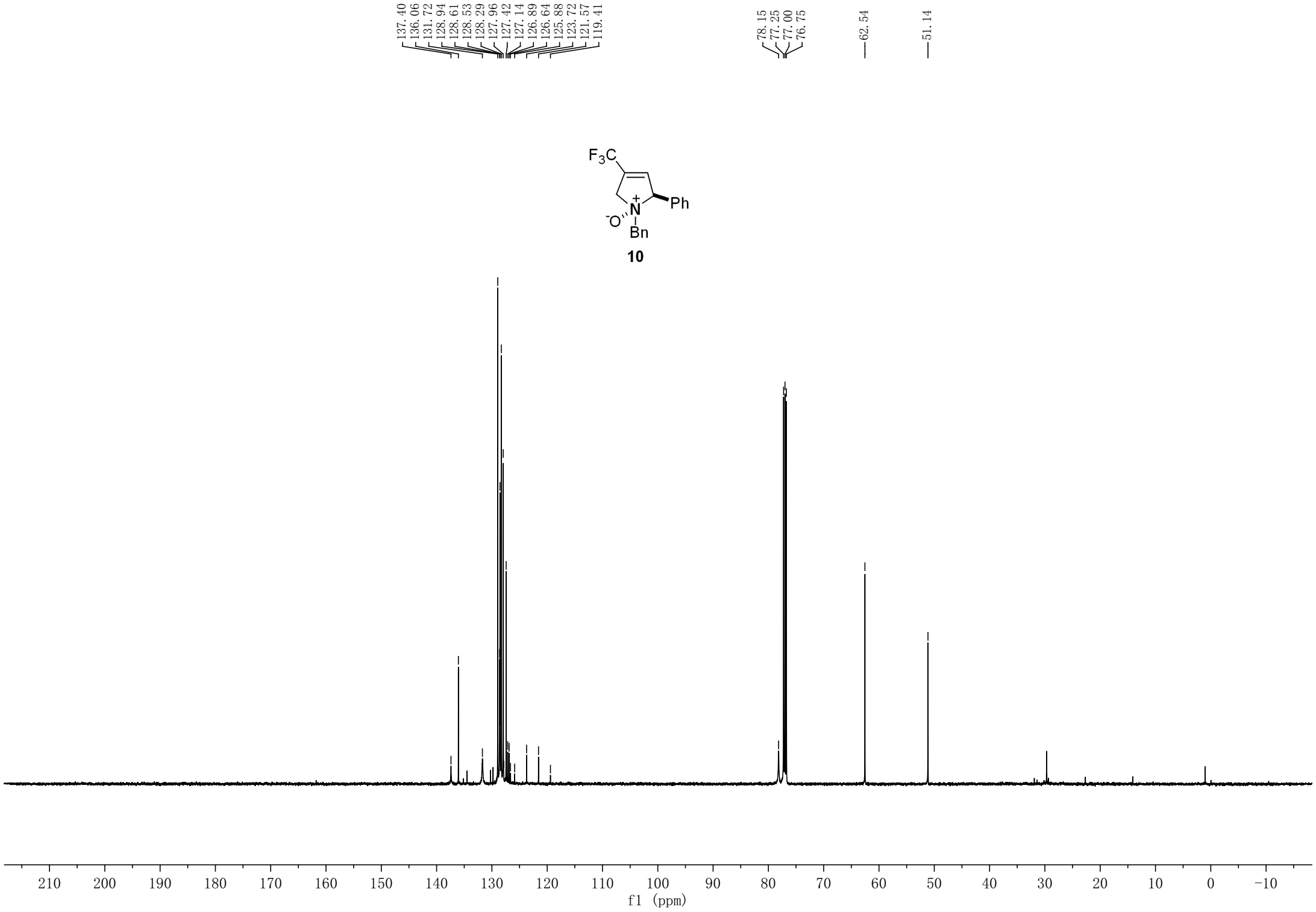

7.26
4.87
3.98
3.97
3.78
3.71
3.69
3.69
3.67
3.67
3.65
3.65
3.64
3.63
3.62
3.31
2.87
2.85
2.85
2.83
2.82
2.29
2.28
2.27
2.25
2.24
1.68
1.67
1.46
F3C
OH
N
Boc
9
0.78
1.07
0.84
2.04
0.99
1.00
1.01
0.80
9.01
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

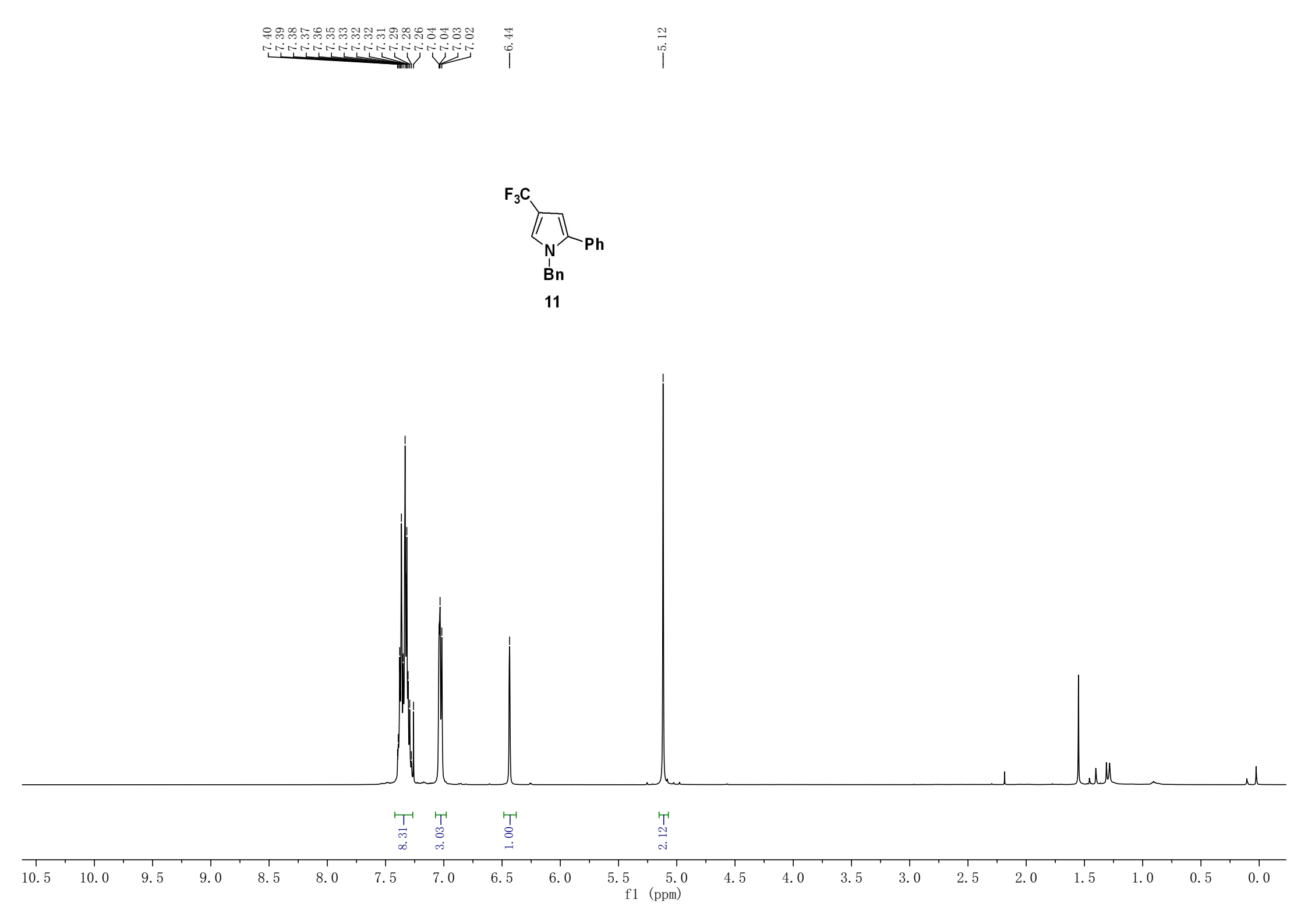

−70.87
F3C
OH
N
Boc
9
20
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

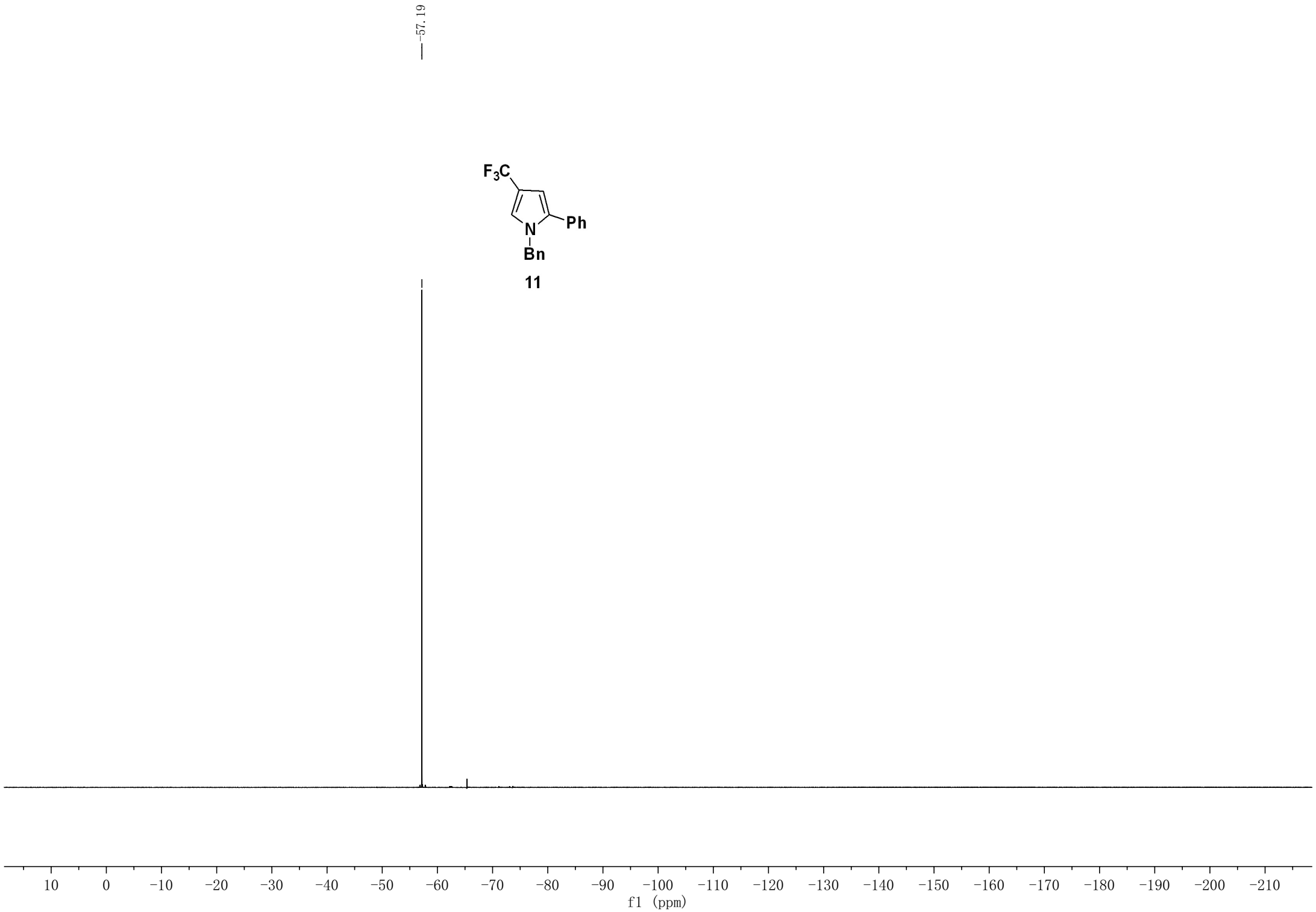

156.15
130.17
127.42
124.67
121.92
81.19
77.32
77.00
76.68
66.50
60.52
46.56
41.33
41.04
40.75
40.46
28.46
28.43
28.29
F3C
OH
N
Boc
9
28.46
28.43
28.29
28.8 28.6 28.4 28.2 28.0 27.8 27.6 27.4
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.36
7.31
7.26
6.59
5.49
4.16
4.14
3.97
3.95
3.51
F3C
Ph
N
O
Bn
10
10.09
1.00
0.98
1.03
1.06
2.08
f1 (ppm)


-68.12
F3C
Ph
N
O
Bn
10
-57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 -81 -82 -83 -84 -85 -86 -87 -88 -89 -90
f1 (ppm)


137.40
136.06
131.72
128.94
128.61
128.53
128.29
127.96
127.42
127.14
126.89
126.64
125.88
123.72
121.57
119.41
78.15
77.25
77.00
76.75
62.54
51.14
F3C
Ph
N
O
Bn
10
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.40
7.39
7.38
7.37
7.36
7.35
7.33
7.32
7.32
7.31
7.29
7.28
7.26
7.04
7.04
7.03
7.02
6.44
5.12
F3C
Ph
N
Bn
11
8.31
3.03
1.00
2.12
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-57.19
F3C
Ph
N
Bn
11
10
0
-10
-20
-30
-40
-50
-60
-70
-80
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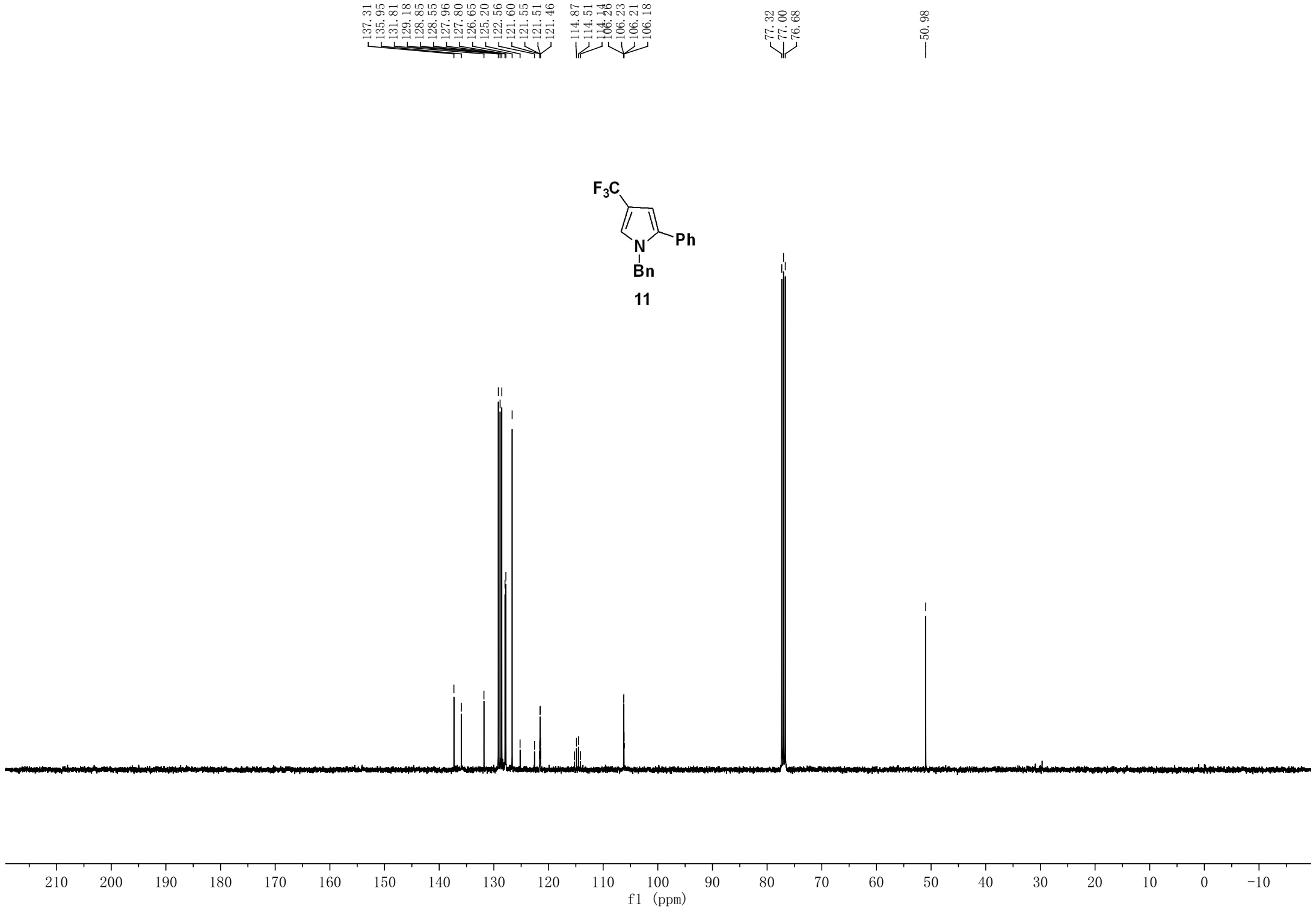
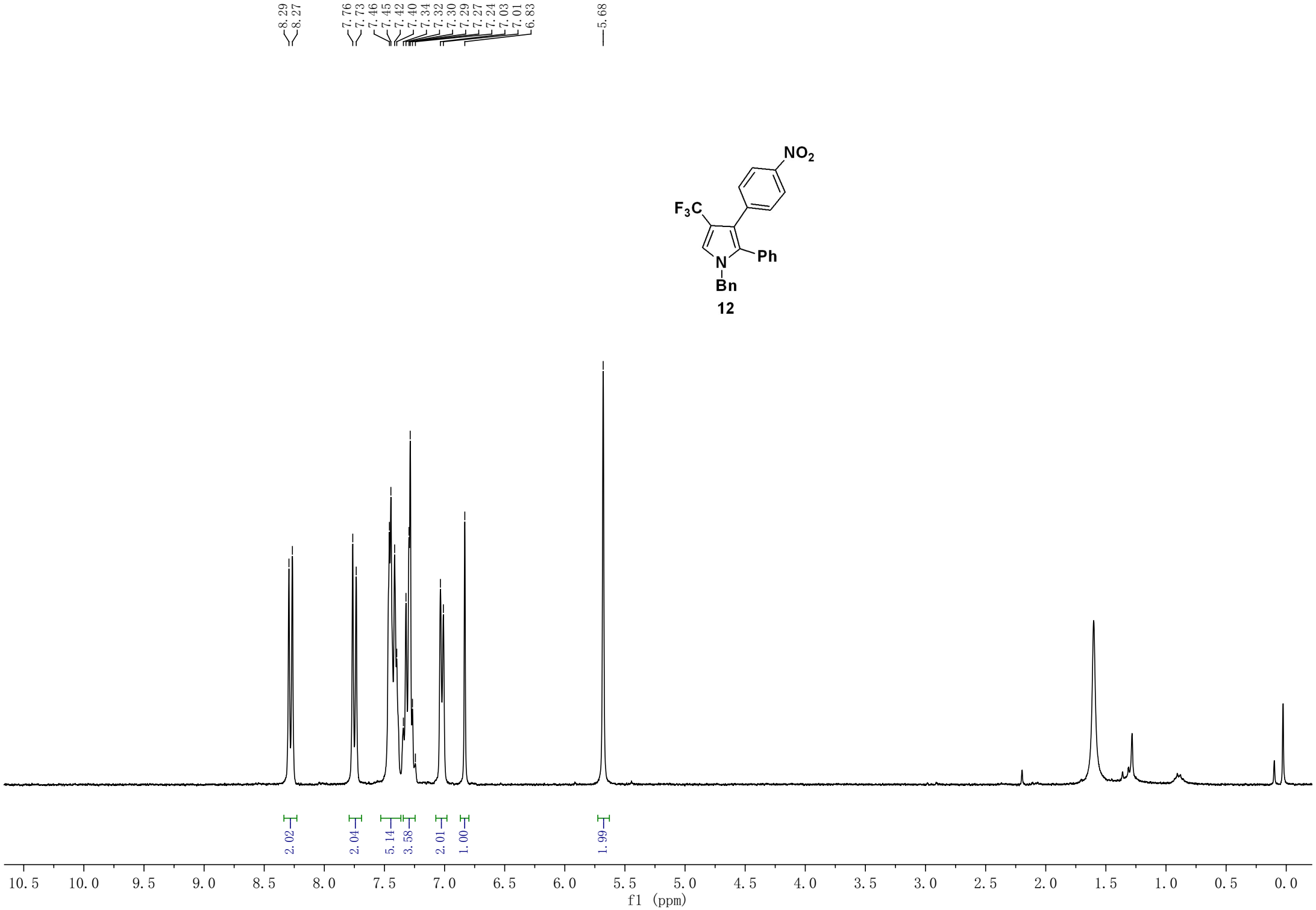
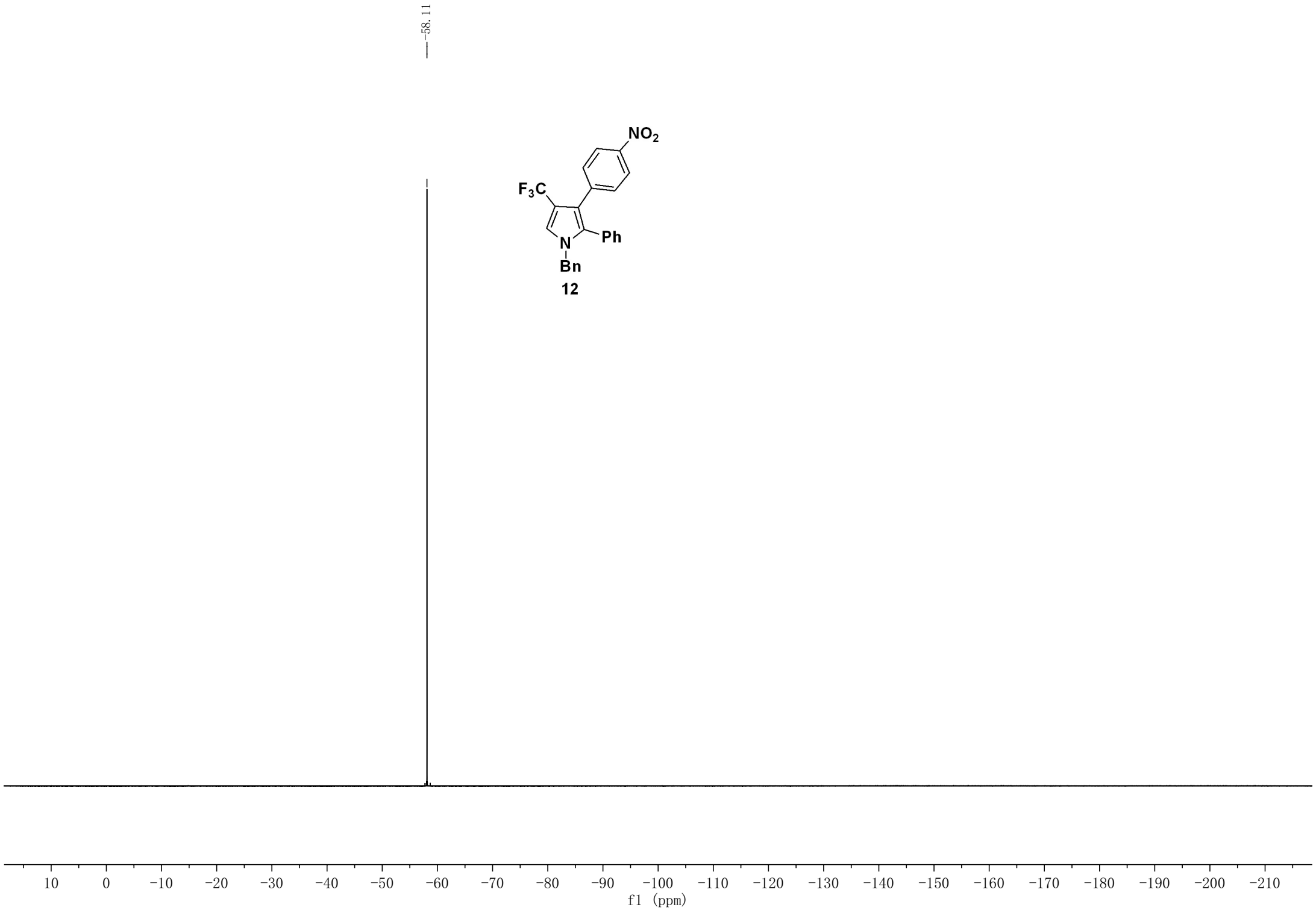
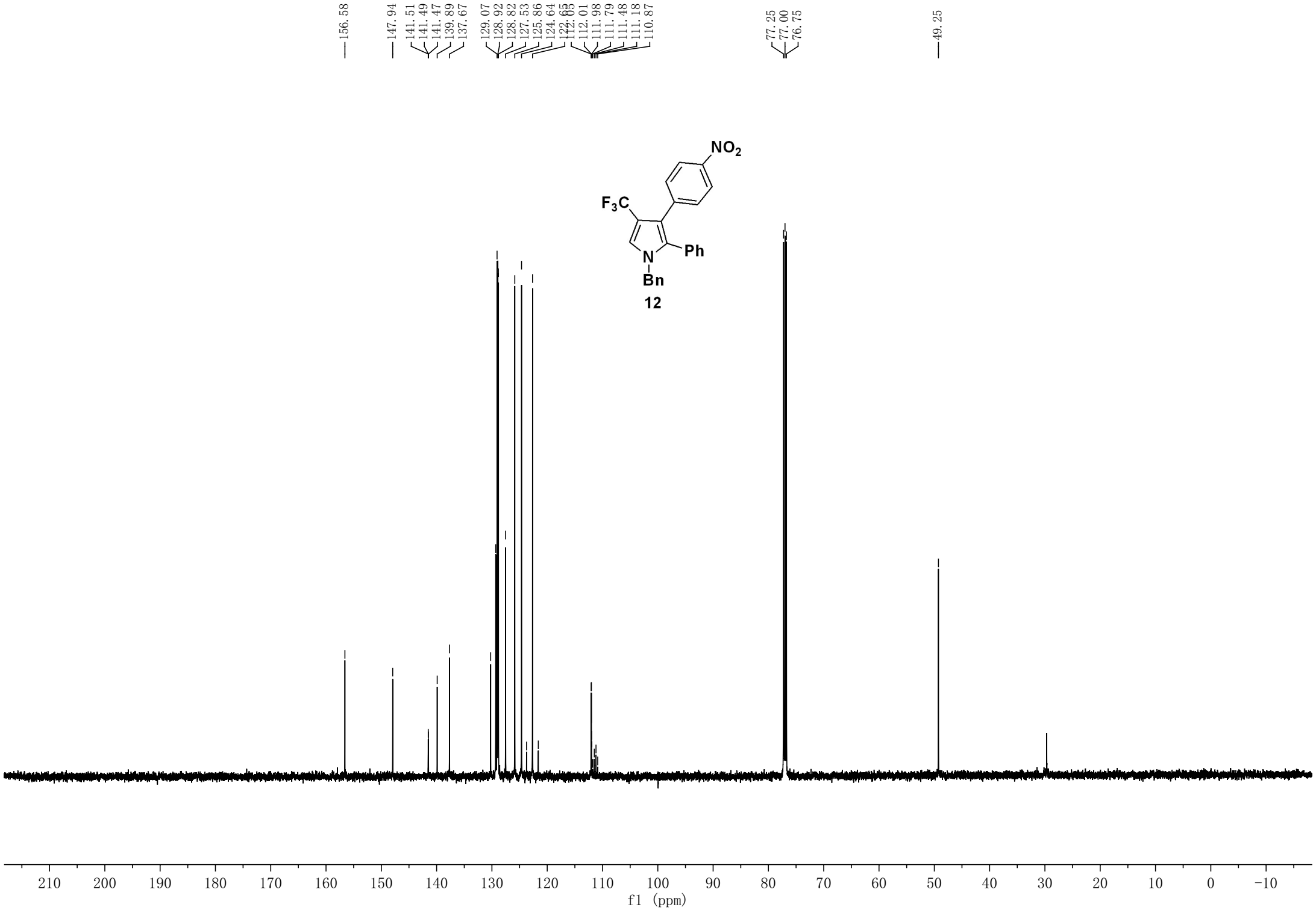
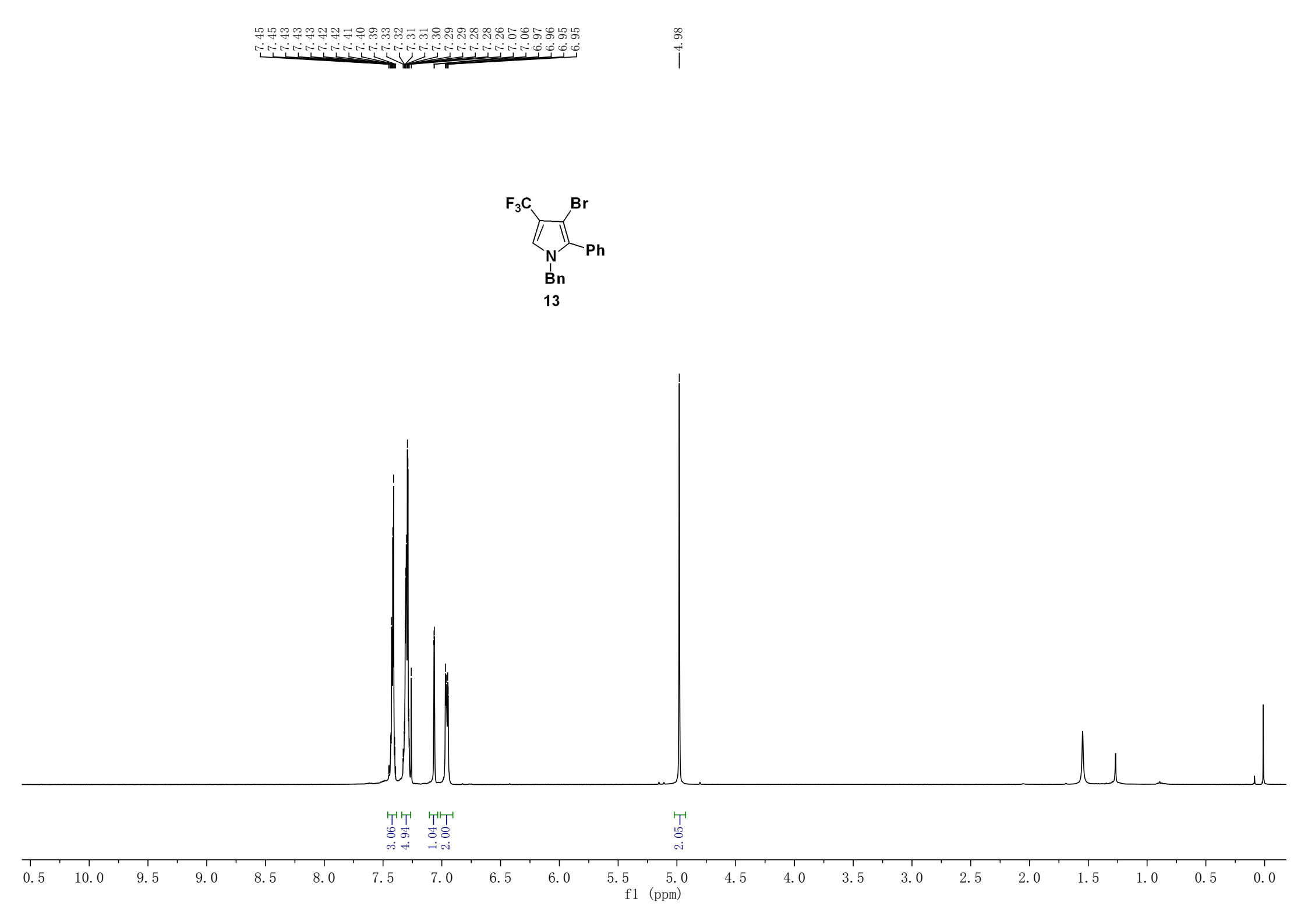
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

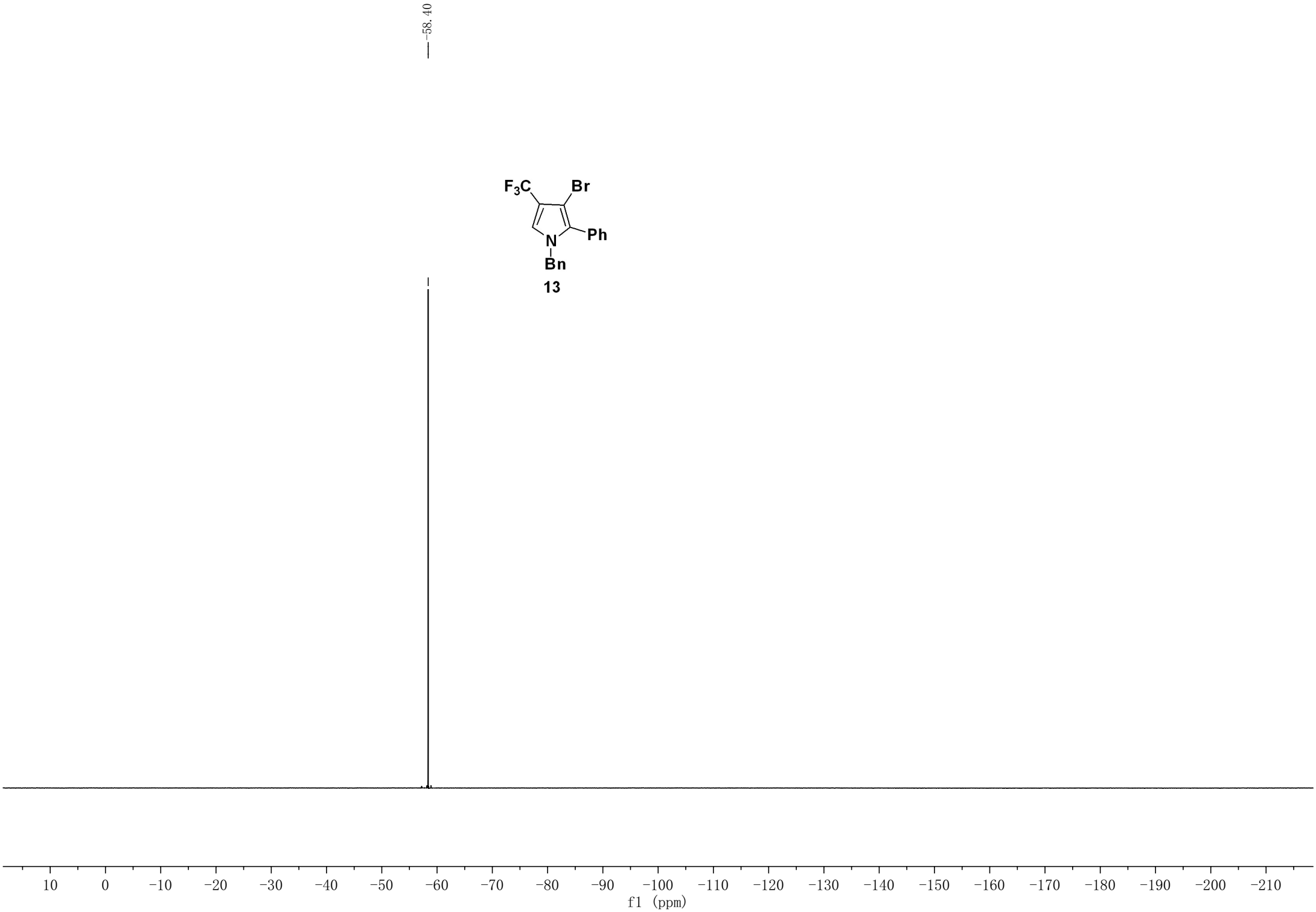

137.31
135.95
131.81
129.18
128.85
128.55
127.96
127.80
126.65
125.20
122.56
121.60
121.55
121.51
121.46
114.87
114.51
106.26
106.23
106.21
106.18
77.32
77.00
76.68
50.98
F3C
Ph
N
Bn
11
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

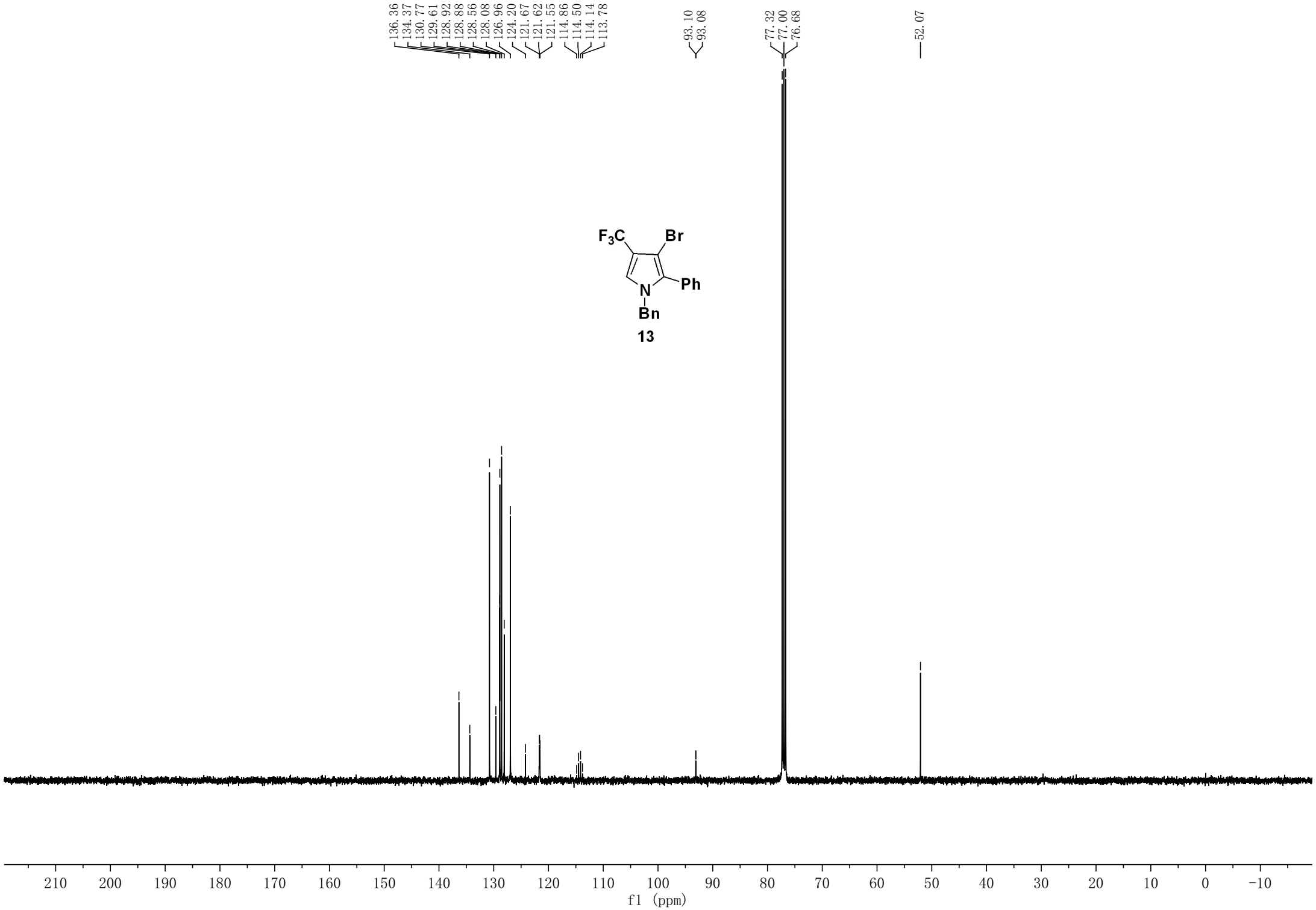

8.29
8.27
7.76
7.73
7.46
7.45
7.42
7.40
7.34
7.32
7.30
7.29
7.27
7.24
7.03
7.01
6.83
5.68
NO2
F3C
Ph
N
Bn
12
2.02
2.04
5.14
3.58
2.01
1.00
1.99
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

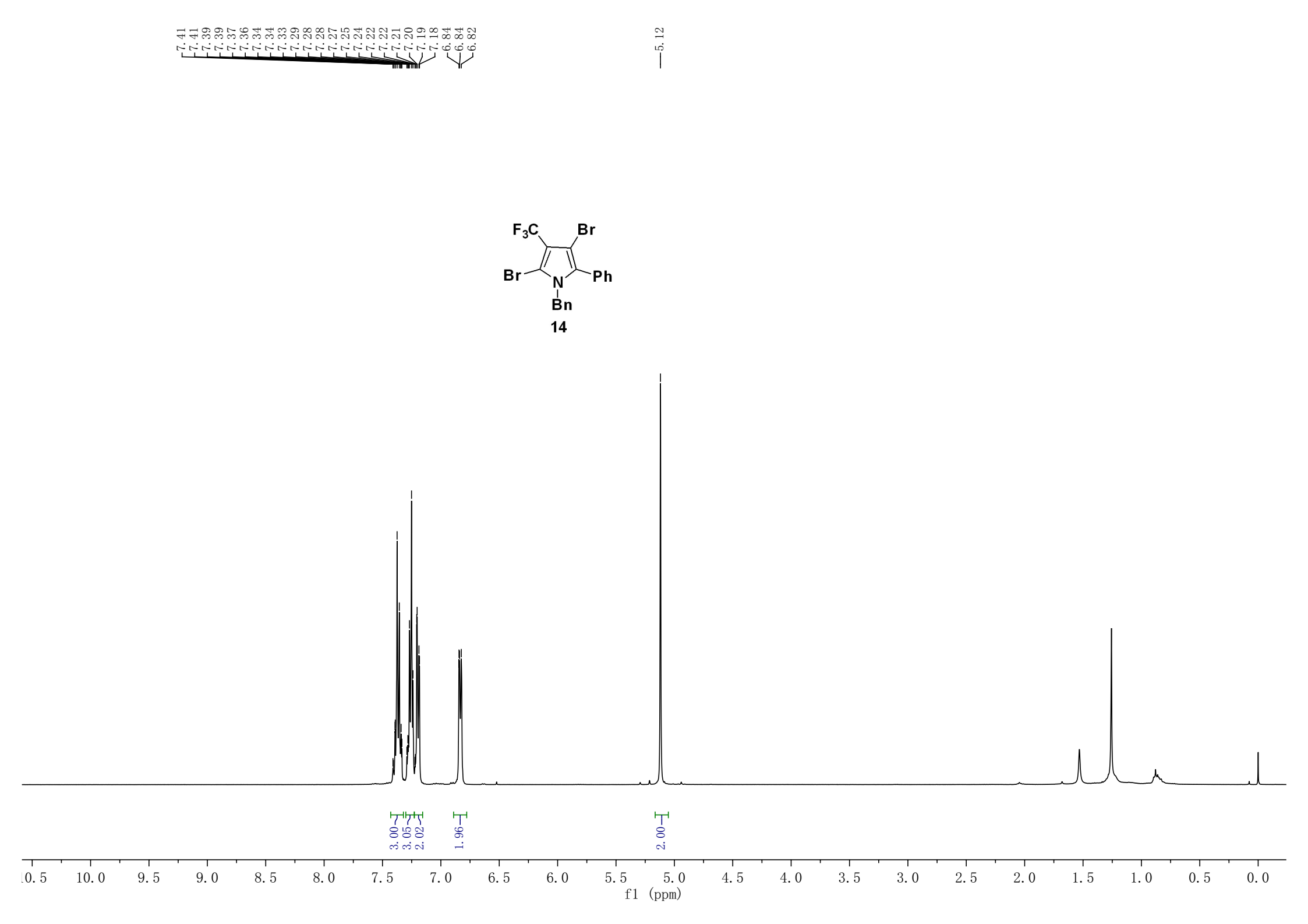

-58.11
NO2
F3C
Ph
N
Bn
12
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

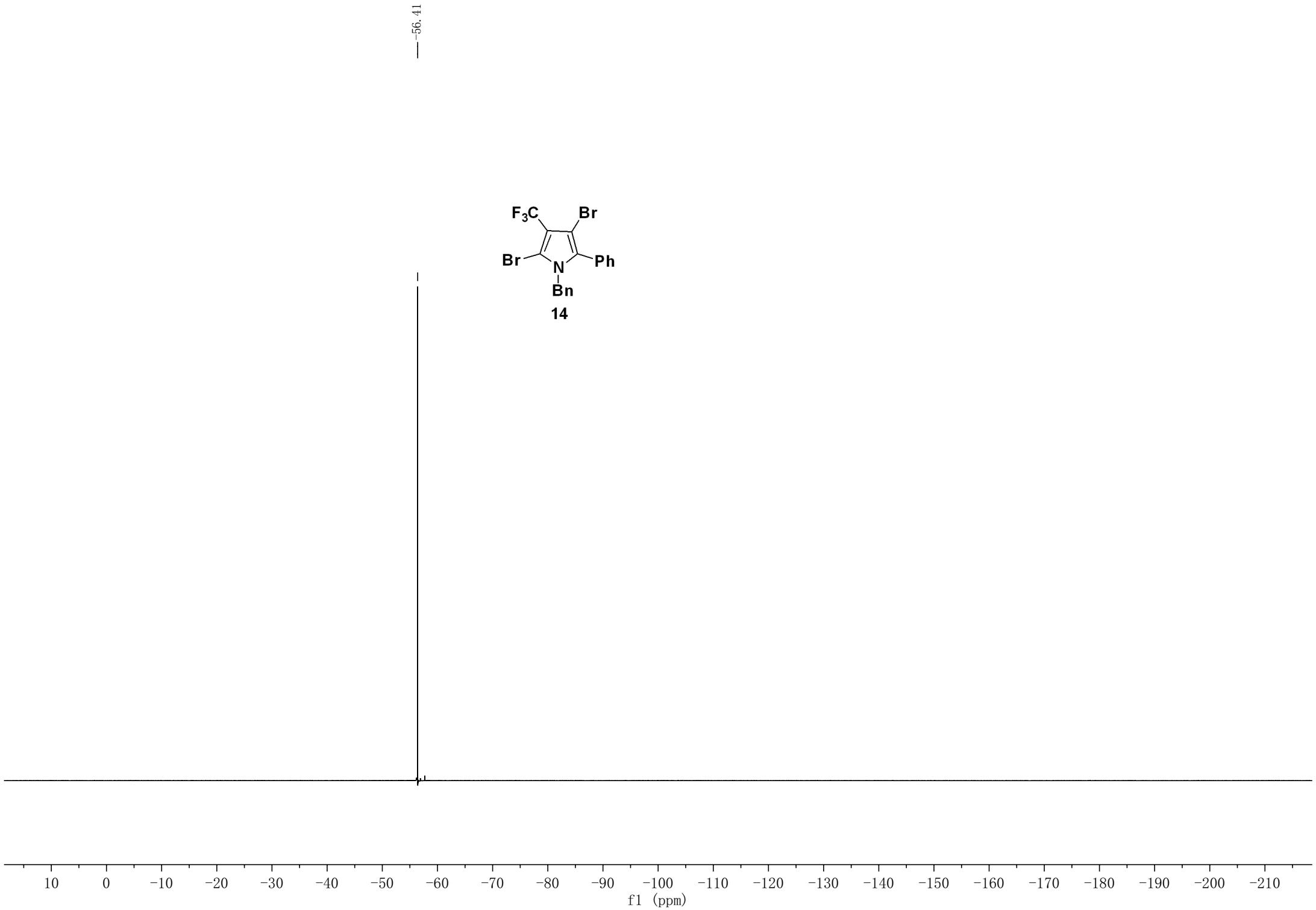

156.58
147.94
141.51
141.49
141.47
139.89
137.67
129.07
128.92
128.82
127.53
125.86
124.64
122.65
122.03
112.01
111.98
111.79
111.48
111.18
110.87
77.25
77.00
76.75
49.25
NO2
F3C
Ph
N
Bn
12
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

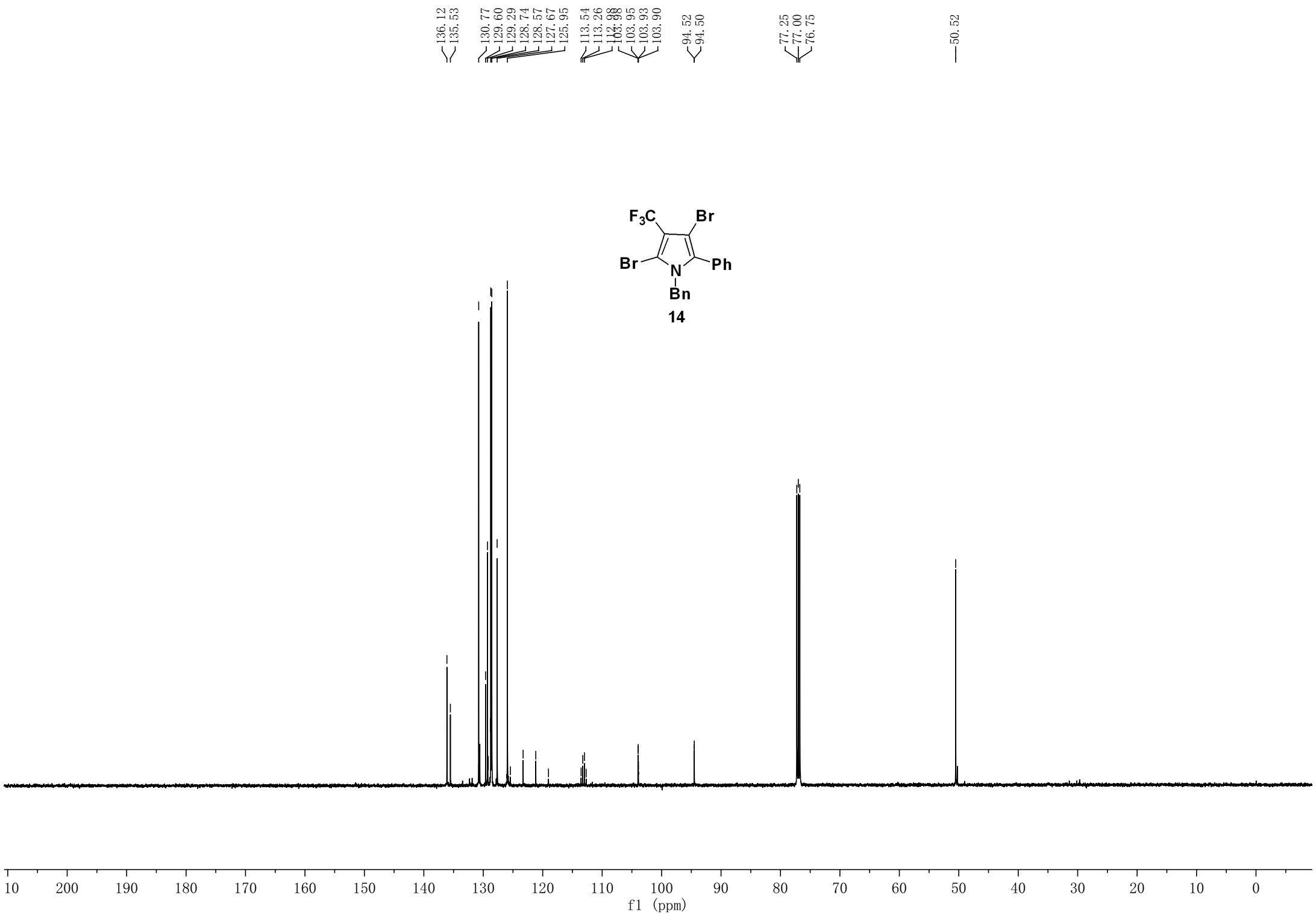

7.45
7.45
7.43
7.43
7.43
7.42
7.42
7.41
7.40
7.39
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.28
7.26
7.07
7.06
6.97
6.96
6.95
6.95
4.98
F3C
Br
Ph
N
Bn
13
3.06
4.94
1.04
2.00
2.05
0.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

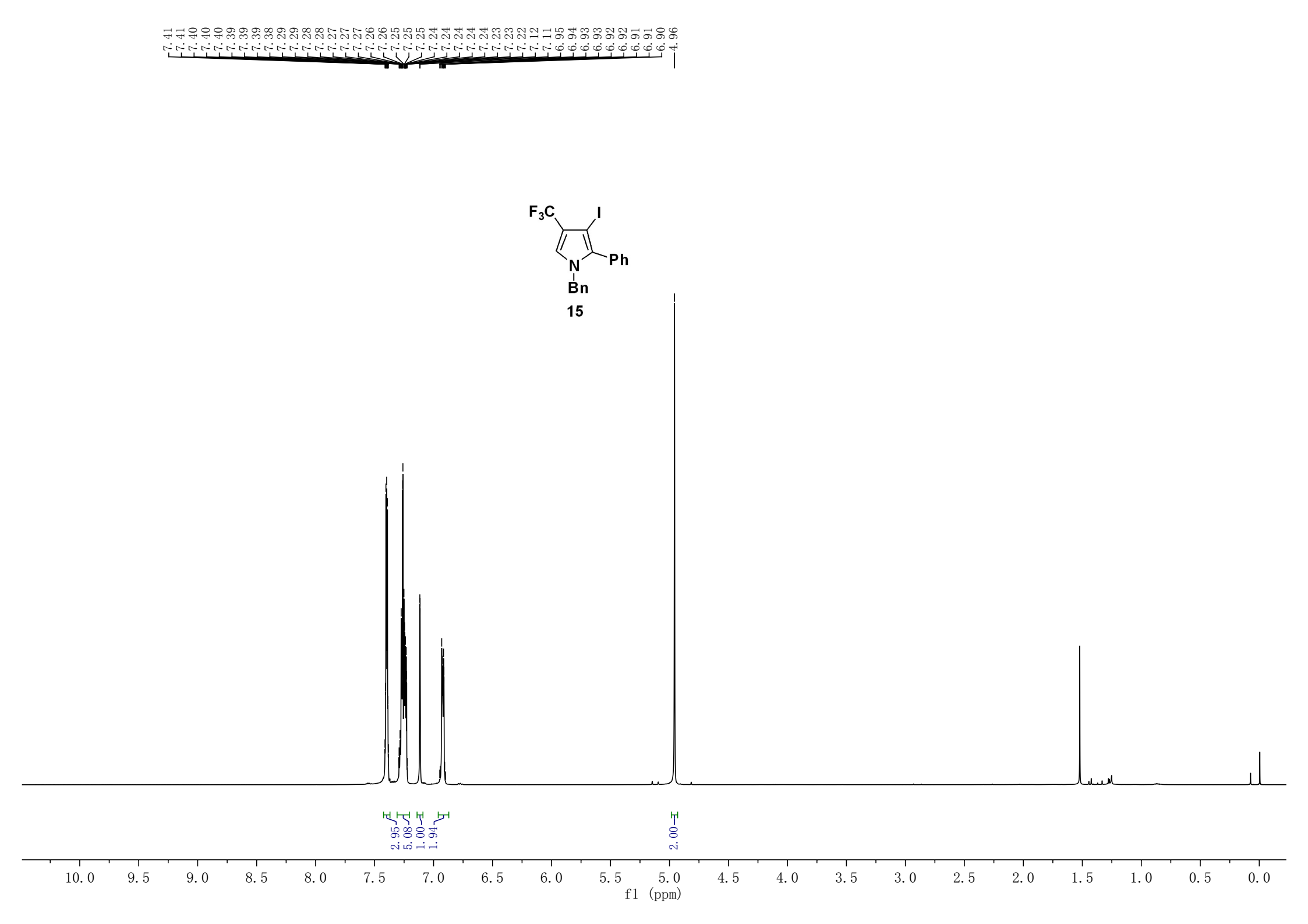

-58.40
F3C
Br
Ph
N
Bn
13
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

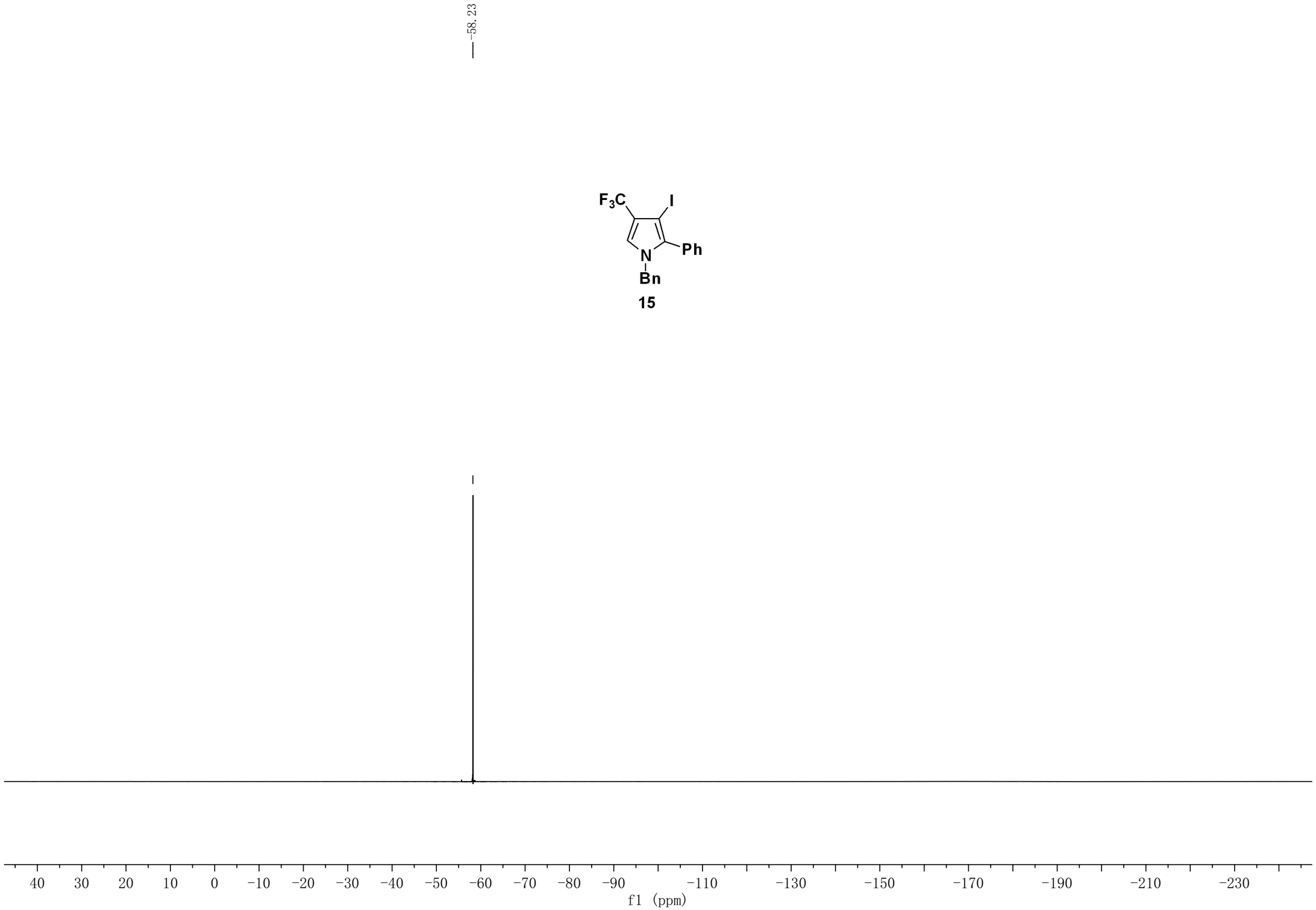

136.36
134.37
130.77
129.61
128.92
128.88
128.56
128.08
126.96
124.20
121.67
121.62
121.55
114.86
114.50
114.14
113.78
93.10
93.08
77.32
77.00
76.68
52.07
F3C
Br
Ph
N
Bn
13
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

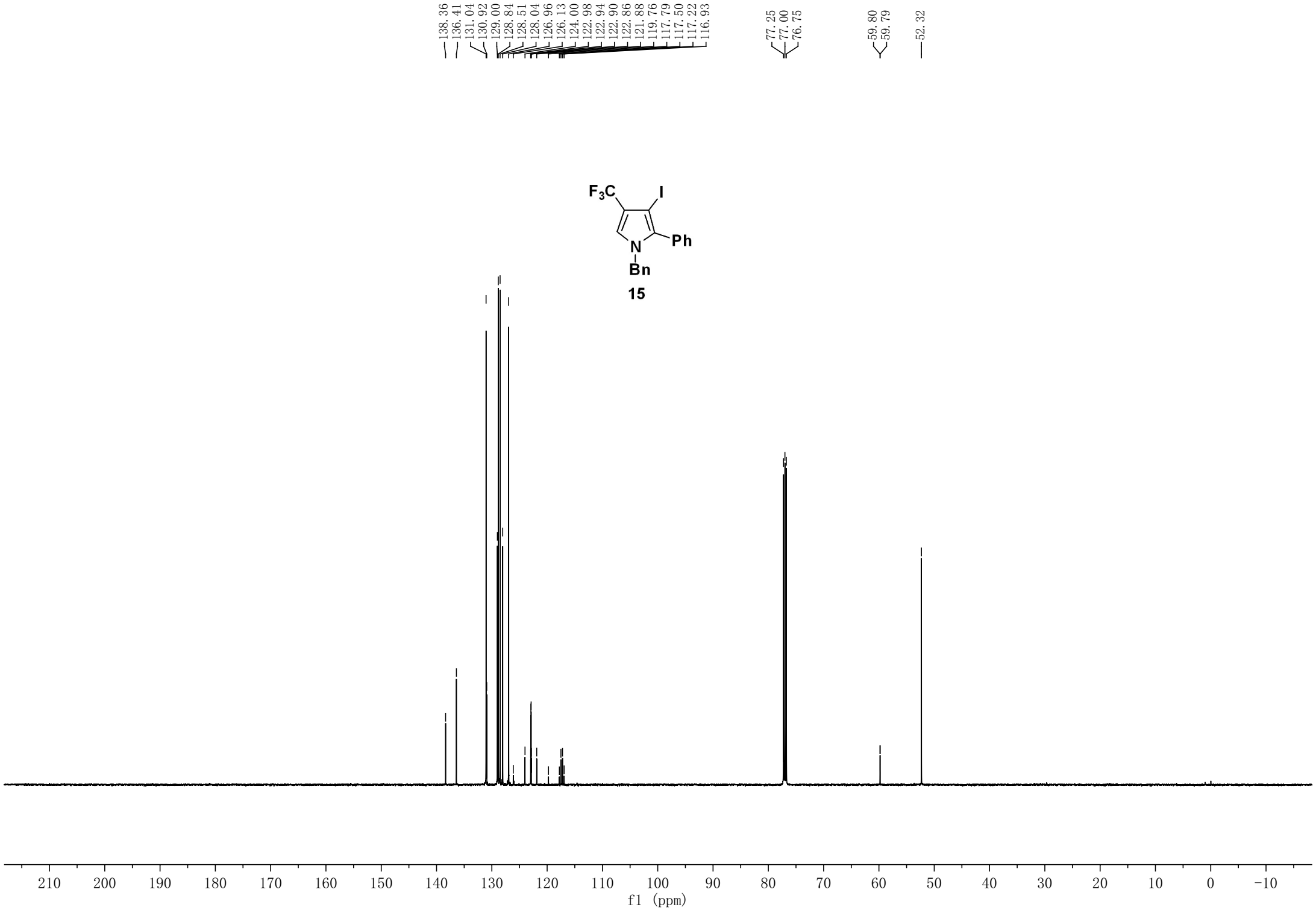

7.41
7.41
7.39
7.39
7.37
7.36
7.34
7.34
7.33
7.29
7.28
7.28
7.27
7.25
7.24
7.22
7.22
7.21
7.20
7.19
7.18
6.84
6.84
6.82
5.12
F3C
Br
Br
Ph
N
Bn
14
3.00
3.05
2.02
1.96
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

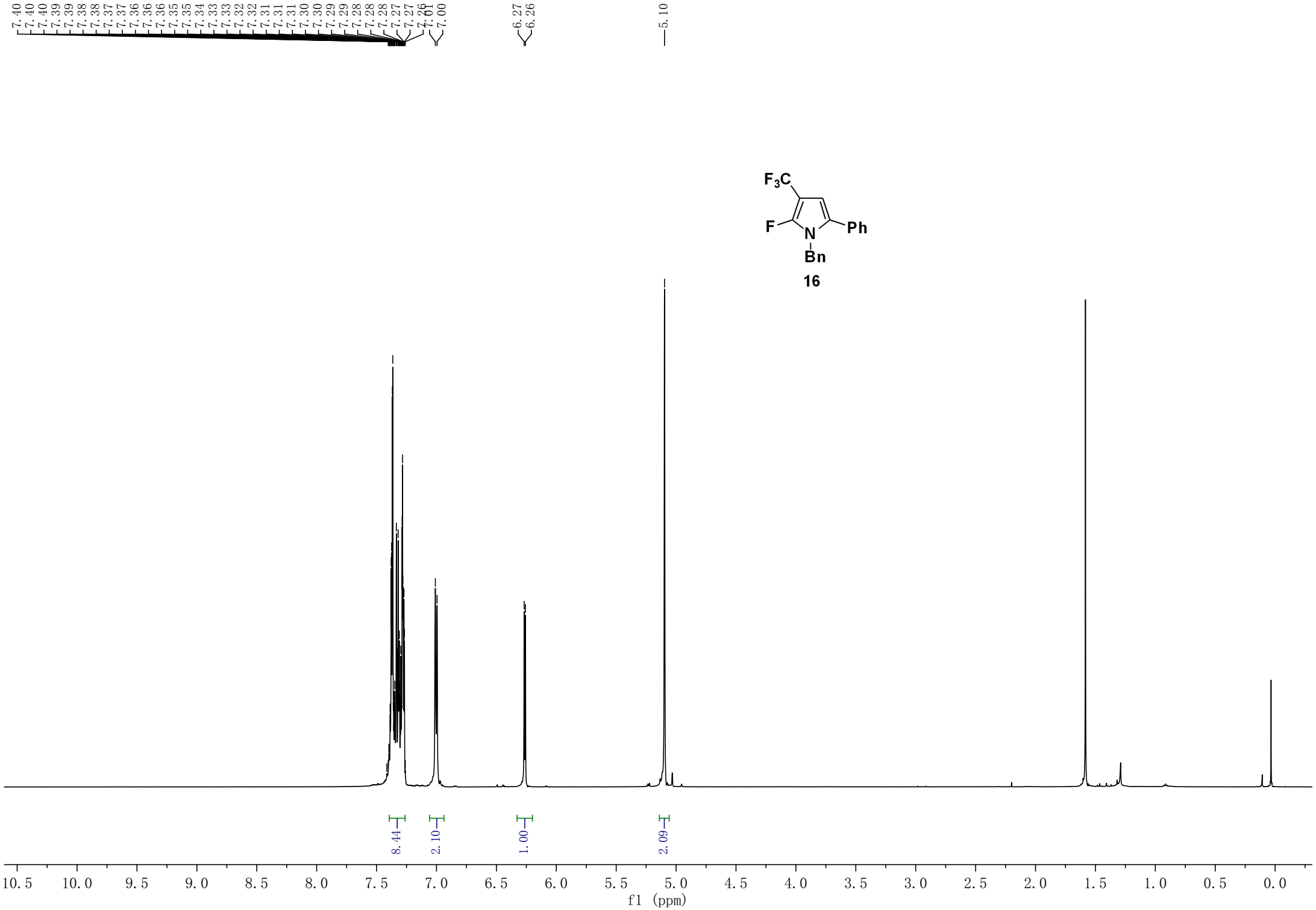

-56.41
F3C
Br
Br
N
Ph
Bn
14
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


136.12
135.53
130.77
129.60
129.29
128.74
128.57
127.67
125.95
113.54
113.26
103.95
103.93
103.90
94.52
94.50
77.25
77.00
76.75
50.52
F3C
Br
Br
Ph
N
Bn
14
f1 (ppm)


7.41 7.41 7.40 7.40 7.40 7.39 7.39 7.39 7.38 7.29 7.29 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.25 7.25 7.25 7.24 7.24 7.24 7.24 7.24 7.23 7.23 7.22 7.12 7.11 6.95 6.94 6.93 6.93 6.92 6.92 6.91 6.91 6.90 4.96
F3C
I
Ph
N
Bn
15
2.95
5.08
1.00
1.94
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


-58.23
F3C
I
Ph
N
Bn
15
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


138.36
136.41
131.04
130.92
129.00
128.84
128.51
128.04
126.96
126.13
124.00
122.98
122.94
122.90
122.86
121.88
119.76
117.79
117.50
117.22
116.93
77.25
77.00
76.75
59.80
59.79
52.32
F3C
I
Ph
N
Bn
15
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.40
7.40
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.36
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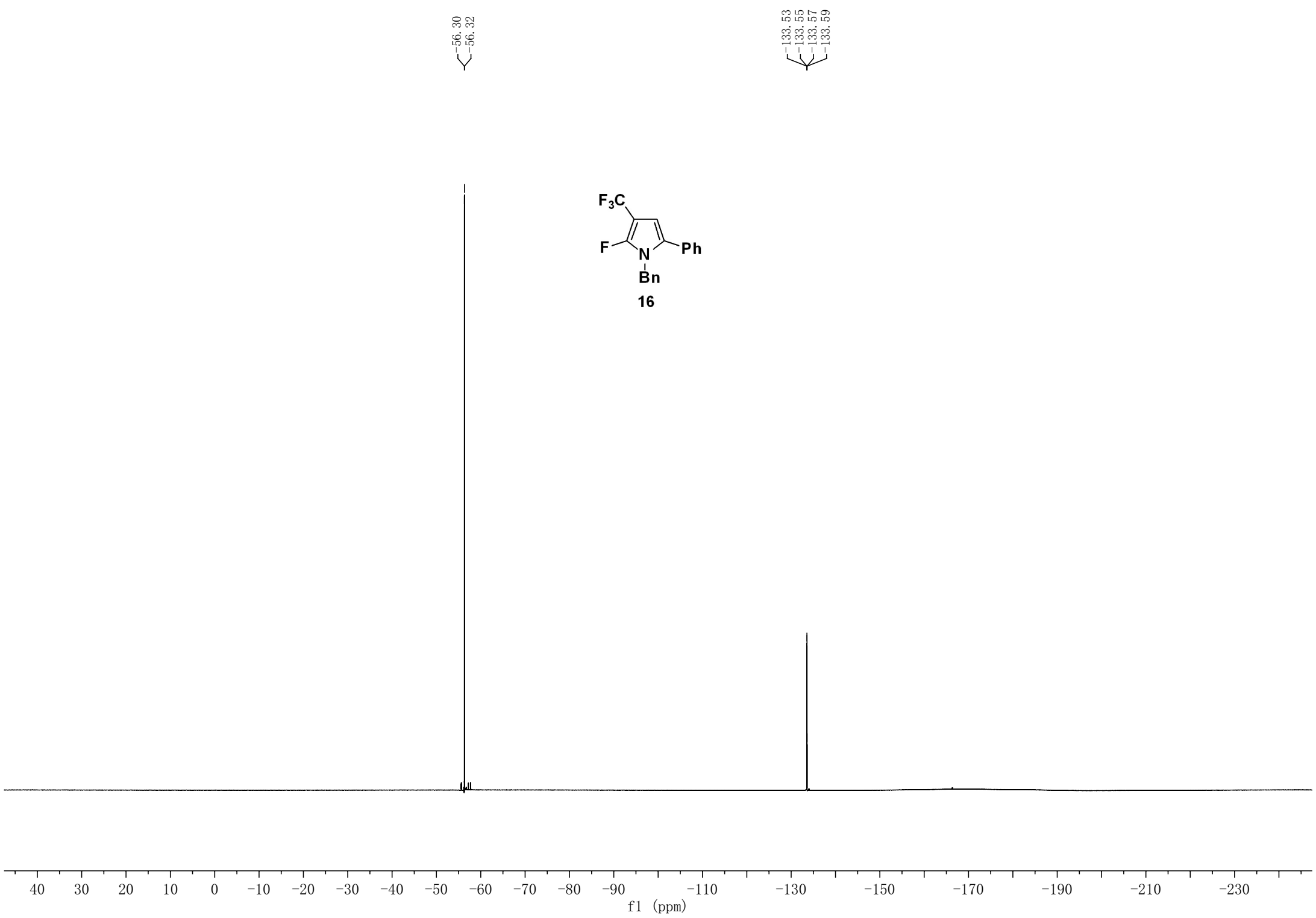
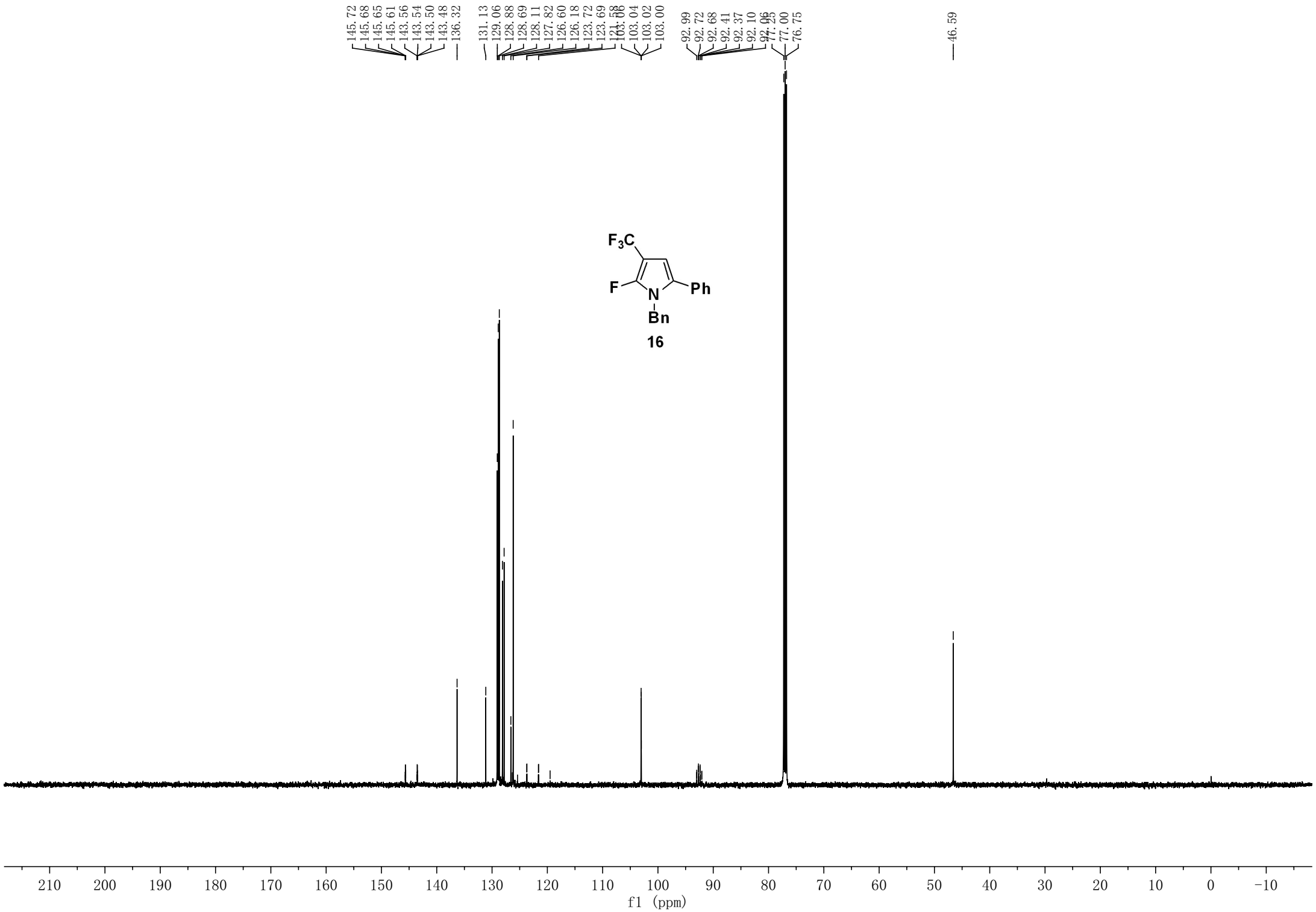
7.35
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.26
7.01
7.00
6.27
6.26
5.10
F3C
F
N
Ph
Bn
16
8.44
2.10
1.00
2.09
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


-56.30
-56.32
-133.53
-133.55
-133.57
-133.59
F3C
F
N
Ph
Bn
16
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)


145.72
145.68
145.65
145.61
143.56
143.54
143.50
143.48
136.32
131.13
129.06
128.88
128.69
128.11
127.82
126.60
126.18
123.72
123.69
103.04
103.02
103.00
92.99
92.72
92.68
92.41
92.37
92.10
77.00
76.75
46.59
F3C
F
N
Ph
Bn
16
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)