Supporting Information

Temperature-Controlled Regioselective Thiolation of 2-Indolylmethanols under Aqueous Micellar Conditions

Shengzhen Zhu,[a] Xiaoji Cao,[b] Yu Zhang, [a] Jinyue Luo,[a] Fei Wang,[a] and Shenlin Huang*[a]

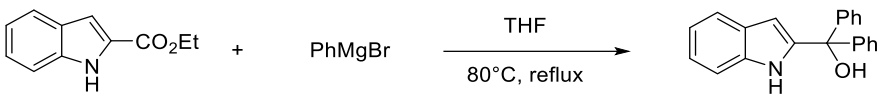
*Corresponding author. Email: shuang@njfu.edu.cn.

I. General Information.

Unless otherwise stated, all glassware was oven dried and all reactions were carried out under an atmosphere of nitrogen and a light-free environment. All reagents were obtained from commercial suppliers and used without further purification. 2-Indolylmethanols were prepared according to reported procedures[1]. 4-acetamidothiophenol were prepared according to reported procedures[2]. DBSA and SDBS were purchased from the supplier, and other surfactants were prepared according to reported procedures[3]. Reactions were monitored using Thin Layer Chromatography (TLC) carried out on Merck silica gel plates (60F-254) using UV light as the visualizing agent and High Performance Liquid Chromatography (HPLC) with UV detection at 254 nm. For HPLC yields, UV response factors relative to an internal standard (Diphenylsulfide). Flash column chromatography was performed using silica gel 60 (200-300 mesh). HRMS data were recorded on Agilent 6500 QTOFMS-ESI or Waters GCT Premier TOFMS-EI. All ^{1}H NMR, ^{13}C NMR spectra were recorded on Bruker DRX-600. Chemical shifts were given in parts per million (ppm, δ), referenced to the solvent peak of $CDCl_3$, defined at δ = 7.26 (^{1}H NMR), defined at δ = 77.16 (^{13}C NMR); or DMSO-d6, defined at δ = 2.50 (^{1}H NMR), defined at δ = 39.52 (^{13}C NMR). Coupling constants were quoted in Hz (J). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br).

II. Substrates Synthesis.

General Procedures A for the Synthesis of 2-Indolylmethanols 1.



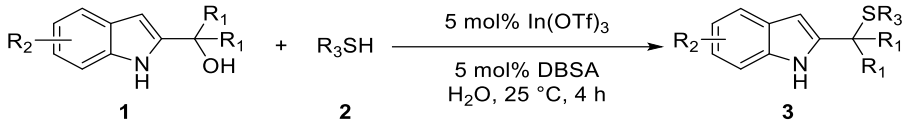
A **B** **1a**

Substrates **1** were synthesized according to the literature method.[1] In a flame-dried Schlenk bottle under nitrogen, phenylmagnesium bromide **B** (20 mL, 3 mol/mL) was added to the Schlenk bottle. Then, in a ice-water bath, the solution of ethyl 1H-indole-2-carboxylate **A** (10 mol) in anhydrous THF (1 mol/mL) was added to the Schlenk bottle. Subsequently, the reaction mixture

was moved to an oil bath, which was refluxed at 80 °C overnight. After the completion of the reaction indicated by TLC, the reaction mixture was quenched by saturated ammonium chloride solution and was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate =20/1) to afford the pure 2-indolylmethanol **1a**.

(1H-indol-2-yl)diphenylmethanol (1a): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.42 – 7.32 (m, 10H), 7.30 (dd, J = 8.1, 0.6 Hz, 1H), 7.20 – 7.17 (m, 1H), 7.12 – 7.09 (m, 1H), 6.27 – 6.10 (m, 1H), 2.92 (s, 1H).

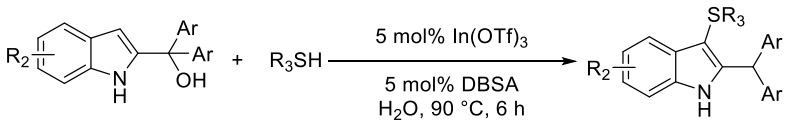
General Procedures B for the Synthesis of Products 3.



1 2 3

2-indolylmethanol **1** (0.3 mmol, 1 eq), thiophenol **2** (0.48 mmol, 1.6 eq) and Indium trifluoromethanesulfonate ($In(OTf)_3$) (0.015 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 3 mL). Then, the mixture was stirred at 25 °C. After the completion of the reaction indicated by TLC (about 4 hours), the reaction mixture was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate =20/1) to afford the pure **3**.

General Procedures C for the Synthesis of Products 4.



1 2 4

2-indolylmethanol **1** (0.3 mmol, 1 eq), thiophenol **2** (0.48 mmol, 1.6 eq) and Indium trifluoromethanesulfonate ($In(OTf)_3$) (0.015 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 3 mL). Then, the mixture was stirred at 90 °C. After the completion of the reaction indicated by TLC (about 6 hours), the reaction mixture was extracted by

ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate =20/1) to afford the pure **4**.

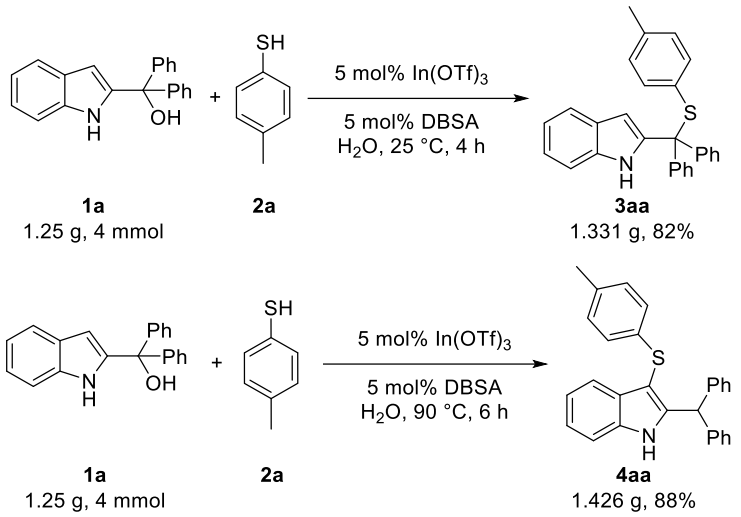
III. Optimization of the Reaction Conditions.

Table S1. Optimization of the reaction conditions

Entry	Catalyst (mol%)	Solvent	T (℃)	Yield[b] (%) **3aa**/**4aa**
1	None	5 mol% DBSA/H_2O	25	69/9
2	HCl(5)	5 mol% DBSA/H_2O	25	76/18
3	$FeCl_3$(5)	5 mol% DBSA/H_2O	25	80/17
4	$AlCl_3$(5)	5 mol% DBSA/H_2O	25	61/7
5	$Cu(OTf)_2$(5)	5 mol% DBSA/H_2O	25	25/45
6	$InCl_3$(5)	5 mol% DBSA/H_2O	25	85/trace
7	**$In(OTf)_3$(5)**	**5 mol% DBSA/H_2O**	**25**	**89(84)[c]/trace**
8	$In(OTf)_3$(10)	5 mol% DBSA/H_2O	25	89/trace
9	$In(OTf)_3$(30)	5 mol% DBSA/H_2O	25	87/trace
10	$In(OTf)_3$(5)	5 mol% SDBS/H_2O	25	65/5
11	$In(OTf)_3$(5)	EtOAc	25	50/14
12	$In(OTf)_3$(5)	CH_2Cl_2	25	51/16
13	$In(OTf)_3$(5)	$CHCl_3$	25	41/21
14	$In(OTf)_3$(5)	2% TPGS-750-M/H_2O	25	22/0
15	$In(OTf)_3$(5)	2% SPGS-550-M/H_2O	25	0/0
16	$In(OTf)_3$(5)	2% DAPGS-550-M/H_2O	25	14/0
17	$In(OTf)_3$(5)	H_2O	25	0/0
18[d]	$In(OTf)_3$(5)	5 mol% DBSA/H_2O	60	60/7
19[d]	$In(OTf)_3$(5)	5 mol% DBSA/H_2O	70	42/26
20[d]	$In(OTf)_3$(5)	5 mol% DBSA/H_2O	80	6/74
21[d]	**$In(OTf)_3$(5)**	**5 mol% DBSA/H_2O**	**90**	**0/91(89)[c]**
22[d]	$In(OTf)_3$(5)	5 mol% DBSA/H_2O	100	0/90

[a]Reaction conditions: **1a** (0.1 mmol), **2a** (0.16 mmol), solvent (1 mL), 4 h. [b]Yields were determined by HPLC analysis with diphenylsulfide as the internal standard. [c]Isolated yield. [d]Run 6 h

IV. Scale-Up Reaction.

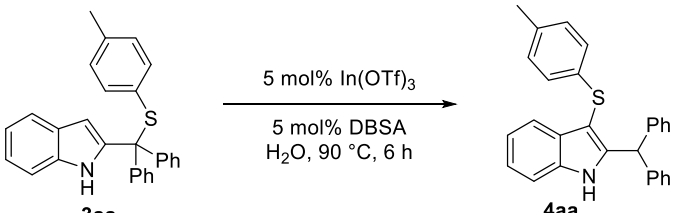


For scale-up reaction, 2-indolylmethanol **1a** (1.25 g, 4 mmol), *p*-thiocresol **2a** (812 mg, 6.4 mmol) and Indium trifluoromethanesulfonate (115 mg, 0.2 mmol) were added to a solution of DBSA (72 mg, 0.2 mmol) in water (0.1 M, 40 mL). Then, the mixture was stirred at 25 °C. After the completion of the reaction indicated by TLC, the reaction mixture was extracted by ethyl acetate for three times. The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel (petroleum ether/ethyl acetate =20/1) to afford the pure **3aa** in 82% yield.

The same procedure was followed by running the reaction at 90 °C for 6 h, **4aa** was isolated in 88% yield.

V. Control Experiment.

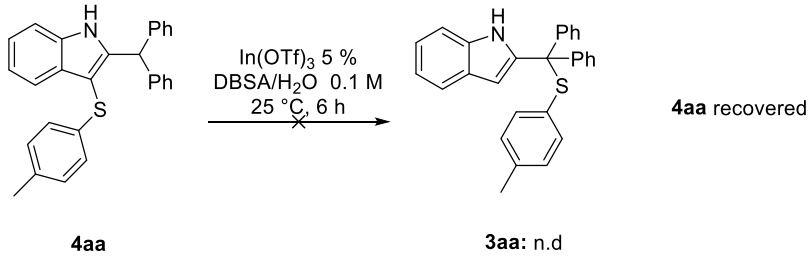
For control experiment, all reactions were carried out on 0.1 mmol scale and yields were determined by HPLC analysis with diphenylsulfide as the internal standard.



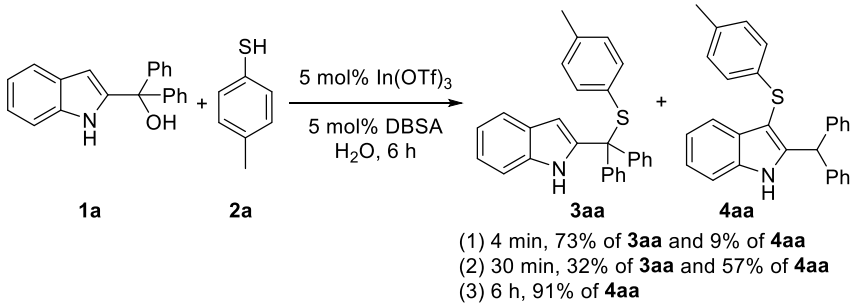
3aa (0.1 mmol, 1 eq) and Indium trifluoromethanesulfonate (0.005 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 3 mL), followed by stirring at 90 °C for 6 h. The yield was determined by HPLC analysis with diphenylsulfide as the internal standard.

The same procedure was followed without $In(OTf)_3$, 77% of **4aa** was detected and no **3aa** recovered.

The replacing of 5 mol% DBSA/H_2O with H_2O, only 2% of **4aa** obtained and 78% of **3aa** recovered.



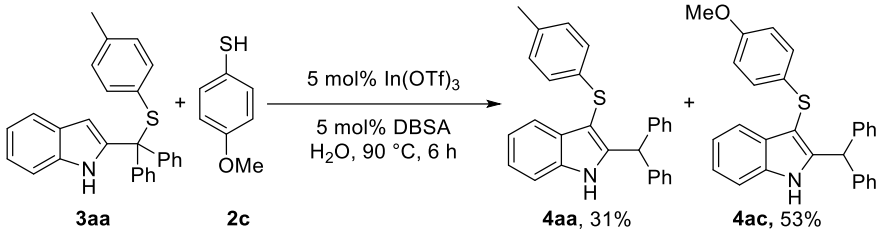
4aa (0.1 mmol, 1 eq) and Indium trifluoromethanesulfonate (0.005 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 1 mL). Then, the mixture was stirred at 25 °C for 4 h. No **3aa** was d etected and only **4aa** recovered.



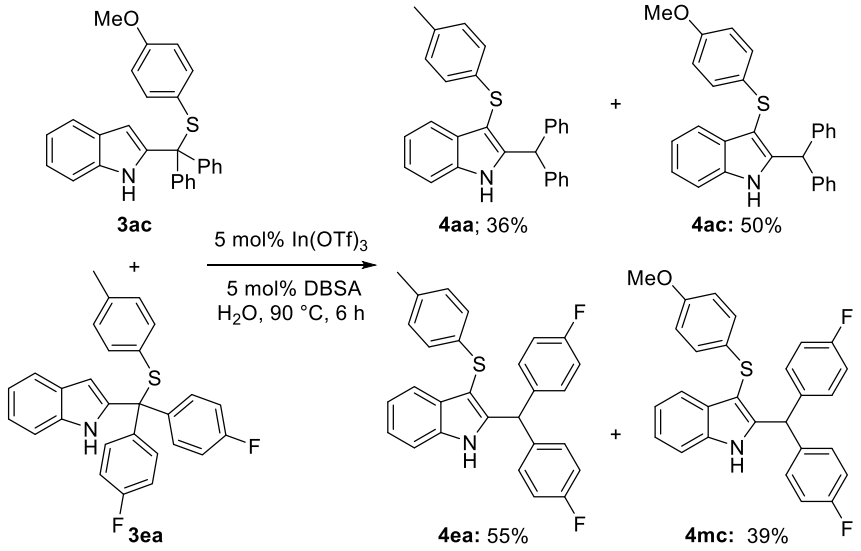
1a (0.1 mmol, 1 eq), **2a** (0.16 mmol, 1.6 eq) and Indium trifluoromethanesulfonate (0.005 mmol, 5 mol%) were added to a solution of DBSA (0.005 mmol, 5 mol%) in water (0.1 M, 1 mL). Then, the mixture was stirred at 90 °C for 4 min. 73% of **3aa** and 9% of **4aa** was detected.

The same procedure was followed by running the reaction at 90 °C for 30 minutes, 32% of **3aa** and 57% of **4aa** was detected.

The same procedure was followed by running the reaction at 90 °C for 6 h, **4aa** was obtained in 91% yield and no **3aa** was detected.



3aa (0.1 mmol, 1 eq), **2c** (0.16 mmol, 1.6 eq) and Indium trifluoromethanesulfonate (0.005 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 1 mL). Then, the mixture was stirred at 90 °C for 6 h. 31% of **4aa** and 53% of **4ac** was detected, respectively.



3ac (0.1 mmol, 1 eq), **3ea** (0.16 mmol, 1.6 eq) and Indium trifluoromethanesulfonate (0.005 mmol, 5 mol%) were added to a solution of DBSA (0.015 mmol, 5 mol%) in water (0.1 M, 1 mL). Then, the mixture was stirred at 90 °C for 6 h. And we obtained **4aa**, **4ac**, **4ea** and **4mc** in 36%, 50%, 55% and 39% yield, respectively.

VI. Recycle Study and Calculation of Green Chemistry Metrics.

Recycle Study:

To a 4 mL vial, the mixture of 2-indolylmethanol **1a** (93.6 mg, 0.3 mmol), thiophenol **2e** (70.8 mg, 0.48 mmol), $In(OTf)_3$ (8.6 mg, 0.015 mmol) was added solvent (3 mL, 5 mol% DBSA in water). Then, the mixture was stirred at 90 °C for 6 h. The reaction mixture was cooled to room temperature, and the desired product precipitated out as solid. The aqueous medium was removed out for the next cycle, while the solid residue is further purified through flash chromatography on silica gel to afford the pure **4ae**.

Reuse of the solvent: Only 2-indolylmethanol **1a** (93.6 mg, 0.3 mmol), thiophenol **2e** (70.8 mg, 0.48 mmol) were added to the solvent, while no additional $In(OTf)_3$ was required.

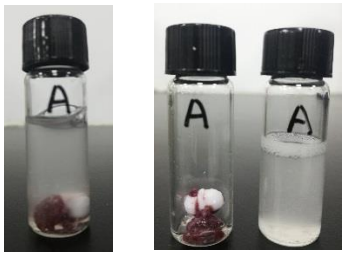


Figure S1. The mixture was cooled to room temperature(left); The solvent was removed(right).

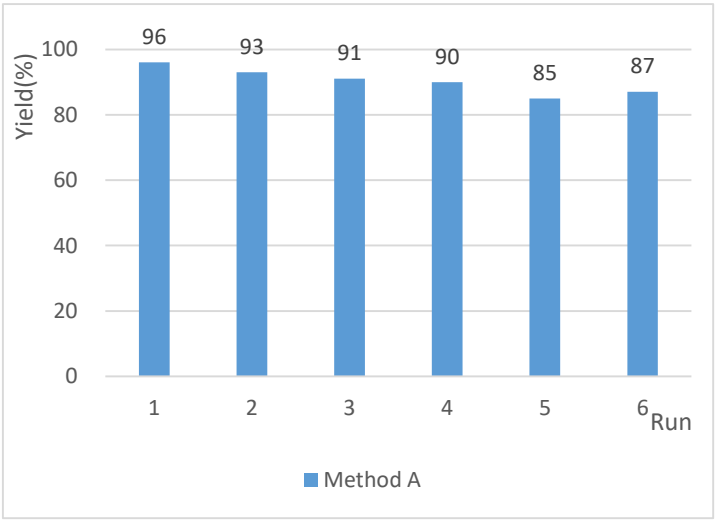
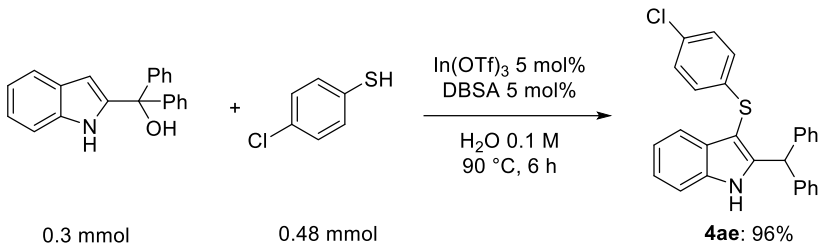


Figure S2. The yield of each run for recycle experiment.

Calculation of Green Chemistry Metrics:

The green chemistry metrics (Atom economy [4], E-factor [5] and Eco-scale [6]) were calculated in this part.



0.3 mmol 0.48 mmol **4ae**: 96%

This work	To a 4 mL vial, the mixture of 2-indolylmethanol **1a** (93.6 mg, 0.3 mmol), thiophenol **2e** (70.8 mg, 0.48 mmol), $In(OTf)_3$ (8.6 mg, 0.015 mmol) was added solvent (3 mL, 5 mol% DBSA in water). Then, the mixture was stirred at 90 °C for 6 h. The reaction mixture was cooled to room temperature, and the desired product precipitated out as solid. The aqueous medium was removed out for the next cycle, while the solid residue is purified through flash chromatography on silica gel (petroleum ether/ethyl acetate =20/1) to afford the pure **4ae**. (**Method A**)	**4ae** 96% 123 mg
	To a 4 mL vial, the mixture of 2-indolylmethanol **1a** (93.6 mg, 0.3 mmol), thiophenol **2e** (70.8 mg, 0.48 mmol), $In(OTf)_3$ (8.6 mg, 0.015 mmol) was added solvent (3 mL, 5 mol% DBSA in water). Then, the mixture was stirred at 90 °C for 6 h. The reaction mixture was cooled to room temperature, and then the reaction mixture was extracted by ethyl acetate for three times (1 mL + 2 X 0.5 mL). The combined organic layer was dried by anhydrous sodium sulfate, which was concentrated under the reduced pressure. The resulted residue was purified through flash chromatography on silica gel to afford the pure **4ae**. (**Method B**)	**4ae** 96% 123 mg

$$\textbf{AE} = \frac{\text{MW of desired product}}{\Sigma \text{ of MW of stoichiometric reactants}} \times 100\%$$

$$= \frac{426}{299.4+144.6} \times 100\% = 95.6\% \quad \text{Method A}$$

$$= \frac{426}{299.4+144.6} \times 100\% = 95.6\% \quad \text{Method B}$$

$$\textbf{PMI} = \frac{\text{total mass used in the process (Kg)}}{\text{mass of product (Kg)}}$$

$$= \frac{(93.6+70.8+8.6+5.4+3000)\ \text{mg}}{123\ \text{mg}} = 25.8 \quad \text{Method A}$$

$$= \frac{(93.6+70.8+8.5+5.4+3000+1794)\ \text{mg}}{123\ \text{mg}} = 40.4 \quad \text{Method B}$$

$$\text{E Factor} = \frac{\text{total of organic wastes (Kg)}}{\text{Product (Kg)}}$$

$$= \frac{0}{123\ \text{mg}} = 0 \quad \text{Method A}$$

$$= \frac{1794\ \text{mg}}{123\ \text{mg}} = 14.6 \quad \text{Method B}$$

This work:

Method A

Parameter	Detail of parameters	Penalty points
1.Yield	96%	2
2. Cost of reactants to obtain 10 mmol of product		
	2-indolylmethanol	1
	4-Chlorothiophenol	1
	$In(OTf)_3$	1
	DBSA	0
	H_2O	0
3. Safety	2-indolylmethanol	0
	4-Chlorothiophenol	5 (N)
	$In(OTf)_3$	0
	DBSA	0
	H_2O	0
4. Technical setup	Common setup	0
5. Temperature/time	Heating > 1 h	3
6. Workup and purification		
	Classical chromatography	10
Eco-scale score		**77**

Method B

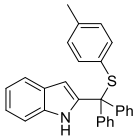
Parameter	Detail of parameters	Penalty points
1.Yield	96%	2
2. Cost of reactants to obtain 10 mmol of product		
	2-indolylmethanol	1
	4-Chlorothiophenol	1
	$In(OTf)_3$	1
	DBSA	0
	H_2O	0
3. Safety	2-indolylmethanol	0
	4-Chlorothiophenol	5 (N)
	$In(OTf)_3$	0
	DBSA	0
	H_2O	0
4. Technical setup	Common setup	0
5. Temperature/time	Heating > 1 h	3
6. Workup and purification		
	Liquid-liquid extraction	3
	Classical chromatography	10
Eco-scale score		**74**

Table S2. Calculation of green chemistry metrics

	AE	PMI	E Factor	Eco-scale
Method A	95.6%	25.8	0	77
Method B	95.6%	40.4	14.6	74

VII. Characterization Data of Products.

2-(diphenyl(p-tolylthio)methyl)-1H-indole (3aa)



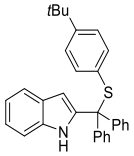
White solid, 100 mg, 83% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.34 (m, 4H), 7.31 – 7.26 (m, 7H), 7.22 – 7.16 (m, 1H), 7.13 – 7.08 (m, 1H), 6.95 – 6.92 (m, 2H), 6.91 (d, *J* = 8.2 Hz, 2H), 6.23 (dd, *J* = 2.0, 0.6 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 141.1, 139.1, 136.1, 135.6, 129.8, 129.5, 128.0, 127.8, 127.5, 122.3, 120.8, 119.9, 110.9, 105.8, 65.8, 21.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{24}NS$: 406.1624, found 406.1623.

2-(((4-(tert-butyl)phenyl)thio)diphenylmethyl)-1H-indole (3ab)



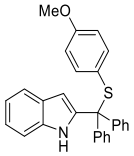
White solid, 101 mg, 76% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.52 (dd, *J* = 7.8, 0.5 Hz, 1H), 7.39 – 7.35 (m, 4H), 7.27 (m, 6H), 7.24 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.19 – 7.16 (m, 1H), 7.12 – 7.08 (m, 3H), 7.00 – 6.95 (m, 2H), 6.22 (dd, *J* = 2.1, 0.7 Hz, 1H), 1.26 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 152.3, 143.4, 141.2, 136.1, 135.3, 130.0, 129.6, 128.0, 127.9, 127.5, 125.8, 122.3, 120.8, 119.9, 110.9, 105.7, 66.0, 34.8, 31.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{31}H_{30}NS$: 448.2093, found 448.2086.

2-(((4-methoxyphenyl)thio)diphenylmethyl)-1H-indole (3ac)



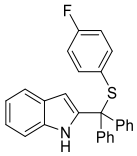
White solid, 117 mg, 92% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.37 – 7.34 (m, 4H), 7.31 – 7.27 (m, 7H), 7.20 (td, *J* = 8.1, 0.9 Hz, 1H), 7.11 (td, *J* = 7.7, 0.6 Hz, 1H), 6.99 – 6.95 (m, 2H), 6.66 – 6.62 (m, 2H), 6.24 (d, *J* = 1.6 Hz, 1H), 3.75 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.6, 143.2, 141.2, 138.1, 136.0, 129.5, 127.9, 127.9, 127.5, 123.6, 122.2, 120.8, 119.9, 114.2, 110.9, 105.7, 66.0, 55.4.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{24}NOS$: 422.1573, found 422.1573.

2-(((4-fluorophenyl)thio)diphenylmethyl)-1H-indole (3ad)



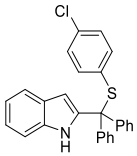
White solid, 101 mg, 82% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.33 (m, 4H), 7.30 – 7.26 (m, 7H), 7.19 (t, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.02 – 6.94 (m, 2H), 6.79 – 6.74 (m, 2H), 6.28 (d, *J* = 1.5 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 163.4 (d, *J* = 250.1 Hz), 143.0, 140.5, 138.0 (d, *J* = 8.4 Hz), 136.1, 129.4, 128.3 (d, *J* = 3.5 Hz), 128.1, 127.9, 127.6, 122.5, 120.8, 120.1, 115.8 (d, *J* = 21.7 Hz), 110.9, 106.0, 66.2.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}FNS$: 410.1373, found 410.1372.

2-(((4-chlorophenyl)thio)diphenylmethyl)-1H-indole (3ae)



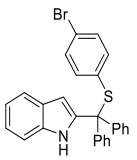
White solid, 114 mg, 89% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.52 (dd, *J* = 7.9, 0.6 Hz, 1H), 7.36 – 7.32 (m, 4H), 7.30 – 7.26 (m, 7H), 7.19 (ddd, *J* = 8.2, 7.1, 1.1 Hz, 1H), 7.10 (td, *J* = 7.6, 0.9 Hz, 1H), 7.06 – 7.01 (m, 2H), 6.94 – 6.90 (m, 2H), 6.30 (dd, *J* = 2.2, 0.8 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.0, 140.2, 136.3, 136.1, 135.0, 132.0, 129.3, 128.8, 128.1, 127.8, 127.7, 122.5, 120.9, 120.1, 111.0, 106.1, 66.2.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}ClNS$: 426.1078, found 426.1072.

2-(((4-bromophenyl)thio)diphenylmethyl)-1H-indole (3af)



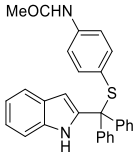
White solid, 120 mg, 85% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.35 – 7.32 (m, 4H), 7.30 – 7.26 (m, 7H), 7.21 – 7.17 (m, 3H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 8.2 Hz, 2H), 6.29 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.0, 140.2, 136.3, 136.1, 132.7, 131.8, 129.3, 128.2, 127. 8, 127.7, 123.2, 122.6, 120.9, 120.1, 111.0, 106.2, 66.1.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{27}H_{21}BrNS$: 470.0573, found 470.0561.

N-(4-(((1H-indol-2-yl)diphenylmethyl)thio)phenyl)acetamide (3ag)



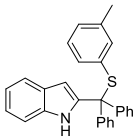
White solid, 82 mg, 61% yield.

^{1}H NMR (600 MHz, DMSO) δ 11.07 (d, *J* = 1.7 Hz, 1H), 9.93 (s, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.25 (m, 12H), 7.10 – 7.03 (m, 1H), 6.99 – 6.92 (m, 1H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.19 (d, *J* = 1.8 Hz, 1H), 1.99 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 168.7, 143.6, 140.9, 140.1, 137.1, 136.1, 129.0, 128.1, 127.4, 127.1, 126.1, 121.7, 120.3, 119.2, 118.7, 111.8, 104.5, 65.9, 24.3.

HRMS-ESI (m/z): [M+Na] $^+$ calculated for $C_{29}H_{24}N_2NaOS$: 471.1502, found 471.1488.

2-(diphenyl(m-tolylthio)methyl)-1H-indole (3ah)



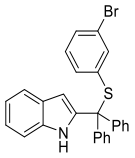
White solid, 97 mg, 80% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.40 – 7.36 (m, 4H), 7.32 – 7.26 (m, 6H), 7.25 (s, 1H), 7.19 – 7.16 (m, 1H), 7.09 (m, 1H), 7.02 (d, *J* = 7.5 Hz, 1H), 6.98 (t, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 7.6 Hz, 1H), 6.75 (s, 1H), 6.22 (d, *J* = 1.7 Hz, 1H), 2.07 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4, 141.0, 138.4, 136.1, 136.0, 133.2, 132.0, 129.5, 129.4, 128.5, 128.0, 127.8, 127.5, 122.3, 120.8, 119.9, 110.9, 105.8, 65.9, 21.2.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{28}H_{24}NS$: 406.1624, found 406.1616.

2-(((3-bromophenyl)thio)diphenylmethyl)-1H-indole (3ai)



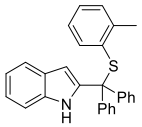
White solid, 119 mg, 85% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.38 – 7.34 (m, 4H), 7.34 – 7.27 (m, 8H), 7.21 – 7.17 (m, 1H), 7.13 – 7.06 (m, 2H), 7.00 – 6.95 (m, 1H), 6.92 (t, *J* = 7.9 Hz, 1H), 6.32 (d, *J* = 1.4 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.9, 140.1, 137.2, 136.2, 135.9, 132.9, 131.4, 129.8, 129.3, 128.2, 127.8, 127.7, 122.6, 122.1, 120.9, 120.1, 111.0, 106.2, 66.4.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}BrNS$: 470.0573, found 470.0556.

2-(diphenyl(o-tolylthio)methyl)-1H-indole (3aj)



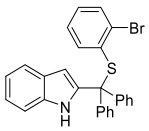
White solid, 95 mg, 78% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.45 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.36 – 7.32 (m, 4H), 7.30 – 7.26 (m, 7H), 7.19 – 7.15 (m, 1H), 7.10 – 7.06 (m, 1H), 6.97 – 6.90 (m, 2H), 6.84 (td, *J* = 7.7, 1.3 Hz, 1H), 6.37 (d, *J* = 1.5 Hz, 1H), 1.55 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.8, 142.9, 140.7, 136.0, 135.4, 132.6, 130.3, 129.4, 128.8, 127.8, 127.7, 127.5, 126.2, 122.2, 120.7, 119.8, 110.8, 105.8, 65.9, 20.6.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{24}NS$: 406.1624, found 406.1637.

2-(((2-bromophenyl)thio)diphenylmethyl)-1H-indole (3ak)



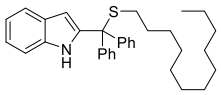
White solid, 99 mg, 70% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 1H), 7.46 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.36 (dd, *J* = 6.7, 2.9 Hz, 4H), 7.32 – 7.27 (m, 7H), 7.18 (dd, *J* = 11.2, 3.9 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.98 – 6.91 (m, 2H), 6.87 – 6.82 (m, 1H), 6.39 (d, *J* = 1.5 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.9, 139.2, 136.3, 136.1, 133.0, 132.9, 130.2, 129.3, 128.22, 128.20, 127.9, 127.4, 126.6, 122.5, 120.8, 120.1, 111.1, 106.5, 66.6.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}BrNS$: 470.0573, found 470.0571.

2-((dodecylthio)diphenylmethyl)-1H-indole (3al).



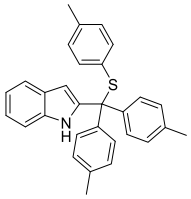
Colourless oil, 134 mg, 93% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.61 – 7.53 (m, 1H), 7.53 – 7.42 (m, 4H), 7.37 – 7.30 (m, 5H), 7.29 – 7.26 (m, 2H), 7.23 – 7.19 (m, 1H), 7.15 – 7.09 (m, 1H), 6.45 – 6.27 (m, 1H), 2.42 – 2.21 (m, 2H), 1.51 – 1.41 (m, 2H), 1.36 – 1.14 (m, 18H), 0.96 – 0.88 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 144.1, 140.8, 136.4, 128.7, 128.3, 127.7, 127.3, 122.3, 120.6, 120.0, 110.9, 105.7, 62.2, 32.1, 29.8, 29.7, 29.5, 29.5, 29.3, 29.1, 28.8, 22.8, 14.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{33}H_{42}NS$: 484.3032, found 484.3019.

2-(di-*p*-tolyl(p-tolylthio)methyl)-1H-indole (3ba)



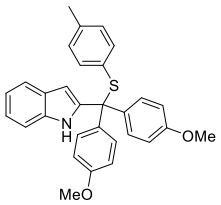
White solid, 95 mg, 73% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 4H), 7.17 – 7.14 (m, 1H), 7.10 – 7.03 (m, 5H), 6.92 (d, *J* = 8.2 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 6.17 (d, *J* = 1.7 Hz, 1H), 2.34 (s, 6H), 2.26 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5, 140.6, 138.9, 137.2, 136.0, 135.4, 130.2, 129.5, 129.4, 128.7, 127.8, 122.1, 120.7, 119.8, 110.9, 105.7, 65.4, 21.3, 21.2.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{30}H_{28}NS$: 434.1937, found 434.1925.

2-(di-*p*-tolyl(p-tolylthio)methyl)-1H-indole (3ca).



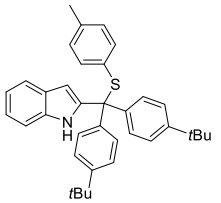
White solid, 95 mg, 68% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.51 (d, *J* = 7.7 Hz, 1H), 7.26 – 7.21 (m, 5H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.09 (t, *J* = 7.3 Hz, 1H), 6.97 – 6.91 (m, 4H), 6.80 (d, *J* = 8.6 Hz, 4H), 6.17 (s, 1H), 3.81 (s, 6H), 2.29 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.8, 141.9, 139.0, 136.0, 135.7, 135.7, 130., 130.1, 129.5, 127.8, 122.2, 120.7, 119.8, 113.2, 110.9, 105.5, 65.0, 55.4, 21.3.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{30}H_{27}NNaO_2S$: 488.1655, found 488.1650.

2-(bis(4-(tert-butyl)phenyl)(p-tolylthio)methyl)-1H-indole (3da)



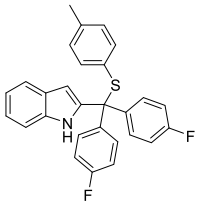
White solid, 113 mg, 73% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.26 – 7.23 (m, 9H), 7.19 – 7.14 (m, 1H), 7.10 – 7.06 (m, 1H), 6.90 (d, *J* = 8.2 Hz, 2H), 6.87 (d, *J* = 8.2 Hz, 2H), 6.25 (d, *J* = 1.5 Hz, 1H), 2.26 (s, 3H), 1.32 (s, 18H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.3, 141.66, 140.4, 138.8, 136.1, 135.6, 130.2, 129.4, 129.1, 127.9, 124.8, 122.1, 120.7, 119.8, 110.9, 105.5, 65.4, 34.6, 31.5, 21.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{36}H_{40}NS$: 518.2876, found 518.2858.

2-(bis(4-fluorophenyl)(p-tolylthio)methyl)-1H-indole (3ea).



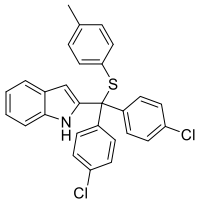
White solid, 106 mg, 80% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.32 – 7.26 (m, 4H), 7.26 – 7.25 (m, 1H), 7.22 – 7.18 (m, 1H), 7.13 – 7.09 (m, 1H), 7.00 – 6.85 (m, 8H), 6.15 (dd, *J* = 2.1, 0.7 Hz, 1H), 2.29 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.0 (d, *J* = 247.9 Hz), 140.7, 139.5, 138.9 (d, *J* = 3.2 Hz), 136.0, 135.8, 131.1 (d, *J* = 8.0 Hz), 129.6, 129.1, 127.6, 122.5, 120.7, 120.0, 114.7 (d, *J* = 21.3 Hz), 110.9, 105.7, 64.5, 21.2.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{22}F_2NS$: 442.1436, found 442.1425.

2-bis(4-chlorophenyl)(p-tolylthio)methyl)-1H-indole (3fa).



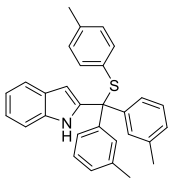
White solid, 101 mg, 71% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.29 – 7.27 (m, 1H), 7.25 – 7.17 (m, 9H), 7.13 – 7.08 (m, 1H), 6.93 (d, *J* = 8.1 Hz, 2H), 6.91 – 6.88 (m, 2H), 6.15 (dd, *J* = 2.2, 0.7 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 141.5, 140.2, 139.8, 136.1, 136.0, 133.7, 130.8, 129.8, 128.8, 128.2, 127.7, 122.7, 120.9, 120.2, 111.0, 106.0, 64.7, 21.4.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{22}Cl_2NS$: 474.0845, found 474.0822.

2-(di-m-tolyl(p-tolylthio)methyl)-1H-indole (3ga)



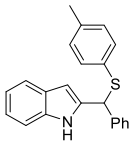
White solid, 98 mg, 75% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.26 (m, 1H), 7.19 – 7.14 (m, 5H), 7.11 (d, *J* = 8.6 Hz, 2H), 7.10 – 7.05 (m, 3H), 6.90 (m, 4H), 6.23 (d, *J* = 1.1 Hz, 1H), 2.27 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.3, 141.3, 139.0, 137.4, 136.0, 135.8, 130.2, 129.8, 129.4, 128.2, 127.9, 127.8, 126.6, 122.1, 120.7, 119.8, 110.9, 105.7, 65.9, 21.7, 21.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{30}H_{28}NS$: 434.1937, found 434.1926.

2-(phenyl(p-tolylthio)methyl)-1H-indole (3ha)



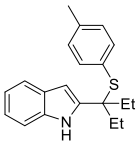
White solid, 57 mg, 57% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.39 (m, 2H), 7.36 – 7.31 (m, 3H), 7.31 – 7.27 (m, 1H), 7.21 – 7.15 (m, 3H), 7.12 – 7.07 (m, 1H), 7.02 (d, *J* = 7.9 Hz, 2H), 6.39 – 6.29 (m, 1H), 5.59 (s, 1H), 2.29 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.8, 137.83, 137.77, 136.4, 132.3, 131.1, 129.9, 128.8, 128.54, 128.50, 127.9, 122.1, 120.6, 120.0, 111.0, 102.9, 52.5, 21.2.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{22}H_{20}NS$: 330.1311, found 330.1304.

2-(3-(p-tolylthio)pentan-3-yl)-1H-indole (3ia).



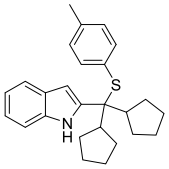
White solid, 58 mg, 62% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39 (dd, *J* = 8.1, 0.6 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.12 – 7.08 (m, 1H), 6.91 (d, *J* = 7.9 Hz, 2H), 6.83 (d, *J* = 8.1 Hz, 2H), 6.18 (dd, *J* = 2.0, 0.6 Hz, 1H), 2.25 (s, 3H), 1.97 (dq, *J* = 14.6, 7.3 Hz, 2H), 1.82 (dq, *J* = 14.6, 7.4 Hz, 2H), 0.95 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.5, 138.7, 136.1, 135.4, 129.4, 128.4, 128.1, 121.9, 120.4, 119.6, 110.8, 102.4, 56.9, 27.4, 21.3, 8.3.

HRMS-ESI (m/z): [M+H] $^{+}$ calculated for $C_{20}H_{24}NS$: 310.1624, found 310.1622.

2-(dicyclopentyl(p-tolylthio)methyl)-1H-indole (3ja).



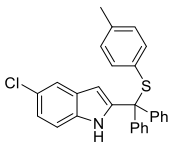
White solid, 95 mg, 82% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.19 (m, 1H), 7.13 (m, 3H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.43 (d, *J* = 1.7 Hz, 1H), 2.60 – 2.53 (m, 2H), 2.27 (s, 3H), 1.86 – 1.80 (m, 2H), 1.75 – 1.63 (m, 4H), 1.53 – 1.36 (m, 10H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 140.1, 137.9, 134.8, 134.3, 130.6, 129.5, 128.7, 121.5, 120.3, 119.7, 110.9, 102.8, 64.6, 49.0, 29.0, 28.9, 25.5, 25.0, 21.2.

HRMS-ESI (m/z): [M+H] $^{+}$ calculated for $C_{26}H_{32}NS$: 390.2250, found 390.2239.

5-chloro-2-(diphenyl(p-tolylthio)methyl)-1H-indole (3ka).



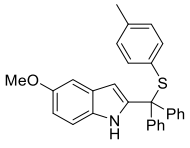
White solid, 110 mg, 84% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.47 (d, *J* = 1.9 Hz, 1H), 7.36 – 7.32 (m, 4H), 7.31 – 7.26 (m, 6H), 7.16 (d, *J* = 8.6 Hz, 1H), 7.12 (dd, *J* = 8.6, 2.0 Hz, 1H), 6.91 (s, 4H), 6.16 (d, *J* = 1.5 Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.1, 142.7, 139.2, 135.6, 134.3, 129.6, 129.5, 129.4, 128.8, 128.1, 127.6, 125.5, 122.6, 120.1, 111. 9, 105.3, 65.7, 21.3.

HRMS-ESI (m/z): [M+H] $^{+}$ calculated for $C_{28}H_{23}ClNS$: 440.1234, found 440.1229.

2-(diphenyl(p-tolylthio)methyl)-5-methoxy-1H-indole (3la).



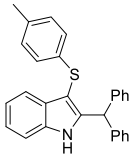
White solid, 110 mg, 85% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.37 – 7.31 (m, 4H), 7.28 – 7.24 (m, 6H), 7.15 (d, *J* = 8.8 Hz, 1H), 6.98 (d, *J* = 2.2 Hz, 1H), 6.96 – 6.87 (m, 4H), 6.84 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.14 (d, *J* = 1.2 Hz, 1H), 3.83 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 154.3, 143.4, 141.8, 139.0, 135.5, 131.2, 129.8, 129.5, 128.2, 127.9, 127.5, 112.5, 111.7, 105.6, 102.4, 65.8, 56.0, 21.3.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{29}H_{26}NOS$: 436.1730, found 436.1718.

2-benzhydryl-3-(*p*-tolylthio)-1H-indole (4aa).



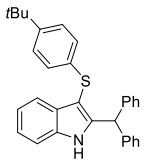
White solid, 108 mg, 89% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.35 – 7.31 (m, 5H), 7.31 – 7.27 (m, 2H), 7.25 – 7.22 (m, 1H), 7.20 – 7.16 (m, 5H), 7.01 – 6.98 (m, 2H), 6.96 (d, *J* = 8.3 Hz, 2H), 6.22 (s, 1H), 2.29 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.0, 141.7, 135.8, 135.1, 134.6, 130.3, 129.5, 129.0, 128.8, 127.0, 126.4, 122.7, 121.0, 119.7, 111.3, 101.4, 48.3, 21.0.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{28}H_{24}NS$: 406.1624, found 406.1615.

2-benzhydryl-3-((4-(tert-butyl)phenyl)thio)-1H-indole (4ab)



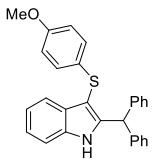
White solid, 122 mg, 91% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.33 – 7.29 (m, 2H), 7.29 – 7.27 (m, 3H), 7.26 – 7.23 (m, 2H), 7.23 – 7.20 (m, 1H), 7.19 – 7.15 (m, 1H), 7.15 – 7.11 (m, 6H), 6.99 – 6.96 (m, 2H), 6.18 (s, 1H), 1.27 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 147.9, 145.0, 141.7, 135.8, 135.2, 130.5, 129.1, 128.8, 127.1, 126.3, 125.8, 122.7, 121.0, 119.8, 111.3, 101.6, 48.3, 34.4, 31.5.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{31}H_{30}NS$: 448.2093, found 448.2091.

2-benzhydryl-3-((4-methoxyphenyl)thio)-1H-indole (4ac).



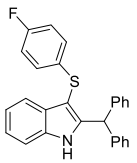
White solid, 122 mg, 97% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.34 – 7.29 (m, 5H), 7.29 – 7.26 (m, 2H), 7.23 – 7.20 (m, 1H), 7.19 – 7.15 (m, 5H), 7.05 – 7.00 (m, 2H), 6.74 – 6.64 (m, 2H), 6.24 (s, 1H), 3.74 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 157.8, 144.6, 141.8, 135.8, 130.3, 129.3, 129.0, 128.9, 128.8, 127.1, 122.7, 121.06, 119.7, 114.5, 111.3, 102.6, 55.4, 48.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{24}NOS$: 422.1573, found 422.1570.

2-benzhydryl-3-((4-fluorophenyl)thio)-1H-indole (4ad).



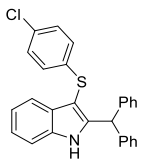
White solid, 119 mg, 97% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.34 – 7.26 (m, 7H), 7.25 – 7.21 (m, 1H), 7.19 – 7.16 (m, 1H), 7.15 (d, *J* = 7.2 Hz, 4H), 6.99 – 6.95 (m, 2H), 6.82 – 6.76 (m, 2H), 6.18 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.9 (d, *J* = 243.7 Hz), 145.2, 141.5, 135.7, 133.6, 130.2, 129.0, 128.9, 128.1 (d, *J* = 7.8 Hz), 127.1, 122.8, 121.2, 119.5, 115.7 (d, *J* = 22.0 Hz), 111.4 , 101.3, 48.4.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}FNS$: 410.1373, found 410.1371.

2-benzhydryl-3-((4-chlorophenyl)thio)-1H-indole (4ae).



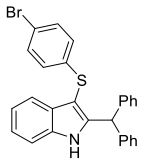
White solid, 123 mg, 96% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.39 – 7.26 (m, 7H), 7.25 – 7.22 (m, 1H), 7.20 – 7.16 (m, 1H), 7.15 (d, *J* = 7.2 Hz, 4H), 7.08 – 7.00 (m, 2H), 6.96 – 6.86 (m, 2H), 6.15 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.4, 141.3, 137.3, 135.7, 130.4, 130.0, 128.9, 128.8, 128.7, 127.3, 127.1, 122.9, 121.2, 119.4, 111.4, 100.3, 48.3.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{27}H_{21}ClNS$: 426.1078, found 426.1060.

2-benzhydryl-3-((4-bromophenyl)thio)-1H-indole (4af).



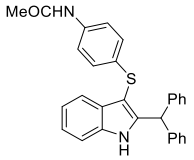
White solid, 124 mg, 88% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.26 (m, 6H), 7.24 – 7.21 (m, 1H), 7.19 – 7.15 (m, 3H), 7.13 (d, *J* = 7.1 Hz, 4H), 6.89 – 6.76 (m, 2H), 6.12 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.5, 141.4, 138.1, 135.8, 131.6, 130.1, 129.0, 128.9, 127.7, 127.2, 123.0, 121.3, 119.5, 118.3, 111.5, 100.2, 48.4.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{27}H_{20}BrNNaS$: 492.0392, found 492.0392.

N-(4-((2-benzhydryl-1H-indol-3-yl)thio)phenyl)acetamide (4ag).



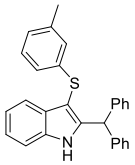
White solid, 98 mg, 73% yield.

^{1}H NMR (600 MHz, DMSO) δ 11.49 (s, 1H), 9.85 (s, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.39 – 7.29 (m, 7H), 7.24 (t, *J* = 7.3 Hz, 2H), 7.19 (d, *J* = 7.5 Hz, 4H), 7.15 – 7.11 (m, 1H), 7.05 – 7.00 (m, 1H), 6.95 – 6.88 (m, 2H), 6.10 (s, 1H), 1.98 (s, 3H).

^{13}C NMR (151 MHz, DMSO) δ 168.1, 145.5, 141.7, 136.9, 136.5, 131.8, 128.8, 128.7, 128.5, 126.7, 124.6, 122.2, 120.1, 119.6, 118.3, 112.1, 99.1, 47.7, 23.9.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{29}H_{24}N_2NaOS$: 471.1502, found 471.1486.

2-benzhydryl-3-(m-tolylthio)-1H-indole (4ah).



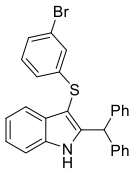
White solid, 113 mg, 93% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.36 – 7.27 (m, 6H), 7.26 – 7.24 (m, 1H), 7.23 – 7.20 (m, 1H), 7.18 – 7.13 (m, 5H), 7.02 – 6.98 (m, 1H), 6.92 – 6.76 (m, 3H), 6.17 (s, 1H), 2.18 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.2, 141.7, 138.5, 138.5, 135.8, 130.4, 129.0, 128.8, 128.6, 127.1, 126.8, 125.8, 123.3, 122.7, 121.0, 119.7, 111.3, 101.0, 48.3, 21.5.

HRMS-ESI (m/z): [M+Na] $^+$ calculated for $C_{28}H_{23}NNaS$: 428.1443, found 428.1429.

2-benzhydryl-3-((3-bromophenyl)thio)-1H-indole (4ai).



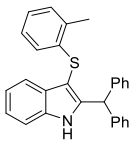
White solid, 134 mg, 95% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.62 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.30 (m, 5H), 7.29 – 7.26 (m, 2H), 7.26 – 7.23 (m, 1H), 7.22 – 7.18 (m, 1H), 7.17 – 7.13 (m, 5H), 7.12 – 7.10 (m, 1H), 6.96 – 6.90 (m, 2H), 6.13 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.8, 141.4, 141.3, 135.7, 130.1, 130.0, 129.0, 128.9, 128.4, 127.8, 127.2, 124.5, 122.94, 122.87, 121.3, 119.4, 111.5, 99.7, 48.4.

HRMS-ESI (m/z): [M+Na] $^+$ calculated for $C_{27}H_{20}BrNNaS$: 492.0392, found 492.0401.

2-benzhydryl-3-(o-tolylthio)-1H-indole (4aj).



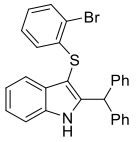
White solid, 115 mg, 94% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.34 – 7.26 (m, 6H), 7.26 – 7.21 (m, 2H), 7.18 – 7.13 (m, 5H), 7.12 (d, *J* = 7.4 Hz, 1H), 6.96 (td, *J* = 7.4, 0.9 Hz, 1H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.66 (d, *J* = 7.9 Hz, 1H), 6.12 (s, 1H), 2.49 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.3, 141.7, 137.9, 135.9, 134.5, 130.3, 129.9, 129.0, 128.8, 127.1, 126.3, 125.3, 124.4, 122.8, 121.0, 119.7, 111.4, 100.3, 48.3, 20.1.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{28}H_{24}NS$: 406.1624, found 406.1622.

2-benzhydryl-3-((2-bromophenyl)thio)-1H-indole (4ak).



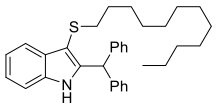
White solid, 139 mg, 98% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.48 – 7.44 (m, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.30 – 7.26 (m, 4H), 7.25 – 7.21 (m, 3H), 7.18 – 7.15 (m, 1H), 7.15 – 7.12 (m, 4H), 6.89 – 6.82 (m, 2H), 6.50 – 6.44 (m, 1H), 6.12 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 146.0, 141.3, 139.8, 135.9, 132.6, 130.0, 129.0, 128.9, 127.4, 127.1, 126.6, 125.6, 123.0, 121.3, 119.9, 119.6, 111.5, 99.9, 48.3.

HRMS-ESI (m/z): [M+Na] $^+$ calculated for $C_{27}H_{20}BrNNaS$: 492.0392, found 492.0369.

2-benzhydryl-3-(dodecylthio)-1H-indole (4al).



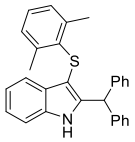
Colourless oil, 116 mg, 80% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.80 (s, 1H), 7.39 – 7.26 (m, 7H), 7.24 – 7.15 (m, 6H), 6.30 (s, 1H), 2.67 – 2.31 (m, 2H), 1.44 – 1.12 (m, 20H), 0.97 – 0.87 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 144.0, 142.2, 135.6, 130.9, 129.1, 128.8, 127.0, 122.3, 120.6, 119.5, 111.2, 104.1, 48.2, 36.1, 32.1, 30.2, 29.8, 29.7, 29.7, 29.5, 29.3, 28.8, 22.8, 14.3.

HRMS-ESI (m/z): [M+Na] $^+$ calculated for $C_{33}H_{41}NNaS$: 506.2852, found 506.2836.

2-benzhydryl-3-((2, 6-dimethylphenyl)thio)-1H-indole (4am).



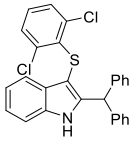
White solid, 112 mg, 89% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.40 – 7.26 (m, 7H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.15 – 7.11 (m, 1H), 7.10 – 6.96 (m, 8H), 5.93 (s, 1H), 2.42 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 141.8, 141.6, 140.3, 135.5, 133.5, 129.7, 128.9, 128.8, 128.4, 127.5, 127.0, 122.2, 120.4, 119. 4, 111.1, 103.8, 48.4, 22.4.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{29}H_{26}NS$: 420.1780, found 420.1776.

2-benzhydryl-3-((2,6-dichlorophenyl)thio)-1H-indole (4an).



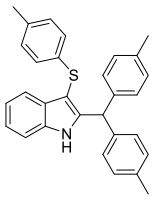
White solid, 120 mg, 87% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.32 – 7.26 (m, 4H), 7.26 – 7.21 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.16 – 7.11 (m, 2H), 7.09 (d, *J* = 7.5 Hz, 4H), 6.95 (t, *J* = 8.0 Hz, 1H), 6.26 (s, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.4, 141.7, 139.7, 135.3, 133.1, 130.0, 128.9, 128.9, 128.81, 128.76, 127.0, 122.3, 120.7, 119. 8, 111.3, 101.7, 48.5.

HRMS-ESI (m/z): [M+H] $^+$ calculated for $C_{27}H_{20}Cl_2NS$: 460.0688, found 460.0681.

2-(di-p-tolylmethyl)-3-(p-tolylthio)-1H-indole (4ba).



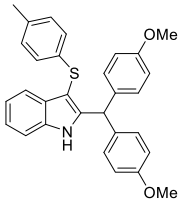
White solid, 109 mg, 84% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.22 – 7.19 (m, 1H), 7.16 – 7.13 (m, 1H), 7.11 (d, *J* = 8.0 Hz, 4H), 7.03 (d, *J* = 8.1 Hz, 4H), 6.96 – 6.92 (m, 4H), 6.09 (s, 1H), 2.35 (s, 6H), 2.27 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.5, 138.9, 136.6, 135.7, 135.3, 134.5, 130.4, 129.5, 129.5, 128.9, 126.4, 122.6, 120.9, 119.6, 111.3, 101.0, 47.6, 21.2, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{30}H_{27}NNaS$: 456.1756, found 456.1739.

2-(bis(4-methoxyphenyl)methyl)-3-(*p*-tolylthio)-1H-indole (4ca).



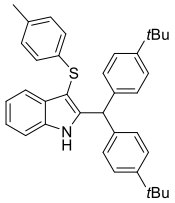
White solid, 123 mg, 88% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.21 – 7.17 (m, 1H), 7.15 – 7.11 (m, 1H), 7.04 (d, *J* = 8.6 Hz, 4H), 6.96 – 6.89 (m, 4H), 6.85 – 6.78 (m, 4H), 6.04 (s, 1H), 3.79 (s, 6H), 2.25 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.6, 145.8, 135.7, 135.2, 134.5, 134.1, 130.4, 130.0, 129.5, 126.4, 122.6, 120.9, 119.6, 114.2, 111.3, 100.9, 55.4, 46.7, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{30}H_{27}NNaO_2S$: 488.1655, found 488.1640.

2-(bis(4-methoxyphenyl)methyl)-3-(*p*-tolylthio)-1H-indole (4da).



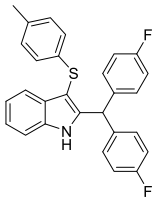
White solid, 127 mg, 82% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.32 – 7.28 (m, 5H), 7.21 – 7.17 (m, 1H), 7.14 – 7.11 (m, 1H), 7.08 (d, *J* = 8.3 Hz, 4H), 6.93 – 6.88 (m, 4H), 6.10 (s, 1H), 2.24 (s, 3H), 1.31 (s, 18H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 149.8, 145.8, 138.7, 135.8, 135.3, 134.4, 130.4, 129.4, 128.6, 126.4, 125.7, 122.5, 120.9, 119.6, 111.3, 101.0, 47.4, 34.6, 31.5, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{36}H_{39}NNaS$: 540.2695, found 540.2677.

2-(bis(4-fluorophenyl)methyl)-3-(*p*-tolylthio)-1H-indole (4ea).



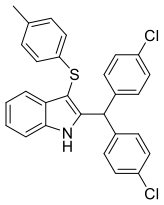
White solid, 114 mg, 86% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.65 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.20 – 7.16 (m, 1H), 7.12 – 7.06 (m, 4H), 7.04 – 6.96 (m, 4H), 6.96 – 6.90 (m, 4H), 6.15 (s, 1H), 2.28 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.9 (d, *J* = 246.2 Hz), 144.3 (s), 137.1 (d, *J* = 3.2 Hz), 135.7, 134.7 (d, *J* = 5.9 Hz), 130.4, 130.4, 130.2, 129.5, 126.4, 122.9, 121.1, 119.7, 115.7 (d, *J* = 21.4 Hz), 111.3, 101.7, 46.8, 20.9.

HRMS-ESI (m/z): $[M+H]^+$ calculated for $C_{28}H_{22}F_2NS$: 442.1436, found 442.1428.

2-(bis(4-chlorophenyl)methyl)-3-(*p*-tolylthio)-1H-indole (4fa).



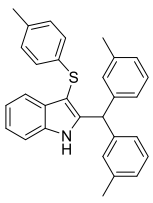
White solid, 121 mg, 85% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.26 (m, 1H), 7.26 – 7.21 (m, 4H), 7.19 – 7.15 (m, 1H), 7.04 – 7.01 (m, 4H), 6.92 – 6.87 (m, 4H), 6.10 (s, 1H), 2.26 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.7, 139.6, 135.8, 134.9, 134.7, 133.2, 130.3, 130.3, 129.5, 129.1, 126.5, 123.1, 121.3, 119.8, 111.4, 102.1, 47.2, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{28}H_{21}Cl_2NNaS$: 496.0664, found 496.0644.

2-(di-m-tolylmethyl)-3-(*p*-tolylthio)-1H-indole (4ga).



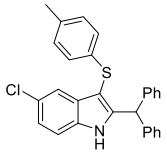
White solid, 104 mg, 80% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.35 (d, *J* = 8.1 Hz, 1H), 7.25 – 7.20 (m, 3H), 7.18 (td, *J* = 7.6, 0.9 Hz, 1H), 7.09 (d, *J* = 7.6 Hz, 2H), 6.99 – 6.93 (m, 8H), 6.12 (s, 1H), 2.30 (s, 6H), 2.28 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.2, 141.7, 138.5, 135.8, 135.3, 134.5, 130.4, 129.8, 129.4, 128.7, 127.8, 126.5, 126.0, 122.6, 120.9, 119.7, 111.3, 101.2, 48.2, 21.6, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{30}H_{27}NNaS$: 456.1756, found 456.1741.

2-benzhydryl-5-chloro-3-(*p*-tolylthio)-1H-indole (4ka).



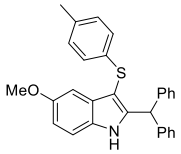
White solid, 121 mg, 92% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.59 (d, *J* = 2.0 Hz, 1H), 7.33 – 7.26 (m, 6H), 7.22 (d, *J* = 8.6 Hz, 1H), 7.15 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 4H), 6.96 – 6.90 (m, 4H), 6.14 (s, 1H), 2.26 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 146.5, 141.4, 134.9, 134.6, 134.1, 131.6, 129.6, 129.0, 128.9, 127.2, 126.9, 126.5, 123.1, 119.2, 112.4, 101.4, 48.3, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{28}H_{22}ClNNaS$: 462.1054, found 462.1034.

2-benzhydryl-5-methoxy-3-(*p*-tolylthio)-1H-indole (4la).



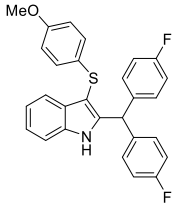
White solid, 119 mg, 91% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.32 – 7.26 (m, 4H), 7.26 – 7.22 (m, 2H), 7.20 (d, *J* = 8.8 Hz, 1H), 7.12 (d, *J* = 7.4 Hz, 4H), 7.06 (d, *J* = 2.3 Hz, 1H), 6.93 (s, 4H), 6.85 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.11 (s, 1H), 3.79 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 155.2, 145.7, 141.7, 135.2, 134.5, 131.2, 130.6, 129.5, 129.0, 128.8, 127.0, 126.2, 112.9, 112.1, 101.2, 100.9, 56.0, 48.4, 21.0.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{29}H_{25}NNaOS$: 458.1549, found 458.1531.

2-(bis(4-fluorophenyl)methyl)-3-((4-methoxyphenyl)thio)-1H-indole (4mc).



White solid, 125 mg, 91% yield.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.24 – 7.20 (m, 1H), 7.18 – 7.15 (m, 1H), 7.08 – 7.04 (m, 4H), 7.01 – 6.93 (m, 6H), 6.67 – 6.63 (m, 2H), 6.16 (s, 1H), 3.73 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 161.9 (d, *J* = 246.3 Hz), 157.9, 144.0, 137.2 (d, *J* = 3.2 Hz), 135.7, 130.5, 130.4, 129.0, 128.8, 122.9, 121.2, 119.7, 115.8 (d, *J* = 21.4 Hz), 114.5, 111.4, 102.8, 55.4, 46.9.

HRMS-ESI (m/z): $[M+Na]^+$ calculated for $C_{28}H_{21}F_2NNaOS$: 480.1204, found 480.1188.

VII. References

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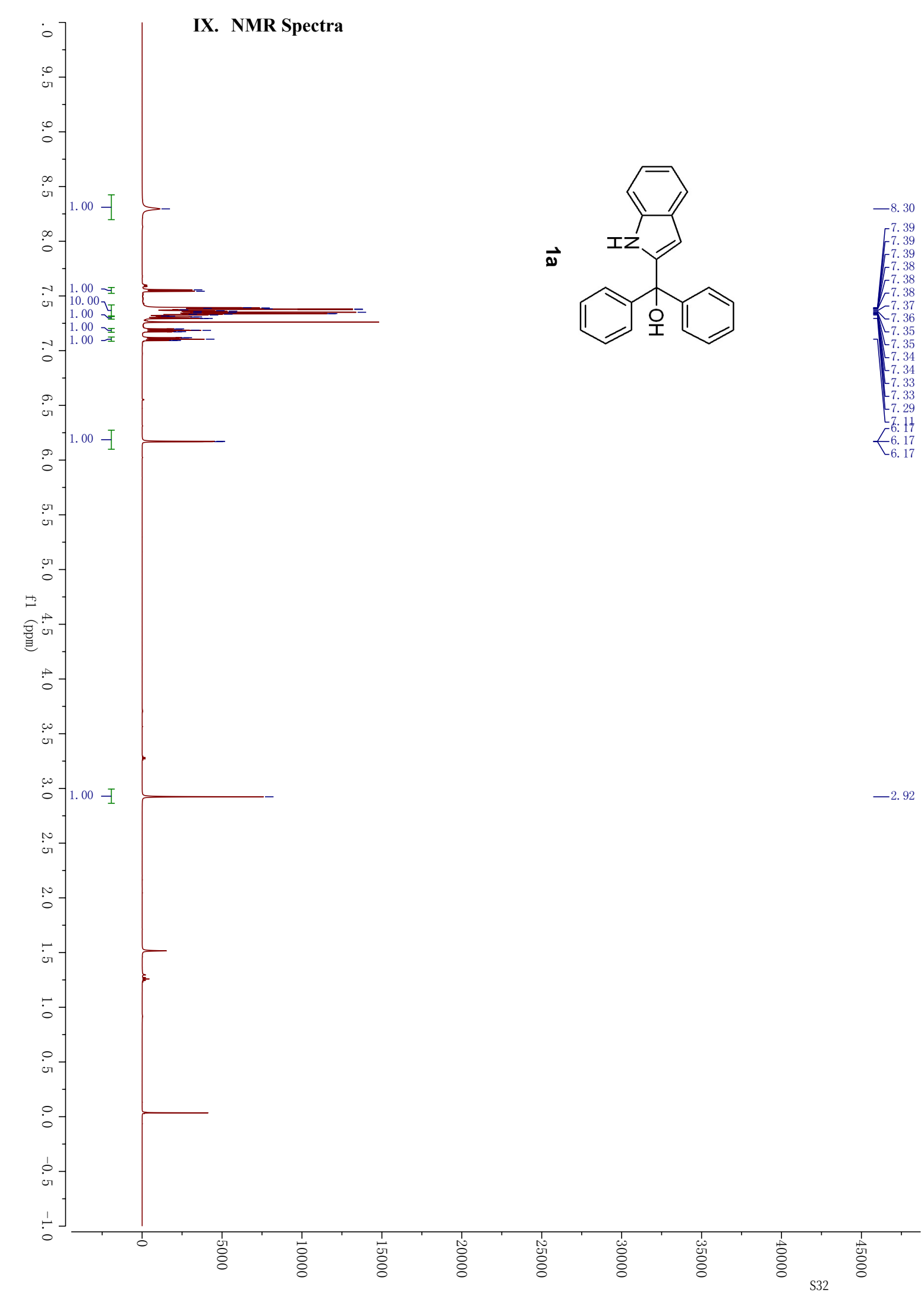
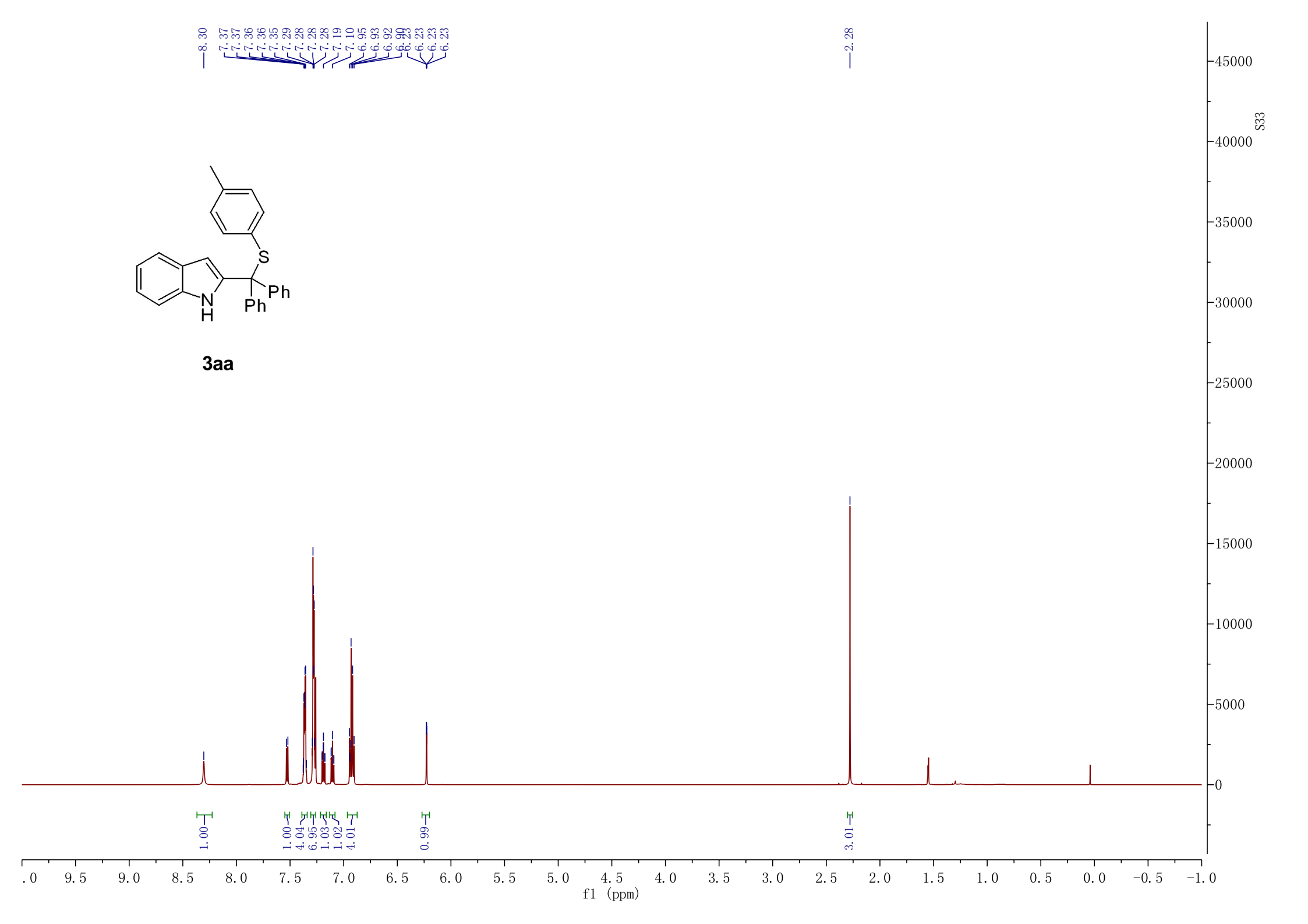
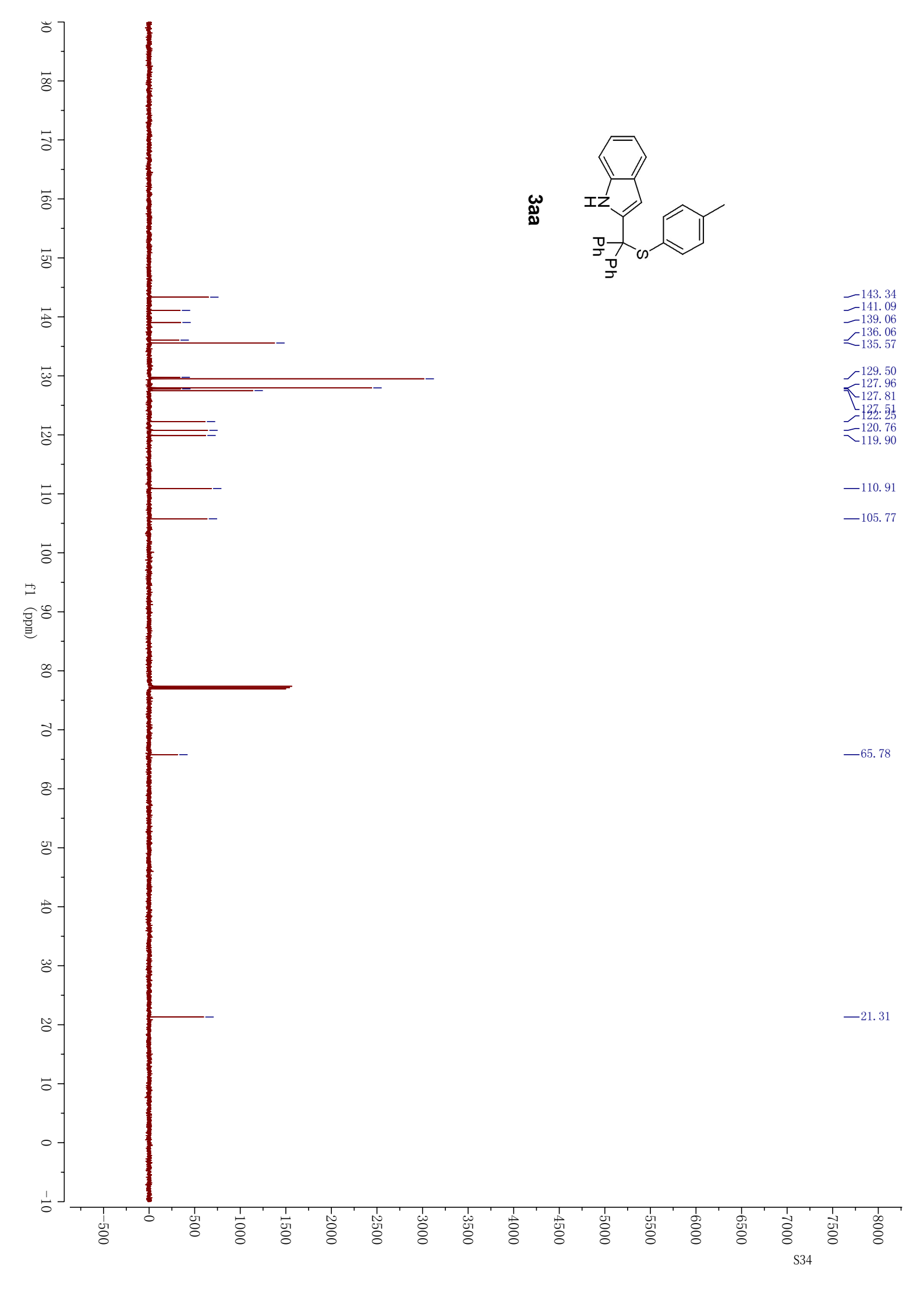
7. P. Sang, Z. Chen, J. Zou and Y. Zhang, *Green Chem.*, 2013, **15**, 2096.
8. P. Wang, S. Tang, P. Huang and A. Lei, *Angew. Chem. Int. Ed.*, 2017, **56**, 3009.

IX. NMR Spectra




8.30
7.37
7.37
7.36
7.36
7.35
7.29
7.28
7.28
7.28
7.19
7.10
6.95
6.93
6.92
6.90
6.23
6.23
6.23
2.28
S
Ph
Ph
N
H
3aa
S33
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1.00
1.00
4.04
6.95
1.03
1.02
4.01
0.99
3.01
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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141.09
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136.06
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127.51
122.25
120.76
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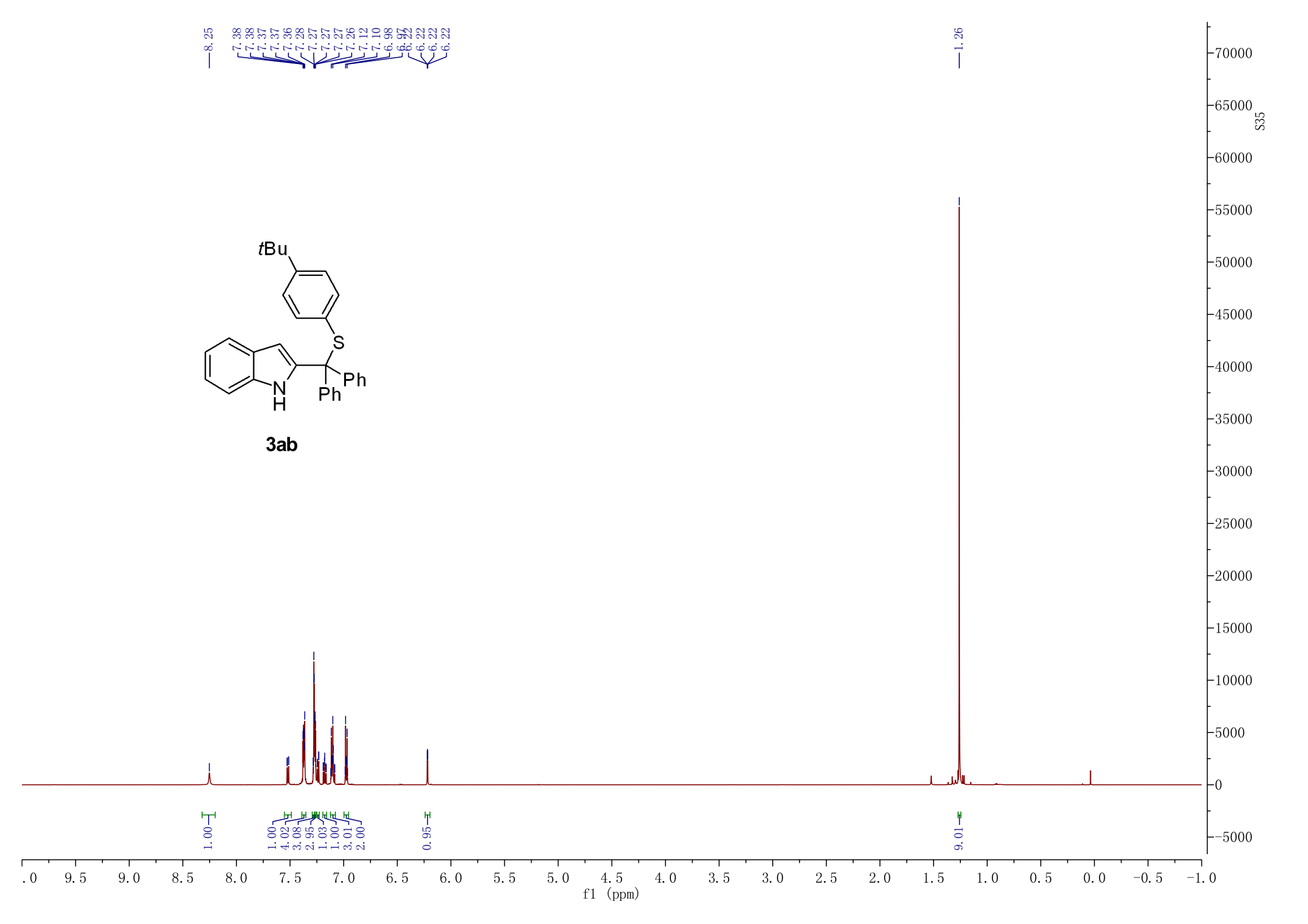
110.91
105.77
65.78
21.31
f1 (ppm)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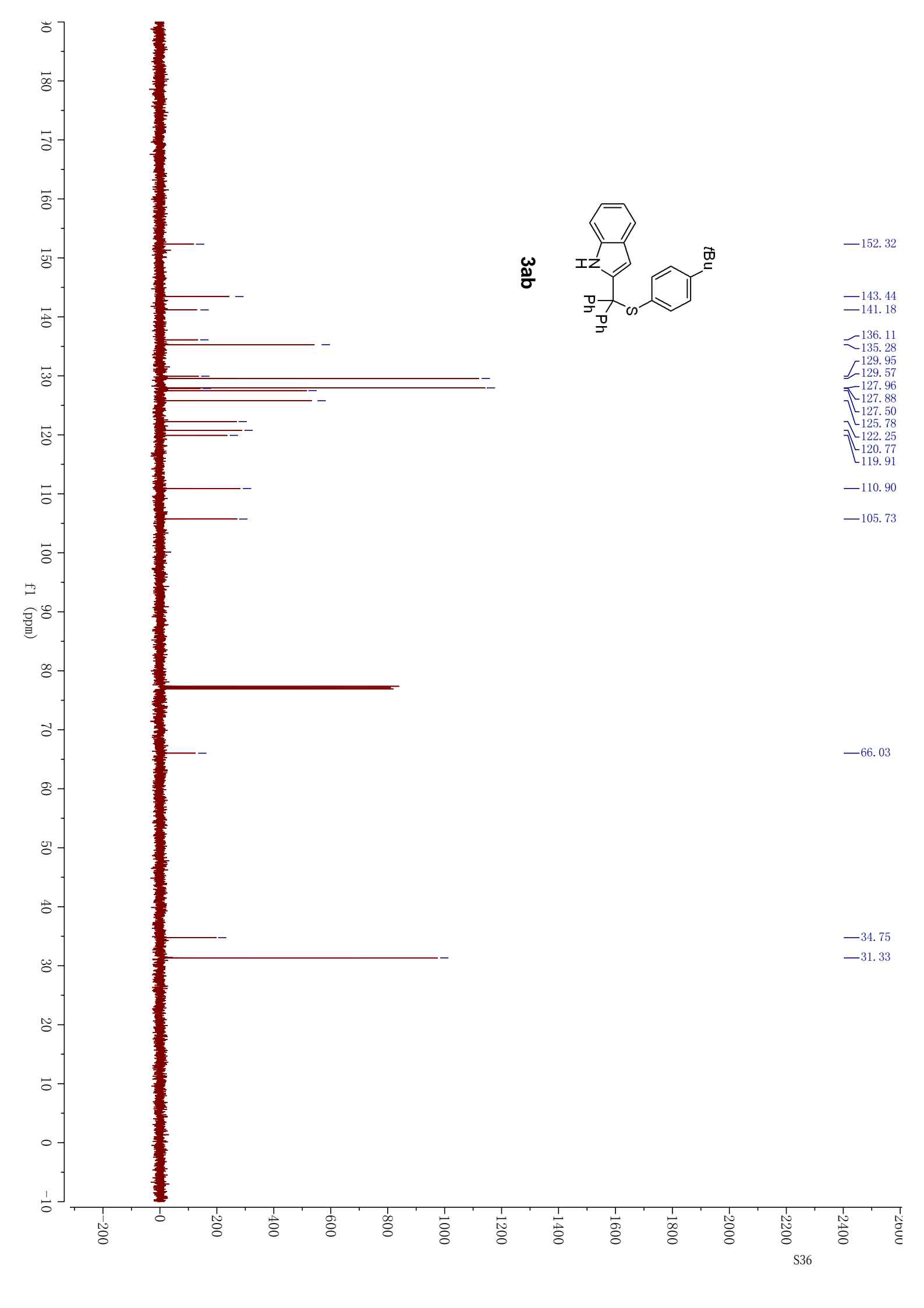
7.38
7.38
7.37
7.37
7.36
7.28
7.27
7.27
7.27
7.26
7.12
7.10
6.98
6.97
6.22
6.22
6.22
1.26
tBu
S
Ph
Ph
N
H
3ab
1.00
1.00
4.02
3.08
2.95
1.03
1.00
3.01
2.00
0.95
9.01
f1 (ppm)
S35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tBu
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H
Ph
Ph
S
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129.95
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110.90
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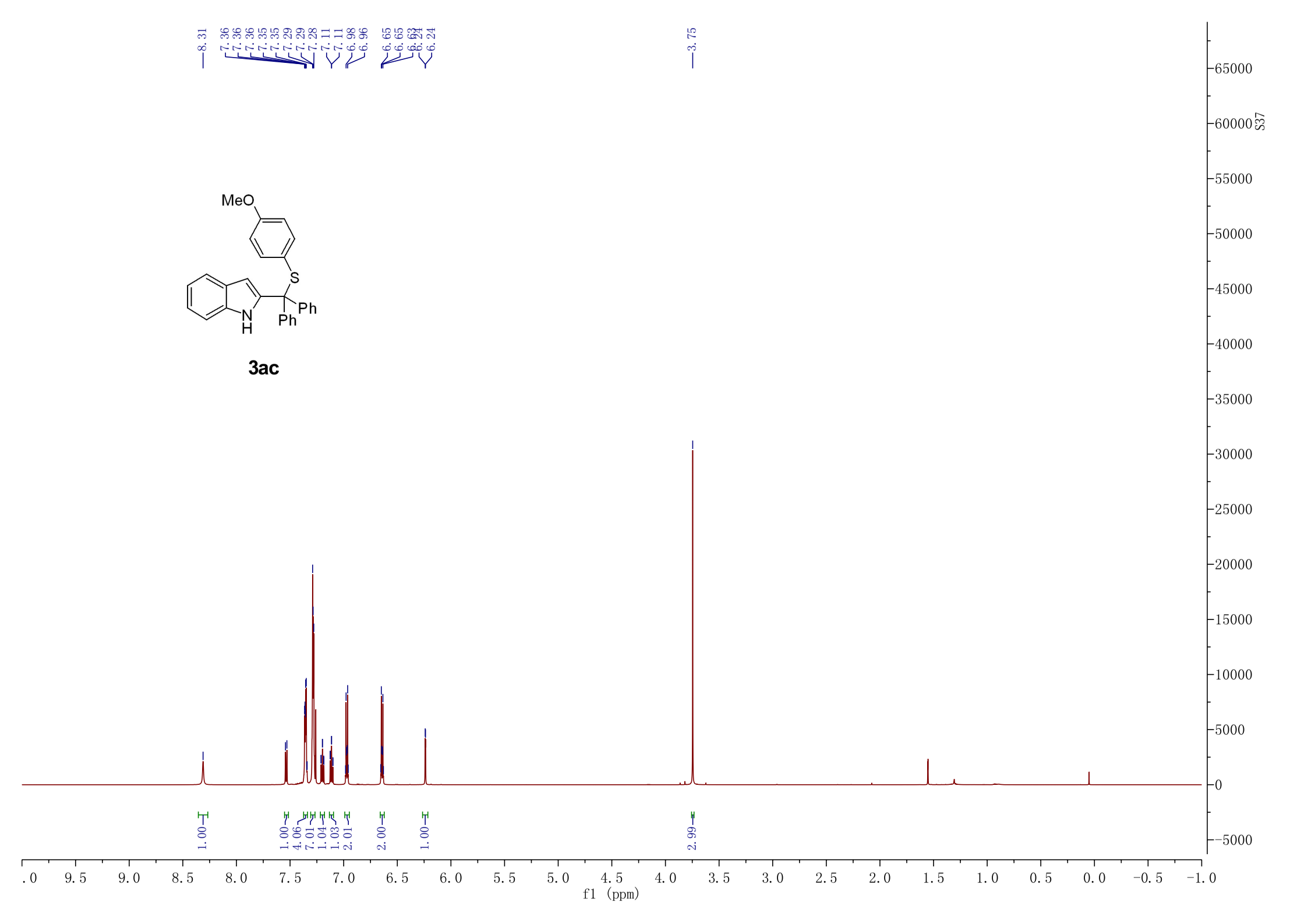
34.75
31.33
f1 (ppm)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7.36
7.36
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7.35
7.35
7.29
7.29
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7.11
7.11
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6.96
6.65
6.65
6.24
6.24
3.75
MeO
S
Ph
Ph
N
H
3ac
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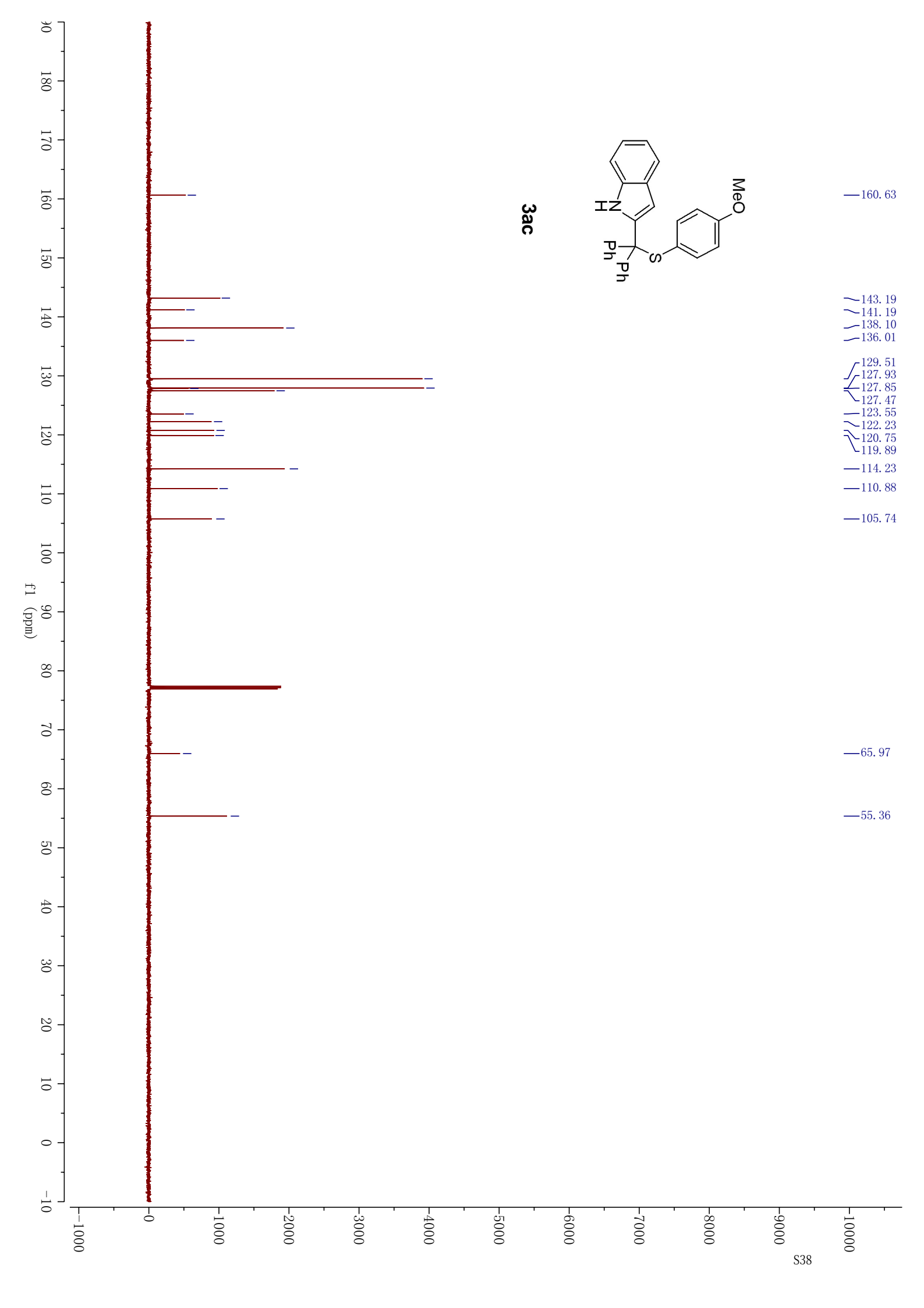
7.01
1.04
1.03
2.01
2.00
1.00
2.99
f1 (ppm)
S37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Ph
Ph
S
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122.23
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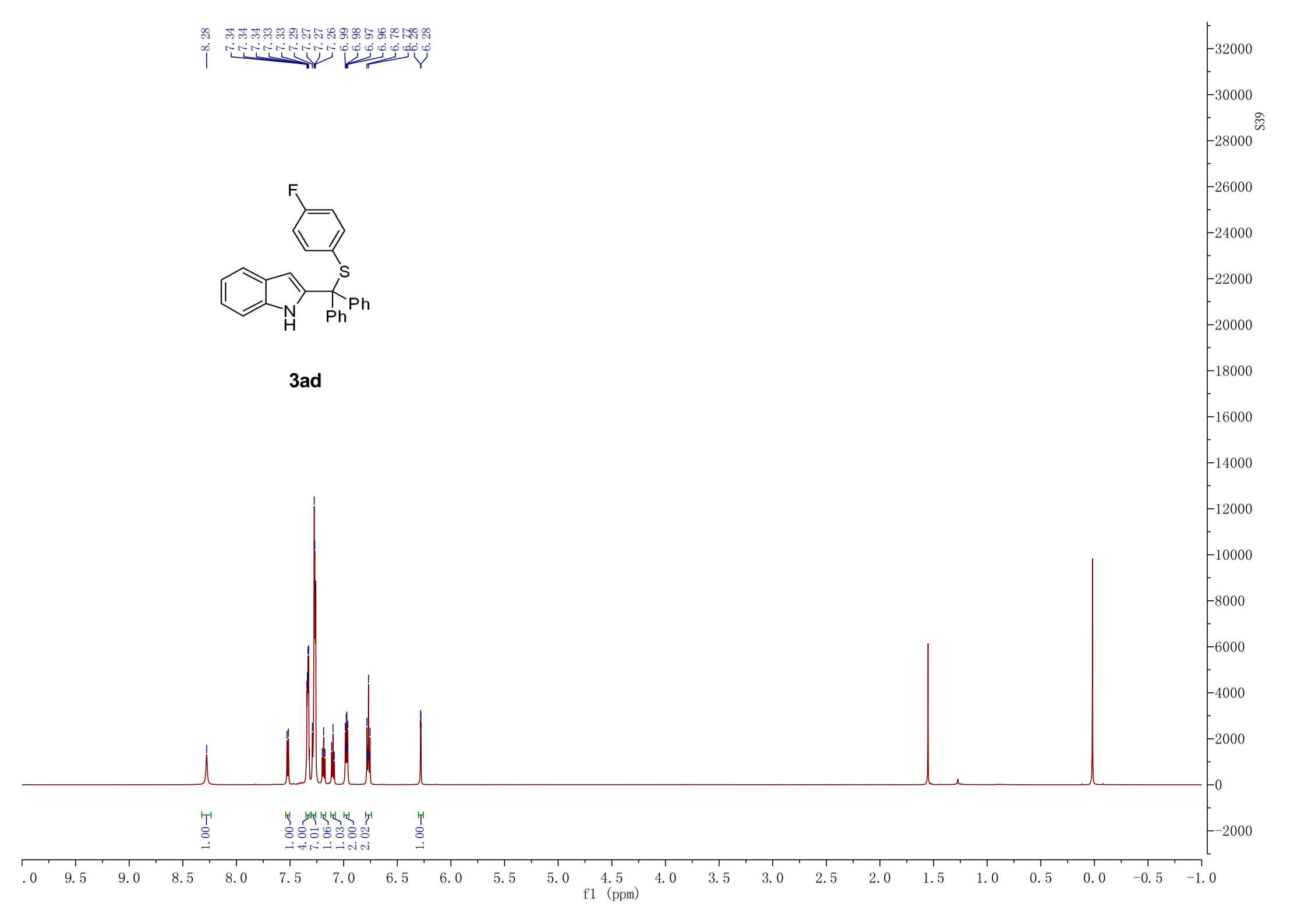
110.88
105.74
65.97
55.36
f1 (ppm)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7.34
7.34
7.33
7.29
7.27
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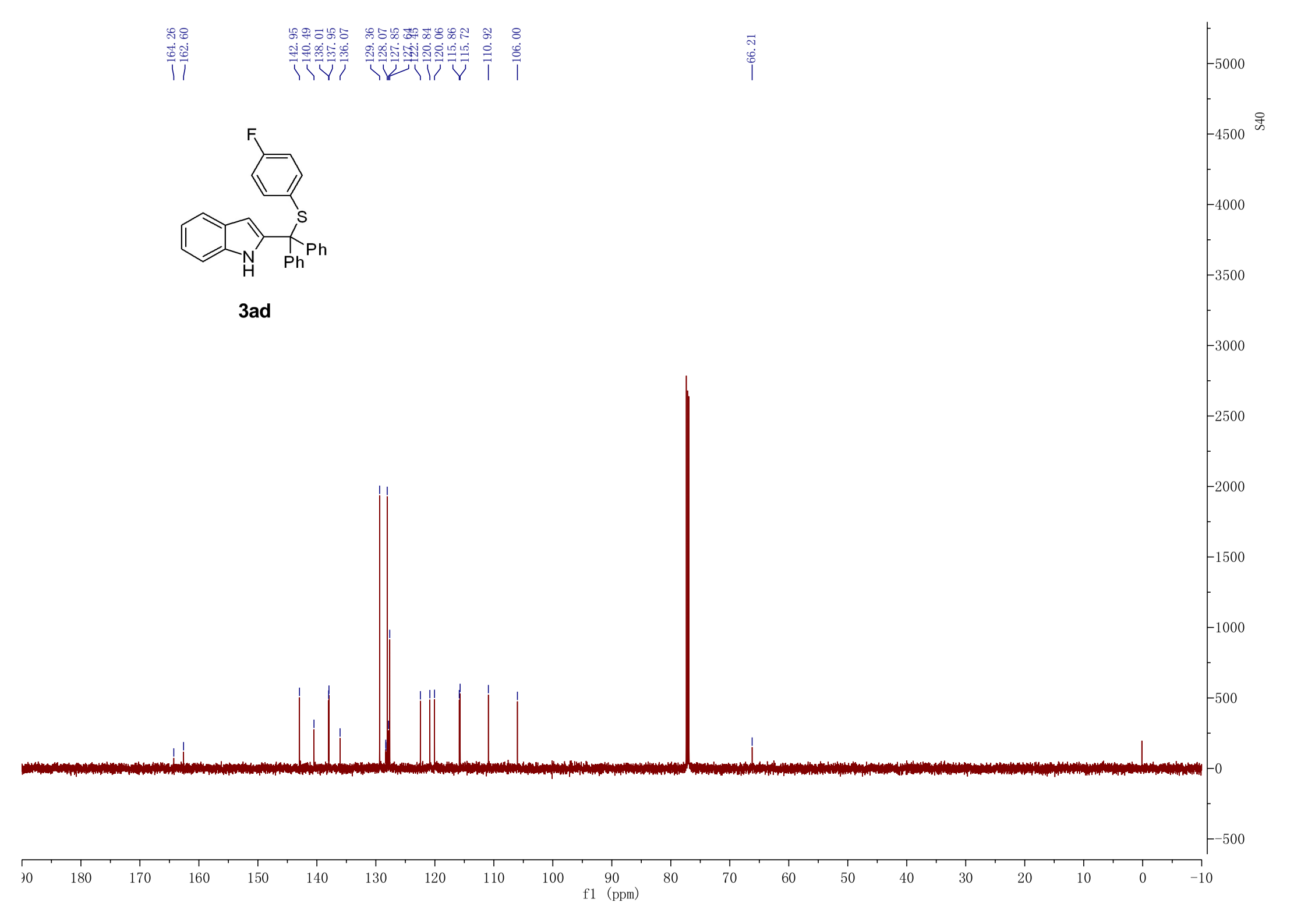
N
H
3ad
S39
f1 (ppm)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137.95
136.07
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127.85
127.64
122.45
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110.92
106.00
66.21
F
S
N
H
Ph
Ph
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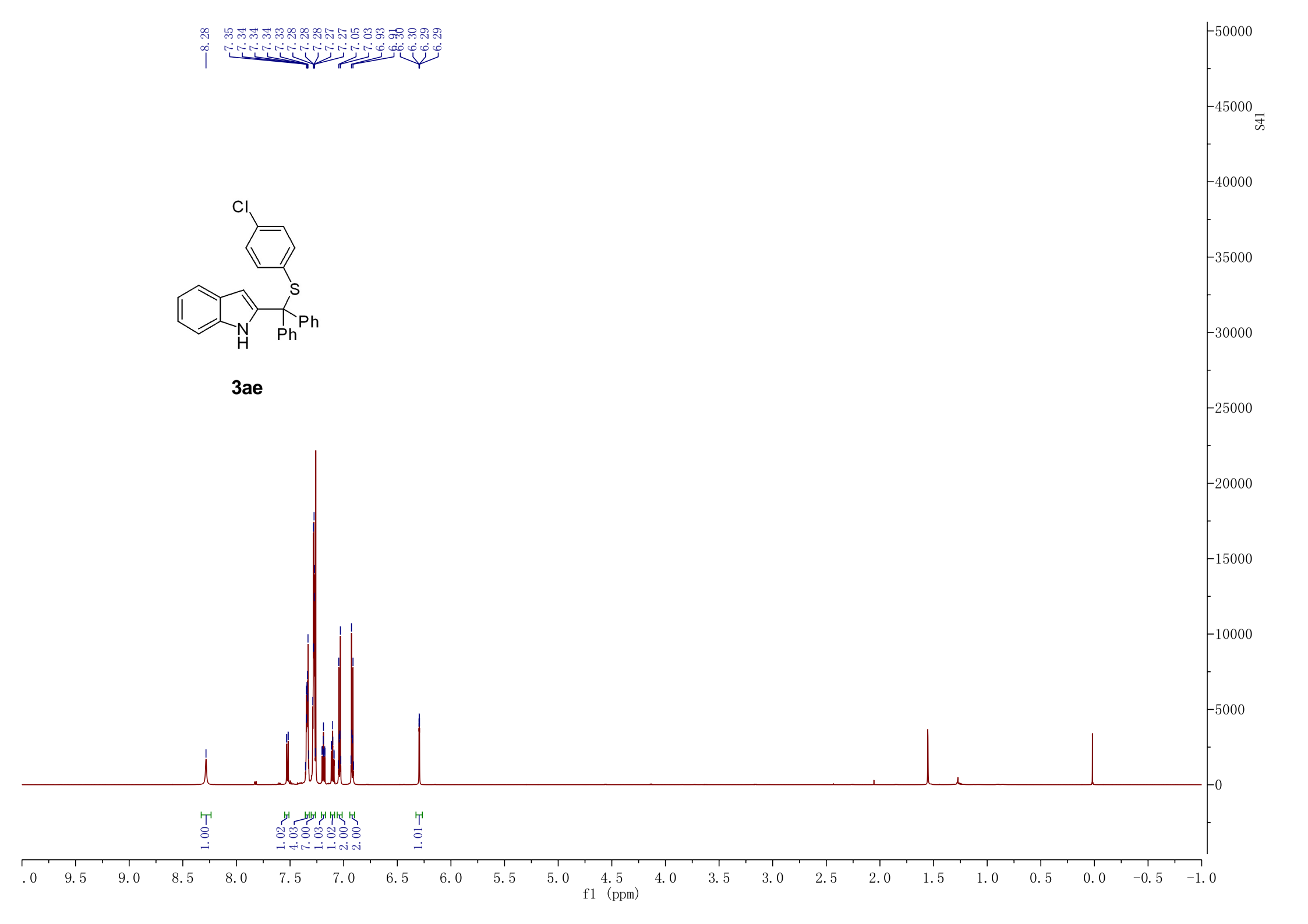
3000
2500
2000
1500
1000
500
0
−500
f1 (ppm)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Cl
S
Ph
Ph
N
H
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40000
35000
30000
25000
20000
15000
10000
5000
0
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1.00
1.02
4.03
7.00
1.03
1.02
2.00
2.00
1.01
.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
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1.5
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0.0
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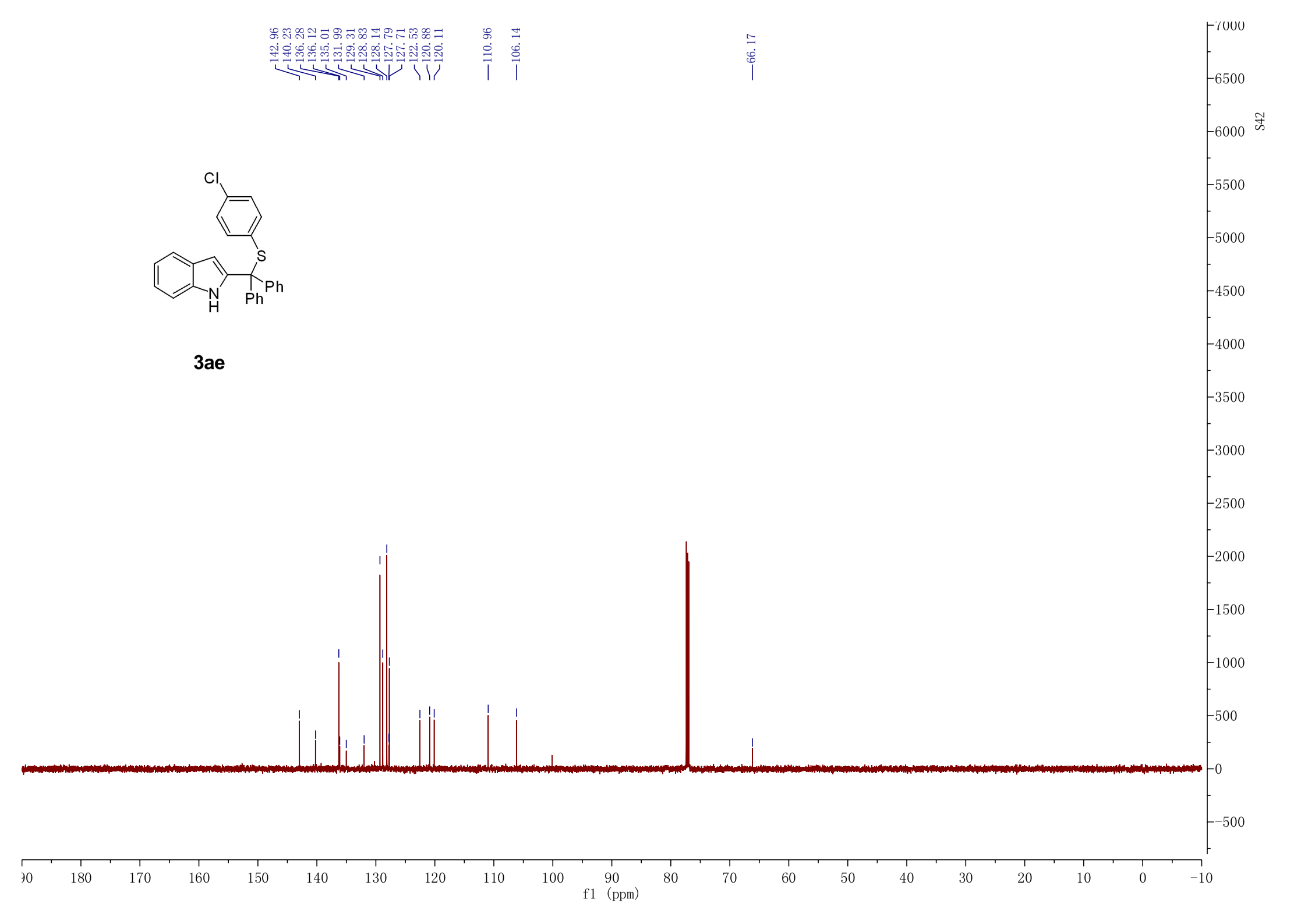
-1.0
f1 (ppm)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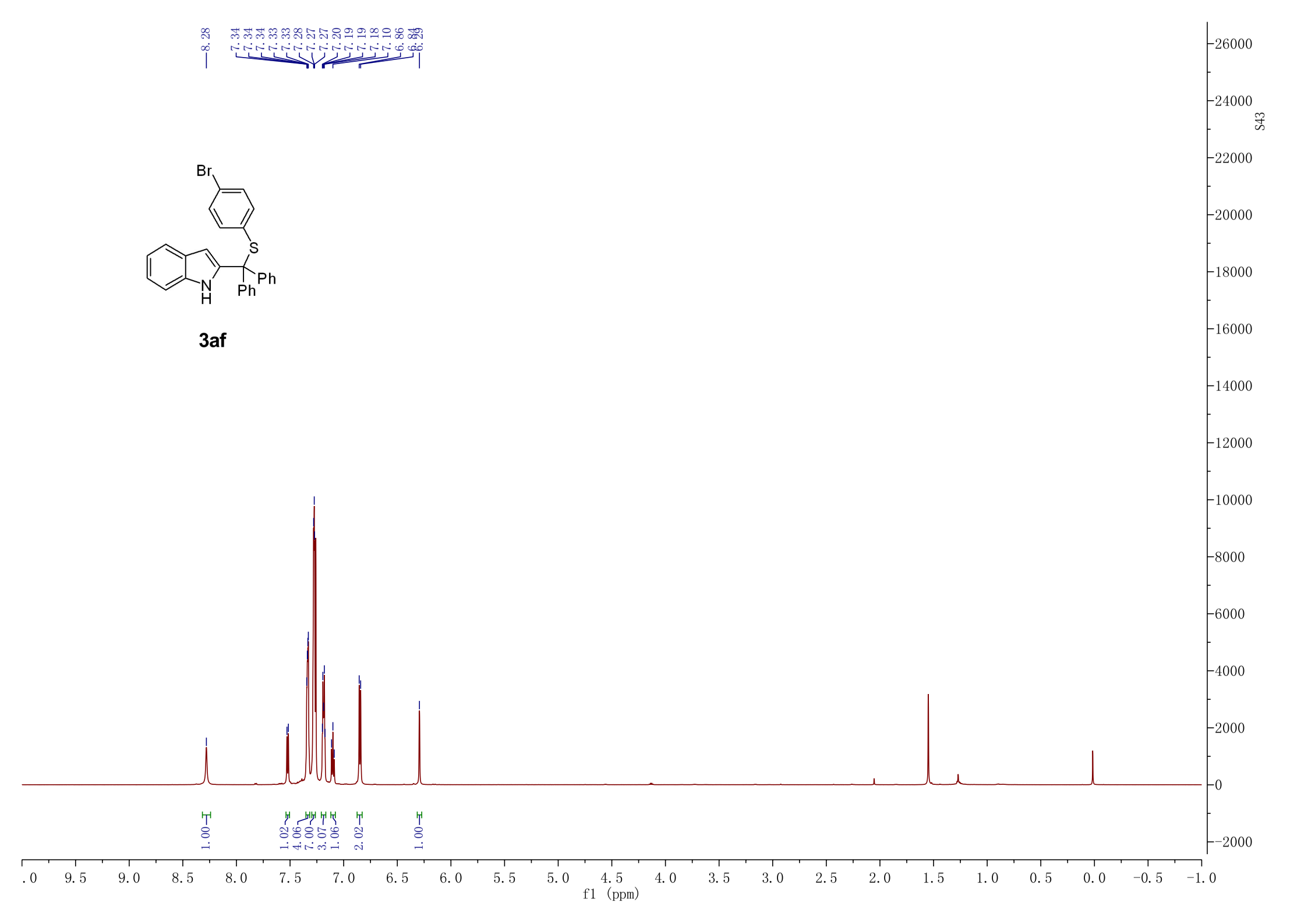
Cl
S
Ph
Ph
N
H
3ae
f1 (ppm)
S42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7.10
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6.29
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Ph
Ph
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3.07
1.06
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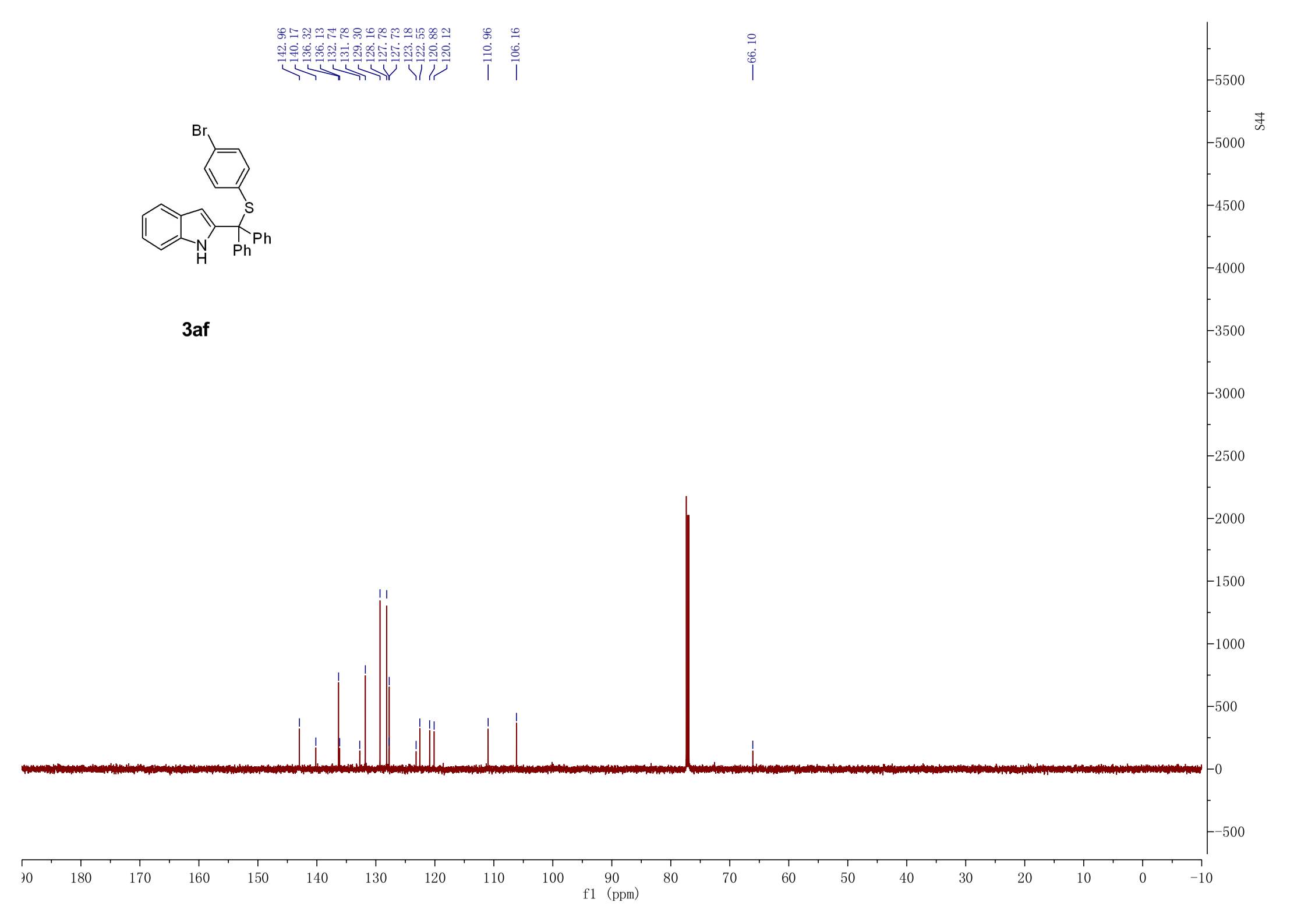
1.00
f1 (ppm)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132.74
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128.16
127.78
127.73
123.18
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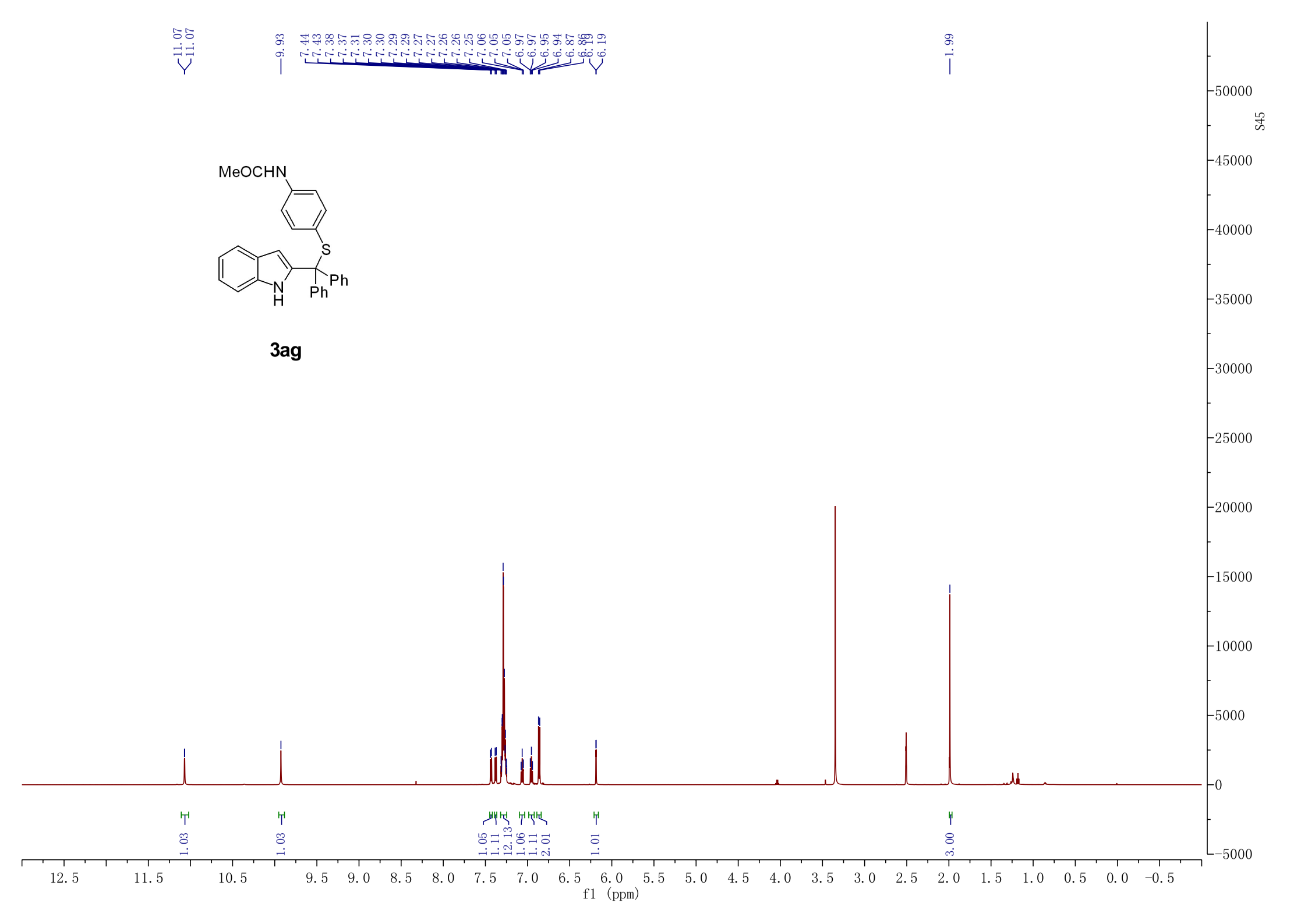
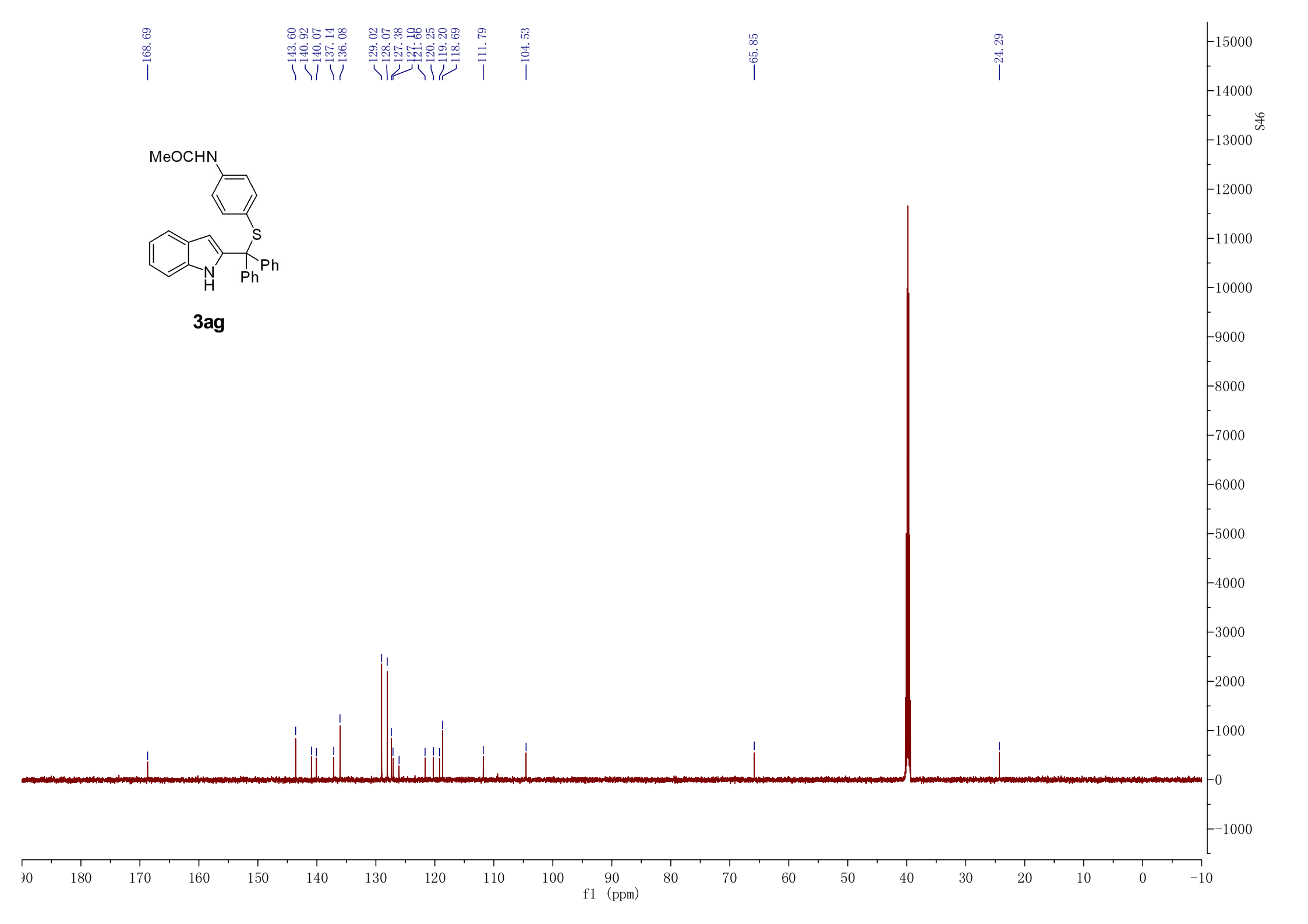
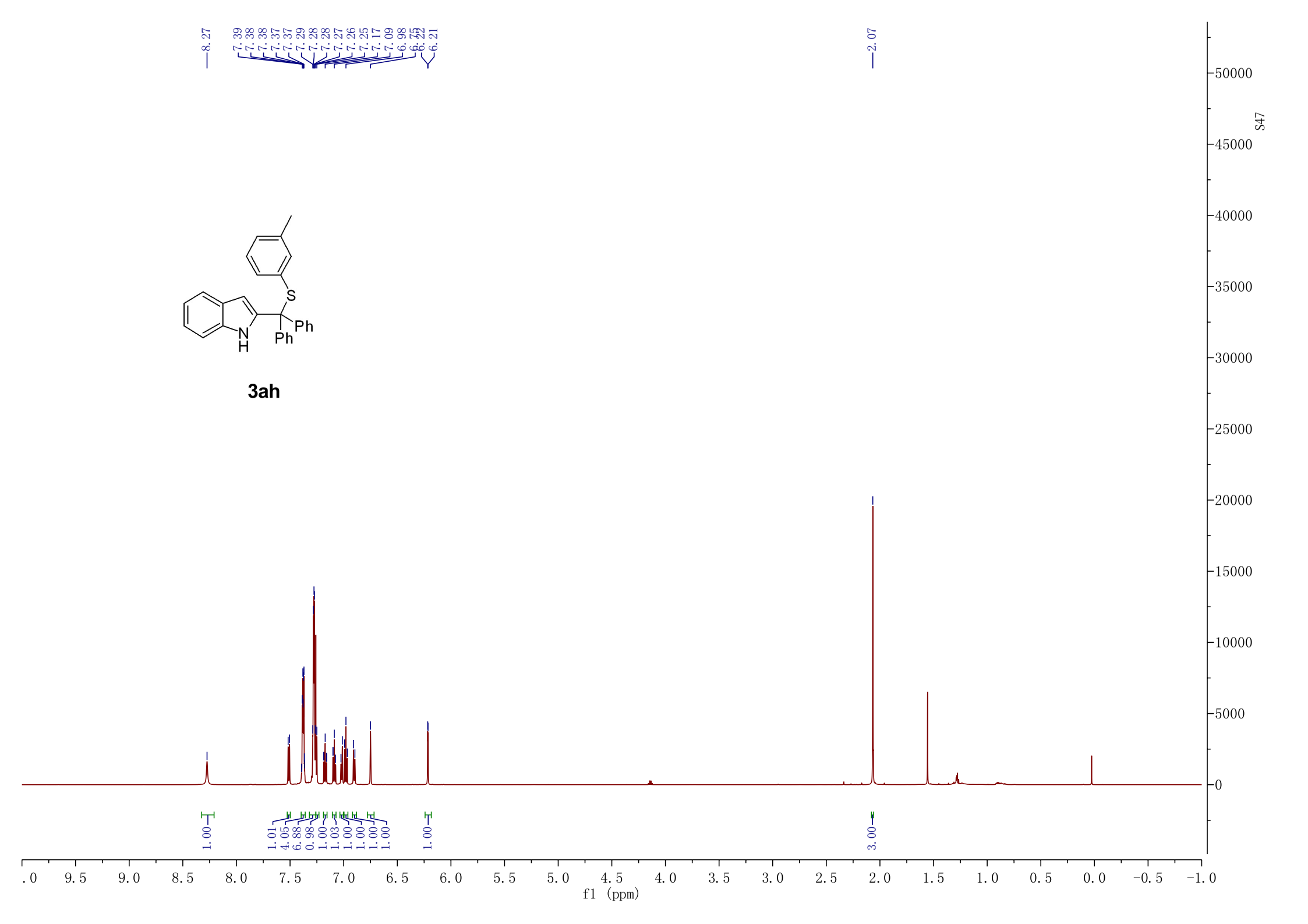
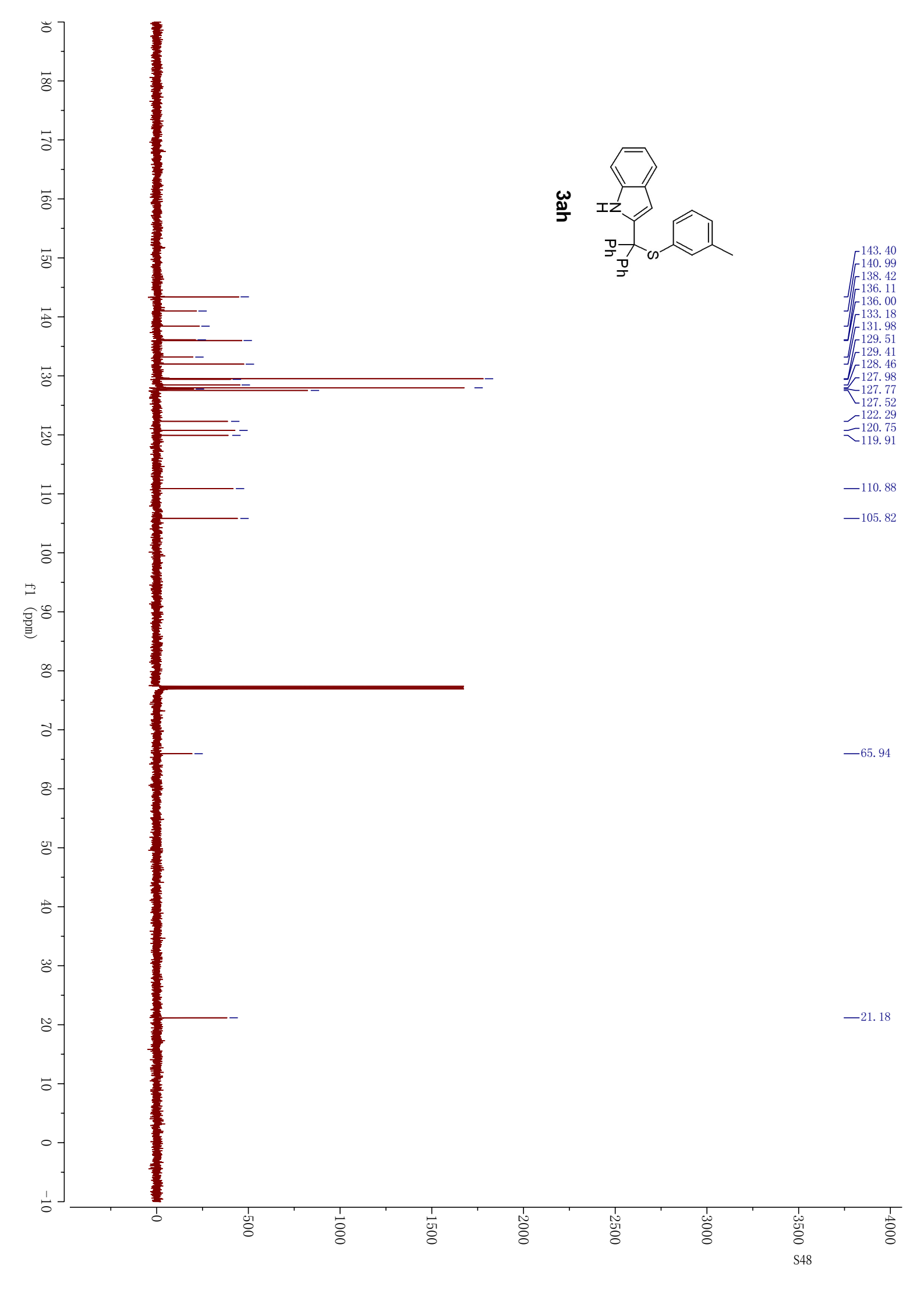
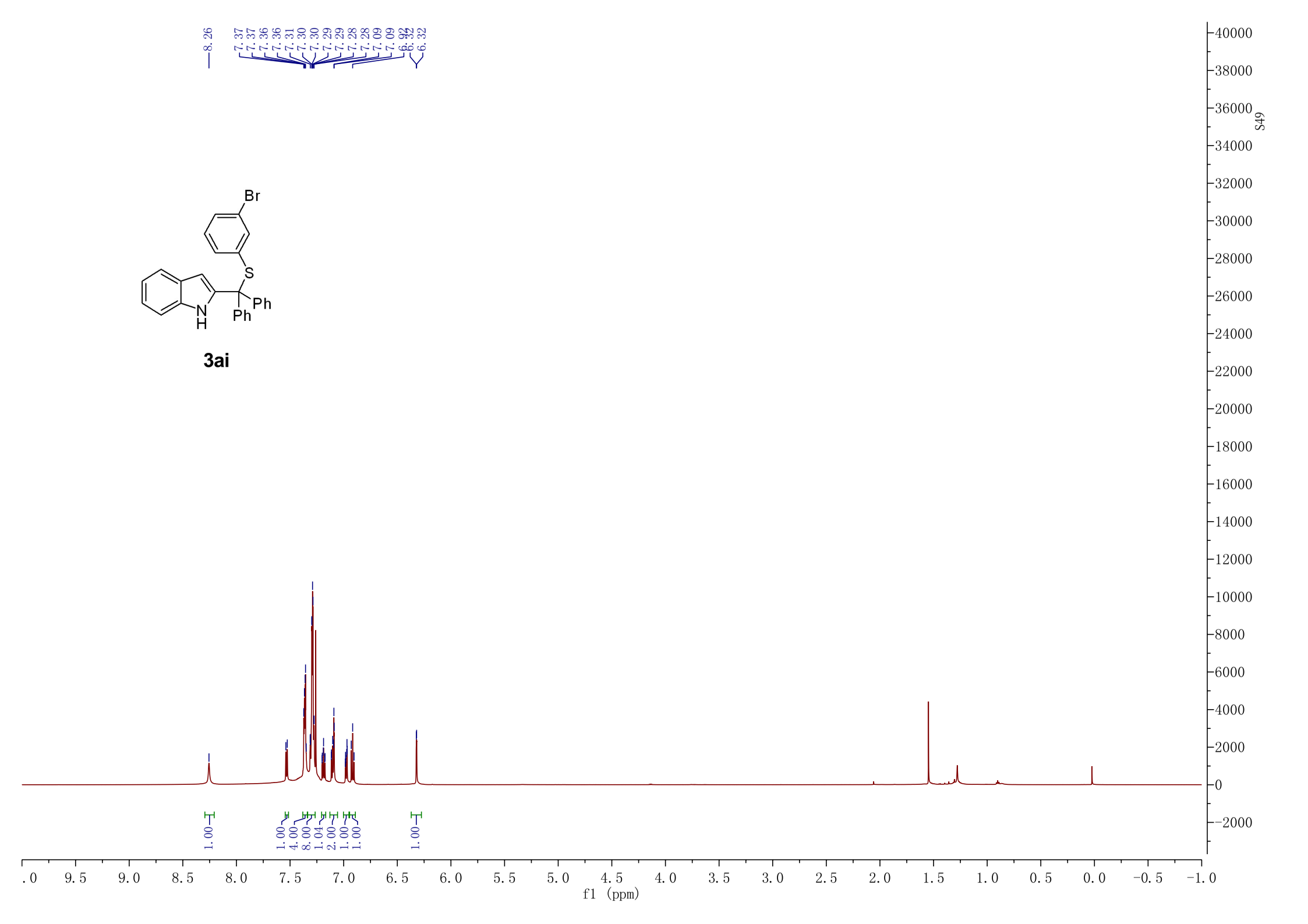
120.88
120.12
110.96
106.16
66.10
Br
S
N
H
Ph
Ph
3af
S44
f1 (ppm)

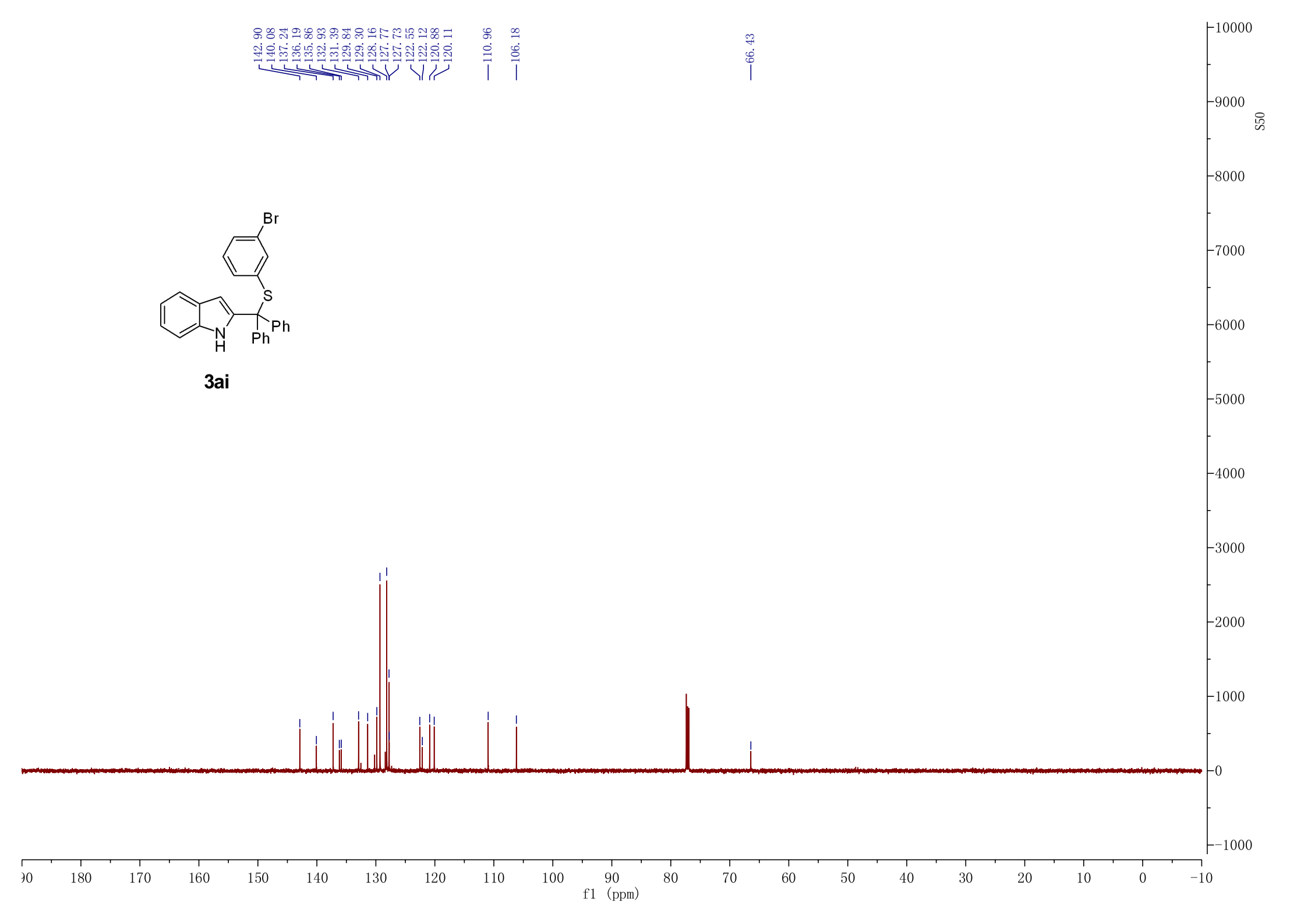

11.07
11.07
9.93
7.44
7.43
7.38
7.37
7.31
7.30
7.30
7.29
7.29
7.27
7.27
7.26
7.26
7.25
7.06
7.05
7.05
6.97
6.97
6.95
6.94
6.87
6.86
6.19
6.19
1.99
MeOCHN
S
N
H
Ph
Ph
3ag
S45
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
1.03
1.03
1.05
1.11
12.13
1.06
1.11
2.01
1.01
3.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

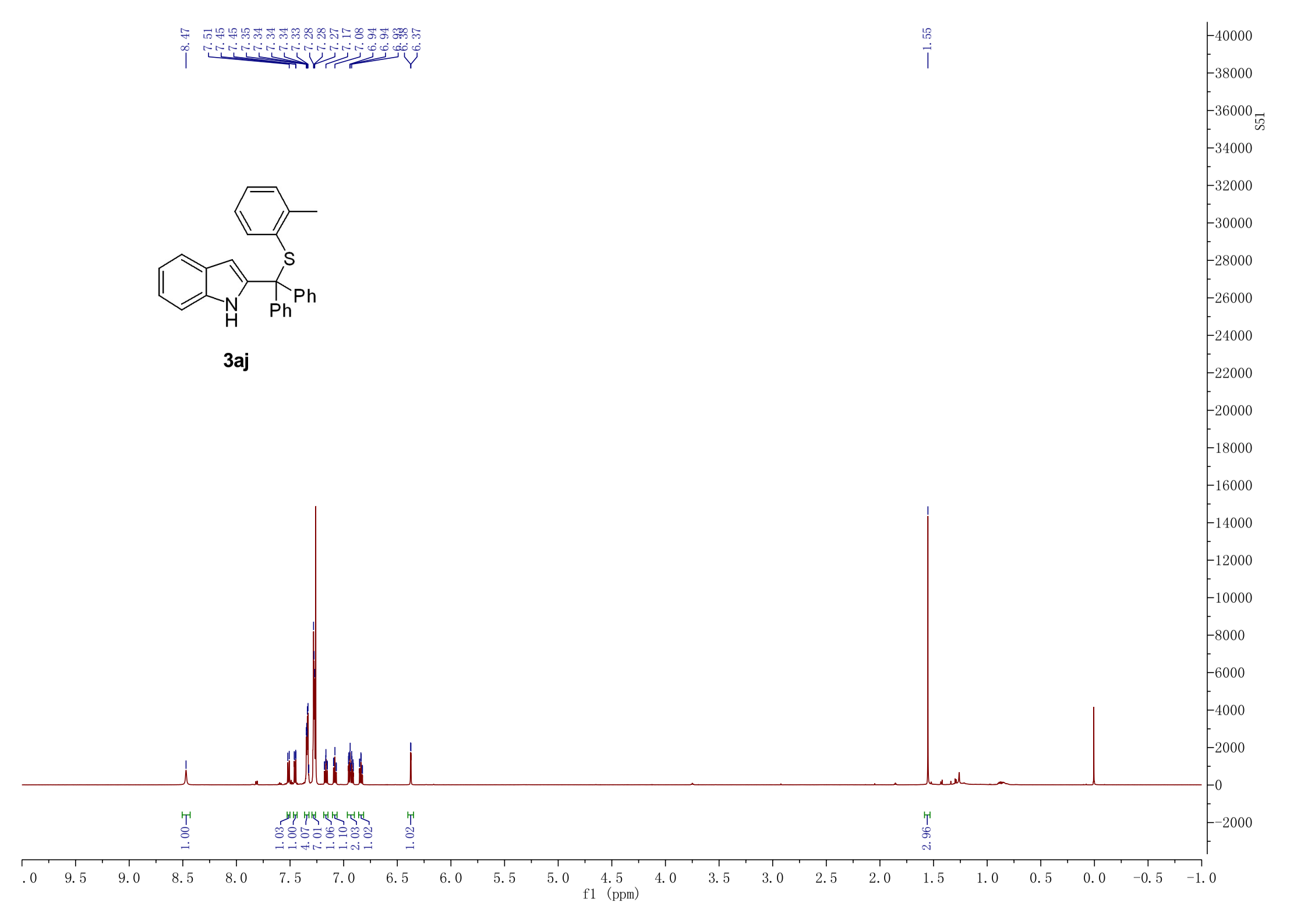

168.69
143.60
140.92
140.07
137.14
136.08
129.02
128.07
127.38
120.25
119.20
118.69
111.79
104.53
65.85
24.29
MeOCHN
S
N
H
Ph
Ph
3ag
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
−1000
S46
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

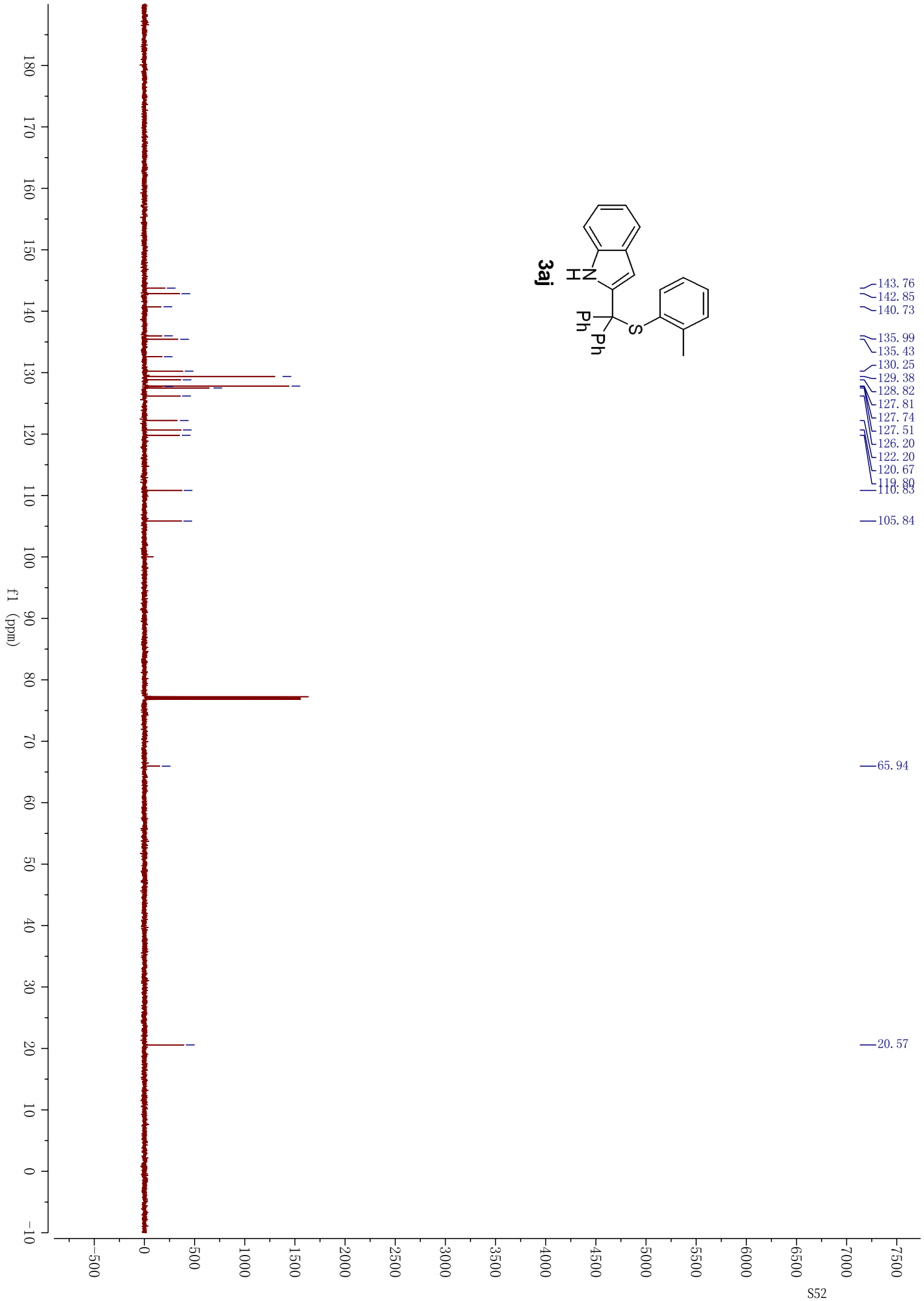

8.27
7.39
7.38
7.38
7.37
7.37
7.29
7.28
7.28
7.27
7.26
7.25
7.17
7.09
6.98
6.75
6.21
2.07
S
Ph
Ph
N
H
3ah
S47
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1.00
1.01
4.05
6.88
0.98
1.00
1.03
1.00
1.00
1.00
1.00
3.00
f1 (ppm)

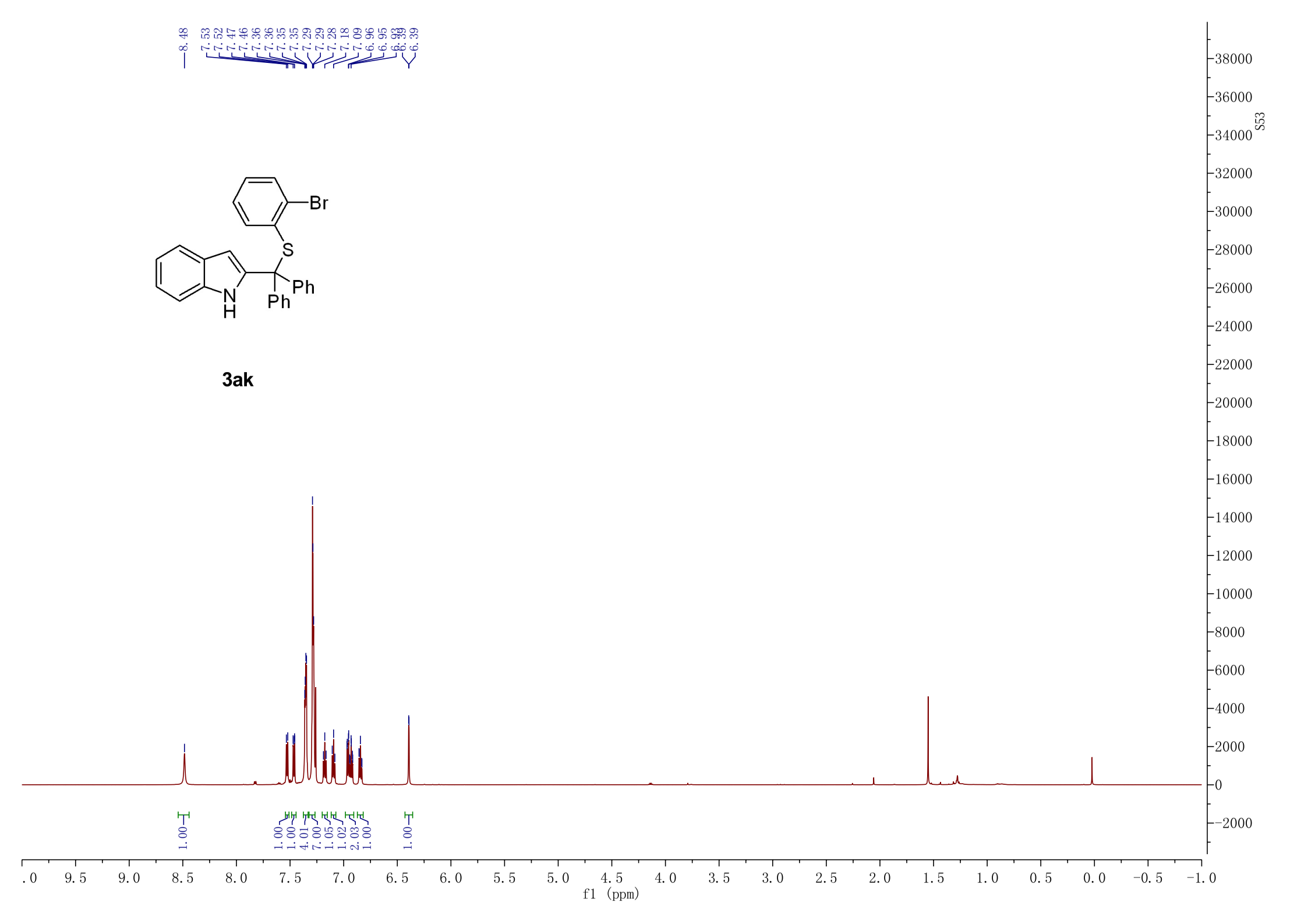

3ah
143.40
140.99
138.42
136.11
136.00
133.18
131.98
129.51
129.41
128.46
127.98
127.77
127.52
122.29
120.75
119.91
110.88
105.82
65.94
21.18
f1 (ppm)

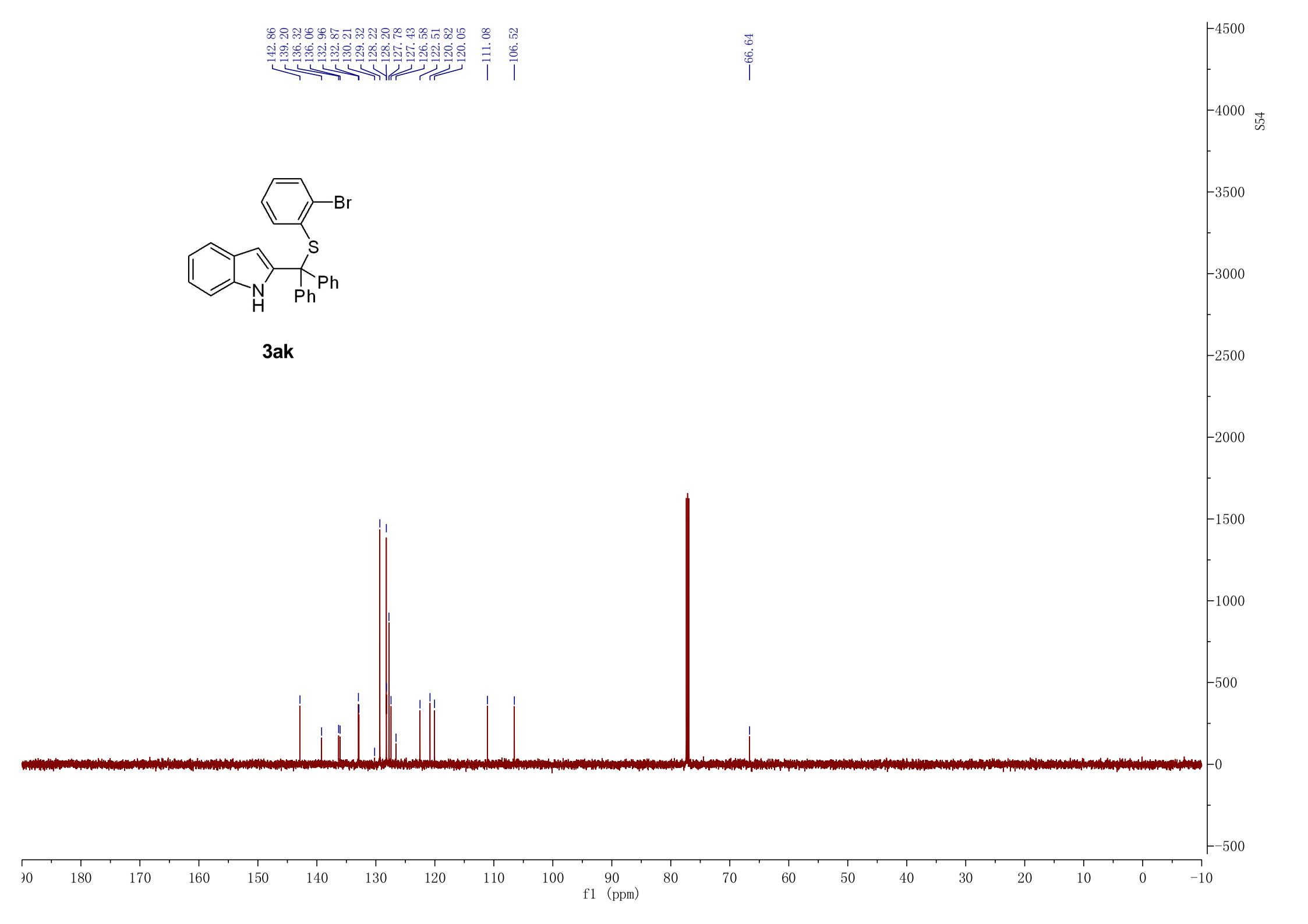

8.26
7.37
7.37
7.36
7.36
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.09
7.09
6.32
6.32
Br
S
Ph
Ph
N
H
3ai
1.00
1.00
4.00
8.00
1.04
2.00
1.00
1.00
1.00
f1 (ppm)

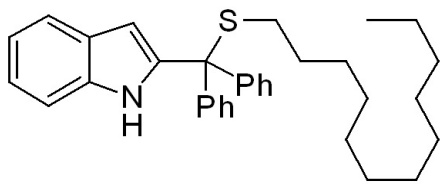

142.90
140.08
137.24
136.19
135.86
132.93
131.39
129.84
129.30
128.16
127.77
127.73
122.55
122.12
120.88
120.11
110.96
106.18
66.43
Br
S
N
H
Ph
Ph
3ai
S50
f1 (ppm)


8.47
7.51
7.45
7.45
7.35
7.34
7.34
7.34
7.33
7.28
7.28
7.27
7.17
7.08
6.94
6.94
6.37
1.55
S
Ph
Ph
N
H
3aj
S51
f1 (ppm)


3aj
143.76
142.85
140.73
135.99
135.43
130.25
129.38
128.82
127.81
127.74
127.51
126.20
122.20
120.67
119.80
110.83
105.84
65.94
20.57
f1 (ppm)

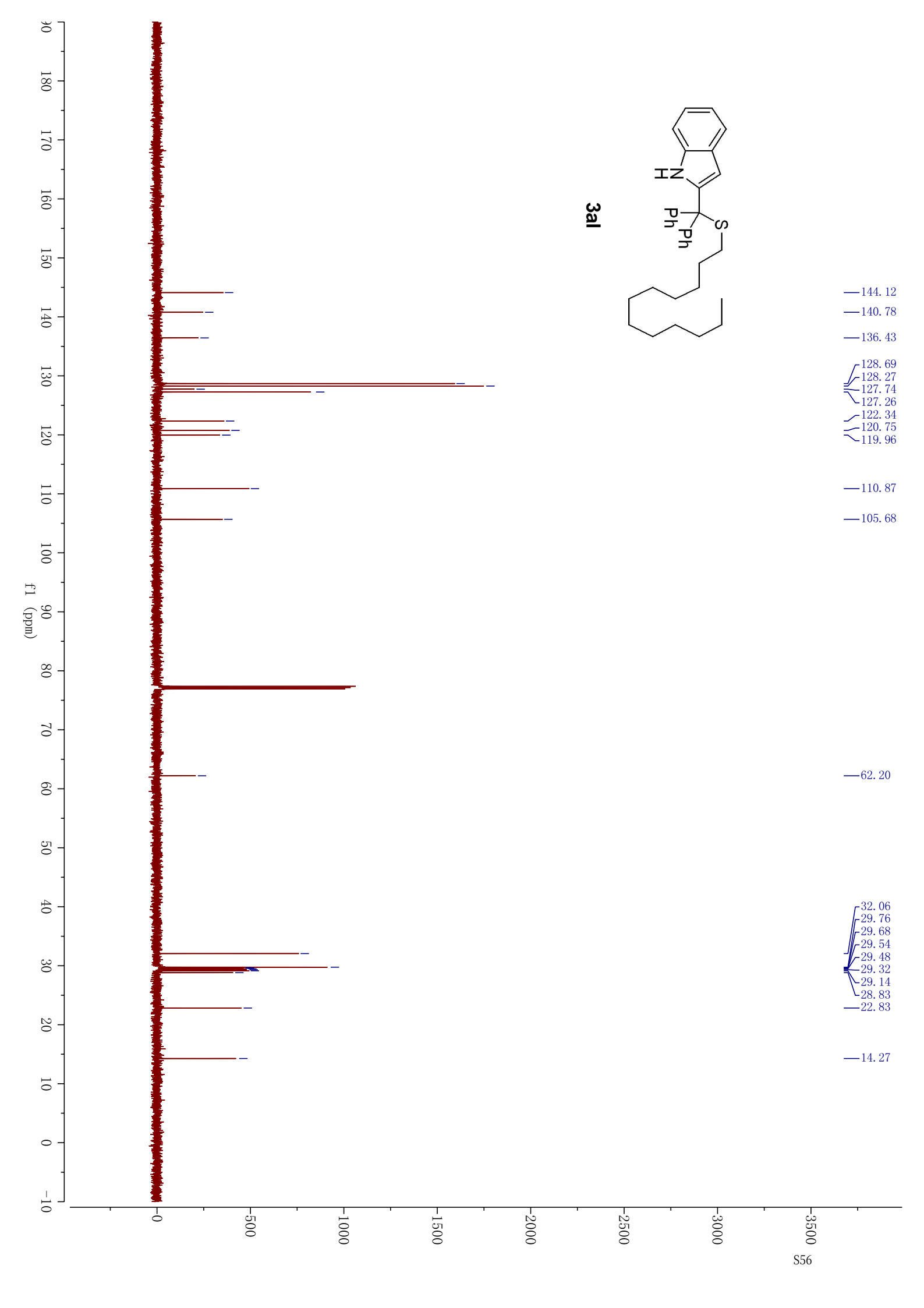

8.48
7.53
7.52
7.47
7.46
7.36
7.36
7.35
7.35
7.29
7.29
7.28
7.18
7.09
6.96
6.95
6.39
6.39
Br
S
Ph
Ph
N
H
3ak
S53
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
1.00
1.00
1.00
4.01
7.00
1.05
1.02
2.03
1.00
1.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

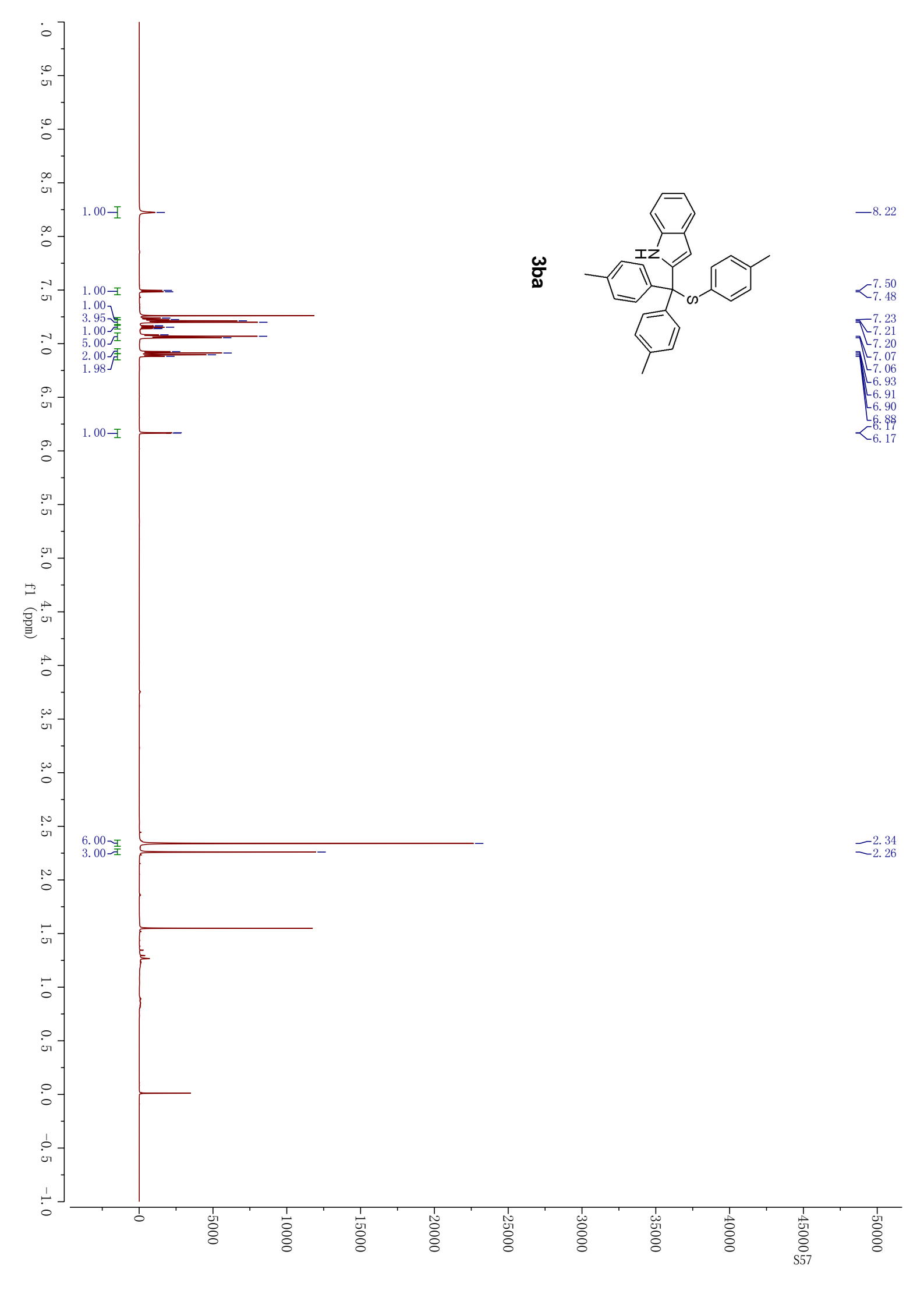

142.86
139.20
136.32
136.06
132.96
132.87
130.21
129.32
128.22
128.20
127.78
127.43
126.58
122.51
120.82
120.05
111.08
106.52
66.64
Br
S
Ph
Ph
N
H
3ak
f1 (ppm)
S54

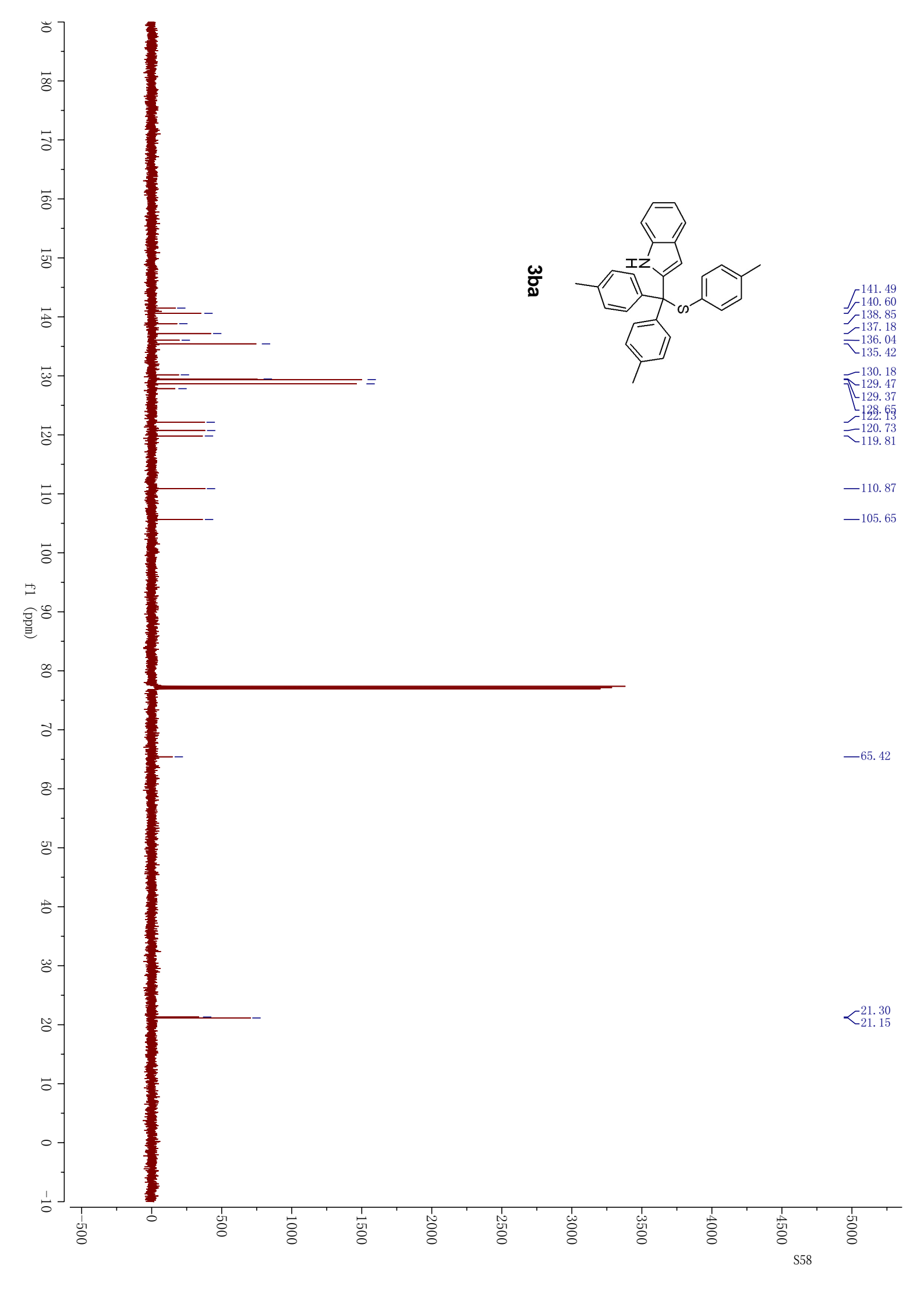

S
Ph
Ph
N
H

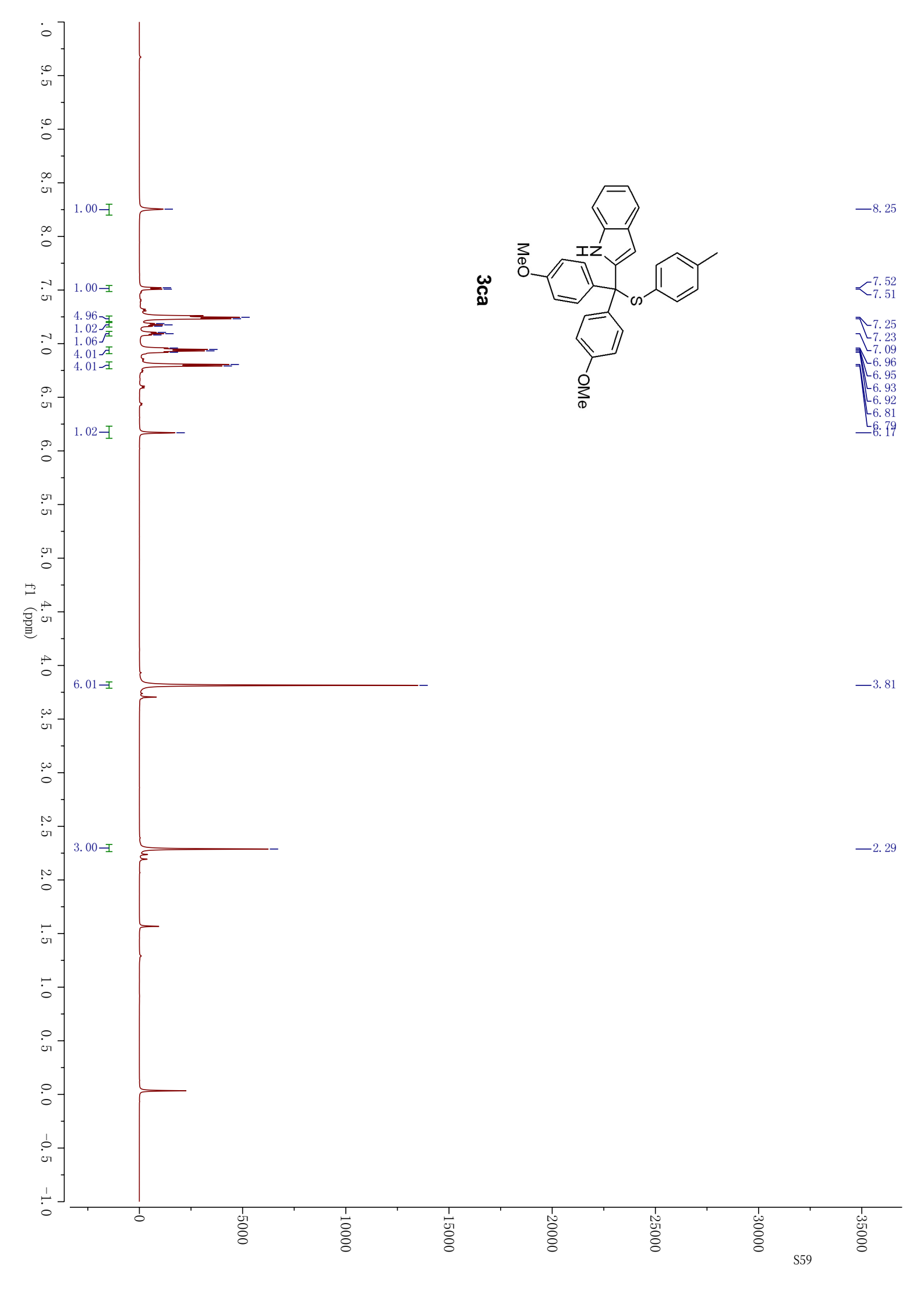
3al

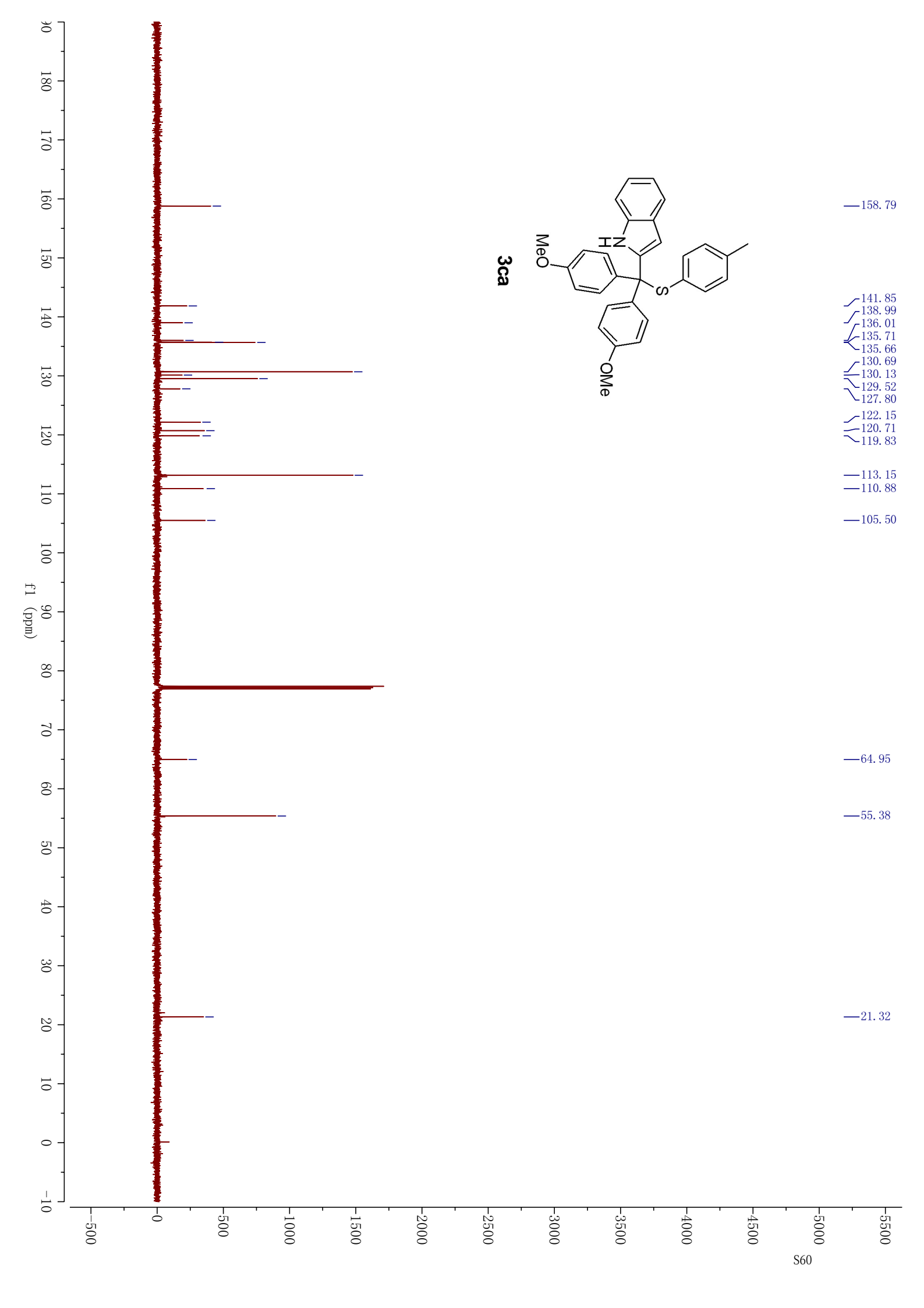
8.40
7.52
7.51
7.51
7.51
7.50
7.49
7.34
7.34
7.33
7.33
7.32
7.31
7.28
7.27
6.35
6.35
6.34
2.34
2.33
2.32
2.32
2.30
1.47
1.46
1.45
1.33
1.31
1.28
1.22
0.94
0.93
0.92
0.92
0.91
0.90
S55
0.93
1.00
4.00
4.92
1.90
1.03
1.01
0.95
2.00
2.01
18.35
3.00
f1 (ppm)

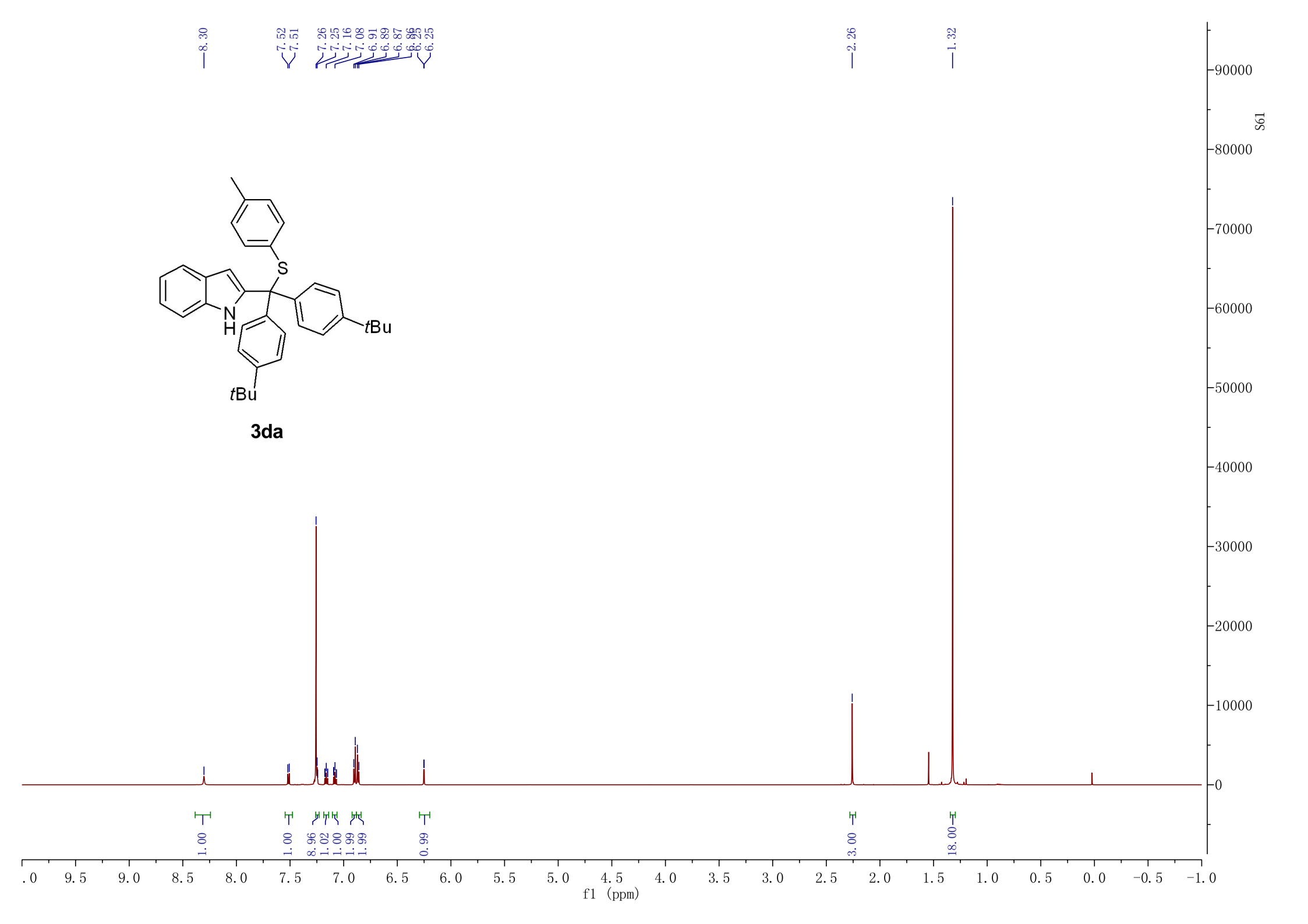

3al
N
H
Ph
Ph
S
144.12
140.78
136.43
128.69
128.27
127.74
127.26
122.34
120.75
119.96
110.87
105.68
62.20
32.06
29.76
29.68
29.54
29.48
29.32
29.14
28.83
22.83
14.27
f1 (ppm)

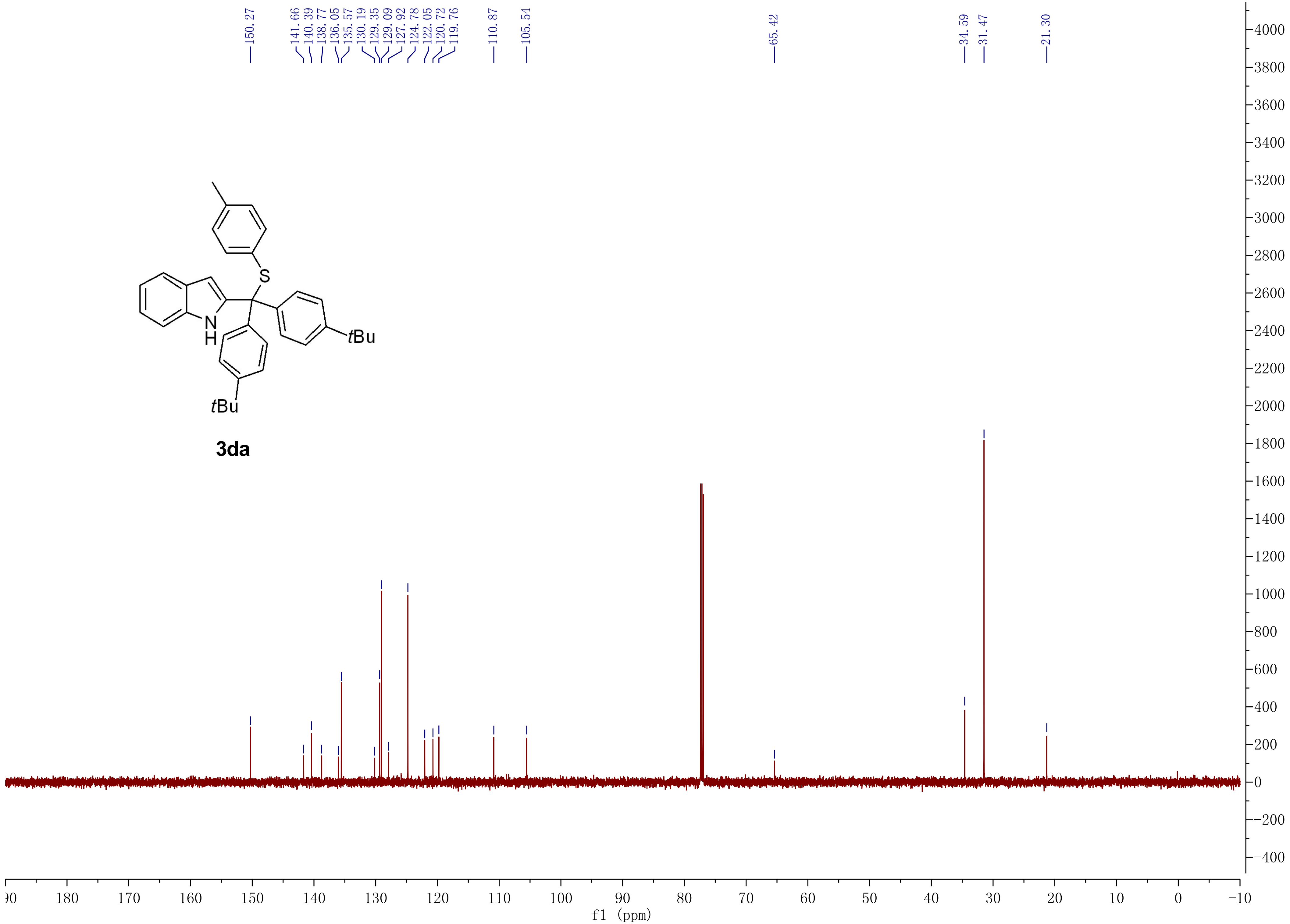

3ba
8.22
7.50
7.48
7.23
7.21
7.20
7.07
7.06
6.93
6.91
6.90
6.88
6.17
6.17
2.34
2.26
1.00
1.00
1.00
3.95
1.00
5.00
2.00
1.98
1.00
6.00
3.00
f1 (ppm)

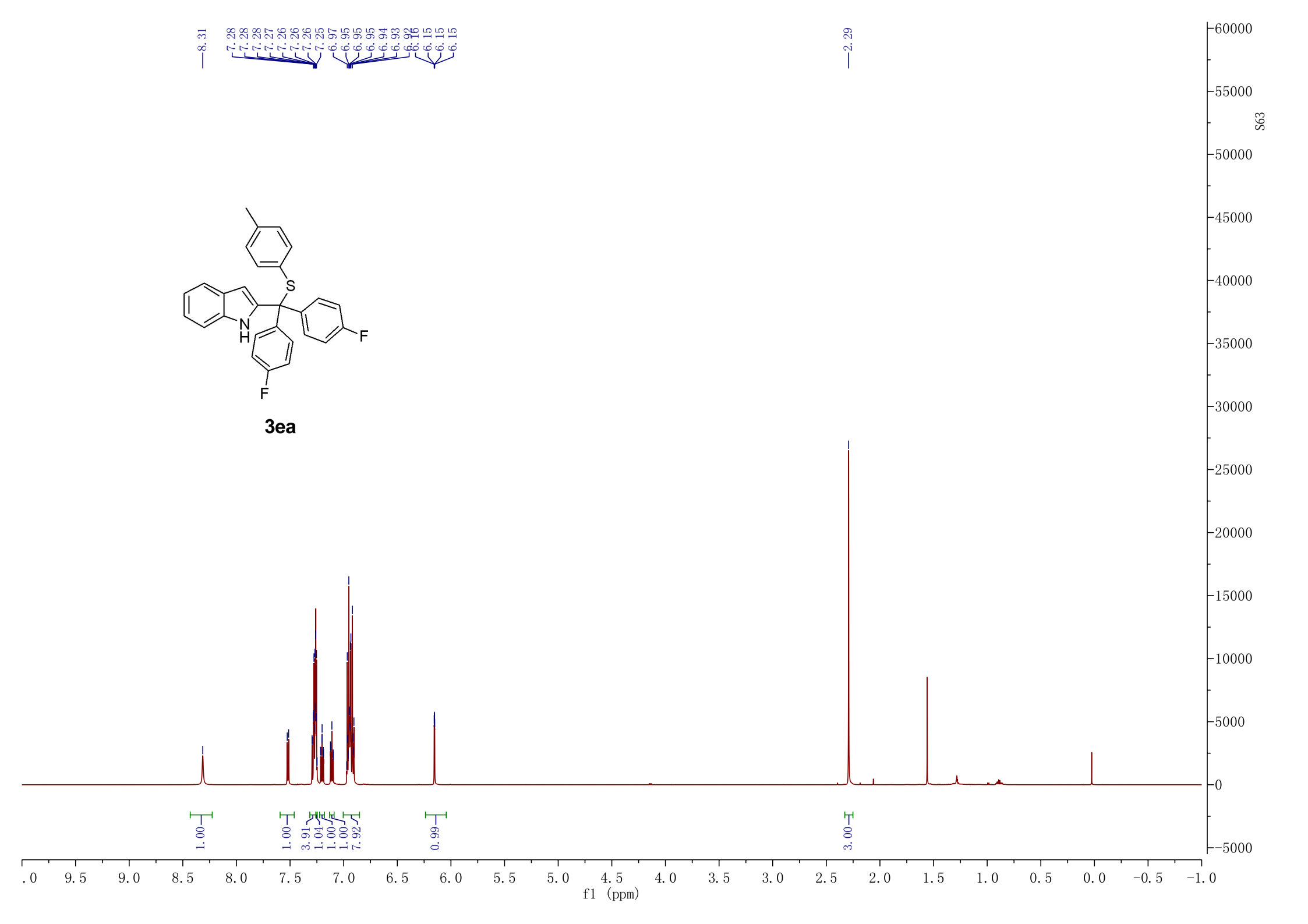

3ba
141.49
140.60
138.85
137.18
136.04
135.42
130.18
129.47
129.37
128.65
122.13
120.73
119.81
110.87
105.65
65.42
21.30
21.15
f1 (ppm)

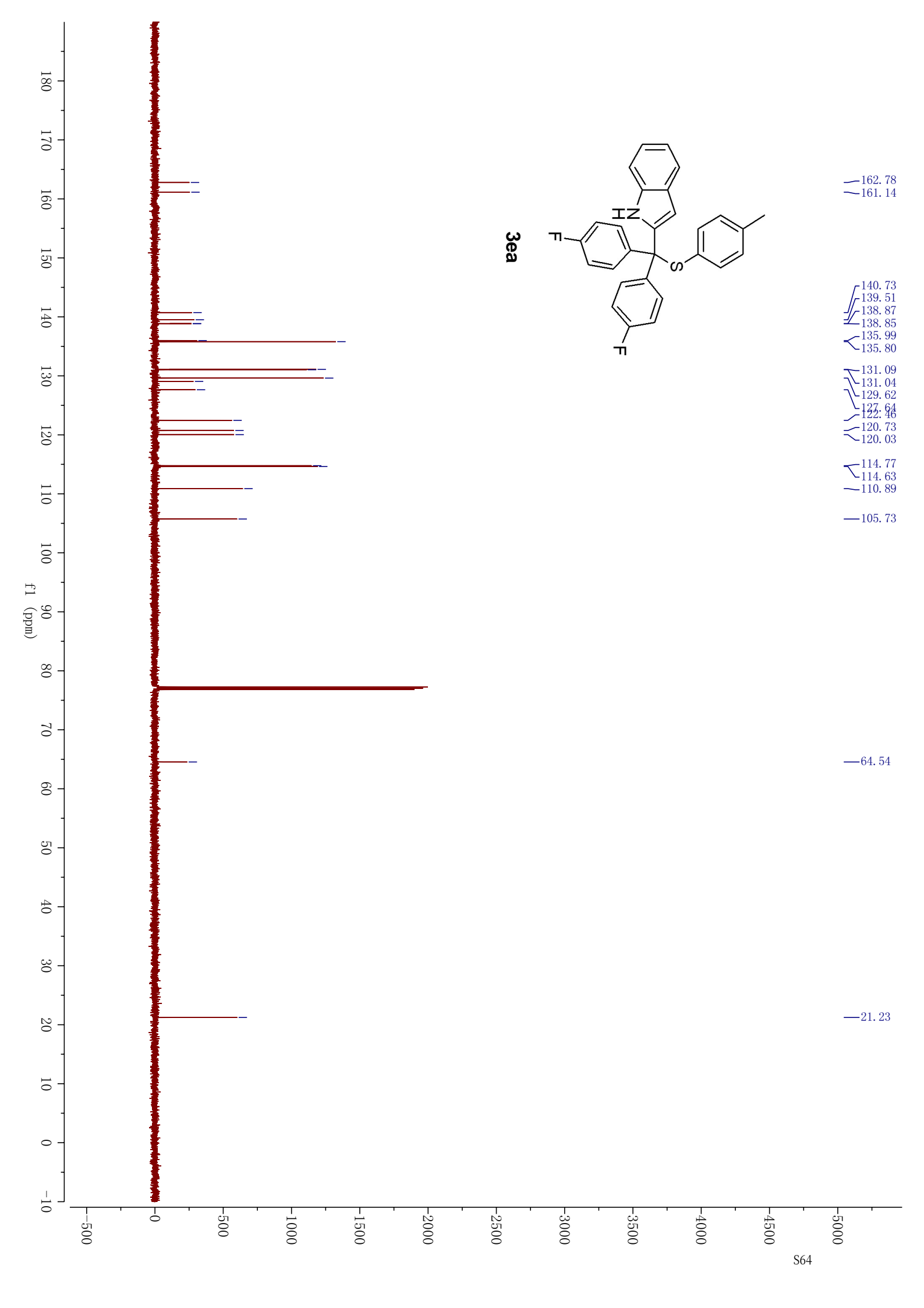

3ca
MeO
OMe
N
H
S
1.00
1.00
4.96
1.02
1.06
4.01
4.01
1.02
6.01
3.00
8.25
7.52
7.51
7.25
7.23
7.09
6.96
6.95
6.93
6.92
6.81
6.79
6.17
3.81
2.29
f1 (ppm)

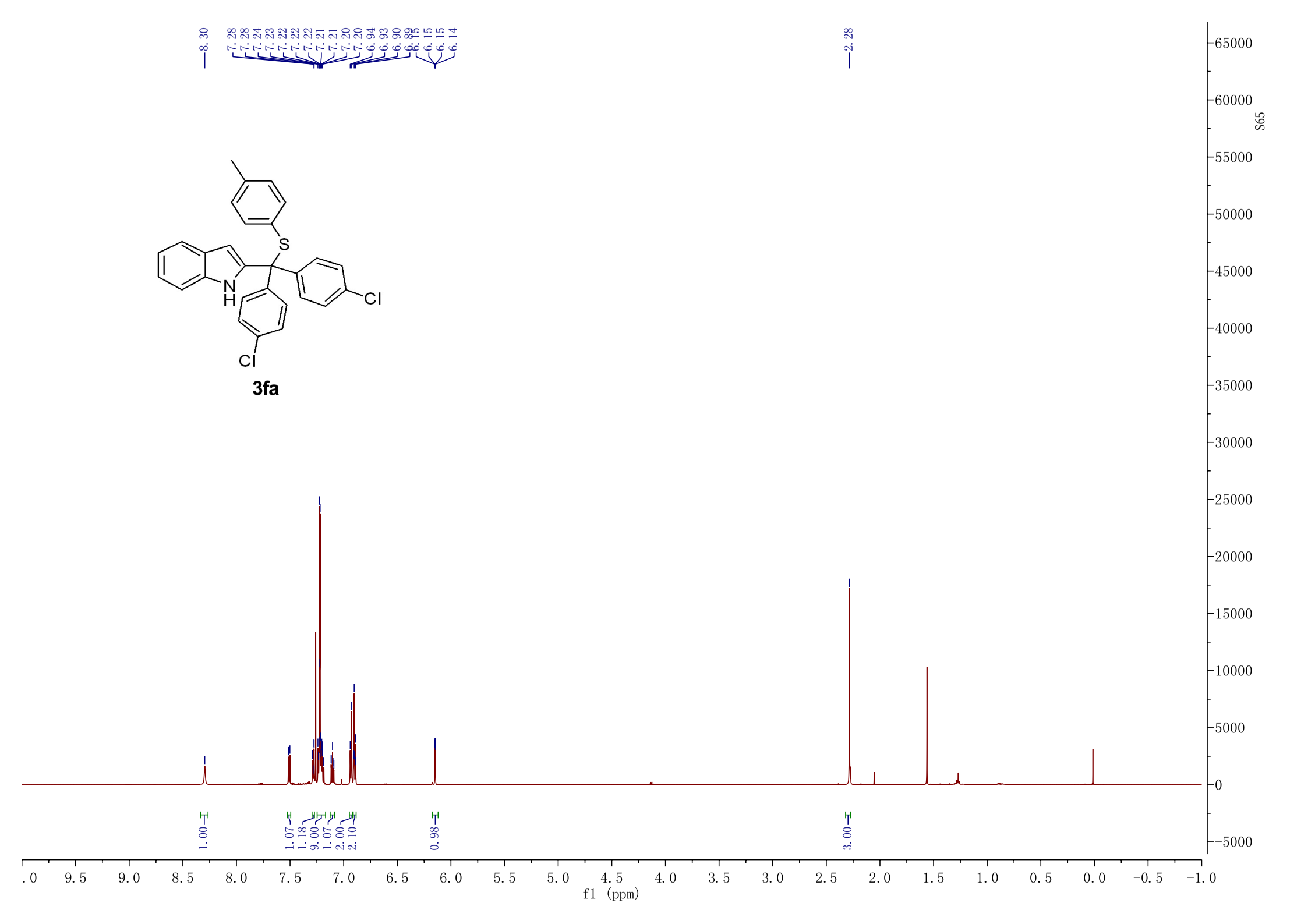

3ca
MeO
OMe
N
H
S
158.79
141.85
138.99
136.01
135.71
135.66
130.69
130.13
129.52
127.80
122.15
120.71
119.83
113.15
110.88
105.50
64.95
55.38
21.32
f1 (ppm)

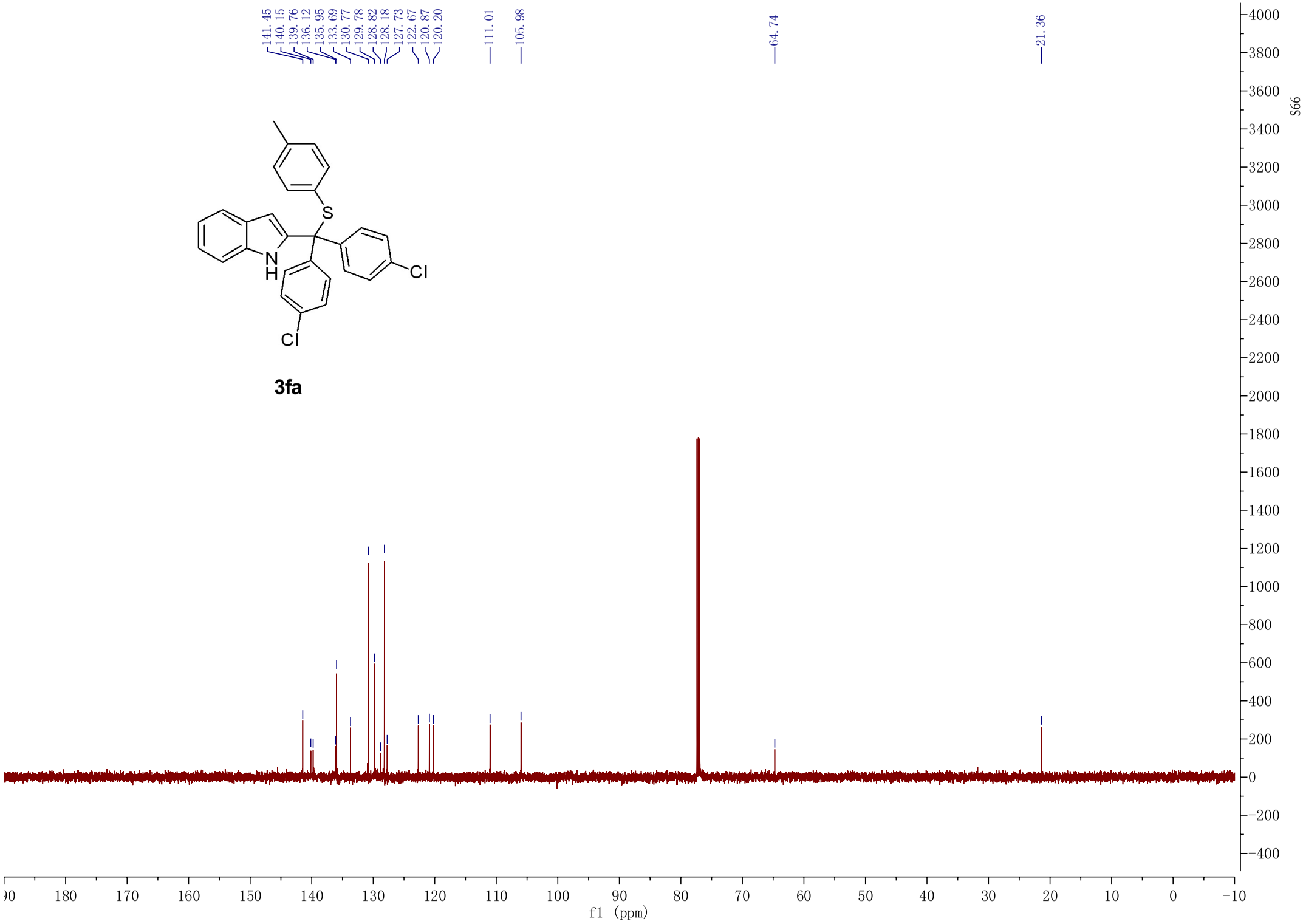

8.30
7.52
7.51
7.26
7.25
7.16
7.08
6.91
6.89
6.87
6.25
2.26
1.32
S
N
H
tBu
tBu
3da
S61
f1 (ppm)
1.00
1.00
8.96
1.02
1.00
1.99
1.99
0.99
3.00
18.00

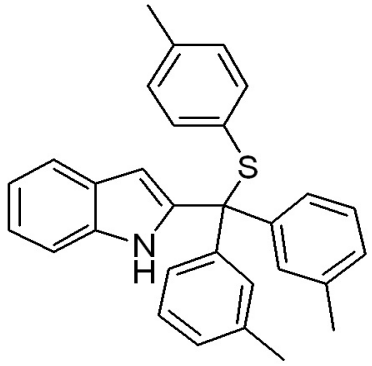

150.27
141.66
140.39
138.77
136.05
135.57
130.19
129.35
129.09
127.92
124.78
122.05
120.72
119.76
110.87
105.54
65.42
34.59
31.47
21.30
S
N
H
tBu
tBu
3da
f1 (ppm)


8.31
7.28
7.28
7.28
7.27
7.26
7.26
7.26
7.25
6.97
6.95
6.95
6.95
6.94
6.93
6.92
6.16
6.15
6.15
6.15
2.29
S
N
H
F
F
3ea
1.00
1.00
3.91
1.04
1.00
7.92
0.99
3.00
f1 (ppm)
S63

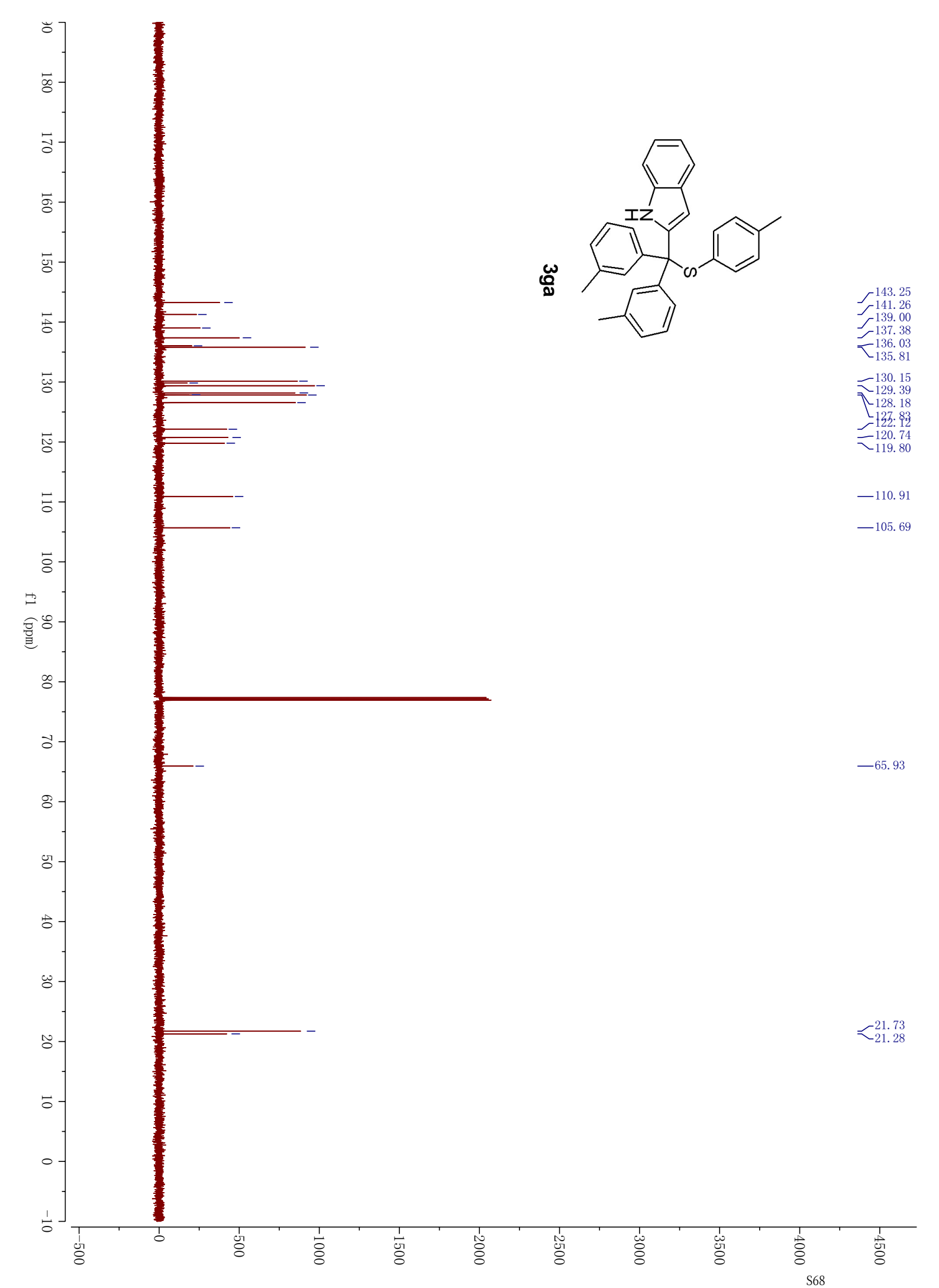

3ea
F
N
H
S
F
162.78
161.14
140.73
139.51
138.87
138.85
135.99
135.80
131.09
131.04
129.62
127.64
122.46
120.73
120.03
114.77
114.63
110.89
105.73
64.54
21.23
f1 (ppm)


8.30
7.28
7.28
7.24
7.23
7.22
7.22
7.22
7.21
7.21
7.20
7.20
6.94
6.93
6.90
6.89
6.15
6.15
6.14
2.28
S
N
H
Cl
Cl
3fa
S65
f1 (ppm)


141.45
140.15
139.76
136.12
135.95
133.69
130.77
129.78
128.82
128.18
127.73
122.67
120.87
120.20
111.01
105.98
64.74
21.36
S
N
H
Cl
Cl
3fa
f1 (ppm)



3ga


3ga
143.25
141.26
139.00
137.38
136.03
135.81
130.15
129.39
128.18
127.83
122.12
120.74
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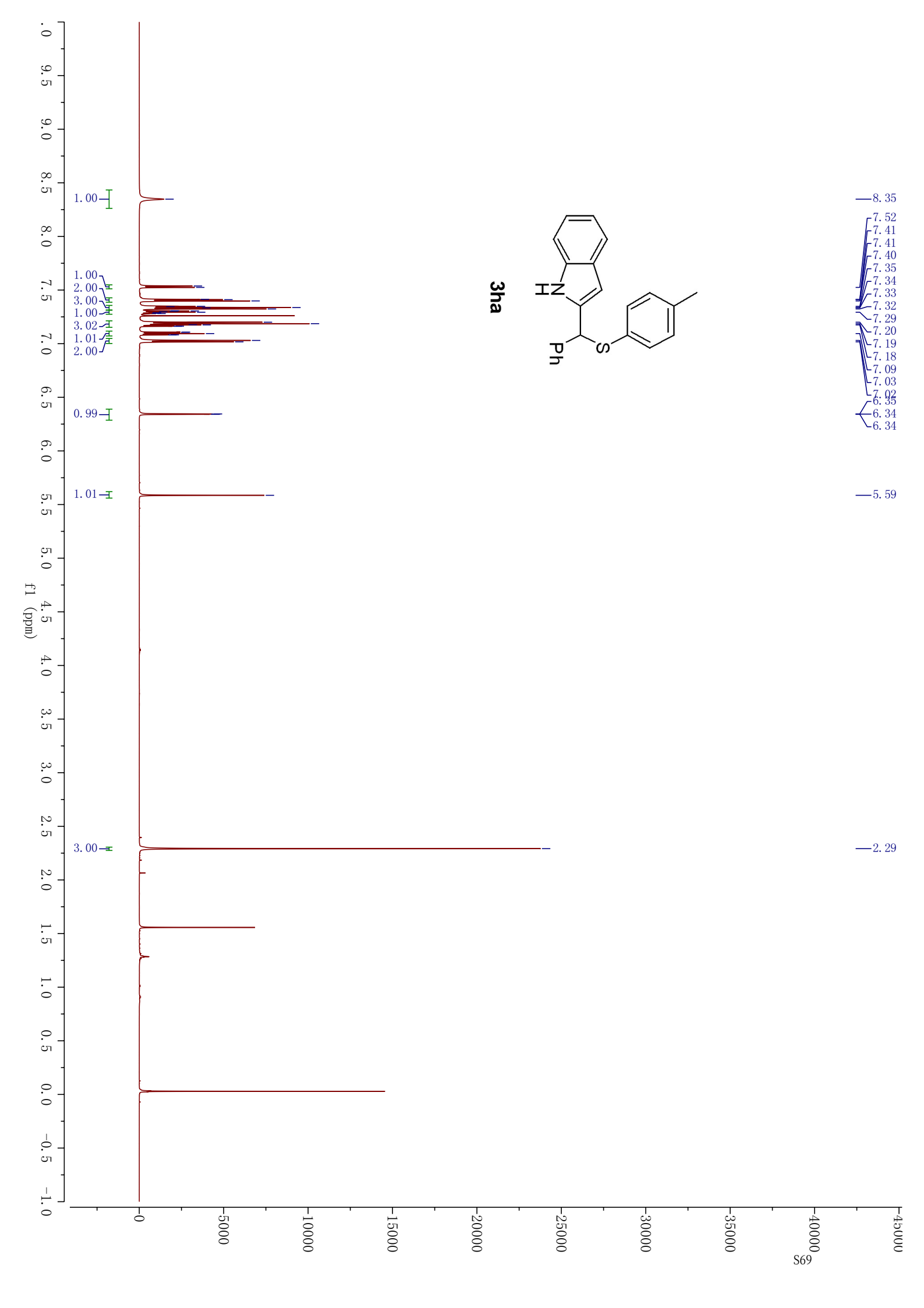
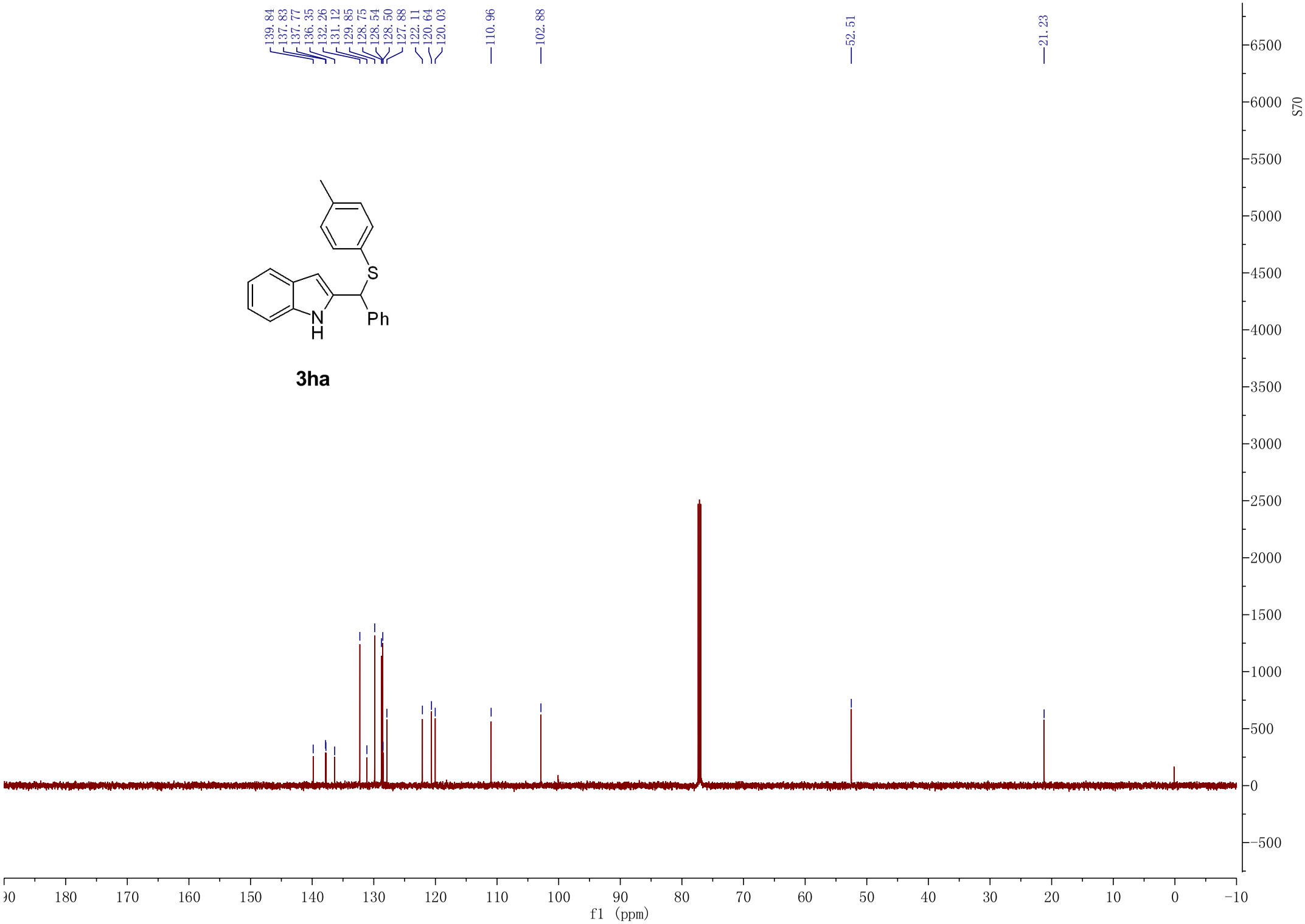
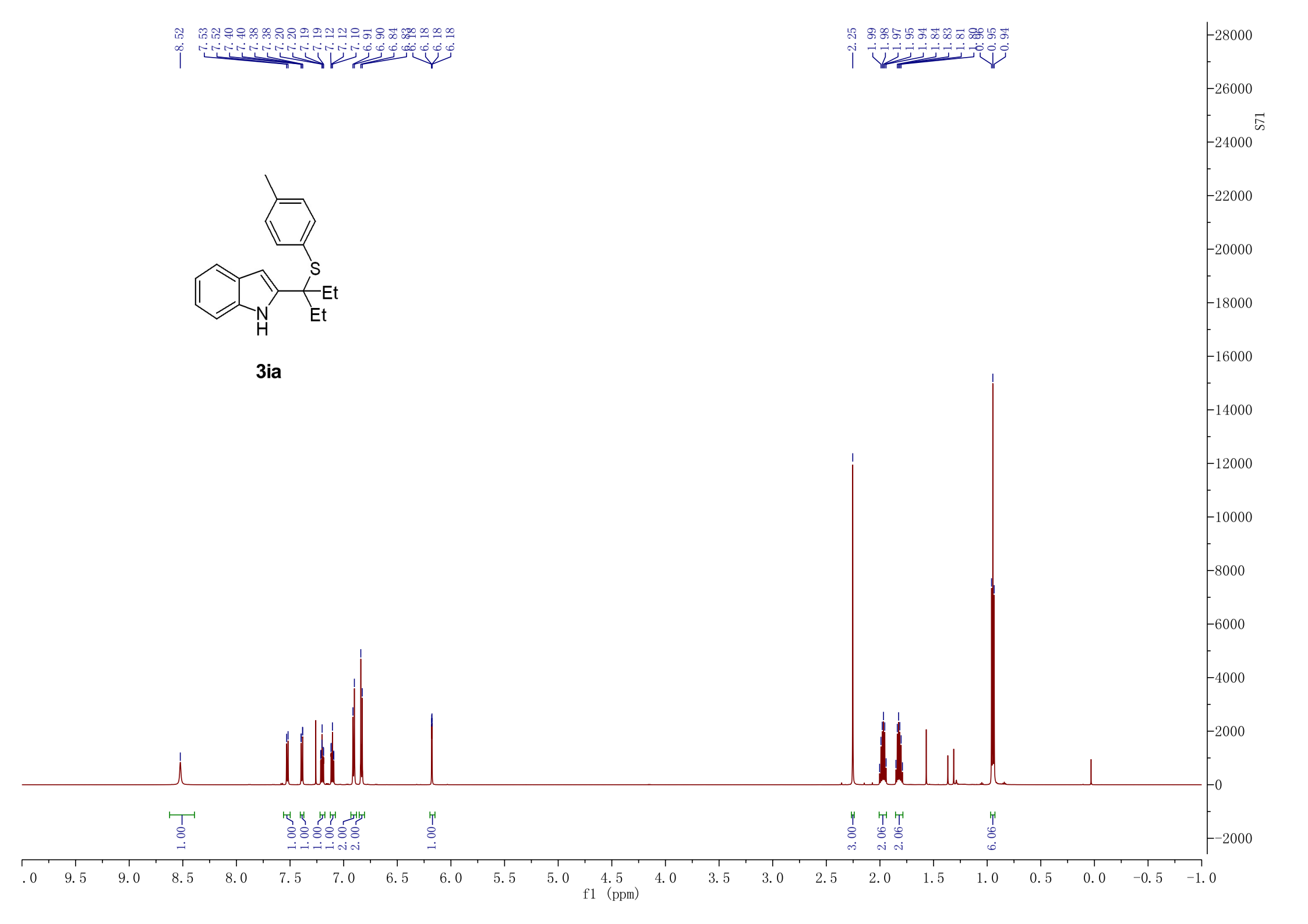
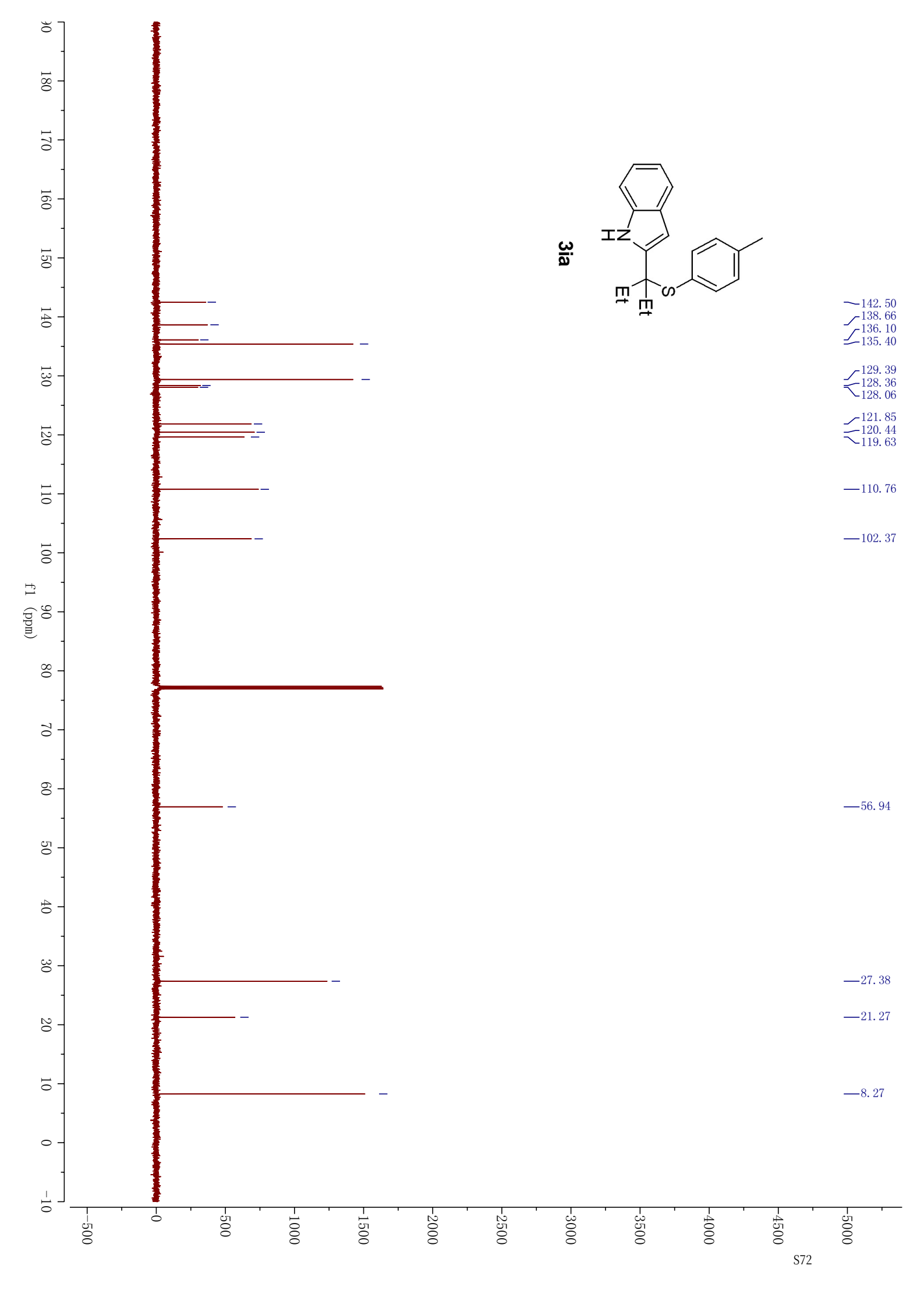
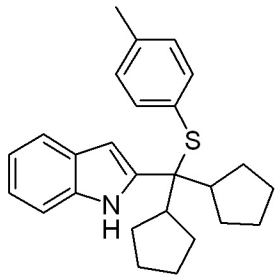
110.91
105.69
65.93
21.73
21.28
f1 (ppm)


3ha
1.00
1.00
2.00
3.00
1.00
3.02
1.01
2.00
0.99
1.01
3.00
8.35
7.52
7.41
7.41
7.40
7.35
7.34
7.33
7.32
7.29
7.20
7.19
7.18
7.09
7.03
7.02
6.35
6.34
6.34
5.59
2.29
f1 (ppm)

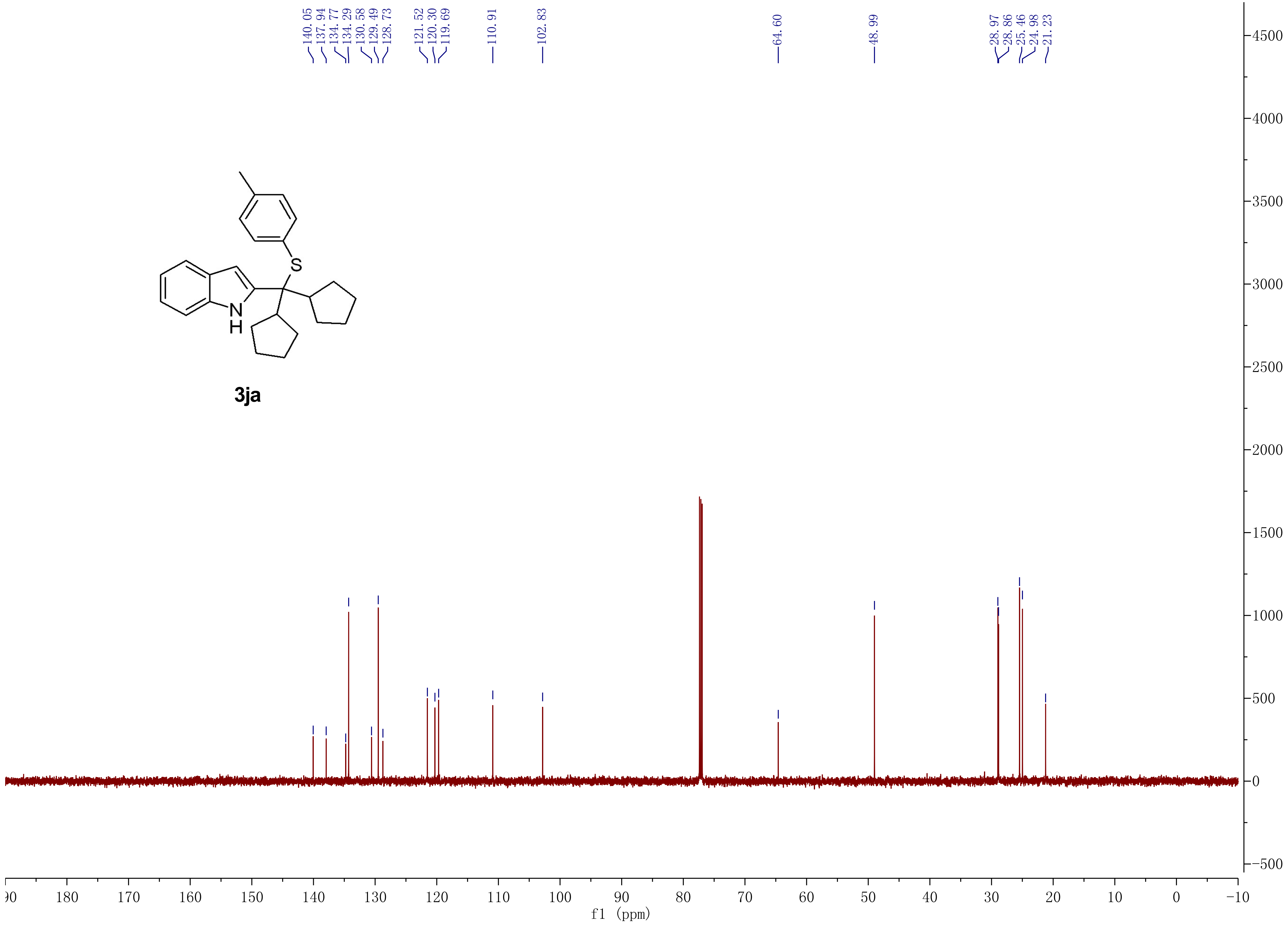

139.84
137.83
137.77
136.35
132.26
131.12
129.85
128.75
128.54
128.50
127.88
122.11
120.64
120.03
110.96
102.88
52.51
21.23
S
N
H
Ph
3ha
S70
f1 (ppm)

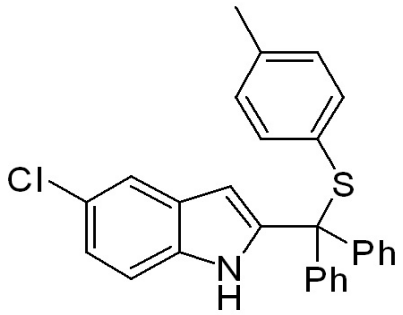

8.52
7.53
7.52
7.40
7.40
7.38
7.38
7.20
7.20
7.19
7.19
7.12
7.12
7.10
6.91
6.90
6.84
6.83
6.18
6.18
6.18
2.25
1.99
1.98
1.97
1.95
1.94
1.84
1.83
1.81
0.95
0.94
S
Et
Et
N
H
3ia
S71
f1 (ppm)


3ia
142.50
138.66
136.10
135.40
129.39
128.36
128.06
121.85
120.44
119.63
110.76
102.37
56.94
27.38
21.27
8.27
f1 (ppm)

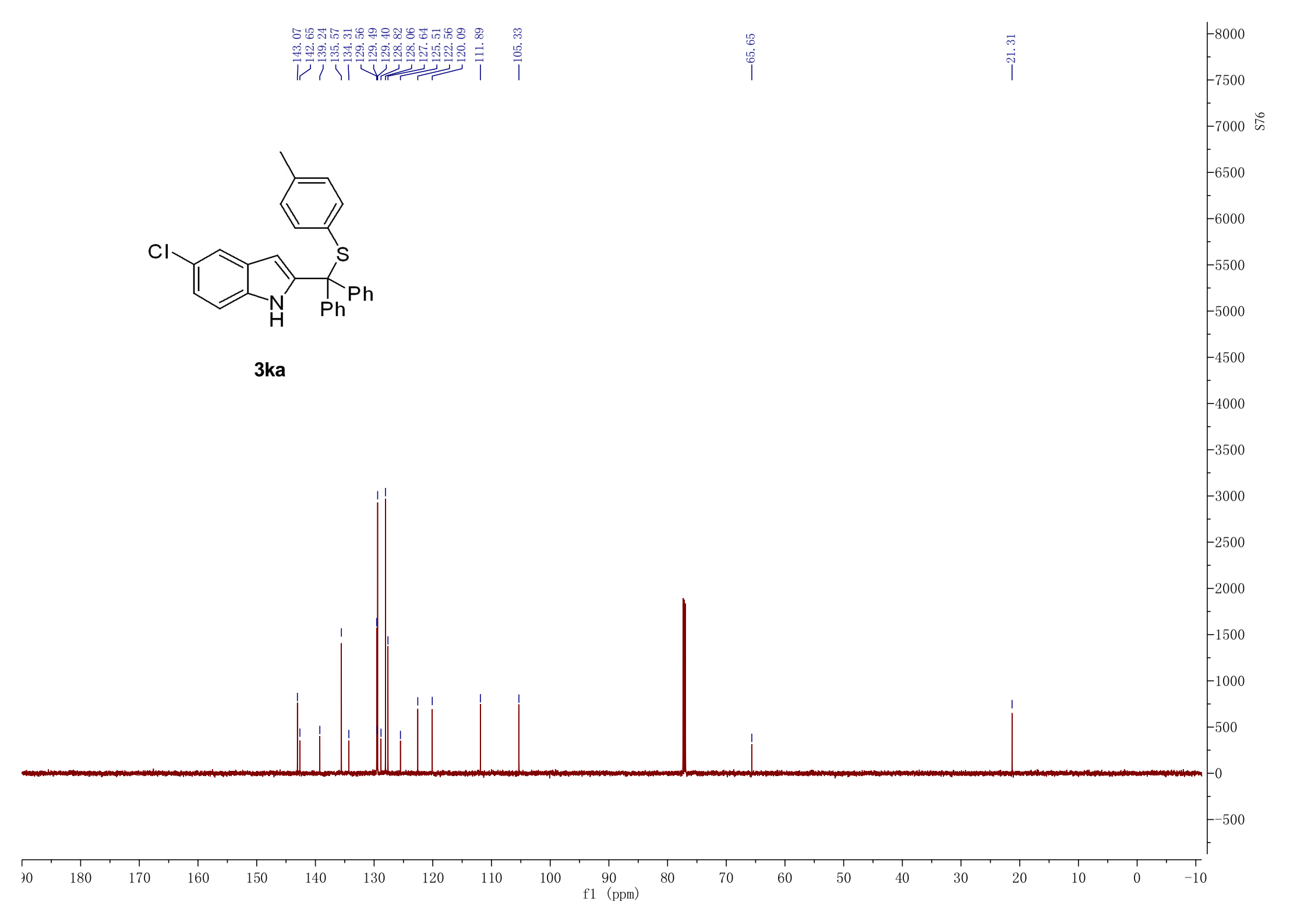


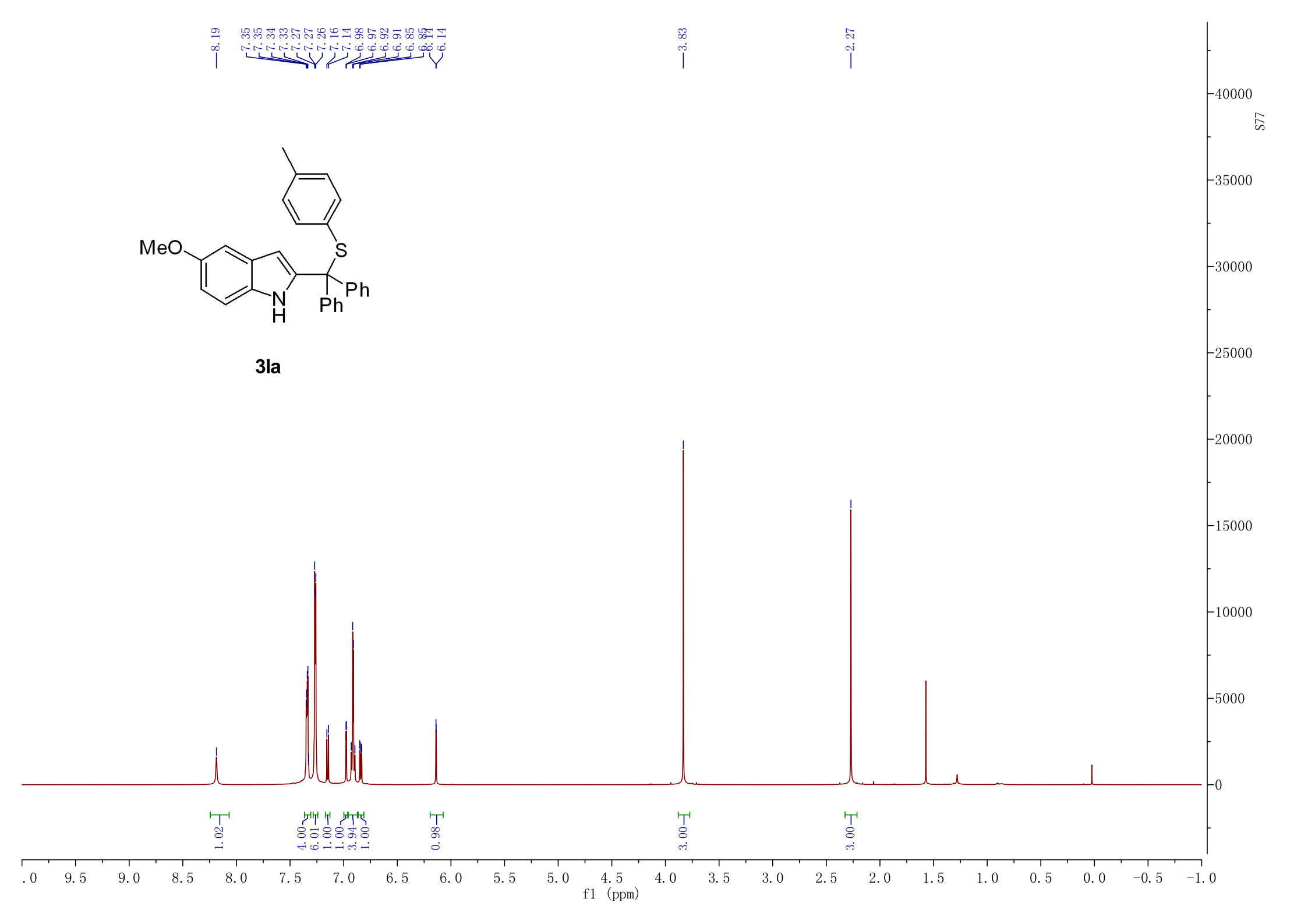
3ja

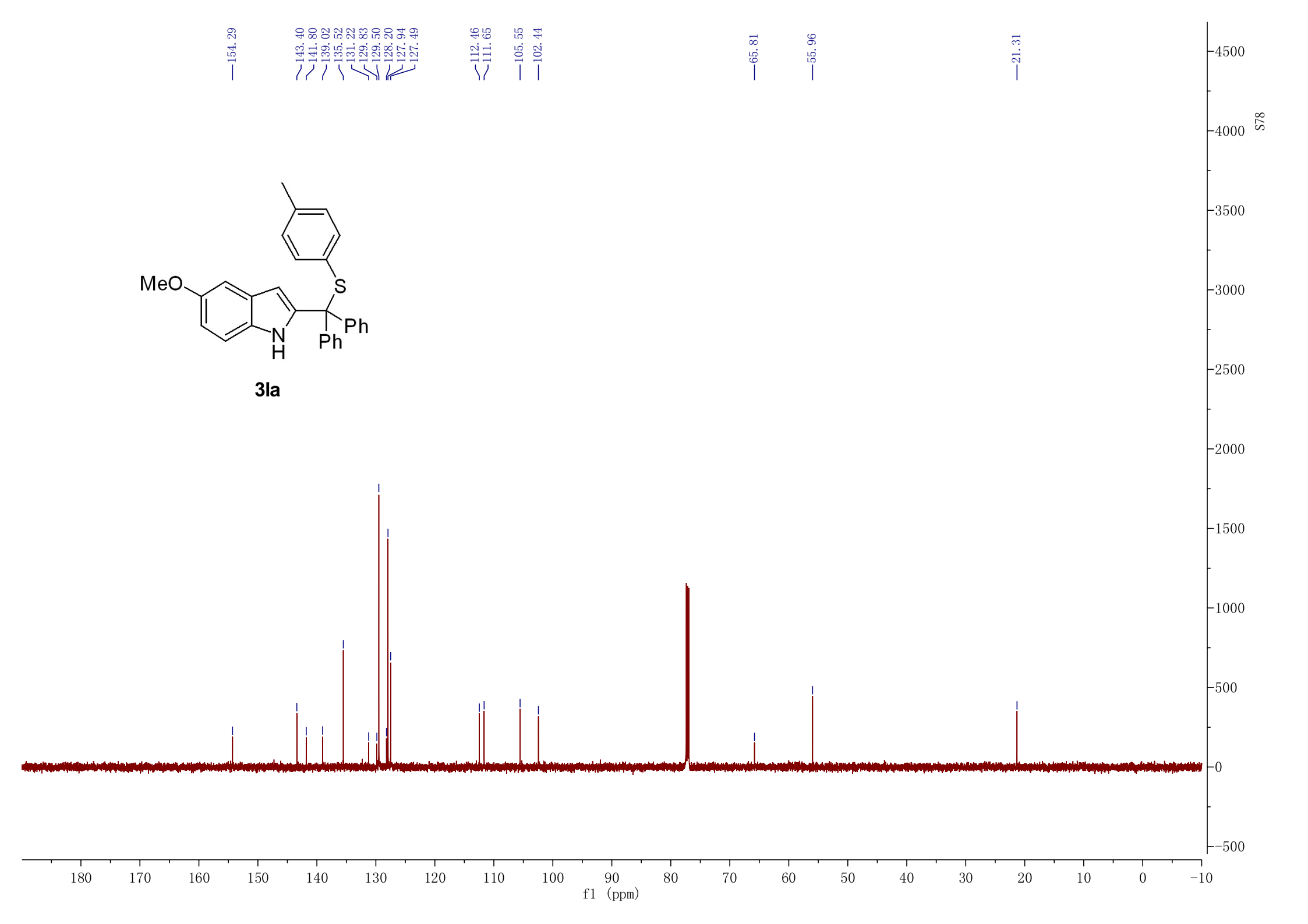

140.05
137.94
134.77
134.29
130.58
129.49
128.73
121.52
120.30
119.69
110.91
102.83
64.60
48.99
28.97
28.86
25.46
24.98
21.23
3ja
f1 (ppm)

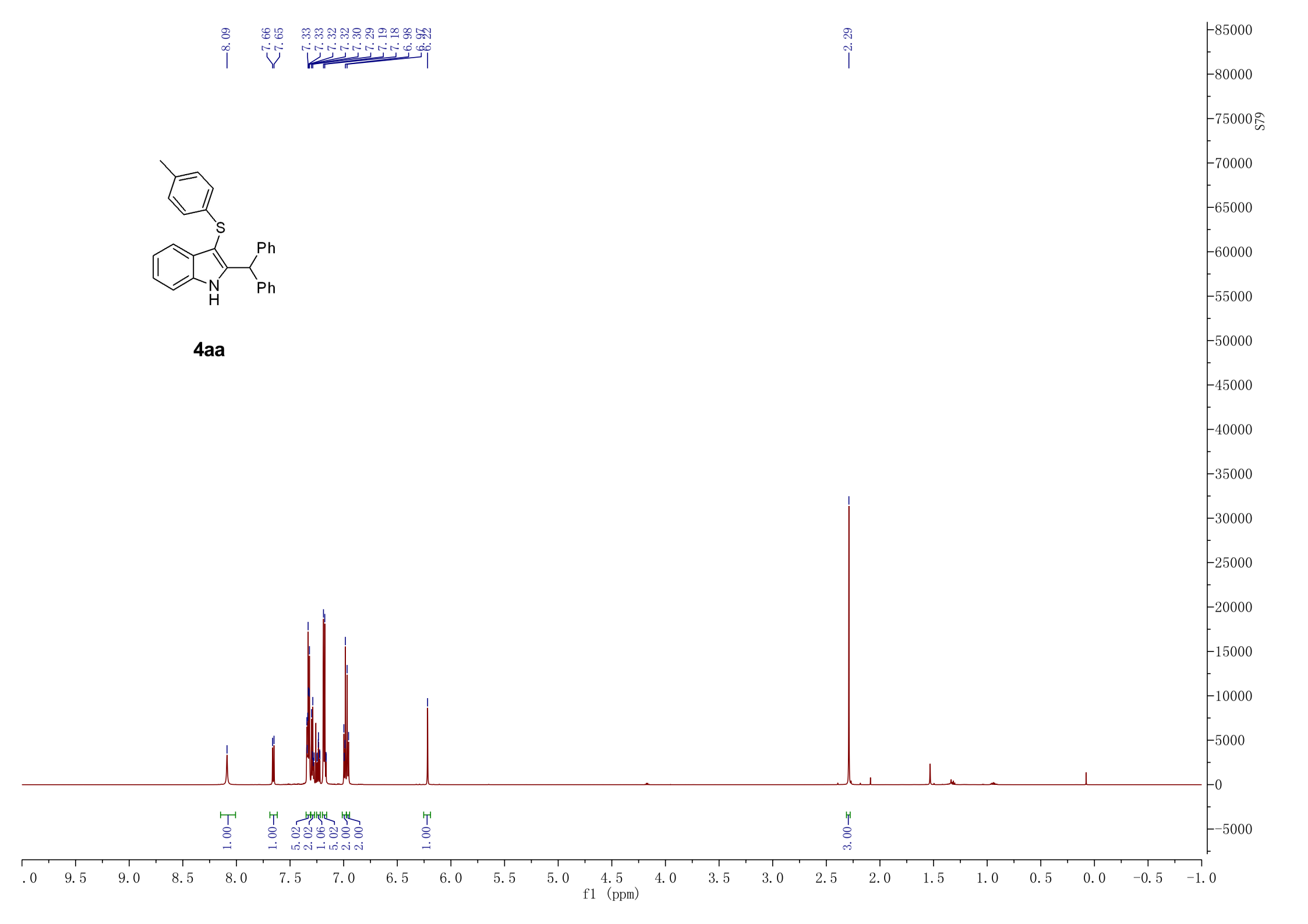


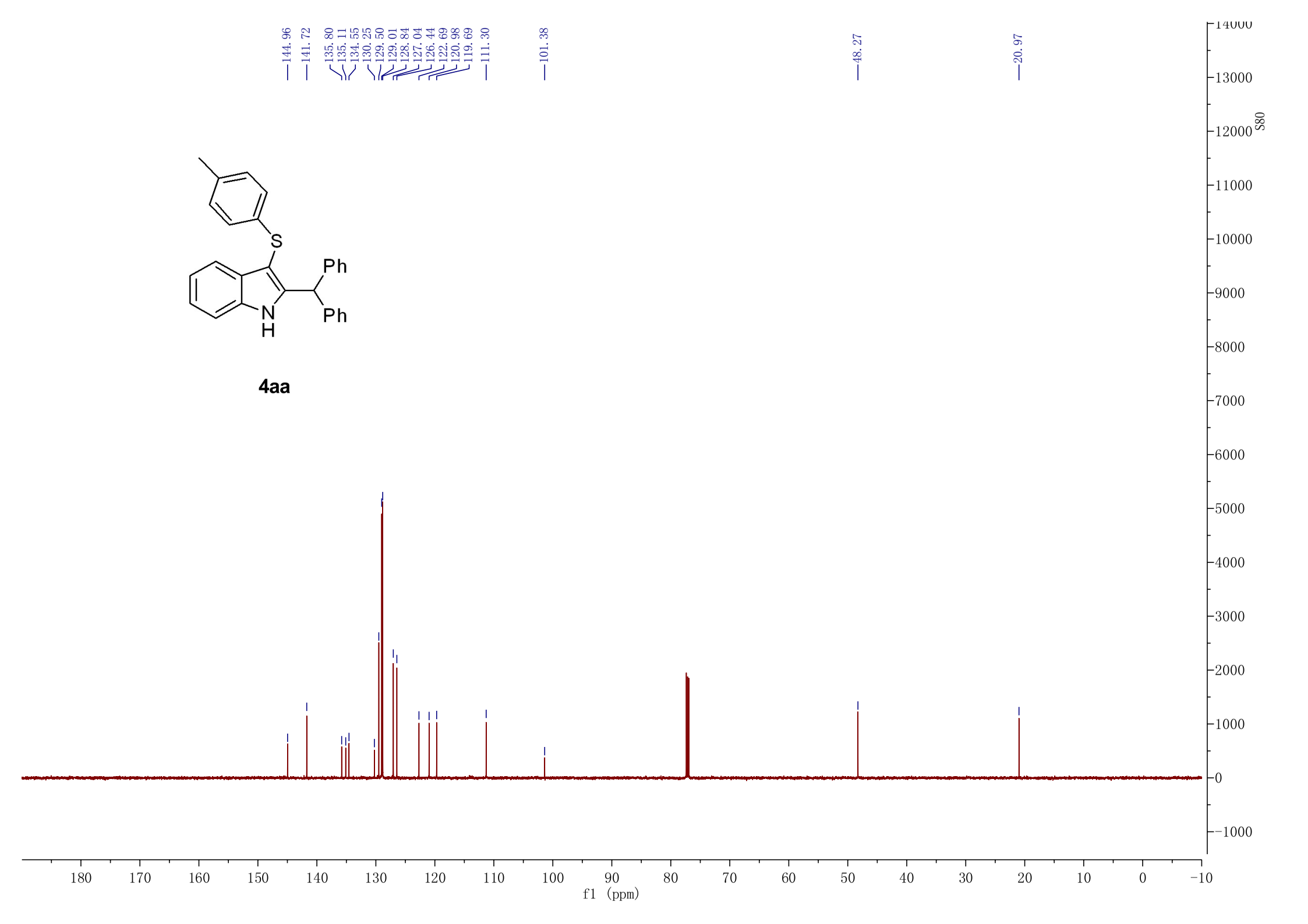
3ka

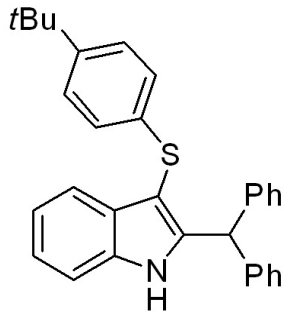

143.07
142.65
139.24
135.57
134.31
129.56
129.49
129.40
128.82
128.06
127.64
125.51
122.56
120.09
111.89
105.33
65.65
21.31
Cl
S
Ph
Ph
N
H
3ka
f1 (ppm)
S76


8.19
7.35
7.35
7.34
7.33
7.27
7.27
7.26
7.16
7.14
6.98
6.97
6.92
6.91
6.85
6.85
6.14
3.83
2.27
MeO
S
Ph
Ph
N
H
3la
S77
40000
35000
30000
25000
20000
15000
10000
5000
0
1.02
4.00
6.01
1.00
1.00
3.94
1.00
0.98
3.00
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

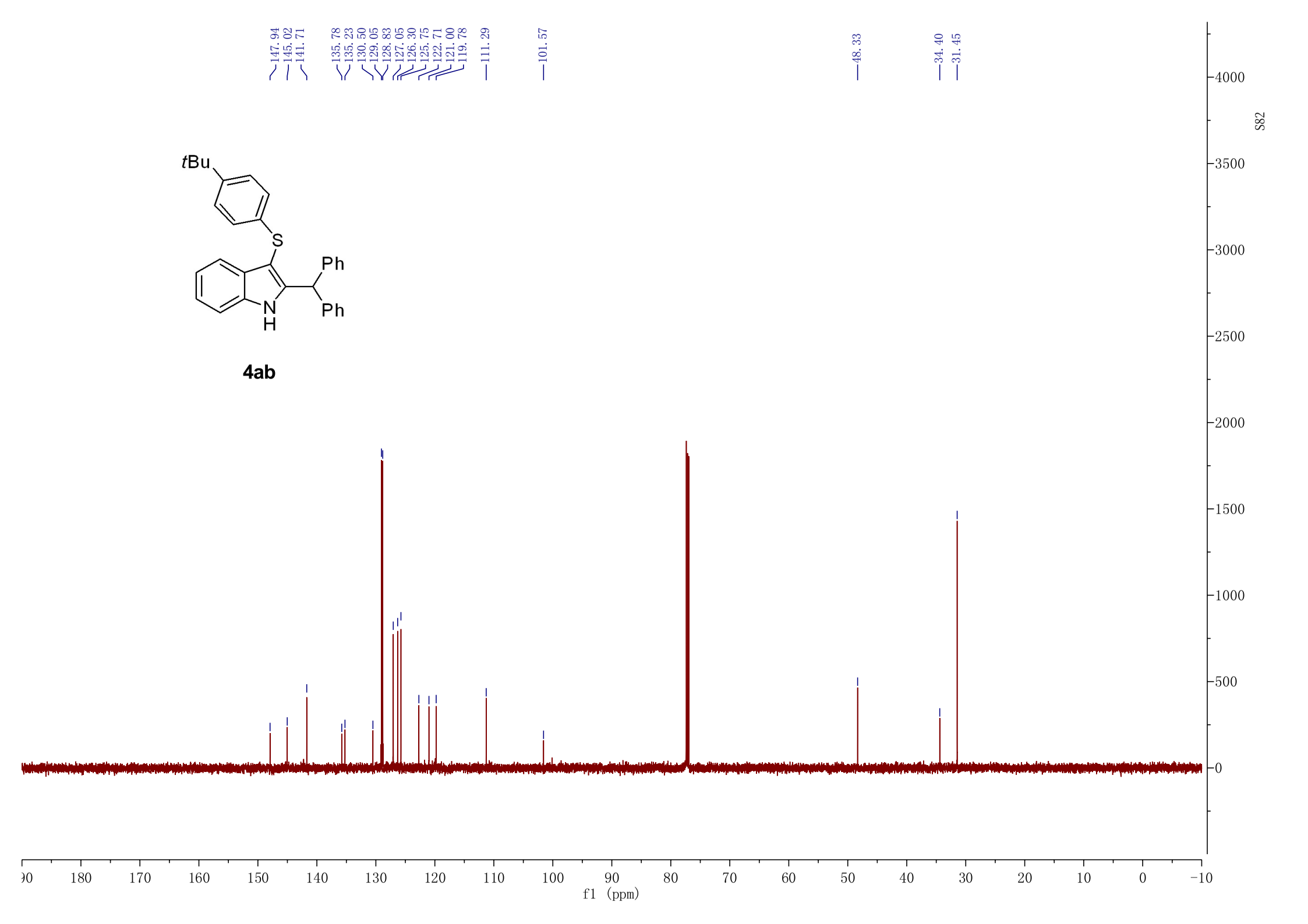

154.29
143.40
141.80
139.02
135.52
131.22
129.83
129.50
128.20
127.94
127.49
112.46
111.65
105.55
102.44
65.81
55.96
21.31
MeO
S
Ph
Ph
N
H
3la
f1 (ppm)
S78

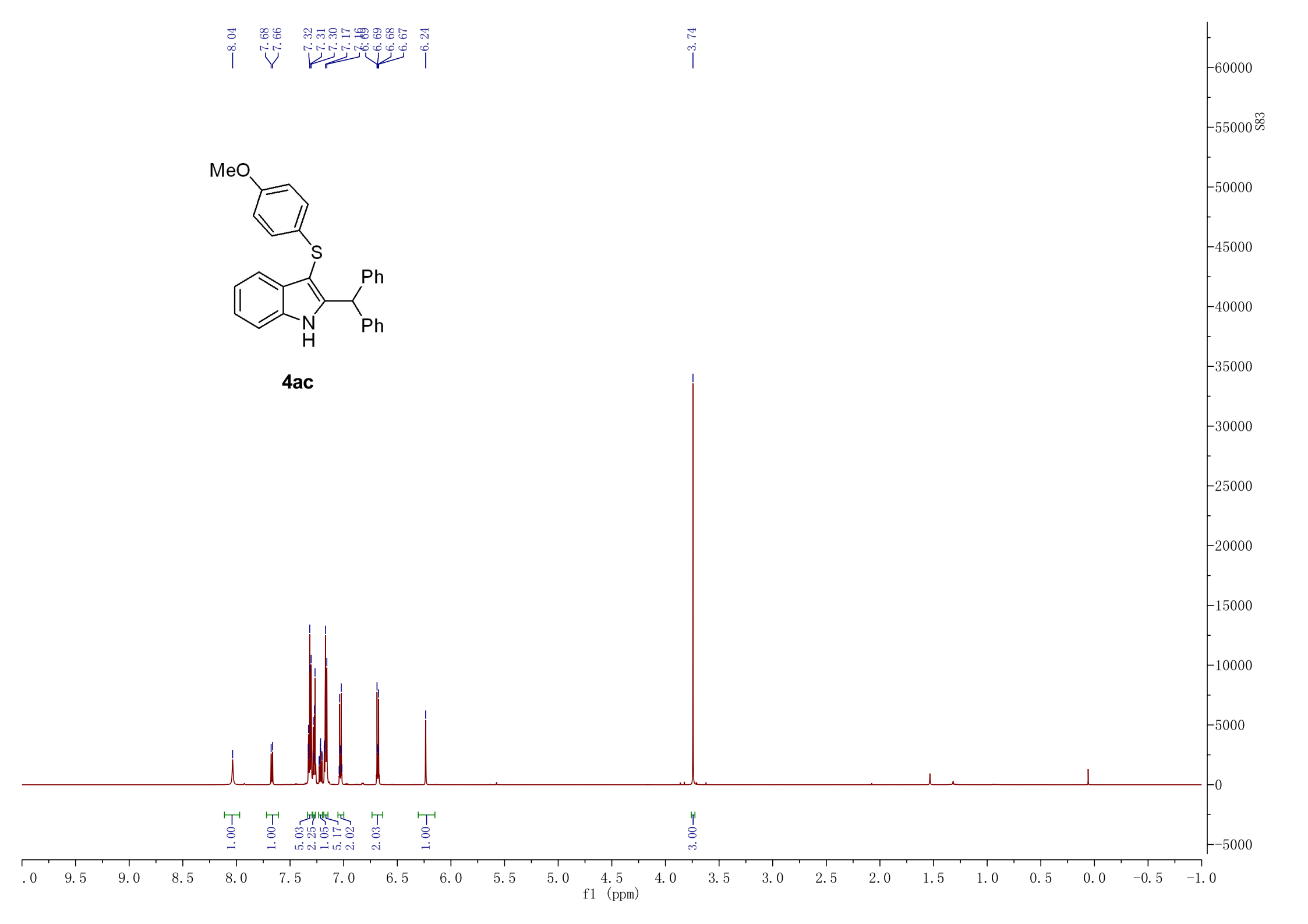

8.09
7.66
7.65
7.33
7.33
7.32
7.32
7.30
7.29
7.19
7.18
6.98
6.97
6.22
2.29
S
Ph
Ph
N
H
4aa
1.00
1.00
5.02
2.02
1.06
5.02
2.00
2.00
1.00
3.00
f1 (ppm)
S79

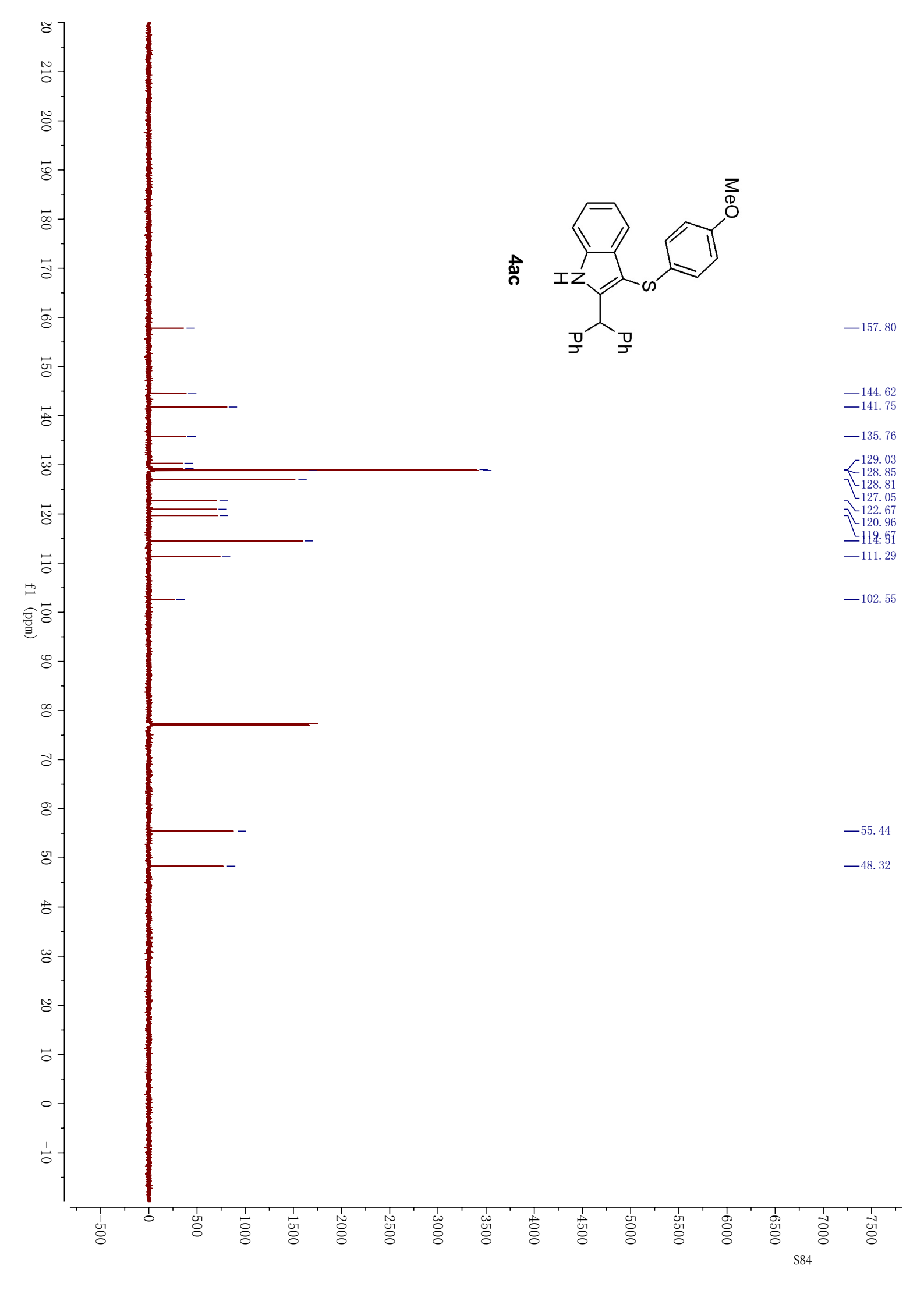

144.96
141.72
135.80
135.11
134.55
130.25
129.50
129.01
128.84
127.04
126.44
122.69
120.98
119.69
111.30
101.38
48.27
20.97
S
Ph
Ph
N
H
4aa
S80
f1 (ppm)

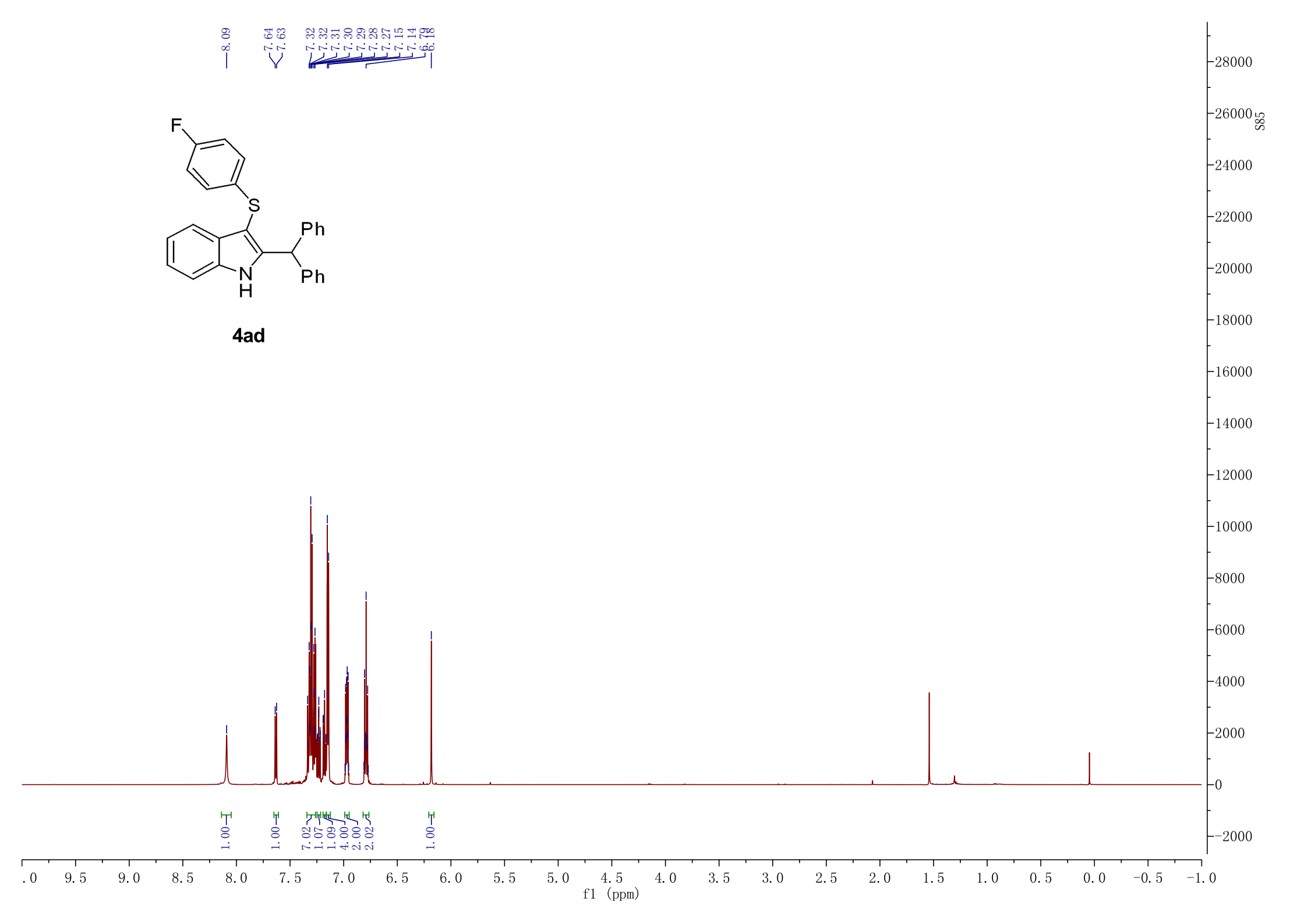


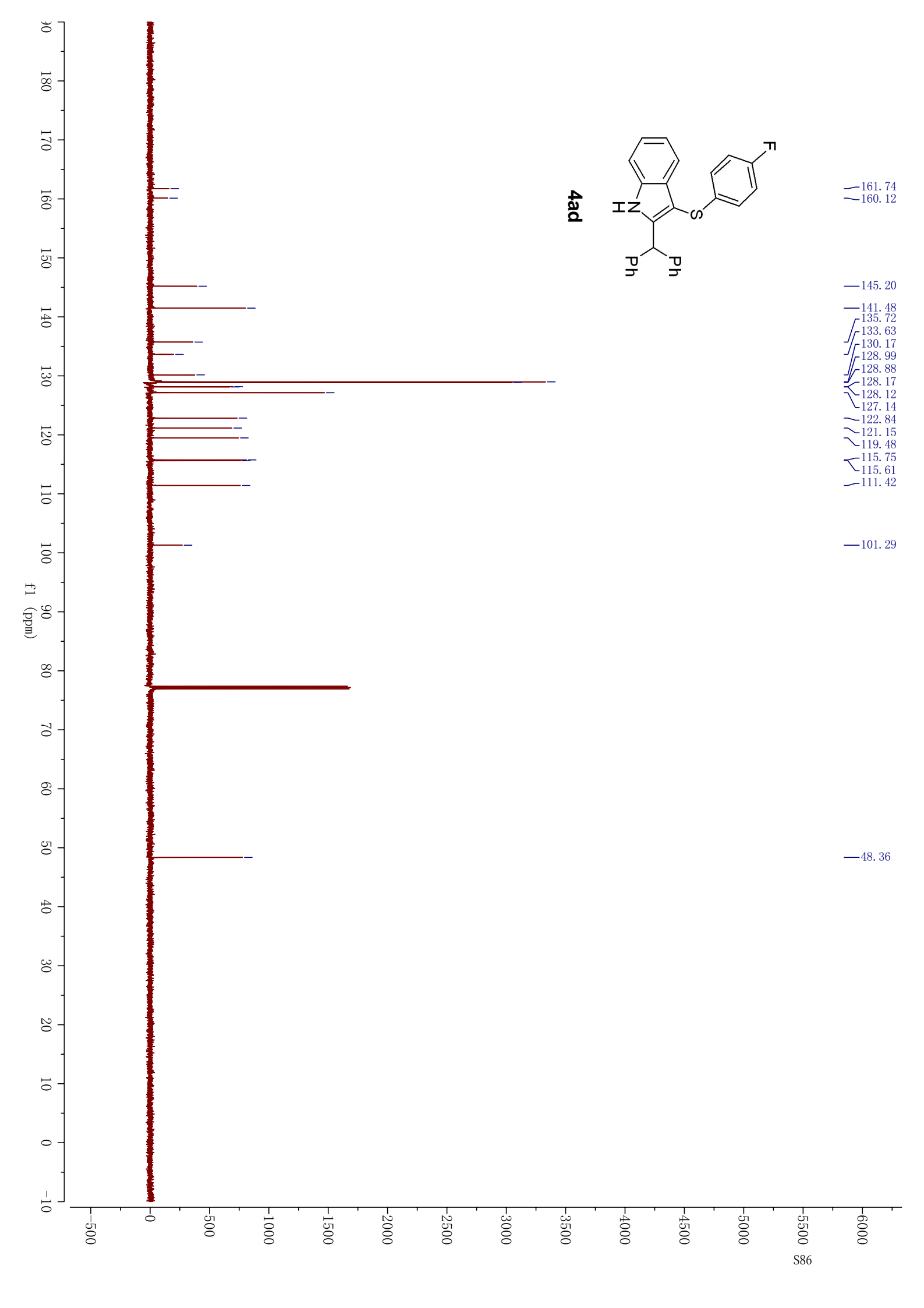
4ab

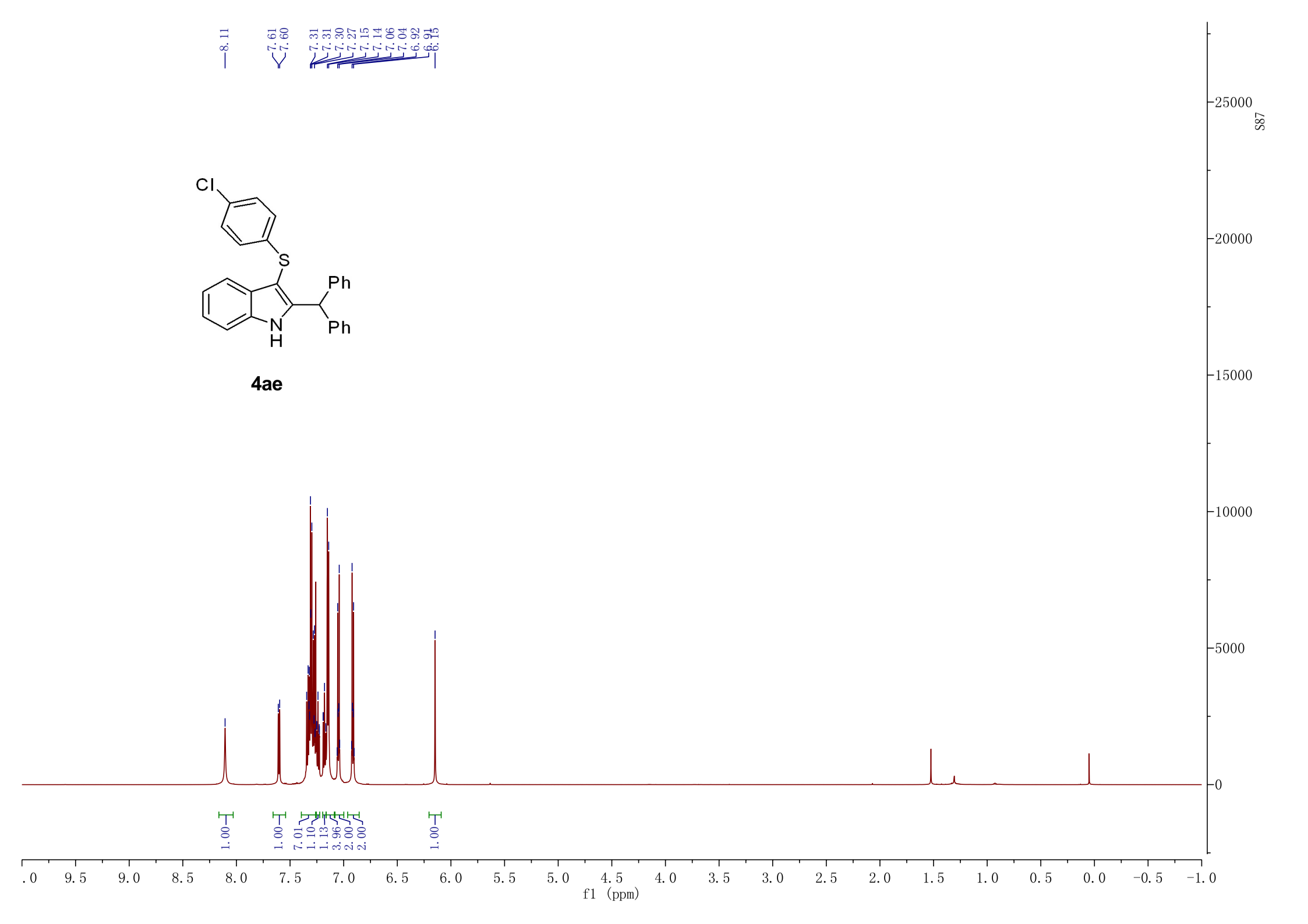

147.94
145.02
141.71
135.78
135.23
130.50
129.05
128.83
127.05
126.30
125.75
122.71
121.00
119.78
111.29
101.57
48.33
34.40
31.45
tBu
S
Ph
Ph
N
H
4ab
S82
4000
3500
3000
2500
2000
1500
1000
500
0
f1 (ppm)

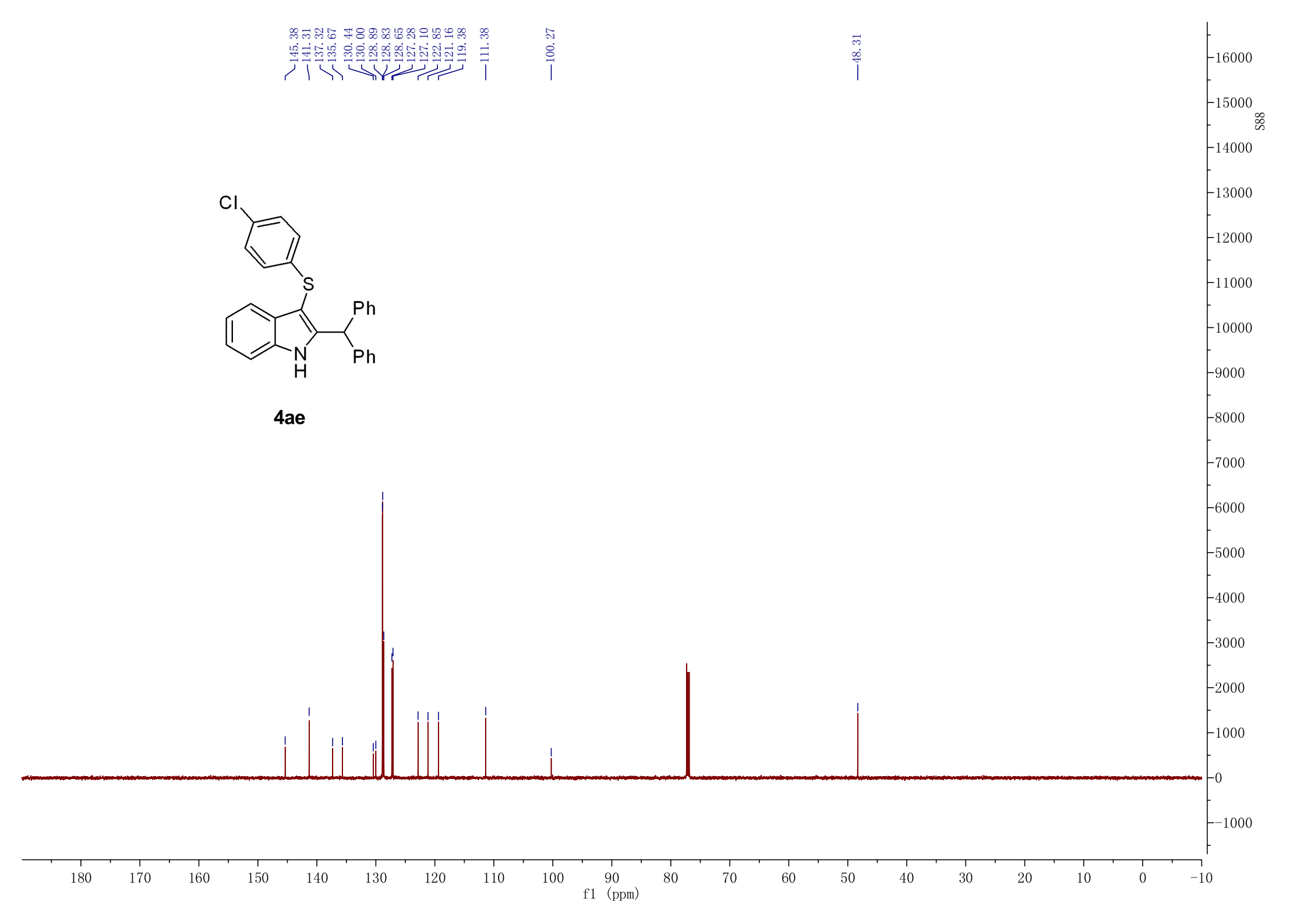

8.04
7.68
7.66
7.32
7.31
7.30
7.17
6.69
6.68
6.67
6.24
3.74
MeO
S
Ph
Ph
N
H
4ac
S83
1.00
1.00
5.03
2.25
1.05
5.17
2.02
2.03
1.00
3.00
f1 (ppm)

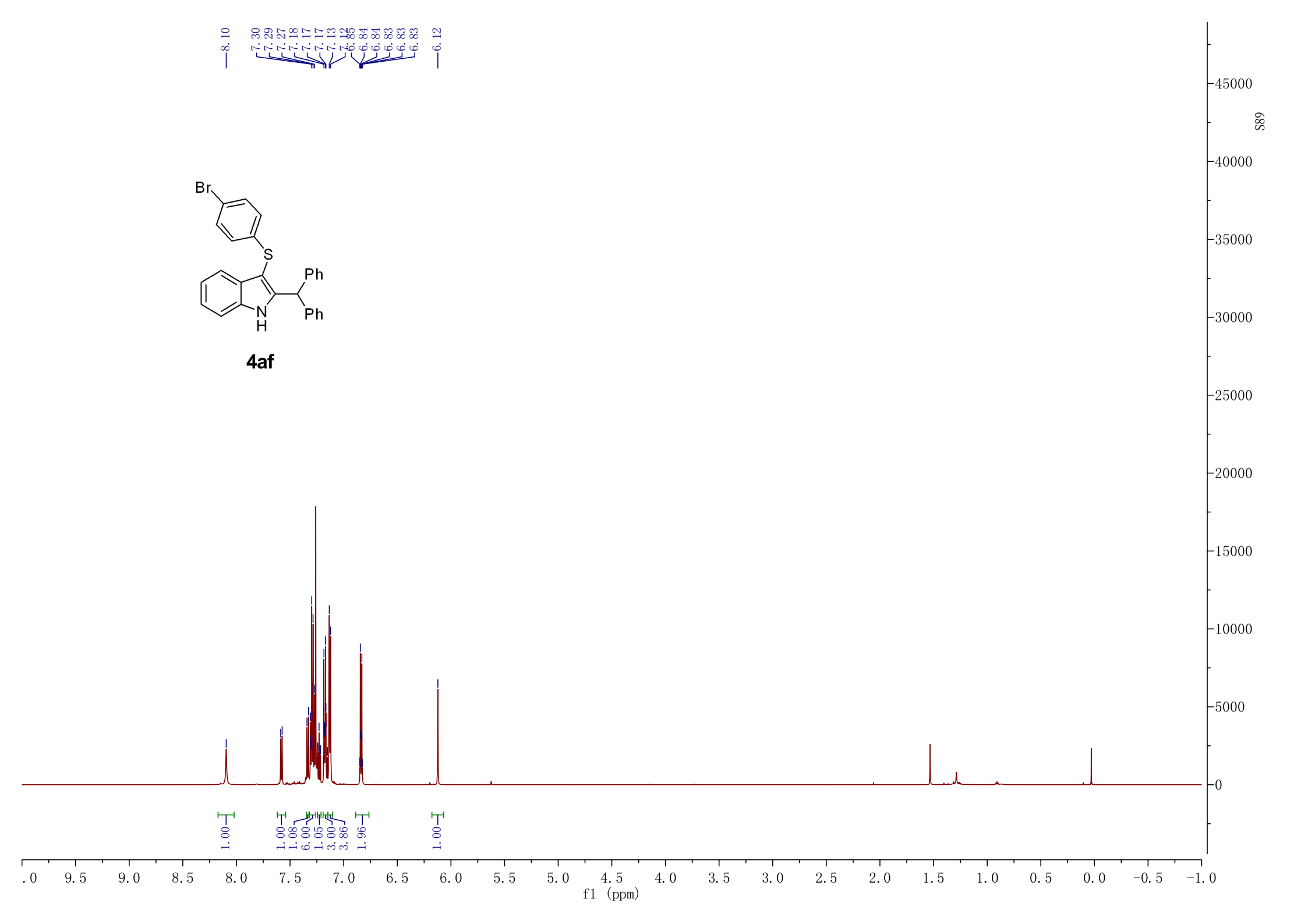

4ac
MeO
N
H
S
Ph
Ph
157.80
144.62
141.75
135.76
129.03
128.85
128.81
127.05
122.67
120.96
119.67
114.51
111.29
102.55
55.44
48.32
f1 (ppm)

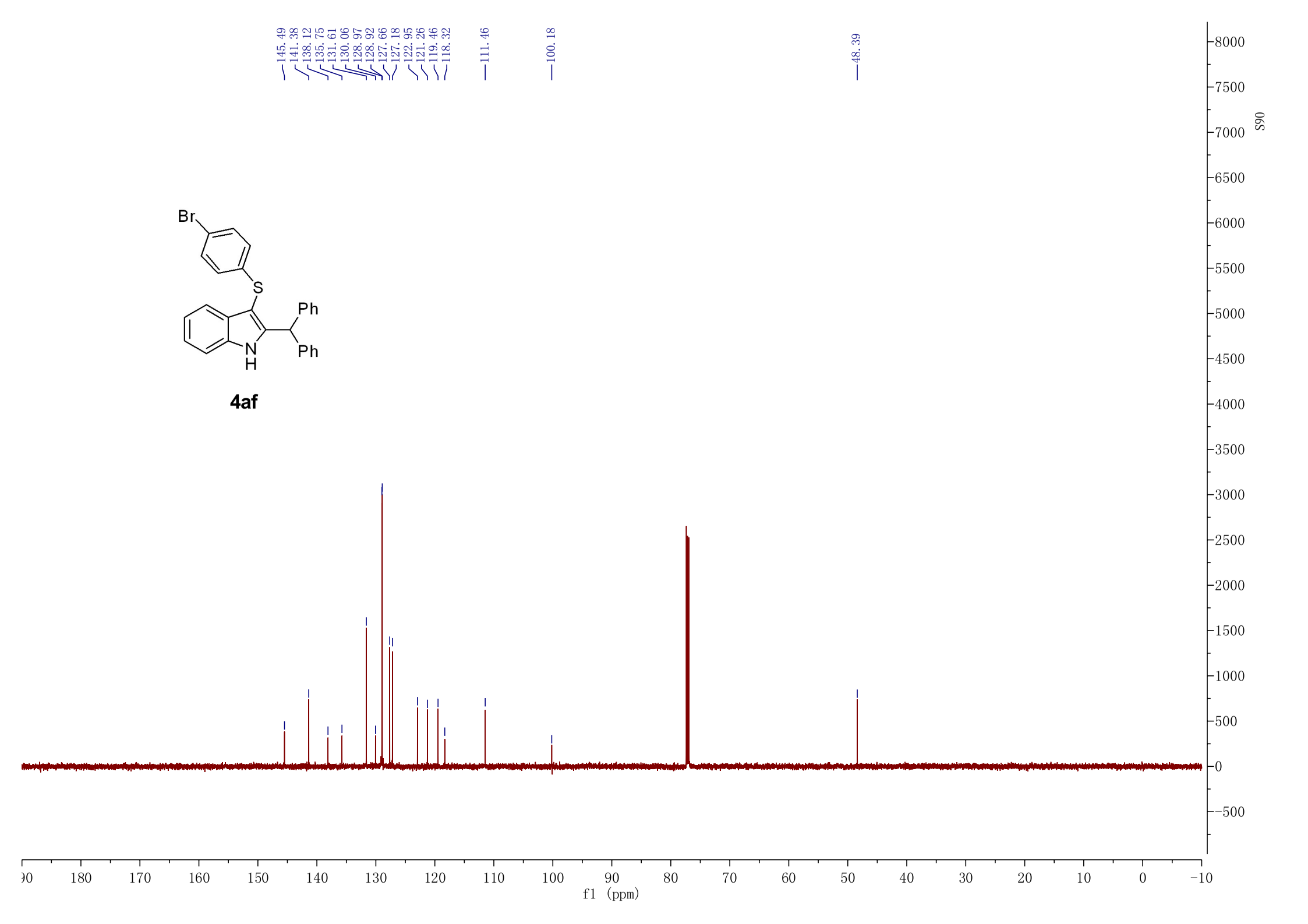

8.09
7.64
7.63
7.32
7.32
7.31
7.30
7.29
7.28
7.27
7.15
7.14
6.79
6.18
F
S
Ph
Ph
N
H
4ad
S85
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
1.00
1.00
7.02
1.07
1.09
4.00
2.00
2.02
1.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

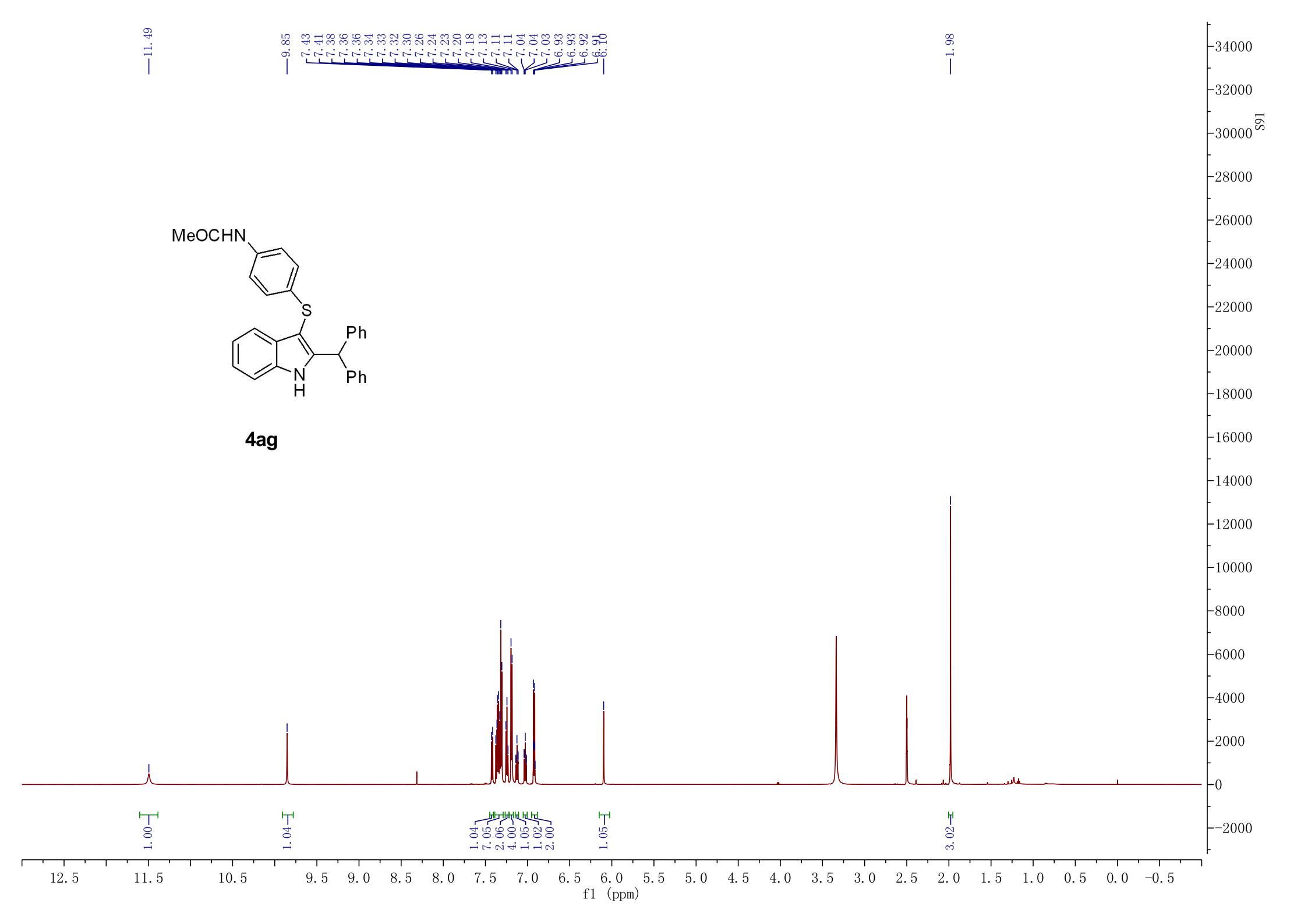

4ad
F
S
N
H
Ph
Ph
161.74
160.12
145.20
141.48
135.72
133.63
130.17
128.99
128.88
128.17
128.12
127.14
122.84
121.15
119.48
115.75
115.61
111.42
101.29
48.36
f1 (ppm)


8.11
7.61
7.60
7.31
7.31
7.30
7.27
7.15
7.14
7.06
7.04
6.92
6.91
6.15
Cl
S
Ph
Ph
N
H
4ae
25000
20000
15000
10000
5000
0
S87
1.00
1.00
7.01
1.10
1.13
3.96
2.00
2.00
1.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


145.38
141.31
137.32
135.67
130.44
130.00
128.89
128.83
128.65
127.28
127.10
122.85
121.16
119.38
111.38
100.27
48.31
Cl
S
Ph
Ph
N
H
4ae
S88
f1 (ppm)


8.10
7.30
7.29
7.27
7.18
7.17
7.17
7.13
7.12
6.85
6.84
6.84
6.83
6.83
6.83
6.12
Br
S
Ph
Ph
N
H
4af
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
S89
1.00
1.00
1.08
6.00
1.05
3.00
3.86
1.96
1.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


145.49
141.38
138.12
135.75
131.61
130.06
128.97
128.92
127.66
127.18
122.95
121.26
119.46
118.32
111.46
100.18
48.39
Br
S
Ph
Ph
N
H
4af
S90
f1 (ppm)


11.49
9.85
7.43
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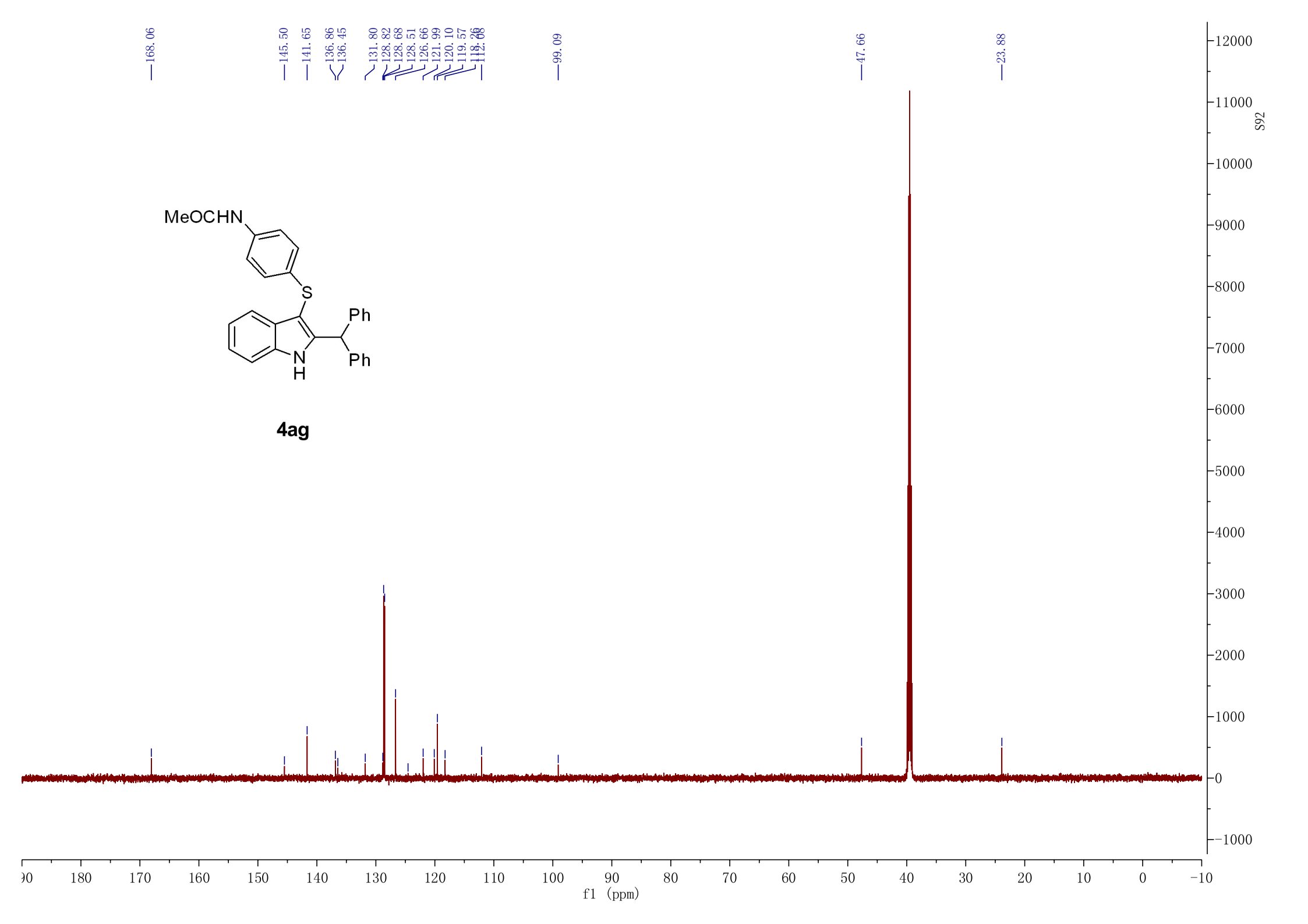
7.38
7.36
7.36
7.34
7.33
7.32
7.30
7.26
7.24
7.23
7.20
7.18
7.13
7.11
7.11
7.04
7.04
7.03
6.93
6.92
6.91
6.10
1.98
MeOCHN
S
Ph
Ph
N
H
4ag
S91
1.00
1.04
1.04
7.05
2.06
4.00
1.05
1.02
2.00
1.05
3.02
f1 (ppm)


168.06
145.50
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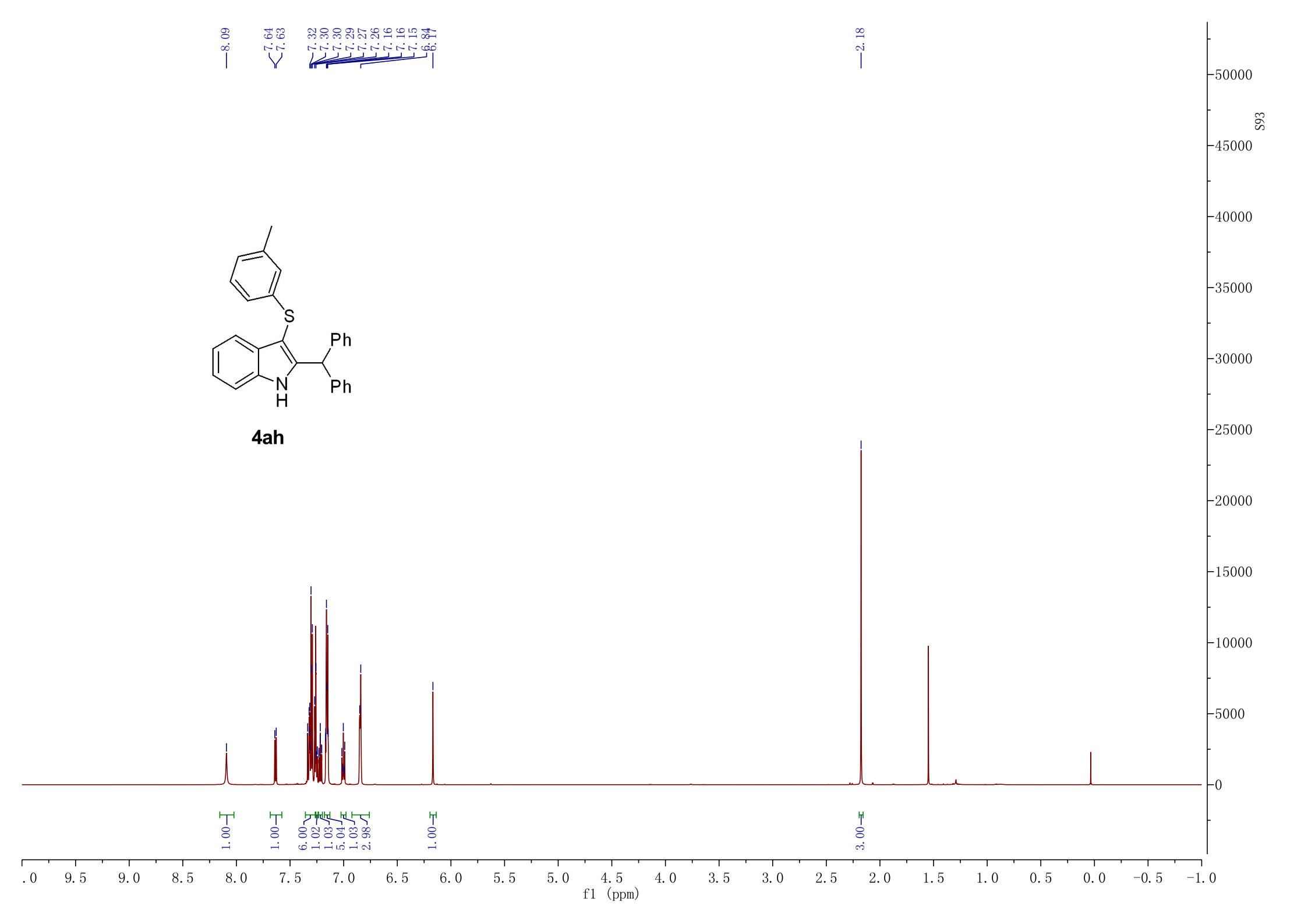
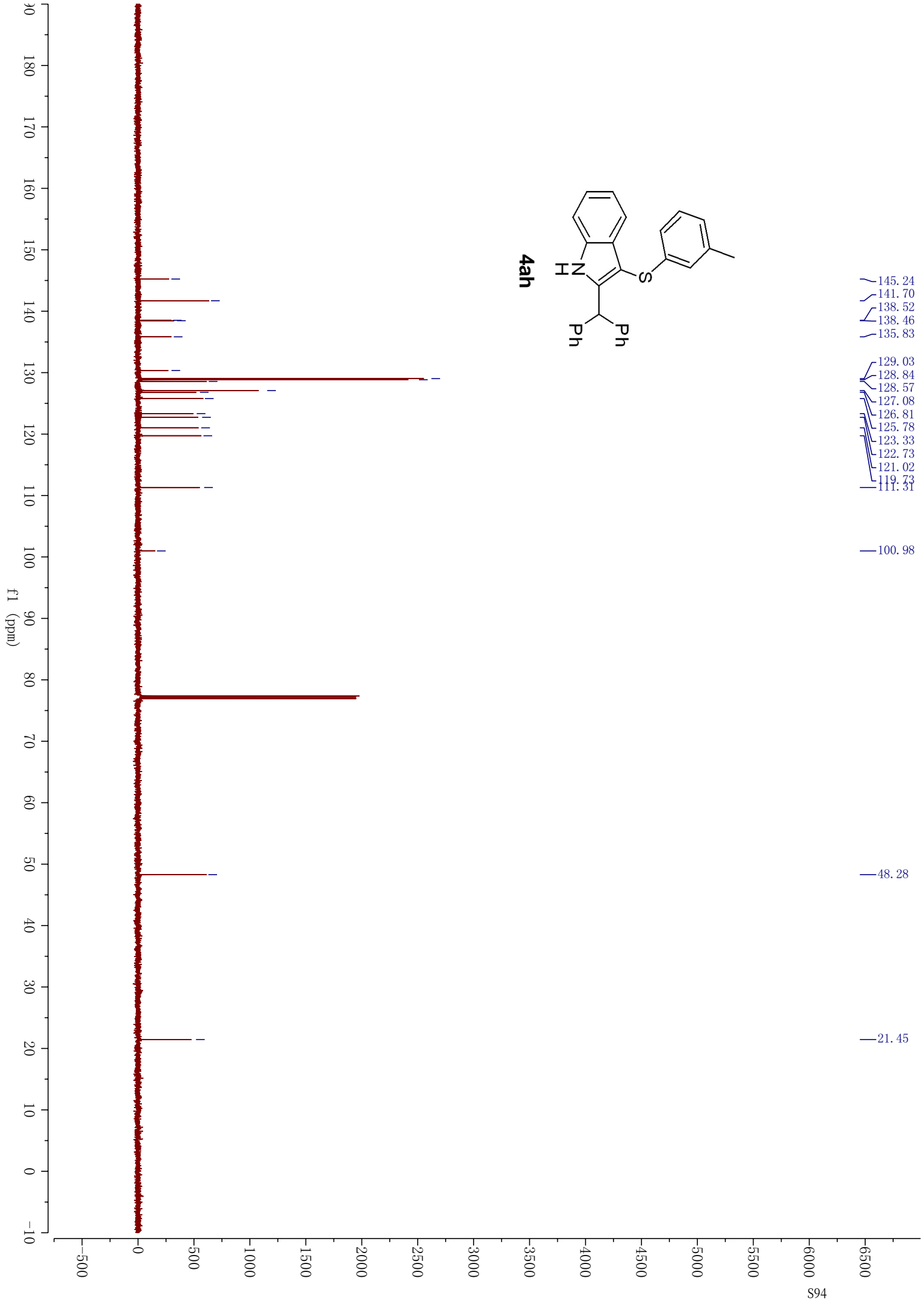
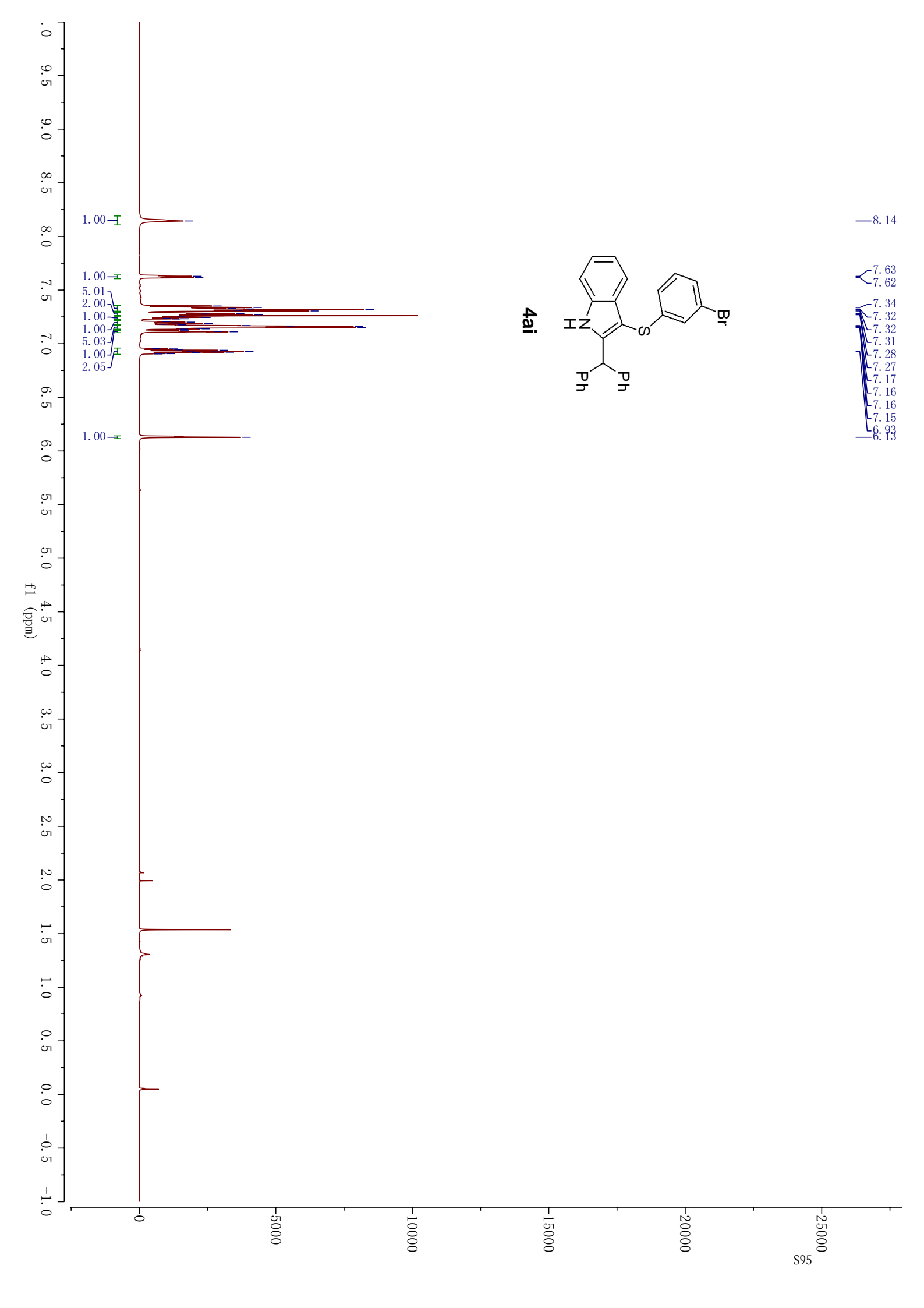
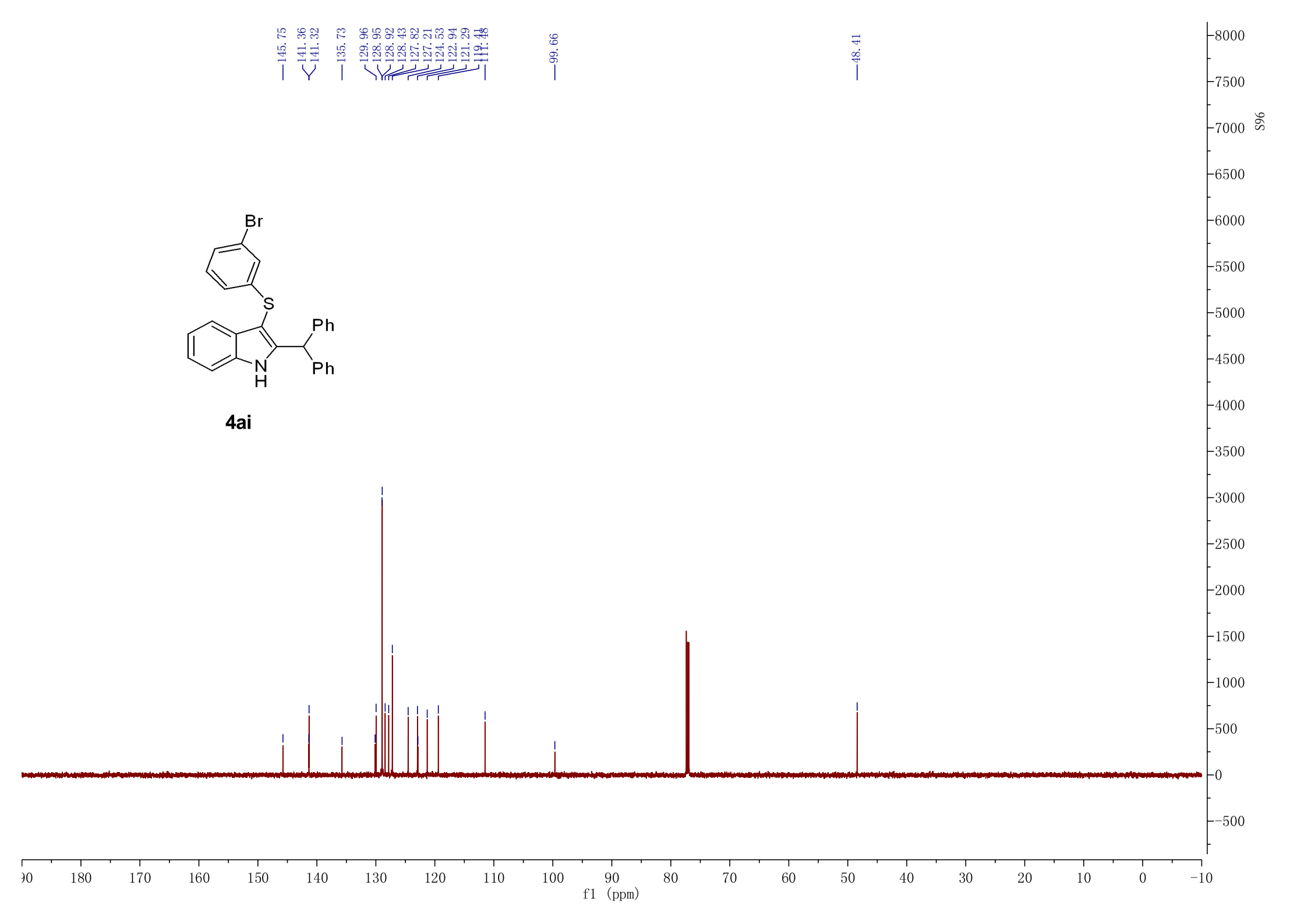
136.86
136.45
131.80
128.82
128.68
128.51
126.66
121.99
120.10
119.57
99.09
47.66
23.88
MeOCHN
S
Ph
Ph
N
H
4ag
S92
f1 (ppm)


8.09
7.64
7.63
7.32
7.30
7.30
7.29
7.27
7.26
7.16
7.16
7.15
6.84
6.17
2.18
S
Ph
Ph
N
H
4ah
S93
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1.00
1.00
6.00
1.02
1.03
5.04
1.03
2.98
1.00
3.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


4ah
N
H
S
Ph
Ph
145.24
141.70
138.52
138.46
135.83
129.03
128.84
128.57
127.08
126.81
125.78
123.33
122.73
121.02
119.73
111.31
100.98
48.28
21.45
f1 (ppm)


4ai
1.00
1.00
5.01
2.00
1.00
1.00
5.03
1.00
2.05
1.00
8.14
7.63
7.62
7.34
7.32
7.32
7.31
7.28
7.27
7.17
7.16
7.16
7.15
6.93
6.13
f1 (ppm)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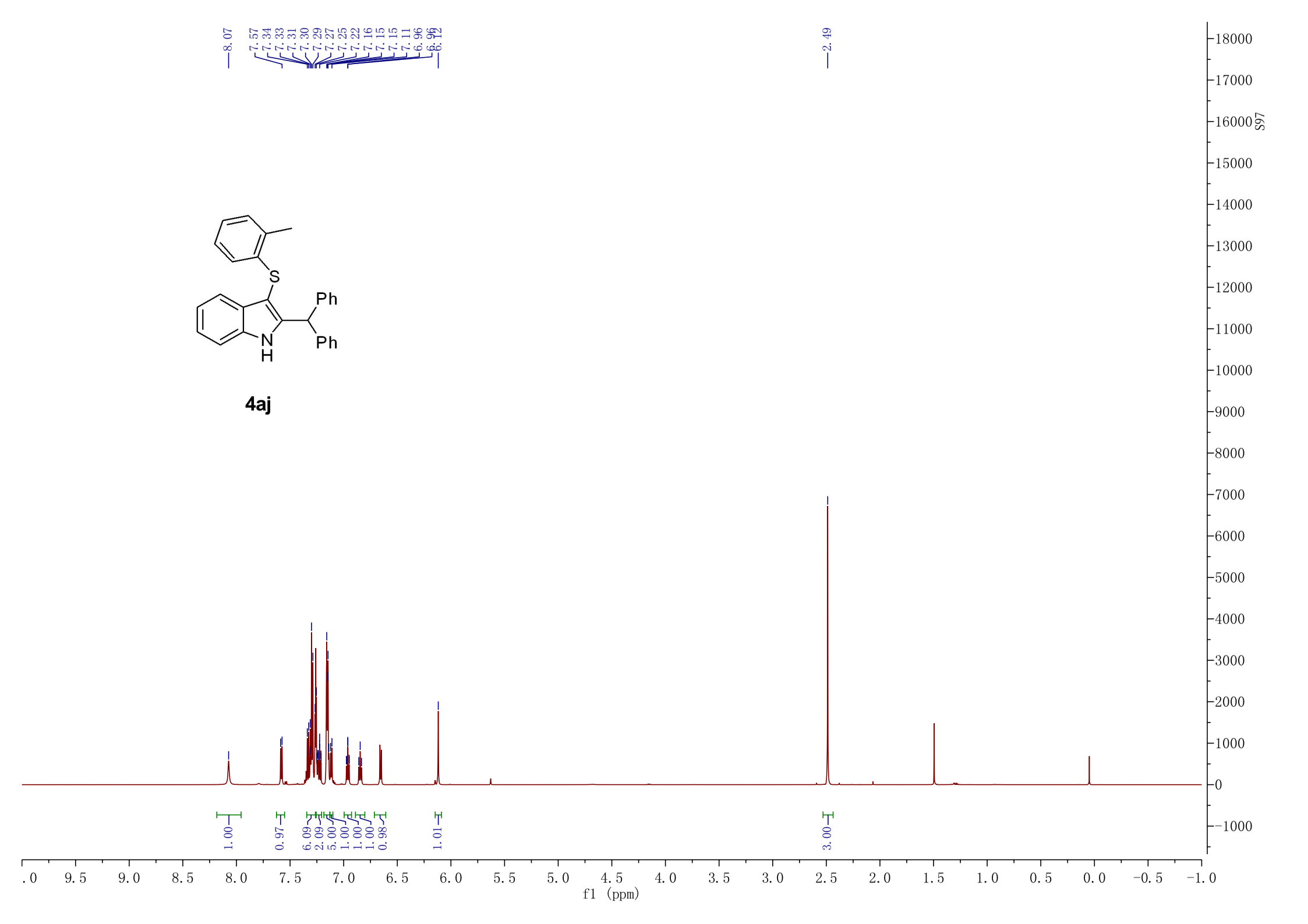
141.32
135.73
129.96
128.95
128.92
128.43
127.82
127.21
124.53
122.94
121.29
99.66
48.41
Br
S
Ph
Ph
N
H
4ai
S96
f1 (ppm)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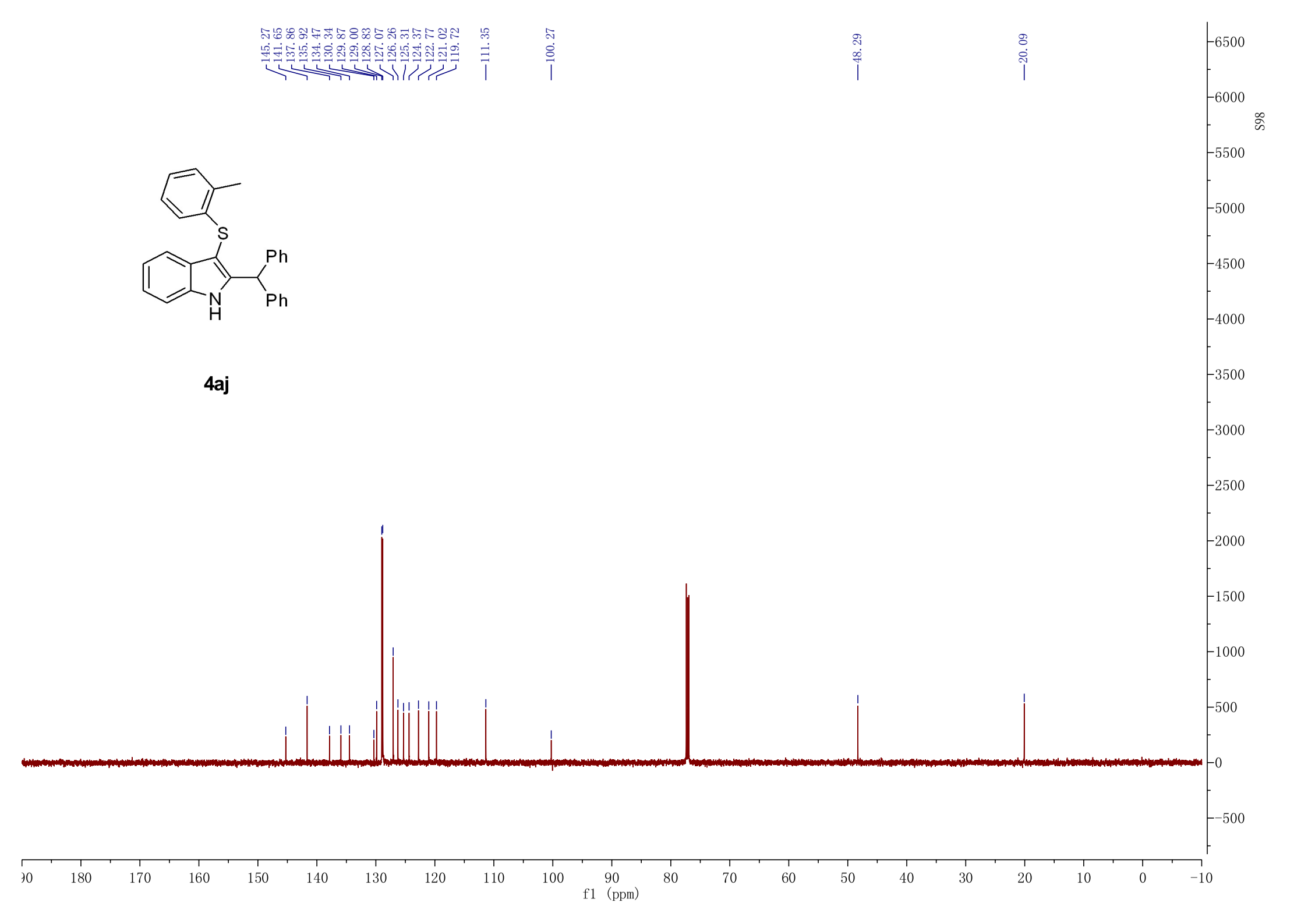
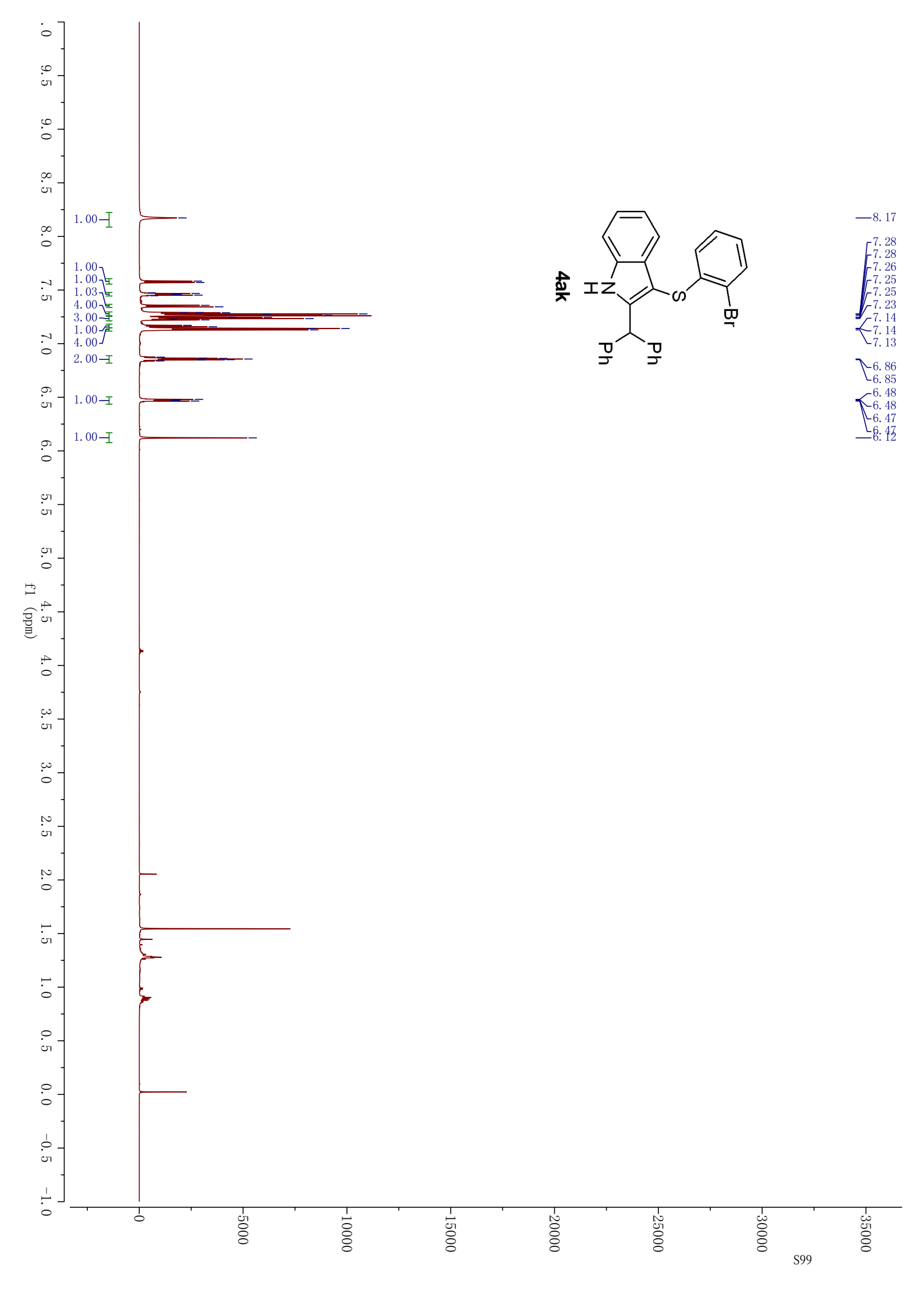
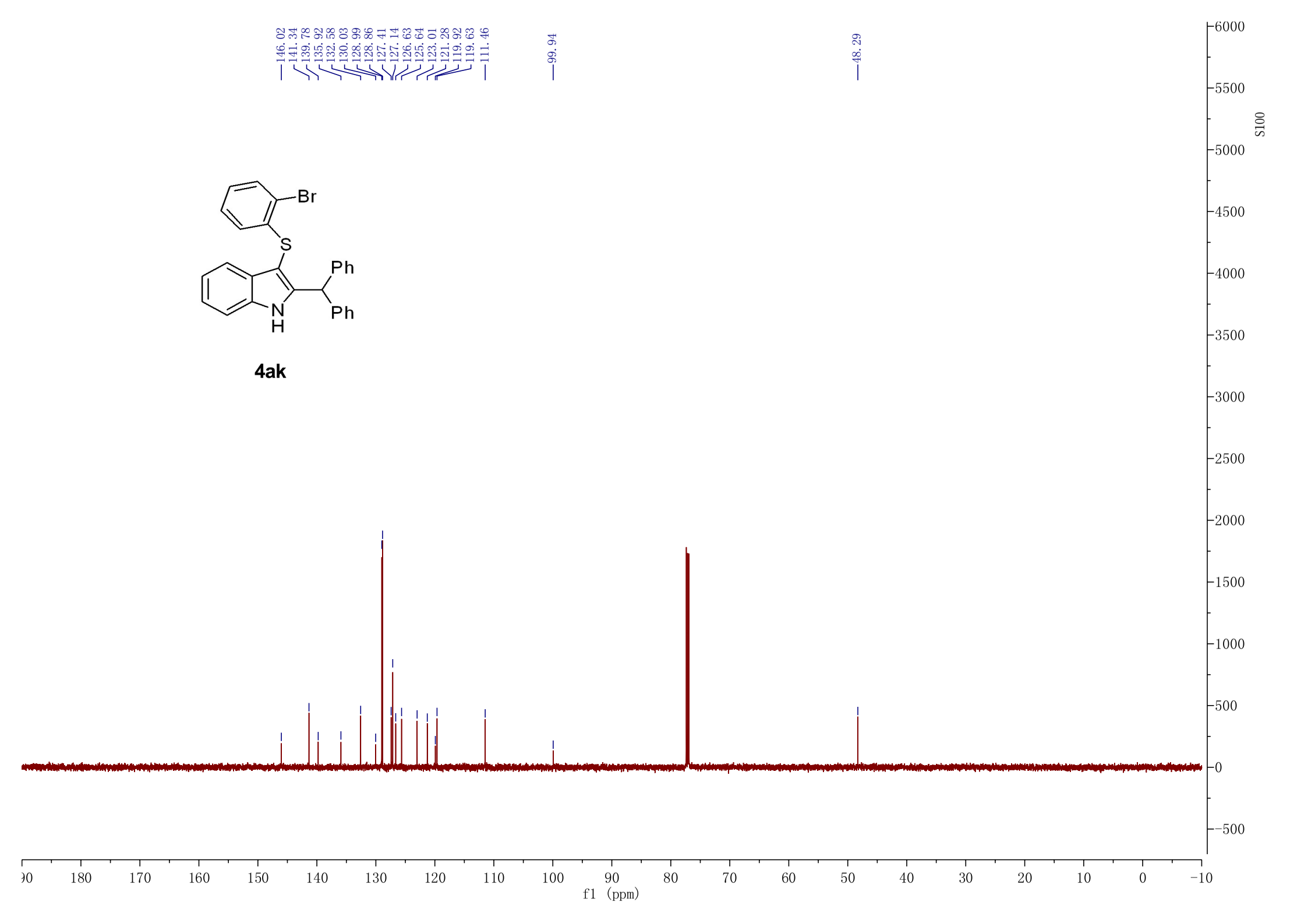
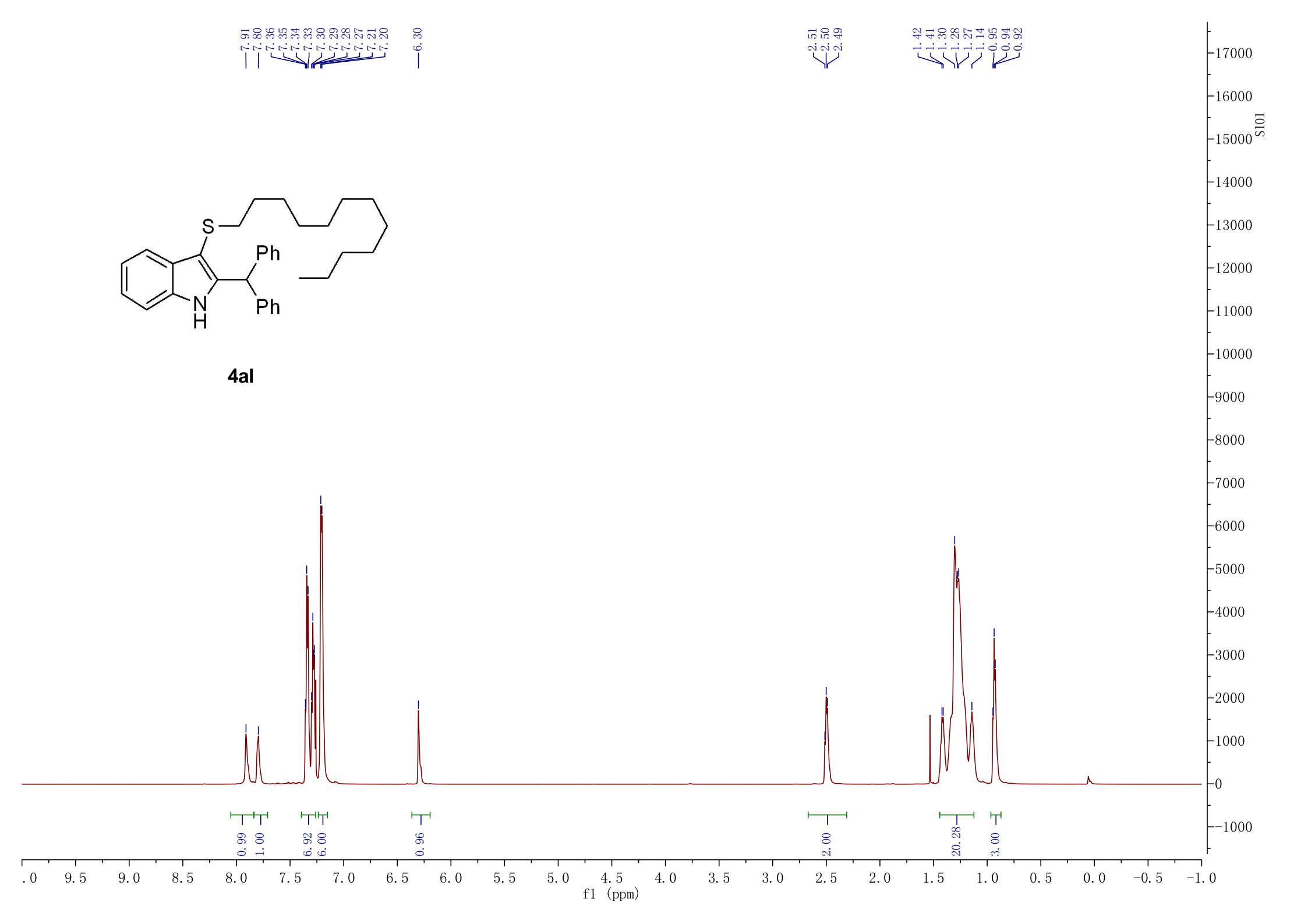
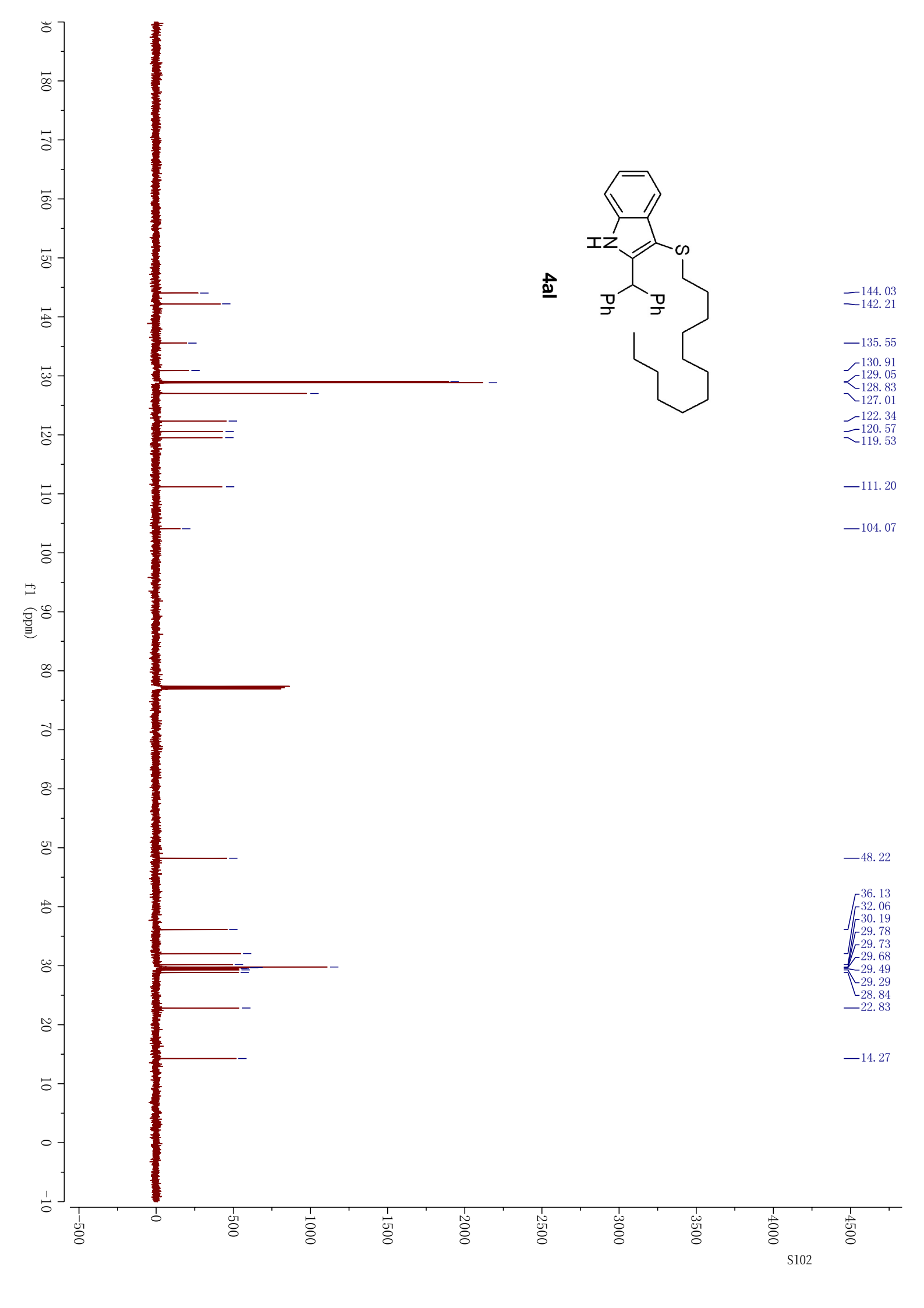
7.57
7.34
7.33
7.31
7.30
7.29
7.27
7.25
7.22
7.16
7.15
7.11
6.96
6.92
2.49
S
Ph
Ph
N
H
4aj
S97
1.00
0.97
6.09
2.09
5.00
1.00
1.00
0.98
1.01
3.00
f1 (ppm)

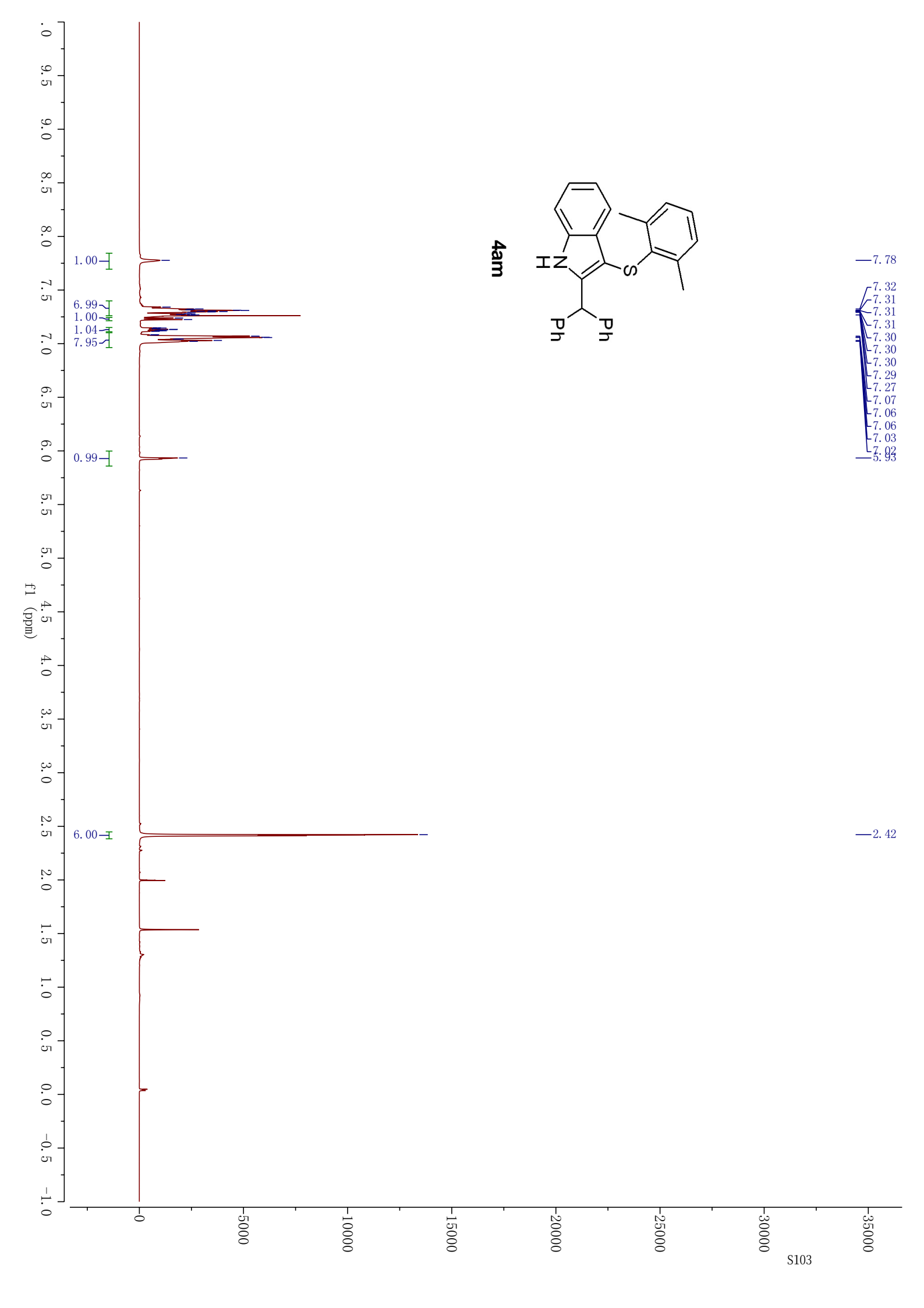

145.27
141.65
137.86
135.92
134.47
130.34
129.87
129.00
128.83
127.07
126.26
125.31
124.37
122.77
121.02
119.72
111.35
100.27
48.29
20.09
S
Ph
Ph
N
H
4aj
S98
f1 (ppm)

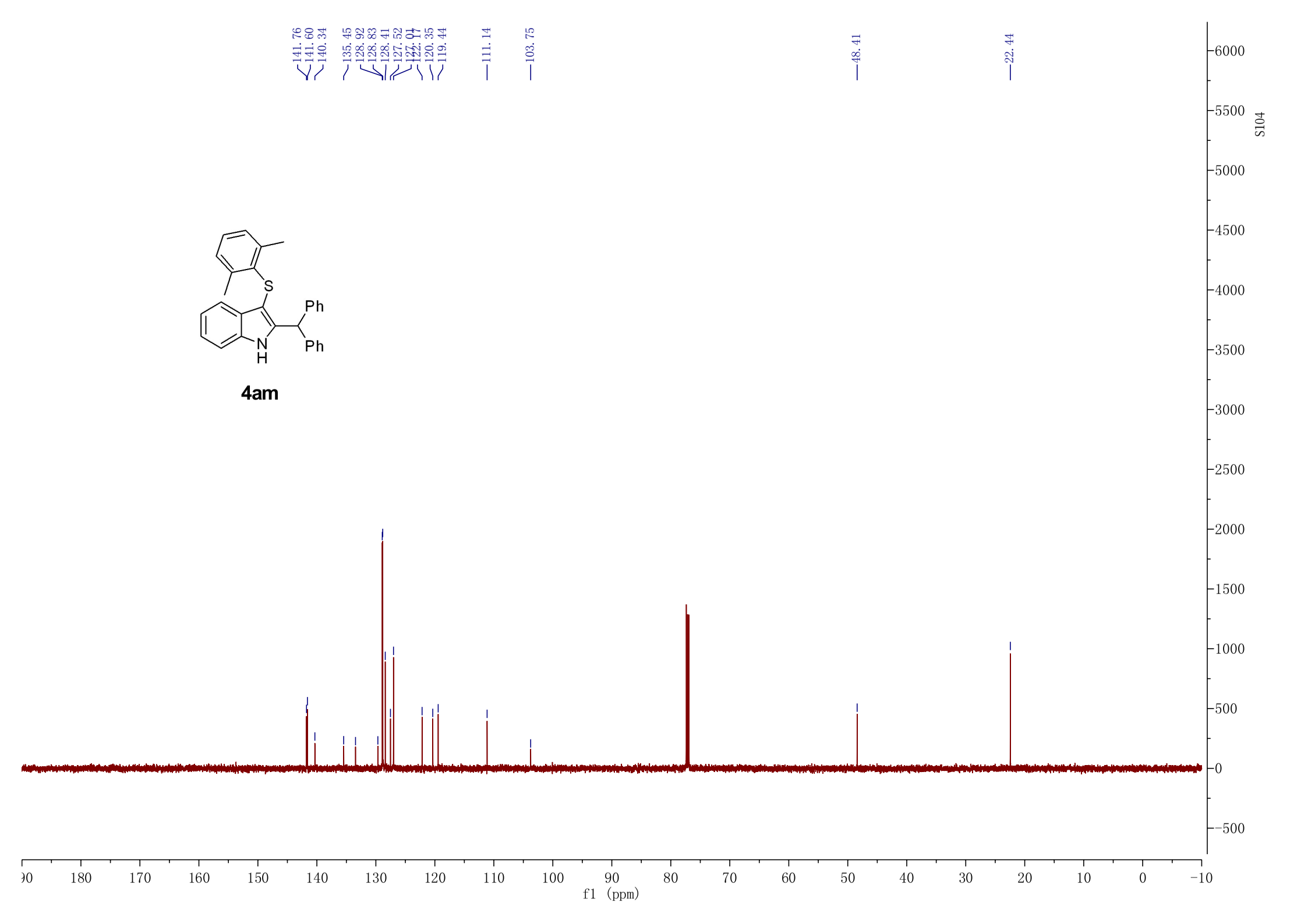

4ak
1.00
1.00
1.00
1.03
4.00
3.00
1.00
4.00
2.00
1.00
1.00
8.17
7.28
7.28
7.26
7.25
7.25
7.23
7.14
7.14
7.13
6.86
6.85
6.48
6.48
6.47
6.47
6.12
f1 (ppm)

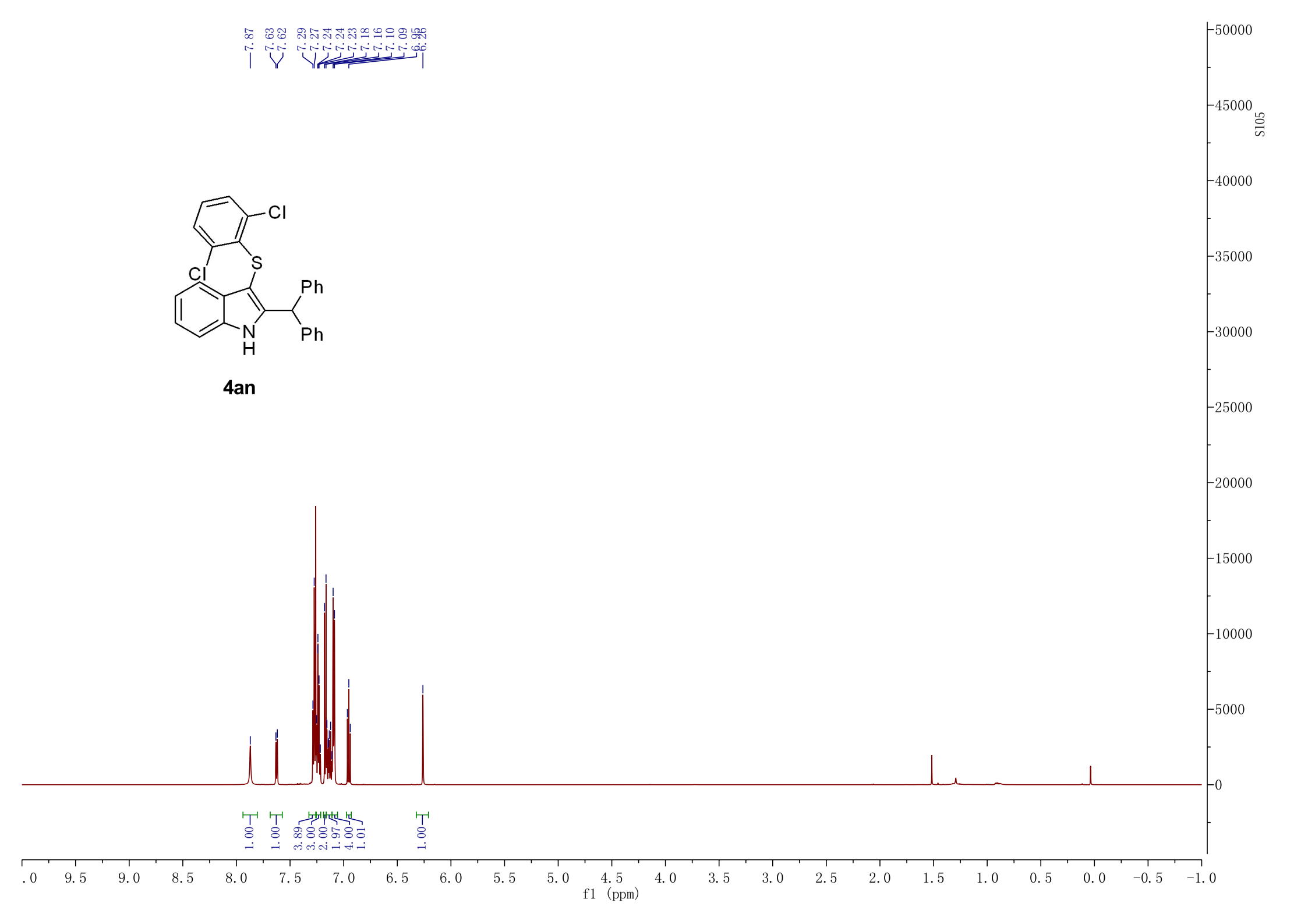

146.02
141.34
139.78
135.92
132.58
130.03
128.99
128.86
127.41
127.14
126.63
125.64
123.01
121.28
119.92
119.63
111.46
99.94
48.29
Br
S
Ph
Ph
N
H
4ak
S100
f1 (ppm)

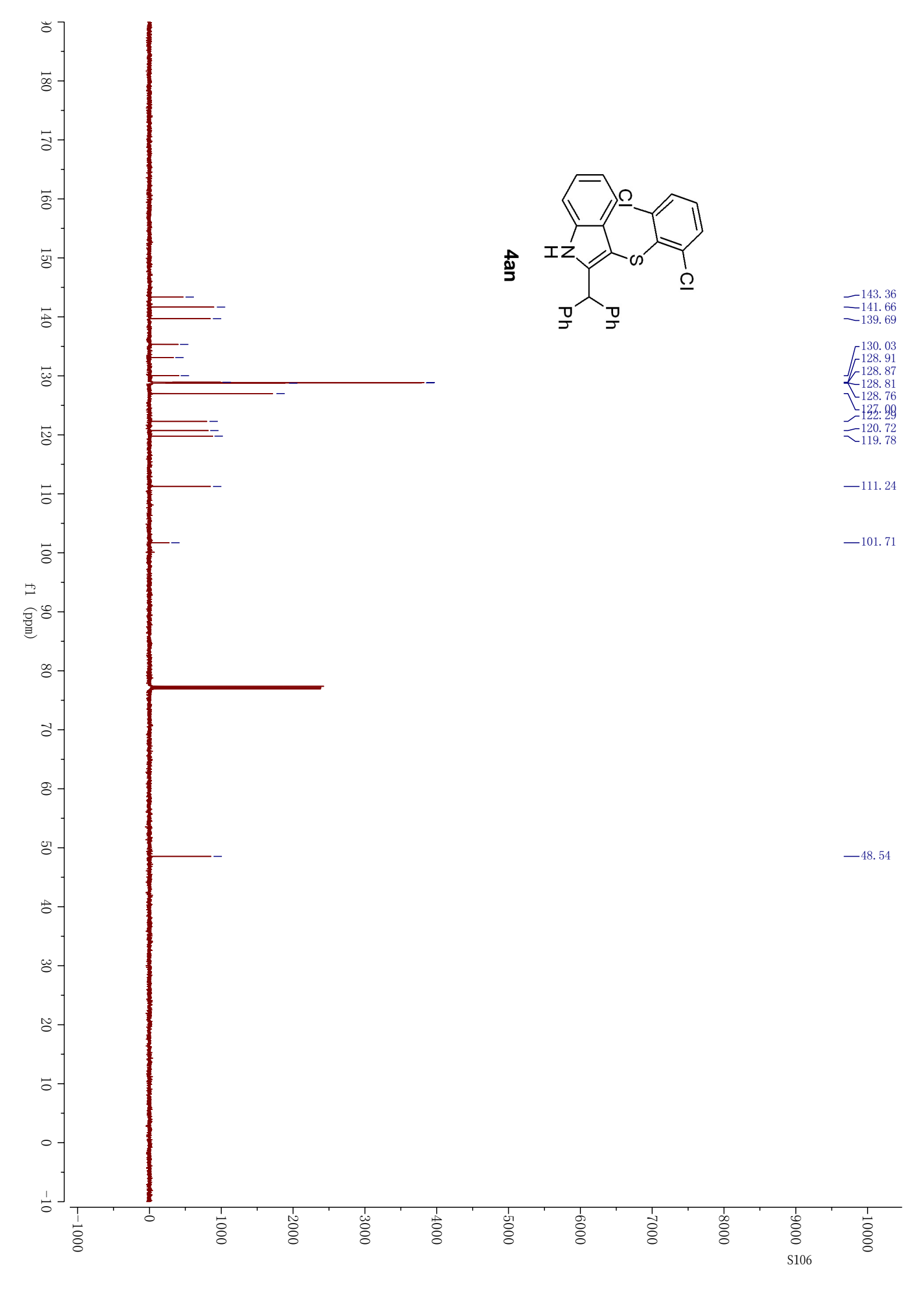

7.91
7.80
7.36
7.35
7.34
7.33
7.30
7.29
7.28
7.27
7.21
7.20
6.30
2.51
2.50
2.49
1.42
1.41
1.30
1.28
1.27
1.14
0.95
0.94
0.92
S
Ph
Ph
N
H
4al
S101
0.99
1.00
6.92
6.00
0.96
2.00
20.28
3.00
f1 (ppm)

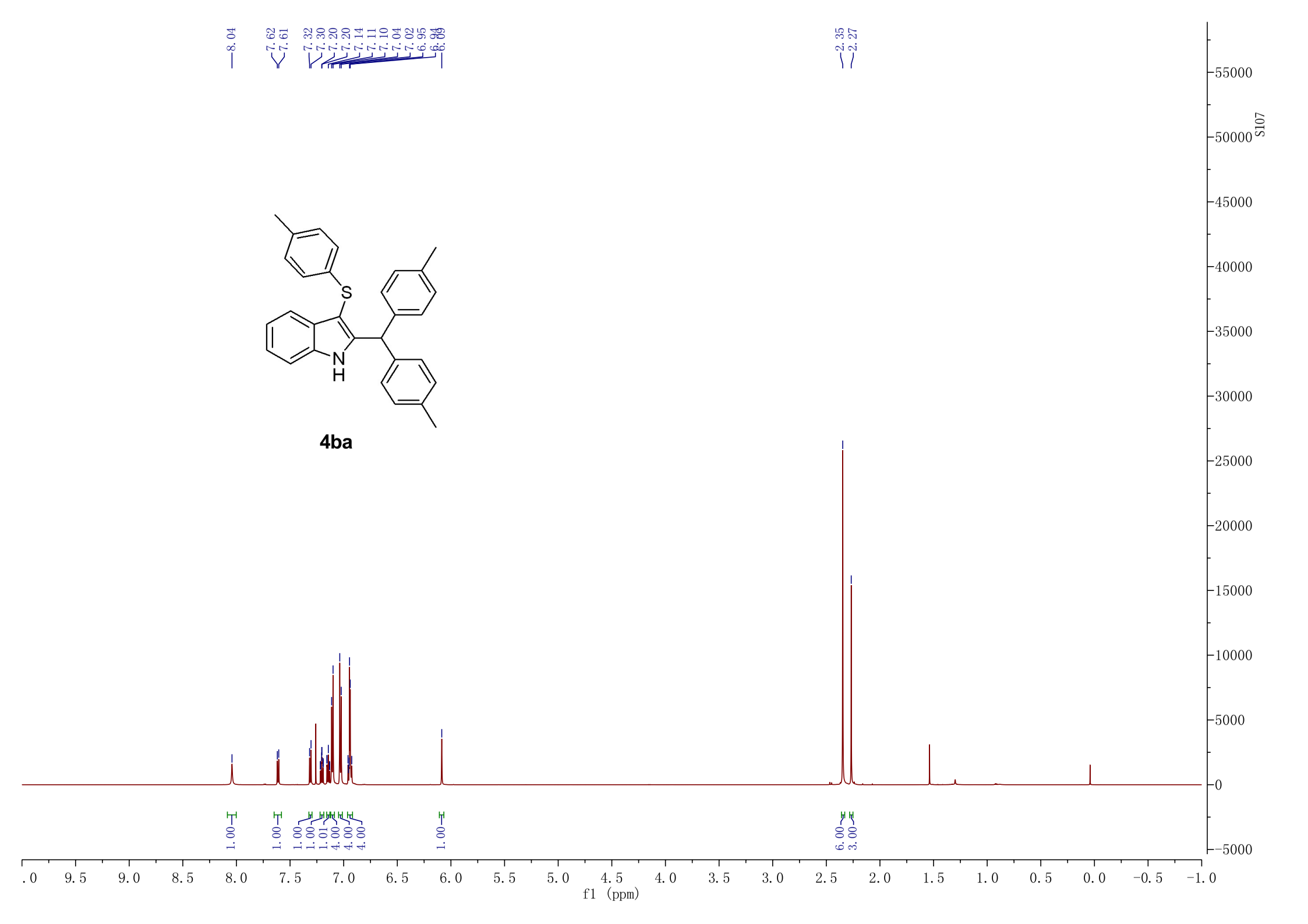

4al
144.03
142.21
135.55
130.91
129.05
128.83
127.01
122.34
120.57
119.53
111.20
104.07
48.22
36.13
32.06
30.19
29.78
29.73
29.68
29.49
29.29
28.84
22.83
14.27
f1 (ppm)

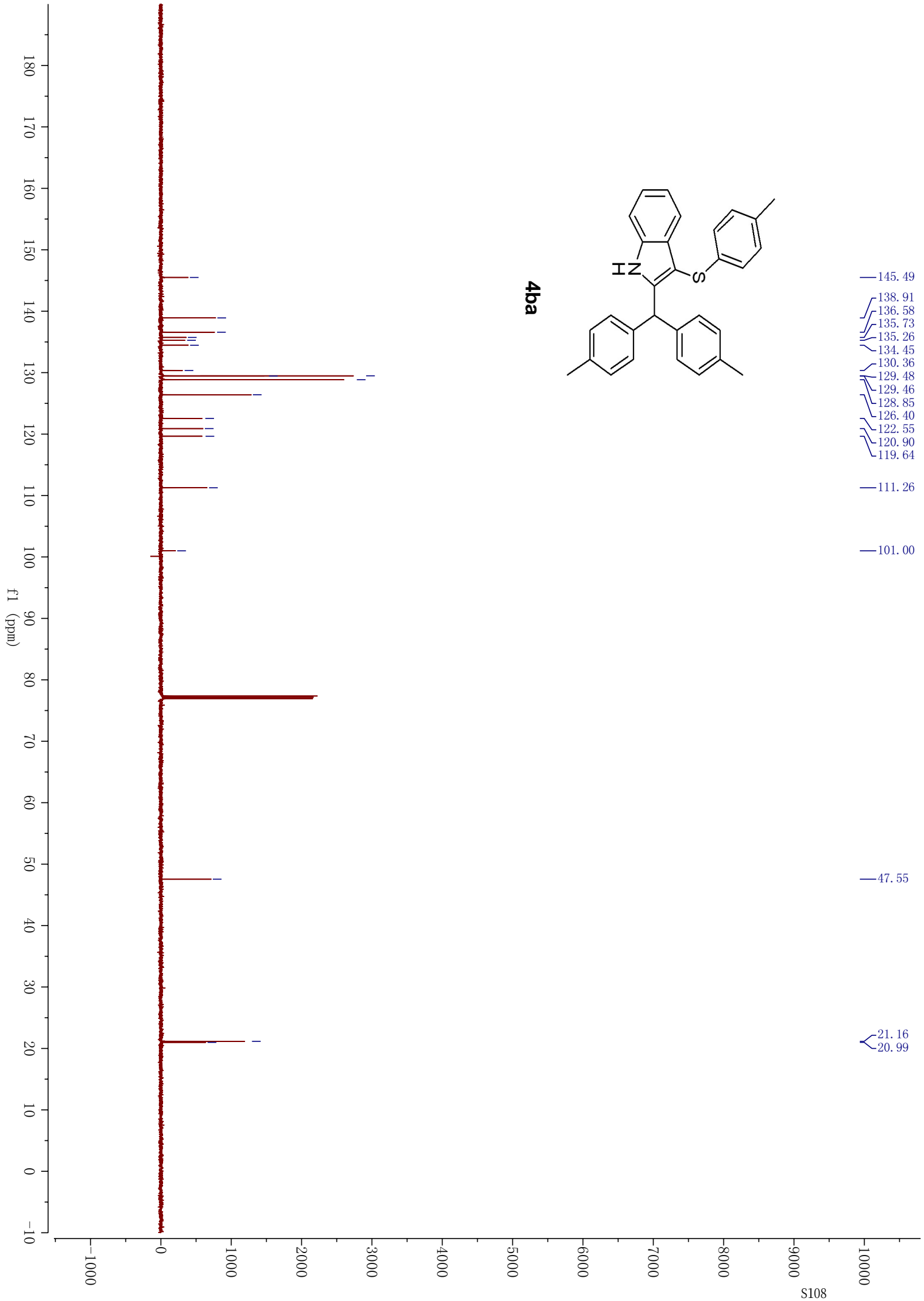

4am
1.00
6.99
1.00
1.04
7.95
0.99
6.00
7.78
7.32
7.31
7.31
7.31
7.30
7.30
7.30
7.29
7.27
7.07
7.06
7.06
7.03
7.02
5.93
2.42
f1 (ppm)

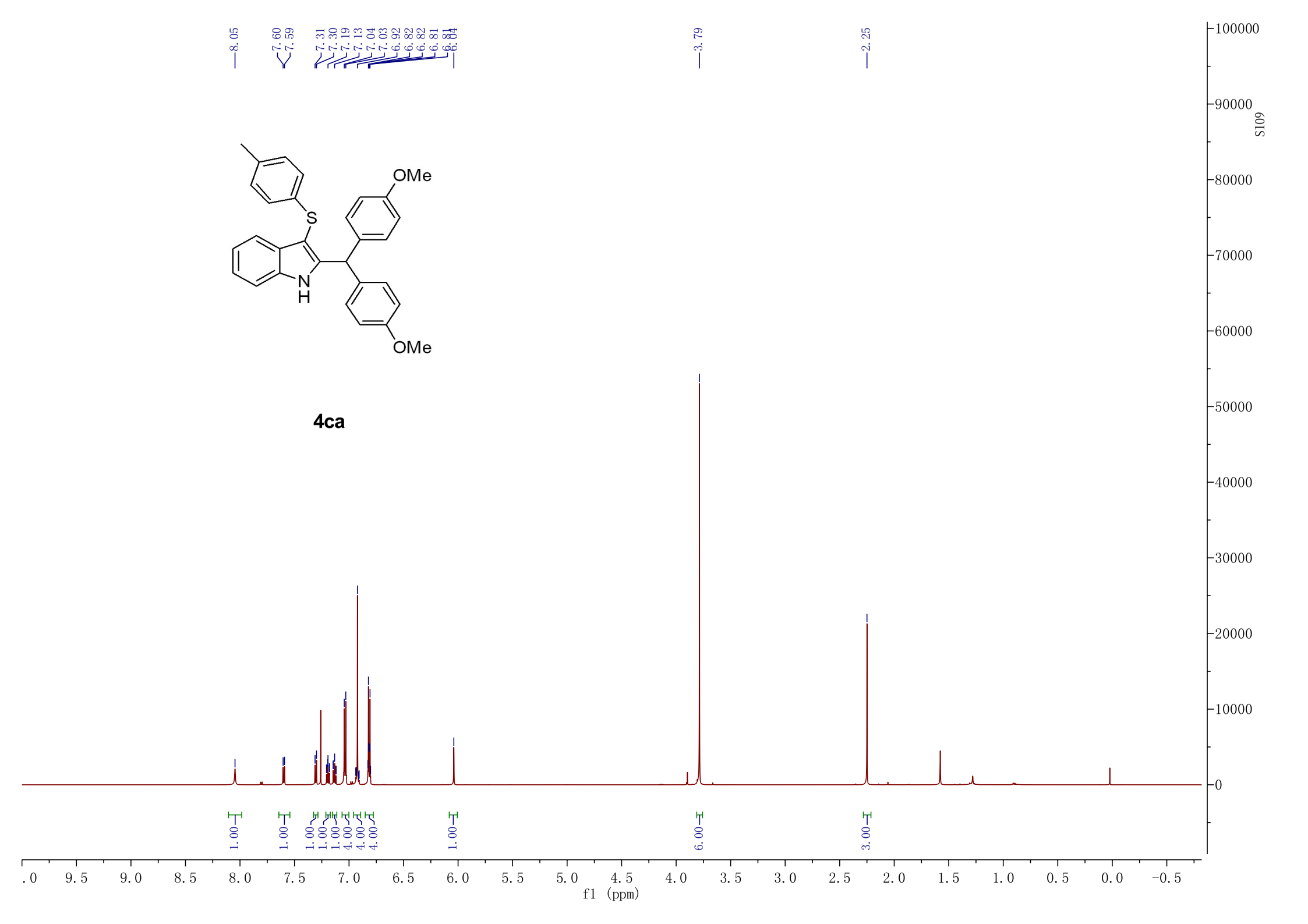

141.76
141.60
140.34
135.45
128.92
128.83
128.41
127.52
122.17
120.35
119.44
111.14
103.75
48.41
22.44
S
Ph
Ph
N
H
4am
S104
f1 (ppm)

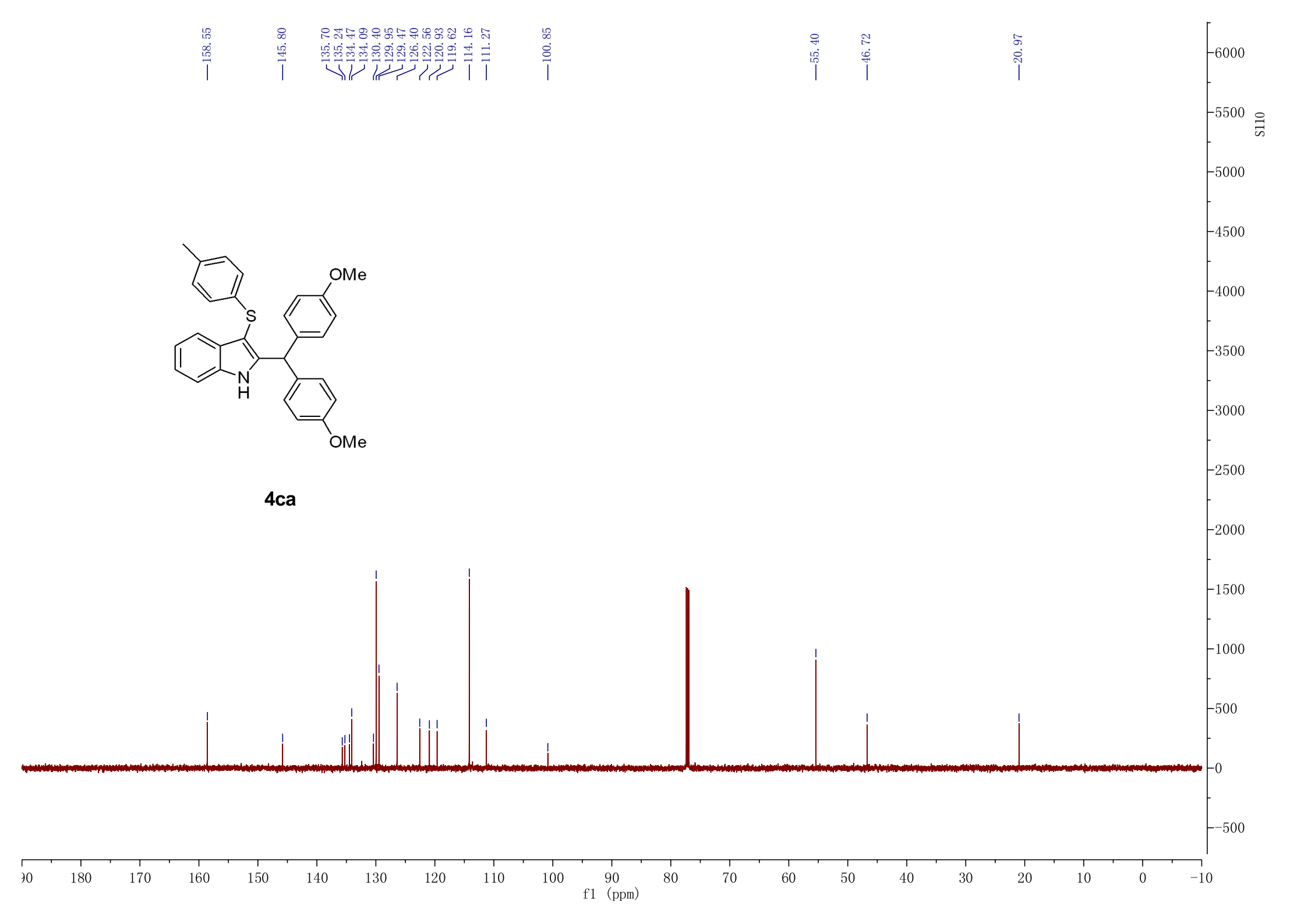

7.87
7.63
7.62
7.29
7.27
7.24
7.24
7.23
7.18
7.16
7.10
7.09
6.95
6.26
Cl
S
Cl
Ph
Ph
N
H
4an
S105
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1.00
1.00
3.89
3.00
2.00
1.97
4.00
1.01
1.00
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

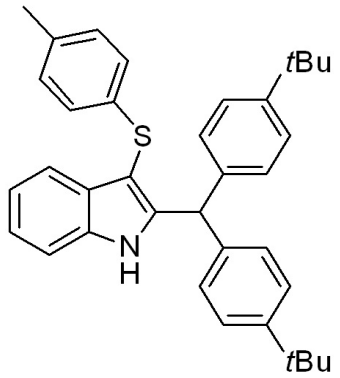

4an
Cl
N
H
S
Cl
Ph
Ph
143.36
141.66
139.69
130.03
128.91
128.87
128.81
128.76
127.00
122.29
120.72
119.78
111.24
101.71
48.54
f1 (ppm)


8.04
7.62
7.61
7.32
7.30
7.20
7.14
7.11
7.10
7.04
7.02
6.95
2.35
2.27
S
N
H
4ba
1.00
1.00
1.00
1.00
1.01
4.00
4.00
4.00
1.00
6.00
3.00
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
S107
f1 (ppm)


4ba
145.49
138.91
136.58
135.73
135.26
134.45
130.36
129.48
129.46
128.85
126.40
122.55
120.90
119.64
111.26
101.00
47.55
21.16
20.99
f1 (ppm)

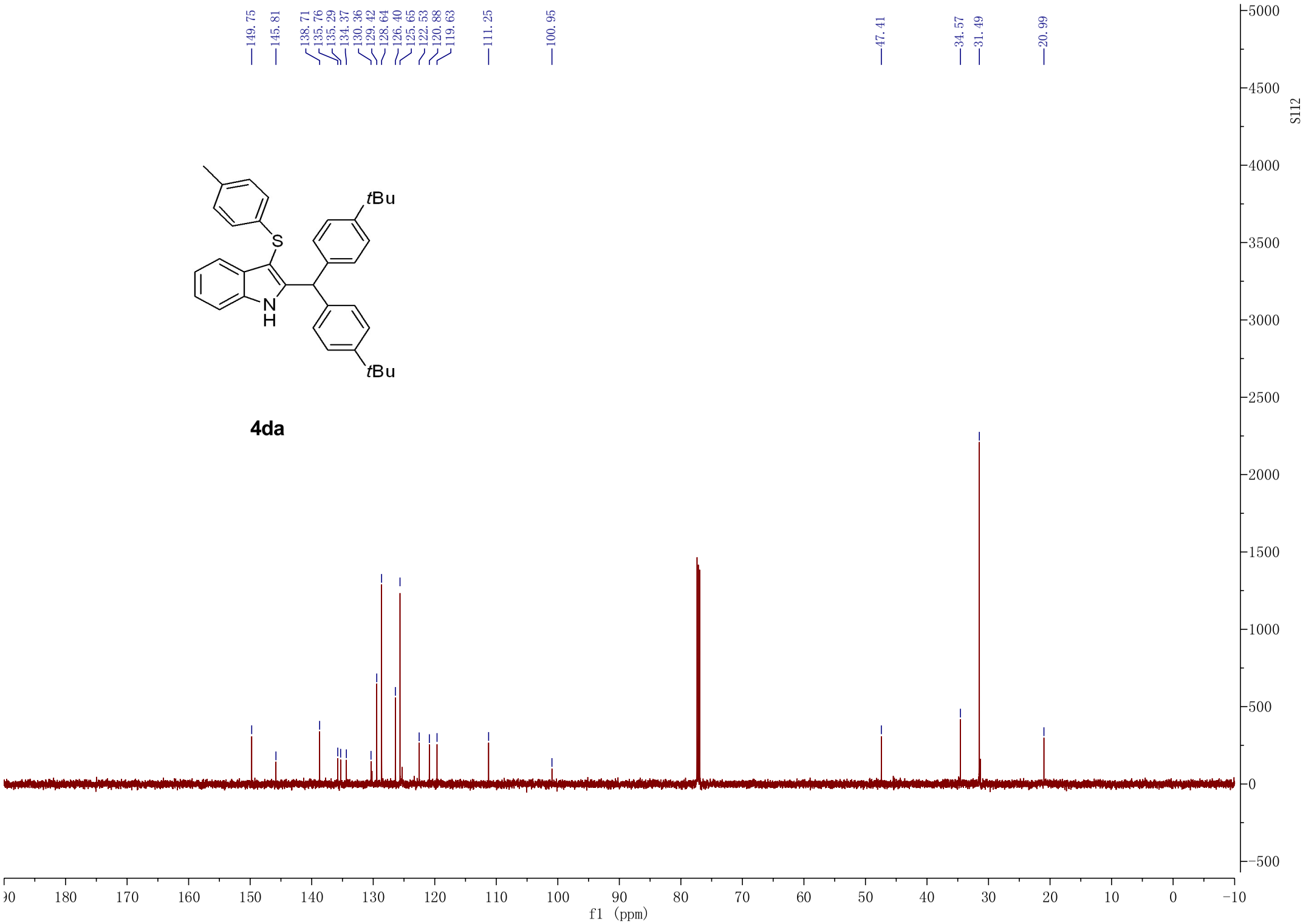

8.05
7.60
7.59
7.31
7.30
7.19
7.13
7.04
7.03
6.92
6.82
6.82
6.81
6.04
3.79
2.25
OMe
S
N
H
OMe
4ca
S109
f1 (ppm)

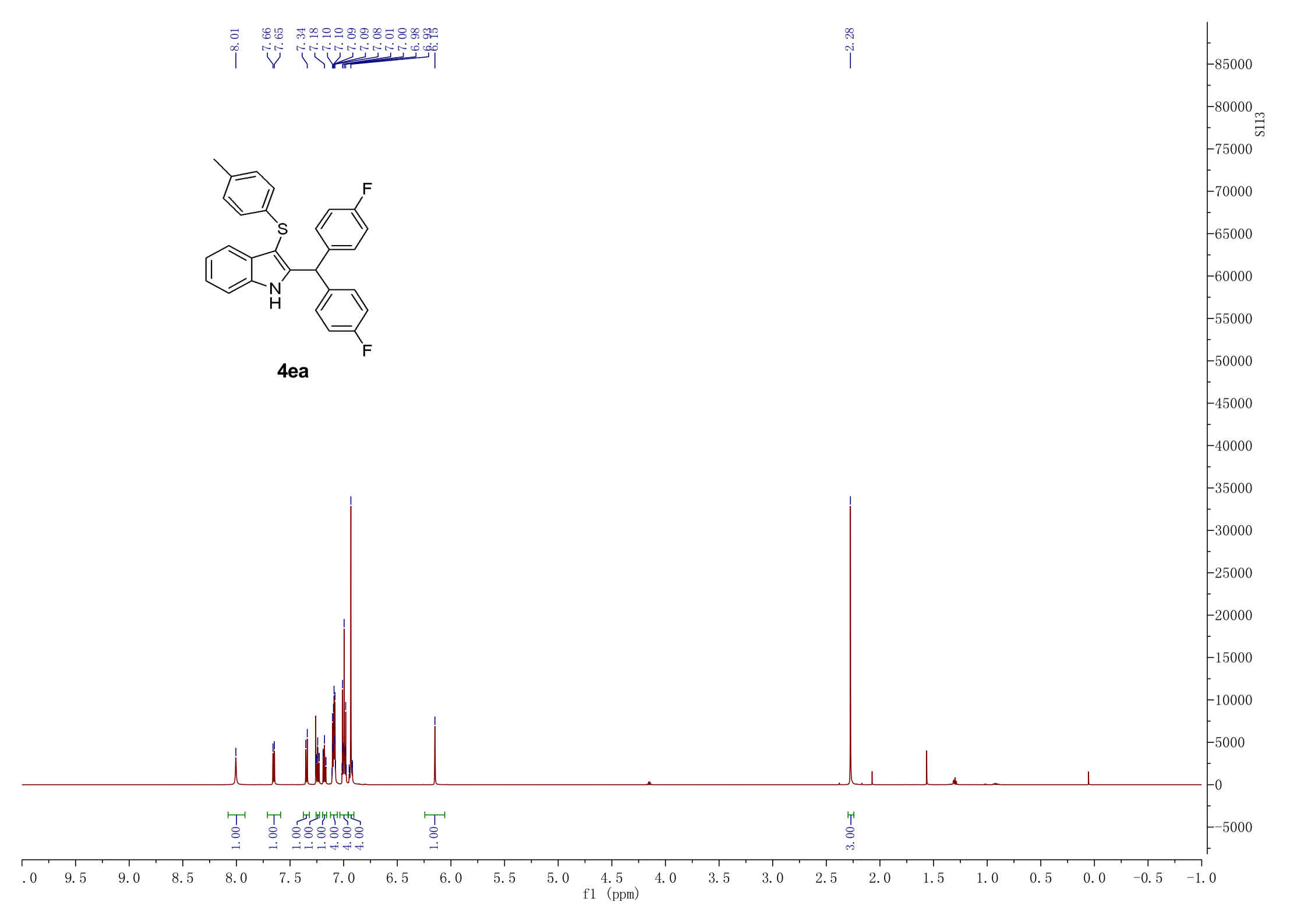

158.55
145.80
135.70
135.24
134.47
134.09
130.40
129.95
129.47
126.40
122.56
120.93
119.62
114.16
111.27
100.85
55.40
46.72
20.97
OMe
S
N
H
OMe
4ca
S110
f1 (ppm)

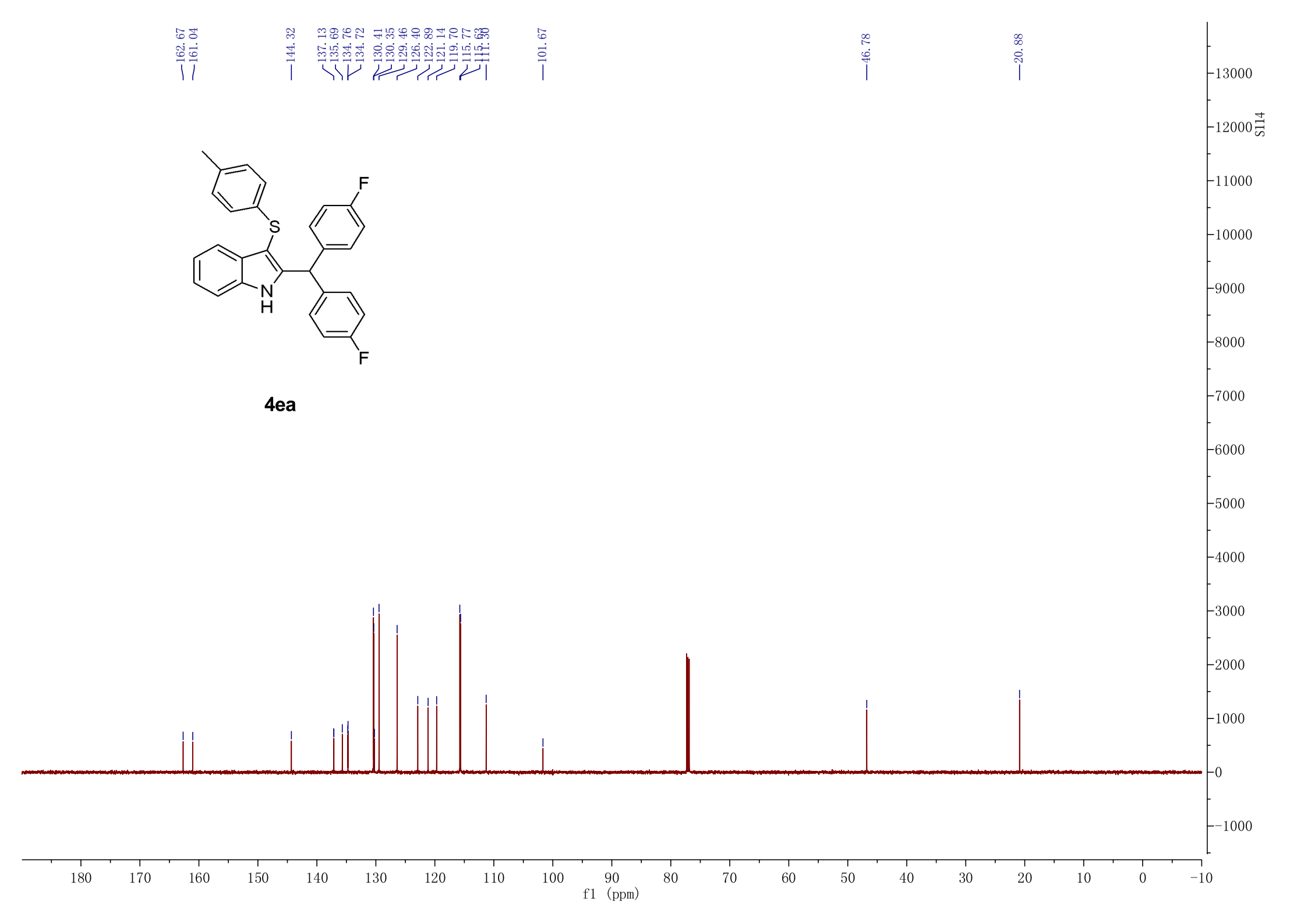

tBu
S
N
H
tBu

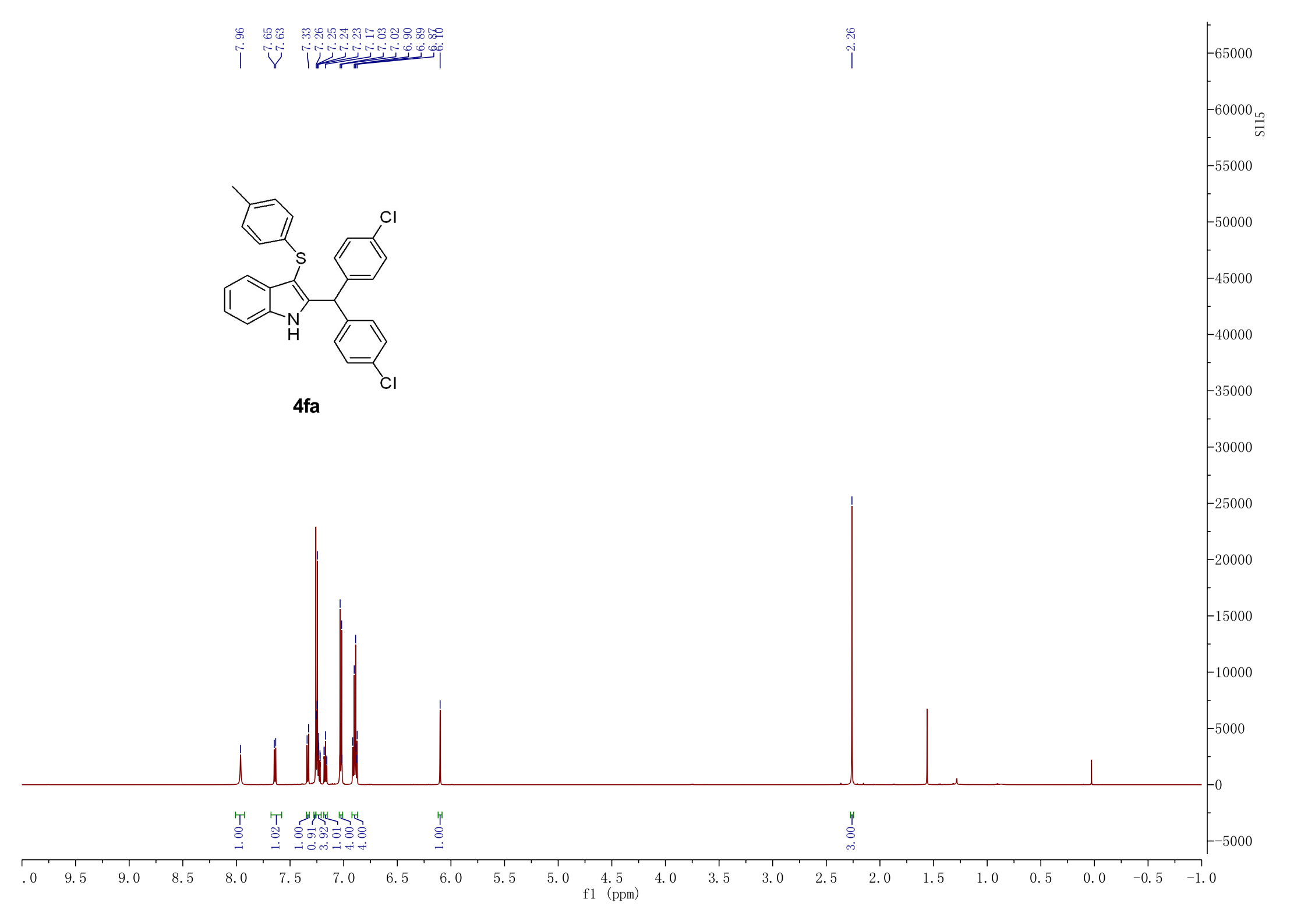
4da

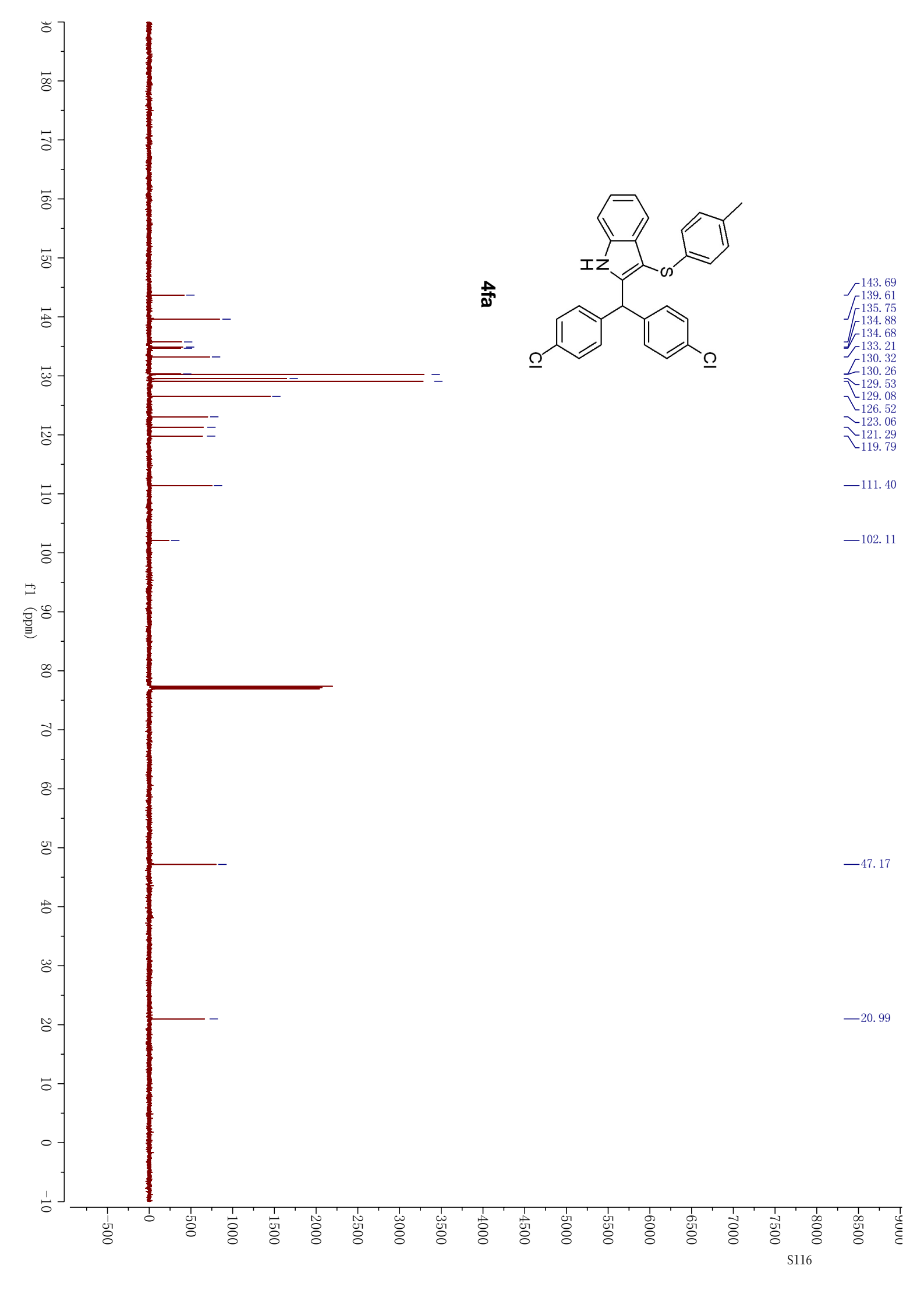
8.11
7.60
7.59
7.32
7.31
7.30
7.29
7.28
7.19
7.13
7.08
7.07
6.90
6.10
2.24
1.31
S111
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
0.96
1.01
5.05
1.05
1.05
4.00
4.00
1.01
3.00
18.03
.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

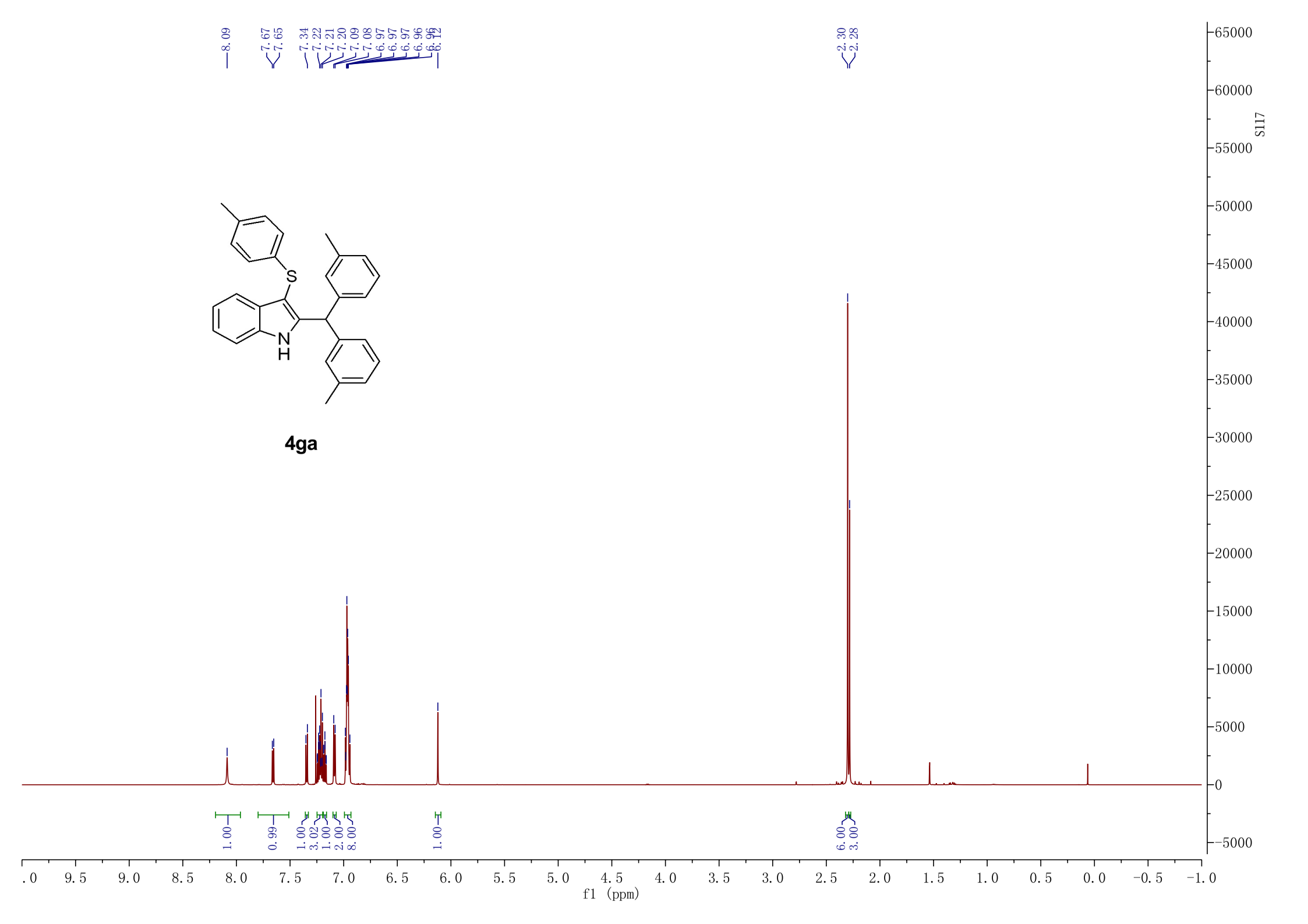

149.75
145.81
138.71
135.76
135.29
134.37
130.36
129.42
128.64
126.40
125.65
122.53
120.88
119.63
111.25
100.95
47.41
34.57
31.49
20.99
tBu
S
N
H
tBu
4da
S112
f1 (ppm)

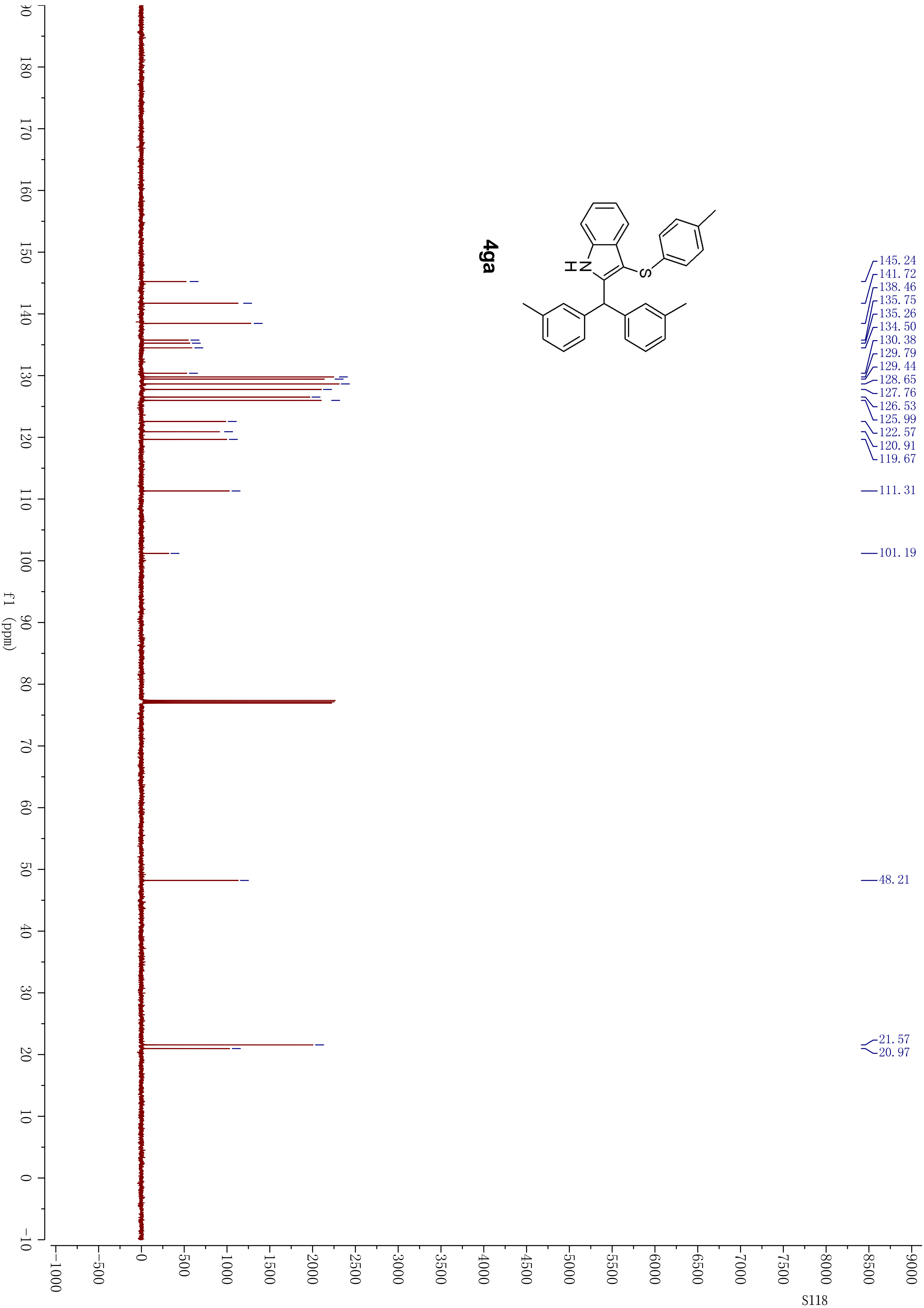

8.01
7.66
7.65
7.34
7.18
7.10
7.10
7.09
7.09
7.08
7.01
7.00
6.98
6.93
6.15
2.28
F
S
N
H
F
4ea
S113
1.00
1.00
1.00
1.00
1.00
4.00
4.00
4.00
1.00
3.00
f1 (ppm)

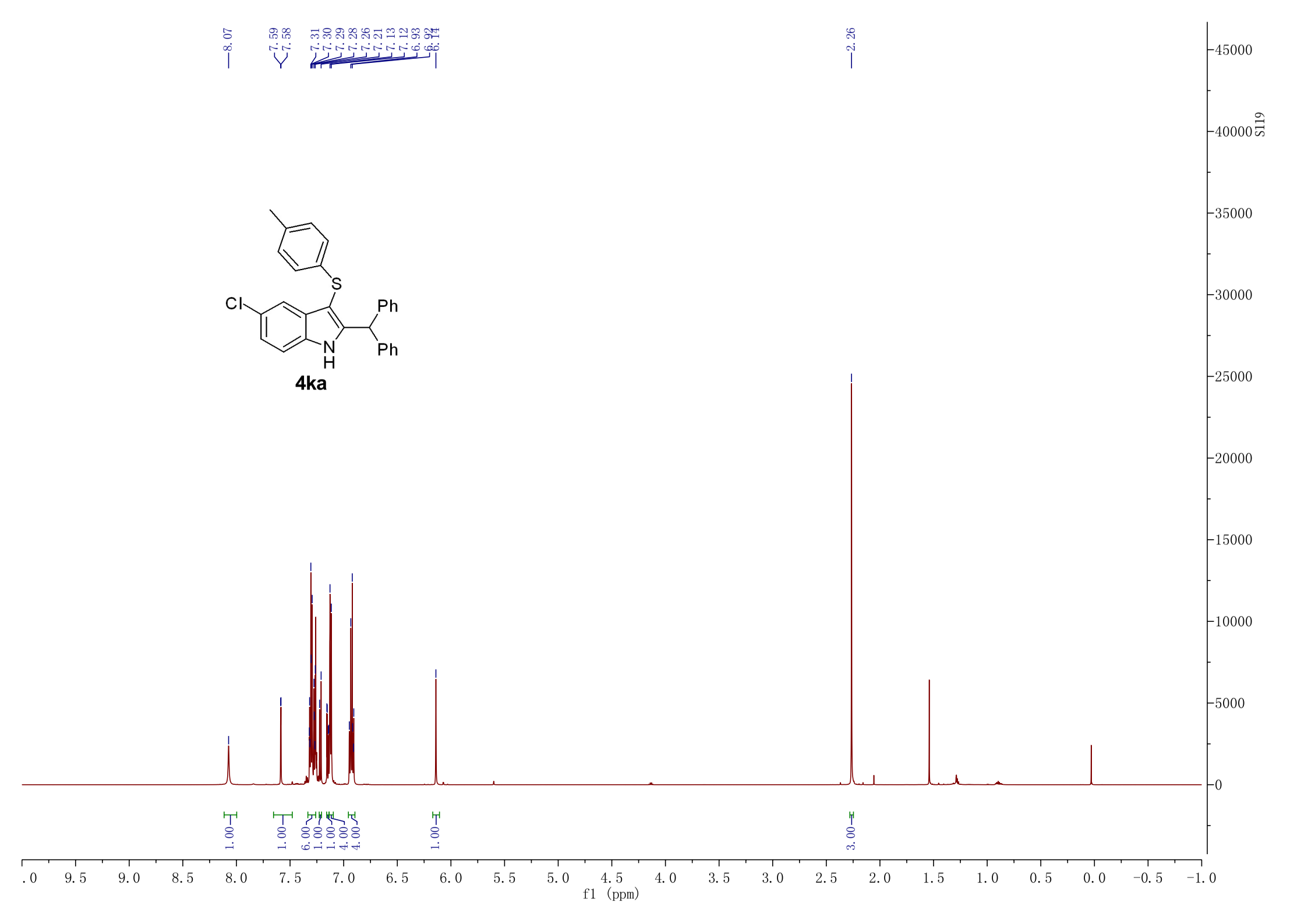

162.67
161.04
144.32
137.13
135.69
134.76
134.72
130.41
130.35
129.46
126.40
122.89
121.14
119.70
115.77
101.67
46.78
20.88
F
S
N
H
F
4ea
S114
f1 (ppm)

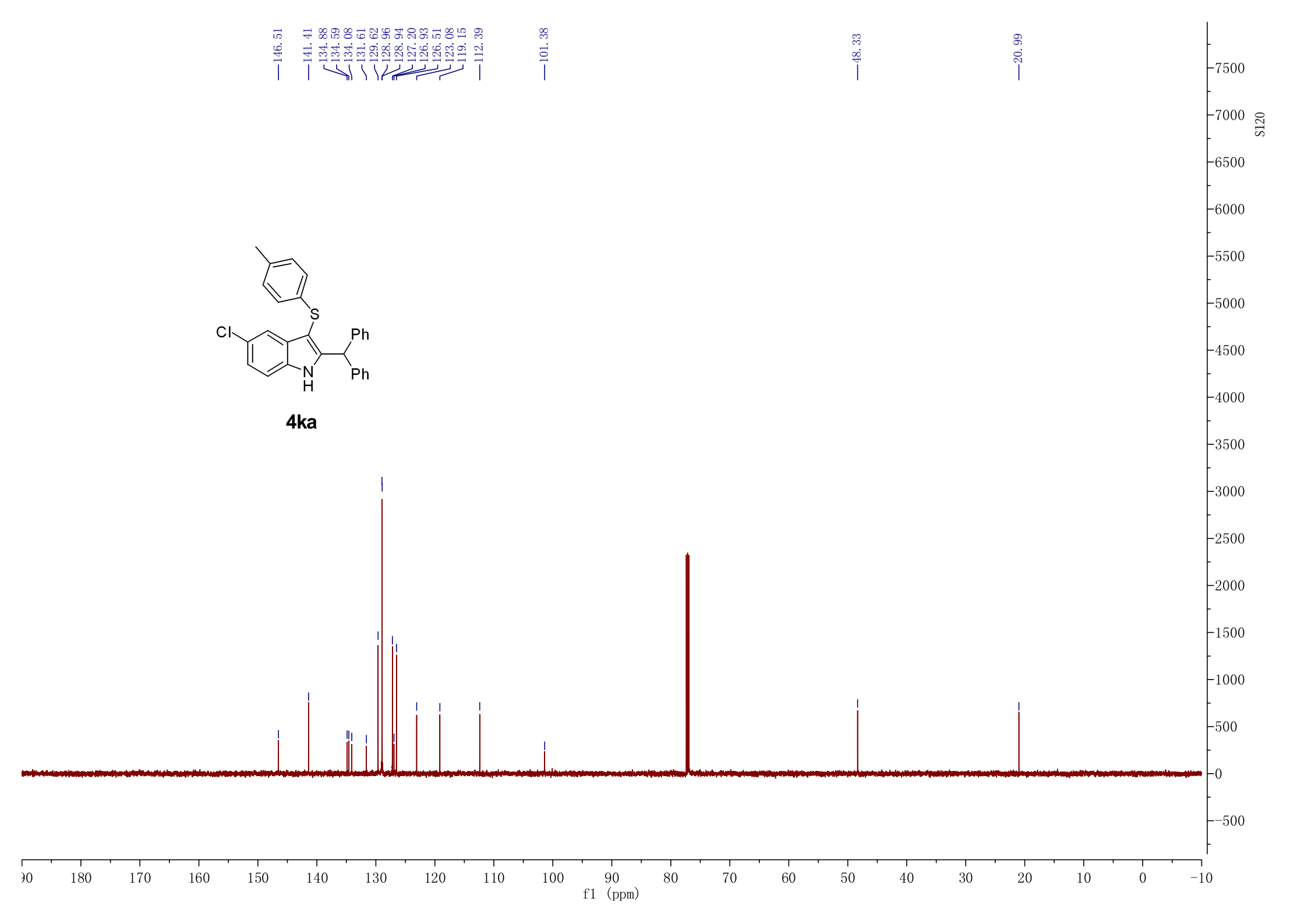

7.96
7.65
7.63
7.33
7.26
7.25
7.24
7.23
7.17
7.03
7.02
6.90
6.89
6.87
6.10
2.26
Cl
S
N
H
Cl
4fa
S115
1.00
1.02
1.00
0.91
3.92
1.01
4.00
4.00
1.00
3.00
f1 (ppm)

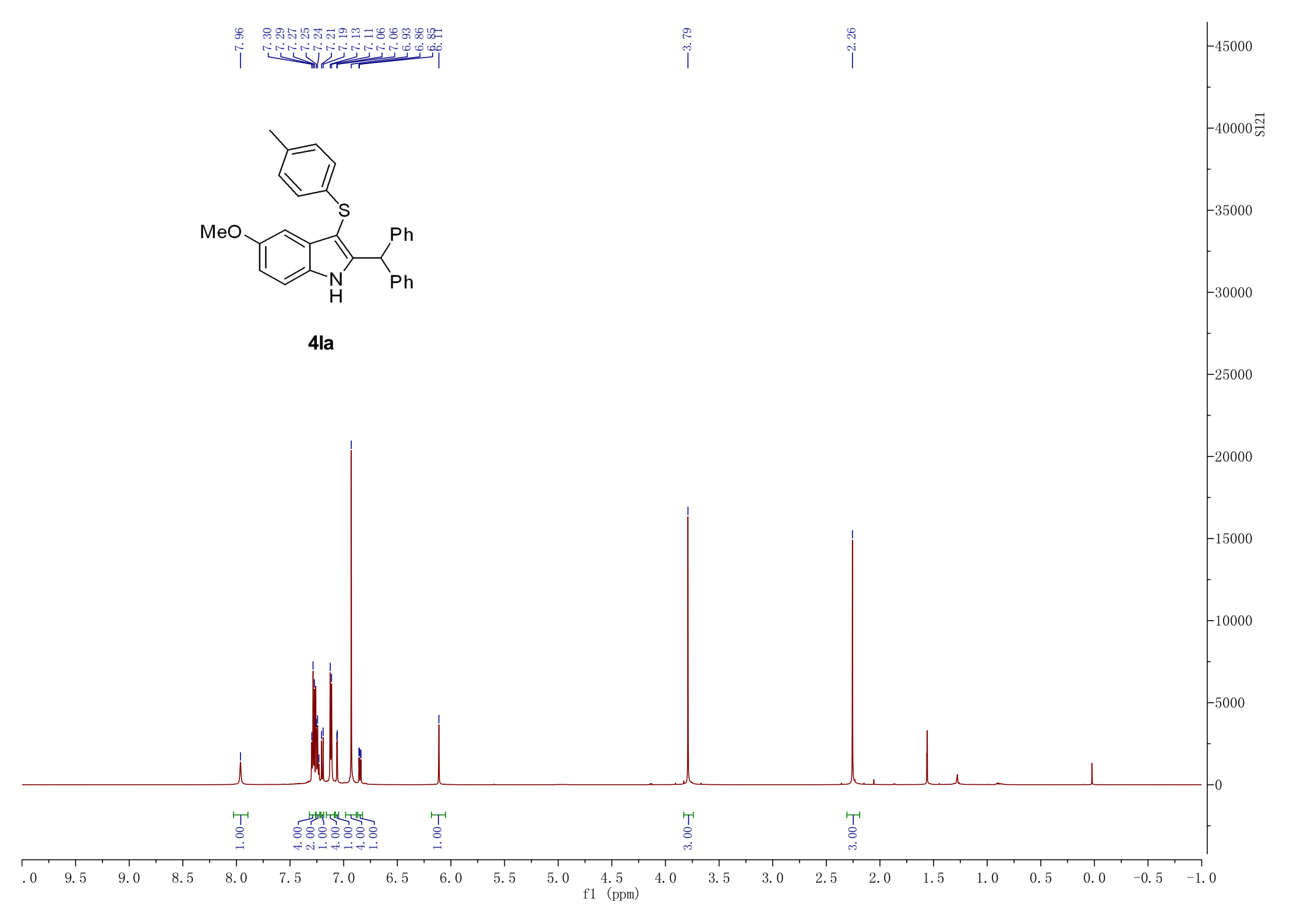

4fa
143.69
139.61
135.75
134.88
134.68
133.21
130.32
130.26
129.53
129.08
126.52
123.06
121.29
119.79
111.40
102.11
47.17
20.99
f1 (ppm)

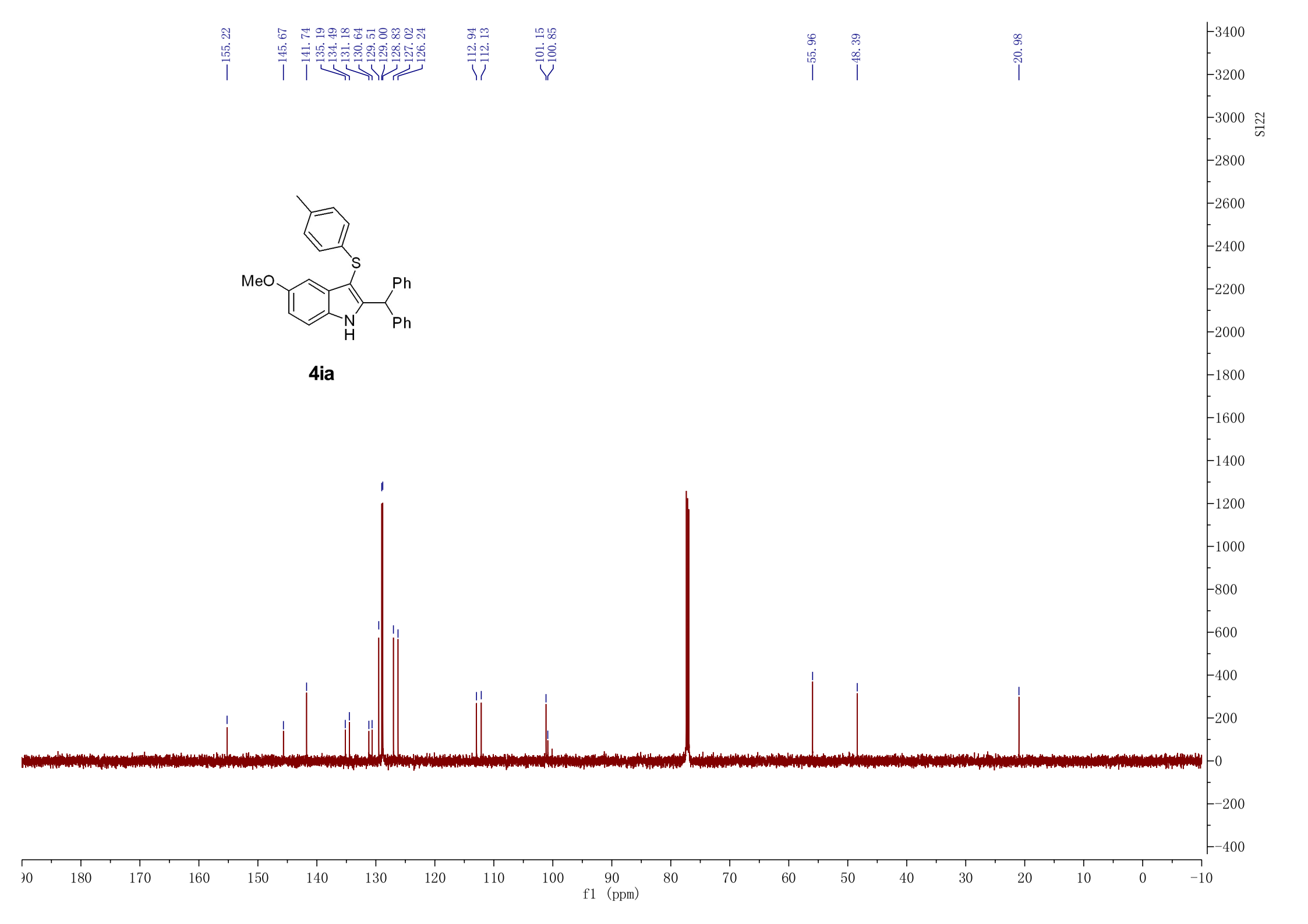

8.09
7.67
7.65
7.34
7.22
7.21
7.20
7.09
7.08
6.97
6.97
6.96
6.96
6.12
2.30
2.28
S
N
H
4ga
S117
1.00
0.99
1.00
3.02
1.00
2.00
8.00
1.00
6.00
3.00
f1 (ppm)

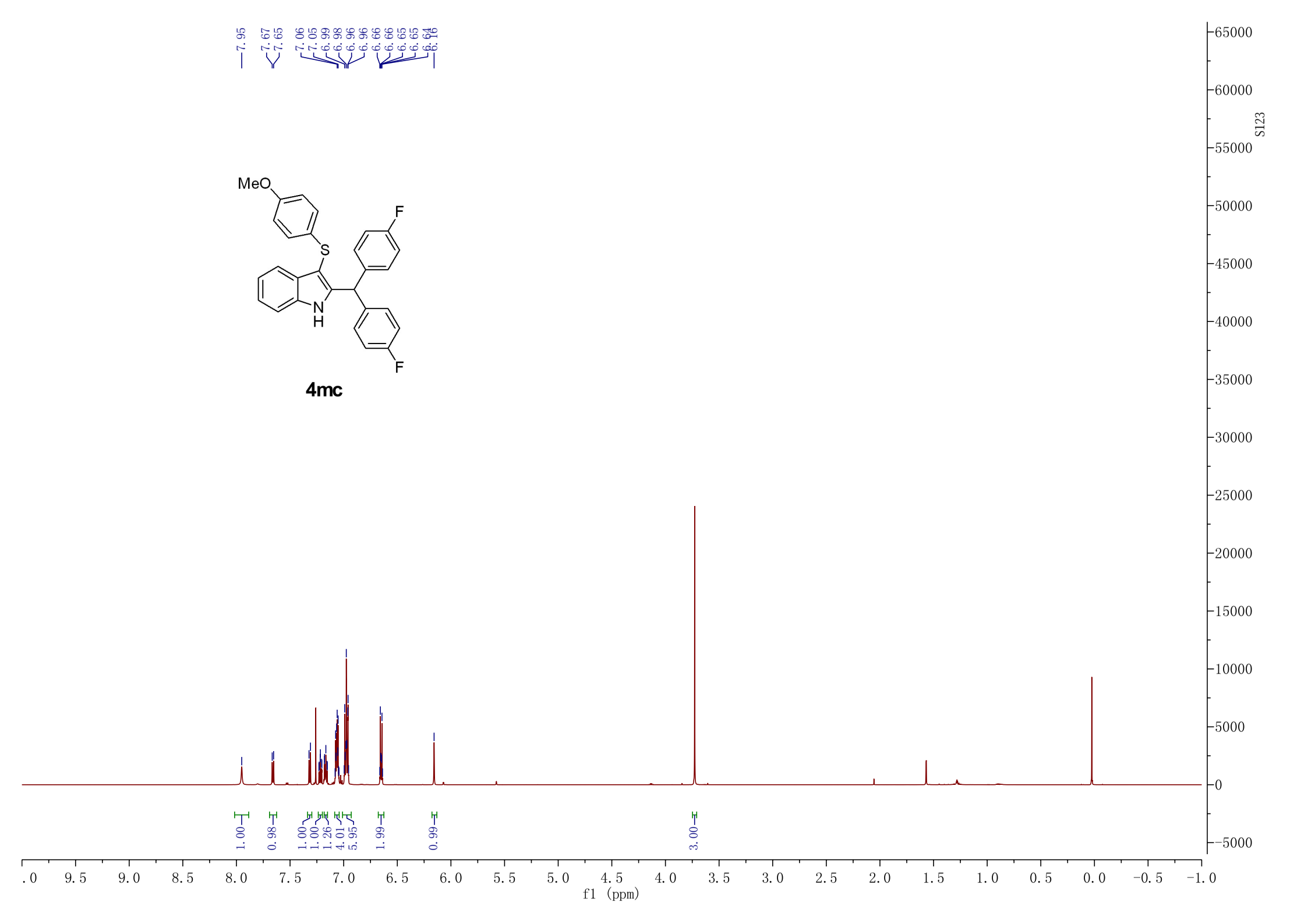

4ga
NH
S
145.24
141.72
138.46
135.75
135.26
134.50
130.38
129.79
129.44
128.65
127.76
126.53
125.99
122.57
120.91
119.67
111.31
101.19
48.21
21.57
20.97
f1 (ppm)

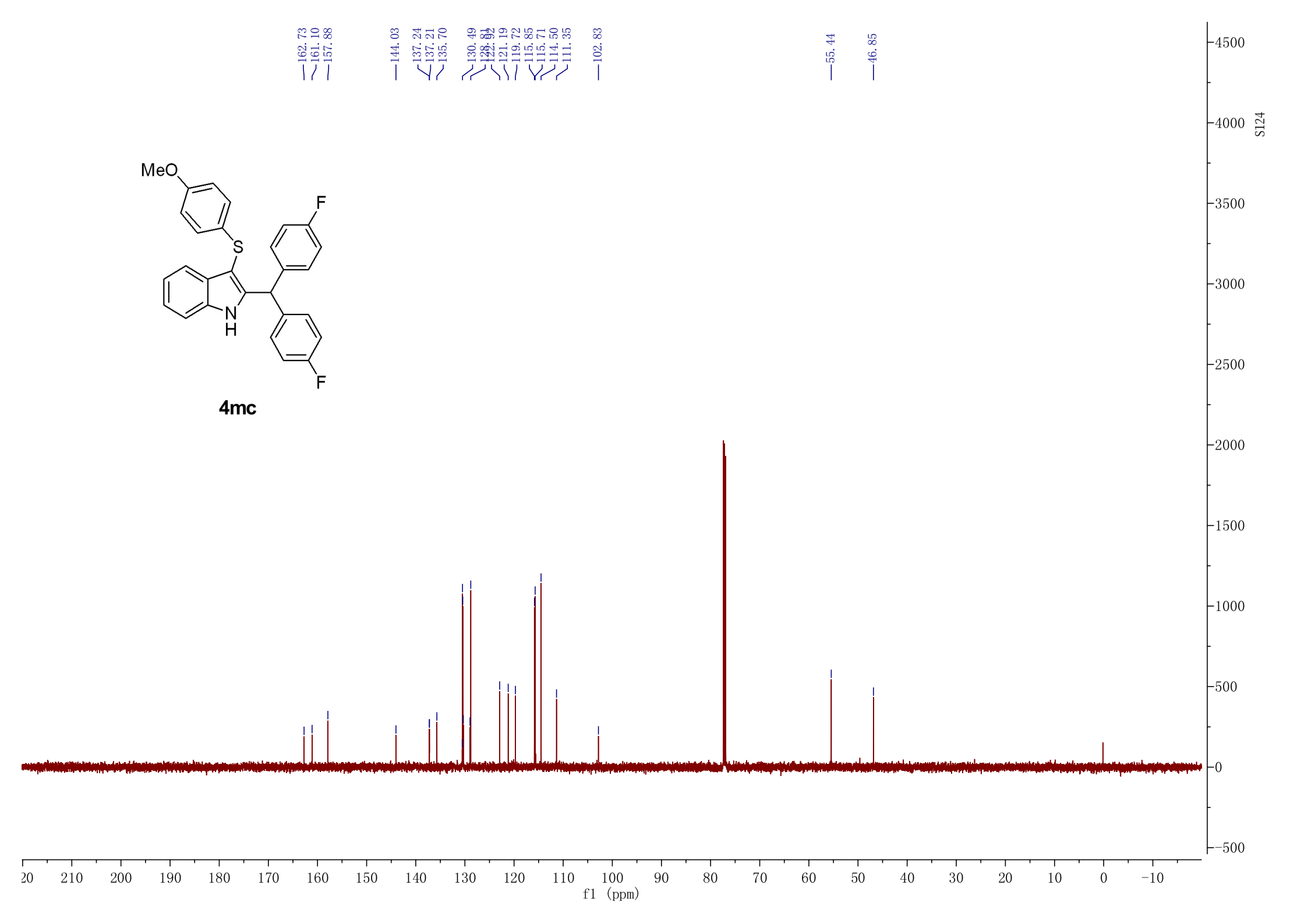

8.07
7.59
7.58
7.31
7.30
7.29
7.28
7.26
7.21
7.13
7.12
6.93
6.92
6.14
2.26
S
Cl
Ph
Ph
N
H
4ka
1.00
1.00
6.00
1.00
1.00
4.00
4.00
1.00
3.00
f1 (ppm)
S119


146.51
141.41
134.88
134.59
134.08
131.61
129.62
128.96
128.94
127.20
126.93
126.51
123.08
119.15
112.39
101.38
48.33
20.99
S
Cl
Ph
Ph
N
H
4ka
S120
f1 (ppm)


7.96
7.30
7.29
7.27
7.25
7.24
7.21
7.19
7.13
7.11
7.06
6.93
6.86
6.85
6.11
3.79
2.26
MeO
S
Ph
Ph
N
H
4la
S121
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
1.00
4.00
2.00
1.00
4.00
1.00
4.00
1.00
1.00
3.00
3.00
f1 (ppm)


155.22
145.67
141.74
135.19
134.49
131.18
130.64
129.51
129.00
128.83
127.02
126.24
112.94
112.13
101.15
100.85
55.96
48.39
20.98
MeO
S
Ph
Ph
N
H
4ia
S122
f1 (ppm)


7.95
7.67
7.65
7.06
7.05
6.99
6.98
6.96
6.96
6.66
6.66
6.65
6.65
6.64
6.16
MeO
S
N
H
F
F
4mc
S123
1.00
0.98
1.00
1.00
1.26
4.01
5.95
1.99
0.99
3.00
f1 (ppm)


162.73
161.10
157.88
144.03
137.24
137.21
135.70
130.49
128.84
128.82
122.92
121.19
119.72
115.85
115.71
114.50
111.35
102.83
55.44
46.85
MeO
S
N
H
F
F
4mc
f1 (ppm)
S124