Visible-Light-Induced Synthesis of Carbazoles by in situ Formation of Photosensitizing Intermediate

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General Considerations

General reagent information

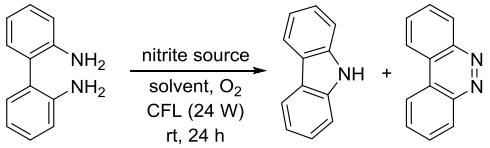
All reagents and solvents including ^{t}BuONO and 1,2-Dichloroethane (DCE) were purchased from Sigma-Aldrich, Alfa Aesar, TCI and Combi Blocks chemical companies. Flash column chromatography was performed using Merck silica gel 60 (70-230 mesh).

General analytical information

The 2,2′-diamino-1,1′-biaryls and carbazole products were characterized by ^{1}H, ^{13}C NMR, and FT-IR spectroscopy. NMR spectra were recorded on a Bruker 600 MHz instrument (600 MHz for ^{1}H NMR and 151 MHz for ^{13}C NMR). Copies of ^{1}H and ^{13}C NMR spectra can be found at the end of the Supporting Information. ^{1}H NMR experiments are reported in units, parts per million (ppm), and were measured relative to residual chloroform (7.26 ppm) or residual DMSO (2.5 ppm) in the deuterated solvent. ^{13}C NMR spectra are reported in ppm relative to deuterochloroform (77.23 ppm) or deuterated DMSO (39.5 ppm), and all were obtained with ^{1}H decoupling. Coupling constants were reported in Hz. FT-IR spectra were recorded on a Nicolet iS 10 ThermoFisher FT-IR spectrometer. Reactions were monitored by ^{1}H-NMR of the crude reaction mixture using bromoform as internal standard and products were detected by GC-MS using the Agilent GC 7890B/5977A inert MSD with Triple-Axis Detector. Mass spectral data of all unknown compounds were obtained from the Korea Basic Science Institute (Daegu) on a Jeol JMS 700 high resolution mass spectrometer. UV−Vis spectra were recorded on a Scinco S-3100 spectrophotometer equipped with a Peltier temperature controller. Melting points of unknown carbazole compounds were recorded on a Stuart SMP30 apparatus.

Optimization Table of Reaction Conditions

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



1a **2a** **S1**

entry	nitrite source (equiv.)	solvent (concentration)	variation	Yield (%)[b]	
				2a	**S1**
1	^{t}BuONO (1.5)	MeCN (0.1 M)	--	47	14
2	^{t}BuONO (1.5)	DMF (0.1 M)	--	30	7
3	^{t}BuONO (1.5)	DMSO (0.1 M)	--	--	trace
4	^{t}BuONO (1.5)	MeOH (0.1 M)	--	--	trace
5	^{t}BuONO (1.5)	TFE (0.1 M)	--	48	20
6	^{t}BuONO (1.5)	DCM (0.1 M)	--	55	8
7	^{t}BuONO (1.5)	DCE (0.1 M)	--	68	11
8	^{t}BuONO (1.5)	DCE (0.1 M)	aerobic atmosphere	38	6
9	^{t}BuONO (1.5)	DCE (0.1 M)	no O_2[c]	--	12
10	^{t}BuONO (1.5)	DCE (0.1 M)	no visible light	trace	10
11	^{t}BuONO (1.5)	DCE (0.1 M)	using UV-cut @ 400 nm	52	9
12	^{t}BuONO (1.5)	DCE (0.1 M)	blue LEDs (21 W)	50	11
13	^{t}BuONO (1.5)	DCE (0.1 M)	white LEDs (21 W)	60	9
14	^{t}BuONO (1.5)	DCE (0.1 M)	CFL (15 W)	65	12
15	^{t}BuONO (1.5)	DCE (0.1 M)	CFL (100 W)	68	10
16	isoamyl nitrite (1.5)	DCE (0.1 M)	--	60	15
17	^{t}BuONO (2)	DCE (0.1 M)	--	66	12
18	**^{t}BuONO (1.3)**	**DCE (0.1 M)**	**--**	**68**	**10**
19	^{t}BuONO (1.1)	DCE (0.1 M)	--	56	8
20	^{t}BuONO (1.3)	DCE (0.2 M)	--	59	9
21	^{t}BuONO (1.3)	DCE (0.5 M)	--	43	8
22	^{t}BuONO (1.3)	DCE (0.05 M)	--	51	5
23	^{t}BuONO (1.3)	DCE (0.1 M)	20 h	66	10
24	^{t}BuONO (1.3)	DCE (0.1 M)	30 h	68	11
25	^{t}BuONO (1.3)	DCE (0.1 M)	TEA (1 equiv.)	--	--
26	^{t}BuONO (1.3)	DCE (0.1 M)	$Ir(ppy)_3$ (1 mol%)	61	12
27	^{t}BuONO (1.3)	DCE (0.1 M)	$Ir(dFppy)_3$ (1 mol%)	65	9
28	^{t}BuONO (1.3)	DCE (0.1 M)	$Ru(bpy)_3$ (1 mol%)	62	10
29	^{t}BuONO (1.3)	DCE (0.1 M)	Eosin Y (1 mol%)	60	15

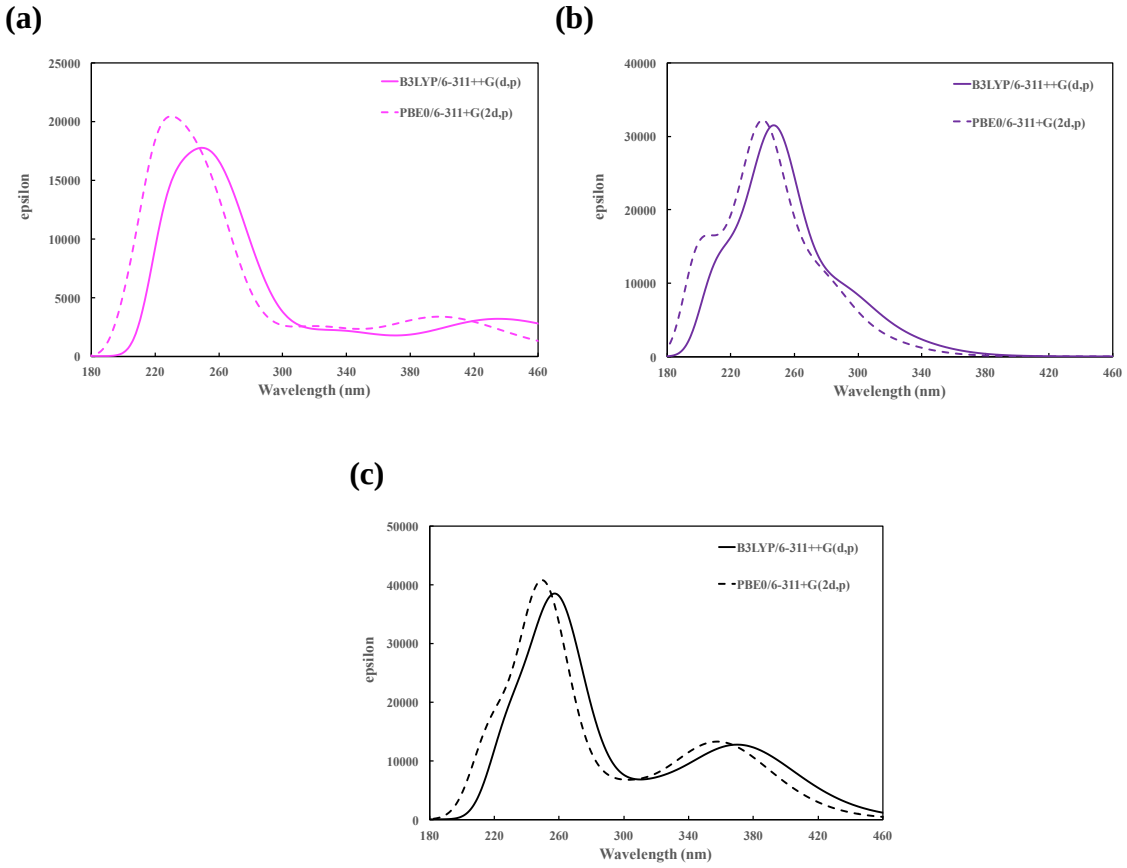
[a]Reaction scale: 0.1 mmol; [b]Yields were determined by ^{1}H NMR of crude reaction mixture using bromoform as the internal standard; [c]Molecular oxygen was effectively removed from the reaction mixture by repeated vacuum-freeze-thaw cycles.

Density Functional Theory (DFT) Calculation Details

All the molecules at ground state are optimized using hybrid B3LYP (Becke, three-parameter, Lee-Yang-Parr) exchange-correlation density functional theory and 6-311++G(d,p) basis. All calculations were performed using GAUSSIAN09 software, and the solvent effect was considered by the polarizable continuum model (IEF-PCM) implemented in GAUSSIAN09 package (with dichloromethane as a solvent). The absence of vibrational normal modes with imaginary frequencies was checked to verify the quality of minimization procedure. With this optimized

geometry at the ground state, a calculation using the time-dependent density functional theory (TD-DFT) with B3LYP functional was performed for the excitation energies (the number of calculated excited states set to 20) with the same level of basis set, 6-311++G(d,p), with IEF-PCM. To verify that our calculations are reasonable without any model dependence, we compare the TD-DFT results obtained from two different funcitonals, B3LYP/6-311++G(d,p) and PBE0/6-311+G(2d,p). These two functionals were known to provide reasonable spectroscopy data for organic dyes. In the figure below (Figure *S1*), we show the comparison for intermediates **I**, **II** and **III**. The agreement between them is fairly good and, therefore, we present only the results from the B3LYP functional in the main text and below in Figures *S2–S4*.

Comparison of TD-DFT results from different functionals, B3LYP and PBE0



Figures *S1*. Comparison of TD-DFT results from different functionals, B3LYP/6-311++G(d,p) and PBE0/6-311+G(2d,p) where (a), (b) and (c) represents Intermediate-**I,** Intermediate-**II** and Intermediate-**III** respectively. Results from the B3LYP and PBE0 functionals are shown in solid and dashed line respectively.

Table *S2*. Selected TD-DFT [B3LYP/6-311++G(d,p)] calculated wavelength, oscillator strength and compositions of major electronic transitions of Intermediate-**I**.

Wavelength	Osc. Strength (*f*)	Major Contributions	
437.82	0.0760	H-1 → L (99%)	
340.00	0.0430	H → L+2 (98%)	
273.89	0.0469	H → L+3 (61%)	H-4 → L (23%)
272.13	0.0619	H-4 → L (58%)	H-3 → L (32%)
267.94	0.0985	H-3 → L (30%)	H → L+3 (28%)
255.14	0.0416	H → L+4 (77%)	H-3 → L (9%)
249.15	0.2385	H-1 → L+2 (74%)	
228.25	0.2609	H → L+5 (49%)	H → L+6 (27%)

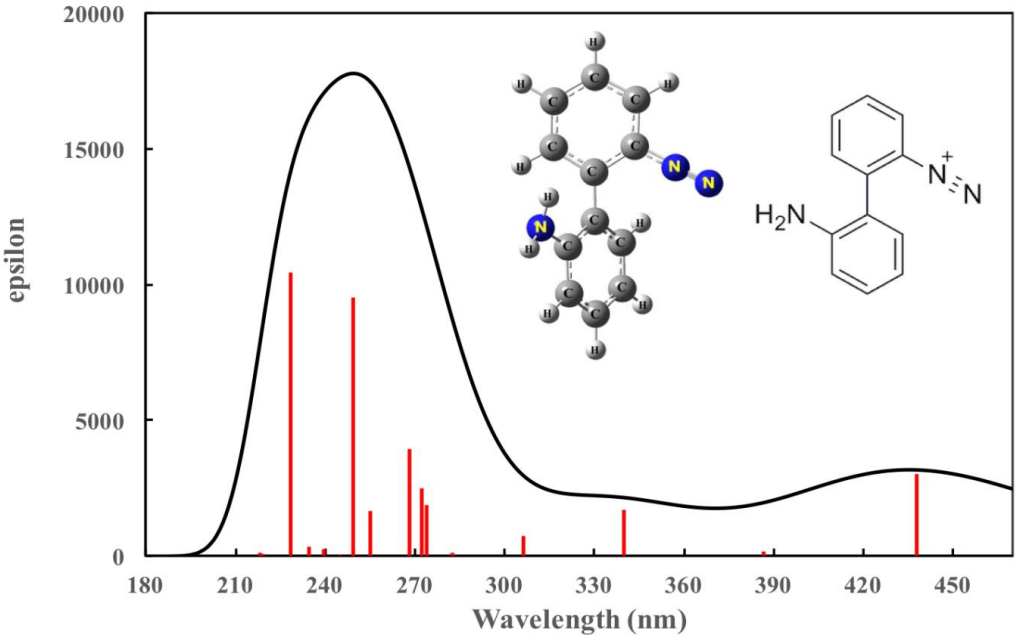


Figure *S2*. Calculated [B3LYP/6-311++G(d,p)] absorption spectrum and structure of Intermediate-**I**

Table *S3*. Selected TD-DFT [B3LYP/6-311++G(d,p)] calculated wavelength, oscillator strength and compositions of major electronic transitions of Intermediate-**II**.

Wavelength	Osc. Strength (*f*)	Major Contributions	
328.81	0.0421	H-1 → L (73%)	H-2 → L (10%)
289.97	0.1929	H → L+1 (50%)	H-2 → L (34%)
251.36	0.1747	H → L+2 (30%)	H-3 → L (30%)
250.55	0.4347	H-1 → L+1 (39%)	H → L+2 (26%)
233.92	0.1089	H-4 → L (33%)	H-2 → L+1 (32%)
228.54	0.0967	H-1 → L+2 (50%)	H-5 → L (13%)
211.33	0.1063	H-1 → L+3 (41%)	H-5 → L (14%)
207.95	0.1022	H-2 → L+2 (19%)	H-3 → L+1 (19%)
		H-1 → L+3 (17%)	

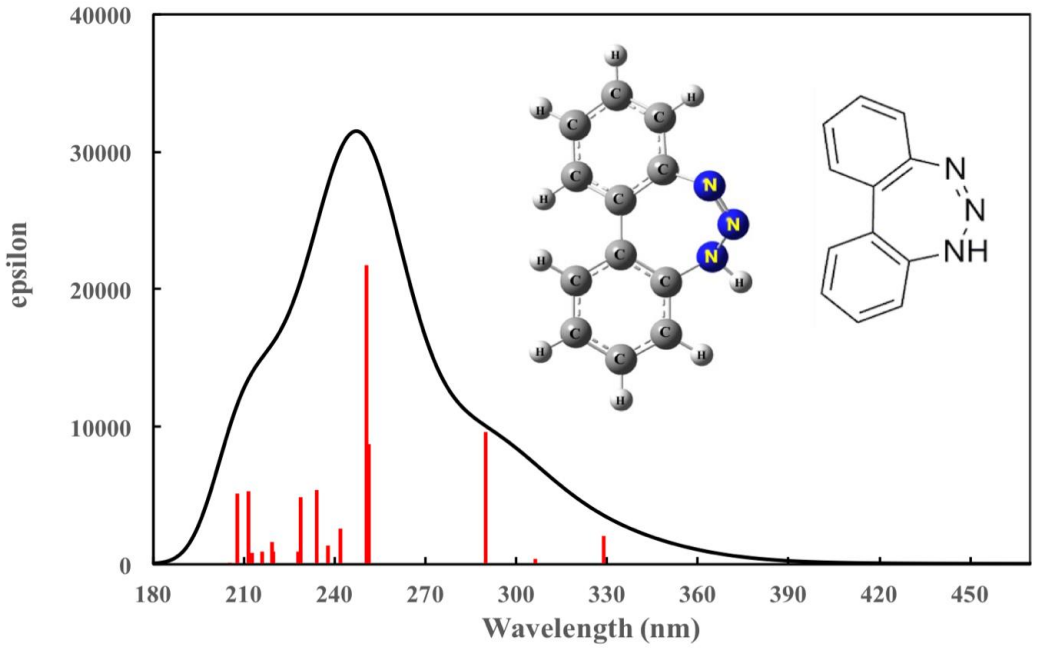


Figure *S3*. Calculated [B3LYP/6-311++G(d,p)] absorption spectrum and structure of Intermediate-**II**.

Table *S4*. Selected TD-DFT [B3LYP/6-311++G(d,p)] calculated wavelength, oscillator strength and compositions of major electronic transitions of Intermediate-**III**.

Wavelength	Osc. Strength (*f*)	Major Contributions	
376.03	0.2562	H → L (93%)	
316.30	0.1183	H-1 → L (83%)	H → L+1 (12%)
266.98	0.1488	H-2 → L (62%)	H → L+2 (31%)
258.45	0.7252	H-1 → L+1 (79%)	
238.47	0.1155	H → L+4 (70%)	H-2 → L+1 (20%)
230.69	0.2258	H-1 → L+2 (53%)	H-4 → L (35%)

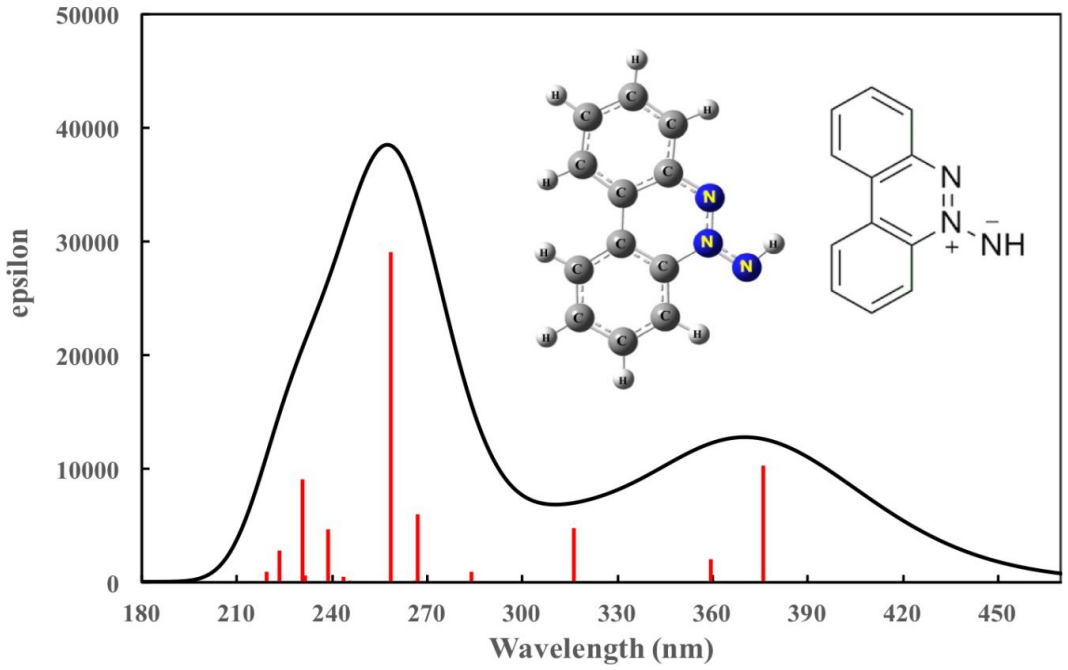


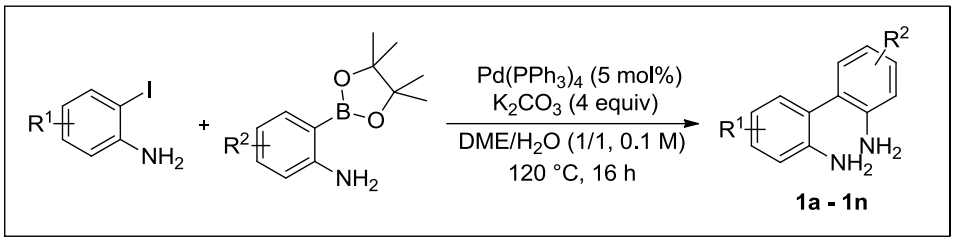
Figure *S4*. Calculated [B3LYP/6-311++G(d,p)] absorption spectrum and structure of Intermediate-**III**.

Experimental Details

1. Preparation of 2,2′-Diaminobiaryls, 1a–1n

For the synthesis of **1a-1n**, we followed a slightly modified synthetic procedure that was reported by the Ritter group for the synthesis of 2-(2-pyridinyl)aniline.[1]

Representative procedure; Synthesis of 2,2′-Diaminobiphenyl **1a**

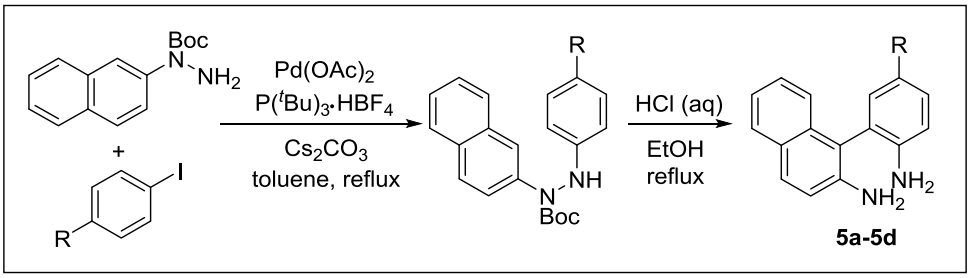


An oven-dried 250 mL round bottom flask equipped with a magnetic stir bar was charged with 2-iodoaniline (5 mmol, 1.10 g) and 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (5 mmol, 1.09 g) in ethylene glycol dimethyl ether (25 mL) mixed with distilled water (25 mL). 5 mol% $Pd(PPh_3)_4$ (0.25 mmol, 0.29 g) and K_2CO_3 (20 mmol, 2.76 g) were added to it. The round bottom flask connected with a reflux column was placed in the oil bath and heated for 16 h at 120 °C. The progress of the reaction was monitored by TLC and gas chromatography. The flask was cooled to room temperature, the reaction mixture was diluted with dichloromethane, and the aqueous phase was extracted with dichloromethane. The combined organic layers were dried over anhydrous $MgSO_4$, and concentrated *in vacuo*. The residue was purified by silica gel flash column chromatography using dichloromethane as the eluent to give the desired product **1a** (0.69 g, 75%).

Other substrates **1b–1n** were synthesized similarly to the synthesis of **1a** by Suzuki-Miyaura coupling process using the corresponding substituted 2-haloanilines and 2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline.

2. Preparation of 2,2′-Diaminobiaryl[2] 5a–5d

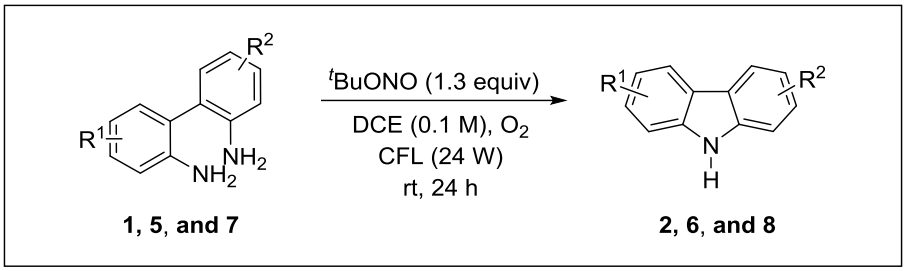
Representative procedure; Synthesis of 1-(2-Aminophenyl)naphthalen-2-amine **5a**



To an oven-dried two neck 100 mL round bottom flask equipped with a magnetic stir bar and a reflux condenser were charged *tert*-butyl 1-(naphthalen-2-yl)hydrazine-1-carboxylate (3.87 mmol, 1.00 g), iodobenzene (3.2 mmol, 0.65 g), 5 mol% $Pd(OAc)_2$ (0.19 mmol, 0.04 g), 5 mol% $P(^tBu)_3{\cdot}HBF_4$ (0.19 mmol, 0.06 g), Cs_2CO_3 (4.64 mmol, 1.51 g) and 30 mL of anhydrous toluene at rt. The resulting mixture was flushed with Ar several times and heated under reflux for 1.5 h. The progress of the reaction was monitored by TLC. The reaction mixture was cooled to room temperature and partitioned into dichloromethane and water. The combined organic layers were dried over anhydrous $MgSO_4$, and concentrated *in vacuo*. The residue was purified by silica gel flash column chromatography (hexane/EtOAc = 30/1) to give *tert*-butyl 1-(naphthalen-2-yl)-2-phenylhydrazine-1-carboxylate (2.18 mmol, 0.73 g) in 68% yield. To a flask charged with the resulting hydrazide product were added 30 mL of ethanol and a few drops of conc. HCl (35%) at rt. The reaction mixture was then heated under reflux for 1 h. The progress of the reaction was monitored by TLC. The reaction mixture was cooled to rt and neutralized by adding $NaHCO_3$(*s*). The mixture was then filtered, concentrated and purified by silica-gel chromatography (2/1 hexane/CH_2Cl_2 → 9/1 EtOAc/MeOH) to afford 1-(2-aminophenyl)naphthalen-2-amine **5a** (1.68 mmol, 0.39 g) in 77% yield.

3. Synthesis of Carbazole Compounds 2a–2n, 6a–6d, and 8

3.1. Representative procedure; Synthesis of *N*–H carbazole 2a

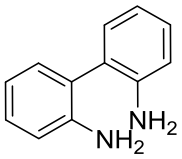


A resealable tube equipped with a magnetic stir bar was charged with [1,1′-biphenyl]-2,2′-diamine **1a** (0.3 mmol, 55 mg), in 1,2-dichloroethane (DCE) (3 mL, 0.1 M). Then ^{t}BuONO [0.4 mmol, 52 μL; considering the purity of ^{t}BuONO (90% purity)] was added to the solution and stirred for 10 min. Oxygen gas was then bubbled through the reaction mixture for 10 minutes and the tube was sealed with a silicone septum screw cap. The tube was then placed under oxygen atmosphere (molecular oxygen balloon) and visible-light irradiation of CFL (24 W) at room temperature. After 24 h, the solvent was evaporated and the reaction mixture was purified by flash column chromatography to furnish the pure *N*–H carbazole product **2a** (34 mg, 68%).

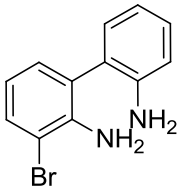
3.2. Representative procedure in 1 mmol scale; Synthesis of 3-methyl-9*H*-carbazole 2j

A resealable tube equipped with a magnetic stir bar was charged with 5-methyl-2,2′-diaminebiphenyl **1j** (1 mmol, 198 mg), in 1,2-dichloroethane (DCE) (10 mL, 0.1 M). Then ^{t}BuONO [1.4 mmol, 172 μL; considering the purity of ^{t}BuONO (90% purity)] was added to the solution and stirred for 15 min. Oxygen gas was then bubbled through the reaction mixture for 15 minutes and the tube was sealed with a silicone septum screw cap. The tube was then placed under oxygen atmosphere (molecular oxygen balloon) and visible-light irradiation of CFL (24 W) at room temperature. After 24 h, the solvent was evaporated and the reaction mixture was purified by flash column chromatography to furnish the pure 3-methyl-9*H*-carbazole **2j** (99 mg, 55%).

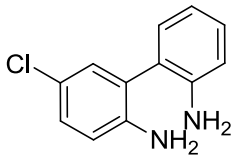
Analytic data for 2,2′-Diaminobiaryl Compounds



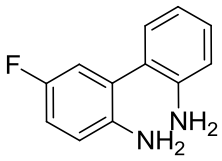
1a (2,2′-Diaminebiphenyl; CAS 1454-80-4)[3]: brown solid (0.69 g, 75%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.20 (ddd, *J* = 8.4, 7.0, 1.8 Hz, 2H), 7.11 (dd, *J* = 7.8, 1.8 Hz, 2H), 6.82 (ddd, *J* = 7.8, 7.0, 1.2 Hz, 2H), 6.76 (dd, *J* = 8.4, 1.2 Hz, 2H), 3.69 (s, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.1, 131.0, 128.8, 124.6, 118.8, 115.6; **IR (neat)**: ν_{max} = 3436, 3348, 3020, 1609, 1482, 1442, 1295, 745 cm^{-1}; ***R*$_f$** 0.40 (dichloromethane).



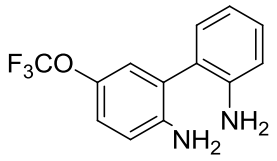
1b (3-Bromo-2,2′-diaminebiphenyl, CAS 306292-43-3)[4]: off-white solid (0.50 g, 38%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.37 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.10 (ddd, *J* = 8.4, 7.8, 1.8 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.96 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.74 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 6.63 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.59 (dd, *J* = 8.4, 7.8 Hz, 1H), 4.08 (bs, 2H), 3.54 (bs, 2H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.0, 142.0, 132.0, 130.8, 130.1, 129.2, 125.5, 123.8, 119.0, 118.7, 115.6, 109.7 ; **IR (neat)**: ν_{max} = 3459, 3368, 3023, 1738, 1610, 1443, 904, 725 cm^{-1}; ***R*$_f$** 0.65 (dichloromethane).



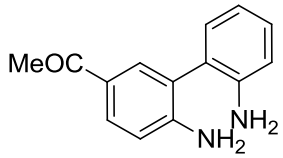
1c (5-Chloro-2,2′-diaminebiphenyl): pale red solid (0.60 g, 55%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.20 (dd, *J* = 7.8, 6.8, 1.8 Hz, 1H), 7.14 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.09 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.83 (ddd, *J* = 7.8, 6.8, 1.2 Hz, 1H), 6.78 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 1H), 3.68 (bs, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.1, 143.0, 131.1, 130.8, 129.4, 128.8, 126.2, 123.4, 123.3, 119.1, 116.8, 115.9; **IR (neat)**: ν_{max} = 3441, 3359, 1613, 1485, 1295, 907, 730 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{12}H_{11}ClN_2$ [M^+] 218.0605, found 218.1; ***R*$_f$** 0.50 (dichloromethane).



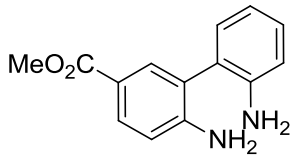
1d (5-Fluoro-2,2′-diaminebiphenyl): brown solid (0.82 g, 80%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.20 (dd, *J* = 8.4, 7.8 1.8 Hz, 1H), 7.10 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.92 – 6.85 (m, 2H), 6.84 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 6.79 (dd, *J* = 8.4, 0.6 Hz, 1H), 6.72 (dd, *J* = 9.0, 4.8 Hz, 1H), 3.73 (bs, 2H), 3.60 (bs, 2H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 156.4 (d, *J* = 237.1 Hz), 144.2, 140.4, 131.1, 129.4, 126.0 (d, *J* = 7.6 Hz), 123.8, 119.1, 117.5 (d, *J* = 22.7 Hz), 116.7 (d, *J* = 9.1 Hz), 116.0, 115.5 (d, *J* = 22.2 Hz); **IR (neat)**: ν_{max} = 3353, 1739, 1490, 1365, 751 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{12}H_{11}FN_2$ [M^+] 202.0906, found 202.1; ***R*$_f$** 0.33 (dichloromethane).



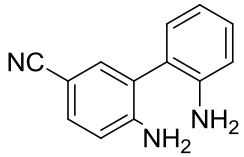
1e (5-Trifluoromethoxy-2,2′-diaminebiphenyl): brown solid (0.81 g, 60%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.15 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 7.01 (d, *J* = 9.0 Hz, 1H), 6.99 (s, 1H), 6.79 (dd, *J* = 7.8, 6.6 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.65 (d, *J* = 9.0 Hz, 1H), 3.68 (bs, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.1, 143.2, 141.2, 131.0, 129.4, 125.4, 124.0, 123.3, 121.9, 120.8 (q, *J* = 255.8 Hz), 119.0, 116.1, 115.9; **IR (neat)**: ν_{max} = 1636, 1457, 1279, 1151, 817, 750 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{13}H_{11}F_3N_2O$ [M^+] 268.0818, found 268.1; $\boldsymbol{R_f}$ 0.82 (dichloromethane).



1f (1-(2′,6-Diamino-[1,1′-biphenyl]-3-yl)ethan-1-one): brown solid (0.91 g, 80%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.77 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.74 (d, *J* = 2.0 Hz, 1H), 7.18 (ddd, *J* = 7.8, 7.8, 1.2 Hz, 1H), 7.08 (dd, *J* = 7.2, 1.2 Hz, 1H), 6.82 (ddd, *J* = 7.8, 7.2, 1.8 Hz, 1H), 6.77 (d, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 8.4 Hz, 1H), 4.29 (bs, 2H), 3.68 (bs, 2H), 2.48 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 196.6, 149.2, 144.2, 132.6, 131.1, 130.0, 129.4, 127.9, 123.2, 119.0, 115.8, 114.5 (overlapped peaks are present), 26.2; **IR (neat)**: ν_{max} = 3353, 1659, 1612, 1293, 1231, 904, 723 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{14}H_{14}N_2O_2$ [M^+] 226.1101, found 226.1; $\boldsymbol{R_f}$ 0.23 (dichloromethane).

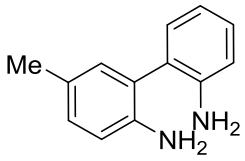


1g (Methyl 2′,6-diamino-[1,1′-biphenyl]-3-carboxylate): brown solid (0.95 g, 78%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.85 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.82 (d, *J* = 1.8 Hz, 1H), 7.18 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.82 (dd, *J* = 7.8, 7.8 Hz, 1H), 6.76 (d, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 8.4 Hz, 1H), 4.19 (bs, 2H), 3.83 (s, 3H), 3.66 (bs, 2H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 167.3, 148.9, 144.2, 133.2, 131.1, 130.9, 129.3, 123.4, 123.3, 119.8, 118.9, 115.8, 114.5, 51.7; **IR (neat)**: ν_{max} = 3366, 1698, 1615, 1307, 1235, 904, 723 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{14}H_{14}N_2O_2$ [M^+] 242.1050, found 242.1; $\boldsymbol{R_f}$ 0.33 (dichloromethane).

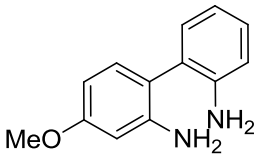


1h (2′,6-Diamino-[1,1′-biphenyl]-3-carbonitrile): gray solid (0.73 g, 69%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.44 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.41 (d, *J* = 1.8 Hz, 1H), 7.22 (ddd, *J* = 8.4, 7.6, 1.2 Hz, 1H), 7.06 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.85 (ddd, *J* = 7.8, 7.6, 1.2 Hz, 1H), 6.80 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.76 (d, *J* = 7.6 Hz, 1H), 4.22 (bs, 2H), 3.64 (bs, 2H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 148.5,

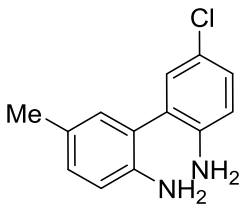
144.1, 135.5, 133.2, 131.1, 130.0, 124.6, 122.0, 120.1, 119.4, 116.1, 115.2, 100.9; **IR (neat)**: ν_{max} = 3362, 2215, 1616, 1490, 669 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{13}H_{11}N_3$ [M^+] 209.0953, found 209.1; $\boldsymbol{R_f}$ 0.30 (dichloromethane).



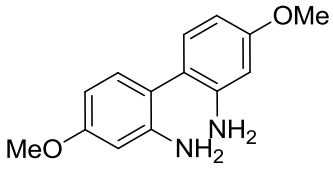
1j (5-Methyl-2,2′-diaminebiphenyl): brown solid (0.40 g, 40%) **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.18 (dd, *J* = 7.8, 7.8 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.96 (s, 1H), 6.84 (dd, *J* = 7.8, 7.8 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 7.8 Hz, 1H), 3.66 (bs, 4H), 2.28 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.3, 141.7, 131.7, 131.2, 129.5, 128.9, 128.2, 125.0, 124.9, 118.9, 115.9, 115.7, 20.6; **IR (neat)**: ν_{max} = 3434, 3349, 1613, 1491, 1297, 751 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{13}H_{14}N_2$ [M^+] 198.1157, found 198.1; $\boldsymbol{R_f}$ 0.40 (dichloromethane).



1k (4-Methoxy-2,2′-diaminebiphenyl, CAS 54147-86-3)[5]: brown solid (0.27 g, 25%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.17 (ddd, *J* = 8.2, 7.8, 1.8 Hz, 1H), 7.11 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.82 (ddd, *J* = 7.8, 7.8, 1.2 Hz, 1H), 6.78 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.42 (dd, *J* = 8.0, 2.4 Hz, 1H), 6.35 (d, *J* = 2.4 Hz, 1H), 3.81 (s, 3H), 3.72 (bs, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 160.5, 145.5, 144.6, 132.0, 131.6, 128.8, 124.5, 118.9, 117.6, 115.6, 104.6, 101.2, 55.4; **IR (neat)**: ν_{max} = 3445, 3358, 1610, 1487, 1296, 1205, 752 cm^{-1}; $\boldsymbol{R_f}$ 0.35 (dichloromethane).

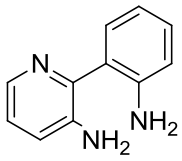


1l (5-Chloro-5′-methoxy-2,2′-diaminebiphenyl): gray solid (0.43 g, 37%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.13 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 7.01 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.91 (d, *J* = 1.8 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.69 (d, *J* = 8.4 Hz, 1H), 3.66 (bs, 4H), 2.28 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 143.0, 141.5, 131.4, 130.7, 130.0, 128.6, 128.4, 126.5, 123.6, 123.2, 116.8, 116.1, 20.6; **IR (neat)**: ν_{max} = 3435, 3352, 1616, 1487, 1285, 813 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{13}H1_3ClN_2$ [M^+] 232.0762, found 232.1; $\boldsymbol{R_f}$ 0.55 (dichloromethane).

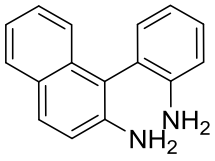


1m (4,4′-Dimethoxy-2,2′-diaminebiphenyl): brown solid (0.43 g, 35%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.01 (d, *J* = 8.0 Hz, 2H), 6.41 (dd, *J* = 8.0, 2.6 Hz, 2H), 6.33 (d, *J* = 2.6 Hz, 2H), 3.80 (s, 6H), 3.75 (bs, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 160.2, 145.7,

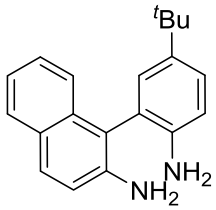
132.2, 117.2, 104.3, 101.0, 55.2; **IR (neat)**: ν_{max} = 3367, 1614, 1497, 1205, 904, 723 cm^{-1}; **MS** *m/z* (EI) calc. for $C_{14}H_{16}N_2O_2$ [M^+] 244.1212, found 244.1; $\boldsymbol{R_f}$ 0.30 (dichloromethane).



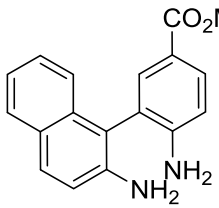
1n (2-(2-Aminophenyl)pyridin-3-amine, CAS 144190-32-9)[6]: brown oil (0.50 g, 54%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.07 (dd, *J* = 4.2, 1.8 Hz, 1H), 7.29 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.15 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 7.04 – 7.00 (m, 2H), 6.80 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 6.76 (dd, *J* = 8.4, 1.2 Hz, 1H), 3.89 (bs, 4H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.9, 143.7, 140.8, 139.6, 129.9, 129.6, 123.2, 123.15, 123.12, 118.6, 116.9; **IR (neat)**: ν_{max} = 3324, 3191, 1611, 1441, 1302, 905, 724 cm^{-1}; $\boldsymbol{R_f}$ 0.13 (dichloromethane).



5a (1-(2-Aminophenyl)naphthalen-2-amine, CAS 93013-27-5)[7]: gray solid (0.39 g, 77%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.72 – 7.67 (m, 2H), 7.27 – 7.19 (m, 4H), 7.10 (dd, *J* = 1.6, 1.2 Hz, 1H), 7.03 (d, *J* = 8.8 Hz, 1H), 6.90 - 6.84 (m, 2H), 3.64 (bs, 4H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 144.8, 141.7, 133.3, 131.7, 130.7, 129.0, 128.9, 128.0, 127.9, 126.5, 123.8, 122.2, 121.2, 118.9, 118.1, 115.6, 115.3; **IR ($CHCl_3$)**: ν_{max} = 3381, 3052, 1620, 1497, 1392, 1291, 1150 cm^{-1}; $\boldsymbol{R_f}$ 0.31 (dichloromethane).

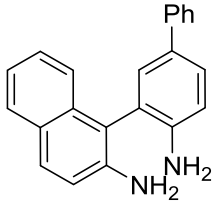


5b (1-(2-Amino-5-(tert-butyl)phenyl)naphthalen-2-amine, CAS 756822-75-0)[7]: gray solid (0.51 g, 80%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.71 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.30 – 7.19 (m, 4H), 6.81 (d, *J* = 8.4 Hz, 1H), 3.62 (bs, 4H); **^{13}C NMR (100 MHz, $CDCl_3$)** δ 142.1, 141.8, 141.7, 133.4, 128.9, 128.5, 128.0, 127.9, 126.4, 125.7, 124.0, 122.1, 120.9, 118.1, 116.0, 115.4, 34.2, 31.7; **IR ($CHCl_3$)**: ν_{max} = 3489, 3369, 3203, 3052, 2961, 2868, 1620, 1501, 1285, 1258, 1210 cm^{-1}.



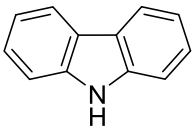
5c (Methyl 4-amino-3-(2-aminonaphthalen-1-yl)benzoate, CAS 756822-77-2)[7]: off-white solid (0.50 g, 79%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.94 (dd, *J* = 2.0, 2.0 Hz, 1H), 7.84 (d, *J* = 2.0 Hz, 1H), 7.73 – 7.70 (m, 2H), 7.30 – 7.20 (m, 3H), 7.03 (d, *J* = 8.8 Hz, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 3.96 (bs, 2H), 3.82 (bs, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** 166.9, 149.3,

141.9, 134.0, 133.1, 131.2, 129.5, 128.00, 127.97, 126.7, 123.5, 122.3, 120.14, 120.12, 118.1, 114.4, 113.8, 51.7; **IR ($CHCl_3$)**: ν_{max} = 3472, 3368, 3213, 3054, 1703, 1617, 1304, 1254, 1147 cm^{-1}; $\boldsymbol{R_f}$ 0.21 (dichloromethane).

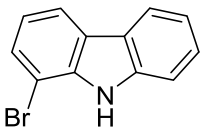


5d (1-(4-Amino-[1,1′-biphenyl]-3-yl)naphthalen-2-amine, CAS 756822-76-1)[7]: gray solid (0.47 g, 69%); **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.74 – 7.70 (m, 2H), 7.56 – 7.52 (m, 3H), 7.41 (d, *J* = 2.4 Hz, 1H), 7.37 – 7.33 (m, 3H), 7.31 – 7.26 (m, 1H), 7.25 – 7.20 (m, 2H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 3.83 (bs, 2H), 3.60 (bs, 2H); **^{13}C NMR (100 MHz, $CDCl_3$)** 114.3, 141.8, 140.6, 133.3, 131.6, 130.2, 129.1, 128.5, 128.0, 127.9, 127.5, 126.6, 126.14, 126.10, 123.8, 122.2, 121.6, 118.1, 116.0, 115.1; **IR ($CHCl_3$)** ν_{max} = 3465, 3374, 3201, 3053, 1615, 1512, 1484, 1303, 1263, 1147 cm^{-1}.

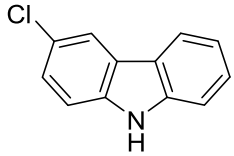
Analytic data for Carbazole Compounds



2a (*N*-H Carbazole, CAS 86-74-8)[8]: white solid (34 mg, 68%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.09 (d, *J* = 7.8 Hz, 2H), 8.04 (bs, 1H), 7.44 – 7.41 (m, 4H), 7.25 (ddd, *J* = 8.4, 6.0, 2.4 Hz, 2H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 139.7, 126.0, 123.6, 120.5, 119.7, 110.8; **IR (neat)**: ν_{max} = 3418, 1450, 1335, 748, 724 cm^{-1}; $\boldsymbol{R_f}$ 0.50 (hexane/EtOAc, 4/1).

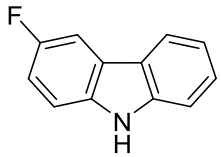


2b (1-Bromo-9*H*-carbazole, CAS 16807-11-7)[9]: off-white solid (45 mg, 61%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.25 (bs, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.47 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.28 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.13 (dd, *J* = 7.8, 7.8 Hz, 1H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 139.3, 138.3, 128.2, 126.8, 124.9, 123.9, 121.1, 120.8, 120.3, 119.6, 111.3, 104.3; **IR (neat)**: ν_{max} = 3409, 1496, 1454, 1320, 905, 749 cm^{-1}; $\boldsymbol{R_f}$ 0.60 (hexane/EtOAc, 4/1).

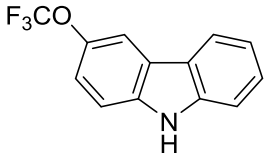


2c (3-Chloro-9*H*-carbazole, CAS 2732-25-4)[10]: off-white solid (36 mg, 60%); **^{1}H NMR (600 MHz, $CDCl_3$)** 8.04 (bs, 1H), 8.03 (s, 1H), 8.02 (d, *J* = 6.6 Hz, 1H), 7.46-7.41 (m, 2H), 7.37 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.34 (d, *J*

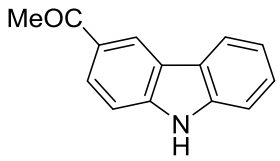
= 8.4 Hz, 1H), 7.25 (ddd, *J* = 8.4, 6.6, 1.8 Hz, 1H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 140.2, 137.9, 126.8, 126.1, 125.2, 124.8, 122.7, 120.7, 120.3, 120.0, 111.74, 111.0; **IR (neat)**: ν_{max} = 3405, 1471, 1270, 904, 726 cm^{-1}; ***R*$_f$** 0.45 (hexane/EtOAc, 4/1).



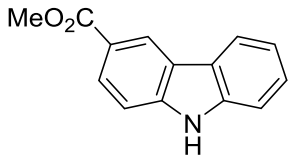
2d (3-Floro-9*H*-carbazole, CAS 391-45-7)[10]: off-white solid (31 mg, 56%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 7.8 Hz, 1H), 8.00 (bs, 1H), 7.73 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.35 (dd, *J* = 9.0, 4.2 Hz, 1H), 7.24 (ddd, *J* = 8.4, 6.0, 2.4 Hz, 1H), 7.16 (ddd, *J* = 9.0, 8.4, 2.4 Hz, 1H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 158.5, 156.9, 140.7, 136.0, 126.6, 123.7 (d, *J* = 127.6 Hz), 120.8, 119.7, 113.8 (d, *J* = 25.5 Hz), 111.3 (d, *J* = 9.06 Hz), 111.1, 106.2 (d, *J* = 23.7 Hz); **IR (neat)**: ν_{max} = 3421, 1496, 1456, 1168, 806, 746, 724 cm^{-1}; ***R*$_f$** 0.42 (hexane/EtOAc, 4/1).



2e (3-Trifluoromethyoxy-9*H*-carbazole): brown solid (52 mg, 70%); mp 158 – 159 °C **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.05 (bs, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.90 (s, 1H), 7.45 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.41 (d, *J* = 7.8 Hz, 1H), 7.36 (d, *J* = 9.0 Hz, 1H), 7.27 (dd, *J* = 9.0, 7.8 Hz, 1H), 7.25 (d, *J* = 6.6 Hz, 1H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 142.8, 140.5, 137.9, 126.9, 124.0, 123.1, 120.8, 120.6 (q, *J* = 255.8 Hz), 120.1, 119.7, 113.4, 111.2, 111.1; **IR (neat)**: ν_{max} = 3417, 1457, 1258, 1163, 903, 723 cm^{-1}; **HRMS** *m/z* (EI) calc. for $C_{13}H_8F_3NO$ [M^+] 251.0558, found 251.05568; ***R*$_f$** 0.45 (hexane/EtOAc, 4/1).

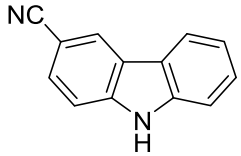


2f (1-(9*H*-Carbazol-3-yl)ethan-1-one, CAS 3215-37-0)[11]: white solid (38 mg, 60%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.74 (s, 1H), 8.36 (bs, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.48–7.47 (m, 2H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.32-7.29 (m, 1H), 2.73 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 198.0, 142.6, 140.2, 129.7, 126.9, 126.8, 123.7, 123.4, 122.1, 120.8, 120.7, 111.2, 110.5, 26.9; **IR (neat)**: ν_{max} = 3286, 1660, 1601, 1361, 1247, 735 cm^{-1}; ***R*$_f$** 0.42 (hexane/EtOAc, 2/1).

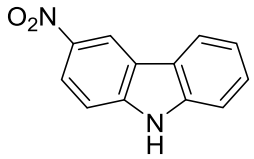


2g (Methyl 9*H*-carbazole-3-carboxylate, CAS 97931-41-4)[12]: off-white solid (42 mg, 62%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.82 (s, 1H), 8.47 (bs, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 8.12 (dd, *J* = 7.8 Hz, 1H), 7.48–7.43 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 1H), 7.29 (dd, *J* = 8.4, 6.6 Hz, 1H), 3.99 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 168.2, 142.5, 140.2, 127.6, 126.8, 123.5,

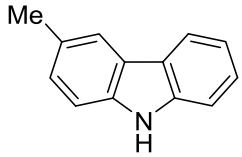
123.3, 123.1, 121.5, 120.8, 120.5, 111.1, 110.4, 52.2; **IR (neat)**: ν_{max} = 3296, 1687, 1604, 1332, 1246, 728 cm^{-1}; $\boldsymbol{R_f}$ 0.28 (hexane/EtOAc, 4/1).



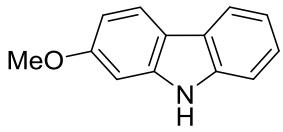
2h (9*H*-Carbazole-3-carbonitrile, CAS 57102-93-9)[8]: off-white solid (37 mg, 64%); **^{1}H NMR (600 MHz, DMSO-d_6)** δ 11.85 (s, 1H), 8.70 (s, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.49 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.24 (dd, *J* = 7.8, 7.2 Hz, 1H); **^{13}C NMR (151 MHz, DMSO-d_6)** δ 142.1, 140.7, 129.0, 127.4, 126.0, 123.1, 122.0, 121.4, 121.0, 120.3, 112.5, 112.0, 100.6; **IR (neat)**: ν_{max} = 3305, 2224, 1734, 1206, 669 cm^{-1}; $\boldsymbol{R_f}$ 0.47 (hexane/EtOAc, 2/1).



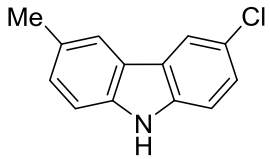
2i (3-Nitro-9*H*-carbazole, CAS 3077-85-8)[13]: pale yellow solid (32 mg, 50%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.44 (bs, 1H), 8.37 (s, 1H), 8.17 – 8.13 (m, 3H), 7.55 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.33 (dd, *J* = 7.8, 6.6 Hz, 1H) ; **^{13}C NMR (151 MHz, $CDCl_3$)** δ 146.1, 141.8, 138.4, 128.7, 128.5, 122.2, 121.7, 121.0, 120.5, 115.2, 111.5, 107.0; **IR (neat)**: ν_{max} = 3377, 2923, 1512, 1341, 1323, 903, 733 cm^{-1}; $\boldsymbol{R_f}$ 0.39 (hexane/EtOAc, 4/1).



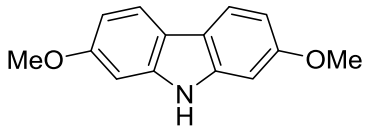
2j (3-Methyl-9*H*-carbazole, CAS 4630-20-0)[8]: off-white solid (35 mg, 65%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.04 (d, *J* = 7.8 Hz, 1H), 7.90 (bs, 1H), 7.86 (s, 1H), 7.42 – 7.36 (m, 2H), 7.29 (d, *J* = 7.8, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.21 (d, *J* = 7.2 Hz, 1H), 2.53 (s, 3H), **^{13}C NMR (151 MHz, $CDCl_3$)** δ 140.0, 137.9, 129.0, 127.4, 125.8, 123.7, 123.4, 120.45, 120.43, 119.4, 110.8, 110.4, 21.6; **IR (neat)**: ν_{max} = 3405, 2918, 1458, 904, 727 cm^{-1}; $\boldsymbol{R_f}$ 0.54 (hexane/EtOAc, 4/1).



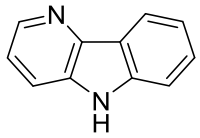
2k (2-Methoxy-9*H*-carbazole, CAS 6933-49-9)[10]: gray solid (15 mg, 26%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ7.97 (d, *J* = 8.4 Hz, 1H), 7.96 (bs, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.34 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.21 (dd, *J* = 7.8, 7.2 Hz, 1H), 6.91 (s, 1H), 6.86 (d, *J* = 7.8 Hz, 1H); 3.90 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 125.3, 141.0, 139.7, 124.8, 121.3, 119.8, 119.7, 117.5, 110.5, 108.4, 94.9, 55.9, 29.3; **IR (neat)**: ν_{max} = 3387, 2917, 1737, 1462, 903, 727 cm^{-1}; $\boldsymbol{R_f}$ 0.36 (hexane/EtOAc, 4/1).



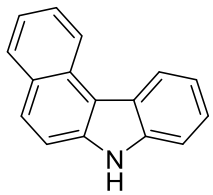
2l (3-Chloro-6-methyl-9*H*-carbazole): off-white solid (42 mg, 66%); mp 163 – 164 °C; **^{1}H NMR (600 MHz, $CDCl_3$)** δ 7.99 (s, 1H), 7.94 (bs, 1H), 7.82 (s, 1H), 7.34(d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.27 (d, *J* = 8.4 Hz, 1H), 2.53 (s, 3H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 138.5, 138.2, 129.4, 128.1, 125.9, 124.9, 124.6, 122.9, 120.6, 120.2, 111.7, 110.7, 21.6; **IR (neat)**: ν_{max} = 3392, 2920, 2852, 1446, 1274, 811, 731 cm^{-1}; **HRMS** *m/z* (EI) calc. for $C_{13}H_{10}ClN$ [M^+] 215.0502, found 215.0500; $\boldsymbol{R_f}$ 0.46 (hexane/EtOAc, 4/1).



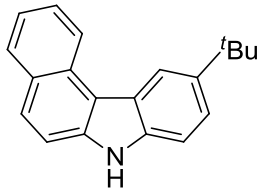
2m (2,7-Dimethoxy-9*H*-carbazole, CAS 61822-18-2)[14]: pale-brown solid (20 mg, 30%); **^{1}H NMR (600 MHz, DMSO-d_6)** δ 10.95 (bs, 1H), 7.83 (d, *J* = 8.4 Hz, 2H), 6.92 (s, 2H), 6.72 (dd, *J* = 8.4 Hz, 2H), 3.80 (s, 6H); **^{13}C NMR (151 MHz, DMSO-d_6)** δ 158.0, 141.4, 120.3, 116.9, 107.7, 95.1, 55.7; **IR (neat)**: ν_{max} = 3379, 1610, 1456, 1023, 1000, 823, 761 cm^{-1}; $\boldsymbol{R_f}$ 0.23 (hexane/EtOAc, 4/1).



2n (5*H*-Pyrido[3,2-*b*]indole, CAS 245-08-9)[8]: brown solid (22 mg, 45%); **^{1}H NMR (600 MHz, DMSO-d_6)** δ 11.42 (bs, 1H), 8.45 (d, *J* = 4.2 Hz, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.50 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.38 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.24 (dd, *J* = 7.8, 7.2 Hz, 1H); **^{13}C NMR (151 MHz, DMSO-d_6)** δ 141.6, 140.9, 133.3, 127.8, 122.0, 120.6, 120.5, 119.7, 118.4, 112.1; **IR (neat)**: ν_{max} = 2921, 1627, 1458, 1394, 889 cm^{-1}; $\boldsymbol{R_f}$ 0.26 (hexane/EtOAc, 2/1).

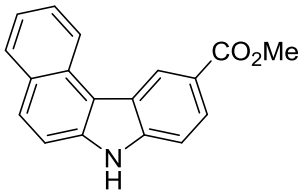


6a (7*H*-Benzo[*c*]carbazole, CAS 205-25-4)[15]: off-white solid (37 mg, 58%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.79 (d, *J* = 8.4 Hz, 1H), 8.57 (d, *J* = 7.8 Hz, 1H), 8.42 (bs, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.72 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.48 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.46 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.39 (dd, *J* = 8.4, 7.8 Hz, 1H); **^{13}C NMR (151 MHz, $CDCl_3$)** δ 138.7, 137.3, 130.2, 129.43, 129.40, 127.6, 127.1, 124.6, 124.2, 123.5, 123.2, 122.3, 120.5, 115.7, 112.8, 111.3; **IR (neat)**: ν_{max} = 3411, 3050, 2924, 1467, 1359, 805, 741 cm^{-1}; $\boldsymbol{R_f}$ 0.38 (hexane/EtOAc, 4/1).

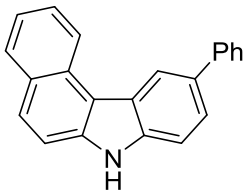


6b (10-(*tert*-Butyl)-7*H*-benzo[*c*]carbazole, CAS 756822-83-0)[15]: brown solid (45 mg, 55%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 8.79 (d, *J* = 8.4 Hz,

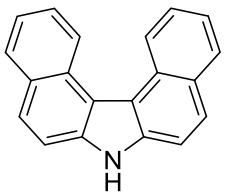
1H), 8.57 (s, 1H), 8.36 (s, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 9.0 Hz, 1H), 7.73 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.48 (dd, *J* = 8.4, 7.2 Hz, 1H), 1.54 (s, 9H); **^{13}C NMR (151 MHz, CDCl$_3$)** δ 143.4, 137.6, 136.8, 130.2, 129.4, 129.4, 127.3, 127.0, 124.1, 123.4, 123.0, 122.7, 118.2, 115.8, 112.9, 110.8, 35.1, 32.3; **IR (neat)**: ν_{max} = 3413, 2959, 1480, 1365, 1286, 908, 805, 735 cm^{-1}; ***R*$_f$** 0.43 (hexane/EtOAc, 4/1).



6c (Methyl 7*H*-benzo[*c*]carbazole-10-carboxylate)[15]: brown solid (50 mg, 61%); mp 243-244 °C; **^{1}H NMR (600 MHz, DMSO-d$_6$)** δ 12.23 (s, 1H), 9.15 (s, 1H), 8.71 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 8.06 (dd, *J* = 8.4, 7.8 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 9.0 Hz, 1H), 7.77 (d, *J* = 7.2 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.51 (dd, *J* = 8.4, 7.2 Hz, 1H), 3.94 (s, 3H).**^{13}C NMR (151 MHz, DMSO-d$_6$)** δ 167.5, 141.9, 138.9, 129.8, 129.5, 129.3, 128.4, 127.8, 125.5, 123.7, 123.6, 123.0, 122.9, 121.2, 114.6, 113.9, 112.0, 52.4; **IR (neat)**: ν_{max} = 3321, 2921, 1697, 1616, 796 cm^{-1}; **HRMS** *m/z* (EI) calc. for $C_{18}H_{13}NO_2$ [M$^+$] 275.0946, found 275.0948; ***R*$_f$** 0.22 (hexane/EtOAc, 4/1).

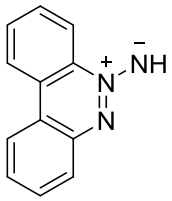


6d (10-Phenyl-7*H*-benzo[*c*]carbazole, CAS 756822-84-1)[15]: off-white solid (61 mg, 70%); **^{1}H NMR (600 MHz, CDCl$_3$)** δ 8.84 (d, *J* = 8.4 Hz, 1H), 8.76 (s, 1H), 8.42 (bs, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 9.0 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 2H), 7.74 (dd, *J* = 7.8, 6.6 Hz, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.60 (dd, *J* = 8.4, 7.8 Hz, 2H), 7.55–7.49 (m, 3H), 7.40 (dd, *J* = 8.4, 7.2 Hz, 1H); **^{13}C NMR (151 MHz, CDCl$_3$)** δ 142.7, 138.1, 137.8, 134.1, 130.2, 129.5, 129.4, 129.0, 127.9, 127.8, 127.1, 126.8, 124.8, 124.3, 123.5, 123.3, 120.9, 115.8, 112.8, 111.5; **IR (neat)**: ν_{max} = 3411, 3049, 2924, 1473, 1288, 906, 804, 734 cm^{-1}; ***R*$_f$** 0.37 (hexane/EtOAc, 4/1).



8 (7*H*-Dibenzo[*c*,*g*]carbazole, CAS 194-59-2)[15]: brown solid (20 mg, 25%); **^{1}H NMR (600 MHz, CDCl$_3$)** δ 9.22 (d, *J* = 8.4 Hz, 2H), 8.78 (bs, 1H), 8.04 (d, *J* = 7.8 Hz, 2H), 7.87 (d, *J* = 8.4 Hz, 2H), 7.70 (dd, *J* = 8.4, 6.6 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.53 (dd, *J* = 7.8, 6.6 Hz, 2H); **^{13}C NMR (151 MHz, CDCl$_3$)** δ 136.4, 130.2, 129.44, 129.39, 127.1, 125.7, 125.4, 123.5, 118.1, 112.8; **IR (neat)**: ν_{max} = 3408, 2924, 1529, 1381, 1322, 801, 740 cm^{-1}; ***R*$_f$** 0.34 (hexane/EtOAc, 4/1).

Analytic data for Benzocinnoline *N*-imide (III)



III (Benzo[*c*]cinnolin-5-ium-5-ylamide, CAS 35393-83-0):[16] yellow solid (12 mg, 20%); **^{1}H NMR (600 MHz, $CDCl_3$)** δ 9.45 (s, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.31 (d, *J* = 7.2 Hz, 1H), 8.11 (d, *J* = 8.4 Hz, 1H), 7.78 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.63 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.51 (dd, *J* = 8.4, 7.2 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.30 (dd, *J* = 8.4, 7.2 Hz, 1H).; **^{13}C NMR (151 MHz, $CDCl_3$)** δ 144.3, 131.7, 130.5, 129.1, 128.1, 124.4, 122.5, 122.4, 121.7, 121.4, 116.2 (overlapped peaks present); **IR (neat)**: ν_{max} = 3189, 2923, 1467, 1384, 1326, 763, 715 cm^{-1}; **HRMS** *m/z* (EI) calc. for $C_{12}H_9N_3$ [M^+] 195.0796, found 195.0796; $\boldsymbol{R_f}$ 0.45 (hexane/EtOAc, 4/1).

References

1. Lee, E.; Hooker, J. M.; Ritter, T. *J .Am. Chem. Soc.* **2012**, *134*, 17456.
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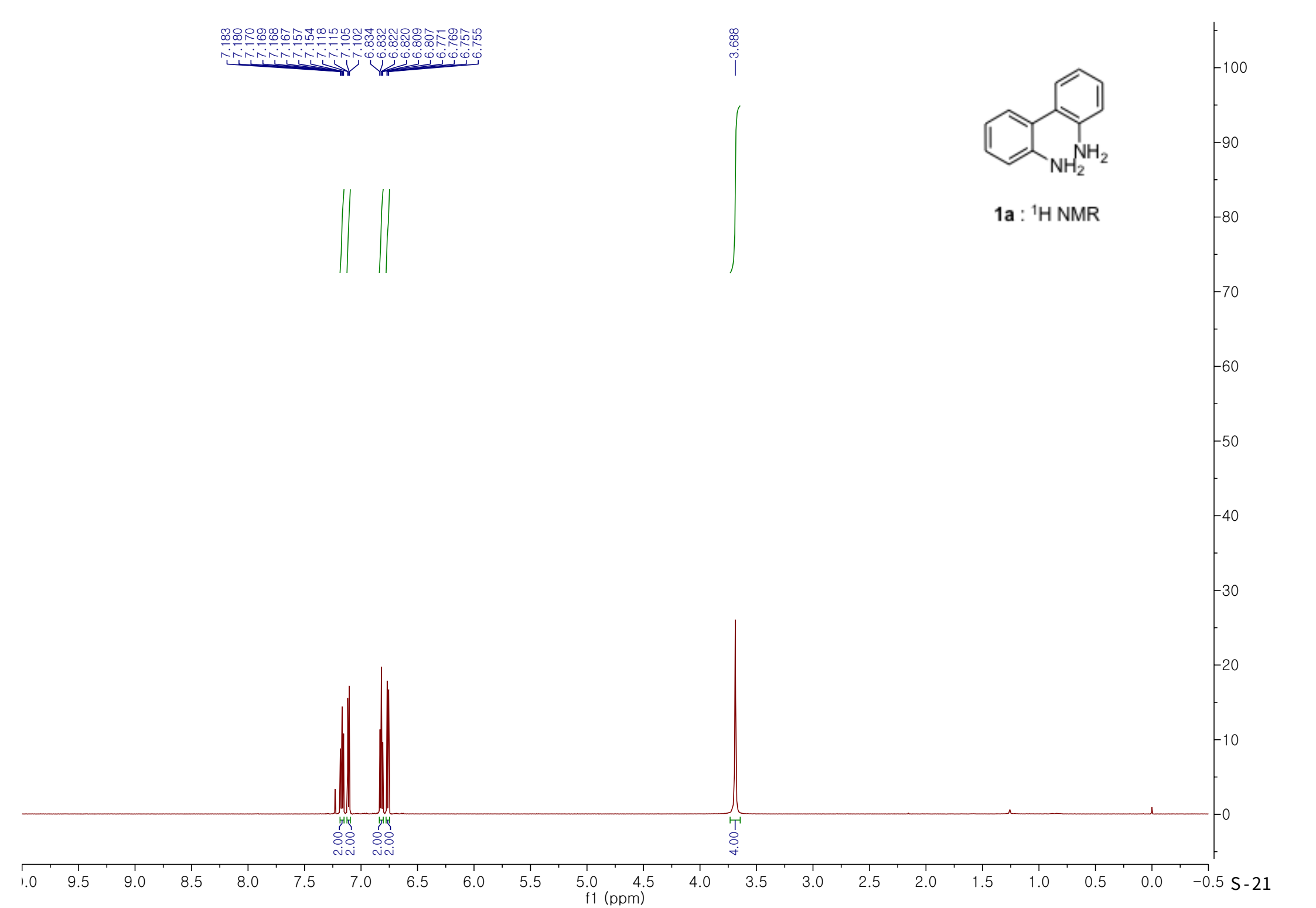
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6.832
6.822
6.820
6.809
6.807
6.771
6.769
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NH2
1a : 1H NMR
2.00
2.00
2.00
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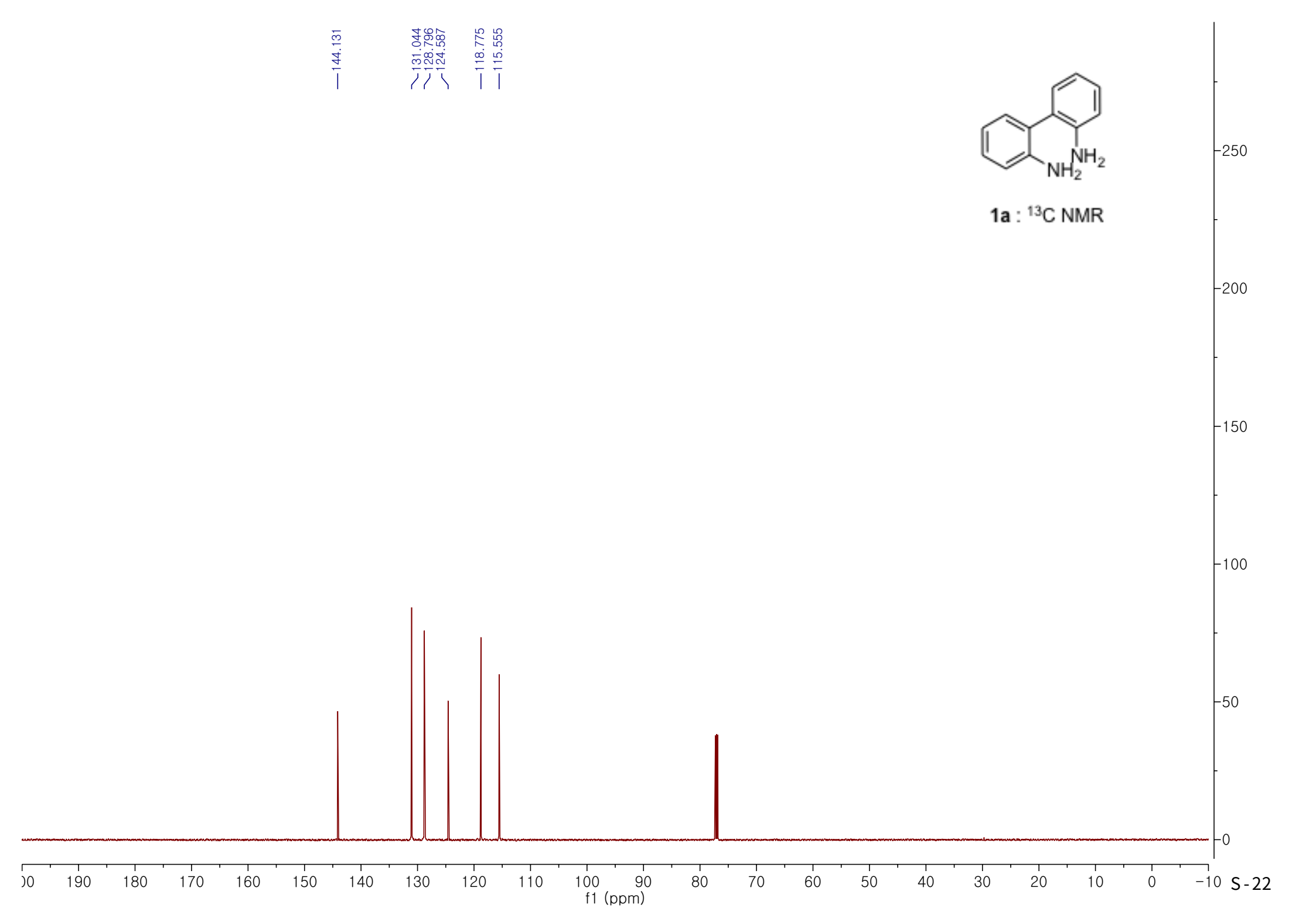
4.00
f1 (ppm)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200
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180
170
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40
30
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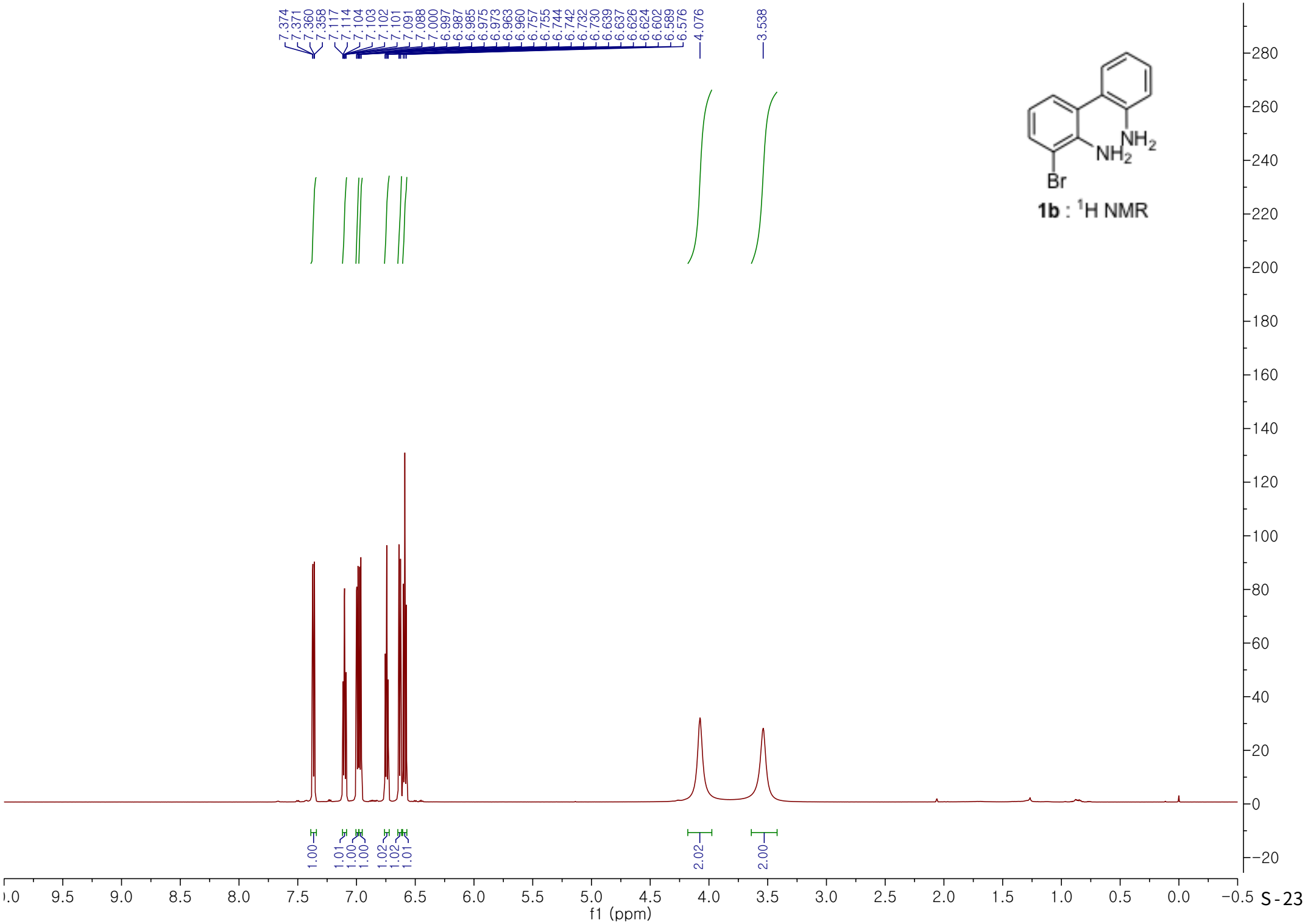
f1 (ppm)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6.963
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6.755
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6.637
6.626
6.624
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6.576
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3.538
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NH2
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1.01
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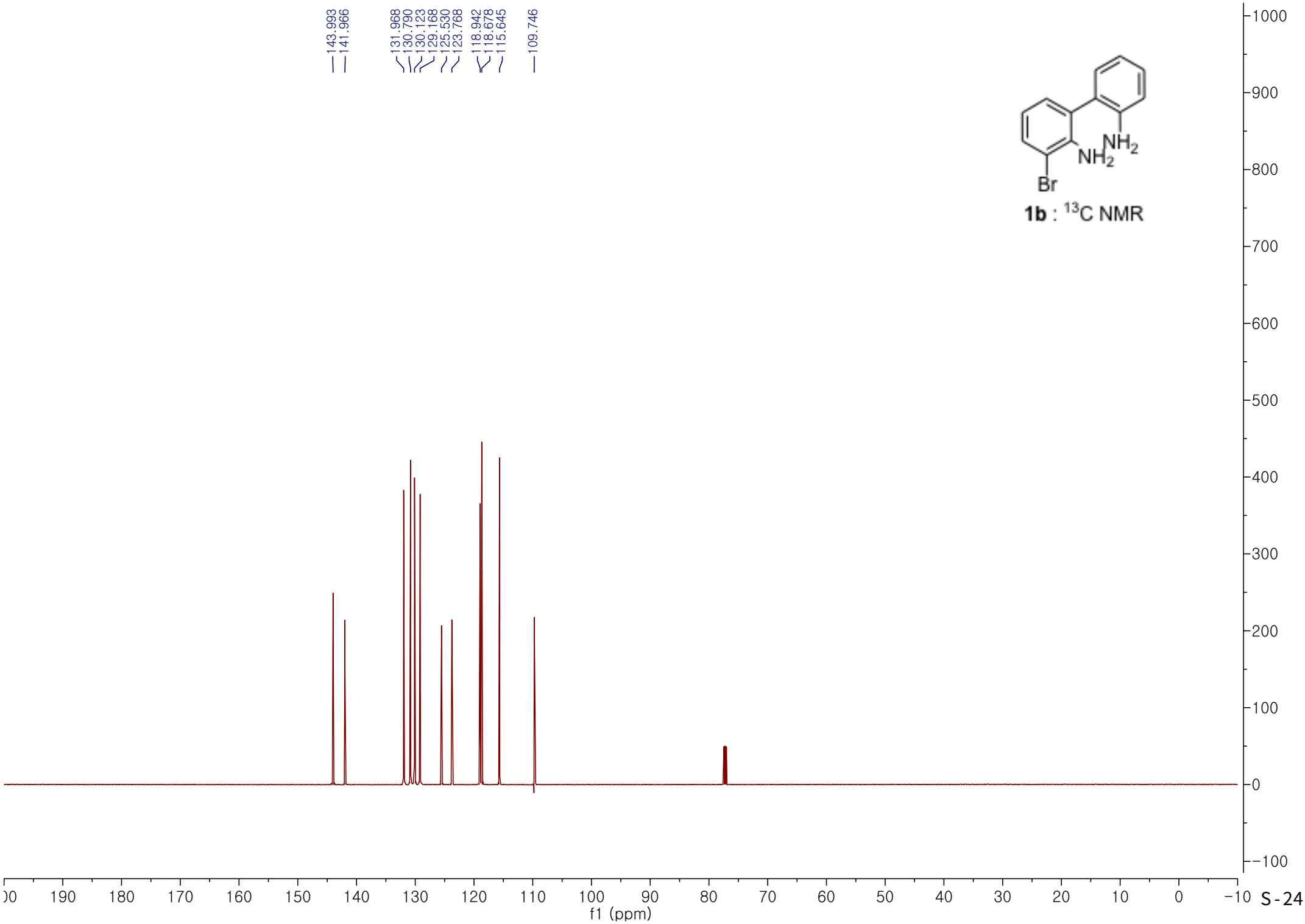
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Br
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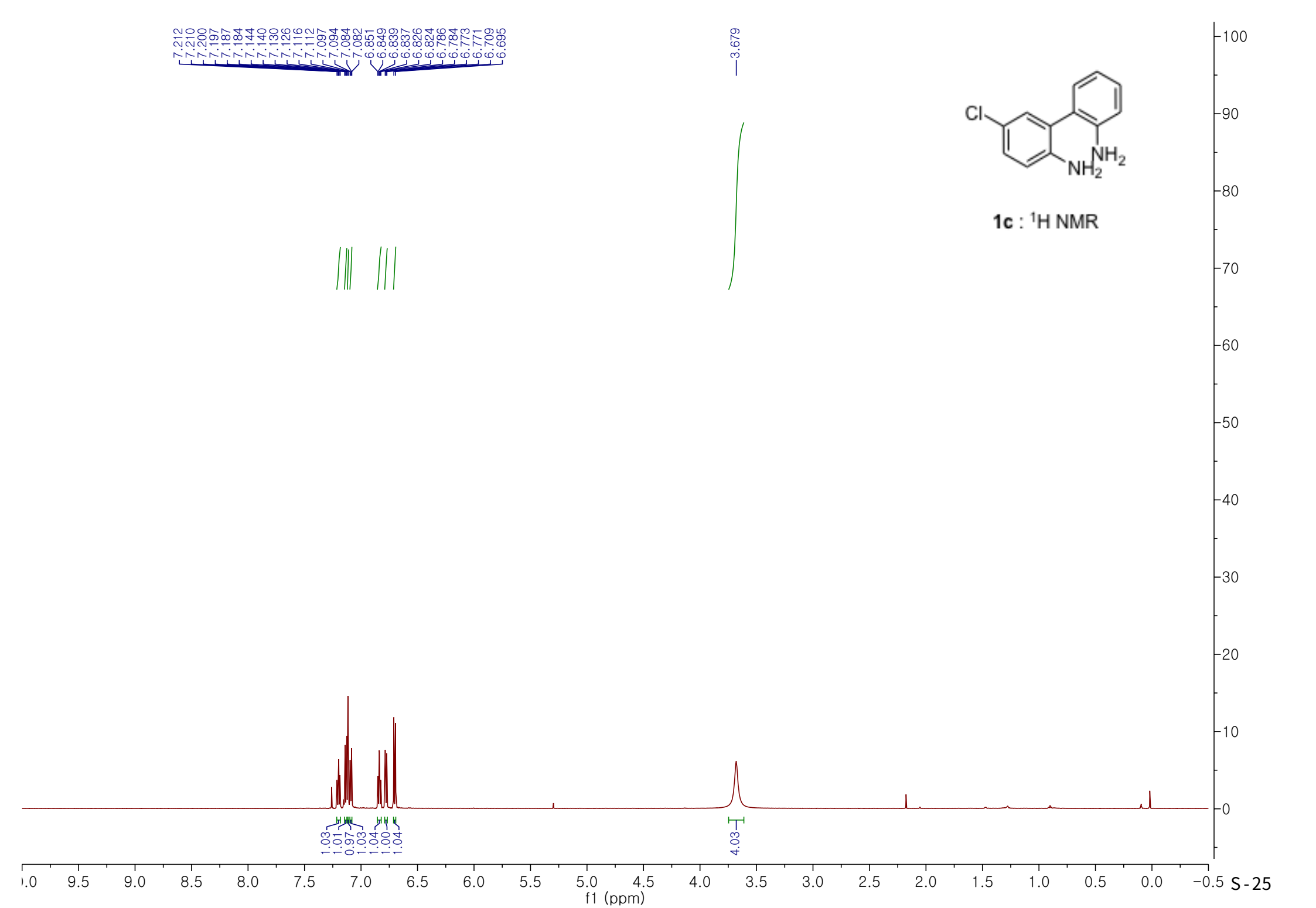
f1 (ppm)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7.094
7.084
7.082
6.851
6.849
6.839
6.837
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6.824
6.786
6.784
6.773
6.771
6.709
6.695
3.679
Cl
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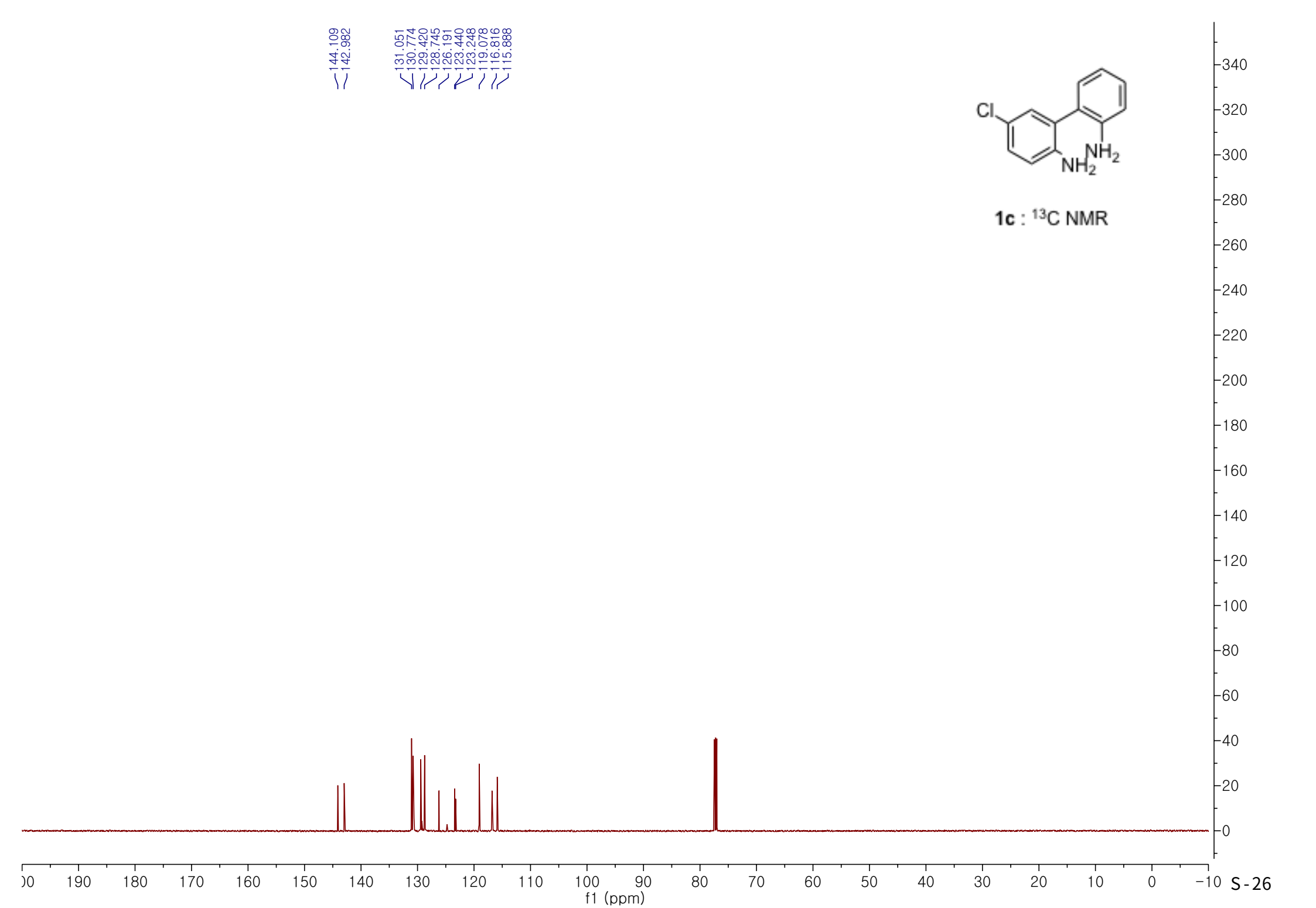
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Cl
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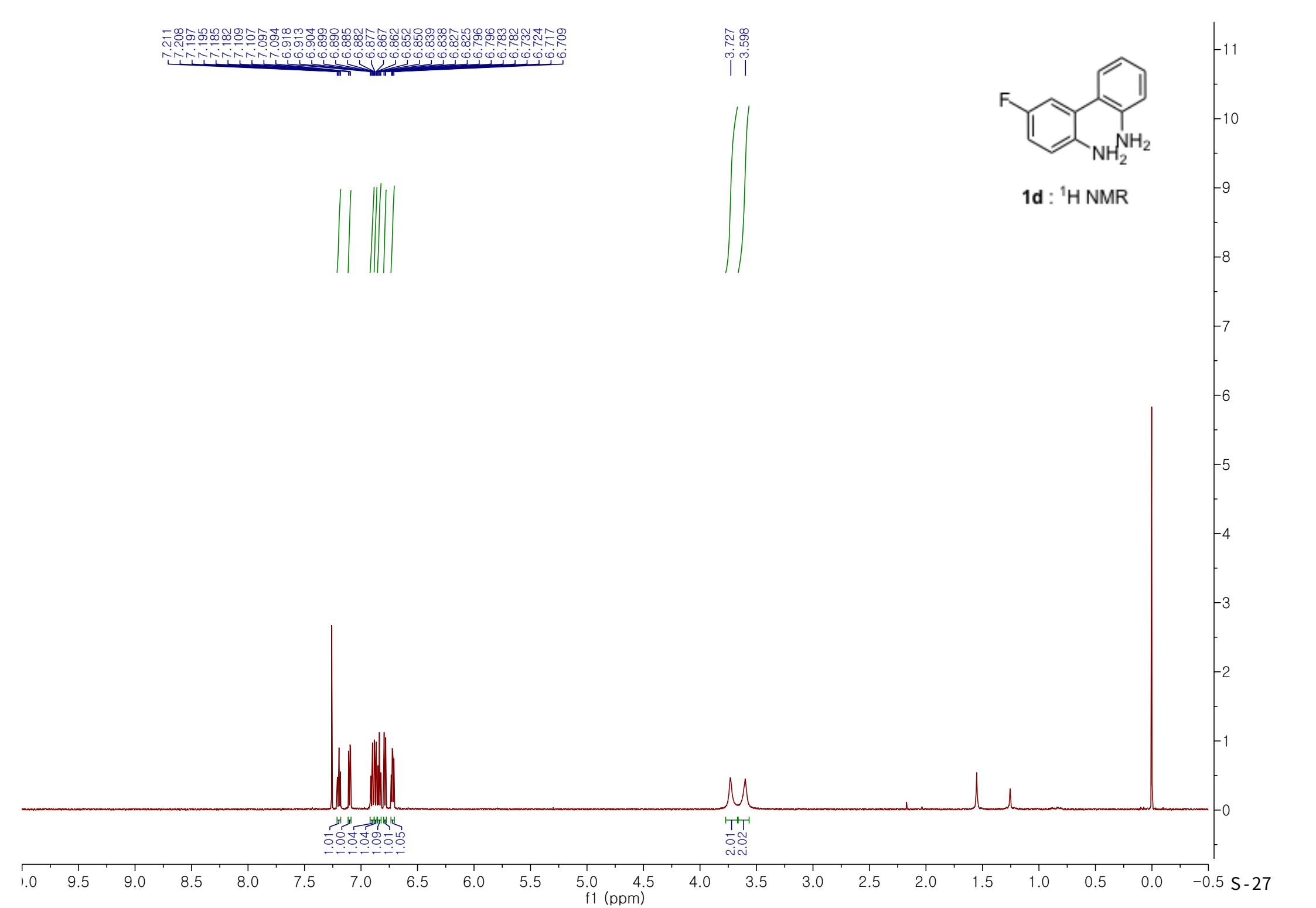
NH2
1c : 13C NMR
f1 (ppm)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6.899
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6.862
6.852
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6.839
6.838
6.827
6.825
6.796
6.796
6.783
6.782
6.732
6.724
6.717
6.709
3.727
3.598
F
NH2
NH2
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1.00
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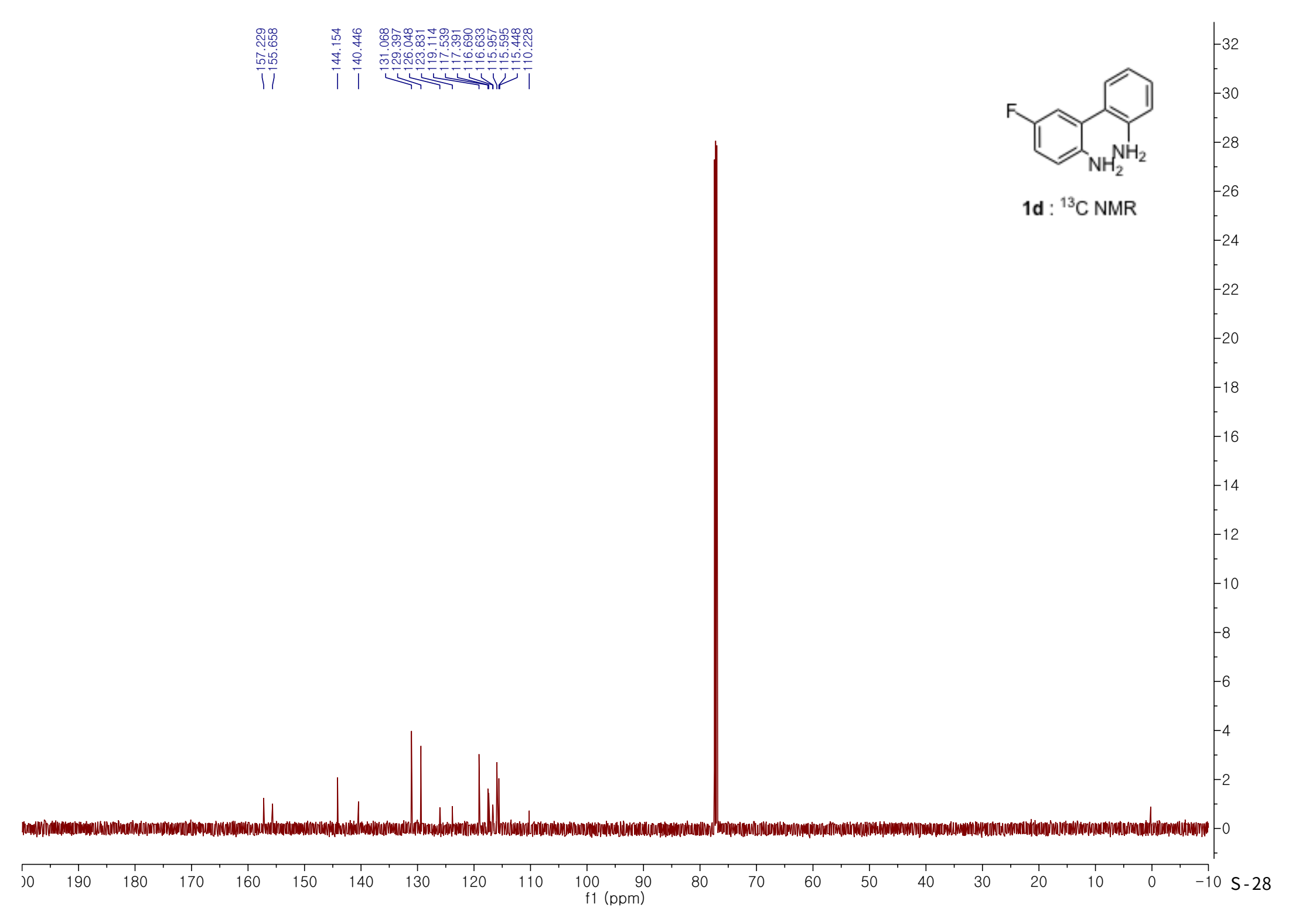
1.04
1.09
1.01
1.05
2.01
2.02
f1 (ppm)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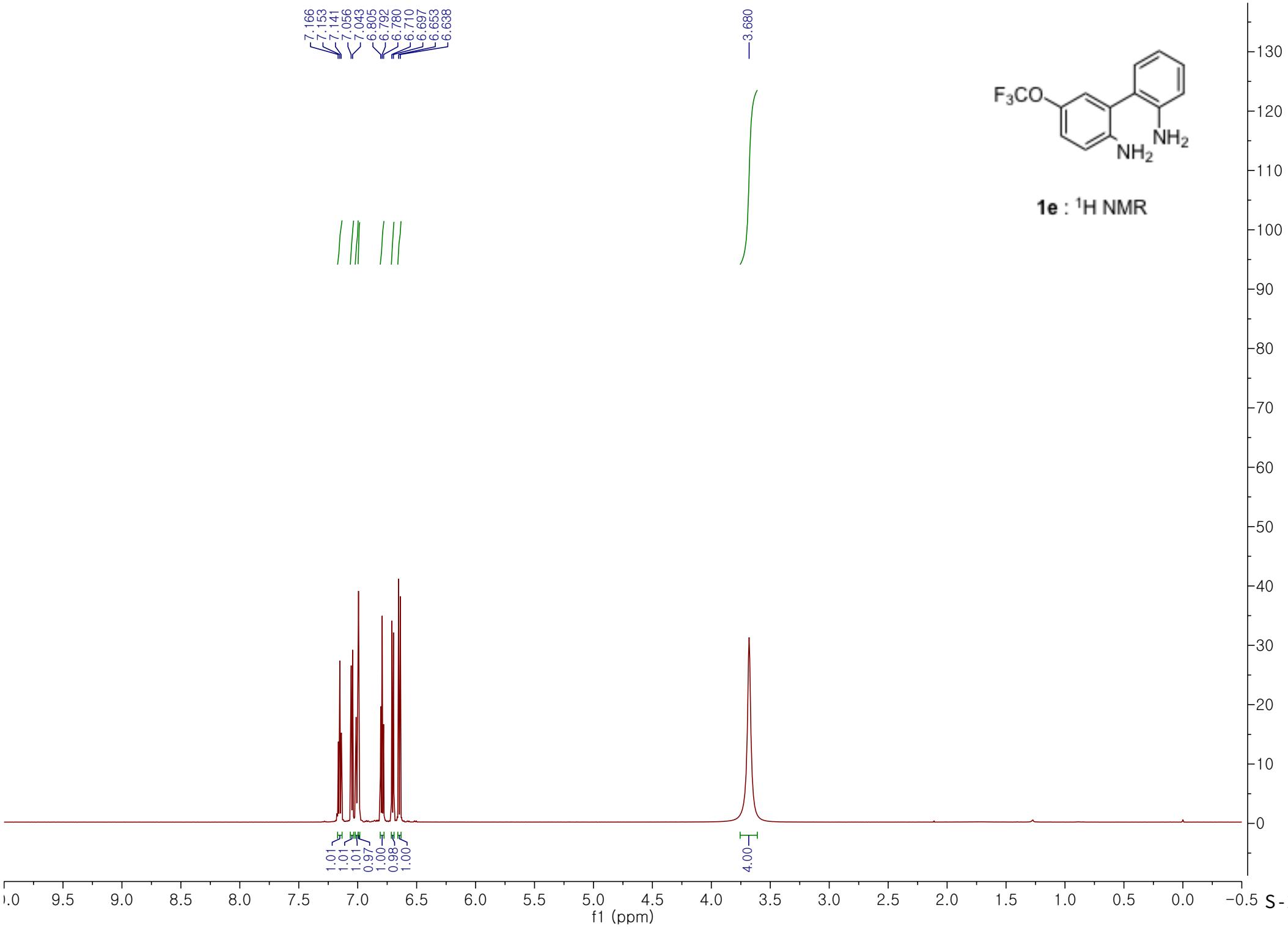
115.595
115.448
110.228
F
NH2
NH2
1d : 13C NMR
f1 (ppm)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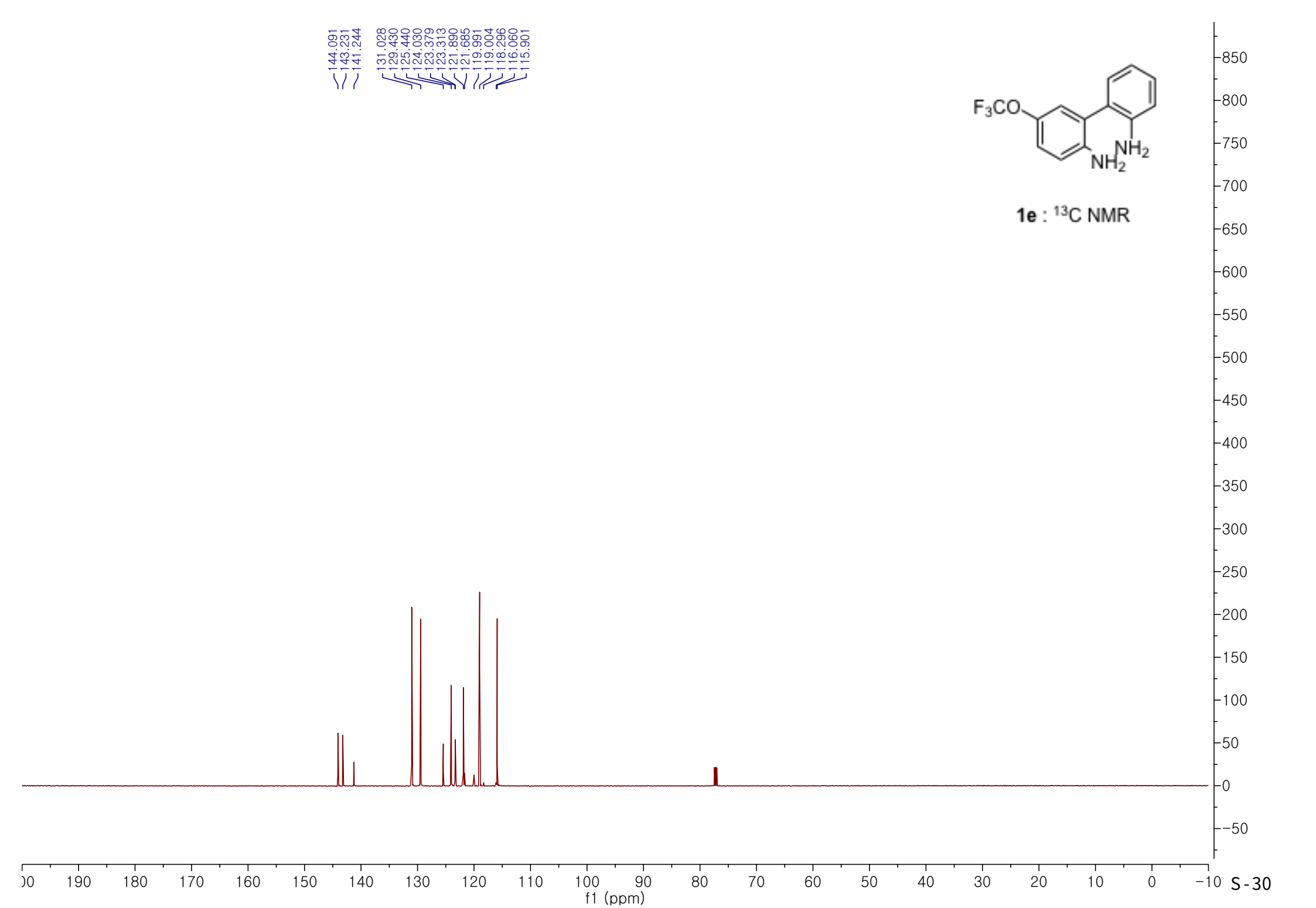
4.00
f1 (ppm)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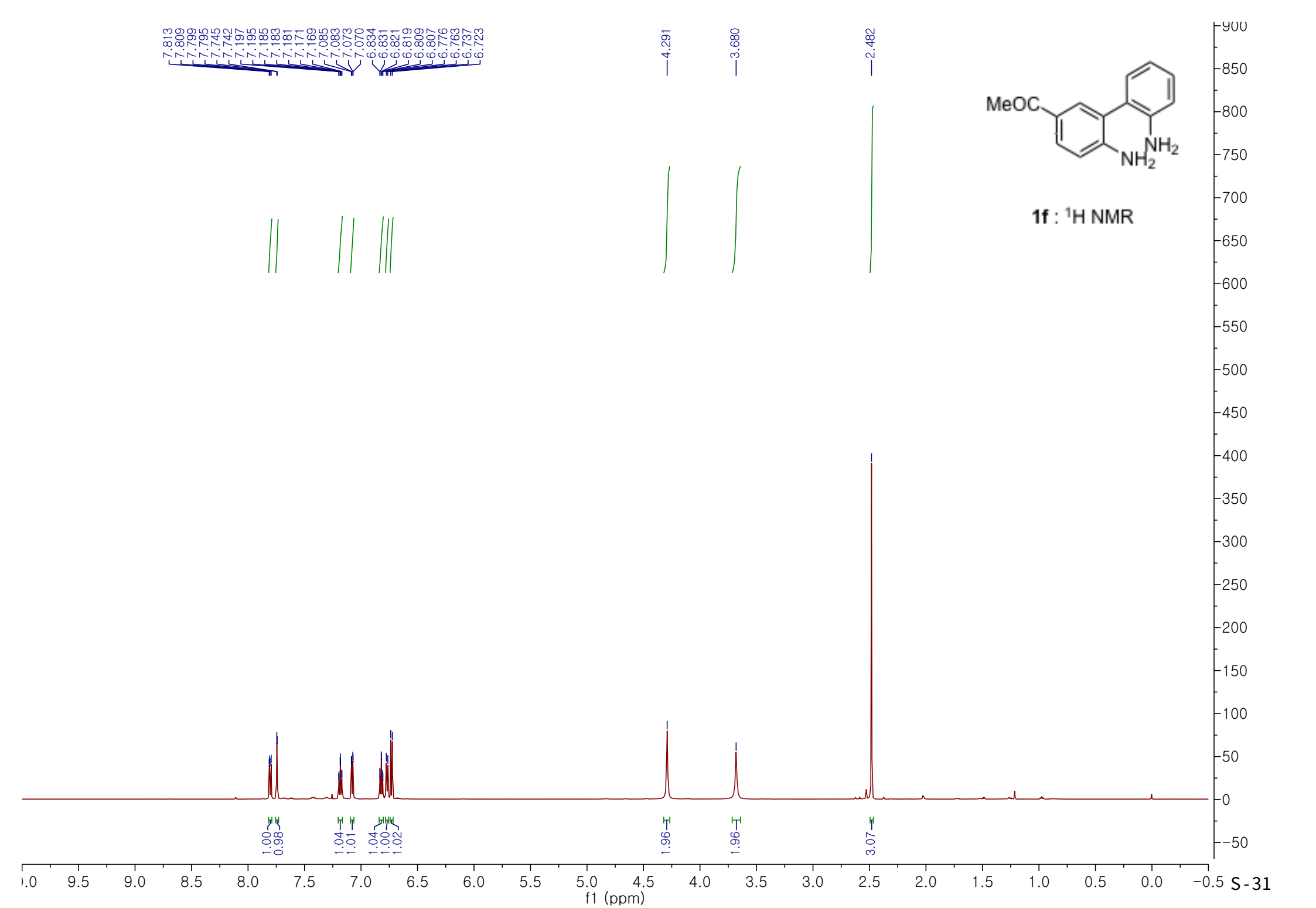
NH2
NH2
1e : 13C NMR
f1 (ppm)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6.809
6.807
6.776
6.763
6.737
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MeOC
NH2
NH2
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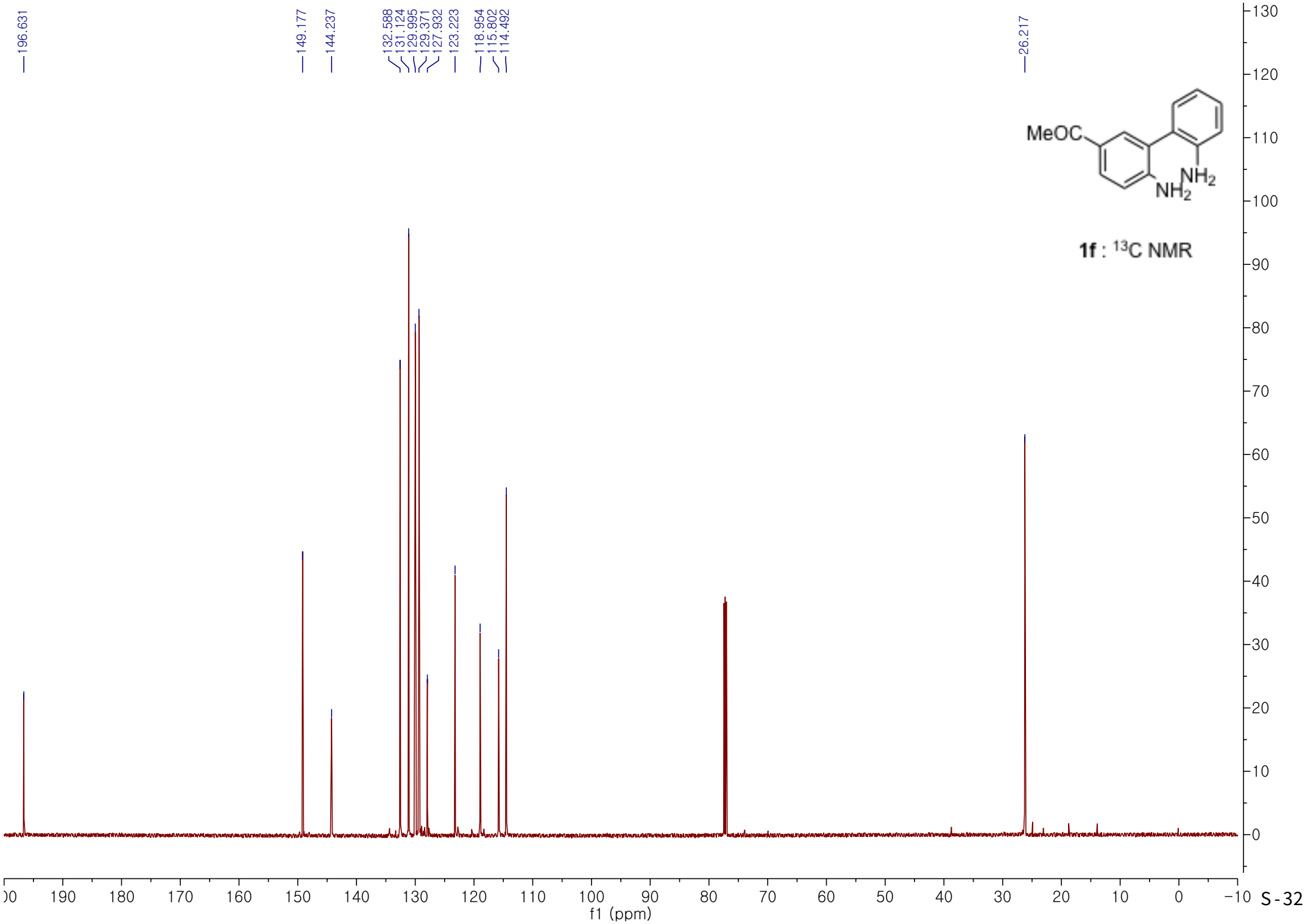
f1 (ppm)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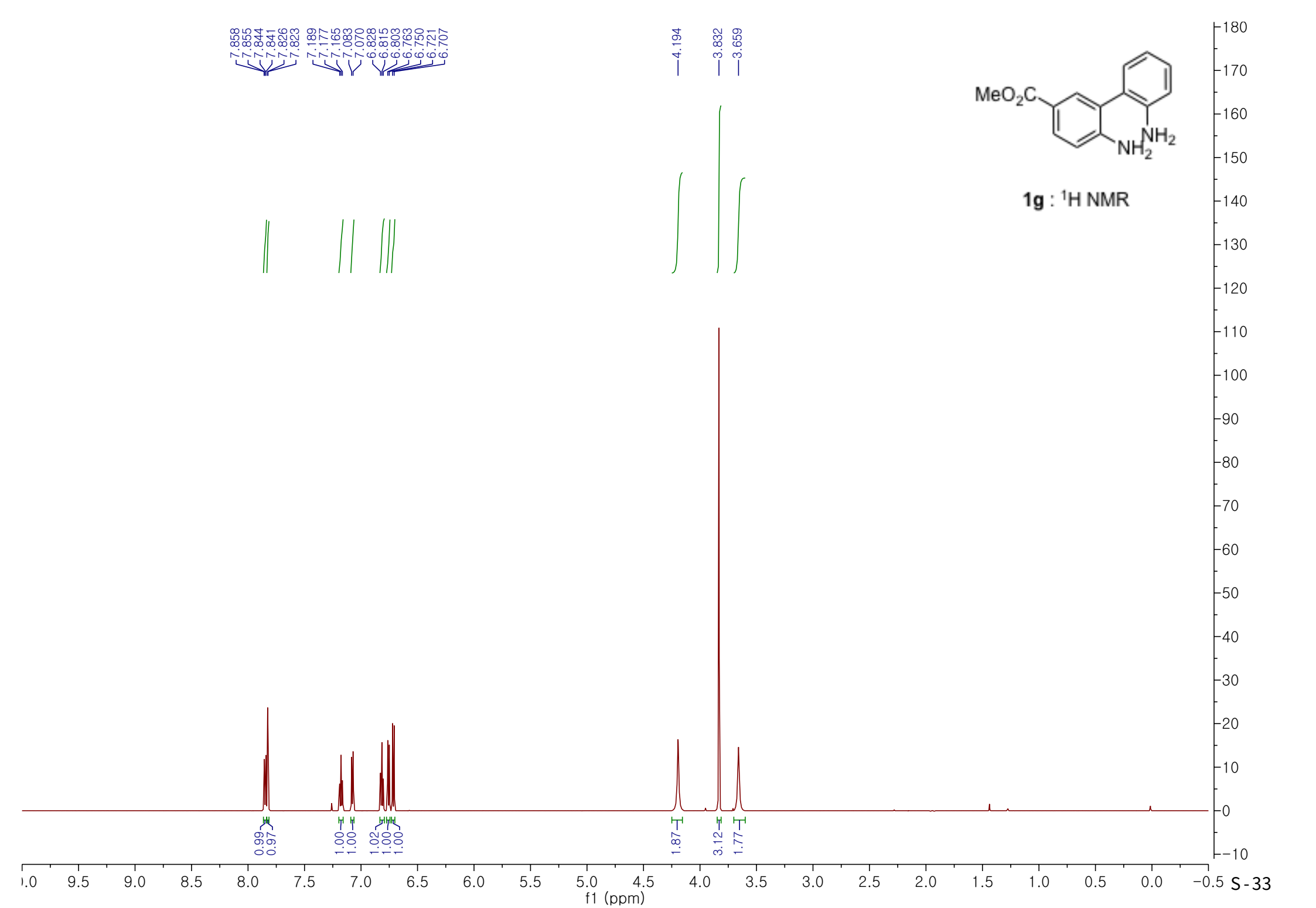
NH2
NH2
1f : 13C NMR
f1 (ppm)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6.707
4.194
3.832
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MeO2C
NH2
NH2
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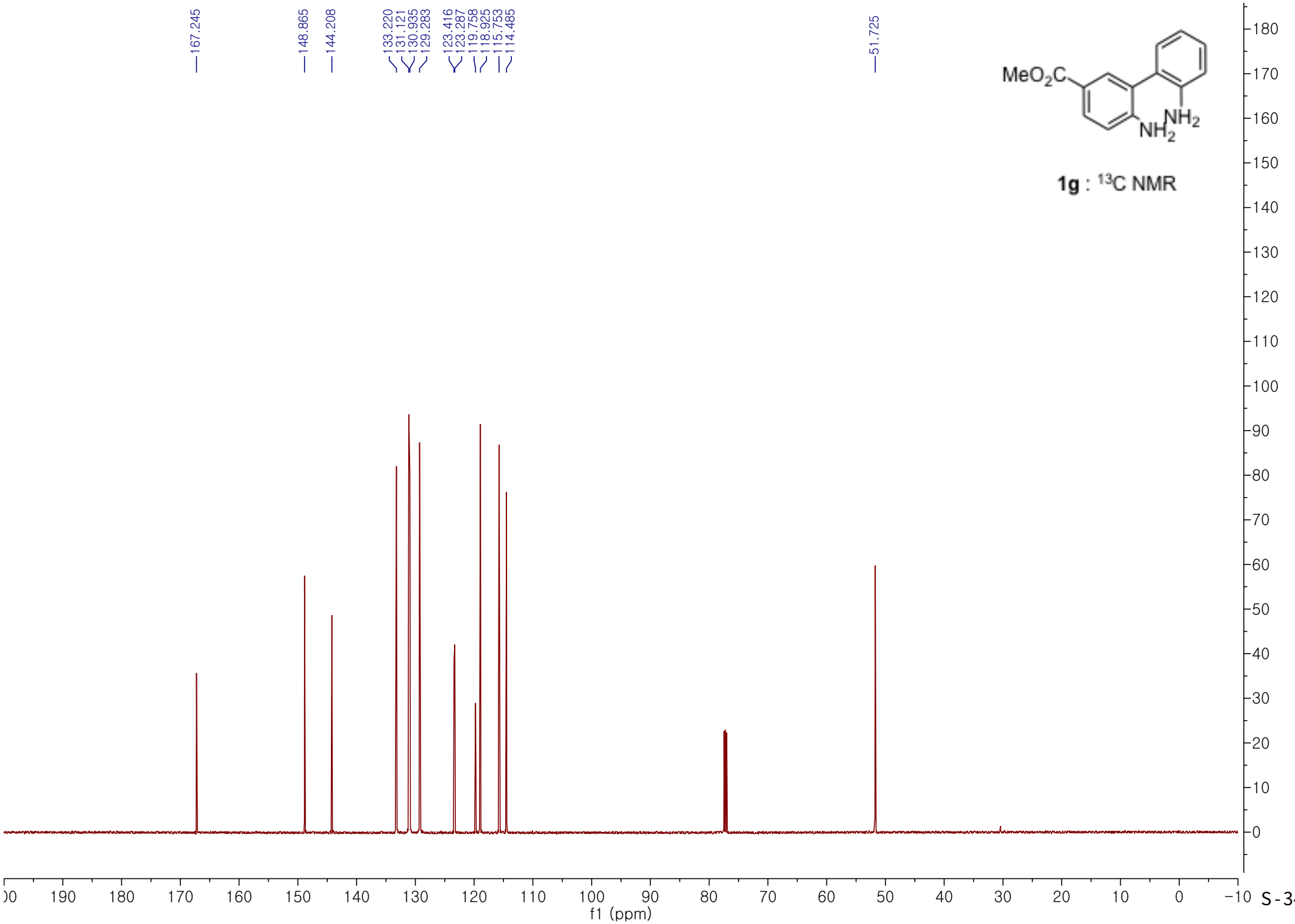
f1 (ppm)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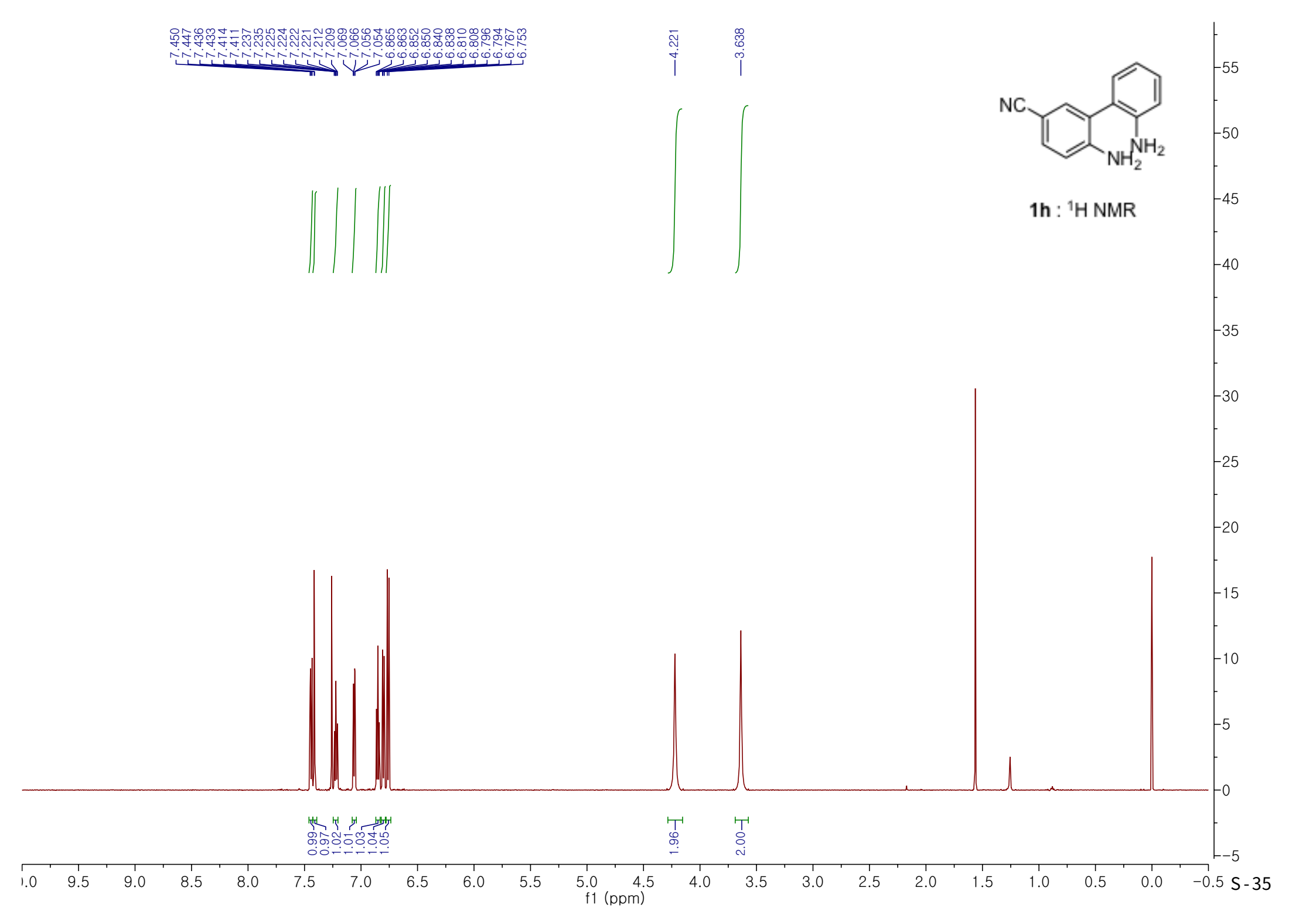
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6.796
6.794
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4.221
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NC
NH2
NH2
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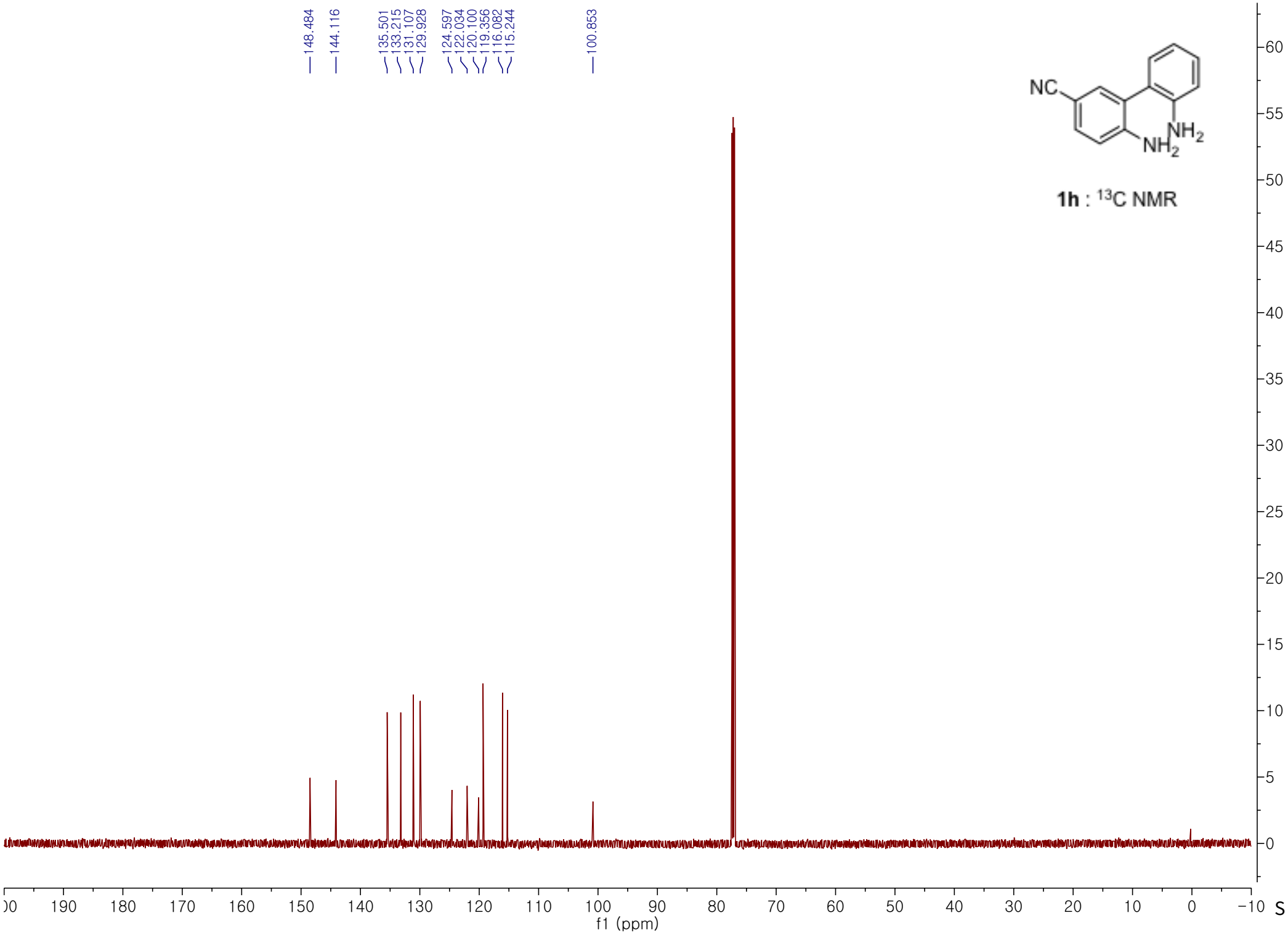
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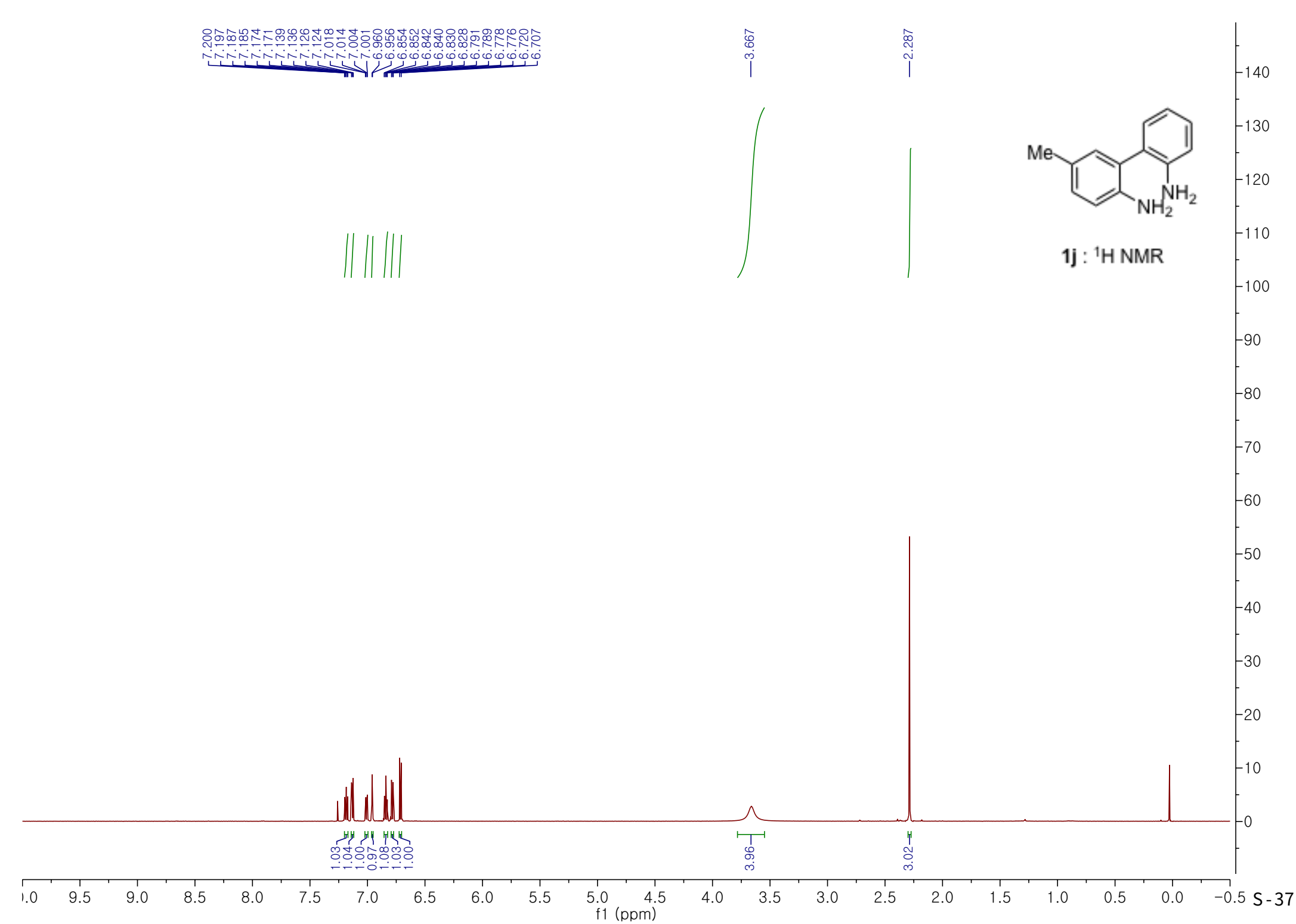
f1 (ppm)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6.789
6.778
6.776
6.720
6.707
3.667
2.287
Me
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NH2
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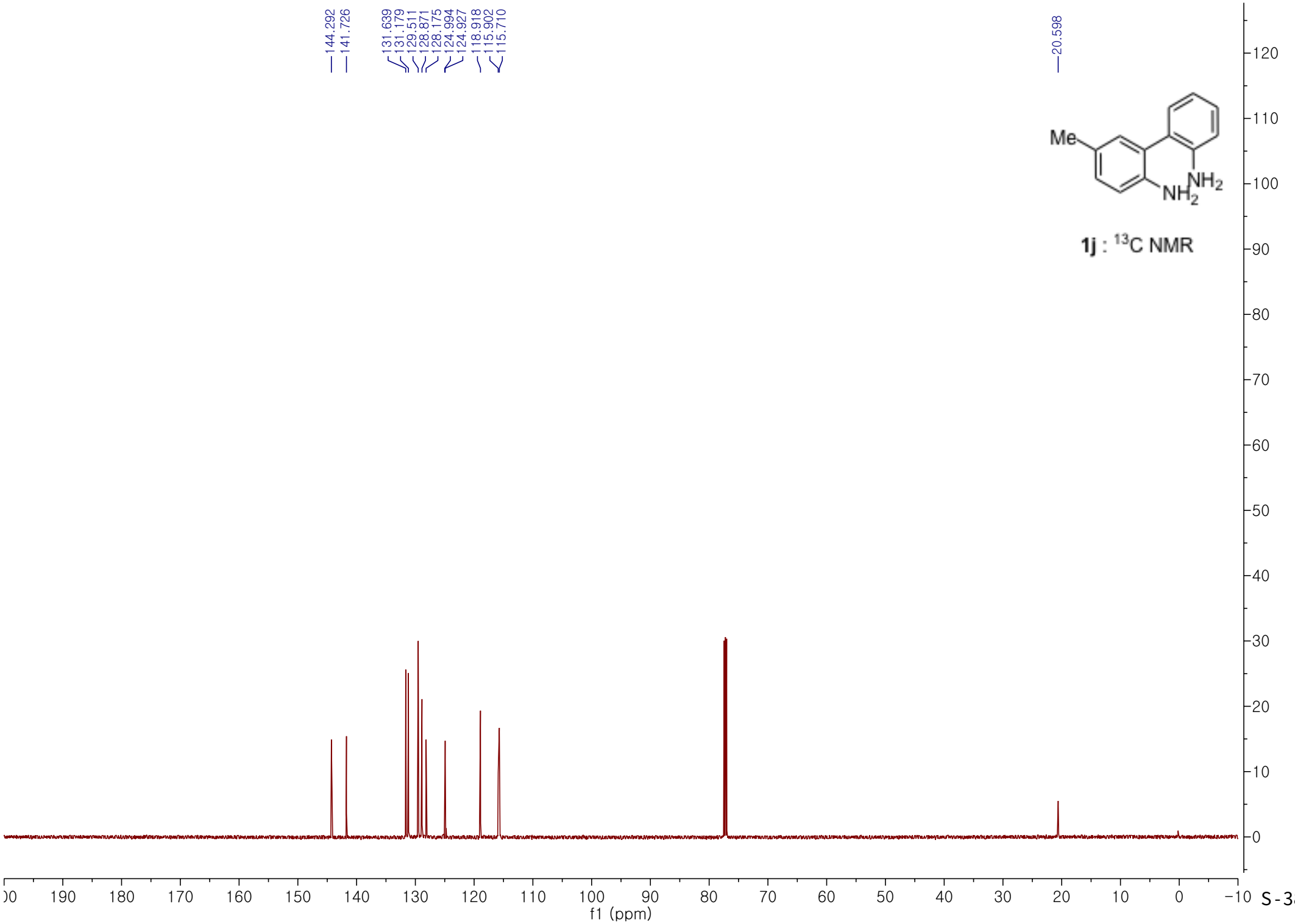
3.02
f1 (ppm)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NH2
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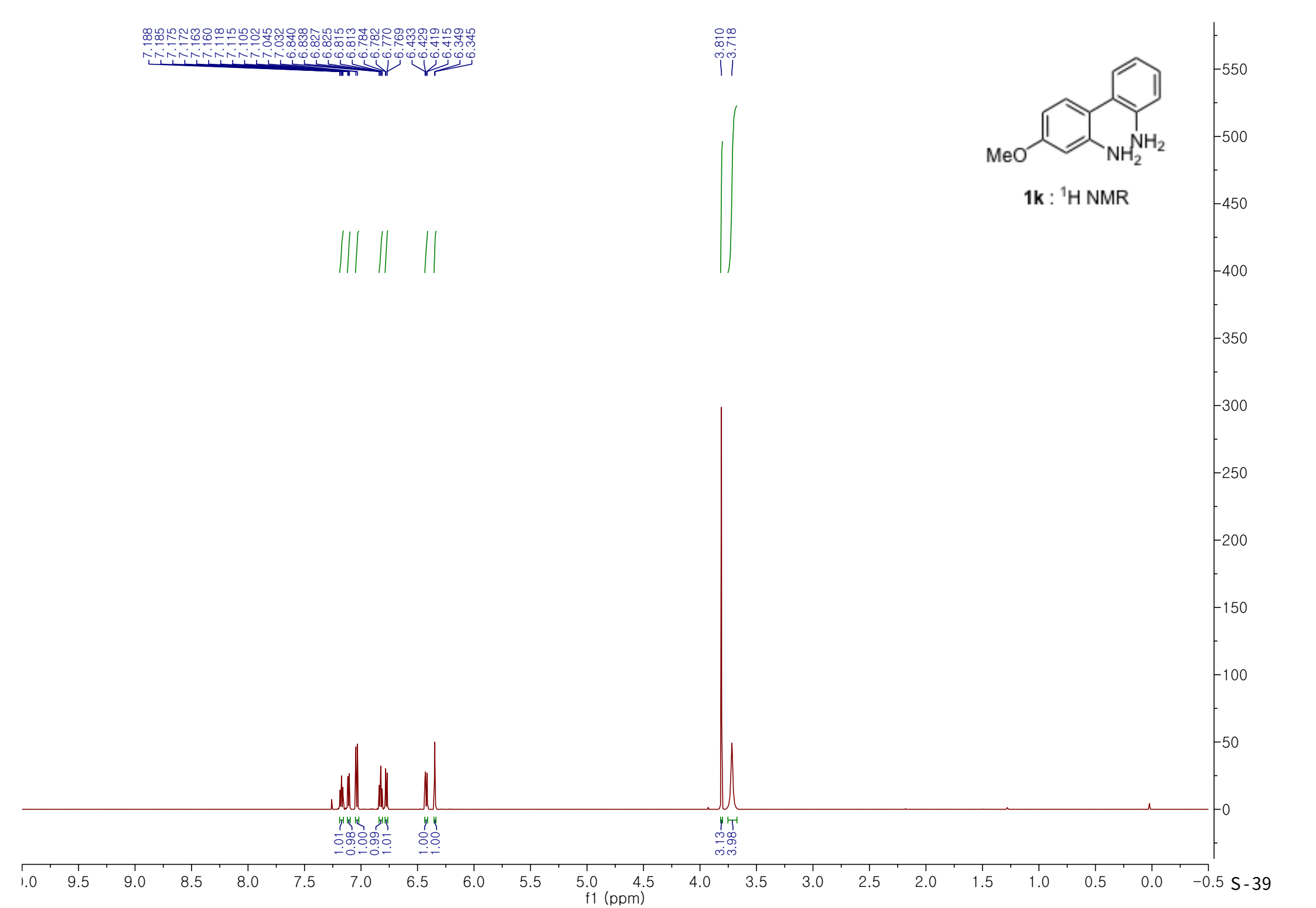
f1 (ppm)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6.770
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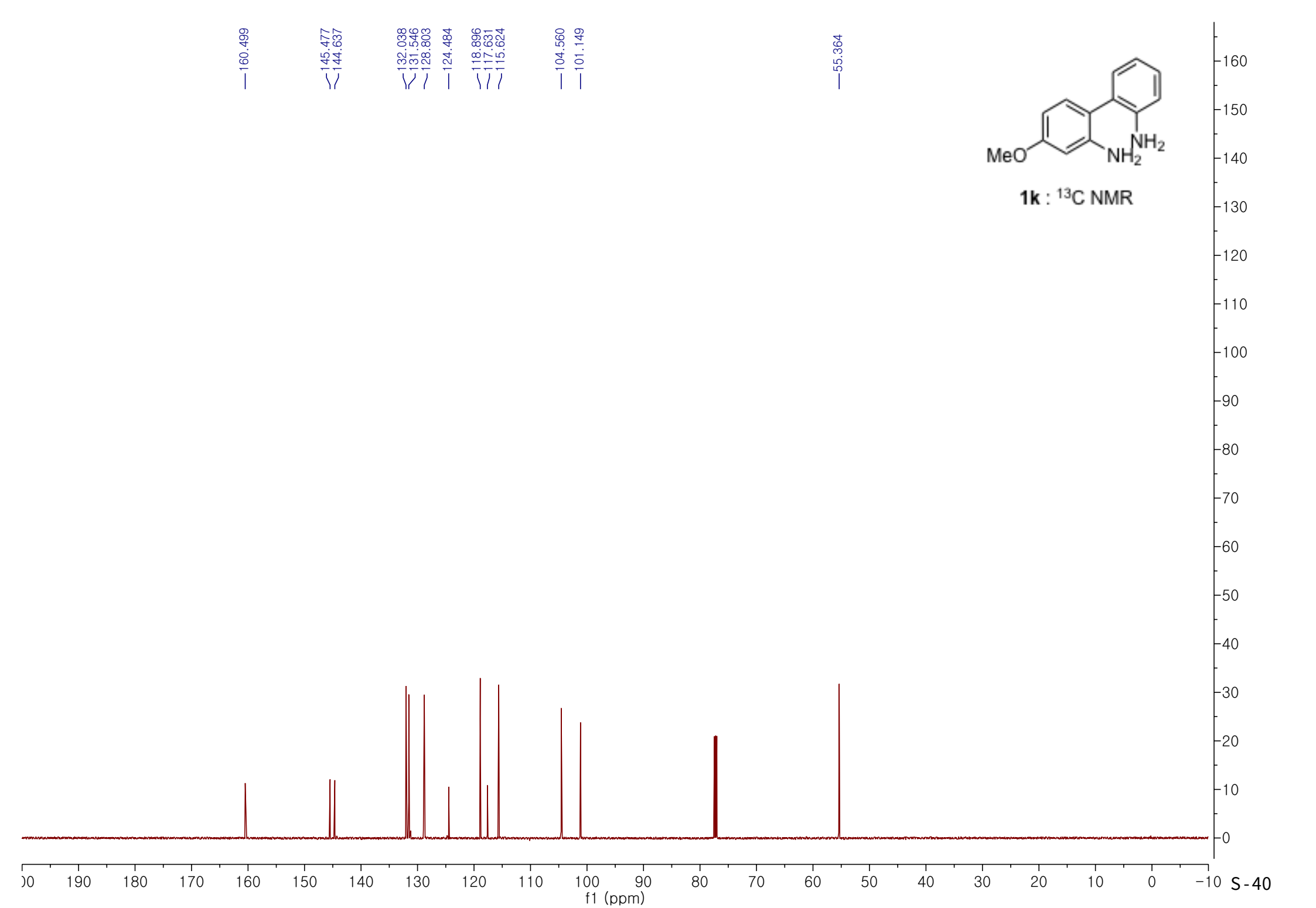
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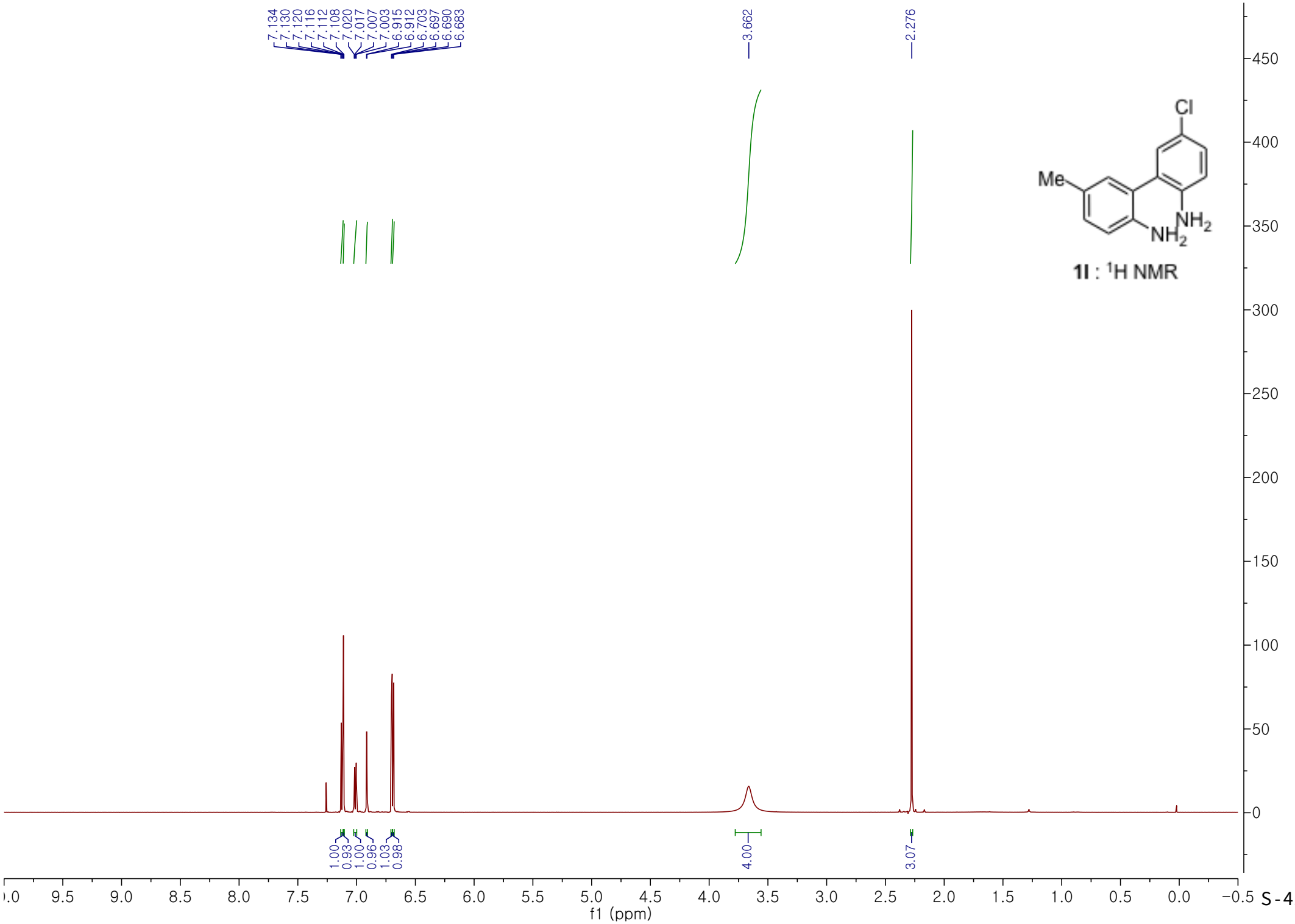
f1 (ppm)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6.697
6.690
6.683
3.662
2.276
Cl
Me
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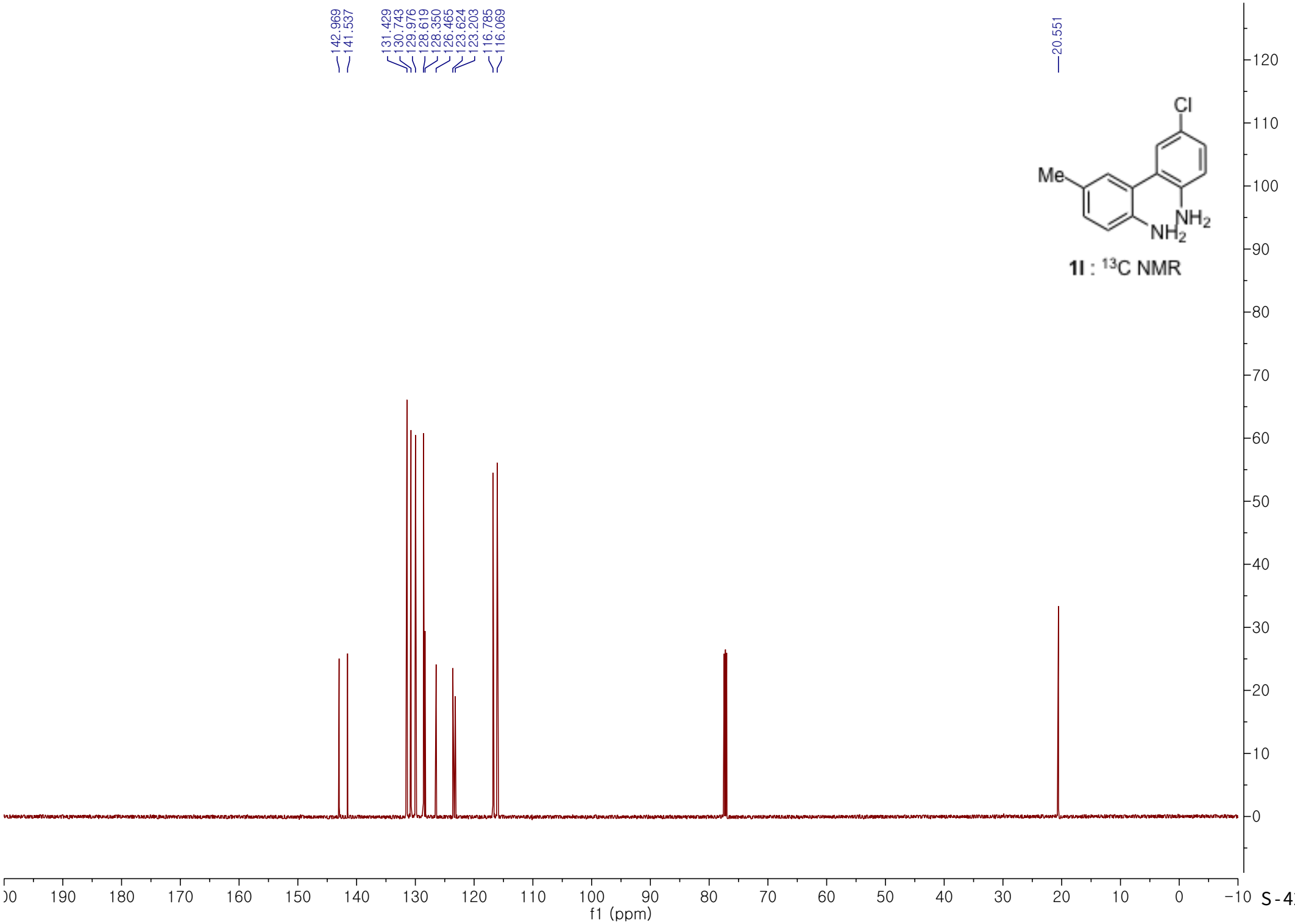
f1 (ppm)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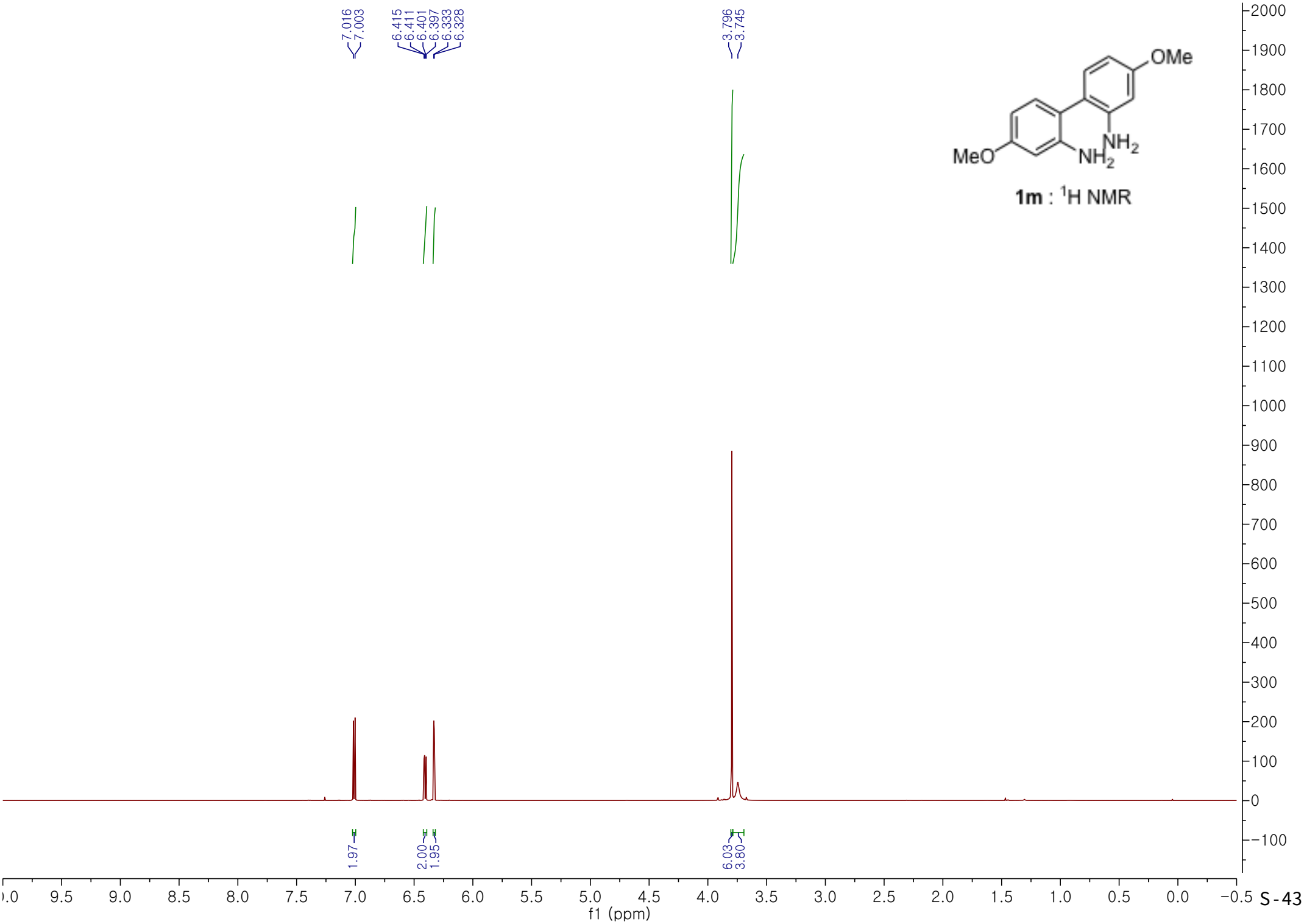
f1 (ppm)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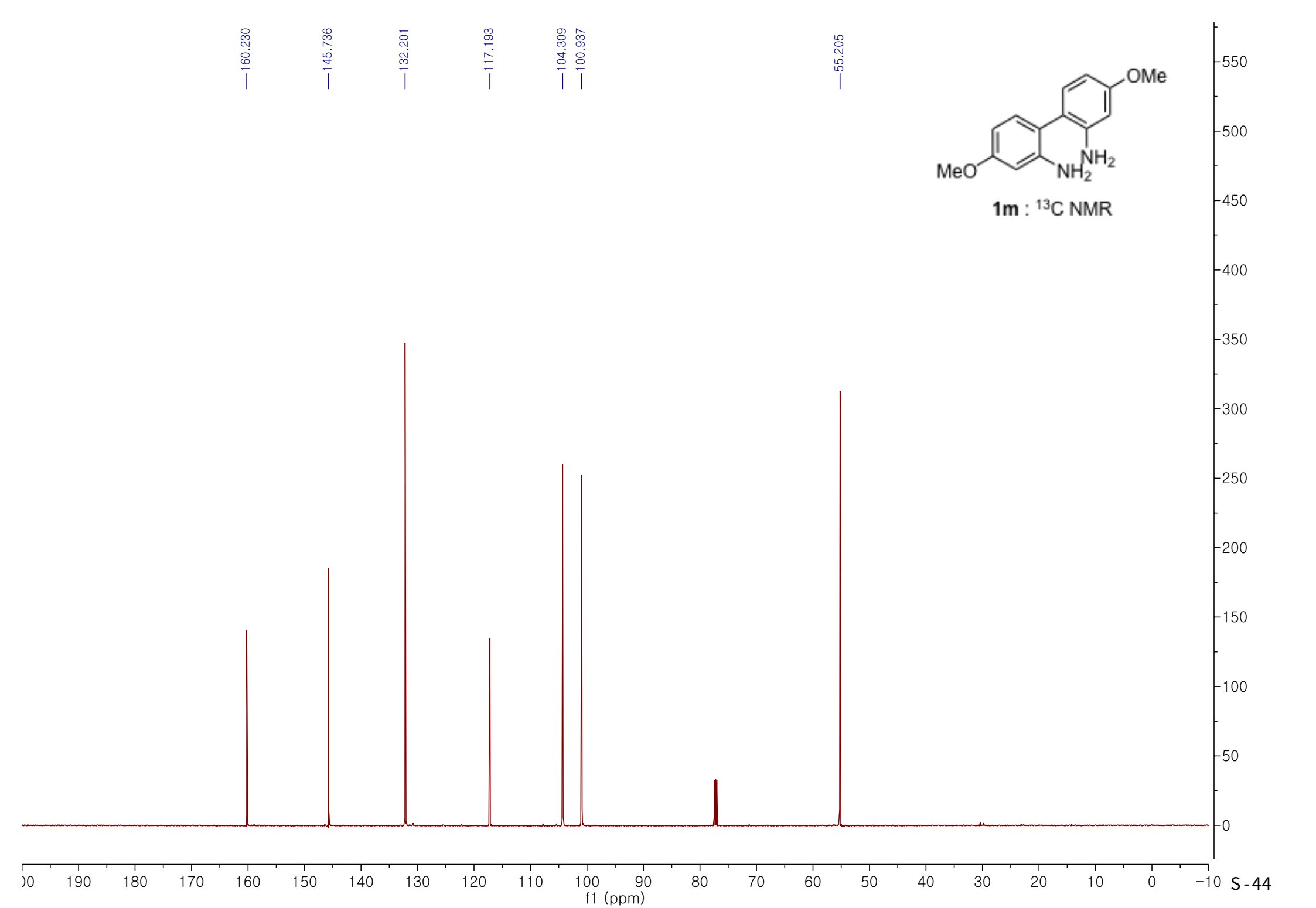
3.80
f1 (ppm)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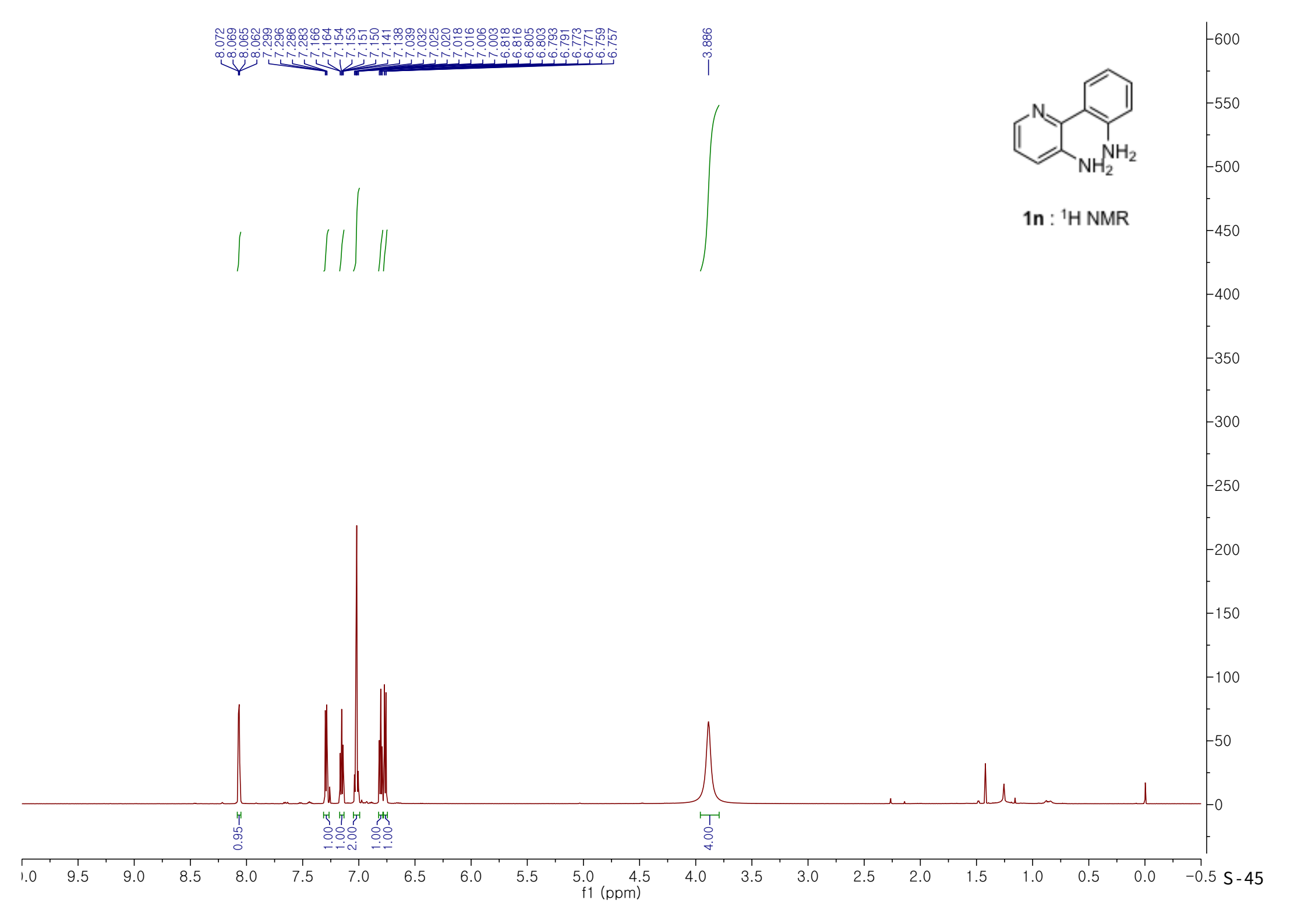
f1 (ppm)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7.151
7.150
7.141
7.138
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7.032
7.025
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7.018
7.016
7.006
7.003
6.818
6.816
6.805
6.803
6.793
6.791
6.773
6.771
6.759
6.757
3.886
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NH2
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1.00
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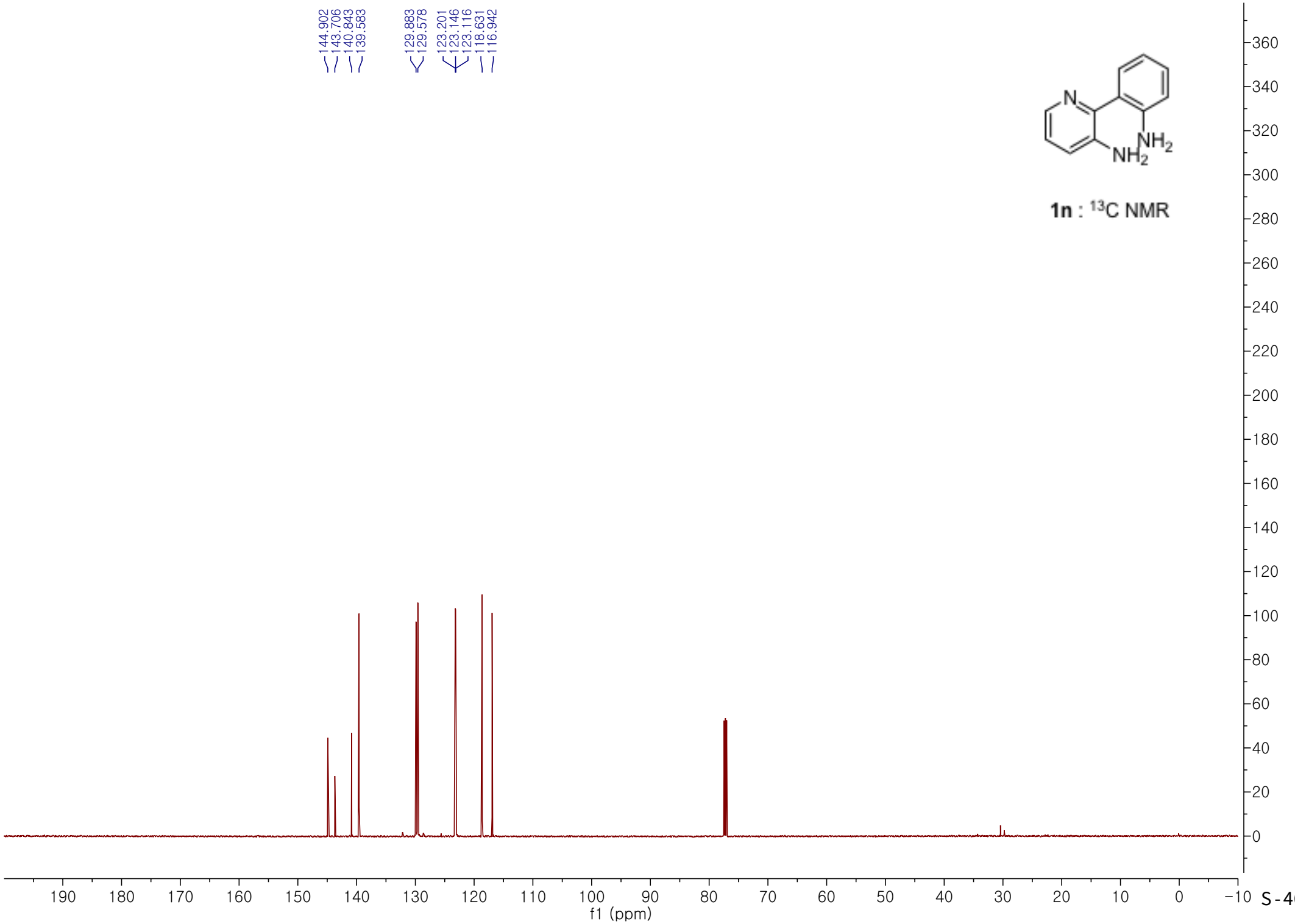
4.00
f1 (ppm)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123.116
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NH2
NH2
1n : 13C NMR
360
340
320
300
280
260
240
220
200
180
160
140
120
100
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60
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0
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170
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150
140
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120
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100
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80
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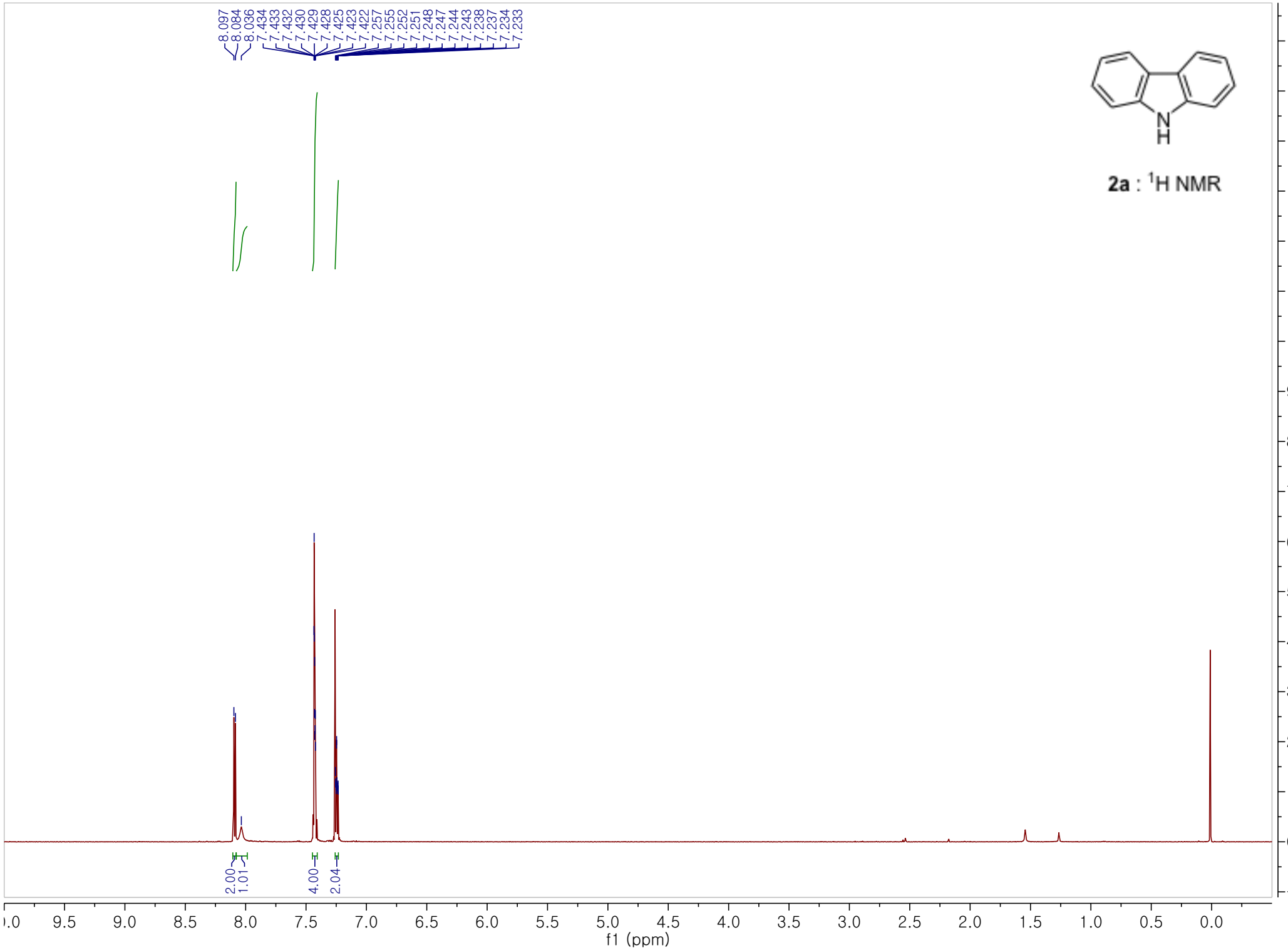
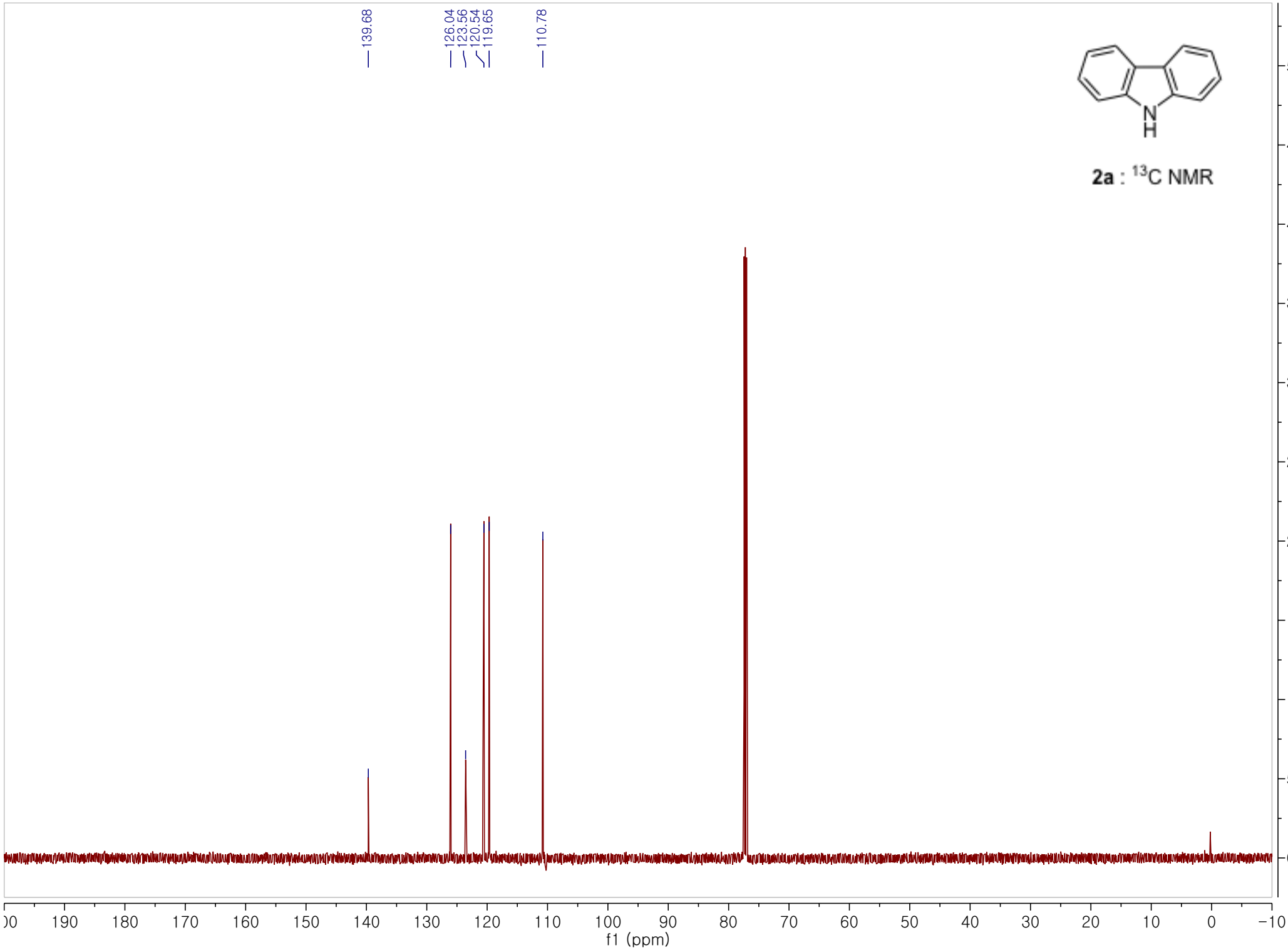
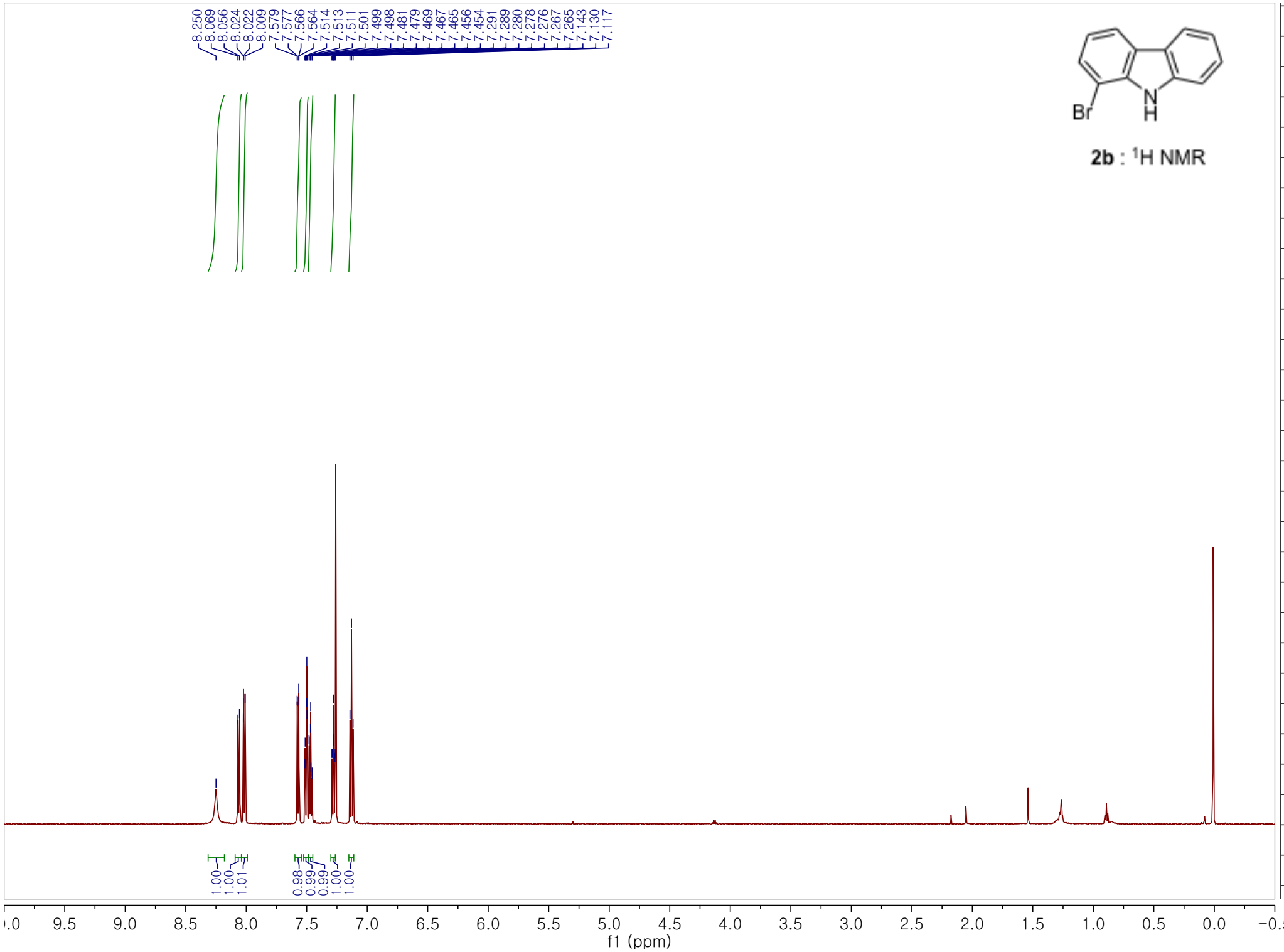
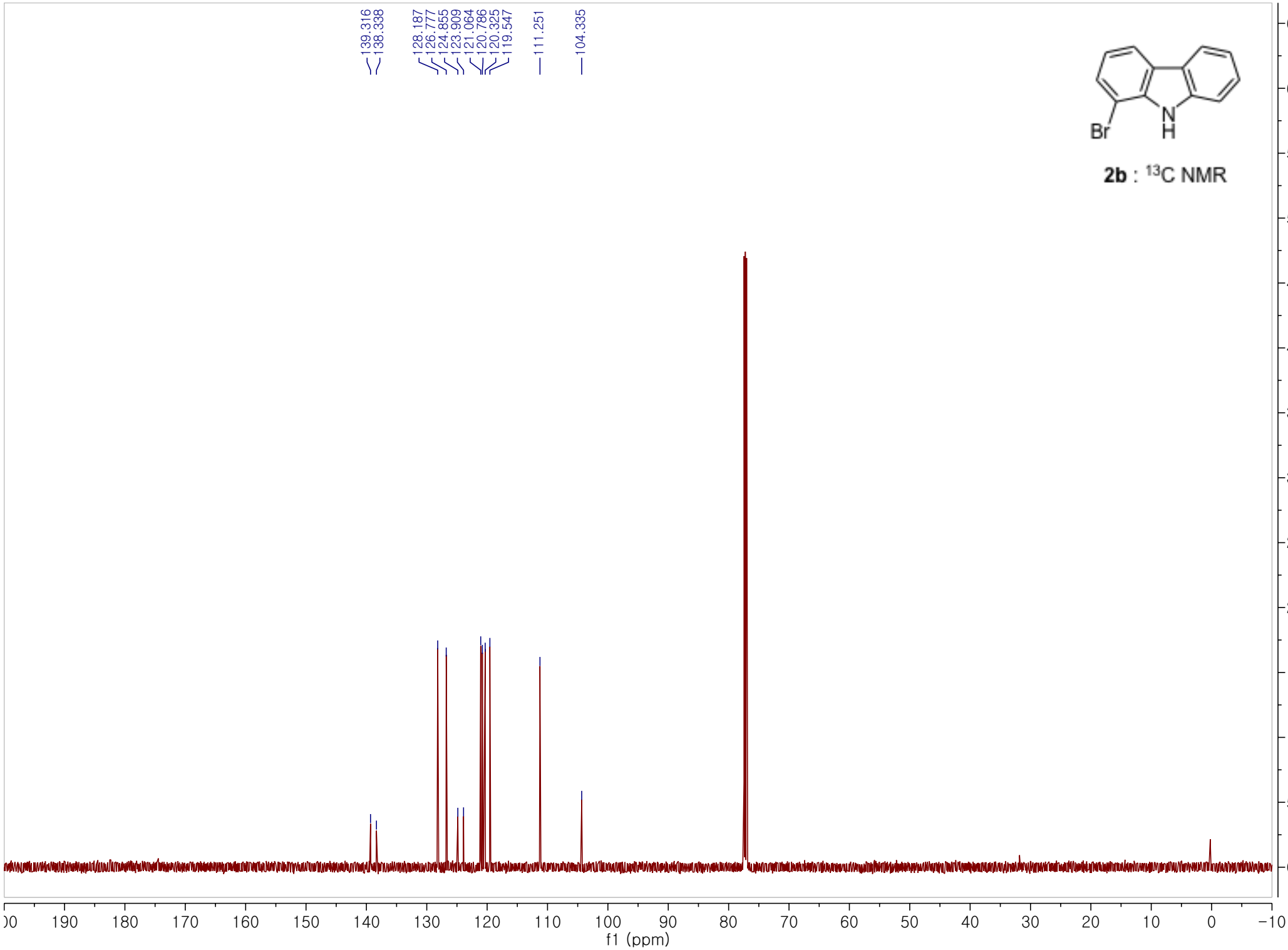
40
30
20
10
0
−10
f1 (ppm)

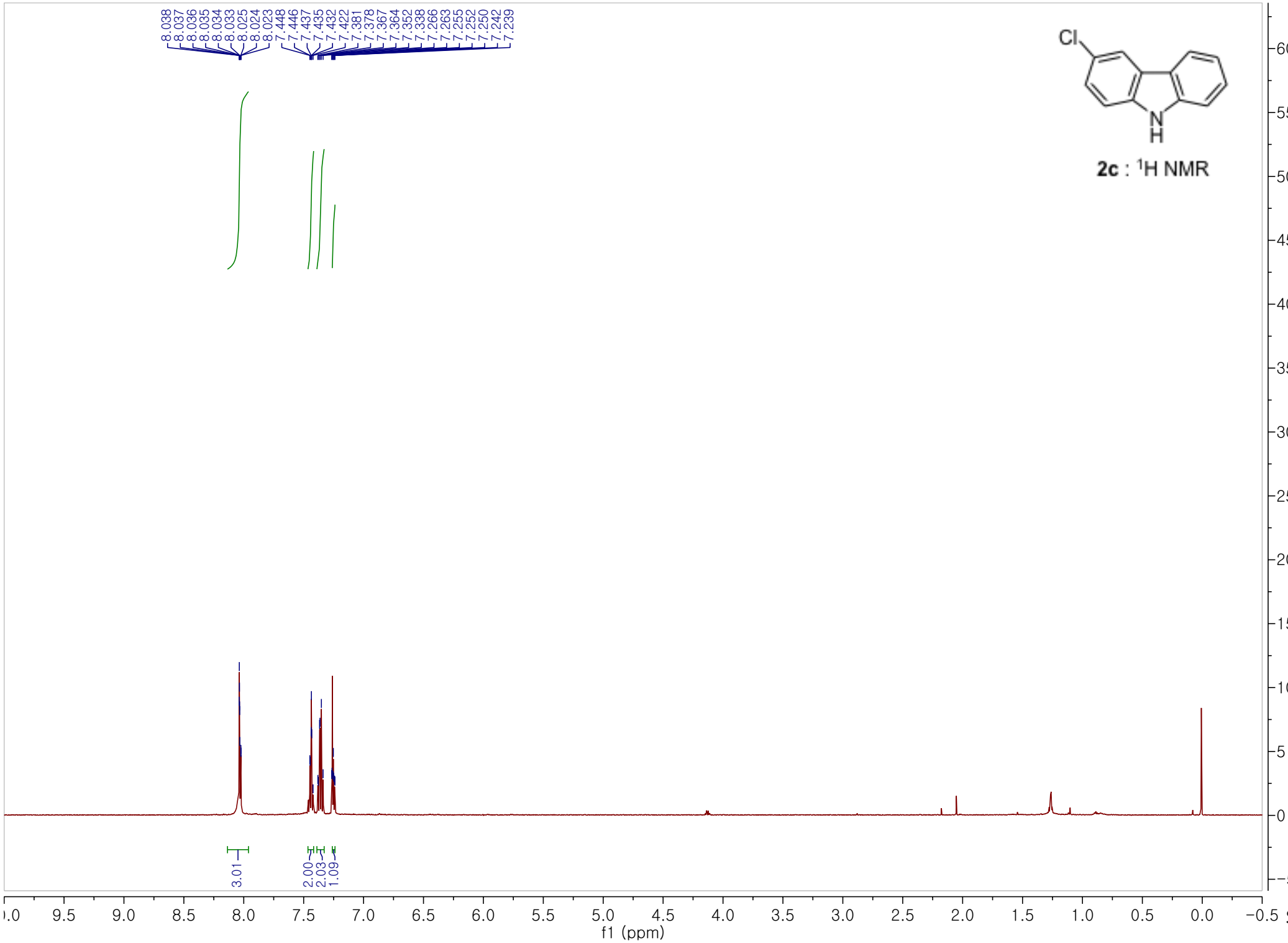

8.097
8.084
8.036
7.434
7.433
7.432
7.430
7.429
7.428
7.425
7.423
7.422
7.257
7.255
7.252
7.251
7.248
7.247
7.244
7.243
7.238
7.237
7.234
7.233
2.00
1.01
4.00
2.04
f1 (ppm)

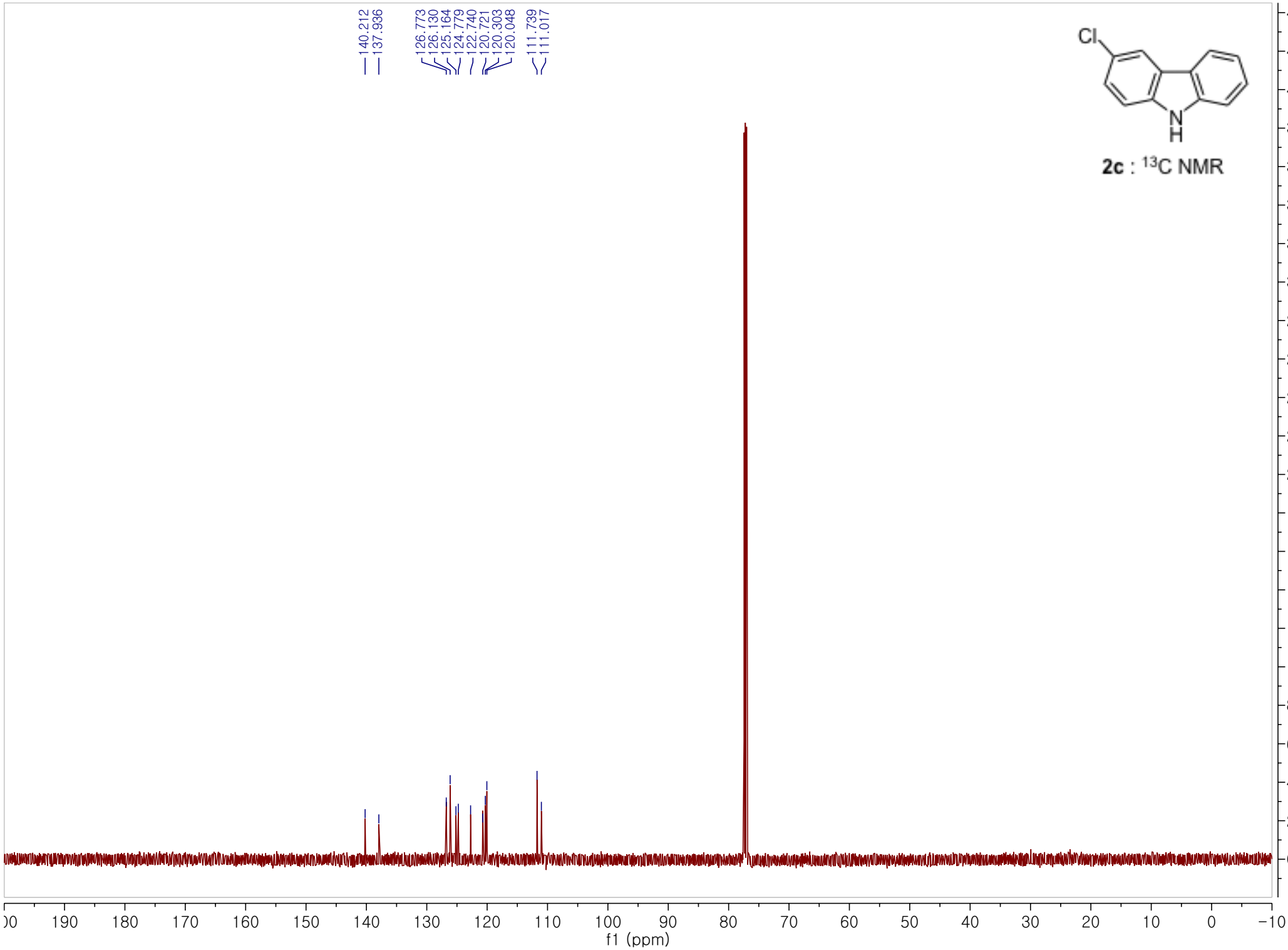
2a : ^{1}H NMR

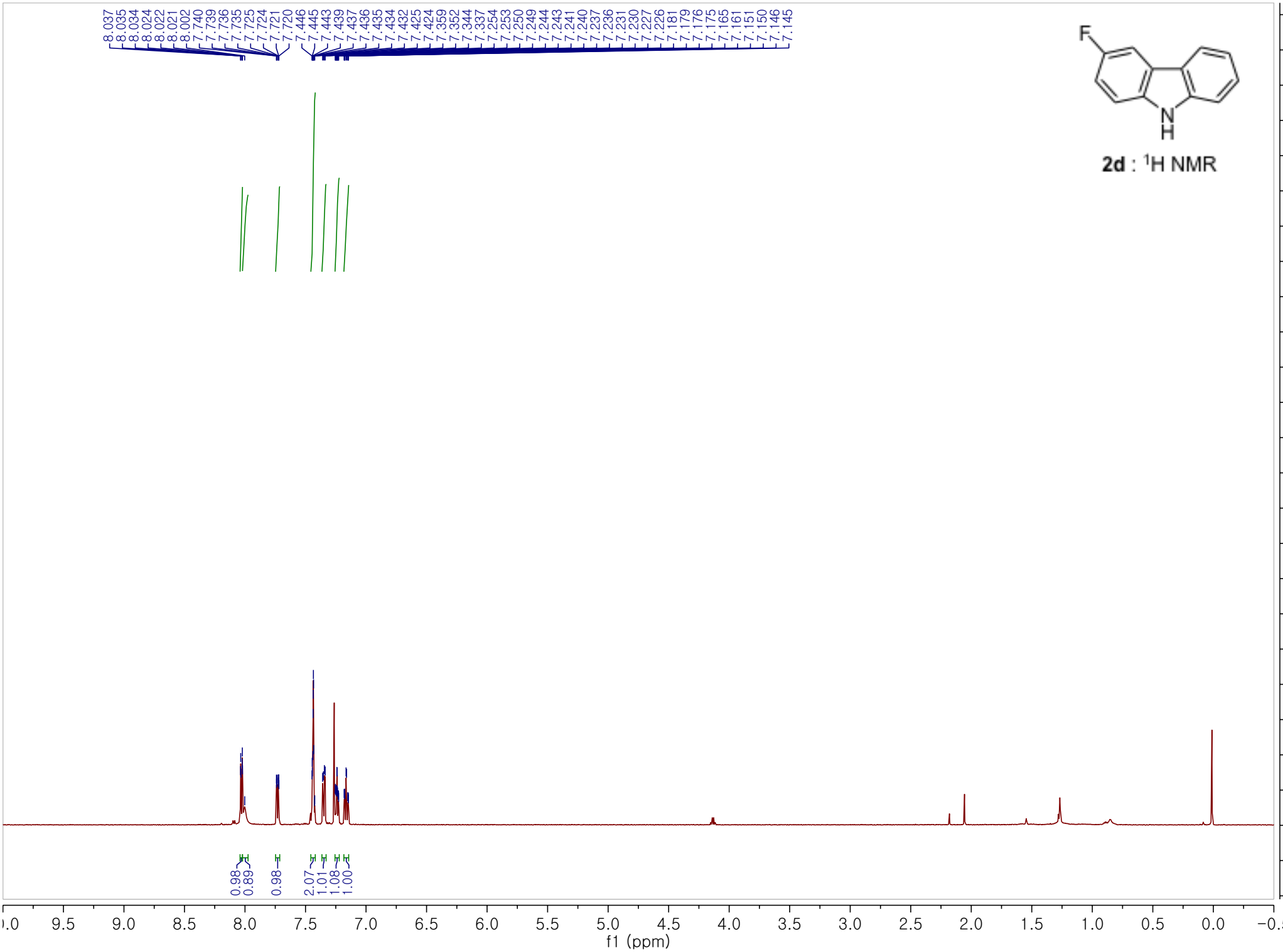

139.68
126.04
123.56
120.54
119.65
110.78
N
H
2a : 13C NMR
f1 (ppm)

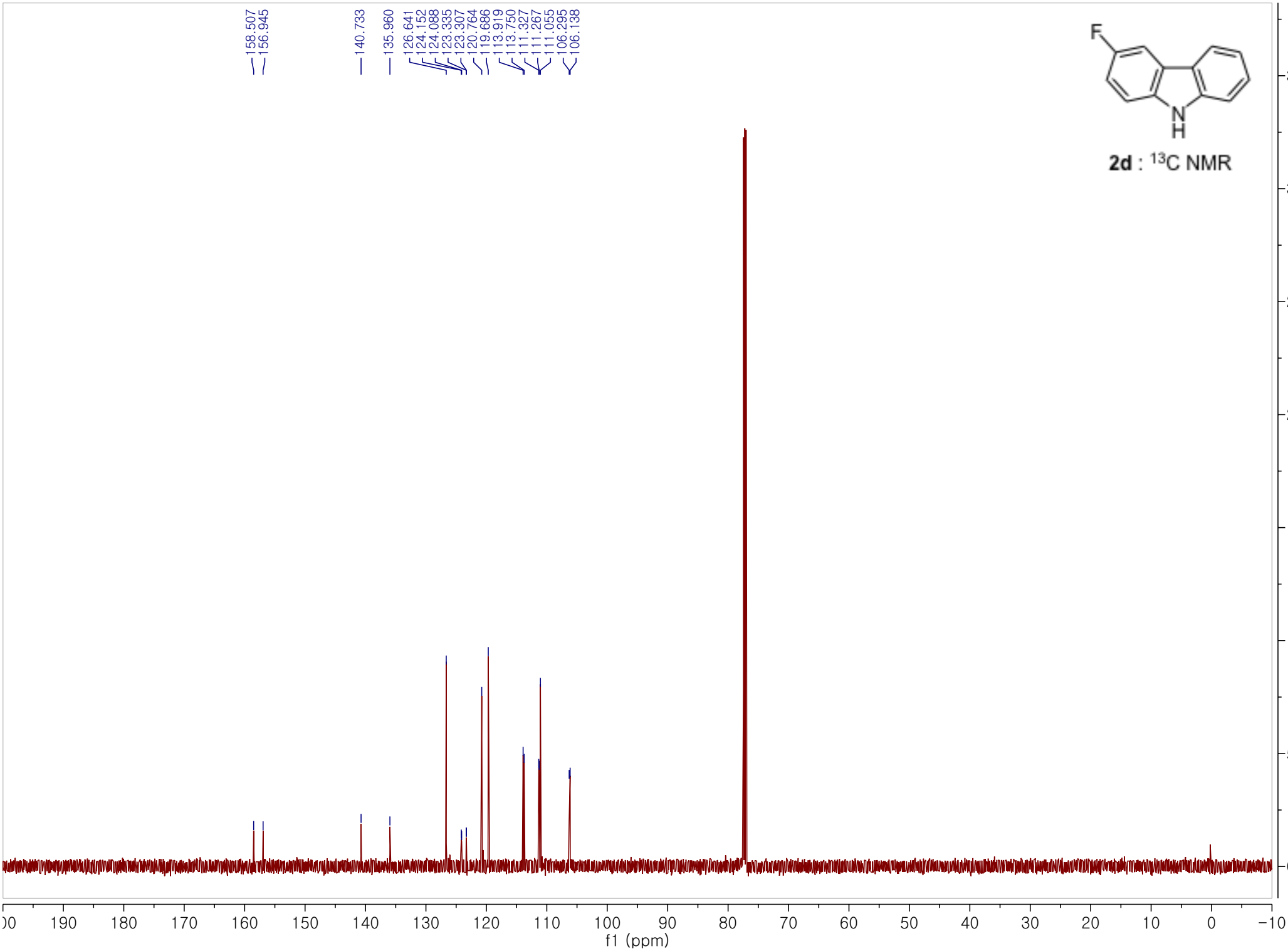

8.250
8.069
8.056
8.024
8.022
8.009
7.579
7.577
7.566
7.564
7.514
7.513
7.511
7.501
7.499
7.498
7.481
7.479
7.469
7.467
7.465
7.456
7.454
7.291
7.289
7.280
7.278
7.276
7.267
7.265
7.143
7.130
7.117
Br
N
H
2b : 1H NMR
1.00
1.00
1.01
0.98
0.99
0.99
1.00
1.00
f1 (ppm)

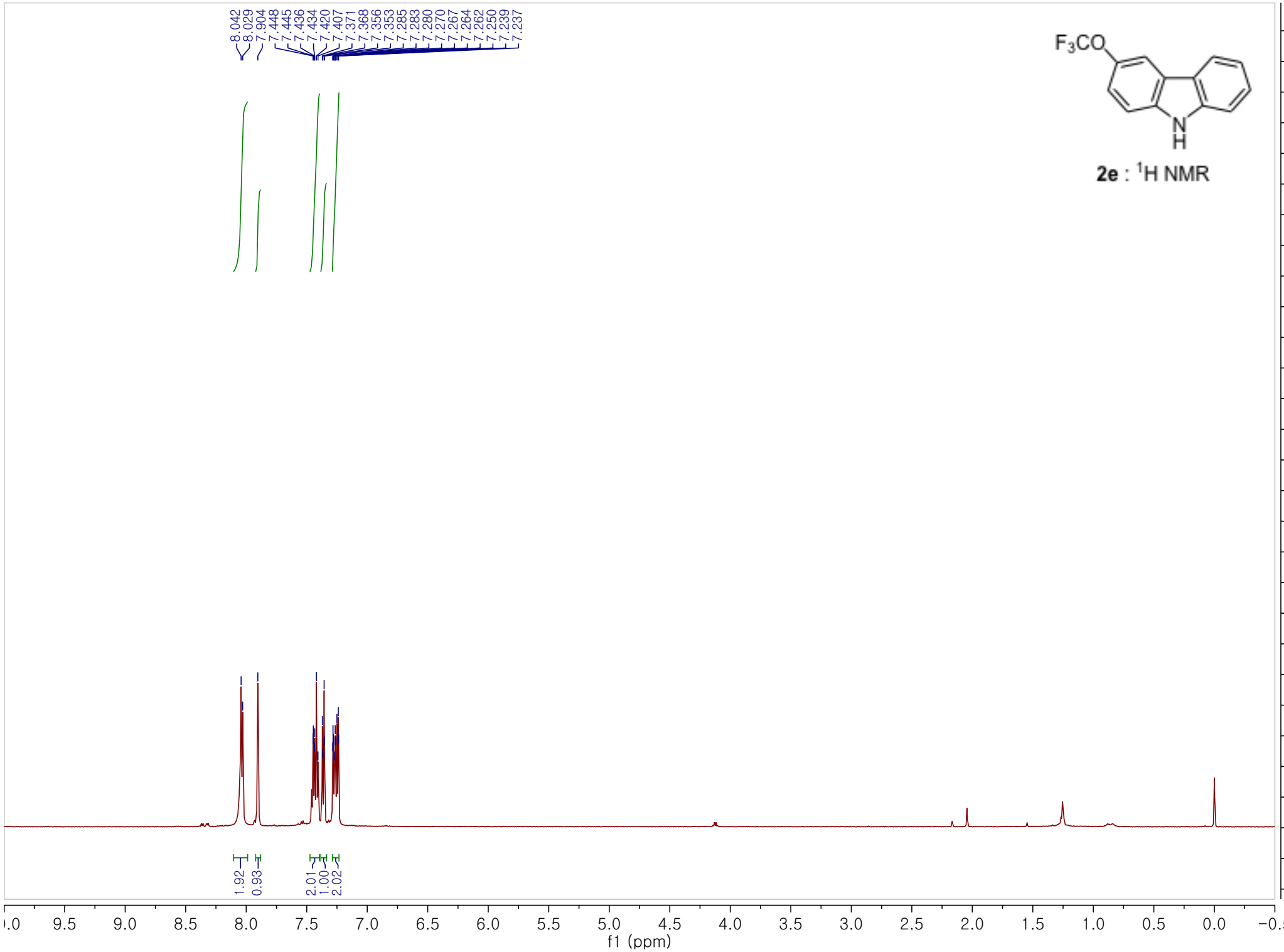

139.316
138.338
128.187
126.777
124.855
123.909
121.064
120.786
120.325
119.547
111.251
104.335
Br
N
H
2b : 13C NMR
f1 (ppm)

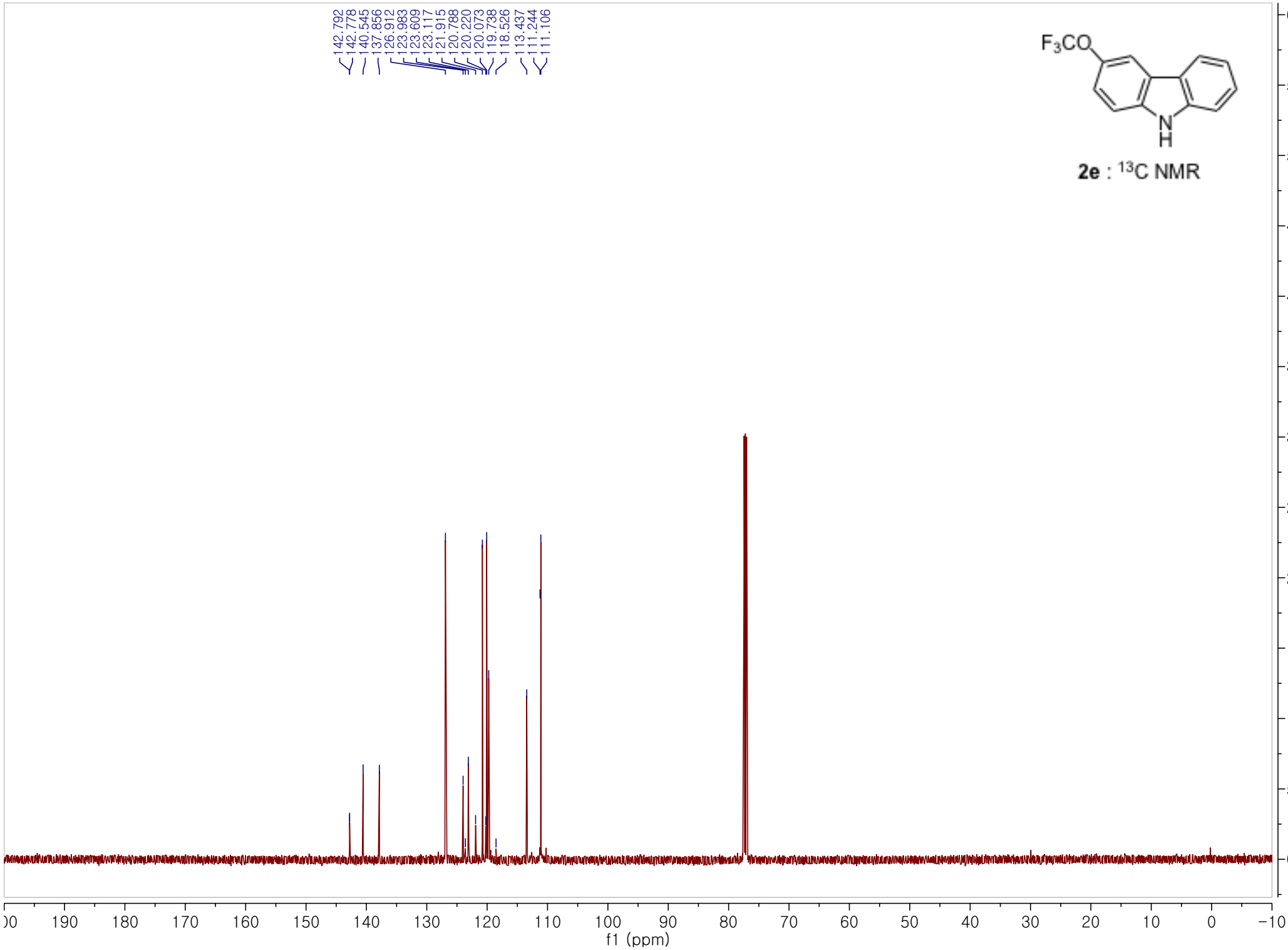

8.038
8.037
8.036
8.035
8.034
8.033
8.025
8.024
8.023
7.448
7.446
7.437
7.435
7.432
7.422
7.381
7.378
7.367
7.364
7.352
7.338
7.266
7.263
7.255
7.252
7.250
7.242
7.239
Cl
N
H
2c : 1H NMR
3.01
2.00
2.03
1.09
f1 (ppm)

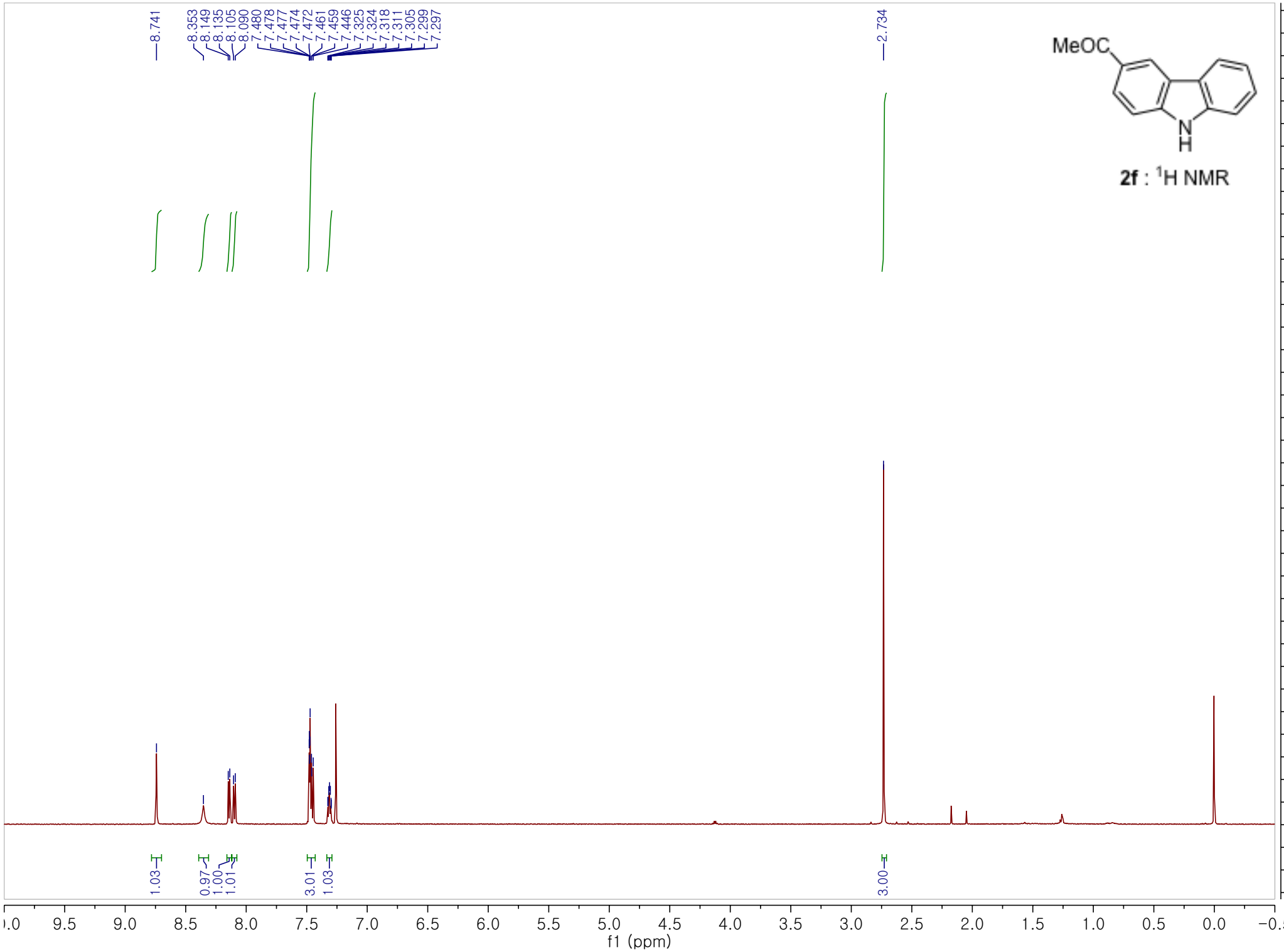

140.212
137.936
126.773
126.130
125.164
124.779
122.740
120.721
120.303
120.048
111.739
111.017
Cl
N
H
2c : 13C NMR
f1 (ppm)

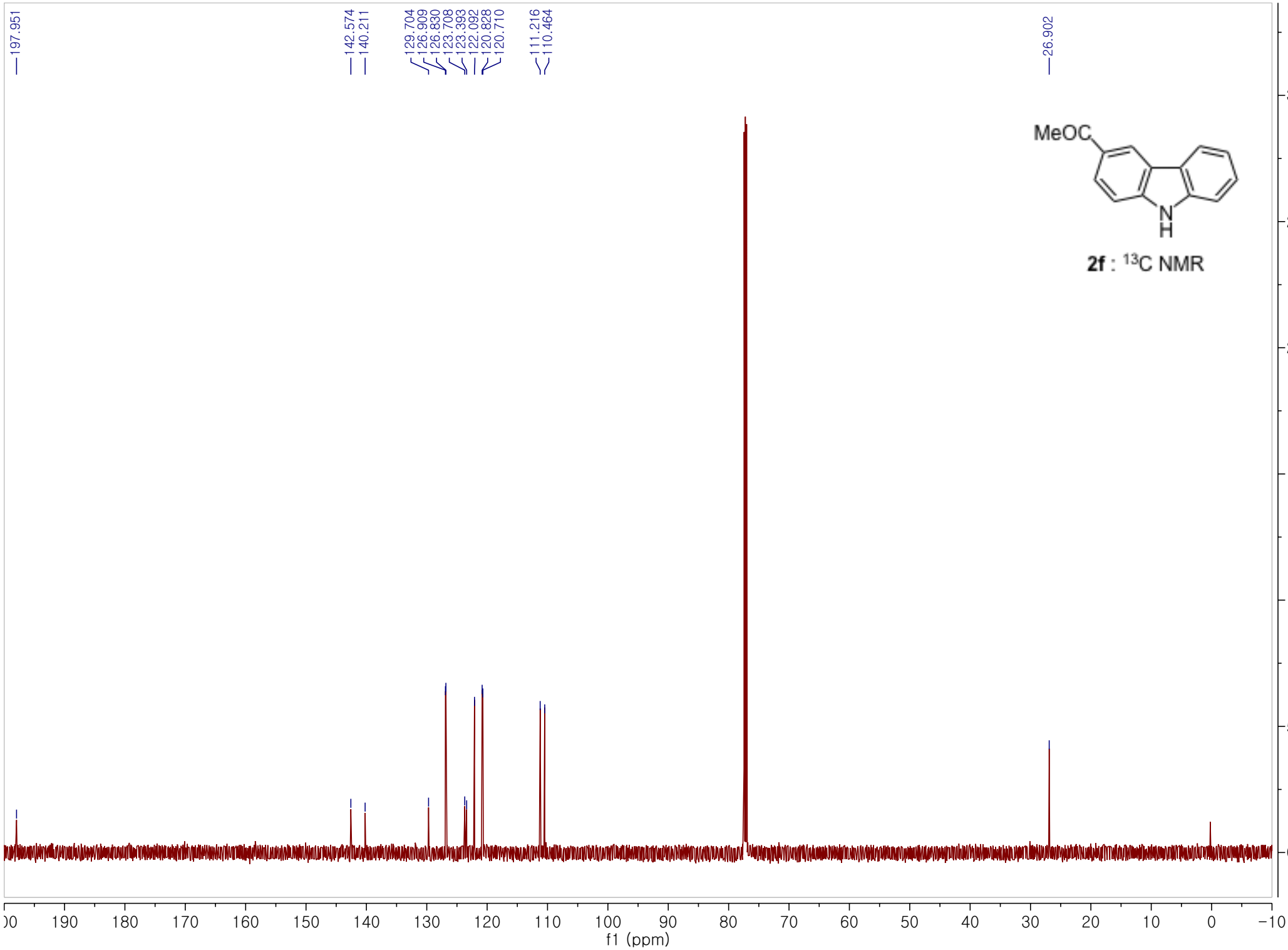

8.037
8.035
8.034
8.024
8.022
8.021
8.002
7.740
7.739
7.736
7.735
7.725
7.724
7.721
7.720
7.446
7.445
7.443
7.439
7.437
7.436
7.435
7.434
7.432
7.425
7.424
7.359
7.352
7.344
7.337
7.254
7.253
7.250
7.249
7.244
7.243
7.241
7.240
7.237
7.236
7.231
7.230
7.227
7.226
7.181
7.179
7.176
7.175
7.165
7.161
7.151
7.150
7.146
7.145
F
N
H
2d : 1H NMR
0.98
0.89
0.98
2.07
1.01
1.08
1.00
f1 (ppm)

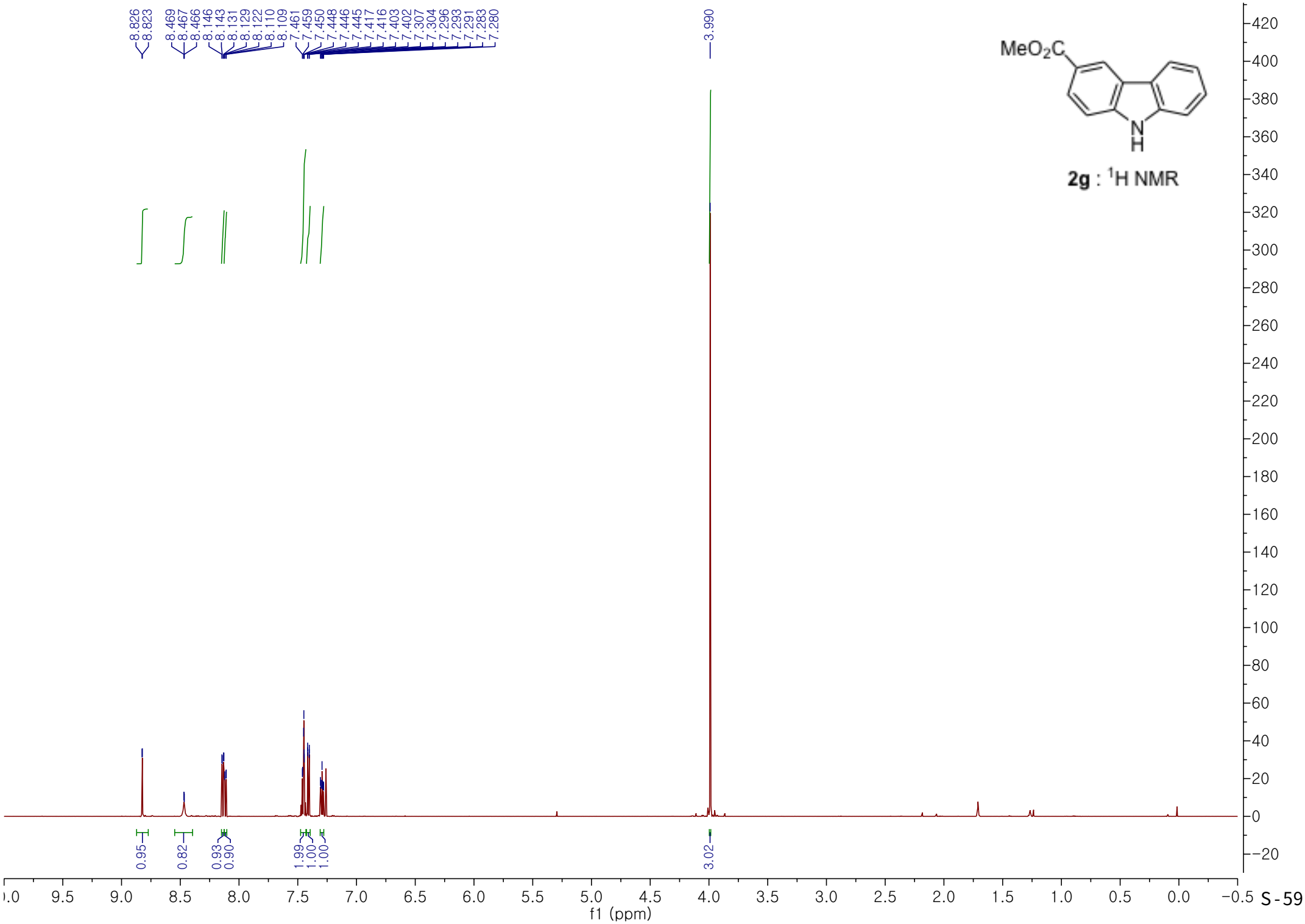

158.507
156.945
140.733
135.960
126.641
124.152
124.088
123.335
123.307
120.764
119.686
113.919
113.750
111.327
111.267
111.055
106.295
106.138
F
N
H
2d : 13C NMR
f1 (ppm)

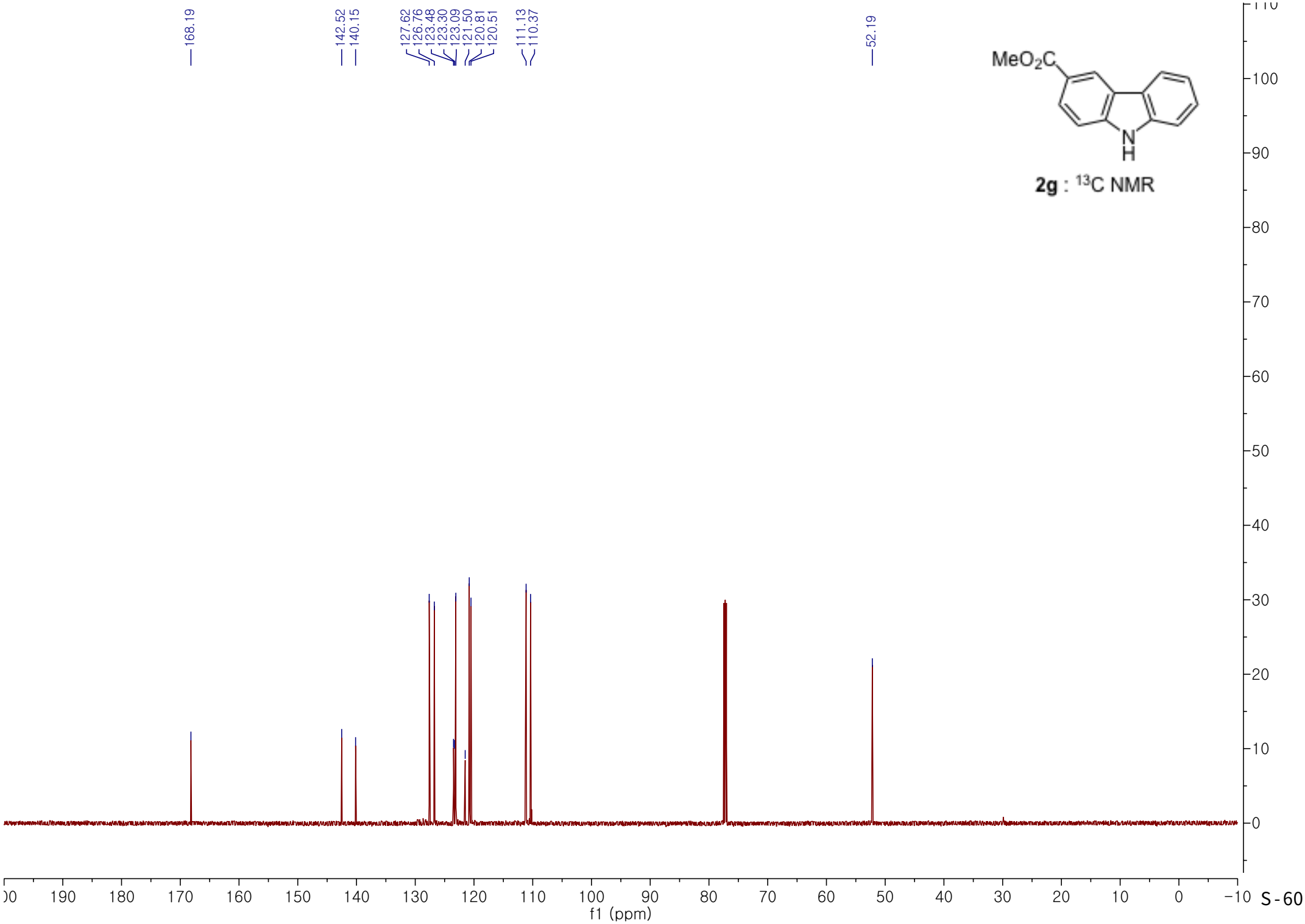

8.042
8.029
7.904
7.448
7.445
7.436
7.434
7.420
7.407
7.371
7.368
7.356
7.353
7.285
7.283
7.280
7.270
7.267
7.264
7.262
7.250
7.239
7.237
F3CO
N
H
2e : 1H NMR
1.92
0.93
2.01
1.00
2.02
f1 (ppm)

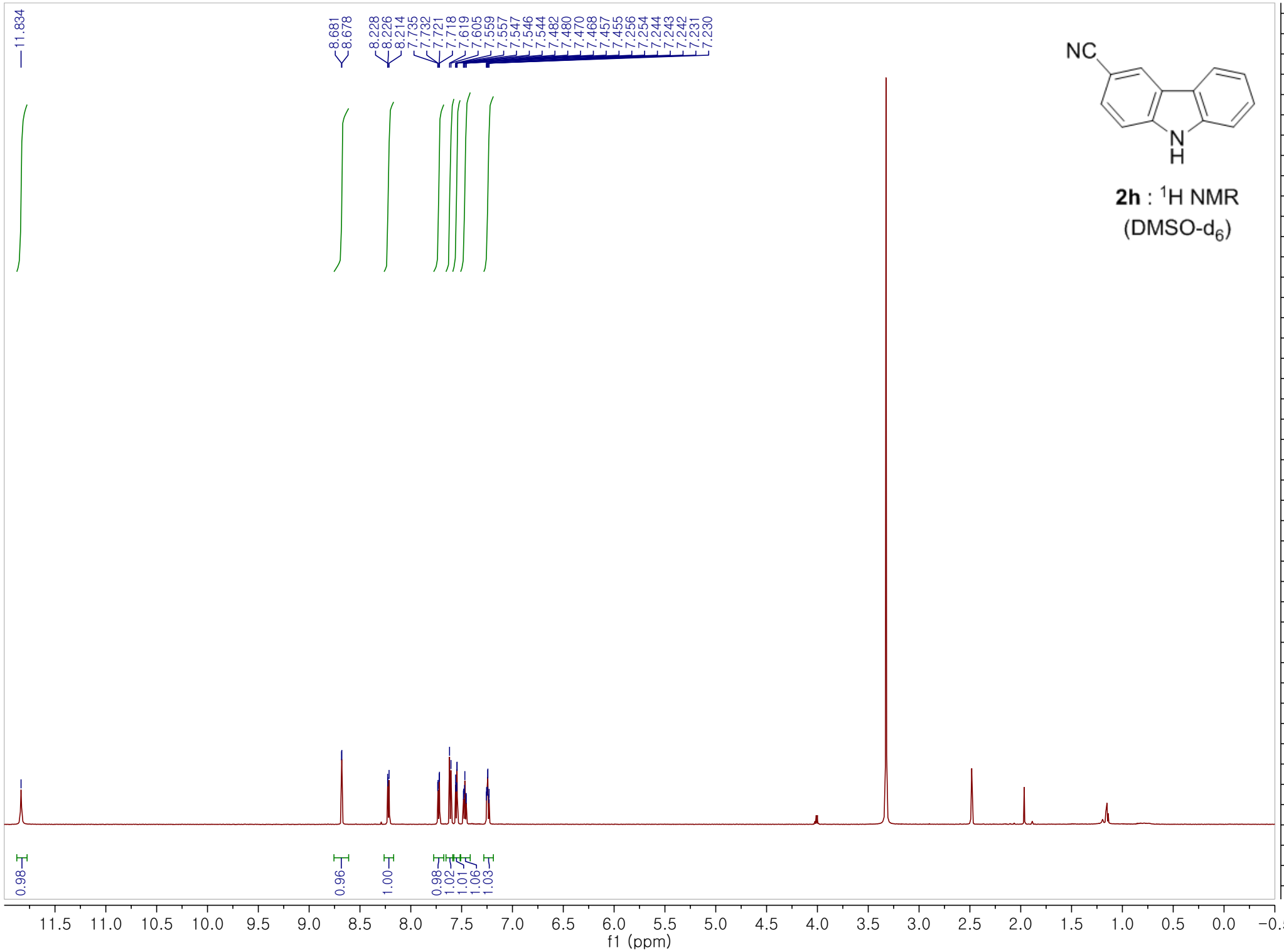

142.792
142.778
140.545
137.856
126.912
123.983
123.609
123.117
121.915
120.788
120.220
120.073
119.738
118.526
113.437
111.244
111.106
F3CO
N
H
2e : 13C NMR
f1 (ppm)

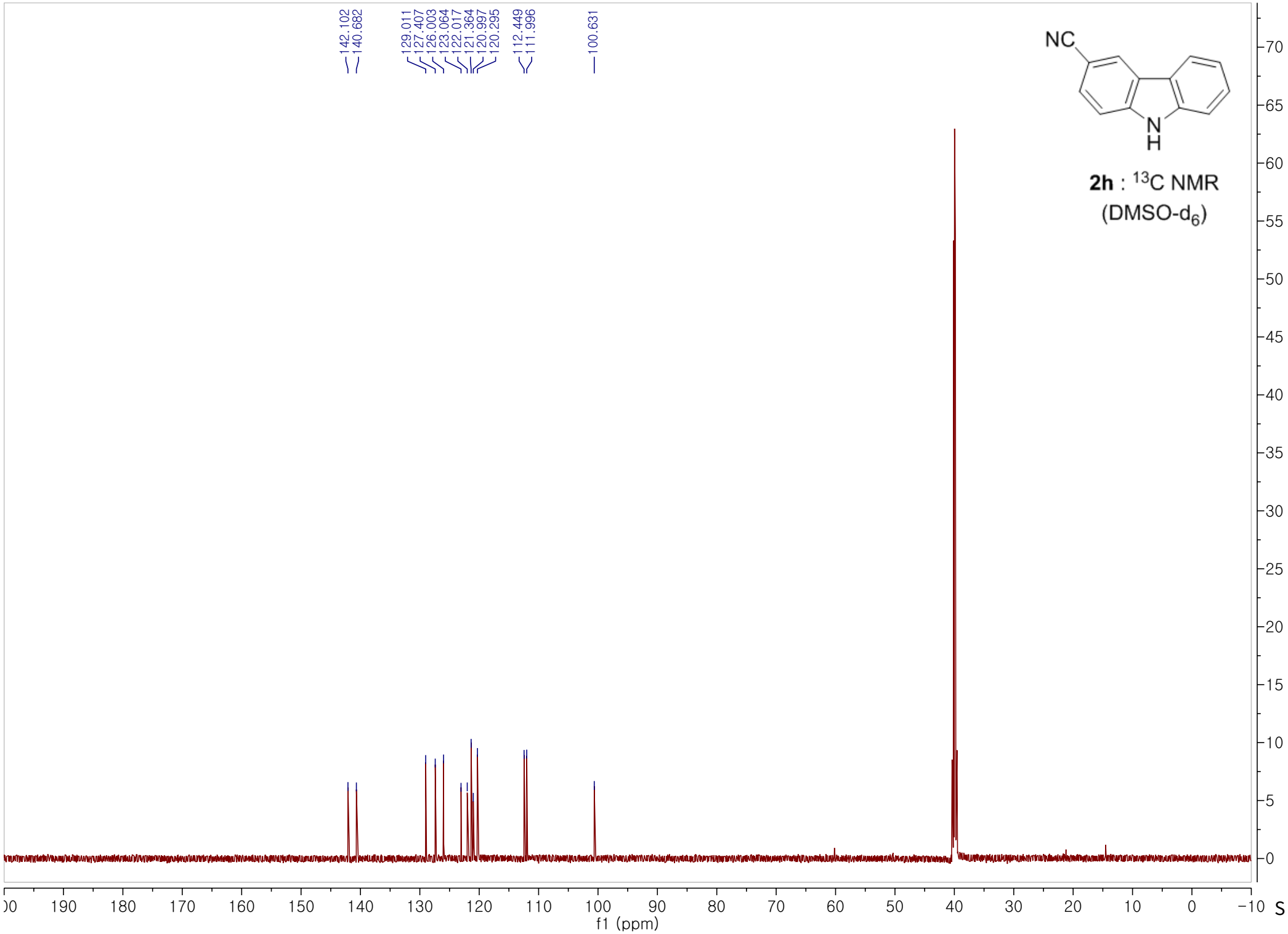

8.741
8.353
8.149
8.135
8.105
8.090
7.480
7.478
7.477
7.474
7.472
7.461
7.459
7.446
7.325
7.324
7.318
7.311
7.305
7.299
7.297
2.734
MeOC
N
H
2f : 1H NMR
1.03
0.97
1.00
1.01
3.01
1.03
3.00
f1 (ppm)

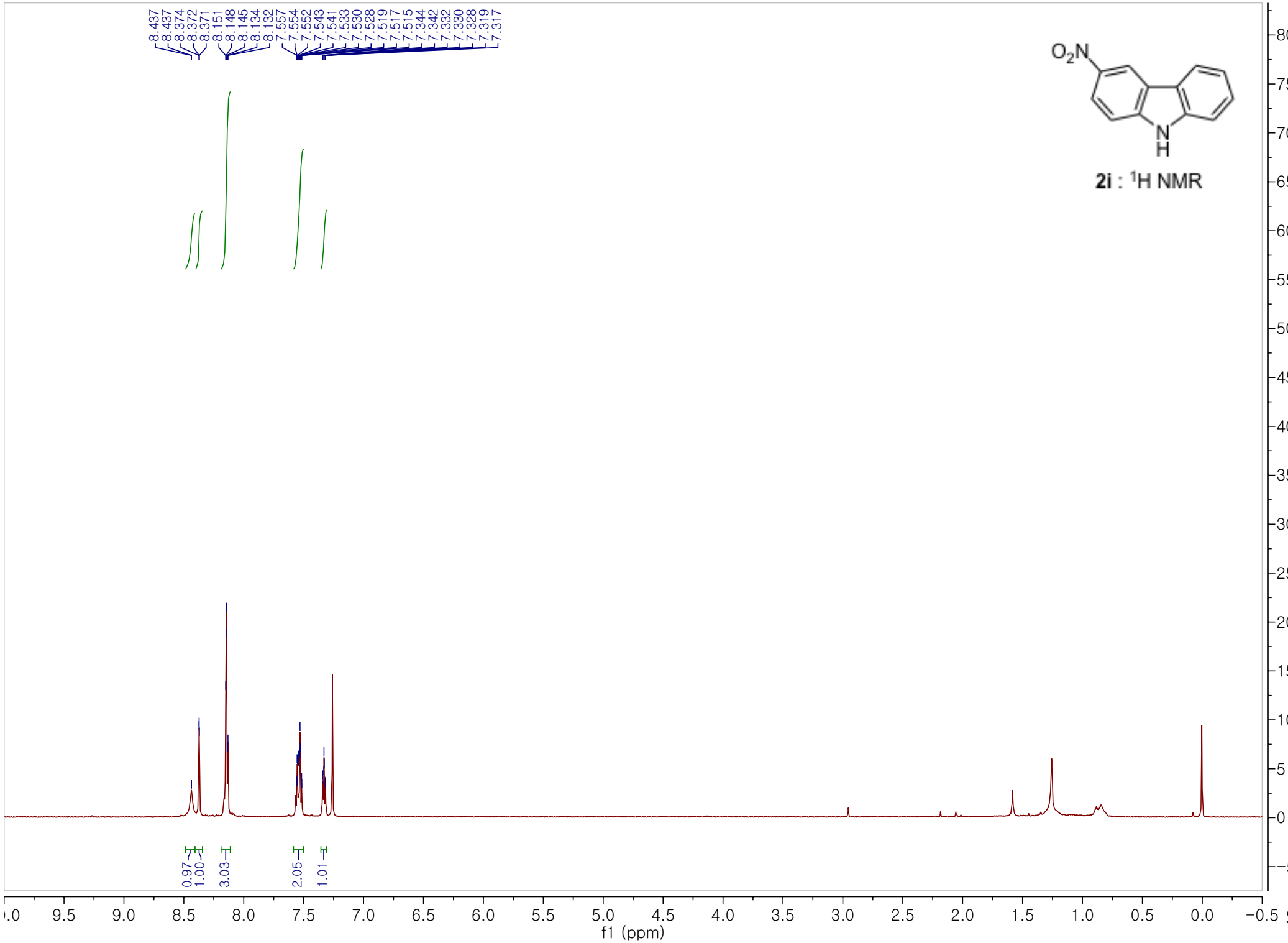

197.951
142.574
140.211
129.704
126.909
126.830
123.708
123.393
122.092
120.828
120.710
111.216
110.464
26.902
MeOC
N
H
2f : 13C NMR
f1 (ppm)

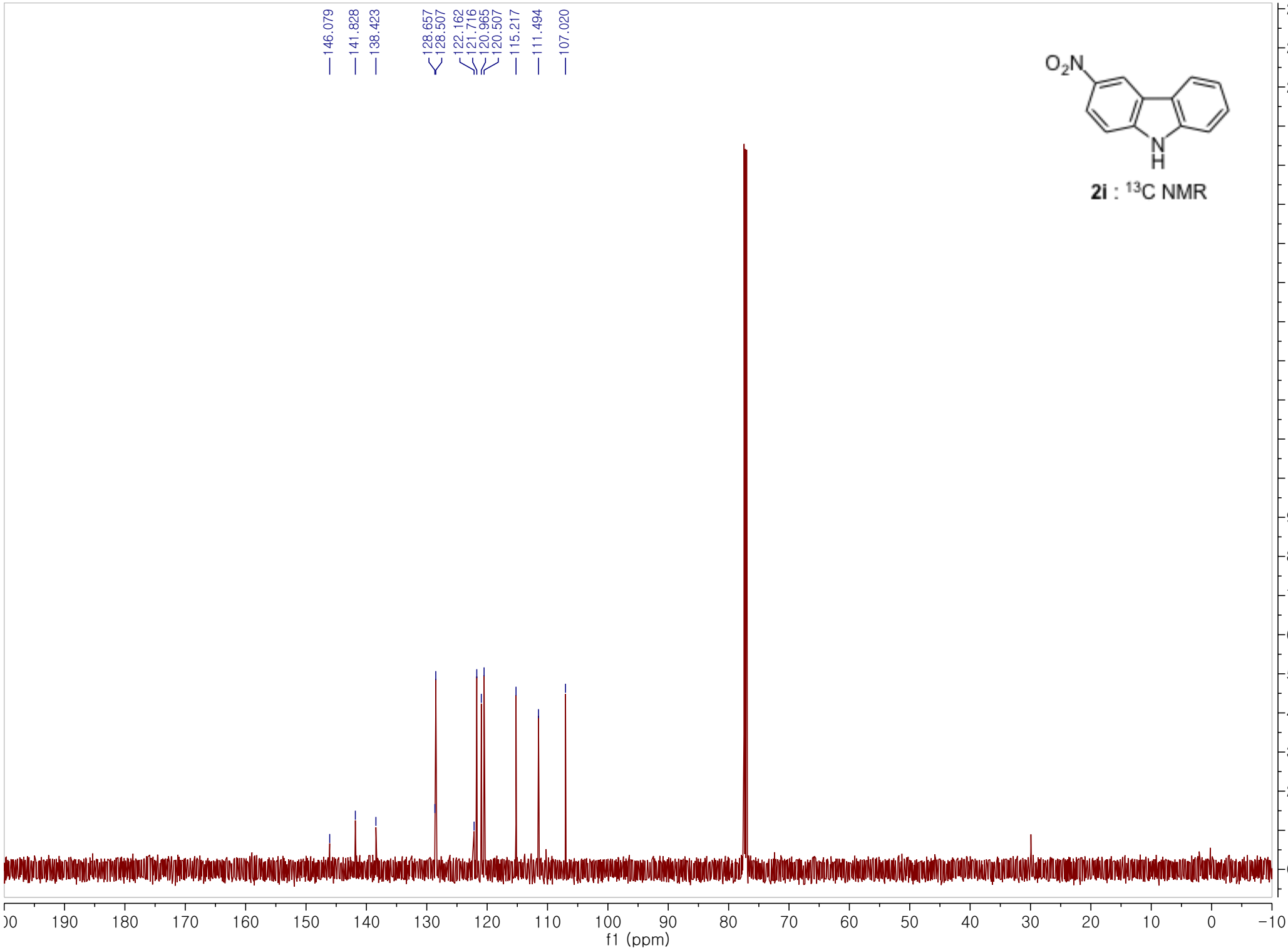

8.826
8.823
8.469
8.467
8.466
8.146
8.143
8.131
8.129
8.122
8.110
8.109
7.461
7.459
7.450
7.448
7.446
7.445
7.417
7.416
7.403
7.402
7.307
7.304
7.296
7.293
7.291
7.283
7.280
3.990
MeO2C
N
H
2g : 1H NMR
0.95
0.82
0.93
0.90
1.99
1.00
1.00
3.02
f1 (ppm)

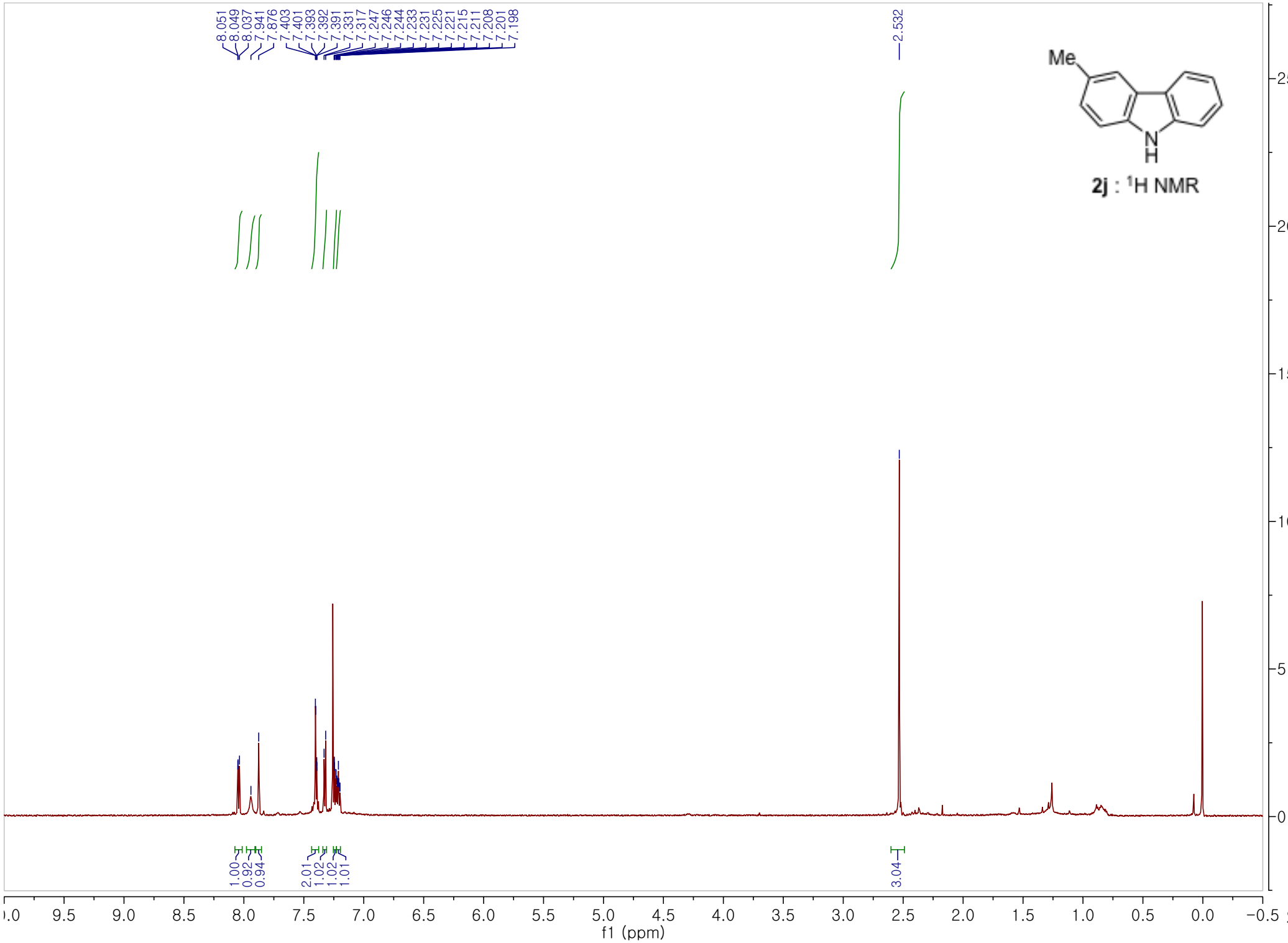

168.19
142.52
140.15
127.62
126.76
123.48
123.30
123.09
121.50
120.81
120.51
111.13
110.37
52.19
MeO2C
N
H
2g : 13C NMR
f1 (ppm)

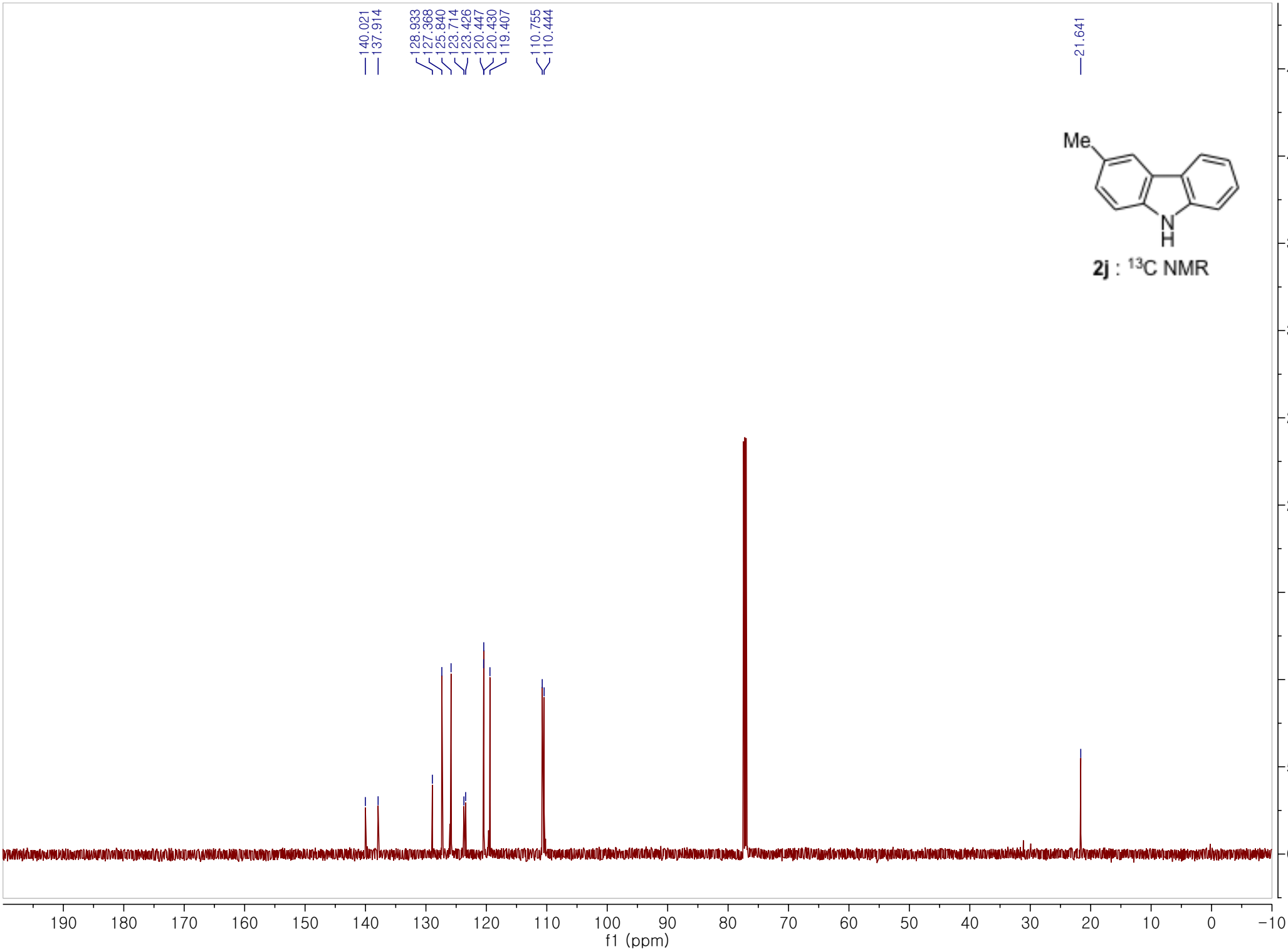

11.834
8.681
8.678
8.228
8.226
8.214
7.735
7.732
7.721
7.718
7.619
7.605
7.559
7.557
7.547
7.546
7.544
7.482
7.480
7.470
7.468
7.457
7.455
7.256
7.254
7.244
7.243
7.242
7.231
7.230
NC
N
H
2h : 1H NMR
(DMSO-d6)
0.98
0.96
1.00
0.98
1.02
1.01
1.06
1.03
f1 (ppm)

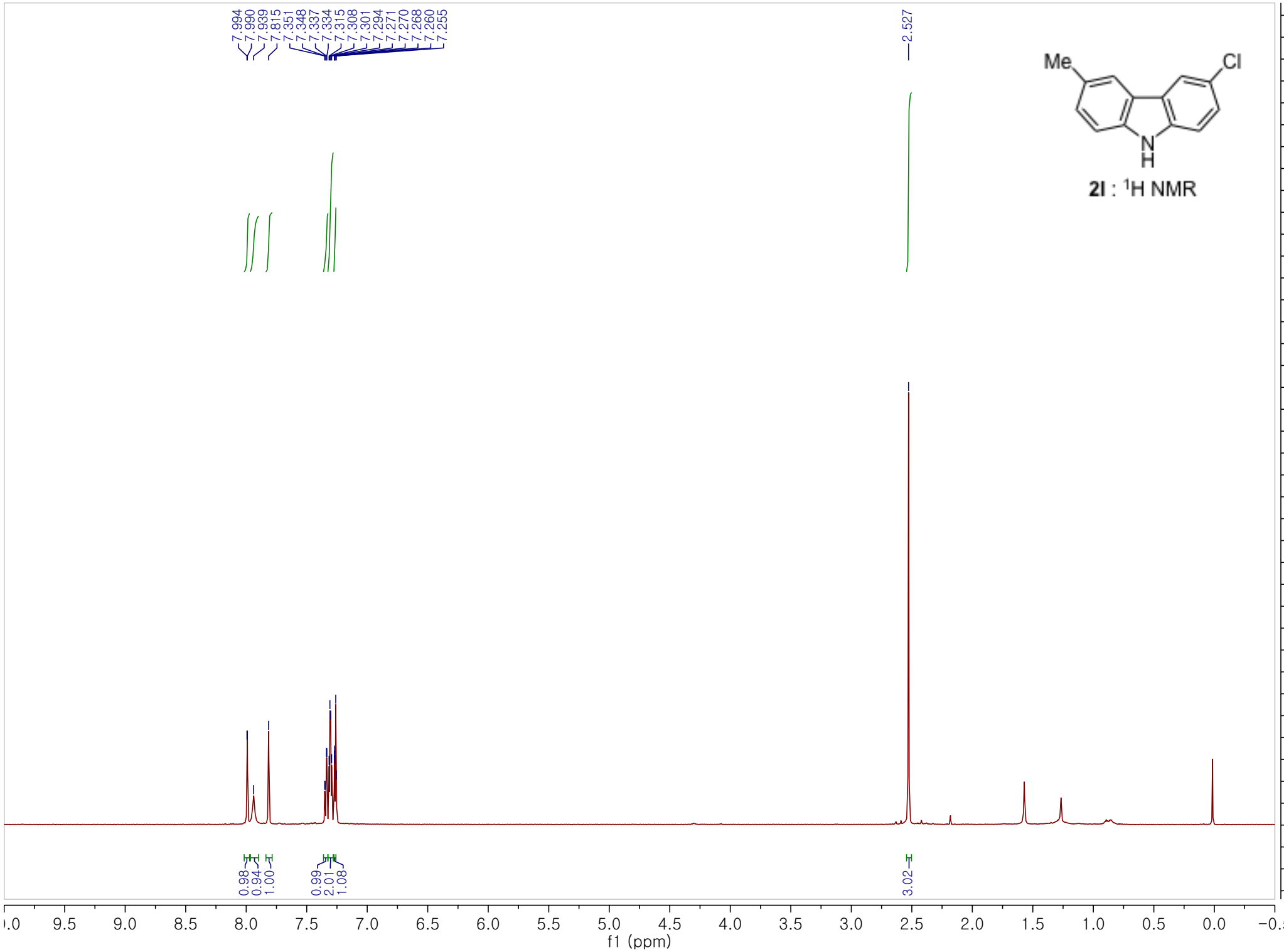

142.102
140.682
129.011
127.407
126.003
123.064
122.017
121.364
120.997
120.295
112.449
111.996
100.631
NC
N
H
2h : 13C NMR
(DMSO-d6)
f1 (ppm)

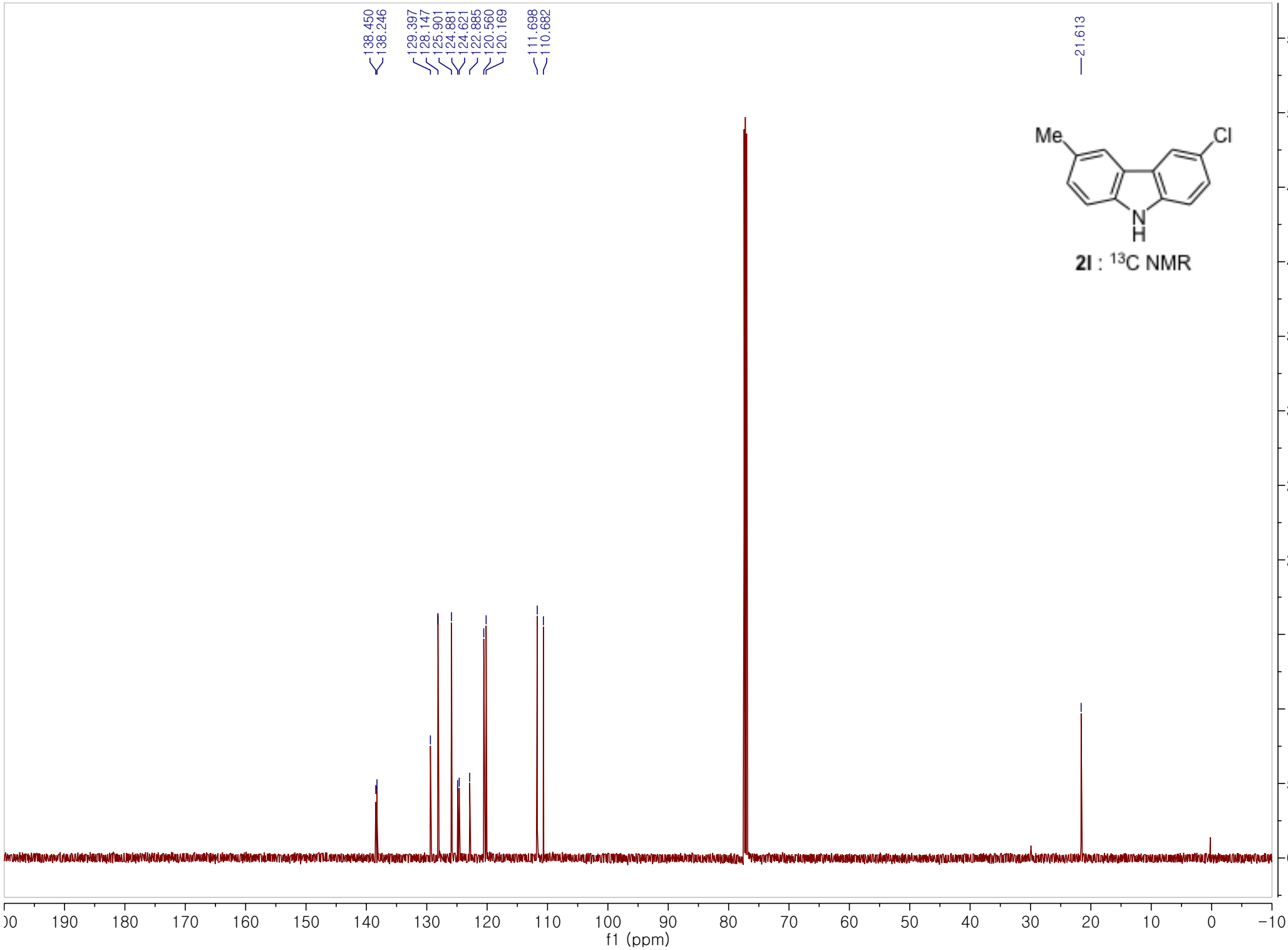

8.437
8.437
8.374
8.372
8.371
8.151
8.148
8.145
8.134
8.132
7.557
7.554
7.552
7.543
7.541
7.533
7.530
7.528
7.519
7.517
7.515
7.344
7.342
7.332
7.330
7.328
7.319
7.317
O2N
N
H
2i : 1H NMR
0.97
1.00
3.03
2.05
1.01
f1 (ppm)

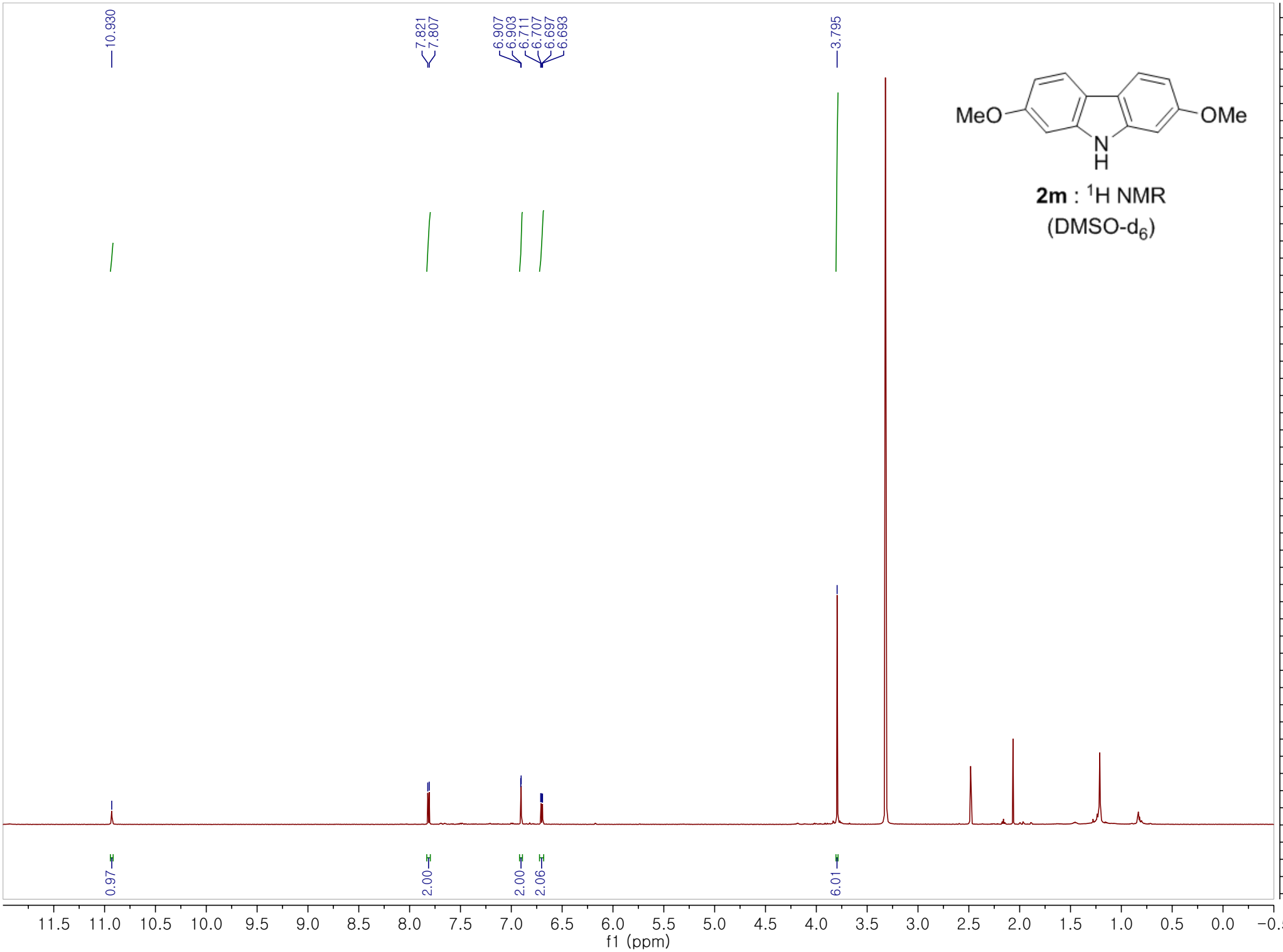

146.079
141.828
138.423
128.657
128.507
122.162
121.716
120.965
120.507
115.217
111.494
107.020
O2N
N
H
2i : 13C NMR
f1 (ppm)

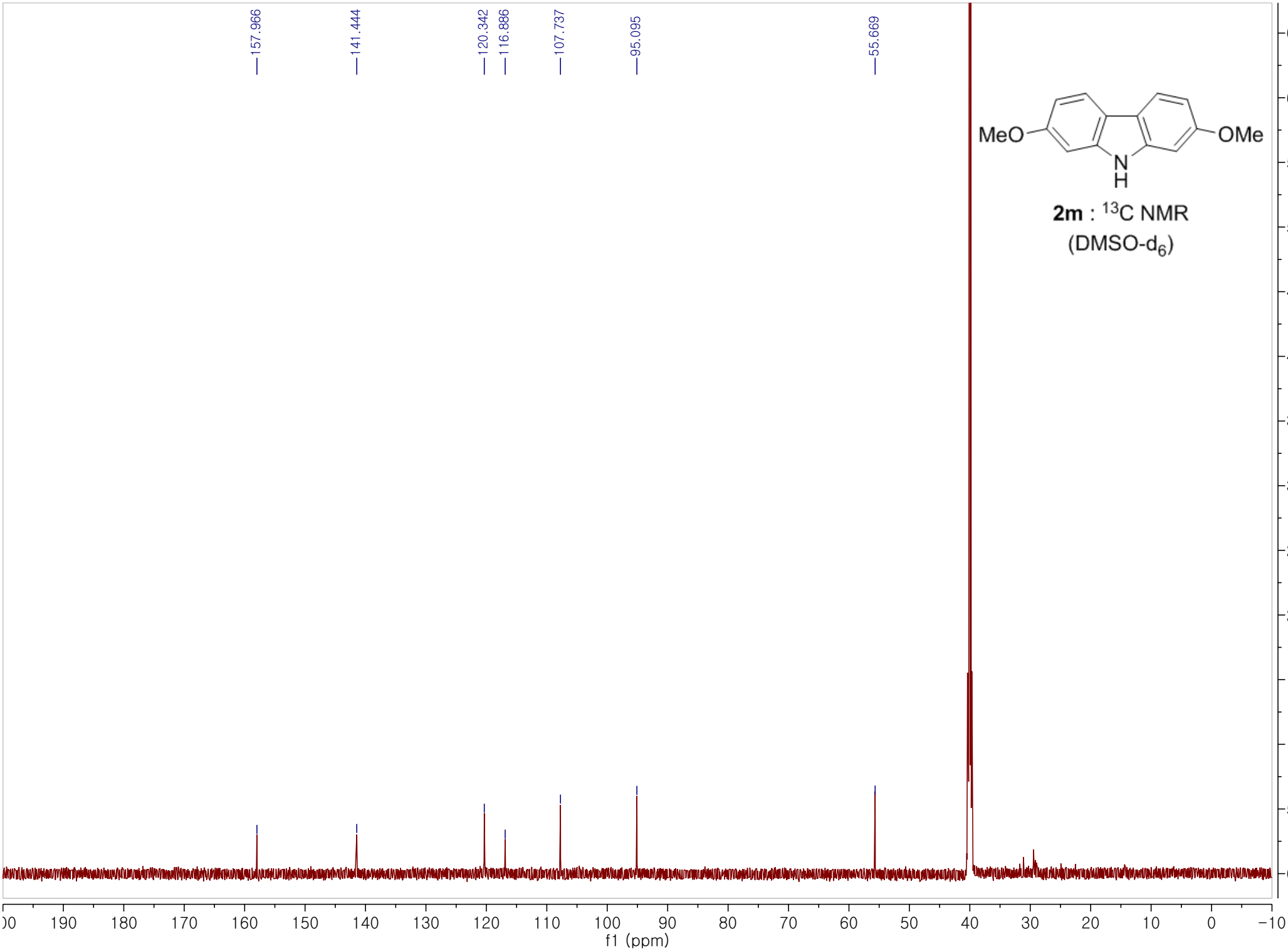

8.051
8.049
8.037
7.941
7.876
7.403
7.401
7.393
7.392
7.391
7.331
7.317
7.247
7.246
7.244
7.233
7.231
7.225
7.221
7.215
7.211
7.208
7.201
7.198
2.532
Me
N
H
2j : 1H NMR
1.00
0.92
0.94
2.01
1.02
1.02
1.01
3.04
f1 (ppm)

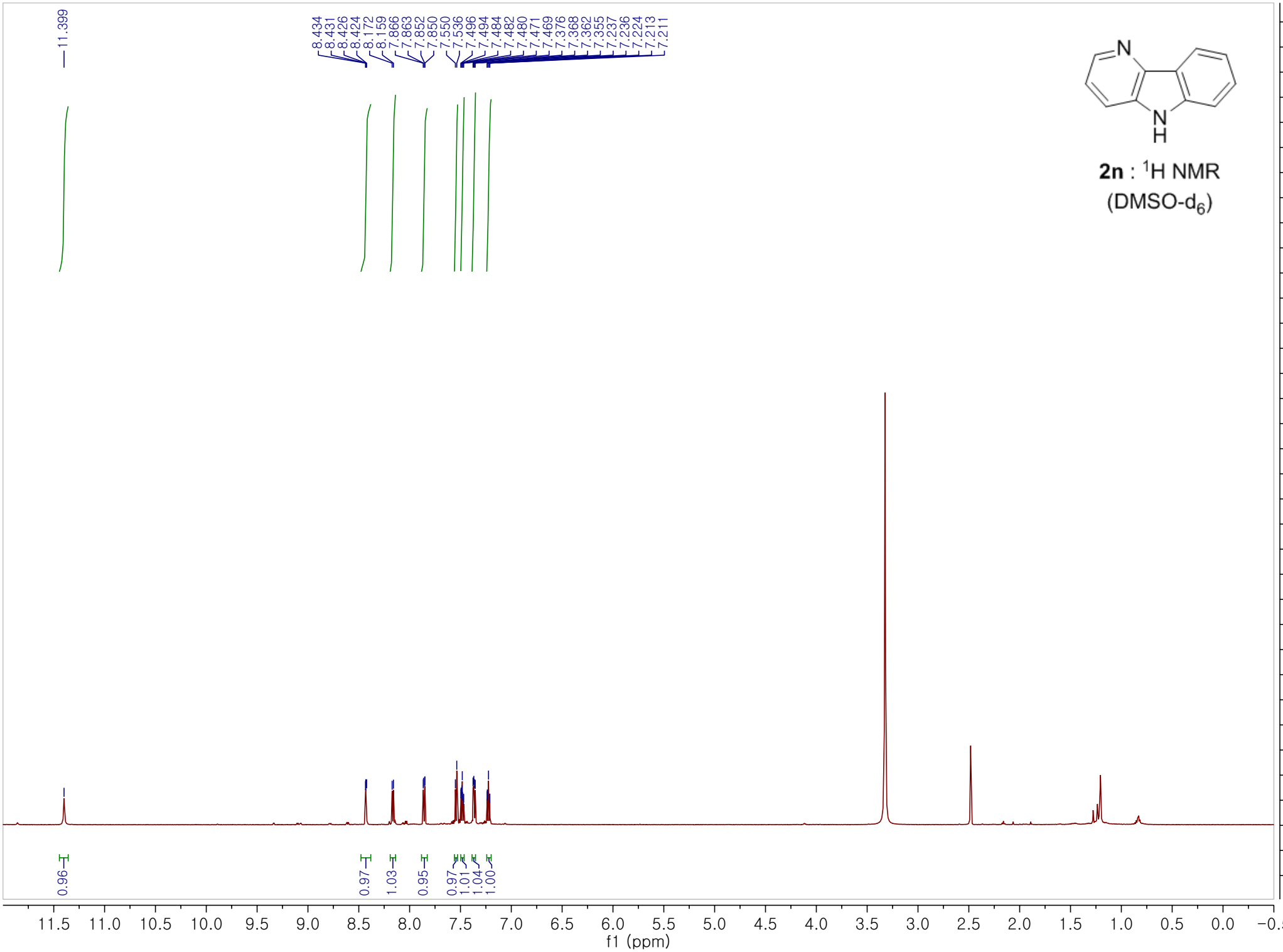

140.021
137.914
128.933
127.368
125.840
123.714
123.426
120.447
120.430
119.407
110.755
110.444
21.641
Me
N
H
2j : 13C NMR
f1 (ppm)

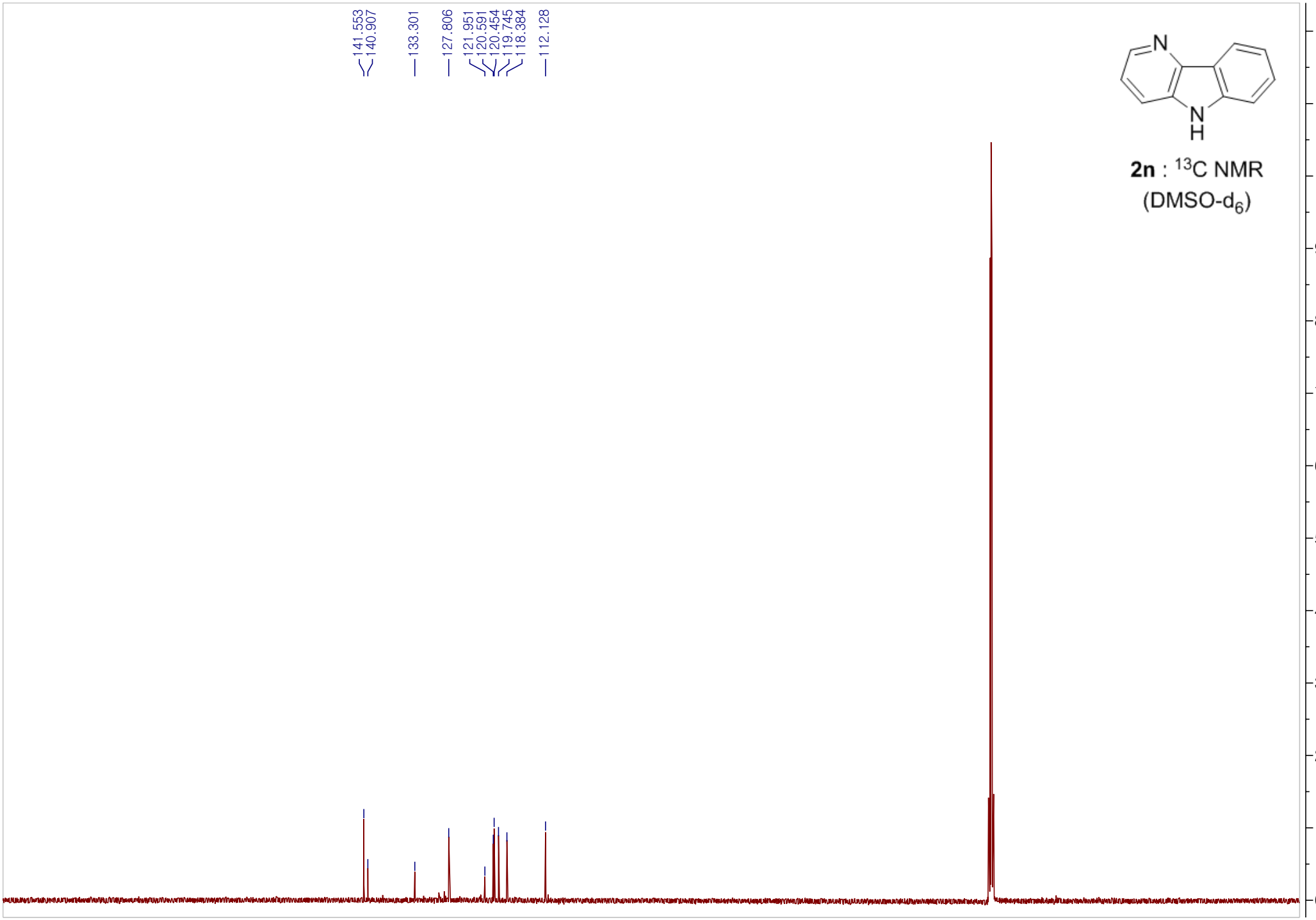

7.994
7.990
7.939
7.815
7.351
7.348
7.337
7.334
7.315
7.308
7.301
7.294
7.271
7.270
7.268
7.260
7.255
2.527
Me
Cl
N
H
2l : 1H NMR
0.98
0.94
1.00
0.99
2.01
1.08
3.02
f1 (ppm)

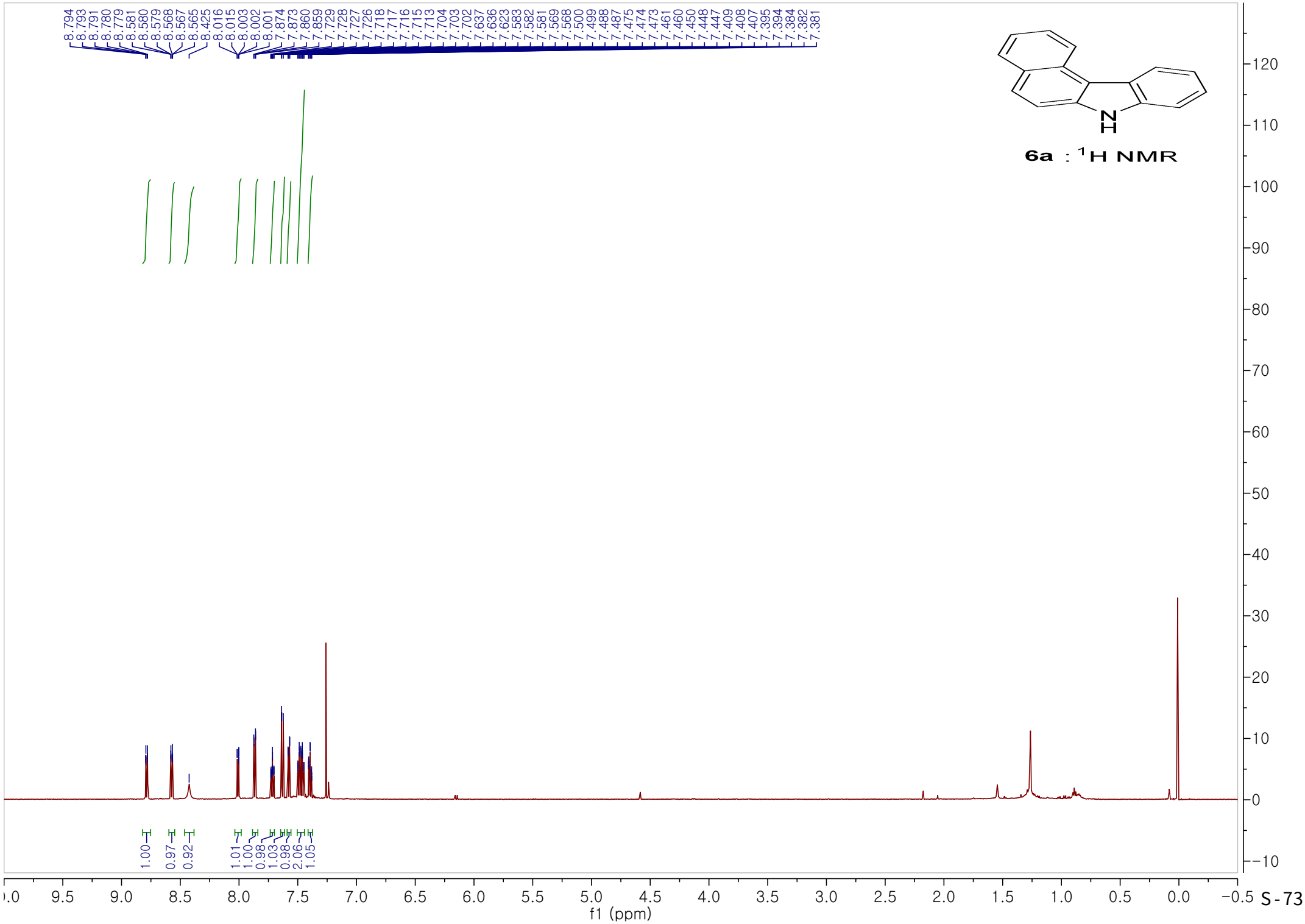

138.450
138.246
129.397
128.147
125.901
124.881
124.621
122.885
120.560
120.169
111.698
110.682
21.613
Me
Cl
N
H
2l : 13C NMR
f1 (ppm)

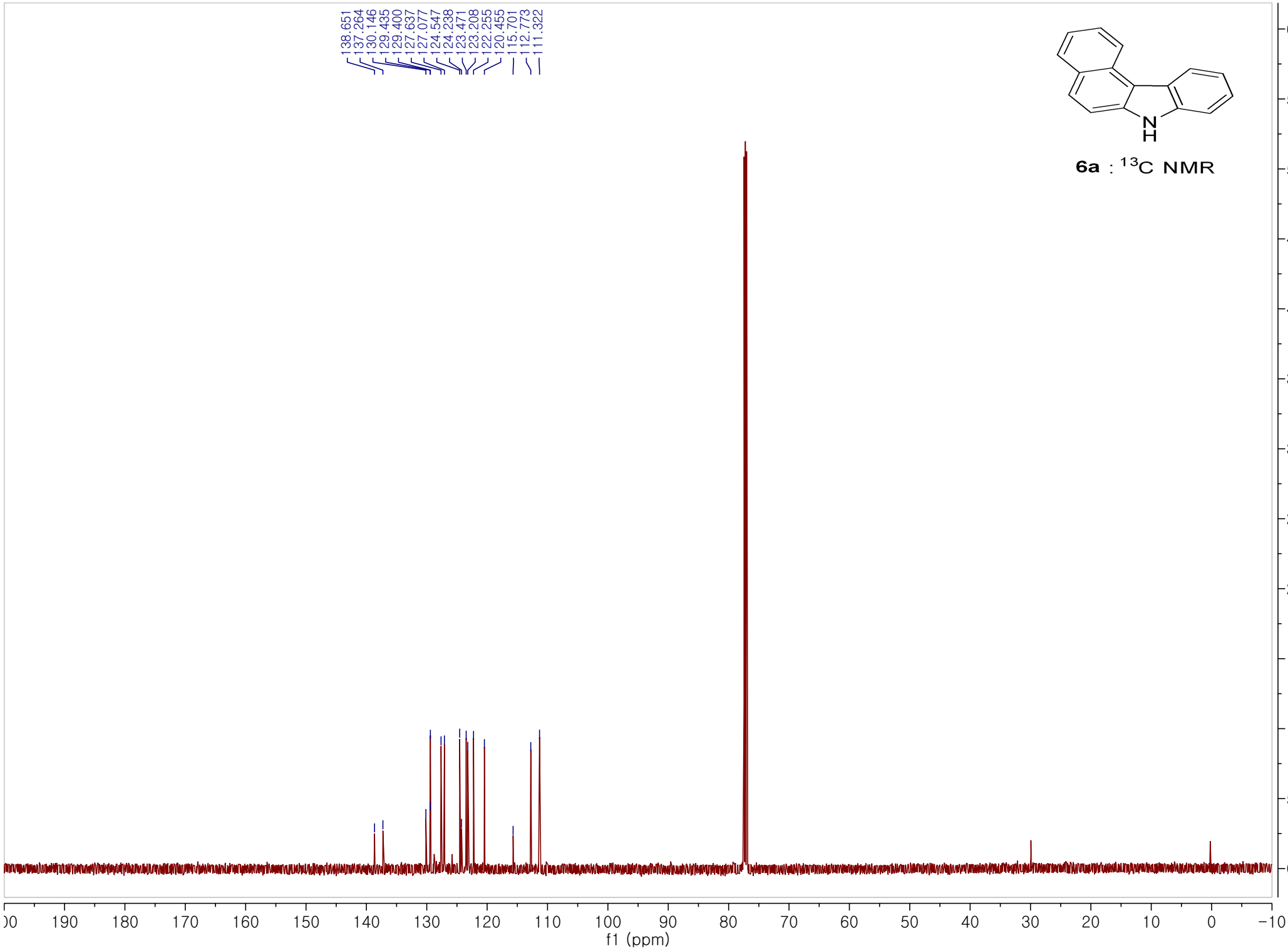

10.930
7.821
7.807
6.907
6.903
6.711
6.707
6.697
6.693
3.795
MeO
OMe
N
H
2m : 1H NMR
(DMSO-d6)
0.97
2.00
2.00
2.06
6.01
f1 (ppm)

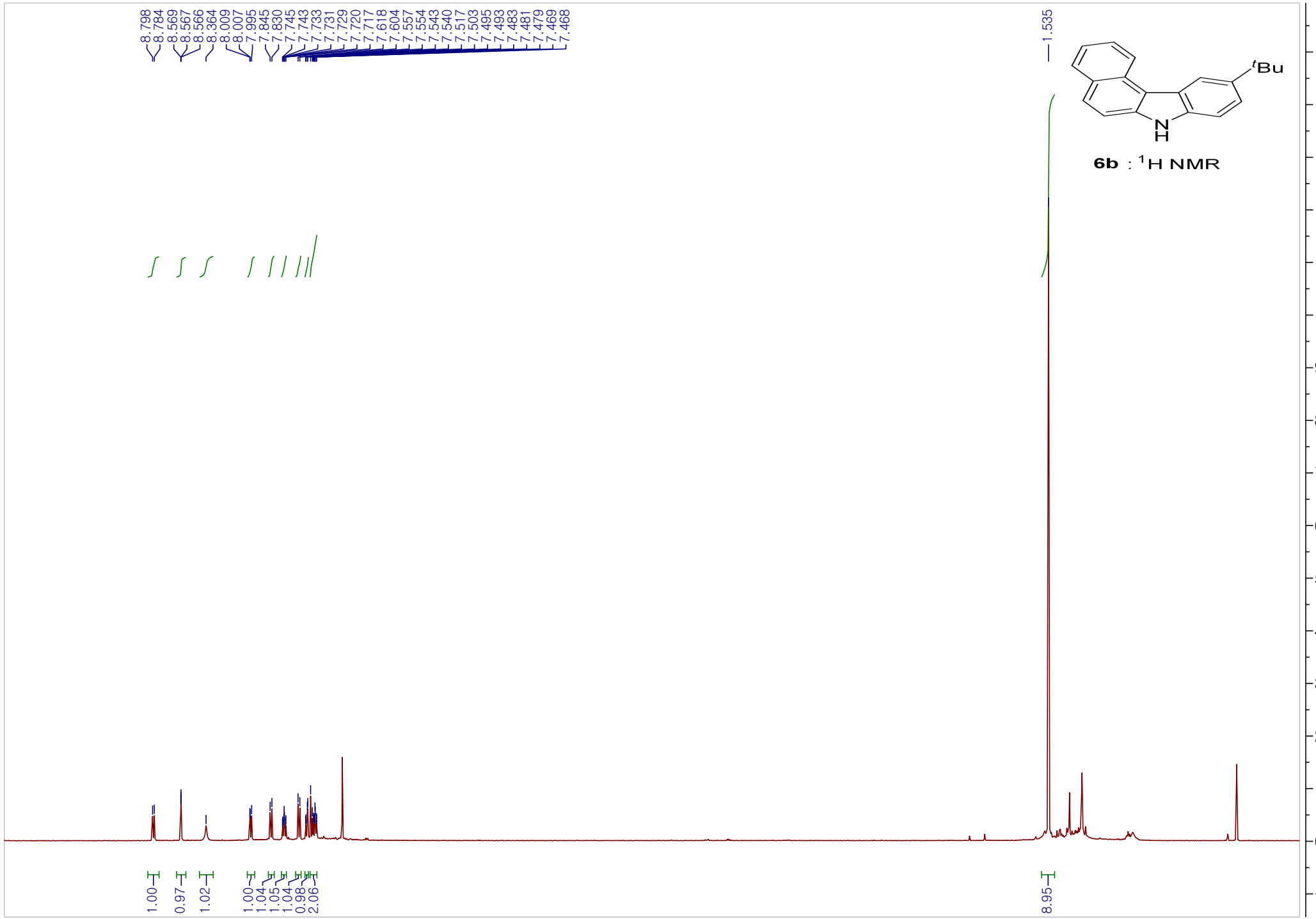

157.966
141.444
120.342
116.886
107.737
95.095
55.669
MeO
OMe
N
H
2m : 13C NMR
(DMSO-d6)
f1 (ppm)

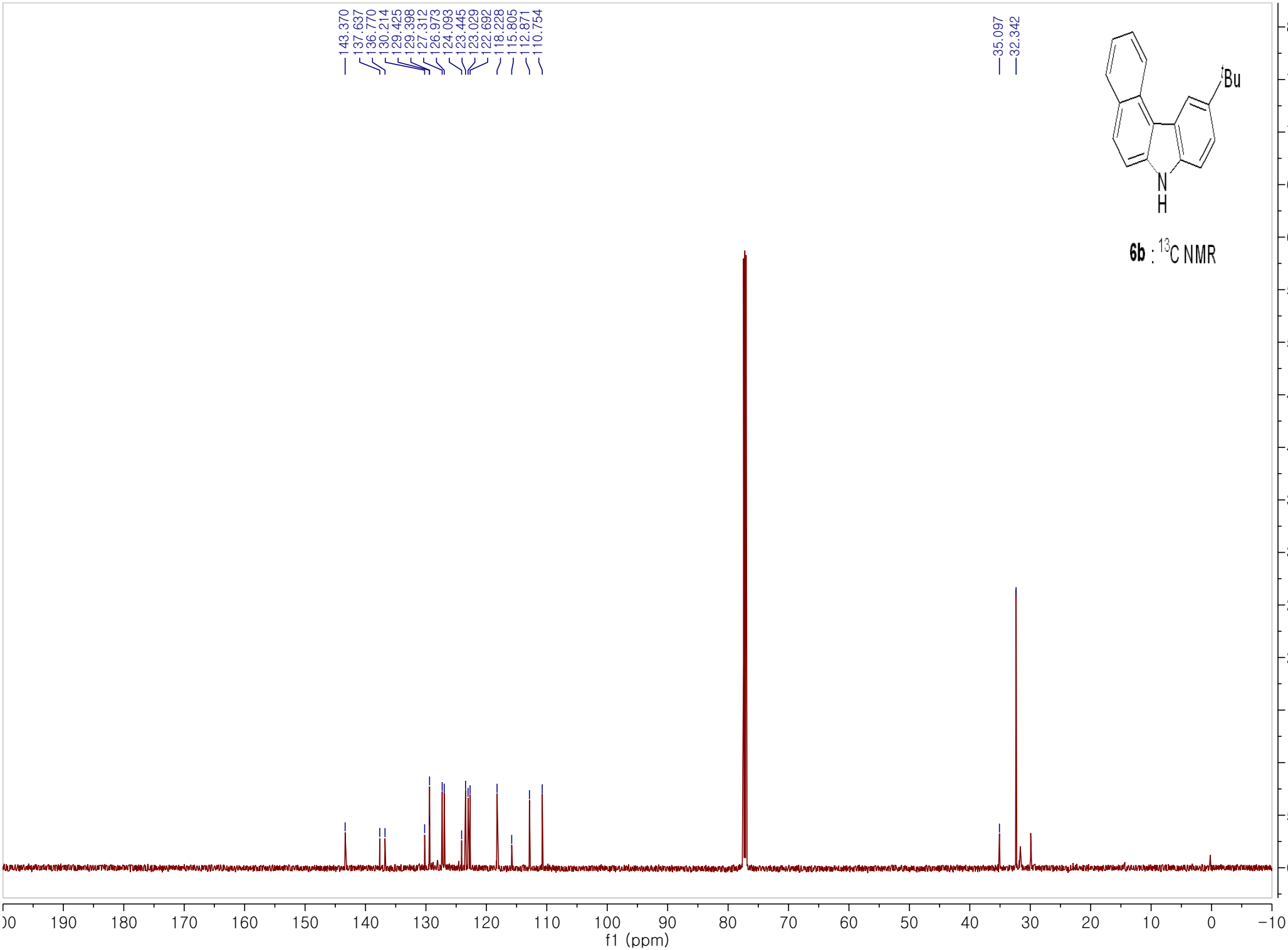

11.399
8.434
8.431
8.426
8.424
8.172
8.159
7.866
7.863
7.852
7.850
7.550
7.536
7.496
7.494
7.484
7.482
7.480
7.471
7.469
7.376
7.368
7.362
7.355
7.237
7.236
7.224
7.213
7.211
N
N
H
2n : 1H NMR
(DMSO-d6)
0.96
0.97
1.03
0.95
0.97
1.01
1.04
1.00
f1 (ppm)

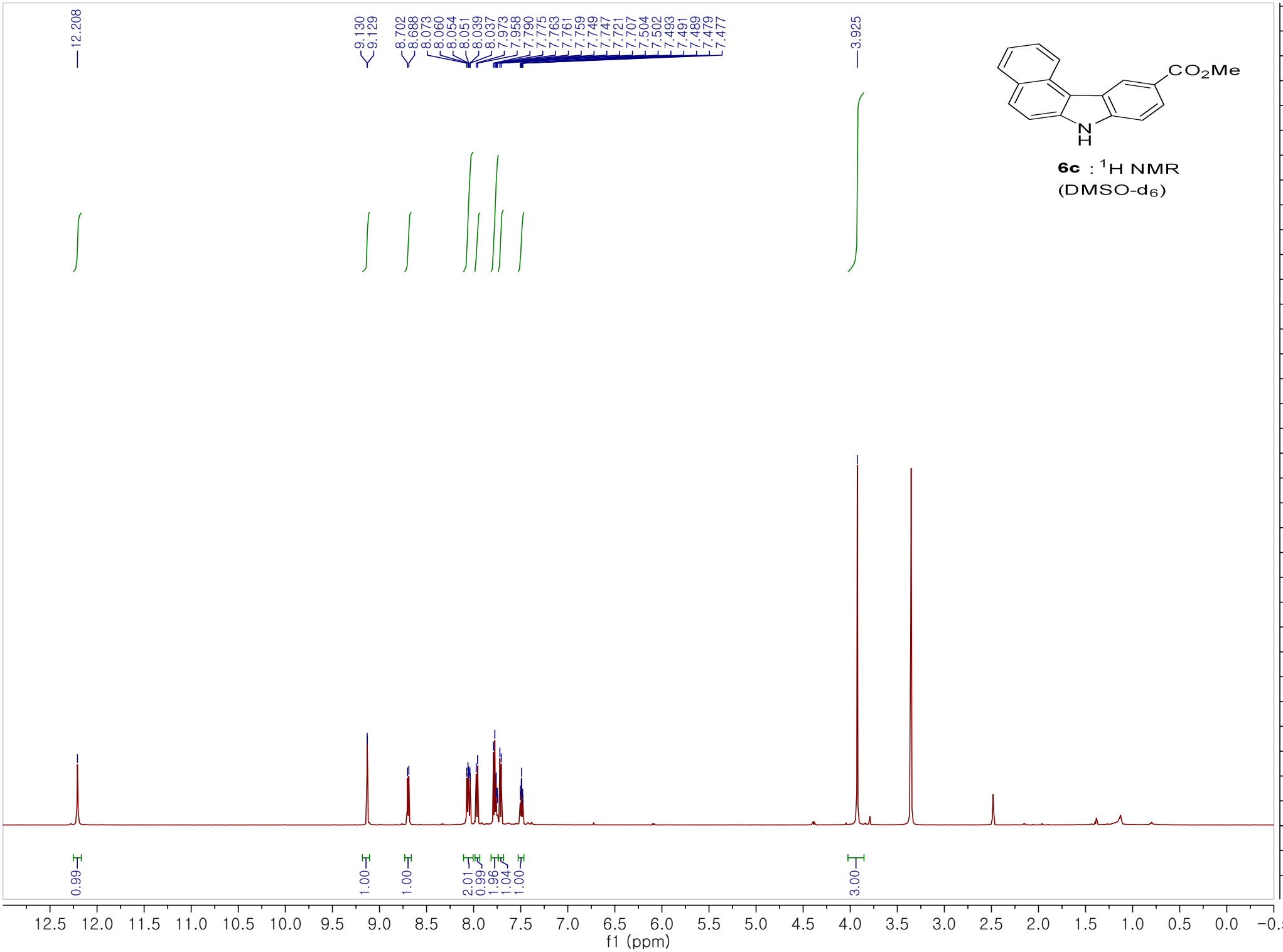

141.553
140.907
133.301
127.806
121.951
120.591
120.454
119.745
118.384
112.128
N
N
H
2n : 13C NMR
(DMSO-d6)
f1 (ppm)

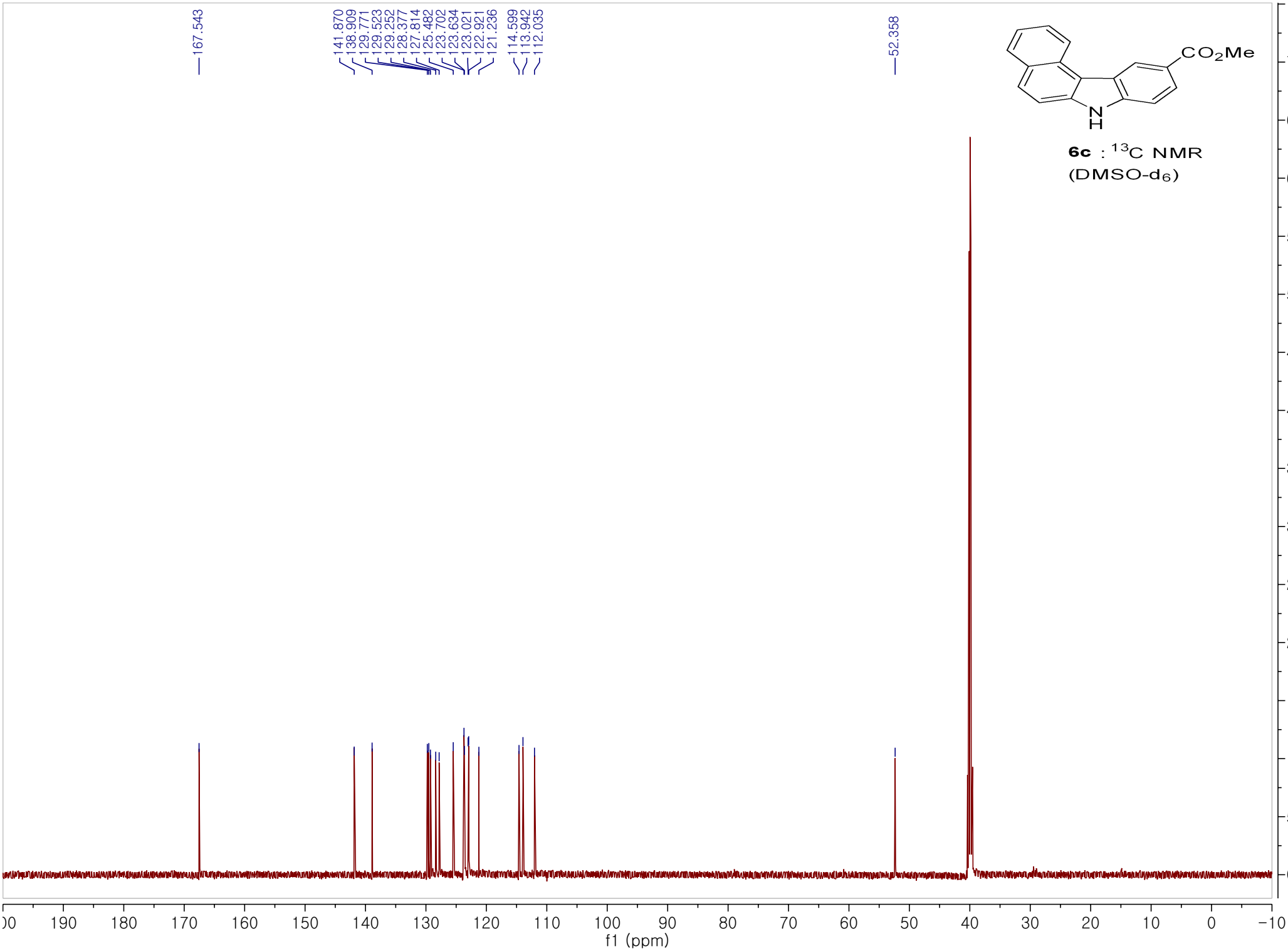

8.794
8.793
8.791
8.780
8.779
8.581
8.580
8.579
8.568
8.567
8.565
8.425
8.016
8.015
8.003
8.002
8.001
7.874
7.873
7.860
7.859
7.729
7.728
7.727
7.726
7.718
7.717
7.716
7.715
7.713
7.704
7.703
7.702
7.637
7.636
7.623
7.583
7.582
7.581
7.569
7.568
7.500
7.499
7.488
7.487
7.475
7.474
7.473
7.461
7.460
7.450
7.448
7.447
7.409
7.408
7.407
7.395
7.394
7.384
7.382
7.381
N
H
6a : 1H NMR
1.00
0.97
0.92
1.01
1.00
0.98
1.03
0.98
2.06
1.05
f1 (ppm)

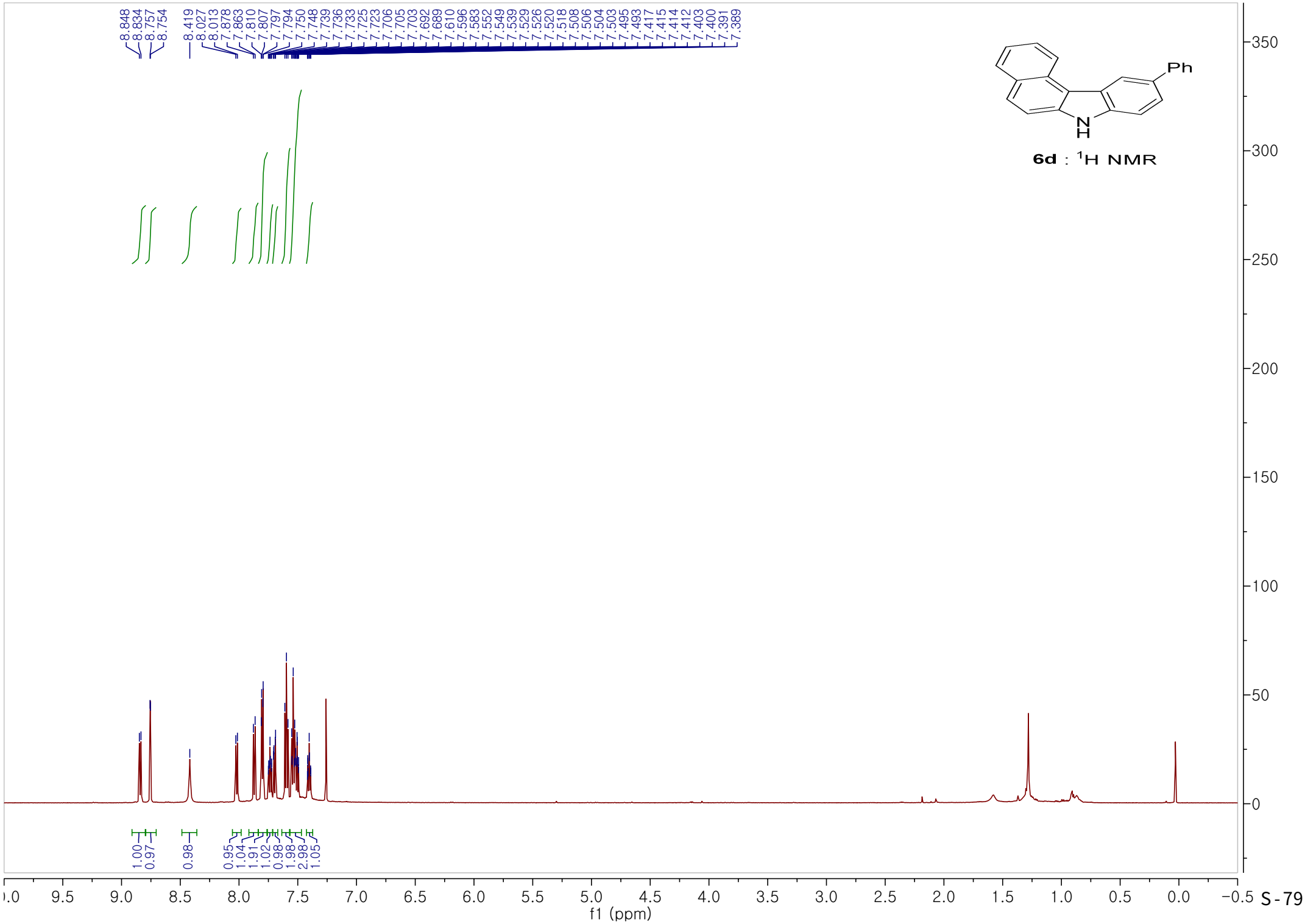

138.651
137.264
130.146
129.435
129.400
127.637
127.077
124.547
124.238
123.471
123.208
122.255
120.455
115.701
112.773
111.322
N
H
6a : 13C NMR
f1 (ppm)

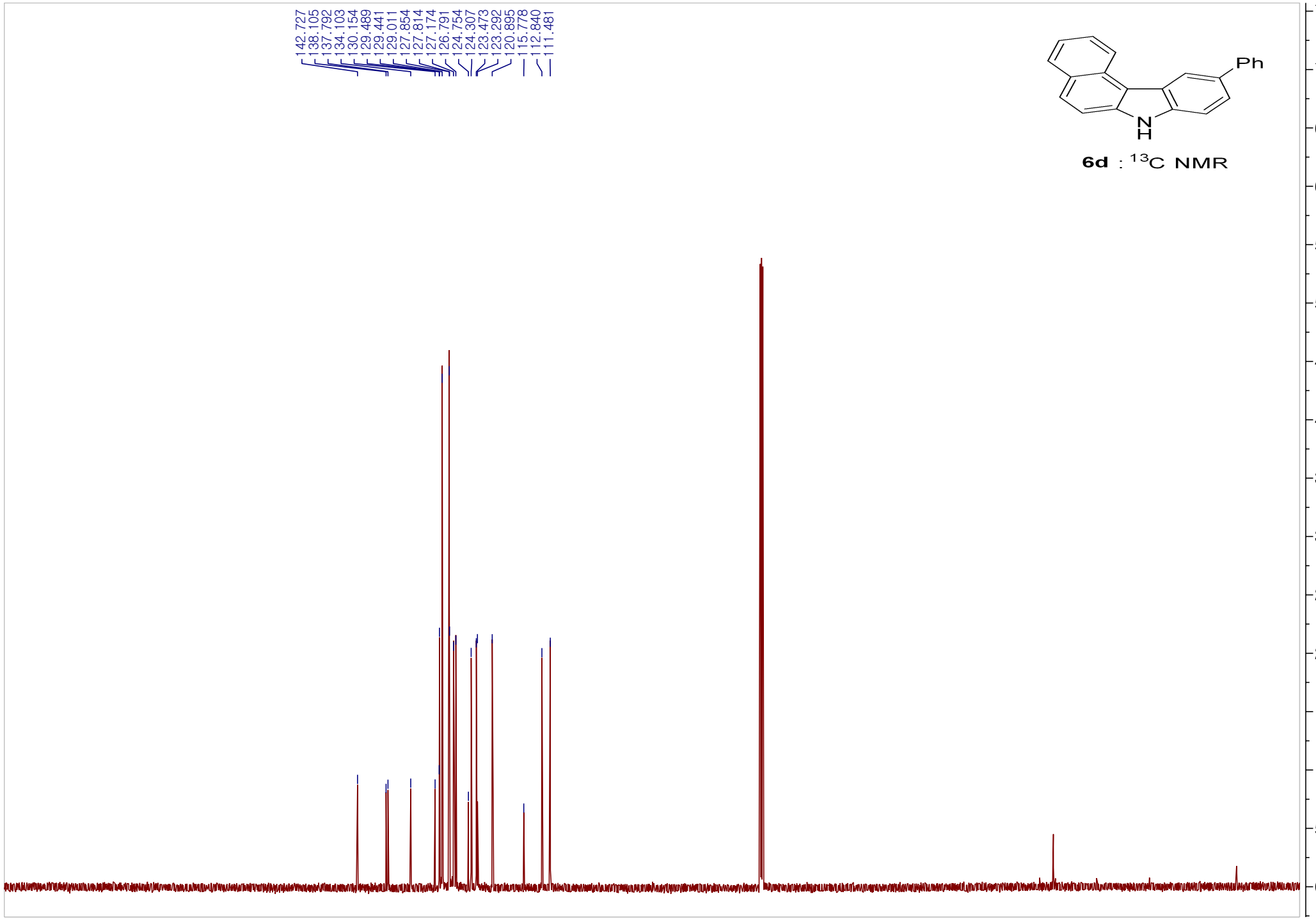

8.798
8.784
8.569
8.567
8.566
8.364
8.009
8.007
7.995
7.845
7.830
7.745
7.743
7.733
7.731
7.729
7.720
7.717
7.618
7.604
7.557
7.554
7.543
7.540
7.517
7.503
7.495
7.493
7.483
7.481
7.479
7.469
7.468
1.535
tBu
N
H
6b : 1H NMR
1.00
0.97
1.02
1.00
1.04
1.05
1.04
0.98
2.06
8.95
f1 (ppm)

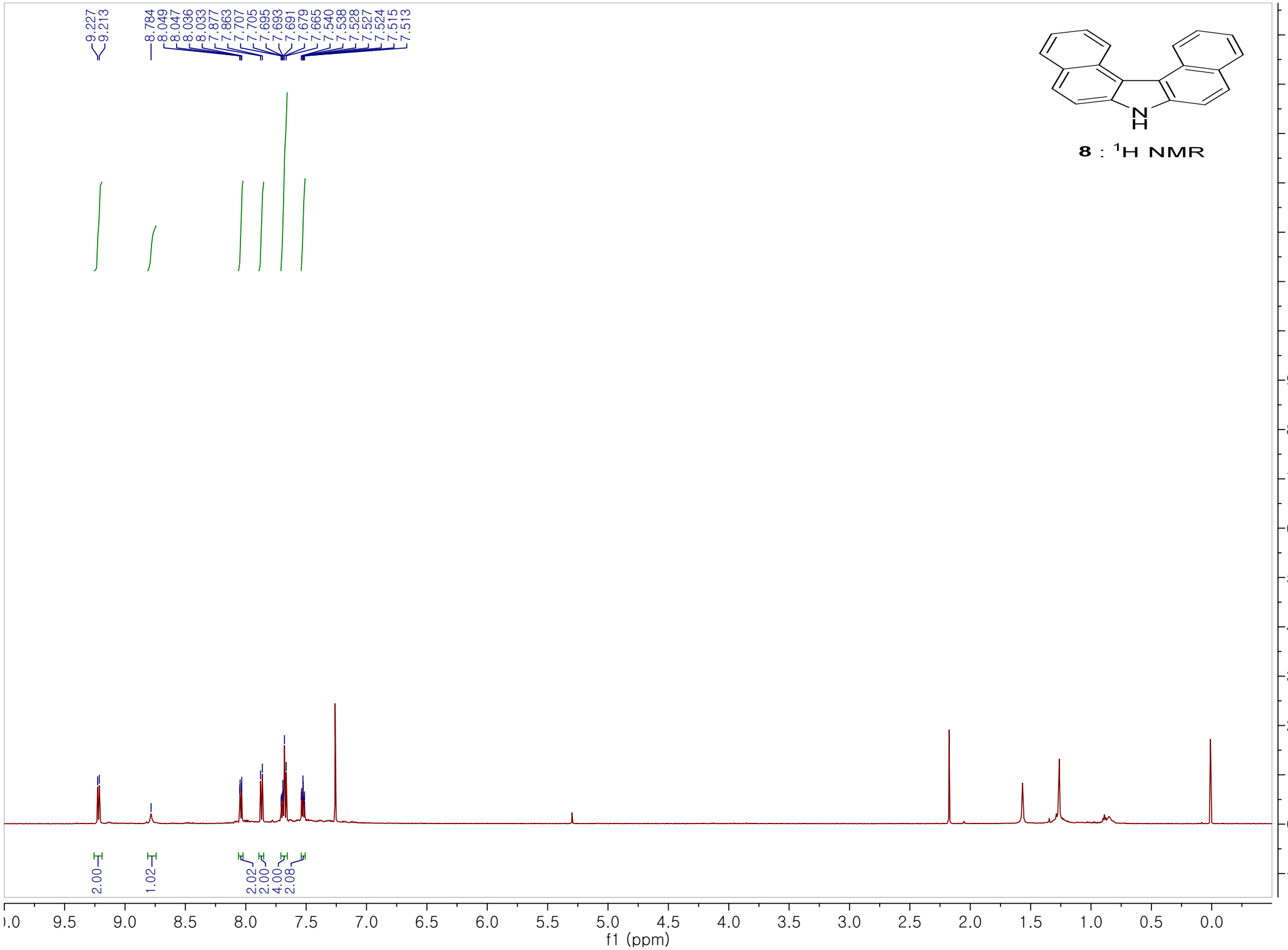

143.370
137.637
136.770
130.214
129.425
129.398
127.312
126.973
124.093
123.445
123.029
122.692
118.228
115.805
112.871
110.754
35.097
32.342
tBu
N
H
6b : 13C NMR
f1 (ppm)

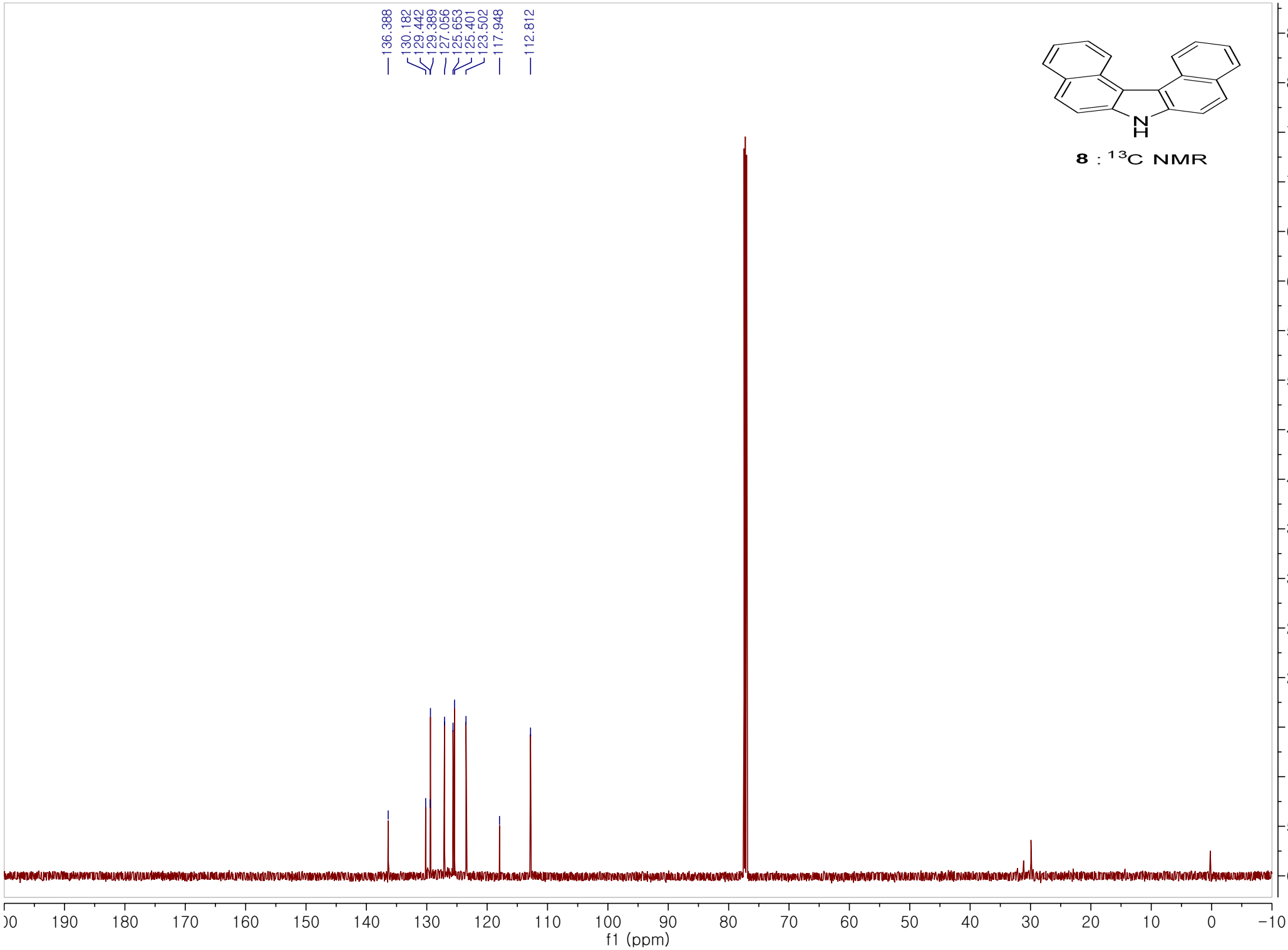

12.208
9.130
9.129
8.702
8.688
8.073
8.060
8.054
8.051
8.039
8.037
7.973
7.958
7.790
7.775
7.763
7.761
7.759
7.749
7.747
7.721
7.707
7.504
7.502
7.493
7.491
7.489
7.479
7.477
3.925
CO2Me
N
H
6c : 1H NMR
(DMSO-d6)
0.99
1.00
1.00
2.01
0.99
1.96
1.04
1.00
3.00
f1 (ppm)

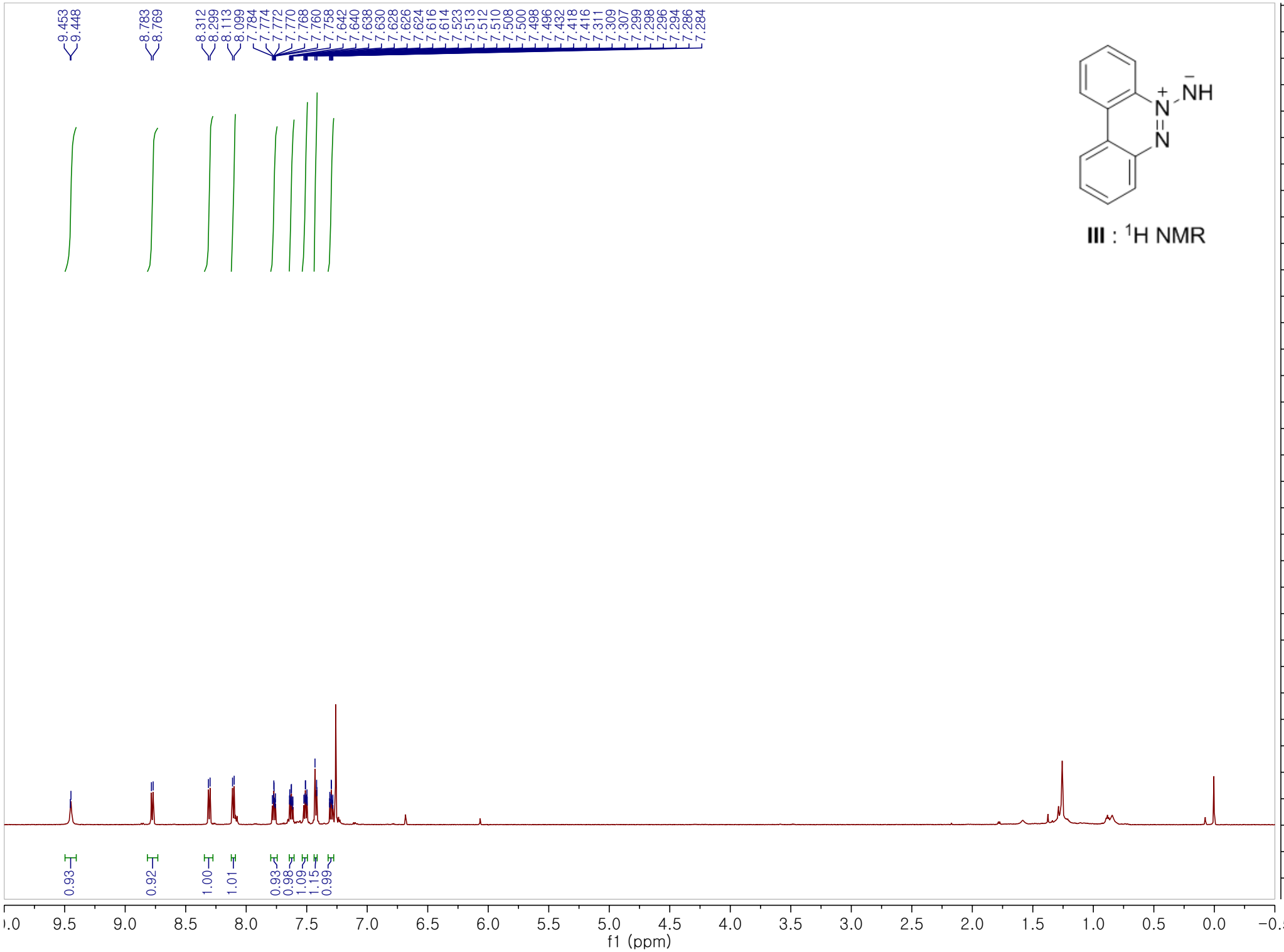

167.543
141.870
138.909
129.771
129.523
129.252
128.377
127.814
125.482
123.702
123.634
123.021
122.921
121.236
114.599
113.942
112.035
52.358
CO2Me
N
H
6c : 13C NMR
(DMSO-d6)
f1 (ppm)

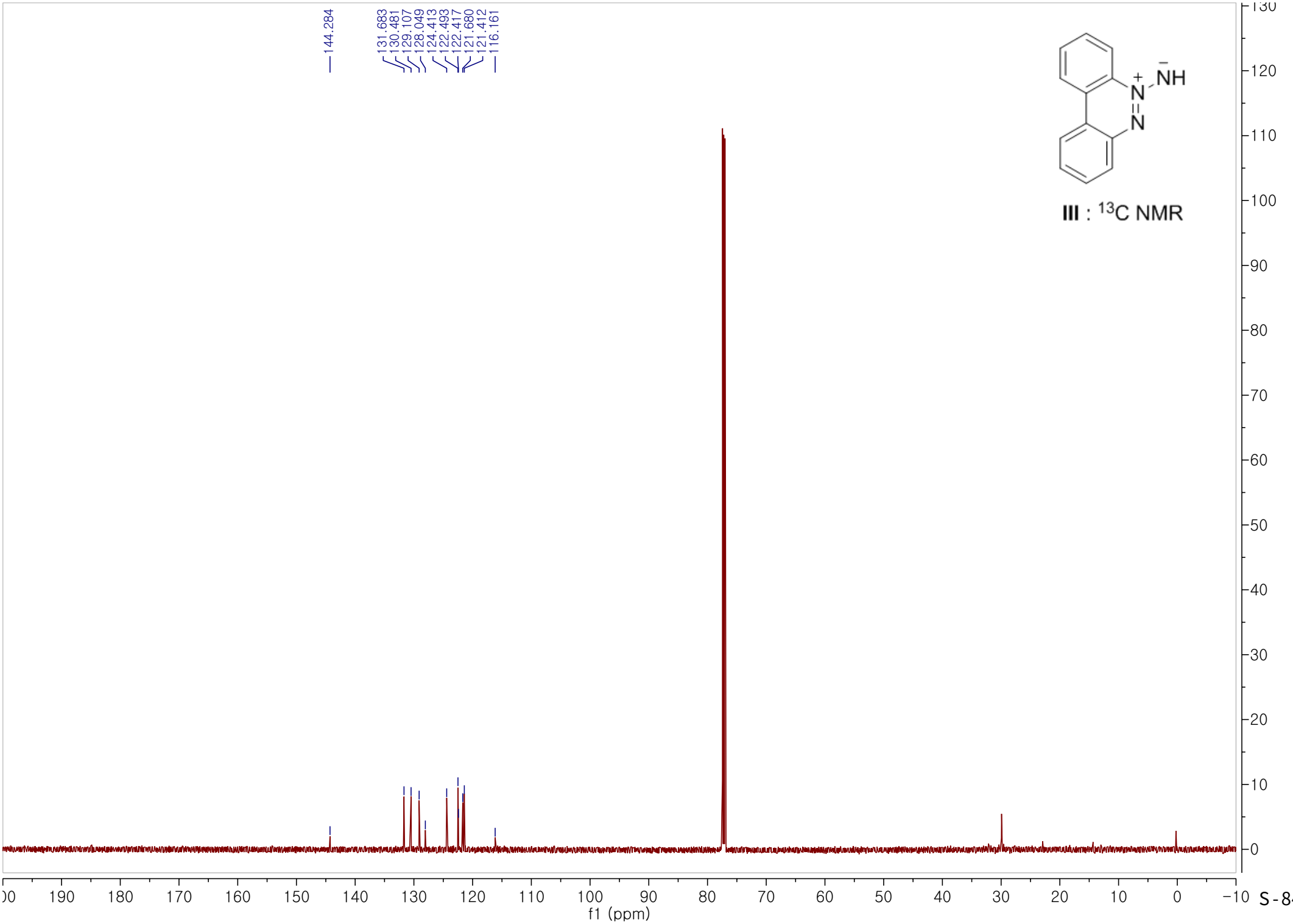

8.848
8.834
8.757
8.754
8.419
8.027
8.013
7.878
7.863
7.810
7.807
7.797
7.794
7.750
7.748
7.739
7.736
7.733
7.725
7.723
7.706
7.705
7.703
7.692
7.689
7.610
7.596
7.583
7.552
7.549
7.539
7.529
7.526
7.520
7.518
7.508
7.506
7.504
7.503
7.495
7.493
7.417
7.415
7.414
7.412
7.403
7.400
7.391
7.389
Ph
N
H
6d : 1H NMR
1.00
0.97
0.98
0.95
1.04
1.91
1.02
0.98
1.98
2.98
1.05
f1 (ppm)


142.727
138.105
137.792
134.103
130.154
129.489
129.441
129.011
127.854
127.814
127.174
126.791
124.754
124.307
123.473
123.292
120.895
115.778
112.840
111.481
Ph
N
H
6d : 13C NMR
f1 (ppm)


9.227
9.213
8.784
8.049
8.047
8.036
8.033
7.877
7.863
7.707
7.705
7.695
7.693
7.691
7.679
7.665
7.540
7.538
7.528
7.527
7.524
7.515
7.513
8 : 1H NMR
2.00
1.02
2.02
2.00
4.00
2.08
f1 (ppm)


136.388
130.182
129.442
129.389
127.056
125.653
125.401
123.502
117.948
112.812
N
H
8 : 13C NMR
f1 (ppm)


9.453
9.448
8.783
8.769
8.312
8.299
8.113
8.099
7.784
7.774
7.772
7.770
7.768
7.760
7.758
7.642
7.640
7.638
7.630
7.628
7.626
7.624
7.616
7.614
7.523
7.513
7.512
7.510
7.508
7.500
7.498
7.496
7.432
7.418
7.416
7.311
7.309
7.307
7.299
7.298
7.296
7.294
7.286
7.284
NH
N
N
III : 1H NMR
0.93
0.92
1.00
1.01
0.93
0.98
1.09
1.15
0.99
f1 (ppm)


144.284
131.683
130.481
129.107
128.049
124.413
122.493
122.417
121.680
121.412
116.161
III : 13C NMR
f1 (ppm)