Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Nitrogen-Centered Radical-Mediated C-H Imidation of Arenes and Heteroarenes via Visible Light Induced Photocatalysis

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Contents

I. General Information

Anisole, phenyl acetate, fluorobenzene, chlorobenzene, bromobenzene, methyl benzoate, 1,4-dimethoxybenzene, methyl *p*-anisate, *o*-xylene, *m*-xylene, *p*-xylene, 1,2-dichlorobenzene, dimethylphthalate, 2-bromo-1,3-dimethylbenzene, mesitylene, 1,3,5-tri-*tert*-butylbenzene, 4-methoxypyridine, 2,6-lutidine, 2,6-di-*tert*-butylpyridine, 2,4,6-collidine, phthalimide, *N*-chlorophthalimide, *N*-bromophthalimide, glacial acetic acid, *tert*-butanol, potassium carbonate, sodium hypochlorite, hydrazine monohydrate and tris[2-(4,6-difluorophenyl)pyridinato-C^2,*N*]iridium(III) ([Ir(dFppy)$_3$]) were purchased from commercial sources and used as received without further purification, unless otherwise noted. Catalysts ([Ir(ppy)$_2$(dtbbpy)]PF_6 [1], [Ir(ppy)$_3$] [2] and [Ir(dFppy)$_3$] [2]) and *N*-chlorophthalimide[3] also could be obtained by using reported procedures. *Tert*-butyl hypochlorite was prepared by using a literature procedure.[4] Benzene, toluene, pyridine and solvents were obtained by passing through activated alumina columns of solvent purification systems from Glass Contour.

The progress of reaction was checked on thin layer chromatography (TLC) plates (Merck 5554 Kiesel gel 60 F254), and the spots were visualized under 254 nm UV light and/or charring after dipping the TLC plate into a vanillin solution (15.0 g of vanillin and 2.5 mL of concentrated sulfuric acid in 250 mL of ethanol), a $KMnO_4$ solution (3.0 g of $KMnO_4$, 20.0 g of K_2CO_3, and 5.0 mL of 5% NaOH solution in 300 mL of water), or a ninhydrin solution (1.5 g of ninhydrin, 5 mL of acetic acid, 500 mL of 95% ethanol). Column chromatography was performed on silica gel (Merck 9385 Kiesel gel 60) using hexanes-EtOAc (v/v).

NMR spectra were obtained on a Bruker DPX-300 (300 MHz), an Agilent 400-MR DD2 Magnetic Resonance System (400 MHz) and a Varian/Oxford As-500 (500 MHz) spectrophotometer. Chemical shift values were recorded as parts per million relative to tetramethylsilane as an internal standard unless otherwise indicated, and coupling constants in Hertz. The following abbreviations (or

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[1] J. D. Slinker, A. A. Gorodetsky, M. S. Lowry, J. Wang, S. Parker, R. Rohl, S. Bernhard and G. G. Malliaras, *J. Am. Chem. Soc.*, 2004, **126**, 2763.

[2] A. B. Tamayo, B. D. Alleyne, P. I. Djurovich, S. Lamansky, I. Tsyba, N. N. Ho, R. Bau and M. E. Thompson, *J. Am. Chem. Soc.*, 2003, **125**, 7377.

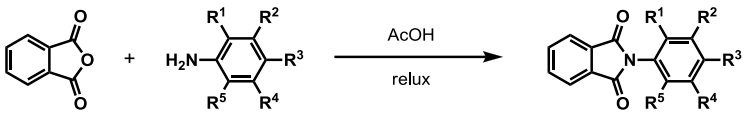
[3] H. Zimmer and L. F. Audrieth, *J. Am. Chem. Soc.*, 1954, **76**, 3856.

[4] H. Du, B. Zhao and Y. Shi, *J. Am. Chem. Soc.*, 2008, **130**, 8590.

combinations thereof) were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad. IR spectra were measured on a Thermo Scientific Nicolet 6700 spectrometer. High resolution mass spectra were recorded on a JEOL JMS-600W, JMS-700, Agilent 6890 Series or a JEOL JMS-AX505WA, HP 5890 Series II spectrometer using electron impact (EI) or fast atom bombardment (FAB) method. (We thank Hyeasuk Shin at National Center for Inter-University Research Facilities and Sungmin Lim at Korea Basic Science Institute for obtaining high resolution mass spectra.) Gas chromatography data were obtained on a Hewlett Packard HP 6890 Series GC systems.

II. General Procedures

A. General procedure for synthesis of authentic samples



Authetic compounds listed in Table 2 were synthesized according to the literature.[5] To a reaction vessel with a magnetic stirring bar were added phthalic anhydride (0.5 mmol), corresponding aniline (0.5 mmol) and glacial acetic acid (2.0 ml). No need to exclude moisture or air. After refluxing for 3–4 h with vigorous stirring, the reaction mixture was cooled to room temperature and addition of water provided the product precipitate. The crude precipitate was then recrystallized from hot ethanol to obtain the pure compound.

B. General procedure for photocatalytic imidation of aromatic compounds

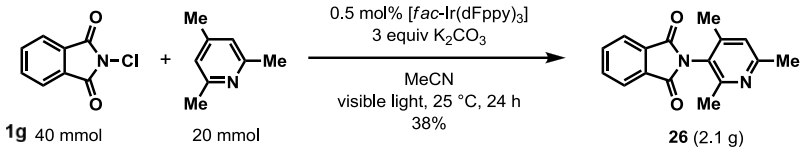
Method A for imidation using N-chlorophthalimide

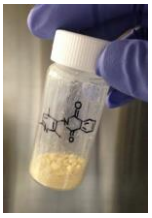
To a reaction vessel with a magnetic stirring bar were added *N*-chlorophthalimide (90.8 mg/0.50 mmol or 181.6 mg/1.00 mmol), potassium carbonate (207.3 mg, 1.50 mmol), and [*fac*-Ir(dFppy)$_3$] (1.9 mg, 0.0025 mmol, 0.5 mol % for the limiting agent). After addition of acetonitrile (5.0 ml), arene/heteroarene substrate (1.00 mmol or 0.50 mmol) and acetic acid (5.7 µl) were added. The

[5] S. M. Capitosti, T. P. Hansen and M. L. Brown, *Biorg. Med. Chem.*, 2004, **12**, 327.

mixture was placed in the irradiation apparatus equipped with a 20 W household compact fluorescent lamp (CFL). After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane. The resulting organic phase was washed with 2 *N* NaOH aqueous solution to remove the remaining phthalimide, dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The resulting crude mixture was purified by flash column chromatography on silica gel, which furnished the title compounds as described.

Gram-scale imidation reaction (26, Table 2)





To a reaction flask with a magnetic stirring bar were added *N*-chlorophthalimide (7.3 g, 40.0 mmol), potassium carbonate (8.3 g, 60.0 mmol), and [*fac*-Ir(dFppy)$_3$] (76.4 mg, 0.10 mmol). After addition of acetonitrile (200 ml), 2,4,6-collidine (2.6 ml, 20.0 mmol) and acetic acid (0.2 ml) were added. The mixture was placed in the irradiation apparatus equipped with 13 W white LED lamps (X2). After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane. The resulting organic phase was washed with 2 *N* NaOH aqueous solution to remove the remaining phthalimide, dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The resulting crude mixture was purified by flash column chromatography on silica gel, which furnished **26** in 38% yield (2.1 g, 7.7 mmol).

Method B for imidation using phthalimide and tert-butyl hypochlorite

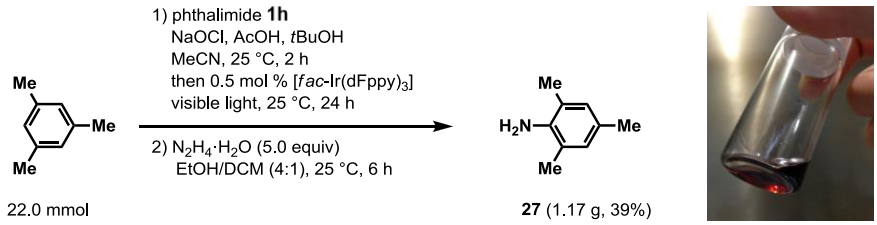
To a reaction vessel with a magnetic stirring bar were added phthalimide (147.1 mg, 1.00 mmol), potassium carbonate (207.3 mg, 1.50 mmol), *tert*-butanol (95.6 µl, 1.00 mmol) and [*fac*-Ir(dFppy)$_3$] (1.9 mg, 0.0025 mmol). After addition of acetonitrile (5.0 ml), *tert*-butyl hypochlorite (113 µl, 1.00 mmol) was added in one portion and the reaction mixture was vigorously stirred at room temperature without light. After 2 h, arene/heteroarene substrate (0.50 mmol) was added and the mixture was placed in the irradiation apparatus equipped with a 20 W CFL. After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane. The resulting organic phase was washed with 2 *N* NaOH

aqueous solution to remove the remaining phthalimide, dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The resulting crude mixture was purified by flash column chromatography on silica gel, which furnished the title compounds as described.

Method C for imidation using phthalimide and sodium hypochlorite

To a reaction vessel with a magnetic stirring bar were added phthalimide (227.0 mg, 1.25 mmol), *tert*-butanol (95.6 µl, 1.00 mmol) and acetonitrile (5.0 ml). Aqueous solution of sodium hypochlorite containing 11–14% chlorine (0.44 ml, 1.00 mmol) and acetic acid (57.2 µl, 1.00 mmol) were slowly added at the same time and the resulting solution was stirred vigorously at room temperature without light. After 2 h, [*fac*-Ir(dFppy)$_3$] (1.9 mg, 0.0025 mmol) and arene/heteroarene substrate (0.50 mmol) were added and the mixture was placed in the irradiation apparatus equipped with a 20 W CFL. After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane. The resulting organic phase was washed with 2 *N* NaOH aqueous solution to remove the remaining phthalimide, dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The resulting crude mixture was purified by flash column chromatography on silica gel, which furnished the title compounds as described.

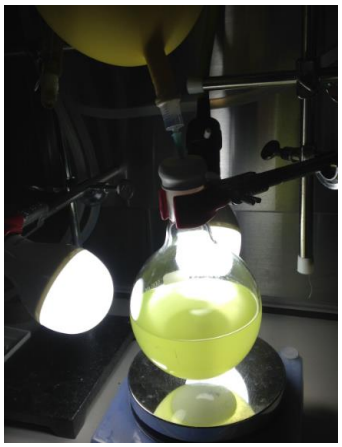
Method D for gram-scale one-pot imidation/hydrazinolysis (Scheme 3)



To a reaction vessel with a magnetic stirring bar were added phthalimide (8.1 g, 55.0 mmol), *tert*-butanol (4.2 ml, 44.0 mmol) and acetonitrile (220 ml). Aqueous solution of sodium hypochlorite containing 11–14% chlorine (21.8 ml, 44.0 mmol) and acetic acid (2.5 ml, 44.0 mmol) were slowly added at the same time and the resulting solution was stirred vigorously at room temperature without light. After 2 h, [*fac*-Ir(dFppy)$_3$] (84.0 mg, 0.11 mmol) and mesitylene (3.1 ml, 22.0 mmol) were added and the mixture was placed in the irradiation apparatus equipped with 13 W white LED lamps (X2). After 24 h, the solvent was evaporated under reduced pressure and the resulting crude mixture

was then dissolved in ethanol/dichloromethane (120 ml/30 ml) which was treated by addition of hydrazine monohydrate (98%, 5.5 ml). After stirring for 6 h at room temperature, the resulting suspension was filtered through a short pad of silica with diethyl ether. The filtrate was washed with 2 *N* NaOH aqueous solution, dried over anhydrous magnesium sulfate, filtered and concentrated carefully under reduced pressure to afford the crude mixture which was purified by flash column chromatography on silica gel using hexanes/ethyl acetate as an eluent, which furnished 2,4,6-trimethylaniline[6] **27** as the product (1.17 g, 8.65 mmol) in 39% yield. Reddish brown oil. R_f 0.68 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.76 (s, 2H), 3.43 (s, 2H), 2.20 (s, 3H), 2.15 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.3, 129.0, 127.3, 122.0, 20.6, 17.8.

1. Chlorination



2. Photocatalytic imidation

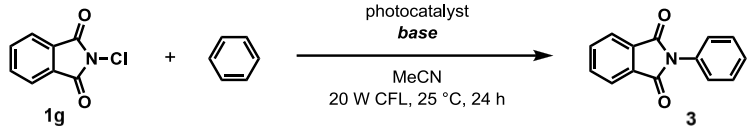
3. Hydrazinolysis

[6] H. Rao, H. Fu, Y. Jiang and Y. Zhao, *Angew. Chem. Int. Ed.*, 2009, **48**, 1114.

III. Optimization of Reaction Conditions

To a reaction vessel with a magnetic stirring bar were added *N*-chlorophthalimide (0.50 mmol), base, and photocatalyst. After addition of acetonitrile, benzene and additional reagents as described were added. The mixture was then placed in the irradiation apparatus equipped with a 20 W household compact fluorescent lamp (CFL). After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane and the resulting organic phase was dried over anhydrous sodium sulfate, filtered, concentrated and analyzed by ^{1}H NMR spectroscopy.

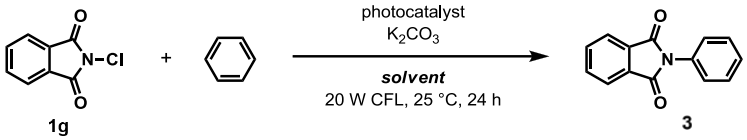
Table S1. Effect of bases



Entry	Photocatalyst	Base	Yield [%]
1	$[Ir(ppy)_2(dtbbpy)]PF_6$	**K_2CO_3**	**26** [a]
2	$[Ir(ppy)_2(dtbbpy)]PF_6$	$NaHCO_3$	12 [a]
3	$[Ir(ppy)_2(dtbbpy)]PF_6$	Na_2CO_3	15 [a]
4	$[Ir(ppy)_2(dtbbpy)]PF_6$	NaH_2PO_4	3 [a]
5	$[Ir(ppy)_2(dtbbpy)]PF_6$	K_2HPO_4	9 [a]
6	$[Ir(ppy)_2(dtbbpy)]PF_6$	KO*t*Bu	0 [a]
7	$[Ir(ppy)_2(dtbbpy)]PF_6$	DIPEA	trace [b]
8	$[Ir(ppy)_2(dtbbpy)]PF_6$	TEA	trace [b]
9	[*fac*-Ir(ppy)$_3$]	**K_2CO_3**	**34** [a]
10	[*fac*-Ir(ppy)$_3$]	Li_2CO_3	13 [c]
11	[*fac*-Ir(ppy)$_3$]	BaO	18 [c]
12	[*fac*-Ir(ppy)$_3$]	MgO	21 [c]
13	[*fac*-Ir(ppy)$_3$]	Ag_2CO_3	trace [c]
14	[*fac*-Ir(ppy)$_3$]	Ag_3PO_4	trace [c]
15	[*fac*-Ir(ppy)$_3$]	AgF	trace [c]
16	[*fac*-Ir(ppy)$_3$]	CsF	23 [c]
17	[*fac*-Ir(ppy)$_3$]	DABCO	0 [c]
18	[*fac*-Ir(ppy)$_3$]	Na-ascorbate	trace [c]
19	[*fac*-Ir(ppy)$_3$]	LiOAc	14 [c]
20	[*fac*-Ir(ppy)$_3$]	NaOAc	28 [c]
21	[*fac*-Ir(ppy)$_3$]	KOAc	26 [c]
22	[*fac*-Ir(ppy)$_3$]	CsOAc	21 [c]
23	[*fac*-Ir(ppy)$_3$]	KOPiv	32 [c]
24	[*fac*-Ir(ppy)$_3$]	CsOPiv	29 [c]

Reaction conditions: *N*-chlorophthalimide (1.0 mmol), benzene (0.5 mmol), photocatalyst (0.005 mmol, 1.0 mol %), base (1.5 mmol) acetonitrile (4.0 mL), 20 W CFL, 25 °C, 24 h. [a] Isolated yield. [b] Reduction of the N–Cl bond provided phthalimide. [c] Yields are based on crude proton NMR spectroscopy.

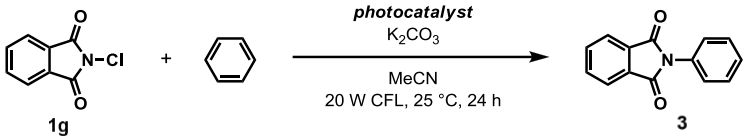
Table S2. Effect of solvents



Entry	Solvent	Yield [%][a]
1	**MeCN**	**26**
2	DMSO	NR
3	DMF	NR
4	DCM	trace
5	DCE	trace
6	NMP	trace
7	THF	trace
8	MeCN/Benzene (7:1)	16
9	benzene	NR
10	MeOH	0[b]
11	EtOH	0[b]
12	*i*PrOH	7
13	*t*BuOH	NR
14	*t*BuOH/MeCN (1:1)	22

Reaction conditions: *N*-chlorophthalimide (1.0 mmol), benzene (0.5 mmol), $[Ir(ppy)_2(dtbbpy)]PF_6$ (0.005 mmol, 1.0 mol %), potassium carbonate (1.5 mmol), acetonitrile (4.0 mL), 20 W CFL, 25 °C, 24 h. [a] Isolated yield. [b] Background reactions between *N*-chlorophthalimide and solvents occurred. NR: no reaction.

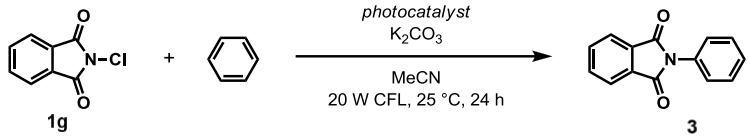
Table S3. Effect of catalysts



Entry	Catalyst	Yield [%][a]
1	**[*fac*-Ir(dFppy)$_3$]**	**39**
2	**[*fac*-Ir(ppy)$_3$]**	**34**
3	$[Ir(ppy)_2(dtbbpy)]PF_6$	26
4	$[Ir(dF(CF_3)ppy)_2(dtbbpy)]PF_6$	17
5	$[Ru(bpy)_3]Cl_2.6H_2O$	7
6	$[Ru(dmb)_3](PF_6)_2$	9
7	$[Ru(phen)_3](PF_6)_2$	5
8	$[Ru(3,4,7,8\text{-Me-phen})_3](PF_6)_2$	13
9	$[Ru(bpz)_3](BArF)_2$	trace
10	$[Ru(4,7\text{-Ph-phen})_3]Cl_2$	6
11	Eosin Y	7
12	Fluorescein	10
13	Rose Bengal	9

Reaction conditions: *N*-chlorophthalimide (1.0 mmol), benzene (0.5 mmol), photocatalyst (0.005 mmol, 1.0 mol %), potassium carbonate (1.5 mmol), acetonitrile (4.0 mL), 20 W CFL, 25 °C, 24 h. [a] Isolated yield. dmb = 4,4'-dimethyl-2,2'-bipyridine

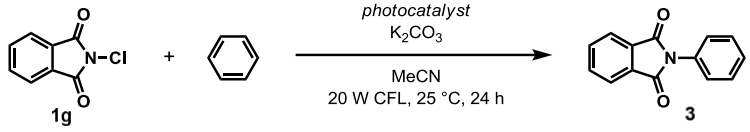
Table S4. Effect of catalyst equivalents and concentrations



Entry	Photocatalyst (mol %)	Concentration (M)	Yield [%][a]
1	[*fac*-Ir(ppy)$_3$] (0.1)	0.125	16
2	[*fac*-Ir(ppy)$_3$] (0.2)	0.125	22
3	[*fac*-Ir(ppy)$_3$] **(0.5)**	0.125	**35**
4	[*fac*-Ir(ppy)$_3$] (1.0)	0.125	34
5	[*fac*-Ir(ppy)$_3$] (3.0)	0.125	22
6	[*fac*-Ir(ppy)$_3$] (5.0)	0.125	15
7	[*fac*-Ir(dFppy)$_3$] **(0.5)**	0.1	**41**
8	[*fac*-Ir(dFppy)$_3$] (0.5)	0.125	38
9	[*fac*-Ir(dFppy)$_3$] (0.5)	0.2	30
10	[*fac*-Ir(dFppy)$_3$] (0.5)	0.5	24

Reaction conditions: *N*-chlorophthalimide (1.0 mmol), benzene (0.5 mmol), potassium carbonate (1.5 mmol), acetonitrile, 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

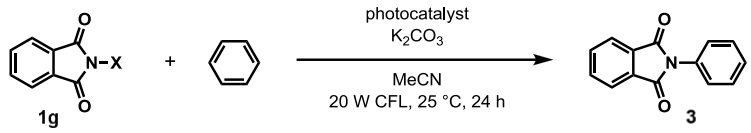
Table S5. Effect of *N*-chlorophthalimide and arene equivalents and concentrations



Entry	*N*-chlorophthalimide equiv (mmol)	Arene equiv	Photocatalyst (mol %)	Solvent (ml)	Yield [%][a]
1	2 (1.0 mmol)	1	[*fac*-Ir(ppy)$_3$] (1.0)	4.0	34
2	2	2	[*fac*-Ir(ppy)$_3$] (1.0)	4.0	22
3	2	5	[*fac*-Ir(ppy)$_3$] (1.0)	4.0	29
4	2	10	[*fac*-Ir(ppy)$_3$] (1.0)	4.0	26
5	2	20	[*fac*-Ir(ppy)$_3$] (1.0)	4.0	31
6	2	1	[*fac*-Ir(dFppy)$_3$] (0.5)	5.0	41
7	1 (0.5 mmol)	1	[*fac*-Ir(dFppy)$_3$] (0.5)	5.0	45
8	1	2	[*fac*-Ir(dFppy)$_3$] (0.5)	5.0	55
9	1	5	[*fac*-Ir(dFppy)$_3$] (0.5)	5.0	37
10	1	10	[*fac*-Ir(dFppy)$_3$] (0.5)	5.0	29

Reaction conditions: *N*-chlorophthalimide, benzene, potassium carbonate (1.5 mmol), acetonitrile, 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

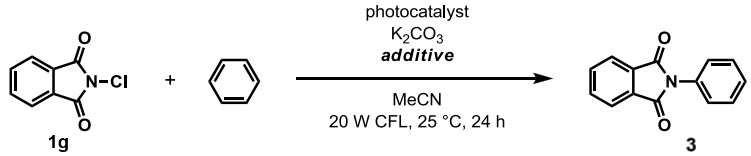
Table S6. Effect of leaving groups



Entry	X	Catalyst	Yield [%][a]
1	I	[*fac*-Ir(ppy)$_3$]	0
2	Br	[*fac*-Ir(ppy)$_3$]	4
3	**Cl**	[*fac*-Ir(ppy)$_3$]	**43 (41[b])**
4	AcO	[*fac*-Ir(ppy)$_3$]	NR
5	TsO	[*fac*-Ir(ppy)$_3$]	22
6	MsO	[*fac*-Ir(ppy)$_3$]	20
7	TfO	[*fac*-Ir(ppy)$_3$]	13
8	PhthN-I-Ph	[*fac*-Ir(ppy)$_3$]	0
9	**Cl**	[*fac*-Ir(dFppy)$_3$]	**55 (54[b])**
10	AcO	[*fac*-Ir(dFppy)$_3$]	NR
11	TsO	[*fac*-Ir(dFppy)$_3$]	33
12	MsO	[*fac*-Ir(dFppy)$_3$]	32
13	TfO	[*fac*-Ir(dFppy)$_3$]	ND

Reaction conditions: *N*-X reagent (0.5 mmol), benzene (1.0 mmol), photocatalyst (0.0025 mmol, 0.5 mol %), potassium carbonate (1.5 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy. [b] Isolated yield. NR: no reaction, ND: not detectable.

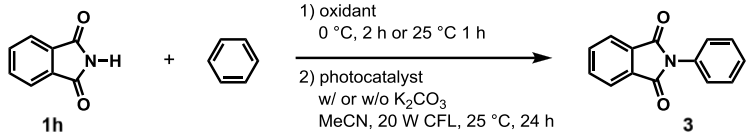
Table S7. Effects of additives



Entry	Catalyst	Additive (equiv)	Yield [%][a]
1	[*fac*-Ir(ppy)$_3$]	none	43
2	[*fac*-Ir(ppy)$_3$]	$AgNO_3$ (1)	NR
3	[*fac*-Ir(ppy)$_3$]	LiCl (1)	8
4	[*fac*-Ir(ppy)$_3$]	$Cu(OAc)_2$ (0.1)	14
5	[*fac*-Ir(ppy)$_3$]	PivOH (1)	47
6	[*fac*-Ir(ppy)$_3$]	PivOH (0.2)	48
7	[*fac*-Ir(ppy)$_3$]	AcOH (1)	27
8	[*fac*-Ir(ppy)$_3$]	AcOH (0.5)	36
9	[*fac*-Ir(ppy)$_3$]	**AcOH (0.2)**	**54**
10	[*fac*-Ir(dFppy)$_3$]	none	55
11	[*fac*-Ir(dFppy)$_3$]	$AgNO_3$ (1)	NR
12	[*fac*-Ir(dFppy)$_3$]	*t*BuOH (1)	55
13	[*fac*-Ir(dFppy)$_3$]	Diphenyl phosphate (0.2)	22
14	[*fac*-Ir(dFppy)$_3$]	TFA (0.2)	36
15	[*fac*-Ir(dFppy)$_3$]	Formic acid (0.2)	40
16	[*fac*-Ir(dFppy)$_3$]	PivOH (0.2)	46
17	[*fac*-Ir(dFppy)$_3$]	**AcOH (0.2)**	**65**

Reaction conditions: *N*-chlorophthalimide (0.5 mmol), benzene (1.0 mmol), photocatalyst (0.0025 mmol, 0.5 mol %), potassium carbonate (1.5 mmol), acetonitrile (5.0 mL), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy. NR: no reaction.

Table S8. Optimization of imidation reactions via *in situ* chlorination of phthalimide

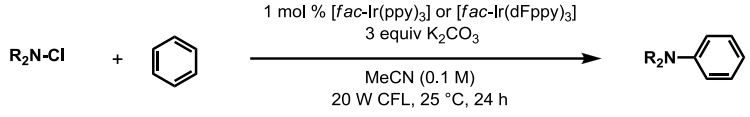


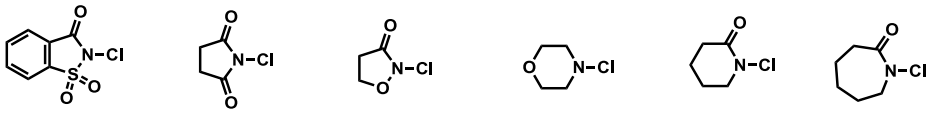
1h **3**

Entry	Catalyst	Oxidant (equiv)	Base (equiv)	Yield [%][a]
1	[*fac*-Ir(ppy)$_3$]	*t*BuOCl (1)	K_2CO_3 (3)	40
2	[*fac*-Ir(ppy)$_3$]	*t*BuOCl (2)	K_2CO_3 (3)	6
3[b]	[*fac*-Ir(ppy)$_3$]	NaOCl (1.5), AcOH (1.5)	–	28
4[c]	[*fac*-Ir(ppy)$_3$]	NaOCl (1.5), AcOH (1.5)	–	30
5[c]	[*fac*-Ir(ppy)$_3$]	NaOCl (1.5), AcOH (1.5)	K_2CO_3 (3)	20
6[b]	[*fac*-Ir(ppy)$_3$]	NaOCl (3), AcOH (3)	–	trace
7[c]	[*fac*-Ir(ppy)$_3$]	NaOCl (3), AcOH (3)	–	trace
8	[*fac*-Ir(dFppy)$_3$]	*t*BuOCl (1)	K_2CO_3 (3)	48
9	[*fac*-Ir(dFppy)$_3$]	*t*BuOCl (1), *t*BuOH (1)	K_2CO_3 (3)	**58**
10[c]	[*fac*-Ir(dFppy)$_3$]	NaOCl (1.5), AcOH (1.5)	–	32
11[c]	[*fac*-Ir(dFppy)$_3$]	NaOCl (1), AcOH (1)	–	39
12[c]	[*fac*-Ir(dFppy)$_3$]	NaOCl (1), AcOH (1), *t*BuOH (1)	–	52

Reaction conditions: phthalimide (0.5 mmol), benzene (1.0 mmol), photocatalyst (0.0025 mmol, 0.5 mol %), potassium carbonate (1.5 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy. [b] Step 1 was carried out at 0 °C for 2 h. [c] Step 1 was carried out at 25 °C for 1 h.

Table S9. Scope of nitrogen sources (*amination with preformed N-chloro compounds)*[a]

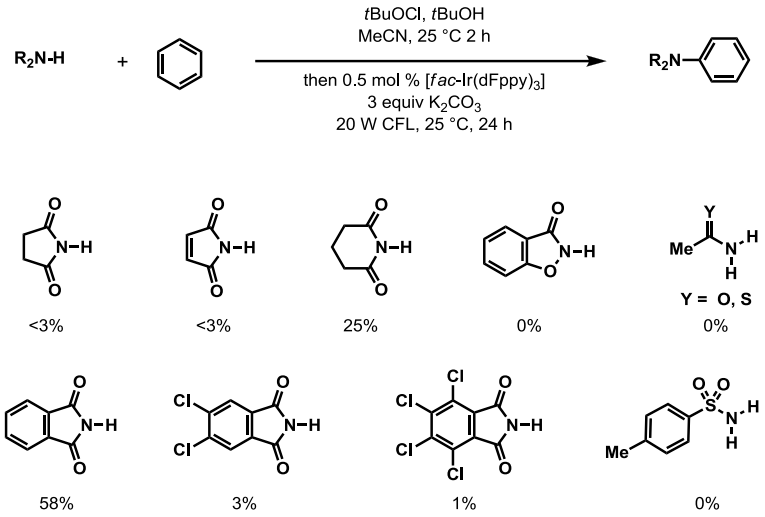




0% 21% 0% 0% 0% 0%

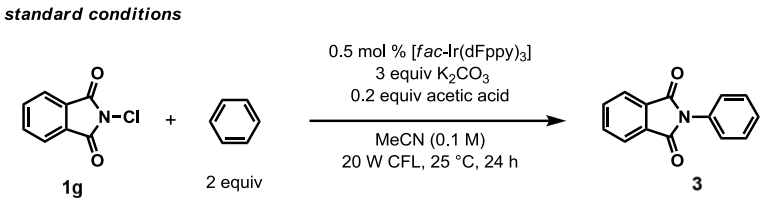
Reaction conditions: *N*-chloro compound (0.5 mmol), benzene (1.0 mmol), photocatalyst (0.005 mmol, 1 mol %), potassium carbonate (1.5 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

Table S10. Scope of nitrogen sources (*in situ chlorination followed by amination)* [a]



Reaction conditions: *N*-reagent (0.5 mmol), benzene (1.0 mmol), photocatalyst (0.0025 mmol, 0.5 mol %), *tert*-butyl hypochlorite (0.5 mmol), *tert*-butanol (0.5 mmol), potassium carbonate (1.5 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

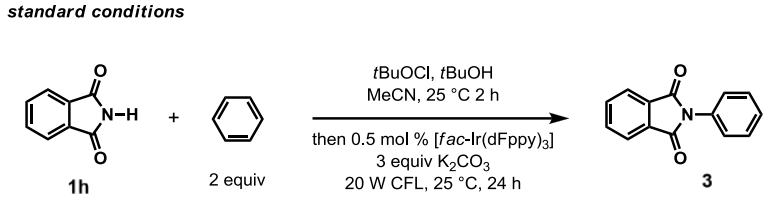
Table S11. Control experiments (conditions using *N*-chlorophthalimide)



Entry	Catalyst	Base	Additive	Visible Light	Yield [%][a]
1	O	O	O	O	65
2	O	O	–	O	55
3	O	O	–	–	trace
4	O	–	–	O	ND
5	O	–	O	O	trace
6	–	O	–	O	8
7	–	O	–	–	trace
8	O	–	–	O	ND
9	–	–	–	O	ND

Reaction conditions: *N*-chlorophthalimide (0.5 mmol), benzene (1.0 mmol), [*fac*-Ir(dFppy)$_3$] (0.0025 mmol, 0.5 mol %), potassium carbonate (1.5 mmol), acetic acid (0.1 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

Table S12. Control experiments (conditions using phthalimide with oxidant)



Entry	Catalyst	Base	*t*BuOCl	*t*BuOH	Visible Light	Yield [%][a]
1	O	O	O	O	O	58
2	O	O	O	–	O	48
3	O	O	–	–	O	NR
4	O	O	O	O	–	trace
5	O	–	O	O	O	trace
6	–	O	O	O	O	7
7	–	O	O	O	–	trace
8	–	–	O	O	O	ND

Reaction conditions: phthalimide (0.5 mmol), benzene (1.0 mmol), [*fac*-Ir(dFppy)$_3$] (0.0025 mmol, 0.5 mol %), *tert*-butyl hypochlorite (0.5 mmol), *tert*-butanol (0.5 mmol), potassium carbonate (1.5 mmol), acetonitrile (5.0 ml), 20 W CFL, 25 °C, 24 h. [a] Yields are based on crude proton NMR spectroscopy.

IV. Supplementary Results

A. Fluorescence quenching experiments

Emission intensities were recorded using a FluoroMate FS-2 fluorescence spectrometer. According to the literature [2], the excitation wavelength was 346 nm for all solutions and the emission intensities were collected at 468 nm. A 0.05 mM solution of [*fac*-Ir(dFppy)$_3$] in acetonitrile was used to prepare the appropriate quencher solutions which were placed in a 1.0 cm quartz cuvette to collect emission spectra. Recorded data were plotted to calculate the Stern-Volmer constants for quenchers.

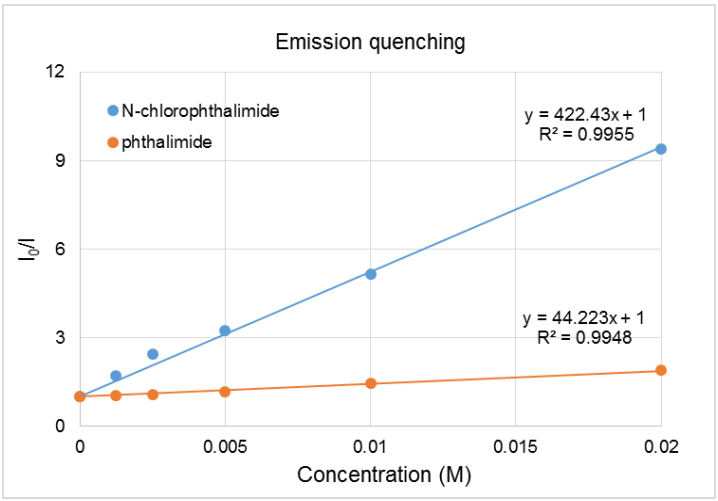
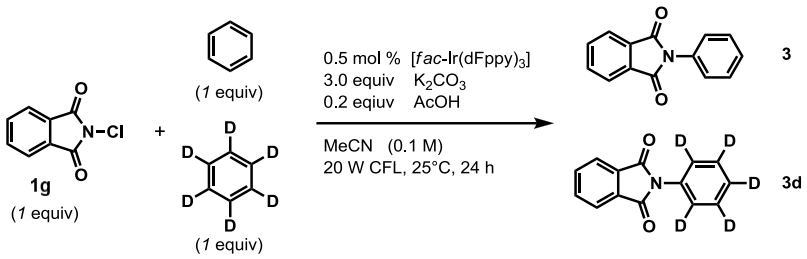


Figure S1. Stern-Volmer Plots of *N*-chlorophthalimide (blue) and phthalimide (orange)

B. Kinetic isotope effect of arene imidation



To a reaction vessel with a magnetic stirring bar were added *N*-chlorophthalimide (90.8 mg, 0.50 mmol), potassium carbonate (207.3 mg, 1.50 mmol), and [*fac*-Ir(dFppy)$_3$] (1.9 mg, 0.0025 mmol, 0.5 mol % for the limiting starting material). After addition of acetonitrile (5.0 ml), benzene (44.6 µl, 0.5 mmol), benzene-d^6 (44.3 µl, 0.5 mmol) and acetic acid (5.7 µl) were added. The mixture was placed in the irradiation apparatus equipped with a 20 W household compact fluorescent lamp (CFL). After 24 h, the reaction was quenched by addition of saturated $Na_2S_2O_3$ aqueous solution and the aqueous phase was then extracted with dichloromethane and the resulting organic phase was dried over anhydrous sodium sulfate, filtered and concentrated under reduced pressure. The resulting crude mixture was purified by flash column chromatography on silica gel, which furnished the title compounds with the KIE value as described by averaging the ratios of proton NMR signals obtained by carrying out the reaction three times. A representative proton NMR spectrum was provided as below.

Reaction run No.	**3/3d**
1	54/46 = 1.17
2	52/48 = 1.08
3	53/47 = 1.13
Average	1.13

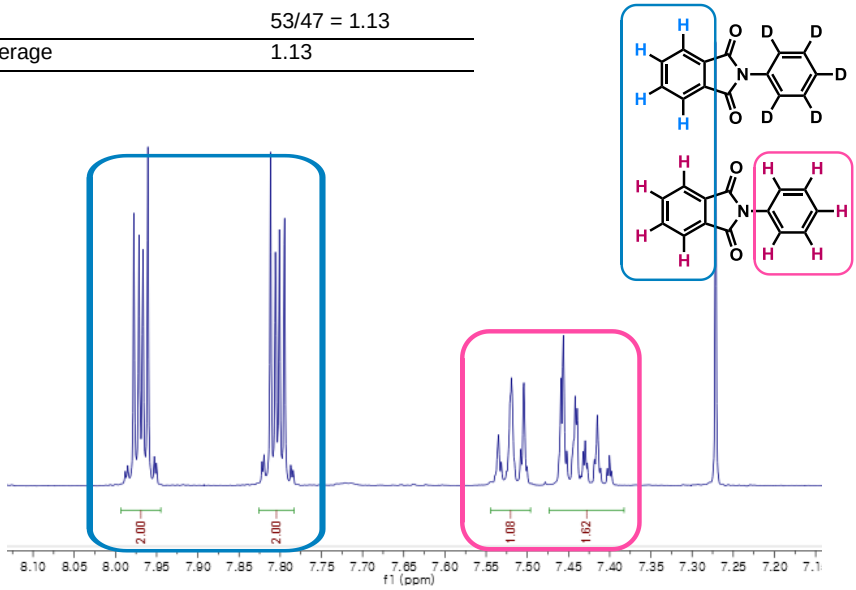


Figure S2. Proton NMR spectra for KIE expetimental analysis

C. Light on-off experiments

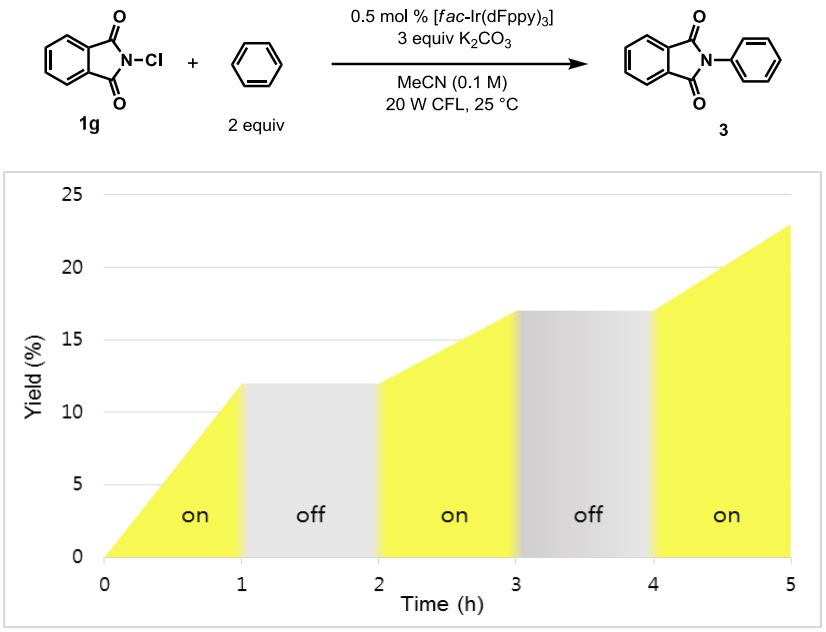


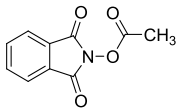
Figure S3. Light on-off experiment

Entry	1 h	2 h	3 h	4 h	5 h	Yield [%][a]
1	On	–	–	–	–	12
2	On	On	–	–	–	19
3	On	On	On	–	–	25
4	On	Off	–	–	–	12
5	On	Off	On	–	–	17
6	On	Off	On	Off	–	17
7	On	Off	On	Off	On	23

Reaction conditions: *N*-chlorophthalimide (0.5 mmol), benzene (1.0 mmol), [*fac*-Ir(dFppy)$_3$] (0.0025 mmol, 0.5 mol %), potassium carbonate (1.5 mmol), acetonitrile (0.1 M), 20 W CFL, 25 °C. [a] Yields are based on crude proton NMR spectroscopy.

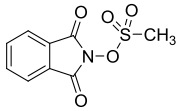
V. Compound Characterization

A. Preparation and characterization of substrates



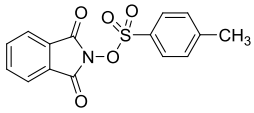
N-acetoxyphthalimide (1,3-dioxoisoindolin-2-yl acetate) (**1a**) [7]

The titled compound was prepared according to the procedure described in the reference literature. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92–7.88 (m, 2H), 7.82–7.78 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 162.1, 135.0, 129.1, 124.2, 17.9.



Phthalimide *N*-mesylate (1,3-dioxoisoindolin-2-yl methanesulfonate) (**1b**) [8]

The titled compound was prepared according to the procedure described in the reference literature. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97–7.91 (m, 2H), 7.88–7.82 (m, 2H), 3.48 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 135.6, 128.7, 124.7, 40.4.



Phthalimide *N*-tosylate (1,3-dioxoisoindolin-2-yl 4-methylbenzenesulfonate) (**1c**) [9]

The titled compound was prepared according to the procedure described in the reference literature. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.94 (m, 2H), 7.89–7.84 (m, 2H), 7.83–7.79 (m, 2H), 7.43–7.39 (m, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.5, 147.2, 135.3, 131.0, 130.3, 129.8, 128.8, 124.5, 22.2.

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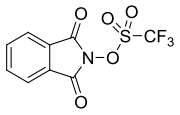
[7] E. Malmström, R. D. Miller and C. J. Hawker, *Tetrahedron*, 1997, **53**, 15225.

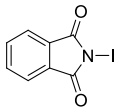
[8] C. L. Chan, E. J. Lien and Z. A. Tokes, *J. Med. Chem.*, 1987, **30**, 509.

[9] M. Chanmiya Sheikh, S. Takagi, A. Ogasawara, M. Ohira, R. Miyatake, H. Abe, T. Yoshimura and H. Morita, *Tetrahedron*, 2010, **66**, 2132.



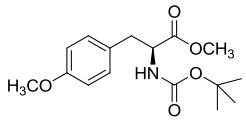
Phthalimide *N*-triflate (1,3-dioxoisoindolin-2-yl trifluoromethanesulfonate) (**1d**) [10]

The titled compound was prepared according to the procedure described in the reference literature. Colorless crystal. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.96 (m, 2H), 7.92–7.88 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 160.5, 136.1, 128.4, 125.1, 120.9, 116.6, 112.3.



N-iodophthalimide (2-iodoisoindoline-1,3-dione) (**1e**) [11]

The titled compound was prepared according to the procedure described in the reference literature. Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.91–7.84 (m, 2H), 7.73–7.65 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.9, 134.0, 133.0, 124.0.



(*S*)-Methyl 2-(*tert*-butoxycarbonylamino)-3-(4-methoxyphenyl)propanoate (**18aa**) [12]

The titled compound was prepared according to the procedure described in the reference literature. Light yellow solid. R_f 0.57 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.04 (d, J = 8.6 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 5.00–4.91 (m, 1H), 4.58–4.48 (m, 1H), 3.79 (s, 3H), 3.71 (s, 3H), 3.03 (qd, J = 14.0, 5.9 Hz, 2H), 1.42 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.6, 158.8, 155.3, 130.5, 128.1, 114.2, 80.1, 55.4, 54.7, 52.4, 37.6, 28.5.

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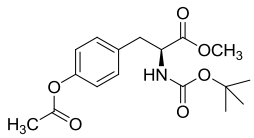
[10] T. M. Chapman and E. A. Freedman, *J. Org. Chem.*, 1973, **38**, 3908.

[11] R. Soundararajan, S. Krishnamurthy, V. S. Srinivasan and T. R. Balasubramanian, *J. Organomet. Chem.*, 1983, **255**, 295.

[12] B. R. Buckley, P. C. B. Page and V. McKee, *Synlett*, 2011,1399.

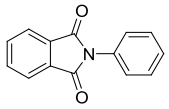


(*S*)-Methyl 3-(4-acetoxyphenyl)-2-(*tert*-butoxycarbonylamino)propanoate (**18ba**)

To a flame dried reaction vessel with a magnetic stirring bar were added *N*-(*tert*-butoxycarbonyl)-*L*-tyrosine methyl ester (1.00 g, 3.55 mmol), triethylamine (0.7 ml, 5.02 mmol) and 4-dimethylaminopyridine (10.0 mg). After addition of dichloromethane (7.1 ml) under N_2 atmosphere, acetyl chloride (0.28 ml, 3.94 mmol) was slowly added and the reaction mixture was stirred at room temperature. After 1.5 h, the reaction mixture was quenched with saturated NH_4Cl aqueous solution and the aqueous layer was extracted with dichloromethane three times. The combined organic layer was dried over magnesium sulfate and concentrated under reduced pressure. The product was purified by flash column chromatography to give white powder (1.10 g, 96%).

R_f 0.41 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.14 (d, *J* = 8.1 Hz, 2H), 7.05–6.97 (m, 2H), 5.07–4.96 (m, 1H), 4.62–4.55 (m, 1H), 3.71 (s, 3H), 3.08 (ddd, *J* = 36.7, 14.0, 5.9 Hz, 2H), 2.29 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 172.4, 169.6, 155.3, 149.9, 133.8, 130.5, 121.8, 80.2, 54.5, 52.5, 37.9, 28.5, 21.3. IR (neat): ν_{max} 3370, 2978, 1752, 1715, 1509, 1439, 1368, 1252, 1217, 1196, 1167, 1105, 1056, 1019, 912, 851, 750 cm^{-1}. HRMS (FAB) calcd. for $C_{17}H_{24}NO_6^+$ ($M+1^+$): 338.1604, found 338.1604.

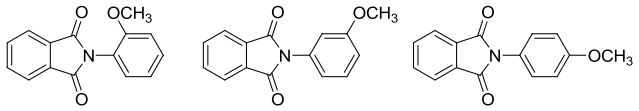
B. Characterizaion of products



N-phenylphthalimide (**3**) [13]

R_f 0.60 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00–7.92 (m, 2H), 7.83–7.77 (m, 2H), 7.54–7.48 (m, 2H), 7.47–7.38 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.5, 134.6, 131.9, 131.8, 129.3, 128.3, 126.8, 123.9.

[13] H. J. Kim, J. Kim, S. H. Cho and S. Chang, *J. Am. Chem. Soc.*, 2011, **133**, 16382.



N-(methoxyphenyl)phthalimide (**4**) [14,15]

Following the general procedure for photocatalytic imidation (*method A*), starting from anisole (109 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **4a**, **4b** and **4c** was afforded as a light yellow solid after column chromatography (52.3 mg, 0.207 mmol, 41%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (15: 1.0: 13).

R_f 0.41 (hexanes-EtOAc, 2:1).

N-(2-methoxyphenyl)phthalimide (**4a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96–7.86 (m, 2H), 7.80–7.70 (m, 2H), 7.48–7.37 (m, 1H), 7.26 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.13–7.00 (m, 2H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 155.6, 134.3, 132.5, 130.9, 130.2, 123.9, 121.1, 120.4, 112.3, 56.0.

N-(3-methoxyphenyl)phthalimide (**4b**)

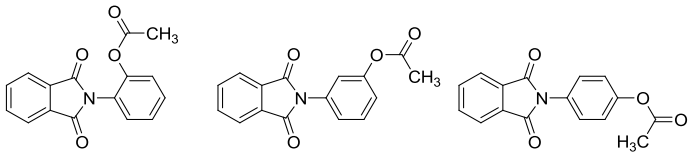
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.90 (m, 2H), 7.84–7.76 (m, 2H), 7.41 (t, *J* = 8.1 Hz, 1H), 7.06–6.86 (m, 3H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 160.2, 134.6, 132.9, 132.0, 130.0, 124.0, 119.1, 114.3, 112.6, 55.7.

N-(4-methoxyphenyl)phthalimide (**4c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.91 (m, 2H), 7.81–7.74 (m, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 3.85 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.8, 159.4, 134.5, 132.0, 128.1, 124.4, 123.9, 114.7, 55.7.

[14] R. Shrestha, P. Mukherjee, Y. Tan, Z. C. Litman and J. F. Hartwig, *J. Am. Chem. Soc.*, 2013, **135**, 8480.

[15] M. V. Khedkar, S. R. Khan, D. N. Sawant, D. B. Bagal and B. M. Bhanage, *Adv. Synth. Catal.*, 2011, **353**, 3415.



5a **5b** **5c**

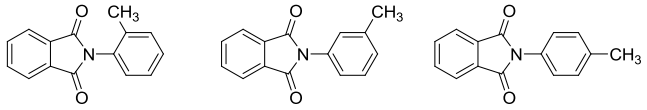
N-(acetoxyphenyl)phthalimide (**5**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from phenyl acetate (127 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **5a**, **5b** and **5c** was afforded as a white solid after column chromatography (64.1 mg, 0.228 mmol, 46%). The structures and the relative ratios of isomers were determined by ^{1}H NMR spectraoscopy described in the reference literature.

Isomeric ratio (3.2: 2.0: 1.0).

R_f 0.37 (hexanes-EtOAc, 2:1).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.94 (m, 2H), 7.85–7.78 (m, 2H), 7.55–7.46 (m, 1.2H), 7.43–7.35 (m, 2H), 7.32 (t, *J* = 2.0 Hz, 0.2H), 7.29–7.23 (m, 0.4H), 7.17 (dd, *J* = 8.2, 1.3 Hz, 0.4H), 2.34 (s, 0.5H), 2.32 (s, 1H), 2.15 (s, 1.6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 169.3, 169.1, 168.2, 167.3, 167.0, 166.7, 151.0, 150.1, 146.5, 134.7, 134.6, 132.8, 132.0, 131.8, 131.7, 130.0, 129.8, 129.6, 129.3, 127.6, 126.4, 124.1, 124.03, 123.99, 123.95, 123.8, 123.6, 122.4, 121.2, 119.8, 21.3, 21.1.



6a **6b** **6c**

N-(methylphenyl)phthalimide (**6**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from toluene (106 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **6a**, **6b** and **6c** was afforded as a white solid after column chromatography (55.9 mg, 0.236 mmol, 47%). In the case following the *method B* starting from toluene (53.1 μl, 0.50 mmol), the isomeric mixture was provided in 46% yield (54.5 mg, 0.230 mmol). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (2.5: 1.0: 1.3).

R_f 0.48 (hexanes-EtOAc, 2:1).

N-(2-methylphenyl)phthalimide (**6a**)

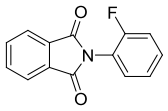
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.93 (m, 2H), 7.83–7.77 (m, 2H), 7.39–7.38 (m, 1H), 7.37 (d, *J* = 1.1 Hz, 1H), 7.36–7.31 (m, 1H), 7.21 (d, *J* = 7.5 Hz, 1H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 136.7, 134.5, 132.2, 131.4, 130.8, 129.7, 128.9, 127.1, 124.0, 18.3.

N-(3-methylphenyl)phthalimide (**6b**)

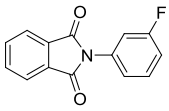
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.79 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.42–7.35 (m, 1H), 7.24–7.19 (m, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 139.3, 134.5, 132.0, 131.7, 129.3, 129.1, 127.5, 124.0, 123.9, 21.6.

N-(4-methylphenyl)phthalimide (**6c**)

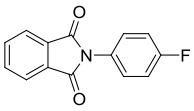
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.79 (dd, *J* = 5.5, 3.0 Hz, 2H), 7.31 (s, 4H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 138.4, 134.5, 132.0, 130.0, 129.2, 126.7, 123.9, 21.4.



7a



7b



7c

N-(fluorophenyl)phthalimide (**7**) [14,16]

Following the general procedure for photocatalytic imidation (*method A*), starting from fluorobenzene (94.2 µl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **7a**, **7b** and **7c** was afforded as a white solid after column chromatography (56.7 mg, 0.235 mmol, 47%). In the case following the *method B* starting from fluorobenzene (47.1 µl, 0.50 mmol), the isomeric mixture was provided in 40% yield (48.6 mg, 0.201 mmol). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (7.4: 4.0: 9.3).

R_f 0.57 (hexanes-EtOAc, 2:1).

N-(2-fluorophenyl)phthalimide (**7a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.93 (m, 2H), 7.84–7.76 (m, 2H), 7.49–7.41 (m, 1H), 7.37 (td, *J* = 7.7, 2.0 Hz, 1H), 7.32–7.23 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.7, 159.3, 156.8, 134.7, 132.1, 131.0, 130.9, 130.1, 124.9, 124.8, 124.1, 119.6, 119.5, 117.1, 116.9. ^{19}F NMR (376 MHz, $CDCl_3$): δ -118.71, -118.73, -118.73, -118.74, -118.75, -118.75, -118.76, -118.77.

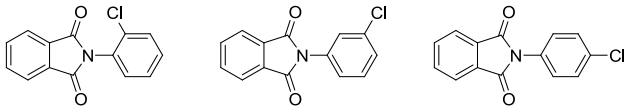
N-(3-fluorophenyl)phthalimide (**7b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.93 (m, 2H), 7.85–7.77 (m, 2H), 7.48 (td, *J* = 8.2, 6.3 Hz, 1H), 7.29 (ddd, *J* = 8.0, 1.9, 0.9 Hz, 1H), 7.27–7.22 (m, 1H), 7.12 (tdd, *J* = 8.4, 2.5, 0.9 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 164.1, 161.6, 134.8, 133.3, 133.2, 131.7, 130.5, 130.4, 124.1, 122.23, 122.19, 115.3, 115.1, 114.3, 114.0. ^{19}F NMR (376 MHz, $CDCl_3$): δ -111.18, -111.20, -111.21, -111.23, -111.23, -111.25.

N-(4-fluorophenyl)phthalimide (**7c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.91 (m, 2H), 7.85–7.76 (m, 2H), 7.47–7.39 (m, 2H), 7.24–7.15 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 163.4, 160.9, 134.7, 131.8, 128.6, 128.5, 127.78, 127.75, 124.0, 116.5, 116.2. ^{19}F NMR (376 MHz, $CDCl_3$): δ -113.06, -113.07, -113.08, -113.08, -113.09, -113.10, -113.10, -113.11, -113.13.

[16] D. C. Chen, H. Q. Ye and H. Wu, *Catal. Commun.*, 2007, **8**, 1527.



8a **8b** **8c**

N-(chlorophenyl)phthalimide (**8**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from chlorobenzene (101 µl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **8a**, **8b** and **8c** was afforded as a white solid after column chromatography (77.0 mg, 0.299 mmol, 60%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (2.3: 1.0: 2.0).

R_f 0.57 (hexanes-EtOAc, 2:1).

N-(2-chlorophenyl)phthalimide (**8a**)

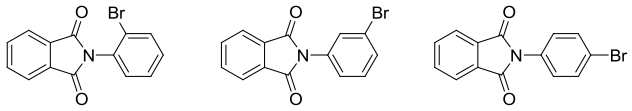
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03–7.93 (m, 2H), 7.86–7.77 (m, 2H), 7.62–7.54 (m, 1H), 7.48–7.40 (m, 2H), 7.39–7.32 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 134.7, 133.4, 132.1, 130.9, 130.7, 129.8, 127.9, 124.2.

N-(3-chlorophenyl)phthalimide (**8b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03–7.93 (m, 2H), 7.86–7.77 (m, 2H), 7.53–7.49 (m, 1H), 7.48–7.42 (m, 1H), 7.41–7.36 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 134.8, 133.0, 131.8, 130.3, 128.4, 126.9, 124.8, 124.1.

N-(4-chlorophenyl)phthalimide (**8c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.92 (m, 2H), 7.84–7.78 (m, 2H), 7.51–7.45 (m, 2H), 7.45–7.39 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 134.8, 134.0, 131.8, 130.4, 129.5, 127.9, 124.1.



9a **9b** **9c**

N-(bromophenyl)phthalimide (**9**) [13,17]

Following the general procedure for photocatalytic imidation (*method A*), starting from bromobenzene (105 µl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **9a**, **9b** and **9c** was afforded as a white solid after column chromatography (65.7 mg, 0.217 mmol, 43%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (3.3: 2.0: 2.7).

R_f 0.57 (hexanes-EtOAc, 2:1).

N-(2-bromophenyl)phthalimide (**9a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.96 (m, 2H), 7.85–7.79 (m, 2H), 7.78–7.73 (m, 1H), 7.50–7.44 (m, 1H), 7.40–7.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 134.7, 133.8, 132.1, 131.6, 131.2, 131.0, 128.7, 124.2, 123.5.

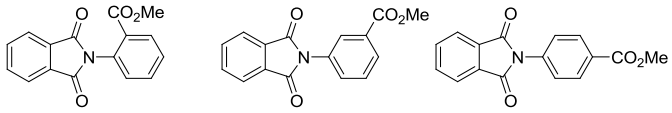
N-(3-bromophenyl)phthalimide (**9b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.92 (m, 2H), 7.86–7.77 (m, 2H), 7.65 (t, J = 1.7 Hz, 1H), 7.57–7.51 (m, 1H), 7.46–7.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 134.8, 133.1, 131.7, 131.3, 130.5, 129.7, 125.3, 124.1, 122.6.

N-(4-bromophenyl)phthalimide (**9c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.93 (m, 2H), 7.84–7.77 (m, 2H), 7.67–7.61 (m, 2H), 7.39–7.33 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.1, 134.8, 132.5, 131.8, 130.9, 128.2, 124.1, 122.0.

[17] M. V. Khedkar, S. R. Khan, K. P. Dhake and B. M. Bhanage, *Synthesis*, 2012, **44**, 2623.



10a **10b** **10c**

N-(methoxycarbonylphenyl)phthalimide (**10**) [18,19]

Following the general procedure for photocatalytic imidation (*method A*), starting from methyl benzoate (136.2 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **10a**, **10b** and **10c** was afforded as a white solid after column chromatography (48.3 mg, 0.172 mmol, 34%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (7.2: 11: 4.0).

R_f 0.48 (hexanes-EtOAc, 2:1).

N-(2-methoxycarbonylphenyl)phthalimide (**10a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21–8.11 (m, 1H), 8.00–7.91 (m, 2H), 7.84–7.75 (m, 2H), 7.69 (ddd, *J* = 7.7, 1.5, 0.8 Hz, 1H), 7.60–7.50 (m, 1H), 7.40 (dd, *J* = 7.9, 1.0 Hz, 1H), 3.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 165.4, 134.5, 133.5, 132.3, 132.0, 131.8, 130.5, 129.3, 128.2, 123.9, 52.5.

N-(3-methoxycarbonylphenyl)phthalimide (**10b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (dd, *J* = 2.7, 1.0 Hz, 1H), 8.09 (ddd, *J* = 7.7, 1.9, 1.0 Hz, 1H), 8.01–7.94 (m, 2H), 7.85–7.79 (m, 2H), 7.69–7.64 (m, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.2, 166.3, 134.8, 132.1, 131.8, 131.5, 131.1, 129.4, 129.3, 127.9, 124.1, 52.6.

N-(4-methoxycarbonylphenyl)phthalimide (**10c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (dd, *J* = 8.7, 2.1 Hz, 2H), 8.00–7.95 (m, 2H), 7.83–7.76 (m, 2H), 7.58 (dd, *J* = 8.5, 1.5 Hz, 2H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 166.5, 136.0, 134.8, 131.7, 130.6, 129.4, 126.1, 124.1, 52.5.

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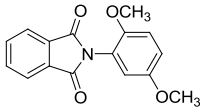
[18] J. Vamecq, P. Bac, C. Herrenknecht, P. Maurois, P. Delcourt and J. P. Stables, *J. Med. Chem.*, 2000, **43**, 1311.

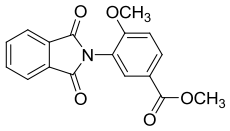
[19] Y. Zhou, A. L. Rodriguez, R. Williams, C. D. Weaver, P. J. Conn and C. W. Lindsley, *Bioorg. Med. Chem. Lett.*, 2009, **19**, 6502.



N-(2,5-dimethoxyphenyl)phthalimide (**11**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 1,4-dimethoxybenzene (138.2 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **11** was afforded as a light yellow solid after column chromatography (62.1 mg, 0.219 mmol, 44%) with *N*-(4-methoxyphenyl)phthalimide (12.3 mg, 0.049 mmol, 10%).

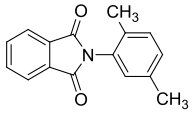
R_f 0.31 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97–7.91 (m, 2H), 7.81–7.72 (m, 2H), 7.00–6.95 (m, 2H), 6.85–6.80 (m, 1H), 3.78 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 153.8, 149.9, 134.3, 132.4, 123.9, 120.9, 116.1, 115.8, 113.4, 56.6, 56.0. IR (neat): ν_{max} 3093, 3009, 2956, 2836, 1786, 1769, 1724, 1510, 1461, 1384, 1278, 1227, 1204, 1114, 1045, 1023, 928, 893, 861, 734 cm^{-1}. HRMS (EI) calcd. for $C_{16}H_{13}NO_4^+$ (M^+): 283.0844, found 283.0845.



N-(2-methoxy-5-methoxycarbonylphenyl)phthalimide (**12**)

Following the general procedure for photocatalytic imidation (*method A*), starting from methyl *p*-anisate (166.0 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **12** was afforded as a colorless crystal after column chromatography (75.0 mg, 0.241 mmol, 48%). In the case following the *method A* starting from methyl *p*-anisate (83.1 mg, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product was provided in 39% yield (60.3 mg, 0.194 mmol) which was not changed in open-air conditions. When the reaction was carried out in the conditions following the *method B* starting from methyl *p*-anisate (83.1 mg, 0.50 mmol), the product yield was 41% (63.7 mg, 0.205 mmol).

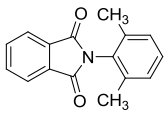
R_f 0.20 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (dd, J = 8.8, 2.1 Hz, 1H), 7.96 (d, J = 2.1 Hz, 1H), 7.92 (dd, J = 5.4, 3.1 Hz, 2H), 7.77 (dd, J = 5.4, 3.1 Hz, 2H), 7.06 (d, J = 8.8 Hz, 1H), 3.87 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.2, 166.2, 159.4, 134.5, 132.9, 132.4, 132.1, 124.0, 123.3, 120.5, 111.8, 56.4, 52.3. IR (neat): ν_{max} 2952, 2844, 1782, 1724, 1611, 1512, 1447, 1377, 1317, 1294, 1273, 1214, 1185, 1148, 1119, 1086, 1022, 985, 915, 881, 830, 795, 767, 720 cm^{-1}. HRMS (EI) calcd. for $C_{17}H_{13}NO_5^+$ (M^+): 311.0793, found 311.0789.



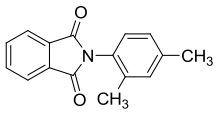
N-(2,5-dimethylphenyl)phthalimide (**13**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from *p*-xylene (123 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **13** was afforded as a white solid after column chromatography (50.1 mg, 0.199 mmol, 40%). In the case following the *method A* starting from *p*-xylene (61.7 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product was provided in 50% yield (63.0 mg, 0.251 mmol).

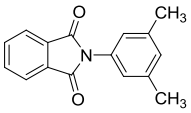
R_f 0.61 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.92 (m, 2H), 7.83–7.75 (m, 2H), 7.29–7.22 (m, 1H), 7.21–7.14 (m, 1H), 7.02 (s, 1H), 2.36 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 136.9, 134.5, 133.5, 132.2, 131.1, 130.54, 130.48, 129.3, 123.9, 21.0, 17.8.



14a



14b



14c

N-(dimethylphenyl)phthalimide (**14**) [20]

Following the general procedure for photocatalytic imidation (*method A*), starting from *m*-xylene (123 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **14a**, **14b** and **14c** was afforded as a white solid after column chromatography (72.2 mg, 0.287 mmol, 57%). In the case following the *method A* starting from *m*-xylene (61.7 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the isomeric mixture was provided in 72% yield (90.8 mg, 0.361 mmol). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (4.0: 9.0: 1.0).

R_f 0.61 (hexanes-EtOAc, 2:1).

N-(2,6-dimethylphenyl)phthalimide (**14a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.94 (m, 2H), 7.84–7.77 (m, 2H), 7.31–7.25 (m, 1H), 7.19 (d, *J* = 7.5 Hz, 2H), 2.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 137.1, 134.5, 132.2, 130.0, 129.7, 128.7, 124.0, 18.3.

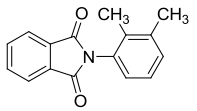
N-(2,4-dimethylphenyl)phthalimide (**14b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.91 (m, 2H), 7.83–7.75 (m, 2H), 7.18 (s, 1H), 7.14 (dd, *J* = 8.5, 0.5 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 2.38 (s, 3H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 139.7, 136.3, 134.5, 132.2, 132.1, 128.6, 128.0, 127.8, 123.9, 21.4, 18.1.

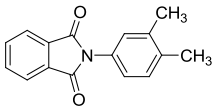
N-(3,5-dimethylphenyl)phthalimide (**14c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.92 (m, 2H), 7.82–7.76 (m, 2H), 7.05 (s, 1H), 7.02 (s, 2H), 2.38 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 139.1, 134.5, 132.0, 131.5, 130.4, 124.7, 123.9, 21.5.

[20] A. A. Kantak, S. Potavathri, R. A. Barham, K. M. Romano and B. DeBoef, *J. Am. Chem. Soc.*, 2011, **133**, 19960.



15a



15b

N-(dimethylphenyl)phthalimide (**15**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from *o*-xylene (121 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **15a** and **15b** was afforded as a white solid after column chromatography (41.5 mg, 0.164 mmol, 33%). In the case following the *method A* starting from *o*-xylene (60.3 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the isomeric mixture was provided in 34% yield (43.1 mg, 0.171 mmol). When the reaction was carried out in the conditions following the *method B* starting from *o*-xylene (121 μl, 1.00 mmol) and phthalimide (73.6 mg, 0.50 mmol), the product yield was 35% (43.9 mg, 0.174 mmol). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (1.0: 1.0).

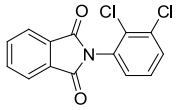
R_f 0.61 (hexanes-EtOAc, 2:1).

N-(2,3-dimethylphenyl)phthalimide (**15a**)

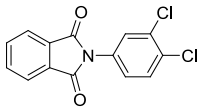
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.91 (m, 2H), 7.84–7.75 (m, 2H), 7.30–7.19 (m, 2H), 7.09–7.01 (m, 1H), 2.36 (s, 3H), 2.08 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.8, 138.6, 135.3, 134.5, 132.3, 131.2, 130.7, 126.48, 126.46, 124.0, 20.7, 14.9.

N-(3,4-dimethylphenyl)phthalimide (**15b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.91 (m, 2H), 7.82–7.75 (m, 2H), 7.29–7.25 (m, 1H), 7.19–7.16 (m, 1H), 7.14 (dd, J = 8.0, 2.2 Hz, 1H), 2.31 (d, J = 2.9 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 137.8, 137.2, 134.5, 132.0, 130.5, 129.3, 127.9, 124.3, 123.8, 20.1, 19.7.



16a



16b

N-(dichlorolphenyl)phthalimide (**16**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from 1,2-dichlorobenzene (113 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **16a** and **16b** was afforded as a white solid after column chromatography (53.7 mg, 0.184 mmol, 37%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

Isomeric ratio (4.0: 4.9).

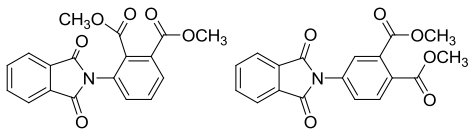
R_f 0.51 (hexanes-EtOAc, 2:1).

N-(2,3-dichlorophenyl)phthalimide (**16a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.81 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.59 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.36 (t, *J* = 8.1 Hz, 1H), 7.31–7.23 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 134.8, 134.5, 132.5, 131.9, 131.6, 131.5, 129.2, 127.9, 124.2.

N-(3,4-dichlorophenyl)phthalimide (**16b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.94 (m, 2H), 7.85–7.78 (m, 2H), 7.64 (d, *J* = 2.4 Hz, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.37 (dd, *J* = 8.6, 2.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.8, 135.0, 133.2, 132.3, 131.7, 131.3, 130.9, 128.4, 125.7, 124.2.



17a 17b

N-(dimethoxycarbonylphenyl)phthalimide (**17**)

Following the general procedure for photocatalytic imidation (*method A*), starting from dimethylphthalate (163 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **17a** and **17b** was afforded as a white solid after column chromatography (46.6 mg, 0.137 mmol, 27%). The structures and the relative ratios of isomers were determined by synthesis of authentic samples and their ^{1}H NMR spectra.

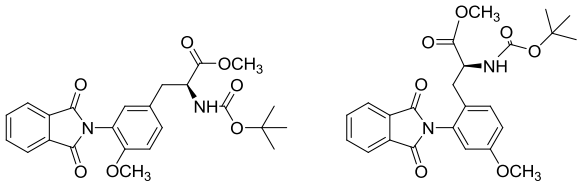
Isomeric ratio (1.0: 1.0).

N-(2,3-dimethoxycarbonylphenyl)phthalimide (**17a**)

R_f 0.21 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.97–7.93 (m, 2H), 7.82–7.79 (m, 2H), 7.66 (t, *J* = 7.9 Hz, 1H), 7.52 (dd, *J* = 7.9, 1.2 Hz, 1H), 3.91 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.1, 166.6, 166.4, 134.8, 133.3, 133.2, 132.99, 131.96, 131.0, 130.7, 130.6, 124.2, 53.2, 53.1. IR (neat): ν_{max} 2953, 2360, 1786, 1726, 1596, 1468, 1433, 1381, 1284, 1235, 1205, 1153, 1133, 1111, 1085, 1066, 914, 885, 763, 717 cm^{-1}. HRMS (EI) calcd. for $C_{18}H_{13}NO_6^+$ (M^+): 339.0743, found 339.0746.

N-(3,4-dimethoxycarbonylphenyl)phthalimide (**17b**)

R_f 0.24 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99–7.96 (m, 2H), 7.93 (d, *J* = 2.1 Hz, 1H), 7.86 (d, *J* = 8.3 Hz, 1H), 7.84–7.81 (m, 2H), 7.72 (dd, *J* = 8.3, 2.1 Hz, 1H), 3.93 (s, 3H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 167.3, 166.7, 135.0, 134.6, 133.1, 131.6, 131.2, 130.0, 128.5, 126.6, 124.3, 53.1, 53.0. IR (neat): ν_{max} 2954, 1782, 1724, 1607, 1468, 1436, 1416, 1376, 1283, 1219, 1192, 1129, 1070, 961, 881, 846, 823, 789, 771, 718 cm^{-1}. HRMS (EI) calcd. for $C_{18}H_{13}NO_6^+$ (M^+): 339.0743, found 339.0749.



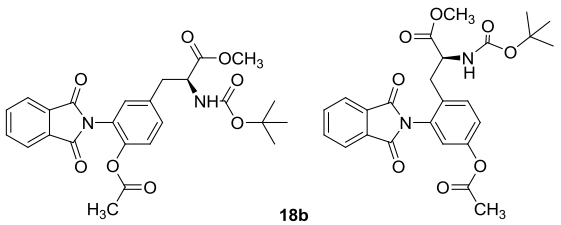
18a

(*S*)-Methyl 2-(*tert*-butoxycarbonylamino)-3-(3-(phthalimidyl)-4-methoxyphenyl)propanoate and (*S*)-methyl 2-(*tert*-butoxycarbonylamino)-3-(2-(phthalimidyl)-4-methoxyphenyl)propanoate (**18a**)

Following the general procedure for photocatalytic imidation (*method A*), starting from (*S*)-methyl 2-(*tert*-butoxycarbonylamino)-3-(4-methoxyphenyl)propanoate **18aa** (309.4 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **18a** was afforded as a light yellow oil after column chromatography (93.1 mg, 0.205 mmol, 40%). In the case following the *method A* starting from **18aa** (154.7 mg, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product was provided in 46% yield (103 mg, 0.228 mmol). The products were characterized as a mixture because they could not be separated into the each of isomers by silica gel chromatography or preparative TLC.

Isomeric ratio (7.1 : 1.0).

R_f 0.22 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99–7.96 (m, 0.28H), 7.95–7.92 (m, 2H), 7.82–7.80 (m, 0.28H), 7.79–7.77 (m, 2H), 7.31–7.28 (m, 0.28H), 7.24–7.20 (m, 1H), 7.02–6.96 (m, 2H), δ 6.72 (d, J = 2.5 Hz, 0.14H), 5.15–5.13 (m, 0.14H), 5.09–5.02 (m, 1H), 4.62–4.55 (m, 1H), 4.49–4.46 (m, 0.14H), 3.80 (s, 0.42H), 3.78 (s, 3H), 3.73 (s, 3H), 3.60 (s, 0.42H), 3.13–3.05 (m, 2H), 2.98–2.93 (m, 0.14H), 2.88–2.84 (m, 0.14H), 1.44 (s, 9H), 1.34 (s, 1.26H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 172.4, 167.9, 167.8, 167.4, 167.3, 159.3, 155.3, 154.6, 134.6, 134.3, 132.4, 132.2, 131.5, 131.4, 131.0, 128.7, 124.1, 124.0, 123.8, 120.4, 116.1, 114.5, 112.4, 80.2, 79.9, 56.1, 55.6, 54.6, 54.0, 52.6, 52.5, 37.5, 33.4, 28.5, 28.4. IR (neat): ν_{max} 3372, 2977, 1782, 1722, 1614, 1513, 1447, 1380, 1287, 1258, 1166, 1112, 1086, 1025, 879, 719 cm^{-1}. HRMS (FAB) calcd. for $C_{24}H_{27}N_2O_7^+$ (M+1$^+$): 455.1818, found 455.1817.



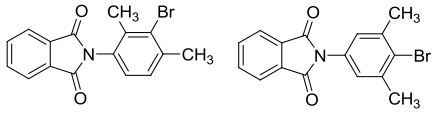
18b

(*S*)-Methyl 3-(4-acetoxy-3-(phthalimidyl)phenyl)-2-(*tert*-butoxycarbonylamino)propanoate and (*S*)-methyl 3-(4-acetoxy-2-(phthalimidyl)phenyl)-2-(*tert*-butoxycarbonylamino)propanoate (**18b**)

Following the general procedure for photocatalytic imidation (*method A*), starting from (*S*)-methyl 3-(4-acetoxyphenyl)-2-(*tert*-butoxycarbonylamino)propanoate **18ba** (337.4 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **18b** was afforded as a light yellow oil after column chromatography (88.0 mg, 0.182 mmol, 36%). In the case following the *method A* starting from **18ba** (168.7 mg, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product was provided in 33% yield (78.6 mg, 0.163 mmol). The products were characterized as a mixture because they could not be separated into the each of isomers by silica gel chromatography or preparative TLC.

Isomeric ratio (1.1: 1.0).

R_f 0.36 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01–7.91 (m, 4H), 7.85–7.77 (m, 4H), 7.41 (d, *J* = 8.6 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.26 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.22 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.15 (s, 1H), 7.03 (d, *J* = 2.4 Hz, 1H), 5.13 (dd, *J* = 41.8, 8.2 Hz, 2H), 4.56 (dd, *J* = 51.8, 7.2 Hz, 2H), 3.73 (s, 3H), 3.60 (s, 3H), 3.15 (d, *J* = 4.4 Hz, 2H), 3.01 (dd, *J* = 14.7, 5.9 Hz, 1H), 2.91 (dd, *J* = 14.7, 7.8 Hz, 1H), 2.27 (s, 3H), 2.12 (s, 3H), 1.43 (s, 9H), 1.33 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.5, 172.2, 168.9, 168.2, 167.6, 167.4, 166.5, 155.4, 155.3, 150.0, 145.4, 134.7, 134.6, 132.9, 132.04, 131.98, 131.7, 131.2, 130.8, 130.3, 124.2, 124.1, 124.0, 123.7, 122.9, 122.5, 80.3, 80.1, 54.4, 53.8, 52.7, 52.5, 37.7, 33.6, 28.5, 28.4, 21.3, 21.1. IR (neat): ν_{max} 3376, 2978, 1768, 1727, 1608, 1505, 1436, 1375, 1241, 1180, 1110, 1015, 887, 721 cm^{-1}. HRMS (FAB) calcd. for $C_{25}H_{27}N_2O_8^+$ (M+1$^+$): 483.1767, found 483.1767.



N-(bromodimethylphenyl)phthalimide (**19**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 2-bromo-1,3-dimethylbenzene (133 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the isomeric mixture of **19a** and **19b** was afforded as a white solid after column chromatography (77.5 mg, 0.235 mmol, 47%). The structures and relative ratios of isomers were determined by isolation of the isomers and assigning their ^{1}H NMR spectra.

Isomeric ratio (4.0: 1.0).

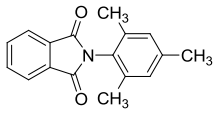
R_f 0.59 (hexanes-EtOAc, 2:1).

N-(3-bromo-2,4-dimethylphenyl) phthalimide (**19a**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.92 (m, 2H), 7.85–7.76 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.0 Hz, 1H), 2.48 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.5, 140.3, 137.3, 134.7, 132.1, 129.1, 129.0, 128.6, 127.5, 124.1, 24.5, 19.7. IR (neat): ν_{max} 1733, 1713, 1481, 1381, 1235, 1110, 887, 721, 695 cm^{-1}. HRMS (EI) calcd. for $C_{16}H_{12}BrNO_2$ (M+): 329.0051, found 329.0050.

N-(4-bromo-3,5-dimethylphenyl)phthalimide (**19b**)

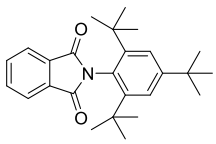
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.91 (m, 2H), 7.84–7.76 (m, 2H), 7.26 (s, 2H), 2.47 (s, 6H). ^{13}C NMR (100 MHz $CDCl_3$): δ 167.4, 139.6, 134.7, 131.9, 130.1, 127.7, 126.4, 124.0, 24.3. IR (neat): ν_{max} 1717, 1590, 1468, 1414, 1378, 1110, 1086, 1031, 857, 711 cm^{-1}. HRMS (EI) calcd. for $C_{16}H_{12}BrNO_2$ (M+): 329.0051, found 329.0051.



N-mesitylphthalimide (**20**) [13]

Following the general procedure for photocatalytic imidation (*method A*), starting from mesitylene (139 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **20** was afforded as a white solid after column chromatography (46.4 mg, 0.175 mmol, 35%). In the case following the *method C* starting from mesitylene (66.0 μl, 0.50 mmol), the product **20** was provided in 52% yield (68.7 mg, 0.259 mmol).

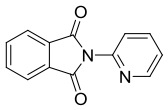
R_f 0.68 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.93 (m, 2H), 7.83–7.77 (m, 2H), 7.01 (s, 2H), 2.33 (s, 3H), 2.12 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.6, 139.6, 136.7, 134.5, 132.2, 129.5, 127.2, 124.0, 21.4, 18.2.



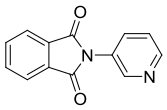
N-(2,4,6-tri-*tert*-butylphenyl)phthalimide (**21**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 1,3,5-tri-*tert*-butylbenzene (246.4 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **21** was afforded as a white solid after column chromatography (19.7 mg, 0.0503 mmol, 10%).

R_f 0.70 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99–7.95 (m, 2H), 7.81–7.77 (m, 2H), 7.55 (s, 2H), 1.35 (s, 9H), 1.28 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.5, 151.0, 148.6, 134.5, 132.9, 125.1, 124.2, 124.1, 37.3, 35.2, 33.1, 31.6. IR (neat): ν_{max} 2949, 2904, 1728, 1710, 1597, 1461, 1439, 1377, 1364, 1275, 1198, 1107, 1078, 882, 764, 750, 723, 701 cm^{-1}. HRMS (EI) calcd. for $C_{26}H_{33}NO_2^+$ (M^+): 391.2511, found 391.2513.



22a



22b

N-(pyridinyl)phthalimide (**22**) [15]

Following the general procedure for photocatalytic imidation (*method A*), starting from pyridine (80.6 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), **22a** (13.8 mg, 0.062 mmol, 12%) and **22b** (29.3 mg, 0.131 mmol, 26%) were afforded as white solid after column chromatography. The structures and relative ratios of isomers were determined by isolation and comparing with synthesized authentic samples by assigning their ^{1}H NMR spectra.

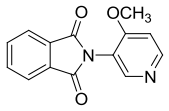
Isomeric ratio (1.0: 2.1).

N-(2-pyridinyl)phthalimide (**22a**)

R_f 0.33 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.73–8.68 (m, 1H), 8.01–7.96 (m, 2H), 7.93–7.87 (m, 1H), 7.84–7.79 (m, 2H), 7.48–7.42 (m, 1H), 7.40–7.35 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9, 149.9, 146.4, 138.5, 134.8, 132.0, 124.2, 123.7, 122.3.

N-(3-pyridinyl)phthalimide (**22b**)

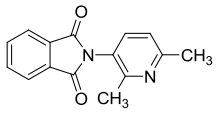
R_f 0.22 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81–8.78 (m, 1H), 8.65 (dd, J = 4.8, 1.5 Hz, 1H), 8.01–7.96 (m, 2H), 7.87–7.81 (m, 3H), 7.47 (ddd, J = 8.2, 4.8, 0.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 149.0, 147.6, 135.0, 133.78, 131.77, 129.0, 124.2, 123.9.



N-(4-methoxypyridin-3-yl)phthalimide (**23**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 4-methoxypyridine (102 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **23** was afforded as a light yellow solid after column chromatography (44.4 mg, 0.175 mmol, 35%). In the case following the *method A* starting from 4-methoxypyridine (50.7 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product **23** was provided in 40% yield (51.2 mg, 0.251 mmol).

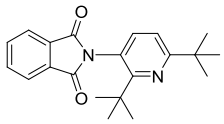
R_f 0.10 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (d, *J* = 5.7 Hz, 1H), 8.41 (s, 1H), 7.99–7.94 (m, 2H), 7.83–7.79 (m, 2H), 6.99 (d, *J* = 5.7 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 161.8, 152.4, 150.8, 134.6, 132.2, 124.1, 117.9, 107.6, 56.1. IR (neat): ν_{max} 2360, 2342, 1717, 1593, 1511, 1433, 1381, 1288, 1192, 1102, 1016, 881, 828, 716 cm^{-1}. HRMS (EI) calcd. for $C_{14}H_{10}N_2O_3^+$ (M^+): 254.0691, found 254.0692.



N-(2,6-dimethylpyridin-3-yl)phthalimide (**24**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 2,6-lutidine (116 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **24** was afforded as a light yellow solid after column chromatography (52.3 mg, 0.207 mmol, 41%). In the case following the *method A* starting from 2,6-lutidine (57.9 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product **24** was provided in 50% yield (63.1 mg, 0.250 mmol).

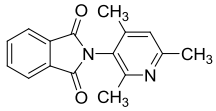
R_f 0.36 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99–7.94 (m, 2H), 7.84–7.80 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 2.60 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.2, 159.2, 156.2, 136.9, 134.8, 132.1, 124.5, 124.1, 121.7, 24.6, 21.4. IR (neat): ν_{max} 2925, 1783, 1764, 1728, 1582, 1474, 1381, 1266, 1229, 1107, 1084, 885, 828, 719 cm^{-1}. HRMS (EI) calcd. for $C_{15}H_{12}N_2O_2^+$ (M^+): 252.0899, found 252.0899.



N-(2,6-di-*tert*-butylpyridin-3-yl)phthalimide (**25**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 2,6-di-*tert*-butylpyridine (224 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **25** was afforded as a white solid after column chromatography (59.2 mg, 0.176 mmol, 35%). In the case following the *method A* starting from 2,6-di-*tert*-butylpyridine (112 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product **25** was provided in 29% yield (48.0 mg, 0.143 mmol).

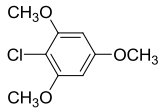
R_f 0.60 (hexanes-EtOAc, 2:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98–7.92 (m, 2H), 7.82–7.76 (m, 2H), 7.24 (dd, *J* = 2.7, 0.9 Hz, 2H), 1.38 (s, 9H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.9, 168.5, 164.7, 139.1, 134.6, 132.4, 124.1, 122.7, 117.4, 39.4, 38.1, 30.6, 30.3. IR (neat): ν_{max} 2960, 2868, 1786, 1766, 1732, 1715, 1587, 1483, 1456, 1383, 1356, 1266, 1226, 1132, 1108, 1084, 904, 887, 831, 761, 721, 706, 690, 530 cm^{-1}. HRMS (EI) calcd. for $C_{21}H_{24}N_2O_2^+$ (M^+): 336.1838, found 336.1837.



N-(2,4,6-trimethylpyridin-3-yl)phthalimide (**26**)

Following the general procedure for photocatalytic imidation (*method A*), starting from 2,4,6-collidine (132 μl, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **26** was afforded as a light yellow solid after column chromatography (48.4 mg, 0.185 mmol, 37%). In the case following the *method A* starting from 2,4,6-collidine (66.0 μl, 0.50 mmol) and *N*-chlorophthalimide (181.6 mg, 1.00 mmol), the product **26** was provided in 45% yield (59.4 mg, 0.226 mmol).

R_f 0.20 (hexanes-EtOAc, 2:1). ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00–7.96 (m, 2H), 7.85–7.81 (m, 2H), 7.02 (s, 1H), 2.55 (s, 3H), 2.36 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.1, 158.9, 156.4, 146.6, 134.8, 132.1, 124.2, 123.8, 123.4, 24.4, 21.1, 17.9. IR (neat): ν_{max} 2925, 1783, 1728, 1602, 1469, 1373, 1317, 1224, 1111, 1087, 1029, 8884, 722 cm^{-1}. HRMS (EI) calcd. for $C_{16}H_{14}N_2O_2^+$ (M^+): 266.1055, found 266.1056.

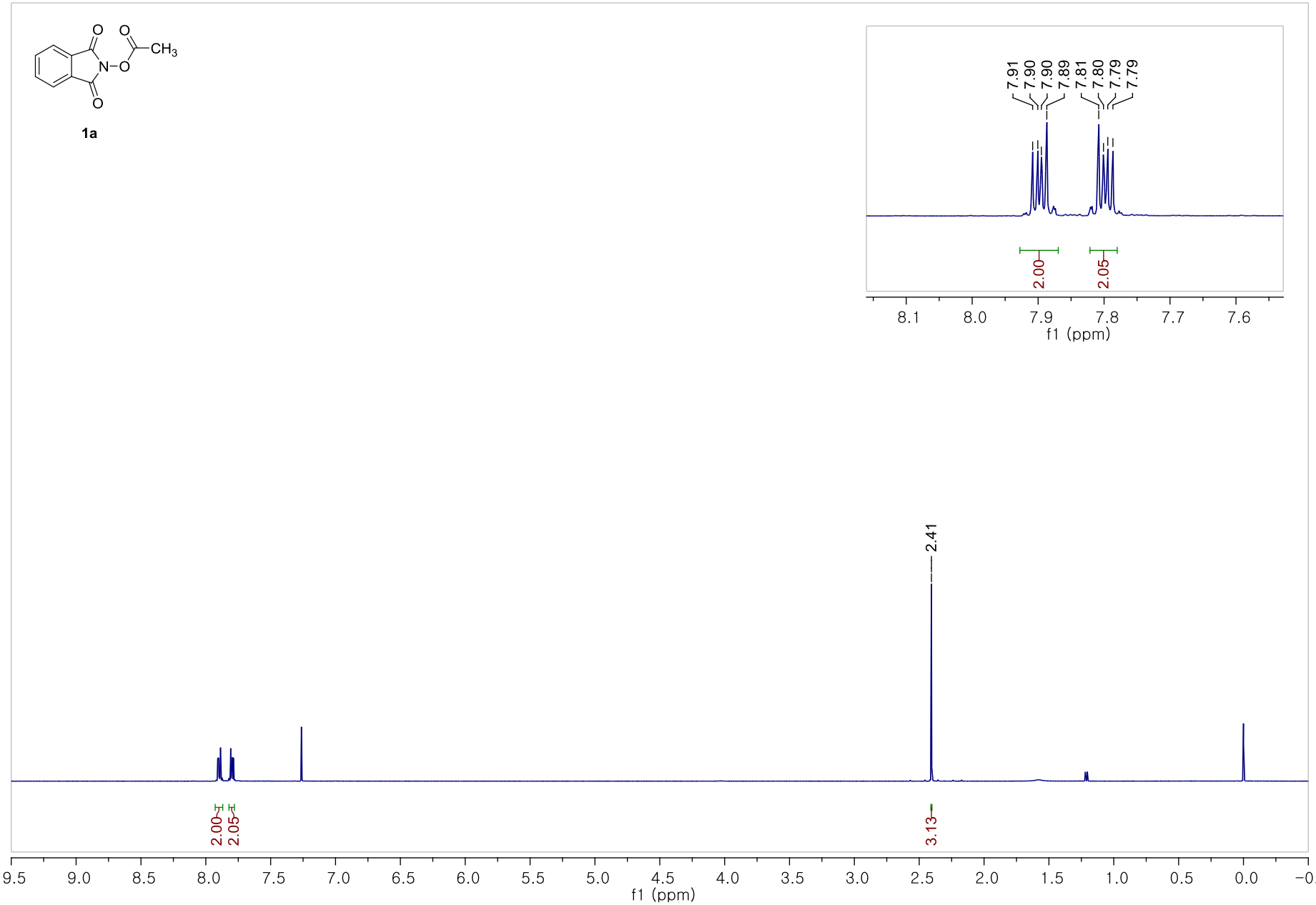


2-Chloro-1,3,5-trimethoxybenzene (**28**) [21]

Following the general procedure for photocatalytic imidation (*method A*), starting from 1,3,5-trimethoxybenzene (168.2 mg, 1.00 mmol) and *N*-chlorophthalimide (90.8 mg, 0.50 mmol), the titled compound **28** was afforded as a light yellow crystal after column chromatography (83.1 mg, 0.410 mmol, 82%).

R_f 0.62 (hexanes-EtOAc, 2:1). ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.18 (s, 2H), 3.85 (s, 6H), 3.81 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.6, 156.7, 102.91, 91.8, 56.5, 55.7.

[21] L. Gu, T. Lu, M. Zhang, L. Tou and Y. Zhang, *Adv. Synth. Catal.*, 2013, **355**, 1077.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7.90
7.89
7.81
7.80
7.79
7.79
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2.05
8.1
8.0
7.9
7.8
7.7
7.6
f1 (ppm)
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2.00
2.05
3.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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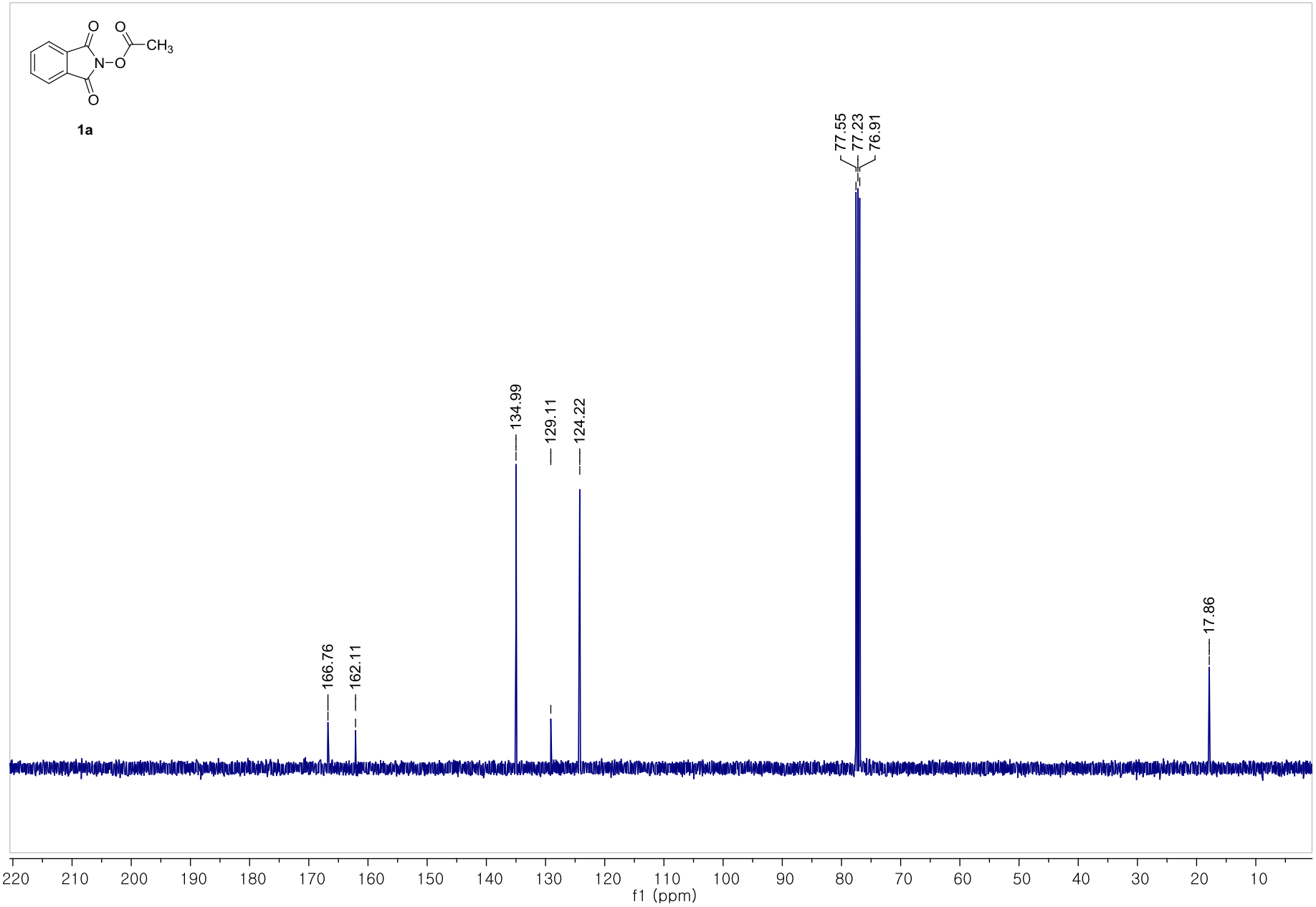
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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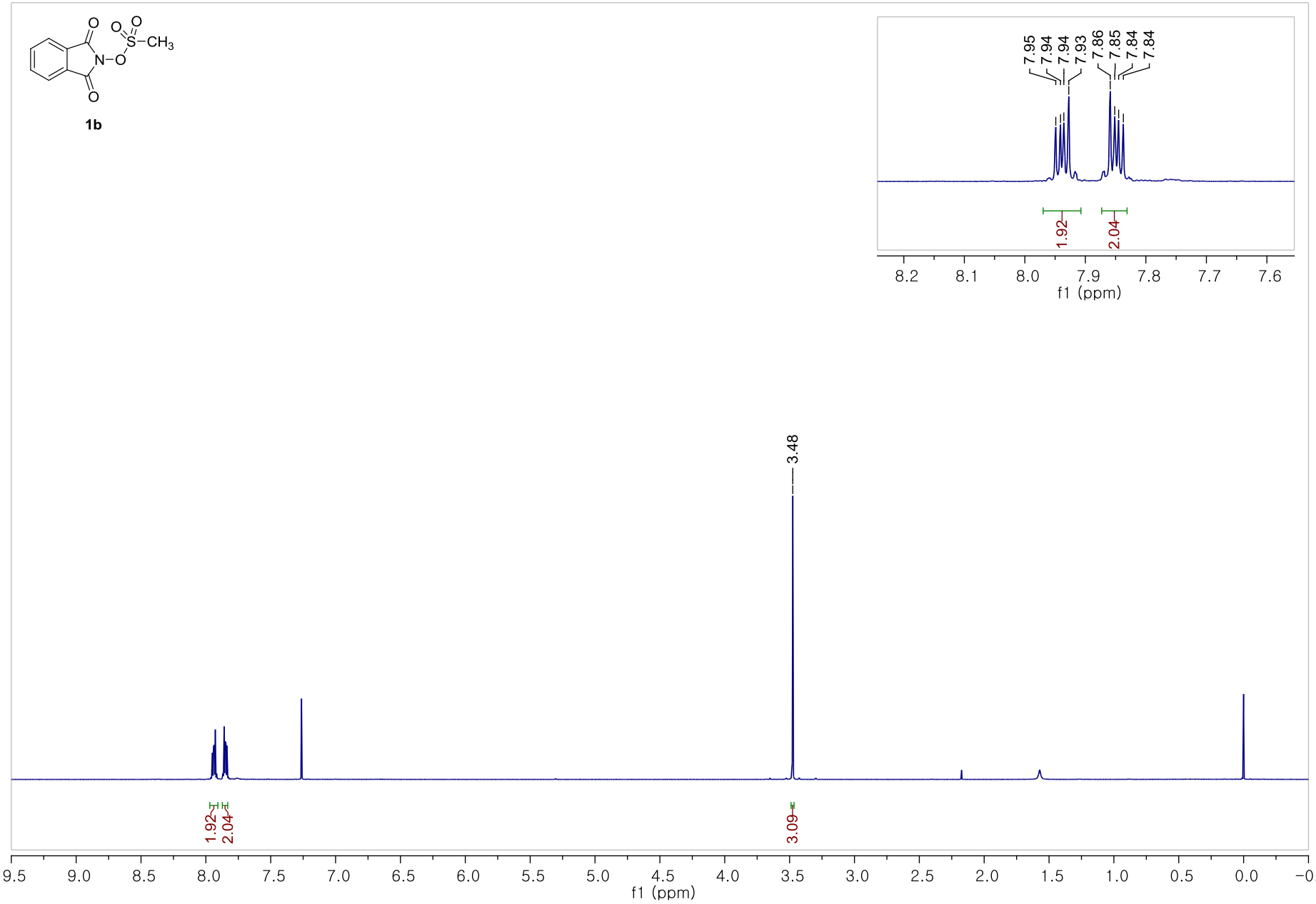
166.76
162.11
134.99
129.11
124.22
77.55
77.23
76.91
17.86
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


1b
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7.94
7.94
7.93
7.86
7.85
7.84
7.84
1.92
2.04
8.2
8.1
8.0
7.9
7.8
7.7
7.6
f1 (ppm)
3.48
1.92
2.04
3.09
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
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1.5
1.0
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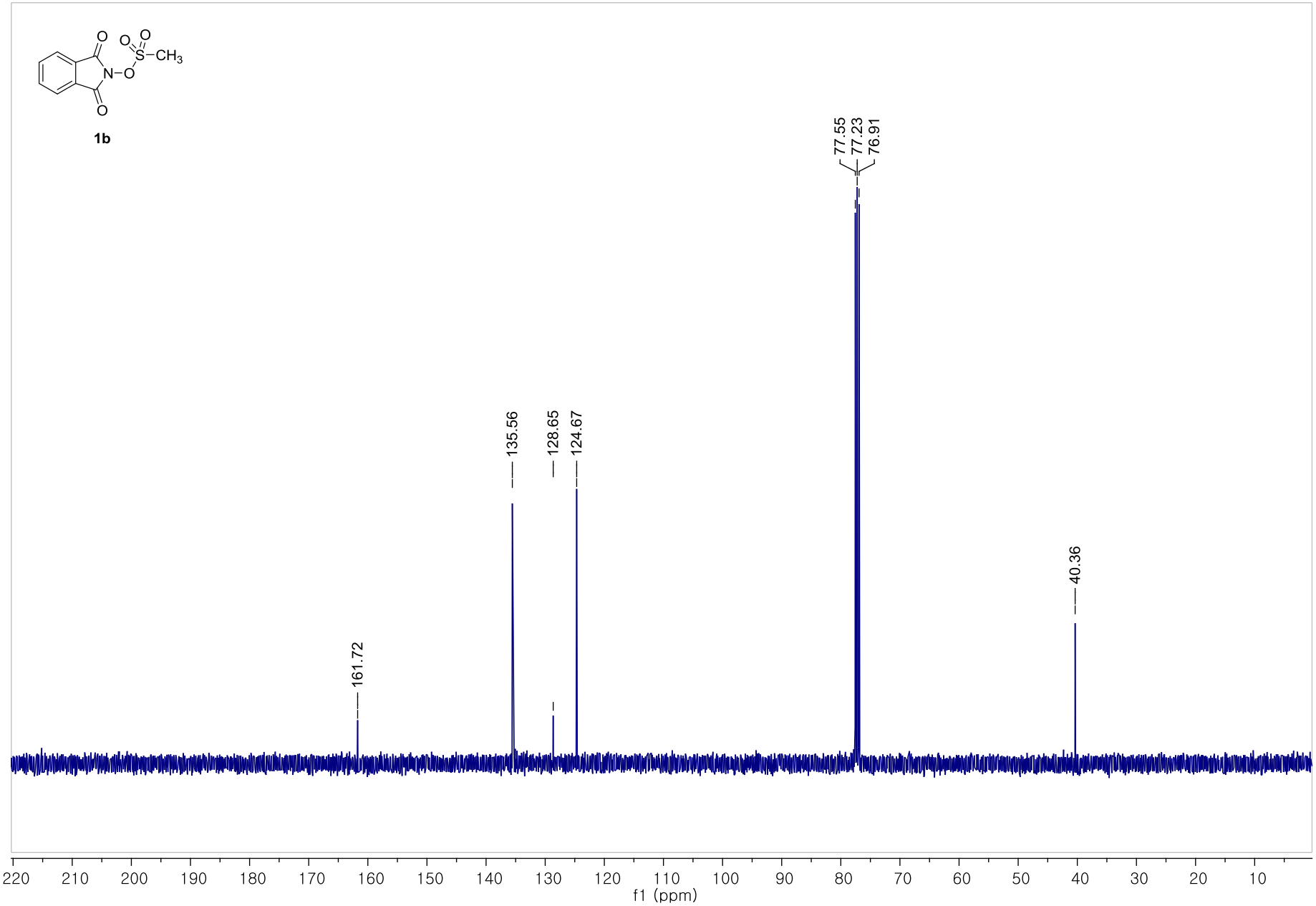
0.0
f1 (ppm)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128.65
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40.36
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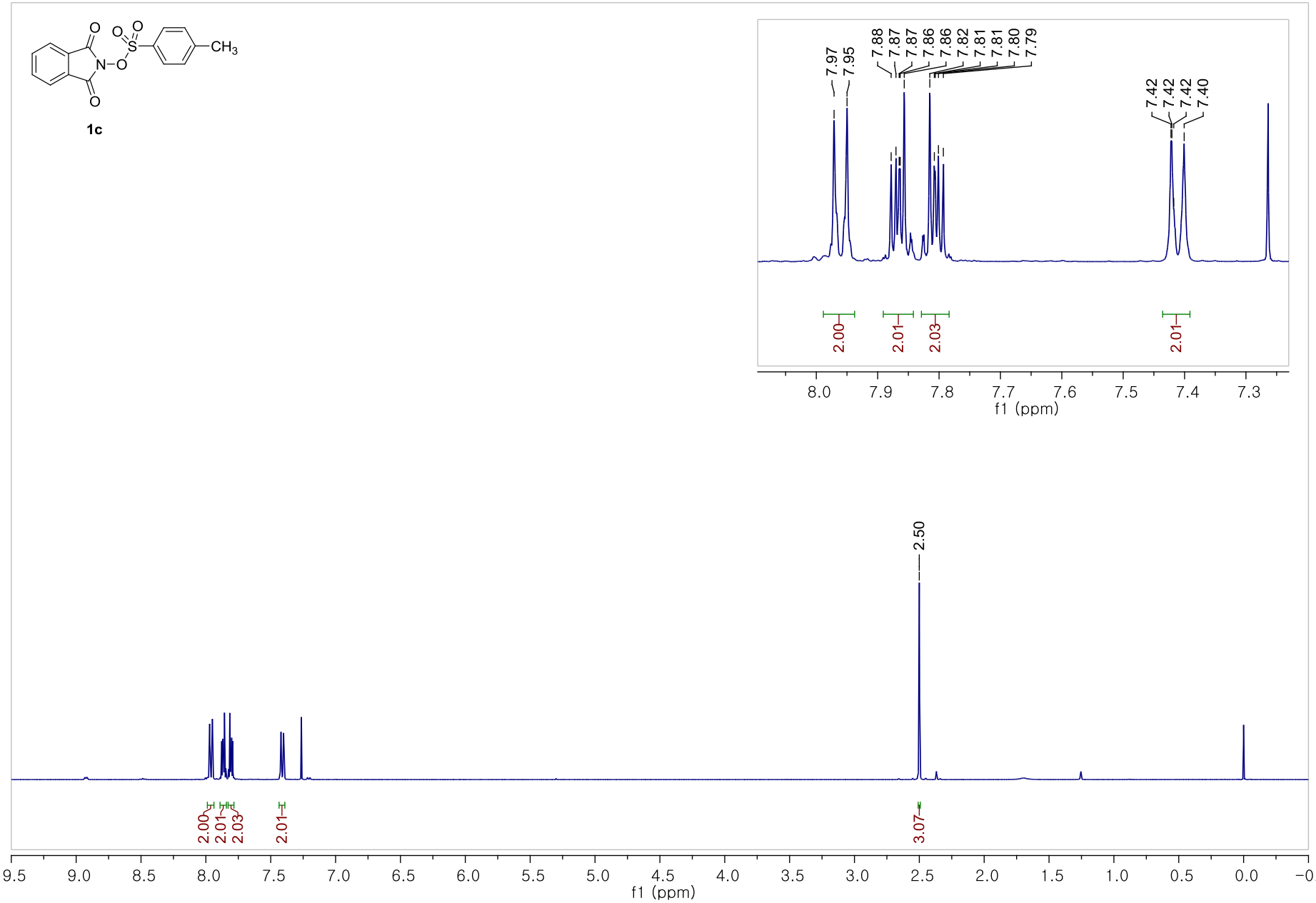
f1 (ppm)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7.82
7.81
7.81
7.80
7.79
7.42
7.42
7.42
7.40
2.00
2.01
2.03
2.01
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)
2.50
2.00
2.01
2.03
2.01
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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2.5
2.0
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1.0
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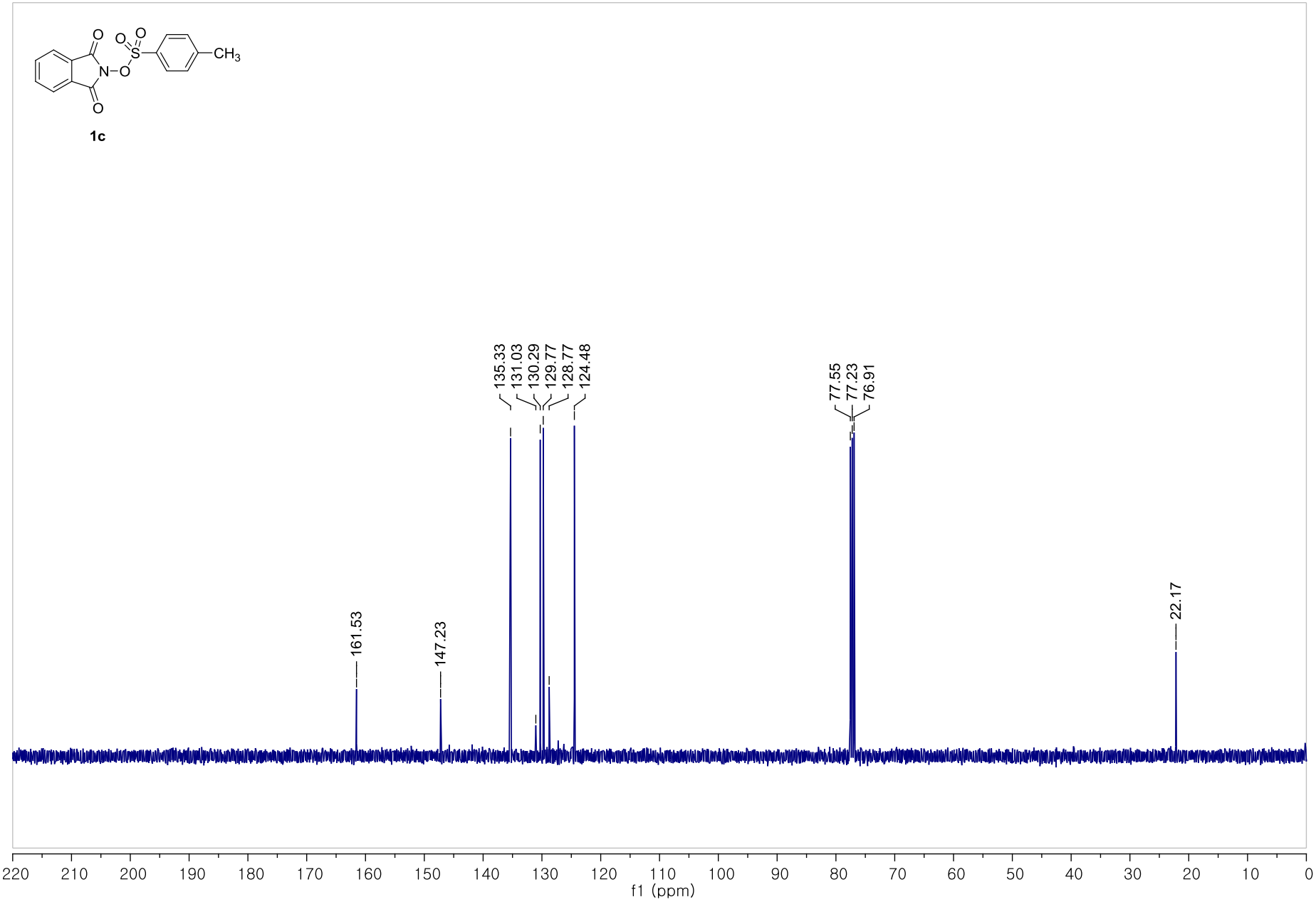
0.0
f1 (ppm)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147.23
135.33
131.03
130.29
129.77
128.77
124.48
77.55
77.23
76.91
22.17
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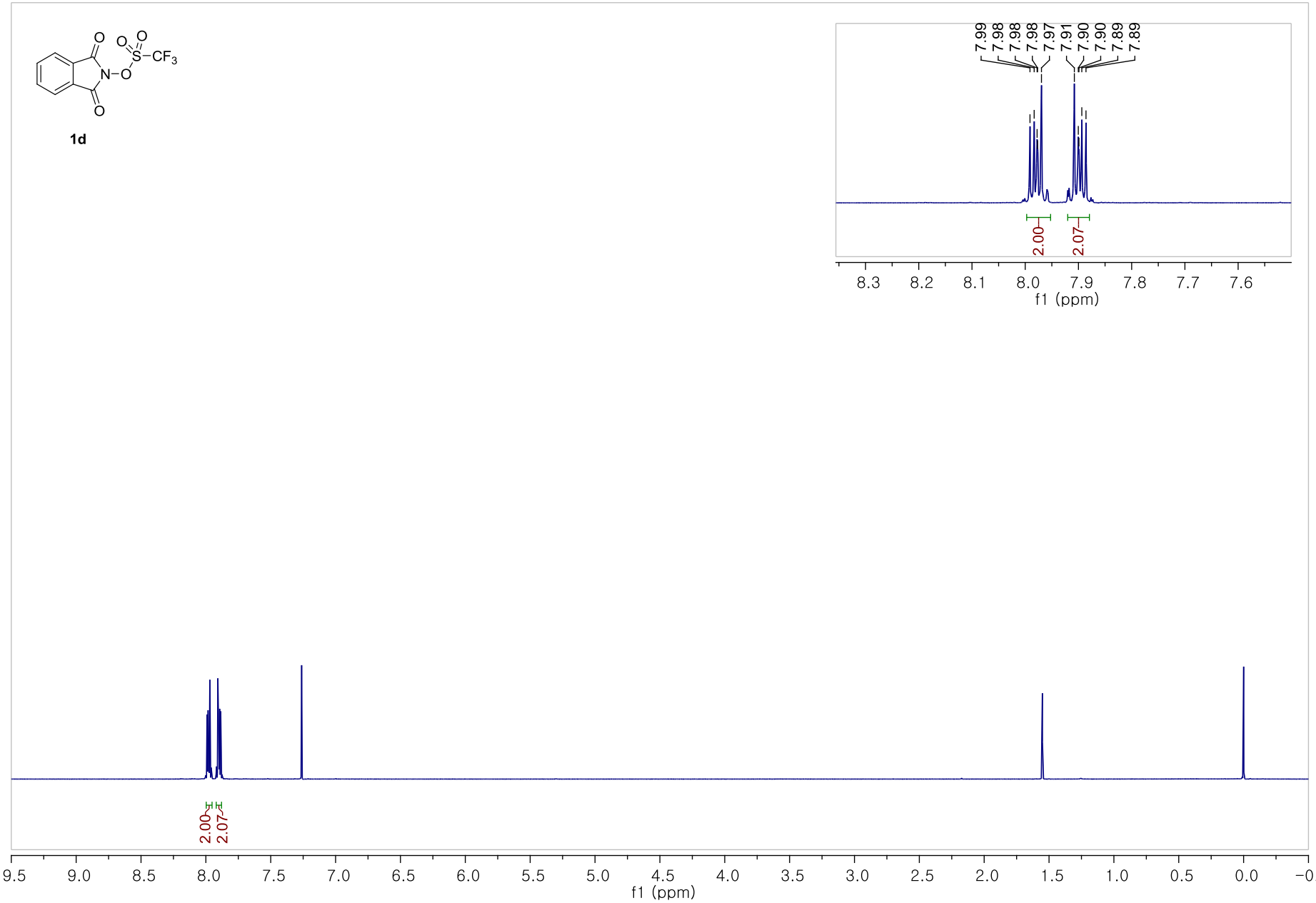
f1 (ppm)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7.98
7.98
7.97
7.91
7.90
7.90
7.89
7.89
2.00
2.07
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
f1 (ppm)
2.00
2.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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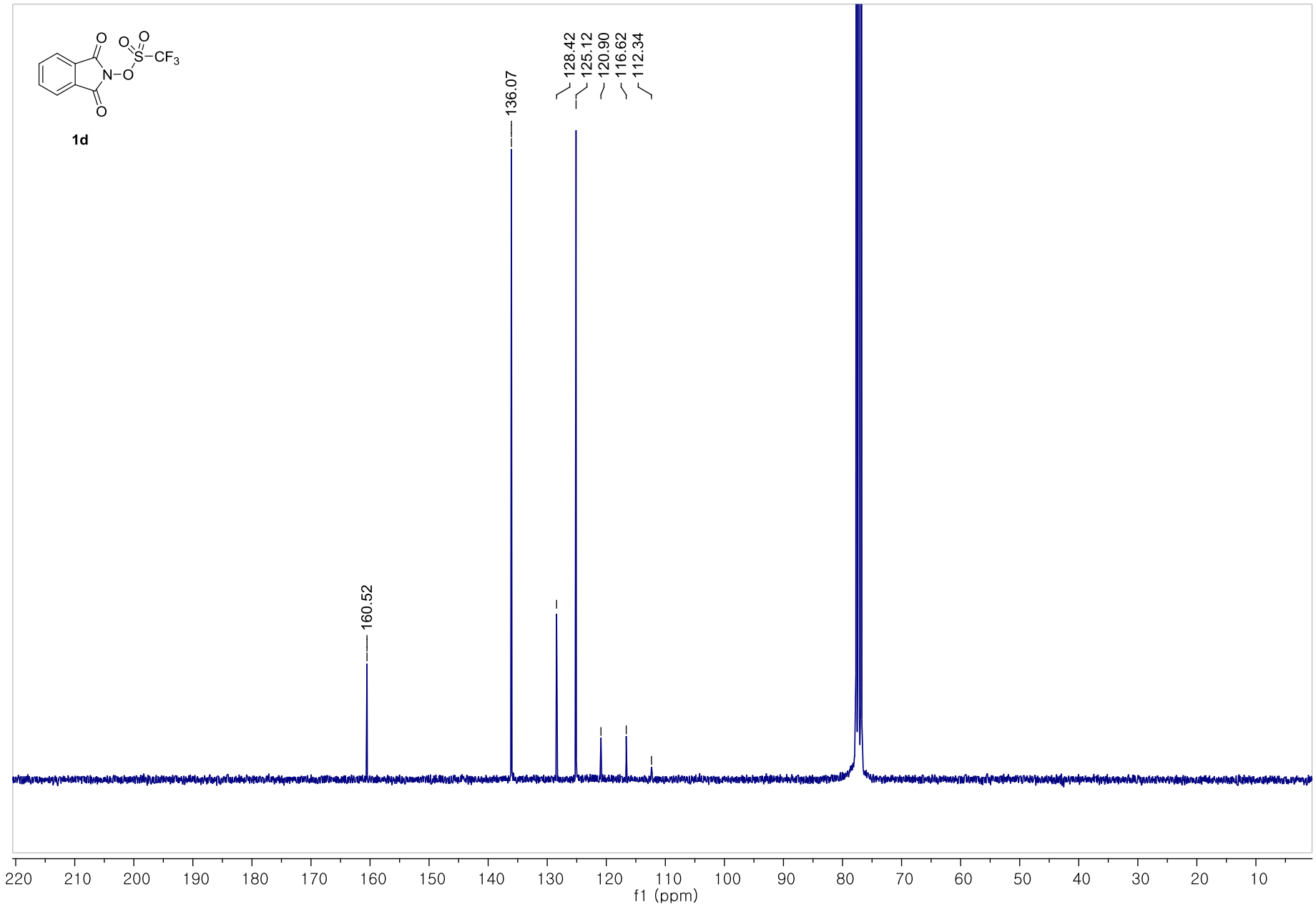
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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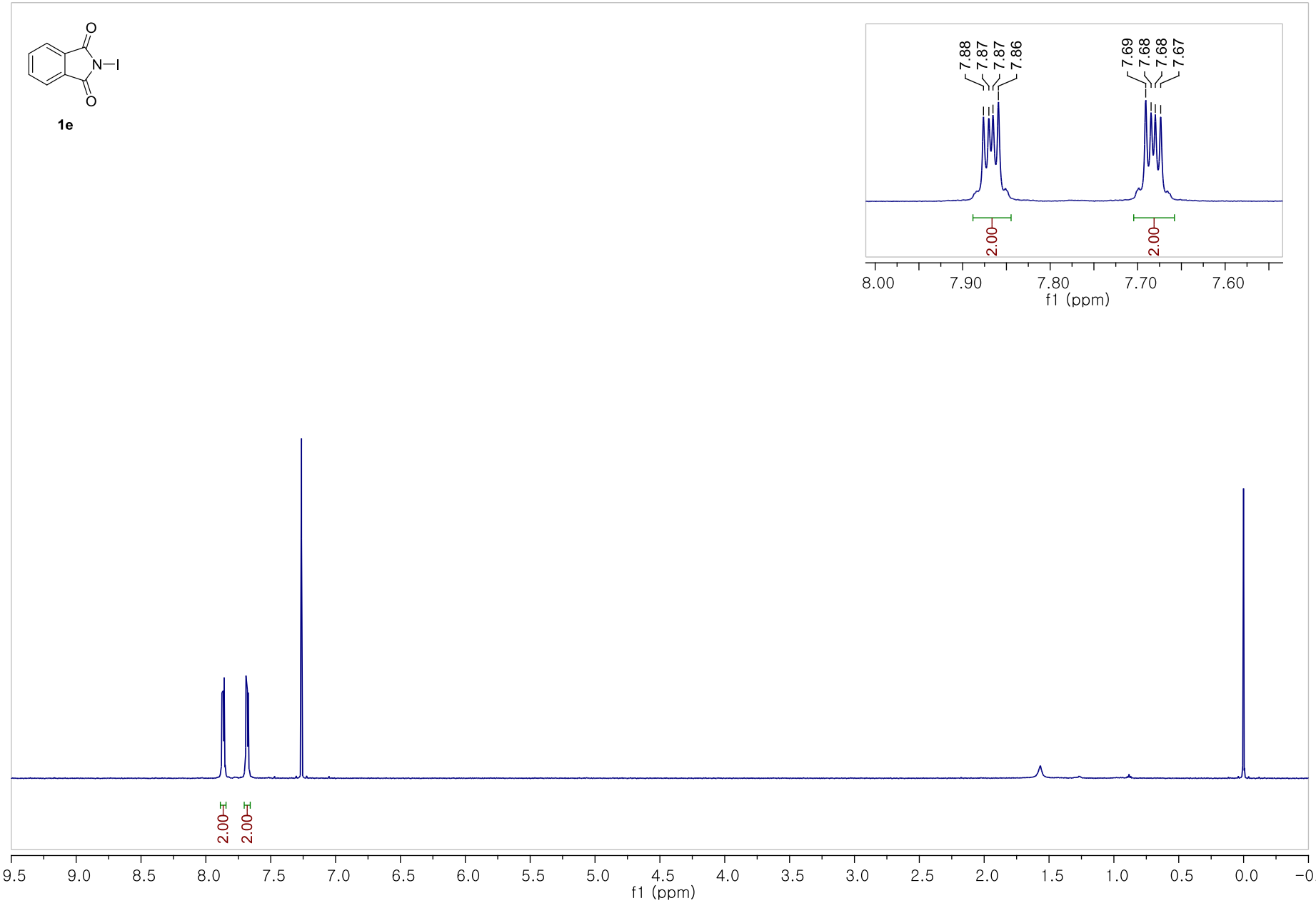
125.12
120.90
116.62
112.34
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


1e
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7.87
7.86
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7.68
7.68
7.67
2.00
2.00
8.00
7.90
7.80
7.70
7.60
f1 (ppm)
2.00
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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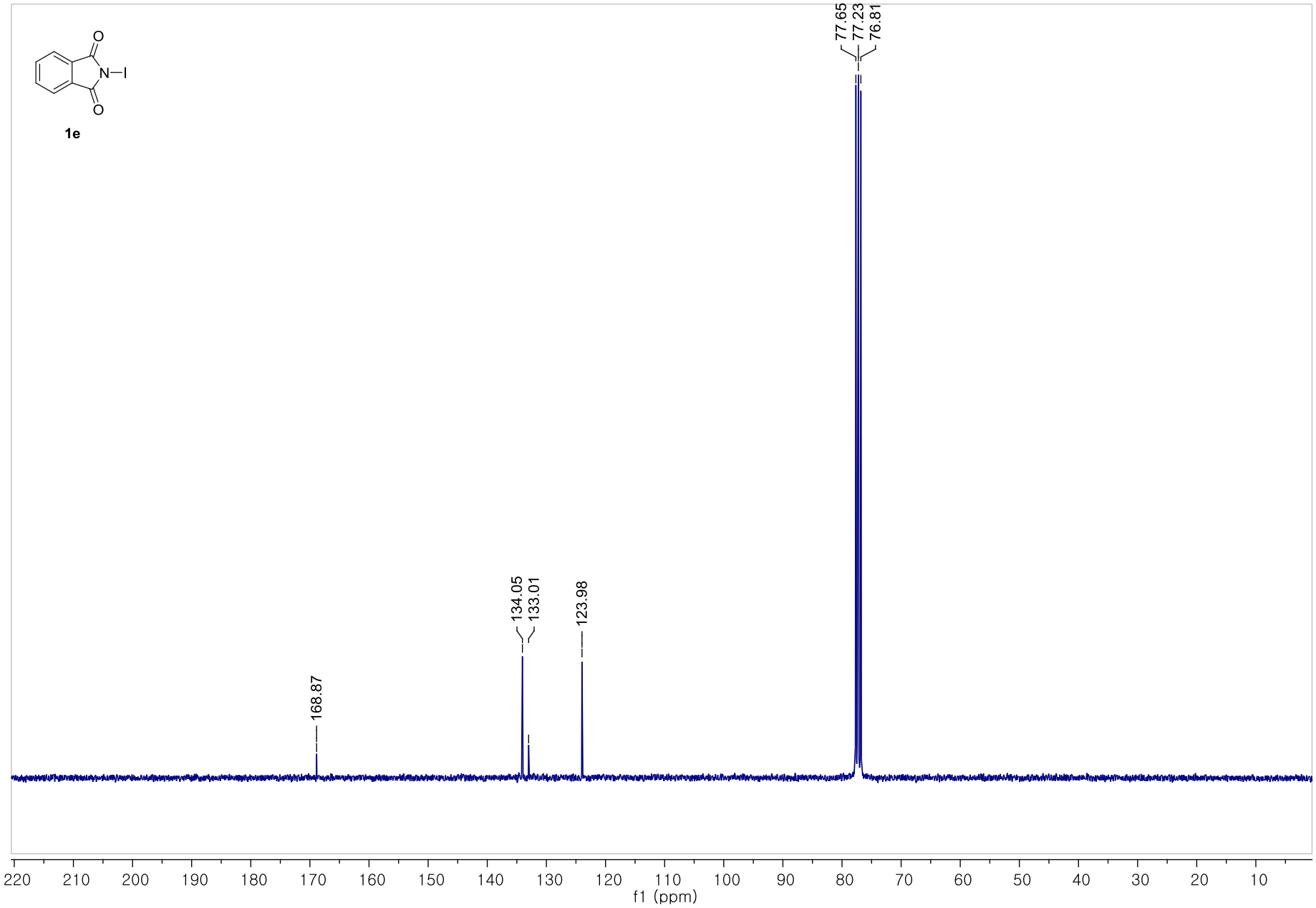
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.01
123.98
168.87
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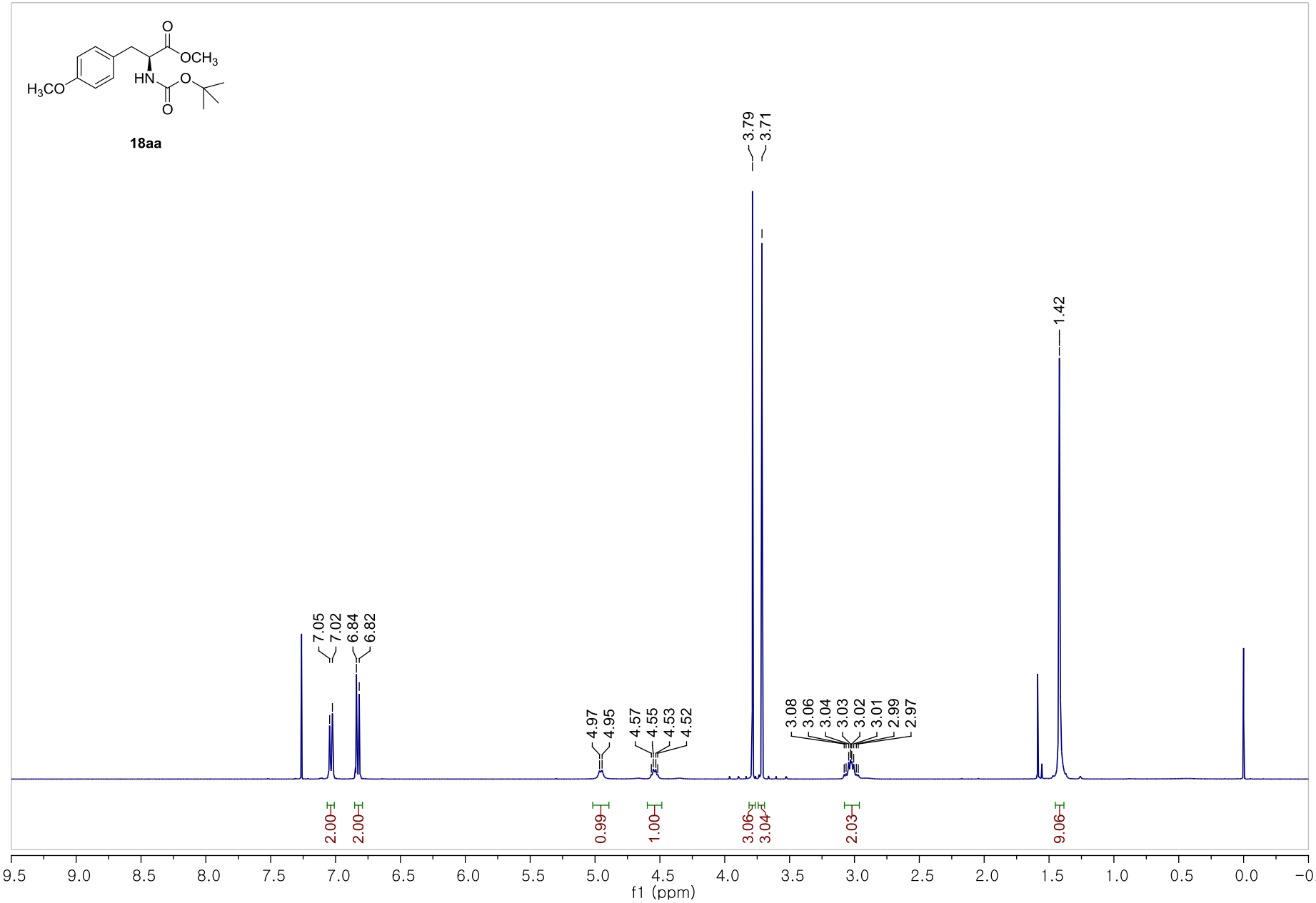
f1 (ppm)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4.97
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4.57
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4.53
4.52
3.79
3.71
3.08
3.06
3.04
3.03
3.02
3.01
2.99
2.97
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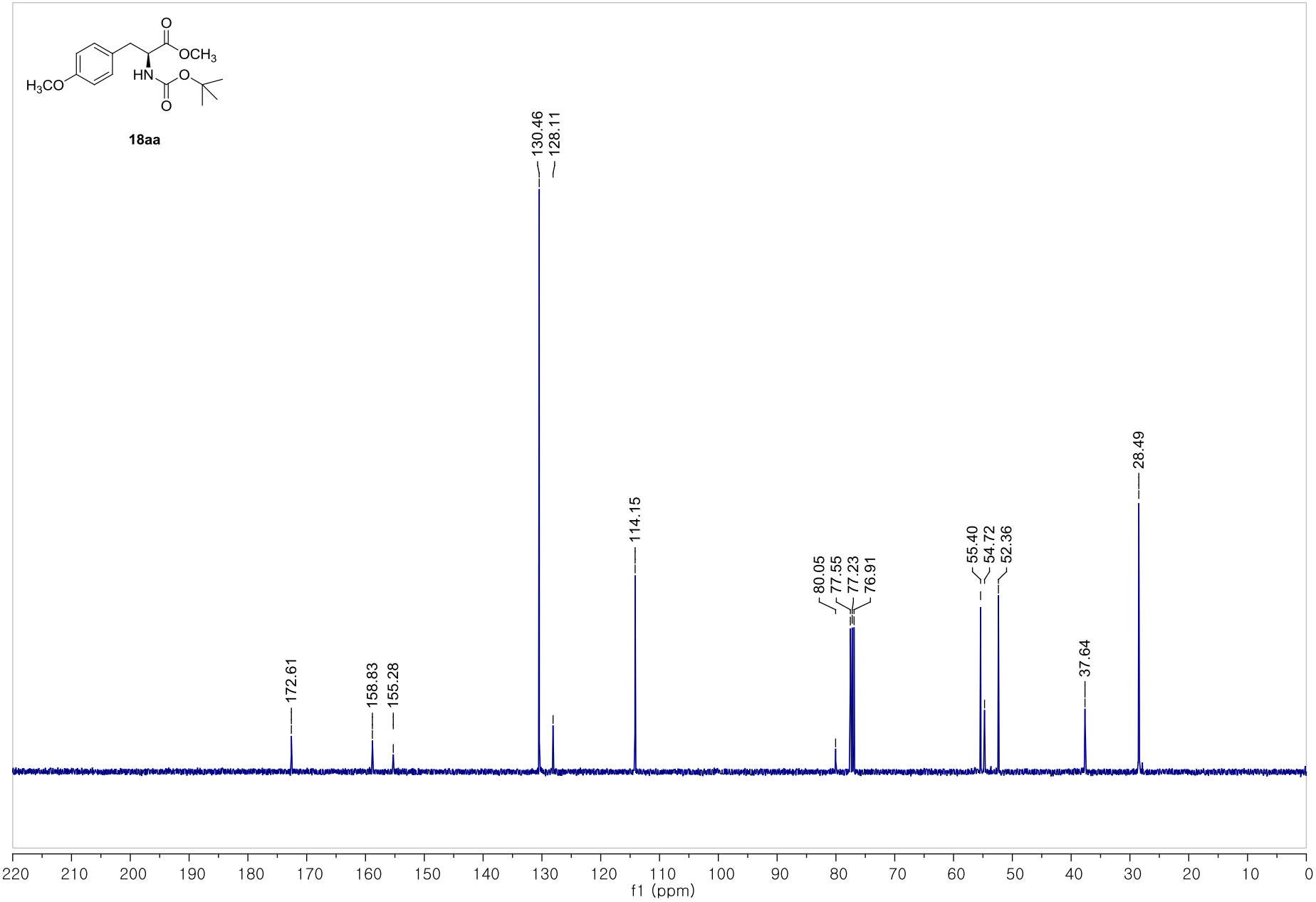
2.00
2.00
0.99
1.00
3.06
3.04
2.03
9.06
f1 (ppm)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37.64
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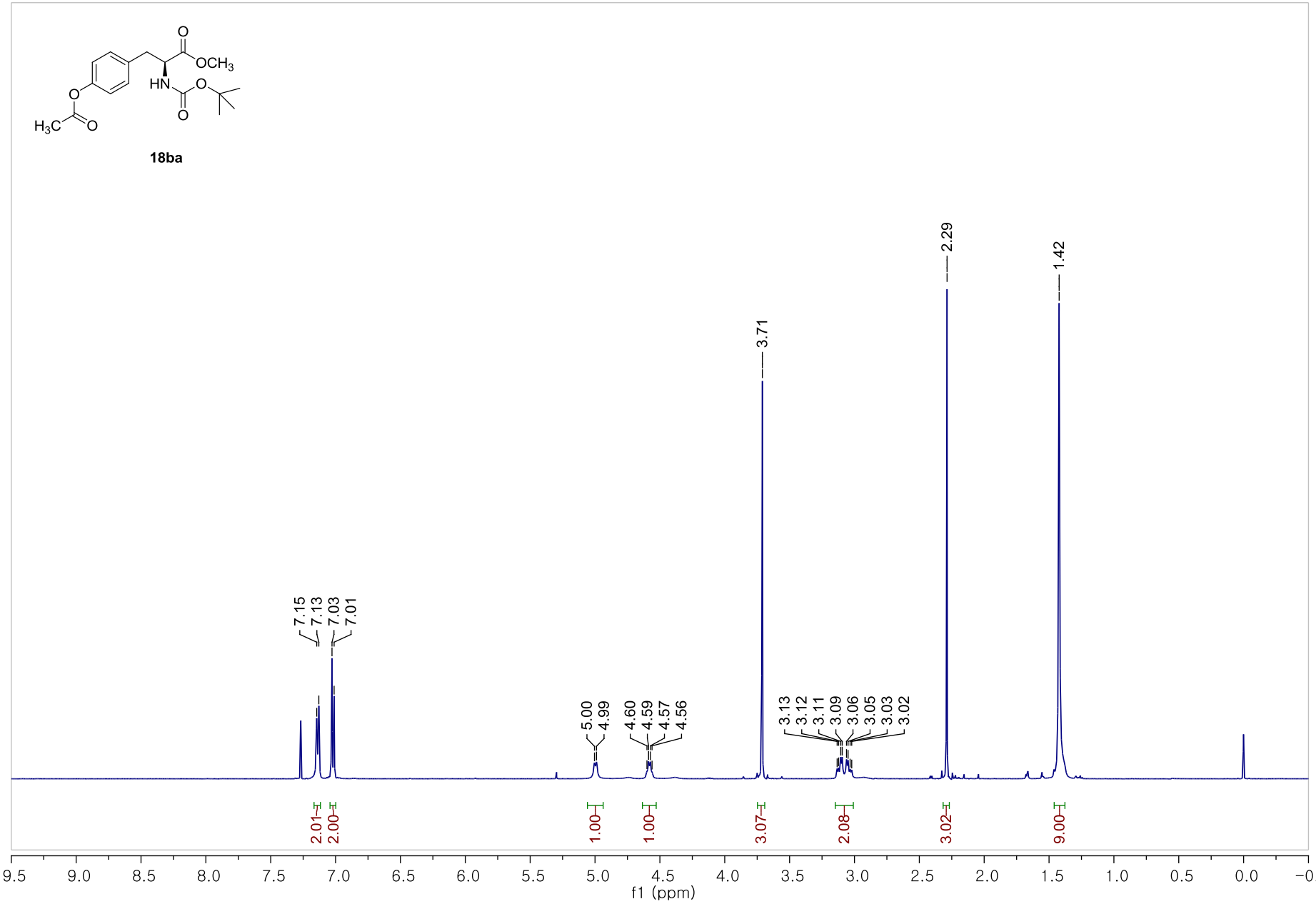
172.61
158.83
155.28
f1 (ppm)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3.13
3.12
3.11
3.09
3.06
3.05
3.03
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1.00
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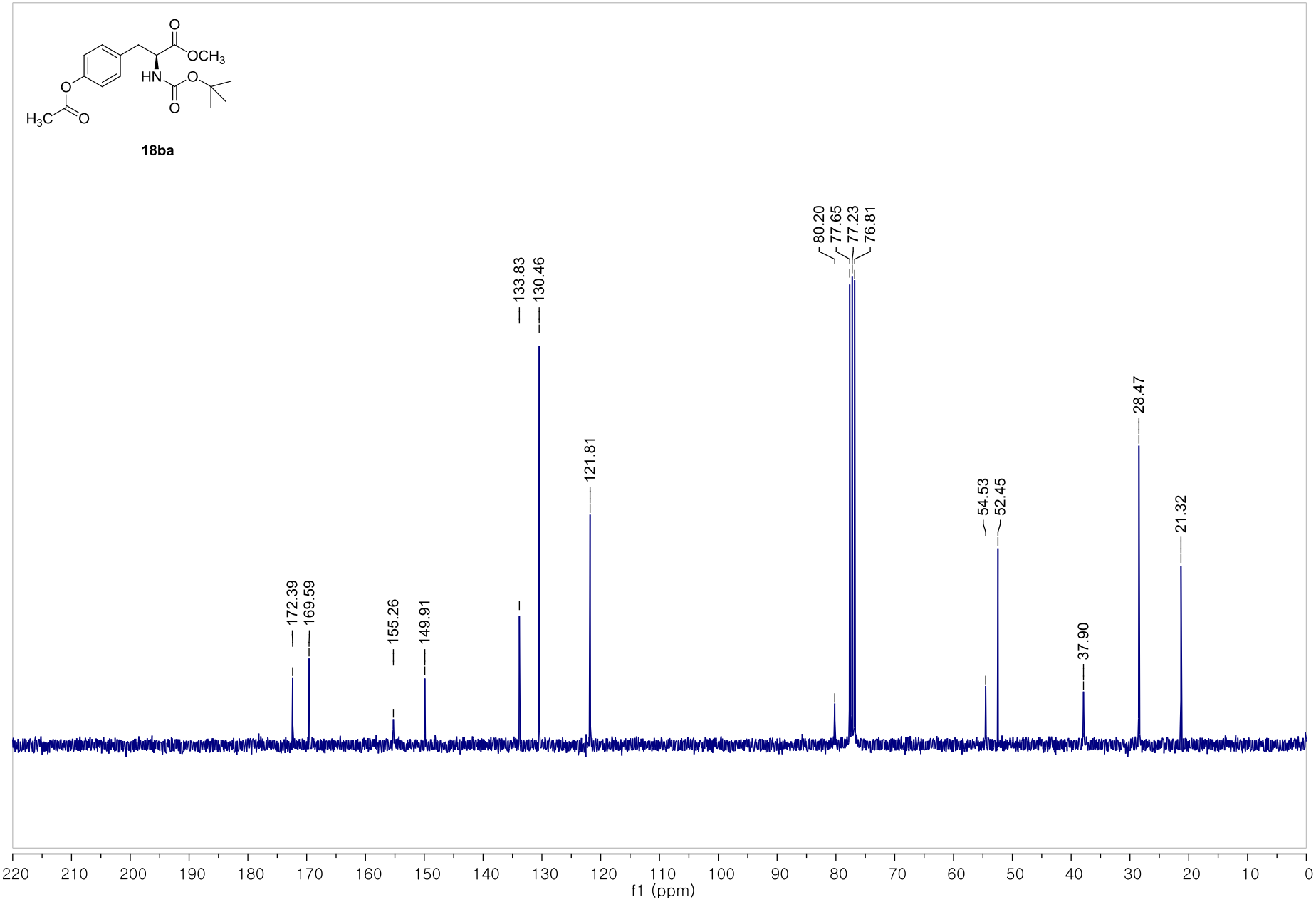
2.08
3.02
9.00
f1 (ppm)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133.83
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77.65
77.23
76.81
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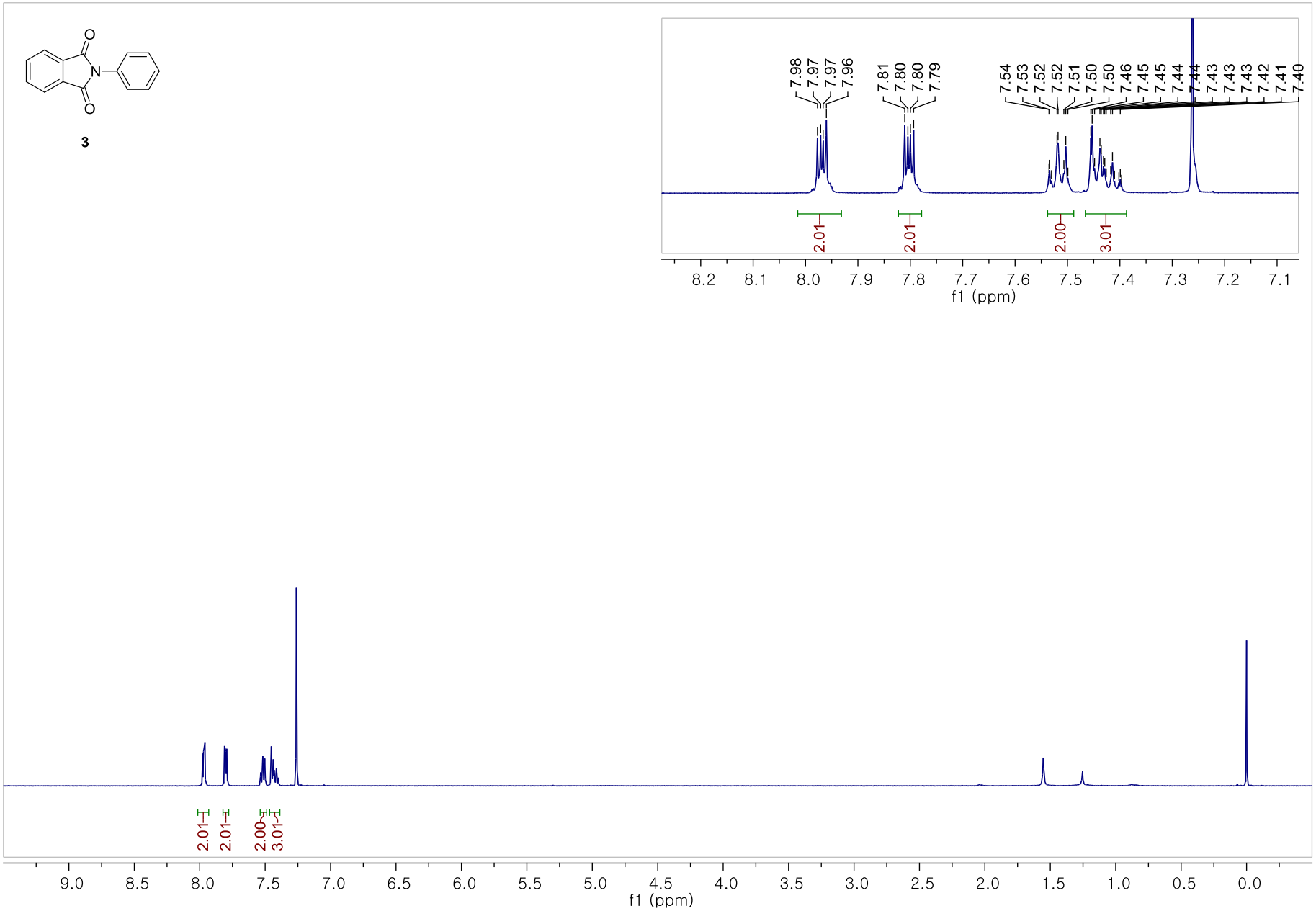
52.45
37.90
28.47
21.32
f1 (ppm)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N
O
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7.96
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7.52
7.52
7.51
7.50
7.50
7.46
7.45
7.45
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7.43
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7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
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2.01
2.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
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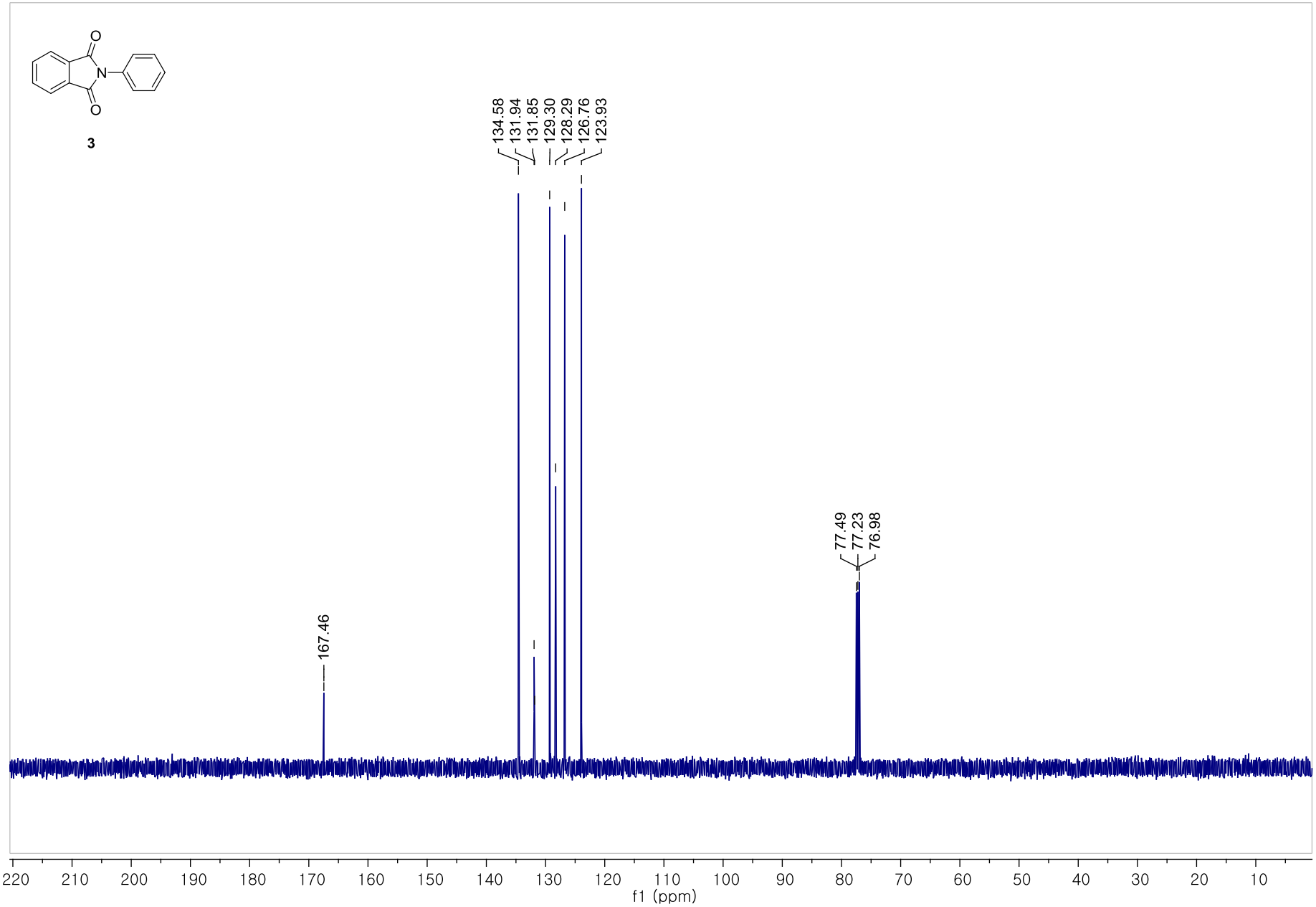
1.0
0.5
0.0
f1 (ppm)


3
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131.85
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128.29
126.76
123.93
77.49
77.23
76.98
167.46
220
210
200
190
180
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140
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120
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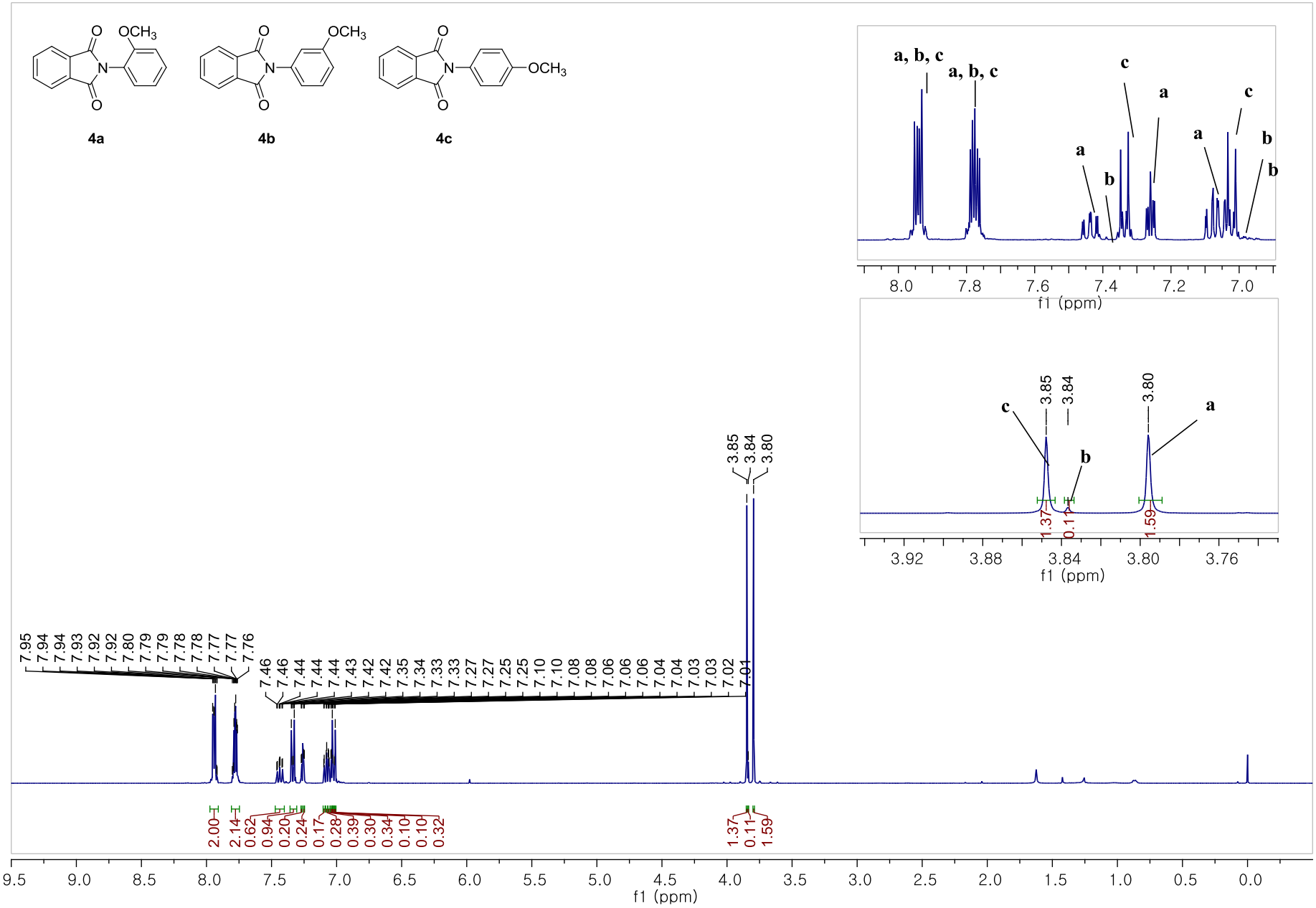
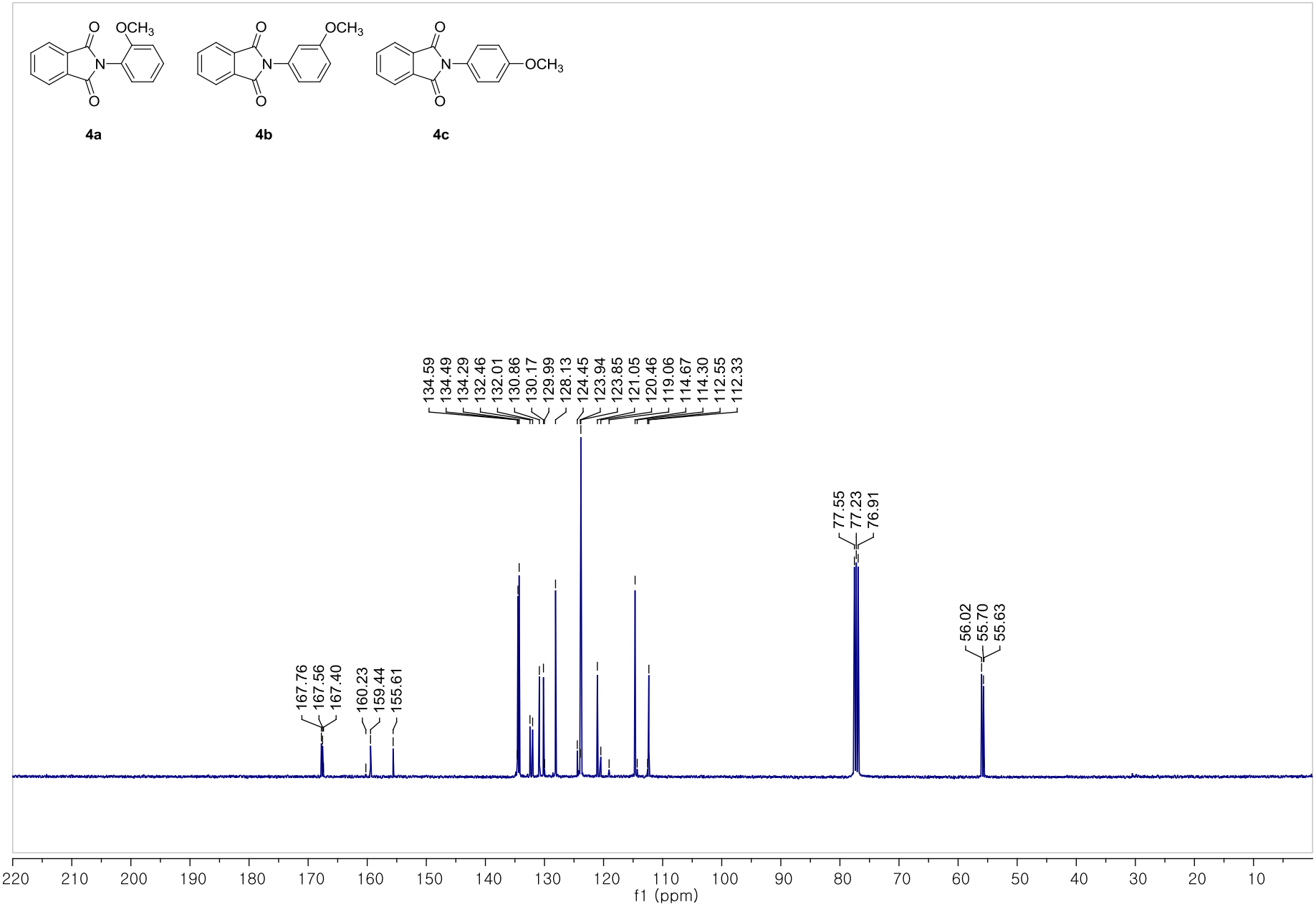
80
70
60
50
40
30
20
10
f1 (ppm)


4a
4b
4c
a, b, c
a, b, c
c
a
c
a
b
b
a
b
f1 (ppm)
c
3.85
3.84
b
3.80
a
1.37
0.11
1.59
f1 (ppm)
7.95 7.94 7.94 7.93 7.92 7.92 7.80 7.79 7.79 7.78 7.78 7.77 7.77 7.76
7.46 7.46 7.44 7.44 7.44 7.43 7.42 7.42 7.35 7.34 7.33 7.33 7.27 7.27 7.25 7.10 7.10 7.08 7.08 7.06 7.06 7.06 7.04 7.04 7.03 7.03 7.02 7.01
3.85 3.84 3.80
2.00 2.14 0.62 0.94 0.20 0.24 0.17 0.28 0.39 0.30 0.34 0.10 0.10 0.32
1.37 0.11 1.59
f1 (ppm)


4a
4b
4c
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134.29
132.46
132.01
130.86
130.17
129.99
128.13
124.45
123.94
123.85
121.05
120.46
119.06
114.67
114.30
112.55
112.33
77.55
77.23
76.91
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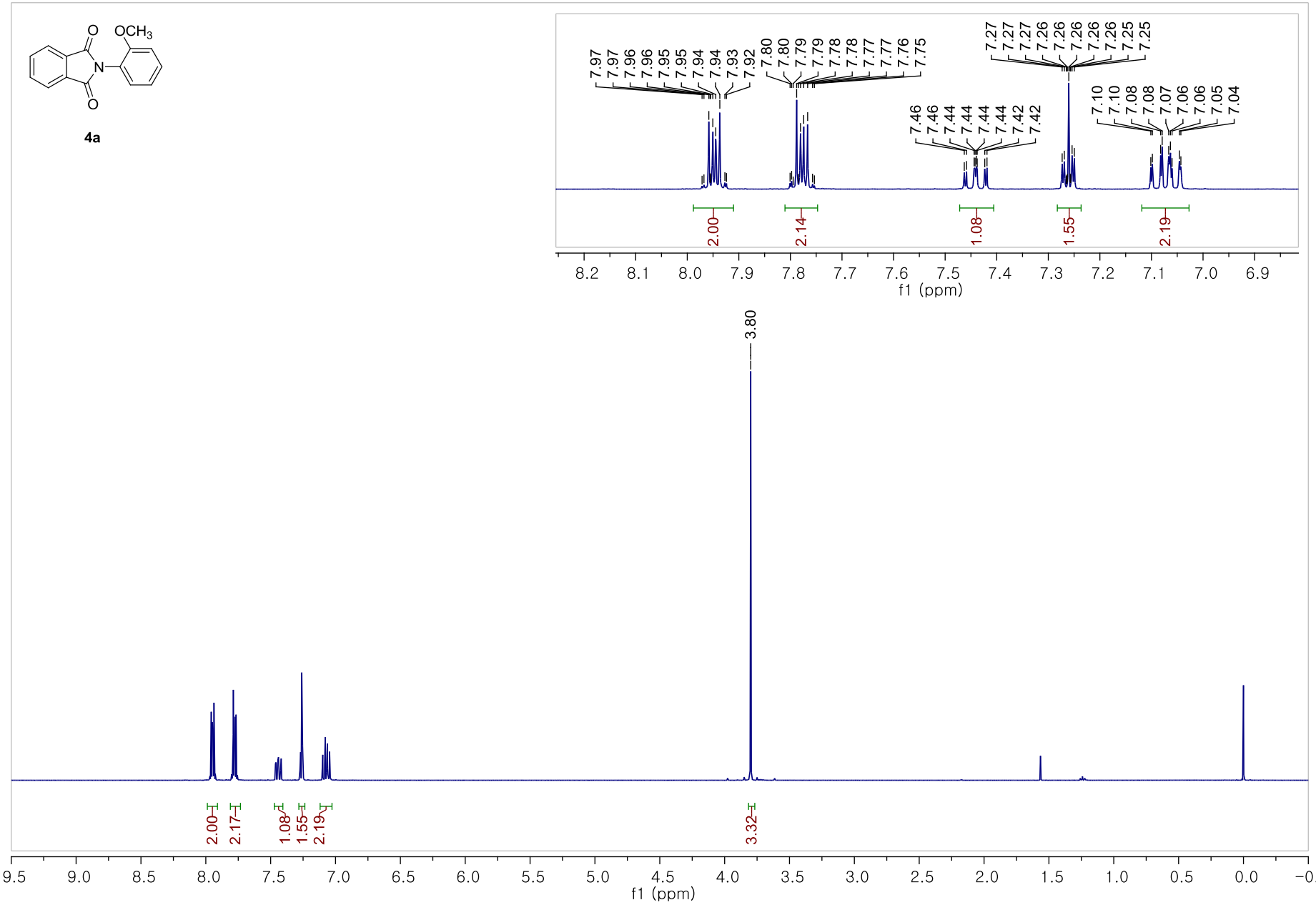
55.70
55.63
167.76
167.56
167.40
160.23
159.44
155.61
f1 (ppm)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OCH3
N
O
4a
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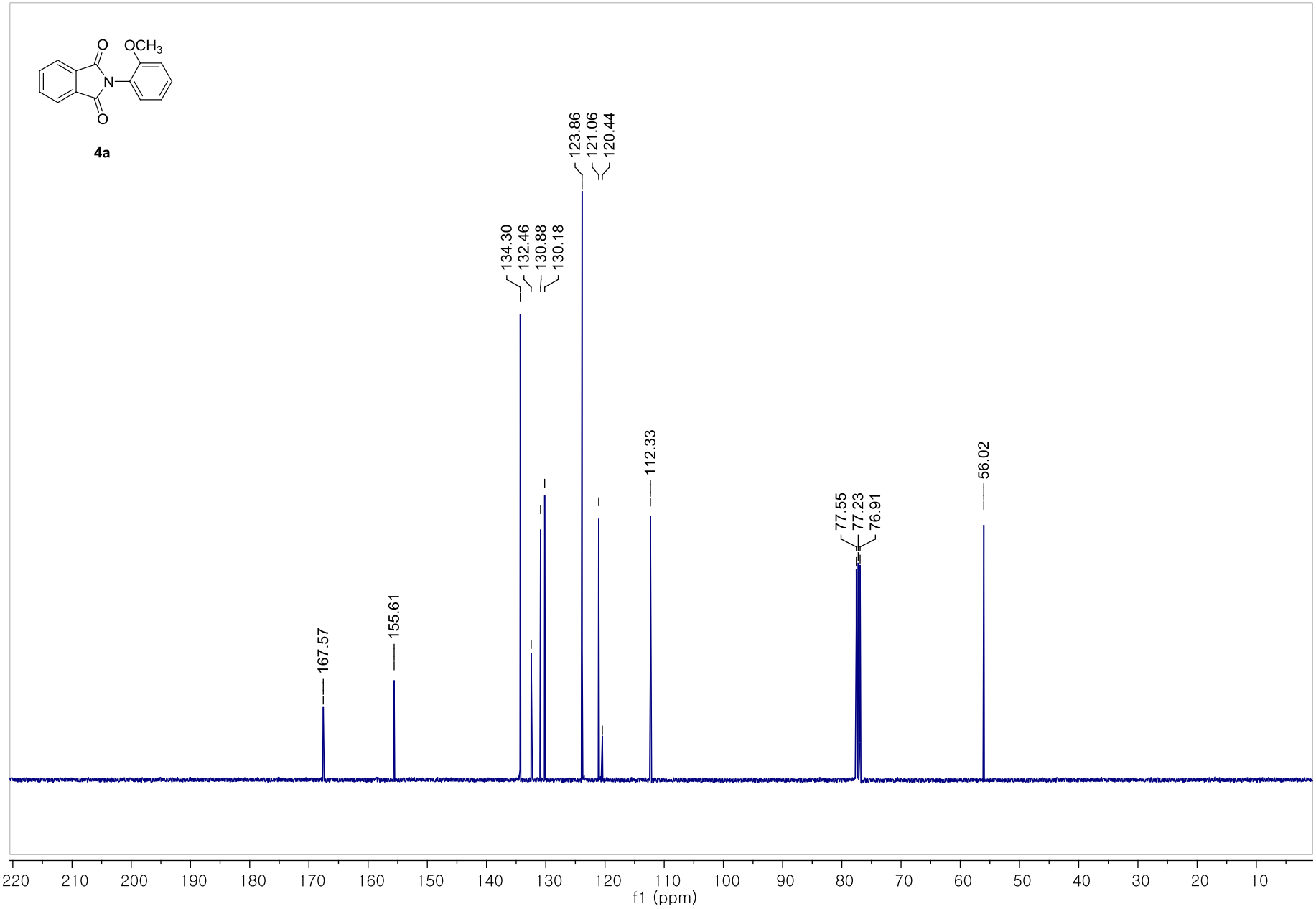
7.80 7.80 7.79 7.79 7.78 7.78 7.77 7.77 7.76 7.75
7.46 7.46 7.44 7.44 7.44 7.44 7.42 7.42
7.27 7.27 7.27 7.26 7.26 7.26 7.26 7.25 7.25
7.10 7.10 7.08 7.08 7.07 7.06 7.06 7.05 7.04
2.00 2.14 1.08 1.55 2.19
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
3.80
2.00 2.17 1.08 1.55 2.19 3.32
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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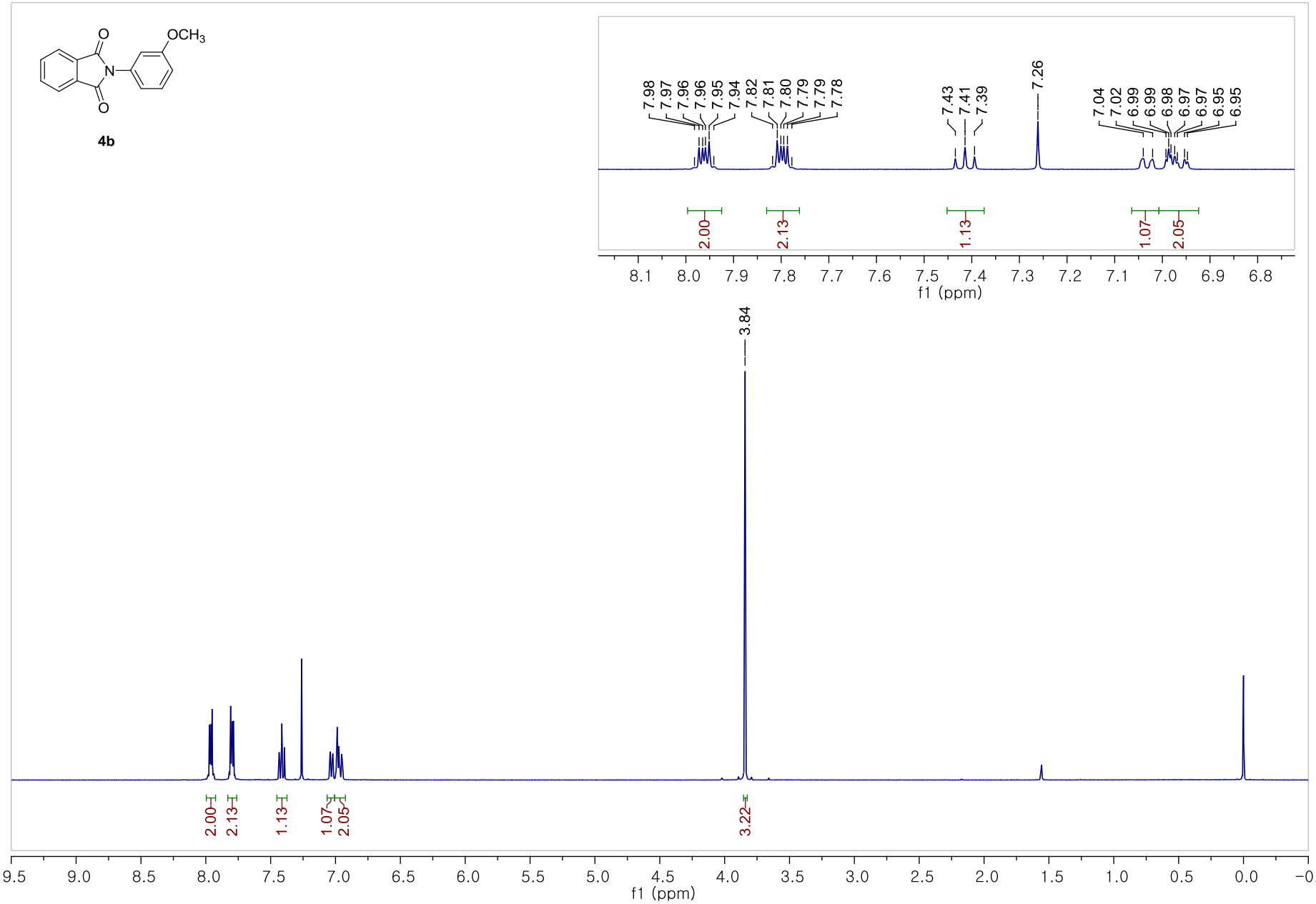
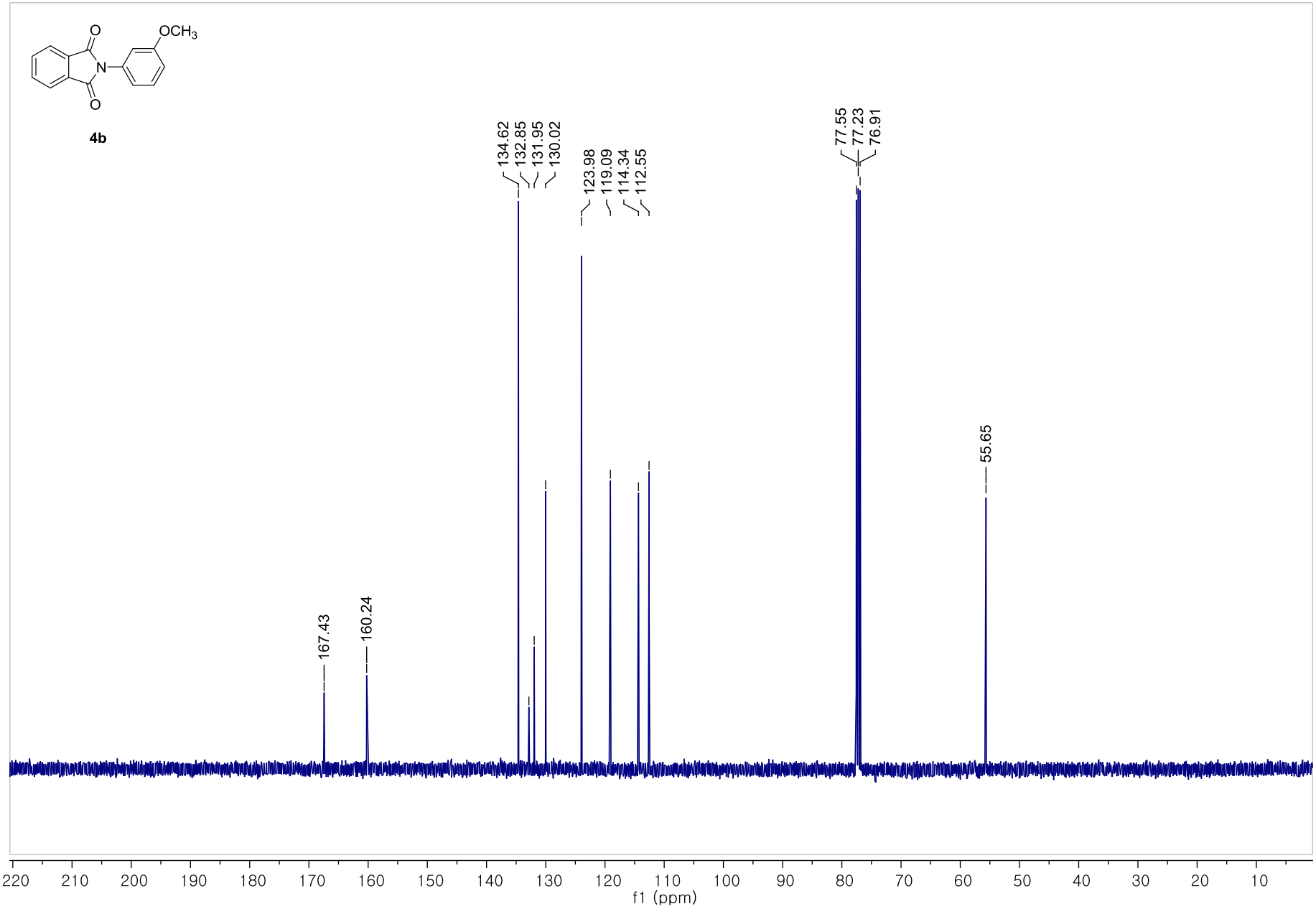
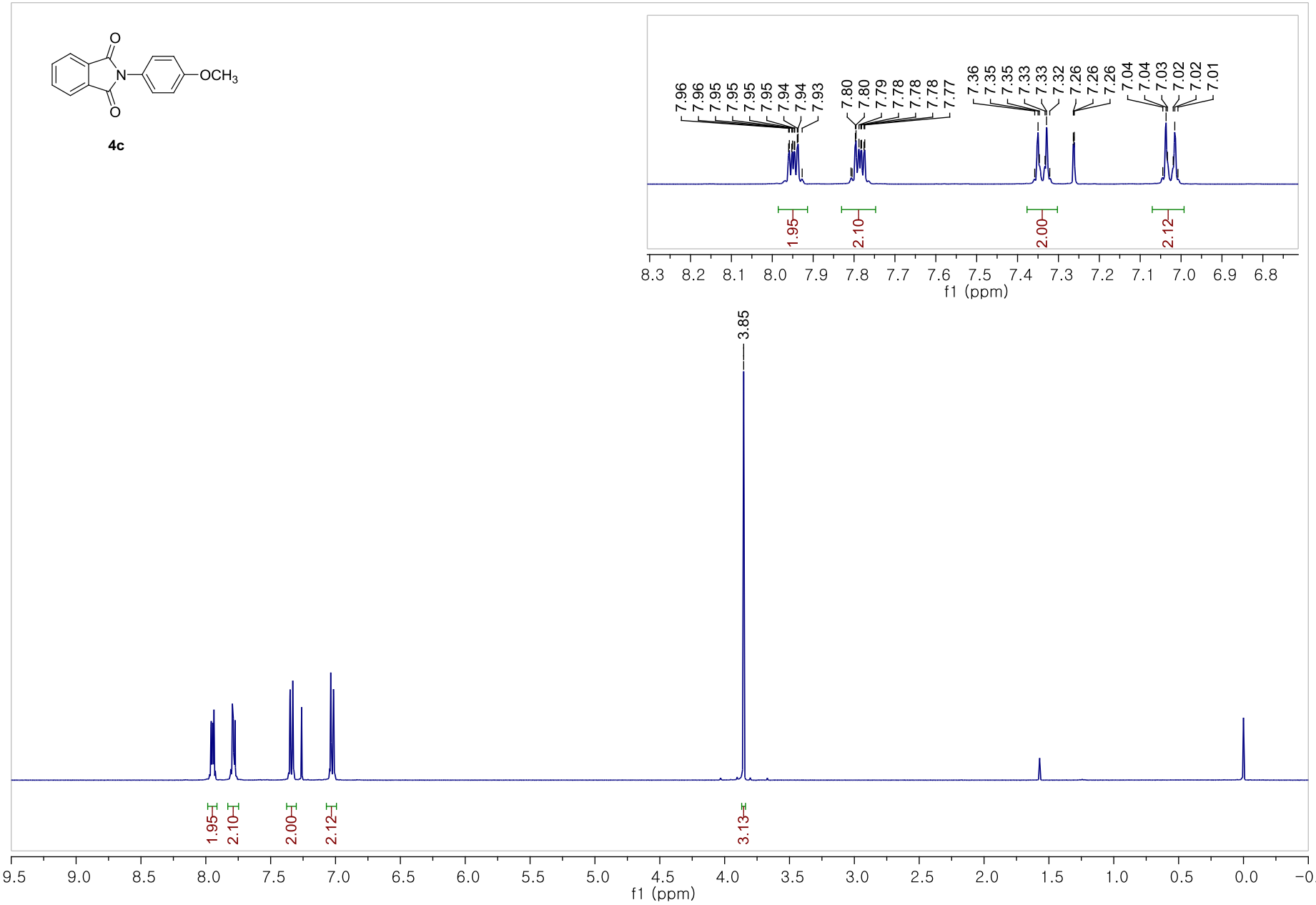
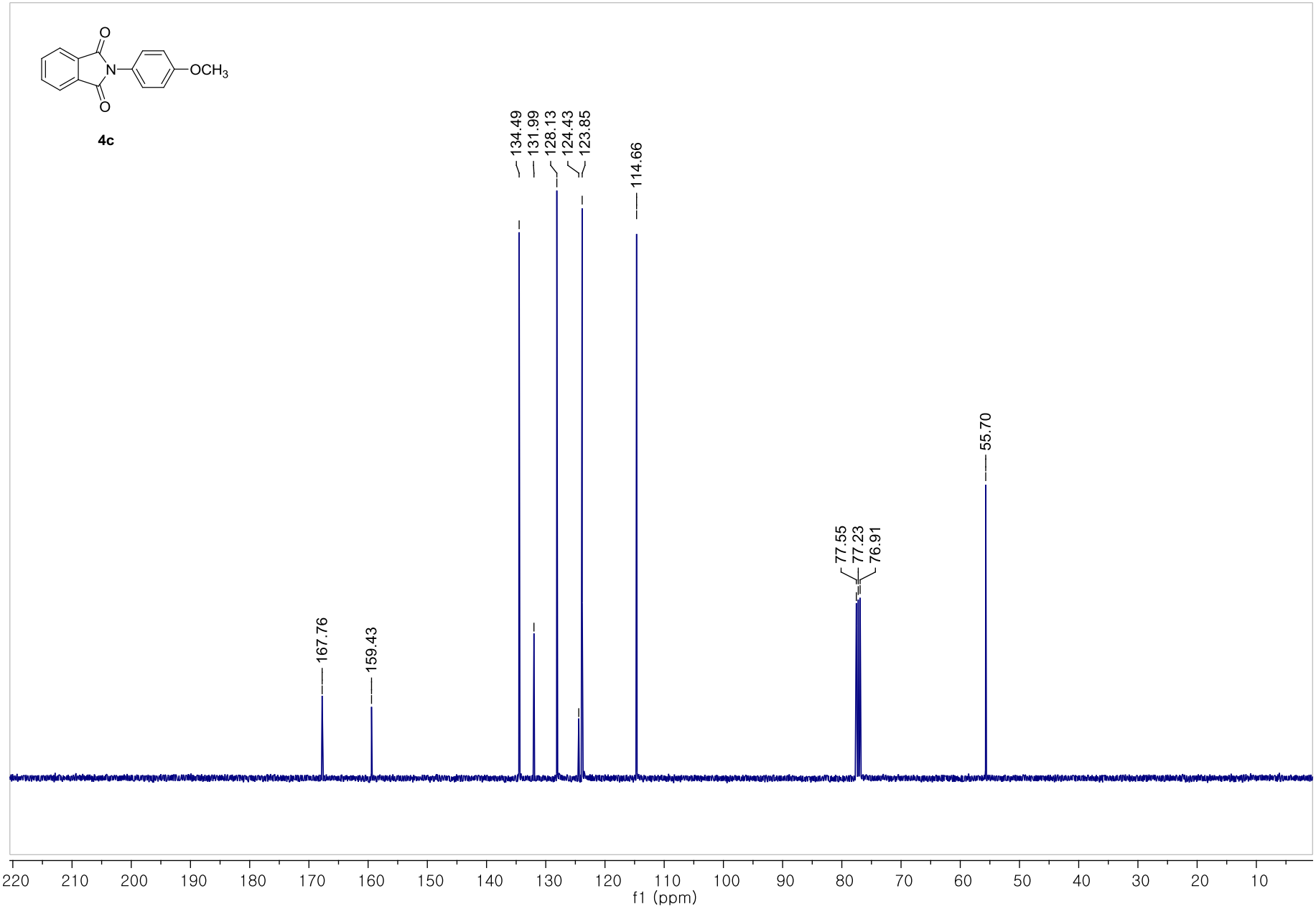
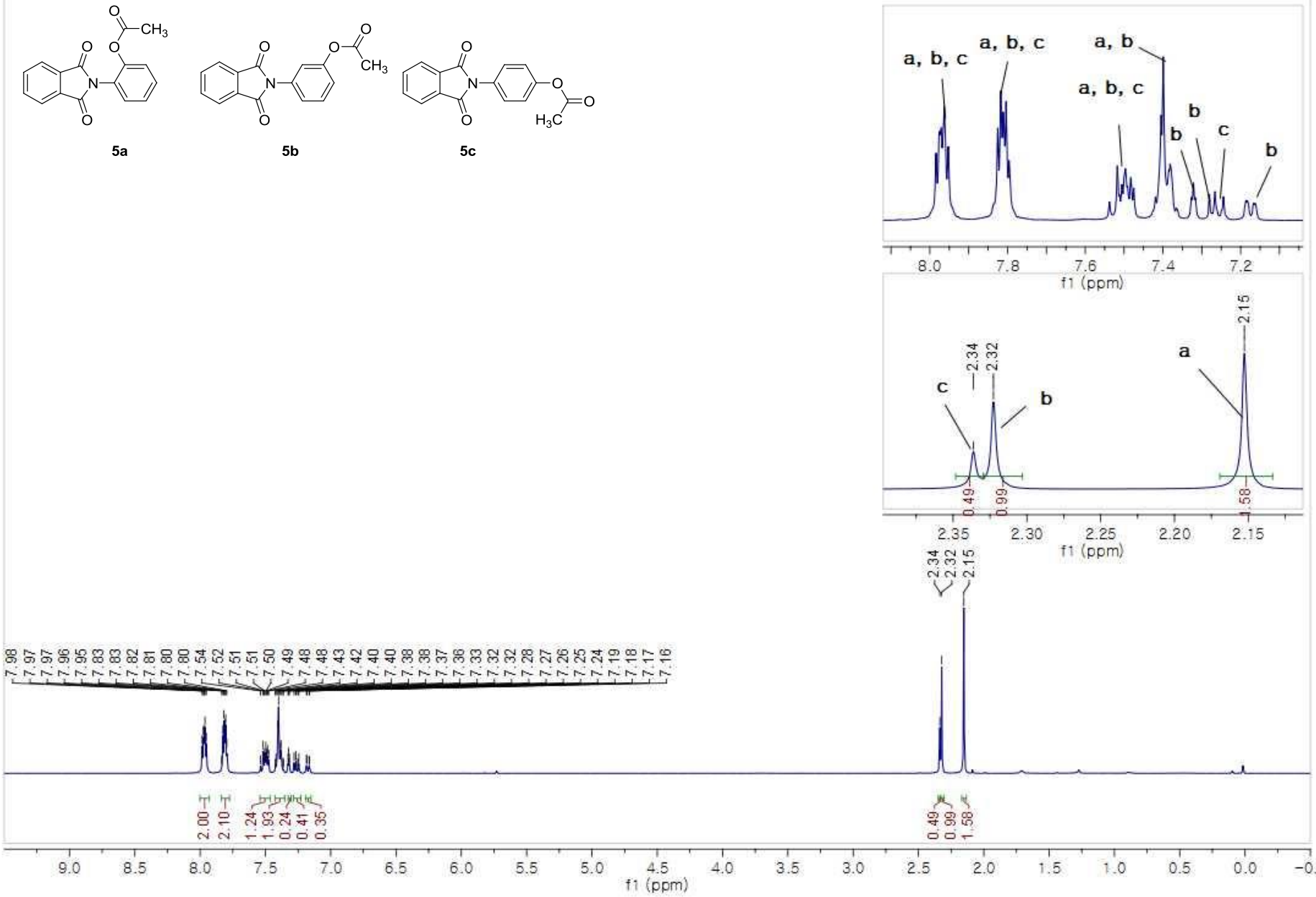
132.46
130.88
130.18
123.86
121.06
120.44
112.33
77.55
77.23
76.91
56.02
f1 (ppm)

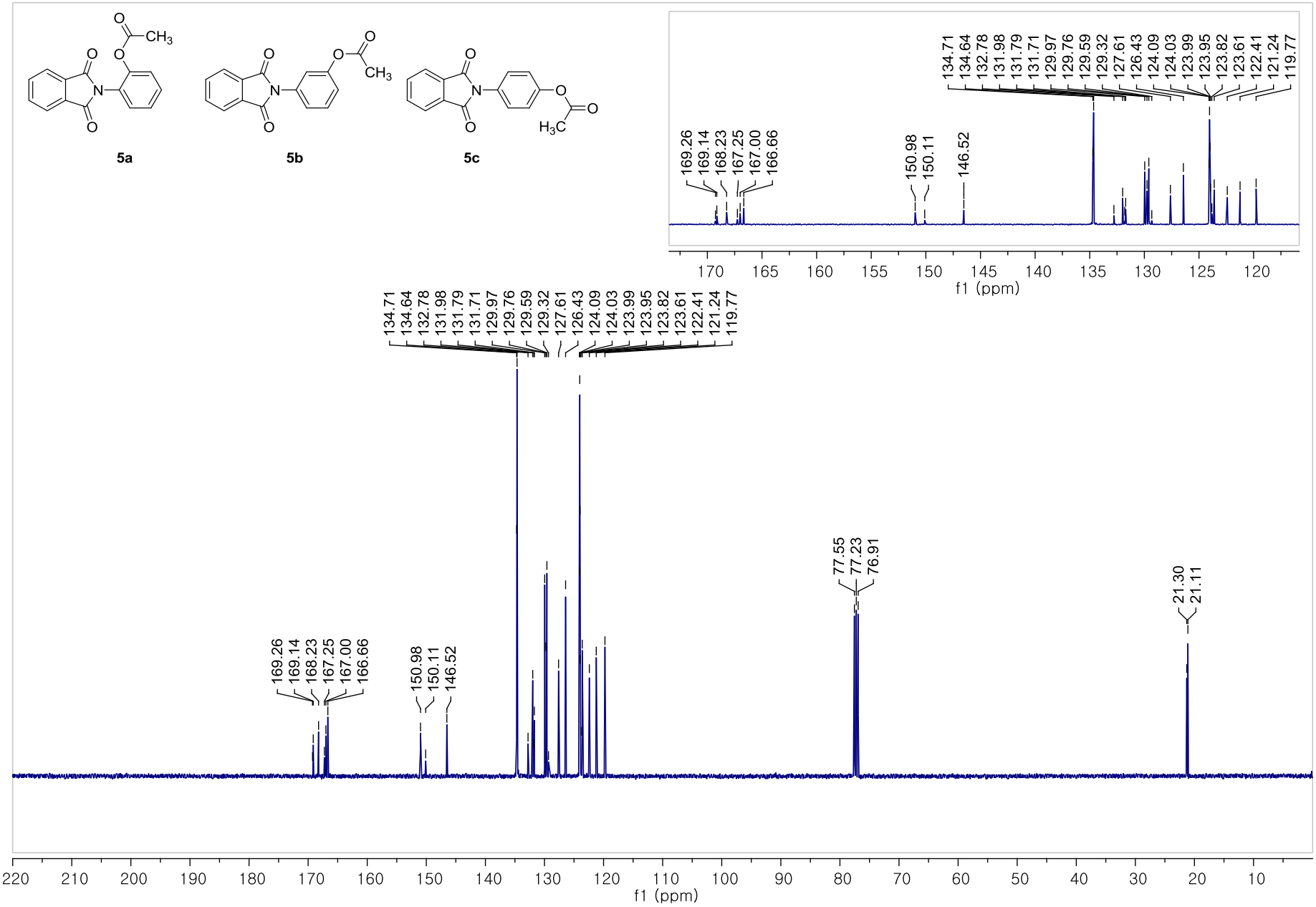

4b
7.98
7.97
7.96
7.96
7.95
7.94
7.82
7.81
7.80
7.79
7.79
7.78
7.43
7.41
7.39
7.26
7.04
7.02
6.99
6.99
6.98
6.97
6.95
6.95
2.00
2.13
1.13
1.07
2.05
f1 (ppm)
3.84
2.00
2.13
1.13
1.07
2.05
3.22
f1 (ppm)

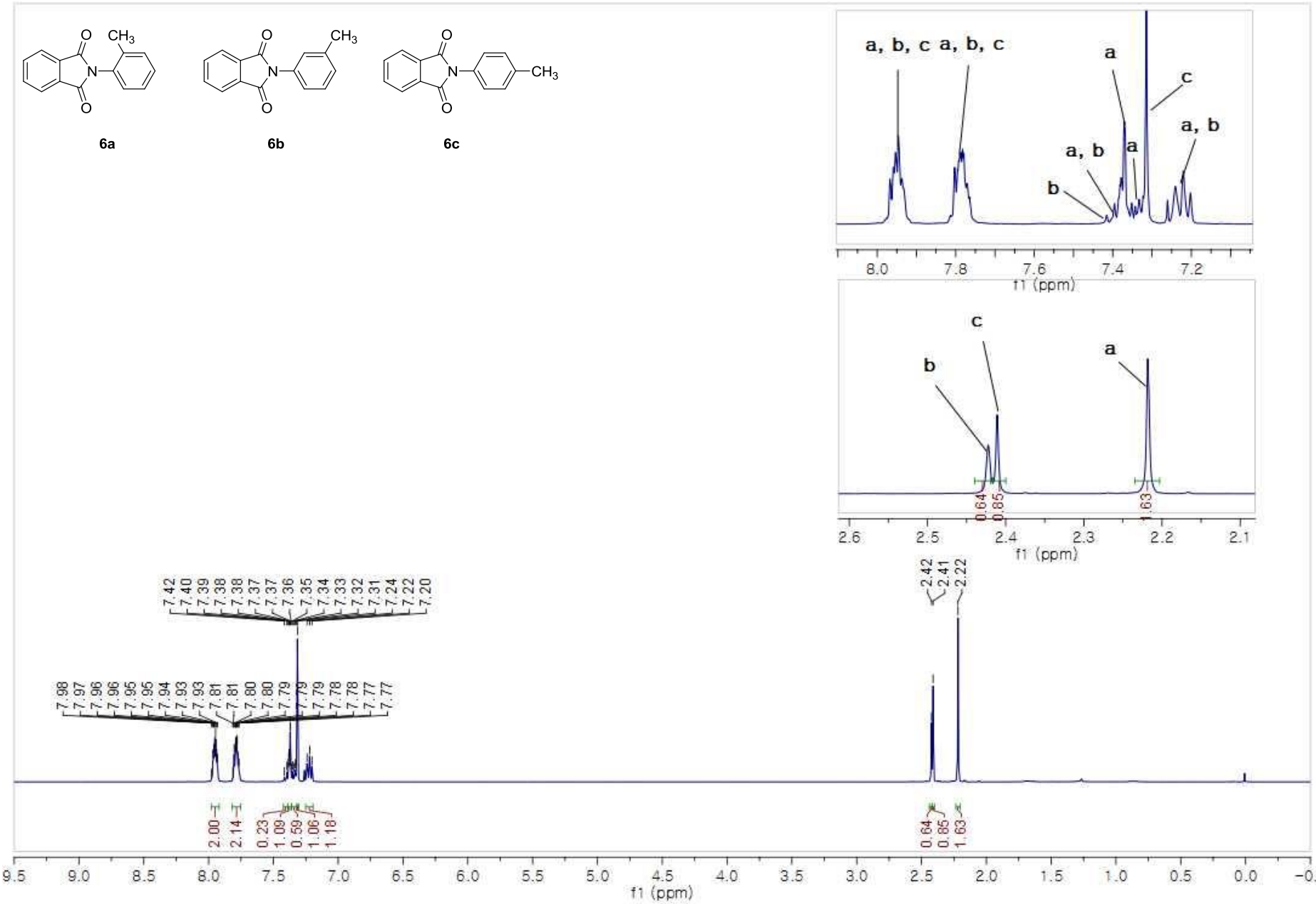

O
OCH3
N
O
4b
134.62
132.85
131.95
130.02
123.98
119.09
114.34
112.55
77.55
77.23
76.91
55.65
167.43
160.24
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

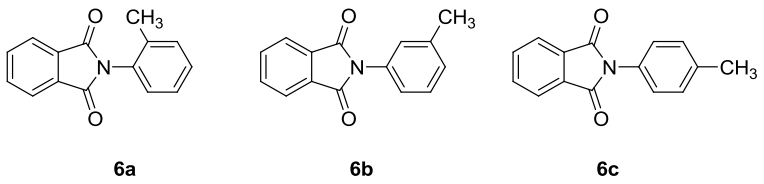

4c
7.96
7.96
7.95
7.95
7.95
7.95
7.94
7.94
7.93
7.80
7.80
7.79
7.78
7.78
7.78
7.77
7.36
7.35
7.35
7.33
7.33
7.32
7.26
7.26
7.26
7.04
7.04
7.03
7.02
7.02
7.01
1.95
2.10
2.00
2.12
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
3.85
1.95
2.10
2.00
2.12
3.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


O
N
OCH3
O
4c
134.49
131.99
128.13
124.43
123.85
114.66
77.55
77.23
76.91
55.70
167.76
159.43
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

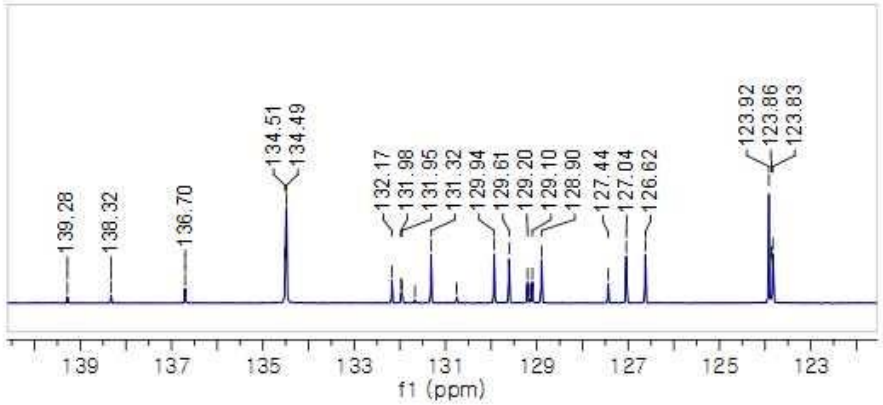

5a
5b
5c
a, b, c
a, b, c
a, b
a, b, c
b
b
c
b
f1 (ppm)
c
2.34
2.32
b
a
2.15
0.49
0.99
1.58
f1 (ppm)
2.34
2.32
2.15
7.98
7.97
7.97
7.96
7.95
7.83
7.82
7.81
7.80
7.80
7.54
7.52
7.51
7.51
7.50
7.49
7.48
7.48
7.43
7.42
7.40
7.40
7.38
7.38
7.37
7.36
7.33
7.32
7.32
7.28
7.27
7.26
7.25
7.24
7.19
7.18
7.17
7.16
2.00
2.10
1.24
1.93
0.24
0.41
0.35
0.49
0.99
1.58
f1 (ppm)

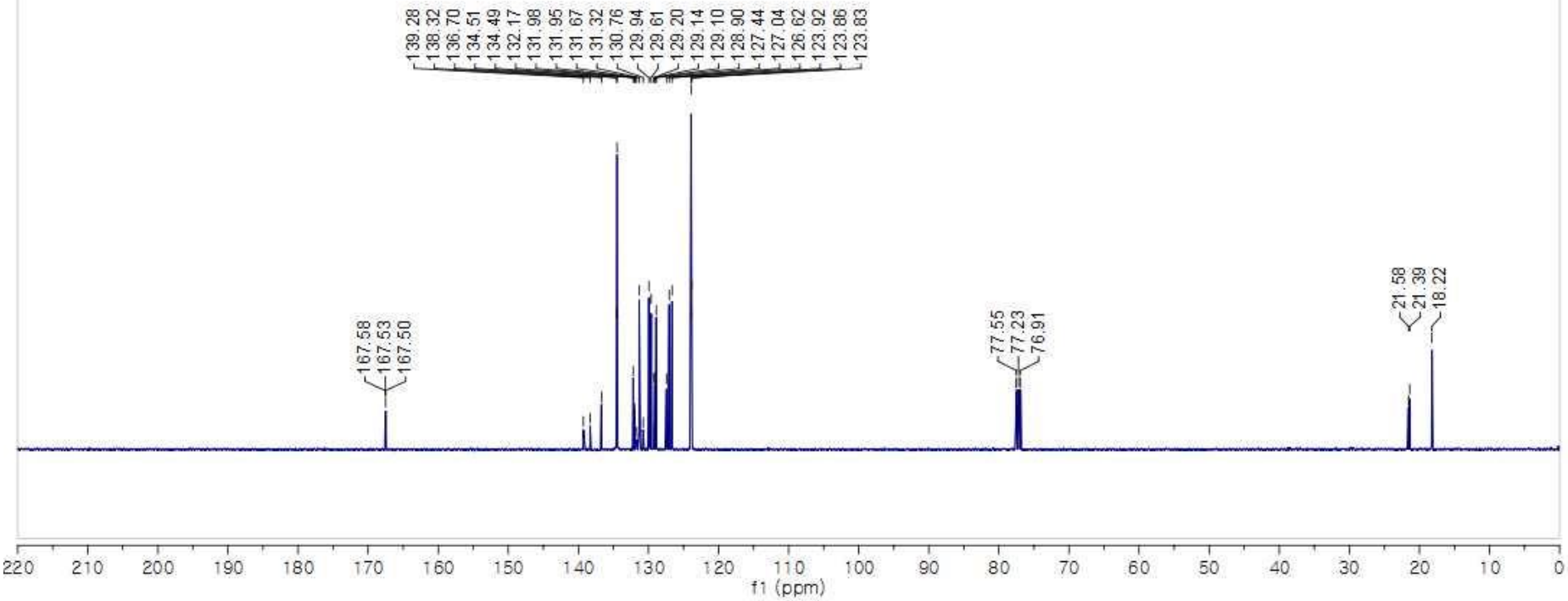

5a
5b
5c
169.26
169.14
168.23
167.25
167.00
166.66
150.98
150.11
146.52
134.71
134.64
132.78
131.98
131.79
131.71
129.97
129.76
129.59
129.32
127.61
126.43
124.09
124.03
123.99
123.95
123.82
123.61
122.41
121.24
119.77
77.55
77.23
76.91
21.30
21.11
f1 (ppm)

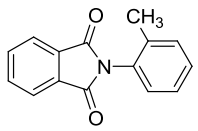

6a
6b
6c
a, b, c a, b, c
a
c
a, b
a, b
a
b
f1 (ppm)
c
b
a
0.64
0.85
1.63
f1 (ppm)
2.42
2.41
2.22
7.42
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.24
7.22
7.20
7.98
7.97
7.96
7.96
7.95
7.95
7.94
7.93
7.93
7.81
7.81
7.80
7.80
7.79
7.79
7.79
7.78
7.78
7.77
7.77
2.00
2.14
0.23
1.09
0.59
1.06
1.18
0.64
0.85
1.63
f1 (ppm)


O
CH3
N
O
O
CH3
N
O
O
CH3
N
O

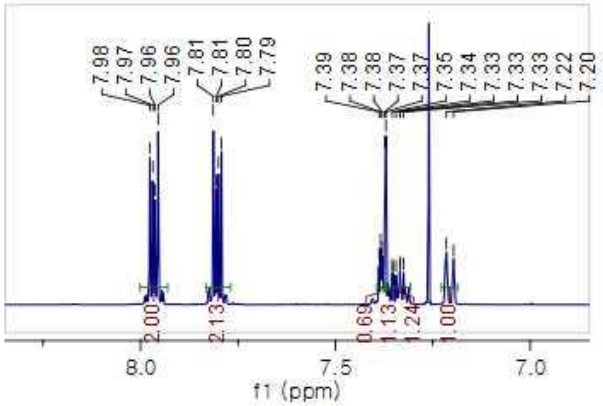
6a **6b** **6c**

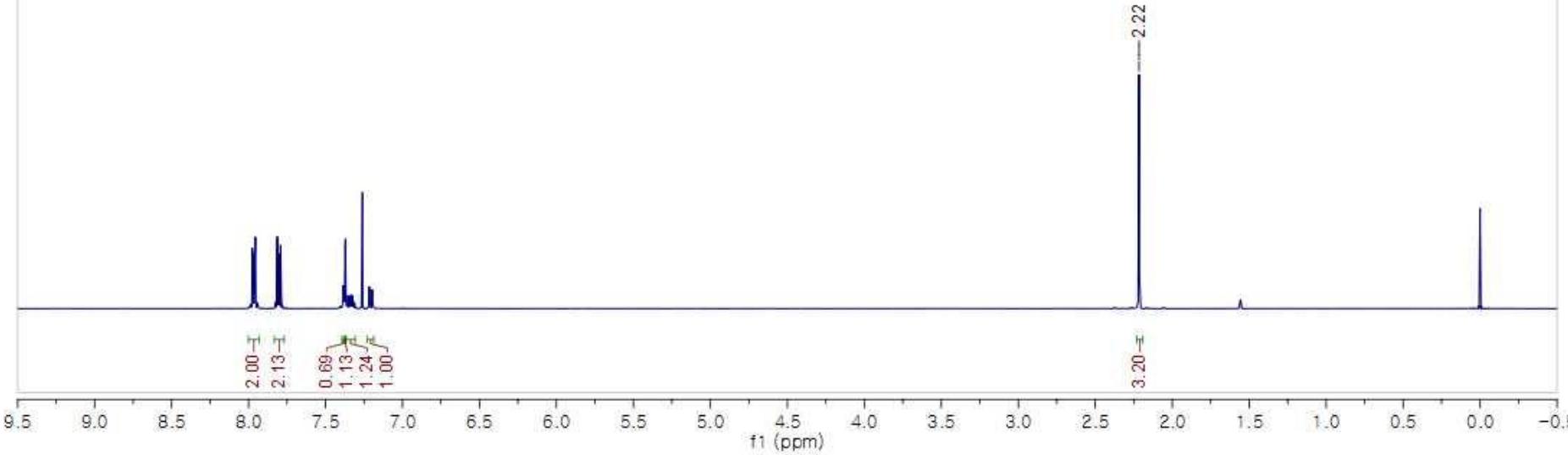

139.28
138.32
136.70
134.51
134.49
132.17
131.98
131.95
131.32
129.94
129.61
129.20
129.10
128.90
127.44
127.04
126.62
123.92
123.86
123.83
139
137
135
133
131
129
127
125
123
f1 (ppm)

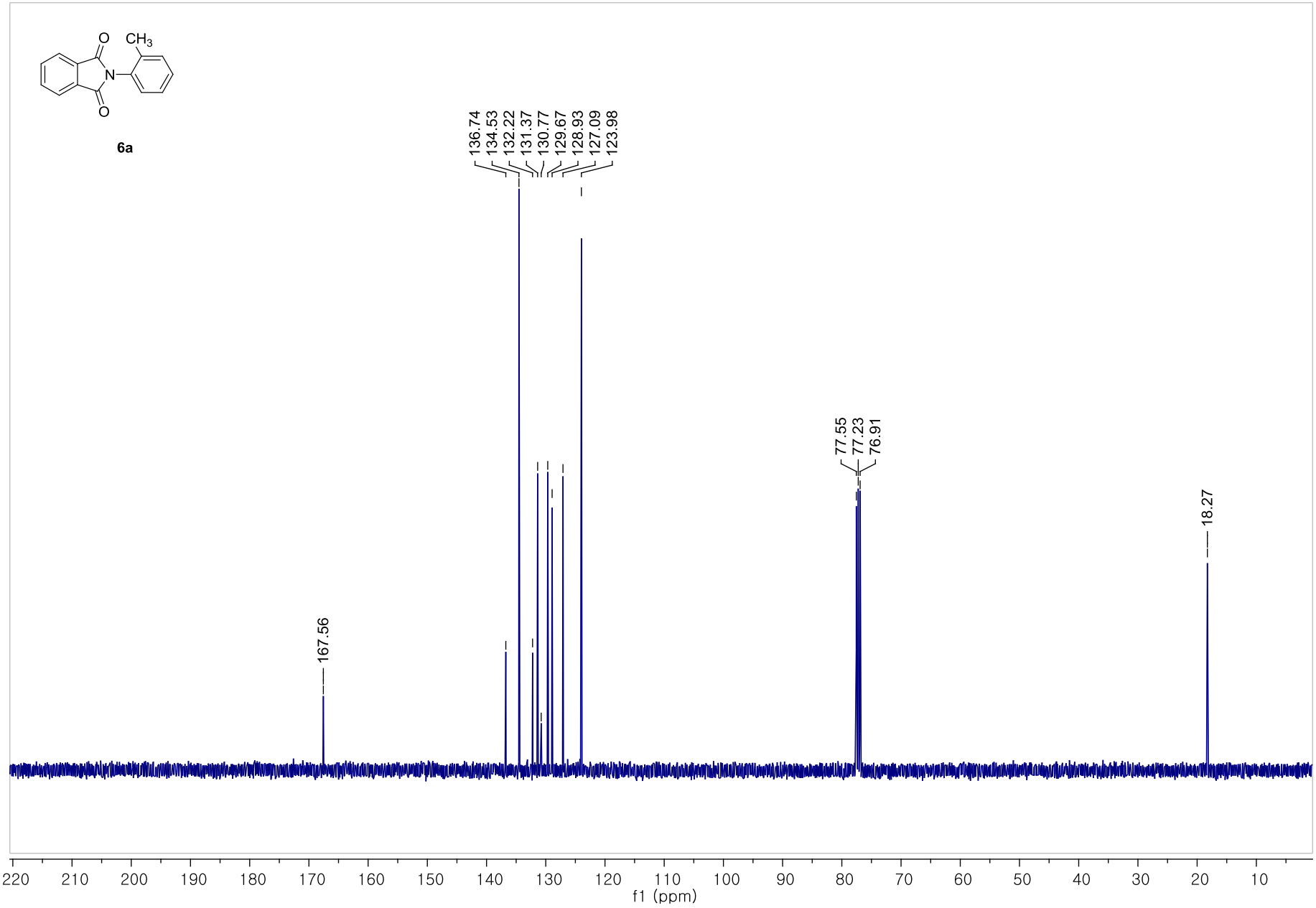

139.28
138.32
136.70
134.51
134.49
132.17
131.98
131.95
131.67
131.32
130.76
129.94
129.61
129.20
129.14
129.10
128.90
127.44
127.04
126.62
123.92
123.86
123.83
167.58
167.53
167.50
77.55
77.23
76.91
21.58
21.39
18.22
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

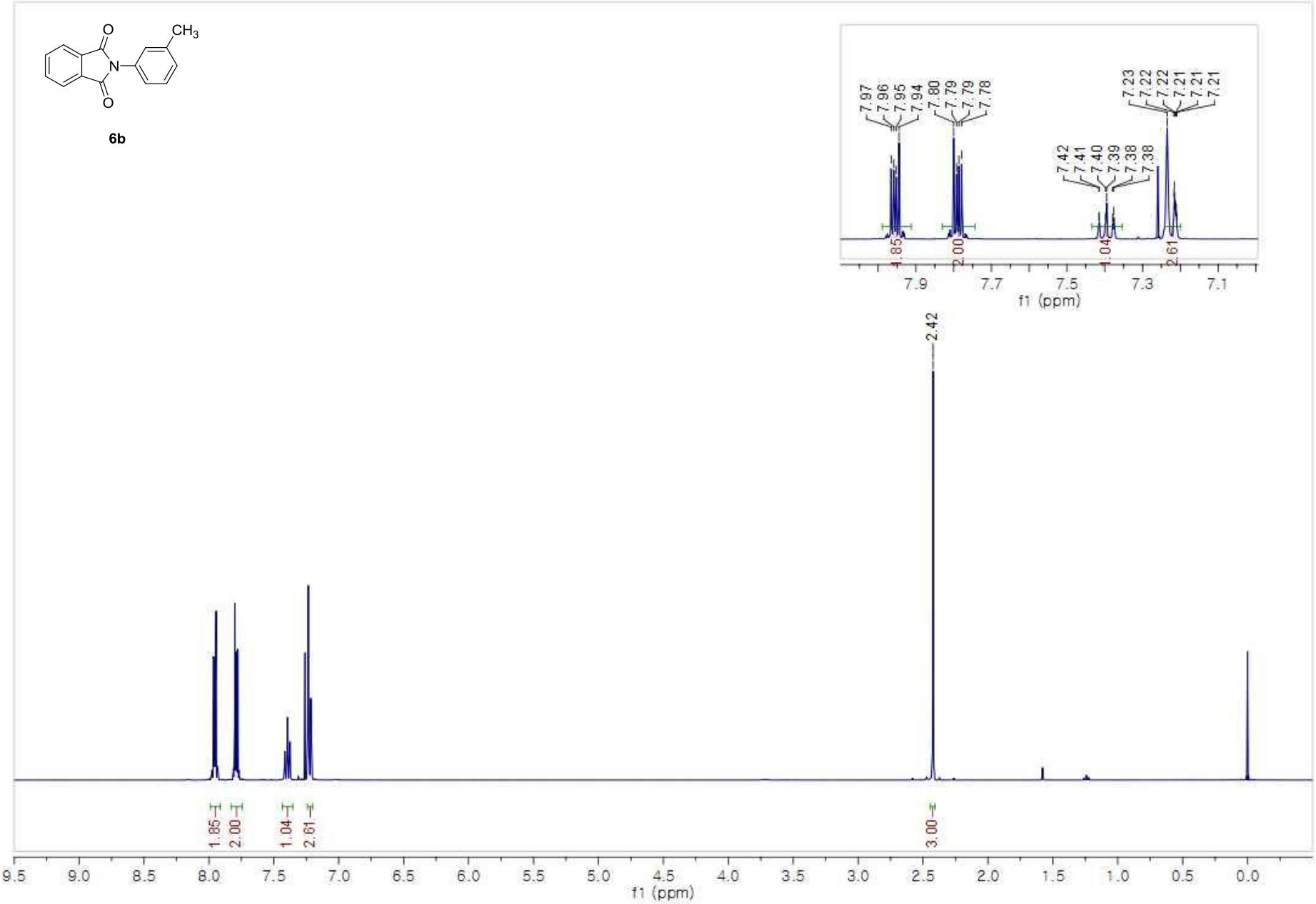

O
CH3
N
O

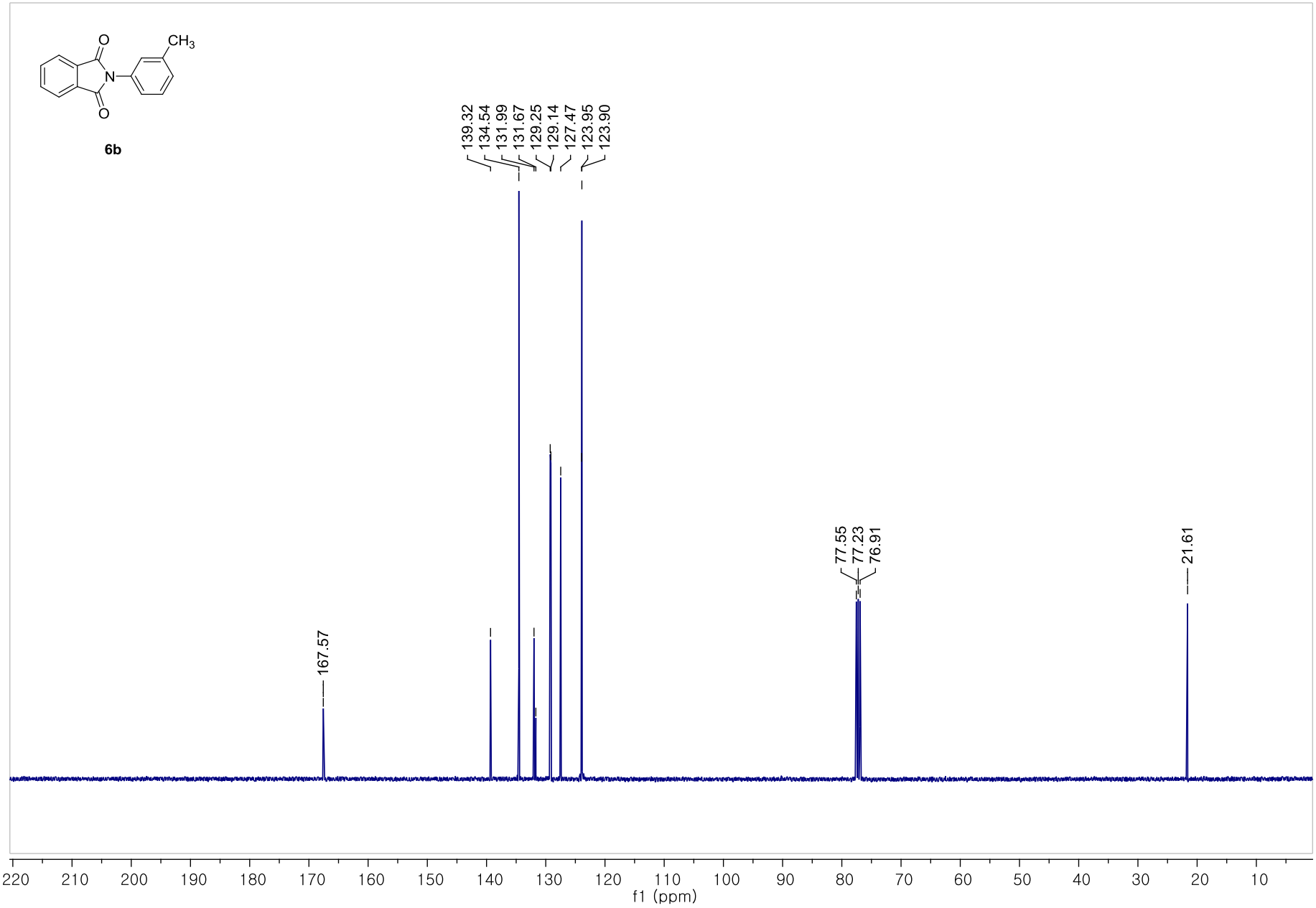
6a

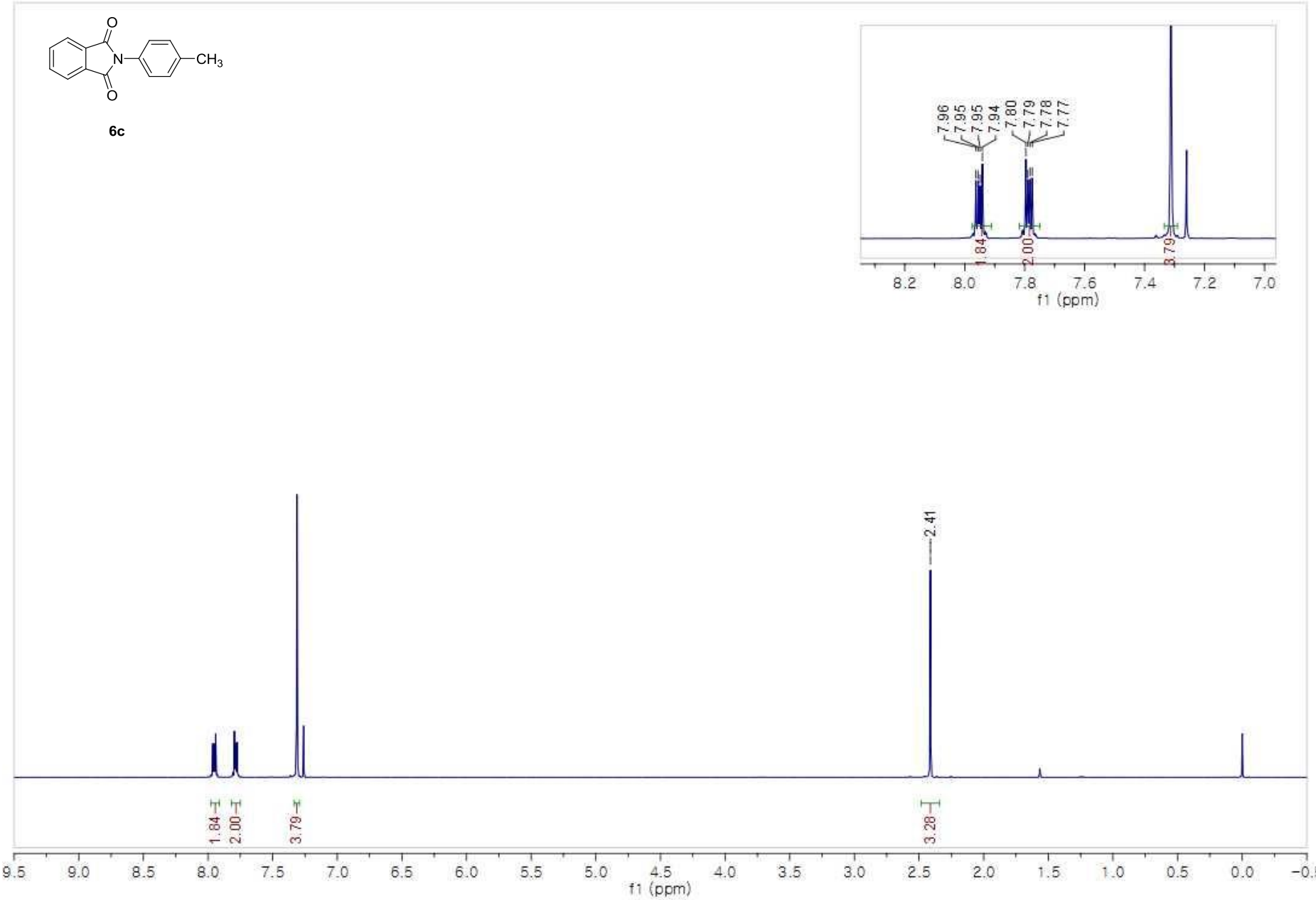

7.98
7.97
7.96
7.96
7.81
7.81
7.80
7.79
7.39
7.38
7.38
7.37
7.37
7.35
7.34
7.33
7.33
7.22
7.20
2.00
2.13
0.69
1.13
1.24
1.00
8.0
7.5
7.0
f1 (ppm)

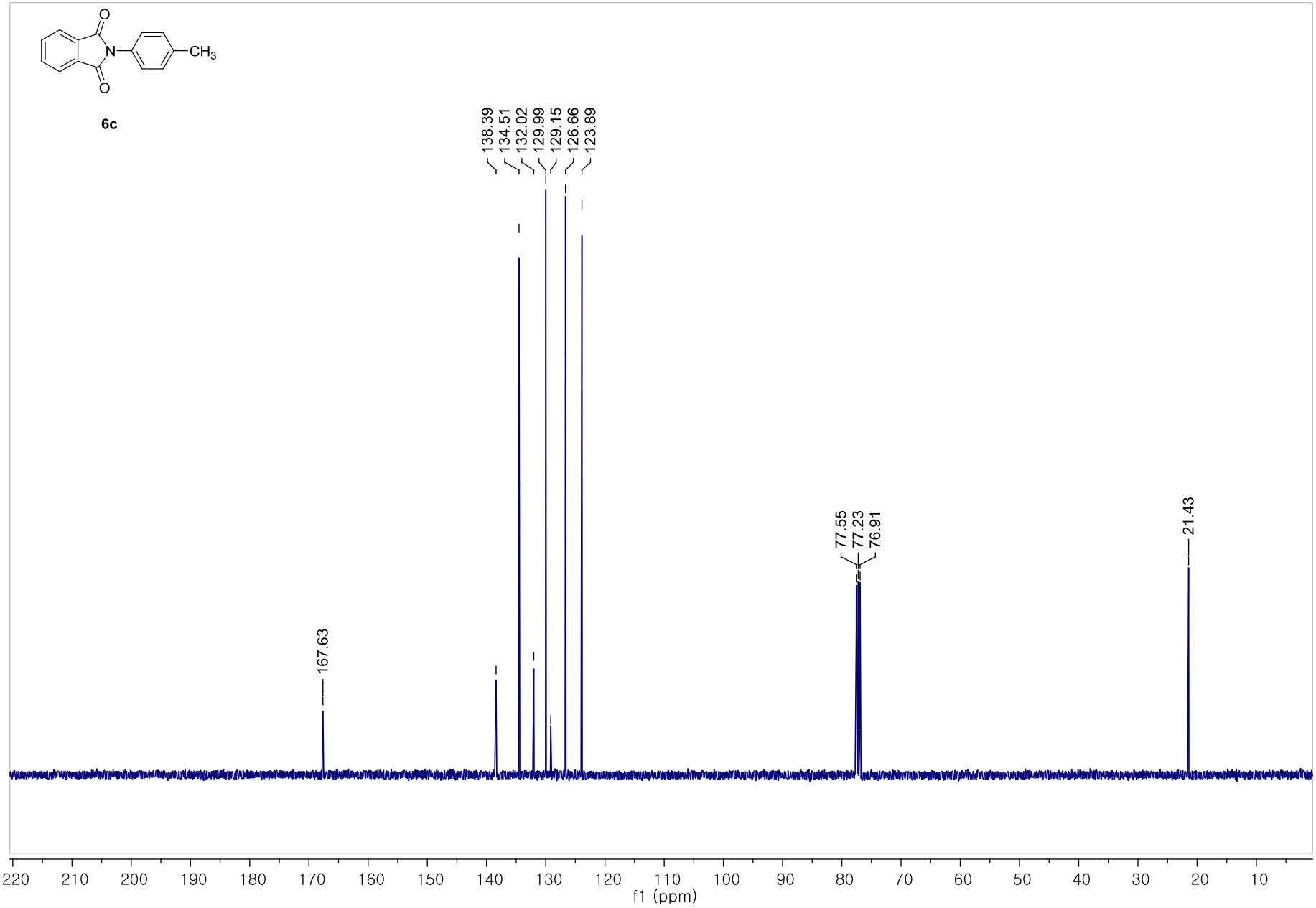

2.22
2.00
2.13
0.69
1.13
1.24
1.00
3.20
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

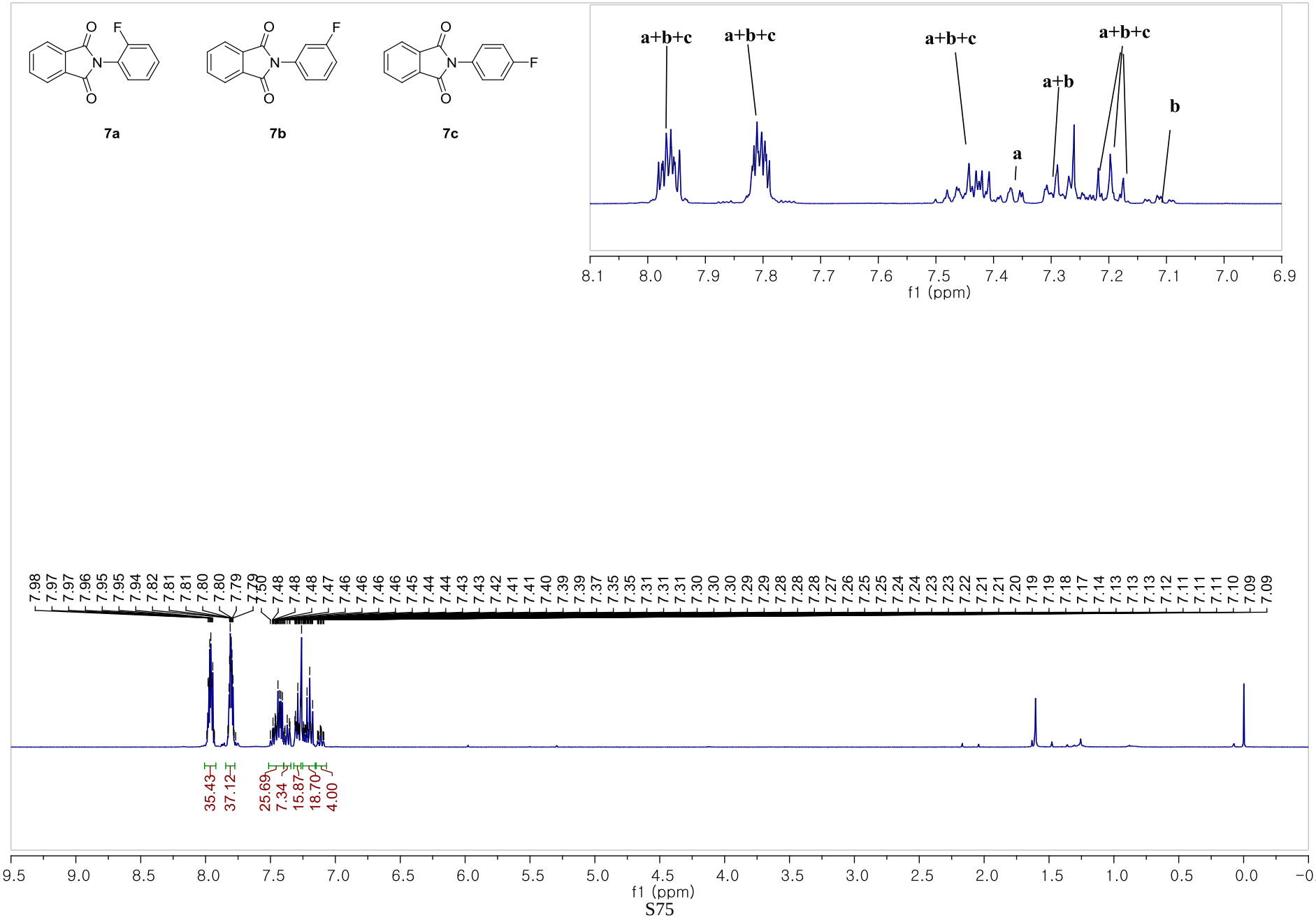

O
CH3
N
O
6a
136.74
134.53
132.22
131.37
130.77
129.67
128.93
127.09
123.98
77.55
77.23
76.91
18.27
167.56
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

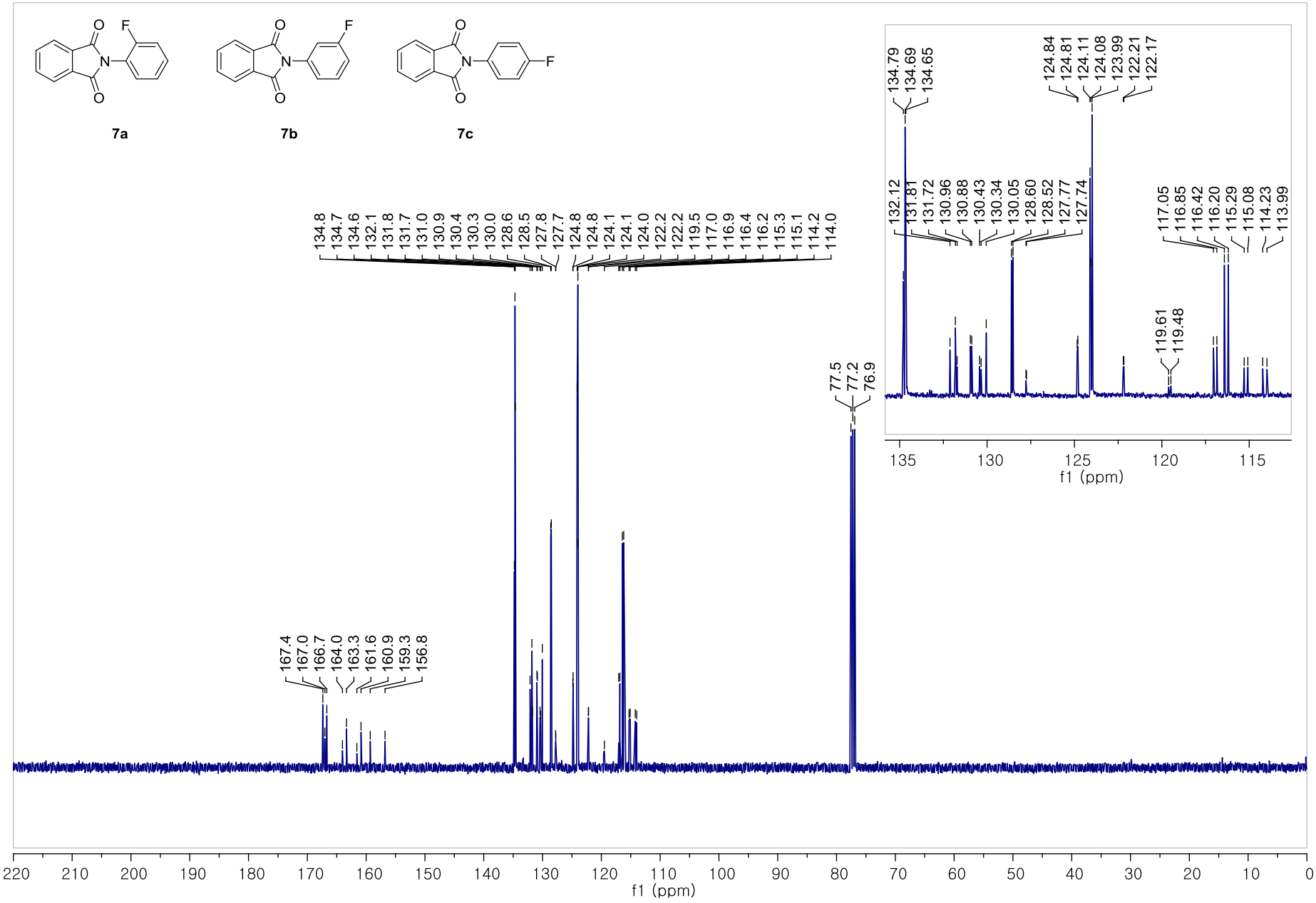

O
CH3
N
O
6b
7.97
7.96
7.95
7.94
7.80
7.79
7.79
7.78
7.42
7.41
7.40
7.39
7.38
7.38
7.23
7.22
7.22
7.21
7.21
7.21
1.85
2.00
1.04
2.61
7.9
7.7
7.5
7.3
7.1
f1 (ppm)
2.42
1.85
2.00
1.04
2.61
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

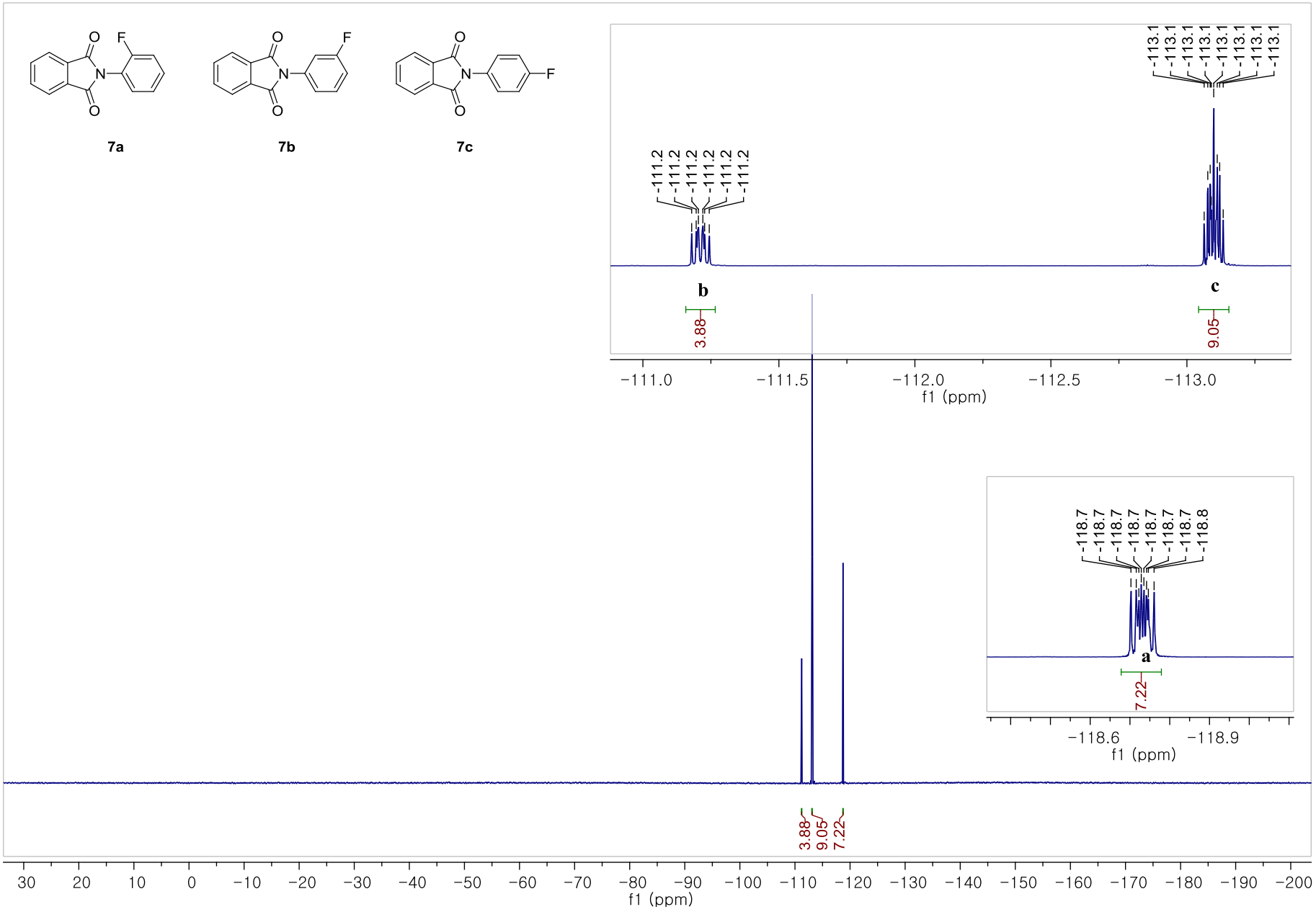

O
CH3
N
O
6b
139.32
134.54
131.99
131.67
129.25
129.14
127.47
123.95
123.90
77.55
77.23
76.91
21.61
167.57
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

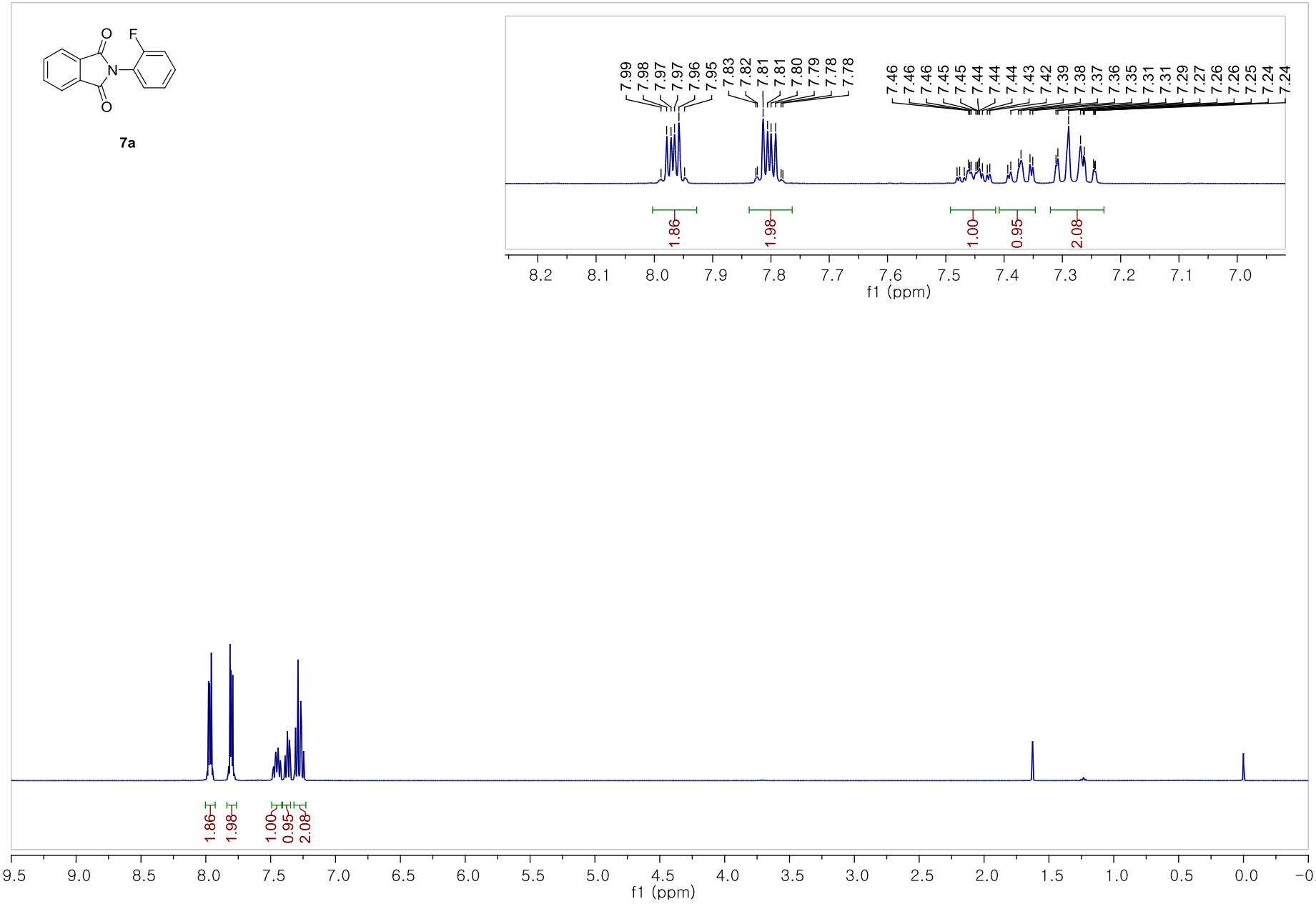

O
N
CH3
O
6c
7.96
7.95
7.95
7.94
7.80
7.79
7.78
7.77
1.84
2.00
3.79
8.2
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)
2.41
1.84
2.00
3.79
3.28
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

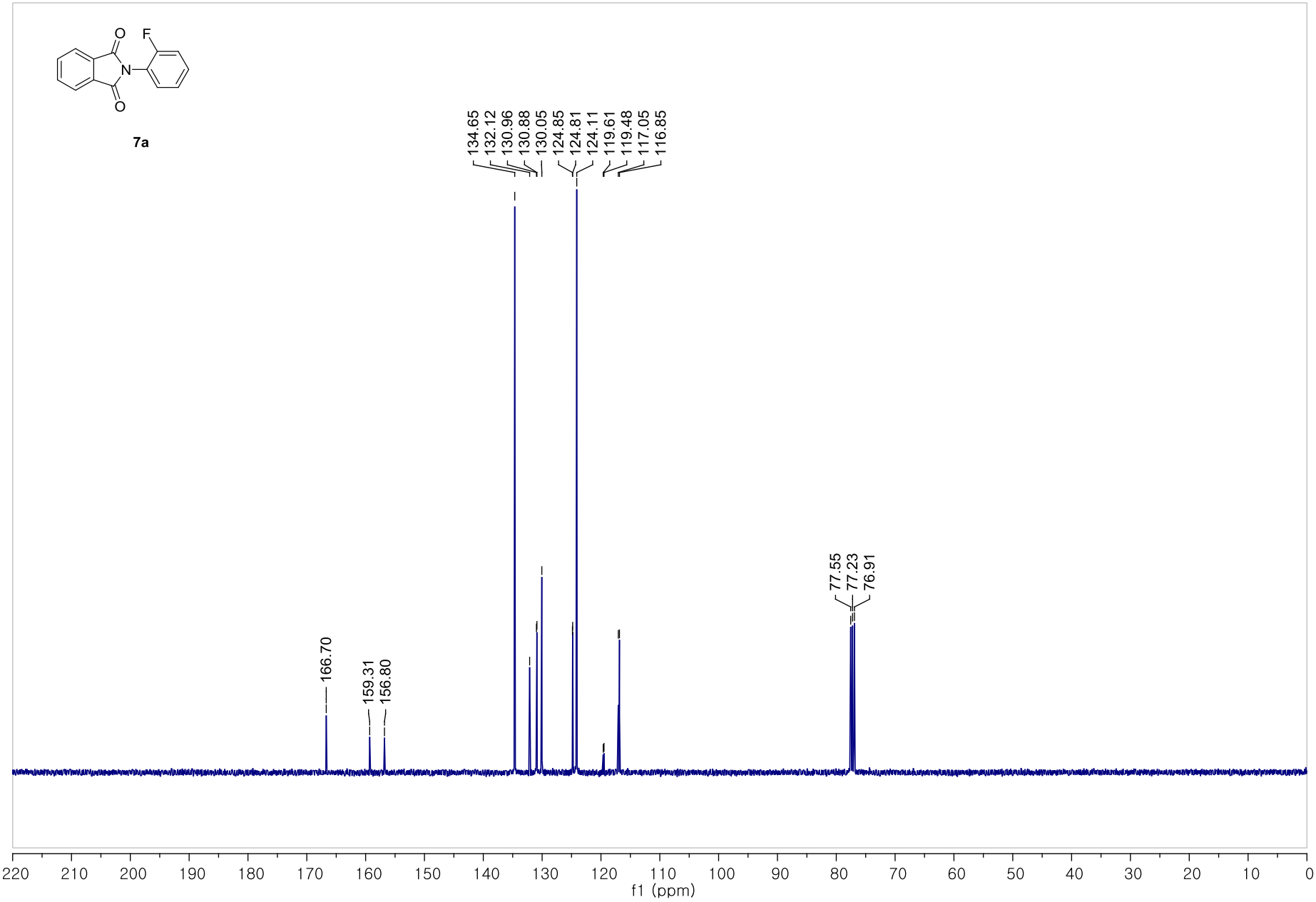

6c
138.39
134.51
132.02
129.99
129.15
126.66
123.89
167.63
77.55
77.23
76.91
21.43
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

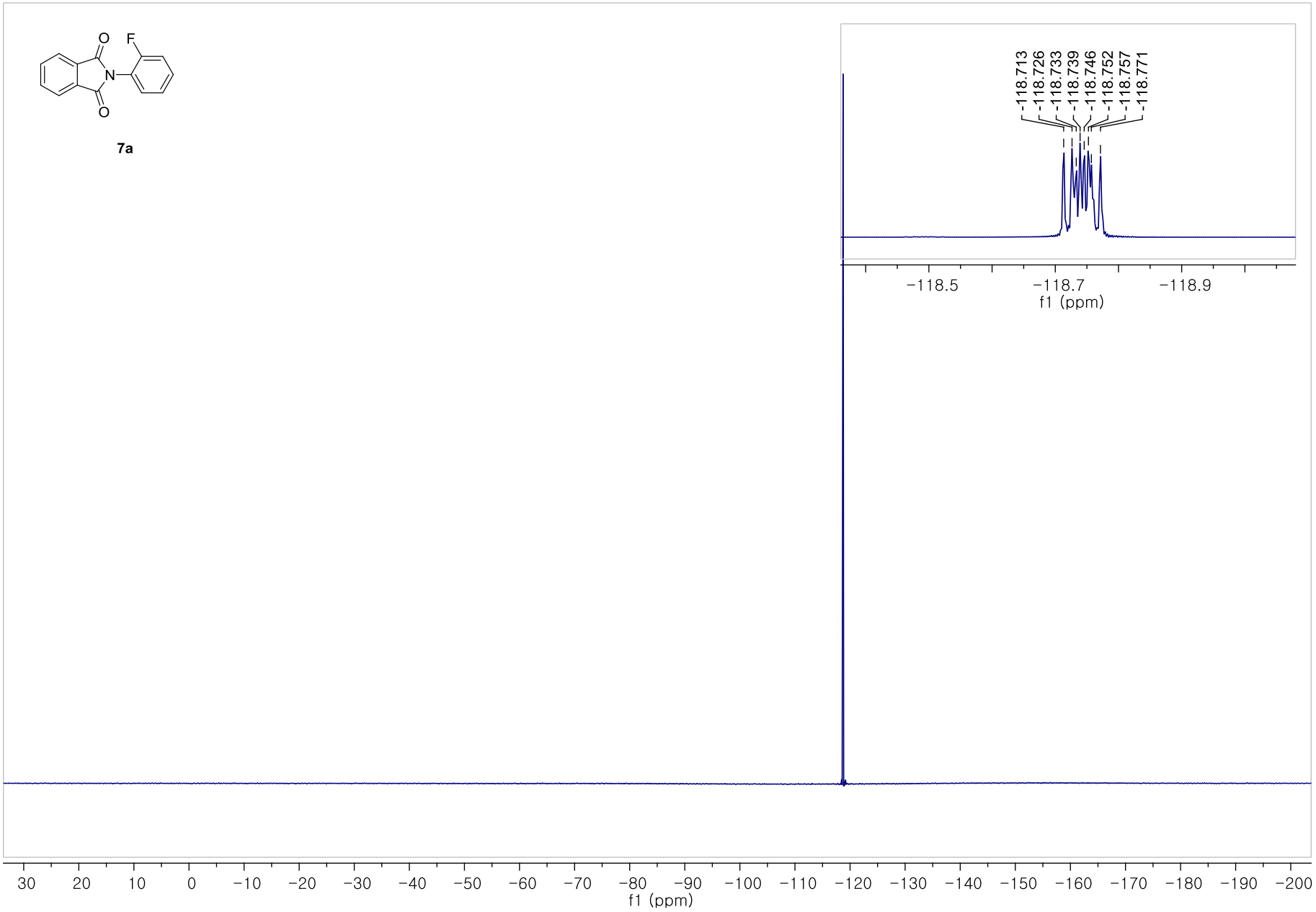

7a
7b
7c
a+b+c
a+b+c
a+b+c
a+b
a+b+c
a
b
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
35.43
37.12
25.69
7.34
15.87
18.70
4.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.
f1 (ppm)

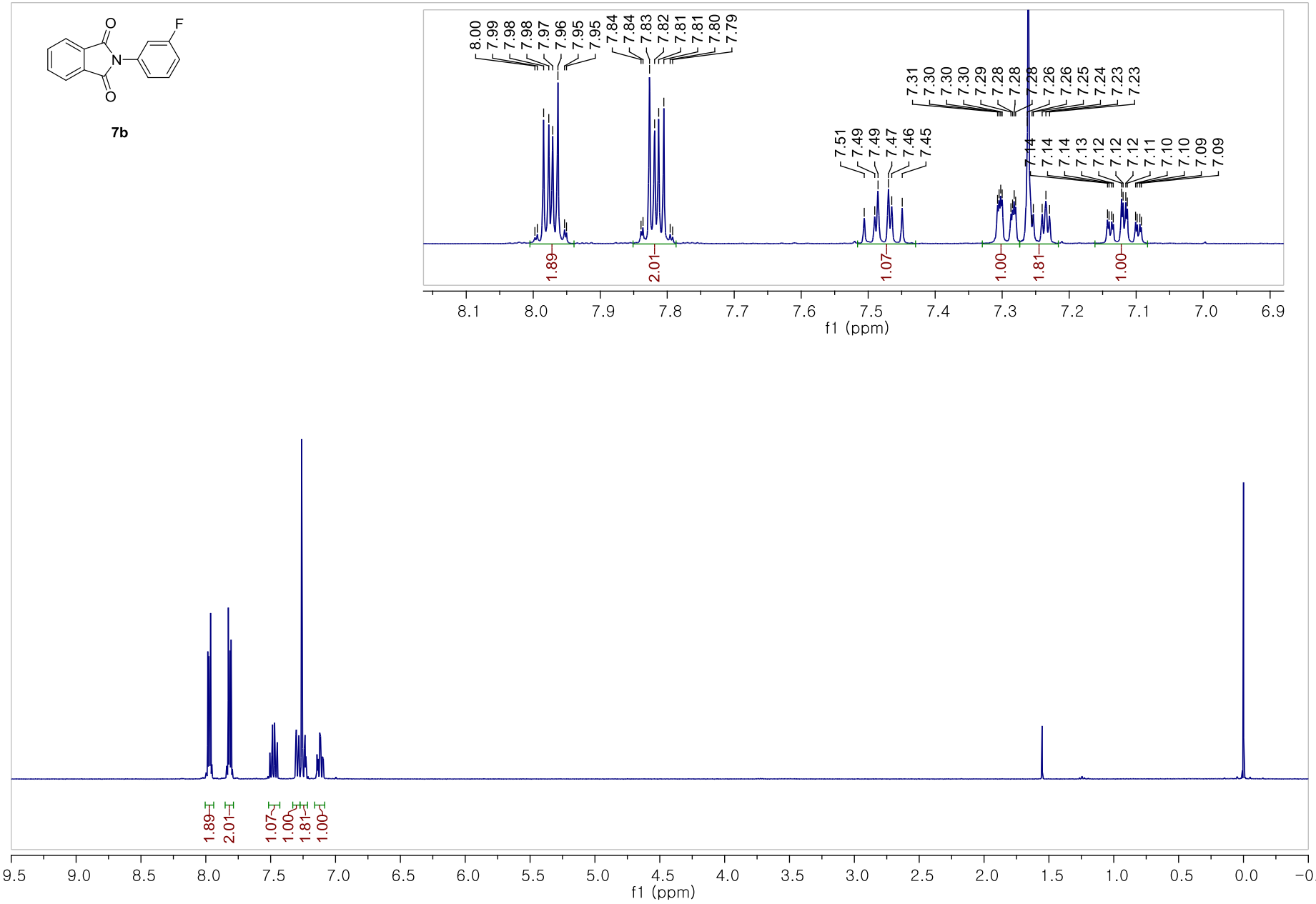

7a
7b
7c
134.8
134.7
134.6
132.1
131.8
131.7
131.0
130.9
130.4
130.3
130.0
128.6
128.5
127.8
127.7
124.8
124.8
124.1
124.1
124.0
122.2
122.2
119.5
117.0
116.9
116.4
116.2
115.3
115.1
114.2
114.0
167.4
167.0
166.7
164.0
163.3
161.6
160.9
159.3
156.8
77.5
77.2
76.9
134.79
134.69
134.65
132.12
131.81
131.72
130.96
130.88
130.43
130.34
130.05
128.60
128.52
127.77
127.74
124.84
124.81
124.11
124.08
123.99
122.21
122.17
119.61
119.48
117.05
116.85
116.42
116.20
115.29
115.08
114.23
113.99
135
130
125
120
115
f1 (ppm)
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

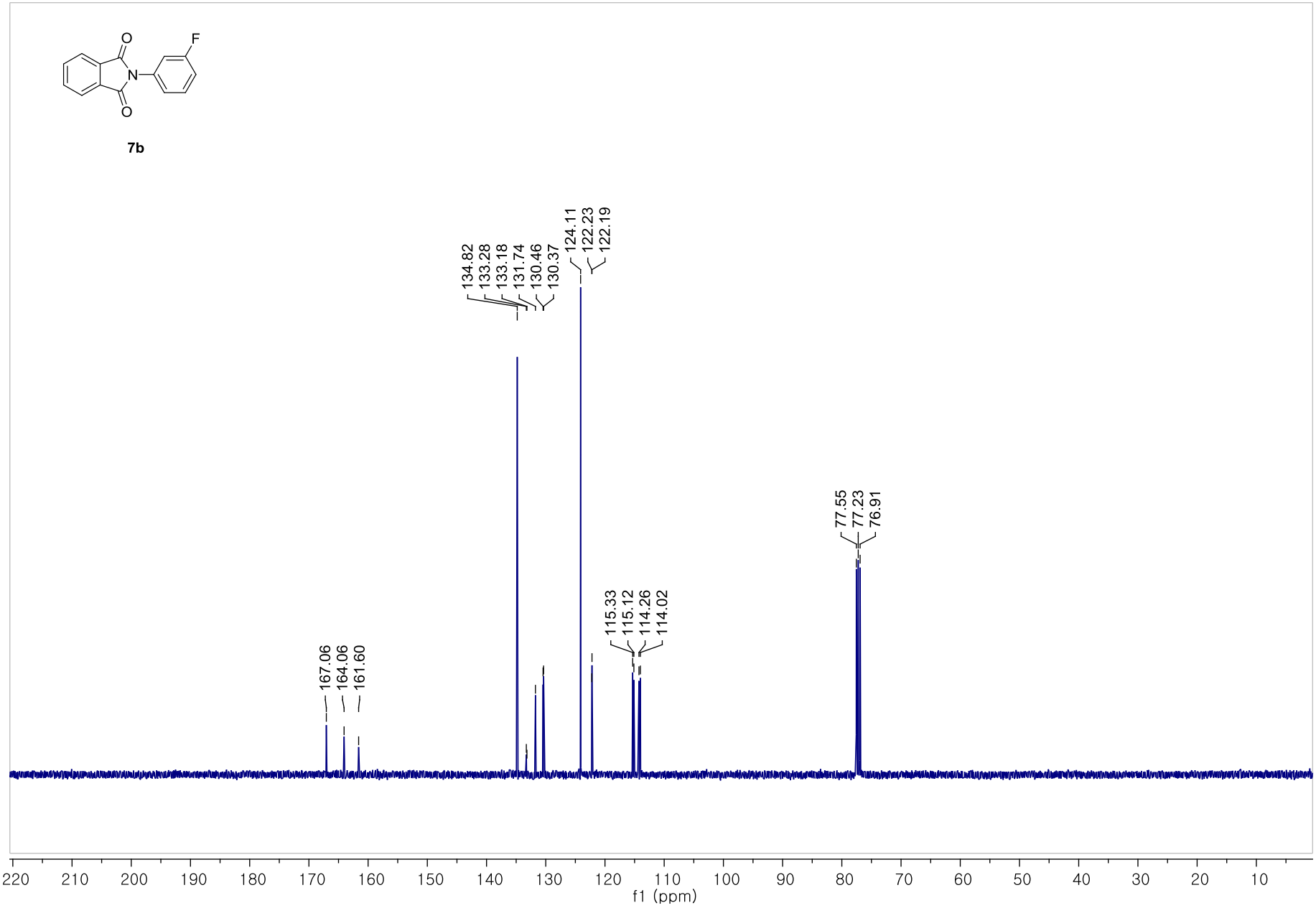

7a
7b
7c
-111.2
-113.1
b
c
3.88
9.05
-111.0
-111.5
-112.0
-112.5
-113.0
f1 (ppm)
-118.7
-118.8
a
7.22
-118.6
-118.9
f1 (ppm)
3.88
9.05
7.22
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

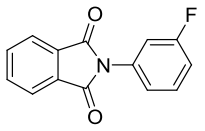

O
F
N
O
O
7a
7.99
7.98
7.97
7.97
7.96
7.95
7.83
7.82
7.81
7.81
7.80
7.79
7.78
7.78
7.46
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.42
7.39
7.38
7.37
7.36
7.35
7.31
7.31
7.29
7.27
7.26
7.26
7.25
7.24
7.24
1.86
1.98
1.00
0.95
2.08
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
1.86
1.98
1.00
0.95
2.08
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


7a
134.65
132.12
130.96
130.88
130.05
124.85
124.81
124.11
119.61
119.48
117.05
116.85
77.55
77.23
76.91
166.70
159.31
156.80
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

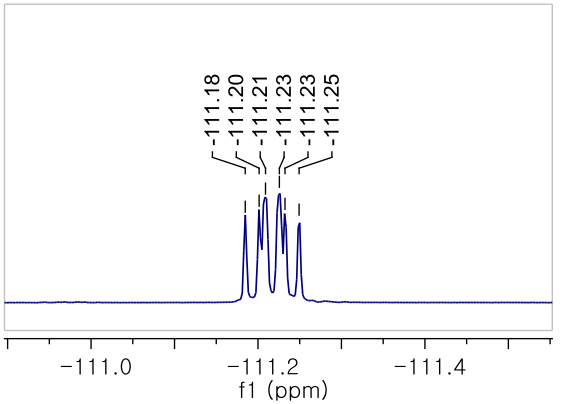

O
F
N
O
7a
-118.713
-118.726
-118.733
-118.739
-118.746
-118.752
-118.757
-118.771
-118.5
-118.7
-118.9
f1 (ppm)
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

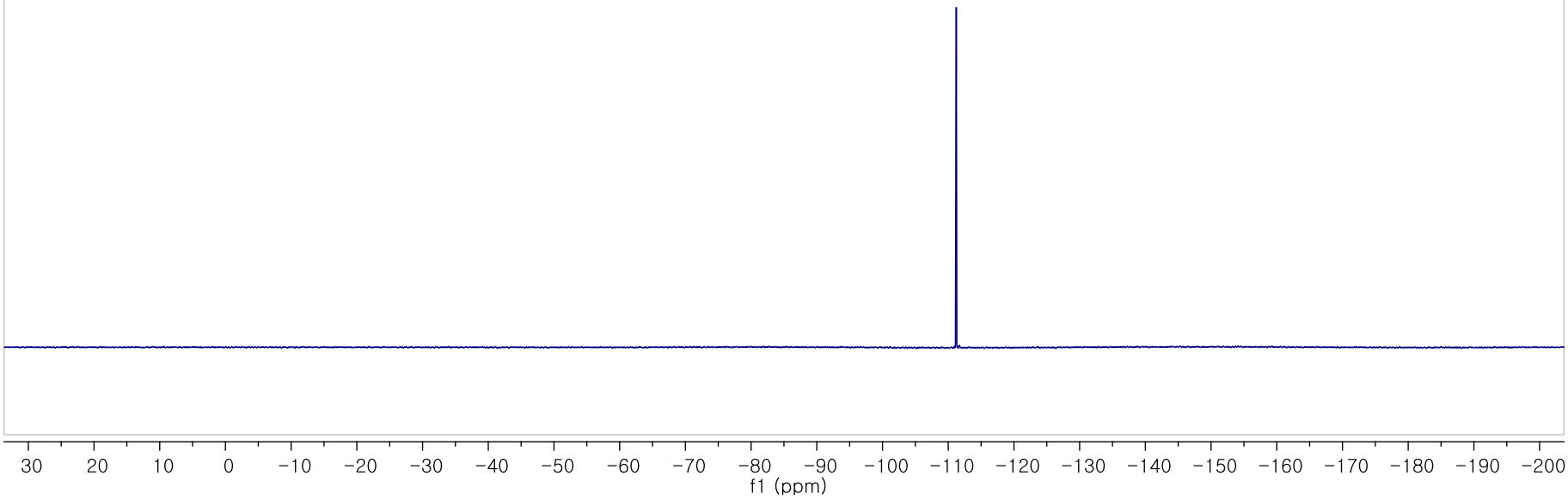

7b
8.00
7.99
7.98
7.98
7.97
7.96
7.95
7.95
7.84
7.84
7.83
7.82
7.81
7.81
7.80
7.79
7.31
7.30
7.30
7.30
7.29
7.28
7.28
7.28
7.26
7.26
7.25
7.24
7.23
7.23
7.51
7.49
7.49
7.47
7.46
7.45
7.14
7.14
7.14
7.13
7.12
7.12
7.12
7.11
7.10
7.10
7.09
7.09
1.89
2.01
1.07
1.00
1.81
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
1.89
2.01
1.07
1.00
1.81
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

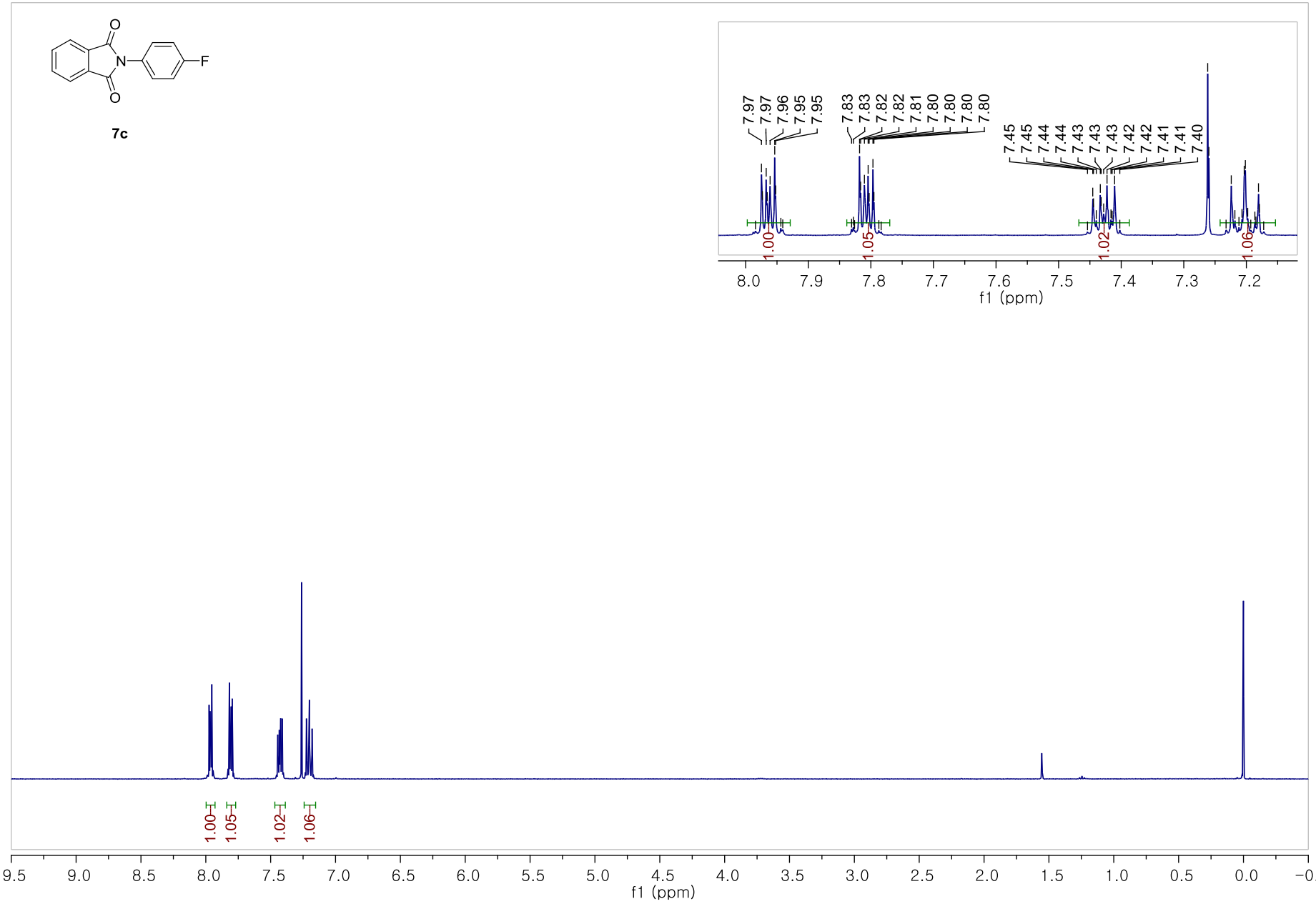

O
F
N
O
7b
134.82
133.28
133.18
131.74
130.46
130.37
124.11
122.23
122.19
115.33
115.12
114.26
114.02
77.55
77.23
76.91
167.06
164.06
161.60
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

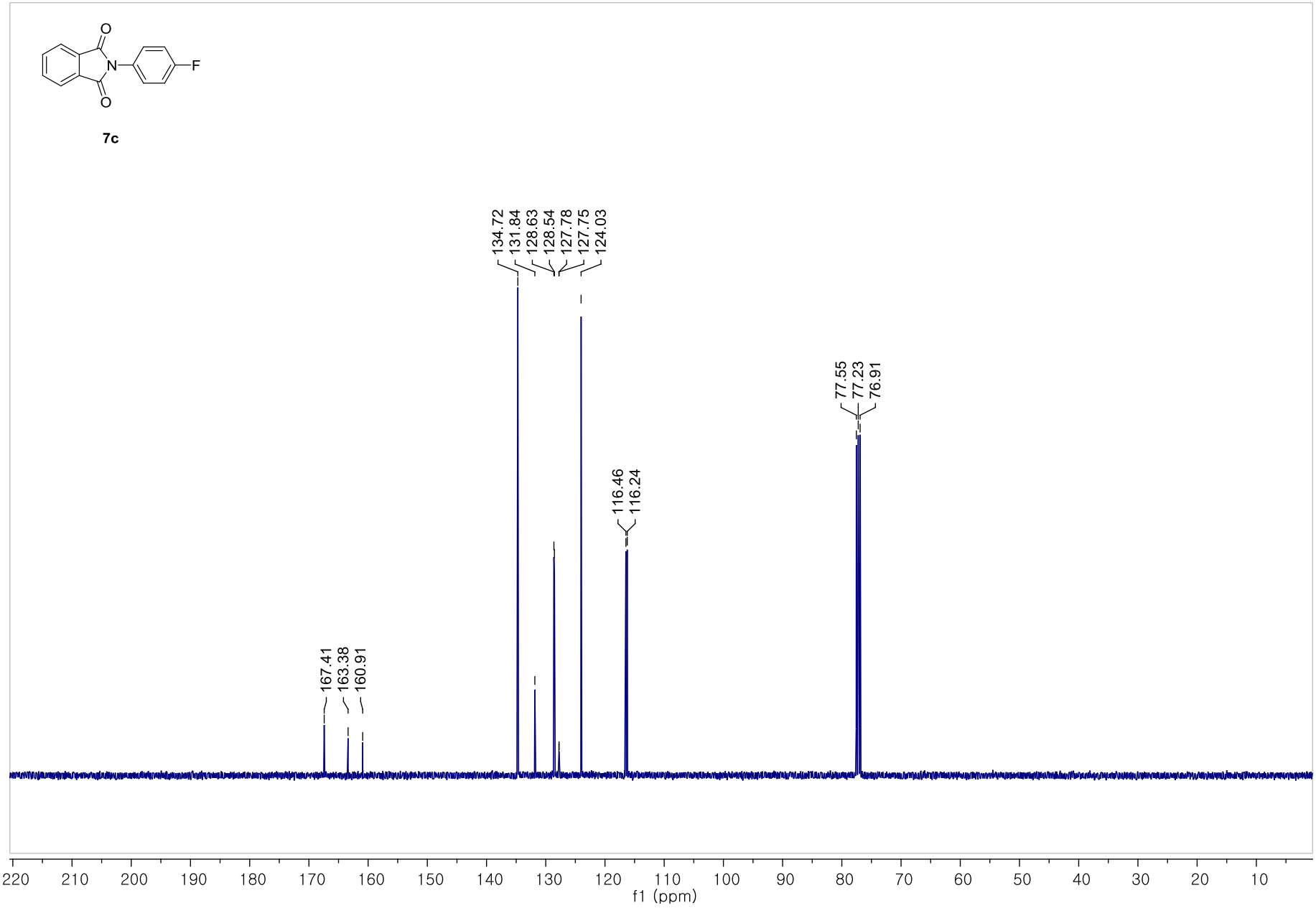

O
F
N
O

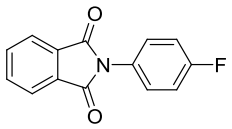
7b


-111.18
-111.20
-111.21
-111.23
-111.23
-111.25
-111.0
-111.2
-111.4
f1 (ppm)

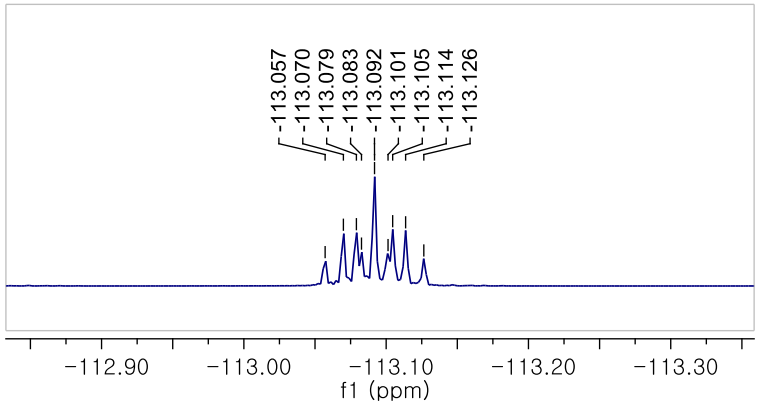

30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

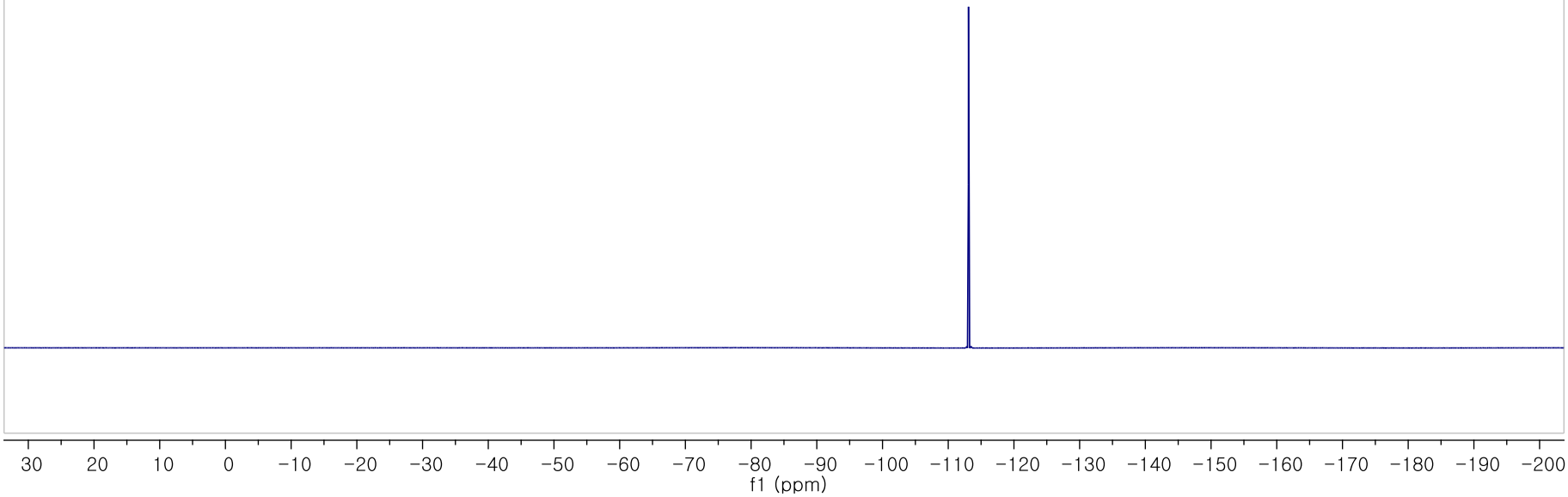

O
N
F
O
7c
7.97
7.97
7.96
7.95
7.95
7.83
7.83
7.82
7.82
7.81
7.80
7.80
7.80
7.80
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.40
1.00
1.05
1.02
1.06
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
1.00
1.05
1.02
1.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

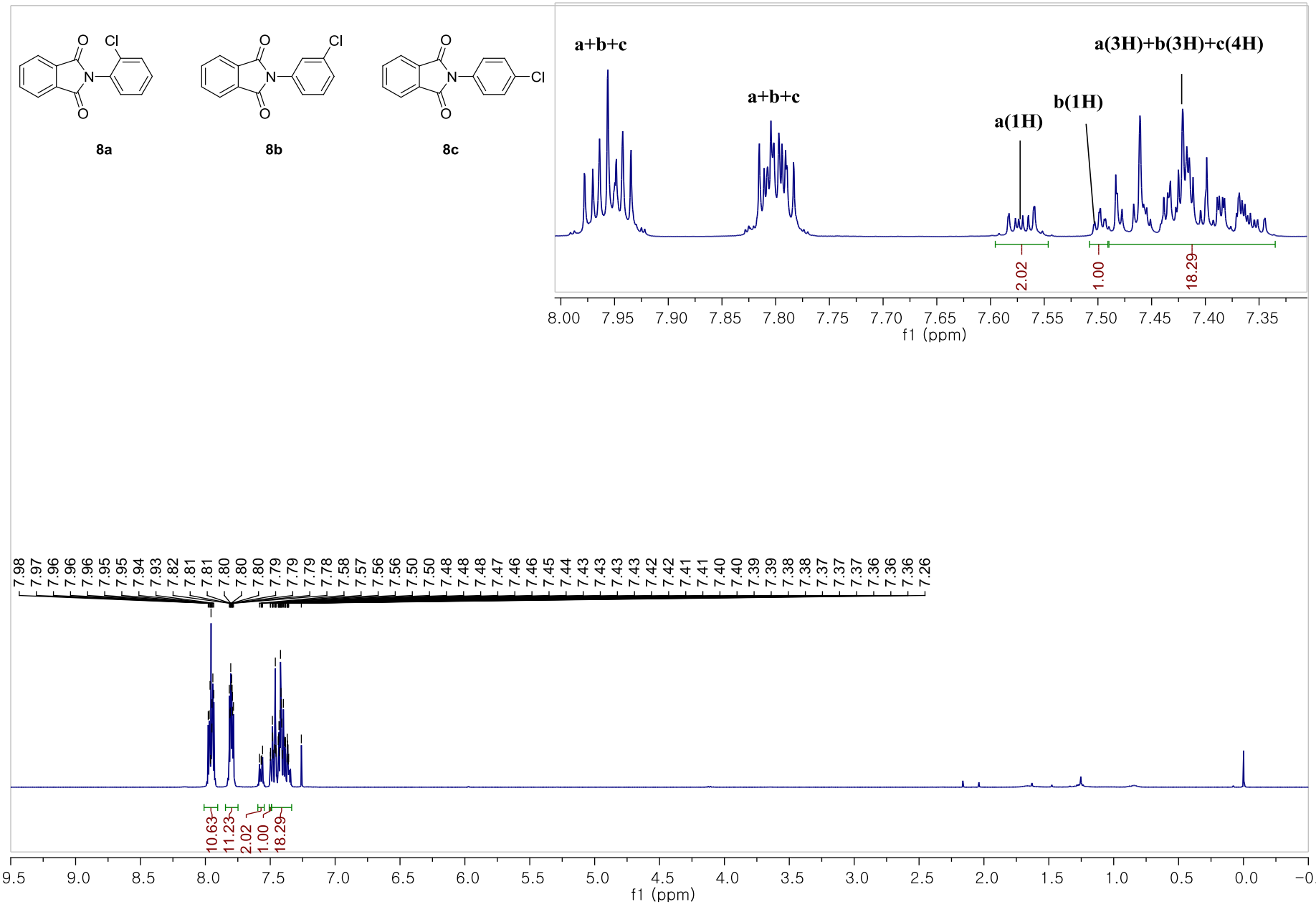

O
N
F
O
7c
134.72
131.84
128.63
128.54
127.78
127.75
124.03
116.46
116.24
77.55
77.23
76.91
167.41
163.38
160.91
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

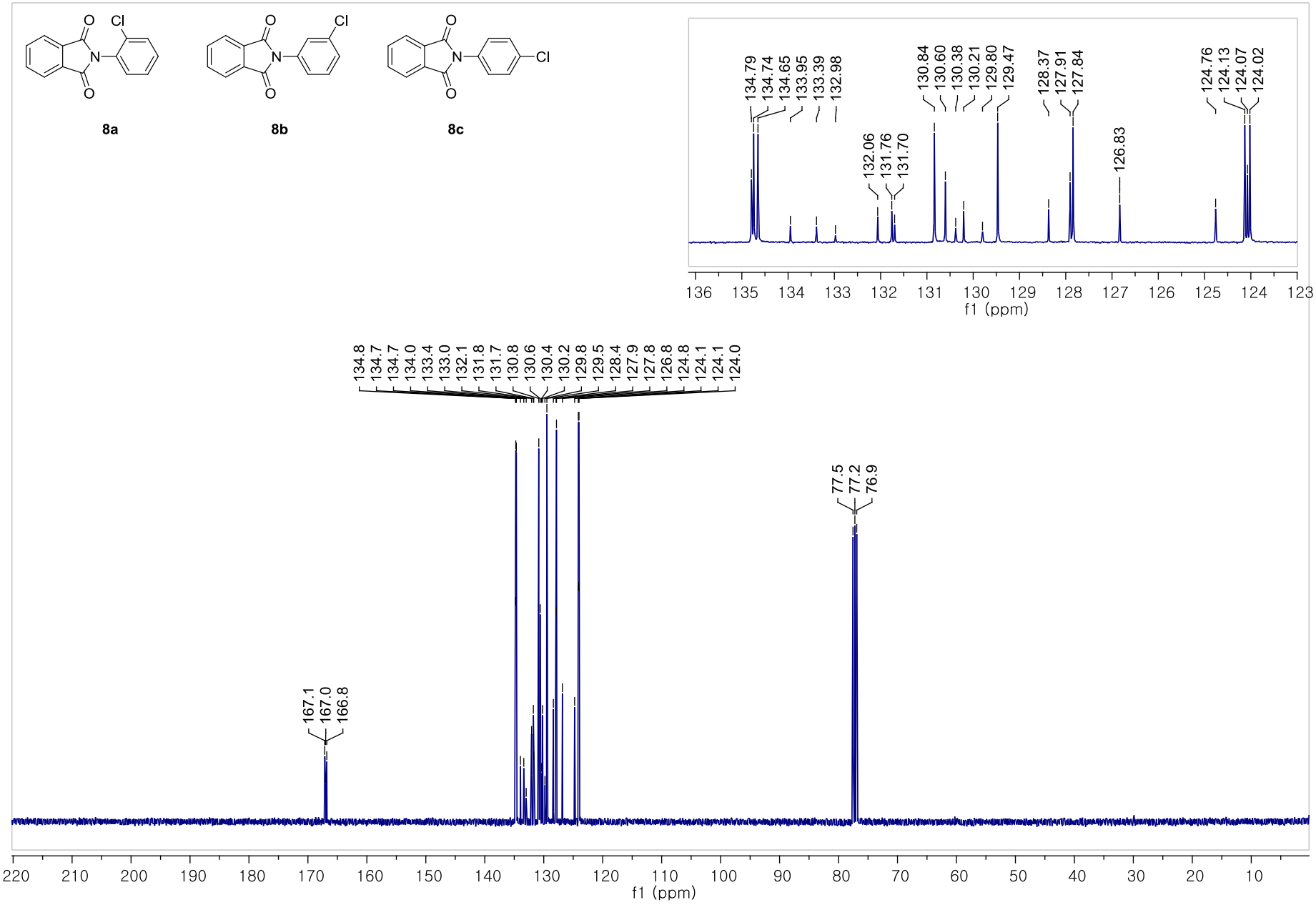

O
N
F
O

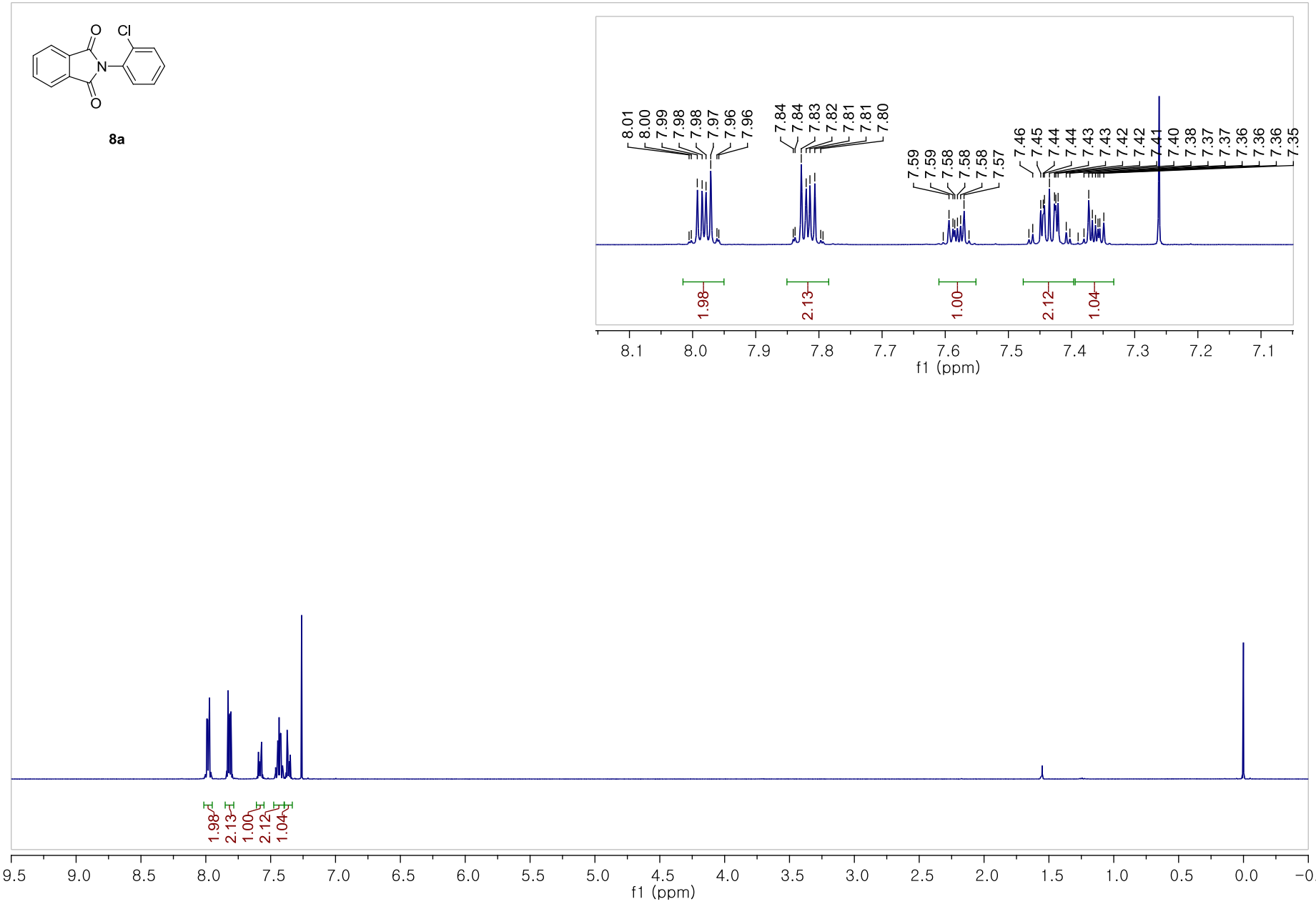
7c

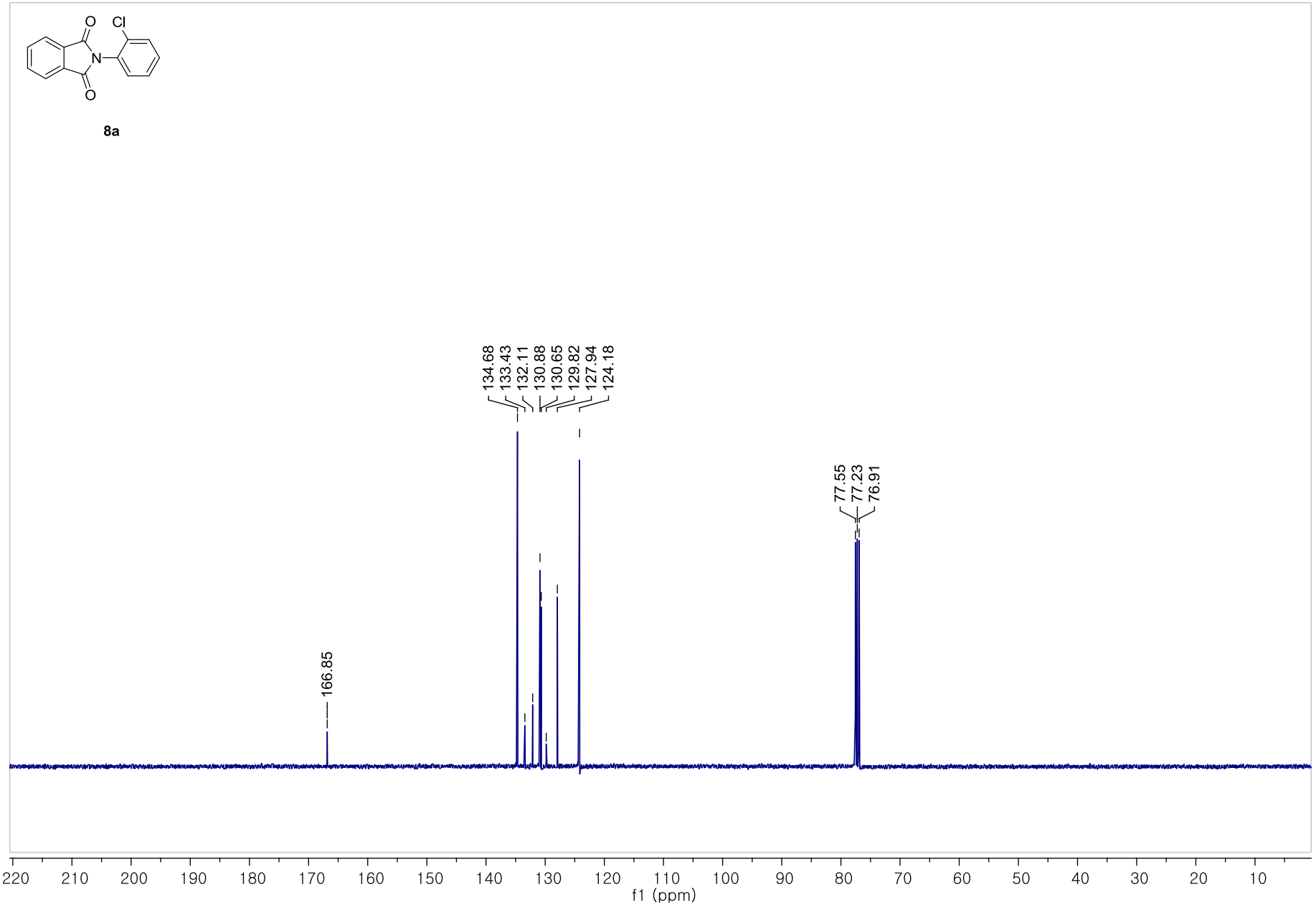

-113.057
-113.070
-113.079
-113.083
-113.092
-113.101
-113.105
-113.114
-113.126
-112.90
-113.00
-113.10
-113.20
-113.30
f1 (ppm)

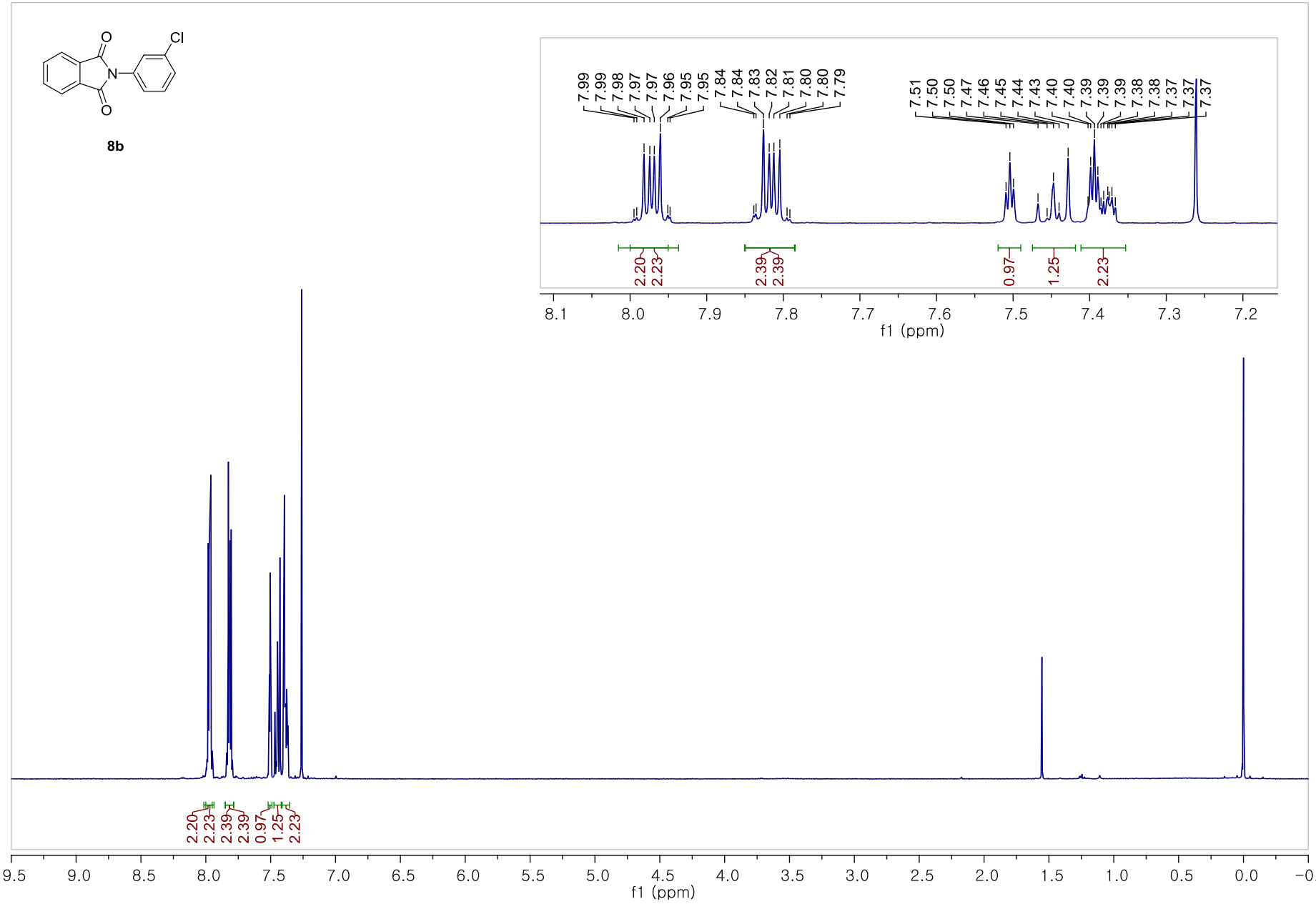

30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

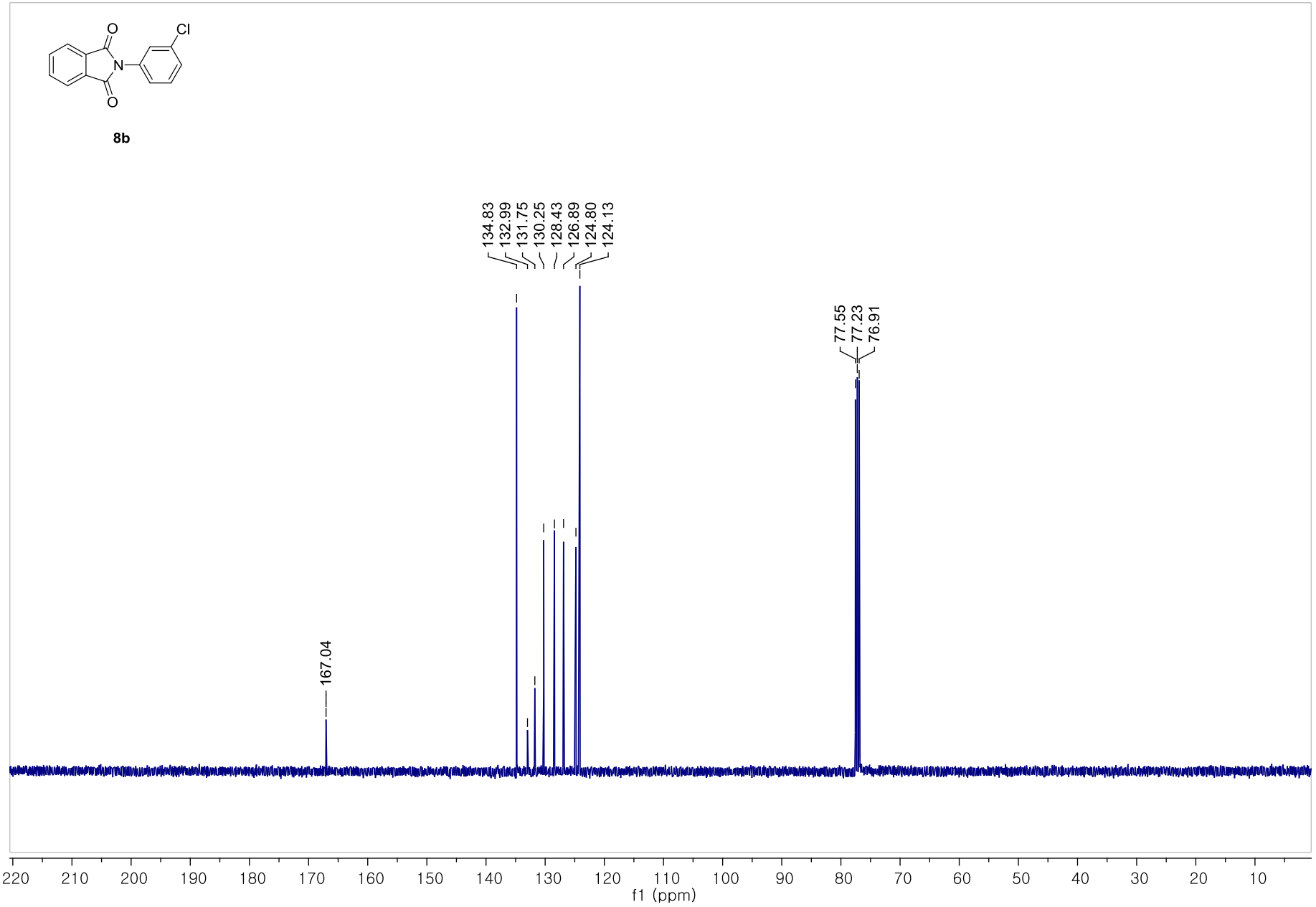

8a
8b
8c
a+b+c
a+b+c
a(1H)
b(1H)
a(3H)+b(3H)+c(4H)
2.02
1.00
18.29
f1 (ppm)
10.63
11.23
2.02
1.00
18.29
f1 (ppm)

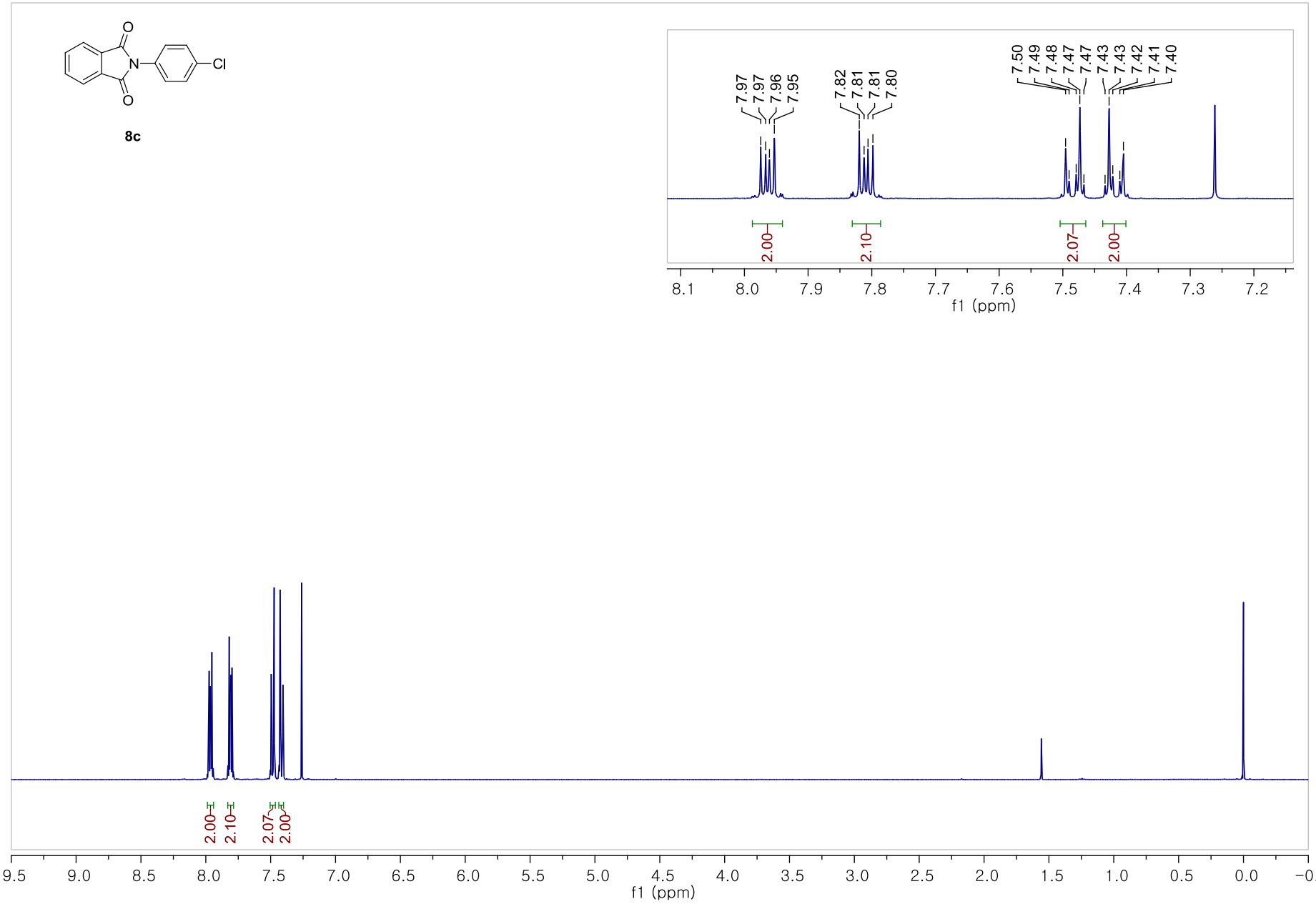

8a
8b
8c
134.79
134.74
134.65
133.95
133.39
132.98
132.06
131.76
131.70
130.84
130.60
130.38
130.21
129.80
129.47
128.37
127.91
127.84
126.83
124.76
124.13
124.07
124.02
f1 (ppm)
134.8
134.7
134.7
134.0
133.4
133.0
132.1
131.8
131.7
130.8
130.6
130.4
130.2
129.8
129.5
128.4
127.9
127.8
126.8
124.8
124.1
124.1
124.0
77.5
77.2
76.9
167.1
167.0
166.8
f1 (ppm)

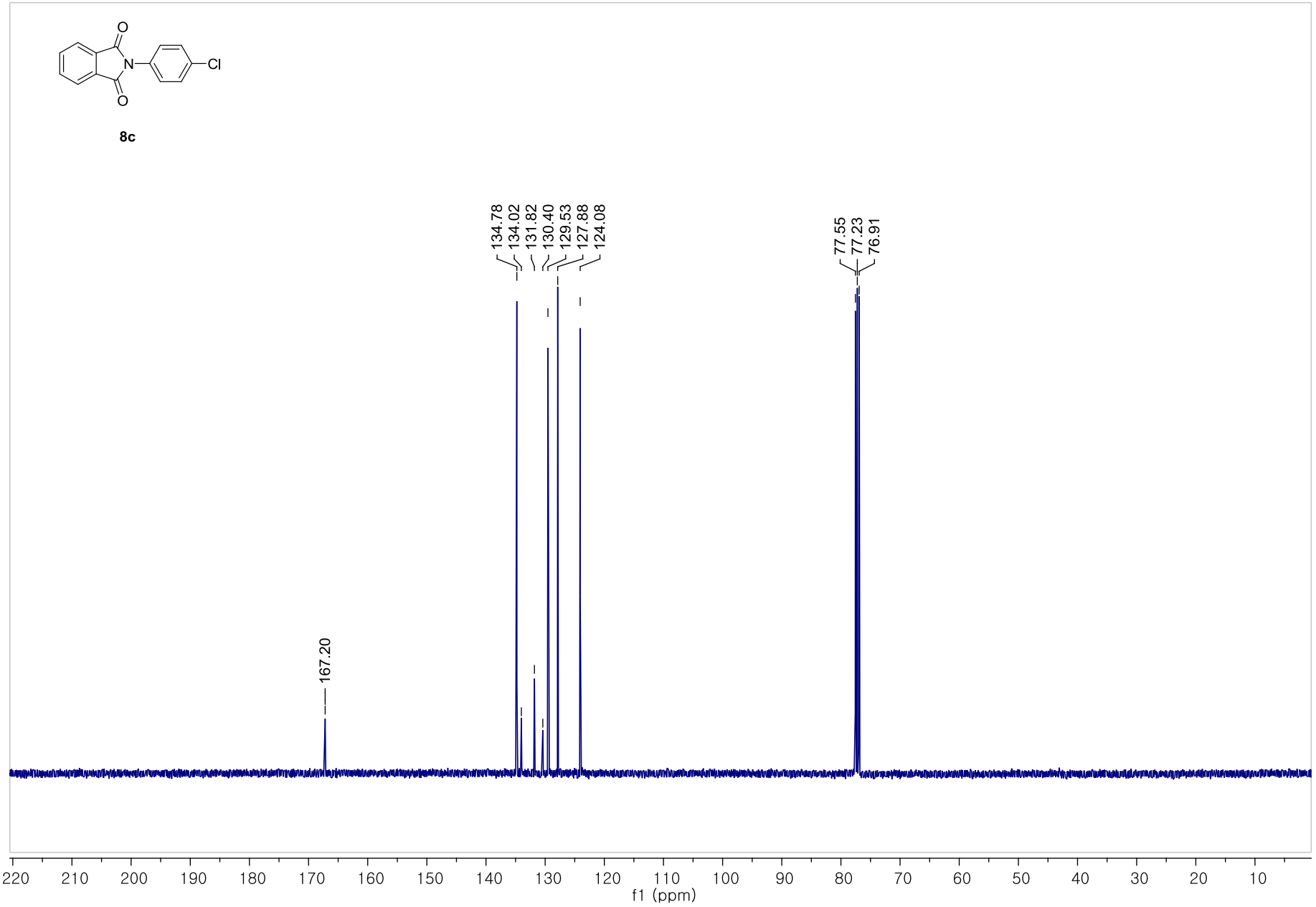

O
Cl
N
O
8a
8.01
8.00
7.99
7.98
7.98
7.97
7.96
7.96
7.84
7.84
7.83
7.82
7.81
7.81
7.80
7.59
7.59
7.58
7.58
7.58
7.57
7.46
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.41
7.40
7.38
7.37
7.37
7.36
7.36
7.36
7.35
1.98
2.13
1.00
2.12
1.04
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
1.98
2.13
1.00
2.12
1.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

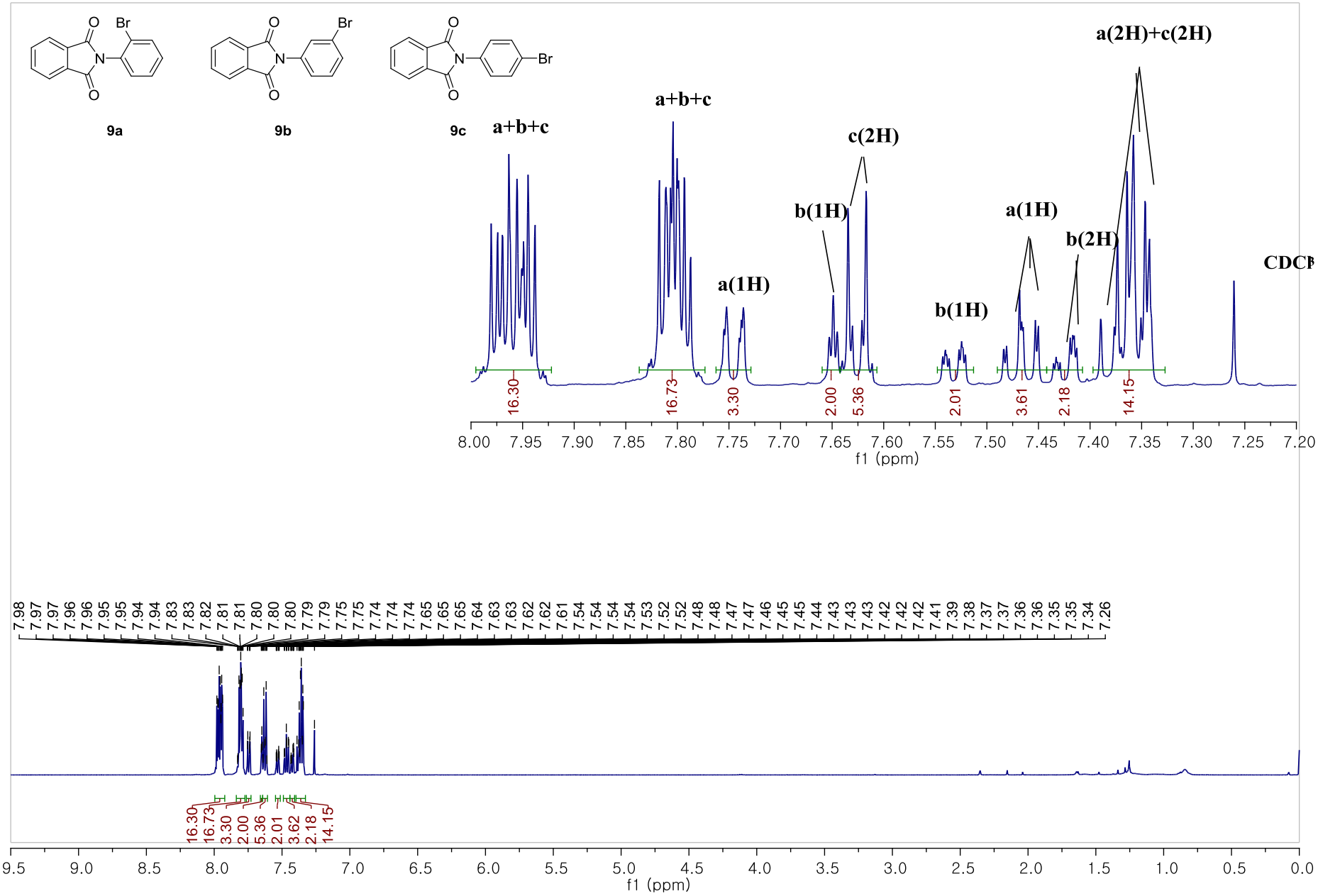

O
Cl
N
O
8a
134.68
133.43
132.11
130.88
130.65
129.82
127.94
124.18
77.55
77.23
76.91
166.85
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

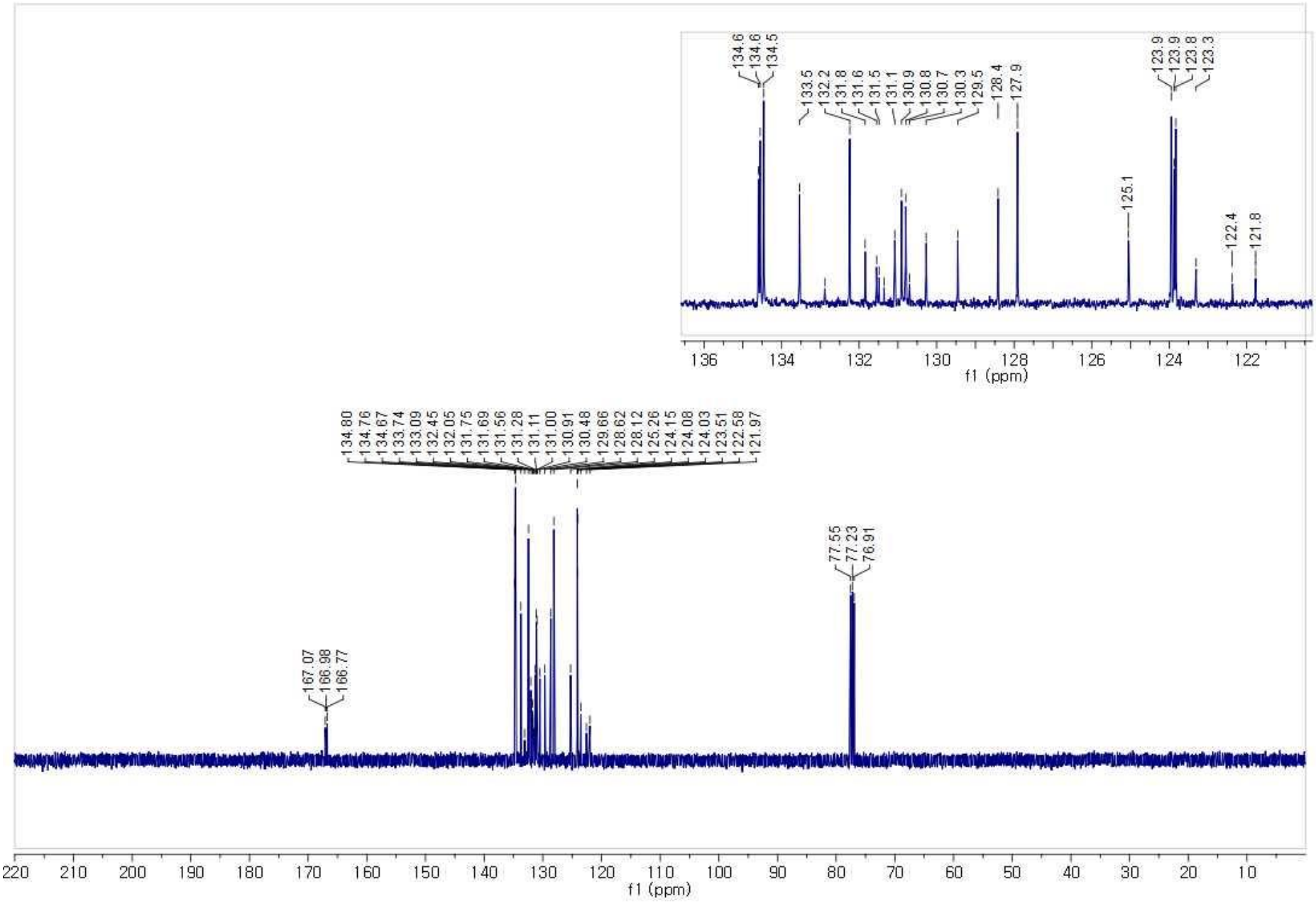

O
N
O
Cl
8b
7.99
7.99
7.98
7.97
7.97
7.96
7.95
7.95
7.84
7.84
7.83
7.82
7.81
7.80
7.80
7.79
7.51
7.50
7.50
7.47
7.46
7.45
7.44
7.43
7.40
7.40
7.39
7.39
7.39
7.38
7.38
7.37
7.37
7.37
2.20
2.23
2.39
2.39
0.97
1.25
2.23
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
2.20
2.23
2.39
2.39
0.97
1.25
2.23
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

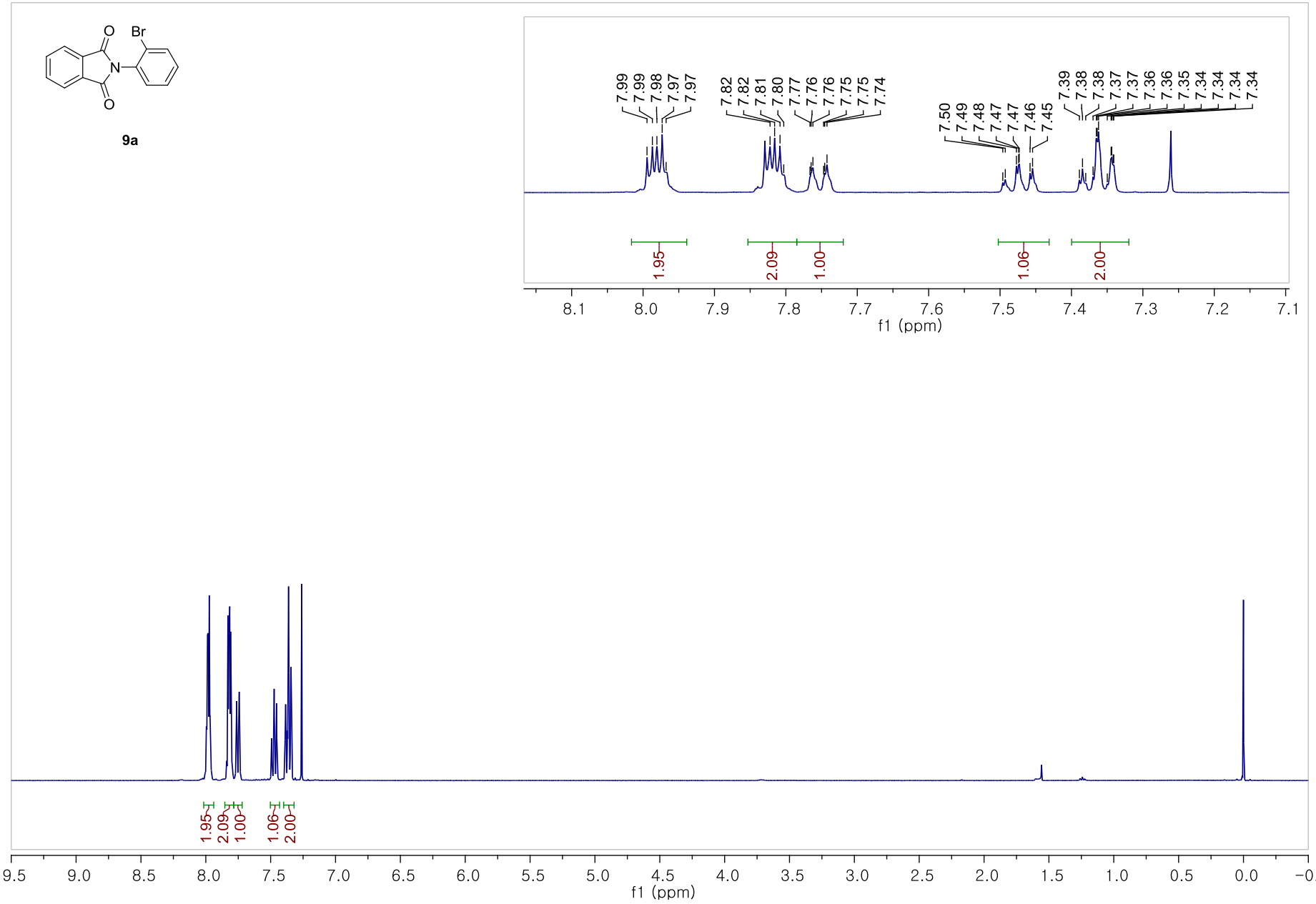

O
Cl
N
O
8b
134.83
132.99
131.75
130.25
128.43
126.89
124.80
124.13
77.55
77.23
76.91
167.04
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

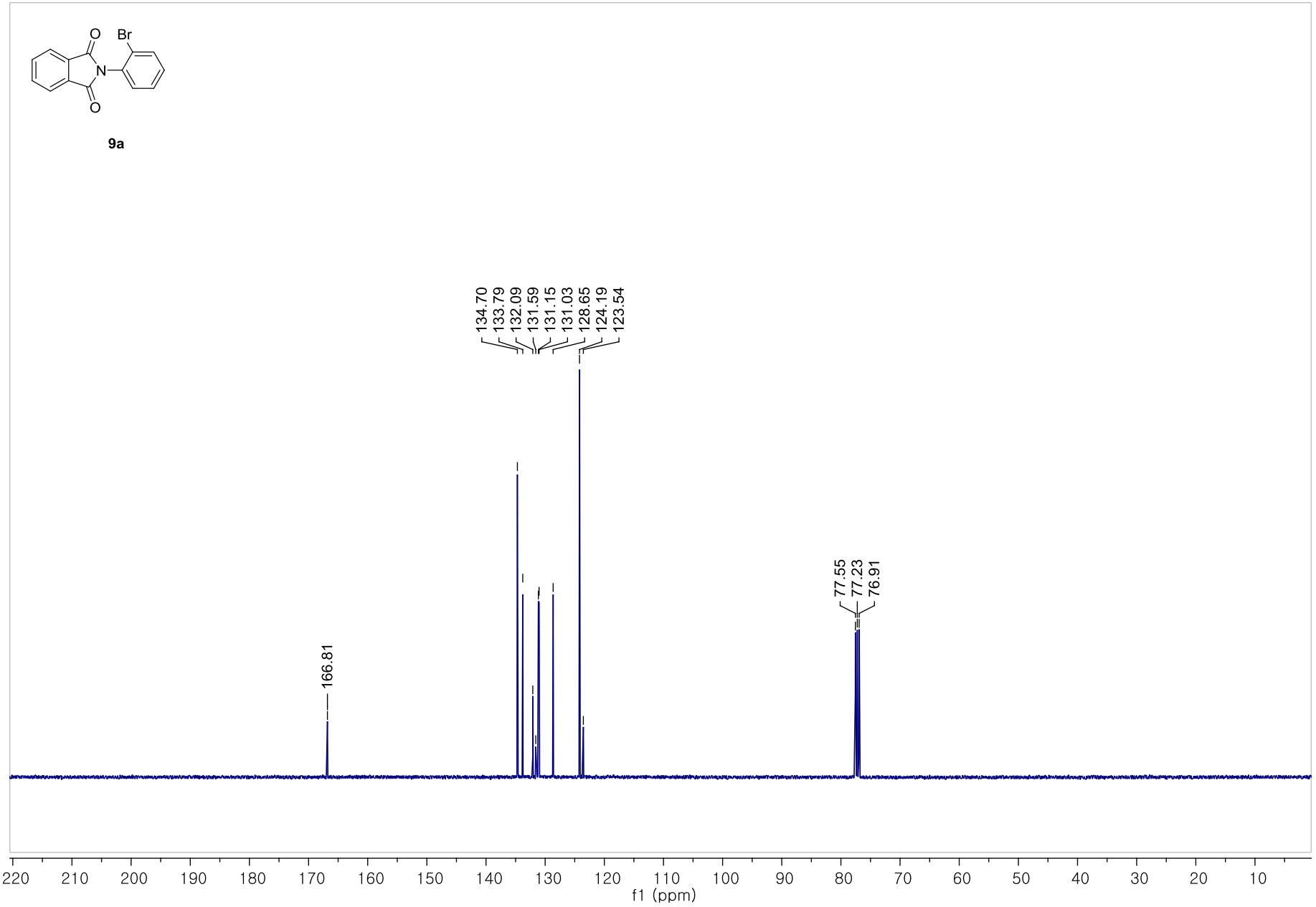

O
N
Cl
O
8c
7.97
7.97
7.96
7.95
7.82
7.81
7.81
7.80
7.50
7.49
7.48
7.47
7.47
7.43
7.43
7.42
7.41
7.40
2.00
2.10
2.07
2.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
2.00
2.10
2.07
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

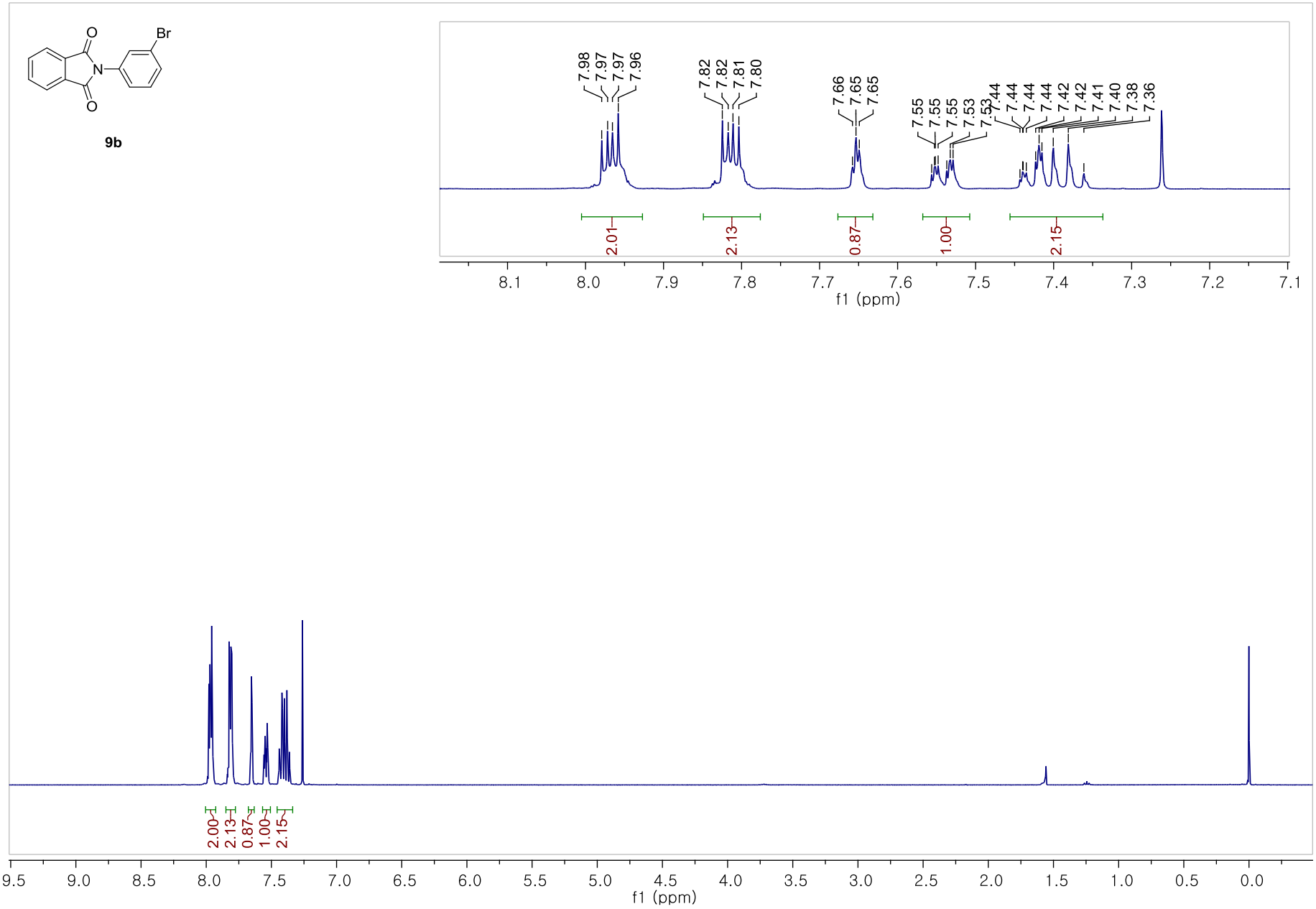

O
N
Cl
O
8c
134.78
134.02
131.82
130.40
129.53
127.88
124.08
77.55
77.23
76.91
167.20
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

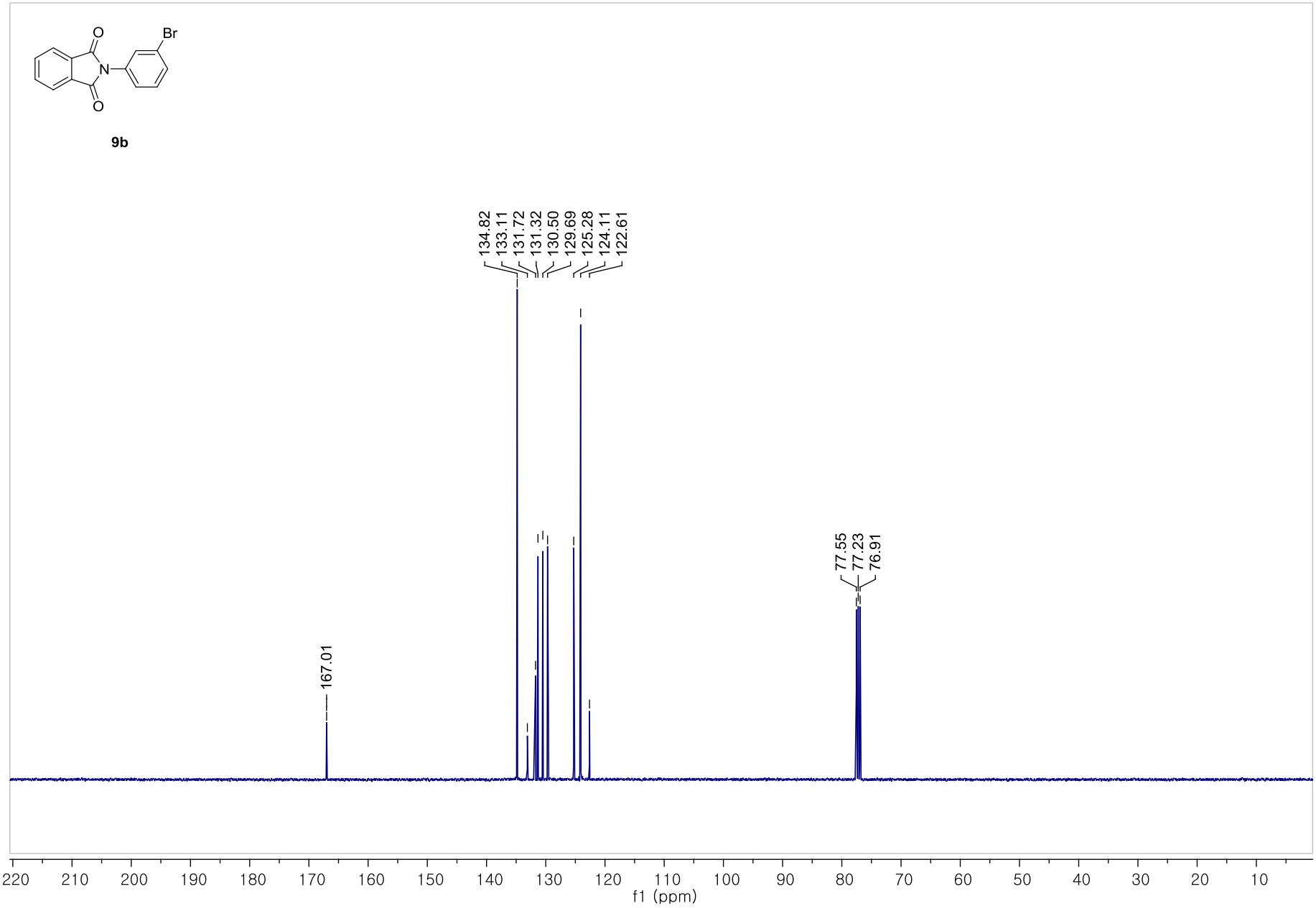

9a
9b
9c
a+b+c
a+b+c
a(1H)
b(1H)
c(2H)
b(1H)
a(1H)
b(2H)
a(2H)+c(2H)
CDCl
16.30
16.73
3.30
2.00
5.36
2.01
3.61
2.18
14.15
f1 (ppm)
16.30
16.73
3.30
2.00
5.36
2.01
3.62
2.18
14.15
f1 (ppm)

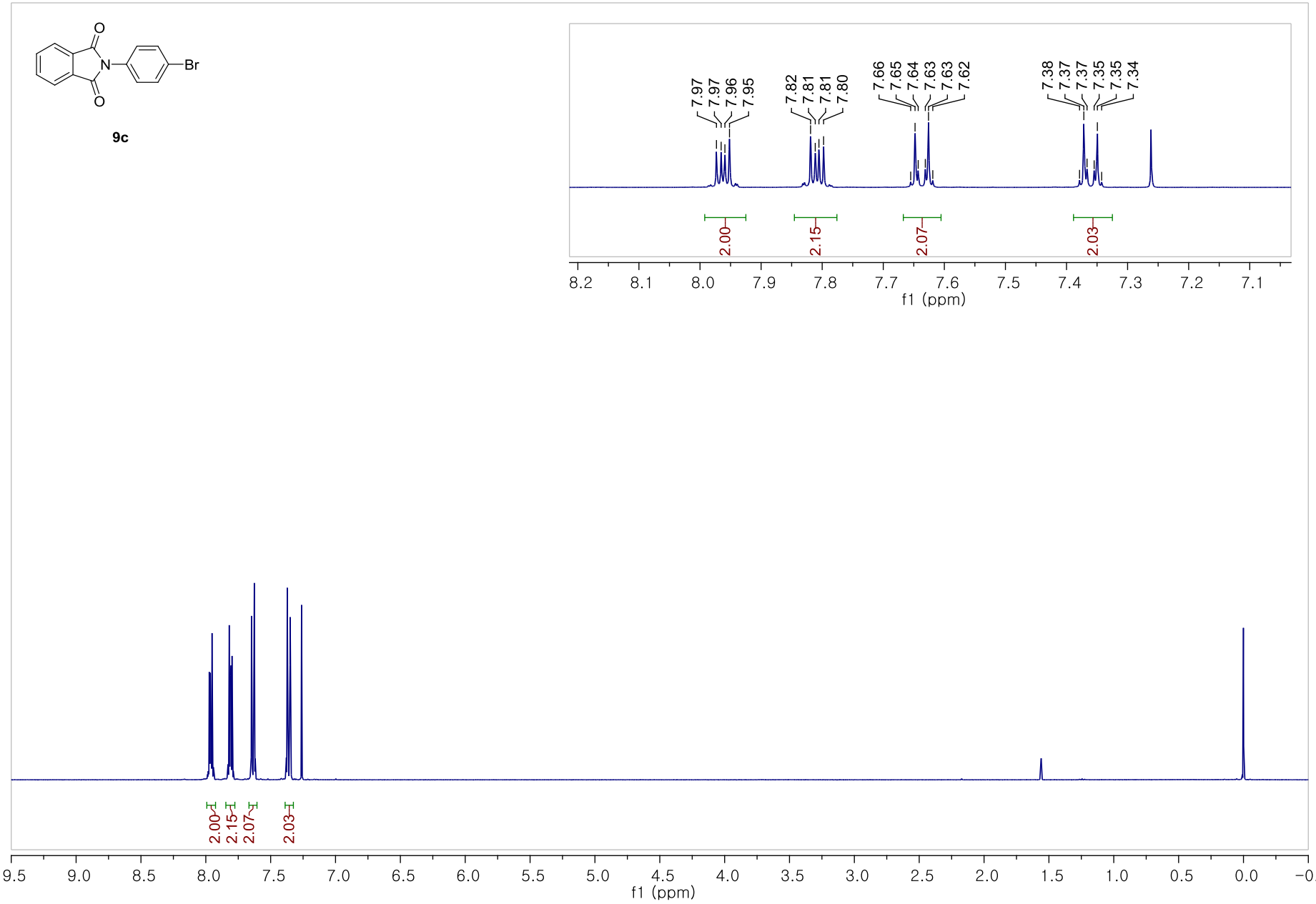

134.6
134.6
134.5
133.5
132.2
131.8
131.6
131.5
131.1
130.9
130.8
130.7
130.3
129.5
128.4
127.9
125.1
123.9
123.9
123.8
123.3
122.4
121.8
136
134
132
130
128
126
124
122
f1 (ppm)
134.80
134.76
134.67
133.74
133.09
132.45
132.05
131.75
131.69
131.56
131.28
131.11
131.00
130.91
130.48
129.66
128.62
128.12
125.26
124.15
124.08
124.03
123.51
122.58
121.97
77.55
77.23
76.91
167.07
166.98
166.77
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

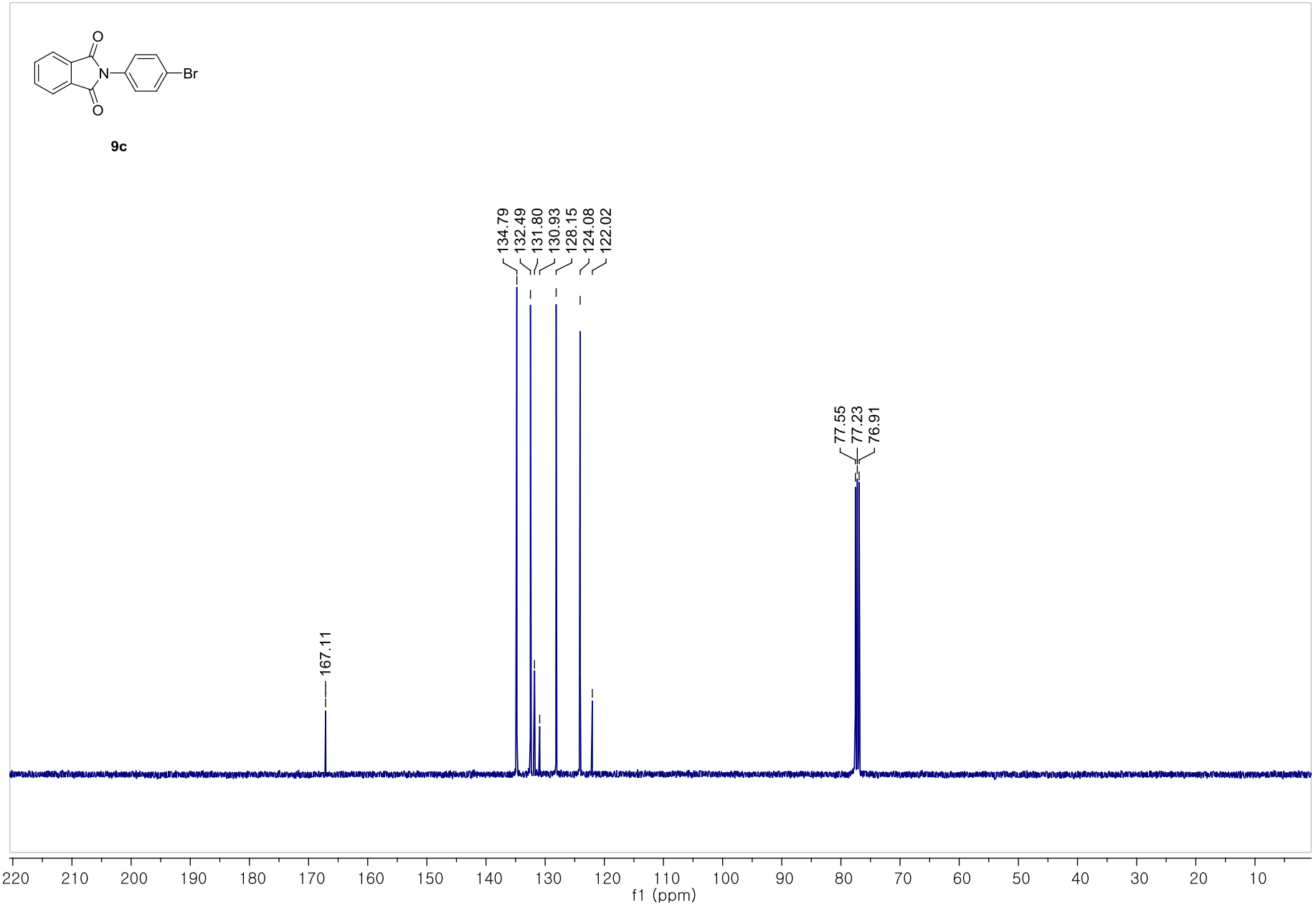

O
Br
N
O
9a
7.99
7.99
7.98
7.97
7.97
7.82
7.82
7.81
7.80
7.77
7.76
7.76
7.75
7.75
7.74
7.50
7.49
7.48
7.47
7.47
7.46
7.45
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.34
7.34
1.95
2.09
1.00
1.06
2.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
1.95
2.09
1.00
1.06
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.
f1 (ppm)

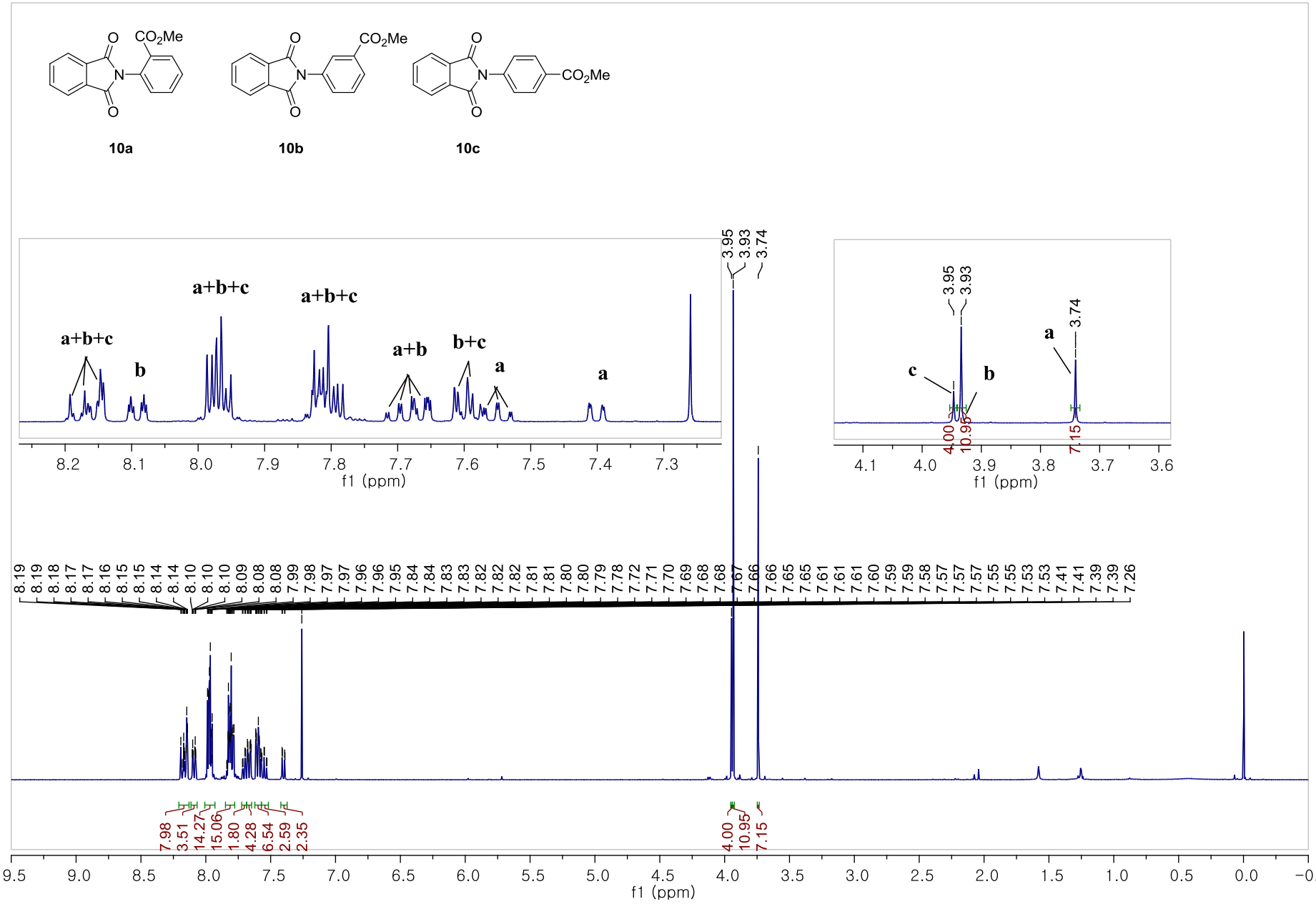

O
Br
N
O
9a
134.70
133.79
132.09
131.59
131.15
131.03
128.65
124.19
123.54
77.55
77.23
76.91
166.81
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

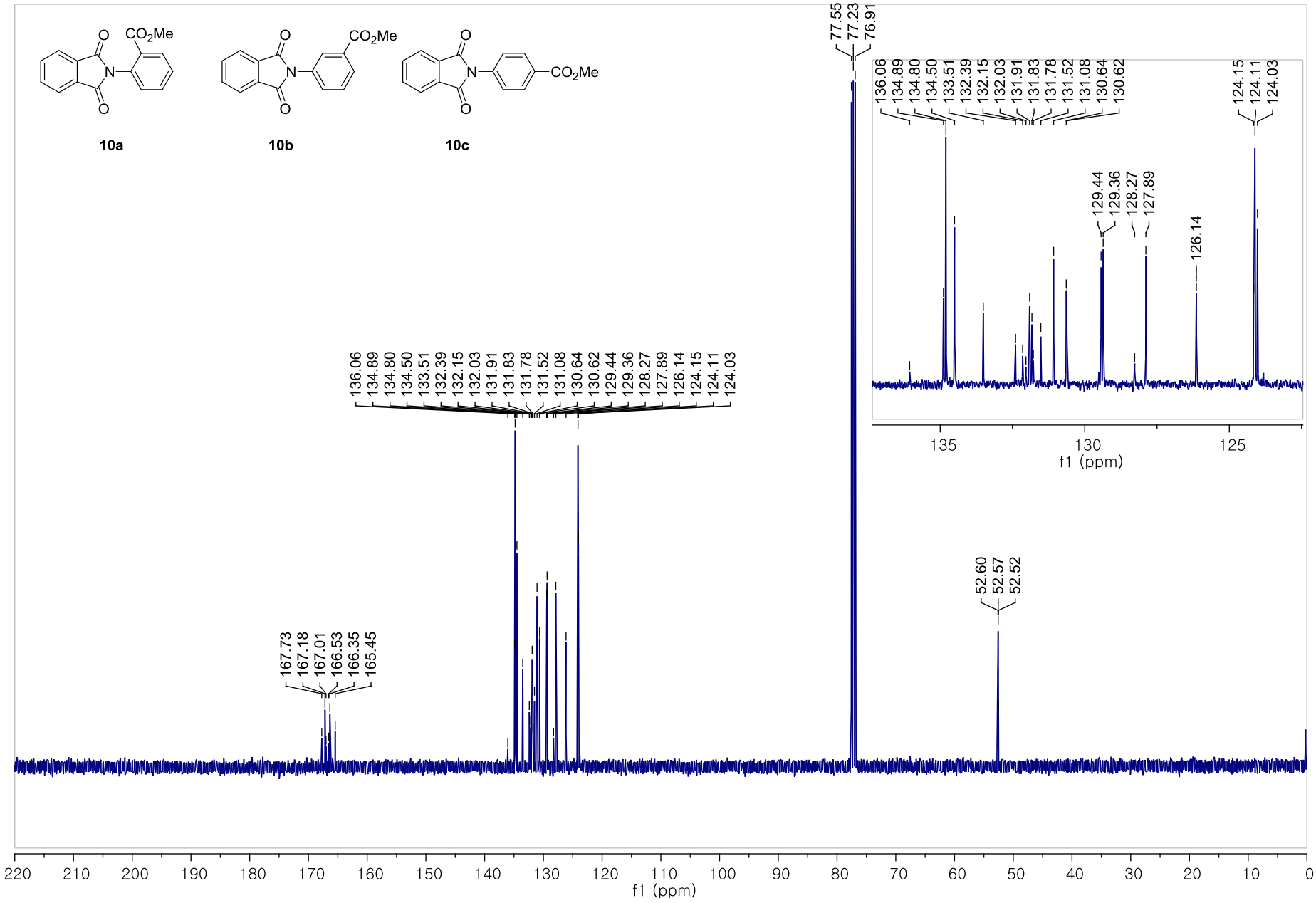

O
Br
N
O
9b
7.98
7.97
7.97
7.96
7.82
7.82
7.81
7.80
7.66
7.65
7.65
7.55
7.55
7.55
7.53
7.53
7.44
7.44
7.44
7.44
7.42
7.42
7.41
7.40
7.38
7.36
2.01
2.13
0.87
1.00
2.15
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.00
2.13
0.87
1.00
2.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

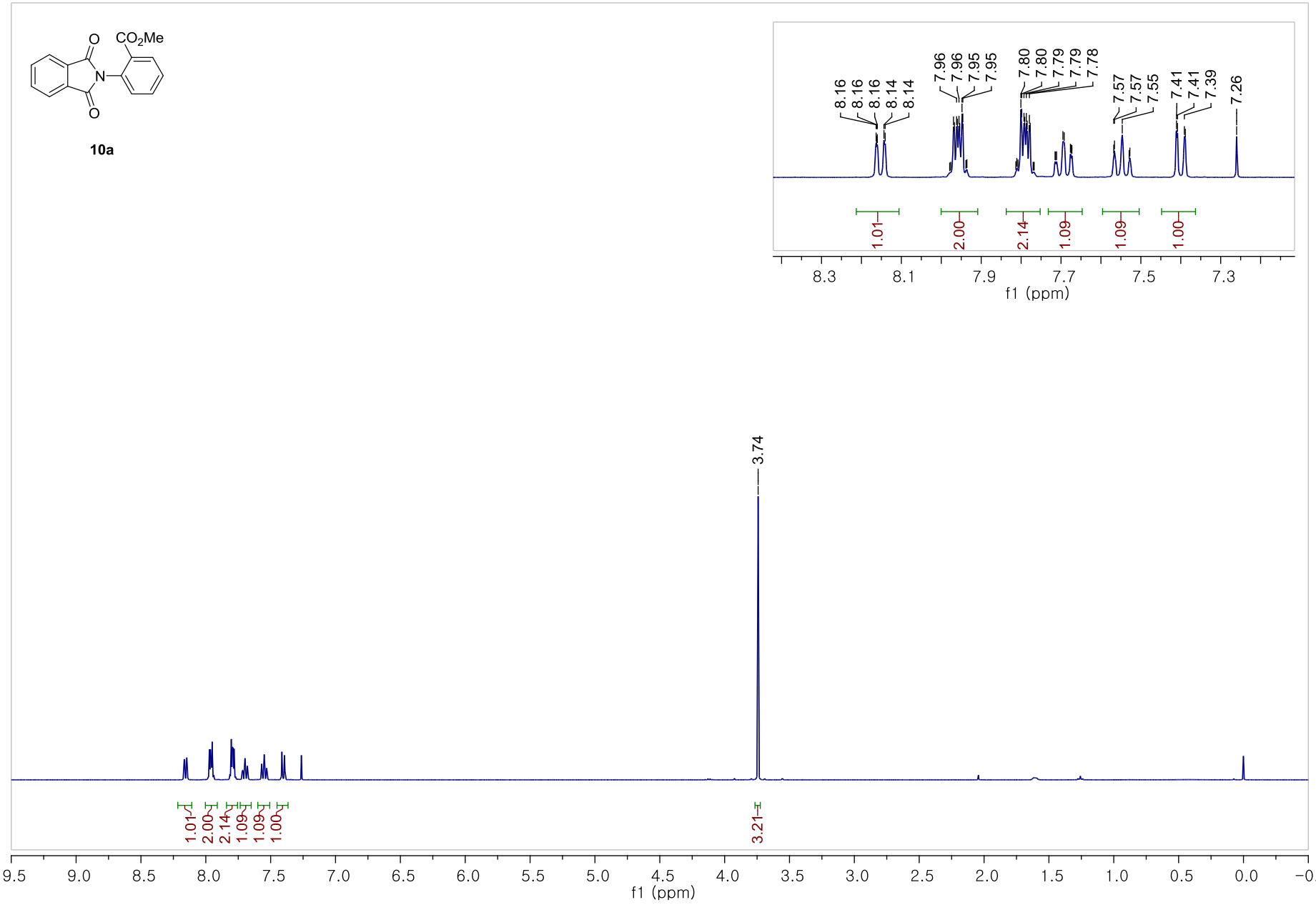

O
Br
N
O
9b
134.82
133.11
131.72
131.32
130.50
129.69
125.28
124.11
122.61
77.55
77.23
76.91
167.01
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

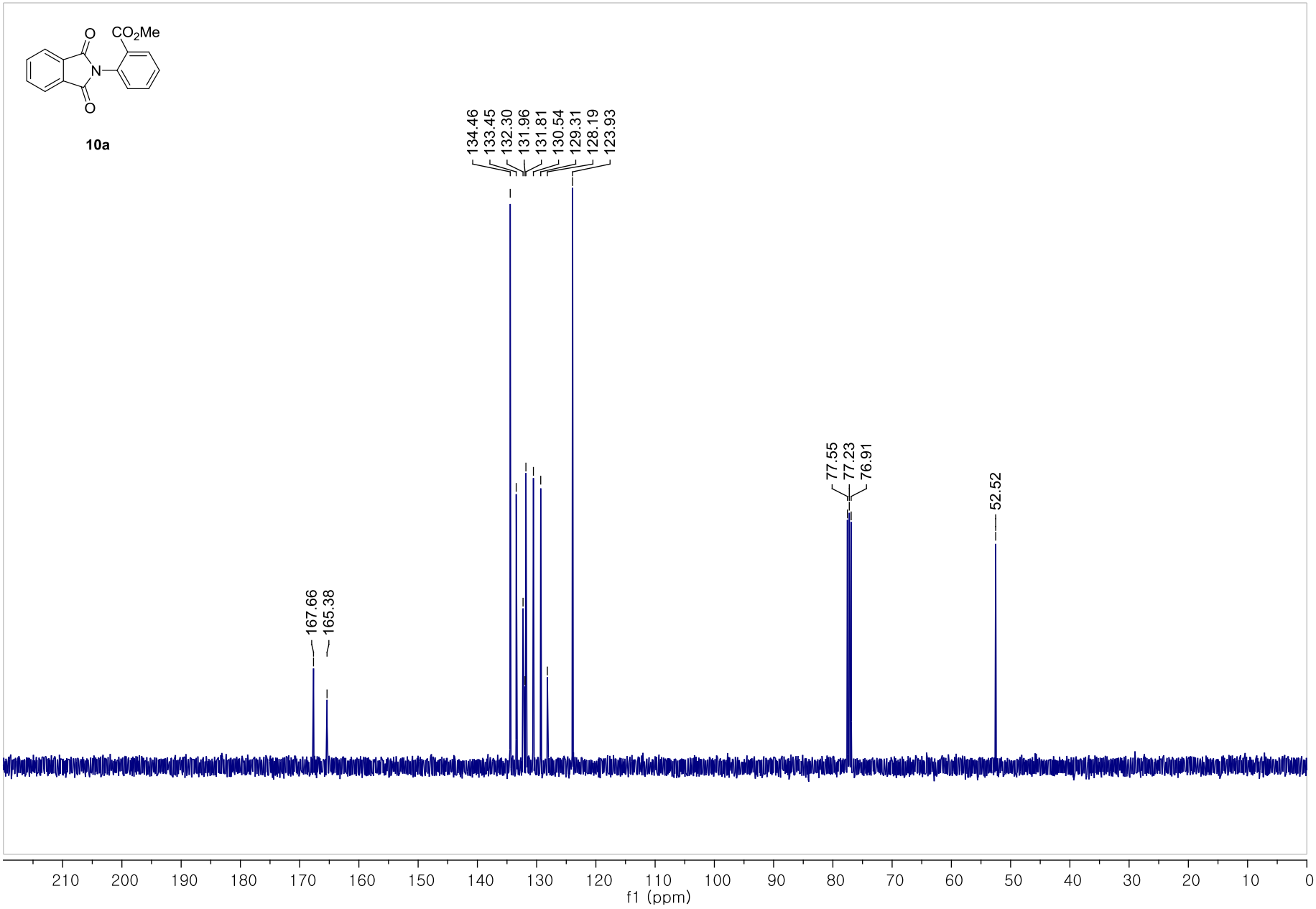

O
N
Br
O
9c
7.97
7.97
7.96
7.95
7.82
7.81
7.81
7.80
7.66
7.65
7.64
7.63
7.63
7.62
7.38
7.37
7.37
7.35
7.35
7.34
2.00
2.15
2.07
2.03
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.00
2.15
2.07
2.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

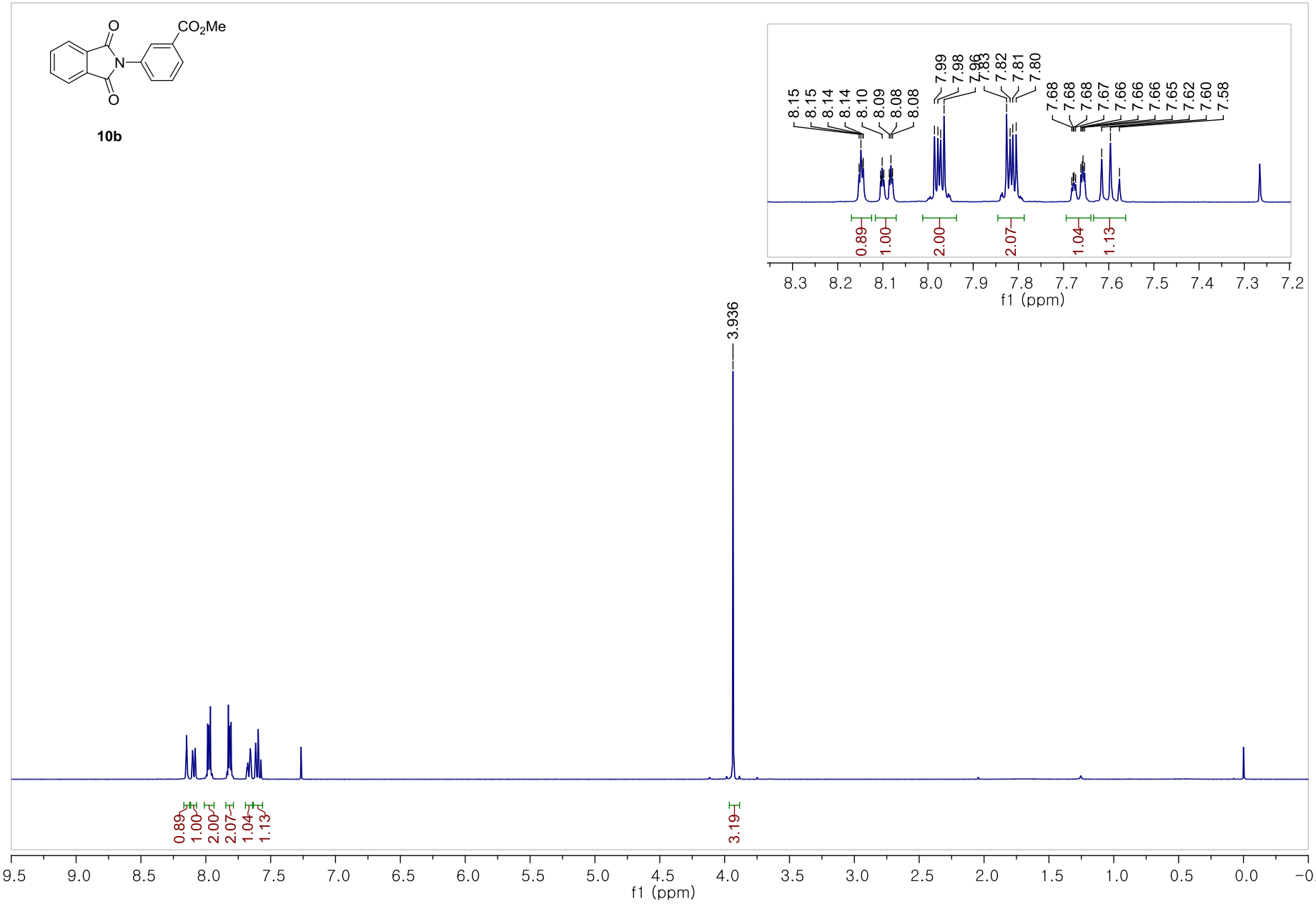

O
N
Br
O
9c
134.79
132.49
131.80
130.93
128.15
124.08
122.02
77.55
77.23
76.91
167.11
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

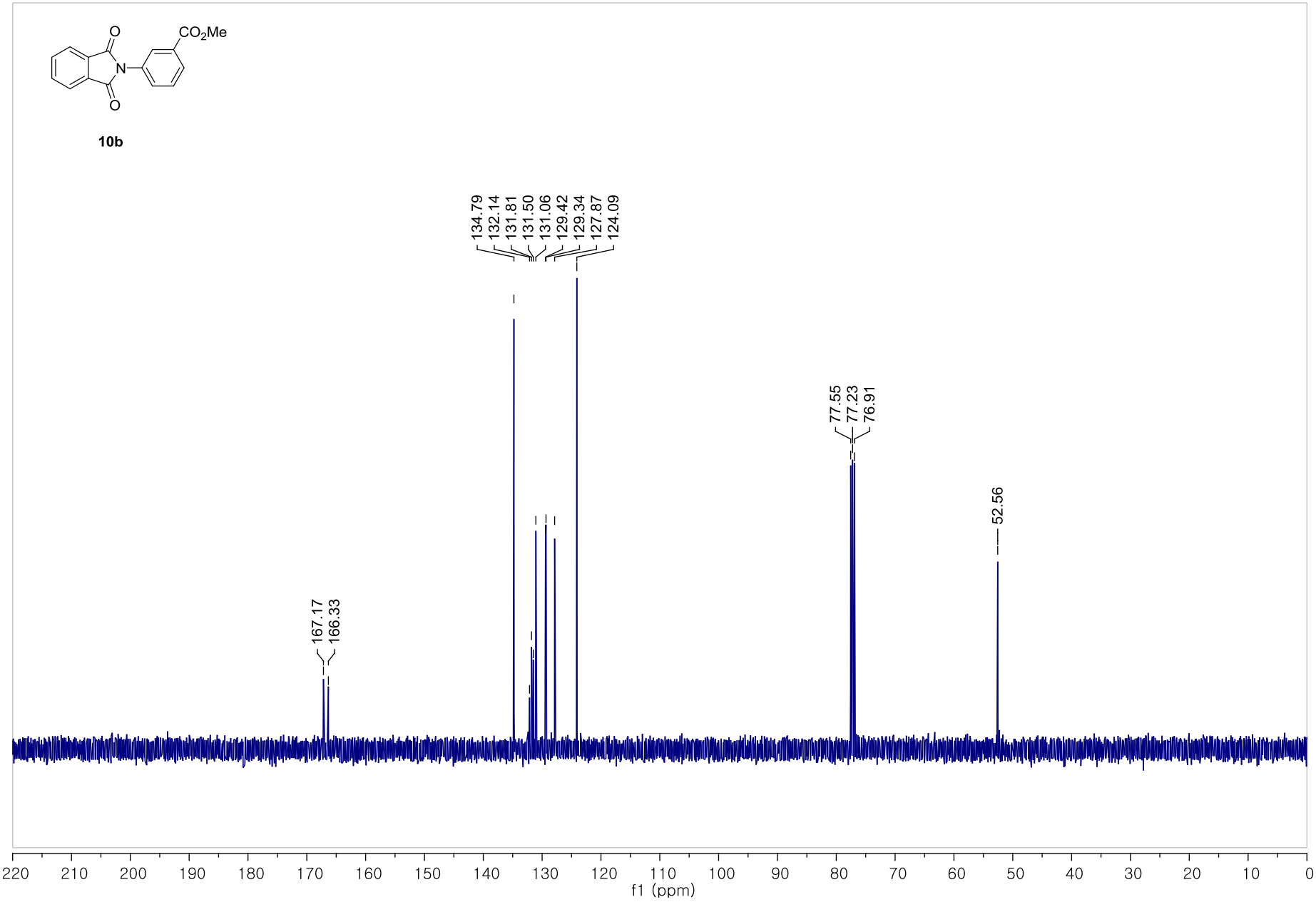

10a
10b
10c
a+b+c
a+b+c
a+b+c
a+b
b+c
a
b
a
c
b
a
3.95
3.93
3.74
4.00
10.95
7.15
f1 (ppm)
7.98
3.51
14.27
15.06
1.80
4.28
6.54
2.59
2.35
4.00
10.95
7.15

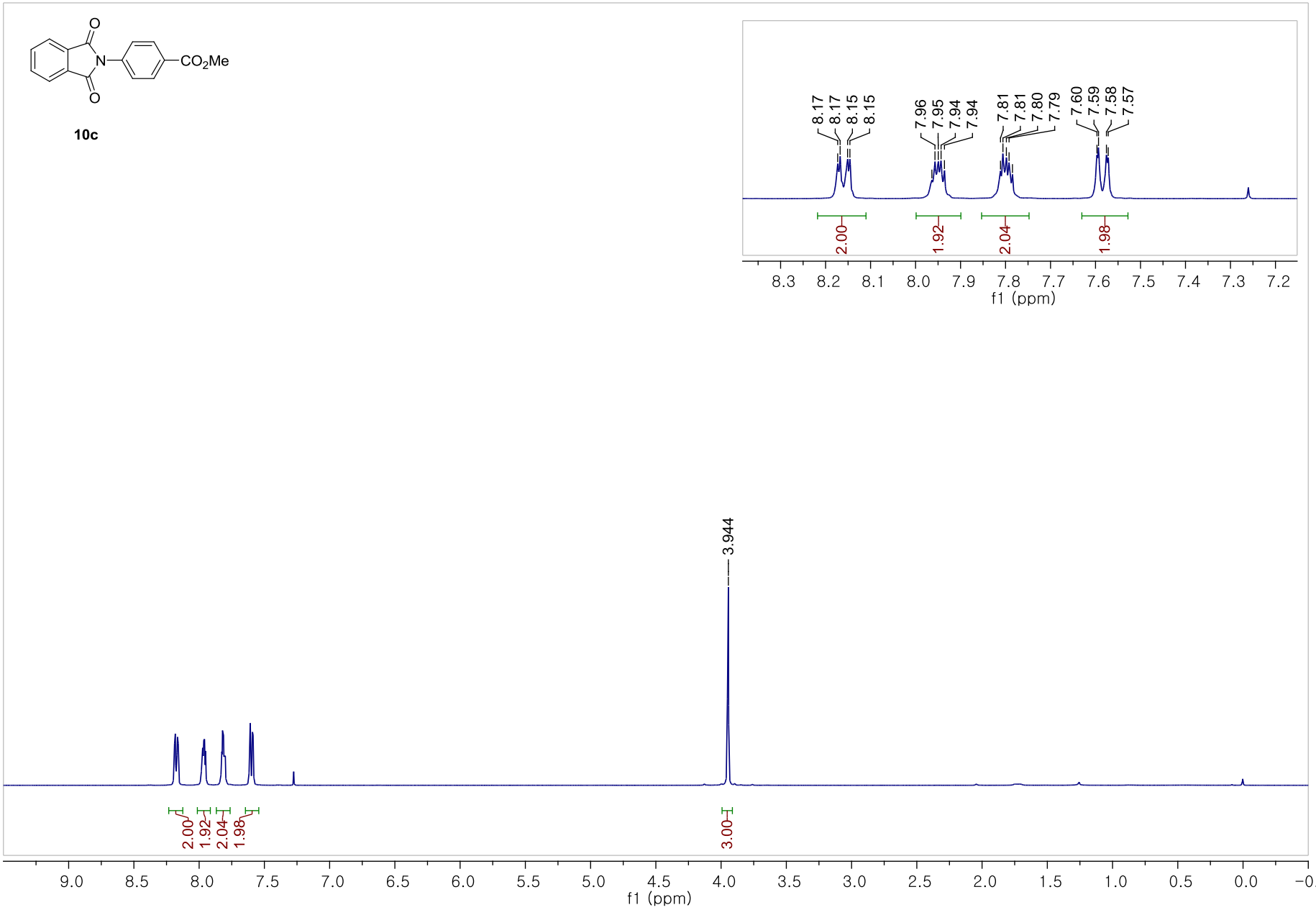

10a
10b
10c
77.55
77.23
76.91
136.06
134.89
134.80
134.50
133.51
132.39
132.15
132.03
131.91
131.83
131.78
131.52
131.08
130.64
130.62
129.44
129.36
128.27
127.89
126.14
124.15
124.11
124.03
52.60
52.57
52.52
167.73
167.18
167.01
166.53
166.35
165.45
f1 (ppm)

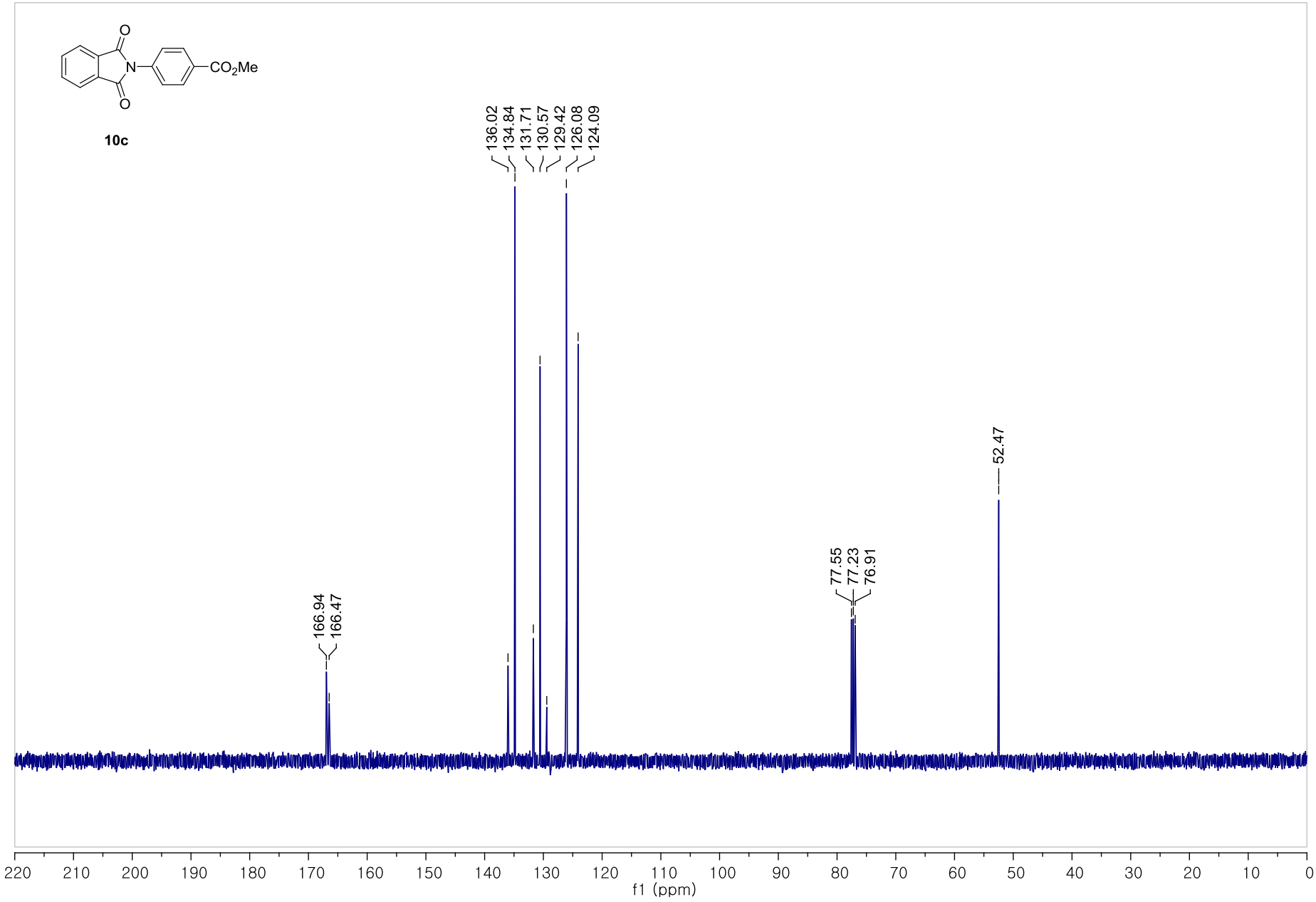

O
CO2Me
N
O
10a
8.16
8.16
8.16
8.14
8.14
7.96
7.96
7.95
7.95
7.80
7.80
7.79
7.79
7.78
7.57
7.57
7.55
7.41
7.41
7.39
7.26
1.01
2.00
2.14
1.09
1.09
1.00
8.3
8.1
7.9
7.7
7.5
7.3
f1 (ppm)
3.74
1.01
2.00
2.14
1.09
1.09
1.00
3.21
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

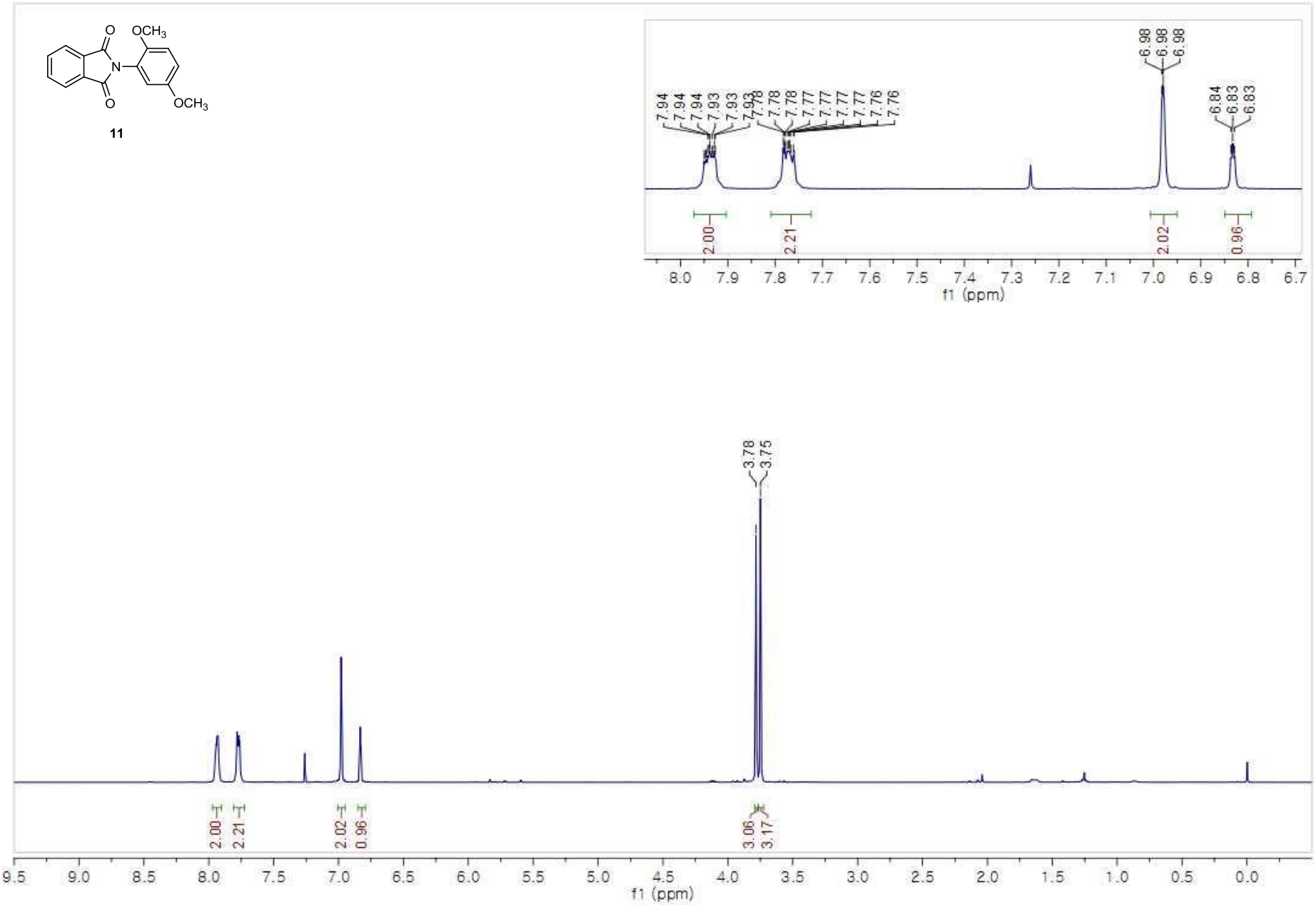

O
CO2Me
N
O
10a
134.46
133.45
132.30
131.96
131.81
130.54
129.31
128.19
123.93
77.55
77.23
76.91
52.52
167.66
165.38
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

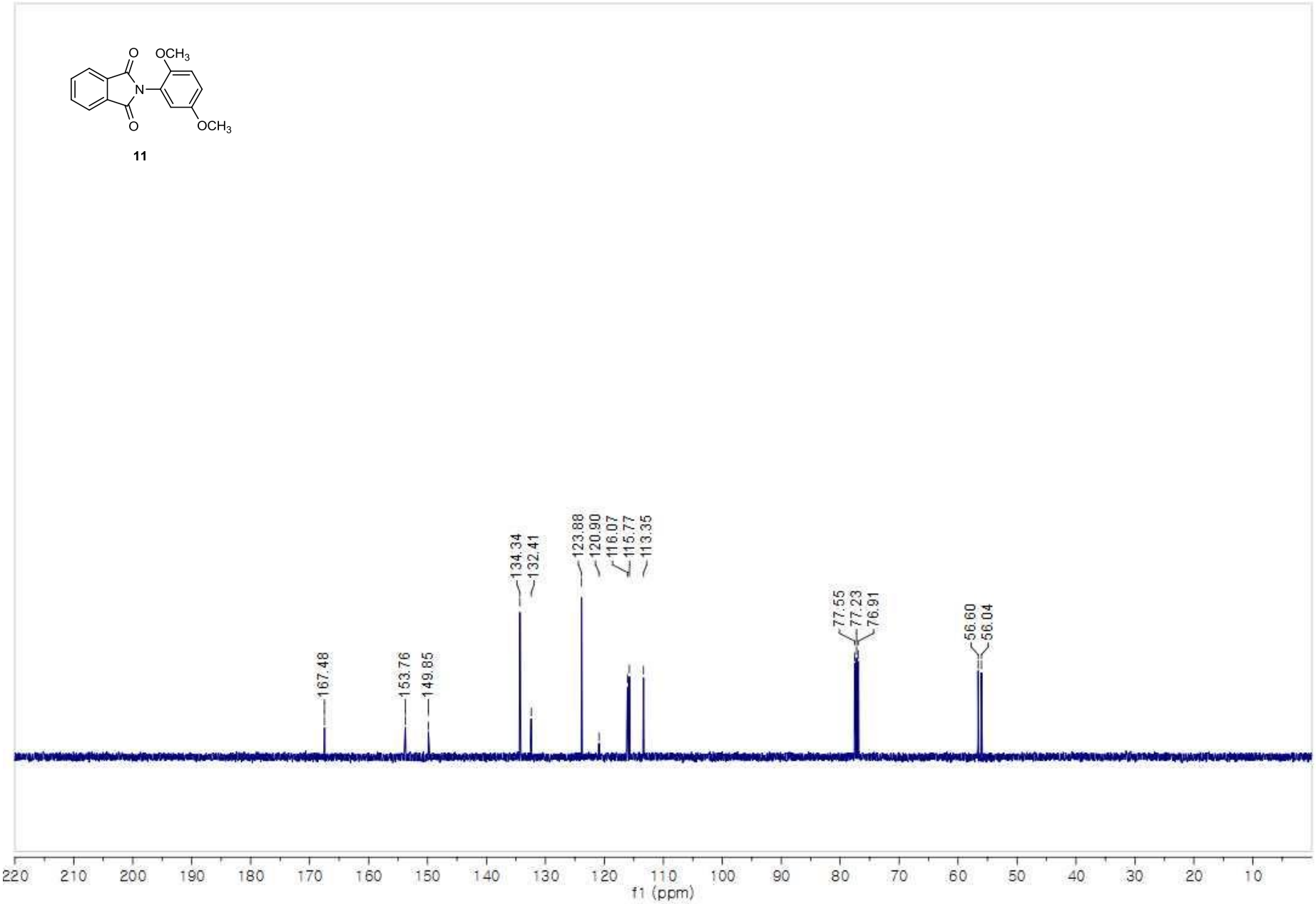

CO2Me
O
N
O
10b
8.15
8.15
8.14
8.14
8.10
8.09
8.08
8.08
7.99
7.98
7.96
7.83
7.82
7.81
7.80
7.68
7.68
7.68
7.67
7.66
7.66
7.66
7.65
7.62
7.60
7.58
0.89
1.00
2.00
2.07
1.04
1.13
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
3.936
3.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

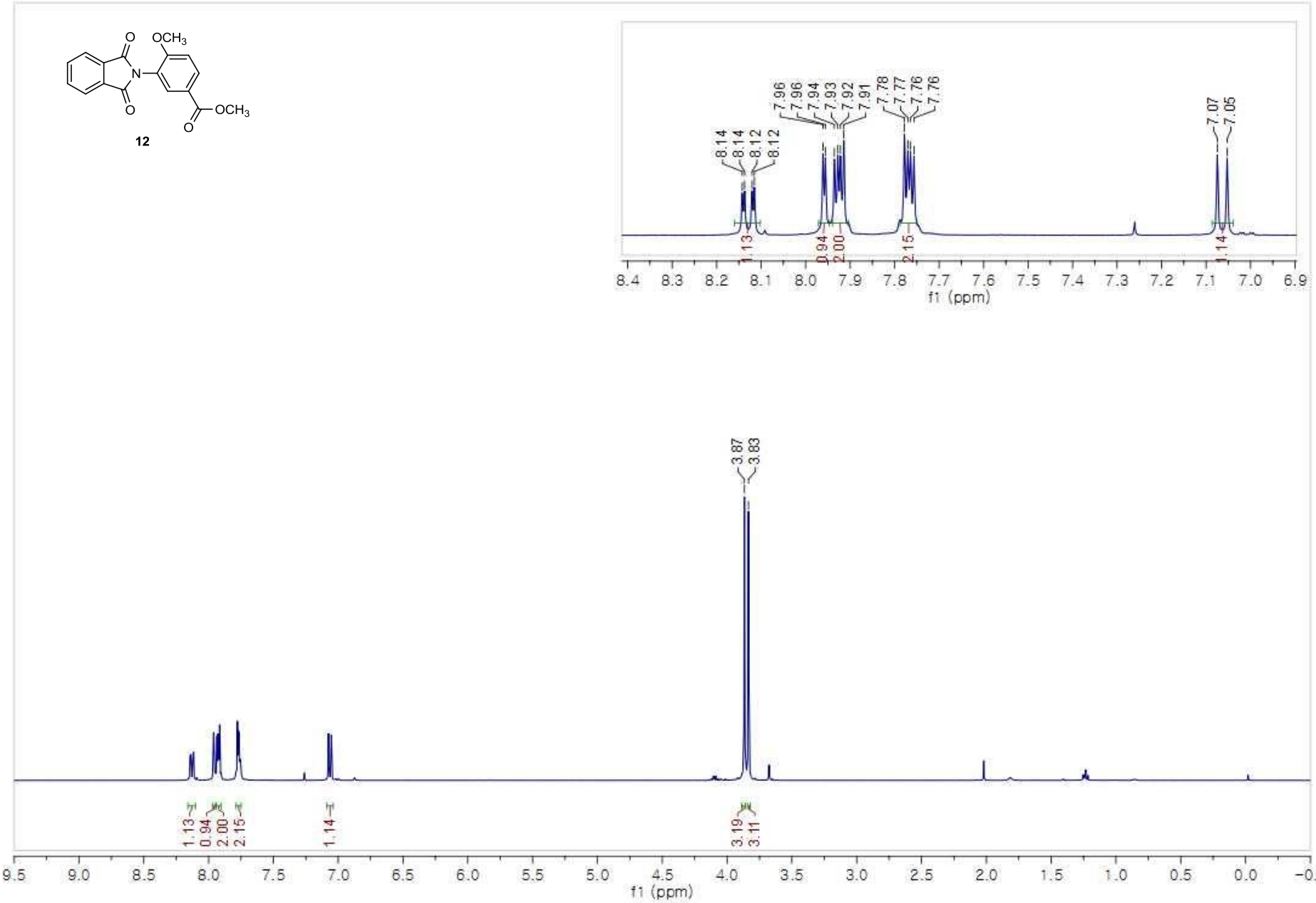

O
CO2Me
N
O
10b
134.79
132.14
131.81
131.50
131.06
129.42
129.34
127.87
124.09
77.55
77.23
76.91
52.56
167.17
166.33
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

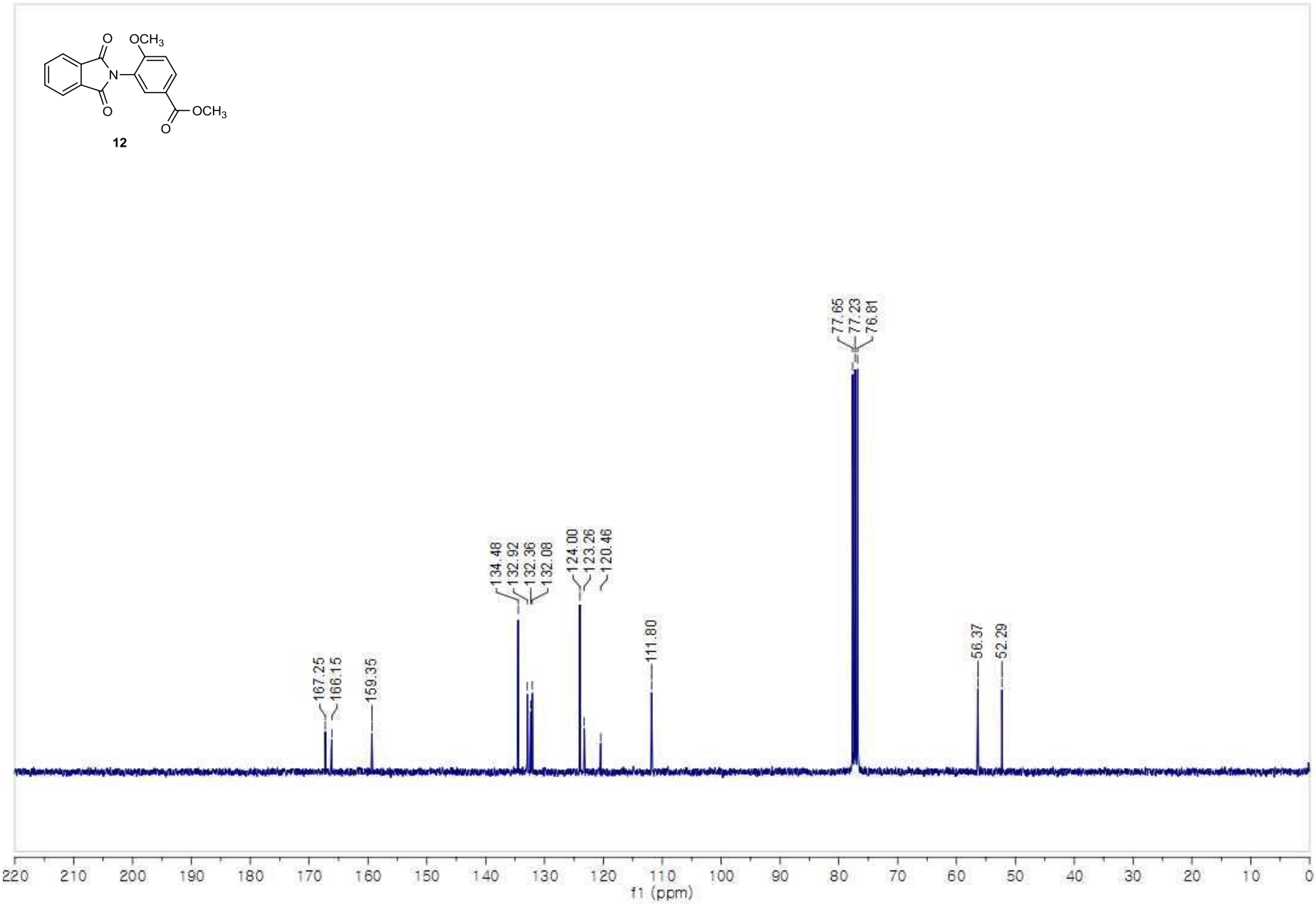

O
N
O
CO2Me
10c
8.17
8.17
8.15
8.15
7.96
7.95
7.94
7.94
7.81
7.81
7.80
7.79
7.60
7.59
7.58
7.57
2.00
1.92
2.04
1.98
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
3.944
2.00
1.92
2.04
1.98
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

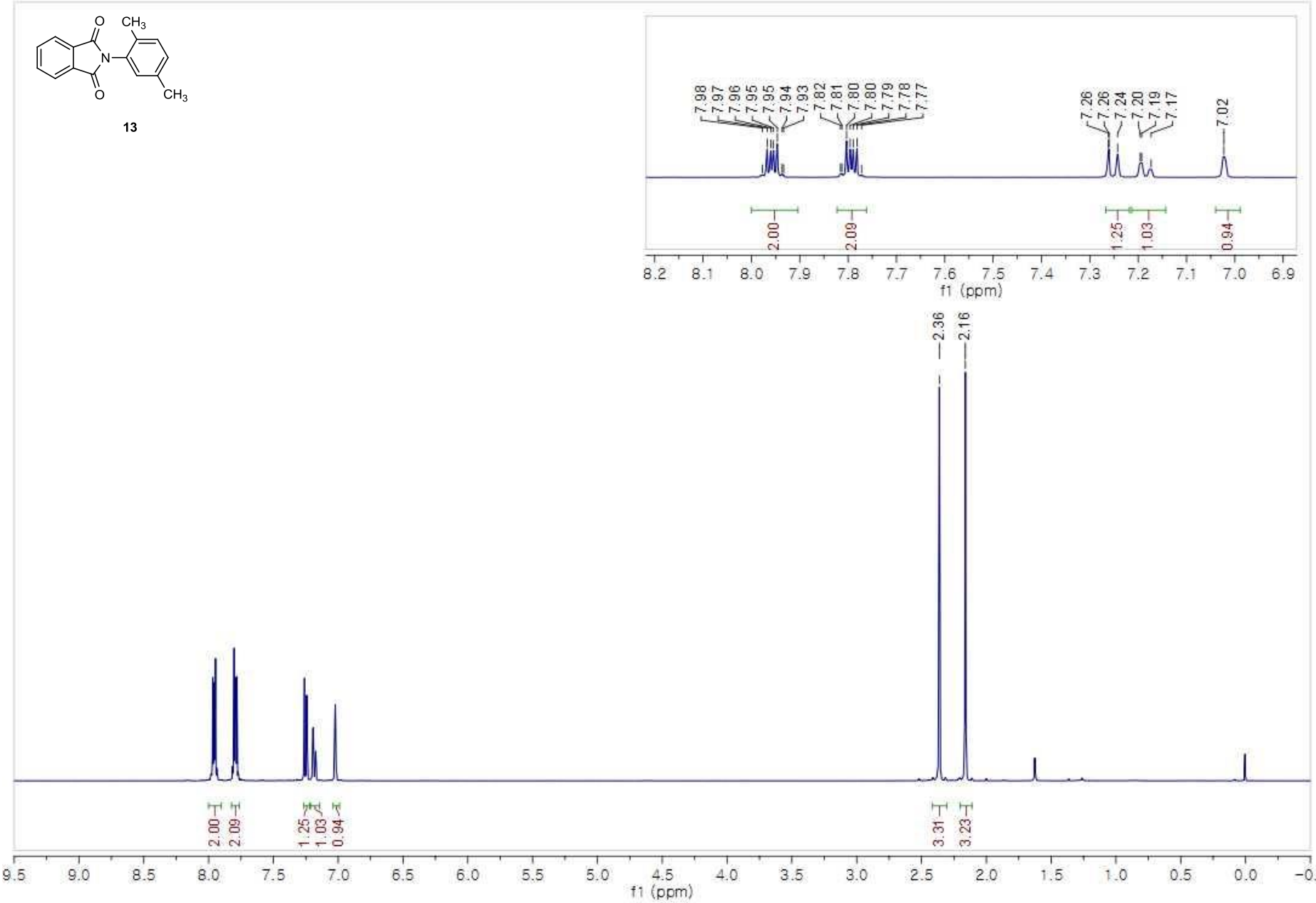

O
N
O
CO2Me
10c
136.02
134.84
131.71
130.57
129.42
126.08
124.09
166.94
166.47
77.55
77.23
76.91
52.47
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

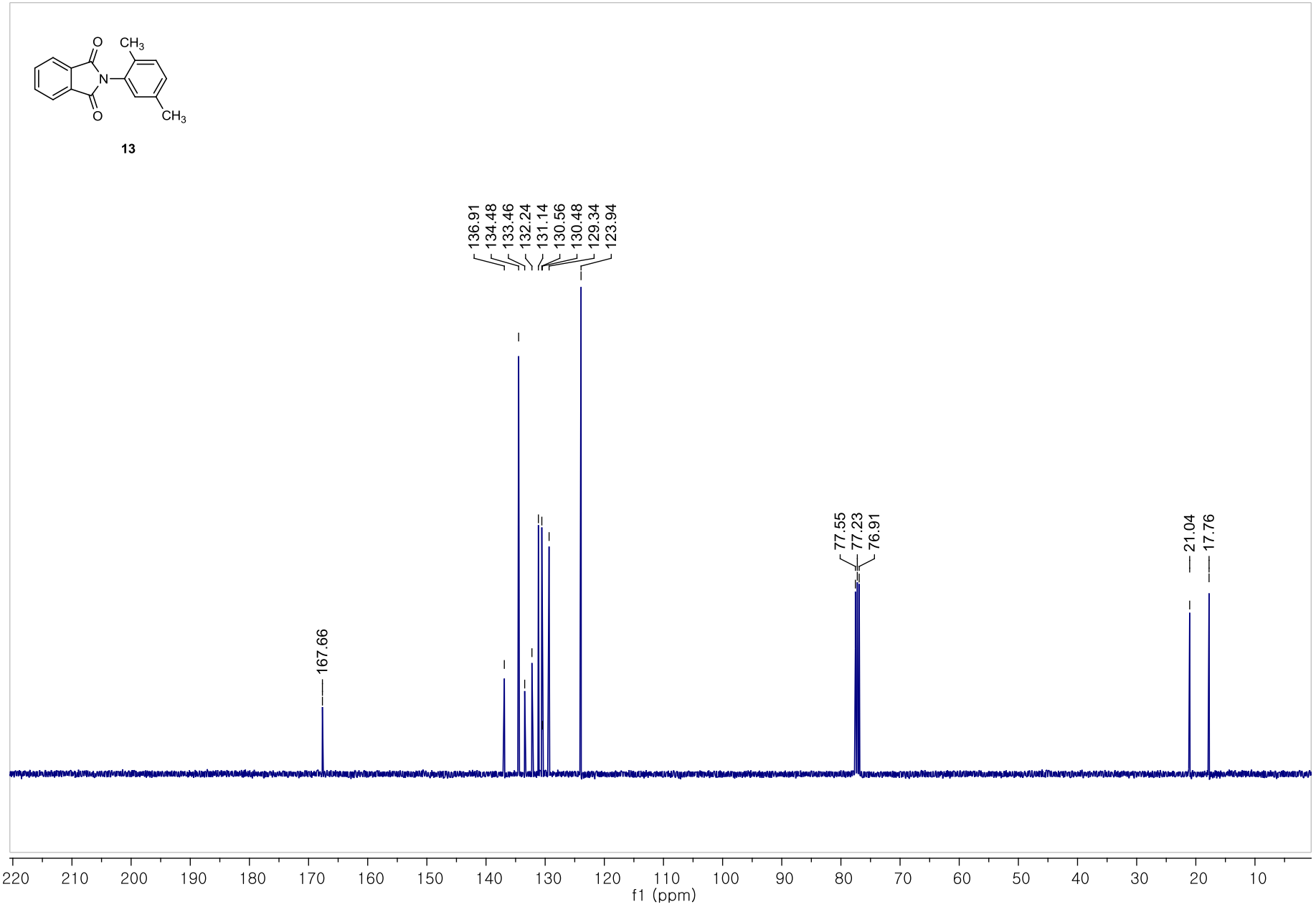

OCH3
OCH3
11
7.94
7.94
7.94
7.93
7.93
7.93
7.78
7.78
7.78
7.77
7.77
7.77
7.77
7.76
7.76
6.98
6.98
6.98
6.84
6.83
6.83
2.00
2.21
2.02
0.96
f1 (ppm)
3.78
3.75
2.00
2.21
2.02
0.96
3.06
3.17
f1 (ppm)

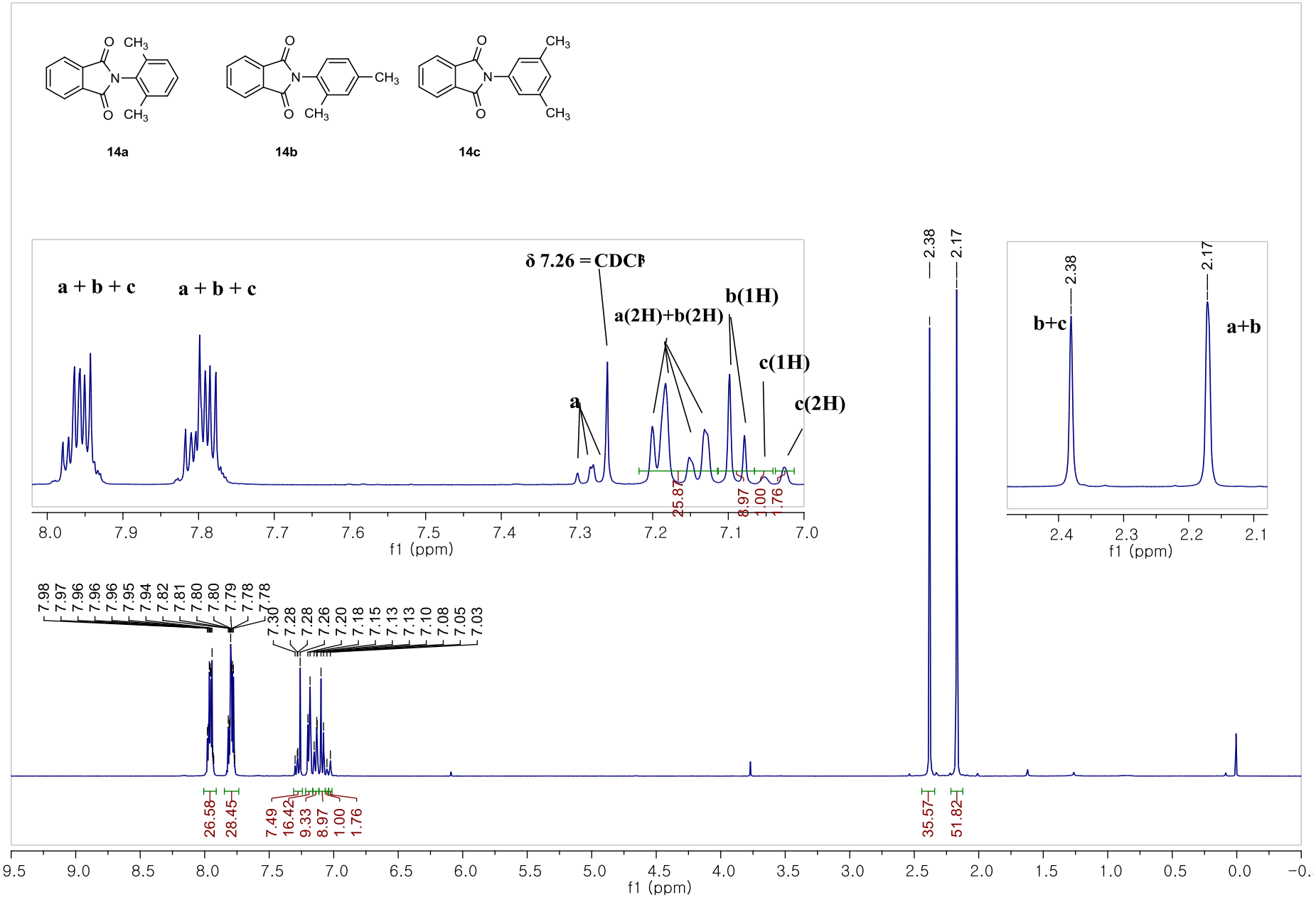

O
OCH3
N
O
OCH3
11
167.48
153.76
149.85
134.34
132.41
123.88
120.90
116.07
115.77
113.35
77.55
77.23
76.91
56.60
56.04
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

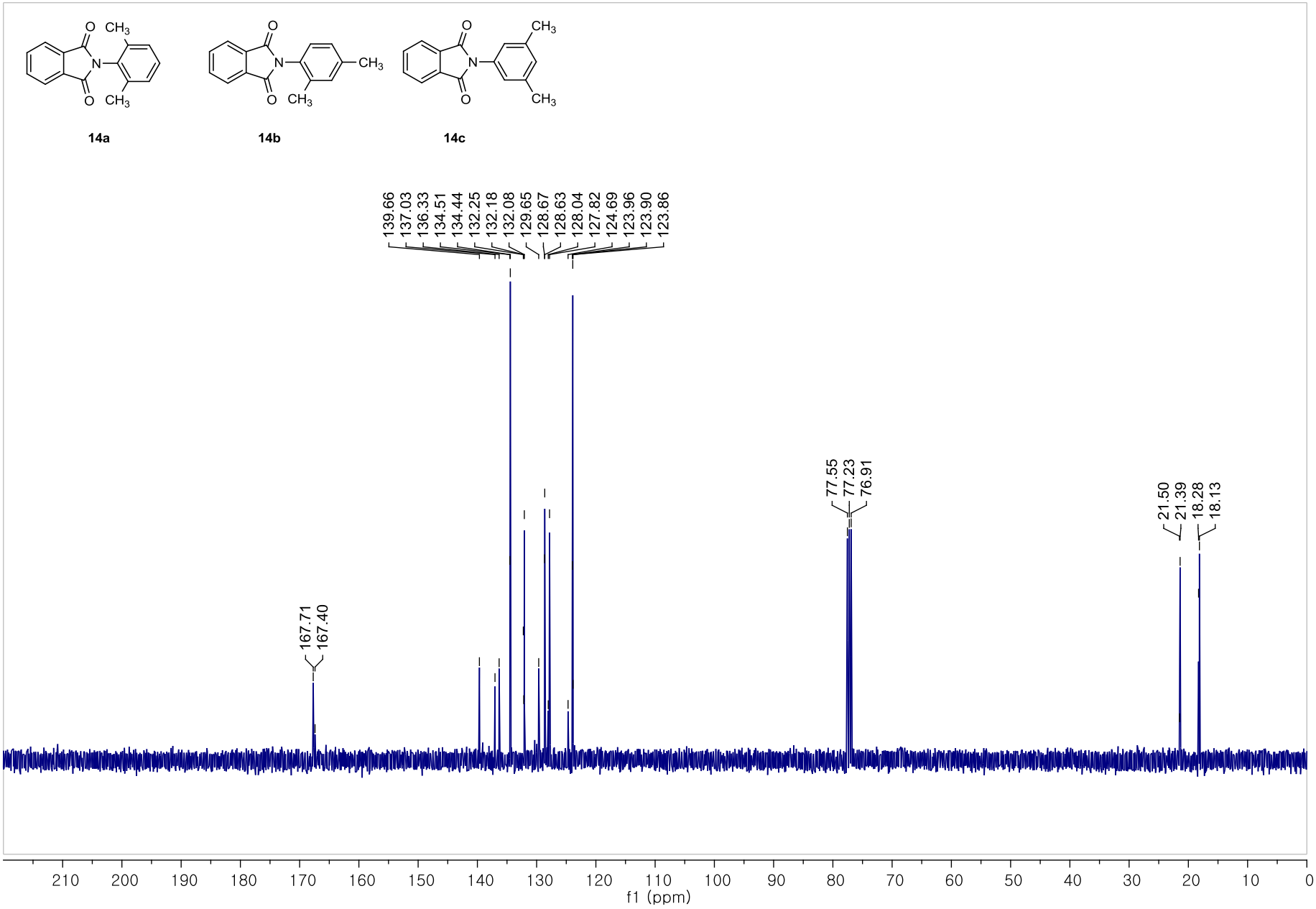

OCH3
O
N
O
OCH3
O
12
8.14
8.14
8.12
8.12
7.96
7.96
7.94
7.93
7.92
7.91
7.78
7.77
7.76
7.76
7.07
7.05
1.13
0.94
2.00
2.15
1.14
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
3.87
3.83
1.13
0.94
2.00
2.15
1.14
3.19
3.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

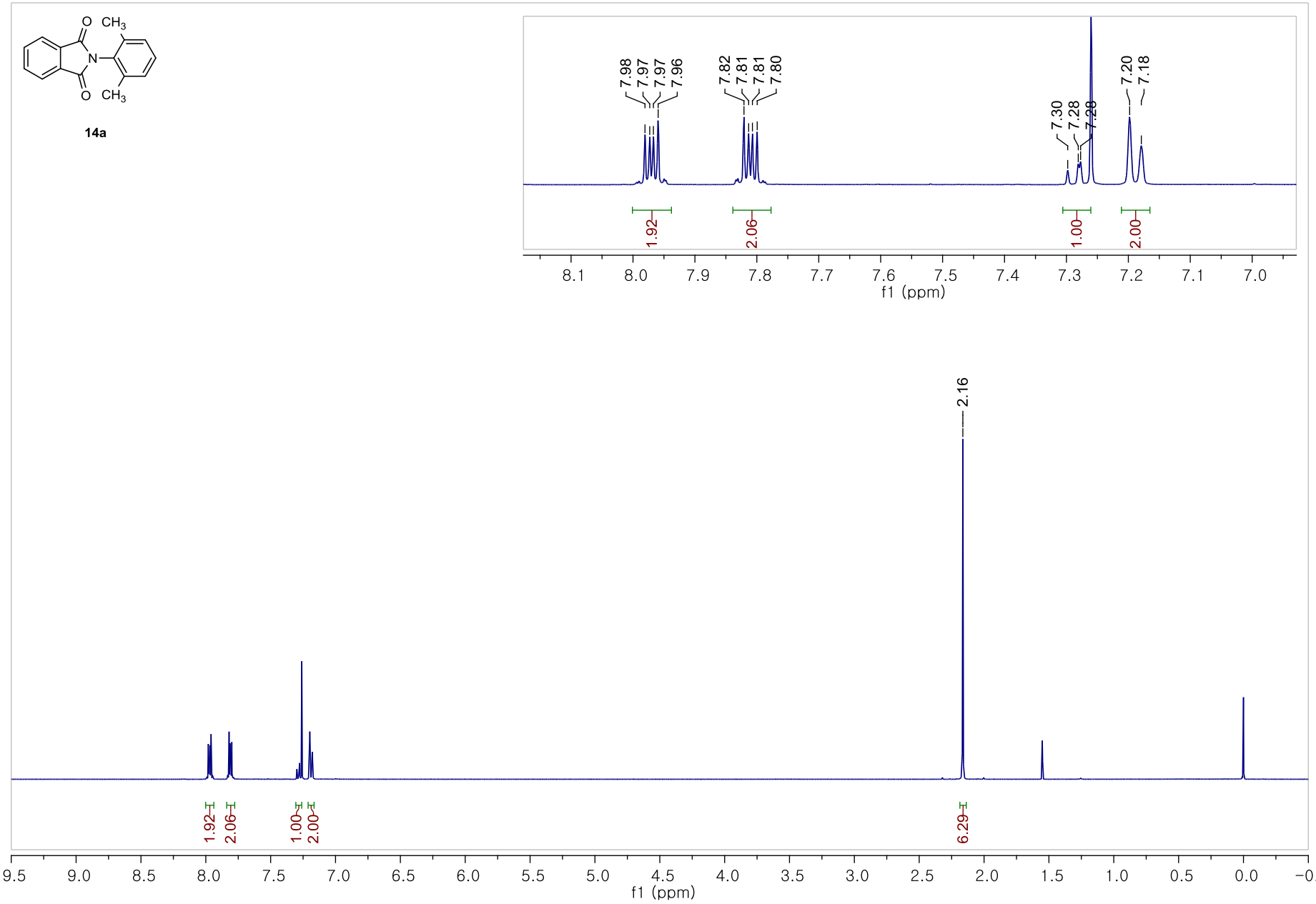

O
OCH3
N
O
O
OCH3
O
12
167.25
166.15
159.35
134.48
132.92
132.36
132.08
124.00
123.26
120.46
111.80
77.65
77.23
76.81
56.37
52.29
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

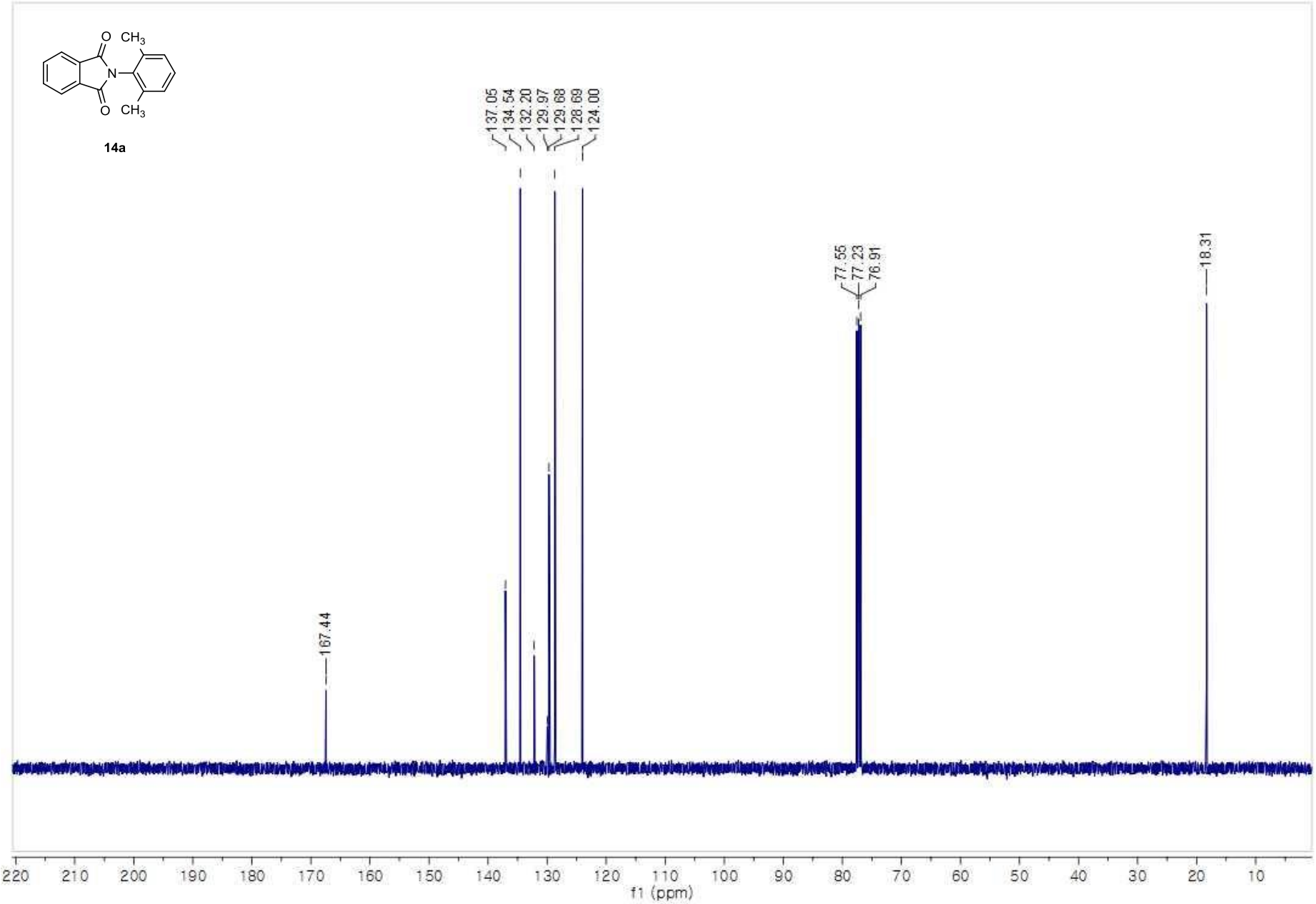

O
CH3
N
O
CH3
13
7.98
7.97
7.96
7.95
7.95
7.94
7.93
7.82
7.81
7.80
7.80
7.79
7.78
7.77
7.26
7.26
7.24
7.20
7.19
7.17
7.02
2.00
2.09
1.25
1.03
0.94
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
2.36
2.16
2.00
2.09
1.25
1.03
0.94
3.31
3.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

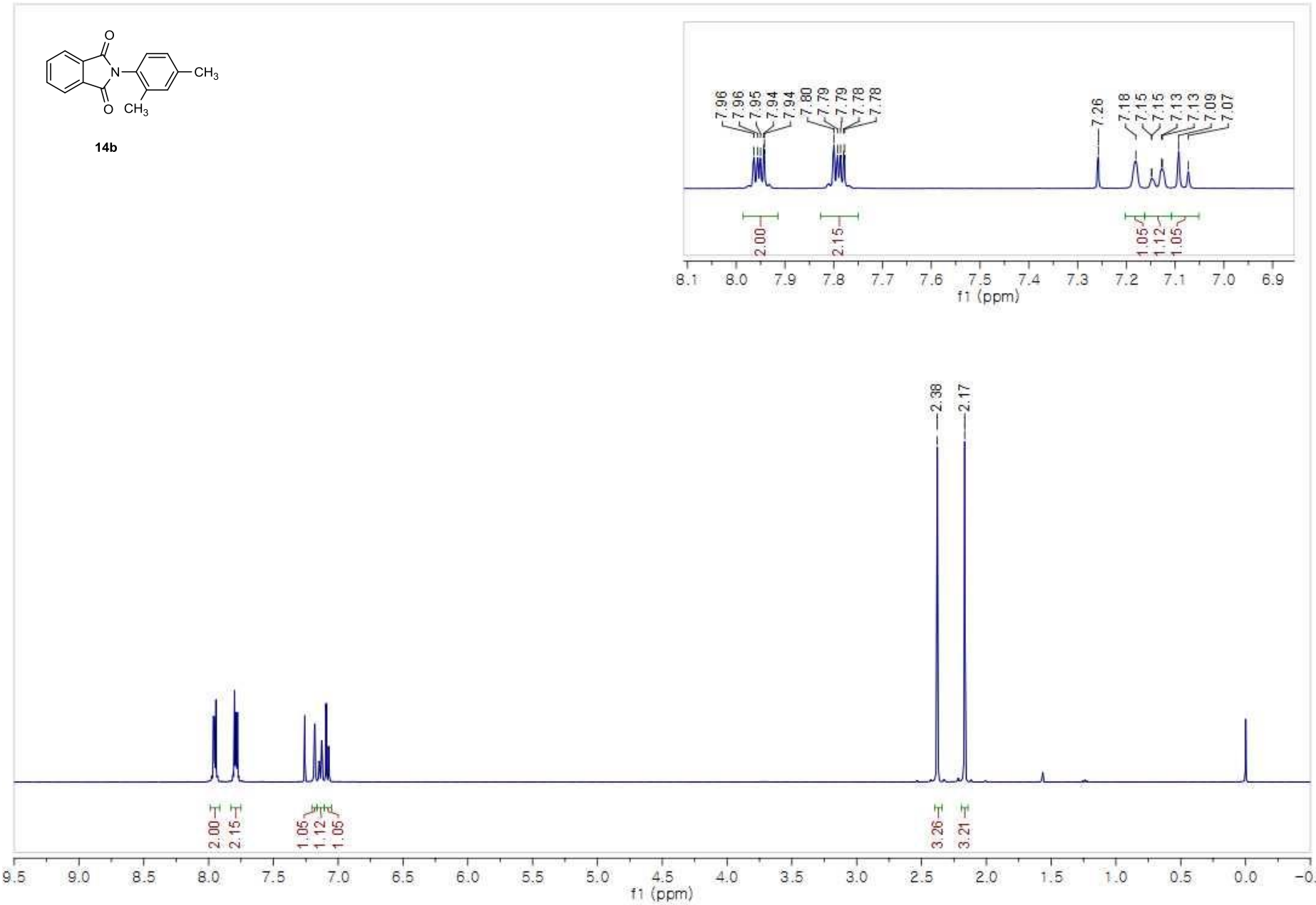

O
CH3
N
O
CH3
13
136.91
134.48
133.46
132.24
131.14
130.56
130.48
129.34
123.94
167.66
77.55
77.23
76.91
21.04
17.76
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

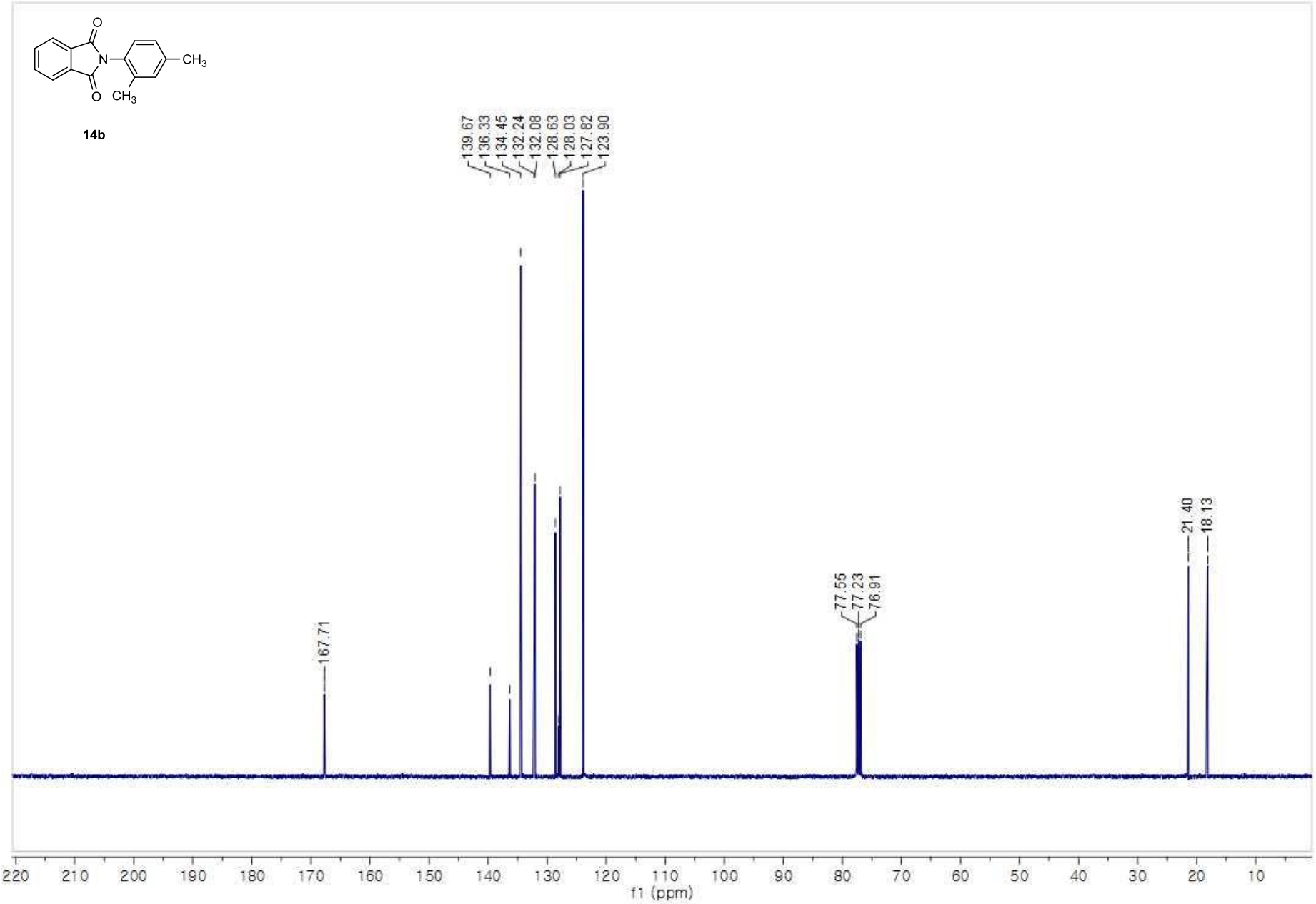

14a
14b
14c
a + b + c
a + b + c
δ 7.26 = CDCl3
a
a(2H)+b(2H)
b(1H)
c(1H)
c(2H)
b+c
a+b
f1 (ppm)

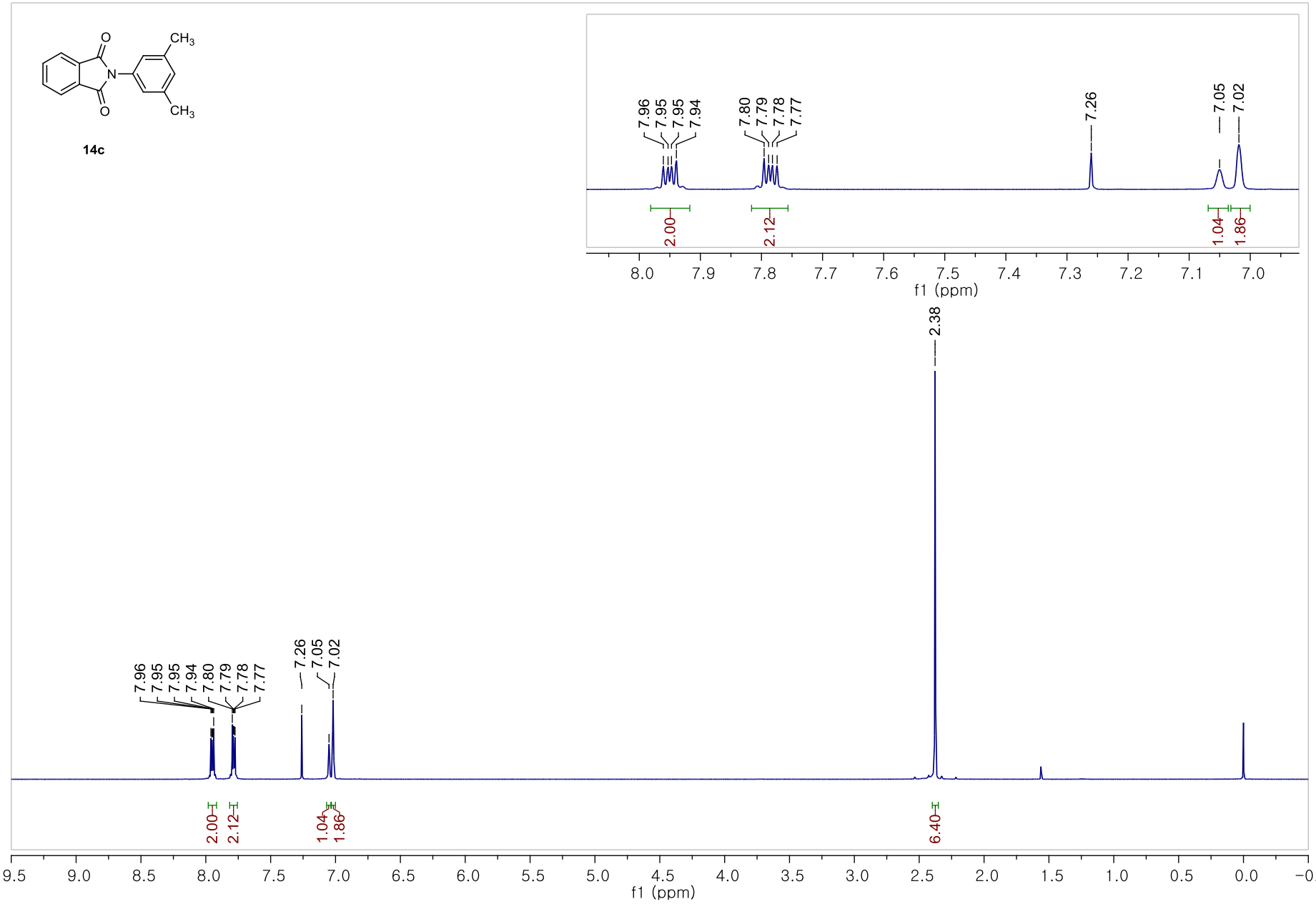

14a
14b
14c
139.66
137.03
136.33
134.51
134.44
132.25
132.18
132.08
129.65
128.67
128.63
128.04
127.82
124.69
123.96
123.90
123.86
167.71
167.40
77.55
77.23
76.91
21.50
21.39
18.28
18.13
f1 (ppm)

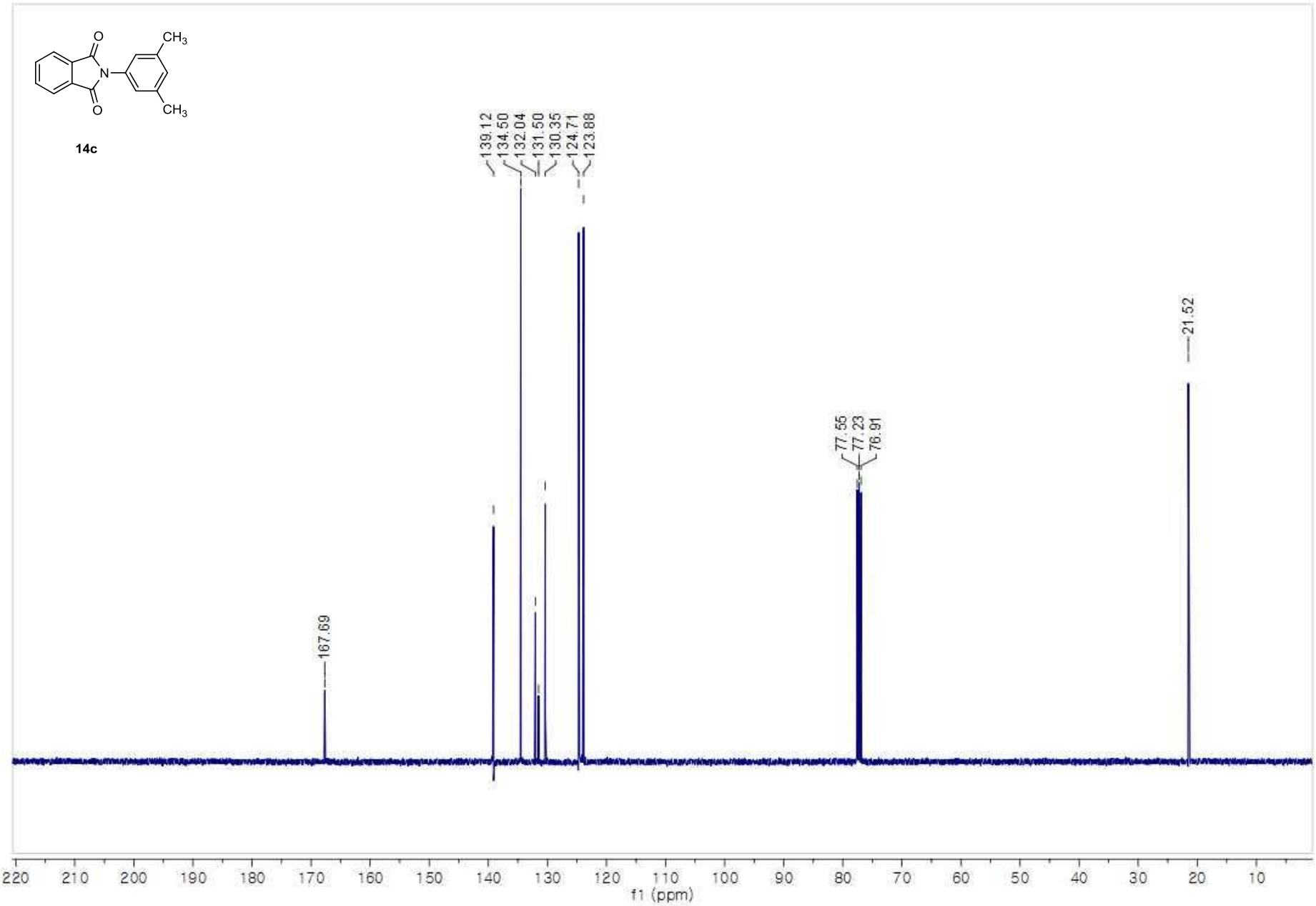

14a
7.98
7.97
7.97
7.96
7.82
7.81
7.81
7.80
7.30
7.28
7.20
7.18
1.92
2.06
1.00
2.00
f1 (ppm)
2.16
6.29
f1 (ppm)

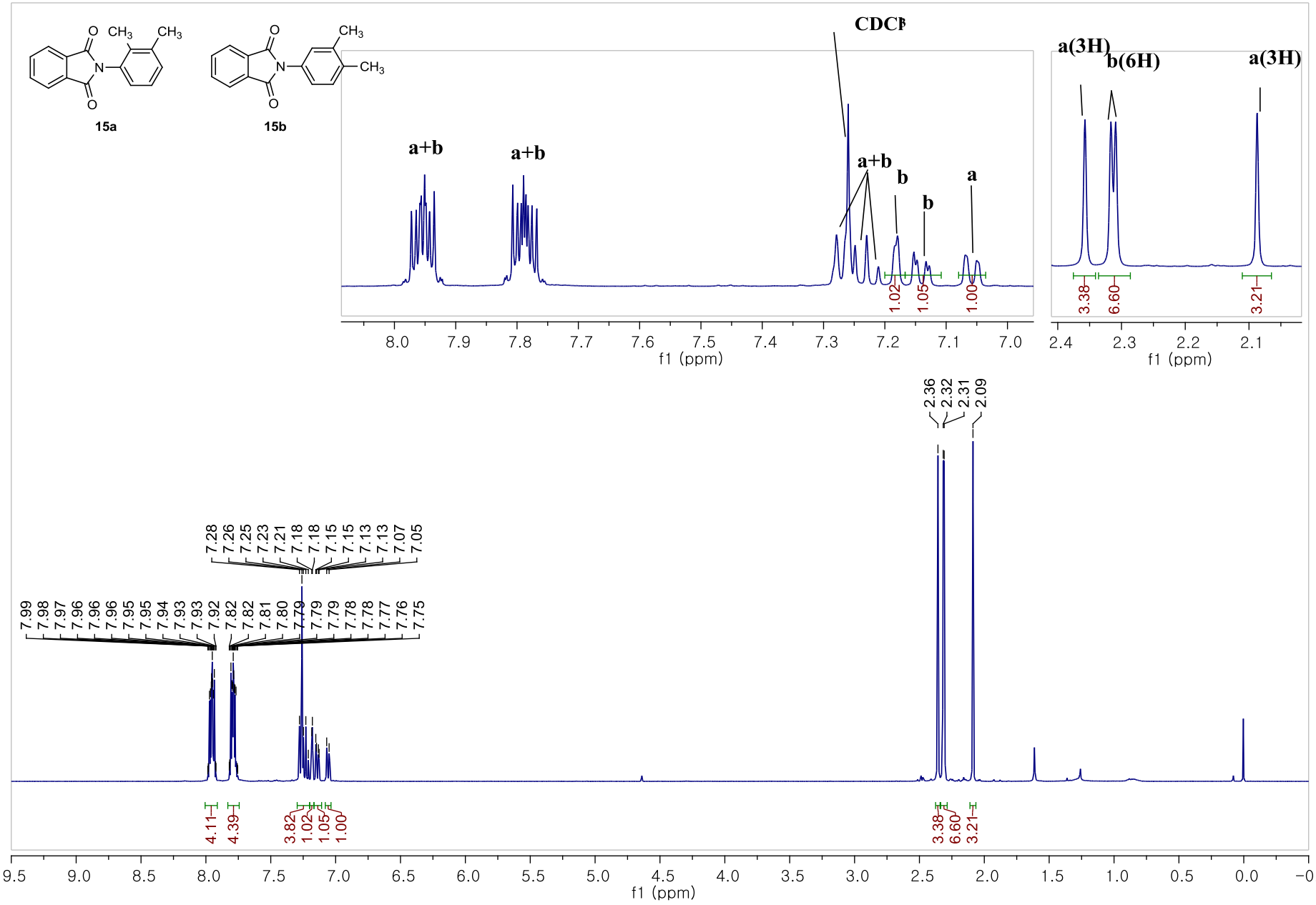

O
CH3
N
O
CH3
14a
137.05
134.54
132.20
129.97
129.68
128.69
124.00
77.55
77.23
76.91
18.31
167.44
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

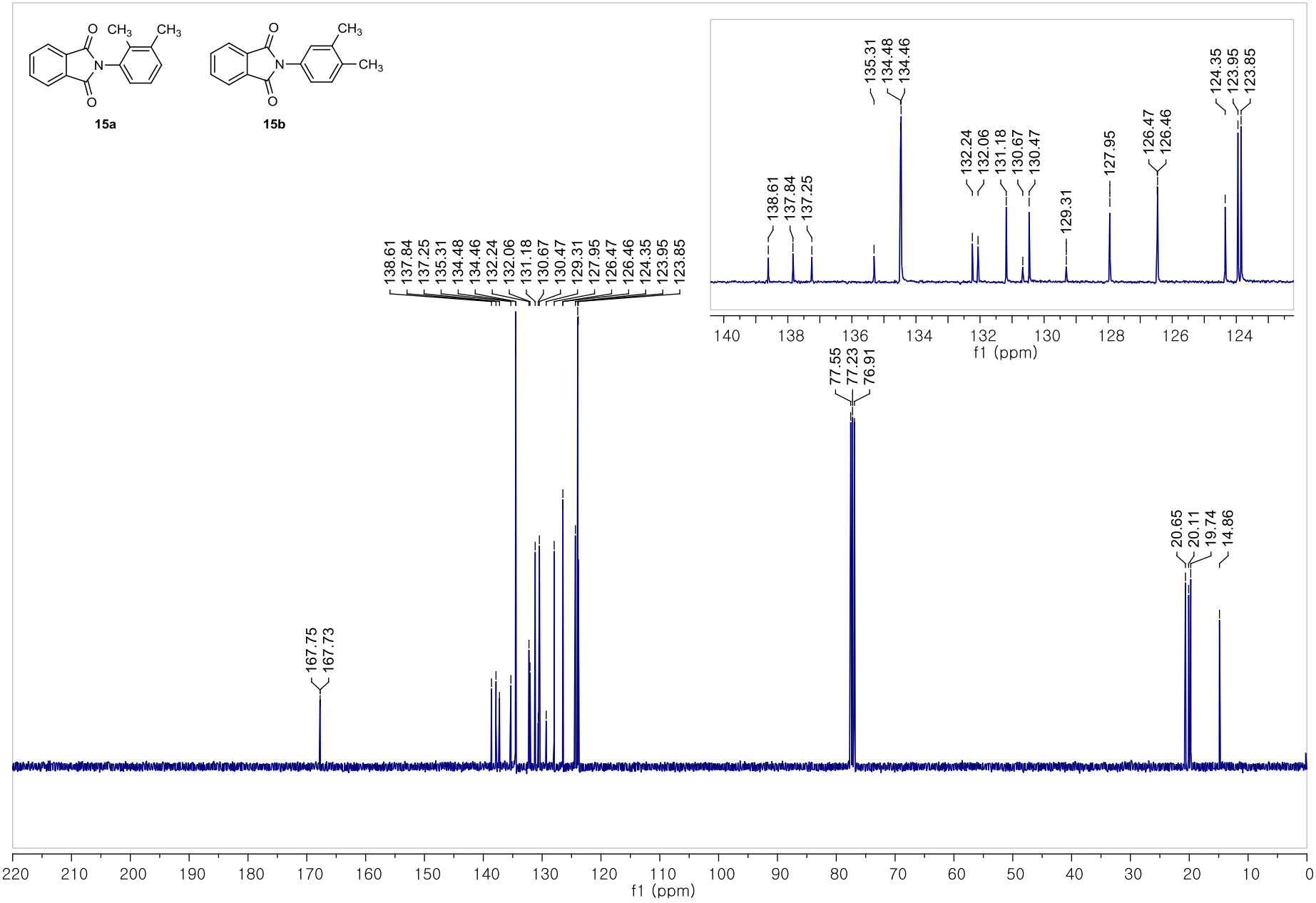

O
N
CH3
O
CH3
14b
7.96
7.96
7.95
7.94
7.94
7.80
7.79
7.79
7.78
7.78
7.26
7.18
7.15
7.15
7.13
7.13
7.09
7.07
2.00
2.15
1.05
1.12
1.05
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
2.38
2.17
2.00
2.15
1.05
1.12
1.05
3.26
3.21
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

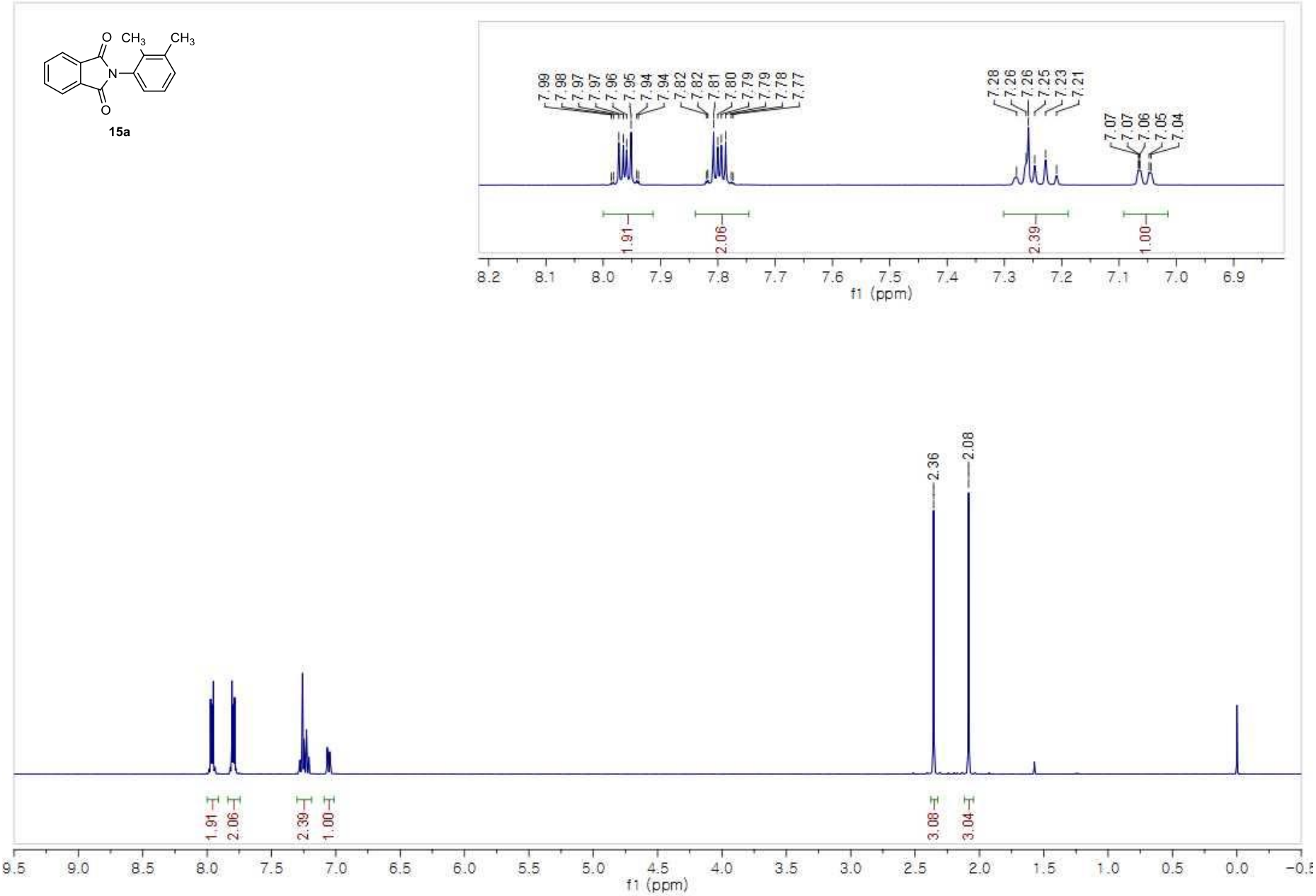

14b
139.67
136.33
134.45
132.24
132.08
128.63
128.03
127.82
123.90
167.71
77.55
77.23
76.91
21.40
18.13
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

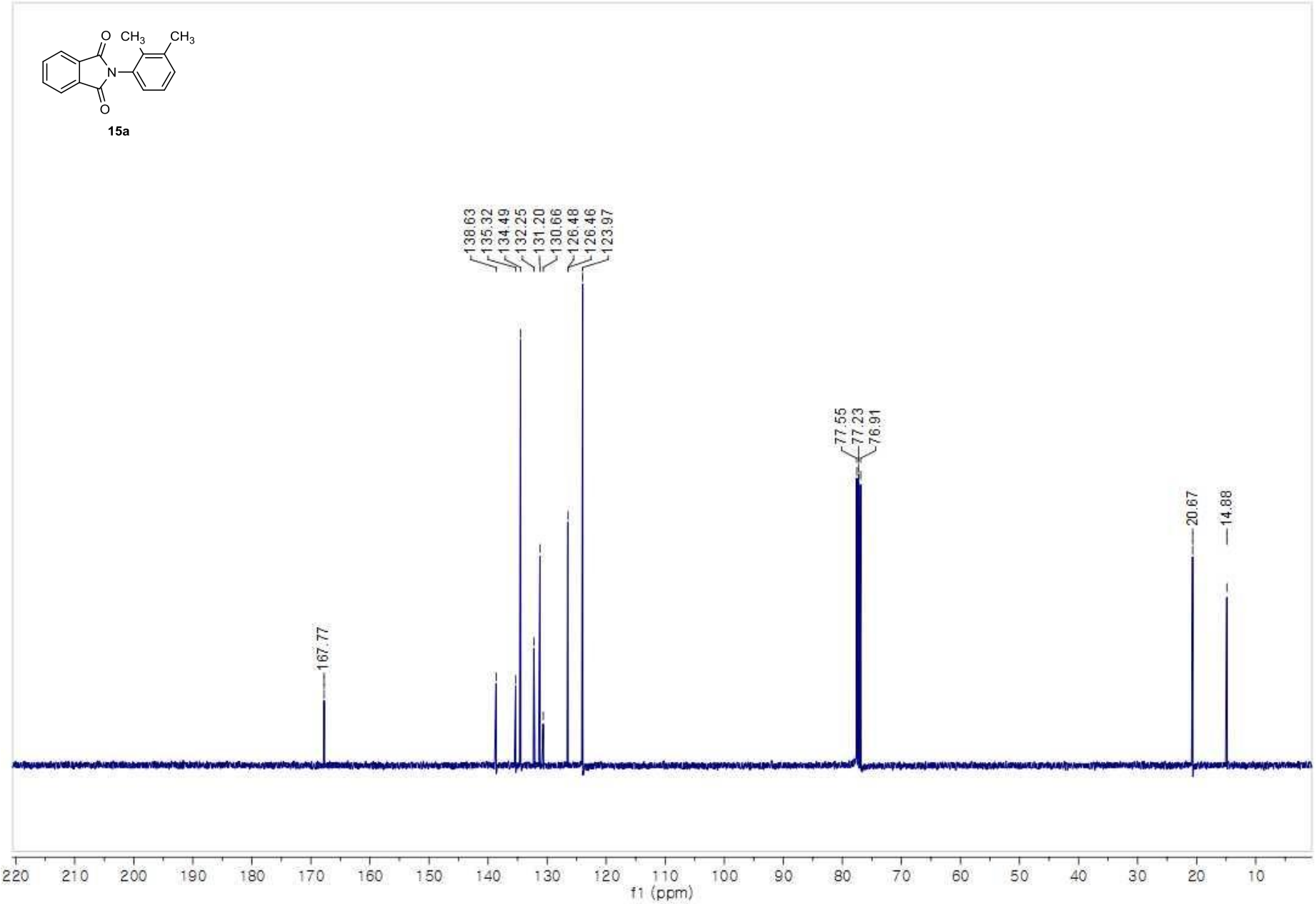

14c
7.96
7.95
7.95
7.94
7.80
7.79
7.78
7.77
7.26
7.05
7.02
2.38
2.00
2.12
1.04
1.86
6.40
f1 (ppm)

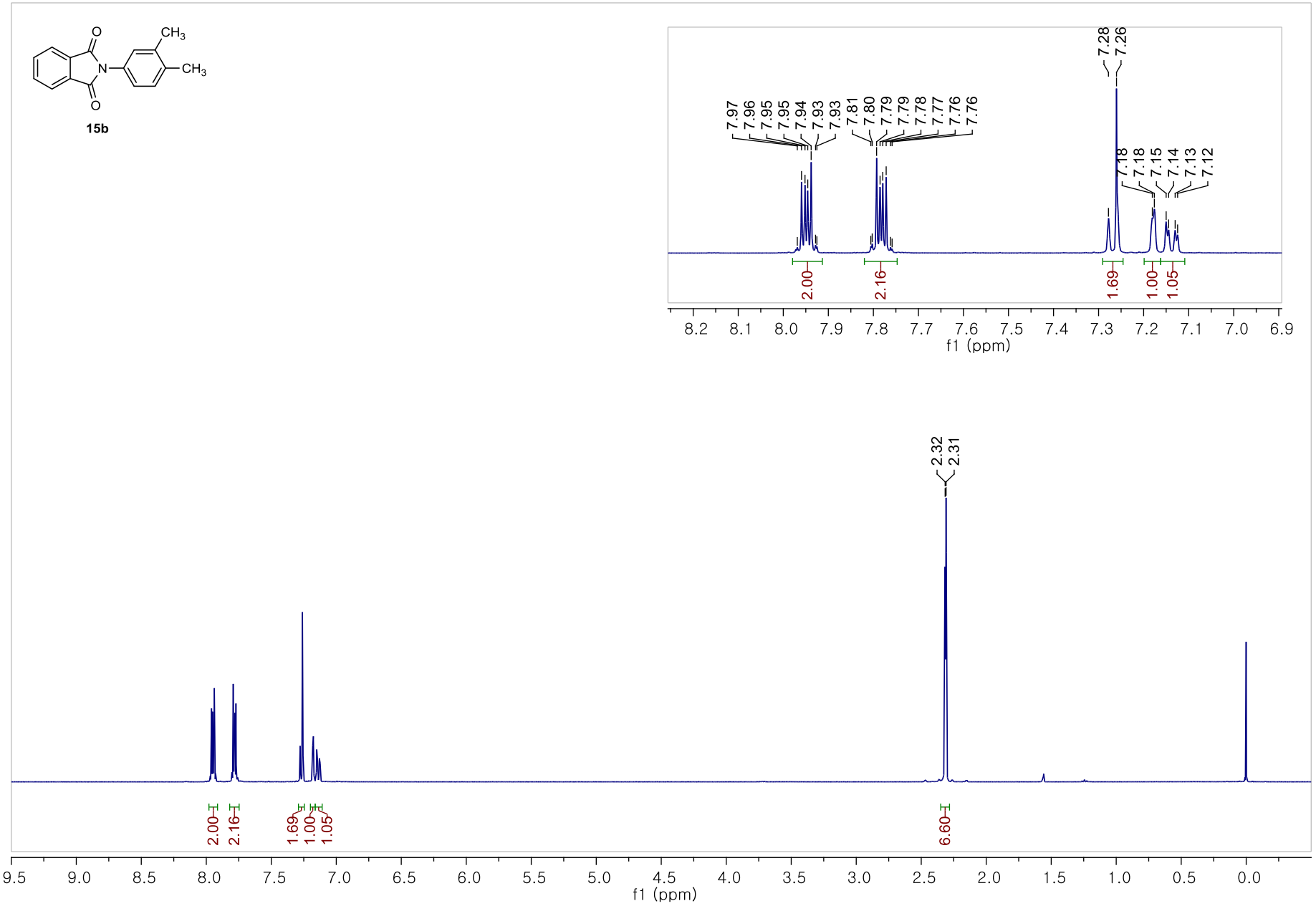

14c
139.12
134.50
132.04
131.50
130.35
124.71
123.88
77.55
77.23
76.91
167.69
21.52
f1 (ppm)

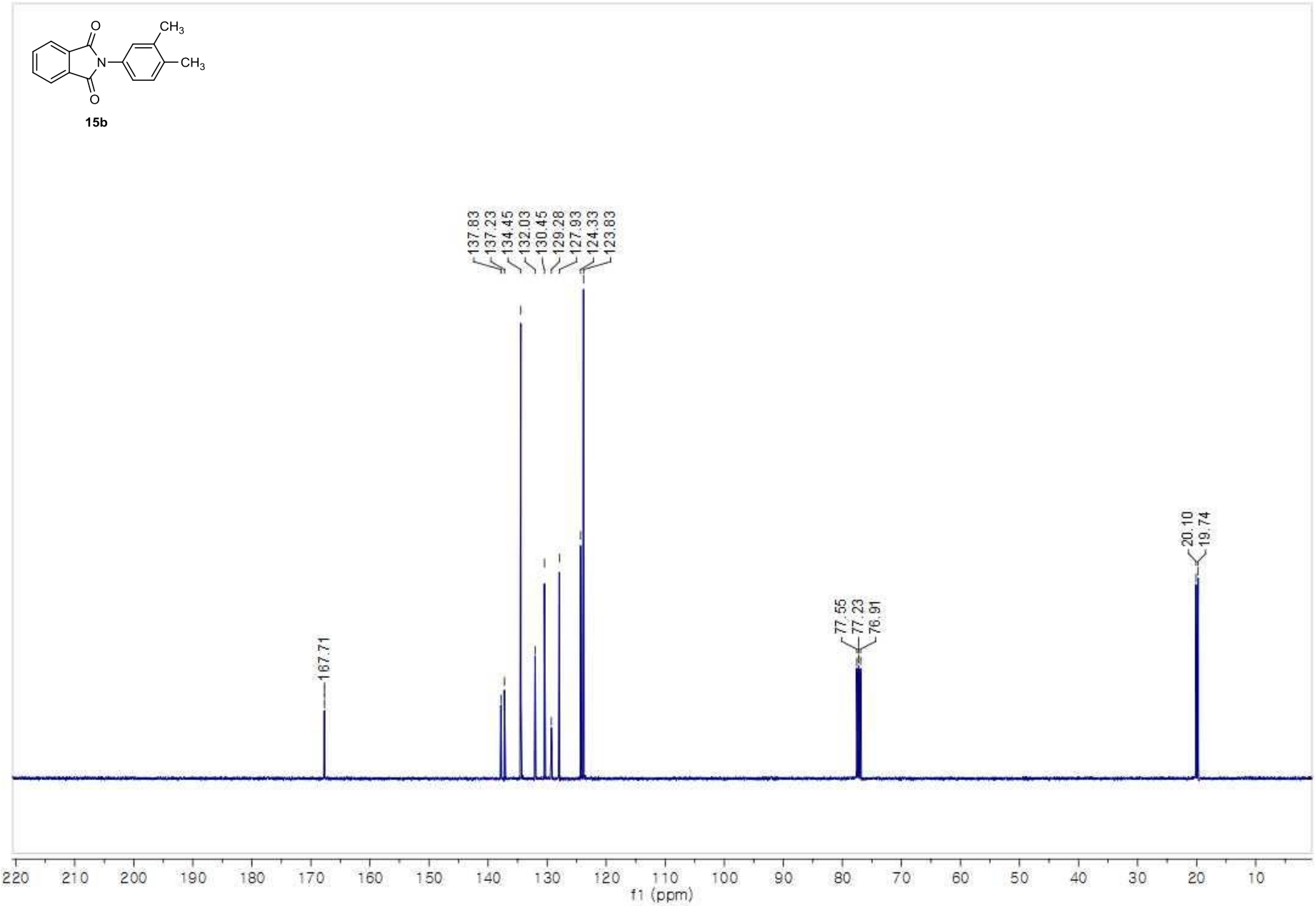

15a
15b
CDCl3
a+b
a+b
a+b
b
b
a
a(3H)
b(6H)
a(3H)
f1 (ppm)
f1 (ppm)
f1 (ppm)

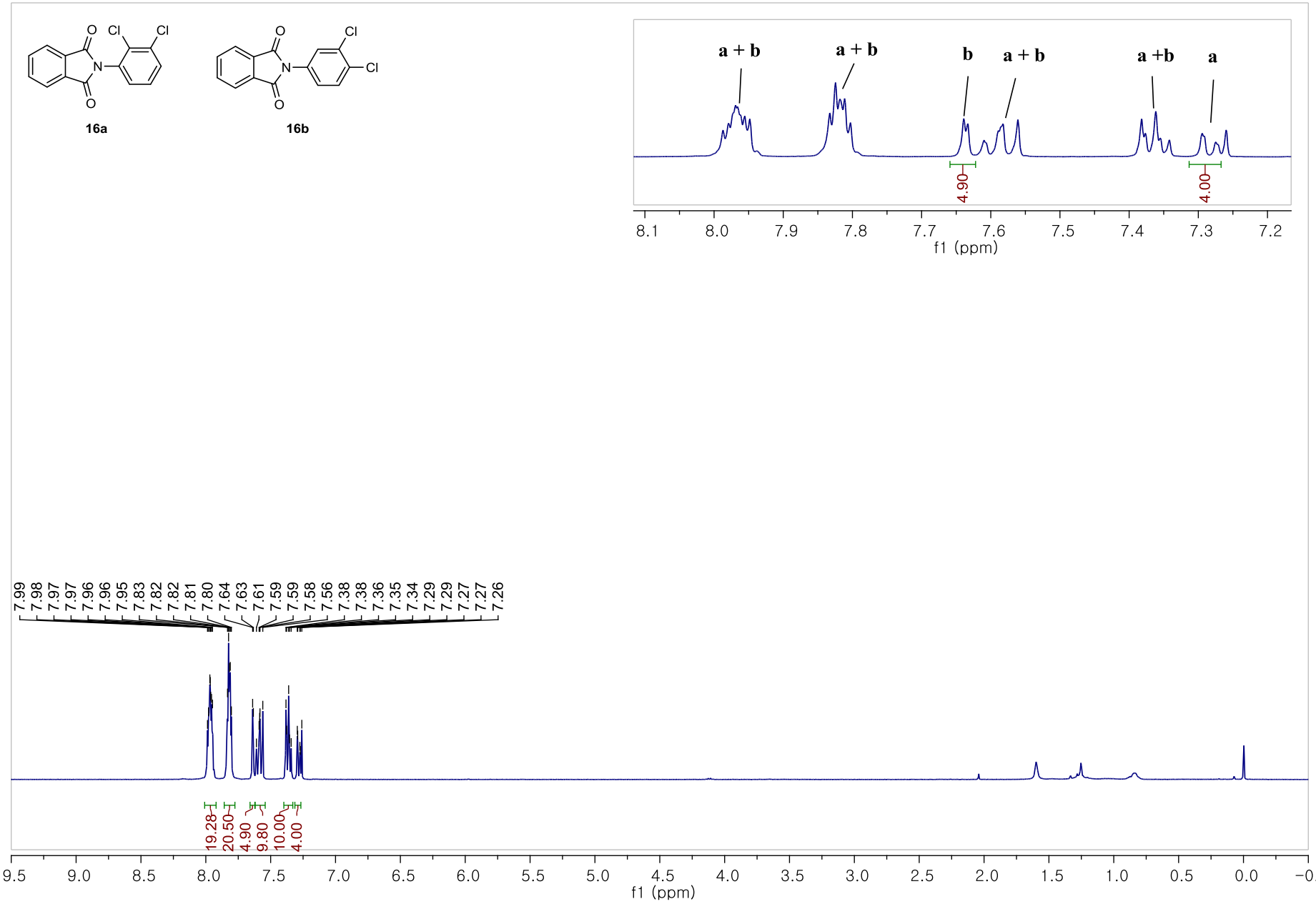

15a
15b
138.61
137.84
137.25
135.31
134.48
134.46
132.24
132.06
131.18
130.67
130.47
129.31
127.95
126.47
126.46
124.35
123.95
123.85
77.55
77.23
76.91
167.75
167.73
20.65
20.11
19.74
14.86
f1 (ppm)

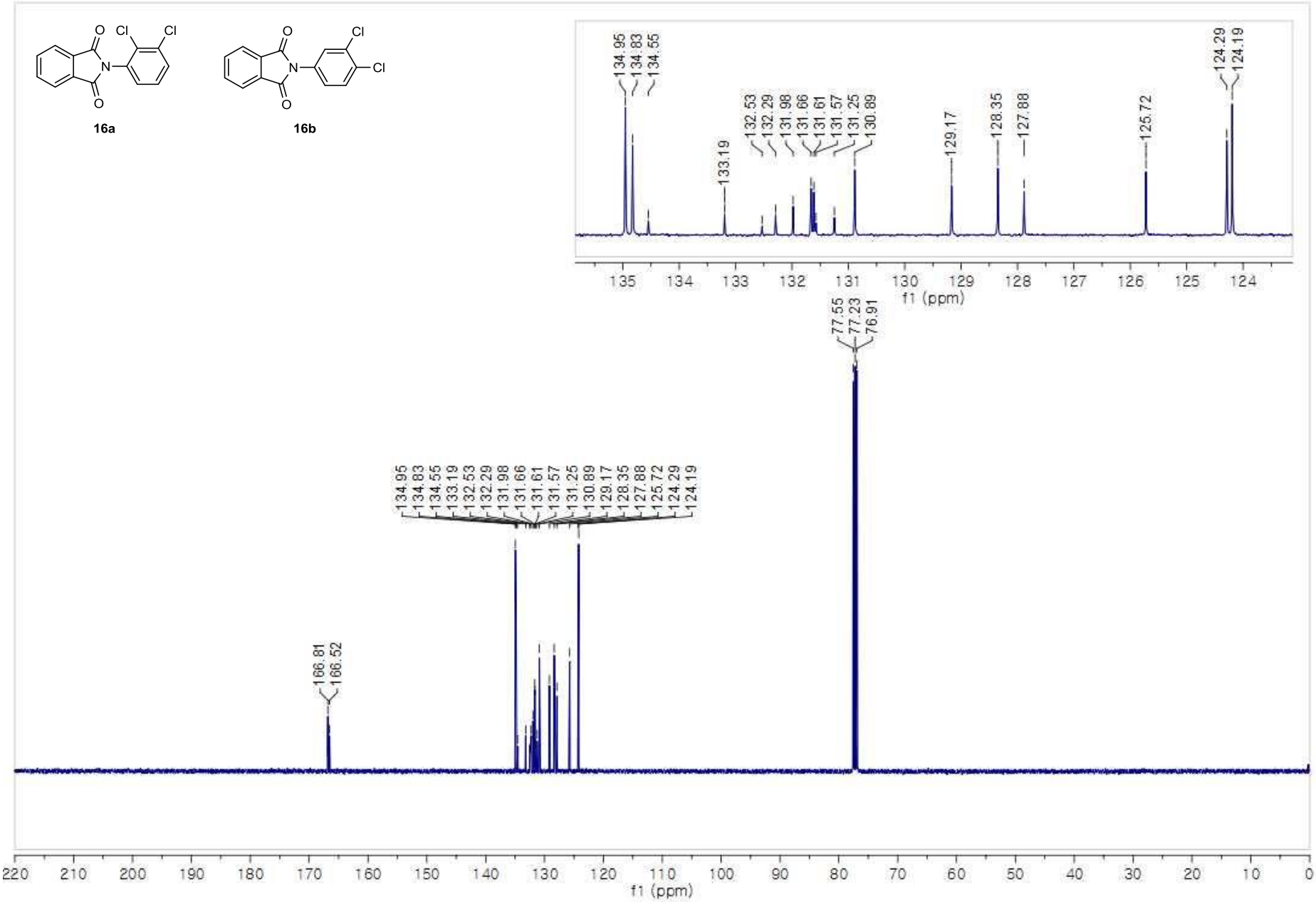

O
CH3
CH3
N
O
15a
7.99
7.98
7.97
7.97
7.96
7.95
7.94
7.94
7.82
7.81
7.80
7.79
7.79
7.78
7.77
7.28
7.26
7.26
7.25
7.23
7.21
7.07
7.07
7.06
7.05
7.04
1.91
2.06
2.39
1.00
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
2.36
2.08
1.91
2.06
2.39
1.00
3.08
3.04
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

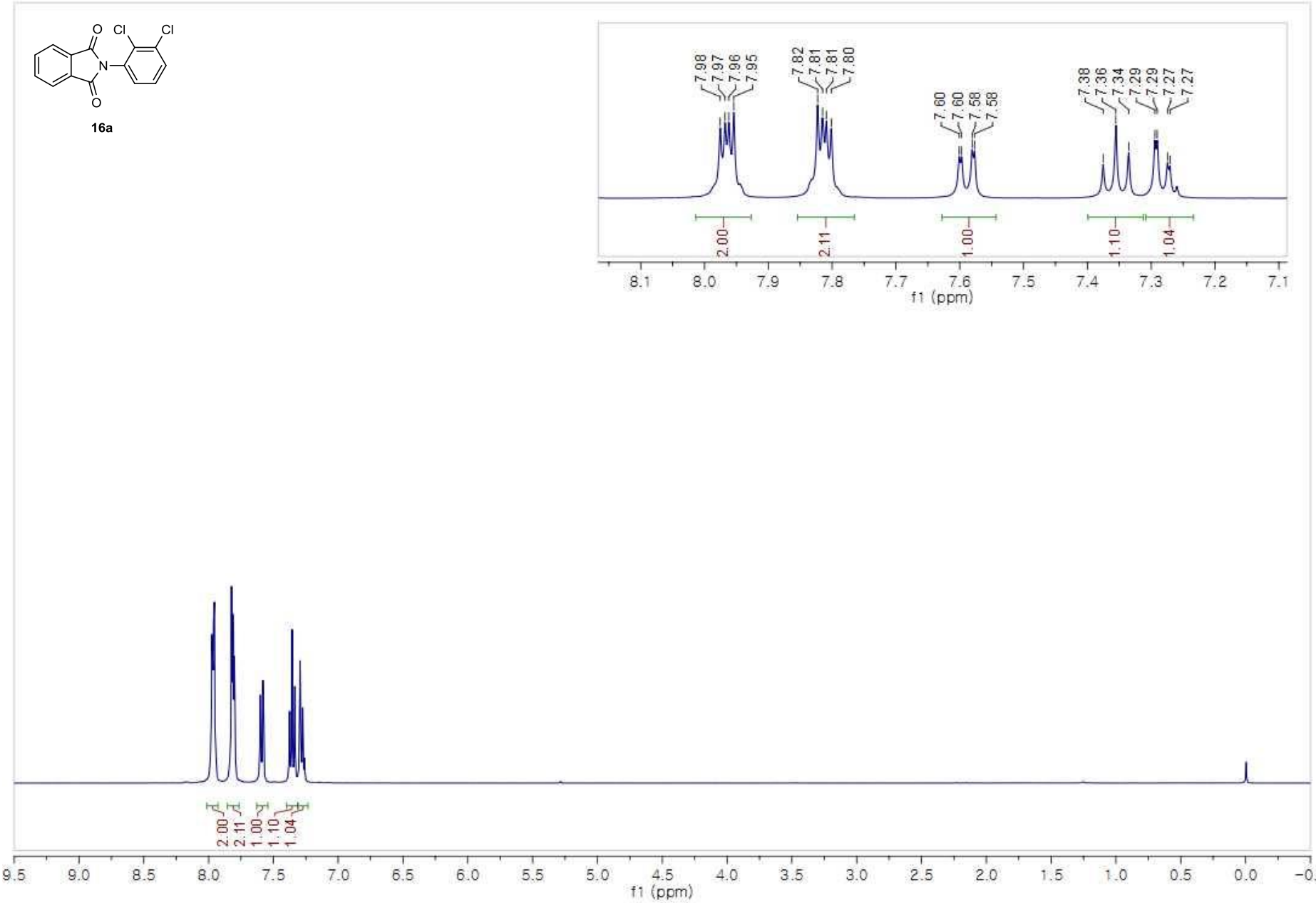

O
CH3
CH3
N
O
15a
138.63
135.32
134.49
132.25
131.20
130.66
126.48
126.46
123.97
77.55
77.23
76.91
20.67
14.88
167.77
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

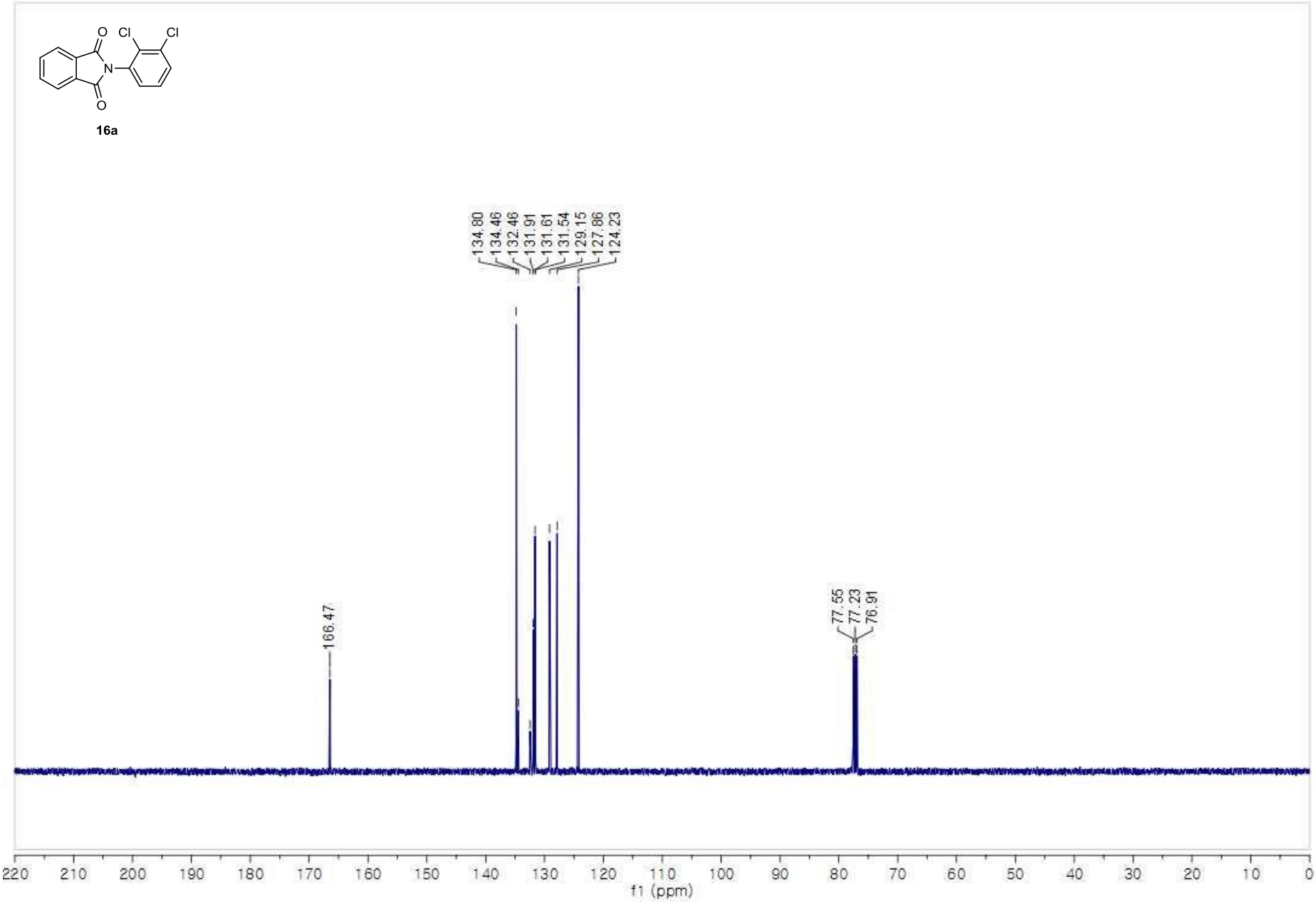

15b
7.97
7.96
7.95
7.95
7.94
7.93
7.93
7.81
7.80
7.79
7.79
7.78
7.77
7.76
7.76
7.28
7.26
7.18
7.18
7.15
7.14
7.13
7.12
2.00
2.16
1.69
1.00
1.05
f1 (ppm)
2.32
2.31
6.60
f1 (ppm)

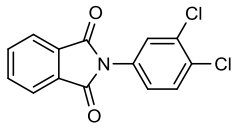

O
CH3
N
CH3
O
15b
137.83
137.23
134.45
132.03
130.45
129.28
127.93
124.33
123.83
167.71
77.55
77.23
76.91
20.10
19.74
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


16a
16b
a + b
a + b
b
a + b
a +b
a
4.90
4.00
f1 (ppm)
7.99 7.98 7.97 7.97 7.96 7.96 7.95 7.83 7.82 7.82 7.81 7.80 7.64 7.63 7.61 7.59 7.59 7.58 7.56 7.38 7.38 7.36 7.35 7.34 7.29 7.29 7.27 7.27 7.26
19.28
20.50
4.90
9.80
10.00
4.00
f1 (ppm)

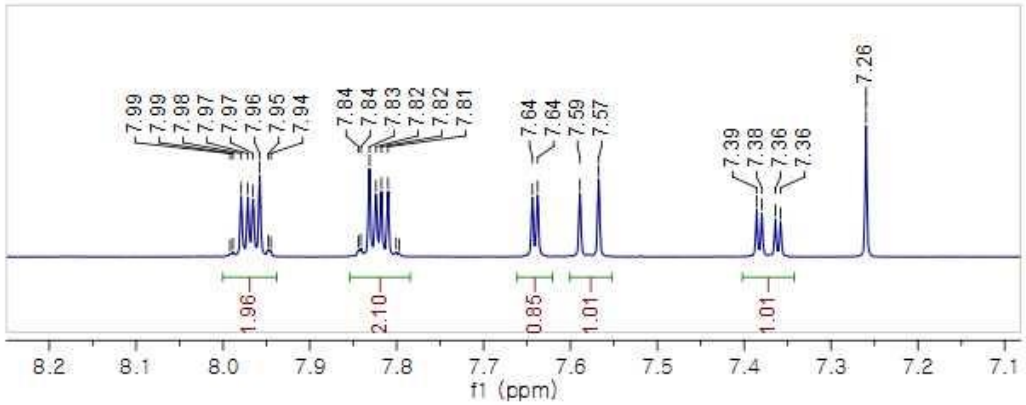

16a
16b
134.95
134.83
134.55
133.19
132.53
132.29
131.98
131.66
131.61
131.57
131.25
130.89
129.17
128.35
127.88
125.72
124.29
124.19
f1 (ppm)
77.55
77.23
76.91
166.81
166.52
f1 (ppm)

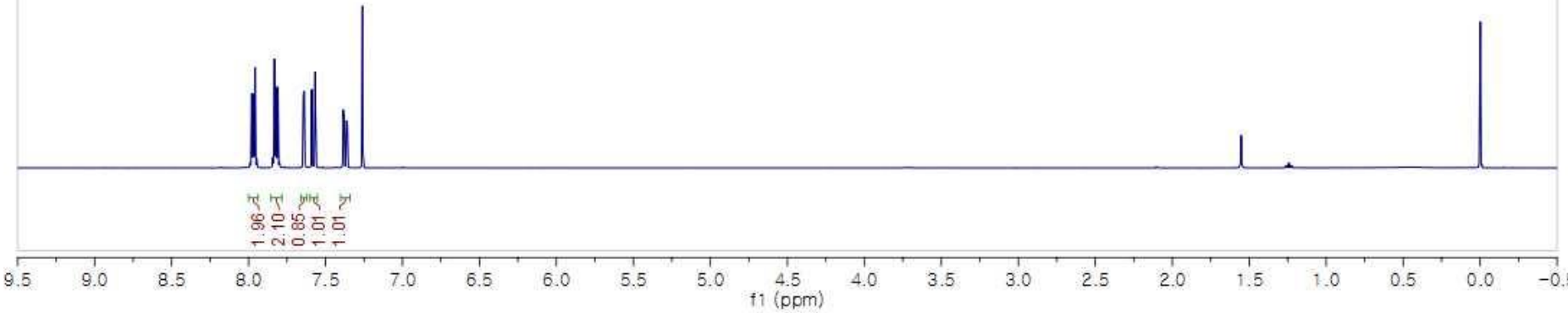

O
Cl
Cl
N
O
16a
7.98
7.97
7.96
7.95
7.82
7.81
7.81
7.80
7.60
7.60
7.58
7.58
7.38
7.36
7.34
7.29
7.29
7.27
7.27
2.00
2.11
1.00
1.10
1.04
f1 (ppm)

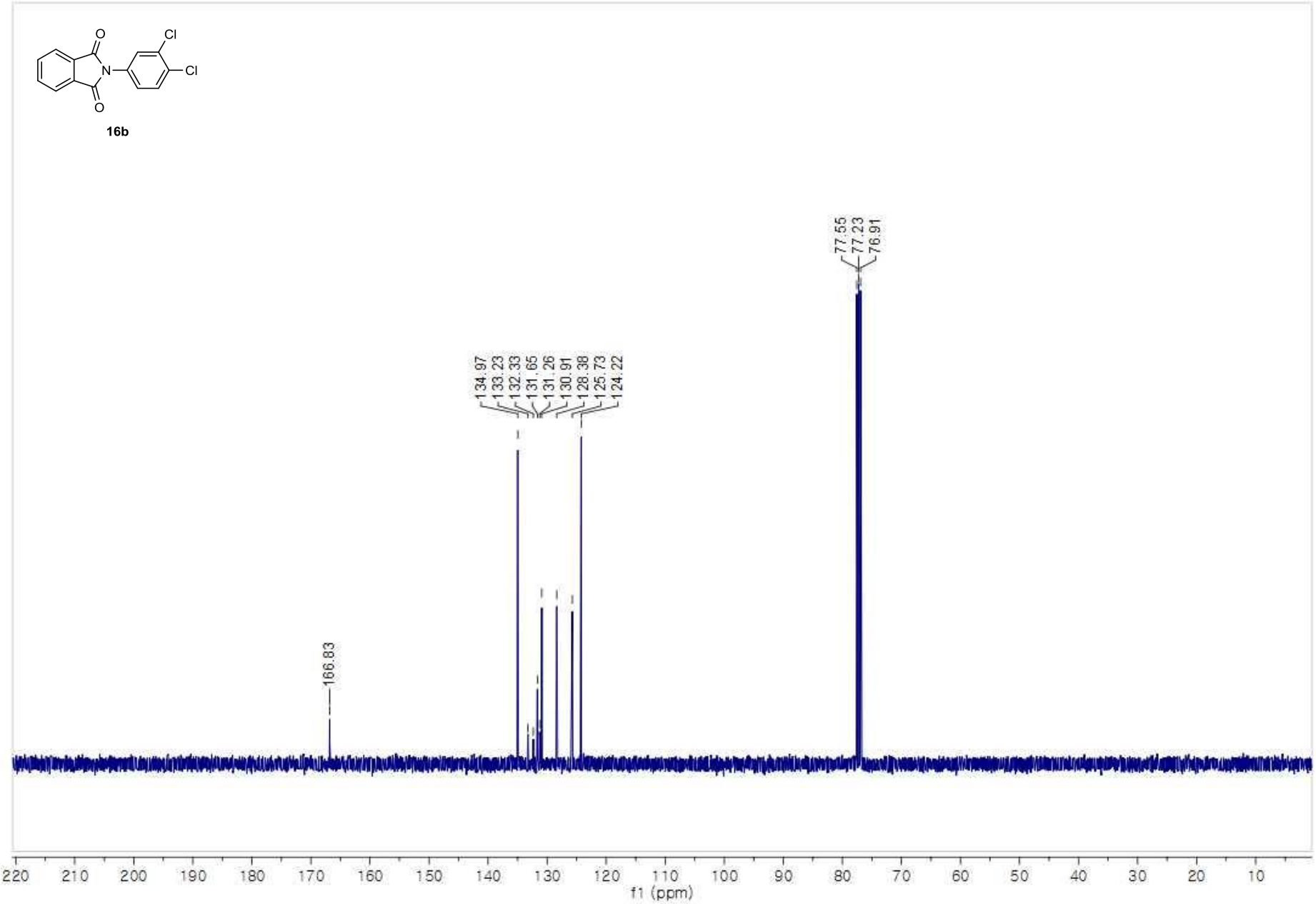

O
Cl
Cl
N
O
16a
134.80
134.46
132.46
131.91
131.61
131.54
129.15
127.86
124.23
166.47
77.55
77.23
76.91
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

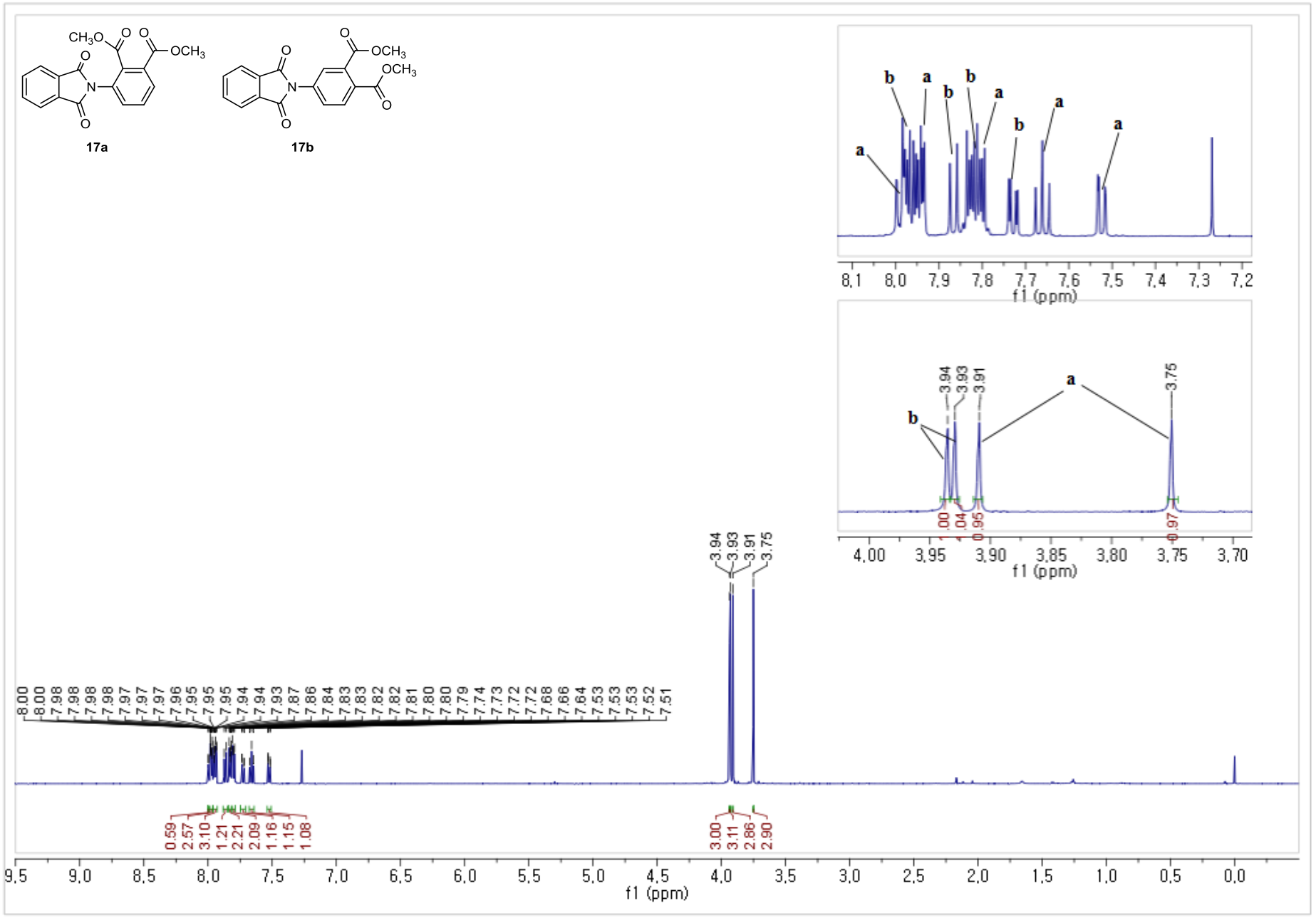

O
Cl
N
Cl
O

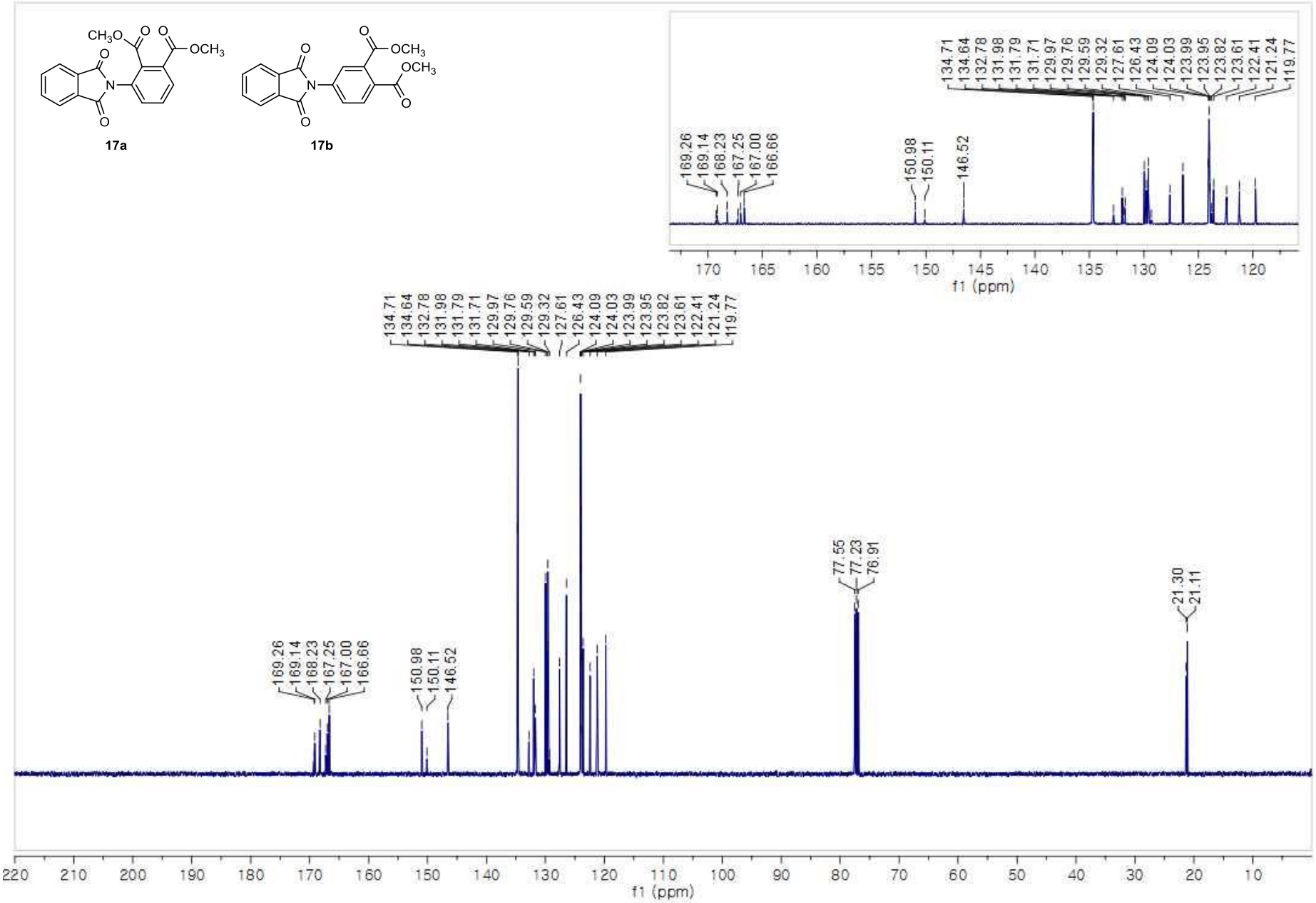
16b

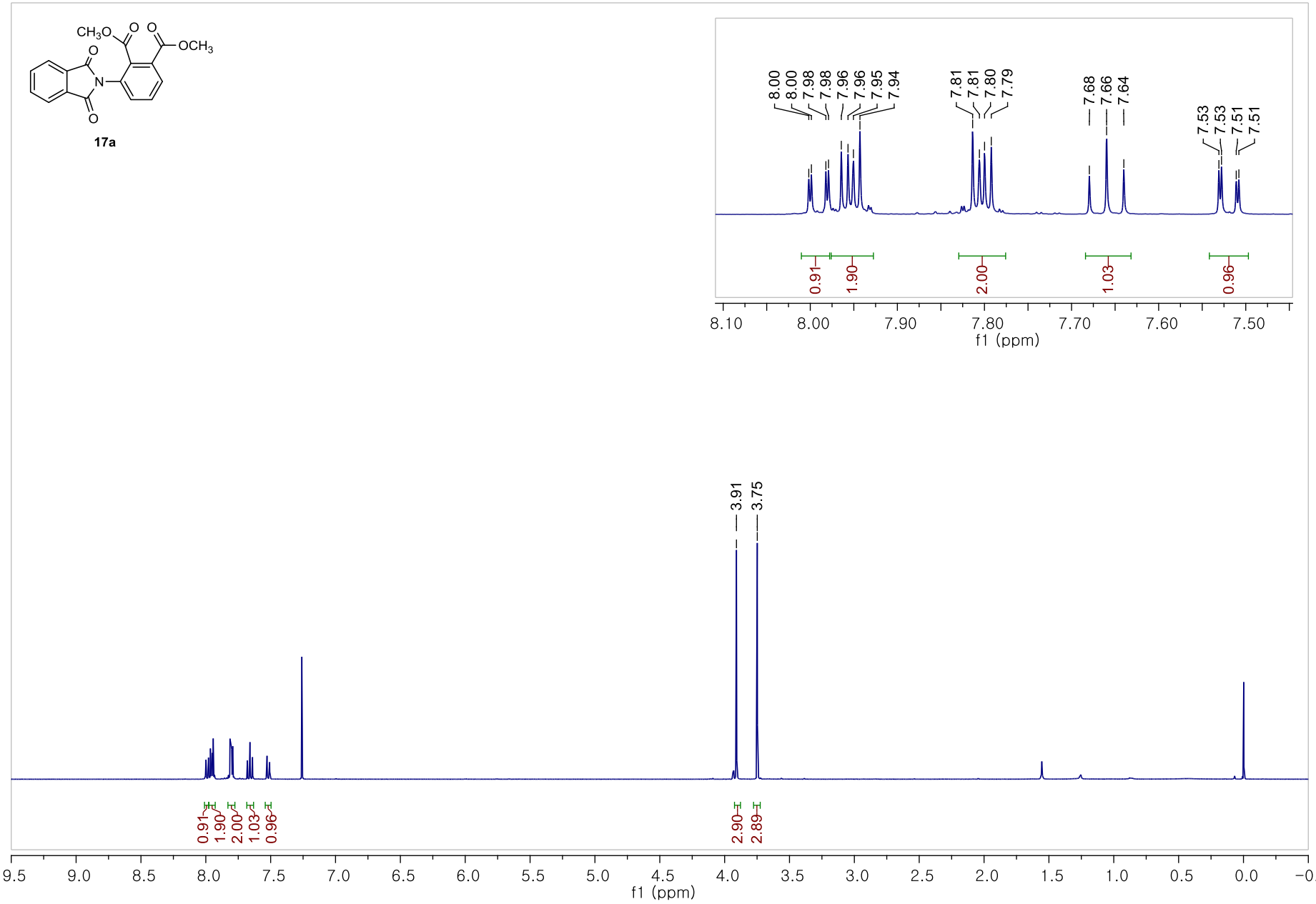

7.99
7.99
7.98
7.97
7.97
7.96
7.95
7.94
7.84
7.84
7.83
7.82
7.82
7.81
7.64
7.64
7.59
7.57
7.39
7.38
7.36
7.36
7.26
1.96
2.10
0.85
1.01
1.01
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)

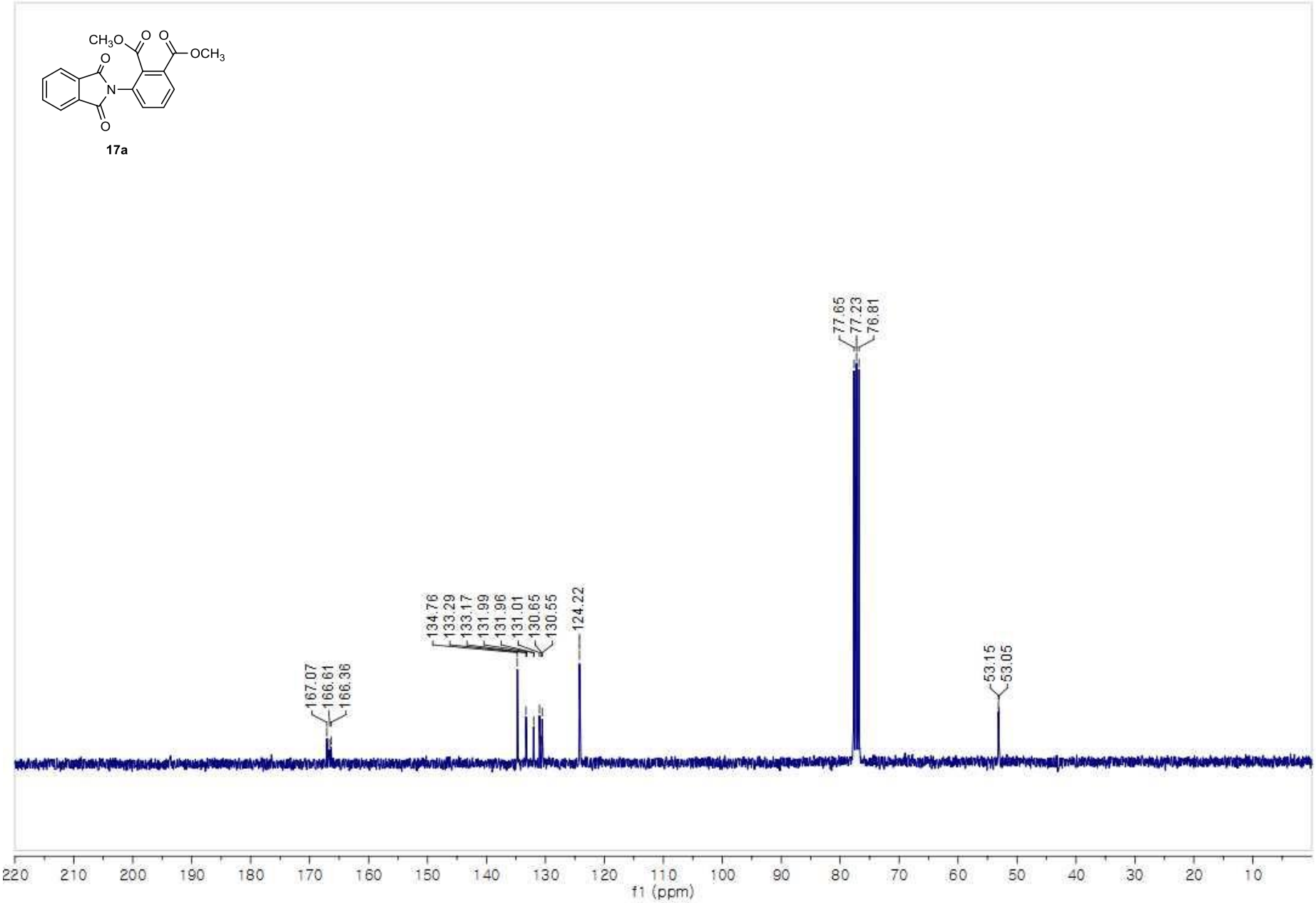

1.96
2.10
0.85
1.01
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

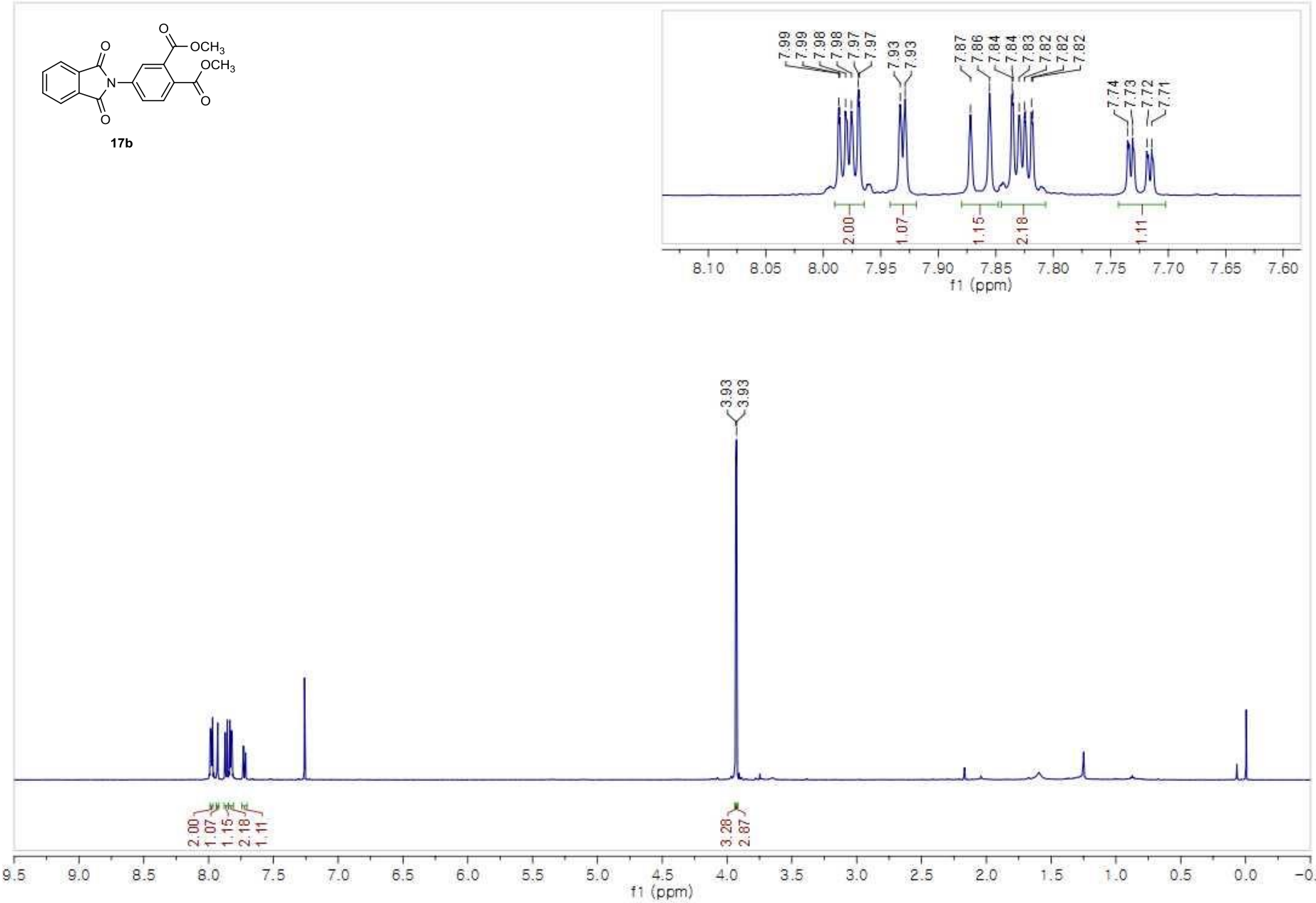

O
Cl
N
Cl
O
16b
77.55
77.23
76.91
134.97
133.23
132.33
131.65
131.26
130.91
128.38
125.73
124.22
166.83
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

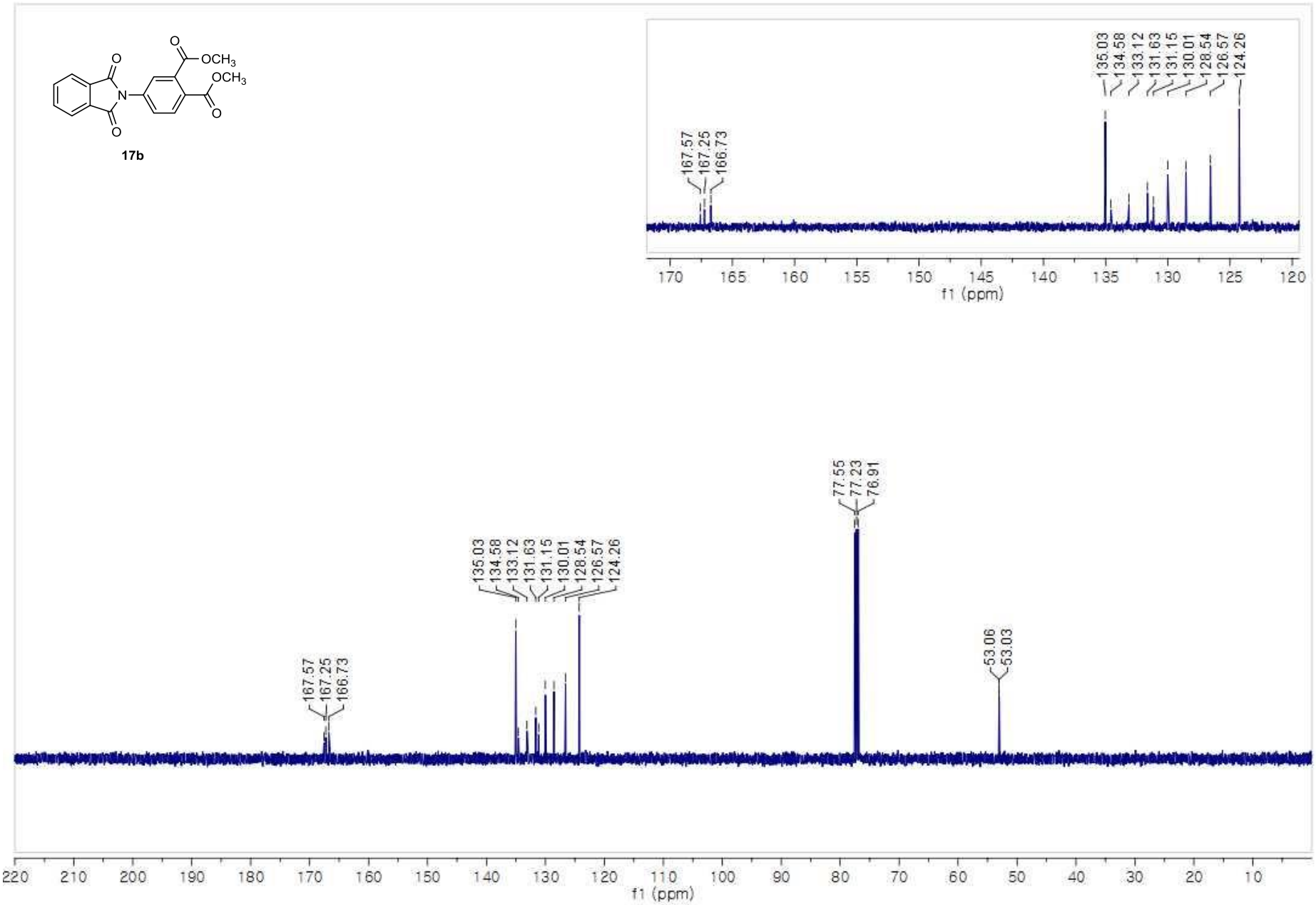

17a
17b
f1 (ppm)

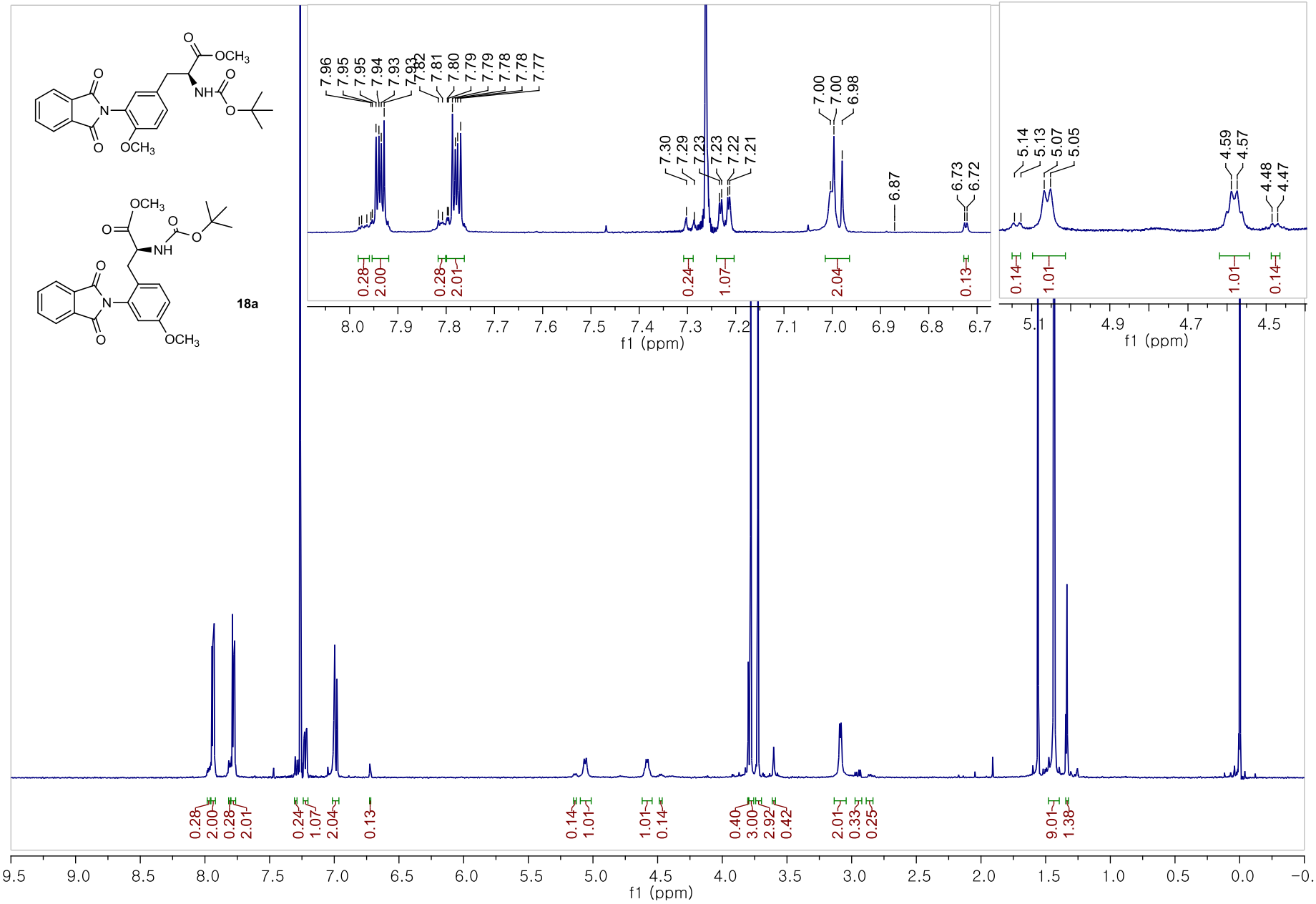

17a
17b
169.26
169.14
168.23
167.25
167.00
166.66
150.98
150.11
146.52
134.71
134.64
132.78
131.98
131.79
131.71
129.97
129.76
129.59
129.32
127.61
126.43
124.09
124.03
123.99
123.95
123.82
123.61
122.41
121.24
119.77
77.55
77.23
76.91
21.30
21.11
f1 (ppm)

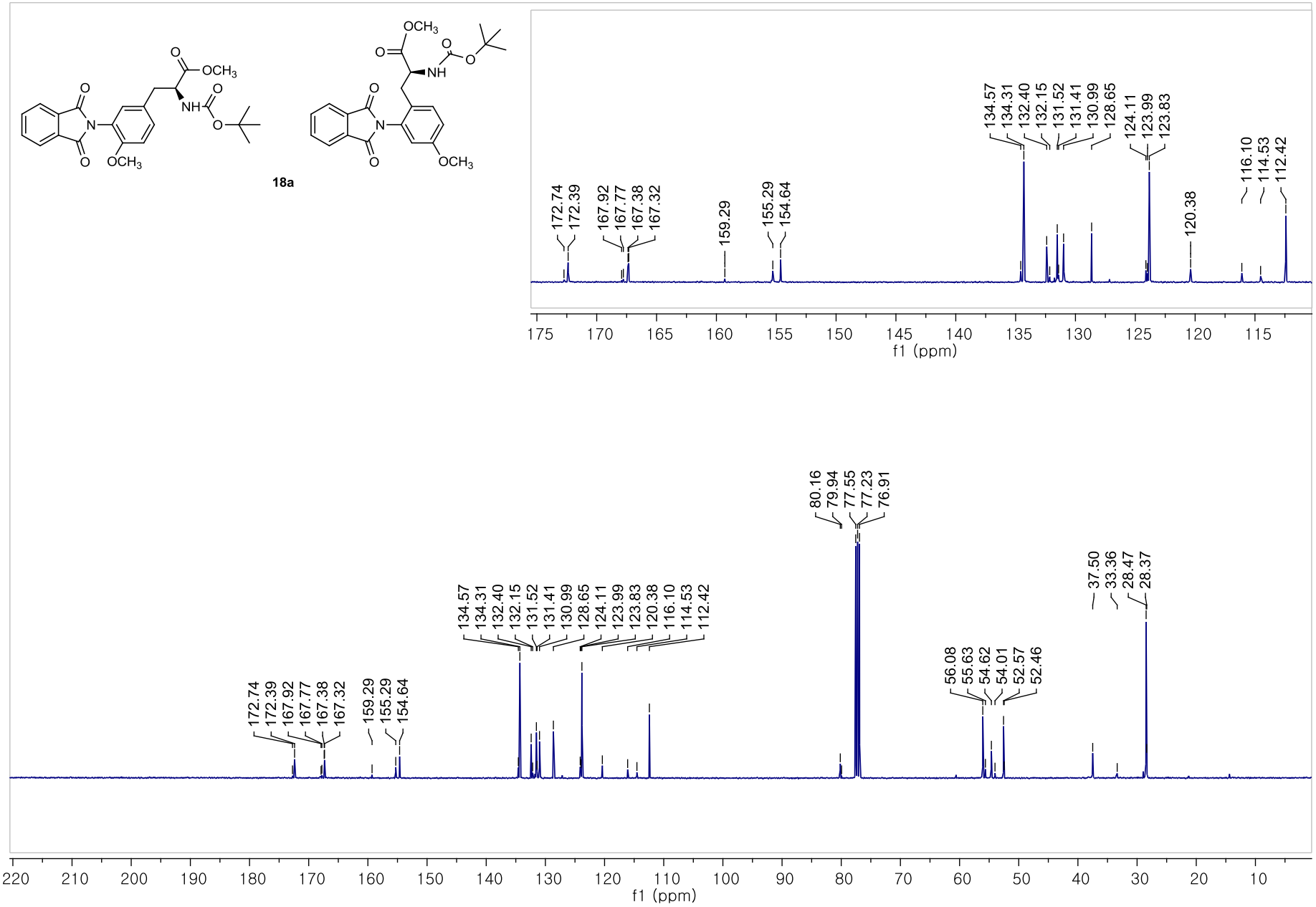

17a
8.00
8.00
7.98
7.98
7.96
7.96
7.95
7.94
7.81
7.81
7.80
7.79
7.68
7.66
7.64
7.53
7.53
7.51
7.51
0.91
1.90
2.00
1.03
0.96
8.10
8.00
7.90
7.80
7.70
7.60
7.50
f1 (ppm)
3.91
3.75
0.91
1.90
2.00
1.03
0.96
2.90
2.89
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

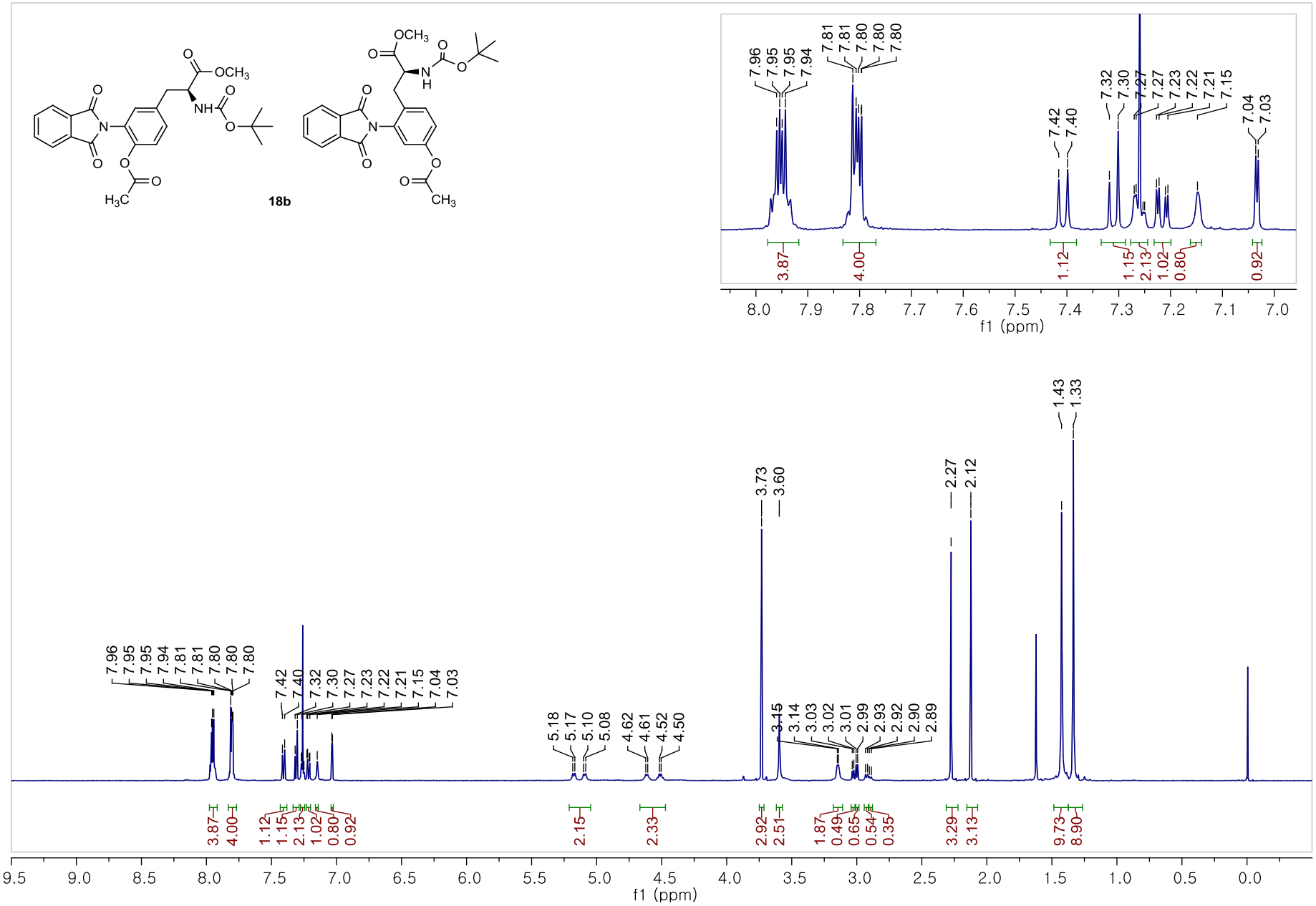

CH3O
O
O
OCH3
O
N
O
17a
167.07
166.61
166.36
134.76
133.29
133.17
131.99
131.96
131.01
130.65
130.55
124.22
77.65
77.23
76.81
53.15
53.05
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

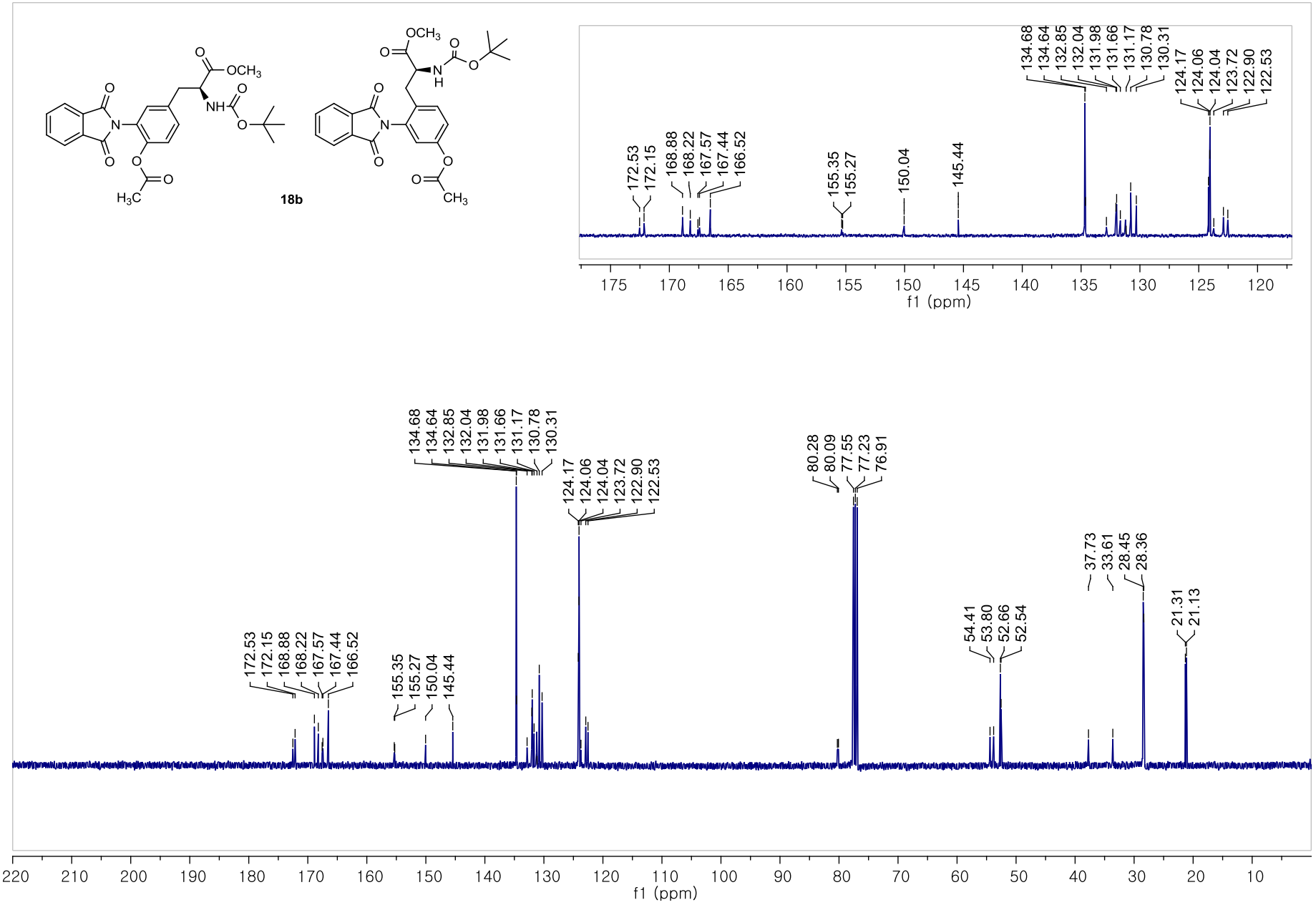

17b
7.99
7.99
7.98
7.98
7.97
7.97
7.93
7.93
7.87
7.86
7.84
7.84
7.83
7.82
7.82
7.82
7.74
7.73
7.72
7.71
2.00
1.07
1.15
2.18
1.11
8.10
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
f1 (ppm)
3.93
3.93
2.00
1.07
1.15
2.18
1.11
3.28
2.87
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

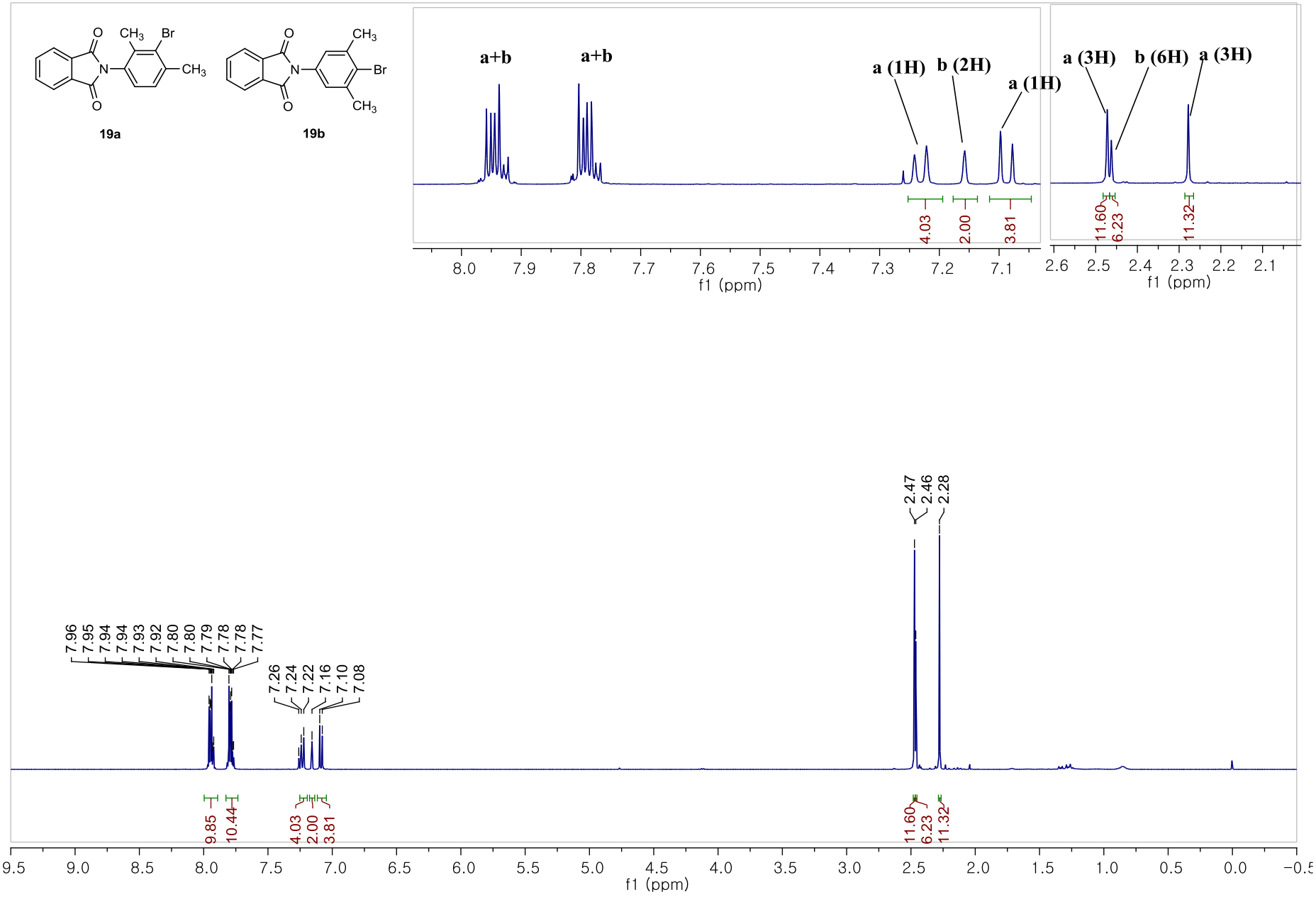

17b
167.57
167.25
166.73
135.03
134.58
133.12
131.63
131.15
130.01
128.54
126.57
124.26
77.55
77.23
76.91
53.06
53.03
f1 (ppm)

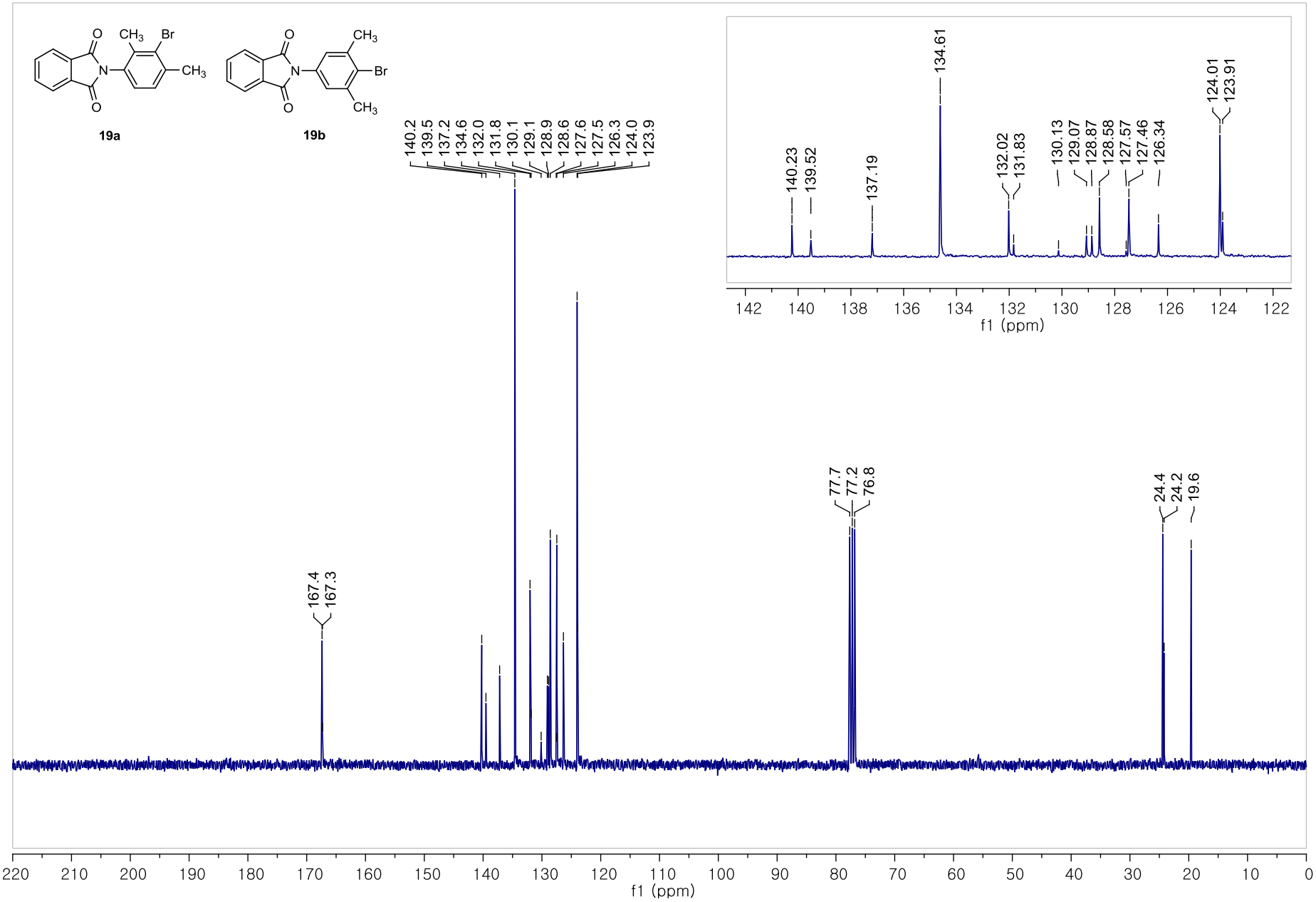

18a
7.96
7.95
7.95
7.94
7.93
7.93
7.82
7.81
7.80
7.79
7.79
7.78
7.78
7.77
7.30
7.29
7.23
7.23
7.22
7.21
7.00
7.00
6.98
6.87
6.73
6.72
5.14
5.13
5.07
5.05
4.59
4.57
4.48
4.47
f1 (ppm)
f1 (ppm)
f1 (ppm)

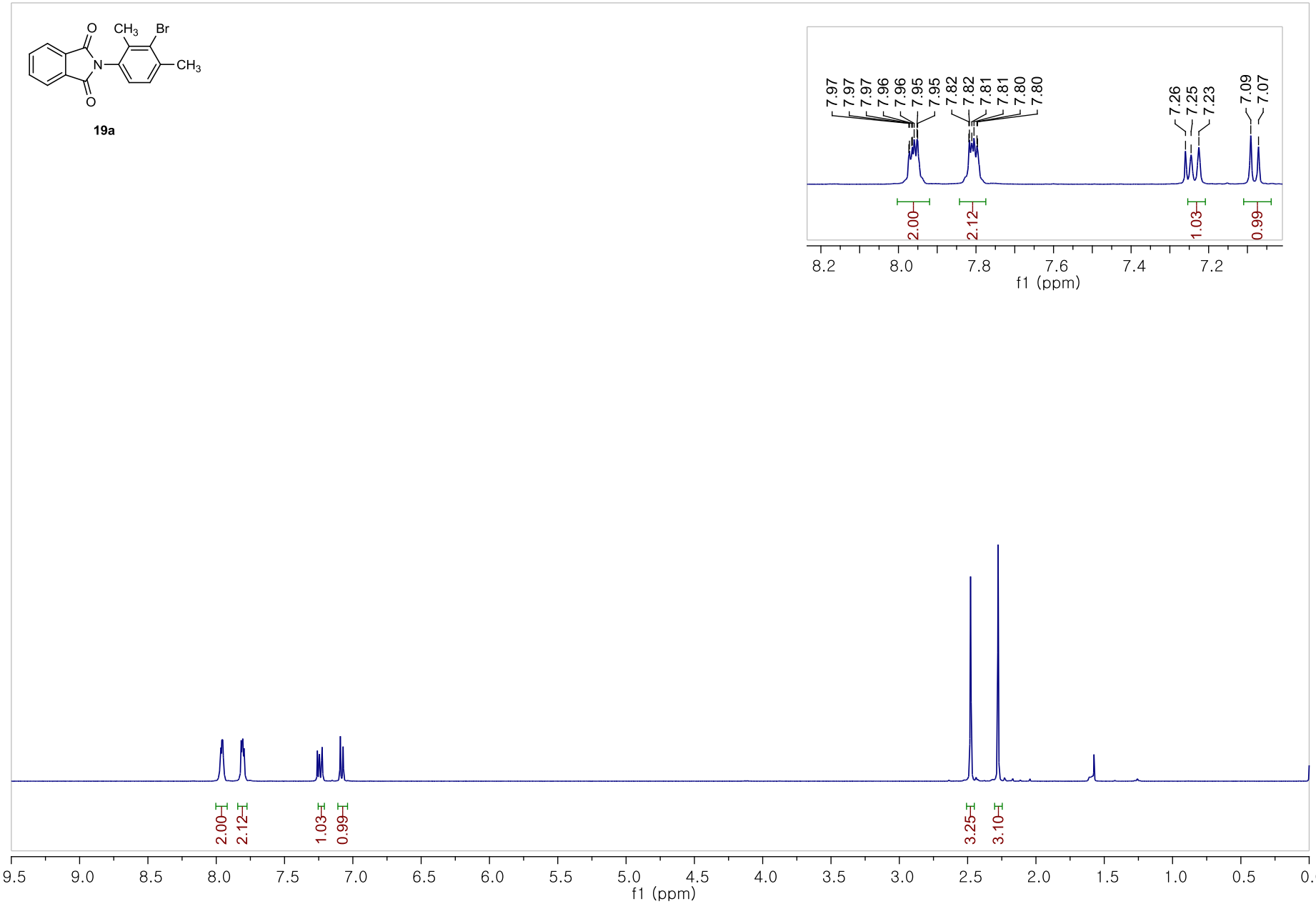

18a
172.74
172.39
167.92
167.77
167.38
167.32
159.29
155.29
154.64
134.57
134.31
132.40
132.15
131.52
131.41
130.99
128.65
124.11
123.99
123.83
120.38
116.10
114.53
112.42
80.16
79.94
77.55
77.23
76.91
56.08
55.63
54.62
54.01
52.57
52.46
37.50
33.36
28.47
28.37
f1 (ppm)

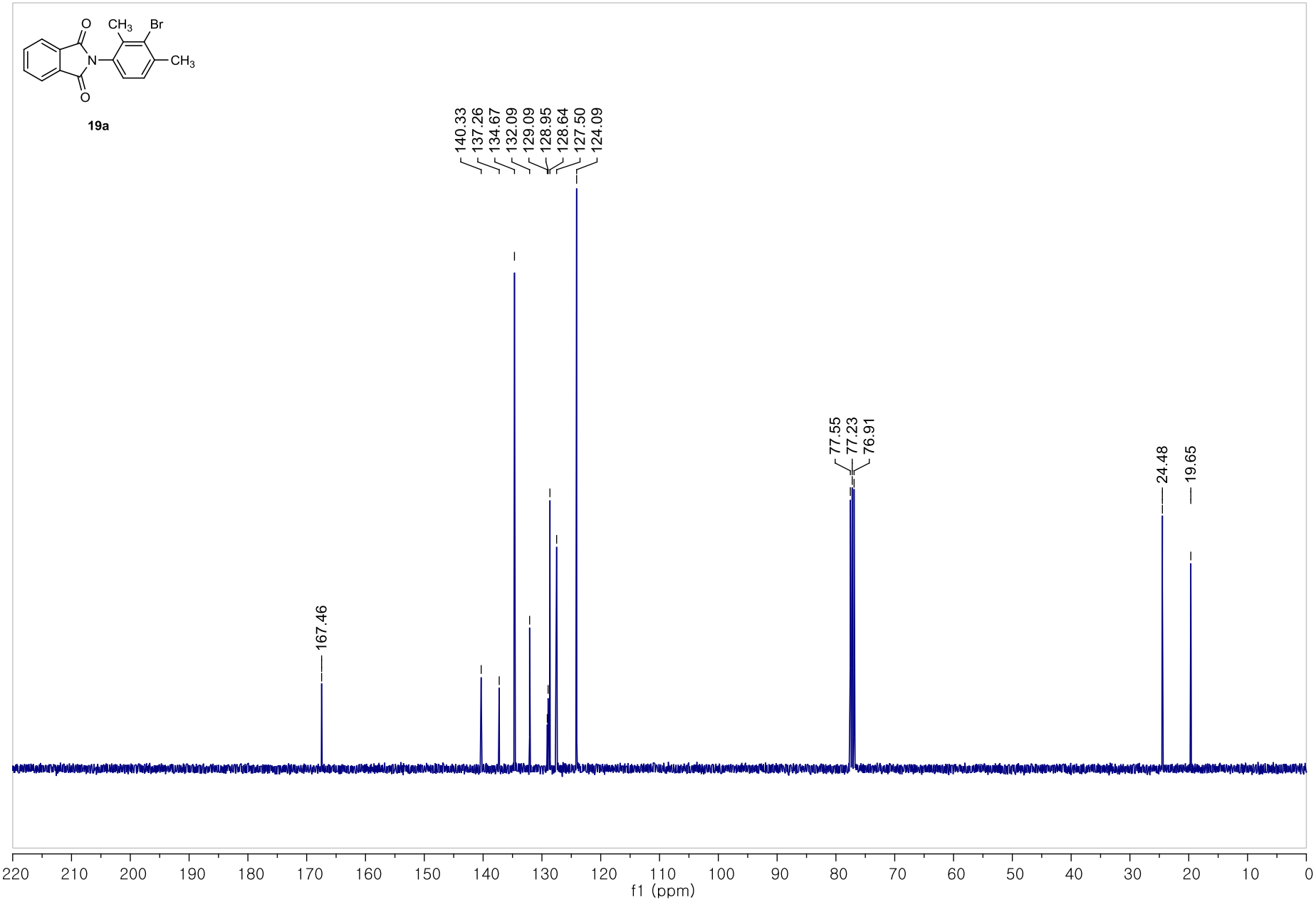

18b
f1 (ppm)

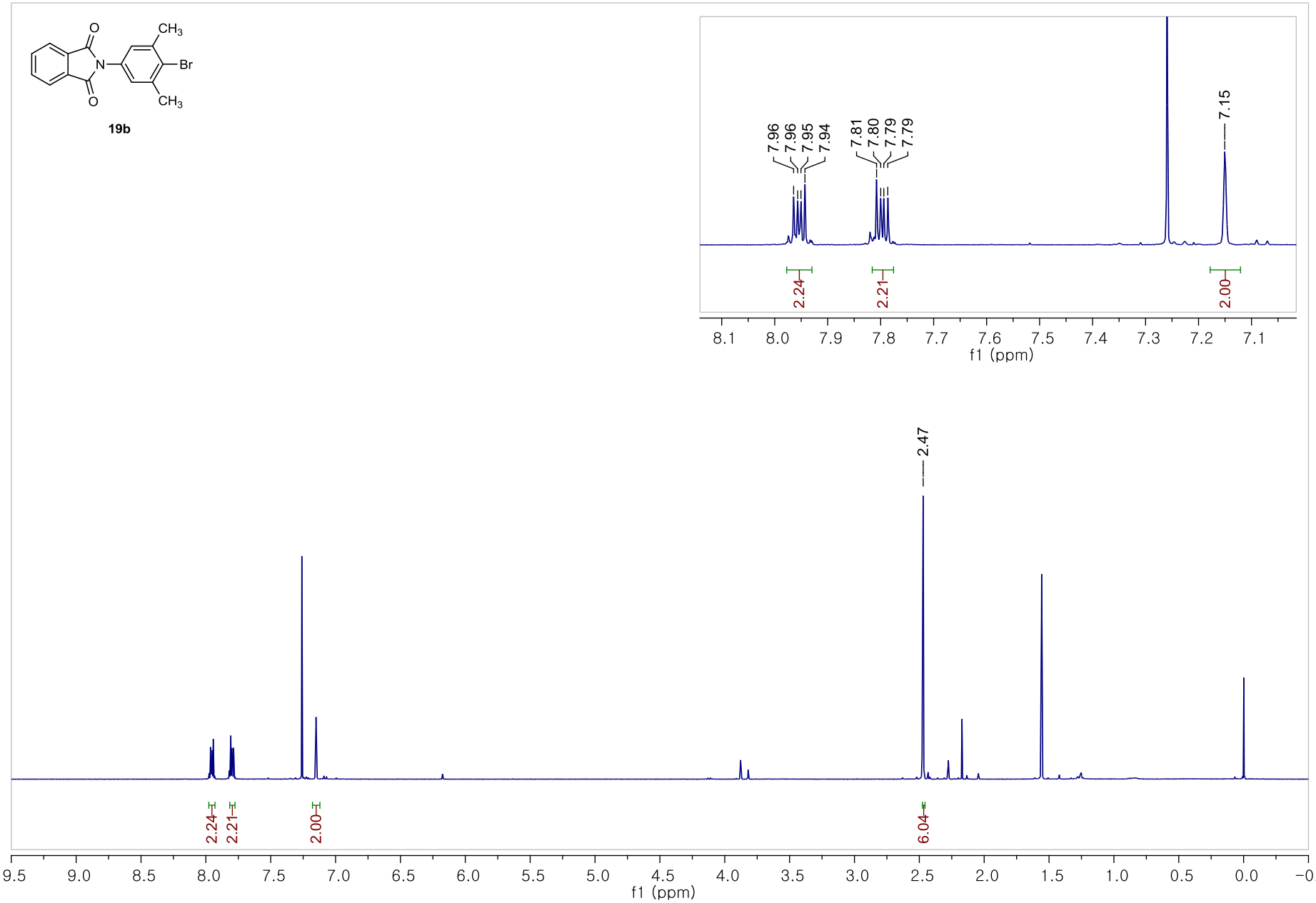

18b
172.53
172.15
168.88
168.22
167.57
167.44
166.52
155.35
155.27
150.04
145.44
134.68
134.64
132.85
132.04
131.98
131.66
131.17
130.78
130.31
124.17
124.06
124.04
123.72
122.90
122.53
80.28
80.09
77.55
77.23
76.91
54.41
53.80
52.66
52.54
37.73
33.61
28.45
28.36
21.31
21.13
f1 (ppm)

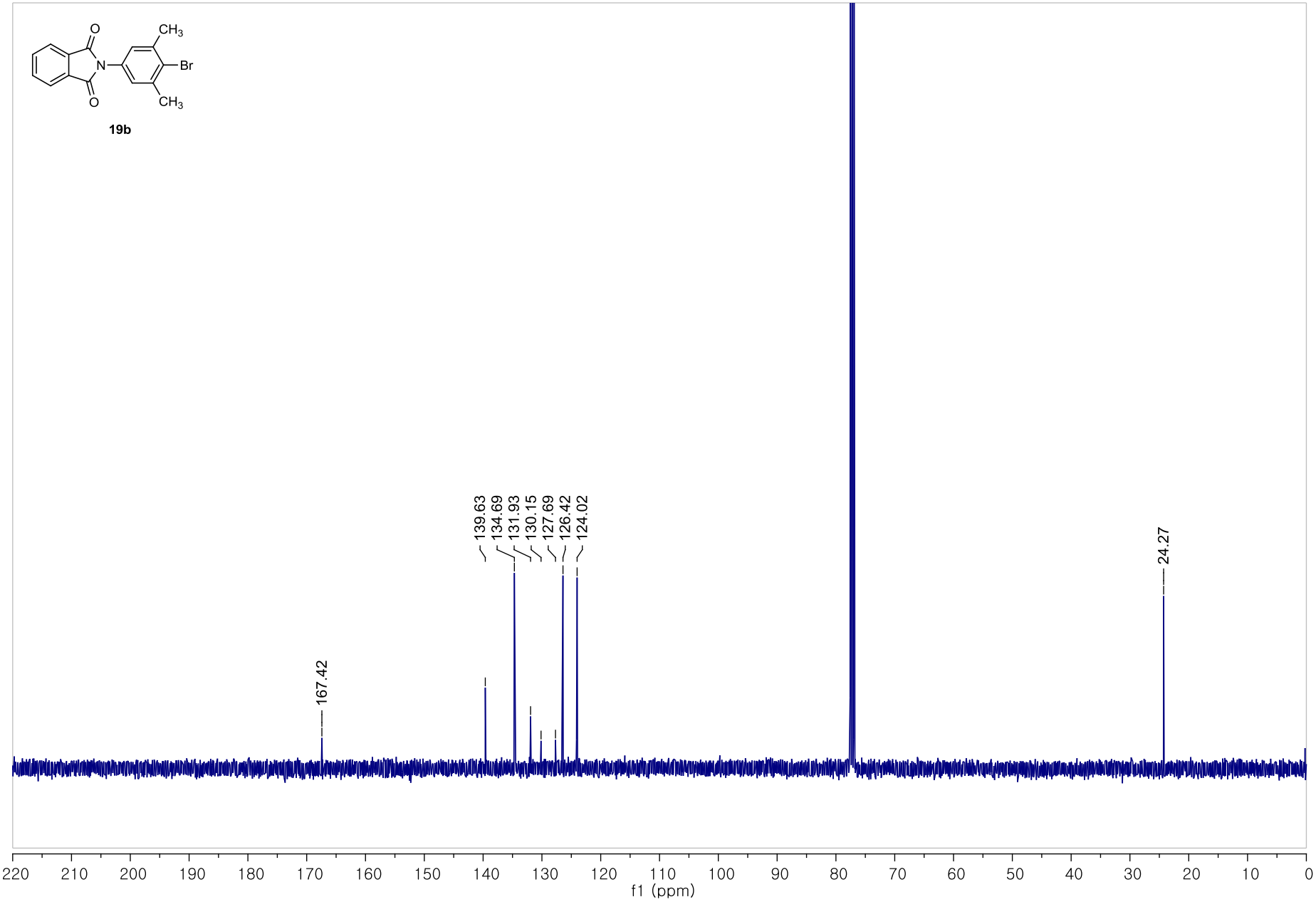

19a
19b
a+b
a+b
a (1H)
b (2H)
a (1H)
a (3H)
b (6H)
a (3H)
4.03
2.00
3.81
11.60
6.23
11.32
f1 (ppm)
7.96
7.95
7.94
7.94
7.93
7.92
7.80
7.80
7.79
7.78
7.78
7.77
7.26
7.24
7.22
7.16
7.10
7.08
2.47
2.46
2.28
9.85
10.44
4.03
2.00
3.81
11.60
6.23
11.32
f1 (ppm)

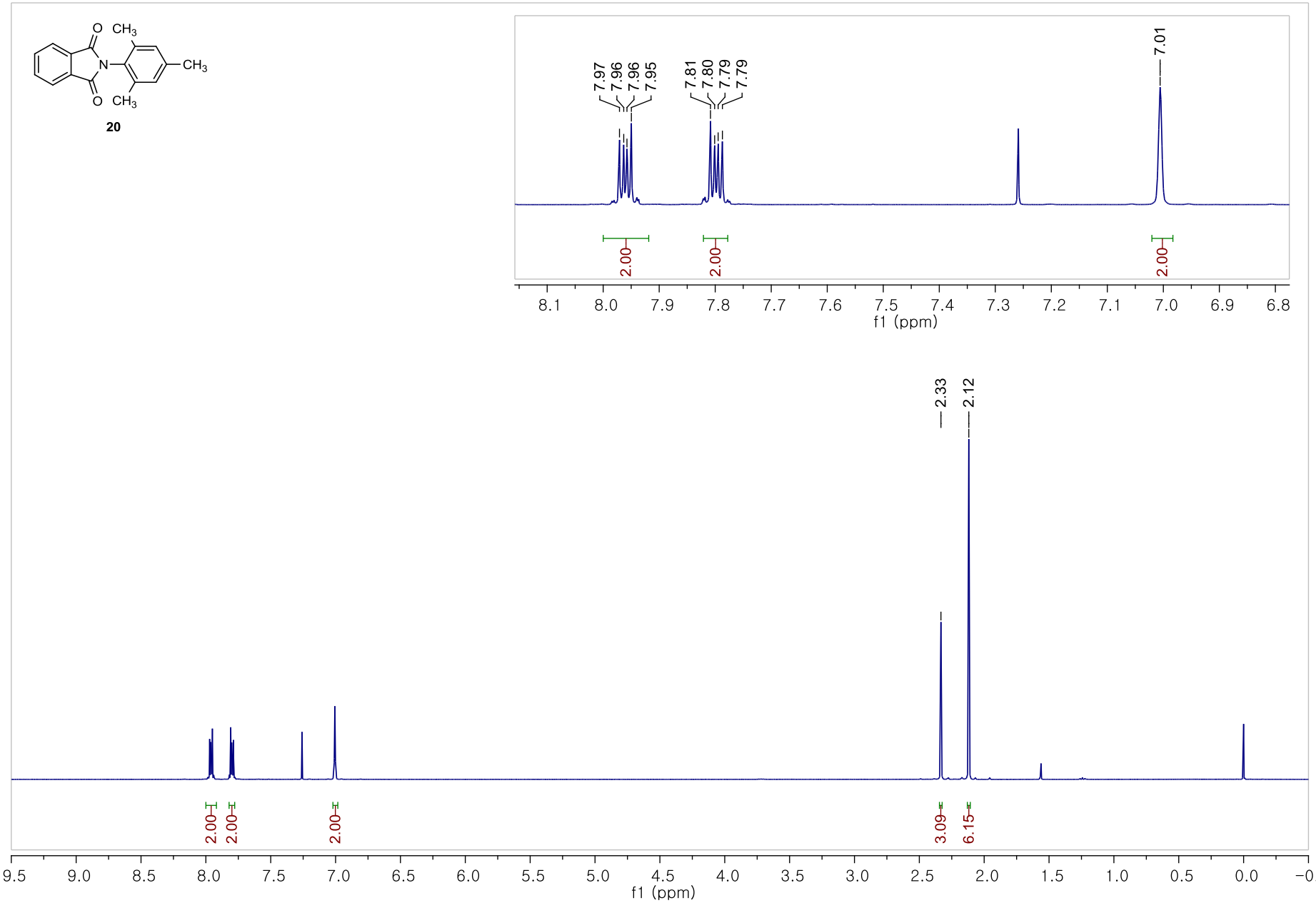

19a
19b
140.2
139.5
137.2
134.6
132.0
131.8
130.1
129.1
128.9
128.6
127.6
127.5
126.3
124.0
123.9
167.4
167.3
77.7
77.2
76.8
24.4
24.2
19.6
140.23
139.52
137.19
134.61
132.02
131.83
130.13
129.07
128.87
128.58
127.57
127.46
126.34
124.01
123.91
f1 (ppm)

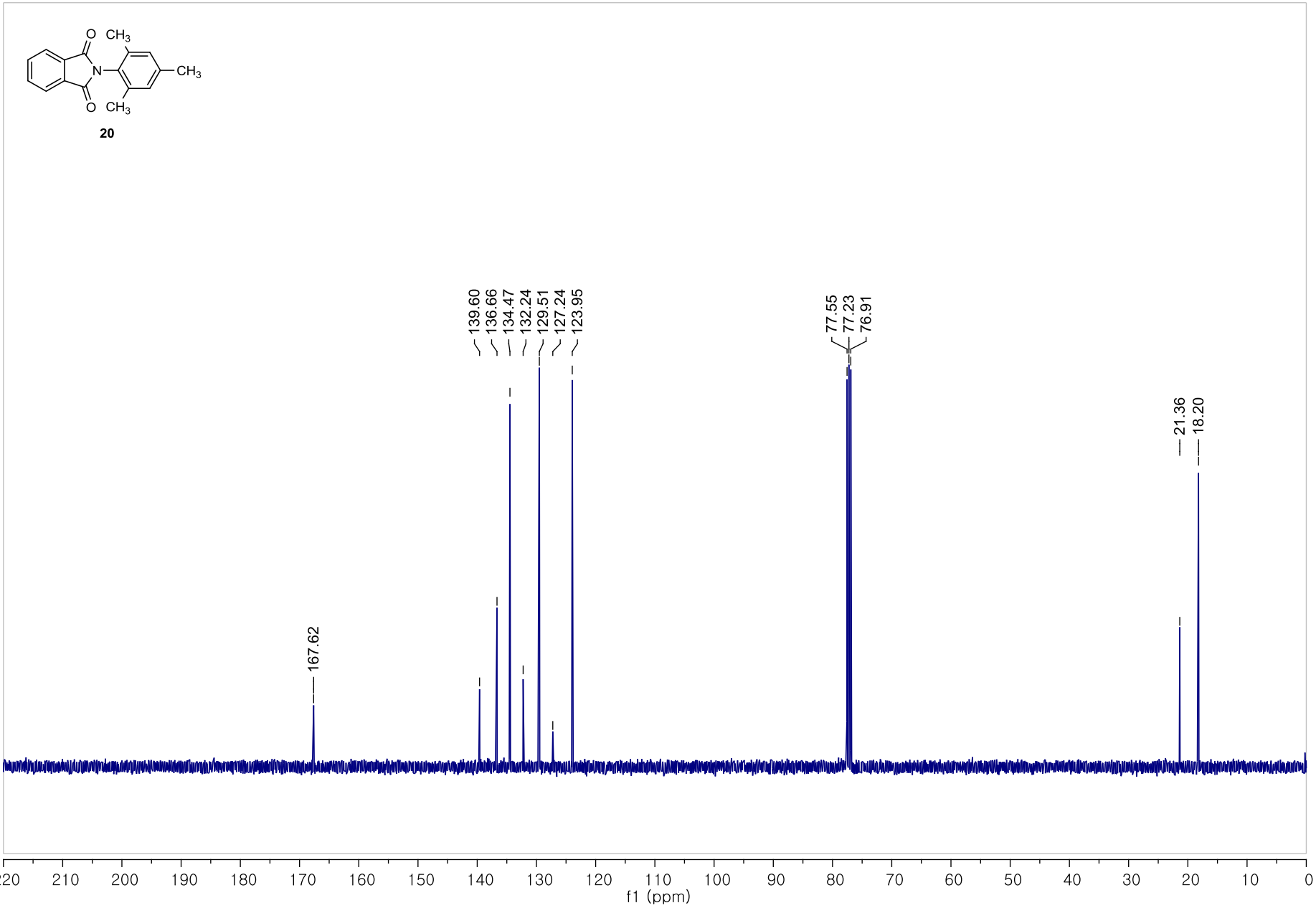

O
CH3
Br
N
CH3
O
19a
7.97
7.97
7.97
7.96
7.96
7.95
7.95
7.82
7.82
7.81
7.81
7.80
7.80
7.26
7.25
7.23
7.09
7.07
2.00
2.12
1.03
0.99
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
2.00
2.12
1.03
0.99
3.25
3.10
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

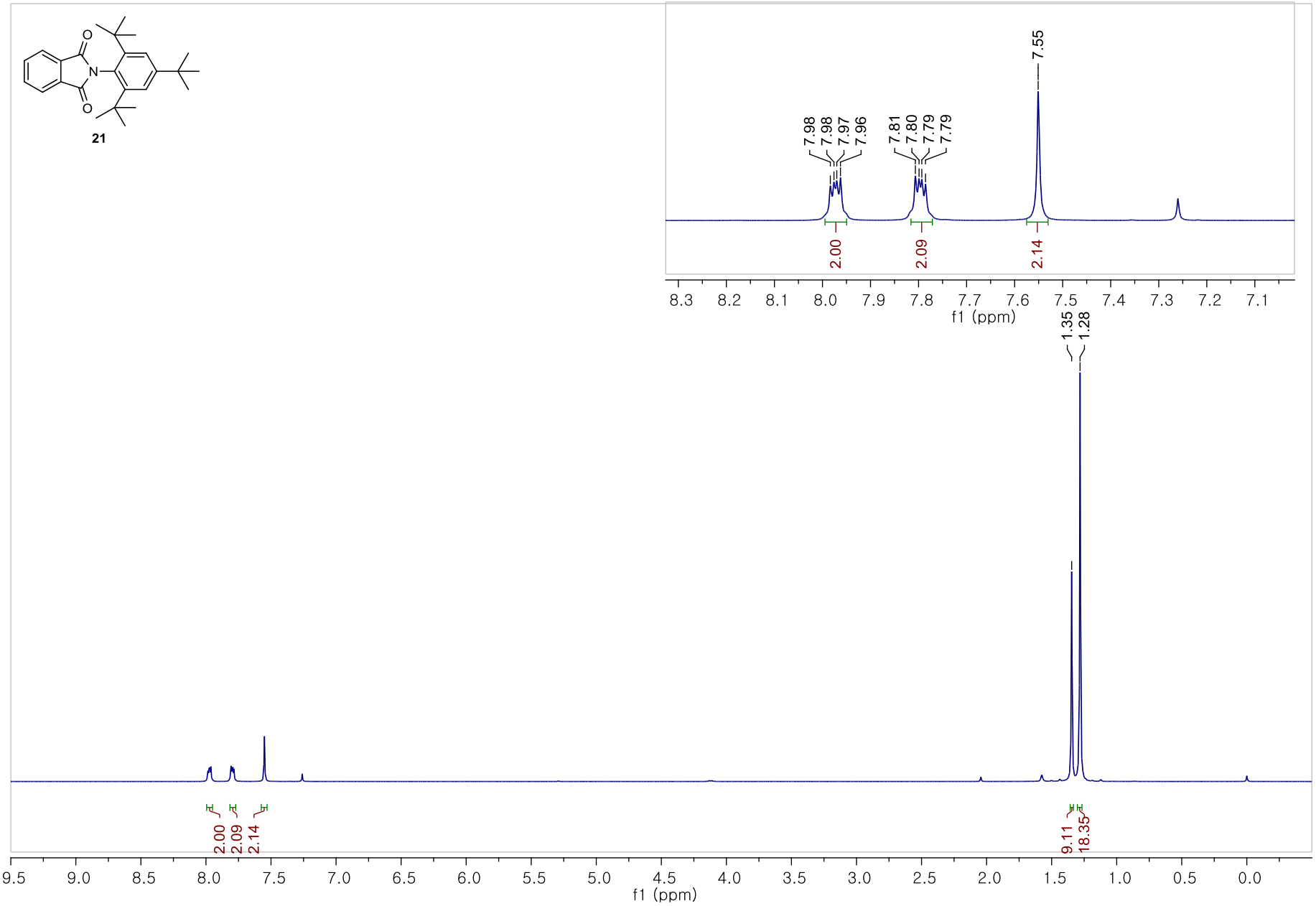

19a
140.33
137.26
134.67
132.09
129.09
128.95
128.64
127.50
124.09
77.55
77.23
76.91
24.48
19.65
167.46
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

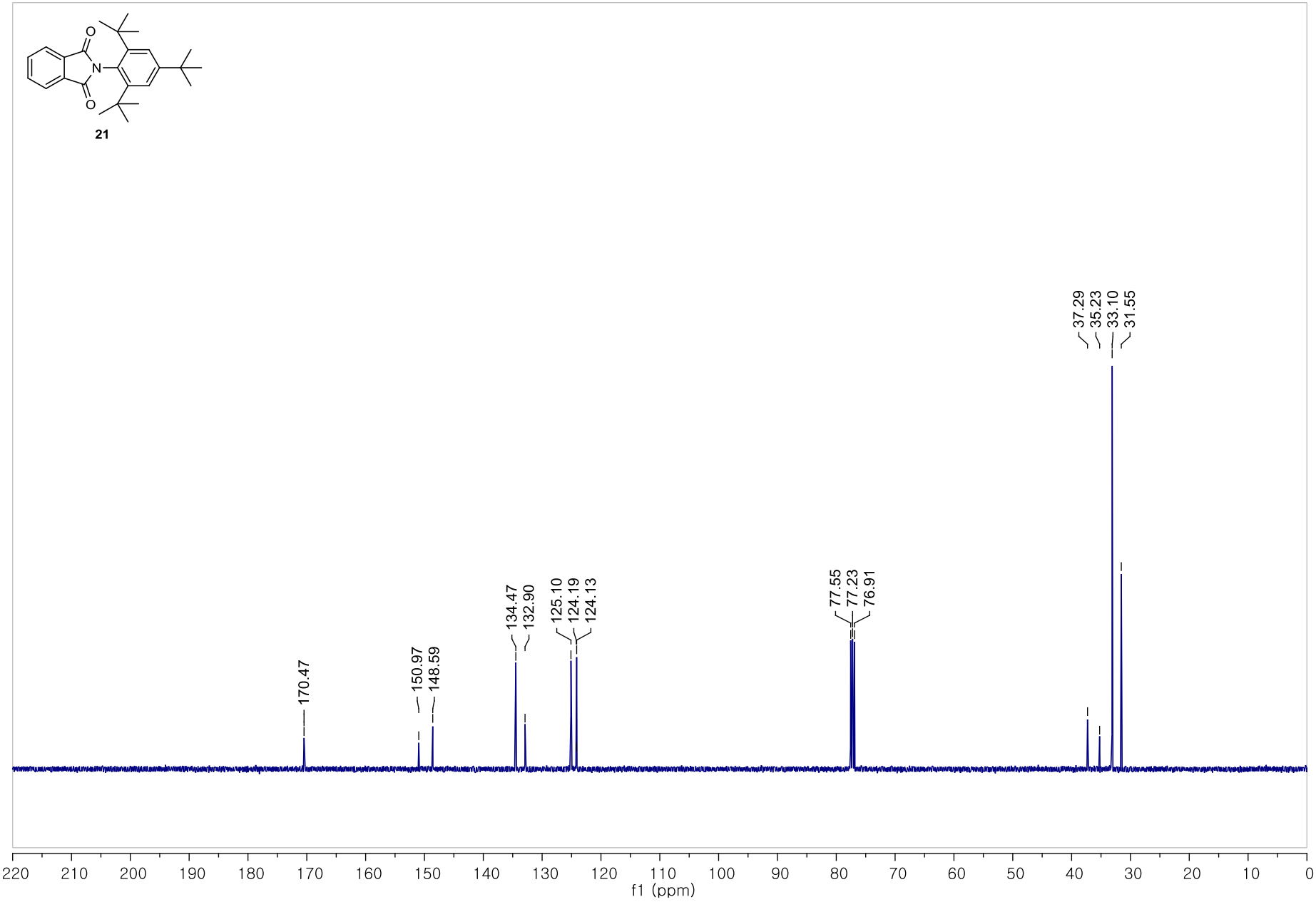

19b
7.96
7.96
7.95
7.94
7.81
7.80
7.79
7.79
7.15
2.24
2.21
2.00
f1 (ppm)
2.47
2.24
2.21
2.00
6.04
f1 (ppm)

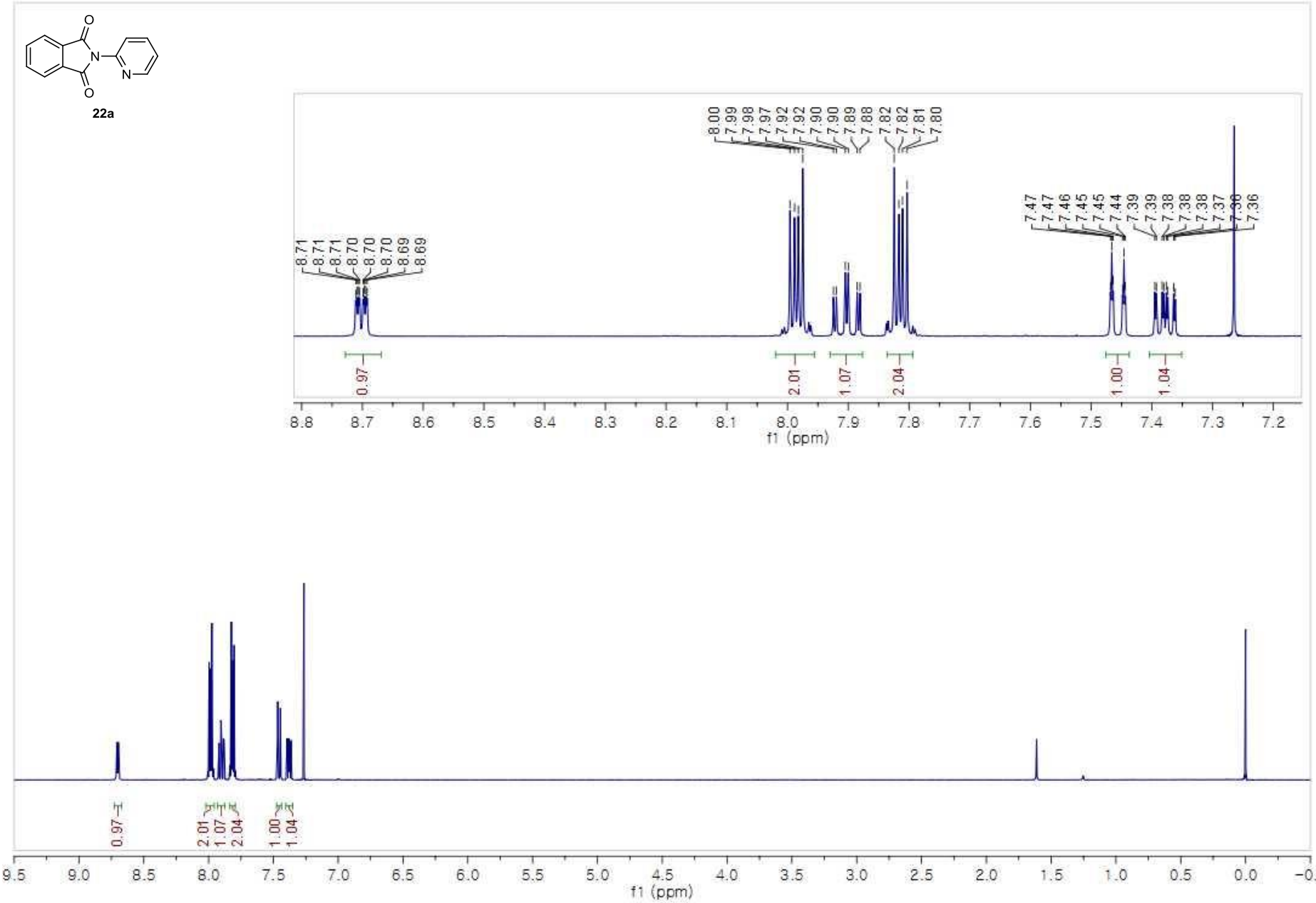

O
CH3
N
Br
O
CH3
19b
167.42
139.63
134.69
131.93
130.15
127.69
126.42
124.02
24.27
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

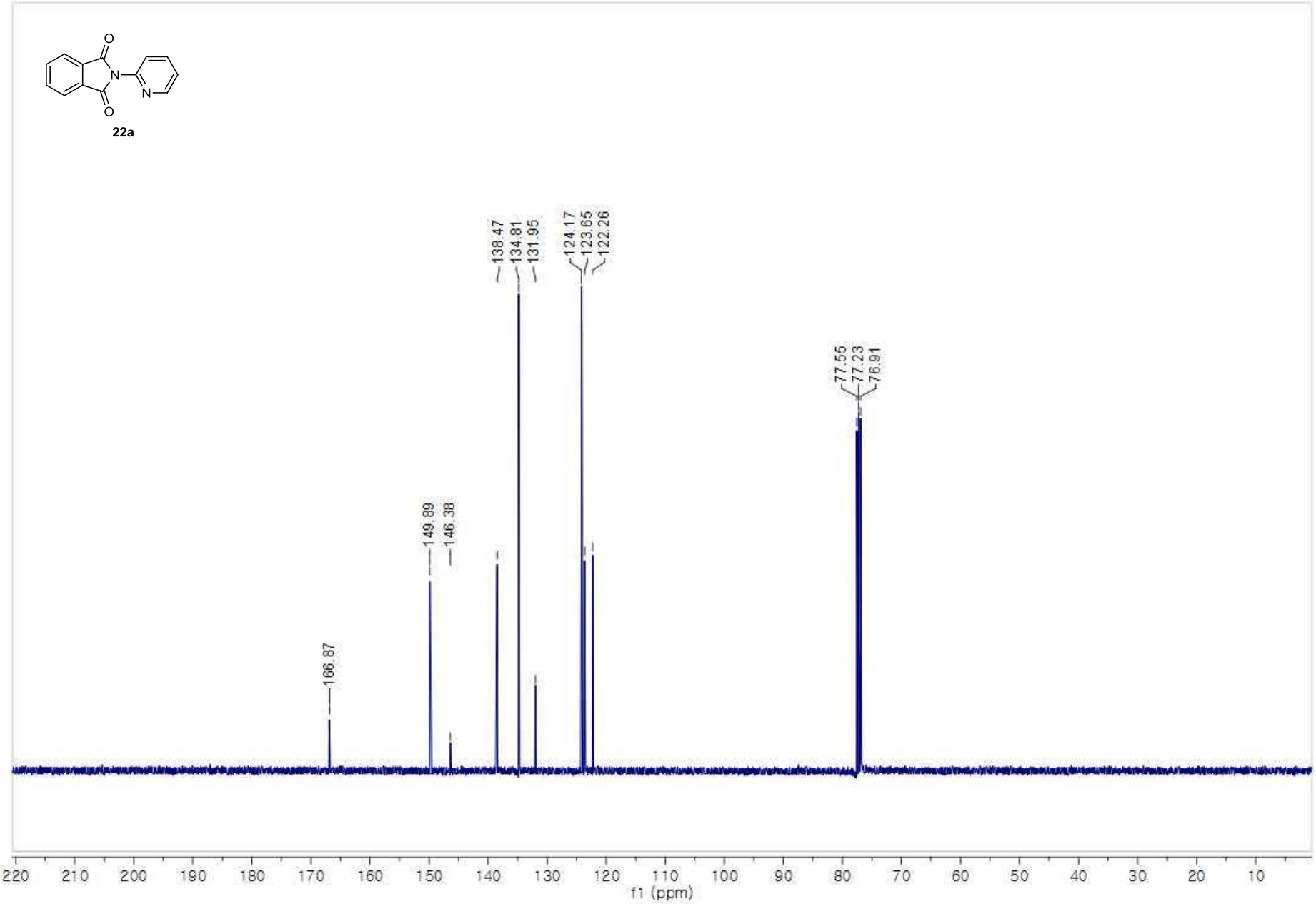

O
CH3
N
CH3
O
CH3
20
7.97
7.96
7.96
7.95
7.81
7.80
7.79
7.79
7.01
2.00
2.00
2.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)
2.33
2.12
2.00
2.00
2.00
3.09
6.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

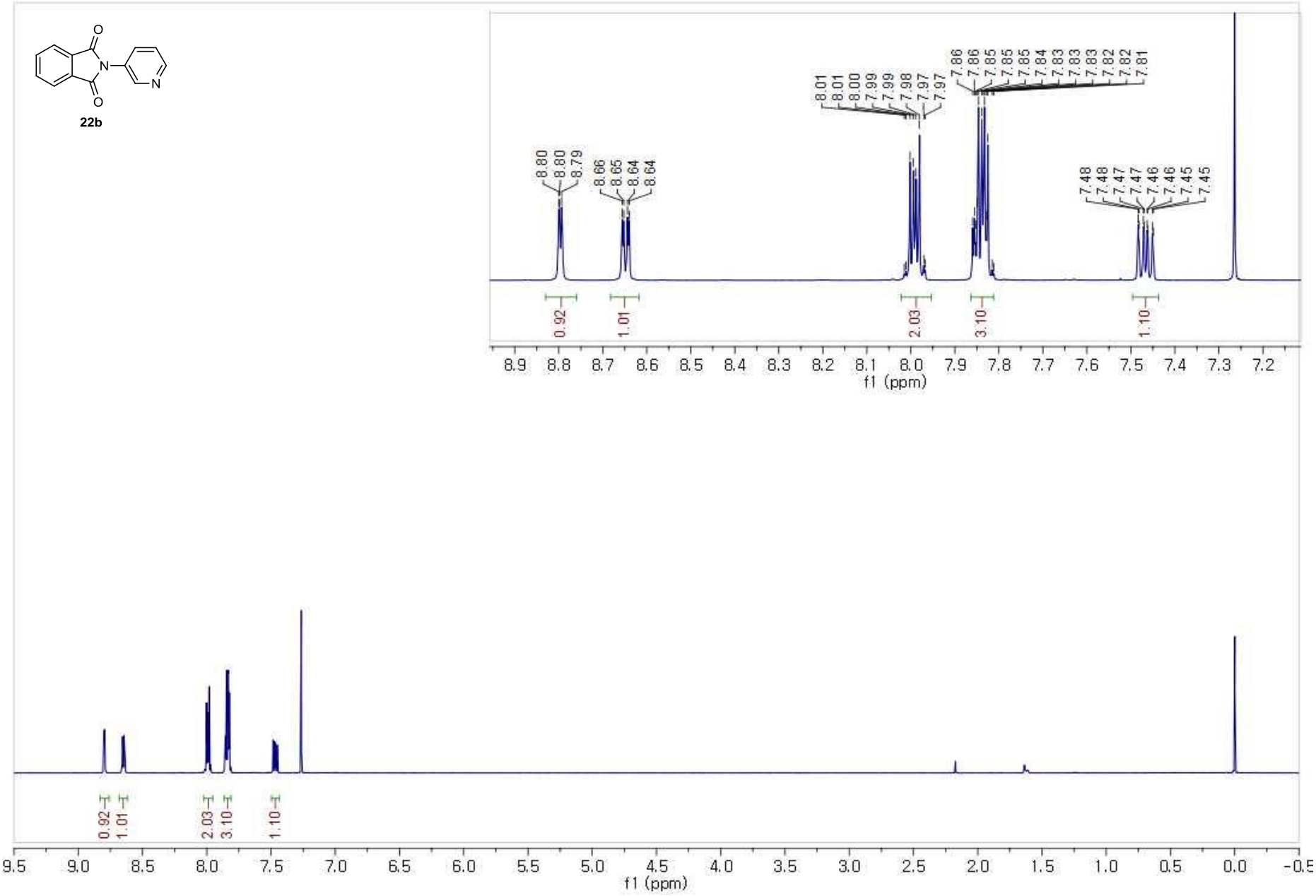

O
CH3
N
CH3
O
CH3
20
139.60
136.66
134.47
132.24
129.51
127.24
123.95
77.55
77.23
76.91
21.36
18.20
167.62
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

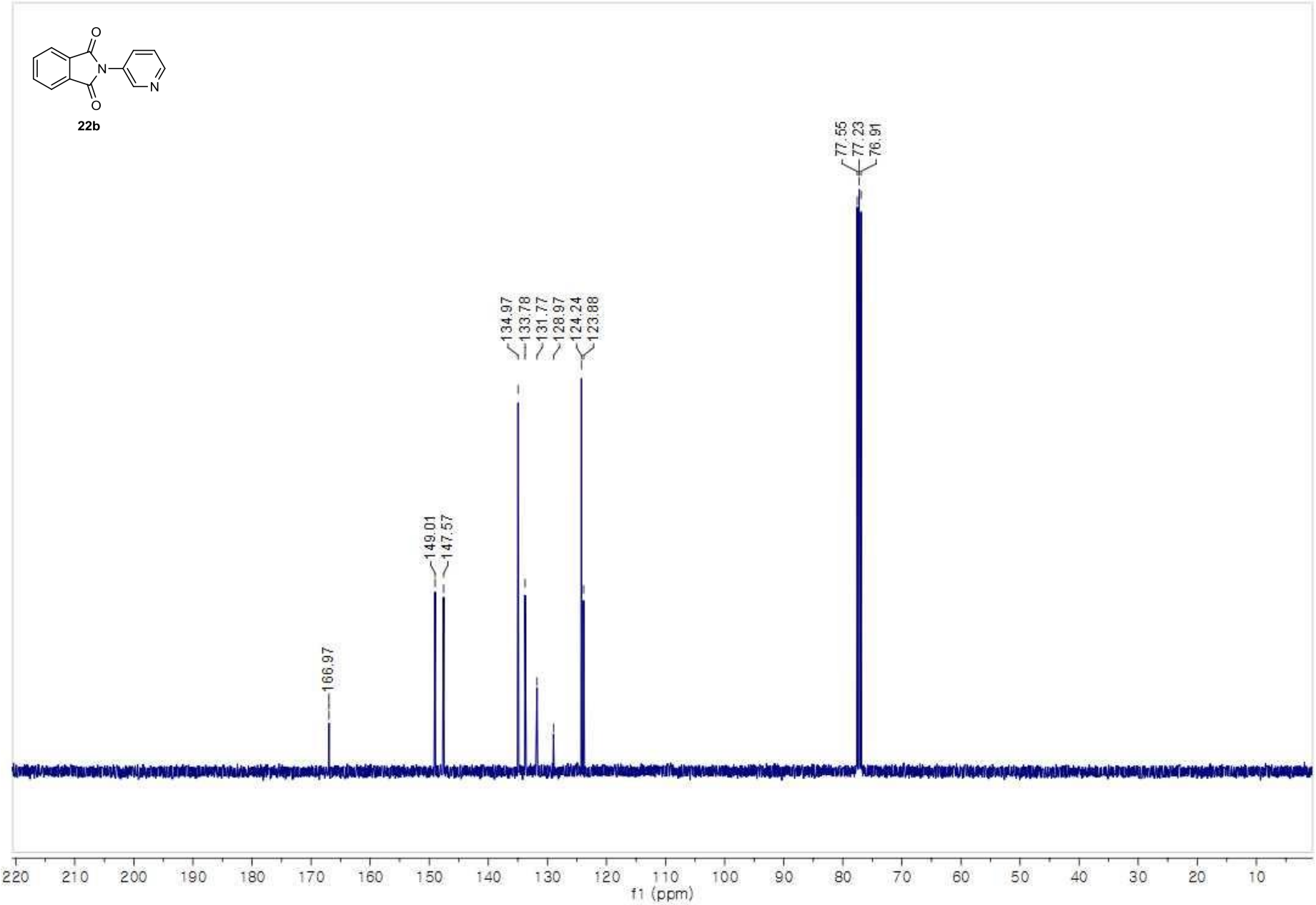

21
7.98
7.98
7.97
7.96
7.81
7.80
7.79
7.79
7.55
2.00
2.09
2.14
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
1.35
1.28
2.00
2.09
2.14
9.11
18.35
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

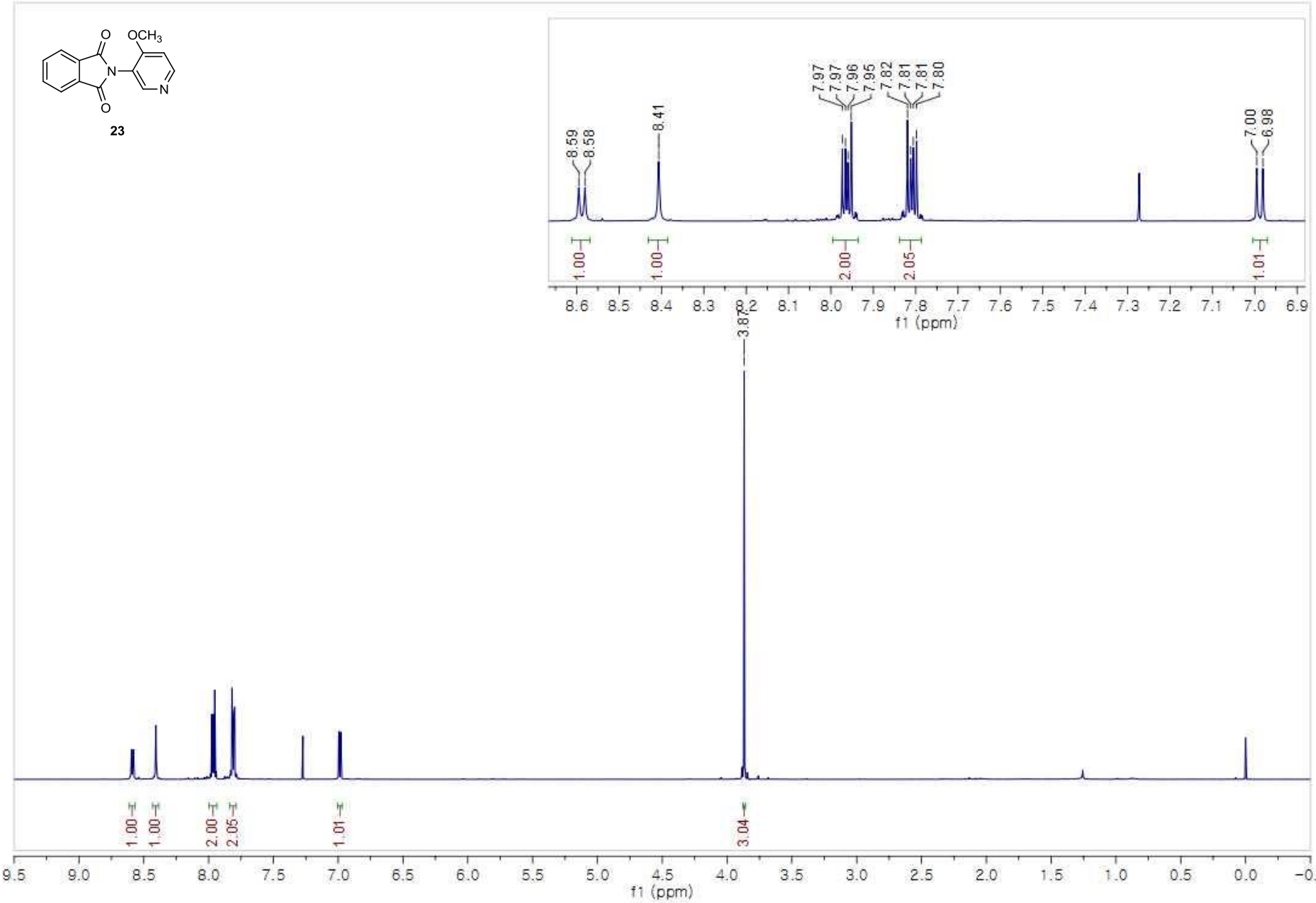

21
170.47
150.97
148.59
134.47
132.90
125.10
124.19
124.13
77.55
77.23
76.91
37.29
35.23
33.10
31.55
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

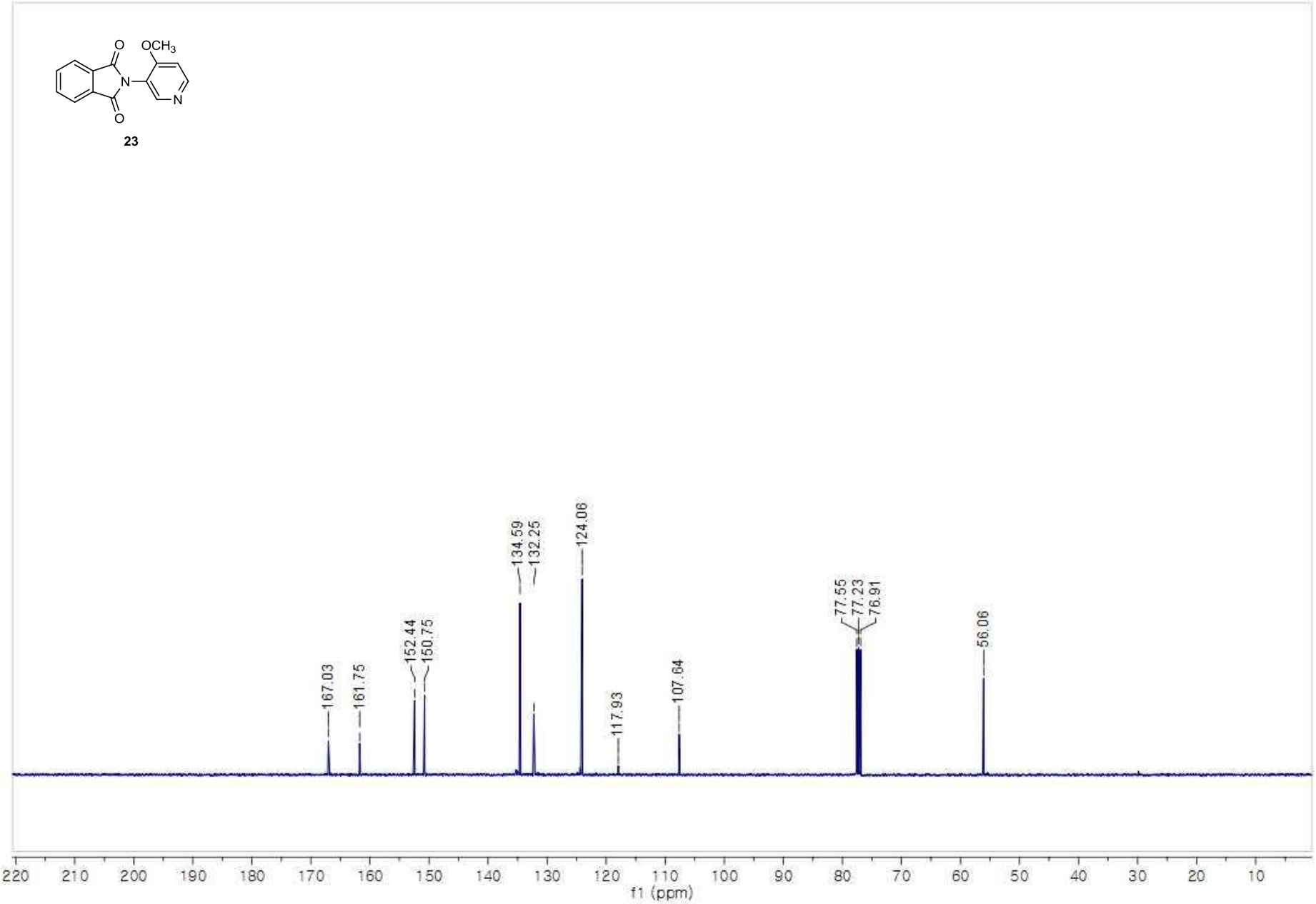

22a
8.71
8.71
8.71
8.70
8.70
8.70
8.69
8.69
8.00
7.99
7.98
7.97
7.92
7.92
7.90
7.90
7.89
7.88
7.82
7.82
7.81
7.80
7.47
7.47
7.46
7.45
7.45
7.44
7.39
7.39
7.38
7.38
7.38
7.37
7.36
7.36
0.97
2.01
1.07
2.04
1.00
1.04
f1 (ppm)
f1 (ppm)

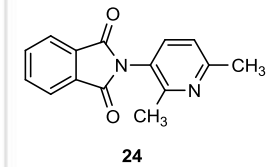

22a
166.87
149.89
146.38
138.47
134.81
131.95
124.17
123.65
122.26
77.55
77.23
76.91
f1 (ppm)


22b
8.80
8.80
8.79
8.66
8.65
8.64
8.64
8.01
8.01
8.00
7.99
7.99
7.98
7.97
7.97
7.86
7.86
7.85
7.85
7.85
7.84
7.83
7.83
7.83
7.82
7.82
7.81
7.48
7.48
7.47
7.47
7.46
7.46
7.45
7.45
0.92
1.01
2.03
3.10
1.10
f1 (ppm)

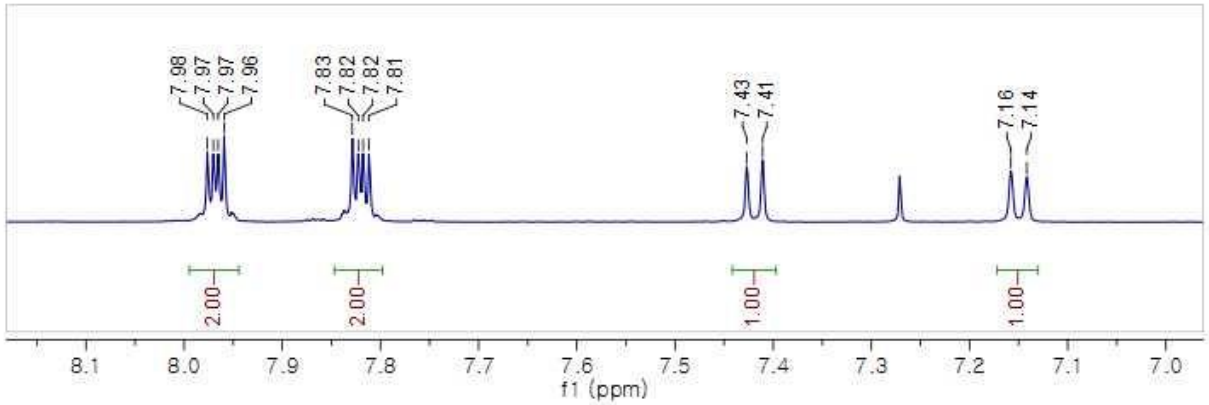

22b
166.97
149.01
147.57
134.97
133.78
131.77
128.97
124.24
123.88
77.55
77.23
76.91
f1 (ppm)

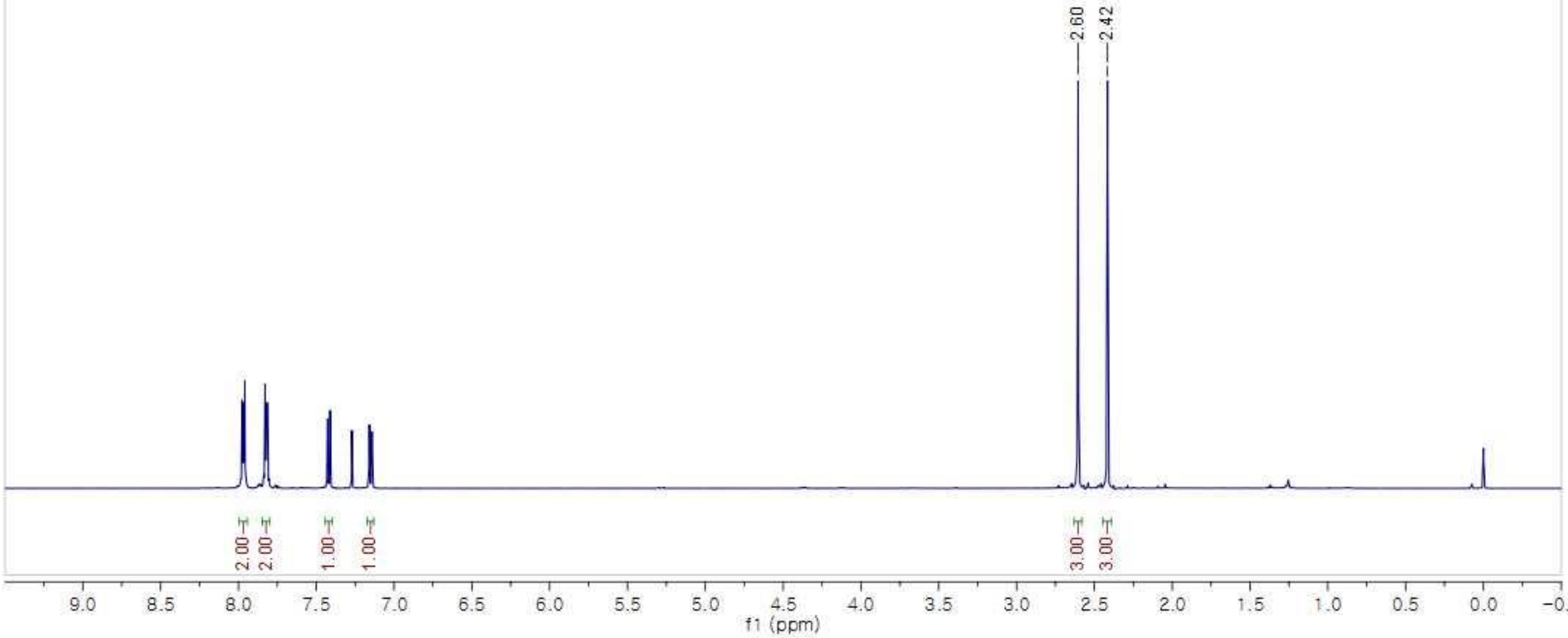

OCH3
O
N
N
O
23
8.59
8.58
8.41
7.97
7.97
7.96
7.95
7.82
7.81
7.81
7.80
7.00
6.98
1.00
1.00
2.00
2.05
1.01
f1 (ppm)
3.87
1.00
1.00
2.00
2.05
1.01
3.04
f1 (ppm)

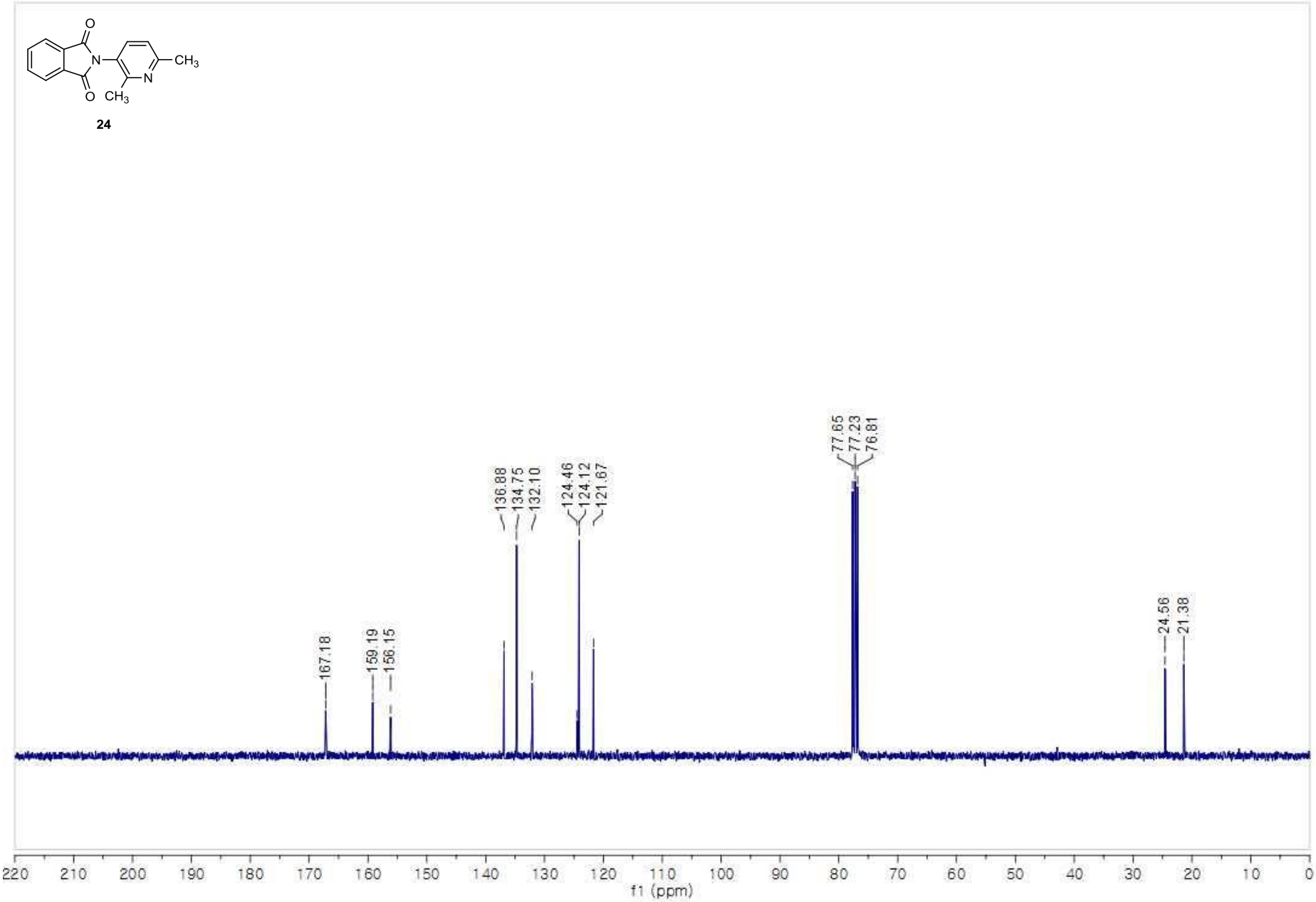

O
OCH3
N
N
O
O
23
167.03
161.75
152.44
150.75
134.59
132.25
124.06
117.93
107.64
77.55
77.23
76.91
56.06
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

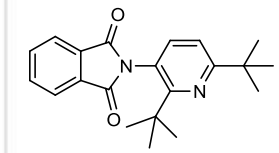

O
N
CH3
N
O
CH3

24

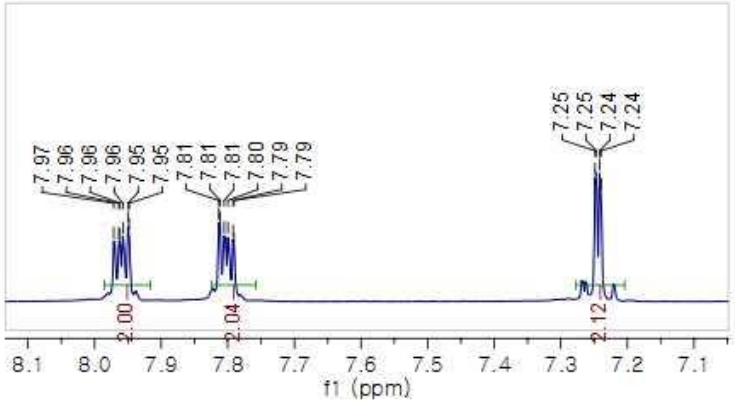

7.98
7.97
7.97
7.96
7.83
7.82
7.82
7.81
7.43
7.41
7.16
7.14
2.00
2.00
1.00
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)

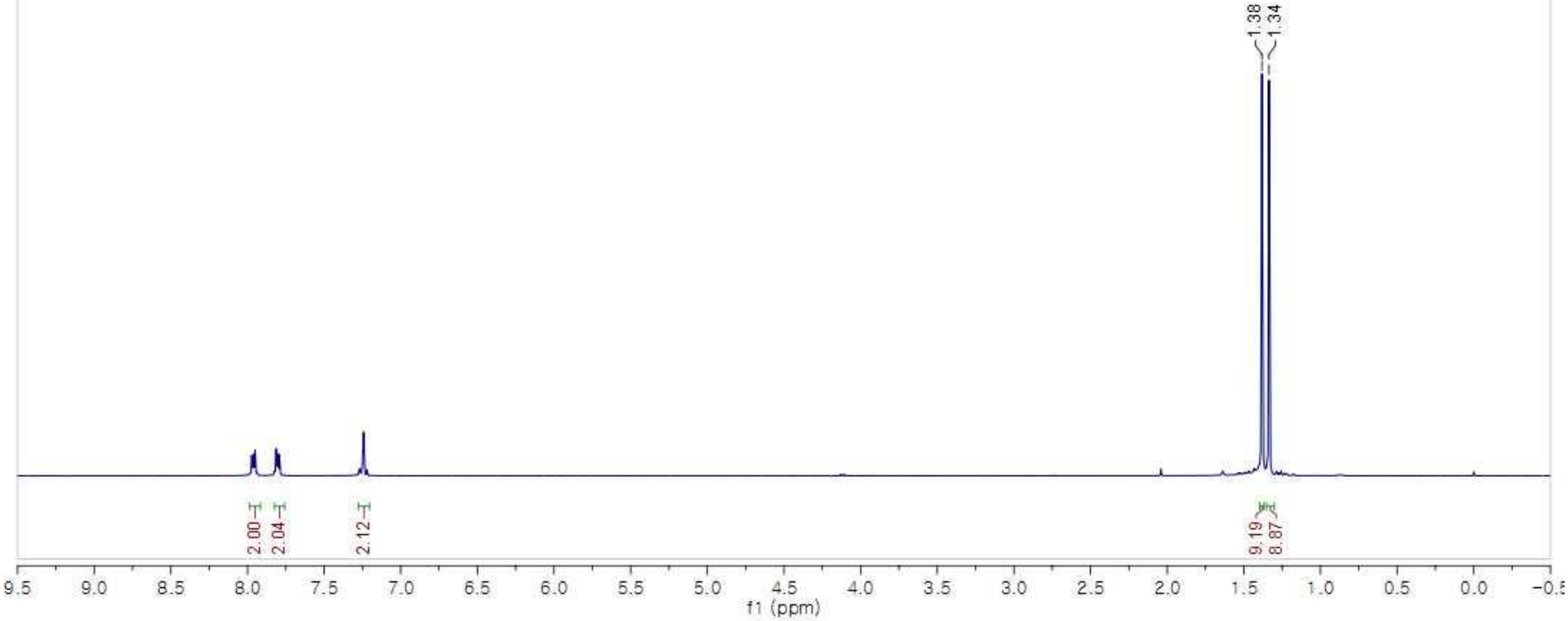

2.60
2.42
2.00
2.00
1.00
1.00
3.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

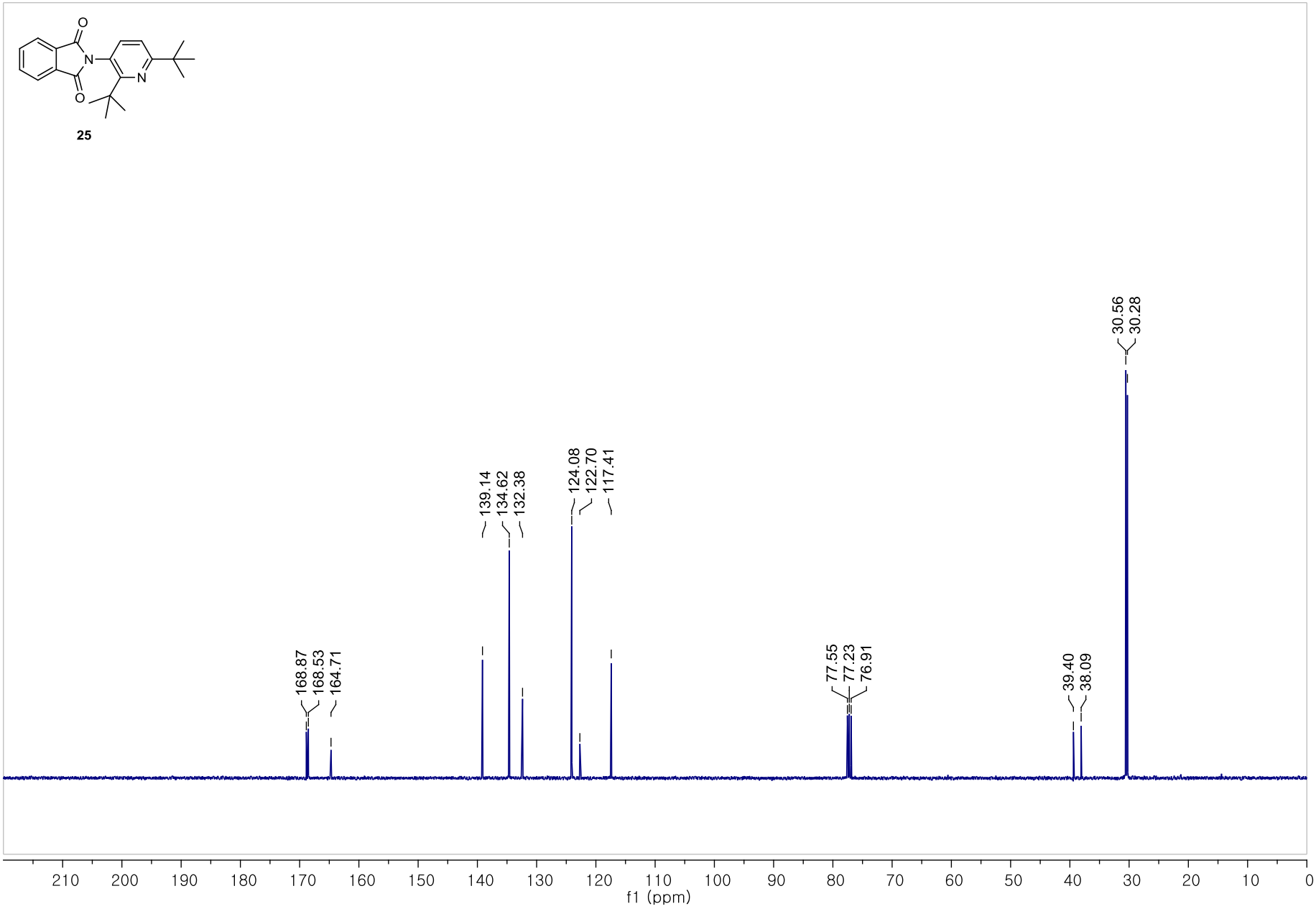

O
N
CH3
N
CH3
O
24
167.18
159.19
156.15
136.88
134.75
132.10
124.46
124.12
121.67
77.65
77.23
76.81
24.56
21.38
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

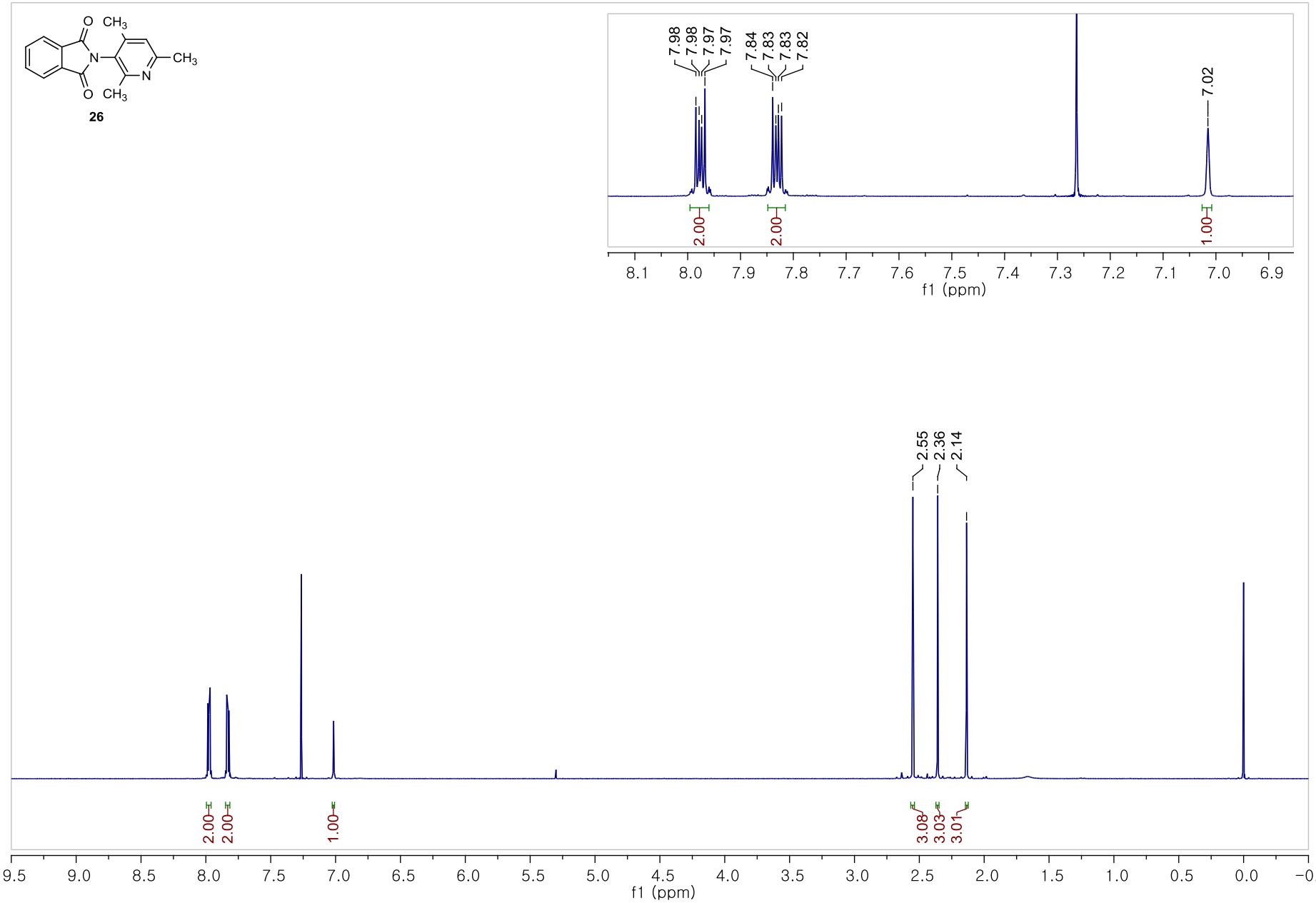


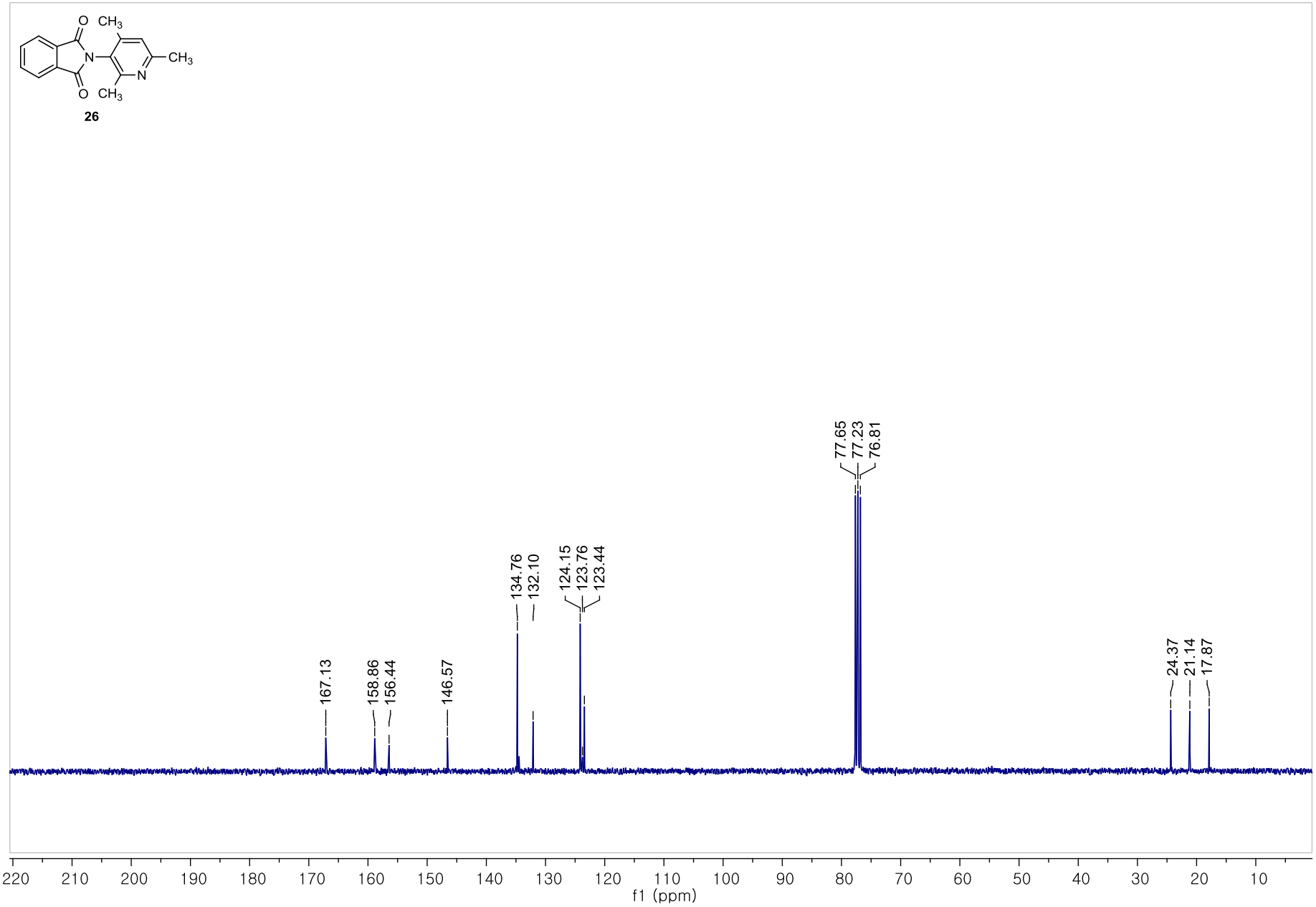
25

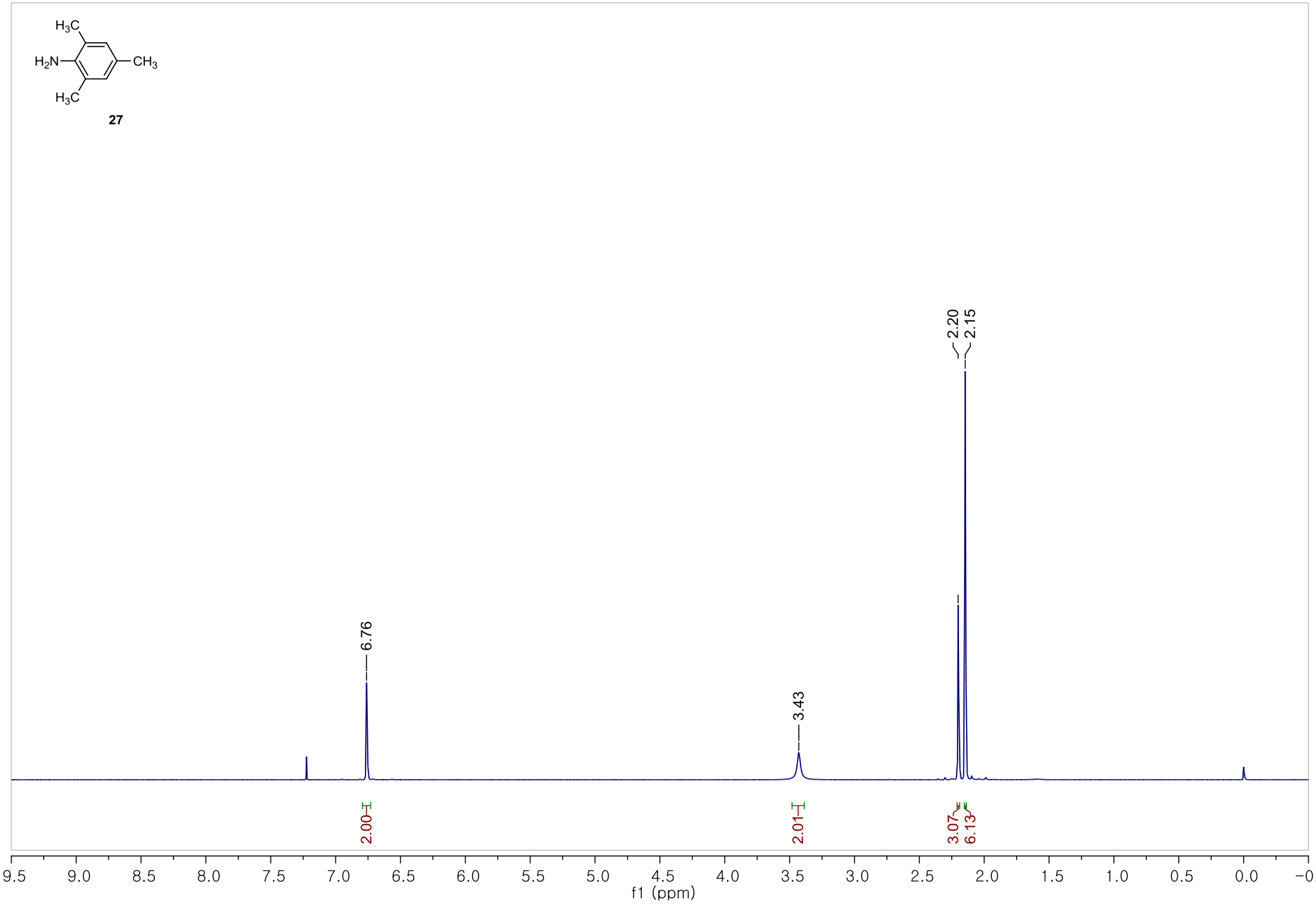

7.97
7.96
7.96
7.96
7.95
7.95
7.81
7.81
7.81
7.80
7.79
7.79
7.25
7.25
7.24
7.24
2.00
2.04
2.12
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)

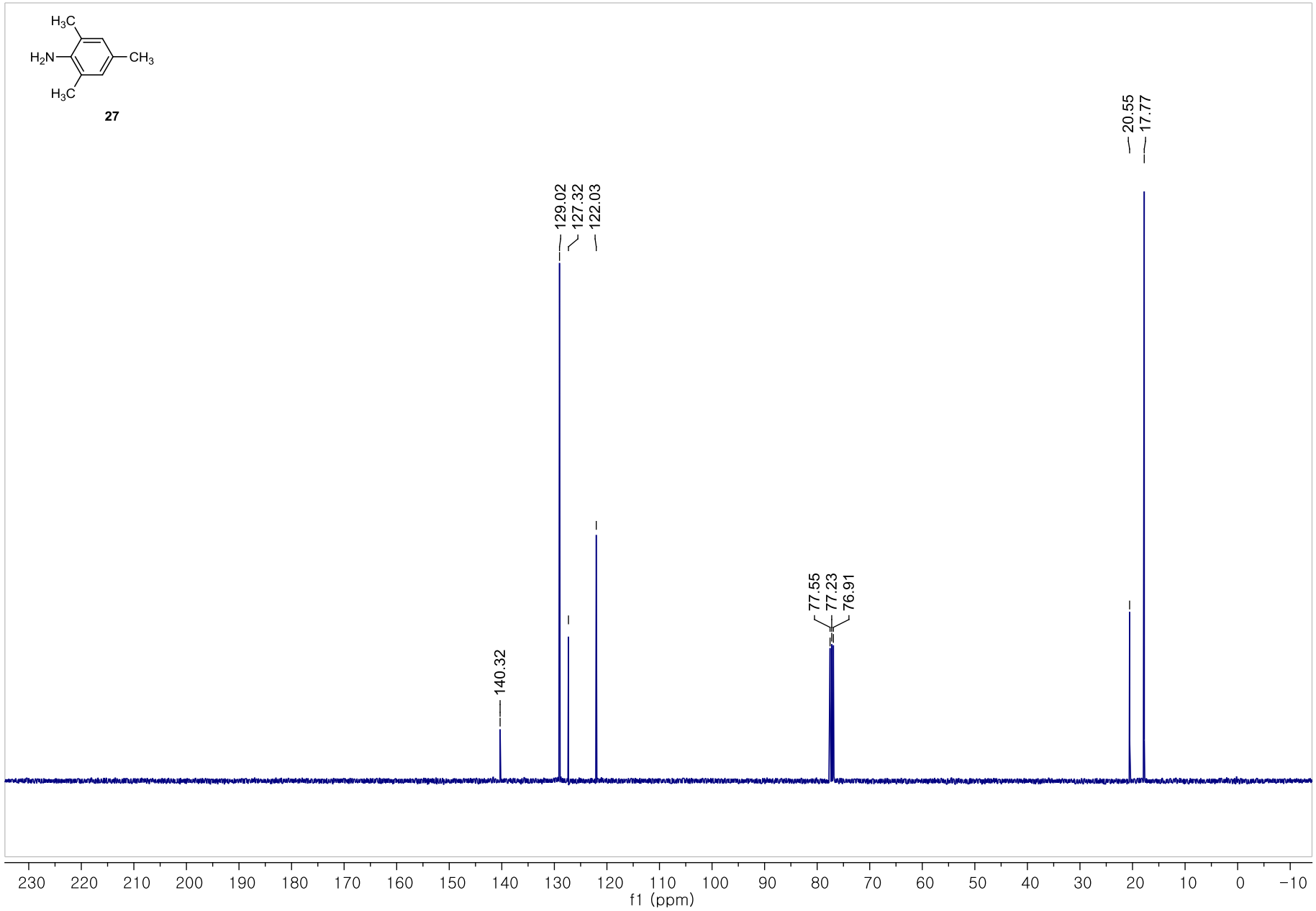

1.38
1.34
2.00
2.04
2.12
9.19
8.87
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

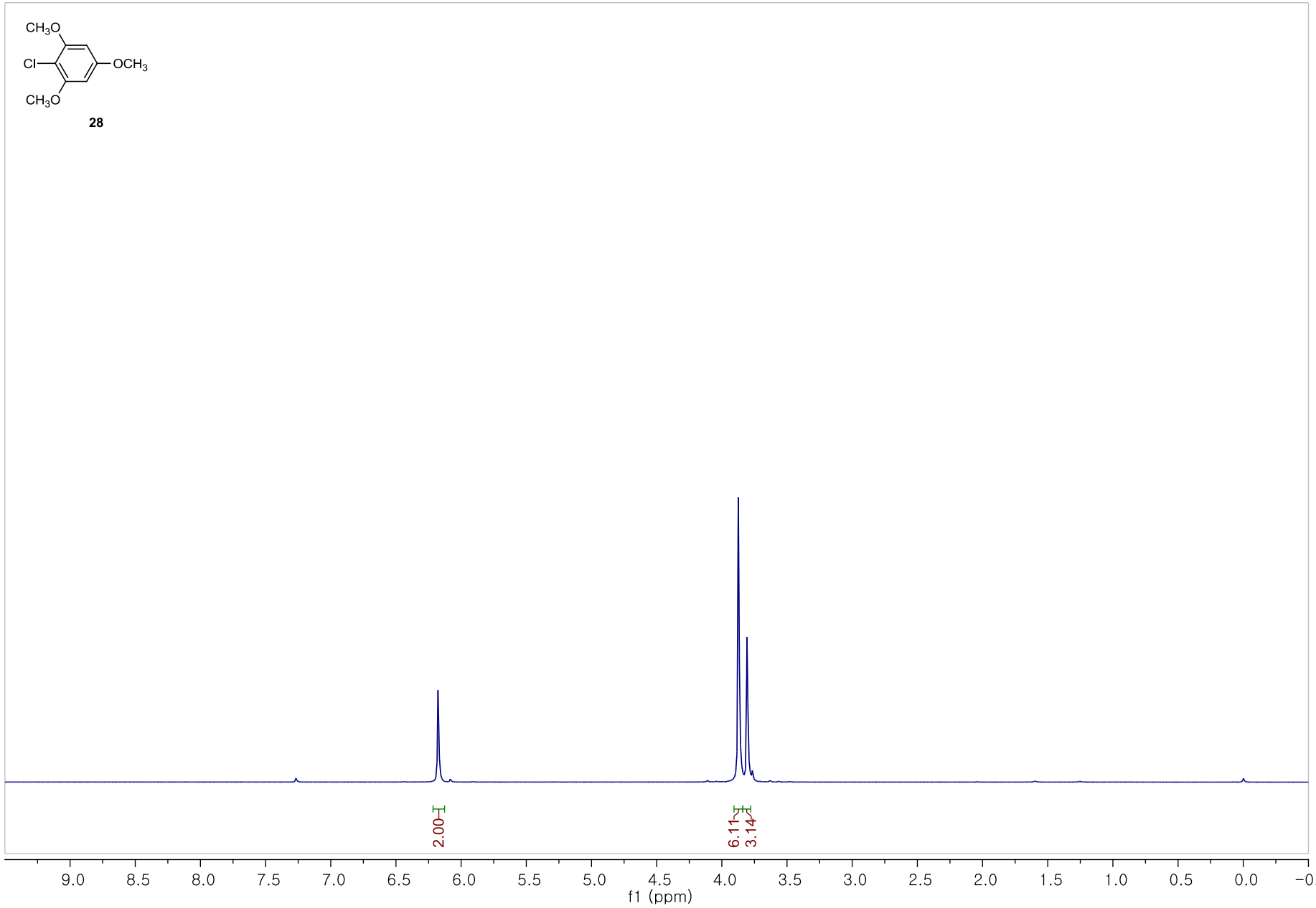

25
168.87
168.53
164.71
139.14
134.62
132.38
124.08
122.70
117.41
77.55
77.23
76.91
39.40
38.09
30.56
30.28
f1 (ppm)

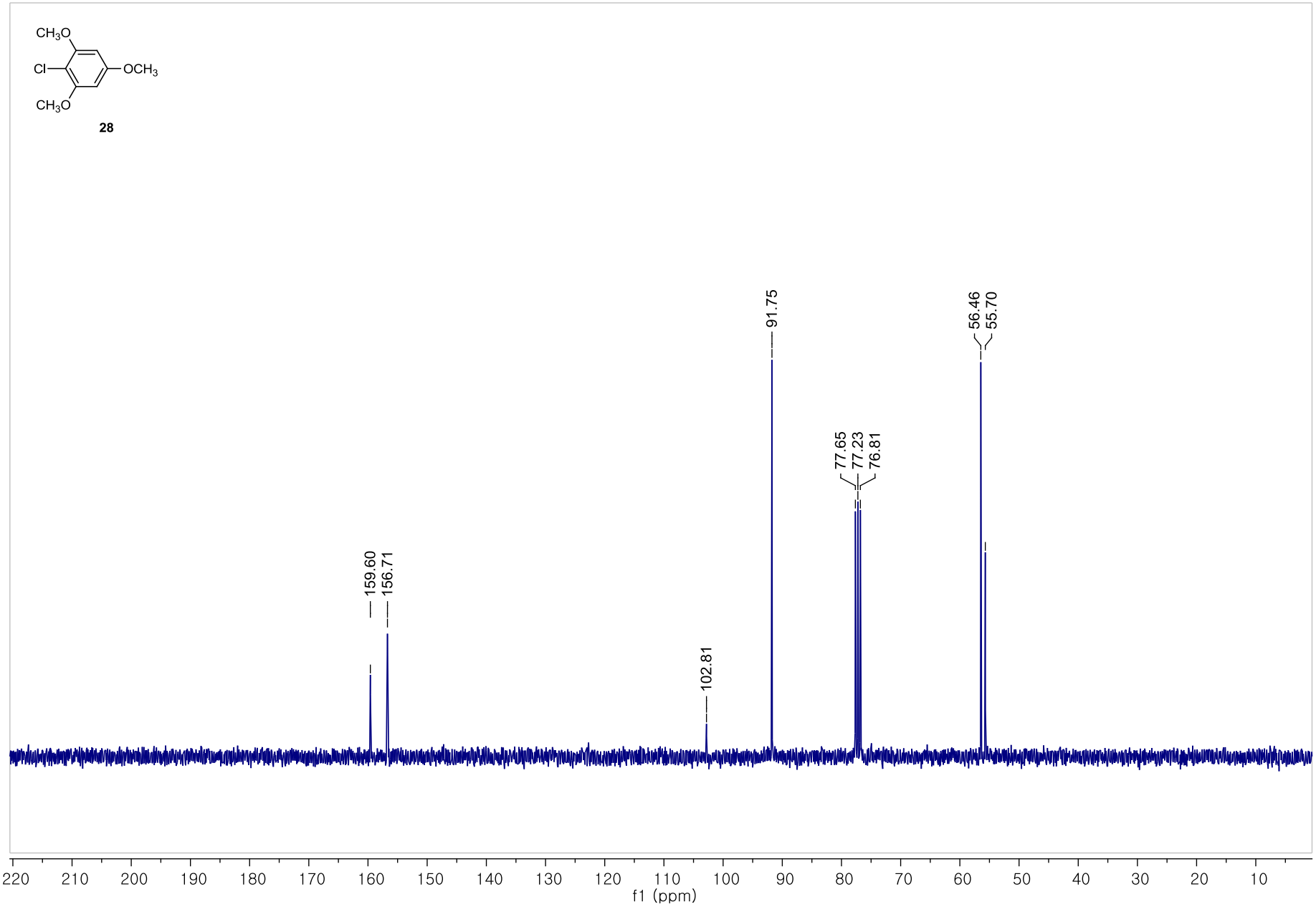

O
CH3
N
CH3
N
O
CH3
26
7.98
7.98
7.97
7.97
7.84
7.83
7.83
7.82
7.02
2.00
2.00
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
f1 (ppm)
2.55
2.36
2.14
2.00
2.00
1.00
3.08
3.03
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


O
CH3
N
CH3
N
O
CH3
O
26
167.13
158.86
156.44
146.57
134.76
132.10
124.15
123.76
123.44
77.65
77.23
76.81
24.37
21.14
17.87
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


H3C
H2N
CH3
H3C
27
6.76
3.43
2.20
2.15
2.00
2.01
3.07
6.13
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


H3C
H2N
CH3
H3C
27
20.55
17.77
129.02
127.32
122.03
77.55
77.23
76.91
140.32
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


CH3O
Cl
OCH3
CH3O
28
2.00
6.11
3.14
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CH3O
Cl
OCH3
CH3O
28
159.60
156.71
102.81
91.75
77.65
77.23
76.81
56.46
55.70
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)