Supporting Information for:

A practical base mediated synthesis of 1,2,4-triazoles enabled by deamination annulation strategy

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CONTENTS

1. General experiment details and materials

Experimental: All non-aqueous reactions and manipulations were using standard Schlenk techniques. All solvents before use were dried and degassed by standard methods and stored under nitrogen atmosphere. All reactions were monitored by TLC with silica gel-coated plates. NMR spectra were recorded on BRUKER Avence III 400 or 500 MHz spectrometers. Chemical shifts were reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (*J*) were reported in Hz and referred to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker MicroTOF-QII mass (ESI). GC analysis were performed on Agilent 7890 with OV-225 column or Hp-5 column. GC-MS analysis were performed with Agilent 7890A/5975C GC-MS system.

2. Optimization of the reaction conditions

Using a nitrogen-filled glove box, an oven-dried pressure tube (38 mL volume) was charged with a magnetic stirring bar, base, benzonitrile (**1a)**, phenyl hydrazine (**2a)** and solvents. Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (design temperature). After design time the reaction was cooled to room temperture, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Purification of the remainder by column chromatography on silica gel gave the corresponding product 1,3,5-triphenyl-1*H*-1,2,4-triazole (**3a**) (petroleum ether/ethyl acetate = 10/1) in the reported yield.

Entry	Parameter
Table S1	Solvent screening
Table S2	Base screening
Table S3	Screening the loading of base
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Table S5	Reaction temperature screening
Table S6	Reaction time screening
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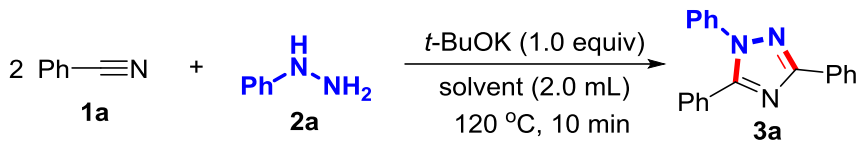
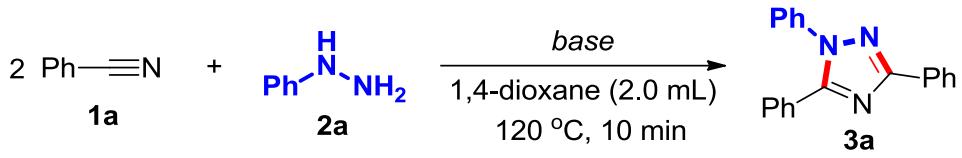
Table S1. Solvent screening [a]



Entry	Solvent	**3a** [%]
1	benzene	12
2	toluene	38
3	xylene	42
4	THF	63
5	2-MeTHF	62
7	diglyme	61
8	**1,4-dioxane**	**84**
9	anisole	56
10	CH_3OH	0
11	CH_3CH_2OH	0
12	*i*-BuOH	<5
13	*t*-BuOH	32
14	*t*-AmOH	41
15	DMF	<5
16	DMAc	11
17	DMSO	8
18	CH_3CN	0
19	CH_3NO_2	0
20	DCM	0
21	DCE	0
22	$CH_3CH_2C(O)OCH_2CH_3$	<5
23	$CHCl_3$	0
24	--	66

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (1.0 mmol), *t*-BuOK (1.0 eqiuv), solvent (2.0 mL), 120 °C, N_2, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

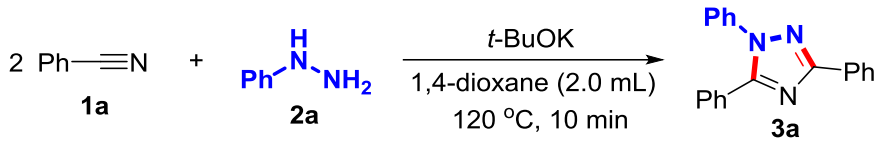
Table S2. Base screening [a]



Entry	Base (1.0 equiv)	**3a** [%]
1	***t*-BuOK**	**84**
2	*t*-BuONa	25
3	*t*-BuOLi	9
4	KHMDS	81
5	NaHMDS	15
6	LiHMDS	0
7	KOH	<5
8	NaOH	0
9	LiOH	0
10	K_2CO_3	0
11	Na_2CO_3	0
12	Li_2CO_3	0
13	$KHCO_3$	0
14	K_3PO_4	0
15	K_2HPO_4	0
16	KH_2PO_4	0
17	KH	72
18	NaH	10
19	NEt_3	0
20	DBU	0
21	Pydine	0
22	KNH_2	73
23	--	0

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (1.0 mmol), base (1.0 equiv), 1,4-dioxane (2.0 mL), 120 °C, N_2, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

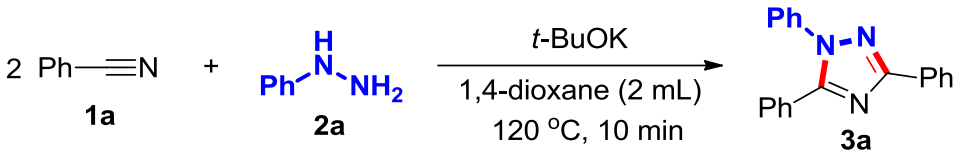
Table S3. Screening the loading of base [a]



Entry	*t*-BuOK (equiv)	**3a** [%]
1	*t*-BuOK (2.0)	70
2	*t*-BuOK (1.6)	76
3	*t*-BuOK (1.4)	80
4	*t*-BuOK (1.2)	83
5	*t*-BuOK (1.0)	84
6	*t*-BuOK (0.9)	83
7	*t*-BuOK (0.8)	85
8	*t*-BuOK (0.7)	84
9	*t*-BuOK (0.6)	84
10	*t*-BuOK (0.5)	83
11	*t*-BuOK (0.4)	83
12	*t*-BuOK (0.3)	82
13	***t*-BuOK (0.2)**	**82**
14	*t*-BuOK (0.15)	62
15	*t*-BuOK (0.1)	43
16	*t*-BuOK (0.05)	21
17	--	0

[a] Reaction conditions: **1a** (0.5 mmol), **2a** (1.0 mmol), *t*-BuOK (x eqiuv), 1,4-dioxane (2.0 mL), 120 °C, N_2, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

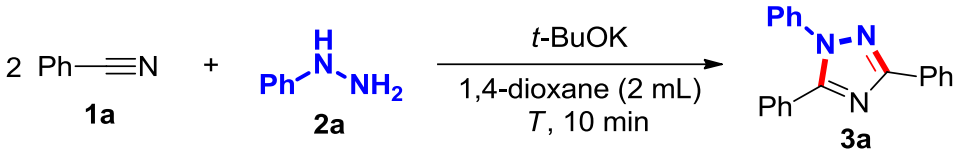
Table S4: Substrate 1a and 2a ratio screening [a]



Entry	**1a** (mmol)	**2a** (mmol)	**3a** (%)
1	0.5	0.5	32
2	0.5	0.6	51
3	0.5	0.7	63
4	0.5	0.8	74
5	0.5	0.9	80
6	0.5	1.0	82
7	0.6	1.0	86
8	0.7	1.0	88
9	0.8	1.0	91
10	0.9	1.0	95
11	**1.0**	**1.0**	**99** (95)[b]
12	1.1	1.0	98
13	1.3	1.0	97
14	1.5	1.0	98
15	2.0	1.0	97

[a] Reaction conditions: **1a** (x mmol), **2a** (x mmol), *t*-BuOK (0.2 mmol), 1,4-dioxane (2.0 mL), 120 °C, N_2, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard. [b] Isolated yield.

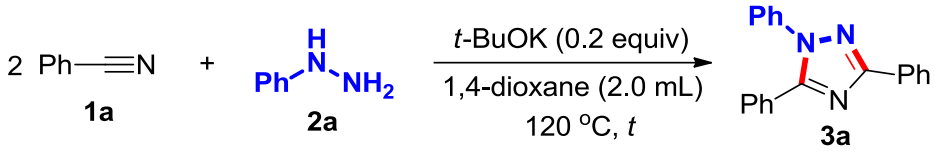
Table S5. Reaction temperature screening [a]



Entry	Temperature (°C)	**3a** [%]
1	rt	7
2	30	10
3	40	16
4	50	24
5	60	53
6	70	77
7	80	90
8	90	91
9	100	95
10	110	96
11	**120**	**99**
12	130	98
13	140	82
14	150	67

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.0 mmol), *t*-BuOK (0.2 mmol), 1,4-dioxane (2.0 mL), N_2, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

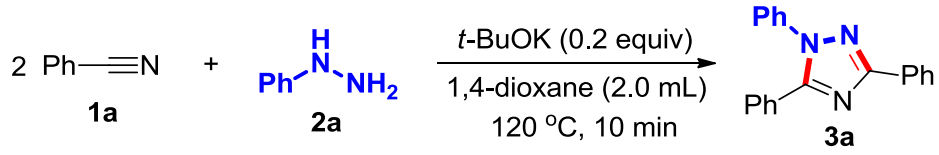
Table S6. Reaction time screening [a]



Entry	Time (min)	**3a** [%]
1	0	0
2	5	66
3	**10**	**99**
4	20	99
5	1h	96
6	15 h	98

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.0 mmol), *t*-BuOK (0.2 mmol), 1,4-dioxane (2.0 mL), N_2, 120 °C. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

Table S7. Reaction system experiments [a]

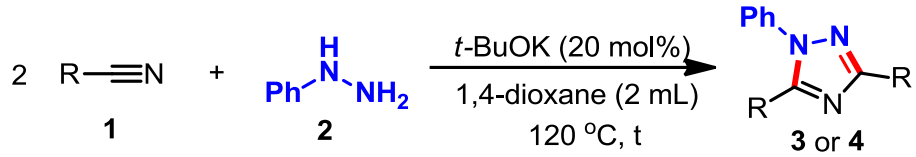


Entry	Reaction system		Additive (equiv)	**3a** [%]
1	air	closed	-	17
2	O_2	closed	-	0
3	N_2	closed	-	99
4	air	Open, reflux	-	0
5	O_2	Open, reflux	-	0
6	N_2	Open, reflux	-	96
7	N_2	closed	H_2O (0.1 mmol)	61
8	N_2	closed	H_2O (0.2 mmol)	31
9	N_2	closed	H_2O (1.0 mmol)	<5

[a] Reaction conditions: **1a** (1.0 mmol), **2a** (1.0 mmol), *t*-BuOK (0.2 mmol), 1,4-dioxane (2.0 mL), 120 °C, 10 min. Yield of **3a** determined by GC-analysis using *n*-dodecane as internal standard.

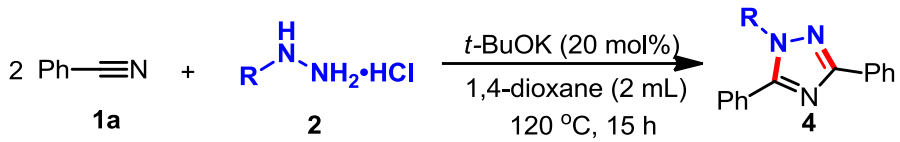
3. General procedure for the synthesis of 1,2,4-triazoles

3.1 The synthesis of 1,2,4-triazoles from various nitriles and hydrazines :



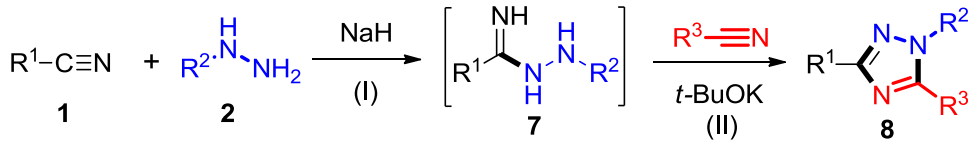
Using a nitrogen-filled glove box, an oven-dried pressure tube (38 mL volume) was charged with a magnetic stirring bar, *t*-BuOK (22 mg, 20 mol%, 0.2 mmol), nitriles (1.0 mmol), hydrazines (1.0 mmol) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 ^{o}C). After design time the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Purification of the remainder by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1 - 1/4, DCM 2%) gave the corresponding products **3** or **4** in the reported yields.

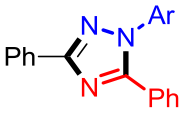
3.2 The synthesis of 1,2,4-triazoles from nitriles and various hydrazines hydrochloride:



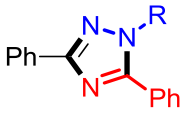
Using a nitrogen-filled glove box, an oven-dried pressure tube (38 mL volume) was charged with a magnetic stirring bar, base, *t*-BuOK (22 mg, 20 mol%, 0.2 mmol), nitriles (1.0 mmol), hydrazine hydrochlorides (**2b, 2c, 2d, 2h, 2i, 2k, 2m, 2o, 2p, 2r, 2s)** and 1,4-dioxane (2 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 ^{o}C). After design time the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Purification of the remainder by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1 - 1/4, DCM 2%) gave the corresponding products **3** or **4** in the reported yields.

3.3 Tandem annulation:

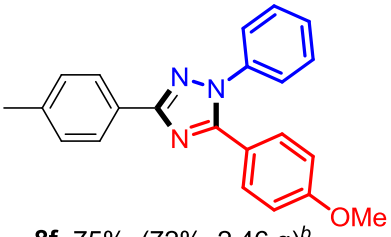




8a, Ar = Ph, 86%
8b, Ar = 3-MePh, 81%
8c, Ar = 4-ClPh, 80%



8d, R = 2-pyridyl, 63%
8e, R = cyclohexyl, 62%

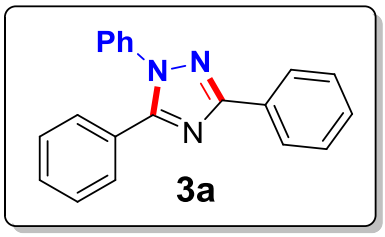


8f, 75%, (72%, 2.46 g)[b]

Under N_2 atmosphere, a solution of NaH (29 mg, 1.2 mmol) in DMSO (1.0 mL) was added hydrazines (1.2 mmol). After 10 min of stirring at room temperature, the mixture of reaction was added drop wise nitriles (1.0 mmol) in DMSO (1.0 mL) and stirred overnight. Then the reaction was quenched with H_2O (2.0 ml), and extracted with DCM (4 X 3 mL). After dried with anhydrous Na_2SO_4, the combined extract was evaporated under reduced pressure to give the intermediate **7**. Then using a nitrogen-filled glove box, an oven-dried pressure tube (38 mL volume) was charged with a magnetic stirring bar, nitriles (0.5 mmol), intermediates **7** (0.5 mmol), *t*-BuOK (22 mg, 20 mol%, 0.2 mmol) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 ^oC). After design time the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Purification of the remainder by column chromatography on silica gel (petroleum ether/ethyl acetate = 100/1 - 1/4, DCM 2%) gave the corresponding products **8** in the reported yields.

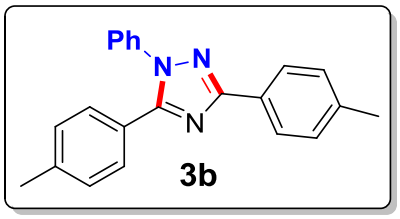
4. Experimental characterization data for products

1,3,5-triphenyl-1*H*-1,2,4-triazole (3a)[1]:



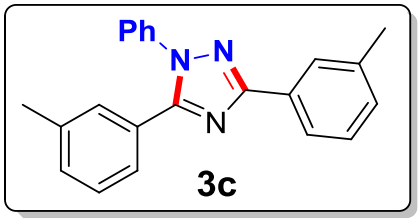
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow solid, 141.1 mg, 95% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.0 Hz, 2H), 7.57 (d, *J* = 7.0 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.45 – 7.40 (m, 7H), 7.37 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.8, 154.6, 138.2, 130.6, 129.9, 129.3, 129.3, 128.9, 128.7, 128.5, 127.9, 126.5, 125.3.

1-phenyl-3,5-di-*p*-tolyl-1*H*-1,2,4-triazole (3b)[2]:



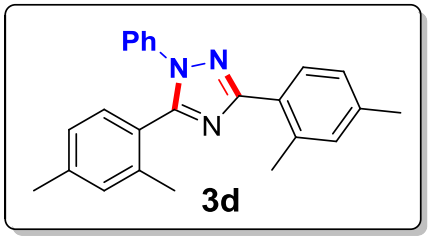
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 156.0 mg, 96% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 6.4 Hz, 2H), 7.37 – 7.27 (m, 7H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 2.29 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.0, 154.8, 140.2, 139.3, 138.5, 129.6, 129.3, 129.2, 128.9, 128.7, 128.1, 126.6, 125.5, 125.2, 21.5, 21.5.

1-phenyl-3,5-di-*m*-tolyl-1*H*-1,2,4-triazole (3c):



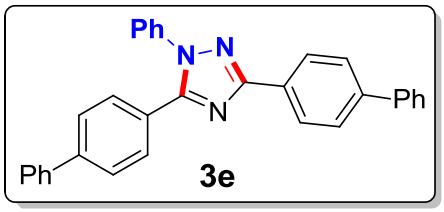
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 152.8 mg, 94% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.39 (s, 1H), 7.33 – 7.26 (m, 5H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.13 – 7.05 (m, 4H), 2.31 (s, 3H), 2.20 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.1, 154.9, 138.7，138.4，138.2, 130.8，130.7，130.2, 129.7, 129.4, 128.8, 128.5，128.4, 128.0, 127.2, 126.0, 125.5, 123.8, 21.4, 21.4; **HRMS** (ESI) calcd. for $C_{22}H_{20}N_3$ [M+H]:326.1657, found: 326.1656.

3,5-bis(2,4-dimethylphenyl)-1-phenyl-1*H*-1,2,4-triazole (3d):



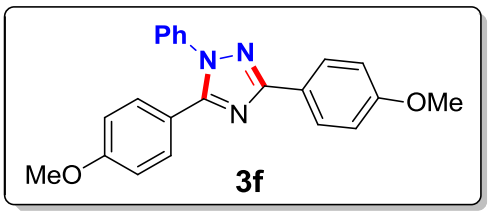
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 169.5 mg, 96% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.6 Hz, 1H), 7.28 – 7.16 (m, 5H), 7.14 – 7.11 (m, 1H), 7.01 (d, *J* = 9.2 Hz, 2H), 6.97 – 6.90 (m, 2H), 2.64 (s, 3H), 2.27 (s, 3H), 2.25 (s, 3H), 2.03 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 153.7, 140.1, 138.7, 138.2, 137.3, 137.1, 132.1, 131.5, 130.2, 129.6, 129.1, 127.7, 127.2, 126.8, 126.6, 125.9, 123.4, 22.1, 21.4, 21.3, 19.8; **HRMS** (ESI) calcd. for $C_{24}H_{24}N_3$ [M+H]:354.1970, found: 354.1966.

3,5-di([1,1'-biphenyl]-4-yl)-1-phenyl-1*H*-1,2,4-triazole (3e):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 208.9 mg, 93% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.67 (dd, *J* = 11.0, 8.0 Hz, 4H), 7.60 (d, *J* = 8.0 Hz, 4H), 7.50 – 7.43 (m, 9H), 7.39 – 7.34 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.8, 154.6, 142.7, 142.1, 140.7, 140.0, 138.4, 129.8, 129.5, 129.4, 128.9, 128.8, 127.9, 127.5, 127.3, 127.2, 127.1, 126.8, 125.6; **HRMS** (ESI) calcd. for $C_{32}H_{24}N_3$ [M+H]:450.1970, found: 450.1974.

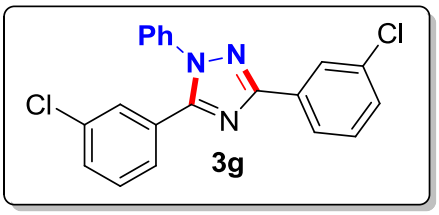
3,5-bis(4-methoxyphenyl)-1-phenyl-1*H*-1,2,4-triazole (3f)[2]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 144.6 mg, 81% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.49 (d, *J* = 9.0 Hz, 2H), 7.43 (s, 5H), 6.98 (d, *J* = 9.0 Hz, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.82 (s, 3H); **^{13}C NMR** (101 MHz,

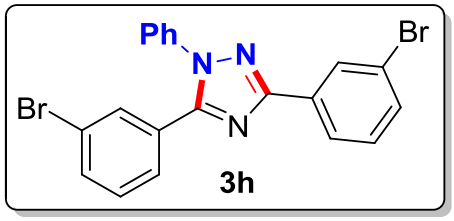
$CDCl_3$) δ 161.6, 160.8, 160.6, 154.5, 138.6, 130.5, 129.4, 128.7, 128.0, 125.5, 123.6, 120.4, 114.0, 55.32.

3,5-bis(3-chlorophenyl)-1-phenyl-1*H*-1,2,4-triazole (3g):



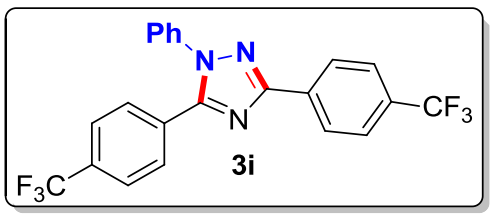
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 115.0 mg, 63% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.08 (s, 1H), 7.63 (s, 1H), 7.48 – 7.43 (m, 3H), 7.41 – 7.36 (m, 5H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.25 – 7.20 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.9, 153.5, 137.9, 134.7, 132.4, 130.2, 129.9, 129.8, 129.6, 129.5, 129.4, 129.3, 129.2, 128.7, 127.8, 126.9, 126.7, 125.4, 124.7; **HRMS** (ESI) calcd. for $C_{20}H_{14}Cl_2N_3$ [M+H]: 366.0565, found: 366.0566.

3,5-bis(3-bromophenyl)-1-phenyl-1H-1,2,4-triazole (3h):



The title compound was prepared according to the general procedure and purified by column chromatography to give a yellow oil, 167.6 mg, 74% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.85 (s, 1H), 7.59 – 7.55 (m, 2H), 7.51 – 7.48 (m, 3H), 7.45 – 7.42 (m, 2H), 7.37 (dd, *J* = 15.6, 7.3 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H);**^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.8, 153.4, 137.8, 133.2, 132.6, 132.5, 132.0, 130.2, 130.1, 129.7, 129.6, 129.4, 127.4, 125.4, 125.1, 122.9, 122.8; **HRMS** (ESI) calcd. for $C_{20}H_{14}Br_2N_3$ [M+H]:453.9554, found: 453.9555.

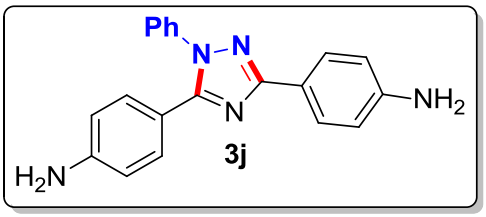
1-phenyl-3,5-bis(4-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (3i):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 88.9 mg,

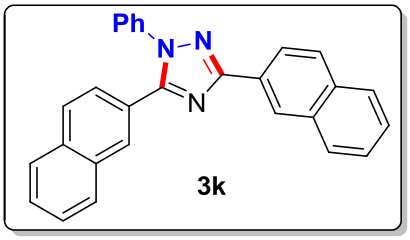
41% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.49 (s, 3H), 7.42 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.1, 153.8, 137.9, 134.0, 132.3, 132.0, 131.6, 131.3, 129.9, 129.7, 129.4, 126.9, 125.9, 125.6, 125.3, 124.9, 123.2, 122.7; **^{19}F NMR** (377 MHz, $CDCl_3$) δ -62.65, -62.98; **HRMS** (ESI) calcd. for $C_{22}H_{14}F_6N_3$ [M+H]:434.1092, found: 434.1094.

4,4'-(1-phenyl-1*H*-1,2,4-triazole-3,5-diyl)dianiline (3j):



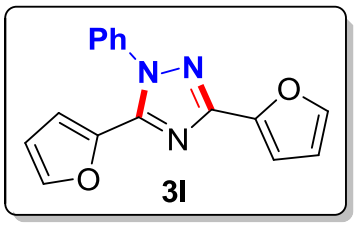
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow solid, 147.2 mg, 90% yield. **^{1}H NMR** (500 MHz, DMSO) δ 7.72 (d, *J* = 8.5 Hz, 2H), 7.54 – 7.42 (m, 3H), 7.39 (d, *J* = 7.0 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 6.60 (d, *J* = 8.5 Hz, 2H), 6.48 (d, *J* = 8.5 Hz, 2H), 5.53 (s, 2H), 5.37 (s, 2H); **^{13}C NMR** (101 MHz, DMSO) δ 161.5, 155.1, 150.8, 150.3, 139.2, 130.1, 129.9, 129.0, 127.6, 126.1, 118.7, 114.9, 114.1, 113.6; **HRMS** (ESI) calcd. for $C_{20}H_{18}N_5$ [M+H]:354.1970, found: 354.1966.

3,5-di(naphthalen-2-yl)-1-phenyl-1*H*-1,2,4-triazole (3k):



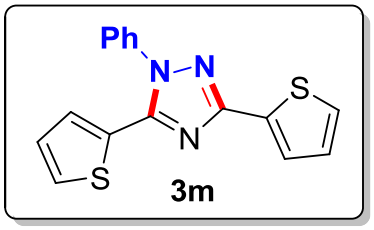
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 170.8 mg, 86% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.41 (d, *J* = 8.5 Hz, 1H), 8.20 (s, 1H), 8.00 (d, *J* = 4.0 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.90 (s, 1H), 7.82 (dd, *J* = 12.5, 8.5 Hz, 3H), 7.59 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.56 – 7.49 (m, 6H), 7.45 – 7.42 (m, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.2, 155.0, 138.4, 134.1, 133.7, 133.5, 132.9, 129.5, 129.4, 129.0, 128.7, 128.50, 128.4, 128.2, 127.9, 127.8, 127.5, 126.8, 126.6, 126.4, 126.1, 125.6, 125.5, 125.4, 124.26. **HRMS** (ESI) calcd. for $C_{28}H_{20}N_3$ [M+H]:398.1657, found: 398.1660.

3,5-di(furan-2-yl)-1-phenyl-1*H*-1,2,4-triazole (3l)[2]:



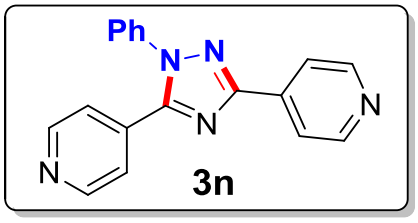
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 110.8 mg, 80% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (q, *J* = 20.0 Hz, 7H), 7.09 (d, *J* = 3.0 Hz, 1H), 6.53 – 6.47 (m, 2H), 6.38 (s, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.4, 146.9, 145.8, 144.5, 143.5, 142.0, 137.7, 129.7, 129.4, 126.2, 113.2, 111.7, 111.6, 110.1.

1-phenyl-3,5-di(thiophen-2-yl)-1H-1,2,4-triazole (3m)[2]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow solid, 51.0 mg, 33% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 3.6 Hz, 1H), 7.57 – 7.52 (m, 5H), 7.41 (m, 2H), 7.15 (dd, *J* = 5.2, 3.6 Hz, 1H), 7.12 (d, *J* = 2.8 Hz, 1H), 6.99 (dd, *J* = 5.2, 3.6 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.2, 150.1, 137.7, 133.2, 130.0, 129.7, 129.3, 129.0, 128.9, 127.7, 127.6, 126.8, 126.8, 126.8, 126.8.

4,4'-(1-phenyl-1*H*-1,2,4-triazole-3,5-diyl)dipyridine (3n):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 124.2 mg, 83% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 (d, *J* = 6.0 Hz, 2H), 8.65 (d, *J* = 6.0 Hz, 2H), 8.08 (d, *J* = 6.0 Hz, 2H), 7.55 – 7.49 (m, 3H), 7.45 – 7.39 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.3, 152.9, 150.4, 150.3, 137.8, 137.5, 134.9, 130.0, 129.9, 125.6, 122.6, 120.7, 100.0; **HRMS** (ESI) calcd. for $C_{18}H_{14}N_5$ [M+H]:300.1249, found: 300.1252.

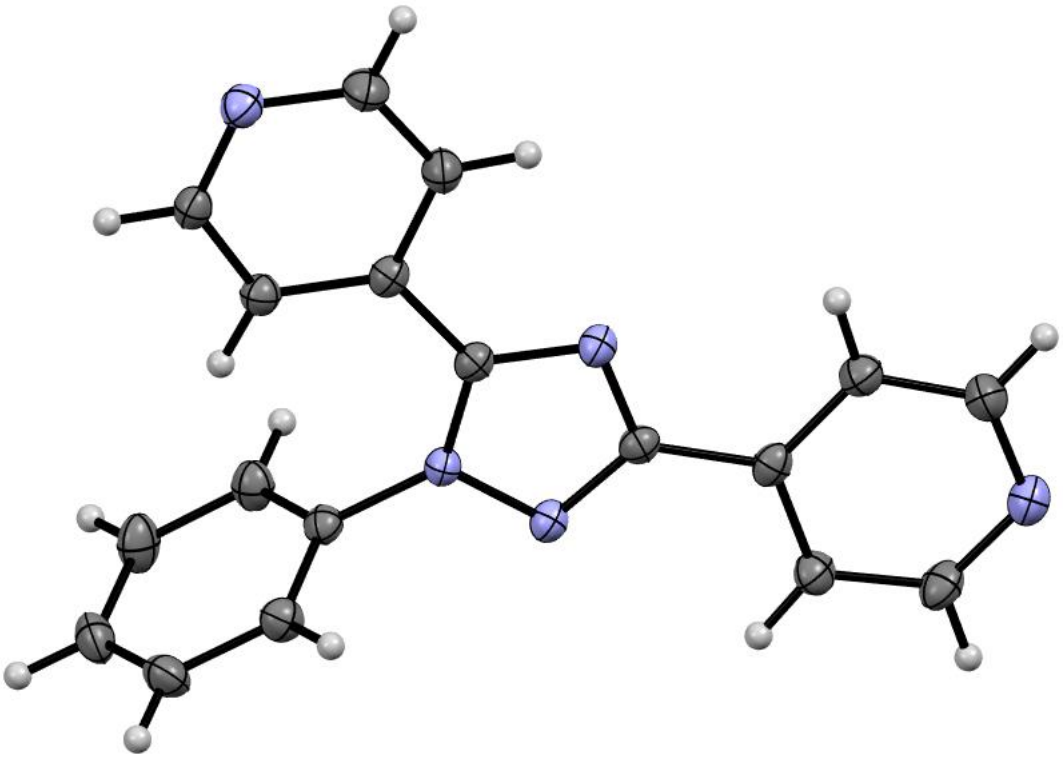
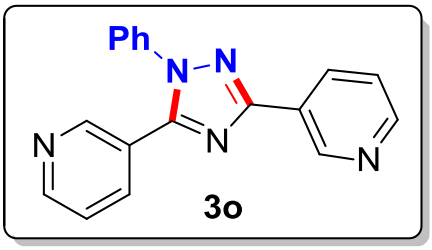


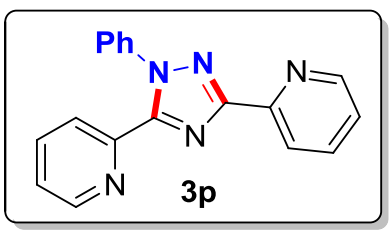
Figure S1. ORTEP drawing of product **3n**

3,3'-(1-phenyl-1*H*-1,2,4-triazole-3,5-diyl)dipyridine (3o):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 140.6 mg, 94% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.44 (s, 1H), 8.77 (s, 1H), 8.65 (m, 2H), 8.47 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.49 – 7.46 (m, 3H), 7.43 – 7.38 (m, 3H), 7.32 (dd, *J* = 8.0, 5.0 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.1, 152.5, 151.0, 150.5, 149.5, 148.0, 137.6, 136.1, 133.9, 129.9, 129.7, 126.5, 125.5, 124.1, 123.5, 123.4; **HRMS** (ESI) calcd. for $C_{18}H_{14}N_5$ [M+H]:300.1249, found: 300.1252.

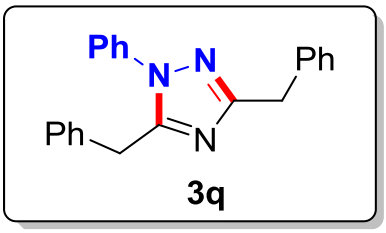
2,2'-(1-phenyl-1*H*-1,2,4-triazole-3,5-diyl)dipyridine (3p):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 124.1 mg, 83% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 4.5

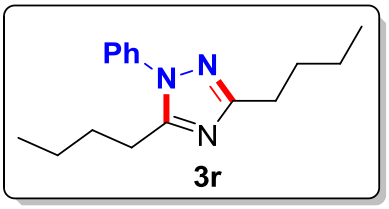
Hz, 1H), 8.48 (d, *J* = 4.5 Hz, 1H), 8.29 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.0 Hz, 1H), 7.80 (dt, *J* = 14.0, 8.0 Hz, 2H), 7.47 (m, 2H), 7.44 – 7.39 (m, 3H), 7.37 – 7.32 (m, 1H), 7.30 (dd, *J* = 4.5, 3.0 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.4, 153.7, 150.1, 149.5, 149.3, 147.3, 138.9, 136.7, 136.6, 128.8, 125.7, 124.5, 124.4, 124.0, 122.0. **HRMS** (ESI) calcd. for $C_{18}H_{14}N_5$ [M+H]: 300.1249, found: 300.1250.

3,5-dibenzyl-1-phenyl-1*H*-1,2,4-triazole (3q):



The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 99.2 mg, 61% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 (m, 5H), 7.29 – 7.20 (m, 4H), 7.19 – 7.12 (m, 4H), 7.02 (d, *J* = 7.0 Hz, 2H), 4.06 (s, 4H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.9, 154.6, 138.2, 137.4, 136.1, 129.3, 129.0, 128.9, 128.7, 128.5, 128.4, 126.9, 126.5, 125.3, 34.8, 32.5; **HRMS** (ESI) calcd. for $C_{22}H_{20}N_3$ [M+H]:326.1657, found: 326.1659.

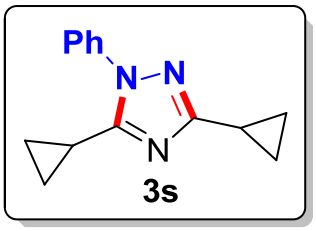
3,5-dibutyl-1-phenyl-1*H*-1,2,4-triazole (3r):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 117.0 mg, 91% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 – 7.34 (m, 5H), 2.80 – 2.65 (m, 4H), 1.74 (d, *J* = 7.5 Hz, 2H), 1.69 (t, *J* = 8.0 Hz, 2H), 1.41 (d, *J* = 7.5 Hz, 2H), 1.33 – 1.28 (m, 2H), 0.93 (t, *J* = 7.5 Hz, 3H), 0.85 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 164.0, 156.2, 137.6, 129.3, 128.6, 125.1, 30.6, 30.0, 29.7, 28.1, 26.2, 22.5, 22.3, 13.8, 13.6; **HRMS** (ESI) calcd. for $C_{16}H_{24}N_3$ [M+H]:258.1970, found: 258.1973.

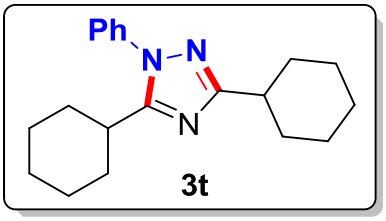
3,5-dicyclopropyl-1-phenyl-1*H*-1,2,4-triazole (3s):

The title compound was prepared according to the general procedure and purified by



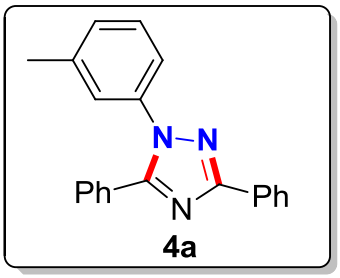
column chromatography to give a white oil, 94.6 mg, 84% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 – 7.20 (m, 5H), 1.93 (dq, *J* = 8.4, 5.2 Hz, 1H), 1.86 – 1.74 (m, 1H), 1.11 – 1.06 (m, 2H), 0.96 – 0.83 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.1, 157.5, 137.7, 129.3, 128.3, 124.8, 9.2, 8.9, 7.7, 7.6; **HRMS** (ESI) calcd. for $C_{16}H_{16}N_3$ [M+H]:226.1344, found: 226.1345.

3,5-dicyclohexyl-1-phenyl-1*H*-1,2,4-triazole (3t):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 143.8 mg, 93% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.52 – 7.33 (m, 5H), 2.74 (m, 2H), 2.07 (d, *J* = 13.5 Hz, 2H), 1.79 (m, 6H), 1.68 (m, 4H), 1.58 (qd, *J* = 12.5, 3.0 Hz, 2H), 1.38 – 1.18 (m, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.8, 159.9, 137.7, 129.3, 128.7, 125.5, 38.0, 35.4, 32.0, 31.8, 26.2, 26.0, 25.9, 25.5; **HRMS** (ESI) calcd. for $C_{20}H_{28}N_3$ [M+H]:310.2283, found: 310.2285.

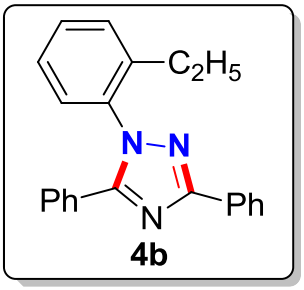
3,5-diphenyl-1-(*m*-tolyl)-1*H*-1,2,4-triazole (4a)[2]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 144.7 mg, 93% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 7.0 Hz, 2H), 7.49 (d, *J* = 7.0 Hz, 2H), 7.38 (m, 2H), 7.32 (m, 2H), 7.28 – 7.22 (m, 3H), 7.16 (m, 2H), 7.04 (d, *J* = 7.5 Hz, 1H), 2.29 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.9, 154.7, 139.7, 138.2, 130.8, 130.0, 129.7, 129.5, 129.1, 129.0, 128.6, 128.5, 128.0, 126.7, 126.1, 122.6, 21.4.

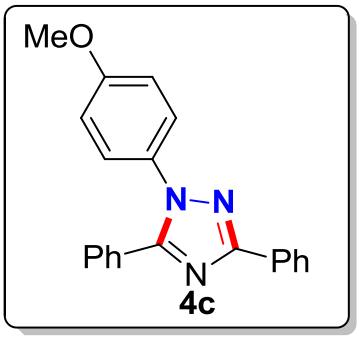
1-(2-ethylphenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4b)[3]:

The title compound was prepared according to the general procedure and purified by



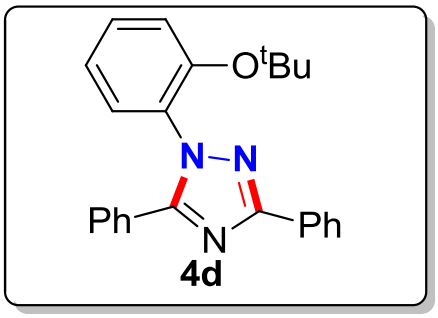
column chromatography to give a light yellow oil, 154.5 mg, 95% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.19 – 8.15 (m, 2H), 7.49 – 7.45 (m, 2H), 7.40 – 7.31 (m, 5H), 7.26 – 7.19 (m, 5H), 2.33 (q, *J* = 7.6 Hz, 2H), 0.96 (t, *J* = 7.6 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.8, 155.4, 141.1, 137.2, 130.9, 130.3, 129.9, 129.8, 129.4, 128.6, 128.5, 128.3, 127.8, 127.7, 127.1, 126.6, 24.1, 14.1.

1-(4-methoxyphenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4c)[3]:



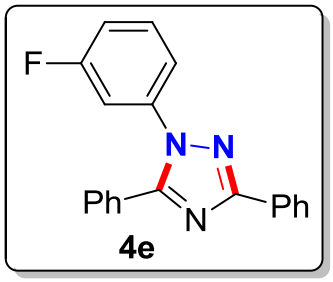
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 140.7 mg, 86% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 6.8 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.40 (m, 5H), 7.39 – 7.35 (m, 3H), 6.97 (d, *J* = 9.0 Hz, 2H), 3.88 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.7, 159.8, 154.7, 131.4, 130.8, 129.9, 129.4, 128.9, 128.6, 128.1, 126.9, 126.6, 114.6, 55.6.

1-(3-(tert-butoxy)phenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4d):



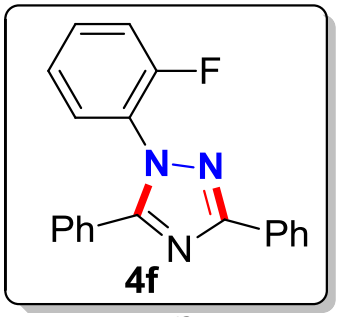
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 129.2 mg, 70% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.0 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.57 (d, *J* = 7.0 Hz, 2H), 7.47 – 7.41 (m, 3H), 7.37 – 7.28 (m, 4H), 7.20 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 8.5 Hz, 1H), 1.05 (s, 9H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.7, 156.4, 150.8, 132.4, 131.1, 130.2, 129.7, 129.2, 128.9, 128.6, 128.3, 128.2, 128.0, 126.6, 123.0, 122.9, 80.5, 28.6; **HRMS** (ESI) calcd. for $C_{24}H_{24}N_3O$ [M+H]: 370.1919, found:370.1927.

1-(3-fluorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4e):



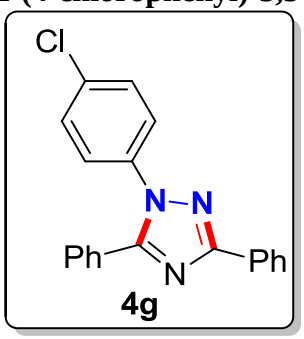
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 137.1 mg, 87% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.23 (d, *J* = 9.0 Hz, 2H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.42 – 7.35 (m, 3H), 7.26 – 7.17 (m, 2H), 7.13 (t, *J* = 8.5 Hz, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 162.70 (d, *J* = 248.7 Hz), 162.2, 154.9, 139.48 (d, *J* = 9.9 Hz), 130.7, 130.6, 130.5, 130.3, 129.6, 129.0, 128.8, 128.7, 128.6, 127.8, 126.7 120.98 (d, *J* = 3.3 Hz), 115.83 (d, *J* = 21.1 Hz), 112.94 (d, *J* = 24.8 Hz); **^{19}F NMR** (377 MHz, $CDCl_3$) δ -110.15; **HRMS** (ESI) calcd. for $C_{20}H_{15}FN_3$.[M+H]:316.1250, found: 316.1251.

1-(2-fluorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4f):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 99.3 mg, 63% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 7.0 Hz, 3H), 7.49 – 7.40 (m, 5H), 7.37 – 7.30 (m, 3H), 7.20 (t, *J* = 9.0 Hz, 1H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 156.6 (d, *J* = 254.1 Hz), 156.4, 131.4 (d, *J* = 7.7 Hz), 130.6, 130.2, 129.6, 128.8, 128.7, 128.6, 128.5, 128.3, 128.2, 127.9, 127.7, 126.7, 125.1 (d, J = 4.1 Hz), 117.1 (d, *J* = 19.3 Hz); **^{19}F NMR** (377 MHz, $CDCl_3$) δ -120.35; **HRMS** (ESI) calcd. for $C_{20}H_{15}FN_3$.[M+H]:316.1250, found: 316.1253.

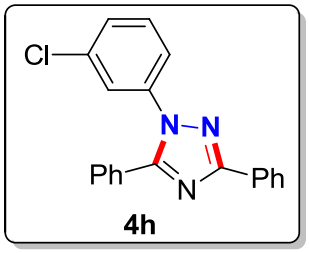
1-(4-chlorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4g)[2]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 150.6 mg, 91% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.0 Hz, 2H), 7.46 (d, *J* = 7.0 Hz, 2H),

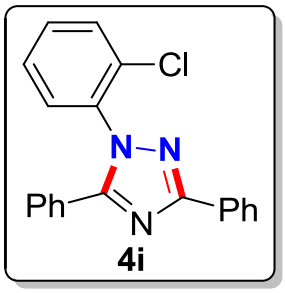
7.36 (m, 4H), 7.29 (m, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.2, 154.9, 136.8, 134.6, 130.6, 130.3, 129.6, 129.0, 128.7, 128.6, 127.9, 126.6, 126.5.

1-(3-chlorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4h)[1]:



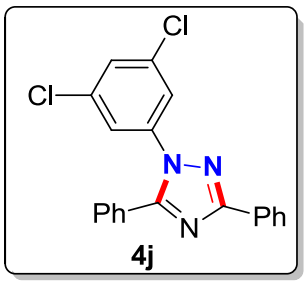
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 130.8 mg, 79% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.0 Hz, 2H), 7.50 – 7.43 (m, 3H), 7.39 – 7.33 (m, 4H), 7.32 – 7.28 (m, 3H), 7.22 (t, *J* = 8.0 Hz, 1H), 7.15 (t, *J* = 6.5 Hz, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.8, 153.5, 137.9, 133.3, 132.6, 132.5.2, 132.0, 130.3, 130.1, 129.7, 129.6, 129.5, 127.4, 125.5, 125.2, 122.9, 122.8.

1-(2-chlorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4i):



The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow solid, 84.6 mg, 51% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.26 – 8.23 (m, 2H), 7.57 – 7.50 (m, 4H), 7.48 – 7.42 (m, 5H), 7.37 (d, *J* = 7.0 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.3, 156.2, 136.4, 132.1, 131.2, 130.7, 130.6, 130.2, 129.6, 129.5, 128.7, 128.6, 128.1, 128.0, 127.7, 126.7; **HRMS** (ESI) calcd. for $C_{20}H_{15}ClN_3$ [M+H]: 332.0955, found: 332.0956.

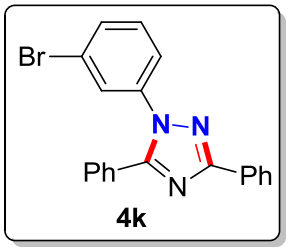
1-(3,5-dichlorophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4j):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 149.7 mg, 82% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.0 Hz, 2H), 7.57 (d, *J* = 7.0 Hz, 2H), 7.46 (m, 6H), 7.41 (t, *J* = 1.5 Hz, 1H), 7.36 (d, *J* = 1.5 Hz, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.4, 155.0, 139.7, 135.6, 132.8, 132.2, 130.7,

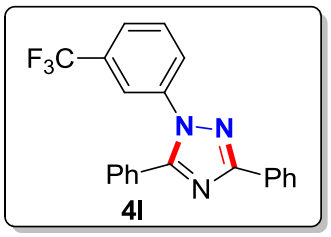
130.3, 129.7, 129.1, 129.0, 128.9, 128.7, 128.6, 126.7, 123.6, 118.8, 112.5; **HRMS** (ESI) calcd. for $C_{20}H_{14}Cl_2N_3$ [M+H]: 366.0565, found: 366.0564.

1-(3-bromophenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4k)[1]:



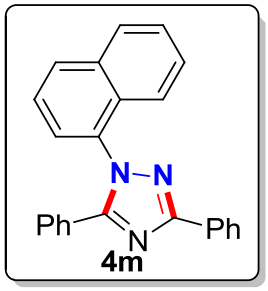
The title compound was prepared according to the general procedure and purified by column chromatography to give a light yellow oil, 125.6 mg, 67% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.0 Hz, 2H), 7.62 (s, 1H), 7.47 (m, 2H), 7.34-7.28 (m, 7H), 7.19 – 7.12 (m, 2H); **^{13}C NMR** (126 MHz, CDCl3) δ 161.1, 153.8, 138.3, 130.8, 129.4, 129.3, 128.5, 128.3, 128.0, 127.7, 127.6, 127.5, 127.3, 126.6, 125.6, 124.4, 122.8, 121.8.

3,5-diphenyl-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4l):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 133.3 mg, 73% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 6.5 Hz, 2H), 7.78 (s, 1H), 7.66 (d, *J* = 7.5 Hz, 1H), 7.59 – 7.51 (m, 4H), 7.50 – 7.43 (m, 4H), 7.39 - 7.36 (m, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.4, 155.0, 138.7, 130.5, 130.4, 130.0, 129.7, 129.1, 128.9, 128.7, 128.2, 127.7, 126.7, 125.3 (d, *J* = 3.6 Hz), 122.2 (d, *J* = 3.9 Hz); **^{19}F NMR** (377 MHz, $CDCl_3$) δ -62.81; **HRMS** (ESI) calcd. for $C_{21}H_{15}F_3N_3$ [M+H]: 366.1218, found: 366.1218.

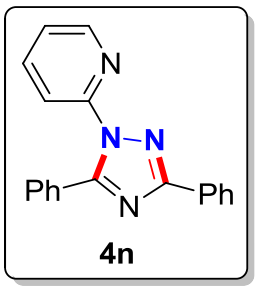
1-(naphthalen-1-yl)-3,5-diphenyl-1*H*-1,2,4-triazole (4m):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 161.4 mg, 93% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 7.0 Hz, 2H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.56 (t, *J* = 7.0 Hz, 1H),

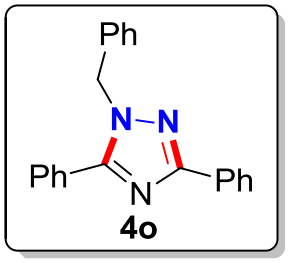
7.52 – 7.43 (m, 8H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.20 (t, *J* = 7.5 Hz, 2H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.3, 156.5, 134.9, 134.4, 130.9, 130.4, 129.9, 129.8, 129.6, 128.7, 128.5, 128.4, 127.9, 127.6, 127.1, 126.8, 125.7, 125.3, 122.9; **HRMS** (ESI) calcd. for $C_{24}H_{18}N_3$ [M+H]: 348.1501, found: 348.1507.

2-(3,5-diphenyl-1*H*-1,2,4-triazol-1-yl)pyridine (4n)[4]:



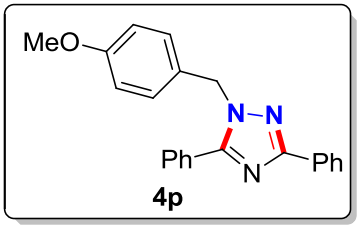
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 110.3 mg, 74% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 4.5 Hz, 1H), 8.17 (d, *J* = 7.5 Hz, 2H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.0 Hz, 3H), 7.37 (t, *J* = 7.0 Hz, 2H), 7.32 (m, 2H), 7.27 (t, *J* = 7.0 Hz, 2H), 7.22 – 7.19 (m, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.1, 155.6, 150.9, 148.9, 138.8, 130.6, 130.0, 129.6, 129.2, 128.6, 128.4, 126.8, 123.8, 119.3.

1-benzyl-3,5-diphenyl-1*H*-1,2,4-triazole (4o)[5]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 135.3 mg, 87% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.5 Hz, 2H), 7.62 (d, *J* = 7.5 Hz, 2H), 7.50 – 7.42 (m, 5H), 7.40 (d, *J* = 7.0 Hz, 1H), 7.36 – 7.28 (m, 3H), 7.21 (d, *J* = 7.5 Hz, 2H), 5.46 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.6, 156.2, 136.1, 131.1, 130.3, 129.0, 129.9, 129.8, 128.6, 128.7, 128.1, 128.0, 126.9, 126.5, 52.8.

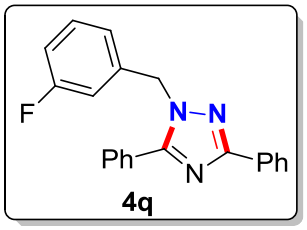
1-(4-methoxybenzyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4p)[6]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 143.3 mg, 84%

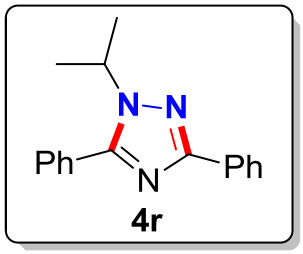
yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 7.0 Hz, 2H), 7.62 (d, *J* = 6.0 Hz, 2H), 7.44 (m, 6H), 7.15 (d, *J* = 8.5 Hz, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 5.38 (s, 2H), 3.78 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.5, 159.4, 155.9, 131.1, 130.2, 129.2, 128.9, 128.6, 128.5, 128.4, 128.1, 126.5, 114.3, 55.3, 52.4.

1-(3-fluorobenzyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4q):



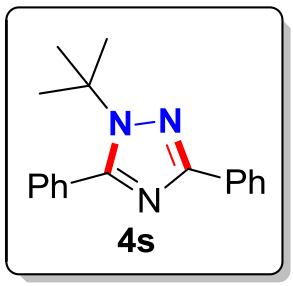
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 120.1 mg, 73% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.0 Hz, 2H), 7.62 (d, *J* = 2.0 Hz, 2H), 7.50 – 7.39 (m, 6H), 7.29 (m, 1H), 7.16 – 7.05 (m, 3H), 5.52 (s, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.8, 159.8 (d, *J* = 247.0 Hz), 156.5, 130.9, 130.3, 129.8 (d, *J* = 7.7 Hz), 129.3, 128.9, 128.8, 128.7, 128.6, 127.8, 126.5, 124.6, 123.3 (d, *J* = 14.3 Hz), 115.5 (d, *J* = 20.9 Hz), 46.8; **^{19}F NMR** (377, MHz, CDCl3) δ -118.25; **HRMS** (ESI) calcd. for $C_{21}H_{17}FN_3$ [M+H]:330.1407, found: 330.1411.

1-isopropyl-3,5-diphenyl-1*H*-1,2,4-triazole (4r)[1]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 126.3 mg, 96% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 7.5 Hz, 2H), 7.62 (d, *J* = 1.5 Hz, 2H), 7.54 – 7.48 (m, 3H), 7.44 (m, 2H), 7.38 (m, 1H), 4.67 (dt, *J* = 13.0, 6.5 Hz, 1H), 1.56 (s, 3H), 1.55 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.2, 154.7, 131.5, 130.0, 128.9, 128.9, 128.6, 128.5, 126.4, 50.7, 29.7, 22.9.

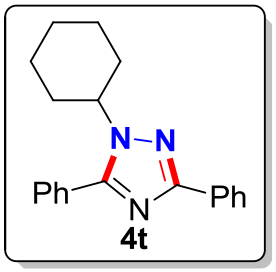
1-(tert-butyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4s)[1]:



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 128.9 mg, 93% yield. **^{1}H NMR** (500 MHz,

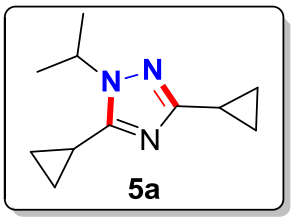
$CDCl_3$) δ 8.30 (d, *J* = 7.0 Hz, 2H), 7.52 (m, 5H), 7.48 – 7.41 (m, 3H), 1.55 (s, 9H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.9, 153.3, 131.1, 130.4, 129.9, 128.8, 128.6, 127.1, 63.5, 30.7; **HRMS** (ESI) calcd. for $C_{18}H_{20}N_3$ [M+H]:278.1657, found: 278.1663.

1-cyclohexyl-3,5-diphenyl-1*H*-1,2,4-triazole (4t)[7]**:**



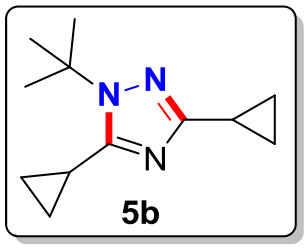
The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 131.9 mg, 87% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.0 Hz, 2H), 7.56 – 7.52 (m, 2H), 7.47 – 7.42 (m, 3H), 7.37 – 7.32 (m, 2H), 7.30 (m, 1H), 4.16 - 4,11 (m, 1H), 2.05 (m, 2H), 1.93 – 1.87 (m, 2H), 1.85 – 1.78 (m, 2H), 1.22 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.0, 154.7, 131.5, 123.0, 129.0, 128.8, 128.5, 126.4, 58.1, 33.2, 29.7, 25.5, 25.0.

3,5-dicyclopropyl-1-isopropyl-1*H*-1,2,4-triazole (5a):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 91.7 mg, 96% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.53 (dt, *J* = 13.6, 6.4 Hz, 1H), 1.86 (m, 1H), 1.70 m, 1H), 1.40 (d, *J* = 6.4 Hz, 6H), 0.96 – 0.89 (m, 4H), 0.82 – 0.75 (m, 4H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.6, 155.5, 49.2, 22.3, 9.0, 7.4, 7.3, 6.2; **HRMS** (ESI) calcd. for $C_{11}H_{18}N_3$ [M+H]:192.1501, found: 192.1495.

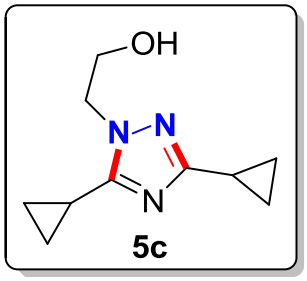
1-(tert-butyl)-3,5-dicyclopropyl-1*H*-1,2,4-triazole (5b):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 94.4 mg, 92% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 2.03 – 1.86 (td, *J* = 8.0, 4.0 Hz, 1H), 1.80 (td, *J* = 8.0, 4.0 Hz, 1H), 1.58 (s, 9H), 1.01 (dd, *J* = 5.0, 2.5 Hz, 2H), 0.90

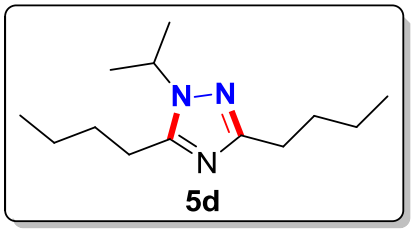
(dd, *J* = 8.0, 2.5 Hz, 2H), 0.82 – 0.62 (m, 4H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.2, 155.8, 58.7, 29.9, 9.3, 8.7, 8.6, 7.0; **HRMS** (ESI) calcd. for $C_{12}H_{20}N_3$ [M+H]:206.1657, found: 206.1653.

2-(3,5-dicyclopropyl-1*H*-1,2,4-triazol-1-yl)ethanol (5c):



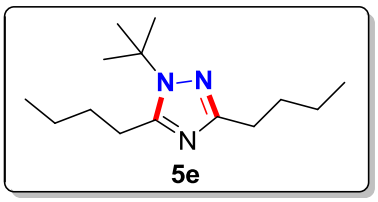
The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 86.9 mg, 90% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.14 (t, *J* = 4.5 Hz, 2H), 3.93 (t, *J* = 4.5 Hz, 2H), 1.91 – 1.74 (m, 2H), 0.99 – 0.93 (m, 4H), 0.83 (m, 4H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.3, 157.8, 61.0, 49.7, 8.9, 7.8, 7.6, 6.2; **HRMS** (ESI) calcd. for $C_{10}H_{16}N_3O$ [M+H]:194.1293, found: 194.1287.

3,5-dibutyl-1-isopropyl-1*H*-1,2,4-triazole (5d):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 101.6 mg, 91% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.31 (q, *J* = 13.6, 6.4 Hz, 1H), 2.65 – 2.56 (m, 4H), 1.63 (q, *J* = 13.2, 4.0 Hz, 4H), 1.39 (d, *J* = 6.4 Hz, 6H), 1.32 (q, *J* = 15.2, 7.6 Hz, 4H), 0.86 (dt, *J* = 10.0, 7.6 Hz, 6H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.1, 154.3, 49.2, 30.9, 30.2, 28.3, 25.7, 22.5, 22.5, 22.4, 13.8, 13.7.; **HRMS** (ESI) calcd. for $C_{13}H_{26}N_3$ [M+H]:224.2127, found: 224.2124.

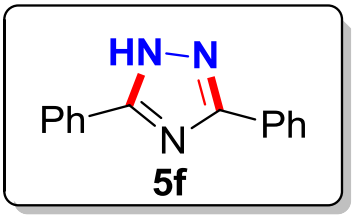
1-(tert-butyl)-3,5-dibutyl-1*H*-1,2,4-triazole (5e):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white oil, 111.6 mg, 94% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.14 – 3.06 (m, 2H), 2.80 – 2.69 (m, 2H), 1.79 (d, *J* = 7.5 Hz, 2H), 1.71 – 1.64 (m, 2H), 1.58 (s, 9H),

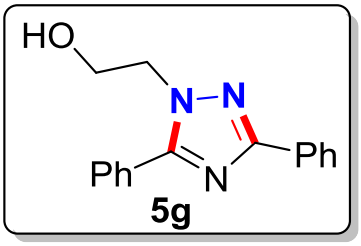
1.37 (dd, *J* = 15.0, 7.5 Hz, 2H), 1.27 (dd, *J* = 15.0, 7.5 Hz, 2H), 0.83 (dt, *J* = 22.0, 7.5 Hz, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.2, 152.9, 64.1, 30.6, 29.7, 28.8, 26.0, 25.0, 22.4, 22.0, 13.4, 13.3; **HRMS** (ESI) calcd. for $C_{14}H_{28}N_3$ [M+H]:238.2283, found: 238.2281.

3,5-diphenyl-1*H*-1,2,4-triazole (5f):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 98.4 mg, 89% yield. **^{1}H NMR** (400 MHz, DMSO) δ 14.53 (s, 1H), 8.15 – 8.00 (m, 4H), 7.63 – 7.41 (m, 6H); **^{13}C NMR** (101 MHz, DMSO) δ 162.1, 155.5, 131.8, 130.7, 129.5, 129.4, 129.2, 127.7, 126.6, 126.3; **HRMS** (ESI) calcd. for $C_{14}H_{12}N_3$ [M+H]:222.1031, found: 222.1031.

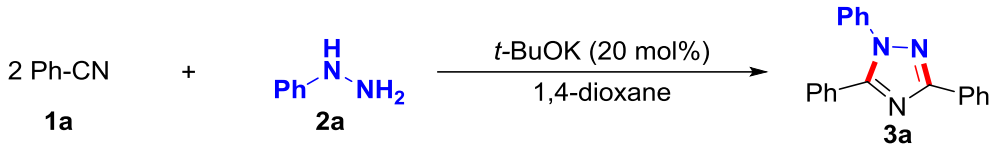
2-(3,5-diphenyl-1*H*-1,2,4-triazol-1-yl)ethanol (5g):



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 107.4 mg, 81% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 6.5 Hz, 2H), 7.72 (d, *J* = 7.0 Hz, 2H), 7.49 – 7.38 (m, 6H), 4.35 – 4.26 (m, 2H), 4.12 – 4.05 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.8, 156.1, 130.5, 129.8, 129.7, 129.3, 128.8, 128.7, 126.8, 126.6, 61.2, 51.3; **HRMS** (ESI) calcd. for $C_{16}H_{16}N_3O$ [M+H]: 266.1297, found: 266.1293.

5. Application

5.1 Gram scale experiments



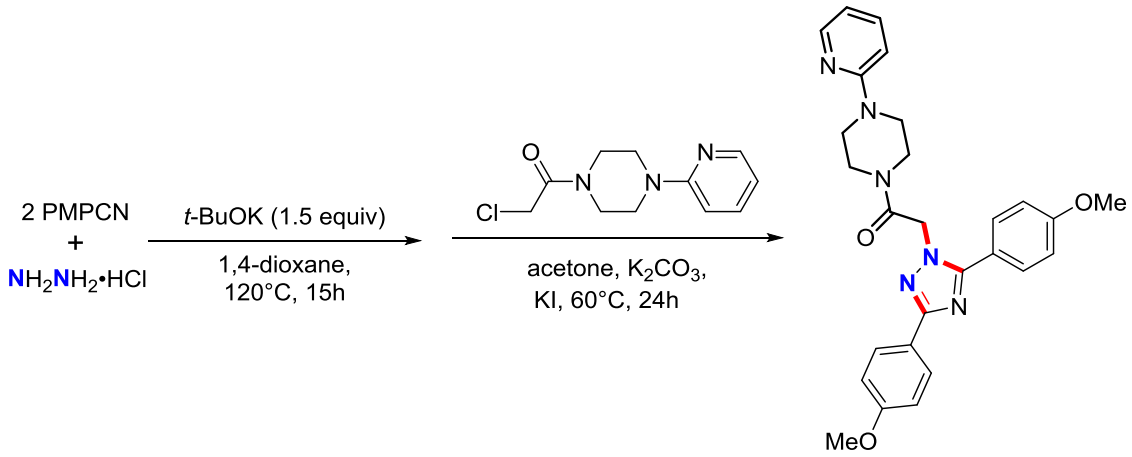
Open system:

10 mmol Scale: Using a nitrogen-filled glove box, an oven-dried Schlenk tube (250 mL volume) was charged with a magnetic stirring bar, *t*-BuOK (2 mmol), **1a** (10 mmol), **2a** (10 mmol) and 1,4-dioxane (50 mL). The tube was sealed, taken out of the glove box and a reflux condenser was attached under argon stream. The mixture was heated to a gentle reflux for an hour under inert atmosphere in an open system at 120 °C (oil bath). After design time the reaction was cooled, quenched with half-saturated brine (1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Then the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (petroleum ether/ethyl acetate = 100/1 - 10/1, DCM 2%) to give the desired product **3a** in 95 % yield (1.41 g).

100 mmol Scale:

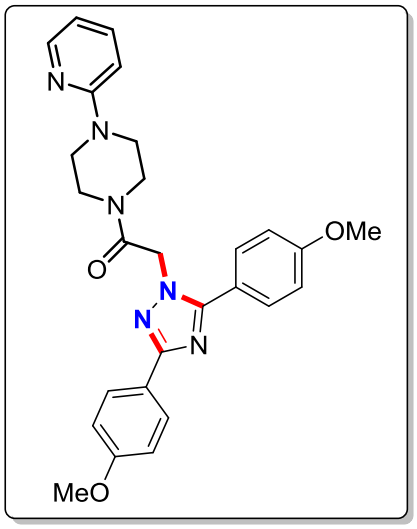
100 mmol Scale: Using a nitrogen-filled glove box, an oven-dried Schlenk tube (2.5 L volume) was charged with a magnetic stirring bar, *t*-BuOK (20 mmol), **1a** (100 mmol), **2a** (100 mmol) and 1,4-dioxane (0.5 L). The tube was sealed, taken out of the glove box and a reflux condenser was attached under argon stream. The mixture was heated to a gentle reflux for two hour under inert atmosphere in an open system at 120 °C (oil bath). After design time the reaction was cooled, quenched with half-saturated brine (5 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC and GC-MS to monitor product formation, respectively. Then the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (petroleum ether/ethyl acetate = 100/1 - 10/1, DCM 2%) to give the desired product **3a** in 94 % yield (13.99 g).

5.2 Synthesis of the mGlu5 receptor of 2-(3,5-bis(4-methoxyphenyl)-1H-1,2,4-triazol-1-yl)-1-(4-(pyridin-2-yl)piperazin-1-yl)ethanone (6a)

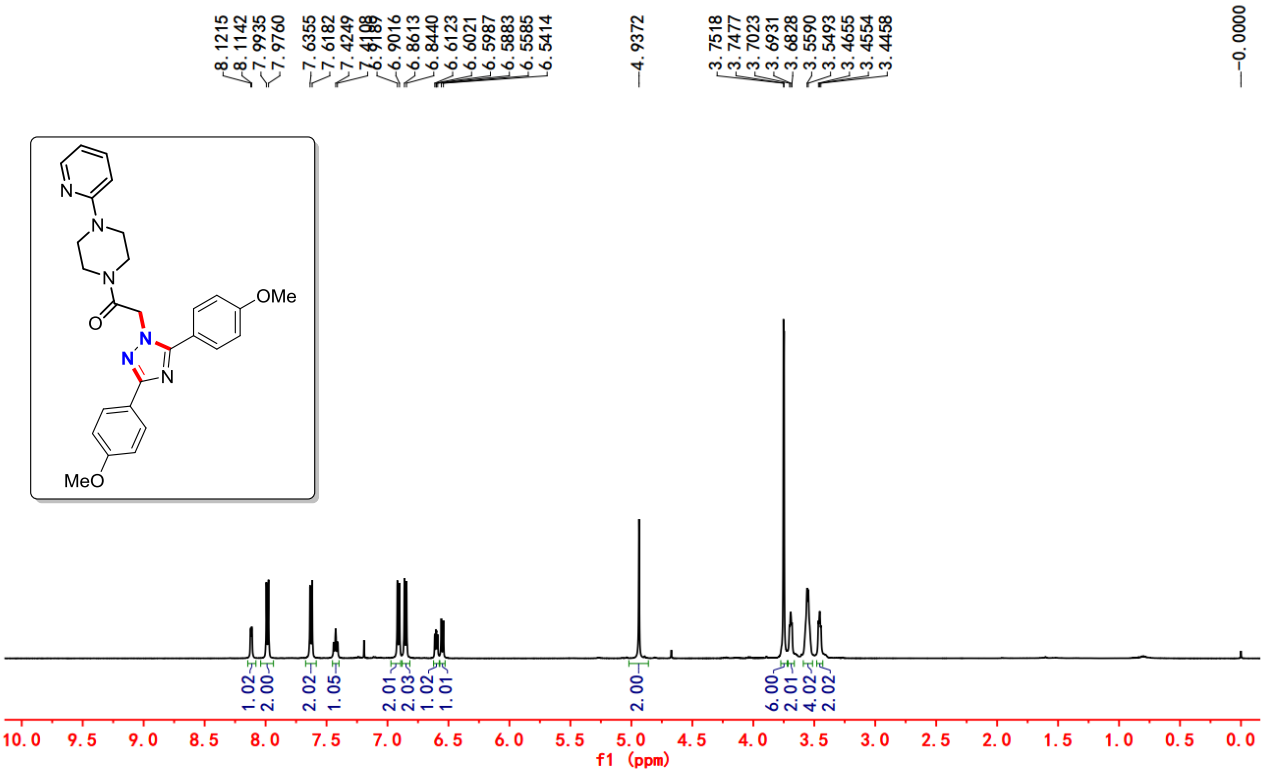


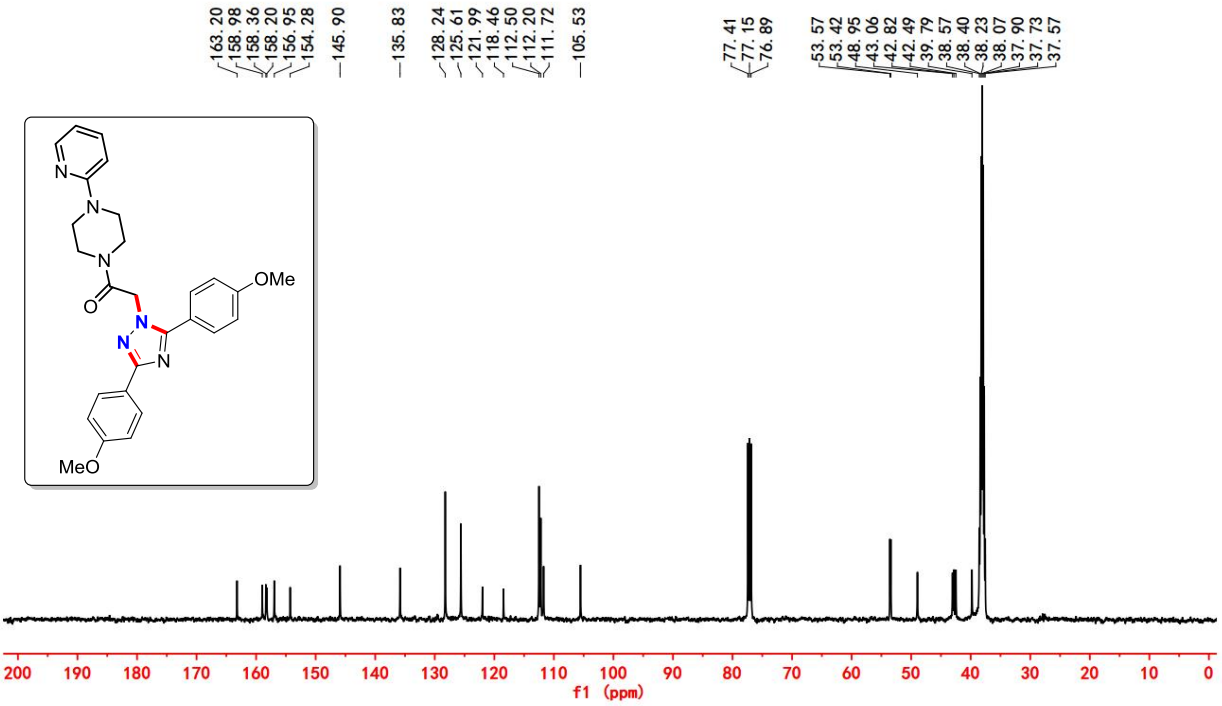
Following our general procedure: In the glove box, a mixture of 4-MeOPhCN (27.0 mg, 0.2 mmol), NH_2NH_2·HCl (14.0 mg, 0.2 mmol), *t*-BuOK (150 mol%) and 1,4-dioxane (0.2 ml) was added into a dry glass tube with a magnetic stirring bar. After being stirred at 120 ^oC (oil bath) for 15 hours, the glass tube was cooled to room temperature. Subsequently, 2-chloro-1-(4-(pyridin-2-yl)piperazin-1-yl) ethan-1-one (120 mg, 0.5 mmol), K_2CO_3 (138 mg, 1.0 mmol), KI (50 mg, 0.3 mmol) and acetone (1.8 mL) were added. The reaction mixture was stirred at 60 ^oC (oil bath) for 24 hours. After the reaction was cooled to room temperture, the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (pentane/ethyl ether = 10/1 - 2/1, DCM 5%) to give the desired product **6a** in 78 % yield (38 mg).

2-(3,5-bis(4-methoxyphenyl)-1H-1,2,4-triazol-1-yl)-1-(4-(pyridin-2-yl)piperazin-1-yl)ethanone (6a)

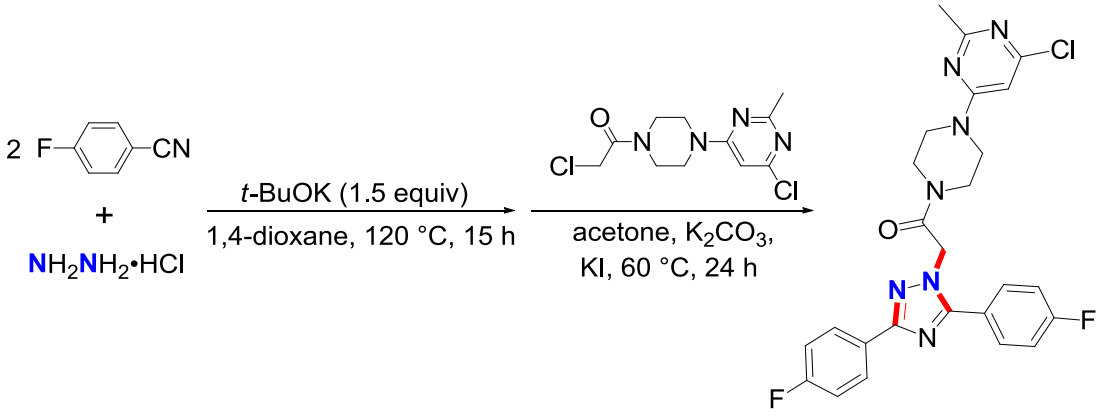


The title compound was prepared according to the general procedure and purified by column chromatography to give the white solid, 38 mg, 78% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 4.0 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.45 – 7.40 (m, 1H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.60 (m, 1H), 6.55 (d, *J* = 8.5 Hz, 1H), 4.94 (s, 2H), 3.75 (s, 6H), 3.74 (s, 6H), 3.71 – 3.66 (m, 2H), 3.55 (d, *J* = 5.0 Hz, 4H), 3.48 – 3.43 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.2, 159.0, 158.4, 158.2, 156.9, 154.3, 145.9, 135.8, 128.2, 125.6, 122.0, 118.5, 112.5, 112.3, 111.7, 105.5, 53.5, 53.4, 48.9, 43.4, 42.9, 42.5, 39.8; **HRMS** (ESI) calcd. for $C_{27}H_{29}N_6O_3$ [M+H]: 485.2301, found: 485.2296.



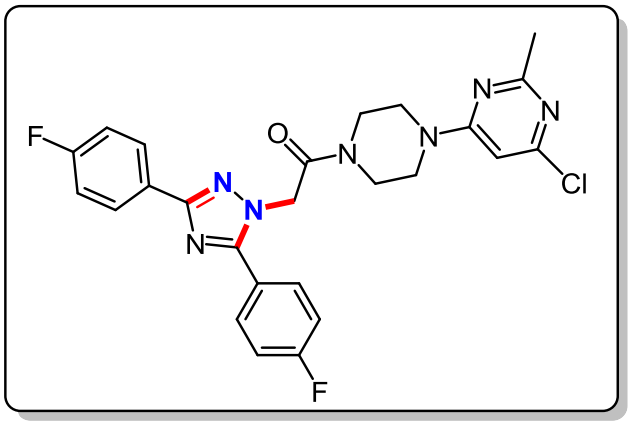

163.20
158.98
158.36
158.20
156.95
154.28
145.90
135.83
128.24
125.61
121.99
118.46
112.50
112.20
111.72
105.53
77.41
77.15
76.89
53.57
53.42
48.95
43.06
42.82
42.49
39.79
38.57
38.40
38.23
38.07
37.90
37.73
37.57
N
N
N
O
N
N
OMe
MeO
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5.3 Synthesis of the mGlu5 receptor of 2-(3,5-bis(4-fluorophenyl)-1H-1,2,4-triazol-1-yl)-1-(4-(6-chloro-2-methylpyrimidin-4-yl)piperazin-1-yl)ethan-1-one (6b)

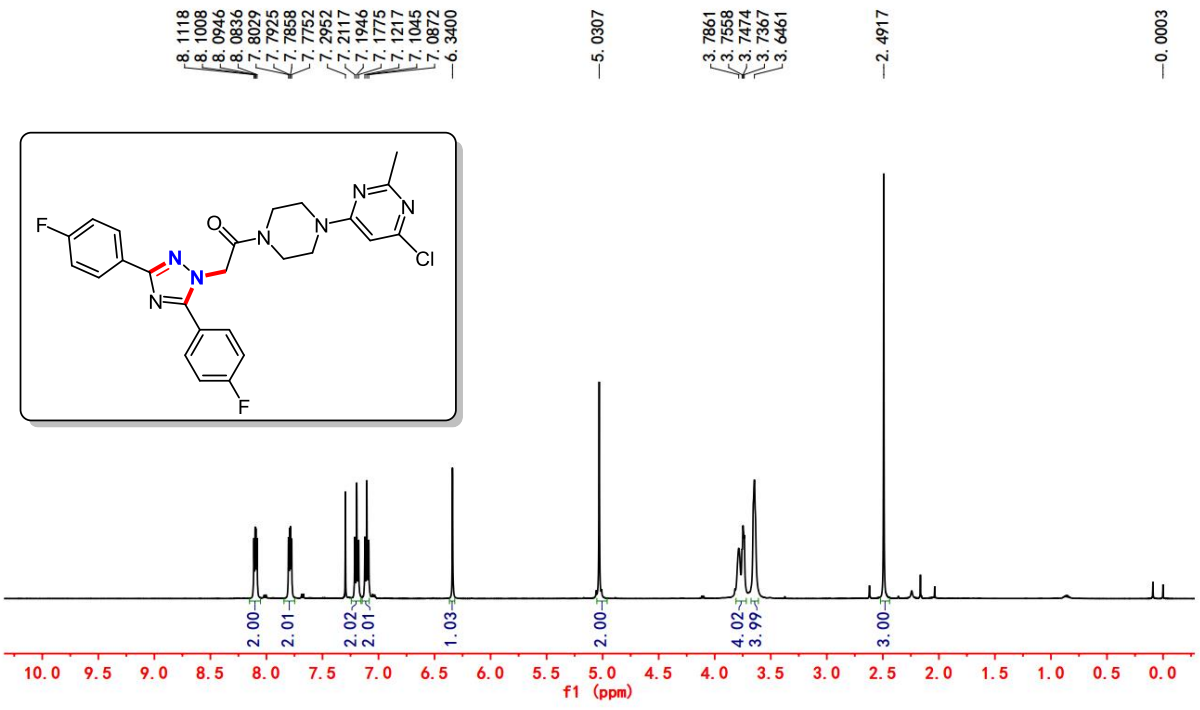


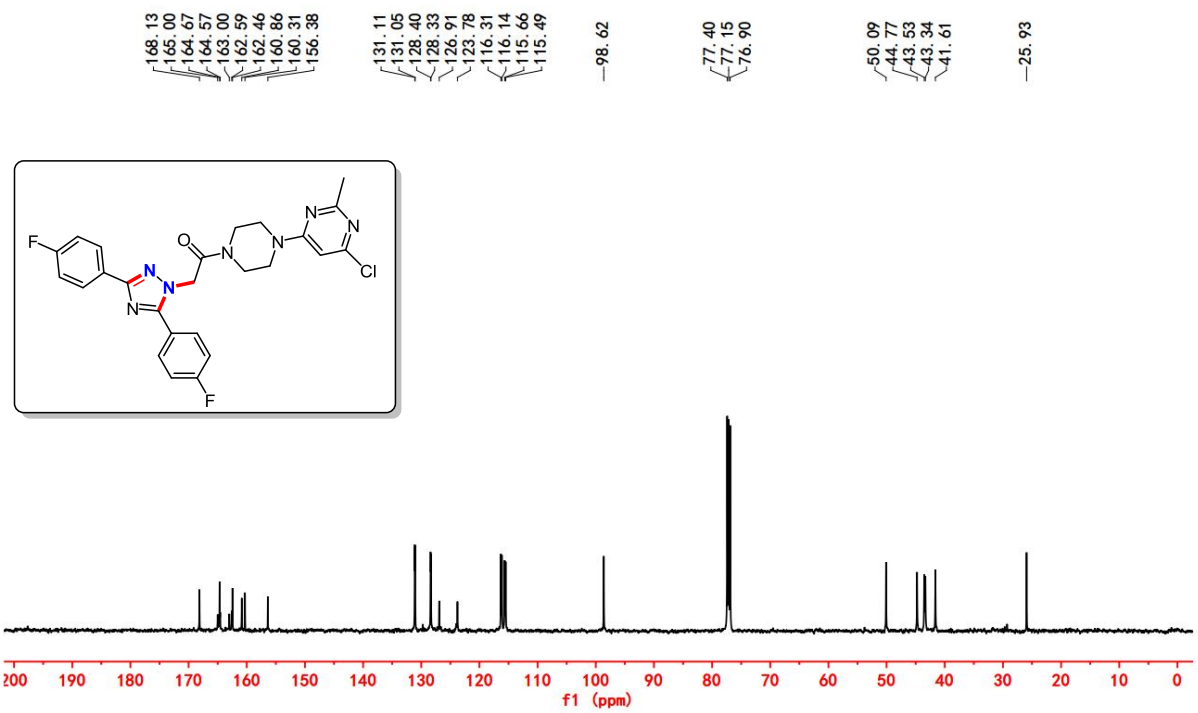
Following our general procedure: In the glove box, a mixture of 4-FPhCN (24.2 mg, 0.2 mmol), $NH_2NH_2 \cdot HCl$ (14.0 mg, 0.2 mmol), *t*-BuOK (150 mol%) and 1,4-dioxane (0.2 ml) was added into a dry glass tube with a magnetic stirring bar. After being stirred at 120 °C (oil bath) for 15 h, the glass tube was cooled to room temperature and added 2-chloro-1-(4-(6-chloro-2-methylpyrimidin-4-yl)piperazin-1-yl)ethan-1-one (145 mg, 0.5 mmol), K_2CO_3 (138 mg, 1.0 mmol), KI (50 mg, 0.3 mmol) and acetone (1.8 mL). The reaction mixture was stirred at 60 °C (oil bath) for 24 h. After the reaction was cooled to room temperture, the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (pentane/ethyl ether = 10/1 - 2/1, DCM 5%) to give the desired product **6b** in 73 % yield.

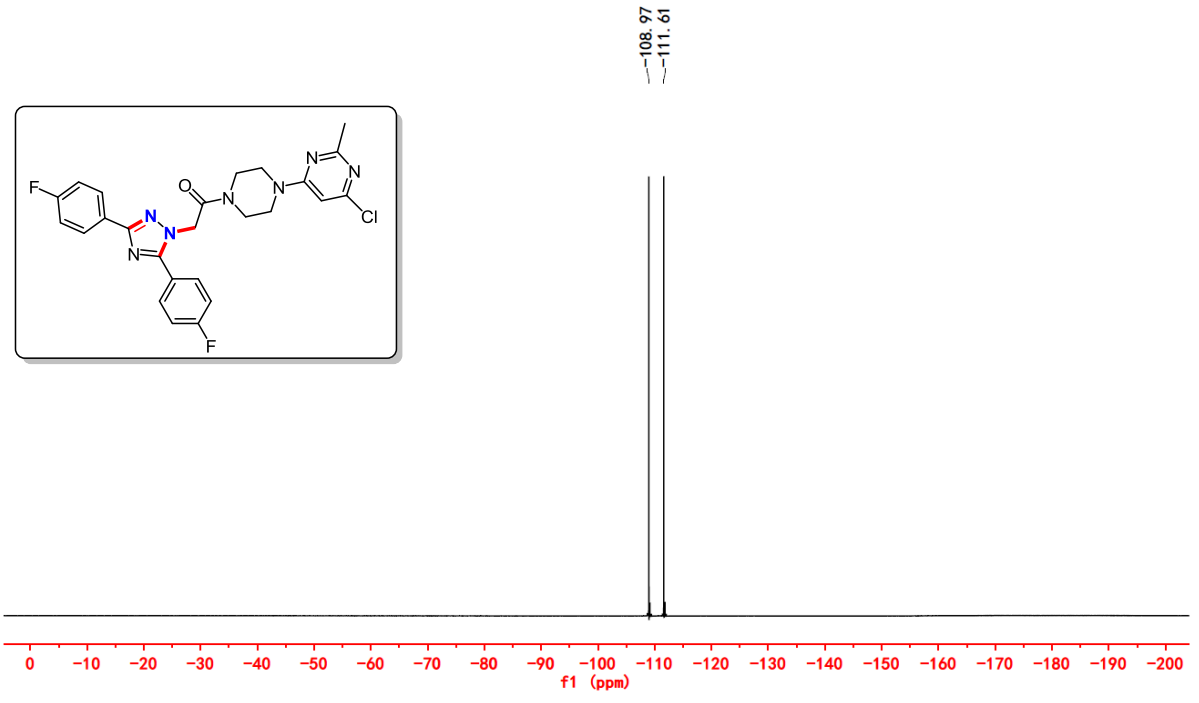
2-(3,5-bis(4-fluorophenyl)-1H-1,2,4-triazol-1-yl)-1-(4-(6-chloro-2-methylpyrimidin-4-yl)piperazin-1-yl)ethan-1-one



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 37.2 mg, 73% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 8.6, 5.5 Hz, 2H), 7.79 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.19 (t, *J* = 8.5 Hz, 2H), 7.10 (t, *J* = 8.6 Hz, 2H), 6.34 (s, 1H), 5.03 (s, 2H), 3.76 (dd, *J* = 14.5, 10.2 Hz, 4H), 3.65 (s, 4H), 2.49 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.1, 165.0, 164.62 (d, *J* = 12.8 Hz), 162.8 (d, J = 52.5 Hz), 162.5, 160.9, 160.3, 156.4, 131.1 (d, *J* = 8.2 Hz), 128.4 (d, *J* = 7.8 Hz), 126.9, 123.8, 116.2 (d, *J* = 21.9 Hz), 115.6 (d, *J* = 21.7 Hz), 115.7, 115.5, 98.6, 50.1, 44.8, 43.5, 43.3, 41.6, 25.9. HRMS (ESI) calcd. for $C_{25}H_{23}ClF_2N_7O$ [M+H]:510.1621, found: 510.1620.

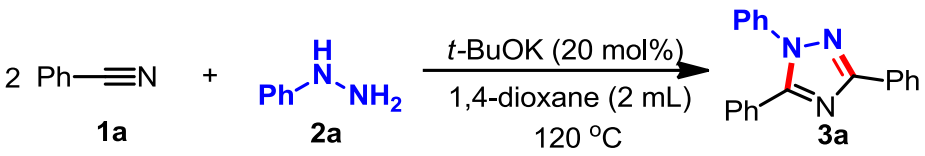



168.13
165.00
164.67
164.57
163.00
162.59
162.46
160.86
160.31
156.38
131.11
131.05
128.40
128.33
126.91
123.78
116.31
116.14
115.66
115.49
98.62
77.40
77.15
76.90
50.09
44.77
43.53
43.34
41.61
25.93
F
O
N
N
N
N
N
Cl
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


108.97
111.61
F
O
N
N
N
N
N
Cl
F
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

6. Mechanistic studies

6.1 Control experiments

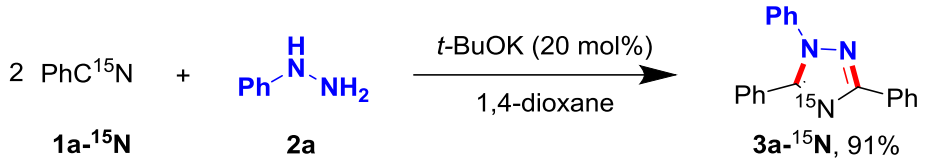


Entry	Reaction condition	Addition	**3a** [%]
1	New seal tube		0
2	New seal tube, 98% *t*-BuOK		96
3	New seal tube, 99.99% *t*-BuOK		94
4	99.99% *t*-BuOK	18-crown-6 (0.2 equiv)	<5
5	99.99% *t*-BuOK	TEMPO (2 equiv)	95
6	99.99% *t*-BuOK	$Ph_2C=CH_2$ (2 equiv)	92

Using a nitrogen-filled glove box, an oven-dried new pressure tube (38 mL volume) was charged with a magnetic stirring bar, PhCN (103 μl, 1.0 mmol), $PhNHNH_2$ (99 μl, 1.0 mmol), *t*-BuOK (20 mol%), addition (0.2 equiv or 2 equiv) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 °C). After 10 min the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC or GC-MS to monitor products formation.

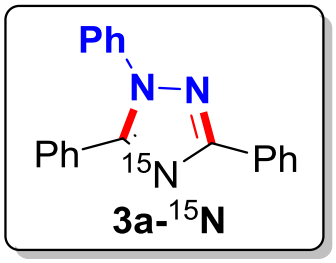
The product of **3a** (entry 3) was analyzed by ICP-MS to analysis and testing the transition metals species. However, the metals (Pd, Rh, Ru, Cu, Co, Ni) in the product **3a** was undetectable (< 0.1 ppm) by ICP-MS analysis.

6.2 ^{15}N-Labeled experiments: PhC^{15}N (1a-^{15}N)

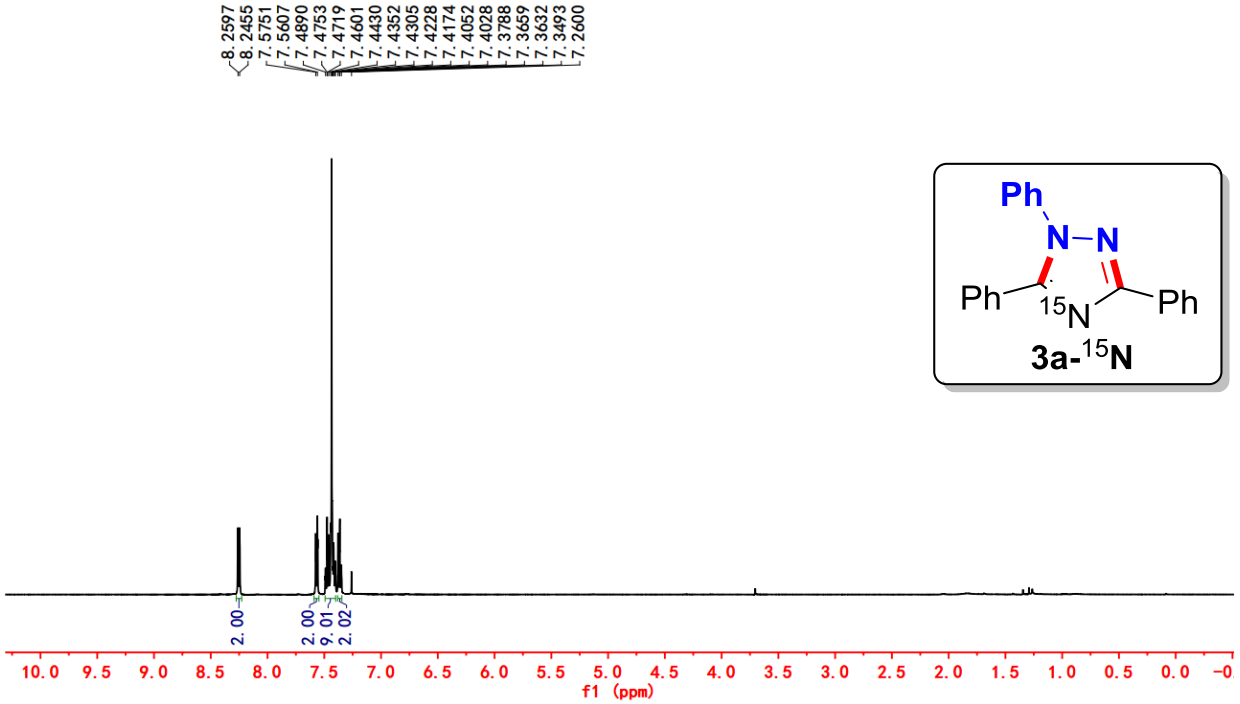


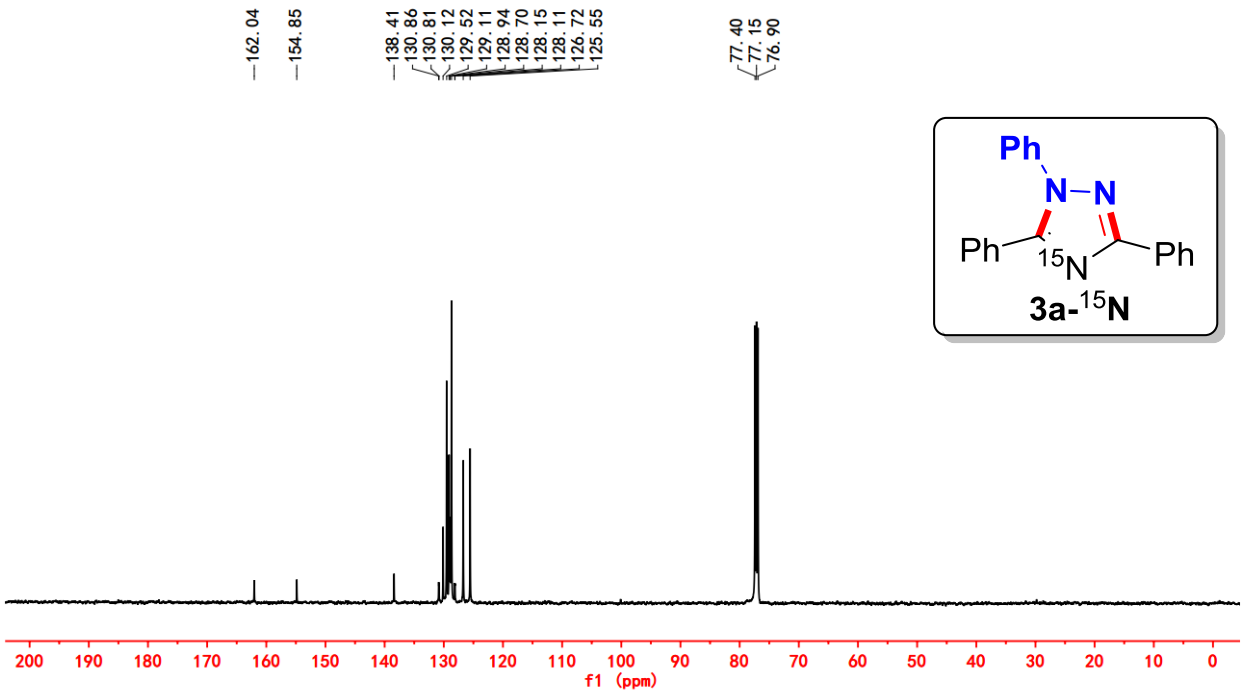
Using a nitrogen-filled glove box, an oven-dried new pressure tube (38 mL volume) was charged with a magnetic stirring bar, PhC^{15}N (103 μl, 1.0 mmol), $PhNHNH_2$ (99 μl, 1.0 mmol), *t*-BuOK (22 mg, 20 mol%, 0.2 mmol) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 °C). After 10 min the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC or GC-MS to monitor products formation. Then the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (pentane/ethyl ether = 10/1 - 2/1, DCM 5%) to give the desired product **3a-^{15}N** in 91 % yield.

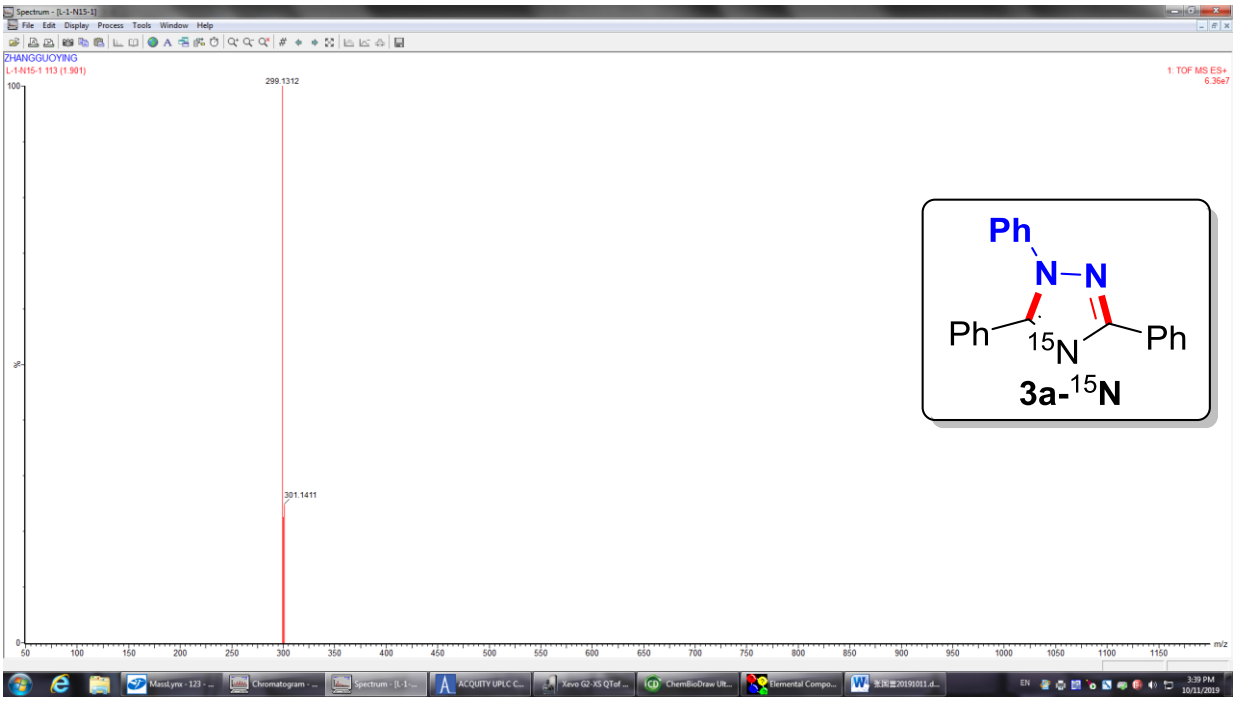
1,3,5-triphenyl-1*H*-1,2,4-triazole (3a-^{15}N):



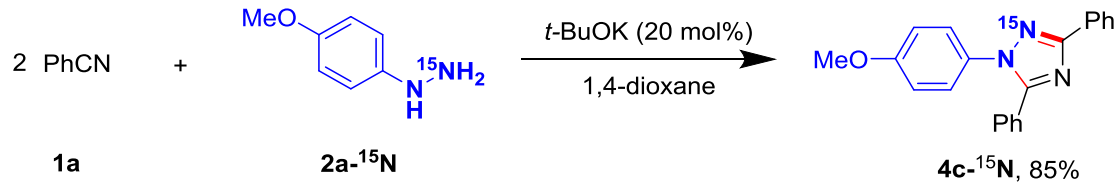
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 136.2 mg, 91% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.0 Hz, 2H), 7.59 (d, *J* = 7.0 Hz, 2H), 7.51 – 7.42 (m, 9H), 7.38 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.9, 154.8, 138.3, 130.7, 130.6, 130.0, 129.4, 128.8, 128.6, 128.1, 128.0, 127.9, 126.6, 125.5; **HRMS** (ESI) calcd. for $C_{20}H_{16}N_2{}^{15}N$ [M+H]:299.1315, found: 299.1312.


8.2597
8.2455
7.5751
7.5607
7.4890
7.4753
7.4719
7.4601
7.4430
7.4352
7.4305
7.4228
7.4174
7.4052
7.4028
7.3788
7.3659
7.3632
7.3493
7.2600
2.00
2.00
9.01
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Ph
N–N
Ph
15N
Ph
3a-15N


162.04
154.85
138.41
130.86
130.81
130.12
129.52
129.11
128.94
128.70
128.15
128.11
126.72
125.55
77.40
77.15
76.90
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Ph
N–N
Ph
15N
Ph
3a-15N

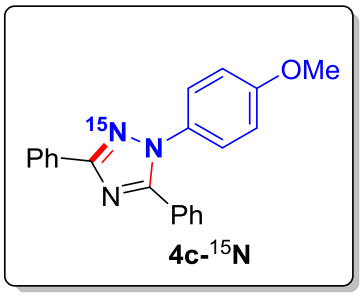


6.3 ^{15}N-Labeled experiments:PMP-NH^{15}NH$_2$ (4p-^{15}N)

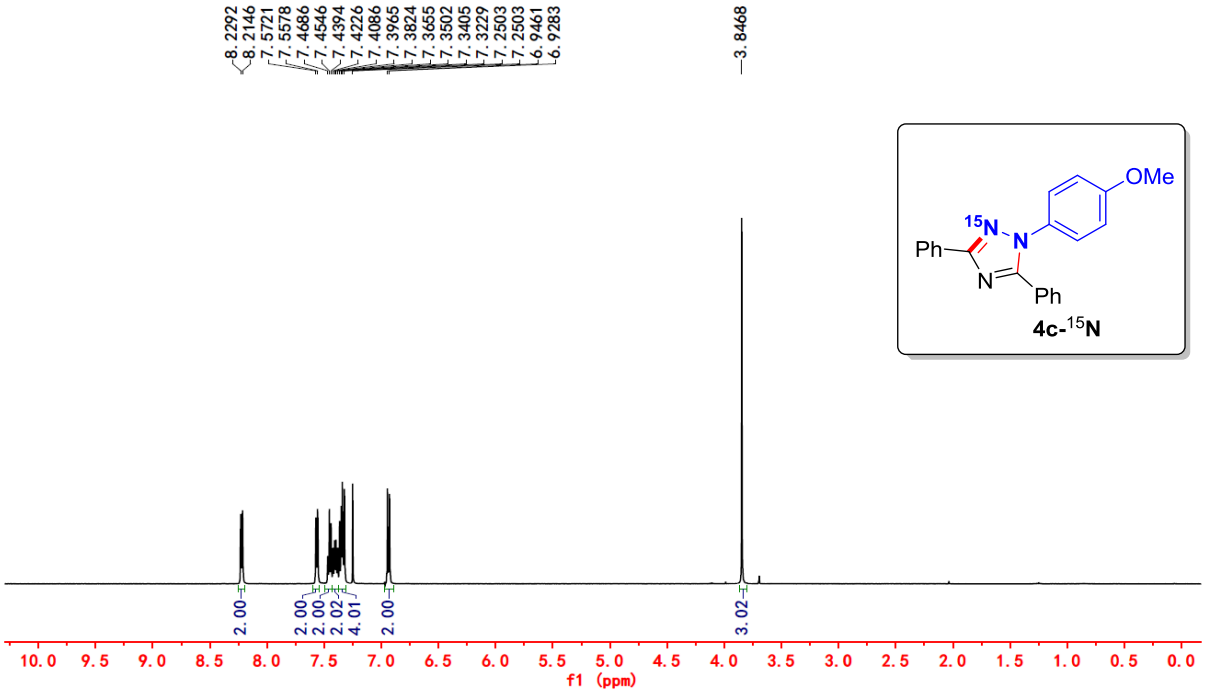


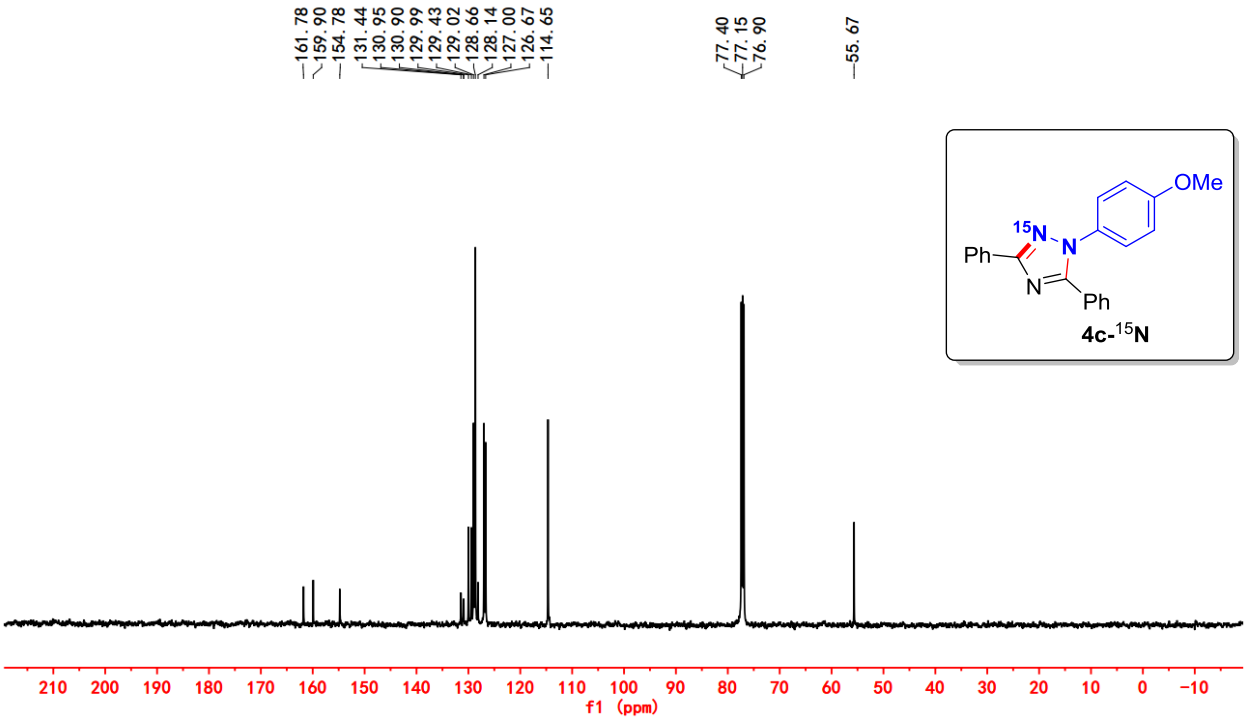
Using a nitrogen-filled glove box, an oven-dried new pressure tube (38 mL volume) was charged with a magnetic stirring bar, PhCN (51 μl, 0.5 mmol), PMPNH^{15}NH$_2$·HCl (87.5 mg, 0.5 mmol), *t*-BuOK (67 mg, 120 mol%, 0.6 mmol) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 ^{o}C). After 15 hours the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC or GC-MS to monitor products formation. Then the corresponding reaction mixture was purified by flash column chromatography on a silica gel column (pentane/ethyl ether = 10/1 - 2/1, DCM 5%) to give the desired product **4c-^{15}N** in 85 % yield.

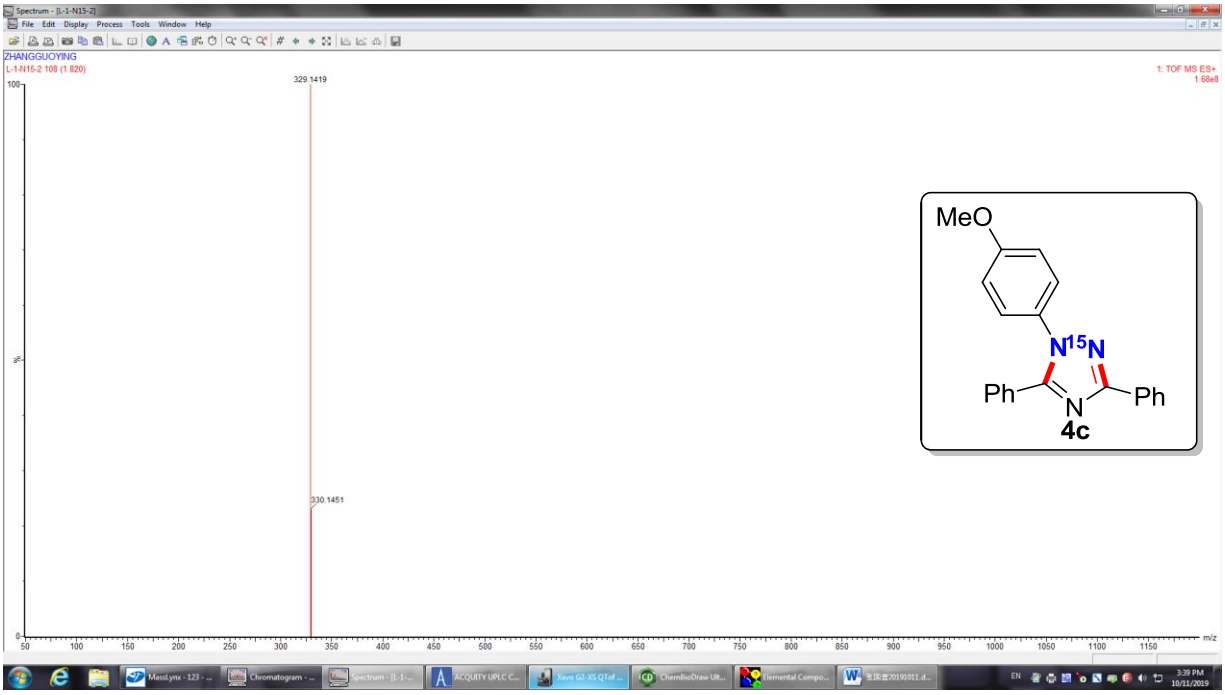
1-(4-methoxyphenyl)-3,5-diphenyl-1*H*-1,2,4-triazole (4c-^{15}N):



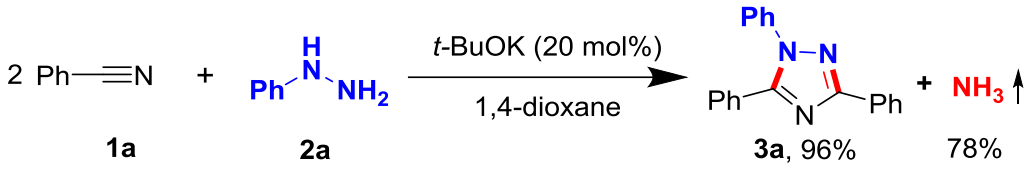
The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 69.7 mg, 85% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.5 Hz, 2H), 7.56 (d, *J* = 7.0 Hz, 2H), 7.45 (m, 2H), 7.40 (m, 2H), 7.34 (m, 4H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.7, 159.8, 154.7, 131.4, 130.8, 130.7, 129.9, 129.3, 128.9, 128.6, 128.1, 126.9, 126.6, 114.7, 55.6; **HRMS** (ESI) calcd. for $C_{21}H_{18}N_2{}^{15}NO$ [M+H]:329.1420, found: 329.1419.




161.78
159.90
154.78
131.44
130.95
130.90
129.99
129.43
129.02
128.66
128.14
127.00
126.67
114.65
77.40
77.15
76.90
55.67
OMe
15N
N
Ph
N
Ph
4c-15N
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)

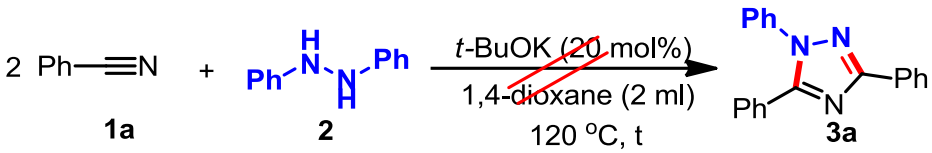

ZHANGGUOYING
329.1419
330.1451
MeO
N15N
Ph
Ph
N
4c

6.4 Analyzed the gas of the reaction



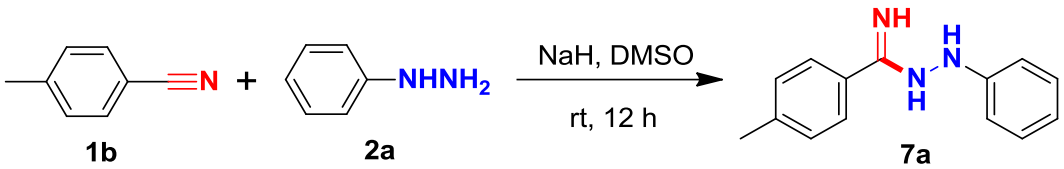
Following our general procedure: In the glove box, a mixture of PhCN (1030 μl, 10 mmol), $PhNHNH_2$ (990 μl, 10 mmol), *t*-BuOK (20 mol%) 1,4-dioxane (10 ml) was added into a dry Schlenk tube with a magnetic stirring bar. The reaction mixture was stirred at 120 °C (oil bath) for 10 min. After the reaction finished, the glass tube was cooled to room temperature. A small aliquot of the gas was analyzed by GC to monitor NH_3 formation. The yield of NH_3 was obtained in 78%. Then, the gas was absorbed with a fresh solution of $Zn(OH)_2$ (1.0 mmol) in H_2O (5 mL). And the white cloudy solution of $Zn(OH)_2$ in H_2O gradually became a clear solution of $[Zn(NH_3)_4](OH)_2$. The yield of NH_3 was obtained in 78%.

6.5 Control experimment



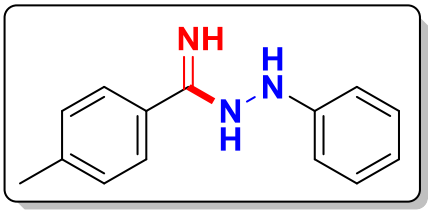
Using a nitrogen-filled glove box, an oven-dried new pressure tube (38 mL volume) was charged with a magnetic stirring bar, PhCN (103 μl, 1.0 mmol), 1,2-diphenylhydrazine (184.2 mg, 1.0 mmol), *t*-BuOK (20 mol%), addition (0.2 equiv or 2 equiv) and 1,4-dioxane (2.0 mL). Then the seal tube was closed tightly with a teflon cap, removed from the glove box and immersed into a pre-heated oil bath (120 °C). After 10 min the reaction was cooled, quenched with half-saturated brine (0.1 mL) and was dried over Na_2SO_4. A small aliquot of the organic phase was analyzed by GC or GC-MS to monitor products formation. The desired compound **3a** was undetected.

6.6 Synthesis of 4-methyl-N'-phenylbenzimidohydrazide

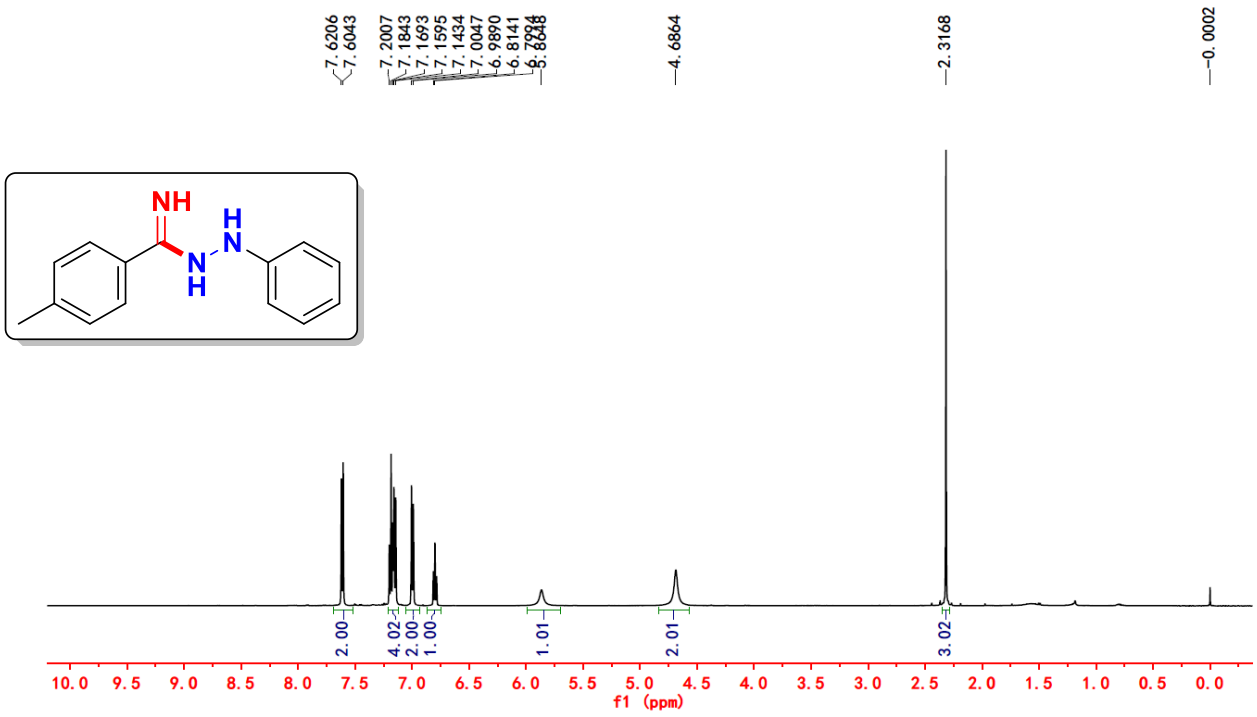


Under N_2 atmosphere, a solution of NaH (29 mg, 1.2 mmol) in DMSO (1 mL) was added $PhNHNH_2$ (0.12 mL, 1.2 mmol). After 10 min of stirring at room temperature, the mixture of reaction was added dropwise 4-MePhCN (117 mg, 1mmol) in DMSO (1 mL) and stirred overnight. Then the reaction was quenched with H_2O (2 ml), and extracted with DCM (4X3 mL). After being dried with anhydrous Na_2SO_4, the combined extract was evaporated under reduced pressure to give a yellow solid (205 mg) in 91% yield.

4-methyl-N'-phenylbenzimidohydrazide



The title compound was prepared according to the general procedure and purified by column chromatography to give a yellow solid, 205 mg, 91% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.21 – 7.12 (m, 4H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.80 (t, *J* = 7.5 Hz, 1H), 5.86 (s, 1H), 4.69 (s, 2H), 2.32 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.4, 147.9, 139.9, 131.4, 129.2, 129.1, 125.8, 120.0, 114.4, 21.4.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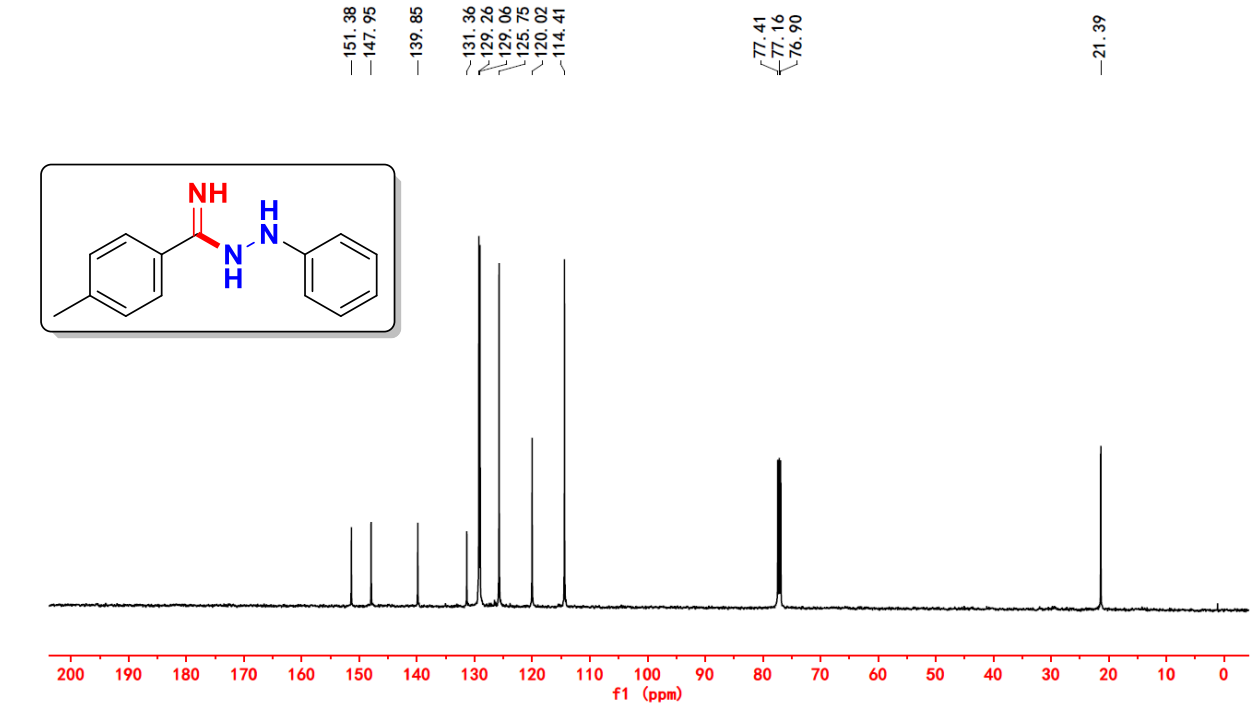
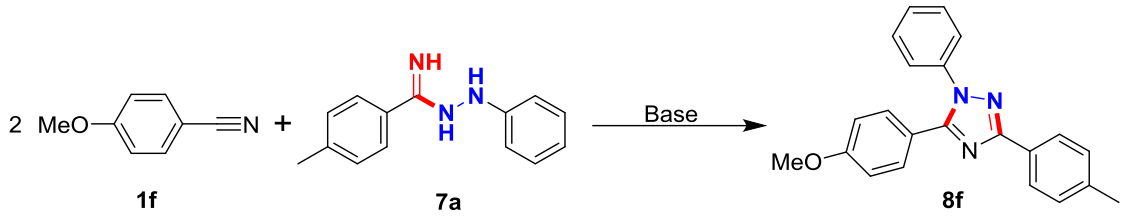
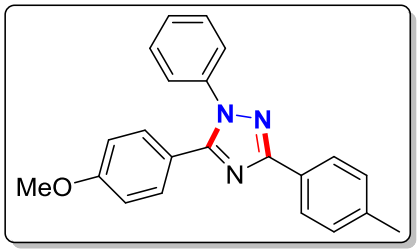
7.6043
7.2007
7.1843
7.1693
7.1595
7.1434
7.0047
6.9890
6.8141
4.6864
2.3168
-0.0002
NH
H
N
N
H
2.00
4.02
2.00
1.00
1.01
2.01
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


151.38
147.95
139.85
131.36
129.26
129.06
125.75
120.02
114.41
77.41
77.16
76.90
21.39
NH
H
N
N
H
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



Following our general procedure: In the glove box, a mixture of PMPCN (67 mg, 0.5 mmol), 4-methyl-N'-phenylbenzimidohydrazide (0.5 mmol, 113 mg), *t*-BuOK (20 mol%) and 1,4-dioxane (2 ml) was added into a dry glass tube with a magnetic stirring bar. The reaction mixture was stirred at 120 °C (oil bath) for 10 min. After the reaction finished, the glass tube was cooled to room temperature and the reaction was quenched with H_2O (0.1 ml). Then the corresponding reaction mixture was purified by flash column chromatography on a silica gel column petroleum ether/ethyl acetate (5/1, v/v) to give the desired product **8a** (141.6 mg, 83%).

5-(4-methoxyphenyl)-1-phenyl-3-(p-tolyl)-1H-1,2,4-triazole



The title compound was prepared according to the general procedure and purified by column chromatography to give a white solid, 141.6 mg, 83% yield. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.42 (s, 5H), 7.25 (s, 2H), 6.86 (d, *J* = 8.5 Hz, 2H), 3.81 (s, 3H), 2.40 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.9, 160.8, 154.5, 139.3, 138.5, 134.0, 130.5, 129.4, 129.3, 128.0, 126.5, 125.5, 120.4, 114.7, 114.0, 55.3, 21.45; HRMS (ESI) calcd. for $C_{22}H_{20}N_3O$ [M+H]: 342.1606, found: 342.1613.

7. Reference

1 Z. Chen, H. Li, W. Dong, M. Miao and H. Ren, *Org. Let.,* 2016, **18**, 1334.

2 M. M. Guru and T. Punniyamurthy, *J. Org. Chem.,* 2012, **77**, 5063.

3 L. Zhang, D. Tang, J. Gao, J. Wang, P. Wu, X. Meng and B. Chen, *Synthesis,* 2016, **22**, 3924.

4 S. V. Kuberkar, *Indian. J. Chem.,* 1991, **30B**, 78.

5 H. Wang, Y. Ren, K. Wang, Y. Man, Y. Xiang, N. Li and B. Tang, *Chem. Commun.,* 2017, **53**, 9644.

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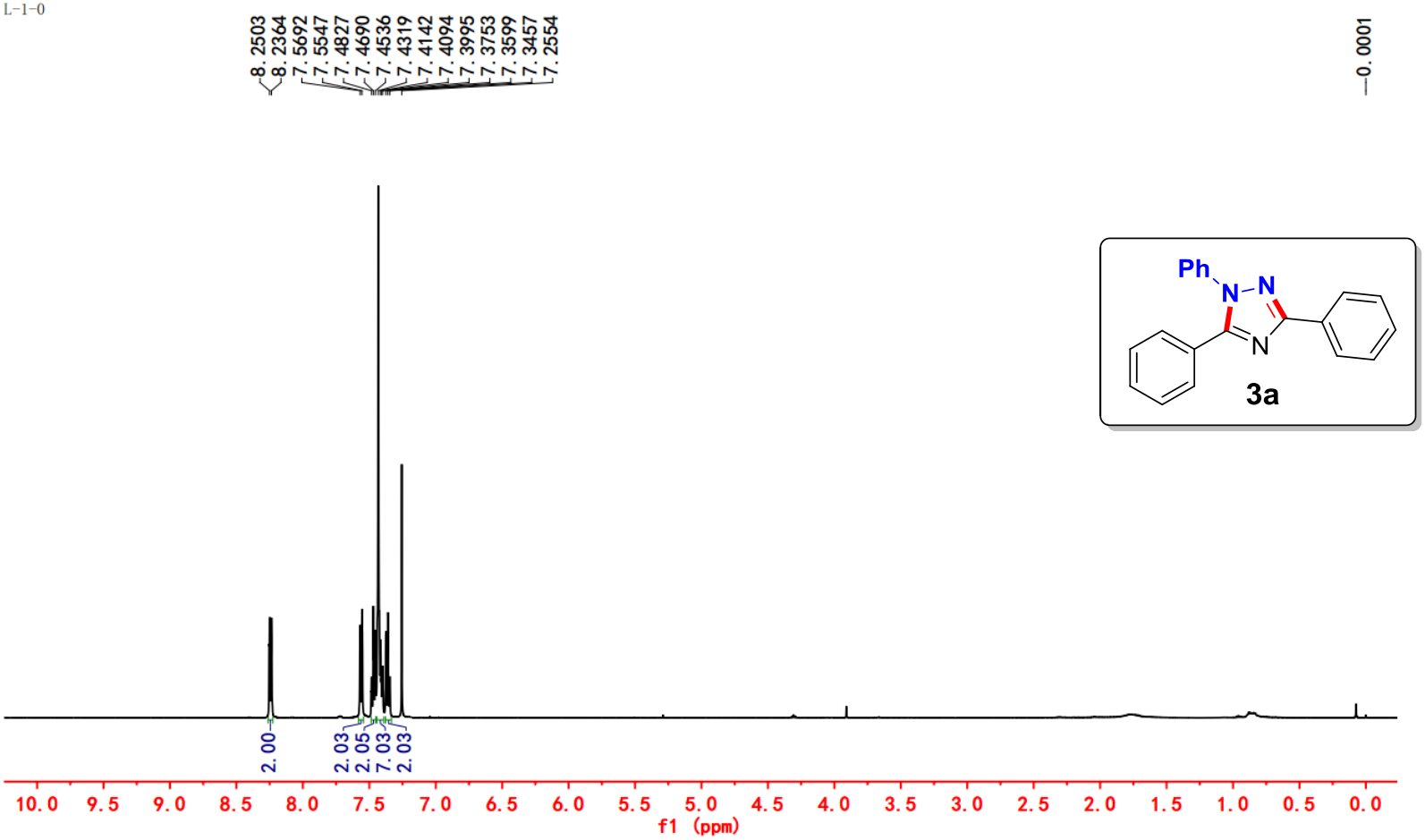
7 J. Kuang, B. Chen and S. Ma, *Org. Chem. Front.*, 2014, **1**, 186.

8. Copies for ^{1}H NMR and ^{13}C NMR of the 1,2,4-triazoles.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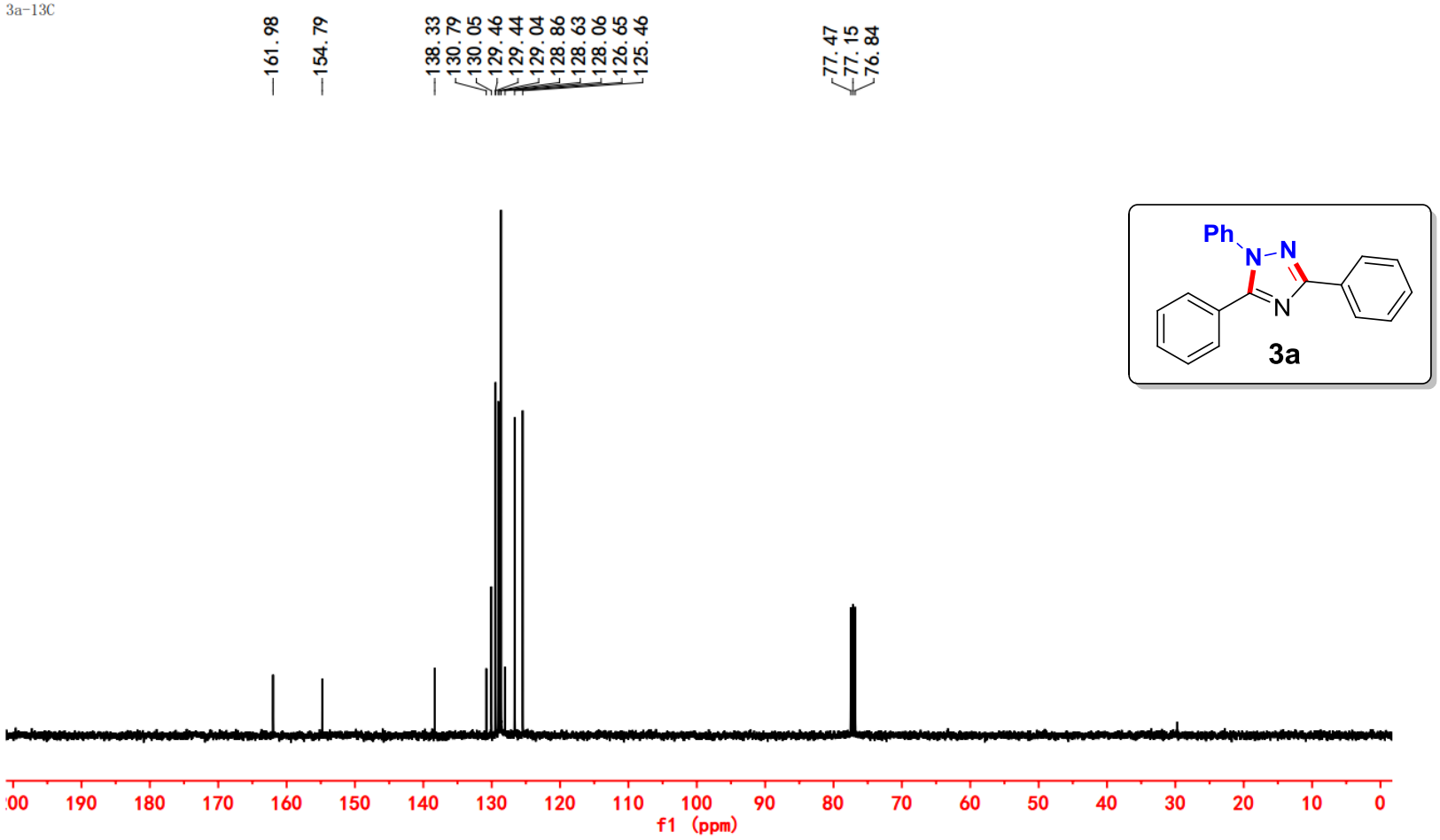
7.4827
7.4690
7.4536
7.4319
7.4142
7.4094
7.3995
7.3753
7.3599
7.3457
7.2554
0.0001
Ph
N
N
N
3a
2.00
2.03
2.05
7.03
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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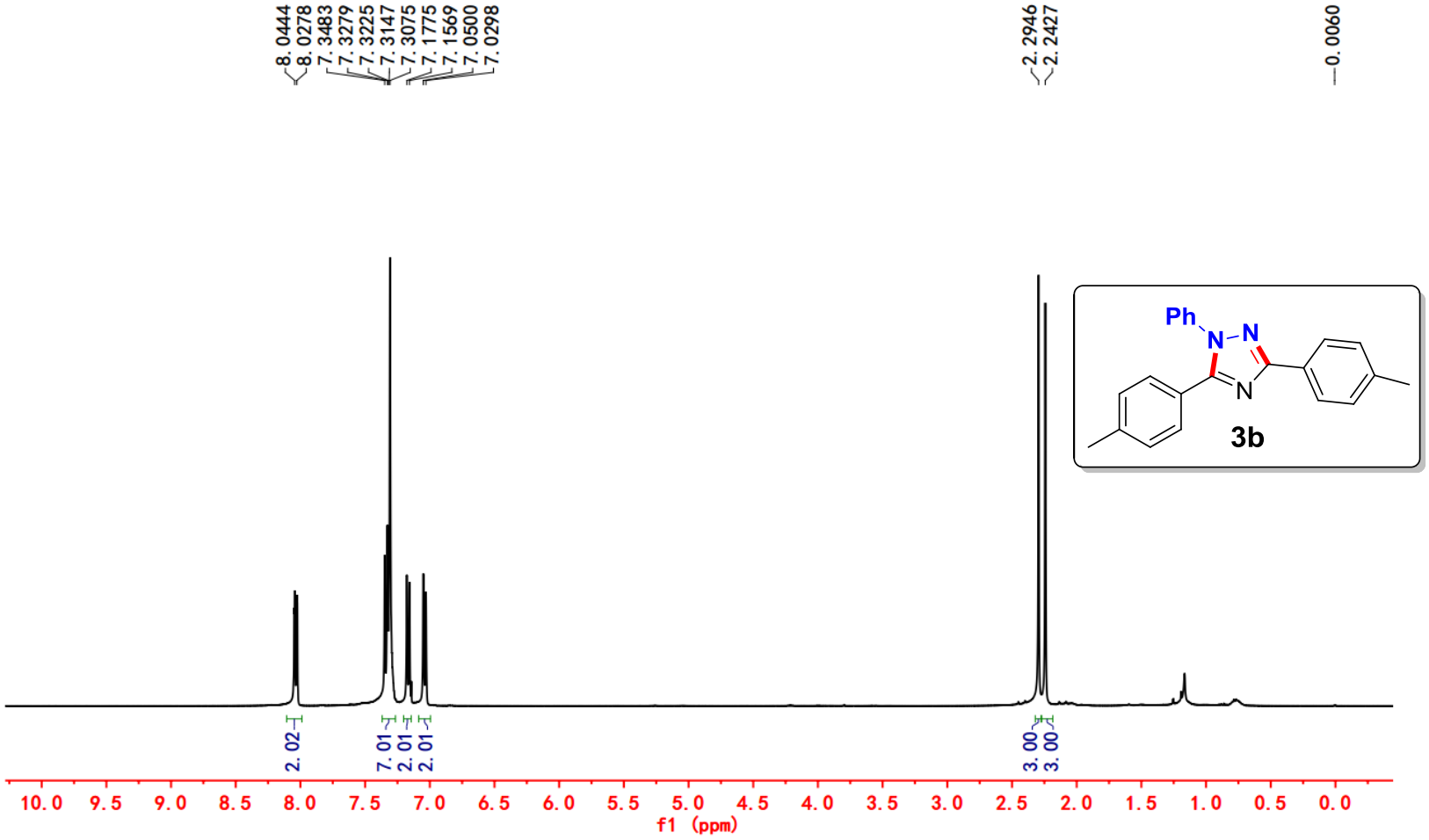
154.79
138.33
130.79
130.05
129.46
129.44
129.04
128.86
128.63
128.06
126.65
125.46
77.47
77.15
76.84
Ph
N
N
N
3a
00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3483
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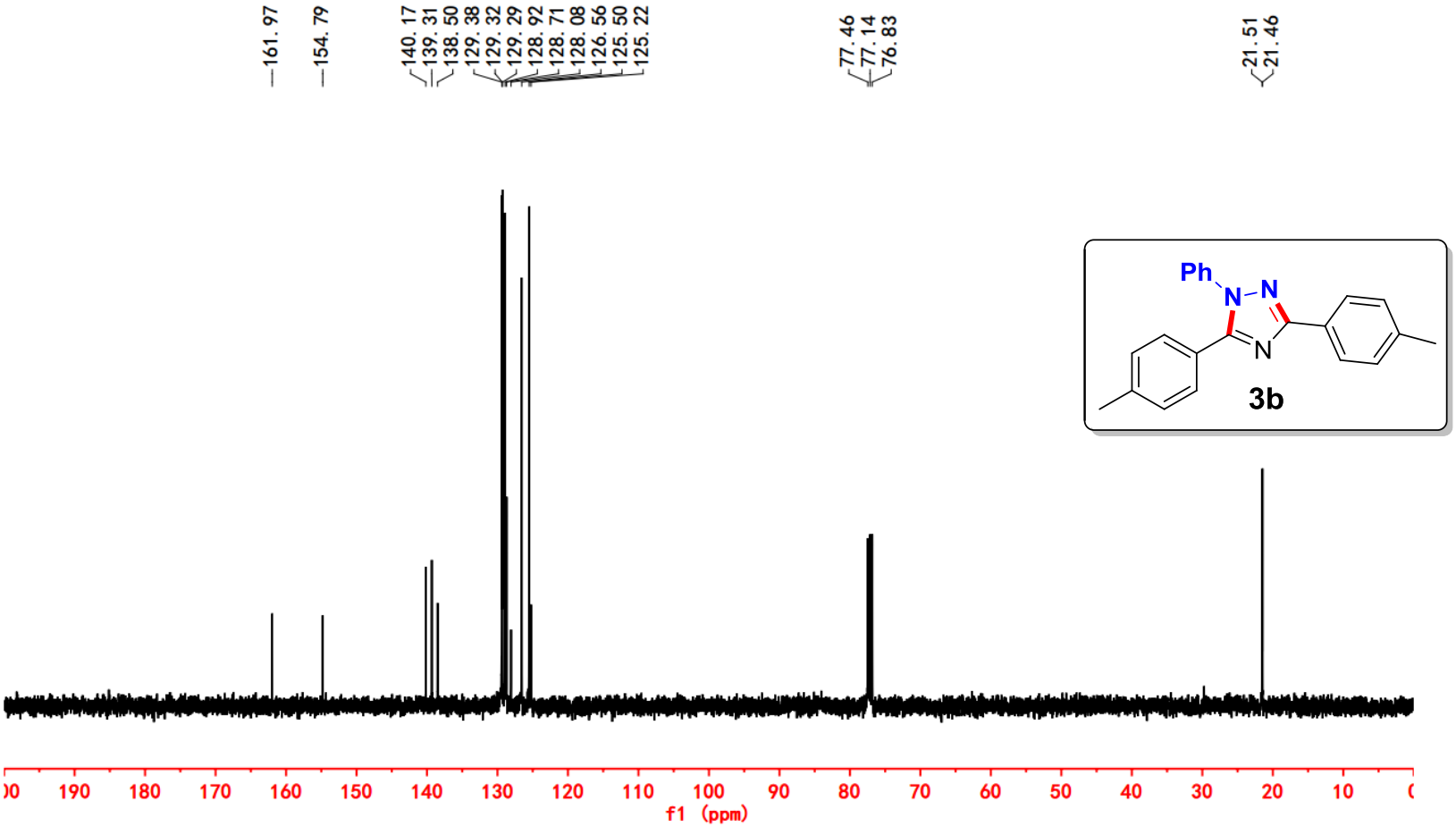
7.0500
7.0298
2.2946
2.2427
0.0060
Ph
N
N
N
3b
2.02
7.01
2.01
2.01
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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140.17
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138.50
129.38
129.32
129.29
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128.71
128.08
126.56
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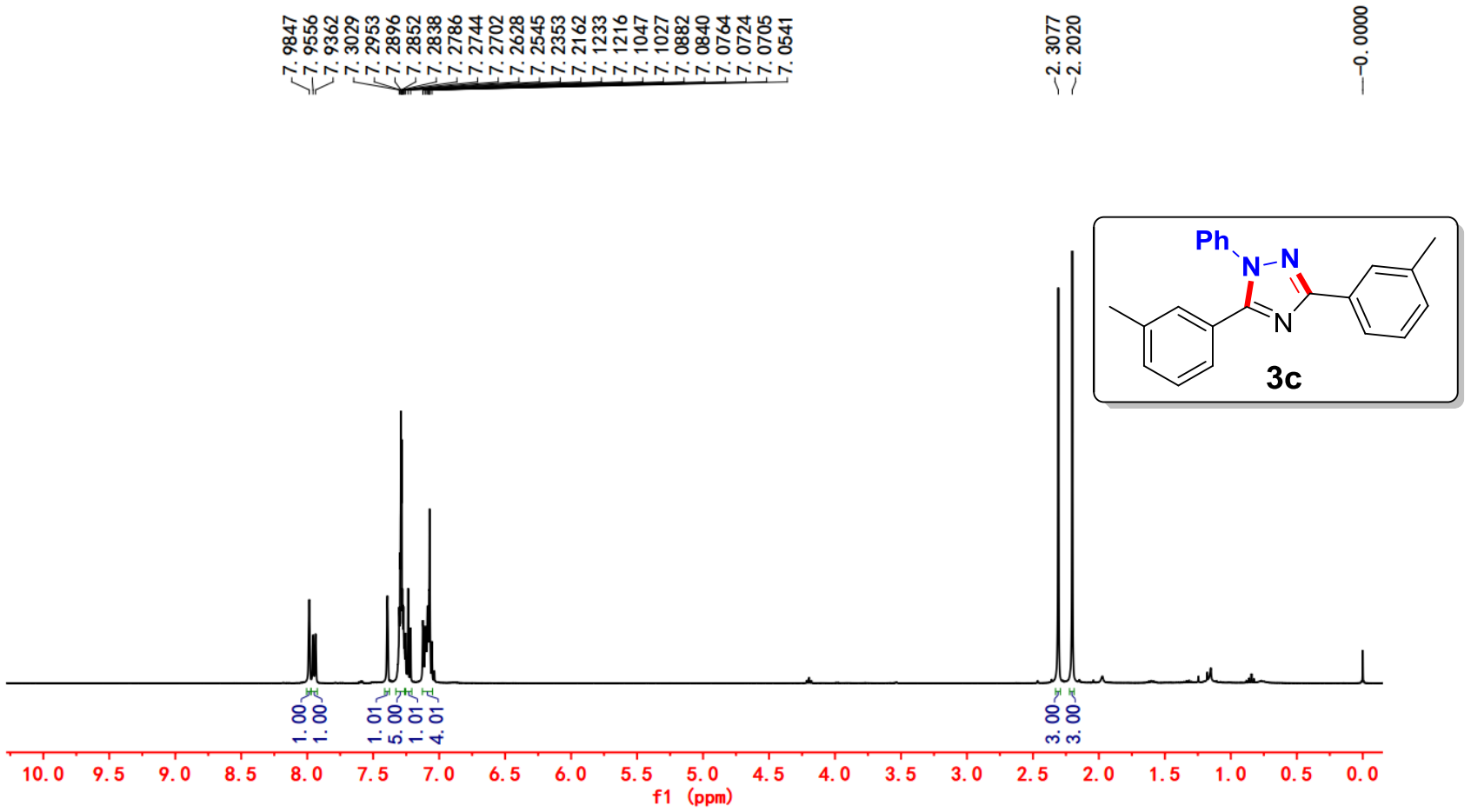
21.46
Ph
N
N
N
3b
f1 (ppm)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7.0764
7.0724
7.0705
7.0541
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1.00
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1.01
5.00
1.01
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3.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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1.0
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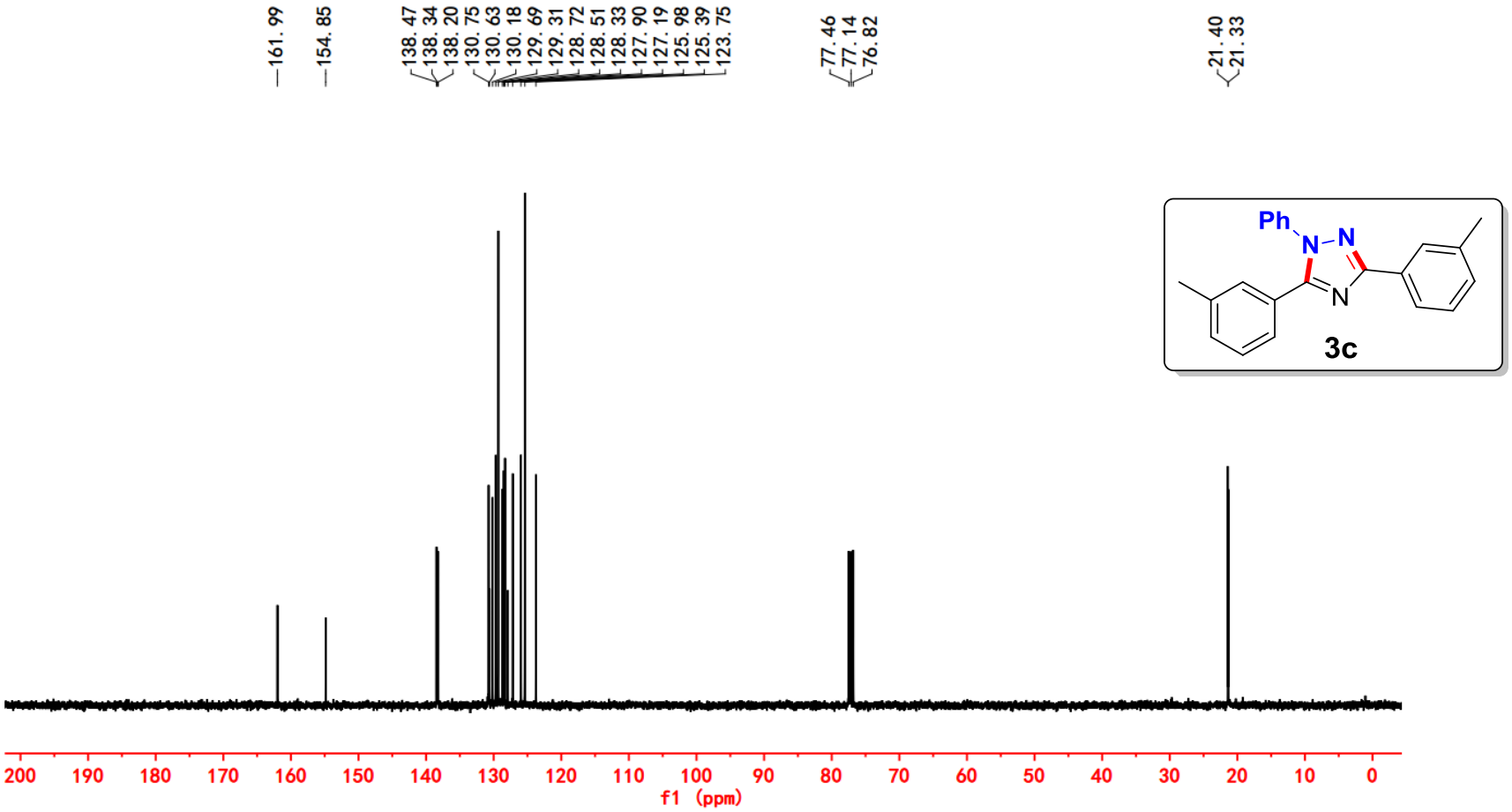
0.0
f1 (ppm)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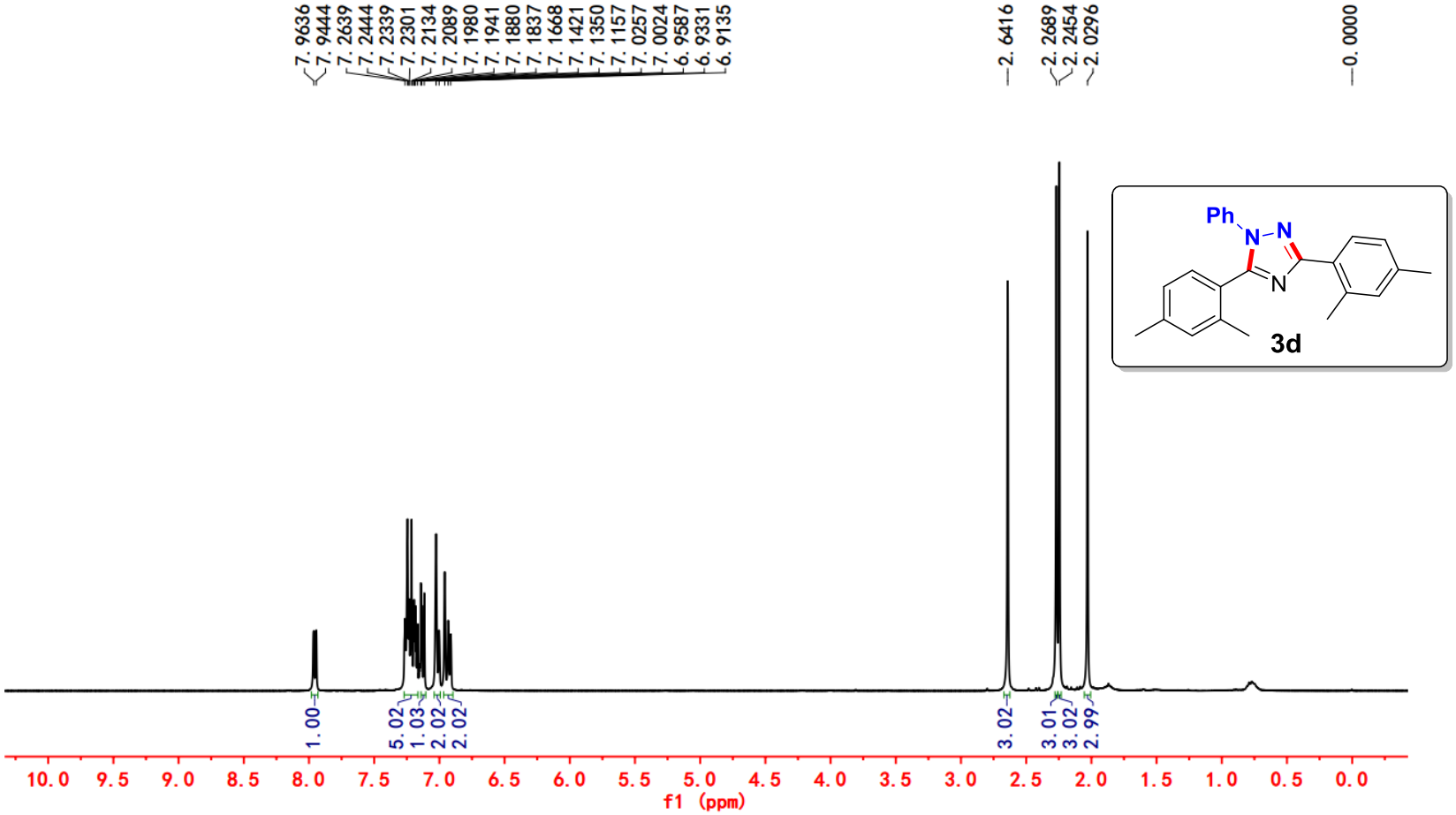
130.18
129.69
129.31
128.72
128.51
128.33
127.90
127.19
125.98
125.39
123.75
77.46
77.14
76.82
21.40
21.33
Ph
N
N
N
3c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.1980
7.1941
7.1880
7.1837
7.1668
7.1421
7.1350
7.1157
7.0257
7.0024
6.9587
6.9331
6.9135
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2.2689
2.2454
2.0296
0.0000
Ph
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N
N
3d
1.00
5.02
1.03
2.02
2.02
3.02
3.01
3.02
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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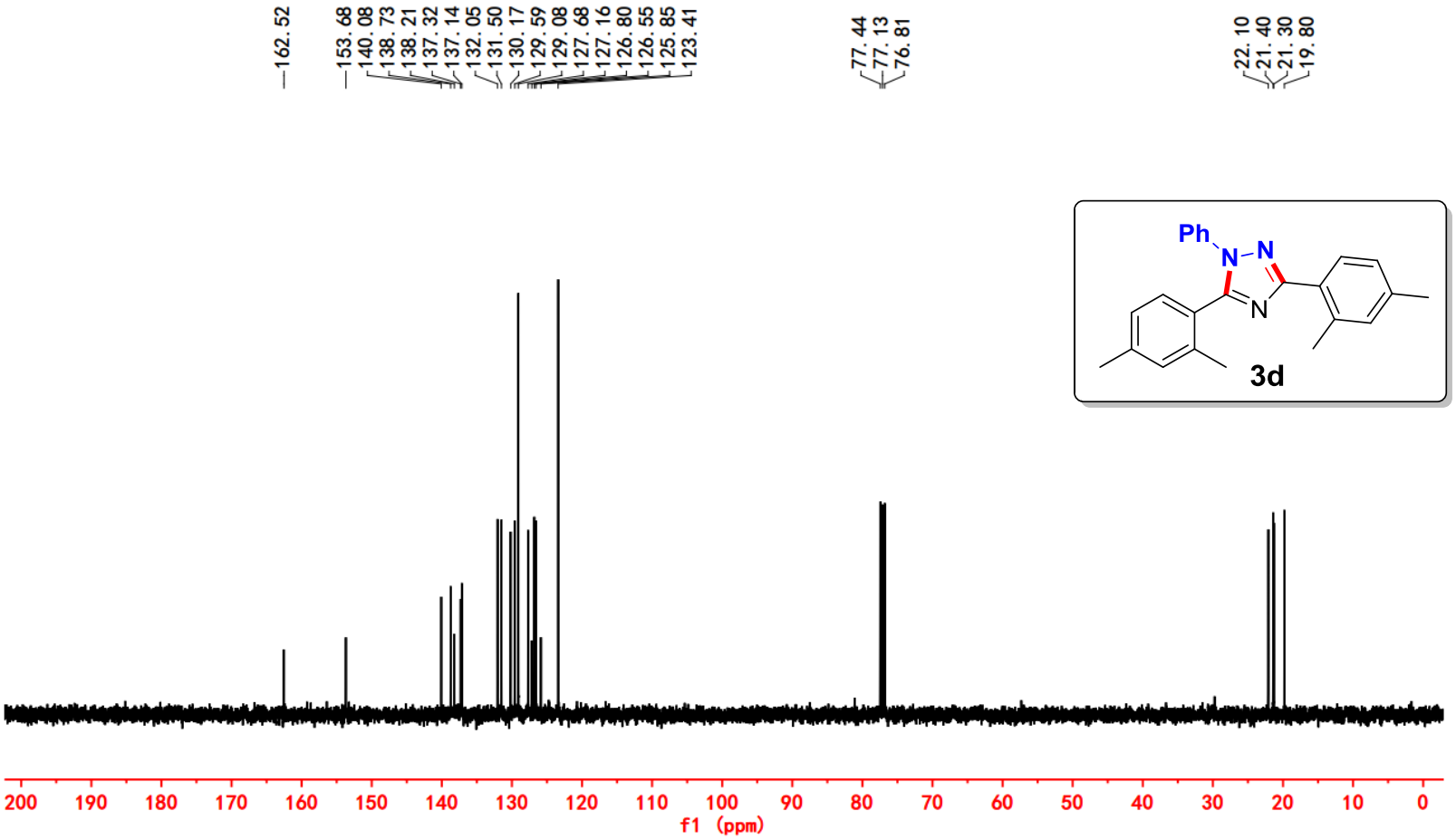
1.0
0.5
0.0
f1 (ppm)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130.17
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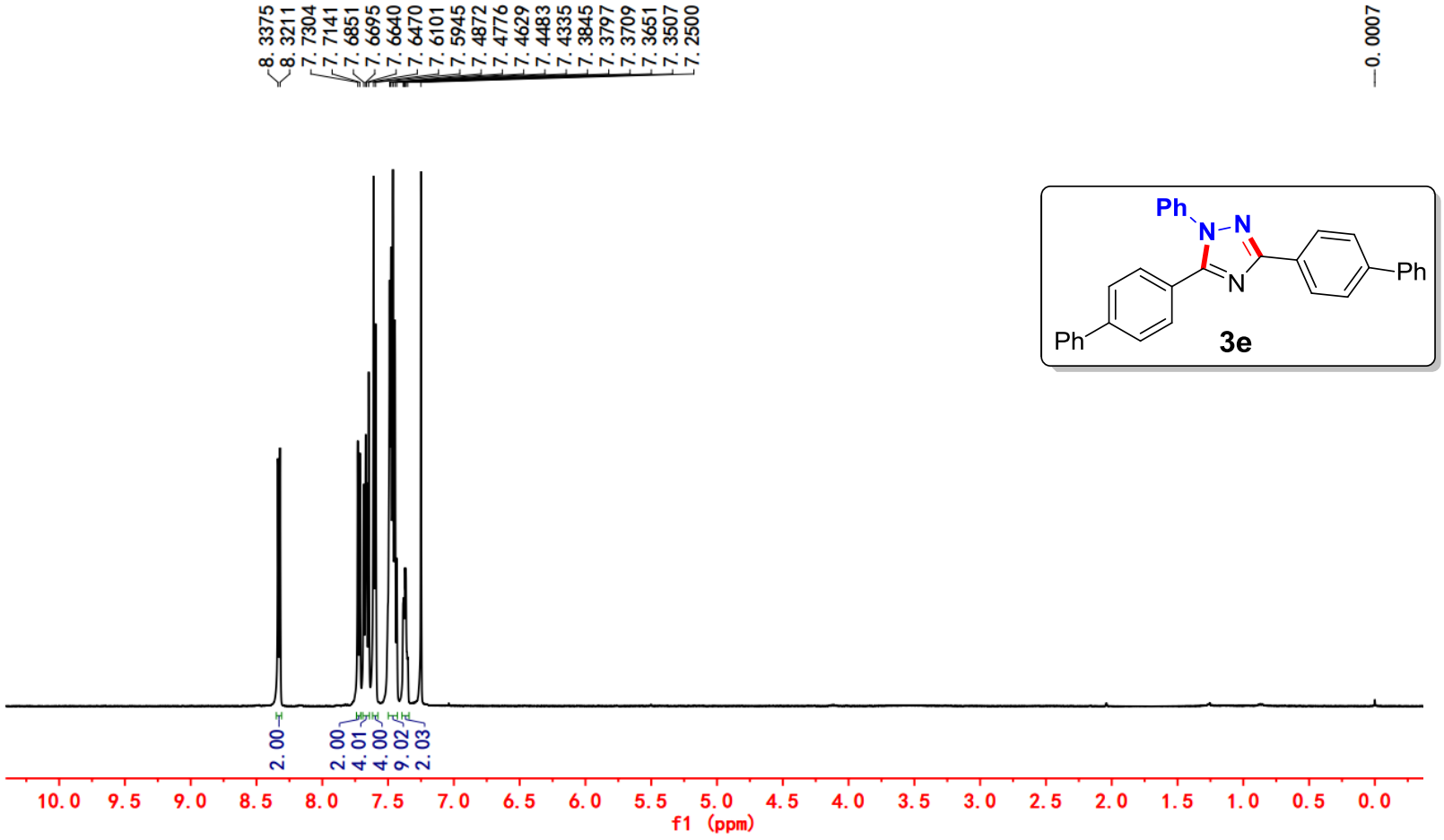
129.08
127.68
127.16
126.80
126.55
125.85
123.41
77.44
77.13
76.81
22.10
21.40
21.30
19.80
Ph
N
N
N
3d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4776
7.4629
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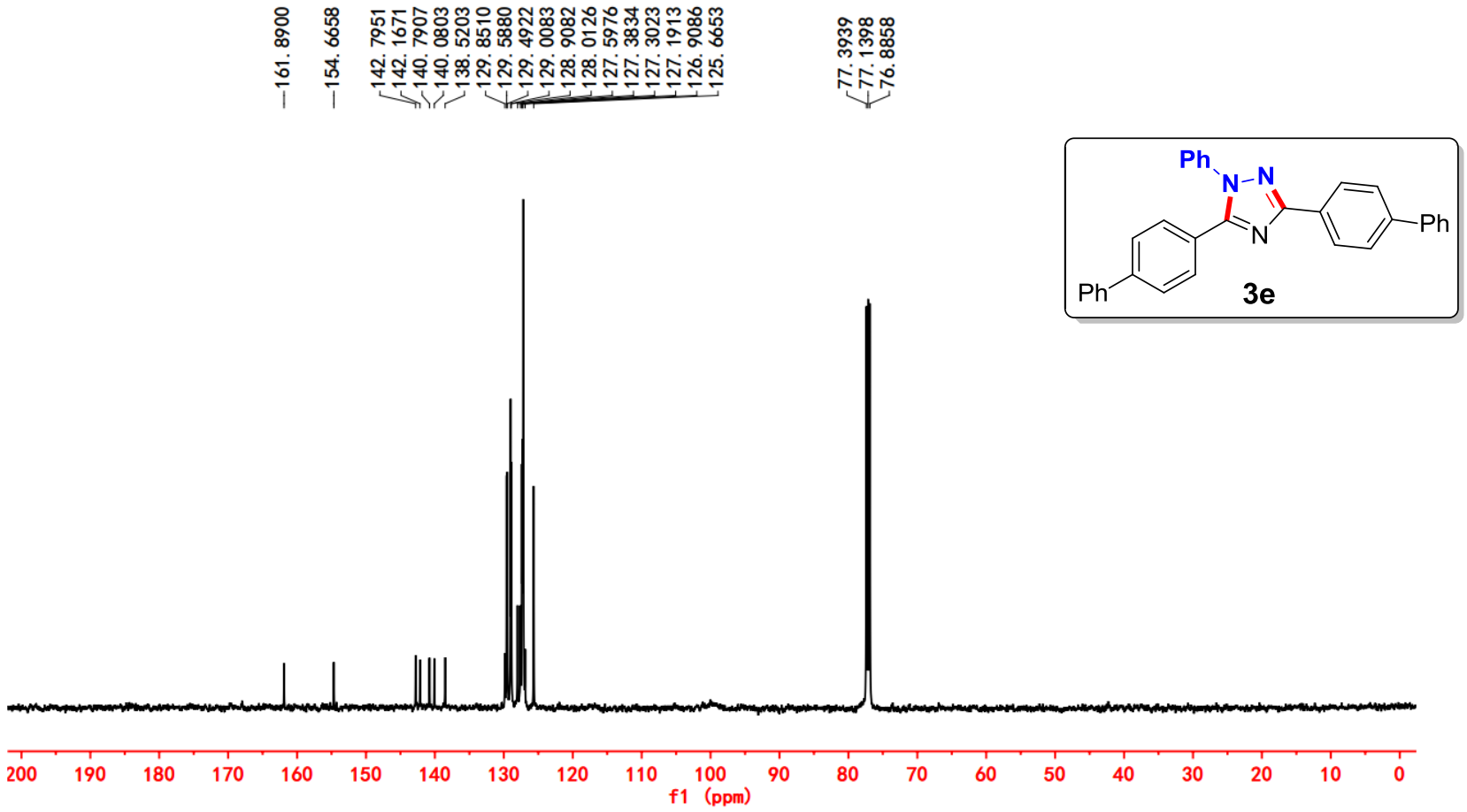
7.4335
7.3845
7.3797
7.3709
7.3651
7.3507
7.2500
0.0007
Ph
N
N
N
Ph
Ph
3e
2.00
2.00
4.01
4.00
9.02
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.0083
128.9082
128.0126
127.5976
127.3834
127.3023
127.1913
126.9086
125.6653
77.3939
77.1398
76.8858
Ph
N
N
N
Ph
Ph
3e
200
190
180
170
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150
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130
120
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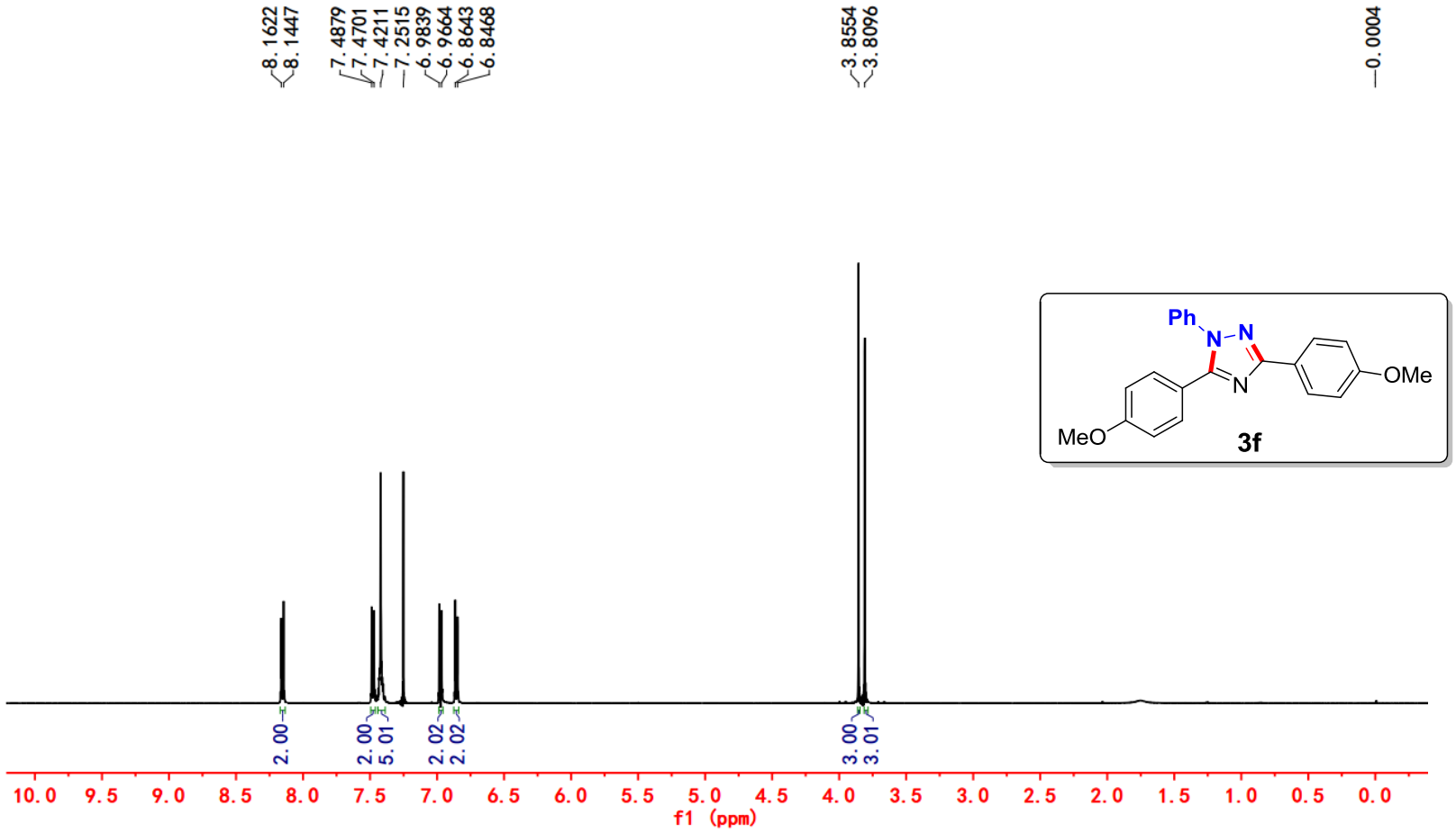
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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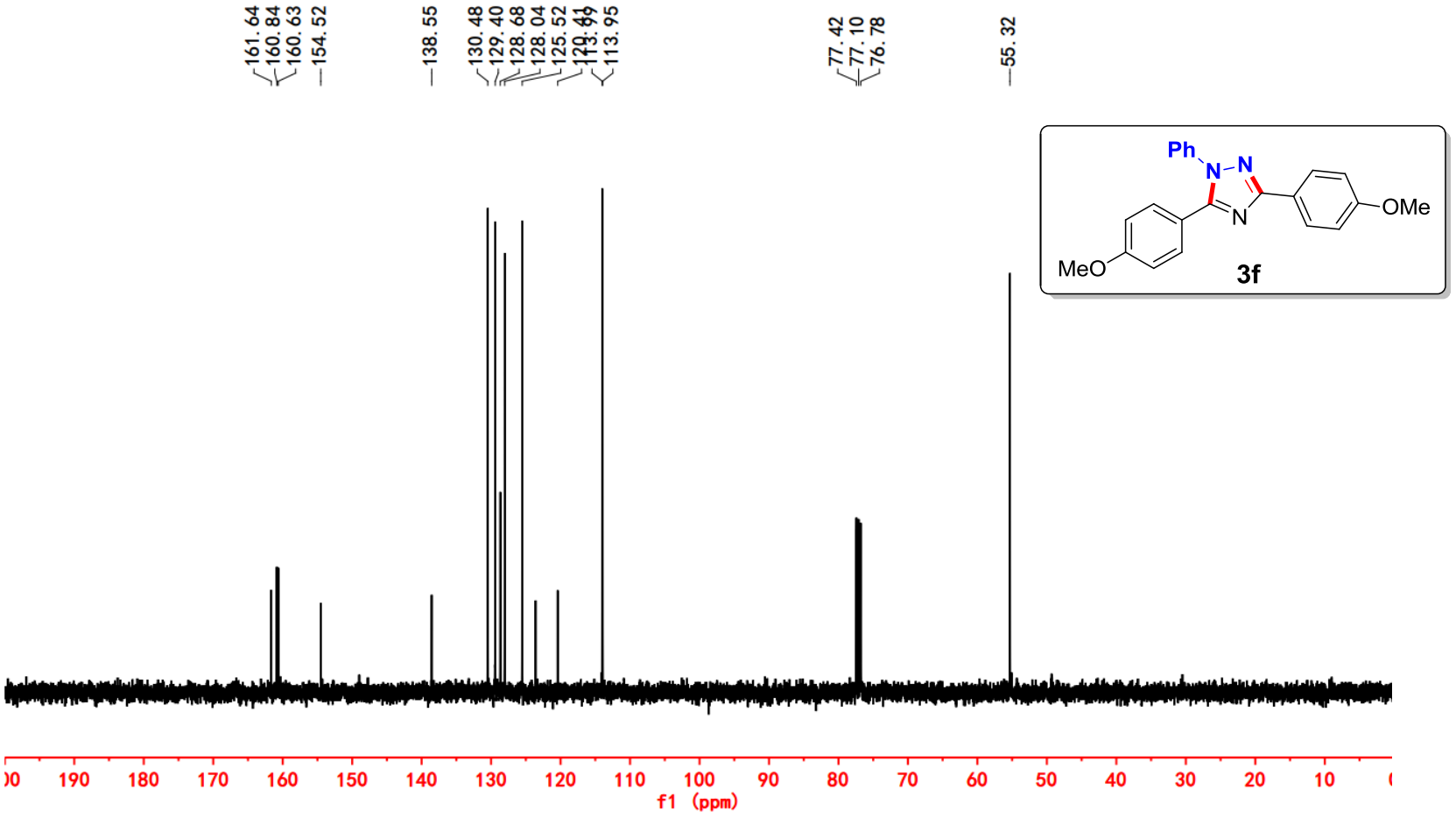
3.8096
0.0004
Ph
N
N
N
OMe
MeO
3f
2.00
2.00
5.01
2.02
2.02
3.00
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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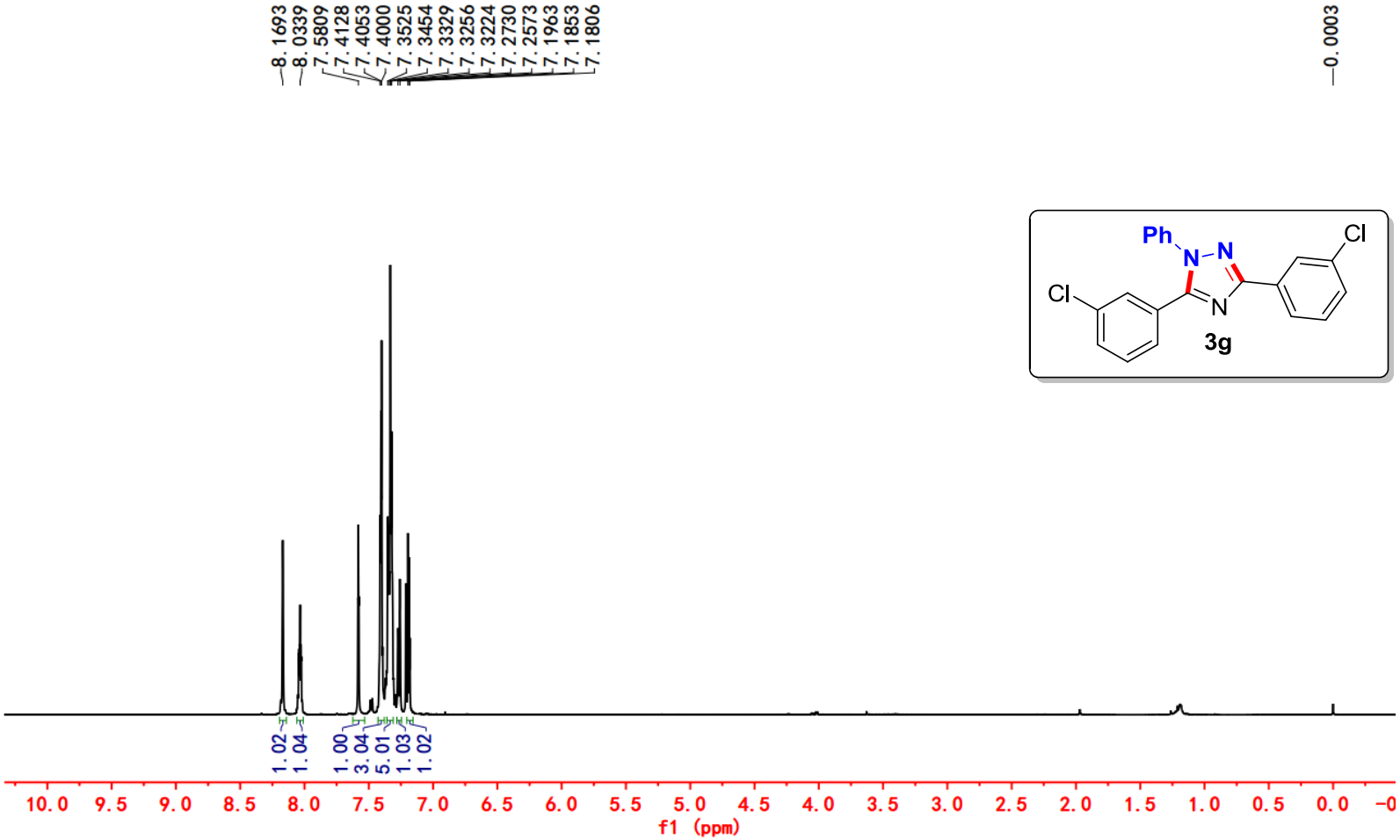
160.84
160.63
154.52
138.55
130.48
129.40
128.68
128.04
125.52
113.95
77.42
77.10
76.78
55.32
Ph
N
N
N
OMe
MeO
3f
f1 (ppm)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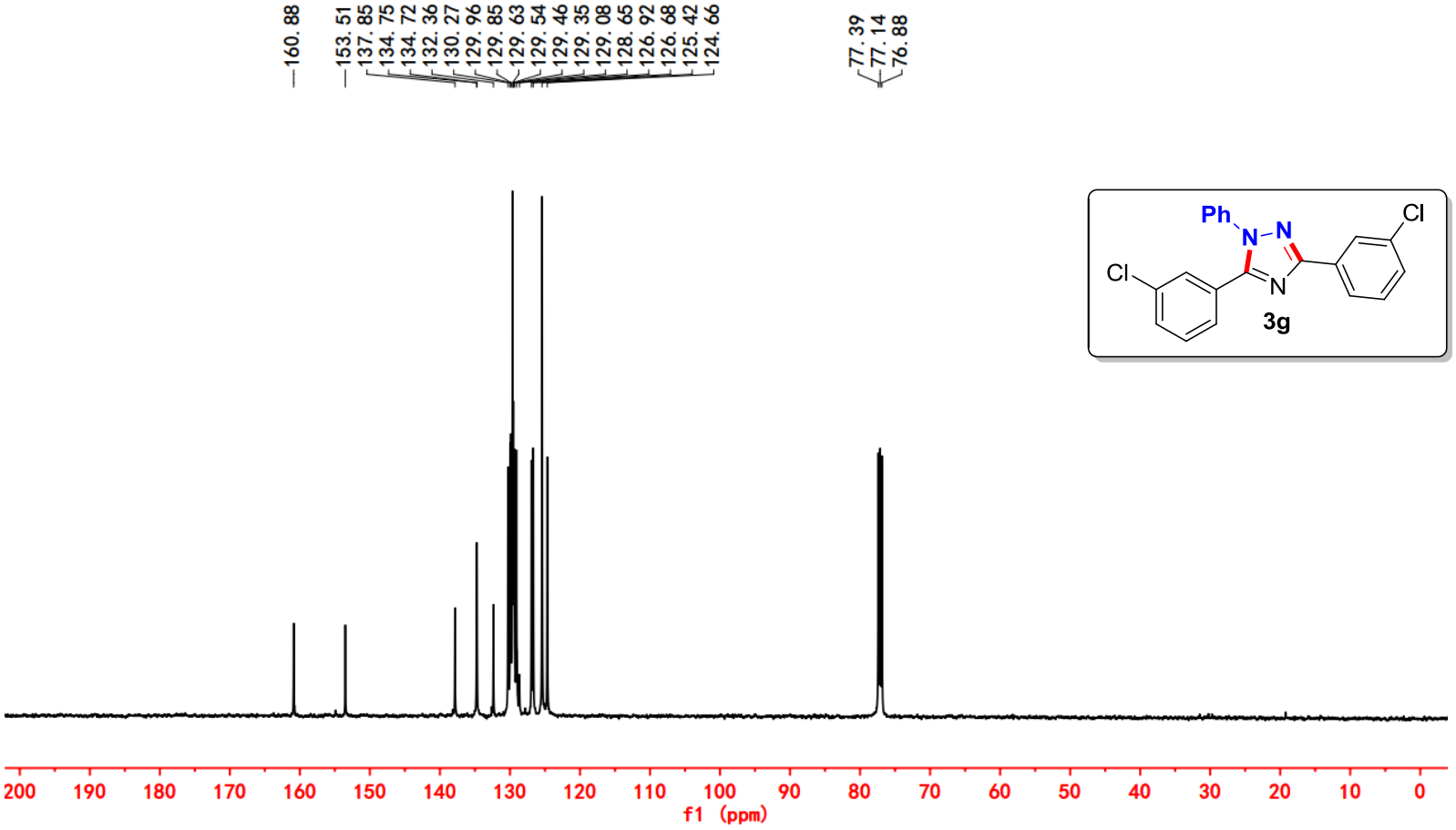
8.0339
7.5809
7.4128
7.4053
7.4000
7.3525
7.3454
7.3329
7.3256
7.3224
7.2730
7.2573
7.1963
7.1853
7.1806
0.0003
Ph
N
N
N
Cl
Cl
3g
1.02
1.04
1.00
3.04
5.01
1.03
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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137.85
134.75
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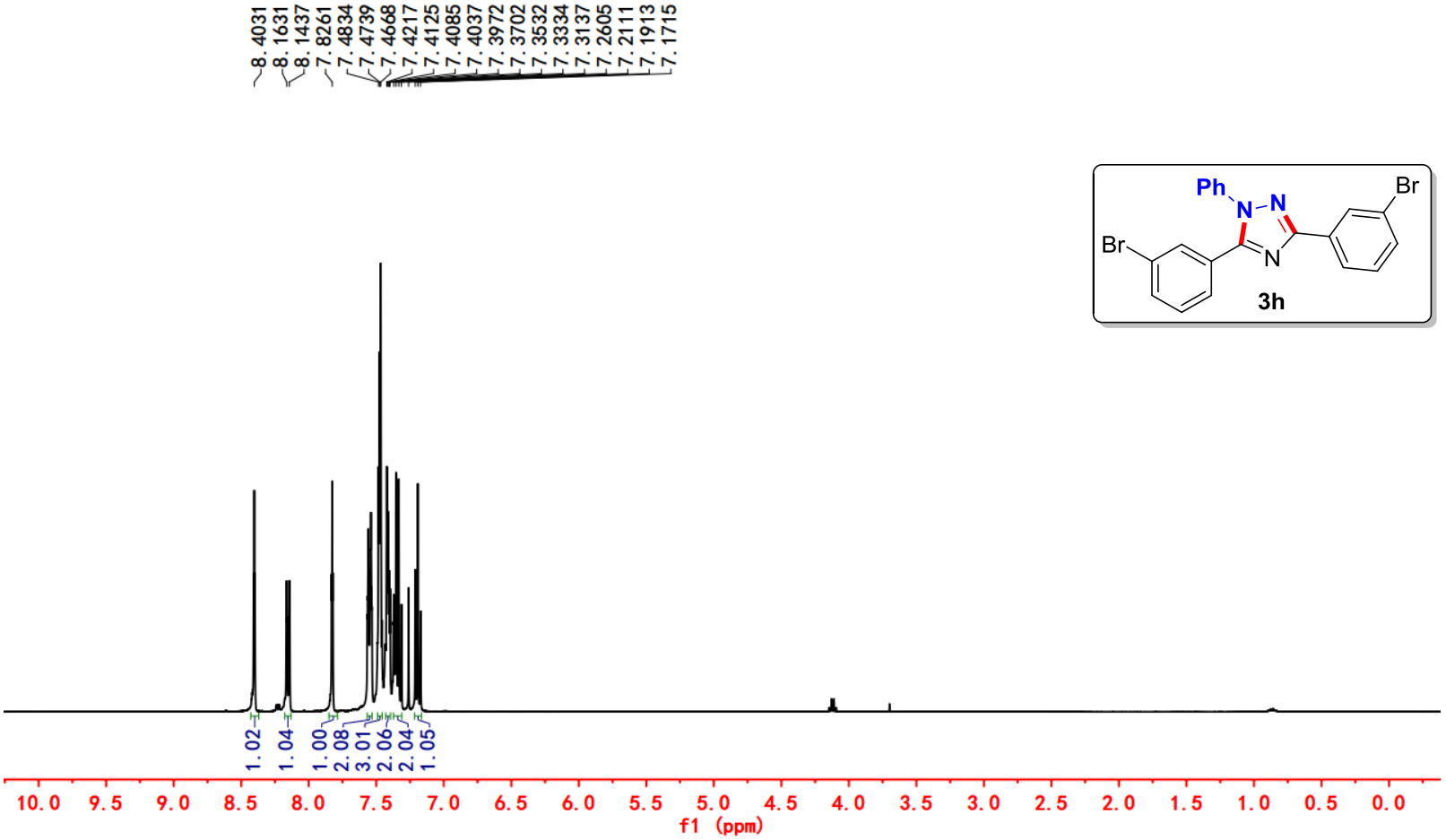
132.36
130.27
129.96
129.85
129.63
129.54
129.46
129.35
129.08
128.65
126.92
126.68
125.42
124.66
77.39
77.14
76.88
Ph
N
N
N
Cl
Cl
3g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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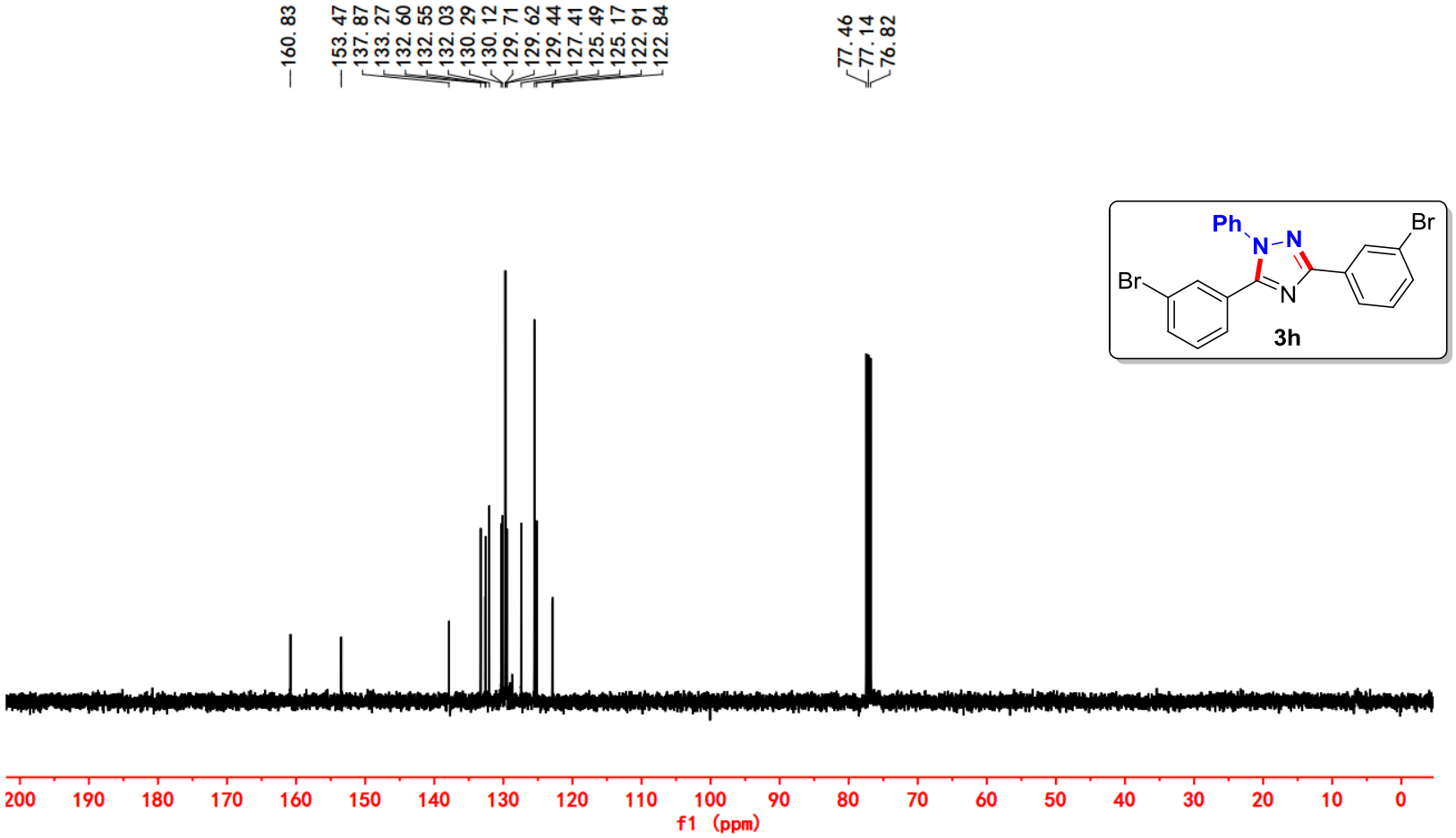
8.1631
8.1437
7.8261
7.4834
7.4739
7.4668
7.4217
7.4125
7.4085
7.4037
7.3972
7.3702
7.3532
7.3334
7.3137
7.2605
7.2111
7.1913
7.1715
Ph
N
N
N
Br
Br
3h
1.02
1.04
1.00
2.08
3.01
2.06
2.04
1.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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153.47
137.87
133.27
132.60
132.55
132.03
130.29
130.12
129.71
129.62
129.44
127.41
125.49
125.17
122.91
122.84
77.46
77.14
76.82
Ph
N
N
N
Br
Br
3h
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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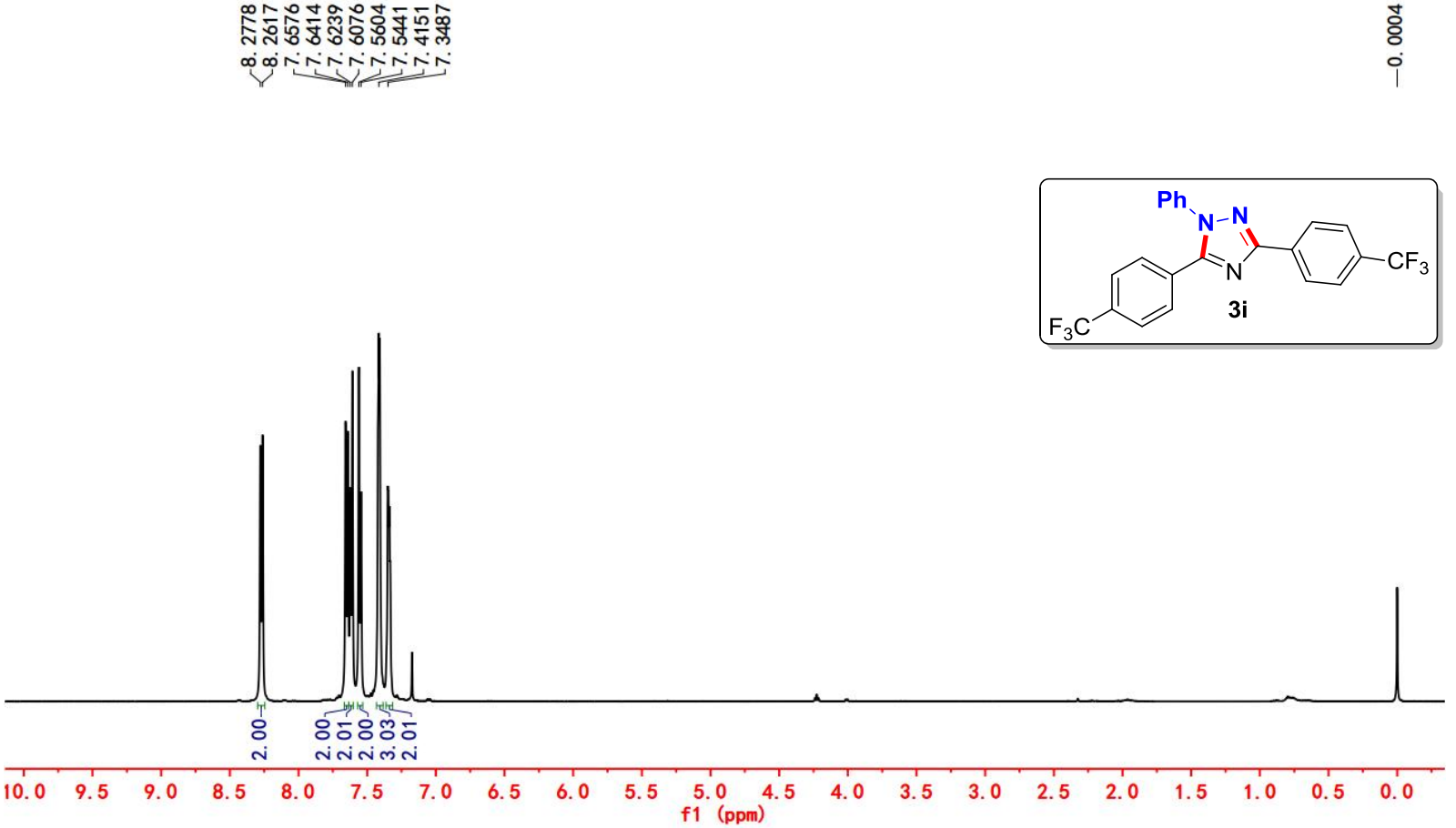
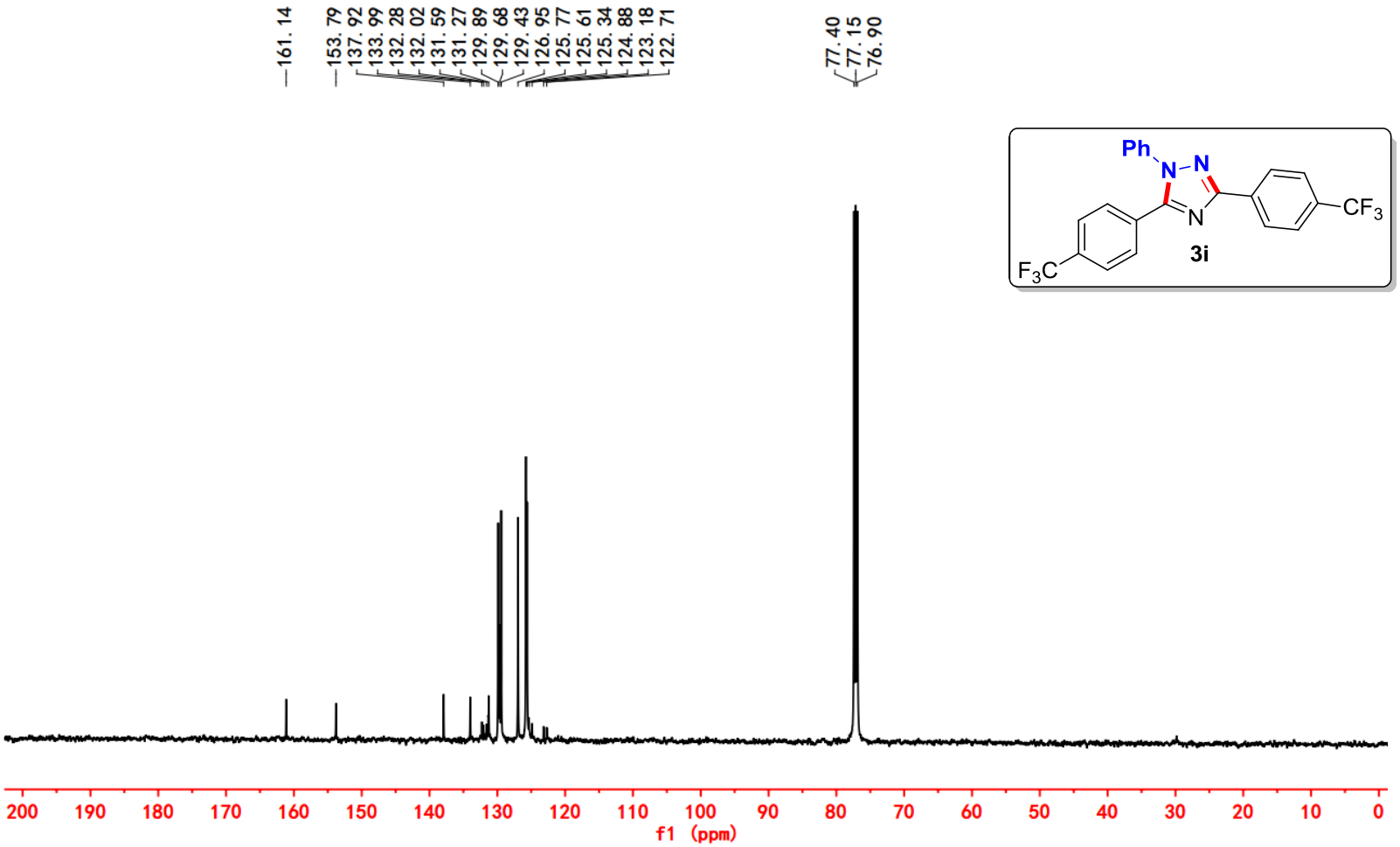
50
40
30
20
10
0
f1 (ppm)


8.2778
8.2617
7.6576
7.6414
7.6239
7.6076
7.5604
7.5441
7.4151
7.3487
0.0004
Ph
N
N
N
CF3
F3C
3i
2.00
2.00
2.01
2.00
3.03
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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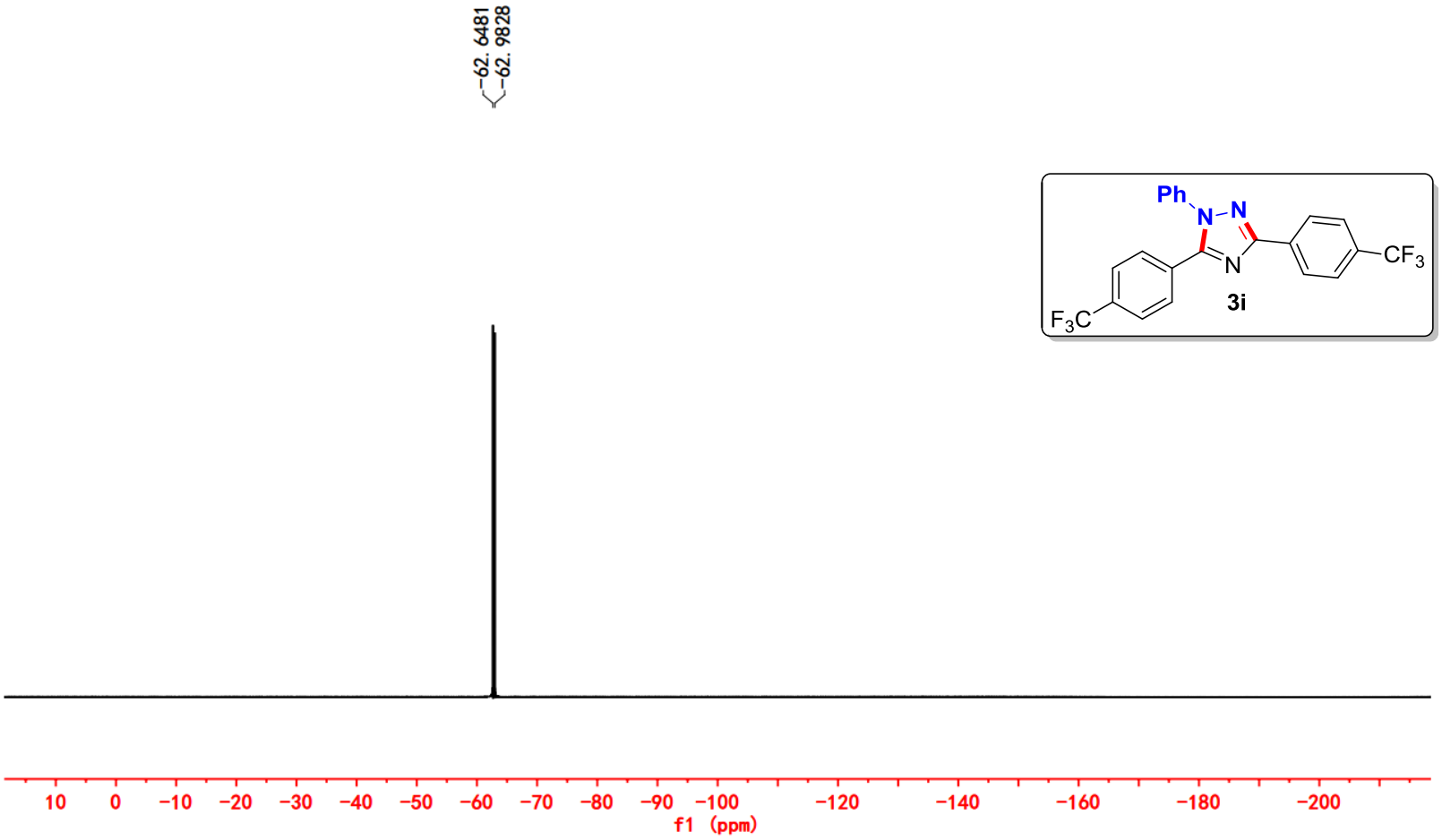
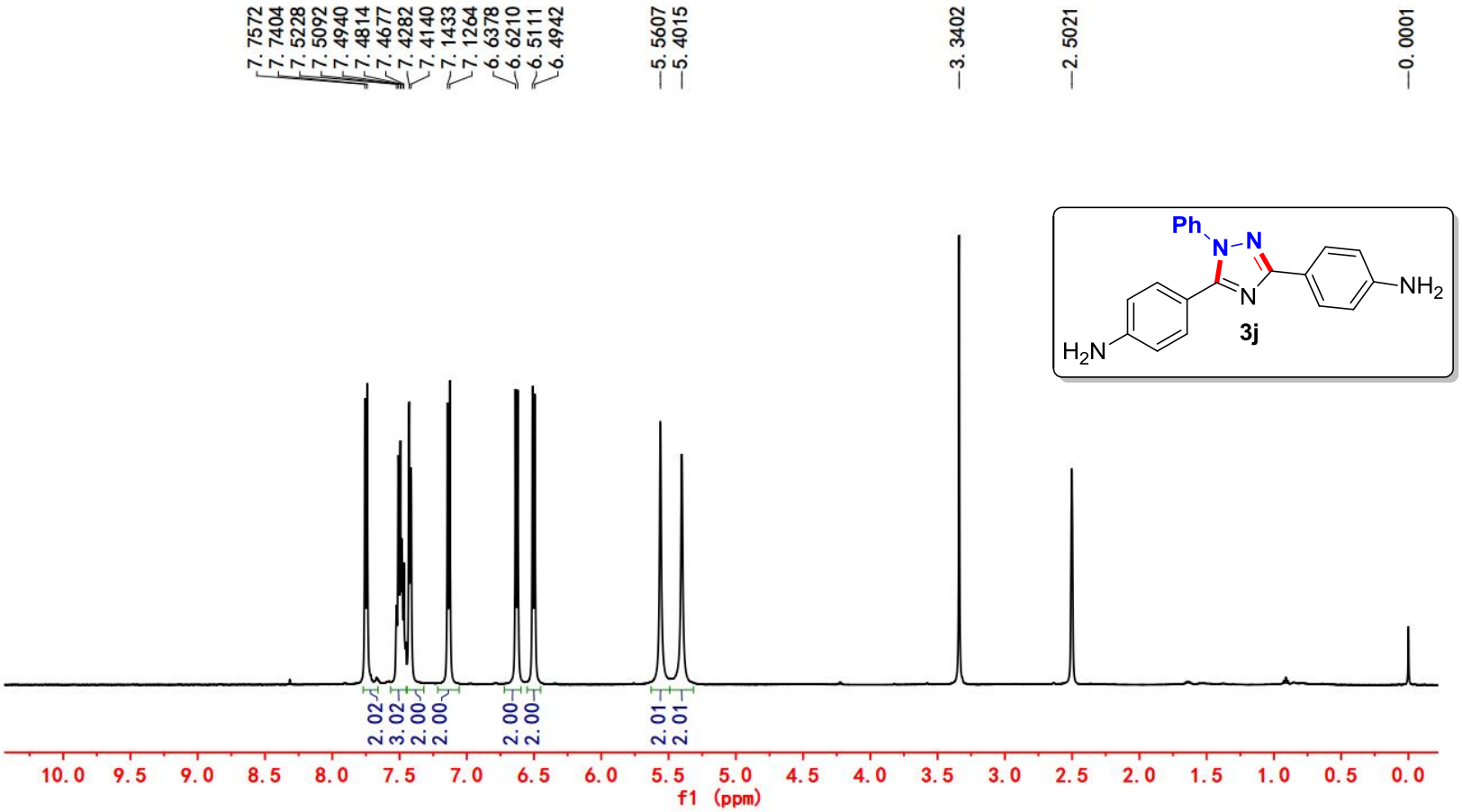
137.92
133.99
132.28
132.02
131.59
131.27
129.89
129.68
129.43
126.95
125.77
125.61
125.34
124.88
123.18
122.71
77.40
77.15
76.90
Ph
N
N
N
CF3
F3C
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.6481
-62.9828
Ph
N
N
N
CF3
F3C
3i
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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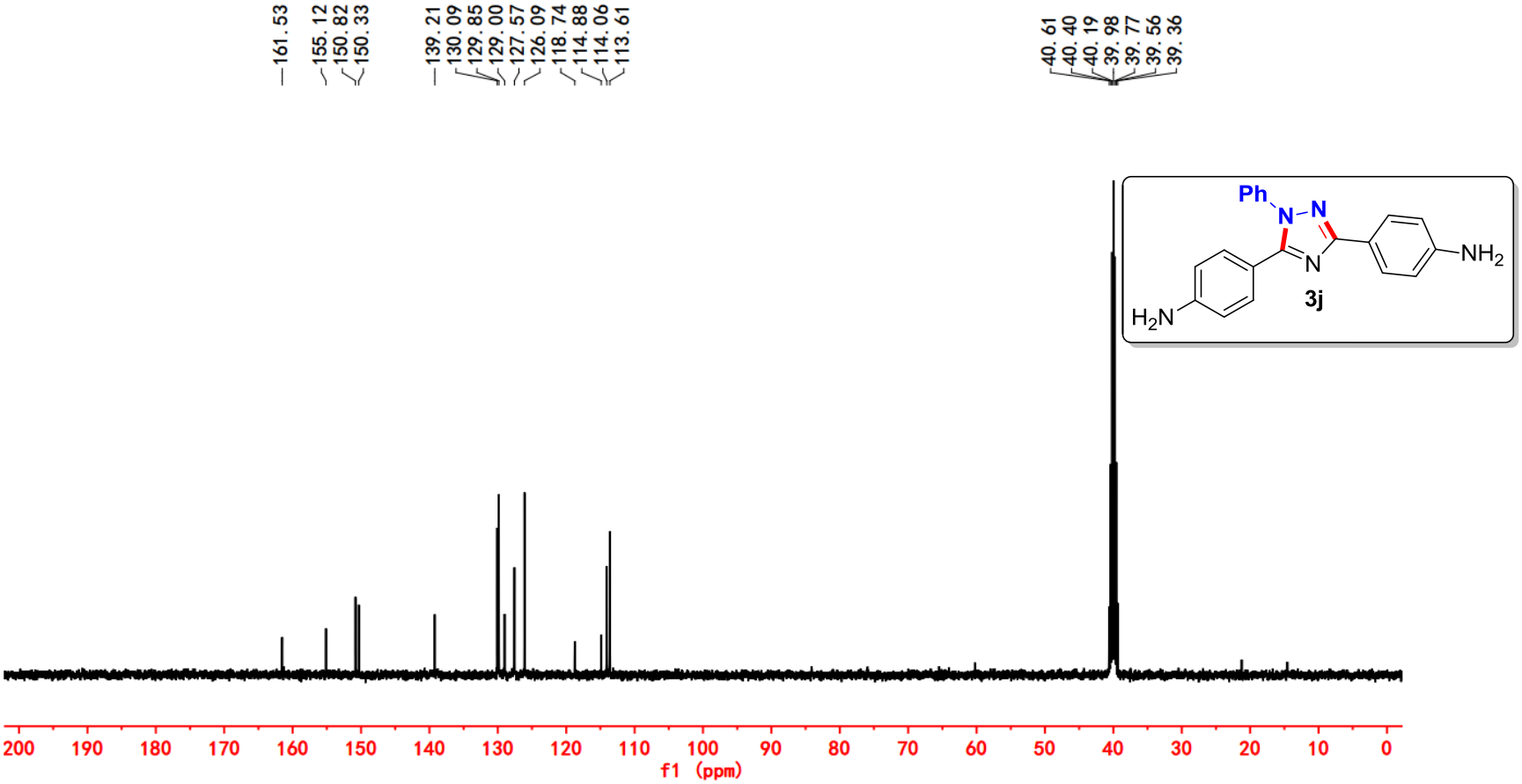
7.7404
7.5228
7.5092
7.4940
7.4814
7.4677
7.4282
7.4140
7.1433
7.1264
6.6378
6.6210
6.5111
6.4942
5.5607
5.4015
3.3402
2.5021
0.0001
Ph
N
N
N
NH2
H2N
3j
2.02
3.02
2.00
2.00
2.00
2.00
2.01
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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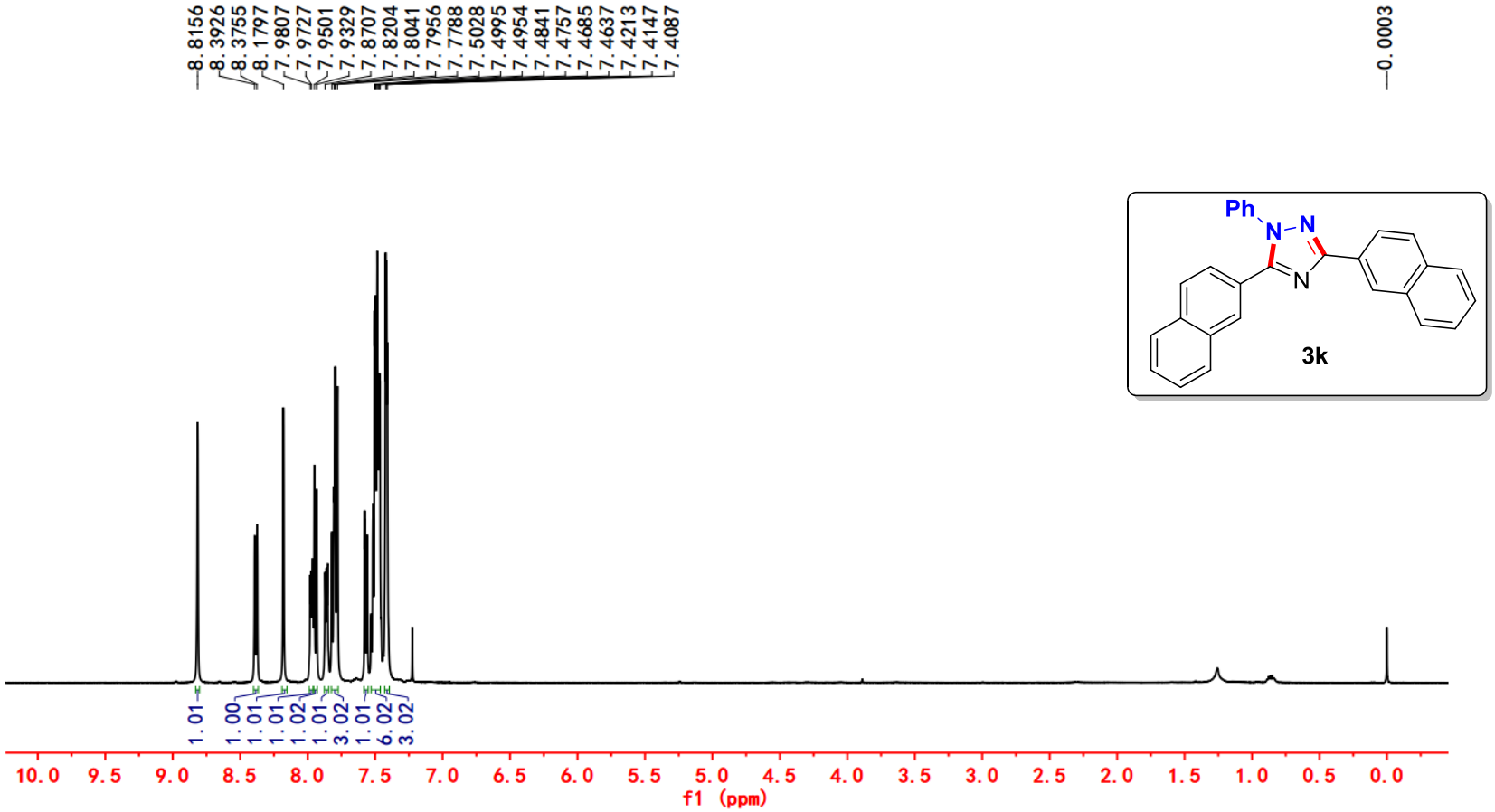
155.12
150.82
150.33
139.21
130.09
129.85
129.00
127.57
126.09
118.74
114.88
114.06
113.61
40.61
40.40
40.19
39.98
39.77
39.56
39.36
Ph
N
N
N
NH2
H2N
3j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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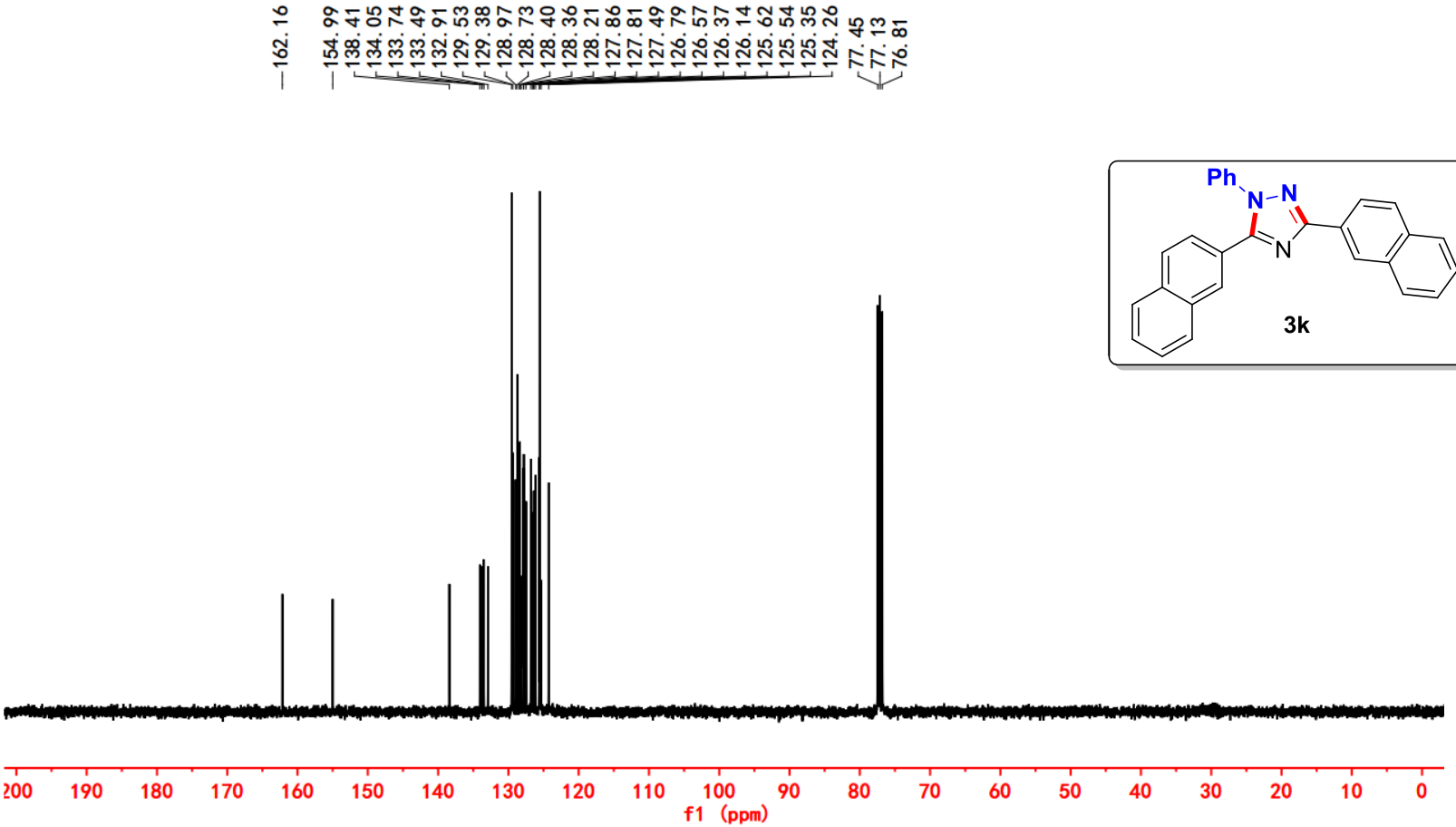
8.3755
8.1797
7.9807
7.9727
7.9501
7.9329
7.8707
7.8204
7.8041
7.7956
7.7788
7.5028
7.4995
7.4954
7.4841
7.4757
7.4685
7.4637
7.4213
7.4147
7.4087
0.0003
Ph
N
N
N
3k
1.01
1.00
1.01
1.01
1.02
1.01
3.02
1.01
6.02
3.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.49
132.91
129.53
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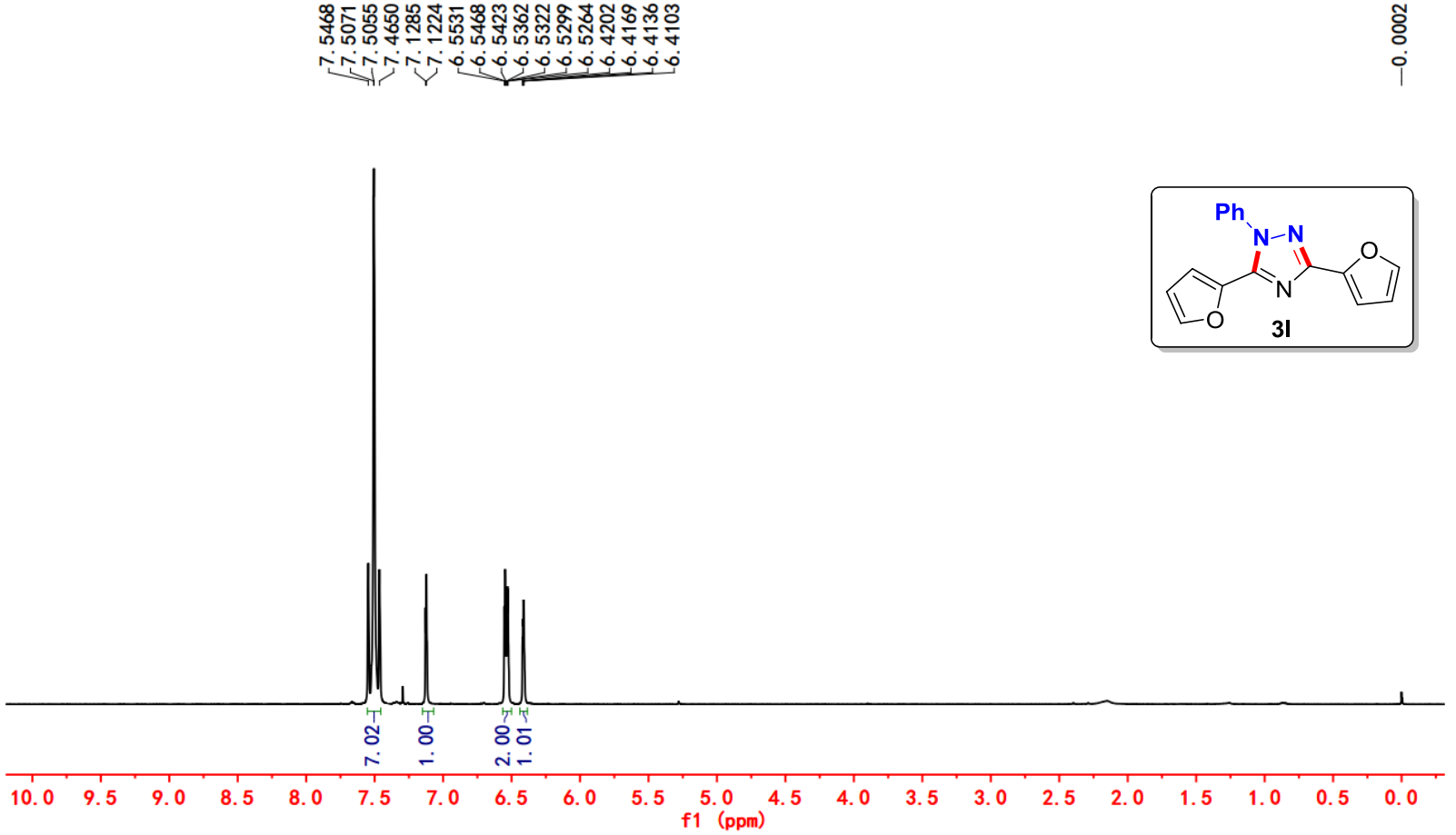
128.97
128.73
128.40
128.36
128.21
127.86
127.81
127.49
126.79
126.57
126.37
126.14
125.62
125.54
125.35
124.26
77.45
77.13
76.81
Ph
N
N
N
3k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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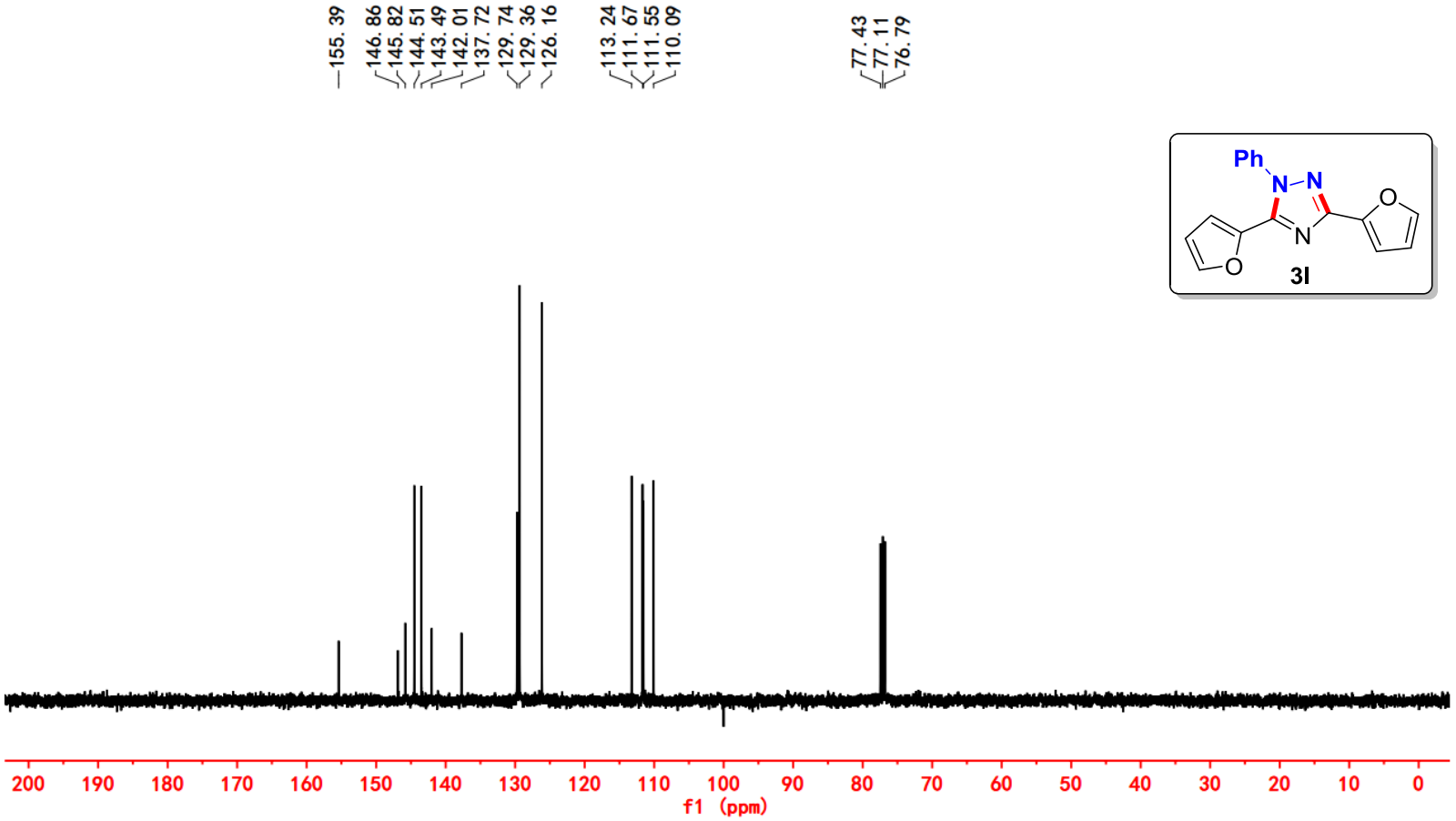
7.5071
7.5055
7.4650
7.1285
7.1224
6.5531
6.5468
6.5423
6.5362
6.5322
6.5299
6.5264
6.4202
6.4169
6.4136
6.4103
0.0002
Ph
N
N
O
N
O
3l
7.02
1.00
2.00
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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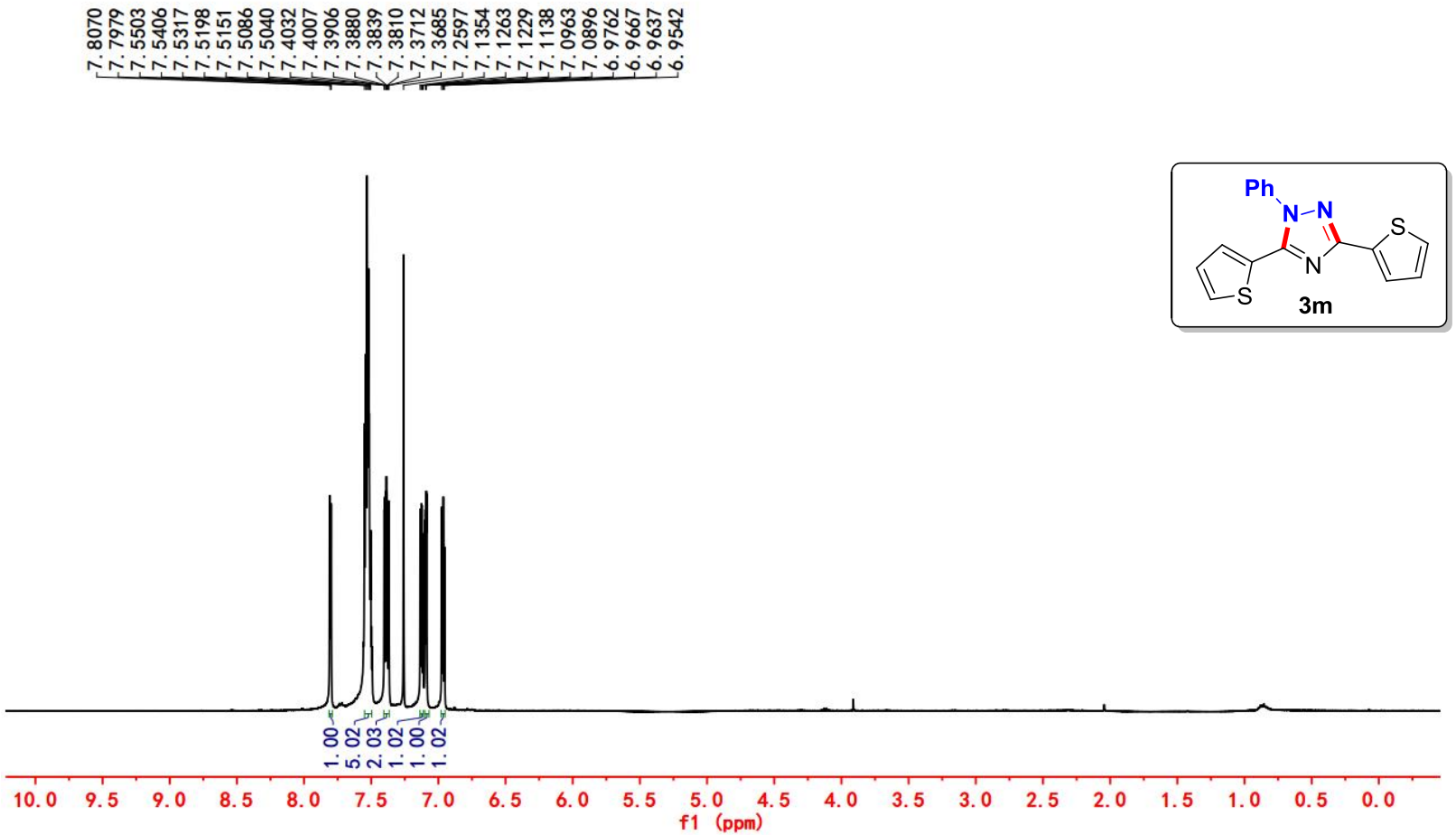
145.82
144.51
143.49
142.01
137.72
129.74
129.36
126.16
113.24
111.67
111.55
110.09
77.43
77.11
76.79
Ph
N
N
O
N
O
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.8070
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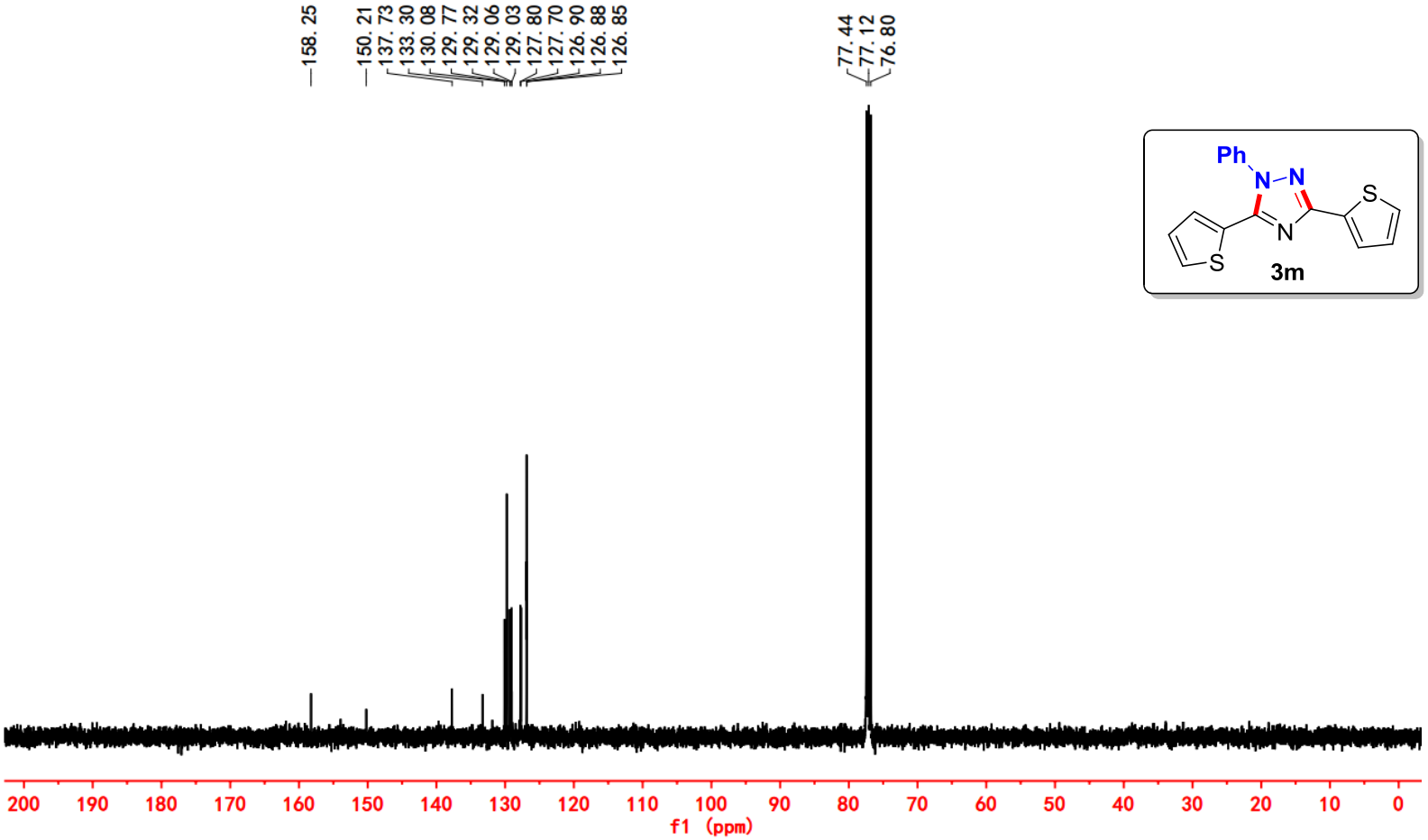
7.5317
7.5198
7.5151
7.5086
7.5040
7.4032
7.4007
7.3906
7.3880
7.3839
7.3810
7.3712
7.3685
7.2597
7.1354
7.1263
7.1229
7.1138
7.0963
7.0896
6.9762
6.9667
6.9637
6.9542
1.00
5.02
2.03
1.02
1.00
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
Ph
N
N
S
N
S
3m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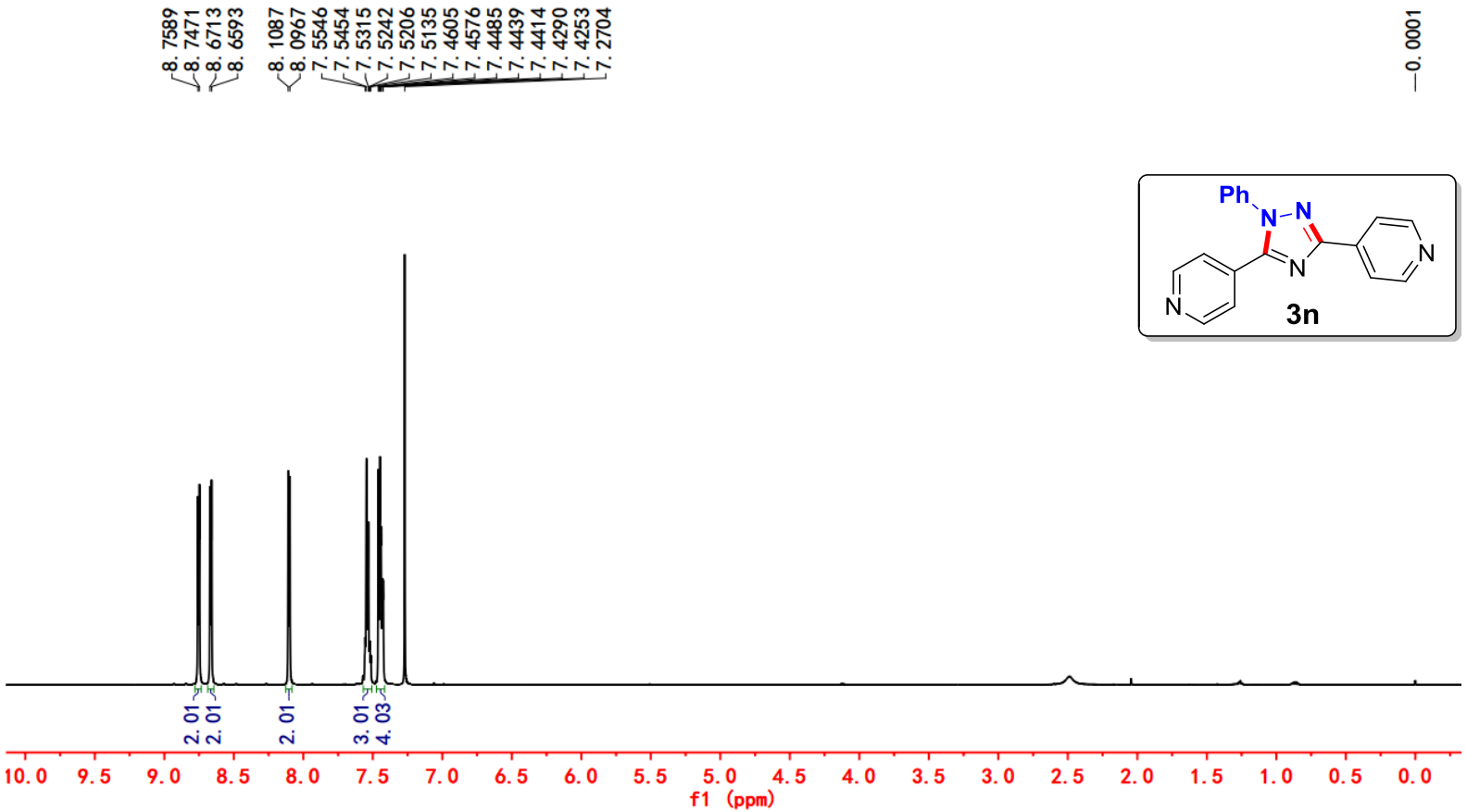
129.77
129.32
129.06
129.03
127.80
127.70
126.90
126.88
126.85
77.44
77.12
76.80
Ph
N
N
S
N
S
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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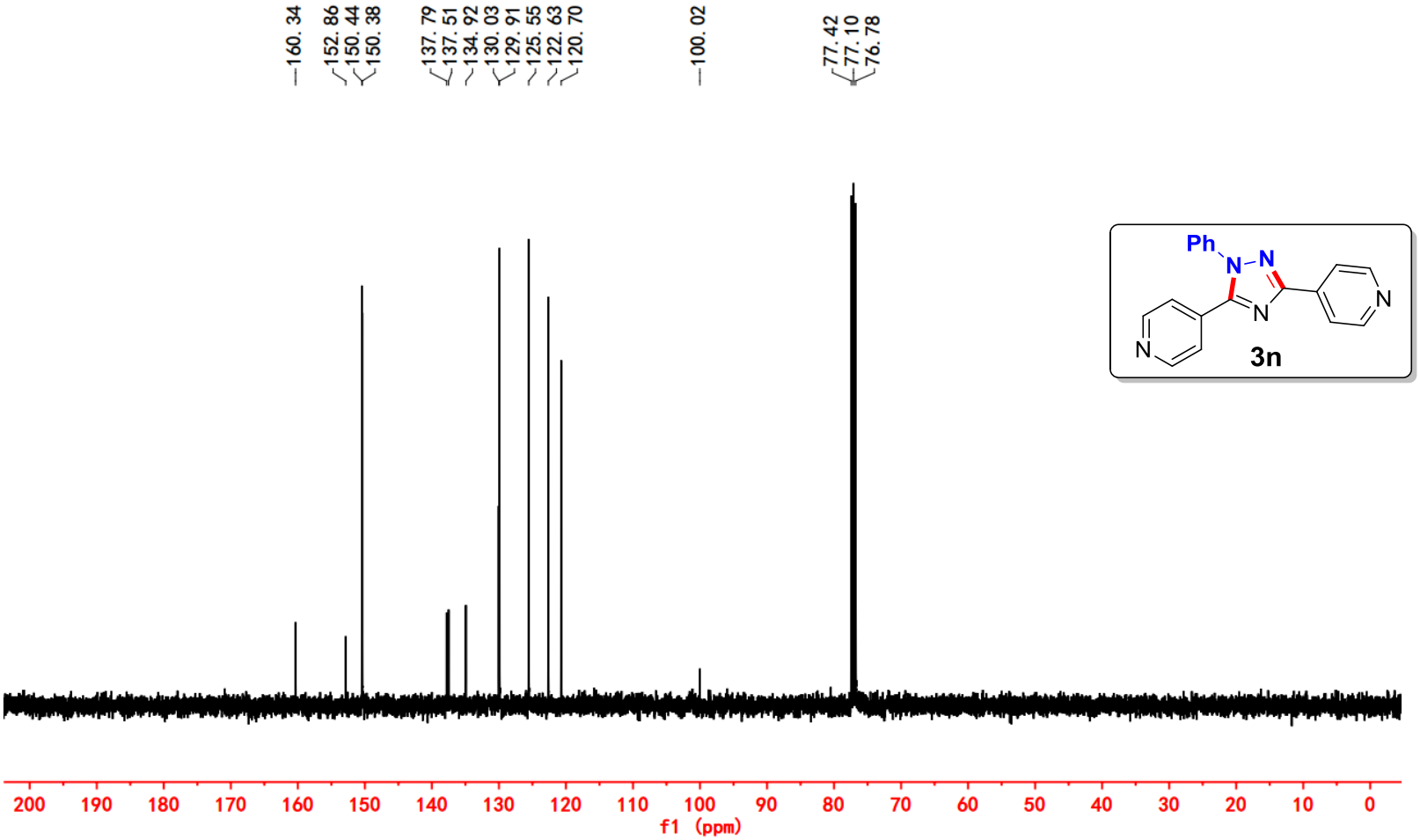
7.5242
7.5206
7.5135
7.4605
7.4576
7.4485
7.4439
7.4414
7.4290
7.4253
7.2704
0.0001
Ph
N
N
N
N
3n
2.01
2.01
2.01
3.01
4.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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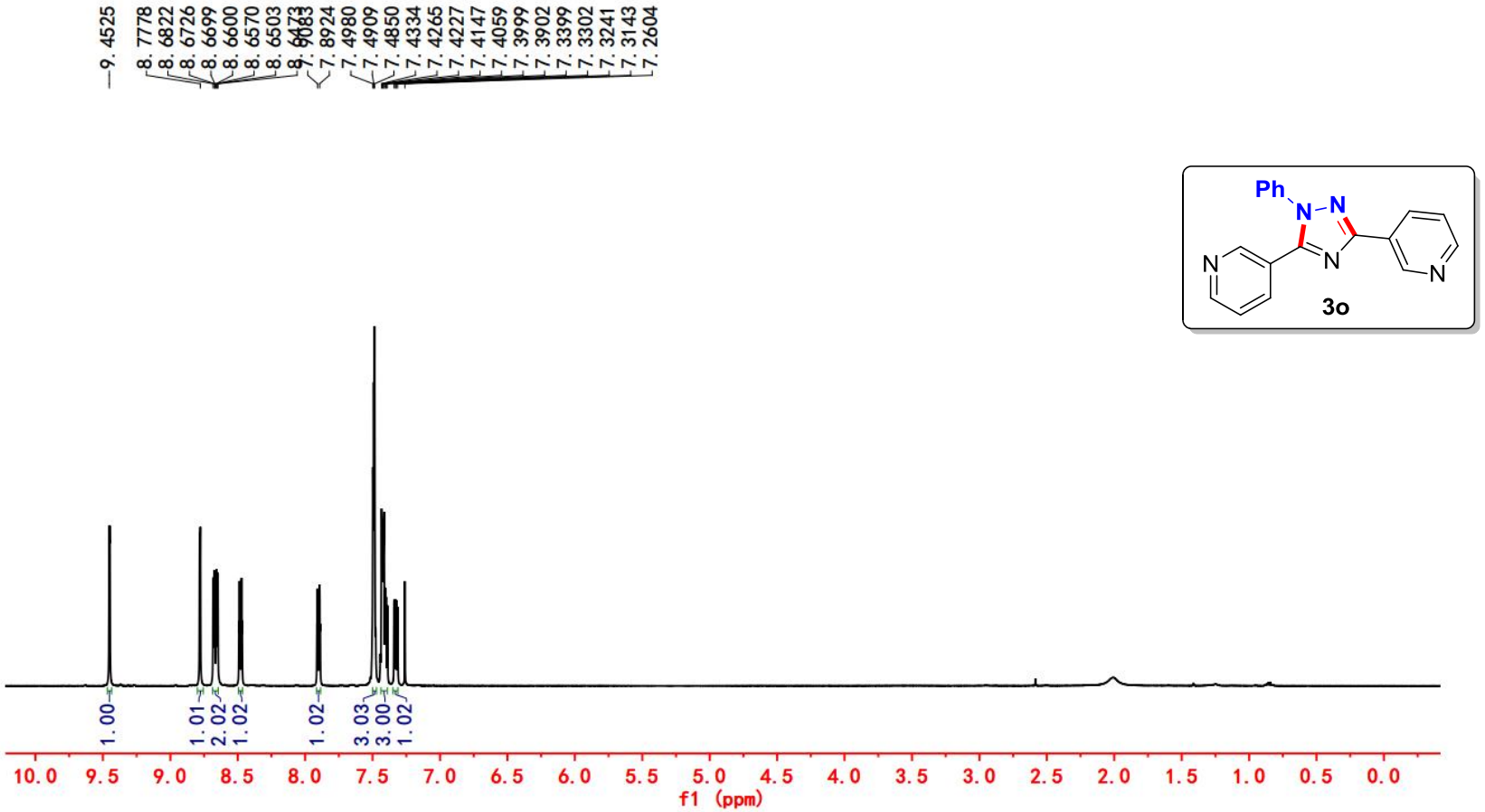
150.44
150.38
137.79
137.51
134.92
130.03
129.91
125.55
122.63
120.70
100.02
77.42
77.10
76.78
Ph
N
N
N
N
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.6600
8.6570
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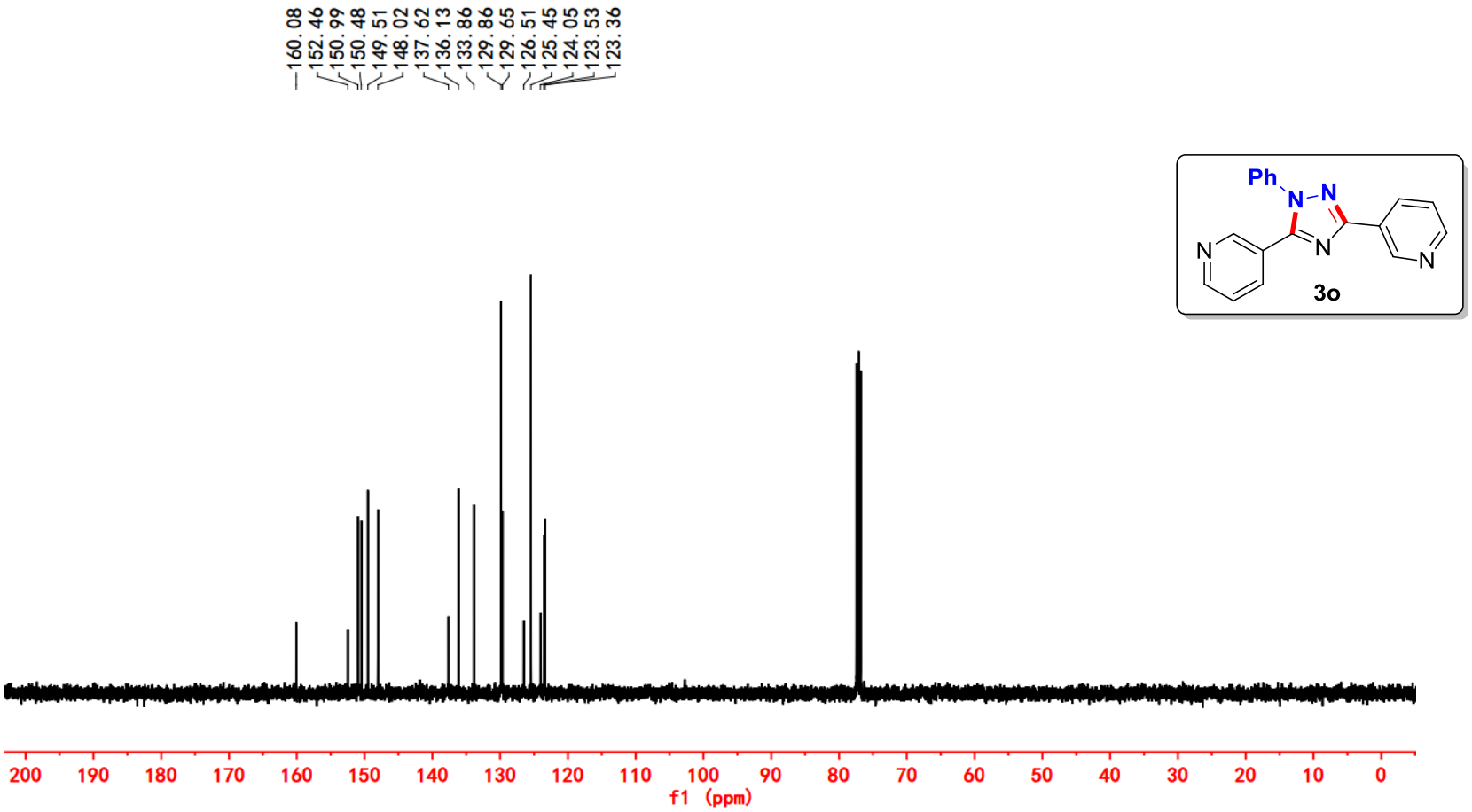
7.4334
7.4265
7.4227
7.4147
7.4059
7.3999
7.3902
7.3399
7.3302
7.3241
7.3143
7.2604
Ph
N
N
N
N
3o
1.00
1.01
2.02
1.02
1.02
3.03
3.00
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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148.02
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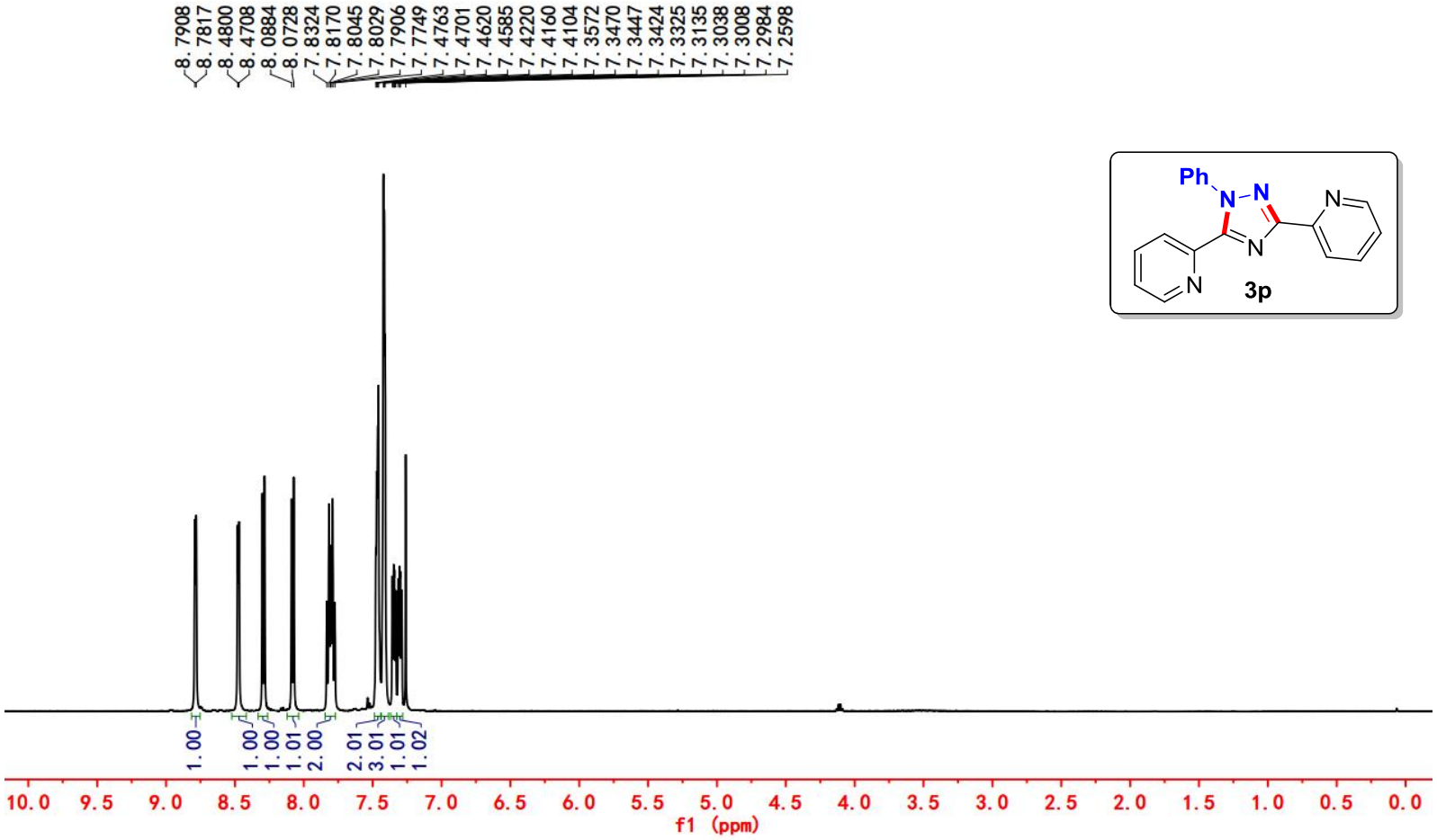
136.13
133.86
129.86
129.65
126.51
125.45
124.05
123.53
123.36
Ph
N
N
N
N
3o
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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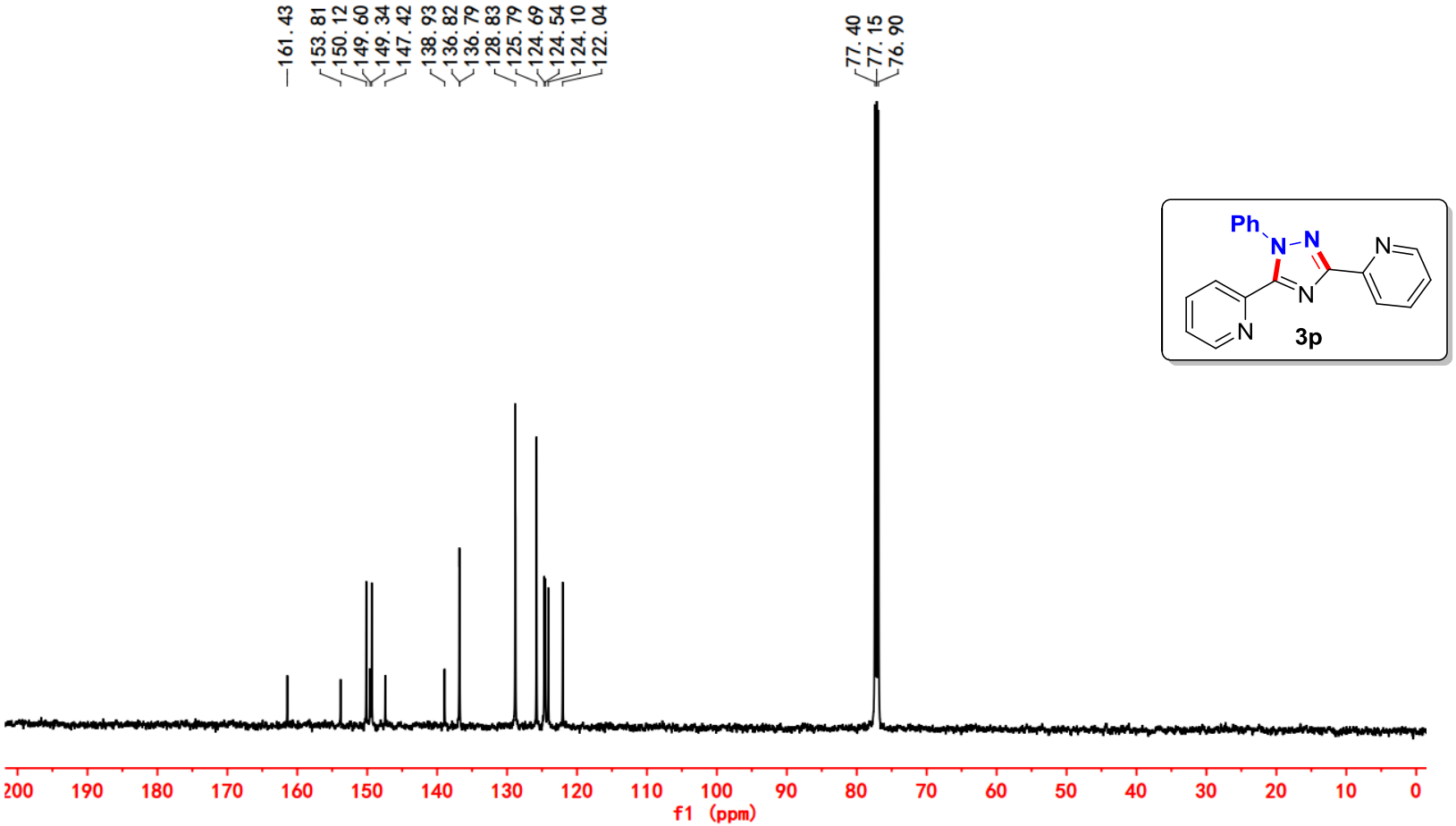
7.4701
7.4620
7.4585
7.4220
7.4160
7.4104
7.3572
7.3470
7.3447
7.3424
7.3325
7.3135
7.3038
7.3008
7.2984
7.2598
Ph
N
N
N
N
N
3p
1.00
1.00
1.00
1.01
2.00
2.01
3.01
1.01
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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149.34
147.42
138.93
136.82
136.79
128.83
125.79
124.69
124.54
124.10
122.04
77.40
77.15
76.90
Ph
N
N
N
N
3p
200
190
180
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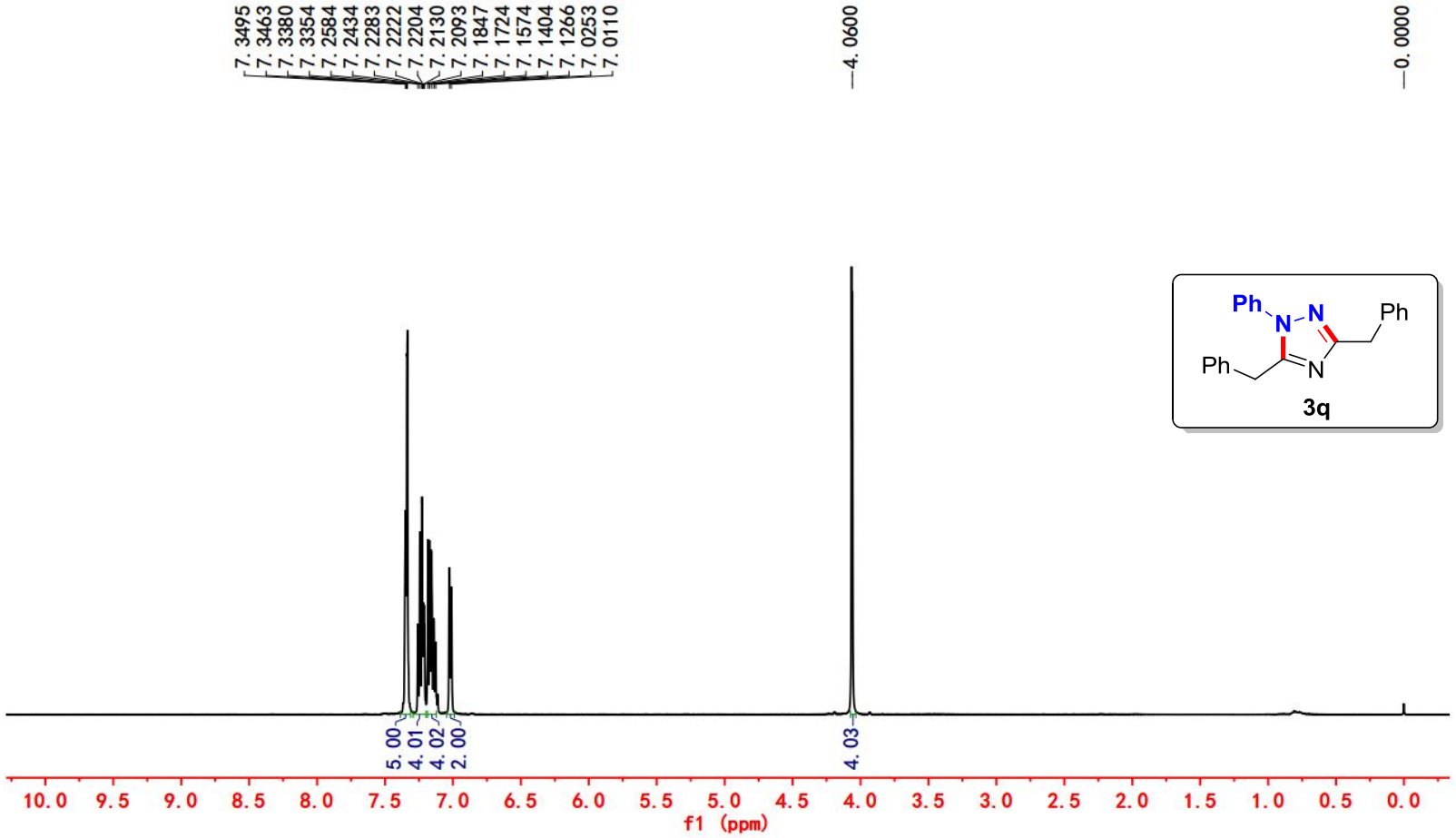
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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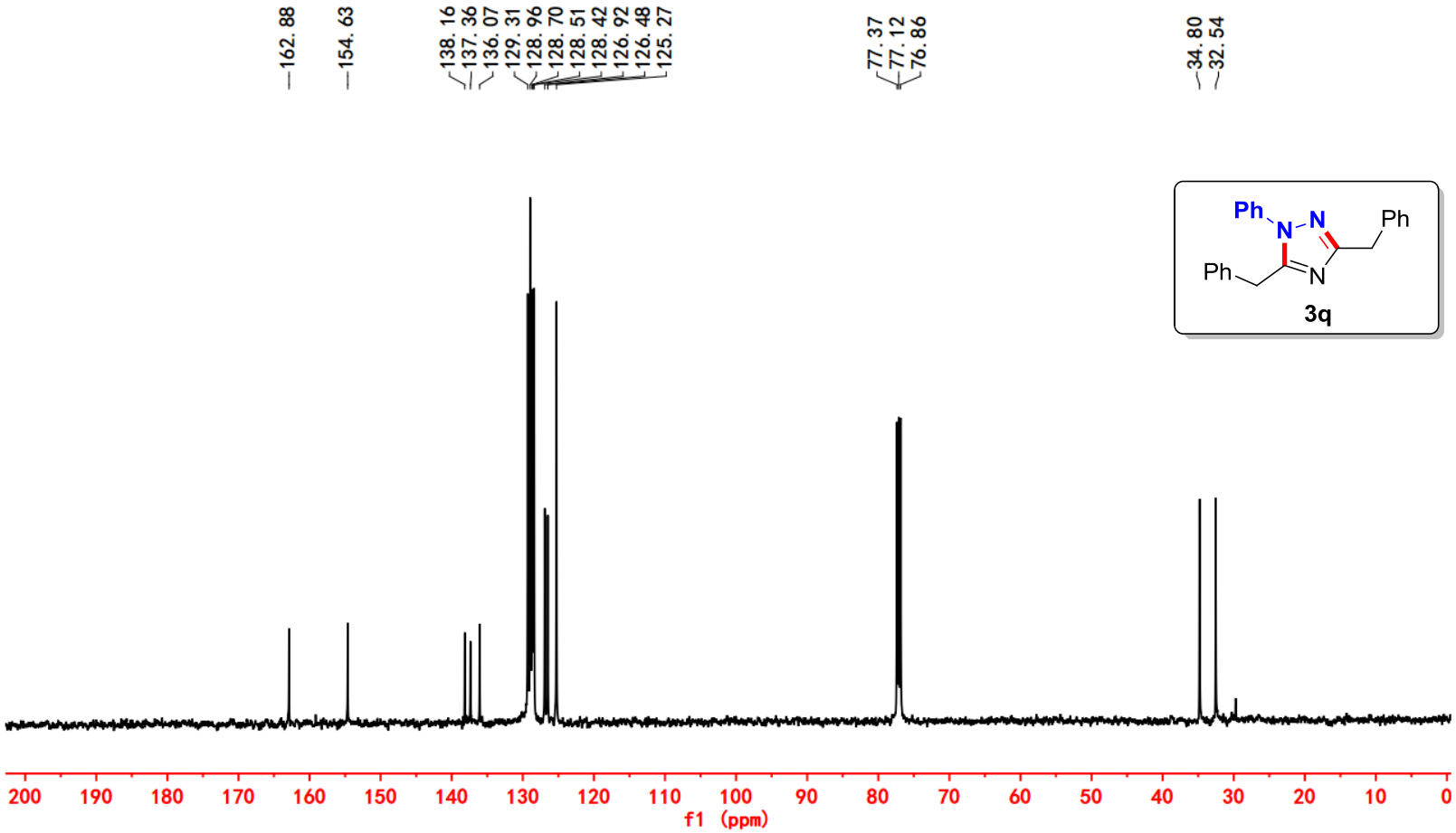
7.1847
7.1724
7.1574
7.1404
7.1266
7.0253
7.0110
4.0600
0.0000
Ph
N
N
Ph
Ph
N
3q
5.00
4.01
4.02
2.00
4.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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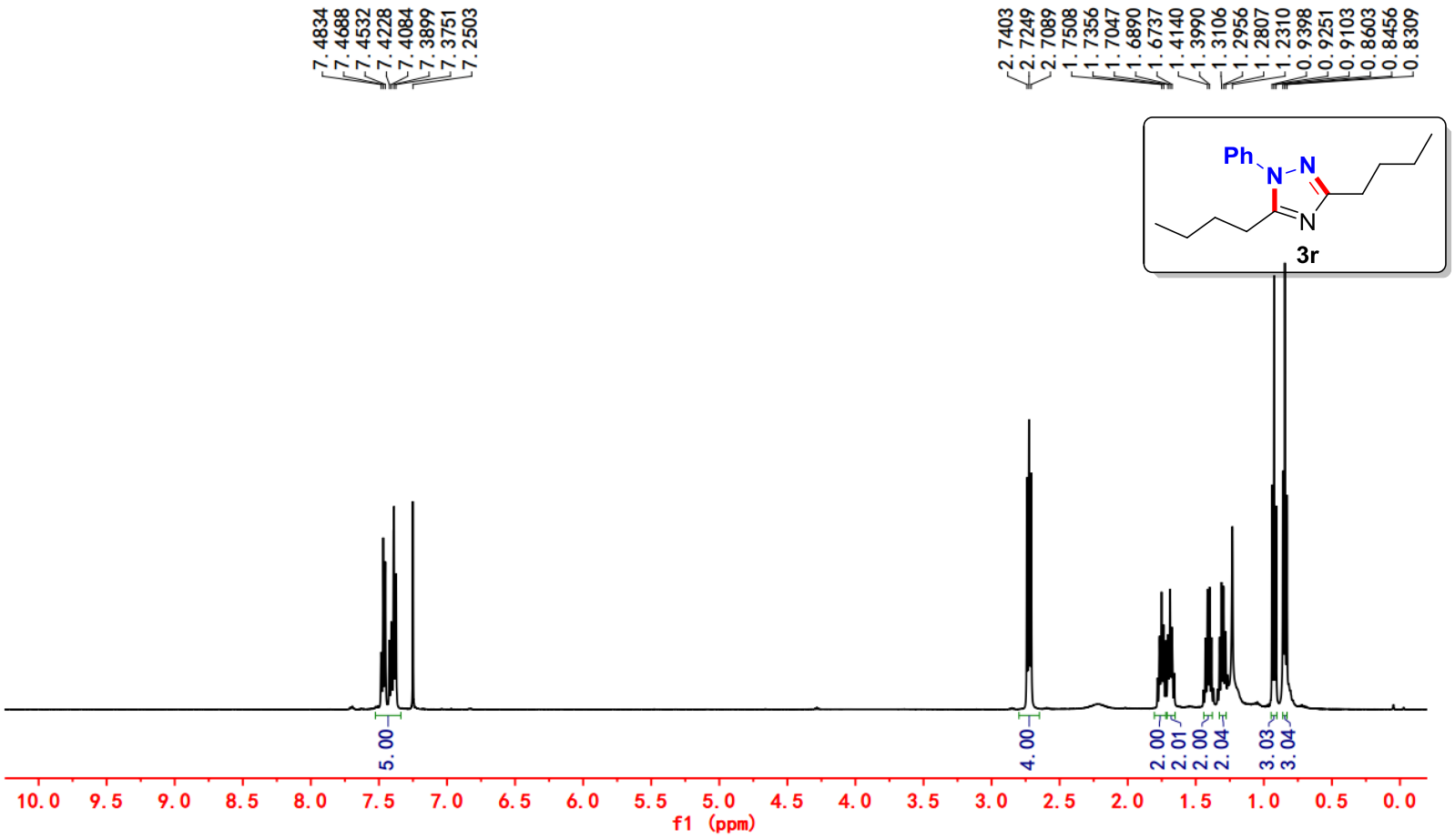
154.63
138.16
137.36
136.07
129.31
128.96
128.70
128.51
128.42
126.92
126.48
125.27
77.37
77.12
76.86
34.80
32.54
Ph
N
N
Ph
Ph
N
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4532
7.4228
7.4084
7.3899
7.3751
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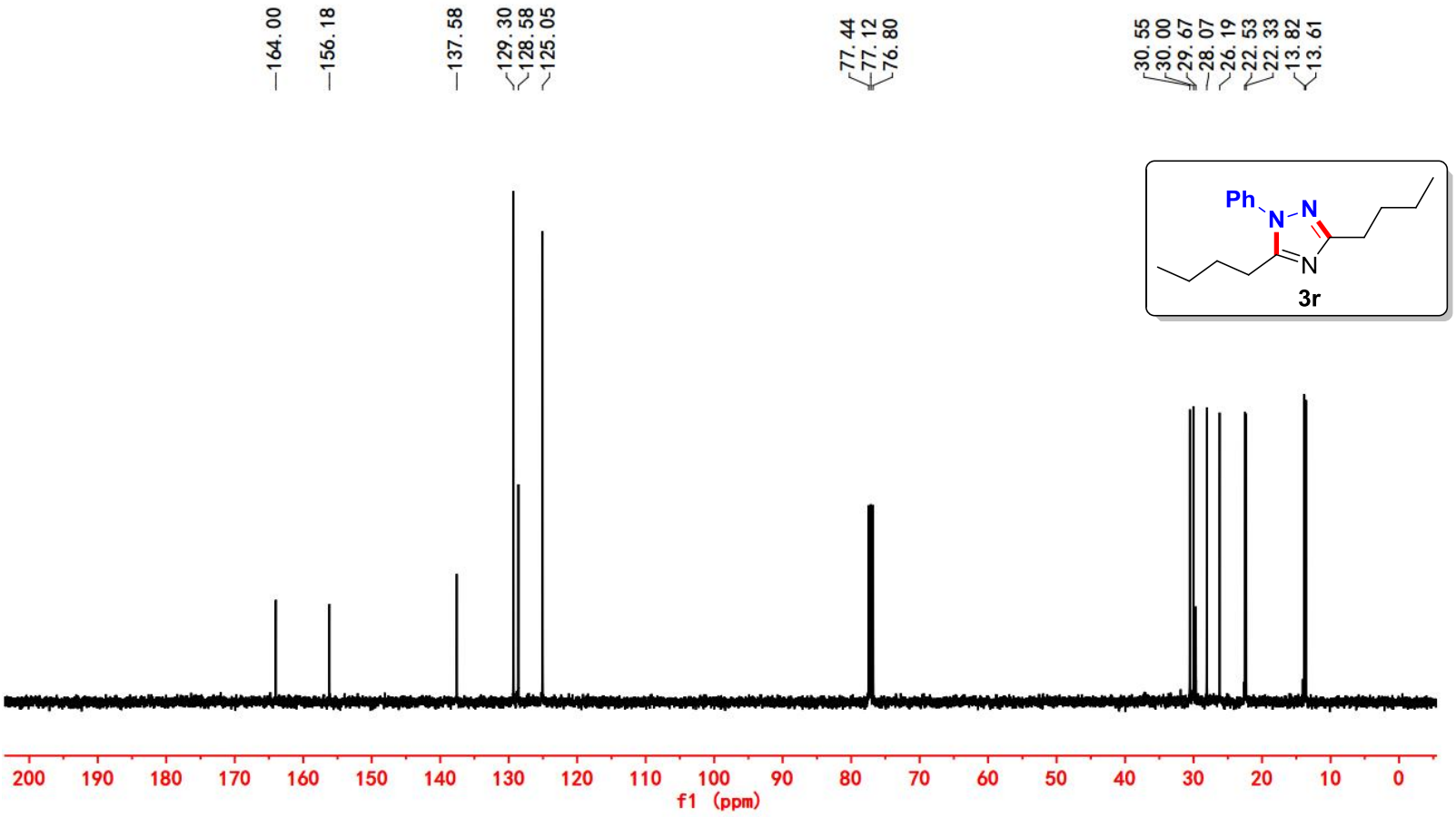
2.7403
2.7249
2.7089
1.7508
1.7356
1.7047
1.6890
1.6737
1.4140
1.3990
1.3106
1.2956
1.2807
1.2310
0.9398
0.9251
0.9103
0.8603
0.8456
0.8309
Ph
N
N
N
3r
5.00
4.00
2.00
2.01
2.00
2.04
3.03
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.58
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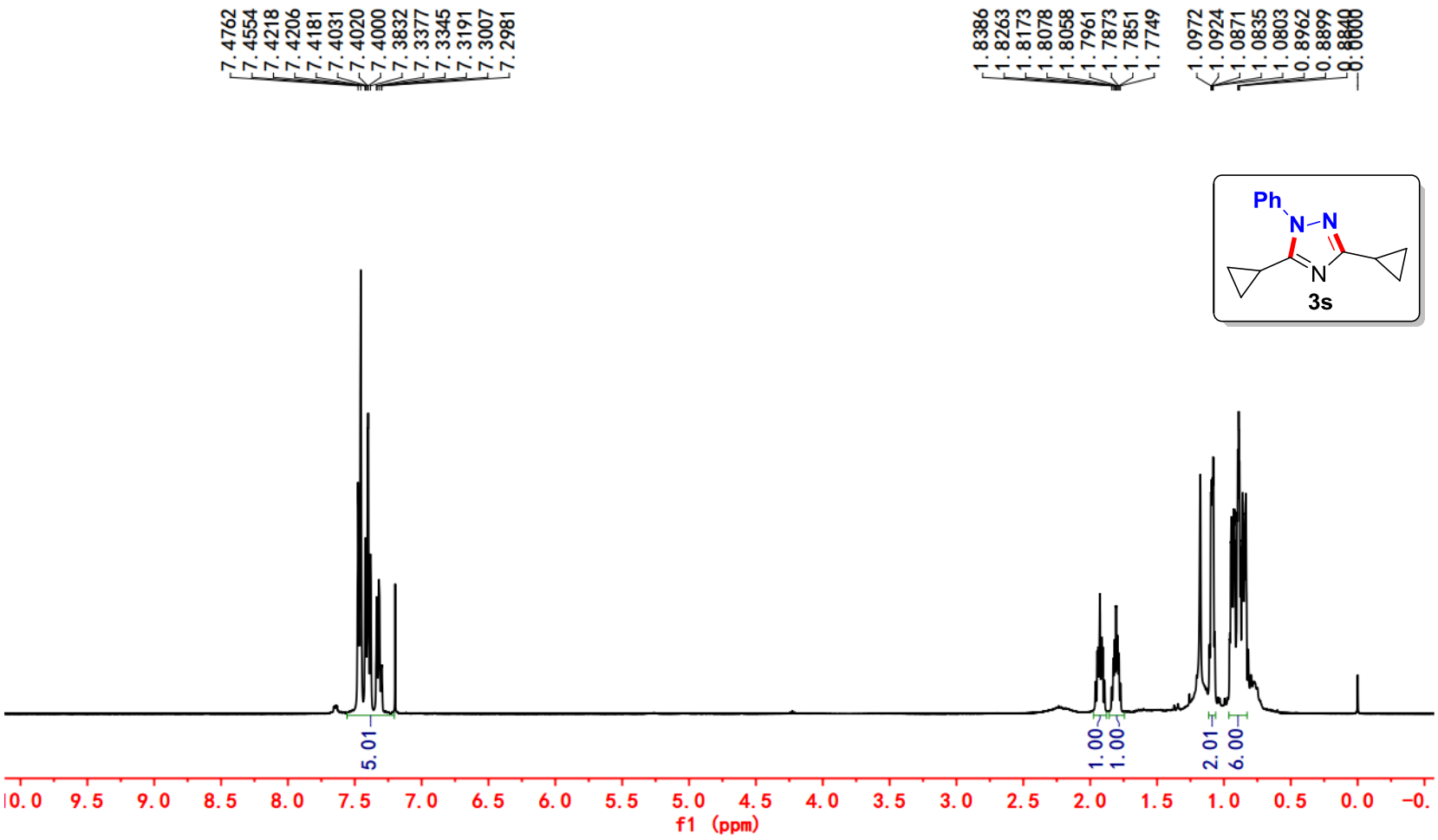
128.58
125.05
77.44
77.12
76.80
30.55
30.00
29.67
28.07
26.19
22.53
22.33
13.82
13.61
Ph
N
N
N
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.4554
7.4218
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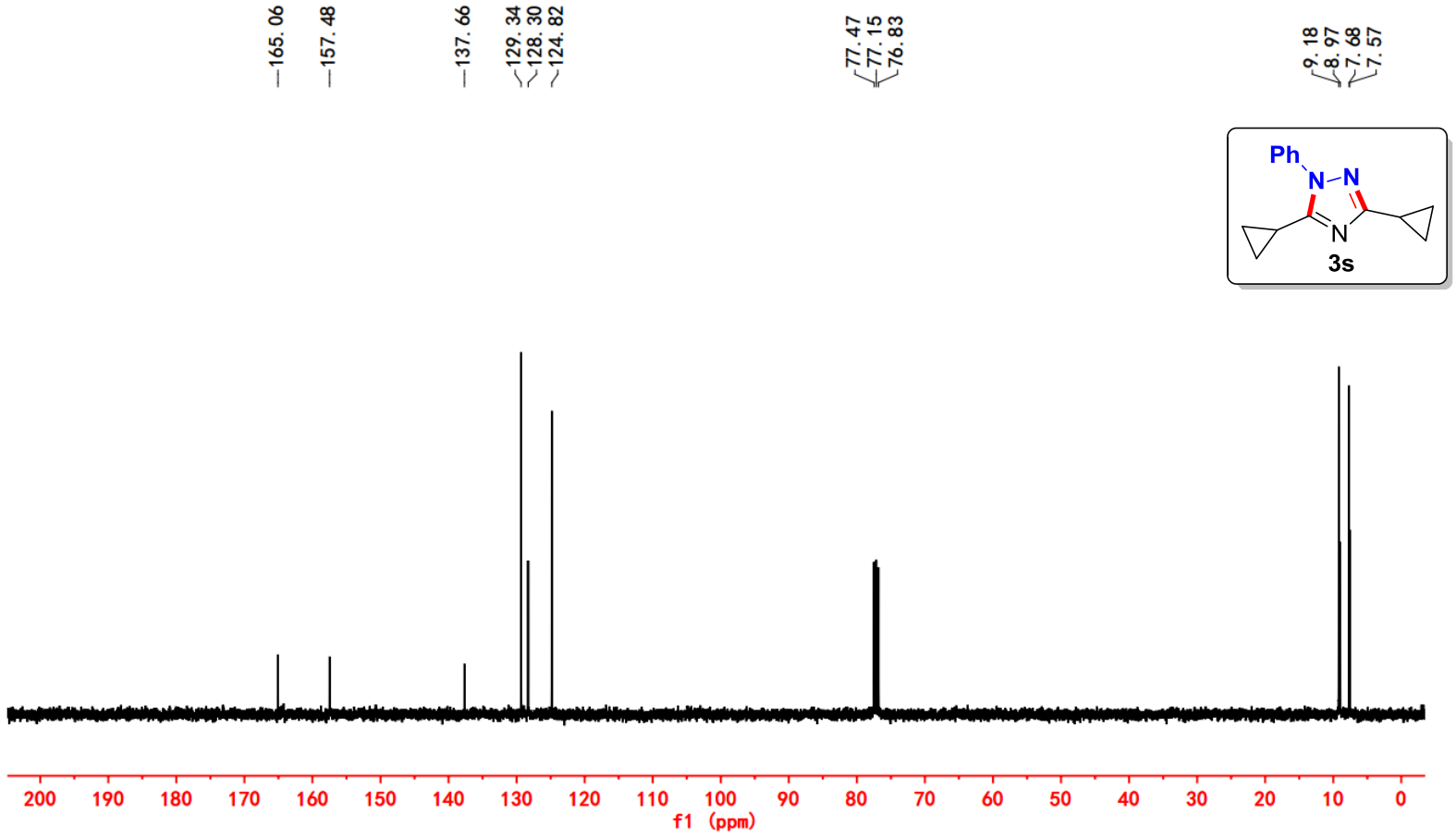
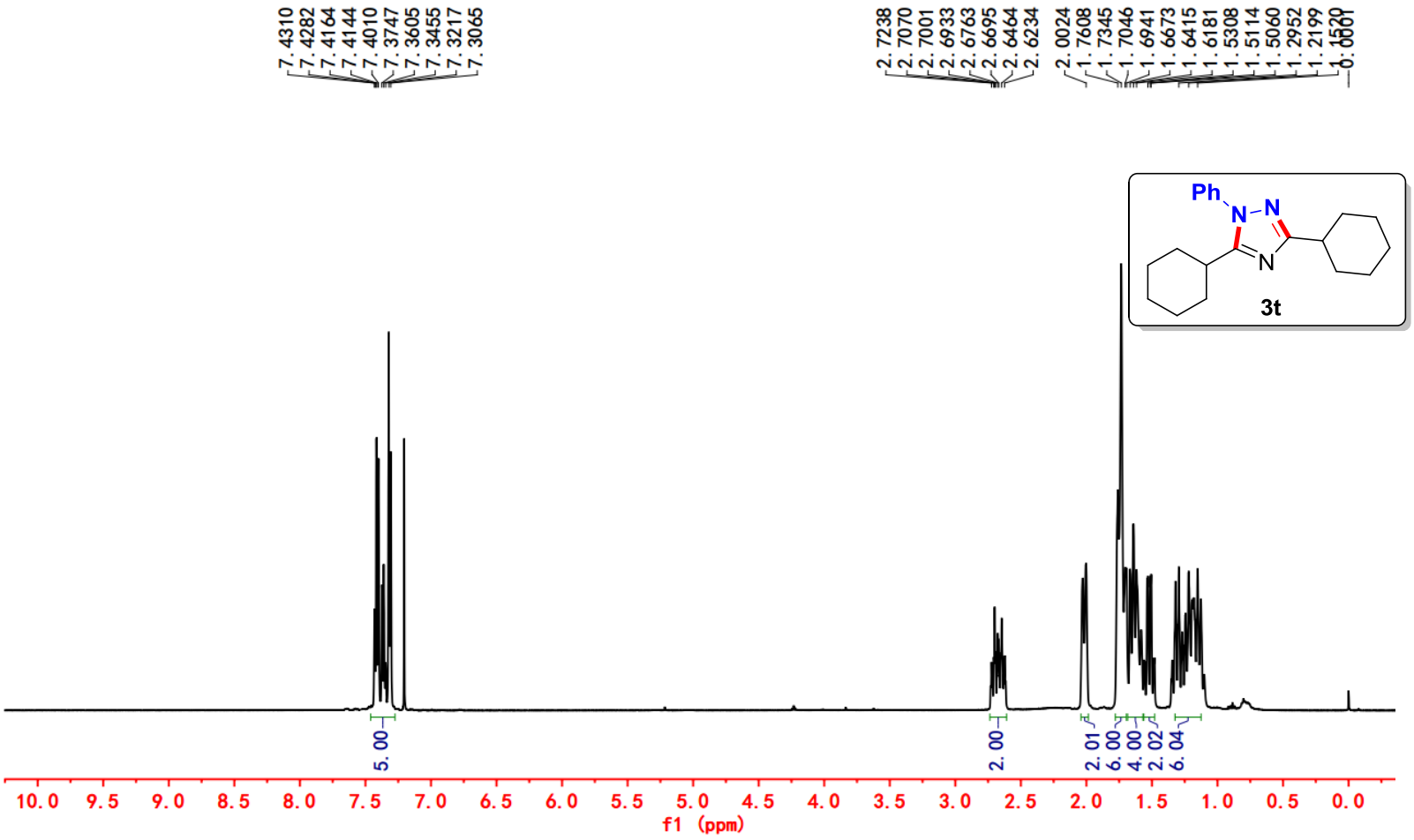
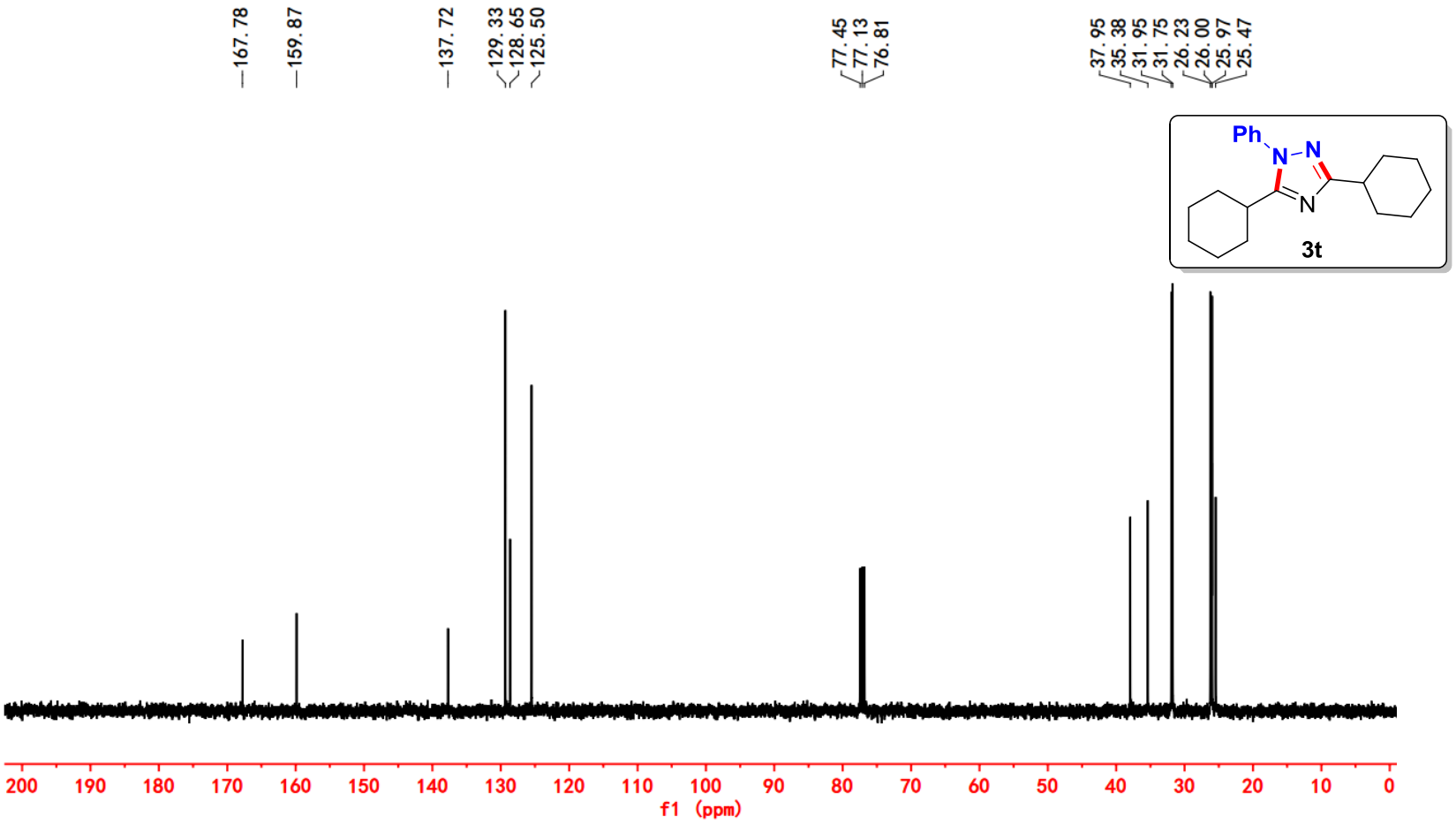
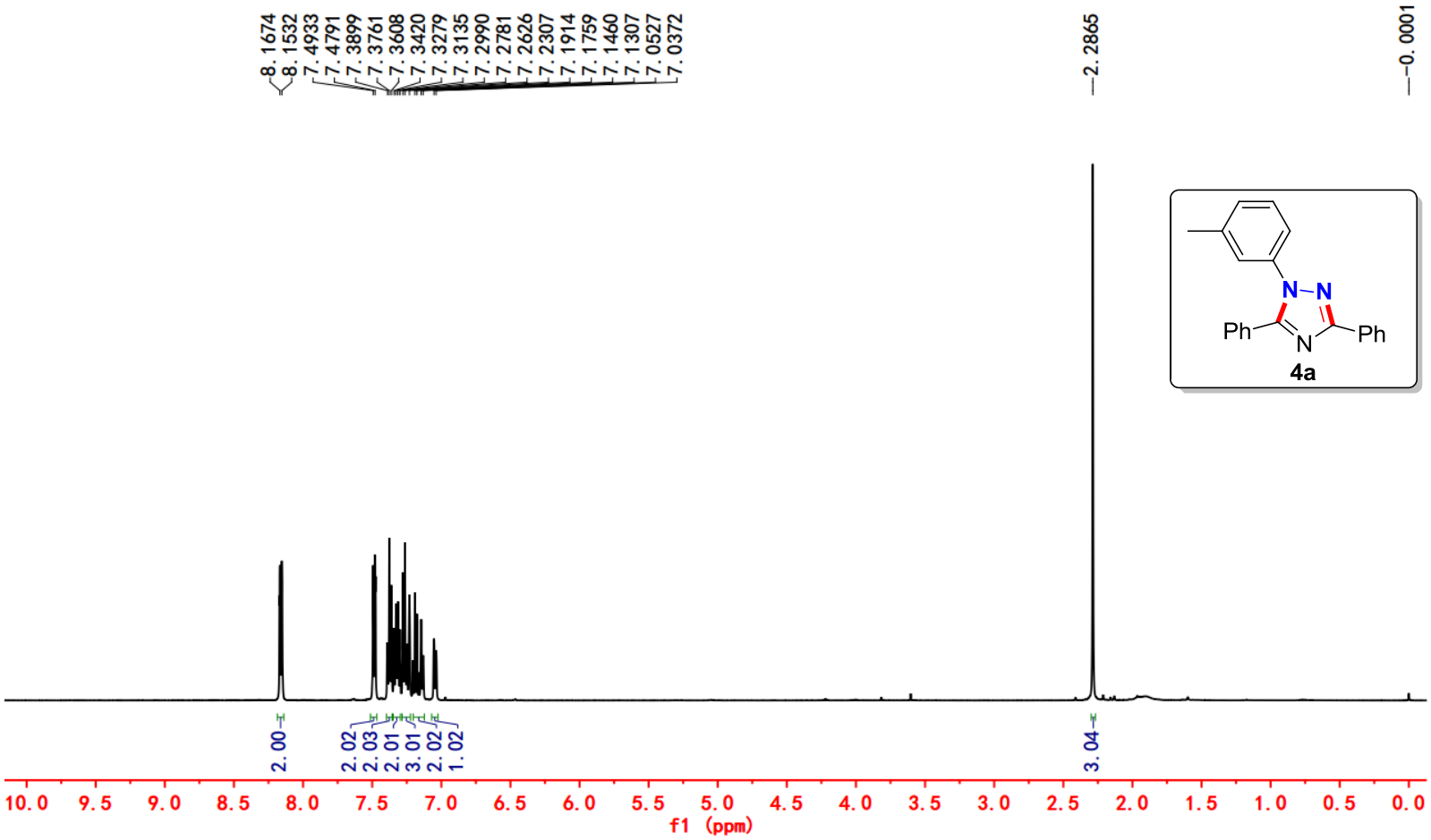
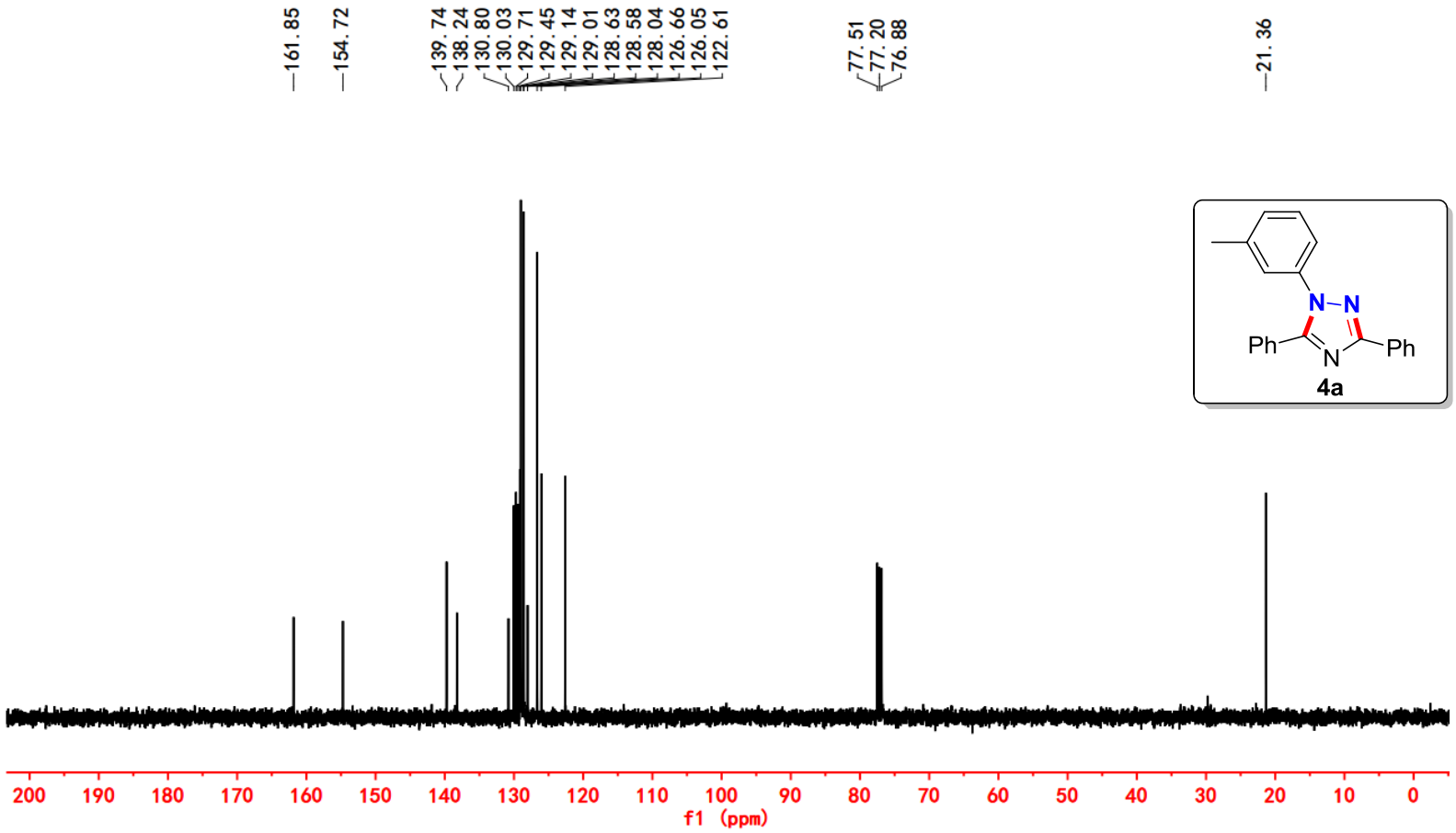
7.4181
7.4031
7.4020
7.4000
7.3832
7.3377
7.3345
7.3191
7.3007
7.2981
1.8386
1.8263
1.8173
1.8078
1.8058
1.7961
1.7873
1.7851
1.7749
1.0972
1.0924
1.0871
1.0835
1.0803
0.8962
0.8899
Ph
N
N
N
3s
5.01
1.00
1.00
2.01
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

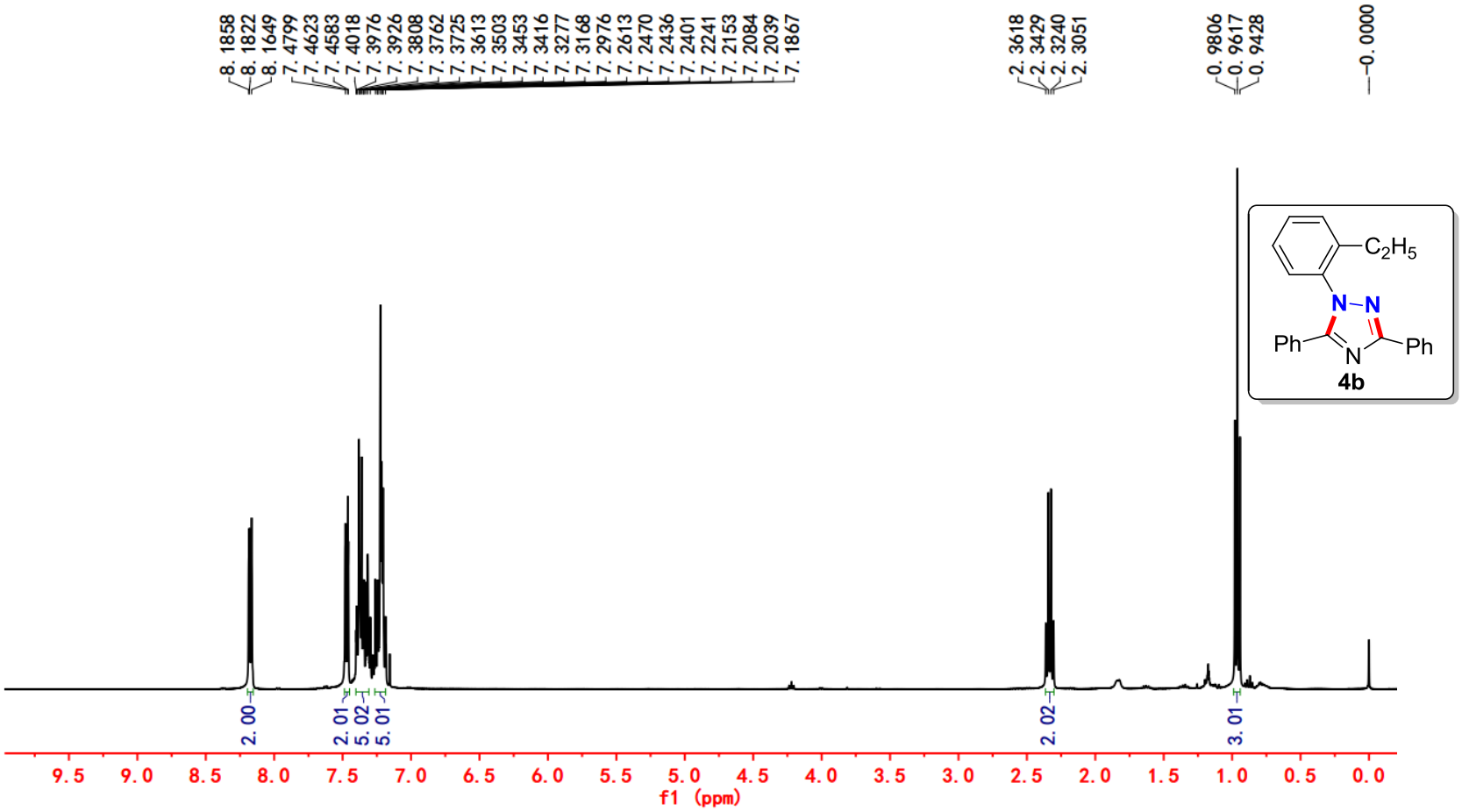

165.06
157.48
137.66
129.34
128.30
124.82
77.47
77.15
76.83
9.18
8.97
7.68
7.57
Ph
N
N
N
3s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.4310
7.4282
7.4164
7.4144
7.4010
7.3747
7.3605
7.3455
7.3217
7.3065
2.7238
2.7070
2.7001
2.6933
2.6763
2.6695
2.6464
2.6234
2.0024
1.7608
1.7345
1.7046
1.6941
1.6673
1.6415
1.6181
1.5308
1.5114
1.5060
1.2952
1.2199
Ph
N
N
N
3t
5.00
2.00
2.01
6.00
4.00
2.02
6.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.78
159.87
137.72
129.33
128.65
125.50
77.45
77.13
76.81
37.95
35.38
31.95
31.75
26.23
26.00
25.97
25.47
Ph
N
N
N
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.1674
8.1532
7.4933
7.4791
7.3899
7.3761
7.3608
7.3420
7.3279
7.3135
7.2990
7.2781
7.2626
7.2307
7.1914
7.1759
7.1460
7.1307
7.0527
7.0372
2.2865
0.0001
Ph
N
N
Ph
4a
2.00
2.02
2.03
2.01
3.01
2.02
1.02
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.85
154.72
139.74
138.24
130.80
130.03
129.71
129.45
129.14
129.01
128.63
128.58
128.04
126.66
126.05
122.61
77.51
77.20
76.88
21.36
N
N
Ph
Ph
4a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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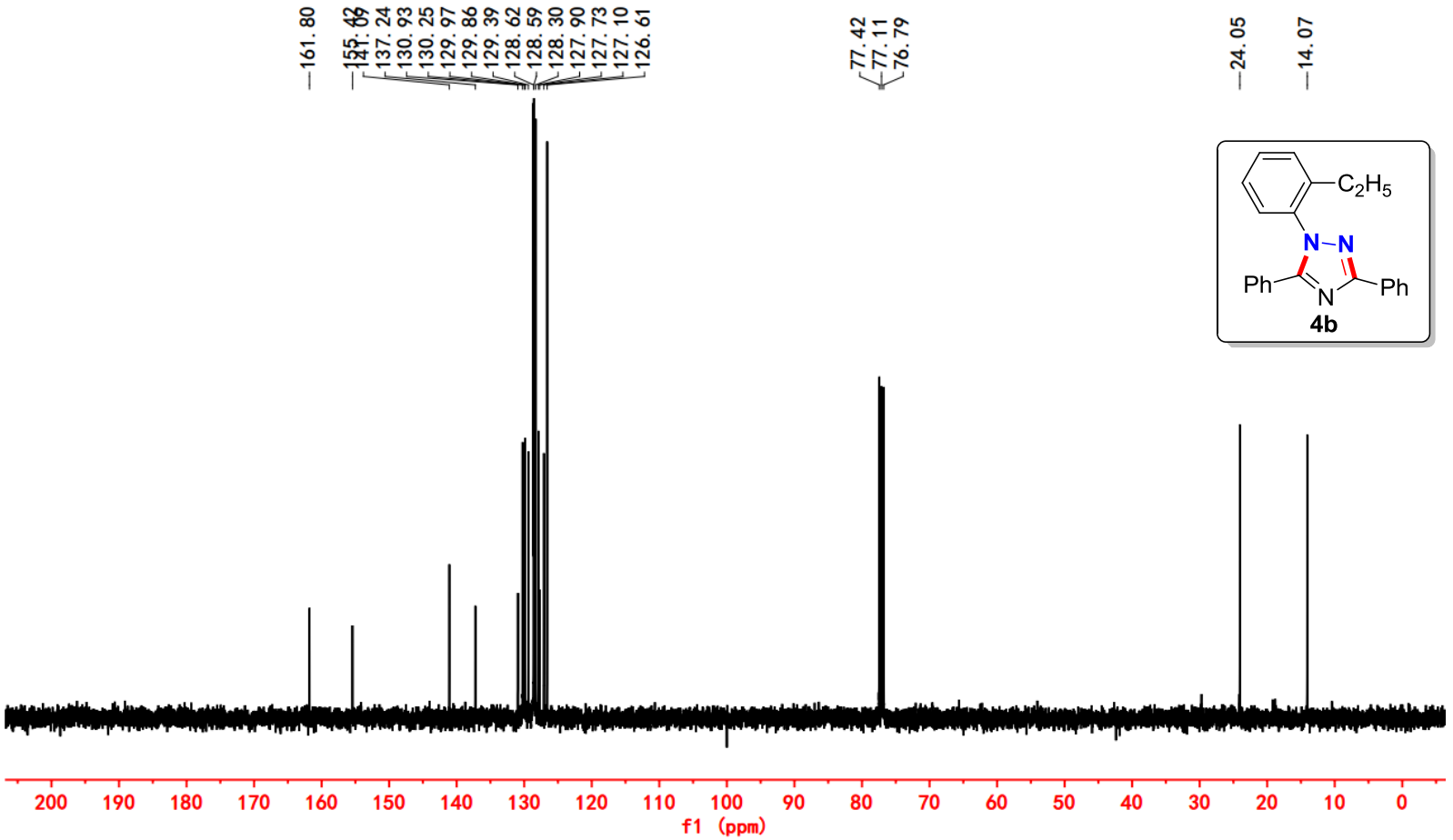
8.1822
8.1649
7.4799
7.4623
7.4583
7.4018
7.3976
7.3926
7.3808
7.3762
7.3725
7.3613
7.3503
7.3453
7.3416
7.3277
7.3168
7.2976
7.2613
7.2470
7.2436
7.2401
7.2241
7.2153
7.2084
7.2039
7.1867
2.3618
2.3429
2.3240
2.3051
0.9806
0.9617
0.9428
0.0000
2.00
2.01
5.02
5.01
2.02
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 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)
C2H5
N–N
Ph
Ph
N
4b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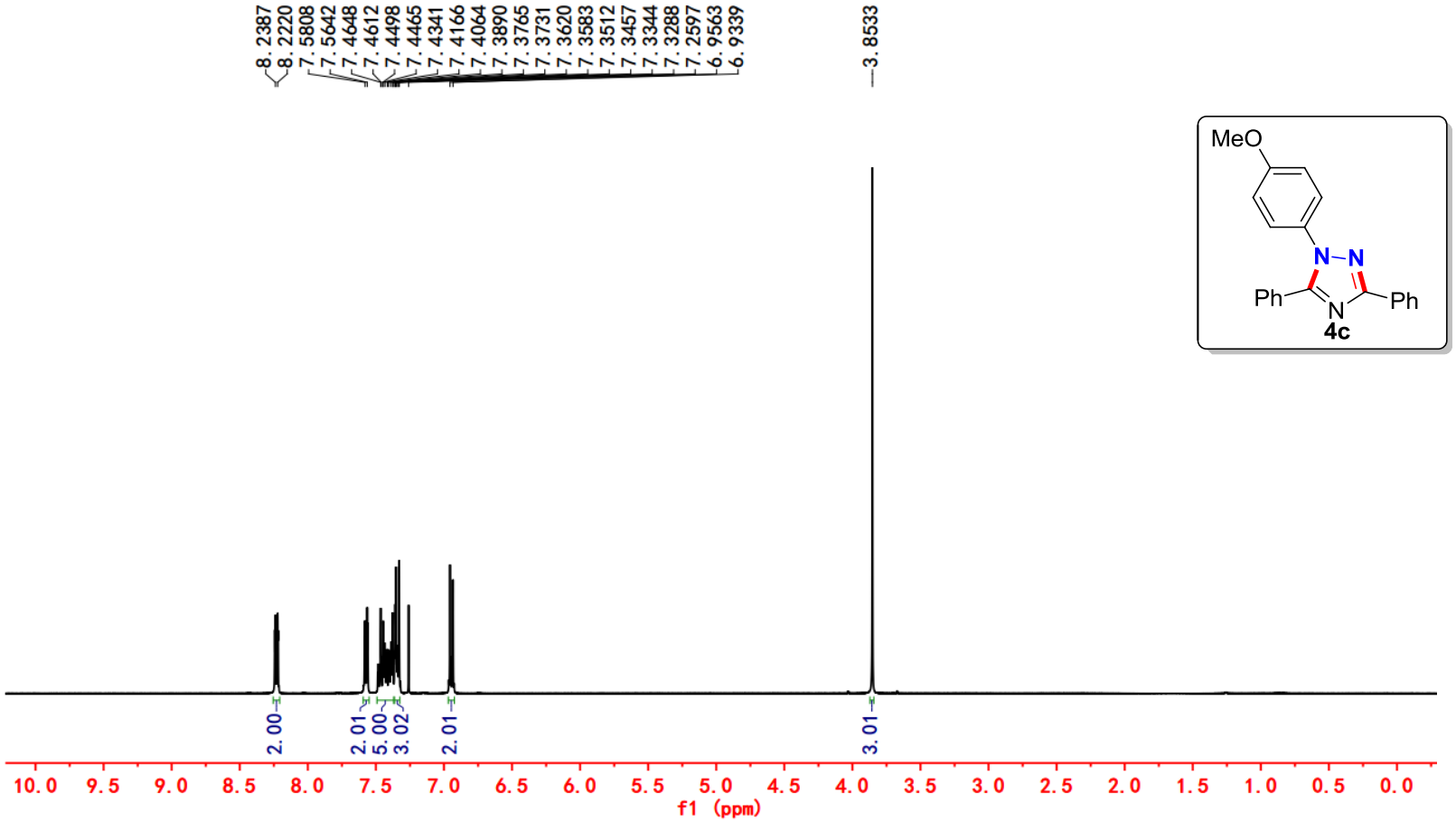
155.42
141.09
137.24
130.93
130.25
129.97
129.86
129.39
128.62
128.59
128.30
127.90
127.73
127.10
126.61
77.42
77.11
76.79
24.05
14.07
C2H5
N
N
Ph
Ph
N
4b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.2387
8.2220
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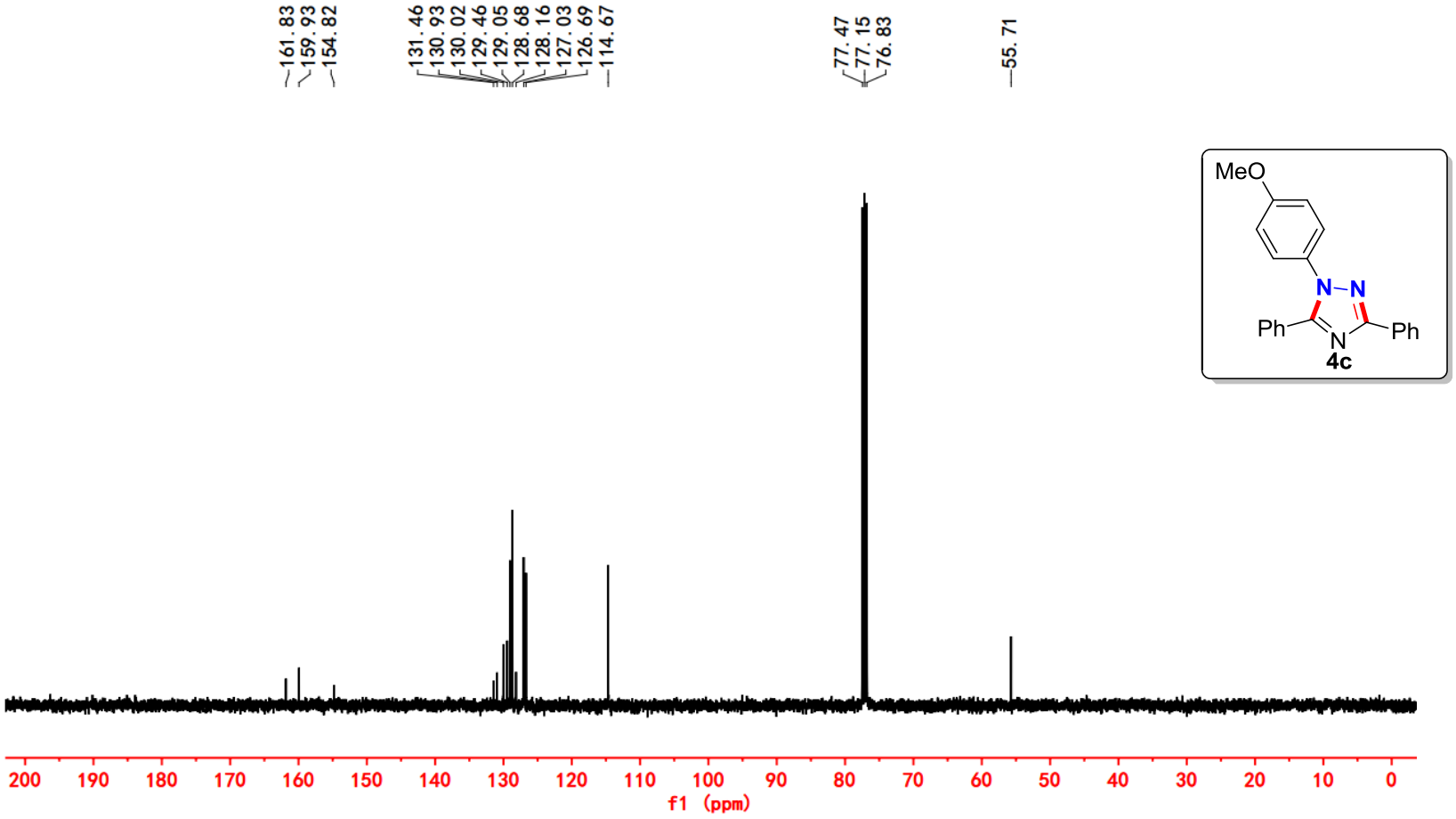
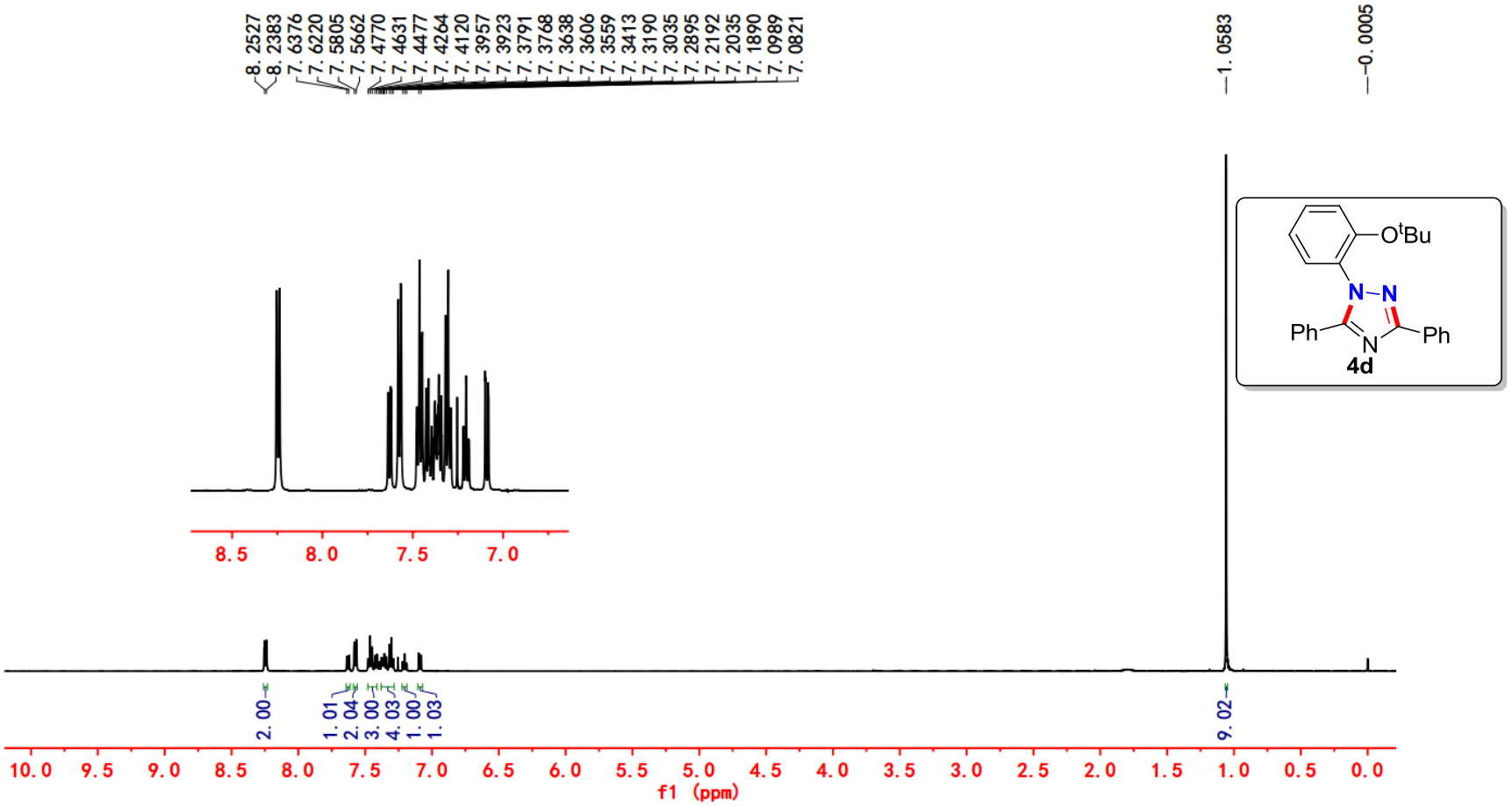
7.5642
7.4648
7.4612
7.4498
7.4465
7.4341
7.4166
7.4064
7.3890
7.3765
7.3731
7.3620
7.3583
7.3512
7.3457
7.3344
7.3288
7.2597
6.9563
6.9339
3.8533
2.00
2.01
5.00
3.02
2.01
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
MeO
N
N
Ph
Ph
N
4c


161.83
159.93
154.82
131.46
130.93
130.02
129.46
129.05
128.68
128.16
127.03
126.69
114.67
77.47
77.15
76.83
55.71
MeO
N
N
Ph
Ph
4c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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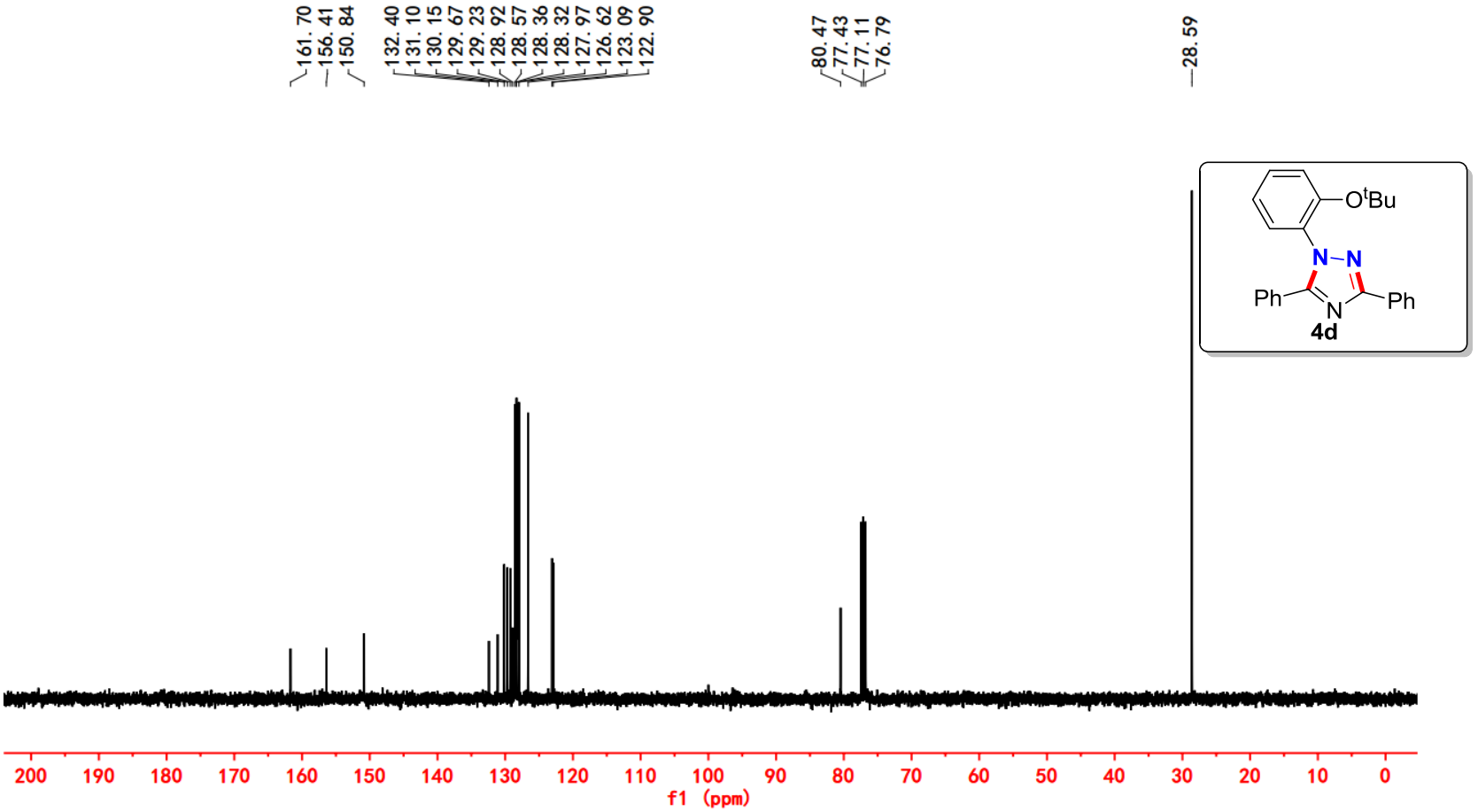
7.6220
7.5805
7.5662
7.4770
7.4631
7.4477
7.4264
7.4120
7.3957
7.3923
7.3791
7.3768
7.3638
7.3606
7.3559
7.3413
7.3190
7.3035
7.2895
7.2192
7.2035
7.1890
7.0989
7.0821
1.0583
0.0005
O^{t}Bu
N–N
Ph
Ph
N
4d
8.5
8.0
7.5
7.0
2.00
1.01
2.04
3.00
4.03
1.00
1.03
9.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.15
129.67
129.23
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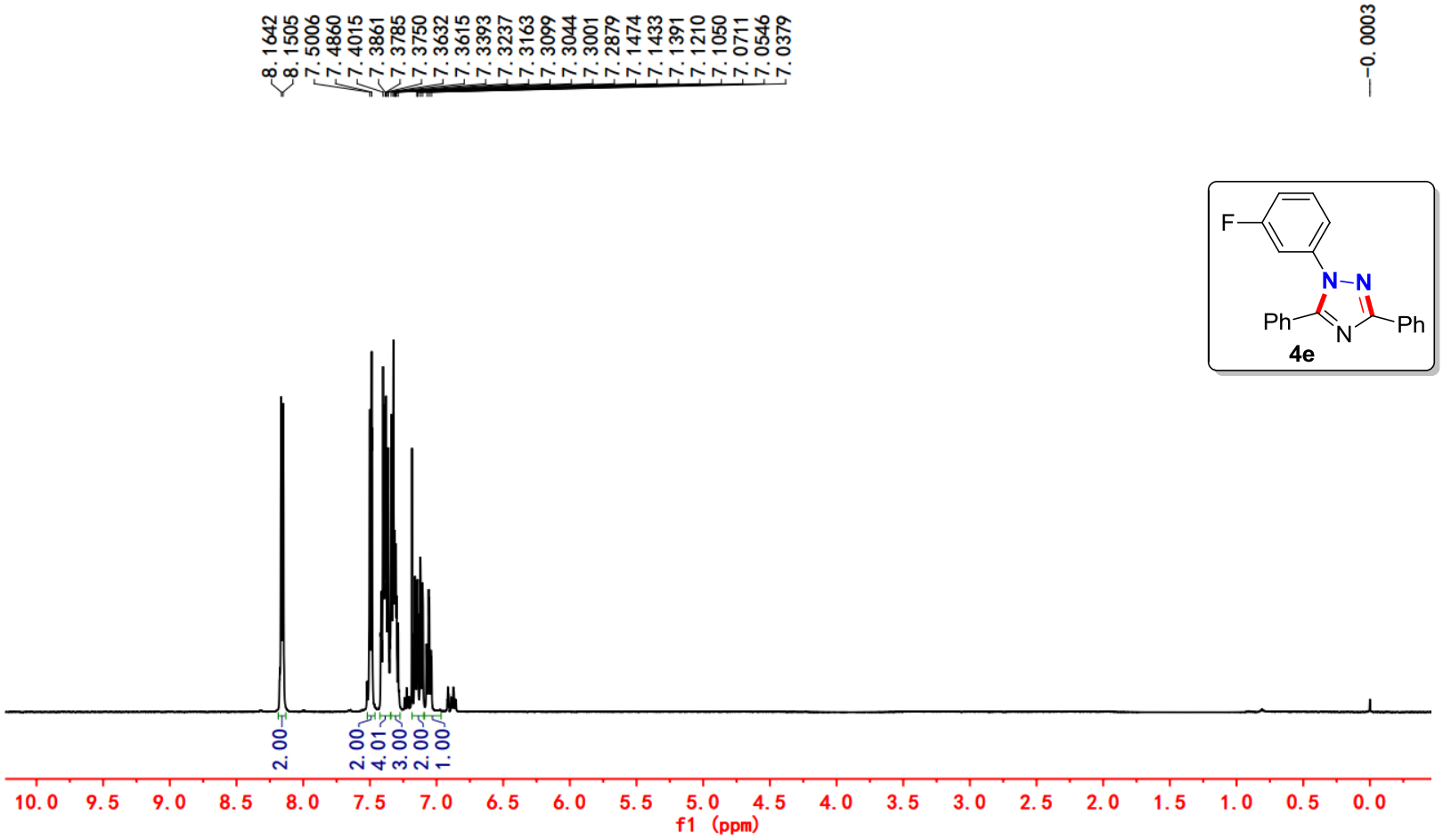
128.57
128.36
128.32
127.97
126.62
123.09
122.90
80.47
77.43
77.11
76.79
28.59
OtBu
N
N
Ph
Ph
N
4d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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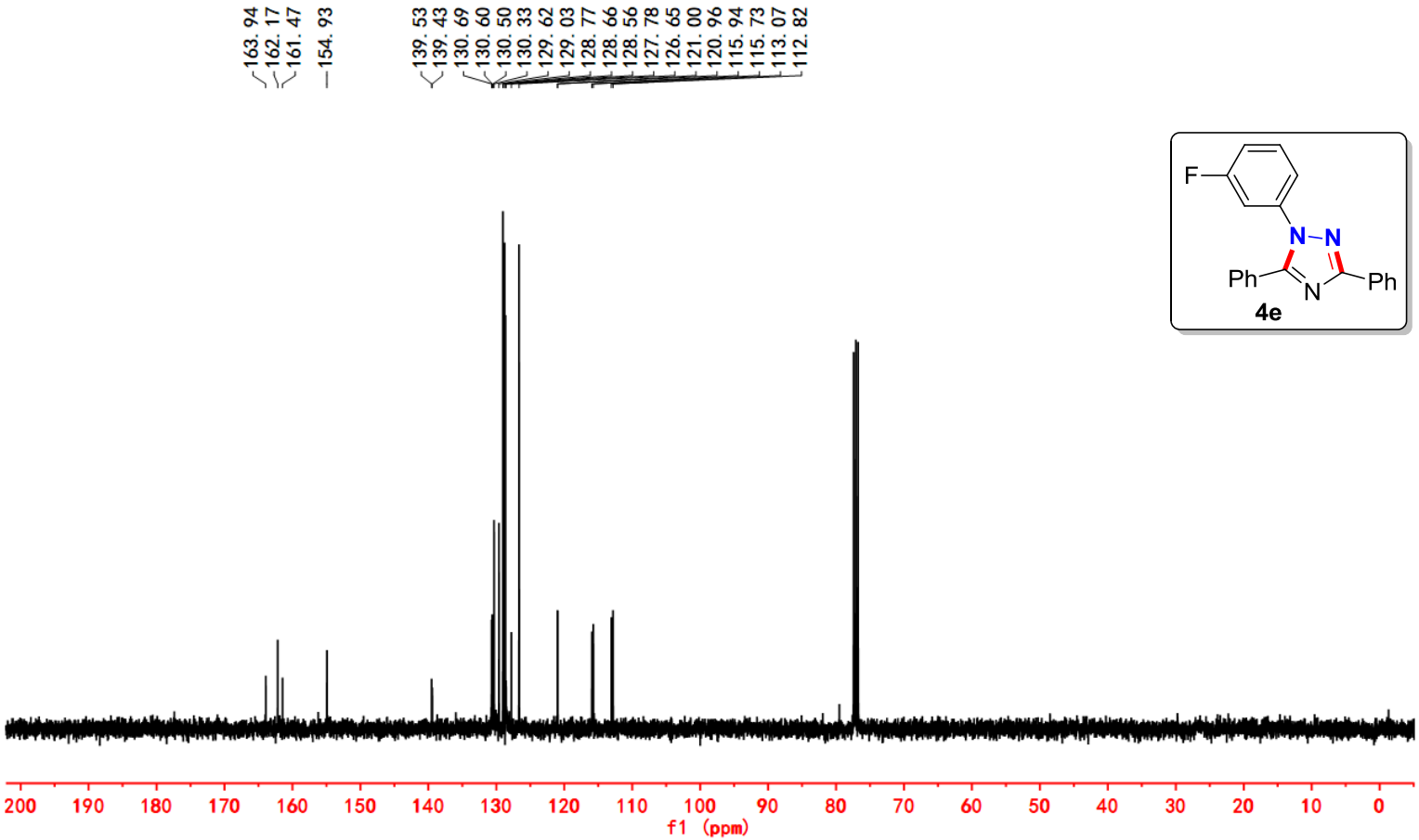
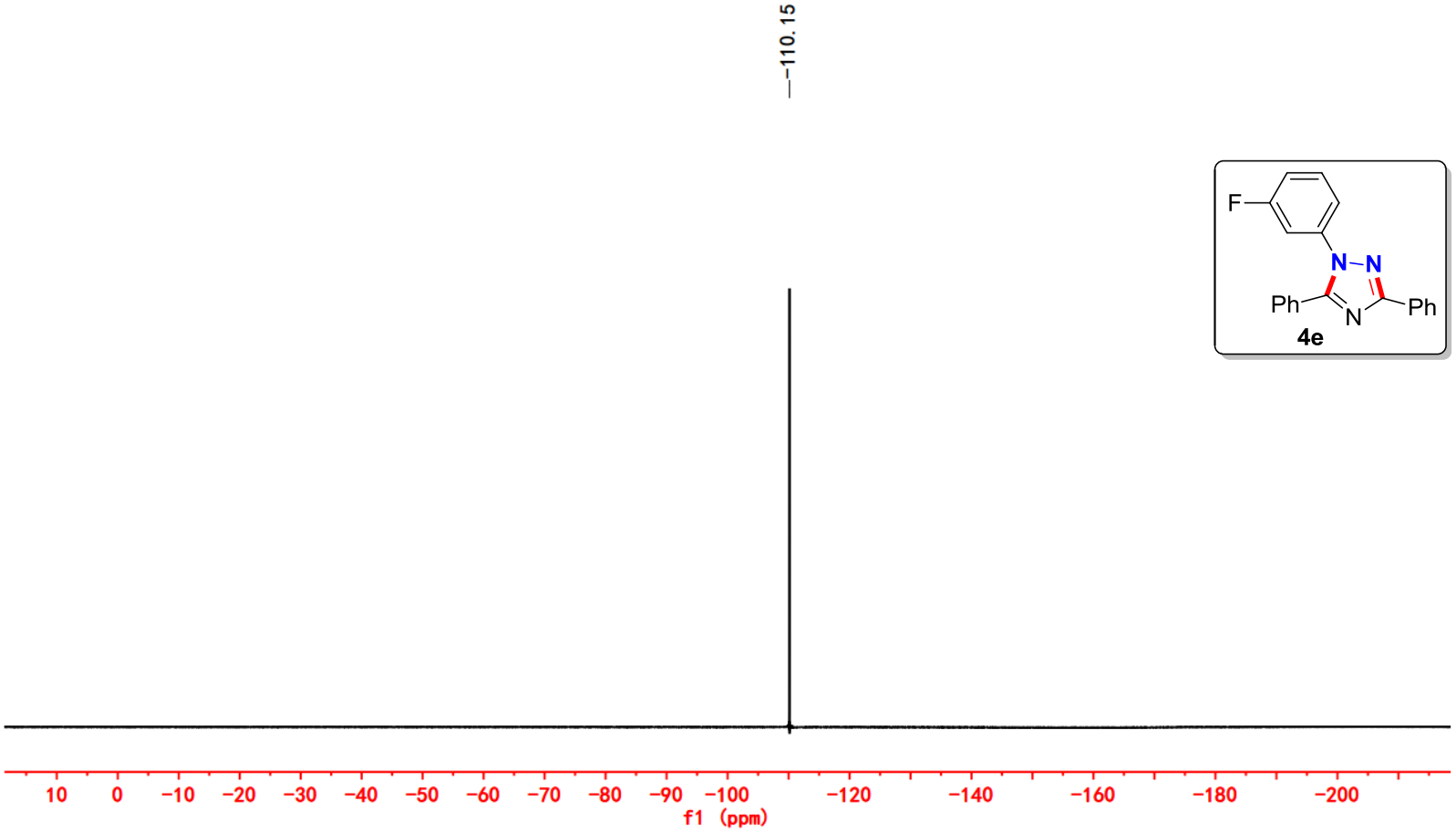
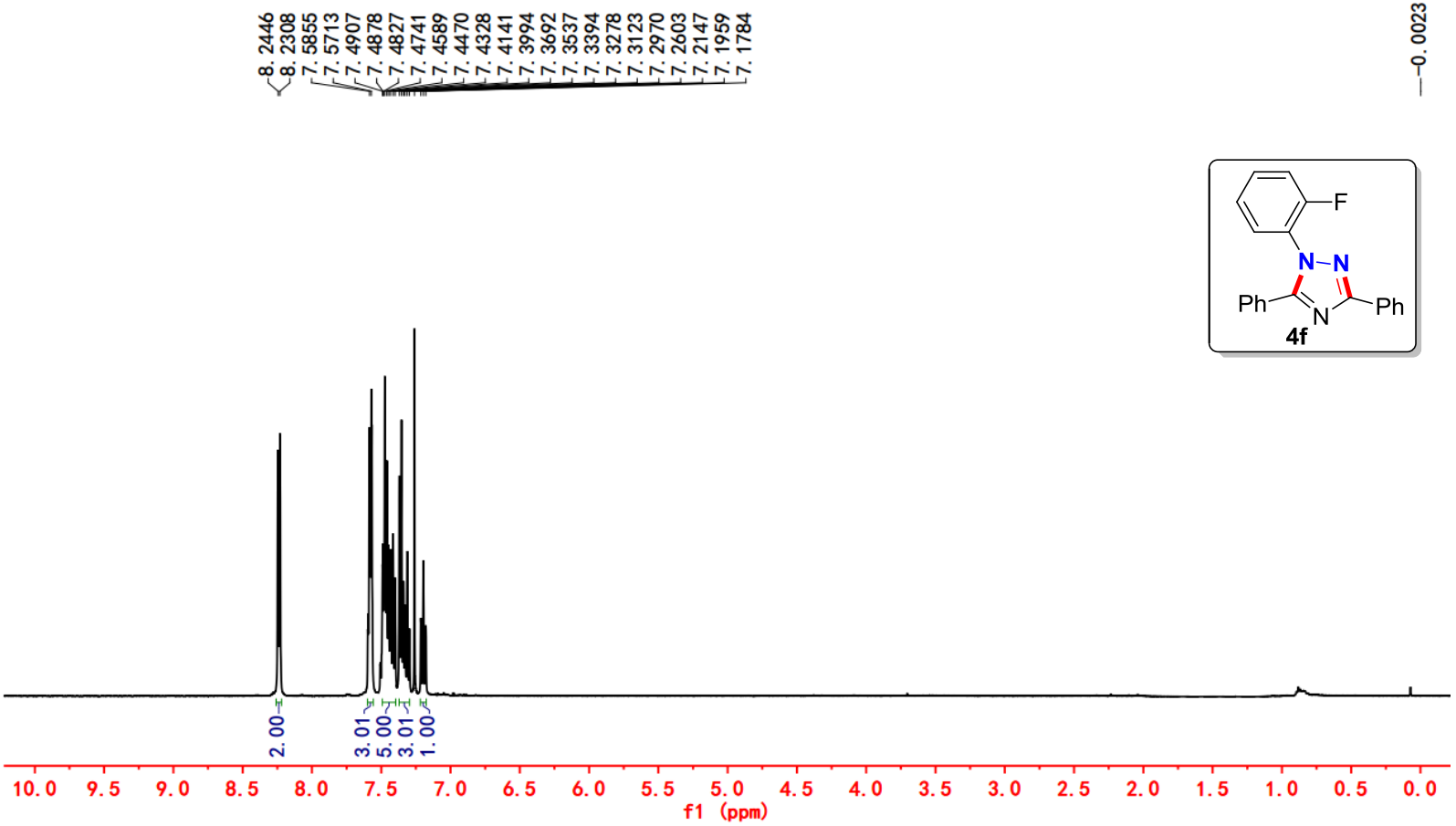
7.4015
7.3861
7.3785
7.3750
7.3632
7.3615
7.3393
7.3237
7.3163
7.3099
7.3044
7.3001
7.2879
7.1474
7.1433
7.1391
7.1210
7.1050
7.0711
7.0546
7.0379
0.0003
F
N
N
Ph
N
Ph
4e
2.00
2.00
4.01
3.00
2.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


163.94
162.17
161.47
154.93
139.53
139.43
130.69
130.60
130.50
130.33
129.62
129.03
128.77
128.66
128.56
127.78
126.65
121.00
120.96
115.94
115.73
113.07
112.82
F
N
N
Ph
Ph
N
4e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-110.15
F
N
N
Ph
N
Ph
4e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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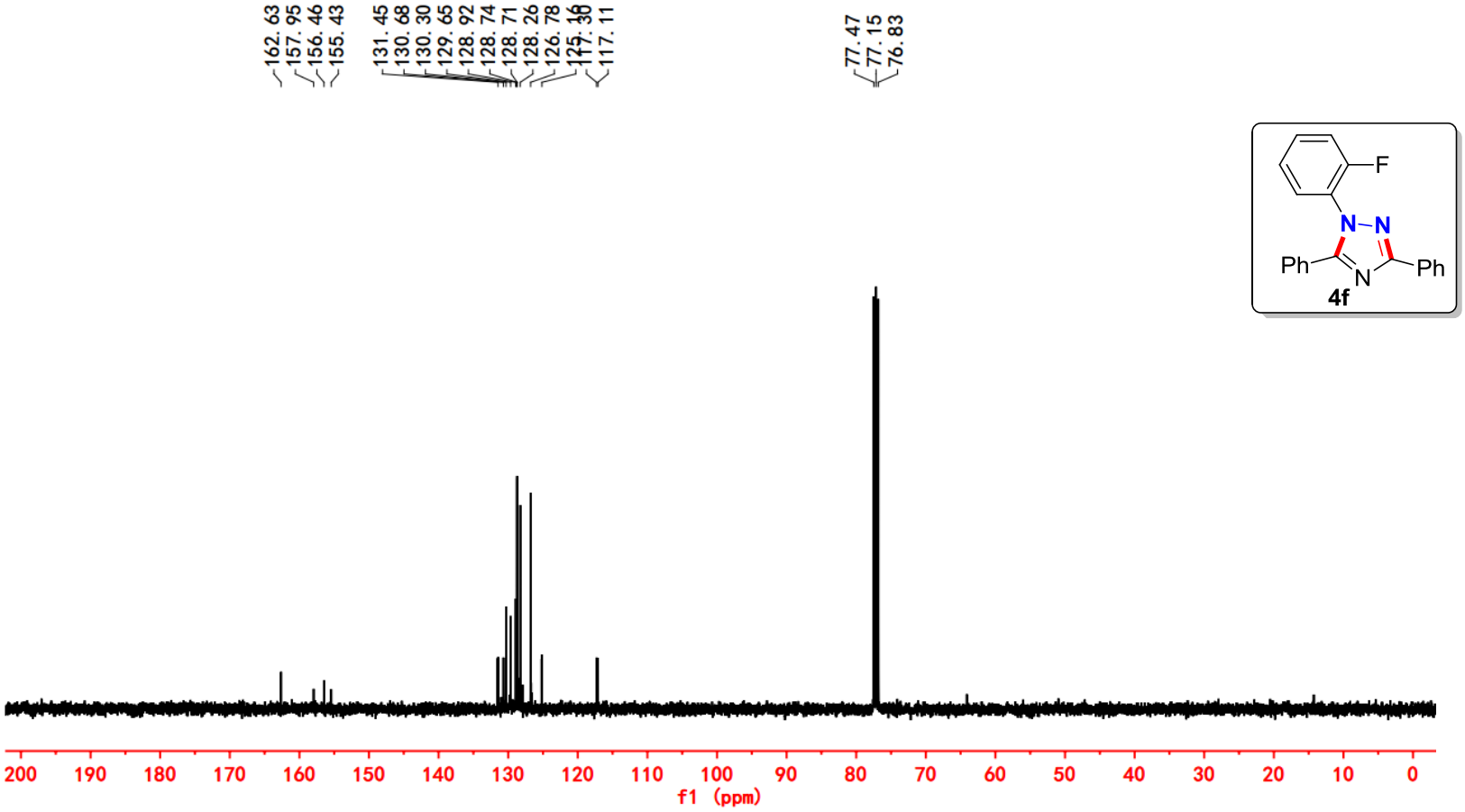
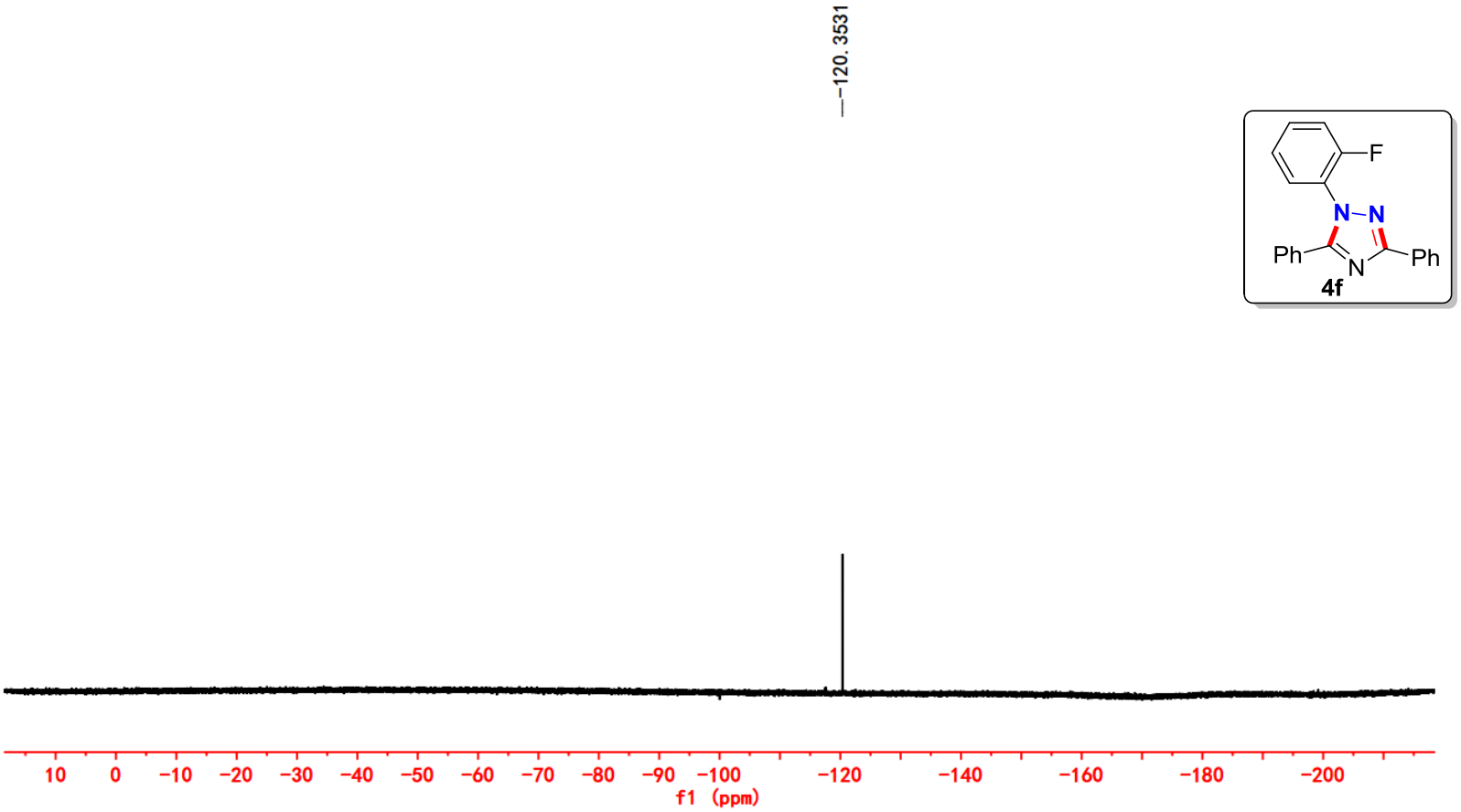
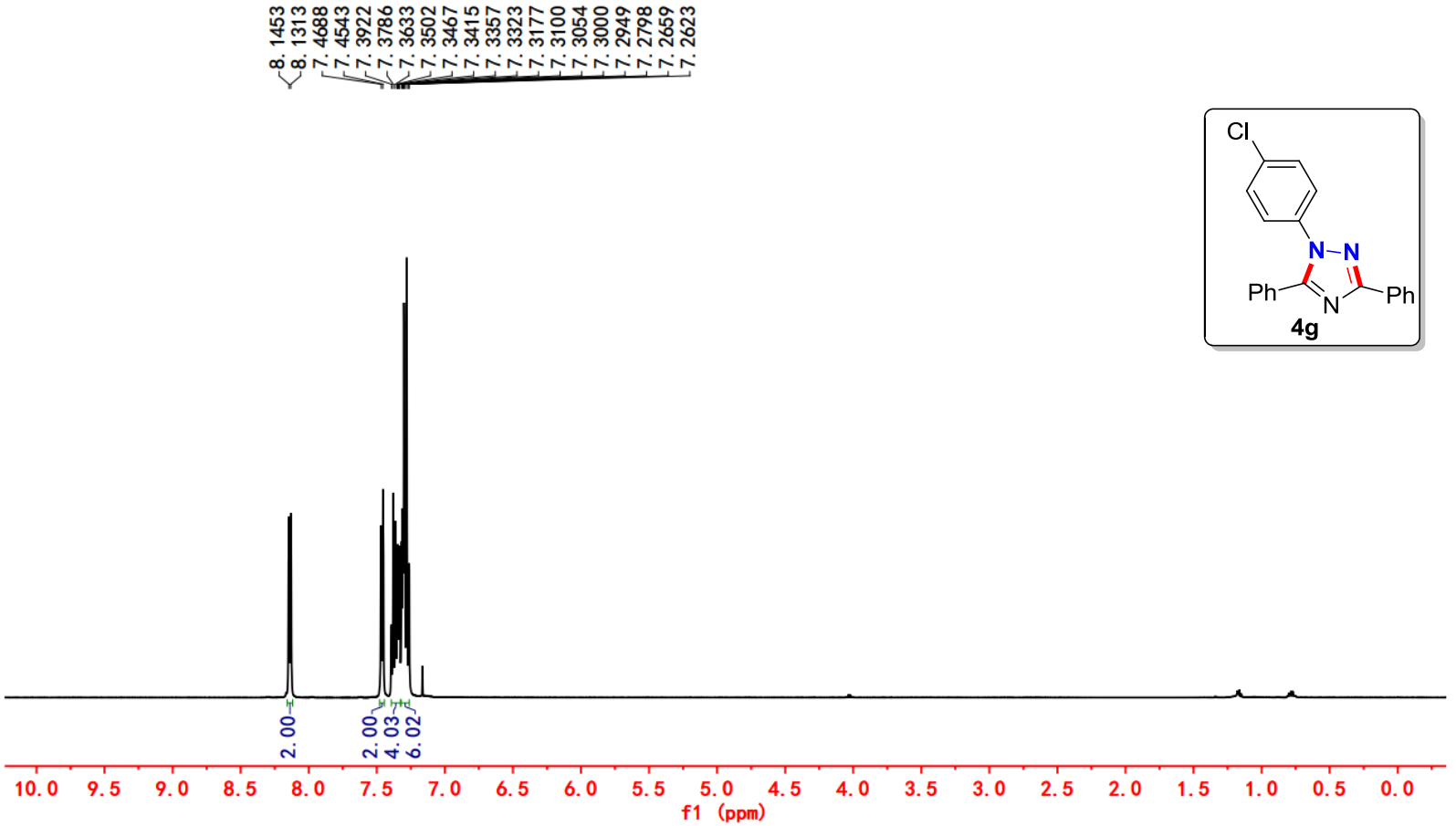
7.5713
7.4907
7.4878
7.4827
7.4741
7.4589
7.4470
7.4328
7.4141
7.3994
7.3692
7.3537
7.3394
7.3278
7.3123
7.2970
7.2603
7.2147
7.1959
7.1784
0.0023
F
N
N
Ph
N
Ph
4f
2.00
3.01
5.00
3.01
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


162.63
157.95
156.46
155.43
131.45
130.68
130.30
129.65
128.92
128.74
128.71
128.26
126.78
125.16
117.30
117.11
77.47
77.15
76.83
F
N
N
Ph
N
Ph
4f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


−120.3531
F
N
N
Ph
N
Ph
4f
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−120
−140
−160
−180
−200
f1 (ppm)


8.1453
8.1313
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7.3922
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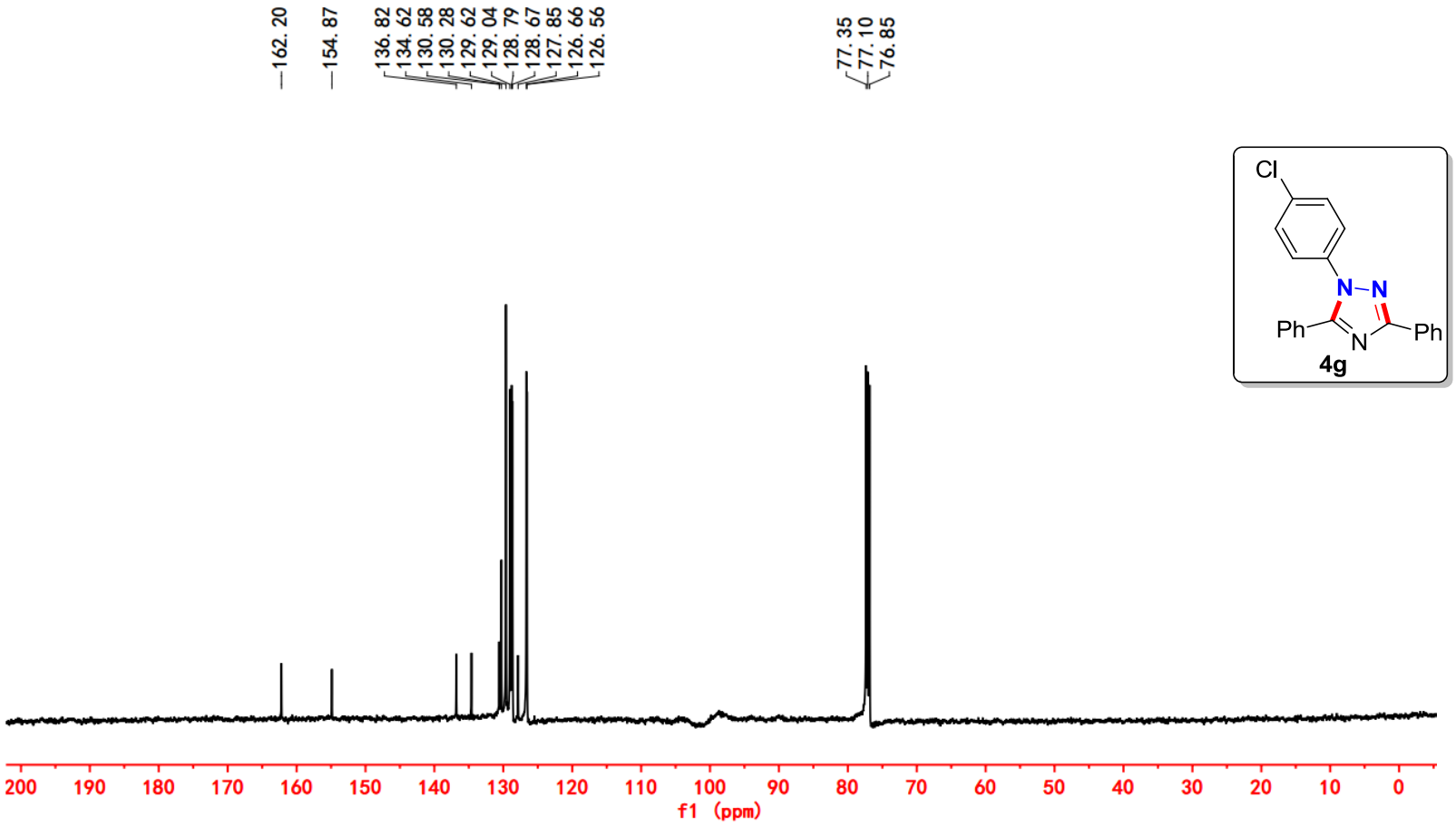
7.3633
7.3502
7.3467
7.3415
7.3357
7.3323
7.3177
7.3100
7.3054
7.3000
7.2949
7.2798
7.2659
7.2623
Cl
N
N
Ph
N
Ph
4g
2.00
2.00
4.03
6.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.04
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128.67
127.85
126.66
126.56
77.35
77.10
76.85
Cl
N
N
Ph
Ph
N
4g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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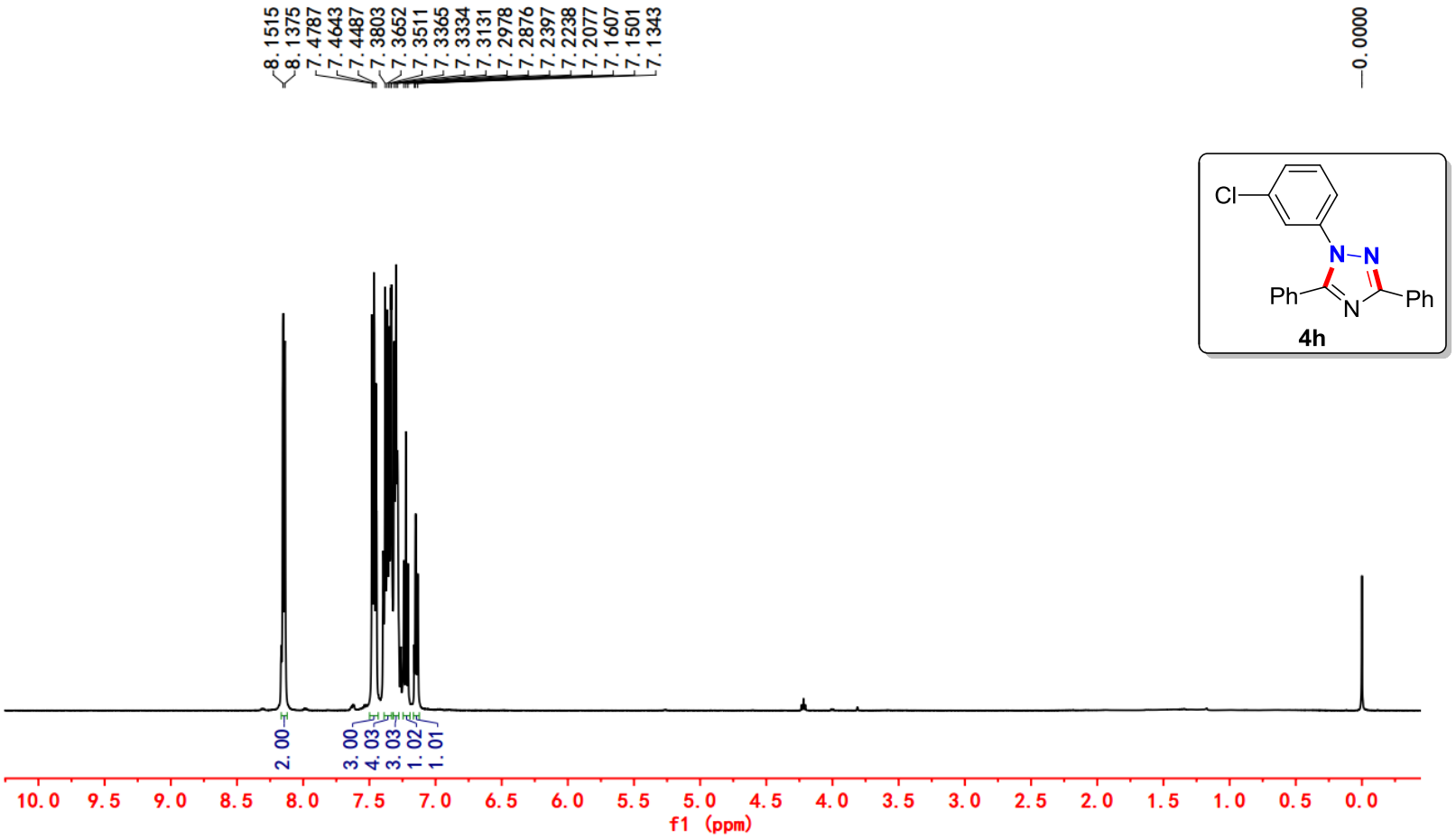
50
40
30
20
10
0
f1 (ppm)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7.4487
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7.3652
7.3511
7.3365
7.3334
7.3131
7.2978
7.2876
7.2397
7.2238
7.2077
7.1607
7.1501
7.1343
0.0000
Cl
N
N
Ph
N
Ph
4h
2.00
3.00
4.03
3.03
1.02
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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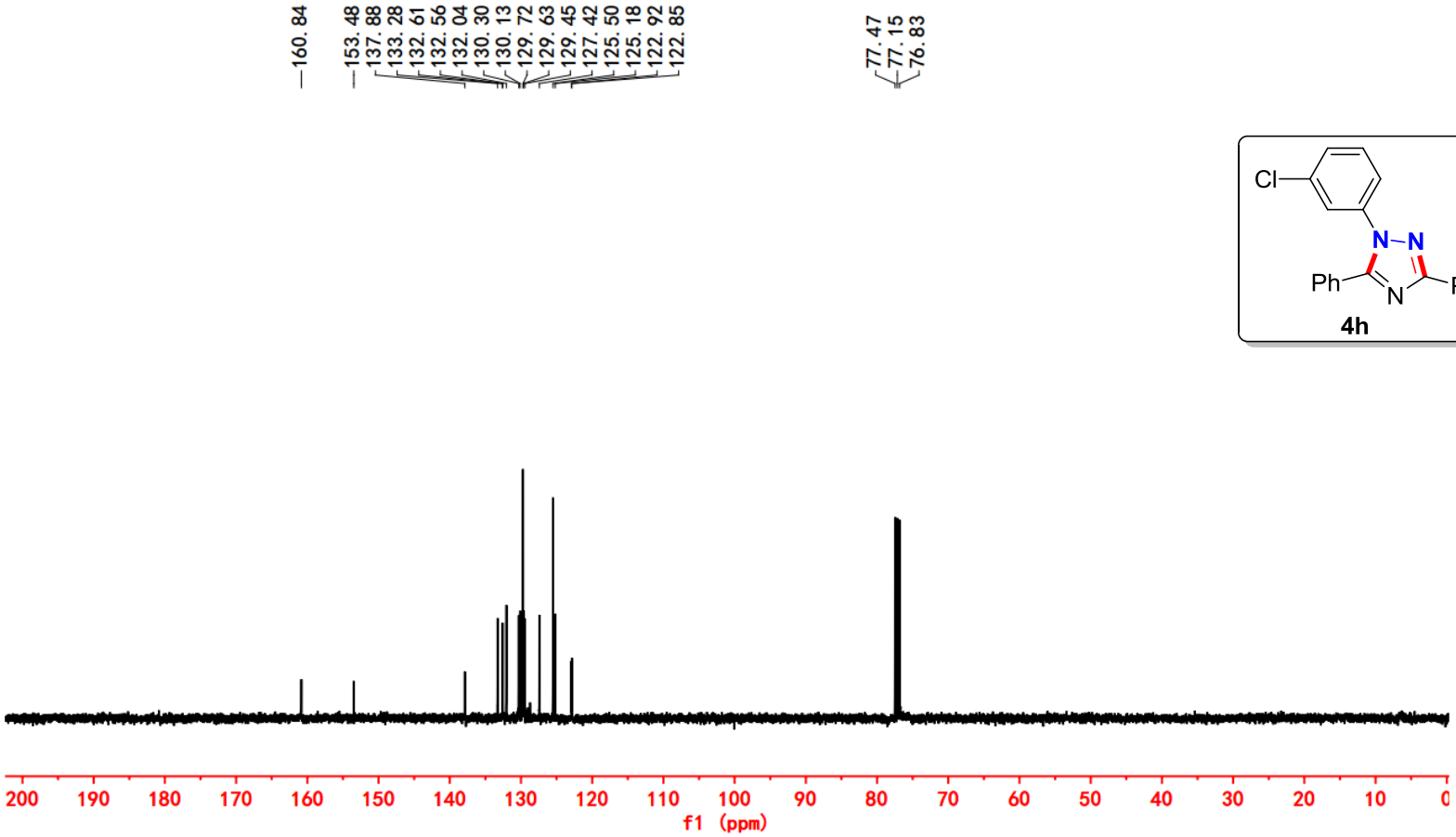
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.30
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129.63
129.45
127.42
125.50
125.18
122.92
122.85
77.47
77.15
76.83
Cl
N
N
Ph
N
Ph
4h
200
190
180
170
160
150
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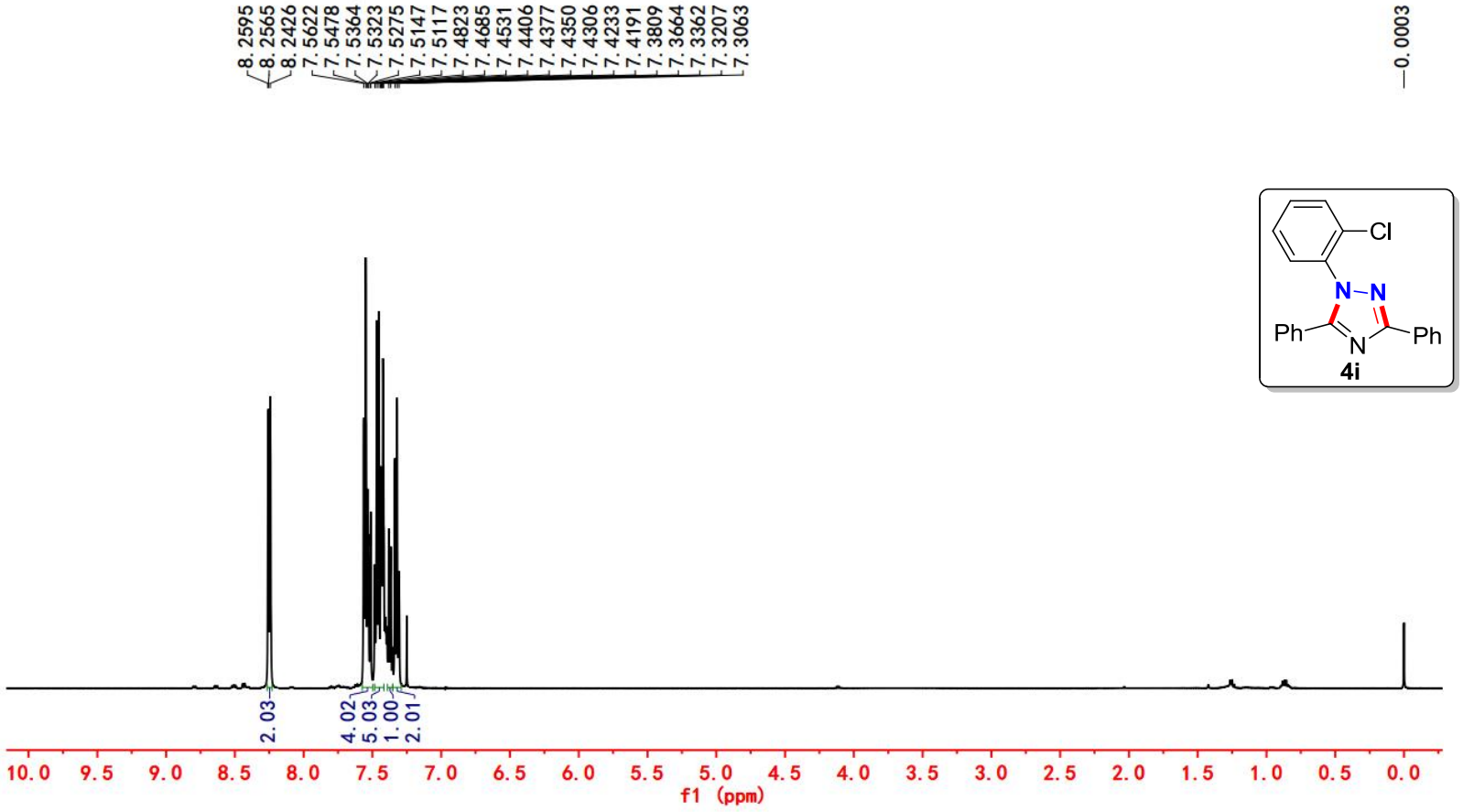
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.2565
8.2426
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7.5364
7.5323
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7.5147
7.5117
7.4823
7.4685
7.4531
7.4406
7.4377
7.4350
7.4306
7.4233
7.4191
7.3809
7.3664
7.3362
7.3207
7.3063
0.0003
Cl
N
N
Ph
Ph
N
4i
2.03
4.02
5.03
1.00
2.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
1.0
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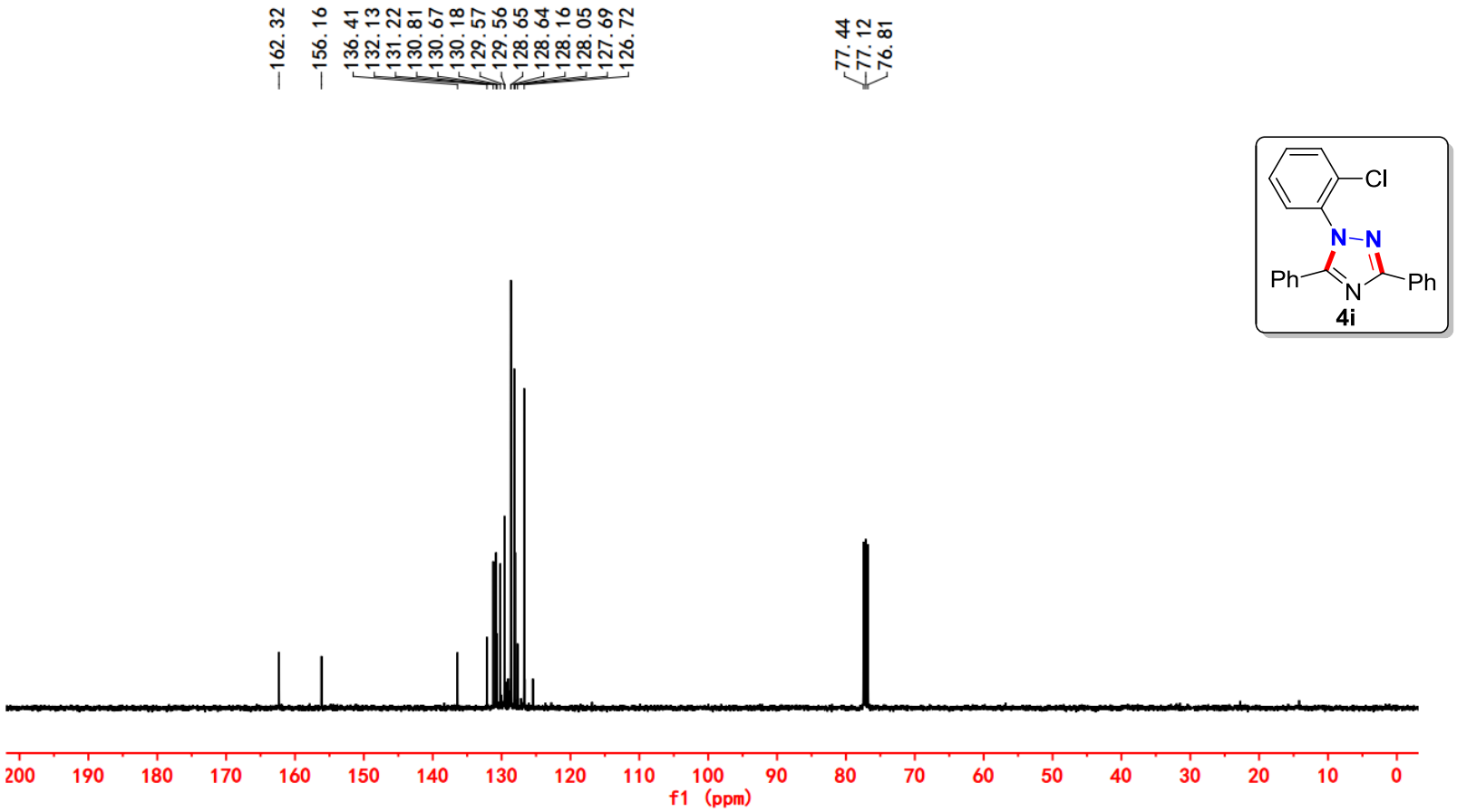
f1 (ppm)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128.16
128.05
127.69
126.72
77.44
77.12
76.81
Cl
N
N
Ph
Ph
N
4i
200
190
180
170
160
150
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120
110
100
90
80
70
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50
40
30
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10
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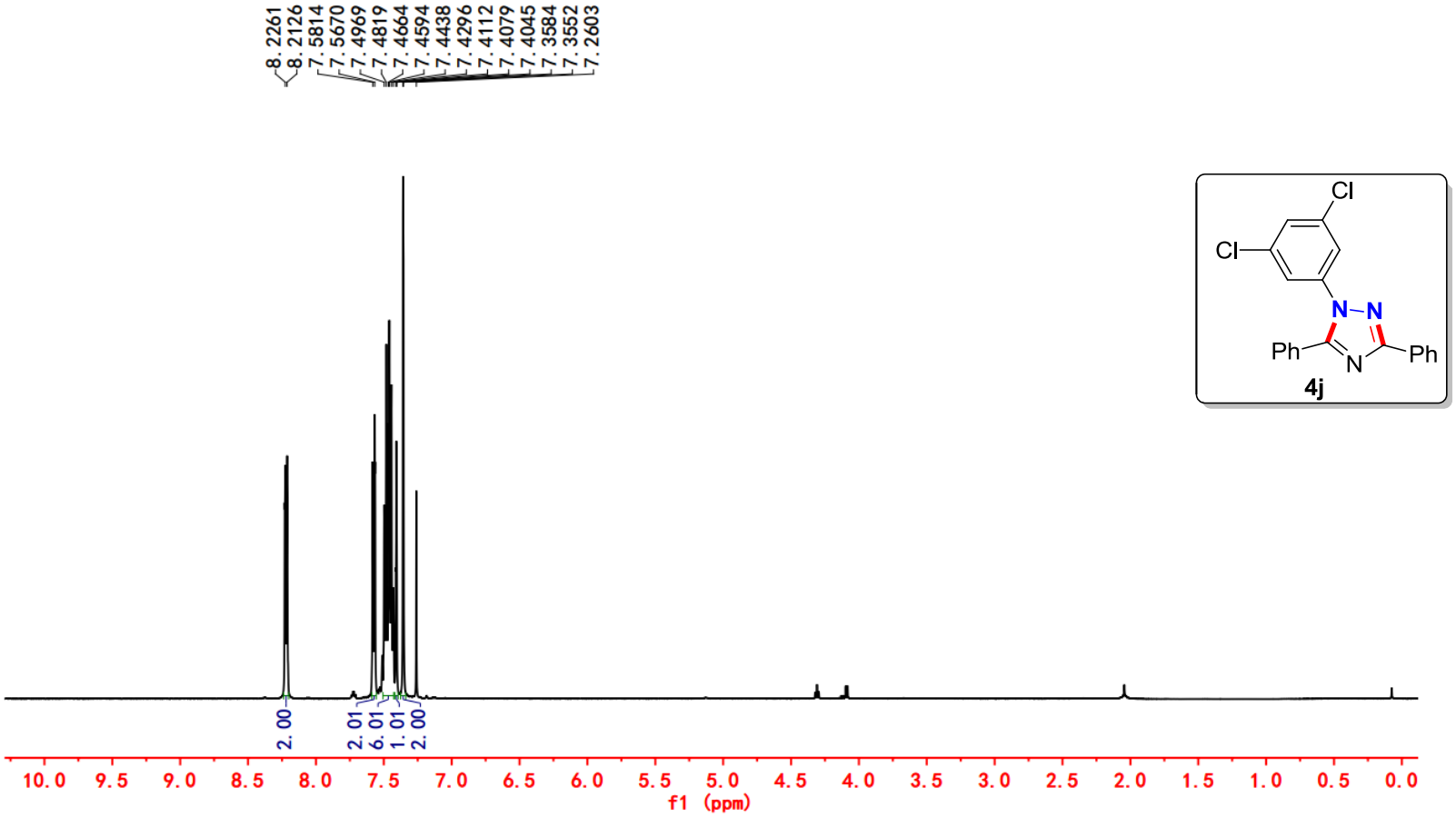
f1 (ppm)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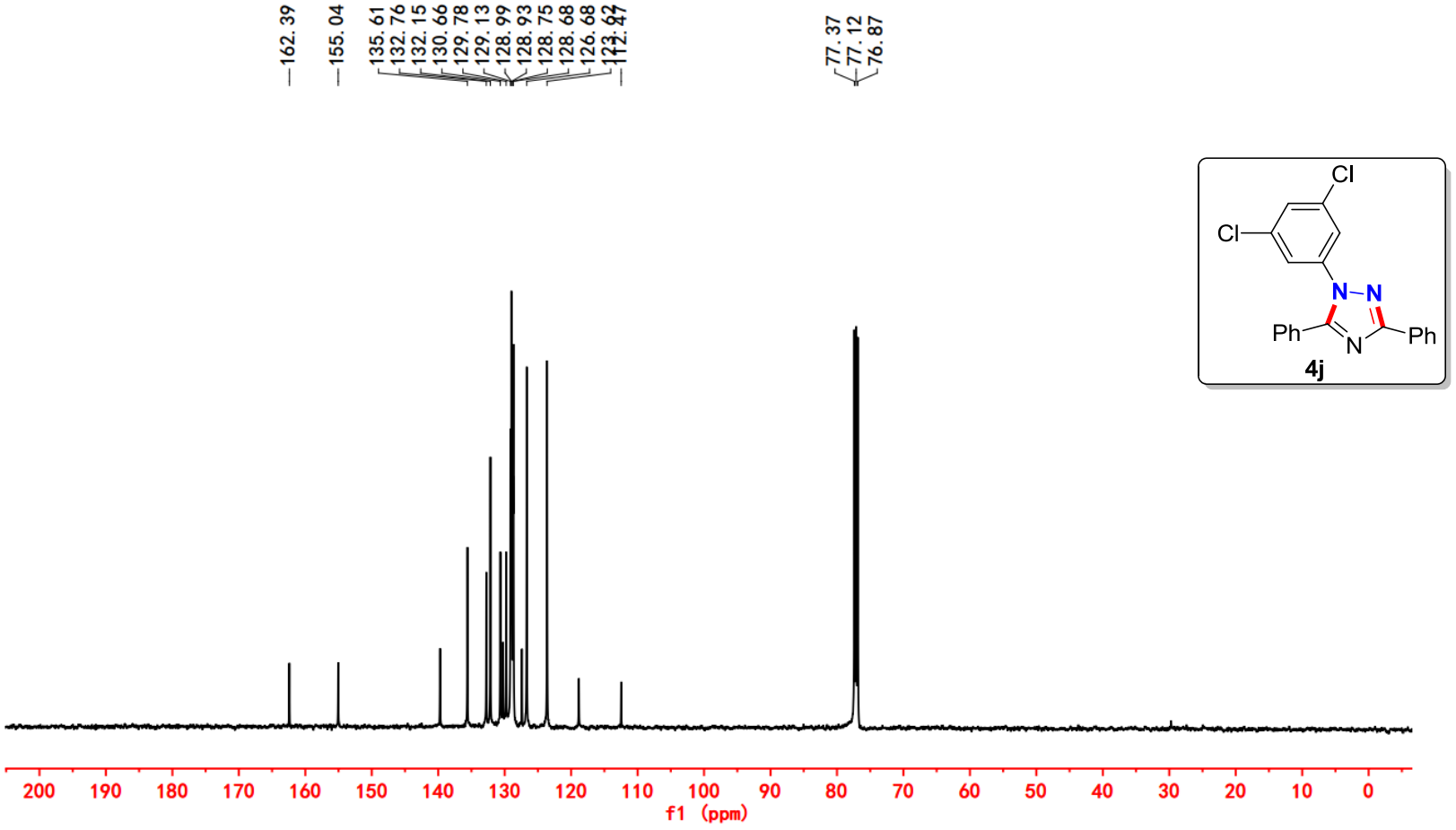
8.2126
7.5814
7.5670
7.4969
7.4819
7.4664
7.4594
7.4438
7.4296
7.4112
7.4079
7.4045
7.3584
7.3552
7.2603
Cl
Cl
N
N
Ph
Ph
N
4j
2.00
2.01
6.01
1.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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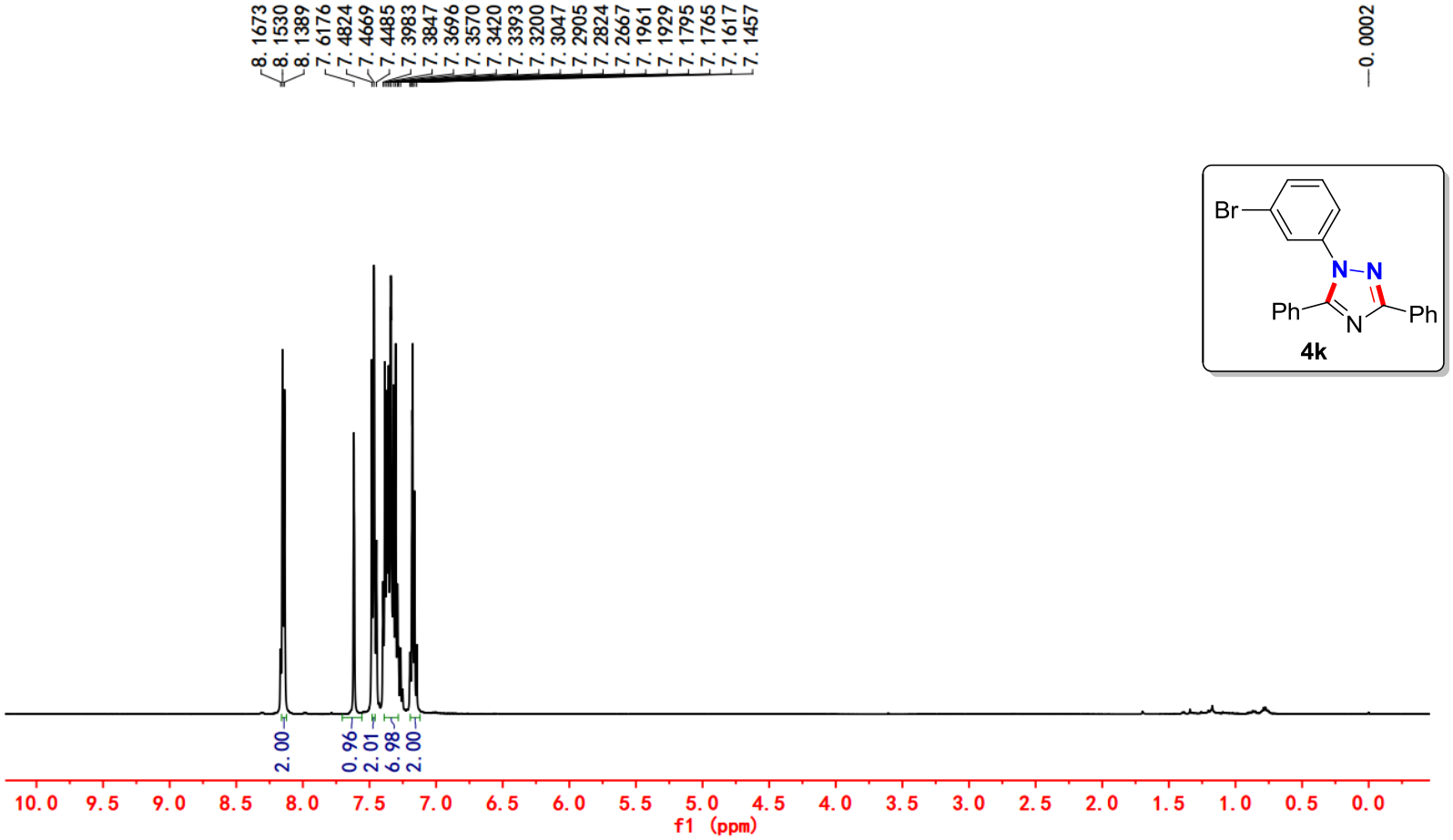
132.76
132.15
130.66
129.78
129.13
128.99
128.93
128.75
128.68
126.68
77.37
77.12
76.87
Cl
Cl
N
N
Ph
Ph
N
4j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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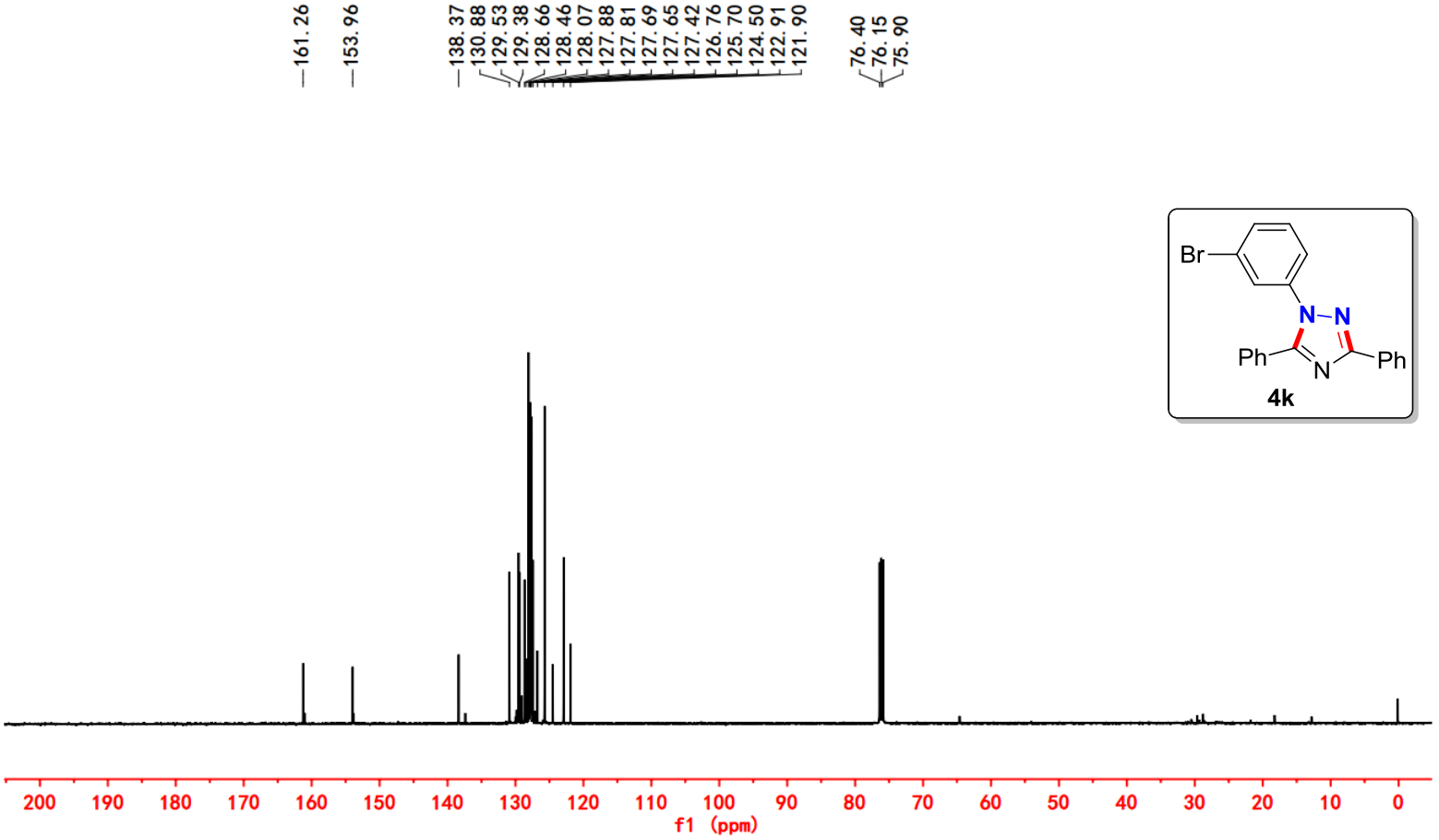
8.1389
7.6176
7.4824
7.4669
7.4485
7.3983
7.3847
7.3696
7.3570
7.3420
7.3393
7.3200
7.3047
7.2905
7.2824
7.2667
7.1961
7.1929
7.1795
7.1765
7.1617
7.1457
0.0002
Br
N
N
Ph
N
Ph
4k
2.00
0.96
2.01
6.98
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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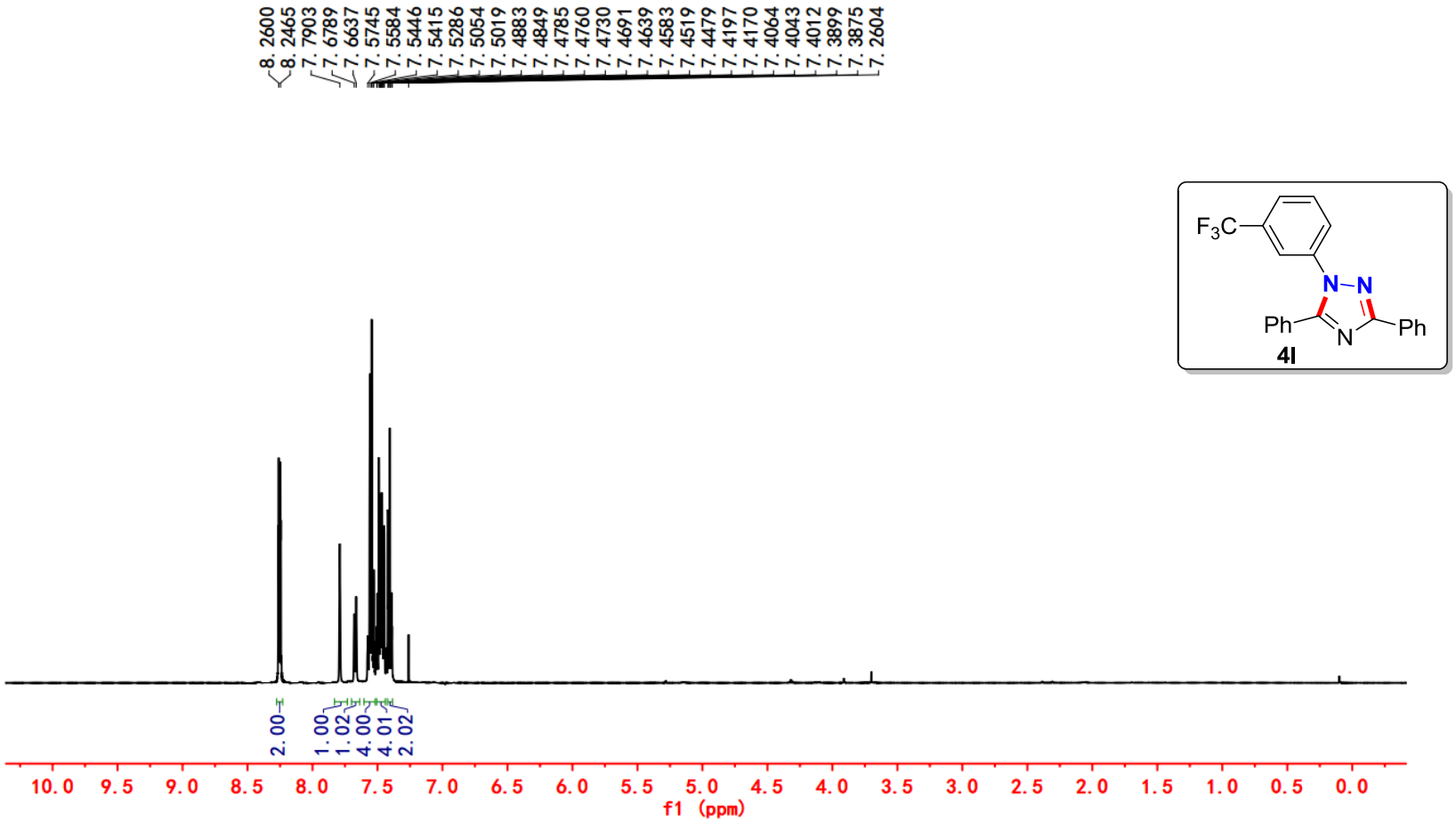
129.38
128.66
128.46
128.07
127.88
127.81
127.69
127.65
127.42
126.76
125.70
124.50
122.91
121.90
76.40
76.15
75.90
Br
N
N
Ph
N
Ph
4k
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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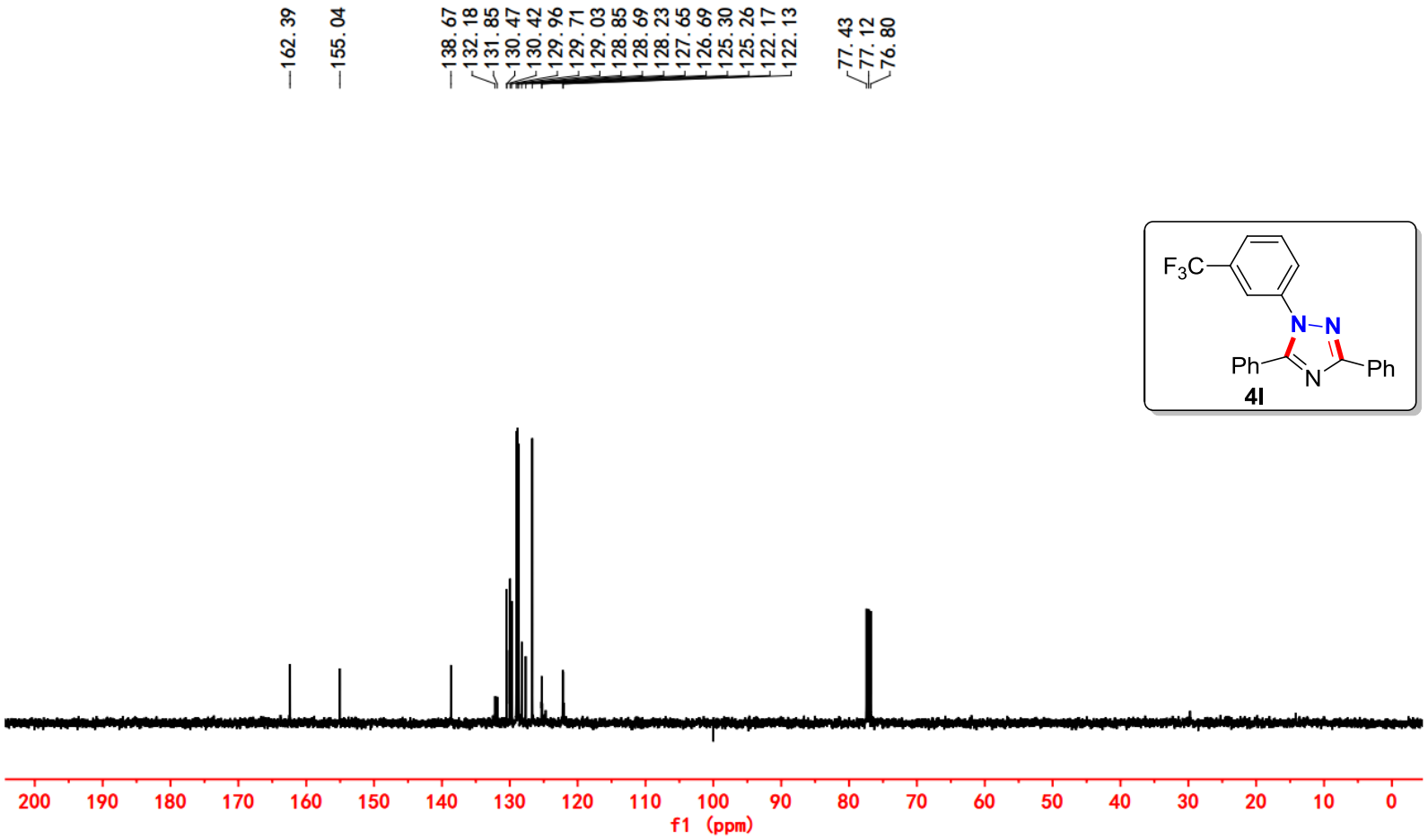
7.5286
7.5054
7.5019
7.4883
7.4849
7.4785
7.4760
7.4730
7.4691
7.4639
7.4583
7.4519
7.4479
7.4197
7.4170
7.4064
7.4043
7.4012
7.3899
7.3875
7.2604
F3C
N
N
Ph
N
Ph
4l
2.00
1.00
1.02
4.00
4.01
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.85
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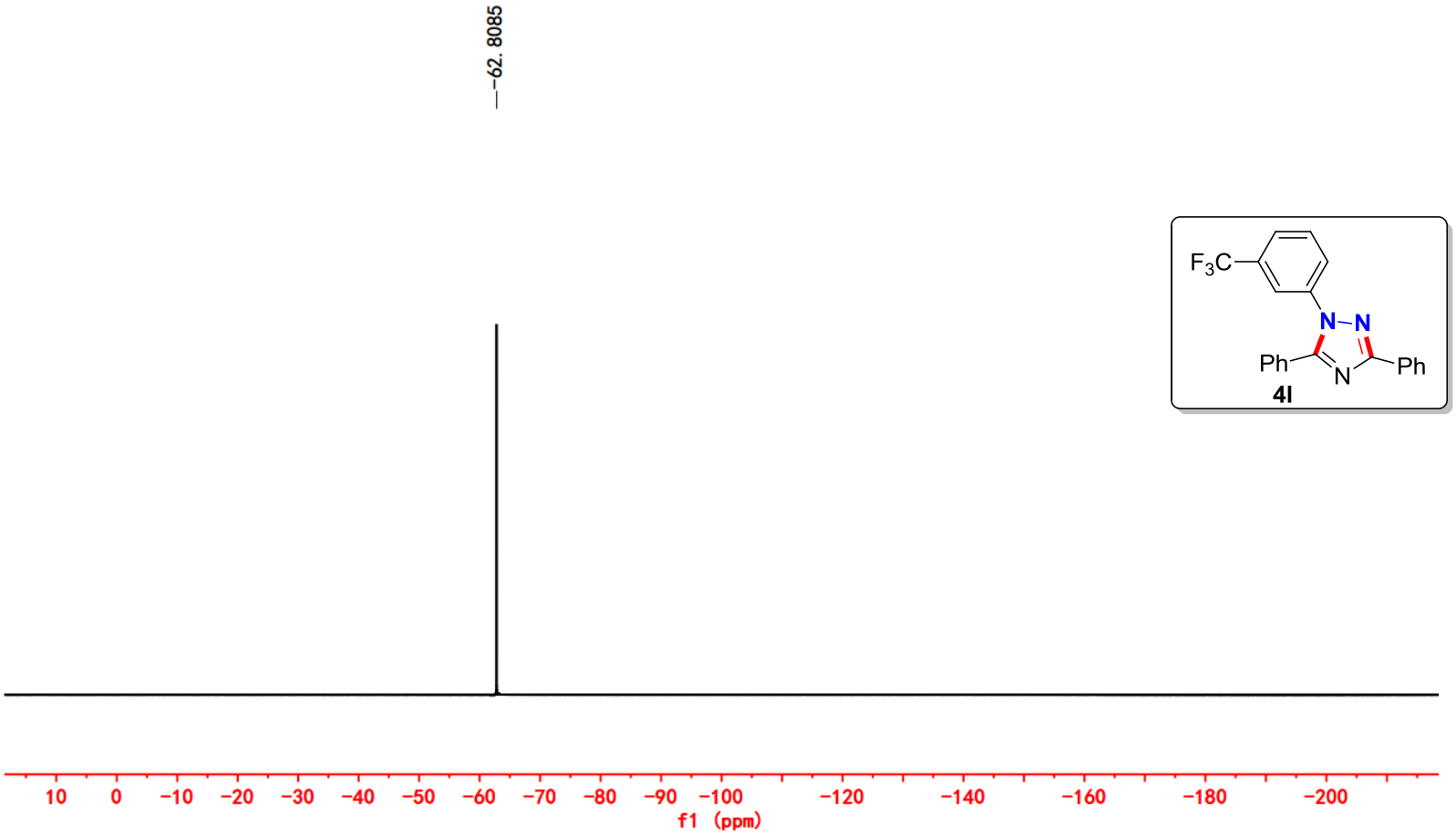
129.71
129.03
128.85
128.69
128.23
127.65
126.69
125.30
125.26
122.17
122.13
77.43
77.12
76.80
F3C
N
N
Ph
N
Ph
4l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-62.8085
F3C
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N
Ph
N
Ph
4l
10
0
-10
-20
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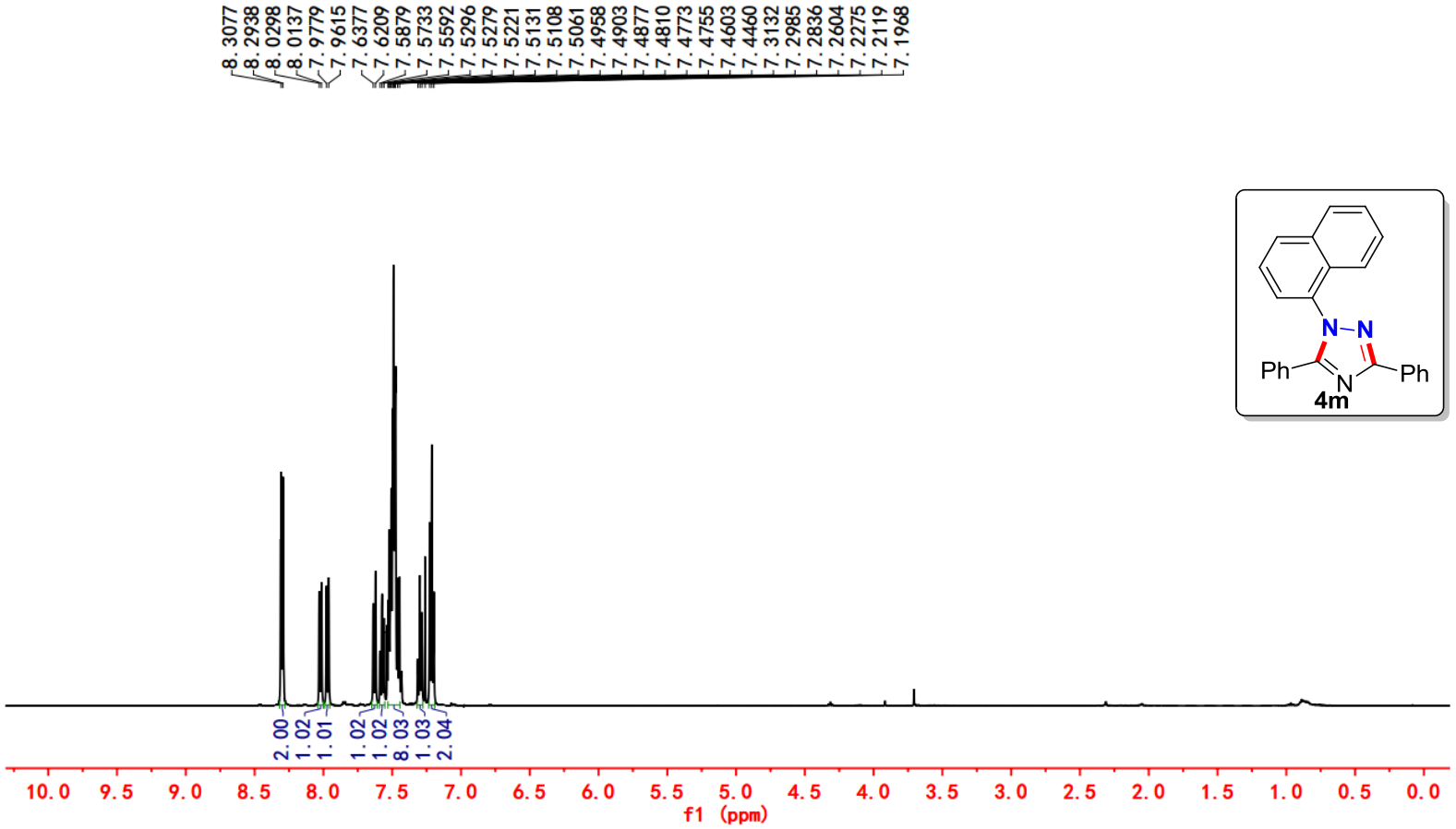
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.9615
7.6377
7.6209
7.5879
7.5733
7.5592
7.5296
7.5279
7.5221
7.5131
7.5108
7.5061
7.4958
7.4903
7.4877
7.4810
7.4773
7.4755
7.4603
7.4460
7.3132
7.2985
7.2836
7.2604
7.2275
7.2119
7.1968
N
N
Ph
Ph
4m
2.00
1.02
1.01
1.02
1.02
8.03
1.03
2.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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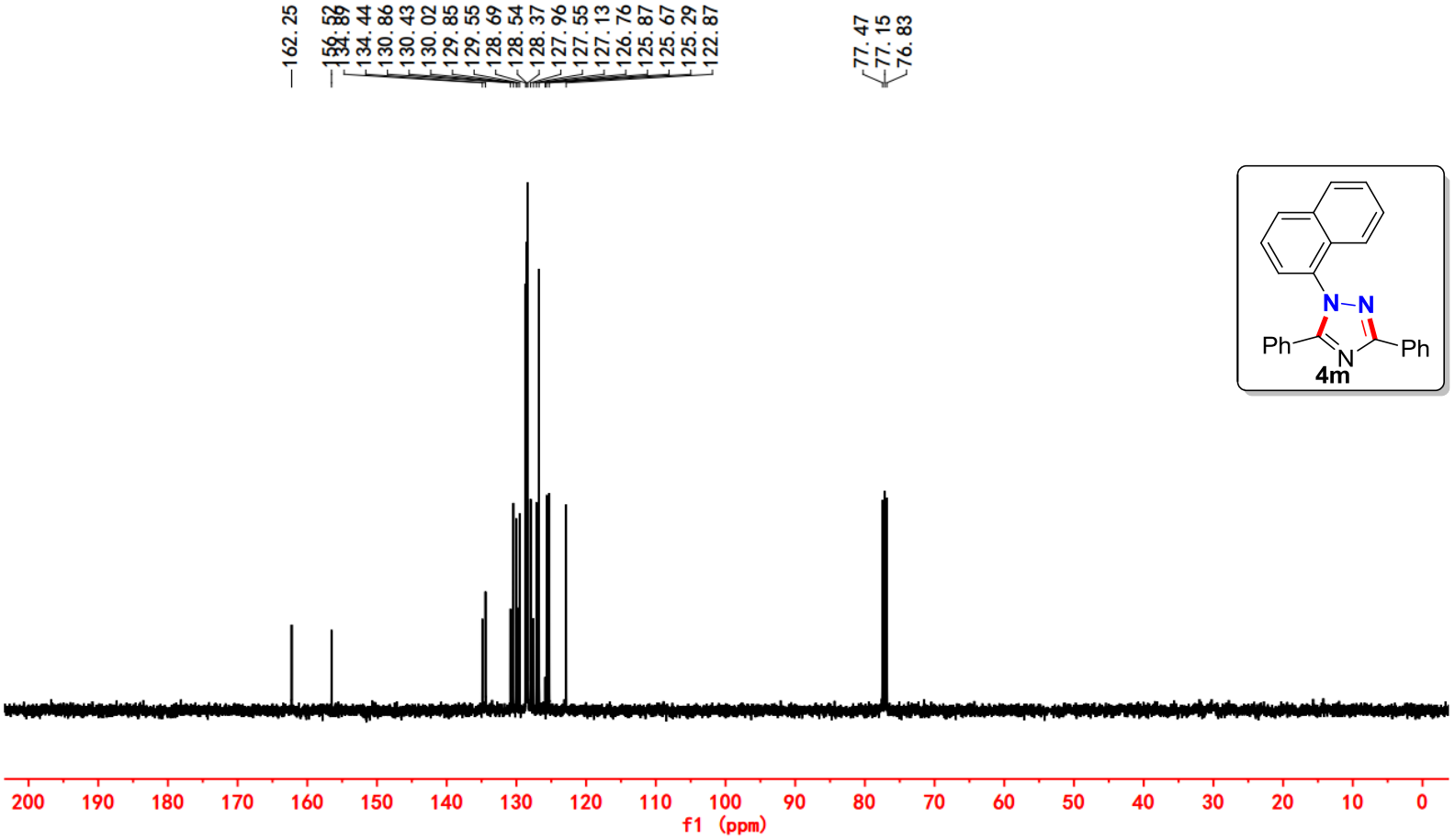
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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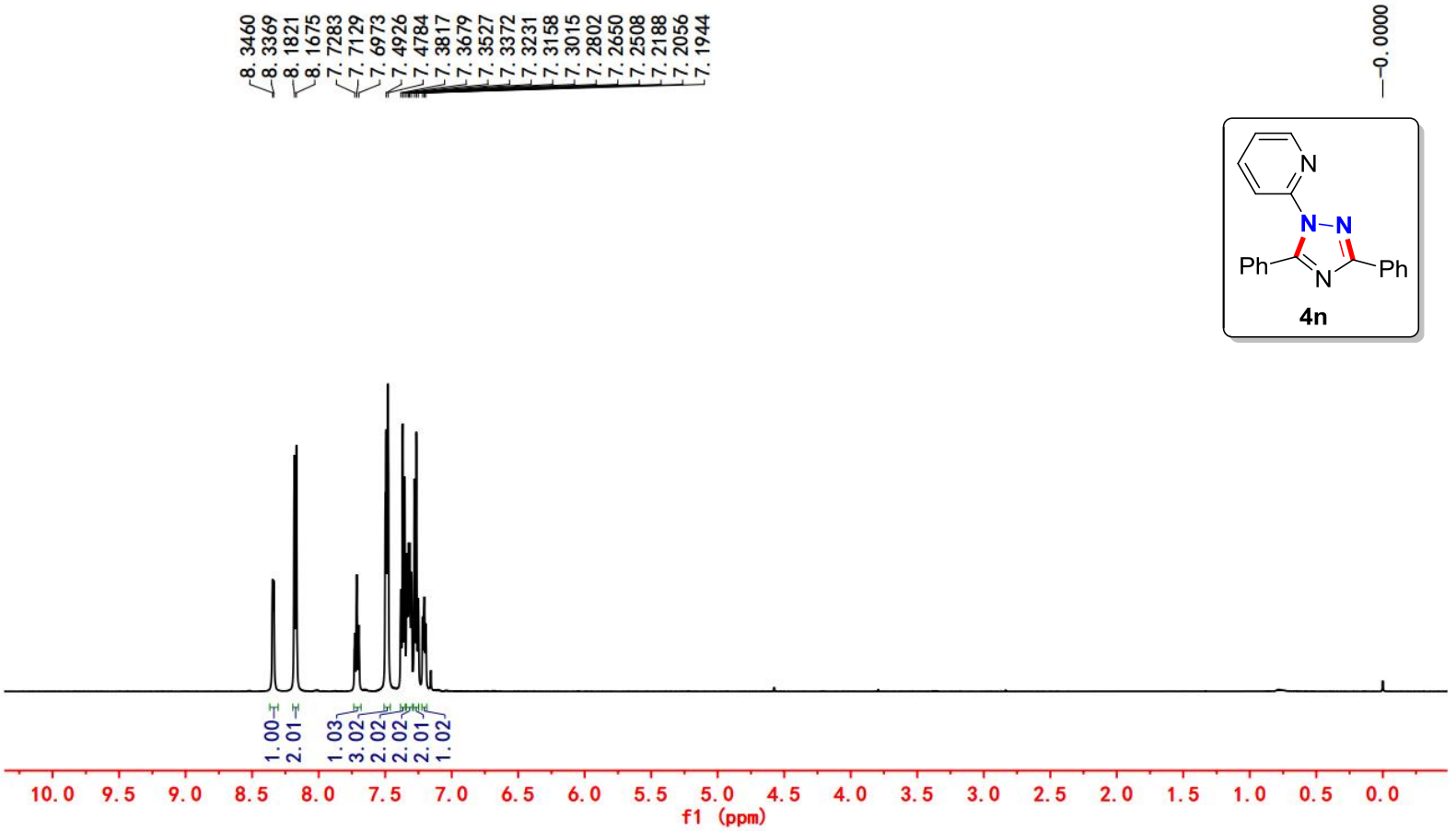
129.55
128.69
128.54
128.37
127.96
127.55
127.13
126.76
125.87
125.67
125.29
122.87
77.47
77.15
76.83
N
N
Ph
Ph
4m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.1675
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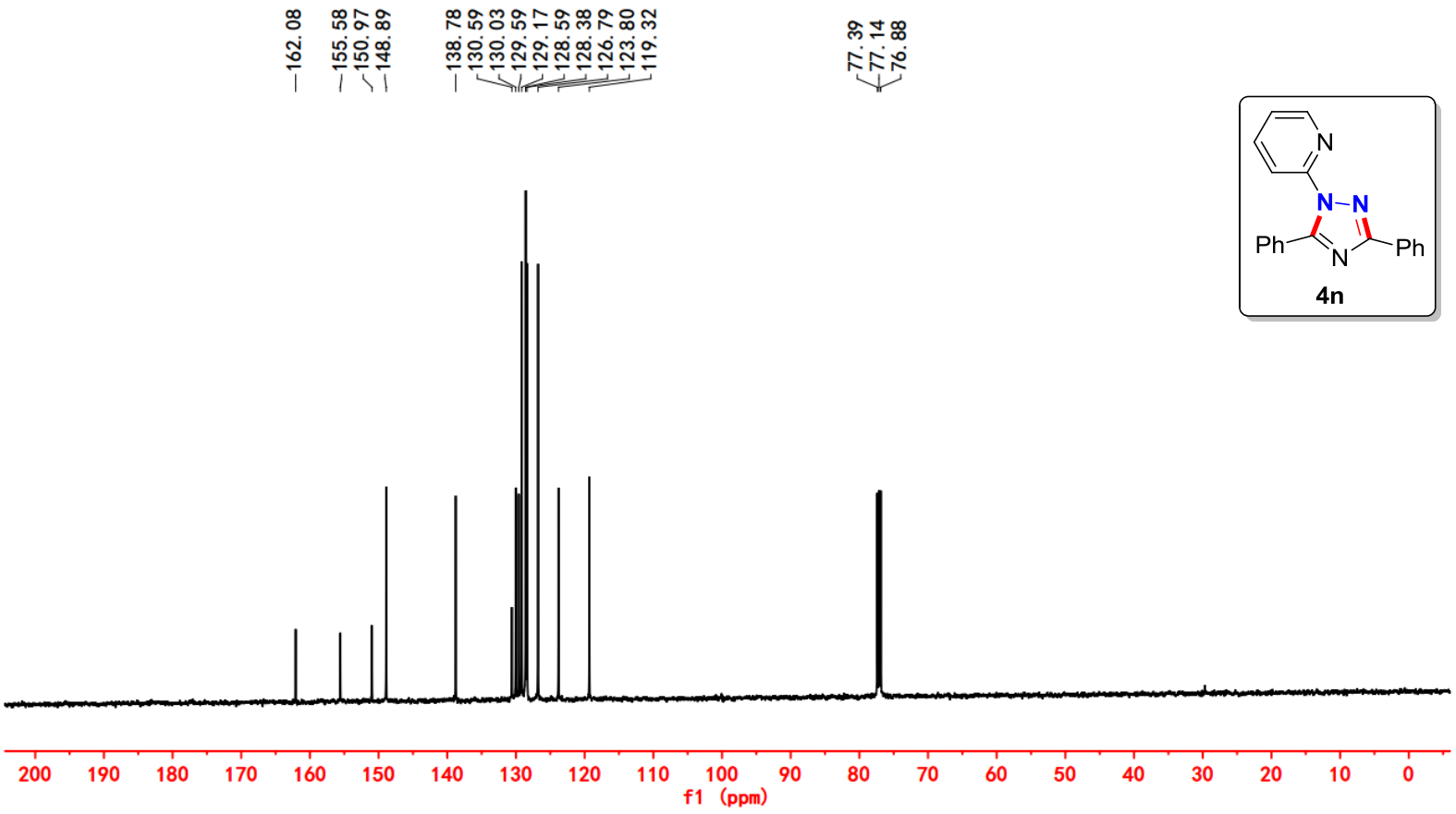
7.7129
7.6973
7.4926
7.4784
7.3817
7.3679
7.3527
7.3372
7.3231
7.3158
7.3015
7.2802
7.2650
7.2508
7.2188
7.2056
7.1944
0.0000
N
N
N
Ph
Ph
4n
1.00
2.01
1.03
3.02
2.02
2.02
2.01
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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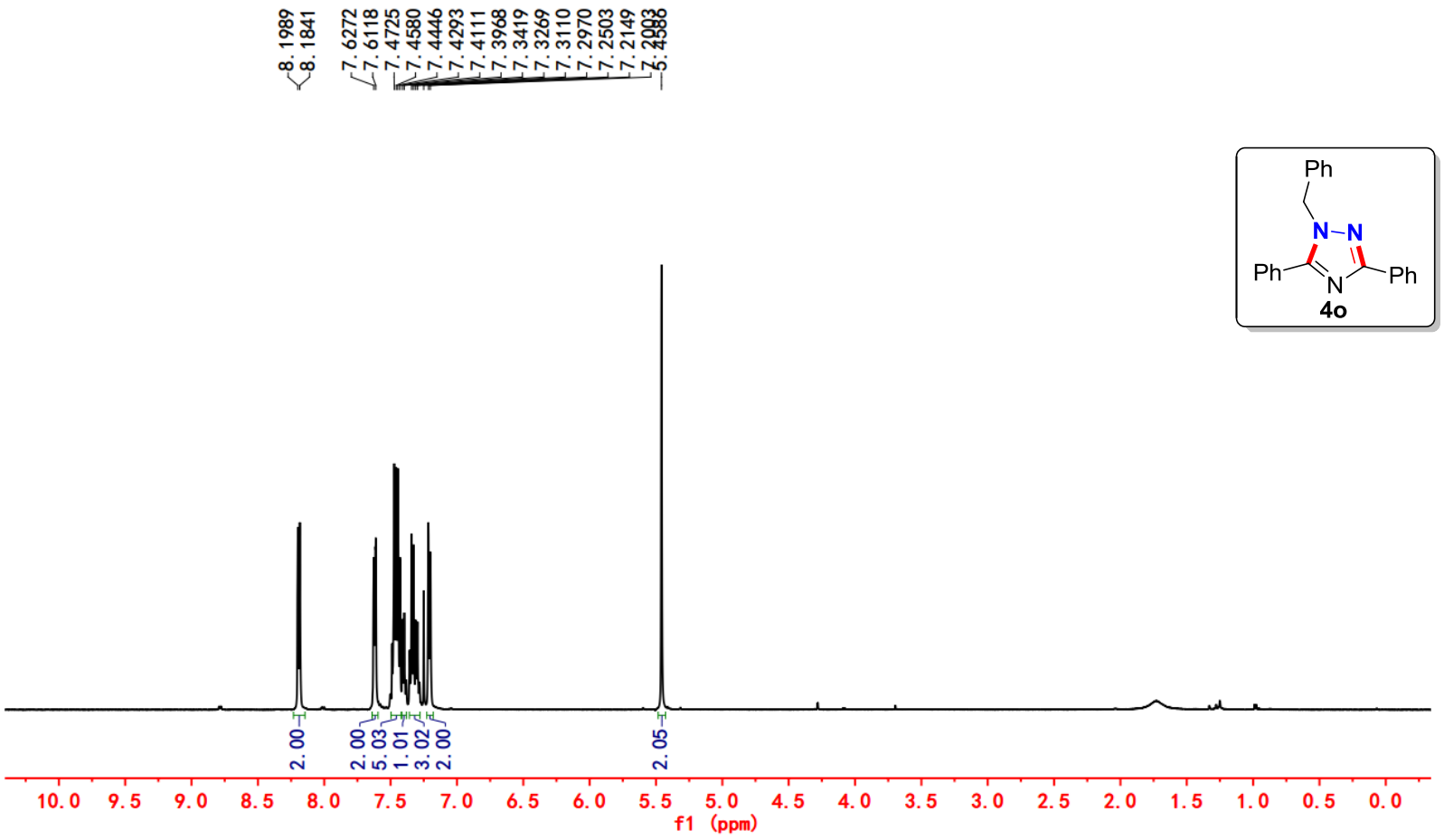
130.59
130.03
129.59
129.17
128.59
128.38
126.79
123.80
119.32
77.39
77.14
76.88
N
N
N
Ph
Ph
4n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3269
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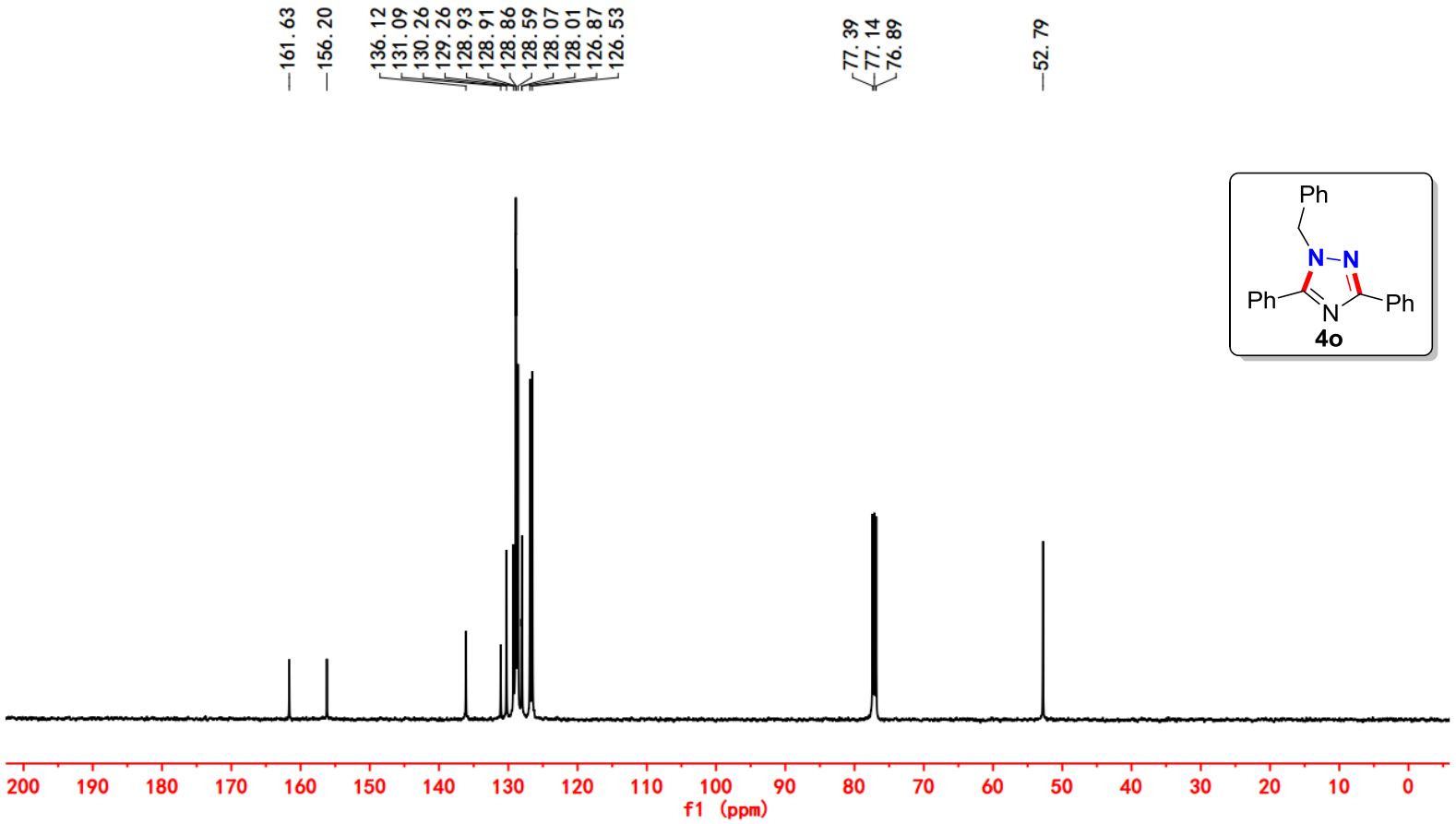
7.2970
7.2503
7.2149
5.4588
Ph
N
N
Ph
Ph
N
4o
2.00
2.00
5.03
1.01
3.02
2.00
2.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.91
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128.59
128.07
128.01
126.87
126.53
77.39
77.14
76.89
52.79
Ph
N
N
Ph
Ph
N
4o
200
190
180
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150
140
130
120
110
100
90
80
70
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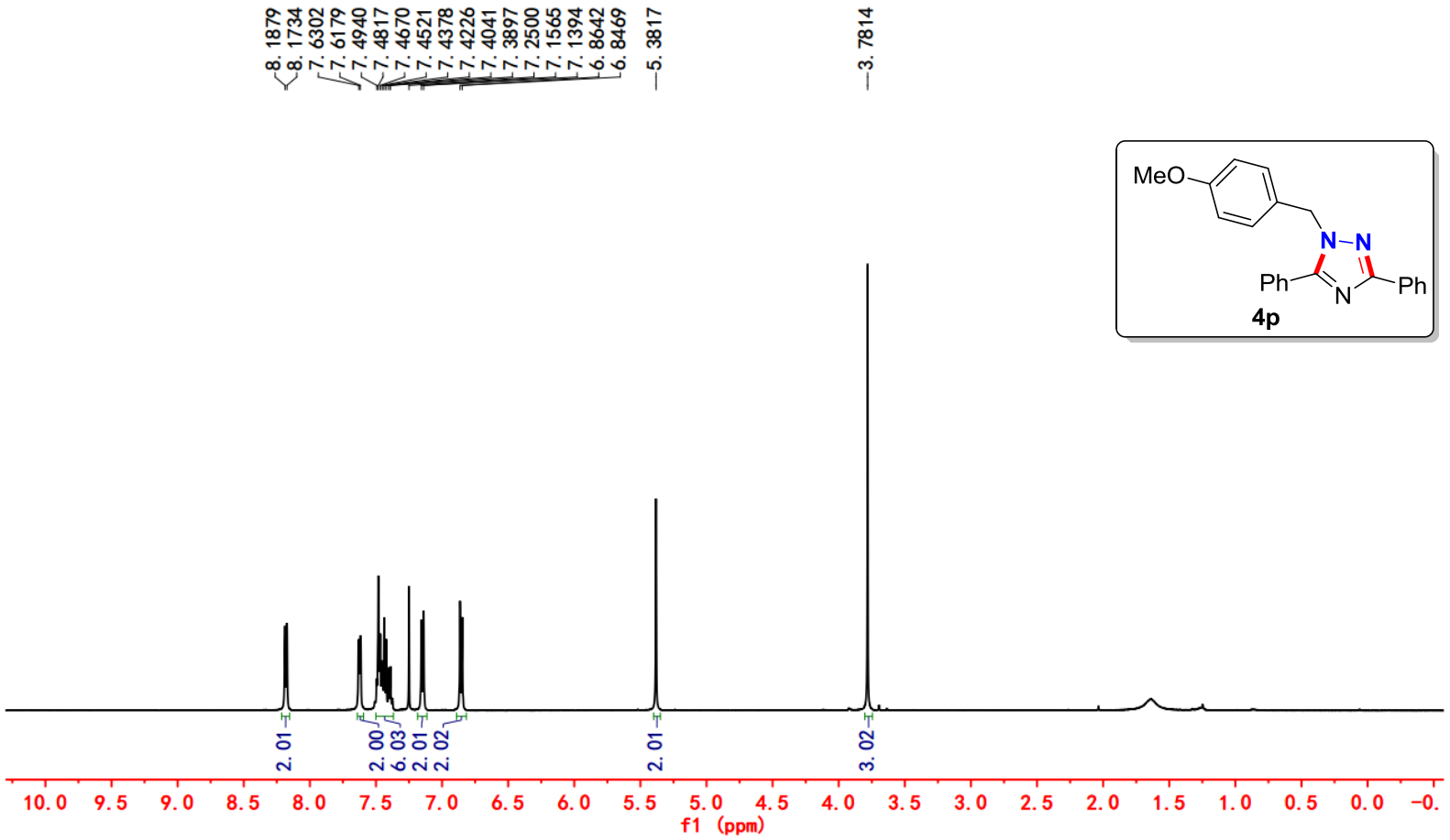
50
40
30
20
10
0
f1 (ppm)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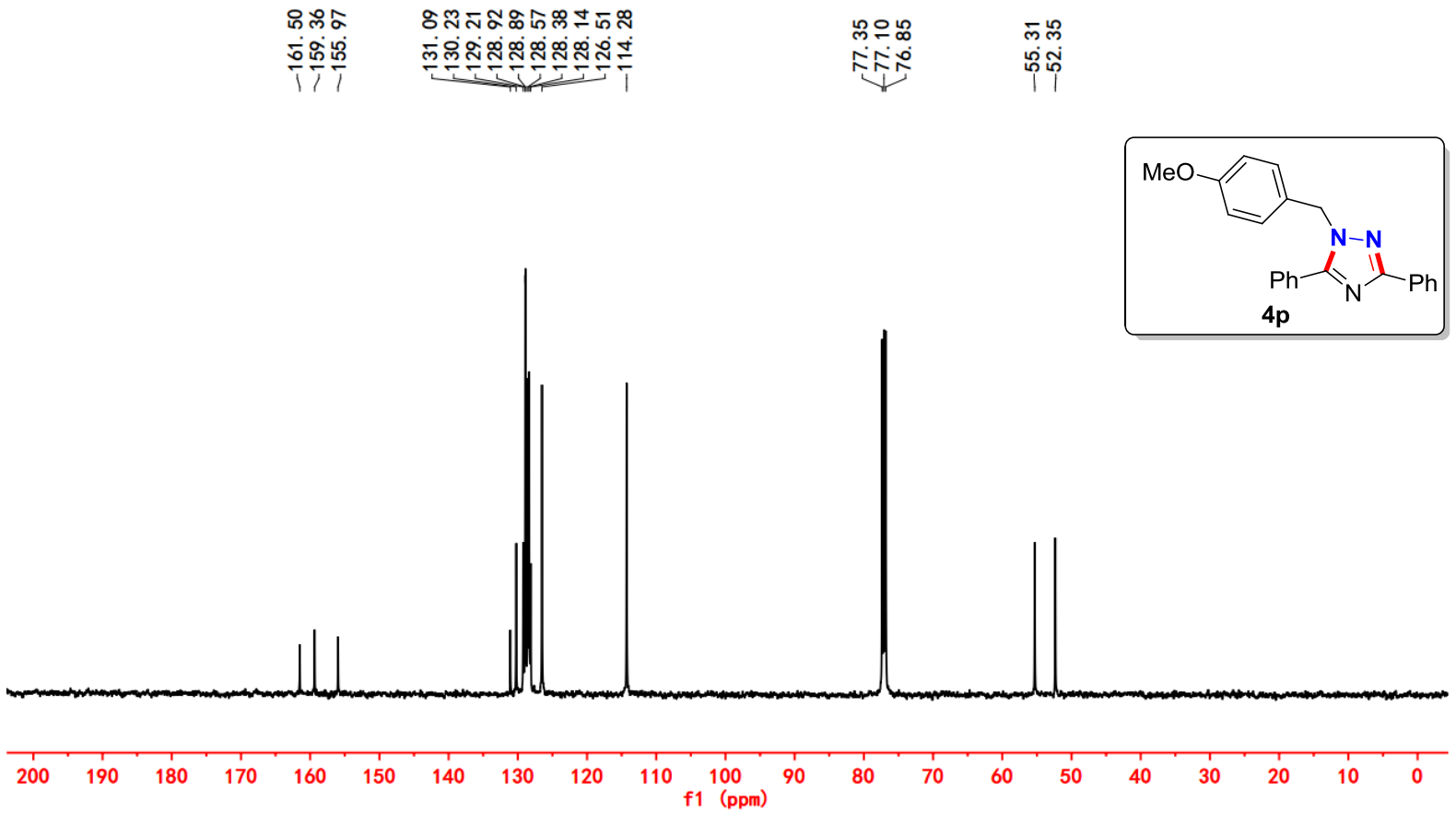
7.4670
7.4521
7.4378
7.4226
7.4041
7.3897
7.2500
7.1565
7.1394
6.8642
6.8469
5.3817
3.7814
MeO
N
N
Ph
N
Ph
4p
2.01
2.00
6.03
2.01
2.02
2.01
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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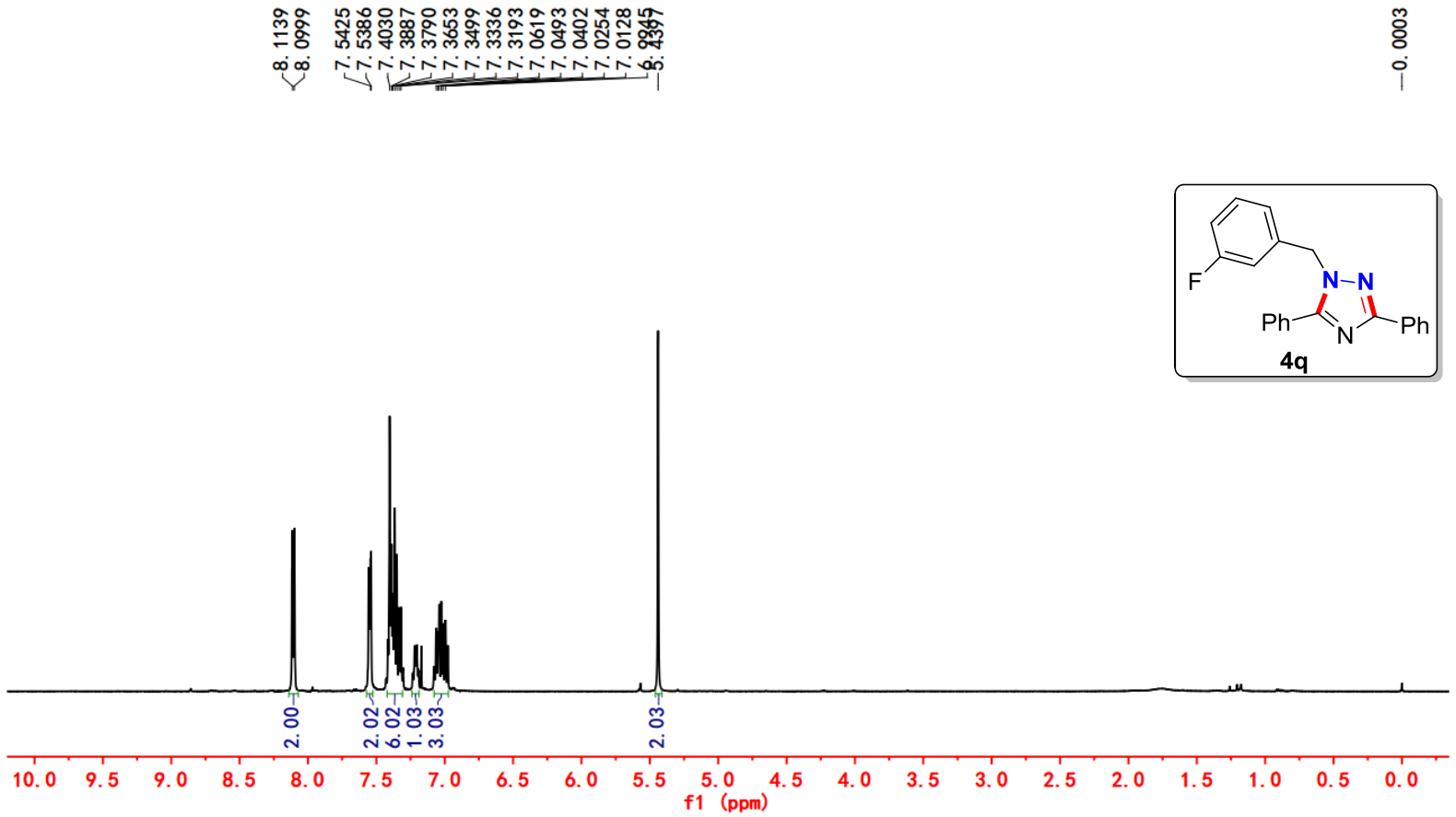
128.89
128.57
128.38
128.14
126.51
114.28
77.35
77.10
76.85
55.31
52.35
MeO
N
N
Ph
N
Ph
4p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.3499
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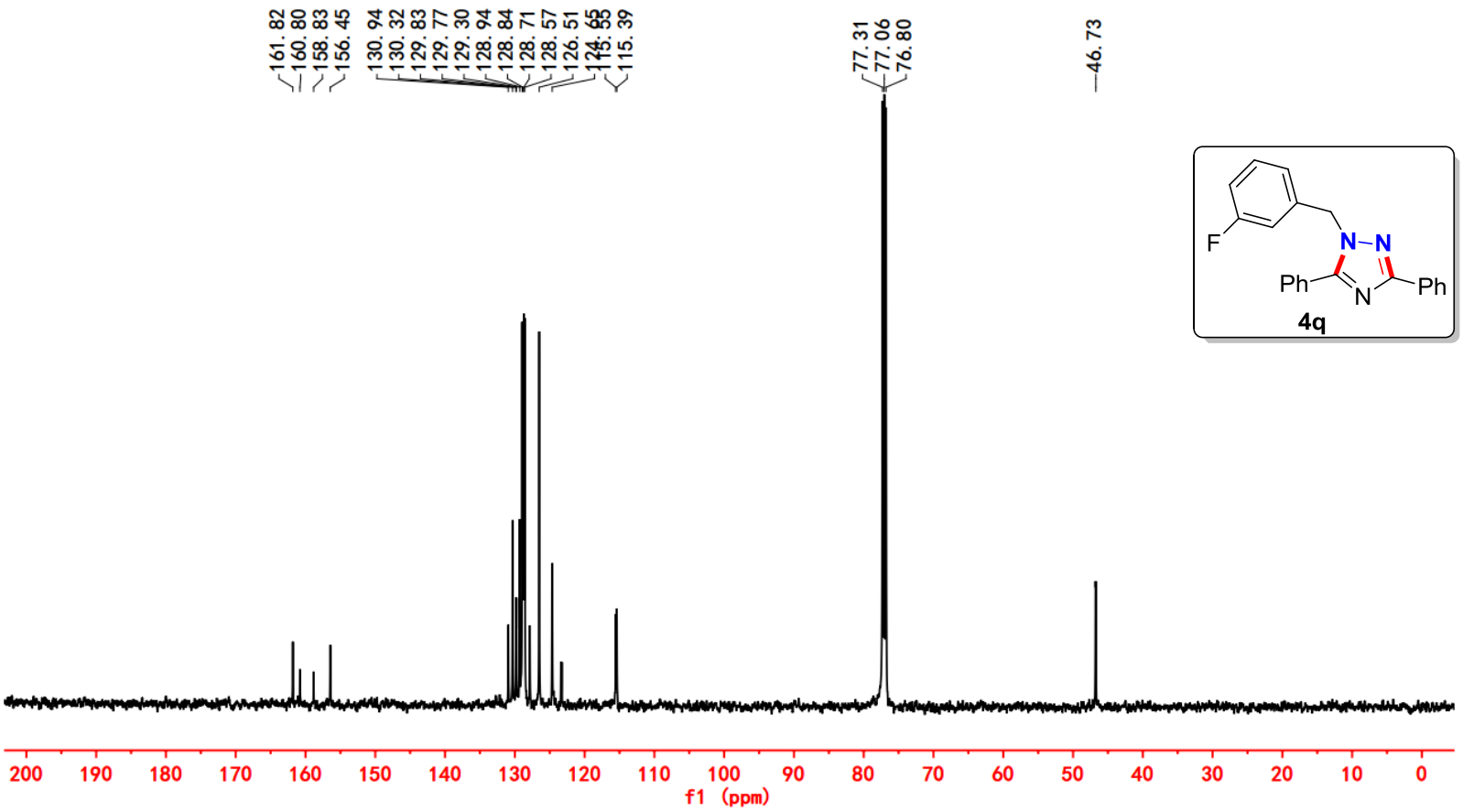
7.3193
7.0619
7.0493
7.0402
7.0254
7.0128
5.4397
0.0003
F
N
N
Ph
N
Ph
4q
2.00
2.02
6.02
1.03
3.03
2.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.71
128.57
126.51
124.65
115.55
115.39
77.31
77.06
76.80
46.73
F
N
N
Ph
N
Ph
4q
200
190
180
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150
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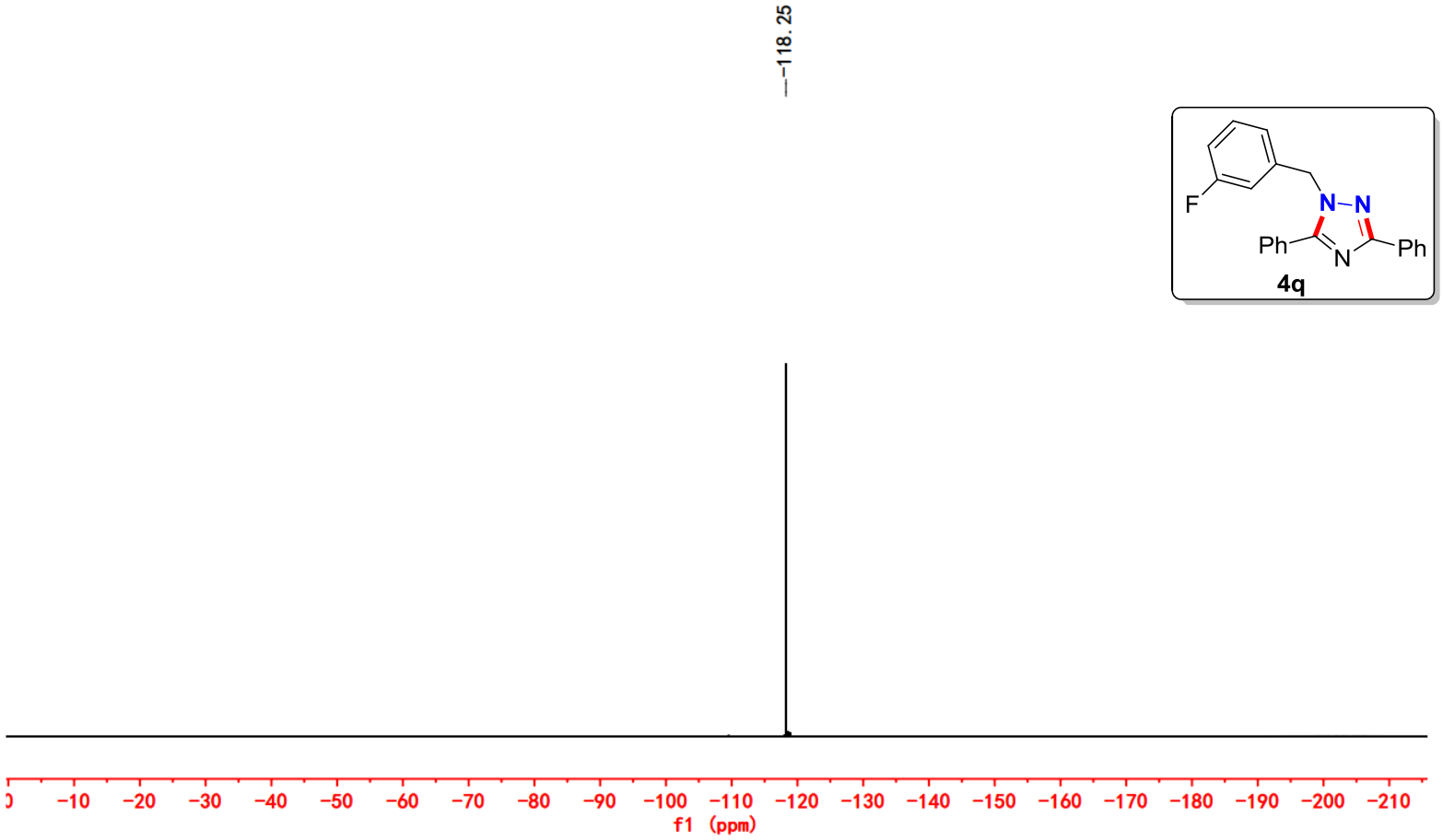
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


−118.25
F
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N
Ph
N
Ph
4q
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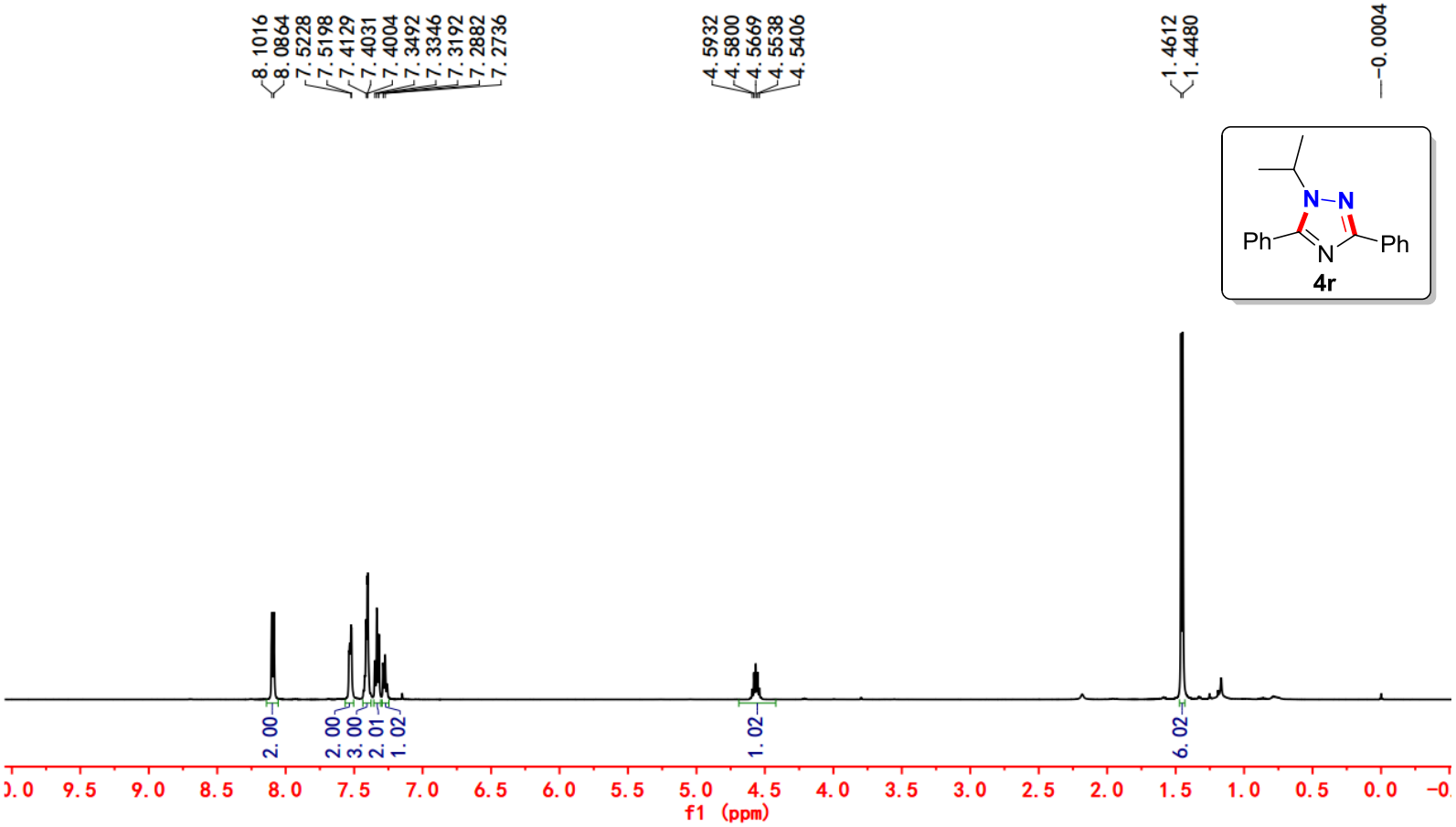
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)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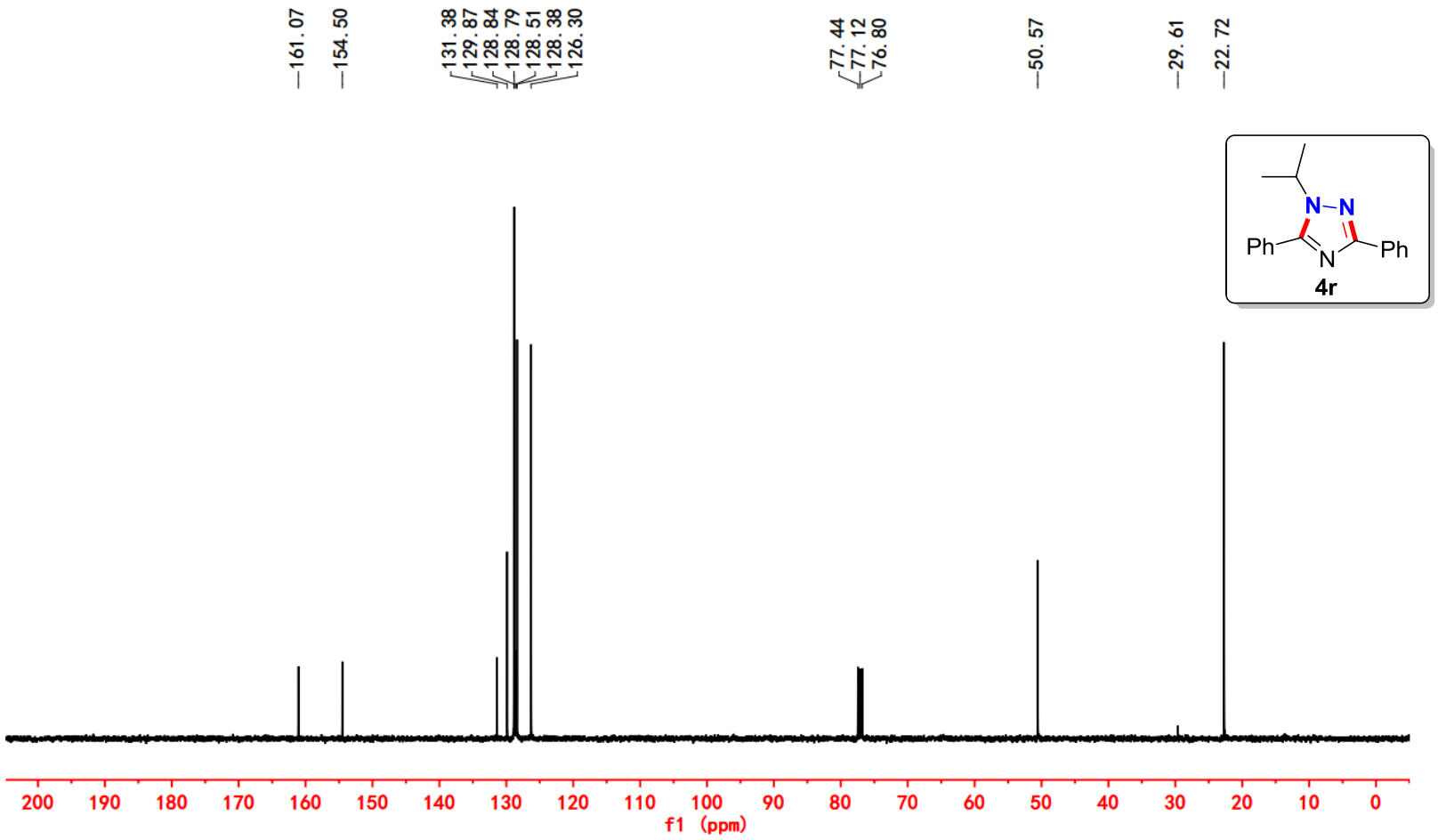
7.4129
7.4031
7.4004
7.3492
7.3346
7.3192
7.2882
7.2736
4.5932
4.5800
4.5669
4.5538
4.5406
1.4612
1.4480
-0.0004
Ph
N
N
Ph
4r
2.00
2.00
3.00
2.01
1.02
1.02
6.02
f1 (ppm)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131.38
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128.84
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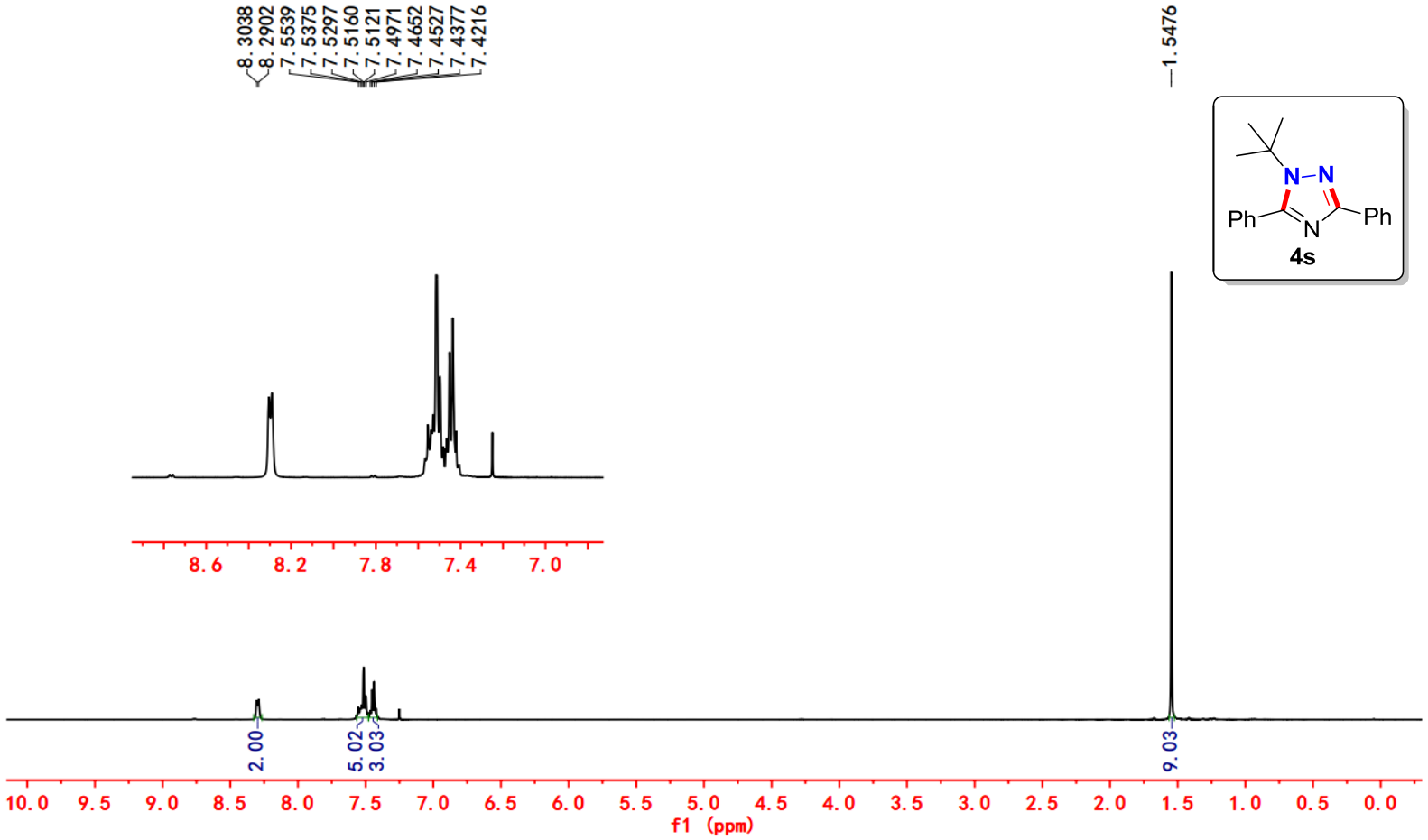
128.51
128.38
126.30
77.44
77.12
76.80
50.57
29.61
22.72
N
N
Ph
N
Ph
4r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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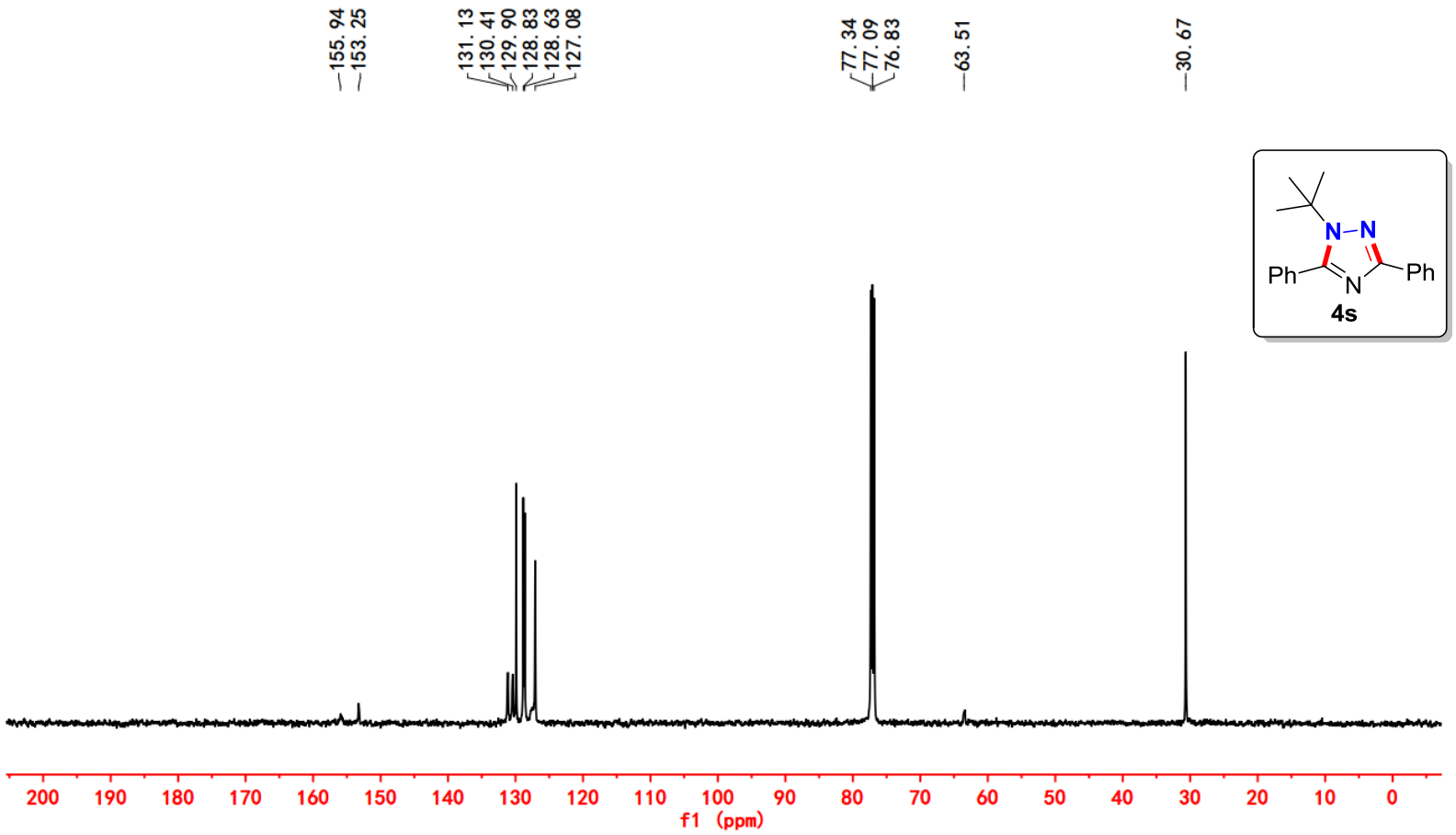
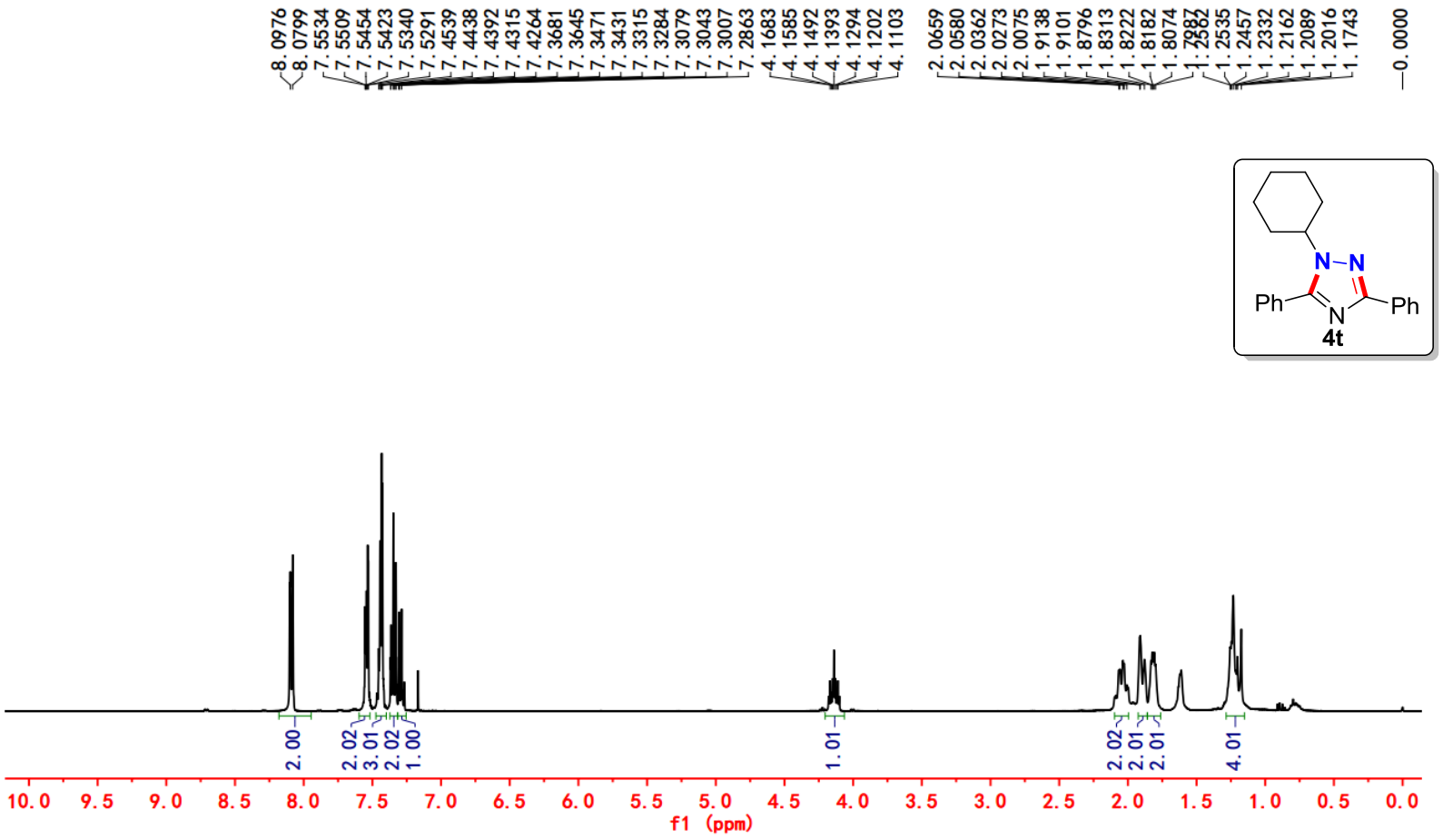
8.2902
7.5539
7.5375
7.5297
7.5160
7.5121
7.4971
7.4652
7.4527
7.4377
7.4216
1.5476
N–N
Ph
Ph
N
4s
8.6
8.2
7.8
7.4
7.0
2.00
5.02
3.03
9.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.94
153.25
131.13
130.41
129.90
128.83
128.63
127.08
77.34
77.09
76.83
63.51
30.67
N
N
Ph
Ph
N
4s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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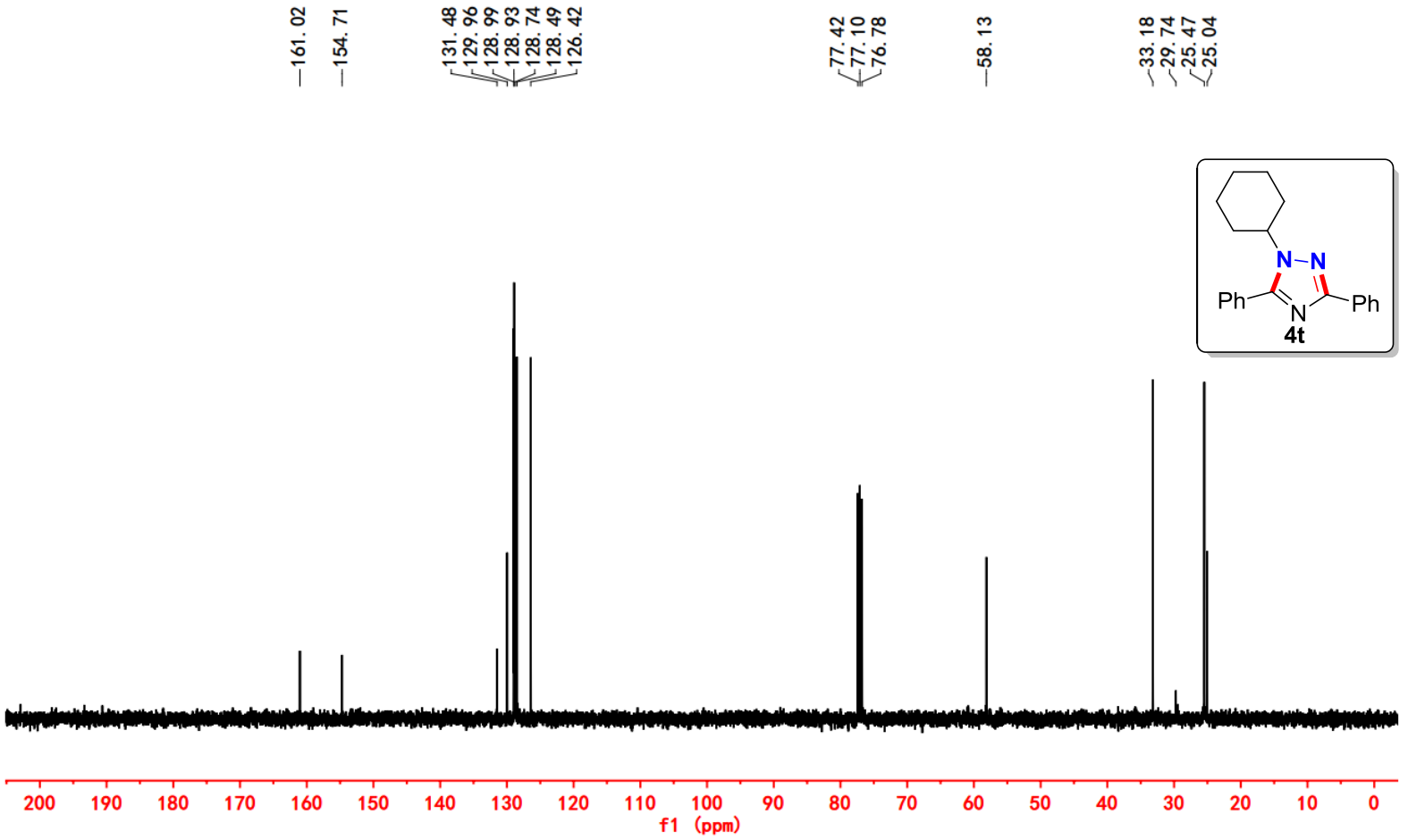
8.0799
7.5534
7.5509
7.5454
7.5423
7.5340
7.5291
7.4539
7.4438
7.4392
7.4315
7.4264
7.3681
7.3645
7.3471
7.3431
7.3315
7.3284
7.3079
7.3043
7.3007
7.2863
4.1683
4.1585
4.1492
4.1393
4.1294
4.1202
4.1103
2.0659
2.0580
2.0362
2.0273
2.0075
1.9138
1.9101
1.8796
1.8313
1.8222
1.8182
1.8074
1.2535
1.2457
1.2332
1.2162
1.2089
1.2016
1.1743
0.0000
N
N
Ph
Ph
N
4t
2.00
2.02
3.01
2.02
1.00
1.01
2.02
2.01
2.01
4.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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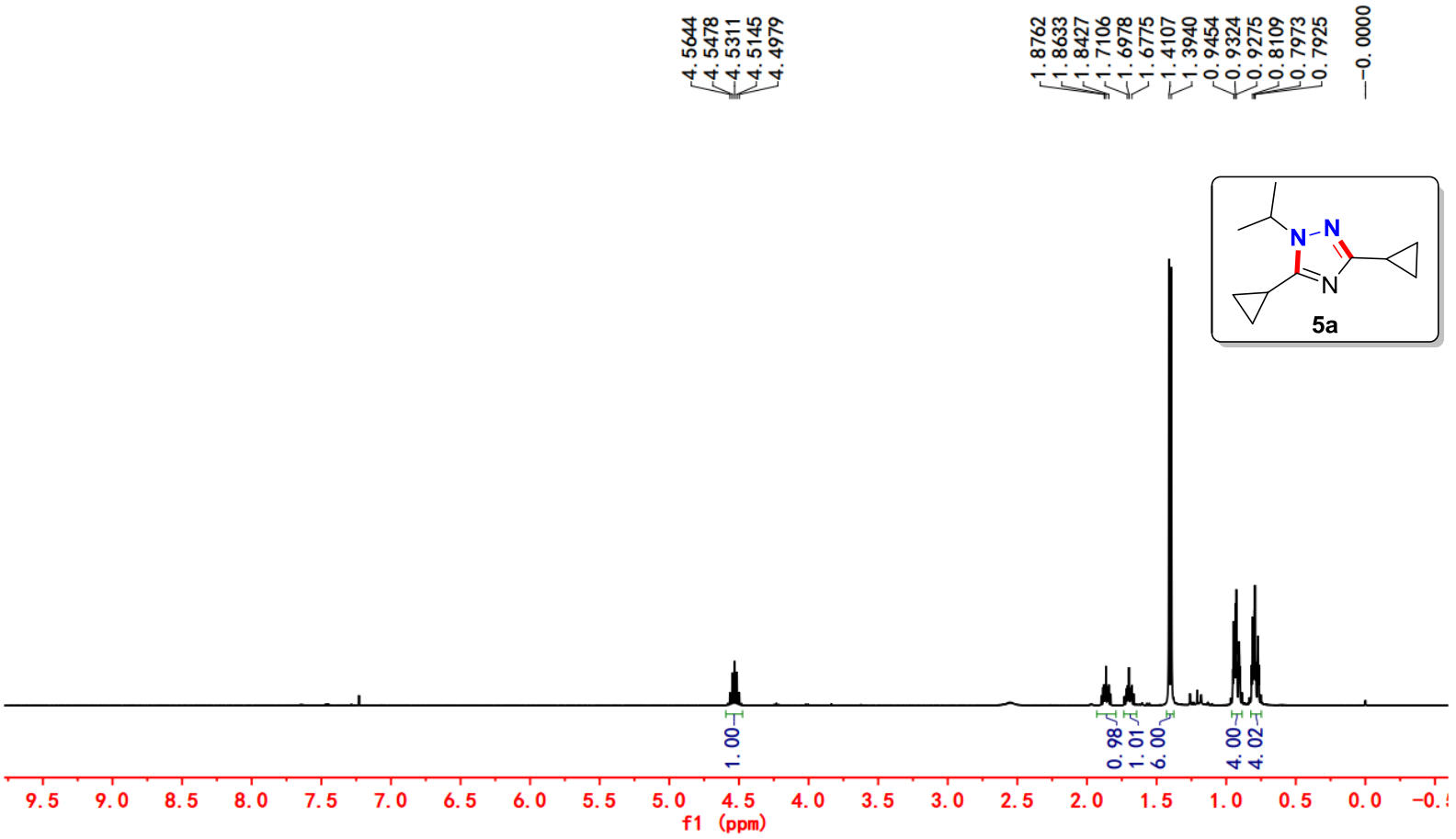
154.71
131.48
129.96
128.99
128.93
128.74
128.49
126.42
77.42
77.10
76.78
58.13
33.18
29.74
25.47
25.04
N
N
Ph
Ph
4t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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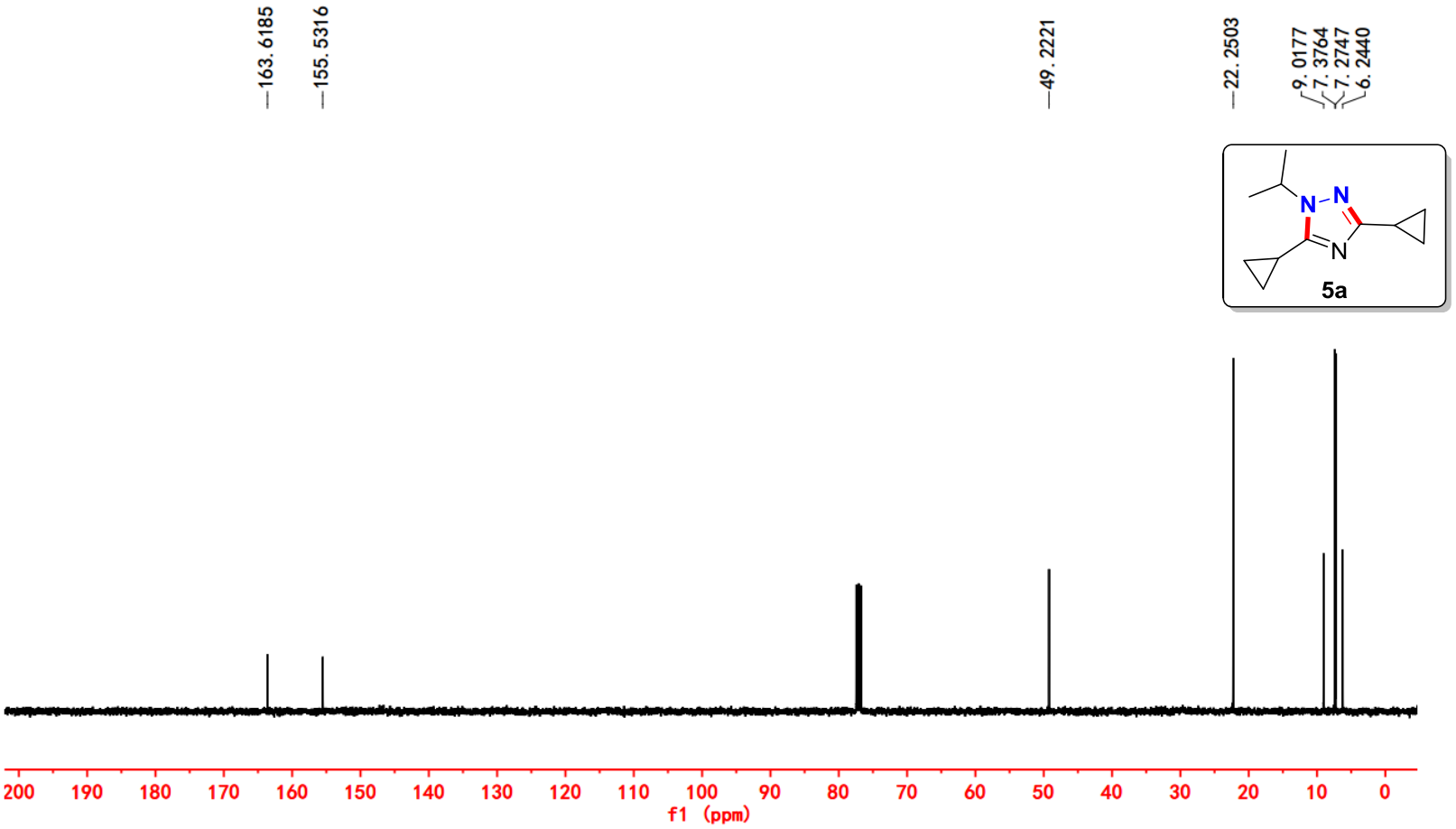
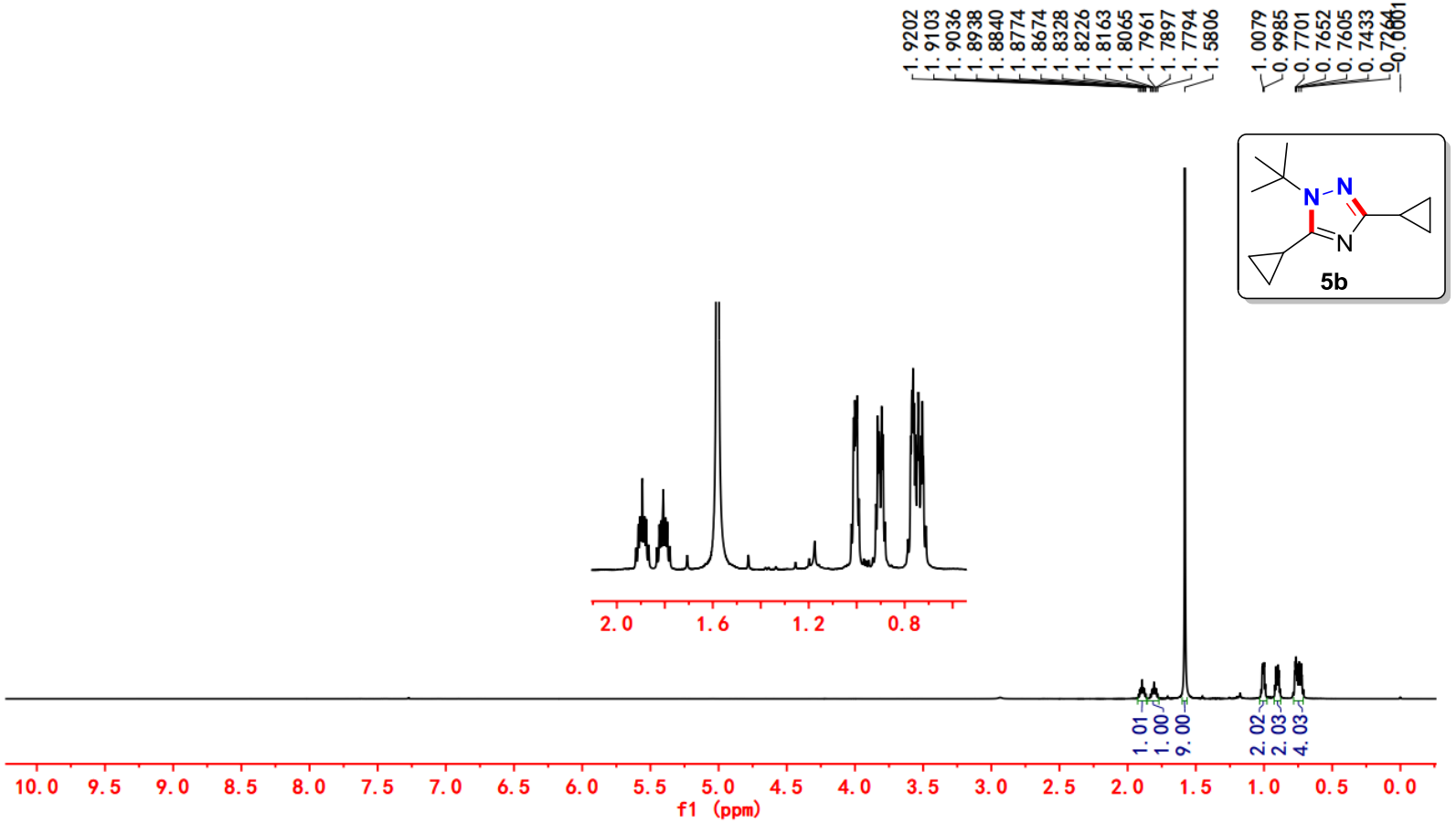
4.5478
4.5311
4.5145
4.4979
1.8762
1.8633
1.8427
1.7106
1.6978
1.6775
1.4107
1.3940
0.9454
0.9324
0.9275
0.8109
0.7973
0.7925
0.0000
5a
1.00
0.98
1.01
6.00
4.00
4.02
f1 (ppm)


163.6185
155.5316
49.2221
22.2503
9.0177
7.3764
7.2747
6.2440
N
N
N
5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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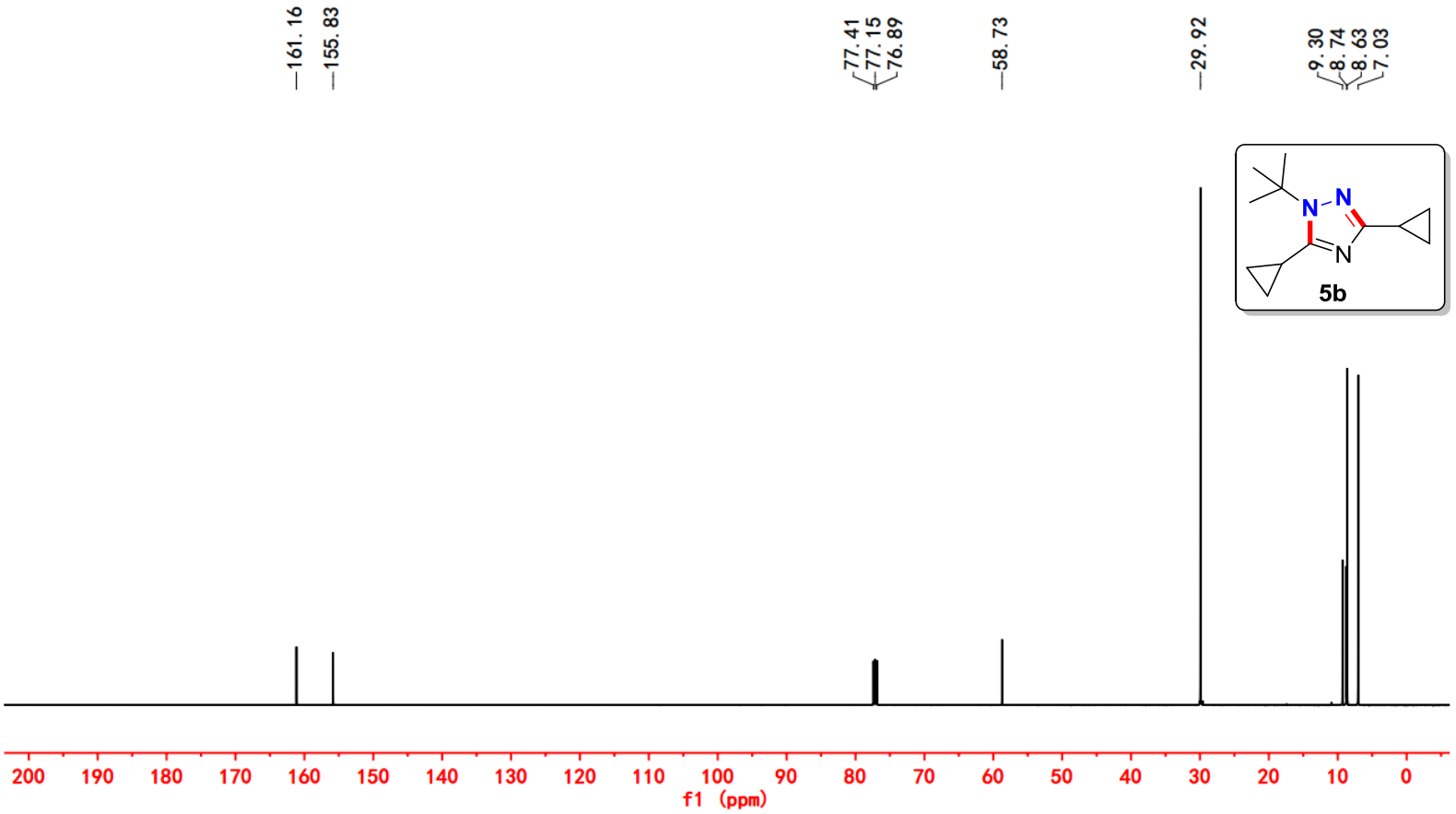
1.9103
1.9036
1.8938
1.8840
1.8774
1.8674
1.8328
1.8226
1.8163
1.8065
1.7961
1.7897
1.7794
1.5806
1.0079
0.9985
0.7701
0.7652
0.7605
0.7433
0.7264
0.0001
N
N
N
5b
2.0
1.6
1.2
0.8
1.01
1.00
9.00
2.02
2.03
4.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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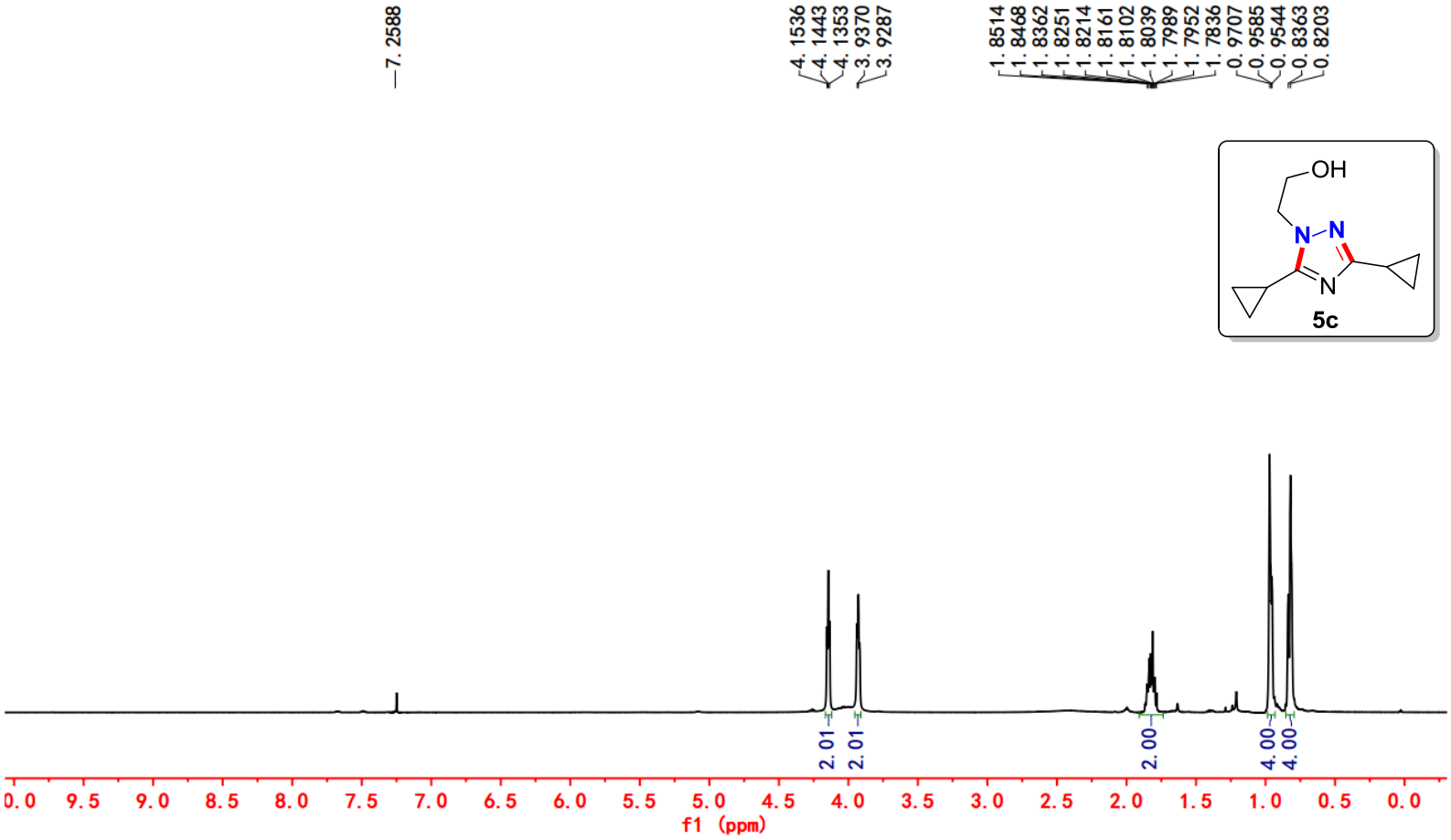
155.83
77.41
77.15
76.89
58.73
29.92
9.30
8.74
8.63
7.03
N
N
N
5b
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.1443
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3.9370
3.9287
1.8514
1.8468
1.8362
1.8251
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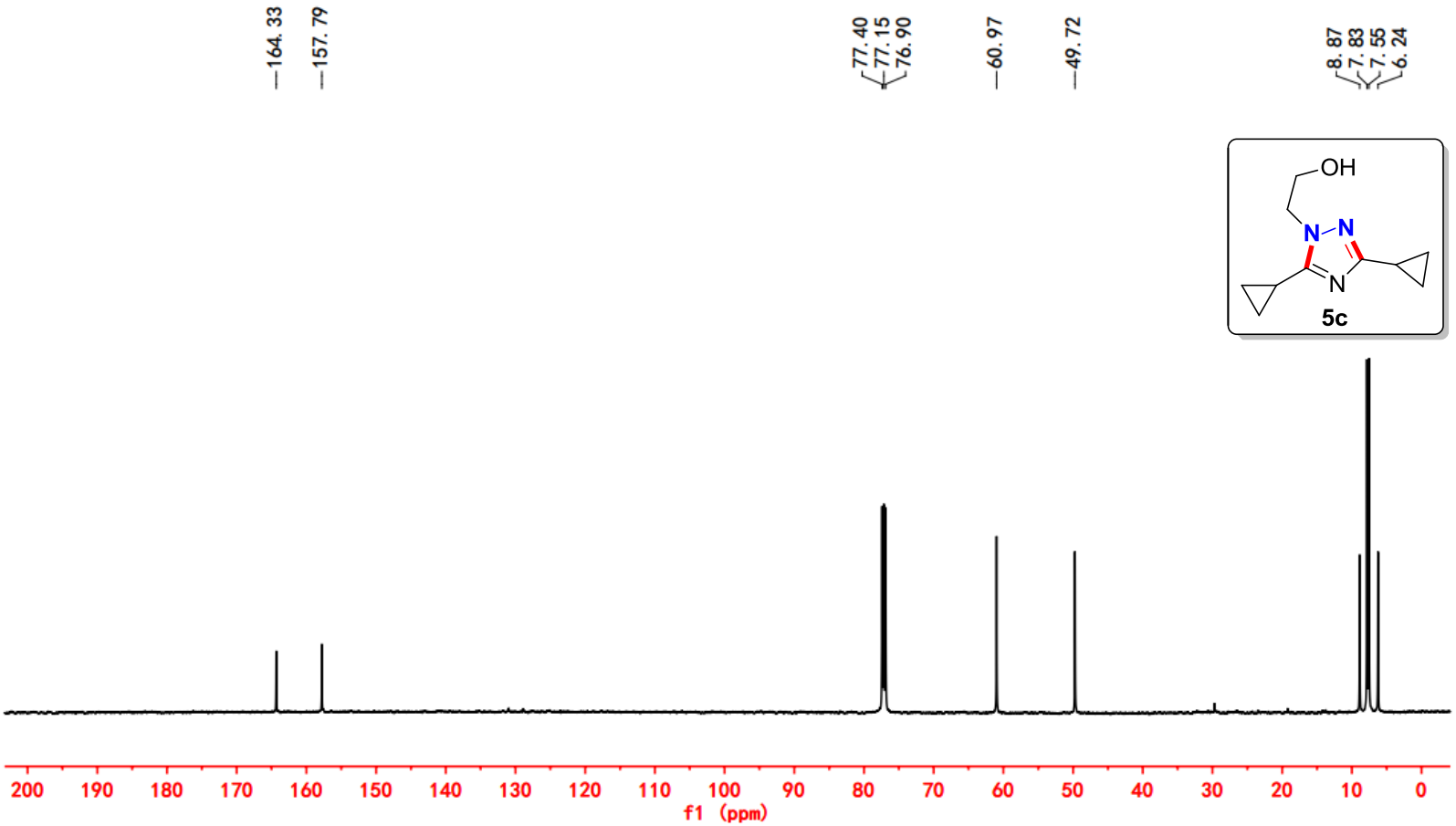
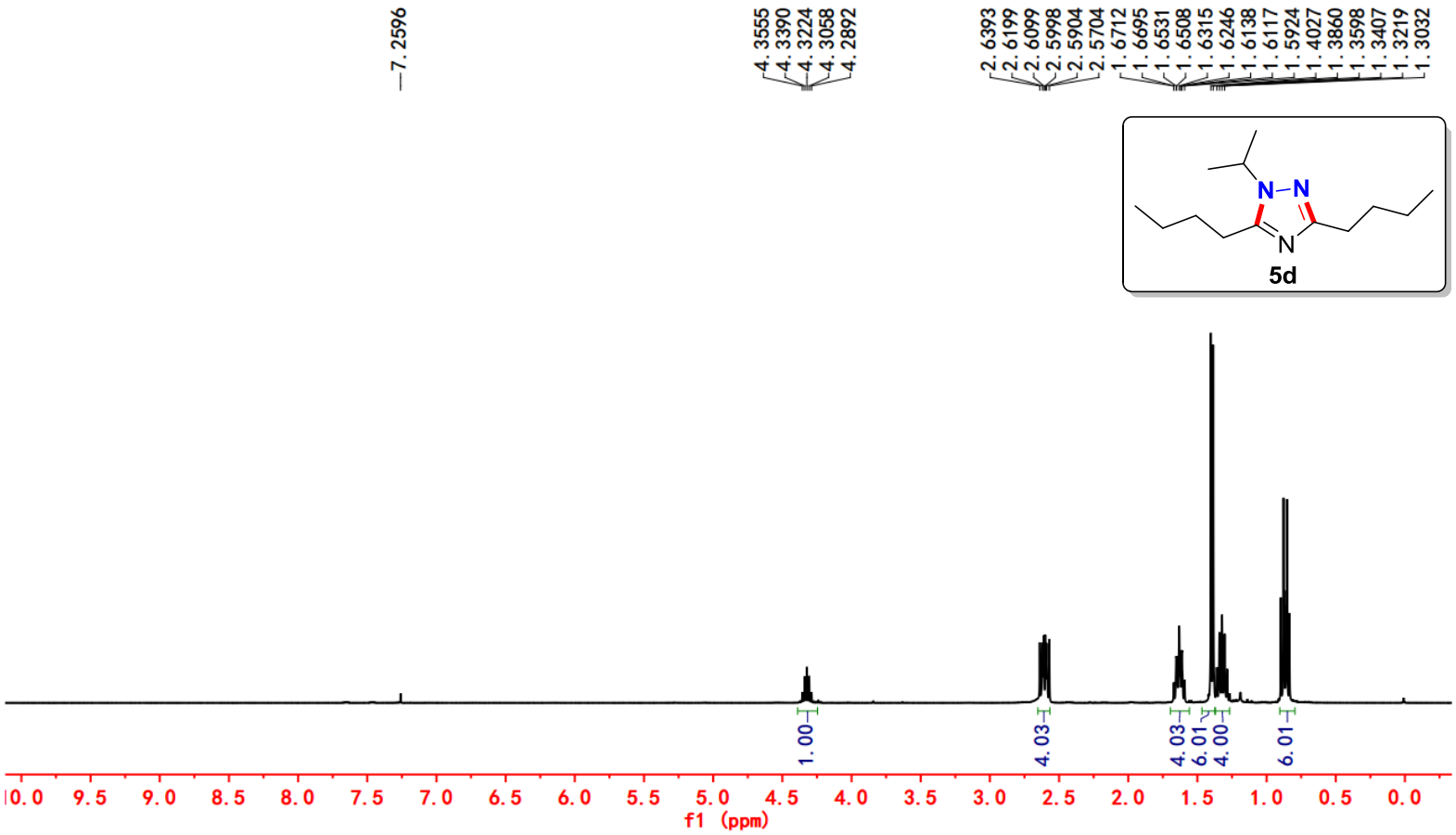
1.8161
1.8102
1.8039
1.7989
1.7952
1.7836
0.9707
0.9585
0.9544
0.8363
0.8203
OH
N
N
N
5c
2.01
2.01
2.00
4.00
4.00
f1 (ppm)


164.33
157.79
77.40
77.15
76.90
60.97
49.72
8.87
7.83
7.55
6.24
OH
N
N
N
5c
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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4.3058
4.2892
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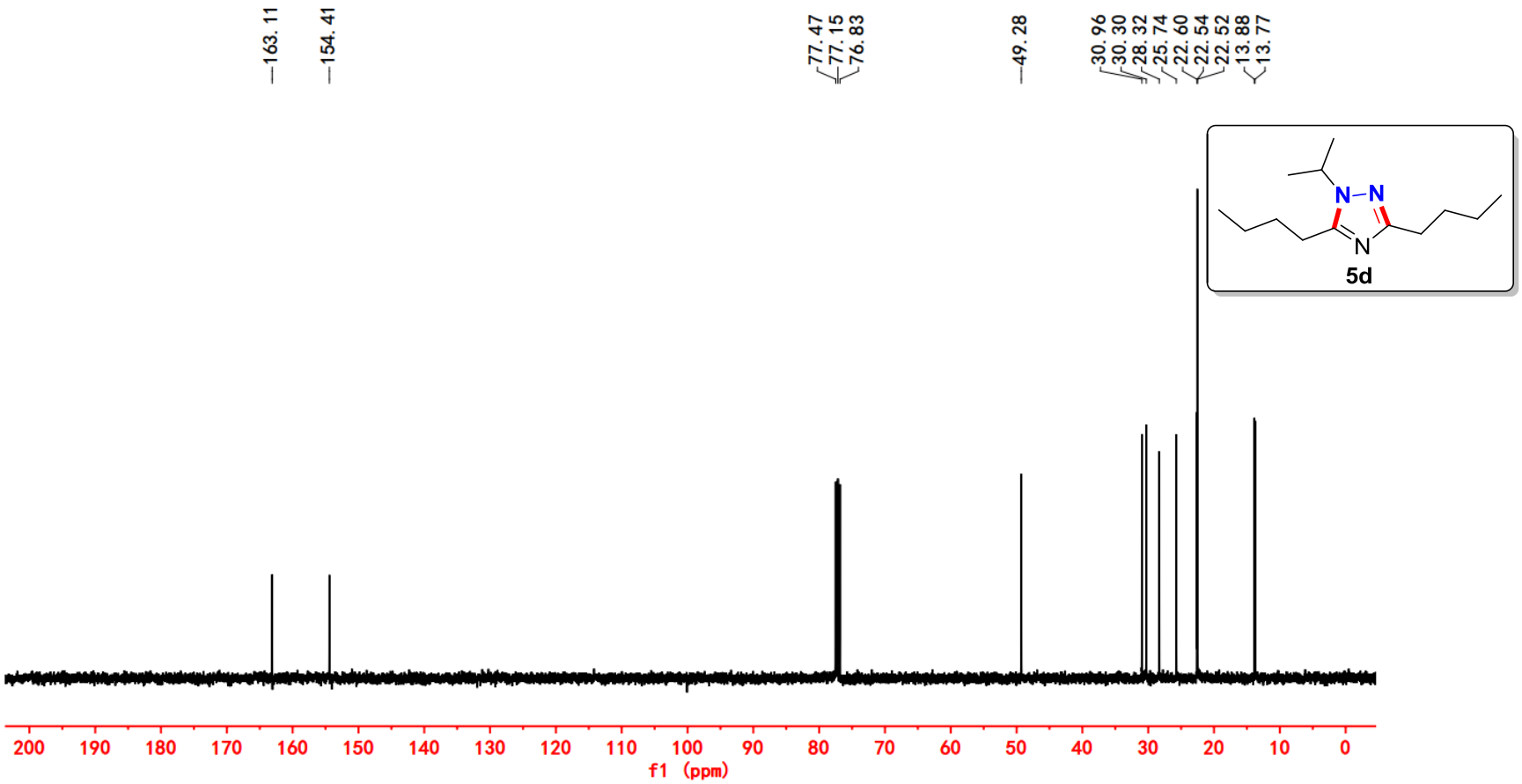
2.6199
2.6099
2.5998
2.5904
2.5704
1.6712
1.6695
1.6531
1.6508
1.6315
1.6246
1.6138
1.6117
1.5924
1.4027
1.3860
1.3598
1.3407
1.3219
1.3032
N
N
N
5d
1.00
4.03
4.03
6.01
4.00
6.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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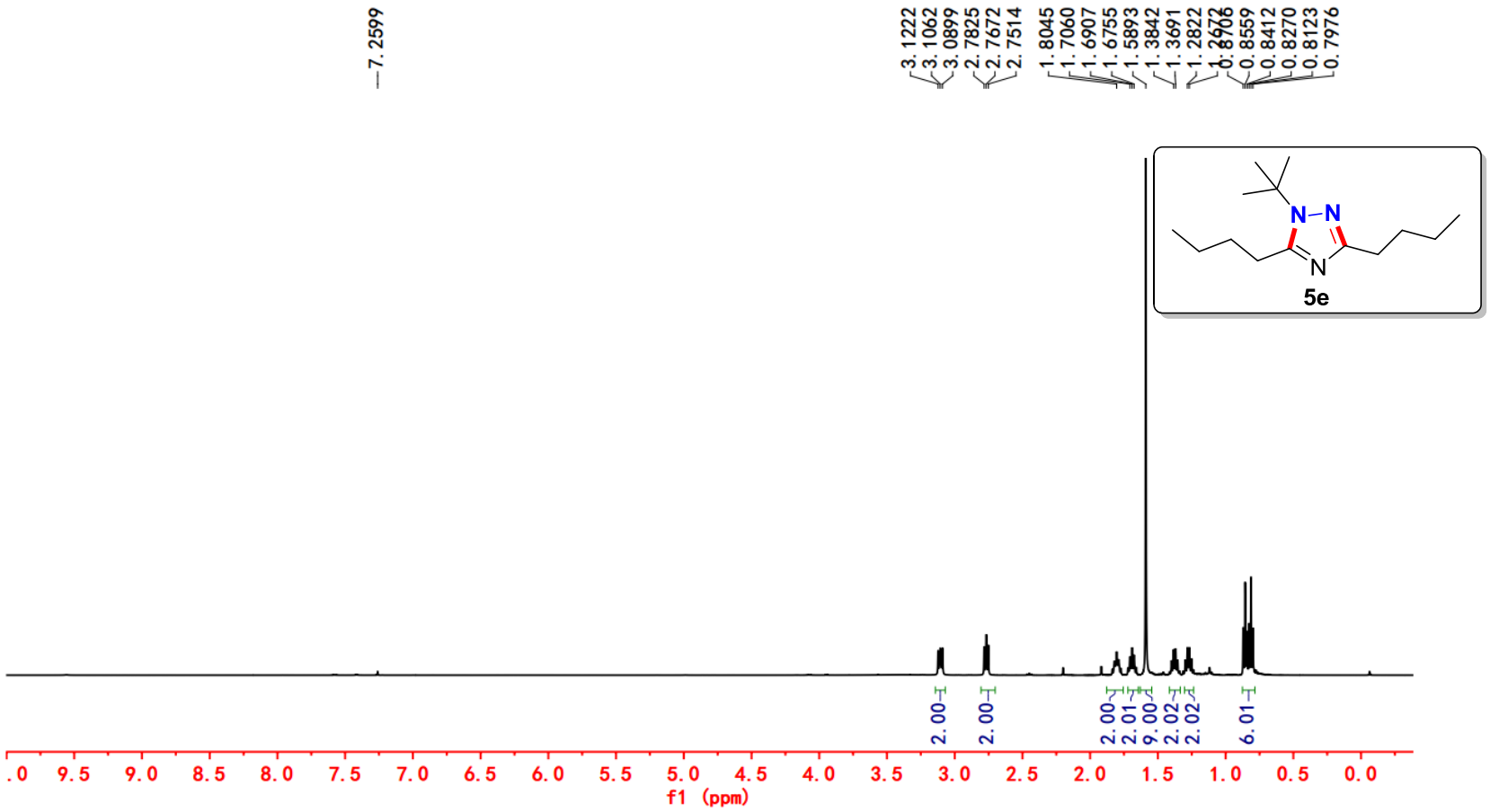
154.41
77.47
77.15
76.83
49.28
30.96
30.30
28.32
25.74
22.60
22.54
22.52
13.88
13.77
N–N
N
5d
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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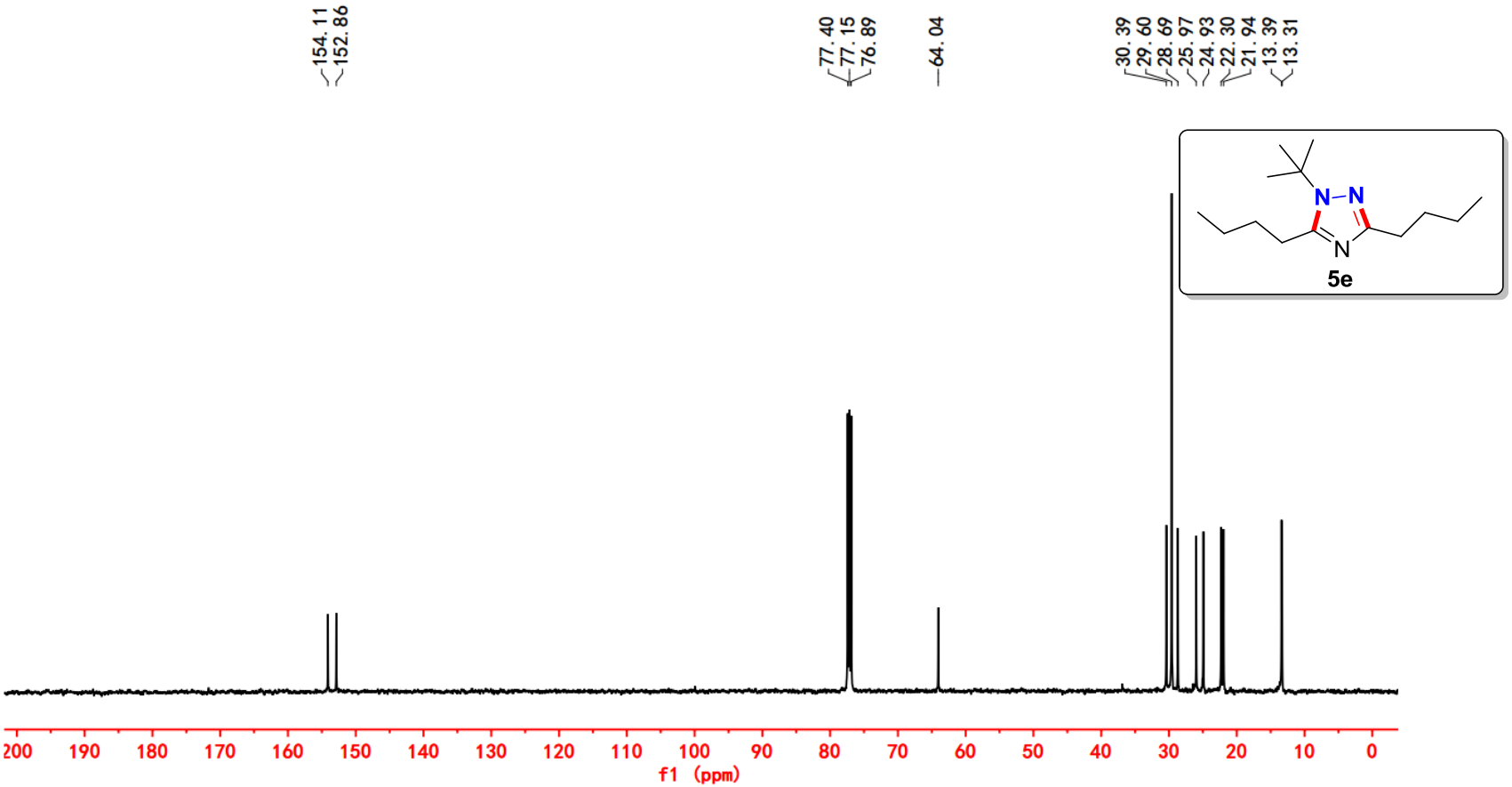
3.1062
3.0899
2.7825
2.7672
2.7514
1.8045
1.7060
1.6907
1.6755
1.5893
1.3842
1.3691
1.2822
1.2672
0.8708
0.8559
0.8412
0.8270
0.8123
0.7976
N–N
N
5e
2.00
2.00
2.00
2.01
9.00
2.02
2.02
6.01
f1 (ppm)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152.86
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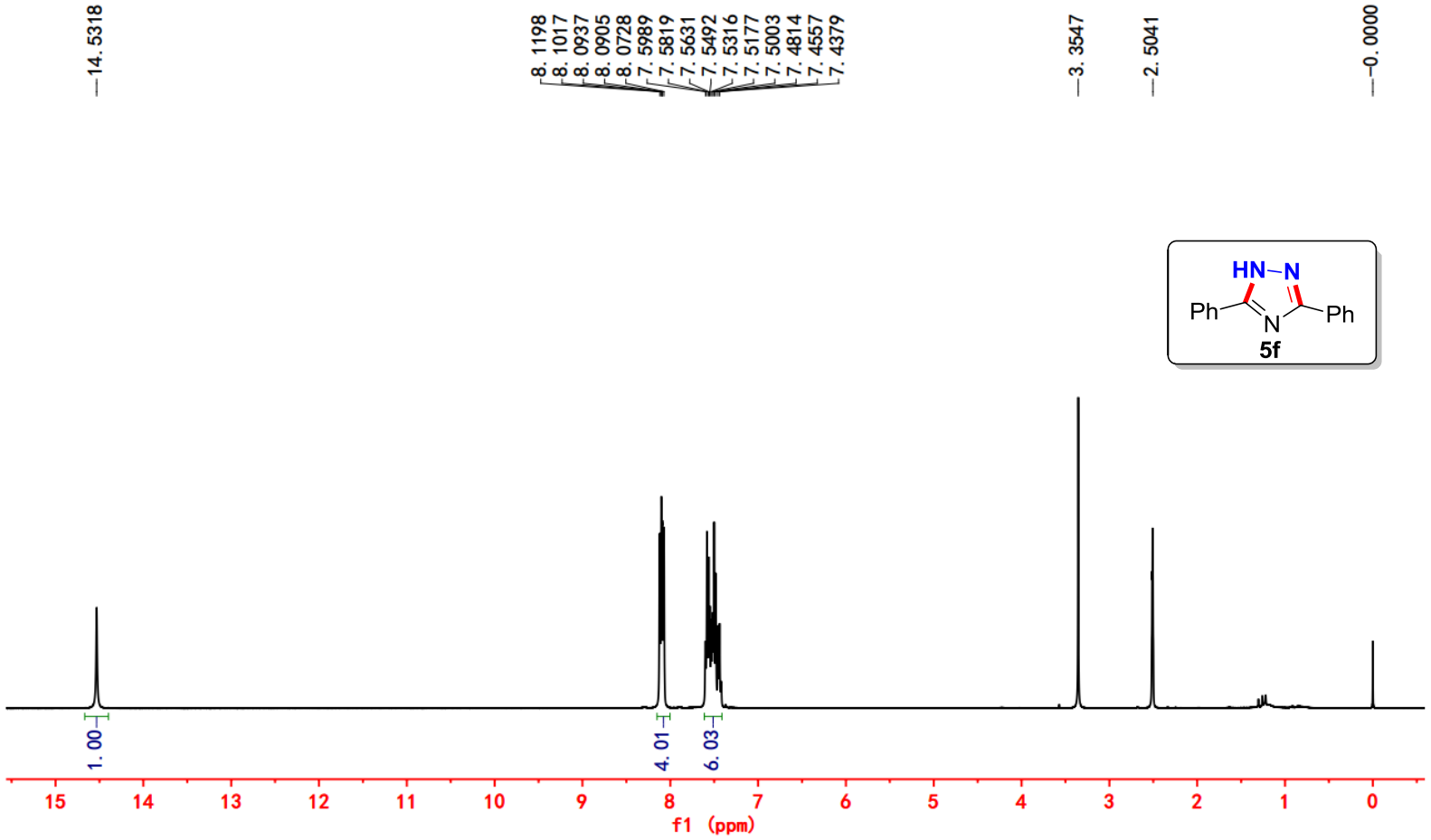
77.15
76.89
64.04
30.39
29.60
28.69
25.97
24.93
22.30
21.94
13.39
13.31
N
N
N
5e
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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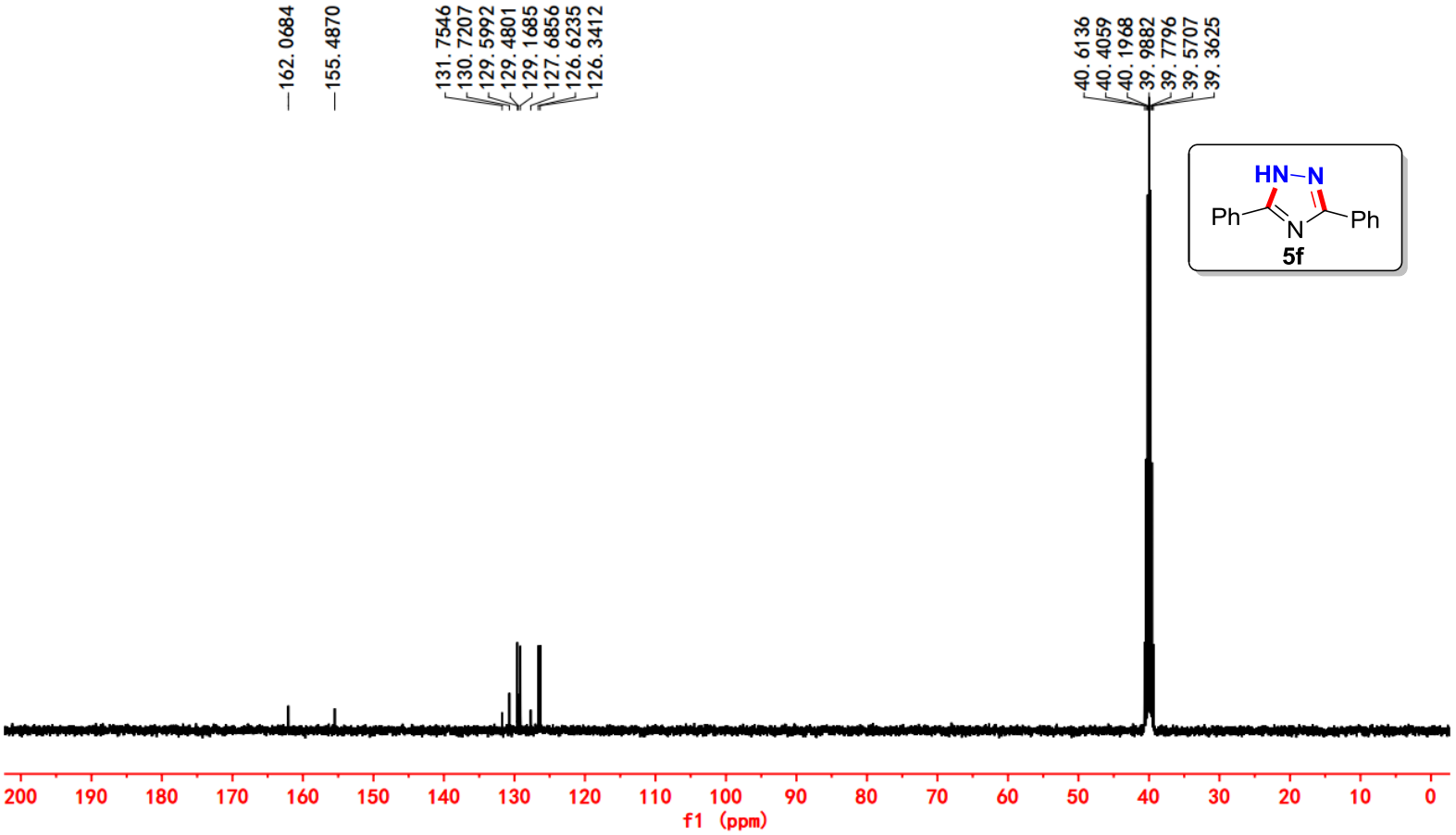
8.1017
8.0937
8.0905
8.0728
7.5989
7.5819
7.5631
7.5492
7.5316
7.5177
7.5003
7.4814
7.4557
7.4379
3.3547
2.5041
0.0000
HN–N
Ph
N
Ph
5f
1.00
4.01
6.03
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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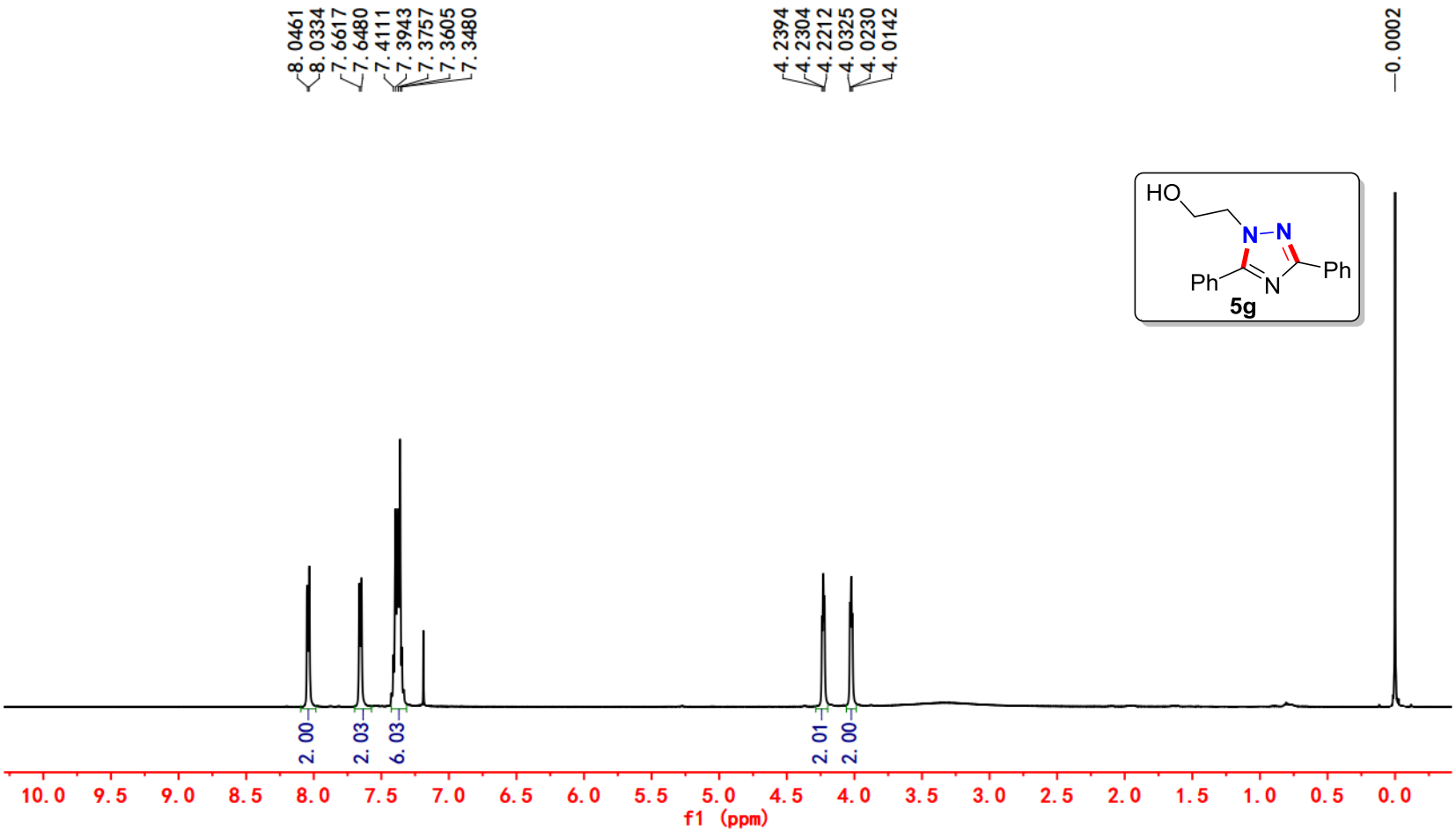
130.7207
129.5992
129.4801
129.1685
127.6856
126.6235
126.3412
40.6136
40.4059
40.1968
39.9882
39.7796
39.5707
39.3625
HN–N
Ph
N
Ph
5f
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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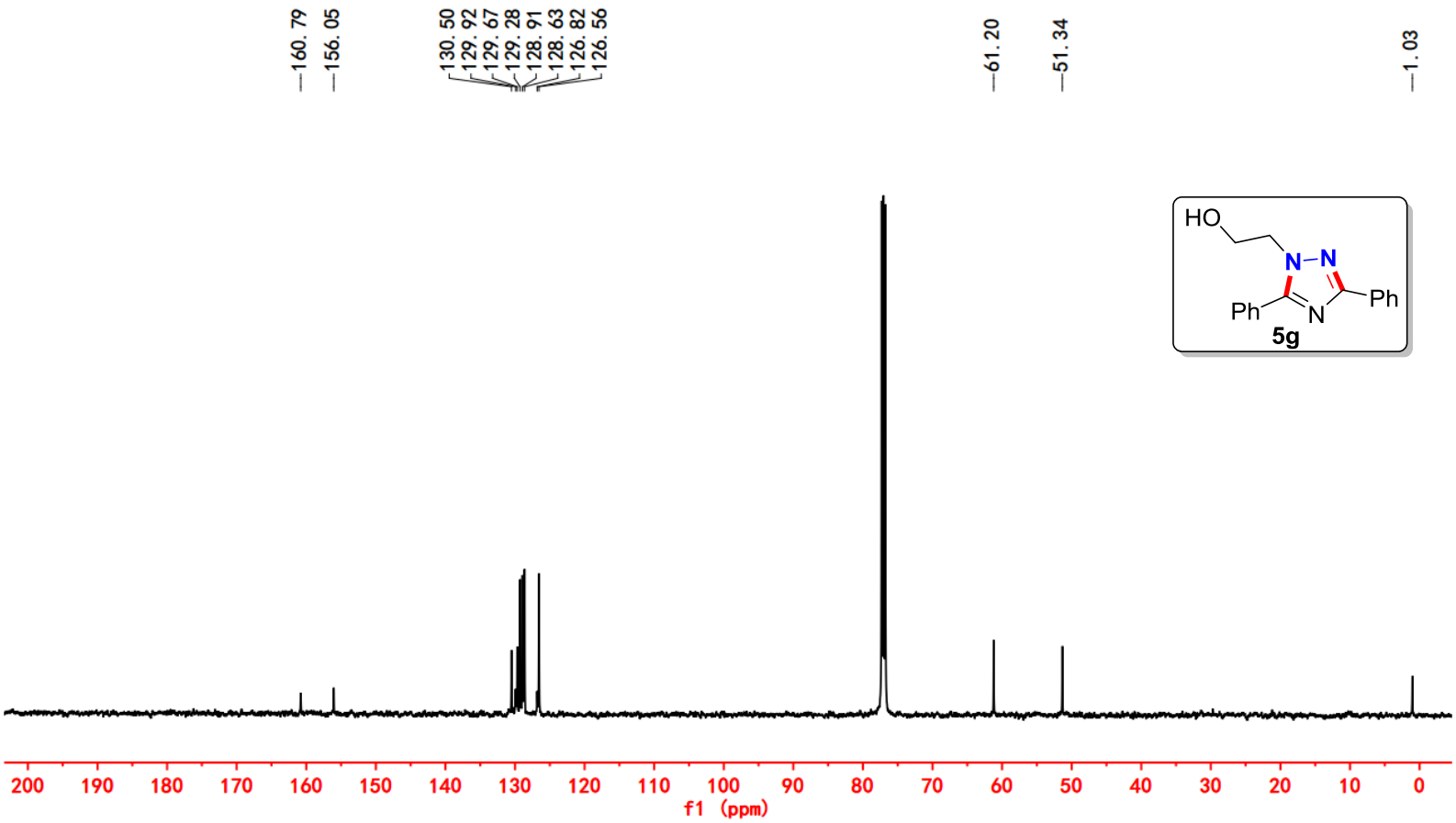
7.3943
7.3757
7.3605
7.3480
4.2394
4.2304
4.2212
4.0325
4.0230
4.0142
0.0002
HO
N
N
Ph
N
Ph
5g
2.00
2.03
6.03
2.01
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.28
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128.63
126.82
126.56
61.20
51.34
1.03
HO
N
N
Ph
N
Ph
5g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)