Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

A concise construction of 4-alkynylquinazolines *via* [4+2] annulation of 4-alkynylbenzoxazinanones with acylhydroxamates under transition-metal-free conditions

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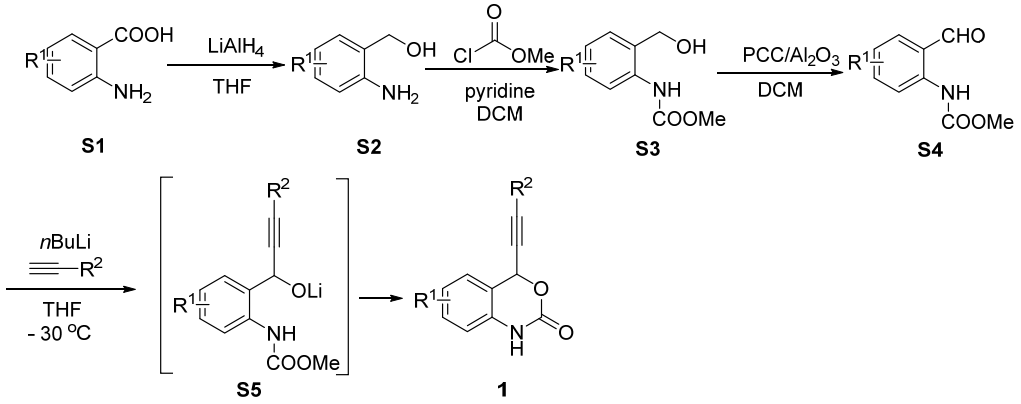
1. General Information

Materials and Reagents: All commercially available chemicals were used as received. All reagents and solvents were obtained from commercial suppliers and used without further purification. All reagents were weighed and handled in air at room temperature. Reactions: All reactions were carried out in air, unless otherwise noted. Melting points were recorded on a RY-1 microscopic melting apparatus and uncorrected. ^{1}H NMR spectra were recorded on 500 MHz and 400 Hz by using a Bruker Avance 500 spectrometer. ^{13}C NMR spectra were recorded on 125 MHz and 100 Hz by using a Bruker Avance 500 spectrometer. Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS). HRMS were performed on an Ultima Global spectrometer with an ESI source.

2. Preparation of Substrates 1 and 2

2.1 Preparation of 4-alkynylquinazolines 1[1]



S1 to **S2**: To a solution of substituted 2-amino-benzoic acid **S1** (5 mmol) in dry THF (4 mL) was added dropwise a solution of $LiAlH_4$ (10 mmol, 3.795g) in THF (1M, 10 mL) while the temperature was maintained at 0 °C. The resulting mixture was allowed to warm to room temperature and was stirred for 2 h. The mixture was then hydrolyzed by addition of water (1 mL) and 5% NaOH (1.5 mL). The resulting suspension was filtered, and the precipitate was washed with ethyl acetate. The combined organic layer was evaporated. The residue was recrystallized from ethyl acetate and petroleum ether, affording the corresponding alcohols **S2** quantitatively as a white or pale yellow solid.

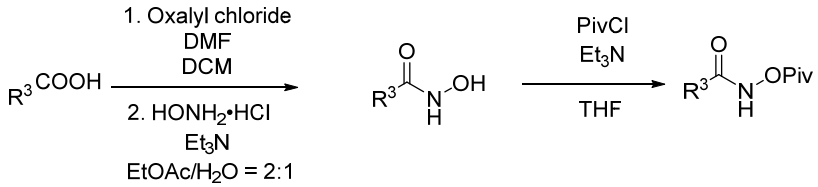
S2 to **S3**: To a solution of above crude product of **S2** in DCM (10 mL), pyridine (5.5 mmol) at 0 °C was added methyl chloroformate (5.5 mmol) dropwise. The resulting mixture was stirred at room temperature for 3 h. The reaction was monitored by TLC (PE/EA = 4:1). The reaction was diluted with brine (10 mL) and extracted with DCM (3×10 mL). The combined organic layer was dried with Na_2SO_4, and evaporated under reduced pressure. The obtained crude product **S3** was used directly without further purification.

S3 to **S4**: To a solution of above crude product of benzyl carbamate **S3** in DCM (15 mL) was added PCC (1.2 g) and Al_2O_3 (3 g). The reaction mixture was stirred at room

temperature for 2 h and then filtered through a bed of silica. The filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (DCM/PE = 1:1) to give product **S4** (75% for 2 steps) as a white solid.

S4 to **1**: Under nitrogen atmosphere, to a solution of substituted terminal alkyne (5 mmol) in dry THF (4 mL) was added dropwise a solution of *n*BuLi (2 mL, 2.5 M in *n*-Hexane) at -30 °C, and the reaction system was stirred for 30 minutes at the same temperature. The mixture was then added dropwise a solution of **S4** (4 mmol, 2 M in THF). The resulting mixture was allowed to warm to room temperature and was stirred for 12 h. Then, the mixture was hydrolyzed by addition of water (1 mL). The reaction was diluted with brine (10 mL) and extracted with DCM (3×10 mL). The combined organic layer was dried with Na_2SO_4, and evaporated under reduced pressure. The crude product was purified by column chromatography on silica gel (PE/EA = 4:1) to give product **1** as a white solid.

2.2 Preparation of Acylhydroxamates 2[2]

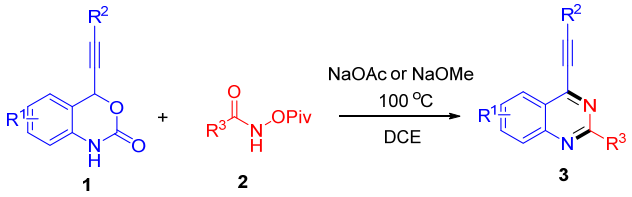


1) To a solution of the carboxylic acids (3.0 mmol, 1.0 eq.) in dry DCM (10 mL) at 0°C was added dropwise oxalyl chloride (0.34 mL, 3.6 mmol, 1.2 eq.) followed by a catalytic amount of dry DMF (2 drops). The reaction was allowed to stir at rt until completion (typically 4 h). The solvent was then removed under reduce pressure to afford the corresponding crude acid chloride.

2) Hydroxylamine hydrochloride (6 mmol, 1.2 eq.) was added to a biphasic mixture of K_2CO_3 (12.0 mmol, 2.0 eq.) in a 2:1 mixture of EtOAc (24 mL) and H_2O (12 mL). The resulting solution was cooled to 0°C followed by dropwise addition of the unpurified acid chloride dissolved in a minimum amount of EtOAc. The flask containing the acid chloride was then rinsed with additional EtOAc. The reaction was allowed to stir for 4 h while reaching rt. Afterwards, the phases were separated and the aqueous phase was extracted twice with EtOAc. The combined organic layers were dried over $MgSO_4$, filtered, and evaporated under reduced pressure. The pure products were obtained without any further purification.

3) Hydroxamic acids (1.0 mmol, 1.0 eq.), Et_3N (1.0 mmol, 1.0 eq.) and PivCl (1.1 mmol, 1.1 eq.) in dry THF (3 mL) was stirred for overnight at rt. EtOAc (2 mL) was added and the reaction was washed with 1 M HCl (2mL), water (2 x 2 mL) and then brine (2 mL). After drying the organic layer over $MgSO_4$, evaporation of the solvent gave a crude product. The crude product was purified by column chromatography on silica gel (PE/EA = 4:1) to give acylhydroxamates **2**.

3. General Procedure for 3

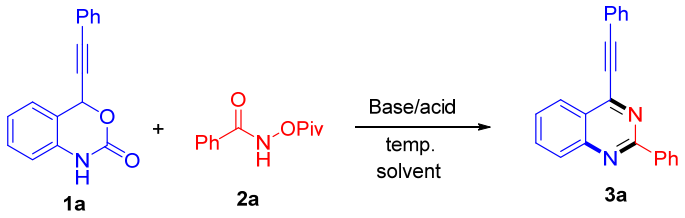


1 2 3

The mixture of 4-alkynylquinazolines **1** (0.20 mmol), acylhydroxamates **2** (0.30 mmol), NaOAc or NaOMe (1 equiv) in DCE (2 mL) was stirred in round-bottomed flask at 100 °C for about 12 h until complete consumption of starting materials as monitored by TLC. Afterwards, the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel using petroleum ether/ethyl acetate (v/v, 30:1) as eluent to give the products **3**.

4. Optimization of Reaction Conditions for 3a

Table S1 Optimization of Reaction Conditions for **3a**[a]



1a 2a 3a

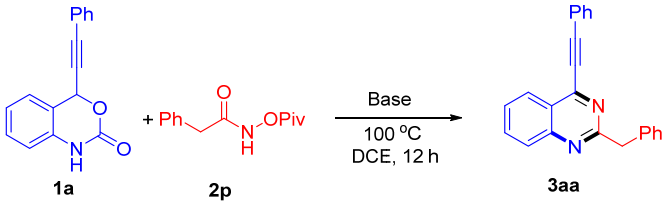
Entry	**1a**:**2a**	Cat.(equiv)	Base/Acid(equiv)	Solvent	Temp	yield[b]
1	1:1	$[Cp^*RhCl_2]_2$ (0.05)	NaOAc (1.0)	DCE	100	73
2	1:1	$[RuCl(p\text{-Cymene})]_2$ (0.05)	NaOAc (1.0)	DCE	100	75
3	1:1	$Cp^*Co(CO)I_2$ (0.3)	NaOAc (1.0)	DCE	100	69
4	1:1	-	NaOAc (1.0)	DCE	100	77
5	1:1	-	NaOAc (1.0)	DCE	rt	0
6	1:1	-	NaOAc (1.0)	DCE	60	43
7	1:1	-	NaOAc (1.0)	DCE	80	57
8	1:1	-	NaOAc (1.0)	DCE	120	69
9	1:1.25	-	NaOAc (1.0)	DCE	100	87
10	**1:1.5**	-	**NaOAc (1.0)**	**DCE**	**100**	**98**
9	1:1.5	-	NaOAc (1.5)	DCE	100	96
10	1:1.5	-	NaOAc (0.5)	DCE	100	78
11	1:1.5	-	$NaOPiv{\bullet}H_2O$ (1.0)	DCE	100	94
12	1:1.5	-	CsOAc (1.0)	DCE	100	93
13	1:1.5	-	K_3PO_4 (1.0)	DCE	100	88
14	1:1.5	-	K_2CO_3 (1.0)	DCE	100	90
15	1:1.5	-	KOtBu (1.0)	DCE	100	85
16	1:1.5	-	$FeCl_3$ (1.0)	DCE	100	trace

17	1:1.5	-	$InCl_3$ (1.0)	DCE	100	trace
18	1:1.5	-	$Zn(OTf)_2$ (1.0)	DCE	100	trace
19	1:1.5	-	AgOTf (1.0)	DCE	100	trace
20	1:1.5	-	NaOAc (1.0)	MeOH	100	42
21	1:1.5	-	NaOAc (1.0)	Toluene	100	87
22	1:1.5	-	NaOAc (1.0)	THF	100	82
23	1:1.5	-	NaOAc (1.0)	DMF	100	78
24	1:1.5	-	NaOAc (1.0)	DMSO	100	62
25	1:1.5	-	NaOAc (1.0)	MeCN	100	87
26	1:1.5	-	NaOAc (1.0)	H_2O	100	41
27	1:1.5	-	NaOAc (1.0)	-	100	46

[a] Reaction conditions: **1a** (0.20 mmol), **2a** (x mmol), base/acid (x equiv), solvent (2 mL), under air, 12 h. [b] Isolated yields. Cp* = pentamethylcyclopentadienyl.

5. Optimization of Reaction Conditions for 3aa

Table S2 Optimization of Reaction Conditions for **3aa**[a]

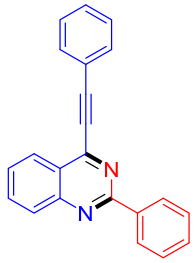


1a 2p 3aa

Entry	Base (equiv)	Solvent	Temp	yield[b]
1	KOH (1.0)	DCE	100	trace
2	KO*t*Bu (1.0)	DCE	100	trace
3	**NaOMe (1.0)**	**DCE**	**100**	**62**
4	K_2CO_3 (1.0)	DCE	100	trace
5	Cs_2CO_3 (1.0)	DCE	100	trace
6	K_3PO_4 (1.0)	DCE	100	trace
7	CsOAc (1.0)	DCE	100	23
8	KOAc (1.0)	DCE	100	16
9	DBU (1.0)	DCE	100	trace
10	Et_3N (1.0)	DCE	100	trace

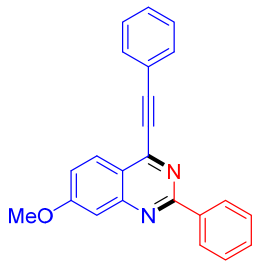
[a] Reaction conditions: **1a** (0.20 mmol), **2p** (1.5 equiv), base (1.0 equiv), DCE (2 mL), in air, 12 h. [b] Isolated yields.

6. Characterization Data of Compounds 3



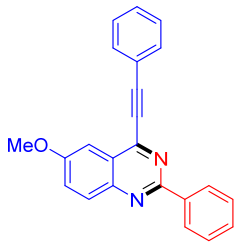
Chemical Formula: $C_{22}H_{14}N_2$

2-Phenyl-4-(phenylethynyl)quinazoline (**3a**): white solid, yield 60.0 mg (98%); CAS: 1619907-97-9. M.p. = 96-97 ºC; **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.66-8.63 (m, 2H, ArH), 8.41-8.38 (m, 1H, ArH), 8.10 (dt, J = 8.5, 0.9 Hz, 1H, ArH), 7.91 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H, ArH), 7.79-7.77 (m, 2H, ArH), 7.65 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H, ArH), 7.56-7.50 (m, 3H, ArH), 7.49-7.43 (m, 3H, ArH); **^{13}C NMR** (100 MHz, CDCl3) δ 160.9, 152.9, 151.0, 137.8, 134.2, 132.6, 130.7, 130.1, 129.1, 128.7, 128.7, 128.6, 127.65, 126.5, 124.0, 121.4, 97.8, 85.7.



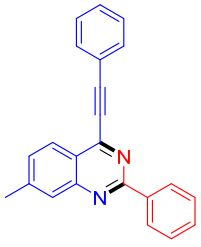
Chemical Formula: $C_{23}H_{16}N_2O$

7-Methoxy-2-phenyl-4-(phenylethynyl)quinazoline (**3b**): white solid, yield 57.9 mg (86%); M.p. = 186-87 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.62-8.58 (m, 2H, ArH), 8.22 (d, J = 9.1 Hz, 1H, ArH), 7.76-7.32 (m, 2H, ArH), 7.54-7.49 (m, 3H, ArH), 7.48-7.40 (m, 3H, ArH), 7.33 (d, J = 2.4 Hz, 1H, ArH), 7.22 (dd, J = 9.0, 2.5 Hz, 1H, ArH), 3.97 (s, 3H, OCH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 164.4, 161.5, 153.4, 151.5, 138.0, 132.5, 130.6, 130.0, 128.7, 128.6, 128.6, 127.8, 121.5, 121.1, 119.6, 106.4, 97.2, 85.7, 55.9. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{17}N_2O^+$, 337.1341, found 337.1342.



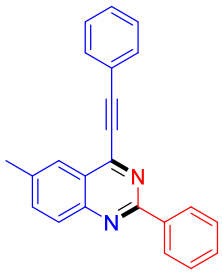
Chemical Formula: $C_{23}H_{16}N_2O$

6-Methoxy-2-phenyl-4-(phenylethynyl)quinazoline (**3c**): white solid, yield 65.3 mg (97%); M.p. = 175-167 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.60-8.59 (m, 2H, ArH), 8.01 (d, J = 9.1 Hz, 1H, ArH), 7.75 (dd, J = 7.7, 1.9 Hz, 2H, ArH), 7.62 (d, J = 2.8 Hz, 1H, ArH), 7.56 (dd, J = 9.2, 2.8 Hz, 1H, ArH), 7.54-7.50 (m, 2H, ArH), 7.49-7.44 (m, 4H, ArH), 4.02 (s, 3H, OCH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 159.2, 158.7, 150.9, 147.3, 138.0, 132.4, 130.6, 130.2, 130.0, 128.7, 128.6, 128.5, 128.3, 127.2, 125.0, 121.6, 103.5, 97.5, 85.8, 55.7. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{17}N_2O^+$, 337.1341, found 337.1342.



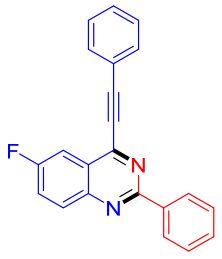
Chemical Formula: $C_{23}H_{16}N_2$

7-Methyl-2-phenyl-4-(phenylethynyl)quinazoline (**3d**): white solid, yield 61.5 mg (96%); CAS: 2287295-47-8. M.p. = 122-123 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.70-8.67(m, 2H, ArH), 8.22 (d, J = 8.1 Hz, 1H, ArH), 7.79-7.50 (m, 2H, ArH), 7.72-7.70 (m, 1H, ArH), 7.56-7.48 (m, 4H, ArH), 7.47-7.41 (m, 3H, ArH), 2.86 (s, 3H, CH_3);**^{13}C NMR** (101 MHz, $CDCl_3$) δ; 159.7, 152.8, 150.0, 138.1, 137.5, 134.0, 132.6, 130.5, 130.0, 128.7, 128.6, 128.5, 127.2, 124.1, 123.9, 121.5, 97.3, 86.0, 77.4, 77.1, 76.7, 17.2.



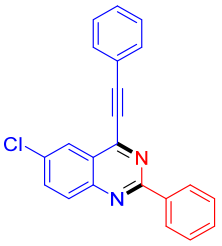
Chemical Formula: $C_{23}H_{16}N_2$

6-Methyl-2-phenyl-4-(phenylethynyl)quinazoline (**3e**): white solid, yield 62.8 mg (98%); M.p. = 197-198 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.68-8.60 (m, 2H, ArH), 8.12 (s, 1H, ArH), 7.99 (d, J = 8.6 Hz, 1H, ArH), 7.79-7.77 (m, 2H, ArH), 7.73 (dd, J = 8.6, 1.9 Hz, 1H, ArH), 7.55-7.49 (m, 3H, ArH),7.48-7.38 (m, 3H, ArH), 2.60 (s, 3H, CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.2, 152.0, 149.6, 138.0, 137.9, 136.5, 132.6, 132.5, 130.4, 130.0, 128.7, 128.7, 128.6, 128.6, 128.5, 125.1, 123.9, 121.5, 97.4, 85.8, 22.0. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{17}N_2^+$, 321.1392, found 321.1391.



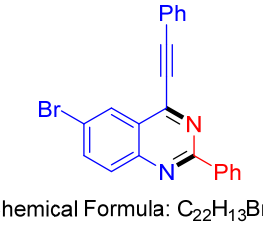
Chemical Formula: $C_{22}H_{13}FN_2$

7-Fluoro-2-phenyl-4-(phenylethynyl)quinazoline (**3f**): white solid, yield 42.8 mg (66%); CAS : 2287295-50-3. M.p. = 160-161 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.63-8.60(m, 2H, ArH), 8.10 (dd, J = 9.2, 5.1 Hz, 1H, ArH), 7.98 (dd, J = 8.3, 2.8 Hz, 1H, ArH), 7.79-7.76 (m, 2H, ArH), 7.67 (td, J = 8.7, 2.8 Hz, 1H, ArH), 7.56-7.50 (m, 3H, ArH), 7.49-7.44 (m, 3H, ArH); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 160.8 (d, $^1J_{C\text{-}F}$ = 252.6 Hz), 160.6 (d, $^5J_{C\text{-}F}$ = 2.8 Hz), 152.3 (d, $^4J_{C\text{-}F}$ = 5.6 Hz), 148.2, 137.5, 132.6, 131.8 (d, $^3J_{C\text{-}F}$ = 8.5 Hz), 130.7, 130.3, 128.7, 128.6, 128.6, 124.6 (d, $^2J_{C\text{-}F}$ = 26.0 Hz), 124.5 (d, $^3J_{C\text{-}F}$ = 9.5 Hz), 121.1, 109.9 (d, $^2J_{C\text{-}F}$ = 23.0 Hz), 98.3, 85.3.



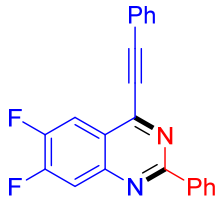
Chemical Formula: $C_{22}H_{13}ClN_2$

6-Chloro-2-phenyl-4-(phenylethynyl)quinazoline (**3g**): white solid, yield 51.8 mg (76%); CAS: 2287295-53-6. M.p. = 210-211 °C.**^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.63-8.60 (m, 2H, ArH), 8.33 (d, J = 2.4 Hz, 1H, ArH), 8.03 (d, J = 8.9 Hz, 1H, ArH), 7.84-7.77 (m, 3H, ArH), 7.56-7.44 (m, 6H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 161.13, 151.98, 149.50, 137.39, 135.19, 133.31, 132.63, 130.91, 130.75, 130.33, 128.69, 128.64, 125.30, 124.38, 121.06, 98.47, 85.17.



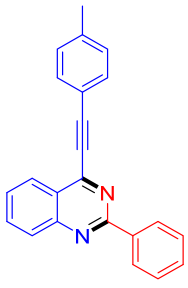
Chemical Formula: $C_{22}H_{13}BrN_2$

6-Bromo-2-phenyl-4-(phenylethynyl)quinazoline (**3h**): white solid, yield 67.0 mg (87%); M.p. = 195-196 °C.**^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.68-8.66 (m, 2H, ArH), 8.55 (s, 1H, ArH), 8.00 (s, 2H, ArH), 7.83 (dd, J = 7.4, 1.8 Hz, 2H, ArH), 7.60-7.50 (m, 6H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.2, 151.8, 149.7, 137.8, 137.4, 132.7, 131.0, 130.8, 130.4, 128.7, 128.7, 124.8, 121.4, 121.1, 98.5, 85.2. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{14}N_2Br^+$, 385.0340, found 385.0340.



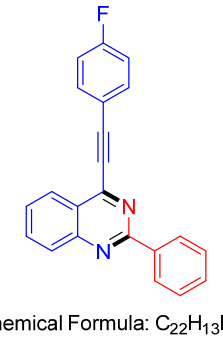
Chemical Formula: $C_{22}H_{12}F_2N_2$

6,7-Difluoro-2-phenyl-4-(phenylethynyl)quinazoline (**3i**): white solid, yield 64.4 mg (94%); M.p. = 169-170 °C.**^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.65-8.63 (m, 2H, ArH), 8.13 (td, J = 9.1, 4.6 Hz, 1H, ArH), 7.86 (ddd, J = 10.8, 7.3, 3.7 Hz, 1H, ArH), 7.81 (d, J = 7.7 Hz, 2H, ArH), 7.60-7.50 (m, 6H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 161.4 (d, $^5J_{C\text{-}F}$ = 2.5 Hz), 155.7 (dd, $^1J_{C\text{-}F}$ = 259.0 Hz, $^2J_{C\text{-}F}$ = 16.1 Hz), 151.9 (d, $^5J_{C\text{-}F}$ = 4.7 Hz), 151.5 (dd, $^1J_{C\text{-}F}$ = 255.0 Hz, $^2J_{C\text{-}F}$ = 15.6 Hz), 148.9 (d, $^2J_{C\text{-}F}$ = 12.0 Hz), 137.2, 132.6, 132.6, 131.0, 130.4, 128.8, 128.7, 128.7, 128.7, 121.0 (d, $^3J_{C\text{-}F}$ = 7.3 Hz), 120.9, 115.4 (d, $^2J_{C\text{-}F}$= 16.7 Hz), 112.5 (d, $^2J_{C\text{-}F}$ = 18.6 Hz), 98.5, 85.0. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{13}N_2F_2^+$, 343.1047, found 343.1046



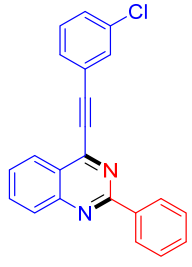
Chemical Formula: $C_{23}H_{16}N_2$

2-Phenyl-4-(*p*-tolylethynyl)quinazoline (**3j**): white solid, yield 60.9 mg (95%); CAS: 2287295-56-9. M.p. = 144-145 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.66-8.63 (m, 2H, ArH), 8.38 (d, J = 8.2 Hz, 1H, ArH), 8.08 (d, J = 8.4 Hz, 1H, ArH), 7.88 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H, ArH), 7.67-7.60 (m, 3H, ArH), 7.55-7.50 (m, 3H, ArH), 7.24 (d, J = 8.0 Hz, 2H, ArH), 2.41 (s, 3H, CH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 160.9, 153.0, 151.0, 140.7, 137.9, 134.2, 132.6, 130.6, 129.4, 129.0, 128.7, 128.6, 127.6, 126.5, 123.9, 118.3, 98.4, 85.3, 21.8.



Chemical Formula: $C_{22}H_{13}FN_2$

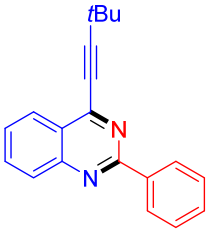
4-((4-Fluorophenyl)ethynyl)-2-phenylquinazoline (**3k**): white solid, yield 46.7 mg (72%);CAS: 2287295-59-2. M.p. = 175-176 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.65-8.62 (m, 2H, ArH), 8.36 (d, J = 8.0 Hz, 1H, ArH), 8.10 (d, J = 8.4 Hz, 1H, ArH), 7.91 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H, ArH), 7.79-7.74 (m, 2H, ArH), 7.64 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H, ArH), 7.56-7.49 (m, 3H, ArH) 7.18-7.12 (m, 2H, ArH); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; δ 163.6 (d, $^1J_{C\text{-}F}$ = 252.6 Hz), 160.9, 152.7, 151.0, 137.8, 134.7 (d, $^3J_{C\text{-}F}$ = 8.7 Hz), 134.3, 130.7, 129.1, 128.7, 128.6, 127.7, 126.3, 123.9, 117.5 (d, $^4J_{C\text{-}F}$ = 3.6 Hz), 116.1 (d, $^2J_{C\text{-}F}$ = 22.3 Hz), 96.6, 85.5 (d, $^5J_{C\text{-}F}$ = 1.5 Hz).



Chemical Formula: $C_{22}H_{13}ClN_2$

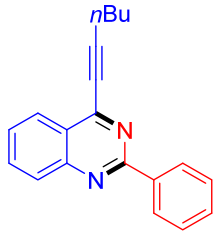
4-((3-Chlorophenyl)ethynyl)-2-phenylquinazoline (**3l**): white solid, yield 57.3 mg (84%); M.p. = 173-174 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.64-8.62 (m, 2H, ArH), 8.35 (d, J = 8.2 Hz, 1H, ArH), 8.10 (d, J = 8.4 Hz, 1H, ArH), 7.92 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H, ArH), 7.76 (t, J = 1.8 Hz, 1H, ArH), 7.56-7.49 (m, 3H, ArH), 7.47-7.44 (m, 1H, ArH), 7.39 (t, J = 7.9 Hz, 1H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 160.9, 152.4, 151.1, 137.7, 134.6, 134.3, 132.3, 130.7, 130.6, 130.4, 129.9, 129.1, 128.7, 128.6, 127.8, 126.3, 123.9, 123.1, 95.7, 86.5. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{14}N_2Cl^+$,

341.0846, found 341.0848.



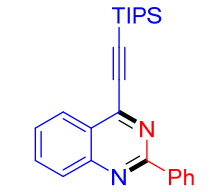
Chemical Formula: $C_{20}H_{18}N_2$

4-(3,3-Dimethylbut-1-yn-1-yl)-2-phenylquinazoline (**3m**): white solid, yield 23.5 mg (41%); M.p. = 112-113 ºC. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.61 (d, J = 6.7 Hz, 1H, ArH), 8.25 (d, J = 8.2 Hz, 1H, ArH), 8.05 (d, J = 8.4 Hz, 1H, ArH), 7.86 (ddd, J = 8.5, 6.9, 1.4 Hz, 1H, ArH), 7.60 (t, J = 7.5 Hz, 1H, ArH), 7.54-7.47 (m, 3H, ArH), 1.49 (s, 9H, *t*Bu); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 160.8, 153.5, 150.8, 137.9, 134.0, 130.5, 128.9, 128.7, 128.5, 127. 5, 126.6, 124.1, 108.4, 76.3, 30.6, 28.6. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{20}H_{19}N_2^+$, 287.1548, found 287.1553.



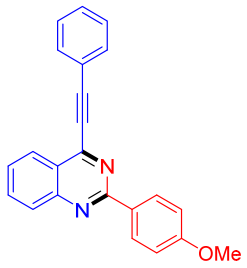
Chemical Formula: $C_{20}H_{18}N_2$

4-(Hex-1-yn-1-yl)-2-phenylquinazoline (**3n**): white solid, yield 38.9 mg (68%); M.p. = 60-61 ºC. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.62-8.59 (m, 2H, ArH), 8.29 (d, J = 8.2 Hz, 1H, ArH), 8.06 (d, J = 8.4 Hz, 1H, ArH), 7.88 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H, ArH), 7.61 (ddd, J = 8.2, 6.8, 1.2 Hz, 1H, ArH), 7.54-7.47 (m, 3H, ArH), 2.67 (t, J = 7.2 Hz, 2H), 1.83 – 1.72 (m, 2H), 1.64 – 1.54 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 160.8, 153.4, 150.9, 137.8, 134.0, 130.5, 128.9, 128.7, 128.5, 127.5, 126.6, 124.0, 100.8, 77.7, 30.3, 22.2, 19.6, 13.6. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{20}H_{19}N_2^+$, 287.1548, found 287.1555.



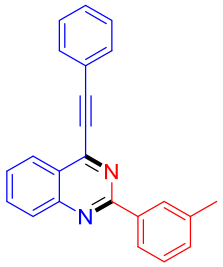
Chemical Formula: $C_{25}H_{30}N_2Si$

2-Phenyl-4-((triisopropylsilyl)ethynyl)quinazoline (**3o**): white solid, yield 54.1 mg (70%); M.p. = 55-56 ºC. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.64 (d, J = 6.4 Hz, 1H, ArH), 8.33 (d, J = 8.2 Hz, 1H, ArH), 8.07 (d, J = 8.4 Hz, 1H, ArH), 7.88 (ddd, J = 8.3, 6.8, 1.4 Hz, 1H, ArH), 7.62 (t, J = 7.6 Hz, 1H, ArH), 7.54-7.48 (m, 3H, ArH), 1.29-1,23 (m, 21H, TIPS); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 160.8, 152.5, 151.0, 137.8, 134.1, 130.6, 129.0, 128.7, 128.6, 127.7, 126.4, 124.1, 102.3, 101.9, 18.8, 11.3. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{25}H_{31}N_2Si^+$, 387.2257, found 387.2260.



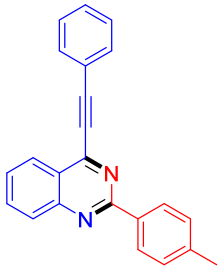
Chemical Formula: $C_{23}H_{16}N_2O$

2-(4-Methoxyphenyl)-4-(phenylethynyl)quinazoline (**3p**): white solid, yield 49.8 mg (74%); M.p. = 175-176 ºC. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.61 (d, J = 8.9 Hz, 2H, ArH), 8.36 (d, J = 8.2 Hz, 1H, ArH), 8.05 (d, J = 8.5 Hz, 1H, ArH), 7.88 (ddt, J = 8.4, 7.0, 1.3 Hz, 1H, ArH), 7.79-7.76 (m, 2H, ArH), 7.61 (ddt, J = 8.2, 6.9, 1.3 Hz, 1H, ArH), 7.48-7.42 (m, 3H, ArH),7.06-7.02 (m, 2H, ArH), 3.90 (s, 3H, OCH_3); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 161.9, 160.7, 152.8, 151.1, 134.2, 132.6, 130.6, 130.4, 130.1, 128.8, 128.6, 127.2, 126.5, 123.7, 121.4, 113.9, 97.5, 85.7, 55.4. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{17}N_2O^+$, 337.1341, found 337.1343.



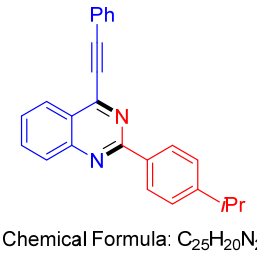
Chemical Formula: $C_{23}H_{16}N_2$

4-(Phenylethynyl)-2-(*m*-tolyl)quinazoline (**3q**): white solid, yield 62.2 mg (97%); CAS: 2287295-64-9. M.p. = 126-127 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.63-8.43 (m, 2H, ArH), 8.39 (d, J = 8.2 Hz, 1H, ArH), 8.10 (d, J = 8.4 Hz, 1H, ArH), 7.90 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H, ArH), 7.80-7.77 (m, 2H, ArH), 7.64 (ddd, J = 8.1, 6.8, 1.1 Hz, 1H), 7.50-7.41 (m, 4H, ArH), 7.32 (d, J = 7.5 Hz, 1H, ArH), 2.50 (s, 3H, CH_3); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 161.1, 152.8, 151.0, 138.2, 137.7, 134.2, 132.6, 131.5, 130.1, 129.2, 129.0, 128.6, 128.5, 127.6, 126.5, 125.9, 123.9, 121.4, 97.8, 85.7, 21.6.



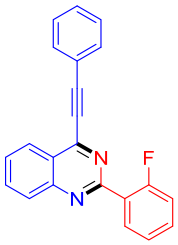
Chemical Formula: $C_{23}H_{16}N_2$

4-(Phenylethynyl)-2-(*p*-tolyl)quinazoline (**3r**): white solid, yield 57.0 mg (89%); CAS: 1619908-09-6. M.p. = 164-165 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.54 (d, J = 8.3 Hz, 2H, ArH), 8.38 (d, J = 8.1 Hz, 1H, ArH), 8.07 (d, J = 8.3 Hz, 1H, ArH), 7.89 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H, ArH), 7.79 - 7.77 (m, 2H, ArH), 7.63 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H, ArH), 7.50-7.43 (m, 3H, ArH) 7.34 (d, J = 8.0 Hz, 2H, ArH), 2.45 (s, 3H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ; 161.0, 152.8, 151.0, 140.9, 135.1, 134.2, 132.6, 130.1, 129.4, 128.9, 128.4, 128.6, 127.4, 126.4, 123.9, 121.4, 97.6, 85.7, 21.5.



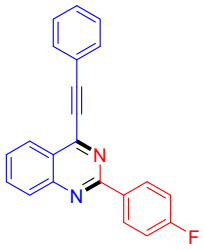
Chemical Formula: $C_{25}H_{20}N_2$

2-(4-Isopropylphenyl)-4-(phenylethynyl)quinazoline (**3s**): white solid, yield 55.8 mg (80%); M.p. = 55-56 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.56 (d, J = 8.1 Hz, 2H, ArH), 8.35 (d, J = 8.2 Hz, 1H, ArH), 8.06 (d, J = 8.4 Hz, 1H, ArH), 7.86 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H, ArH), 7.78-7.70 (m, 2H, ArH), 7.59 (t, J = 7.4 Hz, 1H, ArH), 7.45-7.41 (m, 3H, ArH), 7.39 (d, J = 8.1 Hz, 2H, ArH), 2.99 (hept, J = 7.0 Hz, 1H, CH), 1.31 (d, J = 6.9 Hz, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 161.0, 152.8, 151.8, 151.0, 135.5, 134.2, 132.6, 130.1, 129.0, 128.8, 128.7, 127.4, 126.8, 126.4, 123.8, 121.4, 97.6, 85.8, 34.2, 23.9. **HRMS** (ESI-TOF, [M + H]$^+$): calcd for $C_{25}H_{21}N_2$, 349.1705, found 349.1708



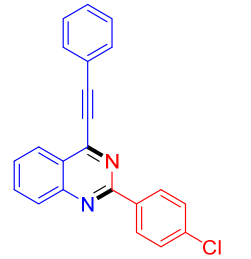
Chemical Formula: $C_{22}H_{13}FN_2$

2-(2-Fluorophenyl)-4-(phenylethynyl)quinazoline (**3t**): white solid, yield 61.6 mg (95%); M.p. = 146-147 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.43 (d, J = 7.7 Hz, 1H, ArH), 8.17-8.12 (m, 2H, ArH), 7.95 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H, ArH), 7.78-7.75 (m, 2H, ArH), 7.71 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H, ArH), 7.49-7.42 (m, 4H, ArH), 7.30 (td, J = 7.6, 1.2 Hz, 1H, ArH),7.24-7.21(m, 1H, ArH); **^{13}C NMR** (125MHz, $CDCl_3$) δ; 161.2 (d, $^1J_{C\text{-}F}$= 254.6 Hz), 159.7 (d, $^4J_{C\text{-}F}$ = 4.0 Hz), 152.9, 150.8, 134.5, 132.6, 132.2 (d, $^5J_{C\text{-}F}$ = 2.0 Hz), 131.6 (d, $^3J_{C\text{-}F}$ J = 8.5 Hz), 130.2, 129.1, 128.7, 128.3, 127.1 (d, $^3J_{C\text{-}F}$ = 10.2 Hz), 126.4, 124.2 (d, $^4J_{C\text{-}F}$ = 3.9 Hz), 123.6, 121.3, 116.8 (d, $^2J_{C\text{-}F}$ = 22.2 Hz), 98.5, 85.5. **HRMS** (ESI-TOF, [M + H]$^+$): calcd for $C_{22}H_{14}N_2F^+$, 325.1141, found 325,1143.



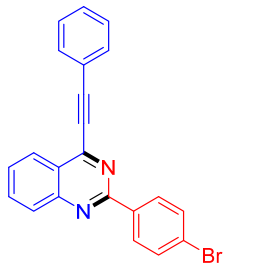
Chemical Formula: $C_{22}H_{13}FN_2$

2-(4-Fluorophenyl)-4-(phenylethynyl)quinazoline (**3u**): white solid, yield 53.8 mg (83%); CAS: 2287295-62-7. M.p. = 152-153°C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.70-8.59 (m, 2H, ArH), 8.38 (ddd, J = 8.3, 1.5, 0.7 Hz, 1H, ArH), 8.07 (dt, J = 8.5, 0.9 Hz, 1H, ArH), 7.90 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H, ArH), 7.79-7.76 (m, 2H, ArH), 7.64 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H, ArH), 7.50-7.43 (m, 3H, ArH),7.23-7.17 (m, 2H, ArH); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 164.7 (d, $^1J_{C\text{-}F}$ = 250.5 Hz), 160.0, 152. 9, 150.9, 134.3, 134.0 (d, $^4J_{C\text{-}F}$ = 2.9 Hz), 132.6, 130.8 (d, $^3J_{C\text{-}F}$ = 8.6 Hz), 130.2, 128.9, 128.7, 127.7, 126.5, 123.8, 121.3, 115.5 (d, $^2J_{C\text{-}F}$ = 21.6 Hz), 97.9, 85.6.



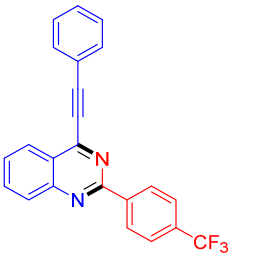
Chemical Formula: $C_{22}H_{13}ClN_2$

2-(4-Chlorophenyl)-4-(phenylethynyl)quinazoline (**3v**): white solid, yield 54.5 mg (80%); CAS: 1619908-11-0. M.p. = 182-183 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.59 (d, J = 8.6 Hz, 2H, ArH), 8.38 (d, J = 7.9 Hz, 1H, ArH), 8.06 (d, J = 8.4 Hz, 1H, ArH), 7.90 (ddd, J = 8.4, 6.8, 1.5 Hz, 1H, ArH), 7.79-7.76 (m, 2H, ArH), 7.65 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H, ArH),7.51-7.43(m, 5H, ArH); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 159.8, 152.9, 150.9, 136.9, 136.3, 134.4, 132.6, 130.2, 130.0, 129.0, 128.8, 128.7, 127.8, 126.5, 123.9, 121.3, 98.1, 85.5.



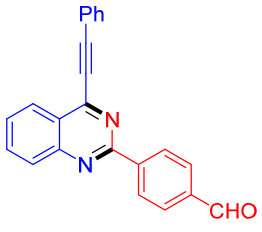
Chemical Formula: $C_{22}H_{13}BrN_2$

2-(4-Bromophenyl)-4-(phenylethynyl)quinazoline (**3x**): white solid, yield 67.0 mg (97%); M.p. = 182-183 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.52 (d, J = 8.6 Hz, 2H, ArH), 8.38 (d, J = 8.2 Hz, 1H, ArH), 8.06 (d, J = 8.4 Hz, 1H, ArH), 7.90 (ddd, J = 8.3, 6.7, 1.5 Hz, 1H, ArH), 7.79 – 7.74 (m, 2H, ArH), 7.67-7.64 (m, 3H, ArH),7.50-7.44 (m, 3H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ; 159.9, 152.9, 150.9, 136.7, 134.4, 132.6, 131.7, 130.3, 130.2, 129.0, 128.7, 127.9, 126.5, 125.5, 124.0, 121.3, 98.1, 85.5. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{14}N_2Br^+$, 385.0340, found 385.0341.



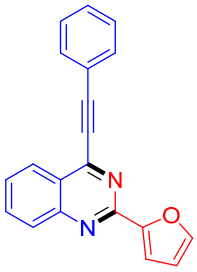
Chemical Formula: $C_{23}H_{13}F_3N_2$

4-(Phenylethynyl)-2-(4-(trifluoromethyl)phenyl)quinazoline (**3w**): white solid, yield 57.7 mg (77%); CAS: 2287295-66-1. M.p. = 158-159 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.76 (d, J = 8.0 Hz, 2H, ArH), 8.40 (d, J = 8.3 Hz, 1H, ArH), 8.10 (dt, J = 8.5, 0.9 Hz, 1H, ArH), 7.93 (ddd, J = 8.4, 6.9, 1.5 Hz, 1H, ArH), 7.78 (dt, J = 7.5, 1.4 Hz, 4H, ArH), 7.68 (ddd, J = 8.2, 6.9, 1.2 Hz, 1H, ArH),7.52-7.43(m, 3H, ArH); **^{13}C NMR** (100 MHz, $CDCl_3$) δ; 159.4, 153.0, 150.9, 141.1, 134.5, 132.6, 132.2 (q, $^2J_{C\text{-}F}$ = 32.3 Hz) , 130.3, 129.2, 129.0, 128.7, 128.3, 126.5, 125.5 (q, $^3J_{C\text{-}F}$ = 3.8 Hz) , 124.2 (q, $^1J_{C\text{-}F}$ = 273.4 Hz), 124.2, 121.2, 98.4, 85.5.



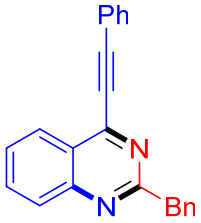
Chemical Formula: $C_{23}H_{14}N_2O$

4-(4-(Phenylethynyl)quinazolin-2-yl)benzaldehyde (**3y**): white solid, yield 65.5 mg (98%); M.p. = 200-201 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 10.16 (s, 1H, CHO), 8.86 (d, J = 8.1 Hz, 1H, ArH), 8.80 (d, J = 8.1 Hz, 1H, ArH), 8.45 (dt, J = 8.4, 1.7 Hz, 1H, ArH), 8.15 (t, J = 9.0 Hz, 1H, ArH), 8.08 (d, J = 8.0 Hz, 1H, ArH), 7.99 (t, J = 7.7 Hz, 1H, ArH), 7.86 – 7.81 (m, 3H, ArH), 7.76-7.72 (m, 1H, ArH),7.56-7.49 (m, 3H, ArH); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.2, 159.5, 153.0, 150.8, 143.3, 141.9, 137.6, 134.6, 132.6, 132.3, 130.3, 129.9, 129.2, 128.7, 128.5, 128.4, 126.5, 124.1, 121.2, 118.9, 113.8, 98.4, 85.5. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{15}N_2O^+$, 335.1184, found 335.1189.



Chemical Formula: $C_{20}H_{12}N_2O$

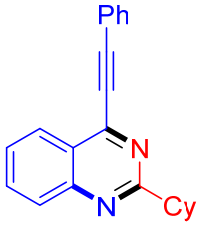
2-(Furan-2-yl)-4-(phenylethynyl)quinazoline (**3z**): white solid, yield 52.2 mg (88%) M.p. = 125-126 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz) δ; 8.37 (dd, J = 8.2, 1.4 Hz, 1H, ArH), 8.11 (d, J = 8.4 Hz, 1H, ArH), 7.91 (ddd, J = 8.5, 6.9, 1.5 Hz, 1H, ArH), 7.78-7.76 (m, 2H, ArH), 7.70 (dd, J = 1.8, 0.9 Hz, 1H, ArH), 7.64 (ddd, J = 8.1, 6.8, 1.2 Hz, 1H, ArH) 7.53-7.52 (m, 1H, ArH), 7.49-7.43 (m, 3H, ArH), 6.62 (dd, J = 3.4, 1.8 Hz, 1H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ; 154.0, 153.1, 152.3, 150.7, 145.4, 134.6, 132.6, 130.2, 128.8, 128.7, 127.6, 126.6, 123.8, 121.2, 114.4, 112.3, 98.4, 85.3. **HRMS** (ESI-TOF, $[M + Na]^+$): calcd for $C_{20}H_{12}N_2ONa^+$, 319.0847, found 319.0845.



3aa

Chemical Formula: $C_{23}H_{16}N_2$

2-Benzyl-4-(phenylethynyl)quinazoline (**3aa**): light yellow soild, yield 39.7 mg (62%). M.p = 98-99 °C **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.35 (d, J = 8.2 Hz, 1H, ArH), 8.01 (d, J = 8.4 Hz, 1H, ArH), 7.88 (ddd, J = 8.5, 6.8, 1.5 Hz, 1H, ArH), 7.76-7.69 (m, 2H, ArH), 7.63 (t, J = 7.6 Hz, 1H, ArH), 7.48-7.41 (m, 5H, ArH), 7.30 (t, J = 7.6 Hz, 2H, ArH), 7.21 (t, J = 7.4 Hz, 1H, ArH), 4.48 (s, 2H, CH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ; 165.8, 153.0, 150.7, 138.5, 134.1, 132.5, 130.1, 129.2, 128.6, 128.5, 128.4, 1276, 126.4, 126.3, 123.5, 121.3, 98.2, 85.4, 46.3. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{23}H_{17}N_2^+$, 321.1392, found 321.1400.

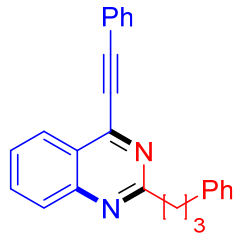


3bb

Chemical Formula: $C_{22}H_{20}N_2$

2-Cyclohexyl-4-(phenylethynyl)quinazoline (**3bb**): light yellow soild, yield 35.6 mg (57%) M.p = 89-90 °C. **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.36 (d, J = 8.2 Hz, 1H, ArH), 8.00 (d, J = 8.4 Hz, 1H, ArH), 7.88 (t, J = 7.7 Hz, 1H, ArH), 7.77-7.70 (m, 2H, ArH), 7.62 (t, J = 7.6 Hz, 1H, ArH), 7.48-7.42 (m, 3H, ArH), 3.08 (tt, J = 11.9, 3.6 Hz, 1H, CH), 2.13-2.10 (m, 2H, Cy), 1.93-1.89 (m, 2H,

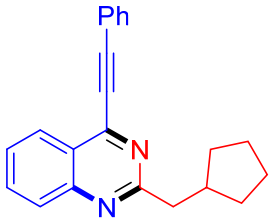
Cy),1.85-1.76 (m, 3H, Cy), 1.50-1.36(m, 3H, Cy); ^{13}C NMR (125 MHz, $CDCl_3$) δ;170.8, 152.7, 150.6, 133.9, 132.5, 130.0, 128.6, 128.5, 127.2, 126.3, 123.7, 121.4, 97.6, 85.5, 47.9, 31.9, 26.3, 26.0. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{21}N_2^+$, 313.1705, found 313.1711.



3cc

Chemical Formula: $C_{25}H_{20}N_2$

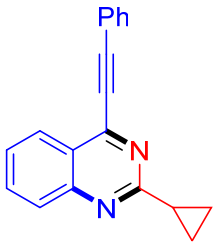
4-(Phenylethynyl)-2-(3-phenylpropyl)quinazoline (**3cc**): light yellow oil, yield 54.4 mg (78%). **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.37 (d, J = 8.2 Hz, 1H, ArH), 7.99 (d, J = 8.4 Hz, 1H, ArH), 7.89 (t, J = 7.7 Hz, 1H, ArH), 7.78-7.70 (m, 2H, ArH), 7.64 (t, J = 7.6 Hz, 1H, ArH), 7.48-7.42 (m, 3H, ArH), 7.29-7.24 (m, 4H, ArH), 7.17 (t, J = 7.0 Hz, 1H, ArH), 3.20 (t, J = 7.8 Hz, 2H, CH_2), 2.79 (t, J = 7.8 Hz, 2H, CH_2), 2.29 (p, J = 7.8 Hz, 2H, CH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ; 167.2, 152.7, 150.6, 142.2, 134.2, 132.6, 130.1, 128.6, 128.6, 128.3, 127.4, 126.4, 125.7, 123.4, 121.3, 98.0, 85.4, 39.7, 35.8, 30.7. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{25}H_{21}N_2^+$, 349.1705, found 349.1705.



3dd

Chemical Formula: $C_{22}H_{20}N_2$

2-(Cyclopentylmethyl)-4-(phenylethynyl)quinazoline (**3dd**): light yellow oil, yield 36.2 mg (58%). **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.36 (d, J = 8.2 Hz, 1H, ArH), 7.99 (d, J = 8.4 Hz, 1H, ArH), 7.87 (t, J = 7.7 Hz, 1H, ArH), 7.76-7.72 (m, 2H, ArH), 7.62 (t, J = 7.6 Hz, 1H, ArH), 7.47-7.41 (m, 3H, ArH), 3.13 (d, J = 7.5 Hz, 2H, CH_2), 2.58 (hept, J = 7.7 Hz, 1H, Cyclopentenyl), 1.91-1.73 (m, 3H, Cyclopentenyl), 1.71-1.65 (m, 2H, Cyclopentenyl), 1.59-1.51(m, 2H, Cyclopentenyl), 1.39-1.32 (m, 1H, Cyclopentenyl); ^{13}C NMR (125 MHz, $CDCl_3$) δ; 167.3, 152.6, 150.5, 134.1, 132.5, 130.1, 128.6, 128.3, 127.3, 126.3, 123.4, 121.3, 97.8, 85.4, 45.8, 39.9, 32.4, 25.1. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{22}H_{21}N_2^+$, 313.1705, found 313.1712.



Chemical Formula: $C_{19}H_{14}N_2$

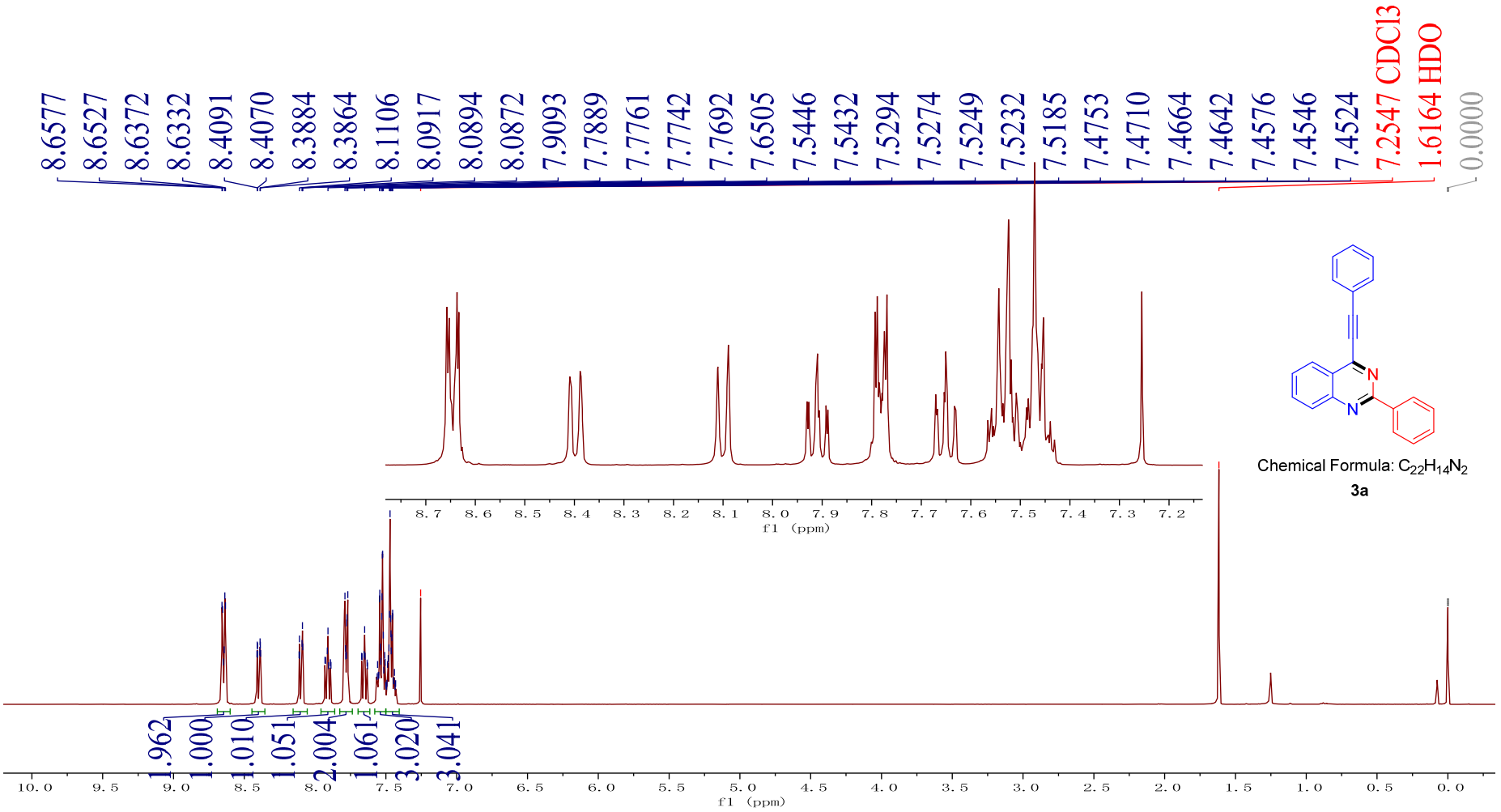
3ee

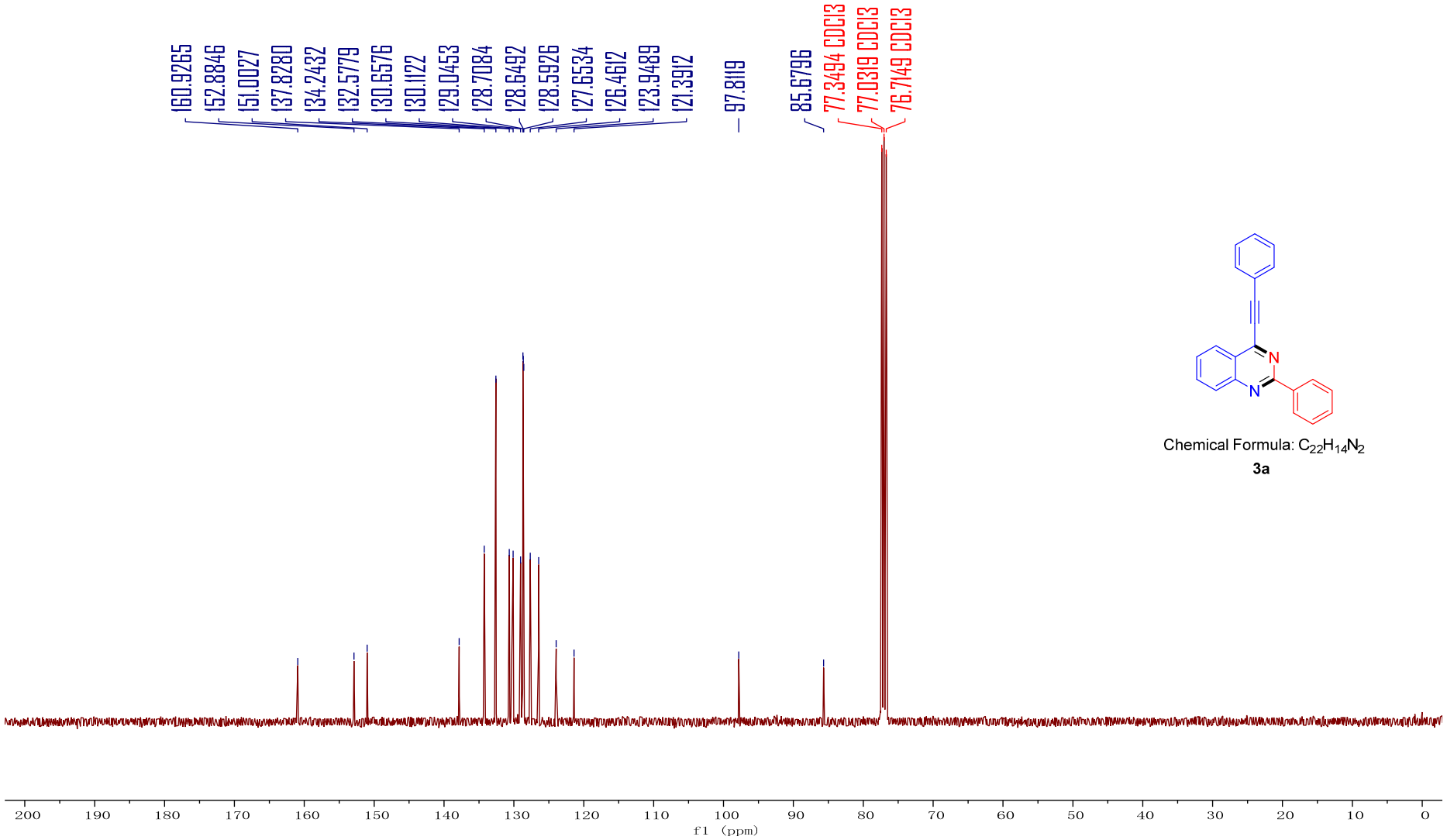
2-Cyclopropyl-4-(phenylethynyl)quinazoline (**3ee**): light yellow oil, yield 22.2 mg (41%). **^{1}H NMR** ($CDCl_3$, 500 MHz) δ; 8.32 (d, J = 8.2 Hz, 1H, ArH), 7.91 (d, J = 8.4 Hz, 1H, ArH), 7.84 (t, J = 7.7 Hz, 1H, ArH), 7.74 (dd, J = 7.5, 1.7 Hz, 2H, ArH), 7.57 (t, J = 7.5 Hz, 1H, ArH), 7.49-7.42 (m, 3H, ArH), 2.43 (tt, J = 8.5, 4.7 Hz, 1H, CH), 1.32 (dt, J = 6.5, 3.5 Hz, 2H, CH_2), 1.14 (dq, J = 7.1, 3.9 Hz, 2H, CH_2); ^{13}C NMR (125 MHz, $CDCl_3$) δ; 168.2, 152.5, 150.7, 134.1, 132.5, 130.0, 128.6, 127.9, 126.7, 126.4, 123.6, 121.4, 97.5, 85.5, 18.7, 10.7. **HRMS** (ESI-TOF, $[M + H]^+$): calcd for $C_{19}H_{15}N_2^+$, 271.1235, found 271.1239.

Reference

1. (a) T.-R. Li, B.-Y. Cheng, Y.-N. Wang, M.-M. Zhang, L.-Q. Lu, W.-J. Xiao, *Angew. Chem. Int. Ed*., **2016**, *55*, 12422–12426. (b) S. Wang, M. Liu, X. Chen, H. Wang, H. Zhai, *Chem. Commun.*, **2018**, *54*, 8375–8378.
2. (a) S. Rakshit, C. Grohmann, T. Besset, F. Glorius, *J. Am. Chem. Soc*., **2011**, *133*, 2350–2353. (b) N. J. Webb, S. P. Marsden, S. A. Raw, *Org. Lett.,* **2014**, *16*, 4718−4721.

7. ^{1}H NMR and ^{13}C NMR Spectra of 3

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128.5926
127.6534
126.4612
123.9489
121.3912
97.8119
85.6796
77.3494 CDCl3
77.0319 CDCl3
76.7149 CDCl3
N
N
Chemical Formula: $C_{22}H_{14}N_2$
3a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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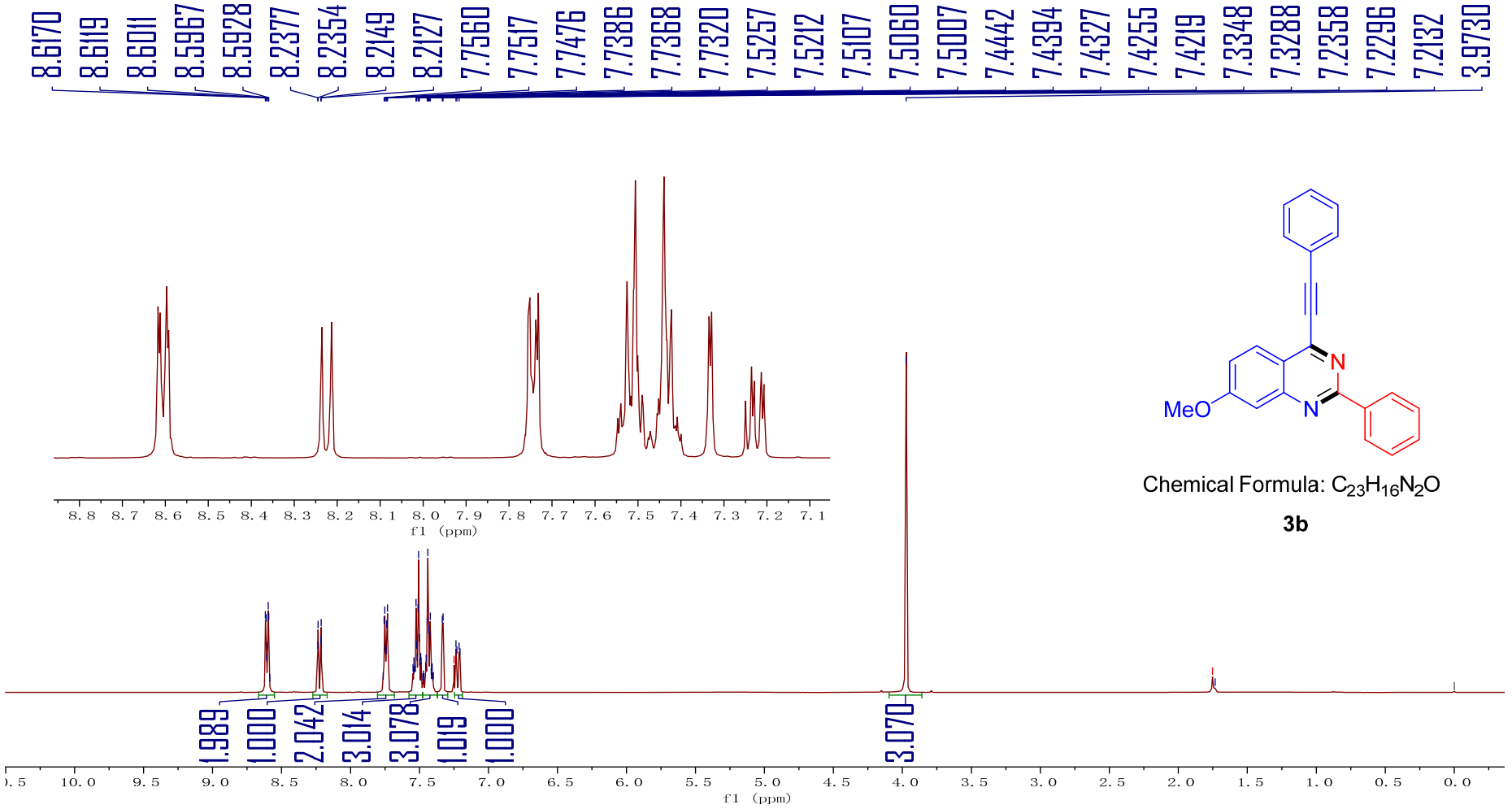
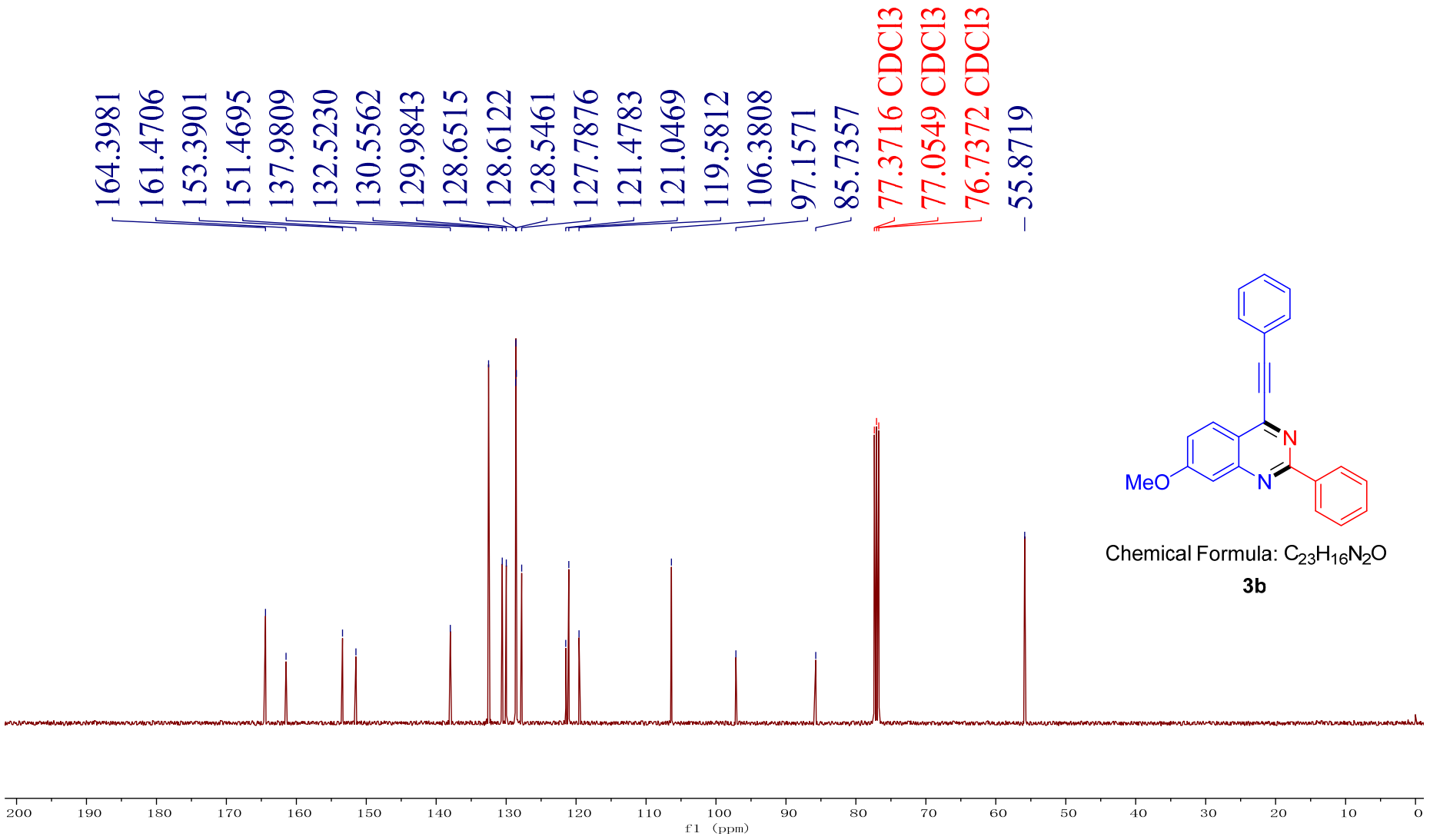
f1 (ppm)



Chemical Formula: $C_{23}H_{16}N_2O$

3b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128.5461
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121.0469
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Chemical Formula: C23H16N2O
3b
200
190
180
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160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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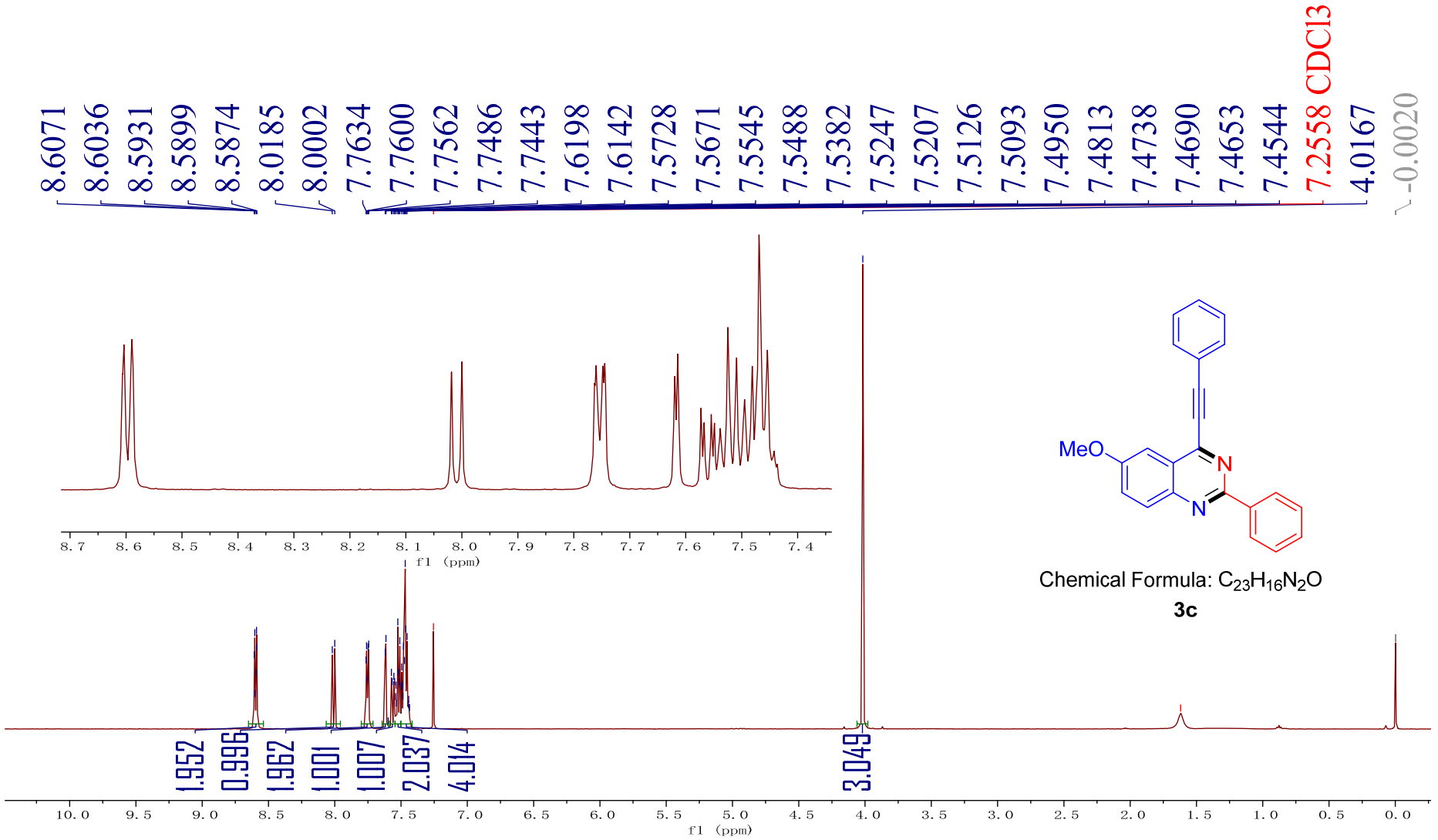
f1 (ppm)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7.5093
7.4950
7.4813
7.4738
7.4690
7.4653
7.4544
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N
N
Chemical Formula: C23H16N2O
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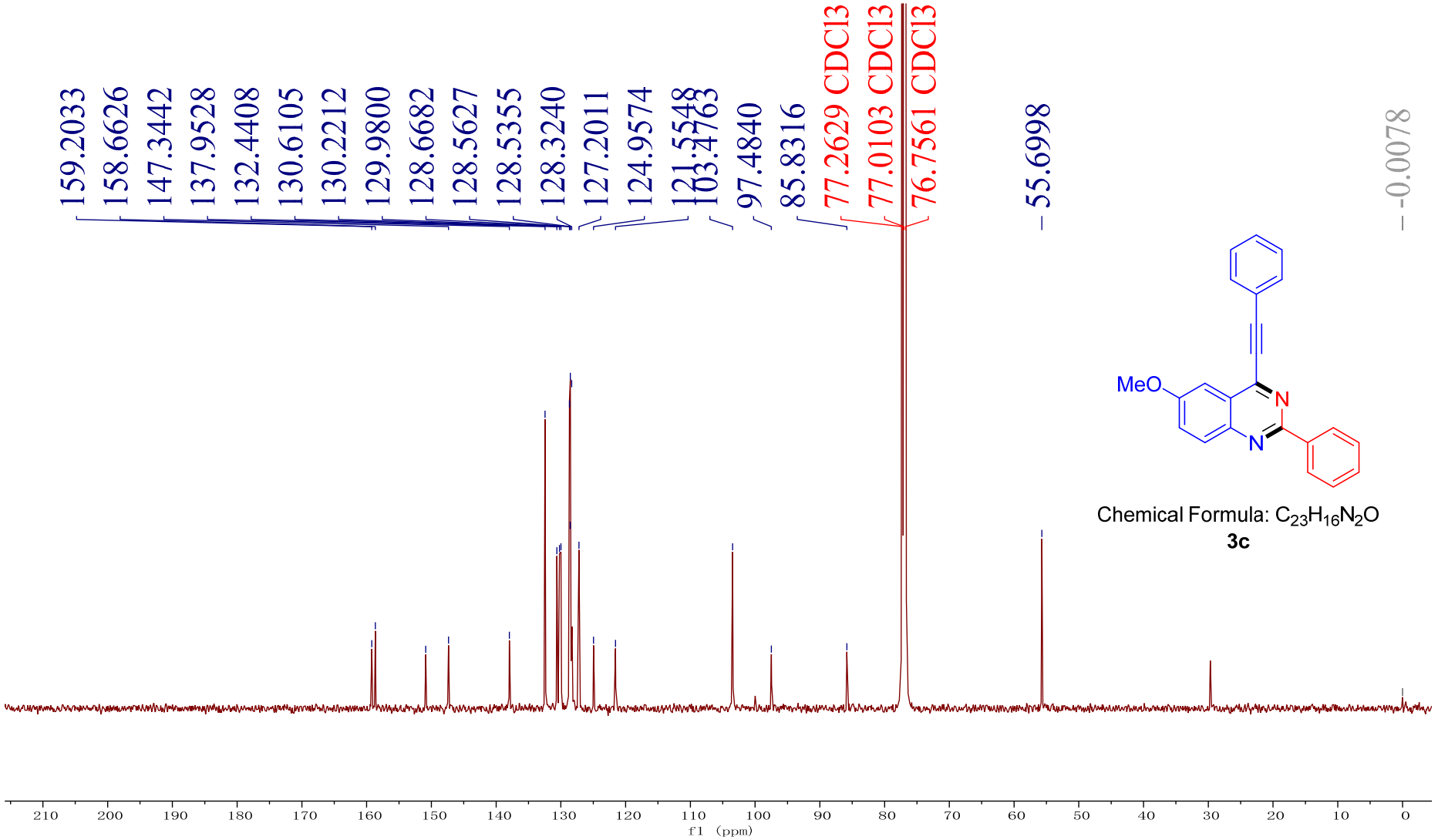
3.049
f1 (ppm)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97.4840
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MeO
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Chemical Formula: $C_{23}H_{16}N_2O$
3c
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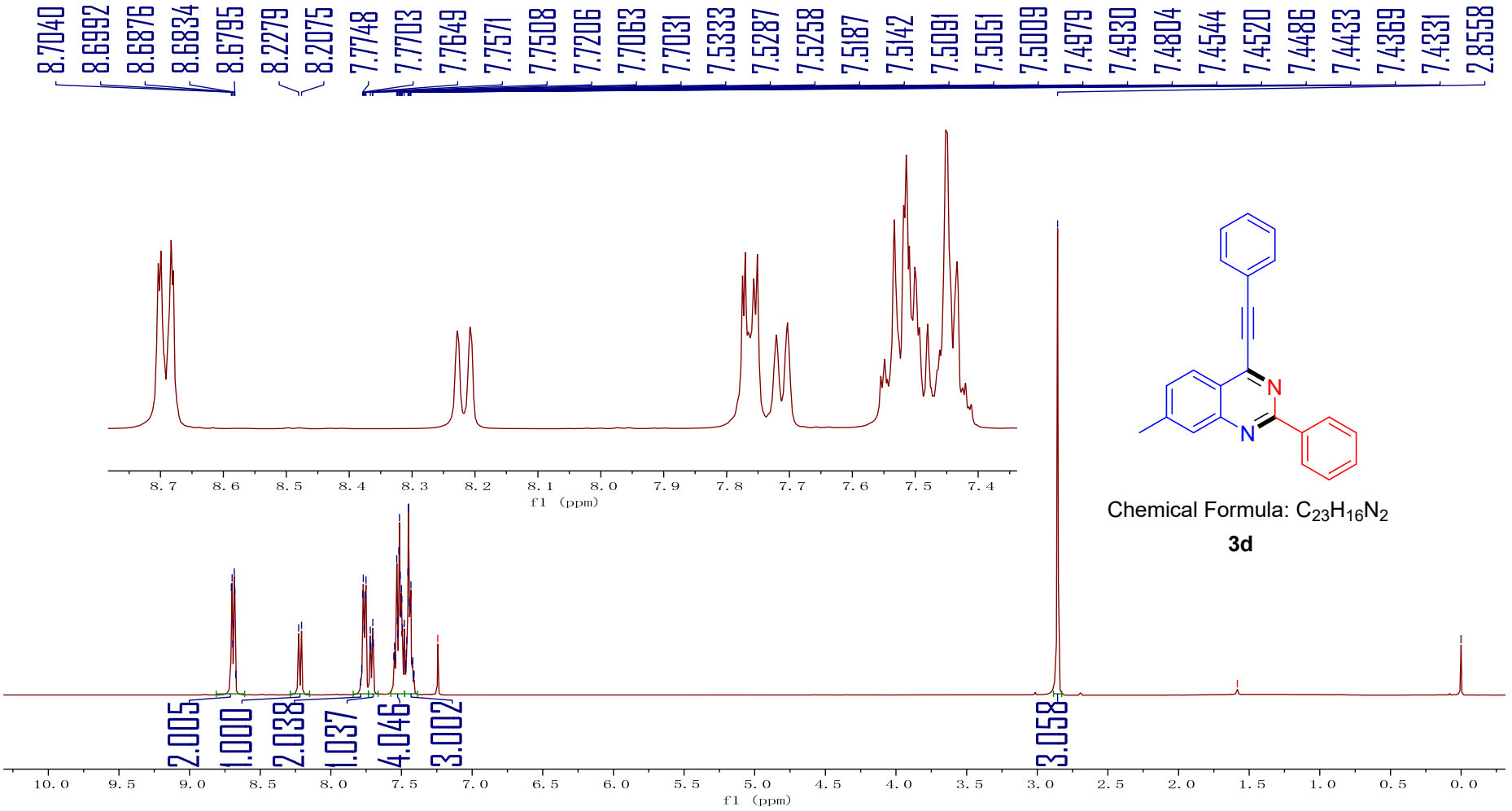
f1 (ppm)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8.6834
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7.5187
7.5142
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7.5009
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7.4930
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7.4433
7.4369
7.4331
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f1 (ppm)
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1.000
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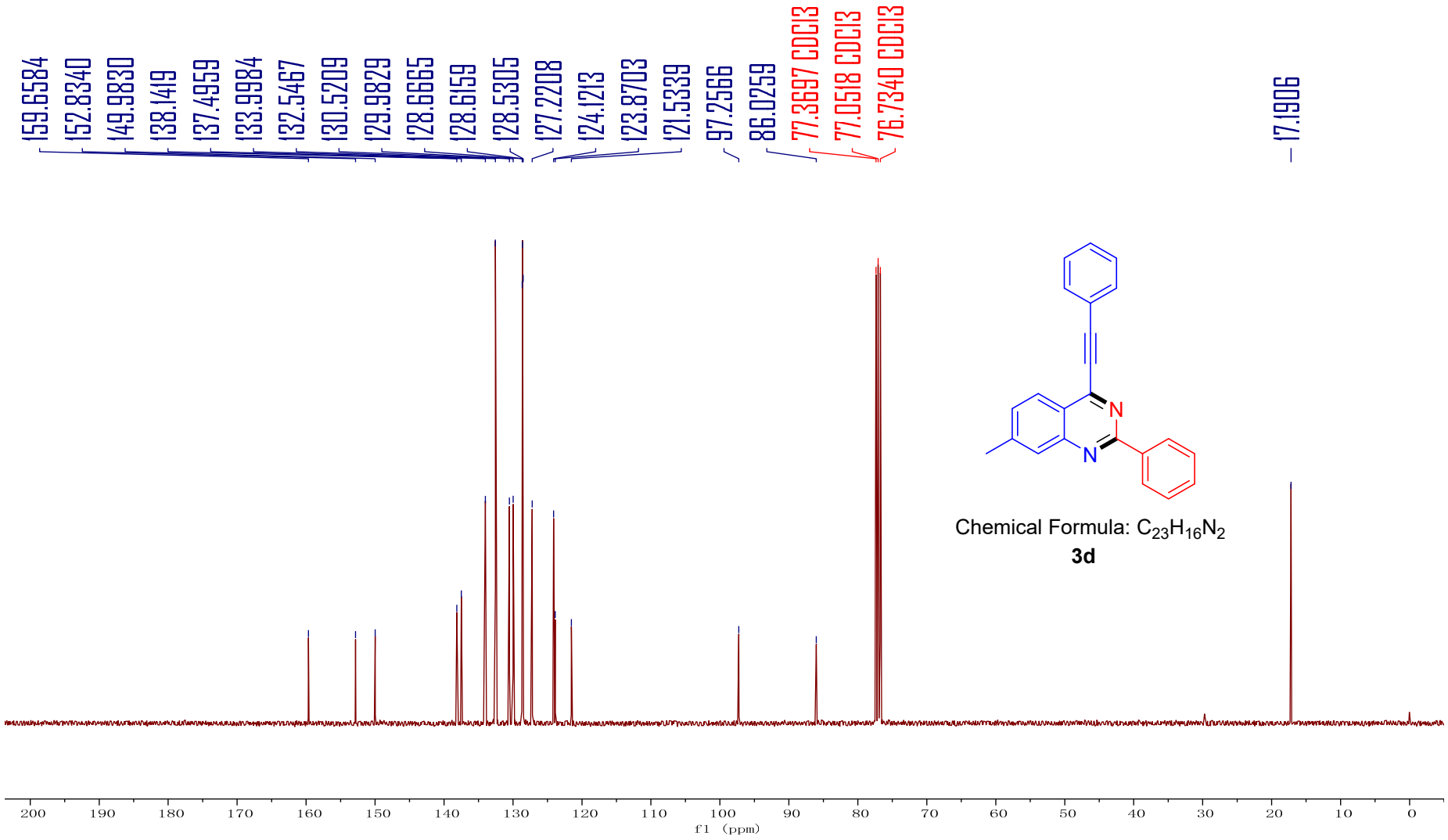
Chemical Formula: $C_{23}H_{16}N_2$
3d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137.4959
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132.5467
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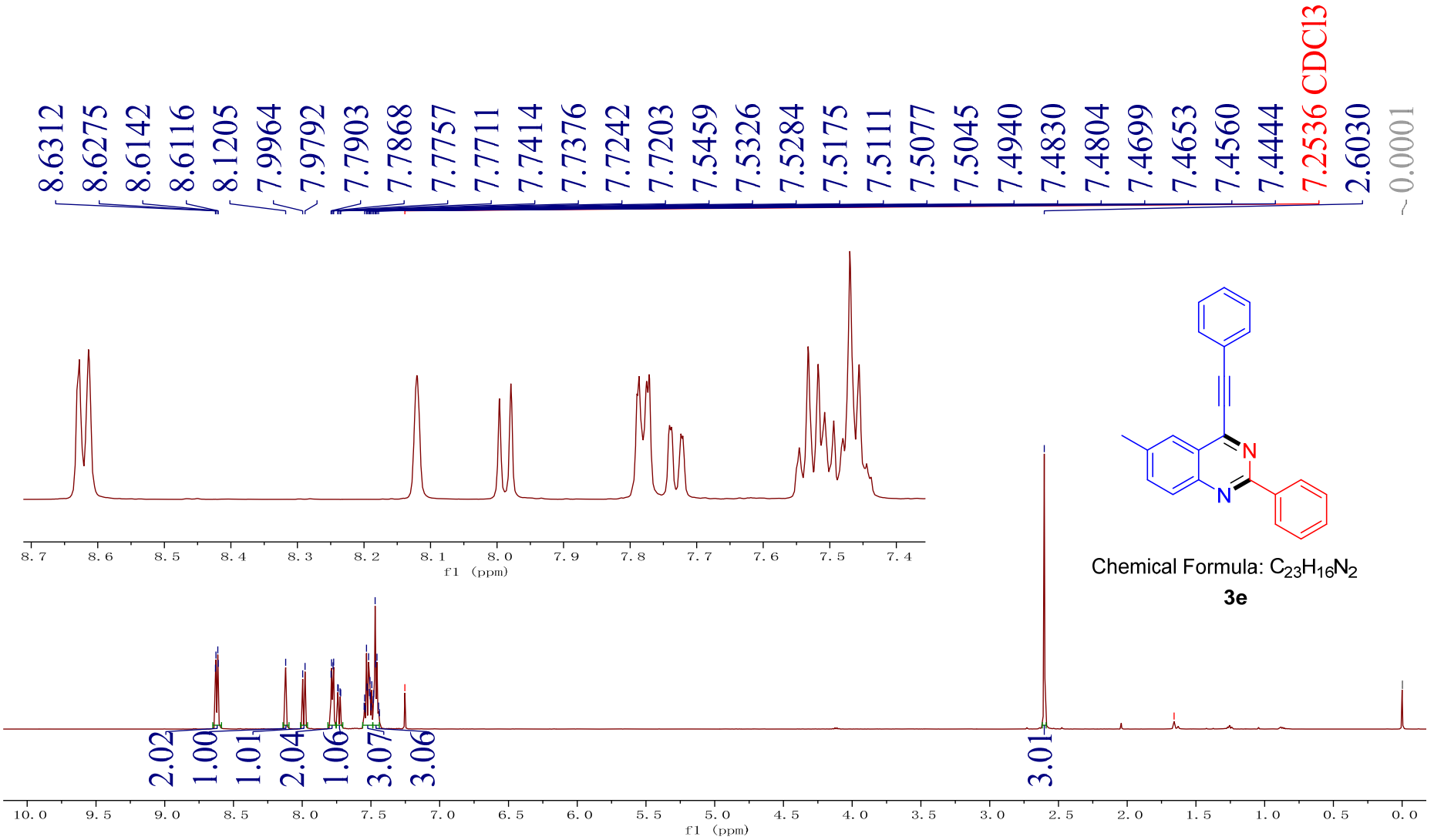
127.2208
124.1213
123.8703
121.5339
97.2566
86.0259
77.3697 CDCl3
77.0518 CDCl3
76.7340 CDCl3
17.1906
N
N
Chemical Formula: $C_{23}H_{16}N_2$
3d
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.4830
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7.4444
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f1 (ppm)
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1.00
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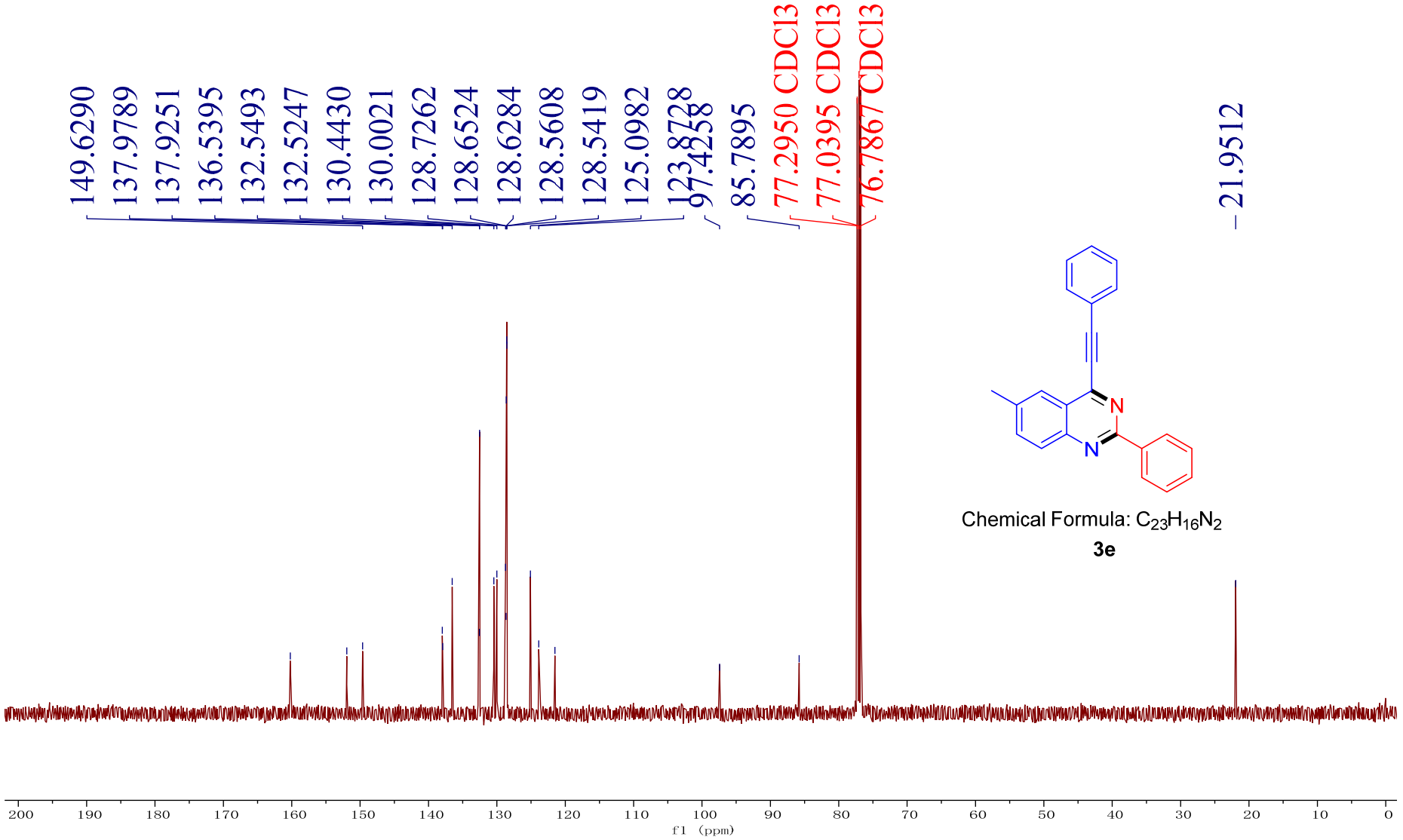
3.06
3.01
f1 (ppm)
N
N
Chemical Formula: C23H16N2
3e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N
N
Chemical Formula: C23H16N2
3e
200
190
180
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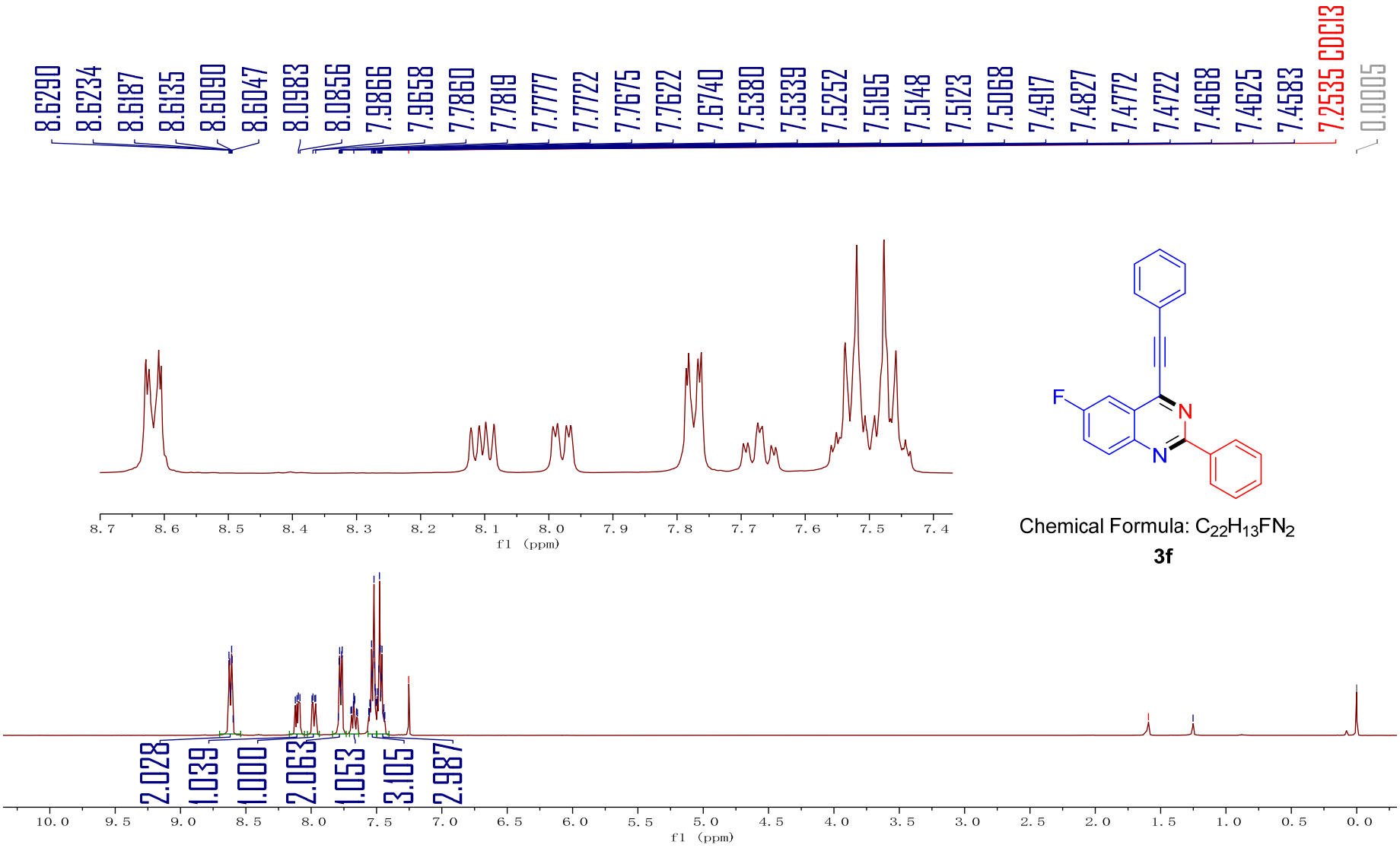
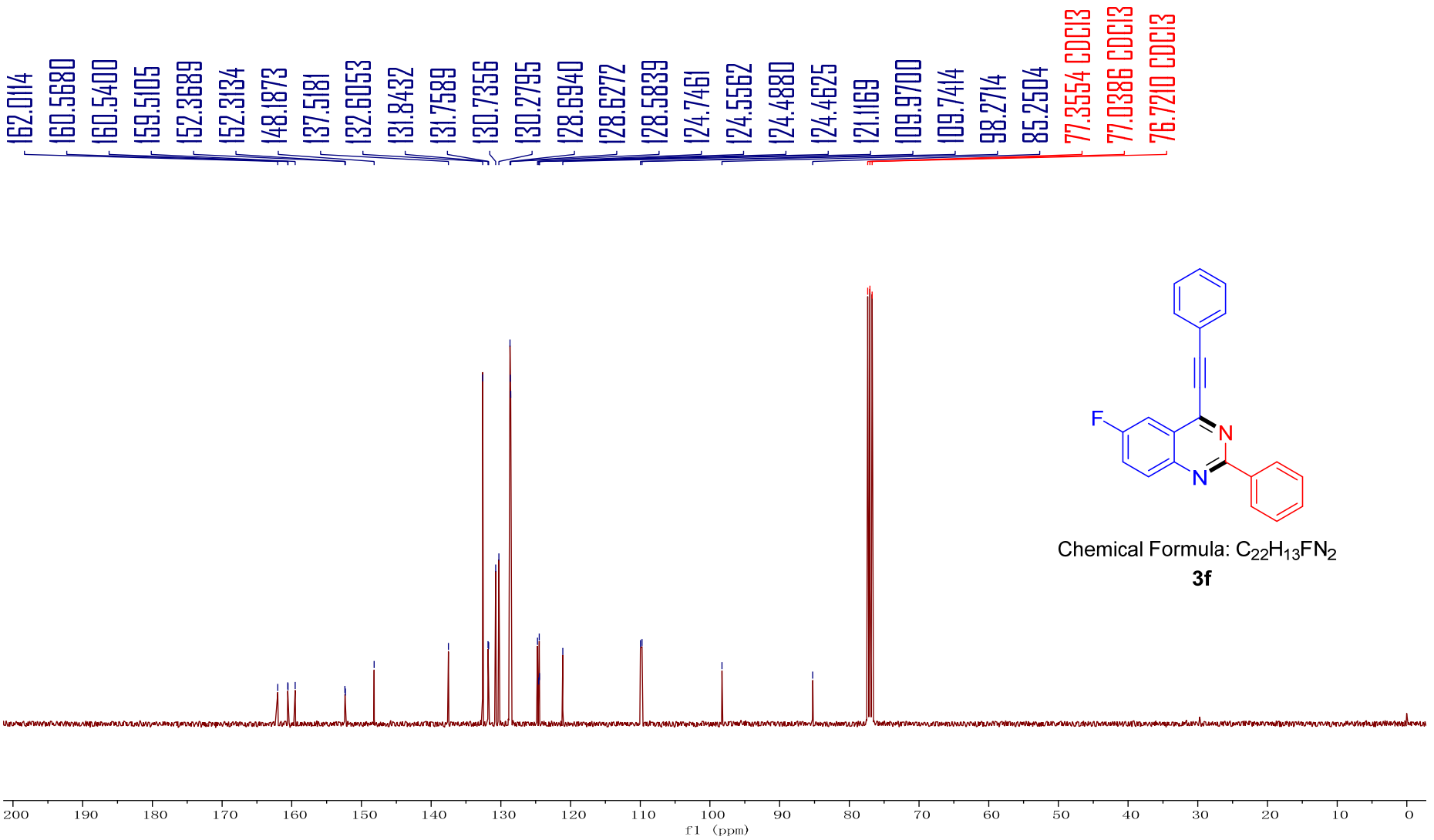
f1 (ppm)



Chemical Formula: $C_{22}H_{13}FN_2$

3f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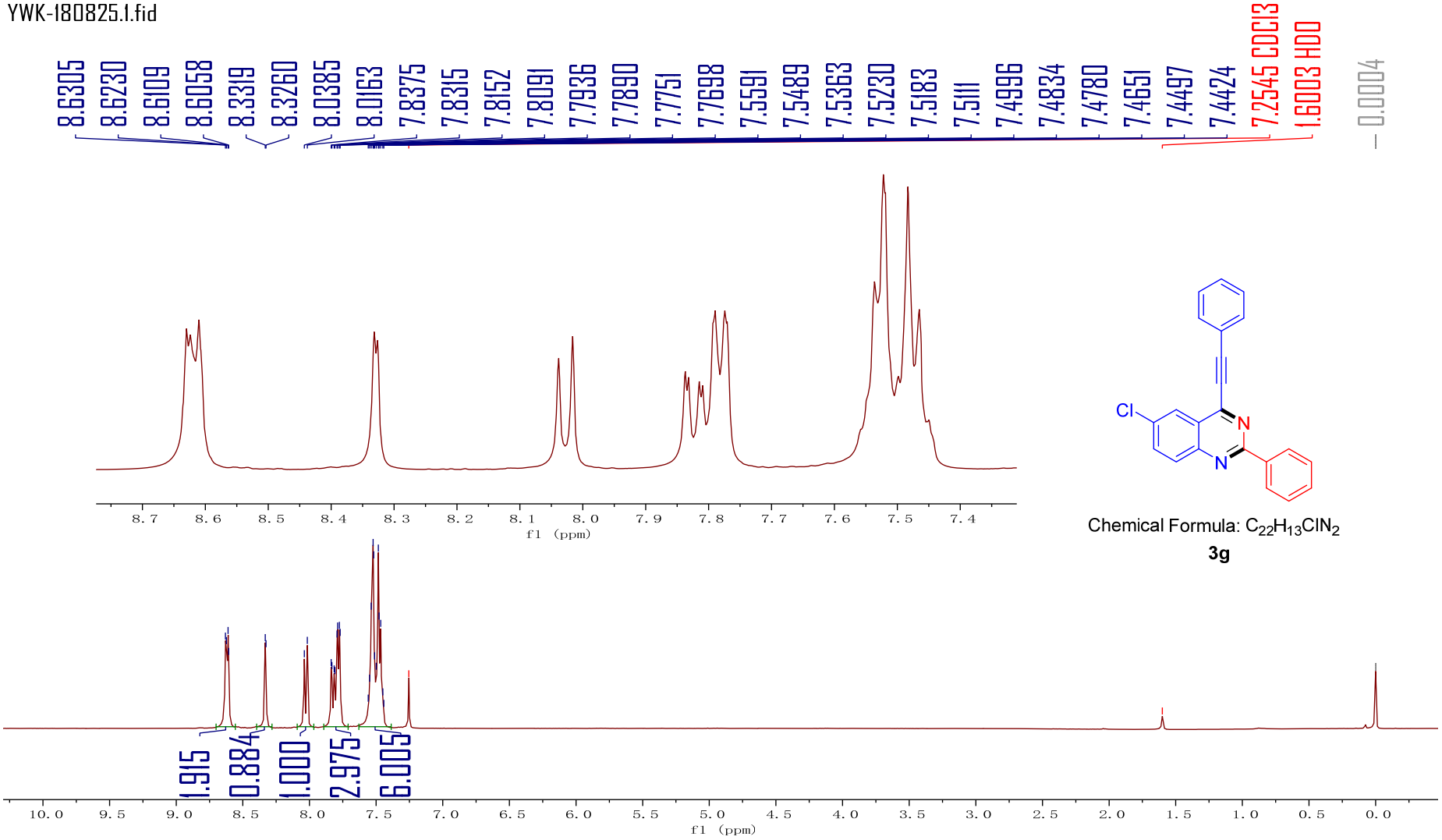
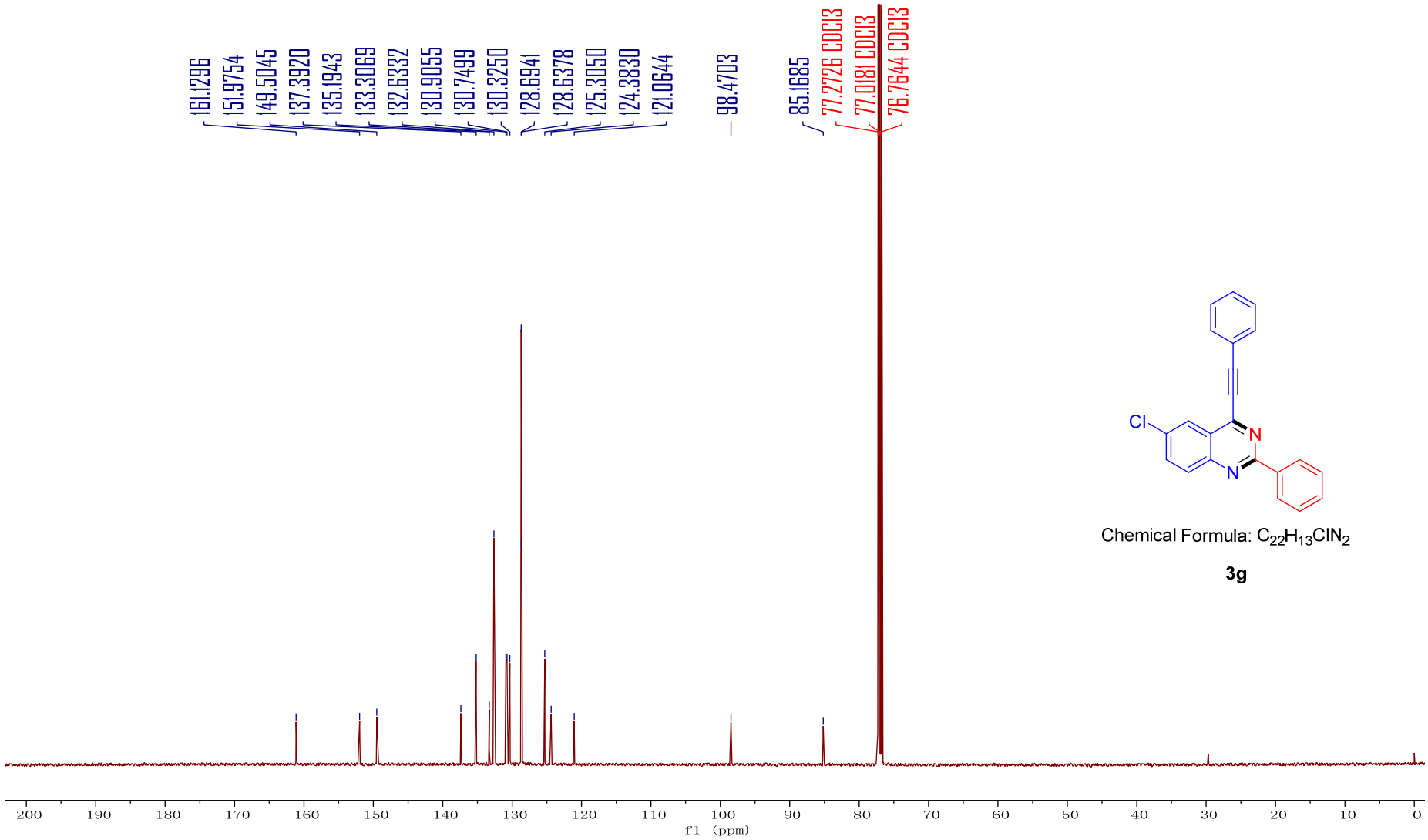
131.7589
130.7356
130.2795
128.6940
128.6272
128.5839
124.7461
124.5562
124.4880
124.4625
121.1169
109.9700
109.7414
98.2714
85.2504
77.3554 CDCl3
77.0386 CDCl3
76.7210 CDCl3
F
N
N
Chemical Formula: $C_{22}H_{13}FN_2$
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

YWK-180825.1.fid



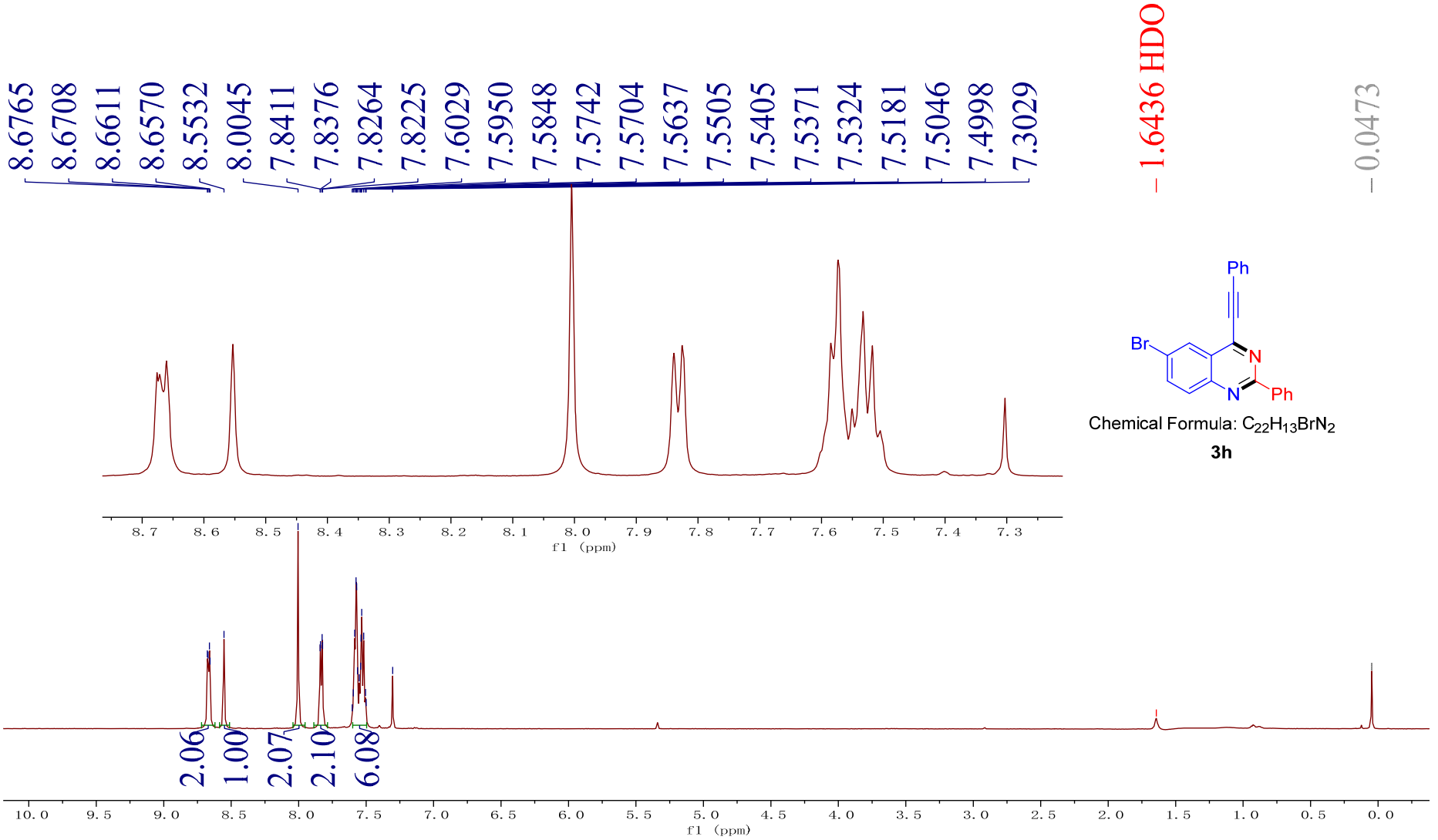
Chemical Formula: $C_{22}H_{13}ClN_2$

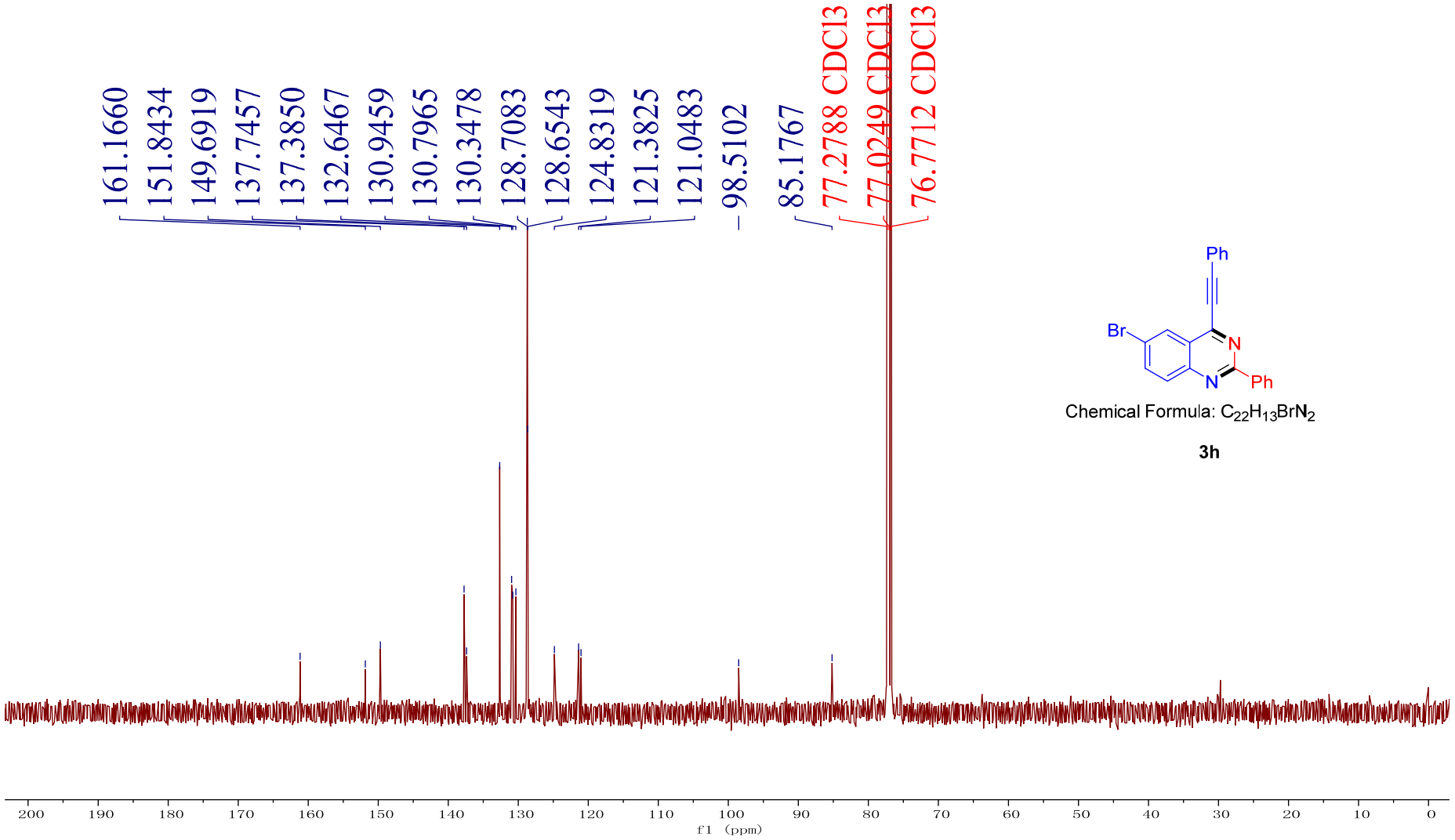
3g

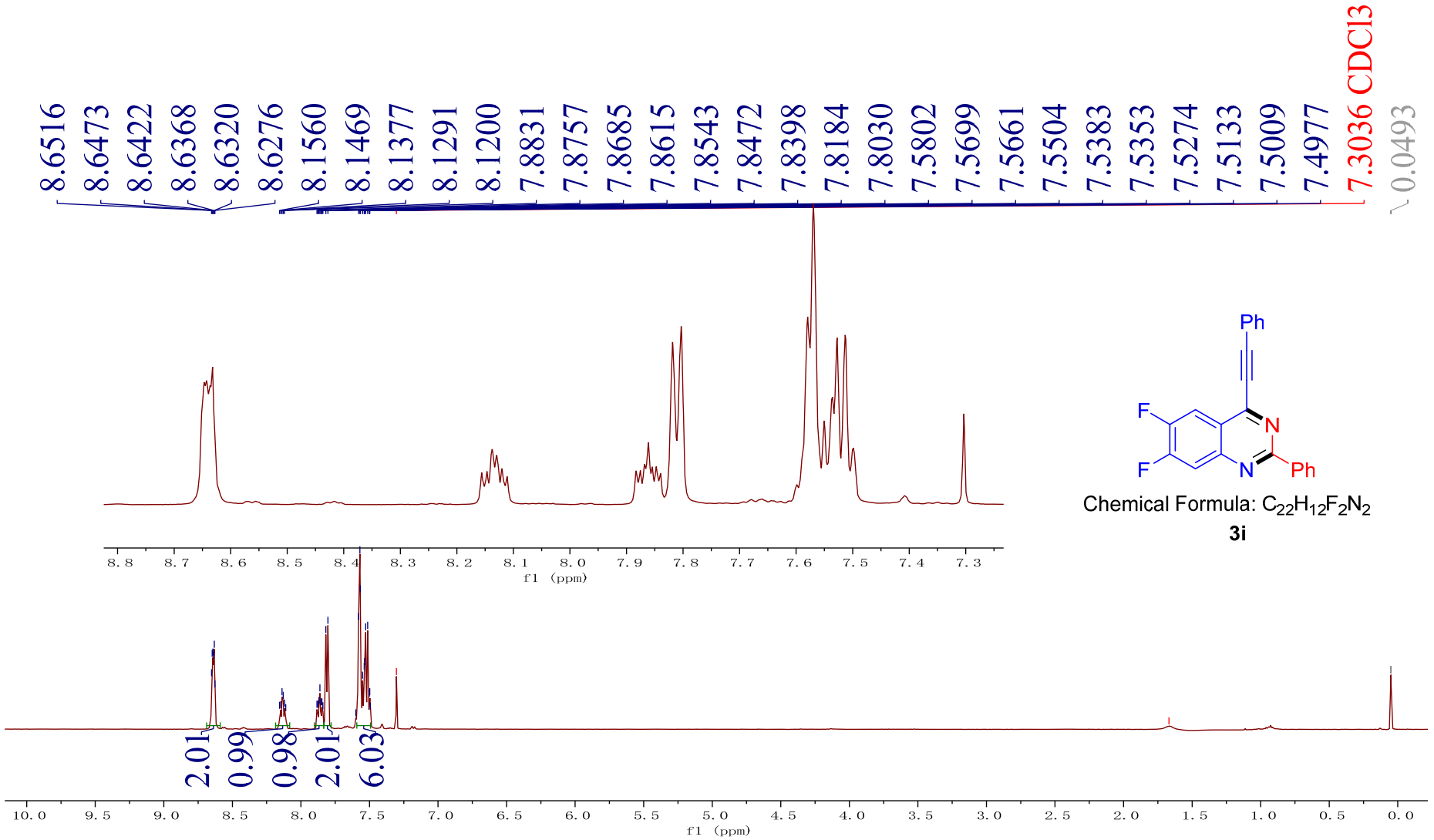


Chemical Formula: $C_{22}H_{13}ClN_2$

3g

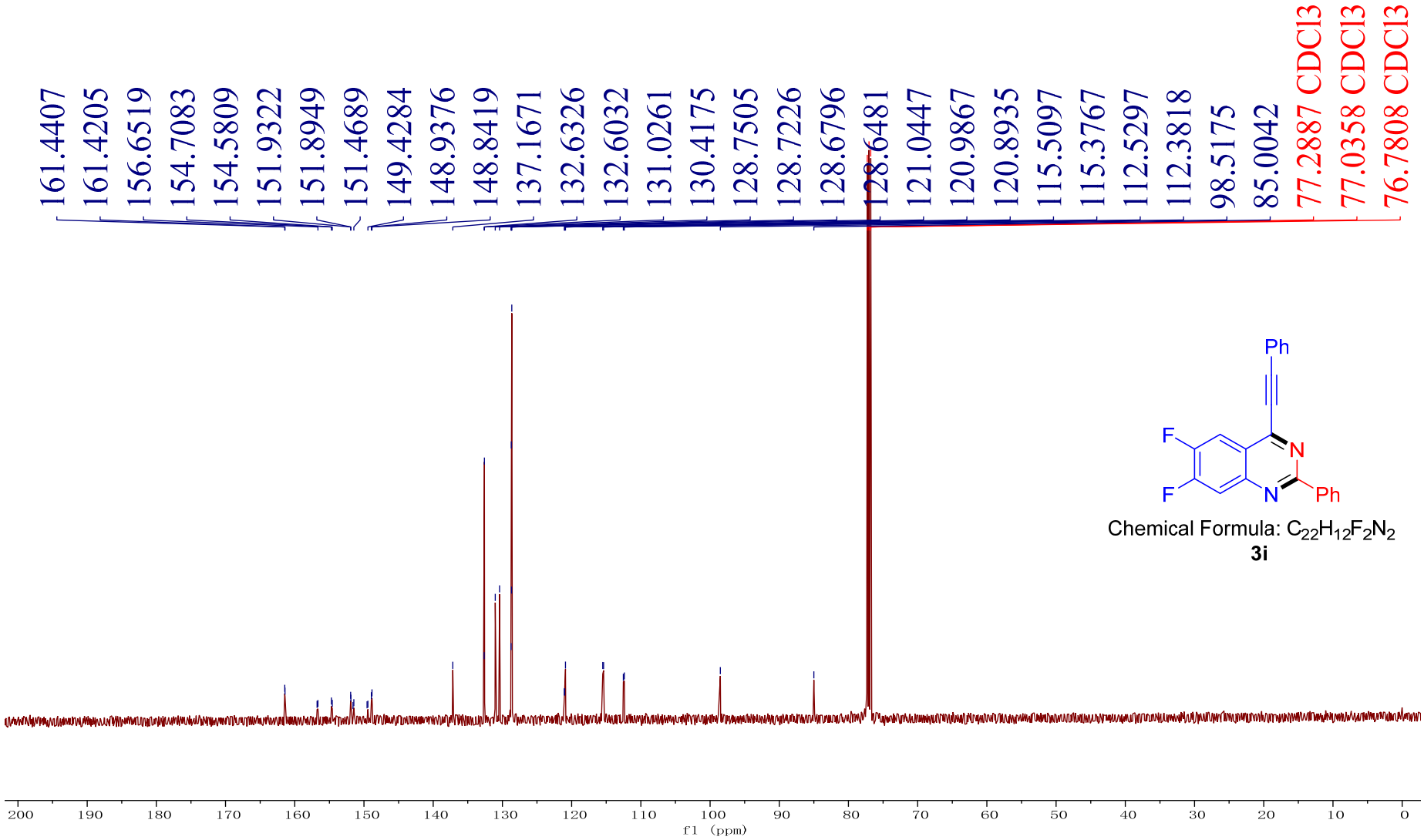

8.6765
8.6708
8.6611
8.6570
8.5532
8.0045
7.8411
7.8376
7.8264
7.8225
7.6029
7.5950
7.5848
7.5742
7.5704
7.5637
7.5505
7.5405
7.5371
7.5324
7.5181
7.5046
7.4998
7.3029
1.6436 HDO
0.0473
Ph
Br
N
N
Ph
Chemical Formula: C22H13BrN2
3h
f1 (ppm)
2.06
1.00
2.07
2.10
6.08
f1 (ppm)


161.1660
151.8434
149.6919
137.7457
137.3850
132.6467
130.9459
130.7965
130.3478
128.7083
128.6543
124.8319
121.3825
121.0483
98.5102
85.1767
77.2788 CDC13
77.0249 CDC13
76.7712 CDC13
Ph
Br
N
N
Ph
Chemical Formula: $C_{22}H_{13}BrN_2$
3h
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



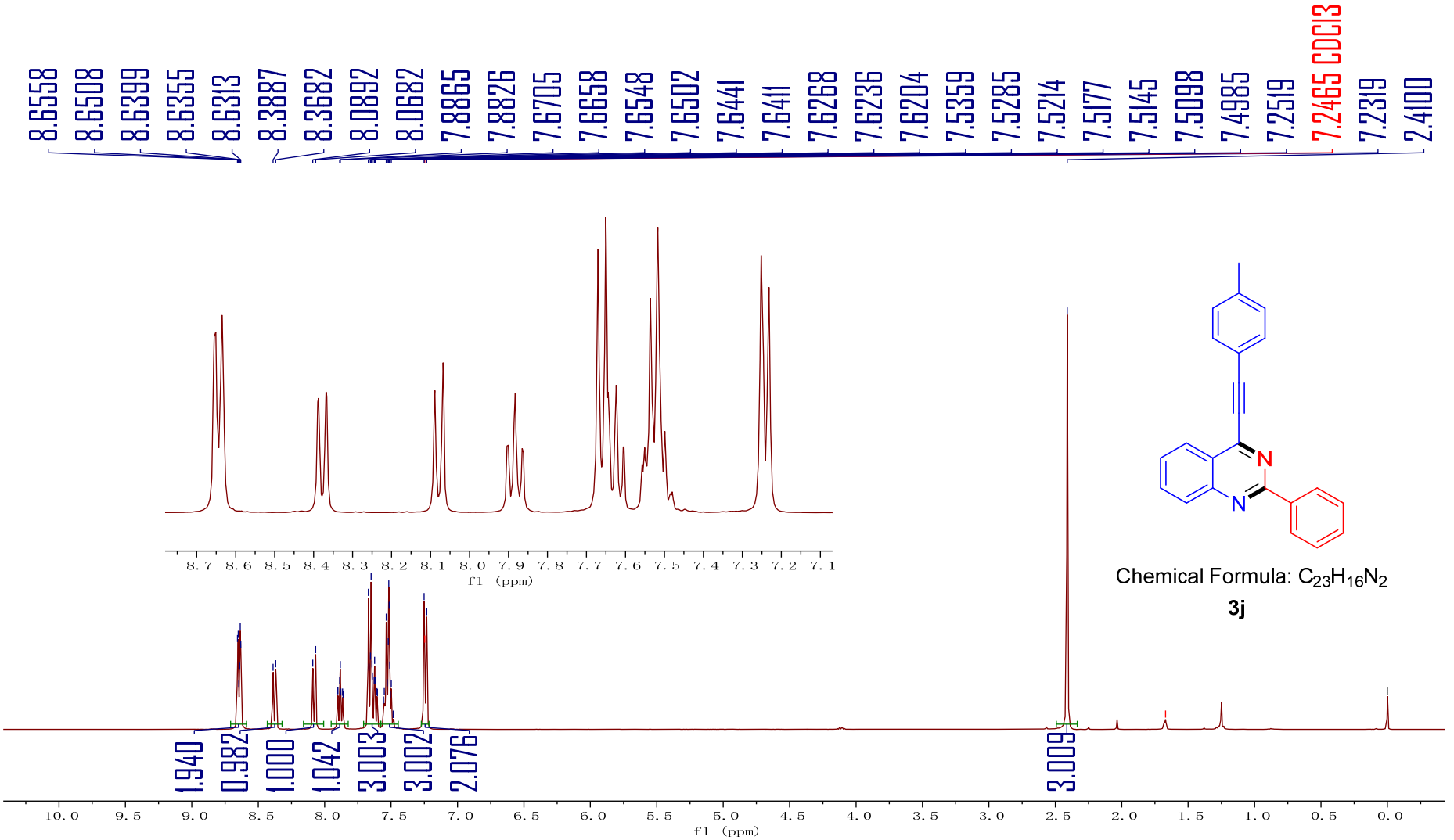
Chemical Formula: $C_{22}H_{12}F_2N_2$

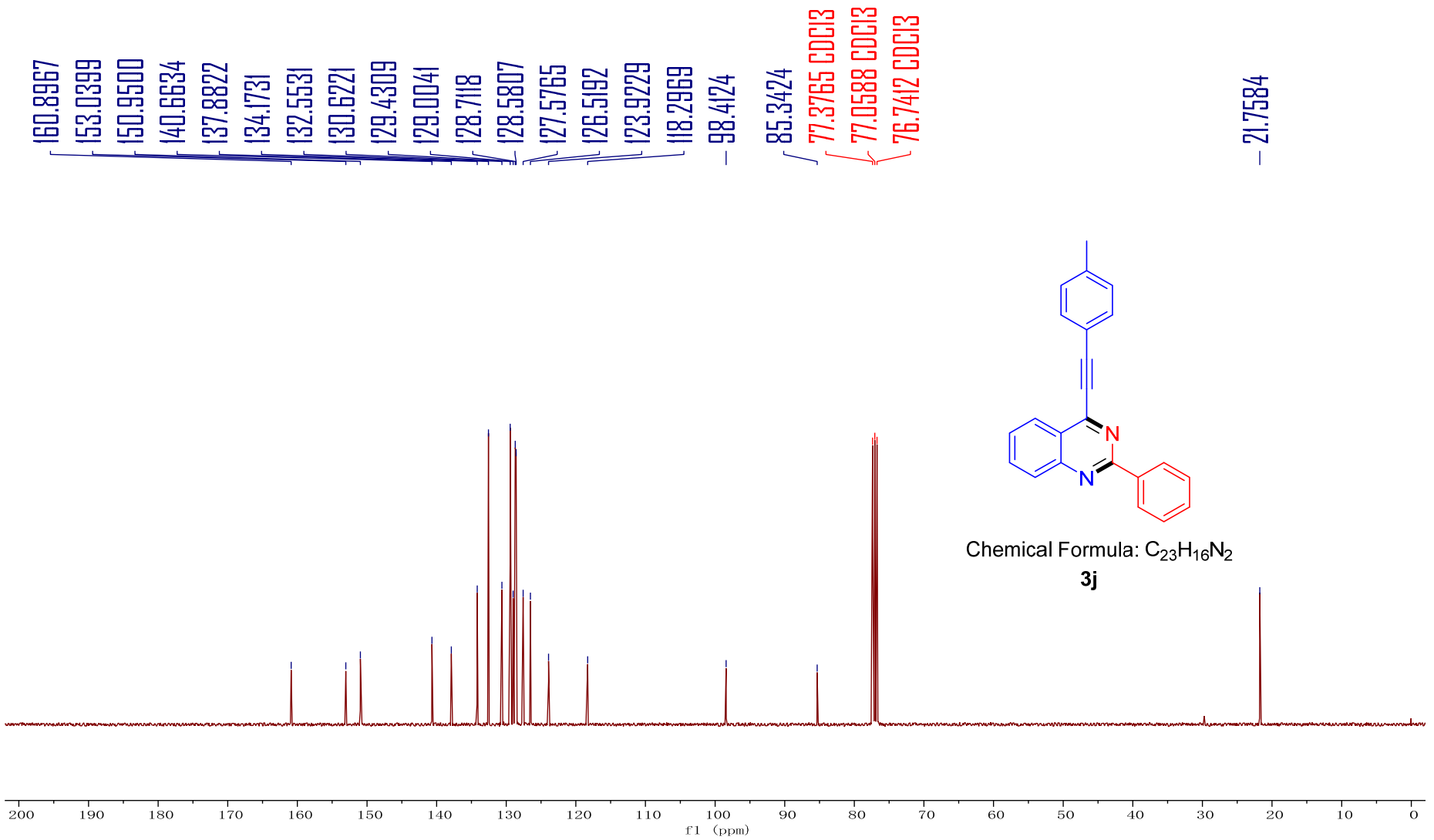
3i



Chemical Formula: $C_{22}H_{12}F_2N_2$

3i


8.6558
8.6508
8.6399
8.6355
8.6313
8.3887
8.3682
8.0892
8.0682
7.8865
7.8826
7.6705
7.6658
7.6548
7.6502
7.6441
7.6411
7.6268
7.6236
7.6204
7.5359
7.5285
7.5214
7.5177
7.5145
7.5098
7.4985
7.2519
7.2465 CDCl3
7.2319
2.4100
1.940
0.982
1.000
1.042
3.003
3.002
2.076
3.009
f1 (ppm)
Chemical Formula: C23H16N2
3j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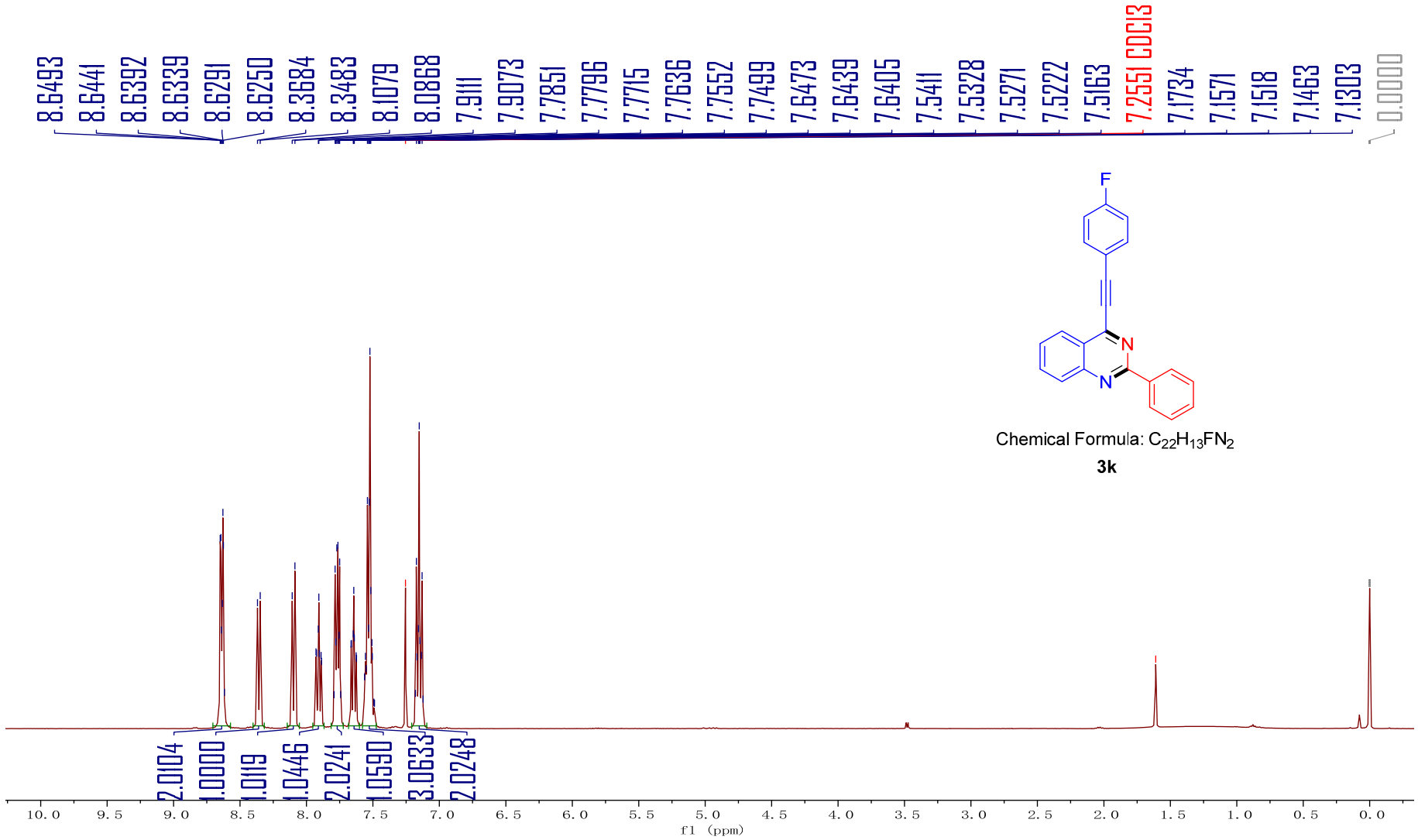
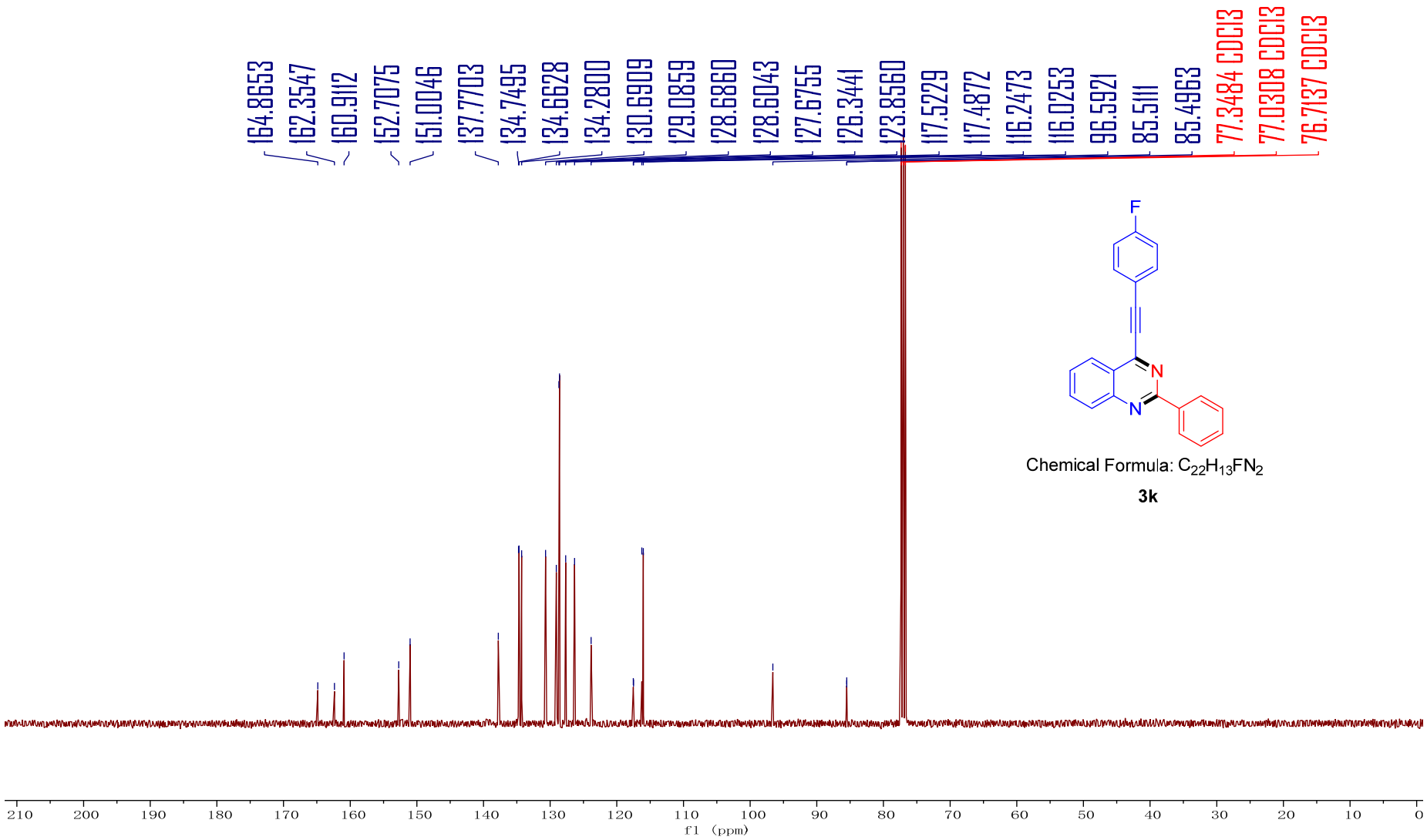
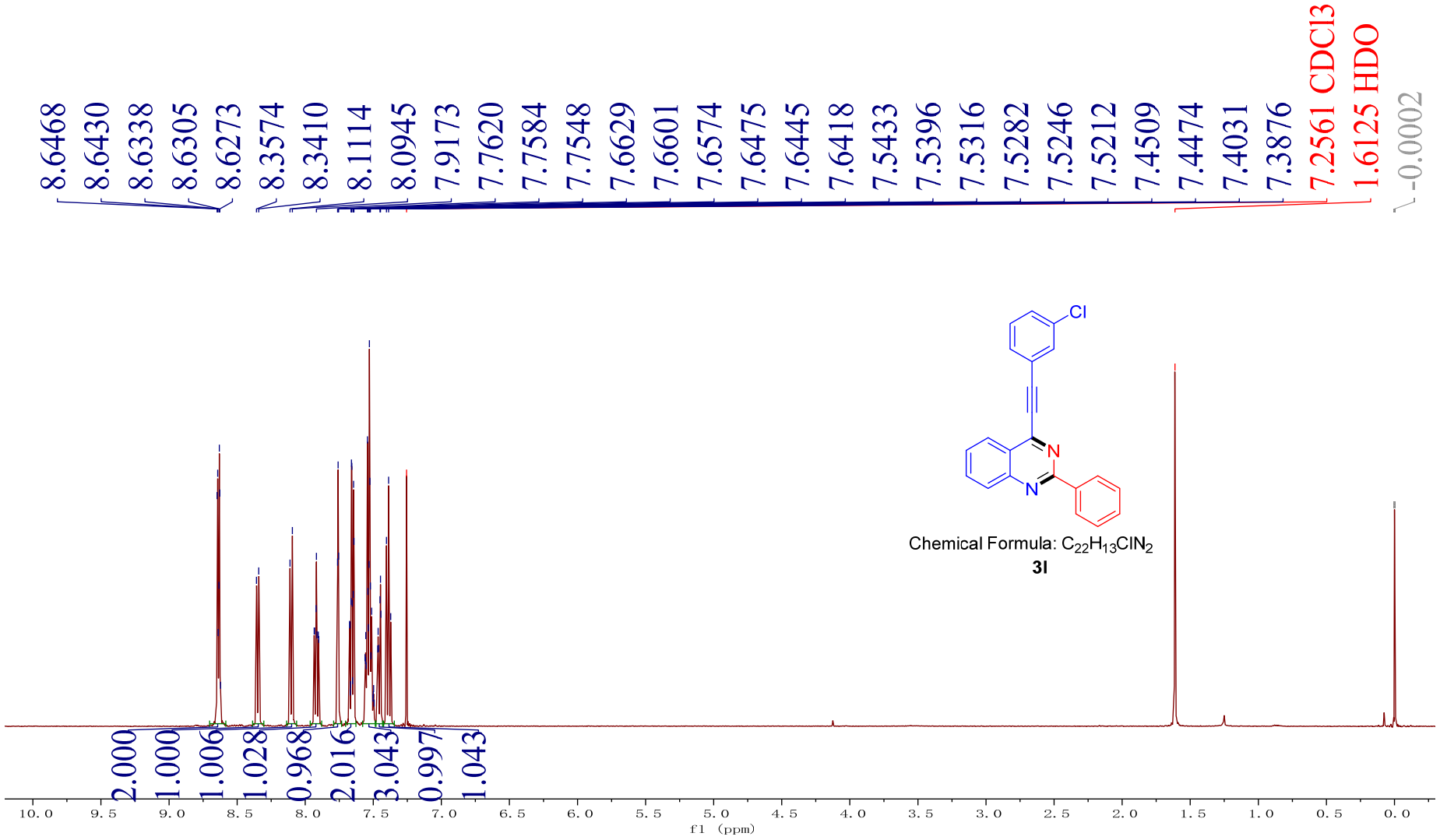
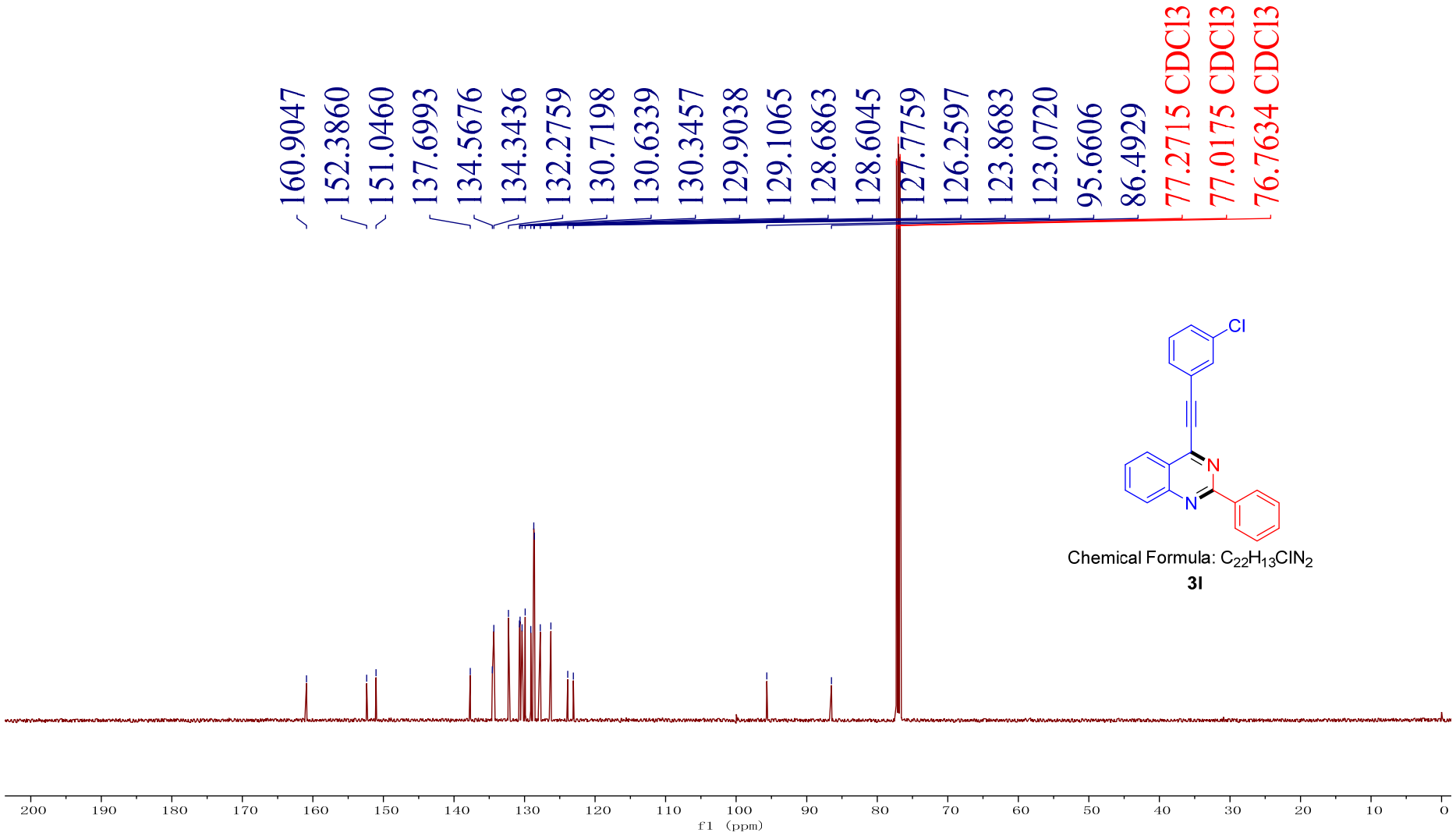
153.0399
150.9500
140.6634
137.8822
134.1731
132.5531
130.6221
129.4309
129.0041
128.7118
128.5807
127.5765
126.5192
123.9229
118.2969
98.4124
85.3424
77.3765 CDCl3
77.0588 CDCl3
76.7412 CDCl3
21.7584
N
N
Chemical Formula: $C_{23}H_{16}N_2$
3j
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.6493
8.6441
8.6392
8.6339
8.6291
8.6250
8.3684
8.3483
8.1079
8.0868
7.9111
7.9073
7.7851
7.7796
7.7715
7.7636
7.7552
7.7499
7.6473
7.6439
7.6405
7.5411
7.5328
7.5271
7.5222
7.5163
7.2551 CDCl3
7.1734
7.1571
7.1518
7.1463
7.1303
0.0000
F
N
N
Chemical Formula: C22H13FN2
3k
2.0104
1.0000
1.0119
1.0446
2.0241
1.0590
3.0633
2.0248
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)

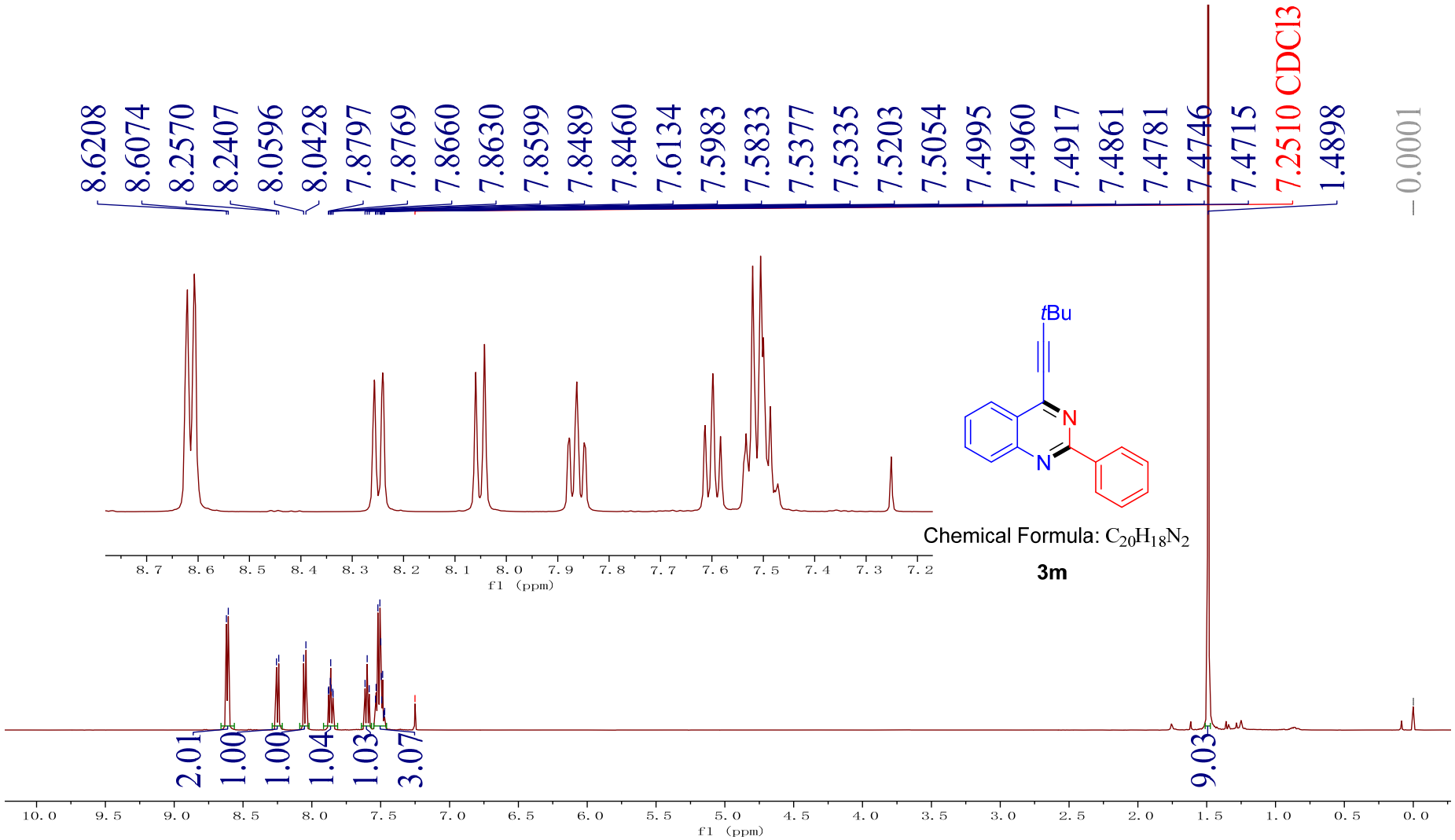

164.8653
162.3547
160.9112
152.7075
151.0046
137.7703
134.7495
134.6628
134.2800
130.6909
129.0859
128.6860
128.6043
127.6755
126.3441
123.8560
117.5229
117.4872
116.2473
116.0253
96.5921
85.5111
85.4963
77.3484 CDCl3
77.0308 CDCl3
76.7137 CDCl3
F
N
N
Chemical Formula: $C_{22}H_{13}FN_2$
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.6468
8.6430
8.6338
8.6305
8.6273
8.3574
8.3410
8.1114
8.0945
7.9173
7.7620
7.7584
7.7548
7.6629
7.6601
7.6574
7.6475
7.6445
7.6418
7.5433
7.5396
7.5316
7.5282
7.5246
7.5212
7.4509
7.4474
7.4031
7.3876
7.2561 CDCl3
1.6125 HDO
-0.0002
Cl
N
N
Chemical Formula: C22H13ClN2
3l
2.000
1.000
1.006
1.028
0.968
2.016
3.043
0.997
1.043
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)



Chemical Formula: $C_{22}H_{13}ClN_2$

3l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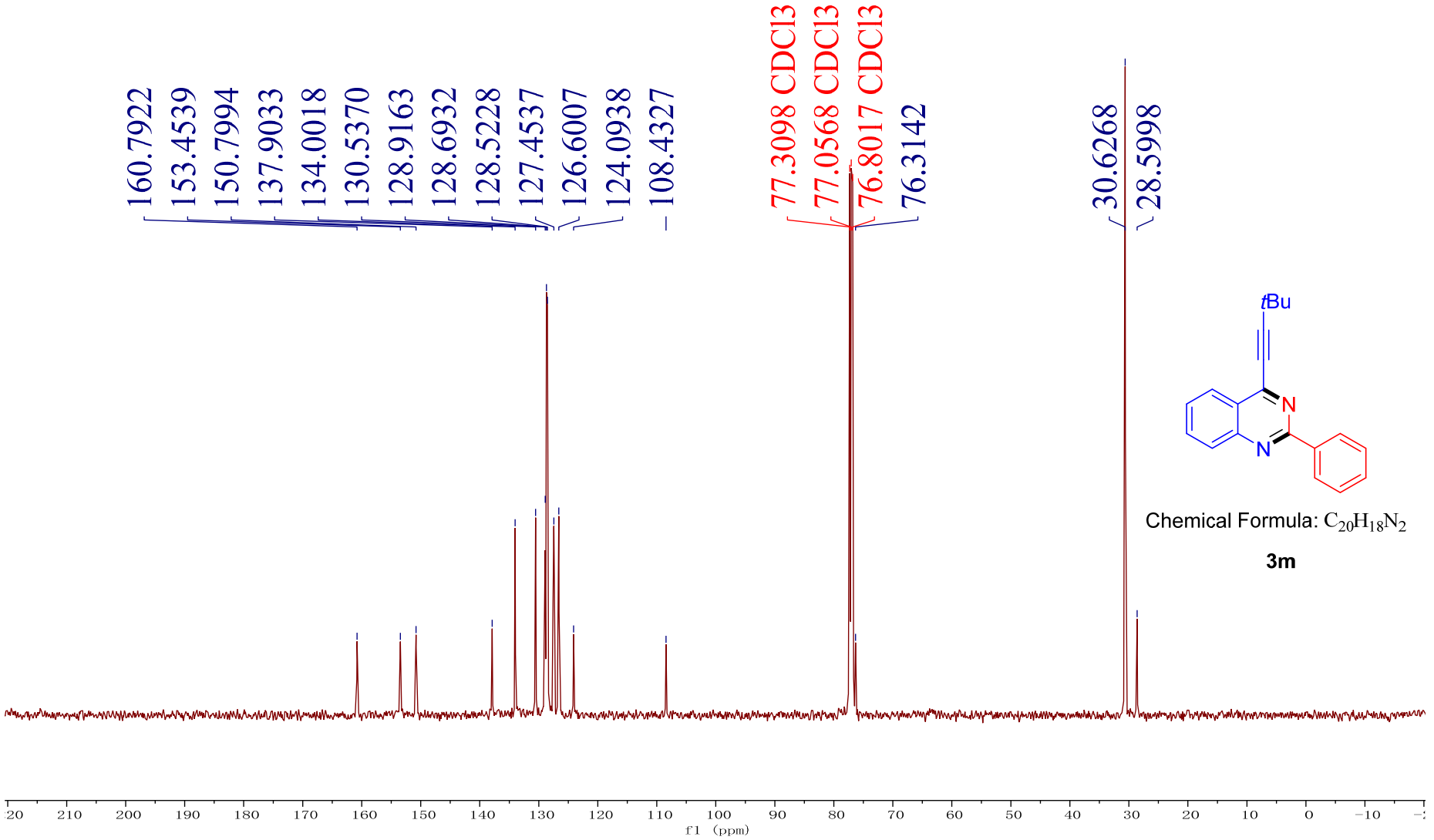
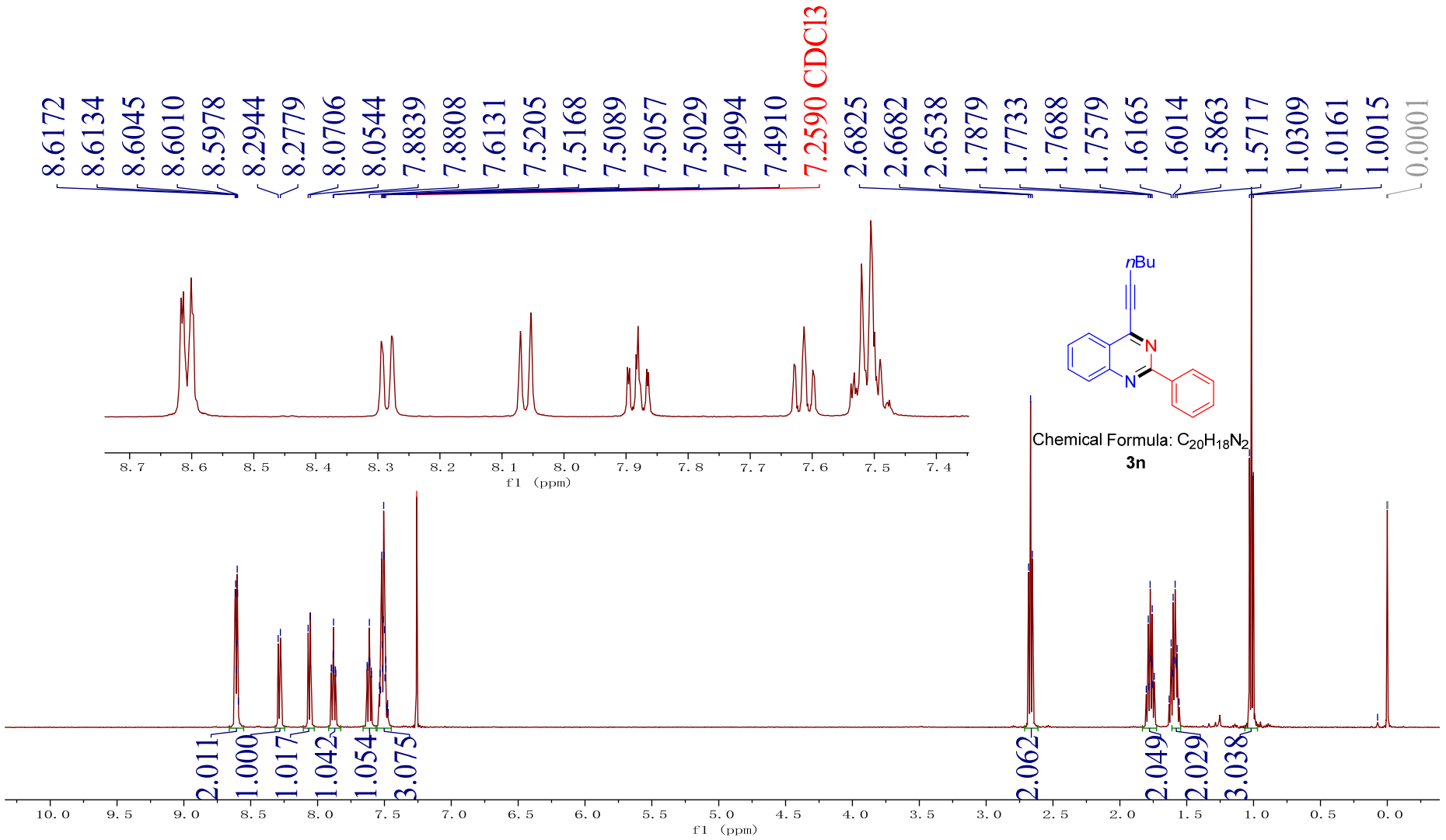
8.6074
8.2570
8.2407
8.0596
8.0428
7.8797
7.8769
7.8660
7.8630
7.8599
7.8489
7.8460
7.6134
7.5983
7.5833
7.5377
7.5335
7.5203
7.5054
7.4995
7.4960
7.4917
7.4861
7.4781
7.4746
7.4715
7.2510 CDCl3
1.4898
0.0001
tBu
N
N
Chemical Formula: C20H18N2
3m
2.01
1.00
1.00
1.04
1.03
3.07
9.03
f1 (ppm)


160.7922
153.4539
150.7994
137.9033
134.0018
130.5370
128.9163
128.6932
128.5228
127.4537
126.6007
124.0938
108.4327
77.3098 CDCl3
77.0568 CDCl3
76.8017 CDCl3
76.3142
30.6268
28.5998
tBu
N
N
Chemical Formula: C20H18N2
3m
f1 (ppm)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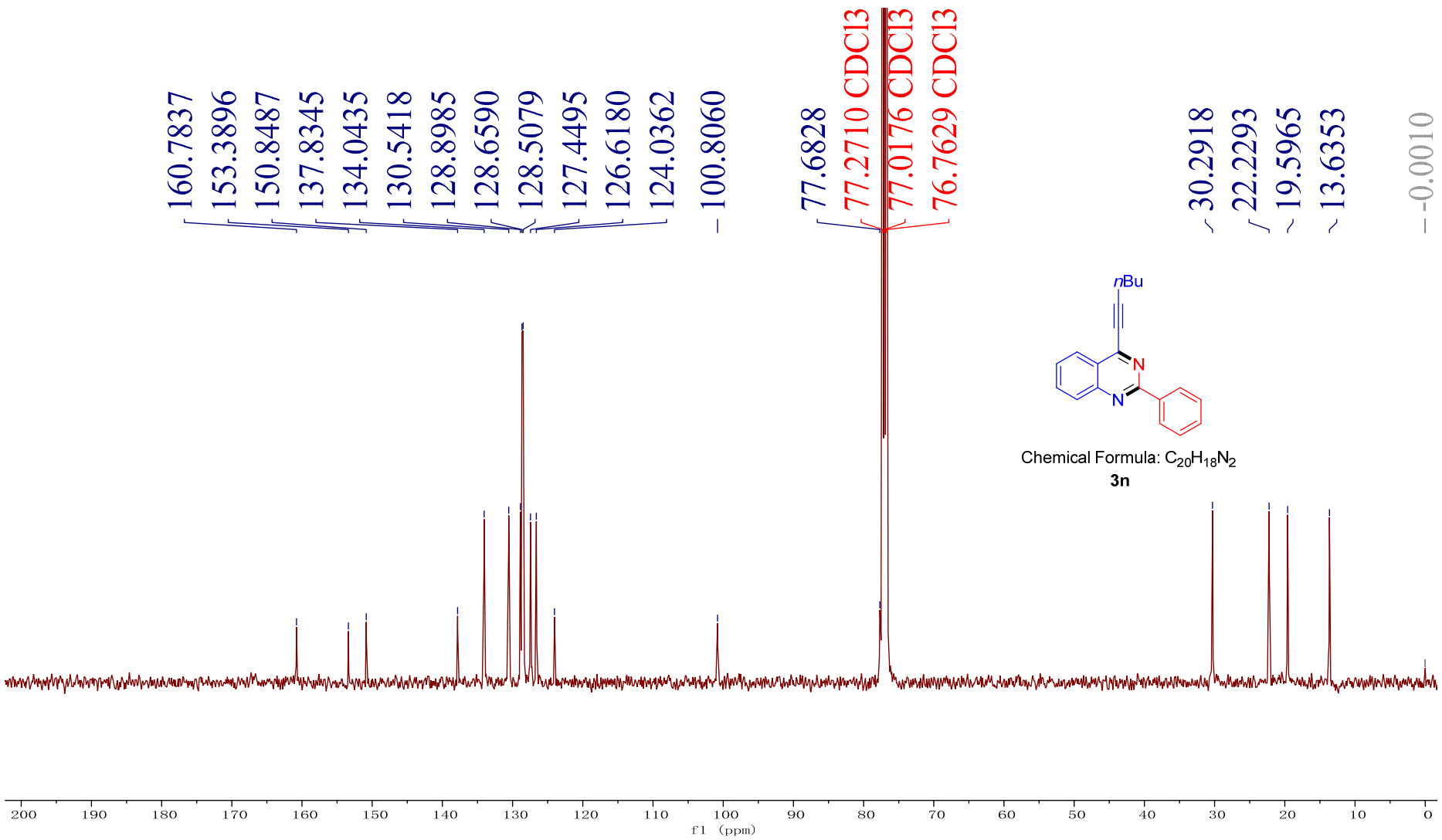
8.6134
8.6045
8.6010
8.5978
8.2944
8.2779
8.0706
8.0544
7.8839
7.8808
7.6131
7.5205
7.5168
7.5089
7.5057
7.5029
7.4994
7.4910
7.2590 CDCl3
2.6825
2.6682
2.6538
1.7879
1.7733
1.7688
1.7579
1.6165
1.6014
1.5863
1.5717
1.0309
1.0161
1.0015
0.0001
nBu
N
N
Chemical Formula: C20H18N2
3n
f1 (ppm)
2.011
1.000
1.017
1.042
1.054
3.075
2.062
2.049
2.029
3.038
f1 (ppm)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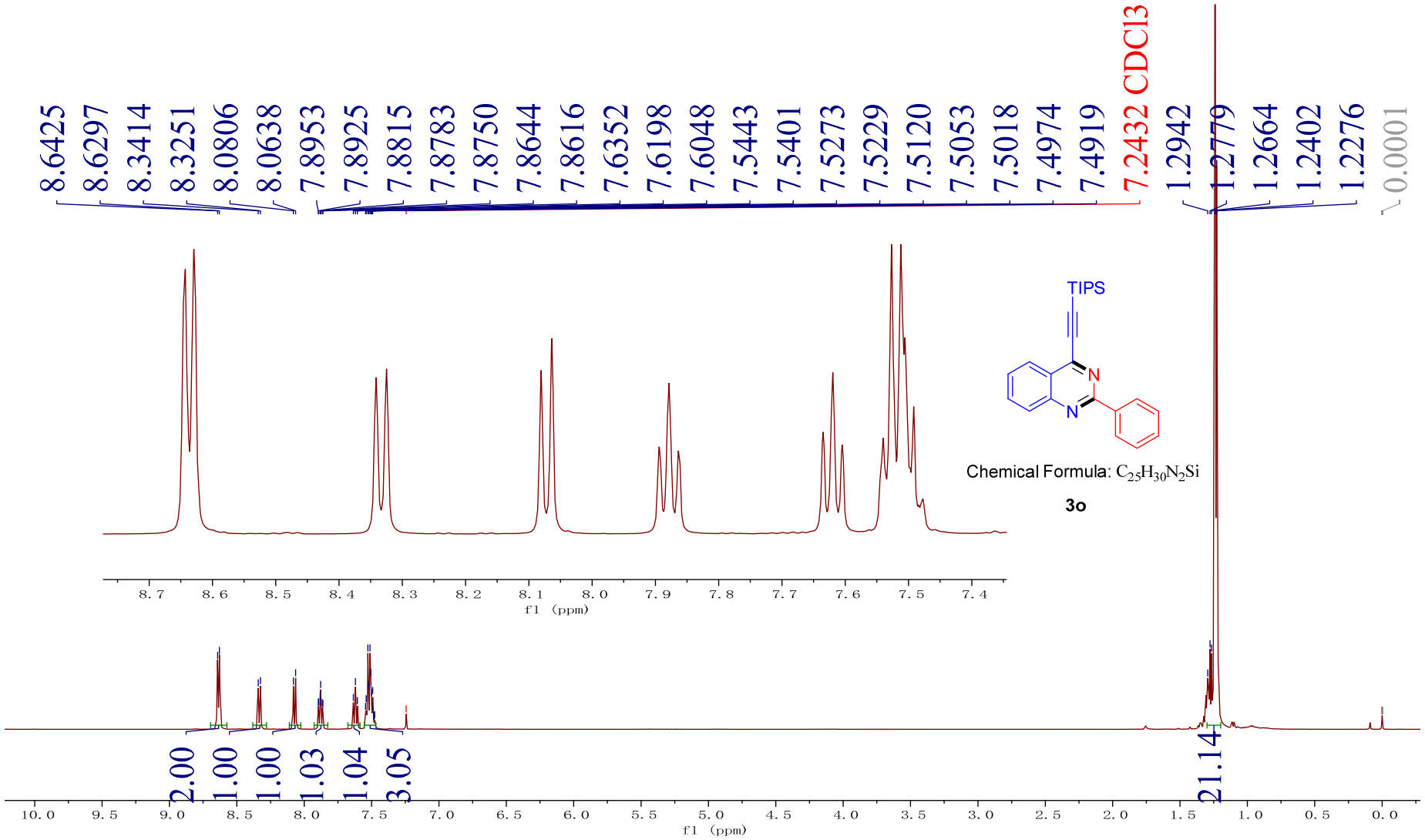
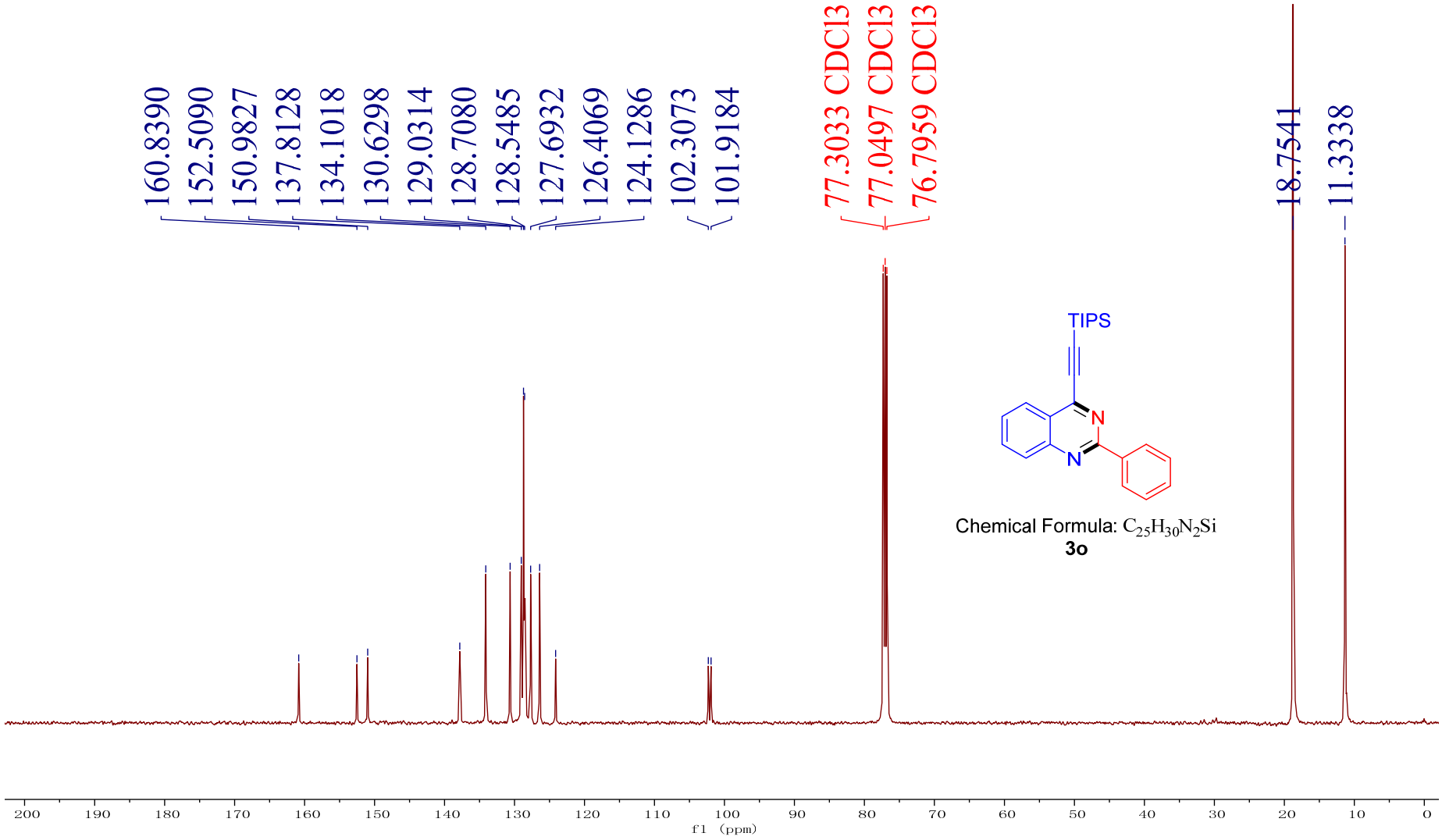
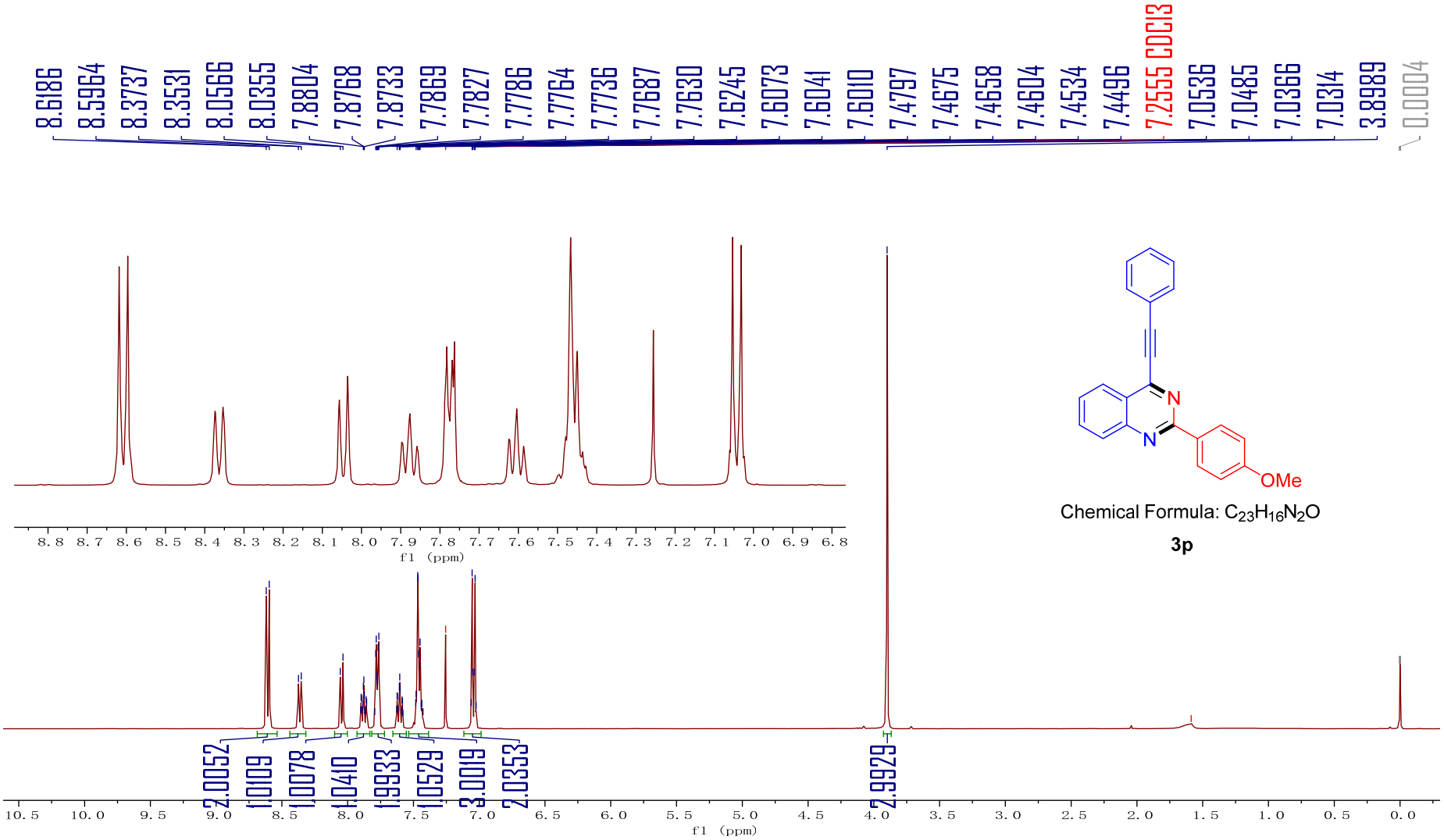
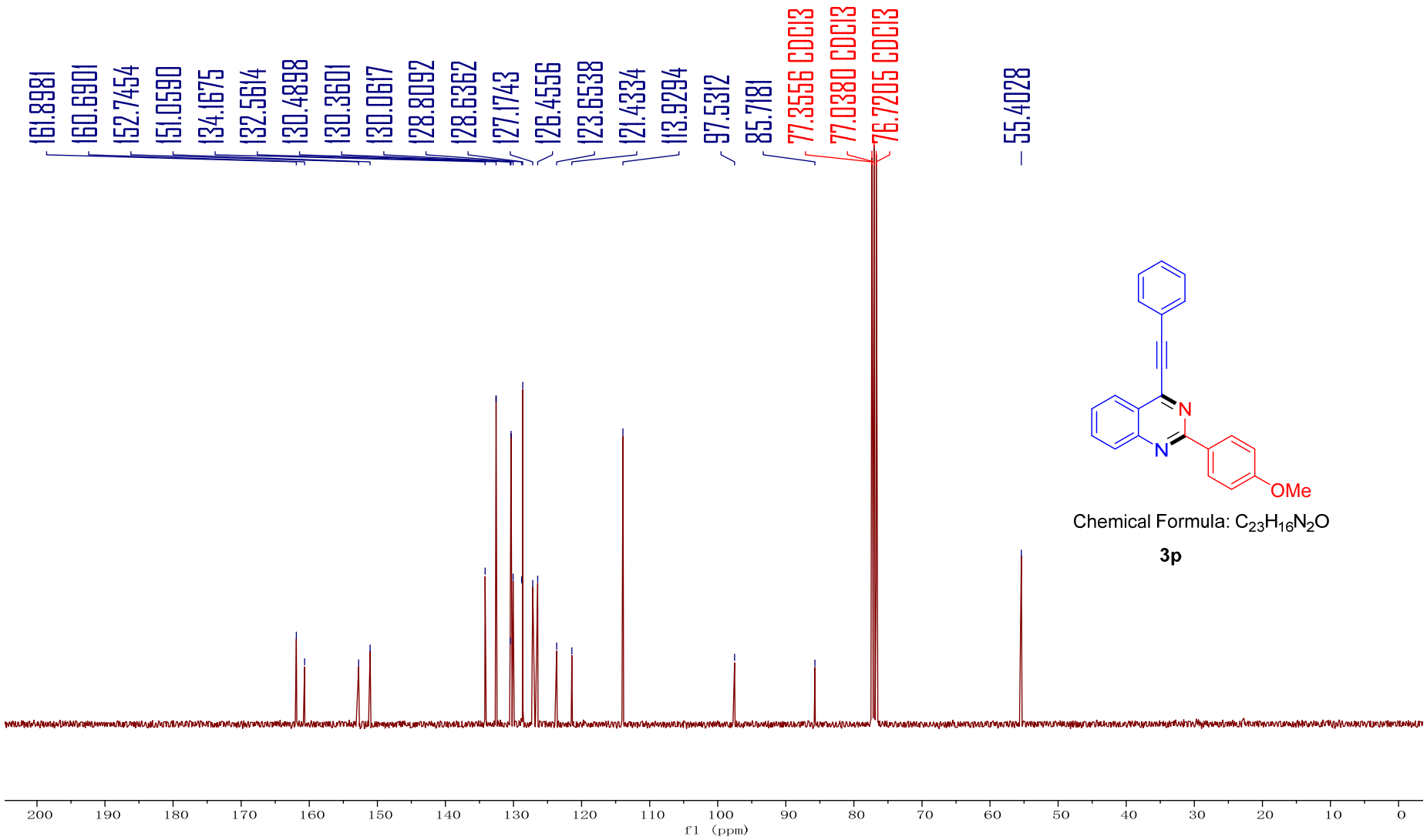
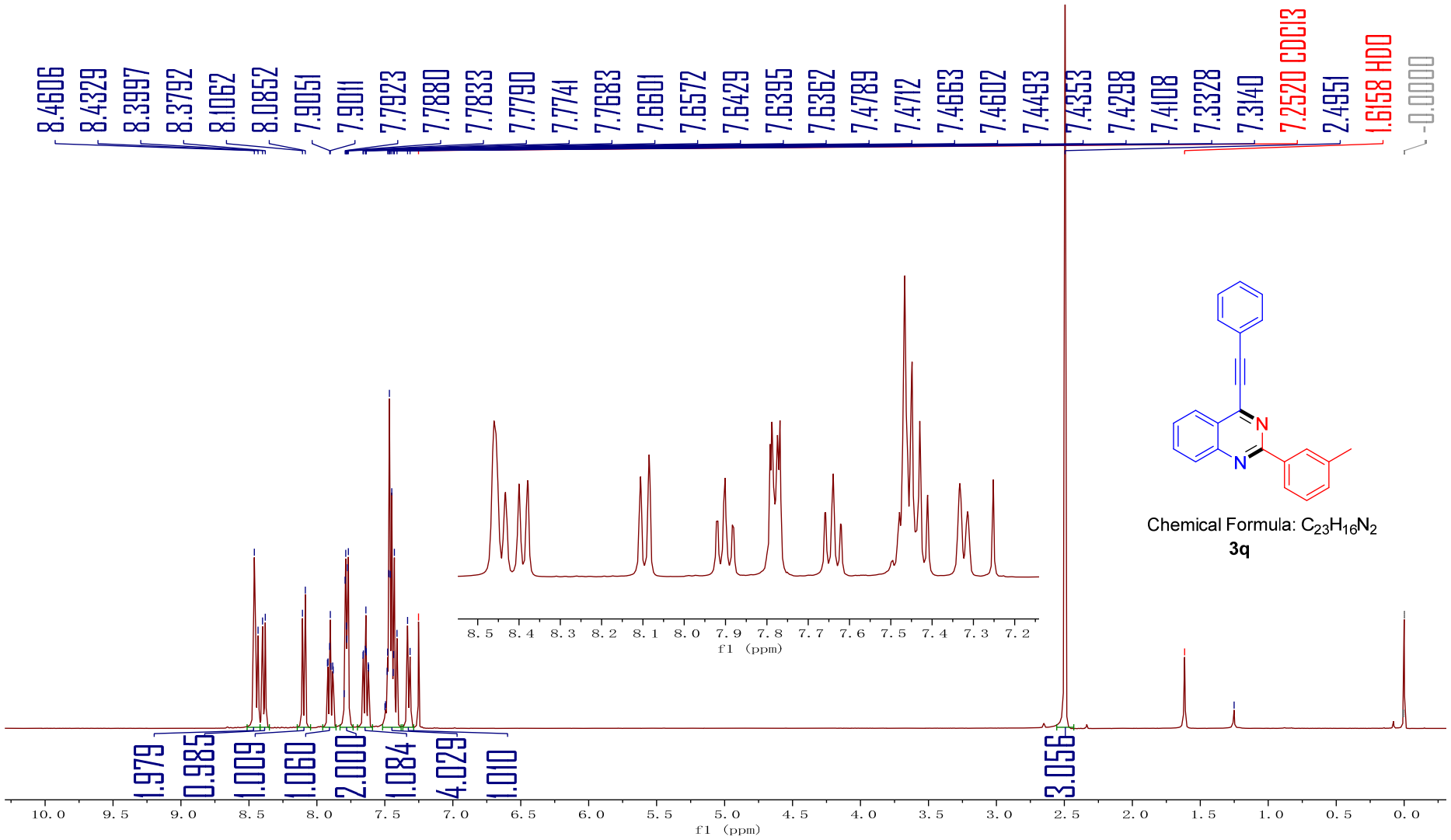
153.3896
150.8487
137.8345
134.0435
130.5418
128.8985
128.6590
128.5079
127.4495
126.6180
124.0362
100.8060
77.6828
77.2710 CDCl3
77.0176 CDCl3
76.7629 CDCl3
30.2918
22.2293
19.5965
13.6353
-0.0010
nBu
N
N
Chemical Formula: C20H18N2
3n
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

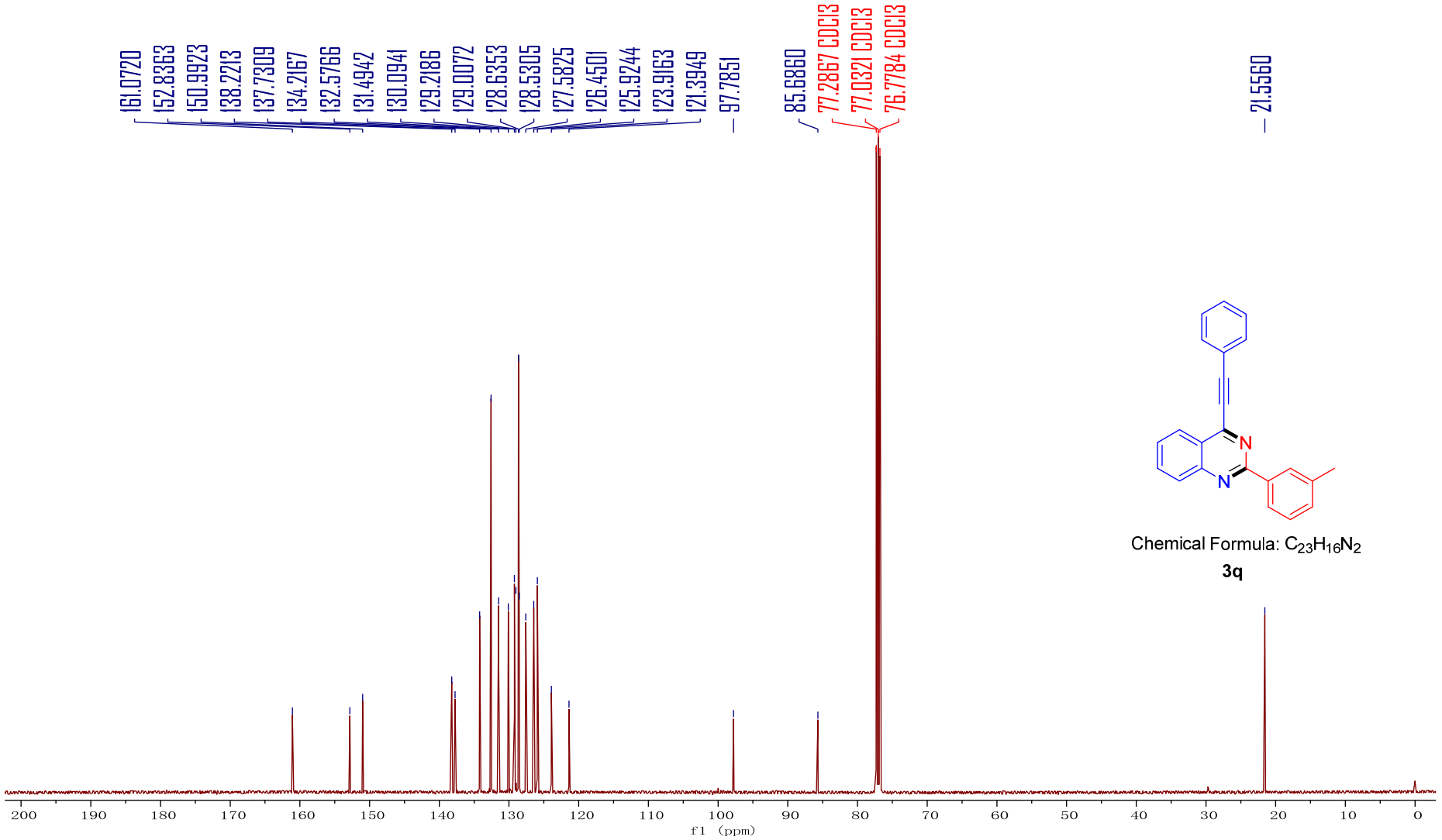

8.6425
8.6297
8.3414
8.3251
8.0806
8.0638
7.8953
7.8925
7.8815
7.8783
7.8750
7.8644
7.8616
7.6352
7.6198
7.6048
7.5443
7.5401
7.5273
7.5229
7.5120
7.5053
7.5018
7.4974
7.4919
7.2432 CDCl3
1.2942
1.2779
1.2664
1.2402
1.2276
0.0001
TIPS
N
N
Chemical Formula: C25H30N2Si
3o
2.00
1.00
1.00
1.03
1.04
3.05
21.14
f1 (ppm)
f1 (ppm)

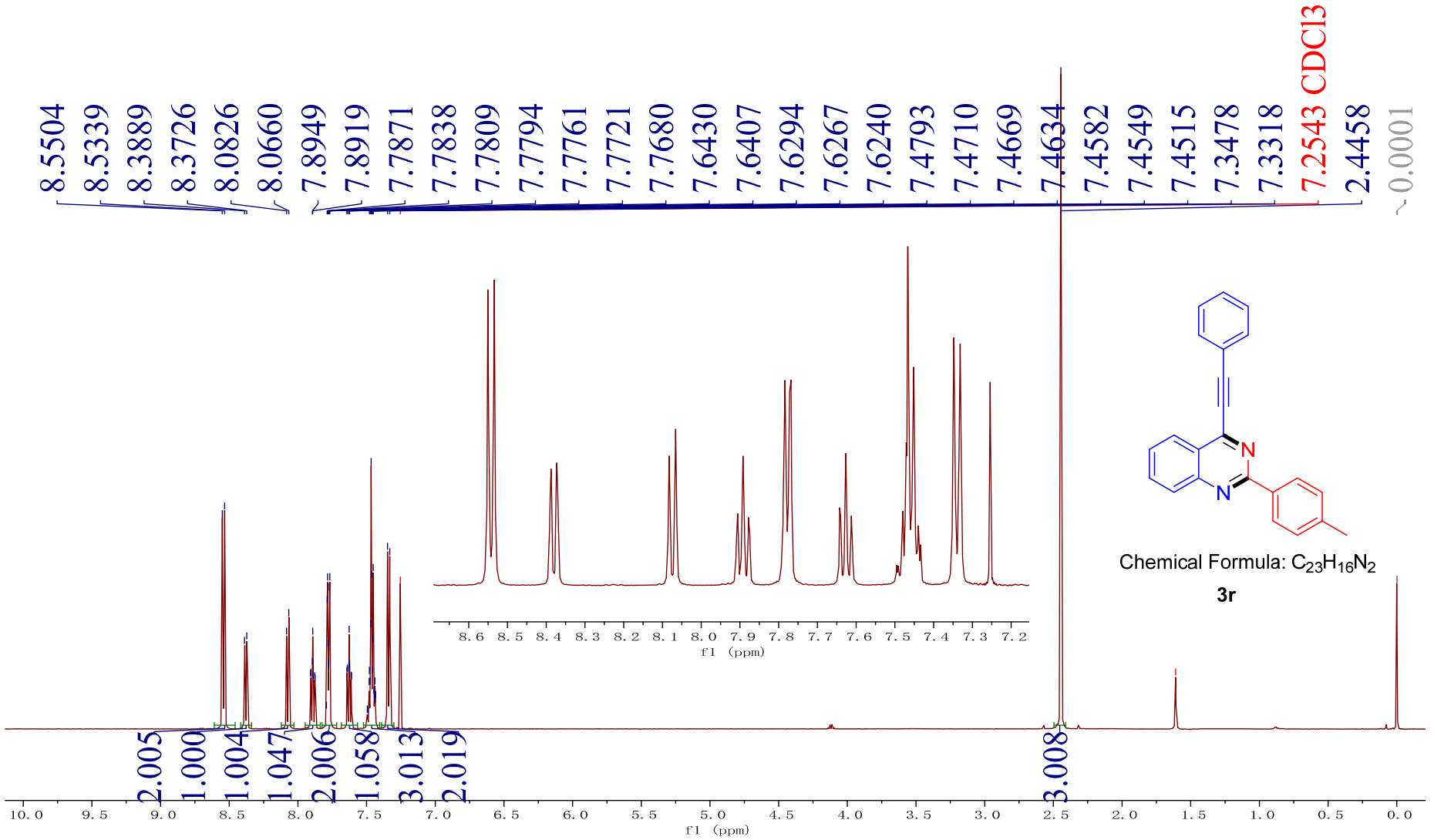

160.8390
152.5090
150.9827
137.8128
134.1018
130.6298
129.0314
128.7080
128.5485
127.6932
126.4069
124.1286
102.3073
101.9184
77.3033 CDCl3
77.0497 CDCl3
76.7959 CDCl3
18.7541
11.3338
TIPS
N
N
Chemical Formula: $C_{25}H_{30}N_2Si$
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.6186
8.5964
8.3737
8.3531
8.0566
8.0355
7.8804
7.8768
7.8733
7.7869
7.7827
7.7786
7.7764
7.7736
7.7687
7.7630
7.6245
7.6073
7.6041
7.6010
7.4797
7.4675
7.4658
7.4604
7.4534
7.4496
7.2555 CDCl3
7.0536
7.0485
7.0366
7.0314
3.8989
0.0004
f1 (ppm)
2.0052
1.0109
1.0078
1.0410
1.9933
1.0529
3.0019
2.0353
2.9929
f1 (ppm)
N
N
OMe
Chemical Formula: C23H16N2O
3p


161.8981
160.6901
152.7454
151.0590
134.1675
132.5614
130.4898
130.3601
130.0617
128.8092
128.6362
127.1743
126.4556
123.6538
121.4334
113.9294
97.5312
85.7181
77.3556 CDCl3
77.0380 CDCl3
76.7205 CDCl3
55.4028
N
N
OMe
Chemical Formula: $C_{23}H_{16}N_2O$
3p
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.4606
8.4329
8.3997
8.3792
8.1062
8.0852
7.9051
7.9011
7.7923
7.7880
7.7833
7.7790
7.7741
7.7683
7.6601
7.6572
7.6429
7.6395
7.6362
7.4789
7.4712
7.4663
7.4602
7.4493
7.4353
7.4298
7.4108
7.3328
7.3140
7.2520 CDCl3
2.4951
1.6158 H2O
-0.0000
1.979
0.985
1.009
1.060
2.000
1.084
4.029
1.010
3.056
f1 (ppm)
Chemical Formula: C23H16N2
3q


161.0720
152.8363
150.9923
138.2213
137.7309
134.2167
132.5766
131.4942
130.0941
129.2186
129.0072
128.6353
128.5305
127.5825
126.4501
125.9244
123.9163
121.3949
97.7851
85.6860
77.2867 CDCl3
77.0321 CDCl3
76.7784 CDCl3
21.5560
N
N
Chemical Formula: C23H16N2
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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8.5339
8.3889
8.3726
8.0826
8.0660
7.8949
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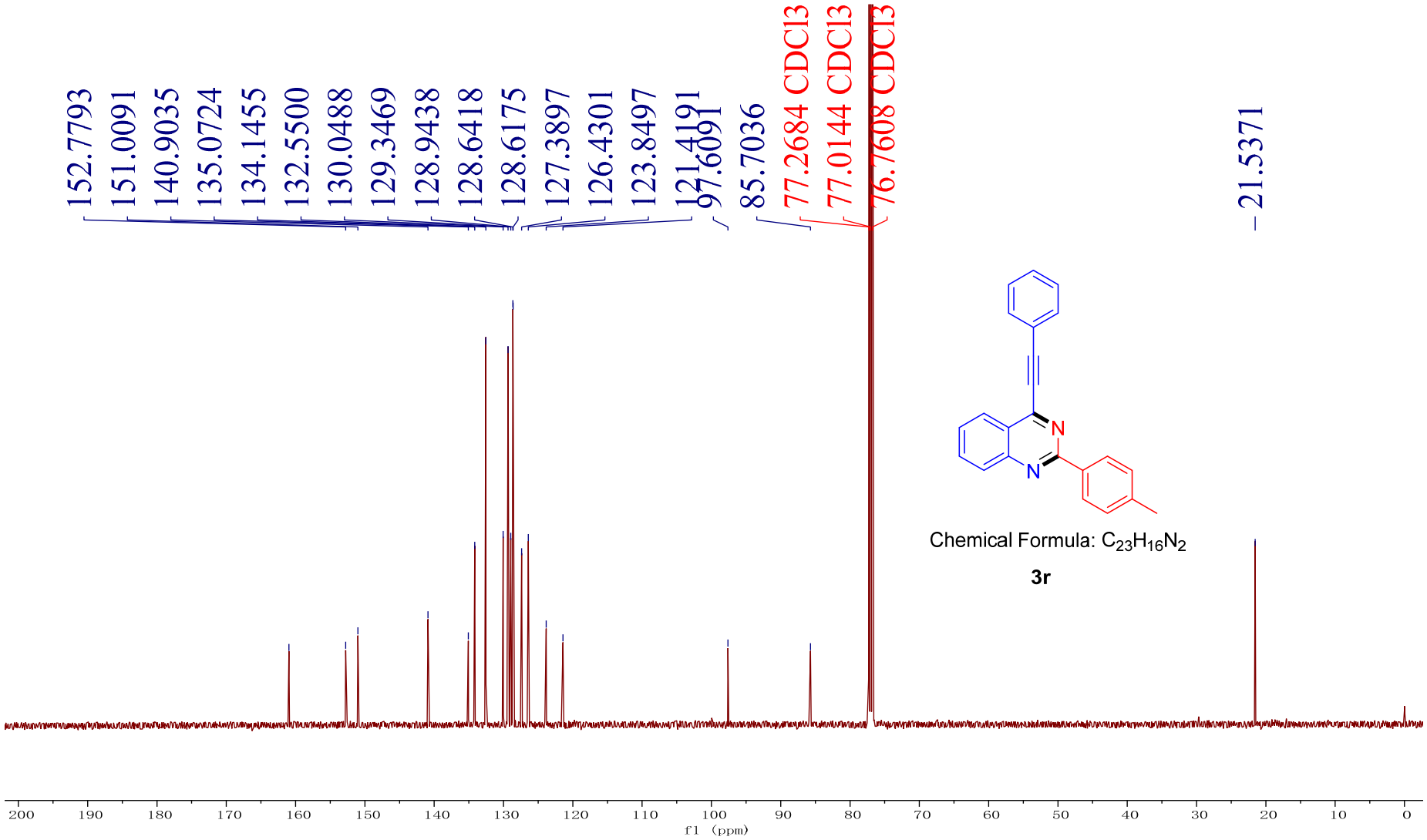
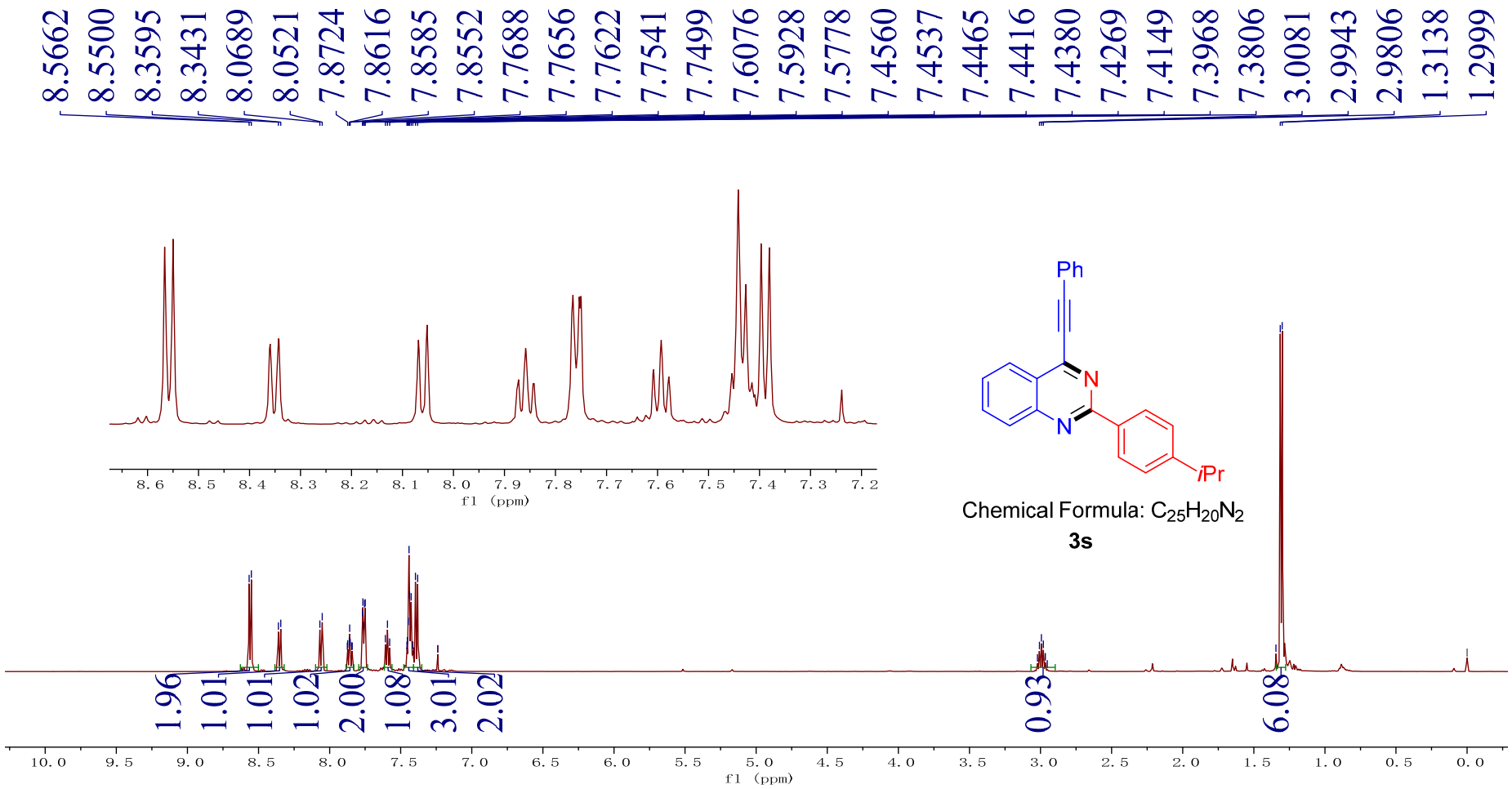
7.7871
7.7838
7.7809
7.7794
7.7761
7.7721
7.7680
7.6430
7.6407
7.6294
7.6267
7.6240
7.4793
7.4710
7.4669
7.4634
7.4582
7.4549
7.4515
7.3478
7.3318
7.2543 CDCl3
2.4458
0.0001
2.005
1.000
1.004
1.047
2.006
1.058
3.013
2.019
3.008
f1 (ppm)
Chemical Formula: C23H16N2
3r


152.7793
151.0091
140.9035
135.0724
134.1455
132.5500
130.0488
129.3469
128.9438
128.6418
128.6175
127.3897
126.4301
123.8497
121.4191
97.6091
85.7036
77.2684 CDCl3
77.0144 CDCl3
76.7608 CDCl3
21.5371
N
N
Chemical Formula: $C_{23}H_{16}N_2$
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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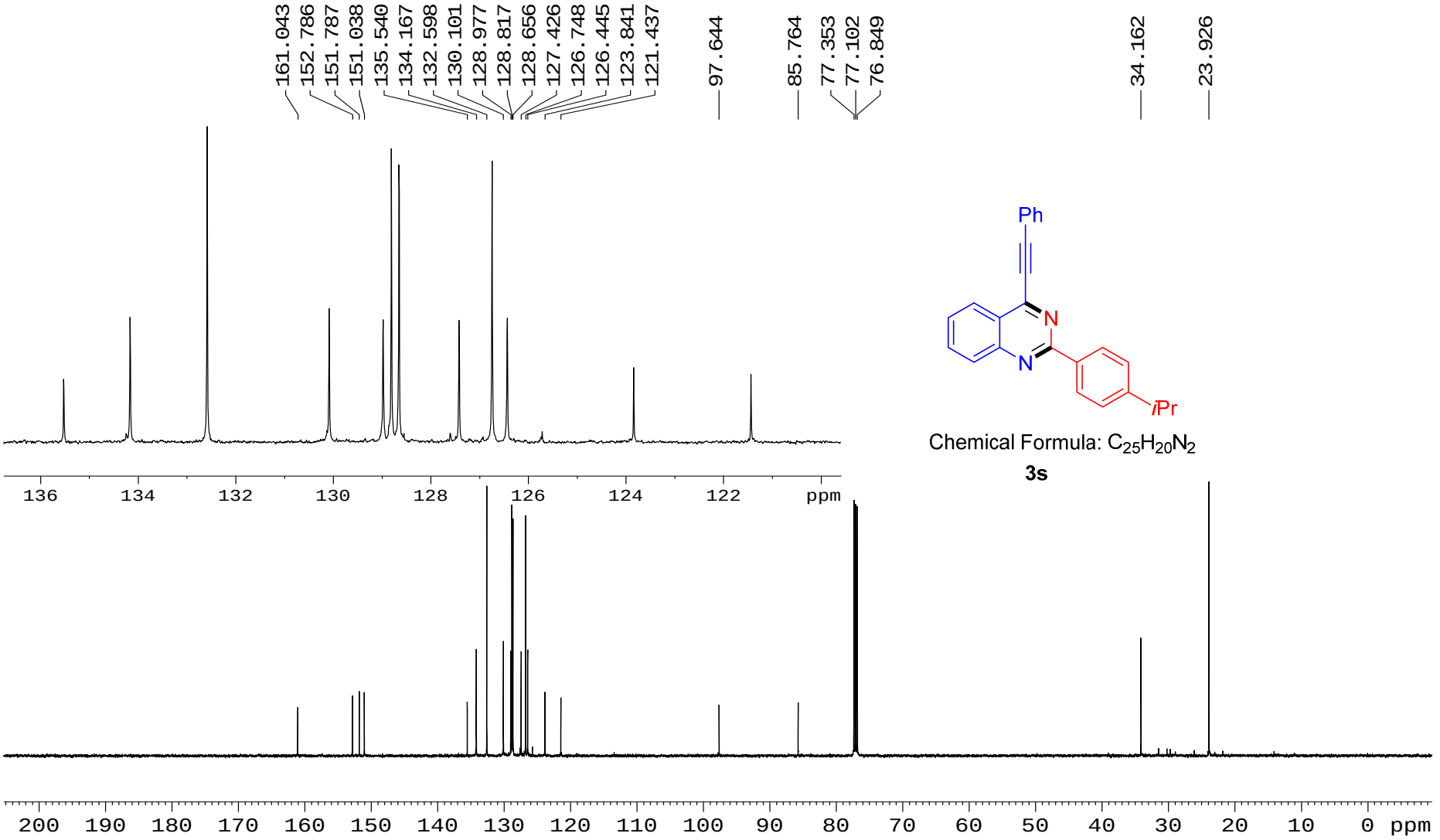
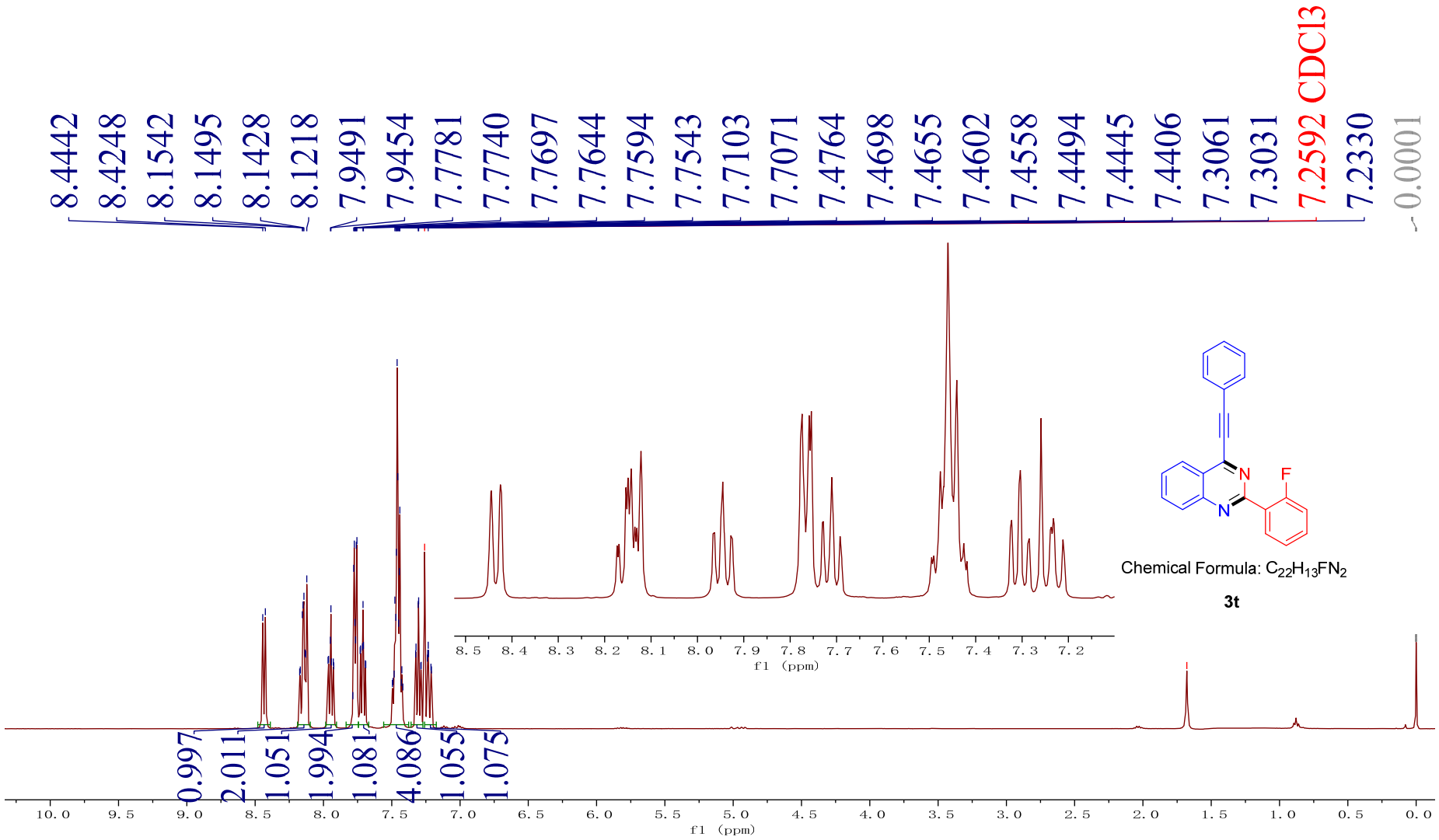
8.5500
8.3595
8.3431
8.0689
8.0521
7.8724
7.8616
7.8585
7.8552
7.7688
7.7656
7.7622
7.7541
7.7499
7.6076
7.5928
7.5778
7.4560
7.4537
7.4465
7.4416
7.4380
7.4269
7.4149
7.3968
7.3806
3.0081
2.9943
2.9806
1.3138
1.2999
f1 (ppm)
Ph
N
N
iPr
Chemical Formula: C25H20N2
3s
1.96
1.01
1.01
1.02
2.00
1.08
3.01
2.02
0.93
6.08
f1 (ppm)


161.043
152.786
151.787
151.038
135.540
134.167
132.598
130.101
128.977
128.817
128.656
127.426
126.748
126.445
123.841
121.437
97.644
85.764
77.353
77.102
76.849
34.162
23.926
Ph
N
N
iPr
Chemical Formula: C25H20N2
3s
136
134
132
130
128
126
124
122
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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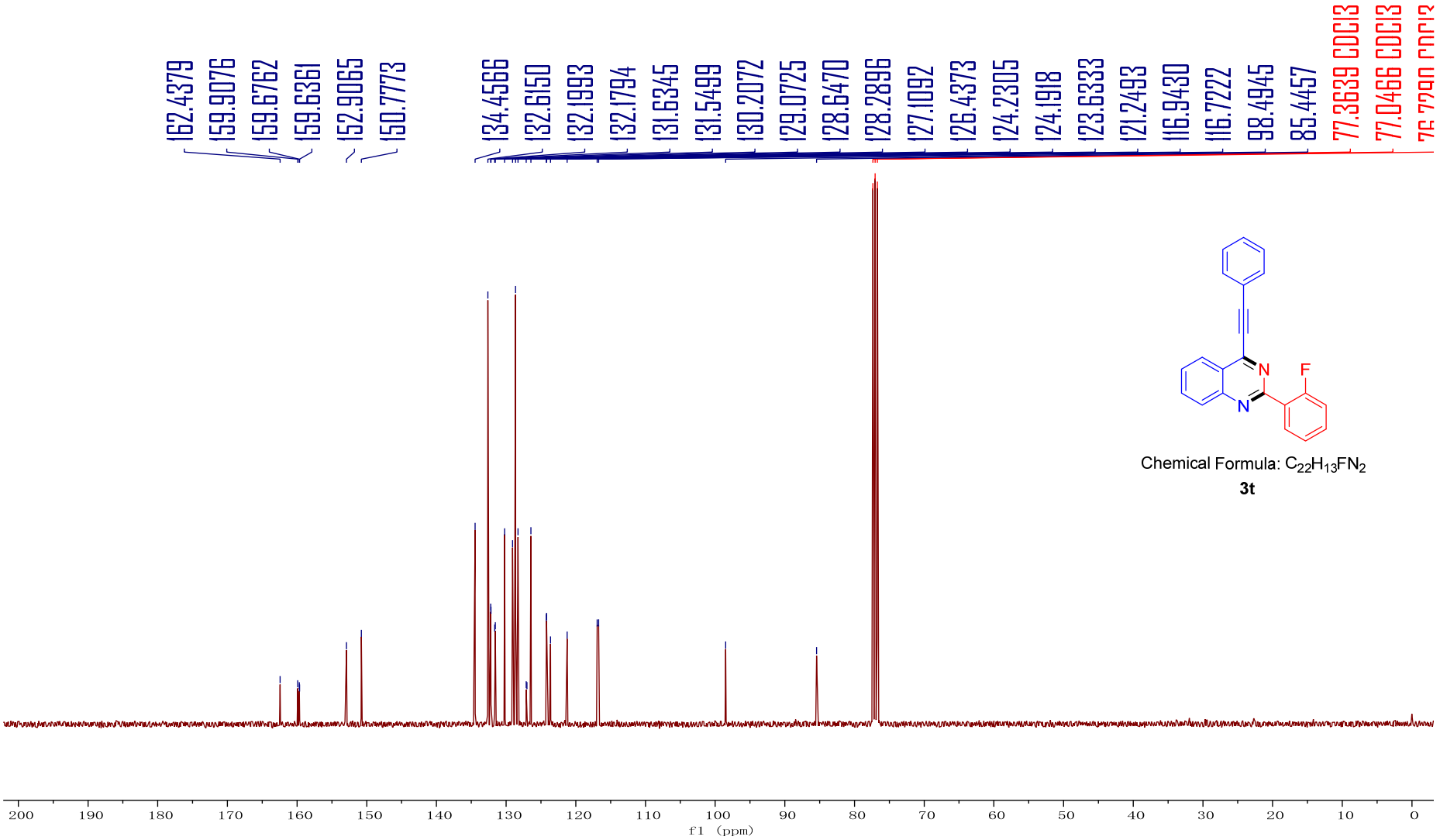
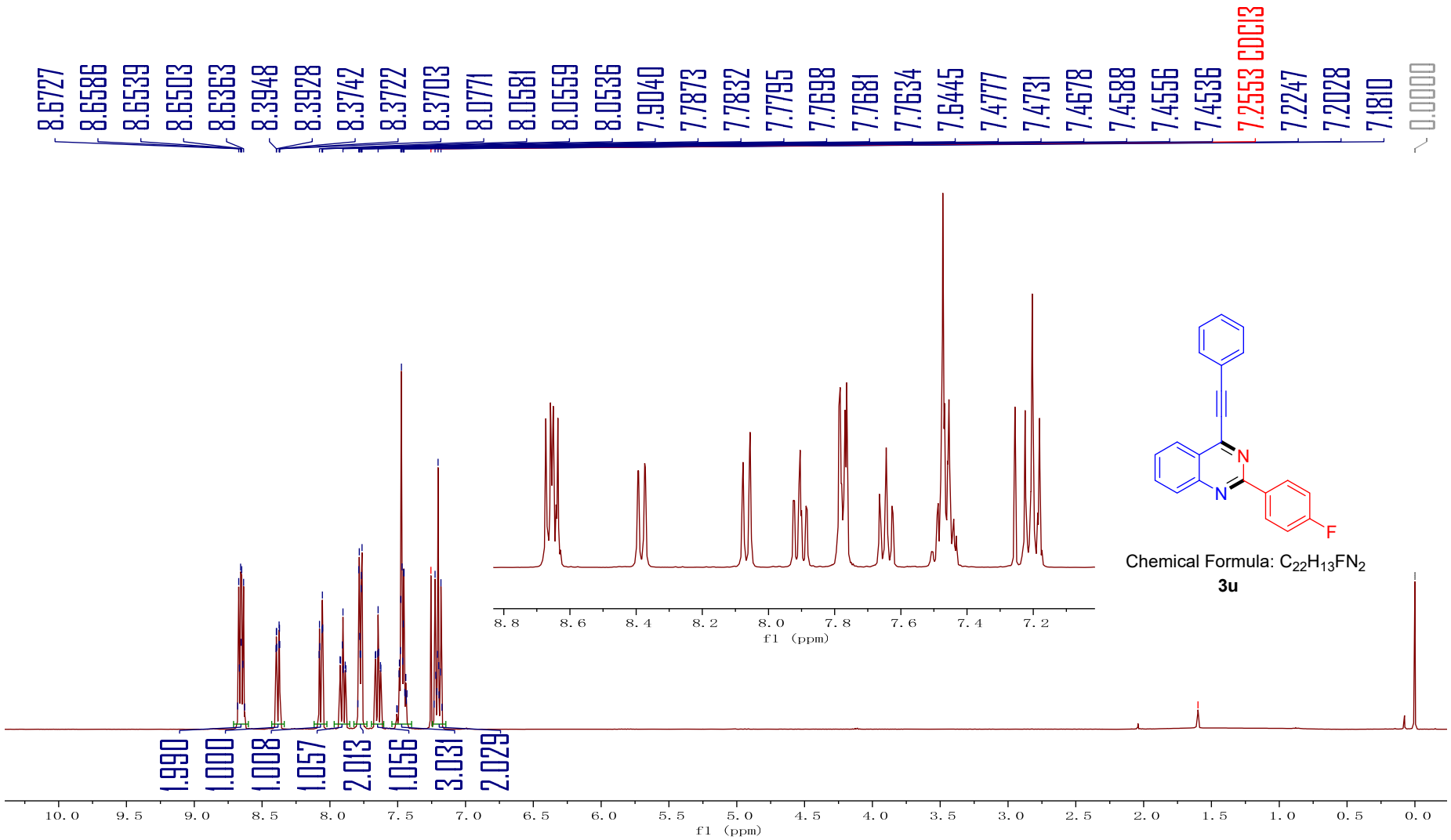
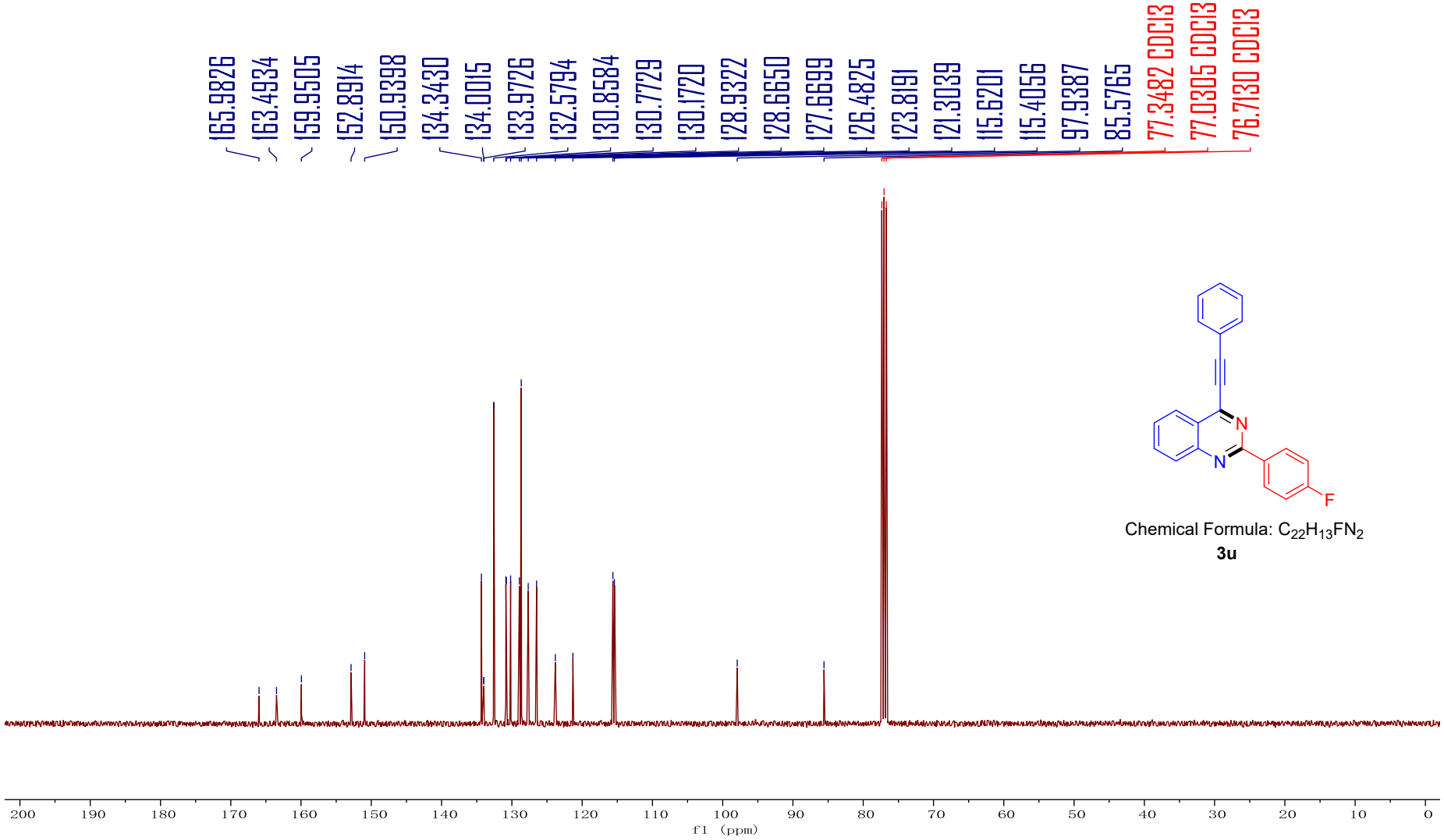
8.4248
8.1542
8.1495
8.1428
8.1218
7.9491
7.9454
7.7781
7.7740
7.7697
7.7644
7.7594
7.7543
7.7103
7.7071
7.4764
7.4698
7.4655
7.4602
7.4558
7.4494
7.4445
7.4406
7.3061
7.3031
7.2592 CDCl3
7.2330
0.0001
0.997
2.011
1.051
1.994
1.081
4.086
1.055
1.075
f1 (ppm)
N
F
N
Chemical Formula: C22H13FN2
3t

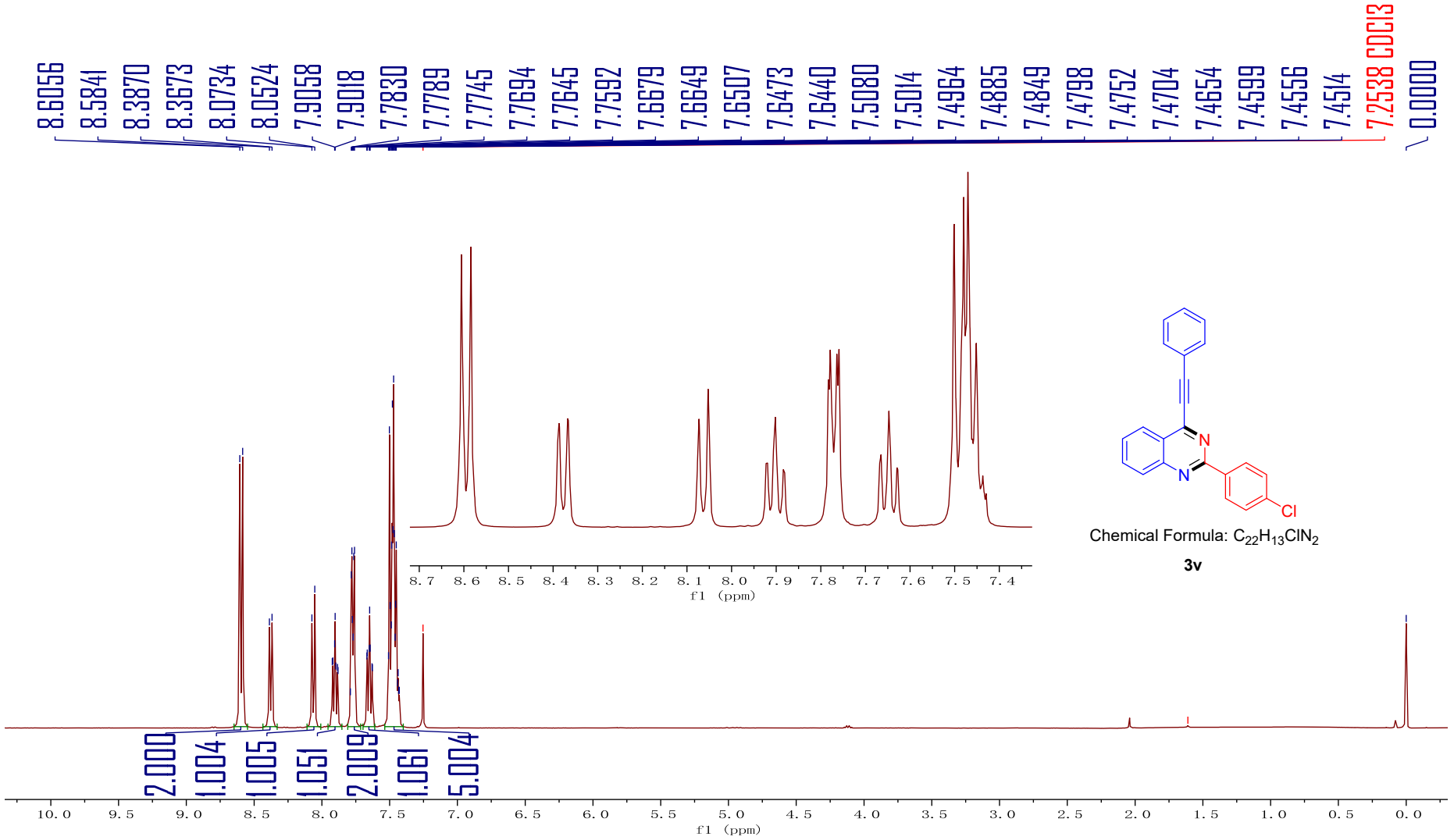

162.4379
159.9076
159.6762
159.6361
152.9065
150.7773
134.4566
132.6150
132.1993
132.1794
131.6345
131.5499
130.2072
129.0725
128.6470
128.2896
127.1092
126.4373
124.2305
124.1918
123.6333
121.2493
116.9430
116.7222
98.4945
85.4457
77.3639 CDCl3
77.0466 CDCl3
76.7293 CDCl3
N
F
N
Chemical Formula: $C_{22}H_{13}FN_2$
3t
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

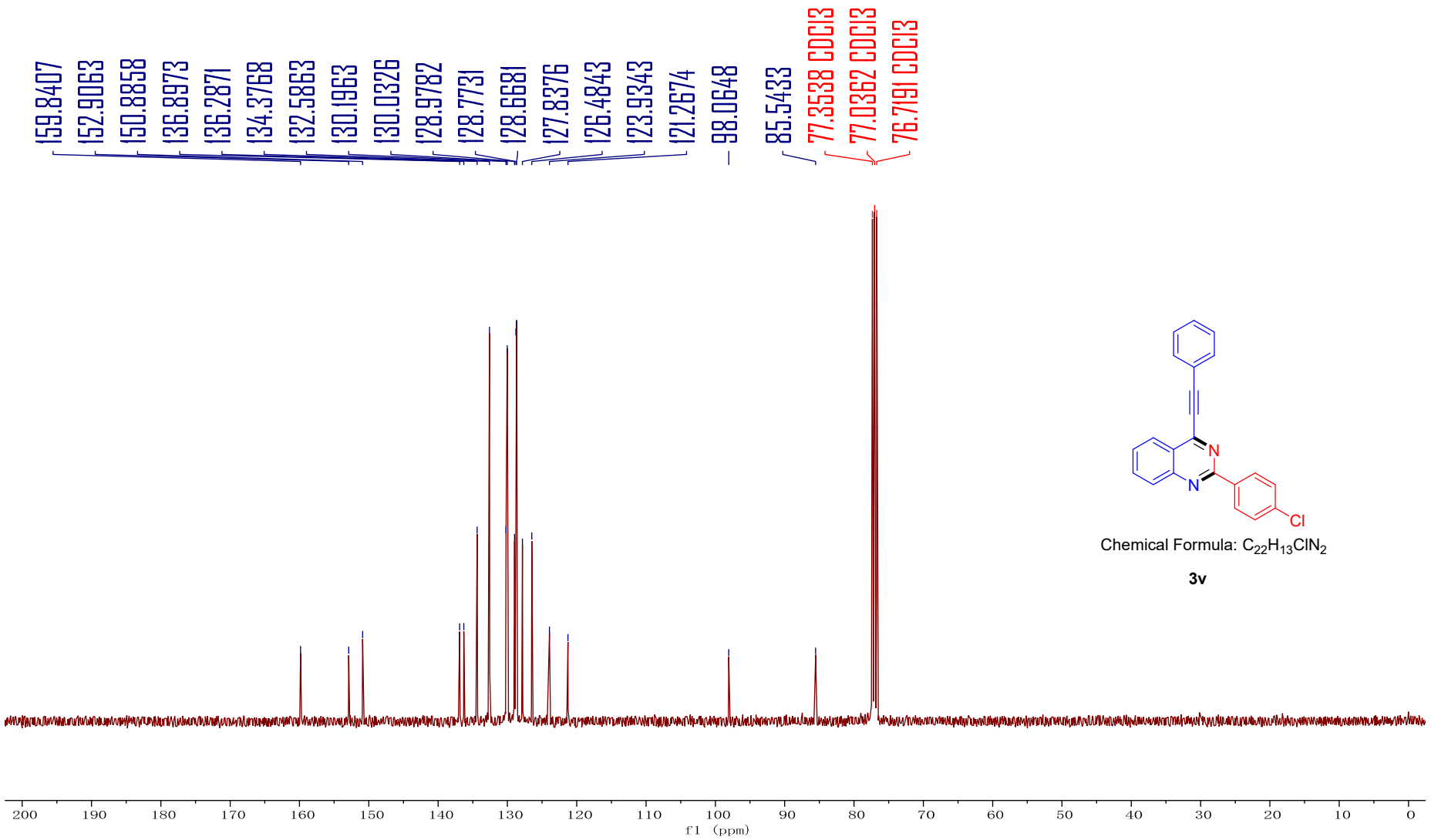

8.6727
8.6586
8.6539
8.6503
8.6363
8.3948
8.3928
8.3742
8.3722
8.3703
8.0771
8.0581
8.0559
8.0536
7.9040
7.7873
7.7832
7.7795
7.7698
7.7681
7.7634
7.6445
7.4777
7.4731
7.4678
7.4588
7.4556
7.4536
7.2553 CDCl3
7.2247
7.2028
7.1810
0.0000
1.990
1.000
1.008
1.057
2.013
1.056
3.031
2.029
f1 (ppm)
f1 (ppm)
N
N
F
Chemical Formula: $C_{22}H_{13}FN_2$
3u

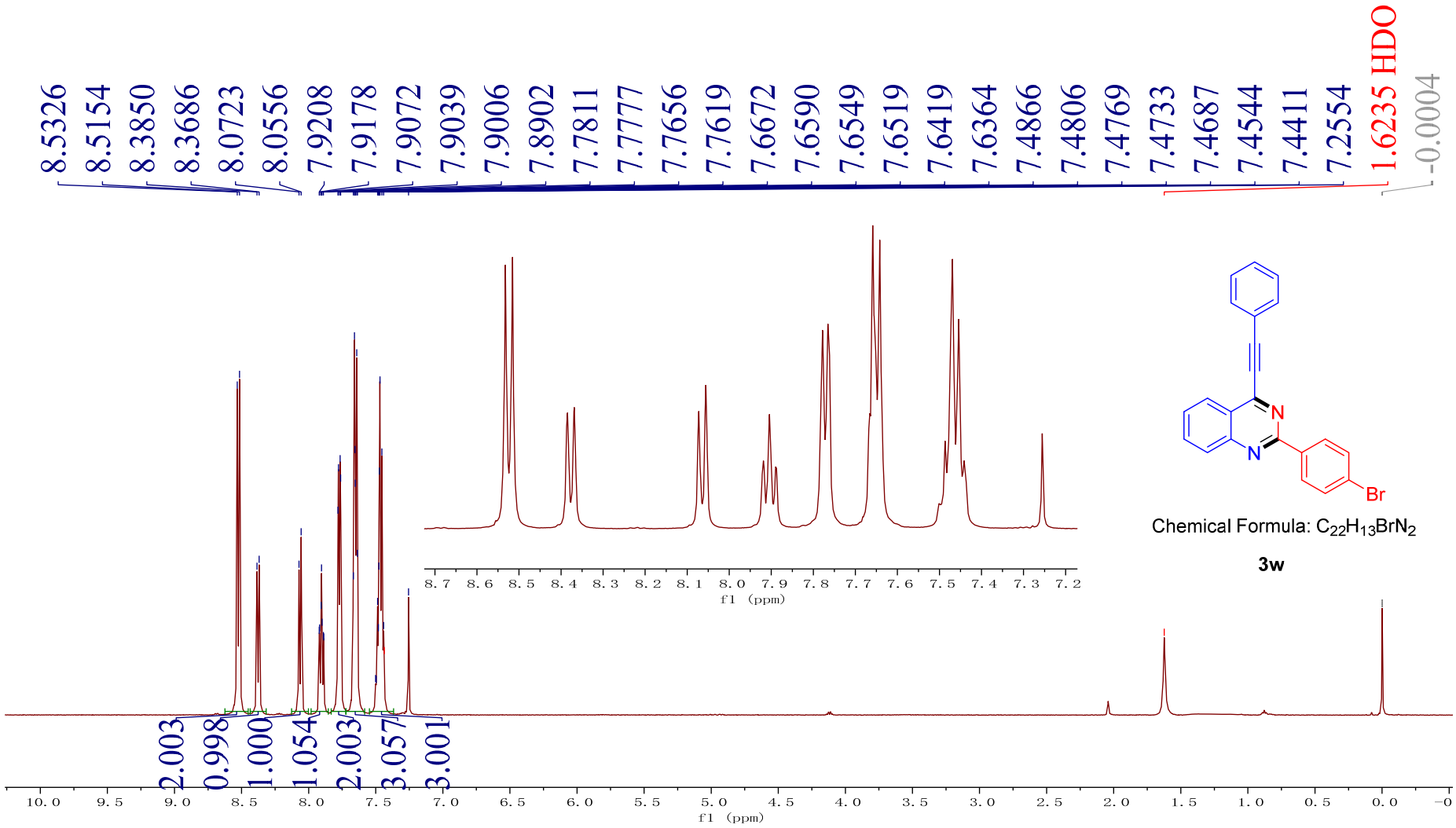


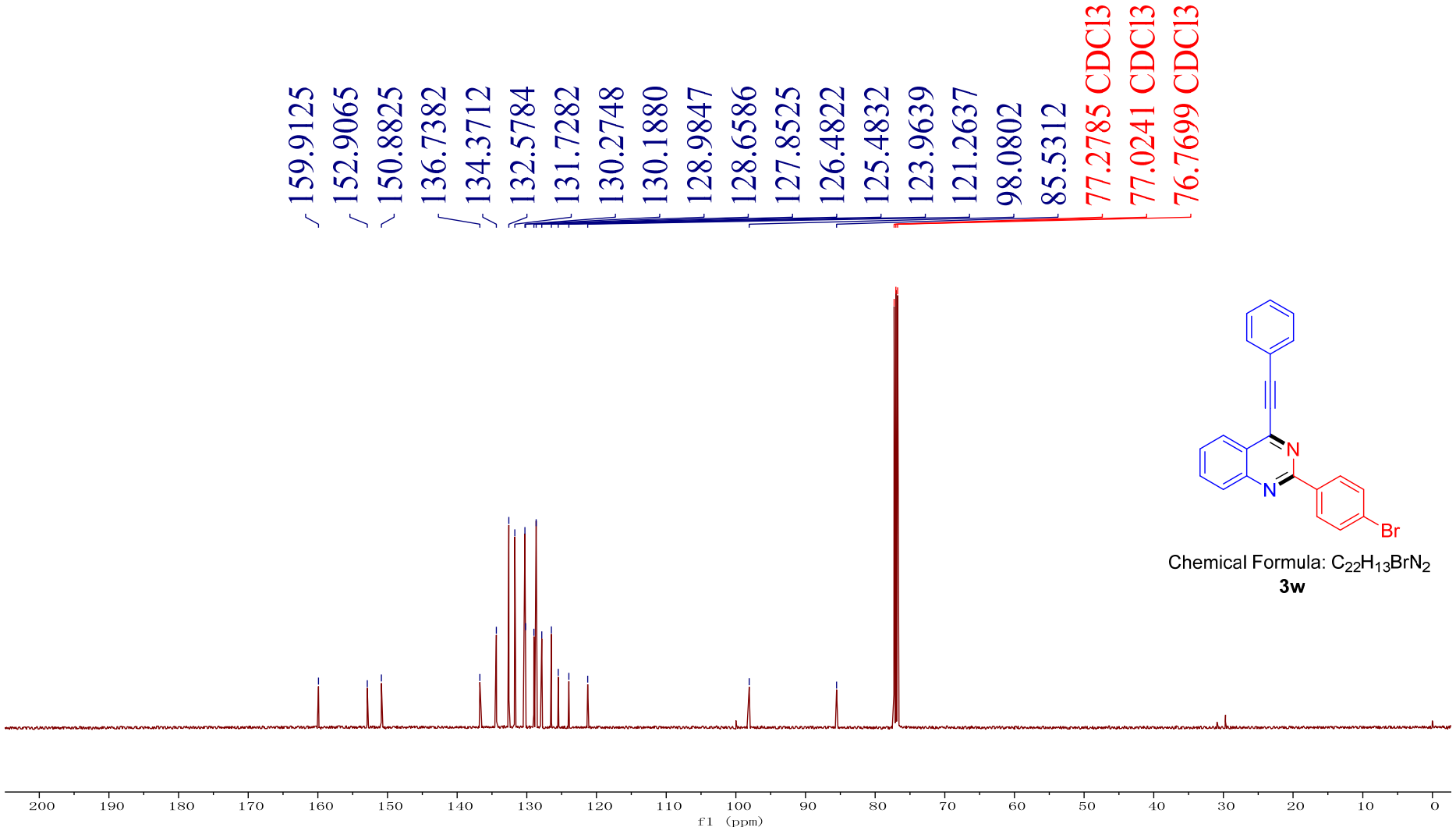
Chemical Formula: $C_{22}H_{13}FN_2$

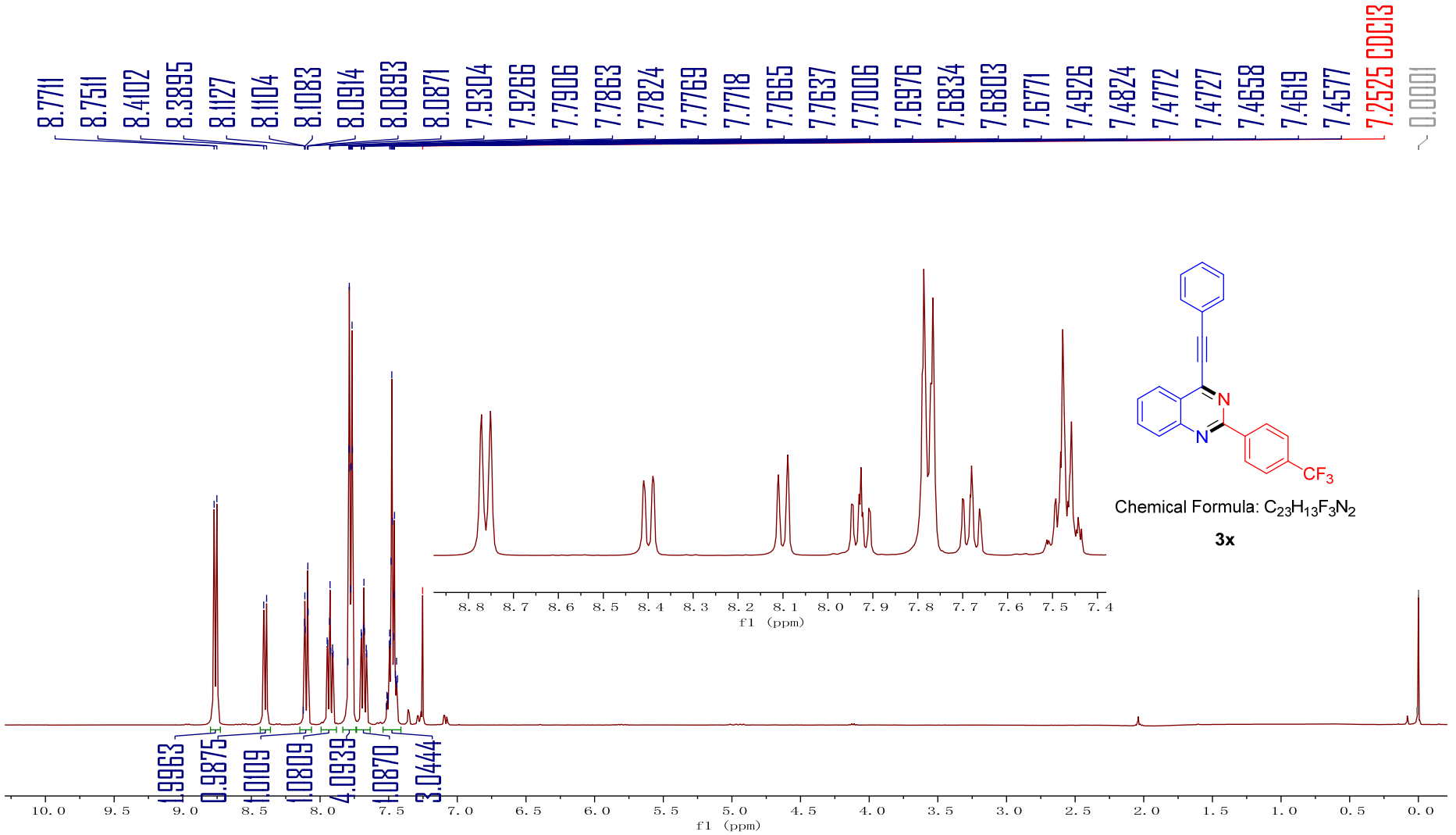
3u

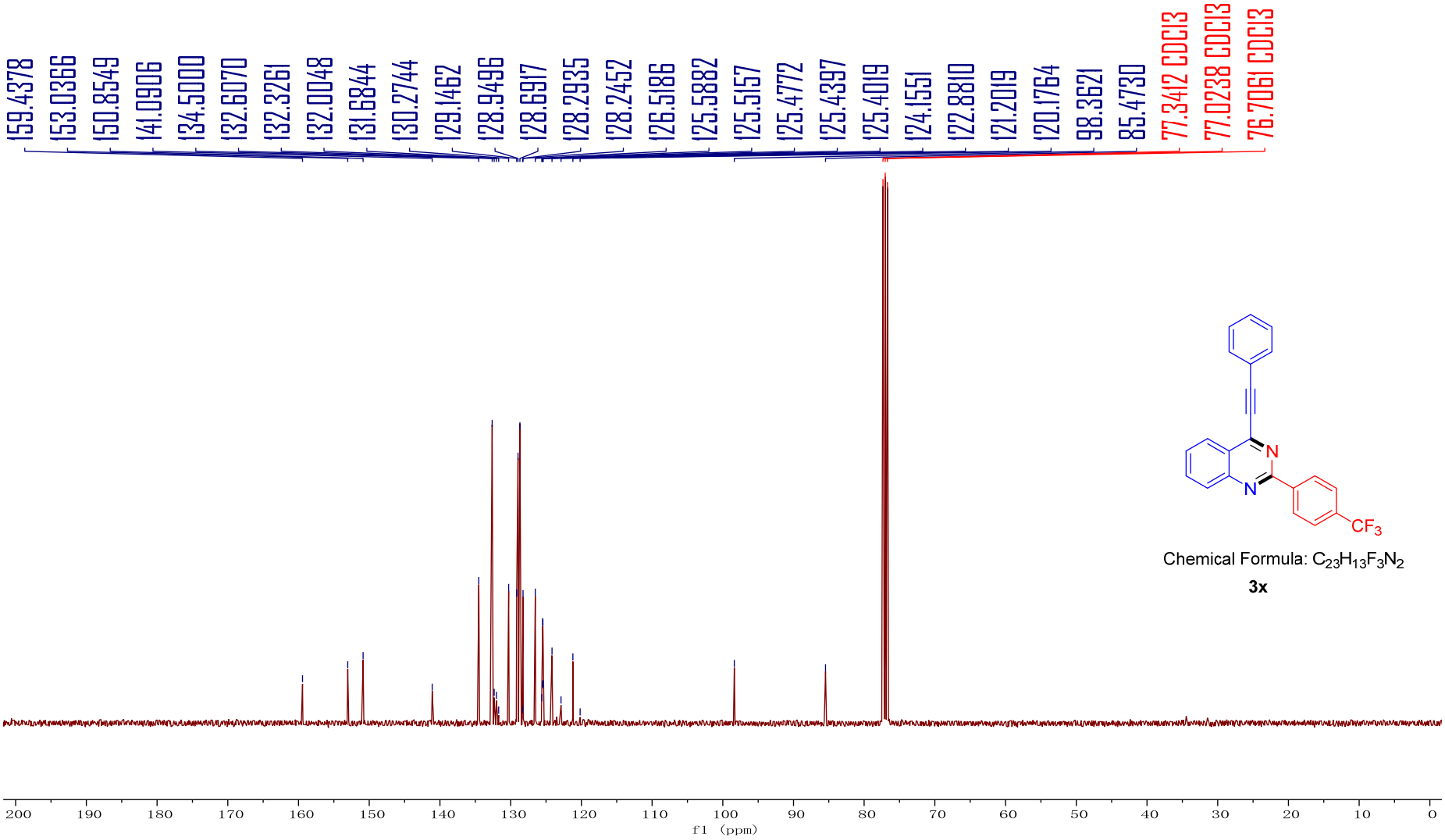

8.6056
8.5841
8.3870
8.3673
8.0734
8.0524
7.9058
7.9018
7.7830
7.7789
7.7745
7.7694
7.7645
7.7592
7.6679
7.6649
7.6507
7.6473
7.6440
7.5080
7.5014
7.4964
7.4885
7.4849
7.4798
7.4752
7.4704
7.4654
7.4599
7.4556
7.4514
7.2538 CDCl3
0.0000
2.000
1.004
1.005
1.051
2.009
1.061
5.004
f1 (ppm)
f1 (ppm)
N
N
Cl
Chemical Formula: $C_{22}H_{13}ClN_2$
3v


159.8407
152.9063
150.8858
136.8973
136.2871
134.3768
132.5863
130.1963
130.0326
128.9782
128.7731
128.6681
127.8376
126.4843
123.9343
121.2674
98.0648
85.5433
77.3538 CDCl3
77.0362 CDCl3
76.7191 CDCl3
N
N
Cl
Chemical Formula: $C_{22}H_{13}ClN_2$
3v
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.5326
8.5154
8.3850
8.3686
8.0723
8.0556
7.9208
7.9178
7.9072
7.9039
7.9006
7.8902
7.7811
7.7777
7.7656
7.7619
7.6672
7.6590
7.6549
7.6519
7.6419
7.6364
7.4866
7.4806
7.4769
7.4733
7.4687
7.4544
7.4411
7.2554
1.6235 HDO
-0.0004
2.003
0.998
1.000
1.054
2.003
3.057
3.001
f1 (ppm)
f1 (ppm)
N
N
Br
Chemical Formula: C22H13BrN2
3w

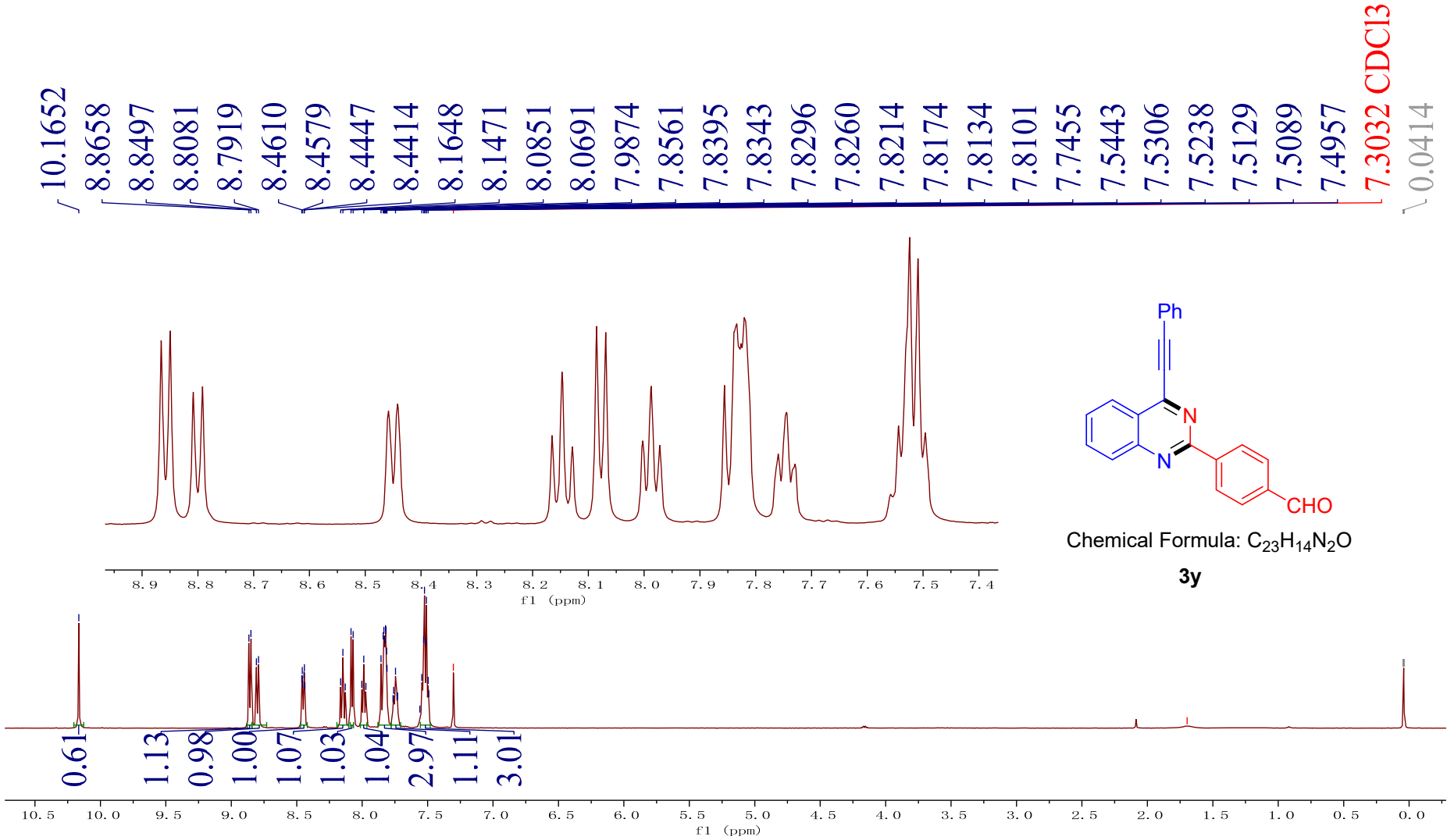

159.9125
152.9065
150.8825
136.7382
134.3712
132.5784
131.7282
130.2748
130.1880
128.9847
128.6586
127.8525
126.4822
125.4832
123.9639
121.2637
98.0802
85.5312
77.2785 CDC13
77.0241 CDC13
76.7699 CDC13
N
N
Br
Chemical Formula: $C_{22}H_{13}BrN_2$
3w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.7711
8.7511
8.4102
8.3895
8.1127
8.1104
8.1083
8.0914
8.0893
8.0871
7.9304
7.9266
7.7906
7.7863
7.7824
7.7769
7.7718
7.7665
7.7637
7.7006
7.6976
7.6834
7.6803
7.6771
7.4926
7.4824
7.4772
7.4727
7.4658
7.4619
7.4577
7.2525 CDCl3
0.0001
1.9963
0.9875
1.0109
1.0809
4.0939
1.0870
3.0444
f1 (ppm)
Chemical Formula: $C_{23}H_{13}F_3N_2$
3x



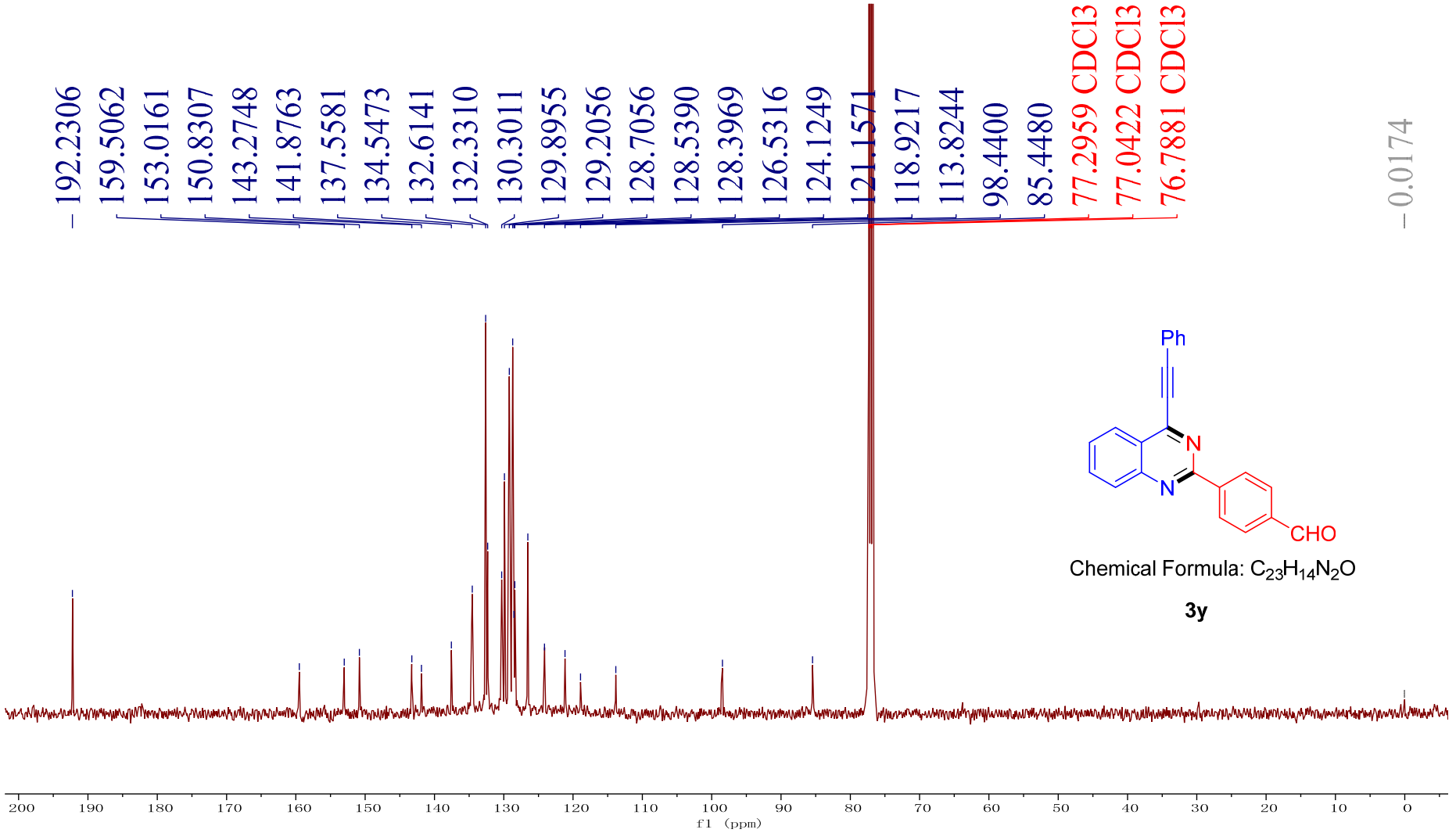
Chemical Formula: $C_{23}H_{13}F_3N_2$

3x



Chemical Formula: $C_{23}H_{14}N_2O$

3y


192.2306
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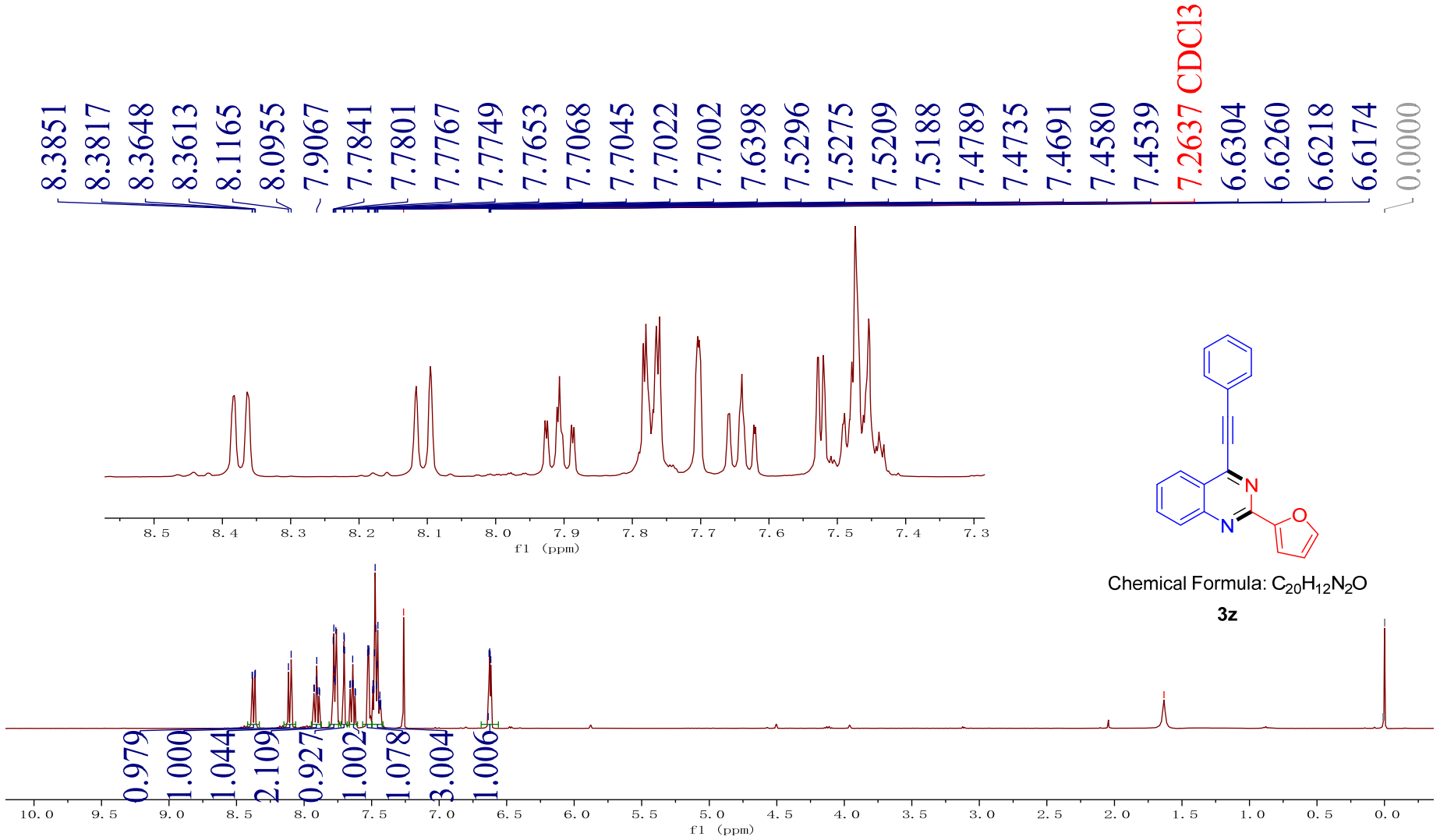
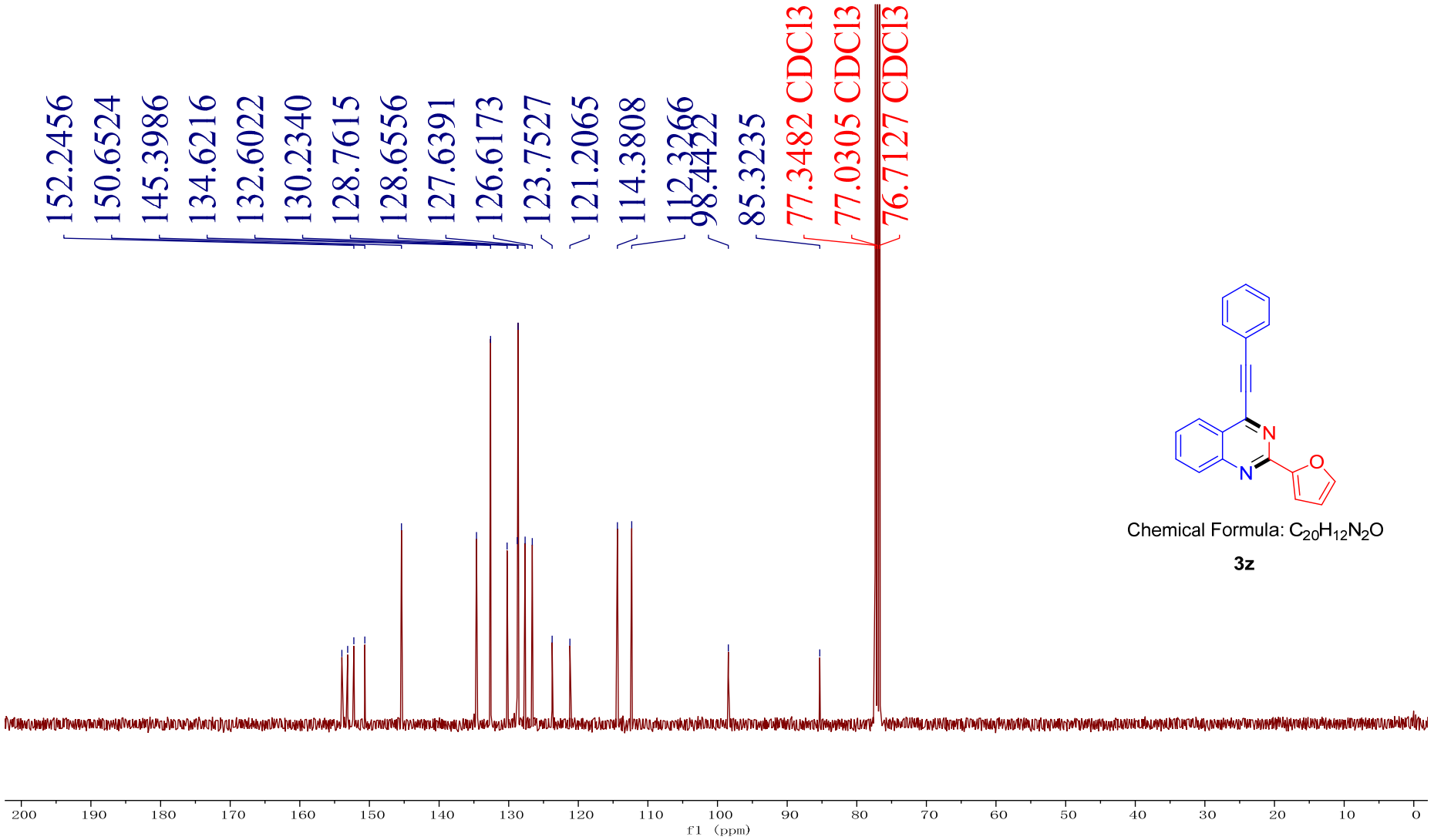
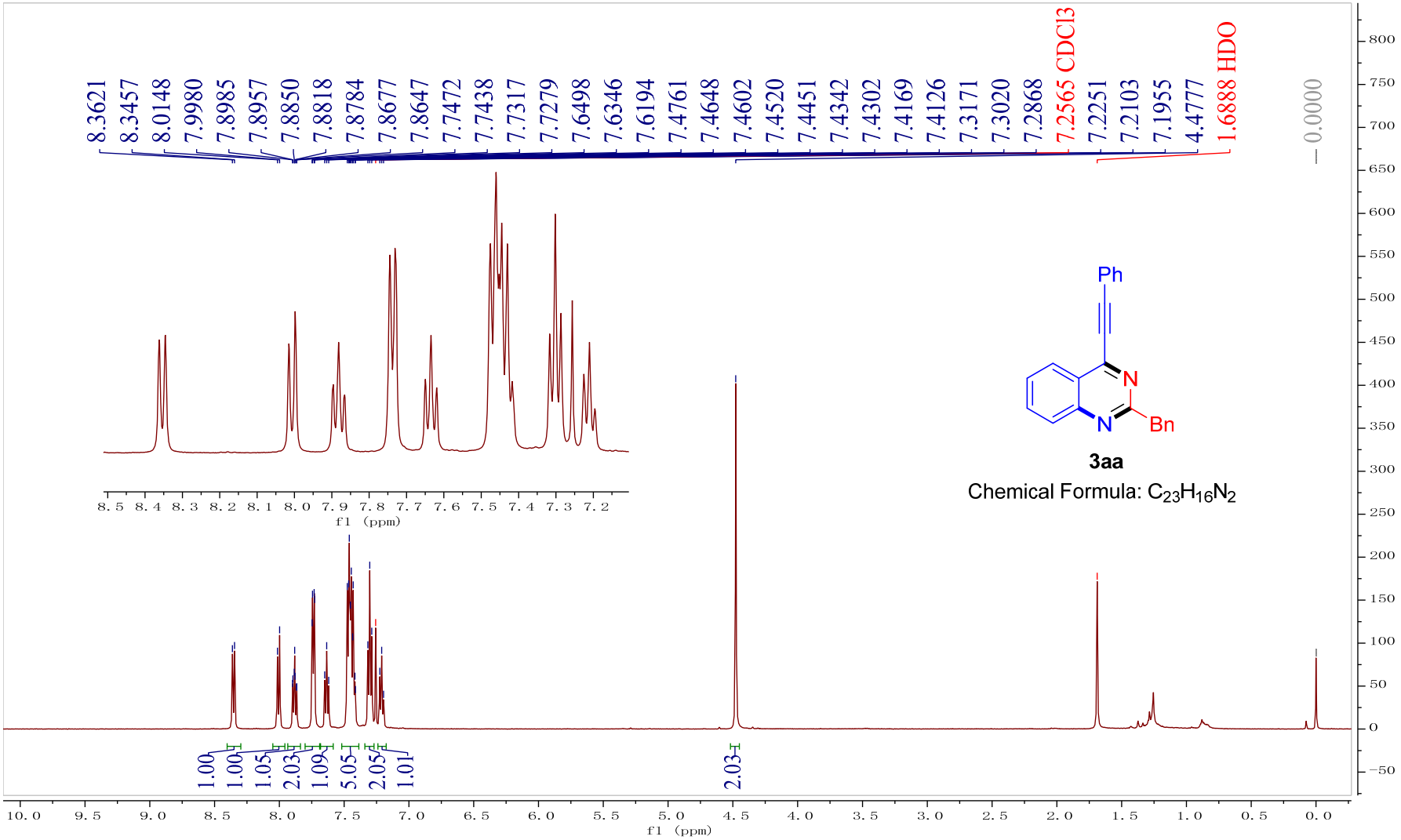
153.0161
150.8307
143.2748
141.8763
137.5581
134.5473
132.6141
132.3310
130.3011
129.8955
129.2056
128.7056
128.5390
128.3969
126.5316
124.1249
121.1571
118.9217
113.8244
98.4400
85.4480
77.2959 CDCl3
77.0422 CDCl3
76.7881 CDCl3
0.0174
Ph
N
N
CHO
Chemical Formula: C23H14N2O
3y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

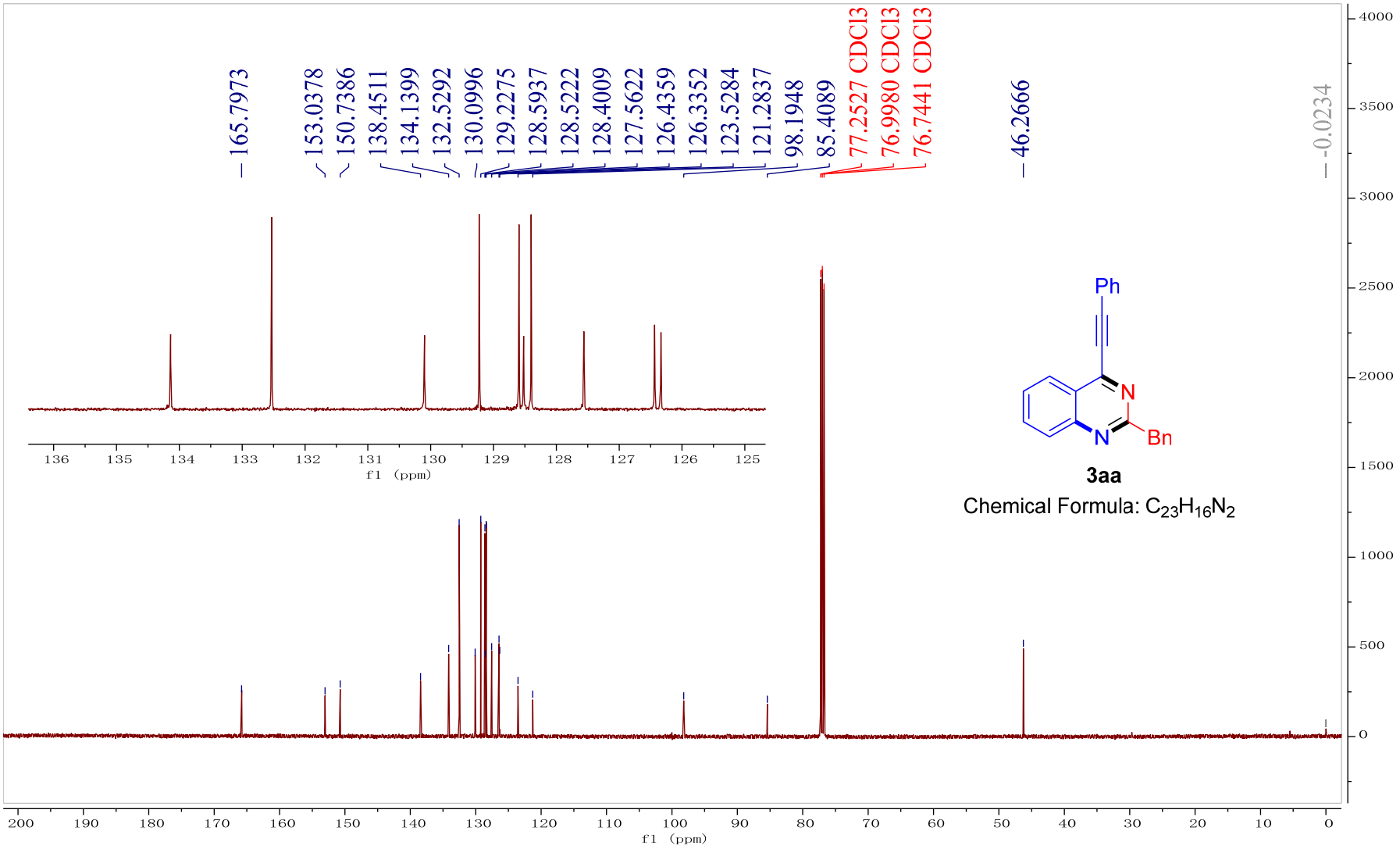

8.3851
8.3817
8.3648
8.3613
8.1165
8.0955
7.9067
7.7841
7.7801
7.7767
7.7749
7.7653
7.7068
7.7045
7.7022
7.7002
7.6398
7.5296
7.5275
7.5209
7.5188
7.4789
7.4735
7.4691
7.4580
7.4539
7.2637 CDCl3
6.6304
6.6260
6.6218
6.6174
0.0000
f1 (ppm)
N
N
O
Chemical Formula: C20H12N2O
3z
0.979
1.000
1.044
2.109
0.927
1.002
1.078
3.004
1.006
f1 (ppm)

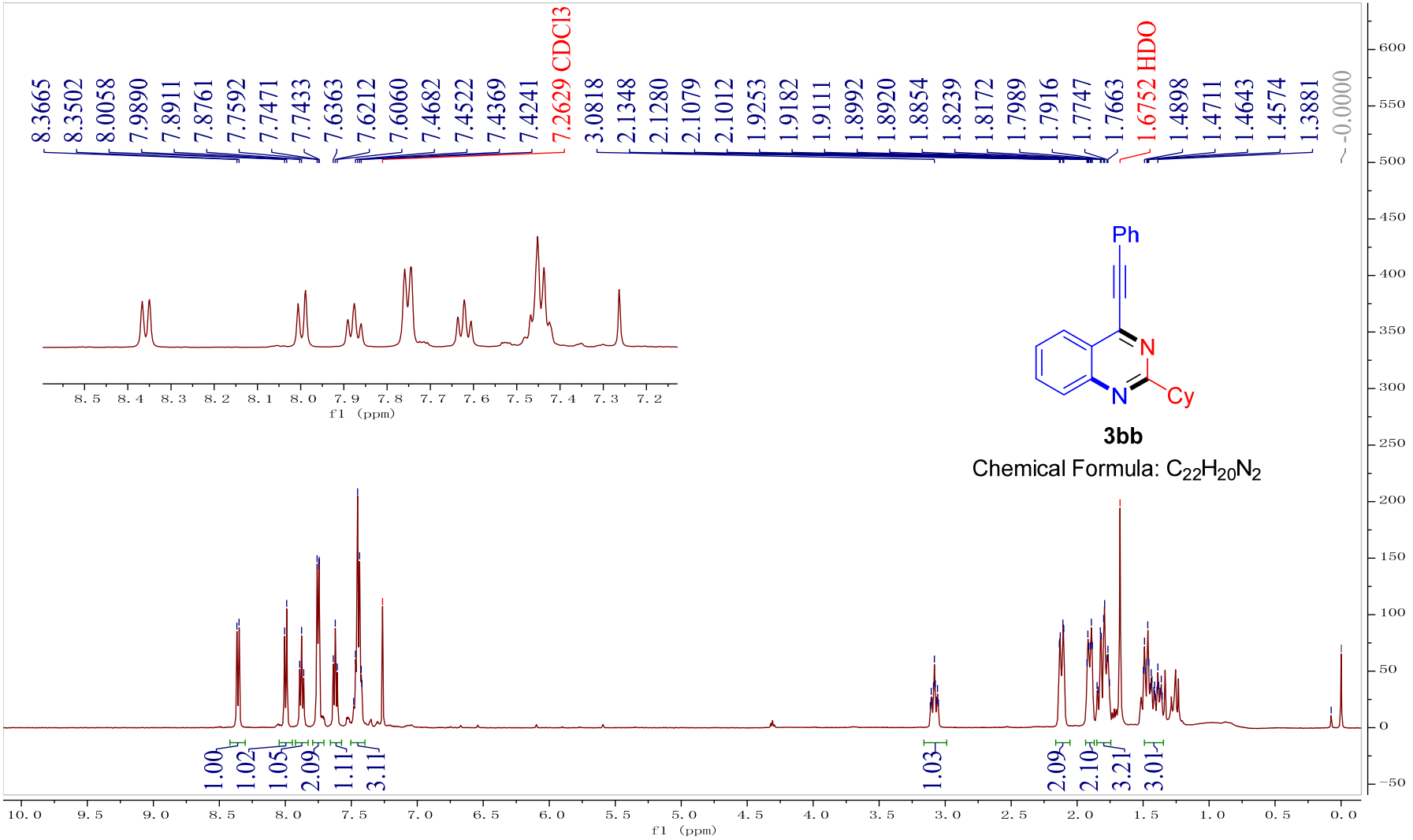


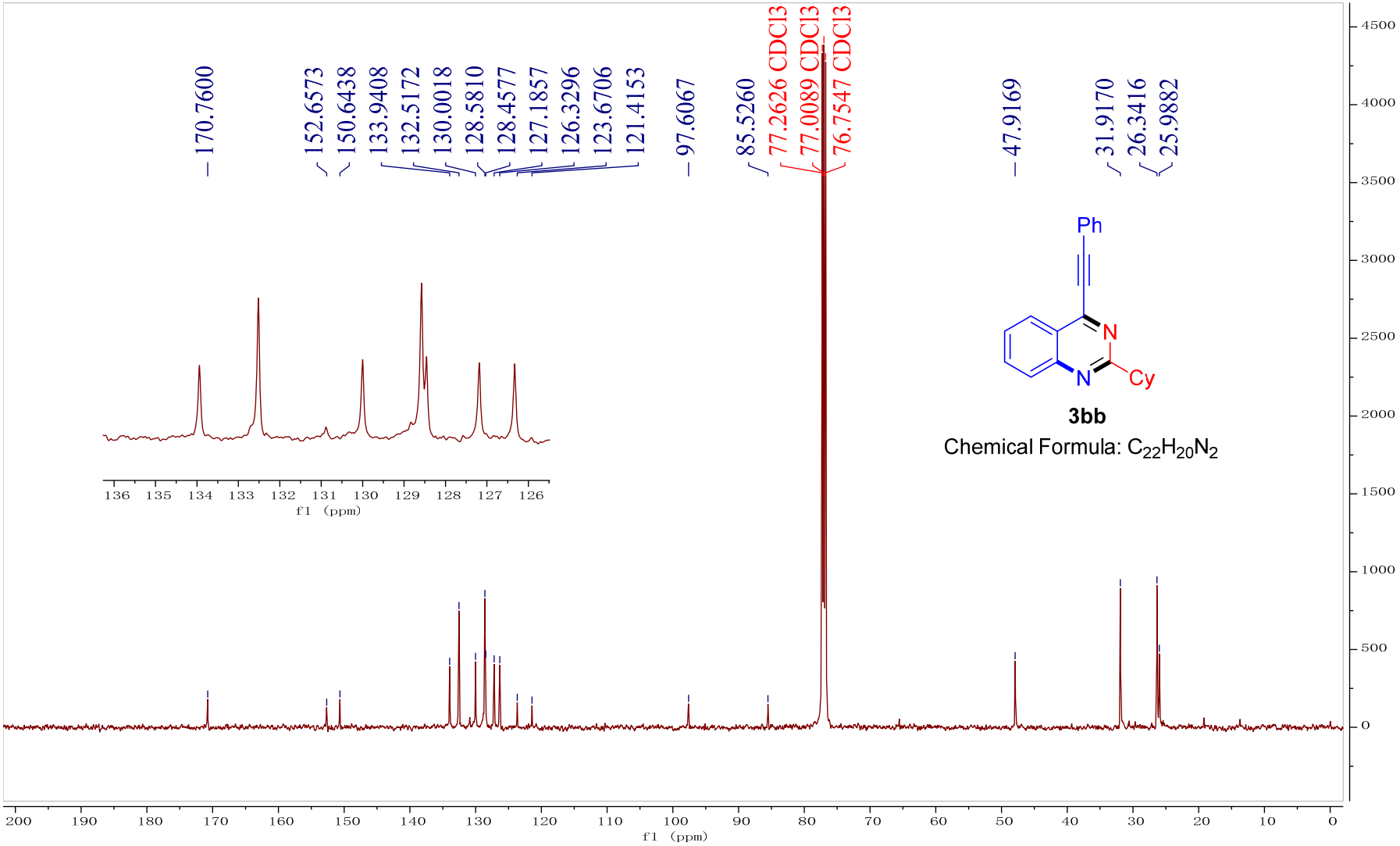
Chemical Formula: $C_{20}H_{12}N_2O$

3z


8.3621
8.3457
8.0148
7.9980
7.8985
7.8957
7.8850
7.8818
7.8784
7.8677
7.8647
7.7472
7.7438
7.7317
7.7279
7.6498
7.6346
7.6194
7.4761
7.4648
7.4602
7.4520
7.4451
7.4342
7.4302
7.4169
7.4126
7.3171
7.3020
7.2868
7.2565 CDCl3
7.2251
7.2103
7.1955
4.4777
1.6888 HDO
0.0000
Ph
N
N
Bn
3aa
Chemical Formula: C23H16N2
f1 (ppm)
1.00
1.00
1.05
2.03
1.09
5.05
2.05
1.01
2.03


165.7973
153.0378
150.7386
138.4511
134.1399
132.5292
130.0996
129.2275
128.5937
128.5222
128.4009
127.5622
126.4359
126.3352
123.5284
121.2837
98.1948
85.4089
77.2527 CDCl3
76.9980 CDCl3
76.7441 CDCl3
46.2666
-0.0234
f1 (ppm)
Ph
N
N
Bn
3aa
Chemical Formula: C23H16N2


8.3665
8.3502
8.0058
7.9890
7.8911
7.8761
7.7592
7.7471
7.7433
7.6363
7.6212
7.6060
7.4682
7.4522
7.4369
7.4241
7.2629 CDCl3
3.0818
2.1348
2.1280
2.1079
2.1012
1.9253
1.9182
1.9111
1.8992
1.8920
1.8854
1.8239
1.8172
1.7989
1.7916
1.7747
1.7663
1.6752 HDO
1.4898
1.4711
1.4643
1.4574
1.3881
~-0.0000
Ph
N
N
Cy
3bb
Chemical Formula: C22H20N2
f1 (ppm)
1.00
1.02
1.05
2.09
1.11
3.11
1.03
2.09
2.10
3.21
3.01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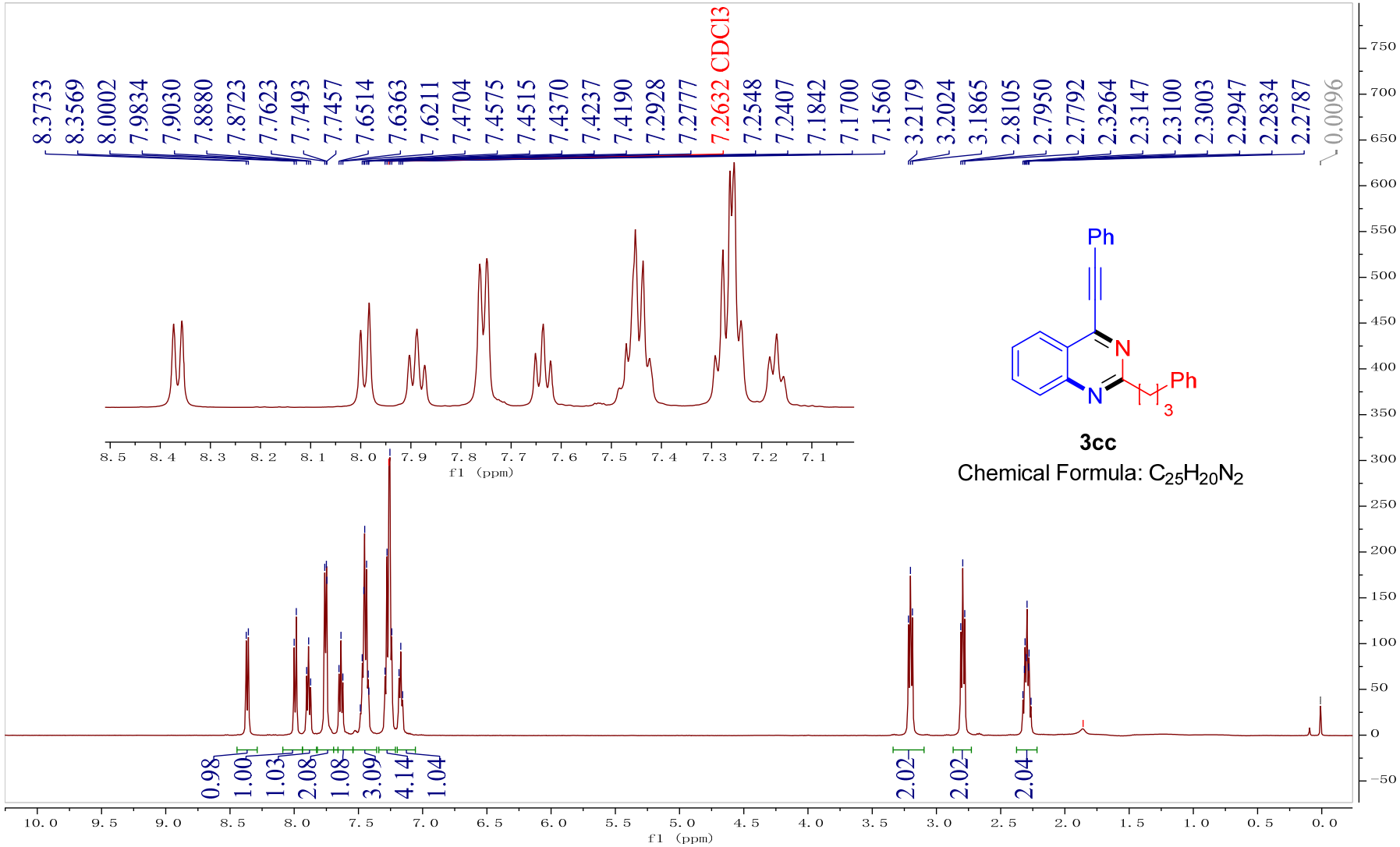
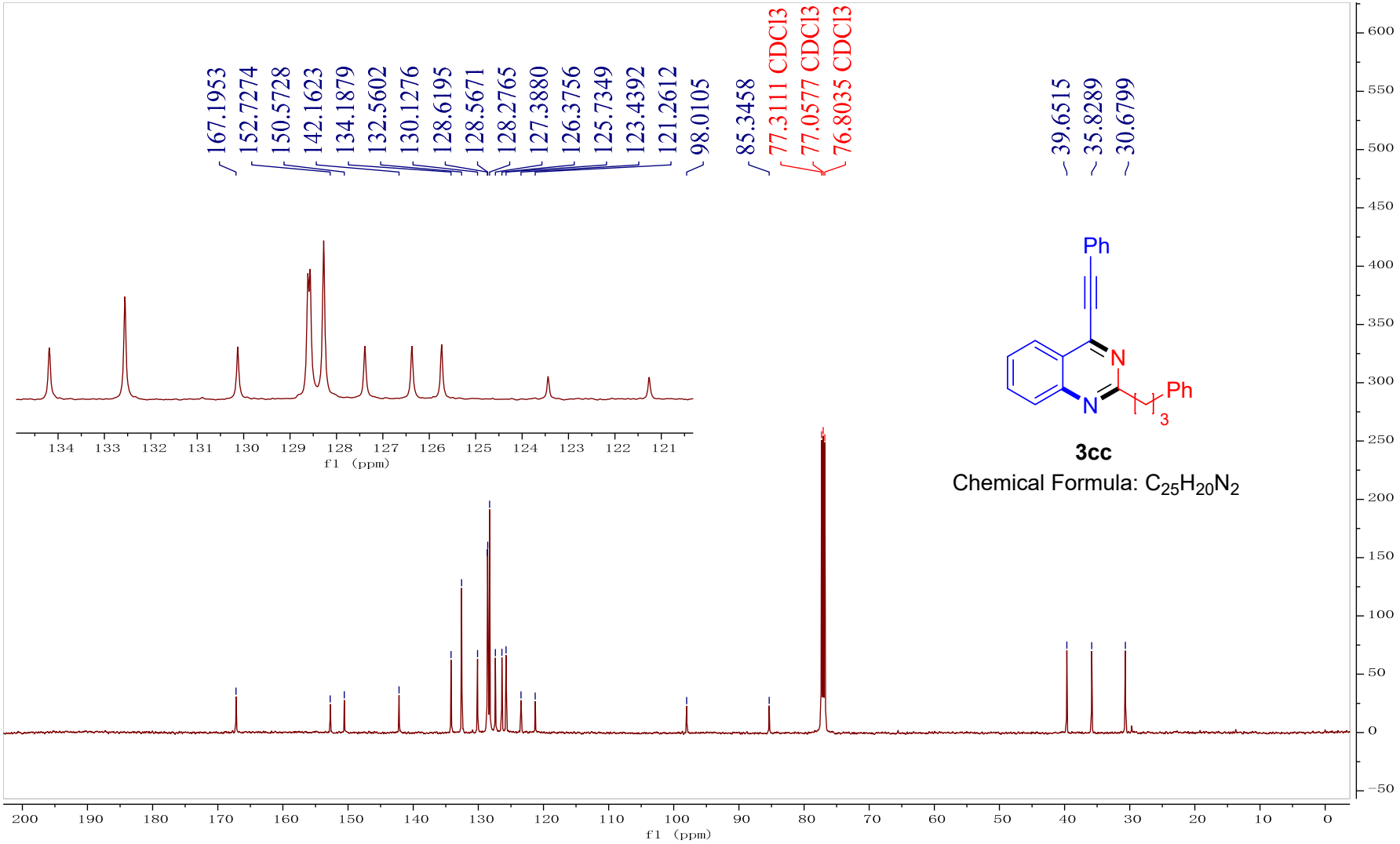
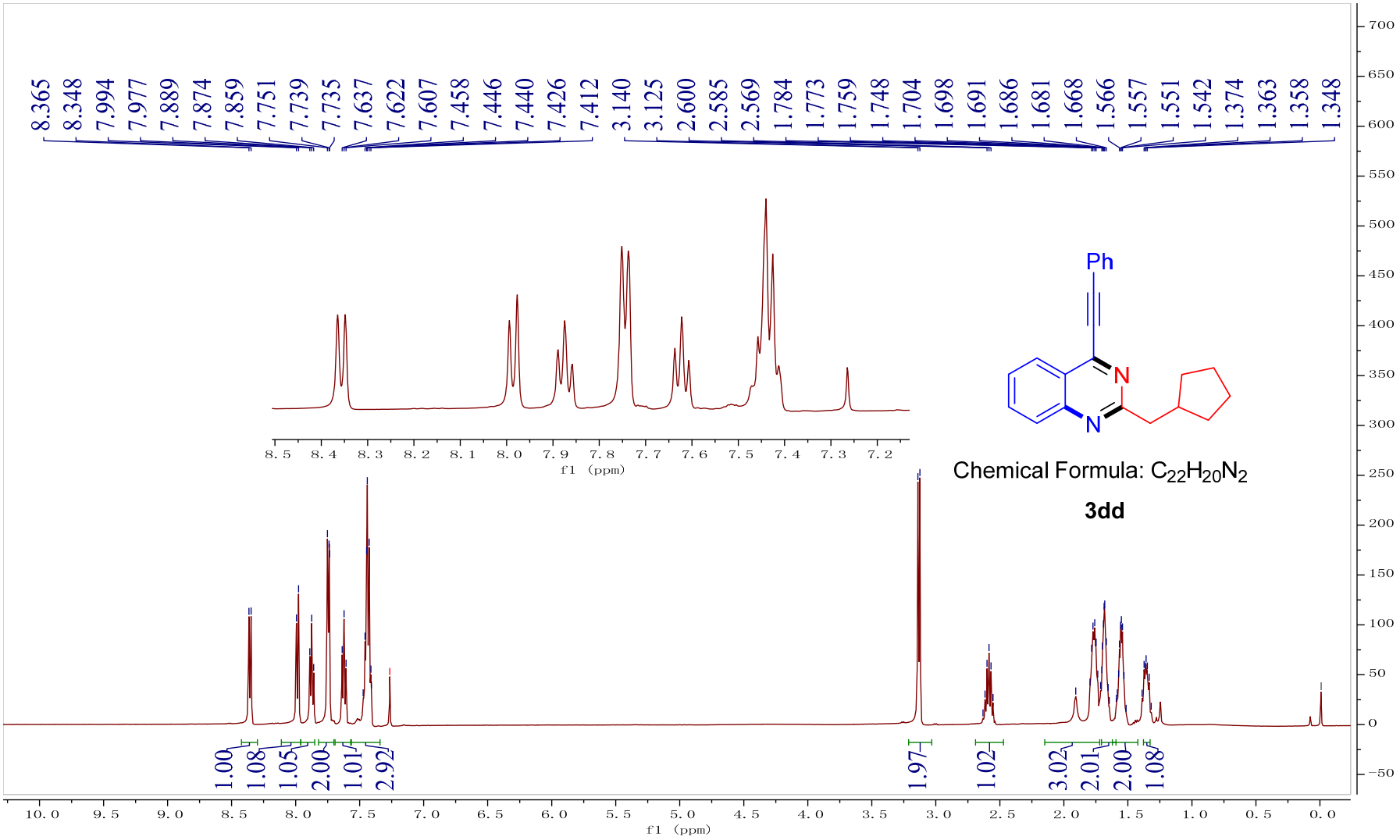
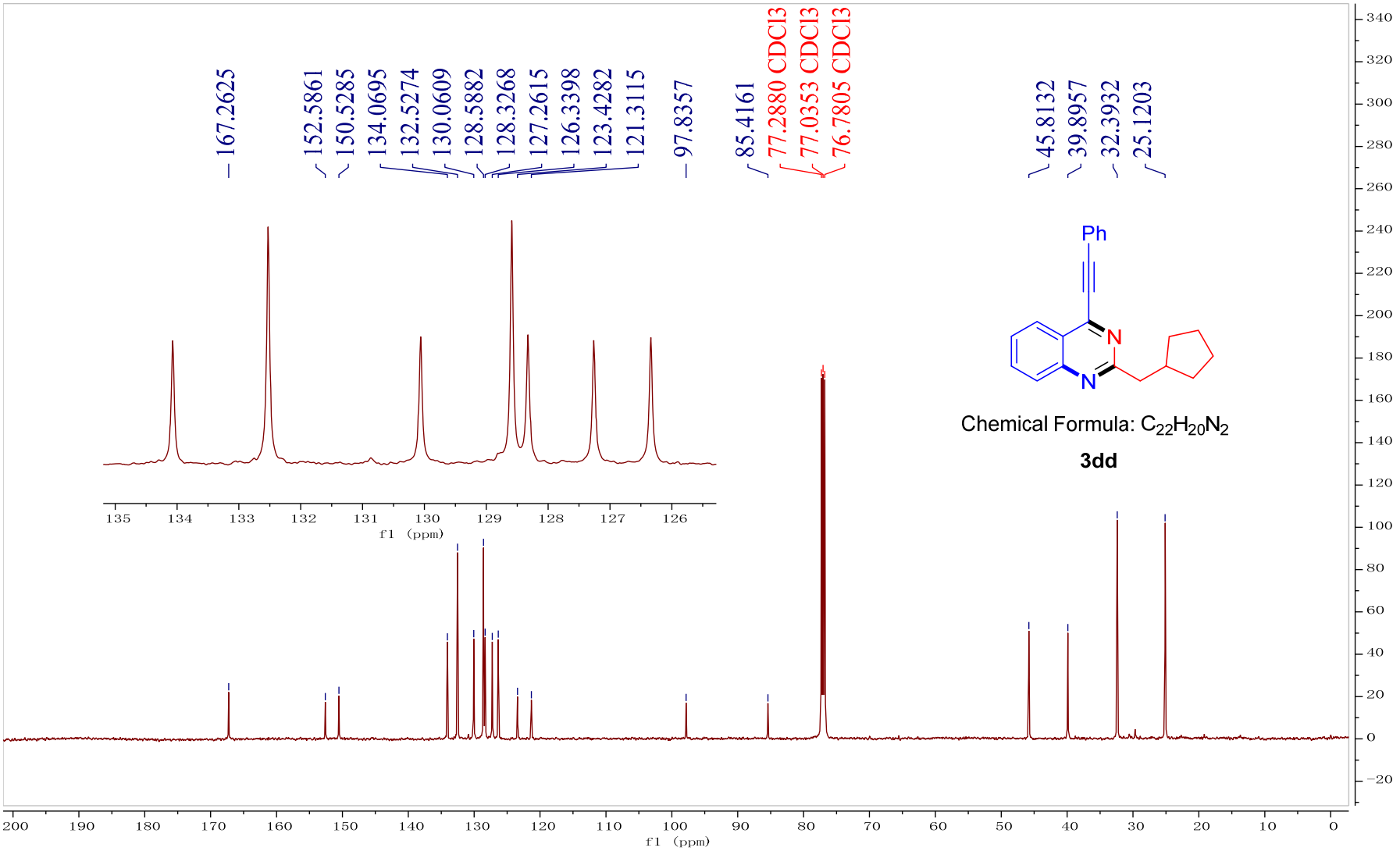
152.6573
150.6438
133.9408
132.5172
130.0018
128.5810
128.4577
127.1857
126.3296
123.6706
121.4153
97.6067
85.5260
77.2626 CDCl3
77.0089 CDCl3
76.7547 CDCl3
47.9169
31.9170
26.3416
25.9882
f1 (ppm)
Ph
N
N
Cy
3bb
Chemical Formula: C22H20N2


8.3733
8.3569
8.0002
7.9834
7.9030
7.8880
7.8723
7.7623
7.7493
7.7457
7.6514
7.6363
7.6211
7.4704
7.4575
7.4515
7.4370
7.4237
7.4190
7.2928
7.2777
7.2632 CDCl3
7.2548
7.2407
7.1842
7.1700
7.1560
3.2179
3.2024
3.1865
2.8105
2.7950
2.7792
2.3264
2.3147
2.3100
2.3003
2.2947
2.2834
2.2787
0.0096
f1 (ppm)
0.98
1.00
1.03
2.08
1.08
3.09
4.14
1.04
2.02
2.02
2.04
f1 (ppm)
Ph
N
N
Ph
3
3cc
Chemical Formula: C25H20N2


167.1953
152.7274
150.5728
142.1623
134.1879
132.5602
130.1276
128.6195
128.5671
128.2765
127.3880
126.3756
125.7349
123.4392
121.2612
98.0105
85.3458
77.3111 CDCl3
77.0577 CDCl3
76.8035 CDCl3
39.6515
35.8289
30.6799
Ph
N
N
Ph
3
3cc
Chemical Formula: C25H20N2
f1 (ppm)
f1 (ppm)


8.365
8.348
7.994
7.977
7.889
7.874
7.859
7.751
7.739
7.735
7.637
7.622
7.607
7.458
7.446
7.440
7.426
7.412
3.140
3.125
2.600
2.585
2.569
1.784
1.773
1.759
1.748
1.704
1.698
1.691
1.686
1.681
1.668
1.566
1.557
1.551
1.542
1.374
1.363
1.358
1.348
f1 (ppm)
Ph
N
N
Chemical Formula: C22H20N2
3dd
1.00
1.08
1.05
2.00
1.01
2.92
1.97
1.02
3.02
2.01
2.00
1.08
f1 (ppm)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152.5861
150.5285
134.0695
132.5274
130.0609
128.5882
128.3268
127.2615
126.3398
123.4282
121.3115
97.8357
85.4161
77.2880 CDCl3
77.0353 CDCl3
76.7805 CDCl3
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32.3932
25.1203
Ph
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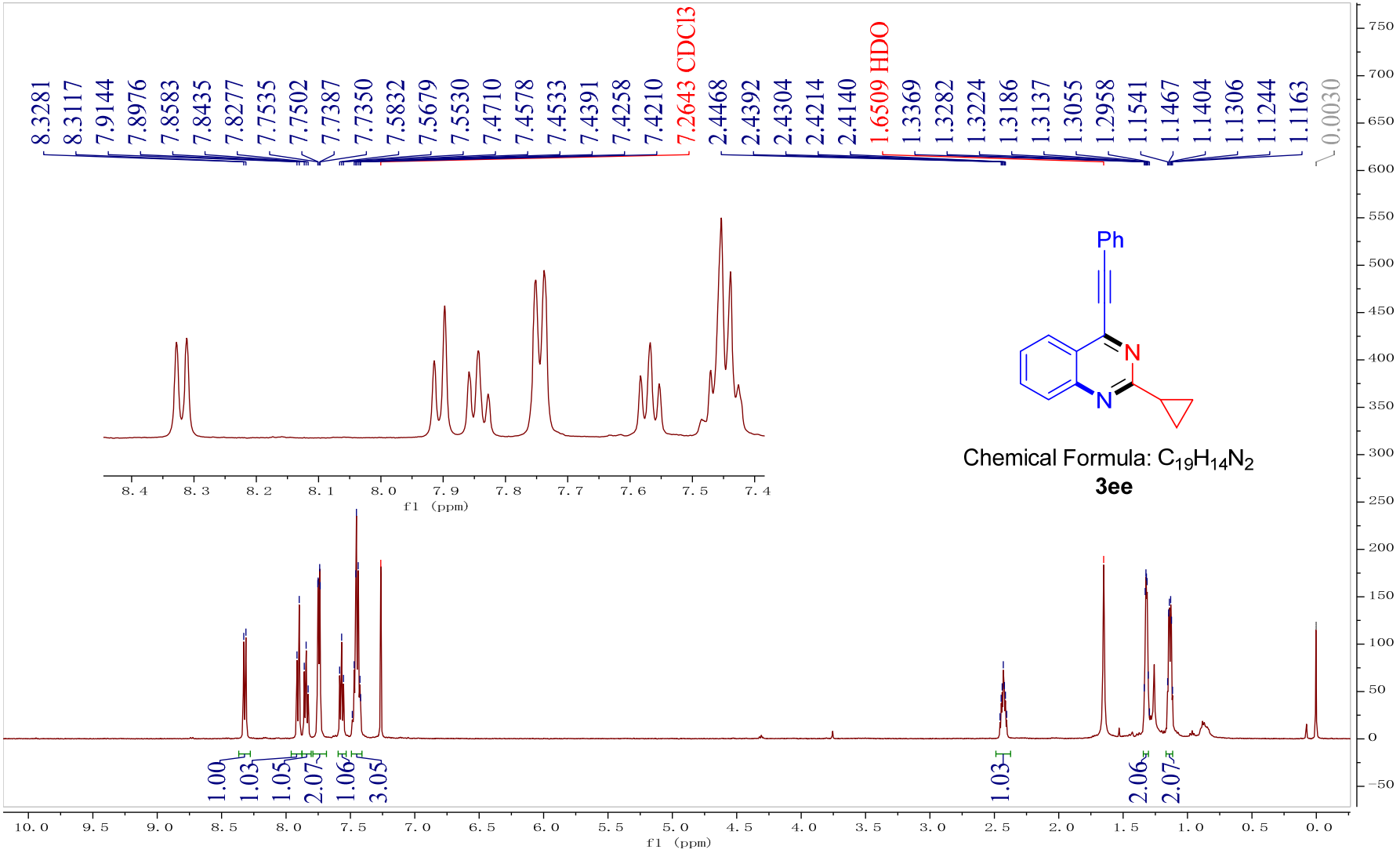
N
Chemical Formula: C22H20N2
3dd
f1 (ppm)
f1 (ppm)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8.3117
7.9144
7.8976
7.8583
7.8435
7.8277
7.7535
7.7502
7.7387
7.7350
7.5832
7.5679
7.5530
7.4710
7.4578
7.4533
7.4391
7.4258
7.4210
7.2643 CDCl3
2.4468
2.4392
2.4304
2.4214
2.4140
1.6509 HDO
1.3369
1.3282
1.3224
1.3186
1.3137
1.3055
1.2958
1.1541
1.1467
1.1404
1.1306
1.1244
1.1163
0.0030
Ph
N
N
Chemical Formula: C19H14N2
3ee
f1 (ppm)
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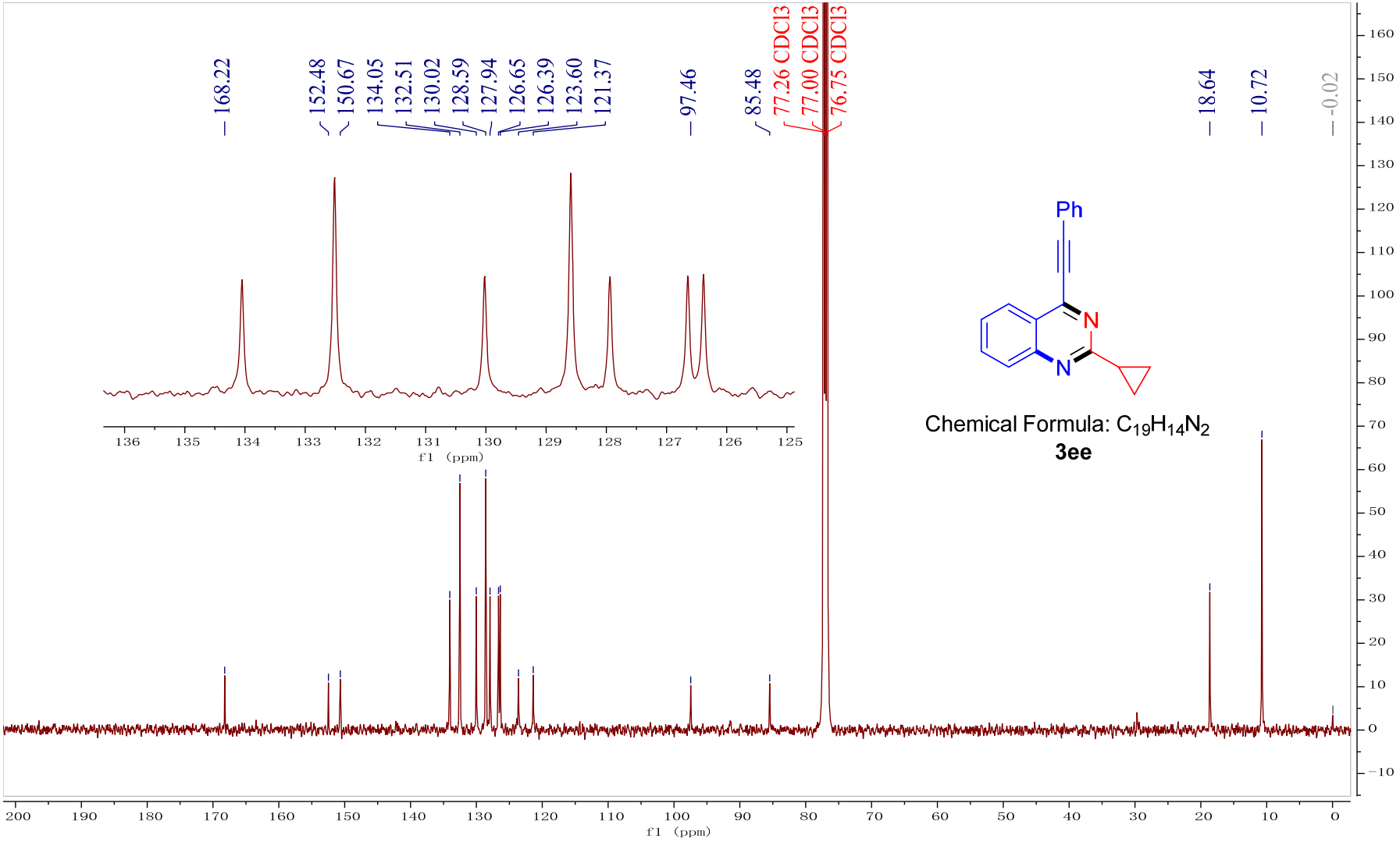
1.03
1.05
2.07
1.06
3.05
1.03
2.06
2.07
f1 (ppm)


168.22
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150.67
134.05
132.51
130.02
128.59
127.94
126.65
126.39
123.60
121.37
97.46
85.48
77.26 CDCl3
77.00 CDCl3
76.75 CDCl3
18.64
10.72
-0.02
Ph
N
N
Chemical Formula: C19H14N2
3ee
f1 (ppm)
f1 (ppm)