Fe-catalyzed Highly Selective Ring Expansion of Alkynylcyclopropyl Alkanols to Cyclobutanols: 1,2-Carbon Shift *Versus* 2,3- C-C Bond Cleavage

Supporting Information

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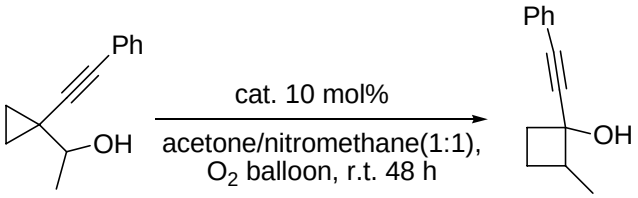
Table of Contents

Table S1. Ring Expansion Reaction of **1a** catalyzed by other catalysts[a]

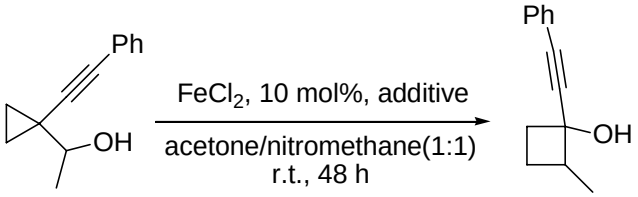


1a **2a**

Entry	Catalyst(10%)	Yield of **2a** (%)[b]
1	$TsOH{\cdot}H_2O$	Trace
2	$AgNO_3$	Trace
3	$CuCl_2{\cdot}2H_2O$	Trace
4	$AuCl_3$	Trace
5	$PtCl_4$	0
6	$Fe(NO_3)_3{\cdot}9H_2O$	Trace
7	$S_C(OTf)_3$	5
8	$AlCl_3$	Trace
9	HOAc	Trace
10	$Cu(OTf)_2$	8
11	$IrCl_3$	7
12	$RhCl_3{\cdot}3H_2O$	Trace
13	$NiCl_2{\cdot}6H_2O$	NR
14	$Ga(OTf)_3$	10
15	$InCl_3$	NR
16	$Mn(OAc)_2{\cdot}2H_2O$	NR
17[c]	HCl	NR
18[c,d]	$FeCl_3$	6
19[e]	$FeCl_3$	36
20	$FeBr_2$	43
21	$Fe(acac)_2$	Trace
22	$Fe(OTf)_3$	15
23	$Fe(OAc)_2$	NR
24	$FeCl_3$/4 ÅMS	NR
25	$Fe_2(SO_4)_3$	NR
26	FeF_3	NR
27	FeF_2	NR

[a] **1a** (37.2 mg, 0.2 mmol), 10 mol% catalyst, 2 mL solvent, under O_2 (1 atm). [b] Isolated yield. [c] The reaction was carried out in 2 mL nitromethane. [d] The reaction was carried out at 40 ℃. [e] The reaction was carried out in 2 mL acetone.

Table S2. The effect of different additives in the $FeCl_2$ catalyzed ring expansion of **1a** to **2a**[a]

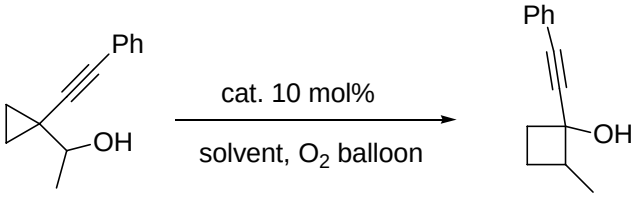


1a **2a**

Entry	additives (eq.)	Yield of **2a** (%)[b]
1	$PhI(OAc)_2$ (0.2)	7
2	BQ (0.2)	32
3	$AgBF_4$ (0.2)	10
4	AgOTf (0.2)	43
5	$AgClO_4$ (0.2)	15
6	$AgNO_3$ (0.2)	trace
7	$^tBuOO^tBu$ (3.0)	38
8	Bipyridine (0.2)	NR
9	H_2O_2 (1.0)	7
10	4-chlorobenzoperoxic acid (1.0)	6
11	H_2O (1.0)	trace
12	Hydroquinone (0.2)	14

[a] **1a** (37.2 mmg, 0.2 mmol), 10 mol% catalyst, 2 mL acetone/nitromethane(1:1), under O_2. [b] Isolated yield.

Table S3. The transformation of **1a** to **2a** in different solvents catalyzed by $FeCl_2$[a]



1a **2a**

Entry	Solvent	T(°C)	time(h)	yield (%)[b]
1	CH_3OH	RT	24	NR
2	CH_3NO_2	RT	16	22
3	DCM	RT	72	16
4	CH_3CN	RT	8	NR
5	DMA	RT	8	NR
6	Toluene	RT	24	trace
7	H_2O	RT	8	NR
8	THF	RT	8	NR
9	DMF	RT	24	NR
10	Dioxane	RT	24	NR
11	$CHCl_3$	RT	24	trace
12[c]	2:1	RT	24	43
13[c]	3:1	RT	48	32
14[c]	10:1	RT	48	30
15[c]	4:1	RT	48	30
16	Acetone	RT	23	40
17	Acetone	reflux	40	6
18[c]	1:1	50	40	10

[a] **1a** (37.2 mmg, 0.2 mmol), $FeCl_2$, 10 mol%, 2 mL solvent, under O_2. [b] Isolated yield. [c] Ratio of acetone/nitromethane.

Experimental section

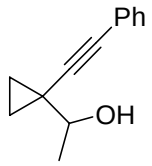
General Remarks.

All manipulations were conducted with a standard Schlenk technique under oxygen atmosphere. ^{1}H-NMR spectra were recorded on a JEOL AL-300 or Bruker AVIII-400 spectrometers. Chemical shifts (in ppm) were referenced to tetramethylsilane (δ = 0 ppm) in $CDCl_3$ as an internal standard. ^{13}C-NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.00 ppm). Mass spectra were recorded using a PE SCLEX QSTAR spectrometer. Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Iron (Ⅱ) chloride (anhydrous, 99.99 %) were purchased from Sream. Some spectra of *cis*-isomers were not obtained due to the less separated amount of *cis*-products.

Substrates **1** are synthesized according to literature procducer[1]

General producer for 1-(1-(Phenylethynyl)cyclopropyl) ethanol (1a):

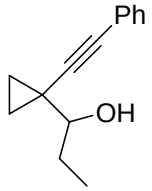
To a solution of 1-cyclopropyl-2-phenylethyne (1.85 g, 13 mmol) in dry THF (100 mL) was added dropwise *n*-BuLi (2.5 M, 15 mmol) in hexane at 0 ^{o}C, The mixture was stirred for 1 h at rt before acetaldehyde was added. After 1 h, the reaction was quenched by addition of 50 mL of water. The mixture was neutralized with 1 N HCl and extracted with diethyl ether (3 x 50 mL). The combined organic layers were dried over Na_2SO_4. After filtration and evaporation, the crude product was purified by column chromatography on silica gel to afford 1.5 g (Yield 63%.) of **1a**.



1a

1)

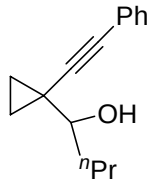
1-(1-(Phenylethynyl)cyclopropyl) ethanol (1a): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.43-7.38(m, 2 H), 7.29-7.25 (m, 3 H), 3.20 (q, *J* = 6.6 Hz, 1 H), 1.90 (brs, 1 H), 1.42 (d, *J* = 6.6 Hz, 3 H), 1.10-0.98 (m, 2 H), 0.94-0.89 (m, 1 H), 0.78-0.73 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.2, 127.7, 123.5, 91.0, 79.3, 73.2, 21.1, 19.9, 14.3, 13.2 ppm; MS (70 eV): m/z (%): 186.2 (6) [M^{+}], 144.1 (100); IR (neat): ν = 3419, 2958, 2927, 2866, 2206, 1716, 1598, 1491, 1446, 756.4, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{13}H_{15}O$ $(M + H)^{+}$: 187.11174, found 187.11143.



1b

2)

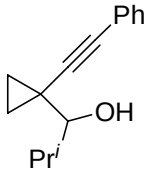
1-(1-(Phenylethynyl)cyclopropyl) propanol (1b): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.40-7.37 (m, 2 H), 7.29-7.25 (m, 3 H), 2.8 (q, *J* = 6.3 Hz, 1 H), 1.80-1.72 (m, 2 H), 1.69 (d, *J* = 6.3 Hz, 1 H), 1.08-0.90 (m, 5 H), 0.91-0.78 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.1, 127.7, 123.5, 91.1, 79.1, 78.9, 28.9, 18.8, 13.9, 13.7, 10.5 ppm; MS (70 eV): m/z (%): 200.2 (8) [M^+], 127.9 (100); IR (neat): ν = 3423, 2964, 2932, 2876, 2361, 2225,1715, 1598, 1491, 1460, 975, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10859.



1c

3)

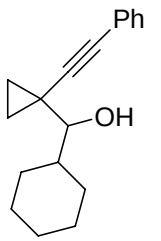
1-(1-(Phenylethynyl)cyclopropyl) butanol (1c): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.47-7.32 (m, 2 H), 7.28-7.26 (m, 3 H), 2.91 (m, 1 H), 1.81-1.74 (m, 3 H), 1.60-1.35 (m, 2 H), 1.10-1.02 (m, 2 H), 0.96 (t, *J* = 7.2 Hz, 3 H), 0.91-0.84 (m, 1 H), 0.83-0.73 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.1, 127.7, 123.5, 91.1, 79.1, 77.2, 38.0, 19.2, 19.1, 14.1, 13.9, 13.8 ppm; MS (70 eV): m/z (%): 214.2 (2) [M^+], 71.0 (100); IR (neat): ν = 3406, 2959, 2932, 2872, 2224, 1717, 1491, 1460, 1030, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{15}H_{18}ONa$ $(M + Na)^+$: 237.12499, found 237.12452.



1d

4)

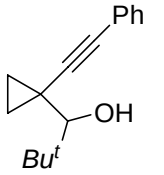
1-(1-(Phenylethynyl)cyclopropyl)-2-methyl propanol (1d): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.41-7.36 (m, 2 H), 7.28-7.24 (m, 3 H), 2.48 (d, *J* = 8.4 Hz, 1 H), 2.20-2.03 (m, 1 H), 1.79 (brs, 1 H), 1.16-1.13 (m, 1 H), 1.08-1.00 (m, 7 H), 0.96-0.82 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.1, 127.6, 123.6, 91.3, 83.2, 78.8, 34.1, 19.5, 19.3, 18.0, 15.6, 13.4 ppm; MS (70 eV): m/z (%): 214.2 (2) [M^+], 105.1 (100); IR (neat): ν = 3447, 2960, 2938, 2874, 2224, 1718, 1599, 1271, 1037, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{15}H_{18}ONa$ $(M + Na)^+$: 237.12499, found 237.1248.



1e

5)

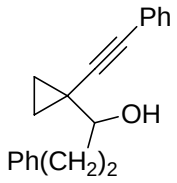
1-Cyclohexyl-(1-(phenylethynyl)cyclopropyl) methanol (1e): solid, mp 42~44 ℃ (*n*-hexane/ethyl aceate); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.43-7.35 (m, 2 H), 7.31-7.24 (m, 3 H), 2.55-2.47 (m, 1 H), 2.18-1.98 (m, 2 H), 1.90-1.56 (m, 6 H), 1.19-1.06 (m, 2 H), 1.04-0.98 (m, 1 H), 0.94-0.73 (m, 5 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.1, 127.6, 123.6, 91.3, 82.3, 78.3, 43.6, 29.7, 29.6, 26.5, 26.2, 25.9, 17.8, 15.5, 13.2 ppm; MS (70 eV): m/z (%): 254.3 (2) [M^+], 43.1 (100) ; IR (neat): ν = 3401, 2927, 2953, 2853, 2225, 2007, 1710, 1449, 1032, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{22}ONa$ $(M + Na)^+$: 277.15629, found 277.15683.



1f

6)

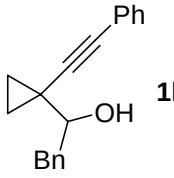
1-(1-(Phenylethynyl)cyclopropyl)-2,2-dimethyl propanol (1f): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.43-7.36 (m, 2 H), 7.31-7.24 (m, 3 H), 2.99 (m, 1 H), 1.92-1.1.62 (m, 2 H), 1.61-1.49 (m, 1 H), 1.09-1.00 (m, 2 H), 0.98-0.75 (m, 9 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.1, 127.7, 123.5, 91.2, 79.2, 75.4, 44.8, 24.4, 23.5, 22.0, 19.5, 14.2, 13.7 ppm; MS (70 eV): m/z (%): 228.1 (1) [M^+], 158 (100); IR (neat): ν = 3395, 2956, 2928, 2870, 2222, 1708, 1598, 1491, 1466, 1071, 1030, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{16}H_{21}ONa$ $(M + Na)^+$: 251.14064, found 251.14152.



1g

7)

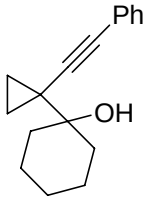
1-(1-(Phenylethynyl)cyclopropyl)-3-phenyl propanol (1g): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.42-7.29 (m, 2 H), 7.29-7.14 (m, 8 H), 2.99-2.68 (m, 3 H), 2.17-2.00 (m, 2 H), 1.78 (d, *J* = 4.2 Hz, 1 H), 1.10-1.00 (m, 2 H), 0.90-0.83 (m, 1 H), 0.80-0.71 (m, 1 H) ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.9, 131.7, 128.4, 128.1, 127.7, 125.8, 123.4, 91.0, 79.3, 76.6, 37.3, 32.1, 19.1, 14.0, 13.8 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 276.2 (6) [M^+] 91.1 (100), IR (neat): ν = 3416, 3060, 3026, 2931, 2862, 2223, 1708, 1600, 1493, 1450, 1077, 1047, 952, 754, 696 cm^{-1}; HRMS m/z (ESI) calcd for $C_{20}H_{20}ONa$ $(M + Na)^+$: 299.14064, found 299.14114.



1h

8)

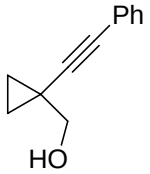
1-Benzyl-1-(1-(phenylethynyl)cyclopropyl) methanol (1h): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.49-7.40 (m, 2 H), 7.35-7.18 (m, 8 H), 3.24-3.15 (m, 2 H), 3.09-2.98 (m, 1 H), 1.84 (brs, 1 H), 1.10-0.80 (m, 3 H), 0.66-0.57 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 138.3, 131.8, 129.5, 128.4, 128.2, 127.8, 126.4, 123.5, 91.2, 78.2, 77.2, 42.3, 18.5, 13.9, 13.7 ppm; MS (70 eV): m/z (%): 262.2 (10) [M^+], 127.9 (100); IR (neat): ν = 3448, 3060, 3028, 2924, 2856, 2220, 1952, 1725, 1600, 1493, 1449, 1267, 1077, 1032, 754, 698 cm^{-1}; HRMS m/z (ESI) calcd for $C_{19}H_{18}ONa$ $(M + Na)^+$: 285.12499, found 285.12459.



1i

9)

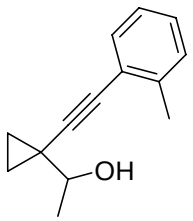
1-(1-(Phenylethynyl)cyclopropyl) cyclohexanol (1i): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.42-7.30 (m, 2 H), 7.29-7.23 (m, 3 H), 1.90-1.76 (m, 2 H), 1.75-1.38 (m, 9 H), 1.05-0.95 (m, 2 H), 0.90-0.80 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.6, 128.1, 127.5, 123.8, 94.1, 77.9, 70.9, 37.5, 34.9, 25.7, 22.9, 22.7, 21.7, 11.1, 8.1 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 240 (1) [M^+], 105 (100) ; IR (neat): ν = 3456, 2934, 2856, 2221, 2010, 1598, 1491, 1445, 1145, 1060, 975, 930, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{17}H_{20}ONa$ $(M + Na)^+$: 263.14064, found 263.1406.



1j

10)

(1-(Phenylethynyl)cyclopropyl) methanol (1j): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.33 (m, 2 H), 7.32-7.24 (m, 3 H), 3.57 (s, 2 H), 1.92 (brs, 1 H), 1.07-1.03 (m, 2 H), 0.92-0.82 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.2, 127.8, 123.3, 92.2, 78.2, 68.8, 15.6, 13.6 ppm; MS (70 eV): m/z (%): 172.2 (12) [M^+], 144.2 (100) ; IR (neat): ν = 3424, 3083, 3061, 3025, 2930, 2862, 2223, 1709, 1493 1453, 1077, 1045, 1033, 755, 696 cm^{-1}; HRMS m/z (ESI) calcd for $C_{12}H_{13}O$ $(M + H)^+$: 173.09609, found 173.09665.

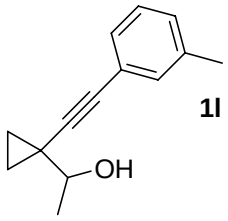


1k

11)

1-(1-(*o*-Tolylethynyl)cyclopropyl) ethanol (1k): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.36 (d, *J* = 7.5 Hz, 1 H), 7.18-7.00 (m, 3 H), 3.21 (q, *J* = 6.3 Hz, 1 H), 2.42 (s, 3 H), 1.83 (brs, 1 H), 1.43 (d, *J* = 6.3

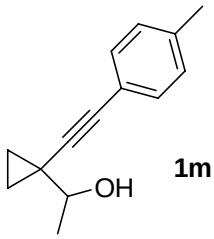
Hz , 3 H), 1.10-0.94 (m, 2 H), 0.93-0.85 (m, 1 H), 0.84-0.70 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 140.1, 131.8, 129.3, 127.7, 125.4, 123.2, 95.04, 78.2, 73.2, 21.2, 20.8, 20.1, 14.5, 13.4 ppm; MS (70 eV): m/z (%): 200.2 (53) [M^+], 115.1 (100) IR (neat): ν = 3345, 2959, 2866, 2220, 1740, 1720, 1486, 1454, 1377, 1161, 1090, 757, 716 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10912.



1l

12)

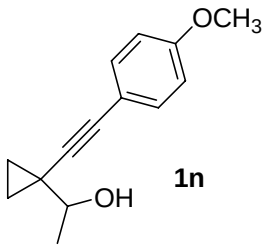
1-(1-(*m*-Tolylethynyl)cyclopropyl) ethanol (12): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.27-7.04 (m, 4 H), 3.25-3.11 (m, 1 H), 2.31 (s, 3 H), 1.79 (d, *J* = 4.2 Hz , 1 H), 1.42 (d, *J* = 6.3 Hz , 3 H), 1.12-0.97 (m, 2 H), 0.96-0.83 (m, 1 H), 0.80-0.71 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 137.8, 132.3, 128.7, 128.6, 128.0, 123.2, 90.6, 79.4, 73.2, 21.1, 19.9, 14.2, 13.2 ppm; MS (70 eV): m/z (%): 200.1 (45), [M^+], 141.1 (100). IR (neat): ν = 3396, 2974, 2926, 2221, 2008, 1720, 1602, 1485, 1449, 1375, 1106, 784, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10933.



1m

13)

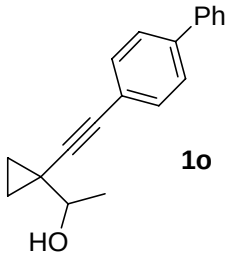
1-(1-(*p*-Tolylethynyl)cyclopropyl) ethanol (1m): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.29 (d, *J* = 7.8 Hz, 2 H), 7.07 (d, *J* = 7.8 Hz, 2 H), 3.18 (q, *J* = 6.3 Hz, 1 H), 2.32 (s, 3 H), 1.93 (brs, 1 H), 1.41 (d, *J* = 6.3 Hz , 3 H), 1.09-0.95 (m, 2 H), 0.94-0.85 (m, 1 H), 0.79-0.70 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 137.7, 131.6, 128.9, 120.3, 90.0, 79.4, 73.3, 21.4, 21.1, 19.9, 14.3, 13.2 ppm; MS (70 eV): m/z (%): 200.2 (5) [M^+], 141.1 (100). IR (neat): ν = 3386, 2972, 2925, 2870, 2221, 1904, 1510, 1450, 1375, 1023, 955, 925, 880, 817, 524 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10905.



1n

14)

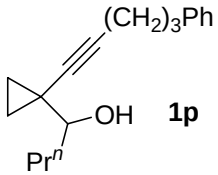
1-(1-((4-Methoxyphenyl)ethynyl)cyclopropyl) ethanol (1n): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.34 (d, *J* = 8.8 Hz, 2 H), 6.81 (d, *J* = 8.8 Hz, 2 H), 3.80 (s, 3 H), 3.18 (q, *J* = 6.3 Hz, 1 H), 1.84 (brs, 1 H), 1.41 (d, *J* = 6.3 Hz, 3 H), 1.05-0.95 (m, 2 H), 0.93-0.84 (m, 1 H), 0.80-0.70 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 159.2, 133.1, 115.6, 113.8, 89.2, 79.1, 73.3, 55.2, 21.1, 18.9, 14.3, 13.1 ppm; MS (70 eV): m/z (%): 216.0 (43) [M^+], 43.1 (100); IR (neat): ν = 3407, 2971, 2932, 2838, 2221, 2006, 1719, 1606, 1510 1287, 1247, 1173, 1032, 925, 833, 749 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{17}O_2$ $(M + H)^+$: 217.12231, found 217.12219.



1o

15)

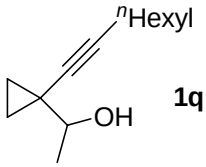
1-(1-(4-Phenyl-phenyl-ethynyl)cyclopropyl) ethanol (1o): solid, mp 52~54 ℃, ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7. 63-7.27 (m, 9 H), 3.28-3.15 (m, 1 H), 1.81 (d, *J* = 6.0 Hz, 1 H), 1.44 (d, *J* = 6.0 Hz, 3 H), 1.15-0.98 (m, 2 H), 0.97-0.94 (m, 1 H), 0.83-0.72 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 140.40, 140.35, 132.1, 128.8, 127.5, 126.9, 126.8, 122.4, 91.7, 79.2, 73.2, 21.2, 20.0, 14.3, 13.3 ppm; MS (70 eV): m/z (%): 262.1 (100) [M^+]; IR (neat): ν = 3351, 2969, 2926, 2881, 2218, 1487, 1447, 1103, 1088, 924, 841, 762, 721, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{19}H_{18}ONa$ $(M + Na)^+$: 285.12499, found 285.12458.



1p

16)

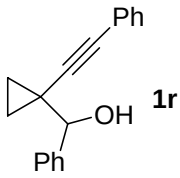
1-(1-(5'-Phenylpent-1-ynyl)cyclopropyl) butanol[2] **(1p)**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.34-7.25 (m, 2 H), 7.23-7.14 (m, 3 H), 2.80 (t, *J* = 6.3 Hz, 1 H), 2.70 (t, *J* = 7.5 Hz, 2 H), 2.17 (t, *J* = 6.9 Hz, 2 H), 1.89-1.60 (m, 5 H), 1.58-1.30 (m, 2 H), 0.99-0.80 (m, 5 H), 0.78-0.70 (m, 1 H), 0.69-0.60 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.7, 128.4, 128.3, 125.8, 81.6, 78.7, 77.2, 37.9, 34.8, 30.6, 19.1, 18.6, 18.2, 14.1, 13.5, 13.2 ppm; MS (70 eV): m/z (%): 256.3 (4) [M^+], 60.1 (100) ; IR (neat): ν = 3462, 3024, 2974, 2932, 2866, 2237, 1738, 1686, 1453, 1376, 1243, 1111, 964, 748, 701 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{24}ONa$ $(M + Na)^+$: 279.17194, found 279.1721.



1q

17)

1-(1-(Oct-1-ynyl)cyclopropyl) ethanol[2] **(1q)**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 3.15-2.96 (m, 1 H), 2.16 (t, *J* = 6.9 Hz, 2 H), 1.47 (q, *J* = 6.9 Hz, 2 H), 1.42-1.20 (m, 10 H), 1.01-0.81 (m, 5 H), 0.80-0.70 (m, 1 H), 0.66-0.54 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 80.7, 79.7, 73.4, 31.3, 29.0, 28.5, 22.5, 21.0, 19.4, 18.8, 14.0, 13.9, 12.6 ppm; MS (70 eV): m/z (%): 194.3 (1) [M^+], 115.1 (100) ; IR (neat): ν = 3376, 2959, 2928, 2859, 2237, 2019, 1723, 1459, 1374, 1096, 1052 cm^{-1}; HRMS m/z (ESI) calcd for $C_{13}H_{23}O$ $(M + H)^+$: 195.17434, found 195.17418.



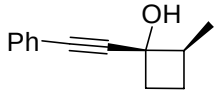
1r

18)

1-Phenyl-(1-(phenylethynyl)cyclopropyl) methanol (1r): liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.52 (d, *J* = 6.9 Hz, 2 H), 7.50-7.02 (m, 8 H), 4.32 (s, 1 H), 2.33 (brs, 1 H), 1.20-0.95 (m, 4 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.6, 131.6, 128.1, 127.9, 127.7, 126.7, 123.4, 91.4, 79.6, 78.2, 19.9, 14.5, 13.2 ppm; MS (70 eV): m/z (%): 248.2 (8) [M^+], 91.1 (100); IR (neat): ν = 3451, 3026, 2958, 2926, 2861, 2237, 1693, 1493, 1450, 1360, 1134, 747, 697 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{16}O$ $(M + H)^+$: 271.10934, found 271.1091.

General producer for 2-Methyl-1-(phenylethynyl) cyclobutanol (2a):

1-(1-(Phenylethynyl)cyclopropyl) ethanol **(1a)** (0.2 mmol, 37.2 mg) was added to the a mixture of $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1. The mixture was stirred at RT for 48 h. The resulting mixture was concentrated and purified by flash chromatography on silica gel (eluent: petroleum ether/ether = 5:1) to afford 25 mg (78 %, based on the conversion, *trans/cis* = 9:1) of **2a**; liquid; and 4.3 mg (12%) of **1a** was recovered.

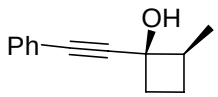


***Trans*-2a**

19)

***Trans*-2-methyl-1-(phenylethynyl) cyclobutanol (*trans*-2a):** liquid**;** ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.38 (m, 2 H), 7.36-7.26 (m, 3 H), 2.58-2.38 (m, 2 H), 2.28 (brs, 1 H), 2.16 (q, *J* = 9.6 Hz, 1 H), 1.99-1.85 (m, 1 H), 1.44-1.24 (m, 1 H), 1.19 (d, *J* = 6.6 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ =

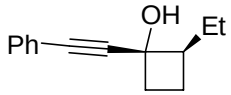
131.7, 128.2, 122.7, 89.8, 86.3, 72.6, 44.0, 36.0, 20.6, 16.1 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%):186.3 (5) [M^+], 144.2 (100); IR (neat): ν = 3396, 2958, 2867, 2224, 1630, 1598, 1090, 756, 691 cm^{-1}; HRMS m/z (ESI) calcd for $C_{13}H_{15}O$ $(M + H)^+$: 187.11174, found 187.11143.



***Cis*-2a**

20)

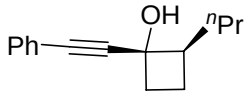
***Cis*-2-methyl-1-(phenylethynyl) cyclobutanol (*cis*-2a):** liquid**;** ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.52-7.40 (m, 2 H), 7.36-7.26 (m, 3 H), 2.82-2.68 (1, 2 H), 2.54-2.40 (m, 1 H), 2.34-2.19 (m, 1 H), 2.16-1.91 (m, 1 H), 1.70-1.51 (m, 1 H), 1.14 (d, *J* = 7.2 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.6, 128.2, 122.8, 92.8, 83.4, 69.4, 42.3, 35.3, 22.7, 13.9 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%):186.3 (2) [M^+], 144.1 (100); IR (neat): ν = 3335, 2958, 2923, 2866, 2222, 1601, 1485, 1451, 1090, 756, 691 cm^{-1}.



***Trans*-2b**

21)

***Trans*-1-(phenylethynyl) -2-ethyl cyclobutanol (*trans*-2b):** The reaction of **1b** (40 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 24 mg (88 %, based on the conversion, *trans/cis* = 6:1) of **2b**, and 12.8 mg (32 %) of **1b** was recovered. ***Trans*-2b:** liquid; ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.49-7.40 (m, 2 H), 7.38-7.24 (m, 3 H), 2.69 (brs, 1 H), 2.44-2.22 (m, 2 H), 2.18-1.97 (m, 1 H), 1.96-1.84 (m, 1 H), 1.80-1.63 (m, 1 H), 1.62-1.44 (m, 1 H), 1.42-1.26 (m, 1 H), 0.94 (t, *J* = 7.5 Hz 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.3, 122.8, 89.9, 86.0, 72.1, 51.0, 35.8, 25.0, 19.0, 11.4 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 200.0 (10) [M^+], 127.7 (100); IR (neat): ν = 3410, 2965, 2931, 2876, 2224, 1491 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10874.

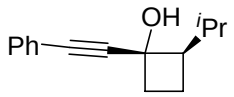


***Trans*-2c**

22)

***Trans*-1-(phenylethynyl)-2-propyl cyclobutanol (*trans*-2c)**: The reaction of **1c** (42.8 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 24.5 mg (57 %, *trans/cis* = 4:1) of **2c**. ***Trans*-2c** liquid; ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.39 (m, 2 H), 7.33-7.31 (m, 3 H), 2.50-2.30 (m, 3 H), 2.12 (q, *J* = 10.2 Hz, 1 H), 1.90-1.80 (m, 1 H), 1.76-1.64, (m, 1 H), 1.55-1.26

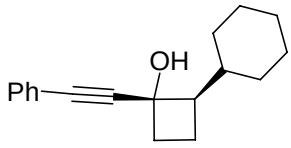
(m, 4 H), 0.93 (t, *J* = 7.2 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.3, 122.8, 90.0, 86.0, 72.2, 49.1, 35.9, 34.1, 20.2, 19.2, 14.3 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 213.9 (4) [M^+], 127.9 (100); IR (neat): ν = 3339, 2956, 2927, 2868, 2228, 1714, 1598, 1491, 1460, 1107, 975, 756, 692 cm^{-1}; HRMS m/z (ESI) calcd for $C_{15}H_{18}ONa$ $(M + Na)^+$: 237.12499, found 237.12461. ***Cis*-2c** liquid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 7.50-7.39 (m, 2 H), 7.35-7.27 (m, 3 H), 2.72-2.60 (m, 1 H), 2.50-2.39 (m, 1 H), 2.25-2.15 (m, 1 H), 2.06-1.91 (m, 1 H), 1.78-1.64 (m, 2 H), 1.50-1.30 (m, 3 H), 1.00-0.90 (m, 4 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 131.6, 128.2, 122.8, 92.8, 83.6, 69.6, 47.3, 35.3, 31.1, 21.9, 20.1, 14.2 ppm;



***Trans*-2d**

23)

***Trans*-1-(phenylethynyl)-2-isopropyl cyclobutanol (*trans*-2d)**: The reaction of **1d** (85.6 mg, 0.4 mmol), $FeCl_2$ (0.04 mmol, 5.1 mg, 10 mol%) and 4 mL acetone/nitromethane = 1/1 afforded 42.0 mg (49 %, *trans/cis* = 2:1) of **2d**. ***Trans*-2d**: solid, mp 56~58 ℃ (*n*-hexane/ethyl aceate); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.40 (m, 2 H), 7.39-7.26 (m, 3 H), 2.40-2.20 (m, 2 H), 2.19-1.80 (m, 4 H), 1.47-1.25 (m, 1 H), 1.03 (d, *J* = 6.3 Hz, 3 H), 0.84 (d, *J* = 6.3 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.7, 128.2, 122.8, 90.1, 85.5, 71.7, 56.9, 35.4, 31.3, 20.3, 19.5, 18.2 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 213.9 (2) [M^+], 144.1 (100); IR (neat): ν = 3333, 2958, 2866, 2224, 1491, 1090, 756, 691 cm^{-1}; HRMS m/z (ESI) calcd for $C_{45}H_{54}O_3Na$ $(3M + Na)^+$: 362.24081, found 362.24226. ***Cis*-2d**: ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.39 (d, *J* = 2.7 Hz, 2 H), 7.36-7.26 (m, 3 H), 2.45-2.30 (m, 1 H), 2.30-2.20 (m, 1 H), 2.18-1.98 (m, 1 H), 1.95-1.75 (m, 4 H), 1.02 (d, *J* = 6.3 Hz, 3 H), 0.83 (d, *J* = 6.3 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.5, 128.22, 128.16, 122.9, 92.8, 83.9, 69.7, 54.4, 34.4, 28.1, 21.9, 20.6, 19.1 ppm.

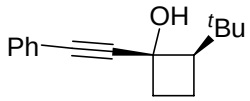


***Trans*-2e**

24)

***Trans*-1-(phenylethynyl)-2-cyclohexyl cyclobutanol (*trans*-2e)**: The reaction of **1e** (102 mg, 0.4 mmol), $FeCl_2$ (0.04 mmol, 5.1 mg, 10 mol%) and 4 mL acetone/nitromethane = 1/1 afforded 38 mg (38 %, *trans/cis* = 4:1) of **2e**. ***Trans*-2e**: solid, mp 96~98 ℃ (*n*-hexane/ethyl aceate); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.52-7.40 (m, 2 H), 7.38-7.25 (m, 3 H), 2.33 (q, *J* = 9.3 Hz, 2 H), 2.20-1.98 (m, 3 H), 1.85-1.50 (m, 6 H), 1.48-1.10 (m, 3 H), 1.05-0.75 (m, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.8, 128.3,

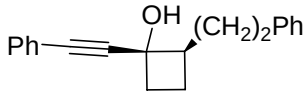
122.9, 90.2, 85.6, 71.8, 55.2, 40.9, 35.5, 31.1, 29.7, 26.6, 26.0, 25.9, 17.7 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 254.3 (5) [M^+], 184.1 (100); IR (neat): ν = 3417, 2968, 2926, 2855, 2219, 2156, 1715, 1451, 1375, 1089, 1028, 928, 808 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{22}ONa$ $(M + Na)^+$: 277.15629, found 277.15683. ***Cis*-2e**: ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.36 (m, 2 H), 7.34-7.24 (m, 3 H), 2.50-2.20 (m, 2 H), 2.15-1.98 (m, 1 H), 1.96-1.80 (m, 4 H), 1.73-1.50 (m, 6 H), 1.10-0.77 (m, 4 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.5, 128.2, 128.1, 122.9, 92.8, 83.9, 69.8, 52.6, 37.5, 34.7, 31.3, 29.2, 26.6, 26.0, 25.6, 21.5 ppm.



***Trans*-2f**

25)

***Trans*-1-(phenylethynyl)-2-tert-butyl cyclobutanol (*trans*-2f):** The reaction of **1f** (45.6 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 6.5 mg (14 %, *trans/cis* >99:1) of **2f**, ***Trans*-2f:** liquid**;** ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.38 (m, 2 H), 7.35-7.26 (m, 3 H), 2.80-2.67 (m, 1 H), 2.54-2.38 (m, 1 H), 2.30-2.13 (m, 1 H), 2.10-1.94 (m, 1 H), 1.87-1.26 (m, 2 H), 1.10-0.80 (m, 9 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.6, 128.2, 122.8, 92.7, 83.7, 69.9, 45.6, 38.0, 35.2, 26.0, 23.0, 22.9, 22.5 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 228.1 (1) [M^+], 142.1 (100); IR (neat): ν = 3418, 3027, 2940, 2222, 1718, 1452, 1079, 756, 697 cm^{-1}; HRMS m/z (ESI) calcd for $C_{16}H_{20}ONa$ $(M + Na)^+$: 277.15629, found 277.15509.

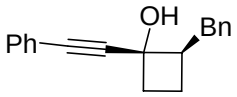


***Trans*-2g**

26)

***Trans*-1-(phenylethynyl)-2-phenethyl cyclobutanol (*trans*-2g)**: The reaction of **1g** (55.2 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 30.0 mg (54 %, *trans/cis* = 2:1) of **2g**. ***Trans*-2g** liquid; ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.52-7.40 (m, 2 H), 7.39-7.10 (m, 8 H), 2.80-2.55 (m, 2 H), 2.52-2.34 (m, 2 H), 2.27 (brs, 1 H), 2.21-1.96 (m, 2 H), 1.95-1.73 (m, 2 H), 1.47-1.30 (m, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 142.4, 131.7, 128.5, 128.4, 128.3, 125.7, 122.7, 89.8, 86.2, 72.1, 48.7, 35.9, 33.8, 33.4, 19.1 ppm (one carbon missing as a result of overlap); MS (70 eV): m/z (%): [M^+], 276.0 (1), 43.2 (100); IR (neat): ν = 3416, 3082, 3060, 3027, 2923, 2220, 1720, 1599, 1493, 1071, 1033, 755, 697 cm^{-1}; HRMS m/z (ESI) calcd for $C_{20}H_{20}ONa$ $(M + Na)^+$: 299.14064, found 299.14151. ***Cis*-2g** liquid; ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.56-7.37 (m, 2 H), 7.35-7.10 (m, 8 H), 2.72-2.53 (m, 3 H), 2.52-2.40 (m, 1 H), 2.28-2.16 (m, 1 H), 2.12-1.90 (m, 3 H), 1.85-1.65 (m, 2 H); ^{13}C NMR

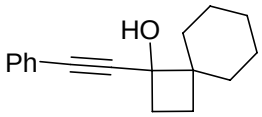
($CDCl_3$, 75.4 MHz): δ = 142.3, 131.6, 128.5, 128.3, 125.7, 122.7, 92.7, 83.8, 69.4, 46.7, 35.3, 33.1, 30.9, 21.7 (two carbons missing as a result of overlap) ppm;



***Trans*-2h**

27)

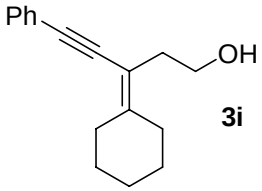
***Trans*-1-(phenylethynyl)-2-benzyl cyclobutanol (*trans*-2h):** The reaction of **1h** (52.4 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 26 mg (50 %, *trans/cis* = 4:1) of **2h**, ***Trans*-2h**: liquid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.51-7.10 (m, 10 H), 3.09-2.95 (m, 2 H), 2.89-2.70 (m, 1 H), 2.60-2.45 (m, 1 H), 2.33-2.25 (m, 1 H), 2.17 (s, 1 H), 2.03-1.80 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 140.0, 131.7, 128.4, 128.1, 128.0, 127.7, 126.7, 122.4, 89.6, 77.2, 74.0, 54.6, 35.5, 29.7, 17.1 ppm; MS (70 eV): m/z (%): 262.2 (28), [M^+], 142.2 (100); IR (neat): ν = 3363, 3092, 3010, 2975, 2219, 1715, 1449, 1370, 1070, 1029, 929, 807, cm^{-1}; HRMS m/z (ESI) calcd for $C_{19}H_{18}ONa$ $(M + Na)^+$: 285.12499, found 285.12459.



2i

28)

1-(Phenylethynyl)- spiro[3.5]nonan-1-ol (2i): The reaction of **1i** (48 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 9.6 mg (20 %) of **2i** and 14 mg (31%) of **3i. 2i:** liquid**;** ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.40 (m, 2 H), 7.35-7.26 (m, 3 H), 2.49-2.30 (m, 1 H), 2.28-2.13 (m, 1 H), 2.07 (brs, 1 H), 1.85-1.10 (m, 12H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 131.6, 128.2, 122.9, 90.8, 85.9, 73.2,, 48.2, 35.4, 33.6, 30.9, 26.0, 25.7, 22.9, 22.5 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 241.2 (4) [M^+ + 1], 158.1 (100); IR (neat): ν = 3448, 3060, 3028, 2931, 2858, 2223, 1720, 1493, 756, 698 cm^{-1}; HRMS m/z (ESI) calcd for $C_{17}H_{20}ONa$ $(M + Na)^+$: 263.14064, found 263.14016.

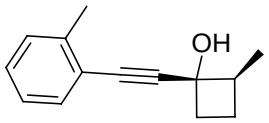


3i

29)

3-Cyclohexylidene-5-phenylpent-4-yn-1-ol (3i): liquid**;** ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.38 (m, 2 H), 7.35-7.26 (m, 3 H), 3.84 (t, *J* = 6.3 Hz, 2 H), 2.55 (t, *J* = 6.6 Hz, 4 H), 2.32 (t, *J* = 6.0 Hz, 2 H), 1.80-1.50 (m, 7 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 151.0, 131.2, 128.2, 127.7, 123.8, 110.0, 92.0,

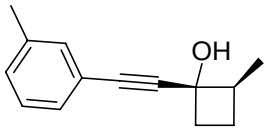
89.6, 61.7, 34.7, 34.2 30.4, 28.1, 28.0, 26.5 ppm; MS (70 eV): m/z (%): 241.3 (3) [M^++2], 144.1 (100); IR (neat): ν = 3426, 3064, 2973, 2928, 2219, 1734, 1376, 1108, 1024, 757 cm^{-1}; HRMS m/z (ESI) calcd for $C_{17}H_{21}O$ $(M + H)^+$: 241.15869, found 241.15897.



***Trans*-2k**

30)

***Trans*-1-(*o*-tolylethynyl)-2-methyl cyclobutanol (*trans*-2k)**: The reaction of **1k** (80 mg, 0.4 mmol), $FeCl_2$ (0.04 mmol, 5.0 mg, 10 mol%) and 4 mL acetone/nitromethane = 1/1 afforded 49.4 mg (62 %, *trans/cis* = 3:1) of **2k**. ***Trans*-2k**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.43 (d, *J* = 7.5 Hz, 1 H), 7.25-7.05 (m, 3 H), 2.57-2.34 (m, 2 H), 2.45 (s, 3 H), 2.18 (q, *J* = 10.2 Hz, 1 H), 1.98-1.85 (m, 1 H), 1.45-1.26 (m, 2 H), 1.20 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 140.1, 132.1, 129.4, 128.3, 125.5, 122.5, 93.8, 85.1, 72.8, 44.0, 36.3, 20.8, 20.7, 16.3 ppm; MS (70 eV): m/z (%): 199.2 (2) [M^+-1], 115.1 (100); IR (neat): ν = 3357, 2959, 2866, 2221, 1740, 1720, 1486, 1454, 1377, 1090, 757, 716 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}ONa$ $(M + Na)^+$: 223.10934, found 223.10914. ***Cis*-2k**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.39 (d, *J* = 7.8 Hz, 1 H), 7.26-7.10 (m, 3 H), 2.76 (q, *J* = 6.9 Hz, 1 H), 2.60-2.40 (m, 1 H), 2.43 (s, 3 H), 2.38-2.20 (m, 1 H), 2.14-1.90 (m, 2 H), 1.72-1.51 (m, 1 H), 1.16 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 140.1, 131.8, 129.4, 128.2, 125.5, 122.5, 96.9, 82.3, 69.4, 42.6, 35.6, 22.7, 20.6, 13.9 ppm;

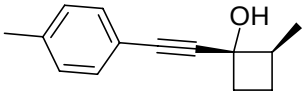


***Trans*-2l**

31)

***Trans*-1-(*m*-tolylethynyl)-2-methyl cyclobutanol (*trans*-2l)**: The reaction of **1l** (40 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 21.2 mg (53 %, *trans/cis* = 3:1) of **2l. *Trans*-2l**: liquid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.35-7.10 (m, 4 H), 2.56-2.25 (m, 3 H), 2.33 (s, 3 H), 2.16 (q, *J* = 9.9 Hz, 1 H), 1.98-1.83 (m, 1 H), 1.45-1.26 (m, 1 H), 1.19 (d, J=6.61 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 138.0, 132.300, 129.2, 128.8, 128.2, 122.5, 89.4, 86.5, 72.6, 44.0, 36.0, 21.2, 20.6, 16.2 ppm; MS (70 eV): m/z (%): 199.9 (18) [M^+], 127.9 (100); IR (neat): ν = 3412, 2961, 2928, 2866, 2220, 1687, 1601, 1485, 1453, 1376, 1094, 785, 691 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{17}O$ $(M + H)^+$: 201.12739, found 201.12669. ***Cis*-2l**: liquid. ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.00 (m, 4 H), 2.74 (q, *J* = 7.2 Hz, 1 H), 2.54-2.35 (m, 1 H), 2.34-2.19 (m, 1 H), 2.32 (s, 3 H), 2.16-1.90

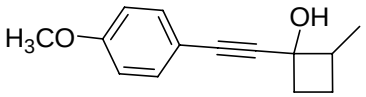
(m, 1 H), 1.70-1.51 (m, 1 H), 1.14 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 137.9, 132.2, 129.1, 128.7, 128.1, 122.6, 92.4, 83.6, 69.4, 42.4, 35.4, 22.7, 21.2, 13.9 ppm;



***Trans*-2m**

32)

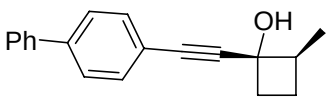
***Trans*-1-(*p*-tolylethynyl)-2-methyl cyclobutanol (*trans*-2m)**: The reaction of **1m** (40 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 24.1 mg (60 %, *trans/cis* = 3:1) of **2m**. ***Trans*-2m**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.35 (d, *J* = 7.8 Hz, 2 H), 7.12 (d, *J* = 7.8 Hz, 2 H), 2.55-2.25 (m, 3 H), 2.35 (s, 3 H), 2.15 (q, *J* = 9.9 Hz, 1 H), 1.97-1.82 (m, 1 H), 1.45-1.26 (m, 1 H), 1.18 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 138.4, 131.6, 129.0, 119.7, 89.0, 86.4, 72.6, 44.0, 36.1, 21.4, 20.6, 16.2 ppm; MS (70 eV): m/z (%): 200.0 (5) [M^+], 141.1 (100); IR (neat): ν = 3436, 2956, 2926, 2870, 2202,1763, 1717, 1492, 1449, 1103, 756, 696 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{17}OH$ $(M + H)^+$: 201.12739, found 201.12741. ***Cis*-2m**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.32 (d, *J* = 7.8 Hz, 2 H), 7.16 (d, *J* = 7.8 Hz, 2 H), 2.74 (q, *J* = 7.2 Hz, 1 H), 2.50-2.37 (m, 1 H), 2.40 (s, 3 H), 2.34-2.18 (m, 1 H), 2.15-1.91 (m, 2 H), 1.70-1.51 (m, 1 H), 1.14 (d, *J* = 7.2 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 138.3, 131.5, 129.0, 119.7, 92.0, 83.5, 69.4, 42.3, 35.4, 22.7, 21.4, 13.9 ppm;



2n

33)

1-((4-Methoxyphenyl)ethynyl)-2-methyl cyclobutanol (2n): liquid**;** The reaction of **1n** (40 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 27 mg (63 %, *trans/cis* = 5:1) of **2n**. ***Trans*-2n**: ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.39 (d, *J* = 8.7 Hz, 2 H), 6.84 (d, *J* = 7.8 Hz, 2 H), 3.82 (s, 3 H), 2.56-2.34 (m, 2 H), 2.29 (brs, 1 H), 1.96-1.85 (m, 2 H), 1.49-1.26 (m, 1 H), 1.18 (d, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 159.6, 133.2, 114.1, 113.9, 88.3, 86.2, 72.7, 55.3, 44.0, 36.1, 20.6, 16.2 ppm; MS (70 eV): m/z (%): 216.2 (5) [M^+], 127.8 (100); IR (neat): ν = 3378, 2958, 2931, 2869, 2221, 1719, 1508, 1457, 1377, 1091, 835 cm^{-1}; HRMS m/z (ESI) calcd for $C_{14}H_{16}O_2Na$ $(M + Na)^+$: 239.10425, found 239.10432; ***Cis*-2n**: ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.79 (d, *J* = 9.0 Hz, 2 H), 6.83 (d, *J* = 9.0 Hz, 2 H), 3.87 (s, 3 H), 2.37 (brs, 1 H), 2.15 (q, *J* = 9.9 Hz, 1 H), 1.96-1.85 (m, 1 H), 1.49-1.26 (m, 3 H), 1.60 (d, *J* = 6.9 Hz, 3 H).



***Trans*-2o**

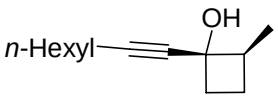
34)

***Trans*-1-(4-phenyl-phenyl-ethynyl)-2-methyl cyclobutanol (*trans*-2o)**: The reaction of **1o** (52.4 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 33.5 mg (64 %, *trans/cis* = 4:1) of **2o**. ***Trans*-2o**: solid, mp 102~104 ℃ (*n*-hexane/ethyl acetate); ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.65-7.26 (m, 9 H), 2.55-2.35 (m, 2 H), 2.31 (d, *J* = 2.4 Hz, 1 H), 2.80 (q, *J* = 9.0 Hz, 1 H), 2.00-1.85 (m, 1 H), 1.45-1.30 (m, 1 H), 1.21 (d, *J* = 6.6 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.1, 140.3, 132.2, 128.8, 127.6, 127.0, 121.6, 90.4, 86.2, 72.7, 44.0, 36.1, 20.7, 16.2 ppm; MS (70 eV): m/z (%): 262.2 (8) [M^+], 220.1 (100); IR (neat): ν = 3400, 2960, 2925, 2865, 2202, 1486, 1109, 842, 767, 695 cm^{-1}; HRMS m/z (ESI) calcd for $C_{19}H_{18}ONa$ $(M + Na)^+$: 285.12499, found 285.12485. ***Cis*-2o**: ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.70-7.28 (m, 9 H), 2.77 (q, *J* = 7.2 Hz, 1 H), 2.60-2.40 (m, 1 H), 2.35-2.20 (m, 1 H), 2.15-1.95 (m, 1 H), 2.00 (brs, 1 H), 1.70-1.60 (m, 1 H), 1.16 (d, *J* = 7.2 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.1, 140.3, 132.1, 128.8, 127.6, 127.0, 121.7, 104.2, 90.4, 86.2, 72.7, 44.0, 36.1, 20.7, 16.2 ppm;

***Trans*-2p**

35)

***Trans*-1-(5′-phenylpent-1-ynyl)-2-propyl cyclobutanol (*trans*-2p):** The reaction of **1p** (51.2 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 29 mg (75 %, based on the conversion, *trans/cis* = 4:1) of **2p**, and 13 mg (25 %) of **1p** was recovered. ***Trans*-2p**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.40-7.25 (m, 2 H), 7.24-7.17 (m, 3 H), 2.75 (t, *J* = 7.5 Hz, 2 H), 2.46-2.15 (m, 3 H), 2.12 (s, 1 H), 2.04 (q, *J* = 10.2 Hz, 1 H), 1.97-1.75 (m, 3 H), 1.68-1.59 (m, 2 H), 1.52-1.20 (m, 4 H), 0.91 (t, *J* = 6.9 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.6, 128.5, 128.3, 125.9, 86.1, 81.5, 72.0, 48.9, 36.1, 34.8, 34.1, 30.4, 20.2, 19.2, 18.2, 14.3 ppm; MS (70 eV): m/z (%): 258.3 (3) [M^+ + 2], 144.1 (100); IR (neat): ν = 3356, 2975, 2927, 2219, 1715, 1367, 1073, 1030, 929, 885, 807 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{25}O$ $(M + H)^+$: 257.18999, found 257.19039.

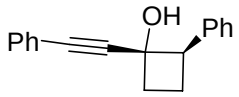


***trans*-2q**

36)

***Trans*-1-(oct-1-ynyl)-2-methyl cyclobutanol (*trans*-2q):** The reaction of **1q** (38.8 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 21 mg (54 %, *trans/cis* = 4:1) of **2q**. ***Trans*-2q**: liquid; ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 2.45-2.30 (m, 1 H), 2.36 (t, *J* = 6.9 Hz, 3 H), 2.11 (s, 1 H), 2.04 (q, *J* = 9.9 Hz, 1 H), 1.90-1.75 (m, 1 H), 1.52 (q, *J* = 7.2 Hz, 2 H), 1.47-1.15 (m, 7

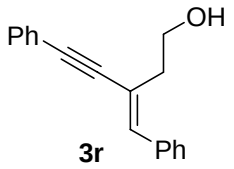
H), 1.09 (d, *J* = 6.6 Hz, 3 H), 0.89 (t, *J* = 6.6 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 87.0, 80.7, 72.4, 43.8, 36.2, 31.3, 28.8, 28.5, 22.6, 20.6, 18.7, 16.0, 14.0 ppm; MS (70 eV): m/z (%): 194.2 (5) [M^+], 177.1 (100); IR (neat): ν = 3443, 2958, 2930, 2860, 2225, 1725, 1458, 1378, 1260, 1100 cm^{-1}; HRMS m/z (ESI) calcd for $C_{13}H_{23}O$ $(M + H)^+$: 195.17434, found 195.17426.



***Trans*-2r**

37)

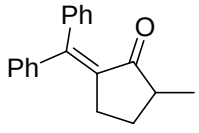
***Trans*-1-(Phenylethynyl)-2-phenyl cyclobutanol (*trans*-2r):** The reaction of **1r** (49.6 mg, 0.2 mmol), $FeCl_2$ (0.02 mmol, 2.5 mg, 10 mol%) and 2 mL acetone/nitromethane = 1/1 afforded 2.3 mg (5%，*trans/cis* > 99:1) of **2r** and 43.8 mg (86%) of **3r. *Trans*-2r:** liquid**;** ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.50-7.26 (m, 5 H), 7.25-7.01 (m, 5 H), 3.72 (t, *J* = 9.6 Hz, 1 H), 3.05-2.44 (m, 2 H), 2.35 (q, *J* = 10.5 Hz, 1 H), 2.18-2.00 (m, 2 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 141.6, 131.6, 128.1, 127.9, 127.7, 126.7, 123.4, 91.4, 79.6, 78.2, 19.9, 14.5, 13.3 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 248.1 (51) [M^+], 91.2 (100); IR (neat): ν = 3408, 3079, 3059, 2973, 2927, 2875, 2225, 1949, 1721, 1601, 1495, 1446, 1122, 1080, 761, 702 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{17}O$ $(M + H)^+$: 249.12739, found 249.12704.



3r

38)

(*E*)-3-Benzylidene-3-phenylethynyl propanol (3r): liquid**;** ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 7.80 (d, *J* = 6.9 Hz, 2 H), 7.43-7.52 (m, 2 H), 7.40-7.24 (m, 6 H), 6.69 (s, 1H), 3.97 (t, *J* = 6.0 Hz, 2 H), 2.67 (t, *J* = 6.0 Hz, 2 H), 1.67 (s, 1 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 136.8, 136.3, 131.5, 128.5, 128.4, 128.2, 128.1, 123.1, 118.1, 96.3, 88.8, 61.3, 42.5 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 248.1 (54) [M^+], 215.1 (100); IR (neat): ν = 3359, 3060, 2953, 2197, 1698, 1598, 1490, 1049, 1027, 755, 691 cm^{-1}; HRMS m/z (ESI) calcd for $C_{18}H_{17}O$ $(M + H)^+$: 249.12739, found 249.12704.



4

39)

2-(diphenylmethylene)-5-methylcyclopentanone (4) was synthesized according to literature procedure[3]

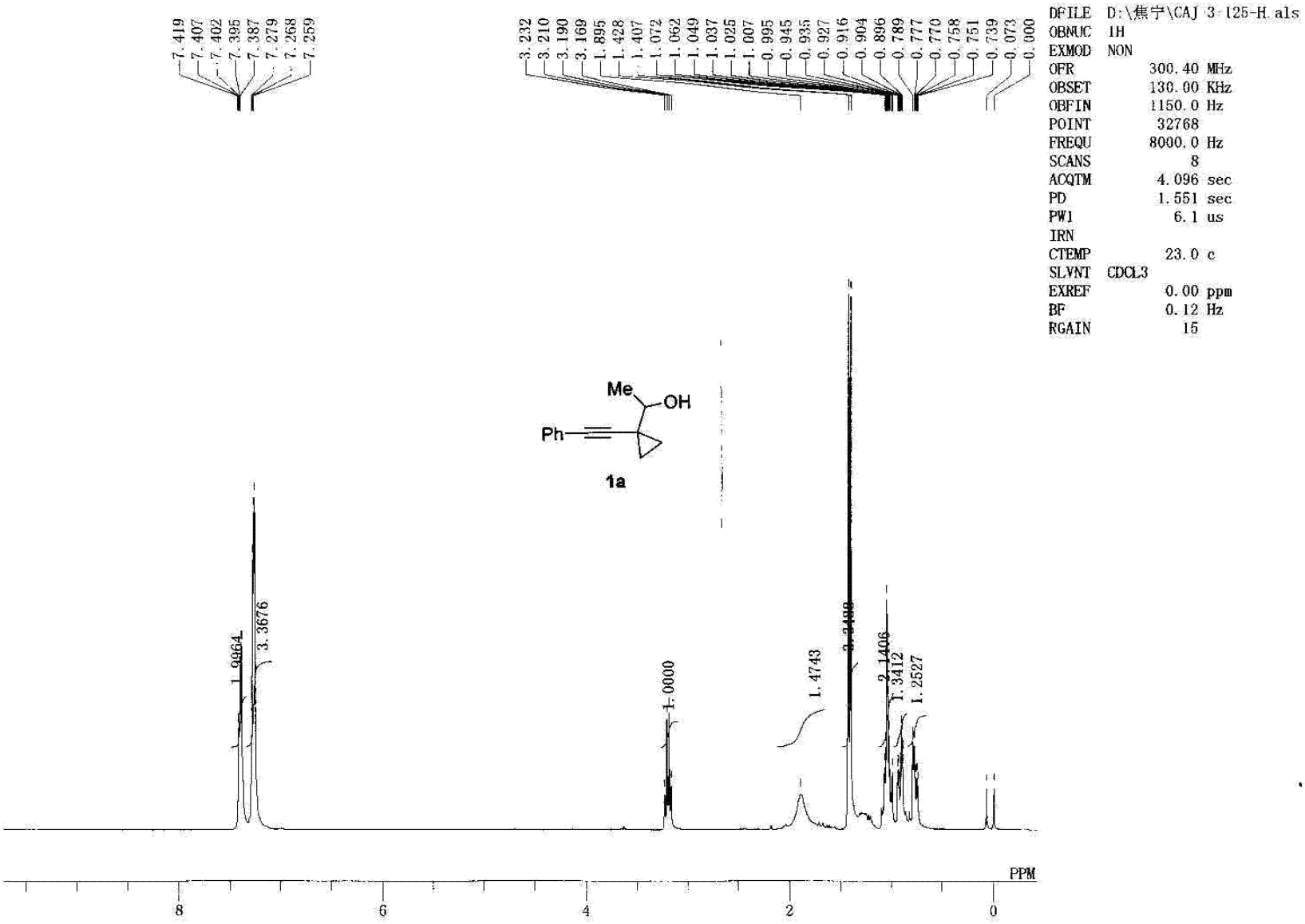
DMF (5 mL), $Pd(OAc)_2$ (11 mg, 0.05 mmol), PPh_3 (26 mg, 0.1 mmol), iodobenzene (204 mg, 1.0 mmol), *i*-Pr_2NEt (130 mg, 1.0 mmol), *n*-Bu_4NCl (277 mg, 1.0 mmol), and **1a** (93 mg, 0.5 mmol) were placed in a standard Schlenk tube under N_2 atmosphere. The Schlenk tube was flushed with N_2 and heated in an oil bath at 80 ℃ for 12 h. The reaction was monitored by TLC to establish completion. The reaction mixture was cooled, diluted with 30 mL of diethyl ether, washed with 40 mL of saturated NaCl, dried (Na_2SO_4), and filtered. The solvent was evaporated under reduced pressure and the product was isolated by chromatography on a sillica gel column to afford 44 mg (67%) 2-(diphenylmethylene)-5-methylcyclopentanone (**4**): solid, mp 84~86 ℃ (*n*-hexane/ethyl acetate); ^1H NMR ($CDCl_3$, 300 MHz): δ = 7.45-7.27 (m, 6 H), 7.26-7.16 (m, 2 H), 7.15-7.09 (m, 2 H), 2.80-2.68 (m, 2 H), 2.41-2.13 (m, 2 H), 1.50-1.34 (m, 1 H), 1.13 (d, *J* = 6.6 Hz, 3 H); ^{13}C NMR ($CDCl_3$, 75.4 MHz): δ = 208.1, 148.5, 141.8, 140.1, 133.8, 129.4, 129.2, 128.2, 128.0, 127.7, 45.0, 30.4, 19.2, 14.9 (one carbon missing as a result of overlap) ppm; MS (70 eV): m/z (%): 262.3 (64) [M^+], 261.3 (100); IR (neat): ν = 2960, 2925, 2868, 1710, 1592, 1443, 1190, 700 cm^{-1}; HRMS m/z (ESI) calcd for $C_{19}H_{19}O$ $(M + H)^+$: 263.14304, found 263.14325.

Reference:

(1) Zhang, J. L.; Schmalz, H. G. *Angew. Chem. Int. Ed.* **2006**, *45*, 6704-6707

(2) Eckhardt, M.; Fu, G. C. *J. Am. Chem. Soc.* **2003**, *125*, 13642-13643.

(3) Larock, R. C.; Reddy, C. K. *Org. Lett*. **2000**, *2*, 3325-3327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7.402
7.395
7.387
7.279
7.268
7.259
3.232
3.210
3.190
3.169
1.895
1.428
1.407
1.072
1.062
1.049
1.037
1.025
1.007
0.995
0.945
0.935
0.927
0.916
0.904
0.896
0.789
0.777
0.770
0.758
0.751
0.739
0.073
0.000
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PD 1.551 sec
PW1 6.1 us
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SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
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Ph
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1.4743
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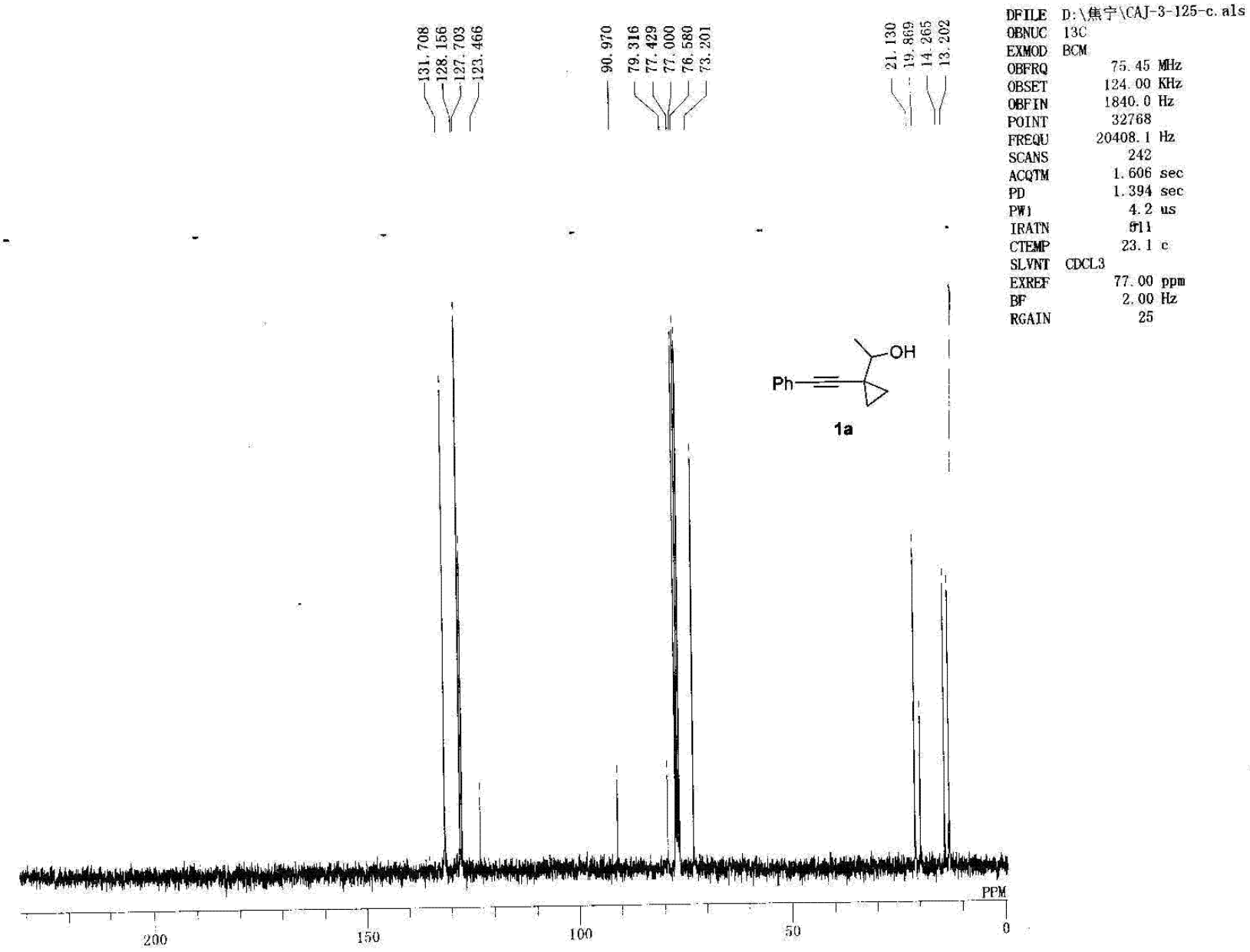
2.1406
1.3412
1.2527
PPM
8
6
4
2
0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127.703
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90.970
79.316
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76.580
73.201
21.130
19.869
14.265
13.202
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POINT 32768
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PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.1 c
SLVNT CDCL3
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Ph
1a
PPM
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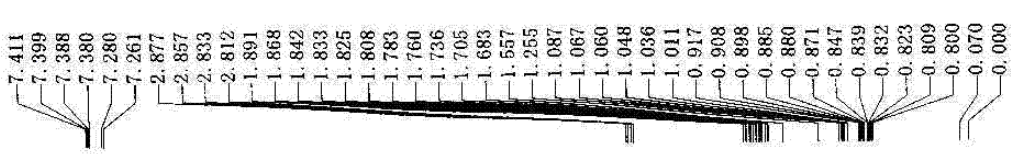
150
100
50
0

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FREQU        8000.0 Hz
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ACQTM         4.096 sec
PD            1.551 sec
PW1             6.1 us
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CTEMP          20.3 c
SLVNT   CDCL3
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RGAIN             22
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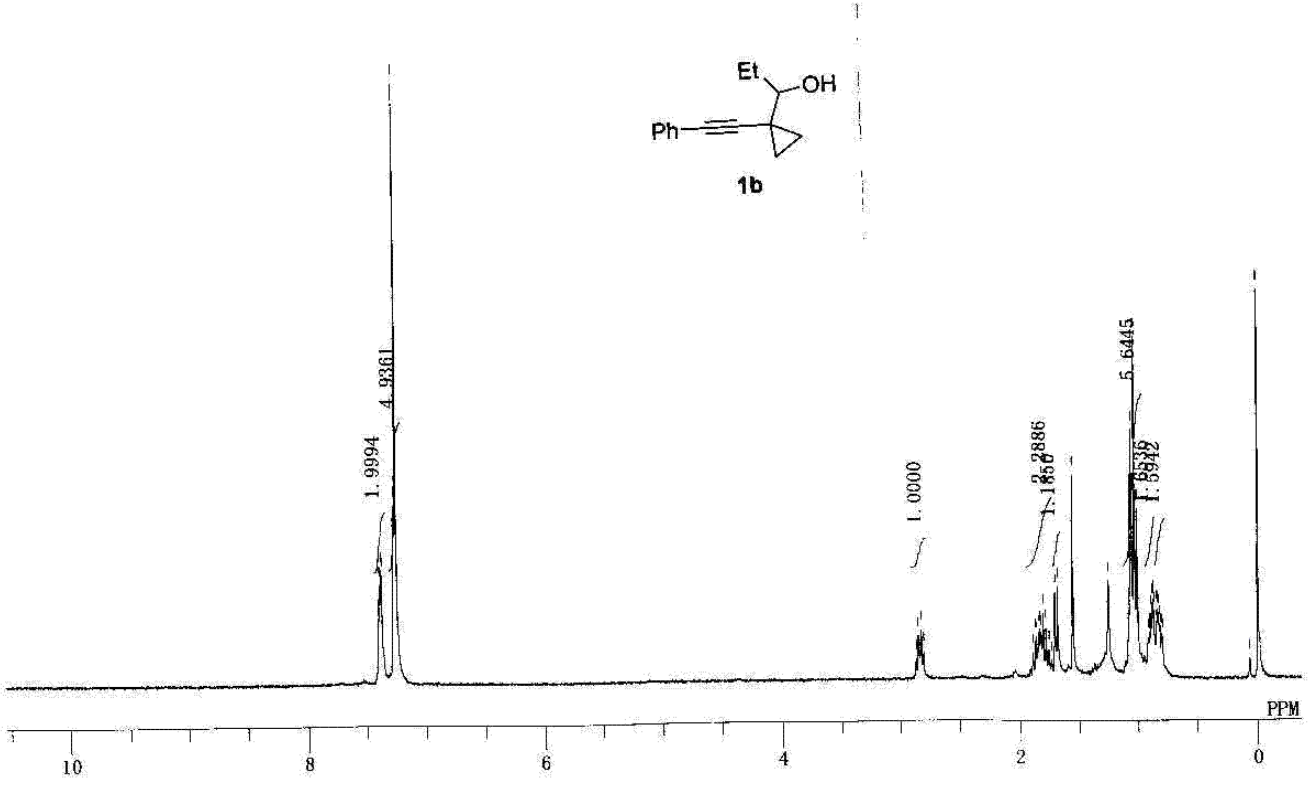

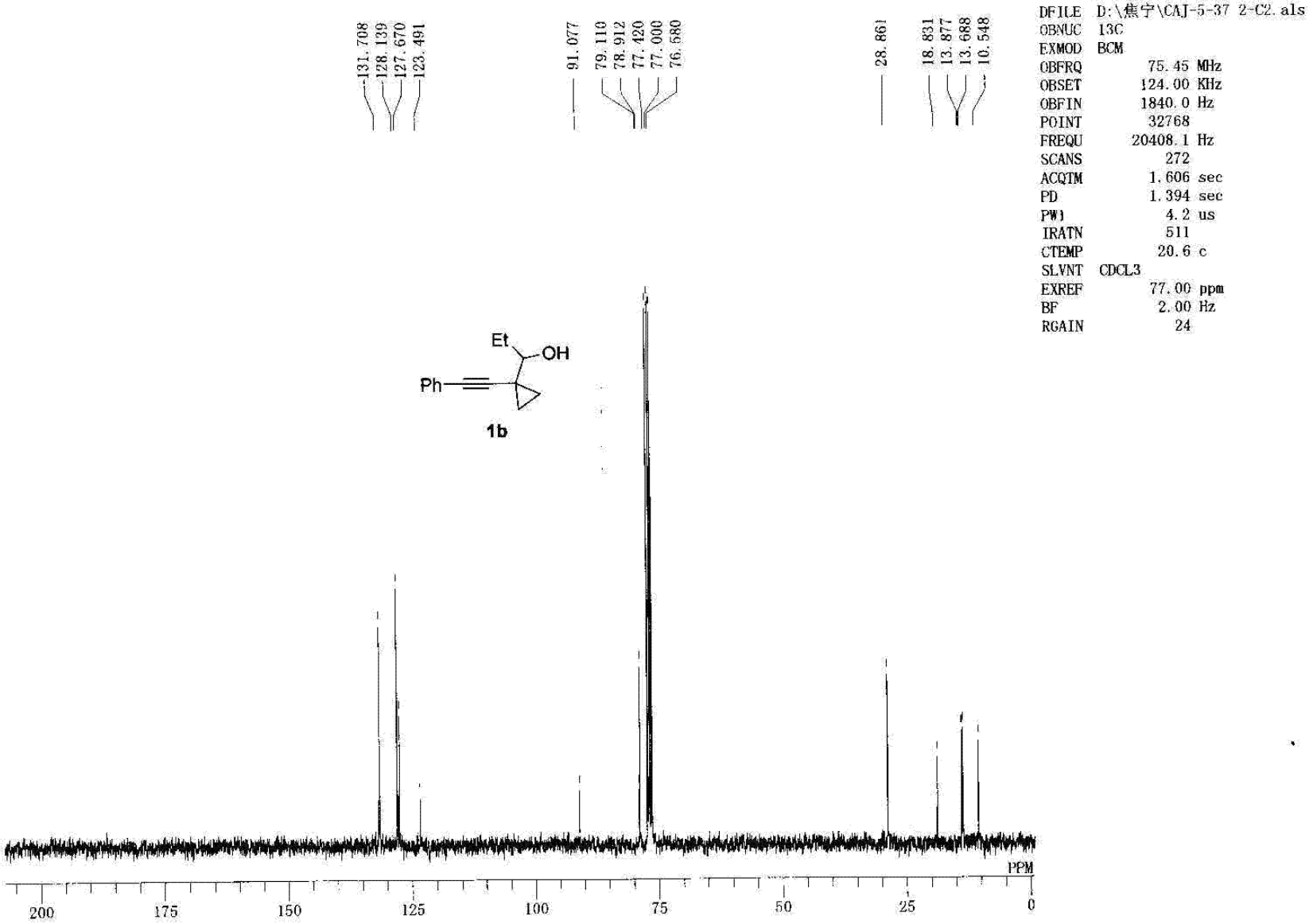
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77.420
77.000
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13.877
13.688
10.548
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OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
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ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
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OH
Ph
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PPM
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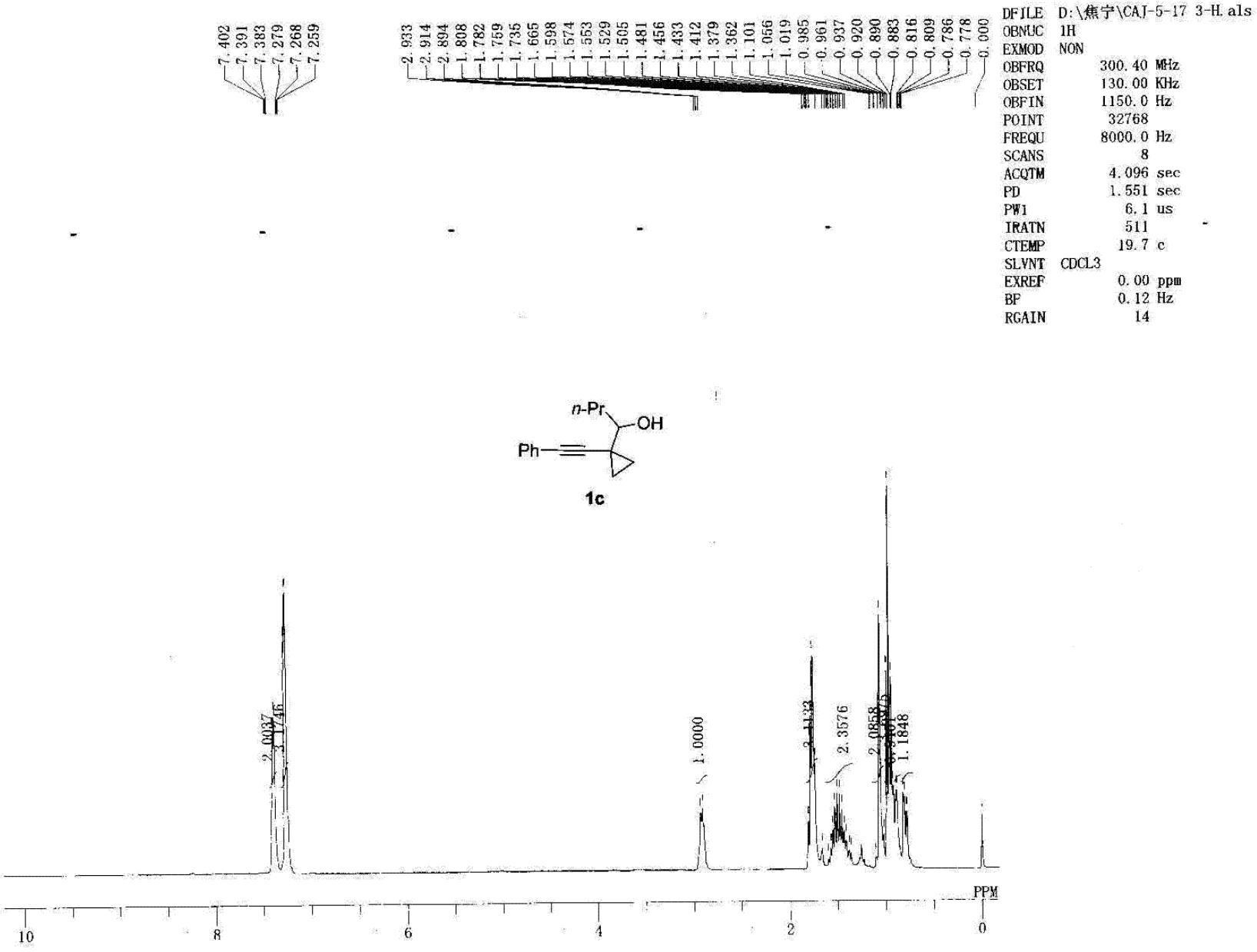
150
125
100
75
50
25
0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2.914
2.894
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1.665
1.598
1.574
1.553
1.529
1.505
1.481
1.456
1.433
1.412
1.379
1.362
1.101
1.056
1.019
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0.961
0.937
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0.890
0.883
0.816
0.809
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PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 19.7 c
SLVNT CDCL3
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BF 0.12 Hz
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n-Pr
OH
Ph
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PPM
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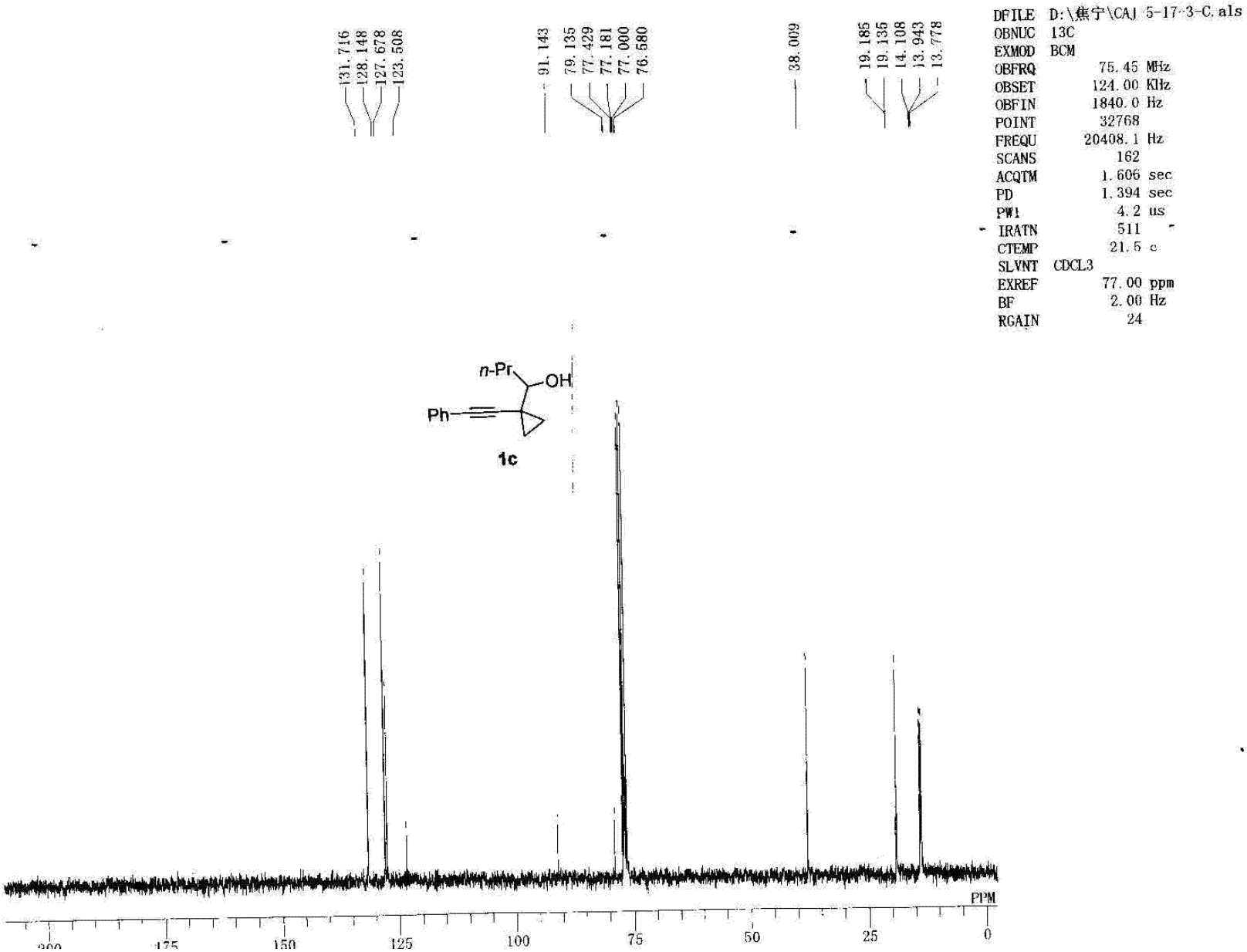
8
6
4
2
0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77.181
77.000
76.580
38.009
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19.136
14.108
13.943
13.778
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PD 1.394 sec
PW1 4.2 us
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CTEMP 21.5 c
SLVNT CDCL3
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Ph
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PPM
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100
75
50
25
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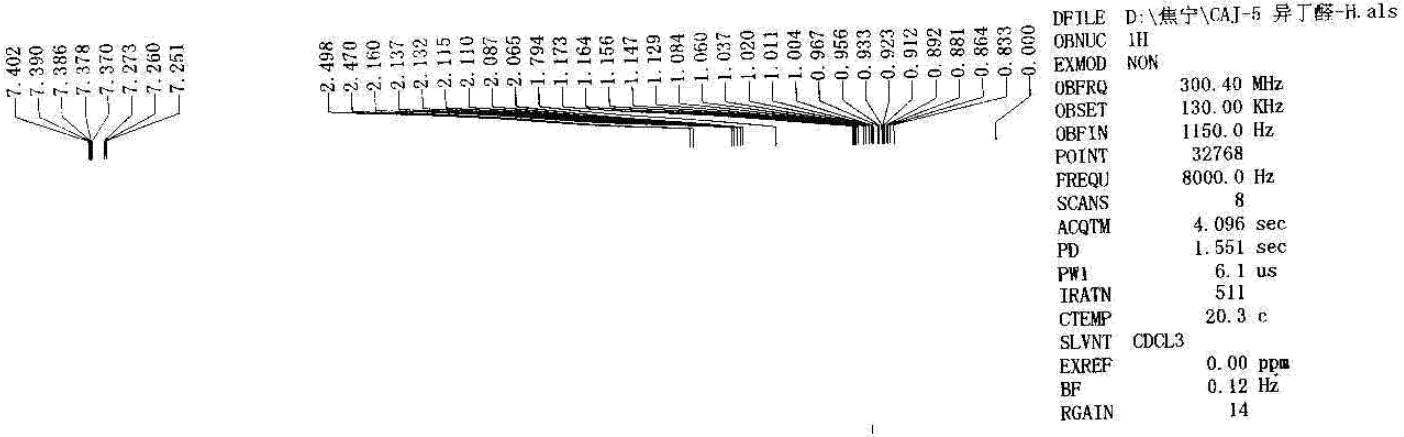
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2.132
2.115
2.110
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2.065
1.794
1.173
1.164
1.156
1.147
1.129
1.084
1.060
1.037
1.020
1.011
1.004
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SLVNT CDCL3
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BF 0.12 Hz
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Ph
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6
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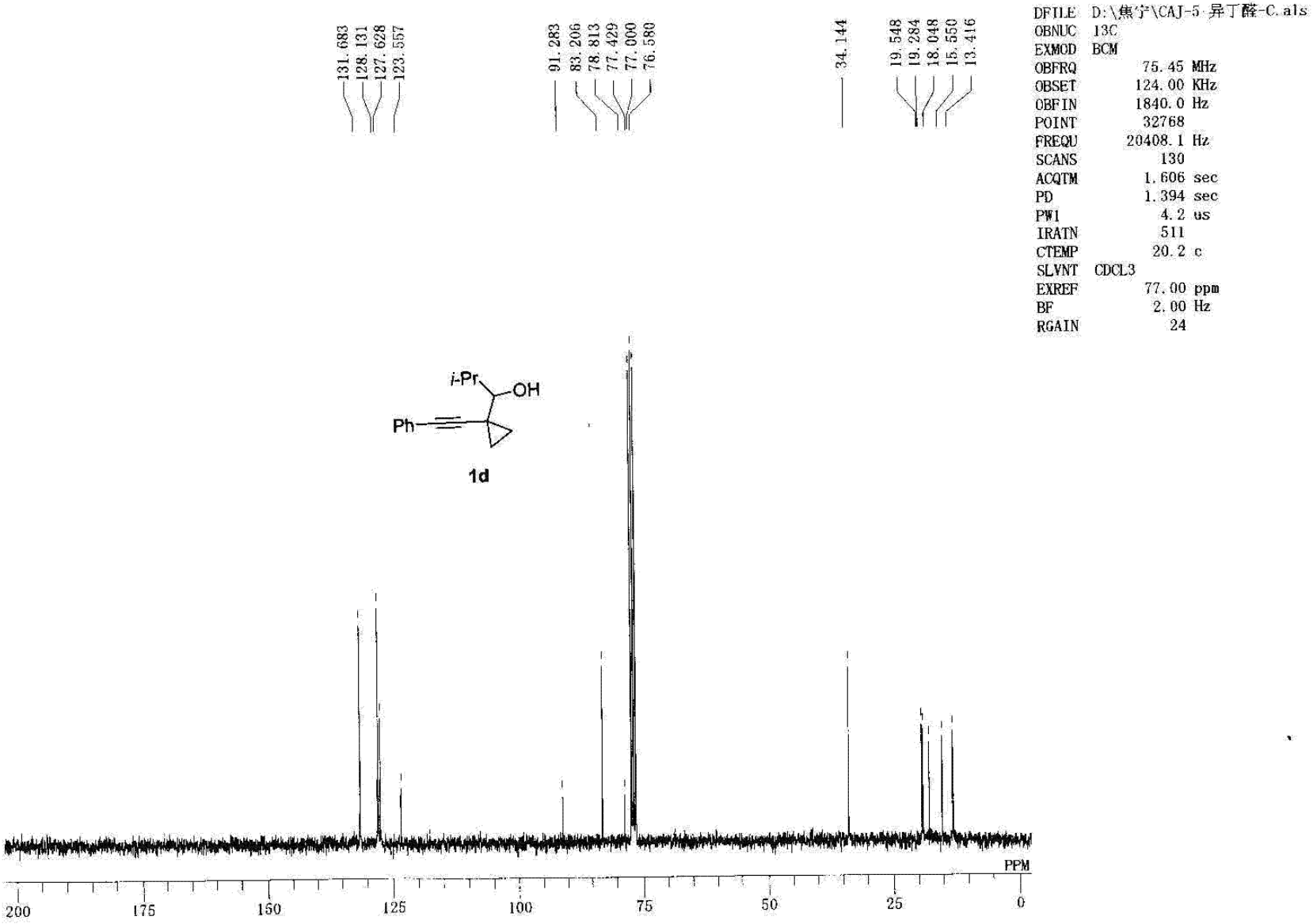
2
0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76.580
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19.284
18.048
15.550
13.416
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OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 130
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
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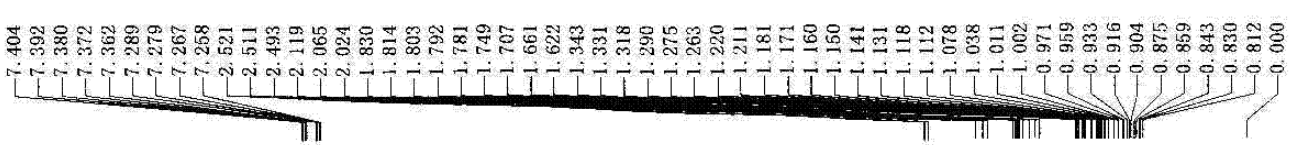
i-Pr
OH
Ph
1d
PPM
200
175
150
125
100
75
50
25
0



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CTEMP	21.8 c
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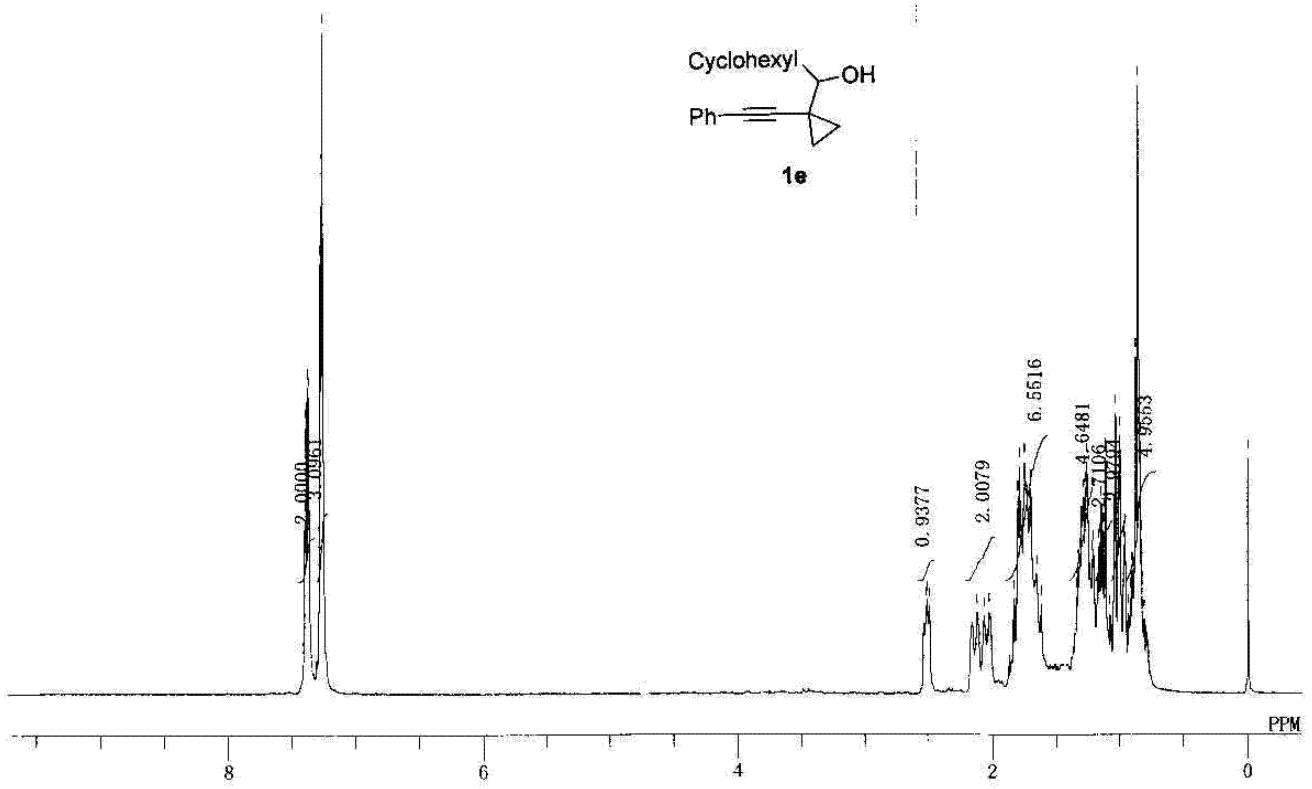
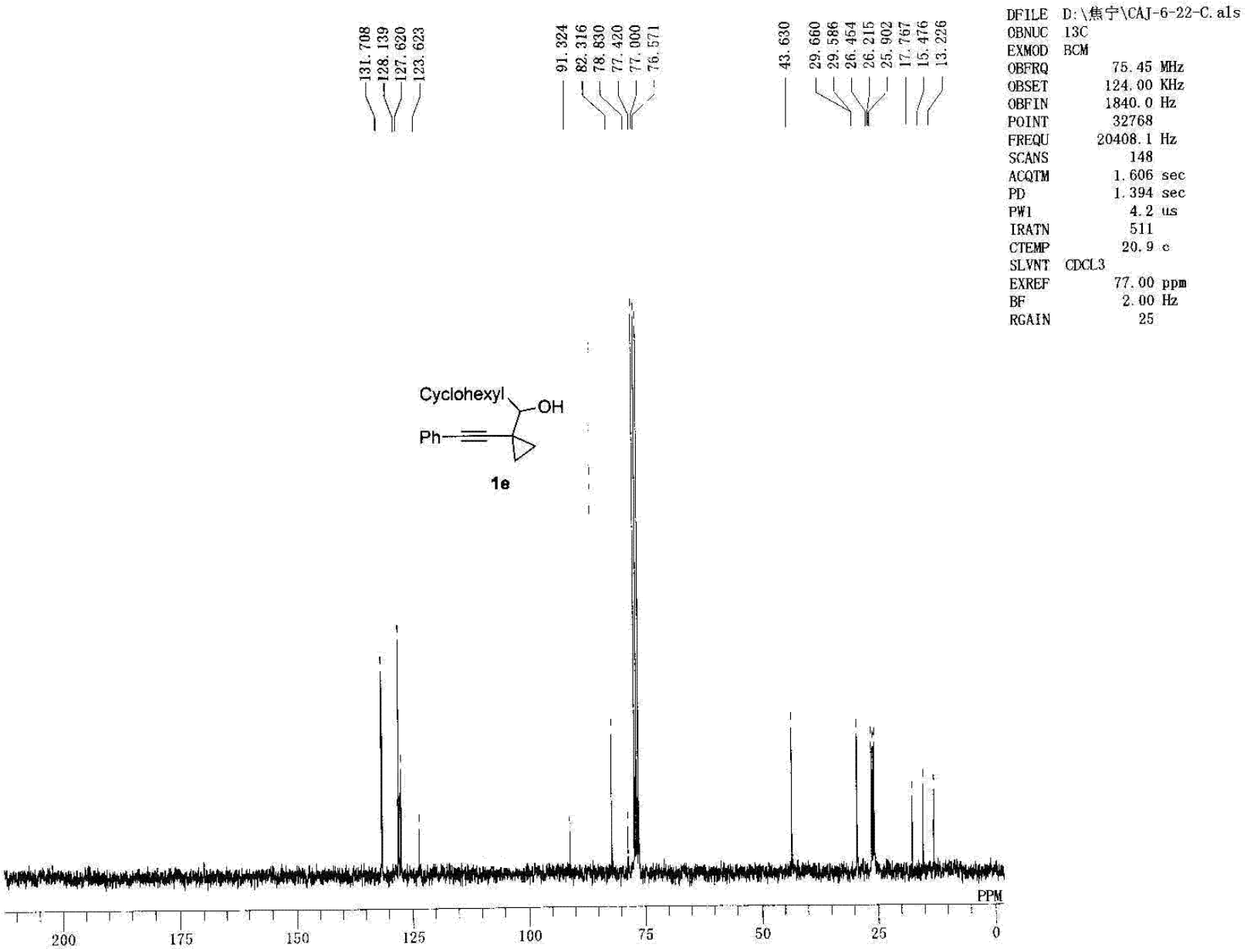
RGAIN	15

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26.454
26.215
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17.767
15.476
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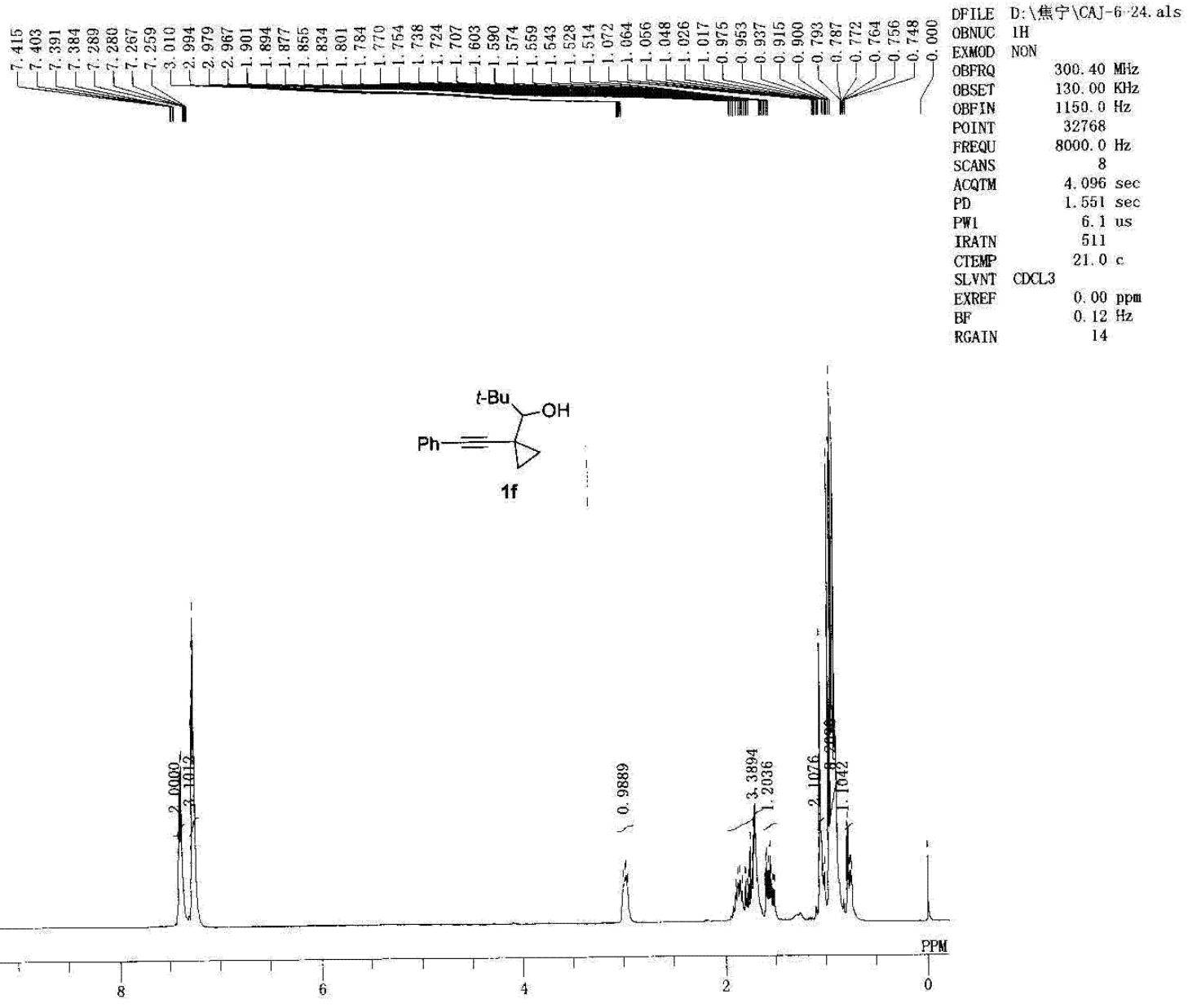
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1.894
1.877
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1.801
1.784
1.770
1.754
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1.724
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1.603
1.590
1.574
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1.528
1.514
1.072
1.064
1.056
1.048
1.026
1.017
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0.900
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PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 21.0 c
SLVNT CDCL3
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BF 0.12 Hz
RGAIN 14
t-Bu
OH
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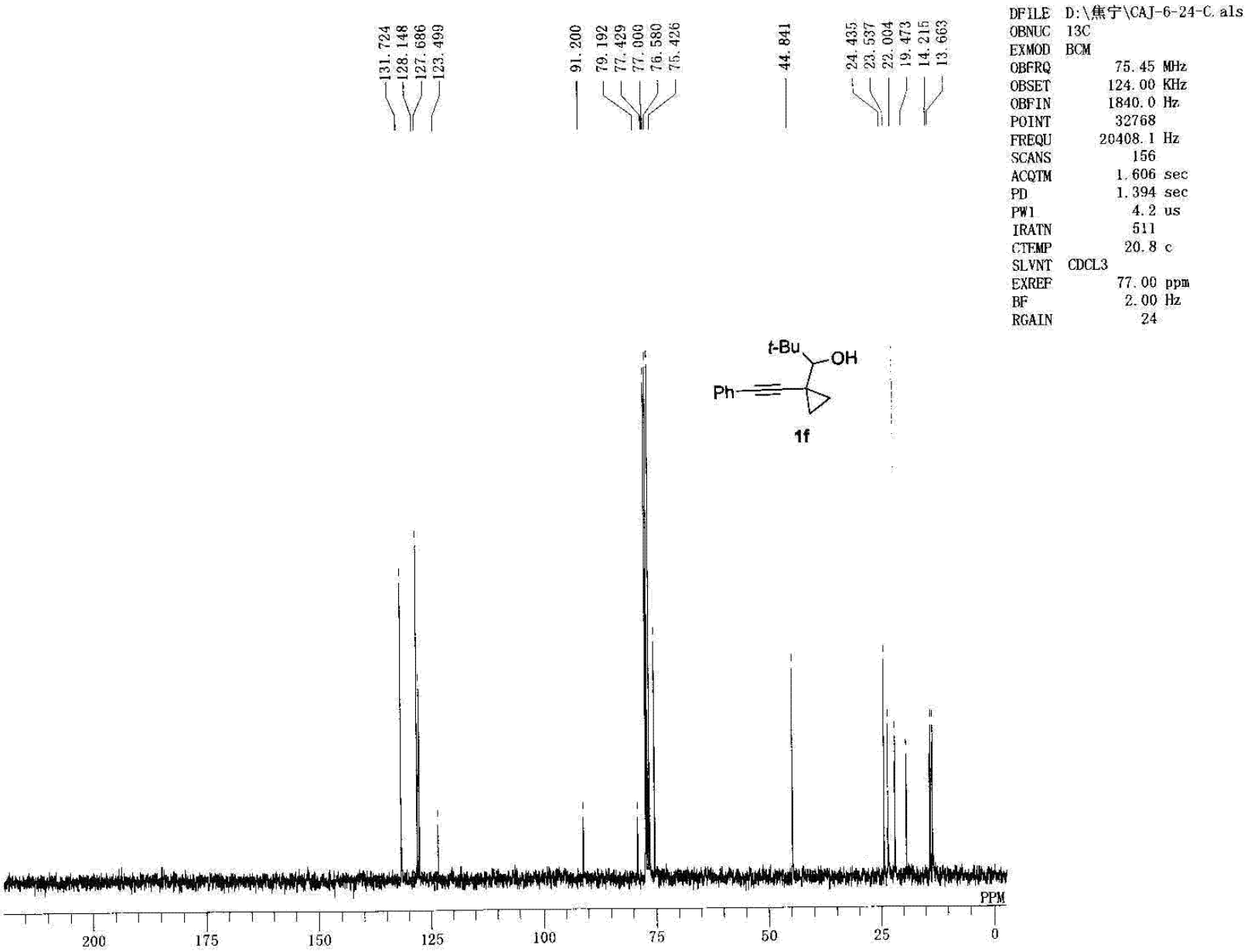
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22.004
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POINT 32768
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SCANS 156
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.8 c
SLVNT CDCL3
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BF 2.00 Hz
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Ph
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PPM
200
175
150
125
100
75
50
25
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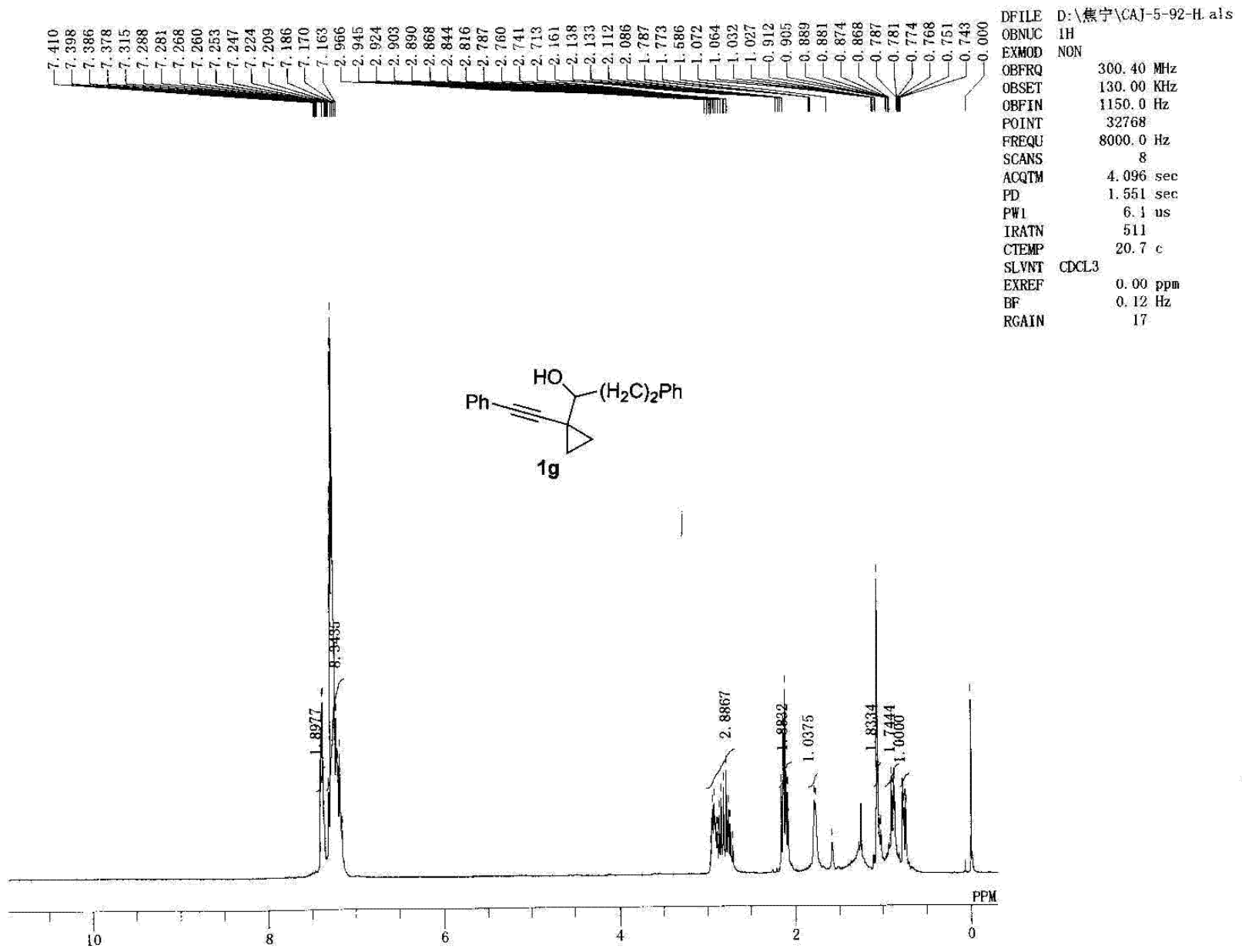
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7.378
7.315
7.288
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7.268
7.260
7.253
7.247
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7.209
7.186
7.170
7.163
2.966
2.945
2.924
2.903
2.890
2.868
2.844
2.816
2.787
2.760
2.741
2.713
2.161
2.138
2.133
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1.586
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1.027
0.912
0.905
0.889
0.881
0.874
0.868
0.787
0.781
0.774
0.768
0.751
0.743
0.000
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OBFIN 1150.0 Hz
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FREQU 8000.0 Hz
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ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
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Ph
1g
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1.0000
PPM
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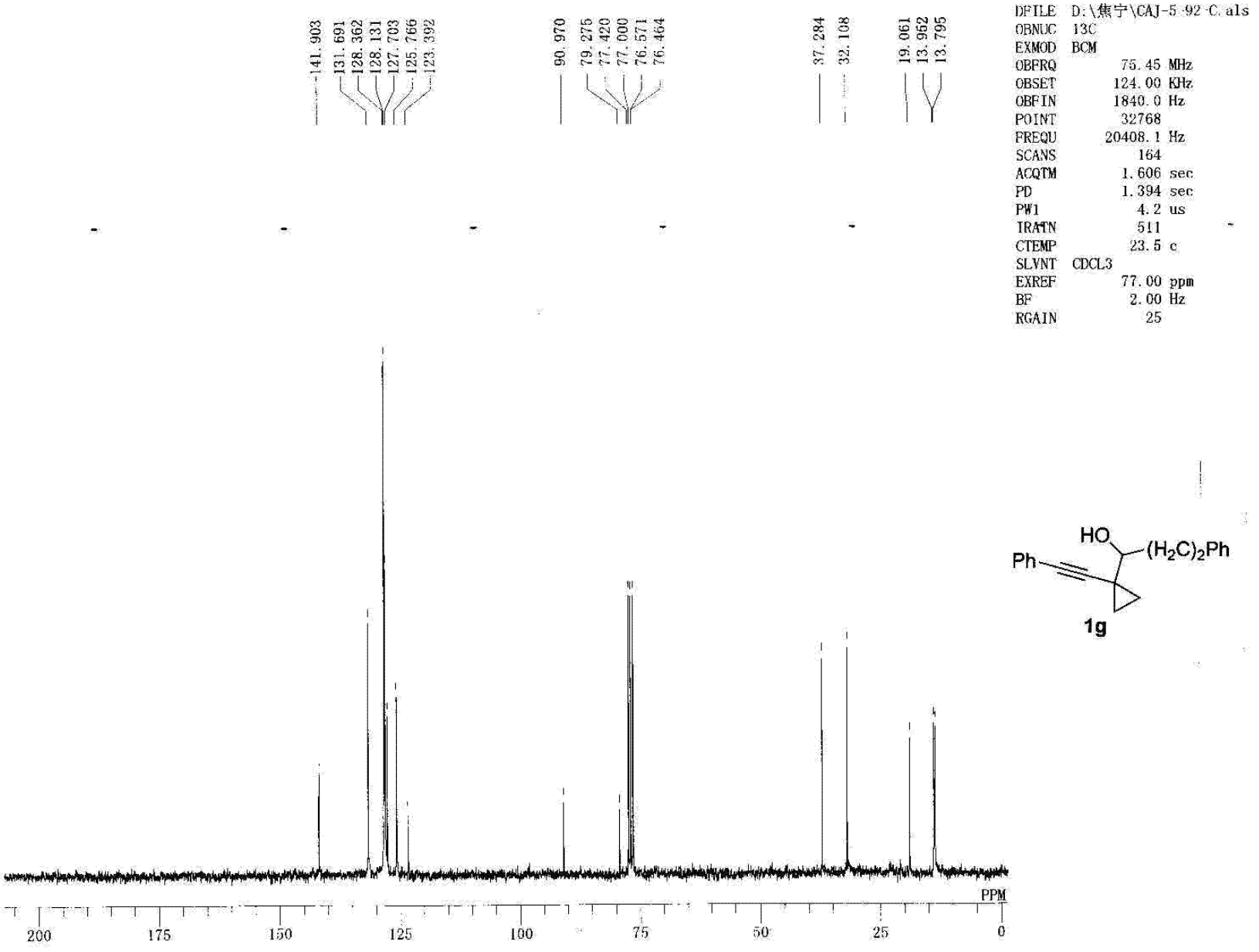
8
6
4
2
0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77.420
77.000
76.571
76.464
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32.108
19.061
13.962
13.795
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EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 164
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PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.5 c
SLVNT CDCL3
EXREF 77.00 ppm
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1g
PPM
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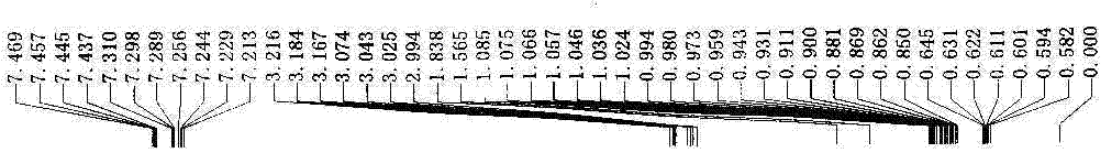
175
150
125
100
75
50
25
0



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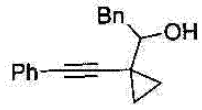
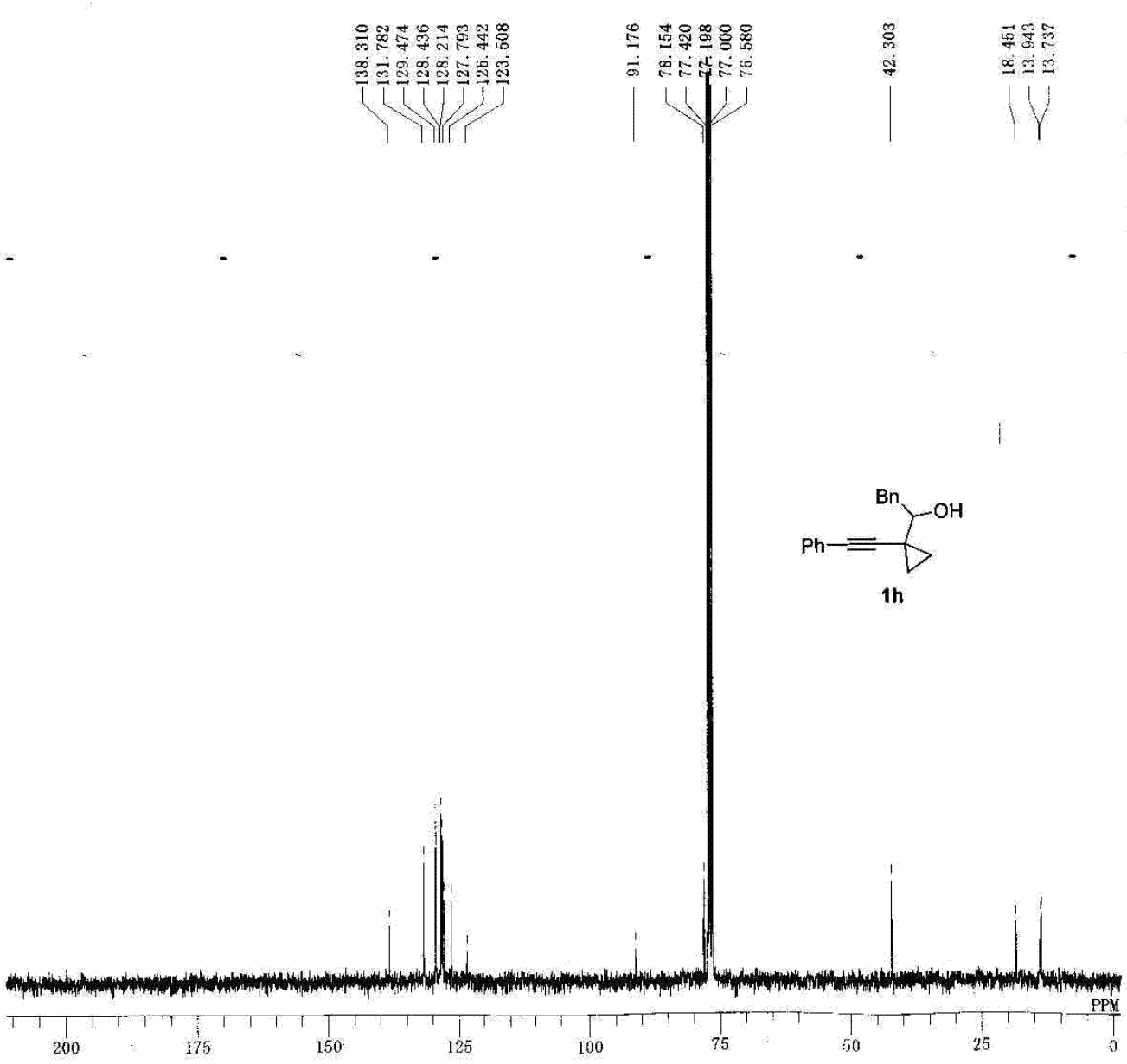
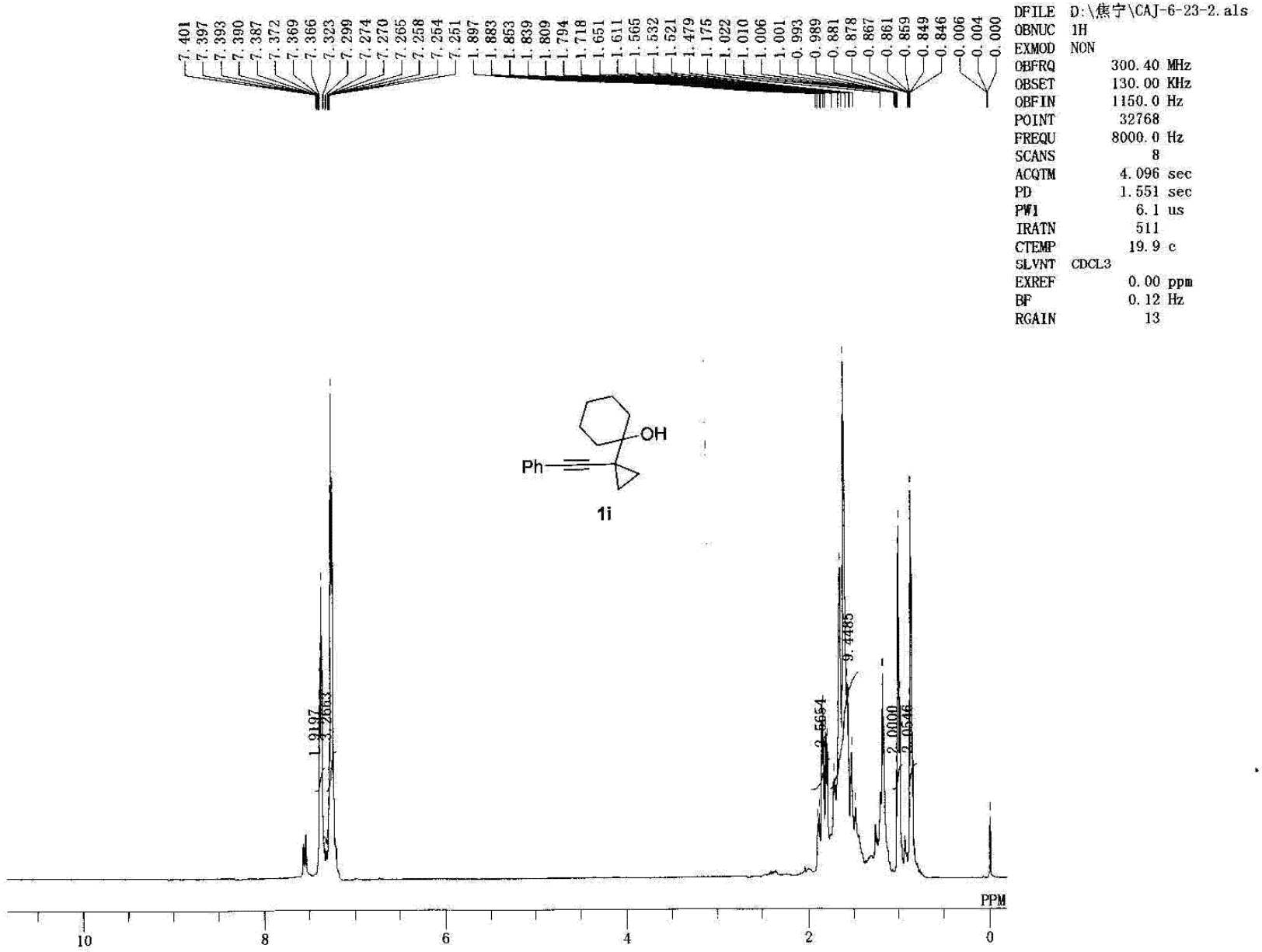
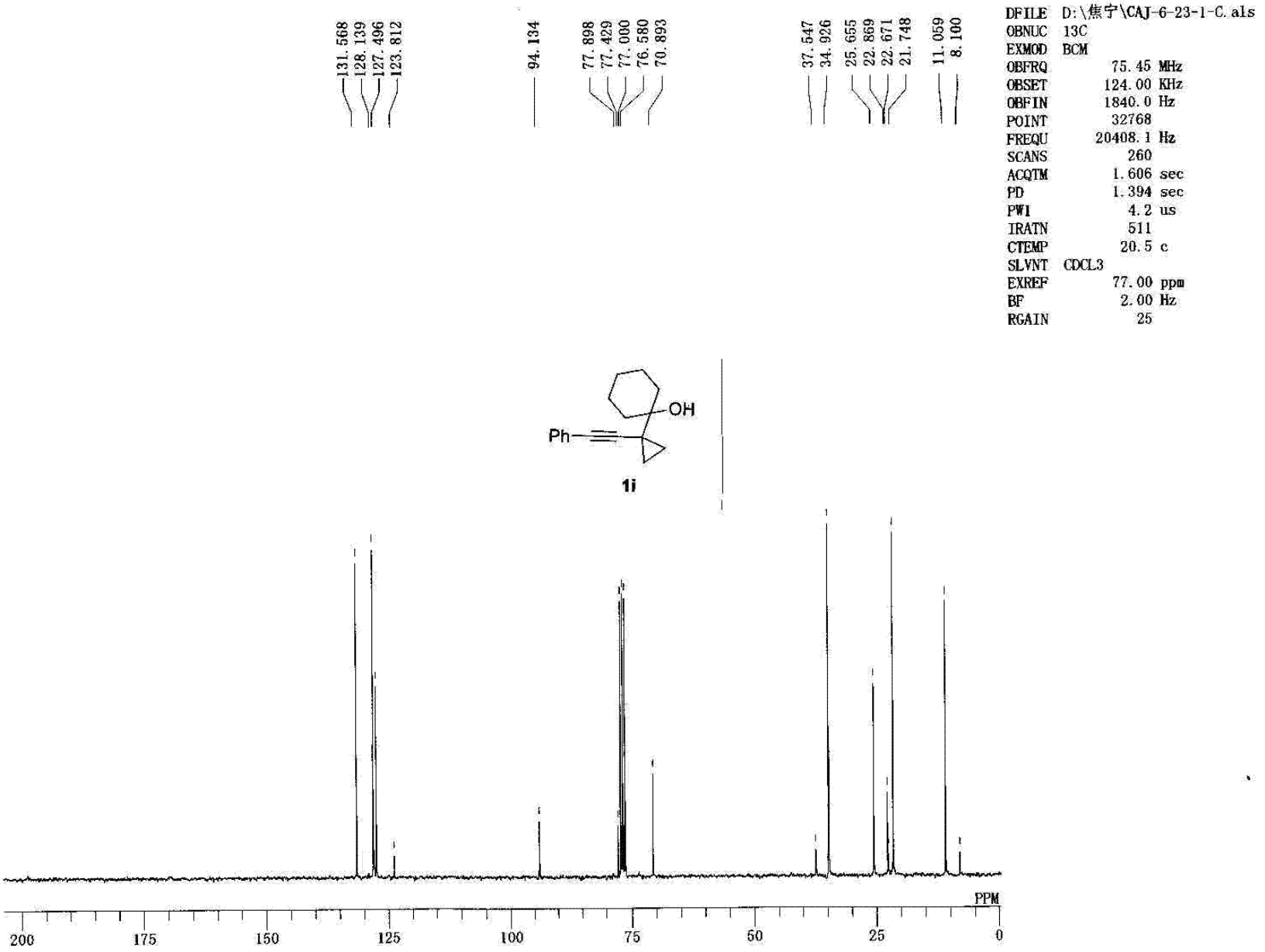
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	21.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	20

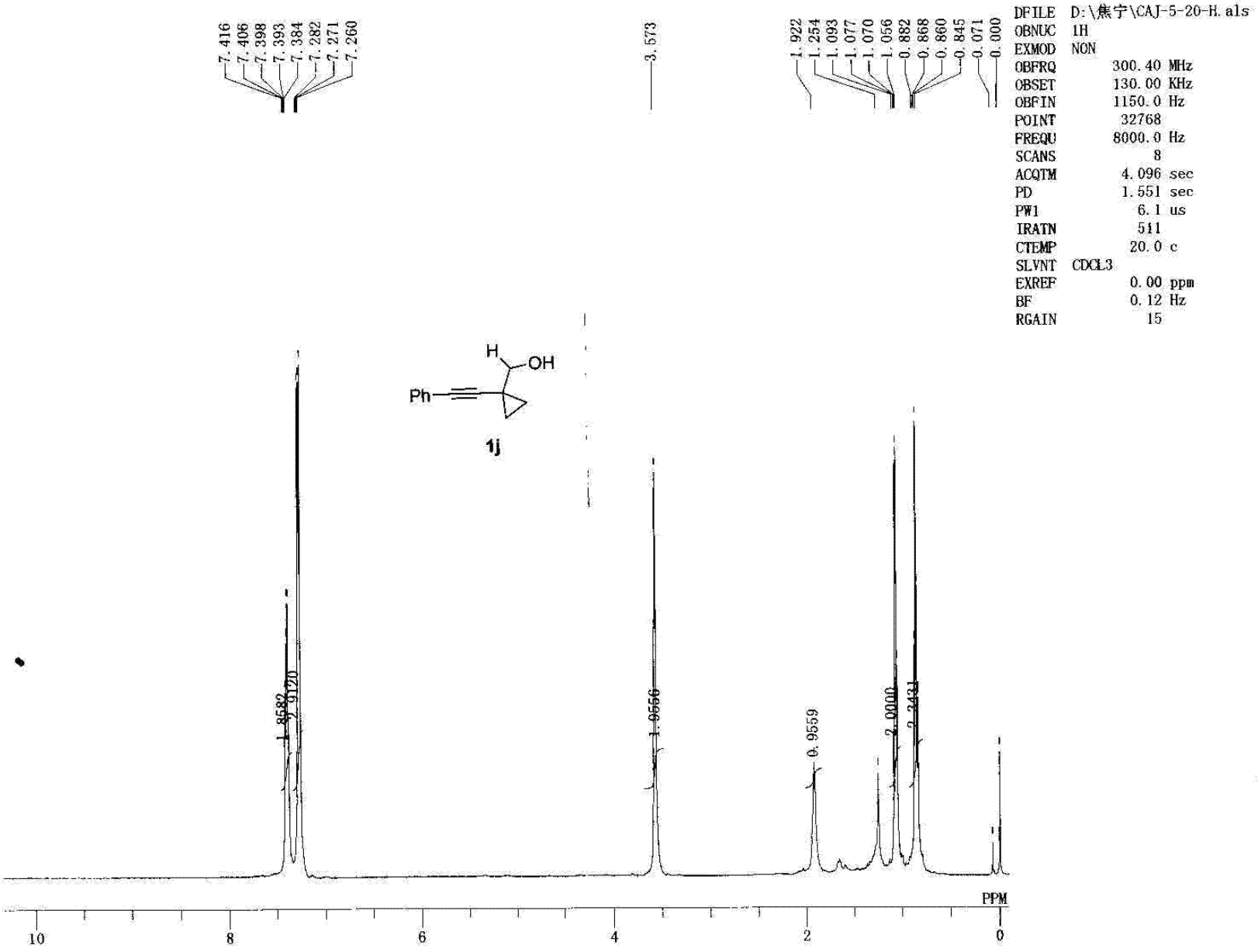


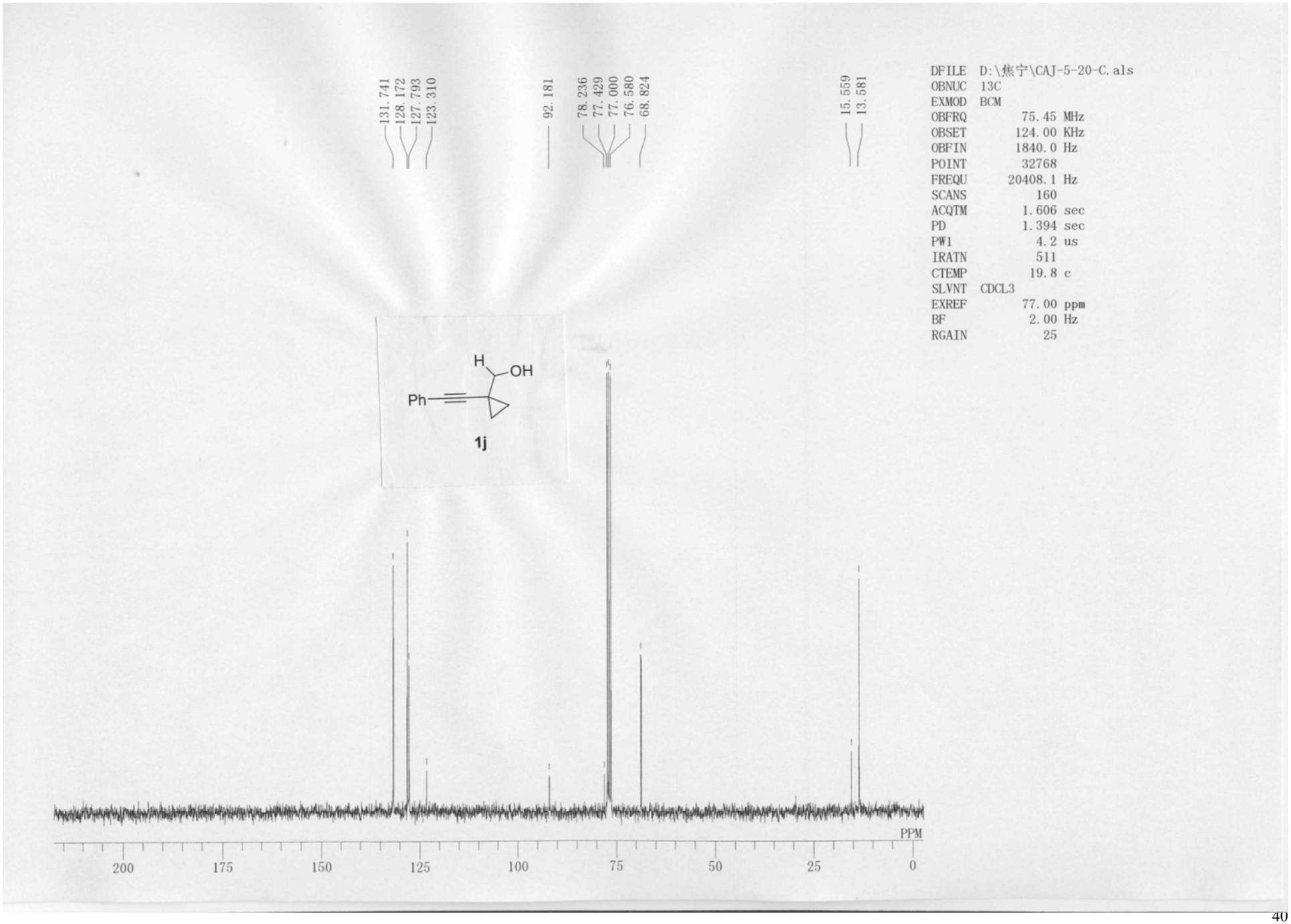
1h

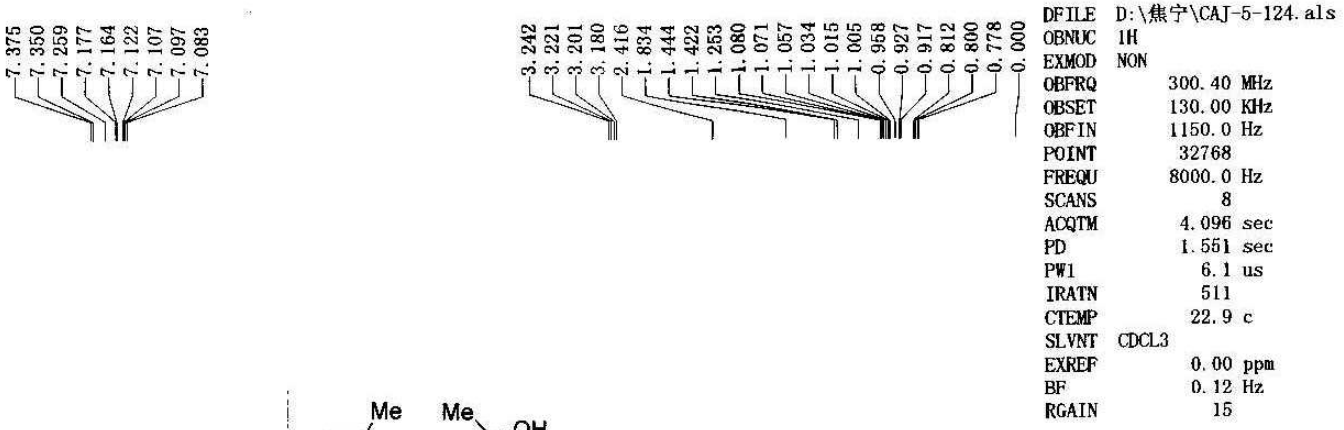

138.310
131.782
129.474
128.436
128.214
127.793
126.442
123.608
91.176
78.154
77.420
77.198
77.000
76.580
42.303
18.451
13.943
13.737
DFILE D:\焦宁\CAJ-5-85-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 412
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 5H
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 26
Bn
OH
Ph
1h
PPM
200
175
150
125
100
75
50
25
0

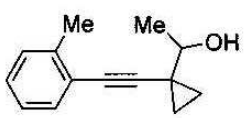

7.401
7.397
7.393
7.390
7.387
7.372
7.369
7.366
7.323
7.299
7.274
7.270
7.265
7.258
7.254
7.251
1.897
1.883
1.853
1.839
1.809
1.794
1.718
1.651
1.611
1.565
1.532
1.521
1.479
1.175
1.022
1.010
1.006
1.001
0.993
0.989
0.881
0.878
0.867
0.861
0.859
0.849
0.846
0.006
0.004
0.000
DFILE D:\焦宁\CAJ-6-23-2.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 19.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13
OH
Ph
1i
1.9197
3.2663
2.5654
9.4485
2.0000
3.0546
PPM
10
8
6
4
2
0


131.568
128.139
127.496
123.812
94.134
77.898
77.429
77.000
76.580
70.893
37.547
34.926
25.655
22.869
22.671
21.748
11.059
8.100
DFILE D:\焦宁\CAJ-6-23-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 260
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Ph
1i
PPM
200
175
150
125
100
75
50
25
0

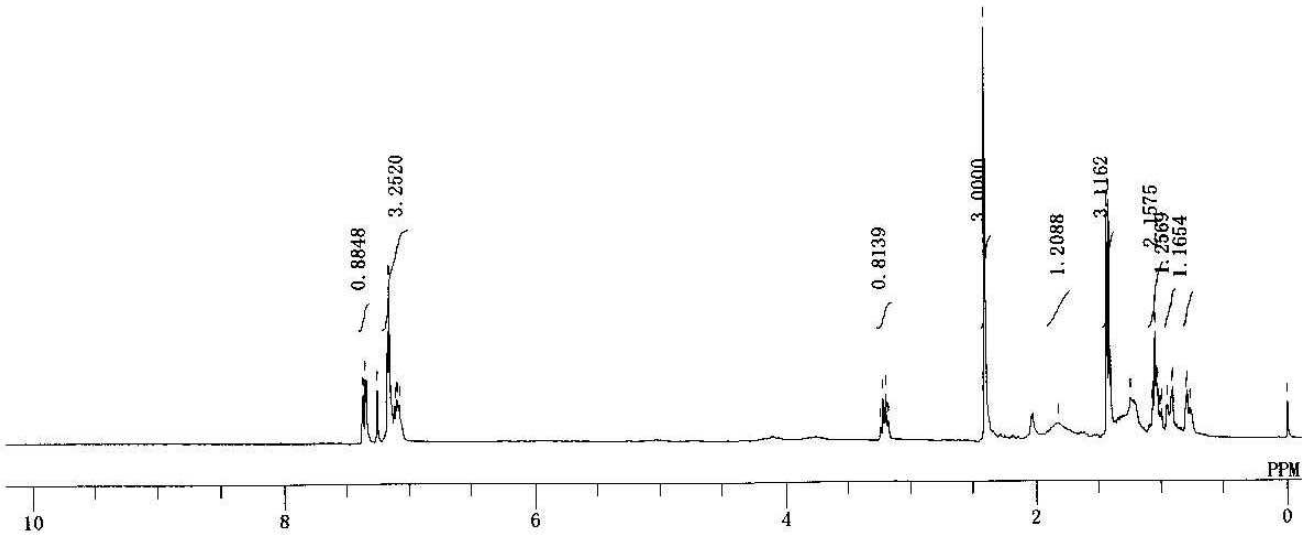

7.416
7.406
7.398
7.393
7.384
7.282
7.271
7.260
3.573
1.922
1.254
1.093
1.077
1.070
1.056
0.882
0.868
0.860
0.845
0.071
0.000
DFILE D:\焦宁\CAJ-5-20-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
H
OH
Ph
1j
1.8582
5.9120
1.0556
0.9559
2.0000
2.2431
PPM
10
8
6
4
2
0

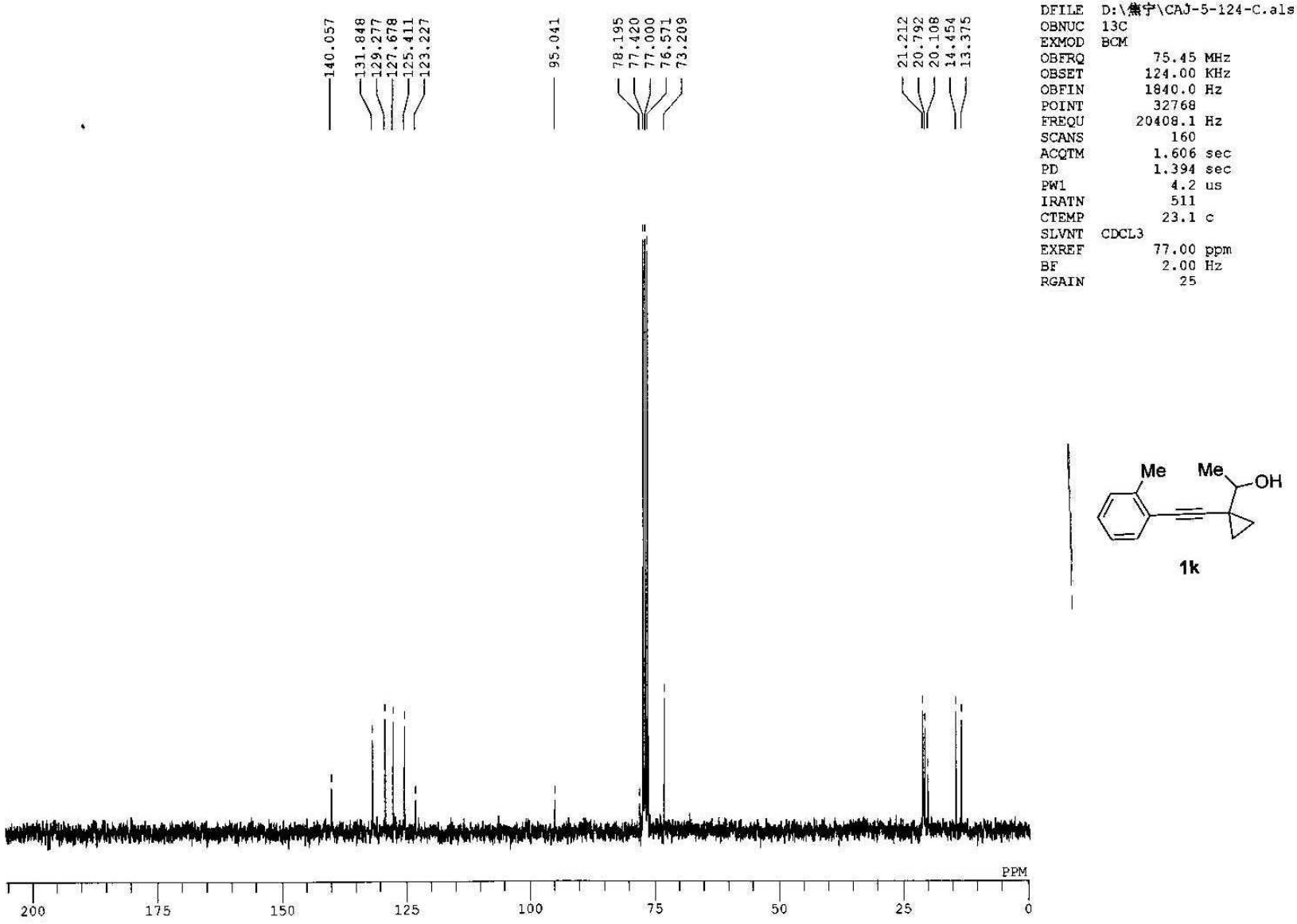


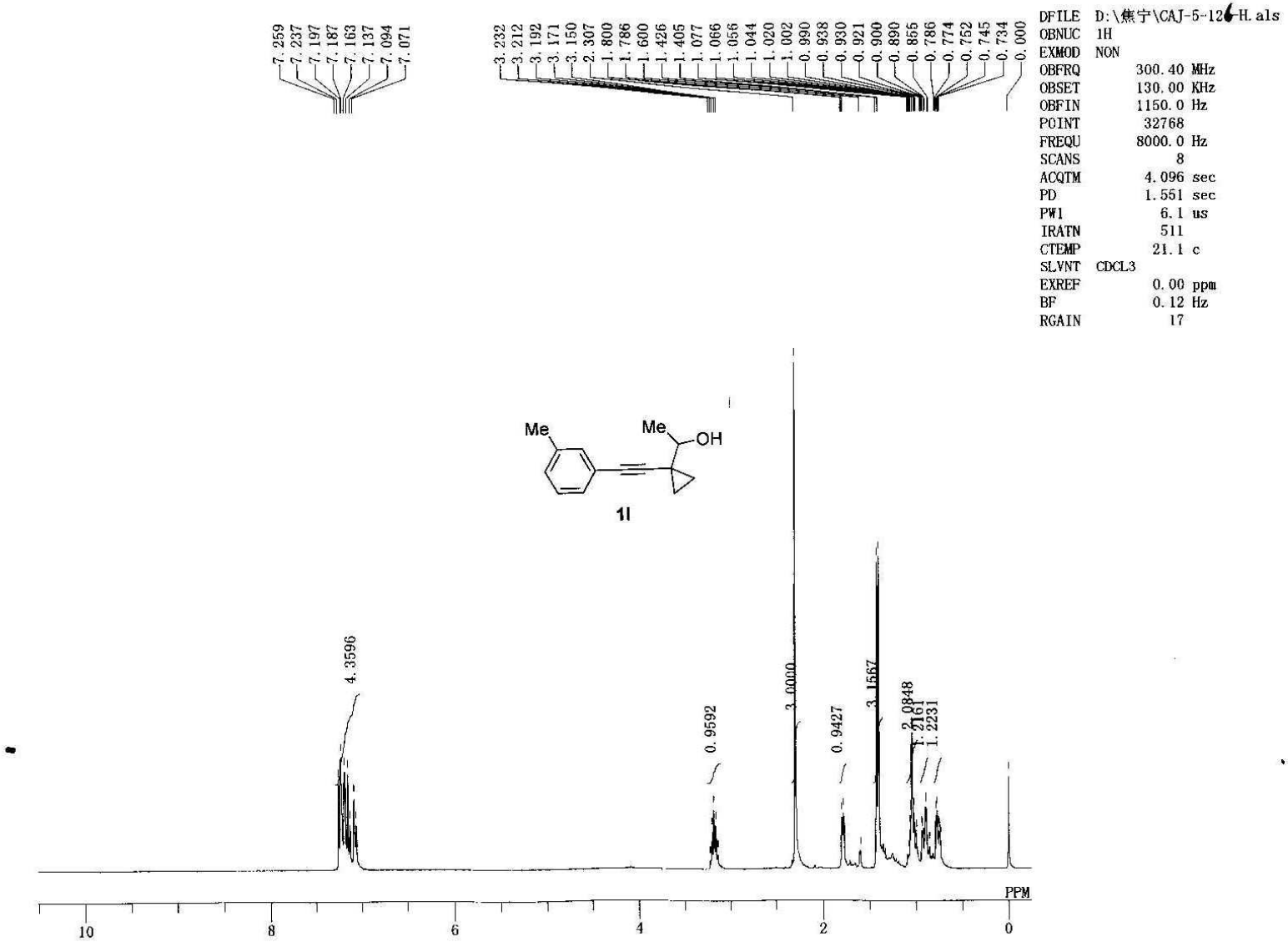

7.375
7.350
7.259
7.177
7.164
7.122
7.107
7.097
7.083
3.242
3.221
3.201
3.180
2.416
1.834
1.444
1.422
1.253
1.080
1.071
1.057
1.034
1.015
1.005
0.958
0.927
0.917
0.812
0.800
0.778
0.000
DFILE D:\焦宁\CAJ-5-124.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15

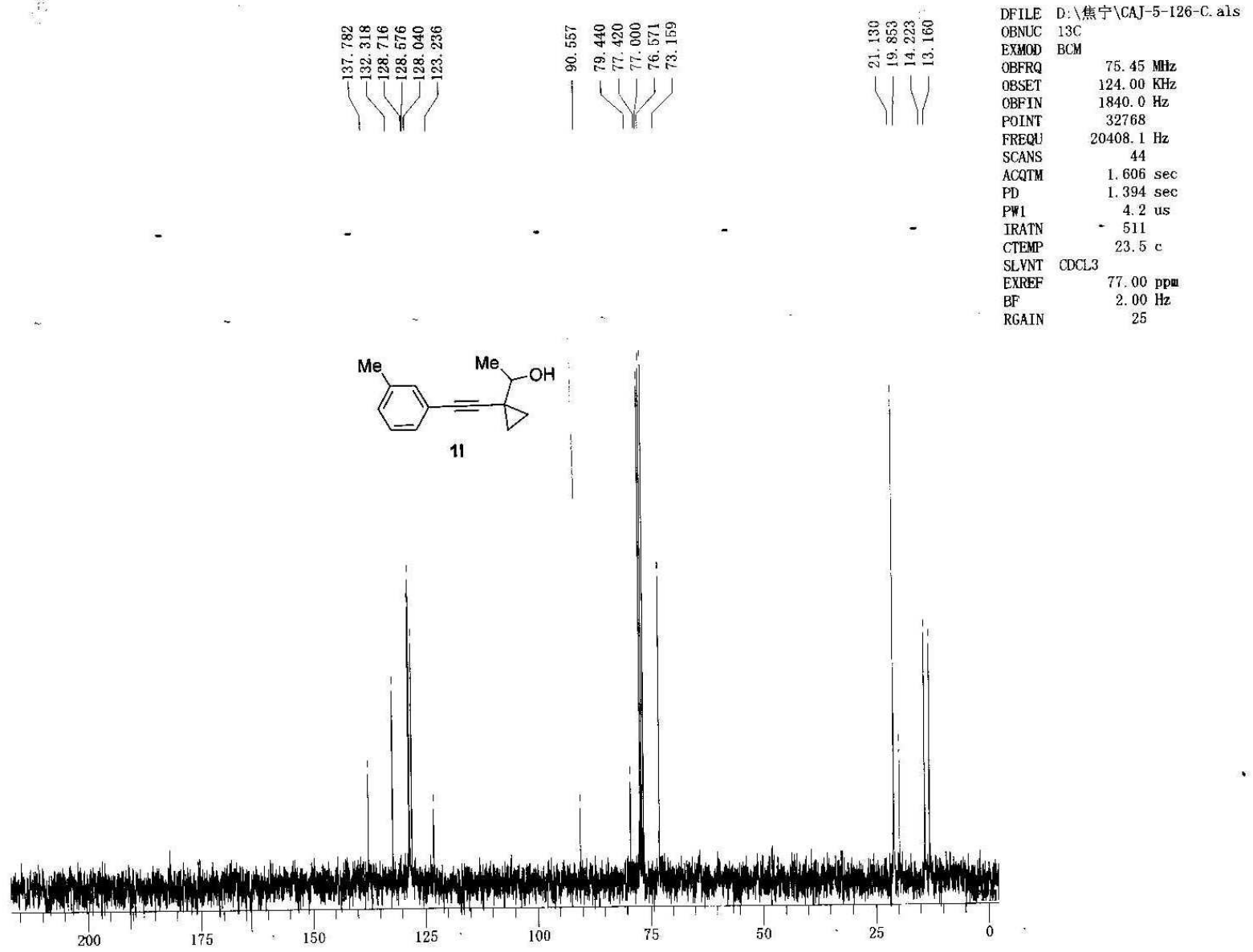

Me
Me
OH

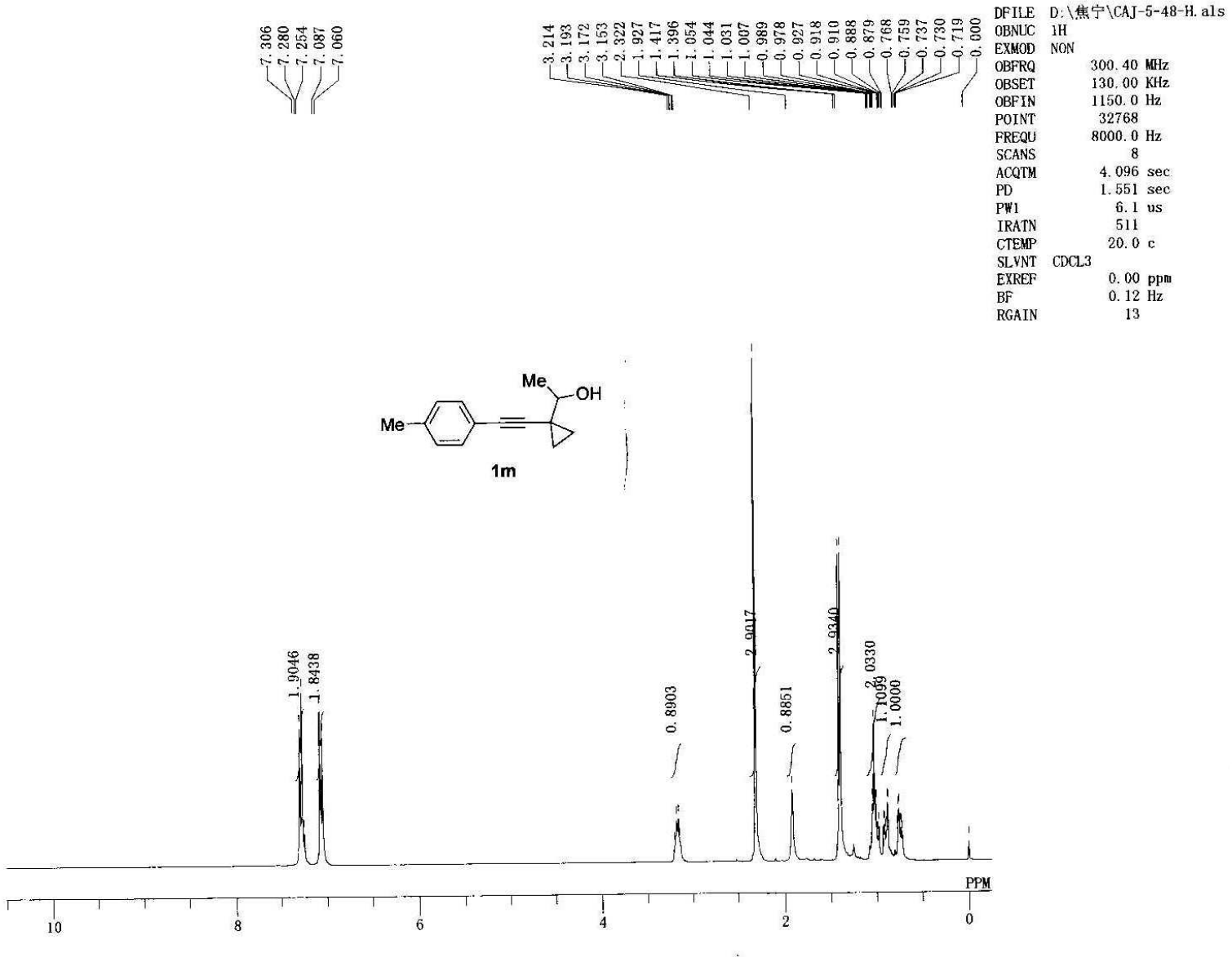
1k

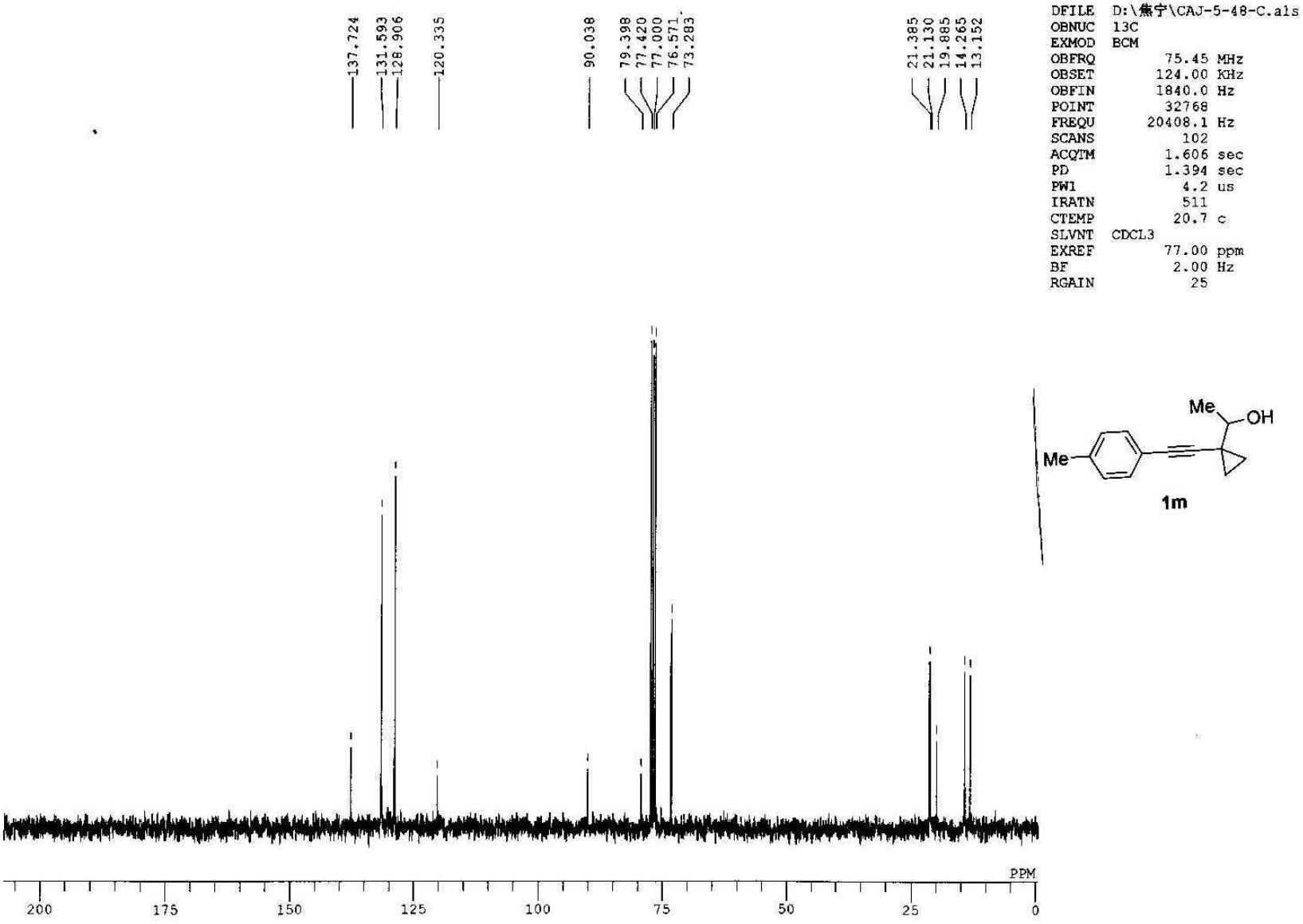

0.8848
3.2520
0.8139
3.0000
1.2088
3.1162
2.1575
2.2569
1.1654
PPM
10
8
6
4
2
0

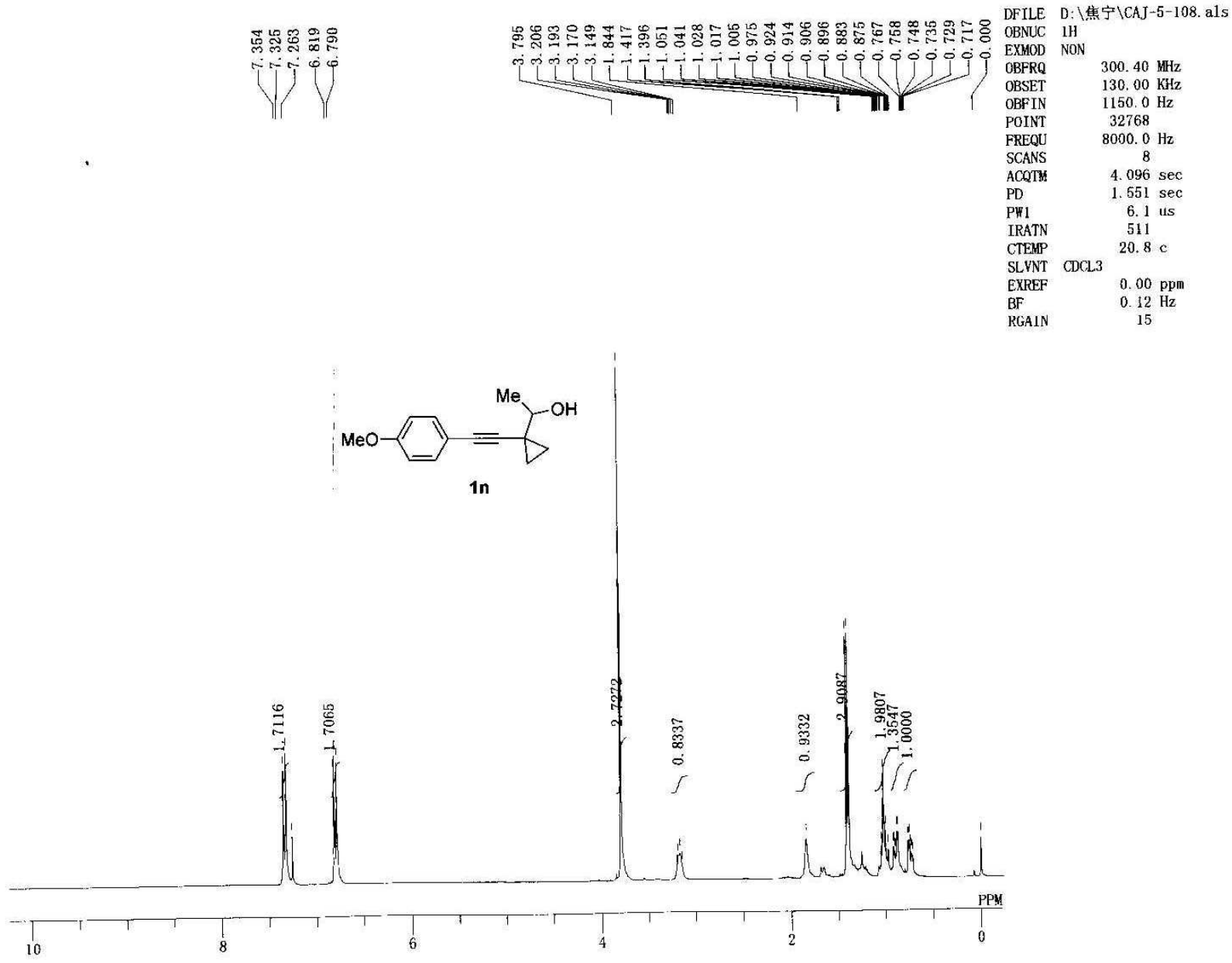

140.057
131.848
129.277
127.678
125.411
123.227
95.041
78.195
77.420
77.000
76.571
73.209
21.212
20.792
20.108
14.454
13.375
DFILE D:\焦宁\CAJ-5-124-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 160
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
Me
OH
1k
PPM
200
175
150
125
100
75
50
25
0

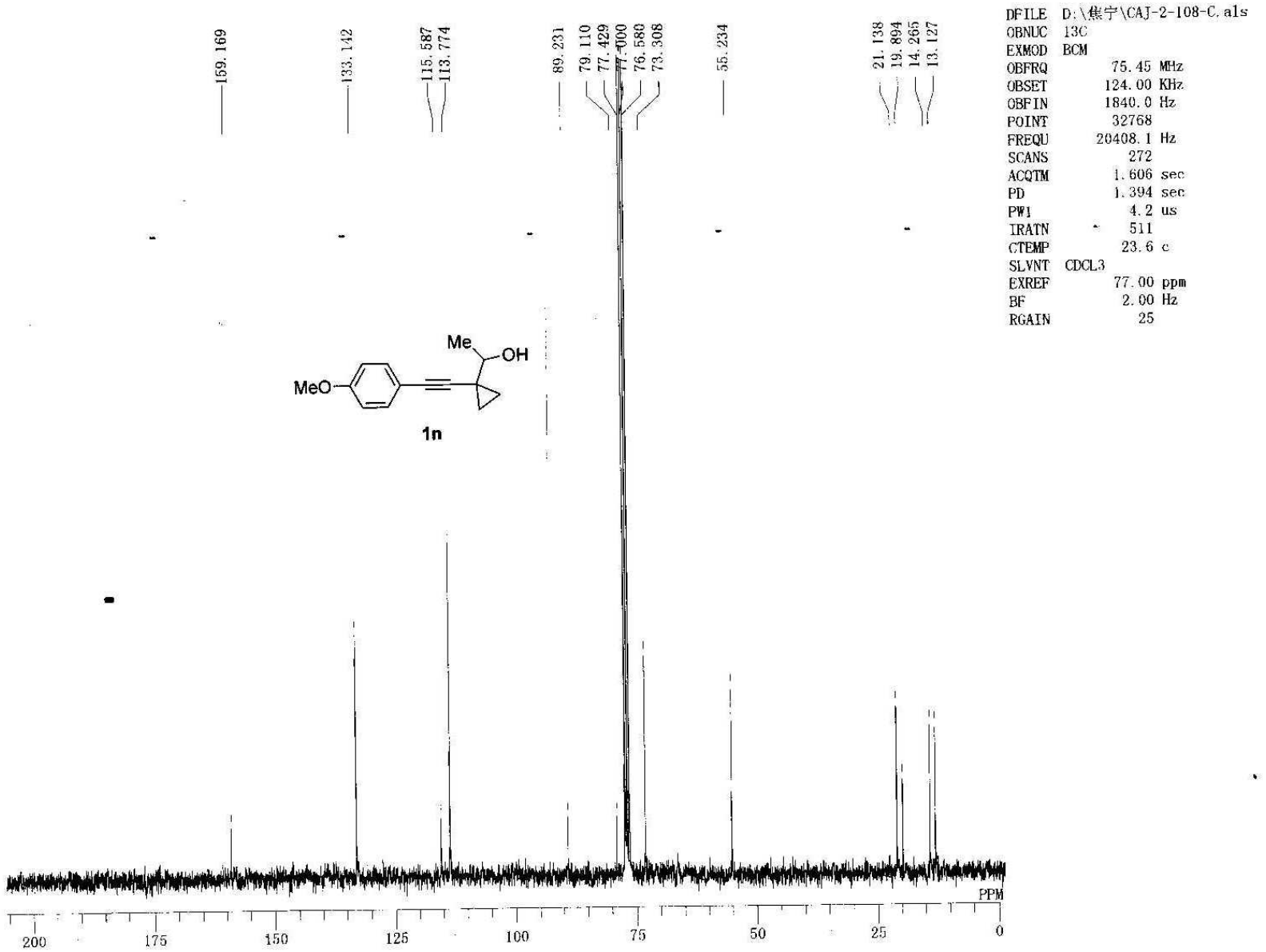

7.259
7.237
7.197
7.187
7.163
7.137
7.094
7.071
3.232
3.212
3.192
3.171
3.150
2.307
1.800
1.786
1.600
1.426
1.405
1.077
1.066
1.056
1.044
1.020
1.002
0.990
0.938
0.930
0.921
0.900
0.890
0.855
0.786
0.774
0.752
0.745
0.734
0.000
DFILE D:\焦宁\CAJ-5-126-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 21.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17
Me
Me
OH
1l
4.3596
0.9592
3.0000
0.9427
3.1567
2.0848
2.2161
1.2231
PPM
10
8
6
4
2
0

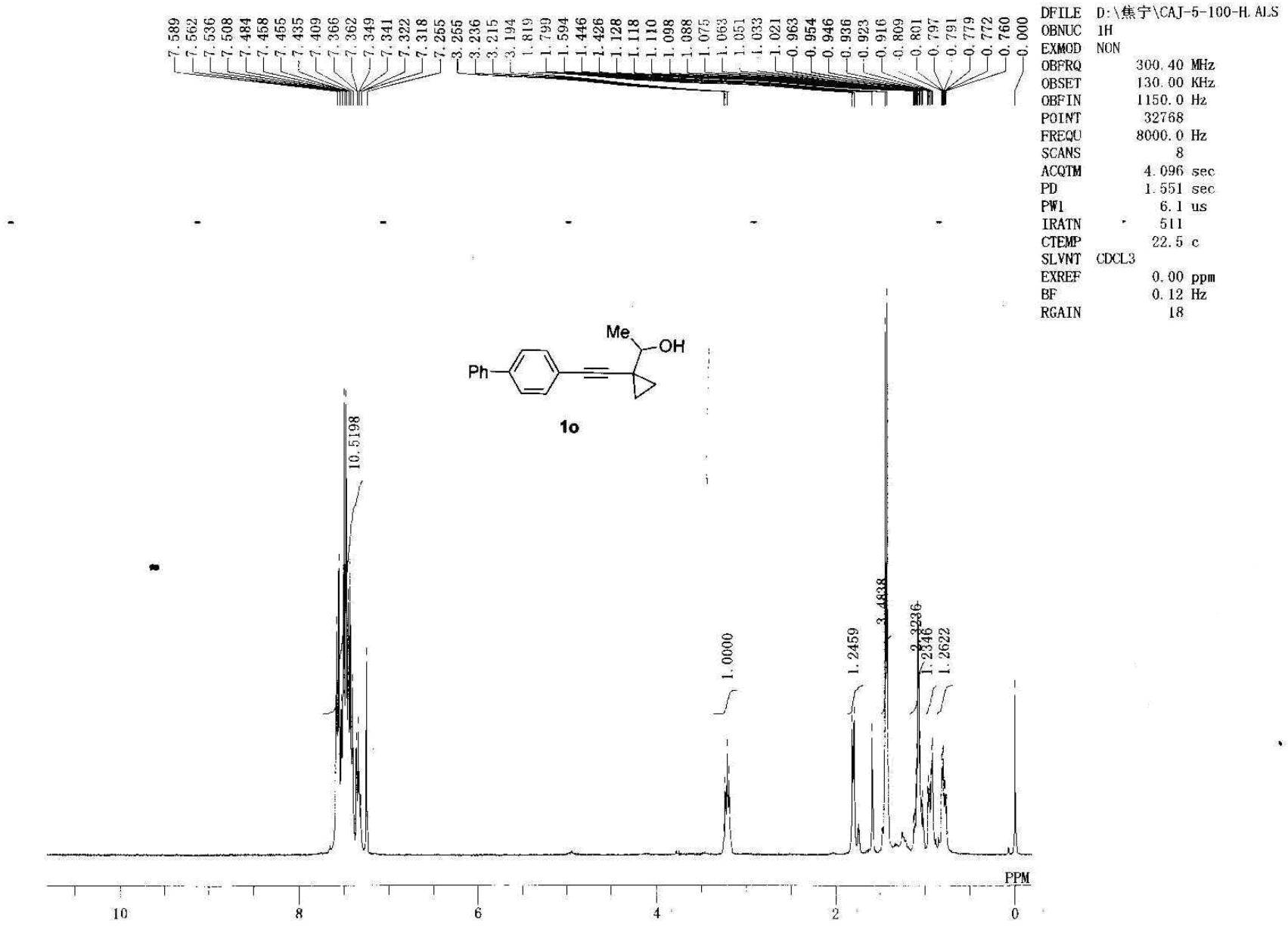

137.782
132.318
128.716
128.576
128.040
123.236
90.557
79.440
77.420
77.000
76.571
73.159
21.130
19.853
14.223
13.160
DFILE D:\焦宁\CAJ-5-126-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 44
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
Me
OH
11
200
175
150
125
100
75
50
25
0

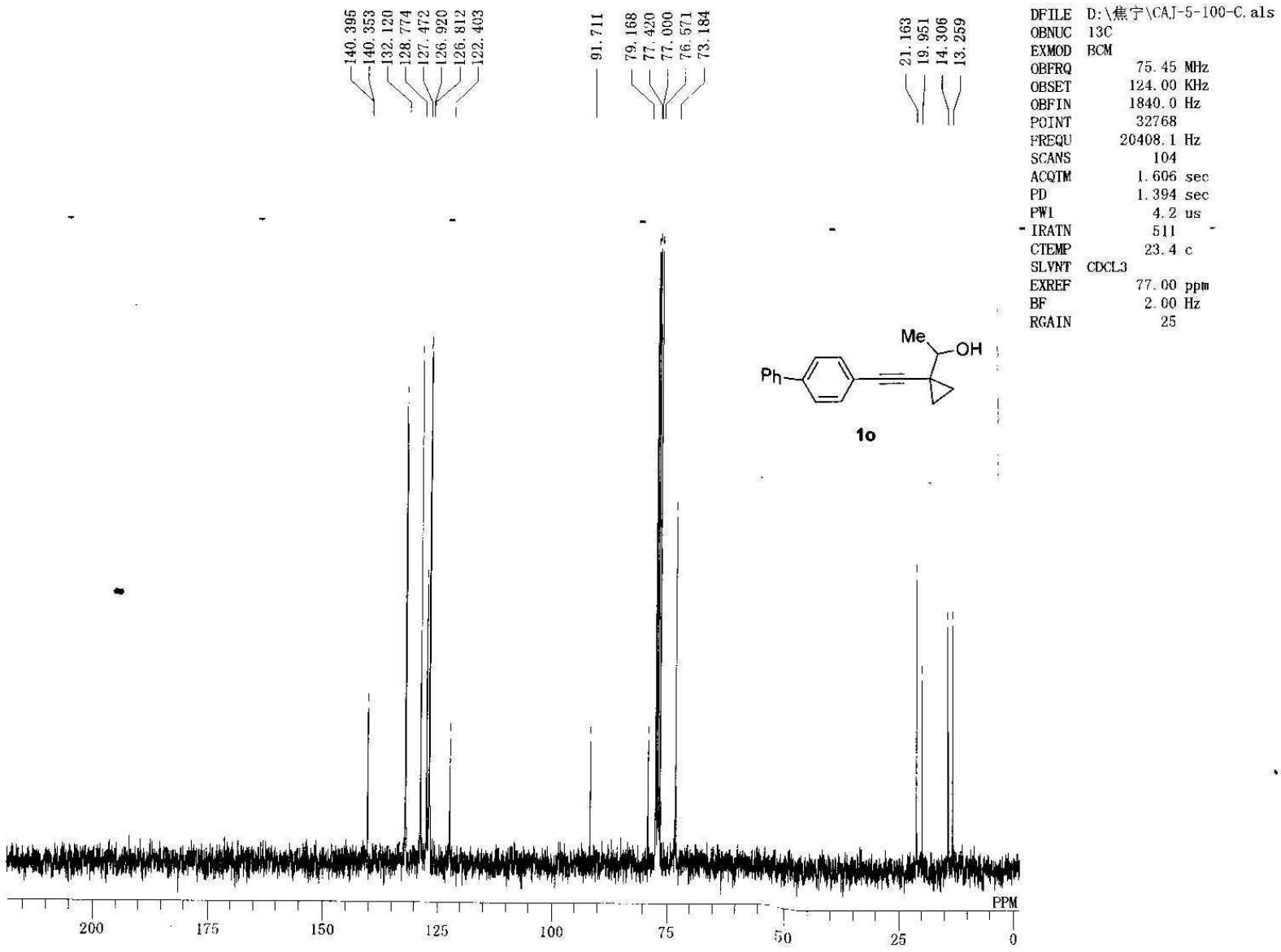

7.306
7.280
7.254
7.087
7.060
3.214
3.193
3.172
3.153
2.322
1.927
1.417
1.396
1.054
1.044
1.031
1.007
0.989
0.978
0.927
0.918
0.910
0.888
0.879
0.768
0.759
0.737
0.730
0.719
0.000
DFILE D:\焦宁\CAJ-5-48-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13
Me
OH
Me
1m
1.9046
1.8438
0.8903
2.9017
0.8851
2.9340
2.0330
1.7099
1.0000
PPM
10
8
6
4
2
0

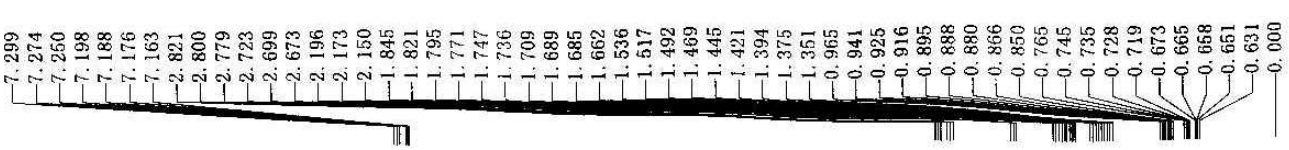

137.724
131.593
128.906
120.335
90.038
79.398
77.420
77.000
76.571
73.283
21.385
21.130
19.885
14.265
13.152
DFILE D:\焦宁\CAJ-5-48-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 102
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
OH
Me
1m
PPM
200
175
150
125
100
75
50
25
0


7.354
7.325
7.263
6.819
6.790
3.795
3.206
3.193
3.170
3.149
1.844
1.417
1.396
1.051
1.041
1.028
1.017
1.005
0.975
0.924
0.914
0.906
0.896
0.883
0.875
0.767
0.758
0.748
0.735
0.729
0.717
0.000
DFILE D:\焦宁\CAJ-5-108.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
Me
OH
MeO
1n
1.7116
1.7065
2.7272
0.8337
0.9332
2.9087
1.9807
1.3547
1.0000
PPM
10
8
6
4
2
0

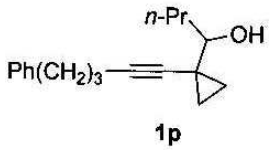

159.169
133.142
115.587
113.774
89.231
79.110
77.429
77.000
76.580
73.308
55.234
21.138
19.894
14.265
13.127
DFILE D:\焦宁\CAJ-2-108-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 272
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
OH
MeO
1n
PPM
200
175
150
125
100
75
50
25
0


7.589
7.562
7.536
7.508
7.484
7.458
7.455
7.435
7.409
7.366
7.362
7.349
7.341
7.322
7.318
7.255
3.255
3.236
3.215
3.194
1.819
1.799
1.594
1.446
1.426
1.128
1.118
1.110
1.098
1.088
1.075
1.063
1.051
1.033
1.021
0.963
0.954
0.946
0.936
0.923
0.916
0.809
0.801
0.797
0.791
0.779
0.772
0.760
0.000
DFILE D:\焦宁\CAJ-5-100-H.ALS
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
Me
OH
Ph
1o
10.5198
1.0000
1.2459
3.4838
2.3236
1.2346
1.2622
PPM
10
8
6
4
2
0

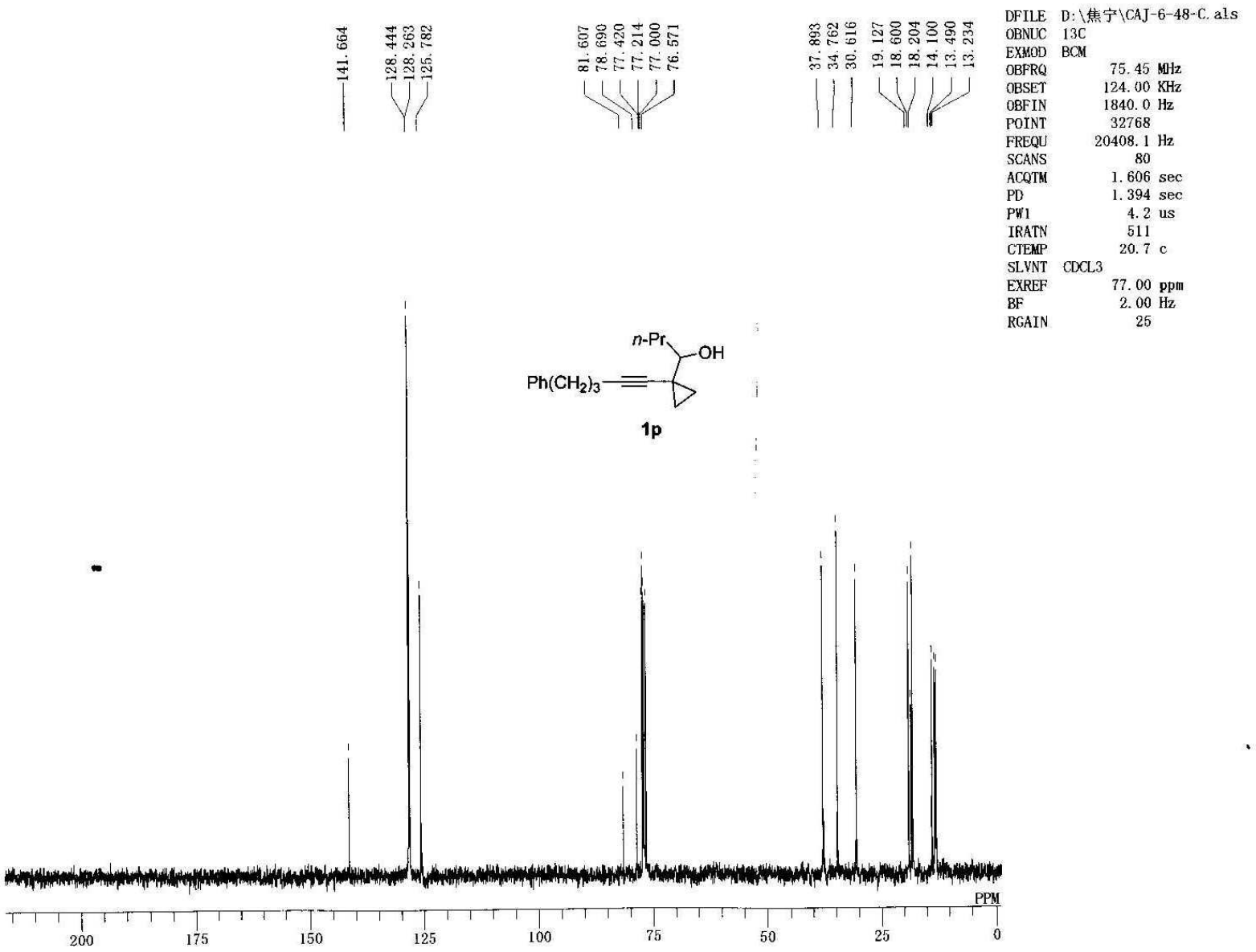

140.395
140.353
132.120
128.774
127.472
126.920
126.812
122.403
91.711
79.168
77.420
77.000
76.571
73.184
21.163
19.951
14.306
13.259
DFILE D:\焦宁\CAJ-5-100-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
PREQU 20408.1 Hz
SCANS 104
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
OH
Ph
1o
200
175
150
125
100
75
50
25
0
PPM

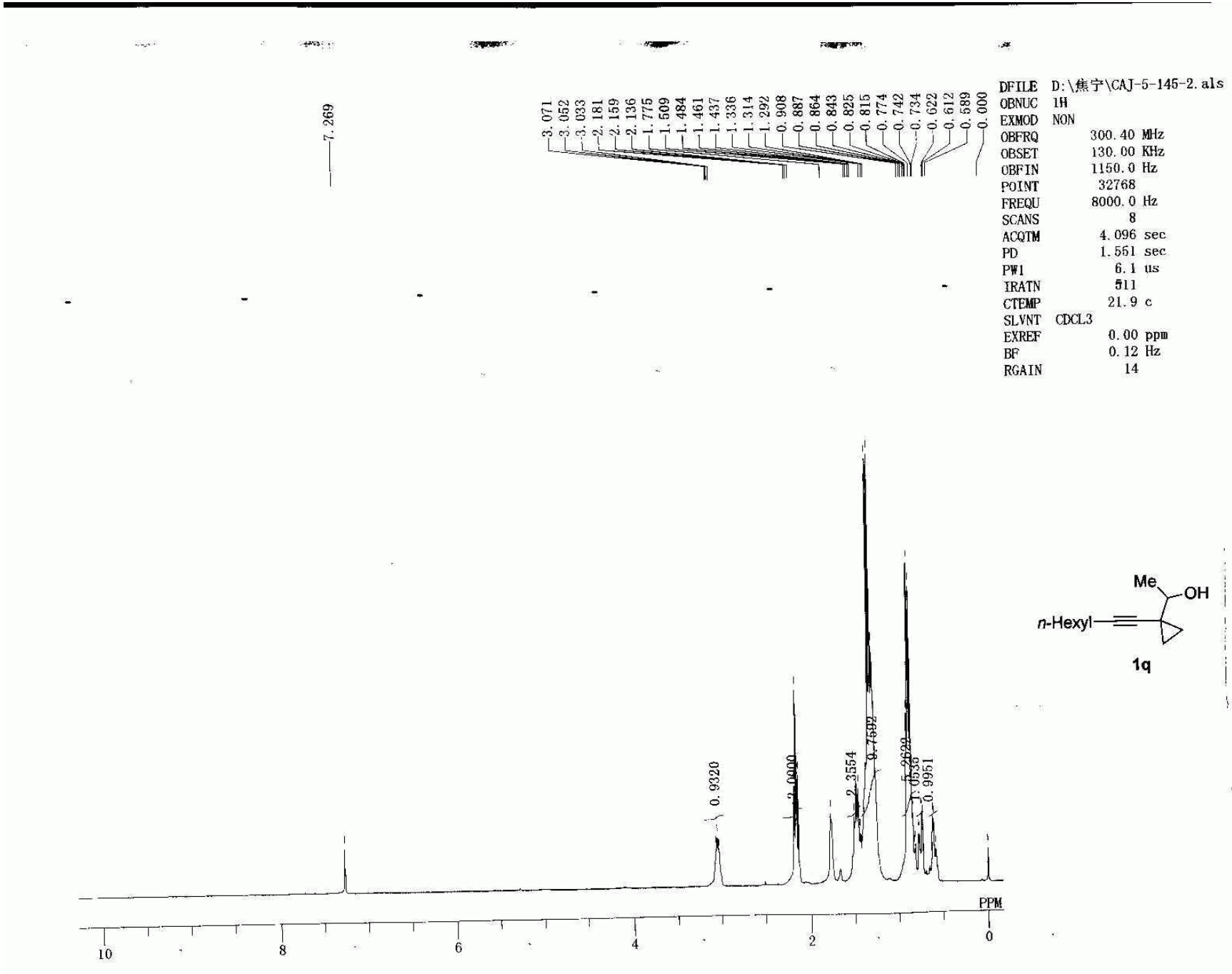


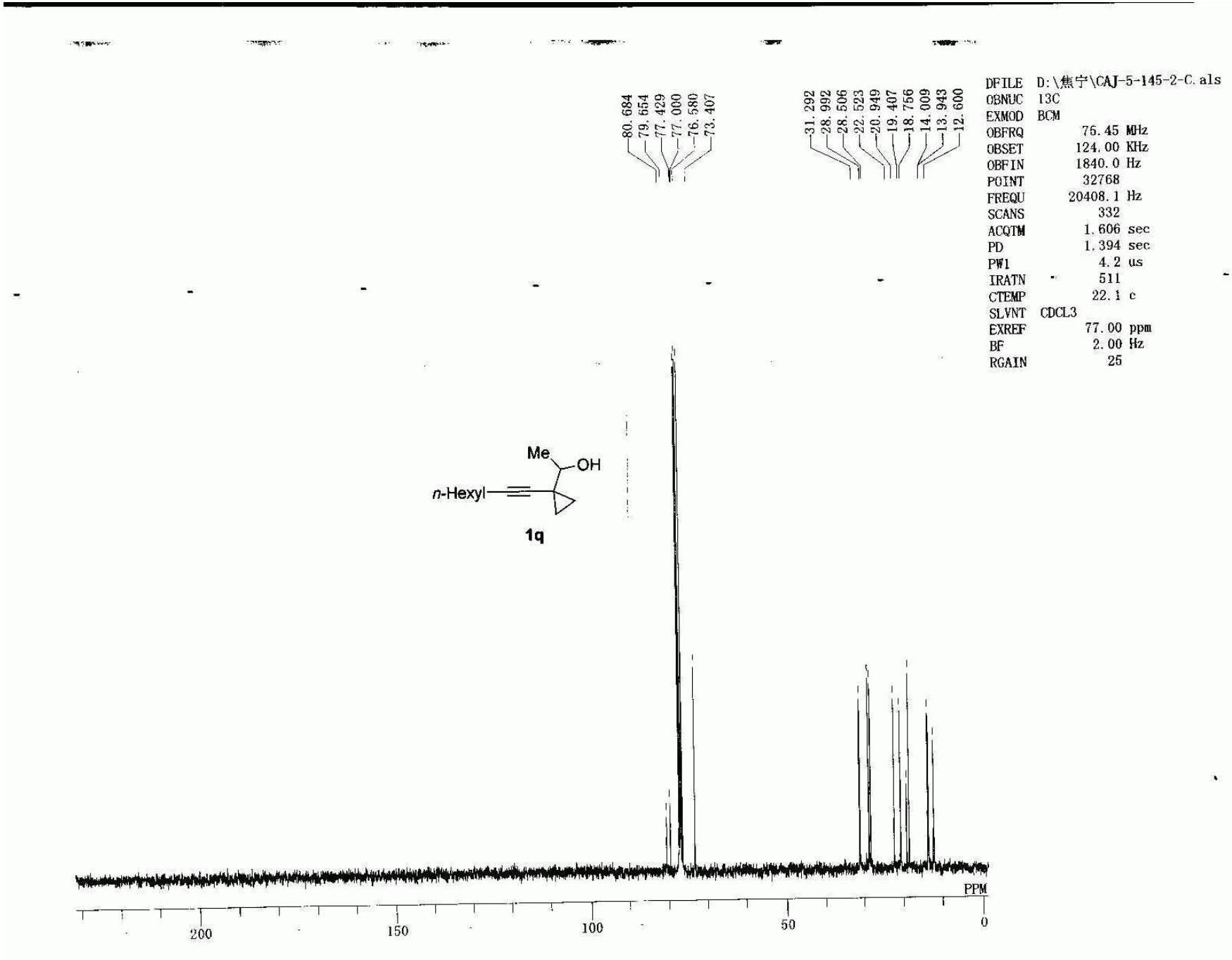

```
DFILE   D:\焦宁\CAJ-6-48.als
OBNUC   1H
EXMOD   NON
OBFRQ        300.40 MHz
OBSET        130.00 KHz
OBFIN        1150.0 Hz
POINT         32768
FREQU        8000.0 Hz
SCANS             8
ACQTM        4.096 sec
PD           1.551 sec
PW1            6.1 us
IRATN             511
CTEMP         21.0 c
SLVNT   CDCL3
EXREF         0.00 ppm
BF            0.12 Hz
RGAIN             12
```

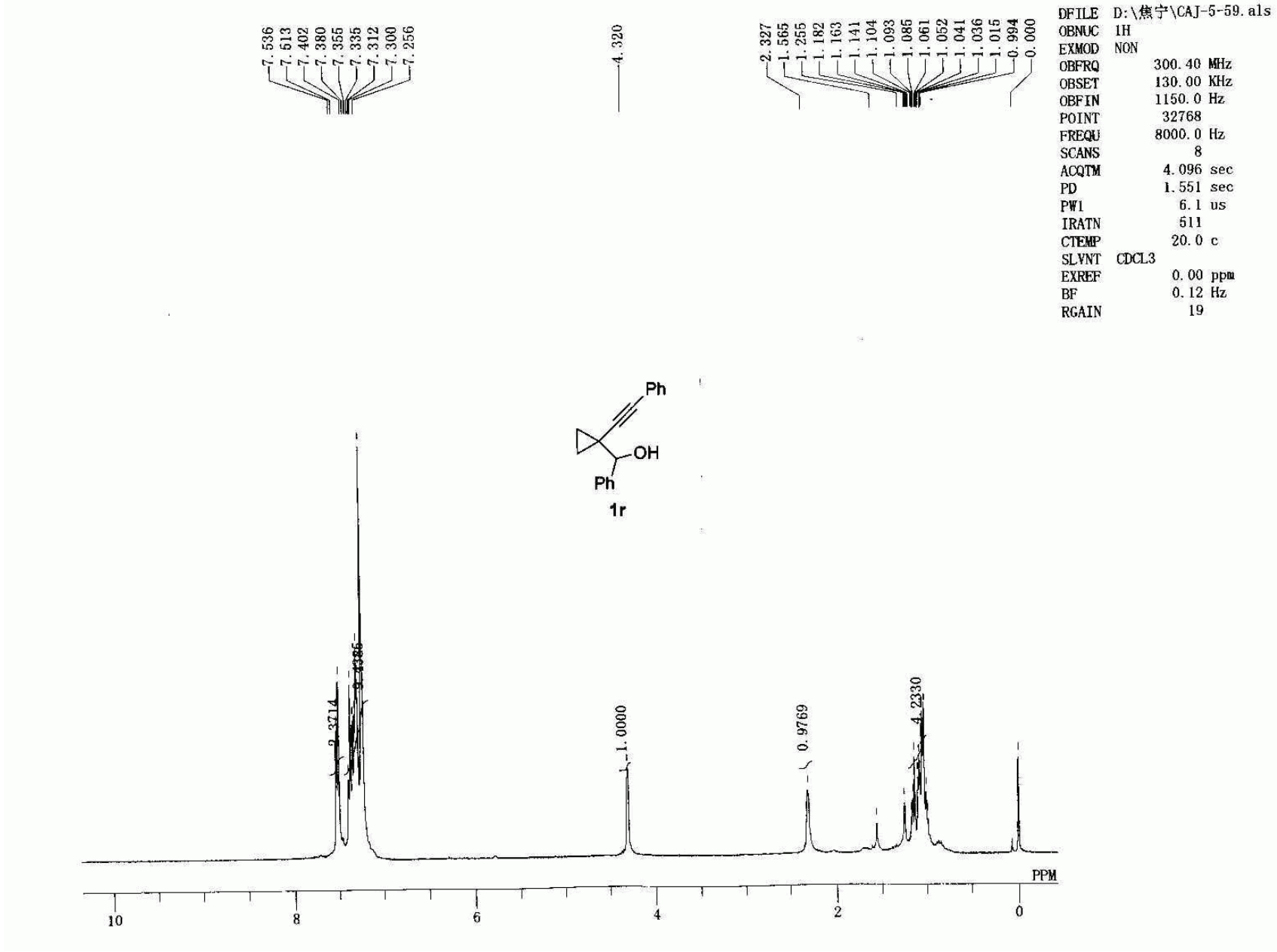


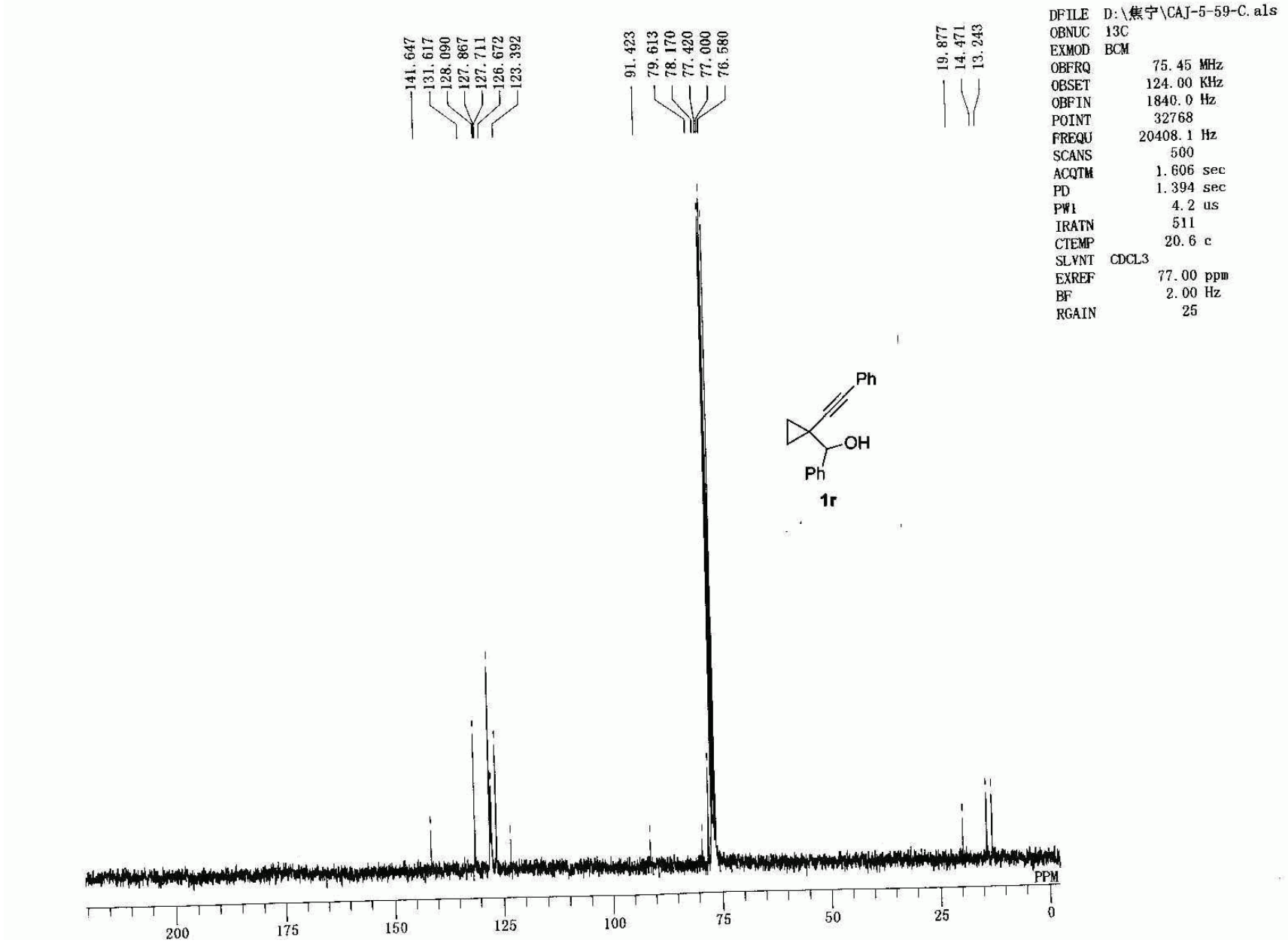
1p

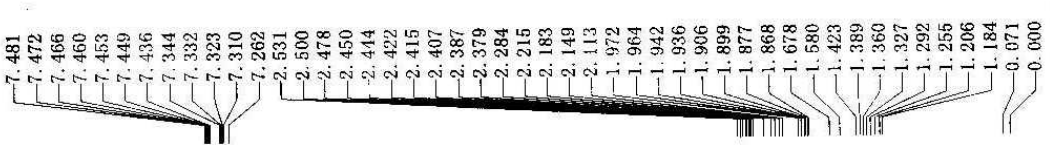

141.664
128.444
128.263
125.782
81.607
78.690
77.420
77.214
77.000
76.571
37.893
34.762
30.616
19.127
18.600
18.204
14.100
13.490
13.234
DFILE D:\焦宁\CAJ-6-48-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 80
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
n-Pr
OH
Ph(CH2)3
1p
PPM
200
175
150
125
100
75
50
25
0


7.269
3.071
3.052
3.033
2.181
2.159
2.136
1.775
1.509
1.484
1.461
1.437
1.336
1.314
1.292
0.908
0.887
0.864
0.843
0.825
0.815
0.774
0.742
0.734
0.622
0.612
0.589
0.000
DFILE D:\焦宁\CAJ-5-145-2.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
0.9320
2.0000
2.3554
0.7692
5.2622
1.0536
0.9951
PPM
10
8
6
4
2
0
Me
OH
n-Hexyl
1q

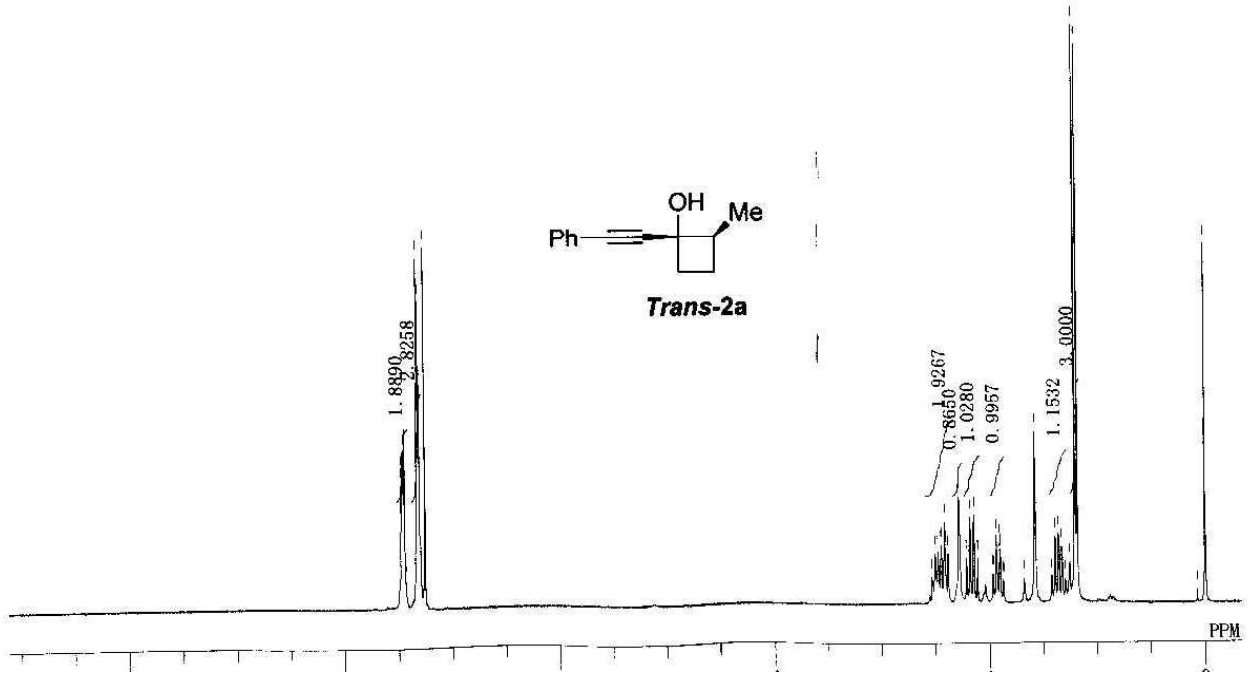

80.684
79.654
77.429
77.000
76.580
73.407
31.292
28.992
28.506
22.523
20.949
19.407
18.756
14.009
13.943
12.600
DFILE D:\焦宁\CAJ-5-145-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 76.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 332
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Me
OH
n-Hexyl
1q
PPM
200
150
100
50
0

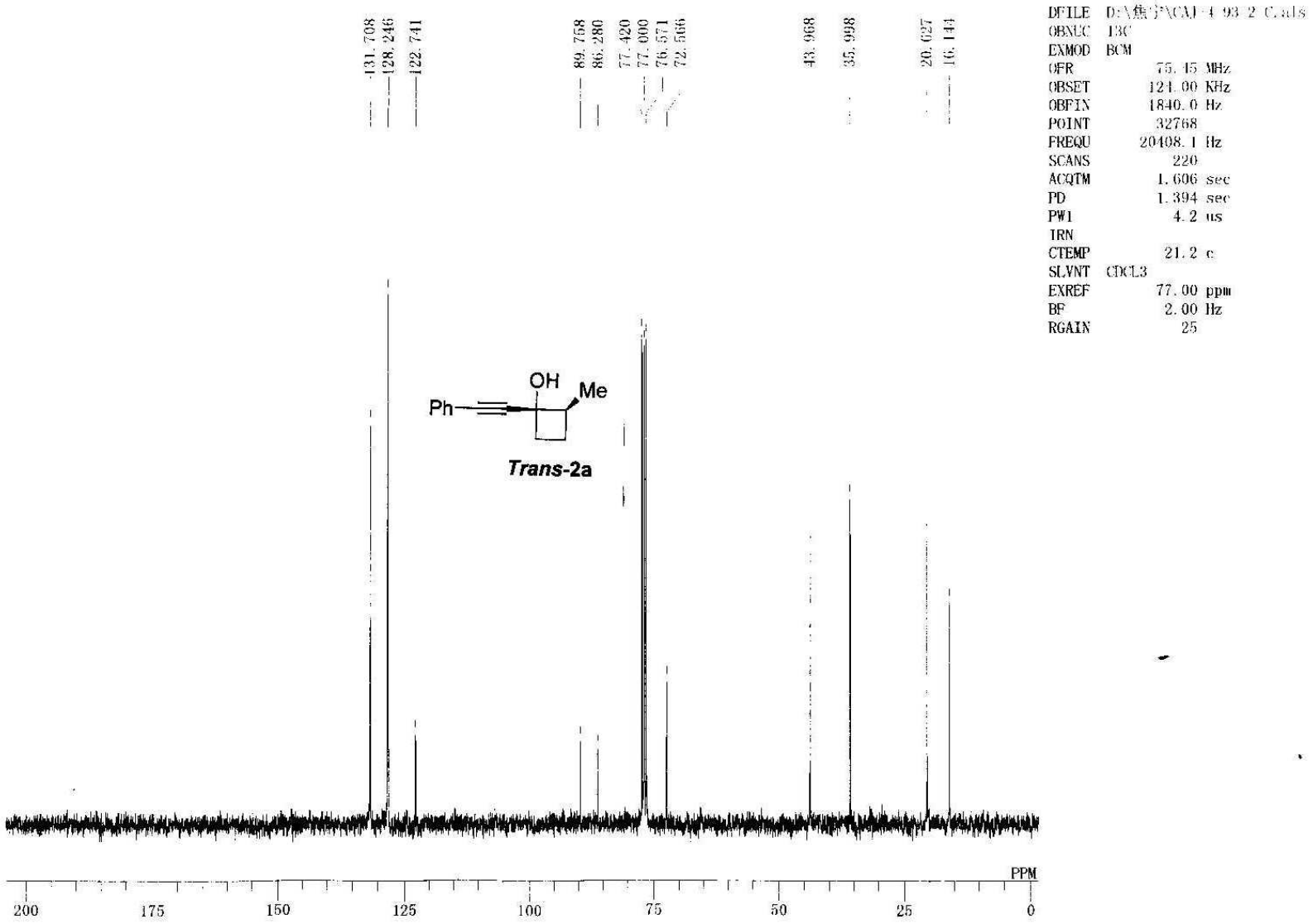

7.536
7.513
7.402
7.380
7.355
7.335
7.312
7.300
7.256
4.320
2.327
1.565
1.255
1.182
1.163
1.141
1.104
1.093
1.086
1.061
1.052
1.041
1.036
1.015
0.994
0.000
DFILE D:\焦宁\CAJ-5-59.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19
Ph
OH
Ph
1r
2.3714
2.3886
1.0000
0.9769
4.2230
PPM
10
8
6
4
2
0

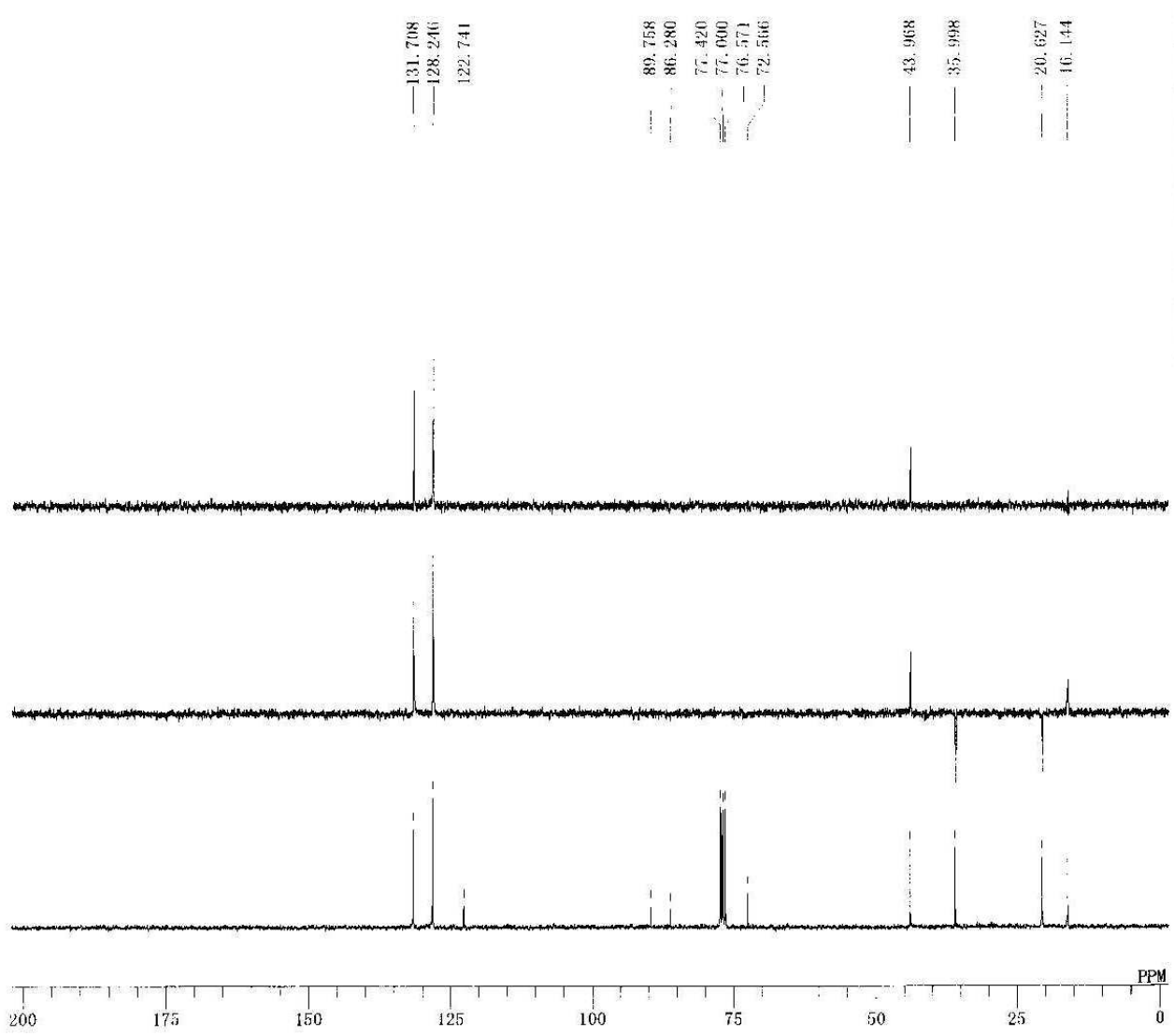

141.647
131.617
128.090
127.867
127.711
126.672
123.392
91.423
79.613
78.170
77.420
77.000
76.580
19.877
14.471
13.243
DFILE D:\焦宁\CAJ-5-59-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 500
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Ph
OH
Ph
1r
PPM
200
175
150
125
100
75
50
25
0



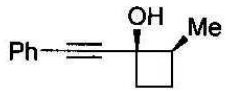
DFILE	D:\焦宁\CAJ-3-131-2.als	
OBNUC	1H	
EXMOD	NON	
OBFRQ	300.40	MHz
OBSET	130.00	KHz
OBFIN	1150.0	Hz
POINT	32768	
FREQU	8000.0	Hz
SCANS	8	
ACQTM	4.096	sec
PD	1.551	sec
PW1	6.1	us
IRATN	511	
CTEMP	20.8	c
SLVNT	CDCL3	
EXREF	0.00	ppm
BF	0.12	Hz
RGAIN	20	



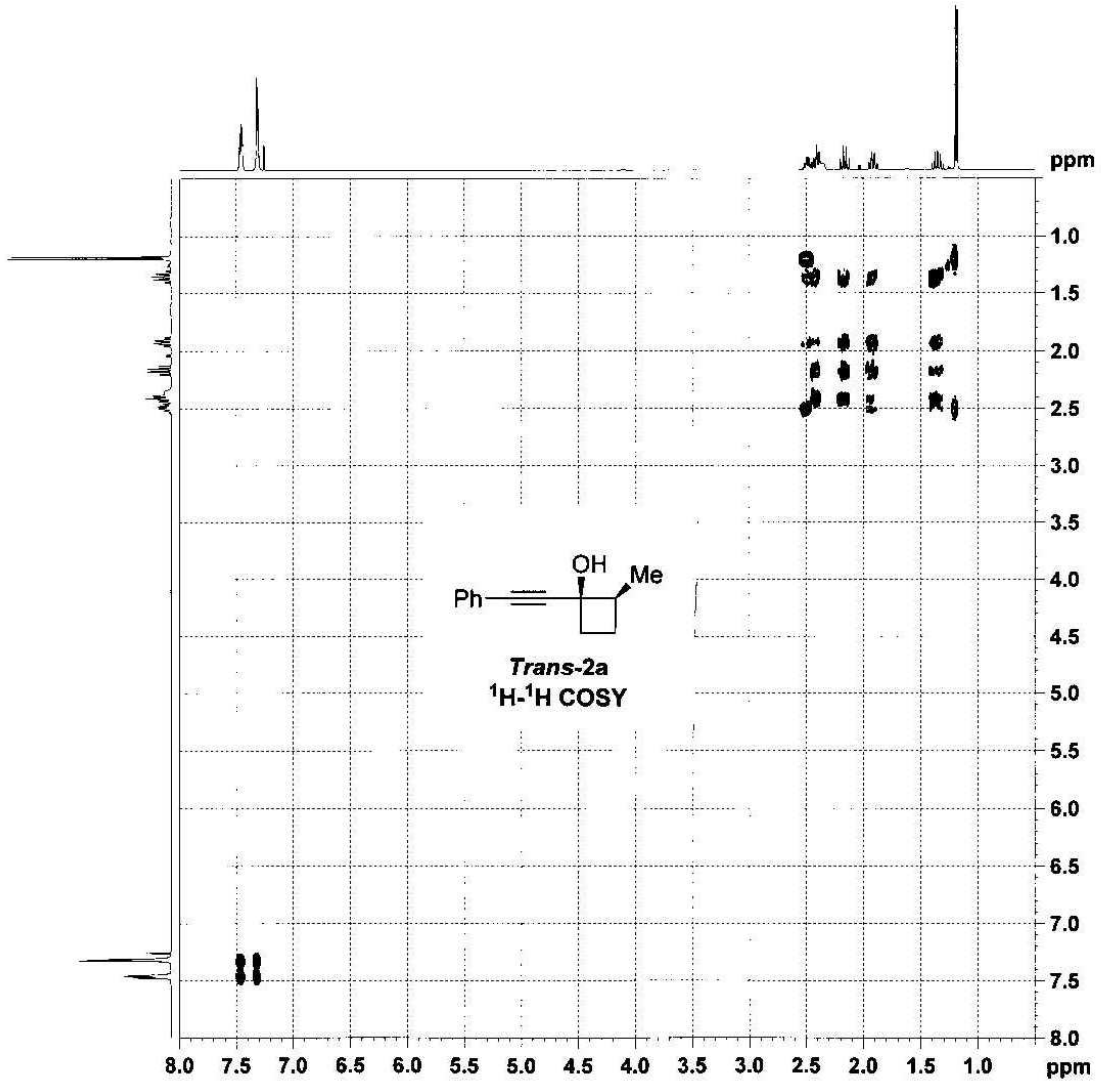

131.768
128.246
122.741
89.758
86.280
77.420
77.000
76.571
72.566
43.968
35.998
20.027
16.144
DFILE D:\焦\CAI-4 93 2 C.als
OBNUC 13C
EXMOD BCM
OFR 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 220
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRN
CTEMP 21.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Me
Ph
Trans-2a
PPM
200
175
150
125
100
75
50
25
0




```
DFILE   D:\集门\CAJ-4-93-2 C.als
OBNUC   13C
EXMOD   BCM
OFR          75.45 MHz
OBSET       124.00 KHz
OBFIN       1810.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS          220
ACQTM        1.606 sec
PD           1.394 sec
PW1            4.2 us
IRN
CTEMP         21.2 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             2.00 Hz
RGAIN            25
```

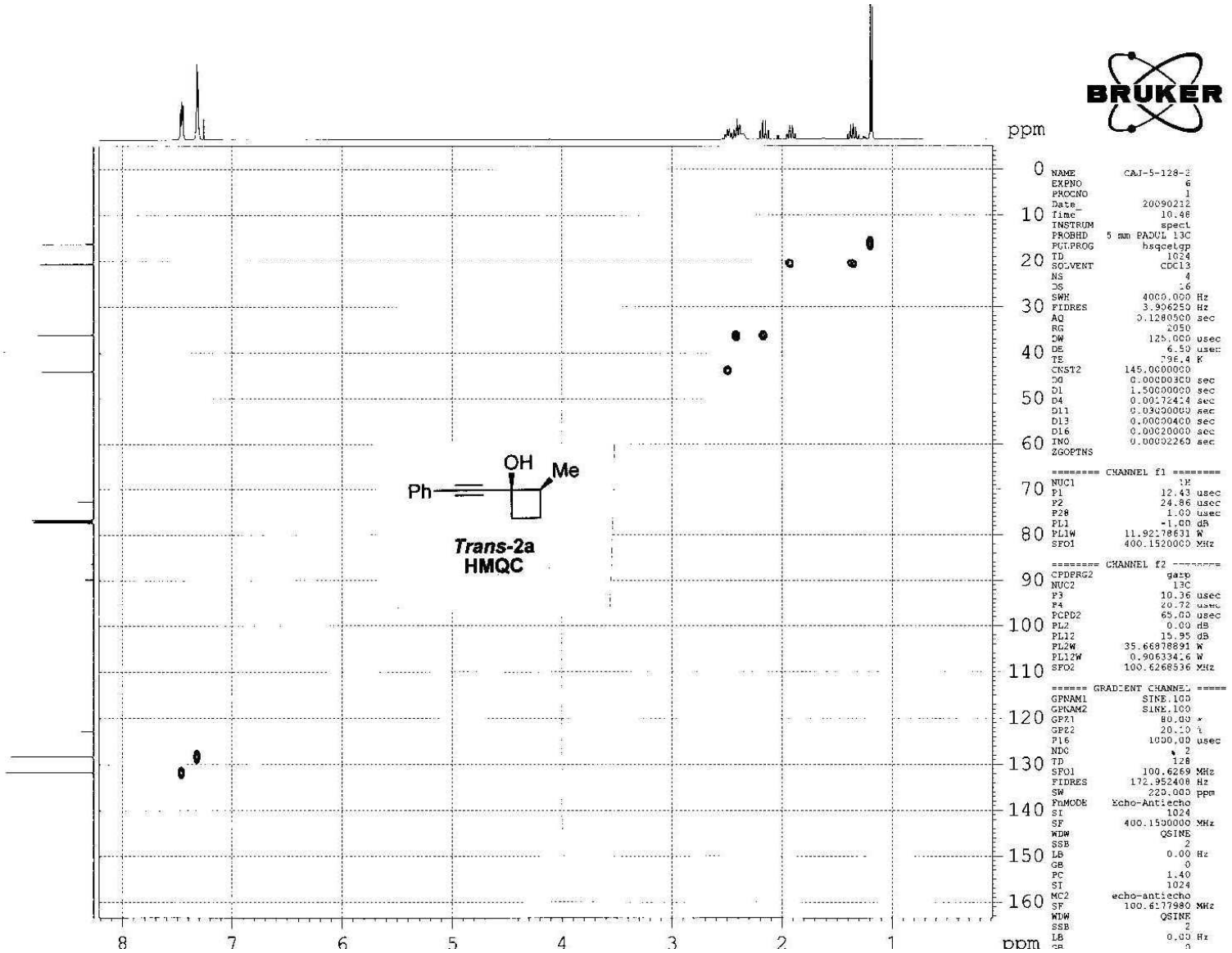


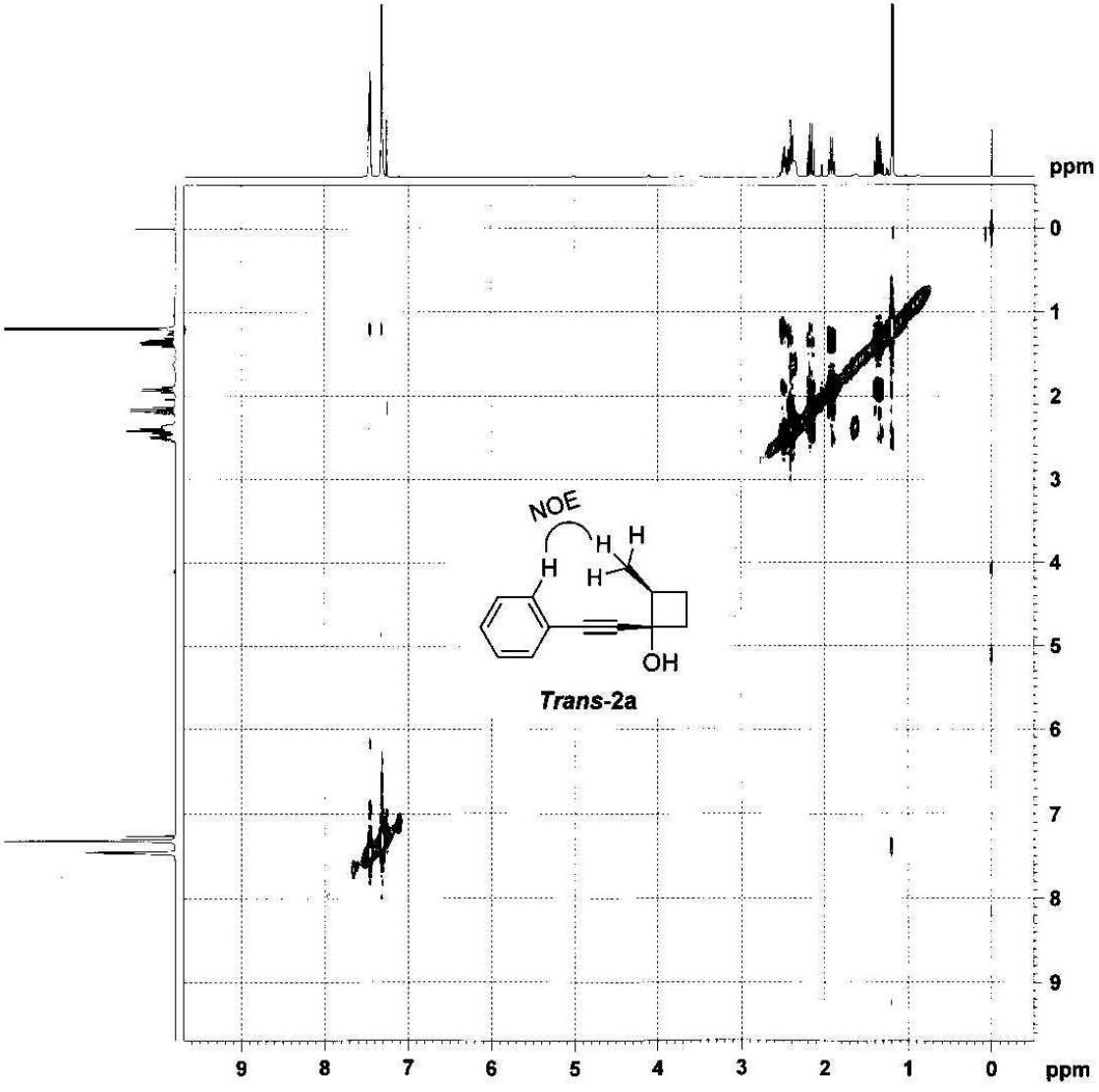
***Trans*-2a**
DEPT



BRUKER

NAME	CAJ-5-128-2	
EXPNO	4	
PROCNO	1	
Date_	20090212	
Time	10.28	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	cosygpmfqf	
TD	2048	
SOLVENT	CDCl3	
NS	4	
DS	16	
SWH	4000.000	Hz
FIDRES	1.953125	Hz
AQ	0.2560500	sec
RG	2050	
DW	125.000	usec
DE	6.50	usec
TE	296.7	K
D0	0.00000300	sec
D1	2.00000000	sec
D13	0.00000400	sec
D16	0.00020000	sec
IN0	0.00024990	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	12.43	usec
PL1	-1.00	dB
PL1W	11.92178631	W
SFO1	400.1520000	MHz
====== GRADIENT CHANNEL =====		
GPNAM1	SINE.100	
GPNAM2	SINE.100	
GPNAM3	SINE.100	
GPZ1	16.00	%
GPZ2	12.00	%
GPZ3	40.00	%
P16	1000.00	usec
ND0	1	
TD	128	
SFO1	400.152	MHz
FIDRES	31.261875	Hz
SW	10.000	ppm
FnMODE	QF	
SI	1024	
SF	400.1500000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	
SI	1024	
MC2	QF	
SF	400.1500000	MHz
WDW	SINE	
SSB	0	

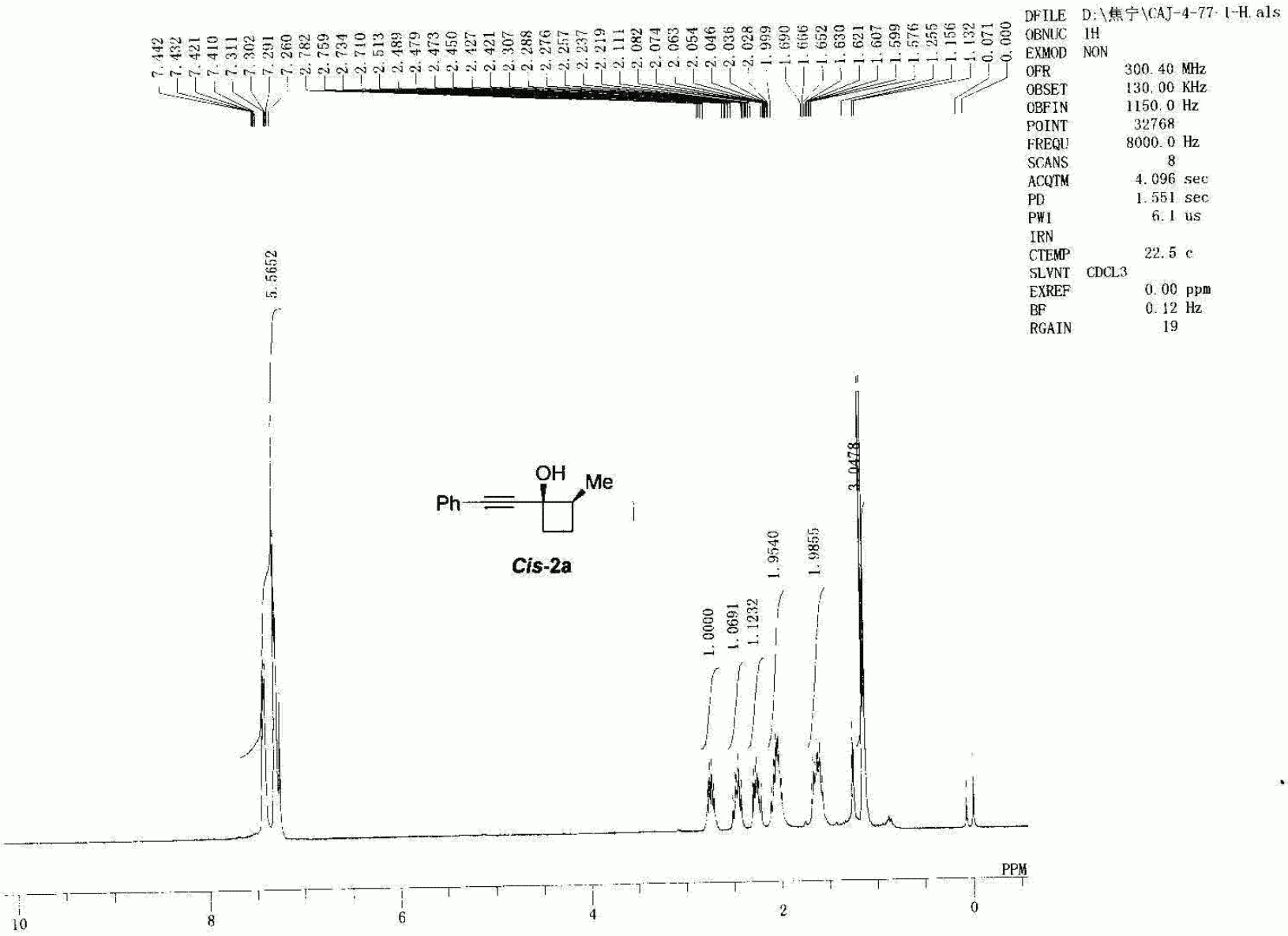

BRUKER
ppm
OH
Me
Ph
Trans-2a
HMQC
8
7
6
5
4
3
2
1
ppm
NAME CAJ-5-128-2
EXPNO 6
PROCNO 1
Date_ 20090212
Time 10.46
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4000.000 Hz
FIDRES 3.906250 Hz
AQ 0.1280500 sec
RG 2050
DW 125.000 usec
DE 6.50 usec
TE 296.4 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00002250 sec
ZGOPTNS
======== CHANNEL f1 ========
NUC1 1H
P1 12.43 usec
P2 24.86 usec
P28 1.00 usec
PL1 -1.00 dB
PL1W 11.92178631 W
SFO1 400.1520000 MHz
======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 10.36 usec
P4 20.72 usec
PCPD2 65.00 usec
PL2 0.00 dB
PL12 15.95 dB
PL2W 35.66878891 W
PL12W 0.90633416 W
SFO2 100.6268536 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
NDO 2
TD 128
SFO1 100.6269 MHz
FIDRES 172.952408 Hz
SW 220.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1500000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 100.6177980 MHz
WDW QSINE
SSB 2
LB 0.00 Hz

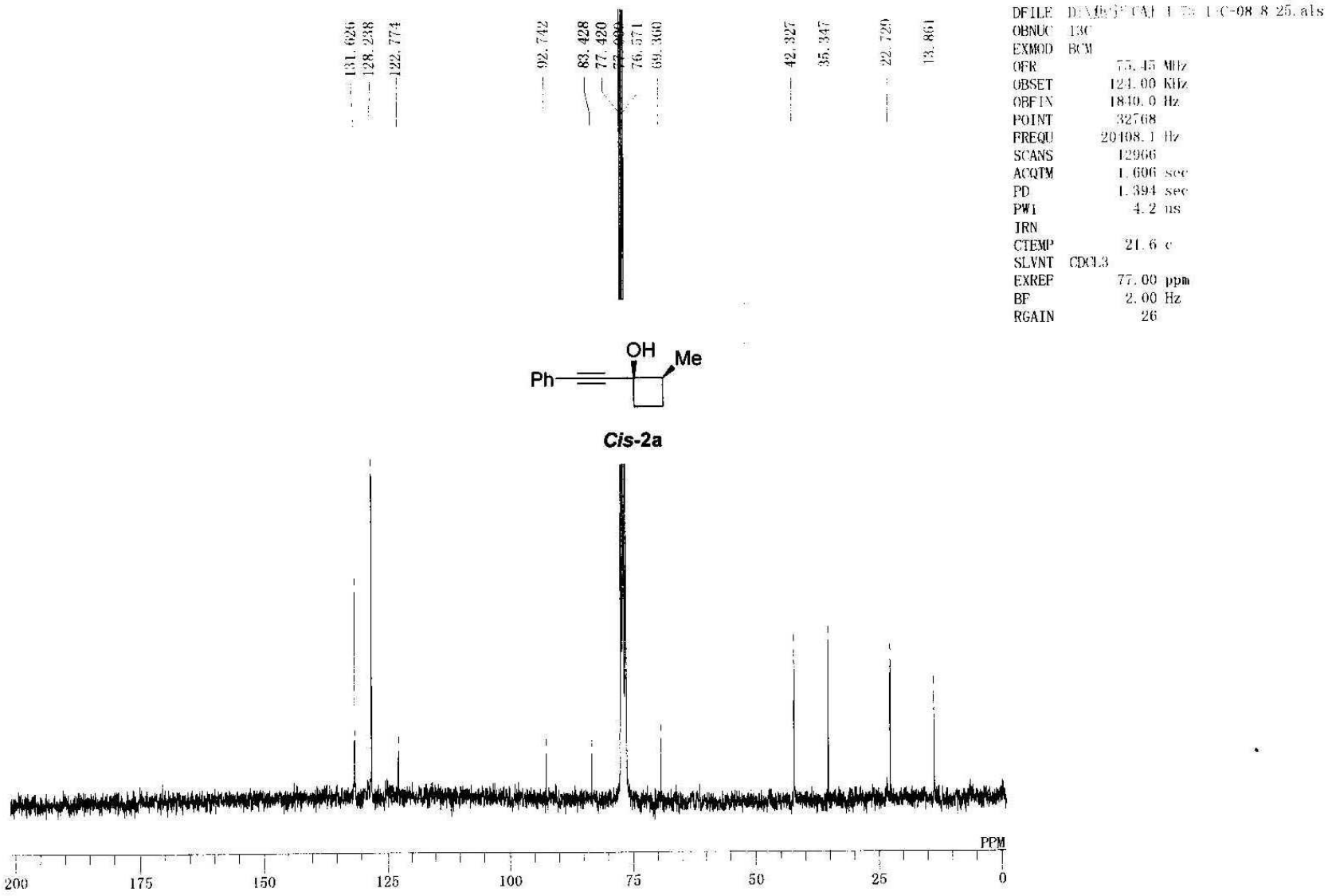


Trans-2a

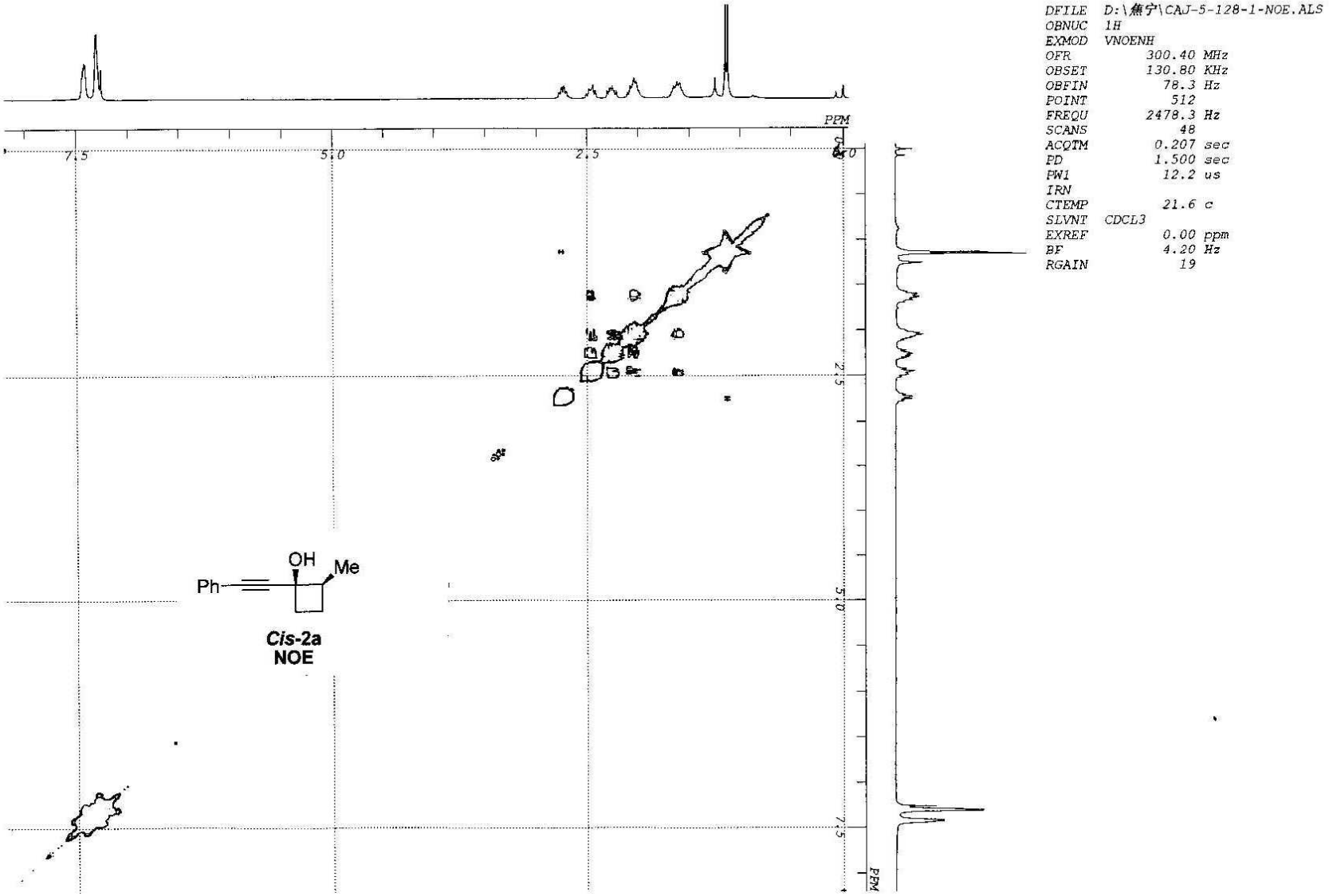
BRUKER

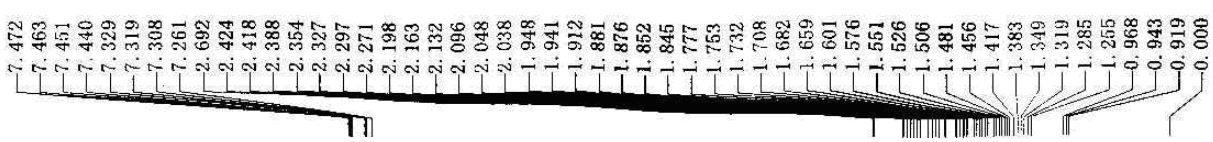
NAME	CAJ-5-128-2	
EXPNO	51	
PROCNO	1	
Date_	20090212	
Time	16.11	
INSTRUM	spect	
PROBHD	5 mm PADUL 13C	
PULPROG	noesyph	
TD	2048	
SOLVENT	CDC13	
NS	160	
DS	16	
SWH	4084.967	Hz
FIDRES	1.994613	Hz
AQ	0.2507252	sec
RG	128	
DW	122.400	usec
DE	6.50	usec
TE	295.9	K
D0	0.00010657	sec
D1	1.00000000	sec
D8	0.69999999	sec
IN0	0.00024480	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	12.43	usec
PL1	-1.00	dB
PL1W	11.92178631	W
SFO1	400.1518420	MHz
ND0	1	
TD	128	
SFO1	400.1518	MHz
FIDRES	31.915401	Hz
SW	10.209	ppm
FnMODE	States-TPPI	
SI	1024	
SF	400.1500049	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	1024	
MC2	States-TPPI	
SF	400.1500044	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	


7.442
7.432
7.421
7.410
7.311
7.302
7.291
7.260
2.782
2.759
2.734
2.710
2.513
2.489
2.479
2.473
2.450
2.427
2.421
2.307
2.288
2.276
2.257
2.237
2.219
2.111
2.082
2.074
2.063
2.054
2.046
2.036
2.028
1.999
1.690
1.666
1.652
1.630
1.621
1.607
1.599
1.576
1.255
1.156
1.132
0.071
0.000
DFILE D:\焦宁\CAJ-4-77-1-H.als
OBNUC 1H
EXMOD NON
OFR 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRN
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19
5.5652
OH
Me
Ph
Cis-2a
1.0000
1.0691
1.1232
1.9540
1.9855
3.0478
PPM
10
8
6
4
2
0

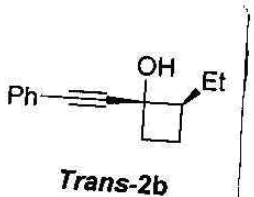

131.626
128.238
122.774
92.742
83.428
77.420
76.571
69.360
42.327
35.347
22.729
13.861
DFILE D:\fb\FCA\1-75-1\C-08_8_25.als
OBNUC 13C
EXMOD BCM
OFR 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 12966
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRN
CTEMP 21.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 26
OH
Me
Ph
PPM
200
175
150
125
100
75
50
25
0

***Cis*-2a**

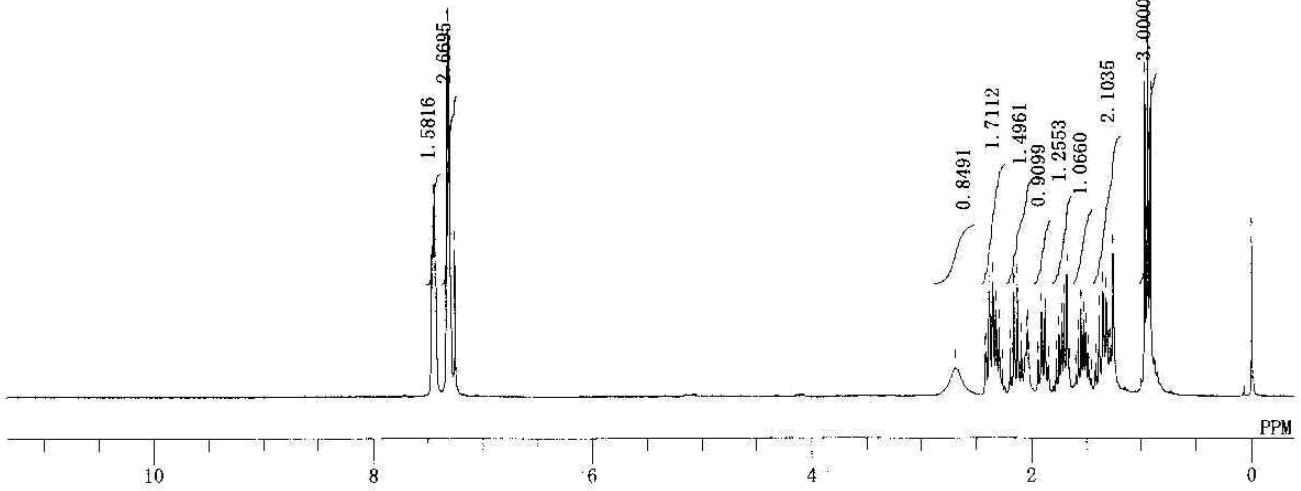

PPM
7.5
5.0
2.5
0.0
OH
Me
Ph
Cis-2a
NOE
DFILE D:\焦宁\CAJ-5-128-1-NOE.ALS
OBNUC 1H
EXMOD VNOENH
OFR 300.40 MHz
OBSET 130.80 KHz
OBFIN 78.3 Hz
POINT 512
FREQU 2478.3 Hz
SCANS 48
ACQTM 0.207 sec
PD 1.500 sec
PW1 12.2 us
IRN
CTEMP 21.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 4.20 Hz
RGAIN 19

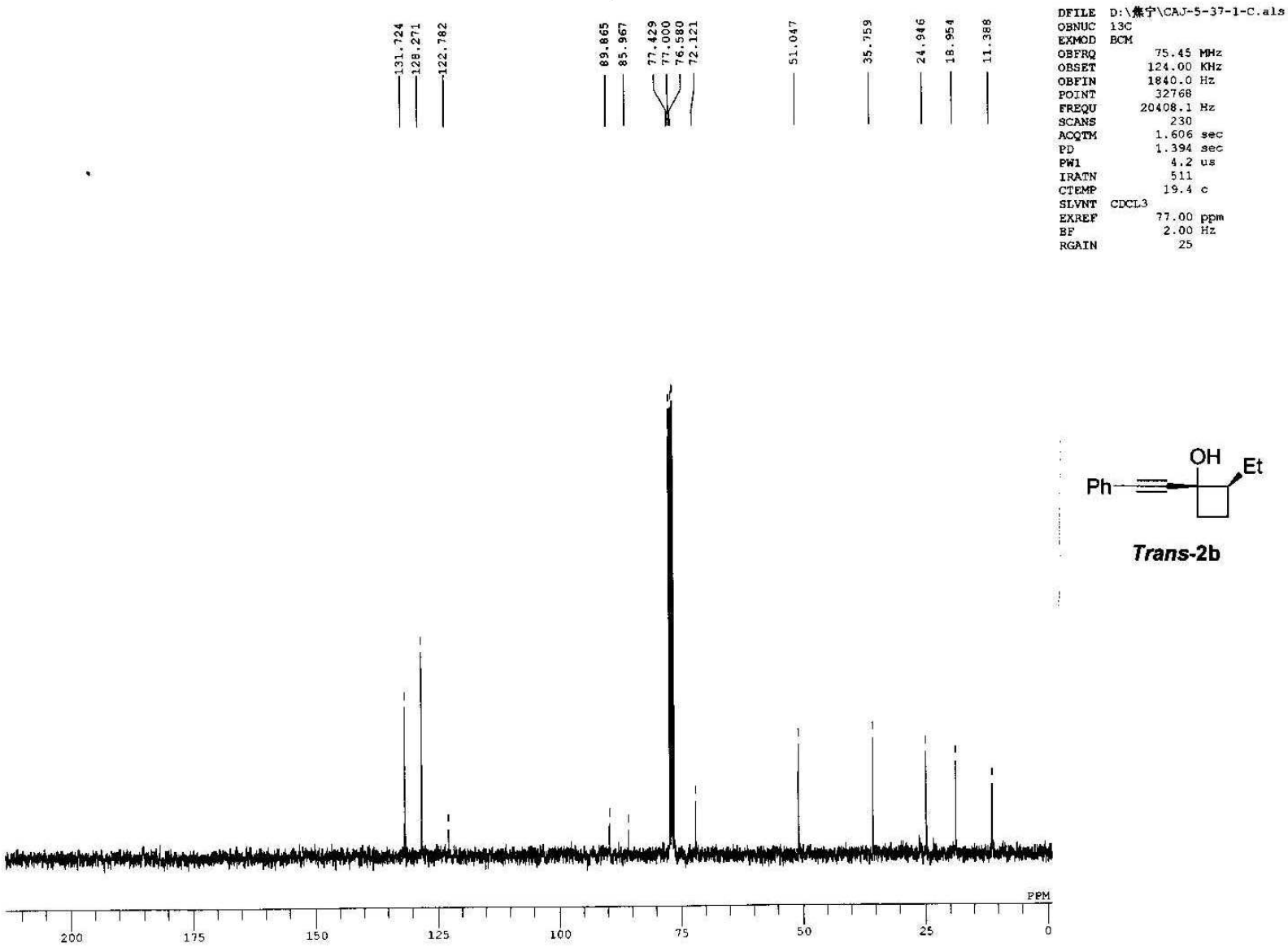


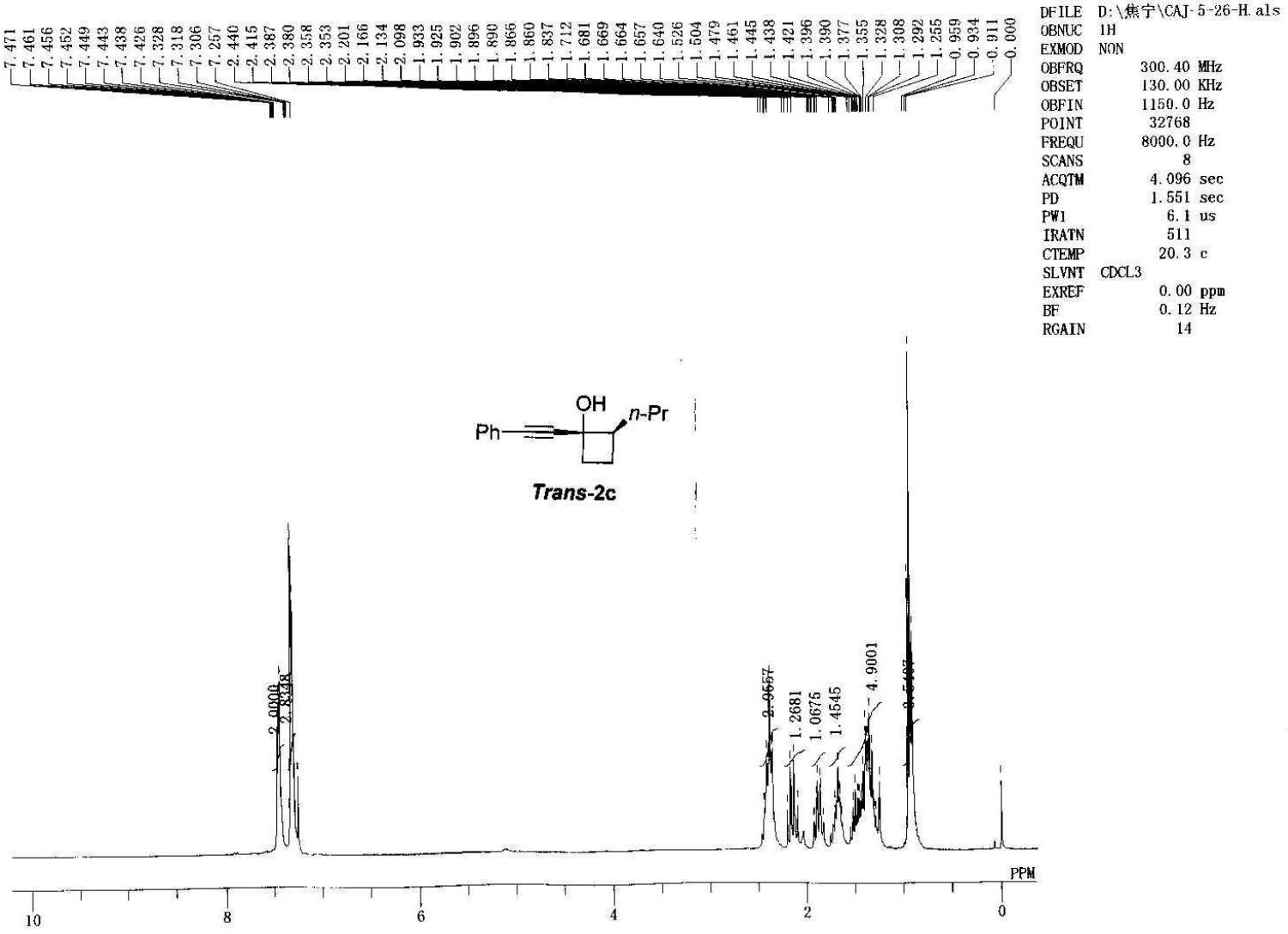
DFILE	D:\焦宁\CAJ-5-37-1-H.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	19.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	16

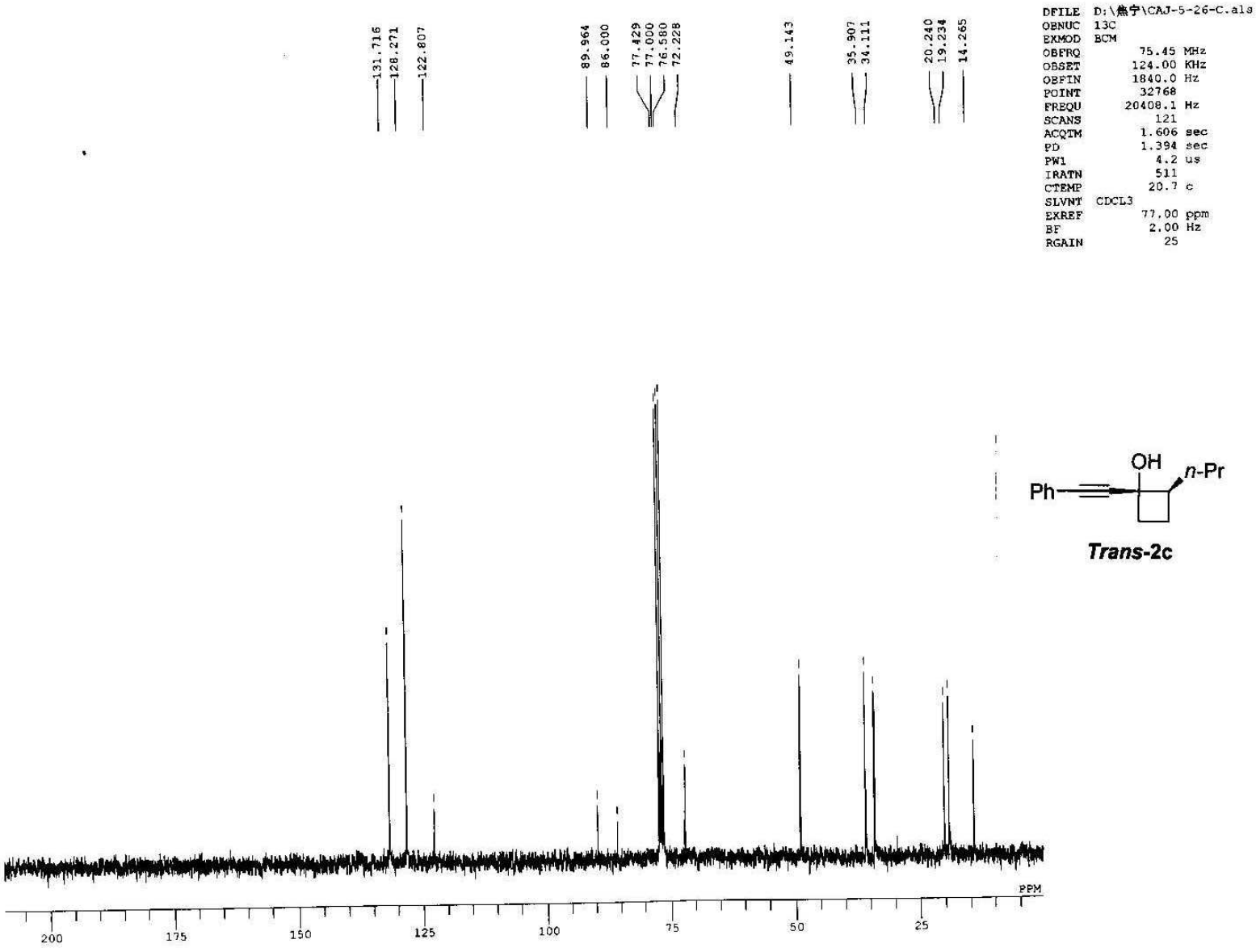


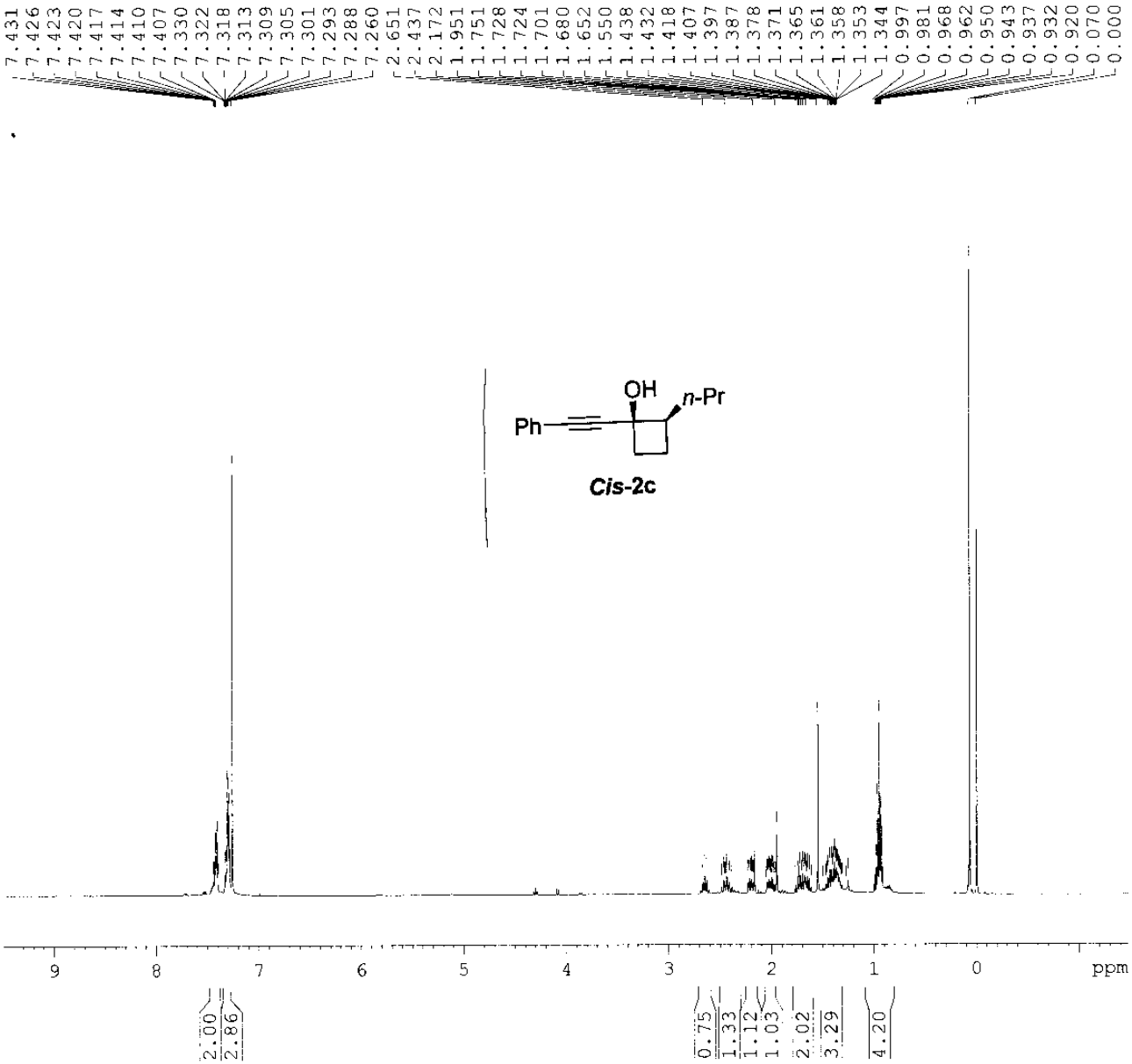
***Trans*-2b**



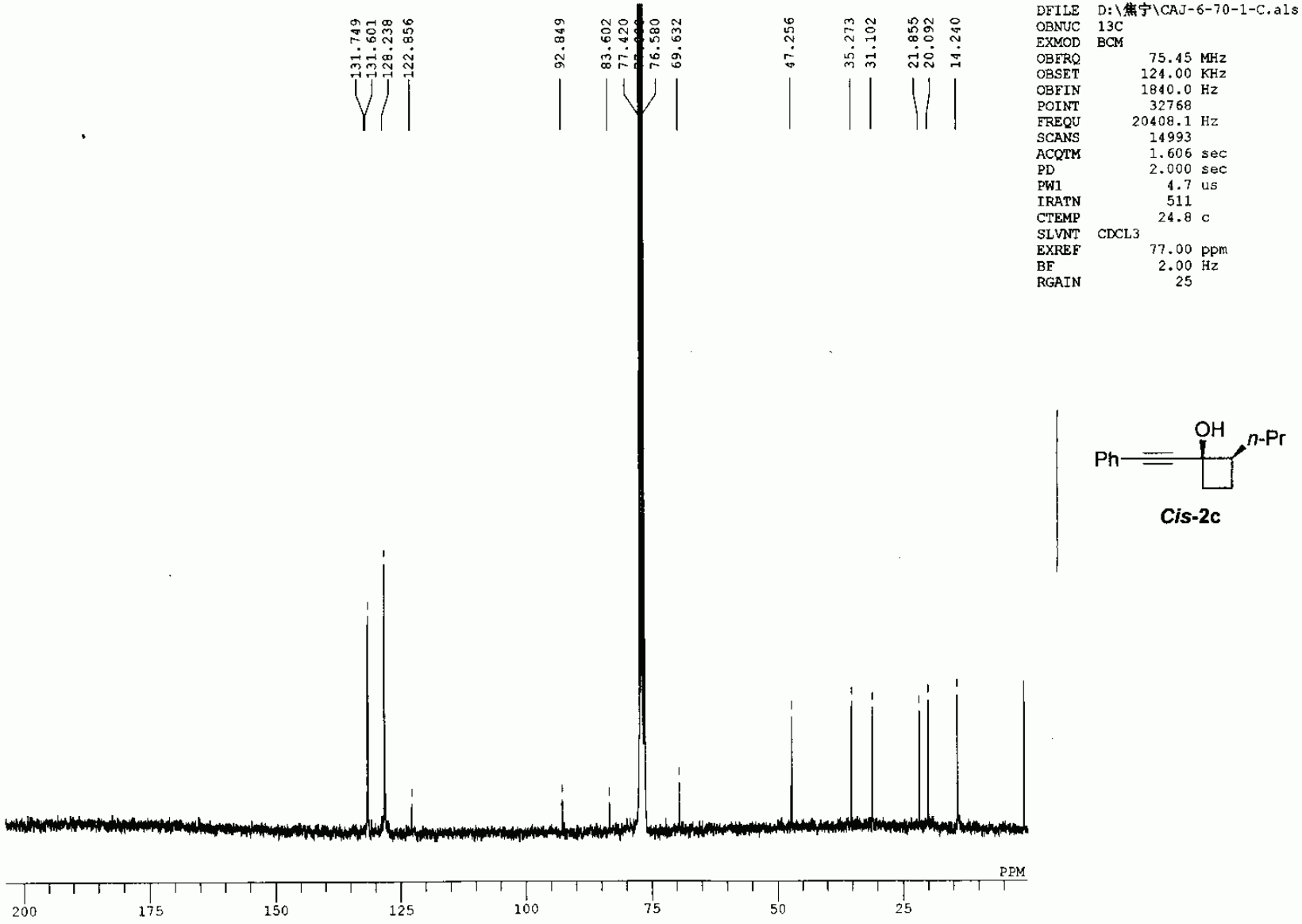

131.724
128.271
122.782
89.865
85.967
77.429
77.000
76.580
72.121
51.047
35.759
24.946
18.954
11.388
DFILE D:\米宁\CAJ-5-37-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 230
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 19.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Et
Ph
Trans-2b
PPM
200
175
150
125
100
75
50
25
0

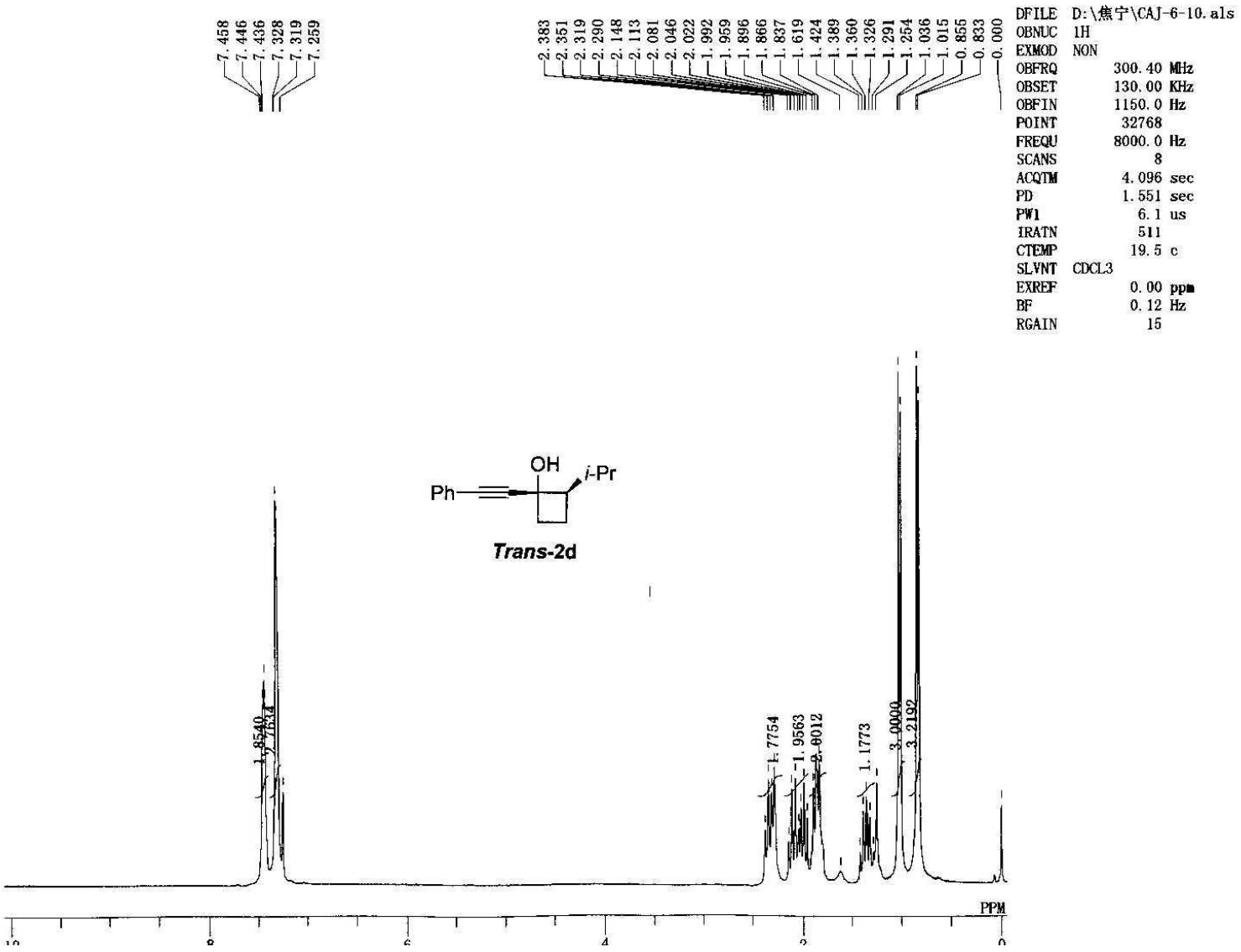

7.471
7.461
7.456
7.452
7.449
7.443
7.438
7.426
7.328
7.318
7.306
7.257
2.440
2.415
2.387
2.380
2.358
2.353
2.201
2.166
2.134
2.098
1.933
1.925
1.902
1.896
1.890
1.866
1.860
1.837
1.712
1.681
1.669
1.664
1.657
1.640
1.526
1.504
1.479
1.461
1.445
1.438
1.421
1.396
1.390
1.377
1.355
1.328
1.308
1.292
1.255
0.959
0.934
0.911
0.000
DFILE D:\焦宁\CAJ-5-26-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
OH
n-Pr
Ph
Trans-2c
2.0000
2.8348
2.9657
1.2681
1.0675
1.4545
4.9001
3.5487
PPM
10
8
6
4
2
0

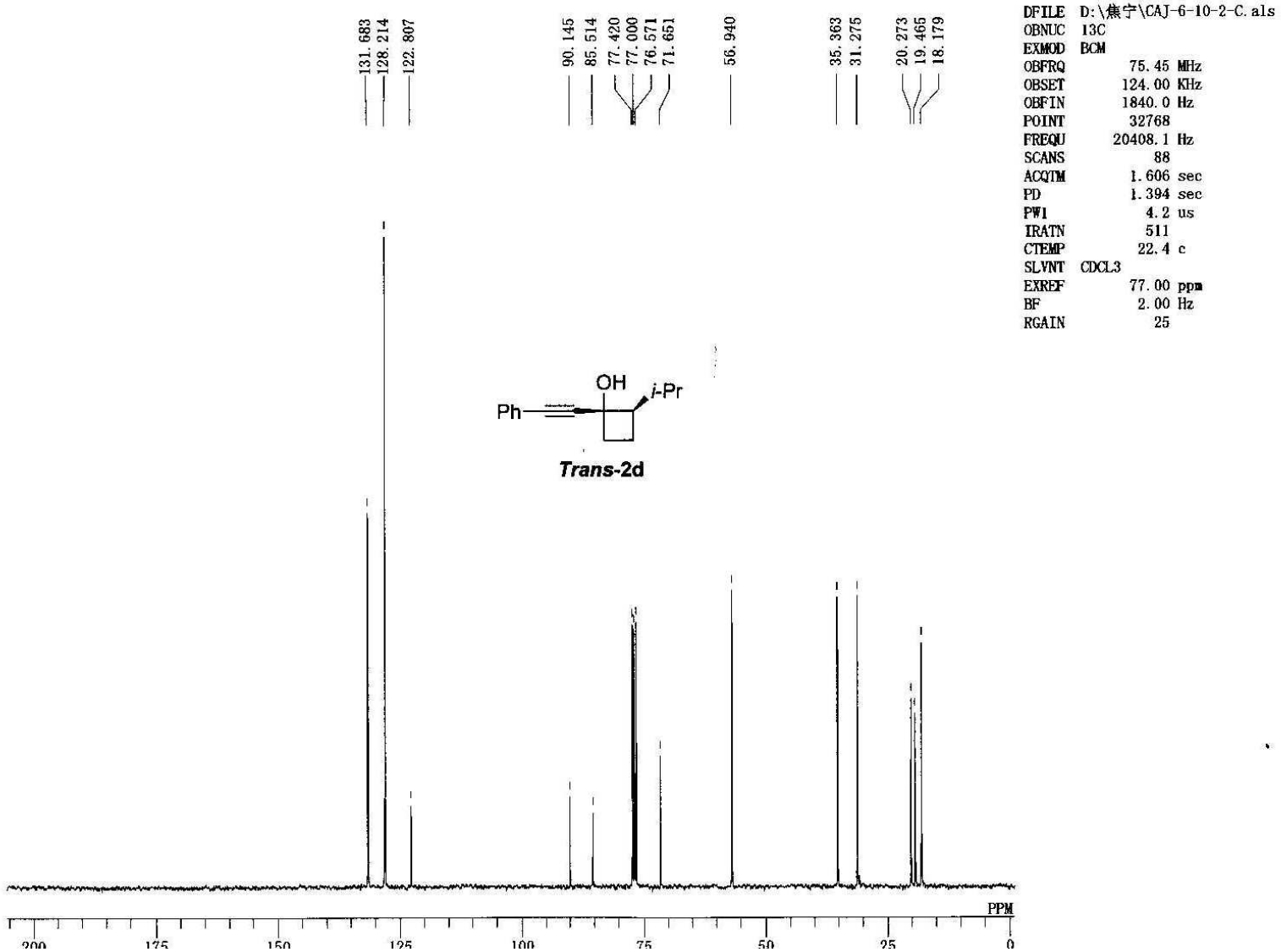

131.716
128.271
122.807
89.964
86.000
77.429
77.000
76.580
72.228
49.143
35.907
34.111
20.240
19.234
14.265
DFILE D:\焦宁\CAJ-5-26-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 121
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
n-Pr
Ph
Trans-2c
PPM
200
175
150
125
100
75
50
25

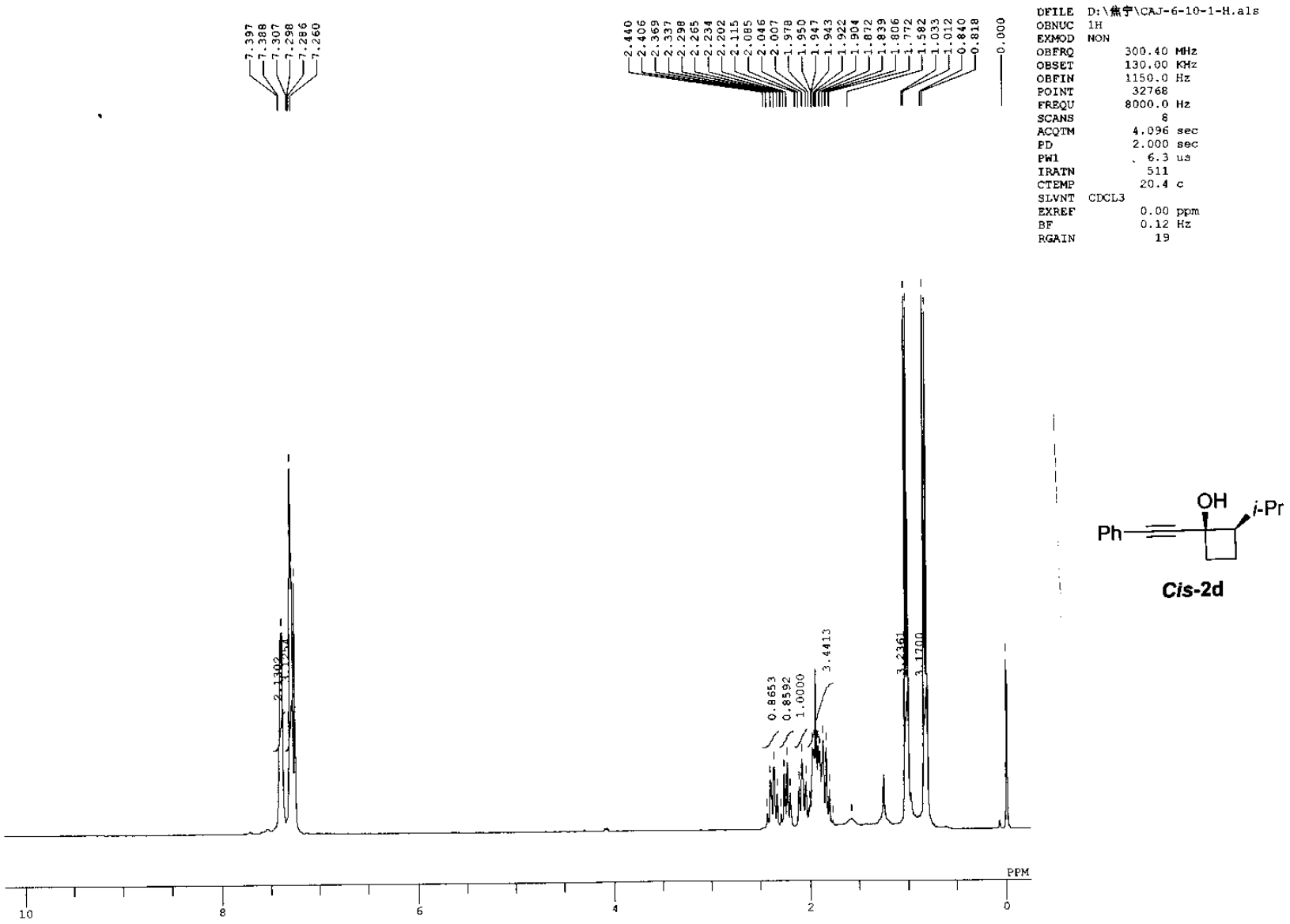


NAME	CAJ-6-70-1
EXPNO	1
PROCNO	1
Date_	20090428
Time	11.06
INSTRUM	spect
PROBHD	5 mm PADUL 13C
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	362
DW	60.800 usec
DE	6.50 usec
TE	293.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.16 usec
PL1	0.00 dB
PL1W	9.46981144 W
SFO1	400.1524711 MHz
SI	32768
SF	400.1500037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



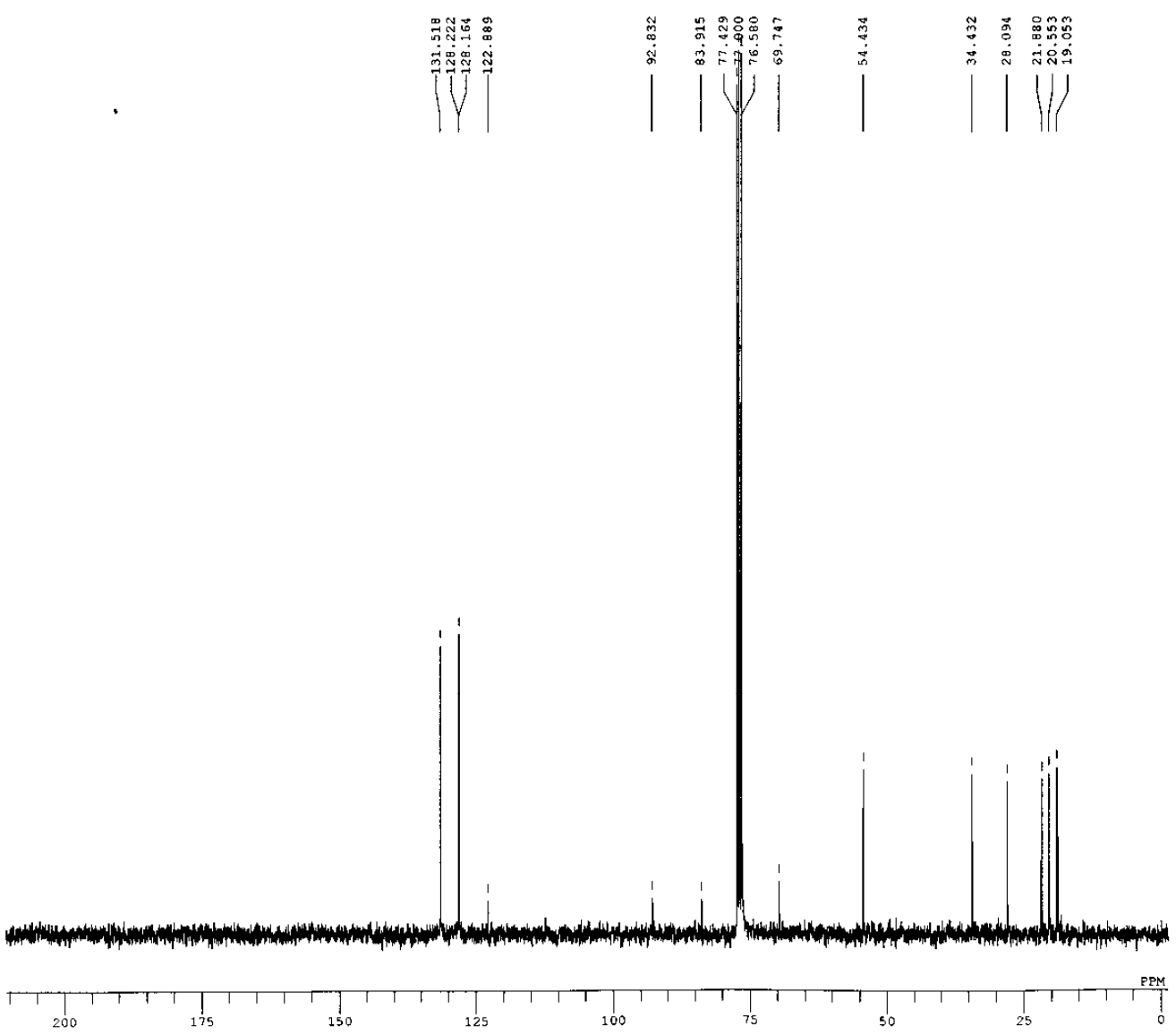

7.458
7.446
7.436
7.328
7.319
7.259
2.383
2.351
2.319
2.290
2.148
2.113
2.081
2.046
2.022
1.992
1.959
1.896
1.866
1.837
1.619
1.424
1.389
1.360
1.326
1.291
1.254
1.036
1.015
0.855
0.833
0.000
DFILE D:\焦宁\CAJ-6-10.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
OH
i-Pr
Ph
Trans-2d
1.8540
1.7754
1.9563
2.0012
1.1773
3.0000
3.2192
PPM


131.683
128.214
122.807
90.145
85.514
77.420
77.000
76.571
71.651
56.940
35.363
31.275
20.273
19.465
18.179
DFILE D:\焦宁\CAJ-6-10-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 88
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
i-Pr
Ph
Trans-2d
PPM
200
175
150
125
100
75
50
25
0

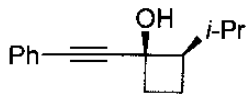

7.397
7.388
7.307
7.298
7.286
7.260
2.440
2.406
2.369
2.337
2.298
2.265
2.234
2.202
2.115
2.085
2.046
2.007
1.978
1.950
1.947
1.943
1.922
1.904
1.872
1.839
1.806
1.772
1.582
1.033
1.012
0.840
0.818
0.000
DFILE D:\焦宁\CAJ-6-10-1-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 2.000 sec
PW1 6.3 us
IRATN 511
CTEMP 20.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19
0.8653
0.8592
1.0000
3.4413
3.2361
3.1700
PPM
10
8
6
4
2
0

OH
i-Pr
Ph

***Cis*-2d**

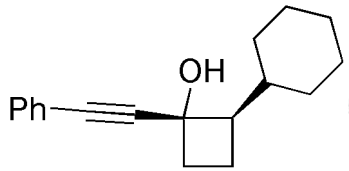



```
DFILE   D:\焦宁\CAJ-6-10-1-C.als
OBNUC   13C
EXMOD   BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU      20408.1 Hz
SCANS          464
ACQTM         1.606 sec
PD            2.000 sec
PW1             4.7 us
IRATN           511
CTEMP          20.5 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             2.00 Hz
RGAIN            24
```

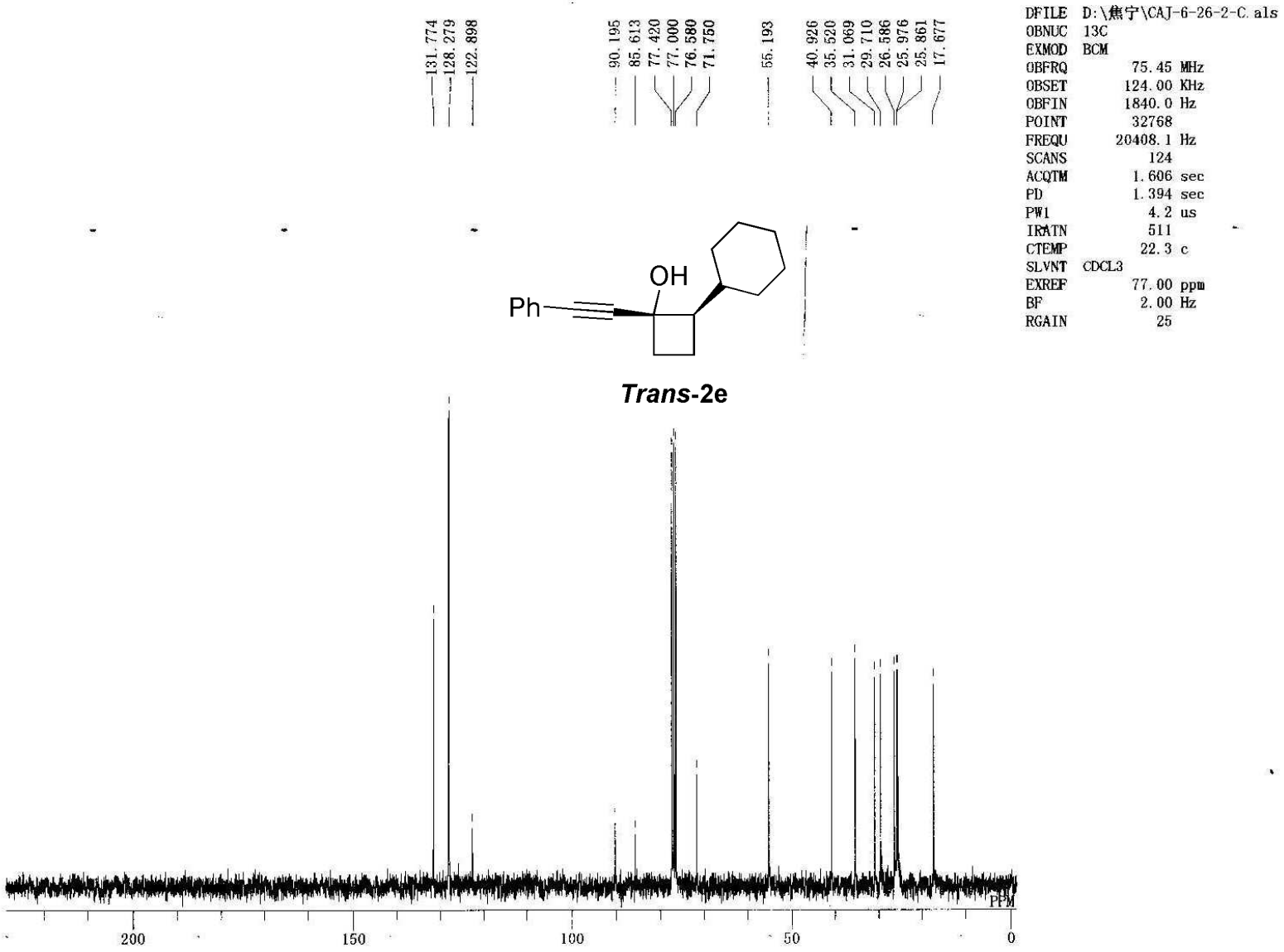


***Cis*-2d**

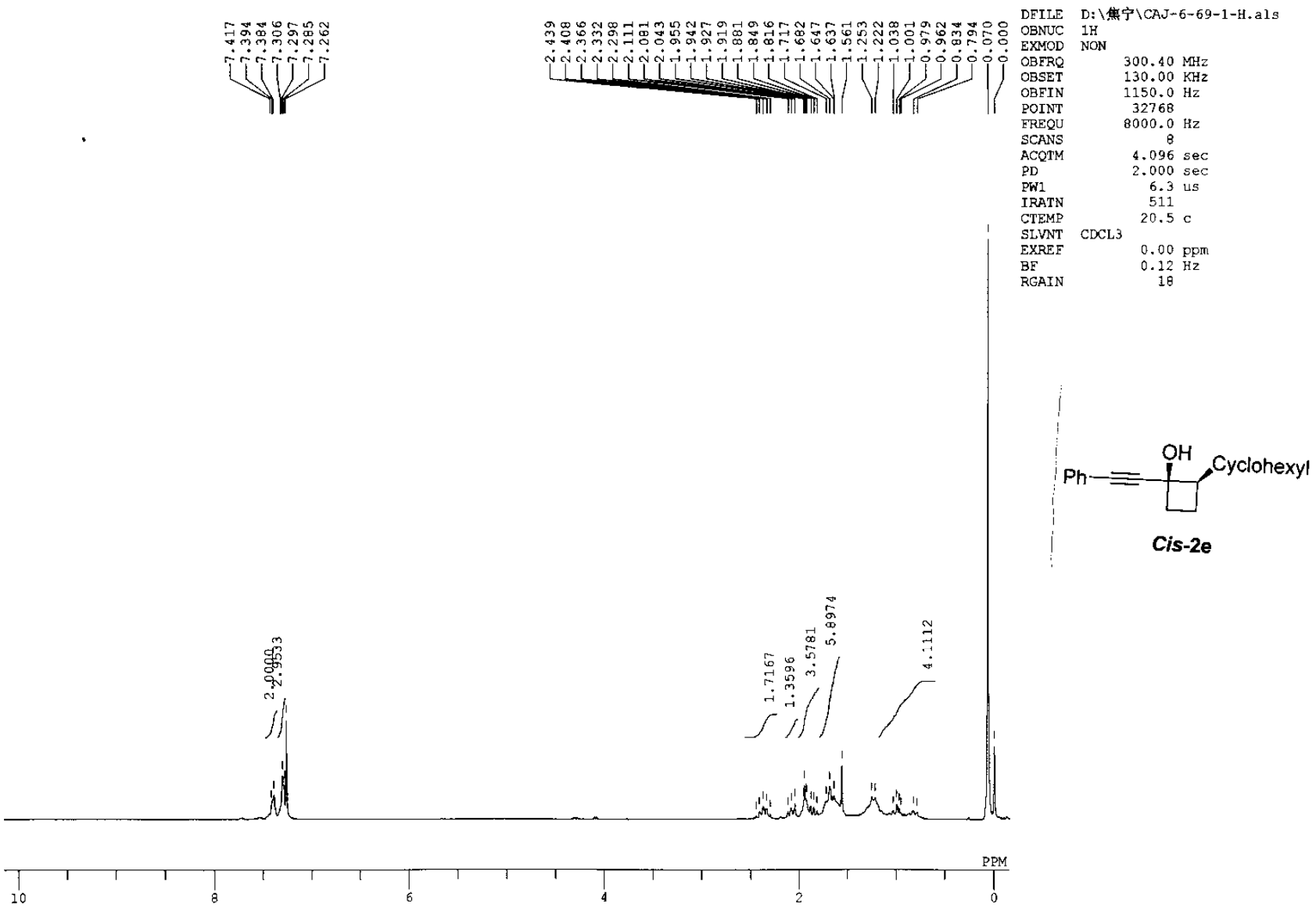
DFILE	D:\焦宁\CAJ-6-26-2.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	22.5 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	14

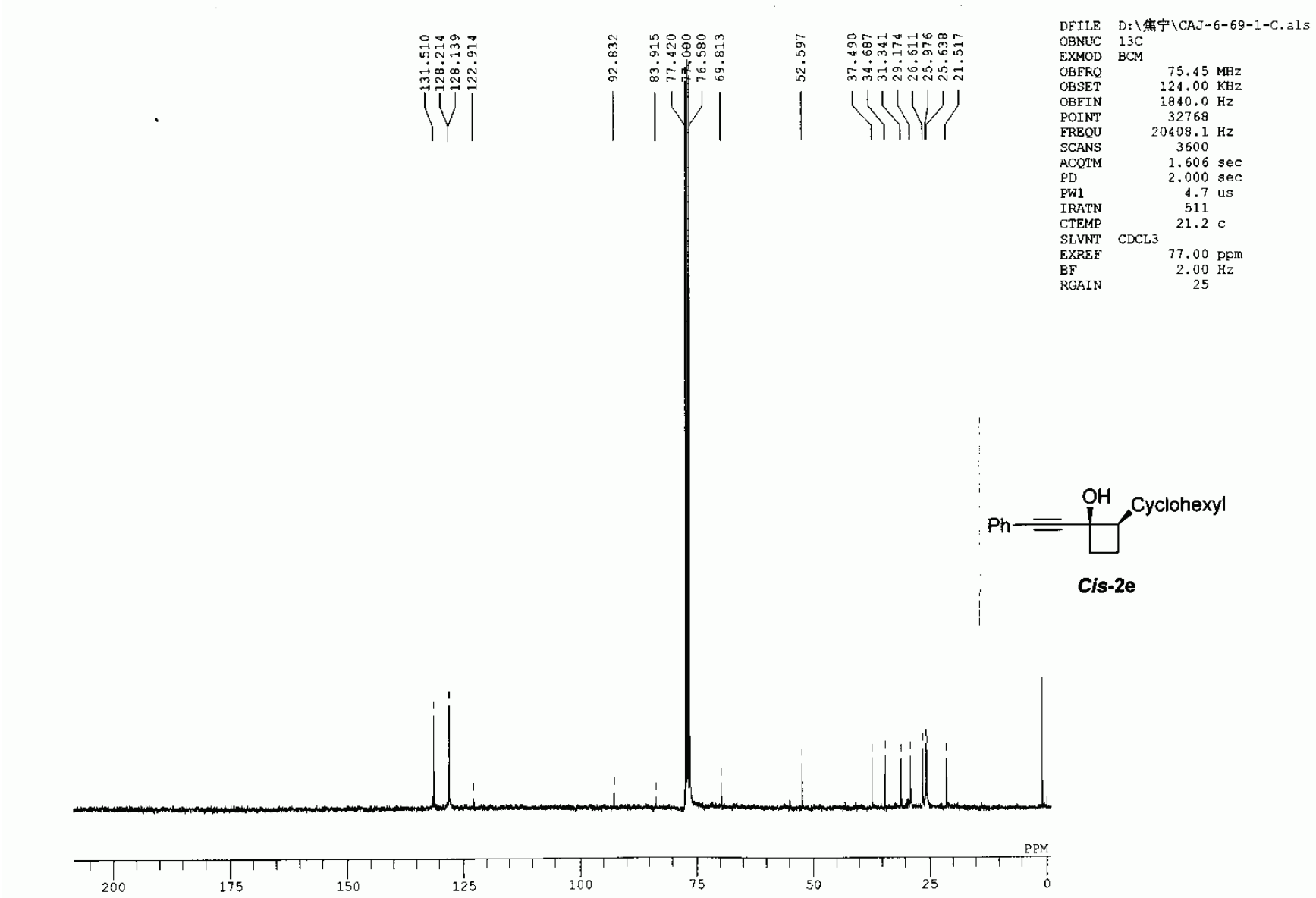


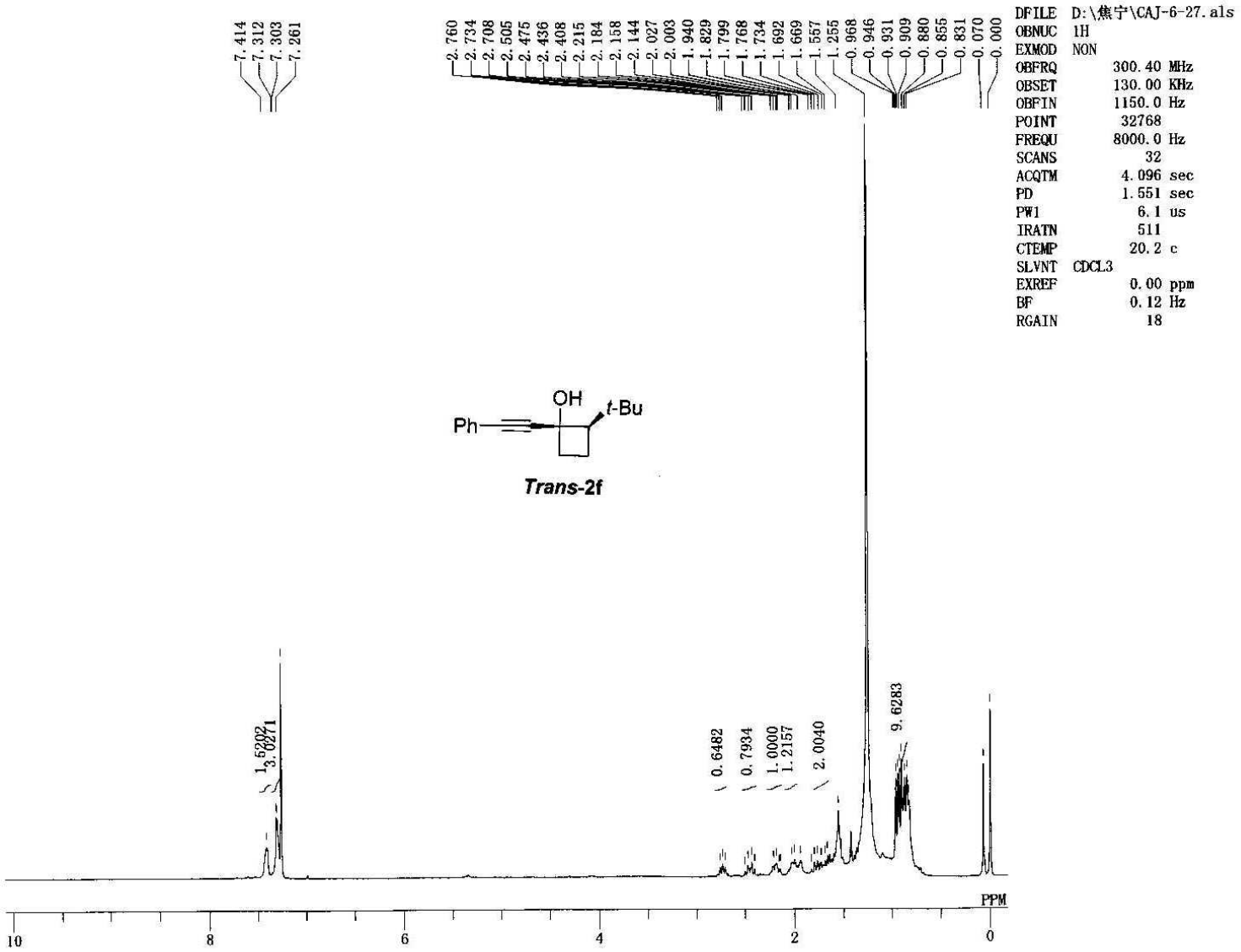
***Trans*-2e**

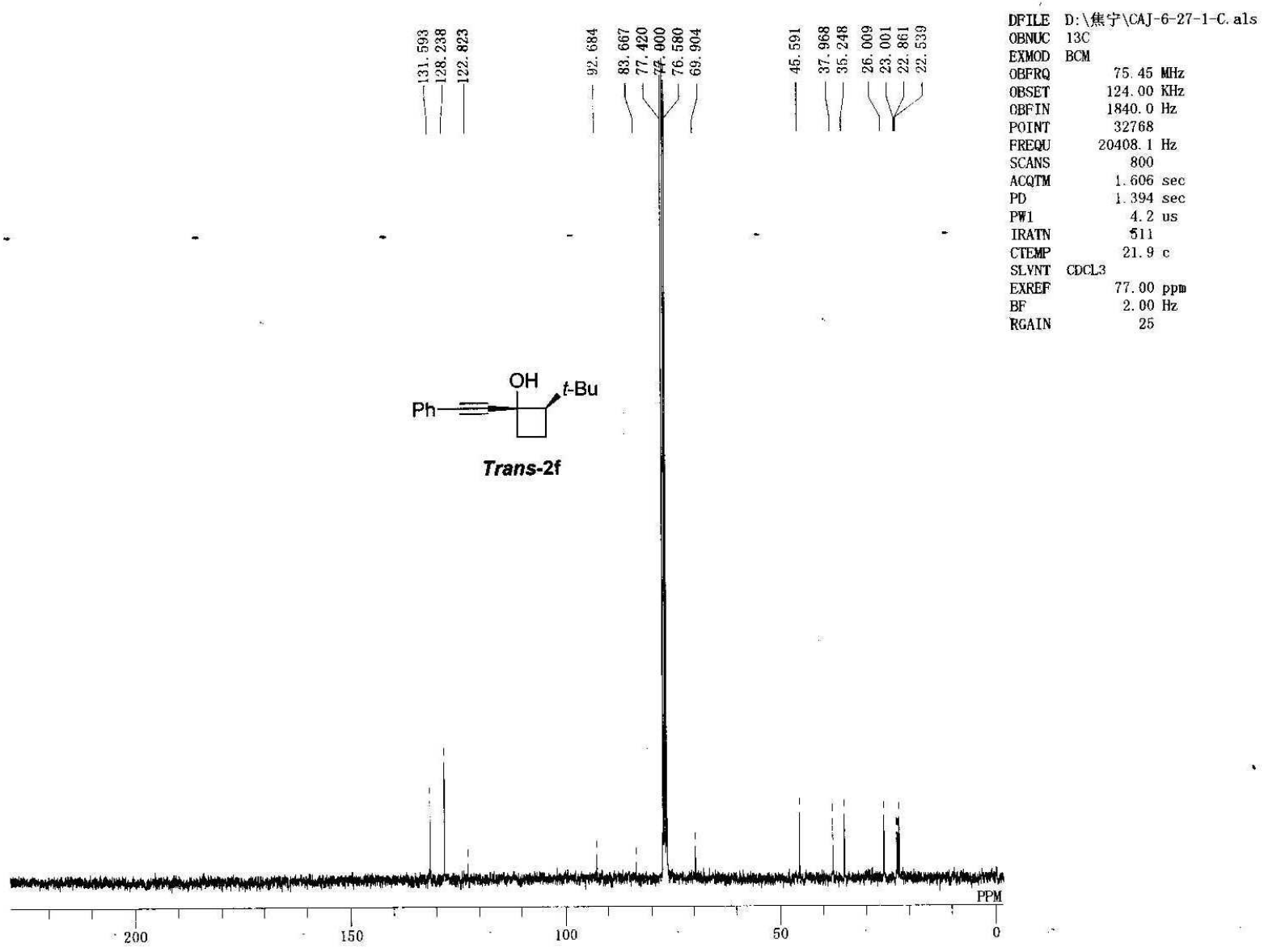

131.774
128.279
122.898
90.195
85.613
77.420
77.000
76.580
71.750
55.193
40.926
35.520
31.069
29.710
26.586
25.976
25.861
17.677
DFILE D:\焦宁\CAJ-6-26-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 124
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Ph
PPM
200
150
100
50
0

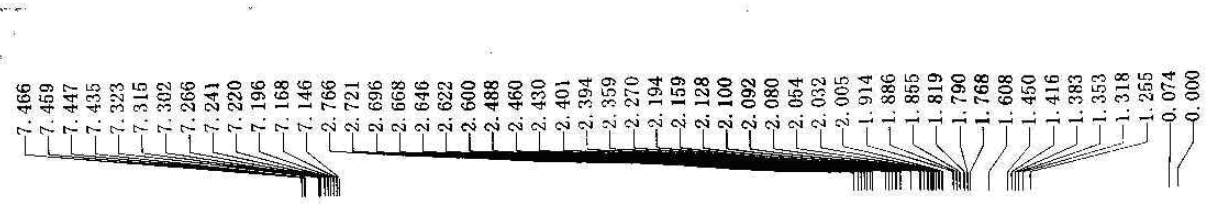
***Trans*-2e**


7.417
7.394
7.384
7.306
7.297
7.285
7.262
2.439
2.408
2.366
2.332
2.298
2.111
2.081
2.043
1.955
1.942
1.927
1.919
1.881
1.849
1.816
1.717
1.682
1.647
1.637
1.561
1.253
1.222
1.038
1.001
0.979
0.962
0.834
0.794
0.070
0.000
DFILE D:\焦宁\CAJ-6-69-1-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 2.000 sec
PW1 6.3 us
IRATN 511
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
2.0000
2.9533
1.7167
1.3596
3.5781
5.8974
4.1112
OH
Ph
Cyclohexyl
Cis-2e
PPM
10
8
6
4
2
0

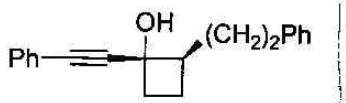

131.510
128.214
128.139
122.914
92.832
83.915
77.420
77.000
76.580
69.813
52.597
37.490
34.687
31.341
29.174
26.611
25.976
25.638
21.517
DFILE D:\焦宁\CAJ-6-69-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 3600
ACQTM 1.606 sec
PD 2.000 sec
PW1 4.7 us
IRATN 511
CTEMP 21.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Cyclohexyl
Ph
Cis-2e
PPM
200
175
150
125
100
75
50
25
0


7.414
7.312
7.303
7.261
2.760
2.734
2.708
2.505
2.475
2.436
2.408
2.215
2.184
2.158
2.144
2.027
2.003
1.940
1.829
1.799
1.768
1.734
1.692
1.669
1.557
1.255
0.968
0.946
0.931
0.909
0.880
0.856
0.831
0.070
0.000
DFILE D:\焦宁\CAJ-6-27.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 32
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
OH
t-Bu
Ph
Trans-2f
1.6202
3.0271
0.6482
0.7934
1.0000
1.2157
2.0040
9.6283
PPM
10
8
6
4
2
0

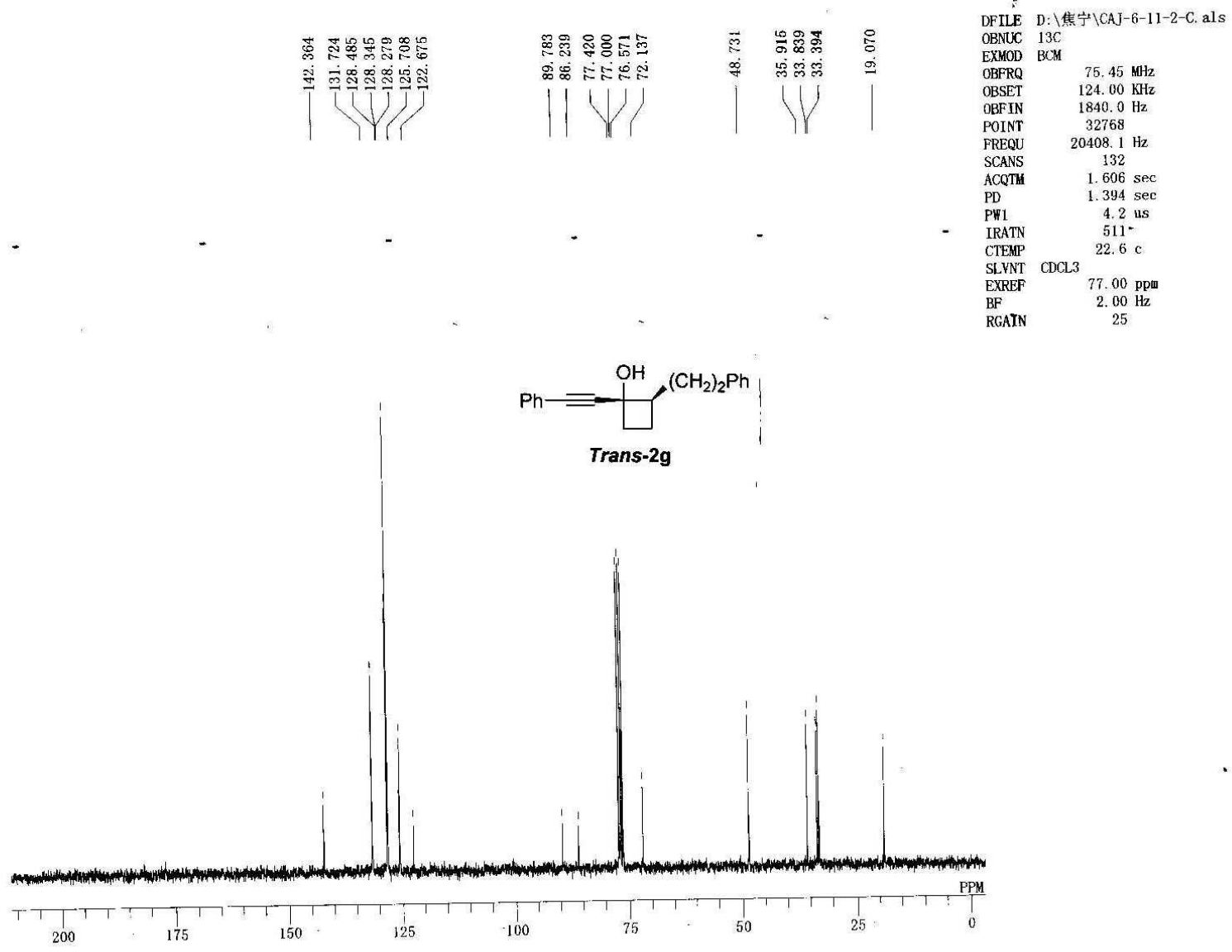

131.593
128.238
122.823
92.684
83.667
77.420
77.000
76.580
69.904
45.591
37.968
35.248
26.009
23.001
22.861
22.539
DFILE D:\焦宁\CAJ-6-27-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 800
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 21.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
t-Bu
Ph
Trans-2f
PPM
200
150
100
50
0

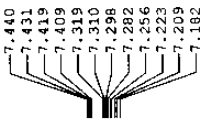


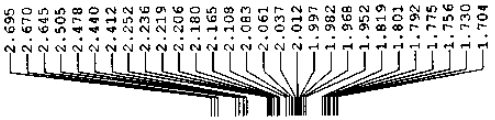
DFILE	D:\焦宁\CAJ-6-11-2.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	22.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	16



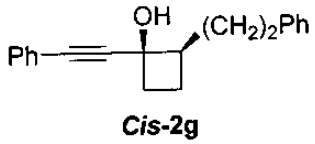
***Trans*-2g**


142.364
131.724
128.485
128.345
128.279
125.708
122.675
89.783
86.239
77.420
77.000
76.571
72.137
48.731
35.916
33.839
33.394
19.070
DFILE D:\焦宁\CAJ-6-11-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 132
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
(CH2)2Ph
Ph
Trans-2g
PPM
200
175
150
125
100
75
50
25
0

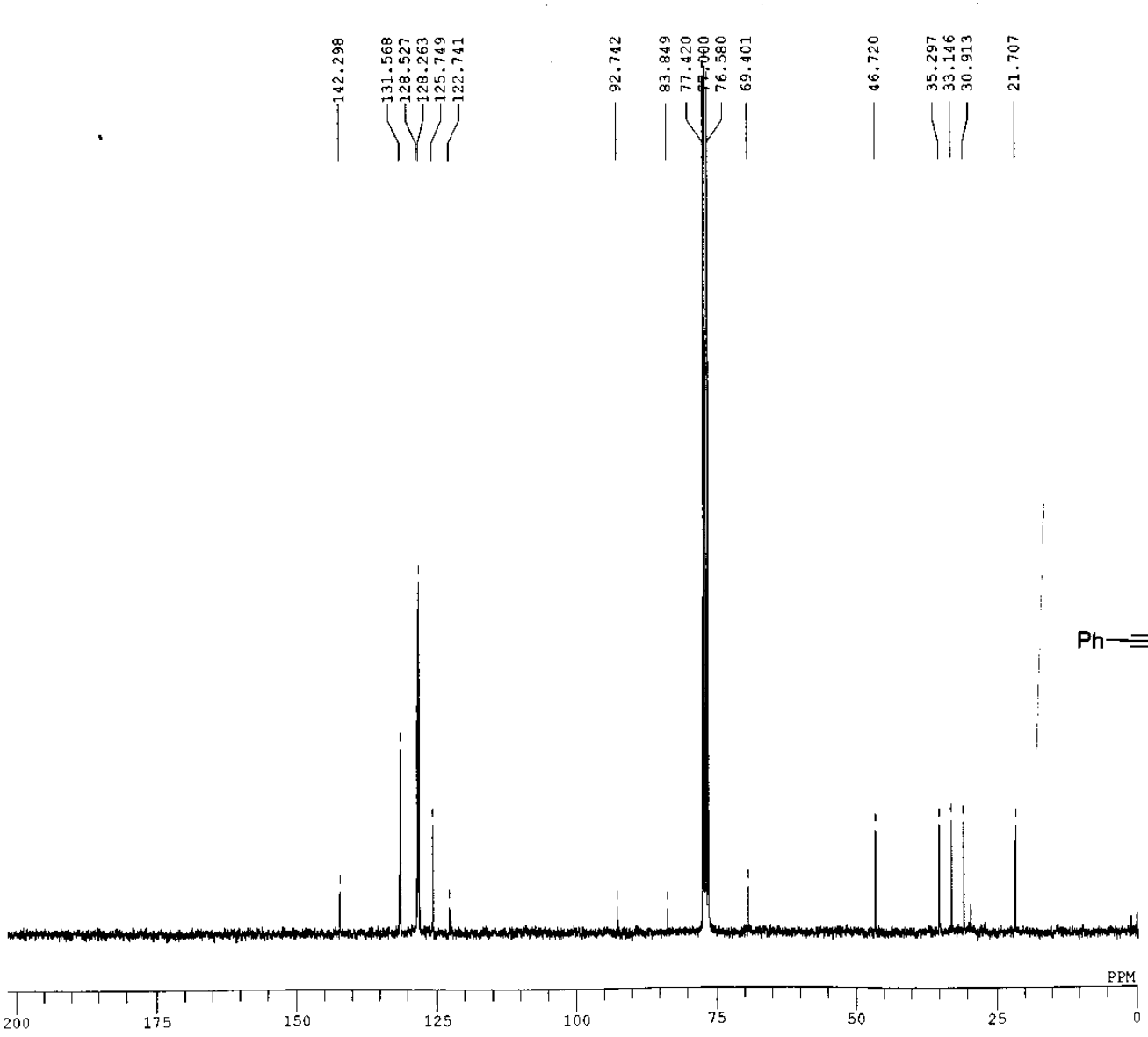




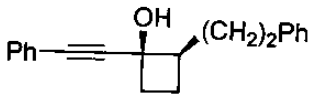

```
DFILE   D:\焦宁\CAJ-6-11-1-H.als
OBNUC   1H
EXMOD   NON
OBFRQ       300.40 MHz
OBSET       130.00 KHz
OBFIN       1150.0 Hz
POINT        32768
FREQU       8000.0 Hz
SCANS             8
ACQTM         4.096 sec
PD            2.000 sec
PW1             6.3 us
IRATN             511
CTEMP          20.5 c
SLVNT   CDCL3
EXREF         0.00 ppm
BF            0.12 Hz
RGAIN             18
```



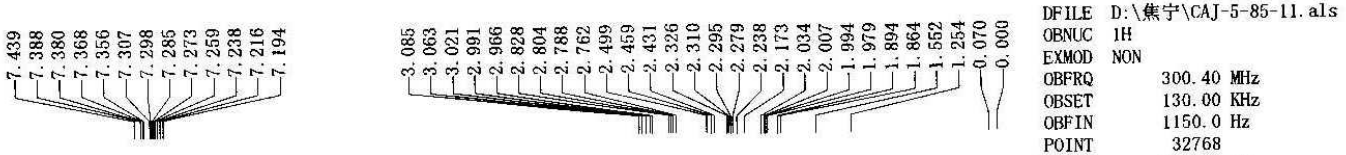
***Cis*-2g**



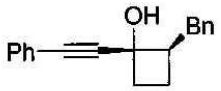
DFILE	D:\焦宁\CAJ-6-11-1-C.als
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	2400
ACQTM	1.606 sec
PD	2.000 sec
PW1	4.7 us
IRATN	511
CTEMP	21.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	2.00 Hz
RGAIN	25



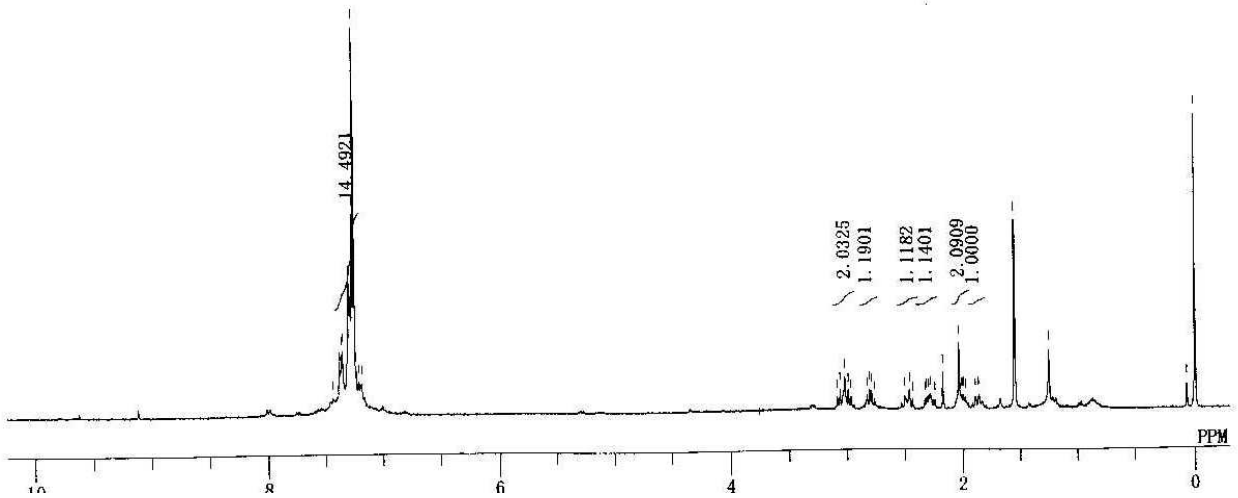
***Cis*-2g**

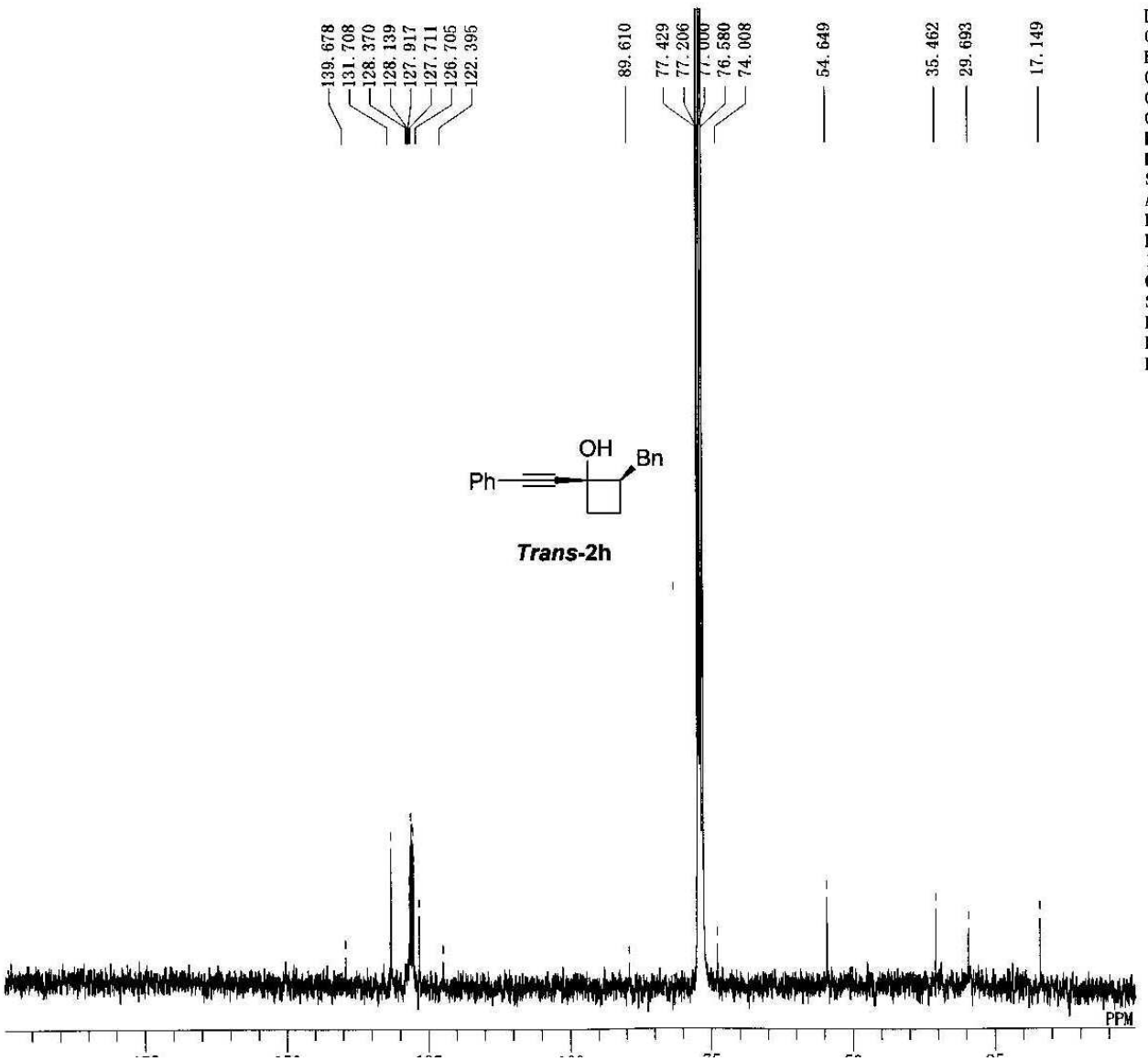


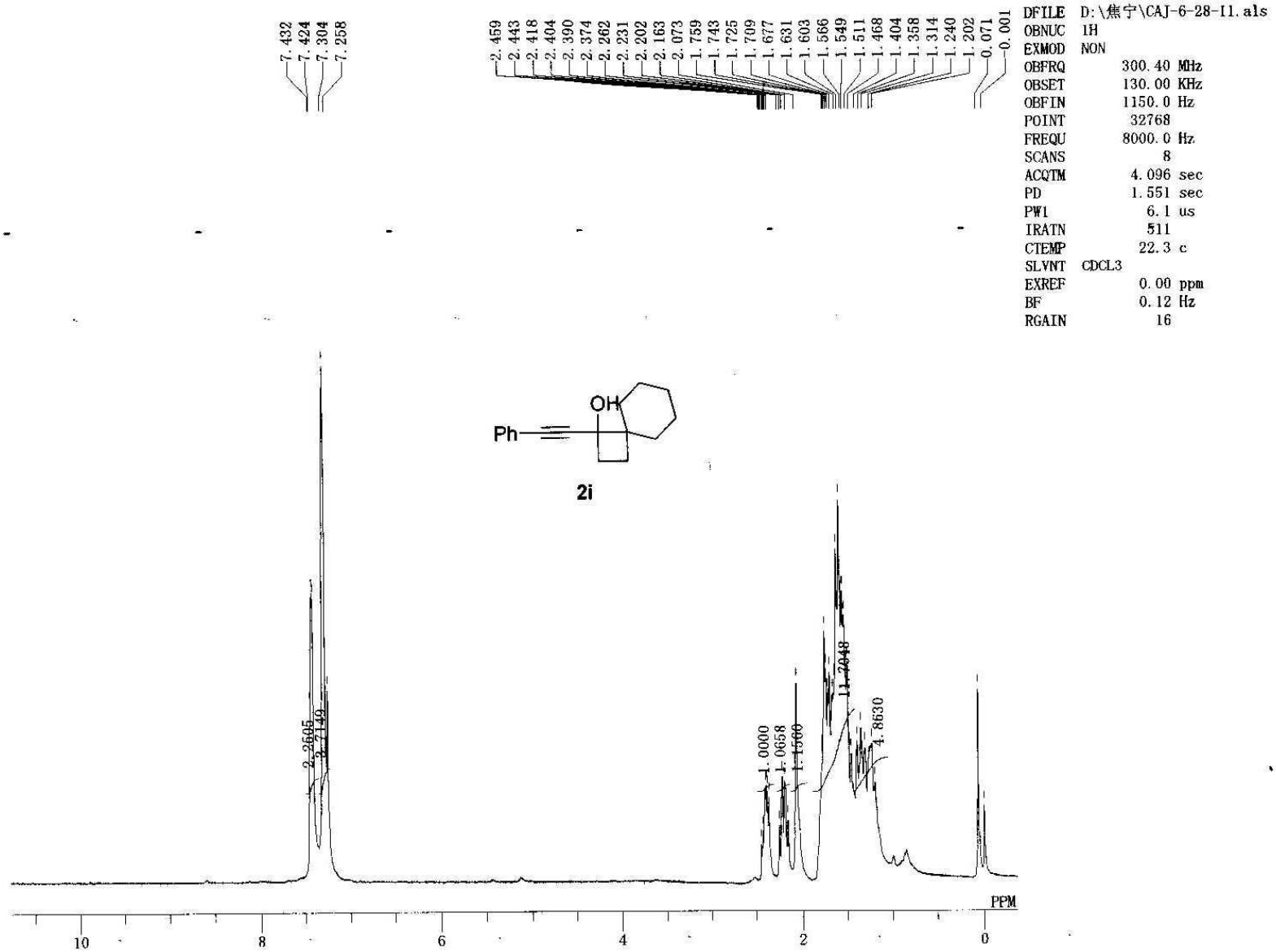
DFILE	D:\焦宁\CAJ-5-85-11.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	21.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	23

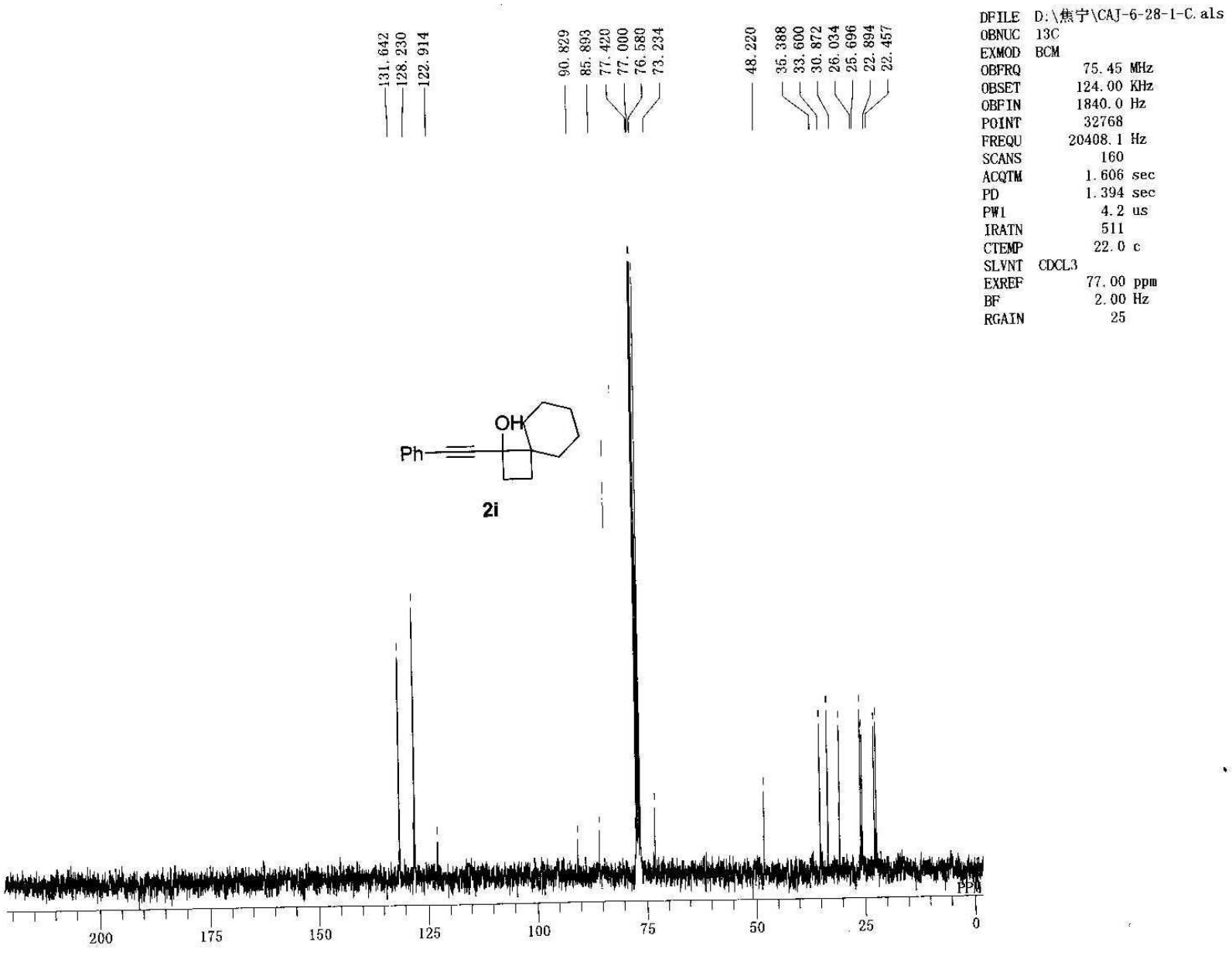


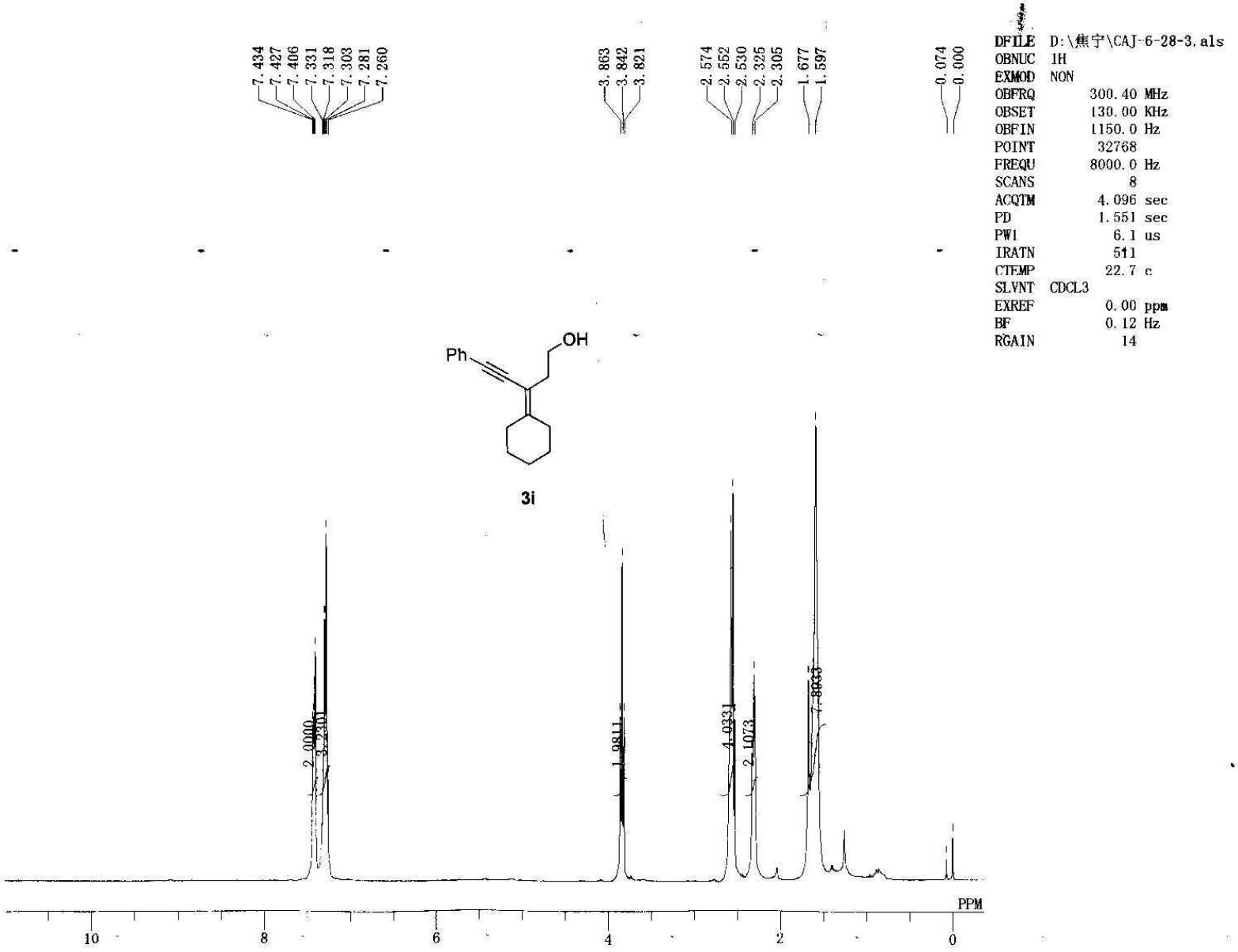
***Trans*-2h**

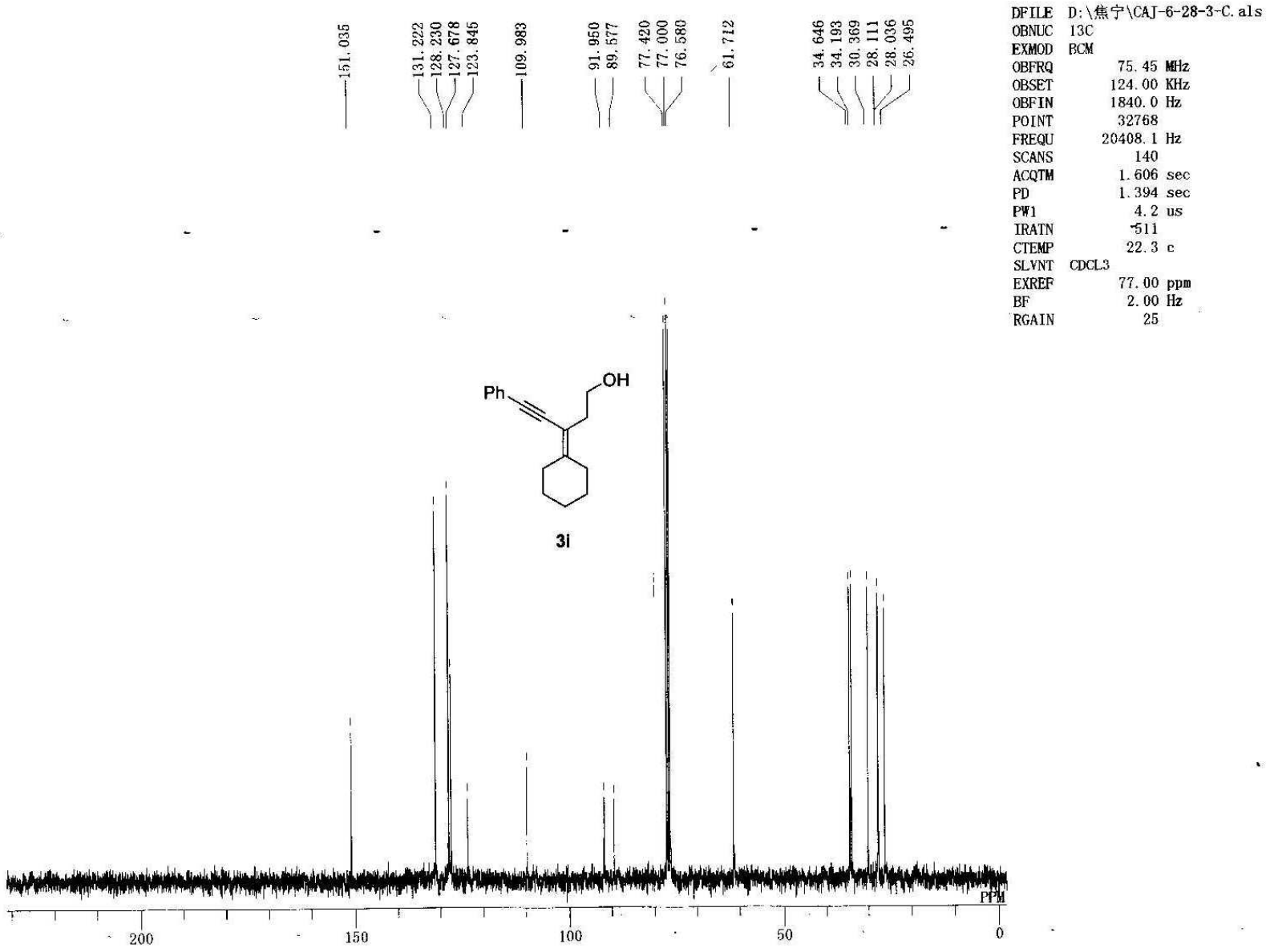


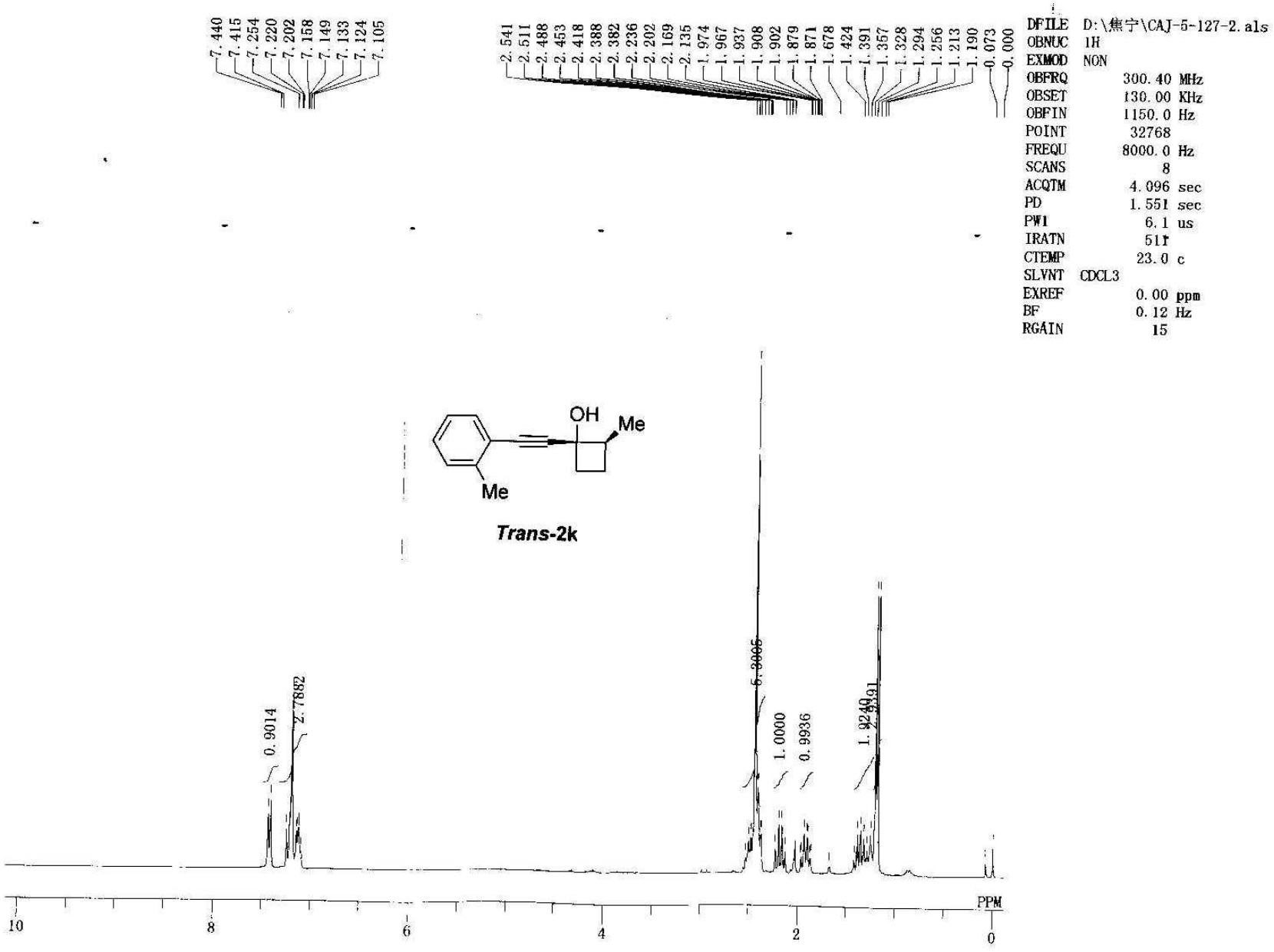

139.678
131.708
128.370
128.139
127.917
127.711
126.705
122.395
89.610
77.429
77.206
76.580
74.008
54.649
35.462
29.693
17.149
DFILE D:\焦宁\CAJ-5-83-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 10300
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Bn
Ph
Trans-2h
PPM

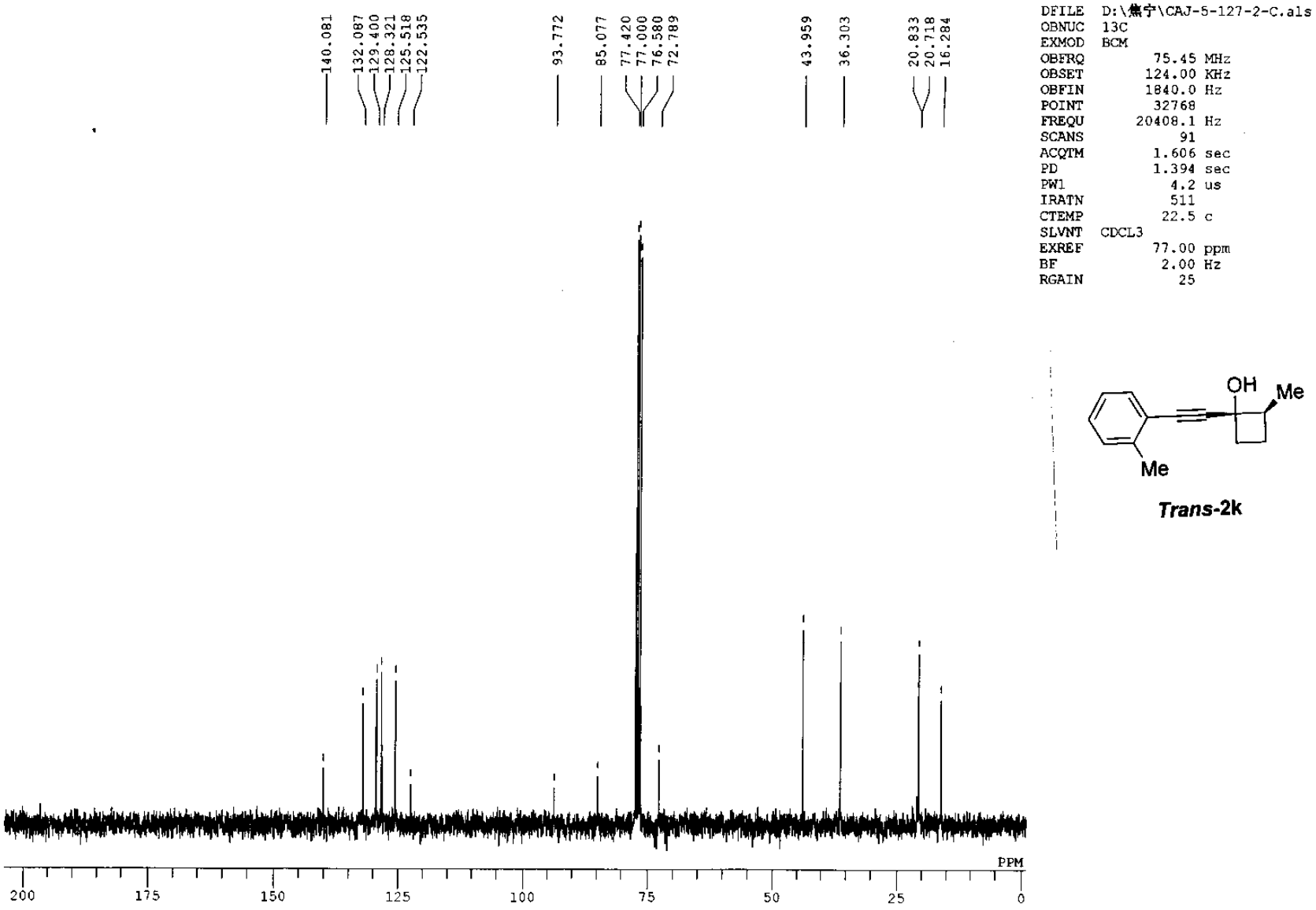

7.432
7.424
7.304
7.258
2.459
2.443
2.418
2.404
2.390
2.374
2.262
2.231
2.202
2.163
2.073
1.759
1.743
1.725
1.709
1.677
1.631
1.603
1.566
1.549
1.511
1.468
1.404
1.358
1.314
1.240
1.202
0.071
0.001
DFILE D:\焦宁\CAJ-6-28-I1.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16
OH
Ph
2i
2.2605
2.2149
1.0000
1.0658
1.1500
4.8630
PPM
10
8
6
4
2
0

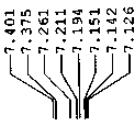

131.642
128.230
122.914
90.829
85.893
77.420
77.000
76.580
73.234
48.220
35.388
33.600
30.872
26.034
25.696
22.894
22.457
DFILE D:\焦宁\CAJ-6-28-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 160
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Ph
2i
PPM
200
175
150
125
100
75
50
25
0

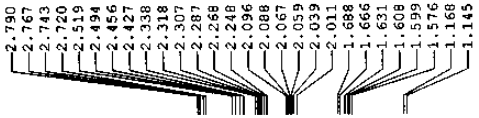

7.434
7.427
7.406
7.331
7.318
7.303
7.281
7.260
3.863
3.842
3.821
2.574
2.552
2.530
2.325
2.305
1.677
1.597
0.074
0.000
DFILE D:\焦宁\CAJ-6-28-3.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
Ph
OH
3i
2.0000
3.3900
1.9811
4.0331
2.1073
7.8633
PPM
10
8
6
4
2
0

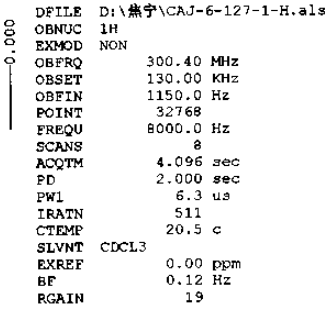

151.035
131.222
128.230
127.678
123.845
109.983
91.950
89.577
77.420
77.000
76.580
61.712
34.646
34.193
30.369
28.111
28.036
26.495
DFILE D:\焦宁\CAJ-6-28-3-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 140
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Ph
OH
3i
200
150
100
50
0
PPM

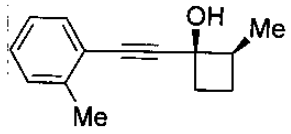

7.440
7.415
7.254
7.220
7.202
7.158
7.149
7.133
7.124
7.105
2.541
2.511
2.488
2.453
2.418
2.388
2.382
2.236
2.202
2.169
2.135
1.974
1.967
1.937
1.908
1.902
1.879
1.871
1.678
1.424
1.391
1.357
1.328
1.294
1.256
1.213
1.190
0.073
0.000
DFILE D:\焦宁\CAJ-5-127-2.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBPIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 51
CTEMP 23.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
OH
Me
Me
Trans-2k
0.9014
2.7882
5.3005
1.0000
0.9936
1.9240
PPM
10
8
6
4
2
0


140.081
132.087
129.400
128.321
125.518
122.535
93.772
85.077
77.420
77.000
76.580
72.789
43.959
36.303
20.833
20.718
16.284
DFILE D:\焦宁\CAJ-5-127-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 91
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Me
Me
Trans-2k
PPM
200
175
150
125
100
75
50
25
0


7.401
7.375
7.261
7.211
7.194
7.151
7.142
7.126

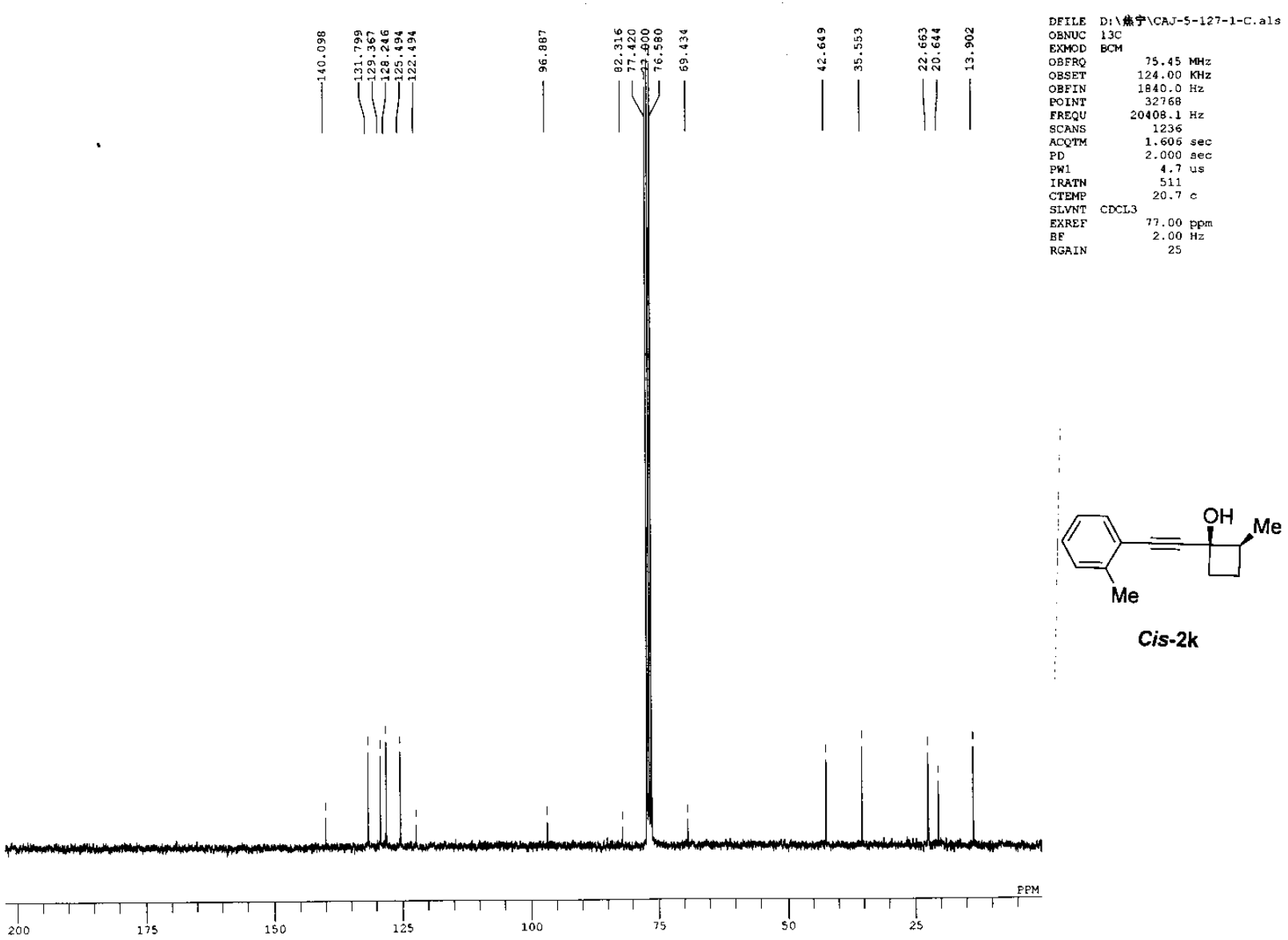

2.790
2.767
2.743
2.720
2.519
2.494
2.456
2.427
2.338
2.318
2.307
2.287
2.268
2.248
2.096
2.088
2.067
2.059
2.039
2.011
1.688
1.666
1.631
1.608
1.599
1.576
1.168
1.145


0.000
DFILE D:\焦宁\CAJ-6-127-1-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 2.000 sec
PW1 6.3 us
IRATN 511
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19

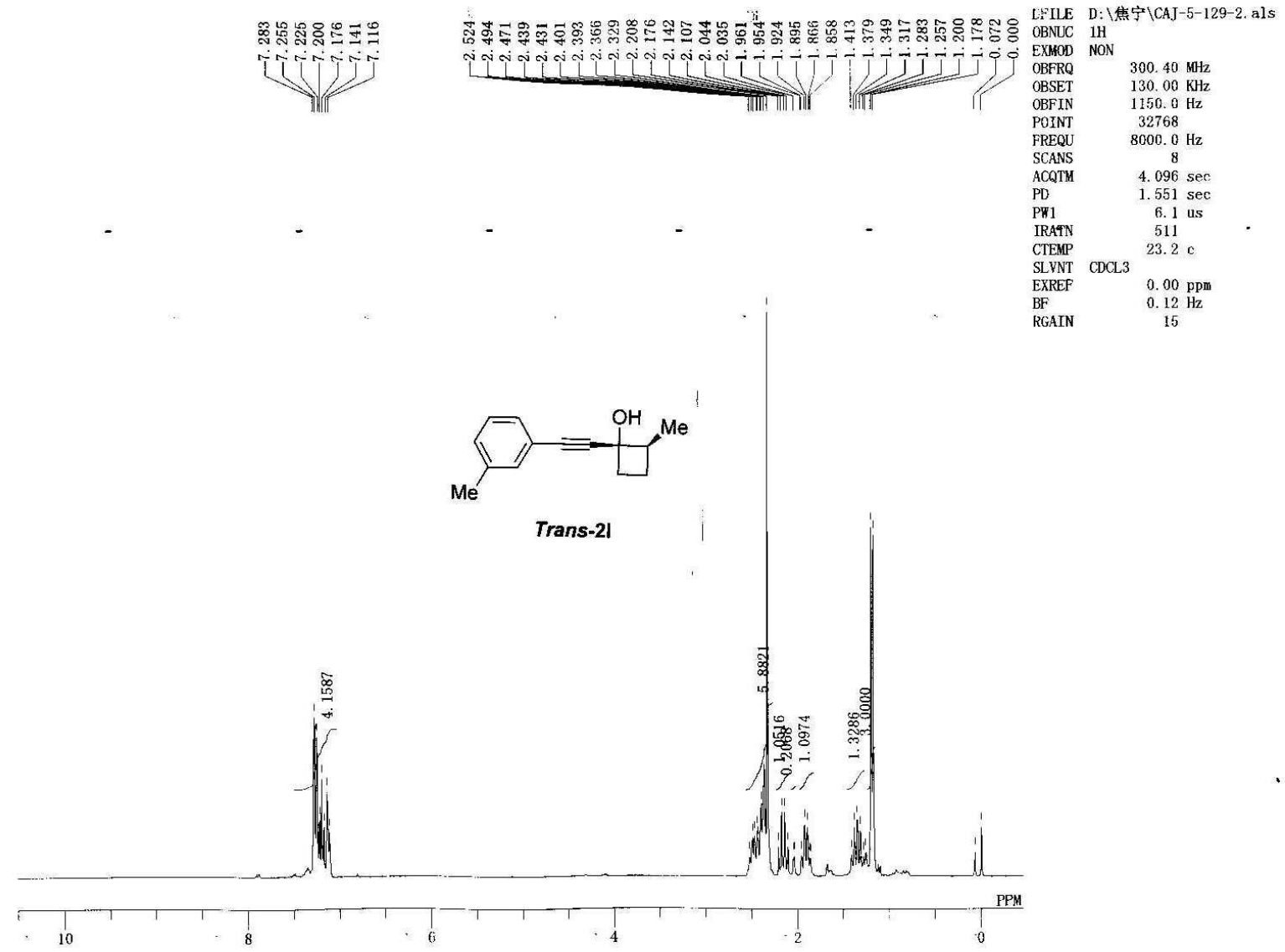

OH
Me
Me

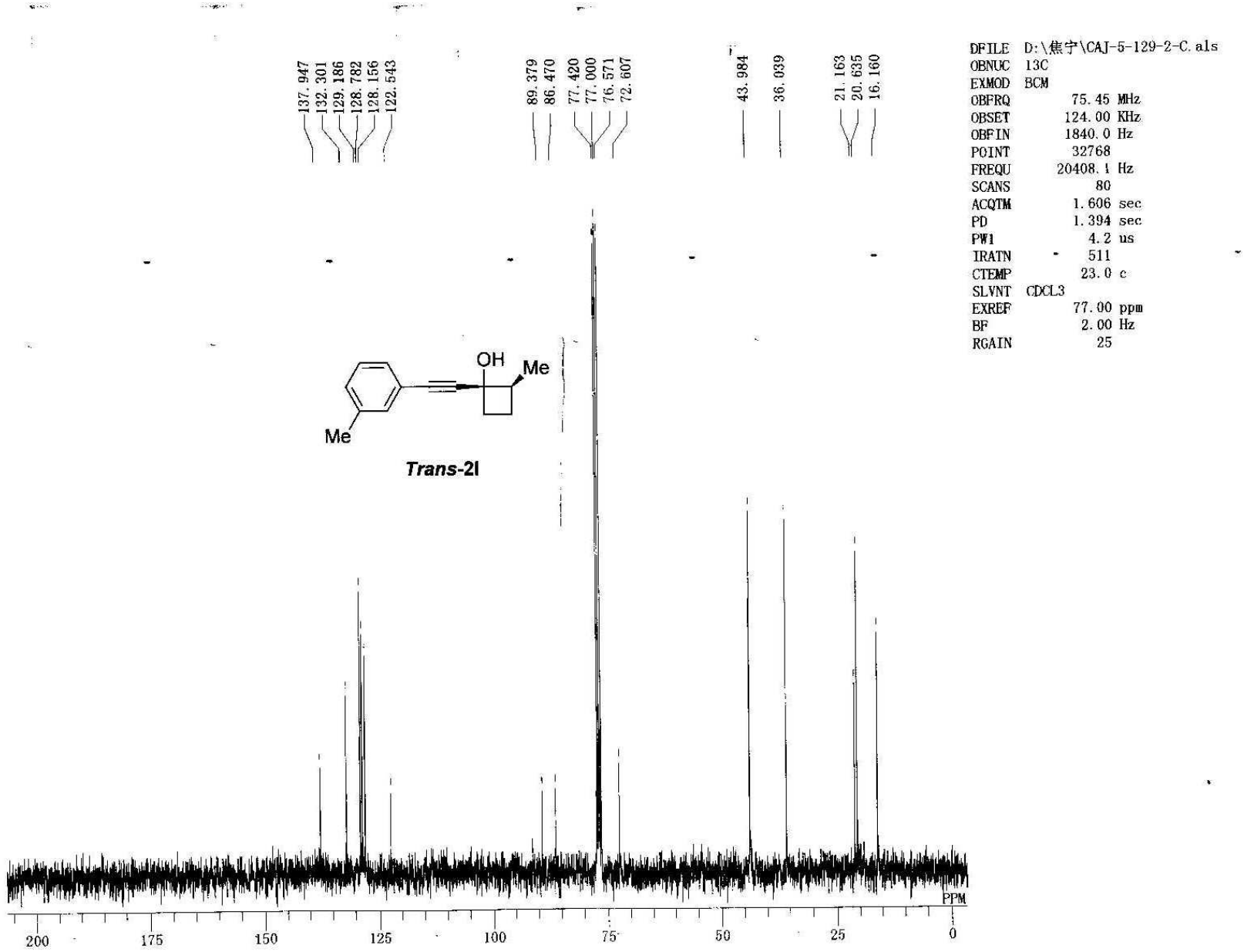
***Cis*-2k**

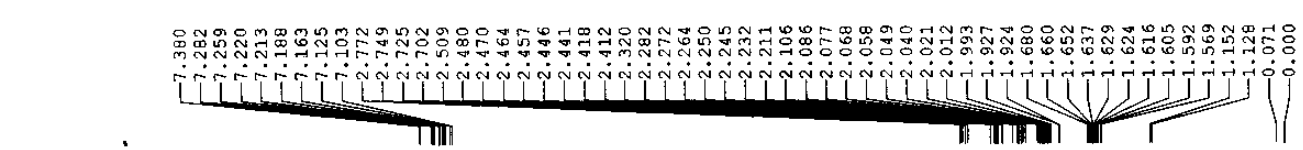
1.0102
2.9723
0.8490
4.2231
1.0000
1.7961
1.3614
3.1917
PPM
10
8
6
4
2
0


140.098
131.799
129.367
128.246
125.494
122.494
96.887
82.316
77.420
77.000
76.580
69.434
42.649
35.553
22.663
20.644
13.902
DFILE D:\焦宁\CAJ-5-127-1-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 1236
ACQTM 1.606 sec
PD 2.000 sec
PW1 4.7 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
LB 2.00 Hz
RGAIN 25
OH
Me
Me
PPM
200
175
150
125
100
75
50
25

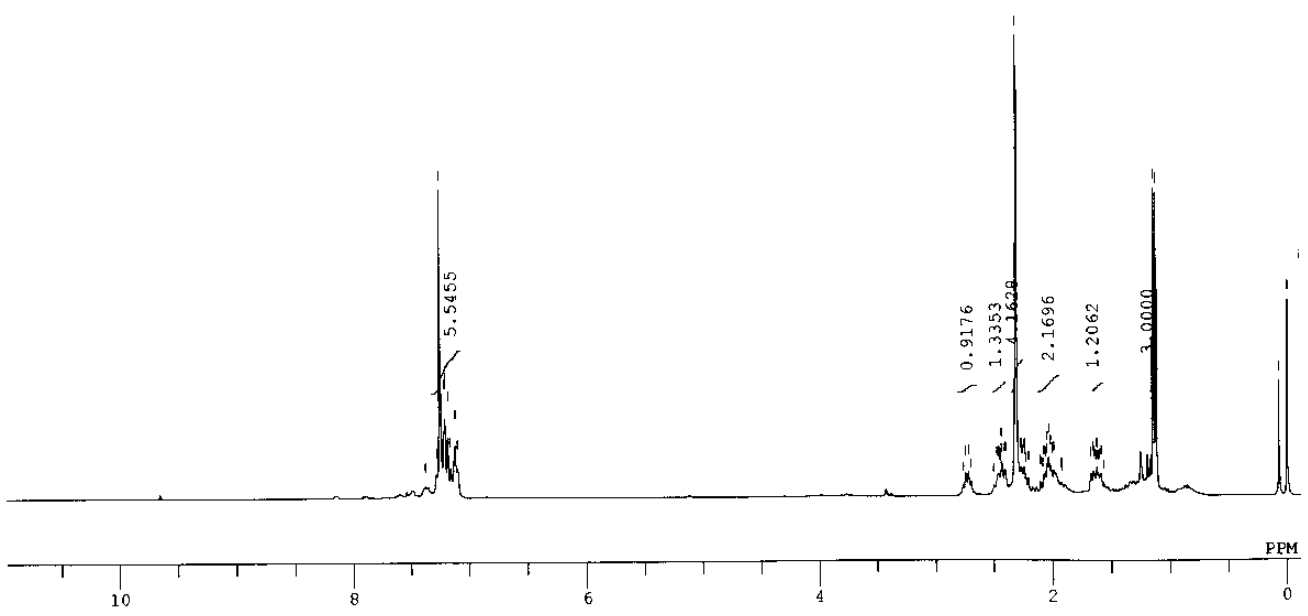
***Cis*-2k**

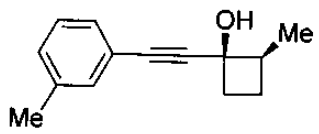

7.283
7.255
7.225
7.200
7.176
7.141
7.116
2.524
2.494
2.471
2.439
2.431
2.401
2.393
2.366
2.329
2.208
2.176
2.142
2.107
2.044
2.035
1.961
1.954
1.924
1.895
1.866
1.858
1.413
1.379
1.349
1.317
1.283
1.257
1.200
1.178
0.072
0.000
DFILE D:\焦宁\CAJ-5-129-2.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 15
OH
Me
Me
Trans-2l
4.1587
5.8821
1.0516
2.0000
1.0974
1.3286
3.0000
PPM
10
8
6
4
2
0


137.947
132.301
129.186
128.782
128.156
122.543
89.379
86.470
77.420
77.000
76.571
72.607
43.984
36.039
21.163
20.635
16.160
DFILE D:\焦宁\CAJ-5-129-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 80
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Me
Me
Trans-2l
PPM
200
175
150
125
100
75
50
25
0

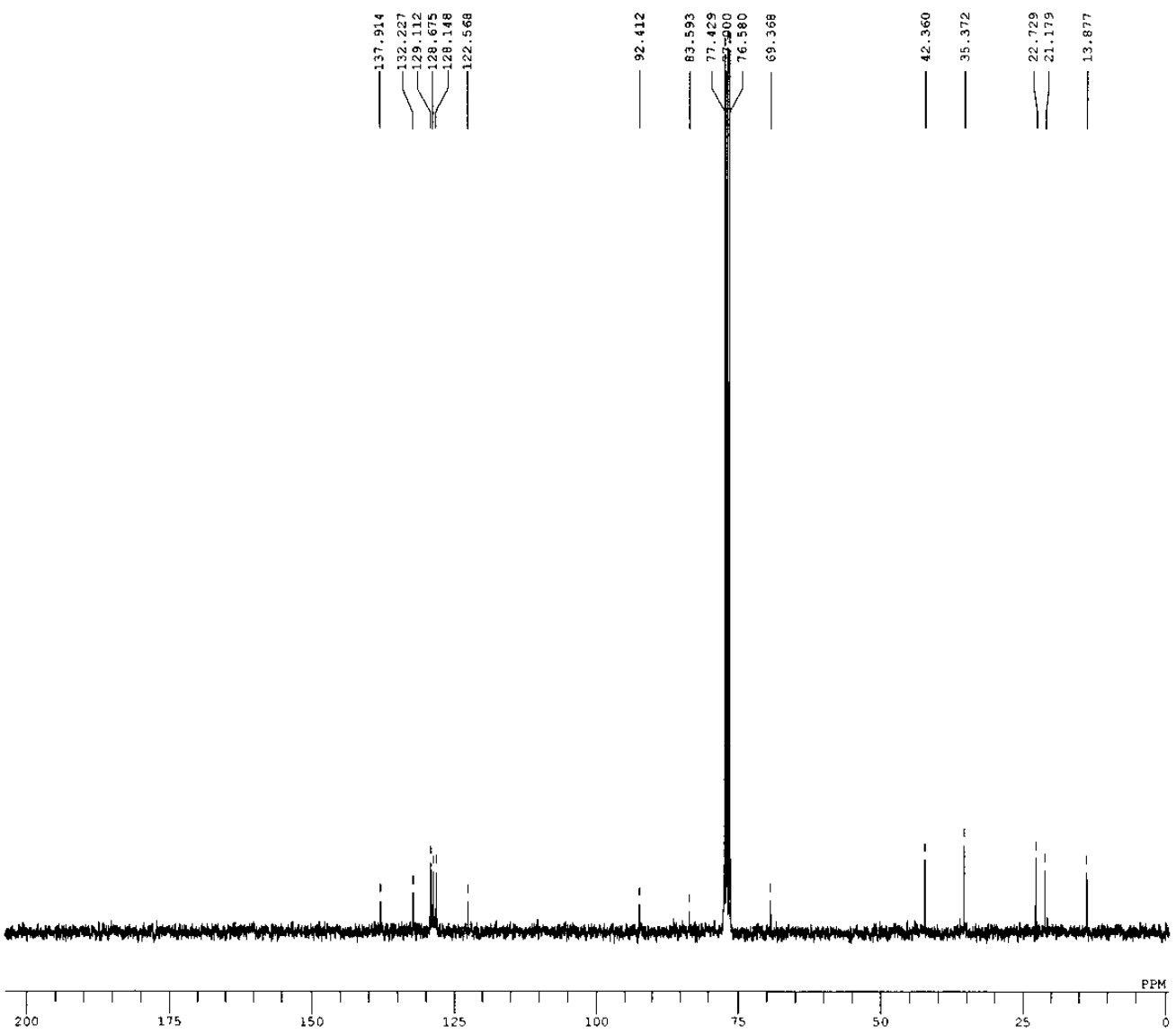


DFILE	D:\焦宁\CAJ-5-129-1.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	23.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
RF	0.12 Hz
RGAIN	19

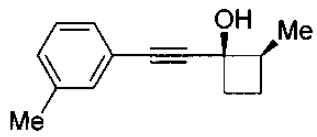




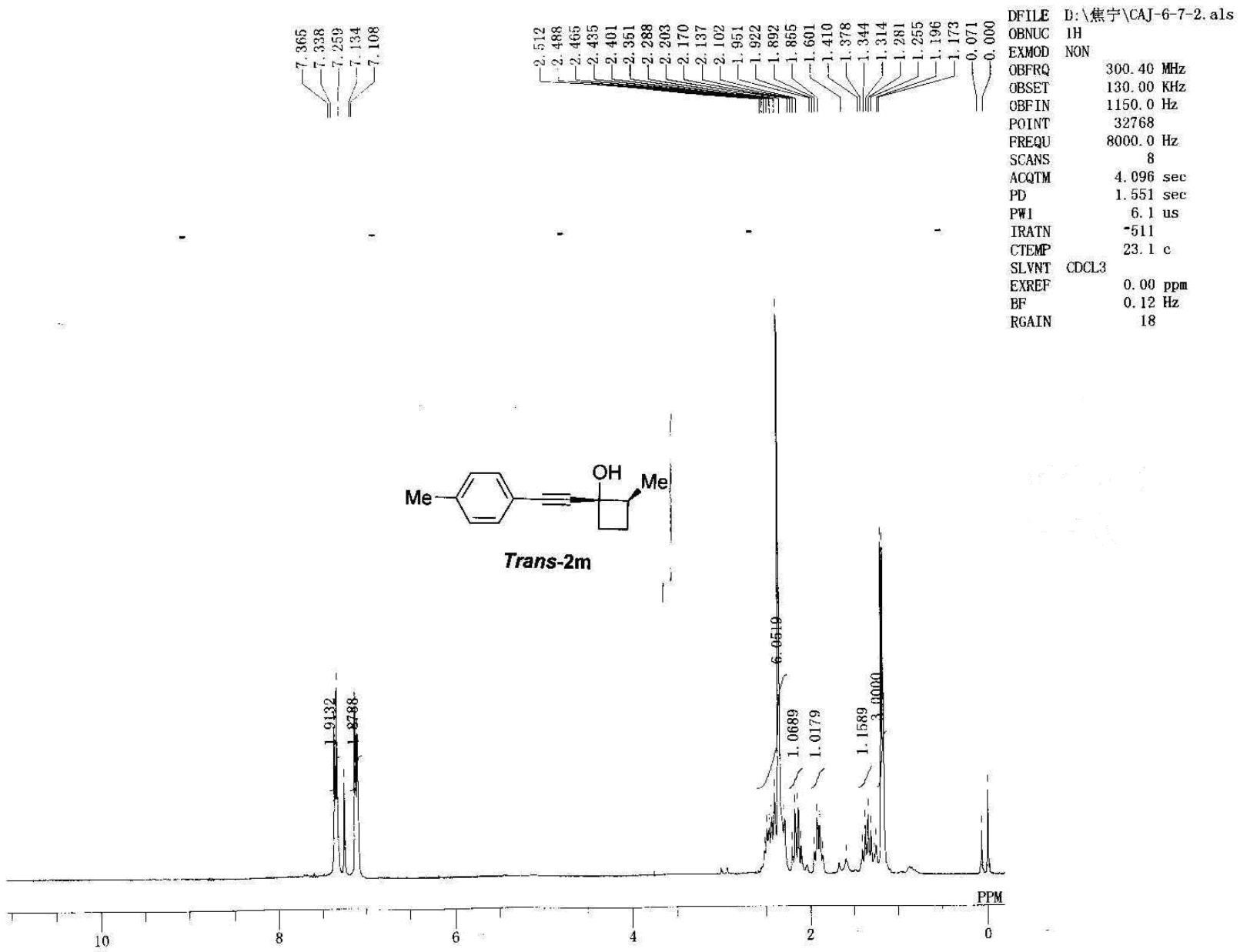
***Cis*-2l**

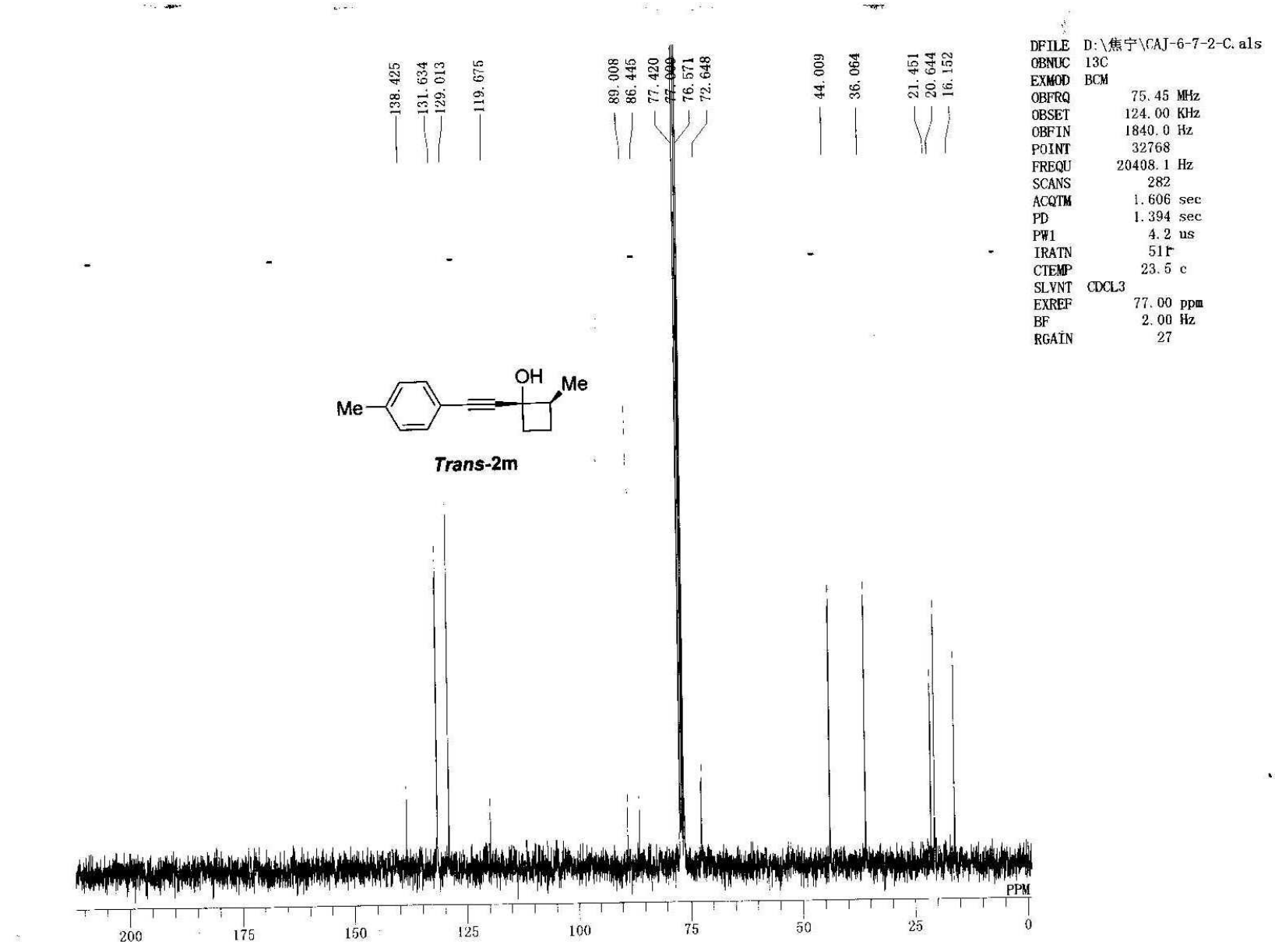


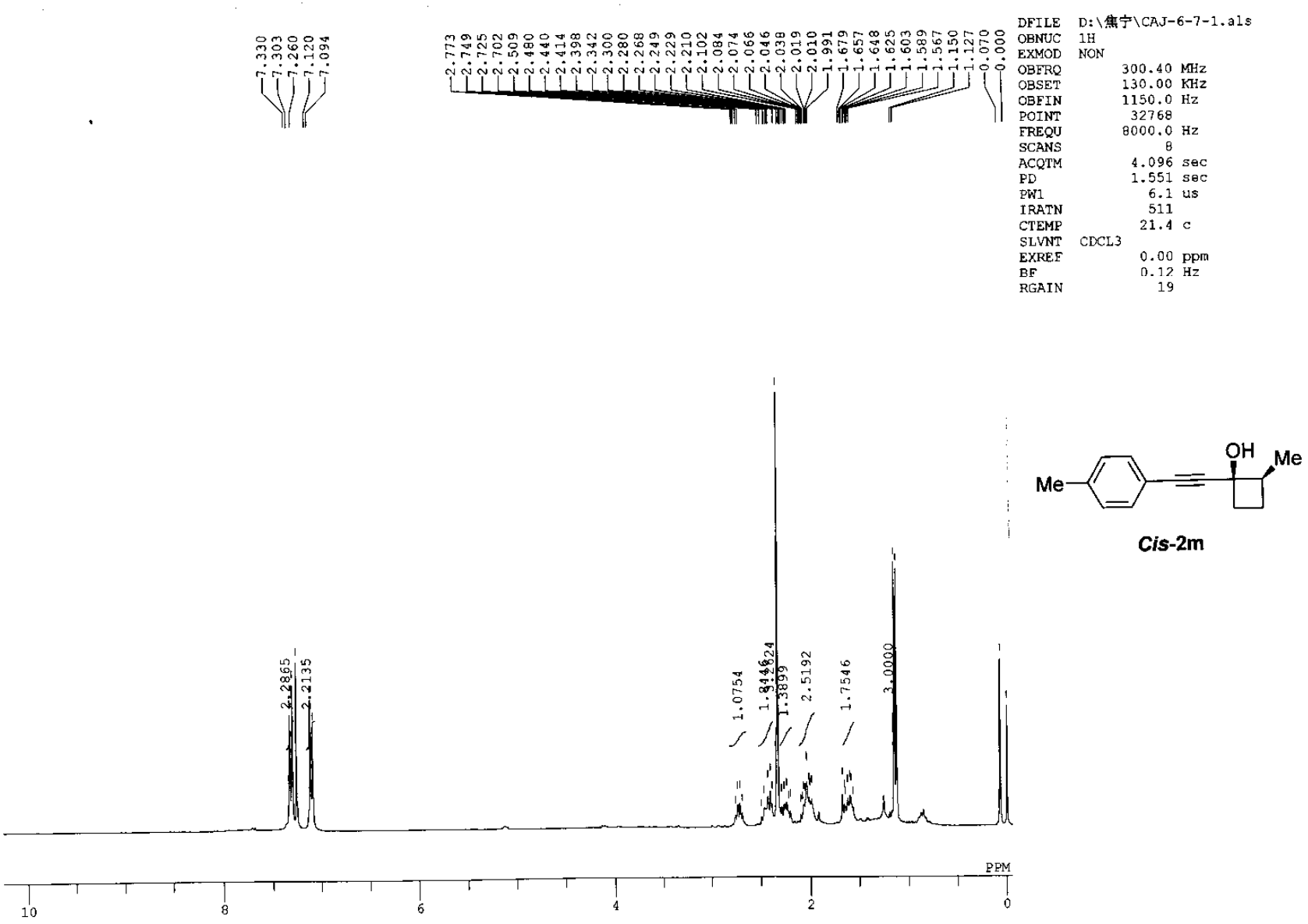

```
DFILE  D:\焦宁\CAJ-5-129-1-C.als
OBNUC  13C
EXMOD  BCM
OBFRQ        75.45 MHz
OBSET       124.00 KHz
OBFIN       1840.0 Hz
POINT        32768
FREQU       20408.1 Hz
SCANS          452
ACQTM         1.606 sec
PD            1.394 sec
PW1             4.2 us
IRATN           511
CTEMP          22.9 c
SLVNT  CDCL3
EXREF         77.00 ppm
BF             2.00 Hz
RGAIN            25
```



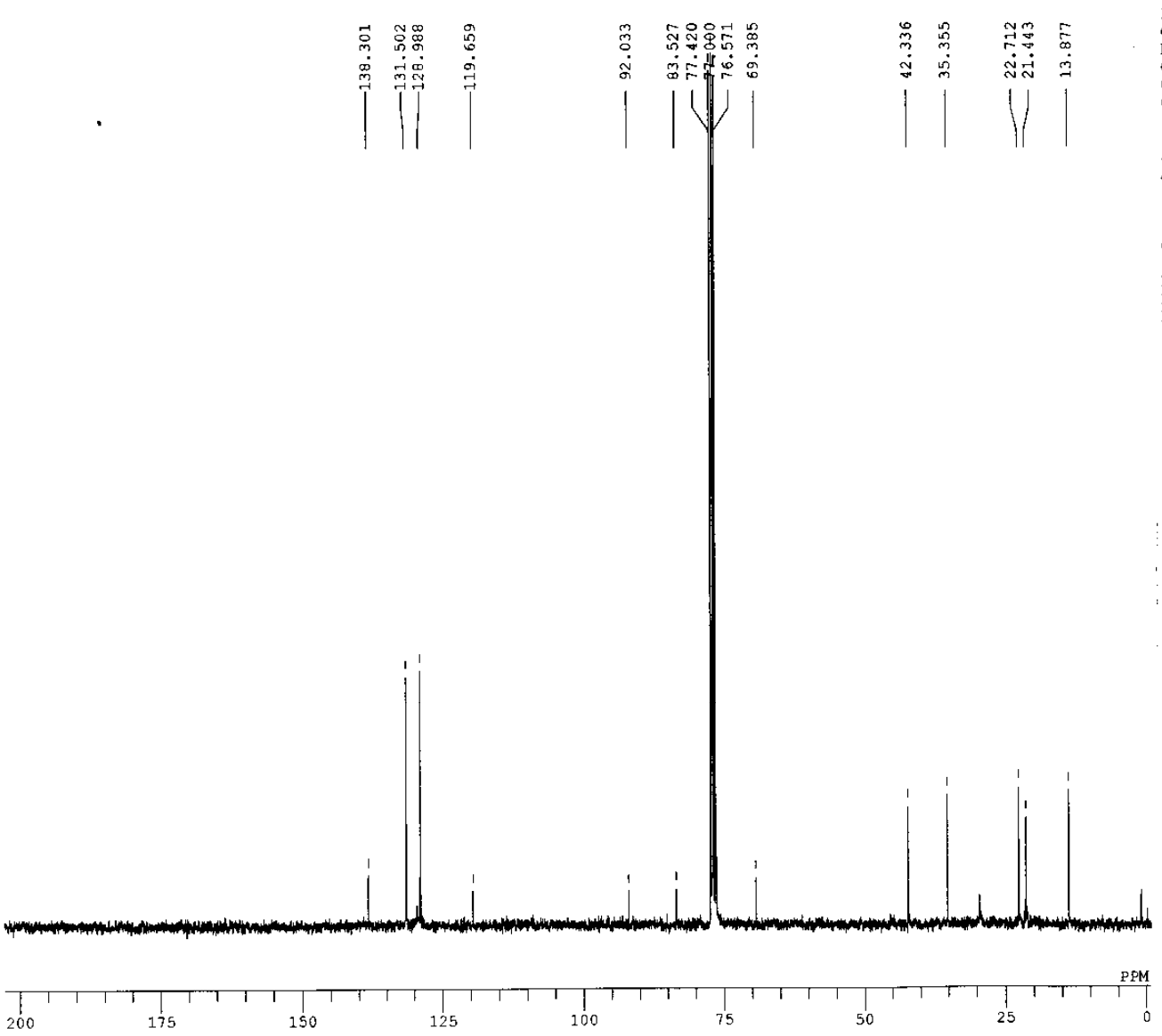
***Cis*-2l**


7.365
7.338
7.259
7.134
7.108
2.512
2.488
2.465
2.435
2.401
2.351
2.288
2.203
2.170
2.137
2.102
1.951
1.922
1.892
1.865
1.601
1.410
1.378
1.344
1.314
1.281
1.255
1.196
1.173
0.071
0.000
DFILE D:\焦宁\CAJ-6-7-2.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 23.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
Me
OH
Me
Trans-2m
1.9132
1.8788
6.0519
1.0689
1.0179
1.1589
3.0000
PPM
10
8
6
4
2
0

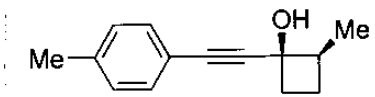

138.425
131.634
129.013
119.675
89.008
86.445
77.420
77.000
76.571
72.648
44.009
36.064
21.451
20.644
16.152
DFILE D:\焦宁\CAJ-6-7-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 282
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 51
CTEMP 23.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 27
OH
Me
Me
Trans-2m
PPM
200
175
150
125
100
75
50
25
0


7.330
7.303
7.260
7.120
7.094
2.773
2.749
2.725
2.702
2.509
2.480
2.440
2.414
2.398
2.342
2.300
2.280
2.268
2.249
2.229
2.210
2.102
2.084
2.074
2.066
2.046
2.038
2.019
2.010
1.991
1.679
1.657
1.648
1.625
1.603
1.589
1.567
1.150
1.127
0.070
0.000
DFILE D:\焦宁\CAJ-6-7-1.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19
2.2865
2.2135
1.0754
1.8446
1.8624
1.3899
2.5192
1.7546
3.0000
PPM
10
8
6
4
2
0
OH
Me
Me

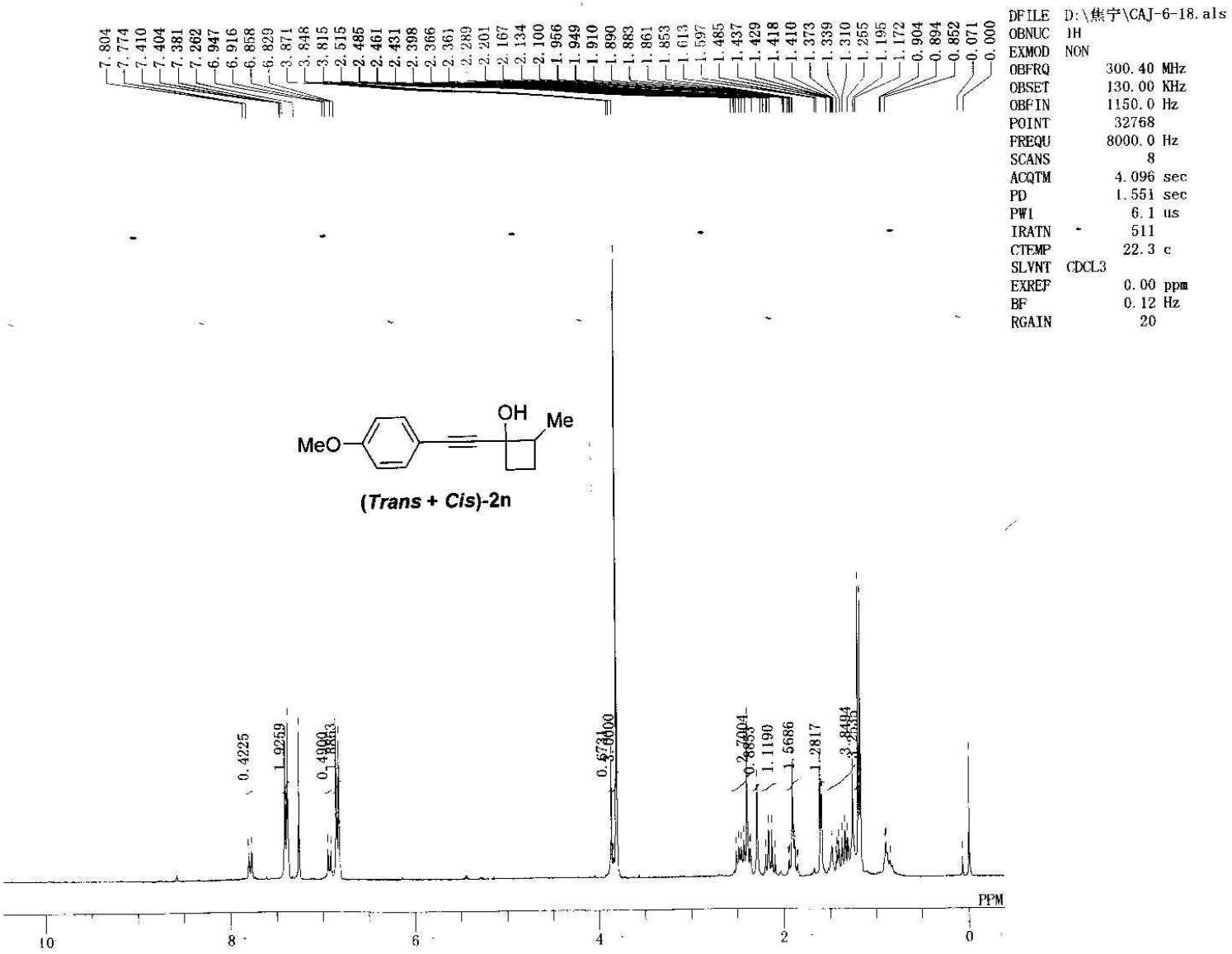
***Cis*-2m**

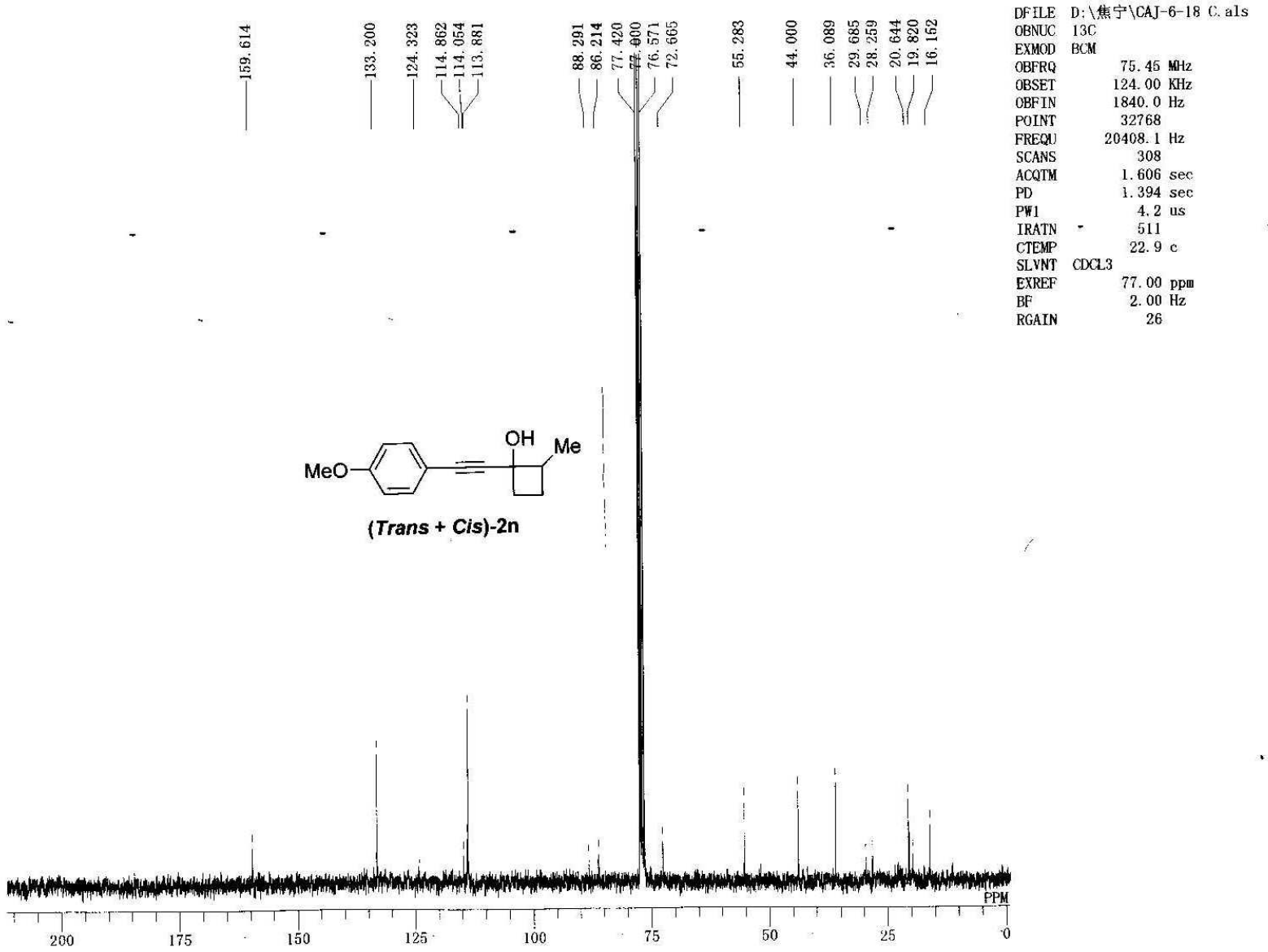


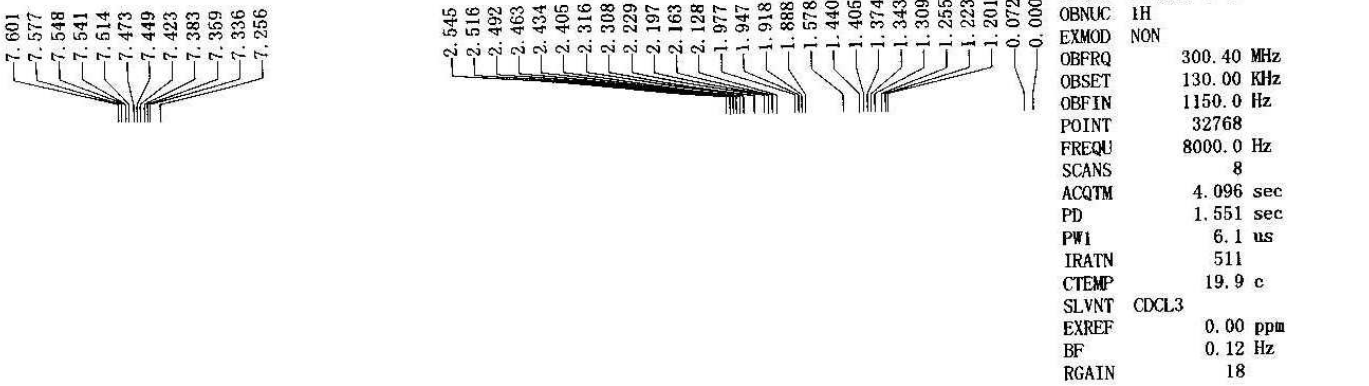

```
DFILE   D:\焦宁\CAJ-6-7-1-C.als
OBNUC   13C
EXMOD   BCM
OBFRQ         75.45 MHz
OBSET        124.00 KHz
OBFIN        1840.0 Hz
POINT         32768
FREQU       20408.1 Hz
SCANS           932
ACQTM          1.606 sec
PD             2.000 sec
PW1              4.7 us
IRATN            511
CTEMP           20.6 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             2.00 Hz
RGAIN              25
```

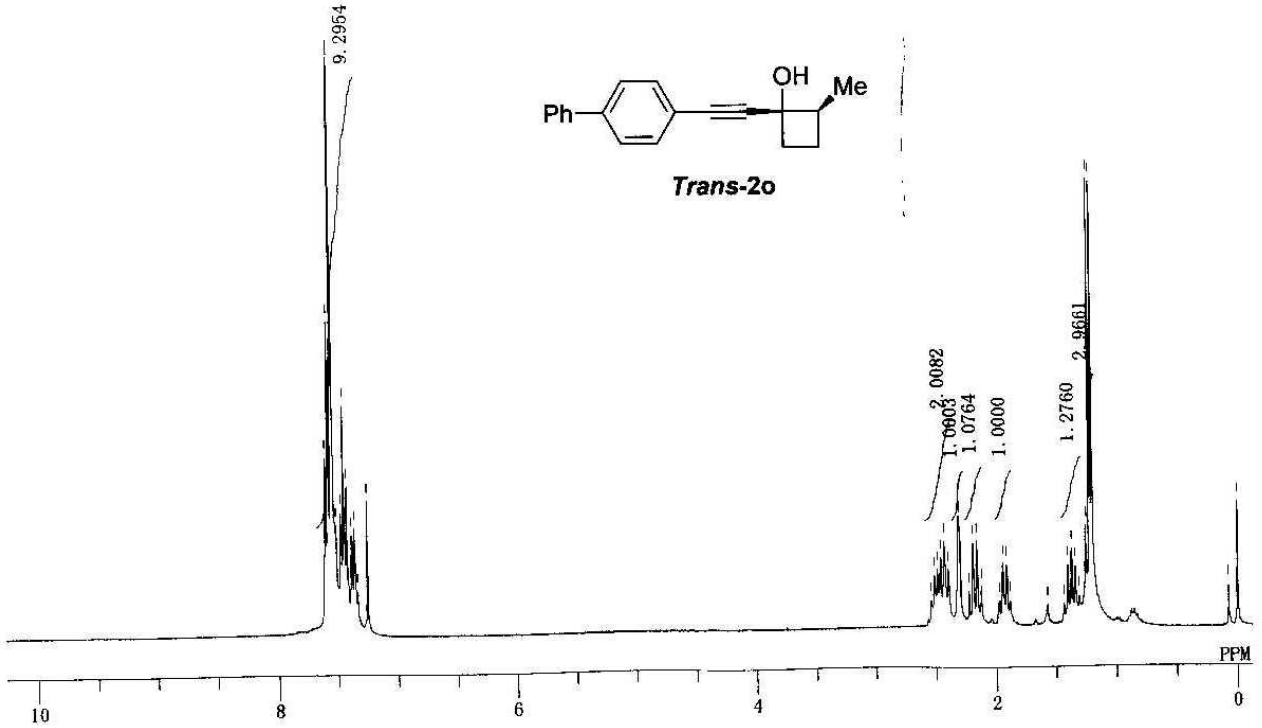


***Cis*-2m**

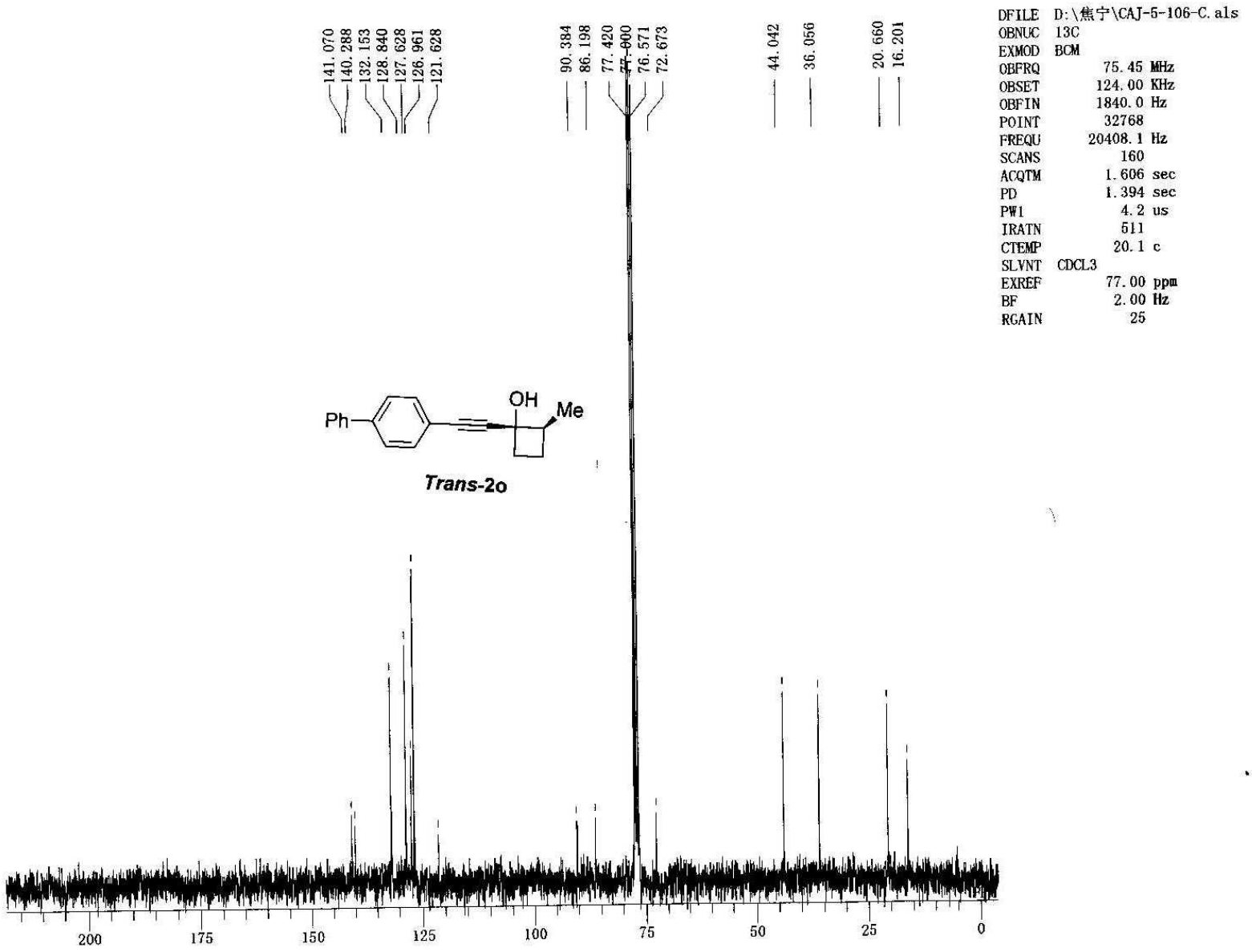

7.804
7.774
7.410
7.404
7.381
7.262
6.947
6.916
6.858
6.829
3.871
3.848
3.815
2.515
2.485
2.461
2.431
2.398
2.366
2.361
2.289
2.201
2.167
2.134
2.100
1.956
1.949
1.910
1.890
1.883
1.861
1.853
1.613
1.597
1.485
1.437
1.429
1.418
1.410
1.373
1.339
1.310
1.255
1.195
1.172
0.904
0.894
0.852
0.071
0.000
DFILE D:\焦宁\CAJ-6-18.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 22.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20
OH
Me
MeO
(Trans + Cis)-2n
0.4225
1.9259
0.4000
0.6721
3.0000
2.4704
0.8853
1.1190
1.5686
1.2817
3.8484
3.2535
PPM
10
8
6
4
2
0

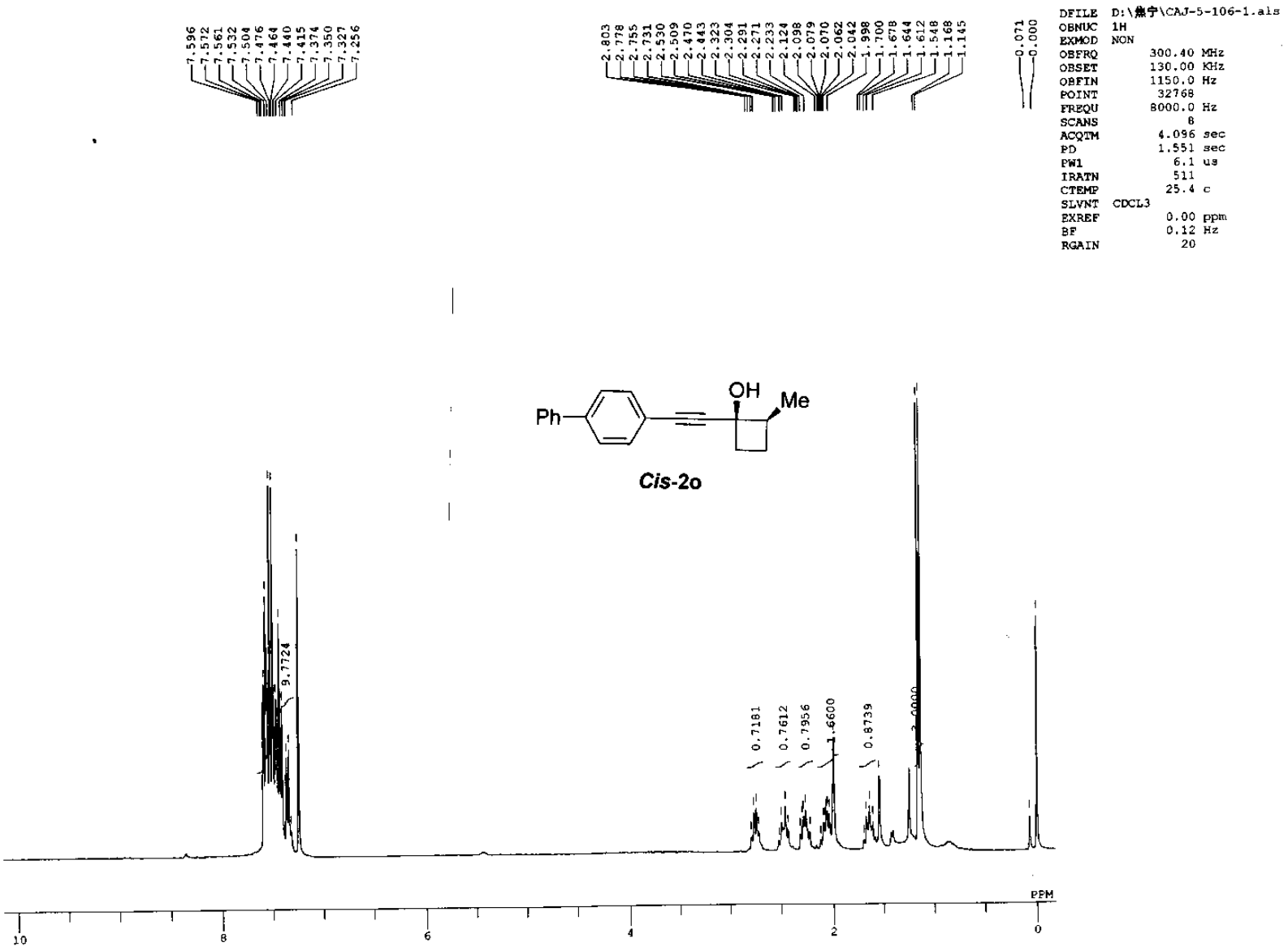

159.614
133.200
124.323
114.862
114.054
113.881
88.291
86.214
77.420
77.000
76.571
72.665
55.283
44.000
36.089
29.685
28.259
20.644
19.820
16.162
DFILE D:\焦宁\CAJ-6-18 C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 308
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 26
OH
Me
MeO
(Trans + Cis)-2n
PPM
200
175
150
125
100
75
50
25
0

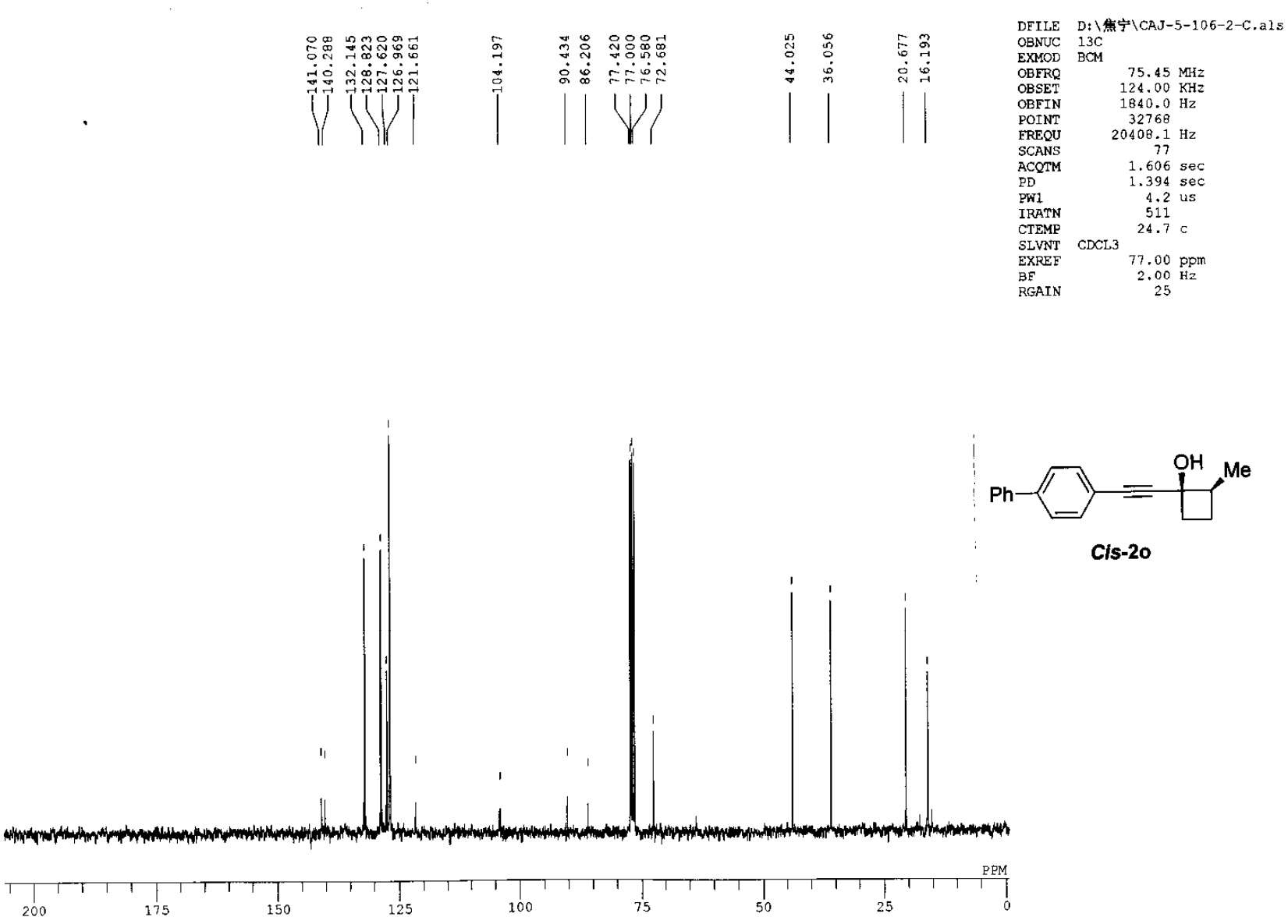

7.601
7.577
7.548
7.541
7.514
7.473
7.449
7.423
7.383
7.369
7.336
7.256
2.545
2.516
2.492
2.463
2.434
2.405
2.316
2.308
2.229
2.197
2.163
2.128
1.977
1.947
1.918
1.888
1.578
1.440
1.405
1.374
1.343
1.309
1.255
1.223
1.201
0.072
0.000
DFILE D:\焦宁\CAJ-5-106-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 19.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18


9.2954
OH
Me
Ph
2.0082
1.0603
1.0764
1.0000
1.2760
2.9661
PPM
10
8
6
4
2
0

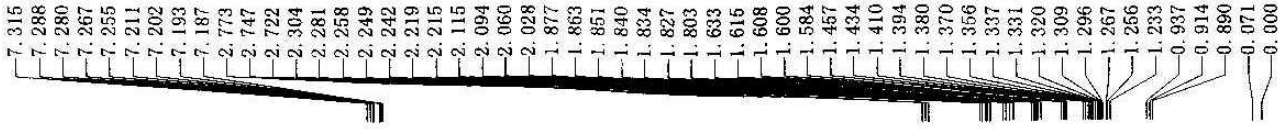
***Trans*-2o**


141.070
140.288
132.153
128.840
127.628
126.961
121.628
90.384
86.198
77.420
77.000
76.571
72.673
44.042
36.056
20.660
16.201
DFILE D:\焦宁\CAJ-5-106-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 160
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Ph
OH
Me
Trans-2o
200
175
150
125
100
75
50
25
0

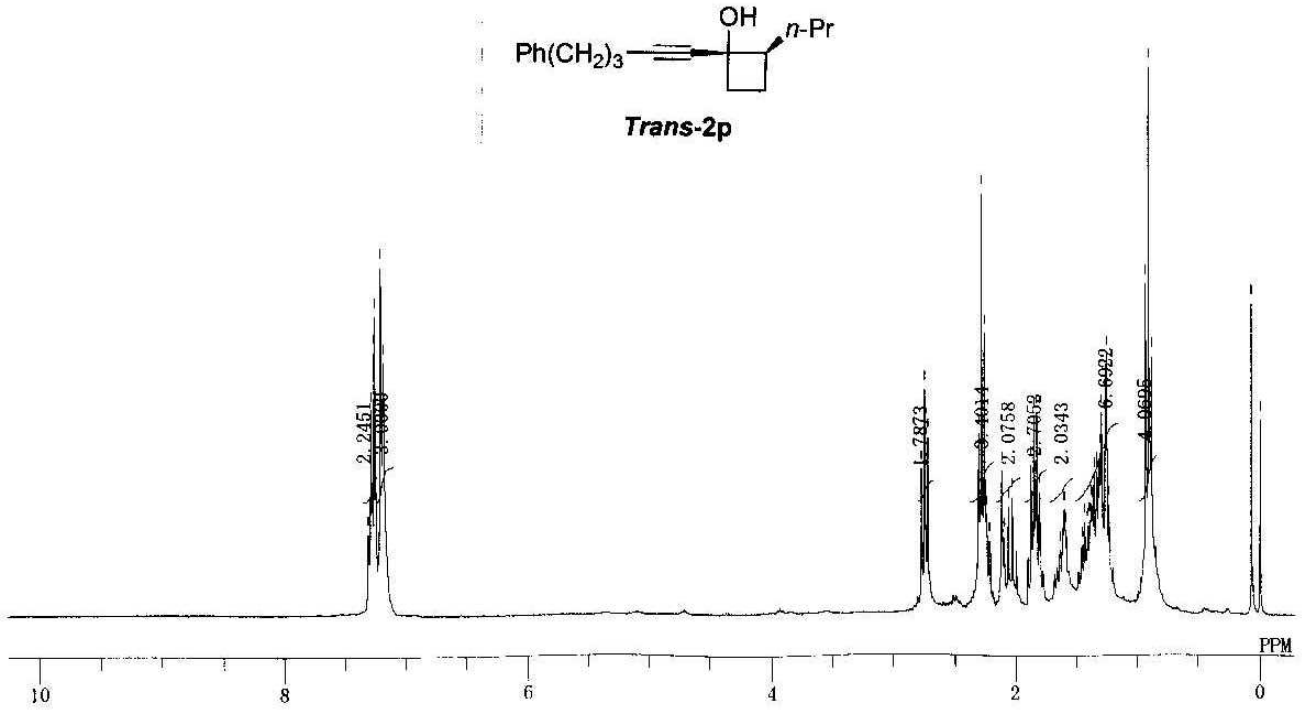

7.596
7.572
7.561
7.532
7.504
7.476
7.464
7.440
7.415
7.374
7.350
7.327
7.256
2.803
2.778
2.755
2.731
2.530
2.509
2.470
2.443
2.323
2.304
2.291
2.271
2.233
2.124
2.098
2.079
2.070
2.062
2.042
1.998
1.700
1.678
1.644
1.612
1.548
1.168
1.145
0.071
0.000
DFILE D:\焦宁\CAJ-5-106-1.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 25.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20
Ph
OH
Me
Cis-2o
9.7724
0.7181
0.7612
0.7956
1.6600
0.8739
3.0000
PPM
10
8
6
4
2
0

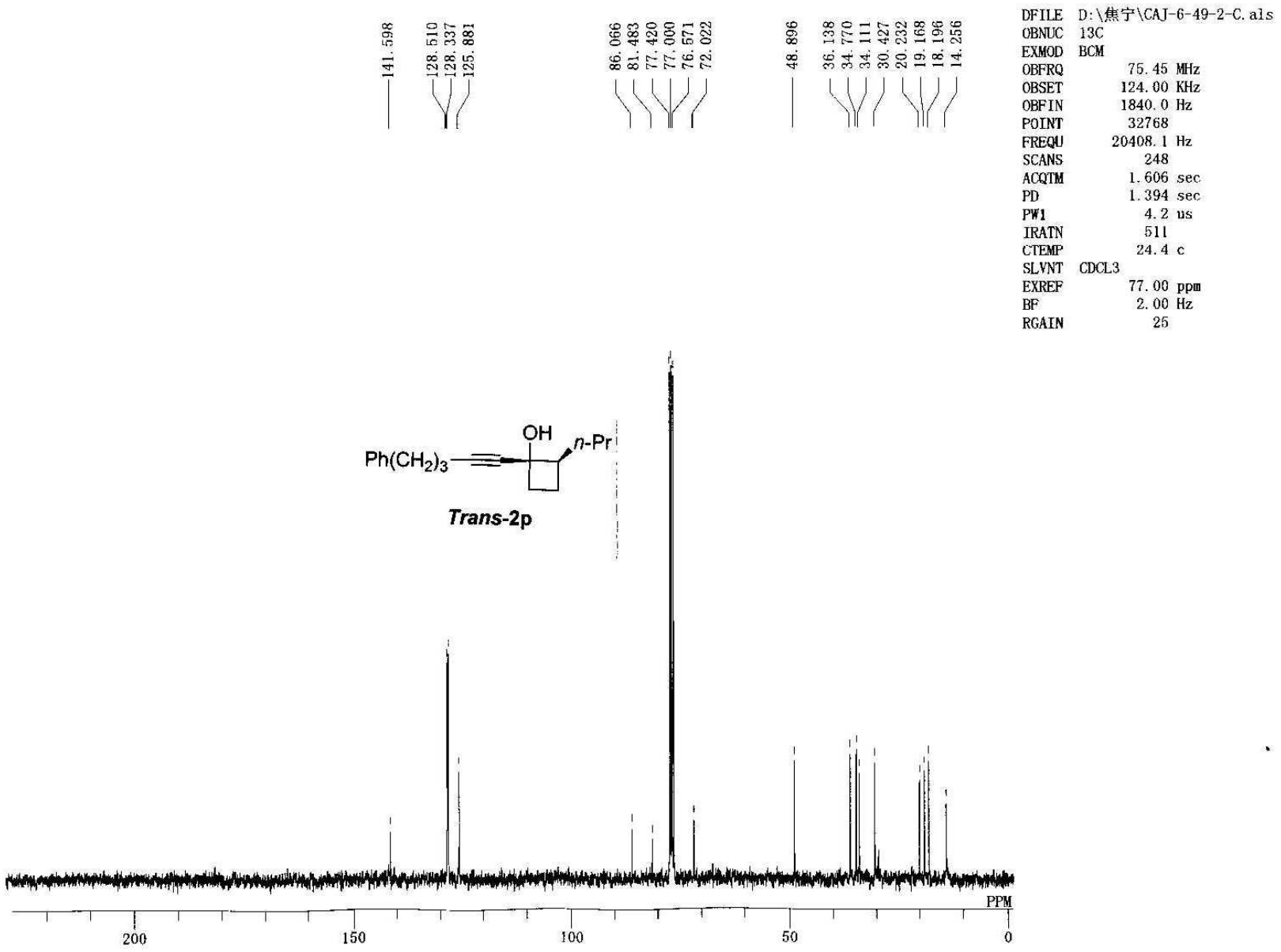

141.070
140.288
132.145
128.823
127.620
126.969
121.661
104.197
90.434
86.206
77.420
77.000
76.580
72.681
44.025
36.056
20.677
16.193
DFILE D:\焦宁\CAJ-5-106-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 77
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 24.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Ph
OH
Me
PPM
200
175
150
125
100
75
50
25
0

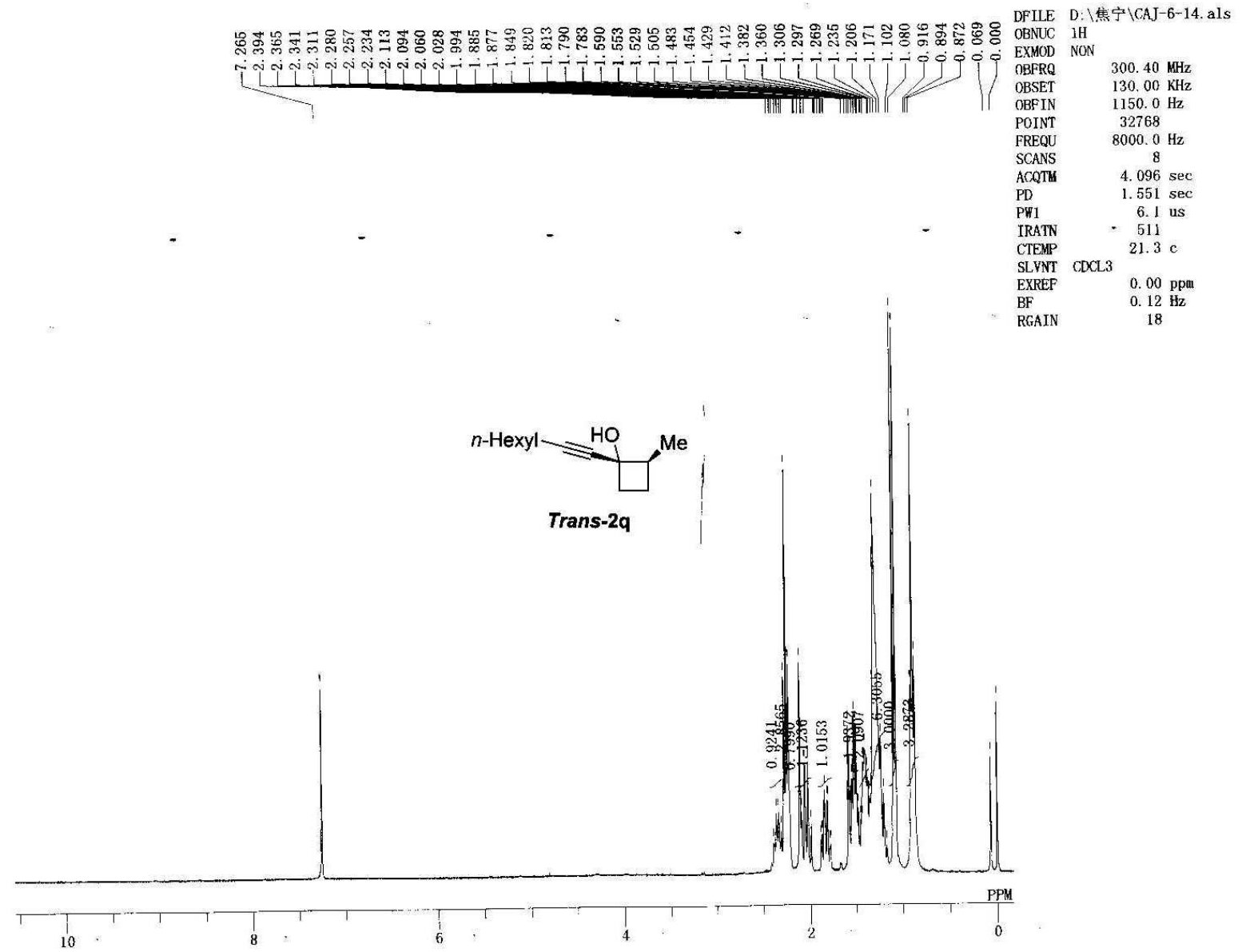
***Cis*-2o**

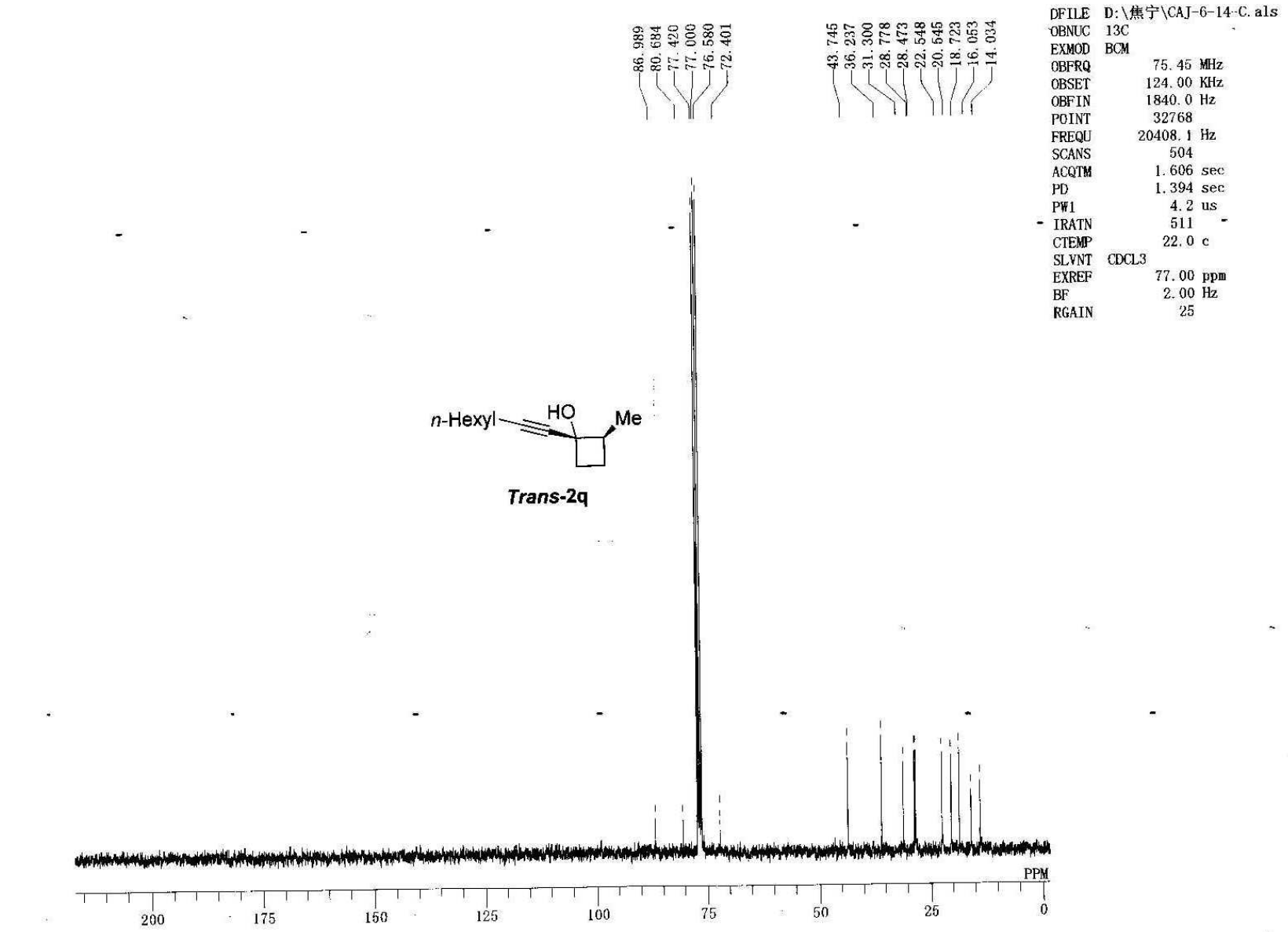


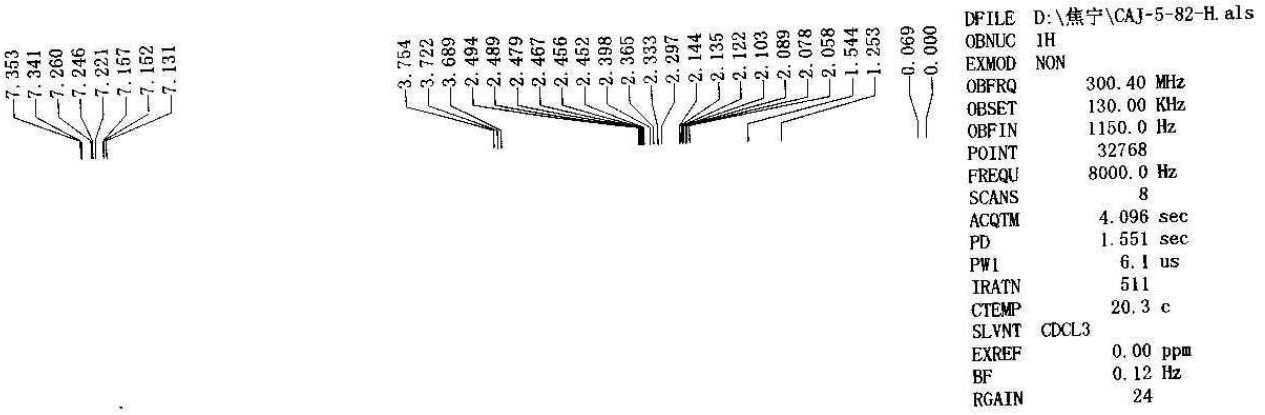
DFILE	D:\焦宁\CAJ-6-49-2.als
OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	8000.0 Hz
SCANS	8
ACQTM	4.096 sec
PD	1.551 sec
PW1	6.1 us
IRATN	511
CTEMP	21.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	15

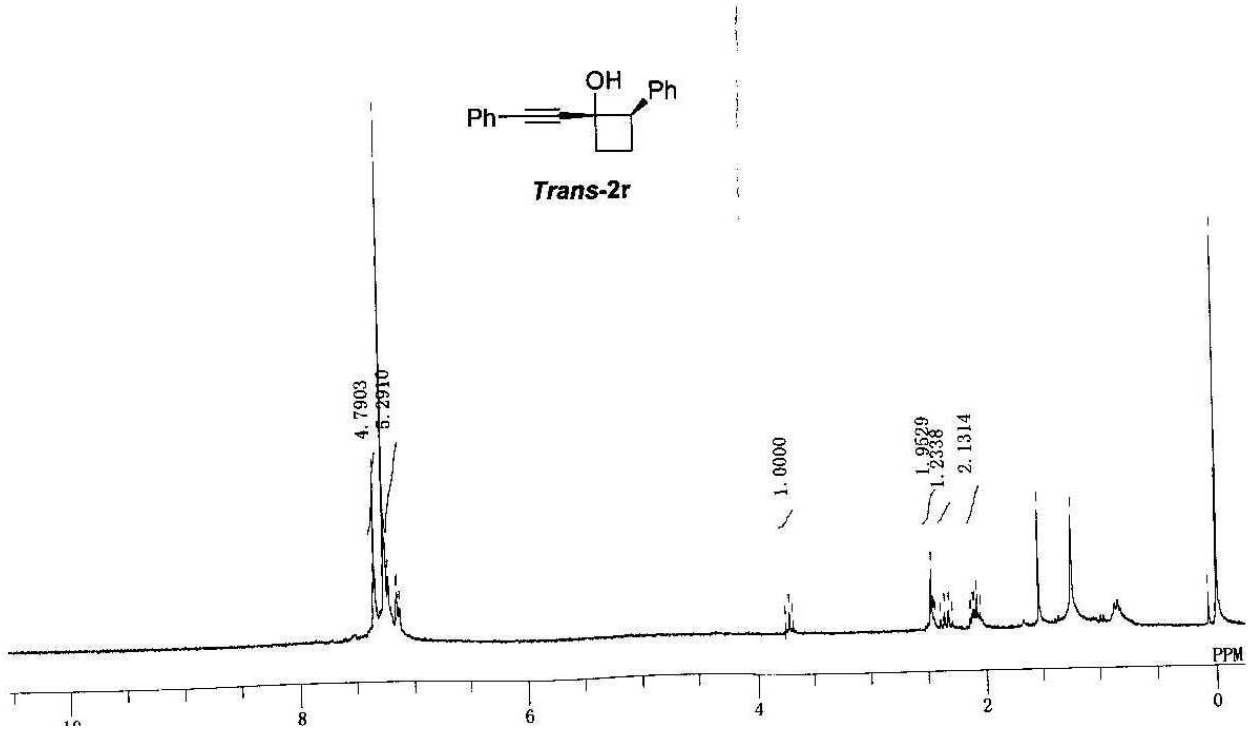



141.598
128.510
128.337
125.881
86.066
81.483
77.420
77.000
76.571
72.022
48.896
36.138
34.770
34.111
30.427
20.232
19.168
18.196
14.256
DFILE D:\焦宁\CAJ-6-49-2-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 248
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 24.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
n-Pr
Ph(CH2)3
Trans-2p
PPM
200
150
100
50
0

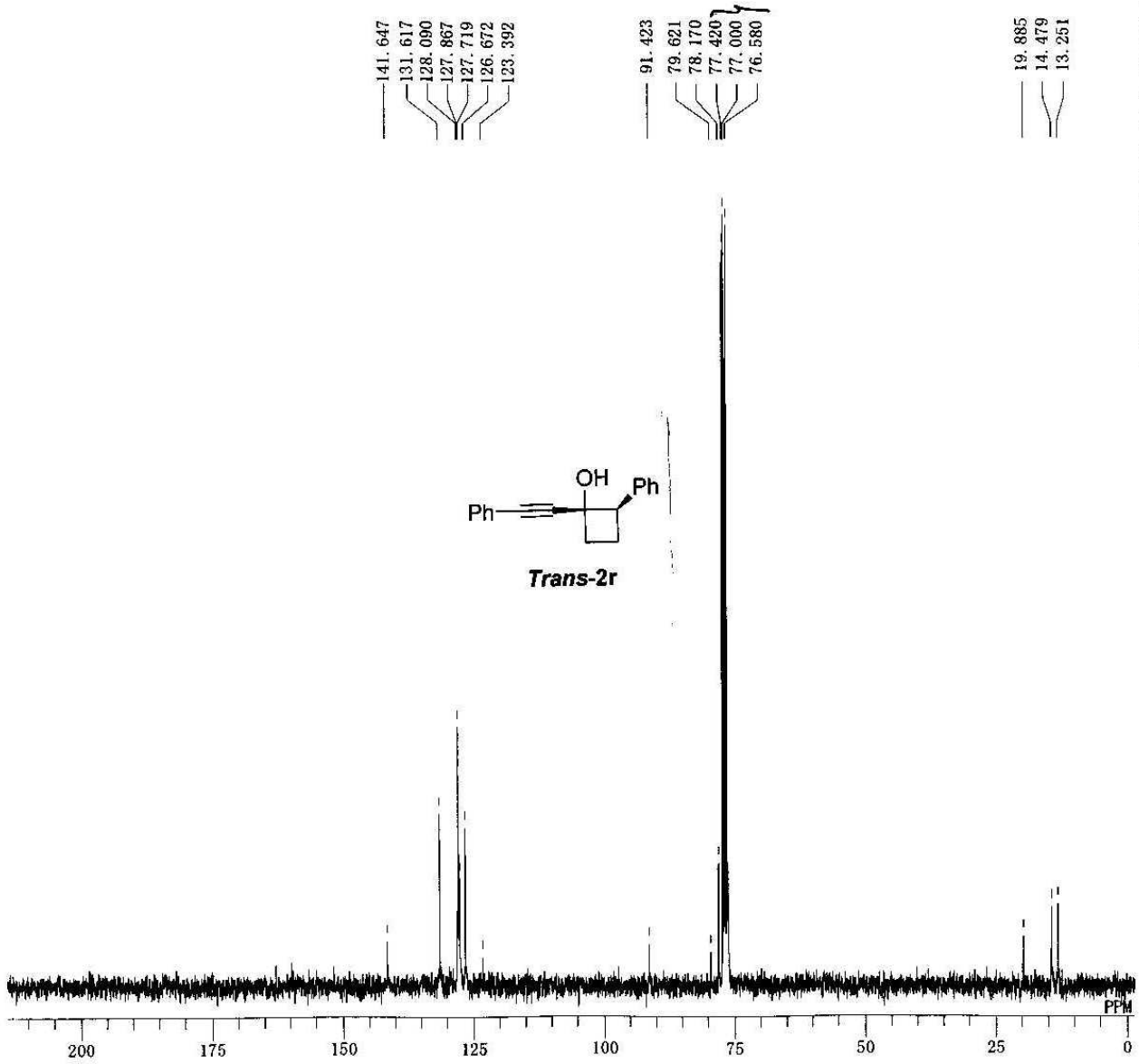

7.265
2.394
2.365
2.341
2.311
2.280
2.257
2.234
2.113
2.094
2.060
2.028
1.994
1.885
1.877
1.849
1.820
1.813
1.790
1.783
1.590
1.553
1.529
1.505
1.483
1.454
1.429
1.412
1.382
1.360
1.306
1.297
1.269
1.235
1.206
1.171
1.102
1.080
0.916
0.894
0.872
0.069
0.000
DFILE D:\焦宁\CAJ-6-14.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
n-Hexyl
HO
Me
Trans-2q
0.8241
0.8565
0.7990
1.3236
1.0153
6.3065
3.0000
3.2872
PPM
10
8
6
4
2
0

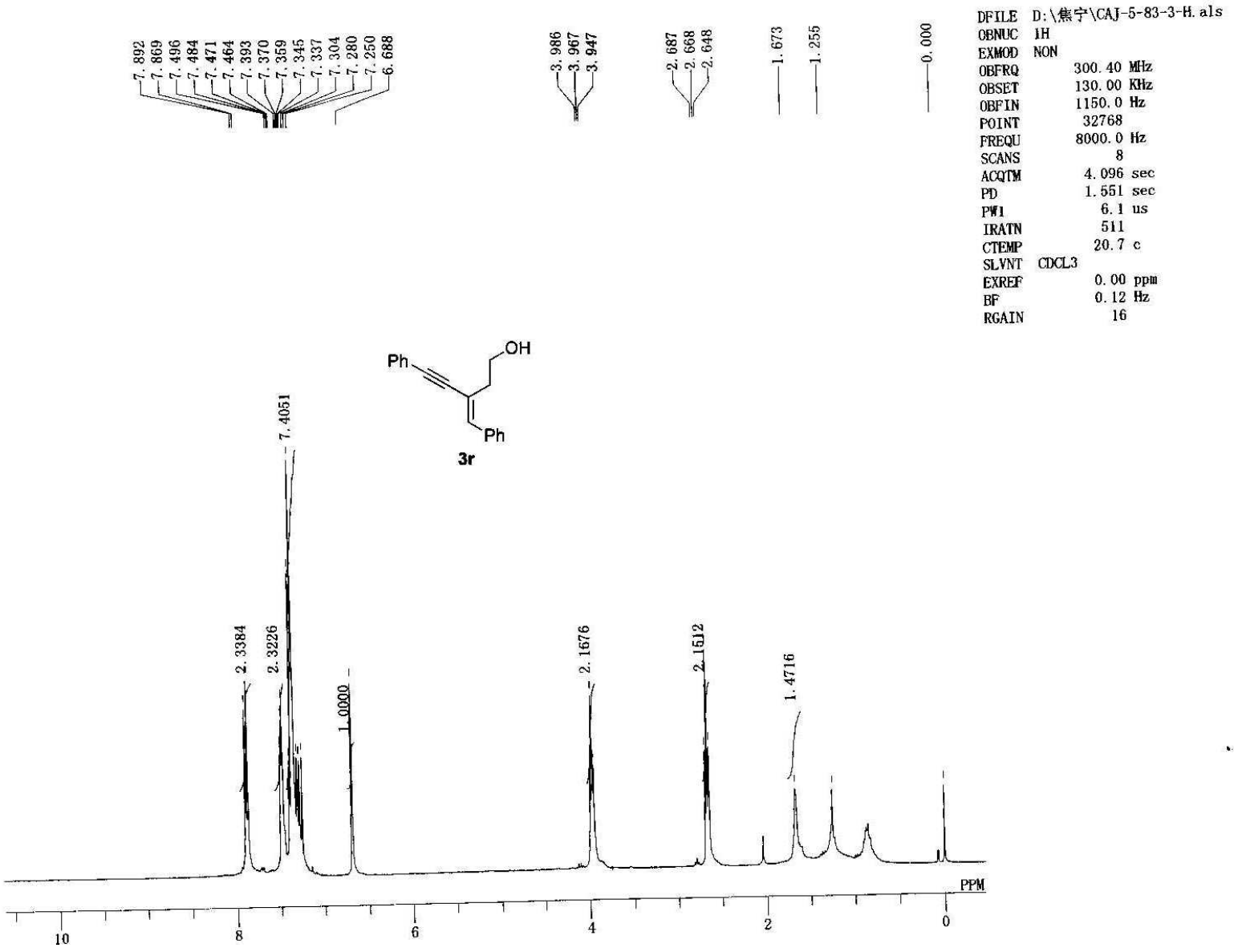

86.989
80.684
77.420
77.000
76.580
72.401
43.745
36.237
31.300
28.778
28.473
22.548
20.545
18.723
16.053
14.034
DFILE D:\焦宁\CAJ-6-14-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 504
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 22.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
n-Hexyl
HO
Me
Trans-2q
PPM
200
175
150
125
100
75
50
25
0

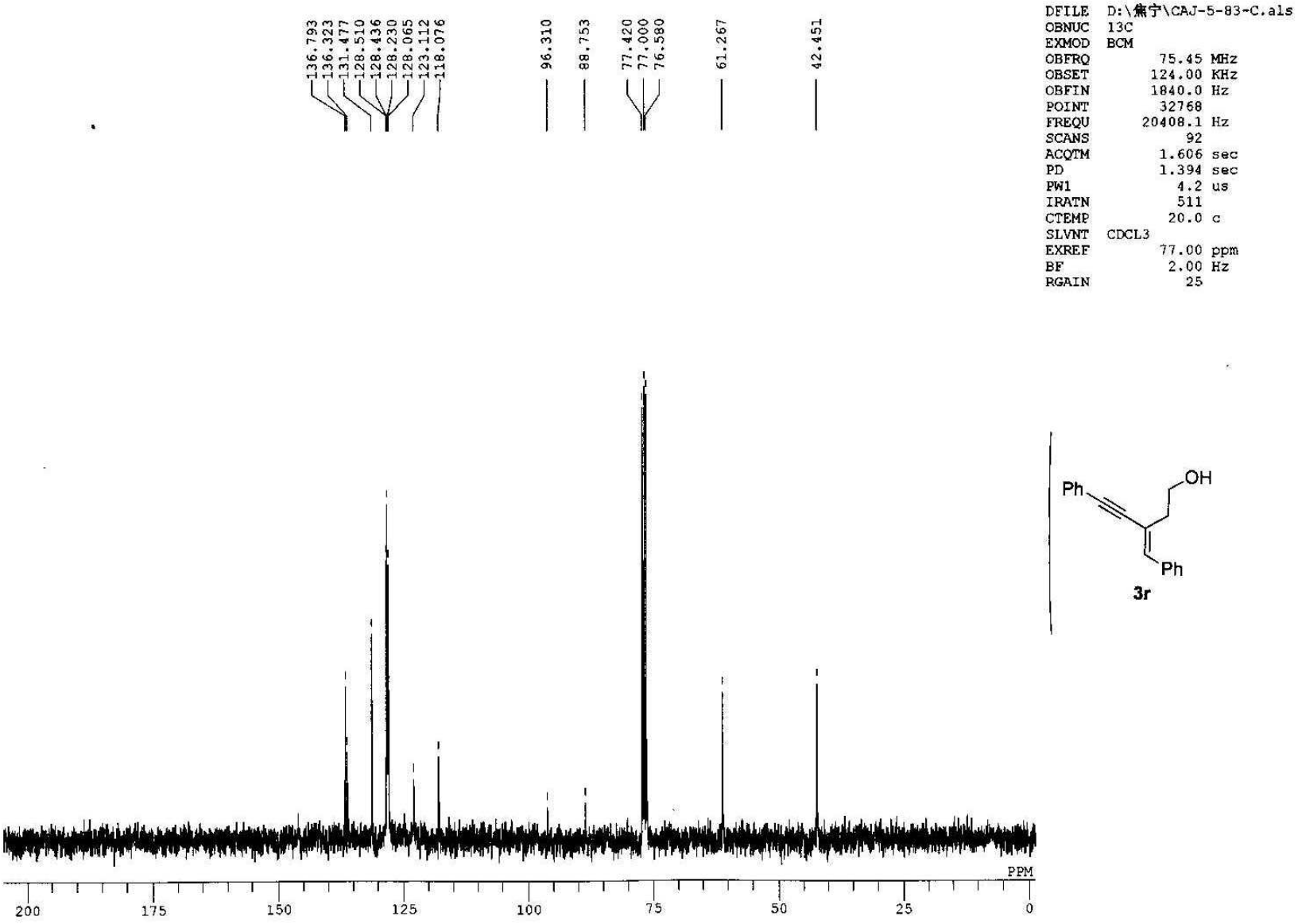

7.353
7.341
7.260
7.246
7.221
7.157
7.152
7.131
3.754
3.722
3.689
2.494
2.489
2.479
2.467
2.456
2.452
2.398
2.365
2.333
2.297
2.144
2.135
2.122
2.103
2.089
2.078
2.058
1.544
1.253
0.069
0.000
DFILE D:\焦宁\CAJ-5-82-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 24

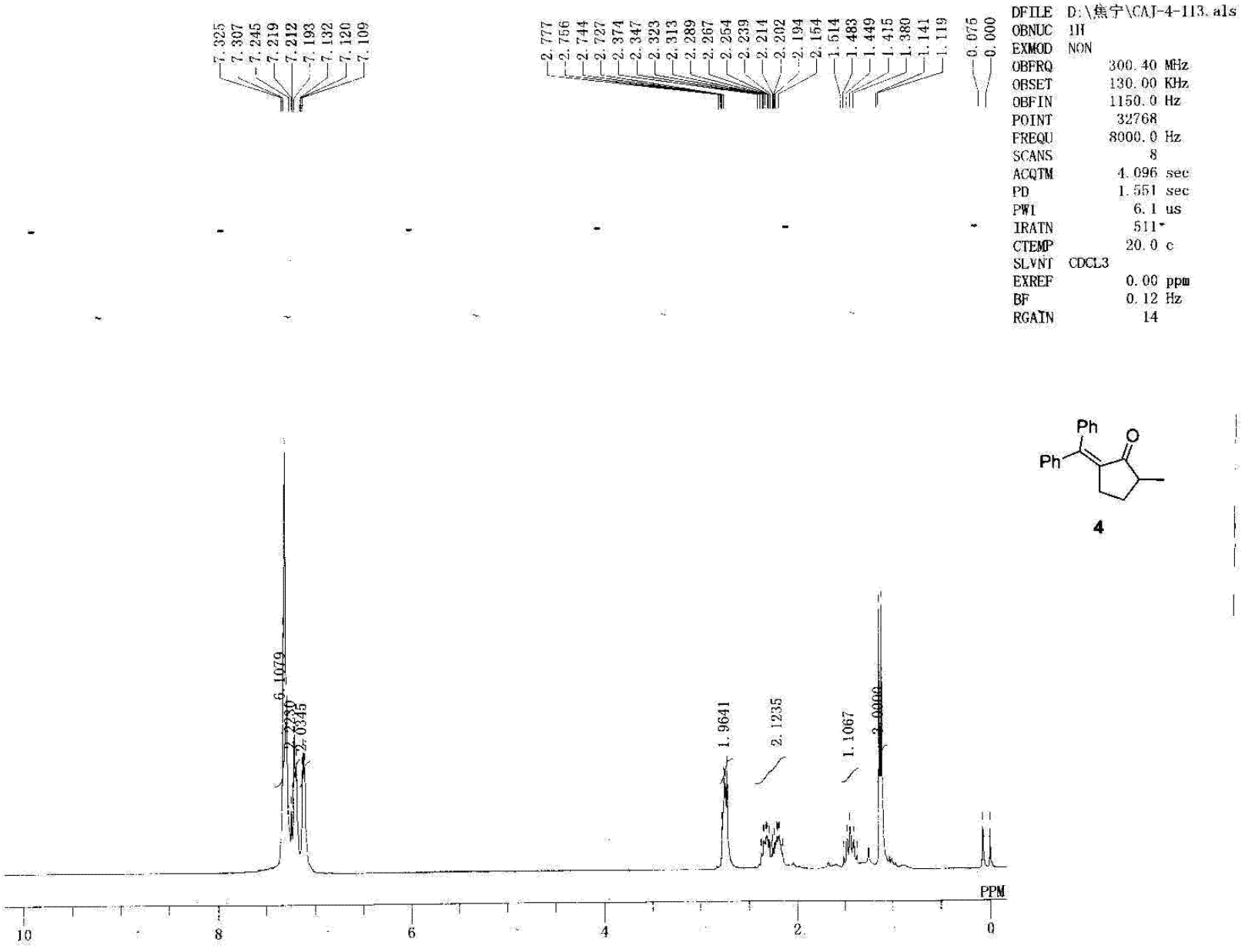

OH
Ph
Ph
4.7903
5.2910
1.0000
1.9529
1.2338
2.1314
PPM
10
8
6
4
2
0

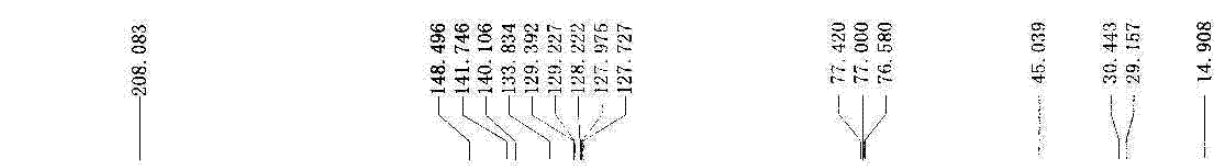
***Trans*-2r**


141.647
131.617
128.090
127.867
127.719
126.672
123.392
91.423
79.621
78.170
77.420
77.000
76.580
19.885
14.479
13.251
DFILE D:\焦宁\CAJ-5-82-C1.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 400
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
OH
Ph
Ph
Trans-2r
PPM
200
175
150
125
100
75
50
25
0

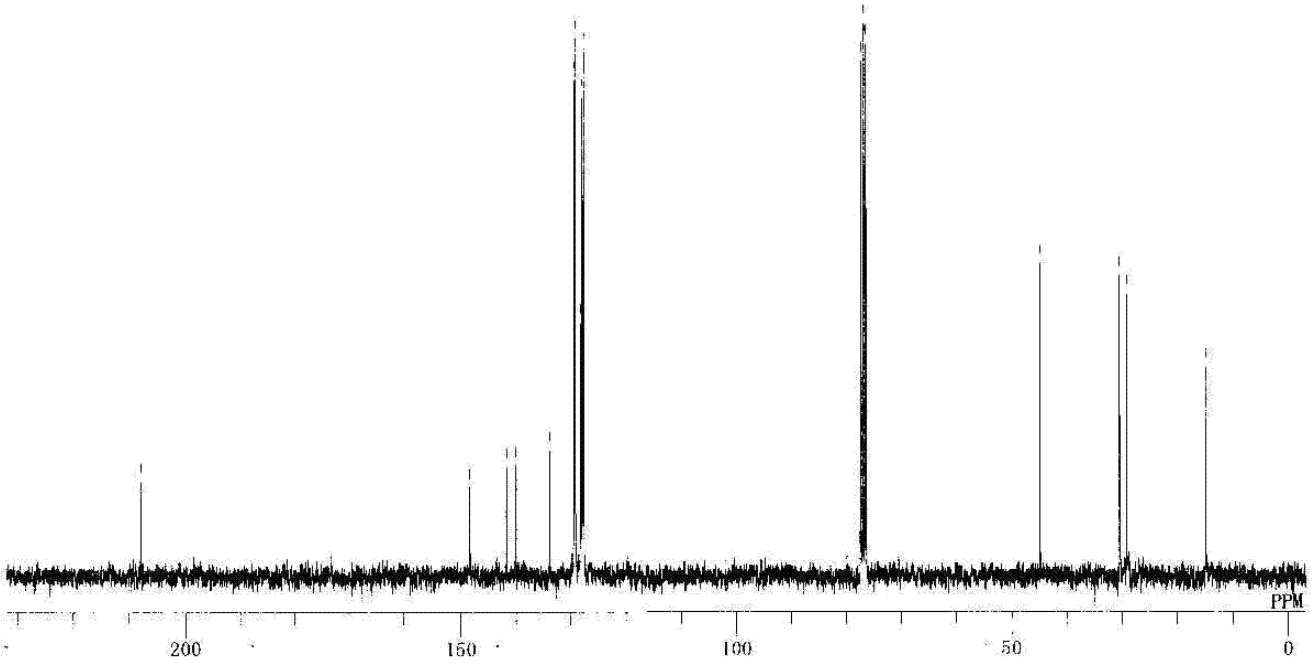

7.892
7.869
7.496
7.484
7.471
7.464
7.393
7.370
7.359
7.345
7.337
7.304
7.280
7.250
6.688
3.986
3.967
3.947
2.687
2.668
2.648
1.673
1.255
0.000
DFILE D:\焦宁\CAJ-5-83-3-H.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16
Ph
OH
Ph
3r
7.4051
2.3384
2.3226
1.0000
2.1676
2.1512
1.4716
PPM
10
8
6
4
2
0

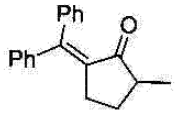

136.793
136.323
131.477
128.510
128.436
128.230
128.065
123.112
118.076
96.310
88.753
77.420
77.000
76.580
61.267
42.451
DFILE D:\焦宁\CAJ-5-83-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 92
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25
Ph
OH
Ph
3r
PPM
200
175
150
125
100
75
50
25
0


7.325
7.307
7.245
7.219
7.212
7.193
7.132
7.120
7.109
2.777
2.756
2.744
2.727
2.374
2.347
2.323
2.313
2.289
2.267
2.254
2.239
2.214
2.202
2.194
2.164
1.514
1.483
1.449
1.415
1.380
1.141
1.119
0.075
0.000
DFILE D:\焦宁\CAJ-4-113.als
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 8000.0 Hz
SCANS 8
ACQTM 4.096 sec
PD 1.551 sec
PW1 6.1 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 14
6.1079
2.2230
2.0345
1.9641
2.1235
1.1067
3.0000
PPM
10
8
6
4
2
0
Ph
Ph
O
4

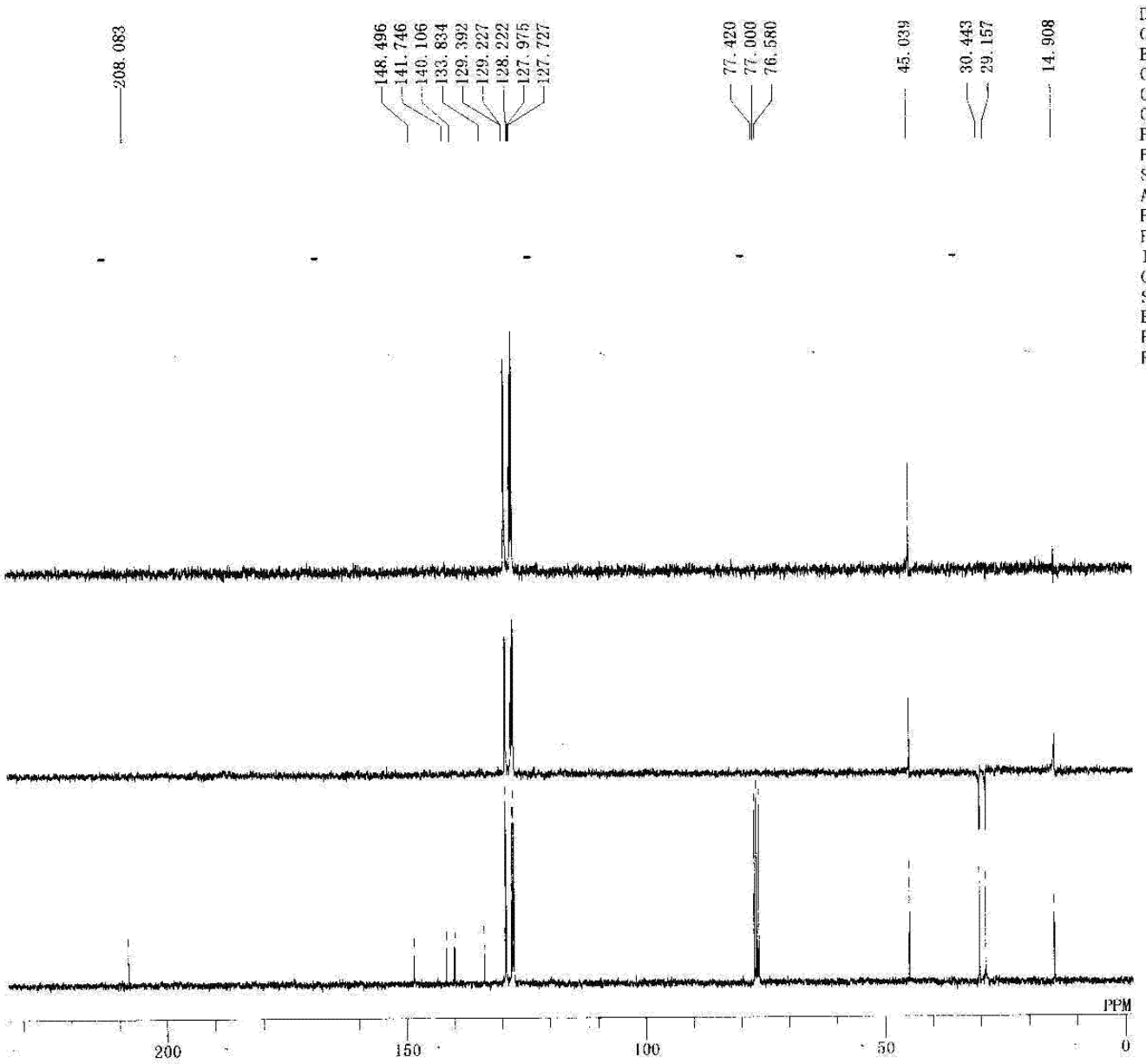


DFILE	D:\焦宁\CAJ-4-113-C.als
OBNUC	13C
EXMOD	BCM
OBFRQ	75.45 MHz
OBSET	124.00 KHz
OBFIN	1840.0 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	84
ACQTM	1.606 sec
PD	1.394 sec
PW1	4.2 us
IRATN	511
CTEMP	20.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	2.00 Hz
RGAIN	25

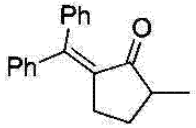




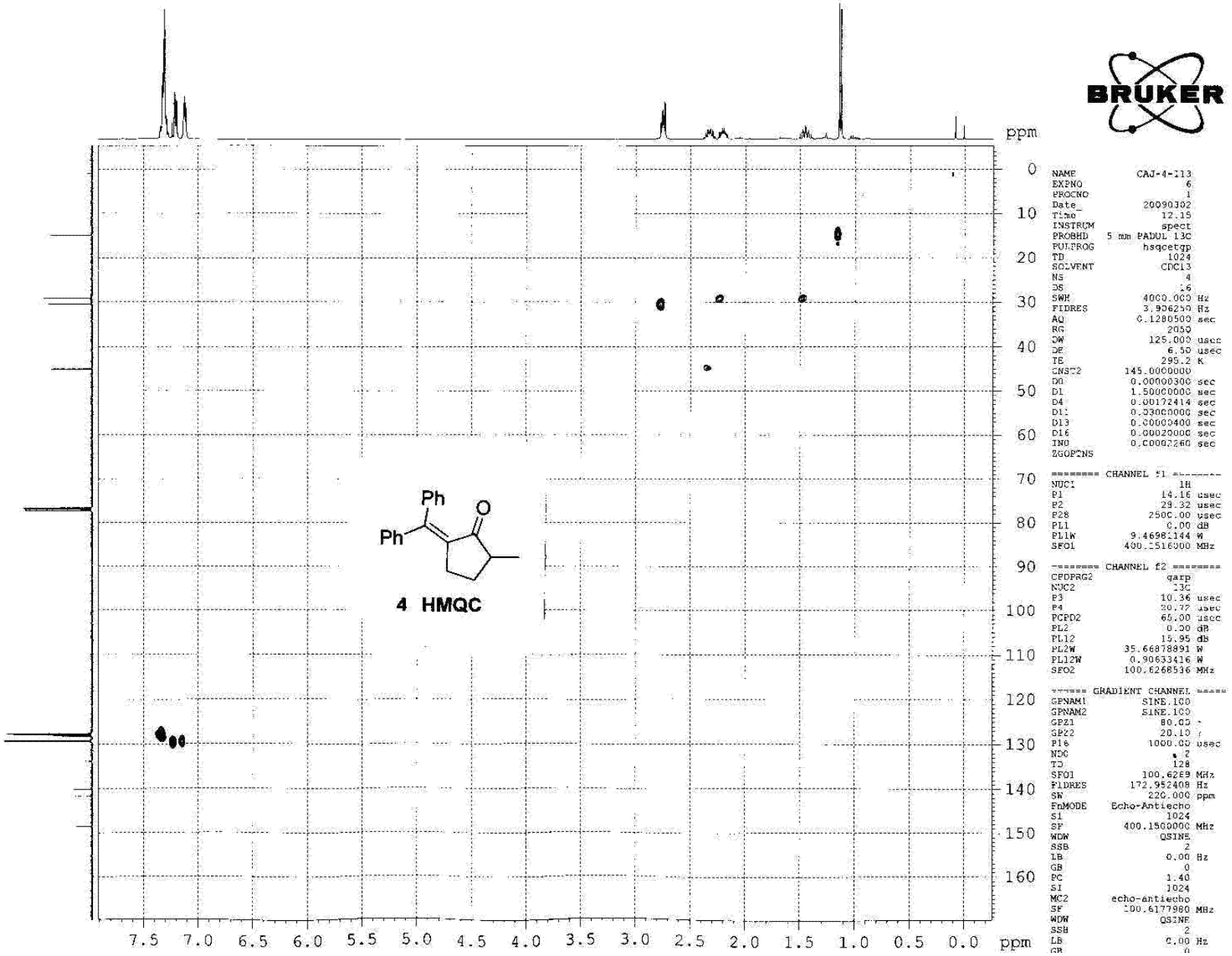
4

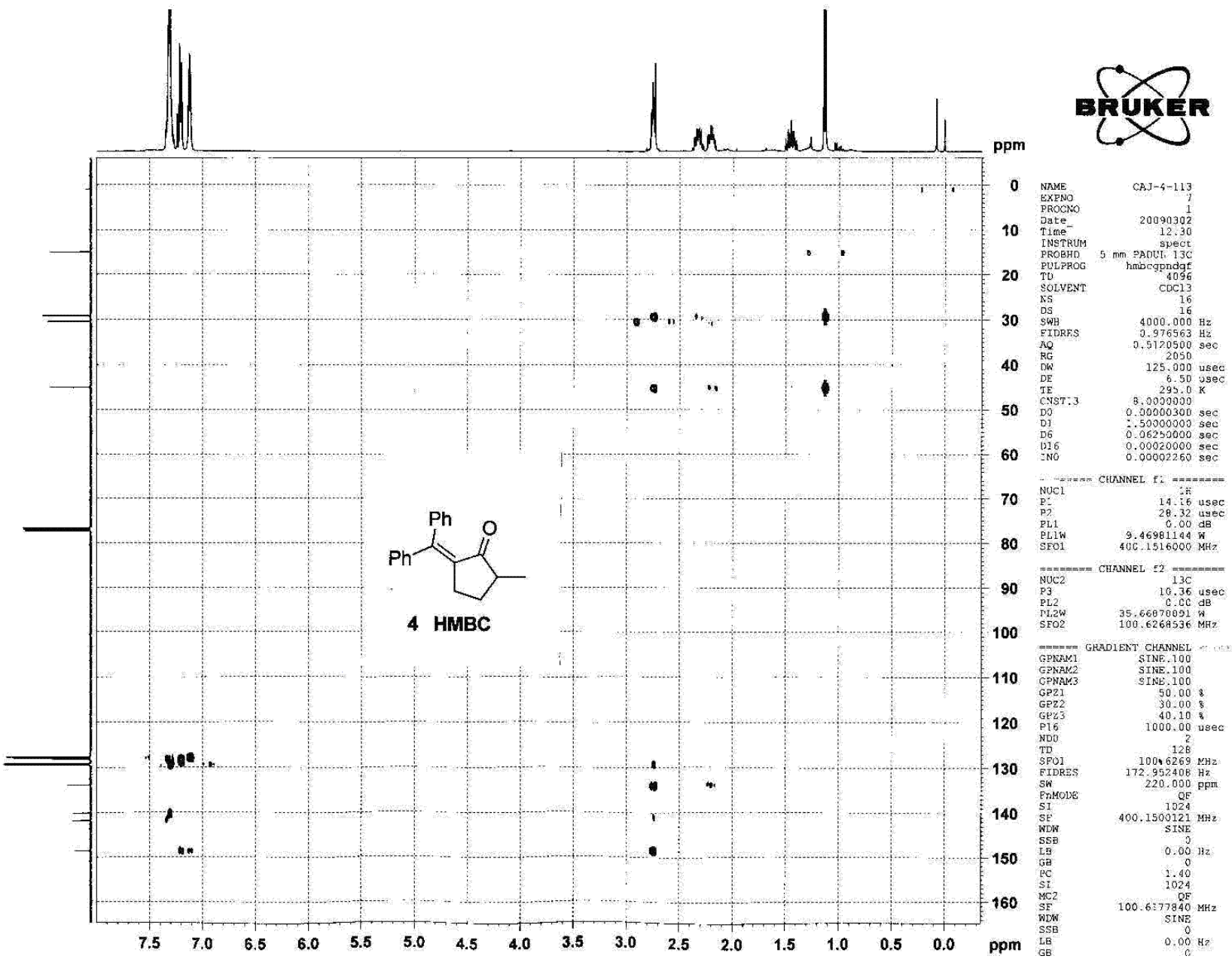


DFILE D:\焦宁\CAJ 4-113-C.als
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 124.00 KHz
OBFIN 1840.0 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 84
ACQTM 1.606 sec
PD 1.394 sec
PW1 4.2 us
IRATN 511
CTEMP 20.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 2.00 Hz
RGAIN 25



4 DEPT


ppm
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 ppm
0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
Ph
Ph
O
4 HMQC
BRUKER
NAME CAJ-4-213
EXPNO 6
PROCNO 1
Date_ 20090302
Time 12.15
INSTRUM spect
PROBHD 5 mm PABBUL 13C
PULPROG hsqcetgp
TD 1024
SOLVENT CDCl3
NS 4
DS 16
SWH 4000.000 Hz
FIDRES 3.906250 Hz
AQ 0.1280500 sec
RG 2050
DW 125.000 usec
DE 6.50 usec
TE 295.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00009400 sec
D16 0.00020000 sec
IN0 0.00002260 sec
ZGOPTNS
======== CHANNEL f1 ========
NUC1 1H
P1 14.16 usec
P2 29.32 usec
P28 2500.00 usec
PL1 0.00 dB
PL1W 9.46981144 W
SFO1 400.1516000 MHz
======== CHANNEL f2 ========
CPDPRG2 garp
NUC2 13C
P3 10.36 usec
P4 20.72 usec
PCPD2 65.00 usec
PL2 0.00 dB
PL12 19.95 dB
PL2W 35.66878891 W
PL12W 0.90633416 W
SFO2 100.6268536 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
NDO 2
TD 128
SFO1 100.6289 MHz
FIDRES 172.952408 Hz
SW 220.000 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1500000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 100.6177980 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0


ppm
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
ppm
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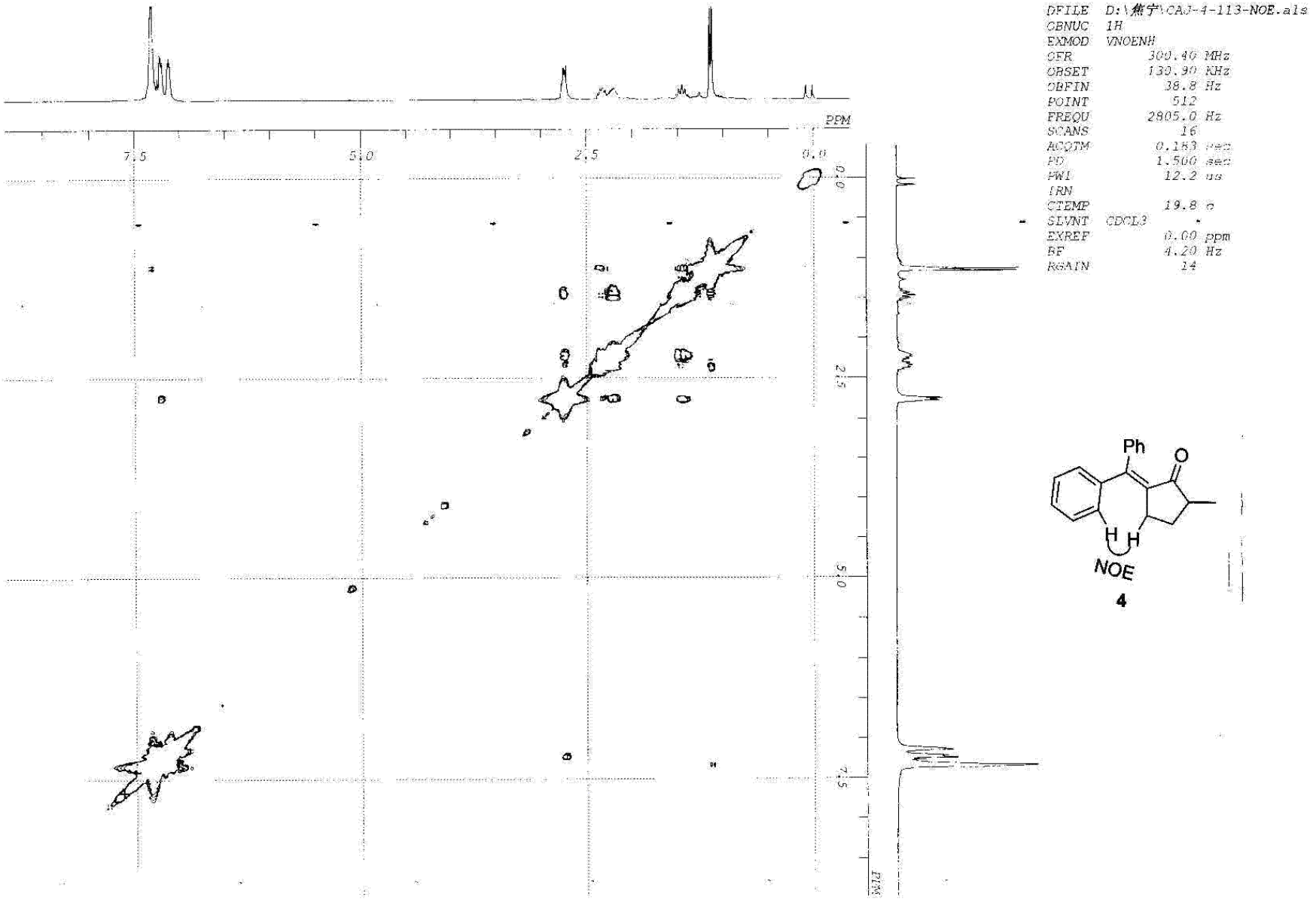
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Ph
O
Ph
4 HMBC
BRUKER
NAME CAJ-4-113
EXPNO 7
PROCNO 1
Date_ 20090302
Time 12.30
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG hmbcgpndqf
TD 4096
SOLVENT CDCl3
NS 16
DS 16
SWH 4000.000 Hz
FIDRES 0.976563 Hz
AQ 0.5120500 sec
RG 2050
DW 125.000 usec
DE 6.50 usec
TE 295.0 K
CNST13 8.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002260 sec
======== CHANNEL f1 ========
NUC1 1H
P1 14.16 usec
P2 28.32 usec
PL1 0.00 dB
PL1W 9.46981144 W
SFO1 400.1516000 MHz
======== CHANNEL f2 ========
NUC2 13C
P3 10.36 usec
PL2 0.00 dB
PL2W 35.66870091 W
SFO2 100.6268536 MHz
====== GRADIENT CHANNEL ======
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
NDO 2
TD 128
SFO1 100.6269 MHz
FIDRES 172.952408 Hz
SW 220.000 ppm
FnMODE QF
SI 1024
SF 400.1500121 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6277840 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0


DFILE D:\焦宁\CAJ-4-113-NOE.als
OBNUC 1H
EXMOD VNOENH
OFR 300.40 MHz
OBSET 130.90 KHz
OBFIN 38.8 Hz
POINT 512
FREQU 2805.0 Hz
SCANS 16
ACQTM 0.183 sec
PD 1.500 sec
PW1 12.2 us
IRN
CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 4.20 Hz
RGAIN 14
PPM
7.5
5.0
2.5
0.0
Ph
O
H
H
NOE
4