Supporting Information

Cationic Ir(I)-Catalyzed sp^3 C-H Bond Alkenylation of Amides with Alkynes

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General

Anhydrous dichloromethane (CH_2Cl_2), acetone, diethyl ether (Et_2O), and chlorobenzene (PhCl) were purchased and dried over activated molecular sieves 4A. All solvents were degassed by argon bubbling prior to use. All reactions were carried out under an atmosphere of argon in oven-dried glassware with a magnetic stirring bar. *racemic*-2,2'-Bis(diphenylphosphino)-binaphthyl (*rac*-BINAP) was purchased from Strem. Amides **1b, c**,[1] and alkynes **1b-e**[2] were prepared by the literature procedures. The other substrates are commercially available.

IR spectra were recorded with a JASCO FT/IR-4100 spectrometer. NMR spectra were recorded with a JEOL AL-400 (400 MHz), Lambda-500 (500 MHz), or Bruker Avance-600 (600 MHz) spectrometer using tetramethylsilane as an internal standard and $CDCl_3$ as a solvent. High-resolution mass spectra (HRMS) were measured on a JEOL JMS-SX102A with FAB (Fast Atomic Bombardment) method.

Experimental Procedures

Preparation of [Ir(cod)$_2$]OTf: To a solution of $[IrCl(cod)]_2$ (400.1 mg, 0.60 mmol) in CH_2Cl_2 (4 mL) was added 1,5-cyclooctadiene (0.22 mL, 0.90 mmol) and a solution of AgOTf (353.1 mg, 1.37 mmol) in acetone (2 mL), and then the resultant solution was stirred for 20 min at ambient temperature. After removal of a precipitate by celite filtration and evaporation of solvents, black solid was formed. This solid was washed with a small amount of cold Et_2O under reduced pressure, and then dried in vacuo over 2 h to give analytically pure $[Ir(cod)_2]OTf$ as a lustrous black solid (96%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ = 2.29-2.35 (m, 8H), 2.49-2.51 (m, 8H), 4.86 (s, 8H). Anal. Calcd for $C_{17}H_{24}F_3O_3SIr$: C, 36.61; H, 4.34. Found: C, 36.52; H, 4.27. $[Ir(cod)_2]BF_4$, $[Ir(cod)_2]PF_6$, and $[Ir(cod)_2]SbF_6$ could be prepared by the similar method.

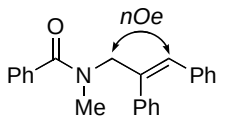
A Typical Experimental Procedure of Ir(I)-Catalyzed Alkenylation of sp^3 C-H bonds (Table 1, entry 3): $[Ir(cod)_2]OTf$ (5.7 mg, 10 μmol) and *rac*-BINAP (6.8 mg, 11 μmol) were placed in a Schlenk tube, which was then evacuated and backfilled with argon (x3). To the reaction vessel were added *N*,*N*-dimethylbenzamide (**1a**) (15.0 mg, 0.1 mmol), diphenylacetylene (**2a**) (36.6 mg, 0.2 mmol), and PhCl (0.2 mL). The solution was then stirred at 135 ˚C for 24 h. After completion of the reaction, the solvent were evaporated. The crude products were purified by thin-layer chromatography (hexane/AcOEt = 1/1) to give analytically pure **3aa** (75%) and **3aa'** (4%).

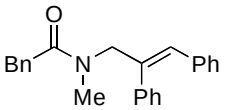
References

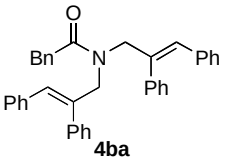
(1) Buswell, M.; Fleming, I.; Ghosh, U.; Mack, S.; Russell, M.; Clark, B. P. *Org. Biomol. Chem.* **2004**, *2*, 3006.

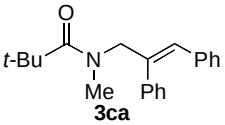
(2) Mio, M. J.; Kopel, L. C.; Braun, J. B.; Gadzikwa, T. L.; Hull, K. L.; Brisbois, R. G.; Markworth, C. J.; Grieco, P. A. *Org. Lett.* **2002**, *4*, 3199.

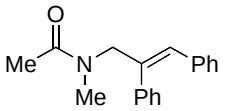
Characterization Table

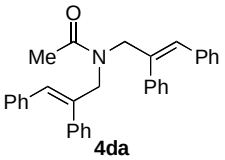
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3aa**	(400 MHz) 2.81, 3.17 (s, 3H), 4.19, 4.67 (s, 2H), 6.49, 6.62 (s, 1H), 6.95-7.30 (m, 15H)	(100 MHz) 33.4, 36.9, 54.0, 59.5, 126.6, 126.9, 127.1, 127.6, 127.7, 128.0, 128.1, 128.2, 128.4, 128.6, 128.9, 129.1, 129.3, 129.5, 135.8, 136.1, 136.1, 136.3, 136.4, 137.4, 137.9, 138.1, 138.3, 138.3, 171.4, 172.4
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1636, 1396, 698	Found m/z 328.1666 [M+H] calcd. for $C_{23}H_{22}NO$: 328.1701
N-methyl-*N*-((*E*)-2,3-diphenylallyl)benzamide		**State:** pale yellow oil

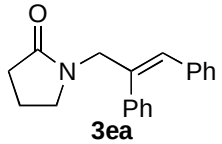
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ba**	(400 MHz) 2.88, 3.05 (s, 3H), 3.58, 3.65 (s, 2H), 4.21, 4.51 (s, 2H), 6.38, 6.43 (s, 1H), 6.91-7.37 (m, 15H)	(100 MHz) 34.0, 34.9, 40.5, 41.3, 54.2, 58.0, 126.5, 126.7, 126.8, 127.1, 127.4, 127.5, 127.8, 127.9, 128.0, 128.3, 128.5, 128.5, 128.6, 128.8, 129.1, 129.1, 129.2, 134.8, 135.1, 135.7, 136.4, 136.7, 138.0, 138.1, 138.6, 170.9, 171.5
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	(CH_2Cl_2) 1646, 1447, 697	Found m/z 342.1850 [M+H] calcd. for $C_{24}H_{24}NO$: 342.1858
N-methyl-2-phenyl-*N*-(2,3-diphenylallyl)acetamide		**State:** colorless oil

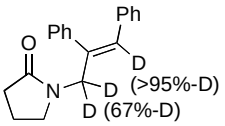
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **4ba**	(400 MHz) 3.54 (s, 2H), 4.11, 4.63 (s, 4H), 6.44, 6.47 (s, 2H), 6.86-7.55 (m, 25H)	(100 MHz) 40.9, 51.3, 54.2, 126.5, 126.9, 127.2, 127.4, 127.6, 127.9, 127.9, 128.1, 128.2, 128.3, 128.4, 128.5, 128.6, 128.9, 129.2, 129.2, 129.2, 131.6, 134.9, 135.7, 136.3, 136.7, 137.9, 138.8, 171.4
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1647, 1445, 695	Found m/z 519.2569 [M] calcd. for $C_{38}H_{33}NO$: 519.2562
2-phenyl-*N*,*N*-bis(2,3-diphenylallyl)acetamide		**State:** yellow oil

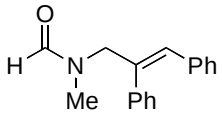
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ca**	(400 MHz) 1.19 (s, 9H), 3.06 (s, 3H), 4.43 (s, 2H), 6.40 (s, 1H), 6.96-7.30 (m, 10H)	(125 MHz) 28.2, 36.4, 38.9, 56.7, 126.7, 126.9, 127.5, 127.9, 128.6, 128.7, 129.2, 136.4, 138.1, 138.6, 177.6
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1632, 1479, 696	Found m/z 308.2024 [M+H] calcd. for $C_{21}H_{26}NO$: 308.2014
N-methyl-*N*-(2,3-diphenylallyl)pivalamide		**State:** colorless oil

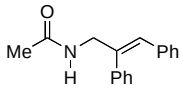
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3da**	(400 MHz) 1.99, 2.00 (s, 3H), 2.92, 3.01 (s, 3H), 4.20, 4.46 (s, 2H), 6.42, 6.47 (s, 1H), 6.94-7.37 (m, 10H)	(100 MHz) 21.1, 21.6, 33.6, 35.3, 54.0, 58.7, 126.7, 127.1, 127.3, 127.4, 127.7, 127.8, 127.8, 128.0, 128.2, 128.5, 128.7, 129.0, 129.1, 129.2, 135.7, 136.4, 136.8, 137.9, 138.2, 138.6, 170.5, 171.1
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1651, 1399, 699	Found m/z 266.1539 [M+H] calcd. for $C_{18}H_{20}NO$: 266.1545
N-methyl-*N*-(2,3-diphenylallyl)acetamide		**State:** colorless oil

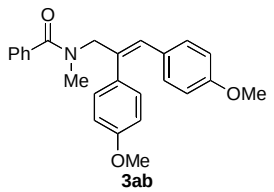
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **4da**	(400 MHz) 1.96 (s, 3H), 4.15, 4.56 (s, 4H), 6.43, 6.51 (s, 2H), 6.94-7.38 (m, 20H)	(100 MHz) 21.3, 51.4, 55.1, 126.8, 127.2, 127.4, 127.5, 127.8, 127.9, 128.1, 128.2, 128.3, 128.6, 128.8, 129.1, 129.2, 129.3, 135.7, 136.4, 136.7, 137.8, 138.4, 138.8, 171.0
	IR (cm^{-1})	**HRMS (FAB^{+}) (m/z)**
	($CDCl_3$) 1651, 1443, 697	Found m/z 444.2320 [M+H] calcd. for $C_{32}H_{30}NO$: 444.2328
N,*N*-bis(2,3-diphenylallyl)acetamide		**State:** yellow oil

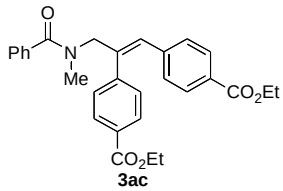
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ea**	(400 MHz) 1.84-1.92 (m, 2H), 2.28 (t, *J* = 8.0, 2H), 3.31 (t, *J* = 7.1, 2H), 4.32 (s, 2H), 6.53 (s, 1H), 6.98-7.31 (m, 10H)	(100 MHz) 17.9, 30.8, 46.8, 50.1, 126.9, 127.6, 127.9, 128.3, 128.5, 128.7, 129.2, 136.3, 137.4, 138.1, 174.8
	IR (cm^{-1})	**HRMS (FAB^{+}) (m/z)**
	(CH_2Cl_2) 1684, 1438, 697	Found m/z 278.1564 [M+H] calcd. for $C_{19}H_{20}NO$: 278.1545
1-(2,3-diphenylallyl)pyrrolidin-2-one		**State:** white solid mp 104-105 ˚C

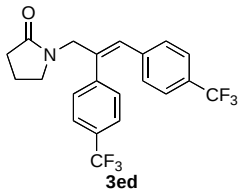
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ea-*d*$_3$**	(400 MHz) 1.84-1.91 (m, 2H), 2.28 (t, *J* = 8.0, 2H), 3.30 (t, *J* = 7.1, 2H), 4.30-4.32 (m, 0.66H), 6.53 (s, <0.05H), 6.98-7.28 (m, 10H)	-
	IR (cm^{-1})	**HRMS (FAB^{+}) (m/z)**
	-	-
-		**State:** white solid

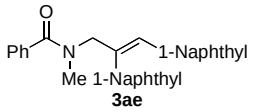
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3fa**	(400 MHz) 2.87, 2.89 (s, 3H), 4.17, 4.40 (s, 2H), 6.54, 6.56 (s, 1H), 6.96-7.35 (m, 10H), 7.89, 7.99 (s, 1H)	(100 MHz) 29.4, 34.1, 51.2, 58.0, 126.9, 127.3, 127.7, 127.9, 127.9, 128.0, 128.3, 128.6, 128.8, 129.1, 129.2, 129.2, 129.7, 135.6, 136.2, 136.6, 136.7, 137.7, 137.8, 162.4, 162.9
	IR (cm^{-1})	**HRMS (FAB^{+}) (m/z)**
	(CH_2Cl_2) 1676, 1395, 698	Found m/z 252.1349 [M+H] calcd. for $C_{17}H_{18}NO$: 252.1388
N-methyl-*N*-(2,3-diphenylallyl)formamide		**State:** pale yellow solid mp 83-84 ˚C

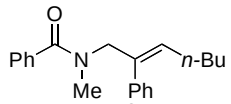
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ga**	(400 MHz) 1.92, 1.97 (s, 3H), 3.64, 3.86 (s, 2H), 6.97 (s, 1H), 7.09-7.39 (m, 10H)	(100 MHz) 23.3, 23.4, 35.0, 42.4, 119.6, 119.6, 121.5, 122.5, 125.7, 126.2, 126.6, 126.7, 127.5, 127.9, 128.2, 128.3, 128.5, 128.8, 128.9, 129.0, 138.0, 138.1, 139.1, 140.5, 167.1, 167.3
	IR (cm^{-1})	**HRMS (FAB^{+}) (m/z)**
	(CH_2Cl_2) 3435, 1647, 1523, 1491, 696	Found m/z 252.1365 [M+H] calcd. for $C_{17}H_{18}NO$: 252.1388
N-(2,3-diphenylallyl)acetamide		**State:** white solid mp 148-150 ˚C

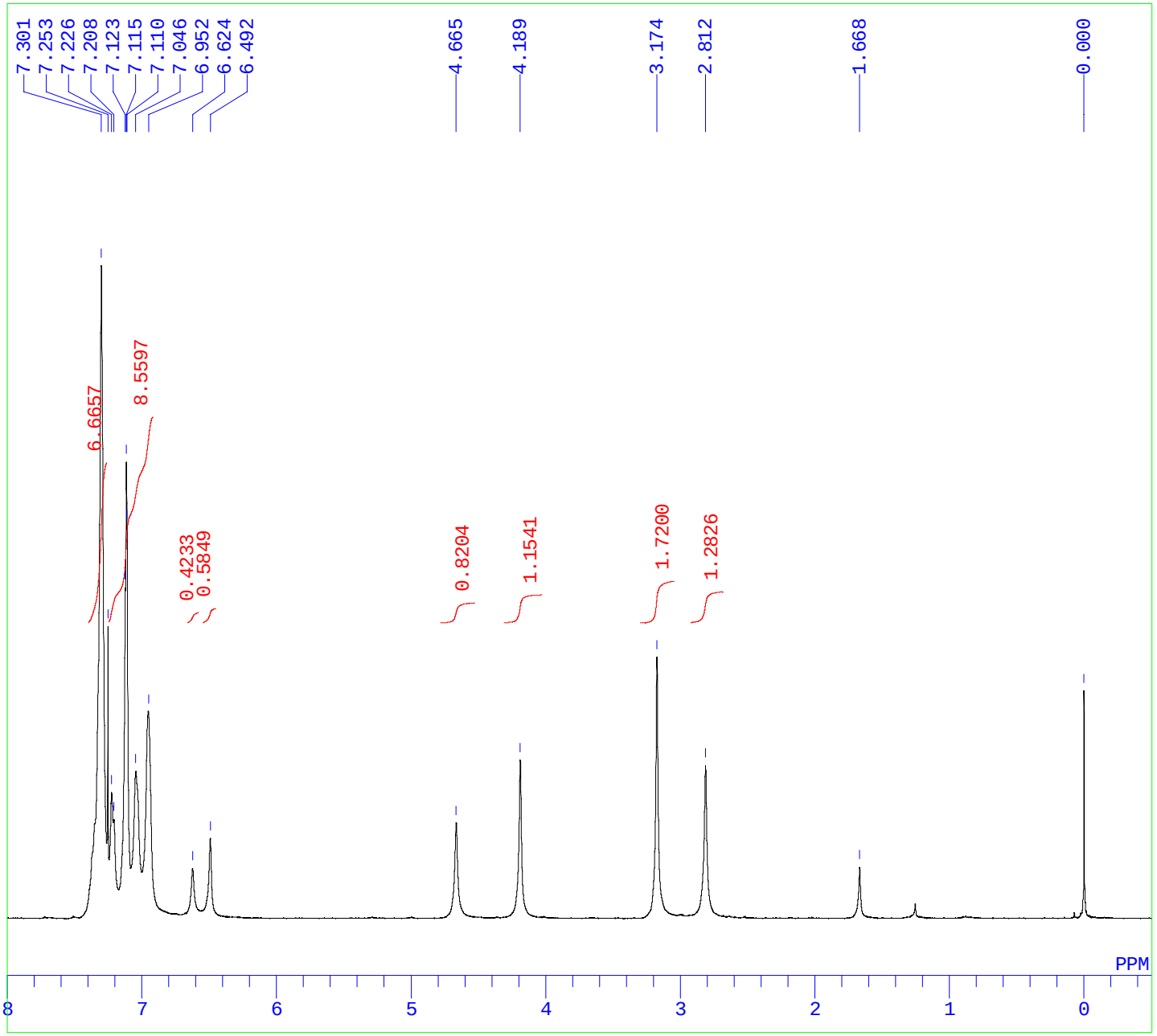
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ab**	(400 MHz) 2.79, 3.14 (s, 3H), 3.74, 3.81 (s, 6H), 4.15, 4.62 (s, 2H), 6.39, 6.52 (s, 1H), 6.66-7.36 (m, 13H)	(125 MHz) 33.2, 36.7, 53.4, 54.0, 54.9, 55.1, 55.2, 59.6, 112.1, 113.5, 114.0, 114.4, 126.7, 127.6, 128.1, 128.3, 128.7, 129.3, 129.3, 129.6, 129.7, 130.1, 130.2, 130.4, 130.5, 130.6, 131.6, 131.8, 132.4, 134.9, 135.6, 136.2, 156.7, 158.4, 158.6, 159.1, 171.3, 172.3
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	(Acetone) 1635, 1509, 1249	Found m/z 388.1908 [M+H] calcd. for $C_{25}H_{26}NO_3$: 388.1913
N-(2,3-bis(4-methoxyphenyl)allyl)-*N*-methylbenzamide		**State:** pale yellow oil

Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ac**	(400 MHz) 1.35, 1.40 (t, *J* = 7.1, 3H), 2.85, 3.17 (s, 3H), 4.26, 4.70 (s, 2H), 4.32, 4.39 (q, *J* = 7.1, 4H), 6.60, 6.73 (s, 1H), 6.99-8.00 (m, 13H)	(125 MHz) 14.3, 14.3, 29.7, 33.5, 33.6, 37.2, 37.2, 53.4, 53.9, 59.0, 60.9, 61.1, 126.4, 126.7, 128.2, 128.2, 128.4, 128.5, 128.5, 128.6, 129.0, 129.1, 129.2, 129.4, 129.6, 129.7, 130.0, 130.2, 136.0, 139.2, 139.6, 140.6, 142.5, 166.2, 171.5, 172.3
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1715, 1636, 1397, 1276, 731	Found m/z 472.2144 [M+H] calcd. for $C_{29}H_{30}NO_5$: 472.2124
N-(2,3-bis(4-(ethoxycarbonyl)phenyl)allyl)-*N*-methylbenzamide		**State:** pale yellow oil

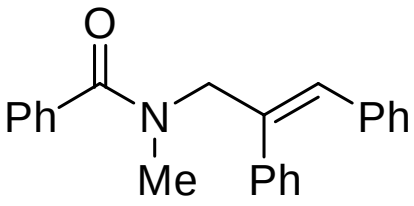
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ed**	(500 MHz) 1.89-1.95 (m, 2H), 2.30 (t, *J* = 8.1, 2H), 3.32 (t, *J* = 7.0, 2H), 4.36 (s, 2H), 6.64 (s, 1H), 7.06 (d, *J* = 8.2, 2H), 7.32 (d, *J* = 8.1, 2H), 7.39 (d, *J* = 8.2, 2H), 7.56 (d, *J* = 8.1, 2H)	(125 MHz) 17.8, 30.6, 46.9, 49.7, 123.9 (q, *J* = 271.8, 2C), 125.1 (q, *J* = 3.8), 125.7 (q, *J* = 3.4), 128.1, 129.1, 129.1 (q, *J* = 32.4), 129.4, 130.1 (q, *J* = 32.7), 138.7, 139.3, 141.3, 175.0
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	(KBr disk) 1682, 1333, 1111, 868, 665	Found m/z 414.1317 [M+H] calcd. for $C_{21}H_{18}F_6NO$: 414.1293
	Anal. (CHN)	
	Found C, 61.03; H, 3.95; N, 3.27	Calcd. For $C_{21}H_{17}F_6NO$ C,61.02; H,4.15; N, 3.39
1-(2,3-bis(4-(trifluoromethyl)phenyl)allyl)pyrrolidin-2-one		**State:** pale yellow solid mp 123-124 ˚C

Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3ae**	(400 MHz) 2.93, 3.16, 3.34, 3.39 (s, 3H), 4.33-4.48, 4.67-4.83 (m, 2H), 6.81-8.29 (m, 20H)	(150 MHz) 33.3, 33.7, 37.4, 38.7, 53.1, 55.6, 57.4, 59.0, 91.4, 92.2, 93.4, 94.5, 120.3, 120.6, 120.8, 121.1, 123.7, 123.8, 123.9, 124.3, 124.4, 125.1, 125.2, 125.3, 125.3, 125.4, 125.5, 125.7, 125.8, 126.0, 126.0, 126.1, 126.2, 126.3, 126.3, 126.4, 126.6, 126.8, 127.0, 127.1, 127.2, 127.6, 127.7, 127.8, 127.9, 128.1, 128.2, 128.3, 128.4, 128.5, 128.6, 128.7, 128.9, 129.2, 129.4, 129.6, 129.7, 130.8, 131.4, 131.5, 131.5, 131.6, 131.8, 131.9, 132.7, 132.7, 133.0, 133.2, 133.3, 133.5, 133.6, 134.3, 135.5, 135.8, 136.2, 136.3, 136.5, 137.2, 138.1, 171.4, 171.7, 172.5, 172.6
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 1635, 1395, 778, 730	Found m/z 450.1790 [M+Na] calcd. for $C_{31}H_{25}NONa$: 450.1834
N-methyl-*N*-(2,3-di(naphthalen-1-yl)allyl)benzamide		**State:** pale yellow oil
We speculate that **3ae** was obtained as a mixture of rotamers derived from axial chirality.		

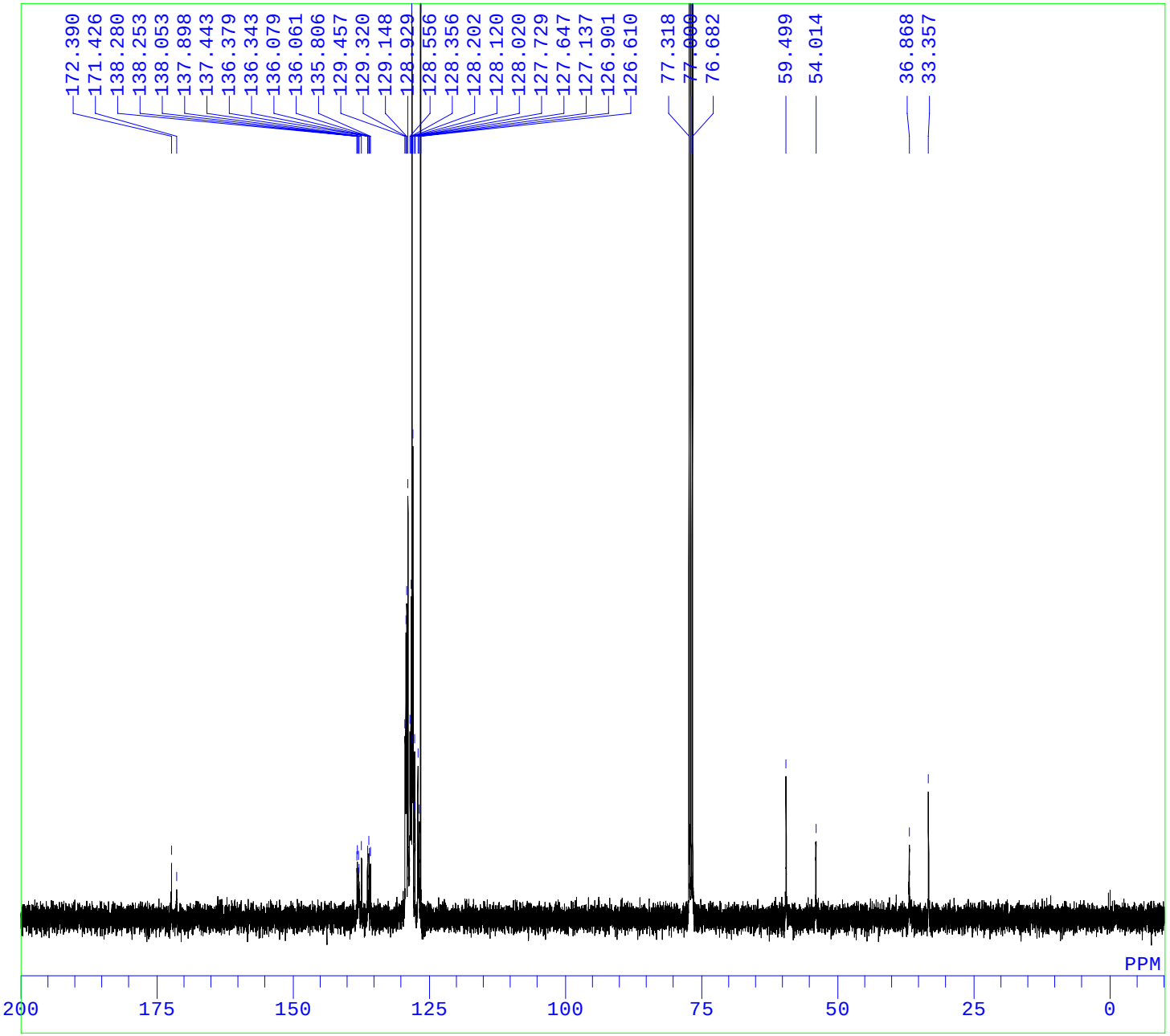
Product	^{1}H NMR ($CDCl_3$) δ, *J* (Hz)	^{13}C NMR ($CDCl_3$) δ, *J* (Hz)
 **3af**	(400 MHz) 0.83 (t, *J* = 6.8, 3H), 1.22-1.37 (m, 4H), 1.94-1.99, 2.08-2.13 (m, 2H), 2.74, 3.08 (s, 3H), 4.03, 4.51 (s, 2H), 5.58, 5.67 (t, *J* = 7.1, 1H), 6.89-7.35 (m, 10H)	(150 MHz) 13.9, 22.2, 28.3, 28.5, 31.9, 32.1, 32.9, 36.6, 53.2, 58.4, 126.6, 127.1, 127.2, 128.1, 128.2, 128.3, 128.4, 128.7, 129.2, 129.3, 130.6, 130.8, 135.8, 136.0, 136.2, 136.6, 138.1, 138.2, 171.2, 172.2
	IR (cm^{-1})	**HRMS (FAB^+) (m/z)**
	($CDCl_3$) 2956, 1637, 1397, 700	Found m/z 308.1988 [M+H] calcd. for $C_{21}H_{26}NO$: 308.2014
N-methyl-*N*-(2-phenylhept-2-enyl)benzamide		**State:** colorless oil



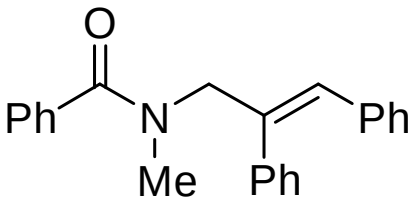

```
DFILE   C:\sp3C-H\3aa-1H.als
COMNT
DATIM   Sun Jan 18 22:16:11 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          25.0 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            15
```



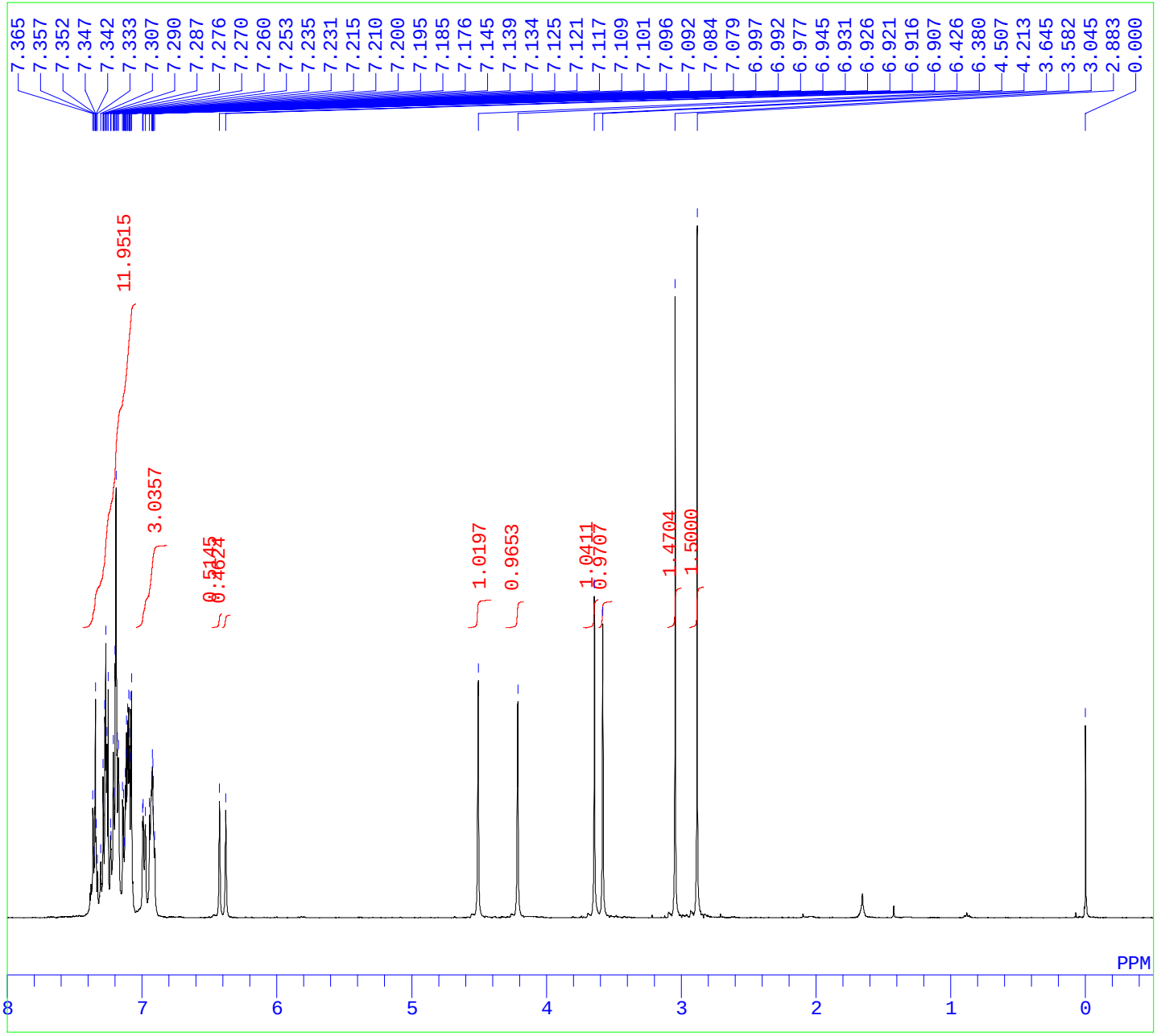
3aa



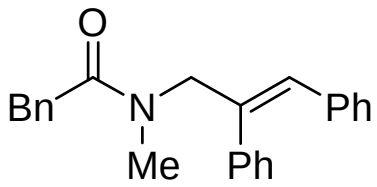

```
DFILE  C:\sp3C-H\3aa-13C.als
COMNT
DATIM  Mon Jan 19 00:34:30 2009
OBNUC  13C
EXMOD  BCM
OBFRQ       100.40 MHz
OBSET       125.00 KHz
OBFIN      10500.0 Hz
POINT        32768
FREQU      29962.5 Hz
SCANS         2840
ACQTM        1.094 sec
PD           1.792 sec
PW1            4.7 us
IRNUC  1H
CTEMP         23.4 c
SLVNT  CDCL3
EXREF        77.00 ppm
BF            0.12 Hz
RGAIN           25
```



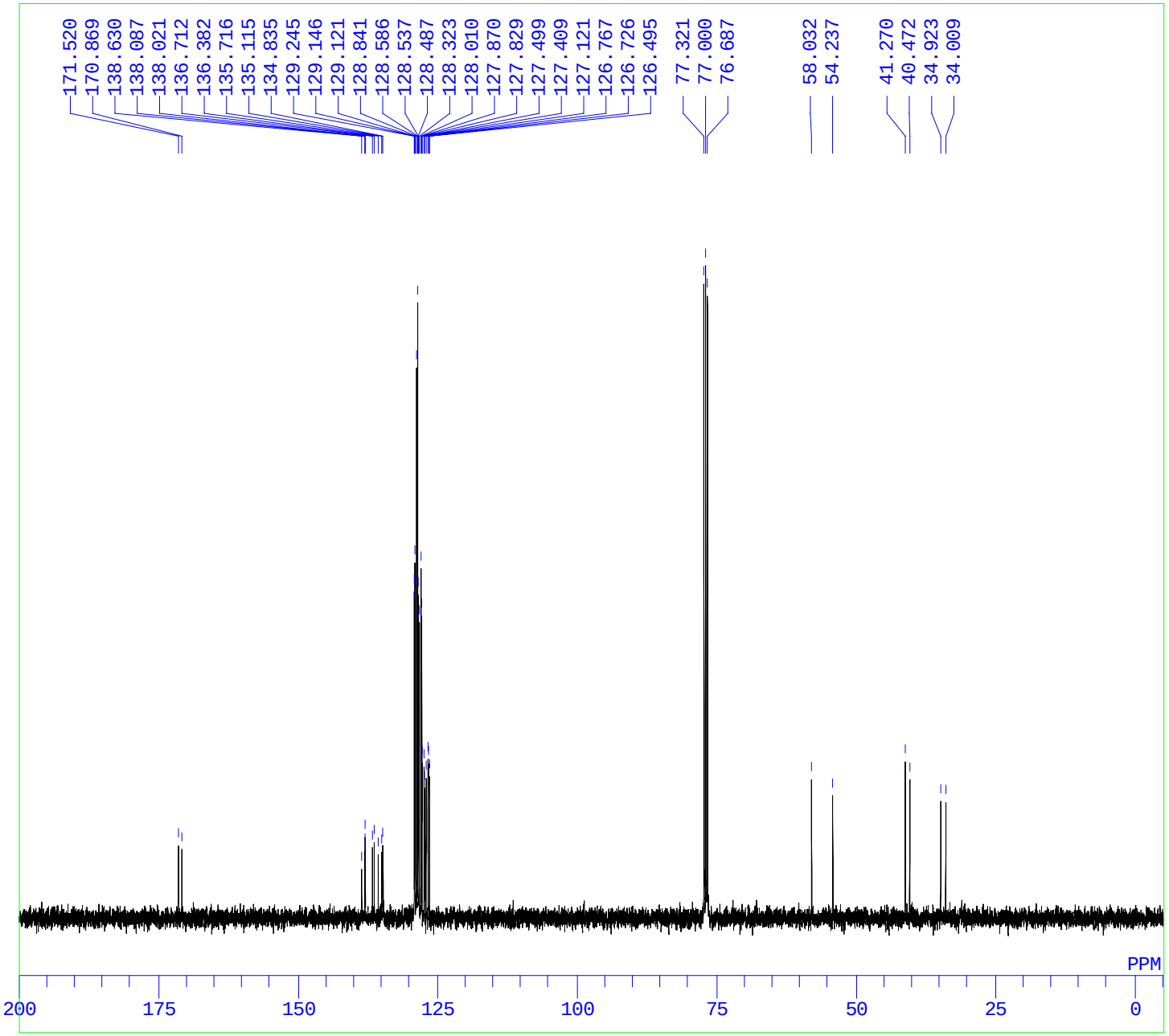
3aa



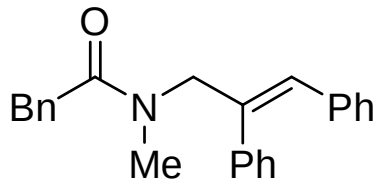

```
DFILE   C:\sp3C-H\3ba-1H.als
COMNT
DATIM   Fri Dec 19 11:24:54 2008
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            1.500 sec
PW1             6.6 us
IRNUC   1H
CTEMP          23.5 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            17
```



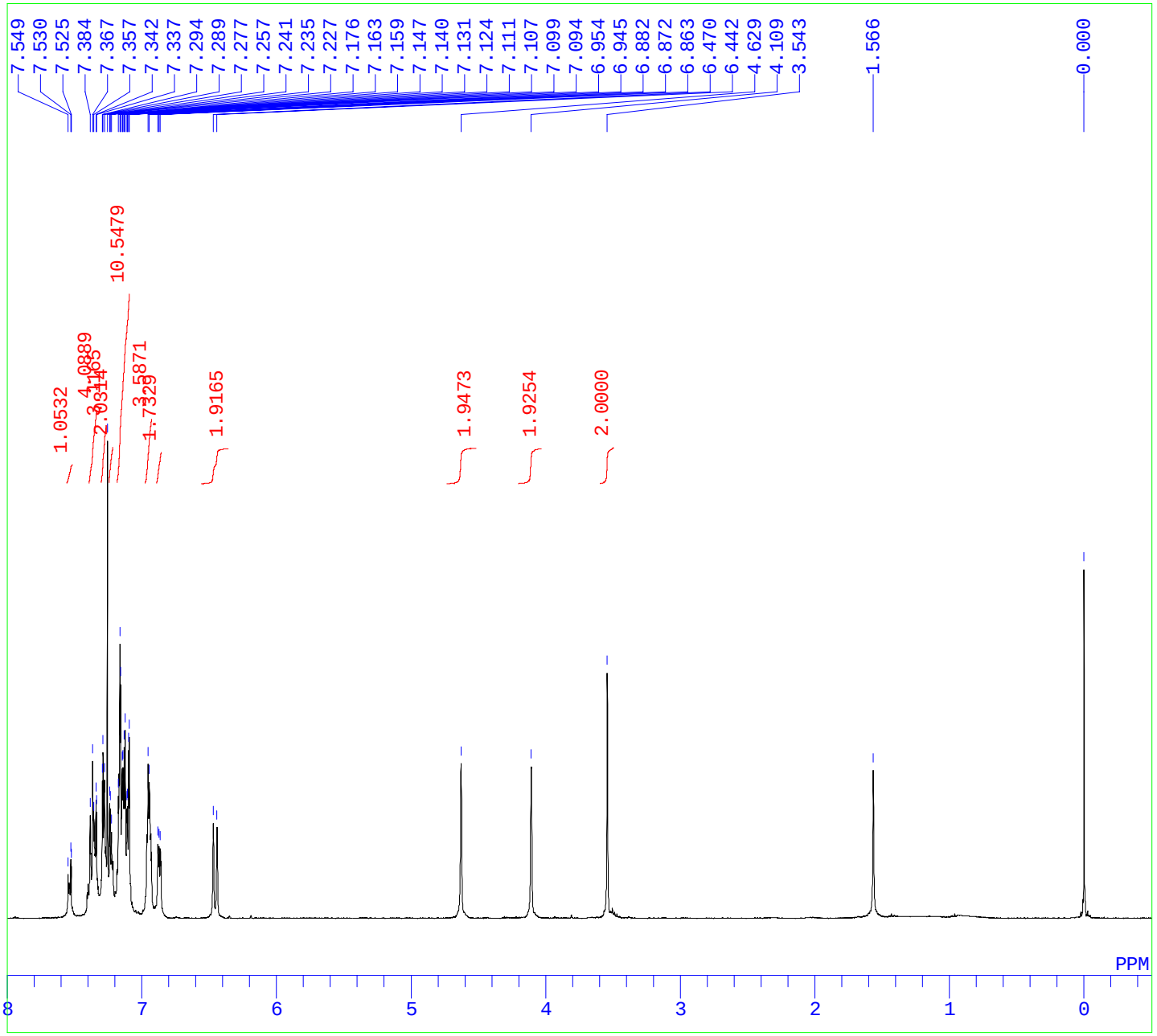
3ba



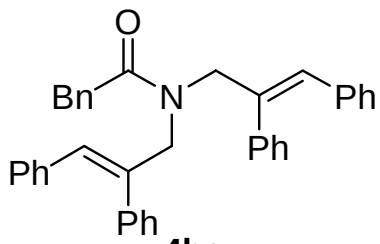

```
DFILE   C:\sp3C-H\3ba-13C.als
COMNT
DATIM   Fri Dec 19 11:41:20 2008
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           309
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          24.9 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



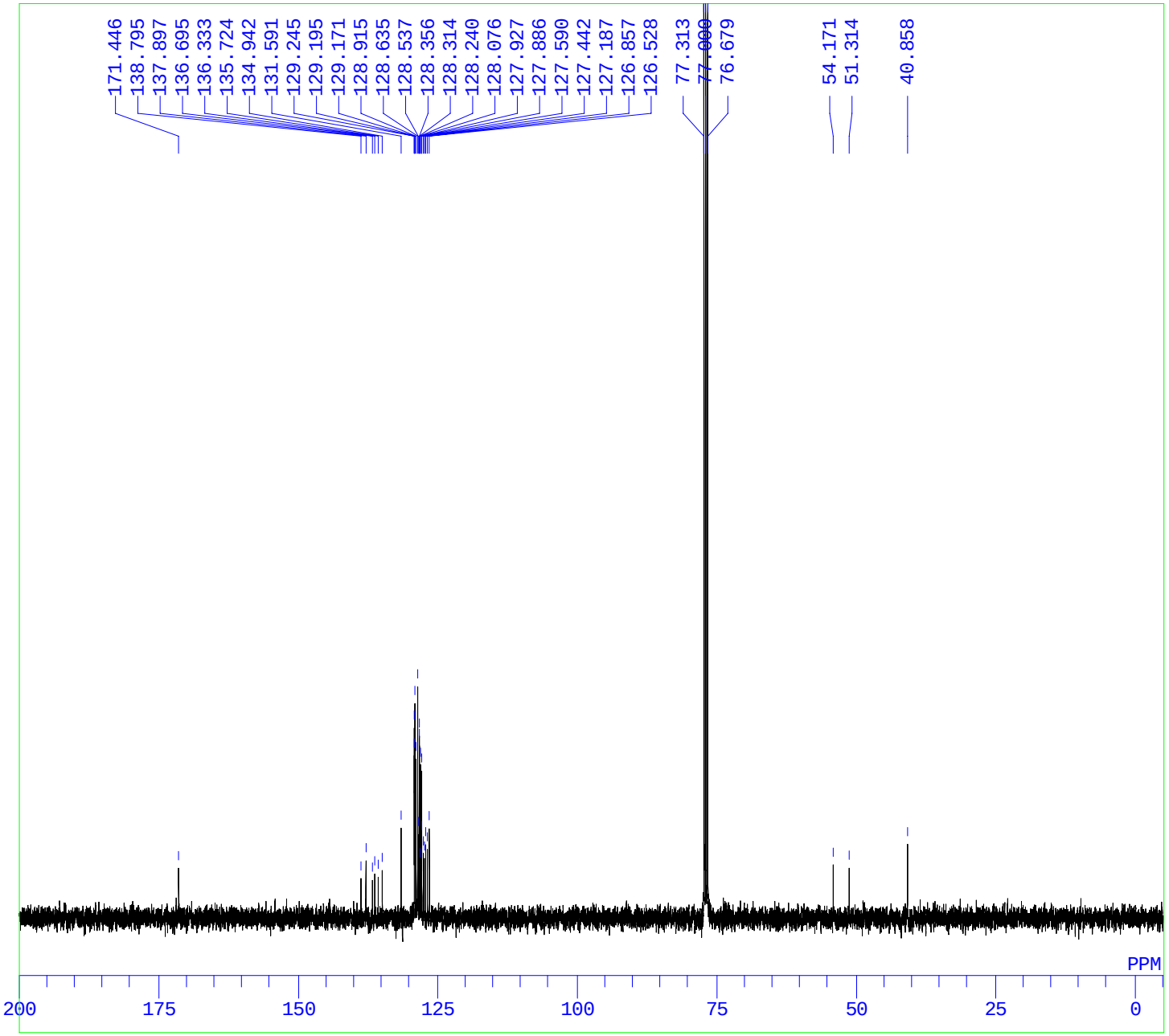
3ba



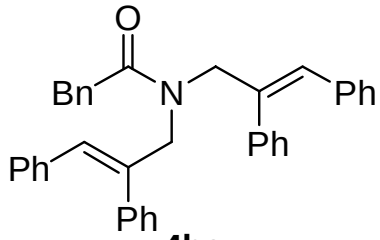

```
DFILE   C:\sp3C-H\4ba-1H.als
COMNT
DATIM   Mon Jan 19 11:33:51 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          22.9 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            18
```



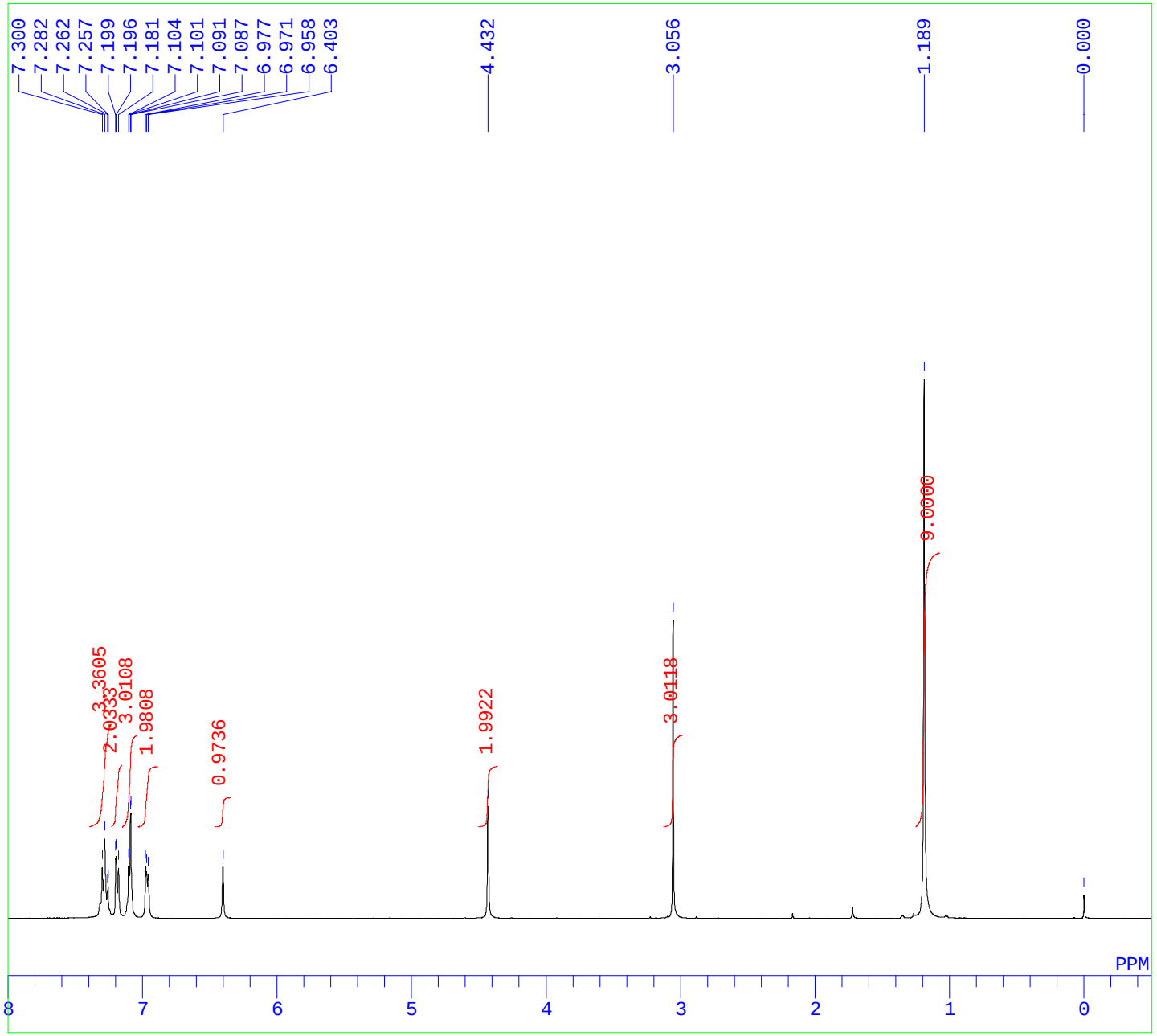
4ba



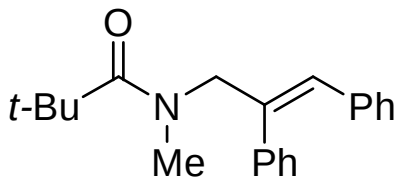

```
DFILE   C:\sp3C-H\4ba-13C.als
COMNT
DATIM   Mon Jan 19 13:01:48 2009
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           501
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          23.9 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            26
```



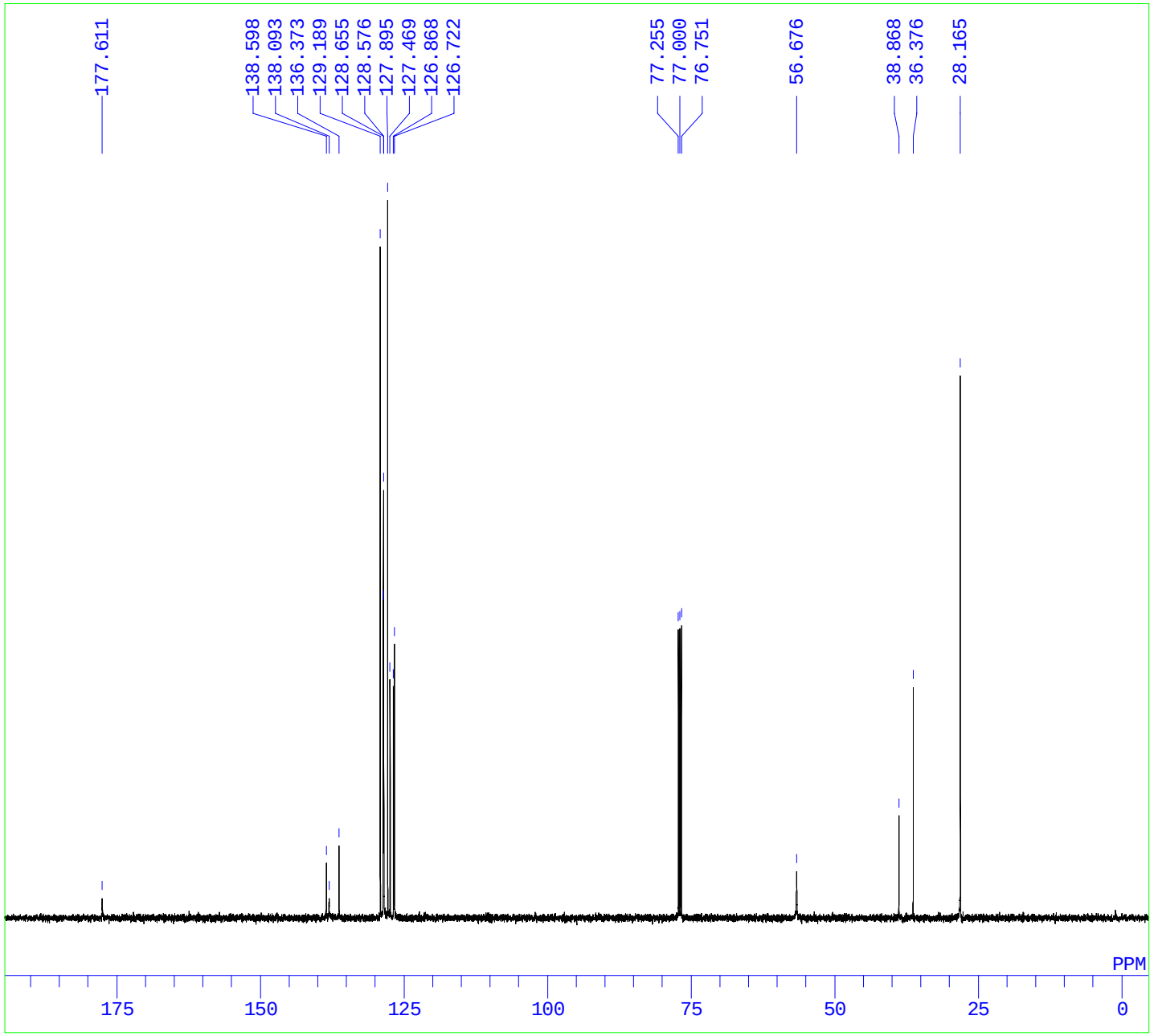
4ba



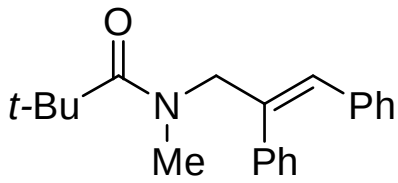

```
DFILE   C:\sp3C-H\3ca-1H.als
COMNT
DATIM   Mon Dec 15 09:49:43 2008
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          23.3 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            15
```



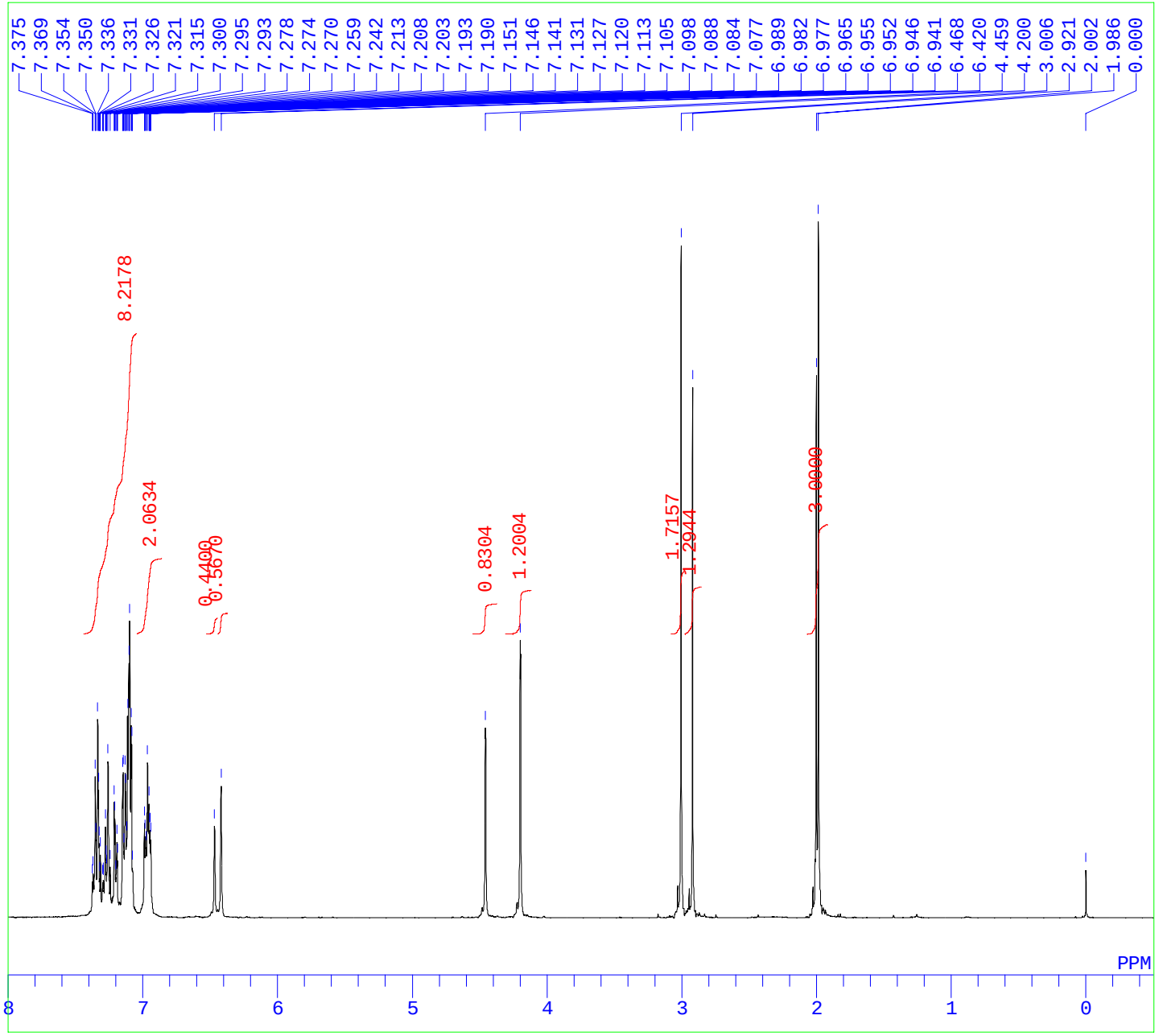
3ca



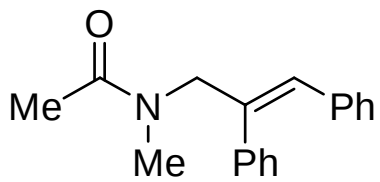

```
DFILE   C:\sp3C-H\3ca-13C.als
COMNT
DATIM   Tue Jan 13 18:47:29 2009
OBNUC   13C
EXMOD   bcm
OBFRQ        125.40 MHz
OBSET        140.00 KHz
OBFIN        2343.8 Hz
POINT         32768
FREQU       25000.0 Hz
SCANS           410
ACQTM         1.311 sec
PD            1.689 sec
PW1             5.5 us
IRNUC   1H
CTEMP          24.8 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            27
```



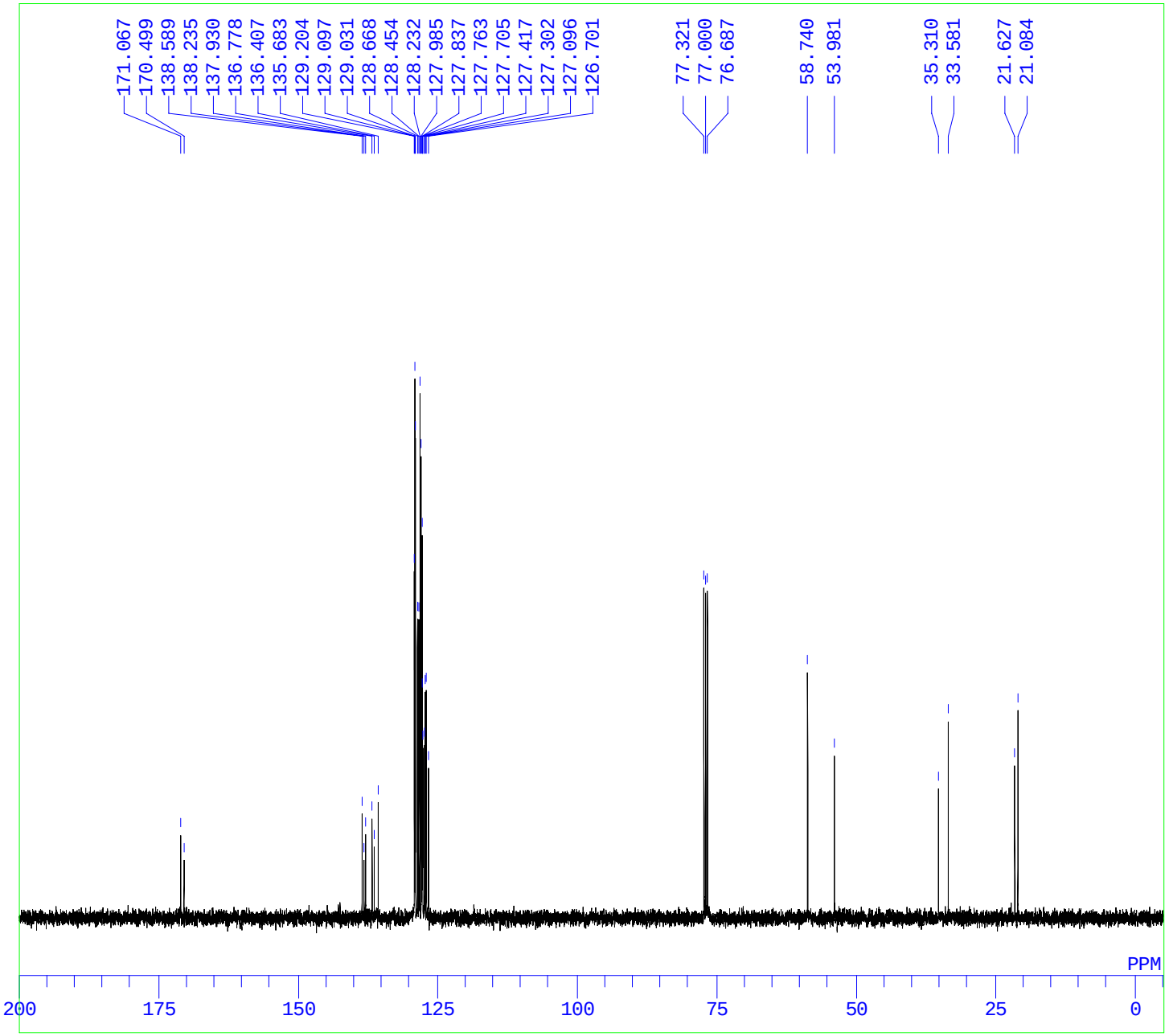
3ca



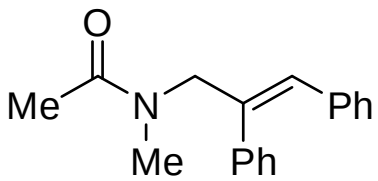

```
DFILE   C:\sp3C-H\3da-1H.als
COMNT
DATIM   Mon Jan 19 11:19:11 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          25.1 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            13
```



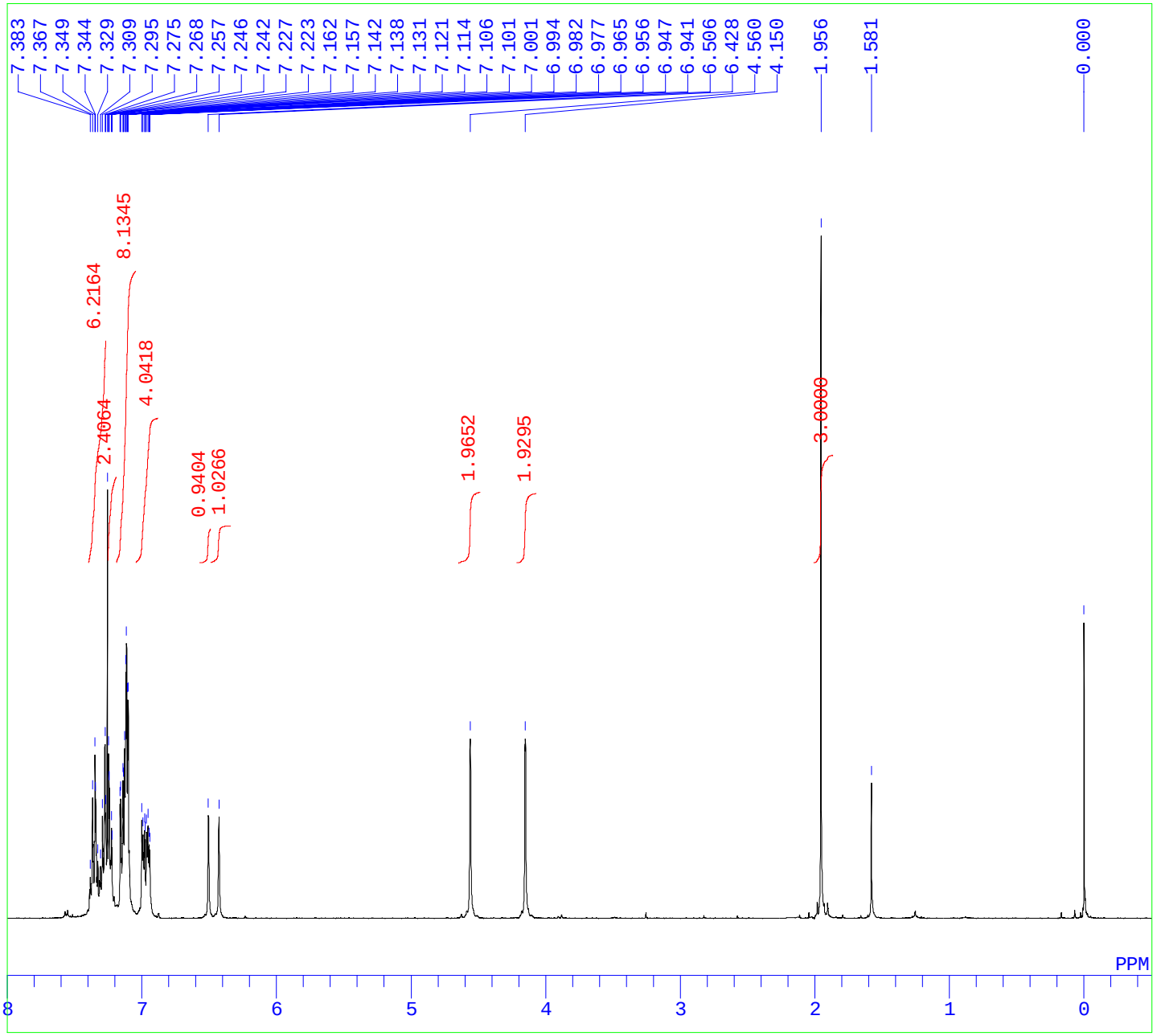
3da



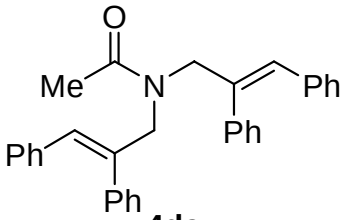

```
DFILE   C:\sp3C-H\3da-13C.als
COMNT
DATIM   Mon Jan 19 11:27:09 2009
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           101
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          23.8 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



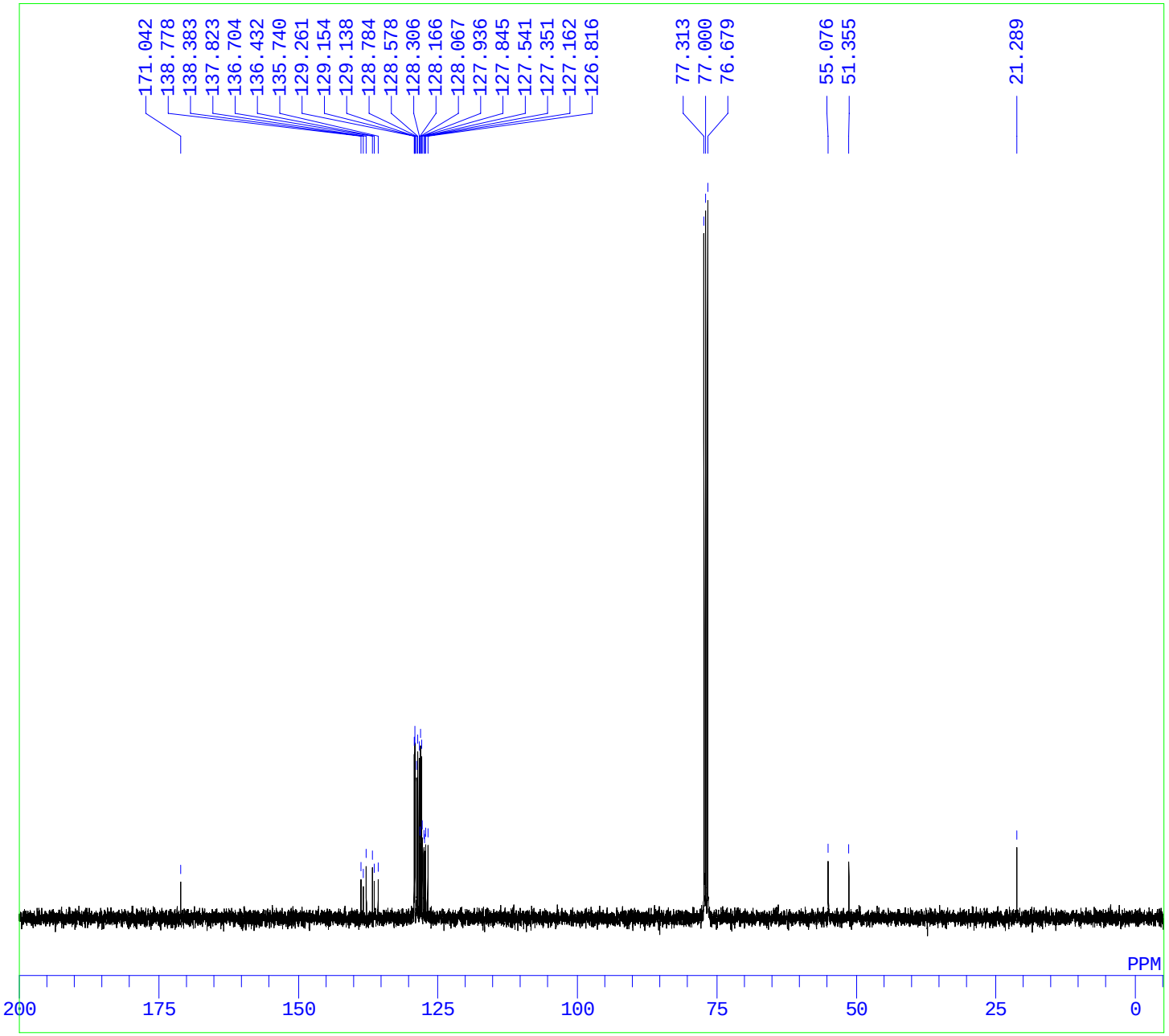
3da



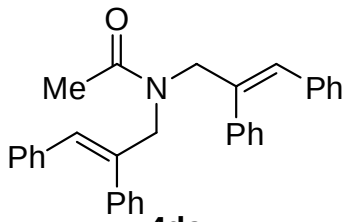

```
DFILE   C:\sp3C-H\4da-1H.als
COMNT
DATIM   Mon Jan 19 12:07:15 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.8 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            18
```



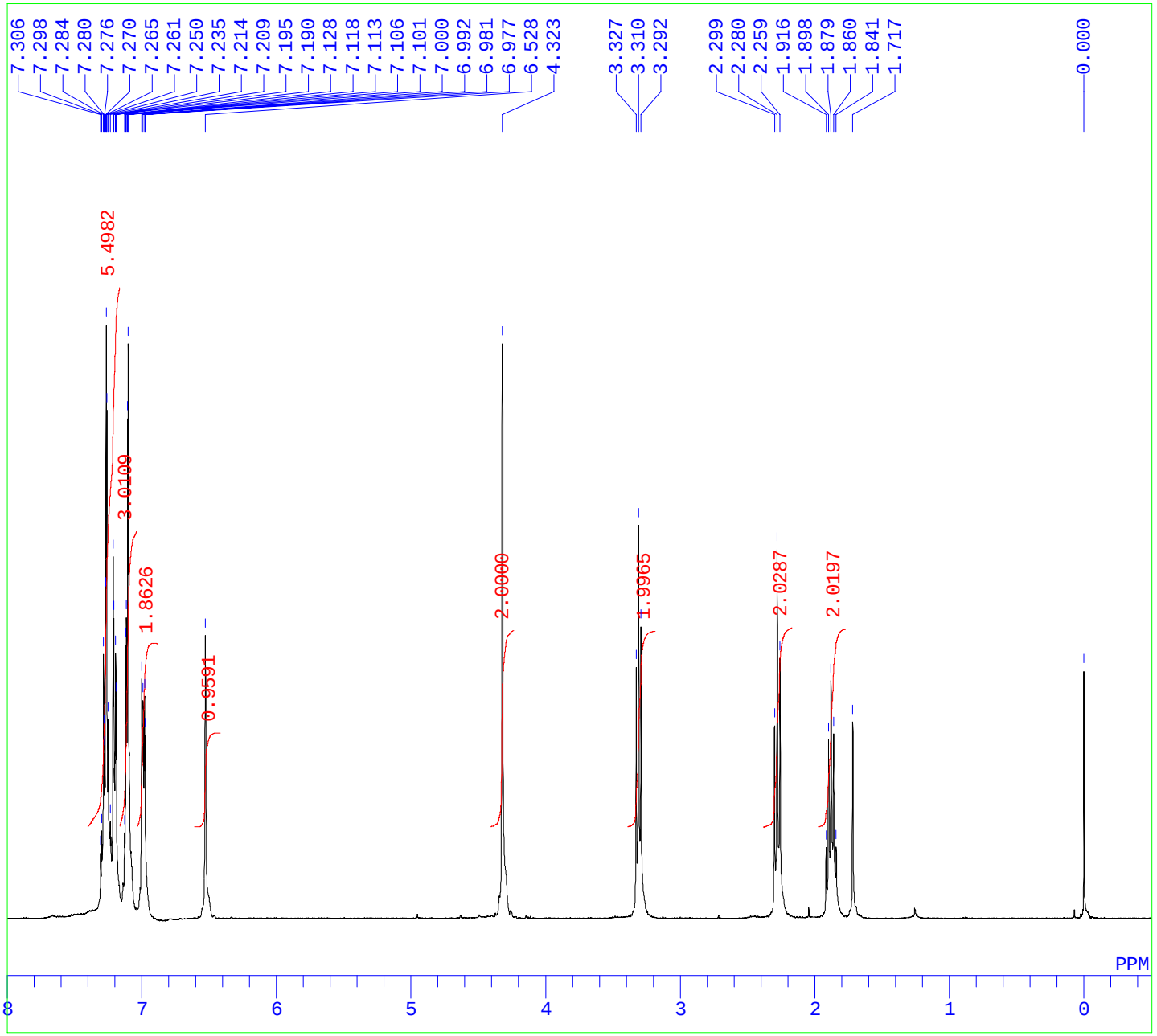
4da



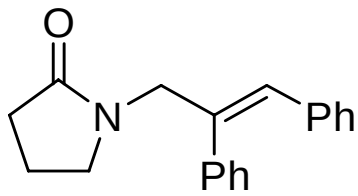

```
DFILE   C:\sp3C-H\4da-13C.als
COMNT
DATIM   Mon Jan 19 12:32:21 2009
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           361
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          23.7 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



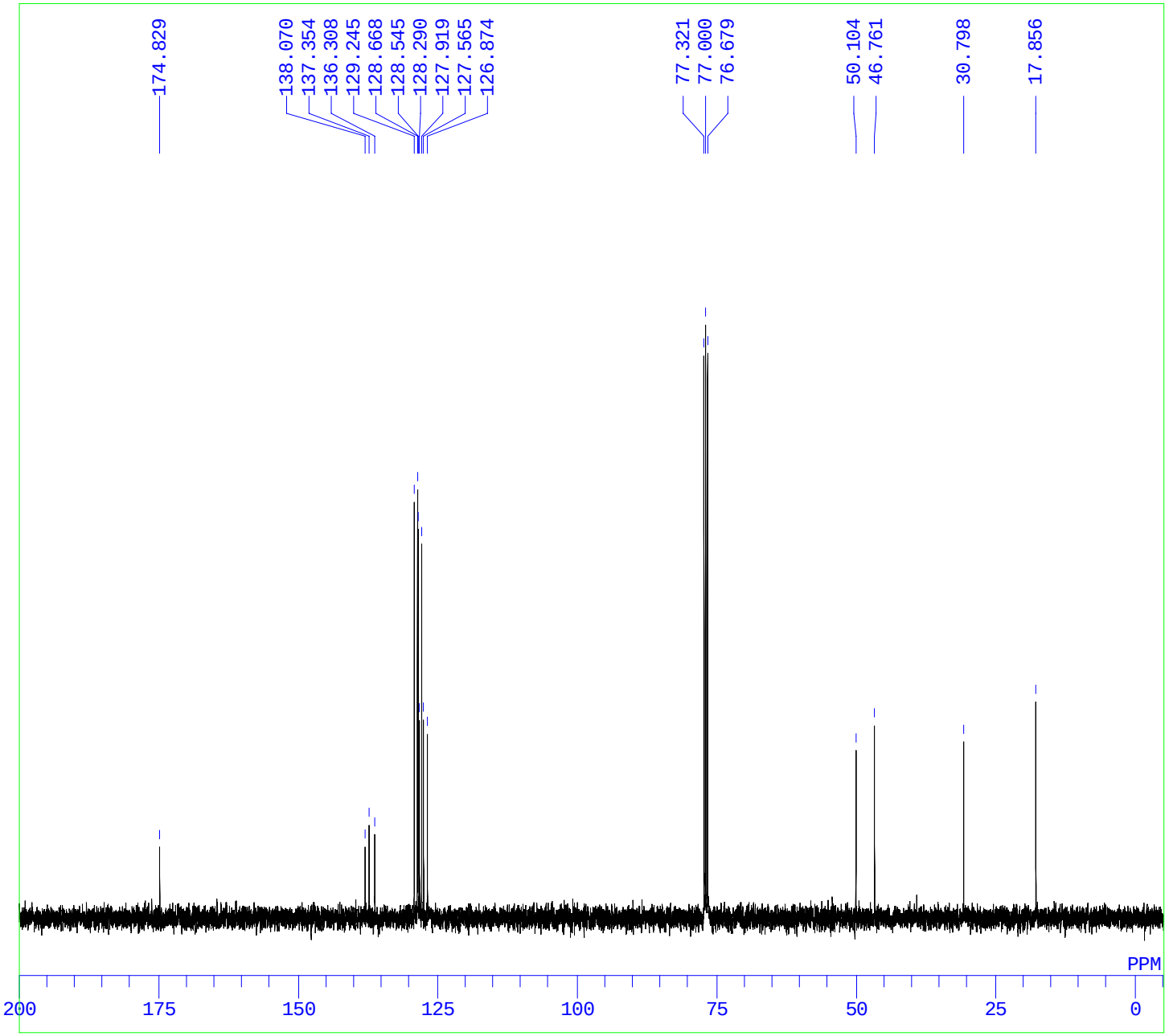
4da



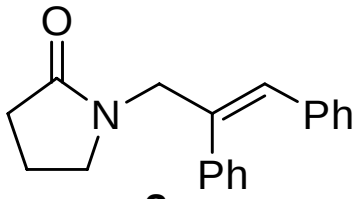

```
DFILE   C:\sp3C-H\3ea-1H.als
COMNT
DATIM   Wed Oct 29 18:05:11 2008
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          23.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            18
```



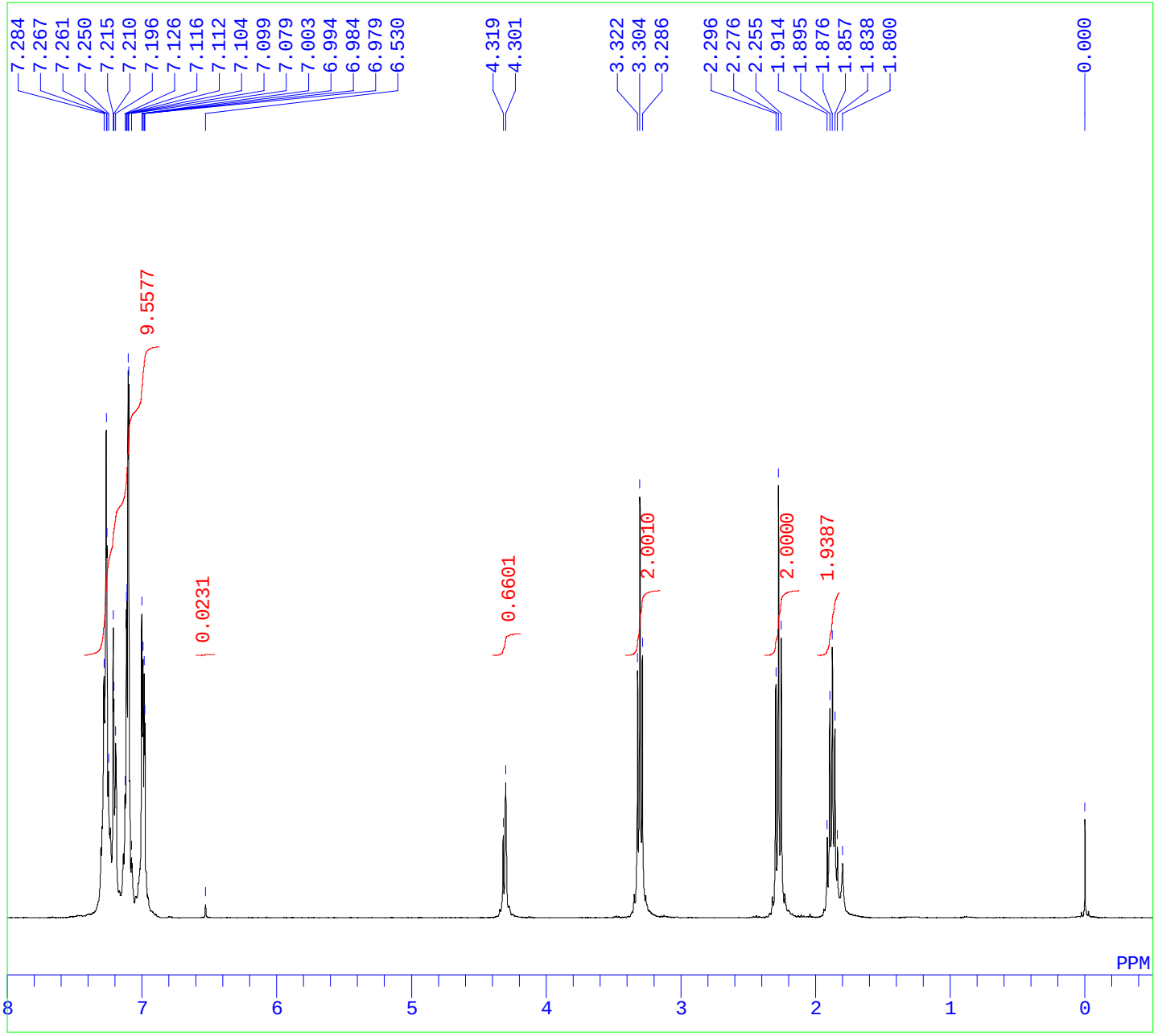
3ea



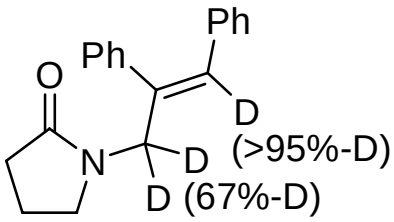

```
DFILE   C:\sp3C-H\3ea-13C.als
COMNT
DATIM   Wed Oct 29 18:13:37 2008
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           121
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          25.2 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



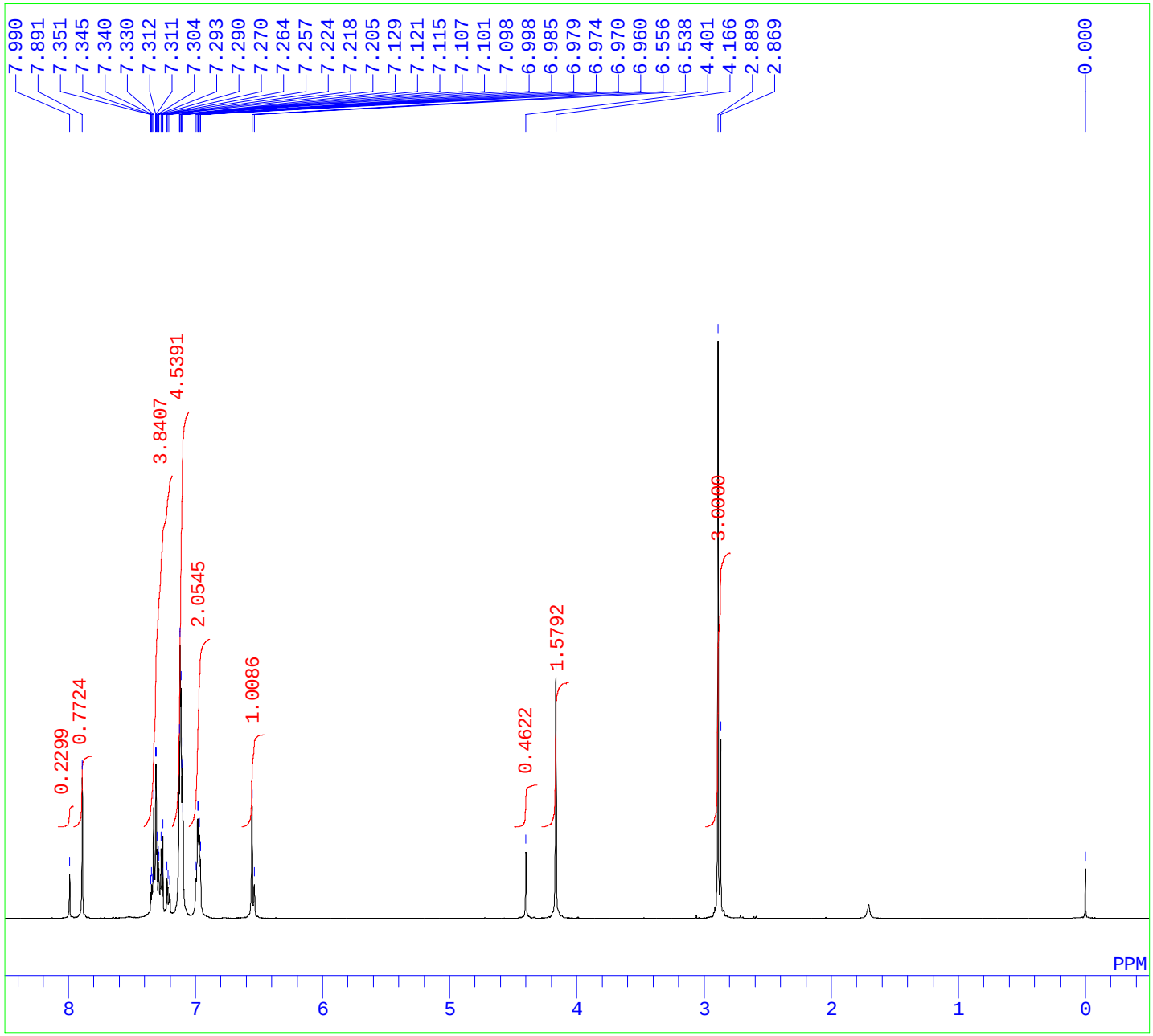
3ea



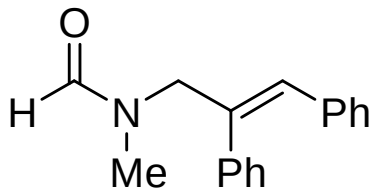

```
DFILE   C:\sp3C-H\3ea-d3-1H.als
COMNT
DATIM   Thu Dec 04 15:08:07 2008
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.1 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            15
```



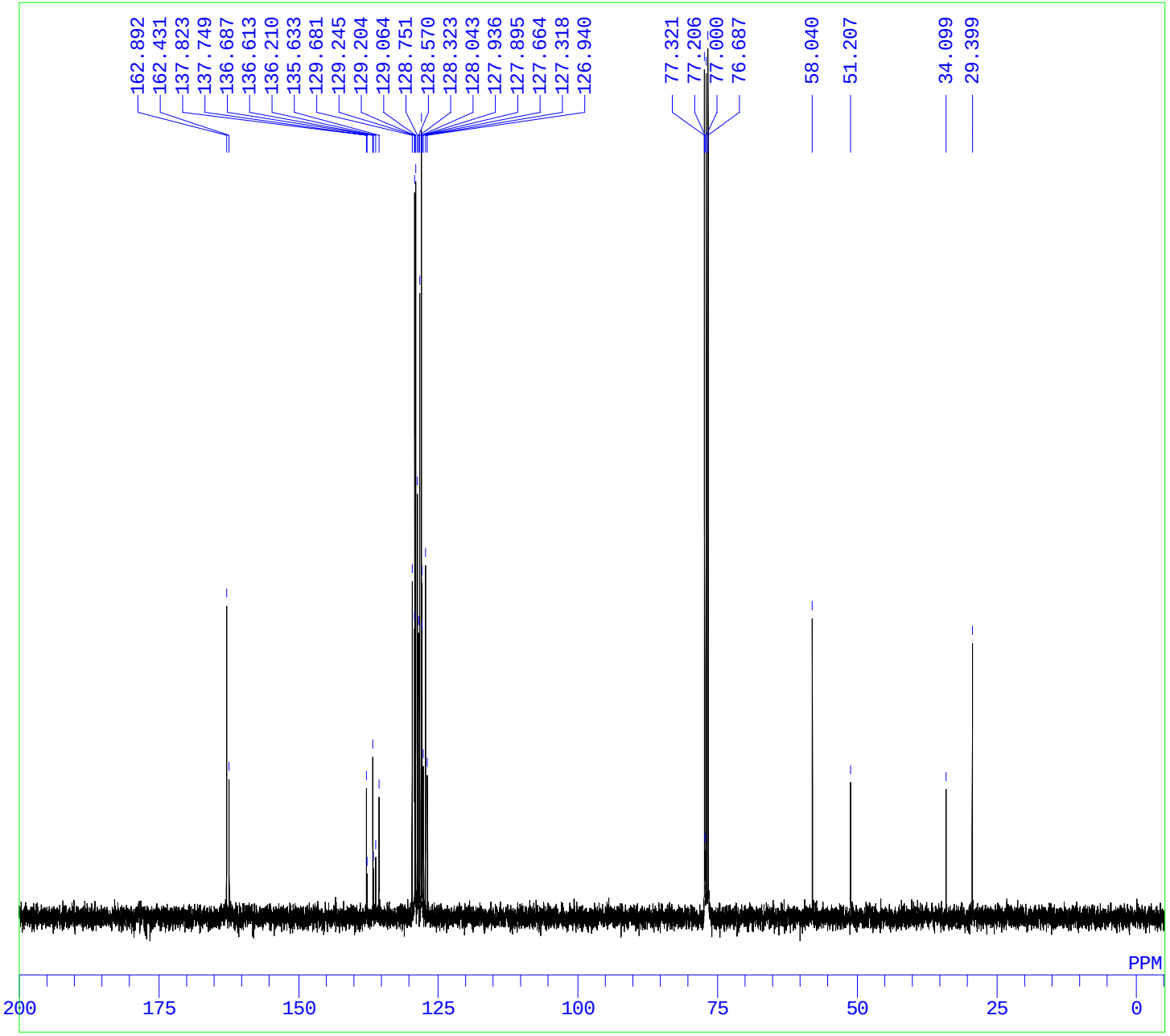
3ea-d_3



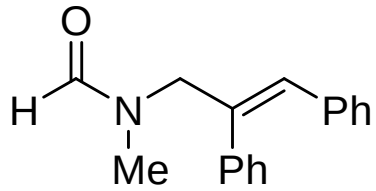

```
DFILE   C:\sp3C-H\3fa-1H.als
COMNT
DATIM   Mon Jan 19 10:56:28 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            17
```



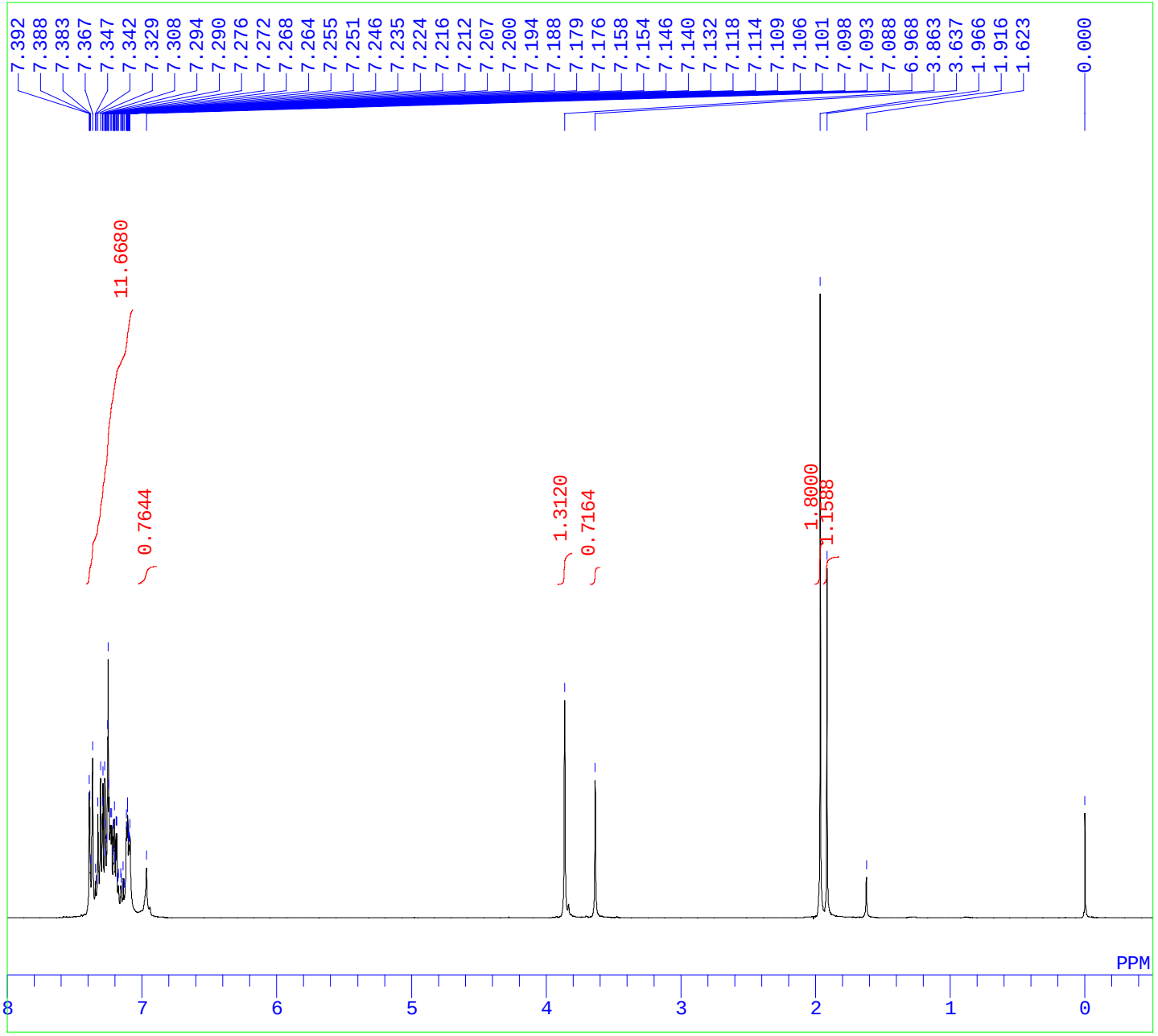
3fa



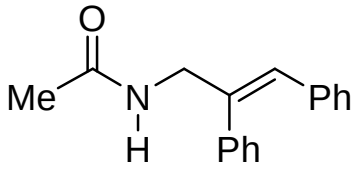

```
DFILE   C:\sp3C-H\3fa-13C.als
COMNT
DATIM   Mon Jan 19 11:13:20 2009
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           241
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          25.3 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



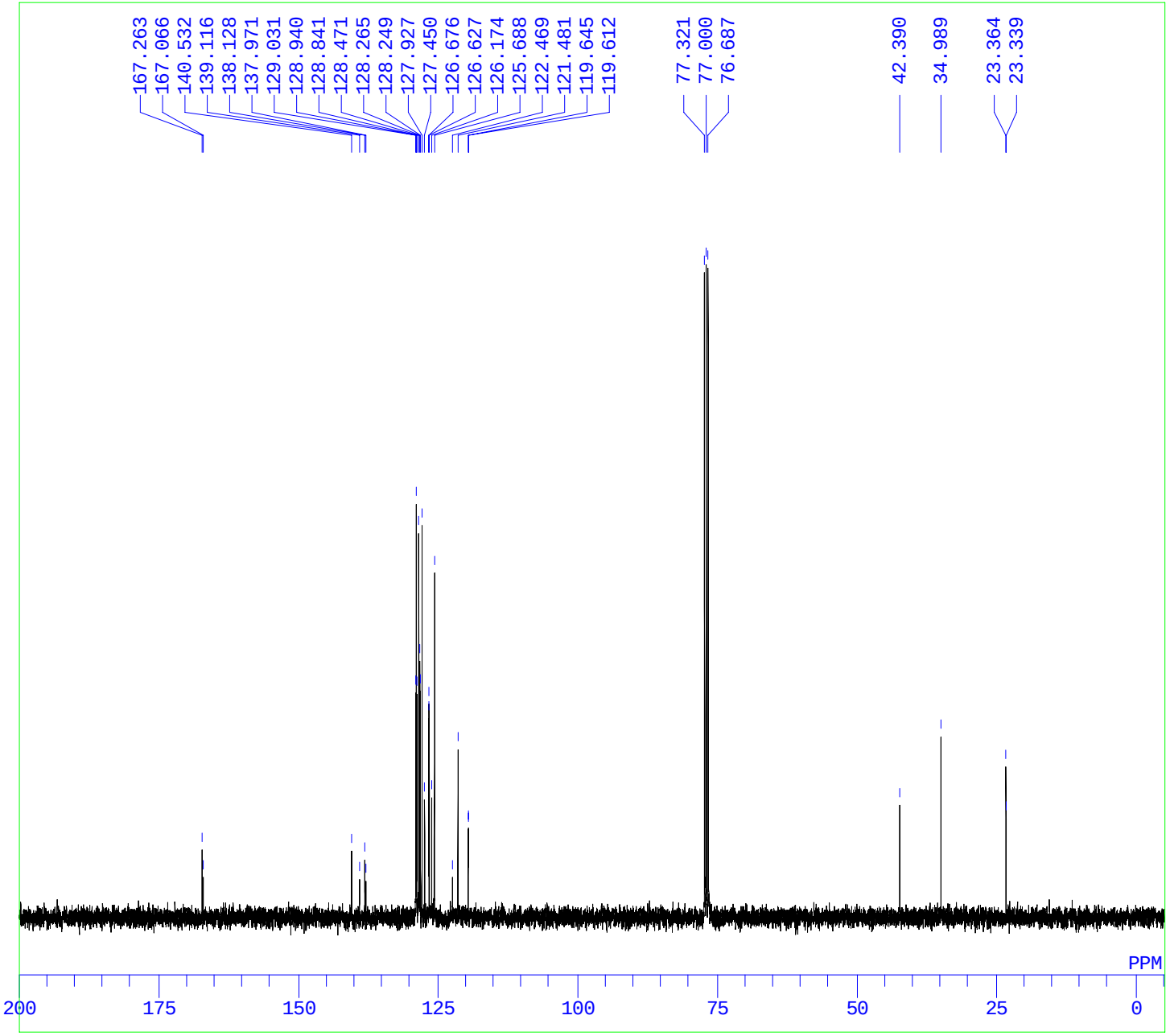
3fa



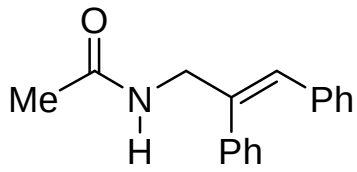

```
DFILE   C:\sp3C-H\3ga-1H.als
COMNT
DATIM   Wed Feb 04 18:35:54 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS             8
ACQTM         4.100 sec
PD            1.500 sec
PW1             6.6 us
IRNUC   1H
CTEMP          27.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            16
```



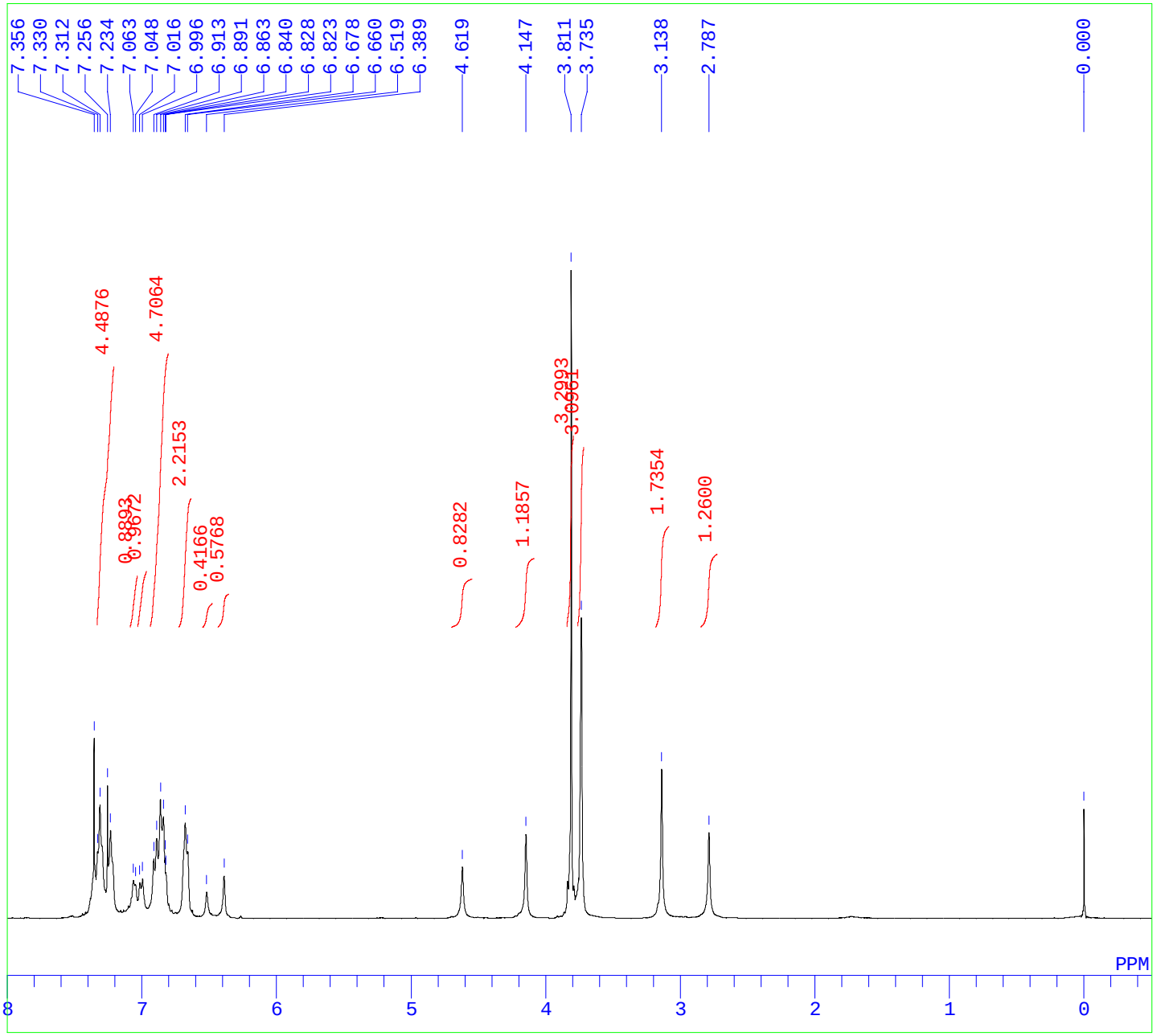
3ga



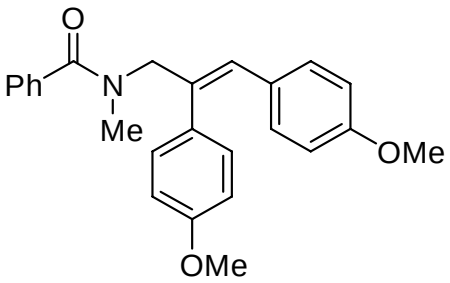

```
DFILE   C:\sp3C-H\3ga-13C.als
COMNT
DATIM   Wed Feb 04 18:50:14 2009
OBNUC   13C
EXMOD   BCM
OBFRQ        100.40 MHz
OBSET        125.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU       27118.6 Hz
SCANS           201
ACQTM         1.208 sec
PD            1.792 sec
PW1             4.7 us
IRNUC   1H
CTEMP          27.7 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            25
```



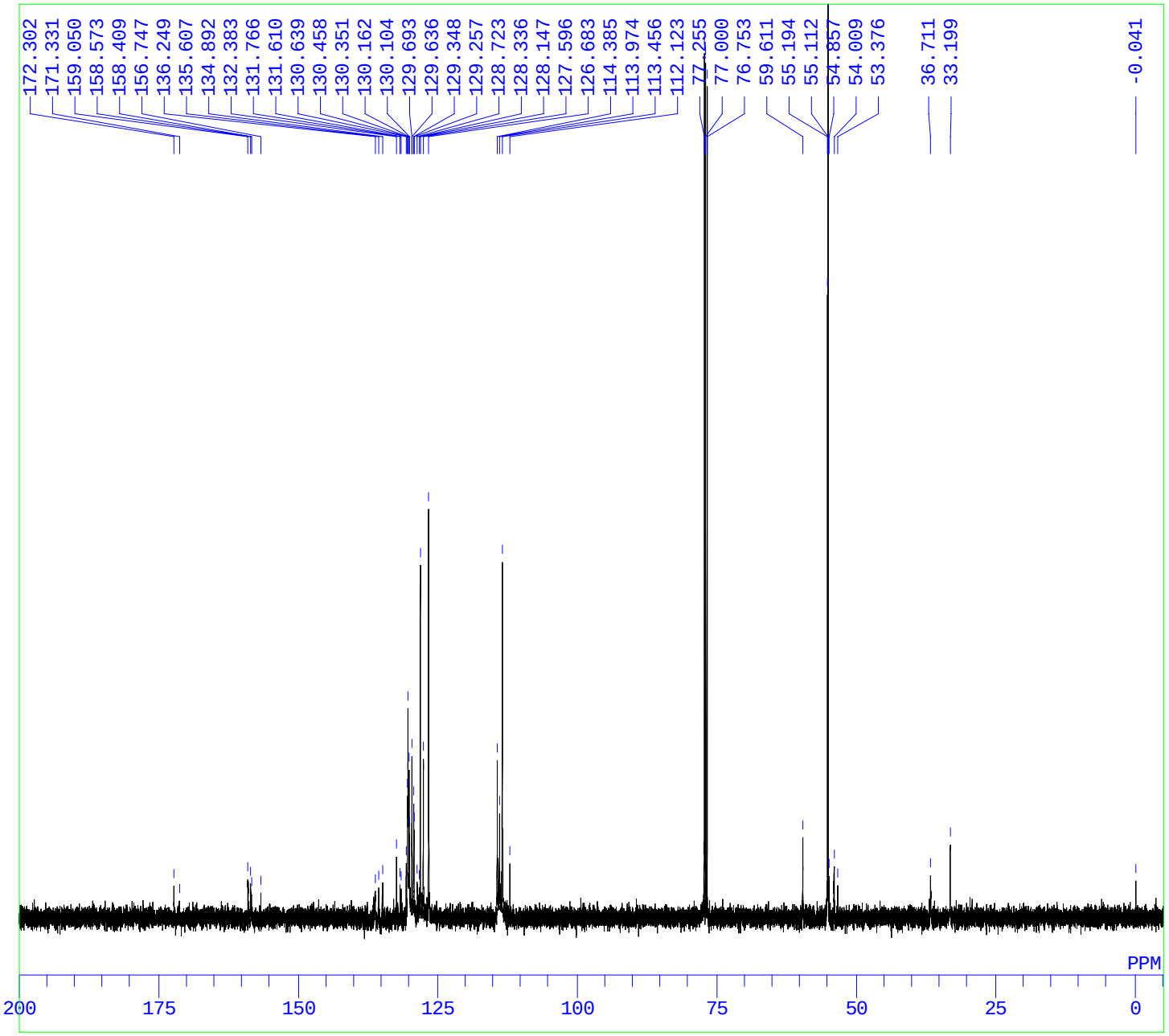
3ga



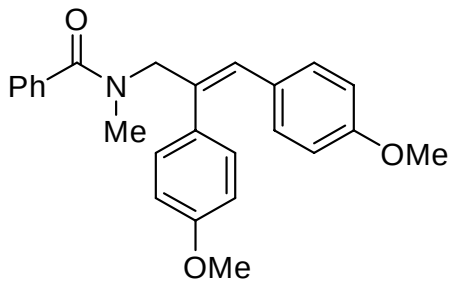

```
DFILE   C:\sp3C-H\3ab-1H.als
COMNT
DATIM   Sat Jan 24 14:52:38 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.8 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            14
```



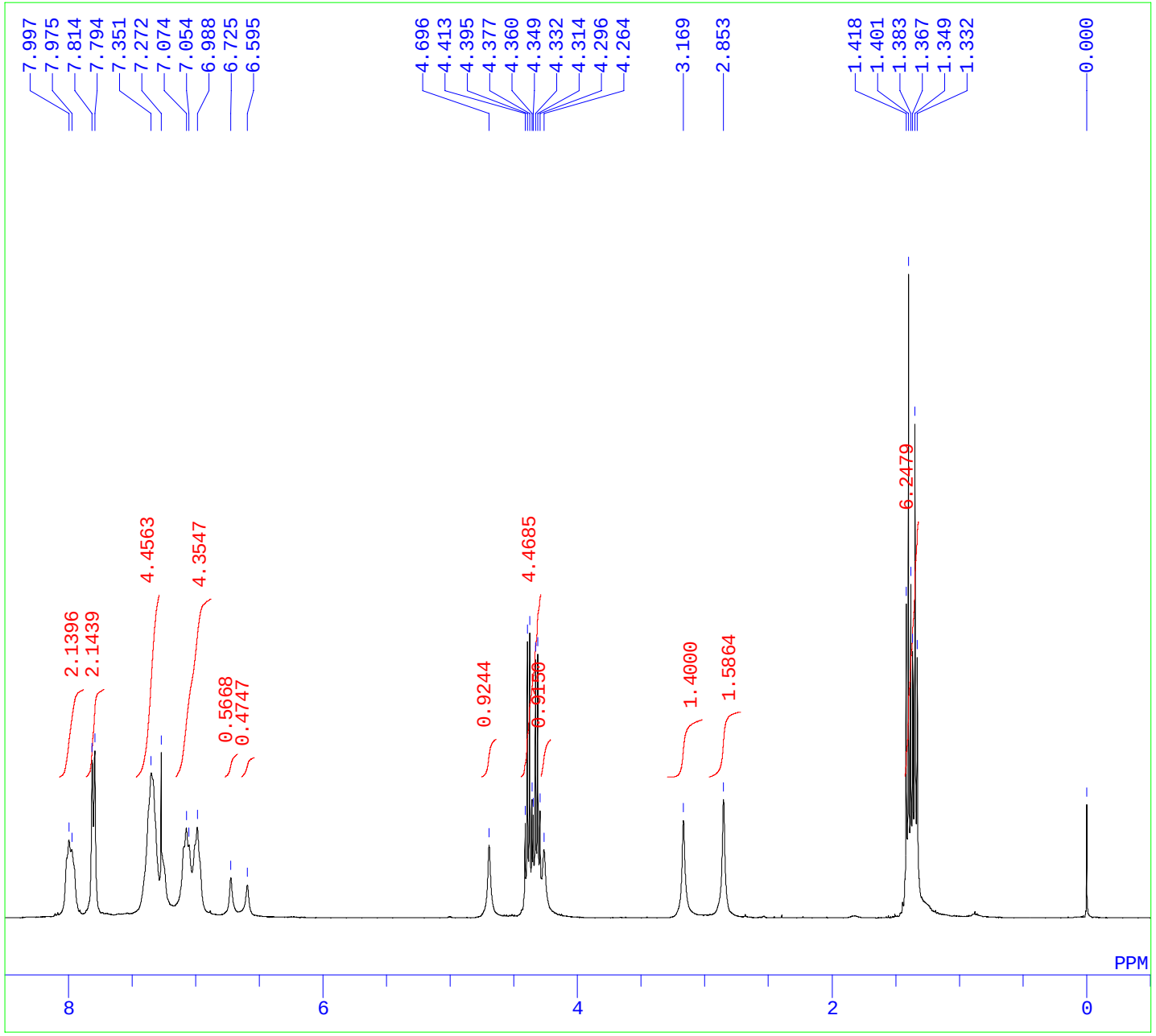
3ab



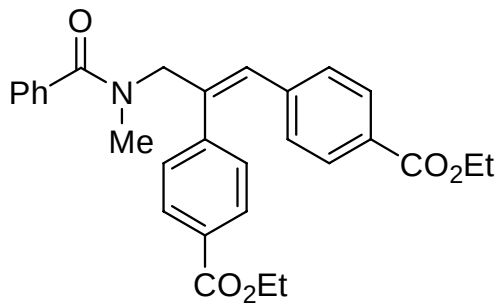

```
DFILE   C:\sp3C-H\3ab-13C.als
COMNT
DATIM   Fri Jan 16 21:50:26 2009
OBNUC   13C
EXMOD   bcm
OBFRQ        125.65 MHz
OBSET        120.00 KHz
OBFIN        7958.0 Hz
POINT         32768
FREQU       33898.3 Hz
SCANS          1200
ACQTM         0.967 sec
PD            2.033 sec
PW1             5.4 us
IRNUC   1H
CTEMP          26.7 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             0.12 Hz
RGAIN            28
```



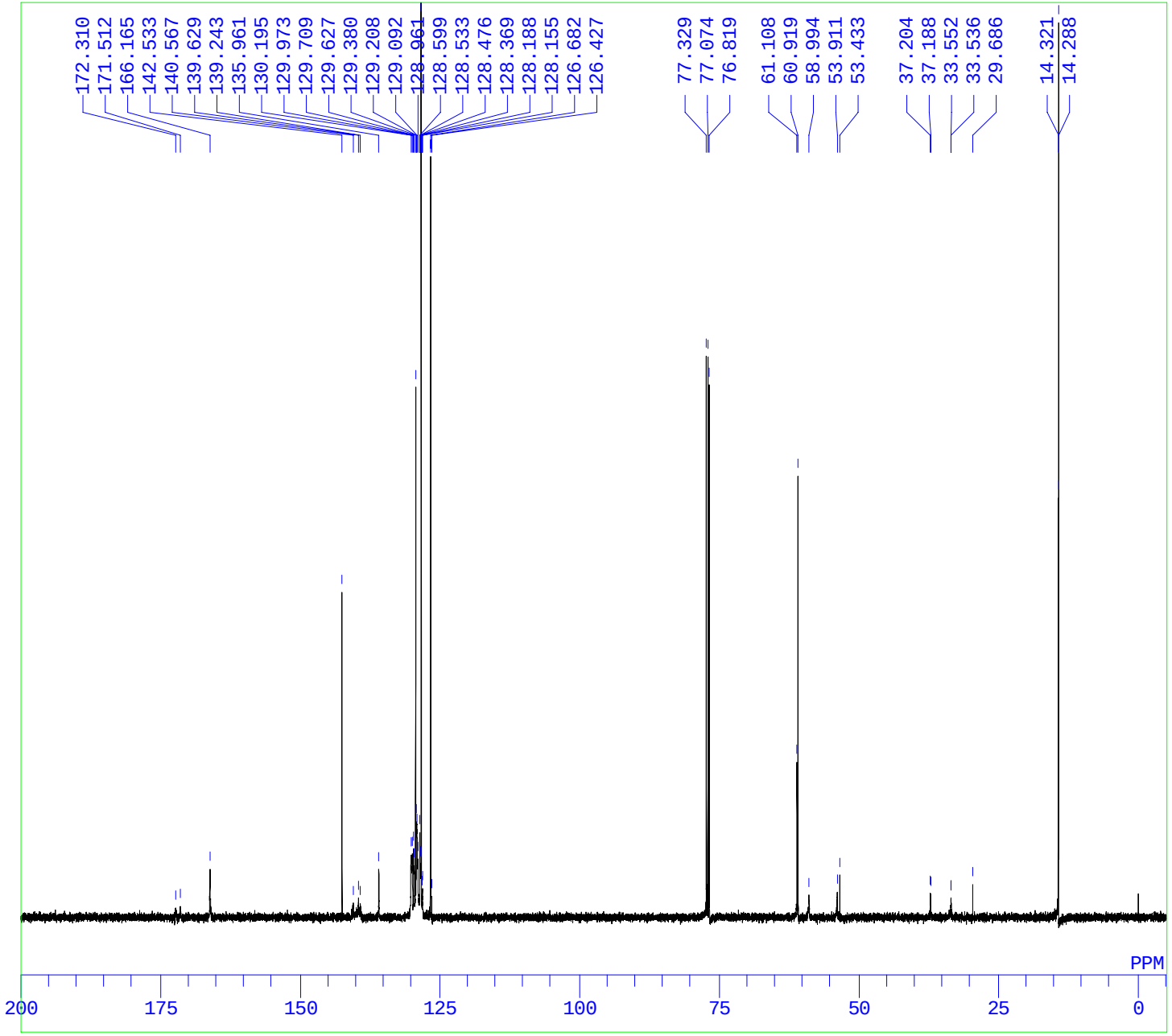
3ab



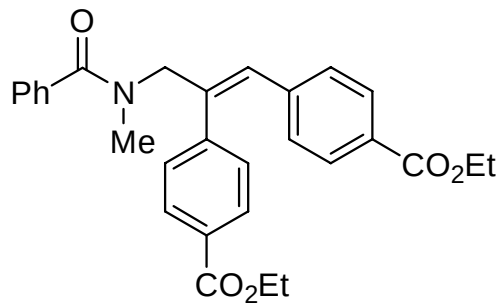

```
DFILE   C:\sp3C-H\3ac-1H.als
COMNT
DATIM   Tue Jan 20 00:14:44 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.2 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            13
```



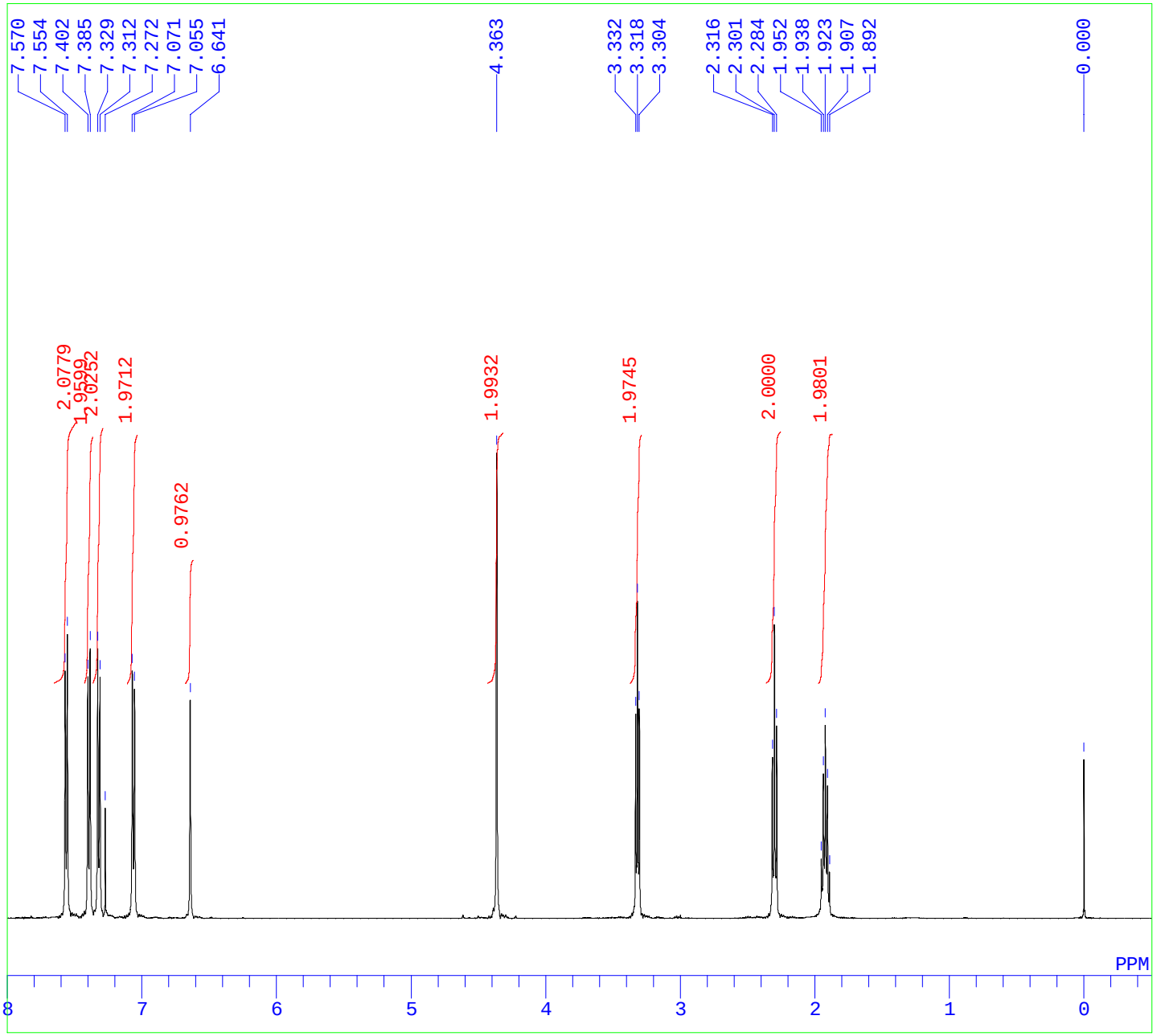
3ac



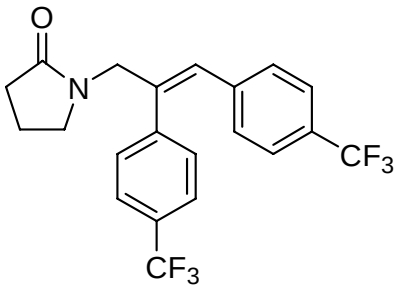

```
DFILE   C:\sp3C-H\3ac-13C.als
COMNT
DATIM   Sat Jan 17 19:54:22 2009
OBNUC   13C
EXMOD   bcm
OBFRQ        125.65 MHz
OBSET        120.00 KHz
OBFIN        7958.0 Hz
POINT         32768
FREQU       33898.3 Hz
SCANS          2001
ACQTM         0.967 sec
PD            2.033 sec
PW1             5.4 us
IRNUC   1H
CTEMP          26.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            28
```



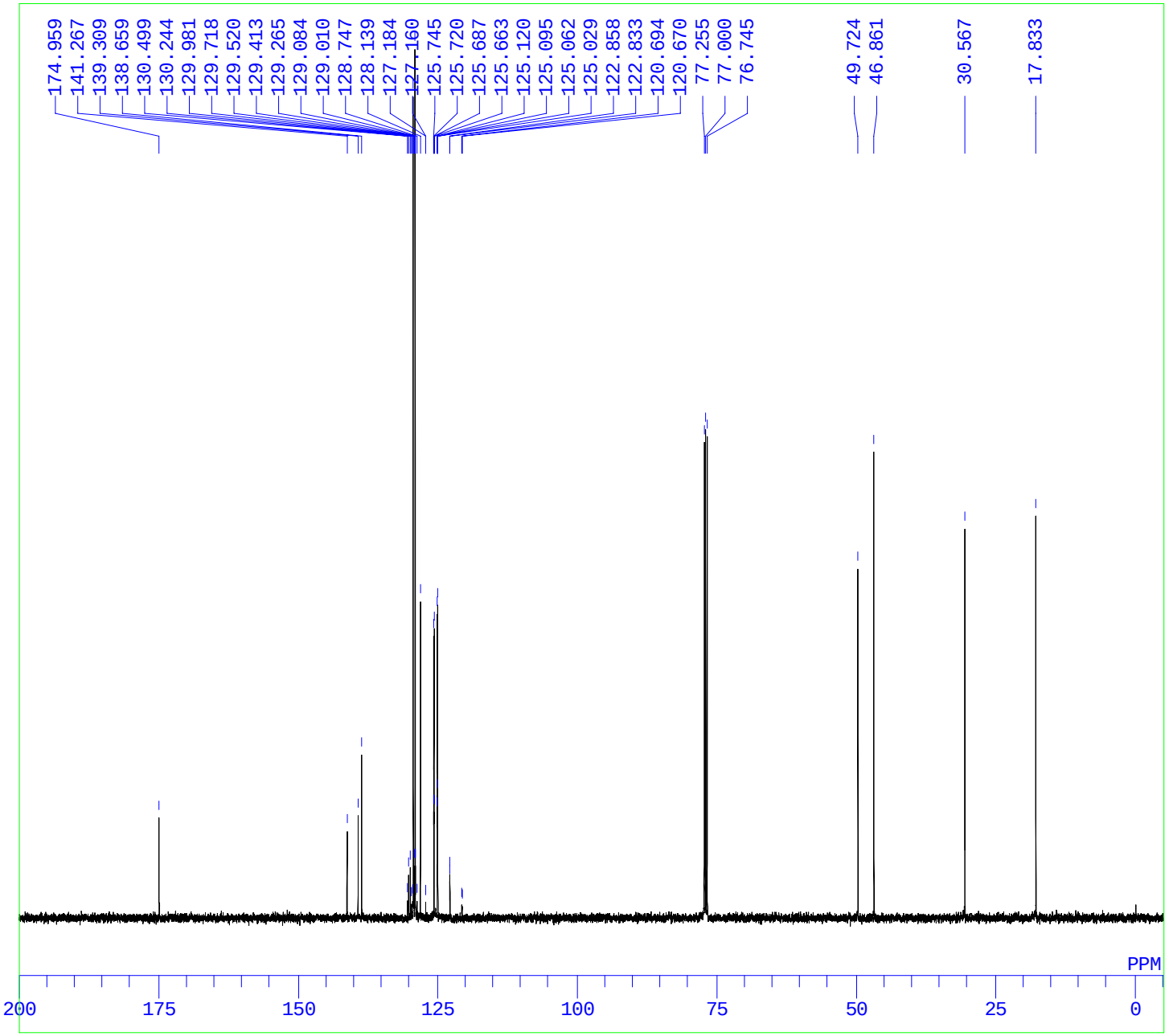
3ac



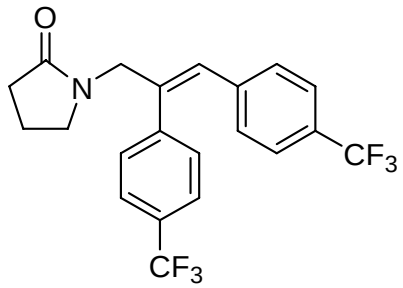

```
DFILE   C:\sp3C-H\3ed-1H.als
COMNT
DATIM   Fri Jan 23 18:11:46 2009
OBNUC   1H
EXMOD   non
OBFRQ        500.00 MHz
OBSET        160.00 KHz
OBFIN        2160.0 Hz
POINT         65536
FREQU       10000.0 Hz
SCANS             4
ACQTM         6.554 sec
PD            0.446 sec
PW1             7.2 us
IRNUC   1H
CTEMP          22.4 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            18
```



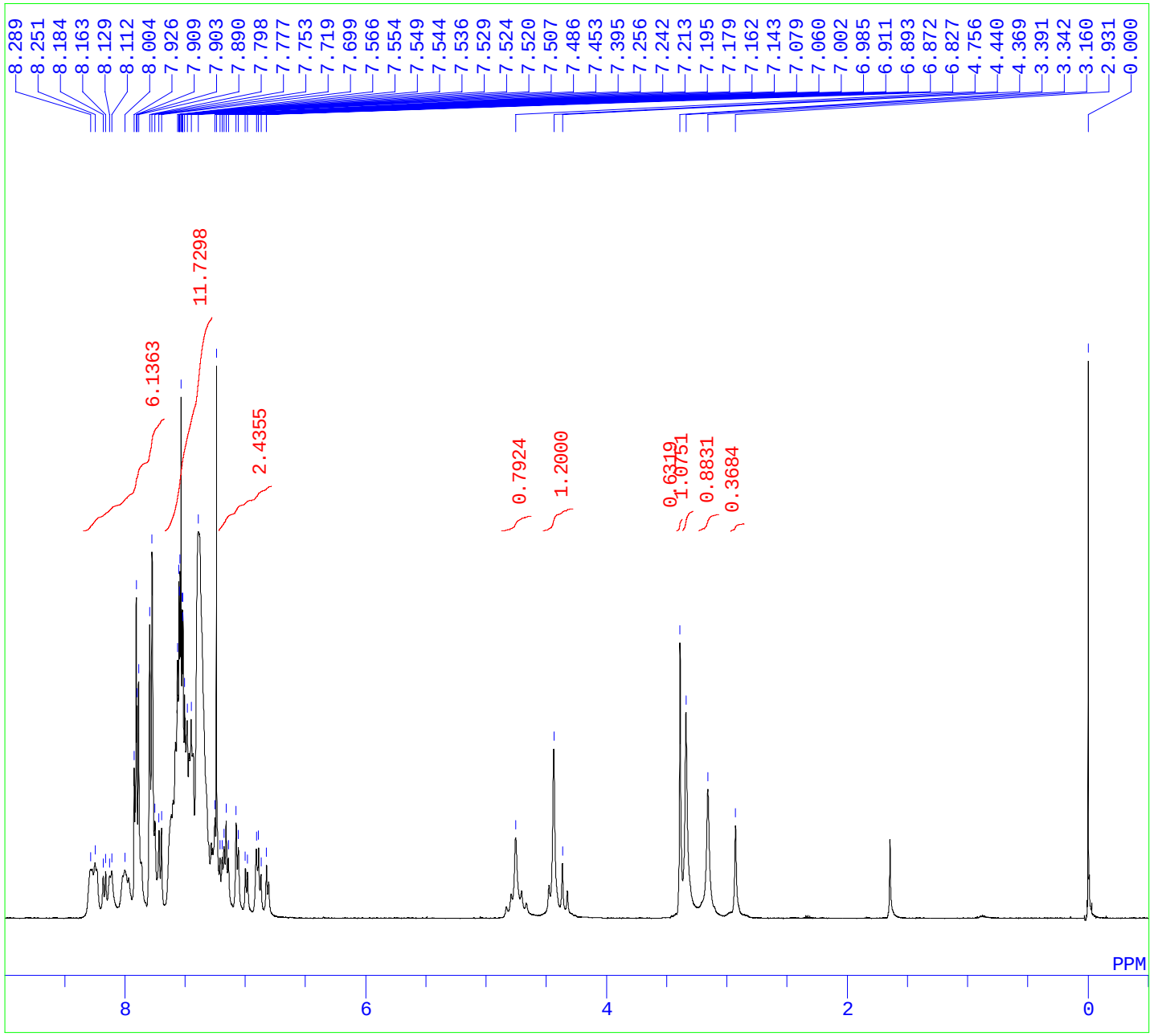
3ed



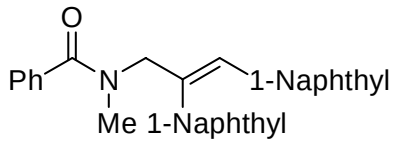

```
DFILE   C:\sp3C-H\3ed-13C.als
COMNT
DATIM   Fri Jan 23 18:44:24 2009
OBNUC   13C
EXMOD   bcm
OBFRQ        125.65 MHz
OBSET        120.00 KHz
OBFIN        7958.0 Hz
POINT         32768
FREQU       33898.3 Hz
SCANS           601
ACQTM         0.967 sec
PD            2.033 sec
PW1             5.4 us
IRNUC   1H
CTEMP          26.3 c
SLVNT   CDCL3
EXREF         77.00 ppm
BF             1.00 Hz
RGAIN            28
```



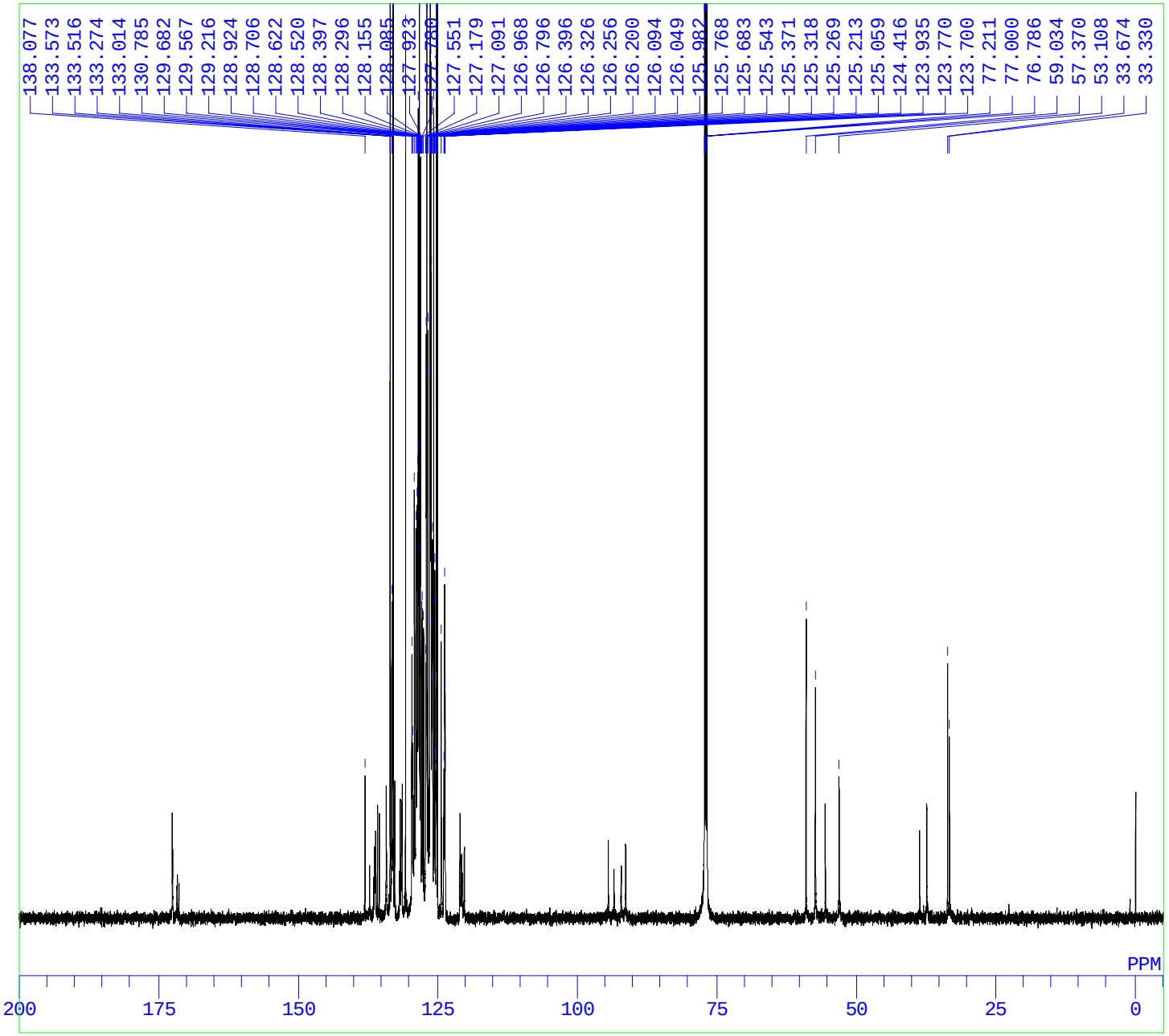
3ed



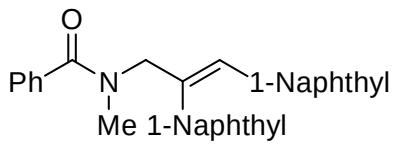

```
DFILE   C:\sp3C-H\3ae-1H.als
COMNT
DATIM   Tue Jan 20 00:21:44 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          24.2 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            15
```



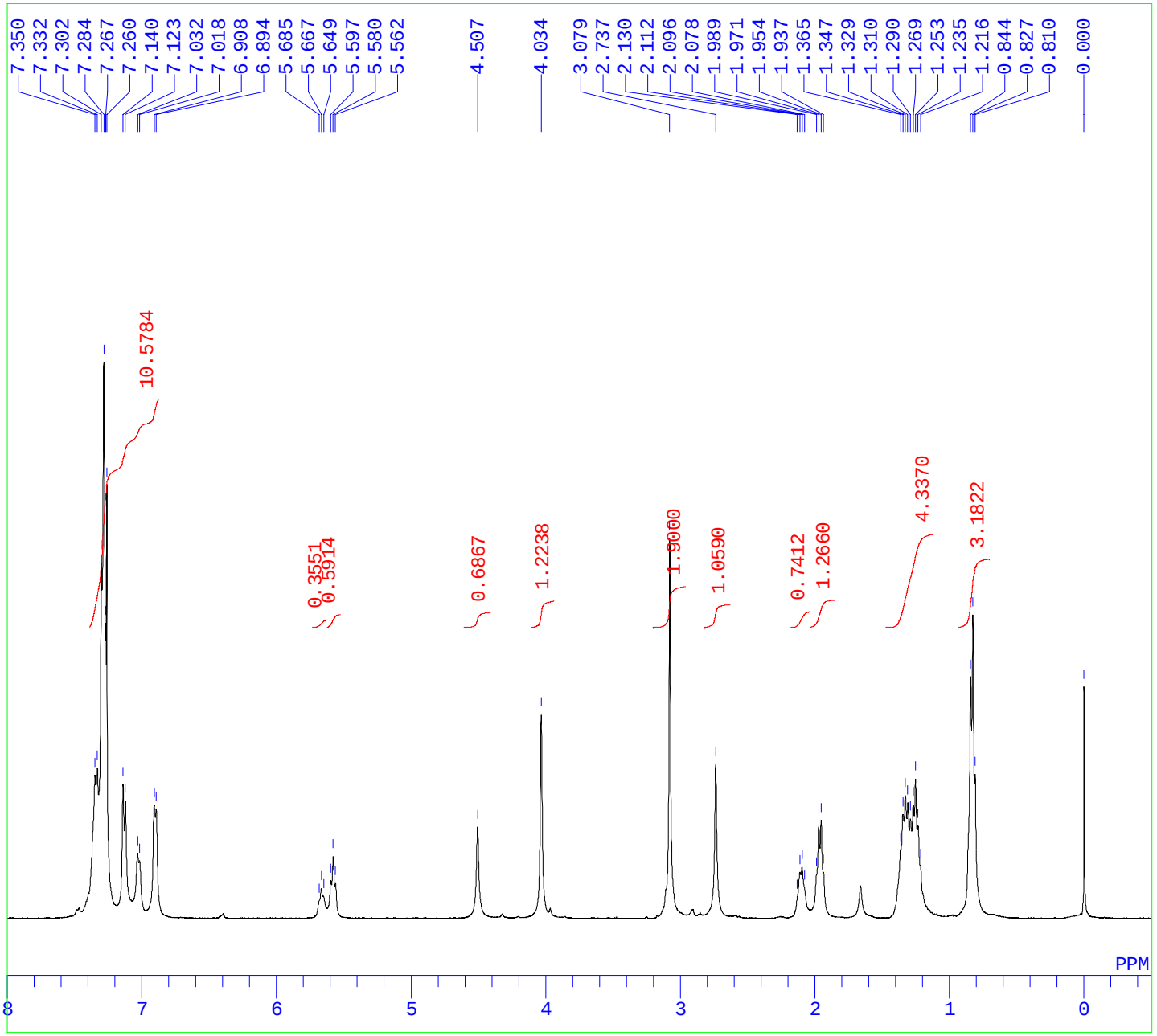
3ae



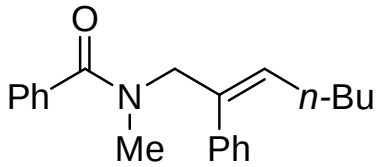

```
DFILE   C:\sp3C-H\3ae-13C.als
COMNT
DATIM
OBNUC   13C
EXMOD
OBFRQ       150.91 MHz
OBSET         8.59 KHz
OBFIN          3.8 Hz
POINT        65536
FREQU      34722.2 Hz
SCANS            8
ACQTM        0.000 sec
PD           0.000 sec
PW1           10.0 us
IRNUC
CTEMP          0.0 c
SLVNT
EXREF        77.00 ppm
BF            0.12 Hz
RGAIN            0
```



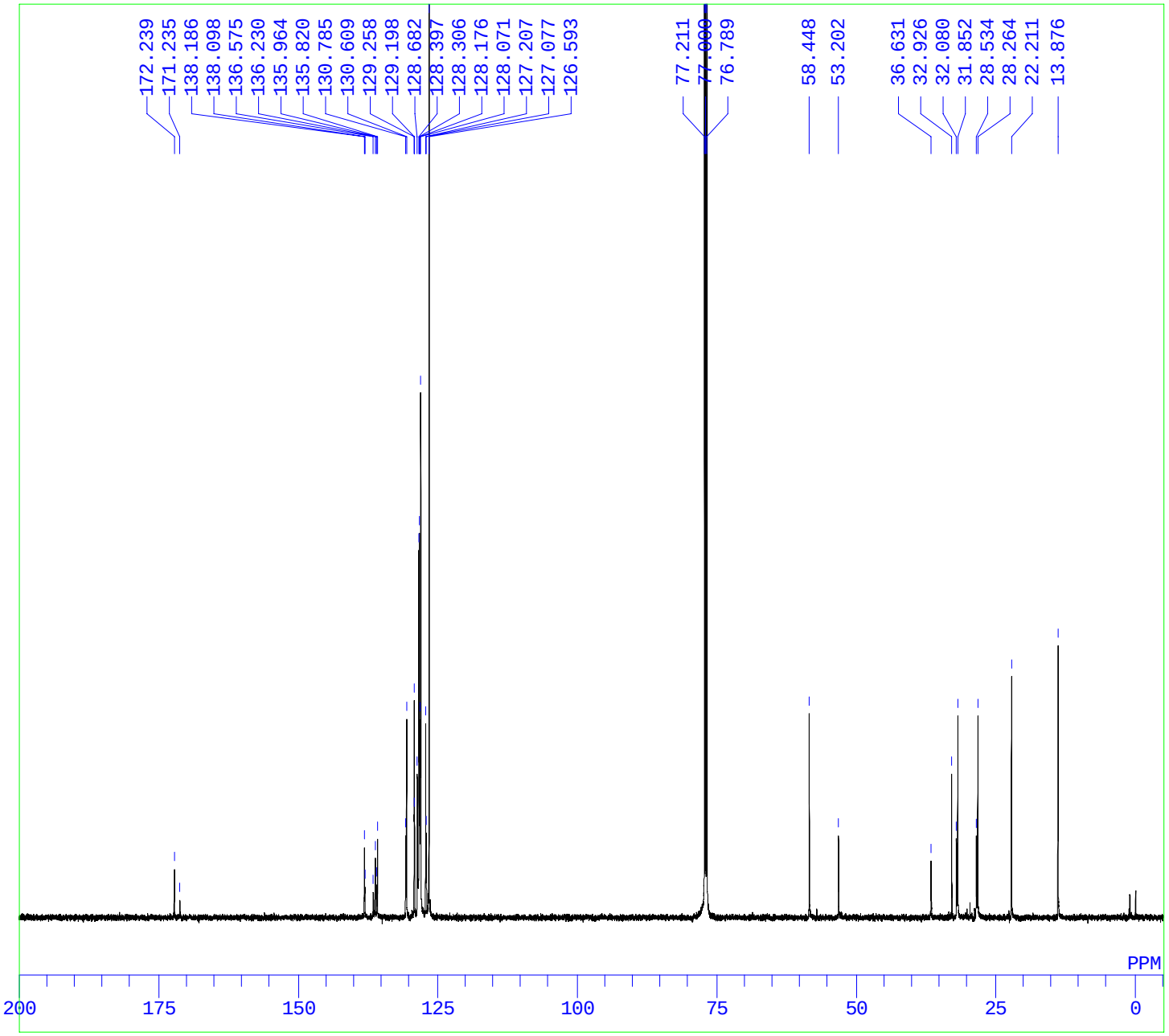
3ae



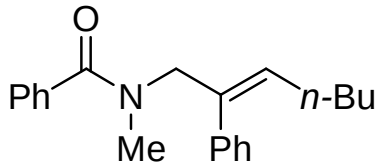

```
DFILE   C:\sp3C-H\3af-1H.als
COMNT
DATIM   Tue Jan 20 15:42:08 2009
OBNUC   1H
EXMOD   NON
OBFRQ        399.65 MHz
OBSET        124.00 KHz
OBFIN       10500.0 Hz
POINT         32768
FREQU        7992.0 Hz
SCANS            16
ACQTM         4.100 sec
PD            2.900 sec
PW1             6.6 us
IRNUC   1H
CTEMP          22.3 c
SLVNT   CDCL3
EXREF          0.00 ppm
BF             0.12 Hz
RGAIN            16
```



3af




```
DFILE   C:\sp3C-H\3af-13C.als
COMNT
DATIM
OBNUC   13C
EXMOD
OBFRQ       150.91 MHz
OBSET         8.59 KHz
OBFIN          3.8 Hz
POINT        65536
FREQU      34722.2 Hz
SCANS            8
ACQTM        0.000 sec
PD           0.000 sec
PW1           10.0 us
IRNUC
CTEMP          0.0 c
SLVNT
EXREF        77.00 ppm
BF            0.12 Hz
RGAIN            0
```



3af