

Radical Carbonylation Reactions of ω -Alkynylamines Leading to α -Methylene Lactams. Synthetic Scope and the Mechanistic Insights

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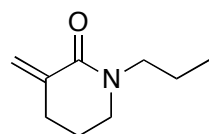
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General information. ^1H NMR spectra were recorded with a JEOL JMN ECP-500 (500 MHz) or JEOL JMN AL-400 (400 MHz) spectrometer in CDCl_3 . Chemical shifts are reported in parts per million (δ) downfield from internal TMS at 0.00. ^{13}C NMR spectra were recorded with a JEOL JMN ECP-500 (125 MHz) or JEOL JMN AL-400 (100 MHz) spectrometer and referenced to the solvent peak at 77.00 ppm. For ^1H -Sn and ^{13}C -Sn coupling constants, the central signals are normally associated with two close pairs of satellites corresponding to both ^{117}Sn and ^{119}Sn isotopes, and average values of the two different coupling constants are reported. Infrared spectra were obtained on a JASCO FT/IR-5300 spectrometer; absorptions are reported in reciprocal centimeters. Both conventional and high resolution mass spectra were recorded with a JEOL MS700 spectrometer. Products were purified by flash chromatography on silica gel (nacalai tesque int. Silica Gel 60, 230-400 mesh). Optical rotations were obtained on JASCO DIP-370 Digital Polarimeter at a wavelength of 589 nm (sodium D line). A single crystal suitable for X-ray crystallography was sealed in glass capillary. All measurements were performed on a Rigaku RAXIS Rapid diffractometer equipped with an imaging plate detector. The frame data were processed using the Rigaku PROCESS-AUTO program,¹ and the reflection data were corrected for absorption with an ABSCOR program.² The structure were solved by direct method and refined on F^2 by full-matrix least-squares method by using SHELX97.³ Anisotropic refinement was applied to all non hydrogen atoms. Hydrogen atoms were found in the final difference Fourier map and have been isotropically refined. Alkynylamines **1a-1j**, **1n**, and **1o** were prepared as previously described.⁴ Alkynylamines **1k**, **1l**, and **1m** were prepared from the corresponding *N*- ω -alkynyl-*N*-(1-phenylethyl) amines.

1. PROCESS-AUTO. *Automatic Data Acquisition and Processing Package for Imaging Plate Diffractometer*, Rigaku Corporation: Tokyo, Japan, 1998.
2. T. Higashi, *ABSCOR, Empirical Absorption Correction based on Fourier Series Approximation*; Rigaku Corporation: Tokyo, Japan, 1998.
3. G. M. Sheldrick, *SHELX97, Program for Crystal Structure Determination*; University of Göttingen: Göttingen, Germany, 1997.
4. a) M. Tojino, Y. Uenoyama, T. Fukuyama, and I. Ryu, *Chem. Comm.* **2004**, 2482. b) Y. Uenoyama, T. Fukuyama, and I. Ryu, *Org. Lett.*, 2007, **9**, 935.

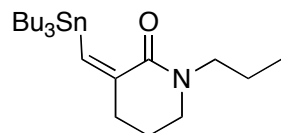
Typical procedure for stannylcarbonylation of alkynylamine 1 (Protocol A); A magnetic stirring bar, AIBN (2,2'-azobisisobutyronitrile, 16.2 mg, 0.1 mmol), benzene (50 mL), Bu_3SnH (170.2 mg, 0.58 mmol), and 4-pentynylpropylamine **1a** (65 mg, 0.52 mmol) were placed in a 100-mL stainless steel autoclave. The autoclave was closed, purged three times with carbon monoxide, pressurized with 75 atm of CO and then heated 90 °C for 3 h. Excess CO was discharged at room temperature. The solvent was removed under reduced pressure. The residue was dissolved into MeOH and TMSCl (5.2 mmol) was added. The reaction mixture was stirred at room temperature for 10 min. After evaporation, the resulting mixture was purified by flash chromatography on SiO_2 to give **2a** (R_f = 0.2, EtOAc/MeOH = 5/1, 71%, 56.5 mg).

1-Propyl-3-methylene-2-piperidinone (2a).



Colorless oil, (R_f = 0.2, hexane/EtOAc = 5/1), ^1H NMR (500 MHz, CDCl_3) δ 0.88 (t, J = 7.3 Hz, 3H), 1.87 (sext, J = 7.3 Hz, 2H), 1.83 (quint, J = 6.0 Hz, 2H), 2.52 (t, J = 6.2 Hz, 2H), 3.30-3.38 (m, 4H), 5.21 (s, 1H), 6.15 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.29, 20.25, 23.19, 30.06, 48.36, 49.26, 121.16, 137.79, 163.91; IR (neat) 1659, 1615 cm^{-1} ; MS (EI) m/z (rel intensity) 153 (M^+ , 22), 139 (36), 124 (61), 110 (100); HRMS (EI) m/z calcd for $\text{C}_9\text{H}_{15}\text{NO}$ (M^+) 153.1153, found 153.1159.

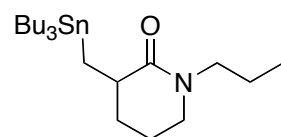
1-Propyl-3-tributylstannylmethylene-2-piperidinone (3a).



E isomer: Colorless oil, (R_f = 0.33, hexane/EtOAc = 5/1). ^1H NMR (500 MHz, CDCl_3) δ 0.89-1.03 (m, 18H), 1.22-1.39 (m, 6H), 1.40-1.68 (m, 6H), 1.82-1.94 (m, 2H), 2.49-2.58 (m, 2H), 3.31-3.42 (m, 4H), 7.40 (s, J ^1H -Sn = 65.4 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 10.09, 11.49, 13.73, 20.45, 23.80, 27.37, 29.22, 32.67, 48.58, 49.78, 139.71, 144.77, 163.46; IR (neat) 1642, 1586 cm^{-1} ; MS (EI), m/z calculated from major ^{120}Sn isotope (rel intensity) 386 (M^+ - C_4H_9 , 100), 272 (46); HRMS (EI) m/z calcd for $\text{C}_{17}\text{H}_{32}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 386.1506, found 386.1509.

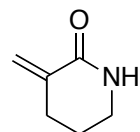
Z isomer: Colorless oil, (R_f = 0.3, hexane/EtOAc = 20/1). ^1H NMR (500 MHz, CDCl_3) δ 0.78-0.92 (m, 18H), 1.23-1.30 (sext, J = 7.3 Hz, 6H), 1.37-1.60 (m, 6H), 1.82-1.87 (m, 2H), 2.61-2.63 (m, 2H), 3.32-3.36 (m, 4H), 6.33 (s, J ^1H -Sn = 71.0 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.3, 11.9, 13.9, 20.42, 23.83, 27.57, 29.45, 33.85, 48.68, 49.27, 143.87, 144.22, 165.09; IR (neat) 1636, 1584; MS (EI), m/z calculated from major ^{120}Sn isotope (rel intensity); 386 (M^+ - C_4H_9 , 100), 272 (48); HRMS (EI) m/z calcd for $\text{C}_{17}\text{H}_{32}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 386.1506, found 386.1513.

1-Propyl-3-tributylstannylmethyl-2-piperidinone (4a).



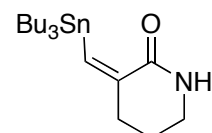
Colorless oil, (R_f = 0.3, hexane/EtOAc = 5/1). ^1H NMR (500 MHz, CDCl_3) δ 0.76-1.11 (m, 19H), 1.24-1.32 (m, 7H), 1.35-1.56 (m, 9H), 1.68-1.78 (m, 1H), 1.82-1.98 (m, 2H), 2.38-2.57 (m, 1H), 3.18-3.30 (m, 4H); ^{13}C NMR (125 MHz, CDCl_3) δ 9.85, 11.38, 13.67, 13.78, 20.38, 21.85, 27.53, 29.32, 31.36, 40.00, 48.21, 49.00, 173.85; IR (neat) 1634 cm^{-1} ; MS (EI), m/z calculated from major ^{120}Sn isotope (rel intensity); 388 (M^+ - C_4H_9 , 67), 350 (100); HRMS (EI) m/z calcd for $\text{C}_{17}\text{H}_{34}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 388.1662, found 388.1664.

3-Methylene-2-piperidinone (2b).



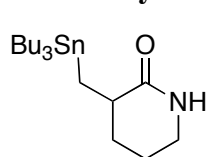
Colorless oil, (R_f = 0.18, EtOAc/MeOH = 19/1), ^1H NMR (500 MHz, CDCl_3) δ 1.87 (quint, J = 6.0 Hz, 2H), 2.57-2.60 (m, 2H), 3.39-3.41 (m, 2H), 5.32 (d, J = 1.4 Hz, 1H), 6.21 (d, J = 1.8 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 23.08, 29.75, 42.63, 122.07, 137.51, 166.04; IR (neat) 1668, 1618 cm^{-1} ; This product is a known compound and was identified by NMR with comparison of literature data (S. Klutchko *et al.* *J. Med. Chem.* **1981**, 24, 104.).

3-Tributylstannylmethylene-2-piperidinone (3b).



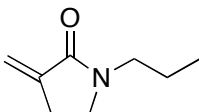
E isomer: Colorless oil, (R_f = 0.38, EtOAc), ^1H NMR (500 MHz, CDCl_3) δ 0.87-0.90 (m, 15H), 1.23-1.46 (m, 6H), 1.61 (quint, J = 7.6 Hz, 6H), 1.92-1.98 (m, 2H), 2.69-2.72 (m, 2H), 3.45-3.52 (m, 2H), 6.54 (bs, 1H), 7.05 (s, J ^1H -Sn = 90.7 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 13.61, 20.23, 22.85, 26.63, 27.98, 30.22, 42.92, 140.55, 154.86, 169.19; MS (EI) m/z calculated from major ^{120}Sn isotope (rel intensity) 344 (M^+ - C_4H_9 , 19), 322, (100), 230 (76), 149 (20); IR (neat) 1641, 1575 cm^{-1} ; HRMS (EI) m/z calcd for $\text{C}_{15}\text{H}_{30}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 344.1037, found 344.1037.
Z isomer: Colorless oil, (R_f = 0.20, hexane/EtOAc = 4/1). ^1H NMR (500 MHz, CDCl_3) δ 0.77-0.92 (m, 15H), 1.28 (sext, J = 7.3 Hz), 1.40-1.49 (m, 6H), 1.66-1.95 (m, 2H), 2.63 (m, 2H), 3.35-3.38 (m, 2H), 6.45 (s, J ^1H -Sn = 69.2 Hz, 1H), 6.85 (bs, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.83, 13.78, 23.63, 27.46, 29.33, 33.29, 42.80, 142.85, 146.17, 166.81; IR (neat) 1663, 1586 cm^{-1} ; MS (EI) m/z calculated from major ^{120}Sn isotope (rel intensity) 344 (M^+ - C_4H_9 , 100), 230 (45); HRMS (EI) m/z calcd for $\text{C}_{14}\text{H}_{26}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 344.1037, found 344.1039.

3-Tributhylstannylmethyl-2-piperidione (4b).



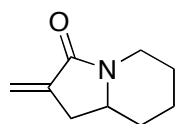
Colorless oil, (R_f = 0.13, hexane/EtOAc = 4/1). ^1H NMR (500 MHz, CDCl_3) δ 0.78-0.89 (m, 15H), 1.14-1.32 (m, 8H), 1.35-1.50 (m, 7H), 1.63-1.73 (m, 1H), 1.81-1.85 (m, 1H), 1.91-1.97 (m, 1H), 2.42 (quint, J = 7.8 Hz, 1H), 3.24-3.26 (m, 2H), 6.70 (bs, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 9.83, 12.93, 13.65, 21.67, 27.40, 29.23, 31.27, 39.49, 42.50, 176.71; IR (neat) 1659 cm^{-1} ; MS (EI) m/z calculated from major ^{120}Sn isotope (rel intensity) 346 (M^+ - C_4H_9 , 27), 324 (100), 230 (33), 198 (22), 151 (52); HRMS (EI) m/z calcd for $\text{C}_{14}\text{H}_{28}\text{NO}^{120}\text{Sn}$ (M^+ - C_4H_9) 346.1193, found 346.1195.

1-Propyl-3-methylene-2-pyrrolidinone (2c).



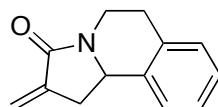
Colorless oil, (R_f = 0.10, hexane/EtOAc = 2/1), ^1H NMR (500 MHz, CDCl_3) δ 0.90 (t, J = 7.3 Hz, 3H), 1.57 (sext, J = 7.5 Hz, 2H), 2.73 (m, 2H), 3.32 (t, J = 7.6 Hz, 2H), 3.37 (t, J = 6.6 Hz, 2H), 5.28 (s, 1H), 5.94 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.28, 20.43, 24.01, 43.94, 44.77, 114.94, 139.89, 167.92; IR (neat) 1686, 1659 cm^{-1} ; MS (EI), m/z (rel intensity) 139 (M^+ , 36), 124 (61), 110 (100); HRMS (EI) m/z calcd for $\text{C}_9\text{H}_{15}\text{NO}$ (M^+) 139.0997, found 139.0982.

1-Oxo-2-methyleneoctahydroindolizine (2d).



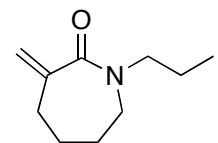
Colorless oil, (R_f = 0.18, Hexane/EtOAc = 1/1), ^1H NMR (500 MHz, CDCl_3) δ 1.08-1.20 (m, 1H), 1.30-1.47 (m, 2H), 1.66-1.69 (m, 1H), 1.84-1.90 (m, 2H), 2.27-2.30 (m, 1H), 2.68-2.73 (m, 1H), 2.86-2.90 (m, 1H), 3.41-4.44 (m, 1H), 4.18-4.20 (m, 1H), 5.21-5.28 (m, 1H), 5.88-5.91 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 23.90, 24.67, 31.84, 33.74, 40.69, 54.50, 115.05, 139.60, 166.84; IR (neat) 1685, 1658 cm^{-1} ; MS (EI) m/z (rel intensity) 151 (M^+ , 100), 122 (34), 110 (19), 95 (21); HRMS (EI) m/z calcd for $\text{C}_9\text{H}_{13}\text{NO}$ (M^+) 151.0997, found 151.0985.

Pyrrolo[2,1-a]isoquinolin-3(2H)-one (2e).



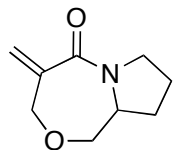
Carbonylation with tributyltin hydride was carried out with V-40 (1,1'-azobis(cyclohexane-1-carbonitrile)) as a radical initiator. Colorless oil, (R_f = 0.18, Hexane/EtOAc = 1/1), ^1H NMR (400 MHz, CDCl_3) δ 2.68-2.83 (m, 2H), 2.98-3.06 (m, 1H), 3.16-3.23 (m, 1H), 3.40 (ddd, J = 16.6, 7.8, 2.0 Hz, 1H), 4.39 (ddd, J = 12.9, 6.1, 2.2 Hz, 1H), 5.36-5.37 (m, 1H), 5.98-6.02 (m, 1H), 7.11-7.26 (m); ^{13}C NMR (100 MHz, CDCl_3) δ 28.35, 33.43, 37.69, 54.05, 115.17, 124.92, 126.80, 126.98, 129.07, 133.64, 137.22, 139.61, 166.33; IR (neat) 1686 cm^{-1} ; MS (EI) m/z (rel intensity) 199 (M^+ , 77), 198 (100), 149 (26), 130 (20); HRMS (EI) m/z calcd for $\text{C}_{13}\text{H}_{13}\text{NO}$ (M^+) 199.0997, found 199.0996.

1-Propyl-3-methylene-2-azacycloheptanone (2f).



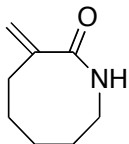
Colorless oil, (R_f = 0.18, hexane/EtOAc = 1/1), ^1H NMR (500 MHz, CDCl_3) δ 0.85 (t, J = 7.3 Hz, 3H), 1.50 (sext, J = 7.5 Hz, 2H), 1.56-1.72 (m, 4H), 2.23-2.29 (m, 2H), 3.19-3.24 (m, 2H), 3.26-3.32 (m, 2H), 5.12 (s, 1H), 5.35 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 11.35, 21.28, 27.82, 28.87, 32.36, 48.97, 49.48, 117.99, 147.78, 172.95; IR (neat) 1644 cm^{-1} ; MS (EI) m/z (relative intensity), 167 (M^+ , 52), 138 (100); HRMS (EI) m/z calcd for $\text{C}_9\text{H}_{15}\text{NO}$ (M^+) 167.1311, found 167.1305.

Hexahydro-4-methylene-(9a-S)-1H,5H-pyrrolo[2,1-c][1,4]oxazepine-5-one (2g).



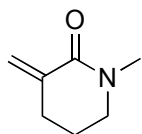
Colorless oil, ($R_f = 0.16$, hexane/EtOAc = 1/1), ^1H NMR (500 MHz, CDCl_3) δ 1.44-1.58 (m, 1H), 1.70-1.81 (m, 1H), 1.82-1.92 (m, 1H), 2.25-2.42 (m, 1H), 3.34 (dd, $J = 11.9, 9.2$ Hz, 1H), 3.40 (ddd, $J = 15.6, 8.7, 6.8$, 1H), 3.81 (ddd, $J = 11.9, 7.8, 3.7$, 1H), 3.82-3.89 (m, 1H), 3.90 (dd, $J = 12.4, 1.8$ Hz, 1H), 4.01 (d, $J = 12.8$ Hz, 1H), 4.30 (d, $J = 12.8$ Hz, 1H), 5.50 (s, 1H), 5.90 (s, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 22.81, 29.67, 47.29, 60.01, 70.54, 73.80, 125.51, 144.22, 169.27; IR (neat) 1647 cm^{-1} ; MS (EI) m/z (rel intensity) 167 (M^+ , 12), 149 (11), 137 (21), 109 (28), 83 (100); HRMS (EI) m/z calcd for $\text{C}_9\text{H}_{13}\text{NO}$ (M^+) 167.0946, found 167.0946.

3-Methylene-2-azacyclooctanone (2h).



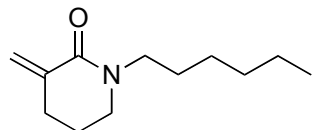
Colorless oil, ($R_f = 0.2$, EtOAc/MeOH = 19/1), ^1H NMR (500 MHz, CDCl_3) δ 1.52-1.61 (m, 6H), 2.37-2.40 (m, 2H), 3.26-3.30 (m, 2H), 4.98-5.13 (m, 1H), 5.14-5.17 (m, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 24.53, 26.22, 31.59, 37.36, 41.54, 114.34, 145.75, 176.31; IR (neat) 1738, 1640 cm^{-1} ; MS (EI) m/z (rel intensity) 139 (M^+ , 14), 111 (100), 67 (62); HRMS (EI) m/z calcd for $\text{C}_{15}\text{H}_{30}\text{N}$ (M^+) 415.1901, found 415.1910.

1-Methyl-3-methylene-2-piperidinone (2j).



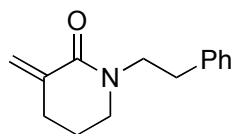
Colorless oil, ($R_f = 0.2$, Hexane/EtOAc = 1/1), ^1H NMR (CDCl_3 , 500 MHz) δ 1.88 (quint, $J = 6.0$ Hz, 2H), 2.55 (t, $J = 6.4$ Hz, 2H), 3.01 (s, 3H), 3.37 (t, $J = 6.0$ Hz, 2H), 5.24 (s, 1H), 6.17 (s, 1H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 23.07, 30.11, 35.09, 50.30, 120.90, 137.82, 164.35; IR (neat) 1657, 1613 cm^{-1} ; EIMS, m/z (rel intensity) 125 (M^+ , 100), 96 (17), 82 (18), 69 (24), 54 (100); HRMS (EI) m/z calcd for $\text{C}_7\text{H}_{11}\text{NO}$ (M^+) 125.0841, found 125.0848.

1-Hexyl-3-methylene-2-piperidinone (2k).



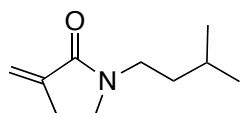
Colorless oil, ($R_f = 0.24$, Hexane/EtOAc = 1/1), ^1H NMR (CDCl_3 , 400 MHz) δ 0.86-0.88 (m, 3H), 1.25-1.34 (m, 6H), 1.54-1.57 (m, 2H), 1.87 (quint, $J = 6.0$ Hz, 2H), 2.53-2.58 (m, 2H), 3.35-3.44 (m, 4H), 5.25 (s, 1H), 6.19 (s, 1H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 13.98, 22.47, 23.23, 26.58, 27.00, 30.08, 31.56, 47.79, 48.36, 121.21, 137.81, 163.85; IR (neat) 1659, 1633 cm^{-1} ; EIMS, m/z (rel intensity) 195 (M^+ , 33), 138 (26), 124 (100), 69 (24), 54 (100); HRMS (EI) m/z calcd for $\text{C}_{12}\text{H}_{21}\text{NO}$ (M^+) 195.1623, found 195.1630.

1-(2-Phenylethyl)-3-methylene-2-piperidinone (2l).



Colorless oil, ($R_f = 0.24$, Hexane/EtOAc = 1/1), ^1H NMR (CDCl_3 , 400 MHz) δ 1.74-1.80 (m, 2H), 2.50-2.55 (m, 2H), 2.91 (t, $J = 7.5$ Hz, 2H), 3.20 (t, $J = 5.9$ Hz, 2H), 3.62 (t, $J = 7.5$ Hz, 2H), 5.26 (s, 1H), 6.22 (s, 1H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 23.10, 29.94, 33.50, 49.33, 50.14, 121.28, 126.24, 128.41, 128.80, 164.02; IR (neat) 1631 cm^{-1} ; EIMS, m/z (rel intensity) 215 (M^+ , 39), 124 (100), 91 (20); HRMS (EI) m/z calcd for $\text{C}_{14}\text{H}_{17}\text{NO}$ (M^+) 215.1310, found 215.1319.

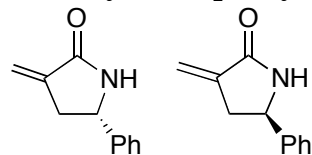
1-(3-Methylbutyl)-3-methylene-2-pyrrolidinone (2m).



Colorless oil. ($R_f = 0.24$, Hexane/EtOAc = 1/1), ^1H NMR (CDCl_3 , 500 MHz) δ 0.94 (d, $J = 6.4$ Hz, 6H), 1.42-1.48 (m, 2H), 1.52-1.65 (m, 1H), 2.74-2.76 (m, 2H), 3.35-3.40 (m, 4H), 5.29 (s, 1H), 5.95 (s, 1H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 22.44, 24.08, 25.87, 35.88, 41.47, 43.82, 114.79, 139.90,

167.71; IR (neat) 1691, 1659 cm^{-1} ; EIMS, m/z (rel intensity) 167 (M^+ , 15), 111 (81), 110 (100), 55 (17); HRMS calcd for $\text{C}_{10}\text{H}_{17}\text{NO}$ (M^+) 167.1310, found 167.1311.

3-Methylene-5-phenyl-2-pyrrolidinone (**2n** and **2o**)

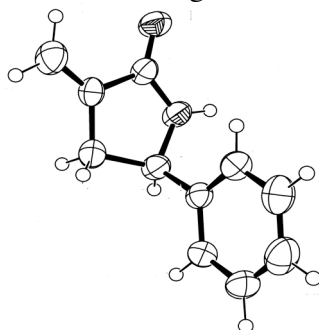


2n: white solid mp = 169-170 $^{\circ}\text{C}$.; (R_f = 0.15, hexane/EtOAc = 1/1), ^1H NMR (CDCl_3 , 500 MHz) δ 2.60-2.69 (m, 1H), 3.22-3.34 (m, 1H), 4.74 (m, 1H), 5.34 (s, 1H), 6.00 (s, 1H), 7.22-7.38 (m, 5H), 7.49 (bs, 1H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 36.89, 54.96, 116.48, 125.76, 128.00, 129.01, 139.05, 142.85, 171.19; IR (KBr) 1656, 1591 cm^{-1} ; EIMS, m/z (rel intensity) 173 (M^+ , 100), 144 (27), 104 (37); HRMS calcd for $\text{C}_{11}\text{H}_{11}\text{NO}$ (M^+) 173.0840, found 173.0843.

2o: white solid, mp = 169-170 $^{\circ}\text{C}$, ^1H -NMR, ^{13}C -NMR, IR and EIMS were identical with those of **2n**. HRMS calcd for $\text{C}_{11}\text{H}_{11}\text{NO}$ (M^+) 173.0840, found 173.0845.

The optical yields were determined by HPLC analysis using a chiral column. HPLC conditions; Chiralcel OD-H; hexane/2-propanol 95/5; flow rate 1.0 mL/min; column temperature 20 $^{\circ}\text{C}$; UV detector 254 nm; retention time for racemate 26.5 and 31.4 min, retention time for (*R*)-isomer (**2o**) 26.5 min in 99% ee, $[\alpha]_{\text{D}}^{18} = -10.0$ ($c = 0.50$, CHCl_3), retention time for (*S*)-isomer (**2n**) 31.4 min in 98% ee, $[\alpha]_{\text{D}}^{18} = 10.0$ ($c = 0.50$ CHCl_3). It should be noted that R isomer has been already known. ((a) Dembele, Y. A.; Belaud, C.; Villieras, J. *Tetrahedron Asymmetry*, **1992**, 3, 511. (b) Frenandes, R. A.; Yamamoto, Y. *J. Org. Chem.* **2004**, 69, 3562.) However, there is discrepancy in spectral and physical data between their data and our data. This led us to examine X-ray analysis of **2o**, which well supported the structure of **2o**. Crystallographic data: $\text{C}_{11}\text{H}_{11}\text{NO}$; $M = 173.21$, orthorhombic, space group $P2_12_12_1$, $a = 8.179(4)$ Å, $b = 9.368(5)$ Å, $c = 12.062(7)$ Å, $\alpha = 90^{\circ}$, $\beta = 90^{\circ}$, $\gamma = 90^{\circ}$, $V = 924.2(7)$ Å³, $Z = 4$, $D_{\text{calcd}} = 1.245$ g/cm³, $T = 296$ K, $\mu(\text{Mo K}\alpha) = 0.080$ mm⁻¹, 9103 reflections measured, 2118 unique ($R_{\text{int}} = 0.0299$), $R1 = 0.0342$, $wR2 = 0.0900$, GOF = 1.023.

ORTEP drawing of **2o**.



DFT Calculations DFT calculations were carried out using the Gaussian 03 programs.⁵ Geometry optimizations were performed using standard gradient techniques at the BHandHLYP level of theory using restricted (RBHandHLYP) and unrestricted (UBHandHLYP) methods for closed- and open-shell systems respectively.⁶ All ground and transition states were verified by vibrational frequency analysis. Standard basis sets were used, as well as the (valence) double- ζ pseudo potential basis sets of Hay and Wadt⁷ supplemented with a single set of d -type polarization functions for the tin (exponent $d(\zeta)_{\text{Sn}} = 0.200$),⁸ together with the double- ζ all-electron basis sets of Dunning⁹ with an additional set of polarization functions (exponents $d(\zeta)_{\text{C}} = 0.75$, $d(\zeta)_{\text{N}} = 0.80$, $d(\zeta)_{\text{O}} = 0.85$ and $p(\zeta)_{\text{H}} = 1.00$) for C, N, O and H were used in this study. We refer to this basis set as DZP throughout this work.

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BHandHLYP/DZP Gaussian Archive entries for the optimized structures involved in the 1,4-hydrogen shift reactions

Substrate of the 1,4-hydrogen shift involving 5-membered ring

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1\NGINC-DUAL1\FOpt\UBHandHLYP\Gen\C5H10N1O1Sn1(2)\MATSU\22-Mar-2009\1\#BHANDHLYP/GEN
SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM
M GEOM=CHECK GUESS=READ\Enol for 1,4-hydrogen transfer in 5-ring\0,2\O\H,1,r1\C,1,r2,2,a1\C,3,r3,1,a2,
2,d1,0\C,4,r4,3,a3,1,d2,0\N,3,r5,1,a4,2,d3,0\C,4,r6,3,a5,1,d4,0\Sn,5,r7,4,a6,3,d5,0\H,5,r8,4,a7,3,d6,0\C,6,r9,3,a8,4,d
7,0\H,6,r10,3,a9,4,d8,0\H,7,r11,4,a10,3,d9,0\H,7,r12,4,a11,3,d10,0\H,10,r13,6,a12,3,d11,0\H,10,r14,6,a13,3,d12,0\H
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,d407,0\H,10,r410,6,a409,3,d408,0\H,10,r411,6,a410,3,d409,0\H,10,r412,6,a411,3,d410,0\H,10,r413,6,a412,3,d411,0\H,10,r414,6,a413,3,d412,0\H,10,r415,6,a414,3,d413,0\H,10,r416,6,a415,3,d414,0\H,10,r417,6,a416,3,d415,0\H,10,r418,6,a417,3,d416,0\H,10,r419,6,a418,3,d417,0\H,10,r420,6,a419,3,d418,0\H,10,r421,6,a420,3,d419,0\H,10,r422,6,a421,3,d420,0\H,10,r423,6,a422,3,d421,0\H,10,r424,6,a423,3,d422,0\H,10,r425,6,a424,3,d423,0\H,10,r426,6,a425,3,d424,0\H,10,r427,6,a426,3,d425,0\H,10,r428,6,a427,3,d426,0\H,10,r429,6,a428,3,d427,0\H,10,r430,6,a429,3,d428,0\H,10,r431,6,a430,3,d429,0\H,10,r432,6,a431,3,d430,0\H,10,r433,6,a432,3,d431,0\H,10,r434,6,a433,3,d432,0\H,10,r435,6,a434,3,d433,0\H,10,r436,6,a435,3,d434,0\H,10,r437,6,a436,3,d435,0\H,10,r438,6,a437,3,d436,0\H,10,r439,6,a438,3,d437,0\H,10,r440,6,a439,3,d438,0\H,10,r441,6,a440,3,d439,0\H,10,r442,6,a441,3,d440,0\H,10,r443,6,a442,3,d441,0\H,10,r444,6,a443,3,d442,0\H,10,r445,6,a444,3,d443,0\H,10,r446,6,a445,3,d444,0\H,10,r447,6,a446,3,d445,0\H,10,r448,6,a447,3,d446,0\H,10,r449,6,a448,3,d447,0\H,10,r450,6,a449,3,d448,0\H,10,r451,6,a450,3,d449,0\H,10,r452,6,a451,3,d450,0\H,10,r453,6,a452,3,d451,0\H,10,r454,6,a453,3,d452,0\H,10,r455,6,a454,3,d453,0\H,10,r456,6,a455,3,d454,0\H,10,r457,6,a456,3,d455,0\H,10,r458,6,a457,3,d456,0\H,10,r459,6,a458,3,d457,0\H,10,r460,6,a459,3,d458,0\H,10,r461,6,a460,3,d459,0\H,10,r462,6,a461,3,d460,0\H,10,r463,6,a462,3,d461,0\H,10,r464,6,a463,3,d462,0\H,10,r465,6,a464,3,d463,0\H,10,r466,6,a465,3,d464,0\H,10,r467,6,a466,3,d465,0\H,10,r468,6,a467,3,d466,0\H,10,r469,6,a468,3,d467,0\H,10,r470,6,a469,3,d468,0\H,10,r471,6,a470,3,d469,0\H,10,r472,6,a471,3,d470,0\H,10,r473,6,a472,3,d471,0\H,10,r474,6,a473,3,d472,0\H,10,r475,6,a474,3,d473,0\H,10,r476,6,a475,3,d474,0\H,10,r477,6,a476,3,d475,0\H,10,r478,6,a477,3,d476,0\H,10,r479,6,a478,3,d477,0\H,10,r480,6,a479,3,d478,0\H,10,r481,6,a480,3,d479,0\H,10,r482,6,a481,3,d480,0\H,10,r483,6,a482,3,d481,0\H,10,r484,6,a483,3,d482,0\H,10,r485,6,a484,3,d483,0\H,10,r486,6,a48
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100563\A14=112.82196463\A15=113.10096183\A16=106.59344187\A17=60.97438042\A18=-62.94664649\A19=178.6821175\Version=x86-Linux-G03RevB.05\HF=-329.64989\S2=0.79768\S2-1=0.\S2A=0.750463\RMSD=4.420e-09\RMSF=2.822e-05\Dipole=0.909499,-1.0012927,0.5632342\PG=C01 [X(C5H10N1O1Sn1)]\@@

Transition state of the 1,4-hydrogen shift involving 5-membered ring

1\N\GINC-DUAL1\FTSUBHandHLYP\Gen\C5H10N1O1Sn1(2)\MATSU\20-Mar-2009\1\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN GEOM=CHECK GUESS=READ OPT=(TS,NOEIGENTEST, READFC,MAXCYCLE=100) NOSYMM\TS for 1,4-hydrogen transfer in 5-ring\0,2\O,-0.0083839243,0.05774075 8,0.0708157253\H,0.0523914405,0.0263553524,1.2493258694\C,1.2631974363,0.0301512384,-0.0460302355\C,2.0281003008,0.0813006113,1.1397998756\C,1.1908592874,0.214513061,2.2853681936\N,2.0170318235,-0.151604 7926,-1.1360104473\C,3.4441681286,-0.2712778558,0.77489966\Sn,0.5652122012,2.1769896324,2.8614396719\H ,1.516886647,-0.3138666816,3.1764246551\C,3.4383286138,-0.1554947599,-0.7763186397\H,1.6629396537,-0.18 19391762,-2.0710157885\H,3.6968798257,-1.2856011379,1.0867690636\H,4.1812585254,0.3950339641,1.215716 8073\H,3.9130082053,0.7690747074,-1.1001001022\H,3.9439713148,-0.9879627268,-1.2567097151\H,0.05938940 98,3.0519195735,1.4883890544\H,1.8213611101,3.0652301766,3.617894287\H,-0.7247957863,2.0586935677,3.97 26300688\Version=x86-Linux-G03RevB.05\HF=-329.6096299\S2=0.755634\S2-1=0.\S2A=0.750026\RMSD=7.40 9e-09\RMSF=2.654e-06\Dipole=1.4238009,-0.4356629,-1.1192199\PG=C01 [X(C5H10N1O1Sn1)]\@@

Product of the 1,4-hydrogen shift involving 5-membered ring

1\N\GINC-DUAL1\FOptUBHandHLYP\Gen\C5H10N1O1Sn1(2)\MATSU\23-Mar-2009\1\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM M GEOM=CHECK GUESS=READ\product for 1,4-hydrogen transfer in 5-ring\0,2\O\C,1,r2\C,2,r3,1,a2\C,3,r4,2,a 3,1,d2,0\N,2,r5,3,a4,4,d3,0\C,3,r6,2,a5,1,d4,0\H,4,r7,3,a6,2,d5,0\H,4,r8,3,a7,2,d6,0\Sn,4,r81,3,a71,2,d61,0\C,5,r9,2,a 8,3,d7,0\H,5,r10,2,a9,3,d8,0\H,6,r11,3,a10,2,d9,0\H,6,r12,3,a11,2,d10,0\H,10,r13,5,a12,2,d11,0\H,10,r14,5,a13,2,d1 2,0\H,9,r15,4,a14,3,d13,0\H,9,r16,4,a15,3,d14,0\H,9,r17,4,a16,3,d15,0\vr2=1.22621207\vr3=1.45288414\vr4=1.473786 91\vr5=1.36405291\vr6=1.49440617\vr7=1.09436935\vr8=1.08802958\vr81=2.17218497\vr9=1.45289923\vr10=1.00199263 \vr11=1.09188027\vr12=1.08882288\vr13=1.0896896\vr14=1.08679397\vr15=1.69546399\vr16=1.69783186\vr17=1.723212 12\vr2=125.65997372\vr3=121.92694973\vr4=107.81204895\vr5=109.00807223\vr6=110.45257001\vr7=111.39732853\vr 71=113.62762743\vr8=113.25361678\vr9=119.77750585\vr10=110.49906791\vr11=112.77758457\vr12=110.96938337\vr a13=111.08559097\vr14=113.78817062\vr15=112.76007676\vr16=102.46410645\vr2=6.1120908\vr3=-174.14653663\vr 4=-179.0363155\vr5=91.23712047\vr6=-150.98837212\vr61=-26.77908539\vr7=-10.44022772\vr8=192.00681958\vr9=- 111.13380694\vr10=129.62768484\vr11=-103.81406539\vr12=135.89555525\vr13=87.10788983\vr14=-45.11903296\vr 15=201.04483841\Version=x86-Linux-G03RevB.05\HF=-329.6861872\S2=0.758398\S2-1=0.\S2A=0.750054\RMS D=7.235e-09\RMSF=3.994e-05\Dipole=-0.5484046,-0.0154413,1.9324678\PG=C01 [X(C5H10N1O1Sn1)]\@@

Substrate of the 1,4-hydrogen shift involving 6-membered ring

1\N\GINC-DUAL1\FOptUBHandHLYP\Gen\C6H12N1O1Sn1(2)\MATSU\23-Mar-2009\1\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM M GEOM=CHECK GUESS=READ\Enol for 1,4-hydrogen transfer in 6-ring\0,2\C\N,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1 ,d1,0\C,4,r4,3,a3,2,d2,0\C,1,r5,2,a4,3,d3,0\O,1,r6,2,a5,3,d4,0\H,2,r7,3,a6,4,d5,0\H,7,r71,1,a61,2,d51,0\H,3,r8,2,a7,1 ,d6,0\H,3,r9,2,a8,1,d7,0\H,4,r10,3,a9,2,d8,0\H,4,r11,3,a10,2,d9,0\H,5,r12,4,a11,3,d10,0\H,5,r13,4,a12,3,d11,0\C,6,r1 4,5,a13,4,d12,0\Sn,16,r15,6,a14,1,d13,0\H,16,r16,6,a15,1,d14,0\H,17,r17,16,a16,6,d15,0\H,17,r18,16,a17,6,d16,0\H ,17,r19,16,a18,6,d17,0\vr1=1.38746581\vr2=1.45689612\vr3=1.52001092\vr4=1.52578651\vr5=1.38453977\vr6=1.366367 49\vr7=1.00700307\vr71=0.95915233\vr8=1.09351079\vr9=1.08775126\vr10=1.08818688\vr11=1.08884055\vr12=1.090615 96\vr13=1.08722727\vr14=1.39528112\vr15=2.10782753\vr16=1.08212926\vr17=1.70391816\vr18=1.70859932\vr19=1.715 04247\vr1=117.69964328\vr2=109.84661139\vr3=110.2565321\vr4=125.98693837\vr5=113.56224032\vr6=113.2392332 1\vr61=109.27456582\vr7=110.97353226\vr8=108.3609311\vr9=109.07008704\vr10=109.20602567\vr11=109.58546528\vr a12=110.13322597\vr13=120.68048023\vr14=127.6095296\vr15=115.31875695\vr16=113.94805774\vr17=113.5453035 7\vr18=105.89211136\vr1=-39.0443693\vr2=58.6101139\vr3=13.20406644\vr4=-170.48907704\vr5=-171.66557394\vr51 =-51.10075643\vr6=81.65415293\vr7=-160.15801401\vr8=180.27401723\vr9=-62.37360004\vr10=69.63084717\vr11=1 86.66296799\vr12=-154.08178271\vr13=1.08810596\vr14=180.58422089\vr15=64.6585792\vr16=-60.90072878\vr17=1 82.30812321\Version=x86-Linux-G03RevB.05\HF=-368.9515584\S2=0.798957\S2-1=0.\S2A=0.750477\RMSD=7. 074e-09\RMSF=2.785e-05\Dipole=0.2813389,-0.0478948,1.6772283\PG=C01 [X(C6H12N1O1Sn1)]\@@

Transition state of the 1,4-hydrogen shift involving 6-membered ring

1\N\GINC-DUAL1\FTSUBHandHLYP\Gen\C6H12N1O1Sn1(2)\MATSU\23-Mar-2009\0\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(TS,NOEIGENTEST,READFC,MAXCYCLE=100) NO SYMM GEOM=CHECK GUESS=READ\TS for 1,4-hydrogen transfer in 6-ring\0,2\O,-0.0050603752,0.03974673

15.0.0749126956\H,0.0603361836,0.0132696552,1.2522074598\C,1.2730912071,0.029066355,-0.0744998341\C,2.0244216164,0.085979978,1.1298224424\C,1.1480516767,0.2556742498,2.2460952143\N,1.8292899906,-0.0468026219,-1.2951367783\C,3.4977617719,-0.1892126705,1.073650788\H,1.4874982161,-0.2126304377,3.1655395304\Sn,0.4531322853,2.2238394488,2.7254448349\C,3.2477682729,-0.3406118619,-1.4416584815\C,4.0472539363,0.2538829141,-0.2868048047\H,1.2072131634,-0.2612469677,-2.0521686997\H,4.012319456,0.3397840989,1.8725983453\H,3.6981305034,-1.2528754589,1.2248640093\H,3.5892317584,0.076257211,-2.3859222528\H,3.4039537938,-1.4207482766,-1.4796960981\H,5.0866015253,-0.0483986335,-0.3972658801\H,4.0126555481,1.3397689847,-0.3540387994\H,1.6276359405,3.1028531223,3.6117302118\H,-0.9493342506,2.1236410272,3.6929923258\H,0.1051631419,3.0884761574,1.2992056245\Version=x86-Linux-G03RevB.05\HF=-368.9185236\S2=0.755097\S2-1=0.\S2A=0.750022\RMSD=6.876e-09\RMSF=6.985e-06\Dipole=1.4183268,-0.5425081,-1.0735448\PG=C01 [X(C6H12N1O1Sn1)]\@\

Product of the 1,4-hydrogen shift involving 6-membered ring

1\N\GINC-DUAL1\FOpt\UBHandHLYP\Gen\C6H12N1O1Sn1(2)\MATSU\23-Mar-2009\1\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM M GEOM=CHECK GUESS=READ\product for 1,4-hydrogen transfer in 6-ring\0,2\C\N,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\C,4,r4,3,a3,2,d2,0\C,1,r5,2,a4,3,d3,0\O,1,r6,2,a5,3,d4,0\H,2,r7,3,a6,4,d5,0\H,3,r8,2,a7,1,d6,0\H,3,r9,2,a8,1,d7,0\H,4,r10,3,a9,2,d8,0\H,4,r11,3,a10,2,d9,0\H,5,r12,4,a11,3,d10,0\H,5,r13,4,a12,3,d11,0\C,6,r14,5,a13,4,d12,0\H,15,r15,6,a14,1,d13,0\H,15,r16,6,a15,1,d14,0\Sn,15,r17,6,a16,1,d15,0\H,18,r18,15,a17,6,d16,0\H,18,r19,15,a18,6,d17,0\H,18,r20,15,a19,6,d18,0\H,1,r1=1.36160122\r2=1.45056984\r3=1.52041544\r4=1.52784083\r5=1.45590123\r6=1.23527914\r7=1.00348575\r8=1.09305893\r9=1.0873662\r10=1.08781049\r11=1.08837893\r12=1.09519239\r13=1.08868327\r14=1.47575676\r15=1.08578621\r16=1.09262063\r17=2.17275049\r18=1.7253115\r19=1.69982478\r20=1.69581699\A1=123.6688418\A2=110.07478008\A3=110.57471485\A4=118.24265362\A5=121.06103351\A6=118.78967076\A7=110.90694211\A8=108.38917506\A9=109.34802607\A10=109.04513277\A11=109.45201619\A12=110.44849713\A13=122.5576972\A14=111.57463587\A15=110.48230912\A16=112.74397064\A17=103.92685434\A18=112.2589407\A19=113.65908572\A20=113.30615592\A21=55.11805733\A22=13.95068201\A23=-166.376639\A24=-195.51350316\A25=83.31169656\A26=-158.93579681\A27=176.86866145\A28=-65.53268863\A29=71.22178218\A30=187.55692703\A31=2=-156.21172335\A32=166.64840124\A33=286.36418912\A34=40.78493806\A35=144.86287571\A36=30.76377436\A37=d18=-100.52892291\Version=x86-Linux-G03RevB.05\HF=-368.9859447\S2=0.758406\S2-1=0.\S2A=0.750052\RMSD=9.706e-09\RMSF=2.113e-05\Dipole=1.2928615,-0.4243473,1.4765586\PG=C01 [X(C6H12N1O1Sn1)]\@\

Substrate of the 1,4-hydrogen shift involving 7-membered ring

1\N\GINC-DUAL1\FOpt\UBHandHLYP\Gen\C7H14N1O1Sn1(2)\MATSU\24-Mar-2009\1\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM M GEOM=CHECK GUESS=READ\Enol for 1,4-hydrogen transfer in 7-ring\0,2\O\H,1,r1\C,1,r2,2,a1\C,3,r3,1,a2,2,d1,0\C,4,r4,3,a3,1,d2,0\N,3,r5,1,a4,2,d3,0\C,6,r6,3,a5,4,d4,0\C,7,r7,6,a6,3,d5,0\C,4,r8,3,a7,1,d6,0\C,9,r9,4,a8,3,d7,0\H,5,r10,4,a9,3,d8,0\Sn,5,r11,4,a10,3,d9,0\H,6,r12,3,a11,1,d10,0\H,7,r13,6,a12,3,d11,0\H,7,r14,6,a13,3,d12,0\H,8,r15,7,a14,6,d13,0\H,8,r16,7,a15,6,d14,0\H,9,r17,4,a16,3,d15,0\H,9,r18,4,a17,3,d16,0\H,10,r19,9,a18,4,d17,0\H,10,r20,9,a19,4,d18,0\H,12,r21,5,a20,4,d19,0\H,12,r22,5,a21,4,d20,0\H,12,r23,5,a22,4,d21,0\H,1,r1=0.95775296\r2=1.36545037\r3=1.3902539\r4=1.40250309\r5=1.37337052\r6=1.45264544\r7=1.52691603\r8=1.52596425\r9=1.52953814\r10=1.0822601\r11=2.10779843\r12=1.00230808\r13=1.08689144\r14=1.0907262\r15=1.0889161\r16=1.09026978\r17=1.08790686\r18=1.09133359\r19=1.08790452\r20=1.08901666\r21=1.70726519\r22=1.70531696\r23=1.71364236\A1=109.12716896\A2=121.66385682\A3=121.56359613\A4=111.24614985\A5=120.08941116\A6=111.84428611\A7=120.74177763\A8=116.62752775\A9=114.581863\A10=130.08162604\A11=112.17172874\A12=108.09093039\A13=109.52133067\A14=109.77673579\A15=108.26822641\A16=106.30613703\A17=109.60127973\A18=108.98809144\A19=108.83917542\A20=107.02818632\A21=113.31285505\A22=112.11867283\A23=45.19741846\A24=10.52613811\A25=-136.35742286\A26=29.42307786\A27=-84.4009193\A28=-167.8666586\A29=23.3497146\A30=-173.68193877\A31=18.93617317\A32=-5.9059236\A33=154.2904173\A34=37.84071898\A35=-79.99915024\A36=163.48452686\A37=144.29754674\A38=-101.95943992\A39=44.35604753\A40=160.17408868\A41=170.40440196\A42=50.5251793\A43=-71.79485326\Version=x86-Linux-G03RevB.05\HF=-408.2362625\S2=0.790137\S2-1=0.\S2A=0.750342\RMSD=8.908e-09\RMSF=5.238e-05\Dipole=0.5544239,0.7537982,-0.6462539\PG=C01 [X(C7H14N1O1Sn1)]\@\

Transition state of the 1,4-hydrogen shift involving 7-membered ring

1\N\GINC-DUAL1\FTSUBHandHLYP\Gen\C7H14N1O1Sn1(2)\MATSU\24-Mar-2009\0\#BHANDHLYP/GEN SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(TS,NOEIGENTEST,READFC,MAXCYCLE=100) NO SYMM GEOM=CHECK GUESS=READ\TS for 1,4-hydrogen transfer in 7-ring\0,2\O,-0.0073132192,-0.0439474001,0.0649846163\H,0.0479435243,-0.0225255593,1.2461254034\C,1.273481788,-0.0075343763,-0.0793244955\C,2.0113896863,-0.0087250493,1.1404085129\C,1.1173980324,-0.2570795999,2.233896375\N,1.7979872713,0.047

4786608,-1.3171133073\N,3.1846914935,-0.3074119079,-1.5701545651\N,4.1716524099,0.7953101141,-1.191494
8689\N,3.4315085266,0.4787021007,1.2623995704\N,3.8774467003,1.4483261039,0.1632318099\N,1.3980251015
,0.2312136885,3.161894814\N,0.4989181308,-2.2605245849,2.6556146992\N,1.1338373933,-0.0031516499,-2.06
58894056\N,3.2784953586,-0.5400202759,-2.62708815\N,3.4210336533,-1.2188353136,-1.0228258575\N,4.17589
04696,1.5653842688,-1.9612706923\N,5.1670859141,0.3509661612,-1.1832055903\N,3.511532422,0.9786902878,
2.2266126085\N,4.1233222222,-0.3664766511,1.3182240554\N,3.1069534202,2.2070509039,0.0402825568\N,4.7
738873289,1.9715283511,0.4920635048\N,-1.0083697153,-2.2631422468,3.4563254429\N,1.6224699757,-3.05804
64616,3.6736196947\N,0.3718967787,-3.1458260246,1.2038818681\N\Version=x86-Linux-G03RevB.05\HF=-408.2
08489\N,0.755388\N,0.750024\N,RMSD=9.543e-09\RMSF=3.046e-06\Dipole=1.3424321,0.3070738,-1.
0682489\PG=C01 [X(C7H14N1O1Sn1)]\@

Product of the 1,4-hydrogen shift involving 7-membered ring

1\N\GINC-DUAL1\FOpt\UBHandHLYP\Gen\C7H14N1O1Sn1(2)\MATSU\27-Mar-2009\1\#BHAndHLYP\GEN
SCF=DIRECT PSEUDO=READ FREQ=NORAMAN OPT=(Z-MATRIX,READFC,MAXCYCLE=100) NOSYM
M GEOM=CHECK GUESS=READ\product for 1,4-hydrogen transfer in 7-ring\0,2\O\N,1,2\N,2,3,1,2\N,3,4,2,3,1,
d2,0\N,2,5,3,4,4,d3,0\N,5,6,2,5,3,4,0\N,6,7,5,6,2,5,0\N,3,8,2,7,1,6,0\N,8,9,3,8,2,7,0\N,4,10,3,9,2,
d8,0\N,4,11,3,10,2,d9,0\N,4,1,3,1,2,d1,0\N,5,12,2,11,1,d10,0\N,6,13,5,12,2,d11,0\N,6,14,5,13,2,d12,0\N,7,
15,6,14,5,d13,0\N,7,16,6,15,5,d14,0\N,8,17,3,16,2,d15,0\N,8,18,3,17,2,d16,0\N,9,19,8,18,3,d17,0\N,9,20,
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36,0\N,13,239,4,238,3,d237,0\N,13,240,4,239,3,d238,0\N,13,241,4,240,3,d239,0\N,13,242,4,241,3,d240,0\N,13,243,4,242,3,d241,0\N,13,244,4,243,3,d242,0\N,13,245,4,244,3,d243,0\N,13,246,4,245,3,d244,0\N,13,247,4,246,3,d245,0\N,13,248,4,247,3,d246,0\N,13,249,4,248,3,d247,0\N,13,250,4,249,3,d248,0\N,13,251,4,250,3,d249,0\N,13,252,4,251,3,d250,0\N,13,253,4,252,3,d251,0\N,13,254,4,253,3,d252,0\N,13,255,4,254,3,d253,0\N,13,256,4,255,3,d254,0\N,13,257,4,256,3,d255,0\N,13,258,4,257,3,d256,0\N,13,259,4,258,3,d257,0\N,13,260,4,259,3,d258,0\N,13,261,4,260,3,d259,0\N,13,262,4,261,3,d260,0\N,13,263,4,262,3,d261,0\N,13,264,4,263,3,d262,0\N,13,265,4,264,3,d263,0\N,13,266,4,265,3,d264,0\N,13,267,4,266,3,d265,0\N,13,268,4,267,3,d266,0\N,13,269,4,268,3,d267,0\N,13,270,4,269,3,d268,0\N,13,271,4,270,3,d269,0\N,13,272,4,271,3,d270,0\N,13,273,4,272,3,d271,0\N,13,274,4,273,3,d272,0\N,13,275,4,274,3,d273,0\N,13,276,4,275,3,d274,0\N,13,277,4,276,3,d275,0\N,13,278,4,277,3,d276,0\N,13,279,4,278,3,d277,0\N,13,280,4,279,3,d278,0\N,13,281,4,280,3,d279,0\N,13,282,4,281,3,d280,0\N,13,283,4,282,3,d281,0\N,13,284,4,283,3,d282,0\N,13,285,4,284,3,d283,0\N,13,286,4,285,3,d284,0\N,13,287,4,286,3,d285,0\N,13,288,4,287,3,d286,0\N,13,289,4,288,3,d287,0\N,13,290,4,289,3,d288,0\N,13,291,4,290,3,d289,0\N,13,292,4,291,3,d290,0\N,13,293,4,292,3,d291,0\N,13,294,4,293,3,d292,0\N,13,295,4,294,3,d293,0\N,13,296,4,295,3,d294,0\N,13,297,4,296,3,d295,0\N,13,298,4,297,3,d296,0\N,13,299,4,298,3,d297,0\N,13,300,4,299,3,d298,0\N,13,301,4,300,3,d299,0\N,13,302,4,301,3,d300,0\N,13,303,4,302,3,d301,0\N,13,304,4,303,3,d302,0\N,13,305,4,304,3,d303,0\N,13,306,4,305,3,d304,0\N,13,307,4,306,3,d305,0\N,13,308,4,307,3,d306,0\N,13,309,4,308,3,d307,0\N,13,310,4,309,3,d308,0\N,13,311,4,310,3,d309,0\N,13,312,4,311,3,d310,0\N,13,313,4,312,3,d311,0\N,13,314,4,313,3,d312,0\N,13,315,4,314,3,d313,0\N,13,316,4,315,3,d314,0\N,13,317,4,316,3,d315,0\N,13,318,4,317,3,d316,0\N,13,319,4,318,3,d317,0\N,13,320,4,319,3,d318,0\N,13,321,4,320,3,d319,0\N,13,322,4,321,3,d320,0\N,13,323,4,322,3,d321,0\N,13,324,4,323,3,d322,0\N,13,325,4,324,3,d323,0\N,13,326,4,325,3,d324,0\N,13,327,4,326,3,d325,0\N,13,328,4,327,3,d326,0\N,13,329,4,328,3,d327,0\N,13,330,4,329,3,d328,0\N,13,331,4,330,3,d329,0\N,13,332,4,331,3,d330,0\N,13,333,4,332,3,d331,0\N,13,334,4,333,3,d332,0\N,13,335,4,334,3,d333,0\N,13,336,4,335,3,d334,0\N,13,337,4,336,3,d335,0\N,13,338,4,337,3,d336,0\N,13,339,4,338,3,d337,0\N,13,340,4,339,3,d338,0\N,13,341,4,340,3,d339,0\N,13,342,4,341,3,d340,0\N,13,343,4,342,3,d341,0\N,13,344,4,343,3,d342,0\N,13,345,4,344,3,d343,0\N,13,346,4,345,3,d344,0\N,13,347,4,346,3,d345,0\N,13,348,4,347,3,d346,0\N,13,349,4,348,3,d347,0\N,13,350,4,349,3,d348,0\N,13,351,4,350,3,d349,0\N,13,352,4,351,3,d350,0\N,13,353,4,352,3,d351,0\N,13,354,4,353,3,d352,0\N,13,355,4,354,3,d353,0\N,13,356,4,355,3,d354,0\N,13,357,4,356,3,d355,0\N,13,358,4,357,3,d356,0\N,13,359,4,358,3,d357,0\N,13,360,4,359,3,d358,0\N,13,361,4,360,3,d359,0\N,13,362,4,361,3,d360,0\N,13,363,4,362,3,d361,0\N,13,364,4,363,3,d362,0\N,13,365,4,364,3,d363,0\N,13,366,4,365,3,d364,0\N,13,367,4,366,3,d365,0\N,13,368,4,367,3,d366,0\N,13,369,4,368,3,d367,0\N,13,370,4,369,3,d368,0\N,13,371,4,370,3,d369,0\N,13,372,4,371,3,d370,0\N,13,373,4,372,3,d371,0\N,13,374,4,373,3,d372,0\N,13,375,4,374,3,d373,0\N,13,376,4,375,3,d374,0\N,13,377,4,376,3,d375,0\N,13,378,4,377,3,d376,0\N,13,379,4,378,3,d377,0\N,13,380,4,379,3,d378,0\N,13,381,4,380,3,d379,0\N,13,382,4,381,3,d380,0\N,13,383,4,382,3,d381,0\N,13,384,4,383,3,d382,0\N,13,385,4,384,3,d383,0\N,13,386,4,385,3,d384,0\N,13,387,4,386,3,d385,0\N,13,388,4,387,3,d386,0\N,13,389,4,388,3,d387,0\N,13,390,4,389,3,d388,0\N,13,391,4,390,3,d389,0\N,13,392,4,391,3,d390,0\N,13,393,4,392,3,d391,0\N,13,394,4,393,3,d392,0\N,13,395,4,394,3,d393,0\N,13,396,4,395,3,d394,0\N,13,397,4,396,3,d395,0\N,13,398,4,397,3,d396,0\N,13,399,4,398,3,d397,0\N,13,400,4,399,3,d398,0\N,13,401,4,400,3,d399,0\N,13,402,4,401,3,d400,0\N,13,403,4,402,3,d401,0\N,13,404,4,403,3,d402,0\N,13,405,4,404,3,d403,0\N,13,406,4,405,3,d404,0\N,13,407,4,406,3,d405,0\N,13,408,4,407,3,d406,0\N,13,409,4,408,3,d407,0\N,13,410,4,409,3,d408,0\N,13,411,4,410,3,d409,0\N,13,412,4,411,3,d410,0\N,13,413,4,412,3,d411,0\N,13,414,4,413,3,d412,0\N,13,415,4,414,3,d413,0\N,13,416,4,415,3,d414,0\N,13,417,4,416,3,d415,0\N,13,418,4,417,3,d416,0\N,13,419,4,418,3,d417,0\N,13,420,4,419,3,d418,0\N,13,421,4,420,3,d419,0\N,13,422,4,421,3,d420,0\N,13,423,4,422,3,d421,0\N,13,424,4,423,3,d422,0\N,13,425,4,424,3,d423,0\N,13,426,4,425,3,d424,0\N,13,427,4,426,3,d425,0\N,13,428,4,427,3,d426,0\N,13,429,4,428,3,d427,0\N,13,430,4,429,3,d428,0\N,13,431,4,430,3,d429,0\N,13,432,4,431,3,d430,0\N,13,433,4,432,3,d431,0\N,13,434,4,433,3,d432,0\N,13,435,4,434,3,d433,0\N,13,436,4,435,3,d434,0\N,13,437,4,436,3,d435,0\N,13,438,4,437,3,d436,0\N,13,439,4,438,3,d437,0\N,13,440,4,439,3,d438,0\N,13,441,4,440,3,d439,0\N,13,442,4,441,3,d440,0\N,13,443,4,442,3,d441,0\N,13,444,4,443,3,d442,0\N,13,445,4,444,3,d443,0\N,13,446,4,445,3,d444,0\N,13,447,4,446,3,d445,0\N,13,448,4,447,3,d446,0\N,13,449,4,448,3,d447,0\N,13,450,4,449,3,d448,0\N,13,451,4,450,3,d449,0\N,13,452,4,451,3,d450,0\N,13,453,4,452,3,d451,0\N,13,454,4,453,3,d452,0\N,13,455,4,454,3,d453,0\N,13,456,4,455,3,d454,0\N,13,457,4,456,3,d455,0\N,13,458,4,457,3,d456,0\N,13,459,4,458,3,d457,0\N,13,460,4,459,3,d458,0\N,13,461,4,460,3,d459,0\N,13,462,4,461,3,d460,0\N,13,463,4,462,3,d461,0\N,13,464,4,463,3,d462,0\N,13,465,4,464,3,d463,0\N,13,466,4,465,3,d464,0\N,13,467,4,466,3,d465,0\N,13,468,4,467,3,d466,0\N,13,469,4,468,3,d467,0\N,13,470,4,469,3,d468,0\N,13,471,4,470,3,d469,0\N,13,472,4,471,3,d470,0\N,13,473,4,472,3,d471,0\N,13,474,4,473,3,d472,0\N,13,475,4,474,3,d473,0\N,13,476,4,475,3,d474,0\N,13,477,4,476,3,d475,0\N,13,478,4,477,3,d476,0\N,13,479,4,478,3,d477,0\N,13,480,4,479,3,d478,0\N,13,481,4,480,3,d479,0\N,13,482,4,481,3,d480,0\N,13,483,4,482,3,d481,0\N,13,484,4,483,3,d482,0\N,13,485,4,484,3,d483,0\N,13,486,4,485,3,d484,0\N,13,487,4,486,3,d485,0\N,13,488,4,487,3,d486,0\N,13,489,4,488,3,d487,0\N,13,490,4,489,3,d488,0\N,13,491,4,490,3,d489,0\N,13,492,4,491,3,d490,0\N,13,493,4,492,3,d491,0\N,13,494,4,493,3,d492,0\N,13,495,4,494,3,d493,0\N,13,496,4,495,3,d494,0\N,13,497,4,496,3,d495,0\N,13,498,4,497,3,d496,0\N,13,499,4,498,3,d497,0\N,13,500,4,499,3,d498,0\N,13,501,4,500,3,d4

2\O\H,1,r1\C,1,r2,2,a1\C,2,r3,1,a2,3,d1,0\C,3,r4,1,a3,2,d2,0\N,3,r5,1,a4,2,d3,0\C,6,r6,3,a5,1,d4,0\C,7,r7,6,a6,3,d5,0\C,5,r8,3,a7,6,d6,0\C,9,r9,5,a8,3,d7,0\C,10,r10,9,a9,5,d8,0\H,4,r11,5,a10,3,d9,0\Sn,4,r12,5,a11,3,d10,0\H,6,r13,3,a12,1,d11,0\H,7,r14,6,a13,3,d12,0\H,7,r15,6,a14,3,d13,0\H,8,r16,7,a15,6,d14,0\H,8,r17,7,a16,6,d15,0\H,9,r18,5,a17,3,d16,0\H,9,r19,5,a18,3,d17,0\H,10,r20,9,a19,5,d18,0\H,10,r21,9,a20,5,d19,0\H,11,r22,10,a21,9,d20,0\H,11,r23,10,a22,9,d21,0\H,13,r24,4,a23,5,d22,0\H,13,r25,4,a24,5,d23,0\H,13,r26,4,a25,5,d24,0\|r1=1.18355526|r2=1.29246335|r3=1.46214443|r4=1.42619215|r5=1.34262218|r6=1.45178479|r7=1.5285342|r8=1.50562178|r9=1.54433794|r10=1.53147937|r11=1.08526138|r12=2.13862557|r13=1.00264638|r14=1.08700997|r15=1.08750386|r16=1.08970318|r17=1.09009177|r18=1.09332512|r19=1.08756404|r20=1.08848442|r21=1.08916233|r22=1.08981976|r23=1.09151836|r24=1.71330649|r25=1.70520761|r26=1.70696215|a1=93.99704897|a2=134.38351684|a3=114.30364455|a4=117.57627556|a5=126.7784953|a6=114.2075321|a7=125.95015753|a8=118.17422782|a9=115.89380004|a10=114.26376449|a11=119.722648|a12=113.75889172|a13=109.07786083|a14=106.59493222|a15=108.06457221|a16=108.23194762|a17=110.48900436|a18=105.30155773|a19=107.07563478|a20=110.09061703|a21=108.50956642|a22=108.37394134|a23=111.38131083|a24=109.97085248|a25=110.437288|d1=-15.04113238|d2=0.50366164|d3=-178.53498121|d4=199.60691963|d5=-100.08614764|d6=21.91119366|d7=34.13332956|d8=-101.11700628|d9=-148.43386114|d10=79.2605039|d11=2.98382119|d12=24.62467285|d13=-220.71505237|d14=-38.08875957|d15=-153.16880722|d16=-92.32156038|d17=-204.76767471|d18=139.86547479|d19=25.06887592|d20=200.71036394|d21=-44.66869372|d22=85.84341334|d23=-34.09112896|d24=205.07707711\\Version=EM64L-G03RevE.01\\HF=-447.4953658\\S2=0.755602\\S2-1=0.\\S2A=0.750026\\RMSD=8.378e-09\\RMSF=6.668e-05\\Thermal=0.\\Dipole=1.4122355,0.3615347,-1.063535\\PG=C01 [X(C8H16N1O1Sn1)]\\@

Product of the 1,4-hydrogen shift involving 8-membered ring

1\N\GINC-I7FOpt\UBHandHLYP\Gen\C8H16N1O1Sn1(2)\HIROSHI\13-Nov-2010\1\#BHAndHLYP/gen pseudo=read freq=NO raman geom=check guess=read OPT=(Z-matrix,calcFC,Maxcycle=100,Maxstep=15) SCF=NoVarAcc Nosymm\\c8 product\0,2\O\C,1,r1\C,2,r2,1,a1\C,3,r3,2,a2,1,d1,0\H,4,r4,3,a3,2,d2,0\N,2,r5,1,a4,3,d3,0\C,6,r6,2,a5,1,d4,0\C,7,r7,6,a6,2,d5,0\C,3,r8,2,a7,6,d6,0\C,9,r9,3,a8,2,d7,0\C,10,r10,9,a9,3,d8,0\Sn,4,r11,3,a10,2,d9,0\H,4,r12,3,a11,2,d10,0\H,6,r13,2,a12,1,d11,0\H,7,r14,6,a13,2,d12,0\H,7,r15,6,a14,2,d13,0\H,8,r16,7,a15,6,d14,0\H,8,r17,7,a16,6,d15,0\H,9,r18,3,a17,2,d16,0\H,9,r19,3,a18,2,d17,0\H,10,r20,9,a19,3,d18,0\H,10,r21,9,a20,3,d19,0\H,11,r22,10,a21,9,d20,0\H,11,r23,10,a22,9,d21,0\H,12,r24,4,a23,3,d22,0\H,12,r25,4,a24,3,d23,0\H,12,r26,4,a25,3,d24,0\|r1=1.23747493|r2=1.46255653|r3=1.47601327|r4=1.08945055|r5=1.35694961|r6=1.45194071|r7=1.52545891|r8=1.50488412|r9=1.53928163|r10=1.53280938|r11=2.18309085|r12=1.08491266|r13=1.00377215|r14=1.08770354|r15=1.08840035|r16=1.08973624|r17=1.09025731|r18=1.09476424|r19=1.09150895|r20=1.08845508|r21=1.08850797|r22=1.08957066|r23=1.09140181|r24=1.69637509|r25=1.69941541|r26=1.72749069|a1=119.2390411|a2=114.24890593|a3=111.98836546|a4=119.92831389|a5=126.7452075|a6=113.67208609|a7=126.00168285|a8=120.34375535|a9=115.95104308|a10=110.27687425|a11=112.24929636|a12=112.33153904|a13=109.06003938|a14=107.32882394|a15=108.06195011|a16=108.66123789|a17=109.3882137|a18=105.00268353|a19=106.29382428|a20=110.53990676|a21=108.52529351|a22=108.31089803|a23=113.63594098|a24=112.0997475|a25=104.13322168|d1=25.01246761|d2=59.98374736|d3=-179.49139239|d4=203.3247013|d5=-108.62817222|d6=39.32269869|d7=9.64724241|d8=-94.08265575|d9=-54.0029968|d10=182.64656953|d11=0.30426828|d12=15.35778235|d13=-229.68593634|d14=-41.81804535|d15=-157.19161976|d16=-117.63320032|d17=-229.06257253|d18=147.37803809|d19=32.75613681|d20=204.75904128|d21=-40.6745246|d22=103.60122402|d23=-27.89397006|d24=218.14971169\\Version=EM64L-G03RevE.01\\HF=-447.5590166\\S2=0.758675\\S2-1=0.\\S2A=0.750056\\RMSD=9.485e-09\\RMSF=5.803e-05\\Thermal=0.\\Dipole=-0.7072549,0.1629213,1.8605772\\PG=C01 [X(C8H16N1O1Sn1)]\\@

BHAndHLYP/6-31G* Gaussian Archive entries for the optimized structures involved in the radical substitution reaction on nitrogen and higher-level calculated single-point energies

N-phenethyl-5-amino-2-methylenepentanoyl radical (K)

BHAndHLYP/6-31G*

1\N\GINC-QUAD\POpt\UBHandHLYP\6-31G(d)\C14H18N1O1(2)\HIROSHI\12-Jan-2011\1\#BHAndHLYP/6-31G* SCF=direct OPT=(Z-matrix,CalcFC,Maxcycle=100) Nosymm\\subst for cyclization with phenethylamine\0,2\C\X,1,1,\O,1,r1,2,90.\C,1,r2,2,a1,3,d1,0\C,4,r3,1,a2,3,d2,0\C,4,r4,1,a3,3,d3,0\C,6,r5,4,a4,1,d4,0\C,7,r6,6,a5,4,d5,0\N,8,r7,7,a6,6,d6,0\H,9,r8,8,a7,7,d7,0\C,9,r81,8,a71,7,d71,0\H,5,r9,4,a8,1,d8,0\H,5,r10,4,a9,1,d9,0\H,6,r11,4,a10,1,d10,0\H,6,r12,4,a11,1,d11,0\H,7,r13,6,a12,4,d12,0\H,7,r14,6,a13,4,d13,0\H,8,r15,7,a14,6,d14,0\H,8,r16,7,a15,6,d15,0\C,11,r17,9,a16,8,d16,0\C,11,r18,9,a17,8,d17,0\H,11,r19,9,a18,8,d18,0\H,20,r20,11,a19,9,d19,0\H,20,r21,11,a20,9,d20,0\H,20,r22,11,a21,9,d20c,0\X,21,1,4,11,90.,20,180.,0\X,21,1,4,26,90.,11,180.,0\C,27,r23,21,a22,20,d21,0\C,27,r24,28,a23,21,d22,0\C,27,r25,29,a24,28,d23,0\C,27,r26,30,a25,29,d24,0\C,27,r27,31,a26,30,d25,0\H,28,r28,21,a27,11,d26,0\H,29,r29,28,a28,21,d27,0\H,30,r30,29,a29,28,d28,0\H,31,r31,30,a30,29,d29,0\H,32,r32,31,a31,30,d30,0\|r1=1.17821566|r2=1.49157859|r3=1.32829694|r4=1.49923957|r5=1.5282239|r6=1.51987634|r7=1.44893843|r8=1.00905549

\r81=1.4577249\r9=1.07740623\r10=1.07912442\r11=1.08815316\r12=1.09059172\r13=1.0910414\r14=1.08797819\r15=1.0878176\r16=1.09905303\r17=1.52821282\r18=1.51269236\r19=1.09788514\r20=1.0866846\r21=1.08690234\r22=1.0864481\r23=1.37763167\r24=1.37867577\r25=1.39349871\r26=1.39169565\r27=1.38531133\r28=1.07738225\r29=1.07842165\r30=1.07813593\r31=1.07830911\r32=1.07948389\aa1=40.77825619\aa2=118.03465557\aa3=116.63706906\aa4=112.74511384\aa5=112.48725885\aa6=110.63571346\aa7=108.79469425\aa71=115.22220503\aa8=120.92519175\aa9=121.58521856\aa10=109.2167985\aa11=108.94342712\aa12=109.01341124\aa13=109.91469936\aa14=108.9440585\aa15=109.48106862\aa16=110.76791567\aa17=109.6273699\aa18=110.8931866\aa19=110.056503\aa20=111.74291586\aa21=110.17460863\aa22=60.13267274\aa23=60.34160423\aa24=60.01709223\aa25=59.65680223\aa26=59.88389125\aa27=119.04162771\aa28=119.71301392\aa29=120.2348963\aa30=120.13950383\aa31=119.67712545\ad1=196.56543402\ad2=-0.25238179\ad3=179.57172148\ad4=-66.15105127\ad5=176.87209295\ad6=177.80883188\ad7=52.59692906\ad71=-185.69434838\ad8=0.23184187\ad9=180.38187434\ad10=-188.59255015\ad11=55.05875749\ad12=55.20806614\ad13=-61.46662344\ad14=58.22391397\ad15=-57.79443995\ad16=70.11601281\ad17=192.26414279\ad18=-49.14338249\ad19=57.10866479\ad20=-63.46466727\ad20c=176.75062866\ad21=80.50089168\ad22=178.38195568\ad23=178.22166423\ad24=178.38794061\ad25=178.44348939\ad26=2.19156522\ad27=180.16953692\ad28=180.05566838\ad29=180.37361092\ad30=180.45309446\\Version=EM64L-G03RevE.01\\HF=-673.8044076\\S2=0.755527\\S2-1=0.\\S2A=0.750022\\RMSD=5.075e-09\\RMSF=1.501e-05\\Thermal=0.\\Dipole=-0.8512308,-0.0885551,0.4879445\\Polar=139.0371571,-1.6799544,133.5095373,32.7520943,-18.9076914,163.836409\\PG=C01 [X(C14H18N1O1)]\\@

BHandHLYP/6-31+G/BHandHLYP/6-31G***
HF=-673.8269034

Transition state for the ring-closure reaction L

BHandHLYP/6-31G*

1\\GINC-QUAD\\FTS\\UBHandHLYP\\6-31G(d)\\C14H18N1O1(2)\\HIROSHI\\12-Jan-2011\\1\\#BHandHLYP/6-31G* SCF=direct OPT=(TS,NoEigenTest,Z-matrix,CalcFC,Maxcycle=100) Nosymm\\TS for cyclization with phenetyla mine\\0,2\\C\\N,1,r1\\C,2,r2,1,a1\\C,3,r3,2,a2,1,d1,\\O\\C,4,r4,3,a3,2,d2,\\O\\C,1,r5,2,a4,3,d3,\\O\\O,1,r6,2,a5,3,d4,\\O\\H,2,r7,3,a6,4,d5,\\O\\C,2,r71,3,a61,4,d51,\\O\\H,3,r8,2,a7,1,d6,\\O\\H,3,r9,2,a8,1,d7,\\O\\H,4,r10,3,a9,2,d8,\\O\\H,4,r11,3,a10,2,d9,\\O\\H,5,r12,4,a11,3,d10,\\O\\H,5,r13,4,a12,3,d11,\\O\\C,6,r14,5,a13,4,d12,\\O\\H,16,r15,6,a14,1,d13,\\O\\H,16,r16,6,a15,1,d14,\\O\\C,9,r17,2,a16,1,d15,\\O\\C,9,r18,2,a17,1,d16,\\O\\H,9,r19,2,a18,1,d17,\\O\\H,19,r20,9,a19,2,d18,\\O\\H,19,r21,9,a20,2,d19,\\O\\H,19,r22,9,a21,2,d20,\\O\\X,20,1,4,9,90,19,180,\\O\\X,20,1,4,25,90,9,180,\\O\\C,26,r23,20,a22,19,d21,\\O\\C,26,r24,27,a23,20,d22,\\O\\C,26,r25,28,a24,27,d23,\\O\\C,26,r26,29,a25,28,d24,\\O\\C,26,r27,30,a26,29,d25,\\O\\H,27,r28,20,a27,9,d26,\\O\\H,28,r29,27,a28,20,d27,\\O\\H,29,r30,28,a29,27,d28,\\O\\H,30,r31,29,a30,28,d29,\\O\\H,31,r32,30,a31,29,d30,\\O\\r1=2.25823542\r2=1.45750671\r3=1.51610784\r4=1.52170597\r5=1.35398962\r6=1.17655291\r7=1.0064264\r71=1.4856871\r8=1.08837862\r9=1.09276315\r10=1.08924538\r11=1.08867688\r12=1.09199982\r13=1.08711828\r14=1.41053201\r15=1.0751075\r16=1.07589564\r17=1.52712529\r18=1.51360394\r19=1.08987058\r20=1.08589986\r21=1.08401829\r22=1.08715316\r23=1.38450229\r24=1.39029069\r25=1.39191861\r26=1.37882615\r27=1.38038285\r28=1.07923994\r29=1.07821059\r30=1.07804654\r31=1.07818188\r32=1.07880275\aa1=111.3255863\aa2=110.23276427\aa3=112.33700206\aa4=104.3507508\aa5=100.10969251\aa6=109.80633908\aa61=115.03221246\aa7=107.96015789\aa8=111.44000049\aa9=108.92042417\aa10=109.88377012\aa11=108.08455497\aa12=108.3987436\aa13=117.92270779\aa14=121.92194961\aa15=119.72725829\aa16=112.61253418\aa17=110.68798282\aa18=107.09944769\aa19=111.02601341\aa20=111.09155138\aa21=109.56295493\aa22=59.85289574\aa23=59.96531437\aa24=59.69224618\aa25=60.07168362\aa26=60.25701084\aa27=119.5607808\aa28=119.79371747\aa29=120.21045187\aa30=120.03775779\aa31=119.85921051\ad1=-43.94256677\ad2=66.53667314\ad3=20.31065918\ad4=-163.66325101\ad5=-149.74517227\ad51=87.7880645\ad6=75.11719901\ad7=-167.57332216\ad8=186.58892308\ad9=-56.937815\ad10=62.44456511\ad11=176.57679522\ad12=-150.84970867\ad13=-3.42213965\ad14=173.32389072\ad15=20.13662452\ad16=-105.25748838\ad17=138.13525147\ad18=55.77823781\ad19=-64.58799624\ad20=175.58925139\ad21=112.66051077\ad22=179.67797507\ad23=179.92031281\ad24=179.7522167\ad25=179.62221433\ad26=0.23188859\ad27=179.9647264\ad28=180.16558141\ad29=179.89761497\ad30=179.72071453\\Version=EM64L-G03RevE.01\\HF=-673.7940561\\S2=0.787945\\S2-1=0.\\S2A=0.750311\\RMSD=2.694e-09\\RMSF=3.678e-05\\Thermal=0.\\Dipole=0.4898516,-0.0074923,1.313475\\Polar=170.6256992,-30.5005285,102.4055788,-30.6114054,1.7996495,172.2301087\\PG=C01 [X(C14H18N1O1)]\\@

BHandHLYP/6-31+G/BHandHLYP/6-31G***
HF=-673.8139062

Intermediate M

BHandHLYP/6-31G*

1\INGINC-QUAD\FOpt\UBHandHLYP\6-31G(d)\C14H18N1O1(2)\HIROSHI\12-Jan-2011\1\#\BHandHLYP/6-31G
* SCF=direct OPT=(Z-matrix,CalcFC,Maxcycle=100) Nosymm\Intermediate for cyclization with phenethylamine\
0,2\N,1,r1\N,2,r2,1,a1\N,3,r3,2,a2,1,d1,0\N,4,r4,3,a3,2,d2,0\N,1,r5,2,a4,3,d3,0\O,1,r6,2,a5,3,d4,0\H,2,r7,3,a6,4,d5,
0\N,2,r7,3,a6,4,d5,0\H,3,r8,2,a7,1,d6,0\H,3,r9,2,a8,1,d7,0\H,4,r10,3,a9,2,d8,0\H,4,r11,3,a10,2,d9,0\H,5,r12,4,a11,
3,d10,0\H,5,r13,4,a12,3,d11,0\N,6,r14,5,a13,4,d12,0\H,16,r15,6,a14,1,d13,0\H,16,r16,6,a15,1,d14,0\N,9,r17,2,a16,1,
d15,0\N,9,r18,2,a17,1,d16,0\H,9,r19,2,a18,1,d17,0\H,19,r20,9,a19,2,d18,0\H,19,r21,9,a20,2,d19,0\H,19,r22,9,a21,2,
d20,0\X,20,1,4,9,90.,19,180.,0\X,20,1,4,25,90.,9,180.,0\N,26,r23,20,a22,19,d21,0\N,26,r24,27,a23,20,d22,0\N,26,r25,
28,a24,27,d23,0\N,26,r26,29,a25,28,d24,0\N,26,r27,30,a26,29,d25,0\H,27,r28,20,a27,9,d26,0\H,28,r29,27,a28,20,d2
7,0\H,29,r30,28,a29,27,d28,0\H,30,r31,29,a30,28,d29,0\H,31,r32,30,a31,29,d30,0\N,1=1.55422306\N,2=1.48324604\N,
3=1.51205484\N,4=1.52134688\N,5=1.39544363\N,6=1.24134983\N,7=1.01342093\N,8=1.53786224\N,9=1.08604538\N,
10=1.08653645\N,11=1.08759604\N,12=1.08917578\N,13=1.09225243\N,14=1.08798901\N,15=1.38399329\N,16=1.07475454\N,
17=1.0773759\N,18=1.52067855\N,19=1.50922339\N,20=1.08494036\N,21=1.08496564\N,22=1.0825194\N,23=1.08644314
\N,24=1.39264993\N,25=1.39238039\N,26=1.38410301\N,27=1.37368913\N,28=1.38476992\N,29=1.07950799\N,30=1.07797
802\N,31=1.0779839\N,32=1.08010714\N,1=114.54259915\N,2=109.25972372\N,3=109.77441759\N,4=1
17.02099581\N,5=110.61123445\N,6=108.00030515\N,7=112.71344846\N,8=107.00479617\N,9=108.36182175\N,10=108.
99519958\N,11=109.64508602\N,12=108.21910225\N,13=109.44000382\N,14=118.43014723\N,15=120.76912332\N,16=1
20.85903073\N,17=112.5708813\N,18=109.3675683\N,19=104.94343119\N,20=111.21195738\N,21=111.00823724\N,22=1
108.0220433\N,23=59.65580852\N,24=59.70648001\N,25=59.8459113\N,26=60.39374791\N,27=60.27449121\N,28=119.7
8240344\N,29=119.84220376\N,30=120.07590699\N,31=120.04353899\N,32=120.8653326\N,1=-54.12693299\N,2=63.47
349176\N,3=27.00137625\N,4=-156.47114348\N,5=-165.1581484\N,6=79.47620265\N,7=-177.878731
72\N,8=184.98193341\N,9=-58.58964945\N,10=76.29190833\N,11=191.17652632\N,12=-165.24861701\N,13=-1.316086
05\N,14=177.50029179\N,15=13.42048833\N,16=-112.9962064\N,17=131.0602276\N,18=58.79941503\N,19=-61.770148
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06932\N,26=0.94644699\N,27=179.87971181\N,28=180.25015626\N,29=180.03189357\N,30=180.27934473\N\Version=E
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BHandHLYP/6-31+G/BHandHLYP/6-31G***
HF=-673.8125744

Product lactam O

BHandHLYP/6-31G*

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0\\H,3,r8,2,a7,1,d6,0\\H,3,r9,2,a8,1,d7,0\\H,4,r10,3,a9,2,d8,0\\H,4,r11,3,a10,2,d9,0\\H,5,r12,4,a11,3,d10,0\\H,5,r13,4,a12
3,d11,0\\C,6,r14,5,a13,4,d12,0\\H,15,r15,6,a14,1,d13,0\\H,15,r16,6,a15,1,d14,0\\r1=1.35898604\\r2=1.44834363\\r3=1.
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23788\\r11=1.08861417\\r12=1.09222823\\r13=1.08687338\\r14=1.32421982\\r15=1.07641503\\r16=1.07849255\\a1=12
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63.8124503\\RMSD=4.601e-09\\RMSF=3.347e-05\\Dipole=1.2269046,-0.0483746,1.0361948\\PG=C01 [X(C6H9N1O
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BHandHLYP/6-31+G/BHandHLYP/6-31G***
HF=-363.8252594

Phenethyl radical (P)

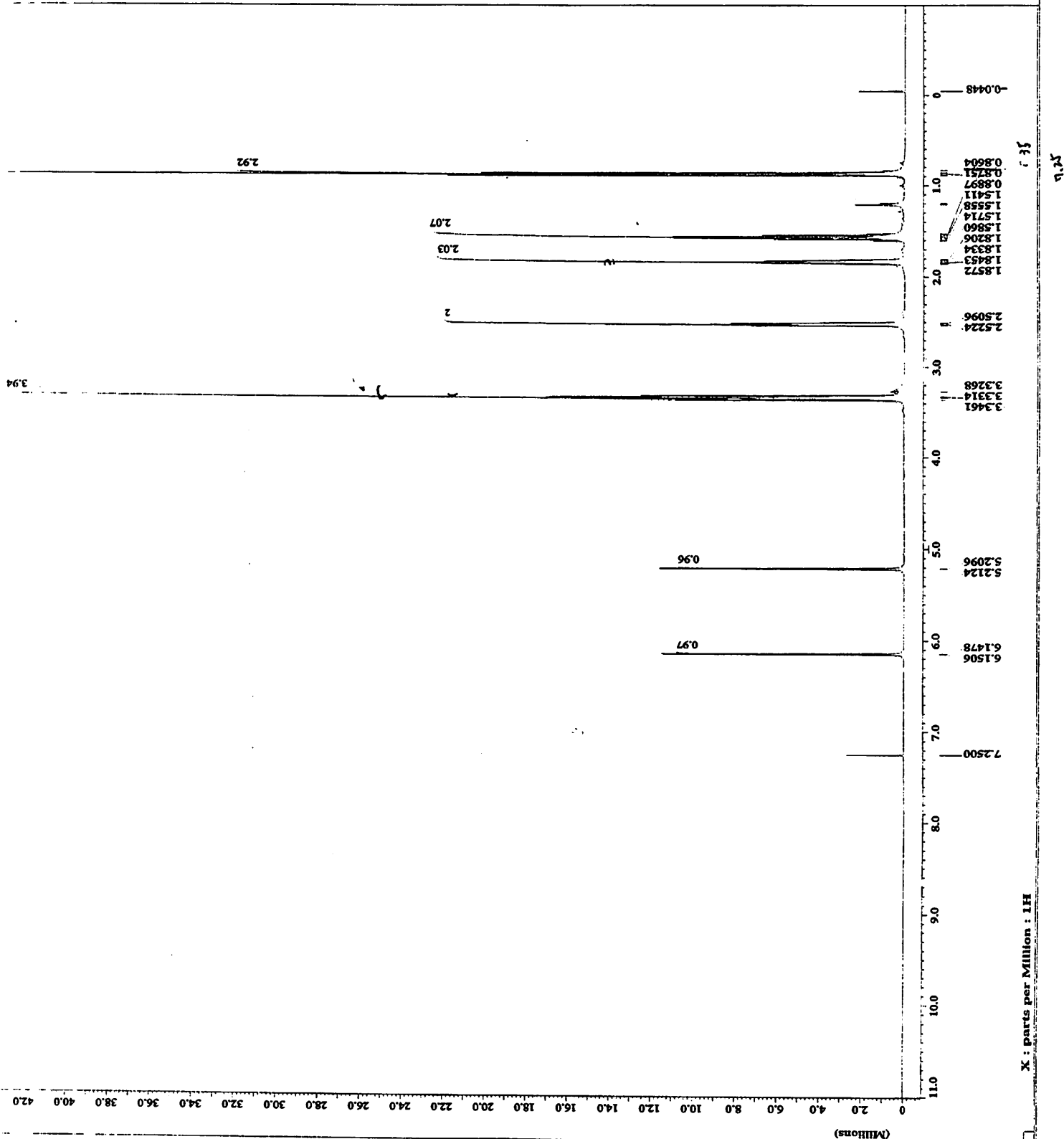
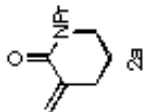
BHandHLYP/6-31G*

1\\INGINC-DUAL1\\POpt\\UBHandHLYP\\6-31G(d)\\C8H9(2)\\MATSU\\12-Jan-2011\\1\\#BHANDHLYP/6-31G* SCF
=DIRECT FREQ=NORAMAN OPT=(Z-MATRIX,CALCFC,MAXCYCLE=100) NOSYMM\\phenethyl radical\\0,
2\\X\\C,1,r1\\C,1,r2,2,a1\\C,1,r3,3,a2,2,d1,0\\C,1,r4,4,a3,3,d2,0\\C,1,r5,5,a4,4,d3,0\\C,1,r6,6,a5,5,d4,0\\C,2,r7,3,a6,4,d5,0\\
C,8,r8,2,a7,3,d6,0\\H,3,r9,2,a8,8,d7,0\\H,4,r10,3,a9,2,d8,0\\H,5,r11,4,a10,3,d9,0\\H,6,r12,5,a11,4,d10,0\\H,7,r13,6,a12,5
d11,0\\H,8,r14,2,a13,3,d12,0\\H,9,r15,8,a14,2,d13,0\\H,9,r16,8,a15,2,d14,0\\H,9,r17,8,a16,2,d15,0\\r1=1.43974015\\r2=
1.38729361\\r3=1.37202934\\r4=1.37792863\\r5=1.38659885\\r6=1.4072121\\r7=1.40910089\\r8=1.49117026\\r9=1.078
94534\\r10=1.07837674\\r11=1.07765809\\r12=1.07847546\\r13=1.07741222\\r14=1.0786105\\r15=1.09119672\\r16=1.0
9119697\\r17=1.08532101\\a1=60.05880089\\a2=59.86524497\\a3=60.88284012\\a4=60.45234266\\a5=59.15579347\\a6
=120.36280514\\a7=124.51399624\\a8=118.69086161\\a9=119.73081379\\a10=120.28726367\\a11=119.79206735\\a12
=119.5587893\\a13=117.42601843\\a14=111.94114338\\a15=111.94115112\\a16=111.01902712\\d1=180.00416704\\d2
=180.00398324\\d3=180.00388729\\d4=180.00390295\\d5=180.00003091\\d6=180.00001753\\d7=0.00002545\\d8=180.
00000065\\d9=179.9999809\\d10=179.99998779\\d11=179.99995581\\d12=0.00019764\\d13=59.84965428\\d14=-59.85
160093\\d15=-180.0009531\\Version=x86-Linux-G03RevB.05\\HF=-310.0360481\\S2=0.843335\\S2-1=0.\\S2A=0.756
159\\RMSD=3.302e-09\\RMSF=3.280e-06\\Dipole=-0.0491113,0.0000089,0.1235134\\PG=C01 [X(C8H9)]\\@

BHandHLYP/6-31+G/BHandHLYP/6-31G***
HF=-310.0455823

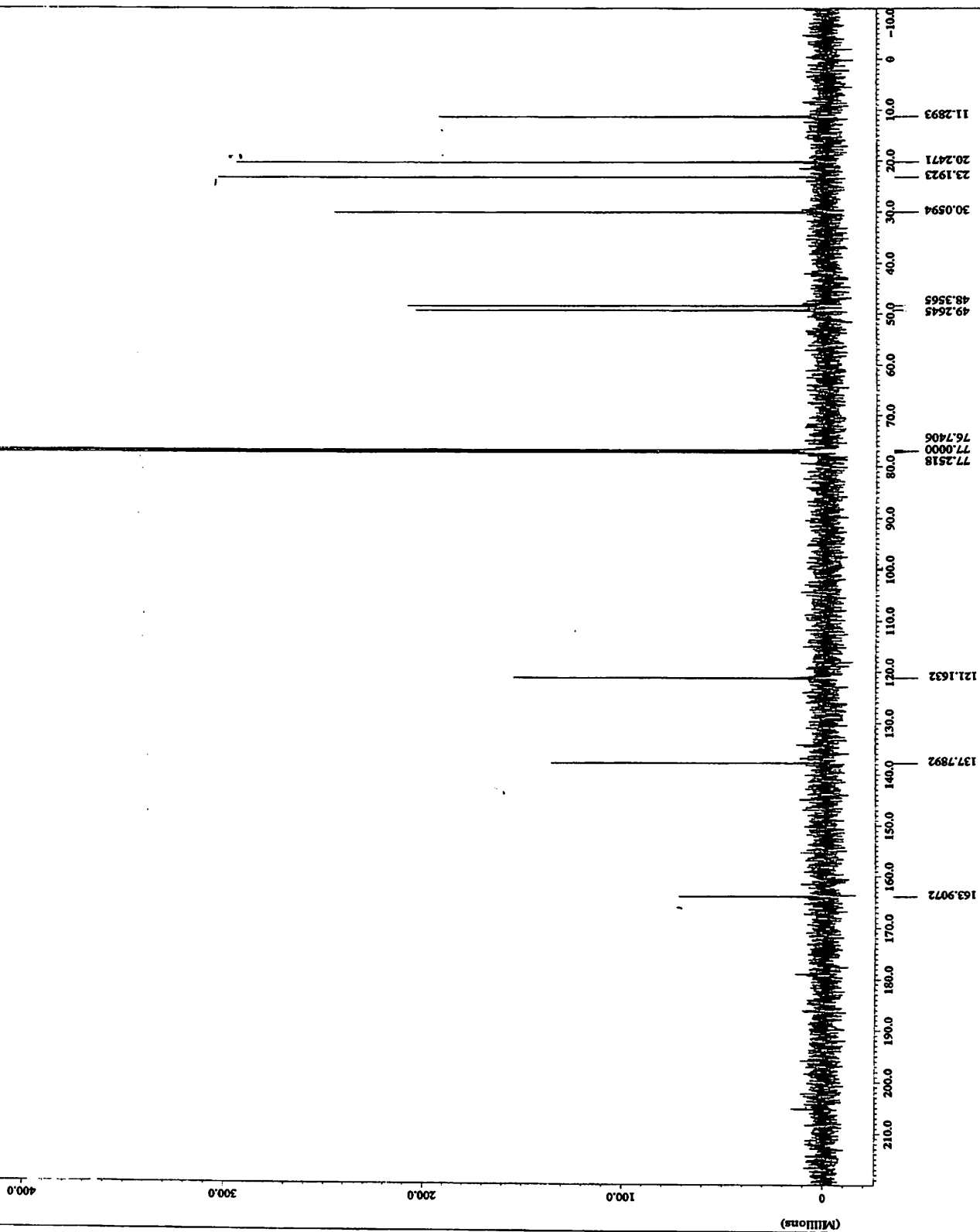
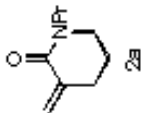
JEOL

ACQUISITION PARAMETERS
File Name - 7JAN-2003 01:25:07
Sample ID - 7JAN-2003 01:25:07
Content - Single Pulse Experiment
Creation Date - 6-JAN-2003 19:16:15
Revision Date - 7-JAN-2003 01:25:07
Spec Site - ECP500
Spec Type - HELIX_RMR
Data Format - 1D COMPLEX
DIN Title - 1H
DIN Size - 16384
DIN Units - [cps]
Scans - 2
Acquisition - 1H
X_Offset - 51(ppm)
X_Freq - 500.15241602(MHz)
X_Sweep - 7.50750751(MHz)
SOLVENT - CDCl3
DIN_Offset - 14(ppm)
Temp_Set - 22.3(C)
Recvr_Gain - 16
Pulse_Program - zgpg30
Field_strength - 11.7473579(T)
Filter_Program - 300MHz
Filter_Offset - 3.7511936(MHz)



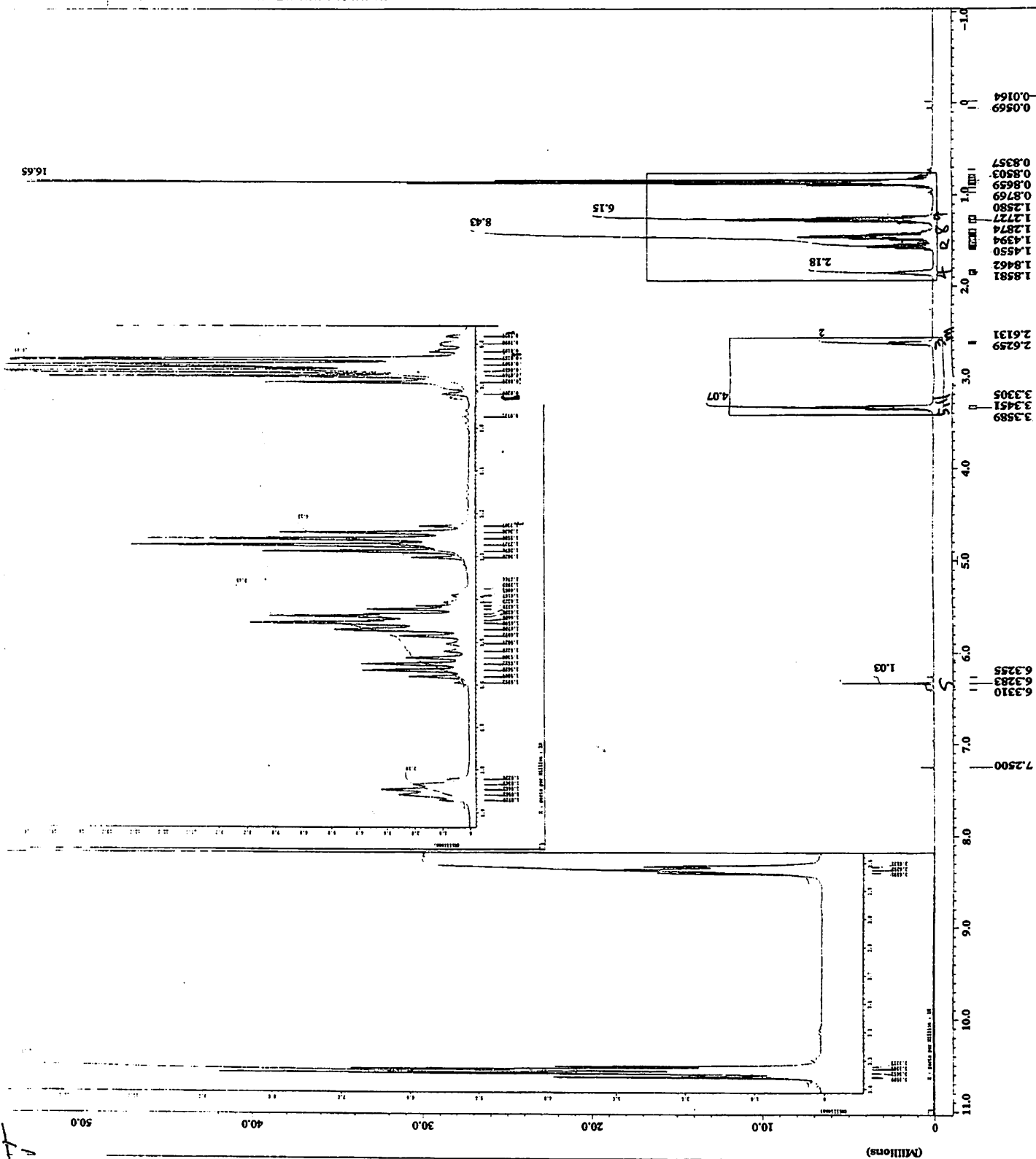
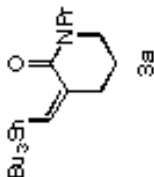
JEOL

--- ACQUISITION PARAMETERS ---
File Name - 1Q_13C_spectrum_419
Author - JEOL LTD.
Sample ID - 419
Chemical - 419
Creation Date - 6-JAN-2003 19:43:52
Revision Date - 7-JAN-2003 09:30:01
Spec Site - ECP500
Spec Type - DRUGA_002
Data Format - 1D COMPLEX
Dimensions - 1
Dim Title - 13C
Dim Site - 12768
Dim Units - 12768
Scans - 122
Mod_return - 1
X_domain - 13C
X_offset - 100 (ppm)
X_sweep - 11.747147 (kHz)
X_resolution - 31.4451088 (kHz)
Solvent - CHLOROFORM-D
Spin_get - 15 (Hz)
Temp_get - 22.9 (C)
Temp_set - 22.9 (C)
Pulse_prog - zgpg30
Pulse_strength - 11.7473578 (W)
Filter_mode - HETCORHET
Filter_width - 15.72066221 (kHz)



JEOL

ACQUISITION PARAMETERS
File Name : 1D_spectrum_8100
Author : J. L. L.
Date : 21-11-13
Experiment : Single Pulse Experiment
Constant : 25-AUG-2003 20:20:10
Creation Date : 25-AUG-2003 11:17:06
Revision Date : 25-AUG-2003 11:17:06
Spec file : 829300
Spec Type : DELTA_800
Data Format : 1D_COMPLEX
Dimensions : 1
D1m Size : 16384
D1m Units : [cps]
Scans : 8
Mod_return : 1
X_offset : 1
X_freq : 500.14241602 [MHz]
X_sweep : 7.50750751 [kHz]
Solvent : CDCl3
Spin_rate : 23.5 [Hz]
Recvr_gain : 13
Field_strength : 11.7473579 [G]
Filter_mode : BORTSMOOTH
Filter_width : 3.7511936 [Hz]



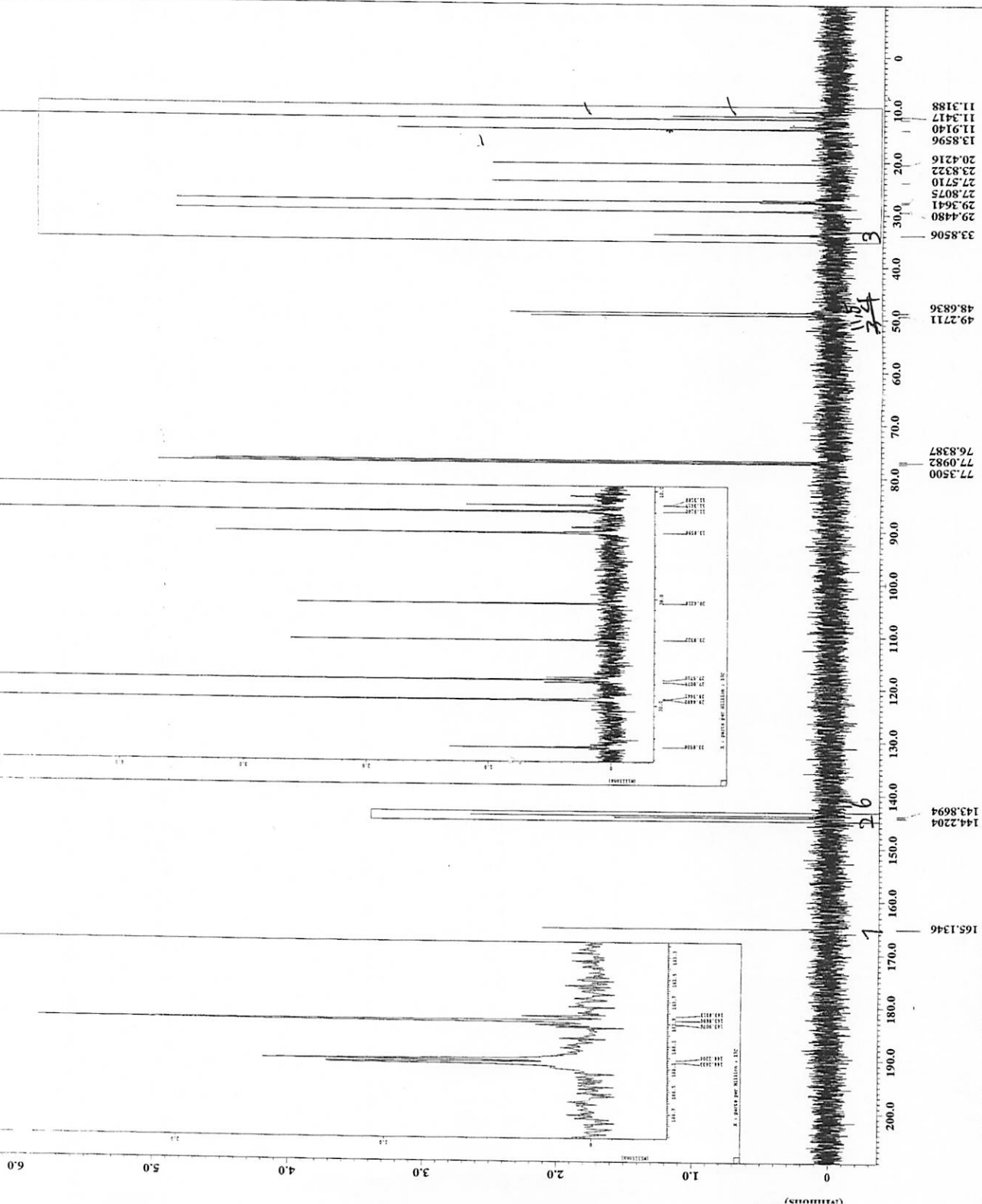
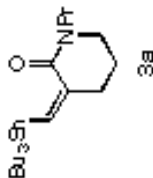
X : parts per Million : 1H

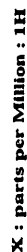
JEOL

```

---- ACQUISITION PARAMETERS ----
File Name      = 1d_13c_spectrum.2236
Author         = JEOL LTD.
Sample ID      = 11-15
Pulse Program  = zgpg30 - Pulse with Broad
Creation Date   = 26-AUG-2003 20:24:17
Revision Date   = 26-AUG-2003 11:22:41
Spec Site      = ECF500

Spec Type      = DELTA NMR
Data Format     = 1D COMPLEX
Dimensions     = X
Dim Title      = 13C
Dim Units      = Hz
Dim Units      = 1000
Scans          = 110
Mod_return     = 1
X_domain       = 13C
X_offset       = 100.625
X_sweep        = 31.446540881 [kHz]
Solvent        = CHLOROFORM-D
Spin_get       = 15 [Hz]
Temp_get       = 25.9 [°C]
Field_strength = 11.7473579 [T]
Filter_mode     = BUTTERWORTH
Filter_width    = 15.72066221 [kHz]
    
```

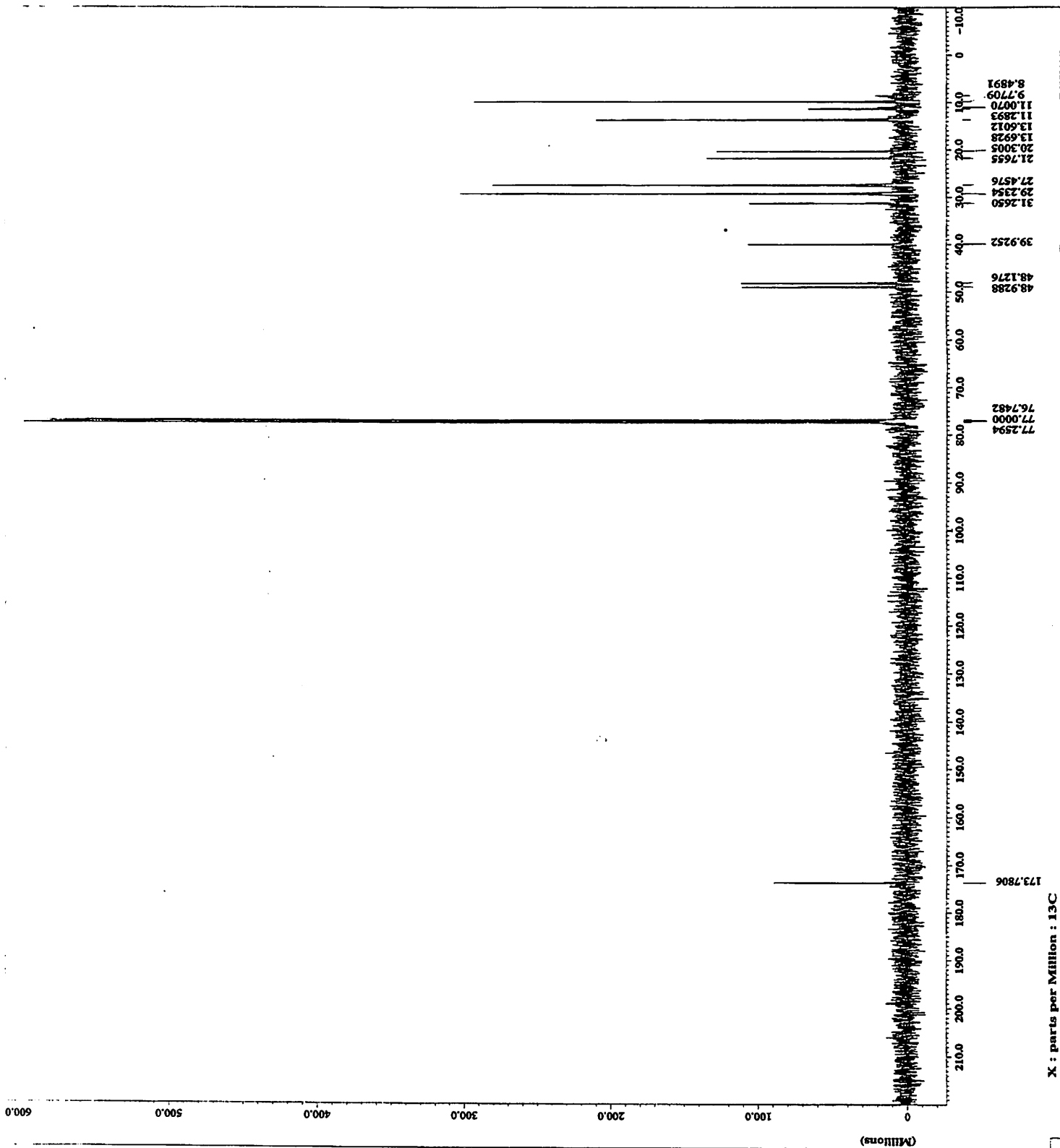
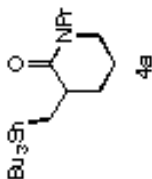


C[Sn](C)(C)C1CCC(CC1)C(=O)N2CCCCC2

```

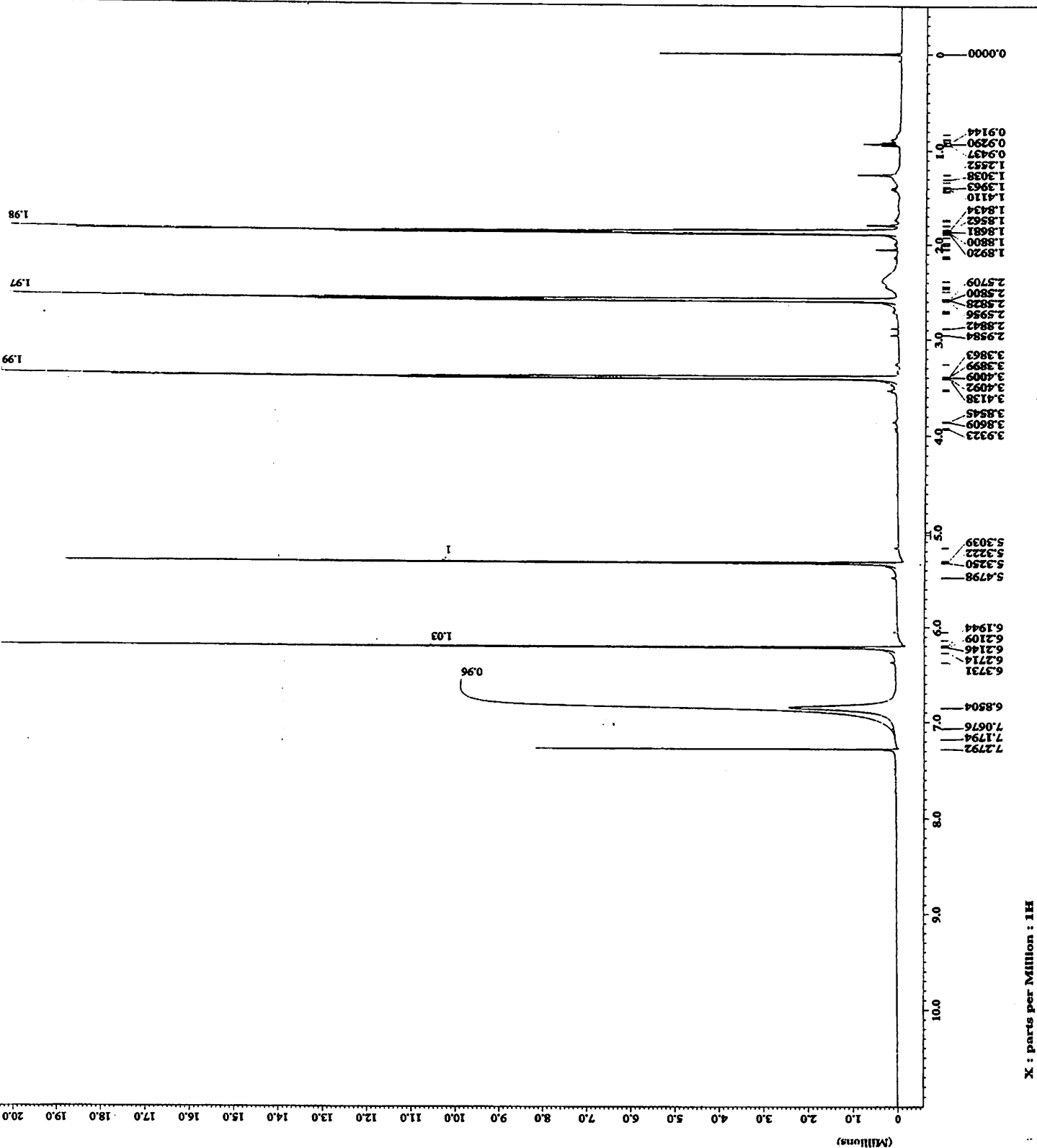
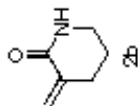
*** ACQUISITION PARAMETERS ***
File Name      = 10_13c_spectrum.1172
Author         = NJOI LRT.
Sample ID      = 13c
Acquisition    = 13c-13c with broad
Creation Date   = 11-APR-2003 17:03:18
Revision       = 12-APR-2003 09:10:07
Dspc site      = ECF500
Spec Type      = 1D NMR
Data Format     = 1D COMPLEX
Dimensions     = 1
Dim 1 title    = 13c
Dim 1 size     = 3789
Dim 2 title    = 13c
Dim 2 size     = 262
Mod-return     = 1
X-domain       = 13c
X-offset       = 100 [ppm]
X-freq         = 125.7617 [MHz]
X-proc         = 1
X-ref          = 13C14454088 [Hz]
Solvent        = CHLOROFORM-D
N1             = 13 [ms]
Sfn            = 37.4 [dB]
Temp_cat       = 1
Temp_gain      = 1
Pulse_prog     = zgpg30
Pulse_width    = 13.7073579 [s]
Filter_mode    = HERTZSUM
Filter_width   = 13.72066221 [Hz]

```



JEOL

----- ACQUISITION PARAMETERS -----
File Name - 1D_SPECTRUM_931
Author - JEOL LTD.
Sample ID - 9856480
Experiment - 1D
Creation Date - 24-JUN-2002 16:39:15
Revision Date - 24-JUN-2002 23:51:44
Spec Site - ECP500
Spec Type - DELTA_500
Data Format - 1D COMPLEX
Dimensions - X
Dim Title - 1H
Dim Size - 6554
Dim Units - (ppm)
Scans - 8
Mod_return - 1
X_domain - 1H
X_offset - 0.0000000000000000
X_sweep - 7.50750751(MHz)
Solvent - CHLOROFORM-D
Spin_rate - 15(Hz)
Temp_get - 25.5(C)
Temp_set - 25.5(C)
Pulse_prog - zgpg30
Field_strength - 31.7473579(T)
Filter_mode - BUTTERWORTH
Filter_width - 3.7511936(KHz)



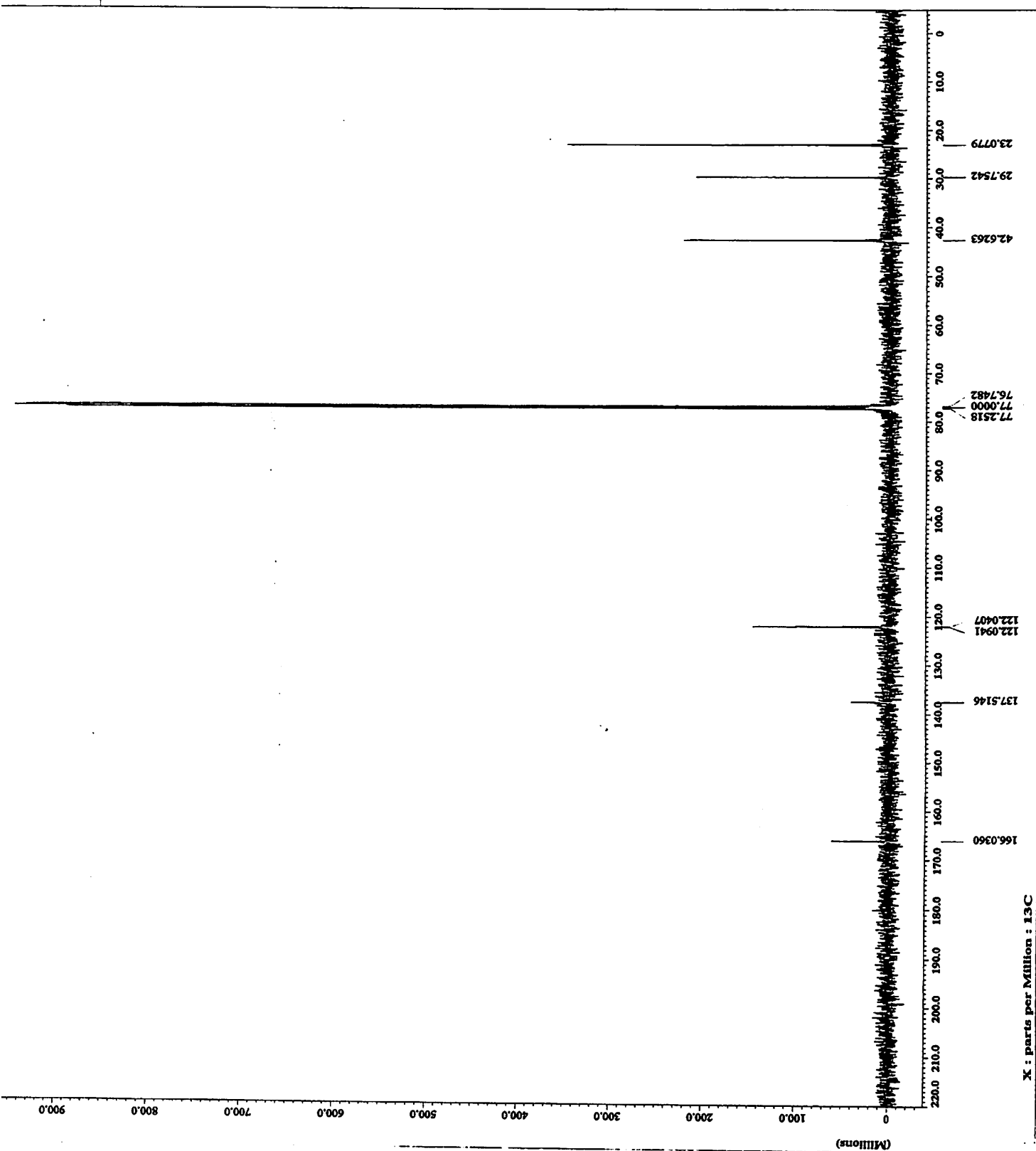
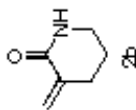
X : parts per Million : 1H

JEOL

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---- ACQUISITION PARAMETERS ----
File Name      - 14.13c_spectrum.331
Author         - JEOL LTD.
Sample ID      - 8885126
Content        - Single Pulse with Broad
Creation Date   - 24-JUN-2002 16:55:06
Revision Date  - 25-JUN-2002 00:19:03
Spec Site      - ECP500

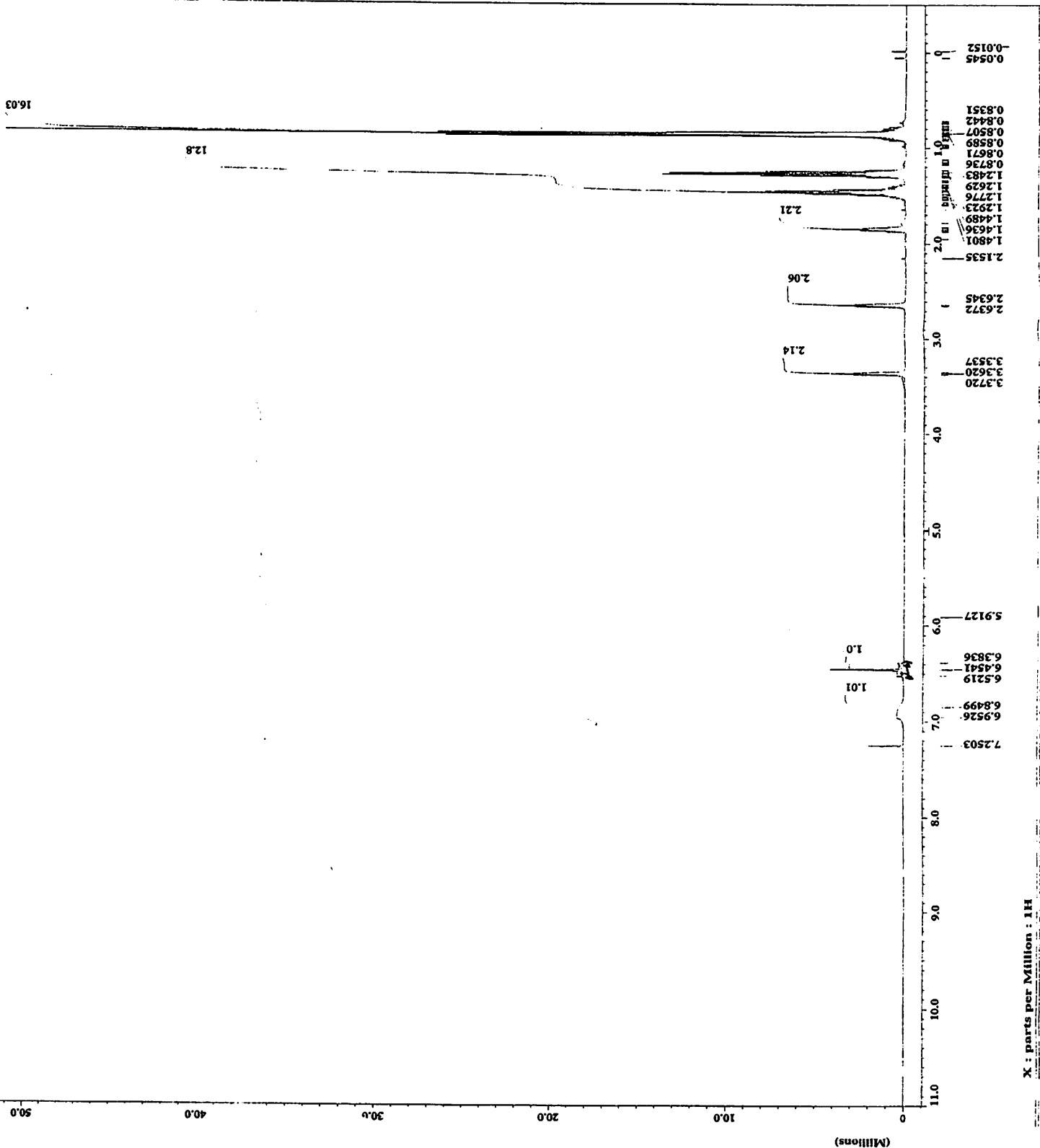
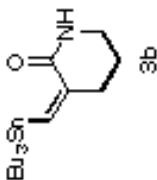
Spec Type      - HETCOR_2D
Pulse Program   - zgpg30
Dimensions     - 13C
Din Title       - 13C
Din Size        - 32768
Din Units       - fpgal
Sfsize          - 400
Mod Return      - 13C
X_domain        - 100 [ppm]
X_offset        - 125.77707547 [kHz]
X_freq          - 125.77707547 [kHz]
X_waltz         - 11.4654088 [kHz]
Spin           - 13C
Spin Set        - 15 [Hz]
Temp Set        - 26.1 [deg]
Recvr Gain      - 29
Field Strength  - 11.7473579 [T]
Filter Set      - HETCOR
Filter Mod      - 15.77066221 [kHz]
    
```



X : parts per Million : ^{13}C

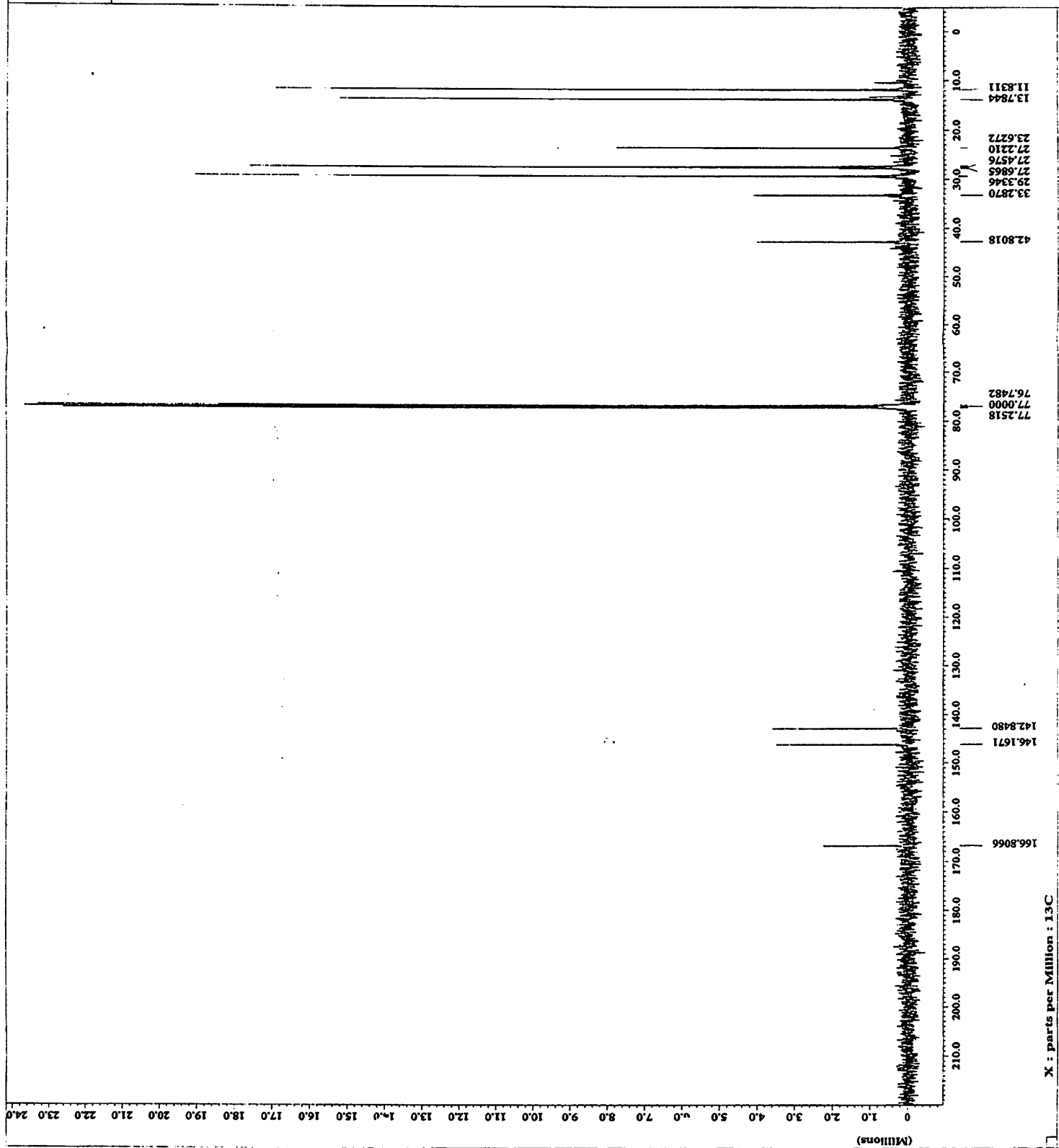
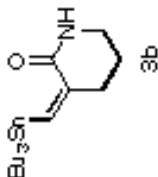
JEOL

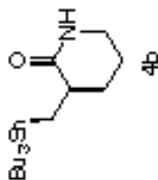
----- ACQUISITION PARAMETERS -----
File Name : 12_Spectrum.104
Sample ID : 01-MI-001-fr.4-12
Content : Single Pulse Experiment
Creation Date : 17-APR-2001 16:32:00
Revision Date : 16-APR-2001 08:33:32
Spec Site : ECP300
Spec Type : DELTA_JMR
Data Format : ID COMPLEX
Pulse Program : 1H
D1a Size : 16384
D1a Units : [ppm]
Scans : 8
Acq_return : 1H
X_offset : 51ppm
X_freq : 500.16241602 [MHz]
X_sweep : 7.50750751 [MHz]
Solvent : CDCl3
P1a : 12.00 [sec]
Temp_pt : 25.4 [deg]
Recvr_gain : 15
Field_strength : 11.7473579 [T]
Filter_mode : BORESCORR
Filter_width : 3.7319936 [MHz]



JEOL

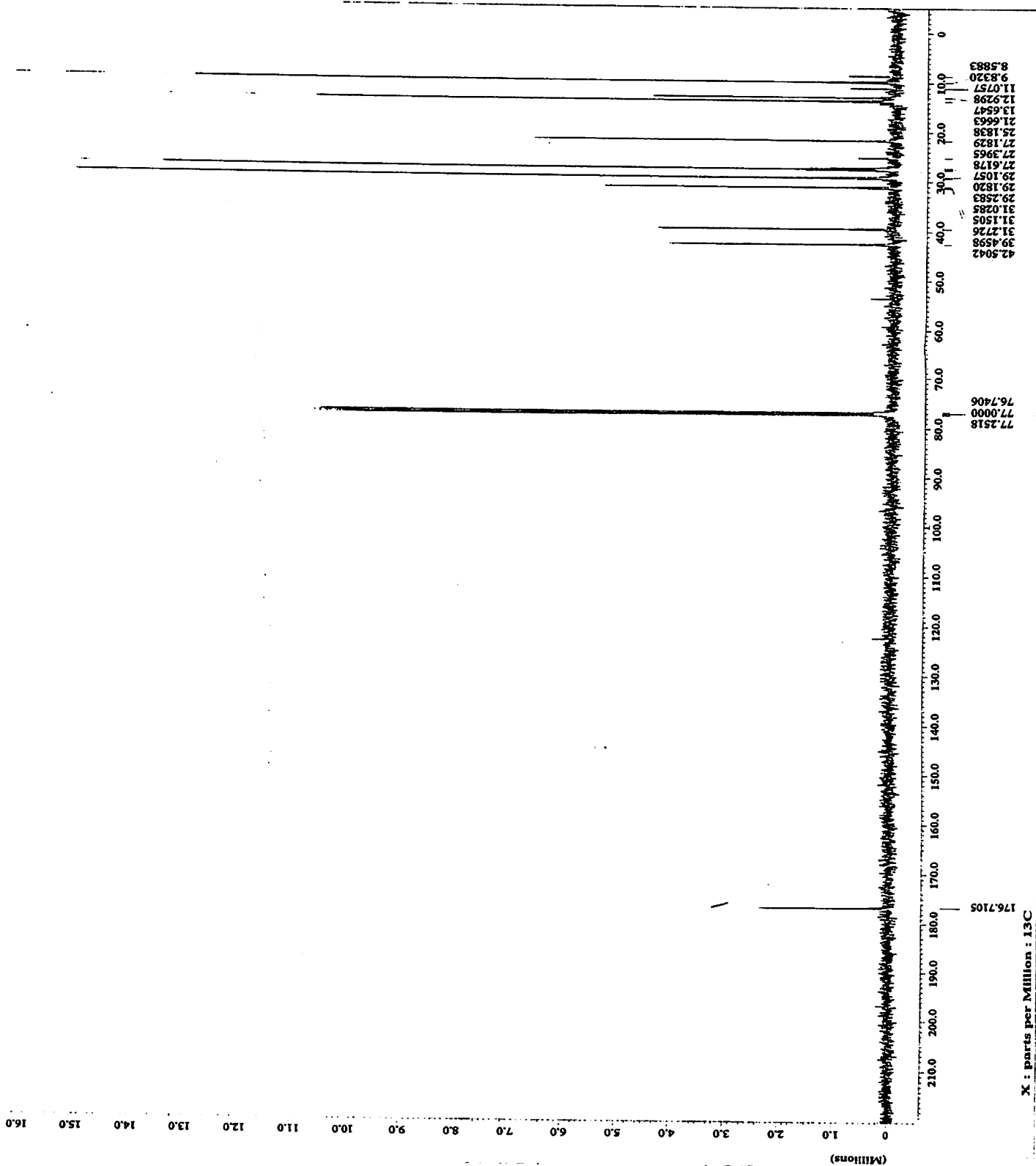
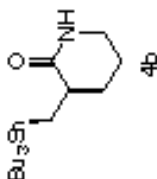
----- ACQUISITION PARAMETERS -----
File Name - 1d_13c_spectrum.52
Author - JTOOL LTD.
Sample ID - 01-mt-001-fr.4-12
Chemical Name - 3b
Creation Date - 17-APR-2001 19:06:00
Revision Date - 18-APR-2001 08:49:59
Spec File - ECP500
Spec Type - DELTA_ROR
Data Format - 1D COMPLEX
Dimensions - X
Dim Title - 13C
Dim Name - 13C
Dim Units - [ppm]
Scans - 400
Mod_return - 1
X_domain - 13C [ppm]
X_offset - 150.1327
X_freq - 125.767547 [MHz]
X_sweep - 31.44554088 [MHz]
Solvent - CHLOROFORM-D
Spin_get - 15 [Hz]
Acq_get - 15.5 [Hz]
Relax_time - 11.747379 [s]
Field_strength - 11.747379 [T]
Filter_mode - BUTTERWORTH
Filter_width - 15.72066231 [Hz]





X : parts per Million : 1H

----- ACQUISITION PARAMETERS -----
File Name - 1d_13c_spectrum.69
Author - JEOL LTD.
Sample ID - 01-MI-006-fr-10-18
Chemical Name - 4b
Creation Date - 23-MAY-2011 13:40:45
Revision Date - 24-MAY-2011 03:05:35
Spec Site - ECP900
Spec Type - DEPTA_900
Data Format - 1D COMPLEX
Dimensions - X
Dim title - 13C
Dim 1 Size - 128K
Dim Units - (ppm)
Scans - 400
Mod_return - 1
X_domain - 13C (ppm)
X_offset - 15 (ppm)
X_freq - 125.76797547 (MHz)
X_sweep - 31.44554088 (kHz)
Solvent - CHLOROFORM-D
Spin_gate - 15 (Hz)
Recp_gate - 15.9 (Hz)
Recp_gain - 11.7473575 (V)
Field_strength - 125.76797547 (MHz)
Filter_mode - BUTTERWORTH
Filter_width - 15.72066231 (kHz)



X : parts per Million : 13C

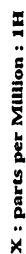
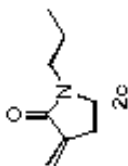
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===== ACQUISITION PARAMETERS =====
File Name      = 1d_spectrum_0003
Author         = JROD LZO.
Sample ID      = RZC-019 fr exoacethyle
Instrument      = RZC-019 Spectrometer
Creation Date   = 20-Mar-2003 21:01:29

Revision Date   = 29-May-2003 10:53:31
Spec Site       = ECF500

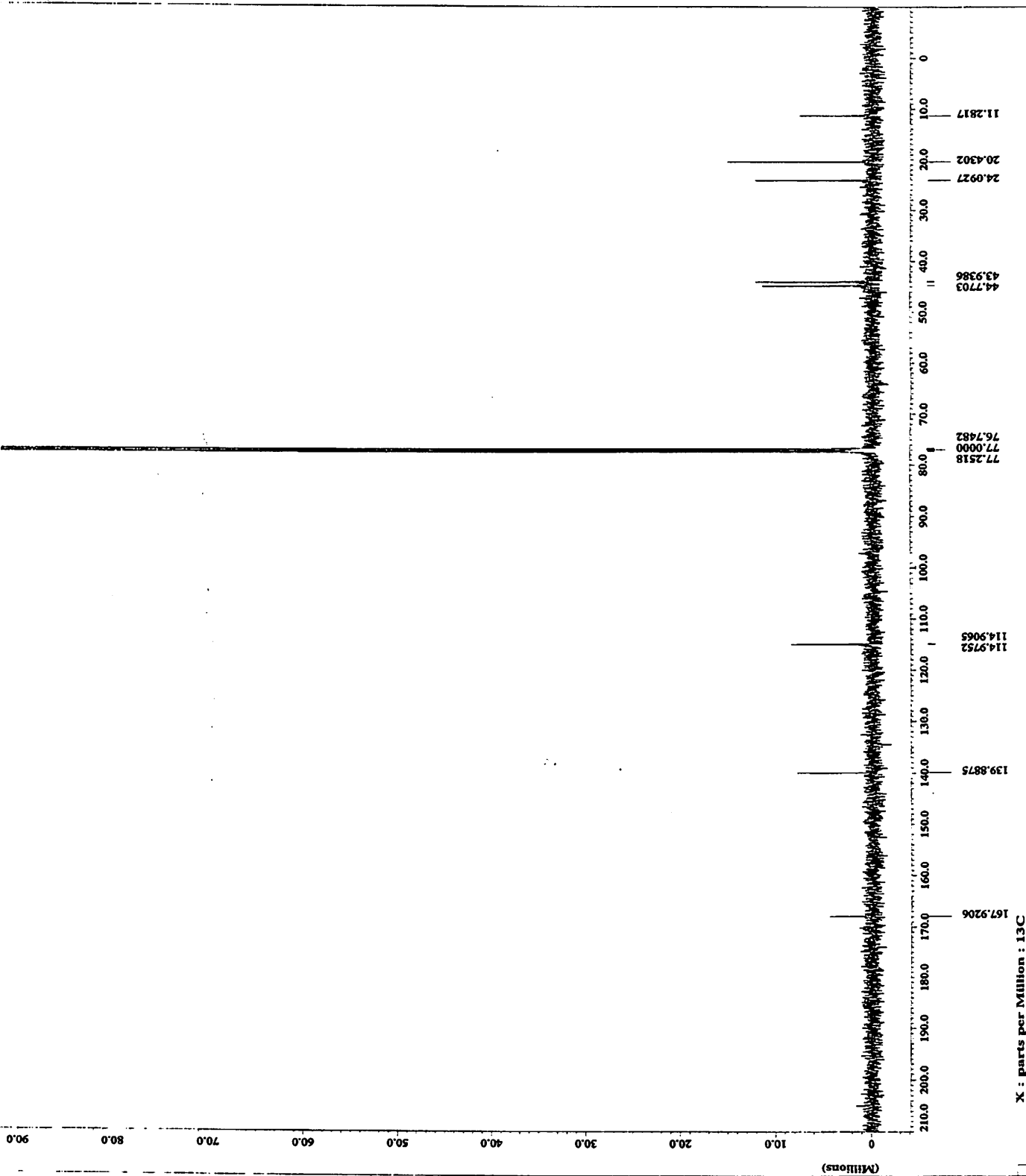
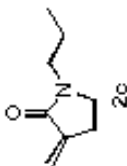
Spec Type       = DZFA_ZDF
Data Format      = 1D COMPLEX
Dimensions      = 1H
DIN title       = 1H
DIN file        = 13984
DIN title       = 13984
DIN file        = 13984
SName           = 1H
Mod_return      = 1
X_domain        = 1H
X_offset        = 5(ppm)
X_resolution     = 4.41603(Hz)
X_sweep         = 7.8575731(Hz)
X_resolution     = 0.00000000(Hz)
BQ_weight       = 14(Hz)
Poin_get        = 24
Poin_get        = 24
Poin_get        = 24
Field_strength  = 11.7473579(T)
Pulse_program    = EPRHNMW03H
Filter_width     = 3.75119936(Hz)

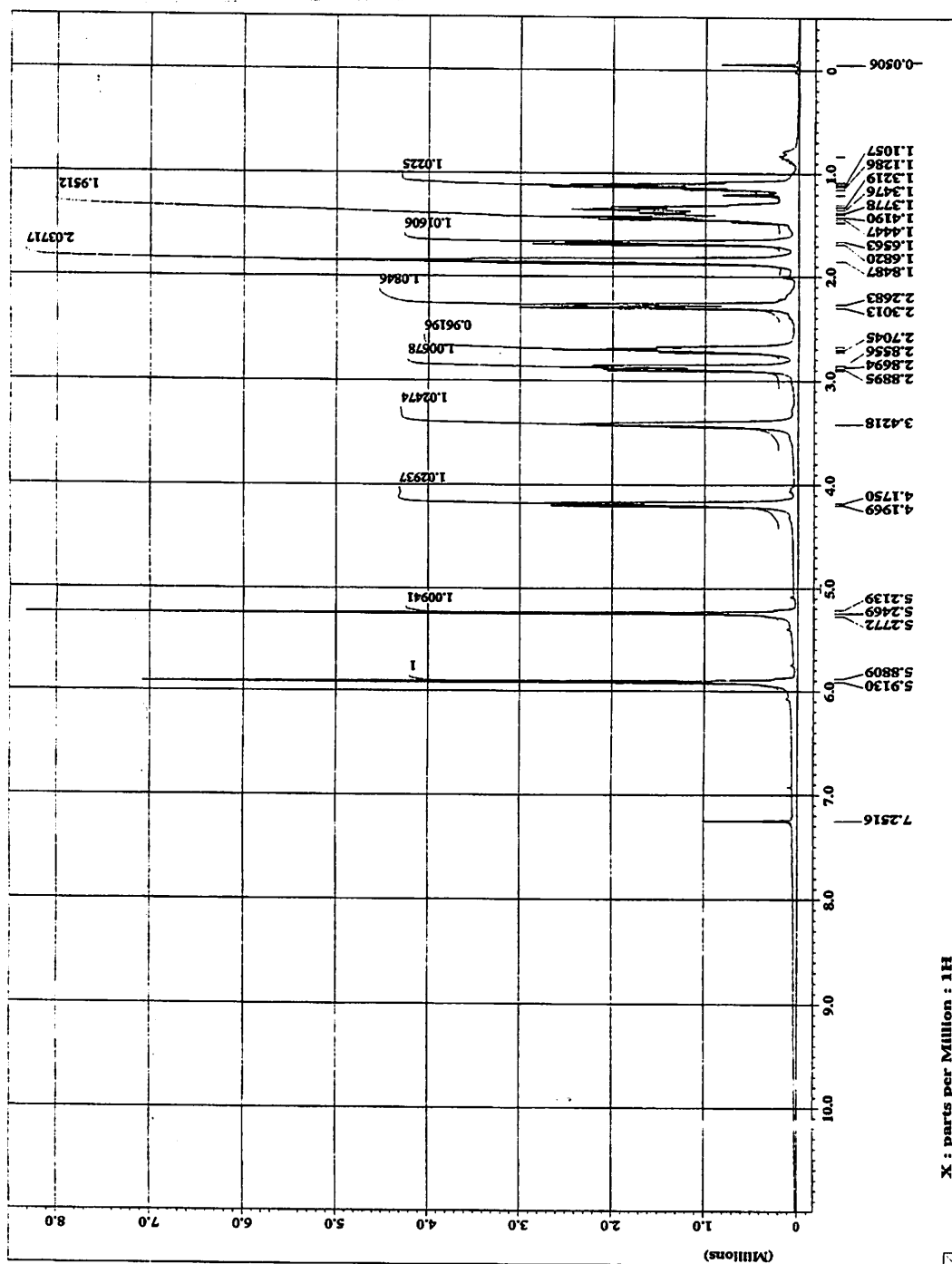
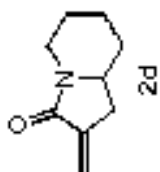
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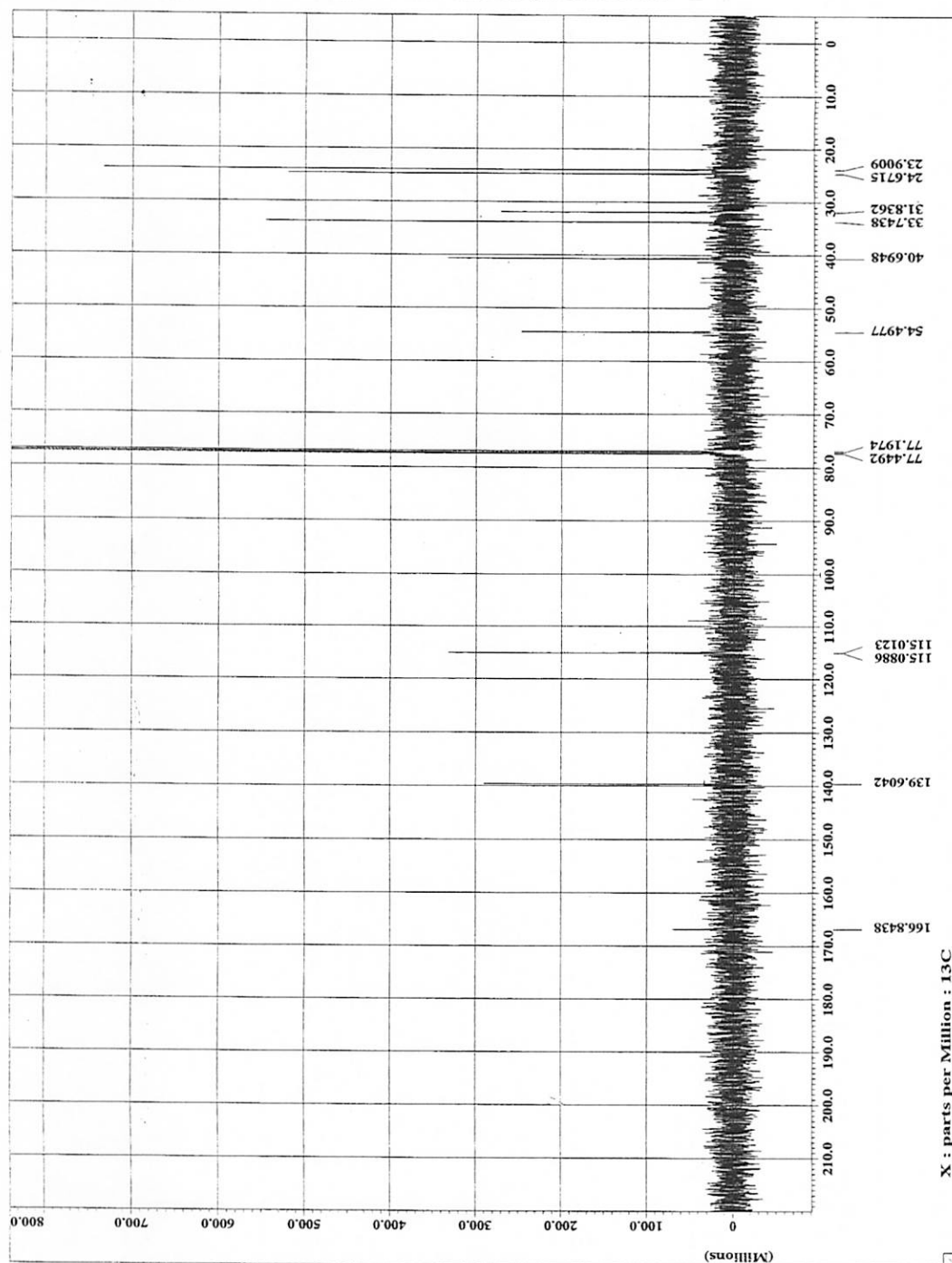
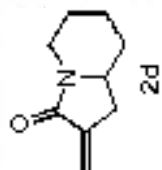


JEOL

----- ACQUISITION PARAMETERS -----
File Name - id_13c_spectrum.1630
Author - JEOL LTD.
Date - 28-MAY-2003 10:54:07
Content - Single Pulse with Broad
Creation Date - 28-MAY-2003 21:37:42
Revision Date - 28-MAY-2003 10:54:07
Spec Site - ECP500
Spec Type - DELTA_XXX
Data Format - ID COMPLEX
Dimensions - X
Dim Size - 32768
Dim Date - [ppm]
Scans - 485
Mod_return - 1
Mod_name - 13C
X_offset - 120.000
X_freq - 125.7777547 (MHz)
X_sweep - 31.44654088 (kHz)
Solvent - CHLOROFORM-D
Spin_get - 4 (Hz)
Spin_set - 21 (Hz)
Recvr_gain - 21
Field_strength - 11.7473579 (T)
Filter_mode - HETZCORH
Filter_width - 15.7266251 (kHz)



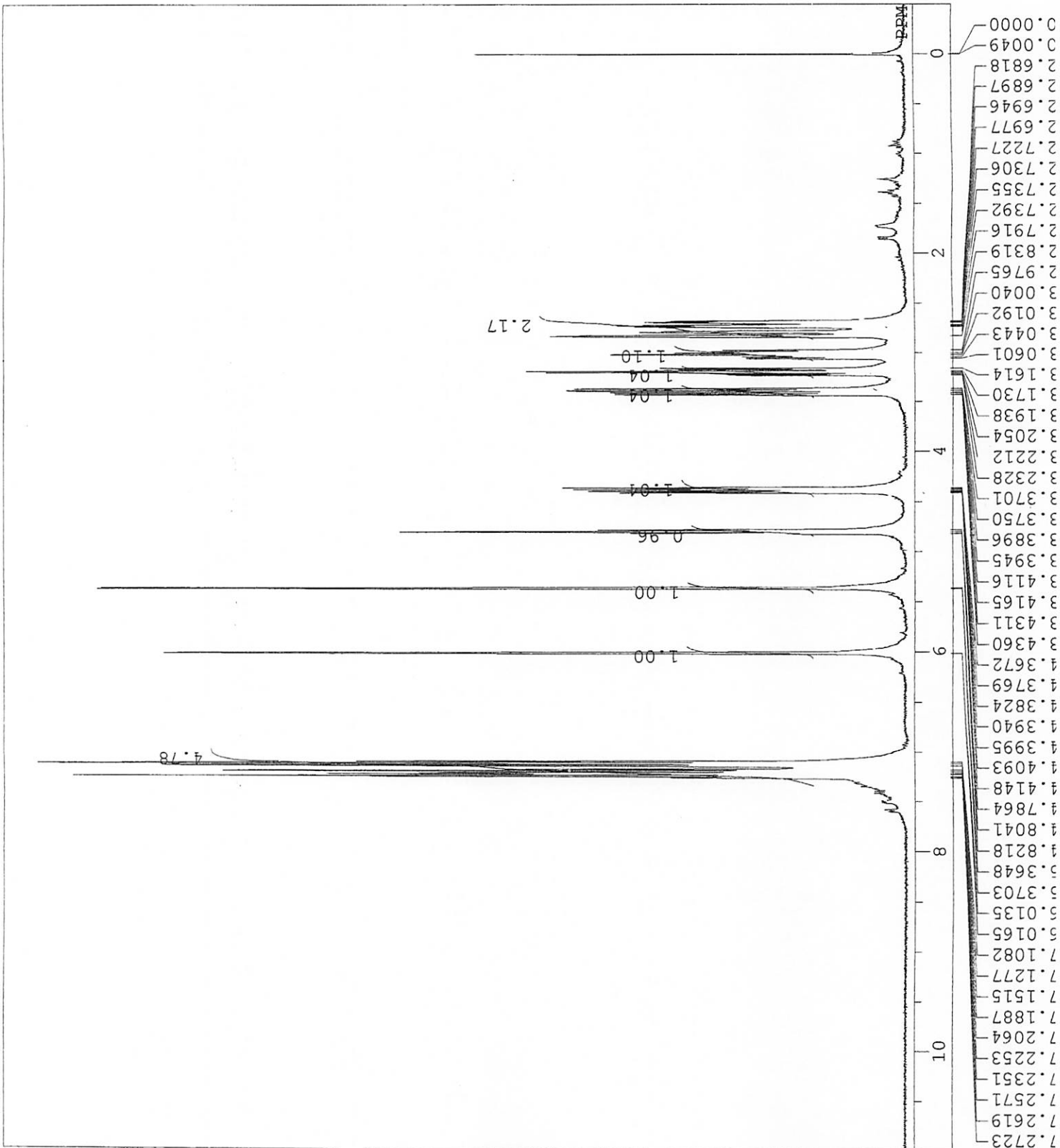
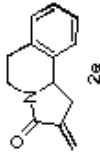




DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
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SCANS
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RGAIN

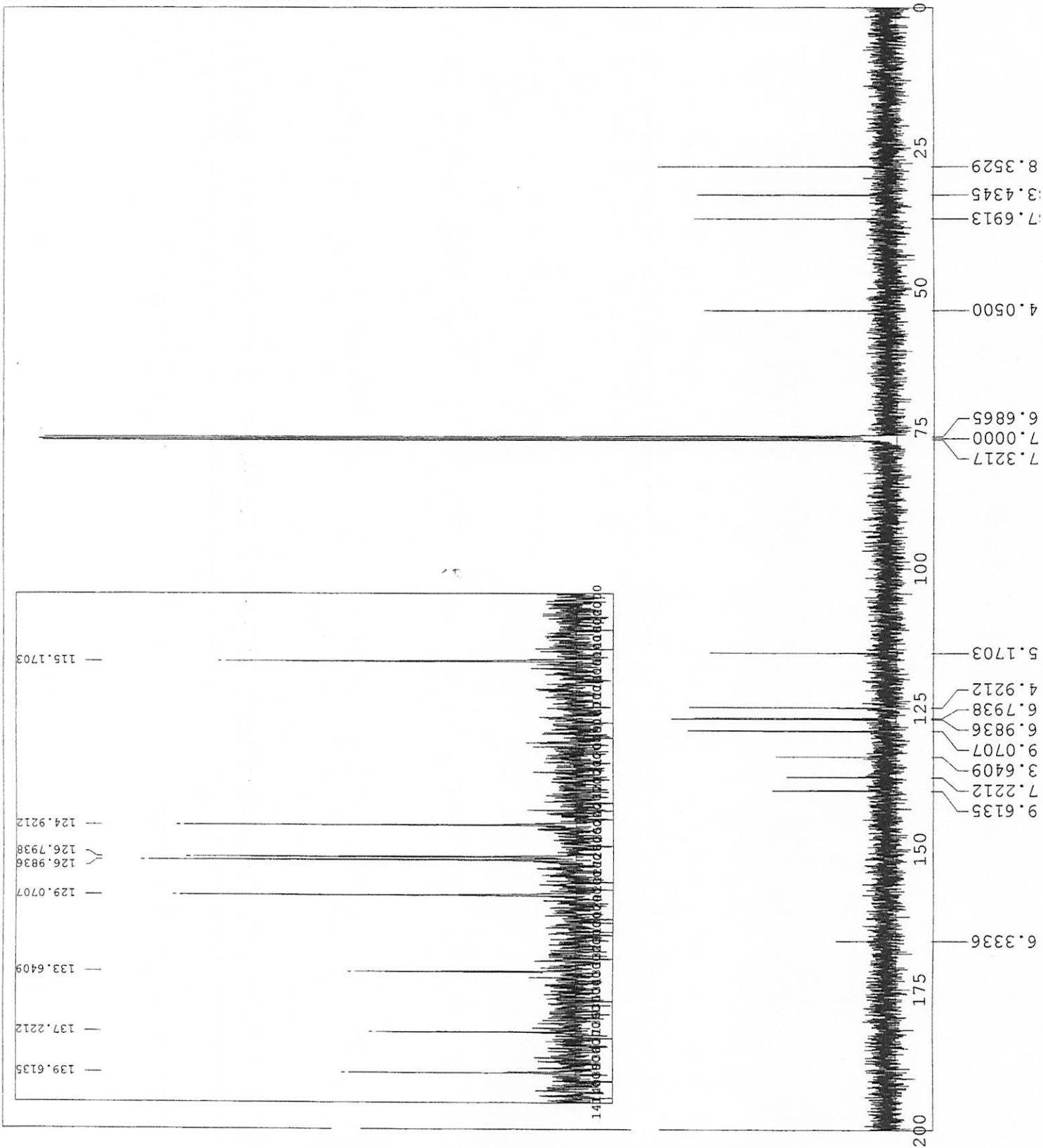
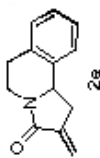
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Sat Mar 20 17:22:14 200
1H
NON

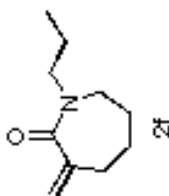
399.65 MHz
124.00 KHz
10500.0 Hz
32768
7993.6 Hz
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4.099 sec
2.901 sec
5.8 us
1H
22.8 c
CDCl3
0.00 ppm
0.12 Hz
13



DFILE C:\WINNMR98\COMMON_DEF
COMNT 04-D1-115-HPLC
DATIM Sat Mar 20 17:46:25 200
OBNUC 13C
EXMOD BCM
OBFRO 100.40 MHz
OBSET 125.00 KHz
OBFIN 10500.0 Hz
POINT 32768
FREQU 27173.9 Hz
SCANS 400
ACQTM 1.206 sec
PD 1.794 sec
PW1 5.5 us
IRNUC 1H
CTEMP 23.9 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

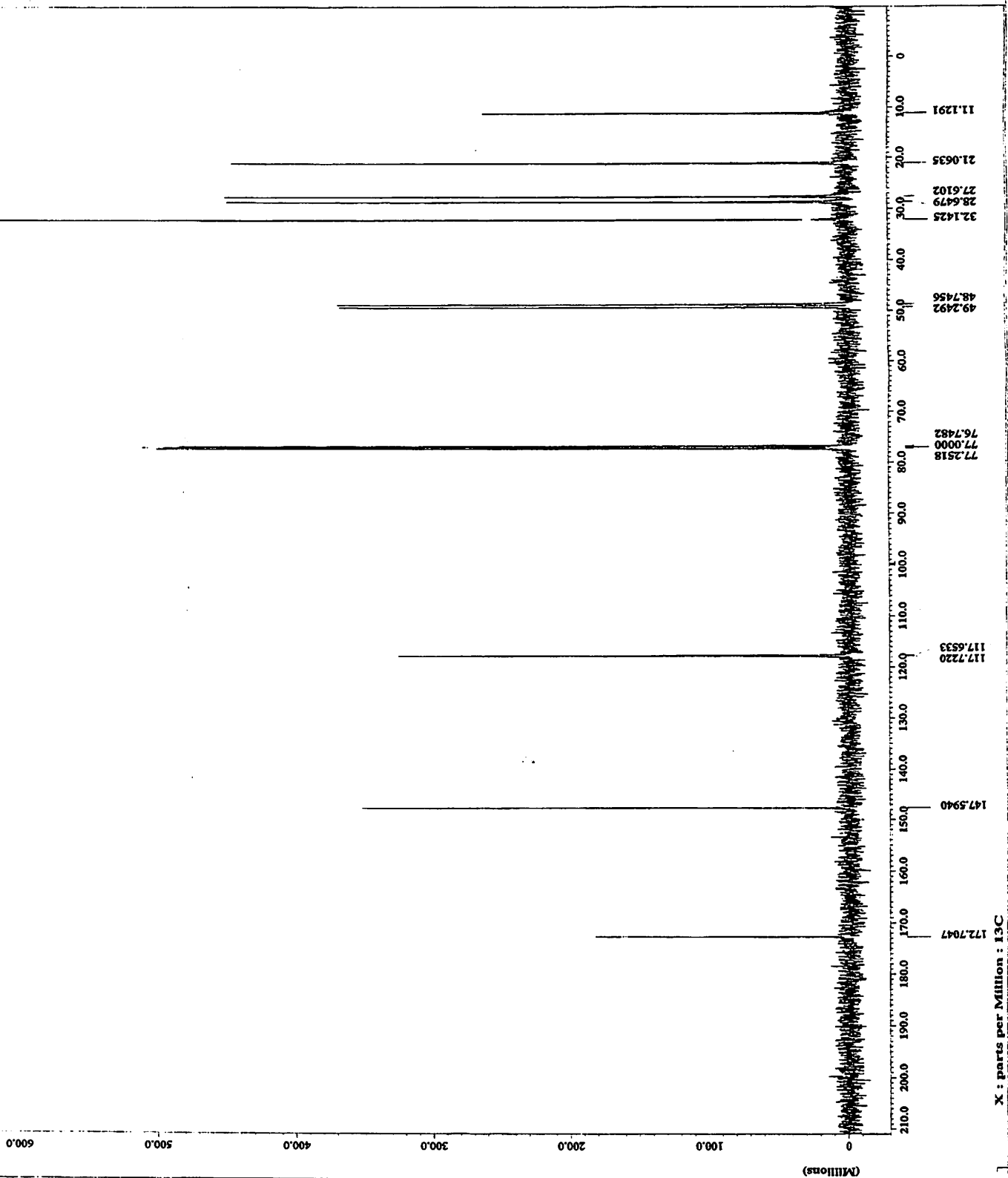
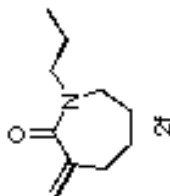
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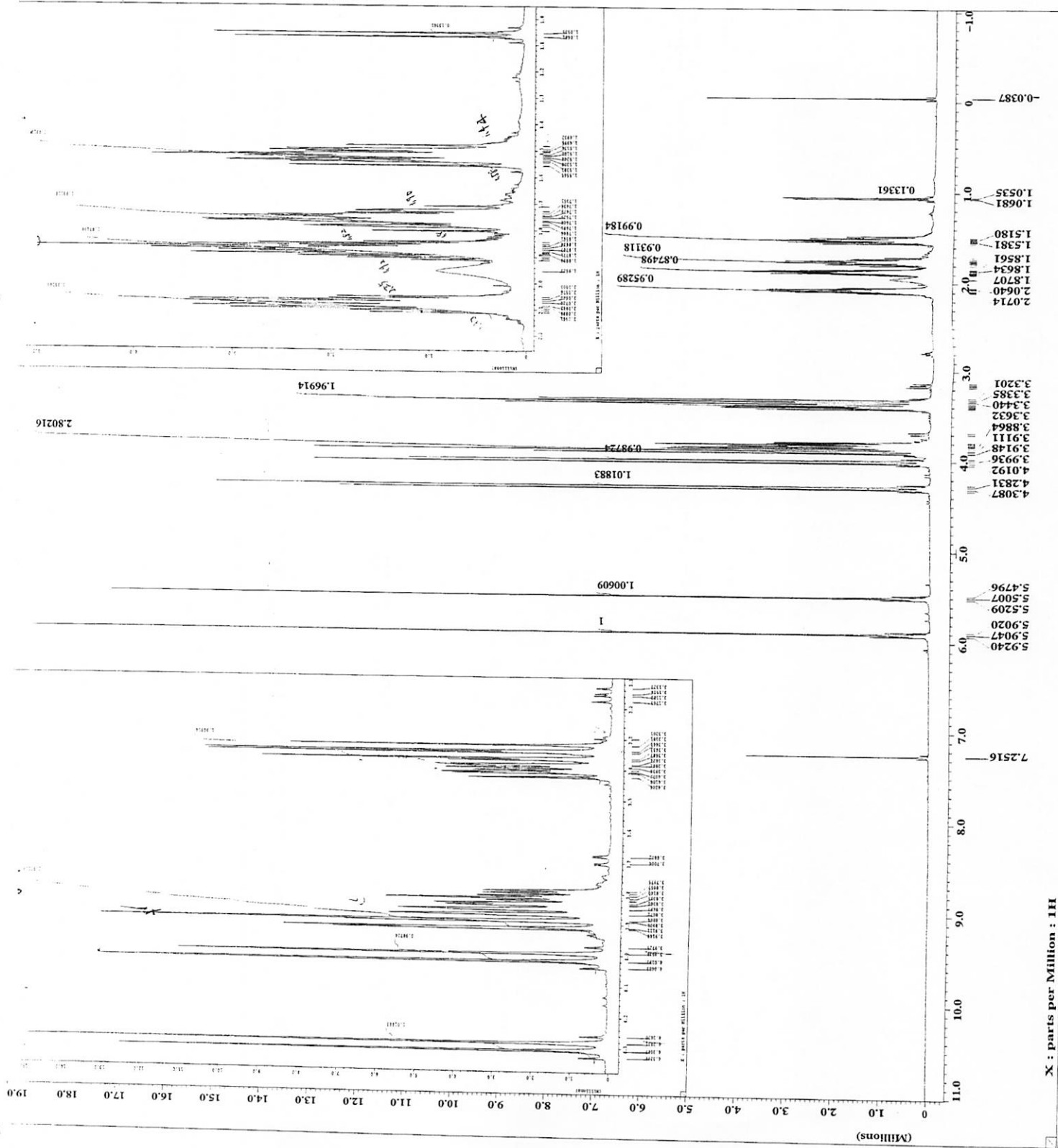
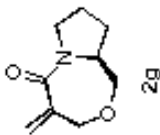
JEOL

--- ACQUISITION PARAMETERS ---
File Name - 1d_13c_spectrum.1905
Author ID - JEOL LTD.
Sample ID - 1172
Content - Single Pulse with Broad
Creation Date - 1-JUL-2003 19:09:44
Revision Date - 2-JUL-2003 09:03:21
Spec Site - RCP300
Spec Type - DELTA_JMR
Data Format - 1D COMPLEX
Dimensions - X
Dim Size - 32768
Dim Units - [ppm]
Scans - 195
Mod_return - 1
X_gain - 100 (ppm)
X_offset - 135.77787547 (MHz)
X_freq - 31.44654088 (MHz)
Solvent - CDCl3
Spin_get - 31 (Hz)
Spin_loss - 25 (Hz)
Recvr_gain - 30
Field_strength - 11.7473379 (T)
Filter_mode - HURTSWORTH
Filter_width - 13.7206622 (Hz)

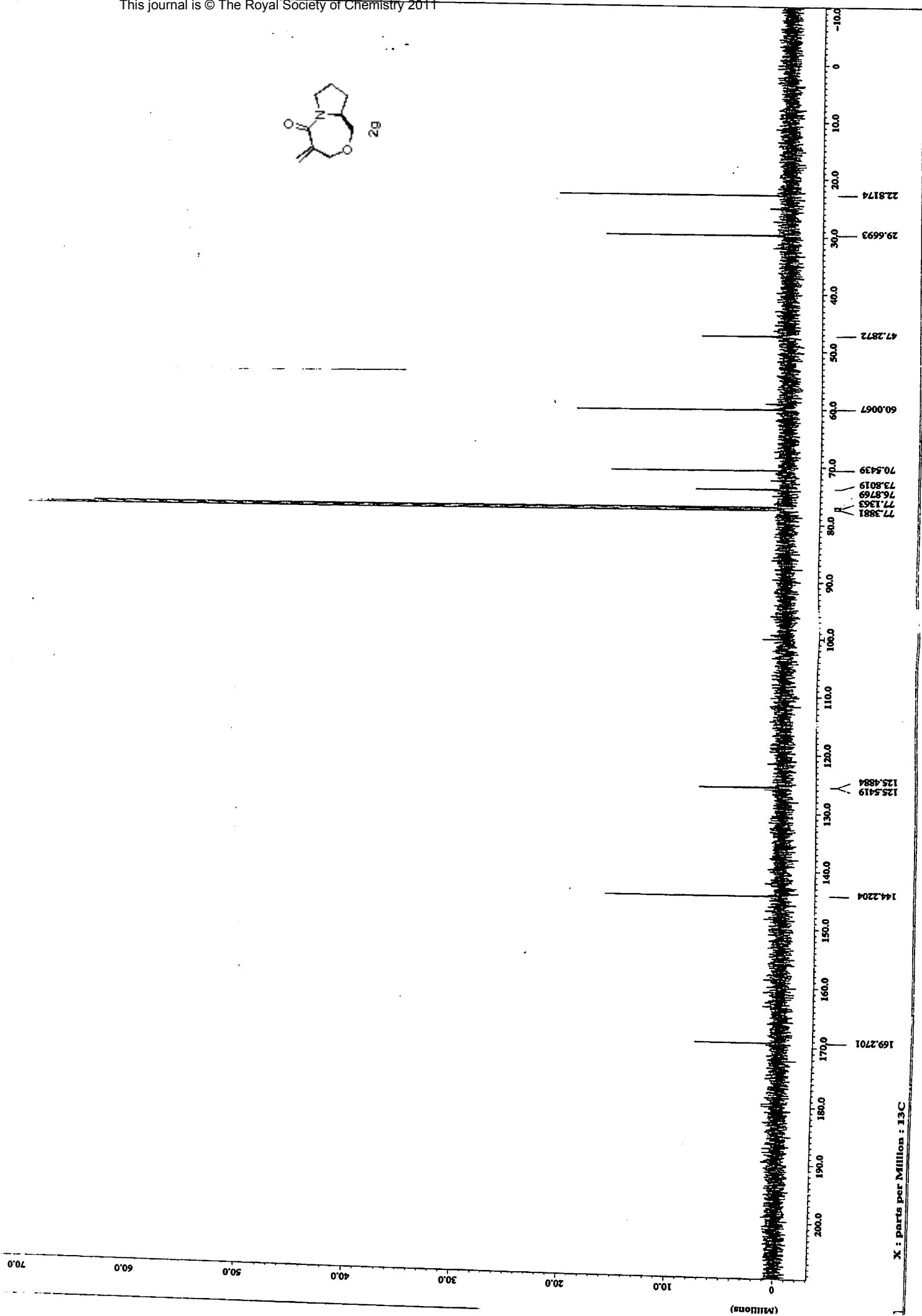
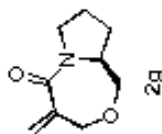


JEOL

ACQUISITION PARAMETERS ---
File Name = 10_spectrum.654
Author = bicyclo
Sample ID = Single Pulse Experiment
Content = 10-MAR-2004 22:29:12
Creation Date = 11-MAR-2004 15:56:18
Revision Date = ECP500
Spec Site =
Spec Type = DELTA_RNR
Data Format = 1D COMPLEX
Data Size = 16384
Data Units = g
Acq. Return = 1H
X.Offset = 5(ppm)
X.Freq = 500.16241602(MHz)
X.Sweep = 7.50750751(kHz)
Spectrum = 100%FORM-D
Spin. rot = 23.1(dc)
Temp. rot = 19
Recvr. Gain = 11.747359(r)
Field_strength = BUTTERWORTH
Filter_Mode = 3.75119936(MHz)
Filter_Width =

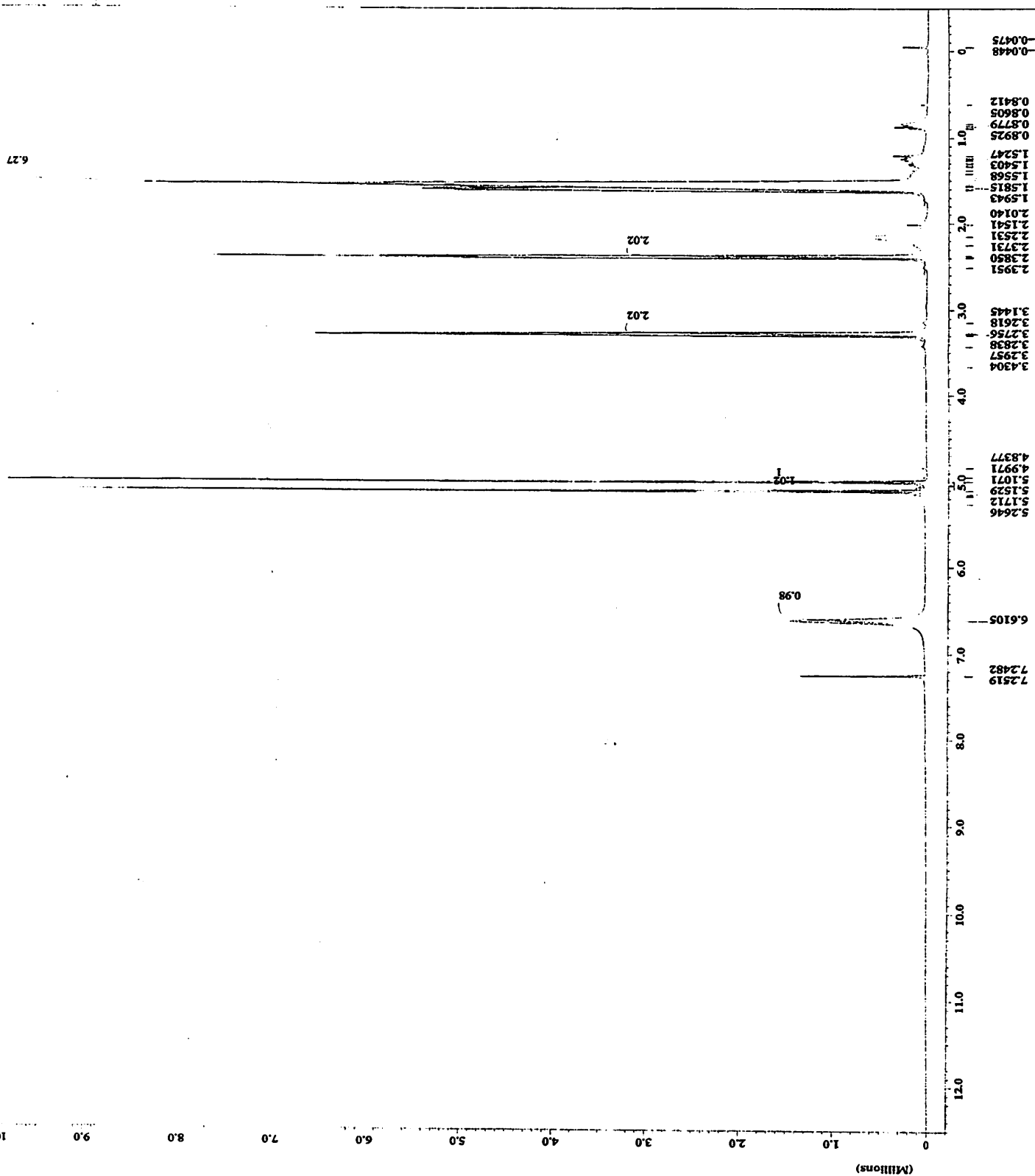
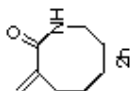


X : parts per Million : 1H



JEOL

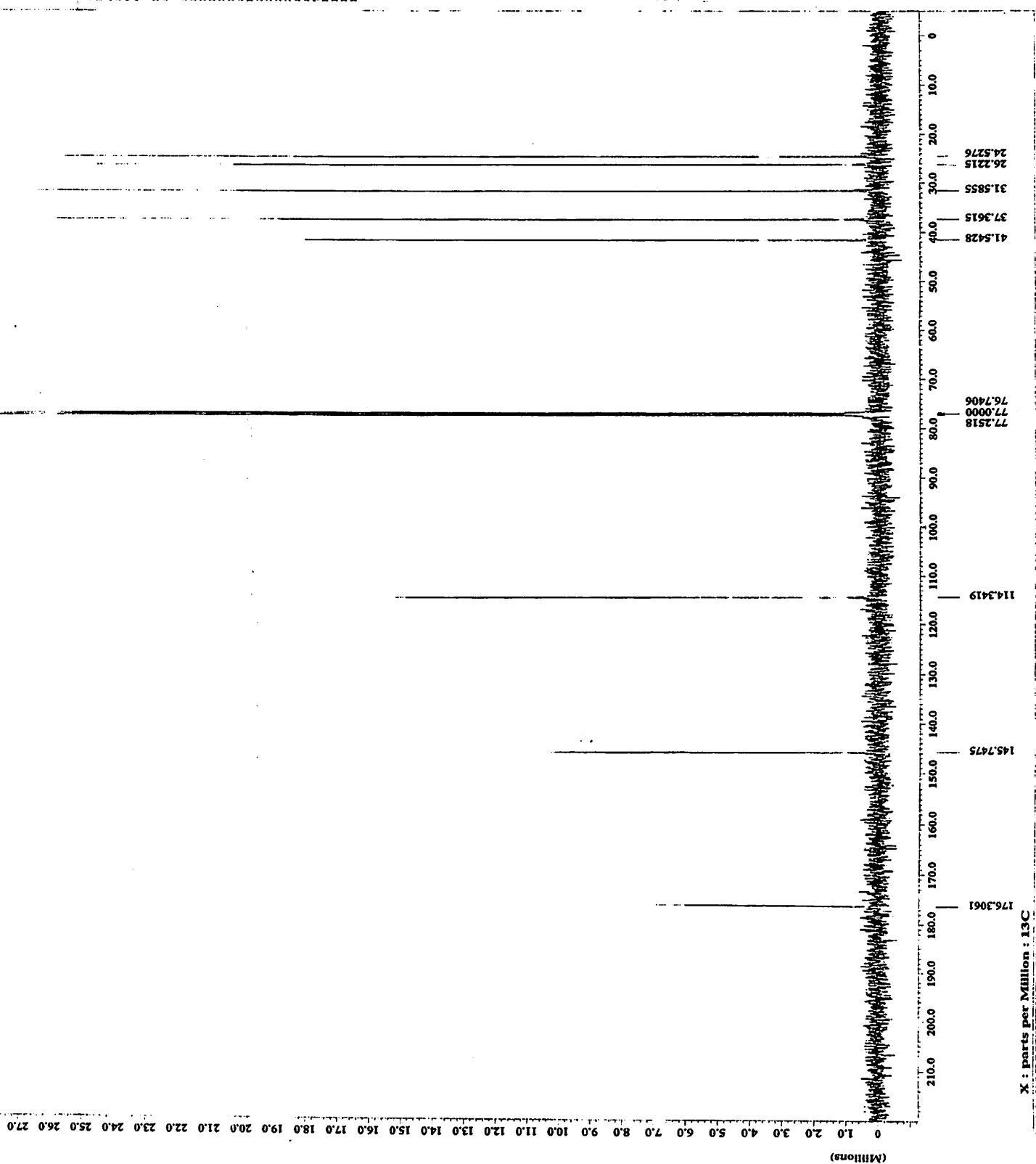
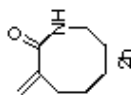
ACQUISITION PARAMETERS
File Name - 1A-017-12-102
Author - JEOL LTD.
Sample ID - 01-017-12-102
Content - Single Pulse Experiment
Creation Date - 25-JUN-2001 12:51:21
Revision Date - 25-JUN-2001 13:15:41
Spec Site - ECP500
Spec Type - 1D Comp
Pulse Program - zgpg30
Dilution - 1
Dilution Volume - 16384
Dilution Site - [ppm]
Dilution Units - [ppm]
Mod Name - 1
X Domain - 1
X Offset - 500.1621602 (MHz)
X Freq - 500.1621602 (MHz)
X Sweep - 1
X Gain - 1
X Gain Set - 15 (dB)
Temp Set - 24 (°C)
Recor Gain - 15
Pulse Length - 11.7473579 (µs)
Pulse Power - 11.7473579 (W)
Pulse Width - 3.75119534 (µs)
Filter Width - 3.75119534 (µs)



X : parts per Million : 1H

JEOL

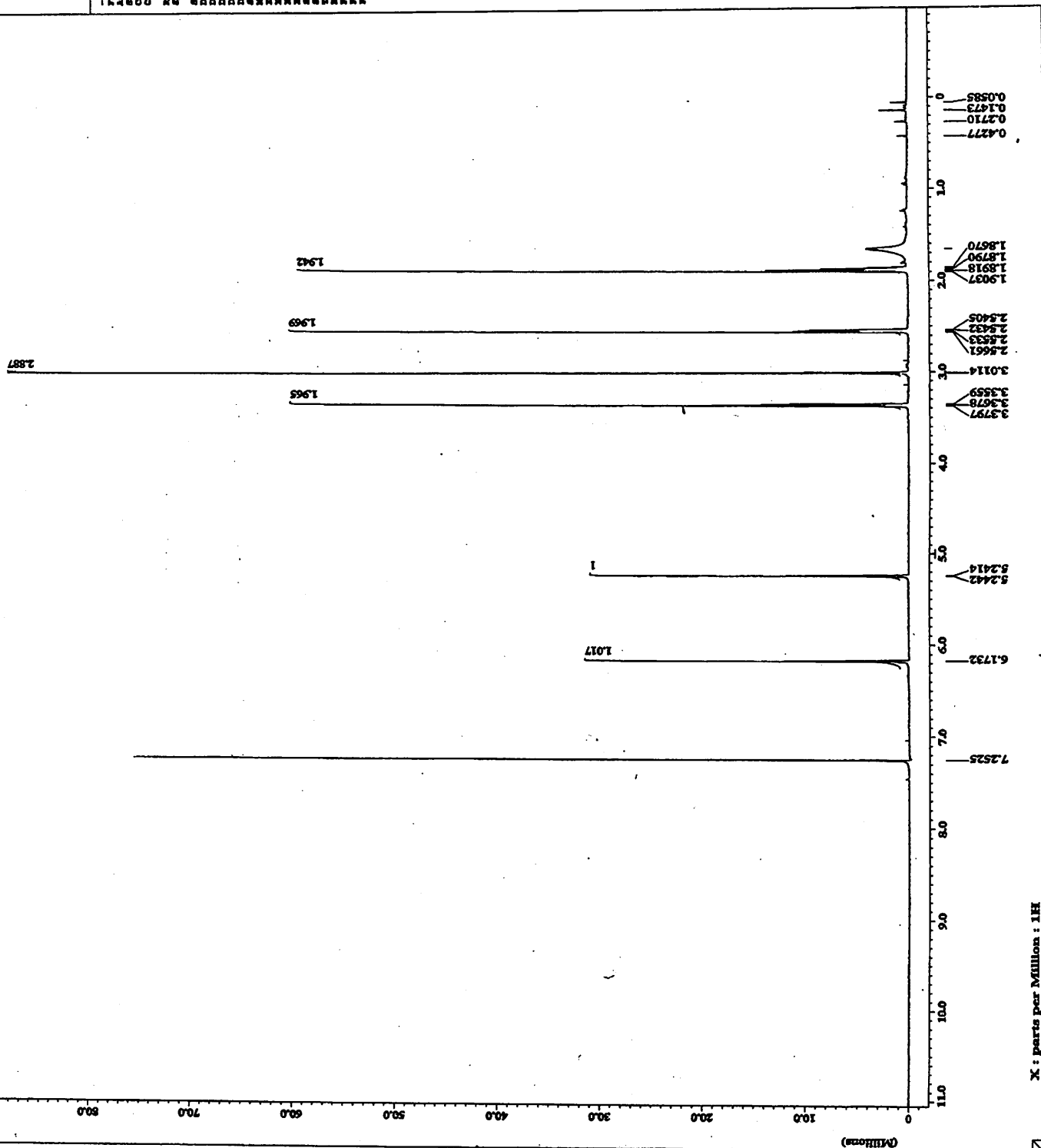
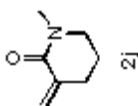
----- ACQUISITION PARAMETERS -----
File Name - 1d_13c_spectrum.123
Author - JROLD LTD.
Sample ID - 01-41-017-cr-37-39
Chemical - 2,2,6,6-tetramethylpiperidine-1-oxyl
Creation Date - 25-JUN-2001 13:06:21
Revision Date - 25-JUN-2001 14:04:54
Spec Site - ECP500
Spec Type - DELTA_800
Data Format - 1D COMPLEX
Dimensions - 1
Dim Title - 13C
Dim Size - 22766
Spectrum - 1
Scan - 400
Mod_return - 1
X_gain - 13C
X_offset - 100 [ppm]
X_freq - 125.7619547 [MHz]
X_solvent - 11.44654088 [MHz]
Solvent - CHLOROFORM-D
Spin_set - 15 [Hz]
Temp_set - 24.8 [C]
Pulse_prog - zgpg30
Pulse_length - 11.7473579 [s]
Filter_mode - HETSPH001
Filter_width - 15.72066231 [Hz]



X : parts per Million : 13C

JEOL

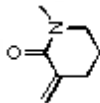
ACQUISITION PARAMETERS
File Name : 1d_spectrum.03
Author :
Date : 2008-04-10
Content : Single Pulse Experiment
Creation Date : 20-04-2008 10:56:40
Revision Date : 20-04-2008 04:43:37
Acq. File : 200804
Acq. Type : 1D
Pulse Program : zgpg30
F2 (MHz) : 500.1361621(MHz)
F1 (MHz) : 7.507507811(MHz)
Solvent : CDCl3
Temp (°C) : 30.0
Acq. Time : 11.747399171
F2 (ppm) : 159.427
F1 (ppm) : 77.000
Filter : zgpg30



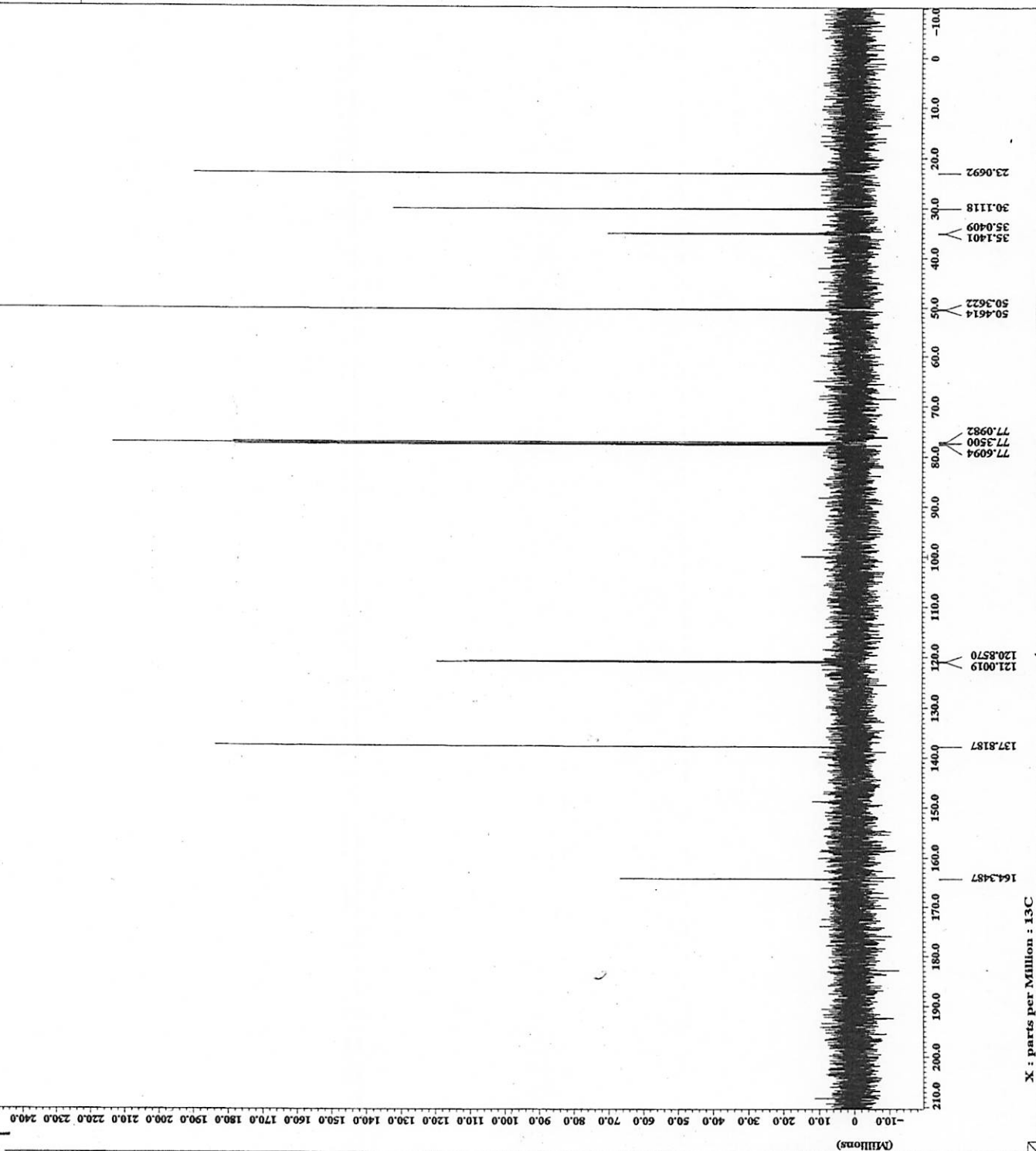
X : parts per Million : 1H

JEOL

----- ACQUISITION PARAMETERS -----
File Name - 1d_13c_spectrum.s61
Sample ID - S881148
Content - Single Pulse with Broad
Creation Date - 7-AUG-2006 13:12:43
Revision Date - 8-AUG-2006 23:41:59
Spec Site - ECP800
Spec Type - DELTA 400
Data Format - ID COMPLEX
Dimensions - 1
Dim 1 Size - 32768
Dim 1 Units - [ppm]
Sca1a - 59
X_offset - 13C
X_offset2 - 100 [ppm]
X_freq - 125.77787547 [MHz]
X_sweep - 31.4656088 [kHz]
SOLVENT - CDCl3
Spin set - 14 [Hz]
Temp_set - 24.3 [deg]
Nuc1r_gain - 30
Pulse length - 12.493159 [us]
Filter mode - HETCOR2D
Filter width - 15.72066221 [kHz]



2]



DFILE
CONNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

C:\NMR\8\COMMON\DEFAULT.AL

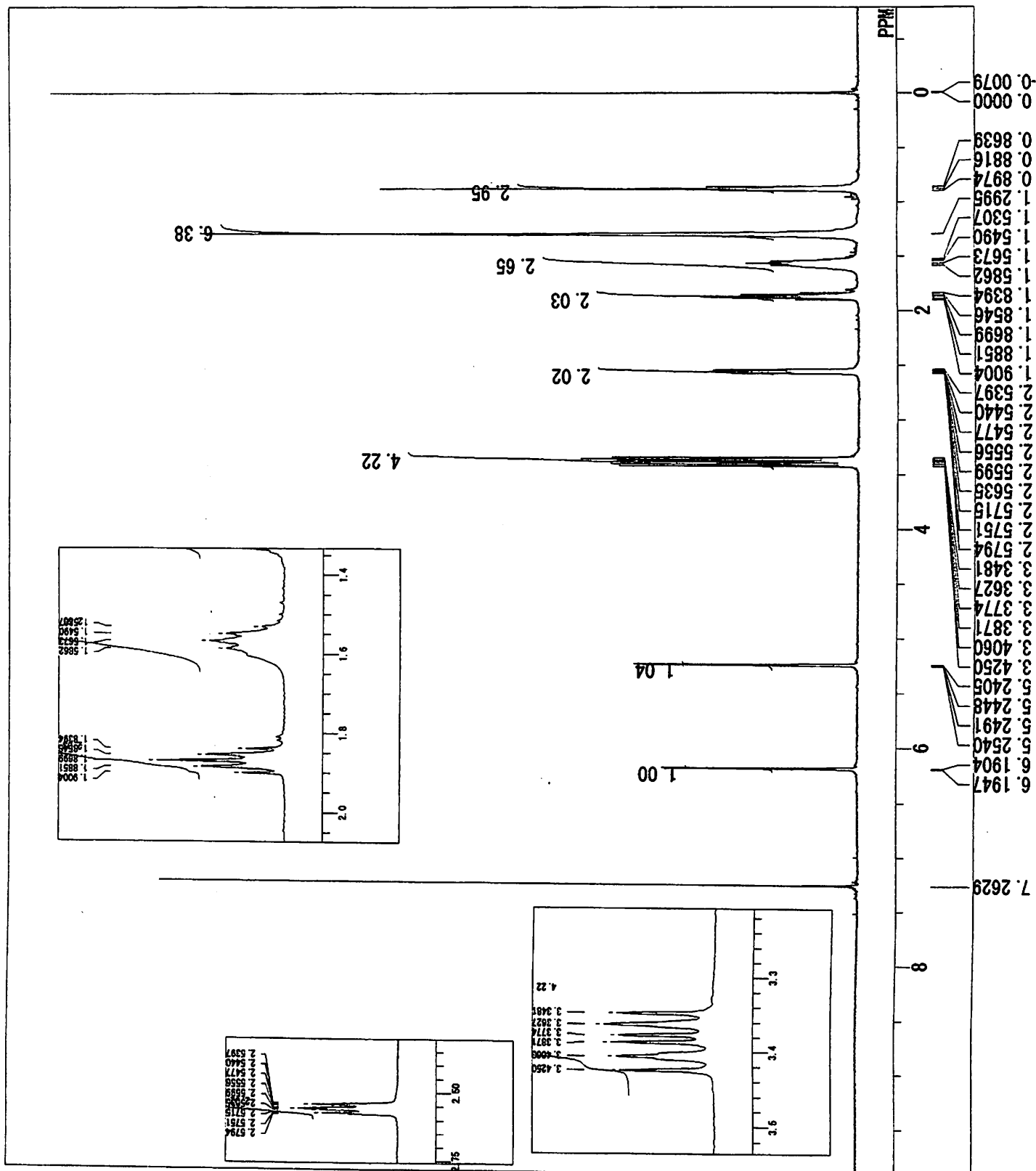
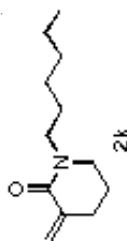
Tue Mar 20 17:32:01 2007

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399.65 MHz
124.00 KHz
10500.00 Hz
32768
7992.01 Hz
8
4.1001 sec
2.9010 sec
5.80 usec
22.4 C
0.00 ppm
0.12 Hz
17

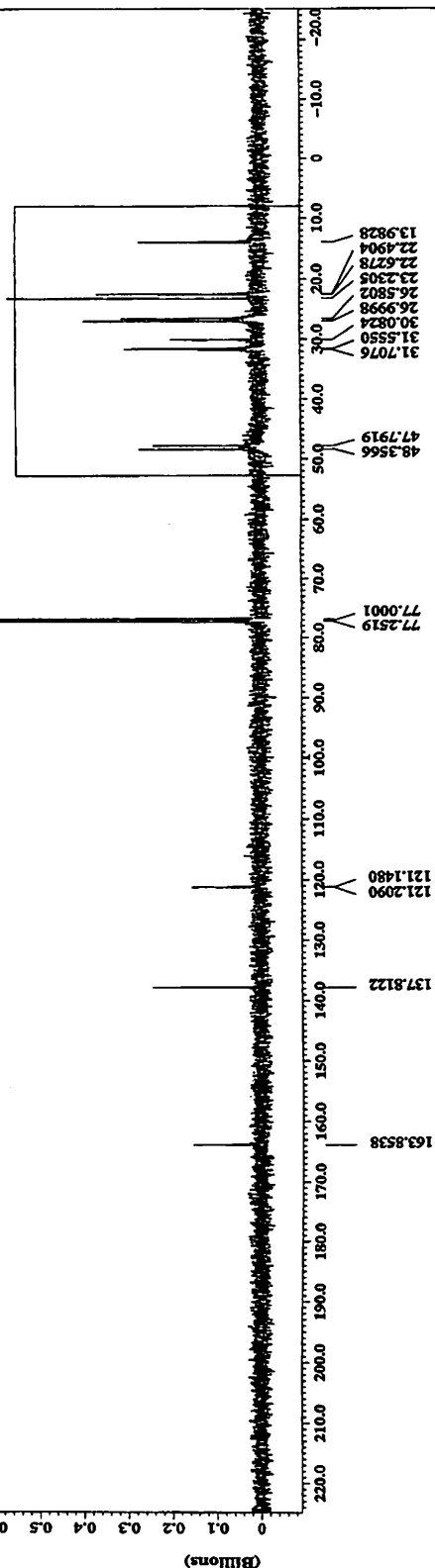
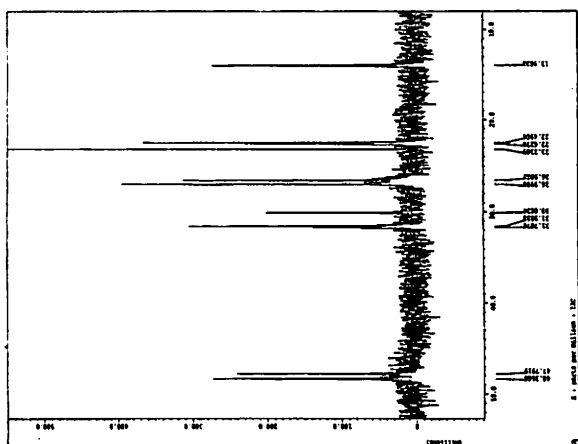
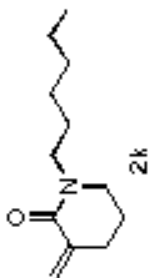
1H

CDCL3





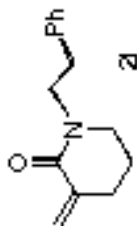
ACQUISITION PARAMETERS
File Name : 1d_13c_spectrum_398
Author : S4604615
Sample ID : Single Pulse with Broad
Creation Date : 23-MAR-2008 23:27:05
Revision Date : 25-MAR-2008 20:07:49
Spec Site : ECP500
Spec Type : DELTA_RN
Data Format : 1D COMPLEX
Dimensions : 1
Dim 1 Title : 13C
Dim 1 Units : [ppm]
Dim 2 Title : 13C
Dim 2 Units : [ppm]
Scales : 1000
Mod Return : 1
X_Correlate : 13C
X_Freq : 125.77787547 [MHz]
X_Sweep : 31.44654088 [kHz]
Solvent : CDCl3
Spin_Prot : 15 [Hz]
Spin_Rec : 20 [Hz]
Solve : 1 [Hz]
Field_Strength : 11.7473579 [T]
Filter_Mode : HETCORNOE
Filter_Width : 15.72066221 [kHz]



X : parts per Million : 13C

Fri Apr 27 17:12:13 2007

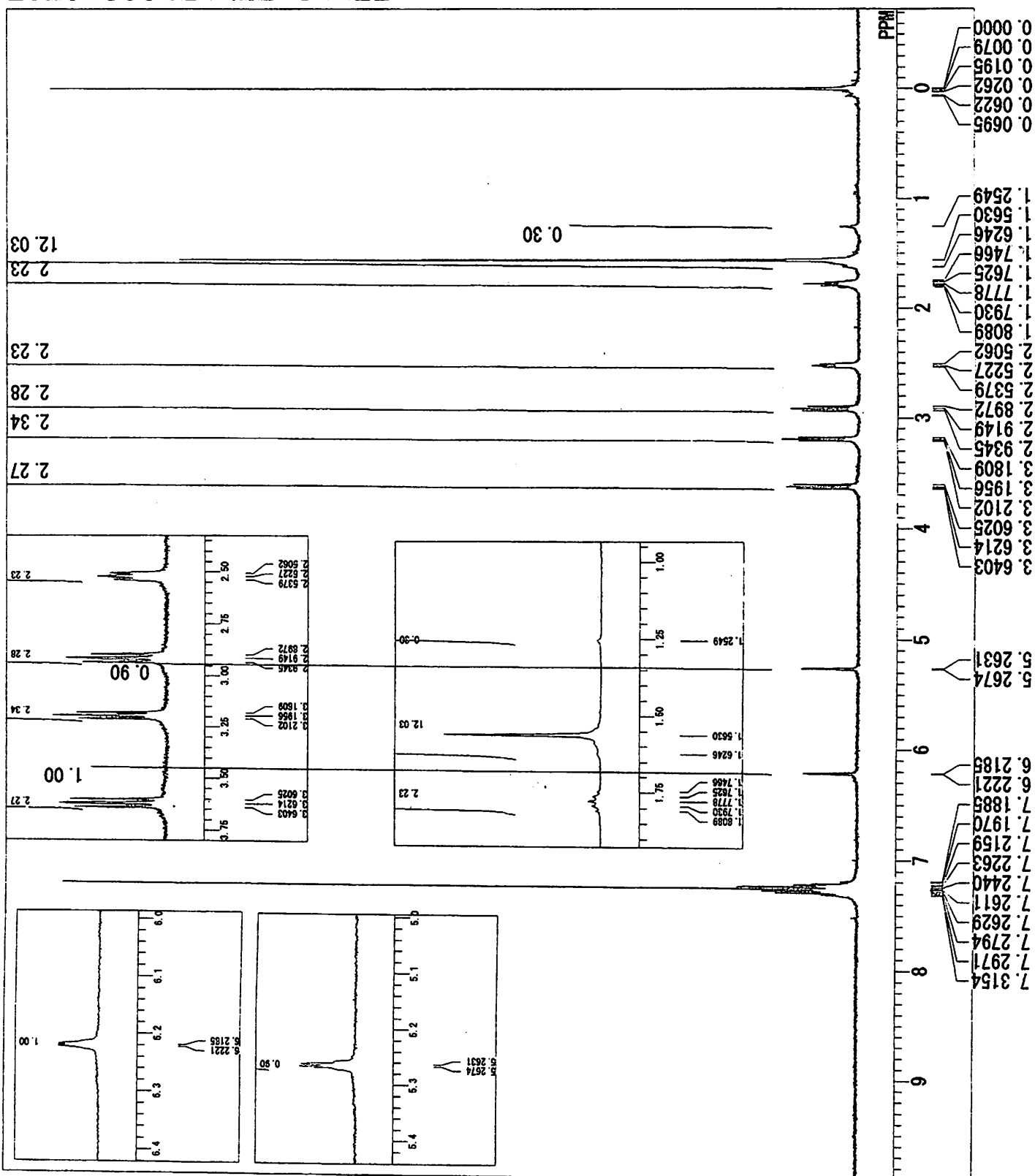
¹ H	399.65 MHz
NON	124.00 KHz
	10500.00 Hz
	32768
	7992.01 Hz
	8
	4.1001 sec
	2.9010 sec
	5.80 usec
¹ H	20.3 °C
CDCL3	0.00 ppm
	0.12 Hz
	21



```

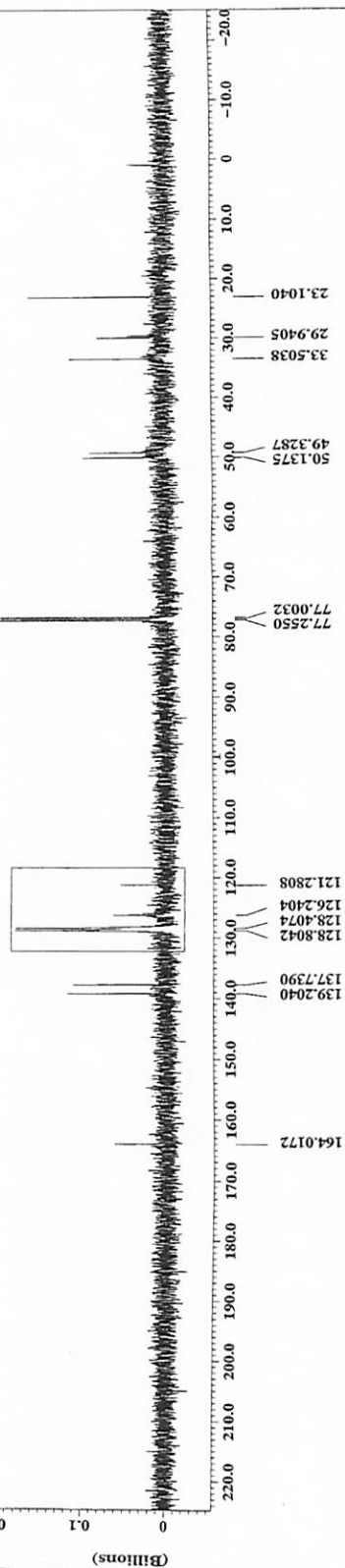
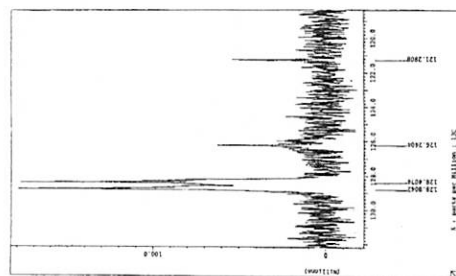
DFILE
COUNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN

```





----- ACQUISITION PARAMETERS -----
File Name = 1d_13c_spectrum_345
Author =
Sample ID = yonamine-phenethyl
Content = Single Pulse with Broad
Creation Date = 18-MAR-2008 11:57:23
Revision Date = 20-MAR-2008 11:18:46
Spec Site = ECP500
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title =
Dim Size = 13C
Scan Units = 32768
Scan Units = 1000000
Mod Return = 489.0
X_Domain = 1
X_Offset = 13C
X_Freq = 100.62517547 [MHz]
X_Freq = 31.44654088 [kHz]
Solvent = CHLOROFORM-D
Spin Get = 14 [Hz]
Temp Get = 22.9 [degC]
Nuc1 Gain = 10
Nuc2 Gain = 10.7473579 [Hz]
Pulse Length = 13.7473579 [Hz]
Filter Mode = BUTTERWORTH
Filter Width = 15.72066221 [kHz]

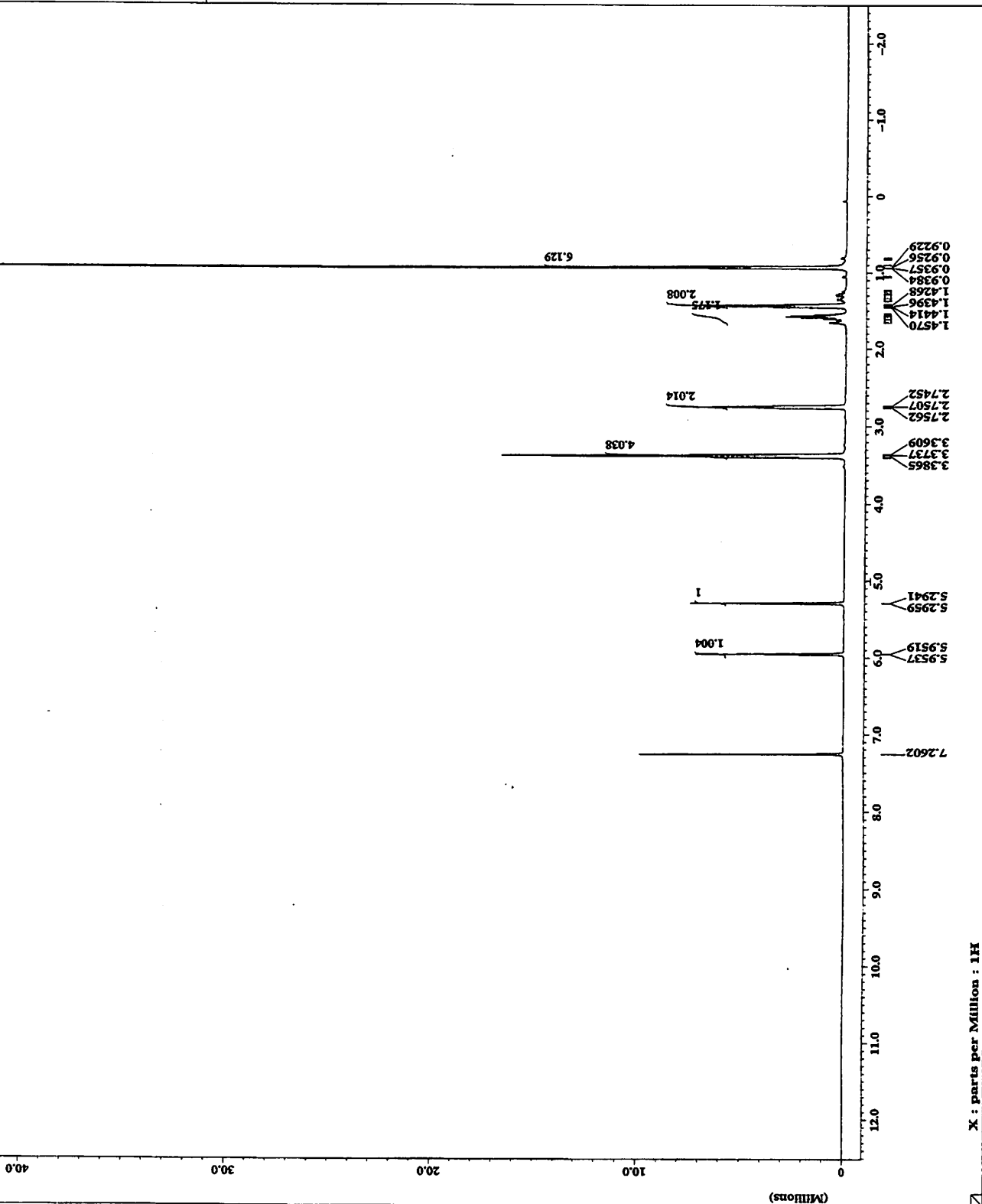
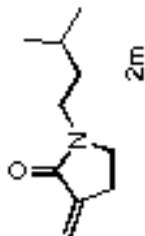


X : parts per Million : 13C

JEOL

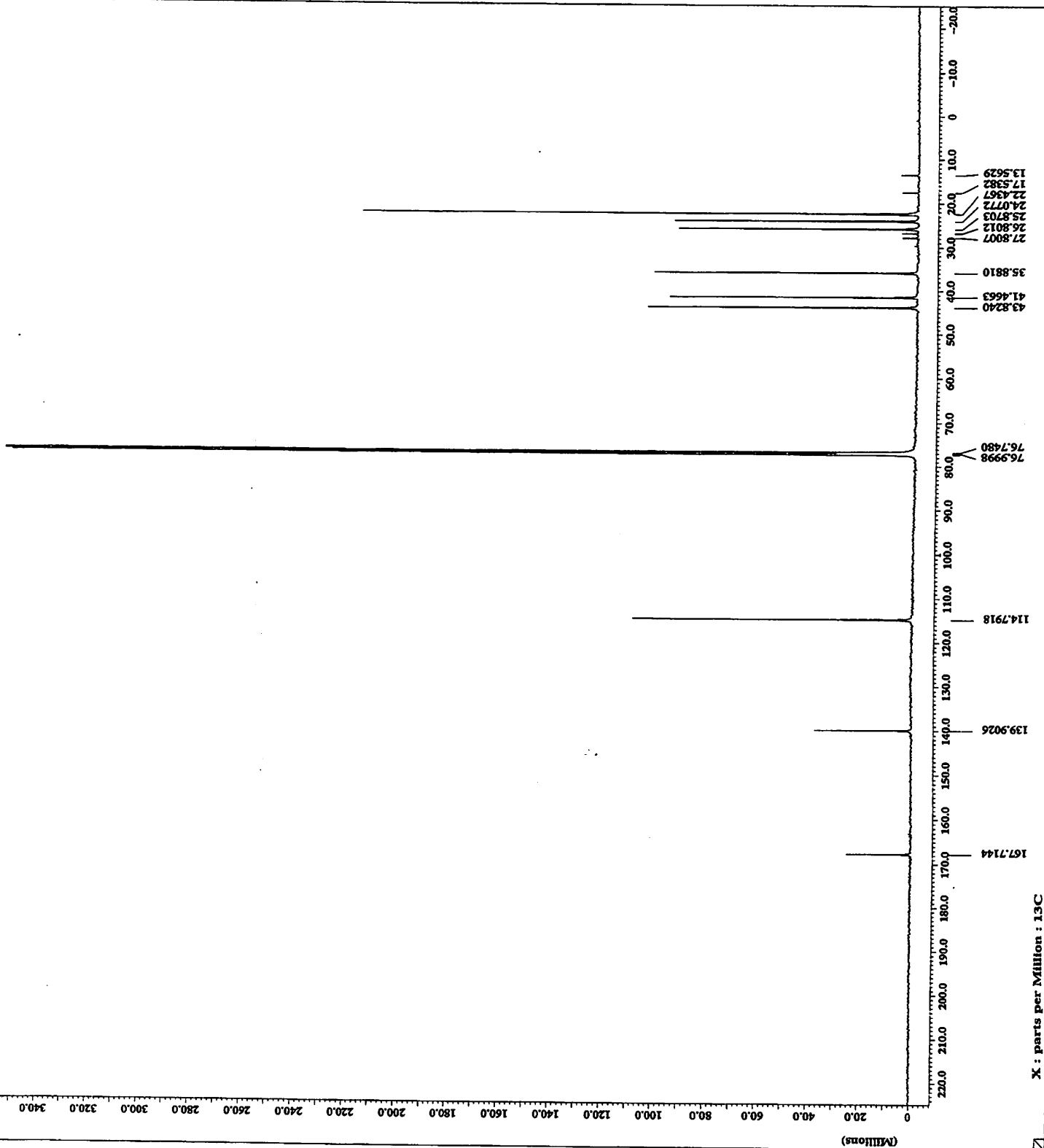
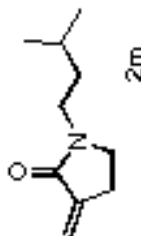
----- PROCESSING PARAMETERS -----
acq_balance
freq : 0.2[Hz]
proc : 2
solventphase
DMS
Reference : 7.255[ppm] : 7.26[ppm]

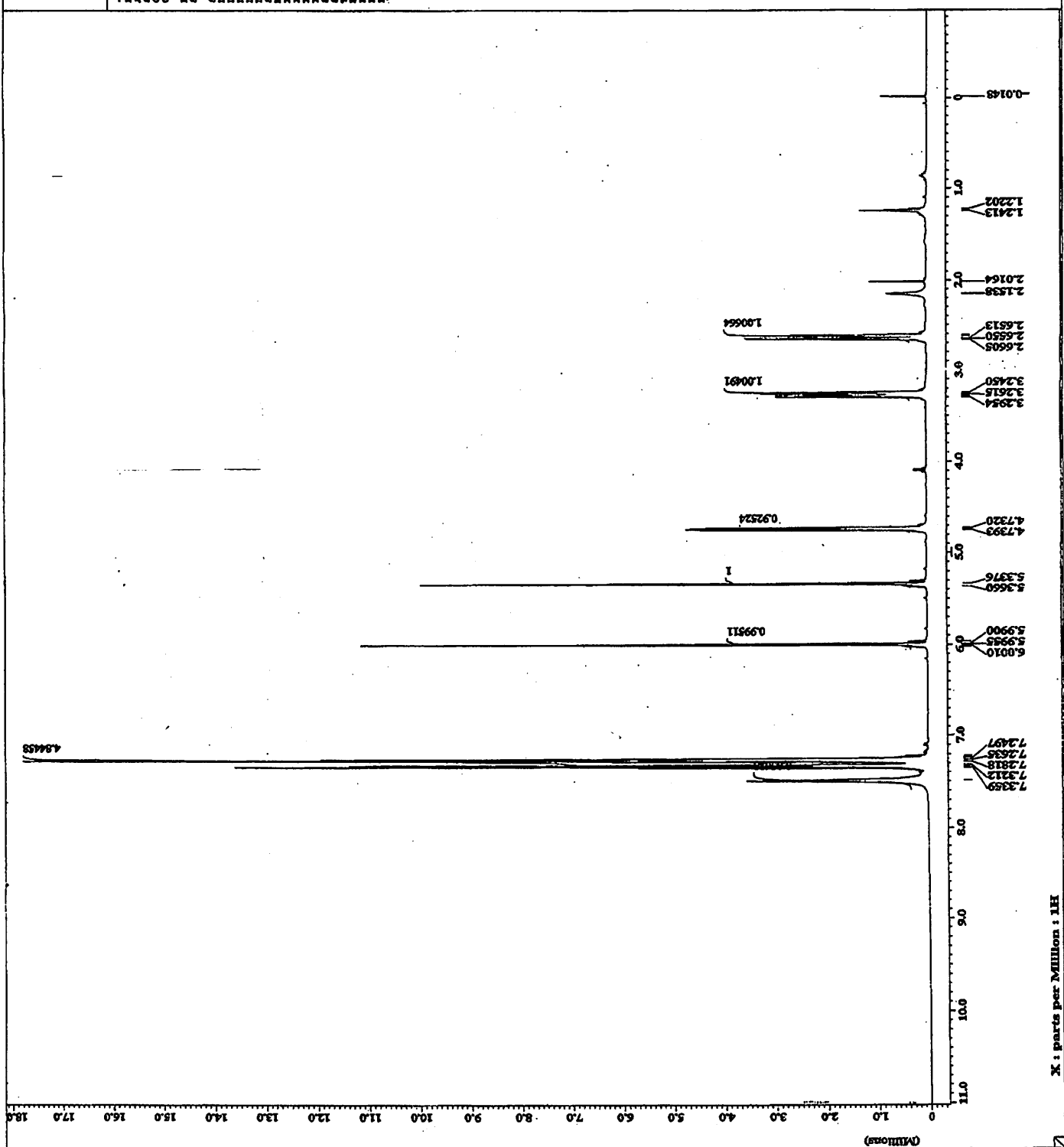
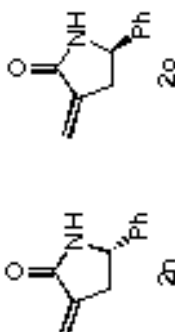
----- ACQUISITION PARAMETERS -----
File Name : 10-Spectrum.24
Author :
Sample ID : test fr.3
Content : Single Pulse Experiment
Creation Date : 7-JUN-2011 17:02:06
Revision Date : 10-JUN-2011 06:26:54
Spec file : KCP300
Spec Type : 1D NMR
Pulse Program : zgpg30
X : 1H
Y : 13C
X Offset : 0
X Freq : 500.13621602[MHz]
Y Freq : 125.760311[MHz]
Solvent : DMSO-d6
Temp_get : 20.5[°C]
Nuc1 : 1H
Nuc2 : 13C
Nuc3 : 15N
Nuc4 : 19F
Nuc5 : 31P
Nuc6 : 77Se
Nuc7 : 151Eu
Nuc8 : 171Yb
Nuc9 : 163La
Nuc10 : 139La
Nuc11 : 133Cs
Nuc12 : 125Te
Nuc13 : 123Sb
Nuc14 : 115In
Nuc15 : 113Cd
Nuc16 : 109Ag
Nuc17 : 107Pd
Nuc18 : 105Te
Nuc19 : 103Rh
Nuc20 : 101Ru
Nuc21 : 99Ru
Nuc22 : 97Mo
Nuc23 : 95Mo
Nuc24 : 93Nb
Nuc25 : 91Zr
Nuc26 : 89Y
Nuc27 : 87Sr
Nuc28 : 85Kr
Nuc29 : 81Br
Nuc30 : 79Br
Nuc31 : 75As
Nuc32 : 71Ga
Nuc33 : 69Ga
Nuc34 : 67Zn
Nuc35 : 65Cu
Nuc36 : 63Cu
Nuc37 : 61Ni
Nuc38 : 59Co
Nuc39 : 57Fe
Nuc40 : 55Fe
Nuc41 : 51V
Nuc42 : 49Ti
Nuc43 : 47Ti
Nuc44 : 45Sc
Nuc45 : 43Ca
Nuc46 : 41Ca
Nuc47 : 39K
Nuc48 : 37K
Nuc49 : 35K
Nuc50 : 33S
Nuc51 : 31P
Nuc52 : 29Si
Nuc53 : 27Al
Nuc54 : 25Mg
Nuc55 : 23Mg
Nuc56 : 21Ne
Nuc57 : 19F
Nuc58 : 17O
Nuc59 : 15N
Nuc60 : 13C
Nuc61 : 12C
Nuc62 : 11B
Nuc63 : 10B
Nuc64 : 9Be
Nuc65 : 7Li
Nuc66 : 6Li
Nuc67 : 3He
Nuc68 : 1H



--- PROCESSING PARAMETERS ---
Sample Name : 14_13c_spectrum_4
Date : 2011-08-08
Time : 10:10:10
F2 : 100.625 MHz
F1 : 125.760 MHz
Reference : TMS
Reference : 77.106 [ppm] : 77 [ppm]

--- ACQUISITION PARAMETERS ---
File Name : 14_13c_spectrum_4
Author : 2011-08-08
Sample ID : 14_13c_spectrum_4
Date : 2011-08-08
Time : 10:10:10
F2 : 100.625 MHz
F1 : 125.760 MHz
Reference : TMS
Reference : 77.106 [ppm] : 77 [ppm]



[illegible]

JEOL

----- ACQUISITION PARAMETERS -----
File Name = 1d_13c_spectrum.f0
Sample ID = E01-020 2 419-13
Content = Single Pulse with Broad
Creation Date = 30-JUN-2004 22:16:51
Revision Date = 1-JUL-2004 18:44:15
Spec file = E01000
Spec Type = 1D 13C NMR
Date Acq = 30-JUN-2004
ID COMPLEX = 1
X = 13C
Dim title = 13C
Dim size = 2768
Dim units = Hz
Scales = 113.0
Mod_return = 1
X_domain = 13C (ppm)
X_offset = 125.77757547 [Hz]
X_freq = 31.44654088 [MHz]
X_resolp = CHLOROFORM-D
Solvent = CDCl3
Pulse_prog = zgpg30
Pulse_set = 231[ac]
Recvr_gain = 18
Field_strength = 11.7473572 [T]
Filter_mode = zgpg30
Filter_width = 15.72662211 [kHz]

