SUPPORTING INFORMATION

Scope of the Ring Opening Metathesis Polymerization (ROMP) Reaction of 1-Substituted Cyclobutenes

Airong Song, Jae Chul Lee, Kathlyn A. Parker* and Nicole S. Sampson*
Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400

Table of Contents

Materials and Methods

Materials and General Procedures. Amino acids and coupling agents used were purchased from Advanced Chem Tech. (Louisville, KY) or PerSeptive Biosystems (Framingham, MA). Solvents and chemical reagents were obtained from Fisher Scientific, Inc. (Springfield, NJ) or Sigma-Aldrich (Milwaukee, WI). Second generation Grubbs' catalyst [$(H_2IMes)(Pcy_3)Cl_2Ru{=}CHPh$] and ethyl 1-bromocyclobutanecarboxylate were purchased from Aldrich (Cat # 569747 and 197297). $(H_2IMes)(3\text{-}Brpyr)_2Cl_2Ru{=}CHPh$ was prepared according to the literature.[1] Cyclobut-1-enecarboxylic acid was synthesized according to the literature.[2,3] CH_2Cl_2 and CH_3OH were dried in a GlassContour solvent pushstill system; benzene, pentane and Et_2O were used without further purification. All reactions were carried out under an Ar atmosphere in oven-dried glassware unless otherwise specified. Analytical thin layer chromatography (TLC) was performed on precoated silica gel plates (60F254), flash chromatography on silica gel-60 (230–400 mesh) and Combi-Flash chromatography on RediSep normal phase silica columns (silica gel-60, 230–400 mesh). TLC spots were detected by UV light and by staining with phosphomolybdic acid (PMA). Inova400, Inova500 and Inova600 MHz NMR Instruments were used to perform NMR analysis, and spectra were recorded in $CDCl_3$ or CD_2Cl_2 unless otherwise noted. ^{1}H-NMR spectra are reported as chemical shift in parts per million (multiplicity, coupling constant in Hz, integration). ^{1}H-NMR data are assumed to be first order. The usual workup for ester or amide coupling reactions was three washes of the CH_2Cl_2 solution with 5% $NaHCO_3$, followed by three washes with 1 N HCl and drying of the CH_2Cl_2 over Na_2SO_4. After evaporation of solvent, the final product was purified by flash silica chromatography or Combi-Flash chromatography

instrument (Teledyne Isco company). LC-MS spectra were acquired on a Waters ACQUITY Ultra Performance Liquid Chromatography system with an SQD detector using a 10 cm×2.1 mm ACQUITY™ BEH C18 (particle size = 1.7 μm) column (Waters Corp, Milford, USA) with elution by a linear gradient of 20-100% *B* at 0.5 mL/min, where *A* = water and *B* = methanol.

PDI (Polydispersity Index) determination. The polymers (before flash column chromatography purification) were dissolved in THF (0.5 mg/mL). An aliquot (100 μL) of the polymer solution was injected and analyzed by gel permeation chromatography using a Phenogel column (300 x 7.80 mm, 5 μm, linear mixed bed, 0-40k MW range). Elution was performed at 0.7 mL/min with THF and detection at 220 nm at 30 °C. Narrowly dispersed polystyrene standards from Aldrich were used as molecular weight calibrants. The number average and weighted average molecular weights were calculated from the chromatogram.

Cyclobut-1-enecarboxylic Acid, 6. The acid was prepared according to the literature (42% yield).[2,3] ^{1}H-NMR (400 MHz) δ 10.23 (bs, 1H), 6.94 (t, J=1.2 Hz, 1H), 2.76 (t, J=3.2 Hz, 2H), 2.51 (td, J=3.2 Hz, 1.2 Hz, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 162.7, 146.5, 138.8, 51.2, 29.3, 27.3.

CB-GlyOMe, 2a. The amide was prepared as previously described (40% yield).[3] ^{1}H-NMR (400 MHz) δ 6.66 (s, 1H), 6.04 (s, 1H), 4.10 (d, J=5.2 Hz, 2H), 3.77 (s, 3H), 2.73 (m, 2H), 2.47 (m, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.6, 162.7, 141.5, 140.9, 52.5, 40.9, 28.6, 26.5.

CB-AlaOMe, 2b. H-Ala-OMe·HCl (0.61 mmol, 77 mg), cyclobut-1-enecarboxylic acid **6** (0.51 mmol, 50 mg) and 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride (EDC·HCl) (0.61 mmol, 117 mg) were dissolved in 2 mL CH_2Cl_2. Diisopropylethyl amine (DIEA) (1.0 mmol, 181 μL) was added at 0 ºC, and the reaction was stirred for 12 h at rt. The usual workup and chromatography

(EtOAc:CH_2Cl_2/2:8) yielded amide **2b** (43 mg, 33%) as a white powder. ^{1}H-NMR (400 MHz) δ 6.65 (s, 1H), 6.11 (s, 1H), 4.66 (m, 1H), 3.76 (s, 3H), 2.72 (m, 2H), 2.47 (m, 2H), 1.44 (d, J=7.2, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 173.9, 162.3, 141.8, 141.2, 52.9, 48.2, 29.1, 26.8, 18.7. HRMS (ESI) calcd. for $C_9H_{14}NO_3$ $[M+H]^+$ 184.0974, found 184.0973.

CB-CONHCH$_2$CH$_2$OMe, 2c. $NH_2CH_2CH_2OCH_3$ (0.61 mmol, 46 mg), cyclobut-1-enecarboxylic acid **6 (**0.51 mmol, 50 mg) and EDC·HCl (0.61 mmol, 117 mg) were dissolved in 2 mL CH_2Cl_2. DIEA (1.0 mmol, 181 μL) was added at 0 ºC, and the reaction was stirred for 12 h at rt. The usual workup and chromatography (EtOAc: CH_2Cl_2/3:7) yielded **2c** (29 mg, 44%) as a white powder. ^{1}H-NMR (400 MHz) δ 6.60 (s, 1H), 5.92 (s, 1H), 3.50 (m, 4H), 3.36 (s, 3H), 2.69 (m, 2H), 2.45 (m, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 162.9, 141.6, 140.6, 71.4, 59.0, 38.9, 28.7, 26.3. HRMS (ESI) calcd. for $C_8H_{14}NO_2$ $[M+H]^+$ 156.1025, found 156.1028.

CB-Glu(OtBu)OMe, 2d. H-Glu(OtBu)-OMe·HCl (0.61 mmol, 155 mg), cyclobut-1-enecarboxylic acid **6 (**0.51 mmol, 50 mg) and EDC·HCl (0.61 mmol, 117 mg) were dissolved in 2 mL CH_2Cl_2. DIEA (1.0 mmol, 181 μL) was added at 0 ºC, and the reaction was stirred for 4 h at rt. The usual workup and chromatography (EtOAc:CH_2Cl_2/3:7) yielded **2d** (64 mg, 42 %) as a white powder. ^{1}H-NMR (500 MHz) δ.6.67 (s, 1H), 6.44 (d, J=7 Hz, 1H), 4.65 (m, 1H), 3.78 (s, 3H), 2.74 (t, J=3.0 Hz, 2H), 2. 48 (d, J=2.5 Hz, 2H), 2.34 (m, 2H), 2.17 (m, 1H), 2.03 (m, 1H), 1.46 (s, 9H). ^{13}C-NMR (100 MHz, CD_2Cl_2) δ 172.8, 163.7, 142.3, 140.8, 81.1, 52.2, 51.7, 31.7, 28.5, 27.6, 26.5, 26.3. HRMS (ESI) calcd. for $C_{15}H_{24}NO_5$ $[M+H]^+$ 298.1654, found 298.1663.

CB-CONHCH$_2$CH$_2$CH$_2$Ph(*p*-CH$_3$), 2e. $NH_2CH_2CH_2CH_2Ph(p\text{-}CH_3)$ (0.61 mmol, 91 mg), cyclobut-1-enecarboxylic acid **6 (**0.51 mmol, 50 mg) and EDC·HCl (0.61 mmol, 117 mg) were

dissolved in 2 mL CH_2Cl_2. DIEA (1.0 mmol, 181 μL) was added at 0 ºC, and the reaction was stirred for 4 h at rt. The usual workup and chromatography (acetone:CH_2Cl_2/1:9) yielded **2e** (29 mg, 25%) as a white powder. ^{1}H-NMR (400 MHz) δ 7.10 (d, J=1.2 Hz, 4H), 6.49 (s, 1H), 3.29 (m, 2H), 2.61-2.64 (m, 4H), 2.43 (m, 2H), 2.31 (s, 3H), 1.82 (m, 2H). ^{13}C-NMR (100 MHz, CD_2Cl_2) δ 162.5, 142.1, 139.6, 138.8, 135.7, 129.4, 129.2, 128.5, 38.9, 33.1, 31.5, 29.9, 28.6, 26.2, 20.9. HRMS (ESI) calcd. for $C_{15}H_{20}NO$ $[M+H]^+$ 230.1545, found 230.1543.

CB-CON(CH$_3$)CH$_2$CO$_2$Me, 3a. $NH(CH_3)CH_2CO_2CH_3$·HCl (0.61 mmol, 85 mg), cyclobut-1-enecarboxylic acid **6** (0.51 mmol, 50 mg), DMAP (0.10 mmol, 13 mg) and EDC·HCl (0.61 mmol, 117 mg) were dissolved in 2 mL CH_2Cl_2. DIEA (1.0 mmol, 181 μL) was added at 0 ºC, and the reaction was stirred for 16 h at rt. The usual workup and chromatography (EtOAc:CH_2Cl_2/1:9) yielded **3a** (12 mg, 13%) as a white powder. ^{1}H-NMR (400 MHz) δ 6.53 (s, 1H), 6.33 (s, 0.47H), 4.22-4.11 (m, 2H+0.94 H), 3.77 (s, 0.94H), 3.74 (s, 2H), 3.22 (s, 3H), 3.03 (s, 1.41H), 2.85 (t, J=3.2 Hz, 2H), 2.78 (t, J=3.2 Hz, 0.94H), 2.48 (t, J=3.2 Hz, 2H), 2.45 (t, J=3.2 Hz, 0.94H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.0, 169.9, 164.5, 164.1, 142.9, 141.1, 140.8, 52.3, 49.9, 37.1, 35.2, 31.6, 27.4. HRMS (ESI) calcd. for $C_9H_{14}NO_3$ $[M+H]^+$ 184.0974, found 184.0975.

CB-CO-piperidine, 3b. Bis(2-oxo-3-oxazolidinyl)phosphinic chloride (BOP-Cl) (0.83 mmol, 211 mg) and cyclobut-1-enecarboxylic acid **6** (0.75 mmol, 74 mg) were dissolved in 3 mL CH_2Cl_2. DIEA (0.75 mmol, 134 μL) was added at 0 ºC, and the reaction was stirred for 2 h at rt. Piperidine (0.91 mmol, 77 mg) and diisopropylethyl amine (DIEA) (0.75 mmol, 134 μL) were added into the solution, which was stirred for another 20 h. The usual workup and chromatography (acetone:CH_2Cl_2/1:9) yielded **3b** (76 mg, 61%) as a white powder. ^{1}H-NMR (500 MHz) δ 6.40 (s, 1H), 3.62 (t, J=2.5 Hz,

4H), 2.85 (t, J=2.5 Hz, 2H), 2.49 (t, J=2.5 Hz, 2H), 1.69-1.58 (m, 6H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 162.9, 141.5, 139.8, 47.0, 43.0, 32.0, 27.4, 24.8. HRMS (ESI) calcd. for $C_{10}H_{16}NO$ $[M+H]^+$ 166.1232, found 166.1233.

CB-CO_2Me, 4a. The methyl ester was prepared as previously described (45% yield).[4] ^{1}H-NMR (400 MHz) δ6.74 (s, 1H), 3.68 (s, 3H), 2.69 (m, 2H), 2.46 (m, 2H). ^{13}C-NMR (100 MHz) δ 162.7, 146.5, 138.8, 51.2, 29.3, 27.3. HRMS (EI) calcd. for $C_6H_8O_2$ $[M]^+$ 112.05243, found 112.05228.

CB-$CO_2CH_2CO_2$Me, 4b. Cyclobut-1-enecarboxylic acid **6** (0.51 mmol, 50 mg) and $BrCH_2CO_2CH_3$ were dissolved in 2 mL dry CH_2Cl_2. KI (0.10 mmol, 17 mg) and DIEA (0.61 mmol, 108 μL) were added into the solution at 0 ºC. The reaction was stirred for 17 h at rt. The usual workup and chromatography (EtOAc:CH_2Cl_2/0.5:9.5) yielded **4b** (46 mg, 53%) as a sticky oil. ^{1}H-NMR (500 MHz) δ 6.92 (s, 1H), 4.69 (s, 2H), 3.79 (s, 3H), 2.80 (m, 2H), 2.53 (m, 2H). ^{13}C-NMR (100 MHz, CD_2Cl_2) δ 168.4, 161.1, 148.4, 137.8, 60.3, 52.2, 29.2, 27.6. HRMS (ESI) calcd. for $C_8H_{10}O_4Na$ $[M+Na]^+$ 193.0477, found 193.0485.

1-Cyclobutenemethanol, 7. 1-Cyclobutenemethanol, **7** was obtained by synthetic procedures previously described in the literature[5] with major modifications using DIBAL-H. Dry Et_2O (4.58 mL) was added to a solution of **4a** (302 mg, 2.70 mmol) in dry CH_2Cl_2 (1.82 mL) and the solution was cooled to -78 °C. DIBAL-H (1.2 mL, 6.74 mmol) was added dropwise to the solution. After stirring at -78 °C for 4 h, the reaction mixuture was poured slowly into a mixture of Et_2O (18.0 mL) and saturated aqueous potassium sodium tartrate (70 mL). The mixture was stirred until both layers turned clear (30 min), and the Et_2O layer was separated. Additional Et_2O (18 mL × 2) was added to the separated aqueous solution to extract the product. The combined Et_2O extracts were dried over anhydrous Na_2SO_4. The

solvent was carefully evaporated under reduced pressure (10 mm Hg) and the residue was further purified by vacuum distillation (25 °C, 0.01 mm Hg) using a Kugelrohr apparatus to yield **7** (92.4 mg, 45% yield). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.93 (m, 1H), 4.09 (m, 2H), 2.52 (m, 2H), 2.42 (m, 2H), 1.37 (t, J=6.0 z, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 148.7, 128.8, 61.6, 29.6, 27.1.

1-Cyclobutenylmethyl acetate, 5a. 3,3-Dimethylaminopyridine (DMAP) (29.1 mg, 0.238 mmol) and DIEA (1.18 mL, 7.14 mmol) were added to a solution of **7** (200 mg, 2.38 mmol) in dry CH_2Cl_2 (5.0 mL) and cooled to 0 °C. Acetyl chloride (339 μL, 4.76 mmol) was added dropwise to the solution at 0 °C. The reaction mixture was stirred at rt for 2 h. After the reaction was complete, iced H_2O (25 mL) was added slowly to the reaction mixture. The mixture was extracted with CH_2Cl_2 (50 mL × 2) and the combined organic extracts were washed with 1N aq HCl (25 mL × 2), 5% aq $NaHCO_3$ (25 mL) and 10% aq NaCl (25 mL). The organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The residue was purified by silica column chromatography with CH_2Cl_2 to afford **5a** (258 mg, 86% yield). The purified fractions were concentrated and diluted with dry CH_2Cl_2 and the solution was stored at -20 °C. ^{1}H-NMR (600 MHz, $CDCl_3$) δ 5.86 (s, 1H), 4.42 (s, 2H), 2.44 (b, 2H), 2.34 (b, 2H), 2.00 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 170.71, 143.61, 131.53, 62.06, 30.05, 27.23, 20.76.

1-Cyclobutenylmethyl trimethyl acetate, 5b. 3,3-Dimethylaminopyridine (DMAP) (13.4 mg, 0.109 mmol) and DIEA (495 μL, 2.84 mmol) were added to a solution of **7** (92 mg, 1.09 mmol) in dry CH_2Cl_2 (4.5 mL) and cooled to 0 °C. Trimethyl acetyl chloride (175 μL, 1.42 mmol) was added dropwise to the solution at 0 °C. The reaction mixture was stirred at rt for 2 h. After the reaction was complete, iced H_2O (25 mL) was added slowly to the reaction mixture. The mixture was extracted with

CH_2Cl_2 (50 mL × 2) and the combined organic extracts were washed with 1N aq HCl (25 mL × 2), 5% aq $NaHCO_3$ (25 mL) and 10% aq NaCl (25 mL). The organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The residue was purified by silica column chromatography with CH_2Cl_2 to afford **5b** (172 mg, 94% yield). The purified fractions were concentrated and diluted with dry CH_2Cl_2 and the solution was stored at -80 °C. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 5.91 (m, 1H), 4.52 (m, 2H), 2.50 (m, 2H), 2.42 (m, 2H), 1.23 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 178.5, 144.2, 130.8, 62.2, 39.1, 30.1, 27.4, 26.7; LRMS (ESI) calcd for $C_{10}H_{17}O_2$ $[M+H]^+$ 169.12, found 169.10.

ROM of Methyl cyclobut-1-enecarboxylate 4a: 9a and 10a. A solution of **4a** (40.0 mg, 0.357 mmol) in dry CH_2Cl_2 (4 mL) was added to a solution of precatalyst **1** (474 mg, 0.536 mmol) in dry CH_2Cl_2 (4 mL) at rt. The solution was stirred at rt for 20 h and ethyl vinyl ether (5 mL, 52.2 mmol) was added to the reaction mixture. After 60 min, the solvent was evaporated and the residue was purified by silica column chromatography with CH_2Cl_2. The purified fractions were evaporated to afford the products **9a** and **10a** (42.1 mg, 55% yield) with *E*/*Z*molar ratio 2.3/1. ^{1}H-NMR (600 MHz, CD_2Cl_2) 1-mer **9a** *Z*-isomer δ 7.36-7.19 (m, 5H), 6.47 (d, J=12.6 Hz, 1H), 6.15 (s, 1H), 5.68 (dt, J=11.4, 7.8 Hz, 1H), 5.60 (s,1H), 3.72 (s, 3H), 2.50 (m, 2H), 2.43 (m, 2H). 1-mer **10a** *E*-isomer δ 7.36-7.19 (m, 5H), 6.42 (d, J=16.2 Hz, 1H), 6.25 (dt, J=22.8, 6.0 Hz, 1H), 6.17 (s, 1H), 5.60 (s, 1H), 3.75 (s, 3H), 2.50 (m, 2H), 2.43 (m, 2H). ^{13}C-NMR (100 MHz, CD_2Cl_2) 1-mer **9a** *Z*-isomer δ 167.9, 140.6, 138.1, 132.1, 130.8, 130.0, 129.3, 128.6, 127.2, 125.5, 52.2, 32.6, 28.0. 1-mer **10a** *E*-isomer δ 168.0, 140.7, 138.1, 131.0, 130.3, 129.0, 128.7, 127.5, 126.5, 52.2, 32.4, 32.3. LC-MS (APCI): Peak time=2.18 min, m/z calcd for $C_{14}H_{16}O_2$ $[M+H]^+$ 217.12, found 217.21, m/z calcd for $C_{14}H_{15}NaO_2$ $[M+Na]^+$ 239.10,

found 239.26， m/z calcd for $C_{13}H_{13}O$ $[M\text{-}CH_3O]^+$ 185.10, found 185.14, m/z calcd for $C_{12}H_{13}$ $[M\text{-}CO_2CH_3]^+$ 157.11, found 157.15.

ROMP of 5a: 13. A solution of **5a** (7.6 mg, 0.06 mmol) in dry CD_2Cl_2 (300 μL) was added to a solution of precatalyst **1** (5.3 mg, 0.006 mmol) in dry CD_2Cl_2 (300 μL) at rt. The reaction was monitored by NMR spectroscopy at rt for 1.5 h and ethyl vinyl ether (300 μL, 3.13 mmol) was added to the reaction mixture. After 30 min, the solvent was evaporated and the residue was purified by silica column chromatography with CH_2Cl_2 and 2% MeOH/CH_2Cl_2. The purified fractions were evaporated to afford the product **13** (6 mg, 73% yield). ^{1}H-NMR (600 MHz, CD_2Cl_2) δ 7.34-7.20 (m, 5H), 6.58 (m, 0.4H), 6.42(m, 0.6H), 6.24 (m, 0.6H), 5.43 (m, 10H), 5.03 (m, 1H), 4.94 (m, 1H), 4.66-4.48 (, 20H), 2.35-1.92 (m, 70H). HRMS (ESI) calcd. for $C_7H_{11}O_2$ $[M+H]^+$ 127.0754, found 127.0752.

ROMP of 1-cyclobutenylmethyl trimethyl acetate 5b: 14. A solution of **5b** (47.4 mg, 0.282 mmol) in dry CH_2Cl_2 (600 μL) was added to a solution of precatalyst **1** (25 mg, 0.0282 mmol) in dry CH_2Cl_2 (2.82 mL) at rt. The solution was stirred at rt for 3 h and ethyl vinyl ether (300 μL, 3.13 mmol) was added to the reaction mixture. After 30 min, the solvent was evaporated and the residue was purified by silica column chromatography with CH_2Cl_2 and 1-2% MeOH/CH_2Cl_2. The purified fractions were evaporated to afford the product **14** (30 mg, 60% yield). ^{1}H-NMR (500 MHz, CD_2Cl_2) δ 7.38-7.12 (m, 10H), 6.62-6.50 (br s, with max. at 6.57, 2H), 6.46-6.32 (br d, with max. at 6.42 and 6.38, 2H), 6.28~6.14 (br m, with max. at 6.24, 2H), 5.62-5.24 (br m, with max. at 5.43, 19H), 4.72~4.95 (br m, with max. at 4.64, 14H), 4.95~4.50 (br m, with max. at 4.57, 8H), 4.50~4.36 (br m, with max. at 4.46, 10H), 2.40~1.94 (br m, with max. at 2.17, 64H), 1.30~1.04 (br s, with max. at 1.18, 144H); ^{13}C-NMR (100 MHz, CD_2Cl_2) δ 139.0-136.5 (with max. at 138.1 and 137.6), 136.0-134.0 (with max. at

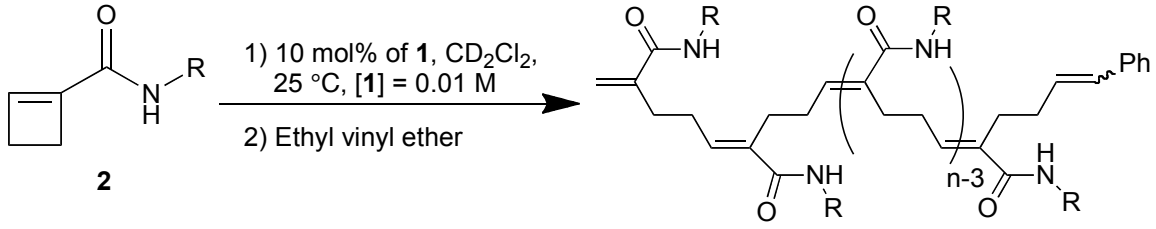
135.1), 131.5-129.3 (with max. at 130.0), 129.3-126.3 (styrenyl carbons), 69.2-67.9 (with max. at 68.4), 64.2-62.8 (with max. at 63.4), 62.8-61.6 (with max. at 62.1), 39.2, 36.4-34.6 (with max. at 35.9 and 35.6), 32.6-30.6 (with max. at 31.4), 29.6-28.2 (with max. at 28.7), 27.5, 27.2-25.8 (with max. at 27.0). ^{1}H-^{13}C gHMQC spectrum, see Table S1.

General Procedure for NMR Tube Reactions. An NMR tube was evacuated for 15 min, and then was purged with Ar for another 15 min. Under an Ar atmosphere, a solution of monomer in CD_2Cl_2 (300 μL) was added to the NMR tube. A solution of precatalyst $(H_2IMes)(3\text{-Br-Py})_2(Cl)_2Ru{=}CHPh$ in CD_2Cl_2 (300 μL) was added to the NMR tube. The stoichiometries of the reactions are indicated in Table S2. After complete mixing of the solution, the NMR tube was placed into the 400 MHz, 500 MHz or 600 MHz NMR spectrometer, and the reaction was monitored for several hours at 25 °C until almost all of the monomer had been consumed. Then the reaction was quenched with ethyl vinyl ether (50 μL), and was monitored for an additional 1 h.

Computational Methods. All the structure optimizations were performed using the hybrid DFT method at the B3LYP level, a combination of Becke's three-parameter hybrid exchange function (B3)[6,7] with the Lee-Yang-Parr correlation function[8] as implemented in Gaussian 03W. The basis sets for the optimization of monomers and their corresponding ring-opened ruthenium carbenes were 6-31G* and LANL2DZ, respectively (Figure 7a). The NBO charge calculations were performed using Hartree-Fock with the 6-31G++* basis set (for cyclobutene monomers) and the LANL2DZ basis set (for ruthenium carbenes). The AIM (atoms in molecule) electron density analysis was performed using the AIMPAC package.[9]

The initial ruthenium-carbene structure was obtained from the crystal structure of $(H_2IMes)(pyridine)_2Cl_2Ru{=}CHPh$,[10] and was modified with GaussianView 3.0. The geometry optimization of the ruthenium-carbenes was performed using the B3LYP/LANL2DZ method (Figure 8).[11-24] To simplify the computation, a methyl and a $CONHCH_3$ group represented the polymer chain and the 1-carbonyl amide group, respectively (Figure 8). The structures of the metallacyclobutane intermediates (Figure 8) were optimized using B3LYP/LANL2DZ in the following way: only one bond in the metallocyclobutane ring was optimized while the other three bond lengths were kept constant, and the partial optimization was continued optimizing each bond in turn until the optimized structure changed little in energy ($\Delta E < 6.3\times10^{-4}$ kcal/mol). Vibrational frequency calculations using B3LYP/LANL2DZ were performed for all model compounds, and there were no imaginary vibrations present in any of the final structures (Figures 7 and S9). Free energies computed for structures (Figure 8) in solvent (CH_2Cl_2) include the electronic energy plus the solvation free energy from the CPCM solvation model based on the UAKS radii using Gaussian 03W.

Figure S1. ROMP of secondary amides **2**. Conversion yield represents the molar ratio of consumed monomer to the initial monomer before ROMP. All the data were collected by comparing the integration of the signals for monomer and the signals for the propagating polymer chains in the ^{1}H NMR spectra.



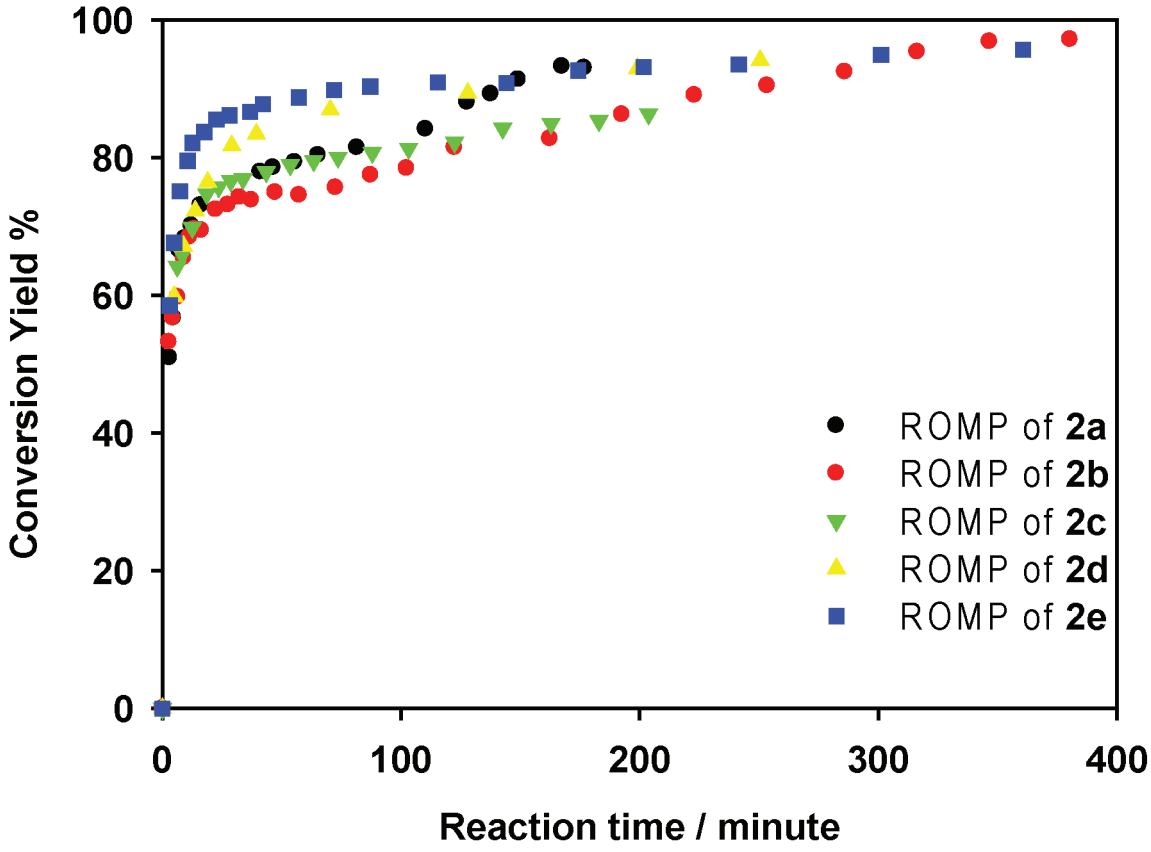
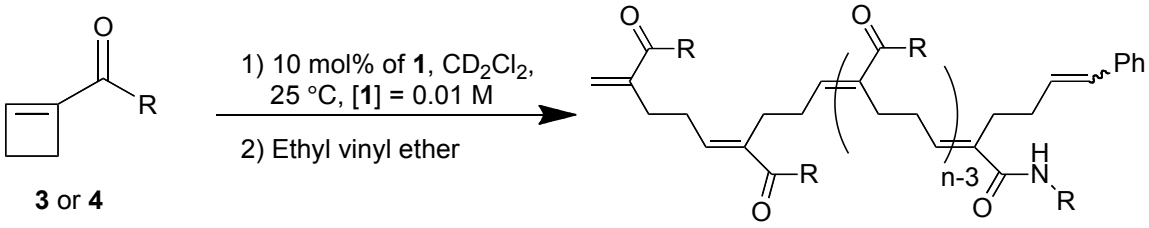


Figure S2. ROM of esters **3** and tertiary amides **4**. Conversion yield represents the molar ratio of consumed monomer to the initial monomer before ROM. All the data were collected by comparing the integration of the signals for monomer and the signals for the propagating polymer chains in the ^{1}H NMR spectra.



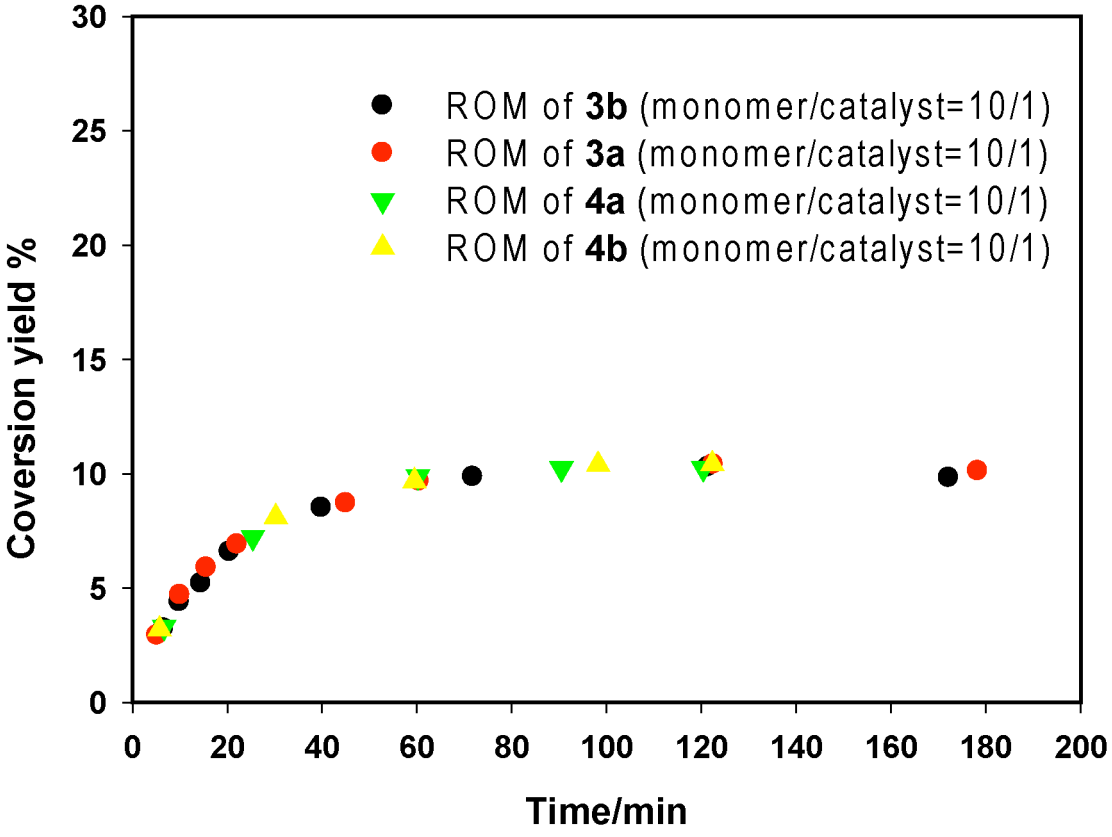


Figure S3. ^{1}H-NMR spectra of ROM of monomer **3b** in CD_2Cl_2 ([**3b**] = 0.1 M, [**1**] = 0.01 M, 25 ºC).

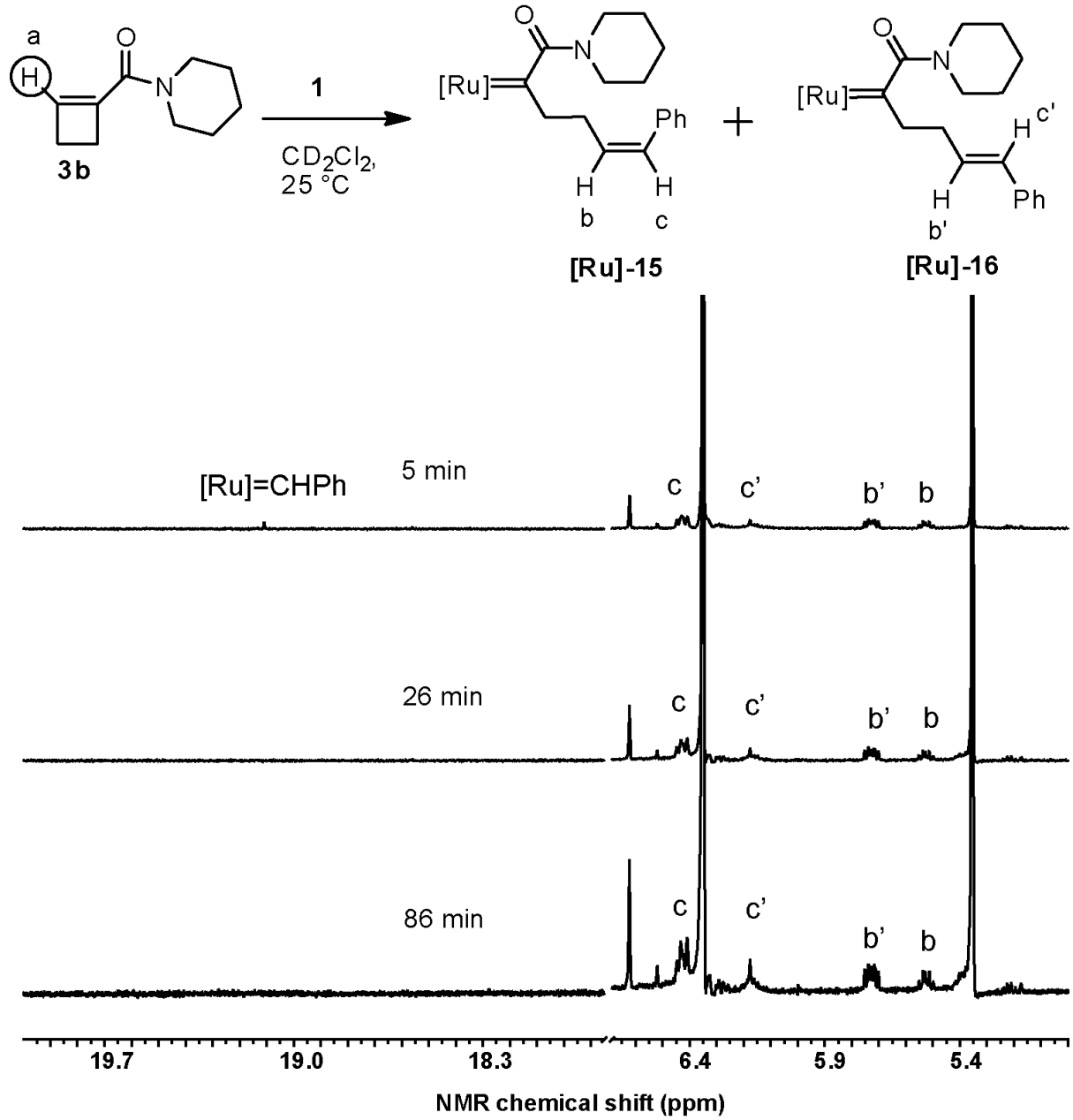
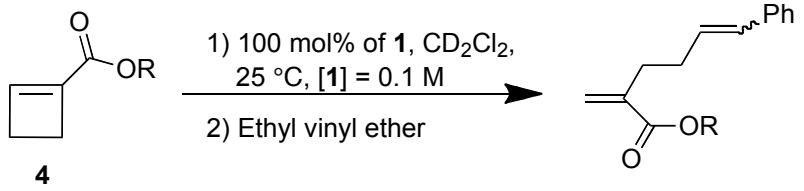


Figure S4. ROM of esters **4**. Conversion yield represents the molar ratio of consumed monomer to the initial monomer before ROM. All the data were collected by comparing the integration of the signals for monomer and the signals for the propagating polymer chains in the ^{1}H NMR spectra.



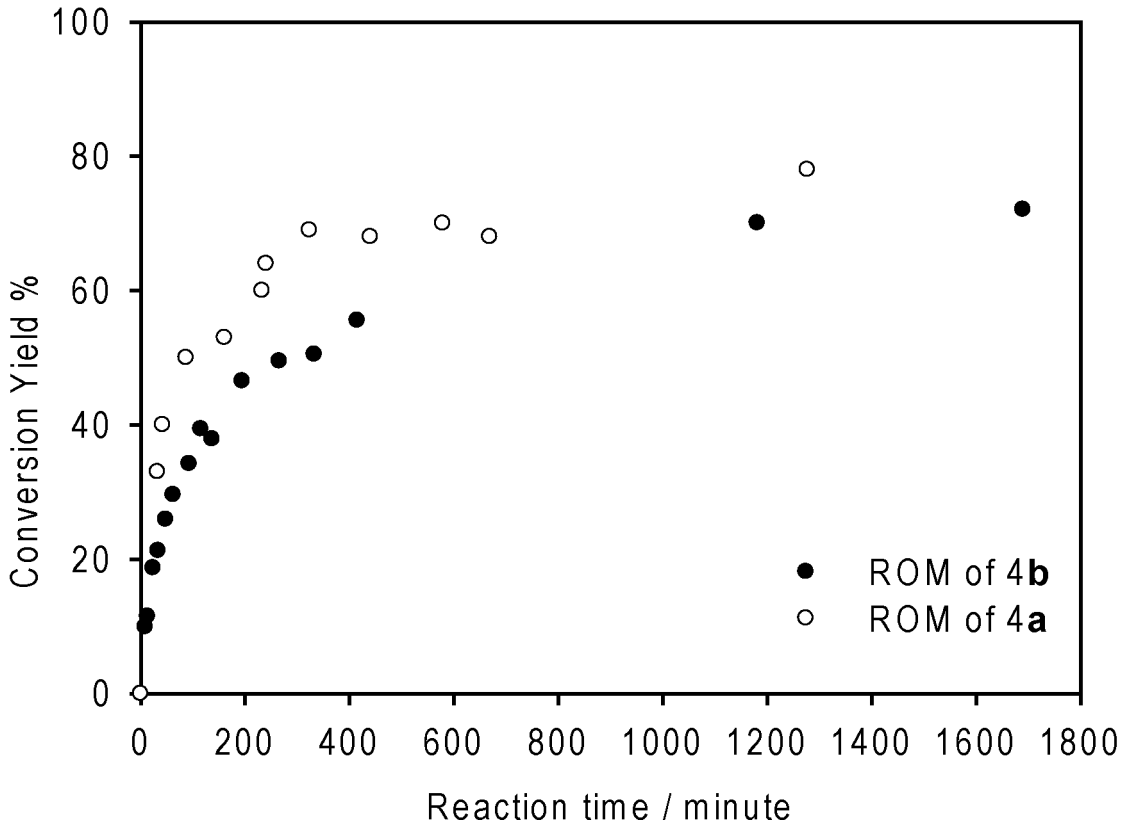


Figure S5. ^{1}H-NMR spectra of ROM of monomer **4a** in CD_2Cl_2 ([**4a**] = 0.1 M, [**1**] = 0.1 M, 25 °C).

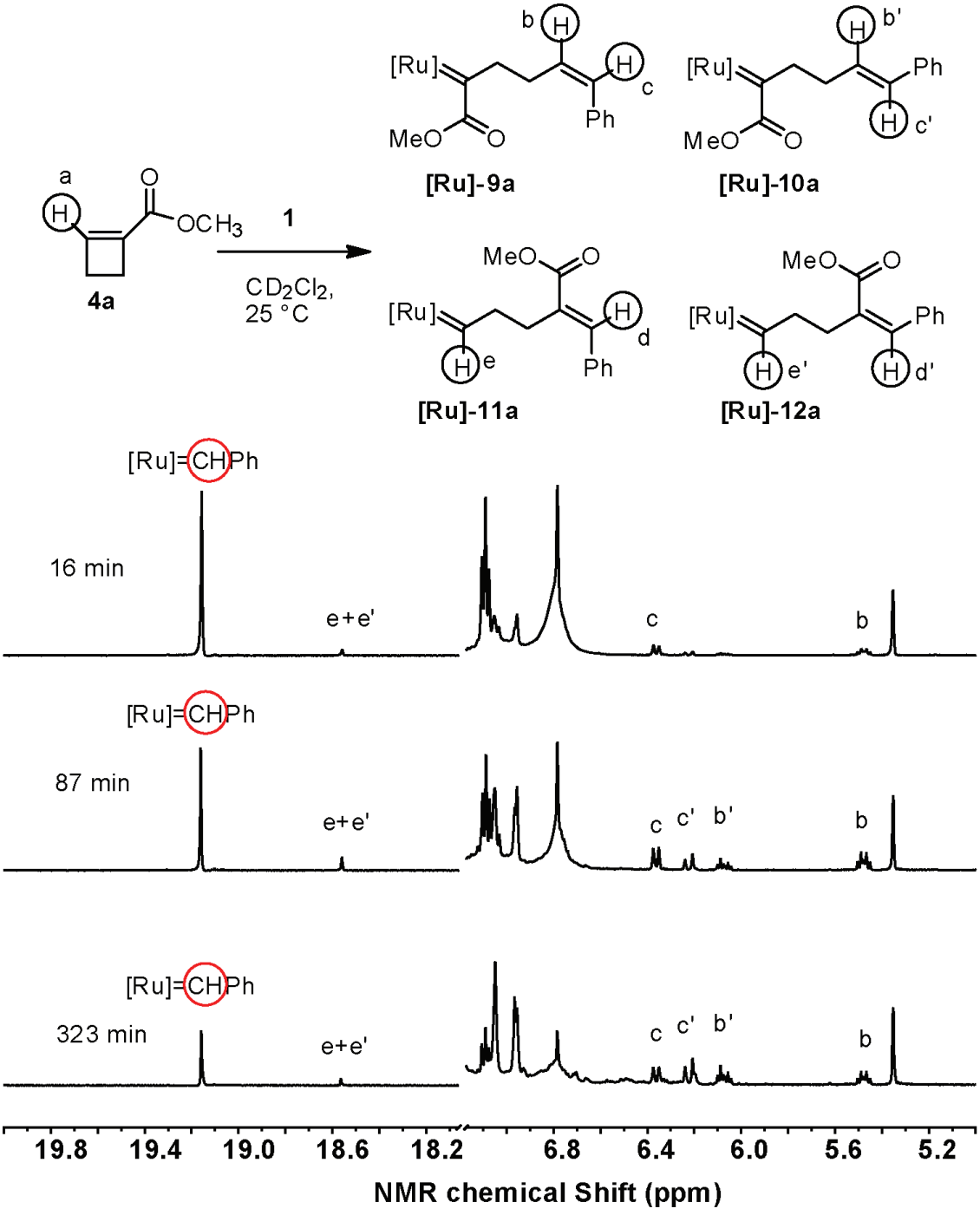
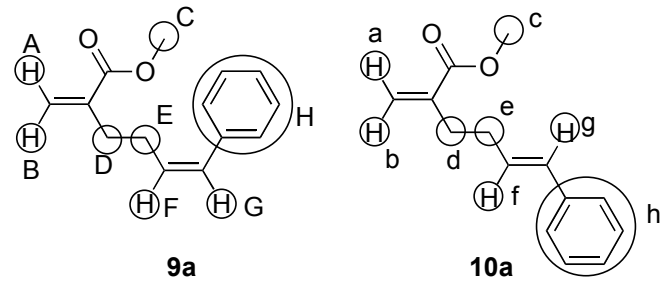


Figure S6. [1]H-NMR spectrum of the 1-mer reaction products **9a** and **10a**.



9a **10a**

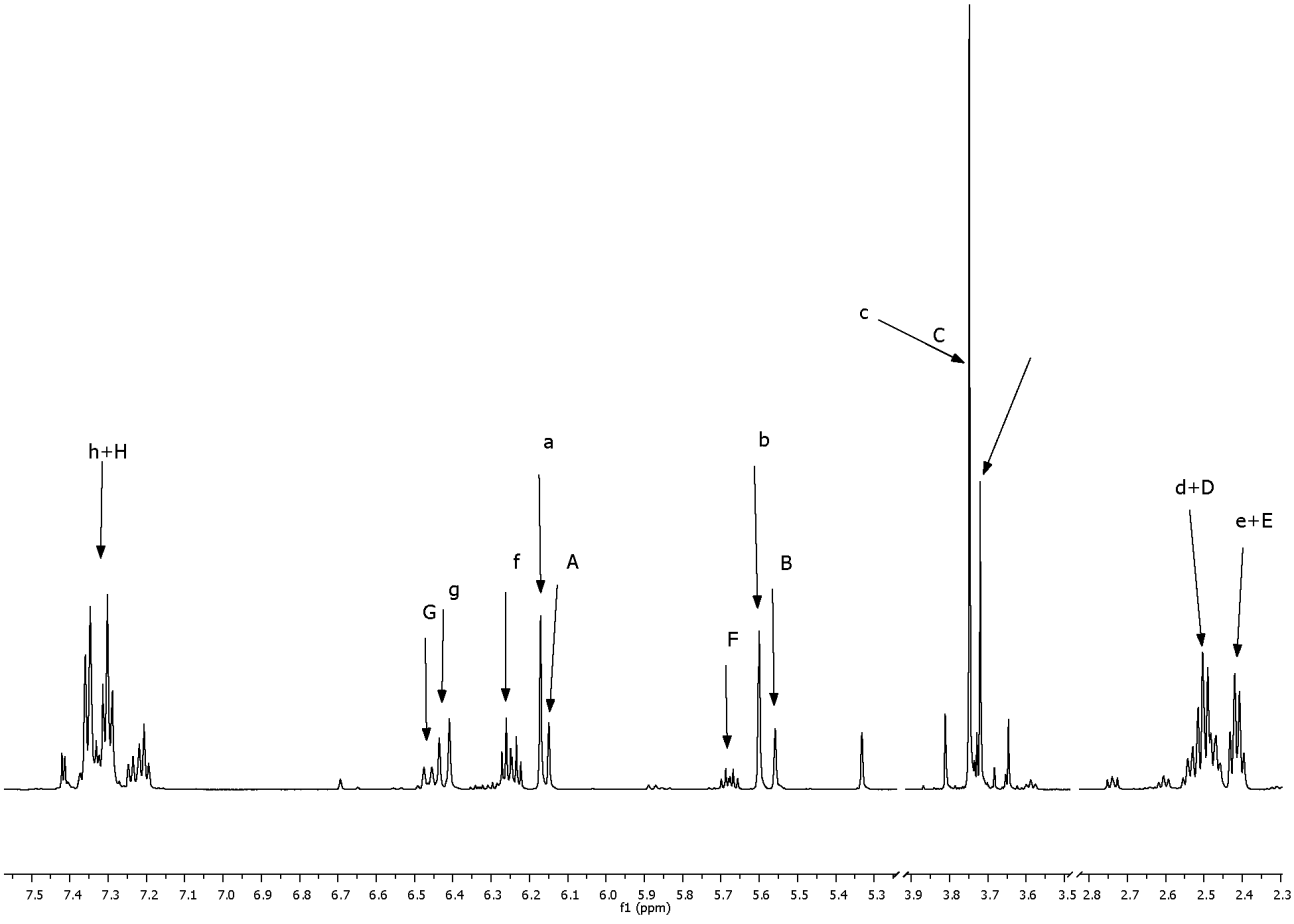
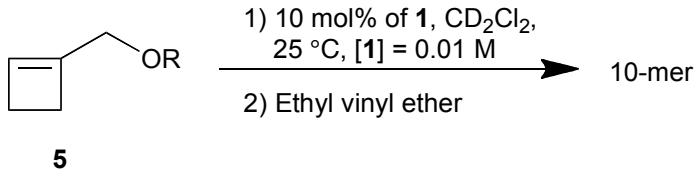


Figure S7. ROMP of carbinol esters **5**. Conversion yield represents the molar ratio of consumed monomer to the initial monomer before ROMP. All the data were collected by comparing the integration of the signals for monomer and the signals for the propagating polymer chains in the ^{1}H NMR spectra.



5

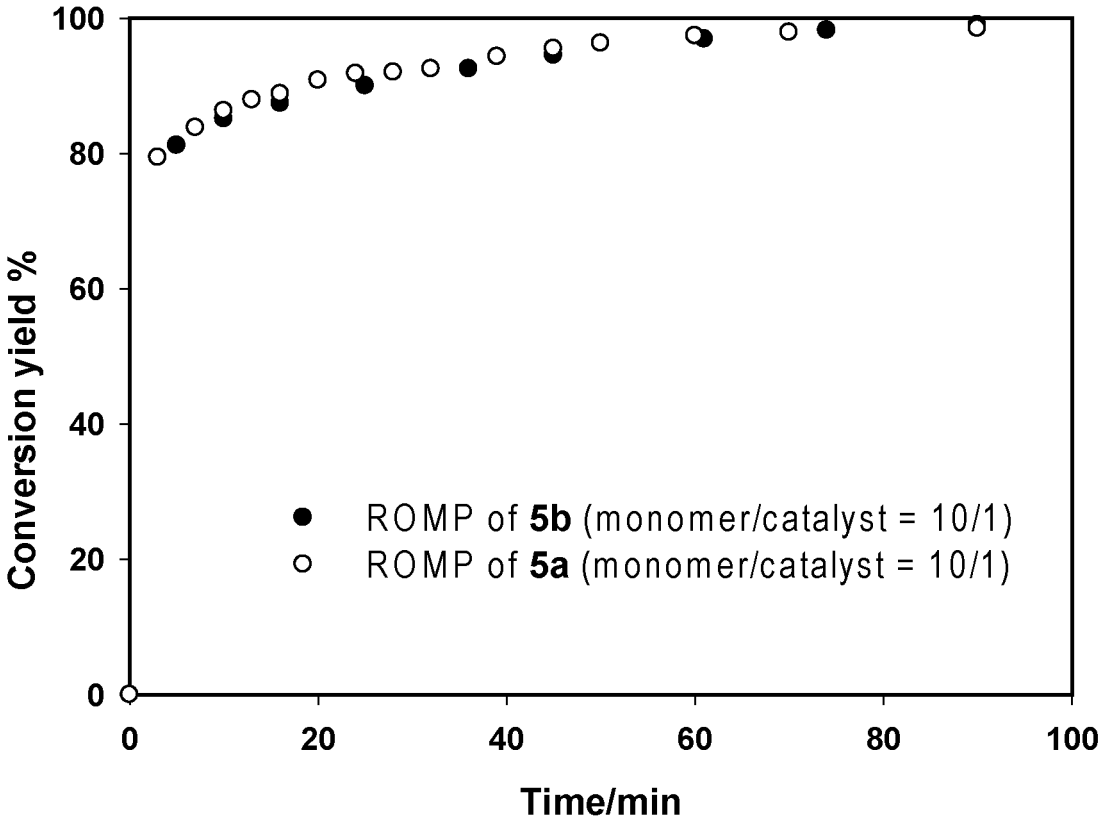


Figure S8. [1]H-NMR spectrum of polymer **13** (R = Ac). The letters indicate the protons in the structure. E, Z: *E*-configuration and *Z*-configuration in the olefins of the structure.

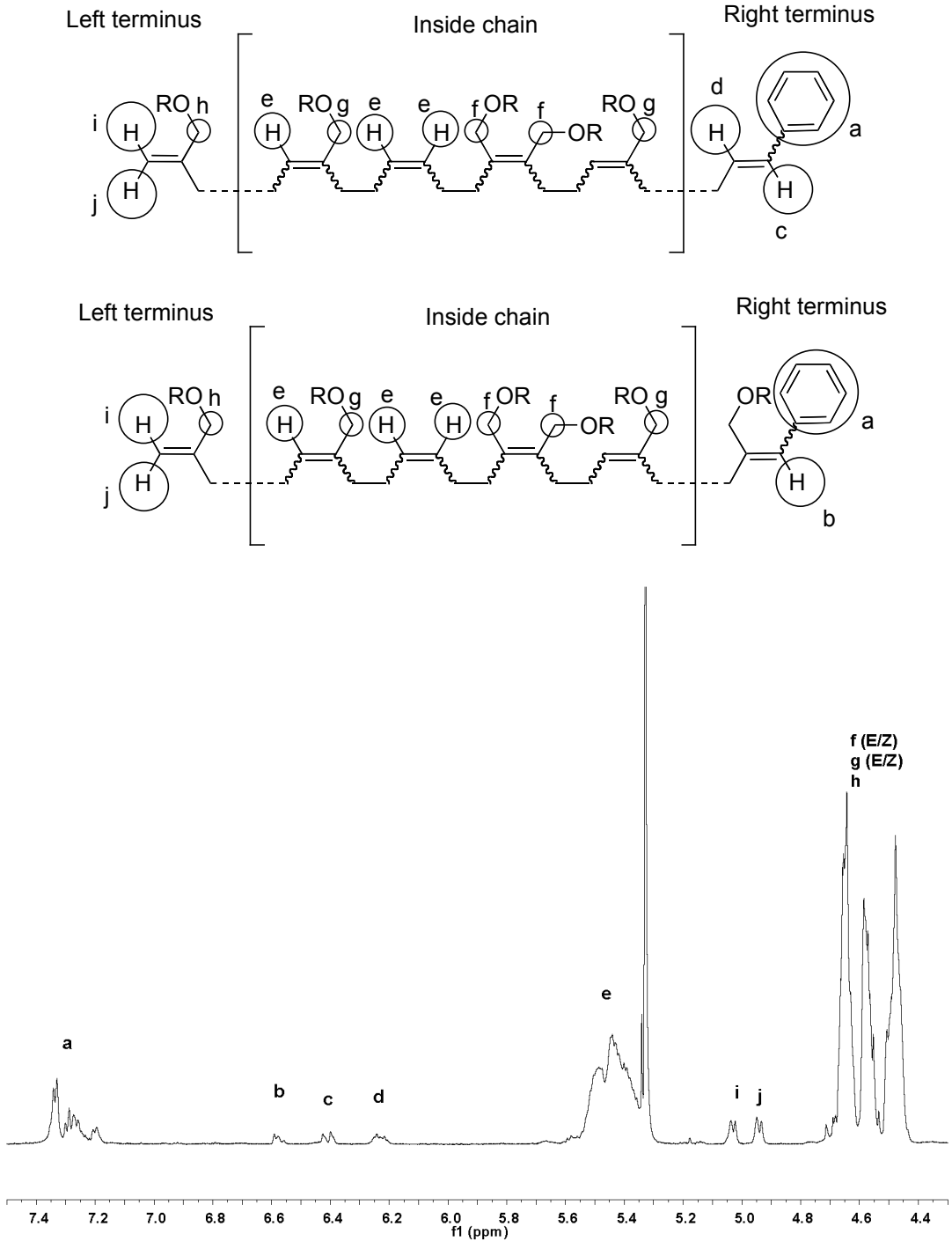
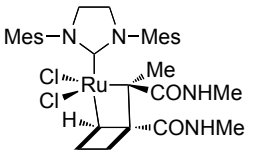
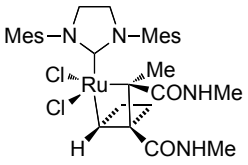


Figure S9. Structures of possible intermediates and ring opened products for ROMP of secondary amides and carbinol esters. To simplify the calculations, the polymer chain and the 1-carbonyl amide group, were modeled as a methyl group and a $CONHCH_3$ substituent, respectively.

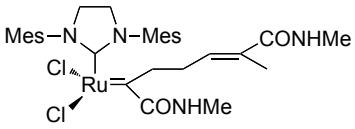
Secondary Amide



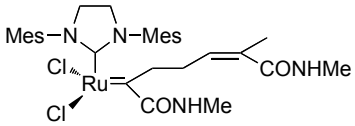
***trans*-IM-2**
-1699.640579 a.u.



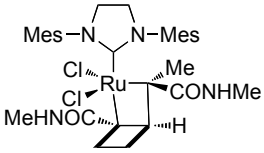
***cis*-IM-2**
-1699.652233 a.u.



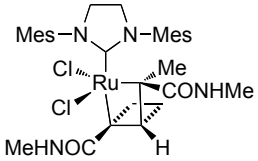
***cis*-RP-1**
-1699.691984 a.u.



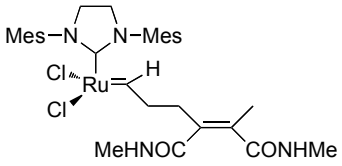
***trans*-RP-1**
-1699.688157 a.u.



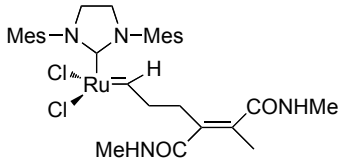
***trans*-IM-1**
-1699.645563 a.u.



***cis*-IM-1**
-1699.655533 a.u.

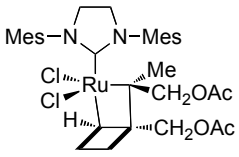


***cis*-RP-2**
-1699.685835 a.u.

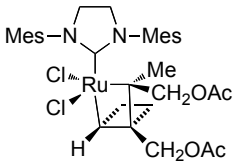


***trans*-RP-2**
-1699.680706 a.u.

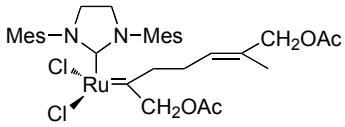
Carbinol Ester



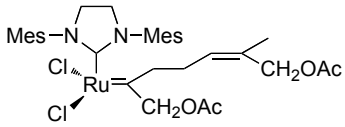
***trans*-IM-2**
-1818.001493 a.u.



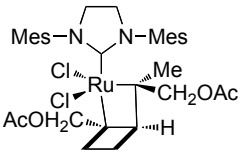
***cis*-IM-2**
-1817.999193 a.u.



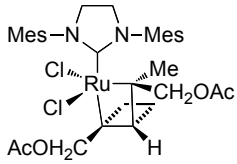
***cis*-RP-1**
-1818.010498 a.u.



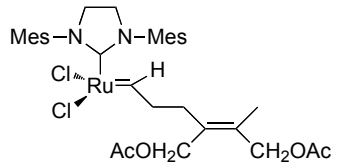
***trans*-RP-1**
-1818.007951 a.u.



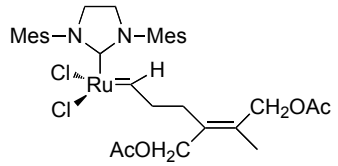
***trans*-IM-1**
-1818.002315 a.u.



***cis*-IM-1**
-1818.004594 a.u.



***cis*-RP-2**
-1818.017043 a.u.



***trans*-RP-2**
-1818.017642 a.u.

Table S1. gHMQC-derived ^{1}H-^{13}C NMR correlation of the 10-mer reaction product **14**.

Assignment	^{1}H-NMR (δ)	^{13}C-NMR (δ)
Phenyl group	7.27	129.0
Inside vinyl group	5.44	130.0
Methylene in the functional group	4.64	63.4
	4.57	62.1
	4.46	68.6
Methylene in the polymer backbone	2.17 (2.40-1.94)	35.7, 31.4, 28.8, 27.0
Trimethyl group	1.18	27.5

Table S2. ROMP reactions monitored by ^{1}H-NMR spectroscopy.[a]

Polymer	Monomer (0.06 mmol)	Catalyst **1**
18	**2a**	0.006 mmol
19	**2b**	0.006 mmol
20	**2c**	0.006 mmol
21	**2d**	0.006 mmol
22	**2e**	0.006 mmol
n/a	**3a**	0.006 mmol
n/a	**3b**	0.006 mmol
9a, 10a	**4a**	0.06 mmol
n/a	**4a**	0.006 mmol
9b, 10b	**4b**	0.06 mmol
n/a	**4b**	0.006 mmol
13	**5a**	0.006 mmol
14	**5b**	0.006 mmol

[a]Reaction conditions: CD_2Cl_2, 25 °C, [**1**] = 0.1 M.

References

(1) Love, J. A.; Morgan, J. P.; Trnka, T. M.; Grubbs, R. H. *Angew. Chem. Int. Ed.* **2002**, 41, 4035-4037.

(2) Campbell, A.; Rydon, H. N. *J. Chem. Soc.* **1953**, 3002-3008.

(3) Lee, J. C.; Parker, K. A.; Sampson, N. S. *J. Am. Chem. Soc.* **2006**, 128, 4578-4579.

(4) Song, A.; Parker, K. A.; Sampson, N. S. *J. Am. Chem. Soc.* **2009**, 131, 3444-5.

(5) Griffin, R. J.; Arris, C. E.; Bleasdale, C.; Boyle, F. T.; Calvert, A. H.; Curtin, N. J.; Dalby, C.; Kanugula, S.; Lembicz, N. K.; Newell, D. R.; Pegg, A. E.; Golding, B. T. *J. Med. Chem.* **2000**, 43, 4071-4083.

(6) Becke, A. D. *J. Chem. Phys.* **1996**, 104, 1040-1046.

(7) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648-5652.

(8) Lee, C. T.; Yang, W. T.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785-789.

(9) http://www.chemistry.mcmaster.ca/aimpac/.

(10) Sanford, M. S.; Love, J. A.; Grubbs, R. H. *Organometallics* **2001**, 20, 5314-5318.

(11) Adlhart, C.; Hinderling, C.; Baumann, H.; Chen, P. *J. Am. Chem. Soc.* **2000**, 122, 8204-8214.

(12) Fomine, S.; Ortega, J. V.; Tlenkopatchev, M. A. *J. Mol. Catal. A-Chem.* **2007**, 263, 121-127.

(13) Hofmann, P.; Volland, M. A. O.; Hansen, S. M.; Eisentrager, F.; Gross, J. H.; Stengel, K. *J. Organomet. Chem.* **2000**, 606, 88-92.

(14) Hoffmann, M.; Marciniec, B. *J. Mol. Model.* **2007**, 13, 477-83.

(15) Cornejo, A.; Fraile, J. M.; Garcia, J. I.; Gil, M. J.; Martinez-Merino, V.; Mayoral, J. A.; Salvatella, L. *Angew. Chem. Int. Ed.* **2005**, 44, 458-461.

(16) Fomine, S.; Tlenkopatchev, M. A. *Appl. Catal. A-Gen.* **2009**, 355, 148-155.

(17) Buchmeiser, M. R.; Wang, D. R.; Zhang, Y.; Naumov, S.; Wurst, K. *Eur. J. Inorg. Chem.* **2007**, 3988-4000.

(18) Straub, B. F. *Adv. Synth. Catal.* **2007**, 349, 204-214.

(19) Chou, H. H.; Lin, Y. C.; Huang, S. L.; Liu, Y. H.; Wang, Y. *Organometallics* **2008**, 27, 5212-5220.

(20) Cantat, T.; Demange, M.; Mezailles, N.; Ricard, L.; Jean, Y.; Le Floch, P. *Organometallics* **2005**, 24, 4838-4841.

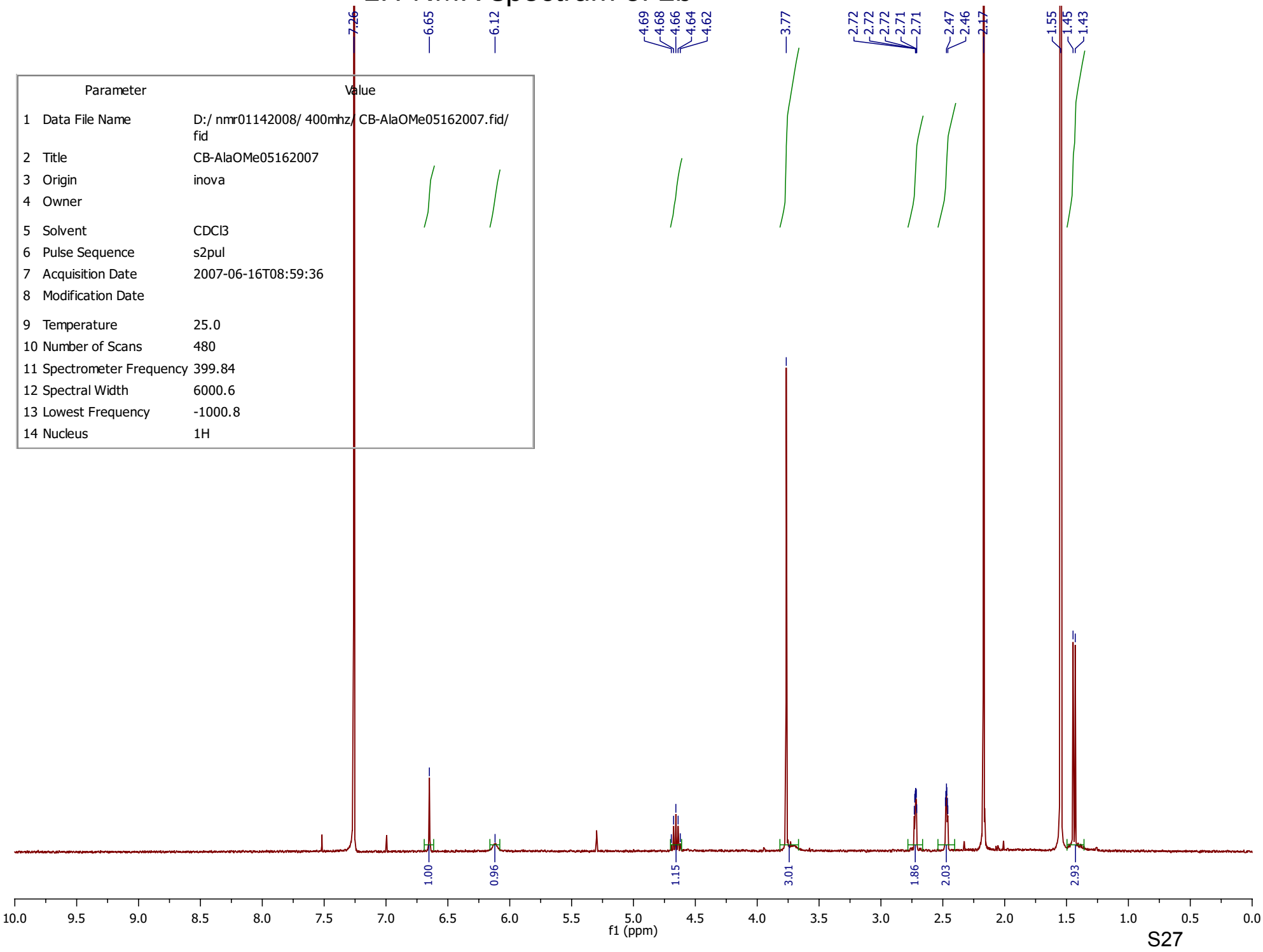
(21) Occhipinti, G.; Bjorsvik, H. R.; Jensen, V. R. *J. Am. Chem. Soc.* **2006**, 128, 6952-6964.

(22) Fomine, S.; Tlenkopatchev, M. A. *Organometallics* **2007**, 26, 4491-4497.

(23) Cabeza, J. A.; Del Rio, I.; Miguel, D.; Perez-Carreno, E.; Sanchez-Vega, M. G. *Dalton Trans.* **2008**, 1937-42.

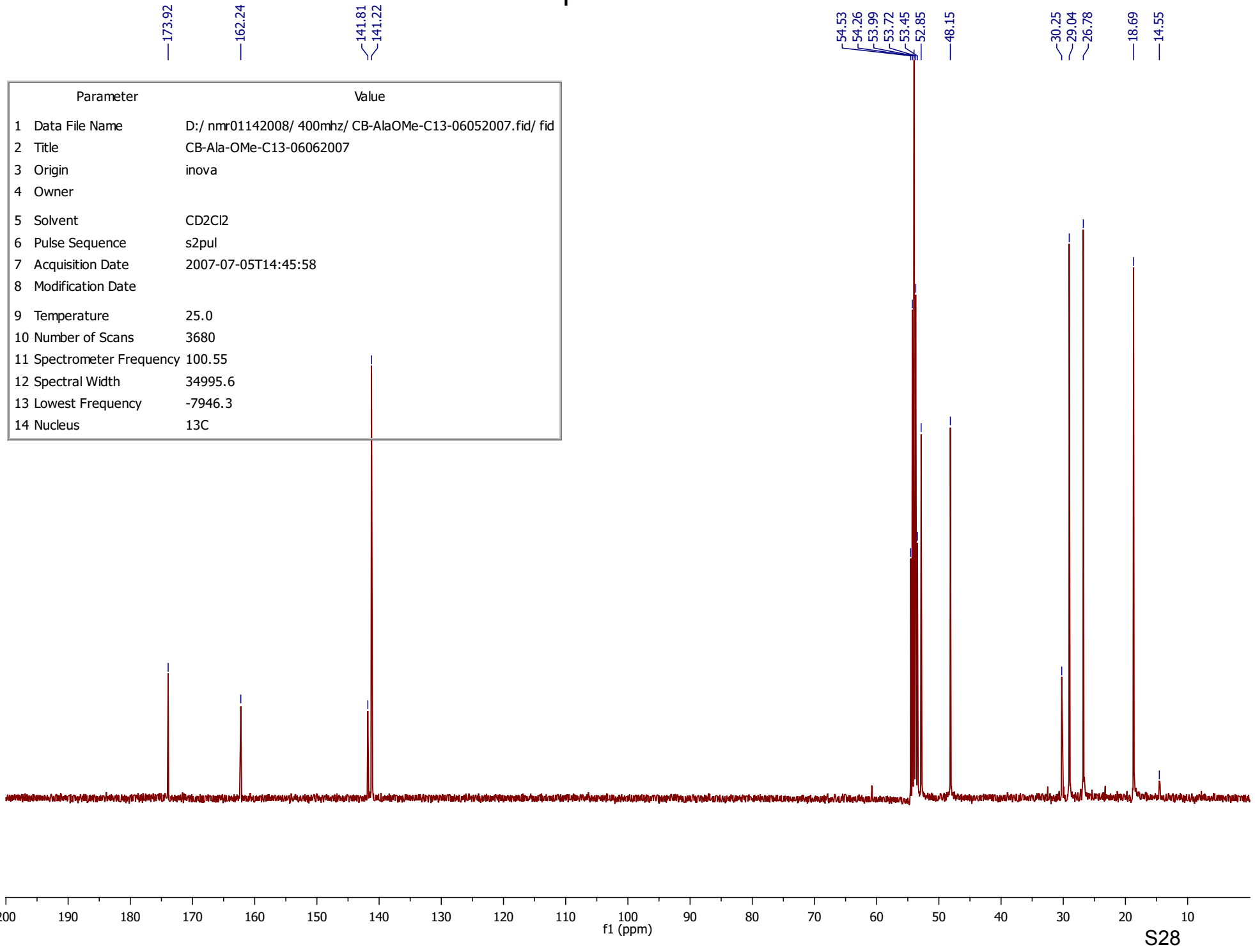
(24) Wang, D.; Wurst, K.; Knolle, W.; Decker, U.; Prager, L.; Naumov, S.; Buchmeiser, M. R. *Angew. Chem. Int. Ed.* **2008**, 47, 3267-3270.

1H-NMR spectrum of 2b



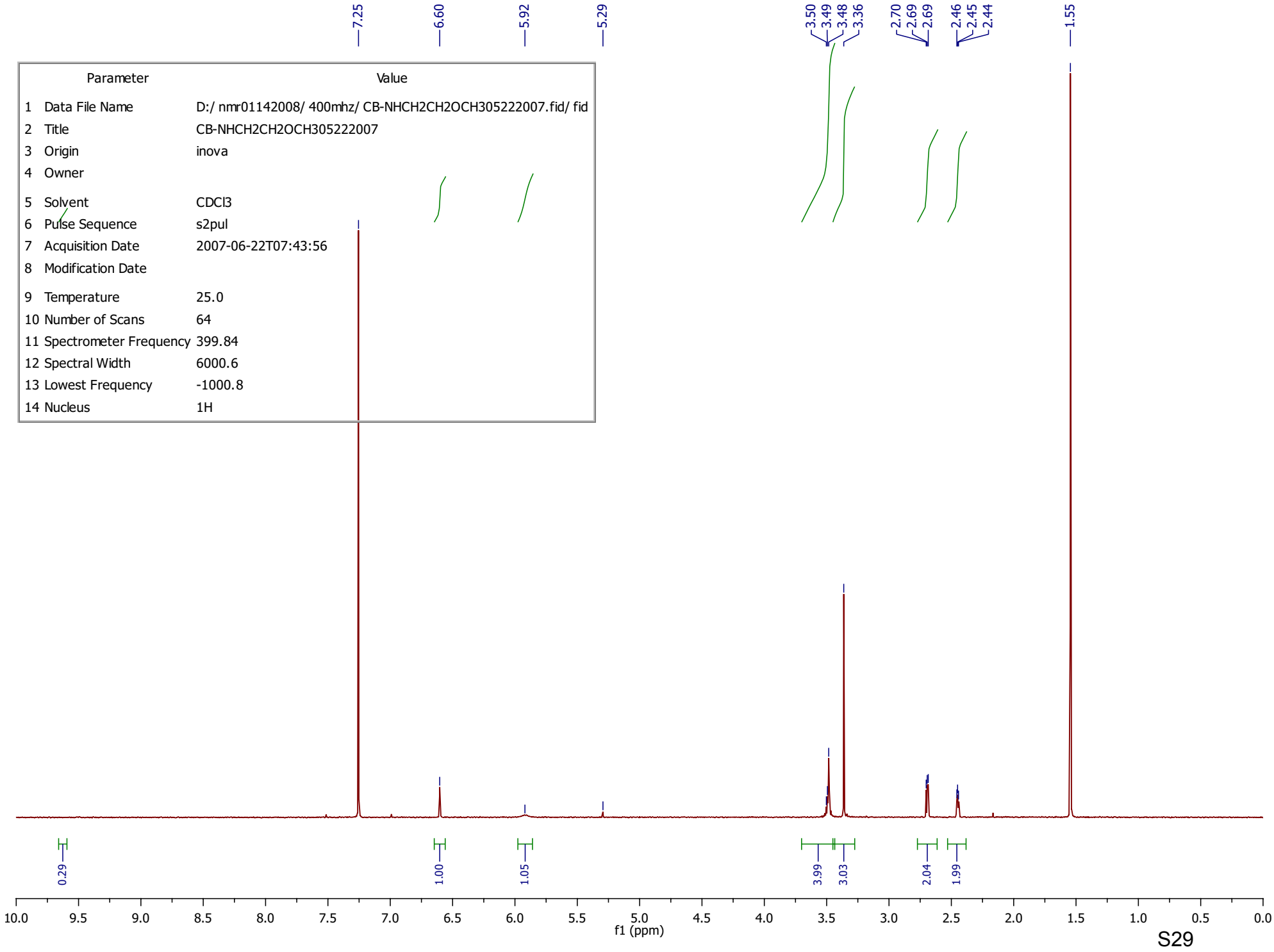
Parameter		Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-AlaOMe05162007.fid/ fid
2	Title	CB-AlaOMe05162007
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-06-16T08:59:36
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	480
11	Spectrometer Frequency	399.84
12	Spectral Width	6000.6
13	Lowest Frequency	-1000.8
14	Nucleus	1H

13C-NMR spectrum of 2b



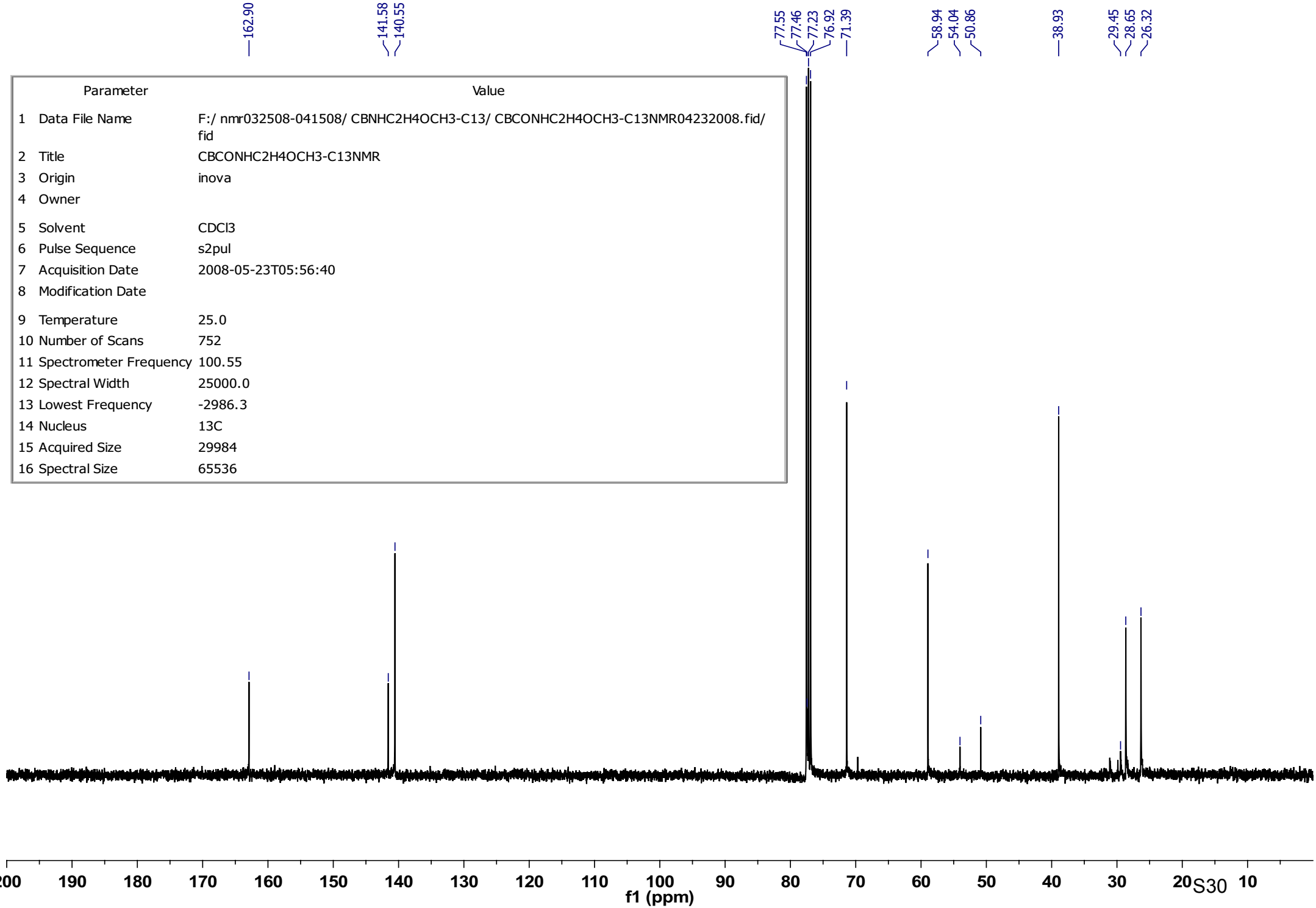
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-AlaOMe-C13-06052007.fid/ fid
2	Title	CB-Ala-OMe-C13-06062007
3	Origin	inova
4	Owner	
5	Solvent	CD2Cl2
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-07-05T14:45:58
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	3680
11	Spectrometer Frequency	100.55
12	Spectral Width	34995.6
13	Lowest Frequency	-7946.3
14	Nucleus	13C

1H-NMR spectrum of 2c



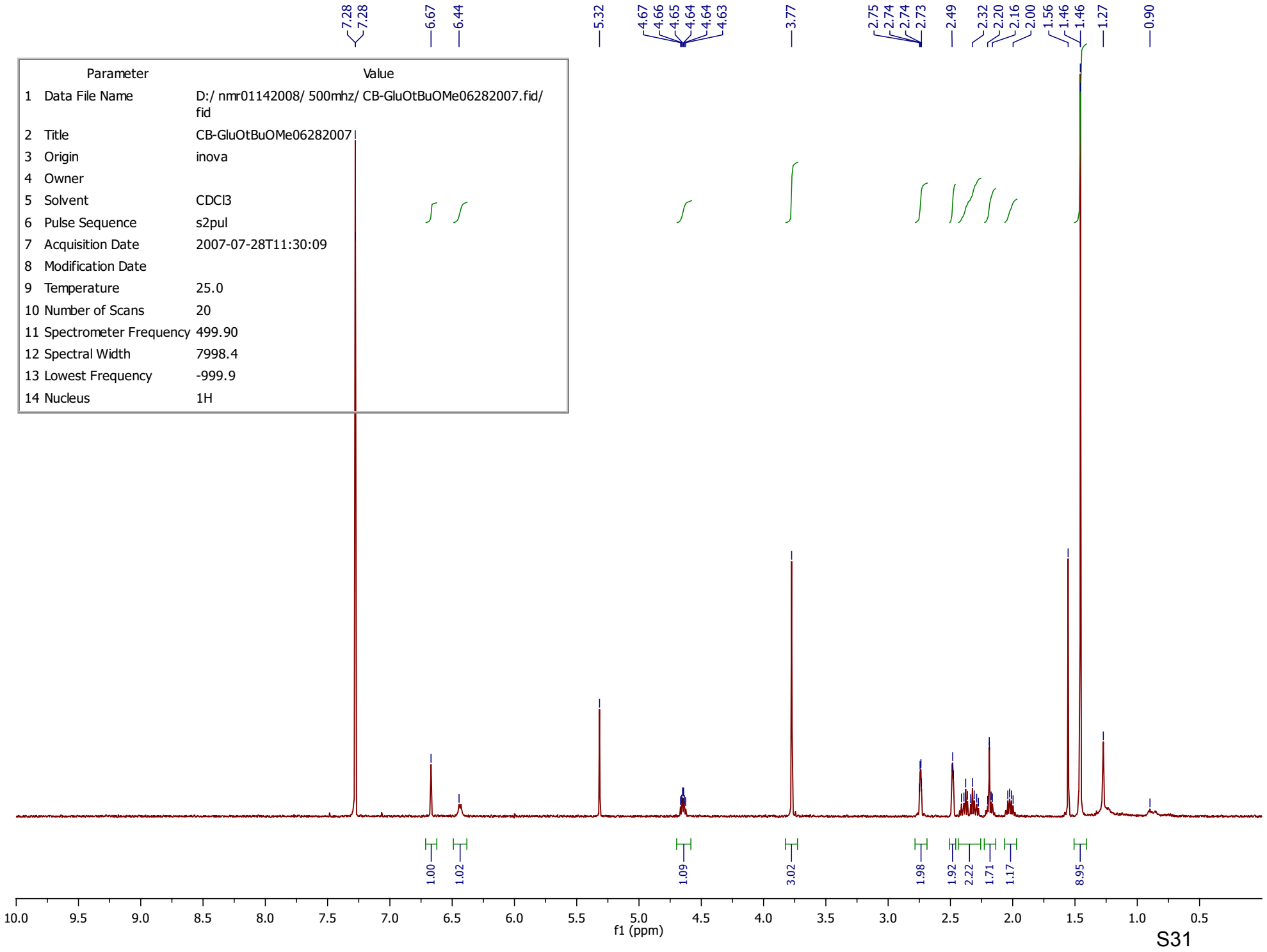
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-NHCH2CH2OCH305222007.fid/ fid
2	Title	CB-NHCH2CH2OCH305222007
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-06-22T07:43:56
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	64
11	Spectrometer Frequency	399.84
12	Spectral Width	6000.6
13	Lowest Frequency	-1000.8
14	Nucleus	1H

13C-NMR spectrum of 2c



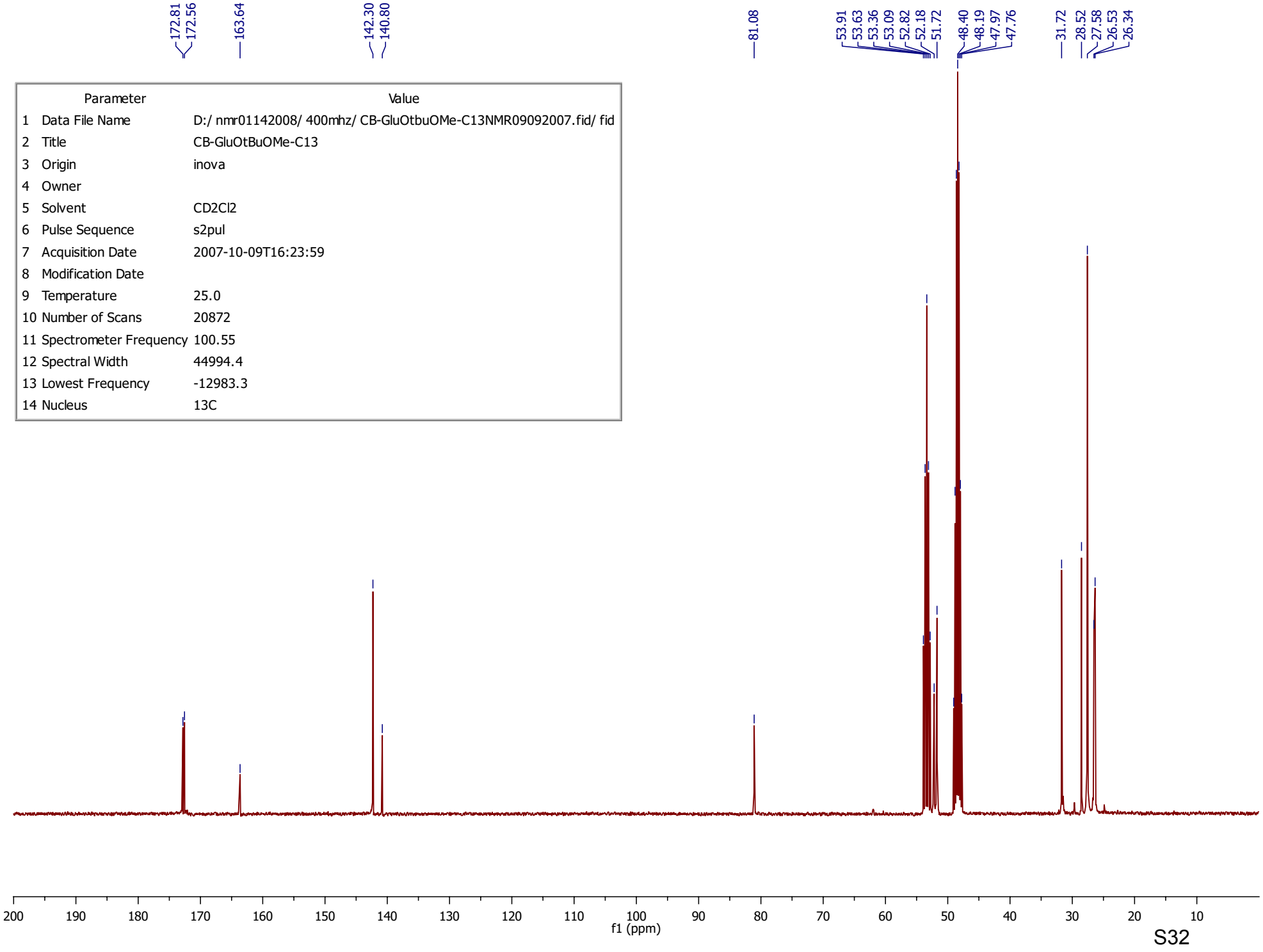
	Parameter	Value
1	Data File Name	F:/ nmr032508-041508/ CBNHC2H4OCH3-C13/ CBCONHC2H4OCH3-C13NMR04232008.fid/ fid
2	Title	CBCONHC2H4OCH3-C13NMR
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2008-05-23T05:56:40
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	752
11	Spectrometer Frequency	100.55
12	Spectral Width	25000.0
13	Lowest Frequency	-2986.3
14	Nucleus	13C
15	Acquired Size	29984
16	Spectral Size	65536

1H-NMR spectrum of 2d



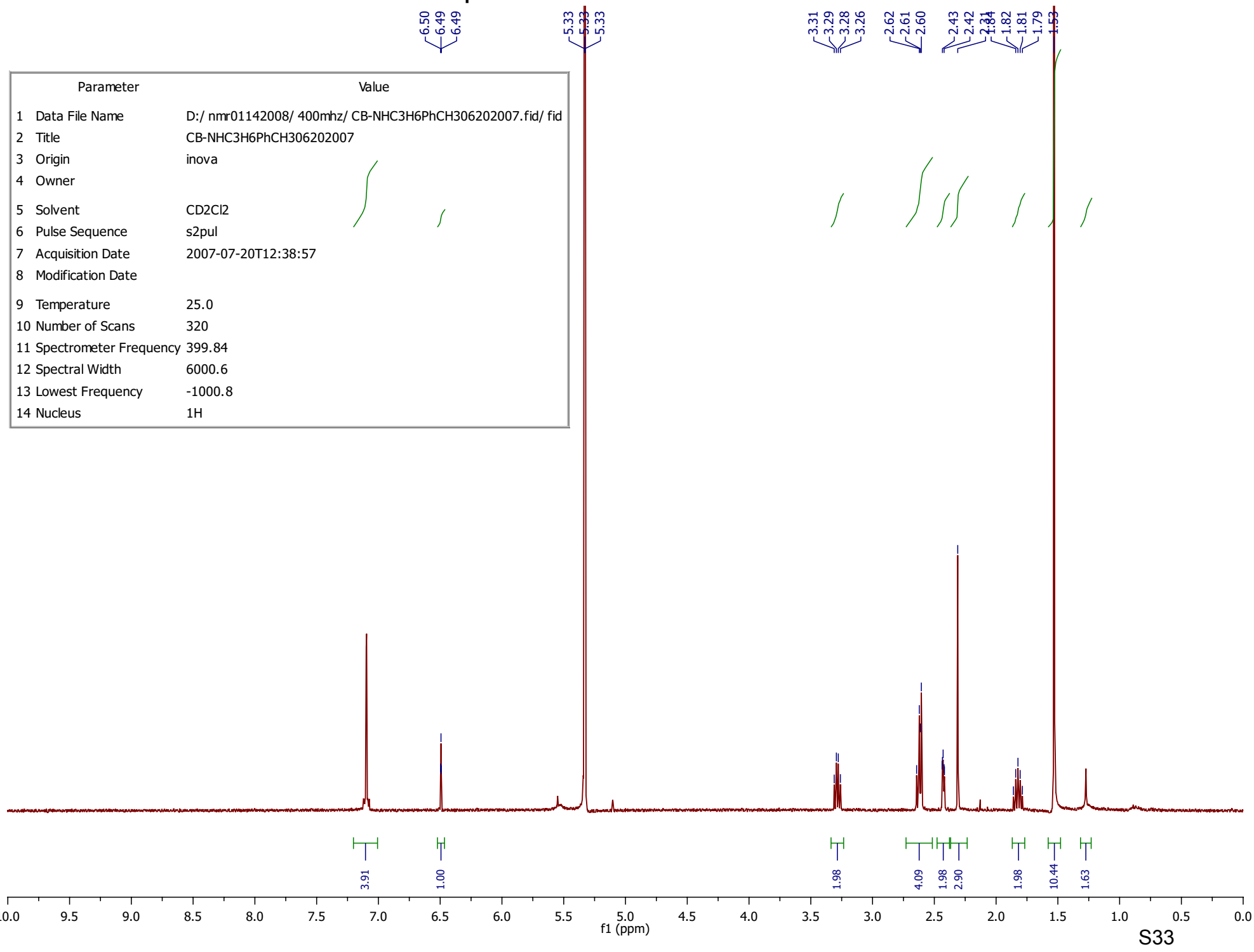
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 500mhz/ CB-GluOtBuOMe06282007.fid/ fid
2	Title	CB-GluOtBuOMe06282007
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-07-28T11:30:09
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	20
11	Spectrometer Frequency	499.90
12	Spectral Width	7998.4
13	Lowest Frequency	-999.9
14	Nucleus	1H

13C-NMR spectrum of 2d



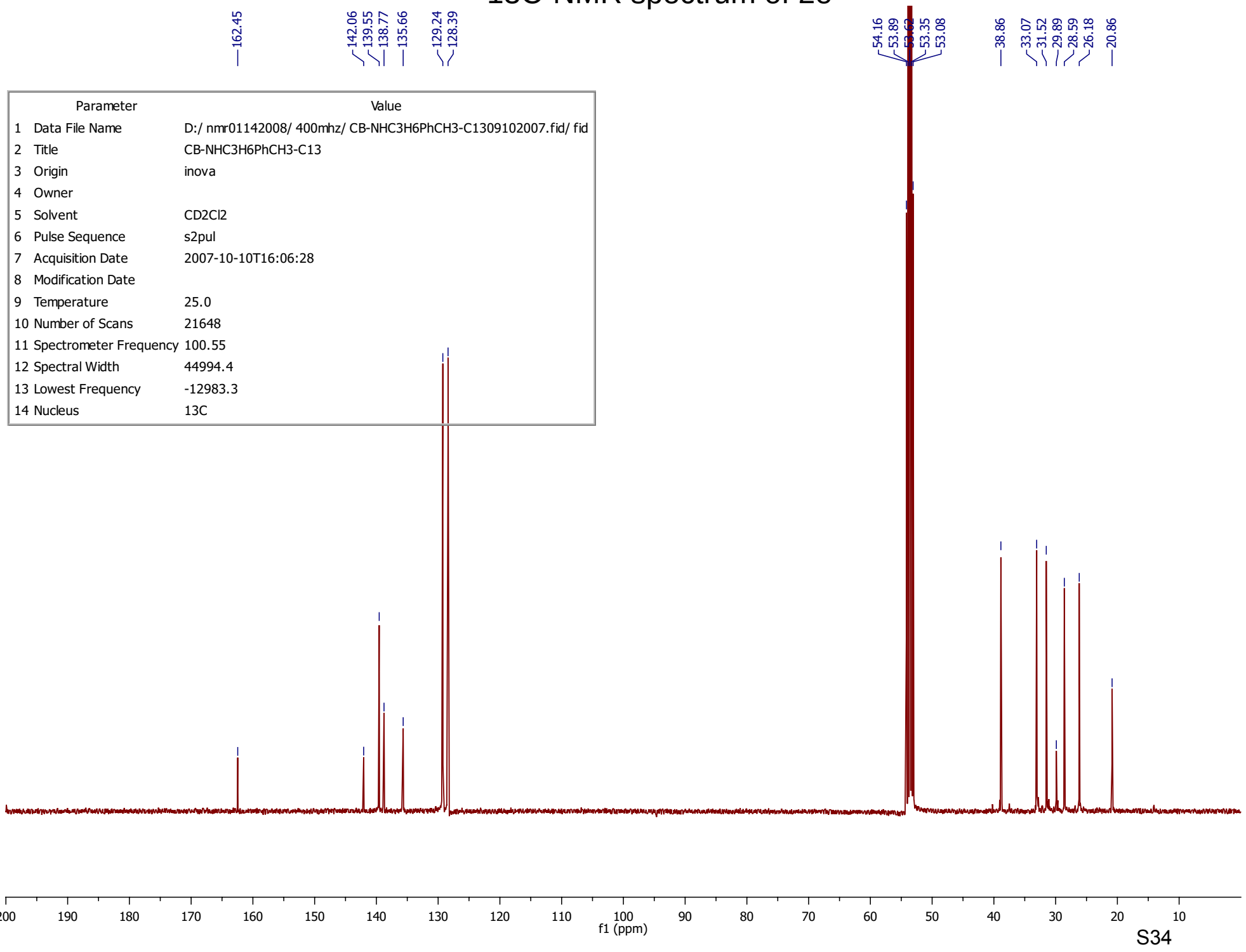
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-GluOtbuOMe-C13NMR09092007.fid/ fid
2	Title	CB-GluOtBuOMe-C13
3	Origin	inova
4	Owner	
5	Solvent	CD2Cl2
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-10-09T16:23:59
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	20872
11	Spectrometer Frequency	100.55
12	Spectral Width	44994.4
13	Lowest Frequency	-12983.3
14	Nucleus	13C

1H-NMR spectrum of 2e



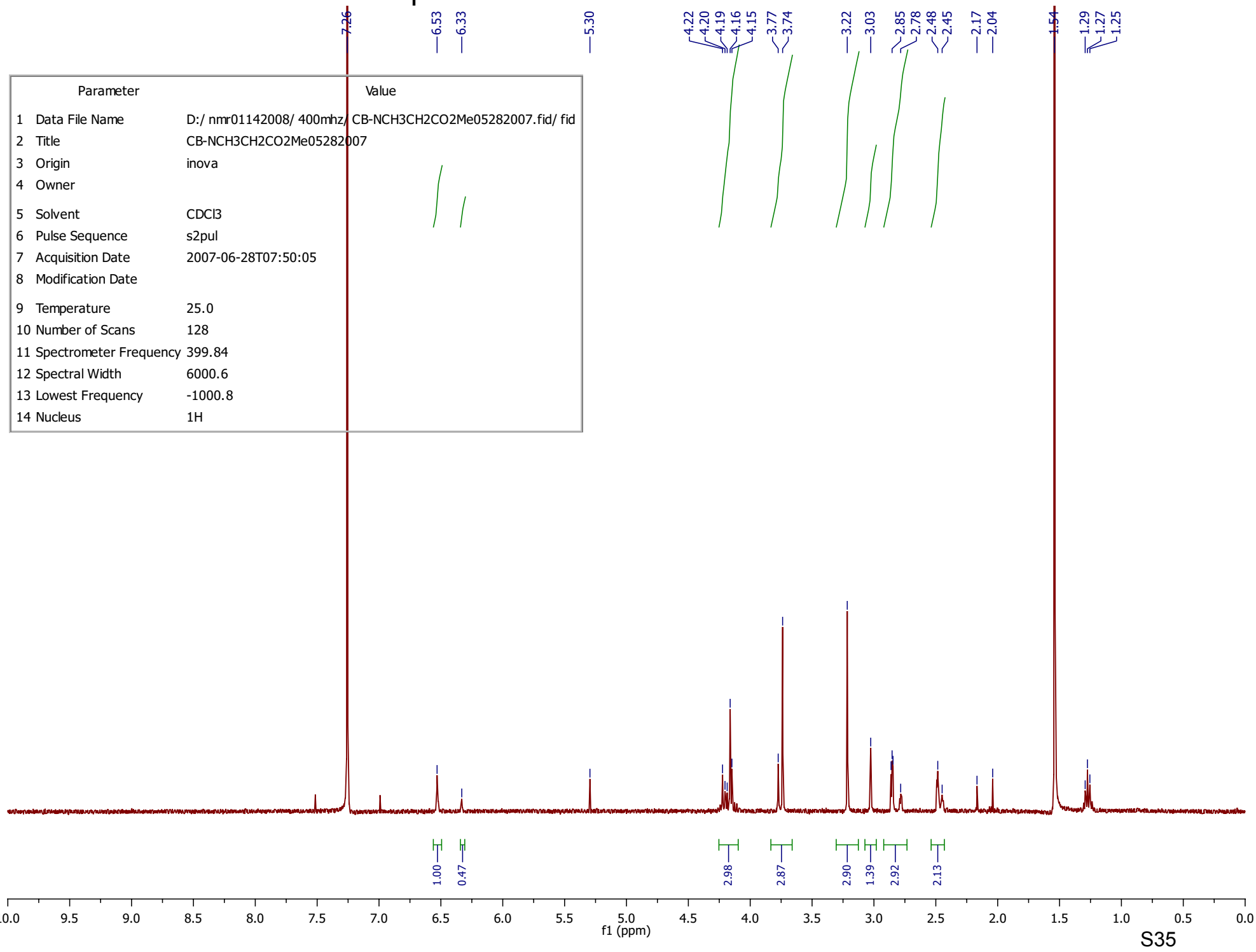
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-NHC3H6PhCH306202007.fid/ fid
2	Title	CB-NHC3H6PhCH306202007
3	Origin	inova
4	Owner	
5	Solvent	CD2Cl2
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-07-20T12:38:57
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	320
11	Spectrometer Frequency	399.84
12	Spectral Width	6000.6
13	Lowest Frequency	-1000.8
14	Nucleus	1H

13C-NMR spectrum of 2e



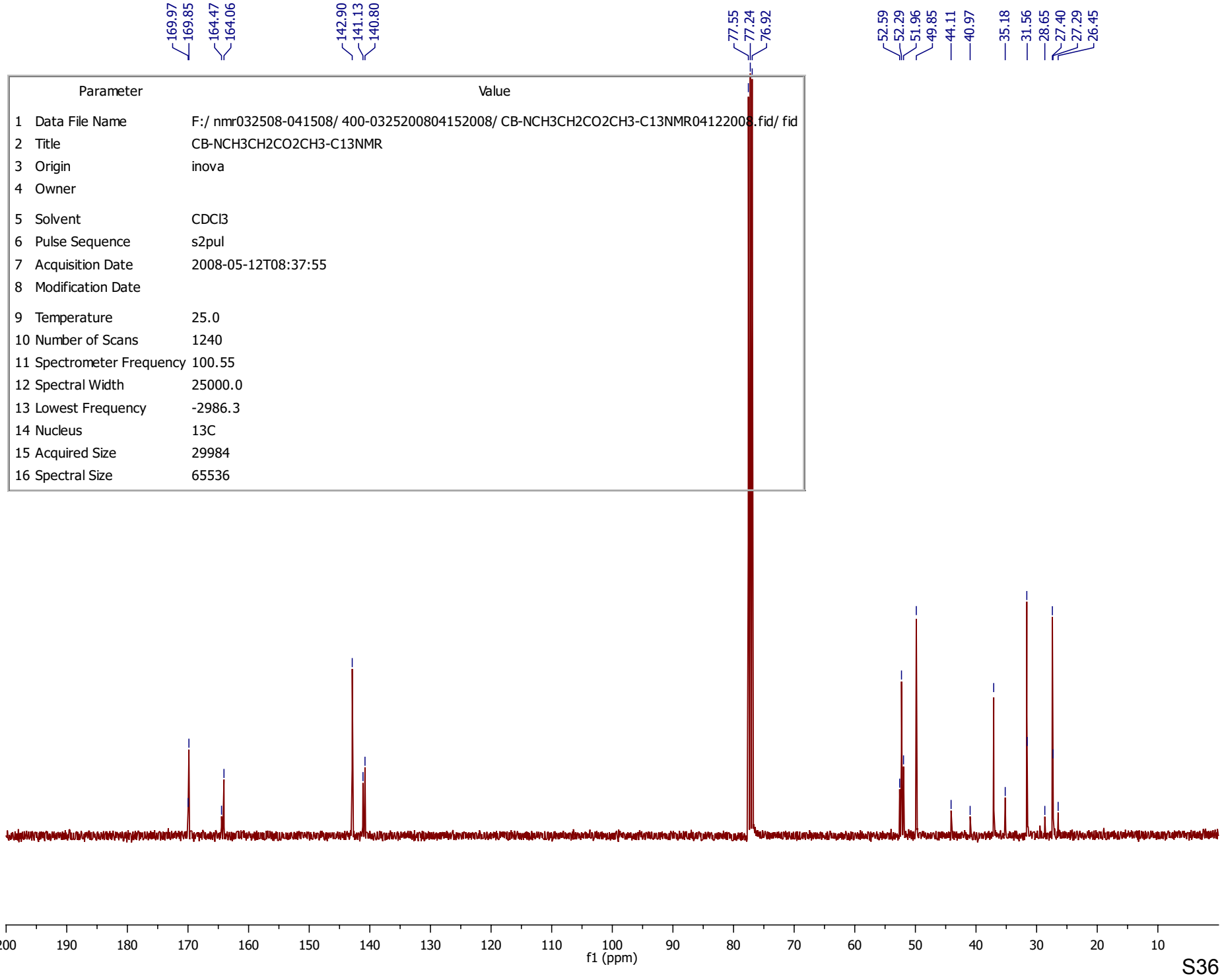
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-NHC3H6PhCH3-C1309102007.fid/ fid
2	Title	CB-NHC3H6PhCH3-C13
3	Origin	inova
4	Owner	
5	Solvent	CD2Cl2
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-10-10T16:06:28
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	21648
11	Spectrometer Frequency	100.55
12	Spectral Width	44994.4
13	Lowest Frequency	-12983.3
14	Nucleus	13C

1H-NMR spectrum of 3a



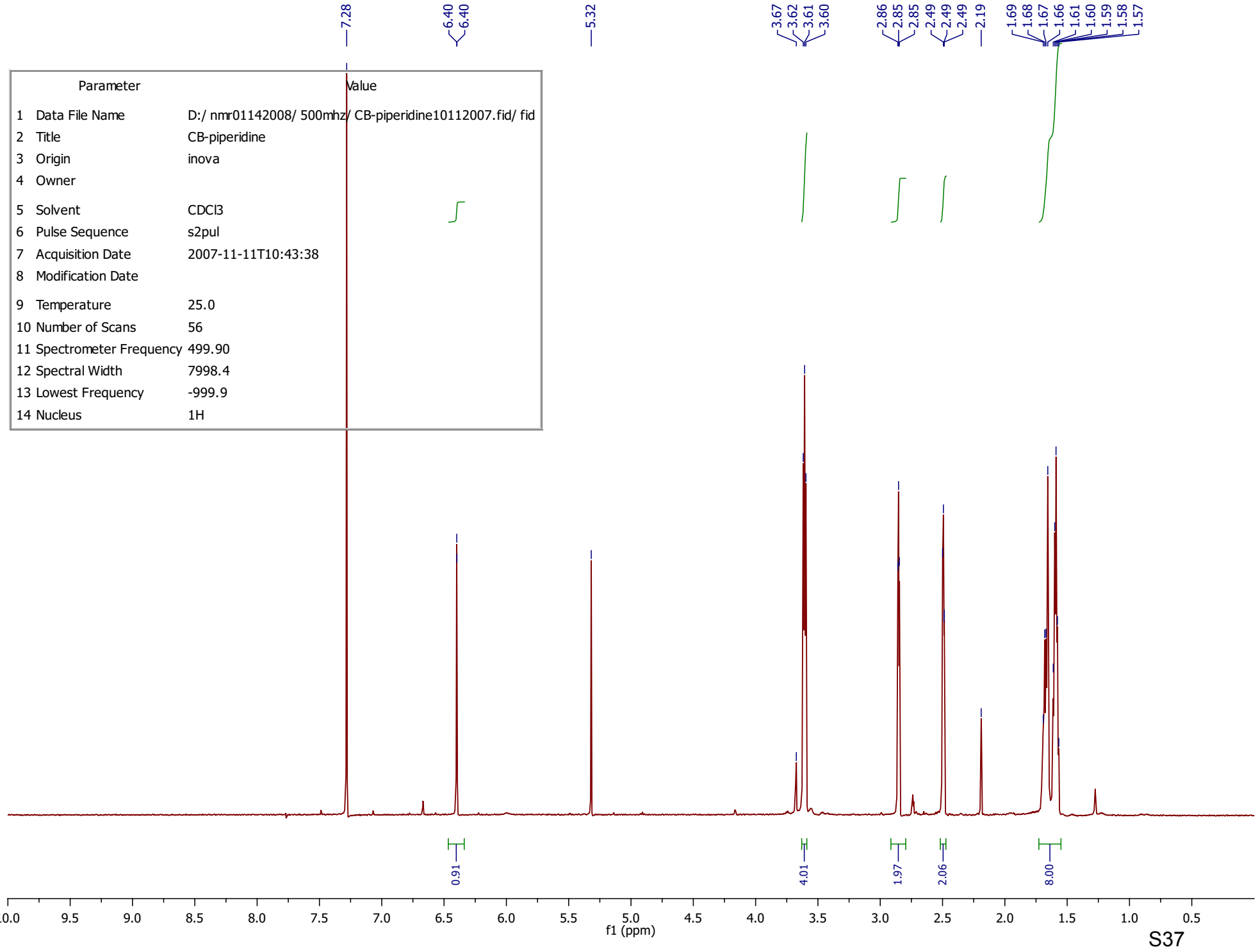
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CB-NCH3CH2CO2Me05282007.fid/ fid
2	Title	CB-NCH3CH2CO2Me05282007
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-06-28T07:50:05
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	128
11	Spectrometer Frequency	399.84
12	Spectral Width	6000.6
13	Lowest Frequency	-1000.8
14	Nucleus	1H

13C-NMR spectrum of 3a



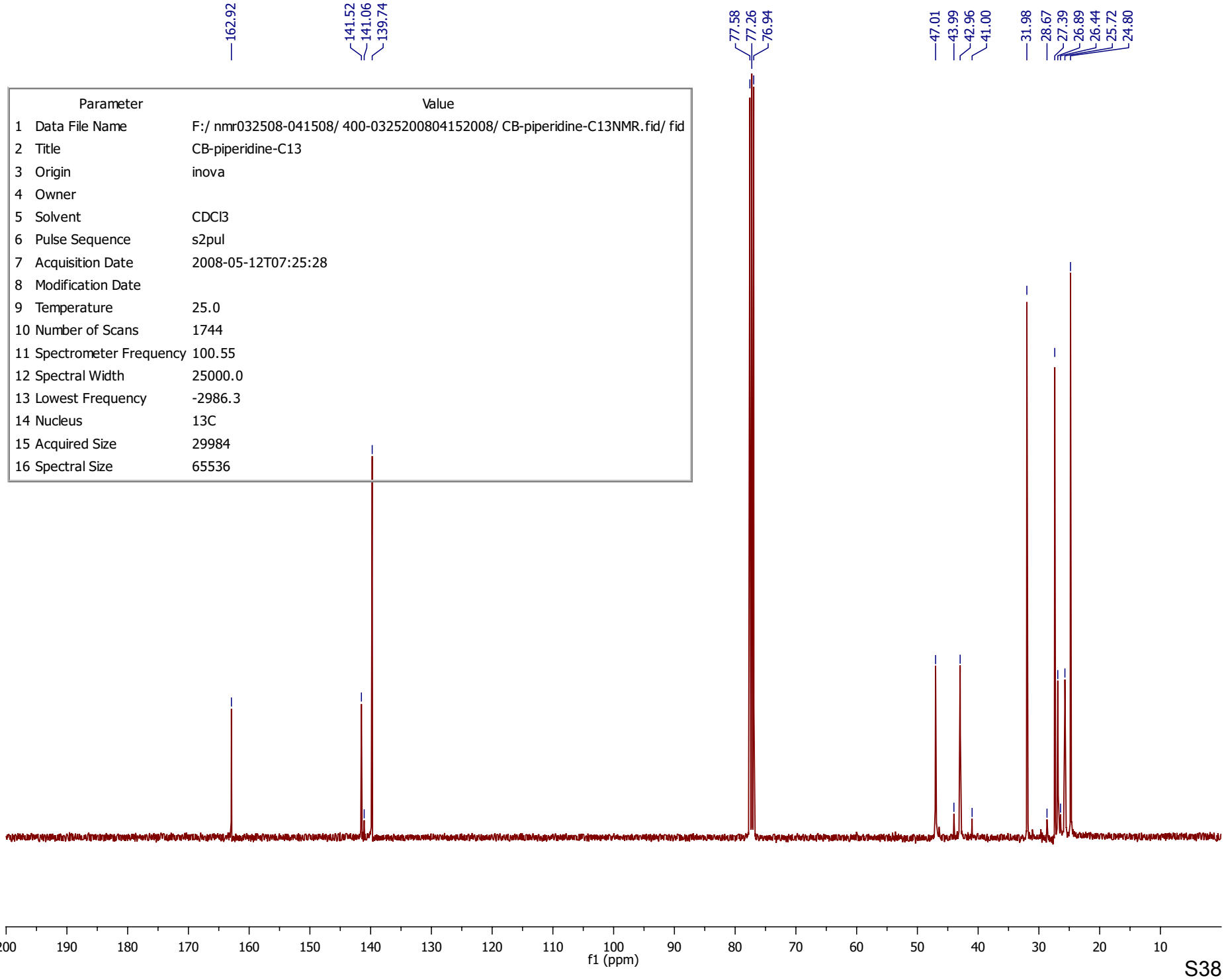
	Parameter	Value
1	Data File Name	F:/ nmr032508-041508/ 400-0325200804152008/ CB-NCH3CH2CO2CH3-C13NMR04122008.fid/ fid
2	Title	CB-NCH3CH2CO2CH3-C13NMR
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2008-05-12T08:37:55
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	1240
11	Spectrometer Frequency	100.55
12	Spectral Width	25000.0
13	Lowest Frequency	-2986.3
14	Nucleus	13C
15	Acquired Size	29984
16	Spectral Size	65536

1H-NMR spectrum of 3b



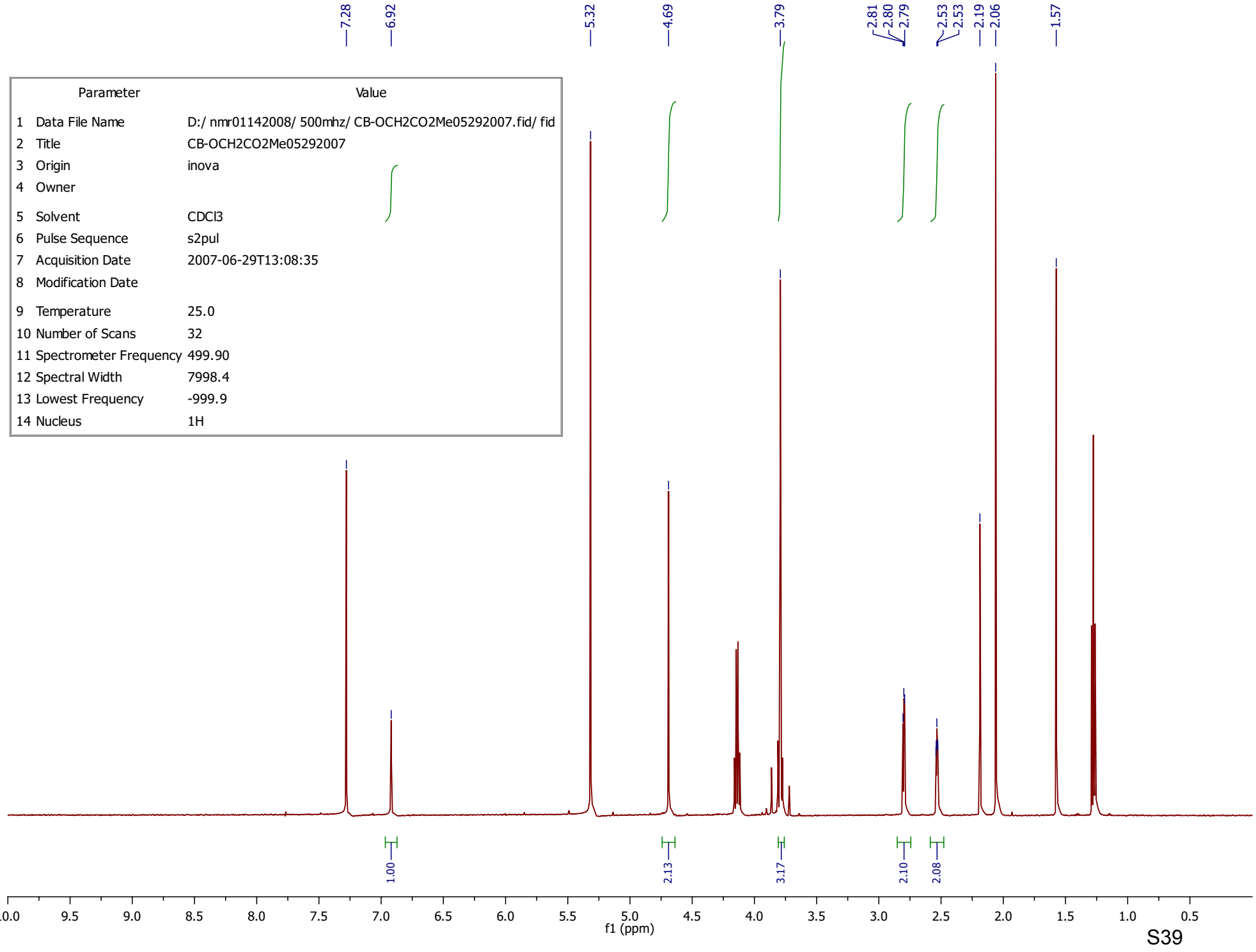
	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 500mhz/ CB-piperidine10112007.fid/ fid
2	Title	CB-piperidine
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-11-11T10:43:38
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	56
11	Spectrometer Frequency	499.90
12	Spectral Width	7998.4
13	Lowest Frequency	-999.9
14	Nucleus	1H

13C-NMR spectrum of 3b



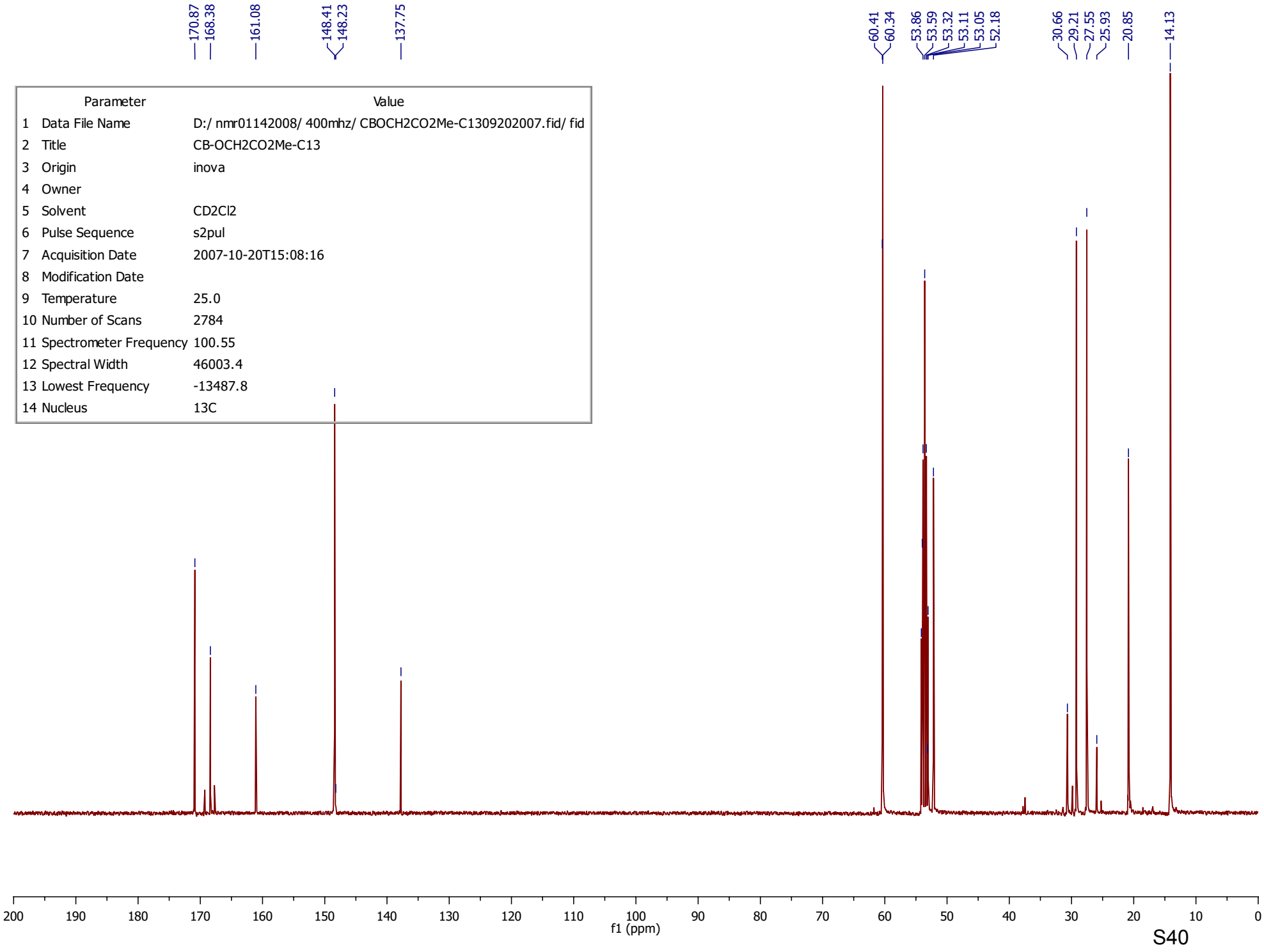
	Parameter	Value
1	Data File Name	F:/ nmr032508-041508/ 400-0325200804152008/ CB-piperidine-C13NMR.fid/ fid
2	Title	CB-piperidine-C13
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2008-05-12T07:25:28
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	1744
11	Spectrometer Frequency	100.55
12	Spectral Width	25000.0
13	Lowest Frequency	-2986.3
14	Nucleus	13C
15	Acquired Size	29984
16	Spectral Size	65536

1H-NMR spectrum of 4b



	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 500mhz/ CB-OCH2CO2Me05292007.fid/ fid
2	Title	CB-OCH2CO2Me05292007
3	Origin	inova
4	Owner	
5	Solvent	CDCl3
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-06-29T13:08:35
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	32
11	Spectrometer Frequency	499.90
12	Spectral Width	7998.4
13	Lowest Frequency	-999.9
14	Nucleus	1H

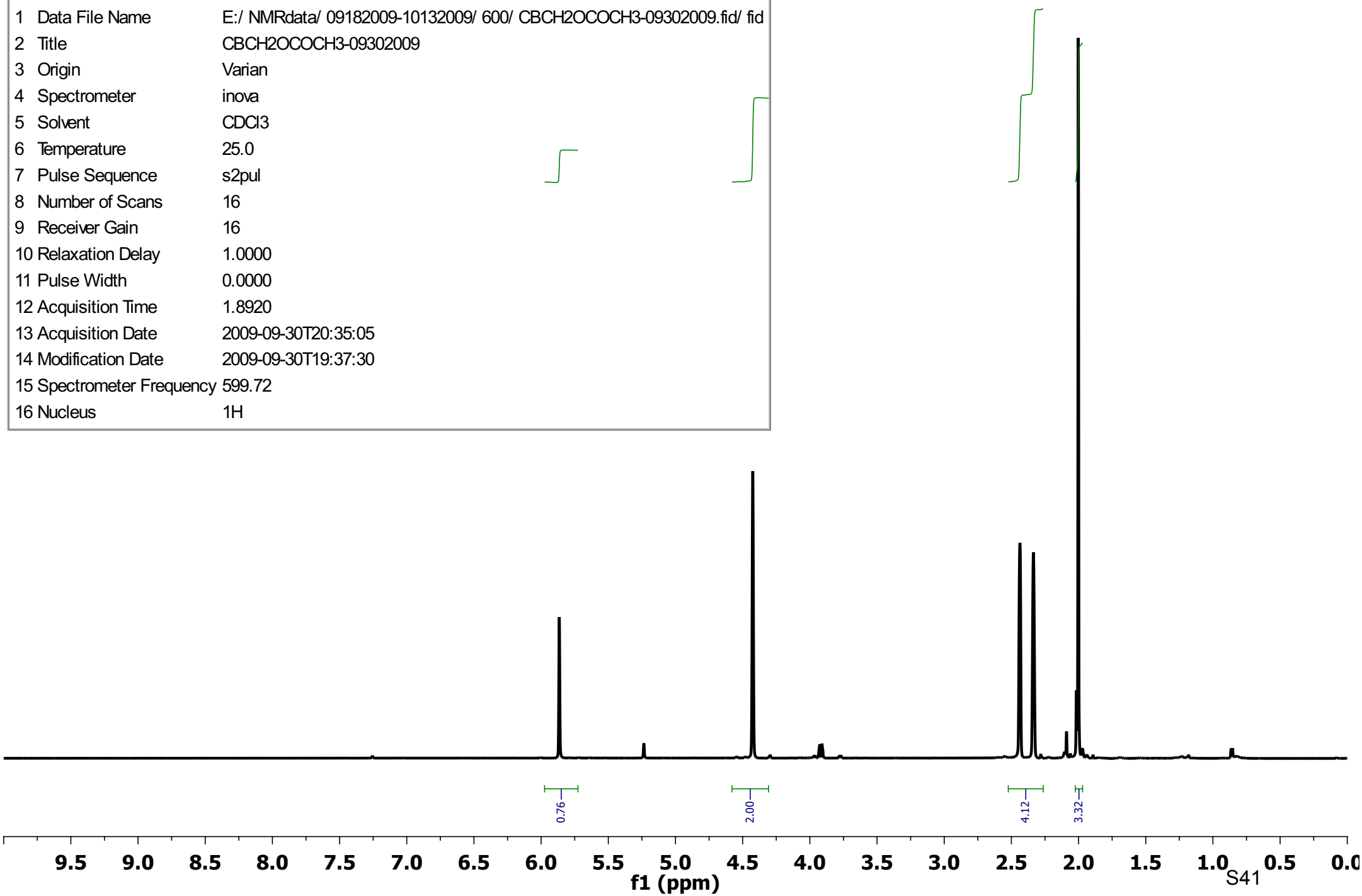
13C-NMR spectrum of 4b



	Parameter	Value
1	Data File Name	D:/ nmr01142008/ 400mhz/ CBOCH2CO2Me-C1309202007.fid/ fid
2	Title	CB-OCH2CO2Me-C13
3	Origin	inova
4	Owner	
5	Solvent	CD2Cl2
6	Pulse Sequence	s2pul
7	Acquisition Date	2007-10-20T15:08:16
8	Modification Date	
9	Temperature	25.0
10	Number of Scans	2784
11	Spectrometer Frequency	100.55
12	Spectral Width	46003.4
13	Lowest Frequency	-13487.8
14	Nucleus	13C

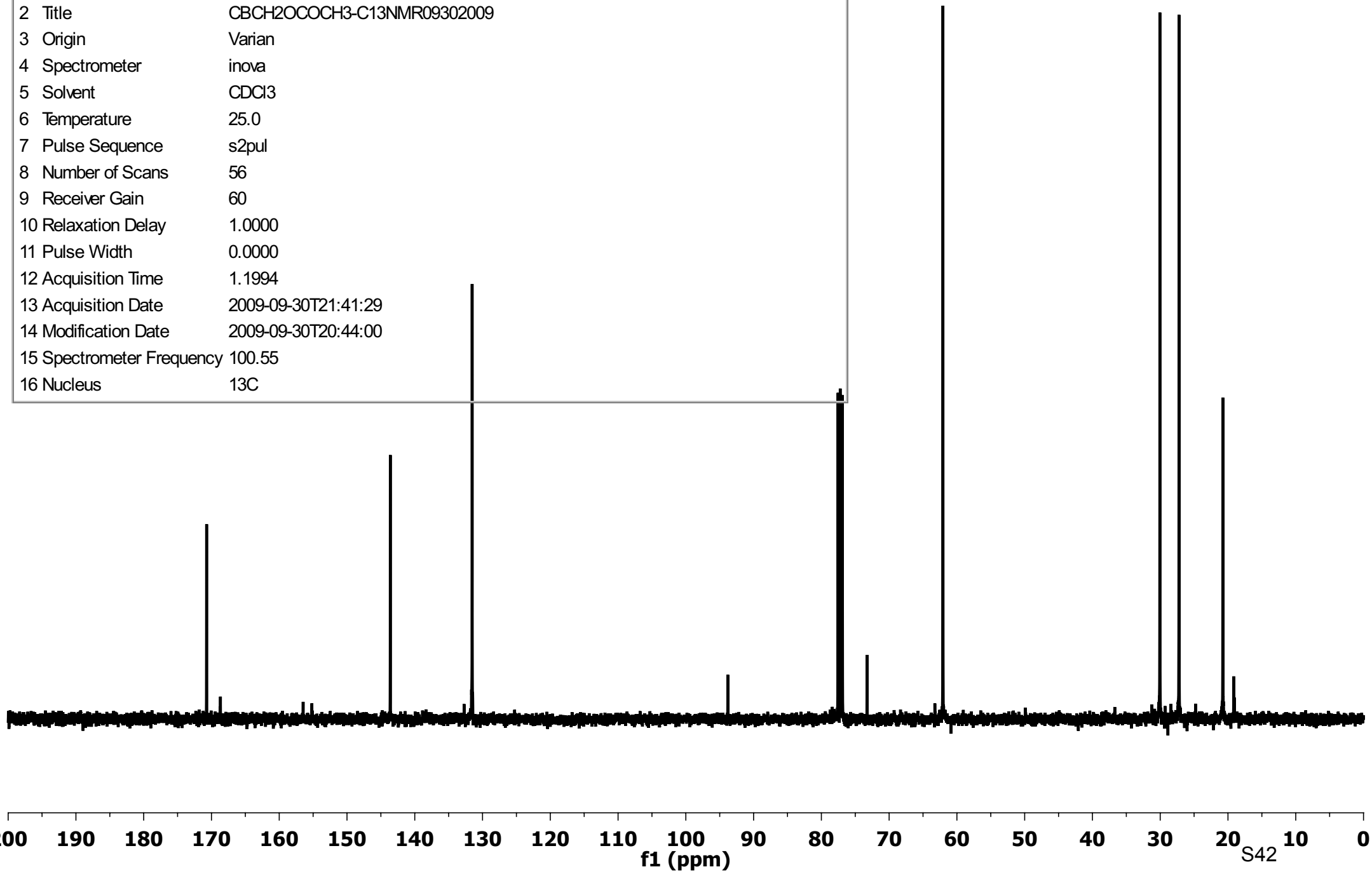
1H-NMR spectrum of 5a

Parameter	Value
1 Data File Name	E:/ NMRdata/ 09182009-10132009/ 600/ CBCH2OCOCH3-09302009.fid/ fid
2 Title	CBCH2OCOCH3-09302009
3 Origin	Varian
4 Spectrometer	inova
5 Solvent	CDCl3
6 Temperature	25.0
7 Pulse Sequence	s2pul
8 Number of Scans	16
9 Receiver Gain	16
10 Relaxation Delay	1.0000
11 Pulse Width	0.0000
12 Acquisition Time	1.8920
13 Acquisition Date	2009-09-30T20:35:05
14 Modification Date	2009-09-30T19:37:30
15 Spectrometer Frequency	599.72
16 Nucleus	1H

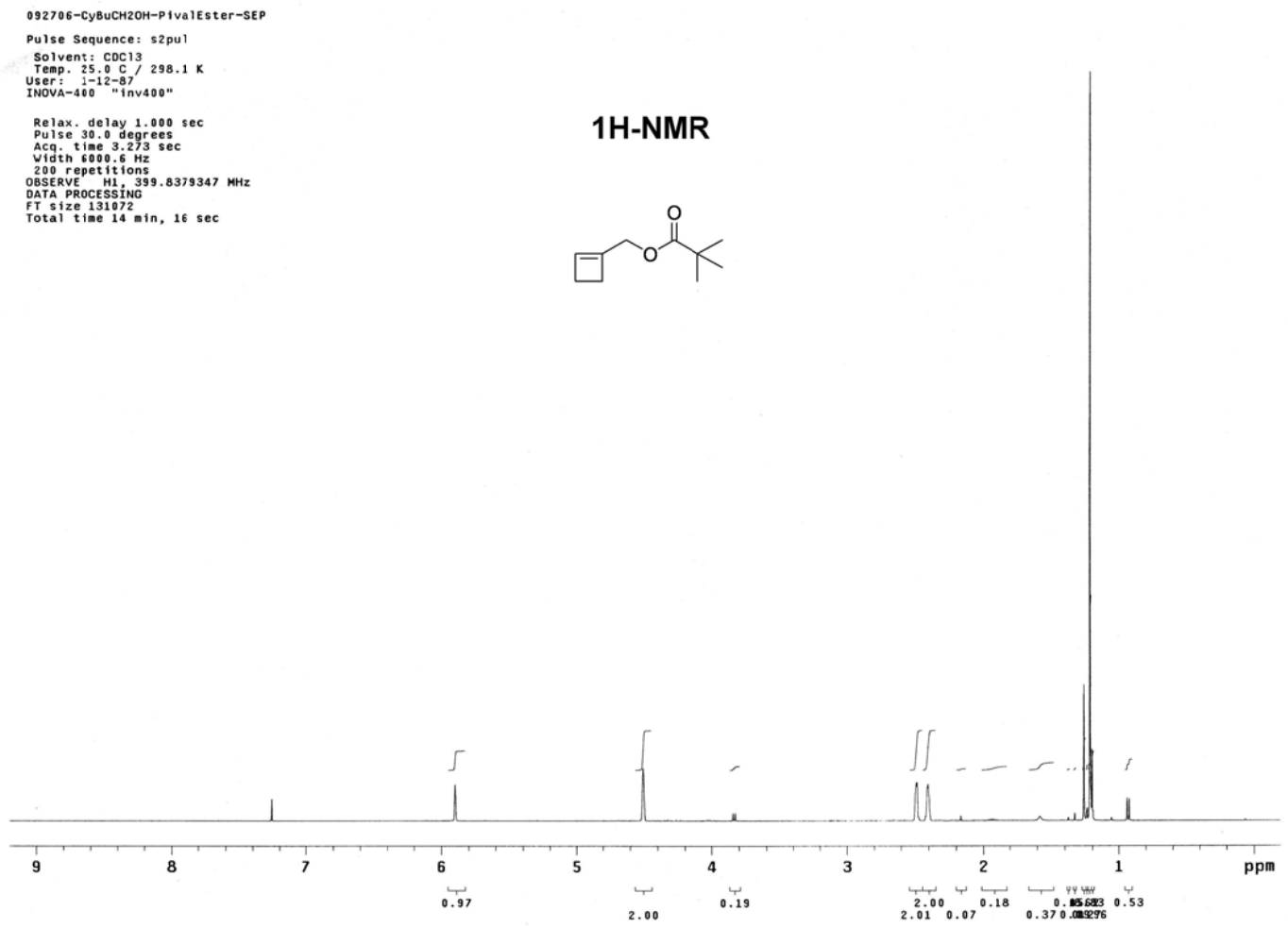


13C-NMR spectrum of 5a

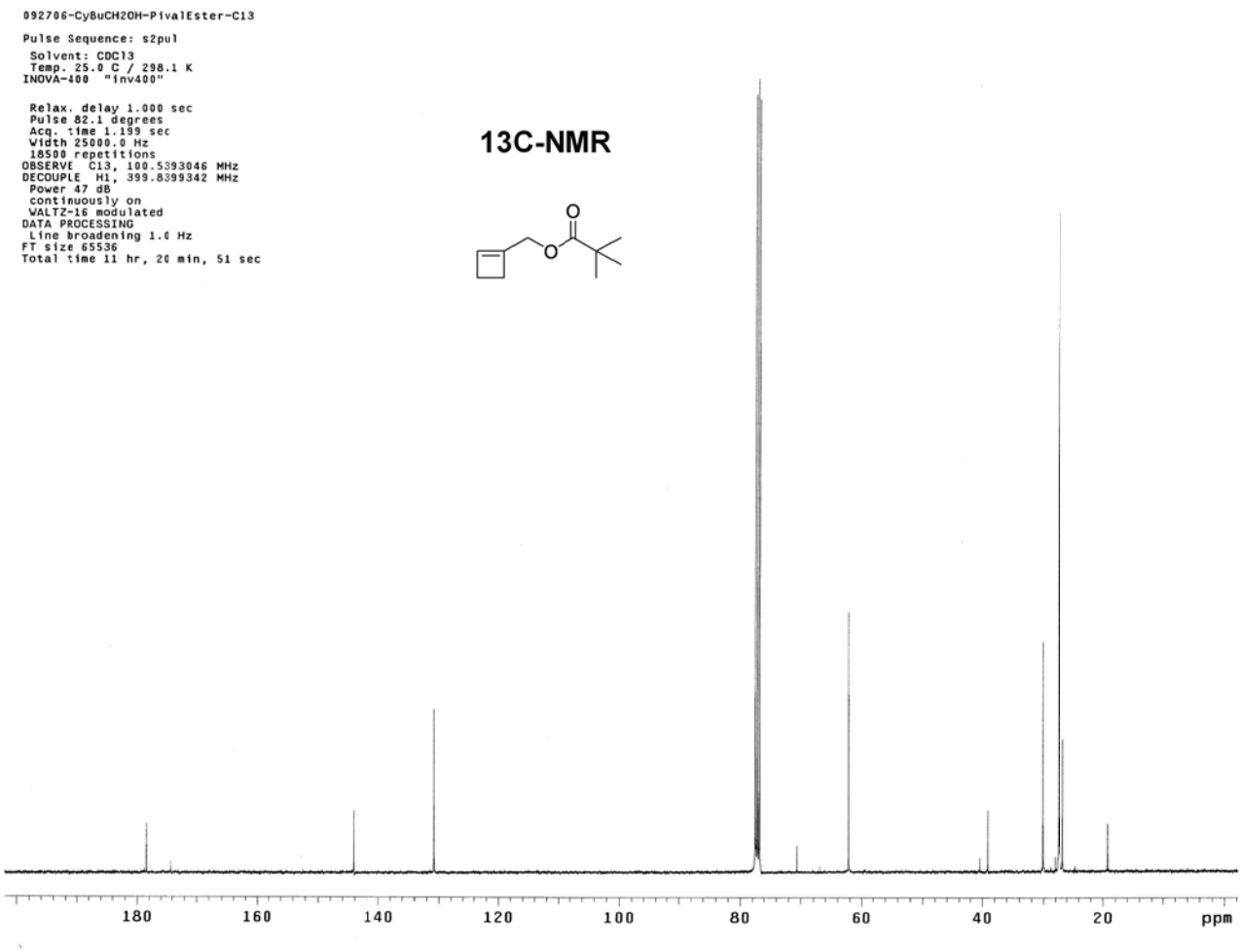
	Parameter	Value
1	Data File Name	E:/ NMRdata/ 09182009-10132009/ 400/ CBCH2OCOCH3-C13NMR09302009.fid/ fid
2	Title	CBCH2OCOCH3-C13NMR09302009
3	Origin	Varian
4	Spectrometer	inova
5	Solvent	CDCl3
6	Temperature	25.0
7	Pulse Sequence	s2pul
8	Number of Scans	56
9	Receiver Gain	60
10	Relaxation Delay	1.0000
11	Pulse Width	0.0000
12	Acquisition Time	1.1994
13	Acquisition Date	2009-09-30T21:41:29
14	Modification Date	2009-09-30T20:44:00
15	Spectrometer Frequency	100.55
16	Nucleus	13C



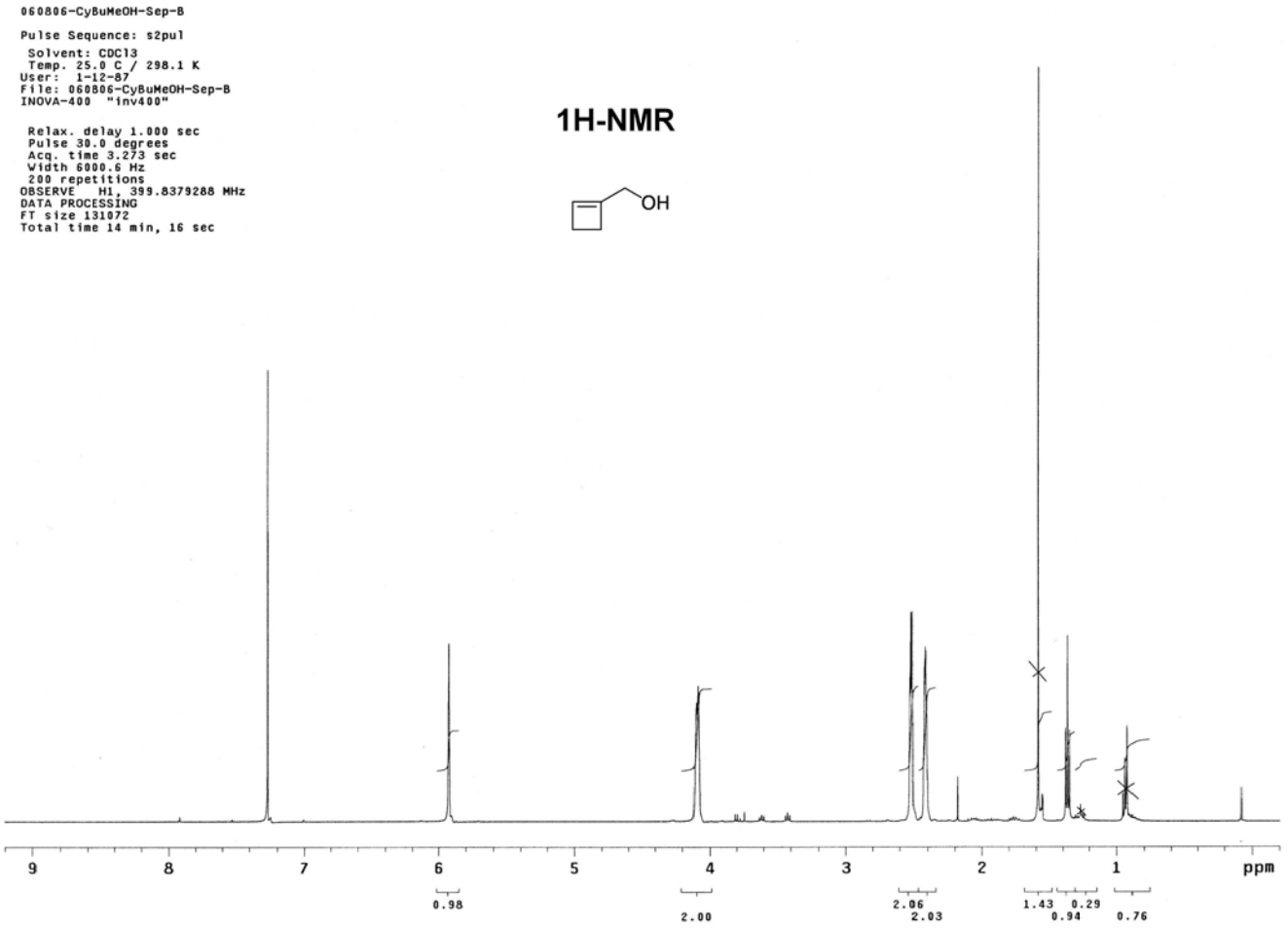
1H-NMR spectrum of 5b



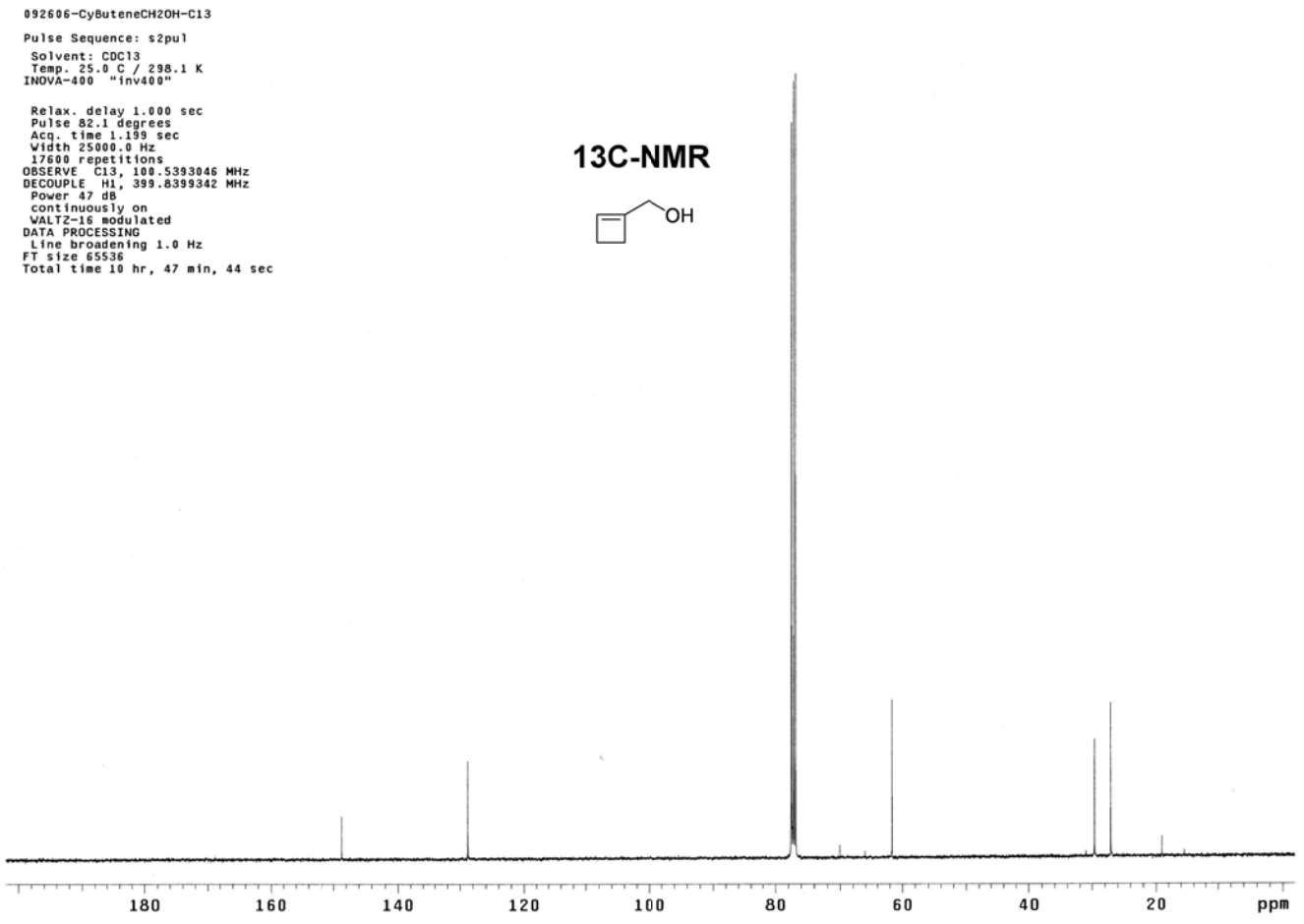
13C-NMR spectrum of 5b



1H-NMR spectrum of 7

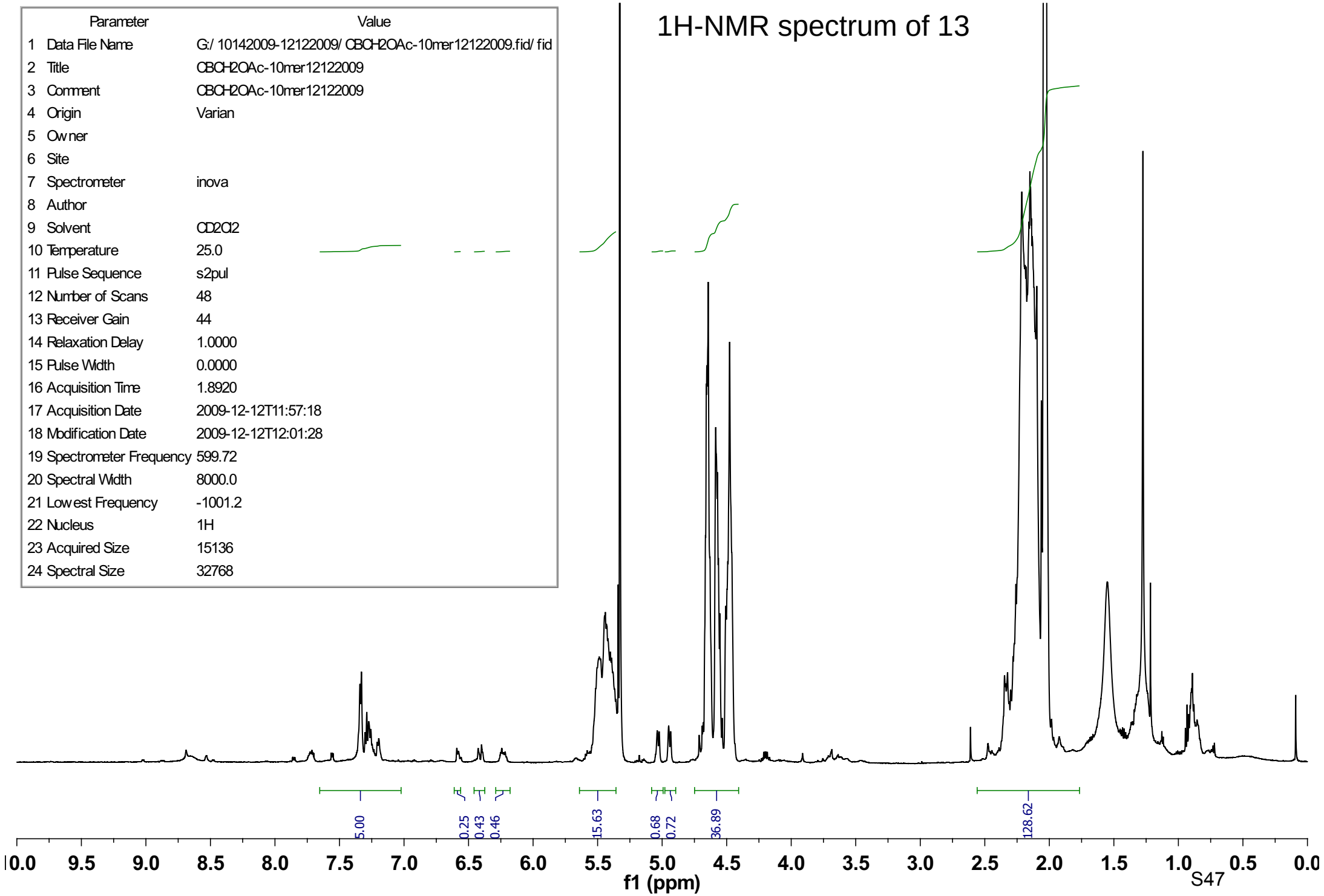


13C-NMR spectrum of 7

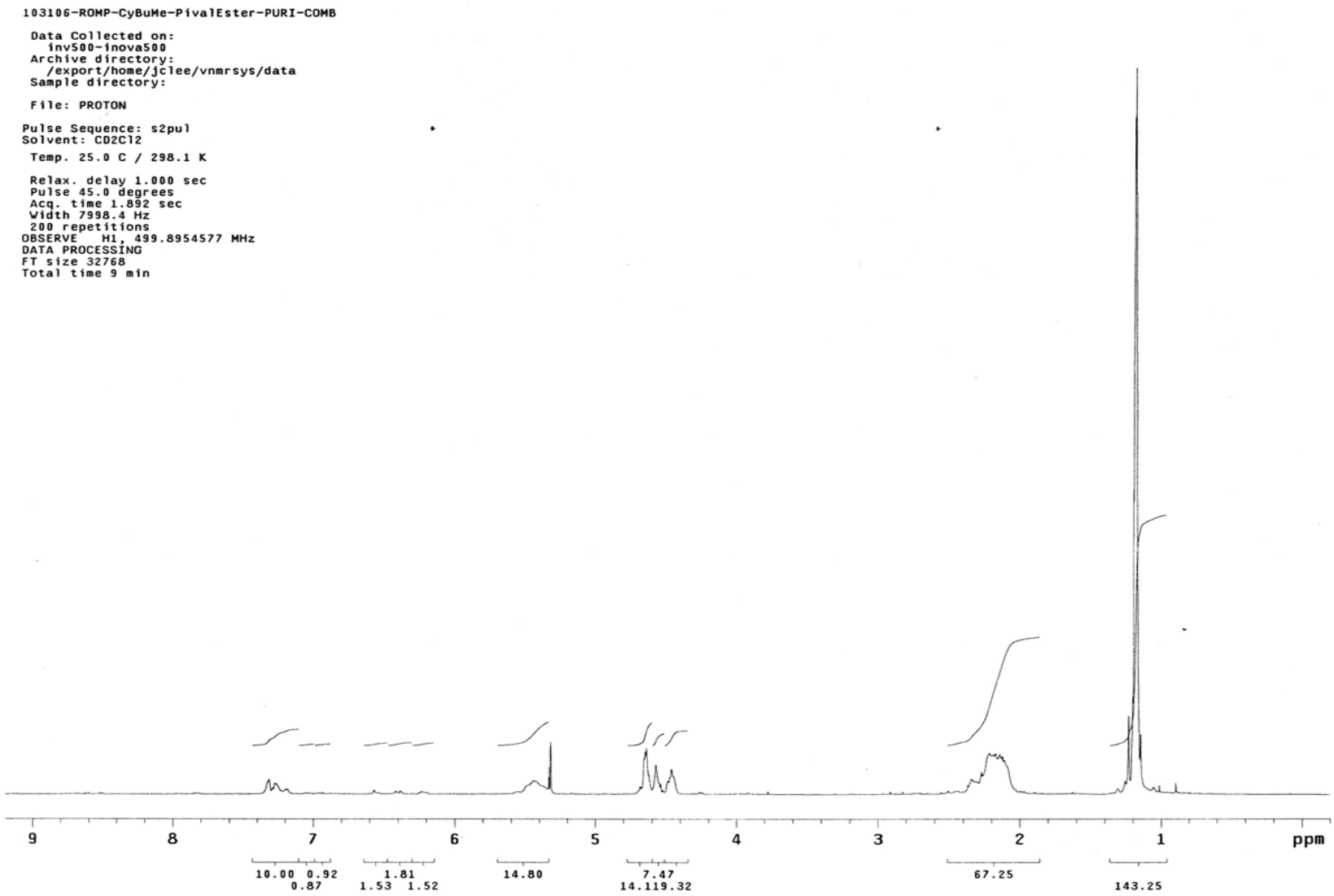


1H-NMR spectrum of 13

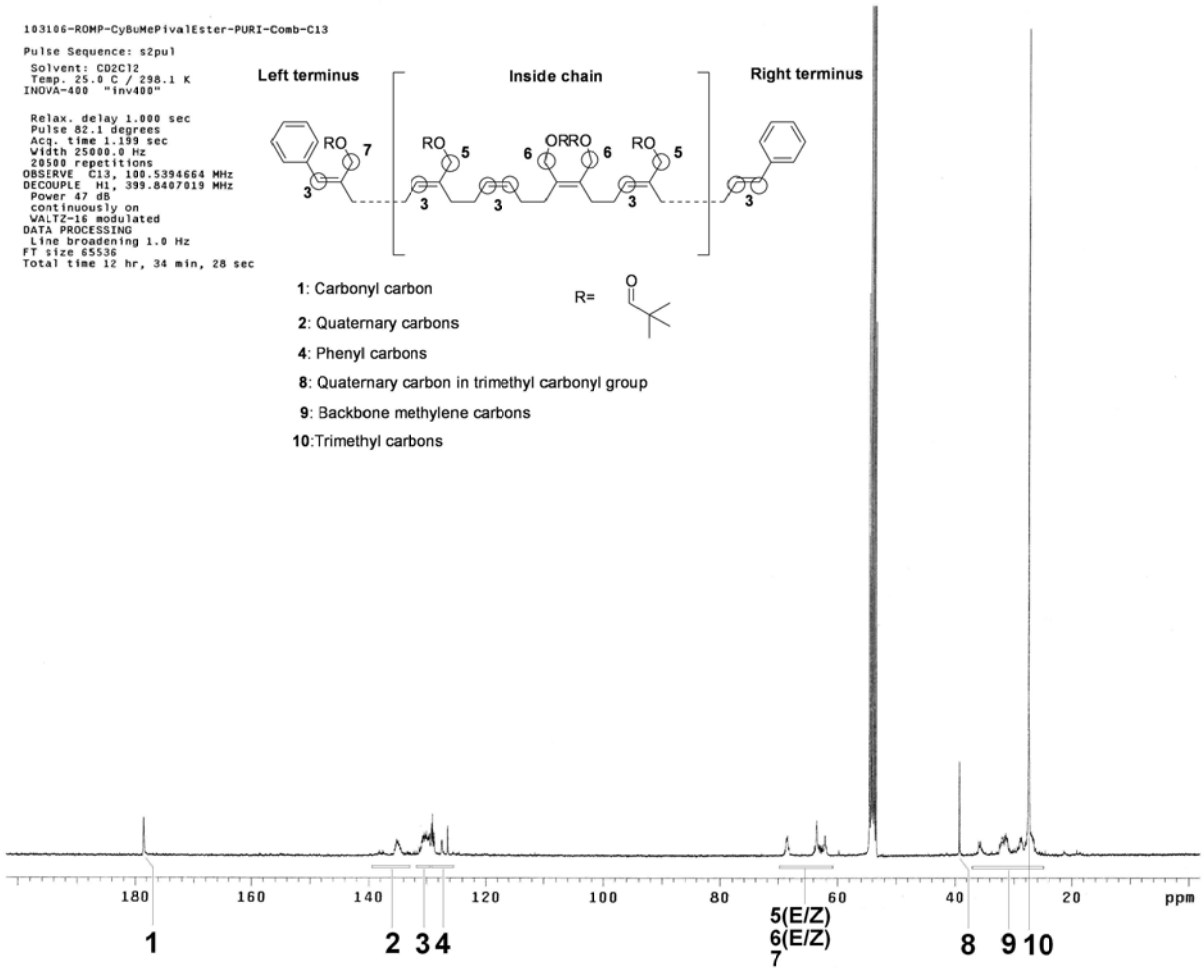
	Parameter	Value
1	Data File Name	G:/ 10142009-12122009/ CBCH2OAc-10mer12122009.fid/ fid
2	Title	CBCH2OAc-10mer12122009
3	Comment	CBCH2OAc-10mer12122009
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	inova
8	Author	
9	Solvent	CD2Cl2
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	48
13	Receiver Gain	44
14	Relaxation Delay	1.0000
15	Pulse Width	0.0000
16	Acquisition Time	1.8920
17	Acquisition Date	2009-12-12T11:57:18
18	Modification Date	2009-12-12T12:01:28
19	Spectrometer Frequency	599.72
20	Spectral Width	8000.0
21	Lowest Frequency	-1001.2
22	Nucleus	1H
23	Acquired Size	15136
24	Spectral Size	32768



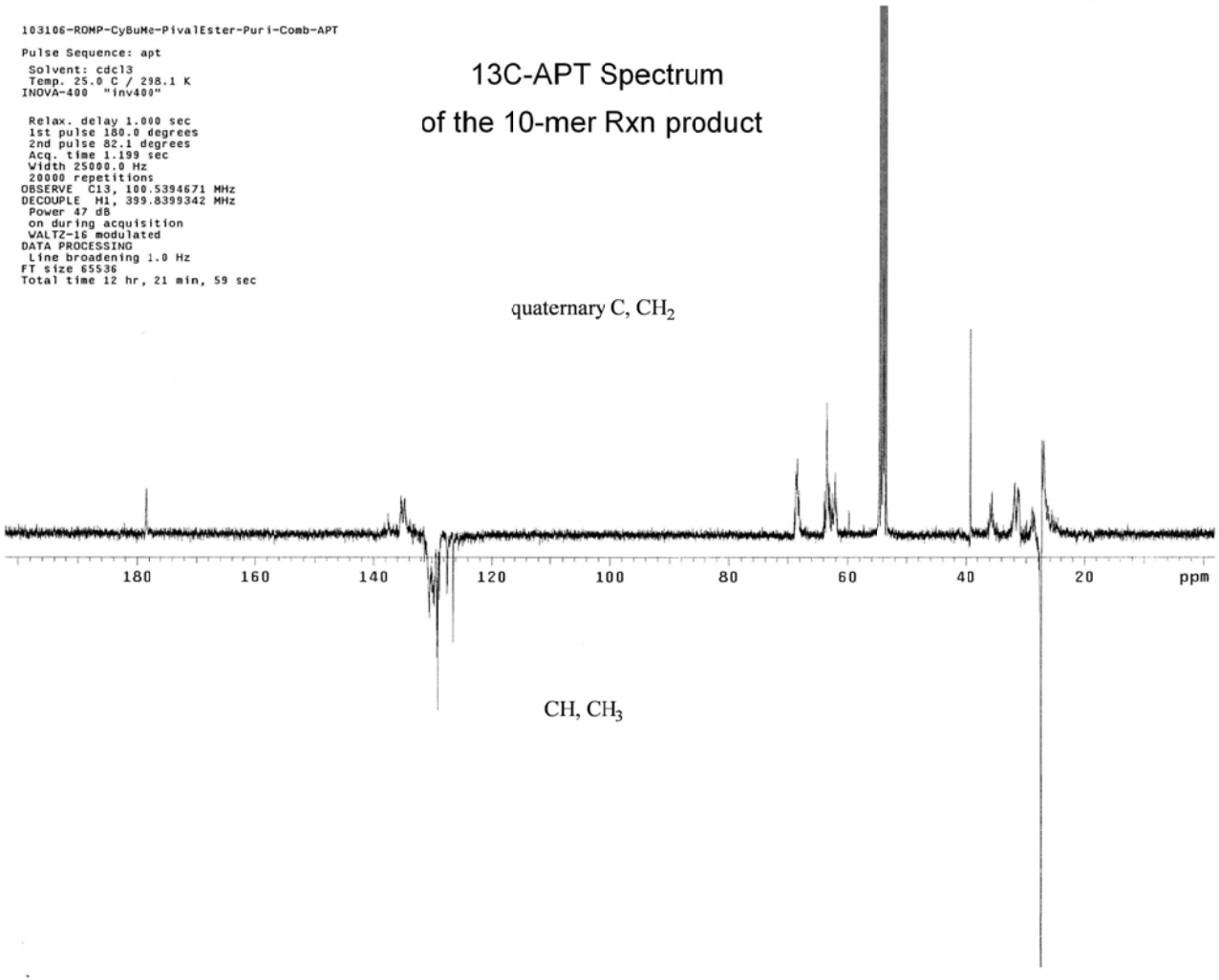
1H-NMR spectrum of 14



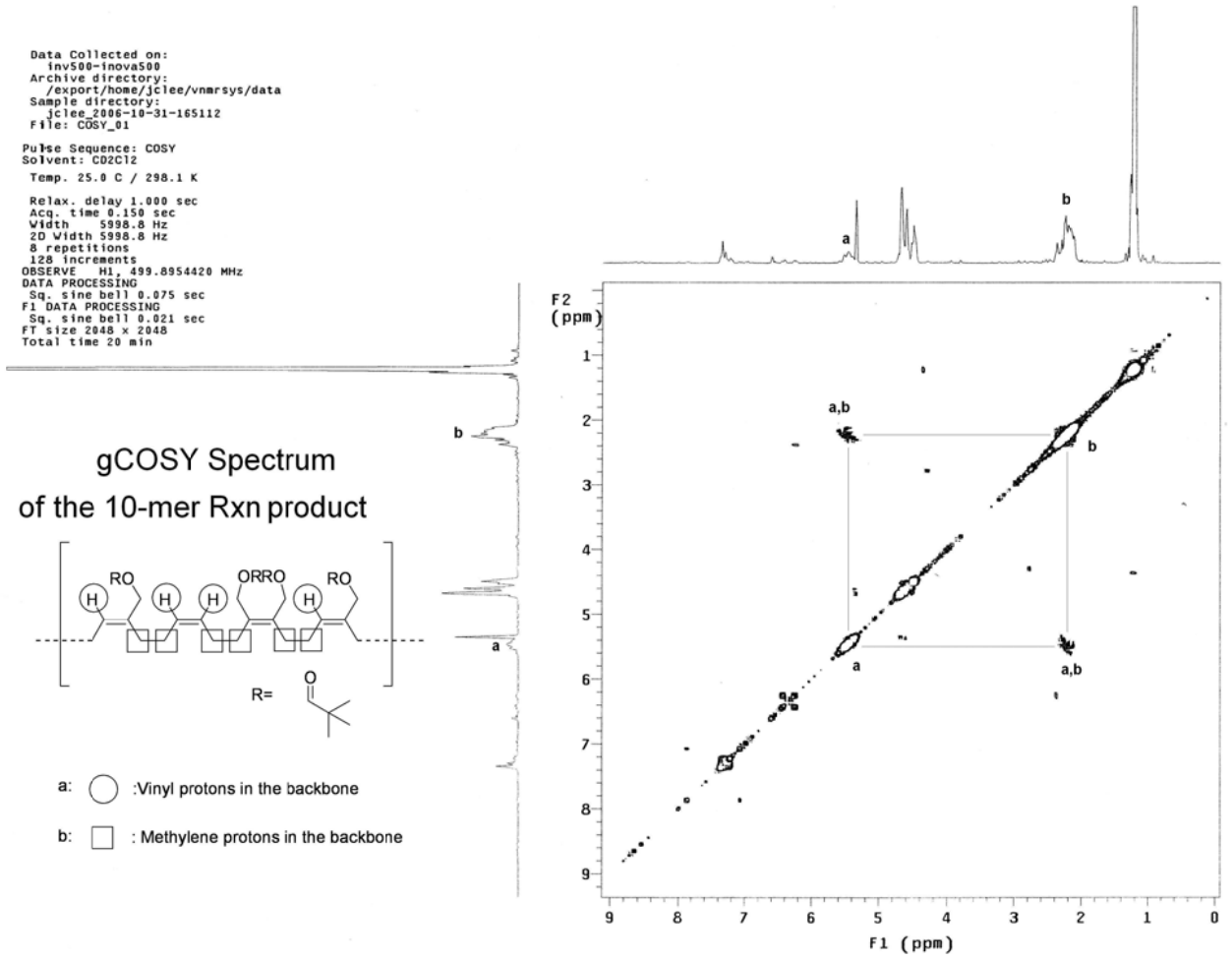
13C-NMR spectrum of 14



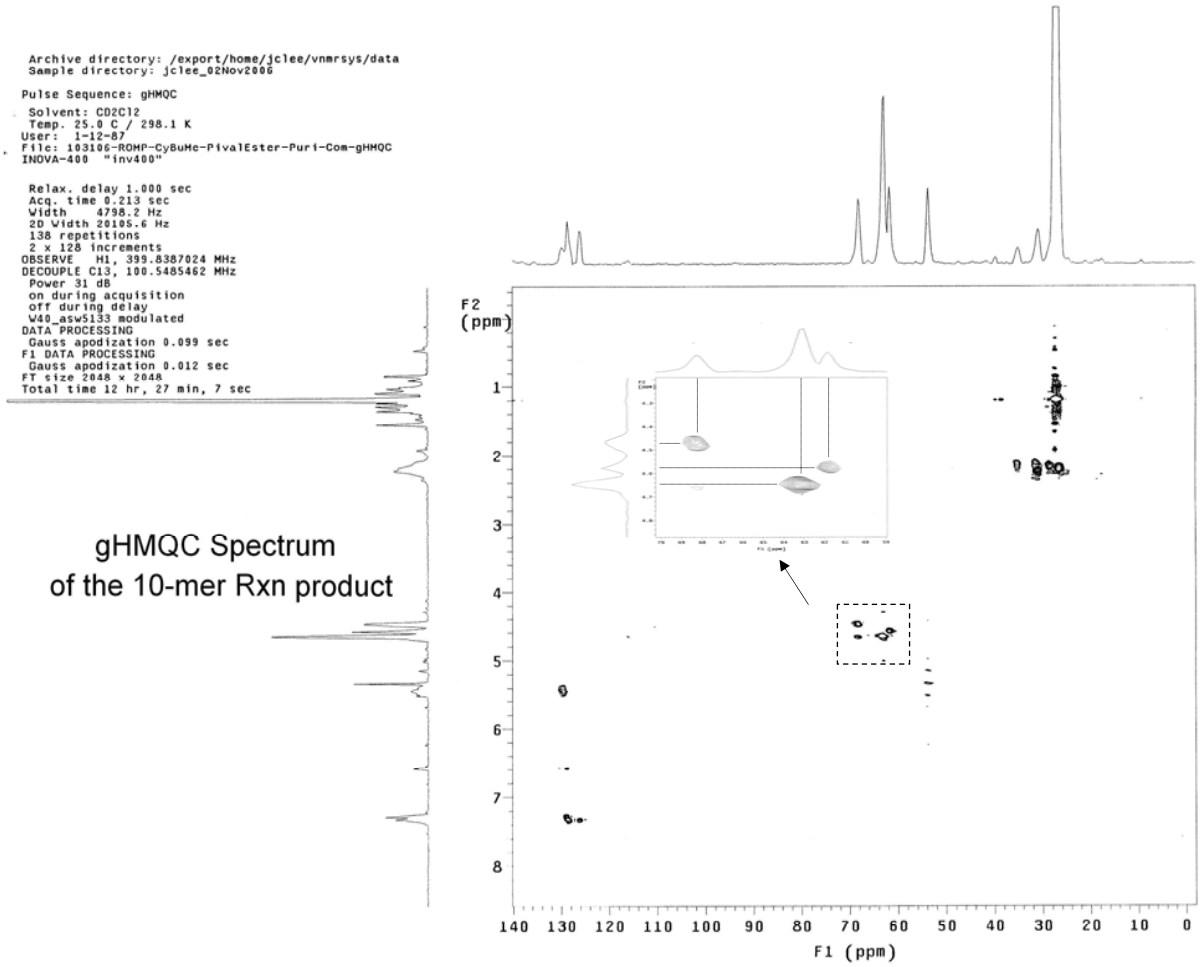
13C-APT spectrum of 14



1H-1H gCOSY spectrum of 14

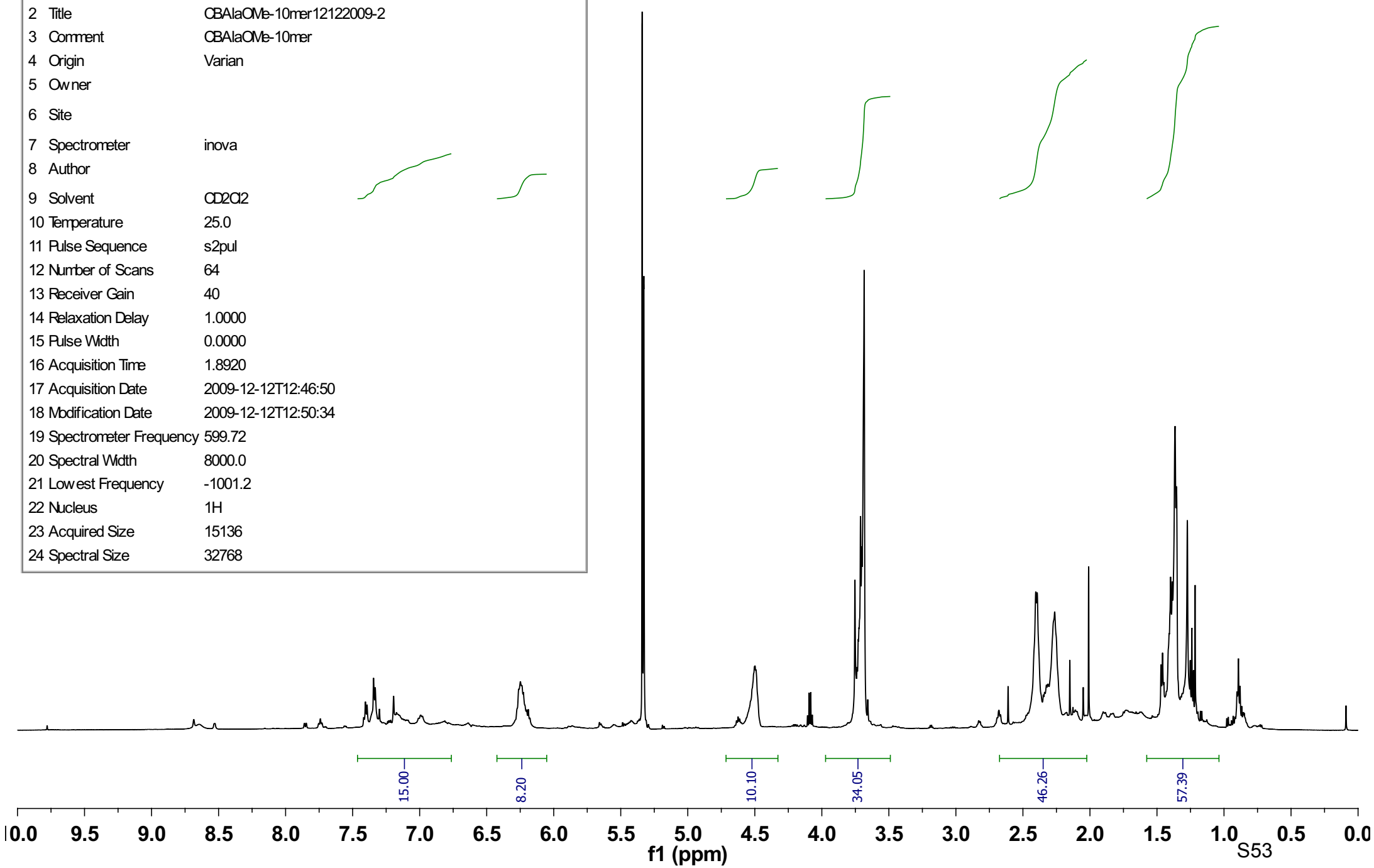


1H-13C gHMQC spectrum of 14



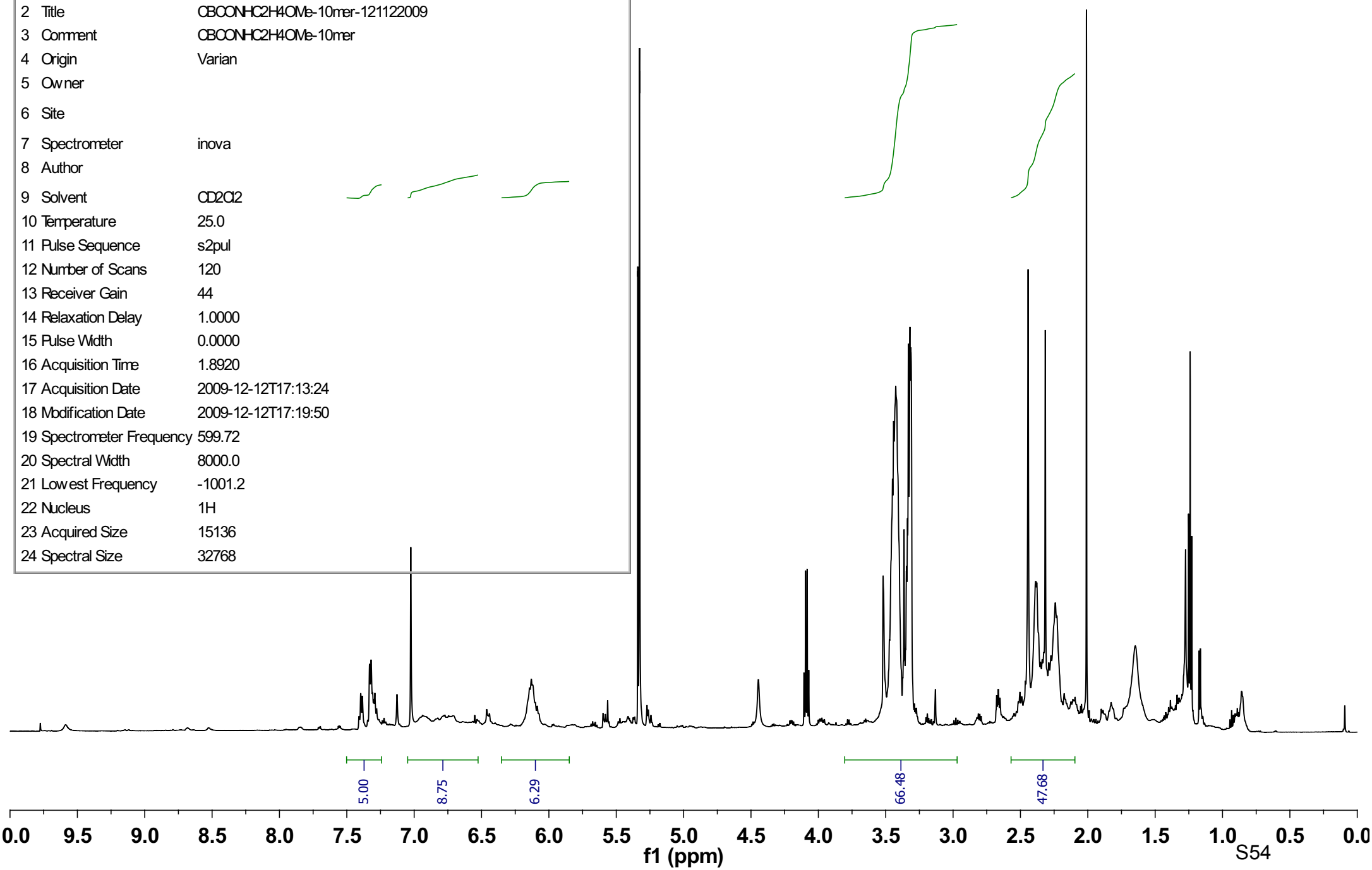
1H-NMR spectrum of 19

Parameter	Value
1 Data File Name	G:/ 10142009-12122009/ CBAlaOMe-10mer12122009-2.fid/ fid
2 Title	CBAlaOMe-10mer12122009-2
3 Comment	CBAlaOMe-10mer
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD2Cl2
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	64
13 Receiver Gain	40
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.8920
17 Acquisition Date	2009-12-12T12:46:50
18 Modification Date	2009-12-12T12:50:34
19 Spectrometer Frequency	599.72
20 Spectral Width	8000.0
21 Lowest Frequency	-1001.2
22 Nucleus	1H
23 Acquired Size	15136
24 Spectral Size	32768



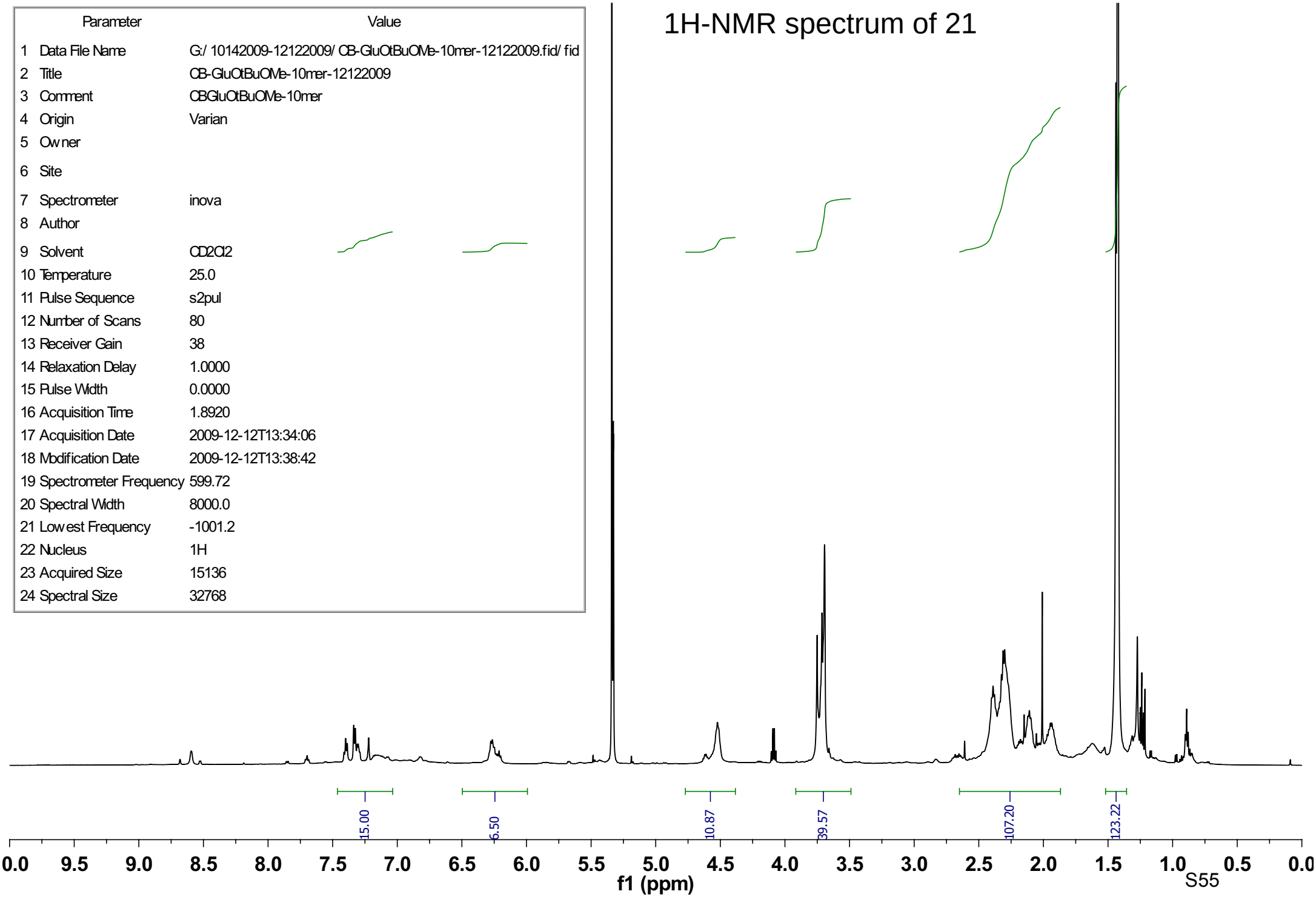
1H-NMR spectrum of 20

	Parameter	Value
1	Data File Name	G:/ 10142009-12122009/ CBCONHC2H4OMe-10mer-121122009.fid/ fid
2	Title	CBCONHC2H4OMe-10mer-121122009
3	Comment	CBCONHC2H4OMe-10mer
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	inova
8	Author	
9	Solvent	CD2Cl2
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	120
13	Receiver Gain	44
14	Relaxation Delay	1.0000
15	Pulse Width	0.0000
16	Acquisition Time	1.8920
17	Acquisition Date	2009-12-12T17:13:24
18	Modification Date	2009-12-12T17:19:50
19	Spectrometer Frequency	599.72
20	Spectral Width	8000.0
21	Lowest Frequency	-1001.2
22	Nucleus	1H
23	Acquired Size	15136
24	Spectral Size	32768



1H-NMR spectrum of 21

	Parameter	Value
1	Data File Name	G:/ 10142009-12122009/ CB-GluOtBuOMe-10mer-12122009.fid/ fid
2	Title	CB-GluOtBuOMe-10mer-12122009
3	Comment	CBGluOtBuOMe-10mer
4	Origin	Varian
5	Owner	
6	Site	
7	Spectrometer	inova
8	Author	
9	Solvent	CD2Cl2
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Number of Scans	80
13	Receiver Gain	38
14	Relaxation Delay	1.0000
15	Pulse Width	0.0000
16	Acquisition Time	1.8920
17	Acquisition Date	2009-12-12T13:34:06
18	Modification Date	2009-12-12T13:38:42
19	Spectrometer Frequency	599.72
20	Spectral Width	8000.0
21	Lowest Frequency	-1001.2
22	Nucleus	1H
23	Acquired Size	15136
24	Spectral Size	32768



1H-NMR spectrum of 22

Parameter	Value
1 Data File Name	G:/ 10142009-12122009/ CB-CONHC3H6PhMe-10mer12122009-2.fid/ fid
2 Title	CB-CONHC3H6PhMe-10mer12122009-2
3 Comment	CBCONHC3H6PhMe-10mer
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	CD2Cl2
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	72
13 Receiver Gain	44
14 Relaxation Delay	1.0000
15 Pulse Width	0.0000
16 Acquisition Time	1.8920
17 Acquisition Date	2009-12-12T13:44:10
18 Modification Date	2009-12-12T13:48:10
19 Spectrometer Frequency	599.72
20 Spectral Width	8000.0
21 Lowest Frequency	-1001.2
22 Nucleus	1H
23 Acquired Size	15136
24 Spectral Size	32768