Electronic Supplementary Information

Spatial effects of oxovanadium-immobilized mesoporous silica on racemization of alcohols and application in lipase-catalyzed dynamic kinetic resolution

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Contents

General considerations

Melting points were determined on a Yanagimoto Melting Point Apparatus and are uncorrected. Infrared (IR) absorption spectra were recorded on a SHIMADZU FTIR-8400S spectrophotometer. ^{1}H and ^{13}C NMR spectra were measured on a JEOL JNM-ECA500 (^{1}H: 500 MHz, ^{13}C: 125 MHz) or JEOL JNM-ECA400, a JEOL AL-300 (^{1}H: 300 MHz, ^{13}C: 75 MHz) instrument with chemical shifts reported in ppm relative to the residual deuterated solvent. Solid ^{13}C NMR spectra were measured on an Agilent (Chemagnetics) CMX 300MHz Infinity NMR spectrometer (^{13}C: 75 MHz) at room temperature. A dipolar decoupled (or the direct detection) magic angle spinning method was used with the magic angle spinning frequency of 5 kHz, and the methine carbon signal of adamantane (38.5 ppm relative to Me_4Si) was used as an external reference. The mass spectra (MS) were measured on a JEOL JMS-S3000 (MALDI), or a JMS-700 (EI) instrument. Yield refers to isolated yields of compounds greater than 95% purity as determined by ^{1}H NMR analysis. ^{1}H NMR and melting points (where applicable) of all known compounds were taken. All new products were further characterized by high resolution mass spectrum (HRMS). HPLC analyses were carried out using a JASCO LC-2000Plus system (HPLC pump: PU-2080, UV detector: MD-2018) equipped with Daicel CHIRALPAK AD-3 and ID, IE columns. All optical active compounds are detected by 254 nm wavelength absorption unless otherwise noted. Optical rotations were measured on a JASCO polarimeter P-1030.

The immobilized *Burkholderia cepacia* lipase, IM (PS-IM), supplied by Amano Enzyme Inc., and MPS2, MPS3 and MPS4, supplied by Taiyo Kagaku Co. Ltd., were used without further purification. Kanto silica gel 60N was used for column chromatography.

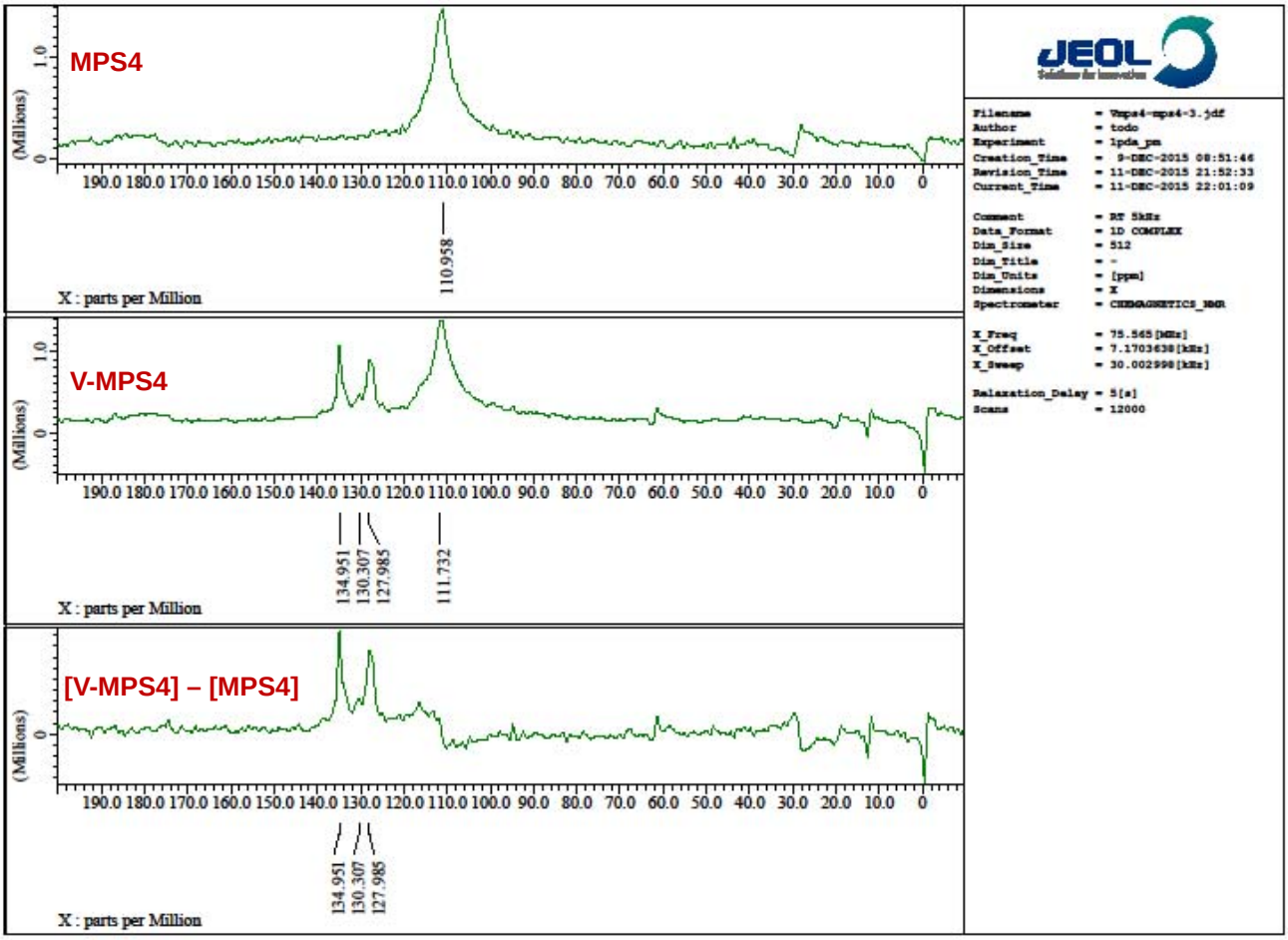
Preparation and structure determination of V-MPS2, V-MPS3 and V-MPS4

Because V-MPS is sensitive to moisture and oxygen, the preparation of V-MPS was slightly modified after the publication of ref. 4c, and the detail is shown below in which all procedure should be operated under anhydrous conditions. MPS (6.3 g), placed in a 2 L-round bottomed flask with an inlet adapter with a 3-way stopcock, was dried in an oven at 150 °C for 12 h, and then the flask was immediately evacuated under reduced pressure (1.0 mmHg) while being cooled down to room temperature over 2 h. This flask was back-filled with argon, to which were added $O=V(OSiPh_3)_3$ (6.7 g, 7.5 mmol) and anhydrous benzene (500 mL) in this order. The reaction mixture was stirred at reflux for 8 h in an argon atmosphere (this process can be conducted by using anhydrous toluene instead of benzene at 80 °C for 8 h), cooled down to room temperature, and concentrated under reduced pressure. The flask was back-filled with argon, and the crude product in the same flask was further dried under reduced pressure (1.0 mmHg) at room temperature for 1 h. After backfill with argon gas, the precipitate was quickly transferred into a centrifuge tube, and the tube was sealed with a rubber septa. A 1:4 mixture of anhydrous hexanes and anhydrous CH_2Cl_2 (total 30 mL) was added, and the mixture was rigorously shacked for 5 min and centrifuged at 3000 rpm for 10 min. The supernatant was discarded using a cannula under the pressure of argon gas. This process was repeated 5 times, and a similar process was performed using anhydrous CH_3CN (30 mL), and the residue was dried under reduced pressure (1.0 mmHg) at room temperature for 12 h to give V-MPS (5.3 g) as an off-white powder.

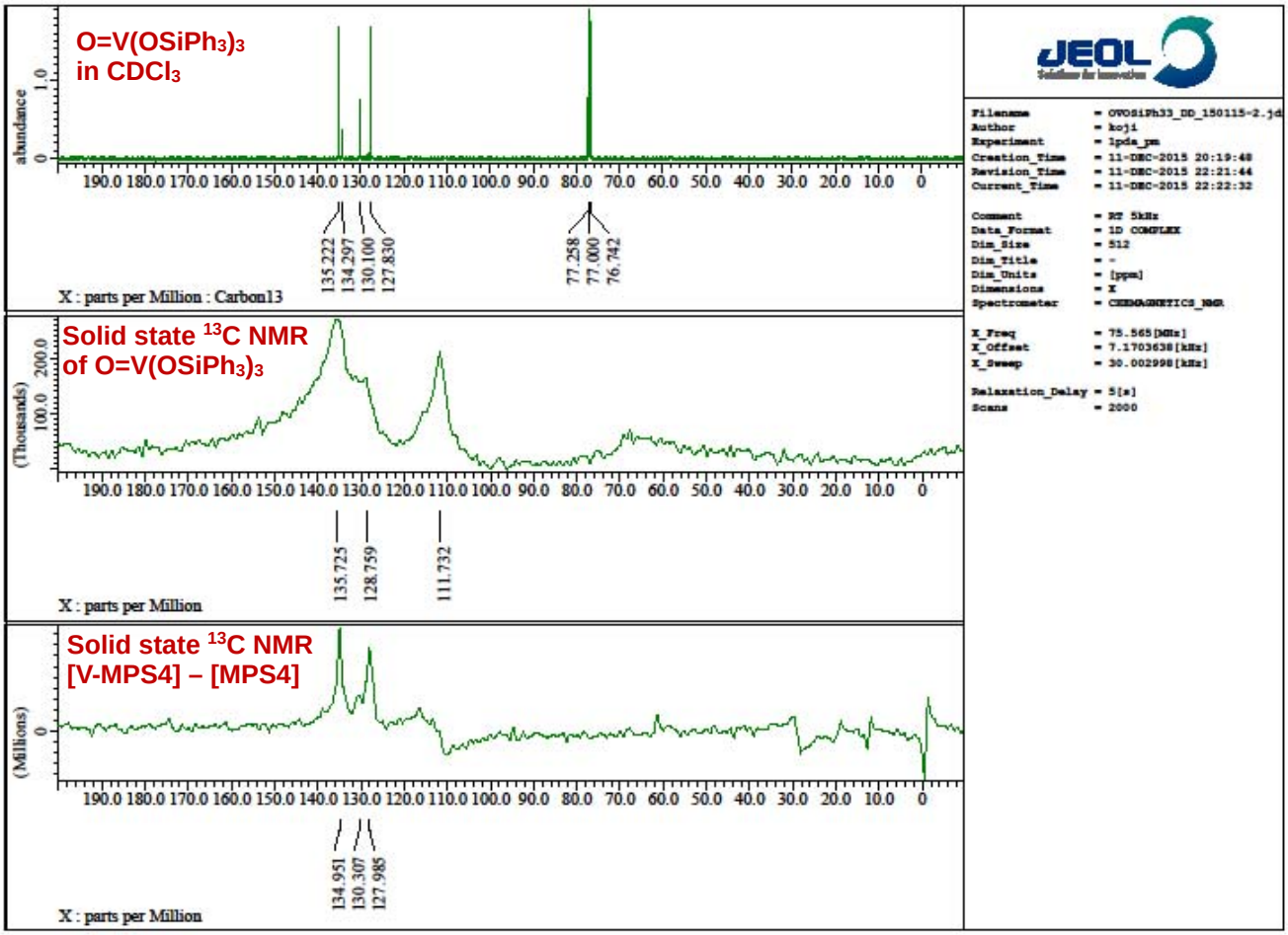
V-MPS2 (5.0 g) was prepared from MPS2 (5.0 g) and $O=V(OSiPh_3)_3$ (5.4 g, 6.0 mmol) according to the abovementioned procedure. V-MPS3, prepared in ref. 4c, was used.

V-MPS2 and V-MPS4 were subjected to the Brunauer–Emmett–Teller (BET), Barrett–Joyner–Halenda (BJH), inductively coupled plasma (ICP), and elemental analyses, and the results are summarized in Table 1.

Solid state ^{13}C NMR of MPS4 and V-MPS4



Comparison of liquid state ^{13}C NMR of $O=V(OSiPh_3)_3$ with solid state ^{13}C NMR of $O=V(OSiPh_3)_3$ and that of [V-MPS4] – [MPS4].

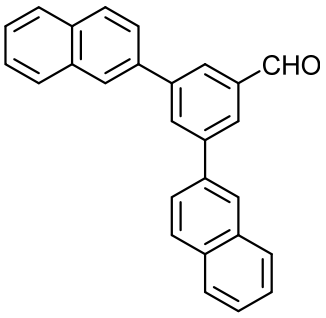


Preparation of racemic substrates (1 and 2)

The known compounds [(±)-**1i**,[1] (±)-**1j**,[1] (±)-**1k**,[1] (±)-**2a**,[1] (±)-**2g**,[1] (±)-**2h**,[1] (±)-**2l**[2] and 2-[2-(2-methoxyethoxy)ethoxy]ethyl 4-methylbenzenesulfonate[3]] were prepared according to the reported methods, and unknown compounds were prepared as follows.

3,5-Di(naphthalen-2-yl)benzaldehyde (5b)

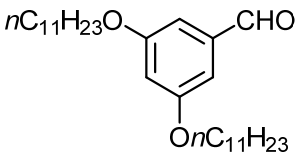
Under an argon atmosphere, to a solution of 3,5-dibromobenzaldehyde (0.50 g, 1.89 mmol), naphthalen-2-ylboronic acid (0.98 g, 5.7 mmol), 2M Na_2CO_3 (7.6 mL, 15 mmol) and THF (20 mL) were added $PdCl_2(dppf)•CH_2Cl_2$ (0.31 g, 0.38 mmol) at room temperature. After stirring at 50 °C for 3 days, the reaction mixture was quenched with 1M HCl followed by the extraction with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 20:1) to give **5b** (0.62 g, 91 %) as a white solid.



Mp 162–163 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.33 (t, *J* = 2.0 Hz, 1H), 8.24 (d, *J* = 2.0 Hz, 2H), 8.19 (d, *J* = 2.0 Hz, 2H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.96 (dd, *J* = 7.0, 2.0 Hz, 2H), 7.92 (dd, *J* = 7.0, 2.0 Hz, 2H), 7.87 (d, *J* = 2.0 Hz, 1H), 7.85 (d, *J* = 2.0 Hz, 1H), 7.58–7.51 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.3, 142.7, 137.6, 137.0, 133.6, 132.9, 132.2, 128.8, 128.3, 127.7, 127.4, 126.6, 126.4, 126.2, 125.2; IR (neat) ν 1695 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{27}H_{18}NaO$ [$(M+Na)^+$] : 358.1353. Found: 358.1352.

3,5-Bisundecyloxybenzaldehyde (5e)

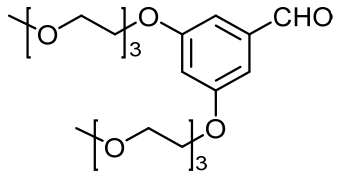
Under an argon atmosphere, to a mixture of 3,5-dihydroxybenzaldehyde (0.20 g, 1.5 mmol) and K_2CO_3 (0.87 g, 6.3 mmol) in DMF (4 mL) was added 1-iodoundecane (1.3 mL, 5.4 mmol) at 65 °C. After stirring at the same temperature for 3 h, the reaction mixture was quenched with H_2O followed by the extraction with Et_2O. The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 20:1) to give **5e** (0.59 g, 91 %) as a pale yellow oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 9.88 (s, 1H), 6.97 (d, *J* = 2.0 Hz, 2H), 6.68 (t, *J* = 2.0 Hz, 1H), 3.97 (t, *J* = 7.0 Hz, 4H), 1.78 (quint, *J* = 7.0 Hz, 4H), 1.45 (quint, *J* = 7.0 Hz, 4H), 1.36–1.24 (m, 28H), 0.88 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 160.7, 138.3, 108.0, 107.5, 68.4, 31.9, 30.0, 29.5, 29.3, 29.1, 26.0, 22.7, 14.1; IR (neat) ν 1728 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{29}H_{51}O_3$ [$(M+H)^+$]: 447.3829. Found: 447.3832.

3,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)benzaldehyde (5f)

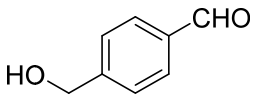
Under an argon atmosphere, to a mixture of 3,5-dihydroxybenzaldehyde (0.50 g, 3.6 mmol) and K_2CO_3 (2.0 g, 14.5 mmol), and potassium iodide (60 mg, 0.36 mmol) in DMF (10 mL) was added 2-[2-(2-methoxyethoxy)ethoxy]ethyl 4-methylbenzenesulfonate[3] (2.3 g, 7.2 mmol) at room temperature. After stirring at 80 °C for 13 h, the reaction mixture was evaporated in vacuo. The residue was purified by column chromatography (CH_2Cl_2/MeOH = 20:1) to give **5f** (1.5 g, 93%) as a colorless oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 7.00 (d, *J* = 2.0 Hz, 2H), 6.74 (t, *J* = 2.0 Hz, 1H), 4.14 (t, *J* = 4.5 Hz, 4H), 3.85 (t, *J* = 4.5 Hz, 4H), 3.72 (t, *J* = 4.5 Hz, 4H), 3.66 (t, *J* = 4.5 Hz, 4H), 3.63 (t, *J* = 4.5 Hz, 4H), 3.53 (t, *J* = 4.5 Hz, 4H), 3.35 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 191.7, 160.3, 138.3, 108.3, 108.0, 71.9, 70.8, 70.6, 70.5, 69.5, 67.8, 58.9; IR (neat) ν 1697 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{21}H_{34}NaO_9$ [$(M+Na)^+$]: 453.2094. Found: 453.2095

4-Hydroxymethylbenzaldehyde (6)

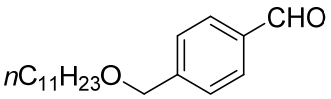
Under an argon atmosphere, sodium borohydride (70 mg, 1.9 mmol) was dropwise added to a solution of terephthalaldehyde (1.0 g, 7. 5 mmol) in a mixture of EtOH (12 mL), H_2O (0.60 mL), and THF (18 mL) at 5 °C over a period of 30 min. After stirring at 0 °C for 10 h, the reaction mixture was neutralized with 1M HCl to about pH5, and the product was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 1:1). to give **6** (0.76 g, 75%) as a white solid



Mp 39–40 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.0 (s, 1H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 4.82 (d, *J* = 6.0 Hz, 2H), ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 147.7, 135.6, 130.0, 126.9, 64.5; IR ($CHCl_3$) ν 3350 cm^{-1}, 1689. HRMS (ESI) *m*/*z* calcd for $C_8H_9O_2$ [$(M+H)^+$]: 137.0597. Found:. 137.0597.

4-Undecyloxymethyl benzaldehyde (7c)

Under an argon atmosphere, triethylsilane (1.4 mL, 8.7 mmol) was dropwise added to a mixture of **6** (1.0 g, 7.2 mmol), 1-undecanol (2mL, 8.7 mmol) and $FeCl_3$ (60 mg, 0.36 mmol) in CH_3NO_2 (36 mL, 0.2 M) over a period of 5.5 h at room temperature. After stirring at the same temperature for 6 h, the reaction mixture was extracted with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. Then, MnO_2 (12.5 g, 0.15 mol) was added to a solution of the residue (7.24 mmol) in CH_2Cl_2 (36 mL, 0.2 M) at 0 °C. After stirring at the same temperature for 12 h, the reaction mixture was filtered through a Celite pad, and the eluent was evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 7:1) to give **7c** (2.30 g, quant) as a colorless oil.

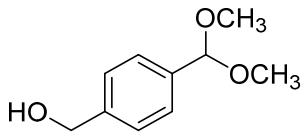


^{1}H NMR (500 MHz, $CDCl_3$) δ 10.0 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 4.58 (s, 2H), 3.50 (t, *J* = 7.0 Hz, 2H), 1.64 (quint, *J* = 7.0 Hz, 2H), 1.38–1.26 (m, 16H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 146.0, 135.6, 129.9, 127.6, 72.1, 71.0, 31.9, 29.7, 29.6, 29.5, 29.3, 26.2, 22.7, 14.1; IR ($CHCl_3$) ν 1705 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{19}H_{31}O_2$ [$(M+H)^+$]: 291.2318. Found: 291.2319.

4-Dimethoxymethylphenyl methanol (8)

Under an argon atmosphere, to a solution of HCl in MeOH (10 %w/w, 53 mg (0.15 mmol) was added to a solution of **6** (0.10 g, 0.72 mmol), $HC(OMe)_3$ (0.59 mL, 5.4 mmol) in MeOH (1.2 mL, 0.6 M) at room temperature. After stirring under reflux conditions for 12 h, the reaction mixture was quenched with $NaHCO_3$ to make the mixture neutral. The reaction

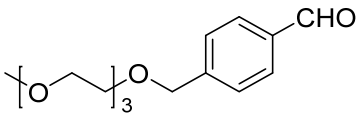
mixture was filtered and the filtrate was evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 1:1) to give **8** (0.10 g, 77%) as a colorless oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 5.39 (s, 1H), 4.71 (d, *J* = 6.0 Hz, 2H), 3.32 (s, 6H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.1, 137.5, 126.9, 126.8, 102.9, 65.1, 52.6 ; IR ($CHCl_3$) ν 3415 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{10}H_{14}NaO_3$ [$(M+Na)^+$]: 205.0834. Found: 205.0835.

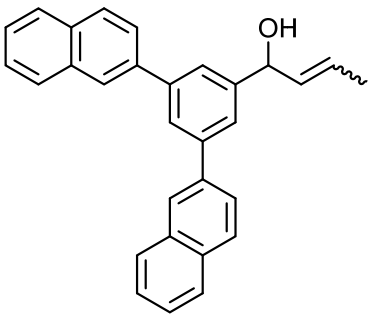
4-(2,5,8,11-Tetraoxadodecyl)benzaldehyde (7d)

Under an argon atmosphere, sodium hydride (210 mg, 5.27 mmol) was added to a mixture of **8** (0.80 g, 4.4 mmol), 2-[2-(2-methoxyethoxy)ethoxy)ethyl 4-methylbenzenesulfonate[3] (1.68 g, 5.3 mmol) and potassium iodide (73 mg, 0.44 mmol) in THF (29 mL) at 0 °C. After stirring under reflux conditions for 1 h, the reaction mixture was quenched with 1M HCl and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 1:5) to give **7d** (1.18 g, 95%) as a red oil.



^{1}H NMR (500 MHz, $CDCl_3$) δ 10.0 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 4.65 (s, 2H), 3.71-3.53 (m, 12H), 3.37 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 145.5, 135.7, 129.9, 127.7, 72.5, 71.9, 70.6, 70.5, 70.0, 59.0; IR ($CHCl_3$) ν 1694 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{15}H_{22}NaO_5$ [$(M+Na)^+$]:305.1356. Found: 305.1359

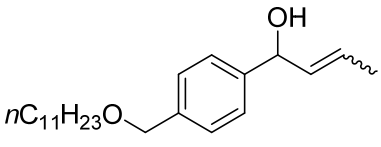
1-(3,5-Di(naphthalen-2-yl)phenyl)but-2-en-1-ol [(±)-2b]



0.59 g, 96% yield, a 1:1 mixture of (*E*)- and (*Z*)-isomers: Prepared from **5b** (0.55 g, 1.53 mmol), 1-propenyl magnesium bromide (0.5 M in THF; 4.6 mL, 2.3 mmol) and THF (15 mL) according to the method for the synthesis of (±)-**2e**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (s, 2H), 7.98 (d, *J* = 8.5 Hz, 2H), 7.95 (s, 1H), 7.95 (d, *J* = 8.5Hz, 2H), 7.90 (d, *J* = 8.5 Hz, 2H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.78 (dd, *J* = 8.5, 2.0 Hz), 7.56–7.50 (m, 4H), 5.96–5.73 (m, 2.5H), 5.37 (dd, *J* = 7.5, 2.5 Hz, 0.5H), 1.90 (dd, *J* = 6.5, 1.5 Hz, 1.5H), 1.79 (d, *J* = 5.5 Hz, 1.5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.0, 144.7, 142.1, 142.0, 138.4, 133.6, 133.6, 132.8, 132.7, 128.5, 128.2, 128.0, 127.6, 126.9, 126.3, 126.0, 125.8, 125.6, 124.3, 124.0, 75.4, 69.6, 17.8, 13.5; IR (neat) ν 3408 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{30}H_{24}NaO$ [$(M+Na)^+$]: 400.1818. Found: 400.1822.

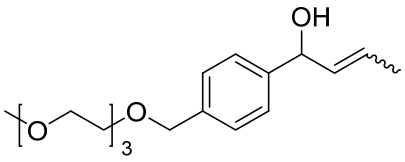
1-(4-((Undecyloxy)methyl)phenyl)but-2-en-1-ol [(±)-2c]



97 mg, 89 % yield, a 1:1 mixture of (*E*)- and (*Z*)-isomers, a colorless oil: Prepared from **7c** (96 mg, 0.33 mmol), 1-propenyl magnesium bromide (0.5 M in THF; 0.99 mL, 0.50 mmol) and THF (1.7 mL, 0.2 M) according to the method for the synthesis of (±)-**2e.**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37–7.31 (m, 4H), 5.75-5.58 (m, 2.5H), 5.16 (dd, *J* = 6.0, 3.5 Hz, 0.5H), 4.49 (s, 2H), 3.45 (t, *J* = 7.0 Hz, 2H), 1.81–1.72 (m, 4H), 1.60 (quint, *J* = 7.0 Hz, 2H), 1.35–1.20 (m, 16H), 0.87 (t, *J* = 7.0 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.0, 142.7, 138.1, 138.0, 133.7, 133.0, 128.0, 127.9, 127.6, 126.5, 126.2, 126.0, 75.2, 72.7, 70.6, 69.4, 32.0, 29.9, 29.7, 29.6, 29.4, 29.6, 29.4, 26.3, 22.8, 17.8, 14.2, 13.5 ; IR ($CHCl_3$) ν 3456, 1653 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{22}H_{36}NaO_2$ [$(M+Na)^+$]:355.2605. Found:. 355.2608

1-(4-(2,5,8,11-Tetraoxadodecyl)phenyl)but-2-en-1-ol [(±)-2d]

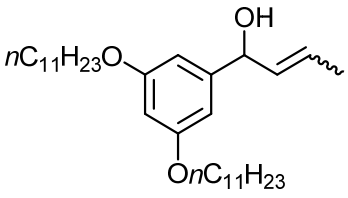


1.12 g, 85% yield, a 1:1 mixture of (*E*)- and (*Z*)-isomers, a colorless oil: Prepared from **7b** (1.14 g, 4.04 mmol), 1-propenyl magnesium bromide (0.5 M in THF; 9.7 mL, 4.9 mmol) and THF (20 mL, 0.2 M) according to the method for the synthesis of (±)-**2e**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.28 (m, 4H), 5.70-5.53(m, 2.5H), 5.11 (d, *J* = 7.0 Hz, 0.5H), 4.55 (s, 2H), 3.67-3.50 (m, 12H), 3.37 (s, 3H), 1.92-1.88 (m, 1H), 1.75 (d, *J* = 6 Hz, 1.5H), 1.69 (d, *J* = 6Hz, 1.5H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.1, 142.8, 137.3, 137.3, 133.6, 132.9, 127.8, 127.8, 127.1, 126.0, 126.0, 125.8, 74.8, 72.8, 71.8, 70.5, 70.4, 69.2, 69.0, 58.9, 17.6, 13.2; IR ($CHCl_3$) ν 3436 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{18}H_{28}NaO_5$ [$(M+Na)^+$]:347.1824. Found: 347.1829

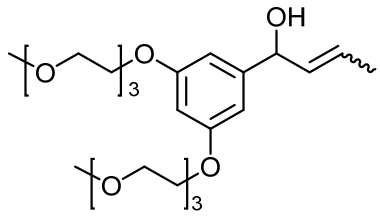
1-(3,5-Bis(undecyloxy)phenyl)but-2-en-1-ol [(±)-2e]

Under an argon atmosphere, to a solution of **5e** (0.59 g, 1.23 mmol) in THF (6 mL) was dropwise added 1-propenyl magnesium bromide (0.5 M in THF; 3.7 mL, 1.84 mmol) at 0 °C. After stirring at the same temperature for 0.5 h, the reaction mixture was quenched with sat. aq. NH_4Cl followed by the extraction with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 10:1) to give (±)-**2e** (0.46 g, 71%, a 1:1 mixture of (*E*)- and (*Z*)-isomers) as a pale yellow oil.



^{1}H NMR (300 MHz, $CDCl_3$) δ 6.53 (d, *J* = 7.0 Hz, 2H), 6.36 (s, 1H), 5.75-5.62 (m, 2H), 5.49 (d, *J* = 7.0 Hz, 0.5H), 5.07 (d, *J* = 6.0 Hz, 0.5H), 3.95 (t, *J* = 6.5 Hz, 4H), 1.83-1.71 (m, 8H), 1.44-1.27 (m, 32H), 0.90 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.5, 146.1, 133.4, 127.5, 104.4, 100.3, 75.3, 69.5, 68.0, 31.9, 29.6, 29.4, 29.3, 29.3, 26.1, 22.7, 17.7, 14.1, 13.4; IR ($CHCl_3$) ν 3389 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{32}H_{57}O_3$ [$(M+H)^+$]: 489.4301. Found: 489.4302.

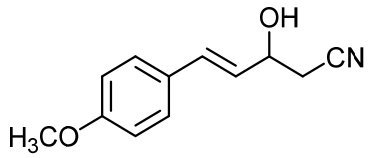
1-(3,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)but-2-en-1-ol [(±)-2f]



0.89 g, 81% yield, a 1:1 mixture of (*E*)- and (*Z*)-isomers, a colorless oil: Prepared from **5f** (1.0 g, 2.3 mmol), 1-propenyl magnesium bromide (0.5 M in THF; 7 mL, 3.5 mmol) and THF (10 mL) according to the method for the synthesis of (±)-**2e**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.48 (d, *J* = 2.0 Hz, 1H), 6.45 (d, *J* = 2.0 Hz, 1H), 6.29 (t, *J* = 2.0 Hz, 1H), 5.67–5.46 (m, 2H), 5.36 (d, *J* = 8.0 Hz, 0.5H), 4.94 (d, *J* = 7.0 Hz, 0.5H), 4.00 (t, *J* = 4.5 Hz, 4H), 3.74 (t, *J* = 4.5 Hz, 4Hz), 3.65–3.61(m, 4H) 3.60–3.54 (m, 8H), 3.47–3.44 (m, 4H), 3.28 (s, 6H), 1.68 (d, *J* = 5.0 Hz, 1.5/3H), 1.61 (d, *J* = 6.5 Hz, 1.5/3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.62, 159.56, 146.2, 145.9, 133.4, 132.8, 126.7, 125.5, 104.6, 104.4, 100.1, 100.0, 74.5, 71.6, 70.4, 70.3, 70.2, 69.4, 68.7, 67.1, 58.6, 17.4, 13.0; IR ($CHCl_3$) ν 3455 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{20}H_{40}NaO_9$ [$(M+Na)^+$]: 495.2570. Found: 495.2565.

(*E*)-1-Cyano-4-(4-methoxyphenyl)but-3-en-2-ol [(±)-1m]

(±)-**1m** was synthesized according to the reported method.[4] Under an argon atmosphere, to a solution of lithium diisopropyamide generated from diisopropylamine (2.1 mL, 15 mmol) and *n*-BuLi (2.6 M in hexanes; 5.7 mL, 15 mmol) in THF (15 mL) was dropwise added a solution of acetonitrile (0.80 mL, 15 mmol) in THF (7.5 mL) at –78 °C. The mixture was stirred for an additional 0.5 h at –78 °C before a solution of 4-methoxycinnamaldehyde (2.4 g, 14.8 mmol) in THF (7.5 mL) was added. After stirring at the same temperature for 16 h, the reaction mixture was quenched with sat. aq. NH_4Cl followed by the extraction with Et_2O. The combined organic layers were dried over $MgSO_4$, and evaporated in vacuo. The residue was purified by column chromatography (hexanes/EtOAc = 3:2) to give (±)-**1m** (2.6 g, 87%) as a white solid.

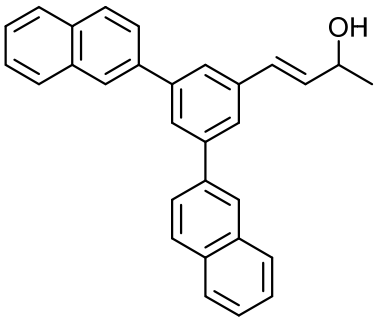


Mp 55–56 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 6.5, 2.0 Hz, 2H), 6.87 (dd, *J* = 6.5, 2.0 Hz, 2H), 6.65 (d, *J* = 15 Hz, 1H) , 6.10 (dd, *J* = 15, 7 Hz, 1H), 4.62-4.58 (m, 1H), 3.81 (s, 3H), 2.70 (dd, *J* = 17, 5.5 Hz, 1H), 2.65 (dd, *J* = 17, 6.5 Hz, 1H), 2.28-2.22 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.9, 132.7, 128.2, 128.0, 125.7, 117.2, 114.1, 69.0, 55.3, 26.4; IR (neat) ν 3447, 2255 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{12}H_{13}NO_2$ [M^+]: 203.0946. Found: 203.0941.

Preparation of (*S*)-1b and (*S*)-1c–f

(*E*)-4-(3,5-Bis(undecyloxy)phenyl)but-3-en-2-ol [(±)-1b]

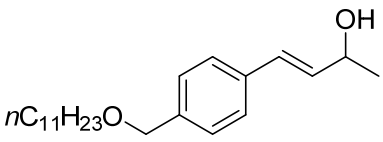
Under an argon atmosphere, to a solution of (±)-**2b** (0.30 g, 0.75 mmol) in CH_3CN (10 mL, 0.08 M) was added $O=V(OSiPh_3)_3$ (67 mg, 0.075 mmol) at room temperature. After stirring at 35 °C for 10 h, the reaction mixture was evaporated in vacuo directly. The residue was purified by column chromatography (hexanes only to hexanes/EtOAc = 4:1) to give (±)-**1b** (279 mg, 93%) as a white solid.



Mp 160–161 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 2.0 Hz, 2H), 7.99–7.92 (m, 5H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.84 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.75 (d, *J* = 2.0 Hz, 2H), 7.57–7.49 (m, 4H), 6.78 (d, *J* = 15.5 Hz, 1H), 6.49 (dd, *J* = 15.5, 6.0 Hz, 1H), 4.63–4.55 (m, 1H), 1.45 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.2, 138.3, 137.9, 134.5, 133.7, 132.8, 129.2, 128.5, 128.2, 127.7, 126.4, 126.1, 126.05, 125.99, 125.6, 124.6, 69.0, 23.5; IR ($CHCl_3$) ν 3383 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{30}H_{24}O$ [M^+]:400.1827. Found: 400.1822.

(*E*)-4-(4-((Undecyloxy)methyl)phenyl)but-3-en-2-ol [(±)-1c]

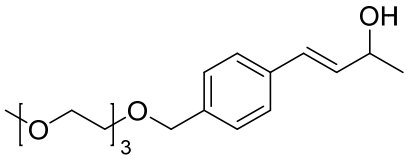
0.50 g, quant, a white solid; Prepared from (±)-**2c** (0.50 g, 1.50 mmol), $O=V(OSiPh_3)_3$ (134 mg, 0.15 mmol) and CH_3CN (19 mL, 0.08 M) according to the method for the synthesis of (±)-**1b**.



Mp 38–39 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8 Hz, 2H), 7.29 (d, *J* = 8 Hz, 2H), 6.57 (d, *J* = 15 Hz, 1H), 6.28 (dd, *J* = 6, 15 Hz, 1H), 4.50-4.48 (m, 3H), 3.45 (t, *J* = 6 Hz, 2H), 1.60 (quint, *J* = 7.0 Hz, 3H), 1.38-1.26 (m, 21H), 0.879 (t, *J* = 6.0 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.2, 135.9, 133.4, 129.1, 127.9, 126.4, 72.5, 70.5, 69.0, 31.9, 29.7, 29.6, 29.5, 29.3, 26.2, 23.4, 22.7, 14.1 ; IR $CHCl_3$) ν 3280 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{22}H_{36}NaO_2$ [$(M+Na)^+$]:355.2607. Found: 355.2608

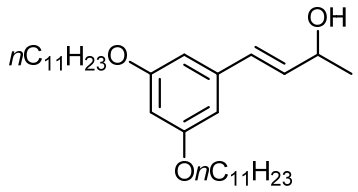
(*E*)-4-(4-(2,5,8,11-Tetraoxadodecyl)phenyl)but-3-en-2-ol [(±)-1d]

0.45 g, 89%, a colorless oil: Prepared from (±)-**2d** (0.50 g, 1.54 mmol), $O=V(OSiPh_3)_3$ (138 mg, 0.154 mmol) and CH_3CN (19.0 mL, 0.08 M) according to the method for the synthesis of (±)-**1b**.



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8 Hz, 2H), 7.30 (d, *J* = 8 Hz, 2H), 6.57 (d, *J* = 16 Hz, 1H), 6.28 (dd, *J* = 16, 6.0 Hz, 1H), 4.55 (s, 2H), 4.49 (m, 1H), 3.67–3.54(m, 12H), 3.38 (s, 3H), 1.38 (d, *J* = 6.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.6, 136.0, 133.5, 129.0, 128.0, 126.4, 72.9, 71.9, 70.6, 70.5, 69.3, 68.8, 59.0, 23.5 ; IR (neat) ν 3450 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{18}H_{28}NaO_5$ [$(M+Na)^+$]:347.1824. Found: 347.1829

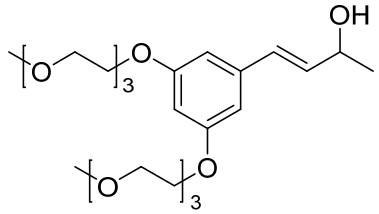
(*E*)-4-(3,5-Bis(undecyloxy)phenyl)but-3-en-2-ol [(±)-1e]



104 mg, quant, a white solid: Prepared from (±)-**2e** (100 mg, 0.21 mmol), O=V(OSiPh$_3$)$_3$ (18.0 mg, 0.020 mmol), CH_3CN (2.5 mL, 0.08 M) according to the method for the synthesis of (±)-**1b**.

Mp 40 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.52-6.45 (m, 3H), 6.37 (t, *J* = 2.0 Hz, 1H), 6.26 (dd, *J* = 16, 6.0 Hz, 1H), 4.50 (quint, *J* = 6.0 Hz, 1H), 3.95 (d, *J* = 7.0 Hz, 4H), 1.81 (quint, *J* = 7.0 Hz, 4H), 1.46–1.27(m, 36H), 0.91 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 138.5, 133.8, 129.5, 105.0, 100.9, 68.9, 68.0, 31.9, 29.6, 29.4, 29.3, 29.2, 26.0, 23.4, 22.7, 14.1; IR ($CHCl_3$) ν 3343 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{32}H_{57}O_3$ [(M+H)$^+$]:489.4292. Found: 489.4302.

(*E*)-4-(3,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)but-3-en-2-ol [(±)-1f]

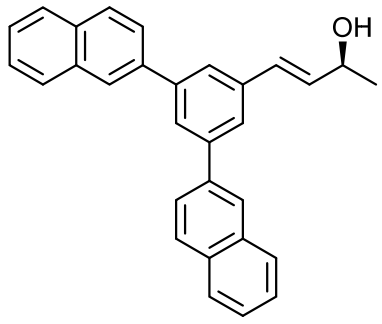


0.78 g, 98% yield, a colorless oil: Prepared from (±)-**2f** (0.80 g, 1.69 mmol), O=V(OSiPh$_3$)$_3$ (151 mg, 0.169 mmol), CH_3CN (10 mL, 0.2 M) according to the method for the synthesis of (±)-**1b**.

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.54 (d, *J* = 2.0 Hz, 2H), 6.47 (d, *J* = 15 Hz, 1H), 6.39 (t, *J* = 2.0, 1H), 6.20 (dd, *J* = 15, 6.0 Hz, 1H), 4.47 (quint, *J* = 6.0 Hz, 1H), 4.10 (t, *J* = 5.0 Hz, 4H), 3.84 (t, *J* = 5.0 Hz, 4H), 3.74-3.64 (m, 12H), 3.55 (m, 4H), 3.37 (s, 6H), 1.36 (d, *J* = 6.0 Hz, 3H) ; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 138.6, 134.1, 129.3, 105.5, 101.1, 71.9, 70.8, 70.6, 70.5, 69.7, 68.8, 67.4, 59.0, 23.4 ; IR ($CHCl_3$) ν 3462 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{24}H_{40}NaO_9$ [(M+Na)$^+$]: 495.2569. Found: 495.2565.

(*S*,*E*)-4-(3,5-Bis(undecyloxy)phenyl)but-3-en-2-ol [(*S*)-1b]

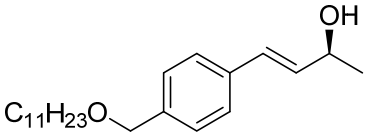
Under an argon atmosphere, to a solution of the alcohol (±)-**1b** (0.30 g, 0.75 mmol) in acetone (10 mL, 0.08 M) were added the immobilized *Candida antartica* lipase B (0.30 g, 1.0 w/w) and vinyl acetate (139 µl, 1.50 mmol) at room temperature. The reaction mixture was stirred at 35 ºC for 13 h and then filtered through a Celite pad. The filtrate was removed under reduced pressure. The residue was purified by column chromatography (silica gel, hexanes/EtOAc = 4:1) to give (*S*)-**1b** (148 mg, 49%, >99% *ee*). The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL ID column (hexanes/2-propanol = 90:10, 1.0 mL/min; retention times 14.3 (*R*), 15.5 min (*S*)).



(*S*)-**1b** was obtained in 49% yield with >99% *ee*.

$[\alpha]_D^{20}$ = –13.4 (*c* 1.33, $CHCl_3$). The spectroscopic data of the obtained product (*S*)-**1b** was in good agreement with (±)-**1b**.

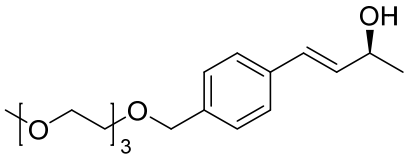
(*S*,*E*)-4-(4-((Undecyloxy)methyl)phenyl)but-3-en-2-ol [(*S*)-1c]



131 mg, 44% yield, >99% *ee* The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 6.1 (*S*), 7.1 min (*R*)): Prepared from **(±)-1c** (300 mg, 0.902 mmol), the immobilized *Candida antartica* lipase B (600 mg, 2.0 w/w), CH_3CN (11 mL, 0.08 M) according to the method for the synthesis of (*S*)-**1b**.

$[\alpha]_D^{19}$ = –16.4 (*c* 0.84, $CHCl_3$) The spectroscopic data of the obtained product (*S*)-**1c** was in good agreement with racemate (±)-**1c**.

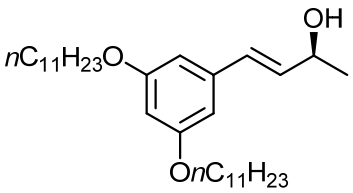
(*S*,*E*)-4-(4-(2,5,8,11-Tetraoxadodecyl)phenyl)but-3-en-2-ol [(*S*)-1d]



132 mg, 53% yield, >99% *ee* The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 80:20, 1.0 mL/min; retention times 12.0 (*S*), 14.8 min (*R*)): Prepared from (±)-**1d** (300 mg, 0.902 mmol), the immobilized *Candida antartica* lipase B (600 mg, 2.0 w/w), CH_3CN (11 mL, 0.08 M) according to the method for the synthesis of (*S*)-**1b**.

$[\alpha]_D^{19}$ = –16.1 (*c* 0.89, $CHCl_3$) The spectroscopic data of the obtained product (*S*)-**1d** was in good agreement with racemate (±)-**1d**.

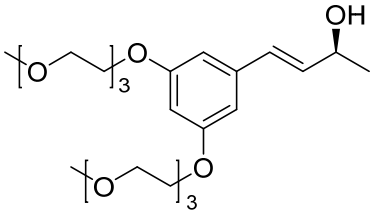
(*S*,*E*)-4-(3,5-Bis(undecyloxy)phenyl)but-3-en-2-ol [(*S*)-1e]



0.52 g, 47% yield, >99% *ee* The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 97.5:2.5, 1.0 mL/min; retention times 12.3 (*S*), 14.2 min (*R*)): Prepared from (±)-**1e** (1.10 g, 2.25 mmol), the immobilized *Candida antartica* lipase B (1.0 g, 1.0 w/w), CH_3CN (28 mL, 0.08 M) according to the method for the synthesis of (*S*)-**1b**.

$[\alpha]_D^{20}$ = –14.5 (*c* 0.32, $CHCl_3$) The spectroscopic data of the obtained product (*S*)-**1e** was in good agreement with racemate (±)-**1e**.

(*S*,*E*)-4-(3,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)but-3-en-2-ol [(*S*)-1f]



0.48 g, 48% yield, >99% *ee* The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 70:30, 1.0 mL/min; retention times 11.6 (*R*), 14.4 min (*S*)): Prepared from (±)-**1f** (1.10 g, 2.25 mmol), the immobilized *Candida antartica* lipase B (1.0 g, 1.0 w/w), CH_3CN (28 mL, 0.08 M) according to the method for the synthesis of (*S*)-**1b**.

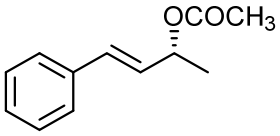
$[\alpha]_D^{20}$ = –10.7 (*c* 0.84, $CHCl_3$) The spectroscopic data of the obtained product (*S*)-**1f** was in good agreement with racemate (±)-**1f**.

DKR of (±)-1 and (±)-2

A typical procedure for DKR (Table 2, Entry 3)

Under an argon atmosphere, to a solution of the alcohol (±)-**2a** (50 mg, 0.33 mmol) in CH_3CN (4.2 mL, 0.08 M) were added the immobilized *Candida antartica* lipase B (CALB) (150 mg, 3.0 w/w), V-MPS4 (17 mg, 3.4 μmol of the vanadium component) and vinyl acetate (62 μL, 0.67 mmol) in this order at room temperature. The reaction mixture was stirred at 35 ºC for 24 h and then filtered through a Celite pad. The filtrate was concentrated under reduced pressure, and the residue was purified by column chromatography (silica gel, hexanes/EtOAc = 10:1) to give (*R*)-**3a** (61 mg, 95%, 98% *ee*). The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 6.1 (*R*), 7.3 min (*S*)).

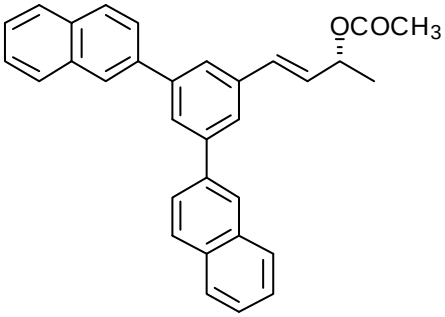
(*R*,*E*)-4-Phenyl-3-buten-2-yl acetate [(*R*)-3a] (Table 2, Entry 4)



(*R*)-**3a** was obtained in 98% yield with 98% *ee*.

A colorless oil. $[\alpha]_D^{27}$ = 117.8 (*c* 0.87, $CHCl_3$) (lit.[1] $[\alpha]_D^{27}$ = +125.1 (*c* 1.0, $CHCl_3$); 99% *ee*). The spectroscopic data of the obtained product (*R*)-**3a** was in good agreement with that in our previous publication.[1]

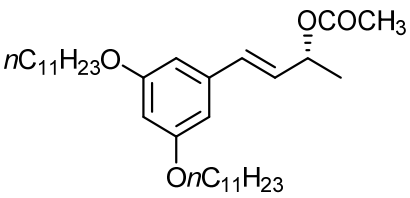
(*R*,*E*)-4-[3,5-Di(naphthalen-2-yl)phenyl)but-3-en-2-yl acetate [(*R*)-3b] (Table 3, entry 2)



(*R*)-**3b** was obtained in quantitative yield with >99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 90:10, 1.0 mL/min; retention times 14.4 (*R*), 17.3 min (*S*)).

A white solid. Mp 67–68 °C. $[\alpha]_D^{26}$ = +79.0 (*c* 0.52, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (s, 2H), 7.98–7.92 (m, 5H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.83 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.74 (d, *J* = 2.0 Hz, 2H), 7.56–7.49 (m, 4H), 6.81 (d, *J* = 16.0 Hz, 1H), 6.40 (dd, *J* = 16.0, 6.5 Hz, 1H), 5.65–5.58 (m, 1H), 2.12 (s, 3H), 1.48 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4, 142.1, 138.2, 137.5, 133.6, 132.7, 131.4, 129.7, 128.5, 128.2, 127.7, 126.4, 126.3, 126.1, 126.0, 125.6, 124.7, 71.0, 21.4, 20.4; IR (neat) ν 1732 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{32}H_{26}NaO_2$ [$(M+Na)^+$]: 465.1817. Found: 465.1825.

(*R*,*E*)-4-(3,5-Bis(undecyloxy)phenyl)but-3-en-2-yl acetate [(*R*)-3e] (Table 3, entry 4)

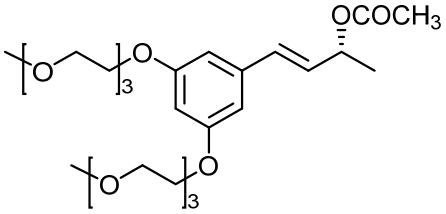


(*R*)-**3e** was obtained in 91% yield with >99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 6.7 (*R*), 9.3 (*S*) min).

A colorless oil. $[\alpha]_D^{27}$ = 54.0 (*c* 0.49, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.54–6.48 (m, 3H), 6.37 (t, *J* = 2.0 Hz, 1H), 6.15 (dd, *J* = 16.0, 7.0 Hz, 1H), 5.54–5.47 (m, 1H), 3.93 (t, *J* = 7.0 Hz, 4H), 2.07 (s, 3H), 1.76 (td, *J* = 7.0 Hz, 4H), 1.48–1.20 (m, 35H), 0.88 (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$)

δ 170.3, 160.4, 138.2, 131.6, 129.1, 105.1, 101.1, 70.9, 68.0, 31.9, 29.60, 29.57, 29.4, 29.33, 29.25, 26.0, 22.7, 21.4, 20.3, 14.1; IR (neat) ν 1740 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{34}H_{58}NaO_4$ [$(M+Na)^+$]: 553.4229. Found: 553.4227.

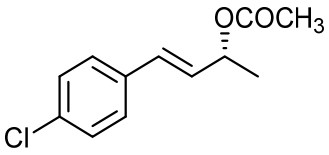
(*R*,*E*)-4-(3,5-Bis(2-(2-(2-methoxyethoxy)ethoxy)ethoxy)phenyl)but-3-en-2-yl acetate [(*R*)-3f] (Table 3, entry 6)



(*R*)-**3f** was obtained in quantitative yield with 99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 70:30, 1.0 mL/min; retention times 11.6 (*R*), 14.4 min (*S*)).

A colorless oil. $[\alpha]_D^{27}$ = +58.5 (*c* 1.04, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 6.53 (d, *J* = 2.0 Hz, 2H), 6.48 (d, *J* = 16.0 Hz, 1H), 6.39 (t, *J* = 2.0 Hz, 1H), 6.13 (dd, *J* = 16.0, 7.0 Hz, 1H), 5.52–5.45 (m, 1H), 4.09 (t, *J* = 4.5 Hz, 4H), 3.83 (t, *J* = 4.5 Hz, 4H), 3.74–3.71 (m, 4H), 3.69–3.63 (m, 8H), 3.56–3.52 (m, 4H), 3.37 (s, 6H), 2.06 (s, 3H), 1.38 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 156.0, 138.2, 131.3, 129.3, 105.5, 101.4, 71.9, 70.8, 70.6, 70.5, 69.6, 67.4, 59.0, 21.3, 20.3; IR (neat) ν 1734 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{26}H_{42}NaO_{10}$ [$(M+Na)^+$]: 537.2675. Found: 537.2670.

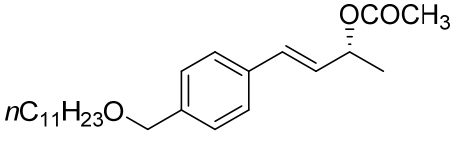
(*R*,*E*)-4-(4-Chlorophenyl)-3-buten-2-yl acetate [(*R*)-3g] (Table 3, entry 8)



(*R*)-**3g** was obtained in 97% yield with 98% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL OD-3 column (hexanes, 0.8 mL/min; retention times 34.8 (*R*), 46.8 min (*S*)).

A colorless oil. $[\alpha]_D^{26}$ = +133.3 (*c* 0.93, $CHCl_3$) (lit.[1] $[\alpha]_D^{27}$ = +131.9 (*c* 0.39, $CHCl_3$); 97% *ee*). The spectroscopic data of the obtained product (*R*)-**3g** was in good agreement with that in our previous publication.[1]

(*R*,*E*)-4-(4-[(Undecyloxy)methyl]phenyl)but-3-en-2-yl acetate [(*R*)-3c] (Table 3, entry 11)

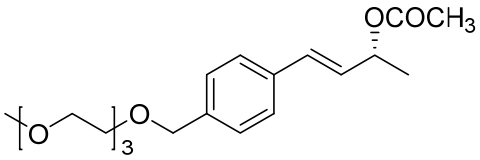


(*R*)-**3c** was obtained in 92% yield with 98% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 6.1 (*R*), 7.1 min (*S*)).

A colorless oil. $[\alpha]_D^{27}$ = 83.0 (*c* 0.87, $CHCl_3$). ^1H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.60 (d, *J* = 16, 1H), 6.20 (dd, *J* = 16, 7.0 Hz, 1H), 5.52 (quint, *J* = 7.0 Hz, 1H), 4.48 (s, 2H), 3.44 (t, *J* = 7.0 Hz 2H), 2.07 (s, 3H), 1.60 (quint, *J* = 7.0 Hz, 2H), 1.60 (quint, *J* = 7.0 Hz, 2H), 1.41 (d, *J* = 7.0 Hz, 3H), 1.36-1.26 (m, 16H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 138.5, 135.6, 131.3, 128.6, 127.8, 126.5, 72.5, 71.0, 70.5, 31.9, 29.7, 29.6, 29.5, 29.3,

26.2, 22.7, 21.4, 20.4, 14.1; IR ($CHCl_3$) ν 1739 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{24}H_{38}NaO_3$ [$(M+Na)^+$]: 397.2718. Found: 397.2713.

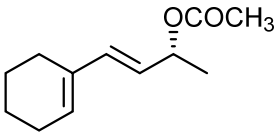
(*R*,*E*)-4-(4-(2,5,8,11-Tetraoxadodecyl)phenyl)but-3-en-2-yl acetate [(*R*)-3d] (Table 3, entry 14)



(*R*)-**3d** was obtained in 90% yield with 98% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 90:10, 1.0 mL/min; retention times 11.8 (*R*), 13.5 (*S*) min).

A colorless oil. $[\alpha]_D^{27}$ = 78.9 (*c* 0.79, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 6.60 (d, *J* = 16.0 Hz, 1H), 6.20 (dd, *J* = 16.0, 7.0 Hz, 1H), 5.52 (quint, *J* = 7.0 Hz, 1H), 4.54 (s, 2H), 3.68–3.53(m, 12H), 3.37 (s, 3H), 2.07 (s, 3H), 1.41 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 138.0, 135.7, 131.2, 128.7, 127.9, 126.5, 72.9, 71.9, 71.0, 70.6, 70.5, 69.4, 59.0, 21.4, 20.3; IR ($CHCl_3$) ν 1730 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{20}H_{30}NaO_6$ [$(M+Na)^+$]: 389.1935. Found: 389.1935.

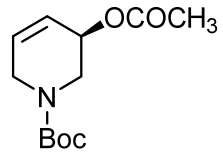
(*R*,*E*)-4-(1-Cyclohexen-1-yl)-3-buten-2-yl acetate [(*R*)-3h] (Table 3, entry 16)



(*R*)-**3h** was obtained in 94% yield with 98% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 4.9 (*R*), 5.9 min (*S*)).

A colorless oil. $[\alpha]_D^{26}$ = +93.3 (*c* 0.98, $CHCl_3$) (lit.[1] $[\alpha]_D^{28}$ = +116.9 (*c* 0.17, $CHCl_3$); 95% *ee*). The spectroscopic data of the obtained product (*R*)-**3h** was in good agreement with that in our previous publication.[1]

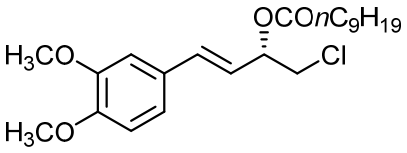
(*R*)-*N*-*tert*-Butoxycarbonyl-5-acetoxy-3-piperidene [(*R*)-3i] (Table 3, entry 18)



(*R*)-**3i** was obtained in 87% yield with 96% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 13.8 (*S*), 15.2 min (*R*)).

A colorless oil. $[\alpha]_D^{26}$ = –97.1 (*c* 0.87, $CHCl_3$) (lit.[1] $[\alpha]_D^{28}$ = –97.0 (*c* 0.65, $CHCl_3$); 97% *ee*). The spectroscopic data of the obtained product (*R*)-**3i** was in good agreement with that in our previous publication.[1]

(*S*,*E*)-1-Chloro-4-(3,4-dimethoxyphenyl)-3-buten-2-yl decanoate [(*S*)-3j] (Table 3, entry 20)

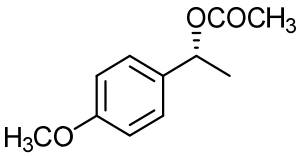


(*S*)-**3j** was obtained in 94% yield with >99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 95:5, 1.0 mL/min; retention times 8.6 (*S*), 12.8 min (*R*)).

A colorless oil. $[\alpha]_D^{26}$ = +48.6 (*c* 0.96, $CHCl_3$) (lit.[1] $[\alpha]_D^{27}$ = +51.4 (*c* 0.81,

$CHCl_3$); 99% *ee*). The spectroscopic data of the obtained product (*S*)-**3j** was in good agreement with that in our previous publication.[1]

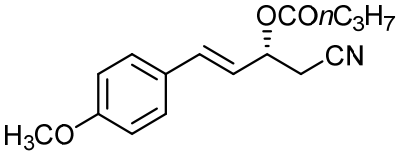
(*R*)-1-(4-Methoxyphenyl)ethyl acetate [(*R*)-3k] (Table 3, entry 22)



(*R*)-**3k** was obtained in 99% yield with >99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 8.6 (*R*), 14.1 min (*S*)).

A colorless oil. $[\alpha]_D^{27}$ = 137.5 (*c* 1.00, $CHCl_3$) (lit.[1] $[\alpha]_D^{28}$ = +124.5 (*c* 0.58, $CHCl_3$); 99% *ee*). The spectroscopic data of the obtained product (*R*)-**3k** was in good agreement with that in our previous publication.[1]

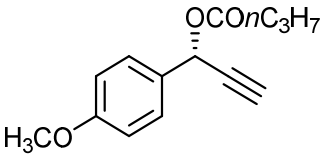
(*R,E*)-1-Cyano-4-(4-methoxyphenyl)but-3-en-2-yl butyrate [(*R*)-3m] (Table 3, entry 26)



(*R*)-**3m** was obtained in 81% yield with >99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 95:5, 1.0 mL/min; retention times 20.1 (*R*), 23.5 min (*S*)).

A yellow oil. $[\alpha]_D^{27}$ = 97.1 (*c* 0.97 $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 9.0, 2.0 Hz, 2H), 6.87 (dd, *J* = 5.0, 2.0 Hz, 2H), 7.00 (d, *J* = 16.0 Hz, 1H), 6.05 (dd, *J* = 16.0, 8.0 Hz, 1H), 5.60 (dt, *J* = 10.0, 8.0 Hz, 1H), 3.82 (s, 3H), 2.83 (dd, *J* = 17.0, 5.0 Hz, 1H), 2.75 (dd, *J* = 17.0, 5.0 Hz, 1H), 2.36 (dt, *J* = 7.0, 2.0 Hz, 2H), 1.69 (sext., *J* = 7.5 Hz, 2H), 0.97 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.4, 160.0, 134.7, 128.2, 127.9, 121.3, 116.1, 114.1, 69.4, 55.3, 36.1, 24.1, 18.3, 13.6; IR (neat) ν 2253, 1739 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{16}H_{19}NNaO_3$ [$(M+Na)^+$]: 296.1257. Found: 296.1257.

(*R*)-1-(4-Methoxyphenyl)prop-2-yn-1-yl butyrate [(*R*)-3n] (Table 3, entry 27)



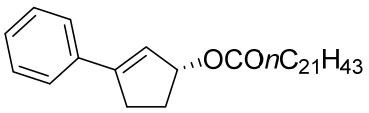
(*R*)-**3n** was obtained in 96% yield with 99% *ee*. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL AD-3 column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 12.0 (*R*), 13.2 min (*S*)).

A colorless oil. $[\alpha]_D^{27}$ = 24.5 (*c* 1.23, $CHCl_3$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8 Hz, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.43 (d, *J* = 2.0 Hz, 1H), 3.81 (s, 3H), 2.63 (d, *J* = 2.0 Hz, 1H), 2.82-2.36 (m, 2H), 1.62-1.70 (m, 2H), 0.93 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.4, 160.1, 129.2, 128.8, 114.0, 80.6, 75.0, 64.7, 55.3, 36.1, 18.3, 13.5; IR (neat) ν 3288, 1733 cm^{-1}. HRMS (ESI) *m*/*z* calcd for $C_{14}H_{17}O_3$ [M^+]: 233.1174. Found: 233.1172

(*R*)-3-Phenylcyclopent-2-en-1-yl docosanoate [(*R*)-3l] (Table 3, entry 23)

Under an argon atmosphere, to a solution of (±)-**2l** (40 mg, 0.25 mmol) in *i*Pr_2O (3.0 mL, 0.08 M) were added immobilized *Candida antartica* lipase B (CALB) (40 mg, 1.0 w/w), V-MPS2 (0.62 g, 12.5 μmol of the vanadium

component) and 2,2,2-trifluoroethyl docosanate (32 mg, 0.075 mmol) at room temperature, and the reaction mixture was stirred at 35 °C for 12 h. 2,2,2-Trifluoroethyl docosanate (32 mg, 0.075 mmol) was added after 12 and 24 h, and the reaction mixture was stirred for total 36 h. The reaction mixture was filtered through a Celite pad. The filtrate was concentrated under reduced pressure, and the residue was purified by column chromatography (silica gel, hexanes/EtOAc/Et_3N = 100:5:1) to give (*R*)-**3l** (95 mg, 79%, 94% *ee*) as a white solid. The optical purity was determined by HPLC analysis at 20 °C, using a CHIRALCEL IE column (hexanes/2-propanol = 99:1, 1.0 mL/min; retention times 6.0 (*R*), 6.7 min (*S*)).



Mp 92–93 °C. $[\alpha]_D^{27}$ = 63.0 (*c* 0.45, $CHCl_3$). ^{1}H NMR (500 MHz, C_6D_6) δ 7.27 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.13–7.04 (m, 3H), 6.30 (d, *J* = 2.0 Hz, 1H), 5.94 (dd, *J* = 7.5, 2.0 Hz, 1H), 2.68–2.59 (m, 1H), 2.33–2.15 (m, 4H), 1.98–1.90 (m, 1H), 1.70–1.61 (m, 2H), 1.40–1.18 (m, 36H), 0.92 (t, *J* =6.5 Hz, 3H); ^{13}C NMR (125 MHz, C_6D_6) δ 173.1, 148.2, 135.7, 128.6, 128.3, 126.5, 124.1, 80.7, 34.7, 32.3, 31.6, 30.5, 30.2, 30.1, 30.0, 29.9, 29.8, 29.7, 29.5, 25.4, 23.1, 14.3; IR ($CHCl_3$) ν 1733 cm^{-1}. HRMS (EI) *m*/*z* calcd for $C_{33}H_{54}O_2$ [$(M+H)^+$]: 482.4124. Found: 482.4130.

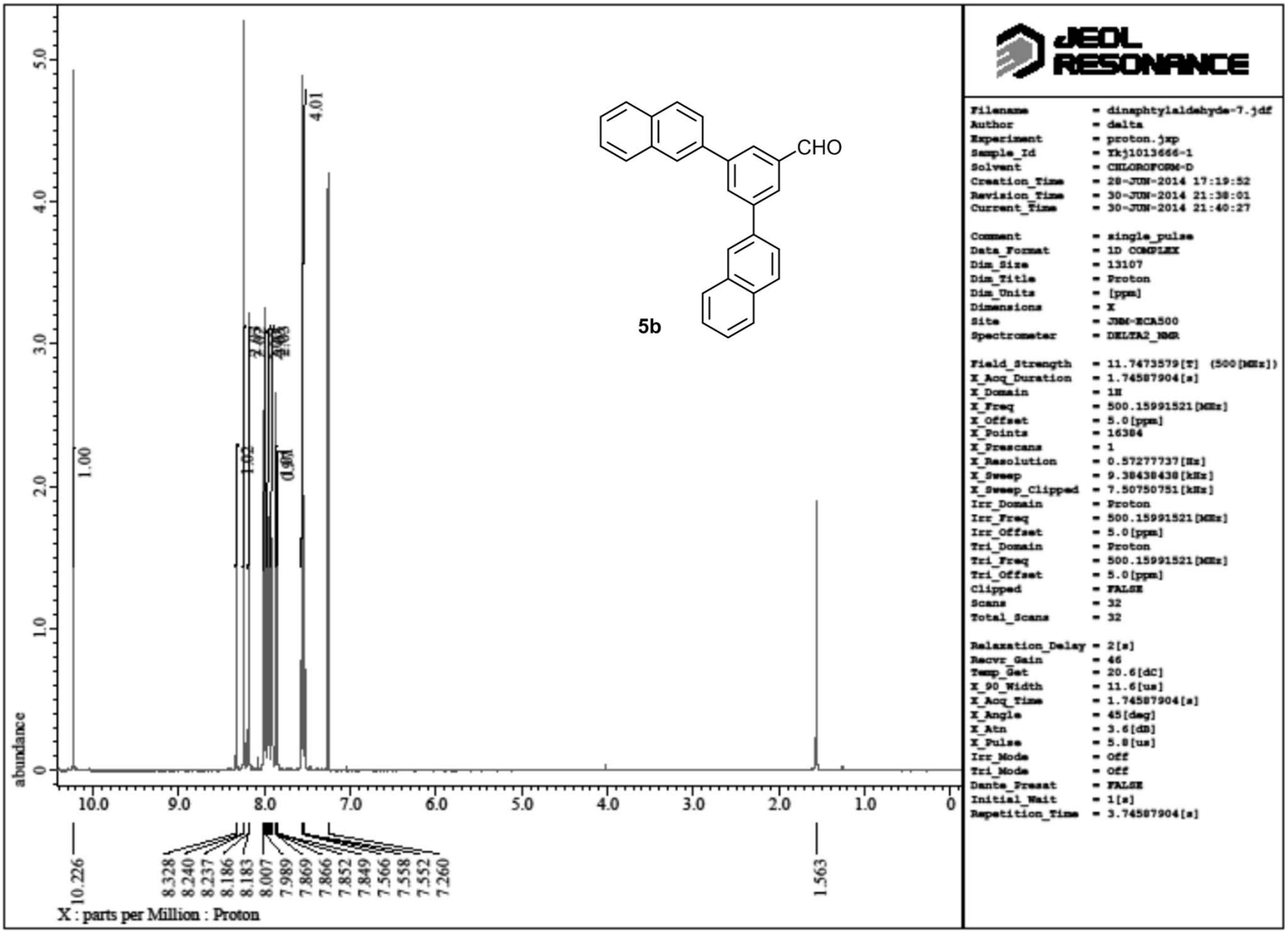
References

1 M. Egi, K. Sugiyama, M. Saneto, R. Hanada, K. Kato, S. Akai, *Angew. Chem. Int. Ed.* 2013, **52**, 3654–3658.

2 J. A. McCubbin, S. Voth, O. V. Krokhin, *J. Org. Chem.* 2011, **76**, 8537–8542. (b) J. A. McCubbin, H. Hosseini, O. V. Krokhin, *J. Org. Chem.* 2010, **75**, 959–962.

3 S. Akai, S. Ishida, K. Hatanaka, T. Ishii, N. Harada, H. Tsukada, N. Oku, *Mol. Pharm.* 2011, **8**, 302–308.

4 A. Träff, R. Lihammar, J.-E. Bäckvall, *J. Org. Chem.* 2011, **76**, 3917–3921.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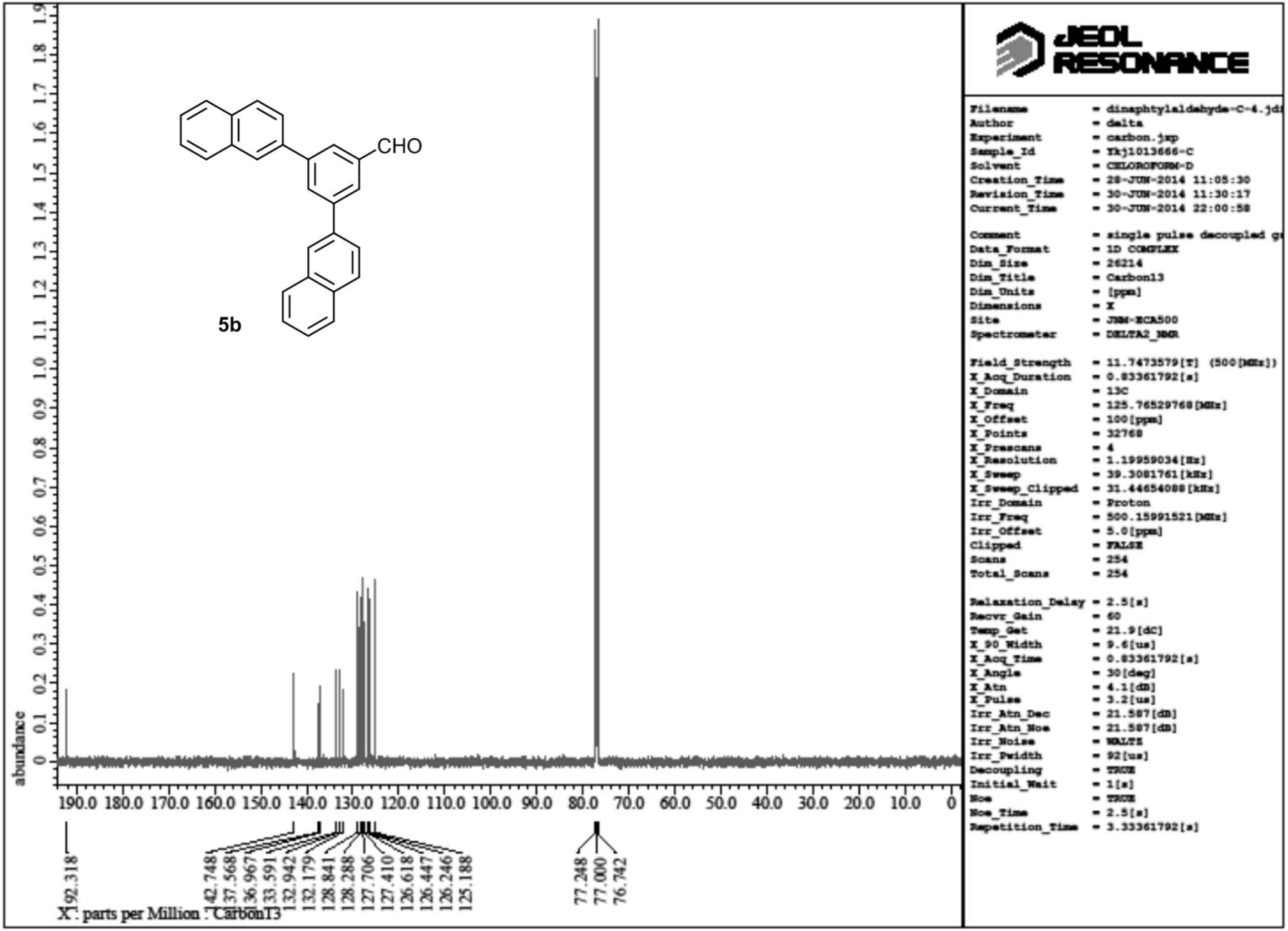
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137.568
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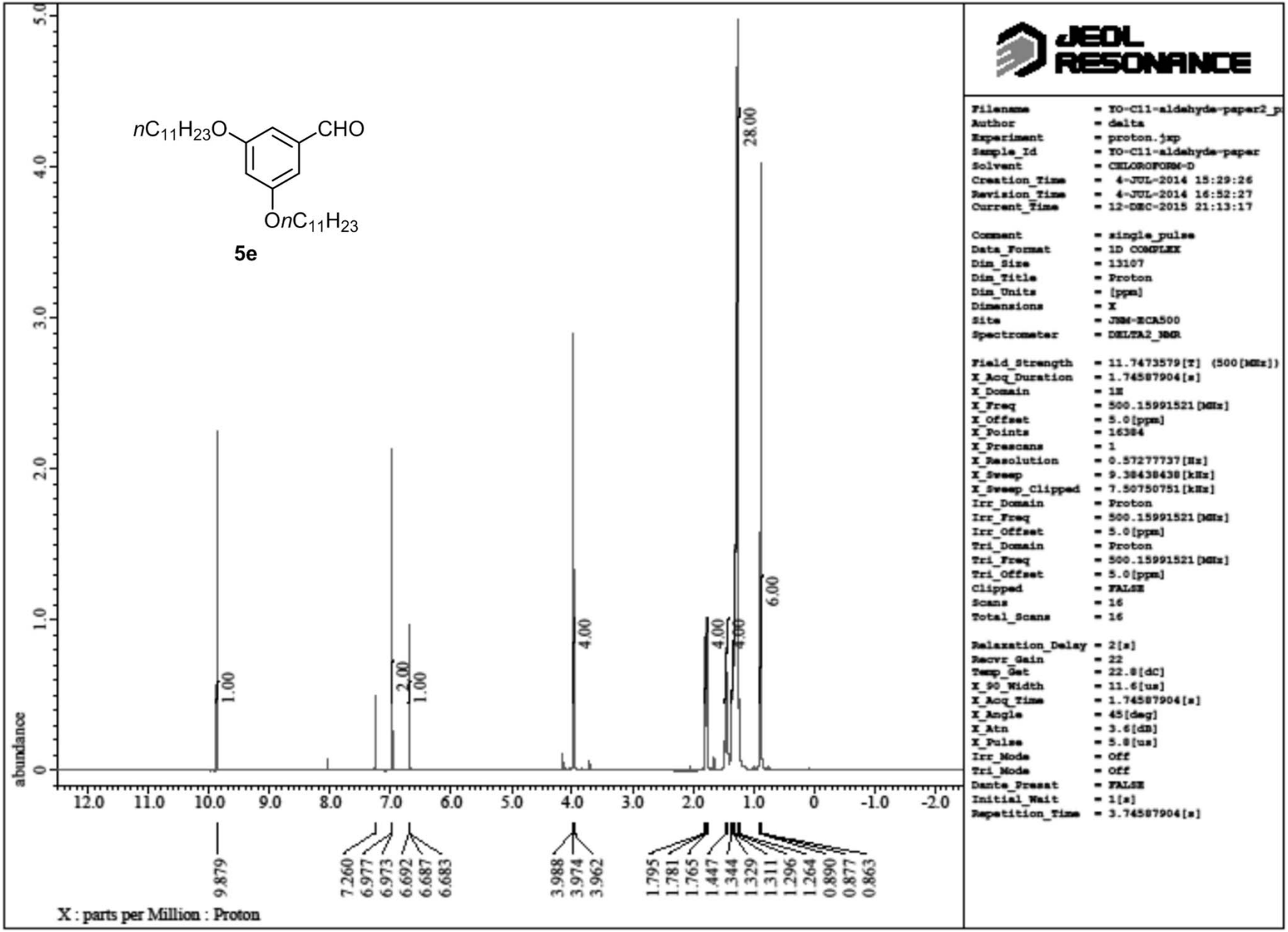
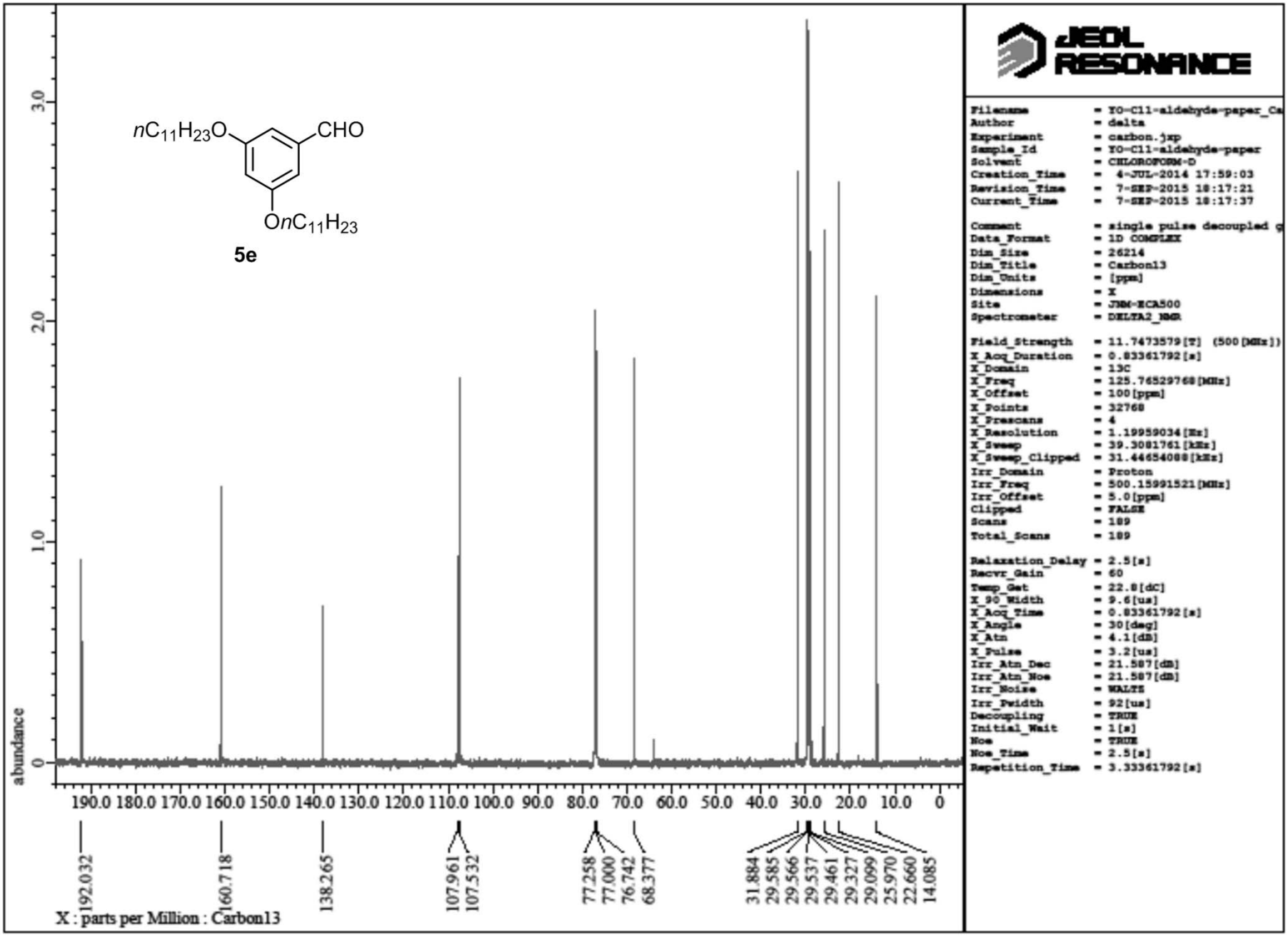
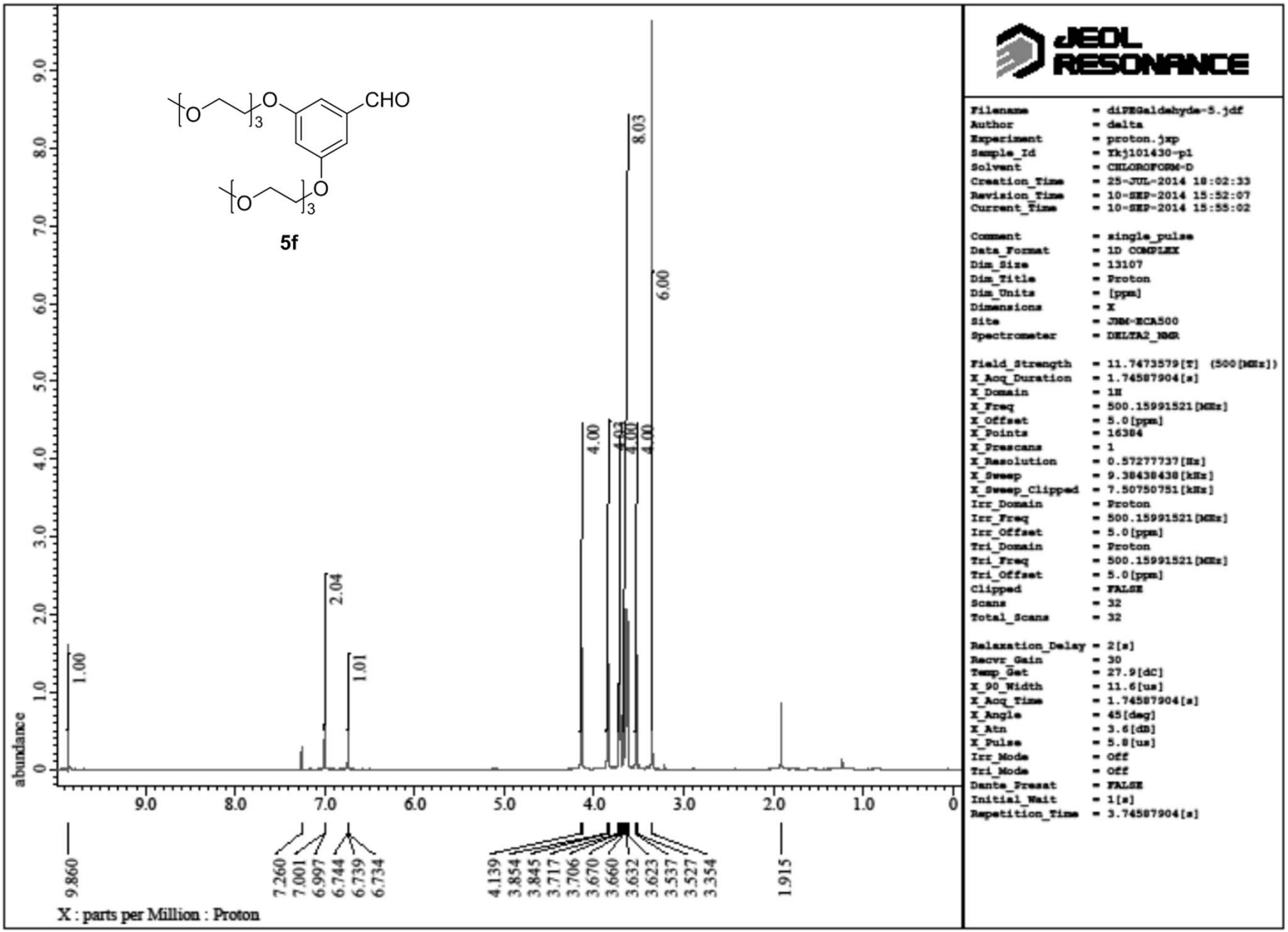
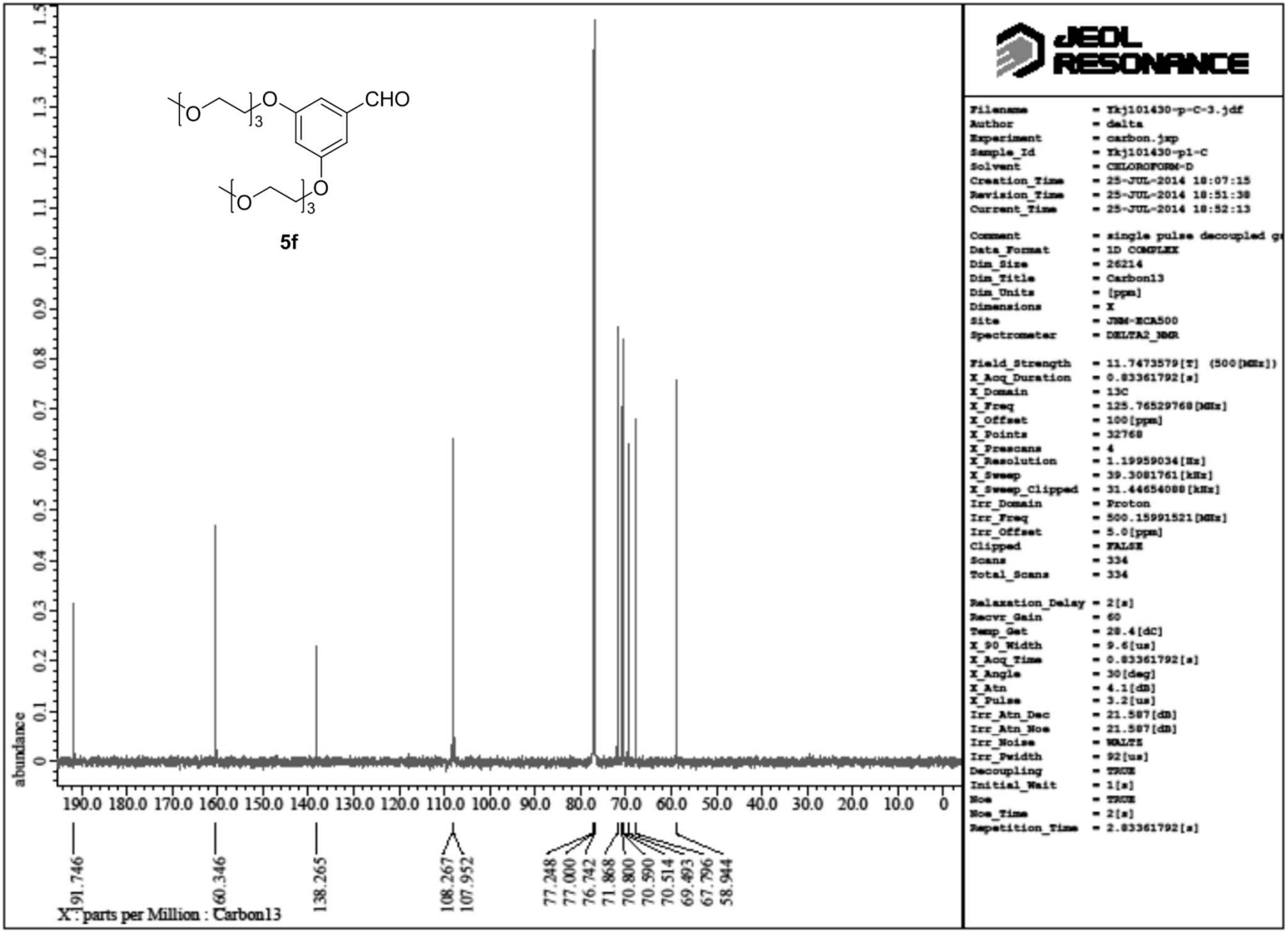
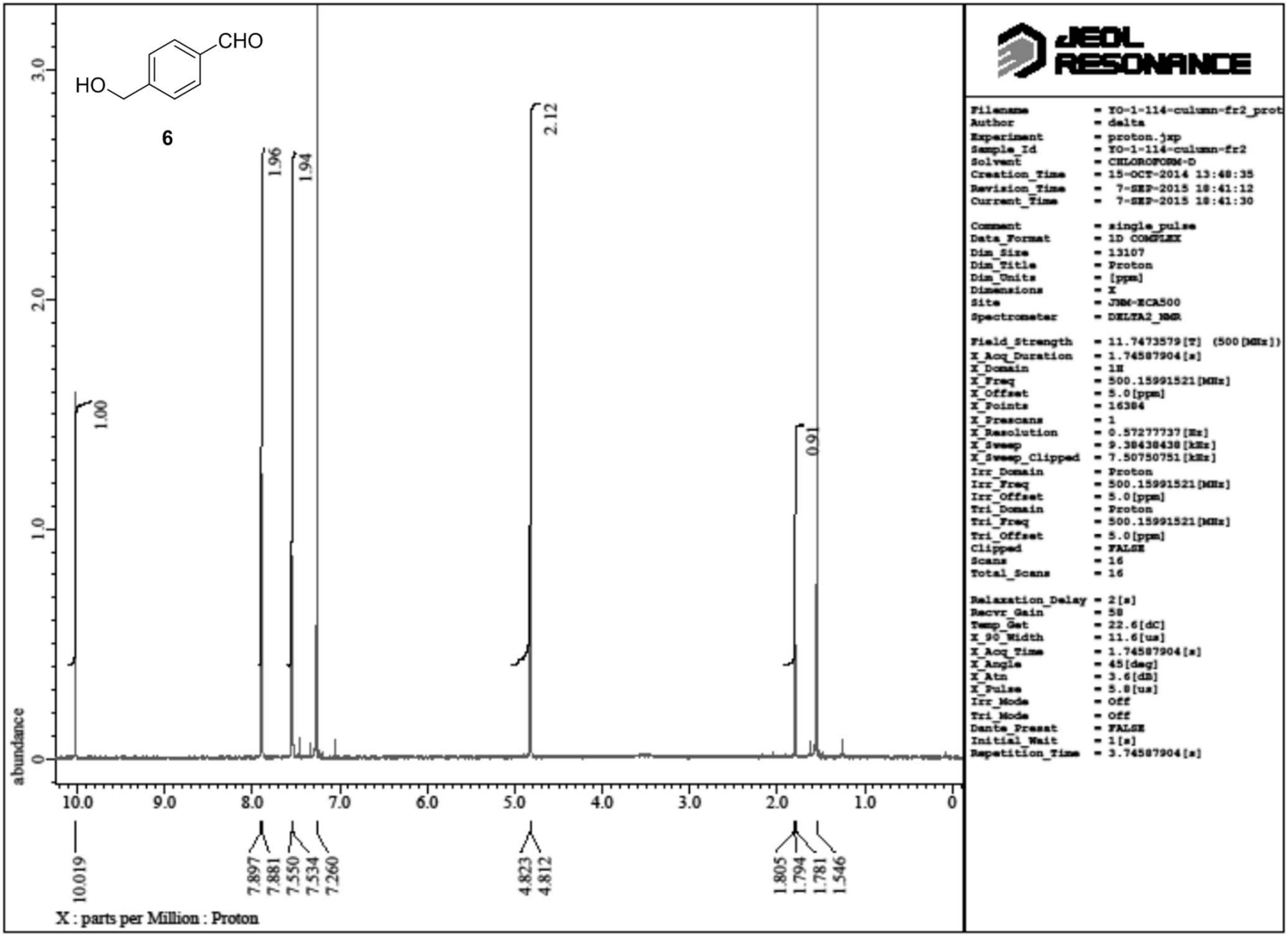
133.591
132.942
132.179
128.841
128.288
127.706
127.410
126.618
126.447
126.246
125.188
77.248
77.000
76.742
X: parts per Million : Carbon13
JEOL RESONANCE
Filename = dinaphtylaldehyde-C-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj1013666-C
Solvent = CHLOROFORM-D
Creation_Time = 28-JUN-2014 11:05:30
Revision_Time = 30-JUN-2014 11:30:17
Current_Time = 30-JUN-2014 22:00:58
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 254
Total_Scans = 254
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 21.9[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

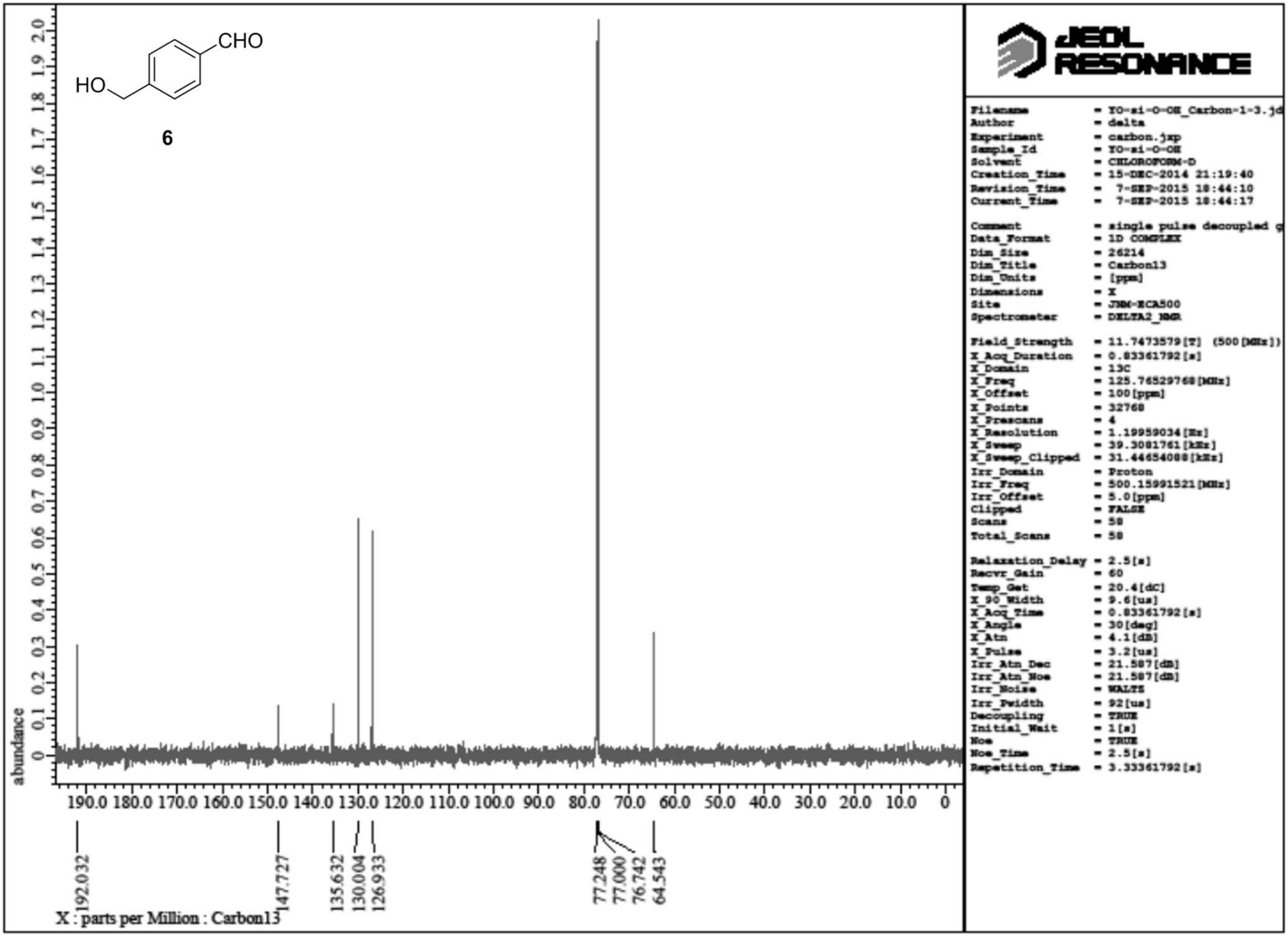

nC11H23O
CHO
OnC11H23
5e
abundance
X : parts per Million : Proton
1.00
2.00
1.00
4.00
4.00
4.00
6.00
28.00
9.879
7.260
6.977
6.973
6.692
6.687
6.683
3.988
3.974
3.962
1.795
1.781
1.765
1.447
1.344
1.329
1.311
1.296
1.264
0.890
0.877
0.863
JEOL RESONANCE
Filename = YO-C11-aldehyde-paper2_p
Author = delta
Experiment = proton.jxp
Sample_Id = YO-C11-aldehyde-paper
Solvent = CHLOROFORM-D
Creation_Time = 4-JUL-2014 15:29:26
Revision_Time = 4-JUL-2014 16:52:27
Current_Time = 12-DEC-2015 21:13:17
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 22
Temp_Get = 22.8[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

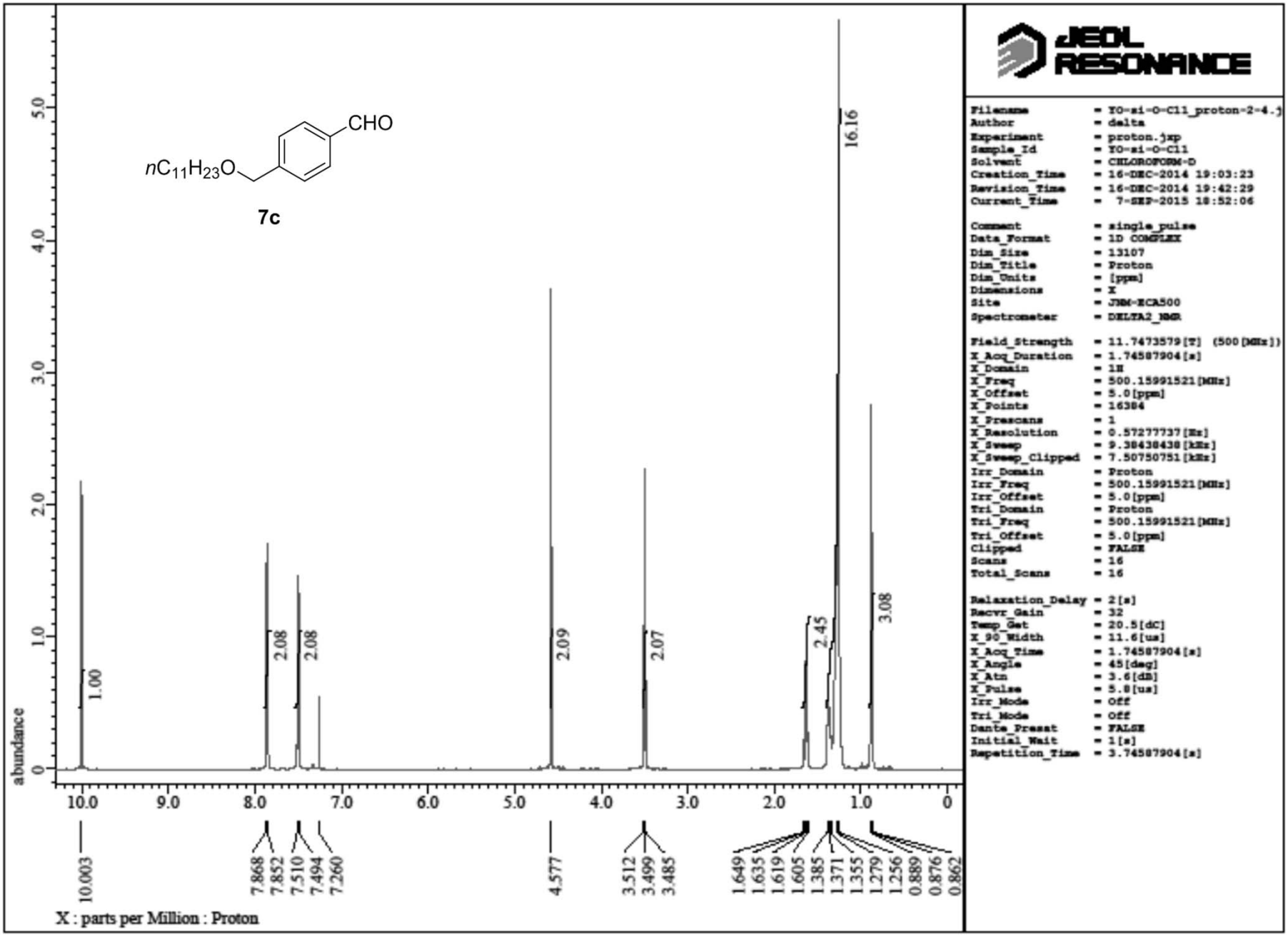

nC11H23O
CHO
OnC11H23
5e
abundance
3.0
2.0
1.0
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
192.032
160.718
138.265
107.961
107.532
77.258
77.000
76.742
68.377
31.884
29.585
29.566
29.537
29.461
29.327
29.099
25.970
22.660
14.085
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-C11-aldehyde-paper_Ca
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-C11-aldehyde-paper
Solvent = CHLOROFORM-D
Creation_Time = 4-JUL-2014 17:59:03
Revision_Time = 7-SEP-2015 18:17:21
Current_Time = 7-SEP-2015 18:17:37
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 189
Total_Scans = 189
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 22.8[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

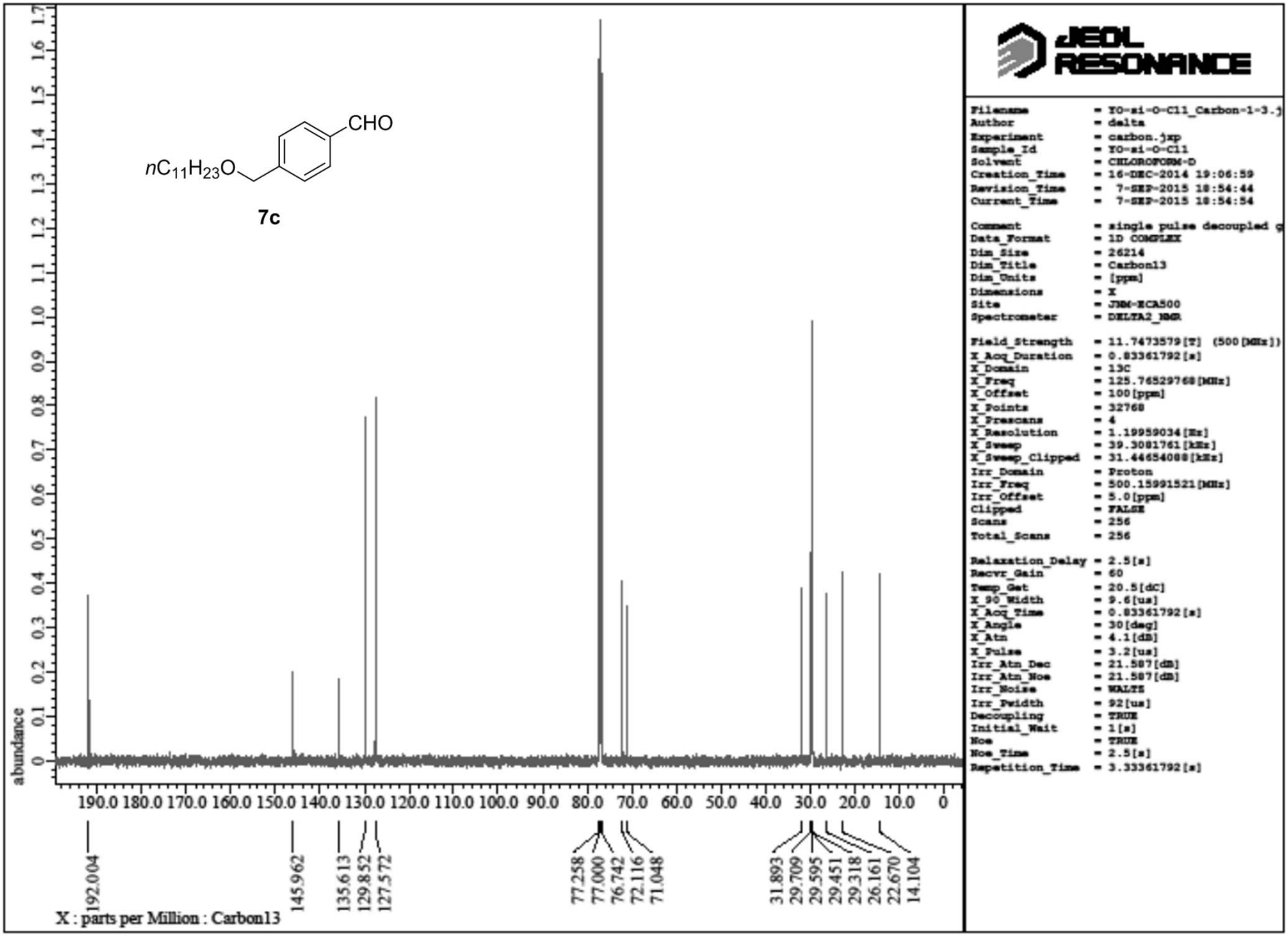

5f
CHO
O
3
abundance
1.00
2.04
1.01
4.00
4.03
4.00
4.00
8.03
6.00
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.860
7.260
7.001
6.997
6.744
6.739
6.734
4.139
3.854
3.845
3.717
3.706
3.670
3.660
3.632
3.623
3.537
3.527
3.354
1.915
X : parts per Million : Proton
JEOL RESONANCE
Filename = diPEGaldehyde-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101430-p1
Solvent = CHLOROFORM-D
Creation_Time = 25-JUL-2014 18:02:33
Revision_Time = 10-SEP-2014 15:52:07
Current_Time = 10-SEP-2014 15:55:02
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 30
Temp_Get = 27.9[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

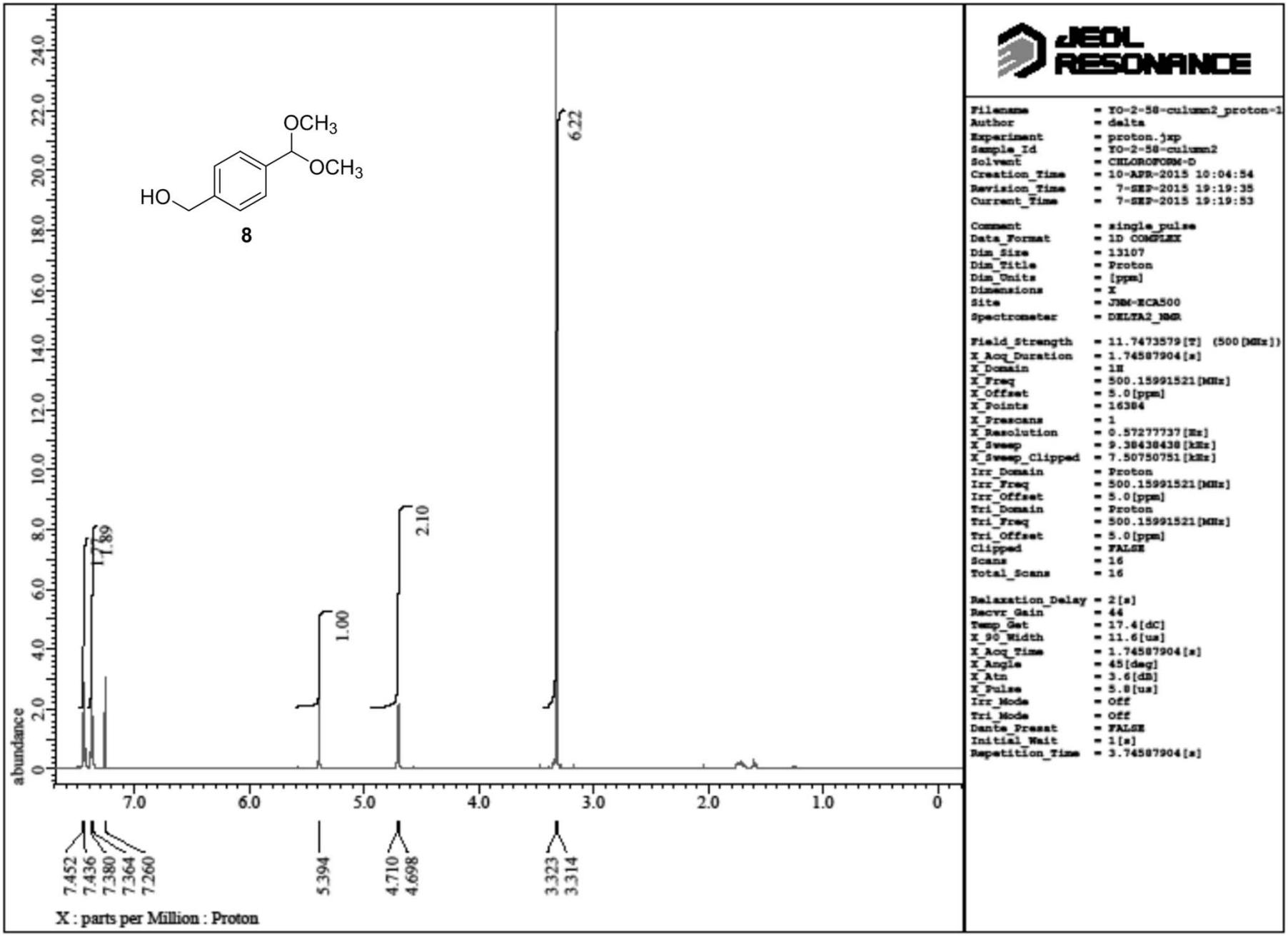

CHO
5f
abundance
X : parts per Million : Carbon13
191.746
160.346
138.265
108.267
107.952
77.248
77.000
76.742
71.868
70.800
70.590
70.514
69.493
67.796
58.944
JEOL RESONANCE
Filename = Ykj101430-p-C-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj101430-p1-C
Solvent = CHLOROFORM-D
Creation_Time = 25-JUL-2014 18:07:15
Revision_Time = 25-JUL-2014 18:51:38
Current_Time = 25-JUL-2014 18:52:13
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 334
Total_Scans = 334
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 28.4[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]

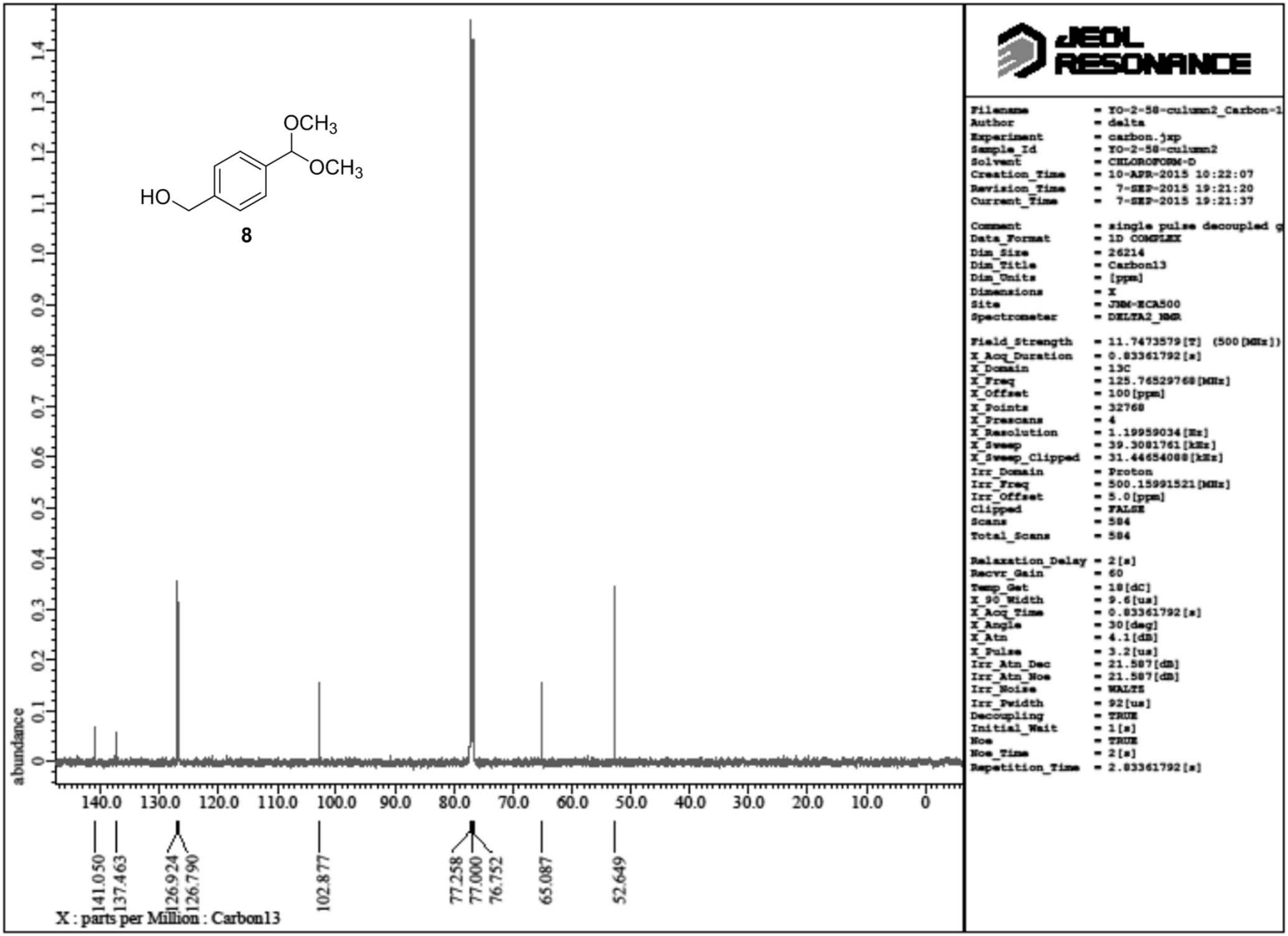

CHO
HO
6
1.96
1.94
2.12
1.00
0.91
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.019
7.897
7.881
7.550
7.534
7.260
4.823
4.812
1.805
1.794
1.781
1.546
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-1-114-column-fr2_prot
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-114-column-fr2
Solvent = CHLOROFORM-D
Creation_Time = 15-OCT-2014 13:48:35
Revision_Time = 7-SEP-2015 18:41:12
Current_Time = 7-SEP-2015 18:41:30
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 22.6[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]


CHO
HO
6
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
192.032
147.727
135.632
130.004
126.933
77.248
77.000
76.742
64.543
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-si-O-OH_Carbon-1-3.jd
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-si-O-OH
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2014 21:19:40
Revision_Time = 7-SEP-2015 18:44:10
Current_Time = 7-SEP-2015 18:44:17
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 58
Total_Scans = 58
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.4[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]


CHO
nC11H23O
7c
abundance
1.00
2.08
2.08
2.09
2.07
2.45
16.16
3.08
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.003
7.868
7.852
7.510
7.494
7.260
4.577
3.512
3.499
3.485
1.649
1.635
1.619
1.605
1.385
1.371
1.355
1.279
1.256
0.889
0.876
0.862
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-si-O-C11_proton-2-4.j
Author = delta
Experiment = proton.jxp
Sample_Id = YO-si-O-C11
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2014 19:03:23
Revision_Time = 16-DEC-2014 19:42:29
Current_Time = 7-SEP-2015 18:52:06
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 32
Temp_Get = 20.5[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

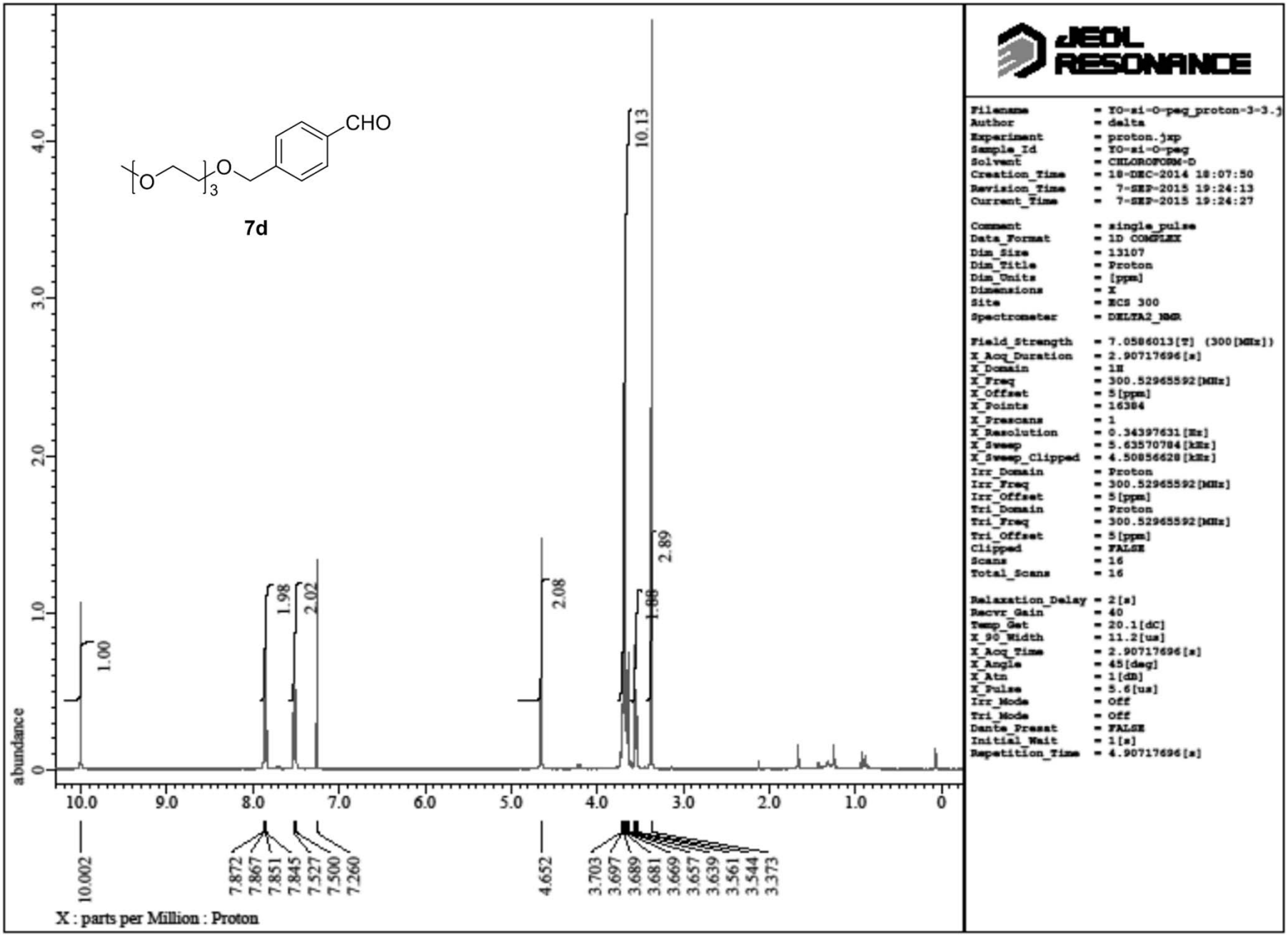

CHO
nC11H23O
7c
abundance
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
192.004
145.962
135.613
129.852
127.572
77.258
77.000
76.742
72.116
71.048
31.893
29.709
29.595
29.451
29.318
26.161
22.670
14.104
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-zi-O-C11_Carbon-1-3.j
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-zi-O-C11
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2014 19:06:59
Revision_Time = 7-SEP-2015 18:54:44
Current_Time = 7-SEP-2015 18:54:54
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 256
Total_Scans = 256
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.5[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

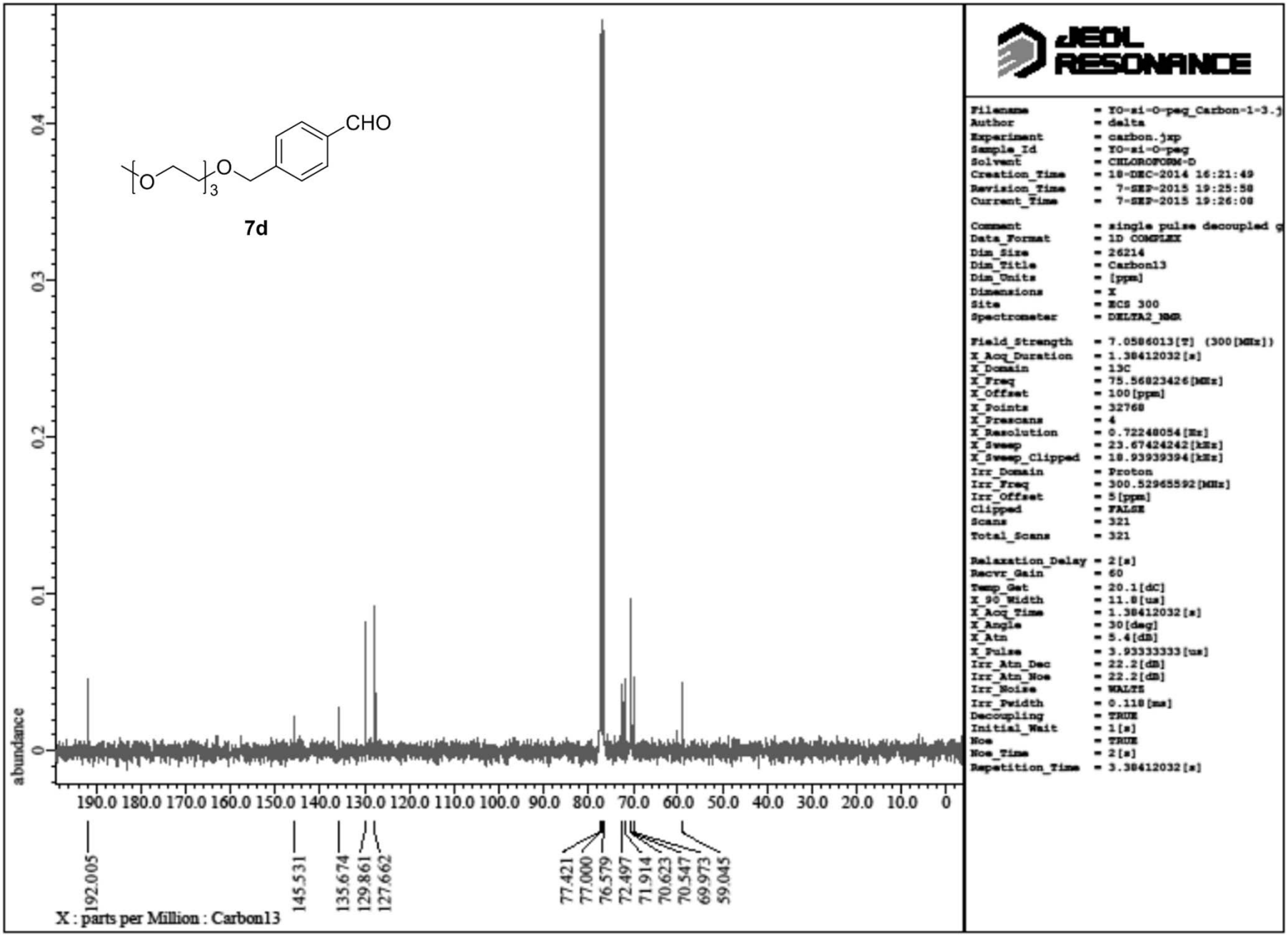

OCH3
OCH3
HO
8
6.22
2.10
1.89
1.77
1.00
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.452
7.436
7.380
7.364
7.260
5.394
4.710
4.698
3.323
3.314
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-2-58-column2_proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = YO-2-58-column2
Solvent = CHLOROFORM-D
Creation_Time = 10-APR-2015 10:04:54
Revision_Time = 7-SEP-2015 19:19:35
Current_Time = 7-SEP-2015 19:19:53
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 44
Temp_Get = 17.4[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

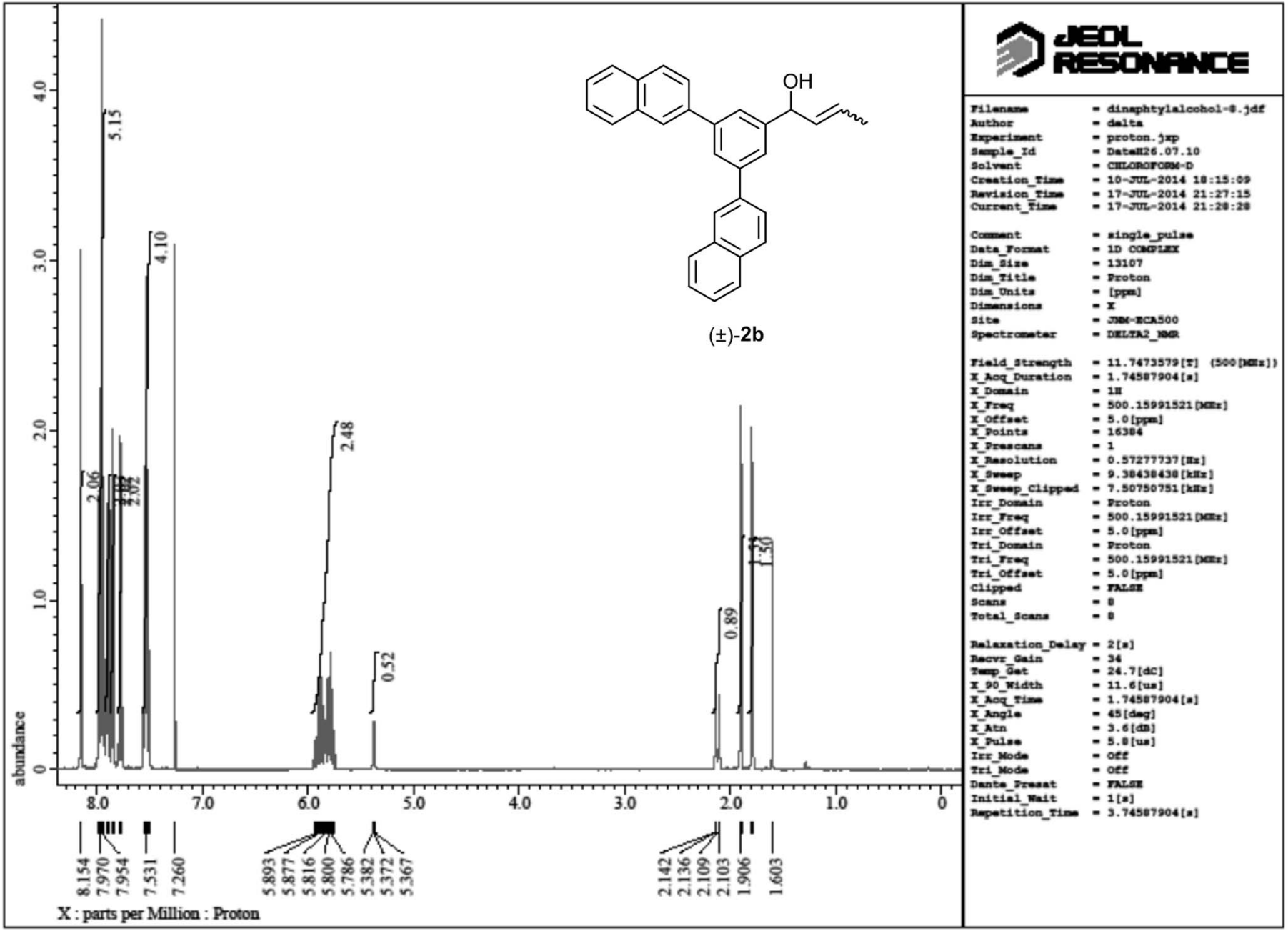


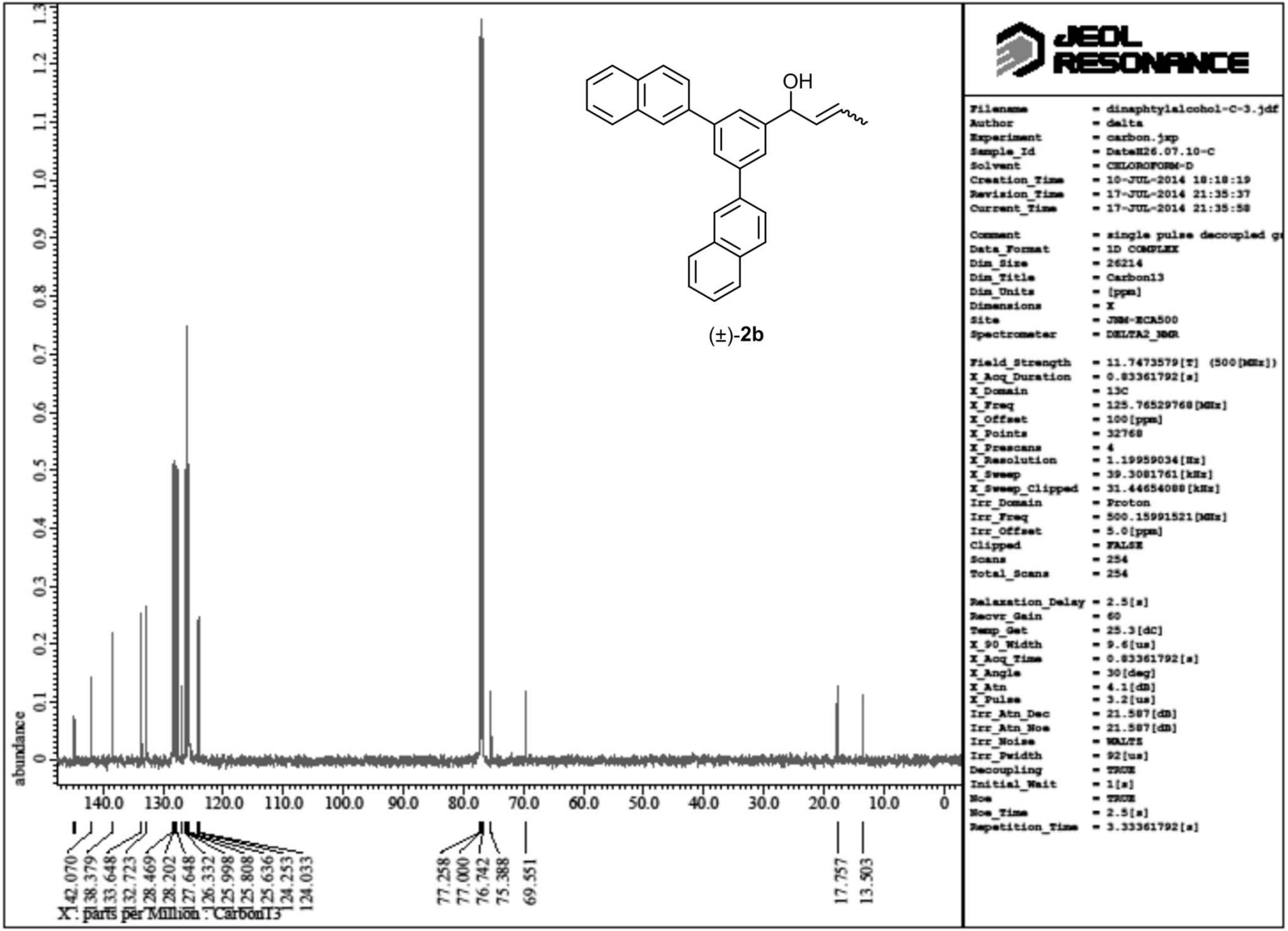
JEOL RESONANCE

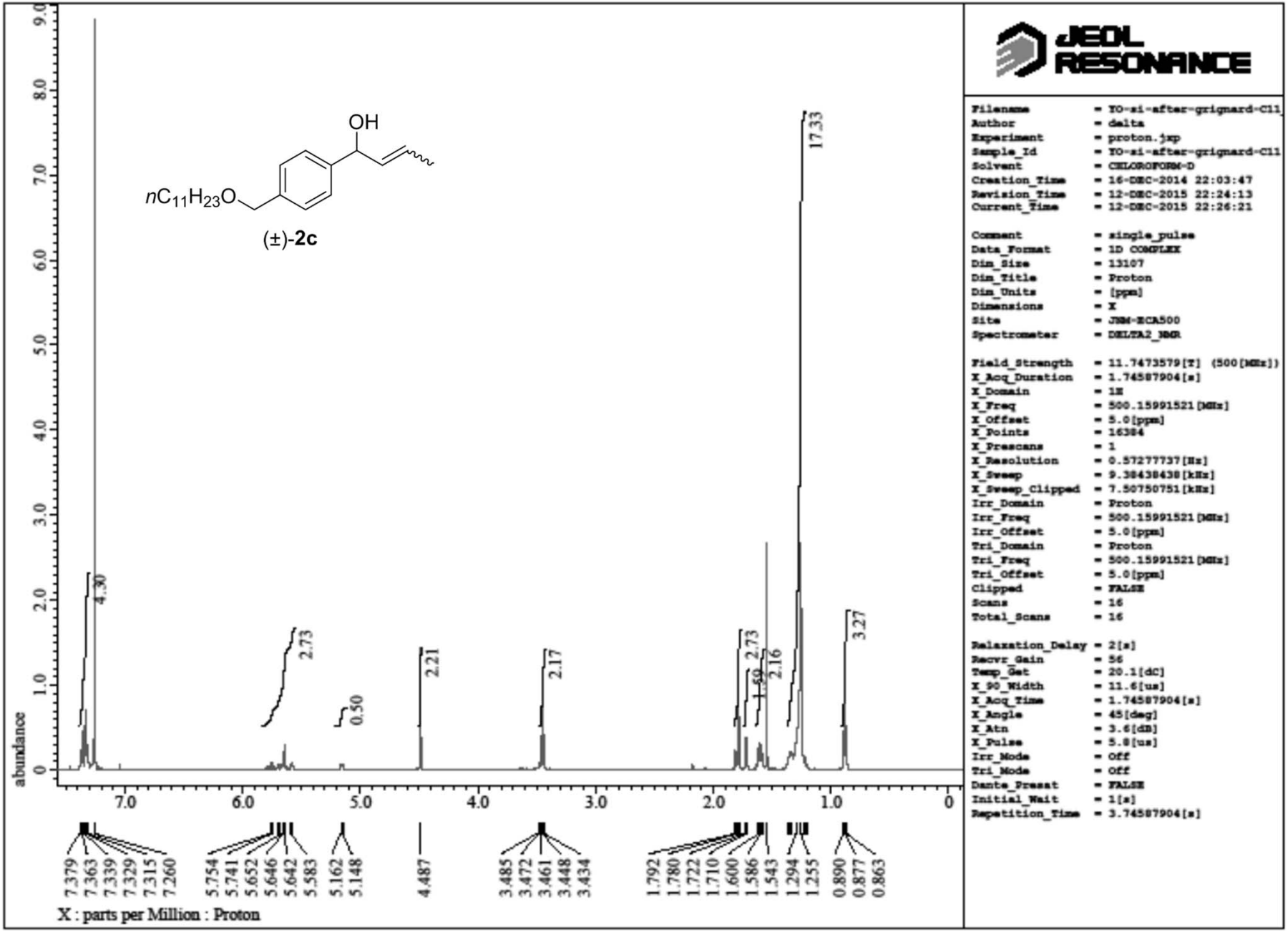
Filename	= YO-2-58-column2_Carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= YO-2-58-column2
Solvent	= CHLOROFORM-D
Creation_Time	= 10-APR-2015 10:22:07
Revision_Time	= 7-SEP-2015 19:21:20
Current_Time	= 7-SEP-2015 19:21:37
Comment	= single pulse decoupled g
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 13C
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
X_Sweep_Clipped	= 31.44654088[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 584
Total_Scans	= 584
Relaxation_Delay	= 2[s]
Recvr_Gain	= 60
Temp_Get	= 18[dC]
X_90_Width	= 9.6[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 4.1[dB]
X_Pulse	= 3.2[us]
Irr_Atn_Dec	= 21.587[dB]
Irr_Atn_Noe	= 21.587[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 92[us]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.83361792[s]

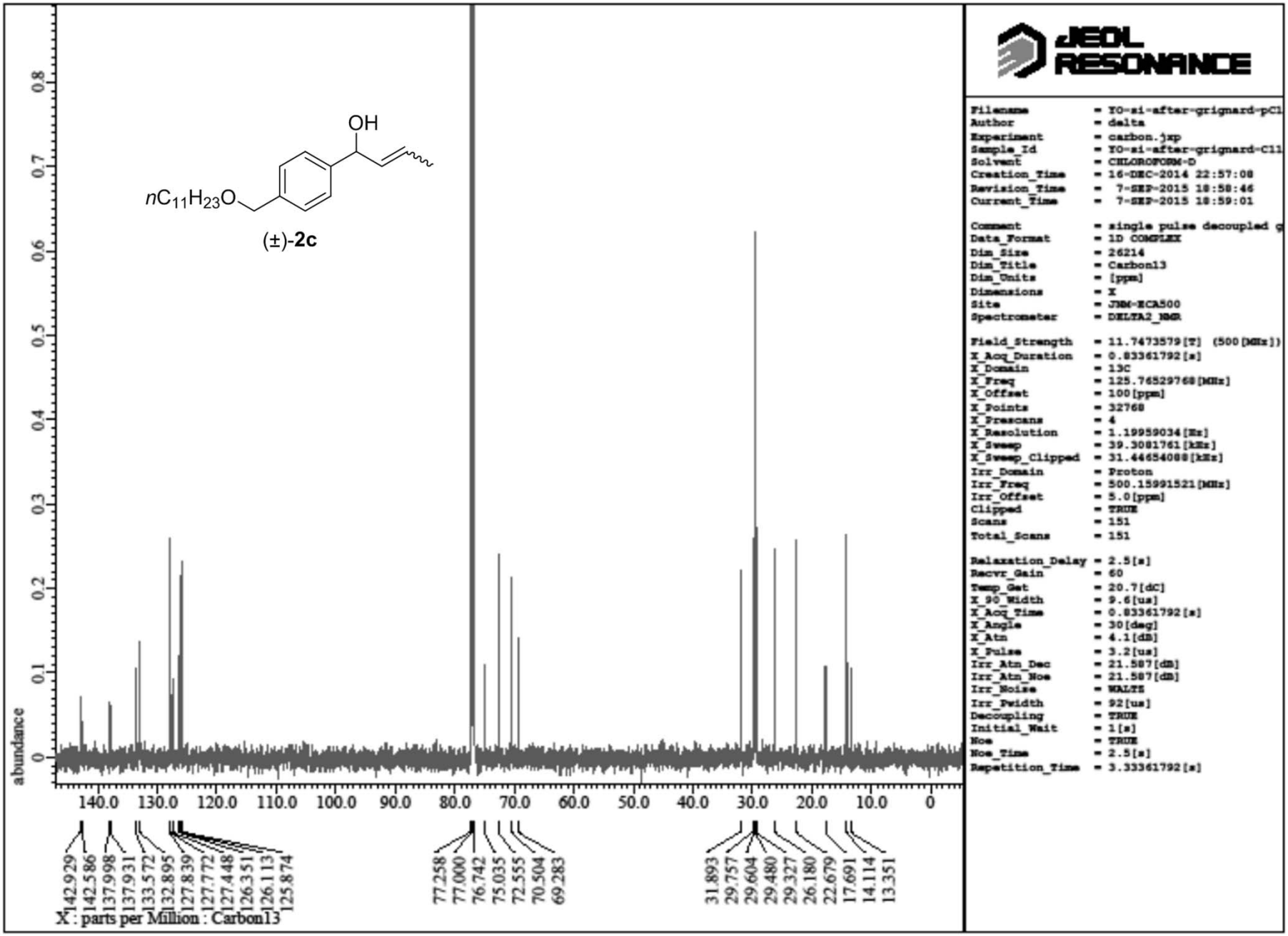

CHO
O
O
3
7d
abundance
4.0
3.0
2.0
1.0
0
10.13
2.89
1.88
2.08
1.98
2.02
1.00
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
10.002
7.872
7.867
7.851
7.845
7.527
7.500
7.260
4.652
3.703
3.697
3.689
3.681
3.669
3.657
3.639
3.561
3.544
3.373
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-si-O-peg_proton-3-3.j
Author = delta
Experiment = proton.jxp
Sample_Id = YO-si-O-peg
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 18:07:50
Revision_Time = 7-SEP-2015 19:24:13
Current_Time = 7-SEP-2015 19:24:27
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 2.90717696[s]
X_Domain = 1H
X_Freq = 300.52965592[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.34397631[Hz]
X_Sweep = 5.63570784[kHz]
X_Sweep_Clipped = 4.50856628[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 300.52965592[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 20.1[dC]
X_90_Width = 11.2[us]
X_Acq_Time = 2.90717696[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5.6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.90717696[s]

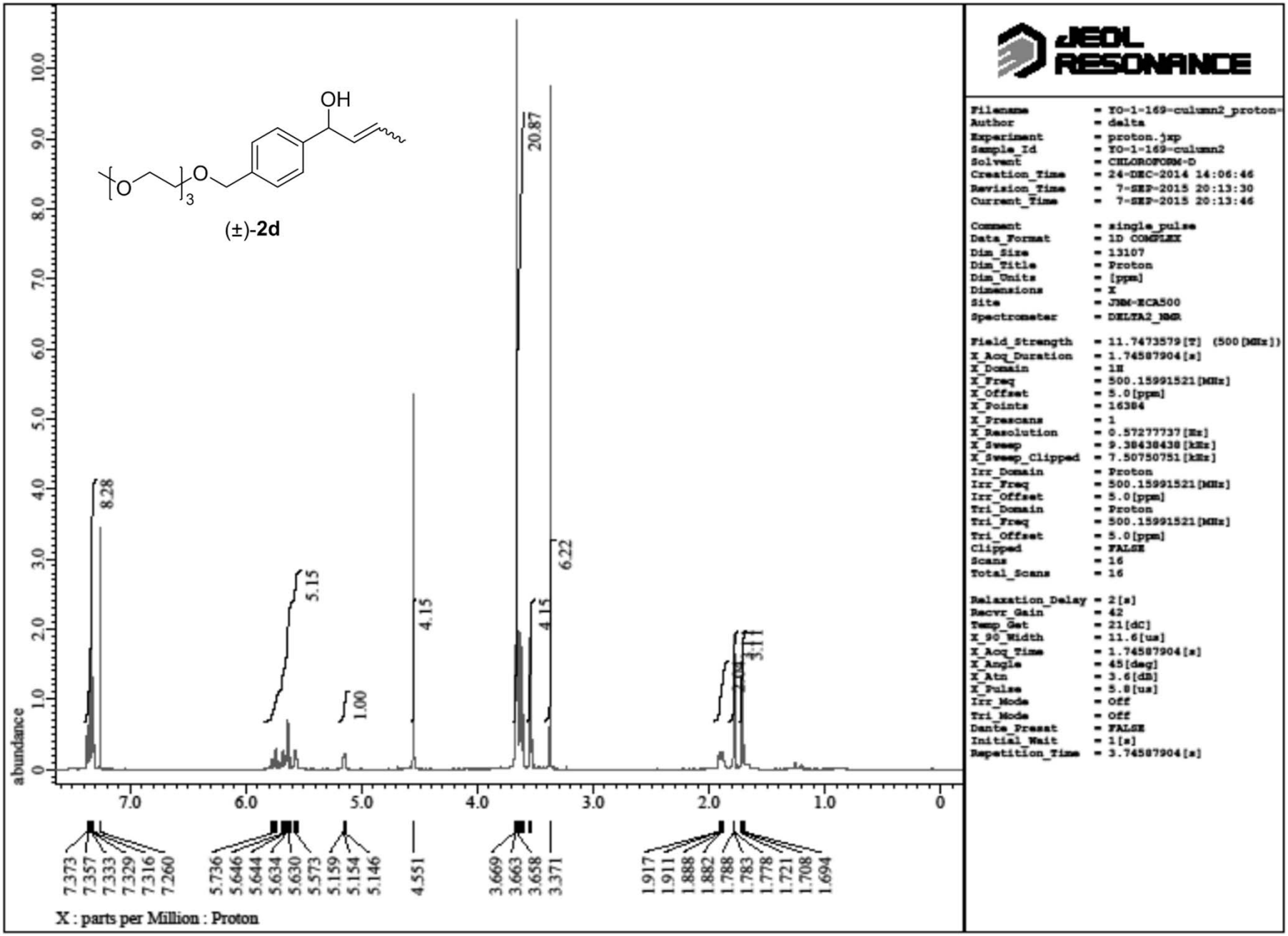

CHO
O
O
3
7d
abundance
0.4
0.3
0.2
0.1
0
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
192.005
145.531
135.674
129.861
127.662
77.421
77.000
76.579
72.497
71.914
70.623
70.547
69.973
59.045
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-zi-O-peg_Carbon-1-3.j
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-zi-O-peg
Solvent = CHLOROFORM-D
Creation_Time = 18-DEC-2014 16:21:49
Revision_Time = 7-SEP-2015 19:25:58
Current_Time = 7-SEP-2015 19:26:08
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 1.38412032[s]
X_Domain = 13C
X_Freq = 75.56823426[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.72248054[Hz]
X_Sweep = 23.67424242[kHz]
X_Sweep_Clipped = 18.93939394[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 321
Total_Scans = 321
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 20.1[dC]
X_90_Width = 11.8[us]
X_Acq_Time = 1.38412032[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.93333333[us]
Irr_Atn_Dec = 22.2[dB]
Irr_Atn_Noe = 22.2[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.118[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.38412032[s]

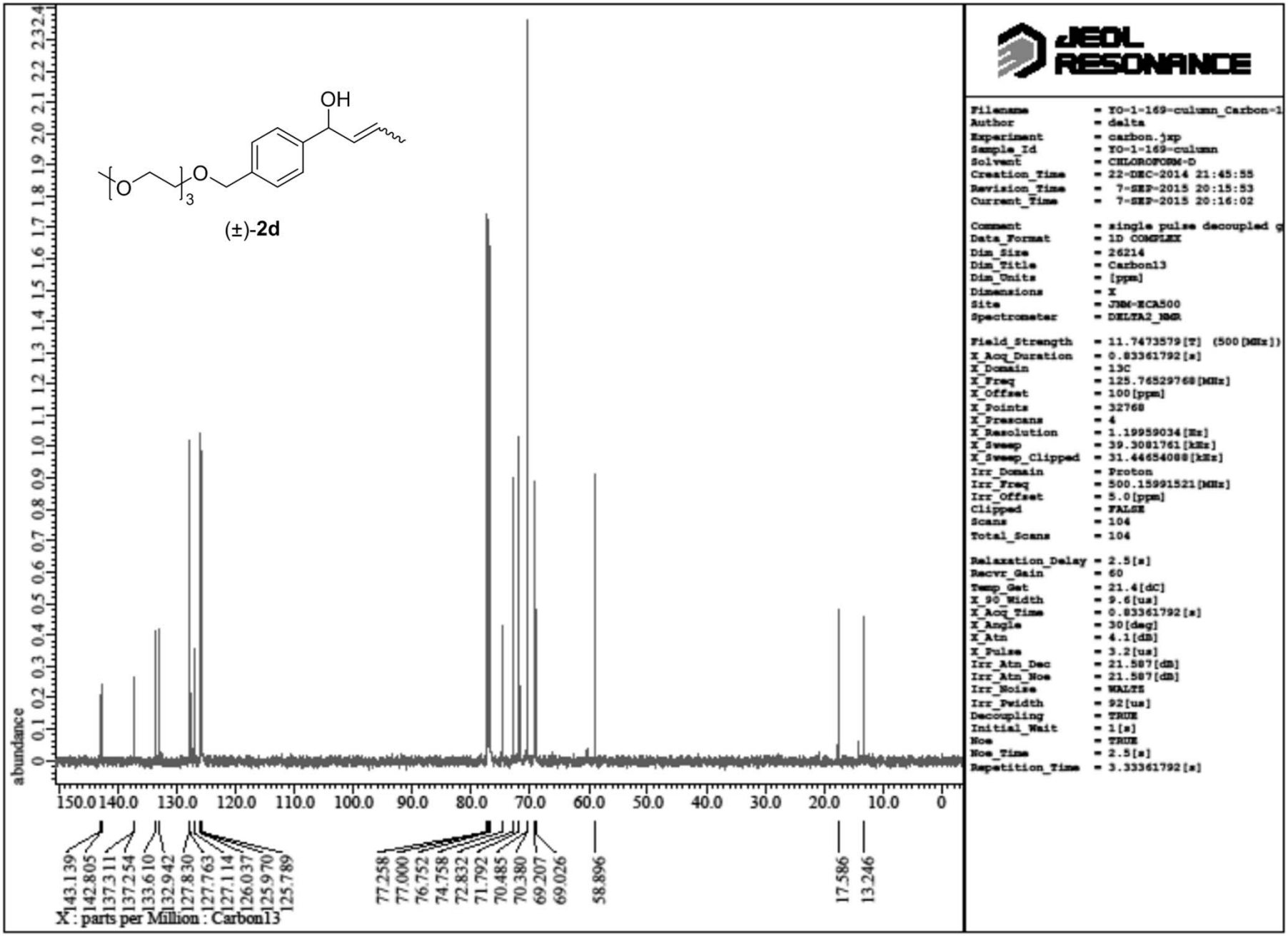

OH
(±)-2b
abundance
X : parts per Million : Proton
5.15
4.10
2.48
0.89
0.52
2.06
1.50
8.154
7.970
7.954
7.531
7.260
5.893
5.877
5.816
5.800
5.786
5.382
5.372
5.367
2.142
2.136
2.109
2.103
1.906
1.603
JEOL RESONANCE
Filename = dinaphtylalcohol-8.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = DateH26.07.10
Solvent = CHLOROFORM-D
Creation_Time = 10-JUL-2014 18:15:09
Revision_Time = 17-JUL-2014 21:27:15
Current_Time = 17-JUL-2014 21:28:28
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 2[s]
Recvr_Gain = 34
Temp_Get = 24.7[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

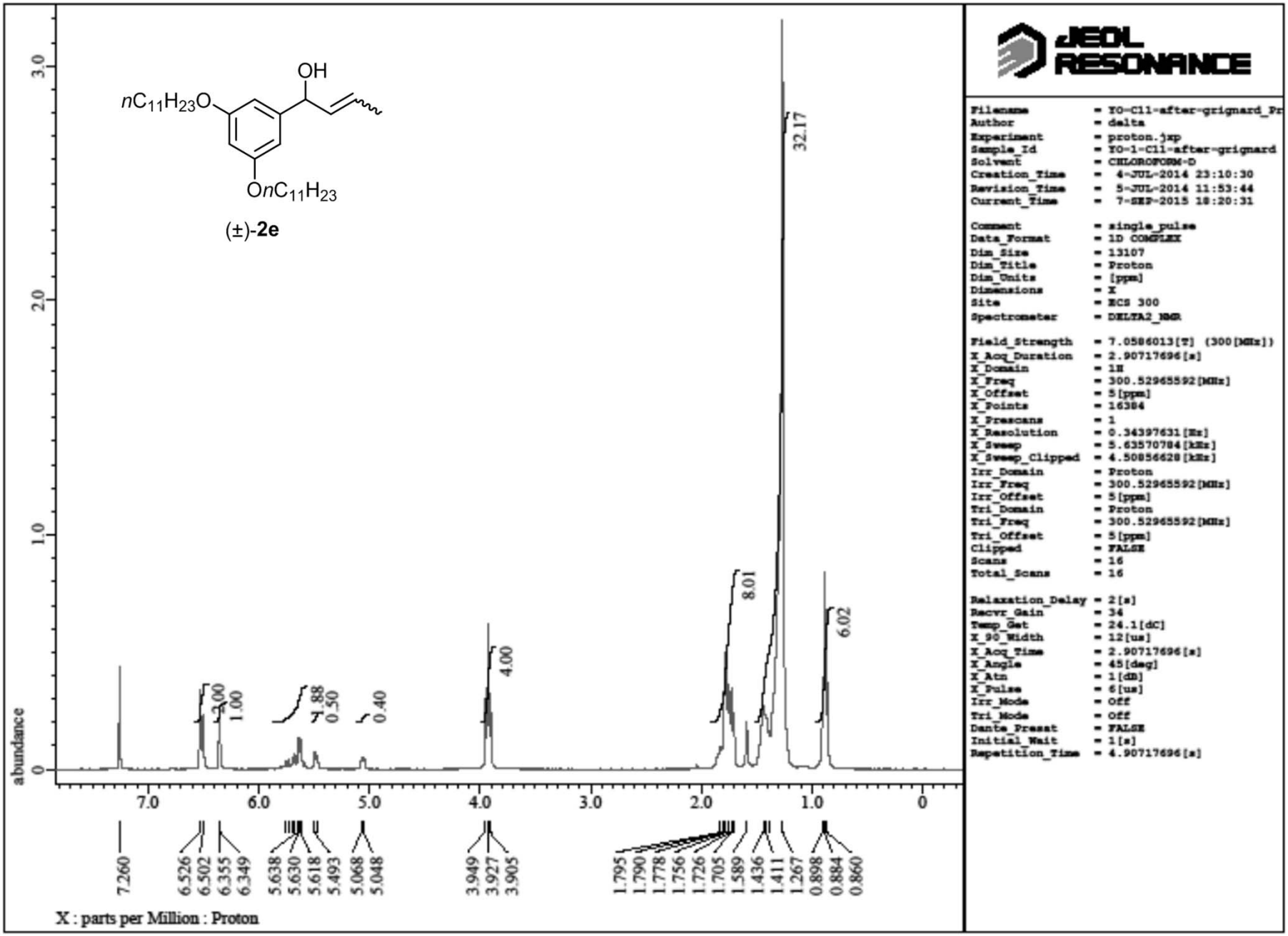

OH
(±)-2b
abundance
X: parts per Million : Carbon13
42.070
38.379
33.648
32.723
28.469
28.202
27.648
26.332
25.998
25.808
25.636
24.253
124.033
77.258
77.000
76.742
75.388
69.551
17.757
13.503
JEOL RESONANCE
Filename = dinaphtylalcohol-C-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = DateN26.07.10-C
Solvent = CHLOROFORM-D
Creation_Time = 10-JUL-2014 18:18:19
Revision_Time = 17-JUL-2014 21:35:37
Current_Time = 17-JUL-2014 21:35:58
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 254
Total_Scans = 254
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 25.3[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

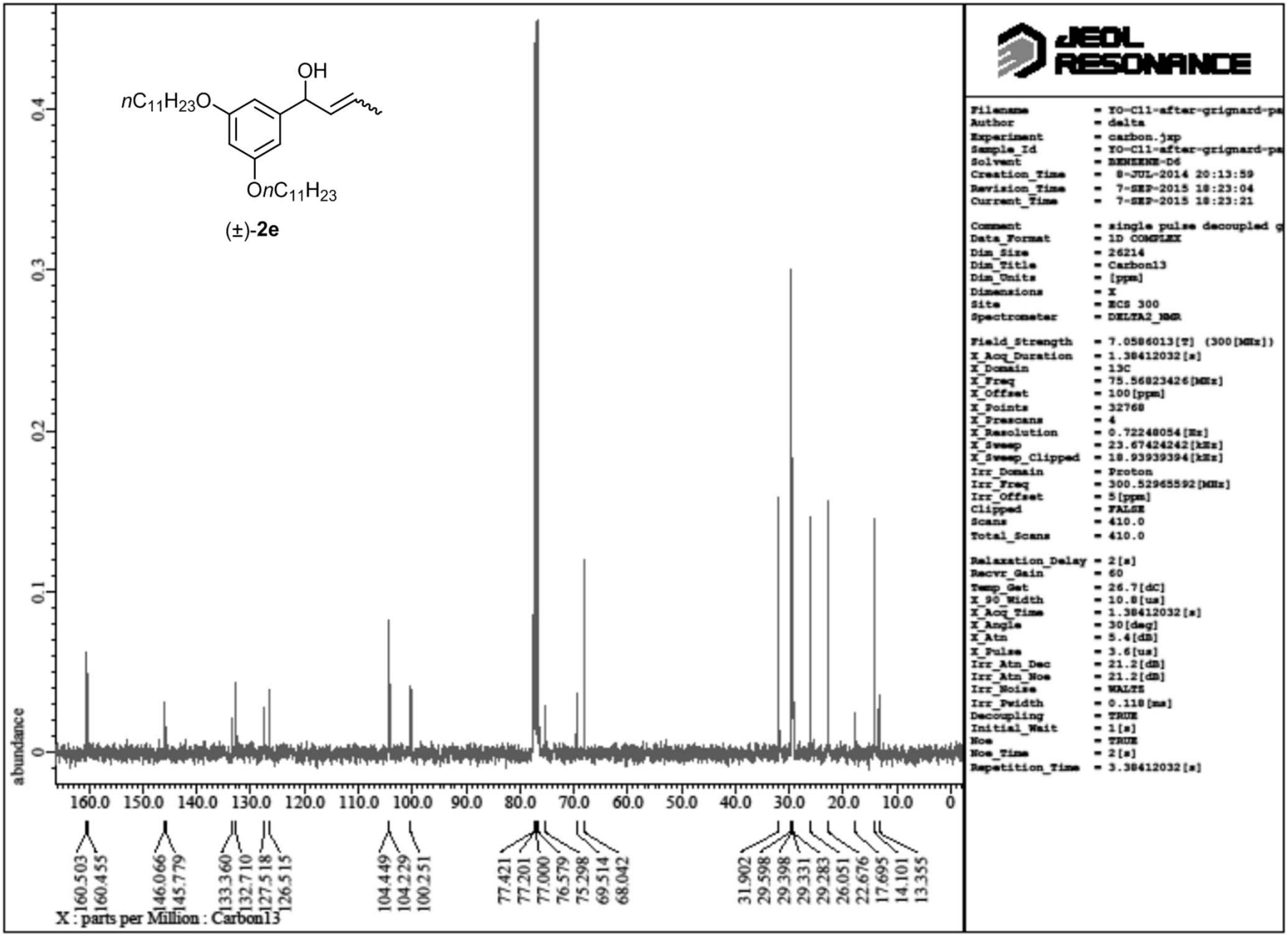

OH
nC11H23O
(±)-2c
abundance
X : parts per Million : Proton
4.30
2.73
0.50
2.21
2.17
1.69
2.73
2.16
17.33
3.27
7.379
7.363
7.339
7.329
7.315
7.260
5.754
5.741
5.652
5.646
5.642
5.583
5.162
5.148
4.487
3.485
3.472
3.461
3.448
3.434
1.792
1.780
1.722
1.710
1.600
1.586
1.543
1.294
1.255
0.890
0.877
0.863
JEOL RESONANCE
Filename = YO-si-after-grignard-C11_
Author = delta
Experiment = proton.jxp
Sample_Id = YO-si-after-grignard-C11
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2014 22:03:47
Revision_Time = 12-DEC-2015 22:24:13
Current_Time = 12-DEC-2015 22:26:21
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 20.1[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

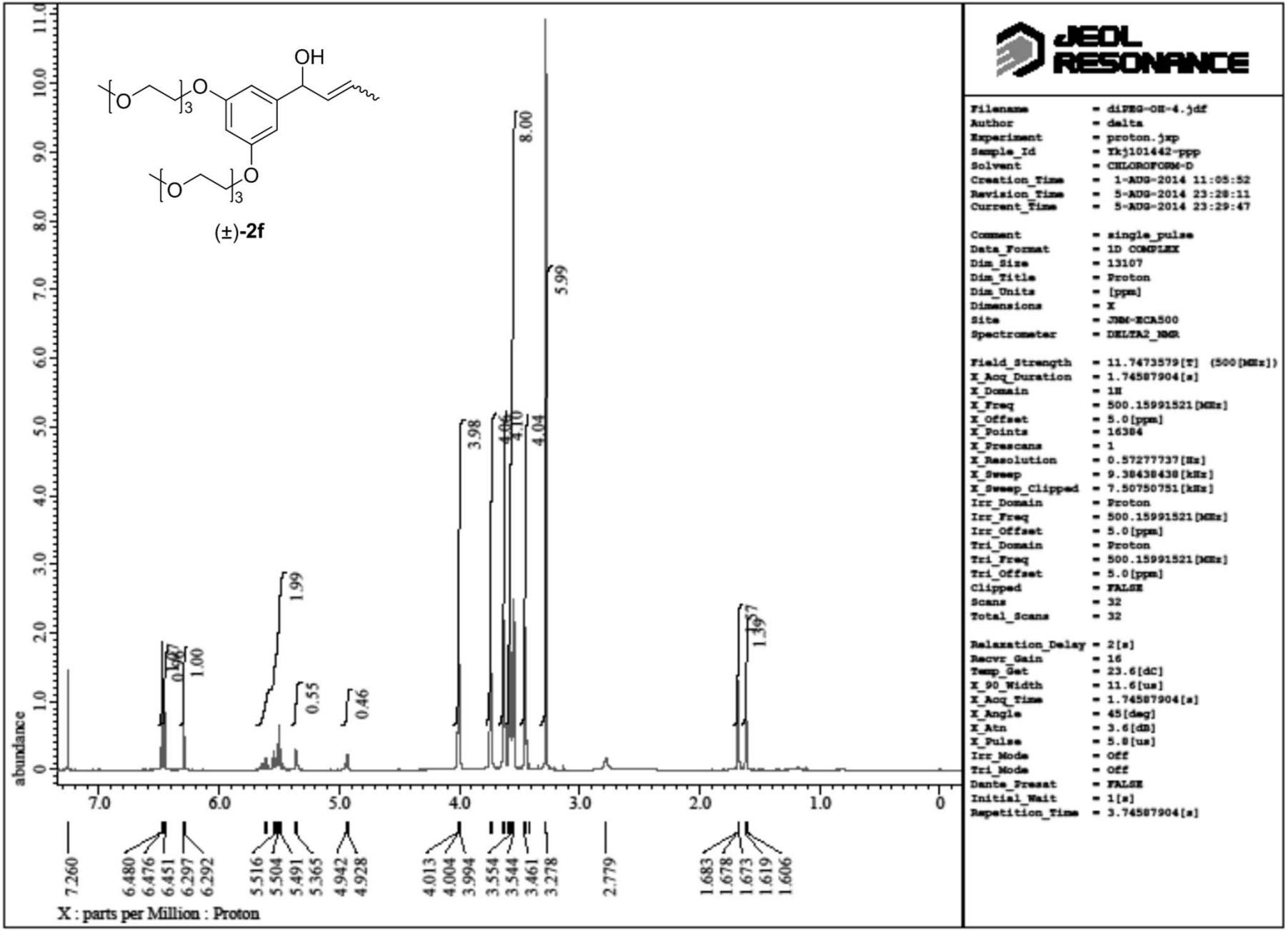

OH
nC11H23O
(±)-2c
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
142.929
142.586
137.998
137.931
133.572
132.895
127.839
127.772
127.448
126.351
126.113
125.874
77.258
77.000
76.742
75.035
72.555
70.504
69.283
31.893
29.757
29.604
29.480
29.327
26.180
22.679
17.691
14.114
13.351
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-si-after-grignard-pCl
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-si-after-grignard-C11
Solvent = CHLOROFORM-D
Creation_Time = 16-DEC-2014 22:57:08
Revision_Time = 7-SEP-2015 18:58:46
Current_Time = 7-SEP-2015 18:59:01
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = TRUE
Scans = 151
Total_Scans = 151
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.7[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

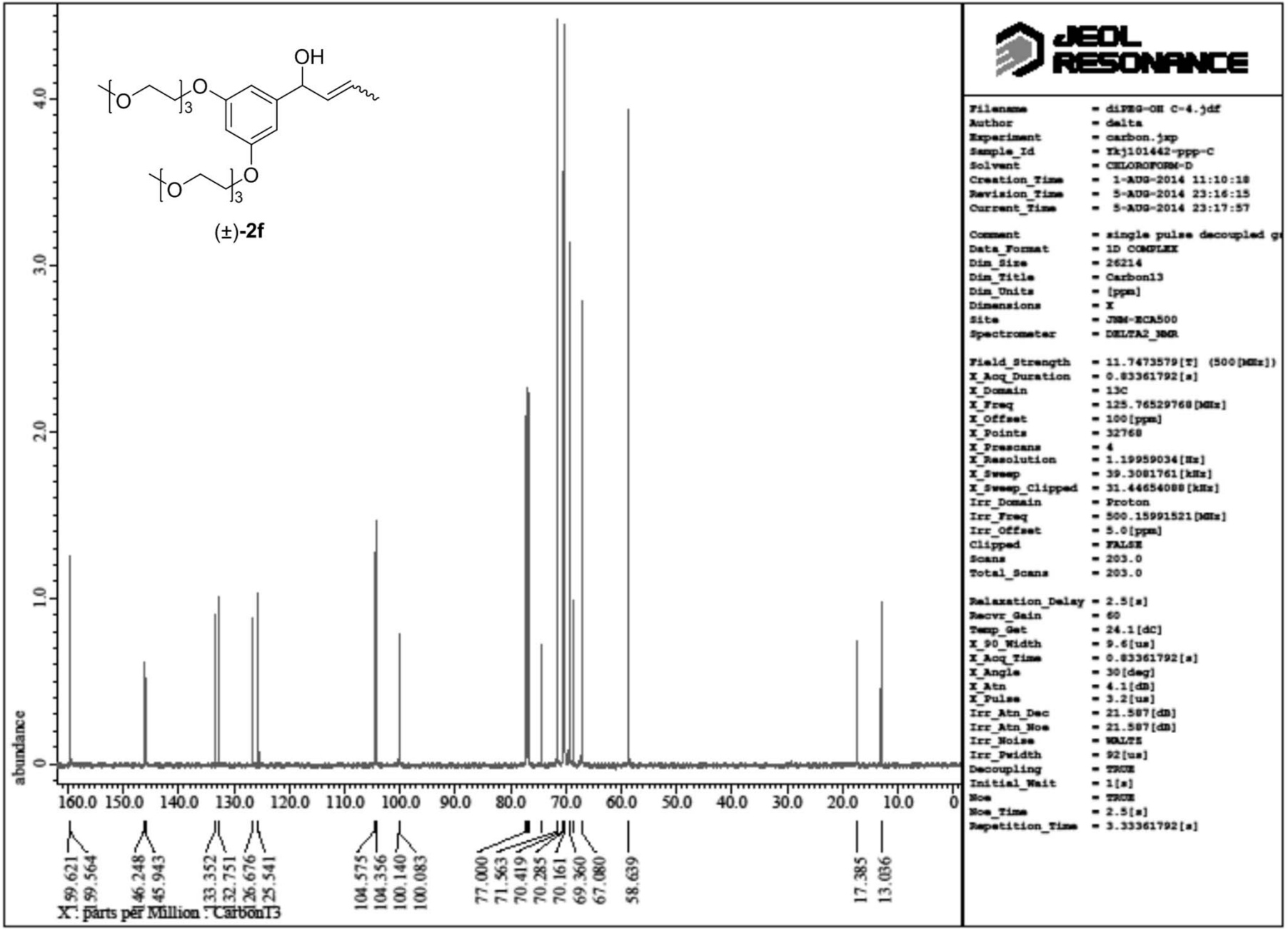

OH
O
O
3
(±)-2d
abundance
8.28
5.15
1.00
4.15
20.87
4.15
6.22
3.11
7.373
7.357
7.333
7.329
7.316
7.260
5.736
5.646
5.644
5.634
5.630
5.573
5.159
5.154
5.146
4.551
3.669
3.663
3.658
3.371
1.917
1.911
1.888
1.882
1.788
1.783
1.778
1.721
1.708
1.694
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-1-169-column2_proton-
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-169-column2
Solvent = CHLOROFORM-D
Creation_Time = 24-DEC-2014 14:06:46
Revision_Time = 7-SEP-2015 20:13:30
Current_Time = 7-SEP-2015 20:13:46
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 42
Temp_Get = 21[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

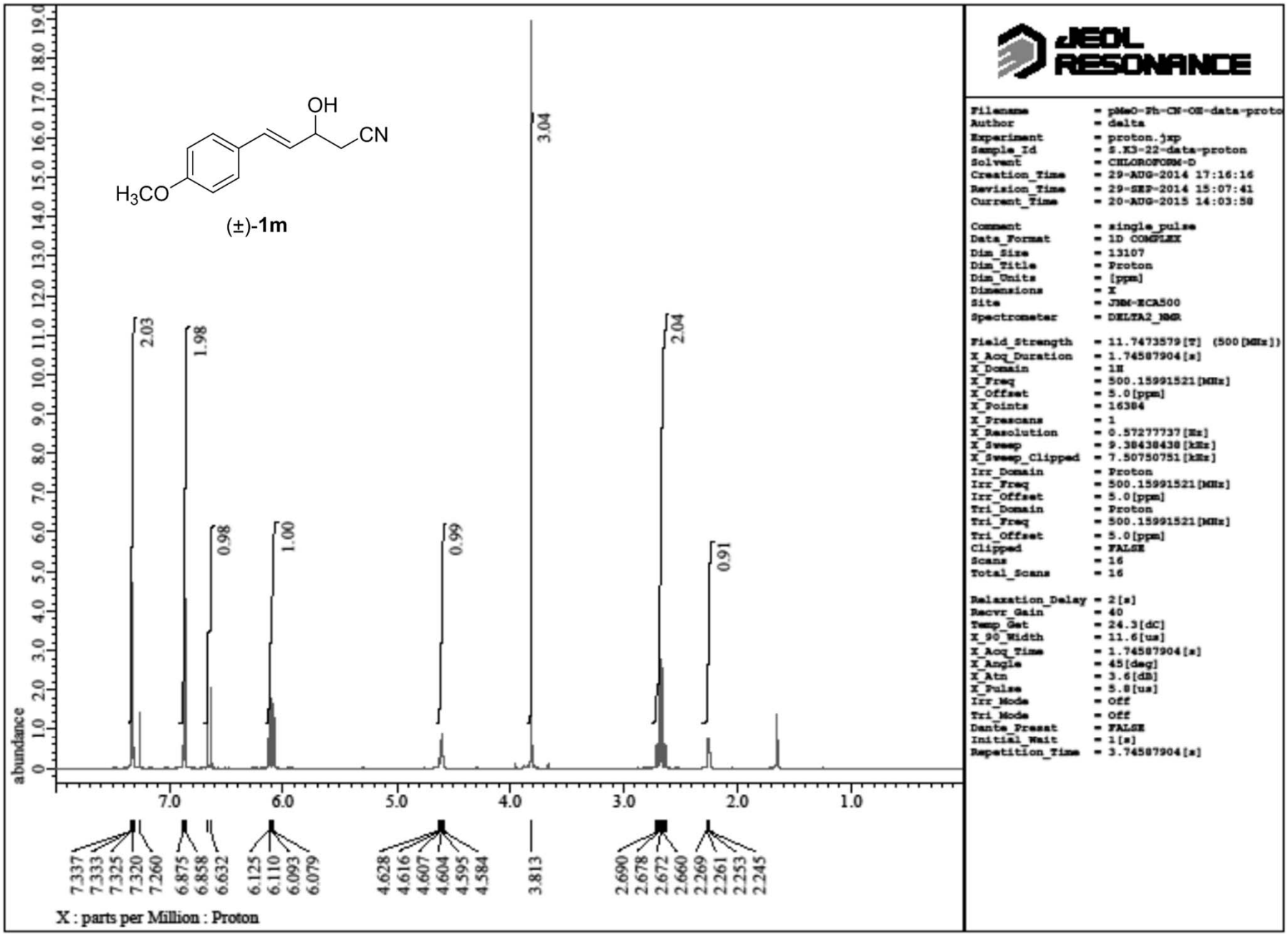

OH
O
O
3
(±)-2d
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.139
142.805
137.311
137.254
133.610
132.942
127.830
127.763
127.114
126.037
125.970
125.789
77.258
77.000
76.752
74.758
72.832
71.792
70.485
70.380
69.207
69.026
58.896
17.586
13.246
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-1-169-column_Carbon-1
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-1-169-column
Solvent = CHLOROFORM-D
Creation_Time = 22-DEC-2014 21:45:55
Revision_Time = 7-SEP-2015 20:15:53
Current_Time = 7-SEP-2015 20:16:02
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 104
Total_Scans = 104
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

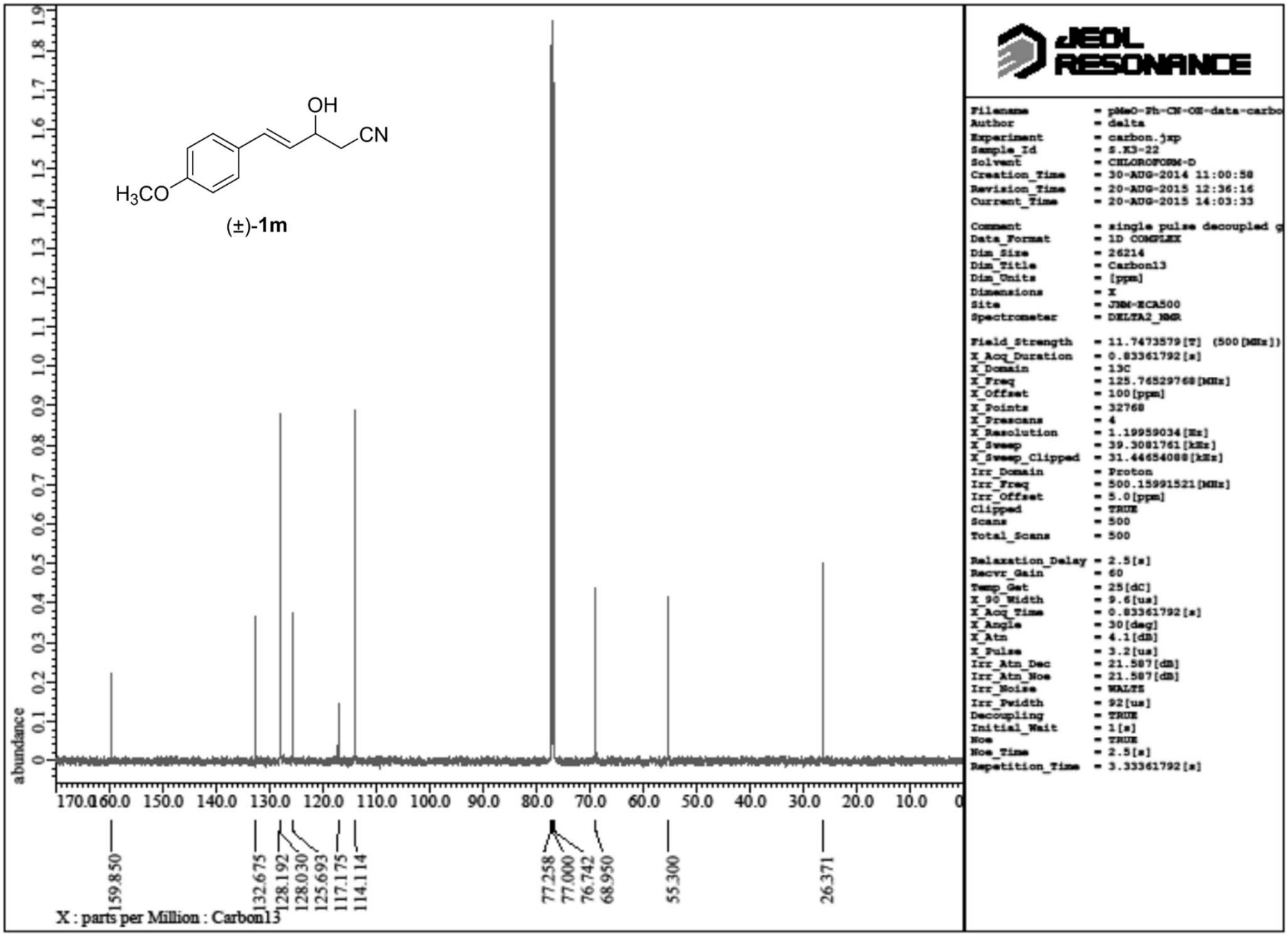

OH
nC11H23O
OnC11H23
(±)-2e
32.17
8.01
6.02
4.00
2.00
1.00
1.88
0.50
0.40
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.260
6.526
6.502
6.355
6.349
5.638
5.630
5.618
5.493
5.068
5.048
3.949
3.927
3.905
1.795
1.790
1.778
1.756
1.726
1.705
1.589
1.436
1.411
1.267
0.898
0.884
0.860
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-C11-after-grignard_Pr
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-C11-after-grignard
Solvent = CHLOROFORM-D
Creation_Time = 4-JUL-2014 23:10:30
Revision_Time = 5-JUL-2014 11:53:44
Current_Time = 7-SEP-2015 18:20:31
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 2.90717696[s]
X_Domain = 1H
X_Freq = 300.52965592[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.34397631[Hz]
X_Sweep = 5.63570784[kHz]
X_Sweep_Clipped = 4.50856628[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 300.52965592[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 34
Temp_Get = 24.1[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.90717696[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.90717696[s]

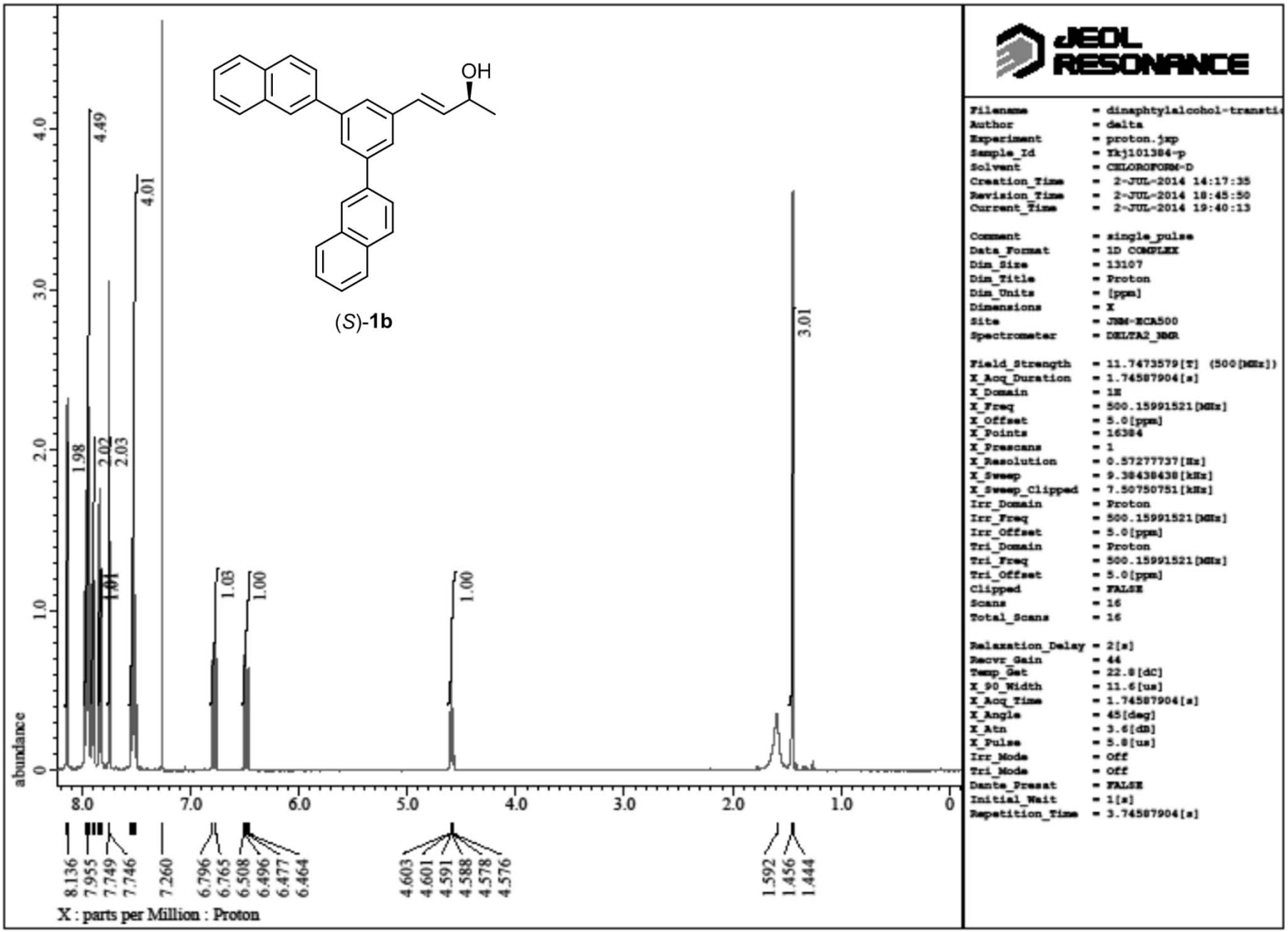

OH
nC11H23O
OnC11H23
(±)-2e
abundance
0.4
0.3
0.2
0.1
0
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
160.503
160.455
146.066
145.779
133.360
132.710
127.518
126.515
104.449
104.229
100.251
77.421
77.201
77.000
76.579
75.298
69.514
68.042
31.902
29.598
29.398
29.331
29.283
26.051
22.676
17.695
14.101
13.355
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-C11-after-grignard-pa
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-C11-after-grignard-pa
Solvent = BENZENE-D6
Creation_Time = 8-JUL-2014 20:13:59
Revision_Time = 7-SEP-2015 18:23:04
Current_Time = 7-SEP-2015 18:23:21
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 1.38412032[s]
X_Domain = 13C
X_Freq = 75.56823426[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.72248054[Hz]
X_Sweep = 23.67424242[kHz]
X_Sweep_Clipped = 18.93939394[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 410.0
Total_Scans = 410.0
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 26.7[dC]
X_90_Width = 10.8[us]
X_Acq_Time = 1.38412032[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.6[us]
Irr_Atn_Dec = 21.2[dB]
Irr_Atn_Noe = 21.2[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.118[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.38412032[s]

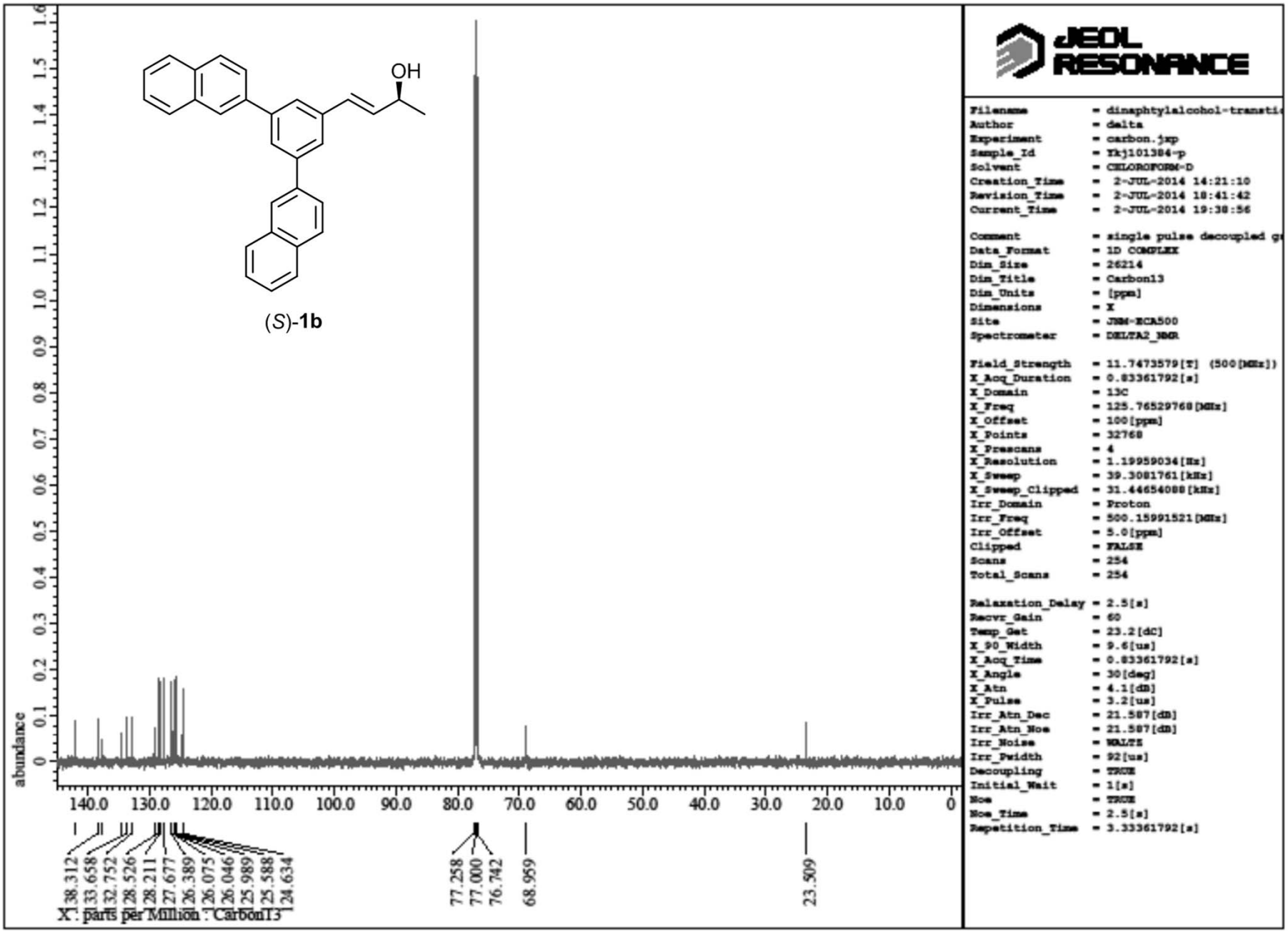

OH
(±)-2f
abundance
X : parts per Million : Proton
JEOL RESONANCE
Filename = diPEG-OH-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101442-ppp
Solvent = CHLOROFORM-D
Creation_Time = 1-AUG-2014 11:05:52
Revision_Time = 5-AUG-2014 23:28:11
Current_Time = 5-AUG-2014 23:29:47
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 16
Temp_Get = 23.6[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

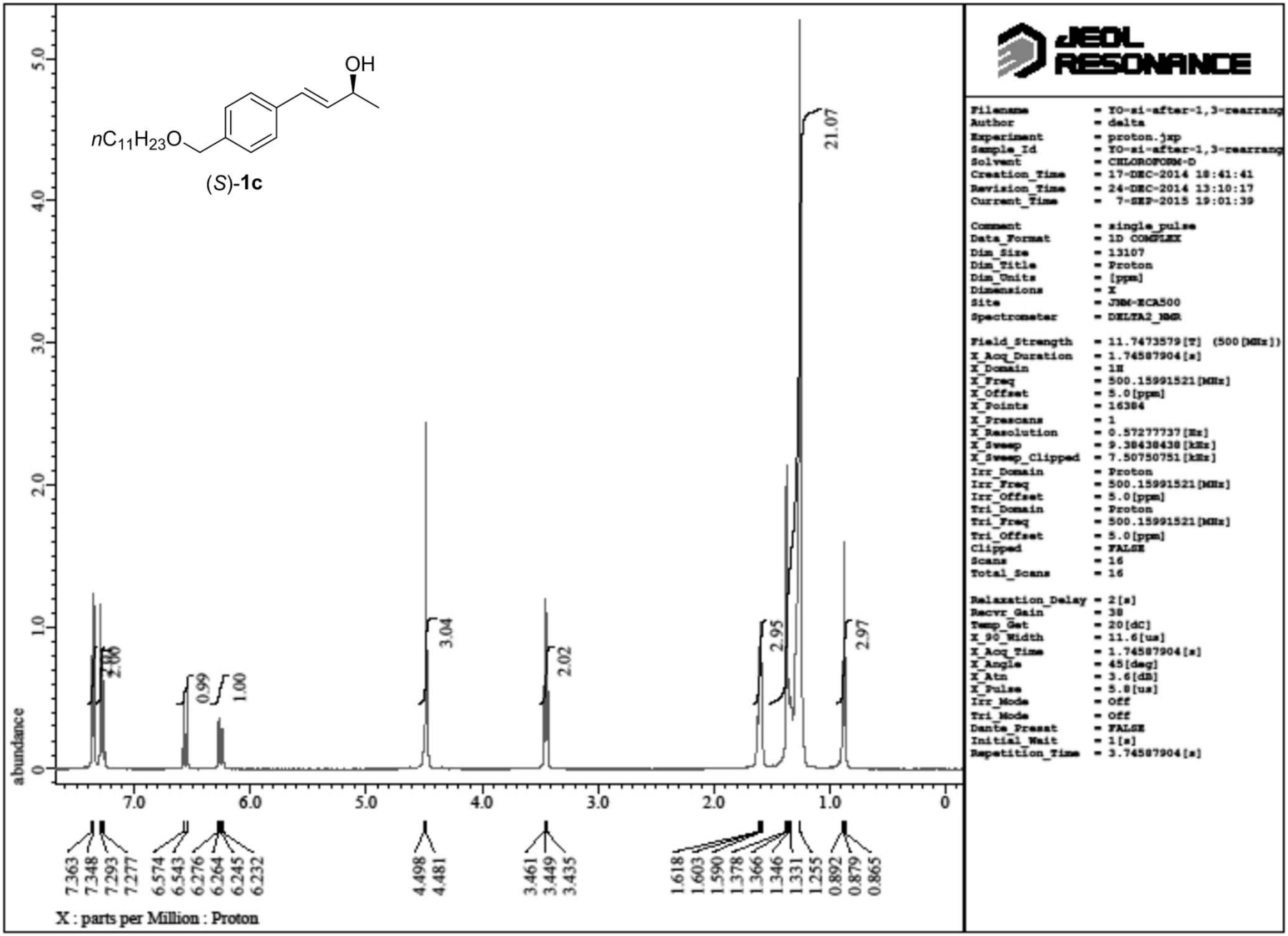

OH
(±)-2f
abundance
4.0
3.0
2.0
1.0
0
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
59.621
59.564
46.248
45.943
33.352
32.751
26.676
25.541
104.575
104.356
100.140
100.083
77.000
71.563
70.419
70.285
70.161
69.360
67.080
58.639
17.385
13.036
X: parts per Million : Carbon13
JEOL RESONANCE
Filename = diPEG-OH C-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj101442-ppp-C
Solvent = CHLOROFORM-D
Creation_Time = 1-AUG-2014 11:10:18
Revision_Time = 5-AUG-2014 23:16:15
Current_Time = 5-AUG-2014 23:17:57
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 203.0
Total_Scans = 203.0
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 24.1[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

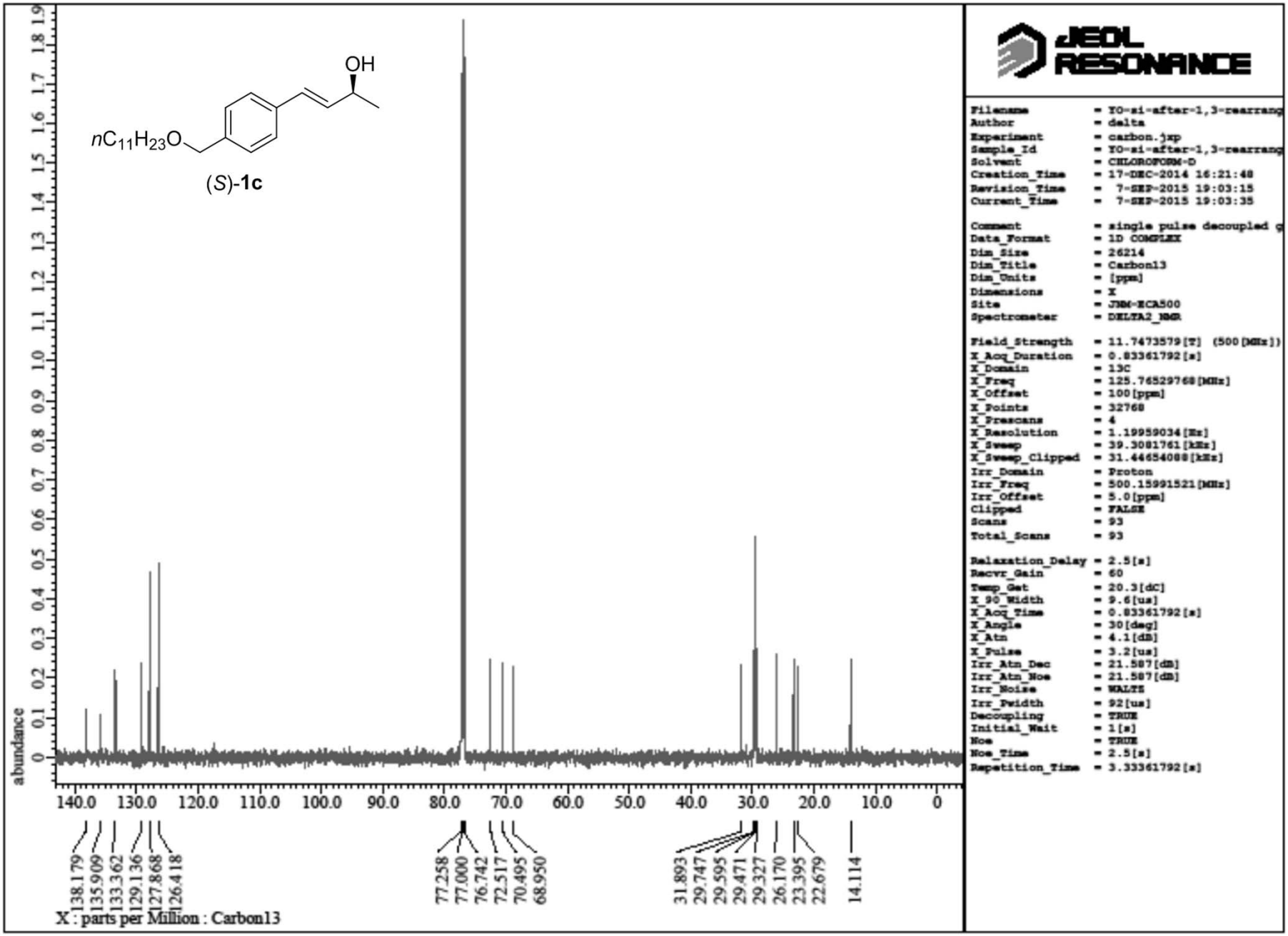

OH
CN
H_3CO
(±)-1m
abundance
2.03
1.98
0.98
1.00
0.99
3.04
2.04
0.91
7.337
7.333
7.325
7.320
7.260
6.875
6.858
6.632
6.125
6.110
6.093
6.079
4.628
4.616
4.607
4.604
4.595
4.584
3.813
2.690
2.678
2.672
2.660
2.269
2.261
2.253
2.245
X : parts per Million : Proton
JEOL RESONANCE
Filename = pMeO-Ph-CH-OH-data-proto
Author = delta
Experiment = proton.jxp
Sample_Id = S.K3-22-data-proton
Solvent = CHLOROFORM-D
Creation_Time = 29-AUG-2014 17:16:16
Revision_Time = 29-SEP-2014 15:07:41
Current_Time = 20-AUG-2015 14:03:58
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 24.3[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

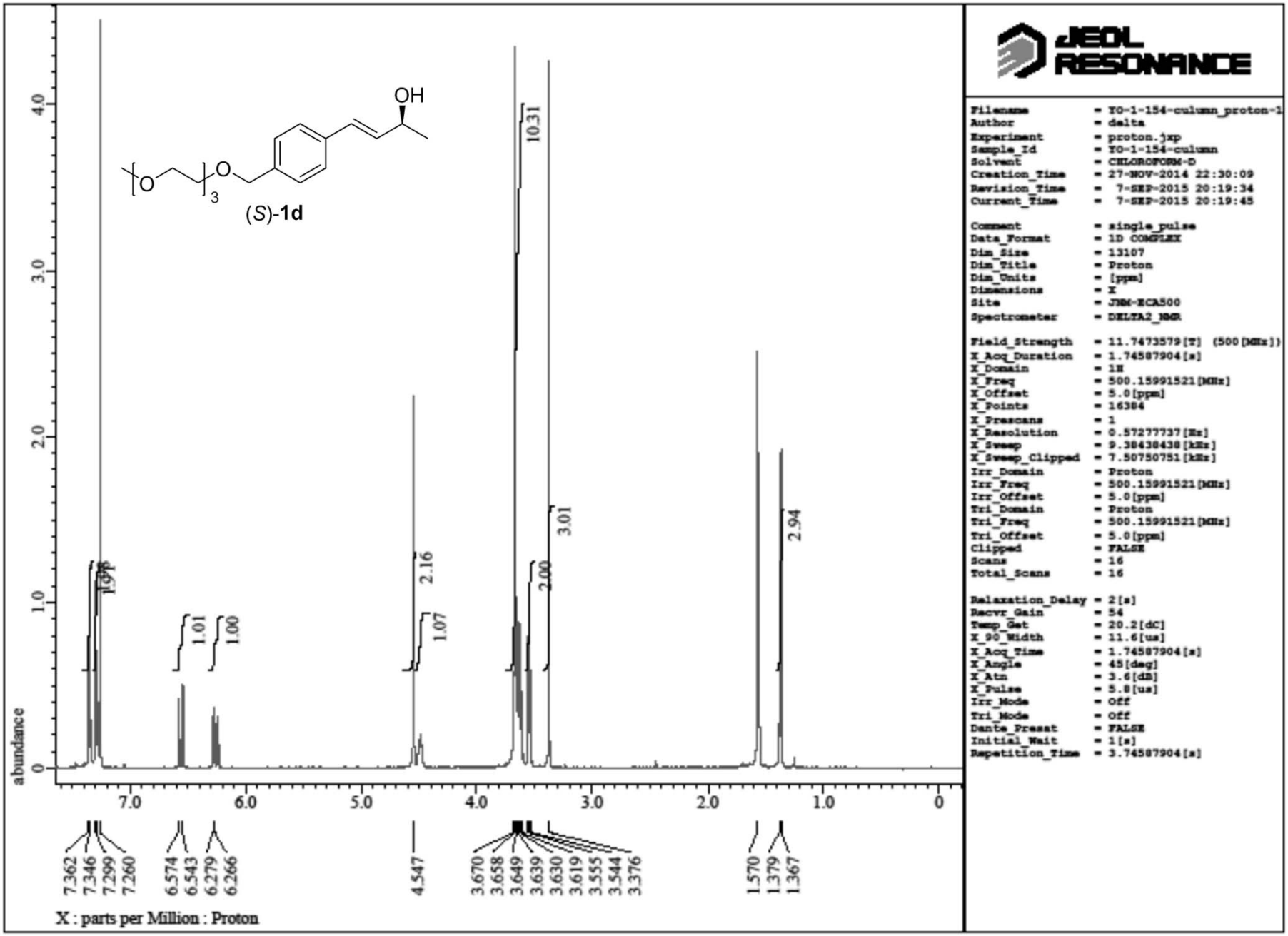

OH
CN
H_3CO
(±)-1m
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
159.850
132.675
128.192
128.030
125.693
117.175
114.114
77.258
77.000
76.742
68.950
55.300
26.371
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = pMeO-Ph-CH-OH-data-carbo
Author = delta
Experiment = carbon.jxp
Sample_Id = S.K3-22
Solvent = CHLOROFORM-D
Creation_Time = 30-AUG-2014 11:00:58
Revision_Time = 20-AUG-2015 12:36:16
Current_Time = 20-AUG-2015 14:03:33
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = TRUE
Scans = 500
Total_Scans = 500
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 25[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

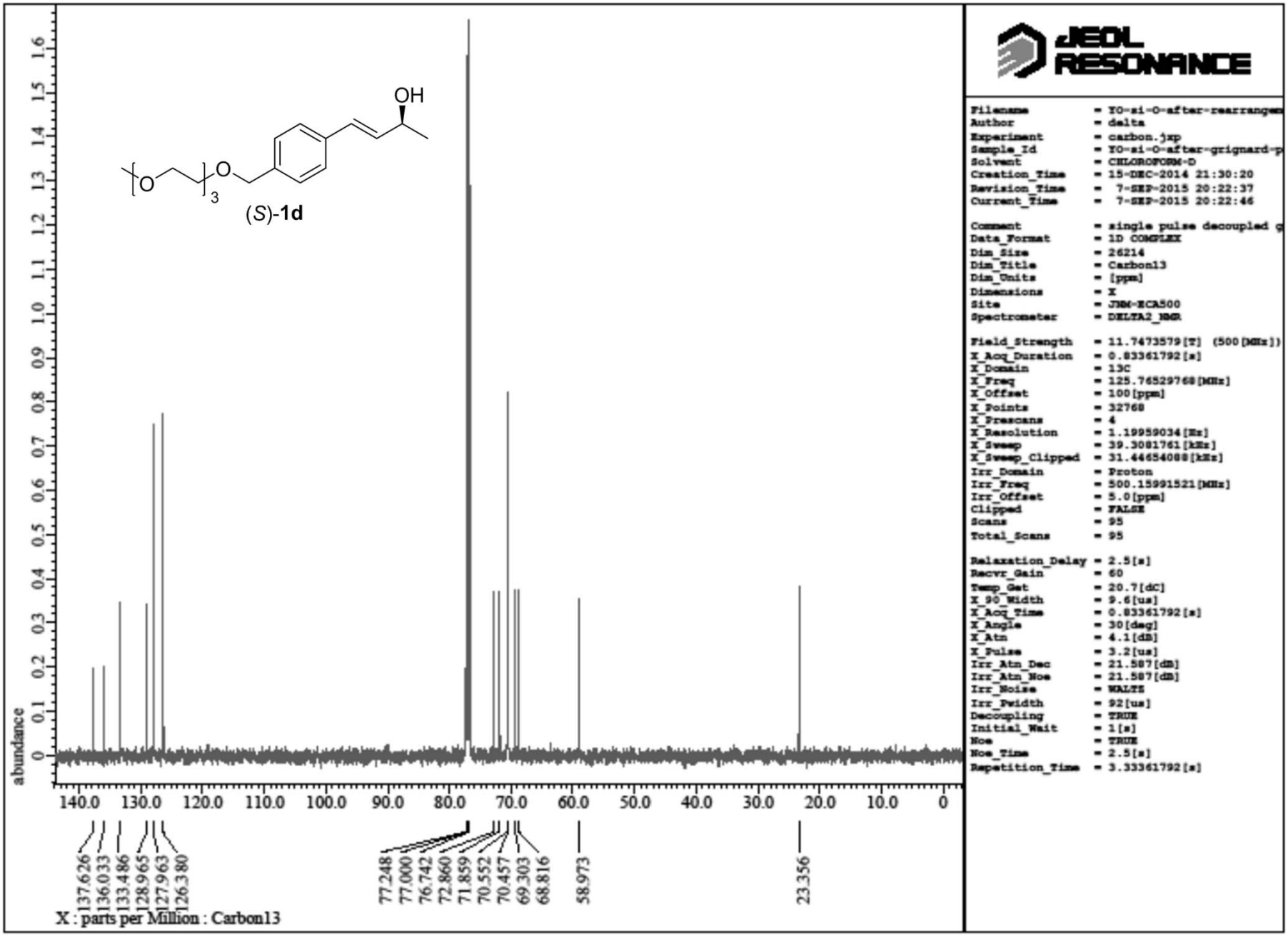

OH
(S)-1b
4.49
4.01
1.98
2.02
2.03
1.01
1.03
1.00
1.00
3.01
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.136
7.955
7.749
7.746
7.260
6.796
6.765
6.508
6.496
6.477
6.464
4.603
4.601
4.591
4.588
4.578
4.576
1.592
1.456
1.444
X : parts per Million : Proton
JEOL RESONANCE
Filename = dinaphtylalcohol-transti
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101384-p
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2014 14:17:35
Revision_Time = 2-JUL-2014 18:45:50
Current_Time = 2-JUL-2014 19:40:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 44
Temp_Get = 22.8[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

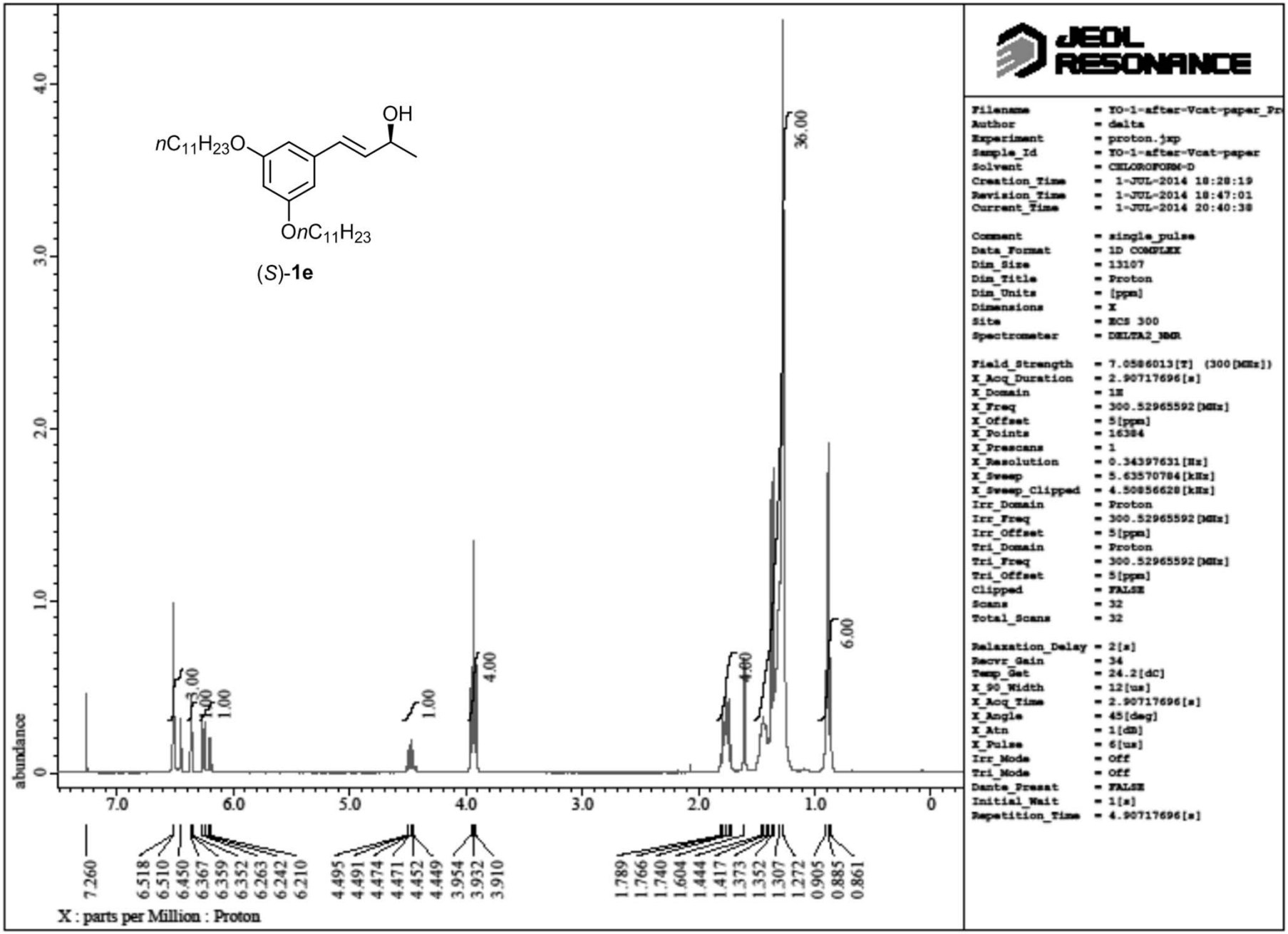

OH
(S)-1b
abundance
X : parts per Million : Carbon13
38.312
33.658
32.752
28.526
28.211
27.677
26.389
26.075
26.046
25.989
25.588
24.634
77.258
77.000
76.742
68.959
23.509
JEOL RESONANCE
Filename = dinaphtylalcohol-transti
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj101384-p
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2014 14:21:10
Revision_Time = 2-JUL-2014 18:41:42
Current_Time = 2-JUL-2014 19:38:56
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 254
Total_Scans = 254
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 23.2[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

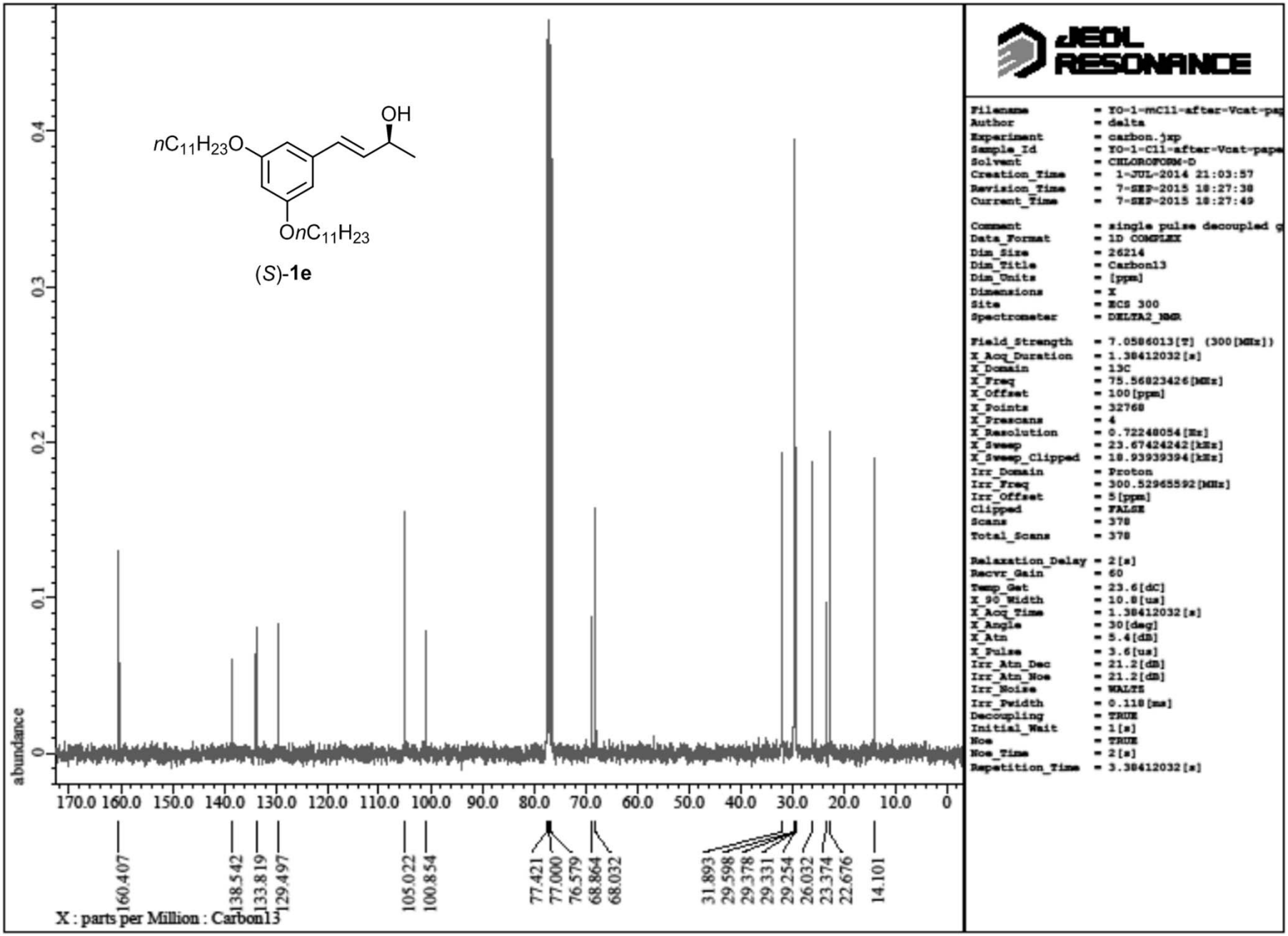

OH
nC11H23O
(S)-1c
abundance
X : parts per Million : Proton
21.07
3.04
2.95
2.97
2.02
0.99
1.00
7.363
7.348
7.293
7.277
6.574
6.543
6.276
6.264
6.245
6.232
4.498
4.481
3.461
3.449
3.435
1.618
1.603
1.590
1.378
1.366
1.346
1.331
1.255
0.892
0.879
0.865
Filename = YO-si-after-1,3-rearrang
Author = delta
Experiment = proton.jxp
Sample_Id = YO-si-after-1,3-rearrang
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2014 18:41:41
Revision_Time = 24-DEC-2014 13:10:17
Current_Time = 7-SEP-2015 19:01:39
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 38
Temp_Get = 20[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

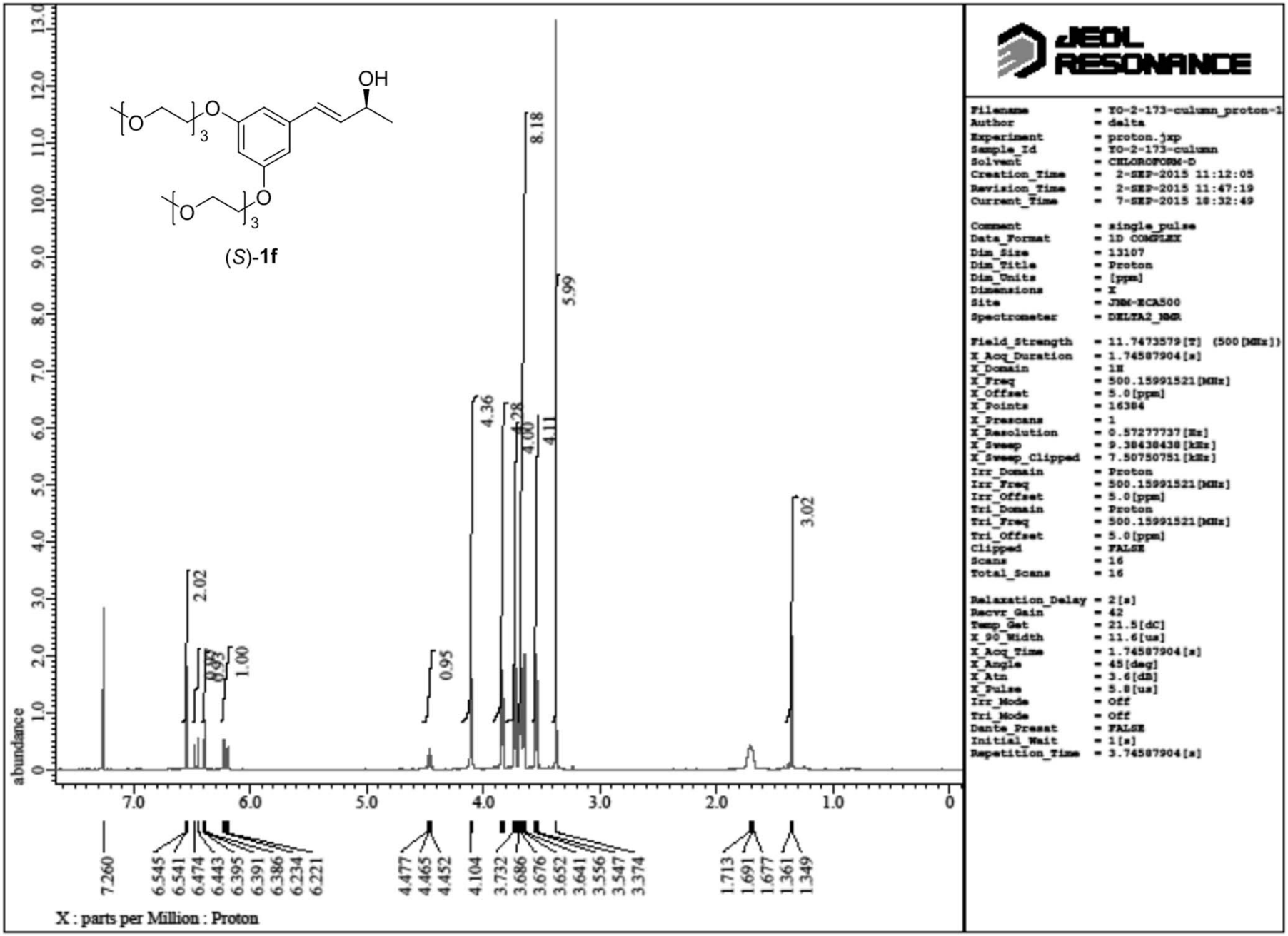

OH
nC11H23O
(S)-1c
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9
140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
138.179
135.909
133.362
129.136
127.868
126.418
77.258
77.000
76.742
72.517
70.495
68.950
31.893
29.747
29.595
29.471
29.327
26.170
23.395
22.679
14.114
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-si-after-1,3-rearrang
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-si-after-1,3-rearrang
Solvent = CHLOROFORM-D
Creation_Time = 17-DEC-2014 16:21:48
Revision_Time = 7-SEP-2015 19:03:15
Current_Time = 7-SEP-2015 19:03:35
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 93
Total_Scans = 93
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.3[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

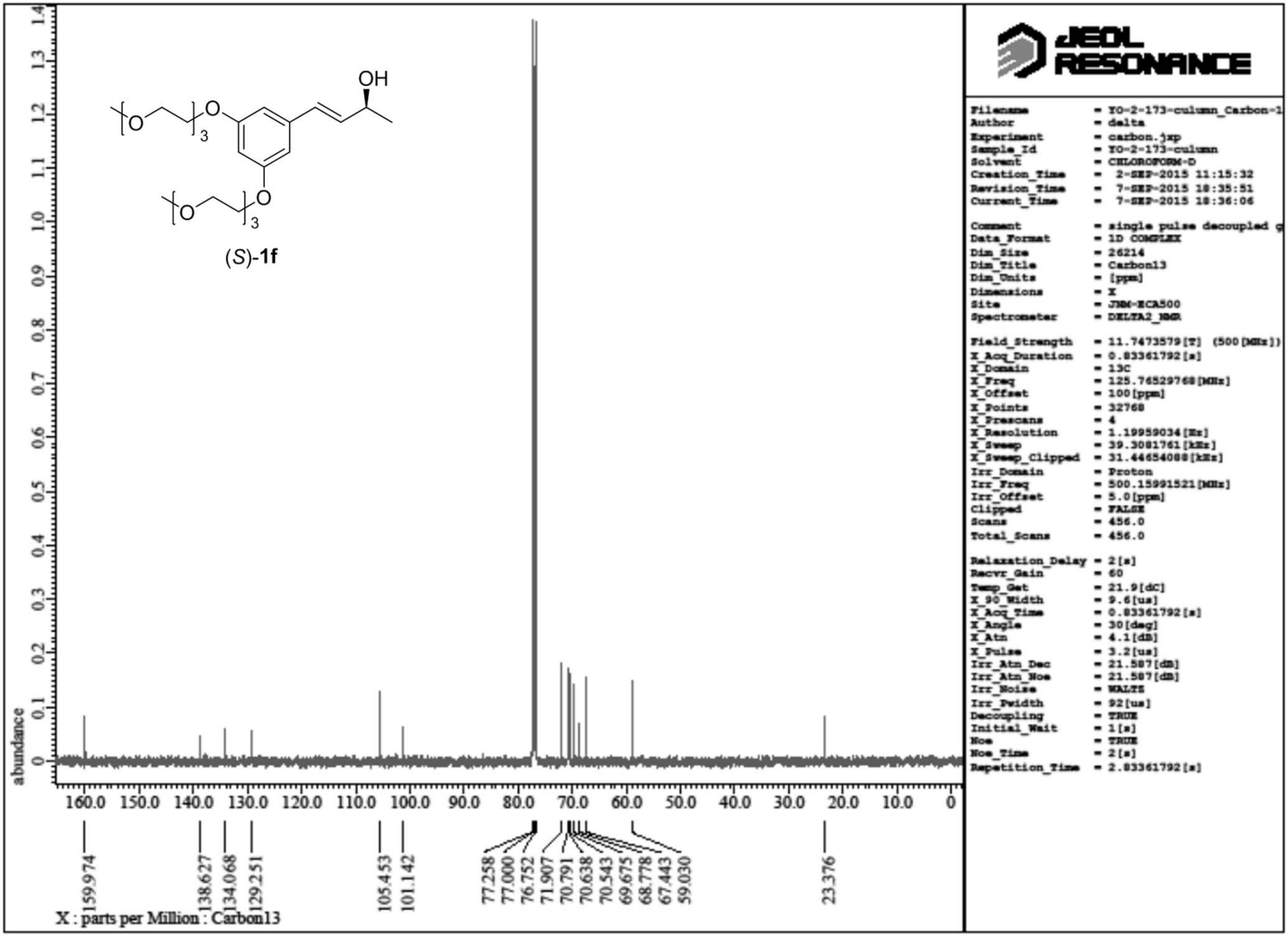

OH
O
O
3
(S)-1d
abundance
4.0
3.0
2.0
1.0
0
10.31
3.01
2.94
2.16
2.00
1.07
1.01
1.00
1.97
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.362
7.346
7.299
7.260
6.574
6.543
6.279
6.266
4.547
3.670
3.658
3.649
3.639
3.630
3.619
3.555
3.544
3.376
1.570
1.379
1.367
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-1-154-culumn_proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-154-culumn
Solvent = CHLOROFORM-D
Creation_Time = 27-NOV-2014 22:30:09
Revision_Time = 7-SEP-2015 20:19:34
Current_Time = 7-SEP-2015 20:19:45
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 54
Temp_Get = 20.2[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

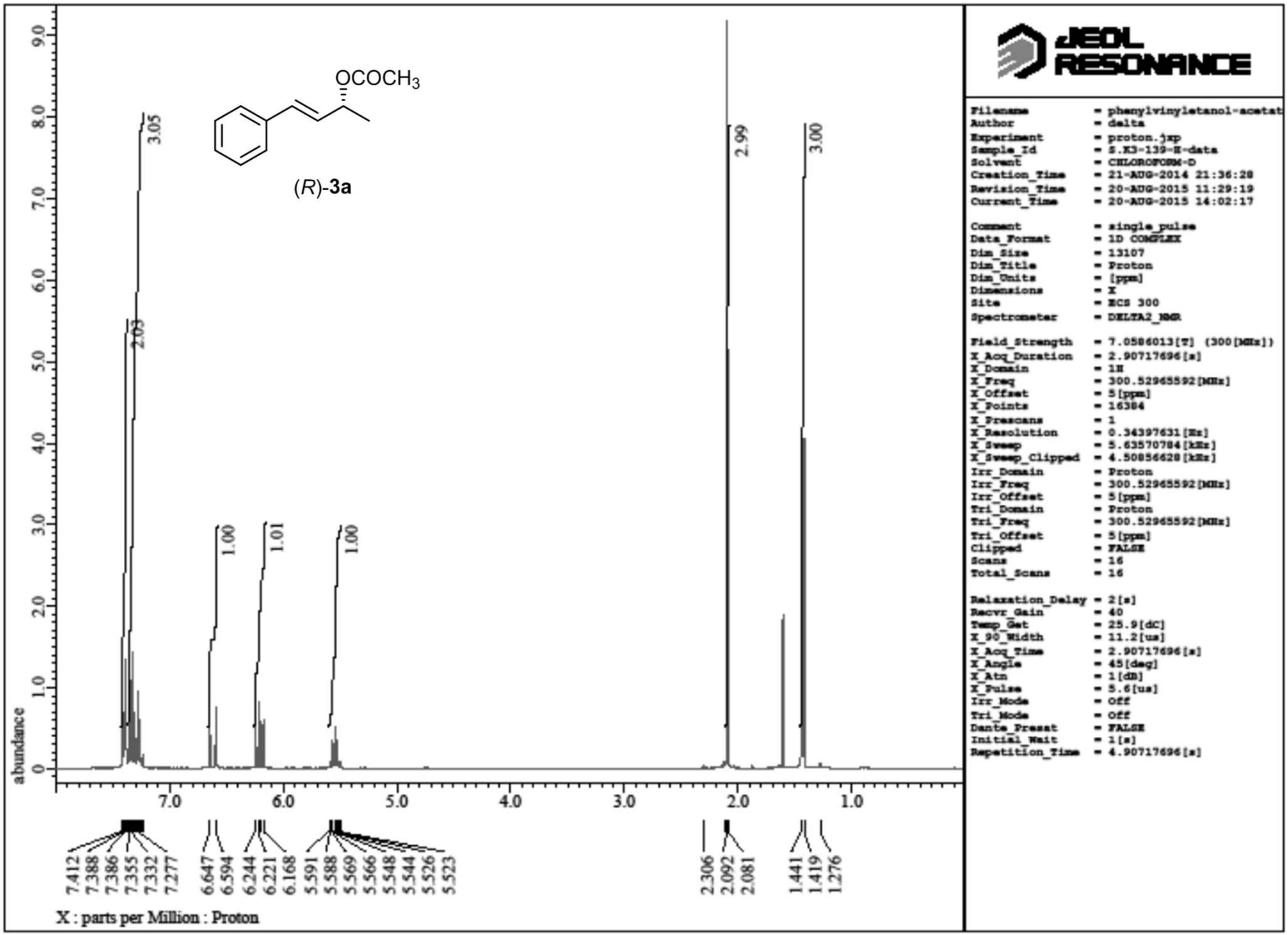

OH
(S)-1d
abundance
X : parts per Million : Carbon13
137.626
136.033
133.486
128.965
127.963
126.380
77.248
77.000
76.742
72.860
71.859
70.552
70.457
69.303
68.816
58.973
23.356
JEOL RESONANCE
Filename = YO-si-O-after-rearrangem
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-si-O-after-grignard-p
Solvent = CHLOROFORM-D
Creation_Time = 15-DEC-2014 21:30:20
Revision_Time = 7-SEP-2015 20:22:37
Current_Time = 7-SEP-2015 20:22:46
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 95
Total_Scans = 95
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.7[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

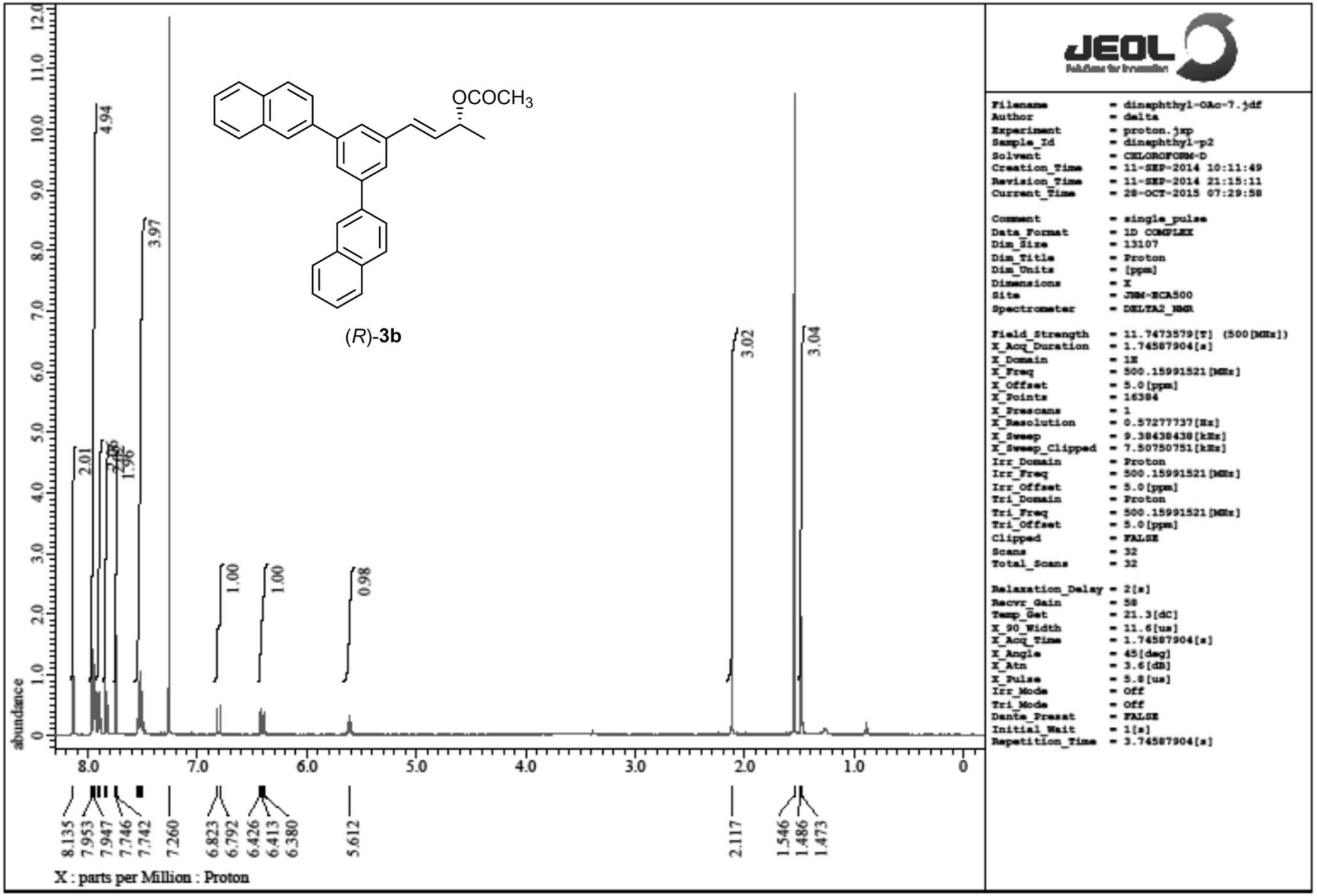

OH
nC11H23O
OnC11H23
(S)-1e
abundance
X : parts per Million : Proton
7.260
6.518
6.510
6.450
6.367
6.359
6.352
6.263
6.242
6.210
4.495
4.491
4.474
4.471
4.452
4.449
3.954
3.932
3.910
1.789
1.766
1.740
1.604
1.444
1.417
1.373
1.352
1.307
1.272
0.905
0.885
0.861
3.00
1.00
1.00
1.00
4.00
4.00
36.00
6.00
JEOL RESONANCE
Filename = YO-1-after-Vcat-paper_Pr
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-after-Vcat-paper
Solvent = CHLOROFORM-D
Creation_Time = 1-JUL-2014 18:28:19
Revision_Time = 1-JUL-2014 18:47:01
Current_Time = 1-JUL-2014 20:40:38
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 2.90717696[s]
X_Domain = 1H
X_Freq = 300.52965592[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.34397631[Hz]
X_Sweep = 5.63570784[kHz]
X_Sweep_Clipped = 4.50856628[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 300.52965592[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 34
Temp_Get = 24.2[dC]
X_90_Width = 12[us]
X_Acq_Time = 2.90717696[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.90717696[s]

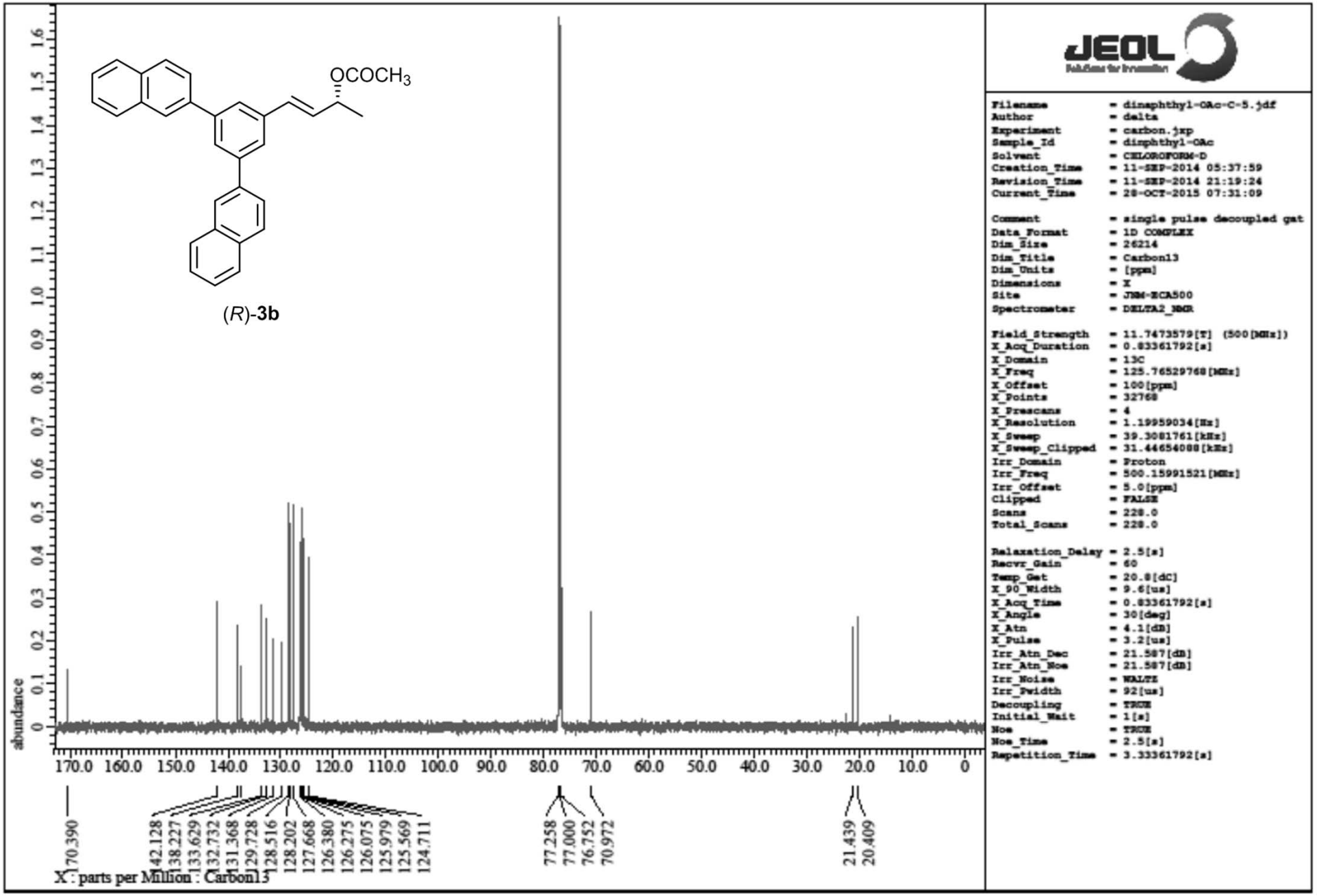

OH
nC11H23O
OnC11H23
(S)-1e
abundance
0
0.1
0.2
0.3
0.4
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
160.407
138.542
133.819
129.497
105.022
100.854
77.421
77.000
76.579
68.864
68.032
31.893
29.598
29.378
29.331
29.254
26.032
23.374
22.676
14.101
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-1-mC11-after-Vcat-pap
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-1-C11-after-Vcat-pape
Solvent = CHLOROFORM-D
Creation_Time = 1-JUL-2014 21:03:57
Revision_Time = 7-SEP-2015 18:27:38
Current_Time = 7-SEP-2015 18:27:49
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 1.38412032[s]
X_Domain = 13C
X_Freq = 75.56823426[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.72248054[Hz]
X_Sweep = 23.67424242[kHz]
X_Sweep_Clipped = 18.93939394[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 378
Total_Scans = 378
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 23.6[dC]
X_90_Width = 10.8[us]
X_Acq_Time = 1.38412032[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.6[us]
Irr_Atn_Dec = 21.2[dB]
Irr_Atn_Noe = 21.2[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.118[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.38412032[s]

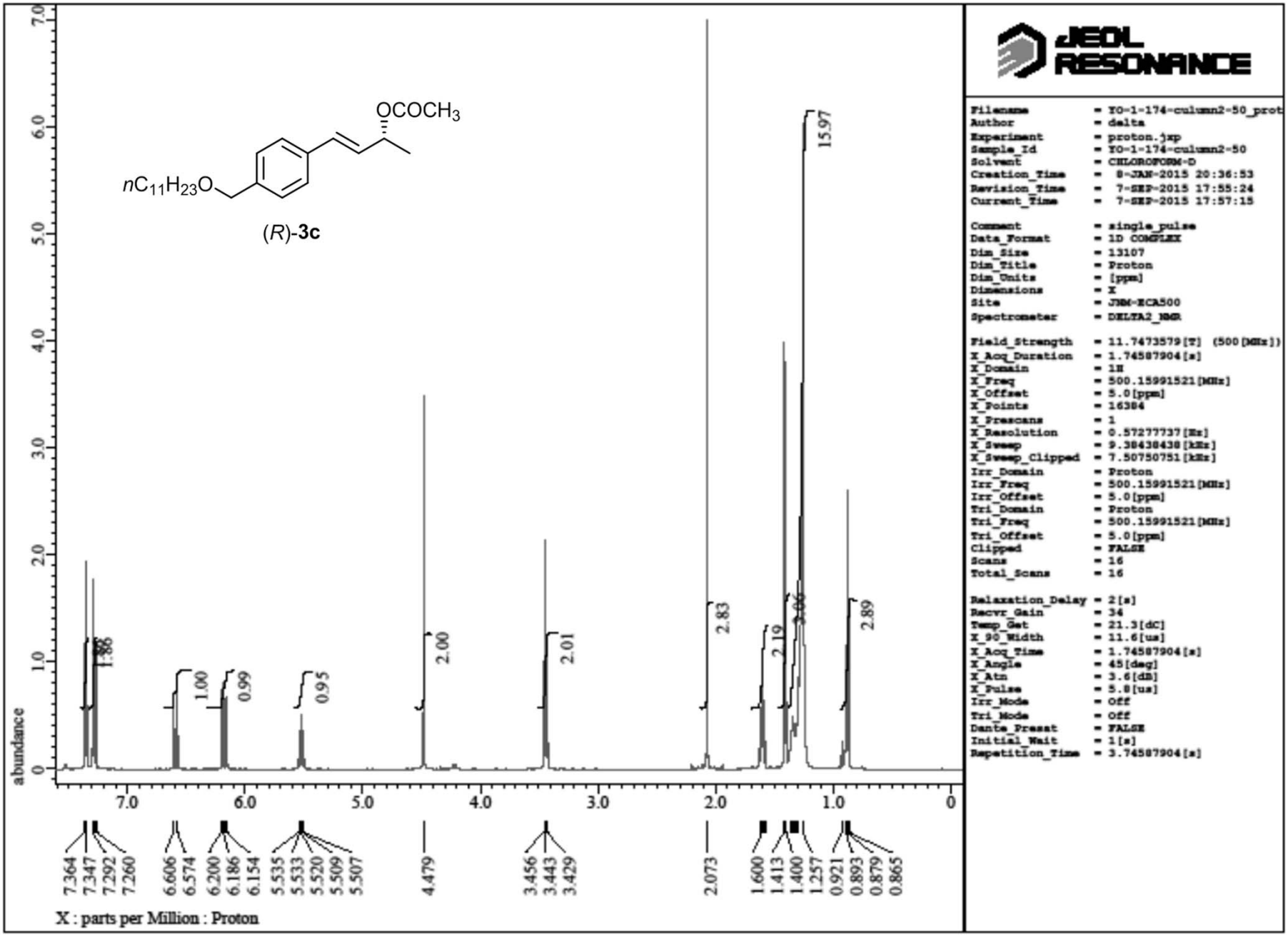

OH
(S)-1f
abundance
X : parts per Million : Proton
Filename = YO-2-173-column_proton-1
Author = delta
Experiment = proton.jxp
Sample_Id = YO-2-173-column
Solvent = CHLOROFORM-D
Creation_Time = 2-SEP-2015 11:12:05
Revision_Time = 2-SEP-2015 11:47:19
Current_Time = 7-SEP-2015 18:32:49
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 42
Temp_Get = 21.5[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

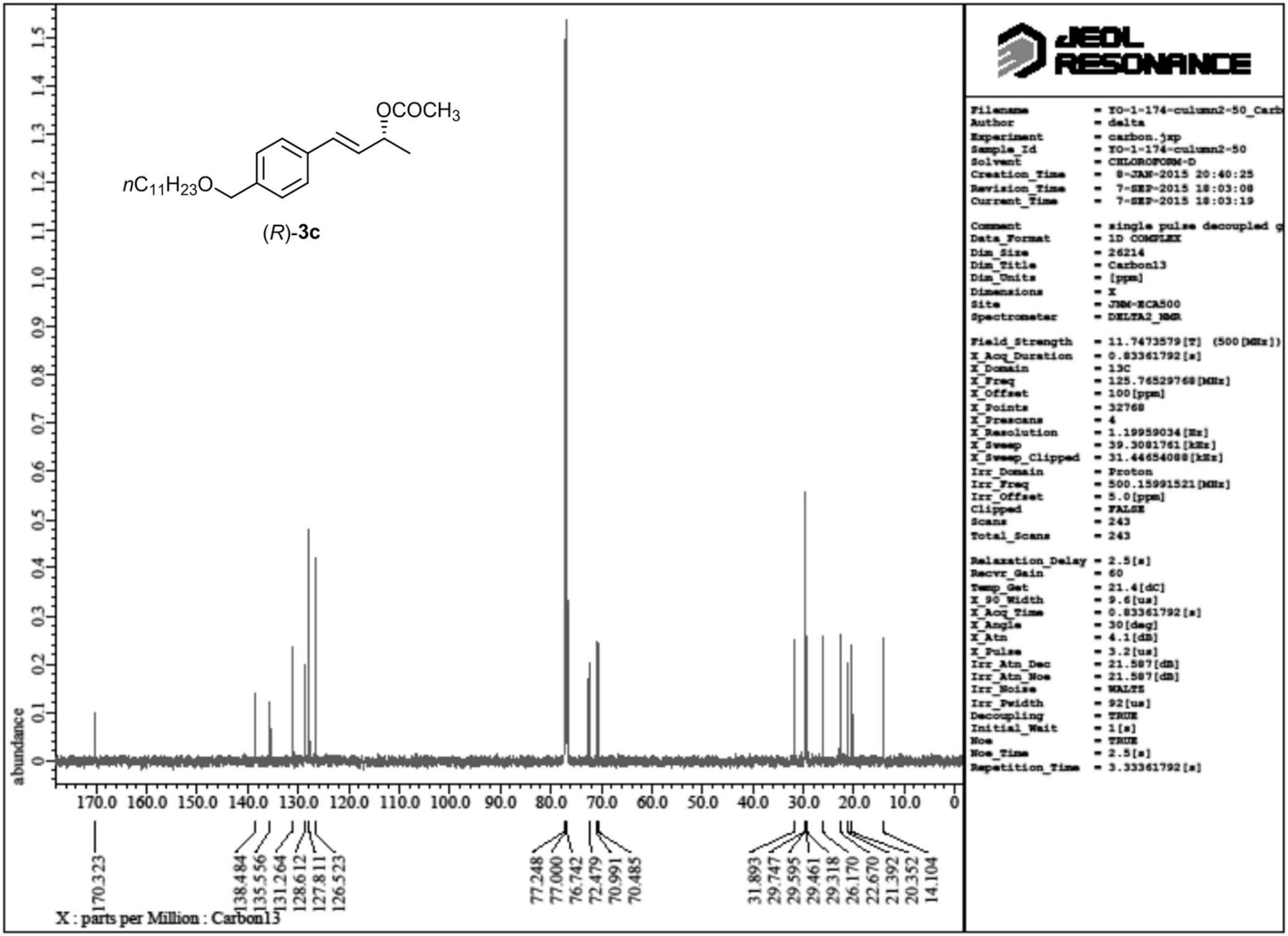

OH
(S)-1f
abundance
X : parts per Million : Carbon13
159.974
138.627
134.068
129.251
105.453
101.142
77.258
77.000
76.752
71.907
70.791
70.638
70.543
69.675
68.778
67.443
59.030
23.376
JEOL RESONANCE
Filename = YO-2-173-column_Carbon-1
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-2-173-column
Solvent = CHLOROFORM-D
Creation_Time = 2-SEP-2015 11:15:32
Revision_Time = 7-SEP-2015 18:35:51
Current_Time = 7-SEP-2015 18:36:06
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 456.0
Total_Scans = 456.0
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 21.9[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]

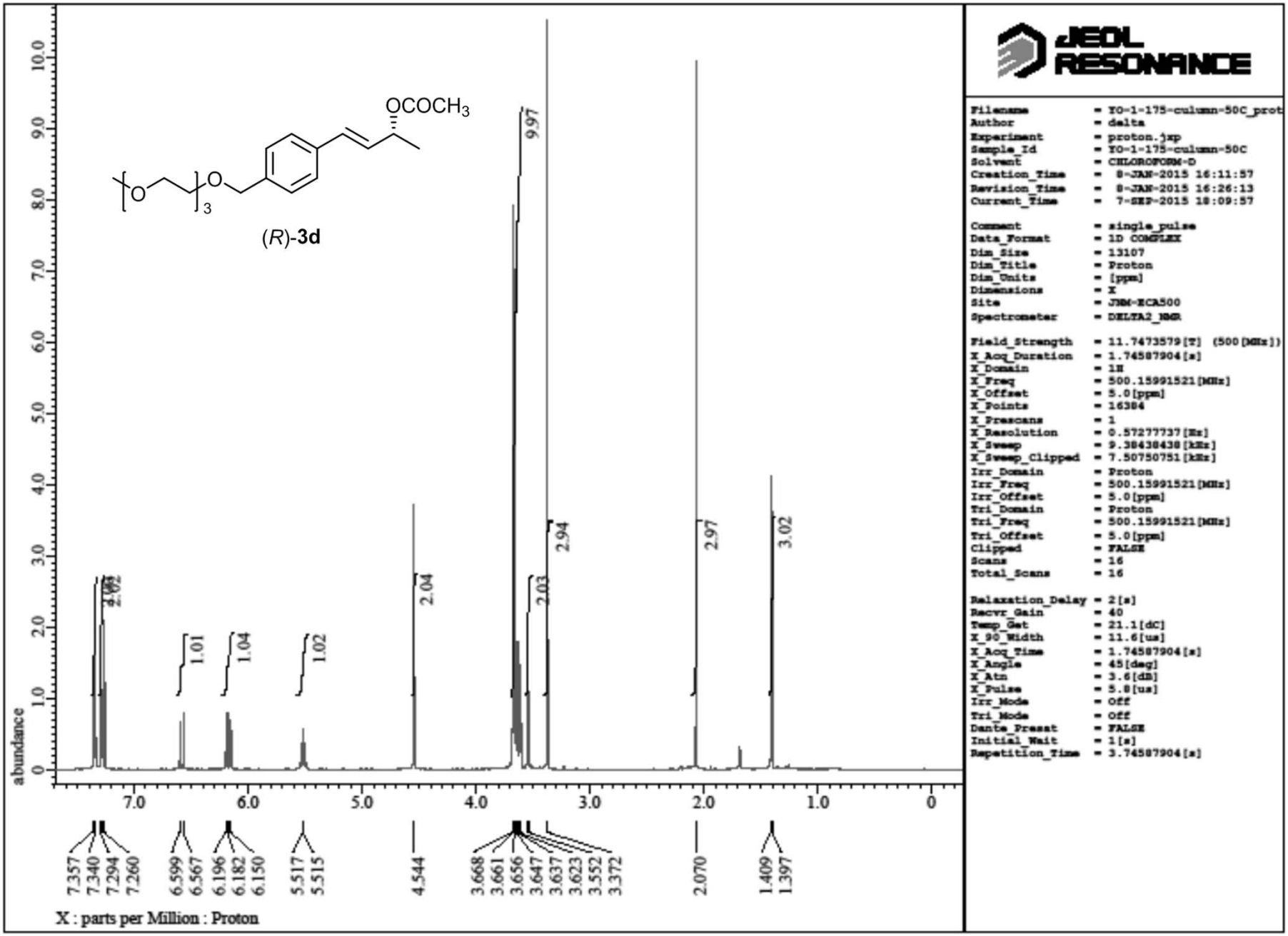

OCOCH3
(R)-3a
3.05
2.03
1.00
1.01
1.00
2.99
3.00
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.412
7.388
7.386
7.355
7.332
7.277
6.647
6.594
6.244
6.221
6.168
5.591
5.588
5.569
5.566
5.548
5.544
5.526
5.523
2.306
2.092
2.081
1.441
1.419
1.276
X : parts per Million : Proton
JEOL RESONANCE
Filename = phenylvinyletanol-acetat
Author = delta
Experiment = proton.jxp
Sample_Id = S.K3-139-H-data
Solvent = CHLOROFORM-D
Creation_Time = 21-AUG-2014 21:36:28
Revision_Time = 20-AUG-2015 11:29:19
Current_Time = 20-AUG-2015 14:02:17
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 2.90717696[s]
X_Domain = 1H
X_Freq = 300.52965592[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.34397631[Hz]
X_Sweep = 5.63570784[kHz]
X_Sweep_Clipped = 4.50856628[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 300.52965592[MHz]
Tri_Offset = 5[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Set = 25.9[dC]
X_90_Width = 11.2[us]
X_Acq_Time = 2.90717696[s]
X_Angle = 45[deg]
X_Atn = 1[dB]
X_Pulse = 5.6[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 4.90717696[s]

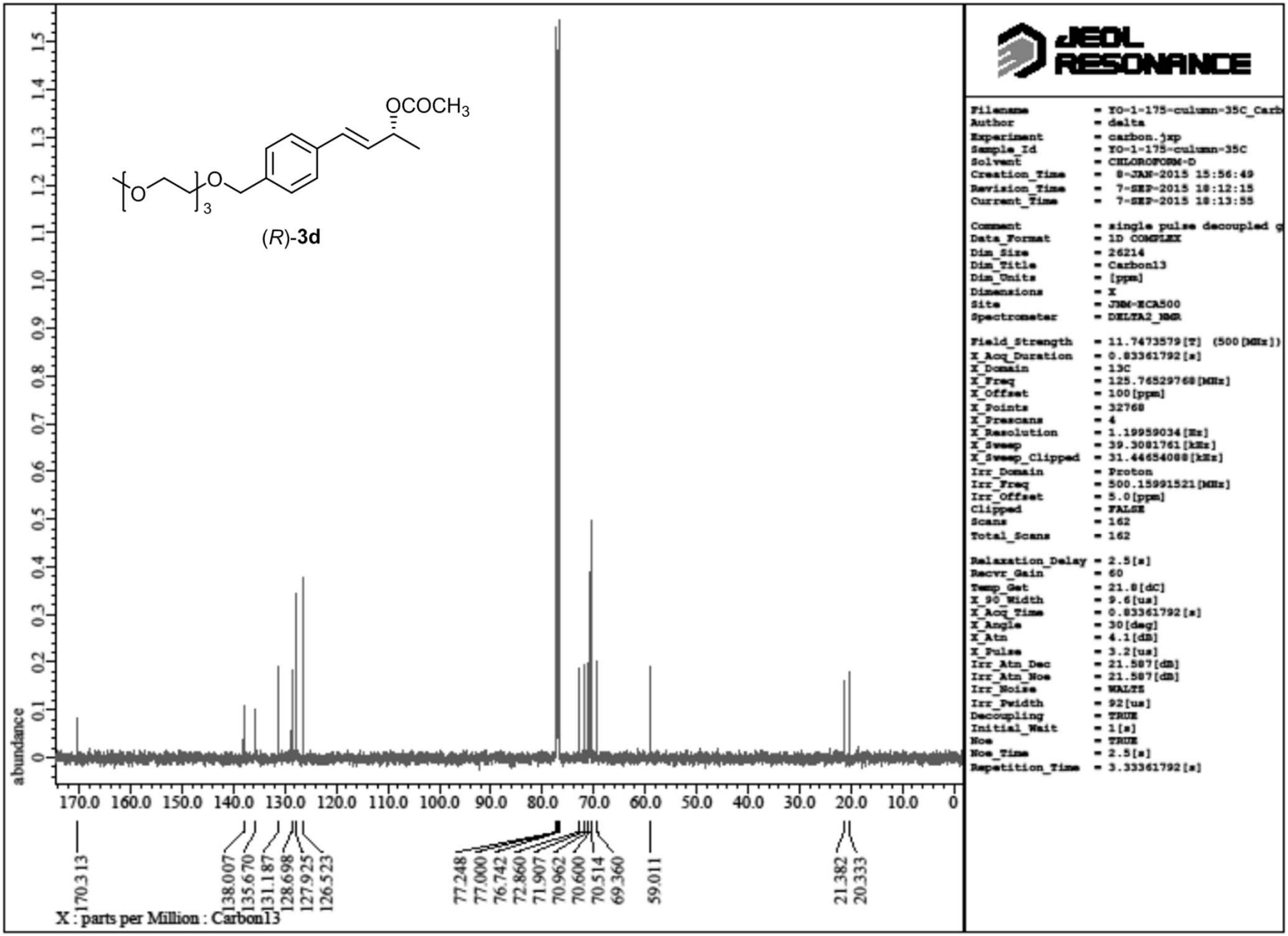

OCOCH3
(R)-3b
4.94
3.97
2.01
1.96
1.00
1.00
0.98
3.02
3.04
abundance
8.135
7.953
7.947
7.746
7.742
7.260
6.823
6.792
6.426
6.413
6.380
5.612
2.117
1.546
1.486
1.473
X : parts per Million : Proton
Filename = dinaphthyl-OAc-7.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = dinaphthyl-p2
Solvent = CHLOROFORM-D
Creation_Time = 11-SEP-2014 10:11:49
Revision_Time = 11-SEP-2014 21:15:11
Current_Time = 28-OCT-2015 07:29:58
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 21.3[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

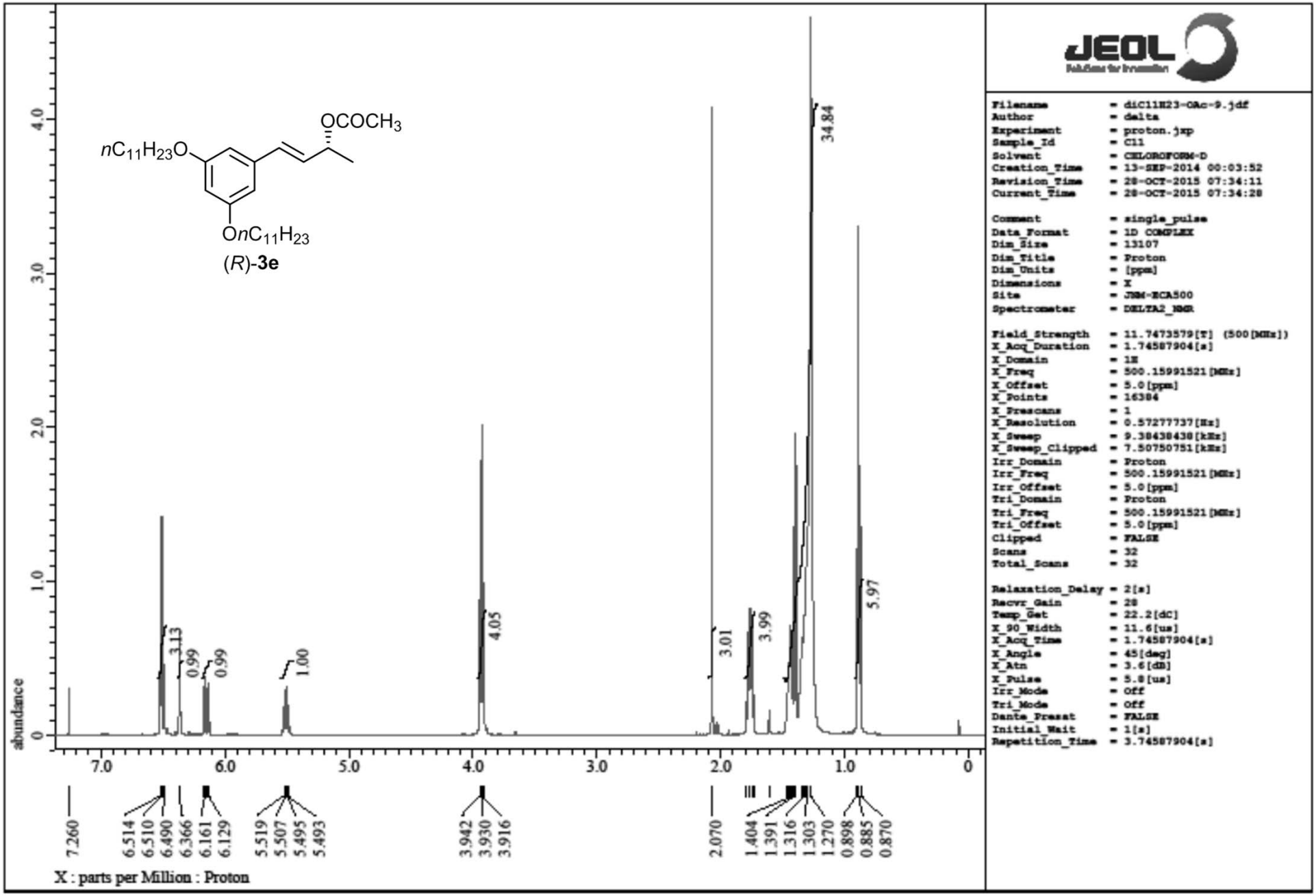

OCOCH3
(R)-3b
abundance
X : parts per Million : Carbon13
170.390
142.128
138.227
133.629
132.732
131.368
129.728
128.516
128.202
127.668
126.380
126.275
126.075
125.979
125.569
124.711
77.258
77.000
76.752
70.972
21.439
20.409
Filename = dinaphthyl-OAc-C-5.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = dinphthyl-OAc
Solvent = CHLOROFORM-D
Creation_Time = 11-SEP-2014 05:37:59
Revision_Time = 11-SEP-2014 21:19:24
Current_Time = 28-OCT-2015 07:31:09
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 228.0
Total_Scans = 228.0
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 20.8[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

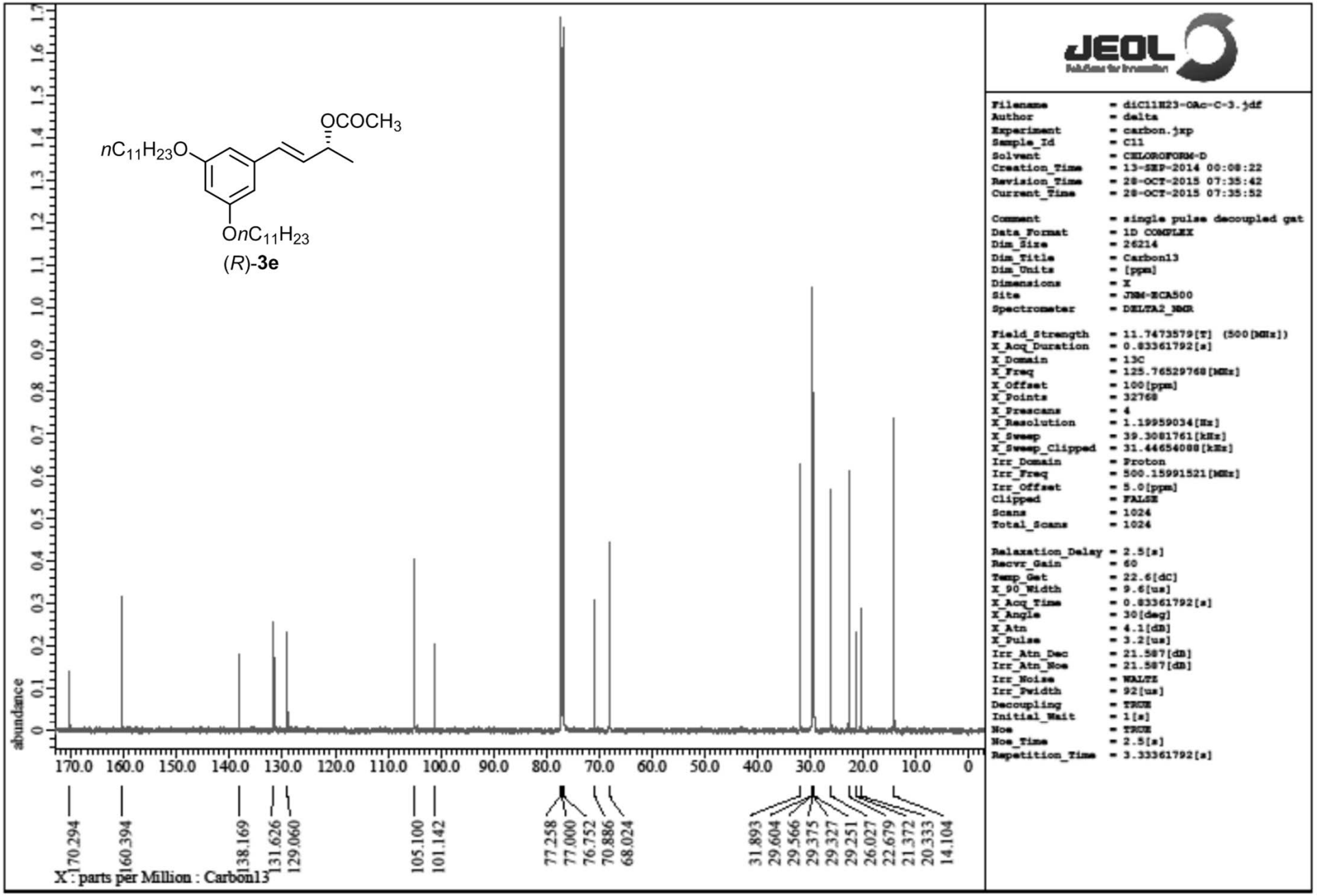

OCOCH3
nC11H23O
(R)-3c
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.00
0.99
0.95
2.00
2.01
2.83
2.19
3.06
2.89
15.97
7.364
7.347
7.292
7.260
6.606
6.574
6.200
6.186
6.154
5.535
5.533
5.520
5.509
5.507
4.479
3.456
3.443
3.429
2.073
1.600
1.413
1.400
1.257
0.921
0.893
0.879
0.865
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-1-174-column2-50_prot
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-174-column2-50
Solvent = CHLOROFORM-D
Creation_Time = 8-JAN-2015 20:36:53
Revision_Time = 7-SEP-2015 17:55:24
Current_Time = 7-SEP-2015 17:57:15
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 34
Temp_Get = 21.3[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

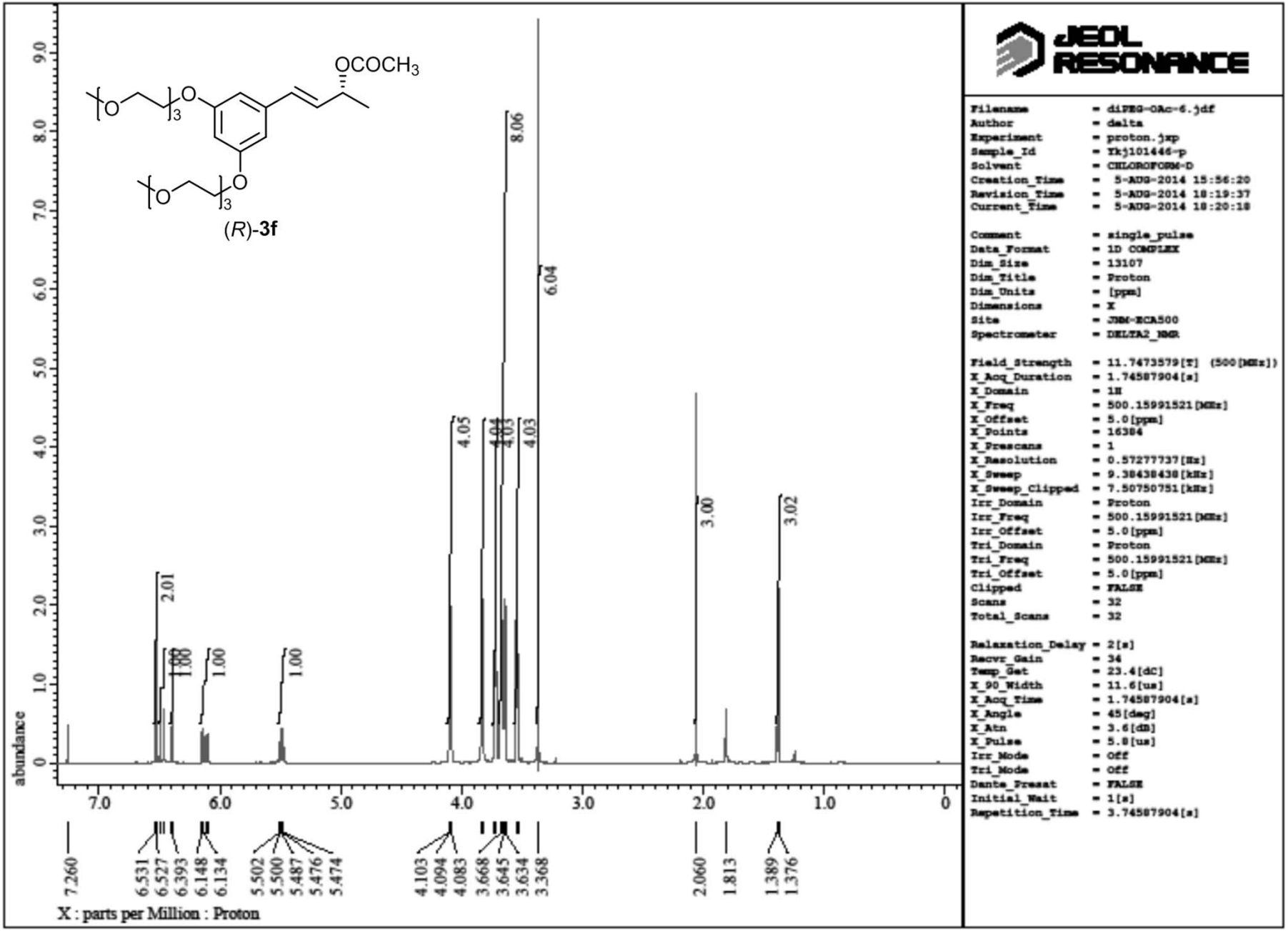

OCOCH3
nC11H23O
(R)-3c
abundance
170.323
138.484
135.556
131.264
128.612
127.811
126.523
77.248
77.000
76.742
72.479
70.991
70.485
31.893
29.747
29.595
29.461
29.318
26.170
22.670
21.392
20.352
14.104
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-1-174-column2-50_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-1-174-column2-50
Solvent = CHLOROFORM-D
Creation_Time = 8-JAN-2015 20:40:25
Revision_Time = 7-SEP-2015 18:03:08
Current_Time = 7-SEP-2015 18:03:19
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 243
Total_Scans = 243
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 21.4[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

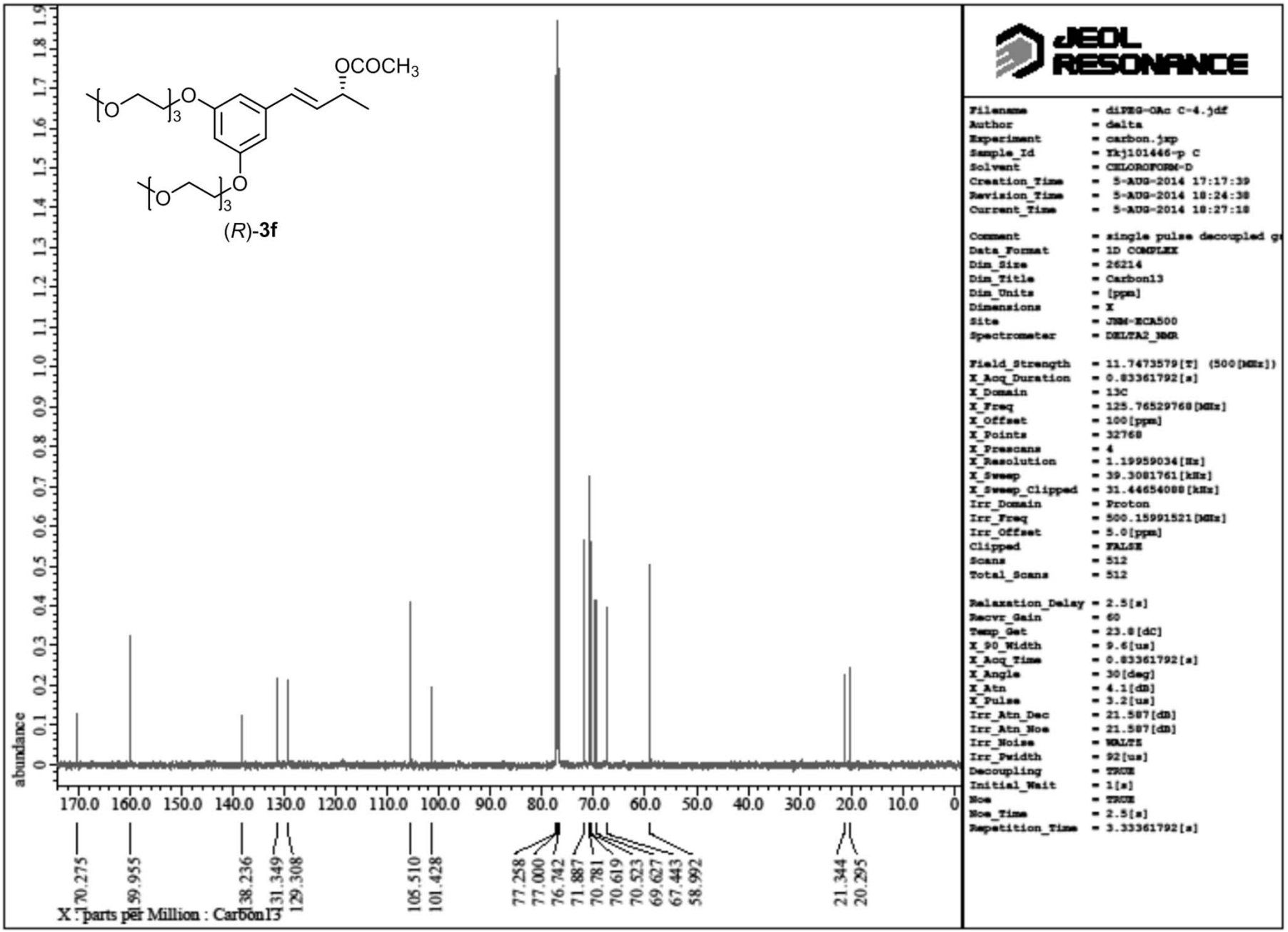

OCOCH3
O
O
3
(R)-3d
abundance
9.97
2.94
2.97
3.02
2.04
2.03
1.01
1.04
1.02
7.357
7.340
7.294
7.260
6.599
6.567
6.196
6.182
6.150
5.517
5.515
4.544
3.668
3.661
3.656
3.647
3.637
3.623
3.552
3.372
2.070
1.409
1.397
X : parts per Million : Proton
JEOL RESONANCE
Filename = YO-1-175-column-50C_prot
Author = delta
Experiment = proton.jxp
Sample_Id = YO-1-175-column-50C
Solvent = CHLOROFORM-D
Creation_Time = 8-JAN-2015 16:11:57
Revision_Time = 8-JAN-2015 16:26:13
Current_Time = 7-SEP-2015 18:09:57
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 21.1[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

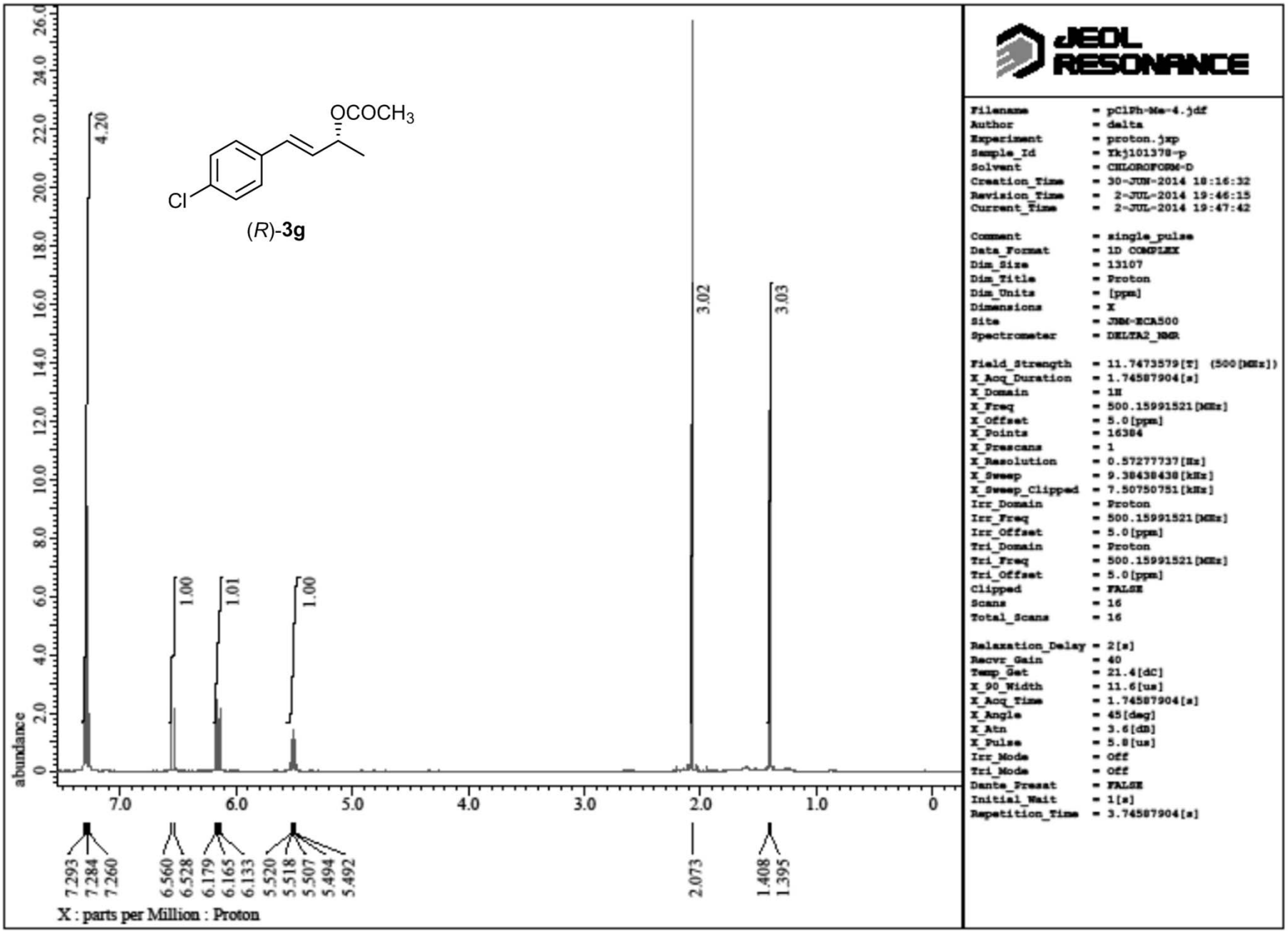

OCOCH3
O
O
3
(R)-3d
abundance
170.313
138.007
135.670
131.187
128.698
127.925
126.523
77.248
77.000
76.742
72.860
71.907
70.962
70.600
70.514
69.360
59.011
21.382
20.333
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = YO-1-175-column-35C_Carb
Author = delta
Experiment = carbon.jxp
Sample_Id = YO-1-175-column-35C
Solvent = CHLOROFORM-D
Creation_Time = 8-JAN-2015 15:56:49
Revision_Time = 7-SEP-2015 18:12:15
Current_Time = 7-SEP-2015 18:13:55
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 162
Total_Scans = 162
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 21.8[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

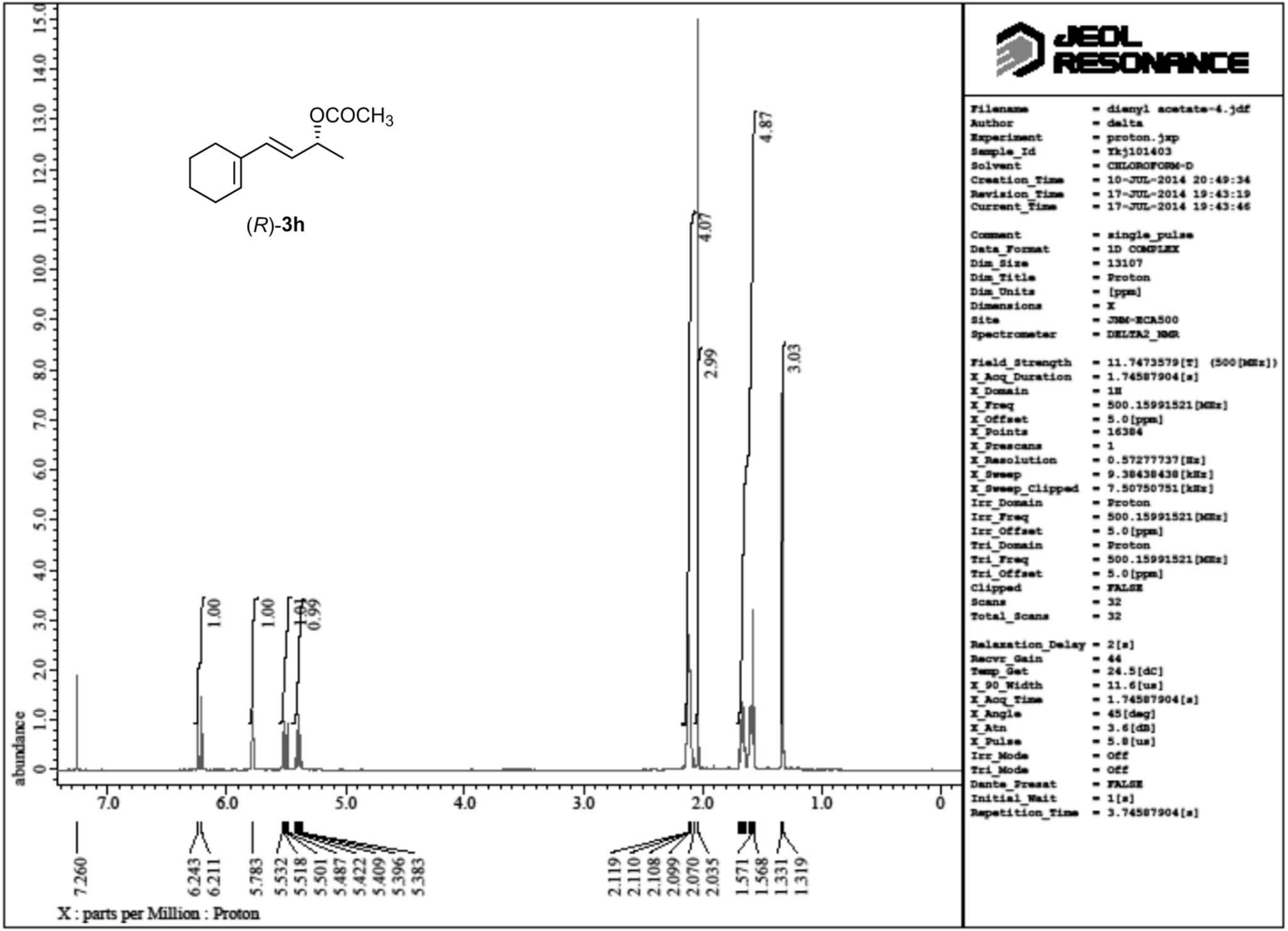

OCOCH3
nC11H23O
OnC11H23
(R)-3e
abundance
34.84
5.97
4.05
3.13
3.01
3.99
0.99
0.99
1.00
7.260
6.514
6.510
6.490
6.366
6.161
6.129
5.519
5.507
5.495
5.493
3.942
3.930
3.916
2.070
1.404
1.391
1.316
1.303
1.270
0.898
0.885
0.870
X : parts per Million : Proton
Filename = diC11H23-OAc-9.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = C11
Solvent = CHLOROFORM-D
Creation_Time = 13-SEP-2014 00:03:52
Revision_Time = 28-OCT-2015 07:34:11
Current_Time = 28-OCT-2015 07:34:28
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 28
Temp_Get = 22.2[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Preset = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

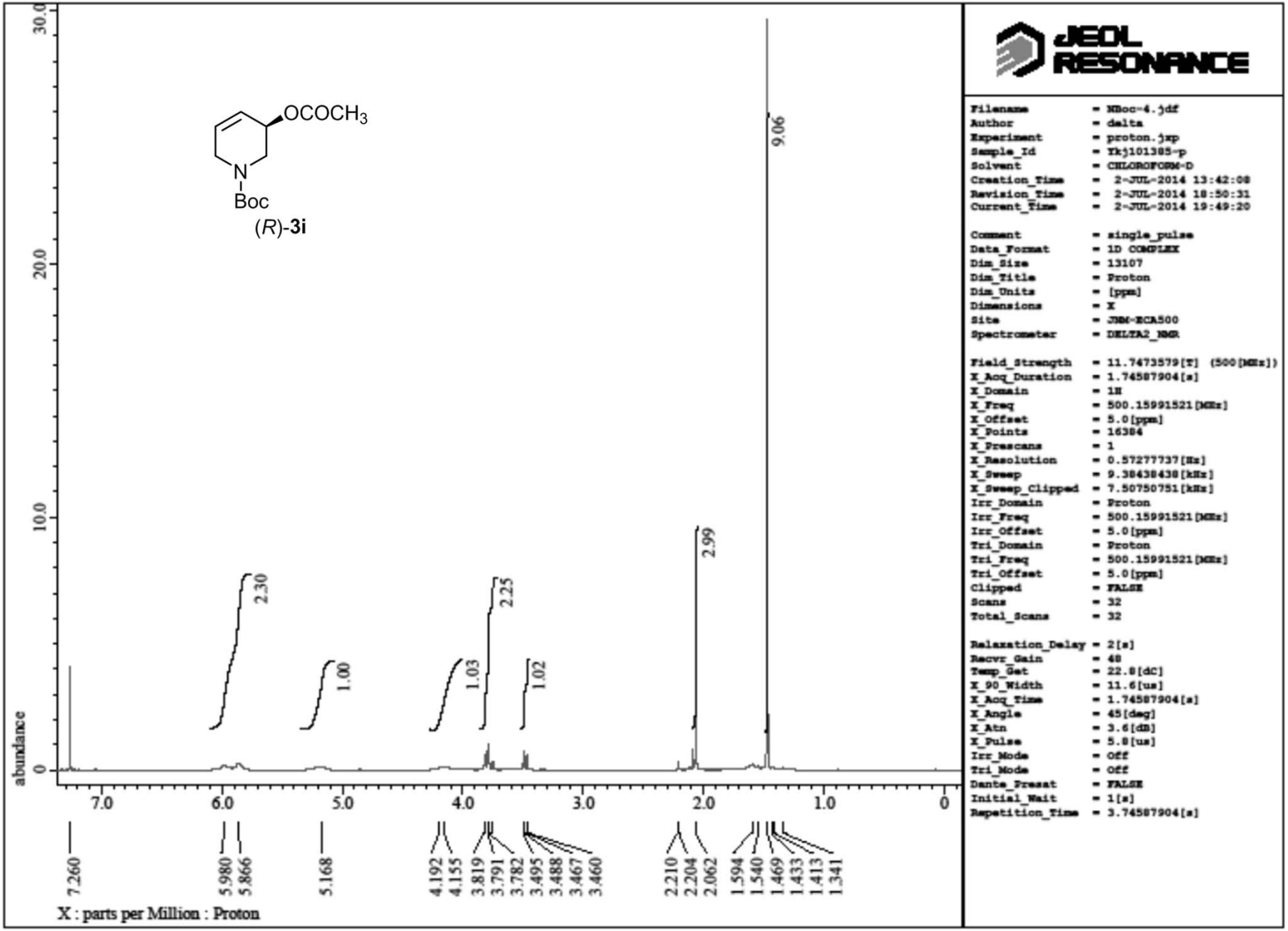

OCOCH3
nC11H23O
OnC11H23
(R)-3e
abundance
X : parts per Million : Carbon13
170.294
160.394
138.169
131.626
129.060
105.100
101.142
77.258
77.000
76.752
70.886
68.024
31.893
29.604
29.566
29.375
29.327
29.251
26.027
22.679
21.372
20.333
14.104
Filename = diC11H23-OAc-C-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = C11
Solvent = CHLOROFORM-D
Creation_Time = 13-SEP-2014 00:08:22
Revision_Time = 28-OCT-2015 07:35:42
Current_Time = 28-OCT-2015 07:35:52
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 22.6[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

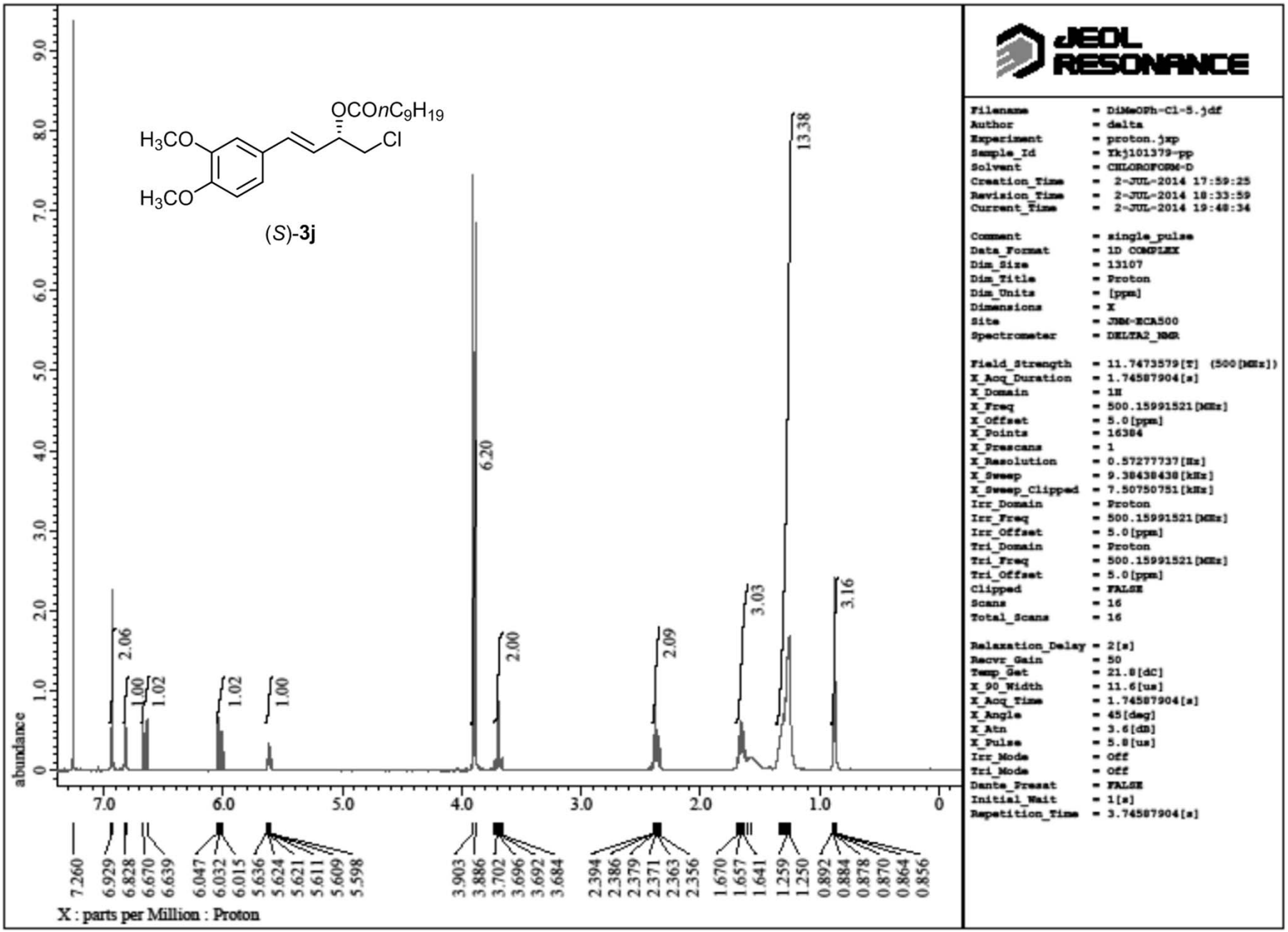

OCOCH3
(R)-3f
abundance
X : parts per Million : Proton
JEOL RESONANCE
Filename = diPEG-OAc-6.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101446-p
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 15:56:20
Revision_Time = 5-AUG-2014 18:19:37
Current_Time = 5-AUG-2014 18:20:18
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 34
Temp_Get = 23.4[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

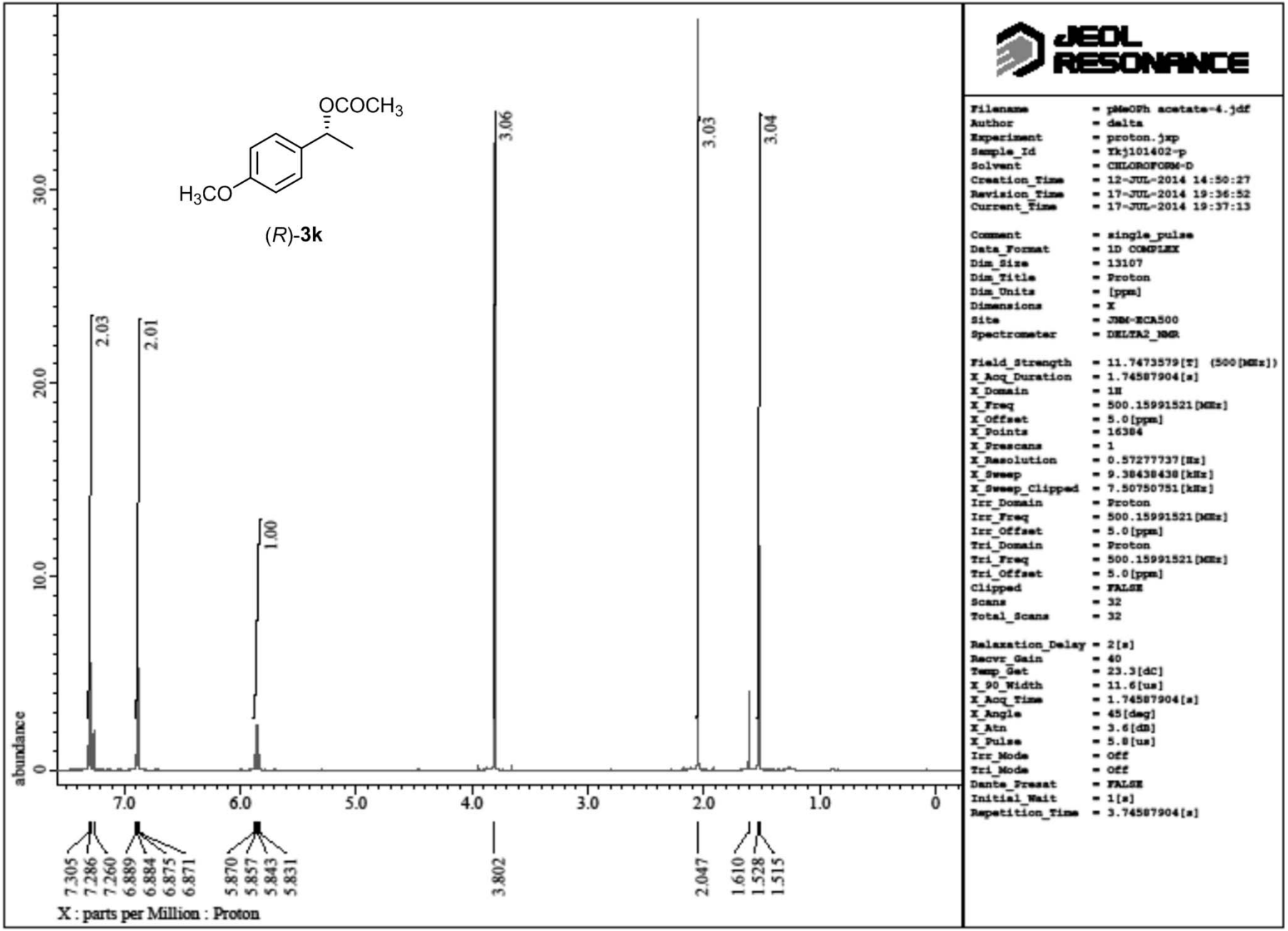

OCOCH3
(R)-3f
abundance
X : parts per Million : Carbon13
170.275
159.955
138.236
131.349
129.308
105.510
101.428
77.258
77.000
76.742
71.887
70.781
70.619
70.523
69.627
67.443
58.992
21.344
20.295
JEOL RESONANCE
Filename = diPEG-OAc C-4.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj101446-p C
Solvent = CHLOROFORM-D
Creation_Time = 5-AUG-2014 17:17:39
Revision_Time = 5-AUG-2014 18:24:38
Current_Time = 5-AUG-2014 18:27:18
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 512
Total_Scans = 512
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 23.8[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]

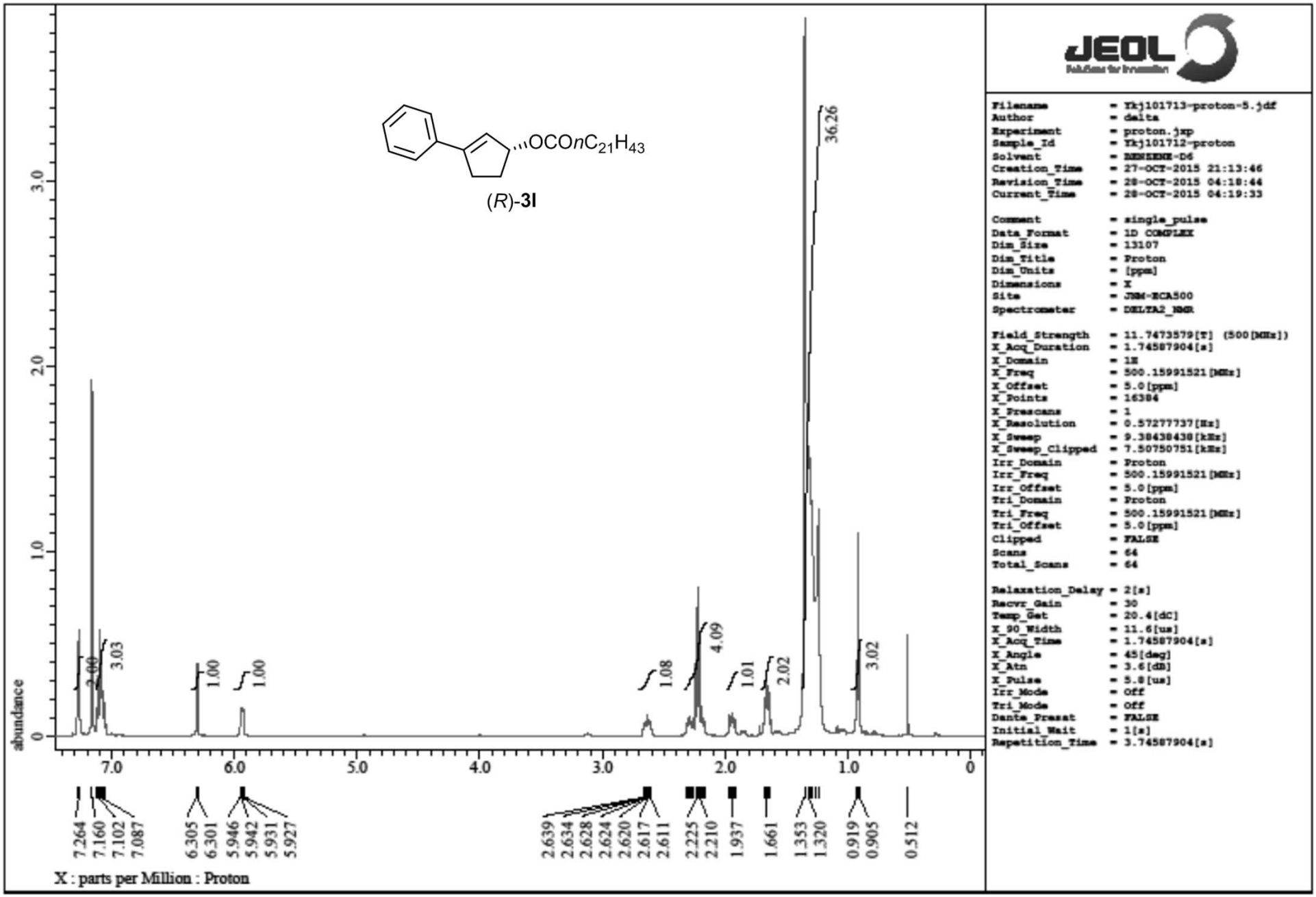

OCOCH3
Cl
(R)-3g
4.20
1.00
1.01
1.00
3.02
3.03
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.293
7.284
7.260
6.560
6.528
6.179
6.165
6.133
5.520
5.518
5.507
5.494
5.492
2.073
1.408
1.395
X : parts per Million : Proton
JEOL RESONANCE
Filename = pClPh-Me-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101378-p
Solvent = CHLOROFORM-D
Creation_Time = 30-JUN-2014 18:16:32
Revision_Time = 2-JUL-2014 19:46:15
Current_Time = 2-JUL-2014 19:47:42
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 21.4[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

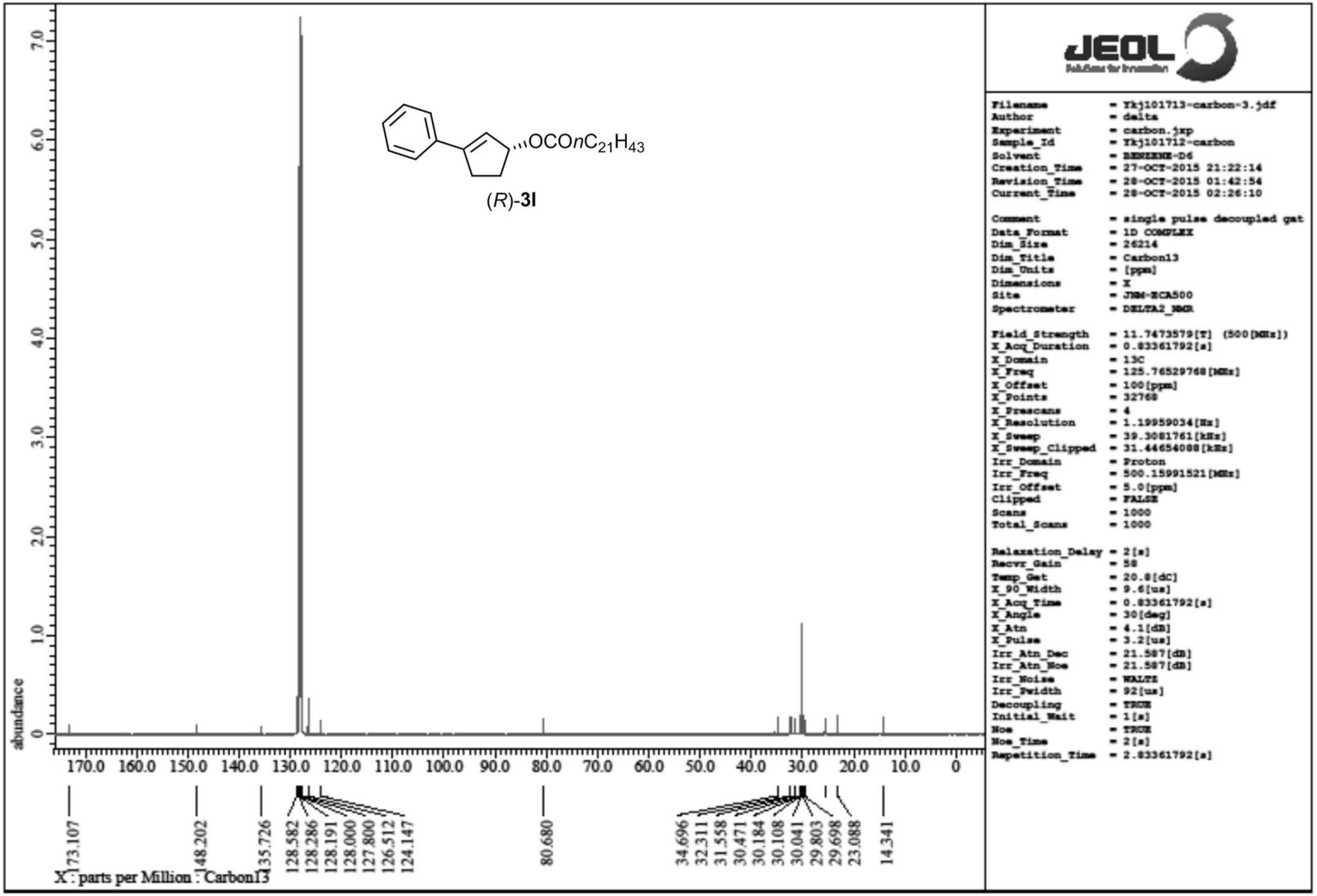

OCOCH3
(R)-3h
abundance
X : parts per Million : Proton
7.260
6.243
6.211
5.783
5.532
5.518
5.501
5.487
5.422
5.409
5.396
5.383
2.119
2.110
2.108
2.099
2.070
2.035
1.571
1.568
1.331
1.319
1.00
1.00
1.01
0.99
4.07
2.99
4.87
3.03
JEOL RESONANCE
Filename = dienyl acetate-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101403
Solvent = CHLOROFORM-D
Creation_Time = 10-JUL-2014 20:49:34
Revision_Time = 17-JUL-2014 19:43:19
Current_Time = 17-JUL-2014 19:43:46
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 44
Temp_Get = 24.5[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

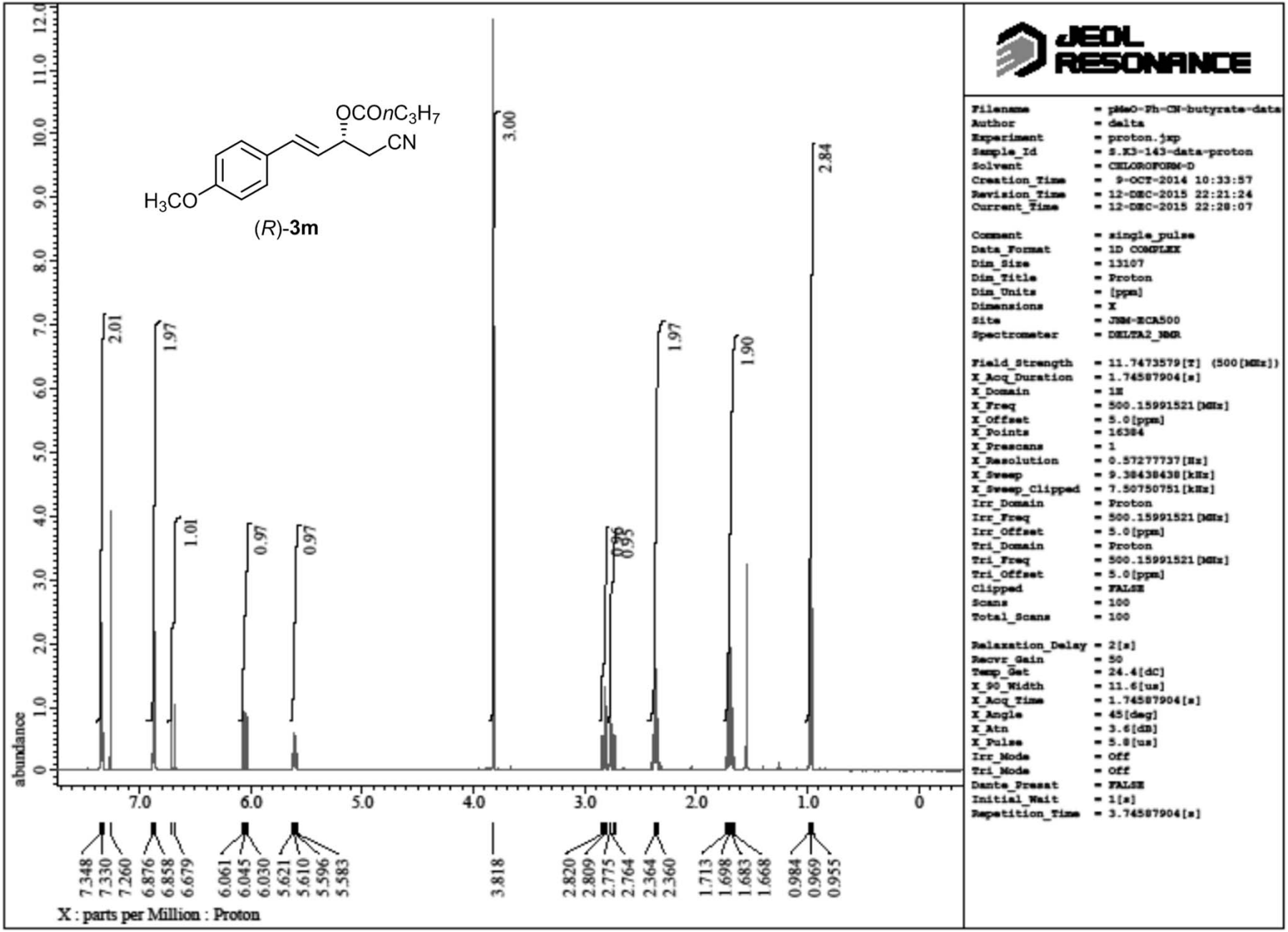

OCOCH3
N
Boc
(R)-3i
9.06
2.99
2.30
2.25
1.00
1.03
1.02
abundance
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.260
5.980
5.866
5.168
4.192
4.155
3.819
3.791
3.782
3.495
3.488
3.467
3.460
2.210
2.204
2.062
1.594
1.540
1.469
1.433
1.413
1.341
X : parts per Million : Proton
JEOL RESONANCE
Filename = NBoc-4.jdf
Author = dalta
Experiment = proton.jxp
Sample_Id = Ykj101385-p
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2014 13:42:08
Revision_Time = 2-JUL-2014 18:50:31
Current_Time = 2-JUL-2014 19:49:20
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 48
Temp_Get = 22.8[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

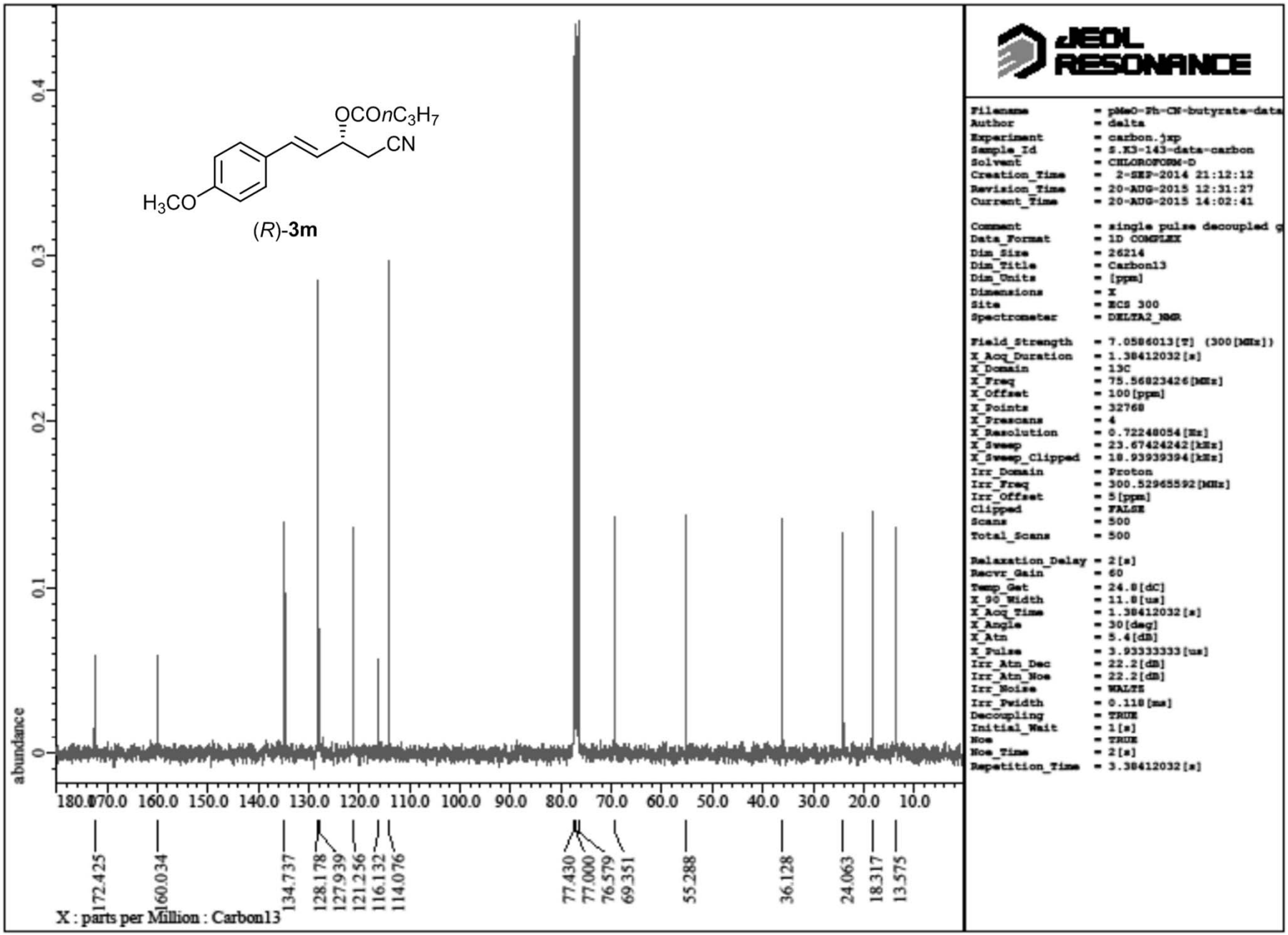

OCOnC_9H_{19}
H_3CO
H_3CO
Cl
(*S*)-**3j**
abundance
X : parts per Million : Proton
JEOL RESONANCE
Filename = DiMeOPh-Cl-5.jdf
Author = dalta
Experiment = proton.jxp
Sample_Id = Ykj101379-pp
Solvent = CHLOROFORM-D
Creation_Time = 2-JUL-2014 17:59:25
Revision_Time = 2-JUL-2014 18:33:59
Current_Time = 2-JUL-2014 19:48:34
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

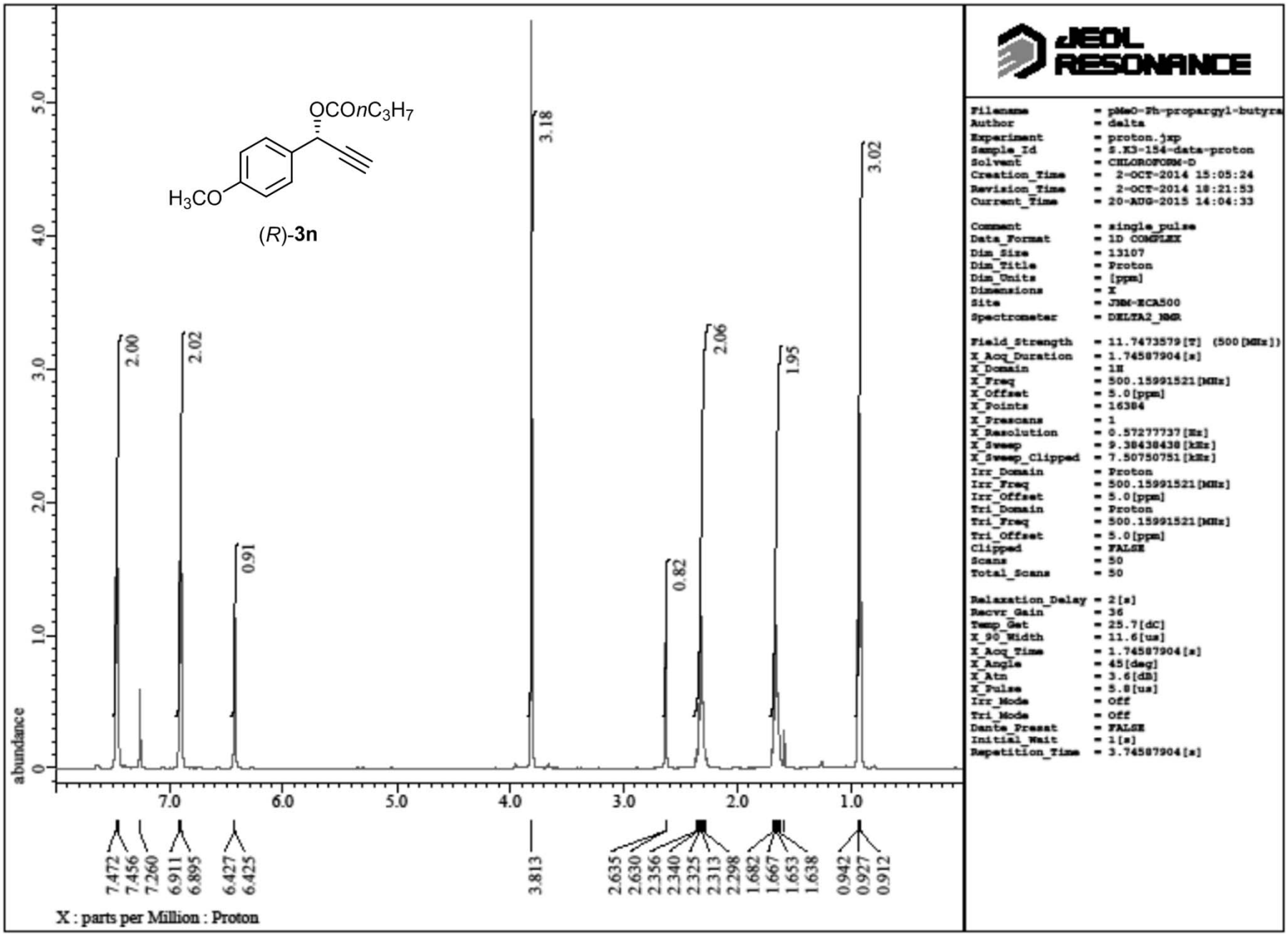

OCOCH3
H3CO
(R)-3k
2.03
2.01
1.00
3.06
3.03
3.04
abundance
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.305
7.286
7.260
6.889
6.884
6.875
6.871
5.870
5.857
5.843
5.831
3.802
2.047
1.610
1.528
1.515
X : parts per Million : Proton
JEOL RESONANCE
Filename = pMeOPh acetate-4.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101402-p
Solvent = CHLOROFORM-D
Creation_Time = 12-JUL-2014 14:50:27
Revision_Time = 17-JUL-2014 19:36:52
Current_Time = 17-JUL-2014 19:37:13
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 32
Total_Scans = 32
Relaxation_Delay = 2[s]
Recvr_Gain = 40
Temp_Get = 23.3[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]

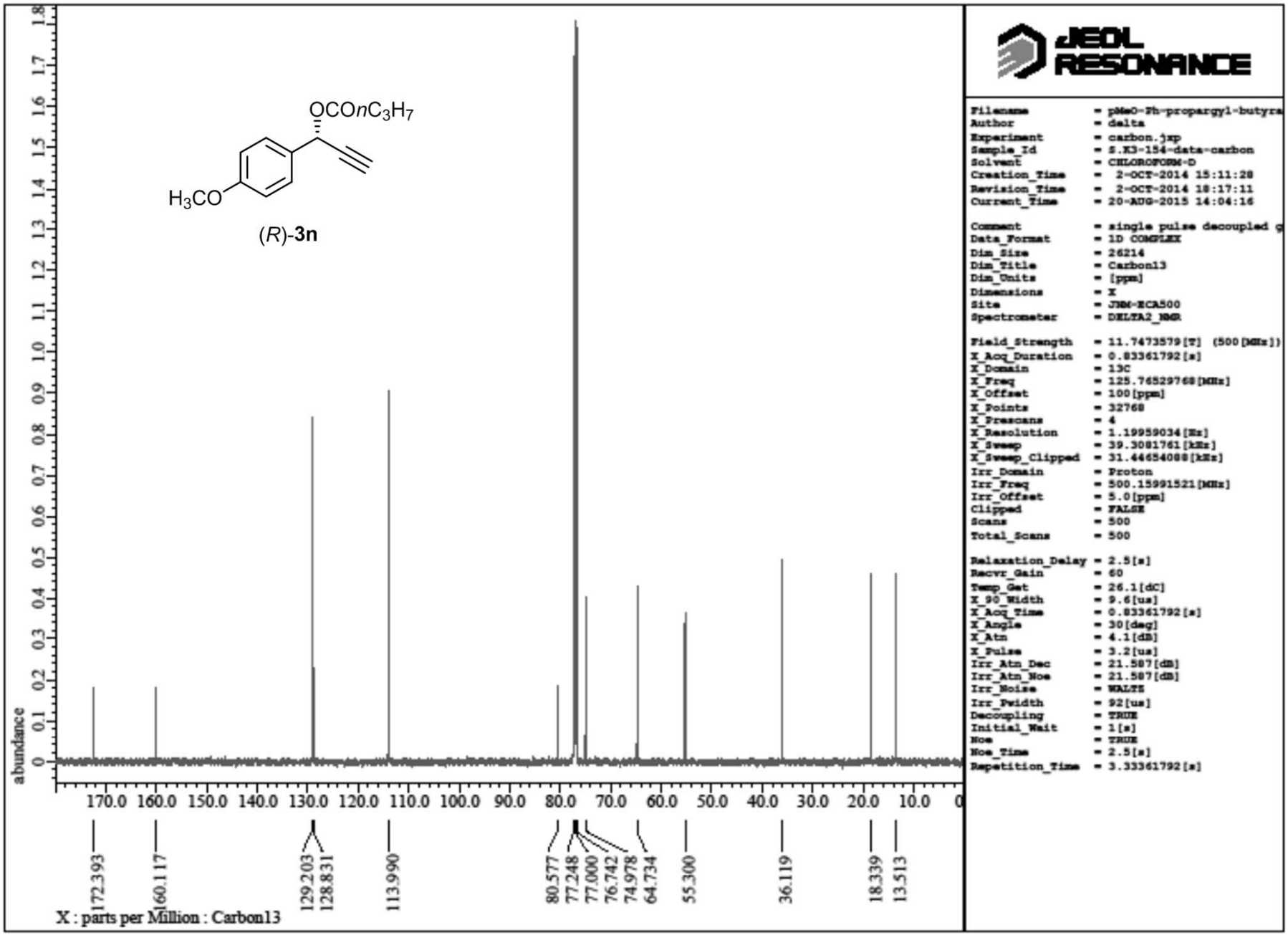

OCO$nC_{21}H_{43}$
(*R*)-**3l**
abundance
X : parts per Million : Proton
7.264
7.160
7.102
7.087
6.305
6.301
5.946
5.942
5.931
5.927
2.639
2.634
2.628
2.624
2.620
2.617
2.611
2.225
2.210
1.937
1.661
1.353
1.320
0.919
0.905
0.512
2.00
3.03
1.00
1.00
1.08
4.09
1.01
2.02
36.26
3.02
Filename = Ykj101713-proton-5.jdf
Author = delta
Experiment = proton.jxp
Sample_Id = Ykj101712-proton
Solvent = BENZENE-D6
Creation_Time = 27-OCT-2015 21:13:46
Revision_Time = 28-OCT-2015 04:18:44
Current_Time = 28-OCT-2015 04:19:33
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 64
Total_Scans = 64
Relaxation_Delay = 2[s]
Recvr_Gain = 30
Temp_Get = 20.4[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]


OCO$nC_{21}H_{43}$
(*R*)-**3l**
abundance
X : parts per Million : Carbon13
173.107
148.202
135.726
128.582
128.286
128.191
128.000
127.800
126.512
124.147
80.680
34.696
32.311
31.558
30.471
30.184
30.108
30.041
29.803
29.698
23.088
14.341
Filename = Ykj101713-carbon-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = Ykj101712-carbon
Solvent = BENZENE-D6
Creation_Time = 27-OCT-2015 21:22:14
Revision_Time = 28-OCT-2015 01:42:54
Current_Time = 28-OCT-2015 02:26:10
Comment = single pulse decoupled gat
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 1000
Total_Scans = 1000
Relaxation_Delay = 2[s]
Recvr_Gain = 58
Temp_Get = 20.8[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]


OCOnC_3H_7
CN
H_3CO
(*R*)-**3m**
abundance
2.01
1.97
1.01
0.97
0.97
3.00
0.96
0.93
1.97
1.90
2.84
7.348
7.330
7.260
6.876
6.858
6.679
6.061
6.045
6.030
5.621
5.610
5.596
5.583
3.818
2.820
2.809
2.775
2.764
2.364
2.360
1.713
1.698
1.683
1.668
0.984
0.969
0.955
X : parts per Million : Proton
JEOL RESONANCE
Filename = pMeO-Ph-CN-butyrate-data
Author = delta
Experiment = proton.jxp
Sample_Id = S.K3-143-data-proton
Solvent = CHLOROFORM-D
Creation_Time = 9-OCT-2014 10:33:57
Revision_Time = 12-DEC-2015 22:21:24
Current_Time = 12-DEC-2015 22:28:07
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 100
Total_Scans = 100
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 24.4[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]


OCOnC_3H_7
CN
H_3CO
(*R*)-**3m**
abundance
0.4
0.3
0.2
0.1
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
172.425
160.034
134.737
128.178
127.939
121.256
116.132
114.076
77.430
77.000
76.579
69.351
55.288
36.128
24.063
18.317
13.575
X : parts per Million : Carbon13
JEOL RESONANCE
Filename = pMeO-Ph-CN-butyrate-data
Author = delta
Experiment = carbon.jxp
Sample_Id = S.K3-143-data-carbon
Solvent = CHLOROFORM-D
Creation_Time = 2-SEP-2014 21:12:12
Revision_Time = 20-AUG-2015 12:31:27
Current_Time = 20-AUG-2015 14:02:41
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = ECS 300
Spectrometer = DELTA2_NMR
Field_Strength = 7.0586013[T] (300[MHz])
X_Acq_Duration = 1.38412032[s]
X_Domain = 13C
X_Freq = 75.56823426[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.72248054[Hz]
X_Sweep = 23.67424242[kHz]
X_Sweep_Clipped = 18.93939394[kHz]
Irr_Domain = Proton
Irr_Freq = 300.52965592[MHz]
Irr_Offset = 5[ppm]
Clipped = FALSE
Scans = 500
Total_Scans = 500
Relaxation_Delay = 2[s]
Recvr_Gain = 60
Temp_Get = 24.8[dC]
X_90_Width = 11.8[us]
X_Acq_Time = 1.38412032[s]
X_Angle = 30[deg]
X_Atn = 5.4[dB]
X_Pulse = 3.93333333[us]
Irr_Atn_Dec = 22.2[dB]
Irr_Atn_Noe = 22.2[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 0.118[ms]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 3.38412032[s]


OCOnC_3H_7
H_3CO
(*R*)-**3n**
abundance
X : parts per Million : Proton
7.472
7.456
7.260
6.911
6.895
6.427
6.425
3.813
2.635
2.630
2.356
2.340
2.325
2.313
2.298
1.682
1.667
1.653
1.638
0.942
0.927
0.912
2.00
2.02
0.91
3.18
0.82
2.06
1.95
3.02
JEOL RESONANCE
Filename = pMeO-Ph-propargyl-butyra
Author = delta
Experiment = proton.jxp
Sample_Id = S.K3-154-data-proton
Solvent = CHLOROFORM-D
Creation_Time = 2-OCT-2014 15:05:24
Revision_Time = 2-OCT-2014 18:21:53
Current_Time = 20-AUG-2015 14:04:33
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 50
Total_Scans = 50
Relaxation_Delay = 2[s]
Recvr_Gain = 36
Temp_Get = 25.7[dC]
X_90_Width = 11.6[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 3.6[dB]
X_Pulse = 5.8[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 3.74587904[s]


OCOnC_3H_7
H_3CO
(*R*)-**3n**
abundance
X : parts per Million : Carbon13
172.393
160.117
129.203
128.831
113.990
80.577
77.248
77.000
76.742
74.978
64.734
55.300
36.119
18.339
13.513
JEOL RESONANCE
Filename = pMeO-Ph-propargyl-butyra
Author = delta
Experiment = carbon.jxp
Sample_Id = S.K3-154-data-carbon
Solvent = CHLOROFORM-D
Creation_Time = 2-OCT-2014 15:11:28
Revision_Time = 2-OCT-2014 18:17:11
Current_Time = 20-AUG-2015 14:04:16
Comment = single pulse decoupled g
Data_Format = 1D COMPLEX
Dim_Size = 26214
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 500
Total_Scans = 500
Relaxation_Delay = 2.5[s]
Recvr_Gain = 60
Temp_Get = 26.1[dC]
X_90_Width = 9.6[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 4.1[dB]
X_Pulse = 3.2[us]
Irr_Atn_Dec = 21.587[dB]
Irr_Atn_Noe = 21.587[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2.5[s]
Repetition_Time = 3.33361792[s]