Supplementary Material (ESI) for Chemical Communications

Formation of Multi-stereogenic Centers

Using a Catalytic Diastereoselective Henry Reaction

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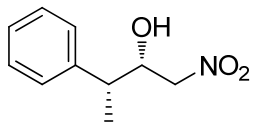
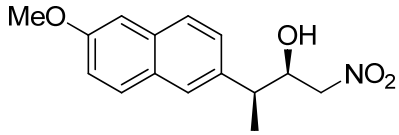
Experimental Section

General Procedure of the (*R,R,R*)-L1-CuCl-Catalyzed Diastereoselective Henry Reaction with Nitromethane. The catalyst was prepared by a complex formation of ligand (*R,R,R*)-**L1** (7.1 mg, 0.011 mol), CuCl (1.0 mg, 0.01 mmol), and pyridine (1 μL, 0.011mmol) in anhydrous dichloromethane (0.5 mL) under Ar. After being stirred for 15 min at room temperature, the solvent was removed under reduced pressure. To the residue were added nitromethane (112 μL, 2 mmol), EtOH (0.4 mL), pyridine (21 μL, 0.26 mmol), and (*S*)-2-phenylpropanal (27 μL, 0.2 mmol) under Ar. The diastereoselective Henry reaction was performed for 19 h at room temperature. Then, the reaction was quenched by the addition of 1N HCl, and the aqueous layer was extracted with dichloromethane. The organic phase was washed with brine, and dried over sodium sulfate. After removal of the solvent under reduced pressure, the residue was purified by column chromatography (using spherical silica gel, *n*-hexane/ethyl acetate =6:1) to afford the adduct (27.6 mg, 71% yield). Diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy and the enantiomeric excess was determined by HPLC analysis.

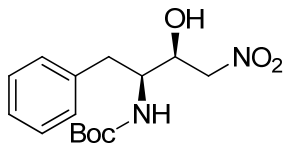
General Procedure of the (*R,R,R*)-L1-CuCl-Catalyzed Diastereoselective Henry Reaction with Nitroethane. The catalyst was prepared by a complex formation of ligand (*R,R,R*)-**L1** (14.2 mg, 0.022 mol) with CuCl (2.0 mg, 0.02 mmol) and pyridine (2 μL, 0.022mmol) in anhydrous dichloromethane (1.0 mL) under Ar. After being stirred for 15 min at room temperature, the solvent was removed under reduced pressure. To the residue were added nitroethane (144 μL, 2 mmol), EtOH (0.4 mL), pyridine (43 μL, 0.53 mmol), and (*S*)-2-phenylpropanal (27 μL, 0.2 mmol) under Ar. The diastereoselective Henry reaction was performed for 19 h at room temperature. Then, the reaction was quenched by the addition of 1N HCl, and the aqueous layer was extracted with dichloromethane. The organic phase was washed with brine, and then dried over sodium sulfate. After removal of the solvent under reduced pressure, the residue was purified by column chromatography (using spherical silica gel, *n*-hexane/ethyl acetate =6:1) to afford the adduct (40.4 mg, 97% yield). Diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy and the enantiomeric excess was determined by HPLC analysis.



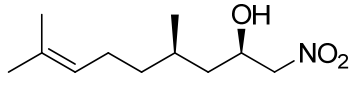
(2*S*,3*R*)-1-nitro-3-phenylbutan-2-ol. IR (ATR) 3420, 1553cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.37-7.18 (m, 5H), 4.43-4.37 (m, 1H), 4.30-4.20 (m, 2H), 2.83 (quintet, 1H, *J*=7.3 Hz), 2.61-2.58 (m, 1H), 1.42 (d, 3H, *J*= 7.3 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 141.94, 129.02, 127.38, 79.40, 73.22, 43.66, 17.37. HRMS (ES-): Exact mass calcd for $C_{10}H_{12}NO_3$ [M – H]-, 194.0823. Found 194.0821. $[\alpha]_D^{26}$ -12.78 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



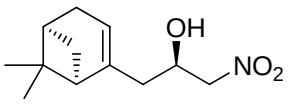
(2*R*,3*S*)-3-(6-methoxynaphthalen-2-yl)-1-nitrobutan-2-ol. IR (ATR) 3566, 2968, 2935, 1606, 1554cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.72 (d, 1H, *J*=8.6 Hz), 7.69 (d, 1H, *J*=9.1 Hz), 7.55 (s, 1H), 7.29-7.10 (m, 3H), 4.46 (dt, 1H, *J*=2.7, 8.2 Hz), 4.32-4.20 (m, 2H), 3.91 (s, 3H), 2.94 (quintet, 1H, *J*=7.3 Hz), 2.77 (br, 1H), 1.47 (d, 3H, *J*=6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.69, 136.95, 133.73, 129.10, 128.92, 127.66, 126.01, 125.74, 119.29, 105.53, 79.48, 73.24, 55.29, 43.59, 17.44. HRMS (ES-): Exact mass calcd for $C_{15}H_{16}NO_4$ [M – H]-, 274.1085. Found 274.1096. $[\alpha]_D^{22}$ +11.45 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



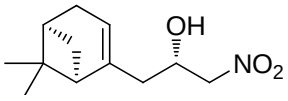
***tert*-butyl ((2*S*,3*S*)-3-hydroxy-4-nitro-1-phenylbutan-2-yl) carbamate**. IR (ATR) 3396, 2979, 2931, 1685, 1556cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.34-7.22 (m, 5H), 4.88 (br, 1H), 4.51-4.40 (m, 2H), 4.32-4.27 (m, 1H), 3.81 (q, 1H, *J*=8.2 Hz), 3.36 (br, 1H), 3.01-2.90 (m, 2H), 1.42 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 155.93, 137.16, 129.20, 128.68, 126.79, 80.27, 79.21, 68.42, 53.86, 38.13, 28.22. HRMS (ES+): Exact mass calcd for $C_{15}H_{22}N_2O_5Na$ [M + H]+, 333.1421. Found 333.1413. $[\alpha]_D^{25}$ -34.80 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



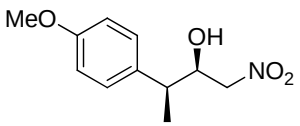
(2*R*,4*R*)-4,8-dimethyl-1-nitronon-7-en-2-ol. IR (ATR) 3734, 2918, 1555cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.12-5.05 (m, 1H), 4.46-4.31 (m, 3H), 2.49 (d, 1H, *J*=4.5 Hz), 2.08-1.90 (m, 2H), 1.69 (s, 3H), 1.66-1.57 (m, 1H), 1.61 (s, 3H), 1.50-1.12 (m, 4H), 0.97 (d, 3H, *J*=6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 131.67, 124.20, 80.76, 66.96, 40.88, 36.27, 28.89, 25.68, 25.17, 19.96, 17.65. HRMS (ES-): Exact mass calcd for $C_{11}H_{20}NO_3$ [M - H]-, 214.1449. Found 214.1452. $[\alpha]_D^{26}$ -0.24 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.



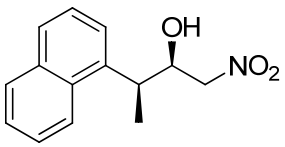
(*R*)-1-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-yl)-3-nitro propan-2-ol. IR (ATR) 3734, 2917, 1556cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.41 (br, 1H), 4.48-4.31 (m, 3H), 2.46-2.04 (m, 8H), 1.29 (s, 3H), 1.13 (d, 1H, *J*=8.6 Hz), 0.85 (s, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 143.03, 121.74, 80.23, 66.47, 45.64, 41.69, 40.45, 37.96, 31.88, 31.36, 26.11, 21.19. HRMS (ES-): Exact mass calcd for $C_{12}H_{18}NO_3$ [M - H]-, 224.1292. Found 224.1296. $[\alpha]_D^{25}$ -19.11 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.



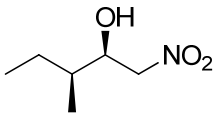
(*S*)-1-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-yl)-3-nitrop ropan-2-ol. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.40 (br, 1H), 4.47-4.32 (m, 3H), 2.46-2.05 (m, 8H), 1.30 (s, 3H), 1.13 (d, 1H, *J*=8.6 Hz), 0.85 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.94, 121.65, 80.38, 66.62, 45.85, 41.85, 40.54, 38.01, 31.81, 31.49, 26.20, 21.25. $[\alpha]_D^{26}$ -21.85 (c 1.00, $CHCl_3$). diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.



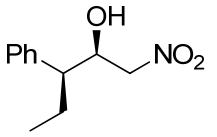
(2*R*,3*S*)-3-(4-methoxyphenyl)-1-nitrobutan-2-ol. IR (ATR) 3456, 2966, 2933, 1553, 1513cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.13-7.10 (m, 2H), 6.90-6.86 (m, 2H), 4.48-4.23 (m, 3H), 3.80 (s, 3H), 2.80 (quintet, 1H, *J*=7.5 Hz), 2.56 (d, 1H, *J*=5.2 Hz), 1.39 (d, 3H, *J*=7.5 Hz). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 158.71, 133.89, 128.34, 114.36, 79.45, 73.43, 55.24, 42.83, 17.49. HRMS (ES-): Exact mass calcd for $C_{11}H_{14}NO_4$ [M – H]-, 224.0928. Found 224.0931. $[\alpha]_D^{23}$ +7.54 (c 1.00, $CHCl_3$). The diastereo ratio was determined by ^{1}H NMR spectroscopy.



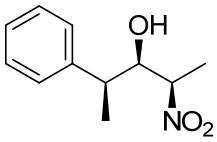
(2*R*,3*S*)-3-(naphthalen-1-yl)-1-nitrobutan-2-ol. IR (ATR) 3539, 3049, 2932, 1553cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.05 (d, 1H, *J*=8.6 Hz), 7.89 (d, 1H, *J*=8.0 Hz), 7.79 (d, 1H, *J*=7.5 Hz), 7.59-7.42 (m, 4H), 4.64 (br, 1H), 4.42-4.34 (m, 1H), 4.25-4.22 (m, 1H), 3.77 (quintet, 1H, *J*=6.9 Hz), 2.57 (br, 1H), 1.55 (d, 3H, *J*=6.9 Hz). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 138.18, 134.08, 131.17, 129.26, 127.76, 126.60, 125.87, 125.57, 124.03, 122.33, 79.30, 73.02, 17.18. HRMS (ES-): Exact mass calcd for $C_{14}H_{14}NO_3$ [M – H]-, 244.0979. Found 244.0984. $[\alpha]_D^{23}$ +67.58 (c 1.00, $CHCl_3$). The diastereo ratio was determined by ^{1}H NMR spectroscopy.



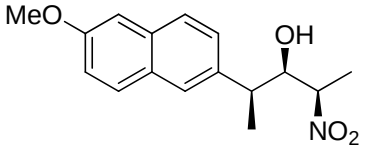
(2*R*,3*S*)-3-methyl-1-nitropentan-2-ol. IR (ATR) 3455, 2964, 2929, 1554cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 4.49-4.39 (m, 2H), 4.30-4.26 (m, 1H), 2.37 (d, 1H, *J*=4.6 Hz), 1.66-1.50 (m, 2H), 1.29-1.18 (m, 1H), 0.96-0.94 (m, 6H). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 79.52, 71.53, 38.20, 25.51, 13.68, 11.54. HRMS (ES-): Exact mass calcd for $C_6H_{12}NO_3$ [M – H]-, 146.0823. Found 146.0817. $[\alpha]_D^{23}$ -3.08 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



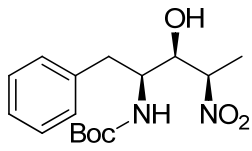
(2*R*,3*S*)-1-nitro-3-phenylpentan-2-ol. IR (ATR) 3555, 2965, 2931, 1553cm^{-1}. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.37-7.13 (m, 5H), 4.58-4.14 (m, 3H), 2.67 (d, 1H, *J*=5.7 Hz), 2.62-2.52 (m, 1H), 2.19-1.60 (m, 2H), 0.77 (t, 3H, *J*=7.5 Hz). ^{13}C-NMR (125 MHz, $CDCl_3$) δ 139.80, 129.04, 128.78, 128.04, 127.43, 79.65, 72.54, 51.61, 24.68, 11.69. HRMS (ES-): Exact mass calcd for $C_{11}H_{14}NO_3$ [M – H]-, 208.0979. Found 208.0980. $[\alpha]_D^{23}$ +2.82 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



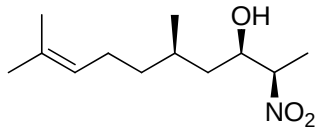
(2*R*,3*R*,4*S*)-2-nitro-4-phenylpentan-3-ol. IR (ATR) 3566, 1549cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.37-7.17 (m, 5H), 4.54-4.47 (m, 1H), 3.90-3.85 (m, 1H), 2.90 (quintet, 1H, *J*= 6.8 Hz), 2.30-2.29 (m, 1H), 1.59 (d, 3H, *J*= 6.8 Hz)), 1.37 (d, 3H, *J*= 6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.62, 128.86, 127.63, 127.17, 84.91, 77.25, 42.19, 16.82, 15.27. HRMS (ES-): Exact mass calcd for $C_{11}H_{14}NO_3$ [M – H]-, 208.0979. Found 208.0978. $[\alpha]_D^{22}$ +41.26 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



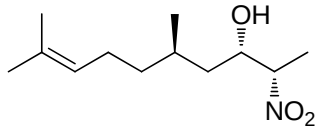
(2*S*,3*R*,4*R*)-2-(6-methoxynaphthalen-2-yl)-4-nitropentan-3-ol IR (ATR) 3734, 1558cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.74-7.69 (m, 2H), 7.58 (s, 1H), 7.32-7.11 (m, 3H), 4.54 (quintet, 1H, *J*= 6.8 Hz), 3.95 (q, 1H, *J*= 6.8 Hz), 3.92 (s, 3H), 3.04 (quintet, 1H, *J*= 6.8 Hz), 2.33 (d, 1H, *J*= 7.3 Hz), 1.59 (d, 3H, *J*= 6.8 Hz), 1.44 (d, 3H, *J*= 6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.69, 137.60, 133.68, 129.18, 128.94, 127.48, 126.19, 119.21, 105.53, 84.92, 55.32, 42.18, 16.87, 15.41. HRMS (ES+): Exact mass calcd for $C_{16}H_{19}NO_4Na$ [M + H]+, 312.1206. Found 312.1205. $[\alpha]_D^{22}$ +35.30 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



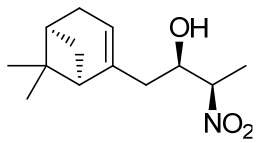
***tert*-butyl ((2*S*,3*R*,4*R*)-3-hydroxy-4-nitro-1-phenylpentan-2-yl) carbamate**. IR (ATR) 3749, 3394, 2979, 2929, 1685, 1556cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.34-7.21 (m, 5H), 4.87 (d, 1H, *J*=9.5 Hz), 4.62-4.55 (m, 1H), 3.96-3.89 (m, 2H), 3.02-2.87 (m, 3H), 1.49 (d, 3H, J=6.8 Hz), 1.40 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 155.77, 137.24, 129.14, 128.76, 126.83, 86.78, 80.19, 72.85, 52.18, 38.68, 28.23, 16.04. HRMS (ES+): Exact mass calcd for $C_{16}H_{24}N_2O_5Na$ [M + H]+, 347.1577. Found 347.1565. $[\alpha]_D^{25}$ -30.77 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR spectroscopy.



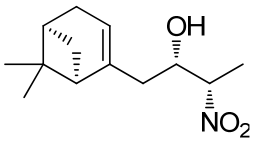
(2*R*,3*R*,5*R*)-5,9-dimethyl-2-nitrodec-8-en-3-ol. IR (ATR) 3566, 2968, 2935, 1606, 1554cm^{-1}. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.12-5.05 (m, 1H), 4.55-4.45 (m, 1H), 4.33-3.94 (m, 1H), 2.18 (d, 1H, *J*=7.3 Hz), 2.09-1.89 (m, 2H), 1.78-1.70 (m, 1H), 1.69 (s, 3H), 1.61 (s, 3H), 1.56 (d, 3H, J=6.8 Hz), 1.51-1.07 (m, 4H), 0.96 (d, 3H, *J*=6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 131.61, 124.31, 87.92, 71.13, 40.49, 35.73, 28.85, 25.67, 25.13, 20.34, 17.63, 16.22. HRMS (ES-): Exact mass calcd for $C_{12}H_{22}NO_3$ [M - H]-, 228.1605. Found 228.1609. $[\alpha]_D^{26}$ +22.30 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.



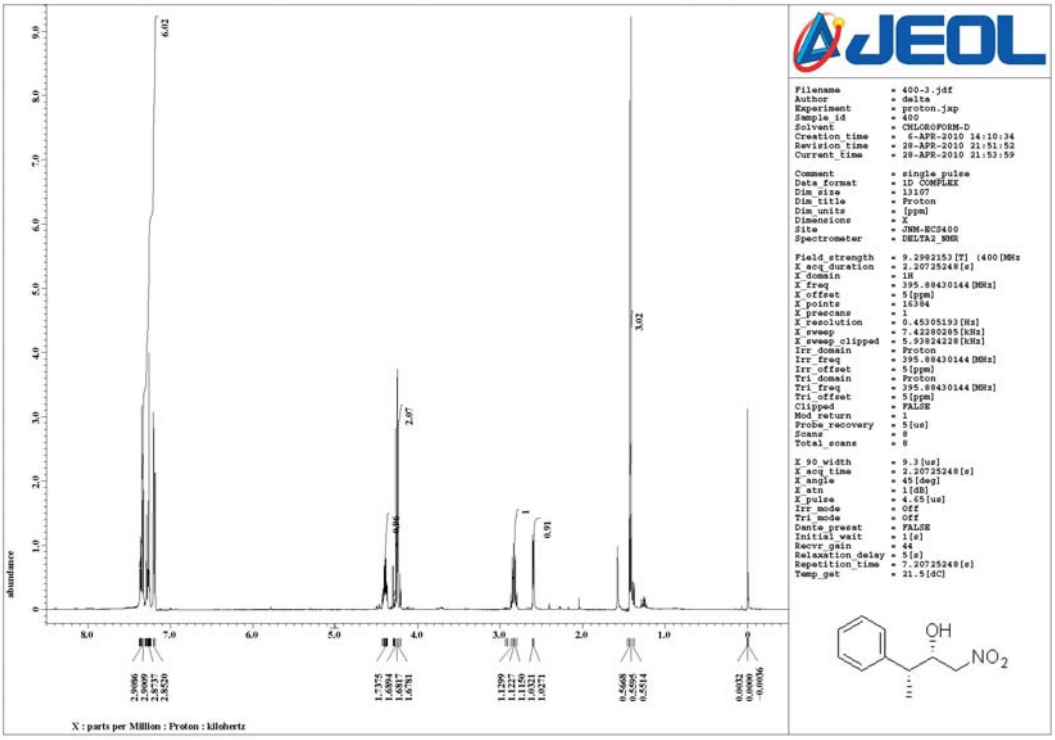
(2*S*,3*S*,5*R*)-5,9-dimethyl-2-nitrodec-8-en-3-ol. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.11-5.05 (m, 1H), 4.55-4.45 (m, 1H), 4.33-3.94 (m, 1H), 2.15 (d, 1H, *J*=6.8 Hz), 2.07-1.92 (m, 2H), 1.80-1.69 (m, 1H), 1.68 (s, 3H), 1.60 (s, 3H), 1.56 (d, 3H, *J*=6.8 Hz), 1.52-1.07 (m, 4H), 0.93 (d, 3H, *J*=6.8 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 131.49, 124.29, 88.33, 70.86, 40.01, 37.78, 28.42, 25.66, 25.34, 18.68, 17.61, 16.18. $[\alpha]_D^{26}$ -13.30 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.

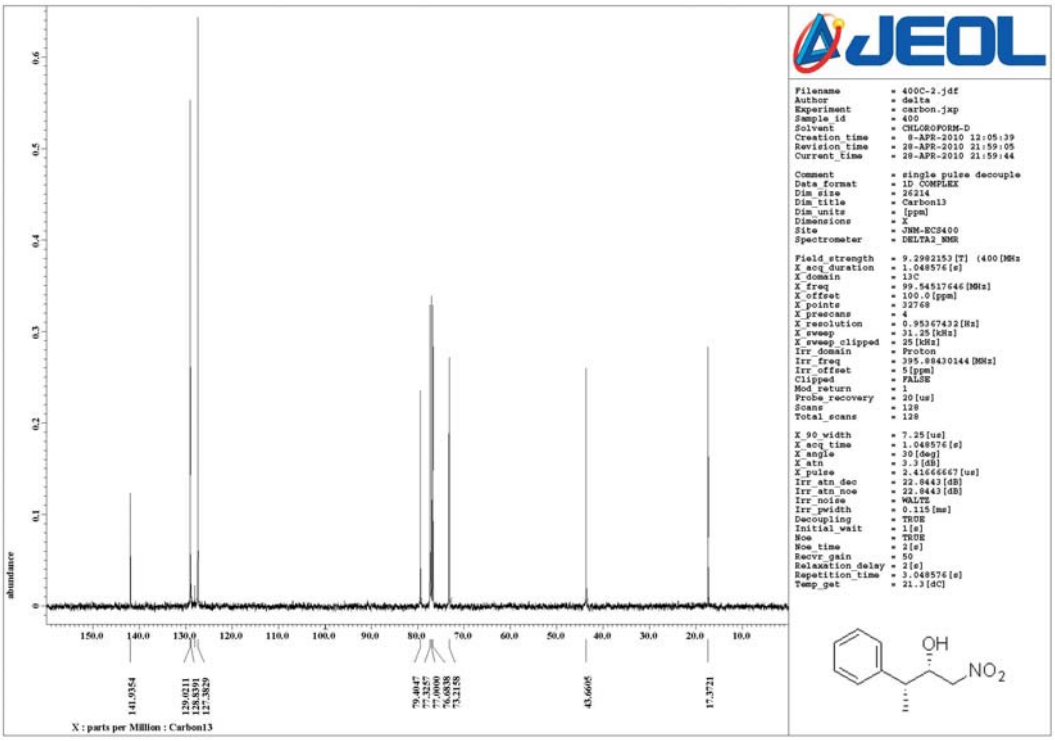


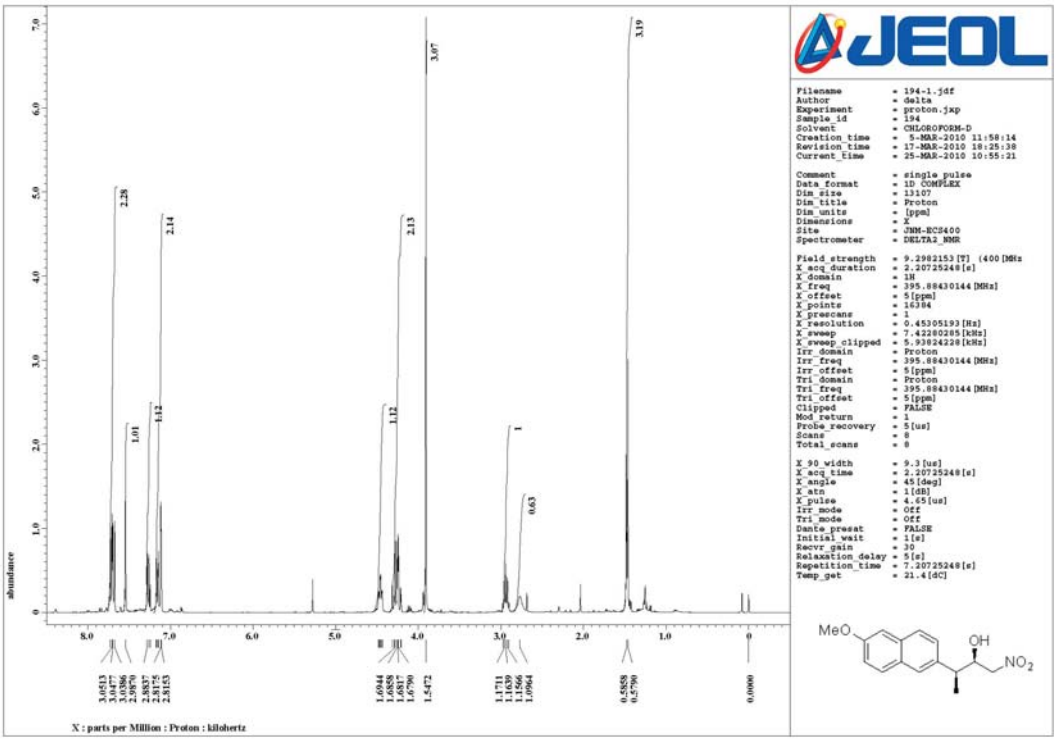
(2*R*,3*R*)-1-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)-3-nitrobutan-2-ol. IR (ATR) 3525, 2985, 2916, 1550cm^{-1} ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.44-5.35 (m, 1H), 4.59-4.48 (m, 1H), 4.22-3.87 (m, 1H), 2.46-2.03 (m, 8H), 1.59-1.54 (m, 3H), 1.30 (s, 3H), 1.11 (d, 1H, J=8.6 Hz), 0.86 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 143.22, 122.20, 87.13, 70.00, 45.38, 40.87, 40.50, 38.08, 31.40, 26.15, 21.14, 21.09, 15.81. HRMS (ES-): Exact mass calcd for $C_{13}H_{20}NO_3$ [M - H]-, 238.1449. Found 238.1454. $[\alpha]_D^{25}$ -9.63 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.

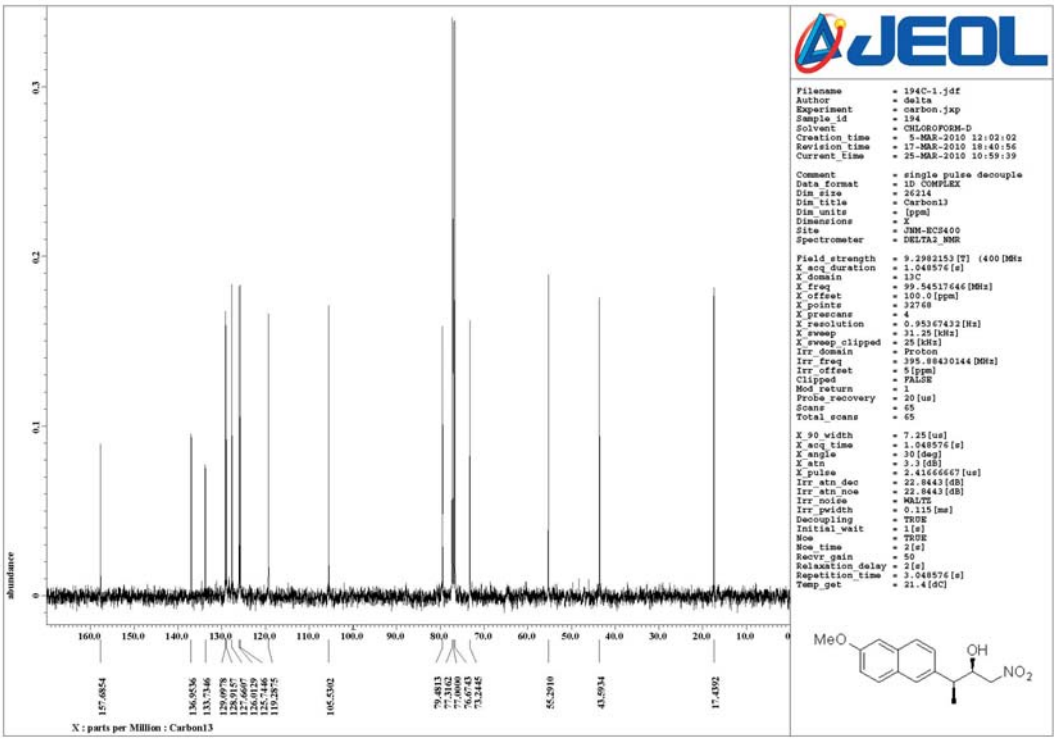


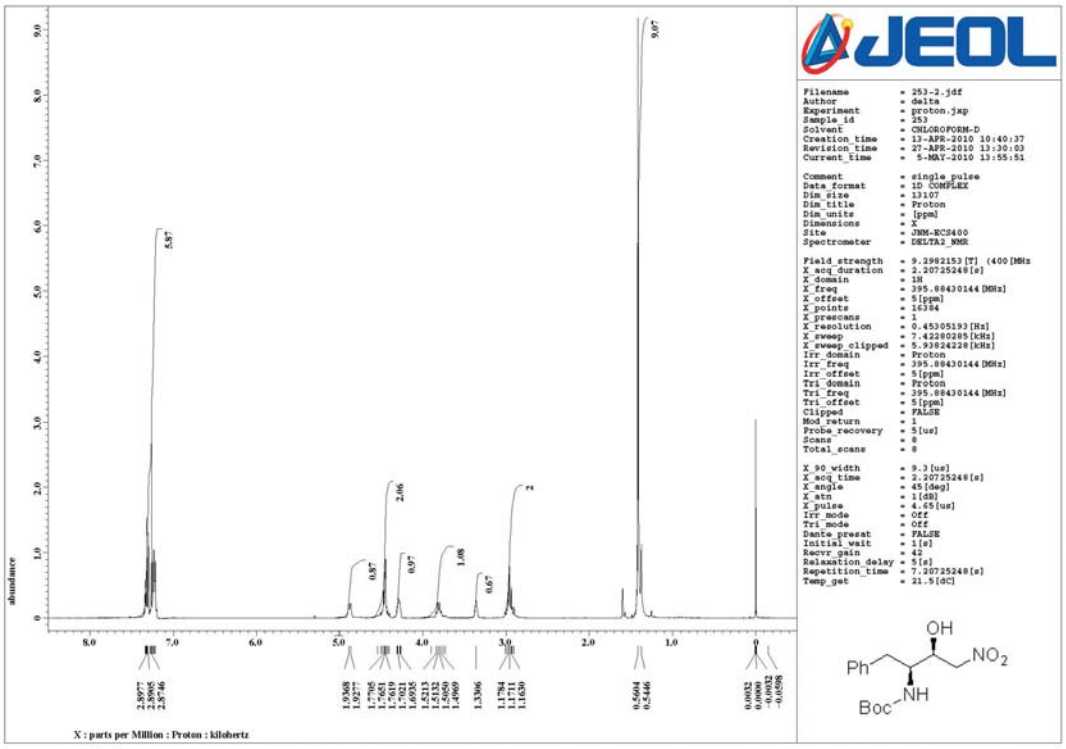
(2*S*,3*S*)-1-((1*R*,5*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)-3-nitrobutan-2-ol. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.44-5.39 (m, 1H), 4.59-4.48 (m, 1H), 4.22-3.87 (m, 1H), 2.46-2.02 (m, 8H), 1.59-1.54 (m, 3H), 1.30 (s, 3H), 1.17 (d, 1H, *J*=8.6 Hz), 0.85 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$) δ 142.84, 121.84, 86.99, 70.27, 45.85, 40.68, 37.74, 31.68, 31.41, 26.08, 21.25, 21.16, 15.96. $[\alpha]_D^{25}$ -29.65 (c 1.00, $CHCl_3$). The diastereoselectivity was determined by ^{1}H NMR and ^{13}C NMR spectroscopy.

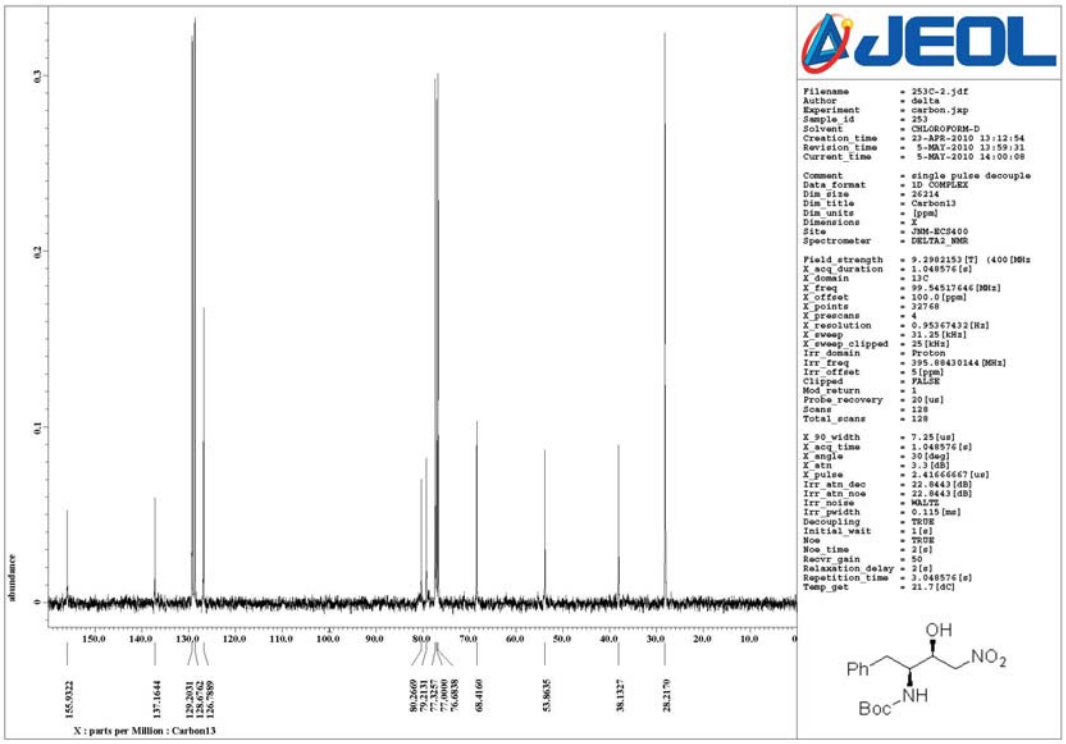

6.02
2.07
0.91
3.02
abundance
X : parts per Million : Proton : kilohertz
Filename = 400-2.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 400
Solvent = CHLOROFORM-D
Creation_time = 6-APR-2010 14:10:34
Revision_time = 28-APR-2010 21:51:52
Current_time = 28-APR-2010 21:53:59
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.5[dC]
OH
NO2

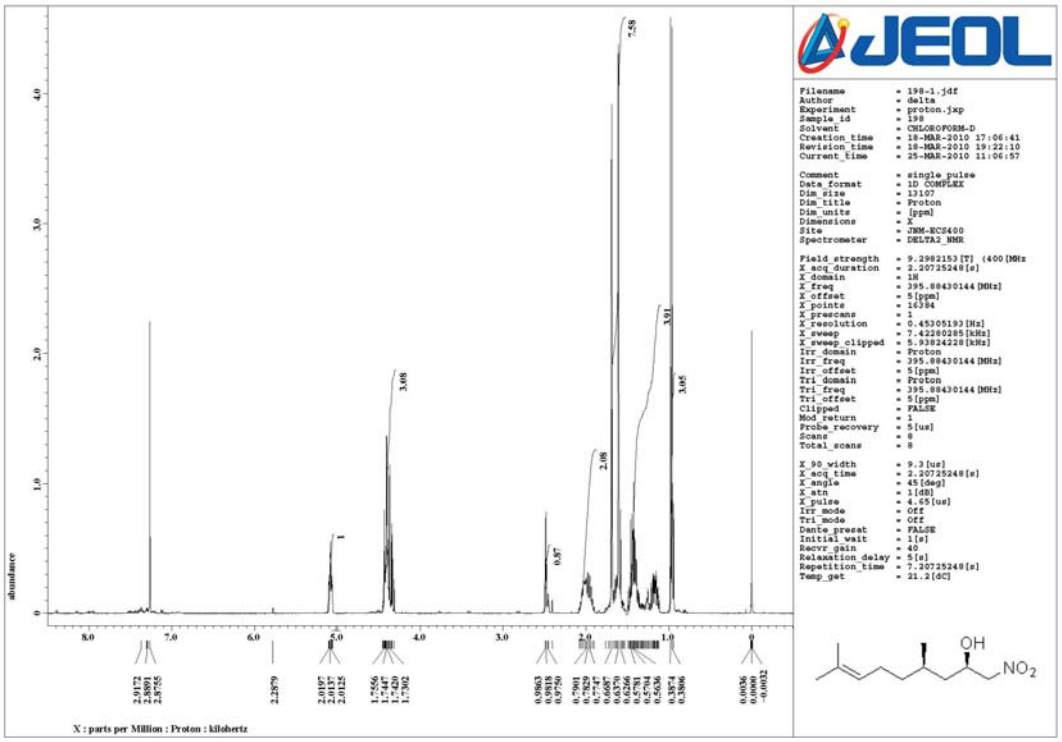

141.9354
129.0211
128.8391
127.3829
79.4047
77.3157
77.0000
76.6838
73.2158
43.6605
17.3721
abundance
X : parts per Million : Carbon13
Filename = 400C-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 400
Solvent = CHLOROFORM-D
Creation_time = 6-APR-2010 12:05:39
Revision_time = 28-APR-2010 21:59:05
Current_time = 28-APR-2010 21:59:44
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.3[dC]
OH
NO2

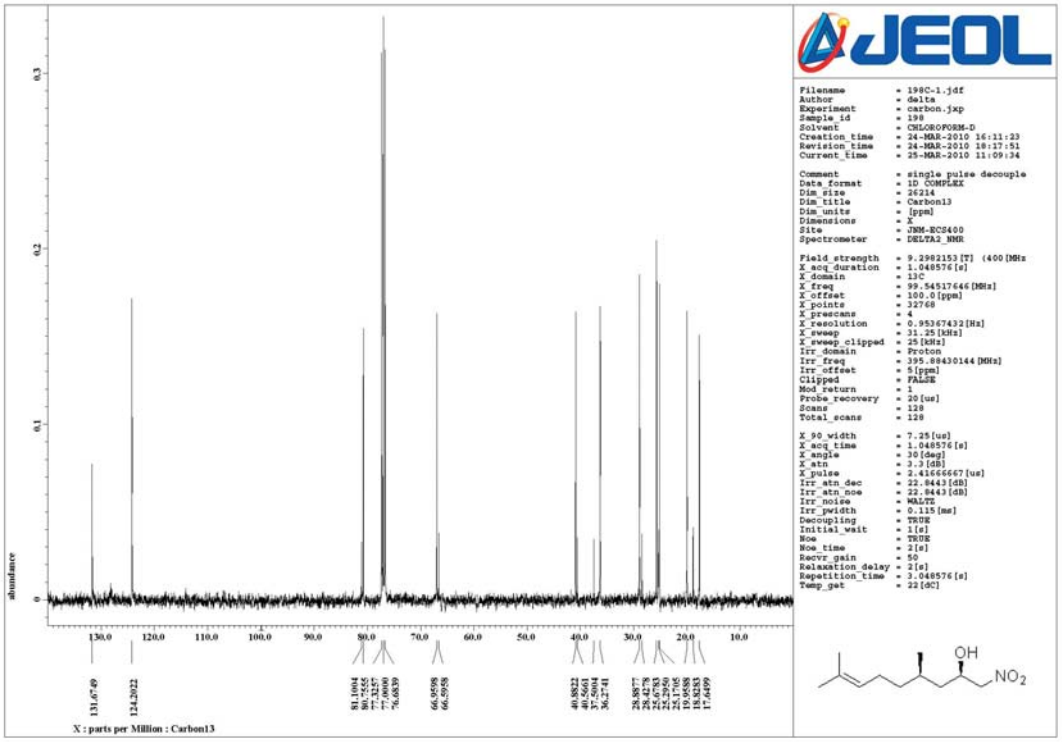

JEOL
Filename = 194-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 194
Solvent = CHLOROFORM-D
Creation_time = 5-MAR-2010 11:58:14
Revision_time = 17-MAR-2010 18:25:38
Current_time = 25-MAR-2010 10:55:21
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153 [T] (400 [MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193 [Hz]
X_sweep = 7.42280265 [kHz]
X_sweep_clipped = 5.93824228 [kHz]
Irr_domain = Proton
Irr_freq = 395.88430144 [MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144 [MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 30
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.4[dC]
MeO
OH
NO2
abundance
X : parts per Million : Proton : kilohertz

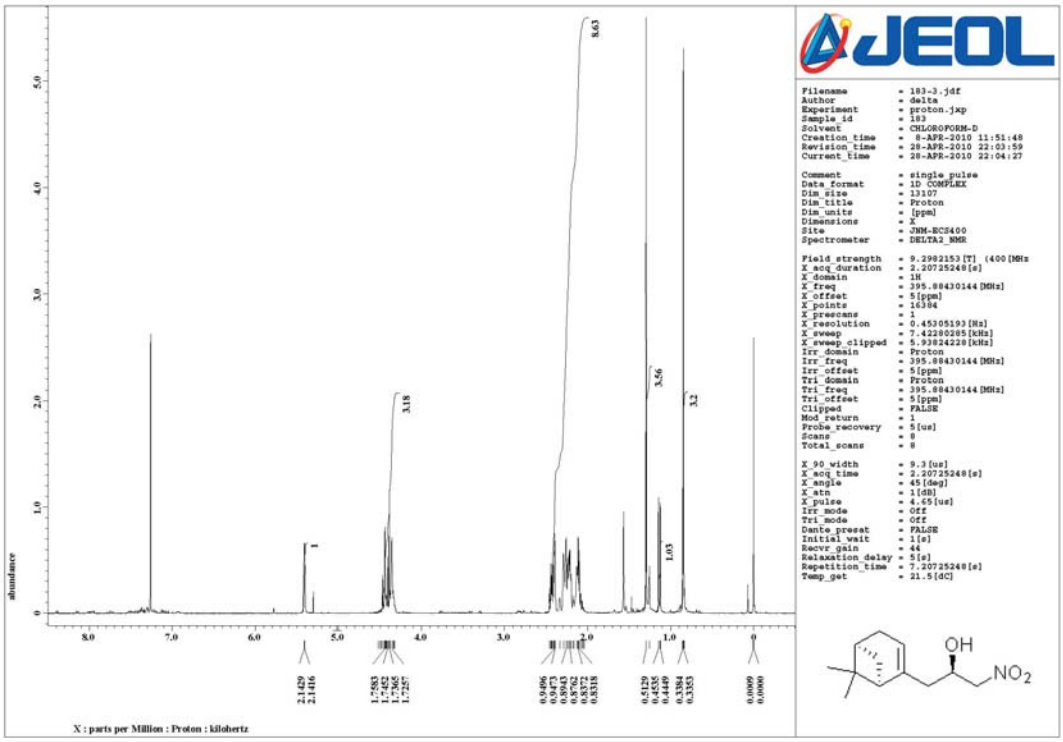

JEOL
Filename = 194C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 194
Solvent = CHLOROFORM-D
Creation_time = 5-MAR-2010 12:02:02
Revision_time = 17-MAR-2010 18:40:56
Current_time = 25-MAR-2010 10:59:39
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153 [T] (400 [MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646 [MHz]
X_offset = 100.0 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432 [Hz]
X_sweep = 31.25 [kHz]
X_sweep_clipped = 25 [kHz]
Irr_domain = Proton
Irr_freq = 395.88430144 [MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 65
Total_scans = 65
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.4[dC]
MeO
OH
NO2
abundance
X : parts per Million : Carbon13

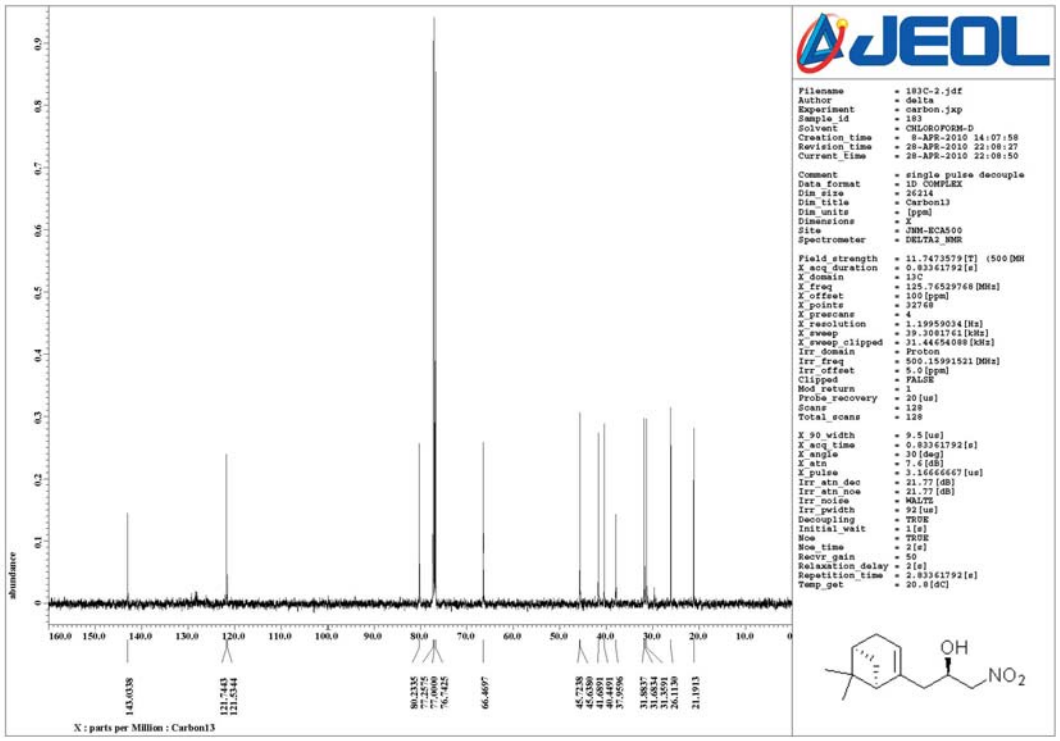

JEOL
Filename = 253-2.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 253
Solvent = CHLOROFORM-D
Creation_time = 13-APR-2010 10:40:37
Revision_time = 27-APR-2010 13:30:03
Current_time = 5-MAY-2010 13:55:51
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.5[dC]
abundance
X : parts per Million : Proton : kilohertz
OH
NO2
Ph
NH
Boc

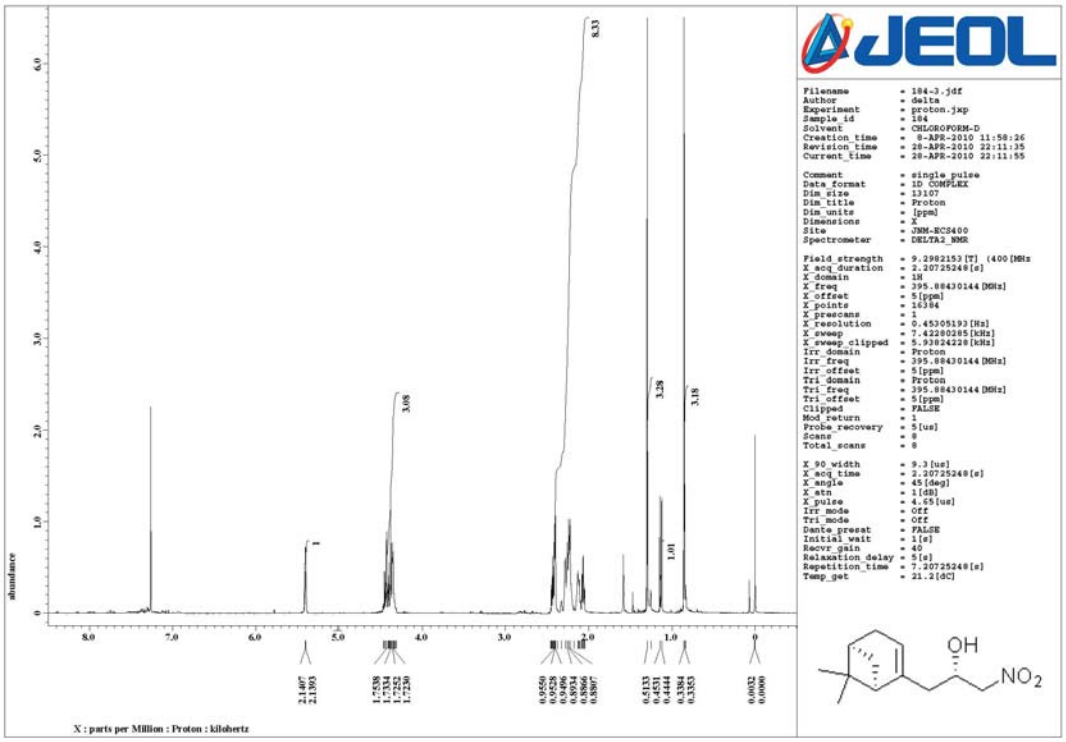

JEOL
Filename = 253C-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 253
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 13:12:54
Revision_time = 5-MAY-2010 13:59:31
Current_time = 5-MAY-2010 14:00:08
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.7[dC]
abundance
X : parts per Million : Carbon13
OH
NO2
Ph
NH
Boc

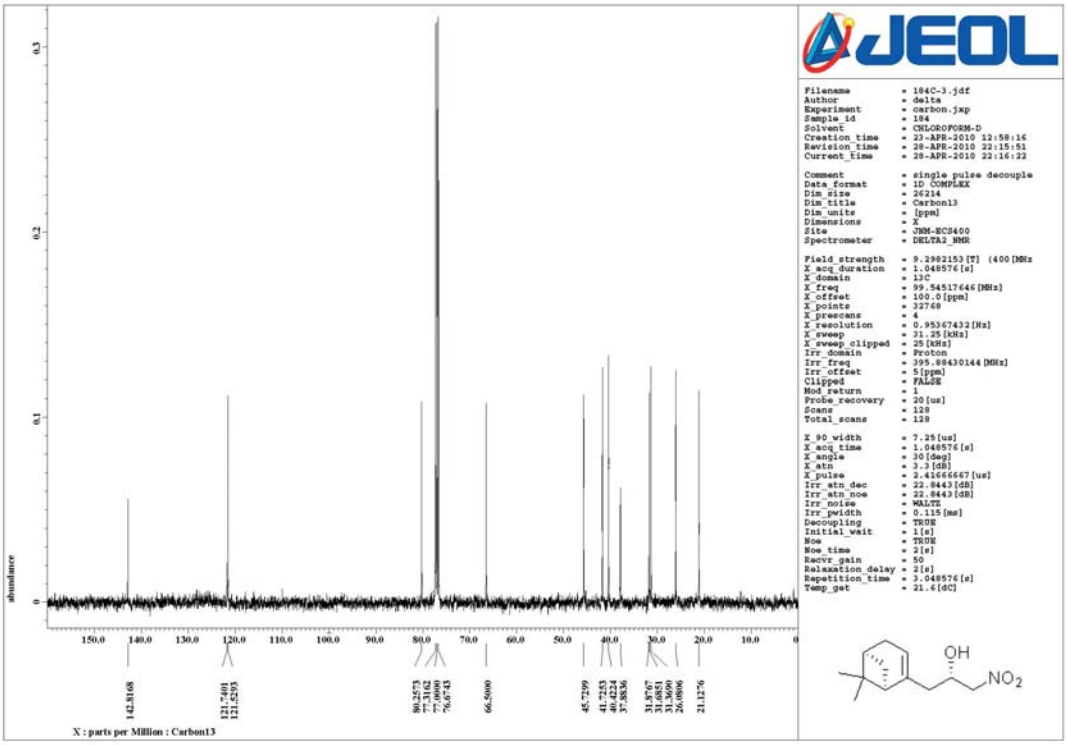

JEOL
Filename = 198-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 198
Solvent = CHLOROFORM-D
Creation_time = 18-MAR-2010 17:06:41
Revision_time = 18-MAR-2010 19:22:10
Current_time = 25-MAR-2010 11:06:57
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.2[dC]
OH
NO2
X : parts per Million : Proton : kilohertz

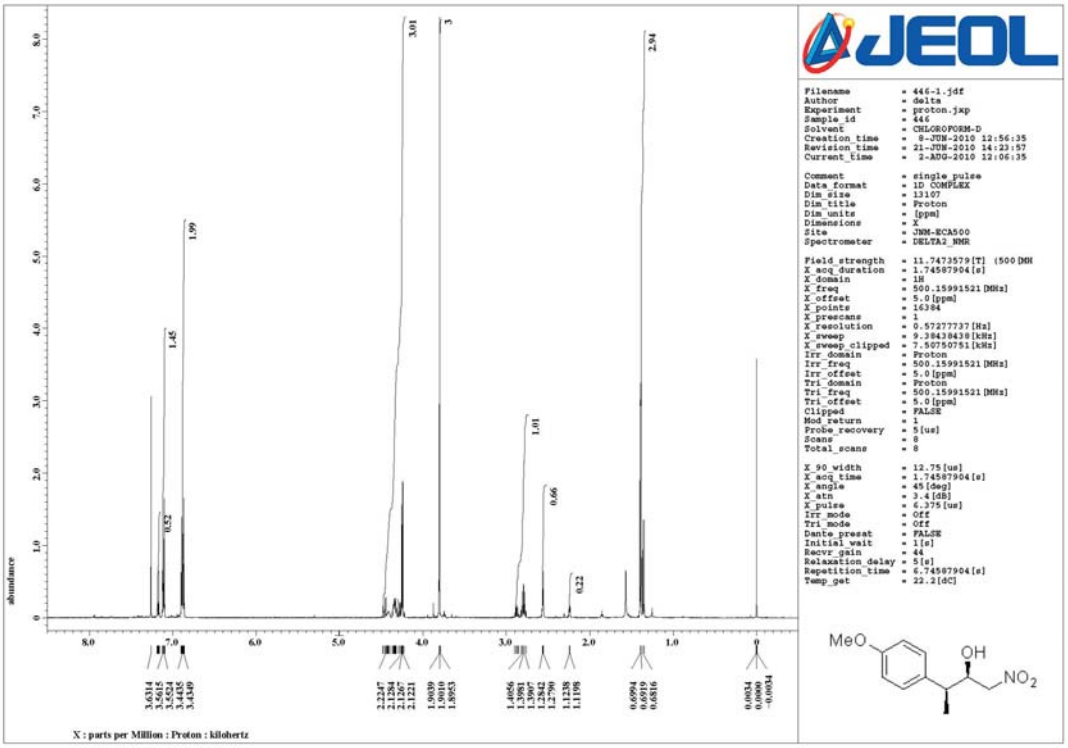

JEOL
Filename = 198C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 198
Solvent = CHLOROFORM-D
Creation_time = 24-MAR-2010 16:11:23
Revision_time = 24-MAR-2010 18:17:51
Current_time = 25-MAR-2010 11:09:34
Comment = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 22[dC]
OH
NO2
X : parts per Million : Carbon13

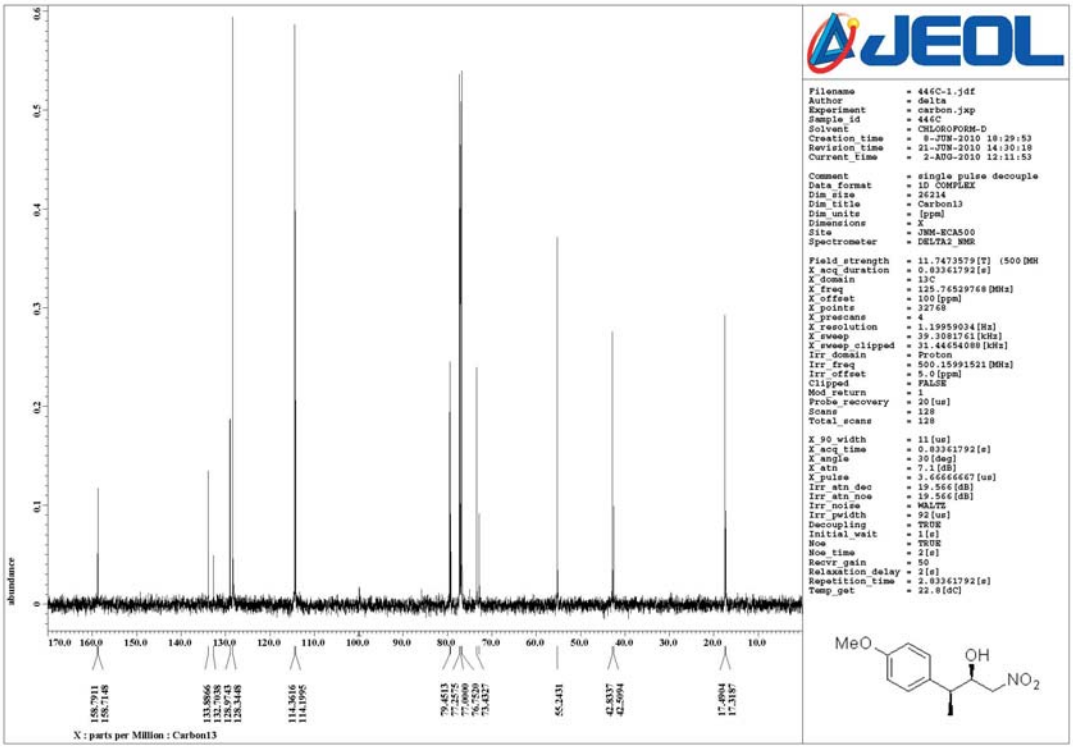

JEOL
Filename = 183-3.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 183
Solvent = CHLOROFORM-D
Creation_time = 8-APR-2010 11:51:48
Revision_time = 28-APR-2010 22:03:59
Current_time = 28-APR-2010 22:04:27
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.5[dC]
OH
NO2
X : parts per Million : Proton : kilohertz

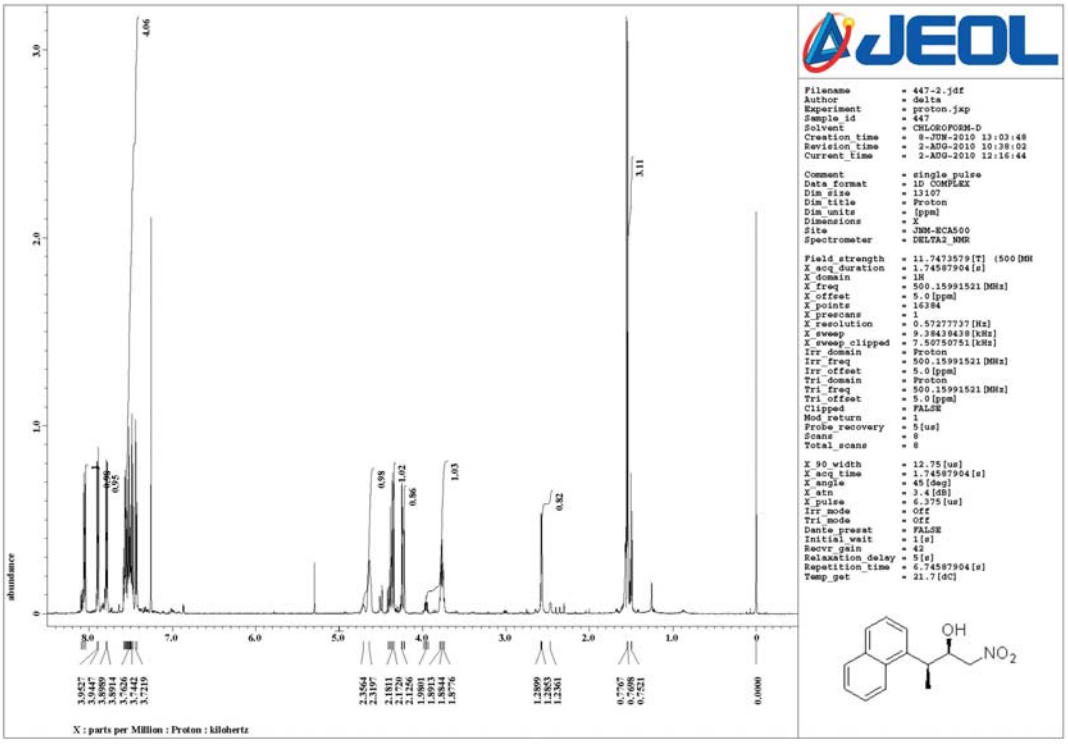

JEOL
Filename = 183C-2.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 183
Solvent = CHLOROFORM-D
Creation_time = 8-APR-2010 14:07:58
Revision_time = 28-APR-2010 22:08:27
Current_time = 28-APR-2010 22:08:50
Comment = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 9.5[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 7.6[dB]
X_pulse = 3.16666667[us]
Irr_atn_dec = 21.77[dB]
Irr_atn_noe = 21.77[dB]
Irr_noise = WALTZ
Irr_pwidth = 92[us]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 20.8[dC]
OH
NO2
X : parts per Million : Carbon13

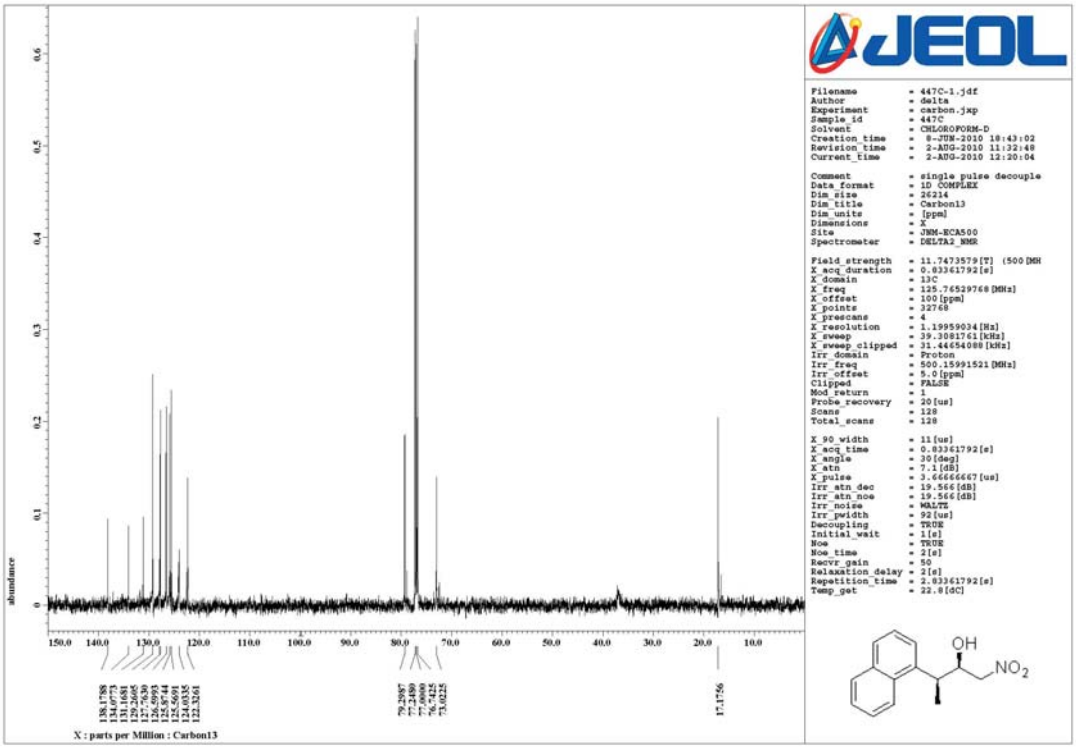

JEOL
Filename = 184-3.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 184
Solvent = CHLOROFORM-D
Creation_time = 8-APR-2010 11:58:26
Revision_time = 28-APR-2010 22:11:35
Current_time = 28-APR-2010 22:11:55
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280265[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.2[dC]
OH
NO2
X : parts per Million : Proton : kilohertz

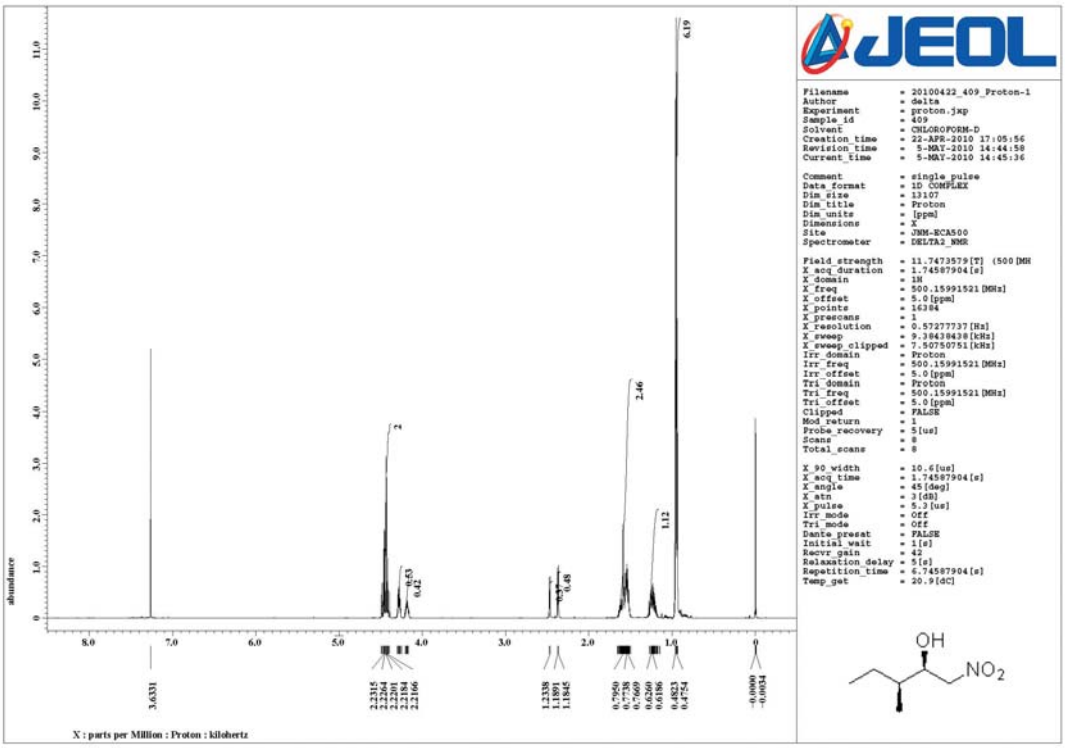

JEOL
Filename = 184C-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 184
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 12:58:16
Revision_time = 28-APR-2010 22:15:51
Current_time = 28-APR-2010 22:16:22
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.6[dC]
OH
NO2
X : parts per Million : Carbon13

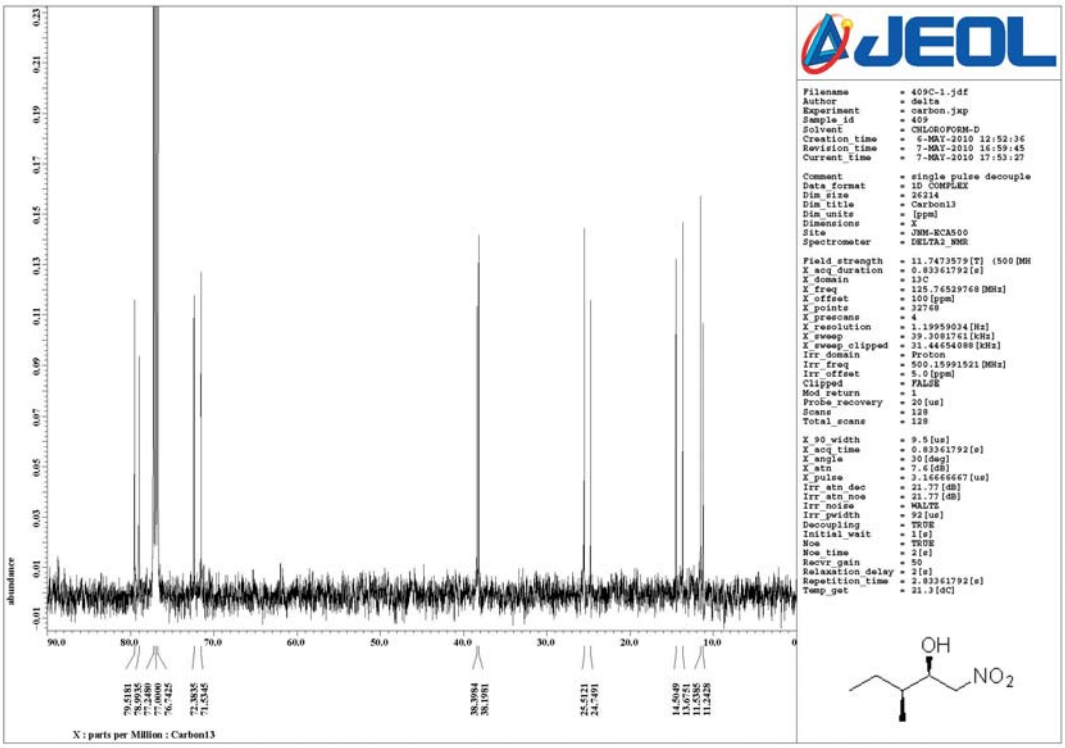

JEOL
Filename = 446-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 446
Solvent = CHLOROFORM-D
Creation_time = 8-JUN-2010 12:56:35
Revision_time = 21-JUN-2010 14:23:57
Current_time = 2-AUG-2010 12:06:35
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 12.75[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_atn = 3.4[dB]
X_pulse = 6.375[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get = 22.2[dC]
MeO
OH
NO2
abundance
X : parts per Million : Proton : kilohertz

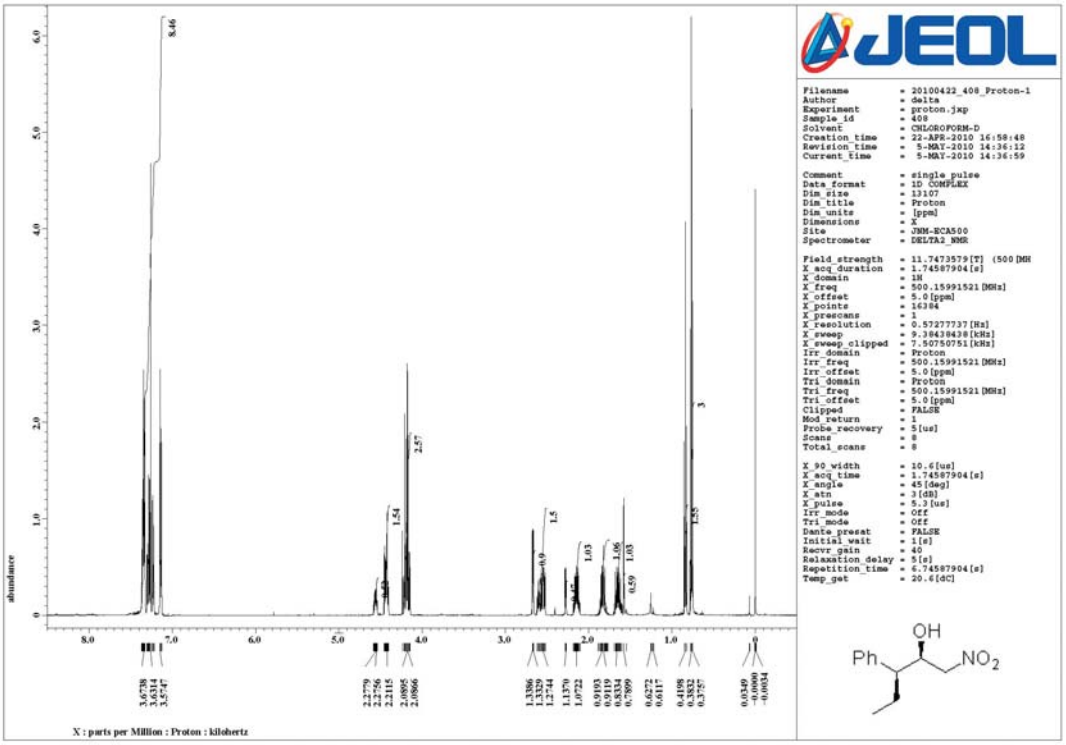

JEOL
Filename = 446C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 446C
Solvent = CHLOROFORM-D
Creation_time = 8-JUN-2010 18:29:53
Revision_time = 21-JUN-2010 14:30:10
Current_time = 2-AUG-2010 12:11:53
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 11[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 7.1[dB]
X_pulse = 3.66666667[us]
Irr_atn_dec = 19.566[dB]
Irr_atn_noe = 19.566[dB]
Irr_noise = WALTZ
Irr_pwidth = 92[us]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 22.8[dC]
MeO
OH
NO2
abundance
X : parts per Million : Carbon13

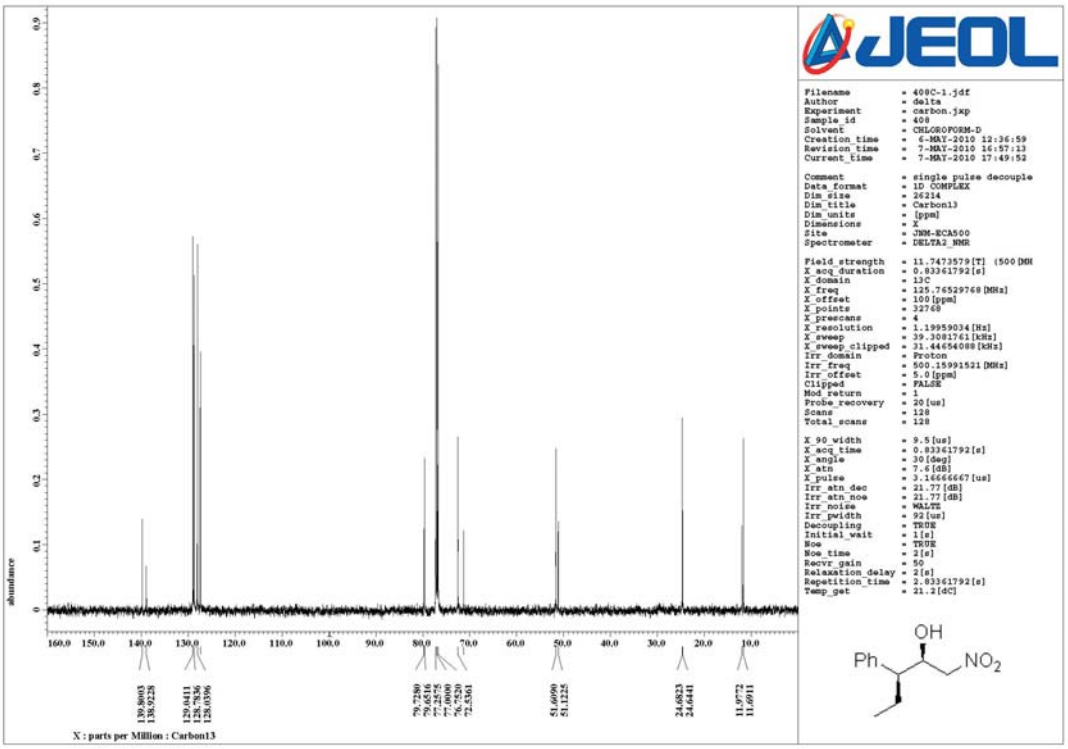

JEOL
Filename = 447-2.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 447
Solvent = CHLOROFORM-D
Creation_time = 8-JUN-2010 13:03:48
Revision_time = 2-AUG-2010 10:38:02
Current_time = 2-AUG-2010 12:16:44
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 12.75[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_atn = 3.4[dB]
X_pulse = 6.375[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get = 21.7[dC]
OH
NO2
abundance
X : parts per Million : Proton : kilohertz

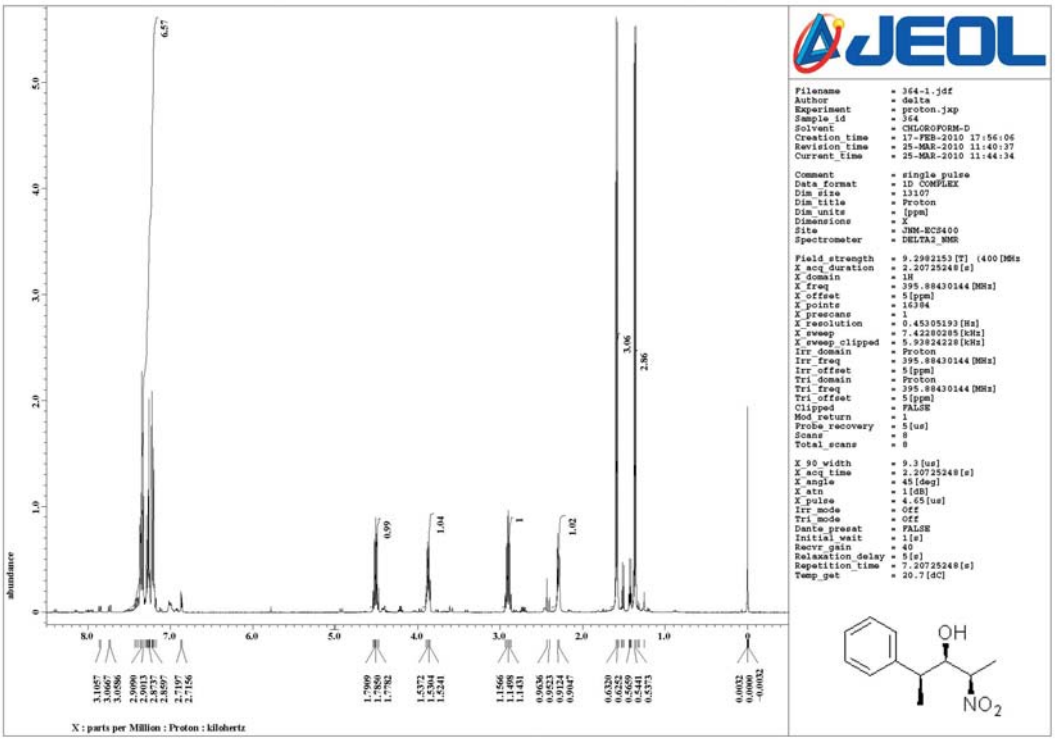

JEOL
Filename = 447C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 447C
Solvent = CHLOROFORM-D
Creation_time = 8-JUN-2010 18:43:02
Revision_time = 2-AUG-2010 11:32:48
Current_time = 2-AUG-2010 12:20:04
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 11[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 7.1[dB]
X_pulse = 3.66666667[us]
Irr_atn_dec = 19.566[dB]
Irr_atn_noe = 19.566[dB]
Irr_noise = WALTZ
Irr_pwidth = 92[us]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 22.8[dC]
OH
NO2
abundance
X : parts per Million : Carbon13

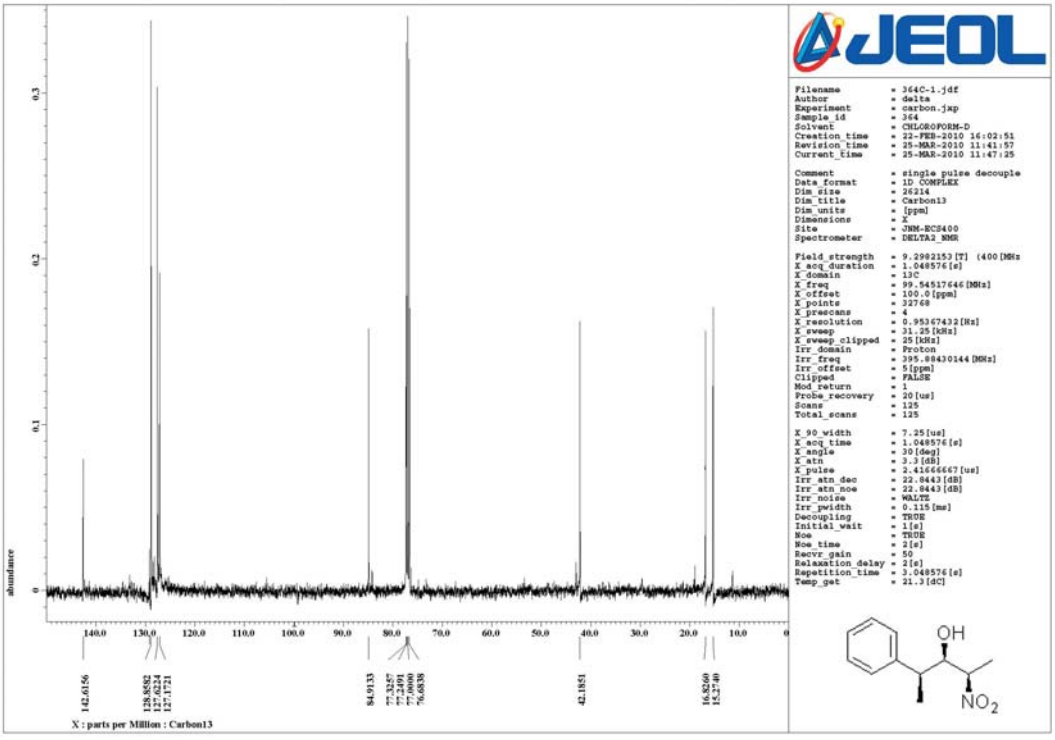

JEOL
Filename = 20100422_409_Proton-1
Author = delta
Experiment = proton.jxp
Sample_id = 409
Solvent = CHLOROFORM-D
Creation_time = 22-APR-2010 17:05:56
Revision_time = 5-MAY-2010 14:44:58
Current_time = 5-MAY-2010 14:45:36
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 5.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get = 20.9[dC]
OH
NO2
abundance
X : parts per Million : Proton : kilohertz

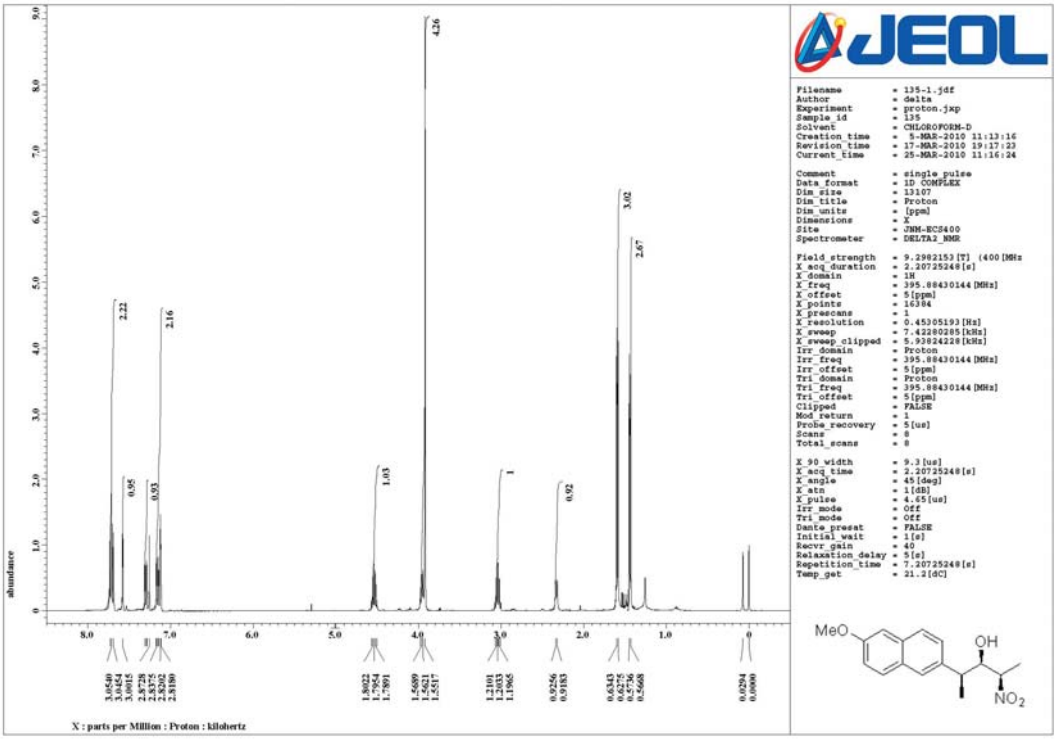

JEOL
Filename = 409C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 409
Solvent = CHLOROFORM-D
Creation_time = 6-MAY-2010 12:52:36
Revision_time = 7-MAY-2010 16:59:45
Current_time = 7-MAY-2010 17:53:27
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 9.5[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 7.4[dB]
X_pulse = 2.16666667[us]
Irr_atn_dec = 21.77[dB]
Irr_atn_noe = 21.77[dB]
Irr_noise = WALTZ
Irr_pwidth = 92[us]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 21.3[dC]
OH
NO2
abundance
X : parts per Million : Carbon13

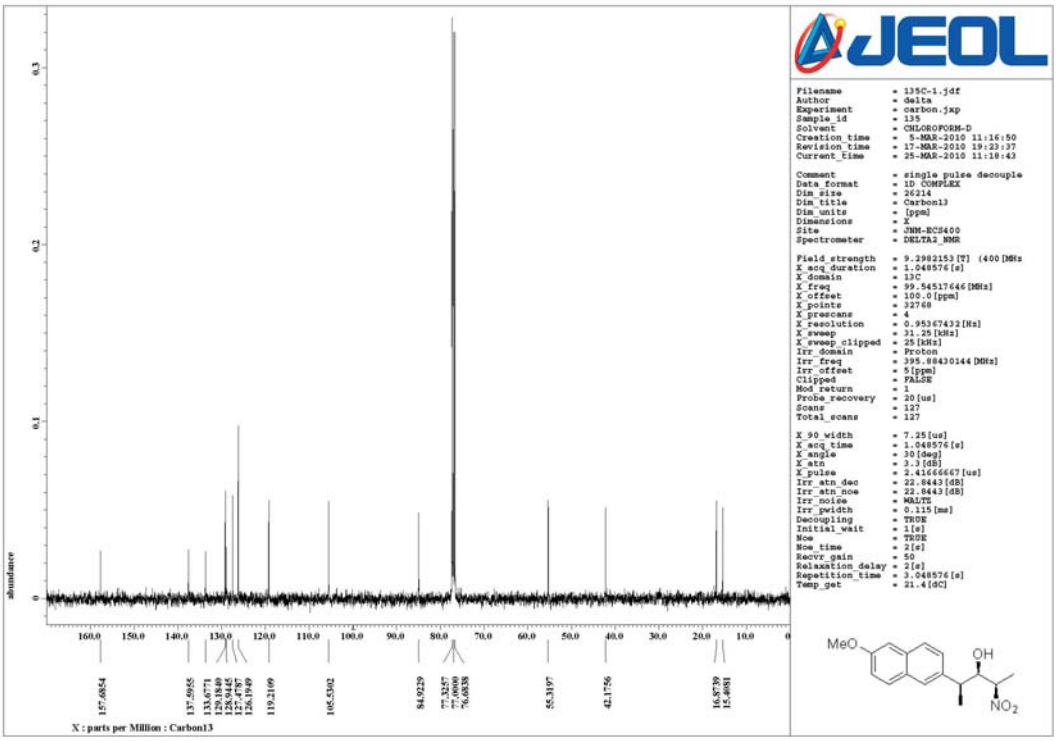

JEOL
Filename = 20100422_408_Proton-1
Author = delta
Experiment = proton.jxp
Sample_id = 408
Solvent = CHLOROFORM-D
Creation_time = 22-APR-2010 16:58:48
Revision_time = 5-MAY-2010 14:36:12
Current_time = 5-MAY-2010 14:36:59
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 10.6[us]
X_acq_time = 1.74587904[s]
X_angle = 45[deg]
X_atn = 3[dB]
X_pulse = 5.3[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 6.74587904[s]
Temp_get = 20.6[dC]
OH
Ph
NO2
abundance
X : parts per Million : Proton : kilohertz

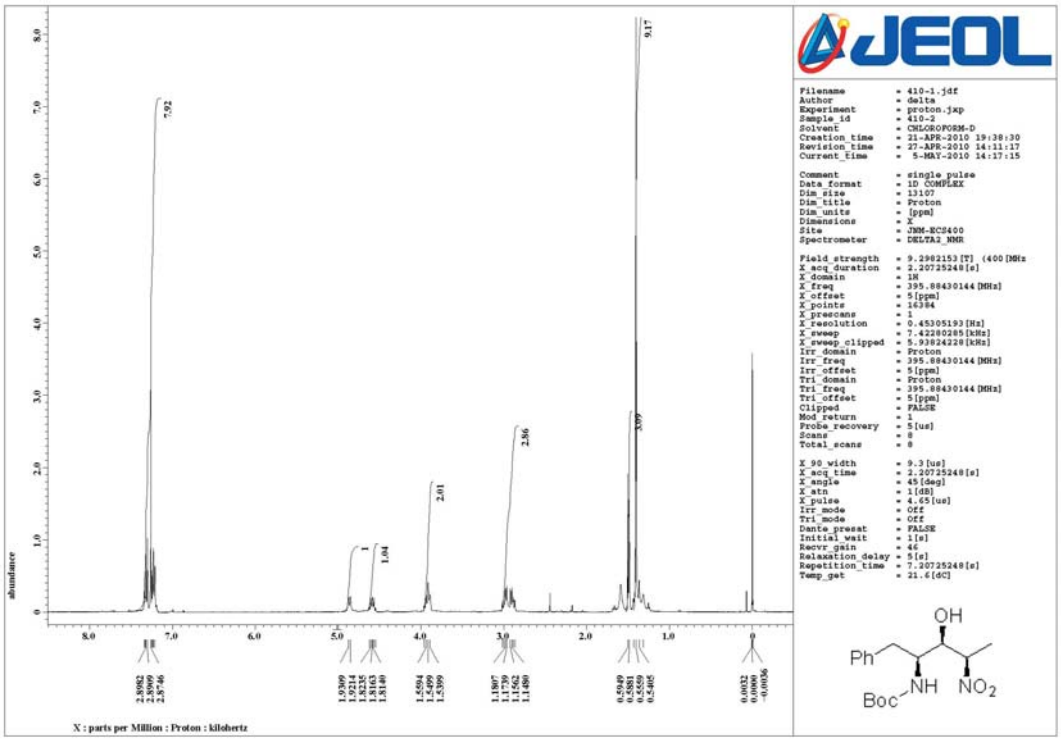

JEOL
Filename = 408C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 408
Solvent = CHLOROFORM-D
Creation_time = 6-MAY-2010 12:36:59
Revision_time = 7-MAY-2010 16:57:13
Current_time = 7-MAY-2010 17:49:52
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR
Field_strength = 11.7473579[T] (500[MH
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
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 9.5[us]
X_acq_time = 0.83361792[s]
X_angle = 30[deg]
X_atn = 7.6[dB]
X_pulse = 3.16666667[us]
Irr_atn_dec = 21.77[dB]
Irr_atn_noe = 21.77[dB]
Irr_noise = WALTZ
Irr_pwidth = 92[us]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 2.83361792[s]
Temp_get = 21.2[dC]
OH
Ph
NO2
abundance
X : parts per Million : Carbon13

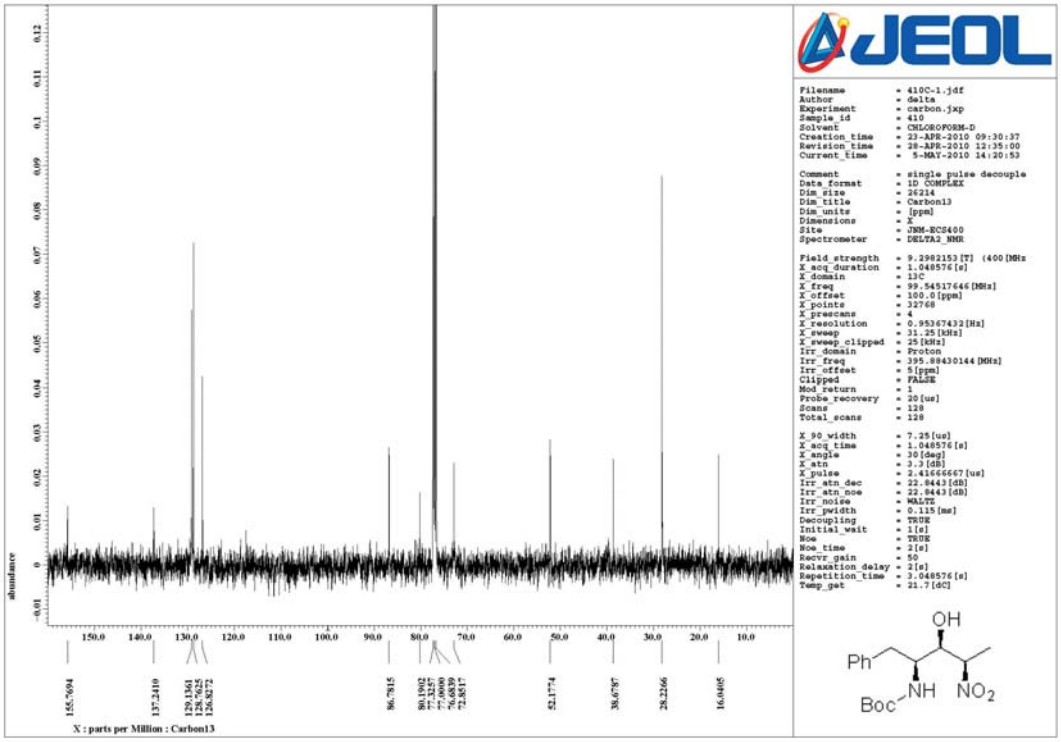

JEOL
Filename = 364-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 364
Solvent = CHLOROFORM-D
Creation_time = 17-FEB-2010 17:56:06
Revision_time = 25-MAR-2010 11:40:37
Current_time = 25-MAR-2010 11:44:34
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.92824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 20.7[dC]
OH
NO2
X : parts per Million : Proton : kilohertz

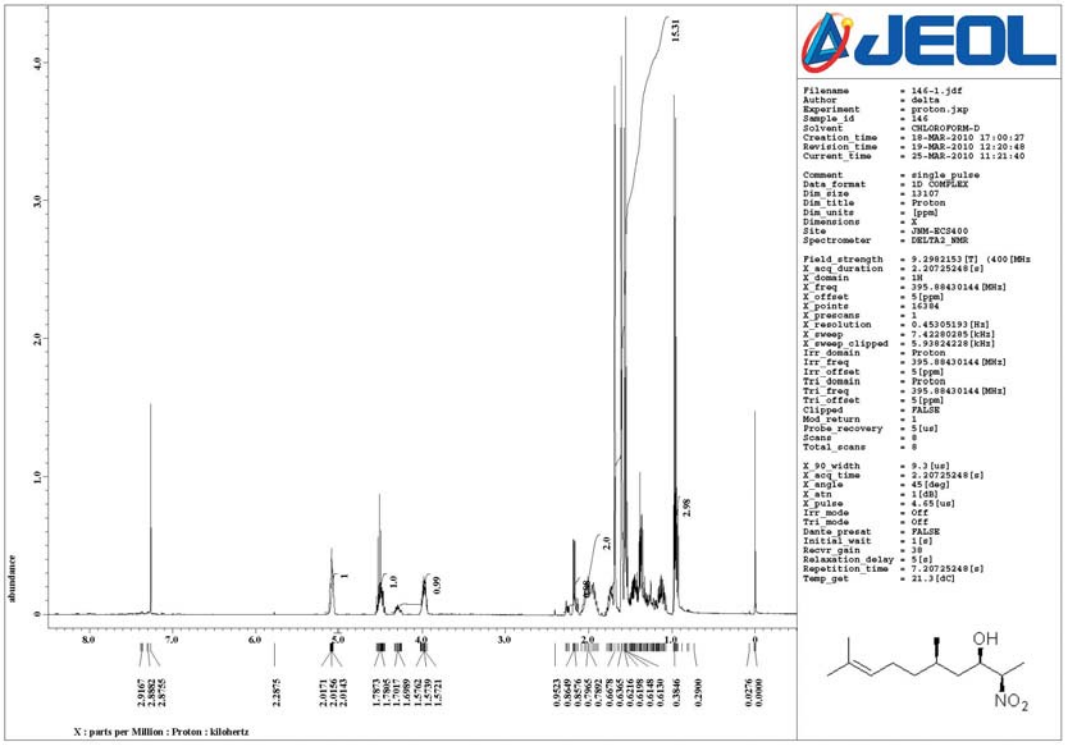

JEOL
Filename = 364C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 364
Solvent = CHLOROFORM-D
Creation_time = 22-FEB-2010 16:02:51
Revision_time = 25-MAR-2010 11:41:57
Current_time = 25-MAR-2010 11:47:25
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 125
Total_scans = 125
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.3[dC]
OH
NO2
X : parts per Million : Carbon13

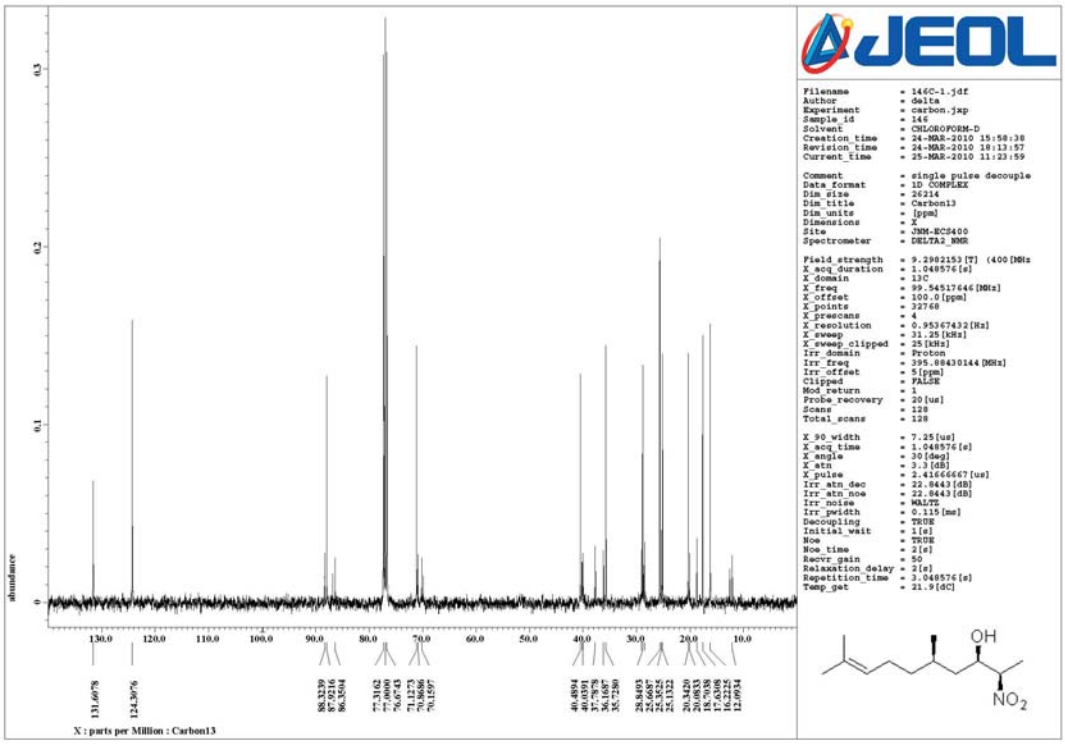

JEOL
Filename = 135-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 135
Solvent = CHLOROFORM-D
Creation_time = 5-MAR-2010 11:13:16
Revision_time = 17-MAR-2010 19:17:23
Current_time = 25-MAR-2010 11:16:24
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153 [T] (400 [MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144 [MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193 [Hz]
X_sweep = 7.42280285 [kHz]
X_sweep_clipped = 5.93824228 [kHz]
Irr_domain = Proton
Irr_freq = 395.88430144 [MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144 [MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 40
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.2[dC]
MeO
OH
NO2
abundance
X : parts per Million : Proton : kilohertz

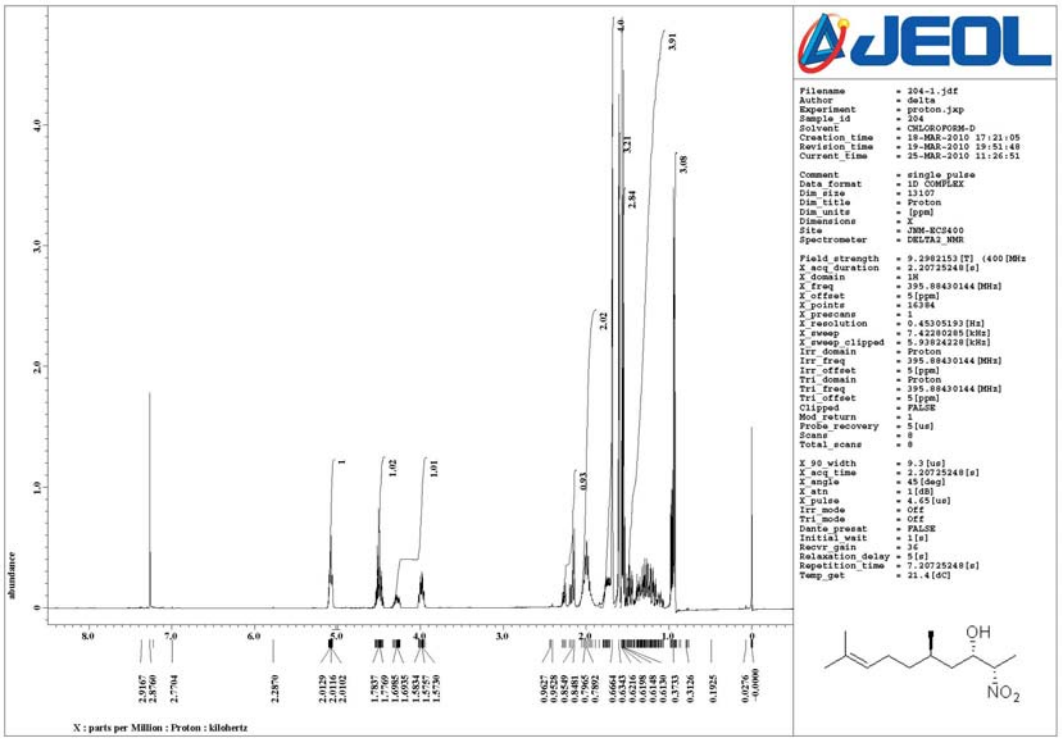

JEOL
Filename = 135C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 135
Solvent = CHLOROFORM-D
Creation_time = 5-MAR-2010 11:16:50
Revision_time = 17-MAR-2010 19:23:37
Current_time = 25-MAR-2010 11:18:43
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153 [T] (400 [MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646 [MHz]
X_offset = 100.0 [ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432 [Hz]
X_sweep = 31.25 [kHz]
X_sweep_clipped = 25 [kHz]
Irr_domain = Proton
Irr_freq = 395.88430144 [MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 127
Total_scans = 127
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.4[dC]
MeO
OH
NO2
abundance
X : parts per Million : Carbon13

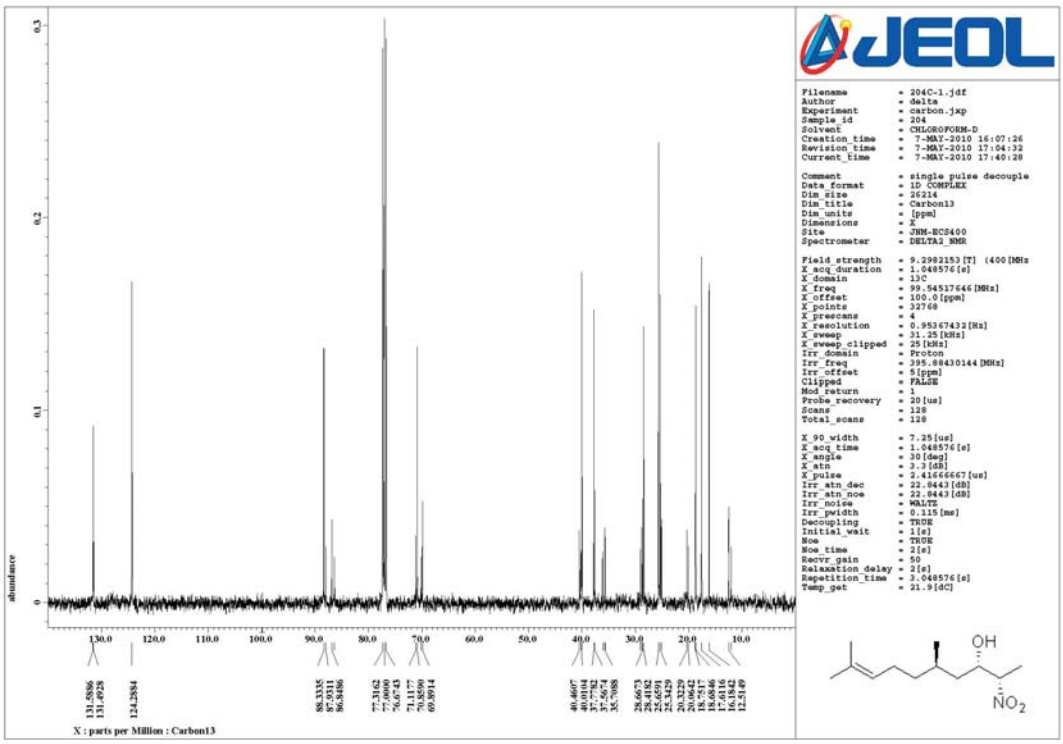

JEOL
Filename = 410-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 410-2
Solvent = CHLOROFORM-D
Creation_time = 21-APR-2010 19:38:30
Revision_time = 27-APR-2010 14:11:17
Current_time = 5-MAY-2010 14:17:15
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 46
Relaxation_delay = 5[s]
Repetition_time = 7.207252480[s]
Temp_get = 21.6[dC]
OH
Ph
NH
NO2
Boc
abundance
X : parts per Million : Proton : kilohertz

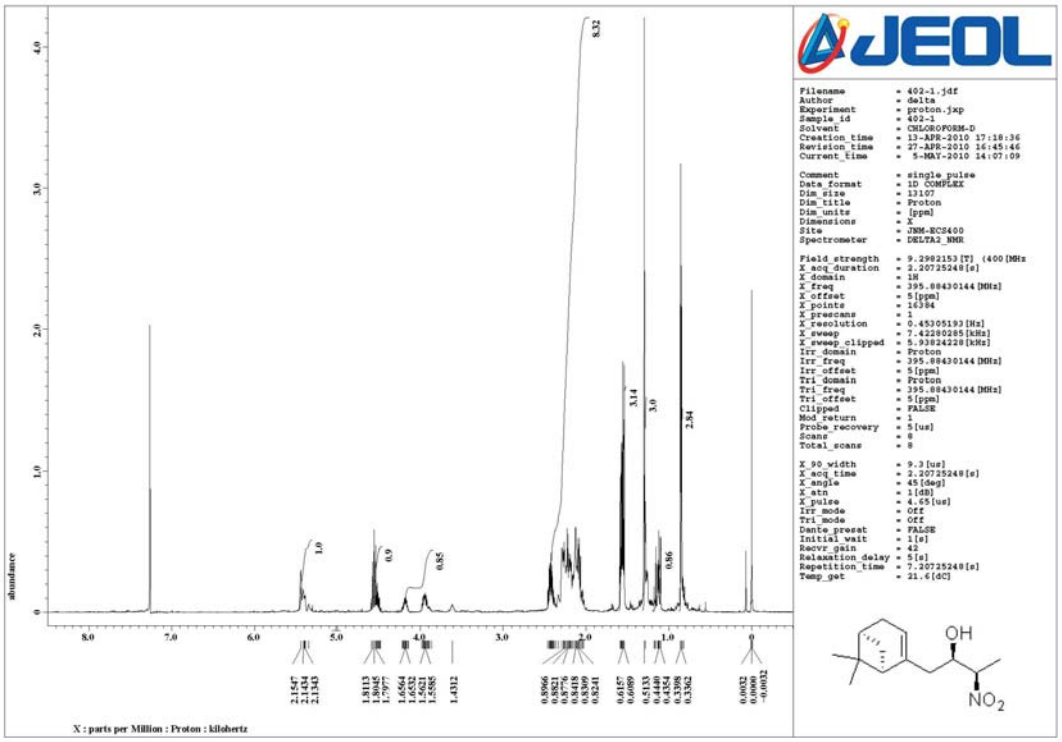

JEOL
Filename = 410C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 410
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 09:30:37
Revision_time = 28-APR-2010 12:35:00
Current_time = 5-MAY-2010 14:20:53
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.7[dC]
OH
Ph
NH
NO2
Boc
abundance
X : parts per Million : Carbon13

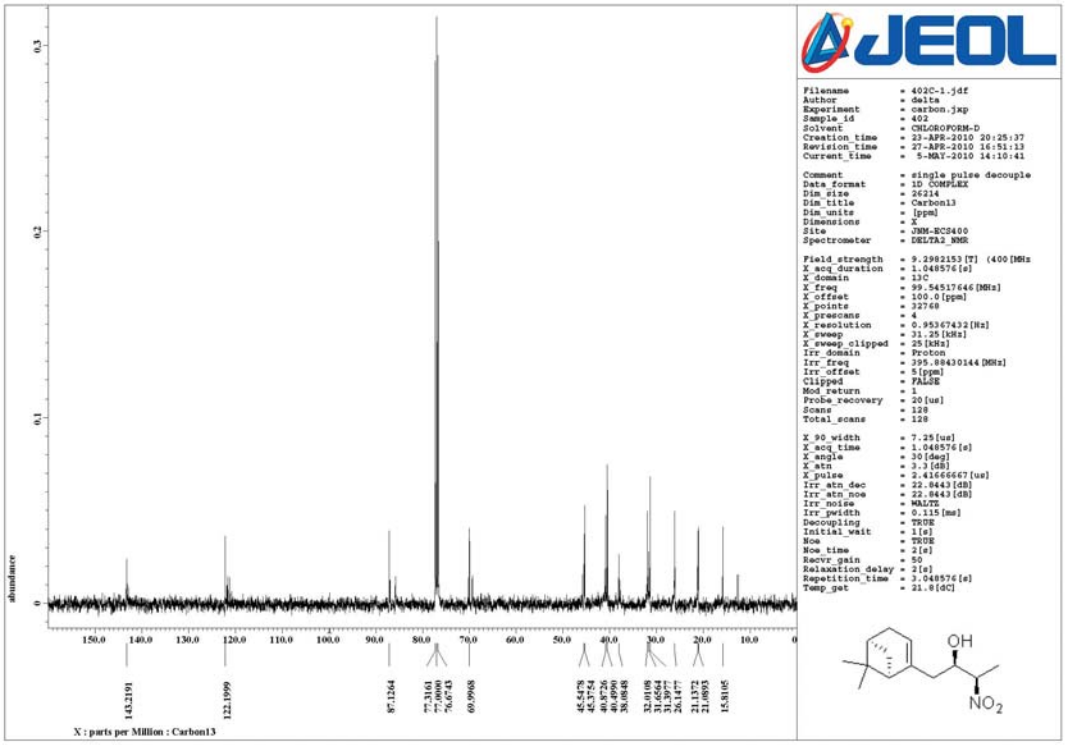

JEOL
Filename = 146-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 146
Solvent = CHLOROFORM-D
Creation_time = 18-MAR-2010 17:00:27
Revision_time = 19-MAR-2010 12:20:48
Current_time = 25-MAR-2010 11:21:40
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 38
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.3[dC]
OH
NO2
X : parts per Million : Proton : kilohertz

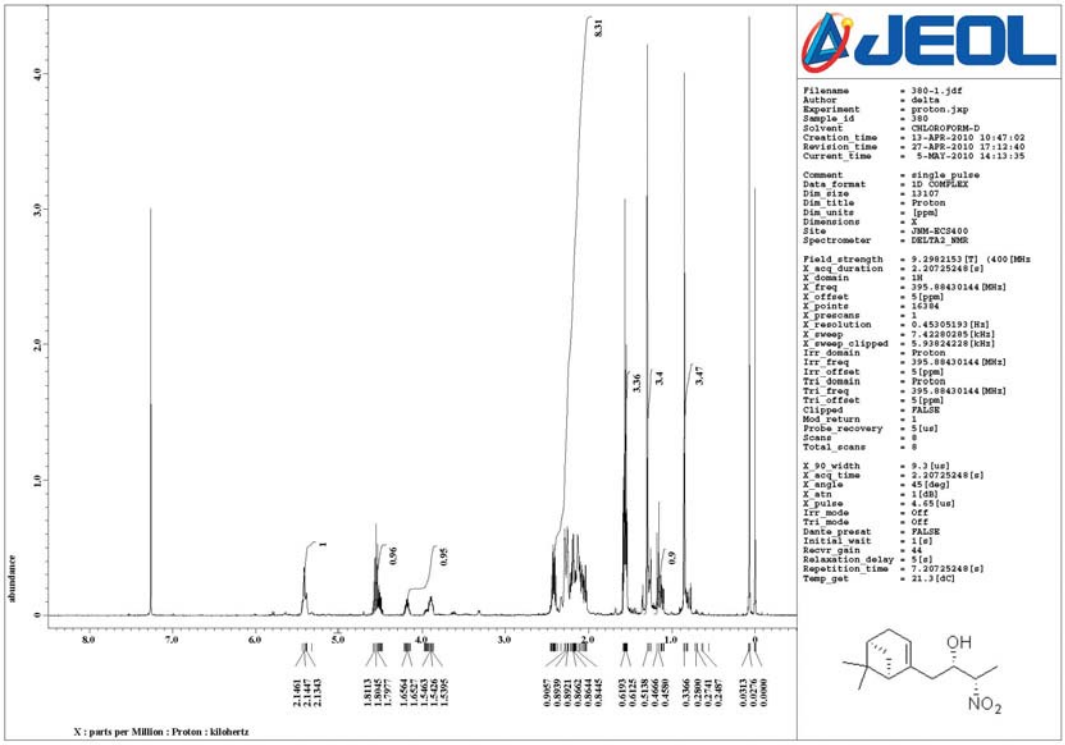

JEOL
Filename = 146C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 146
Solvent = CHLOROFORM-D
Creation_time = 24-MAR-2010 15:58:38
Revision_time = 24-MAR-2010 18:13:57
Current_time = 25-MAR-2010 11:23:59
Comment = single_pulse_decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.0443[dB]
Irr_atn_noe = 22.0443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.9[dC]
OH
NO2
X : parts per Million : Carbon13

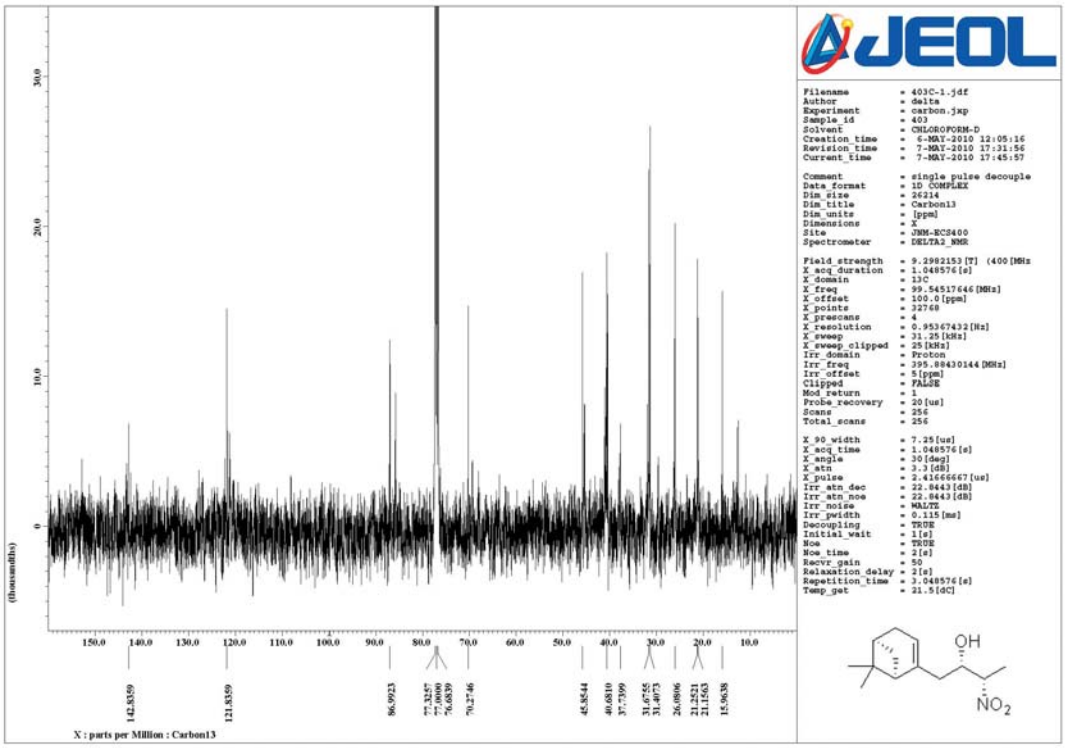

JEOL
Filename = 204-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 204
Solvent = CHLOROFORM-D
Creation_time = 18-MAR-2010 17:21:05
Revision_time = 19-MAR-2010 19:51:48
Current_time = 25-MAR-2010 11:26:51
Comment = single pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 36
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.4[dC]
OH
NO2
X : parts per Million : Proton : kilohertz


JEOL
Filename = 204C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 204
Solvent = CHLOROFORM-D
Creation_time = 7-MAY-2010 16:07:26
Revision_time = 7-MAY-2010 17:04:32
Current_time = 7-MAY-2010 17:40:28
Comment = single pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.0443[dB]
Irr_atn_noe = 22.0443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.9[dC]
OH
NO2
X : parts per Million : Carbon13


JEOL
Filename = 402-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 402-1
Solvent = CHLOROFORM-D
Creation_time = 13-APR-2010 17:18:36
Revision_time = 27-APR-2010 16:45:46
Current_time = 5-MAY-2010 14:07:09
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 42
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.6[dC]
OH
NO2
X : parts per Million : Proton : kilohertz


JEOL
Filename = 402C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 402
Solvent = CHLOROFORM-D
Creation_time = 23-APR-2010 20:25:37
Revision_time = 27-APR-2010 16:51:13
Current_time = 5-MAY-2010 14:10:41
Comment = single_pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 128
Total_scans = 128
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.0443[dB]
Irr_atn_noe = 22.0443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.8[dC]
OH
NO2
X : parts per Million : Carbon13


JEOL
Filename = 380-1.jdf
Author = delta
Experiment = proton.jxp
Sample_id = 380
Solvent = CHLOROFORM-D
Creation_time = 13-APR-2010 10:47:02
Revision_time = 27-APR-2010 17:12:40
Current_time = 5-MAY-2010 14:13:35
Comment = single_pulse
Data_format = 1D COMPLEX
Dim_size = 13107
Dim_title = Proton
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 2.20725248[s]
X_domain = 1H
X_freq = 395.88430144[MHz]
X_offset = 5[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45305193[Hz]
X_sweep = 7.42280285[kHz]
X_sweep_clipped = 5.93824228[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Tri_domain = Proton
Tri_freq = 395.88430144[MHz]
Tri_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 5[us]
Scans = 8
Total_scans = 8
X_90_width = 9.3[us]
X_acq_time = 2.20725248[s]
X_angle = 45[deg]
X_atn = 1[dB]
X_pulse = 4.65[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Recvr_gain = 44
Relaxation_delay = 5[s]
Repetition_time = 7.20725248[s]
Temp_get = 21.3[dC]
OH
NO2
abundance
X : parts per Million : Proton : kilohertz


JEOL
Filename = 403C-1.jdf
Author = delta
Experiment = carbon.jxp
Sample_id = 403
Solvent = CHLOROFORM-D
Creation_time = 6-MAY-2010 12:05:16
Revision_time = 7-MAY-2010 17:31:56
Current_time = 7-MAY-2010 17:45:57
Comment = single_pulse decouple
Data_format = 1D COMPLEX
Dim_size = 26214
Dim_title = Carbon13
Dim_units = [ppm]
Dimensions = X
Site = JNM-ECS400
Spectrometer = DELTA2_NMR
Field_strength = 9.2982153[T] (400[MHz
X_acq_duration = 1.048576[s]
X_domain = 13C
X_freq = 99.54517646[MHz]
X_offset = 100.0[ppm]
X_points = 32768
X_prescans = 4
X_resolution = 0.95367432[Hz]
X_sweep = 31.25[kHz]
X_sweep_clipped = 25[kHz]
Irr_domain = Proton
Irr_freq = 395.88430144[MHz]
Irr_offset = 5[ppm]
Clipped = FALSE
Mod_return = 1
Probe_recovery = 20[us]
Scans = 256
Total_scans = 256
X_90_width = 7.25[us]
X_acq_time = 1.048576[s]
X_angle = 30[deg]
X_atn = 3.3[dB]
X_pulse = 2.41666667[us]
Irr_atn_dec = 22.8443[dB]
Irr_atn_noe = 22.8443[dB]
Irr_noise = WALTZ
Irr_pwidth = 0.115[ms]
Decoupling = TRUE
Initial_wait = 1[s]
Noe = TRUE
Noe_time = 2[s]
Recvr_gain = 50
Relaxation_delay = 2[s]
Repetition_time = 3.048576[s]
Temp_get = 21.5[dC]
OH
NO2
(thousandths)
X : parts per Million : Carbon13