Supporting Information

Stereospecific Synthesis of Dienones Via a Torquoselective Retro-Nazarov Reaction

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Experimental Section

General Information

All reactions were carried out under argon atmosphere in flame-dried or oven-dried glassware. Chromatographic separations were carried out using Silicycle ultra pure silica gel(230-400 mesh). Analytical thin layer chromatography was performed on EM reagent 0.25 nm silicagel 60-F plates. Infrared spectra were recorded on a Perkin Elmer 1600 series FT-IR spectrometer, max cm^{-1} . Bands are Characterized as broad (br), strong (s), medium (m), and weak (w). ^1H NMR spectra were recorded on a Bruker ARX-250 (250 MHz), DRX-300 (300 MHz), DRX-500 (500 MHz) spectrometer and were reported in ppm (δ) from tetramethylsilane (TMS : δ 0.0 ppm). ^{13}C NMR spectra were recorded on a Bruker ARX-250 (62.5 MHz), DRX-300 (75 MHz), DRX-500 (125 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from tetramethylsilane with solvent resonance as the internal standard (CDCl_3 : δ 77.0 ppm).

General Procedure for the Formation of *cis*-1-Methyl-vinylother from Isomerization¹ with *sec*-BuLi

***cis*-1-Methylvinyl-adamantylether.** To a solution of Allyladamantylether (0.575 g, 2.99 mmol) in dry THF (6 mL) was added dropwise the *sec*-BuLi (1.3 M in cyclohexane/hexane(92:8), 2.8 mL, 3.58 mL). The resulting reaction mixture was stirred at this temperature for 1 hr then quenched with sat- NH_4Cl (aq, 5 mL) at $-65\text{ }^{\circ}\text{C}$. The reaction flask was put into $0\text{ }^{\circ}\text{C}$ ice bath and increased temperature slowly to reach bath temperature. The reaction mixture was extracted with ether (3 x 15 mL). The collected organic layer was dried with anhyd. Na_2SO_4 and the solvent was removed in vacuo. The flash chromatography on silica gel (3% triethylamine in n-pentane) gave the desired compound (350 mg, 61 %).

cis-1-Methylvinyl –adamantylether : 61 % ; ^1H NMR (300.13 MHz, CDCl_3), δ 6.30 (dq, $J = 6.3, 1.7$ Hz, 1 H), 4.46 (q, 6.3 Hz, 1 H), 2.17 (br. s, 3 H), 1.83 (d, $J = 2.9$ Hz, 6 H), 1.70 - 1.58 (br. m, 6 H), 1.60 (dd, $J = 6.8, 1.7$ Hz, 3 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 138.1, 102.3, 74.6, 41.8, 36.2, 30.5, 9.3. 9 ; IR (neat) : 3047 (w), 2908 (s), 2851 (s), 1658 (m), 1450 (w), 1405 (w), 1348 (w), 1245 (m), 1115 (s), 1078 (s), 1041 (w), 718 (w) cm^{-1} .

General Procedure for the Formation of α -Chloro-dienone Compound, Z,Z-1-(Adamantyl)-2-chloro-5-methyl-1,4-pentadiene-3-one from [2+2] Cycloaddition², Diazomethane ring expansion³ and the Retro-Nazarov reaction.⁴

Entry 8, Table 1

To a stirred mixture of cis-1-Methylvinyl-adamantylether (243 mg, 1.26 mmol), Zn-Cu⁵ (1.73 g, 26.5 mmol) and dry ether (11 mL) at 0 °C under N_2 was added dropwise the solution of freshly distilled trichloroacetylchloride⁵ in ether (5 mL) over 1 hr. After reaction, the reaction mixture was filtered with celite filter and was partially concentrated under reduced pressure and added hexane to precipitate the zinc chloride. The mixture was stored in the freezer during several hours then celite filtration. The filtrate was washed successively with a cold- NaHCO_3 (aq), water, and brine then dried over anhydrous sodium sulfate. Evaporation of the solvent under reduced pressure gave the crude [2+2] cyclo adduct. To a solution of this crude [2+2] cyclo adduct in Et_2O (4 mL) was added CH_2N_2 (0.4 M, 9.4 mL, 3.79 mmol) solution in Et_2O at 0 °C under N_2 atmosphere. The resulting mixture was stirred for 1 hr at 0 °C then evaporated the solvent under reduced pressure gave the crude α, α - dichlorocyclopentanone compound. This

crude α, α - dichlorocyclopentanone was dissolved in hexafluoro-2-propanol (10 mL). To this reaction mixture was added dropwise 2,2,6,6-tetramethylpiperidine (0.232 mL, 1.37 mmol) at room temperature and the mixture was refluxed, After 3 hrs, the mixture was cooled to room temperature and hexafluoro-2-propanol was removed on a rotary evaporator. To the residue was added ethyl ether (30 mL). This solution was washed with 1N-HCl (aq), sat-NaHCO₃ (aq) and brine (20 mL each). The solution was dried over MgSO₄ and the solvent was removed in vacuo. The flash chromatography (hexanes (11):Ether(1)) gave the desired product, Z,Z-1- (Adamantyl)-2-chloro-5-methyl-1,4-pentadiene-3-one, **Entry 8, Table 1** (white solid, 187 mg, 52.6 % in 3 steps, m.p : 123-125 °C). This product was recrystallized from ether and hexanes.

The General Procedure⁶ for the Preparation of 1-(3-phenyl-1-propyl)-1-butyne from 3-phenyl-1-propanol and Conversion to (E)- and (Z)-1-(3-phenyl-1-propyl)-1-butene.

1-(3-phenyl-1-propyl)-1-butyne

To a suspension of potassium hydride (3.93 g of 30% in mineral oil, theoretically 1.18g, 29.3 mmol, The mineral oil was removed by washing with dry pentane (3 x 10 mL)) in anhydrous THF (10 mL) was added dropwise the solution of 3-phenyl-1-propanol (2 g, 14.6 mmol) in anhydrous THF (3 mL) under argon atmosphere at room temperature. The mixture was stirred at room temperature for 1 hr then cooled to -50 °C. A solution of trichloroethylene (1.45 mL, 16.1 mmol) in anhydrous THF (8 mL) was added dropwise by syringe over 15 min, after which the reaction mixture was allowed to warm to room temperature and was stirred for 1 hr. The resulting dark brown solution was quenched carefully with MeOH (3 mL) and sat-NH₄Cl (aq, 20 mL) at 0 °C ice bath. The phases were separated and the aqueous phase was extracted with pentane (3 x 50 mL). The combined organic phases were dried over sodium sulfate, and filtered with silica gel pad twice with hexanes. The solvent was removed by rotary evaporation to give a transparent oily liquid (3.18 g, 94%). This intermediate was dissolved in anhydrous THF (32 mL) and cooled to -70 °C and treated dropwise with n-BuLi (14.3 mL, 2.4 M in hexanes, 34.4 mmol) under argon atmosphere and warmed slowly to 0 °C over a period of 2.5 hr. The reaction mixture was stirred at 0 °C additional 30 min and was cooled again to -40 °C

and treated dropwise with a solution of ethyl iodide (3.3 mL, 41.2 mmol) in HMPA (6.5 mL). The solution was stirred at room temperature for 3 hr, whereupon it was quenched by cold *sat*-NH₄Cl (aq). The phases were separated and the aqueous phase was extracted with pentane (3 x 70 mL). The combined organic phases were washed with water (3 x 50 mL), dried over sodium sulfate, and filtered. Concentration by rotary evaporation and chromatography on deactivated silicagel with 3% of triethylamine in n-hexanes provided 1-(3-phenyl-1-propyl)-1-butyne (2.11 g, oily liquid, 76%).

1-(3-phenyl-1-propyl)-1-butyne : 76% ; ¹H NMR (250.13 MHz, CDCl₃), δ 7.37 (m, 2 H), 7.25 (m, 3H), 4.02 (t, J = 6.3 Hz, 2 H), 2.78 (t, J = 7.3 Hz, 2 H), 2.20 (q, J = 7.5 Hz, 2 H), 2.0 (m, 2 H), 1.18 (t, J = 7.5 Hz, 3 H) ; ¹³C NMR (62.9 MHz, CDCl₃), δ 140.9, 128.41, 128.40, 125.9, 88.9, 77.0, 38.6, 31.4, 30.3, 15.0, 10.9 ; IR (neat) : 3084 (w), 3060 (w), 3027 (m), 2970 (s), 2933 (s), 2880 (m), 2267 (s), 1495 (m), 1454 (s), 1380 (w), 1237 (s), 1004 (m), 890 (w), 747 (m), 698 (s) cm⁻¹.

(E)-1-(3-phenyl-1-propyl)-1-butene

To the suspension of LAH (95%, 0.24 g, 5.99 mmol) in anhydrous THF (6 mL) was added dropwise by syringe the solution of 1-(3-phenyl-1-propyl)-1-butyne (0.376 g, 1.99 mmol) in anhydrous THF (3 mL) under argon atmosphere at room temperature. The septum was replaced with a reflux condenser connected to an argon –filled ballon and the mixture was refluxed for 4 hr. After the flask was allowed to cool to room temperature, it was placed in an ice bath and the reaction mixture quenched by slow addition of aqueous 10% NaOH (0.4 mL), followed by water (0.5 mL). The resulting mixture was stirred for 30 min, after which the solid material was removed by filtration through Celite pad, which was rinsed with diethyl ether (3 x 10 mL). Concentration by rotary evaporation and short length (1 inch) of chromatography on deactivated silicagel using 3% of TEA in hexanes provided (*E*)-1-(3-phenyl-1-propyl)-1-butene (0.371 g, 98%).

(E)-1-(3-phenyl-1-propyl)-1-butene : 98% ; ¹H NMR (300.13 MHz, CDCl₃), δ 7.34 (m, 2 H), 7.25 (m, 3 H), 6.30 (d, J = 12.6 Hz, 1 H), 4.87 (ddd, J = 12.6, 7.0, 6.6 Hz, 1 H), 3.70 (t, J = 6.3 Hz, 2 H), 2.77 (t, J = 7.4 Hz, 2 H), 1.98 (m, 4 H), 1.01 (t, J = 8.6 Hz, 3 H) ; ¹³C NMR (75.5 MHz, CDCl₃), δ 145.5, 141.6, 128.4, 128.3, 125.8, 106.0, 68.0, 32.1, 30.9, 21.0, 15.3 ; IR (neat) : 3084 (w), 3060 (w), 3027 (m), 2953 (s), 2925 (s), 2868 (m), 1670 (m), 1654 (s), 1495 (w), 1454 (m), 1254 (w), 1180 (s), 1127 (m), 1029 (w), 931 (m), 747

(m), 698 (s) cm^{-1} .

(Z)-1-(3-phenyl-1-propyl)-1-butene

The mixture of 1-(3-phenyl-1-propyl)-1-butyne (0.184 g, 0.977 mmol), pyridine (2.7 mL) and 5% Pd-BaSO₄ (20.3 mg, 0.096 mmol) was stirred for 19 hr at room temperature, under a hydrogen-filled balloon, whereupon the hydrogen was replaced with argon, and the reaction mixture was filtered through Celite pad. The filtrate was diluted with n-pentane (20 mL) and washed with sat-CuSO₄(aq, 5 x 15 mL) and the water (1 X 10 mL). The organic phase was dried over sodium sulfate and the solvent was removed by rotary evaporation. Chromatography on deactivated silicagel using 3% of TEA in hexanes : ethyl ether (20 : 1) provided (Z)-1-(3-phenyl-1-propyl)-1-butene (0.132 g, 71 %). Proton NMR indicated the presence of ca. 8% of the E-isomer.

(Z)-1-(3-phenyl-1-propyl)-1-butene : 71% ; ¹H NMR (250.13 MHz, CDCl₃), δ 7.36 (m, 2 H), 7.25 (m, 3 H), 5.94 (dt, J = 6.24, 1.34 Hz, 1 H), 4.42 (q, J = 7.13 Hz, 1 H), 3.77 (t, J = 6.40 Hz, 2 H), 2.77 (t, J = 7.31 Hz, 2 H), 2.18 (dq, J = 7.50, 1.38 Hz, 2 H), 1.98 (m, 2 H), 1.05 (t, J = 7.50 Hz) ; ¹³C NMR (62.9 MHz, CDCl₃), δ 144.2, 141.6, 128.5, 128.3, 125.8, 108.9, 70.9, 31.9, 31.3, 17.4, 14.5 ; IR (neat) : 3080 (w), 3060 (w), 3027 (m), 2958 (s), 2929 (s), 2864 (s), 1658 (s), 1601 (w), 1495 (m), 1454 (m), 1372 (m), 1245 (m), 1139 (s), 1098 (s), 1066 (m), 1025 (w), 739 (s), 694 (s) cm^{-1} .

Z,Z-1-(t-Butoxy)-2-chloro-5-ethyl-1,4-pentadiene-3-one (Entry 1, Table 1) : 50.7% in 3 steps ; ¹H NMR (250.13 MHz, CDCl₃), δ 7.88 (s, 1 H), 6.47 (dt, J = 11.60, 1.6 Hz, 1 H), 6.15 (dt, J = 11.60, 7.40 Hz, 1 H), 2.53 (double quintet, J = 7.40, 1.60 Hz, 2 H), 1.44 (s, 9 H), 1.05 (t, 3 H) ; ¹³C NMR (62.9 MHz, CDCl₃), δ 186.0, 151.7, 149.2, 123.1, 113.9, 81.8, 28.1, 23.0, 13.5 ; IR (neat) : 3047 (w), 2974 (s), 2944 (m), 2876 (w), 1756 (w), 1658 (s), 1613 (s), 1462 (m), 1372 (s), 1270 (s), 1217 (s), 1143 (s), 976 (m), 886 (m), 845 (m)

cm⁻¹ ; HRMS calcd for C₁₁H₁₇ClO₂Na[M+Na]⁺ 239.0809, Found 239.0810.

Z,Z-1-(t-Butoxy)-2-chloro-5-propyl-1,4-pentadiene-3-one (Entry 2, Table 1) : 54% in 3 steps ; ¹H NMR (250.13 MHz, CDCl₃), δ 7.87 (s, 1 H), 6.49 (dt, J = 11.60, 1.65 Hz, 1 H), 6.15 (dt, J = 11.60, 7.40 Hz, 1 H), 2.49 (dq, J = 7.40, 1.65 Hz, 1 H), 1.50 – 1.30 (m, 2 H), 1.43 (s, 9 H), 0.92 (t, 3 H) ; ¹³C NMR (62.9 MHz, CDCl₃), δ 186.1, 151.8, 147.8, 123.8, 114.0, 81.8, 31.6, 28.2, 22.4, 13.8; IR (neat) : 3051 (w), 2974 (s), 2929 (m), 2872 (m), 1662 (s), 1609 (s), 1580 (s), 1462 (w), 1372 (s), 1266 (s), 1213 (s), 1143 (s), 935 (m), 853 (s), 735 (m) cm⁻¹ ; HRMS calcd for C₁₂H₁₉ClO₂Na[M+Na]⁺ 253.0965, Found 253.0964.

Z,Z-1-(t-Butoxy)-2-chloro-5-butyl-1,4-pentadiene-3-one (Entry 3, Table 1) : 52% in 3 steps ; ¹H NMR (300.13 MHz, CDCl₃), δ 7.87 (s, 1 H), 6.48 (dt, J = 11.60, 1.60 Hz, 1 H), 6.15 (dt, J = 11.60, 7.40 Hz, 1 H), 2.51 (dq, J = 7.40, 1.60 Hz, 2 H), 1.43 (s, 9 H), 1.40 – 1.29 (m, 4 H), 0.89 (t, 3 H) ; ¹³C NMR (75.5 MHz, CDCl₃), δ 186.0, 151.8, 148.0, 123.6, 114.0, 81.8, 31.3, 29.3, 28.2, 22.4, 13.8; IR (neat) : 3039 (w), 2958 (s), 2929 (s), 2872 (m), 1654 (s), 1613 (s), 1466 (m), 1372 (s), 1270 (s), 1213 (s), 1143 (s), 939 (m), 857 (s), 759 (m) cm⁻¹ ; HRMS calcd for C₁₃H₂₁ClO₂Na[M+Na]⁺ 267.1122, Found 267.1115.

Z,Z-1-(t-Butoxy)-2-chloro-5-heptyl-1,4-pentadiene-3-one (Entry 4, Table 1) : 56.8% in 3 steps ; ^1H NMR (500.13 MHz, CDCl_3), δ 7.86 (s, 1 H), 6.47 (dt, $J = 11.60, 1.60$ Hz, 1 H), 6.15 (dt, $J = 11.60, 7.5$ Hz, 1 H), 2.50 (dq, $J = 7.50, 1.50$ Hz, 2 H), 1.42 (s, 9 H), 1.30 – 1.24 (m, 9 H), 0.86 (t, 3 H) ; ^{13}C NMR (125.75 MHz, CDCl_3), δ 186.1, 151.7, 148.2, 123.6, 114.0, 81.8, 31.8, 29.7, 29.3, 29.2, 29.0, 28.2, 22.6, 14.0; IR (neat) : 2958 (m), 2925 (s), 2851 (m), 1658 (m), 1613 (s), 1466 (w), 1372 (m), 1270 (m), 1217 (m), 1147 (s), 939 (w), 857 (m), 808 (w), 755 (m) cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{27}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 309.1591, Found 309.1587.

Z,Z-1-(t-Butoxy)-2-chloro-5-ethylbenzene-1,4-pentadiene-3-one (Entry 5, Table 1) : 52% in 3 steps ; ^1H NMR (300.13 MHz, CDCl_3), δ 7.86 (s, 1 H), 7.31 – 7.15 (m, 5 H), 6.54 (dt, $J = 11.60, 1.60$ Hz, 1 H), 6.19 (dt, $J = 11.60, 7.0$ Hz, 1 H), 2.95 – 2.85 (m, 2 H), 2.82 – 2.75 (m, 2 H), 1.44 (s, 9 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 185.8, 151.7, 146.9, 141.2, 128.5, 128.3, 125.9, 124.0, 114.0, 81.9, 35.1, 31.0, 28.3; IR (neat) : 3027 (w), 2978 (m), 2929 (m), 2855 (w), 1723 (m), 1658 (m), 1609 (s), 1450 (w), 1368 (m), 1266 (m), 1213 (m), 1143 (s), 943 (w), 853 (m), 743 (m) cm^{-1} ; HRMS calcd for $\text{C}_{17}\text{H}_{21}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 315.1122, Found 315.1113.

Z,Z-1- (Adamantyl)-2-chloro-5-butyl-1,4-pentadiene-3-one (Entry 6, Table 1) : 55.9% in 3 steps, ^1H NMR (250.13 MHz, CDCl_3), δ 7.99 (s, 1 H), 6.47 (dt, $J = 11.60$, 1.63 Hz, 1 H), 6.15 (dt, $J = 11.60$, 7.50 Hz, 1 H), 2.51 (dq, $J = 7.50$, 1.33 Hz, 2 H), 2.26 (single, broad, 3 H), 1.94 (d, $J = 2.90$ Hz, 6 H), 1.76 – 1.54 (m, 6 H), 1.49 – 1.25 (m, 4 H), 0.89 (t, 3 H) ; ^{13}C NMR (62.9 MHz, CDCl_3), δ 186.0, 150.9, 147.8, 123.6, 113.9, 81.1, 41.9, 35.6, 31.3, 30.7, 29.4, 22.4, 13.8; IR (neat) : 3051 (w), 2913 (s), 2855 (s), 1658 (m), 1601 (s), 1450 (w), 1356 (w), 1278 (m), 1204 (s), 1176 (m), 1155 (m), 1102 (w), 1049 (s), 967 (w), 894 (w), 735 (m) cm^{-1} ; HRMS calcd for $\text{C}_{19}\text{H}_{27}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 345.1591, Found 345.1598.

Z,Z-1- (Adamantyl)-2-chloro-5-ethylbenzene-1,4-pentadiene-3-one (Entry 7, Table 1) : 51% in 3 steps ; ^1H NMR (300.13 MHz, CDCl_3), δ 7.97 (s, 1 H), 7.35 – 7.10 (m, 5 H), 6.52 (dt, $J = 11.60$, 1.61 Hz, 1 H), 6.19 (dt, $J = 11.60$, 7.0 Hz, 1 H), 2.95 – 2.84 (m, 2 H), 2.83 – 2.76 (m, 2 H), 2.27 (s, br, 3 H), 1.95 (d, $J = 2.81$ Hz, 6H), 1.75 – 1.62 (m, 6 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 185.8, 150.8, 146.6, 141.2, 128.4, 128.3, 125.9, 124.1, 113.9, 81.2, 41.9, 35.7, 35.1, 31.0, 30.7; IR (neat) : 3056 (w), 3027 (w), 2913 (s), 2851 (s), 1658 (m), 1609 (s), 1576 (m), 1450 (m), 1356 (w), 1278 (m), 1200 (s), 1151 (m), 1045 (s), 967 (m), 878 (w), 735 (m), 698 (w) cm^{-1} ; HRMS calcd for $\text{C}_{23}\text{H}_{27}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 393.1591, Found 393.1601.

Entry 8, Table 1

***Z,Z*-1- (Adamantyl)-2-chloro-5-methyl-1,4-pentadiene-3-one (Entry 8, Table 1) :**
 52.6 % in 3 steps, mp : 123-125 °C ; ^1H NMR (500.13 MHz, CDCl_3), δ 8.0 (s, 1H), 6.51 (dq, $J = 11.58, 1.71$ Hz, 1 H), 6.27 (dq, $J = 11.58, 7.2$ Hz, 1 H), 6.27 (br. s, 6 H), 2.05 (dd, $J = 7.2, 1.71$ Hz, 3 H), 1.95 (d. $J = 2.4$ Hz, 6 H), 1.69 (m, 6H) ; ^{13}C NMR (125.75 MHz, CDCl_3), δ 186.0, 151.0, 142.0, 124.7, 113.9, 81.2, 41.9, 35.6, 30.7, 15.8; IR (neat) : 3051 (s), 2986 (w), 2913 (s), 2855 (w), 1654 (w), 1609 (s), 1417 (w), 1266 (s), 1200 (m), 1049 (w), 894 (w) cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{21}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 303.1122, Found 303.1125.

***Z,Z*-1- (*l*-Menthyl)-2-chloro-5-methyl-1,4-pentadiene-3-one (Entry 9, Table 1) :**
 52.1% in 3 steps ; ^1H NMR (300.13 MHz, CDCl_3), δ 7.73 (s, 1 H), 6.48 (dq, $J = 11.58, 1.70$ Hz, 1 H), 6.24 (dq, $J = 11.58, 7.20$ Hz, 1 H), 3.84(dt, $J = 10.84, 4.51$ Hz, 1 H), 2.04 (dd, $J = 7.20, 1.70$ Hz, 3 H), 2.20 – 1.95 (m, 2 H), 1.75 – 1.65 (m, 2 H), 1.55 – 1.40 (m, 2 H), 1.22 (m, 1 H), 1.1 – 0.95 (m, 1 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 185.8, 156.0, 142.2, 124.5, 113.5, 86.7, 47.3, 41.6, 33.8, 31.5, 25.9, 23.5, 21.8, 20.5, 16.4, 15.9; IR (neat) : 3051 (w), 2953 (s), 2925 (s), 2868 (m), 1658 (m), 1613 (s), 1454 (m), 1368 (m), 1262 (s), 1204 (s), 1143 (m), 1090 (m), 984 (m), 792 (w), 139 (s) cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{25}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 307.1435, Found 307.1431.

Z,Z-1- (β-Cholesterol)-2-chloro-5-methyl-1,4-pentadiene-3-one (Entry 10, Table 1) :

58.4% in 3 steps ; ^1H NMR (500.13 MHz, CDCl_3), δ 7.75 (s, 1 H), 6.49 (dq, J = 11.60, 1.73 Hz, 1 H), 6.25 (dq, J = 11.60, 7.20 Hz, 1 H), 3.98 (hep, J = 5.14 Hz, 1 H), 2.05 (dd, J = 7.20, 1.73 Hz, 3 H), 2.0- 1.92 (m, 2 H), 1.85 – 1.76 (m, 2 H), 1.73 –1.63 (m, 2 H), 1.62 – 1.45 (m, 5 H), 1.37 – 1.19 (m, 9 H), 1.18 – 1.03 (m, 7 H), 1.03 – 0.94 (m, 4 H), 0.89 (d, J = 6.60 Hz, 3 H), 0.86 (dd, J = 6.60, 2.20 Hz, 6 H), 0.84 (s, 3 H), 0.65 (s, 3 H) ; ^{13}C NMR (125.75 MHz, CDCl_3), δ 185.8, 155.7, 142.4, 124.5, 113.6, 85.5, 56.4, 56.3, 54.1, 44.7, 42.5, 39.9, 39.5, 36.6, 36.1, 35.7, 35.4, 34.9, 31.9, 28.5, 28.4, 28.2, 27.9, 24.1, 23.8, 22.8, 22.5, 21.2, 18.6, 15.9, 12.2, 12.0; IR (neat) : 3051 (w), 2933 (s), 2868 (m), 1666 (w), 1621 (s), 1585 (m), 1442 (w), 1364 (w), 1262 (s), 1213 (m), 1155 (w), 972 (w), 914 (w), 739 (s), 702 (m) cm^{-1} HRMS calcd for $\text{C}_{33}\text{H}_{53}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 539.3626, Found 539.3655.

Z,Z-1- (α-Cholesterol)-2-chloro-5-methyl-1,4-pentadiene-3-one (Entry 11, Table 1) :

54.8% in 3 steps ; ^1H NMR (300.13 MHz, CDCl_3), δ 7.70 (s, 1 H), 6.50 (dq, J = 11.60, 1.70 Hz, 1 H), 6.25 (dq, J = 11.60, 7.20 Hz, 1 H), 4.32 (br, 1 H), 2.06 (dd, J = 7.20, 1.70 Hz, 3 H), 2.0- 1.92 (m, 1 H), 1.90 – 1.75 (m, 3 H), 1.75 –1.62 (m, 2 H), 1.59 – 1.44 (m, 7 H), 1.39 – 1.29 (m, 5 H), 1.29 – 1.15 (m, 5 H), 1.14 – 1.00 (m, 8 H), 0.90 (d, J = 6.50 Hz, 3 H), 0.87 (dd, J = 6.60, 1.18 Hz, 6 H), 0.84 (s, 3 H), 0.65 (s, 3 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 185.9, 155.7, 142.3, 124.5, 114.1, 81.8, 56.3, 56.2, 53.9, 42.5, 39.8, 39.5, 39.3, 36.1, 35.8, 35.7, 35.4, 33.7, 32.3, 31.7, 28.3, 28.2, 27.9, 26.9, 24.1, 23.8, 22.8, 22.5, 20.7, 18.6, 15.9, 12.0, 11.4; IR (neat) : 3093 (w), 2933 (s), 2868 (m), 1605 (m), 1658 (s), 1446 (m), 1364 (m), 1262 (m), 1209 (s), 1155 (m), 1029 (w), 972 (m), 906 (m), 849 (w), 763

(m), 739 (s), 702 (w) cm^{-1} HRMS calcd for $\text{C}_{33}\text{H}_{53}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 539.3626, Found 539.3627.

Z,Z-1- (3-Phenylpropyl)-2-chloro-5-methyl-1,4-pentadiene-3-one (Entry 12, Table 1) : 50.8% in 3 steps, ^1H NMR (300.13 MHz, CDCl_3), δ 7.63 (s, 1 H), 7.30 (m, 2 H), 7.21 (m, 3 H), 6.43 (dt, $J = 11.56, 1.64$ Hz, 1 H), 6.16 (dt, $J = 11.56, 7.40$ Hz, 1 H), 4.14 (t, $J = 6.40$ Hz, 2 H), 2.77 (t, $J = 7.30, 2$ H), 2.53 (dq, $J = 7.50, 1.64$ Hz, 2 H), 2.10 (q, $J = 6.40$ Hz, 2 H), 1.06 (t, $J = 7.50$ Hz, 3 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 185.6, 156.6, 149.8, 140.4, 128.5, 128.4, 126.2, 122.7, 113.9, 74.7, 31.3, 31.0, 23.1, 13.5; IR (neat) : 3023 (m), 2962 (s), 2933 (s), 2872 (m), 1654 (m), 1613 (s), 1450 (w), 1372 (w), 1200 (s), 1164 (s), 1021 (m), 906 (w), 796 (w), 730 (m), 694 (m) cm^{-1} HRMS calcd for $\text{C}_{16}\text{H}_{19}\text{ClO}_2^+[\text{M}]^+$ 278.1068, Found 278.1042.

Z,E-1 - (1-Menthyl)-2-chloro-5-ethyl-1,4-pentadiene-3-one (Entry 1, Table 2) : 52.1% in 3 steps ; ^1H NMR (500.13 MHz, CDCl_3), δ 7.79 (s, 1 H), 7.03 (dt, $J = 15.30, 6.50$ Hz, 1 H), 6.72 (dt, $J = 15.30, 1.65$ Hz, 1 H), 3.88 (dt, $J = 15.3, 4.5$ Hz, 1 H), 2.30 (double quintet, $J = 8.0, 1.6$ Hz, 2 H), 2.05 (m, 2 H), 1.72 (m, 2 H), 1.55 (m, 1 H), 1.45 (m, 1 H), 1.23 (q, $J = 12.1$ Hz, 1 H), 1.11 (t, 3 H), 1.05 (m, 1 H), 0.95 (dd, $J = 11.9, 6.5$ Hz, 6 H), 0.95 – 0.85 (m, 1 H), 0.82 (d, $J = 6.9$ Hz, 3 H) ; ^{13}C NMR (125.75 MHz, CDCl_3), δ 184.3, 155.4, 149.8, 123.4, 112.5, 86.6, 47.3, 41.7, 33.8, 31.5, 25.9, 25.7, 23.5, 21.9, 20.5, 16.4, 12.3; IR (neat) : 3051 (w), 2958 (s), 2929 (s), 2872 (m), 1658 (m), 1621 (s), 1585 (m), 1454 (w), 1343 (w), 1262 (s), 1245 (m), 1204 (m), 1176 (m), 1143 (m), 1094 (w), 980

(m), 845 (w), 739 (s), 702 (m) cm^{-1} HRMS calcd for $\text{C}_{17}\text{H}_{27}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 321.1591, Found 321.1595.

Z, E-1- (Cyclohexyl)-2-chloro-5-ethyl-1,4-pentadiene-3-one (Entry 2, Table 2) :
 58.6% in 3 steps ; ^1H NMR (300.13 MHz, CDCl_3), δ 7.78 (s, 1 H), 7.0 (dt, $J = 15.3$, 1.60 Hz, 1 H), 6.70 (dt, $J = 15.3$, 6.50 Hz, 1 H), 4.0 (m, 1 H), 2.26 (dq, $J = 7.40$, 1.60 Hz, 2 H), 1.96 – 1.90 (m, 2 H), 1.89 – 1.72 (m, 2 H), 1.70 – 1.50 (m, 3 H), 1.45 – 1.25 (m, 3 H), 1.09 (t, $J = 7.40$ Hz, 3 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 184.2, 154.9, 149.8, 123.3, 112.8, 84.1, 32.2, 25.7, 24.9, 23.3, 12.3; IR (neat) : 3051 (w), 2937 (s), 2855 (m), 1662 (m), 1454 (w), 1372 (m), 1266 (m), 1249 (m), 1209 (s), 1115 (w), 1037 (w), 1008 (m), 972 (w), 906 (w), 735 (s), 702 (w) cm^{-1} ; HRMS calcd for $\text{C}_{13}\text{H}_{19}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 265.0965, Found 265.0965.

Z,E-1 - (Adamantyl)-2-chloro-5-ethyl-1,4-pentadiene-3-one (Entry 3, Table 2):
 53.3% in 3 steps, mp : 174-176 $^{\circ}\text{C}$; ^1H NMR (300.13 MHz, CDCl_3), δ 8.03 (s, 1 H), 7.02 (dt, $J = 15.3$, 6.5 Hz, 1 H), 6.73 (dt, $J = 15.3$, 1.6 Hz, 1 H), 2.35 – 2.20 (m, 5 H), 1.95 (br. s, 6 H), 1.67 (br. s, 6 H), 1.10 (t, 3 H) ; ^{13}C NMR (75.5 MHz, CDCl_3), δ 184.6, 150.2, 149.7, 123.7, 112.9, 81.2, 41.9, 35.7, 30.7, 25.7, 12.4; IR (neat) : 3043 (w), 2996 (m), 2913 (s), 2851 (m), 1654 (m), 1597 (s), 1454 (w), 1356 (m), 1266 (s), 1200 (s), 1045 (m), 967 (w), 894 (w), 730 (s) cm^{-1} ; HRMS calcd for $\text{C}_{17}\text{H}_{23}\text{ClO}_2\text{Na}[\text{M}+\text{Na}]^+$ 317.1278, Found 317.1265.

Z,E-1 – (2-Phenylpropyl)-2-chloro-5-ethyl-1,4-pentadiene-3-one (Entry 4, Table 2): 52% in 3 steps, mp : 63-65 °C ; ^1H NMR (250.13 MHz, CDCl_3), δ 7.68 (s, 1 H), 7.30-7.10 (m, 5 H), 7.05 (dt, $J = 15.3, 6.4$ Hz, 1 H), 7.63 (dt, $J = 15.3, 1.6$ Hz, 1 H), 4.14 (t, $J = 6.40$ Hz, 2 H), 2.76 (t, $J = 7.25$ Hz, 2 H), 2.28 (dq, $J = 7.40, 1.50$ Hz, 2 H), 2.09 (q, $J = 6.40, 2$ H), 1.10 (t, 7.40 Hz, 3H) ; ^{13}C NMR (62.9 MHz, CDCl_3), δ 184.1, 156.0, 150.1, 140.4, 128.5, 128.4, 126.2, 123.2, 113.0, 74.7, 31.3, 31.0, 25.7, 12.3 ; IR (neat) : 3047 (w), 2962 (s), 2876 (m), 1658 (m), 1621 (s), 1491 (w), 1450 (m), 1384 (m), 1262 (s), 1200 (s), 1164 (s), 1008 (m), 902 (w), 739 (s), 698 (s) cm^{-1} ; HRMS calcd for $\text{C}_{16}\text{H}_{19}\text{ClO}_2^+[\text{M}]^+$ 278.1068, Found 278.1042.

Z,E-1 – (Methoxy)-2-chloro-5-cyclohexyl-1,4-pentadiene-3-one (Entry 5-trans, Table 2) : 44.7% in 3 steps ; ^1H NMR (250.13 MHz, CDCl_3), δ 7.62 (s, 1 H), 6.93 (dd, $J = 15.40, 6.83$ Hz, 1 H), 6.63 (dd, $J = 15.40, 1.31$ Hz, 1 H), 3.99 (s, 3 H), 2.15 (m, 1 H), 1.75 (m, 5 H), 1.19 (m, 5 H), ; ^{13}C NMR (62.9 MHz, CDCl_3), δ 184.3, 156.8, 153.9, 121.5, 113.0, 62.5, 40.8, 31.7, 25.8, 25.6; IR (neat) : 3051 (w), 2929 (s), 2851 (m), 1666(m), 1621 (s), 1446 (m), 1266 (s), 1139 (m), 1029 (w), 735 (s) cm^{-1} ; HRMS calcd for $\text{C}_{12}\text{H}_{17}\text{ClO}_2^+[\text{M}]^+$ 228.0911, Found 228.0935.

Z,Z-1 – (Methoxy)-2-chloro-5-cyclohexyl-1,4-pentadiene-3-one (Entry 5-cis, Table 2) :

After isolation, 8.6% in 3 steps ; ^1H NMR (250.13 MHz, CDCl_3), δ 7.60 (s, 1 H), 6.35 (dd, $J = 11.60, 8.10$ Hz, 1 H), 5.98 (dd, $J = 11.60, 9.86$ Hz, 1 H), 3.99 (s, 3 H), 3.00 (m, 1 H), 1.69 (m, 4 H), 1.25 (m, 6 H), ; ^{13}C NMR (62.9 MHz, CDCl_3), δ 185.3, 157.4, 153.7, 121.1, 114.1, 62.5, 37.9, 32.3, 25.8, 25.3; IR (neat) : 3035 (w), 2925 (s), 2847 (m), 1756 (w), 1650(m), 1621 (s), 1446 (m), 1372 (m), 1258 (m), 1225 (s), 1139 (s), 992 (w), 910 (w), 796 (m) cm^{-1} ; HRMS calcd for $\text{C}_{12}\text{H}_{17}\text{ClO}_2^+[\text{M}]^+$ 228.0911, Found 228.0935.

References

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S 16

cis-1-Methylvinyl-adamantylether

7.27408
6.31935
6.31379
6.30813
6.30241
6.29858
6.29290
6.28725
6.28167

4.50819
4.48586
4.46414
4.44205
4.41977

2.17953
1.83118
1.82145
1.69545
1.65117
1.64754
1.64456
1.61730
1.61162
1.59479
1.58912

0.01163

1.0000

0.9929

3.0638

6.2908

5.8343

3.6369

Current Data Parameters
NAME dr-IV-068-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040519

Time 11.06

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SMH 6172.839 Hz

FIDRES 0.168360 Hz

AQ 2.6542580 sec

RG 101.6

DM 81.000 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 7.05 usec

PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768

SF 300.1300022 MHz

MDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 8.00 cm

F1P 10.422 ppm

F1 3127.95 Hz

F2P -0.398 ppm

F2 -119.45 Hz

PPMCM 0.54100 ppm/cm

HZCM 162.37012 Hz/cm

ppm

S 17

cis-1-Methylvinyl-adamantylether

138.114

102.311

77.420

76.997

76.573

74.563

41.839

36.230

30.554

9.297

ppm

Current Data Parameters
NAME dr-IV-069-a1
EXRNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040519

Time 11.11

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 133

DS 4

SWH 18832.393 HZ

FIDRES 0.287360 HZ

AQ 1.7400308 sec

RG 22528

DM 26.550 usec

DE 6.00 usec

TE 297.1 K

D1 1.29999995 sec

d11 0.03000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 5.00 dB
SF01 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677520 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 11.00 cm
FIP 184.611 ppm
F1 13932.17 HZ
F2P -4.790 ppm
F2 -361.48 HZ
PPMCH 9.47004 ppm/cm
HZCM 714.68237 HZ/cm

Current Data Parameters
NAME dr-V-049-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041203
Time 14.17
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 128
DE 96.000 use
TE 137.14 use
D1 300.0 K
D1 1.00000000 sec
P1 8.70 use
SF01 250.1315321 MHz
NUCLEUS 1H

1-(3-phenyl-1-propyl)-1-butyne

S 18

ppm

7.39631
7.39092
7.38436
7.37197
7.36703
7.36118
7.35661
7.34968
7.33402
7.28844
7.27537
7.27302
7.26283
7.25121
7.24521

4.05366
4.02850
4.00329
2.81483
2.78572
2.75374
2.25591
2.22581
2.19614
2.16641
2.14839
2.12341
2.11724
2.09820
2.09189
2.08834
2.07296
2.06619
2.06256
2.03699
1.21239
1.18267
1.15269

Integral

2.0116
3.0367

2.0000

2.0614

2.0500
2.0762

2.9779

F2 - Processing parameters
SI 16384
SF 250.130049 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.50
1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.328 ppm
F1 2583.28 Hz
F2P -0.450 ppm
F2 -112.51 Hz
PPMCM 0.53888 ppm
HZCM 134.78973 Hz/

ppm

8

6

4

2

0

Current Data Parameters
 NAME dr-V-049-a1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041203
 Time 14.21

INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 172
 DS 4

SMH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DW 29.000 use
 DE 41.43 use
 TE 300.0 K

D12 0.00002000 sec
 DL5 23.00 dB
 CPDPRG waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 6.00 use

SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters

SI 32768
 SF 62.8952471 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 12.00 cm
 F1P 212.739 ppm
 F1 13380.26 Hz
 F2P -8.341 ppm
 F2 -524.59 Hz
 PPMCM 11.05398 ppm
 HZCM 695.24268 Hz/

ppm

1-(3-phenyl-1-propyl)-1-butyne

S 19

ppm 200 150 100 50 0

140.919

128.415

128.400

125.995

88.988

77.533

77.003

76.516

38.641

31.427

30.337

15.050

10.902

ppm

S 20

(E)-1-(3-phenyl-1-propyl)-1-butene

7.37209
7.34422
7.33488
7.32171
7.26745
7.25484
7.24597
7.22473
6.33024
6.28826

4.91784
4.89444
4.87261
4.85256
4.82912

3.72357
3.70255
3.68145

2.80134
2.77655
2.75004
2.05996
2.03889
2.03340
2.00918

1.99006
1.98686
1.98243
1.96877
1.95719
1.94786
1.92576
1.06713
1.04253
1.01771
0.07925

1.99006
1.98686
1.98243
1.96877
1.95719
1.94786
1.92576
1.06713
1.04253
1.01771
0.07925

Current Data Parameters
NAME dr-V-052-a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041207
Time 12.38
INSTRUM drvx300
PROBHD 5 mm Multinucl
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 45.3
DM 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.05 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.30

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 10.314 ppm
F1 3095.54 Hz
F2P -0.386 ppm
F2 -115.86 Hz
PPMCM 0.53500 ppm/cm
HZCM 160.56992 Hz/cm

Integral

2.2466
3.5429

0.9850

1.0000

2.3872

2.3420

4.4204

3.3216

ppm

8

6

4

2

0

S 21

(E)-1-(3-phenyl-1-propyl)-1-butene

145.509	
141.626	
128.419	
128.309	
125.800	
106.069	
77.423	
76.999	
76.574	
68.053	
32.116	
30.911	
21.088	
15.315

Current Data Parameters
NAME dr-V-052-a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041207
Time 12.42

INSTRUM drx300
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80

DS 4
SMH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400008 sec
RG 22528
DN 26.550 usec
DE 6.00 usec
TE 297.1 K
D1 1.29999995 sec
D11 0.03000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 5.00 dB
SF01 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 188.227 ppm
F1 14205.04 Hz
F2P -5.740 ppm
F2 -433.17 Hz
PPMCM 9.659832 ppm/cm
HZCM 731.91034 Hz/cm

Current Data Parameters
NAME dr--V-053-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041209
Time 12.43
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 256
DW 96.000 use
DE 137.14 use
TE 300.0 K
D1 1.00000000 sec
P1 8.70 use
SF01 250.1315321 MHz
NUCLEUS 1H

F2 - Processing parameters

SI 16384
SF 250.1300049 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.50

1D NMR plot parameters

CX 20.00 cm
CY 9.00 cm
F1P 10.443 ppm
F1 2612.22 Hz
F2P -0.353 ppm
F2 -88.40 Hz
PPMCM 0.53964 ppm
HZCM 135.03087 Hz/

ppm

7.37240
7.36609
7.35562
7.33930
7.32958
7.31500
7.26569
7.25137
7.23925
7.21955
5.96452
5.95913
5.95333
5.93987
5.93419
5.92869
4.46750
4.43905
4.41358
4.38505
3.79662
3.77112
3.74567
3.69864
3.47359
2.80231
2.77310
2.74113
2.22481
2.21940
2.19511
2.18973
2.16548
2.15977
2.04805
2.02259
2.01660
2.00458
1.99737
1.99061
1.98802
1.97145
1.96171
1.08118
1.06663
1.05106
1.03721
1.02087
1.00759
0.99805

(Z)-1-(3-phenyl-1-propyl)-1-butene

S 22

Integral

2.5996
3.9553

0.1004
1.0336

0.0794
1.0000

2.1909
0.2891
0.3401

2.6757

2.1448
2.9733

4.0412

ppm

8

6

4

2

0

Current Data Parameters
 NAME gr-v-053-a1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20041209
 Time 12.49
 INSTRUM arx250
 PROBHD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 49
 DS 4
 SWH 17241.379 Hz
 FIDRES 0.467702 Hz
 AQ 1.0691060 sec
 RG 22800
 DW 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.00002000 sec
 DL5 23.00 dB
 CPDPRG waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 6.00 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters

SI 32768
 SF 62.8952440 MHz
 WDM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 9.00 cm
 F1P 170.907 ppm
 F1 10749.24 Hz
 F2P -11.084 ppm
 F2 -697.12 Hz
 PPMCM 9.09954 ppm
 HZCM 572.31805 Hz

(Z)-1-(3-phenyl-1-propyl)-1-butene

S 23

Current Data Parameters
 NAME dr-III-136-a2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20040226
 Time 14.57
 INSTRUM apx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1430
 DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

F2 - Processing parameters

SI 16384
 SF 250.130049 MHz
 WDM EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters

CX 20.00 cm
 CY 30.00 cm
 F1P 10.328 ppm
 F1 2583.28 Hz
 F2P -0.392 ppm
 F2 -98.04 Hz
 PPMCM 0.53599 ppm
 HZCM 134.06638 Hz/

S 24
 Entry 1, Table 1

ppm

S 25

Entry 1, Table 1

186.052

151.731
149.221

123.113

113.958

81.777
77.337
76.915
76.491

28.180

23.014

13.516

Current Data Parameters
NAME dr-III-136-a2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040226

Time 16.08

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 473

DS 4

SWH 18832.393 Hz

FIDRES 0.287360 Hz

AQ 1.7400308 sec

RG 22528

DM 26.550 usec

DE 6.00 usec

TE 297.1 K

D1 1.2999995 sec

d11 0.0300000 sec

D31 0.0000000 sec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 8.50 usec
PL1 5.00 dB
SF01 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 wa1tc216
NUC2 ¹H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SF02 300.1312005 MHz

F2 - Processing parameters

SI 32768

SF 75.4677571 MHz

MDM EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 11.00 cm

F1P 224.287 ppm

F1 16926.42 Hz

F2P -6.962 ppm

F2 -525.40 Hz

PPMCM 11.56244 ppm/cm

HZCM 872.59113 Hz/cm

F2 - Acquisition Parameters

Date_ 20040309

Time 13.33

INSTRUM arx250

PROBHD 5 mm QNP 1H

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SMH 5208.333 Hz

FIDRES 0.158946 Hz

AQ 3.1457779 sec

RG 715

DW 96.000 use

DE 137.14 use

TE 300.0 K

D1 1.0000000 sec

P1 8.70 use

SF01 250.1315321 MHz

NUCLEUS 1H

F2 - Processing parameters

SI 16384

SF 250.1300049 MHz

WDW EM

SSB 0

LB 0.20 Hz

GB 0

PC 1.50

10 NMR plot parameters

CX 20.00 cm

CY 30.00 cm

F1P 10.675 ppm

F1 2670.09 Hz

F2P -0.373 ppm

F2 -93.22 Hz

PPMCM 0.55237 ppm

HZCM 138.16553 Hz/

ppm

S 26

Entry 2, Table 1

Current Data Parameters
NAME dr-IV-006-a1
EXPNO 2
PROCNO 1

ppm

Entry 2, Table 1

F2 - Acquisition Parameters
Date_ 20040309

Time 13.38
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 36864
SOLVENT CDCl3
NS 894
DS 4

SMH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
OW 29.000 use
DE 41.43 use
TE 300.0 K

D12 0.00002000 sec
DL5 23.00 dB
CPDPRG waltz16
P31 103.00 use
D1 1.00000000 sec
P1 5.35 use

SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters
SI 32768
SF 62.8952413 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 225.522 ppm
F1 14184.26 Hz
F2P -3.934 ppm
F2 -247.41 Hz
PPKCM 11.47279 ppm
HZCM 721.56362 Hz/

ppm

7.8757

6.5104

6.5049

6.4717

6.4662

6.4607

6.1998

6.1749

6.1501

6.1363

Entry 3, Table 1

2.5299

2.5259

2.5061

2.5012

1.4330

1.4113

1.3987

1.3943

1.3857

1.3750

1.3713

1.3505

1.3245

1.2981

0.9172

0.8938

0.8775

0.8699

0.0053

F2 - Acquisition Parameters

Date_ 20040308

Time 14.27

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 6172.839 Hz

FIDRES 0.168380 Hz

AQ 2.6542580 sec

RG 114

DW 81.000 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 ¹H

P1 7.05 usec

PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768

SF 300.1300022 MHz

MDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 20.00 cm

F1P 10.441 ppm

F1 3133.58 Hz

F2P -0.295 ppm

F2 -88.69 Hz

PPMCM 0.53681 ppm/cm

HZCM 161.11330 Hz/cm

S 28

Integral

1.000

1.033

1.085

2.107

11.459

4.242

3.646

ppm

8

6

4

2

0

ppm

S 29

Entry 3, Table 1

Current Data Parameters
NAME dr-IV-001-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040308
Time 14.32

INSTRUM drx300

PROBHD 5 mm Multinucl

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 202

DS 4

SWH 18832.393 Hz

FIDRES 0.287360 Hz

AQ 1.7400308 sec

RG 22528

DM 26.550 usec

DE 6.00 usec

TE 297.1 K

D1 1.29999955 sec

d11 0.03000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 5.00 dB

SFO1 75.4760107 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 100.00 usec

PL2 120.00 dB

PL12 25.60 dB

SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768

SF 75.4677514 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 7.00 cm

F1P 224.547 ppm

F1 16946.09 Hz

F2P -3.907 ppm

F2 -294.83 Hz

PPMCM 11.42271 ppm/cm

HZCM 862.04614 Hz/cm

ppm

S 30

Integral

ppm

7.8676

7.2601

6.4910

6.4678

6.1769

6.1620

6.1537

6.1470

6.1387

6.1238

Entry 4, Table 1

2.5259

2.5229

2.5109

2.5085

2.4959

2.4936

2.4811

1.4364

1.4268

1.4073

1.3923

1.2933

1.2816

1.2784

1.2694

1.2666

1.2566

1.2477

0.8757

0.8620

0.8480

1.000

1.026

1.060

2.150

12.338

9.778

3.395

Current Data Parameters

NAME dr-III-113a1

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20040113

Time 14.35

INSTRUM DRX500

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 57344

SOLVENT CDCl3

NS 16

DS 2

SWH 10330.578 Hz

FIDRES 0.180151 Hz

AQ 2.7754996 sec

RG 90.5

DW 48.400 usec

DE 6.00 usec

TE 296.7 K

D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 13.25 usec

PL1 -3.00 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SF 500.1300131 MHz

SI 32768

WDW EM

SSB 0

LB 0.20 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 55.00 cm

F1P 10.325 ppm

F1 5163.76 Hz

F2P -0.427 ppm

F2 -213.39 Hz

PPMCM 0.53757 ppm/cr

HZCM 268.85733 Hz/cm

ppm

S 31

186.119

151.762

148.171

123.578

114.044

81.833

77.255

77.000

76.748

31.760

29.707

29.281

29.170

29.073

28.256

22.594

14.060

-0.036

Entry 4, Table 1

Current Data Parameters
NAME dr-II-113a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040113
Time 14.44

INSTRUM DRX500

PROBHD 5 mm Multinuc]

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 247

DS 4

SMH 39681.812 Hz

FIDRES 0.605495 Hz

AQ 0.8258188 sec

RG 16384

DW 12.600 usec

DE 6.00 usec

TE 298.0 K

D1 2.00000000 sec

d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C

P1 8.10 usec

PL1 3.00 dB

SFO1 125.7713108 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 88.00 usec

PL2 0.00 dB

PL12 21.00 dB

SFO2 500.1320005 MHz

F2 - Processing parameters

SI 32768

SF 125.7577935 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 10.00 cm

F1P 226.123 ppm

F1 28436.77 Hz

F2P -5.294 ppm

F2 -665.80 Hz

PPMCM 11.57088 ppm/cm

HZCM 1455.12891 Hz/cm

S 32

7.86188
7.29321
7.29008
7.28627
7.27371
7.26644
7.23149
7.21493
7.20885
7.19108
6.56462
6.52603
6.22003
6.18122

Entry 5, Table 1

2.90970
2.90514
2.88500
2.88091
2.87624
2.85890
2.80948
2.78665

1.59007
1.44479
1.42223

0.01580

Integral

ppm

8

6

4

2

0

0.9517

6.1296

1.0000

1.0337

2.0842

2.1598

9.2862

Current Data Parameters
NAME dr-IV-008-a2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041129

Time 14.22

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 6172.839 Hz

FIDRES 0.188380 Hz

AQ 2.6542580 sec

RG 362

DW 81.000 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 ¹H

P1 7.05 usec

PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768

SF 300.1300022 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 16.00 cm

F1P 10.423 ppm

F1 3128.15 Hz

F2P -0.259 ppm

F2 -77.82 Hz

PPMCM 0.53410 ppm/cm

HZCM 160.29822 Hz/cm

ppm

S 33

Entry 5, Table 1

Current Data Parameters
NAME dr-IV-009-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040310
Time 12.37

INSTRUM drx300
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 401
DS 4

SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 22528
DM 26.550 usec
DE 5.00 usec

TE 297.1 K
D1 1.29959995 sec
d11 0.03000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 5.00 dB
SFO1 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677514 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.50

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 234.138 ppm
F1 17669.89 Hz
F2P -15.406 ppm
F2 -1162.69 Hz
PPMCM 12.47723 ppm/cm
HZCM 941.62878 Hz/cm

Current Data Parameters
NAME dr-IV-038-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040415
Time 15.42

INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zg30

TD 32768
SOLVENT CDCl3

NS 16
DS 2

SWH 5208.333 Hz
FIDRES 0.158946 Hz

AQ 3.1457779 sec
RG 512

DW 96.000 use
DE 137.14 use

TE 300.0 K
D1 1.00000000 sec

P1 8.70 use
SF01 250.1315321 MHz

NUCLEUS 1H

F2 - Processing parameters
SI 16384

SF 250.1300033 MHz
WDW EM

SSB 0
LB 0.20 Hz

GB 0
PC 1.50

1D NMR plot parameters
CX 20.00 cm

CY 6.00 cm
F1P 10.537 ppm

F1 2635.51 Hz
F2P -0.575 ppm

F2 -143.94 Hz
PPMCM 0.55560 ppm

HZCM 138.97235 Hz/

S 34

Entry 6, Table 1

F2 - Acquisition Parameters

Date_ 20040415
Time 15.47
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zgdc30
TD 36864
SOLVENT CDCl3
NS 825
DS 4
SWH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
DW 29.000 use
DE 41.43 use
TE 300.0 K
D12 0.00002000 sec
DL5 23.00 dB
CPDPRG waltz16
P31 103.00 use
D1 1.00000000 sec
P1 5.35 use
SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 62.8952424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 9.00 cm
F1P 227.712 ppm
F1 14321.97 Hz
F2P -4.507 ppm
F2 -283.46 Hz
PPMCM 11.61092 ppm
HZCM 730.27185 Hz/

S 35

Entry 6, Table 1

ppm

S 36

Entry 7, Table 1

7.97976
7.31351
7.29272
7.28939
7.28565
7.27375
7.26587
7.23095
7.22250
7.21794
7.21438
7.20858
7.19849
7.19044
6.55635
6.55096
6.51765
6.51242
6.50748
6.20992
6.17129
2.90686
2.90186
2.89700
2.89300
2.87733
2.87277
2.85566
2.85115
2.84660
2.80668
2.78448
2.27796
1.95199
1.94260
1.74429
1.70234
1.69219
1.67949
1.63790
1.58922
1.44687
0.01524

Integral

0.9576

2.4688

2.9994

0.9994

1.0000

2.0358

2.1055

3.1041

6.3427

6.5086

8

6

4

2

0

Current Data Parameters
NAME gr-IV-061-a2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040730
Time 15.44
INSTRUM drx300
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.188360 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 7.05 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
SF 300.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.30

1D NMR plot parameters

CX 20.00 cm
CY 8.00 cm
F1P 10.380 ppm
F1 3115.31 Hz
F2P -0.414 ppm
F2 -124.33 Hz
PPMCM 0.53971 ppm/cm
HZCM 161.98232 Hz/cm

ppm

S 37

185.796

150.889

146.644

141.192

128.457

128.322

125.937

124.154

113.960

81.256

77.420

77.197

76.997

76.574

41.960

35.690

35.129

31.071

30.767

Entry 7, Table 1

ppm 200 175 150 125 100 75 50 25 0

Current Data Parameters
 NAME dr-IV-061-a2
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20040730
 Time 15.50

INSTRUM drx300
 PROBD 5 mm Multinuc1

PULPROG zgpgc30
 TD 65536

SOLVENT CDCl3
 NS 613

DS 4
 SMH 18932.393 Hz

FIDRES 0.287360 Hz
 AQ 1.7400308 sec

RG 22528
 DM 26.550 usec

DE 6.00 usec
 TE 297.1 K

D1 1.29999995 sec
 d11 0.03000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====
 NUC1 13C

P1 8.50 usec
 PL1 5.00 dB

SFO1 75.4760107 MHz

===== CHANNEL f2 =====
 CPOPRG2 waltz16

NUC2 1H
 PCPR2 100.00 usec

PL2 120.00 dB
 PL12 25.60 dB

SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768

SF 75.4677514 MHz
 MDM EM

SSB 0
 LB 1.00 Hz

GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm

CY 12.00 cm
 F1P 214.524 ppm

F1 16189.63 Hz
 F2P -6.038 ppm

F2 -455.67 Hz
 PPMQM 11.02809 ppm/cm
 HZCM 832.26483 Hz/cm

ppm

8.00482

7.28653

6.52773

6.52431

6.50456

6.50119

6.28497

6.27615

6.27055

6.26180

6.25618

6.24739

2.27428

2.06455

2.06110

2.05013

2.04669

1.95269

1.94794

1.72836

1.70217

1.67239

1.64778

0.00668

Entry 8, Table 1

S 38

Integral

ppm

0.9972

1.0000

1.0187

3.3352

3.1052

6.7377

7.6484

Current Data Parameters

NAME dr-IV-093-a1

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20040614

Time 11.23

INSTRUM DRX500

PROBHD 5 mm Multinucl

PULPROG zg30

TD 57344

SOLVENT CDCl3

NS 16

DS 2

SWH 10330.578 Hz

FIDRES 0.180151 Hz

AQ 2.7754996 sec

RG 64

DW 48.400 usec

DE 6.00 usec

TE 296.7 K

D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 ¹H

P1 13.25 usec

PL1 -3.00 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SI 32768

SF 500.1300000 MHz

WDW EM

SSB 0

LB 0.20 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 8.00 cm

F1P 10.472 ppm

F1 5237.42 Hz

F2P -0.368 ppm

F2 -184.16 Hz

PPMCM 0.54202 ppm/cr

HZCM 271.07913 Hz/cm

S 39

Entry 8, Table 1

186.073
151.004
142.003
124.692
113.950
81.177
77.250
76.996
76.741
41.910
35.640
30.720
15.866

Current Data Parameters
NAME dr-IV-093-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040614
Time 11.28
INSTRUM DRX500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 114
DS 4
SWH 39681.812 Hz
FIDRES 0.605496 Hz
AQ 0.8258188 sec
RG 16384
DM 12.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 8.10 usec
PL1 3.00 dB
SF01 125.7713108 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 0.00 dB
PL12 21.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577983 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 8.00 cm
F1P 226.660 ppm
F1 26506.78 Hz
F2P -8.471 ppm
F2 -1065.26 Hz
PPMCM 11.75754 ppm/cm
HZCM 1478.60181 Hz/cm

ppm

S 41

Entry 9, Table 1

7.75331
7.74888
7.28686
6.52889
6.52544
6.52189
6.51856
6.50577
6.50224
6.49881
6.49543
6.30776
6.29338
6.28463
6.27896
6.27019
6.26460
6.25572
3.89055
3.88151
3.86873
3.85983
3.84701
3.83804
2.07756
2.07390
2.06310
2.05949
2.05487
1.72698
1.72083
1.67135
1.25948
1.23657
0.97420
0.96111
0.95616
0.95037
0.93635
0.82711
0.81317
0.01380

Integral

0.9954

1.0000

1.0004

1.1009

4.4160

0.8805

2.3187

1.1137

1.1812

1.2901

1.2836

7.7728

0.9815

3.5283

ppm

8

6

4

2

0

Current Data Parameters

NAME dr-1V-096-a2

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20040729

Time 15.46

INSTRUM DRX500

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 57344

SOLVENT CDCl3

NS 16

DS 2

SWH 10330.578 Hz

FIDRES 0.180151 Hz

AQ 2.7754996 sec

RG 64

DW 48.400 usec

DE 6.00 usec

TE 296.7 K

D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 13.25 usec

PL1 -3.00 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SI 32768

SF 500.1300000 MHz

WDW EM

SSB 0

LB 0.20 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 7.00 cm

F1P 10.426 ppm

F1 5214.22 Hz

F2P -0.339 ppm

F2 -169.60 Hz

PPMCM 0.53824 ppm/cr

HZCM 269.19104 Hz/cm

Current Data Parameters
NAME dr-IV-096-a2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040729
Time 15.52
INSTRUM DRX500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 122
DS 4
SWH 39681.812 Hz
FIDRES 0.605496 Hz
AQ 0.8258188 sec
RG 16384
DM 12.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 8.10 usec
PL1 3.00 dB
SF01 125.7713108 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 0.00 dB
PL12 21.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577947 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 8.00 cm
F1p 204.684 ppm
F1 25740.60 Hz
F2p -3.764 ppm
F2 -473.39 Hz
PPMCM 10.42241 ppm/cm
HZCM 1310.69958 Hz/cm

Entry 9, Table 1

S 42

ppm

S 43

Entry 10, Table 1

7.75053
7.26756
6.51127
6.50788
6.50435
6.50099
6.48819
6.48471
6.48126
6.47786
6.28786
6.27343
6.26468
6.25899
6.25030
6.24460
6.23593
4.01211
3.99966
3.98938
3.97905
3.96662
2.05815
2.05469
2.04371
2.04031
1.33268
1.32301
1.31871
1.11872
1.11037
0.90633
0.89324
0.87169
0.86719
0.85845
0.85399
0.84215
0.65131
0.00003

0.999

1.000

0.999

1.106

3.107

2.447

2.405

3.567

5.385

10.087

7.885

4.548

4.221

10.966

4.566

ppm

Integral

8

6

4

2

0

Current Data Parameters
NAME dr-IV-088-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040608
Time 15.37

INSTRUM DRX500

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 57344

SOLVENT CDCl3

NS 16

DS 2

SWH 10330.578 HZ

FIDRES 0.180151 HZ

AQ 2.7754996 sec

RG 64

DW 48.400 usec

DE 6.00 usec

TE 296.7 K

D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 13.25 usec

PL1 -3.00 dB

SFO1 500.1330885 MHz

F2 - Processing parameters

SI 32768

SF 500.1300096 MHz

WDW EM

SSB 0

LB 0.20 HZ

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 10.00 cm

F1P 10.324 ppm

F1 5163.29 HZ

F2P -0.390 ppm

F2 -195.19 HZ

PPMCM 0.53571 ppm/cr

HZCM 267.92398 HZ/cm

S 44

185.860

155.676

142.382

124.493

113.609

85.492

77.253

77.000

76.746

56.373

56.253

44.702

42.548

39.475

36.132

35.747

35.407

34.950

28.198

27.976

24.163

23.805

22.789

22.534

21.225

18.638

15.930

12.252

12.030

Entry 10, Table 1

ppm

Current Data Parameters
NAME dr-IV-088-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040608
Time 15.44
INSTRUM DRX500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 146
DS 4
SWH 39681.812 Hz
FIDRES 0.605496 Hz
AQ 0.8258188 sec
RG 16384
DM 12.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.10 usec
PL1 3.00 dB
SF01 125.7713108 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00 usec
PL2 0.00 dB
PL12 21.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577947 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 226.116 ppm
F1 28435.88 Hz
F2P -5.881 ppm
F2 -739.63 Hz
PPMCH 11.55988 ppm/cm
HZCM 1458.77527 Hz/cm

ppm

S 45

7.70467
7.27437
6.53324
6.52756
6.49467
6.48896
6.29346
6.26954
6.25492
6.24567
6.23098

4.32427
4.24346

2.07731
2.07168
2.05338
2.04779
1.62062
1.56956
1.35639
1.33111
1.13081
1.10286
0.91927
0.89763
0.88410
0.88015
0.86212
0.85820
0.81331
0.65879

Entry 11, Table 1

Integral

0.9870

1.0000

1.0074

1.0538

3.0222

1.2993

2.9654

2.1851

8.4765

5.8011

6.6583

9.7275

4.2485

7.3990

3.8428

1.1907

3.7500

ppm

8

6

4

2

0

Current Data Parameters

NAME dr-IV-104-a1

EXPNO 1

PROCNO 1

F2 - Acquisition Parameters

Date_ 20040706

Time 17.43

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SWH 6172.839 Hz

FIDRES 0.188380 Hz

AQ 2.6542580 sec

RG 114

DW 81.000 usec

DE 6.00 usec

TE 300.0 K

D1 1.00000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 7.05 usec

PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768

SF 300.1300022 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 9.00 cm

F1P 10.403 ppm

F1 3122.40 Hz

F2P -0.416 ppm

F2 -125.00 Hz

PPMCM 0.54100 ppm/cm

HZCM 162.37012 Hz/cm

ppm

S 46

185.933

155.728

142.302

124.545

114.122

Entry 11, Table 1

- 81.847
- 77.425
- 77.001
- 76.578
- 56.335
- 56.222
- 53.916
- 42.547
- 39.491
- 39.289
- 36.142
- 35.801
- 35.687
- 35.416
- 28.284
- 28.216
- 27.985
- 23.836
- 22.799
- 22.541
- 20.771
- 18.638
- 15.937
- 12.047
- 11.383

Current Data Parameters
NAME dr-1V-104-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040706
Time 17.52

INSTRUM drx300
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 164
DS 4
SWH 18832.393 HZ
FIDRES 0.287360 HZ
AQ 1.7400308 sec
RG 22528
DM 26.550 usec
DE 6.00 usec
TE 297.1 K
D1 1.29999955 sec
d11 0.03000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 5.00 dB
SFO1 75.4760107 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677508 MHz
WDW EM
SSB 0
LB 1.00 HZ
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 11.00 cm
F1P 205.945 ppm
F1 15542.20 HZ
F2P -4.326 ppm
F2 -326.46 HZ
PPHQM 10.51354 ppm/cm
HZCM 793.43304 HZ/cm

ppm

7.63288
7.33834
7.32174
7.31585
7.29560
7.29103
7.27372
7.24694
7.24247
7.22294
7.21720
7.21233
7.20382
7.19002
6.46044
6.42739
6.42190
6.41645
6.18062
6.15599
6.14211
5.86545
4.16350
4.14202
4.12057
2.79743
2.77311
2.74762
2.56963
2.56416
2.54465
2.53919
2.51971
2.51425
2.14379
2.12228
2.10061
2.09625
2.07301
2.05102
1.08619
1.06112
1.03599
0.01708

Entry 12, Table 1

Integral

0.9728
2.1211
3.1932

1.0000
1.0271

2.1142

2.1927
2.0592

2.2193

3.0635

Current Data Parameters
NAME dr-V-059-aat
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041214
Time 19.44

INSTRUM drx300
PROBHD 5 mm Multinuc1

PULPROG zg30
TD 32768

SOLVENT CDCl3
NS 16

DS 2
SWH 6172.839 Hz

FIDRES 0.188380 Hz
AQ 2.6542580 sec

RG 143.7
DM 81.000 usec

DE 6.00 usec
TE 300.0 K

D1 1.00000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 7.05 usec

PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
SF 300.130022 MHz

WDW EM
SSB 0

LB 0.30 Hz
GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm
CY 6.00 cm

F1P 10.289 ppm
F1 3087.95 Hz

F2P -0.323 ppm
F2 -96.97 Hz

PPMCM 0.53059 ppm/cm
HZCM 159.24614 Hz/cm

S 47

ppm

8

6

4

2

0

S 48

185.574
156.572
149.813
140.376
128.511
128.410
126.184
122.760
113.997

77.423
76.999
76.575
74.731

31.355
31.011
23.104
13.533

Entry 12, Table 1

Current Data Parameters
NAME dr-v-059-aat
EXFNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041214
Time 19.51

INSTRUM dr-x300

PROBHD 5 mm Multinucl

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 139

DS 4

SMH 18832.393 HZ

FIDRES 0.287360 HZ

AQ 1.7400308 sec

RG 22528

DM 26.550 usec

DE 6.00 usec

TE 297.1 K

D1 1.29999995 sec

d11 0.03000000 sec

Q31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 13C

P1 8.50 usec

PL1 5.00 dB

SFO1 75.4760107 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 100.00 usec

PL2 120.00 dB

PL12 25.60 dB

SFO2 300.1312005 MHz

F2 - Processing Parameters

SI 32768

SF 75.4677542 MHz

MDM EM

SSB 0

LB 1.00 HZ

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CV 7.00 cm

F1P 207.628 ppm

F1 15669.20 HZ

F2P -4.527 ppm

F2 -341.68 HZ

PPMCM 10.60776 ppm/cm

HZCM 800.54362 HZ/cm

ppm

7.79890
7.28673
7.06292
7.04992
7.03700
7.03240
7.01943
7.00643
6.73842
6.73520
6.73197
6.70796
6.70469
6.70139

3.90431
3.89534
3.88253
3.87364
3.86083
3.85186

2.30841
2.30522
2.29529
2.29338
2.29060
2.28056
2.27741

1.25177
1.12675
1.11185
1.09705
0.97007
0.95702
0.95140
0.94629
0.93223
0.82499
0.81107
0.01055

Entry 1, Table 2

S 49

Current Data Parameters
NAME dr-IV-120-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040728
Time 10.14
INSTRUM DRX500
PROBHD 5 mm Multinuc1
PULPROG zg30
TD 57344
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.180151 Hz
AQ 2.7754996 sec
RG 64
DM 48.400 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec

===== CHANNEL f1 =====

NUC1 1H
P1 13.25 usec
PL1 -3.00 dB
SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 8.00 cm
F1P 10.485 ppm
F1 5244.02 Hz
F2P -0.399 ppm
F2 -199.40 Hz
PPMCM 0.54420 ppm/cm
HZCM 272.17102 Hz/cm

F2 - Acquisition Parameters

Date_ 20040728
Time 10.20
INSTRUM DRX500
PROBHD 5 mm Multinuc1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 109
DS 4
SMH 39561.812 Hz
FIDRES 0.605496 Hz
AQ 0.8258188 sec
RG 16384
DW 12.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec

===== CHANNEL f1 =====

NUC1 13C
P1 8.10 usec
PL1 3.00 dB
SF01 125.7713108 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 98.00 usec
PL2 0.00 dB
PL12 21.00 dB
SF02 500.1320005 MHz

F2 - Processing parameters

SI 32768
SF 125.7577959 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters

CX 20.00 cm
CY 8.00 cm
F1P 225.493 ppm
F1 28357.46 Hz
F2P -6.916 ppm
F2 -869.73 Hz
PPMCM 11.62042 ppm/cm
HZCM 1461.35901 Hz/cm

ppm

Entry 1, Table 2

S 50

ppm

S 51

7.7873
7.2740
7.0604
7.0389
7.0174
7.0096
6.9881
6.9666
6.7215
6.7163
6.7109
6.6707
6.6654
6.6600

Entry 2, Table 2

4.1059
4.0888
4.0757
4.0626
4.0455
2.2964
2.2913
2.2702
2.2668
2.2501
2.2450
1.9320
1.9215
1.7931
1.6211
1.5890
1.5784
1.5590
1.3761
1.3338
1.3078
1.1156
1.0909
1.0661

1.0215

0.9664

1.0000

1.0461

2.0967

2.1565

2.3252

3.3009

3.4799

3.1543

Current Data Parameters
NAME dr-IV-131-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040811
Time 14.24

INSTRUM drx300
PROBHD 5 mm Multinuc1

PULPROG zg30
TD 32768

SOLVENT CDCl3
NS 16

DS 2
SWH 6172.839 Hz

FIDRES 0.188380 Hz
AQ 2.6542580 sec

RG 101.6
DW 81.000 usec

DE 6.00 usec
TE 300.0 K

D1 1.00000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 1H

P1 7.05 usec

PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters

SF 32768

SF 300.1300022 MHz

MDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.30

1D NMR plot parameters

CX 20.00 cm

CY 9.00 cm

F1P 10.531 ppm

F1 3160.75 Hz

F2P -0.458 ppm

F2 -137.59 Hz

PPMCH 0.54949 ppm/cm

HZCM 164.91699 Hz/cm

ppm

8

6

4

2

0

S 52

184.277

154.952

149.788

123.392

112.871

84.139

77.420

76.996

76.573

32.259

25.681

24.979

23.309

12.295

Entry 2, Table 2

Current Data Parameters
NAME dr-IV-131-a1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040811

Time 14.29

INSTRUM drx300

PROBHD 5 mm Multinuc1

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 86

DS 4

SWH 18932.393 Hz

FIDRES 0.287360 Hz

AQ 1.7400308 sec

RG 22528

DM 26.550 usec

DE 6.00 usec

TE 297.1 K

D1 1.29999995 sec

d11 0.03000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====

NUC1 ¹³C

P1 8.50 usec

PL1 5.00 dB

SFO1 75.4760107 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 ¹H

PCPD2 100.00 usec

PL2 120.00 dB

PL12 25.60 dB

SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768

SF 75.4677531 MHz

MDN EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 9.00 cm

F1P 210.905 ppm

F1 15916.54 Hz

F2P -5.248 ppm

F2 -396.02 Hz

PPMCM 10.80764 ppm/cm

HZCM 815.62823 Hz/cm

ppm

8.03949
7.27373
7.06605
7.04442
7.02286
7.01515
6.99352
6.97199
6.75932
6.75413
6.74880
6.70842
6.70319
6.69791

2.31494
2.30990
2.28851
2.28508
2.26880
2.26384
2.24453
2.23904
1.95952
1.95007
1.73727
1.68602
1.67746
1.65298
1.63500
1.13255
1.10784
1.08305
0.00450

Entry 3, Table 2

Integral

0.9982

1.0000

1.0220

5.5244

6.4041

7.7183

3.3290

Current Data Parameters
NAME dr-IV-138-a2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040907

Time 12.37
INSTRUM drx300

PROBHD 5 mm Multinucl
PULPROG zg30

TD 32768
SOLVENT CDCl3

NS 16
DS 2

SMH 6172.839 Hz
FIDRES 0.188380 Hz

AQ 2.6542580 sec
RG 203.2

DW 81.000 usec
DE 6.00 usec

TE 300.0 K
D1 1.00000000 sec

D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 7.05 usec
PL1 0.00 dB

SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768

SF 300.1300022 MHz
WDW EM

SSB 0
LB 0.30 Hz

GB 0
PC 1.30

1D NMR plot parameters
CX 20.00 cm

CY 6.00 cm
F1P 10.405 ppm

F1 3122.71 Hz
F2P -0.350 ppm

F2 -104.99 Hz
PPMCM 0.53772 ppm/cm

HZCM 161.38499 Hz/cm

S 53

ppm

8

6

4

2

0

Entry 3, Table 2

184.607

150.216
149.719

123.682

112.975

81.166
77.426
77.002
76.579

41.949
35.697
30.767
25.753

12.400

Current Data Parameters
NAME dr-IV-138-a2
EXRNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040907
Time 12.42
INSTRUM drx300
PROBHD 5 mm Multinuc1
PULPROG zgpgc30
TD 65536
SOLVENT CDCl3
NS 110
DS 4
SMH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 22528
DM 26.550 usec
DE 6.00 usec
TE 297.1 K
D1 1.29999955 sec
d11 0.03000000 sec
D31 0.00000000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 5.00 dB
SF01 75.4760107 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 25.60 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677514 MHz
MDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 7.00 cm
F1P 213.784 ppm
F1 16133.78 Hz
F2P -4.346 ppm
F2 -327.99 Hz
PPHMK 10.90649 ppm/cm
HZCM 823.08826 Hz/cm

S 55

Entry 3, Table 2

Current Data Parameters
NAME dr-V-056-aa1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041213
Time 11.02

INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5208.333 Hz
FIDRES 0.156946 Hz
AQ 3.145779 sec
RG 512
DW 96.000 use
DE 137.14 use
TE 300.0 K
D1 1.0000000 sec
P1 8.70 use
SF01 250.131521 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 16384
SF 250.1300049 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.50

1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.301 ppm
F1 2576.59 Hz
F2P -0.440 ppm
F2 -110.17 Hz
PPMCM 0.53707 ppm
HZCM 134.33809 Hz/

Entry 4, Table 2

S 56

Current Data Parameters
 NAME dr-V-056-aa1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20041213
 Time 11.05
 INSTRUM arx250
 PROBD 5 mm QNP 1H
 PULPROG zgpg30
 TD 36864
 SOLVENT CDCl3
 NS 108
 DS 4
 SWH 17241.379 HZ
 FIDRES 0.467702 HZ
 AQ 1.0691060 sec
 RG 22800
 DM 29.000 use
 DE 41.43 use
 TE 300.0 K
 D12 0.00002000 sec
 DL5 23.00 dB
 CPDPRG waltz16
 P31 103.00 use
 D1 1.00000000 sec
 P1 5.00 use
 SF01 62.9023694 MHz
 NUCLEUS 13C
 D11 0.03000000 sec

F2 - Processing parameters

SI 32768
 SF 62.8952440 MHz
 WDW EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

1D NMR plot parameters

CX 20.00 cm
 CY 10.00 cm
 F1P 205.092 ppm
 F1 12899.29 HZ
 F2P -6.386 ppm
 F2 -401.66 HZ
 PPMCM 10.57389 ppm
 HZCM 665.04755 HZ

77.554
 77.046
 76.537
 74.738

31.353
 31.017
 25.700

12.268

184.155
 156.051
 150.139
 140.400
 128.505
 128.406
 126.169
 123.235
 113.046

Entry 4, Table 2

S 57

ppm

Current Data Parameters
NAME dr-V-058-a1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041221
Time 14.43
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 512
DM 96.000 use
DE 137.14 use
TE 300.0 K
D1 1.00000000 sec
P1 8.70 use
SF01 250.131521 MHz
NUCLEUS 1H

F2 - Processing parameters

SI 16384
SF 250.130049 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.50

1D NMR plot parameters

CX 20.00 cm
CY 12.50 cm
F1P 10.450 ppm
F1 2613.85 Hz
F2P -0.568 ppm
F2 -142.06 Hz
PPMCM 0.55090 ppm
HZCM 137.79565 Hz/

Entry 5-trans, Table 2

S 58

F2 - Acquisition Parameters

Date_ 20041221
Time 14.46
INSTRUM srx250
PROBHD 5 mm GNP 1H
PULPROG zgpg30
TD 36864
SOLVENT CDCl3
NS 164
DS 4
SWH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
DM 29.000 use
DE 41.43 use
TE 300.0 K
D12 0.00002000 sec
D15 23.00 dB
CPDPRG waltz16
P31 103.00 use
D1 1.00000000 sec
P1 6.00 use
SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 62.8952440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 10.00 cm
F1P 205.524 ppm
F1 12926.50 Hz
F2P -4.452 ppm
F2 -280.01 Hz
PPMCM 10.49884 ppm
HZCM 660.32538 Hz/

ppm

184.337
156.824
153.931
121.542
113.039
77.494
76.986
76.478
62.465
40.817
31.696
25.832
25.624

Entry 5-trans, Table 2

S 59

ppm
175
150
125
100
75
50
25

Current Data Parameters
 NAME dr-v-058-aat-1m
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20041221
 Time 16.01

INSTRUM apx250
 PROBHD 5 mm QNP 1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 16
 DS 2
 SMH 5208.333 Hz
 FIDRES 0.158946 Hz
 AQ 3.1457779 sec
 RG 1024
 DW 96.000 use
 DE 137.14 use
 TE 300.0 K
 D1 1.00000000 sec
 P1 8.70 use
 SF01 250.1315321 MHz
 NUCLEUS 1H

Entry 5-cis, Table 2

S 60

F2 - Processing parameters
 SI 16384
 SF 250.1300049 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 F1P 10.646 ppm
 F1 2662.80 Hz
 F2P -0.490 ppm
 F2 -122.48 Hz
 PPMCM 0.55677 ppm
 HZCM 139.26418 Hz/

Current Data Parameters
NAME dr-V-058--aa1-m
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20041221
Time 16.05
INSTRUM arx250
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 36864
SOLVENT CDCl3
NS 2314
DS 4
SWH 17241.379 Hz
FIDRES 0.467702 Hz
AQ 1.0691060 sec
RG 22800
DM 29.000 use
DE 41.43 use
TE 300.0 K
D12 0.00002000 sec
D15 23.00 dB
CPDPRG waltz16
P31 103.00 use
D1 1.00000000 sec
P1 6.00 use
SF01 62.9023694 MHz
NUCLEUS 13C
D11 0.03000000 sec

F2 - Processing parameters

SI 32768
SF 62.8952440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
CY 10.00 cm
F1P 209.131 ppm
F1 13153.36 Hz
F2P -3.679 ppm
F2 -231.39 Hz
PQCM 10.64051 ppm
HZCM 669.23773 Hz/

Entry 5-cis, Table 2

S 61