A Practical Synthesis of Triaryl and Triheteroarylmethanes by the Reaction of Aldehydes and Activated Arenes Promoted by Gold (III) chloride

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Supporting Information

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2-15: Experimental procedures and Characterization data
16-55: ¹H and ¹³C NMR spectra

Experimental section

General

All reactions were carried out in oven-dried glassware under argon atmosphere. Progress of reaction was monitored by Thin Layer Chromatography (visualization was effected by exposure to UV light or iodine), while purification was effected by silica gel column chromatography. NMR data were collected at room temperature in CDCl_3 or $(\text{CD}_3)_2\text{SO}$ at an operating frequency of 300 MHz (75 MHz for ^{13}C NMR). IR spectra were recorded on Bomem MB Series FT-IR spectrophotometer. Melting points were recorded on a Buchi melting point apparatus and are uncorrected. Elemental analyses were done using Perkin Elmer-2400 CHNS analyzer. High Resolution Mass Spectra were recorded under EI/HRMS (at 5000 resolution) using JOEL JMS 600H mass spectrometer.

Procedure A

To a solution of **1a** (246mg, 3mmol) and **2a** (106mg, 1mmol) in acetonitrile (2.5mL) was added a solution of AuCl_3 (3.1mg, 1 mol%) in acetonitrile (1mL) under an atmosphere of argon. After stirring the reaction mixture at room temperature for 12 h, it was filtered to remove insoluble impurities. The residue was purified by silica gel column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures) to afford 234mg (93%) of **3a** as a colorless liquid.

Compound 3a

IR (neat) ν_{max} : 3031, 2923, 1558, 1491, 1449, 1384, 1017, 945, 775, 729 cm^{-1} . **^1H NMR** (CDCl_3) δ 2.24 (s, 6H), 5.30 (s, 1H), 5.82-5.85 (uneven triplet, 4H, $J_1 = 2.9$ Hz, $J_2 = 3.9$ Hz), 7.22-7.31 (m, 5H). **^{13}C NMR** (CDCl_3) δ 13.5, 45.0, 106.0, 108.1, 126.8, 128.3, 139.9, 151.1, 152.7. HRMS Calcd for $\text{C}_{17}\text{H}_{16}\text{O}_2$: 252.1150. Found: 252.1153.

Compound 3b

Following procedure A with **1a** (3mmol) and **2b** (1mmol) in presence of AuCl₃ (1 mol%), **3b** was obtained as a colorless liquid in 90% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 2923, 1561, 1451, 1220, 1025, 950, 775cm⁻¹. **¹H NMR** (CDCl₃) δ 2.26 (s, 9H), 5.33 (s, 1H), 5.87 (s, 3H), 5.93 (s, 3H). **¹³C NMR** (CDCl₃) δ 13.6, 39.3, 106.4, 107.9, 150.8, 151.3. HRMS (EI) Calcd for C₁₆H₁₆O₃: 256.1099. Found: 256.1093.

Compound 3c

Following procedure A with **1a** (3mmol) and **2c** (1mmol) in presence of AuCl₃ (1 mol%), **3c** was obtained as a colorless liquid in 76% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 3105, 2921, 1608, 1560, 1444, 1216, 1018, 950, 775, 698cm⁻¹. **¹H NMR** (CDCl₃) δ 2.26 (s, 6H), 5.56 (s, 1H), 5.87 (s, 2H), 5.95 (s, 2H), 6.87-6.93 (m, 2H), 7.17 (d, 1H, J = 4.9 Hz). **¹³C NMR** (CDCl₃) δ 40.4, 106.4, 108.1, 124.7, 125.8, 126.7, 143.4, 151.6, 152.4. HRMS (EI) Calcd for C₁₅H₁₄O₂S: 258.0718. Found: 258.0729.

Compound 3d

Following procedure A with **1a** (3mmol) and **2d** (1mmol) in presence of AuCl₃ (1 mol%), **3d** was obtained as a colorless liquid in 77% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 3424, 2923, 1616, 1606, 1461, 1340, 1220, 1025, 779, 739cm⁻¹. **¹H NMR** (CDCl₃) δ 2.25 (s, 6H), 5.58 (s, 1H), 5.85 (s, 2H), 5.89 (s, 2H), 6.93 (s, 1H), 7.03 (uneven triplet, 1H, $J_1 = 7.6$ Hz, $J_2 = 7.3$ Hz), 7.14 (uneven triplet, 1H, $J_1 = 7.9$ Hz, $J_2 = 7.1$ Hz), 7.28 (d, 1H, $J = 8.1$ Hz), 7.47 (d, 1H, $J = 7.9$ Hz), 7.91 (s, 1H). **¹³C NMR** (CDCl₃) δ 13.7, 36.8, 106.1, 107.5, 111.1, 115.1, 119.4, 119.6, 122.0, 122.9, 126.5, 136.4, 150.9, 153.0. HRMS (EI) Calcd for C₁₉H₁₇NO₂: 291.1259 Found: 291.1261.

Compound 3e

Following procedure A with **1a** (3mmol) and **2e** (1mmol) in presence of AuCl₃ (1 mol%), **3e** was obtained as a colorless liquid in 65% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 2964, 2923, 1558, 1450, 1383, 1218, 1022, 960, 775cm⁻¹. **¹H NMR** (CDCl₃) δ 0.88 (d, 6H, $J = 6.9$ Hz), 2.24-2.32 (m, 7H), 3.66

(d, 1H, $J = 7.8$ Hz), 5.82 (s, 2H), 5.93 (s, 2H). ^{13}C NMR (CDCl_3) δ 13.5, 20.7, 31.9, 46.3, 105.9, 106.9, 150.1, 153.3. HRMS (EI) Calcd for $\text{C}_{14}\text{H}_{18}\text{O}_2$: 218.1307. Found: 218.1474.

Compound 3f

Following procedure A with **1b** (3mmol) and **2b** (1mmol) in presence of AuCl_3 (1 mol%), **3f** was obtained as a colorless viscous liquid in 92% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures). IR (neat) ν_{max} : 3410, 3246, 3057, 2923, 1622, 1463, 1343, 1224, 1025, 747 cm^{-1} . ^1H NMR (CDCl_3) δ 2.15 (s, 3H), 5.78 (s, 1H), 5.80 (s, 2H), 6.54 (s, 2H), 6.96-6.98 (m, 2H), 7.04-7.13 (m, 4H), 7.41-7.46 (m, 4H). ^{13}C NMR (CDCl_3) δ 12.7, 59.0, 104.9, 105.8, 110.4, 115.3, 117.4, 118.2, 120.0, 122.3, 125.7, 135.7, 154.7. HRMS (EI) Calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}$: 326.1419. Found: 326.1452.

Compound 3g

Following procedure A with **1b** (3mmol) and **2c** (1mmol) in presence of AuCl₃ (1 mol%), **3g** was obtained as a colorless crystalline solid (turning brown on storage) in 99% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 185-187 °C. **IR** (KBr) ν_{max} : 3414, 3078, 3028, 1616, 1451, 1416, 1335, 1210, 1095, 1000, 840, 780, 739, 724cm⁻¹. **¹H NMR** (CDCl₃+DMSO-*d*₆) δ 6.11 (s, 1H), 6.87-6.94 (m, 6H), 7.04-7.09 (m, 3H), 7.37 (dd, 4H, $J_1 = 7.8$ Hz, $J_2 = 13.8$ Hz), 9.85 (s, 2H). **¹³C NMR** (CDCl₃+DMSO-*d*₆) δ 34.6, 110.7, 117.9, 118.6, 120.5, 122.5, 122.7, 124.1, 125.5, 125.9, 136.1, 148.7. HRMS (EI) Calcd for C₂₁H₁₆N₂S: 328.1034 Found: 328.1022.

Compound 3h

Following procedure A with **1b** (3 mmol) and **2d** (1 mmol) in presence of AuCl₃ (1 mol%), **3h** was obtained as a colorless crystalline solid (turning brown on storage) in 78% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 234-236 °C. **IR** (KBr) ν_{max} : 3404, 3053, 1606, 1455, 1415, 1335, 1215, 1090, 1010, 799, 604cm⁻¹. **¹H NMR** (CDCl₃+DMSO-*d*₆) δ 6.09 (s, 1H), 6.78 (s, 3H), 6.86-6.89 (m, 3H), 7.03-7.06 (m, 3H), 7.30-7.33 (m, 3H), 7.40-7.43 (m, 3H), 9.67 (s, 1H). **¹³C NMR** (CDCl₃+DMSO-*d*₆) δ 30.8, 110.9, 118.0, 118.5, 119.3, 120.6, 123.1, 126.7, 136.4. HRMS (EI) Calcd for C₂₅H₁₉N₃: 361.1579. Found: 361.1573.

Compound 3i

Following procedure A with **1b** (3mmol) and **2e** (1mmol) in presence of AuCl₃ (1 mol%), **3i** was obtained as a colorless crystalline solid in 76% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 62-64 °C. **IR** (KBr) ν_{max} : 3419, 3023, 1601, 1455, 1425, 1335, 1100, 1005, 744, 704, 579cm⁻¹. **¹H NMR** (CDCl₃) δ 1.01 (d, 6H, J = 6.6 Hz), 2.61-2.68 (m, 1H), 4.24 (d, 1H, J = 8.1 Hz), 6.99-7.13 (m, 6H), 7.25-7.29 (m, 2H), 7.61 (d, 2H, J = 7.8 Hz), 7.85 (s, 2H). **¹³C NMR** (CDCl₃) δ 21.8, 32.9, 41.1, 111.1, 118.9, 119.3, 119.5, 121.4, 121.7, 127.4, 136.0. HRMS (EI) Calcd for C₂₀H₂₀N₂: 288.1626. Found: 288.1632.

Compound 3j

Following procedure A with **1c** (3 mmol) and **2a** (1 mmol) in presence of AuCl₃/3AgOTf (1 mol%), **3j** was obtained as a colorless liquid in 70% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 3066, 2920, 1654, 1559, 1539, 1437, 1222, 1032 cm⁻¹. **¹H NMR** (CDCl₃) δ 2.42 (s, 6H), 5.65 (s, 1H), 6.56 (t, 4H, J = 3.0 Hz), 7.22-7.30 (m, 5H). **¹³C NMR** (CDCl₃) δ 15.4, 47.8, 124.5, 125.7, 126.9, 128.3, 128.4, 138.9, 143.8, 145.2. HRMS (EI) Calcd for C₁₇H₁₆S₂: 284.0693. Found: 284.0692.

Compound 3k

Following procedure A with **1c** (3mmol) and **2c** (1mmol) in presence of AuCl₃/3AgOTf (1 mol%), **3k** was obtained as a colorless liquid in 32% yield after purification by column chromatography (100-200 mesh silica gel, 95:5 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 3063, 2920, 2853, 1414, 1229, 1265, 1040, 805, 703 cm⁻¹. **¹H NMR** (CDCl₃) δ 2.42 (s, 6H), 5.89 (s, 1H), 6.55 (s, 2H), 6.66 (s, 2H), 6.90 (d, 2H, J = 2.2 Hz), 7.17 (d, 1H, J = 2.8 Hz). **¹³C NMR** (CDCl₃) δ 15.4, 42.9, 124.5, 125.5, 125.6, 126.5, 139.1, 144.9, 147.5. HRMS (EI) Calcd for C₁₅H₁₄S₃: 290.0258 Found: 290.0199.

Compound 3l

Following procedure A with **1d** (3mmol) and **2a** (1mmol) in presence of AuCl₃ (1 mol%), **3l** was obtained as a colorless crystalline solid in 93% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 203-205 °C. **IR** (KBr) ν_{max} : 3053, 3018, 2933, 1616, 1476, 1370, 1330, 1225, 1119, 1010, 699cm⁻¹. **¹H NMR** (CDCl₃) δ 3.67 (s, 6H), 5.85 (s, 1H), 6.49 (s, 2H), 6.96 (uneven triplet, 2H, $J_1 = 7.2$ Hz, $J_2 = 7.5$ Hz), 7.14-7.19 (m, 3H), 7.23-7.36 (m, 8H). **¹³C NMR** (CDCl₃) δ 32.8, 40.4, 109.2, 118.5, 118.9, 120.3, 121.7, 126.3, 127.7, 128.4, 128.9, 137.7, 144.6. HRMS (EI) Calcd for C₂₅H₂₂N₂: 350.1783 Found: 350.1772.

Compound 3m

Following procedure A with **1d** (3mmol) and **2b** (1mmol) in presence of AuCl₃ (1 mol%), **3m** was obtained as a colorless crystalline solid in 85% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent

mixtures), Mp – 168-170 °C. **IR** (KBr) ν_{max} : 3119, 3049, 2934, 1616, 1541, 1481, 1326, 1236, 1155, 1015, 960 cm^{-1} . **^1H NMR** (CDCl_3) δ 2.26 (s, 3H), 3.70 (s, 6H), 5.84 (s, 2H), 5.85 (s, 1H), 6.70 (s, 2H), 7.00 (uneven triplet, 2H, $J_1 = 6.9$ Hz, $J_2 = 7.8$ Hz), 7.17 (uneven triplet, 2H, $J_1 = 8.1$ Hz, $J_2 = 6.9$ Hz), 7.25 (d, 2H, $J = 8.4$ Hz), 7.46 (d, 2H, $J = 7.8$ Hz). **^{13}C NMR** (CDCl_3) δ 13.8, 32.6, 34.0, 106.0, 107.2, 109.0, 116.1, 118.8, 119.9, 121.4, 127.3, 127.6, 137.3, 150.4, 155.5. HRMS (EI) Calcd for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}$: 354.1732 Found: 354.1747.

Compound 3n

Following procedure A with **1e** (3mmol) and **2d** (1mmol) in presence of AuCl_3 (1 mol%), **3n** was obtained as a colorless crystalline solid in 64% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 225-227 °C. **IR** (KBr) ν_{max} : 3414, 3379, 3048, 2918, 1616, 1461, 1331, 1200, 1125, 1010, 745 cm^{-1} . **^1H NMR** (CDCl_3) δ 2.25 (s, 6H), 6.16 (s, 1H), 6.80 (s, 1H), 6.97-7.00 (m, 1H), 7.08-7.22 (m, 8H), 7.38 (d, 1H, $J = 8.2$ Hz), 7.52-7.54 (m, 2H), 7.70 (s, 2H), 8.07 (s, 1H). **^{13}C NMR** (CDCl_3) δ 8.5, 32.4, 107.1, 110.8, 111.3, 114.8, 118.2, 118.9, 119.6, 121.0, 122.0, 124.0, 129.3, 134.3, 135.3, 136.7. HRMS (EI) Calcd for $\text{C}_{27}\text{H}_{23}\text{N}_3$: 389.1892. Found: 389.1888.

Compound 4a

Following procedure A with **1f** (3mmol) and **2a** (1mmol) in presence of AuCl₃/3AgOTf (1 mol%), **4a** was obtained as a colorless crystalline solid in 45% yield (85% when conducted at 50 °C) after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 190-192 °C. **IR** (KBr) ν_{max} : 2946, 2843, 1596, 1464, 1424, 1229, 1132, 954, 817cm⁻¹. **¹H NMR** (CDCl₃) δ 3.47 (s, 12H), 3.76 (s, 6H), 6.06 (s, 4H), 6.16 (s, 1H), 6.98-7.10 (m, 5H). **¹³C NMR** (CDCl₃) δ 37.0, 54.9, 56.0, 91.8, 114.2, 124.0, 126.9, 127.7, 145.6, 159.1, 159.7. HRMS (EI) Calcd for C₂₅H₂₈O₆: 424.1886. Found: 424.1836.

Compound 4b

Following procedure A with **1f** (3mmol) and **2f** (1mmol) in presence of AuCl₃/3AgOTf (1 mol%), **4b** was obtained as a colorless crystalline solid in 80% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate

solvent mixtures), Mp – 152-154 °C. **IR** (KBr) ν_{max} : 3068, 2948, 2837, 1606, 1521, 1465, 1416, 1350, 1230, 1120, 1040, 950, 849, 810 cm^{-1} . **^1H NMR** (CDCl_3) δ 3.52 (s, 12H), 3.79 (s, 6H), 6.08 (s, 4H), 6.22 (s, 1H), 7.15 (d, 2H, $J = 8.1$ Hz), 8.00 (d, 2H, $J = 8.7$ Hz). **^{13}C NMR** (CDCl_3) δ 37.4, 55.3, 56.0, 91.6, 112.4, 112.6, 128.6, 145.4, 155.0, 159.8, 160.0. Anal. Calcd for $\text{C}_{25}\text{H}_{27}\text{NO}_8$: C, 63.96; H, 5.80; N, 2.98. Found: C, 64.07; H, 5.58; N, 3.13.

Compound 5a

Following procedure A with **1b** (5mmol) and **2g** (1mmol) in presence of AuCl_3 (2 mol%), **5a** was obtained as a brown solid in 95% yield after purification by column chromatography (neutral alumina, 70:30 hexane: ethyl acetate solvent mixtures), Mp – 180 °C (decomp.). **IR** (KBr) ν_{max} : 3409, 3053, 1706, 1656, 1456, 1415, 1340, 1245, 1005, 1000, 739 cm^{-1} . **^1H NMR** (CDCl_3) δ 5.73 (s, 2H), 6.17 (s, 4H), 7.00 (uneven triplet, 4H, $J_1 = 7.2$ Hz, $J_2 = 7.1$ Hz), 7.13 (uneven triplet, 4H, $J_1 = 7.7$ Hz, $J_2 = 7.0$ Hz), 7.17-7.29 (m, 12H), 7.35 (d, 4H, $J = 7.8$ Hz). **^{13}C NMR** (CDCl_3) δ 39.7, 111.1, 118.5, 119.0, 119.6, 121.2, 123.6, 126.9, 128.3, 136.5, 141.7. HRMS (FAB) Calcd for $\text{C}_{40}\text{H}_{30}\text{N}_4$: 566.25. Found: 566.28.

Compound 5b

Following procedure A with **1a** (5 mmol) and **2g** (1 mmol) in presence of AuCl₃ (2 mol%), **5b** was obtained as a colorless crystalline solid in 51% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures), Mp – 158-160 °C. **IR** (KBr) ν_{max} : 3108, 2923, 1611, 1561, 1445, 1215, 1160, 1025, 965, 769, 649 cm⁻¹. **¹H NMR** (CDCl₃) δ 2.24 (s, 12H), 5.30 (s, 2H), 5.86 (s, 8H), 7.17 (s, 4H). **¹³C NMR** (CDCl₃) δ 13.6, 44.7, 106.0, 108.1, 128.4, 138.6, 151.3, 152.8. HRMS (EI) Calcd for C₂₈H₂₆O₄: 426.1831. Found: 426.1837.

Compound 6a

Following procedure A with **1b** (8 mmol) and **2h** (1 mmol) in presence of AuCl₃ (3 mol%), **6a** was obtained as a light pink solid in 35% yield after purification by column chromatography (neutral alumina, 50:50 hexane: ethyl acetate solvent mixtures), Mp – 120 °C (decomp.). **IR** (KBr) ν_{max} : 3414, 2923, 2853, 1596, 1506, 1415, 1340, 1185, 1100, 1025, 744cm⁻¹. **¹H NMR** (DMSO-*d*₆) δ 5.76 (s, 3H), 6.62 (s, 6H), 6.91-6.93 (m, 12H), 7.04-7.14 (m, 12H), 7.28-7.35 (m, 12H), 9.04 (s, 6H). **¹³C NMR** (acetone-*d*₆) δ 40.5, 112.2, 119.3, 120.0, 120.3, 122.0, 122.7, 124.3, 124.4, 124.6, 128.1, 129.5, 130.3, 130.8, 138.0, 138.1, 140.2, 146.9. HRMS (FAB) Calcd for C₆₉H₅₁N₇: 977.42 Found: 977.53.

Following procedure A with **1a** (8 mmol) and **2h** (1 mmol) in presence of AuCl₃ (3 mol%), **6b** was obtained as a viscous liquid in 63% yield after purification by column chromatography (100-200 mesh silica gel, 90:10 hexane: ethyl acetate solvent mixtures). **IR** (neat) ν_{max} : 2923, 1601, 1556, 1506, 1275, 1215, 1020, 775, 950cm⁻¹. **¹H NMR** (CDCl₃) δ 2.26 (s, 18H), 5.24 (s, 3H), 5.85 (s, 12H), 6.98-7.08 (m, 12H). **¹³C NMR** (CDCl₃) δ 13.7, 44.5, 106.1, 108.1, 124.0, 129.1, 134.2, 146.5, 151.2, 153.0. HRMS (FAB) Calcd for C₅₁H₄₅NO₆: 767.33 Found: 767.37.

Current Data Parameters
NAME Thirumalai
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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PROBHD 5 mm Multinu
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TD 32768
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NS 8
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SWH 4194.631 Hz
FIDRES 0.128010 Hz
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RG 362
DW 119.200 usec
DE 169.96 usec
TE 300.0 K
D1 1.00000000 sec
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SF01 300.1316784 MHz
NUC1 1H
PL1 0.00 dB

F2 - Processing parameters
SI 16384
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 5.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.572 ppm
F1 3172.95 Hz
F2P -0.825 ppm
F2 -247.54 Hz
PPMCM 0.56983 ppm/cm
HZCM 171.02454 Hz/cm

Current Data Parameters

NAME Thirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

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Time 10.23
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PROBHD 5 mm Multinu
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TD 32768
SOLVENT CDCl3
NS 443
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2048
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
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PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
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NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

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LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

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F1 17318.72 Hz
F2P -10.563 ppm
F2 -797.20 Hz
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HZCM 905.79620 Hz/cm

3b

Current Data Parameters
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 EXPNO 1
 PROCNO 1

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 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 362
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
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 P1 11.00 usec
 SFO1 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 40.00

1D NMR plot parameters
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 F1 3236.32 Hz
 F2P -1.107 ppm
 F2 -332.17 Hz
 PPMCM 0.59449 ppm/cm
 HZCM 178.42419 Hz/cm

Current Data Parameters
NAME Thirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050707
Time 11.28
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 40
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2048
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 6.00000000 sec
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SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 75.4677503 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 203.801 ppm
F1 15380.39 Hz
F2P 5.108 ppm
F2 385.45 Hz
PPMCM 9.93466 ppm/cm
HZCM 749.74664 Hz/cm

Current Data Parameters
 NAME Thirumalai
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050323
 Time 15.41
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TO 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 256
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SF01 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300117 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 10.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.870 ppm
 F1 3262.47 Hz
 F2P -1.112 ppm
 F2 -333.74 Hz
 PPMCM 0.59911 ppm/cm
 HZCM 179.81059 Hz/cm

Current Data Parameters

NAME Thirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050407
Time 16.16
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 359
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 1149.4
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 3.00000000 sec
P1 12.50 usec
SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 75.4677341 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 229.825 ppm
F1 17344.34 Hz
F2P -10.224 ppm
F2 -771.61 Hz
PPMCM 12.00244 ppm/cm
HZCM 905.79712 Hz/cm

Current Data Parameters
 NAME Thirumalai
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050328
 Time 9.00
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT D2O
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 322.5
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SF01 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 40.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.824 ppm
 F1 3248.51 Hz
 F2P -1.158 ppm
 F2 -347.70 Hz
 PPMCM 0.59911 ppm/cm
 HZCM 179.81059 Hz/cm

Current Data Parameters
NAME Thirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050707
Time 11.42
INSTAUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDC13
NS 101
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2048
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 6.00000000 sec
P1 12.50 usec
SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 75.4677525 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 206.881 ppm
F1 15612.83 Hz
F2P -7.360 ppm
F2 -555.41 Hz
PPMCM 10.71202 ppm/cm
HZCM 808.41217 Hz/cm

Current Data Parameters
 NAME saumini
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date 20050819
 Time 12.28
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22468
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 7812.500 Hz
 FIDRES 0.347717 Hz
 AQ 1.4380020 sec
 RG 64
 DW 64.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300327 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

Current Data Parameters
 NAME sauminil3C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050825
 Time_ 14.48
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT CDC13
 NS 58
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 1625.5
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 6.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677536 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

Current Data Parameters
 NAME Thirumalai
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050401
 Time 16.03
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 64
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SFO1 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300439 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 10.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.698 ppm
 F1 3210.88 Hz
 F2P -1.044 ppm
 F2 -313.27 Hz
 PPMCM 0.58710 ppm/cm
 HZCM 176.20775 Hz/cm

Current Data Parameters
 NAME Thirumalai13c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050707
 Time 10.58
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zgdc
 TD 32768
 SOLVENT CDC13
 NS 959
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 1448.2
 DW 27.600 usec
 DE 9.43 usec
 TE 300.0 K
 D11 0.03000000 sec
 PL12 17.20 dB
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 SF02 300.1312700 MHz
 NUC2 ¹H
 PL2 120.00 dB
 D1 3.00000000 sec
 P1 12.50 usec
 SF01 75.4760204 MHz
 NUC1 ¹³C
 PL1 -6.00 dB

F2 - Processing parameters
 SI 16384
 SF 75.4678045 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 211.167 ppm
 F1 15936.33 Hz
 F2P -7.426 ppm
 F2 -560.44 Hz
 PPMCM 10.92968 ppm/cm
 HZCM 824.83856 Hz/cm

Current Data Parameters
 NAME saumini
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050912
 Time 10.46
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22468
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 7812.500 Hz
 FIDRES 0.347717 Hz
 AQ 1.4380020 sec
 RG 256
 DW 64.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299406 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 20.00

Current Data Parameters
 NAME saumini13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050901
 Time_ 16.19
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT cdcl3
 NS 218
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 2896.3
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677928 MHz
 WDW EM
 SSB 0
 -- --

Current Data Parameters
 NAME Thirumalai
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050318
 Time 16.20
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 812.7
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SF01 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1299328 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 5.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.401 ppm
 F1 3421.73 Hz
 F2P -1.024 ppm
 F2 -307.44 Hz
 PPMCM 0.62126 ppm/cm
 HZCM 186.45883 Hz/cm

Current Data Parameters
 NAME saumini13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050901
 Time 14.19
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT cdcl3
 NS 542
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 3649.1
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677768 MHz
 WDW EM
 SSB 0
 --

Current Data Parameters
 NAME Thirumalai
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051001
 Time 11.46
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22468
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 4789.272 Hz
 FIDRES 0.213160 Hz
 AQ 2.3457091 sec
 RG 287.4
 DW 104.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1315007 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300116 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 5.00

136.003
127.364
121.650
121.439
120.544
119.457
119.278
118.899
111.149

77.425
76.990
76.564

41.062

32.914

21.825

0.093

Current Data Parameters
NAME saumini13C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050824
Time_ 15.58
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 387
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2298.8
DW 27.600 usec
DE 9.00 usec
TE 0.0 K
D1 3.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 17.23 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.50

Current Data Parameters
 NAME saumini
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050928
 Time_ 17.17
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22468
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 7812.500 Hz
 FIDRES 0.347717 Hz
 AQ 1.4380020 sec
 RG 181
 DW 64.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

Current Data Parameters

NAME saumini13C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date 20050929
Time 11.06
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 192
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2298.8
DW 27.600 usec
DE 9.00 usec
TE 0.0 K
D1 3.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 17.23 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677525 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.50

Current Data Parameters
 NAME Thirumalai
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050405
 Time 11.38
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 181
 DW 119.200 usec
 DE 189.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SFO1 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters

SI 16384
 SF 300.1300178 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 10.00

1D NMR plot parameters

CX 20.00 cm
 F1P 10.730 ppm
 F1 3220.37 Hz
 F2P -1.160 ppm
 F2 -348.11 Hz
 PPMCM 0.59449 ppm/cm
 HZCM 178.42419 Hz/cm

Current Data Parameters
NAME Thirumalai13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050706
Time 16.22
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 412
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 1290.2
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 3.00000000 sec
P1 12.50 usec
SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 75.4677514 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 209.383 ppm
F1 15801.67 Hz
F2P -5.479 ppm
F2 -413.50 Hz
PPMCM 10.74312 ppm/cm
HZCM 810.75885 Hz/cm

Current Data Parameters
 NAME Thirumalai
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050420
 Time 15.00
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 287.4
 DW 111.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SF01 300.1316957 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300156 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0.
 PC 40.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 11.011 ppm
 F1 3304.64 Hz
 F2P -0.903 ppm
 F2 -271.10 Hz
 PPMCM 0.59570 ppm/cm
 HZCM 178.78696 Hz/cm

Current Data Parameters
NAME Ihirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050428
Time 14.15
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 646
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 1149.4
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 3.00000000 sec
P1 12.50 usec
SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters
SI 16384
SF 75.4677352 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 229.810 ppm
F1 17343.23 Hz
F2P -10.239 ppm
F2 -772.71 Hz
PPMCM 12.00244 ppm/cm
HZCM 905.79712 Hz/cm

Current Data Parameters
 NAME saumini
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050906
 Time_ 15.30
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22468
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 7812.500 Hz
 FIDRES 0.347717 Hz
 AQ 1.4380020 sec
 RG 228.1
 DW 64.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318008 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300162 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

Current Data Parameters
 NAME sauminil3C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050901
 Time_ 12.44
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT cdcl3
 NS 204
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 3649.1
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 6.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677508 MHz
 WDW EM
 SSB 0

Current Data Parameters
 NAME Thirumalai
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050426
 Time 12.04
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 574.7
 DW 111.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SFO1 300.1316957 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300082 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 10.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.479 ppm
 F1 3144.96 Hz
 F2P -1.310 ppm
 F2 -393.29 Hz
 PPMCM 0.58945 ppm/cm
 HZCM 176.91238 Hz/cm

Current Data Parameters
 NAME saumini13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050901
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT cdc13
 NS 248
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 4597.6
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677580 MHz
 WDW EM
 SSB 0

Current Data Parameters
 NAME Thirumalai
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050328
 Time 9.16
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4194.631 Hz
 FIDRES 0.128010 Hz
 AQ 3.9059956 sec
 RG 574.7
 DW 119.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SFO1 300.1316784 MHz
 NUC1 1H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300142 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 10.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.615 ppm
 F1 3185.82 Hz
 F2P -0.988 ppm
 F2 -296.40 Hz
 PPMCM 0.58012 ppm/cm
 HZCM 174.11137 Hz/cm

Current Data Parameters

NAME Thirumalai13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050428
Time 13.29
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 562
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2580.3
DW 27.600 usec
DE 9.43 usec
TE 300.0 K
D11 0.03000000 sec
PL12 17.20 dB
CPDPRG2 waltz16
PCPD2 80.00 usec
SF02 300.1312700 MHz
NUC2 1H
PL2 120.00 dB
D1 3.00000000 sec
P1 12.50 usec
SF01 75.4760204 MHz
NUC1 13C
PL1 -6.00 dB

F2 - Processing parameters

SI 16384
SF 75.4677564 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 20.00 cm
F1P 229.529 ppm
F1 17322.04 Hz
F2P -10.520 ppm
F2 -793.91 Hz
PPMCM 12.00244 ppm/cm
HZCM 905.79742 Hz/cm

Current Data Parameters
 NAME saumini
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20050712
 Time 12.33
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 181
 DW 81.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

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

NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
 SF 300.1300079 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

Current Data Parameters
 NAME saumini13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameter
 Date 20050728
 Time 13.35
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT CDC13
 NS 454
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 se
 RG 1149.4
 DW 27.600 us
 DE 9.00 us
 TE 0.0 K
 D1 6.00000000 se
 d11 0.03000000 se
 MCREST 0.00000000 se
 MCWRK 0.01500000 se

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 us
 PL1 -6.00 dB
 SFO1 75.4760204 MH

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 us
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MH

F2 - Processing parameters
 SI 32768
 SF 75.4677313 MH
 WDW EM
 SSB 0

Current Data Parameters
 NAME Thirumalai
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050511
 Time 12.08
 INSTRUM dpx300
 PROBHD 5 mm Multinu
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 4496.403 Hz
 FIDRES 0.137219 Hz
 AQ 3.6438515 sec
 RG 322.5
 DW 111.200 usec
 DE 169.96 usec
 TE 300.0 K
 D1 1.00000000 sec
 P1 11.00 usec
 SFO1 300.1316507 MHz
 NUC1 ¹H
 PL1 0.00 dB

F2 - Processing parameters
 SI 16384
 SF 300.1300120 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB *0
 PC 10.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.719 ppm
 F1 3217.07 Hz
 F2P -1.099 ppm
 F2 -329.96 Hz
 PPMCM 0.59092 ppm/cm
 HZCM 177.35164 Hz/cm

141.703
136.523
128.282
126.872
123.622
121.217
119.575
119.028
118.513
111.117

77.427
77.002
76.577

39.739

-0.082

Current Data Parameters
NAME saumini13C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050901
Time_ 16.47
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgdc
TD 32768
SOLVENT cdcl3
NS 307
DS 0
SWH 18115.941 Hz
FIDRES 0.552855 Hz
AQ 0.9044468 sec
RG 2896.3
DW 27.600 usec
DE 9.00 usec
TE 0.0 K
D1 3.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 12.50 usec
PL1 -6.00 dB
SFO1 75.4760204 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 17.23 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677613 MHz
WDW EM
SSB 0
-- --

Current Data Parameters

NAME Thirumalai
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20050509
Time 12.52
INSTRUM dpx300
PROBHD 5 mm Multinu
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 362
DW 111.200 usec
DE 169.96 usec
TE 300.0 K
D1 1.00000000 sec
P1 11.00 usec
SFO1 300.1316507 MHz
NUC1 1H
PL1 0.00 dB

F2 - Processing parameters

SI 16384
SF 300.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 5.00

1D NMR plot parameters

CX 20.00 cm
F1P 10.478 ppm
F1 3144.65 Hz
F2P -0.914 ppm
F2 -274.25 Hz
PPMCM 0.56957 ppm/cm
HZCM 170.94485 Hz/cm

Current Data Parameters
NAME: thirumalai13c
EXPNO: 2
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20050526
Time: 14.46
INSTRUM: dpx300
PROBHD: 5 mm Multinu
PULPROG: zgpg
TD: 32768
SOLVENT: CDCl3
NS: 584
DS: 0
SWH: 18115.941 Hz
FIDRES: 0.552855 Hz
AQ: 0.9044468 sec
RG: 2896.3
DW: 27.600 usec
DE: 9.43 usec
TE: 300.0 K
D11: 0.03000000 sec
PL12: 17.20 dB
CPDPRG2: waltz16
PCPD2: 80.00 usec
SF02: 300.1312700 MHz
NUC2: 13C
PL2: 120.00 dB
D1: 3.00000000 sec
P1: 12.50 usec
SF01: 75.4760204 MHz
NUC1: 13C
PL1: -6.00 dB

F2 - Processing parameters
SI: 16384
SF: 75.4677508 MHz
WDW: EM
SSB: 0
LB: 0.20 Hz
GB: 0
PC: 1.00

1D NMR plot parameters
CX: 20.00 cm
F1P: 229.602 ppm
F1: 17327.57 Hz
F2P: -10.447 ppm
F2: -788.38 Hz
PPMCM: 12.00245 ppm/cm
HZCM: 905.79779 Hz/cm

Current Data Parameters
 NAME Thirumalai13C
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051001
 Time_ 14.46
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT CDC13
 NS 1200
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 2580.3
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4676793 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.25

Current Data Parameters
 NAME saumini
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050714
 Time_ 16.13
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg30
 TD 22400
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.274739 Hz
 AQ 1.8199580 sec
 RG 161.3
 DW 81.000 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300122 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

6b

Current Data Parameters
 NAME sauminil3C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date 20050720
 Time 11.35
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgdc
 TD 32768
 SOLVENT CDCl3
 NS 558
 DS 0
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 3649.1
 DW 27.600 usec
 DE 9.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 12.50 usec
 PL1 -6.00 dB
 SFO1 75.4760204 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 120.00 dB
 PL12 17.23 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677470 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40