Supporting Information

PART - 1

Cobalt-Catalyzed Aryl-Sulfur Bond Formation

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(See **PART 2** of the supporting information for ^1H and ^{13}C NMR spectra for all compounds in **Table 3**)

Experimental Section

General: All reactions were conducted under nitrogen atmosphere on a dual-manifold Schlenk line unless otherwise mentioned and in oven-dried glass wares. Acetonitrile was dried with CaH_2 and distilled prior to use. Co(dppe)I_2 ¹ was prepared by reported procedure. Other reagents were commercially available and used as purchased.

General Procedure for the Synthesis of Diphenylsulfide (entry 1, table 2): To a solution of $\text{CoI}_2(\text{dppe})$ (0.0050 mmol), zinc (0.750 mmol), pyridine (0.50 mmol) and iodobenzene (0.50 mmol) were added thiophenol (0.50 mmol) and CH_3CN (2.0 mL). The reaction mixture was allowed to stir at 80 °C for 10 h. At the end of the reaction, the reaction mixture was diluted with CH_2Cl_2 , filtered through Celite and silica gel. The filtrate was concentrated and the residue was purified through a silica gel column using Ethyl acetate and hexane as eluent to give pure Diphenylsulfide.

References:

1. McKinney, Ronald J. *Inorg. Chem.* 21, **1982**, 2051 – 2056.

Diphenyl sulfide (entry 1, Table 2): colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 7.21-7.23 (m, 1H), 7.27-7.29 (m, 3H), 7.33-7.34 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 127.0 (2C), 129.1 (4C), 131.0 (4C), 135.7 (2C); **HRMS** calcd for $\text{C}_{12}\text{H}_{10}\text{S}$ 186.0503 found 186.0505. **Registry Number:** [139-66-2].

Phenyl *p*-tolyl sulfide (entry 2, Table 2): colorless oil. ^1H NMR (400 MHz, CDCl_3): δ 2.33 (s, 3H), 7.12 (d, J = 8.4 Hz, 2H), 7.15-7.20 (m, 1H), 7.25 (m, 4H), 7.28 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.1, 126.4, 129.0 (2C), 129.8 (2C), 130.0 (2C), 131.3, 132.3 (2C), 137.1, 137.5; **HRMS** calcd for $\text{C}_{13}\text{H}_{12}\text{S}$ Exact Mass: 200.066 found 200.0658. **Registry Number:** [3699-01-2].

1-Methoxy-4-(phenylthio)benzene (entry 3, Table 2): colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 3.81 (s, 3H), 6.88 (d, J = 8.8 Hz, 2H), 7.10-7.16 (m, 3H), 7.20-7.22 (m, 2H), 7.40 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 55.3, 115.0 (2C), 124.3, 125.7, 128.2 (2C), 128.9 (2C), 135.3 (2C), 138.6, 159.8; **HRMS** calcd for $\text{C}_{13}\text{H}_{12}\text{OS}$ 216.0609 found 216.0616. **Registry Number:** [5633-57-8].

4-Phenylsulfanylacetophenone (entry 4, Table 2): yellow solid, mp 63.0 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.53 (s, 3H), 7.18 (d, $J = 2.4$ Hz, 2H), 7.37-7.40 (m, 3H), 7.47-7.49 (m, 2H), 7.81(d, $J = 2.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 26.4, 127.5, 128.8, 128.9, 129.7, 132.1, 133.8, 134.5, 144.9 197.1; **HRMS** calcd for $\text{C}_{14}\text{H}_{12}\text{OS}$ 228.0608 found 228.0609. **Registry Number:** [10169-55-8].

4-Phenylsulfanylbenzoic acid methyl ester (entry 5, Table 2): colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 1.35 (t, $J = 7.2$ Hz, 3H), 4.33 (q, $J = 7.2$ Hz, 2H), 7.20 (d, $J = 2.4$ Hz, 2H), 7.35-7.38 (m, 3H), 7.45-7.47 (m, 2H), 7.87 (d, $J = 2.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 14.3, 60.9, 127.6 (2C), 127.9, 128.5, 129.5 (2C), 123.0 (2C), 132.5, 133.5 (2C), 144.0, 166.1; **HRMS** calcd for $\text{C}_{15}\text{H}_{14}\text{O}_2\text{S}$ 258.0714 found 258.0716. **Registry Number:** [10129-07-4].

4-(Phenylthio)benzonitrile (entry 6, Table 2): colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.15 (dt, $J = 8.8$ Hz, 2H), 7.40-7.43 (m, 3H), 7.46 (dt, $J = 8.8$ Hz, 2H), 7.48-7.51 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 108.6, 118.7, 127.2 (2C), 129.3,

129.8 (2C), 130.8, 132.3 (2C), 134.4 (2C), 145.6 ; **HRMS** calcd for C₁₃H₉NS 211.0456, found 211.0455. **Registry Number:** [51238-46-1].

(4-Fluorophenyl)(phenyl)sulfide (entry 7, Table 2): colorless oil; **¹H NMR** (400MHz, CDCl₃): δ 7.01 (ddt, *J* = 8.8 Hz, 2H), 7.20-7.22 (m, 1H), 7.23-7.29 (m, 4H), 7.36 (ddt, *J* = 8.8 Hz, 2H); **¹³C NMR** (100 MHz, CDCl₃): δ 116.3, 116.5, 126.7, 129.2 (2C), 129.9 (2C), 130.2, 134.0, 134.1, 136.6, 161.1, 163.6; **HRMS** calcd for C₁₂H₉FS 204.0409 found 204.0409. **Registry Number:** [330-85-8].

4-(Phenylthio)benzenamine (entry 8, Table 2): white solid, mp 90.0 °C; **¹H NMR** (400MHz, CDCl₃): δ 3.79 (bs, 2H), 6.66 (dt, *J* = 8.8 Hz, 2H), 7.06-7.11 (m, 3H), 7.17-7.21 (m, 2H), 7.29 (dt, *J* = 8.8 Hz, 2H); **¹³C NMR** (100 MHz, CDCl₃): δ 115.8 (2C), 120.5, 125.2, 127.3 (2C), 128.8 (2C), 136.1 (2C), 139.7, 147.0; **HRMS** calcd for C₁₂H₁₁NS 201.0612 found 201.0611. **Registry Number:** [1135-14-4].

4-Phenylsulfanylphenol (entry 9, Table 2): colorless oil; **¹H NMR** (400MHz, CDCl₃): δ 4.81 (bs, 1H), 6.81 (dt, *J* = 8.8Hz, 2H), 7.11-7.17 (m, 3H), 7.20-7.22 (m,

2H), 7.35 (dt, $J = 8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 116.5 (2C), 124.6, 125.9, 128.3 (2C), 128.9 (2C), 135.5 (2C), 138.4, 155.8; **HRMS** calcd for $\text{C}_{12}\text{H}_{10}\text{OS}$ 202.0452 found 202.0451. **Registry Number:** [5633-55-6].

1-Methoxy-2-(phenylthio)benzene (entry10, Table 2): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 3.86 (s, 3H), 6.85-6.90 (m, 2H), 7.07 (dd, $J = 8.0$ Hz, 1H), 7.20-7.26 (m, 2H), 7.27-7.32 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3): δ 55.9, 110.8, 121.2, 124.1, 127.0, 128.3, 129.1 (2C), 131.4 (2C), 131.6, 134.5, 157.3; **HRMS** calcd for $\text{C}_{13}\text{H}_{12}\text{OS}$ 216.0609 found 216.0610. **Registry Number:** [14065-22-6].

(2-(Phenylthio)phenyl)methanol (entry11, Table 2): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 2.03 (t, $J = 6.2$ Hz, 1H), 4.76 (d, $J = 6.2$ Hz, 2H), 7.19-7.26 (m, 6H), 7.27-7.32 (m, 2H), 7.33 (d, $J = 1.2$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 63.6, 126.6, 128.5 (2C), 128.5, 129.2 (2C), 129.4 (2C), 132.4, 140.0, 136.0, 142.4; **HRMS** calcd for $\text{C}_{13}\text{H}_{12}\text{OS}$ 216.0609 found 216.0606. **Registry Number:** [1527-14-6].

1-Naphtylphenyl sulfide (entry12, Table 2): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 7.12-7.23 (m, 5H), 7.42 (dd, $J = 8.4$ Hz, 1H), 7.49-7.52 (m, 2H), 7.65 (dd, $J = 7.2$ Hz, 1H), 7.84-7.88 (m, 2H), 8.35-8.37 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 125.6, 125.8, 126.0, 126.4, 126.9, 128.5, 128.9 (2C), 129.0 (2C), 129.1, 131.2, 132.5, 133.5, 134.2, 136.9; **HRMS** calcd for $\text{C}_{16}\text{H}_{12}\text{S}$ 236.0660 found 236.0655.

Registry Number: [7570-98-1].

(Phenanthren-9-yl)(phenyl)sulfide (entry13, Table 2): white solid, mp 141.8 °C; ^1H NMR (400MHz, CDCl_3): δ 7.14-7.22 (m, 5H), 7.57-7.61 (m, 2H), 7.65-7.69 (m, 2H), 7.80 (dd, $J = 8.0, 1.2$ Hz, 1H), 8.00 (s, 1H), 8.44 (dd, $J = 8.0, 1.2$ Hz, 1H), 8.70 (dd, $J = 16.4, 8.4$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 122.7, 123.0, 126.2, 126.5, 127.0, 127.1, 127.2, 127.4, 128.5, 128.9 (2C), 129.1 (2C), 129.6, 130.7, 131.1, 131.6, 131.7, 134.0, 136.7; **HRMS** calcd for $\text{C}_{20}\text{H}_{14}\text{S}$ 286.0816 found 286.0817. **Registry Number:** [16336-55-3].

5-Phenylsulfanylindole (entry14, Table 2): white solid, mp 92.3 °C; ^1H NMR

(400MHz, CDCl₃): δ 6.53 (m, 1H), 7.06-7.23 (m, 6H), 7.30-7.39 (m, 2H), 7.84 (dd, J = 0.8 Hz, 1H), 8.22 (brs, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 102.8, 112.1, 123.0, 125.1, 125.3, 127.3, 127.7 (2C), 128.2, 128.8 (2C), 128.9, 135.6, 139.7; **HRMS** calcd for C₁₄H₁₁NS 225.0612 found 225.0607 .

(Z)-Ethyl 3-(phenylthio)acrylate (entry15, Table 2): colorless oil; ¹H NMR (400MHz, CDCl₃): δ 1.31 (t, J = 7.2 Hz , 3H), 4.24 (q, J = 7.2 Hz , 2H), 5.89 (d, J = 10.4 Hz, 1H), 7.25 (d, J = 10.4 Hz 1H), 7.32-7.38 (m, 3H), 7.47-7.49 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 14.3, 60.3, 113.3, 128.2, 129.3 (2C), 131.0 (2C), 136.1, 149.7, 166.5; **HRMS** calcd for C₁₁H₁₂O₂S 208.0558 found 208.0558. **Registry Number:** [13733-59-0].

Mesityl(phenyl)sulfide (entry 16, Table 2): colorless oil; ¹H NMR (400MHz, CDCl₃): δ 2.30 (s, 3H), 3.64 (s, 6H), 6.88-6.91 (m, 2H), 6.99 (s, 2H), 7.01-7.05 (m, 1H), 7.13-7.17 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 21.1, 21.7 (2C), 124.5, 125.5 (2C), 127.0, 128.8 (2C), 129.3 (2C), 138.4, 139.3, 143.7 (2C); **HRMS** calcd for C₁₅H₁₆S 228.0973 found 228.0970. **Registry Number:** [33667-80-0].

4-(Phenylthio)benzaldehyde (entry 19, Table 2): yellow oil; $^1\text{H NMR}$ (400MHz, CDCl_3): δ 7.22 (d, $J = 8.8$ Hz, 2H), 7.40-7.43 (m, 3H), 7.49-7.53 (m, 2H), 7.70 (d, $J = 8.8$ Hz, 2H), 9.89 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 127.2 (2C), 129.1, 129.8 (2C), 130.1 (2C), 131.3, 133.7, 134.3 (2C), 147.2, 191.2; **HRMS** calcd for $\text{C}_{13}\text{H}_{10}\text{OS}$ 214.0452 found 214.0449. **Registry Number:** [1208-88-4].

***N,N*-Dimethyl-4-(phenylthio)benzenamine (entry 20, Table 2):** white solid, mp 69.2 °C; $^1\text{H NMR}$ (400MHz, CDCl_3): δ 2.97 (s, 6H), 6.69 (dt, $J = 8.8$ Hz, 2H), 7.04-7.10 (m, 3H), 7.16-7.20 (m, 2H), 7.37 (dt, $J = 8.8$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 40.3 (2C), 112.9 (2C), 117.4, 124.9, 126.8 (2C), 128.7 (2C), 136.1 (2C), 140.3, 150.6; **HRMS** calcd for $\text{C}_{14}\text{H}_{15}\text{NS}$ 229.0925 found 229.0924. **Registry Number:** [42881-80-1].

2-(Phenylthio)pyridine (entry 21, Table 2): colorless oil; $^1\text{H NMR}$ (400MHz, CDCl_3): δ 6.93 (d, $J = 8.4$ Hz, 1H), 6.60- 6.99 (m, 1H), 7.39-7.45 (m, 4H), 7.56-7.60

(m, 2H), 8.41 (d, $J = 4.9$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 119.9, 121.3, 129.1, 129.6 (2C), 131.1, 134.9 (2C), 136.7, 149.6, 161.5; **HRMS** calcd for $\text{C}_{11}\text{H}_9\text{NS}$ 187.0456 found 187.0451. **Registry Number:** [3111-54-4].

2-(Phenylthio)furan (entry 22, Table 2): colorless oil; ^1H NMR (400MHz, CDCl_3): δ 6.46 (dd, $J = 3.2, 1.2$ Hz, 1H), 6.73 (dd, $J = 3.2, 1.2$ Hz, 1H), 7.13-7.17 (m, 3H) 7.21-7.26 (m, 2H), 7.57 (dd, $J = 2.0, 0.8$ Hz, 1H) ; ^{13}C NMR (100 MHz, CDCl_3): δ 111.8, 119.5, 126.3, 127.5 (2C), 129.0 (2C), 136.3, 143.1, 146.5; **HRMS** calcd for $\text{C}_{10}\text{H}_8\text{OS}$ 176.0296 found 176.0292. **Registry Number:** [16003-14-8].

1-Methoxy-4-*p*-tolylsulfanyl-benzene (entry 1, Table 3): colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 2.28 (s, 3H), 3.79 (s, 3H), 6.85 (dt, $J = 8.8$ Hz, 2H), 7.04 (d, $J = 8.4$ Hz, 2H), 7.11 (d, $J = 8.4$ Hz, 2H), 7.34 (dt, $J = 8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 20.9, 55.3, 114.8 (2C), 125.6, 129.3 (2C), 129.7 (2C), 134.3 (3C), 136.1, 159.4 ; **HRMS** calcd for $\text{C}_{14}\text{H}_{14}\text{OS}$ 230.0765 found 230.0767. **Registry Number :** [6013-47-4].

Di-*p*-tolylsulfide (entry 2, Table 3): white solid, mp 56.1 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.30 (s, 6H), 7.08 (d, $J = 8.4\text{Hz}$, 4H), 7.21 (d, $J = 8.4\text{ Hz}$, 4H) ; ^{13}C NMR (100 MHz, CDCl_3): δ 21.0, 129.9 (2C), 131.0 (2C), 132.7, 136.8; **HRMS** calcd for $\text{C}_{14}\text{H}_{14}\text{S}$ 214.0816 found 214.0815. **Registry Number:**[620-94-0].

(4-Chlorophenyl)(*p*-tolyl)sulfide (entry 3, Table 3): white solid, mp 71.4 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.33 (s, 3H), 7.12-7.16 (m, 4H), 7.20 (dt, $J = 8.8\text{ Hz}$, 2H), 7.27 (dt, $J = 8.0\text{Hz}$, 2H) ; ^{13}C NMR (100 MHz, CDCl_3): δ 21.1, 129.1 (2C), 130.2 (2C), 130.7, 130.8 (2C), 132.3, 132.5 (2C); **HRMS** calcd for $\text{C}_{11}\text{H}_{11}\text{ClS}$ 234.0270 found 234.0270. **Registry Number:**[22865-55-0].

4-*p*-Tolylsulfanyl-phenol (entry 4, Table 3): white solid, mp 64.0 °C; ^1H NMR (400 MHz, CDCl_3): δ 2.28 (s, 3H), 5.79 (brs, 1H), 6.79 (d, $J = 8.8\text{ Hz}$, 2H), 7.04 (d, $J = 8.0\text{ Hz}$, 2H), 7.10 (d, $J = 8.0\text{ Hz}$, 2H), 7.29 (d, $J = 8.8\text{ Hz}$, 2H) ; ^{13}C NMR (100 MHz, CDCl_3): δ 20.9, 116.3 (2C), 125.9, 129.5 (2C), 129.8 (2C), 133.9, 134.3 (2C), 136.3,

155.2; **HRMS** calcd for C₁₃H₁₂OS 216.0609 found 216.0608. **Registry**

Number:[5633-57-8].

(2-Isopropylphenyl)(p-tolyl)sulfide (entry 5, Table 3): colorless oil; **¹H NMR** (400 MHz, CDCl₃): δ 1.20 (d, *J* = 6.8 Hz, 6H), 2.30 (s, 3H), 3.52 (h, *J* = 6.8 Hz 1H), 7.04-7.09 (m, 3H), 7.14 (dt, *J* = 8.4 Hz, 2H), 7.17 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.23 (td, *J* = 7.6, 1.2 Hz, 1H), 7.30 (dd, *J* = 7.6, 1.2 Hz, 1H) ; **¹³C NMR** (100 MHz, CDCl₃): δ 21.0, 23.4 (2C), 30.5, 125.8, 126.4, 127.7, 129.9 (2C), 130.7 (2C), 132.4, 132.8, 133.9, 136.6, 149.3; **HRMS** calcd for C₁₆H₁₈S 242.1129 found 242.1134.

Phenethyl(p-tolyl)sulfide (entry 6, Table 3): colorless oil; **¹H NMR** (400 MHz, CDCl₃): δ 2.31 (s, 3H), 2.88 (dd, *J* = 8.4, 7.2 Hz, 2H), 3.10 (dd, *J* = 8.4, 7.2 Hz, 2H), 7.09-7.11 (m, 2H), 7.16-7.22 (m, 3H), 7.26-7.30 (m, 4H) ; **¹³C NMR** (100 MHz, CDCl₃): δ 20.9, 35.69, 35.73, 126.3, 128.4 (2C), 128.4 (2C), 129.6 (2C), 130.0 (2C), 132.5, 136.1, 140.3; **HRMS** calcd for C₁₄H₁₆S 228.0973 found 228.0972. **Registry**
Number:[27846-23-7].

Hexyl(*p*-tolyl)sulfide (entry 7, Table 3): colorless oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 0.86 (t, 6.8 Hz, 3H), 1.21-1.31 (m, 4H), 1.35-1.42 (m, 2H), 1.59 (p, $J = 7.2$ Hz, 2H), 2.30 (s, 3H), 2.85 (t, $J = 7.2$ Hz, 2H), 7.07 (d, $J = 8.0$ Hz, 2H), 7.22 (d, $J = 8.0$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 14.0, 21.0, 22.5, 28.5, 29.2, 31.4, 34.3, 129.6 (2C), 129.7 (2C), 133.2, 135.8; **HRMS** calcd for $\text{C}_{13}\text{H}_{20}\text{S}$ 208.1286 found 208.1283.

Registry Number:[5342-83-6].

Cyclohexyl(*p*-tolyl)sulfide (entry 8, Table 3): colorless oil; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 1.30-1.34 (m, 5H), 1.57-1.58 (m, 1H), 1.72-1.75 (m, 2H), 1.92-1.96 (m, 2H), 2.30 (s, 3H), 2.98-2.99 (m, 1H), 7.07 (d, $J = 8.0$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 21.1, 25.8, 26.1 (2C), 33.4 (2C), 47.1, 129.5 (2C), 131.2, 132.8 (2C), 136.8; **HRMS** calcd for $\text{C}_{13}\text{H}_{18}\text{S}$ 206.1129 found 206.1129.

Registry Number:[59693-93-5].

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AQ         1.4418420 sec
RG         64
DE         22.000 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.30 usec
PL1        1.00 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.70 dB
PL13       18.70 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178024 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
  
```

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Ph-S-OMe

7.410
7.388
7.240
7.216
7.197
7.156
7.137
7.117
7.099
6.892
6.870

entry 3-table 2

3.805

Current Data Parameters
NAME Ph-S-OMe
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060530
Time_ 17.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSE 0
LB 0.00 Hz
GB 0
PC 1.00

entry 3-table 2

Current Data Parameters
 NAME Ph-S-4OMe
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060612
 Time_ 23.44
 INSTRU spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG 45.2
 DW 22.000 usec
 DE 6.00 usec
 TE 300.0 K
 DI 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.30 usec
 PL1 1.00 dB
 SFO1 100.6288660 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.40 dB
 PL12 15.70 dB
 PL13 18.70 dB
 SFO2 400.1516010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6178048 MHz
 WDM EM
 SSB G
 LB 3.00 Hz
 GB 0
 PC 1.00

```

185 exp2 std1h
date SAMPLE 6 2006
solvent CDC13
file exp
ACQUISITION exp
sfrq 400.447 dnm 0
in H1 dnm 0
at 2.728 dnm 200
np 32768 dmf PROCESSING
sw 6006.0 lb 0.10
fb 3400 wfile
bs 4 proc
tpwr 59 fn 65536
pw 6.8 werr
d1 1.000 wexp
tof 596.3 wbs
nt 100 wnt
ct 16
alock n
gain not used
FLAGS
il n
in n
dp y
SP -0.0
vp 4004.3
vs 100
sc 0
wc 250
h2mm 2.91
ls 150.87
rfl 3307.1
rfp 2899.2
th 8
ins 10.000
nm ph

```

7.180
 7.186
 7.197
 7.202
 7.240
 7.373
 7.378
 7.386
 7.390
 7.401
 7.468
 7.473
 7.482
 7.493
 7.790
 7.795
 7.807
 7.812

13C OBSERVE
exp3 std13c
197 61

SAMPLE		DEC. & VT	
date	8 2006	dfrq	400.446
solvent	CDCl3	dn	H1
file	exp	dwr	41
ACQUISITION		dof	0
sfrq	100.703	dm	nyy
tn	0.13	dmm	w
at	0.738	dmf	9700
np	40302	lb	1.00
sw	25252.5	wtfile	1.00
fb	14000	proc	ft
bs	4	fn	65536
tpwr	59		
pw	4.9		
d1	0.500	werr	
d2	1.500	wexp	
tof	1546.8	wbs	
nt	1000	wnt	
ct	320		
alock	not used		
gain	n		
il	n		
in	n		
dp	y		
DISPLAY		sp	-0.2
wp	21145.0	vs	50
sc	0	wc	250
hzmh	84.58	is	500.00
rfl	9329.4	rfl	7753.3
th	3	ins	100.000
nm	no	ph	

134.486
133.835
132.098
129.656
128.868
128.761
127.467

77.314
77.000
76.679

26.426

entry 4-table 2

1.535
1.368
1.351
1.333

entry 5-table 2

C13

entry 5-table 2

Current Data Parameters
 NAME COOEt-S-Ph
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060621
 Time_ 1.11
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65336
 SOLVENT CDCl3
 NS 201
 DS 0
 SWH 22727.273 Hz
 FIDRES 0.346791 Hz
 AQ 1.4418420 sec
 RG 64
 DM 22.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 c11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.30 usec
 PL1 1.00 dB
 SFO1 100.6288660 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -2.40 dB
 PL12 15.70 dB
 PL13 18.70 dB
 SFO2 400.1516010 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6178068 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.00

Ph-S-4CN

7.514
7.509
7.505
7.502
7.499
7.496
7.492
7.488
7.485
7.482
7.475
7.470
7.465
7.453
7.448
7.443
7.432
7.426
7.423
7.419
7.415
7.407
7.402
7.241
7.161
7.157
7.152
7.140
7.135
7.130

entry 6-table 2

1.541

Current Data Parameters
NAME Ph-S-4-CN
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060706
Time 14.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.98
2.07
2.97
2.00

4-CN

145.62
134.39
132.27
130.76
129.84
129.30
127.24
118.69
108.62

77.32
77.01
76.69

entry 6-table 2

Current Data Parameters
NAME 082906
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060829
Time 9.08
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 470
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DE 22.000 usec
TE 300.0 K
DI 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178097 MHz
WDW EN
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

7.379
7.373
7.365
7.361
7.356
7.349
7.343
7.288
7.274
7.269
7.267
7.252
7.250
7.240
7.237
7.217
7.213
7.211
7.203
7.196
7.031
7.025
7.014
7.009
7.004
6.993
6.987

entry 7-table 2

Current Data Parameters	
NAME	4-F
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	20060608
Time	23:41
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	512
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
===== CHANNEL f1 =====	
NUC1	1H
PU1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
F2 - Processing parameters	
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

4-F
163.60
161.14
136.62
134.10
134.02
130.18
129.93
129.16
126.74
116.49
116.27
77.32
77.00
76.69

entry 7-table 2

Current Data Parameters
NAME 060812
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060813
Time_ 12.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1032
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
P2 2.40 dB
PL2 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178027 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

Ph-S-4NH2

7.311
7.304
7.299
7.287
7.282
7.276
7.240
7.207
7.203
7.188
7.175
7.170
7.112
7.109
7.104
7.091
7.074
7.060
7.057
6.679
6.672
6.667
6.656
6.651
6.644

3.790

1.527

entry 8-table 2

Current Data Parameters
NAME Ph-S-4NH2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060603
Time 16.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5539540 sec
RG 1150
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

4-NH2

147.01
139.67
136.09
128.77
127.26
125.21
120.46
115.83

77.32
77.00
76.69

entry 8-table 2

Current Data Parameters
NAME exp290
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060812
Time 15.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65336
SOLVENT CDC13
NS 776
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178013 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

Ph-S-OH

7.346
7.340
7.333
7.235
7.223
7.220
7.218
7.207
7.202
7.201
7.197
7.166
7.163
7.157
7.145
7.143
7.138
7.129
7.124
7.106
6.830
6.822
6.817
6.806
6.801
6.793
4.814

entry 9-table 2

Current Data Parameters
NAME Ph-S-OH
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060530
Time 18.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 724
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

OH-C13

```

Current Data Parameters
NAME      OH-C13
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20060531
Time      21.16
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        75
DS        0
SWH       22727.273 Hz
FIDRES    0.346791 Hz
AQ        1.4418420 sec
RG        64
DM        22.000 usec
DE        6.00 usec
TE        300.0 K
D1        2.00000000 sec
d11       0.03000000 sec
DELTA     1.89999998 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        10.30 usec
PL1       1.00 dB
SFO1      100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.40 dB
PL12      15.70 dB
PL13      18.70 dB
SFO2      400.1516010 MHz

F2 - Processing parameters
SI        32768
SF        100.6178021 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.00
  
```

2OMe

7.312
7.309
7.304
7.292
7.287
7.277
7.273
7.257
7.253
7.248
7.240
7.236
7.221
7.219
7.205
7.201
7.077
7.073
7.058
7.053
6.902
6.899
6.881
6.879
6.874
6.871
6.855
6.852
6.836
6.833
3.857

entry 10-table 2

Current Data Parameters
NAME 2OMe
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060602
Time_ 0.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 512
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500169 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

2-OMe

157.30
134.49
131.60
131.43
129.10
128.31
127.02
124.06
121.21
110.84
76.68
77.32
77.00
55.85

entry 10-table 2

Current Data Parameters
NAME exp290
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060812
Time 14.17
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 874
DS 0
SWH 23727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 32
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178042 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

entry 11-table 2

1-naphthene

Current Data Parameters
NAME 1-naphthene
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20060602
Time_ 0.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

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

NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters

SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

136.86
134.16
133.53
132.49
131.16
129.14
129.02
128.91
128.50
126.89
126.37
126.06
125.76
125.57

77.31
77.00
76.68

entry 12-table 2

```
Current Data Parameters
NAME      0814
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20060814
Time_     22.20
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD         65536
SOLVENT
NS         81
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4418420 sec
RG         50.8
DW         22.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.30 usec
PL1        1.00 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.70 dB
PL13       18.70 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI         32768
SF         100.6178153 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00
```

200 180 160 140 120 100 80 60 40 20 ppm

9-phnatherene

entry 13-table 2

Current Data Parameters
 NAME phnatherene
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060527
 Time_ 21.22
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5559540 sec
 RG 912
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.40 dB
 SFO1 400.1528010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1500168 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

136.66
134.01
131.68
131.59
131.06
130.67
129.63
129.10
128.85
128.51
127.43
127.20
127.08
126.99
126.53
126.15
122.99
122.65

77.32
77.01
76.69

entry 13-table 2

Current Data Parameters
NAME 0815
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060815
Time_ 15.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 196
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178020 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1-naphthene

```

Current Data Parameters
NAME      060606
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20060606
Time      17.49
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zg30
TD        32768
SOLVENT   NS
NS        8
DS        0
SWH        6410.256 Hz
FIDRES     0.195625 Hz
AQ         2.5559540 sec
RG         1030
DW         78.000 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         10.00 usec
PL1        -2.40 dB
SFO1       400.1528010 MHz

F2 - Processing parameters
SI         16384
SF         400.1500161 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

entry 14-table 2

C13

139.68
135.64
128.86
128.77
128.22
127.68
127.34
125.29
125.07
123.04
112.06
102.83

77.32
77.00
76.68

entry 14-table 2

Current Data Parameters
NAME 0825
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060825
Time_ 21.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 470
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 4
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.628860 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178020 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

7.487
7.468
7.378
7.372
7.356
7.337
7.317
7.265
7.241

5.906
5.880

4.263
4.246
4.228
4.210

1.545
1.327
1.309
1.291

Current Data Parameters
NAME cis-COOEt
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060608
Time_ 14.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SF01 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500161 MHz
WDW EM
SSB 0
LB 0
GB 0
PC 1.00

C13

entry 15-table 2

Current Data Parameters
NAME Ph-S-COOEt
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060821
Time 0.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 241
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Ph-S-trimethyl

entry 16-table 2

2.364
2.301

Current Data Parameters
NAME Trimethyl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060615
Time_ 23.38
INSTRUM Spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

trimethyl

143.71
139.25
138.39
129.31
128.84
126.95
125.45
124.45

77.32
77.01
76.69

21.69
21.12

entry 16-table 2

Current Data Parameters
NAME 060812
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20060813
Time 11.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1420
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 50.8
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
PI 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

4-CHO

1.553

entry 19-table 2

Current Data Parameters
NAME 071906
EXNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060720
Time 15.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 645
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

entry 19-table 2

Current Data Parameters
NAME 0809
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060809
Time_ 16.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 190
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178041 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

N, N-Dimethyl

entry 20-table 2

2.974

Current Data Parameters
 NAME 072406
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060724
 Time_ 19.55
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 6410.256 Hz
 FIDRES 0.195625 Hz
 AQ 2.5539540 sec
 RG 456
 DW 78.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.00 usec
 PL1 -2.40 dB
 SFO1 400.1528010 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1500168 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

N,N-Dimethyl

entry 20-table 2

Current Data Parameters
NAME 0822
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060823
Time 10.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 189
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 25.4
DM 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SFO1 100.6288660 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178067 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

2-pyridine

8.402
8.400
7.599
7.597
7.594
7.593
7.588
7.586
7.583
7.579
7.575
7.574
7.570
7.561
7.454
7.449
7.435
7.433
7.430
7.428
7.422
7.417
7.413
7.411
7.408
7.400
7.396
7.394
7.390
7.385
7.240
6.990
6.980
6.977
6.973
6.972
6.962
6.959
6.958
6.956
6.858
6.857
6.856

entry 21- table 2

1.566

Current Data Parameters
NAME 072406
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060724
Time 20.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

1.01
2.09
4.19
1.04
1.00

C13

161.52
149.56
136.68
134.93
131.07
129.61
129.06
121.34
119.86

77.32
77.01
76.69

entry 21- table 2

Current Data Parameters
NAME 0908
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060908
Time 14.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 910
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 45.2
DM 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.30 usec
PL1 1.00 dB
SF01 100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.70 dB
PL13 18.70 dB
SFO2 400.1516010 MHz

F2 - Processing parameters
SI 32768
SF 100.6178013 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

6.454
6.459
6.462
6.467
6.728
6.730
6.736
6.739
7.127
7.130
7.134
7.137
7.141
7.146
7.149
7.154
7.157
7.160
7.165
7.167
7.169
7.171
7.213
7.218
7.219
7.226
7.228
7.232
7.235
7.237
7.240
7.248
7.252
7.256
7.258
7.262
7.564
7.566
7.569
7.571

entry 22-table 2

1.548
1.235

Current Data Parameters
NAME furan
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060808
Time_ 9.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 575
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SF01 400.1528010 MHz

F2 - Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

146.47
143.07
136.28
129.02
127.51
126.30
119.45
111.84

77.32
77.00
76.69

entry 22-table 2

```

Current Data Parameters
NAME      methyl
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20060823
Time      15.51
INSTRUM   spect
PROBHD    5 mm DUL 13C-1
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS         208
DS         0
SWH        22727.273 Hz
FIDRES     0.346791 Hz
AQ         1.4418420 sec
RG         45.2
DE         22.000 usec
TE         300.0 K
D1         2.0000000 sec
d11        0.0300000 sec
DELTA     1.89999998 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.30 usec
PL1        1.00 dB
SFO1       100.6288660 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -2.40 dB
PL12       15.70 dB
PL13       18.70 dB
SFO2       400.1516010 MHz

F2 - Processing parameters
SI          32768
SF         100.6178062 MHz
WDW         EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.00
  
```