Supporting Information

**[3+2] Cross-Coupling Reactions of Aziridines with Isocyanates
Catalyzed by Nickel(II) Iodide**

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Analytical Methods

^1H NMR spectra were recorded on a JEOL JNM-EX270L FT NMR SYSTEM (270 MHz), a JEOL JNM-AL300 FT NMR SYSTEM (300 MHz), or a Bruker AM-600 (600 MHz). Chemical Shifts were reported in delta unit (δ relative to chloroform-*d* (7.24 ppm for ^1H NMR and 77.0 ppm for ^{13}C NMR)). Multiplicity is indicated by s (single), d (doublet), t (triplet), and m (multiplet). Coupling constants, *J*, are reported in Hz. IR spectra were recorded on a JASCO FT/IR-410 (FT-IR). Elemental analyses were measured by YANACO CHN-recorder MT-6. Thin layer chromatography (TLC) was performed using Merck silica gel 60F-254 plates.

General procedure

Aziridines **1a**¹, **1b-c**,² **1e**,^{3,4} **1f**,³ **1g**,¹ and **1h**⁵ were prepared as reported in the literature. Aziridine **1d**⁶ was prepared from 2-aziridin-1-yl-ethanol (commercially available). Isocyanates **2a-e** were commercially available and used without further purification. Column chromatography was performed with silica gel 60N (spherical, neutral, 63-210 mm, purchased from Kanto Kagaku Co., LTD).

1a

^1H NMR (600 MHz, CDCl_3) 7.27-7.17 (m, 5H), 3.30 (s, 2H), 1.74-1.73 (m, 2H), 1.20-1.19 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3) 139.3, 128.3, 128.0, 127.0, 65.3, 27.5.

1b

^1H NMR (600 MHz, CDCl_3) 2.15 (t, *J* = 7.2 Hz, 2H), 1.68-1.67 (m, 2H), 1.55-1.50 (m, 2H), 1.38-1.35 (m, 2H), 1.04-1.03 (m, 2H), 0.90 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3) 61.8, 32.0, 27.1, 20.5, 14.0.

1c

^1H NMR (300 MHz, CDCl_3) 1.46-1.45 (m, 2H), 1.35-1.33 (m, 2H), 0.93 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) 52.5, 26.2, 20.1.

1g

^1H NMR (300 MHz, CDCl_3) 7.27-7.22 (m, 2H), 7.04-6.94 (m, 3H), 2.11 (s, 4H); ^{13}C NMR (150 MHz, CDCl_3) 155.1, 128.9, 122.3, 121.0, 27.5.

Preparation of aziridine **1d**

To a mixture of 2-aziridin-1-yl-ethanol (1.0 ml, 12.5 mmol) in THF (20 ml) was slowly added NaH (0.75 g, 18.7 mmol) at 0 °C. Then, TBSCl (2.8 g, 18.7 mmol) was slowly added. When the exothermic reaction had subsided, the resulting solution allowed to warm to r.t, and stirred for 3 h. Then, the mixture was quenched with water, extracted with dichloromethane, and the combined organic phases were dried over sodium sulfate. Evaporation of the solvent gave oil, which was further purified by silica gel column chromatography (CH_2Cl_2 / MeOH, 30:1) to yield **1d** (1.4 g, 7.0

mmol, 56 %).

yellow oil; ^1H NMR (600 MHz, CDCl_3) 3.79 (t, $J = 6.0$ Hz, 2H), 2.34 (t, $J = 6.0$ Hz, 2H), 1.72-1.71 (m, 2H), 1.17-1.16 (m, 2H), 0.90 (s, 9H), 0.07 (s, 6H); ^{13}C NMR (150 MHz, CDCl_3) 63.6, 63.0, 26.9, 25.9, 18.3, -5.4.

Nickel catalyzed cross coupling aziridines **1** with isocyanates **2**

A Representative Procedure. To a purple mixture of NiI_2 (0.0312 g, 0.1 mmol) in dry toluene (3.5 mL) was added a solution of **1** (1 mmol) in dry toluene (3.5 mL) under an argon atmosphere at r.t. Then, compound **2** (1.5 mmol) was added, and the mixture was stirred at 100 °C. The progress of the reaction was monitored by TLC and/or GC-MS, and the mixture was stirred until the starting material **1** disappeared. The mixture was passed through a short column of alumina (CH_2Cl_2). Evaporation of the solvent gave oil, which was further purified by silica gel column chromatography (hexane / AcOEt) to give **3** or **4**.

Nickel catalyzed isomerization of **3**

To a purple mixture of NiI_2 (0.0312 g, 0.1 mmol) in dry toluene (3.5 mL) was added a solution of **3fa** (0.294 g, 1 mmol) in dry toluene (3.5 mL) under an argon atmosphere at r.t., and the mixture was stirred for 16 h at 100 °C. The mixture was passed through a short column of alumina (CH_2Cl_2). Evaporation of the solvent gave oil, which was further purified by silica gel column chromatography (hexane / AcOEt) to give **4fa**.

white solid, mp 98-99 °C; ^1H NMR (300 MHz, CDCl_3) 7.39-6.93 (m, 10H), 4.57 (s, 2H), 4.29 (t, $J = 7.2$ Hz, 2H), 3.36 (t, $J = 7.5$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) 153.2, 147.8, 136.7, 128.6, 128.5, 128.3, 127.6, 123.4, 122.0, 64.4, 49.2, 45.1; IR (KBr) 3426, 2856, 2370, 1673, 1592, 1488, 1448, 1355, 1263, 1170 cm^{-1} ; Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}$: C, 76.16; H, 6.39; N, 11.10. Found: C, 75.92; H, 6.44; N, 10.94.

1-Benzyl-3-phenylimidazolidin-2-one **4aa**

white solid, mp 117-118 °C; ¹H NMR (300 MHz, CDCl₃) 7.52 (d, *J* = 8.1 Hz, 2H), 7.31-7.18 (m, 7H), 6.97 (t, *J* = 7.5 Hz, 1H), 4.41 (s, 2H), 3.71 (dd, *J* = 7.8, 9.9 Hz, 2H), 3.28 (dd, *J* = 6.0, 8.1 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) 157.7, 140.5, 136.8, 128.8, 128.6, 128.2, 127.5, 122.3, 117.3, 48.1, 42.3, 41.2; IR (KBr) 3060, 3029, 2898, 1689, 1596, 1484, 1428, 1361, 1268, 1209, 1155, 1089 cm⁻¹; Anal. Calcd for C₁₆H₁₆N₂O: C, 76.16; H, 6.39; N, 11.10. Found: C, 75.96; H, 6.50; N, 11.06.

(*Z*)-*N*-(3-butyloxazolidin-2-ylidene)benzenamine **3ba**

yellow oil; ¹H NMR (600 MHz, CDCl₃) 7.21 (t, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 7.8 Hz, 1H), 6.93 (t, *J* = 7.8 Hz, 2H), 4.28 (t, *J* = 7.2 Hz, 2H), 3.48 (t, *J* = 7.8 Hz, 2H), 3.36 (t, *J* = 7.8 Hz, 2H), 1.62-1.57 (m, 2H), 1.42-1.36 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃) 153.3, 148.1, 128.4, 123.4, 121.8, 64.3, 45.7, 44.9, 29.4, 20.0, 13.9; IR (neat) 2959, 2929, 2870, 1675, 1590, 1479, 1429, 1366, 1261, 1195, 1117, 1028 cm⁻¹; HRMS Calcd for C₁₃H₁₈N₂O: 218.1419. Found: 218.1410.

(*Z*)-*N*-(3-*tert*-Butyloxazolidin-2-ylidene)-benzenamine **3ca**

yellow oil; ¹H NMR (600 MHz, CDCl₃) 7.22 (t, *J* = 7.8 Hz, 2H), 7.00 (d, *J* = 7.8 Hz, 2H), 6.93 (t, *J* = 7.2 Hz, 1H), 4.15 (t, *J* = 7.2 Hz, 2H), 3.50 (t, *J* = 7.8 Hz, 2H), 1.49 (s, 9H); ¹³C NMR (150 MHz, CDCl₃) 151.1, 148.5, 128.4, 123.2, 121.5, 63.4, 53.6, 44.4, 27.0; IR (neat) 2973, 2907, 1683, 1590, 1478, 1398, 1360, 1293, 1245, 1141, 1049, 980 cm⁻¹; HRMS Calcd for C₁₃H₁₈N₂O: 218.1419. Found: 218.1421.

1-*tert*-Butyl-3-phenylimidazolidin-2-one **4ca**

white solid, mp 90-91 °C; ^1H NMR (270 MHz, CDCl_3) 7.52-7.49 (m, 2H), 7.32-7.26 (m, 2H), 7.02-6.96 (m, 1H), 3.68 (dt, $J = 1.0, 7.5$ Hz, 2H), 3.47 (dt, $J = 1.0, 7.3$ Hz, 2H), 1.40 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) 158.0, 140.7, 128.7, 122.2, 117.6, 53.5, 42.1, 40.0, 27.5; IR (KBr) 2980, 2954, 2865, 1686, 1597, 1506, 1455, 1400, 1361, 1323, 1249, 1156, 1020, 895 cm^{-1} ; Anal. Calcd for $\text{C}_{13}\text{H}_{18}\text{N}_2\text{O}$: C, 71.53; H, 8.31; N, 12.83. Found: C, 71.28; H, 8.33; N, 12.62.

{3-[2-(*tert*-Butyldimethylsiloxy)ethyl]-oxazolidin-2-ylidene}-benzenamine **3da**

yellow oil; ^1H NMR (600 MHz, CDCl_3) 7.21 (t, $J = 8.4$ Hz, 2H), 7.00 (d, $J = 7.2$ Hz, 2H), 6.93 (t, $J = 7.2$ Hz, 1H), 4.28 (t, $J = 7.8$ Hz, 2H), 3.86 (t, $J = 5.4$ Hz, 2H), 3.67 (t, $J = 7.8$ Hz, 2H), 3.49 (t, $J = 4.8$ Hz, 2H), 0.89 (s, 9H), 0.07 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3) 153.0, 148.0, 129.0, 128.9, 128.4, 128.2, 123.4, 121.9, 64.6, 61.9, 47.7, 47.7, 25.9, 18.2, -5.4; IR (neat) 3056, 2954, 2928, 2884, 2857, 1681, 1591, 1544, 1478, 1361, 1256, 1196, 1104 cm^{-1} ; HRMS Calcd for $\text{C}_{17}\text{H}_{28}\text{N}_2\text{O}_2\text{Si}$: 320.1920. Found: 320.1919.

(*Z*)-*N*-(3-benzyl-5-phenyloxazolidin-2-ylidene)benzenamine **3ea**

white solid, mp 88-90 °C; ^1H NMR (300 MHz, CDCl_3) 7.39-7.16 (m, 14H), 6.95 (tt, $J = 7.2, 1.2$ Hz, 1H), 5.45 (t, $J = 7.8$ Hz, 1H), 4.72 (d, $J = 14.7$ Hz, 1H), 4.53 (d, $J = 14.7$ Hz, 1H), 3.71 (t, $J = 8.4$ Hz, 1H), 3.26 (dd, $J = 8.7, 7.8$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) 152.7, 147.4, 138.6, 136.6, 128.7, 128.7, 128.5, 128.3, 127.6, 125.8, 123.6, 122.0, 77.4, 52.6, 49.3; IR (KBr) 3030, 2865, 2361, 1681, 1590, 1496, 1477, 1236, 1020 cm^{-1} ; Anal. Calcd for $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}$: C, 80.46; H, 6.14; N, 8.53. Found: C, 80.37; H, 6.24; N, 8.44.

1-Benzyl-3,4-diphenylimidazolidin-2-one **4ea**

white solid, mp 134-136 °C; ^1H NMR (300 MHz, CDCl_3) 7.37 (d, $J = 7.8$ Hz, 2H), 7.22-7.11 (m, 13H), 6.89 (t, $J = 7.5$ Hz, 1H), 4.37 (s, 2H), 4.54 (d, $J = 14.7$ Hz, 1H), 4.33 (d, $J = 14.7$ Hz, 1H), 3.66 (t, $J = 9.0$ Hz, 1H), 3.03 (dd, $J = 9.0, 5.7$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) 158.2, 140.4, 139.2, 136.7, 129.0, 128.6, 128.5, 128.2, 128.0, 127.6, 126.0, 122.9, 119.8, 57.6, 50.9, 48.0; IR (KBr) 3061, 3038, 1691, 1598, 1503, 1441, 1352, 1256, 1142 cm^{-1} ; Anal. Calcd for $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}$: C, 80.46; H, 6.14; N, 8.53. Found: C, 80.76; H, 6.23; N, 8.37.

(Z)-N-(3-Butyl-5-phenyloxazolidin-2-ylidene)benzenamine **3fa**

yellow oil; ^1H NMR (270 MHz, CDCl_3) 7.22-7.01 (m, 9H), 6.80 (tt, $J = 7.8, 1.6$ Hz, 1H), 5.24 (t, $J = 7.6$ Hz, 1H), 3.61 (t, $J = 9.3$ Hz, 1H), 3.32-3.14 (m, 3H), 1.51-1.40 (m, 2H), 1.27-1.13 (m, 2H), 0.85 (t, $J = 8.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3) 152.7, 140.6, 147.9, 139.0, 128.7, 128.6, 128.4, 125.7, 123.6, 121.7, 77.1, 53.1, 44.8, 29.4, 20.0, 13.9; IR (neat) 3060, 3031, 2958, 2926, 2862, 1681, 1591, 1493, 1455, 1425, 1370, 1330, 1287, 1230, 1195 cm^{-1} ; Anal. Calcd for $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}$: C, 77.52; H, 7.53; N, 9.52. Found: C, 77.35; H, 7.53; N, 9.46.

1-Butyl-3,4-diphenylimidazolidin-2-one **4fa**³

white solid; ^1H NMR (600 MHz, CDCl_3) 7.42 (d, $J = 8.4$ Hz, 2H), 7.33-7.25 (m, 5H), 7.19 (t, $J = 9.0$ Hz, 2H), 6.94 (t, $J = 7.2$ Hz, 1H), 5.18 (dd, $J = 9.0, 5.4$ Hz, 1H), 3.87 (t, $J = 9.0$ Hz, 1H), 3.32 (t, $J = 7.2$ Hz, 2H), 3.21 (dd, $J = 8.4, 6.0$ Hz, 1H), 1.54-1.49 (m, 2H), 1.39-1.33 (m, 2H), 0.93 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3) 158.3, 140.7, 139.4, 129.1, 128.5, 128.0, 126.0, 122.7, 119.6, 57.6, 51.5, 43.6, 29.5, 19.9, 13.7.

white solid, mp 116-117 ° C (lit.⁷ 115-116 ° C); ¹H NMR (600 MHz, CDCl₃) 7.78 (d, *J* = 8.4 Hz, 2H), 7.38 (t, *J* = 8.4 Hz, 2H), 7.28 (t, *J* = 7.2 Hz, 2H), 7.11-7.09 (m, 3H), 7.01 (t, *J* = 7.2 Hz, 1H), 4.45 (t, *J* = 7.8 Hz, 2H), 4.05 (t, *J* = 7.8 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃) 149.1, 147.4, 139.7, 128.8, 128.5, 123.2, 123.0, 122.5, 118.8, 63.7, 46.4.

white solid; ¹H NMR (600 MHz, CDCl₃) 7.60 (d, *J* = 7.8 Hz, 4H), 7.38 (t, *J* = 7.8 Hz, 4H), 7.10 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 4H); ¹³C NMR (150 MHz, CDCl₃) 140.0, 128.9, 123.1, 118.1, 42.0.

yellow oil; ¹H NMR (300 MHz, CDCl₃) 7.34-7.12 (m, 10H), 4.45 (s, 2H), 4.41 (s, 2H), 4.09 (t, *J* = 7.2 Hz, 2H), 3.12 (t, *J* = 7.8 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) 154.9, 142.2, 136.8, 128.4, 128.1, 127.9, 127.3, 127.2, 125.9, 64.1, 49.8, 49.3, 45.7; IR (neat) 3060, 3026, 2905, 2852, 1697, 1603, 1583, 1539, 1493, 1452, 1351, 1259, 1192 cm⁻¹. HRMS Calcd for C₁₇H₁₈N₂O: 266.1419. Found: 266.1415.

light yellow solid, mp 84-85 °C; ¹H NMR (300 MHz, CDCl₃) 7.38-7.26 (m, 6H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.80 (d, *J* = 8.7 Hz, 2H), 4.56 (s, 2H), 4.28 (t, *J* = 8.1 Hz, 2H), 3.76 (s, 3H), 3.34 (t, *J* = 7.5 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃) 154.8, 153.1, 140.9, 136.8, 128.6, 128.3, 127.6, 124.1, 113.9, 64.5, 55.4, 49.3, 45.3; IR (KBr) 3059, 3000, 2946, 2830, 1680, 1573, 1507, 1485, 1454, 1435, 1356, 1293, 1266, 1241, 1203, 1180, 1124, 1105 cm⁻¹; Anal. Calcd for C₁₇H₁₈N₂O₂: C, 72.32; H, 6.43; N, 9.92. Found: C, 72.20; H, 6.65; N, 9.82.

1-((Z)-4-(3-benzyloxazolidin-2-ylideneamino)phenyl)ethanone **3ad**

white solid, mp 80-81 °C; ^1H NMR (600 MHz, CDCl_3) 7.87 (d, $J = 8.4$ Hz, 2H), 7.36-7.29 (m, 5H), 7.14 (d, $J = 8.4$ Hz, 2H), 4.59 (s, 2H), 4.34 (t, $J = 7.2$ Hz, 2H), 3.41 (t, $J = 7.8$ Hz, 2H), 2.54 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) 153.8, 153.1, 136.3, 131.0, 129.4, 128.7, 128.3, 127.8, 123.4, 64.8, 49.1, 45.1, 26.4; IR (KBr) 3063, 3029, 2911, 1671, 1590, 1556, 1486, 1451, 1427, 1411, 1380, 1354, 1294, 1271, 1205, 1172, 1116, 1089, 1065, 1025 cm^{-1} ; Anal. Calcd for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2$: C, 73.45; H, 6.16; N, 9.52. Found: C, 73.1; H, 6.36; N, 9.41.

(Z)-N-(3-benzyloxazolidin-2-ylidene)naphthalen-1-amine **3ae**

yellow solid, mp 85-86 °C; ^1H NMR (270 MHz, CDCl_3) 8.24 (t, $J = 5.1$ Hz, 1H), 7.78 (t, $J = 4.3$ Hz, 1H), 7.51-7.24 (m, 9H), 7.19 (d, $J = 6.2$ Hz, 1H), 4.74 (s, 2H), 4.29 (t, $J = 7.0$ Hz, 2H), 3.43 (t, $J = 7.8$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3) 153.1, 144.2, 136.8, 134.3, 129.5, 128.7, 128.3, 127.7, 127.7, 125.9, 125.5, 124.7, 124.2, 122.0, 117.6, 64.5, 49.4, 45.3; IR (KBr) 3041, 2975, 2923, 2879, 2358, 1662, 1568, 1488, 1358, 1267, 1098, 1014, 938 cm^{-1} ; Anal. Calcd for $\text{C}_{20}\text{H}_{16}\text{N}_2\text{O}$: C, 79.44; H, 6.00; N, 9.26. Found: C, 79.43; H, 5.98; N, 9.20.

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¹H and ¹³C spectra

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 EXMOD NON
 OBSRO 270.05 MHz
 OBSRT 112.00 KHz
 OBSIN 5800.0 Hz
 POINT 32768
 PREOU 5405.4 Hz
 SCANS 8
 ACQTM 6.062 sec
 PD 0.935 sec
 PW1 6.0 us
 IRNTC 1H
 CTENP 20.9 c
 SLVNT CDCL3
 EXREF 7.24 ppm
 BP 0.12 Hz
 RGAIN 21

FILE C:\Documents and Settings\Admin\My Docu
 NAME 4ca
 DATE 10/10/2007
 INSTR Bruker Avance DPX 500
 PROC 13C
 OBPRO 150.91 MHz
 OBSRT 7.89 KHz
 OBSFQ 8.8 Hz
 POINT 32768
 PREOU 35971.2 Hz
 SCANS 8
 ACQTM 0.000 sec
 PD 0.000 sec
 PW1 10.0 us
 INTC 0.0 c
 CTMP 77.00 ppm
 SLVT EXREF
 BP 0.12 Hz
 RGAIN 0

FILE C:\Documents and Settings\Admin\My Documents\Chemistry\NMR\3da C13.a1s
 NAME 3da
 DATE 10/10/2007
 TIME 15:09
 INSTR 13C
 PULPROG zgpg30
 PROCNO 1
 F2 150.91 MHz
 F1 7.89 KHz
 OBSRV 32768
 POINT 1
 PREP 35971.2 Hz
 SCANS 8
 ACQTM 0.000 sec
 PD 0.000 sec
 PM1 10.0 uA
 INTC 0.0 c
 CTMP 77.00 ppm
 SLVT 0.12 Hz
 EXREF 0
 RGAIN 0

PRF1 C:\Documents and Settings\adm\My Docu
 COUNT Tue Dec 21 15:31:11 2004
 DATUM
 ORNTC 1H
 EXMOD NON
 OBPRO 300.40 MHz
 OBSRT 130.00 KHz
 OBSIN 1150.0 Hz
 POINT 32768
 PREOU 6020.4 Hz
 SCANS 8
 ACQTM 5.443 sec
 PD 1.554 sec
 PW1 5.5 us
 IRNTC 1H
 CTEMP 20.4 C
 SLVNT CDCL3
 EXREF 7.24 ppm
 BP 0.12 Hz
 RGAIN 18

PRF C:\Documents and Settings\Admin\My Docu
 CONT Tue Dec 21 16:26:44 2004
 DATM 13C
 ORNT 13C
 EXNO BCM
 OBPRO 75.45 MHz
 OBSRT 124.00 KHz
 OBFIN 1840.0 Hz
 POINT 32768
 PREOU 204 08.1 Hz
 SCANS 1072
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 5.0 ua
 IRNTC 1H
 CTMP 20.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BP 0.12 Hz
 RGAIN 25

PRF1 C:\Documents and Settings\Admin\My Documents\Chemistry\4a\4a.a1s
 COMPT fms-052-4-1
 DATIM Tbu Nov 25 14:04:09 2004
 OBNTC 1H
 EXMOD NON
 OBPRO 300.40 MHz
 OBSRT 130.00 KHz
 OBSIN 1150.0 Hz
 POINT 32768
 PREOU 6013.2 Hz
 SCANS 8
 ACQTM 5.449 sec
 PD 1.551 sec
 PW1 5.5 us
 IRNTC 1H
 CTENC 21.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BP 0.12 Hz
 RGAIN 17

C:\Documents and Settings\Admin\My Documents\Chemistry\4a\4a C13.als
fms-052-4-1

PF1 C:\Documents and Settings\Admin\My Documents\Chemistry\4a\4a C13.als
NAME fms-052-4-1
DATE NOV 25 14:25:31 2004
PROC 13C
INSTR BNM
PULPRO 75.45 MHz
PROBHD 124.00 KHz
OBPNT 1840.0 Hz
POINT 32768
PREOU 20408.1 Hz
SCANS 402
ACQTM 1.606 sec
PD 1.394 sec
PW1 5.0 us
IRNTC 1H
CTEMP 22.5 c
SLVNT CDCl3
EXREF 77.00 ppm
BP 0.12 Hz
RGAIN 25

C:\Documents and Settings\Admin\My Documents\ftmura\NMR\fil\^3fa.a1s
 fms-03s-2

PR1E C:\Documents and Settings\Admin\My Documents\ftmura\NMR\Docu
 COMPT fms-03s-2
 DATE Tue Jun 29 17:33:19 2004
 PROC 1H
 EXNO 1
 EXNO2 NON
 OBSFREQ 270.05 MHz
 OBSFREQ2 112.00 KHz
 OBSFREQ3 5800.0 Hz
 POINT 32768
 PREOU 5405.4 Hz
 SCANS 8
 ACQTM 6.062 sec
 PD 0.935 sec
 PW1 5.5 us
 IRNTC 1H
 CTMP 21.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BP 0.12 Hz
 RGAIN 9

PRF C:\Documents and Settings\Admin\My Documents\Chemistry\3fa C13.a1a
 COMPT 13C
 DATUM
 OBPRO 150.91 MHz
 OBSRT 7.89 KHz
 OBFIN 8.8 Hz
 POINT 32768
 FREOU 35971.2 Hz
 SCANS 8
 ACQTM 0.000 sec
 PD 0.000 sec
 PW1 10.0 us
 IRNDC 0.0 c
 CTMP
 SLVNT
 EXREF 77.00 ppm
 BP 0.12 Hz
 RGAIN 0

C:\Documents and Settings\Admin\My Documents\mura\NMR\fil\^3ab.a1s
fms-02-2

PRF1 C:\Documents and Settings\Admin\My Docu
 COMPT fms-02-2 14:12:18 2004
 DATUM F-1 Jun 04
 ORNOC 1H
 EXMOD NON
 OBPRO 300.40 MHz
 OBSRT 130.00 KHz
 OBPIN 1150.0 Hz
 POINT 32768
 PREOU 6020.4 Hz
 SCANS 8
 ACQTM 5.443 sec
 PD 1.554 sec
 PW1 5.5 us
 IRNOC 1H
 CTENP 19.4 C
 SLVNT CDCL3
 EXREF 7.24 ppm
 BP 0.12 Hz
 RGAIN 8

C:\Documents and Settings\Admin\My Documents\Chemistry\fil\^13ab C13.als
 fma-075-2

FILE C:\Documents and Settings\Admin\My Docu
 NAME fma-075-2
 DATE Thu May 06 16:41:01 2004
 INSTR 13C
 PROC BCM
 EXPRO 75.45 MHz
 OBSRT 124.00 KHz
 OBSIN 1840.0 Hz
 POINT 32768
 PREOU 204 08.1 Hz
 SCANS 116
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 4.0 us
 INTC 1H
 CTMP 21.2 c
 STVT CDCL3
 EXREF 77.00 ppm
 BP 0.12 Hz
 RGAIN 25

PRF1 C:\Documents and Settings\adm\my Docu
 t6-089-4
 COUNT 16
 DATE 14-Apr-07 14:46:24 2005
 PULPROG zgpg30
 OBSN 1
 EXNO 1
 EXMOD NON
 OBPRO 300.40 MHz
 OBSRT 130.00 KHz
 OBFIN 1150.0 Hz
 POINT 32768
 PREOU 6013.2 Hz
 SCANS 8
 ACQTM 5.449 sec
 PD 1.551 sec
 PW1 5.5 us
 IRNTC 1H
 CTEMP 20.5 C
 SLYNT CDCl3
 EXREF 7.24 ppm
 BP 0.12 Hz
 RGAIN 21

PROB	13C
NAME	13C
DATE	
TIME	
INSTR	150.91 MHz
PROBHD	7.89 KHz
PULPROG	8.8 Hz
PC	32768
PD	35971.2 Hz
PR	8
RG	0.000 sec
RGAIN	0.000 sec
RGAIN	10.0 ua
RGAIN	0.0 c
RGAIN	77.00 ppm
RGAIN	0.12 Hz
RGAIN	0

FILE C:\Documents and Settings\Admin\My Documents\3ad\3ad.alc
 NAME 3ad
 DATE 11/11/2011
 TIME 11:11:11
 INSTR 1H
 PULPROG zgpg30
 PROCNO 1
 F2 600.13 MHz
 F1 3.70 KHz
 AQ 3.2768
 SFO 32768
 POU 8389.3 Hz
 SCANS 8
 ACQ 0.000 sec
 PD 0.000 sec
 PM 10.0 us
 INTC 0.0 c
 CTMP 7.24 ppm
 SLVT 0.12 Hz
 EXRF 0
 RGAIN 0

FILE C:\Documents and Settings\Admin\My Documents\Chemistry\3ad\13C.als
 NAME 3ad
 DATE 10/10/2007
 TIME 15:09:15
 INSTR 13C
 PULPROG zgpg30
 PROCNO 1
 F2 150.91 MHz
 F1 7.89 KHz
 AQ 8.8 Hz
 SFO 32768
 POINT 1
 PREP 35971.2 Hz
 SCANS 8
 ACQ 0.000 sec
 PD 0.000 sec
 PM 10.0 us
 INTC 0.0 c
 CTMP 77.00 ppm
 SLVT 0.12 Hz
 EXREF 0
 RGAIN 0

PRF1 C:\Documents and Settings\adamr\My Documents\ftmrm\NMR\fil\73aeal3.sals
 COMPT fm7-045-6
 DATUM Thu May 26 20:03:56 2005
 PNTM 1H
 EXMOD NON
 OBSRO 270.05 MHz
 OBSRT 112.00 KHz
 OBSIN 5800.0 Hz
 POINT 32768
 PREOU 5405.4 Hz
 SCANS 8
 ACQTM 6.062 sec
 PD 0.935 sec
 PW1 6.0 us
 IRNTC 1H
 CTEMP 22.7 c
 SLYNT CDCl3
 EXREF 7.24 ppm
 BP 0.12 Hz
 RGAIN 20

FILE C:\Documents and Settings\Admin\My Documents\Chemistry\3ae 13C.als
 NAME 3ae
 DATE 10/10/2007
 TIME 10:10:10
 INSTR 13C
 PULPROG zgpg30
 PROCNO 1
 F2 150.91 MHz
 F1 7.89 KHz
 AQ 8.8 Hz
 POINT 32768
 PREP 35971.2 Hz
 SCANS 8
 ACQ 0.000 sec
 PD 0.000 sec
 PM 10.0 us
 INTC 0.0 c
 CTMP 77.00 ppm
 SLVT 0.12 Hz
 EXREF 0
 RGAIN 0