Electronic Supplementary Information

Intramolecular Azide-Alkyne [3+2] Cycloaddition: Versatile Route to New Heterocyclic Structural Scaffolds

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Characterization data for the new compounds

(*S*)-(1-Azido-2-(prop-2-ynyloxy)ethyl)benzene (3): Colorless oil; $[\alpha]_D$ 71.6 (*c* 1.1, $CHCl_3$); IR (thin film) 2359, 2341 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.44-7.35 (m, 5H), 4.77 (dd, *J* = 8.6, 4.2 Hz, 1H), 4.26 (dd, *J* = 8.4, 2.4 Hz, 2H), 3.80 (dd, *J* = 10.1, 4.2 Hz, 1H), 3.74 (dd, *J* = 10.1, 8.6 Hz, 1H), 2.48 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 136.4, 128.9, 128.8, 128.1, 127.1, 127.0, 79.1, 75.1, 73.5, 65.1, 58.6. HRMS (ESI, *m/z*) calculated for $C_{11}H_{12}N_3O$ (MH^+) 202.0980, found 202.0938.

(*S*)-(1-Azido-2-(but-2-ynyloxy)ethyl)benzene (4): Colorless oil; $[\alpha]_D$ 97.2 (*c* 1.4, $CHCl_3$) IR (thin film) 2241, 2098 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.44-7.35 (m, 5H), 4.76 (dd, *J* = 8.8, 4.4 Hz, 1H), 4.27-4.19 (m, 2H), 3.77 (dd, *J* = 10, 8.8 Hz, 1H), 3.70 (dd, *J* = 10, 8.8 Hz, 1H), 1.87 (t, *J* = 2.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.7 MHz) δ 136.6, 129.0, 128.8, 128.6, 127.1, 127.0, 83.2, 74.5, 733, 65.2, 59.1, 3.7. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 2216.1137, found 216.1124.

(*S*)-7-Phenyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-C][1,4]oxazine (5). White solid; mp. 90-91 °C; $[\alpha]_D$ 67.9 (*c* 1.2, $CHCl_3$); IR (thin film) 2359, 2343 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.62 (s, 1H), 7.42-7.35 (m, 3H), 7.17-7.14 (m, 2H), 5.66 (t, *J* = 5.0 Hz, 1H), 5.10 (d, *J* = 15.1 Hz, 1H), 5.04 (d, *J* = 15.1 Hz, 1H), 4.30 (dd, *J* = 12.1, 4.3 Hz, 1H), 4.08 (dd, *J* = 12.1, 5.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 136.6, 131.3, 129.0, 128.9, 128.8, 128.1, 127.0 (2C), 70.6, 62.6, 59.8. HRMS (ESI, *m/z*) calculated for $C_{11}H_{12}N_3O$ (MH^+) 202.0980, found 202.0925.

(*S*)-3-Methyl-7-phenyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-C][1,4]oxazine (6). White solid; mp. 101-103 °C; $[\alpha]_D$ 77.1 (*c* 0.8, $CHCl_3$); ^1H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.31 (m, 3H), 7.13-7.10 (m, 2H), 5.56 (t, *J* = 4.5 Hz, 1H), 4.96 (d, *J* = 14.8 Hz, 1H), 4.89 (d, *J* = 14.8 Hz, 1H), 4.20 (dd, *J* = 12.1, 4.3 Hz, 1H), 3.99 (dd, *J* = 12.1, 5.5 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 135.5, 135.4, 135.2, 134.5, 128.5, 127.6,127.4,127.2, 68.8, 61.2, 58.5, 8.0. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 216.1137, found 216.1126.

(*R*)-(2-Azido-1-(prop-2-ynyloxy)ethyl)benzene (7). Colorless oil; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.44-7.34 (m, 5H), 4.79 (dd, *J* = 8.2, 3.9 Hz, 1H), 4.25 (dd, *J* = 15.8, 2.4 Hz, 1H), 3.98 (dd, *J* = 15.8, 2.3 Hz, 1H), 3.58 (dd, *J* = 12.6, 8.2 Hz, 1H), 3.29 (dd, *J* = 12.6, 3.9Hz, 1H), 2.47 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 137.6, 129.1, 128.9, 128.6, 127.2, 127.0, 79.8, 79.1, 74.9,56.4, 55.9. HRMS (ESI, *m/z*) calculated for $C_{11}H_{12}N_3O$ (MH^+) 202.0980, found 202.0990.

(*R*)-(2-Azido-1-(but-2-ynyloxy)ethyl)benzene (8). Colorless oil; IR (thin film) 2221, 2110 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.42-7.33 (m, 5H), 4.74 (dd, *J* = 8.1, 4.2 Hz, 1H), 4.19 (dd, *J* = 15.2, 2.3 Hz, 1H), 3.95 (dd, *J* = 15.2, 2.3 Hz, 1H), 3.56 (dd, *J* = 12.9, 8.1 Hz. 1H), 3.30 (dd, *J* = 12.9, 4.0 Hz, 1H), 1.88 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 138.1, 128.8 (2C), 128.6, 127.0, 83.0, 79.5, 74.6, 56.7, 56.3, 3.7. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 216.1137, found 216.1129.

(*R*)-6-Phenyl-6,7-dihydro-4*H*-[1,2,3]triazolo[5,1-*c*][1,4]oxazine (9). White solid; mp. 136-137 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.58 (s, 1H), 7.51-7.43 (m, 5H), 5.27 (d, *J*=15.2 Hz, 1H), 5.03 (d, *J*=15.2 Hz, 1H), 4.91 (dd, *J* = 10.6, 3.4 Hz, 1H), 4.76 (dd, *J*=13.1, 3.3 Hz, 1H), 4.33 (dd, *J*=13.1, 10.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 136.9, 130.4, 129.1, 129.0, 128.8, 128.2, 126.3, 126.1, 75.7, 62.3, 51.1. HRMS (ESI, *m/z*) calculated for $C_{11}H_{12}N_3O$ (MH^+) 202.0980, found 202.0980.

(*R*)-3-Methyl-6-phenyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazine (10). White solid; mp. 100-102 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.31 (m, 3H), 7.13-7.10 (m, 2H), 5.56 (t, *J*=4.5 Hz, 1H), 4.96 (d, *J*=14.8 Hz, 1H), 4.89 (d, *J*=14.8 Hz, 1H), 4.20 (dd,

J=12.1, 4.3 Hz, 1H), 3.99 (dd, *J*=12.1, 5.5 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 135.5, 135.4, 135.2, 134.5, 128.5, 127.6, 127.4, 127.2, 68.8, 61.2, 58.5, 8.0. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 216.1137, found 202.1126.

(*S*)-(2-Azido-3-(prop-2-ynyloxy)propyl)benzene (12). Colorless oil; $[\alpha]_D$ -3.9 (*c* 1.3, $CHCl_3$); IR (thin film) 2120, 2111 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38-7.22 (m, 5H), 4.20-4.16 (m, 2H), 3.81-3.70 (m, 1H), 3.63 (dd, *J* = 10, 2.2 Hz, 1H), 3.54 (dd, *J* = 9.9, 6.2 Hz, 1H), 2.93 (dd, *J* = 13.7, 6.5 Hz, 1H), 2.82 (dd, *J* = 14, 7 Hz, 1H), 2.48 (t, *J* = 2.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.7 MHz) δ 137.4, 128.9, 128.7, 128.6, 126.9, 83.5, 74.6, 71.1, 62.8, 59.3, 37.5. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 216.1137, found 216.1127.

(*S*)-(2-Azido-3-(but-2-ynyloxy)propyl)benzene (13). Colorless oil; $[\alpha]_D$ -11.2 (*c* 1.4, $CHCl_3$); IR (thin film) 2123, 2102 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37-7.25 (m, 5H), 4.19-4.18 (m, 2H), 3.80-3.74 (m, 1H), 3.63 (dd, *J* = 10, 4 Hz, 1H), 3.54 (dd, *J* = 9.6, 6.4 Hz, 1H), 2.93 (dd, *J* = 14, 6.4 Hz, 1H), 2.82 (dd, *J* = 14, 8 Hz, 1H), 1.877 (t, *J* = 2.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.7 MHz) δ 137.2, 129.5, 129.4, 128.9, 128.6, 126.8, 83.1, 74.6, 71.0, 62.6, 59.1, 37.3, 8.8. HRMS (ESI, *m/z*) calculated for $C_{13}H_{16}N_3O$ (MH^+) 230.1217, found 230.1208.

(*S*)-7-Benzyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazine (14). White solid; mp. 118-120 °C; $[\alpha]_D$ -49.5 (c 1.1, CHCl3); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.54 (s, 1H), 7.40-7.36 (m, 2H), 7.33-7.28 (m, 3H), 4.98-4.82 (m, 2H), 4.76-4.71 (m, 1H), 3.93-3.84 (m, 2H), 3.66 (dd, *J* = 13.6, 4 Hz, 1H), 3.14 (dd, *J* = 14, 3.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.7 MHz) δ 135.9, 130.5, 129.5, 128.9, 128.2, 127.3, 66.0, 62.5, 56.9, 38.5, 29.7. HRMS (ESI, *m/z*) calculated for $C_{12}H_{14}N_3O$ (MH^+) 216.1137, found 216.1145.

(*S*)-7-Benzyl-3-methyl-6,7-dihydro-4H-[1,2,3]triazolo[5,1-c][1,4]oxazine (15). White solid; mp. 133-134 °C; $[\alpha]_D$ -40.6 (*c* 0.9, $CHCl_3$); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38-7.27 (m, 5H), 4.90-4.79 (m, 2H), 4.69-4.64 (m, 1H), 3.89-3.79 (m, 2H), 3.63 (dd, *J* = 13.6, 4 Hz, 1H), 3.11 (dd, *J* = 13.6, 4.2 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.7

MHz) δ 136.9, 135.9, 129.5, 128.9, 127.2, 126.9, 65.8, 62.3, 56.8, 38.4, 10.1. HRMS (ESI, *m/z*) calculated for $C_{13}H_{16}N_3O$ (MH^+) 230.1217, found 230.1206.

1-Azido-2-(but-2-ynyloxy)cyclohexane (20). Colorless oil; IR (thin film) 2241, 2096 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 4.27 (q, *J* = 2.3, 2H), 3.38-3.26 (m, 2H), 2.20-2.10 (m, 1H), 2.05-1.96 (m, 1H), 1.88 (t, *J* = 2.3 Hz, 3H), 1.78-1.69 (m, 2H), 1.35-1.22 (m, 4H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 82.2, 80.1, 75.3, 64.4, 57.2, 30.4, 30.3, 24.0, 23.7, 3.71. HRMS (ESI, *m/z*) calculated for $C_{10}H_{16}N_3O$ (MH^+) 194.1293, found 194.1290.

5a,6,7,8,9,9a-Hexahydro-4*H*-benzo[*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (21). As the precursor azidoalkyne **19** was found to undergo partial cyclization during chromatographic purification, it was subjected directly to the cycloaddition reaction step to afford the product **21** as a white solid; mp. 102-104 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.50 (s, 1H), 5.11 (d, *J* = 15.0 Hz, 1H), 4.91 (d, *J* = 15.0 Hz, 1H), 4.02-3.94 (m, 1H), 3.45 (ddd, *J* = 11.0, 9.4, 4.0 Hz, 1H), 3.08-3.01 (m, 1H), 2.22-2.15 (m, 1H), 2.00-1.90 (m, 2H), 1.70-1.40 (m, 4H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 130.8, 128.3, 78.6, 62.3, 61.1, 30.4, 28.1, 24.0, 23.9. HRMS (ESI, *m/z*) calculated for $C_9H_{14}N_3O$ (MH^+) 180.1137, found 180.1133.

3-Methyl-5a,6,7,8,9,9a-hexahydro-4*H*-benzo[*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (22). White solid; mp. 126-127 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 4.99 (d, *J*=14.8 Hz, 1H), 4.82 (d, *J*=14.82 Hz, 1H), 3.96-3.88 (m, 1H), 3.40 (ddd, *J*=11.0, 9.4, 4.0 Hz, 1H), 3.05-2.98 (m, 1H), 2.26 (s, 3H), 2.21-2.15 (m, 1H), 1.98-1.91 (m, 2H), 1.65-1.40 (m, 4H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 137.0, 127.3, 78.5, 62.1, 61.2, 30.2, 28.0, 24.0, 23.6, 10.0. HRMS (ESI, *m/z*) calculated for $C_{10}H_{16}N_3O$ (MH^+) 194.1293, found 194.1289.

1-Azido-2-(prop-2-ynyloxy)-2,3-dihydro-1*H*-indene (29). Colorless oil; IR (thin film) 2361, 2339, 2094 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.39-7.24 (m, 4H), 4.84 (d, *J* = 5.3 Hz, 1H), 4.44 (ddd, *J* = 7.8, 6.3, 5.3 Hz, 1H), 4.36 (t, *J* = 2.5 Hz, 2H), 3.37 (dd, *J* = 16.0, 7.1 Hz, 1H), 2.95 (dd, *J* = 16.0, 6.3 Hz, 1H), 2.53 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 139.5, 137.9, 129.2, 127.5, 125.2, 125.0, 124.6, 85.0, 79.3, 75.0, 69.8, 57.4, 36.5. HRMS (ESI, *m/z*) calculated for $C_{12}H_{12}N_3O$ (MH^+) 214.0980, found 214.0982.

1-Azido-2-(but-2-ynyloxy)-2,3-dihydro-1*H*-indene (30). Colorless oil; IR (thin film) 2361, 2341, 2095 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.39-7.24 (m, 4H), 4.83 (d, *J* = 5.3 Hz, 1H), 4.43 (ddd, *J* = 7.0, 6.3, 5.3 Hz, 1H), 4.31 (quin, *J* = 2.3 Hz, 2H), 3.35 (dd, *J* = 15.9, 7.0 Hz, 1H), 2.94 (dd, *J* = 15.9, 6.3 Hz, 1H), 1.91 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 139.6, 138.0, 129.1, 127.6, 127.4, 125.2, 125.0, 124.6, 84.5, 69.8, 57.9, 36.7, 3.8. HRMS (ESI, *m/z*) calculated for $C_{13}H_{14}N_3O$ (MH^+) 228.1137, found 228.1145.

1-Azido-2-(but-2-ynyloxy)-1,2,3,4-tetrahydronaphthalene (32). Colorless oil; IR (thin film) 2223, 2098 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.42-7.37 (m, 1H), 7.28-7.22 (m, 2H), 7.17-7.10 (m, 1H), 4.56 (d, *J* = 6.1 Hz, 1H), 4.32-4.28 (m, 2H), 4.05-3.96 (m, 1H), 2.98-2.90 (m, 1H), 2.87-2.78 (m, 1H), 2.24-2.15 (m, 1H), 2.00-1.92 (m, 1H), 1.90 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 135.4, 131.3, 128.2, 127.7, 127.0, 125.4, 81.1, 75.7, 73.9, 62.3, 55.9, 25.0, 23.7, 2.9. HRMS (ESI, *m/z*) calculated for $C_{14}H_{16}N_3O$ ($M + H^+$) 242.1293, found 242.1289.

4,5a,6,10b-Tetrahydroindeno[2,1-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (33). White solid; mp. 164-165 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.15 (d, *J* = 6.4 Hz, 1H), 7.61 (s, 1H), 7.41-7.35 (m, 3H), 5.33 (d, *J* = 15.1 Hz, 1H), 5.28 (d, *J* = 9.2 Hz, 1H), 5.15 (d, *J* = 15.1 Hz, 1H), 4.11 (ddd, *J* = 13.8, 11.1, 9.2 Hz, 1H), 3.28 (dd, *J* = 14.0, 6.6 Hz, 1H), 3.13 (dd, *J* = 13.8, 11.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 137.5, 135.0, 130.8, 129.0, 128.8, 128.7, 125.9, 125.4, 83.1, 83.0, 64.2, 33.6. HRMS (ESI, *m/z*) calculated for $C_{12}H_{12}N_3O$ (MH^+) 214.0980, found 214.0978.

3-Methyl-4,5a,6,10b-Tetrahydroindeno[2,1-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (34). White solid; mp. 168-170 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ 8.13 (d, *J* = 6.9 Hz, 1H), 7.39-7.34 (m, 3H), 5.22 (d, *J* = 14.7 Hz, 1H), 5.21 (d, *J* = 5.0 Hz, 1H), 5.05 (d, *J* = 14.7 Hz, 1H), 4.08 (ddd, *J* = 11.0, 6.6, 5.0 Hz, 1H), 3.27 (dd, *J* = 14.0, 6.6 Hz, 1H), 3.10 (dd, *J* = 14.0, 11.0 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 137.5, 135.1, 129.6, 128.7, 127.8, 127.2, 125.6, 125.2, 83.0, 64.2, 64.1, 33.6, 10.2. HRMS (ESI, *m/z*) calculated for $C_{13}H_{14}N_3O$ (MH^+) 228.1137, found 228.1125.

5a,6,7,11b-Tetrahydro-4*H*-naphtho[2,1-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (35). As the precursor azidoalkyne **31** was found to undergo partial cyclization during chromatographic purification, it was subjected directly to the cycloaddition reaction step to afford the product **35** as a white solid; mp. 121-122 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.54 (t, *J* = 3.4 Hz, 1H), 7.61 (s, 1H), 7.35-7.28 (m, 2H), 7.27-7.18 (m, 1H), 5.33 (d, *J* = 9.4 Hz, 1H), 5.18 (d, *J* = 14.8 Hz, 1H), 4.93 (d, *J* = 14.8 Hz, 1H), 3.90 (m, 1H), 3.18-3.07 (m, 2H), 2.48-2.36 (m, 1H), 2.18-2.07 (m, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 135.6, 132.3, 132.0, 128.5, 128.2, 128.1, 127.7, 126.5, 62.7 (2C), 61.5, 27.4, 26.2. HRMS (ESI, *m*/*z*) calculated for $C_{13}H_{14}N_3O$ (MH^+) 228.1137, found 228.1133.

3-Methyl-5a,6,7,11b-Tetrahydro-4*H*-naphtho[2,1-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (36). White solid; mp. 92-94 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.55-8.47 (m, 1H), 7.35-7.28 (m, 2H), 7.25-7.18 (m, 1H), 5.27 (d, *J* = 9.7 Hz, 1H), 5.04 (d, *J* = 14.6 Hz, 1H), 4.83 (d, *J* = 14.6 Hz, 1H), 3.87-3.81 (m, 1H), 3.18-3.06 (m, 2H), 2.49-2.35 (m, 1H), 2.33 (s, 3H), 2.14-2.04 (m, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 135.8, 134.5, 131.1, 127.7, 127.4, 127.0, 126.6, 125.4, 61.5 (2C), 60.3, 26.3, 25.2, 9.0. HRMS (ESI, *m*/*z*) calculated for $C_{14}H_{16}N_3O$ (MH^+) 242.1293, found 242.1285.

3-Azido-4-(prop-2-ynyloxy)tetrahydrofuran (43). Colorless oil; IR (thin film) 2241, 2104 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.40-4.20 (m, 3H), 4.12-4.00 (m, 3H), 3.85 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.83 (dd, *J* = 10.2, 2.3 Hz, 1H), 2,53 (t, *J* = 2.3 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 83.0, 78.8, 75.8, 72.4, 71.6, 64.9, 57.2. HRMS (ESI, *m*/*z*) calculated for $C_7H_{10}N_3O$ (MH^+) 168.0733, found 168.0743.

3-Azido-4-(but-2-ynyloxy)tetrahydrofuran (44). Colorless oil; IR (thin film) 2237, 2101 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.25-4.19 (m, 3H), 4.10-3.99 (m, 3H), 3.84 (dd, *J* = 10.6, 2.2 Hz, 1H), 3.81 (dd, *J* = 10.2, 2.5 Hz, 1H), 1.89 (t, *J* = 2.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 83.7, 82.5, 74.2, 71.9, 70.9, 65.1, 57.7, 3.63. HRMS (ESI, *m*/*z*) calculated for $C_8H_{12}N_3O$ (MH^+) 182.0929, found 182.0934.

***tert*-Butyl 3-azido-4-(prop-2-ynyloxy)pyrrolidine-1-carboxylate (45).** Light yellow oil; IR (thin film) 2106, 1694 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz; rotameric mixture) δ 4.28

(dd, *J* = 16.0, 2.4 Hz, 1H), 4.21 (d, *J* = 16.0 Hz, 1H), 4.16-4.05 (m, 2H), 3.70-3.57 (m, 2H), 3.53-3.36 (m, 2H), 2.52 (br s, 1H), 1.50 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz; rotameric mixture) δ 154.2, 80.6, 79.9, 78.8, 75.5, 63.5, 57.0, 49.4, 48.7, 28.4. HRMS (ESI, *m/z*) calculated for $C_{12}H_{19}N_4O_3$ (MH^+) 267.1457, found 267.1459.

***tert*-Butyl 3-azido-4-(but-2-ynyloxy)pyrrolidine-1-carboxylate (46).** Light yellow oil; IR (thin film) 2224, 2106, 1702 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz; rotameric mixture) δ 4.23 (dq, *J* = 15.4, 2.3 Hz, 1H), 4.16 (m, 1H), 4.12 (dd, *J* = 4.6, 2.3 Hz, 1H), 4.06 (dd, *J* = 5.6, 2.8 Hz, 1H), 3.70-3.56 (m, 2H), 3.52-3.38 (m, 2H), 1.89 (t, *J* = 2.3 Hz, 3H), 1.48 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz; rotameric mixture) δ 154.2, 83.7, 80.2, 79.9, 74.2, 63.6, 57.6, 49.5, 48.7, 28.5, 3.64. HRMS (ESI, *m/z*) calculated for $C_{13}H_{20}N_4O_3Na$ (MNa^+) 303.1433, found 303.1429.

5a,6,8,8a-Tetrahydro-4*H*-furo[3,4-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (47). Low melting solid; IR (thin film) 2359, 2341 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.59 (s, 1H), 5.32 (d, *J* = 15.2Hz. 1H), 5.11 (d, *J* = 15.2 Hz, 1H), 4.72 (dd, *J* = 8.0, 7.28 Hz, 1H), 4.43 (td, *J* = 9.6, 7.4 Hz, 1H), 4.22 (t, *J* = 7.3 Hz, 1H), 4.10 (m, 2H), 3.86 (dd, *J* = 10.0, 7.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 130.7, 128.9, 79.6, 65.9, 65.6, 64.3, 60.0. HRMS (ESI, *m/z*) calculated for $C_7H_{10}N_3O$ (MH^+) 168.0733, found 168.0756.

3-Methyl-5a,6,8,8a-Tetrahydro-4*H*-furo[3,4-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine (48). Low melting solid; IR (thin film) 2359, 2341,1753 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.21 (d, *J* = 15.0 Hz, 1H), 5.00 (d, *J* = 15.0 Hz, 1H), 4,69 (t, *J*=7.5 Hz, 1H), 4.38 (td, *J* = 9.6, 7.5 Hz, 1H), 4.21 (t, *J* = 7.5 Hz, 1H), 4.12-4.02 (m, 2H), 3.83 (dd, *J* = 10.0, 7.7 Hz, 1H), 2.30 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 137.8, 127.2, 79.7, 65.7, 65.0, 64.0, 58.4, 10.0. HRMS (ESI, *m/z*) calculated for $C_8H_{12}N_3O$ (MH^+) 182.0929, found 182.0931.

***tert*-Butyl 5a,6,8,8a-tetrahydropyrrolo[3,4-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine-7(4*H*)-carboxylate (49).** White solid; mp. 153-155 °C. ^{1}H NMR ($CDCl_3$, 400 MHz; rotameric mixture) δ 7.59 (s, 1H), 5.17 (d, *J* = 15.3 Hz, 1H), 5.09 (d, *J* = 15.3 Hz, 1H), 4.44 (dd, *J* = 9.9, 7.5 Hz, 1H), 4.37-4.28 (m, 1H), 4.01-3.94 (m, 2H), 3.57 (t, *J* = 10.3 Hz, 1H), 3.43-3.36 (m, 1H), 1.54 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz; rotameric mixture) δ 154.2,

130.5, 128.9, 80.7, 78.1, 63.9, 58.2, 45.6, 45.3, 28.3. HRMS (ESI, *m/z*) calculated for $C_{12}H_{19}N_4O_3$ (MH^+) 267.1457, found 267.1460.

***tert*-Butyl 3-methyl-5a,6,8,8a-tetrahydropyrrolo[3,4-*b*][1,2,3]triazolo[1,5-*d*][1,4]oxazine-7(4*H*)-carboxylate (50).** White solid; mp. 178-179 °C. ^{1}H NMR ($CDCl_3$, 400 MHz; rotameric mixture) δ 5.20 (d, *J* = 15.3 Hz, 1H), 5.00 (d, *J* = 15.3 Hz, 1H), 4.41 (dd, *J* = 9.9, 7.5 Hz, 1H), 4.32-4.23 (m, 1H), 3.99-3.89 (m, 2H), 3.54 (t, *J* = 10.3 Hz, 1H), 3.40-3.35 (m, 1H), 2.30 (s, 3H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz; rotameric mixture) δ 154.3, 137.9, 127.0, 80.7, 77.6, 63.8, 58.2, 45.6, 45.3, 28.4, 10.2. HRMS (ESI, *m/z*) calculated for $C_{13}H_{21}N_4O_3$ (MH^+) 281.1614, found 281.1602.

(*S*)-*tert*-Butyl 2-azido-1-phenylethyl(prop-2-ynyl)carbamate (53). Colorless oil; IR (thin film) 2218, 2102, 1690 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.55-7.27 (m, 5H), 4.87-4.75 (m, 1H), 4.0-3.82 (m, 2H), 3.63-3.40 (m, 2H), 2.50 (br s, 1H), 1.52 (br s, 9h); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 157.1, 132.3, 129.7, 128.2, 128.0, 120.9, 114.9, 83.6, 73.7, 65.1, 56.3, 51.8, 38.4, 30.3, 28.5. HRMS (ESI, *m/z*) calculated for $C_{16}H_{21}N_4O_2$ (MH^+) 301.1587, found 301.1595.

(*S*)-*tert*-Butyl 2-azido-1-phenylethyl(but-2-ynyl)carbamate (54). Colorless oil; IR (thin film) IR (thin film) 2123, 2102, 1695 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37-7.25 (m, 5H), 4.19-4.18 (m, 2H), 3.80-3.74 (m, 1H), 3.63 (dd, *J* = 10, 4 Hz, 1H), 3.54 (dd, *J* = 9.6, 6.4 Hz, 1H), 2.93 (dd, *J* = 14, 6.4 Hz, 1H), 2.82 (dd, *J* = 14, 8 Hz, 1H), 1.88 (t, *J* = 2.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 125.7 MHz) δ 137.2, 129.5, 129.4, 128.9, 128.6, 126.8, 83.1, 74.6, 71.0, 62.6, 59.1, 37.3, 3.6. HRMS (ESI, *m/z*) calculated for $C_{17}H_{23}N_4O_2$ (MH^+) 315.1821, found 315.1819.

(*S*)-*tert*-Butyl 6-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-*a*]pyrazine-5(4*H*)-carboxylate (55). Low melting solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.67 (s, 1H), 7.40-7.30 (m, 3H), 7.15-6.85 (m, 2H), 5.88-5.70 (m, 1H), 5.40-3.75 (m, 4H), 1.20 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 153.8, 131.0, 129.2, 128.9 (3C), 128.4, 126.5, 126.0, 59.6, 48.4, 39.1, 29.7, 27.9(3C). HRMS (ESI, *m/z*) calculated for $C_{16}H_{21}N_4O_2$ (MH^+) 301.1664, found 301.1657.

(*S*)-*tert*-Butyl3-Methyl-6-phenyl-6,7-dihydro-[1,2,3]triazolo[1,5-*a*]pyrazine-5(4*H*)-carboxylate (56). White soild; mp. 154-156 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40-7.25 (m, 3H), 7.35-6.80 (m, 2H), 5.76 (br s, 1H), 5.17 (d, *J* = 16.7 Hz, 1H), 4.80-3.70 (m, 3H), 2.35 (s, 3H), 1.49 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 153.9, 137.8, 131.0, 128.9 , 128.8, 128.3, 126.0, 81.0, 59.6, 48.3, 38.9, 27.9, 10.1. HRMS (ESI, *m/z*) calculated for $C_{17}H_{23}N_4O_2$ (MH^+) 315.1281, found 315.1281.

***tert*-Butyl 3-methyl-5a,6,7,8,9,9a-hexahydro-[1,2,3]triazolo[1,5-*a*]quinoxaline-5(4*H*)-carboxylate (60).** As the precursor azidoalkyne **59** was found to undergo partial cyclization during chromatographic purification, it was subjected directly to the cycloaddition reaction step to afford the product **60** as a white solid; mp. 166-167 °C; ^{1}H NMR ($CDCl_3$, 500 MHz, rotameric mixture) δ 5.23 (br s, 1H), 4.37 (s, 1H), 4.17 (d, *J* = 13.2 Hz, 1H), 3.11 (d, *J* = 11.4 Hz, 1H), 2.22 (s, 3H), 1.81-1.70 (m, 1H), 1.69-1.55 (m, 2H), 1.53-1.47 (m, 1H), 1.45 (s, 9H), 1.40-1.01 (m, 4H) ; ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 154.2, 138.2, 126.3, 81.2, 56.0, 52.2, 50.7, 37.2, 29.7, 28.4, 27.3, 24.6, 24.2, 19.1, 10.2. HRMS (ESI, *m/z*) calculated for $C_{15}H_{25}N_4O_2$ (MH^+) 293.1977, found 293.1978.

***tert*-Butyl 1-methyl-5,6,10b,12-tetrahydrobenzo[*f*][1,2,3]triazolo[1,5-*a*]quinoxaline-11(4a*H*)-carboxylate (64).** As the precursor azidoalkyne **63** was found to undergo partial cyclization during chromatographic purification, it was subjected directly to the cycloaddition reaction step to afford the product **64** as a white solid; mp. 161-163 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, mixture of rotamers) δ 7.25-7.14 (m, 3H), 7.03 (br s, 2H), 5.95 & 5.74 (d, *J* = 3.8 Hz, 1H), 5.10 & 4.91 (d, *J* = 16.7 Hz, 1H), 4.82 (br s, 1H), 3.79 & 3.68 (d, *J* = 16.9 Hz, 1H), 3.35-3.17 (m, 1H), 2.78-2.52 (m, 2H), 2.35-2.24 (m, 1H), 2.17 (s, 3H), 1.57 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, mixture of rotamers) δ 154.9, 137.7, 130.7, 129.4, 127.9, 127.2, 126.9, 126.8, 81.8, 54.1, 52.4, 36.4, 28.4, 25.0, 23.1, 10.1. HRMS (ESI, *m/z*) calculated for $C_{19}H_{25}N_4O_2$ (MH^+) 341.1977, found 341.1967.

***tert*-Butyl 3-azido-1,2,3,4-tetrahydronaphthalen-2-ylcarbamate (67).** Viscous oil; ^{1}H NMR ($CDCl_3$, 400 MHz, rotameric mixture) δ 7.49-7.01 (m, 4H), 4.65 (br s, 1H), 3.97 (br s, 1H), 3.88 (br s, 1H), 3.32-3.16 (m, 2H), 2.93 (dd, *J* = 17.0, 7.3 Hz, 1H), 2.73 (dd, *J*

= 16.8, 7.4 Hz, 1H), 1.49 (br s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 155.3, 149.9, 135.8, 134.4, 132.8, 130.9, 129.9, 129.4, 128.8, 127.7, 126.5, 120.1, 80.1, 61.3, 59.7, 53.3, 49.7, 34.6, 33.5, 29.7, 28.4, 26.0, 25.1, 21.8. HRMS (ESI, *m/z*) calculated for $C_{15}H_{20}N_4O_2Na$ (MNa^+) 311.1484, found 311.1490.

***tert*-Butyl 3-methyl-5a,6,11,11a-tetrahydrobenzo[*g*][1,2,3]triazolo[1,5-*a*]quinoxaline-5(4*H*)-carboxylate (69).** As the precursor azidoalkyne **63** was found to undergo partial cyclization during chromatographic purification, it was subjected directly to the cycloaddition reaction step to afford the product **69** as a white solid; mp. 172-174 °C; ^{1}H NMR ($CDCl_3$, 400 MHz, mixture of rotamers) δ 7.39-7.15 (m, 4H), 5.22 (d, *J* = 15.8 Hz, 1H), 4.44-4.37 (m, 1H), 4.18 (d, *J* = 15.8 Hz, 1H), 4.05 (dd, *J* = 16.4, 5.0 Hz, 1H), 3.89-3.80 (m, 1H), 3.68-3.53 (m, 2H), 3.15-3.06 (m, 1H), 2.36 (s, 3H), 1.48 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 154.8, 138.4, 137.9, 133.9, 133.5, 131.9, 129.9, 127.8, 127.0, 126.2, 126.1, 81.5, 61.3, 56.9, 56.5, 43.9, 37.2, 35.0, 32.3, 29.7, 28.4, 27.8, 26.1, 10.1. $C_{19}H_{25}N_4O_2$ (MH^+) 341.1977, found 341.1988.

***tert*-Butyl (3*R*,4*R*)-4-hydroxytetrahydrofuran-3-ylcarbamate (70).** Viscous oil; $[\alpha]_D$ -2.7 (*c* 0.7 $CHCl_3$); IR (thin film) 3410, 1700 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 5.01 (br s, 1H), 4.39 (br s, 1H), 4.25 (br s, 1H), 4.12-3.97 (m, 2H), 3.80 (d, *J* = 8.0 Hz, 1H), 3.52 (d, *J* = 7.7 Hz, 1H), 2.12 (d, *J* = 4.4 Hz 1H), 1.48 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 155.8, 80.1, 74.5, 70.9, 70.4, 53.6, 28.4. HRMS (ESI, *m/z*) calculated for $C_9H_{17}NO_4Na$ (MNa^+) 226.1055, found 226.1065.

***tert*-Butyl (3*S*,4*S*)-4-azidotetrahydrofuran-3-ylcarbamate (71).** White solid; mp. 86-87 °C; $[\alpha]_D$ -4.2 (*c* 1.1 $CHCl_3$); IR (thin film) 2099, 1697 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.74 (br s, 1H), 4.25-4.00 (m, 4H), 3.74 (d, *J* = 8.2 Hz, 1H), 3.67 (d, *J* = 9.7 Hz, 1H), 1.50 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 154.9, 80.4, 71.5, 71.1, 66.3, 57.2, 28.3. HRMS (ESI, *m/z*) calculated for $C_9H_{17}N_4O_3$ (MH^+) 229.1301, found 229.1313.

***tert*-Butyl (3*S*,4*S*)-4-azidotetrahydrofuran-3-yl(prop-2-ynyl)carbamate (72).** Colorless oil; IR (thin film) 2106, 1693 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.43-4.38 (m, 1H), 4.37-4.32 (m, 1H), 4.19 (dd, *J* = 9.8, 6.4 Hz, 1H), 4.10-3.95 (m, 4H), 3.67 (dd, *J*

= 9.8, 4.3 Hz, 1H), 2.27 (t, *J* = 2.4 Hz, 1H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 154.3, 81.8, 80.2, 71.8, 71.5, 68.8, 65.3, 63.4, 35.1, 28.4. HRMS (ESI, *m/z*) calculated for $C_{12}H_{18}N_4O_3Na$ (MNa^+) 289.1277, found 289.1291.

***tert*-Butyl (3*S*,4*S*)-4-azidotetrahydrofuran-3-yl(but-2-ynyl)carbamate (73).** Colorless oil; IR (thin film) 2224, 2104, 1697 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.40-4.35 (m, 2H), 4.16 (dd, *J* = 9.8, 6.4 Hz, 1H), 4.15-3.93 (m, 4H), 3.67 (dd, *J* = 9.8, 4.3 Hz, 1H), 1.83 (t, *J* = 2.4 Hz, 3H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 154.4, 81.3, 79.4, 75.3, 71.8, 68.9, 65.1, 63.3, 35.8, 28.4, 3.5. HRMS (ESI, *m/z*) calculated for $C_{13}H_{20}N_4O_3Na$ (MNa^+) 303.1433, found 303.1432.

(5a*S*,8a*S*)-*tert*-Butyl 5a,6,8,8a-tetrahydrofuro[3,4-*e*][1,2,3]triazolo[1,5-*a*]pyrazine-5(4*H*)-carboxylate (74). White solid; mp. 134-135 °C; $[\alpha]_D$ -35.3° (*c* 0.78 $CHCl_3$); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.65 (s, 1H), 4.87 (d, *J* = 16.8 Hz, 1H), 4.76 (d, *J* = 16.8 Hz, 1H), 4.73 (t, *J* = 7.7 Hz, 1H), 4.63-4.55 (m, 1H), 4.52 (dd, *J* = 10.0, 7.5 Hz, 1H), 4.21 (t, *J* = 9.2 Hz, 1H), 4.17 (t, *J* = 9.2 Hz, 1H), 3.65 (dd, *J* = 10.3, 6.8 Hz, 1H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 154.3, 131.4, 129.9, 82.3, 69.1, 65.3, 60.5, 60.0, 41.9, 28.3. HRMS (ESI, *m/z*) calculated for $C_{12}H_{19}N_4O_3$ (MH^+) 267.1457, found 267.1447.

(5a*S*,8a*S*)-*tert*-Butyl 3-methyl-5a,6,8,8a-tetrahydrofuro[3,4-*e*][1,2,3]triazolo[1,5-*a*]pyrazine-5(4*H*)-carboxylate (75). White solid; mp. 157-158 °C; $[\alpha]_D$ -31.3° (*c* 1.1 $CHCl_3$); ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.76 (d, *J* = 16.6 Hz, 1H), 4.69 (t, *J* = 7.8 Hz, 1H), 4.62 (d, *J* = 16.6 Hz, 1H), 4.60-4.52 (m, 1H), 4.50 (dd, *J* = 10.0, 7.4 Hz, 1H), 4.19 (dd, *J* = 9.8, 8.5 Hz, 1H), 4.14 (t, *J* = 9.4 Hz, 1H), 3.63 (dd, *J* = 10.2, 6.8 Hz, 1H), 2.33 (s, 3H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 154.5, 138.8, 127.9, 82.2, 69.3, 65.3, 60.6, 60.0, 41.7, 28.3, 10.2. HRMS (ESI, *m/z*) calculated for $C_{13}H_{21}N_4O_3$ (MH^+) 281.1614, found 281.1624.

(5a*S*,8a*S*)-4,5,5a,6,8,8a-Hexahydrofuro[3,4-*e*][1,2,3]triazolo[1,5-*a*]pyrazine TFA salt (76). Light yellow solid; mp. 248 °C (decomp); ^{1}H NMR (MeOD, 500 MHz) δ 7.84 (s, 1H), 4.98 (d, *J* = 16.5 Hz, 1H), 4.87-4.75 (m, 3H), 4.35 (t, *J* = 7.5 Hz, 1H), 4.17-4.11 (m, 2H), 3.99 (dd, *J* = 10.4, 7.9 Hz, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 130.4, 128.7, 65.7,

64.5, 58.0, 56.6, 41.2. HRMS (ESI, *m*/*z*) calculated for $C_7H_{11}N_4O$ (free amine) (MH^+) 167.0933, found 167.0933.

(5a*S*,8a*S*)-3-Methyl-4,5,5a,6,8,8a-hexahydrofuro[3,4-*e*][1,2,3]triazolo[1,5-*a*]pyrazine TFA salt (77). Light yellow solid; ^{1}H NMR (MeOD, 400 MHz) δ 4.86 (d, *J* = 16.2 Hz, 1H), 4.80-4.72 (m, 2H), 4.64 (d, *J* = 16.2 Hz, 1H), 4.33 (t, *J* = 7.5 Hz, 1H), 4.14-4.03 (m, 2H), 3.96 (dd, *J* = 10.4, 7.9 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 139.4, 125.3, 65.7, 64.6, 58.2, 57.0, 40.9, 8.3. HRMS (ESI, *m*/*z*) calculated for $C_8H_{13}N_4O$ (free amine) (MH^+) 181.1089, found 181.1094.

***tert*-Butyl (1*R*,2*S*)-2-hydroxy-1,2,3,4-tetrahydronaphthalen-1-ylcarbamate (78).** White solid; mp. (CH_2Cl_2–hexane) 111-112 °C; $[\alpha]_D$ 20.7 (*c* 1.2 $CHCl_3$). IR (thin film) 3400, 1711, 1693 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz, rotameric mixture) δ 7.36-7.32 (m, 1H), 7.25-7.20 (m, 2H), 7.16-7.11 (m, 1H), 4.96 (br s, 2H), 4.19 (d, *J* = 8.6 Hz, 1H), 3.05-2.90 (m, 1H), 2.85-2.75 (m, 2H), 2.08-1.90 (m, 2H), 1.48 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 157.1, 136.4, 134.8, 129.4, 128.7, 127.7, 126.5, 80.2, 69.6, 53.0, 28.4, 26.8, 26.2. HRMS (ESI, *m*/*z*) calculated for $C_{15}H_{21}NO_3Na$ (MNa^+) 286.1419, found 286.1411.

***tert*-Butyl (1*R*,2*R*)-2-azido-1,2,3,4-tetrahydronaphthalen-1-ylcarbamate (79).** White solid; mp. 81-82 °C; $[\alpha]_D$ 29.5 (*c* 0.8 $CHCl_3$); IR (thin film) 2095, 1686 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz, rotameric mixture) δ 7.36-7.28 (m, 1H), 7.26-7.21 (m, 2H), 7.14-7.10 (m, 1H), 4.80-4.74 (m, 2H), 3.88 (br s, 1H), 3.02-2.80 (m, 2H), 2.19-2.12 (m, 1H), 2.06-1.95 (m, 1H), 2.20-2.10 (m, 1H), 2.04-1.94 (m, 1H), 1.52 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 154.4, 134.8, 129.1, 127.8, 127.7, 126.7, 125.7, 79.1, 60.3, 52.3, 27.4, 25.0, 24.1. HRMS (ESI, *m*/*z*) calculated for $C_{15}H_{20}N_4O_2Na$ (MNa^+) 311.1484, found 311.1482.

(4a*R*,10b*R*)-*tert*-Butyl 1-methyl-5,6,10b,12-tetrahydrobenzo[*f*][1,2,3]triazolo[1,5-*a*]quinoxaline-11(4a*H*)-carboxylate (80). White solid; mp. 164-166 °C; $[\alpha]_D$ -14.1 (*c* 0.8 $CHCl_3$); ^{1}H NMR ($CDCl_3$, 400 MHz, rotameric mixture) δ 7.47-7.42 (m, 1H), 7.28-7.16 (m, 3H), 5.43 (d, *J* = 16.5 Hz, 1H), 4.63 (dd, *J* = 10.2, 2.3 Hz, 1H), 4.53 (d, *J* = 10.5

Hz, 1H), 4.35 (d, *J* = 16.6 Hz, 1H), 3.30 (br d, *J* = 12.9 Hz, 1H), 3.22-3.03 (m, 2H), 2.34 (s, 3H), 2.01 (dd, *J* = 12.4, 5.5 Hz, 1H), 1.08 (s, 9H); ^{13}C NMR ($CDCl_3$, 125.8 MHz, rotameric mixture) δ 155.1, 138.4, 133.9, 133.5, 128.9, 127.8, 127.0, 126.2, 126.1, 81.6, 61.3, 57.0, 43.9, 27.8, 27.7, 26.1, 10.1. HRMS (ESI, *m/z*) calculated for $C_{19}H_{25}N_4O_2$ (MH^+) 341.1977, found 341.1974.

(4a*R*,10b*R*)-1-Methyl-4a,5,6,10b,11,12-hexahydrobenzo[*f*][1,2,3]triazolo**[1,5-*a*]quinoxaline TFA salt (81).** Light yellow solid; mp. 272 °C (decomp); ^{1}H NMR (MeOD, 400 MHz) δ 7.57 (d, *J* = 6.5 Hz, 1H), 7.40-7.31 (m, 3H), 4.94-4.85 (m, 2H), 4.69 (d, *J* = 16.0 Hz, 1H), 4.60 (dd, *J* = 11.4, 2.9 Hz, 1H), 3.35-3.24 (m, 1H), 3.23-3.12 (m, 2H), 2.31 (s, 3H), 2.28-2.16 (m, 1H); ^{13}C NMR (MeOD, 125.8 MHz) δ 139.4, 136.0, 129.8, 129.1, 128.3, 126.7, 123.9, 123.7, 57.7, 56.3, 39.1, 26.7, 24.2, 8.2. HRMS (ESI, *m/z*) calculated for $C_{14}H_{17}N_4$ (MH^+) 241.1453, found 241.1446.

1-Azido-1-((prop-2-ynyloxy)methyl)cyclohexane (84). Colorless oil; IR (thin film) 2106 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.21 (d, *J* = 2.4 Hz, 2H), 3.50 (s, 2H), 2.45 (t, *J* = 2.4 Hz, 1H), 1.76-1.38 (m, 9H), 1.33-1.23 (m, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 80.1, 76.6, 74.7, 63.2, 58.7, 31.8, 31.5, 25.5, 22.3, 21.8. HRMS (ESI, *m/z*) calculated for $C_{10}H_{16}N_3O$ (MH^+) 194.1293, found 194.1302.

1-Azido-1-((but-2-ynyloxy)methyl)cyclohexane (85). Colorless oil; IR (thin film) 2106 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.10 (q, *J* = 2.3 Hz, 2H), 3.47 (s, 2H), 1.86 (t, *J* = 2.3 Hz, 3H), 1.76-1.68 (m, 2H), 1.66-1.53 (m, 5H), 1.48-1.38 (m, 2H), 1.33-1.22 (m, 1H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 82.7, 75.4, 74.9, 63.3, 59.3, 31.8, 31.7, 25.4, 21.8, 21.6, 3.7. HRMS (ESI, *m/z*) calculated for $C_{11}H_{18}N_3O$ (MH^+) 208.1450, found 208.1555.

4,6-Dihydrospiro[[1,2,3]triazolo[5,1-*c*][1,4]oxazine-7,1'-cyclohexane] (86). White solid; mp. 78-79 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 (s, 1H), 4.89 (s, 2H), 3.94 (s, 2H), 2.36-2.27 (m, 2H), 1.95-1.85 (m, 4H), 1.78-1.70 (m, 1H), 1.53-1.40 (m, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 130.0, 127.8, 70.3, 69.7, 60.3, 34.1, 34.0, 25.0, 22.5, 22.3. HRMS (ESI, *m/z*) calculated for $C_{10}H_{16}N_3O$ (MH^+) 194.1293, found 194.1300.

3-Methyl-4,6-Dihydrospiro[[1,2,3]triazolo[5,1-*c*][1,4]oxazine-7,1'-cyclohexane] (87). White solid; mp. 116-117 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.79 (s, 2H), 3.88 (s, 2H), 2.35-2.23 (m, 2H), 2.23 (s, 3H), 1.95-1.82 (m, 4H), 1.78-1.68 (m, 1H), 1.50-1.36 (m, 3H); ^{13}C NMR ($CDCl_3$, 125.8 MHz) δ 136.5, 128.3, 70.1, 62.6, 60.1, 34.0, 33.9, 25.1, 22.5, 22.4, 10.1. HRMS (ESI, *m*/*z*) calculated for $C_{11}H_{18}N_3O$ (MH^+) 208.1450, found 208.1457.

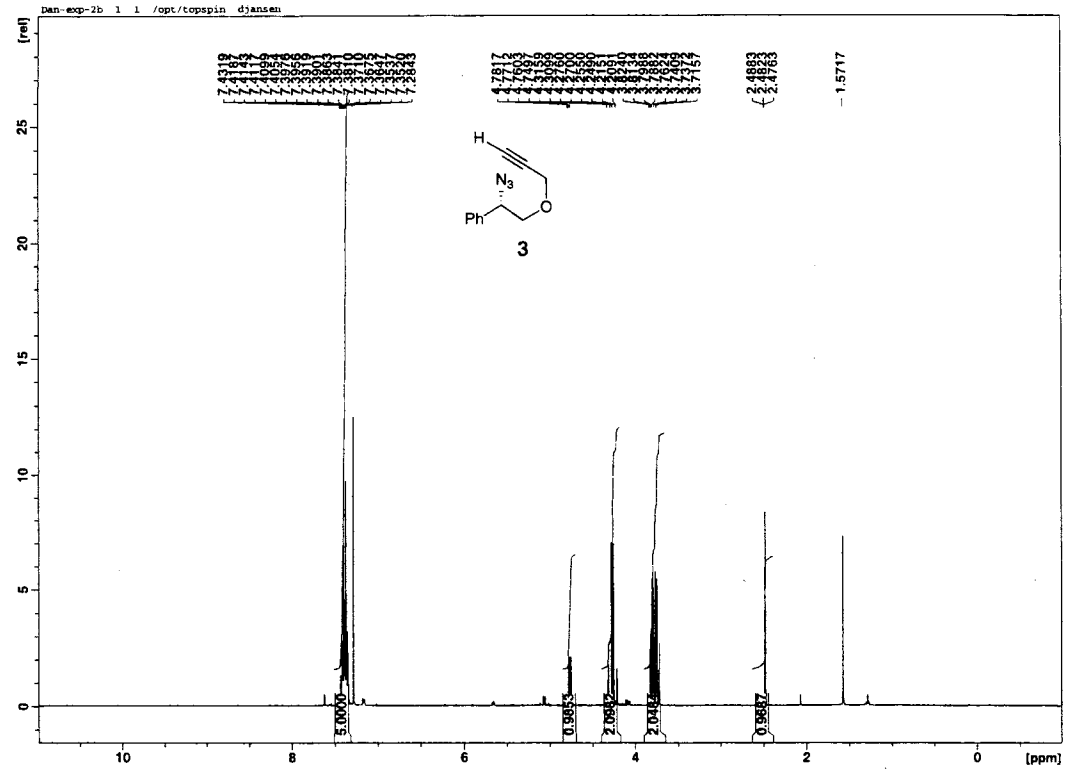
Electronic Supplementary Information

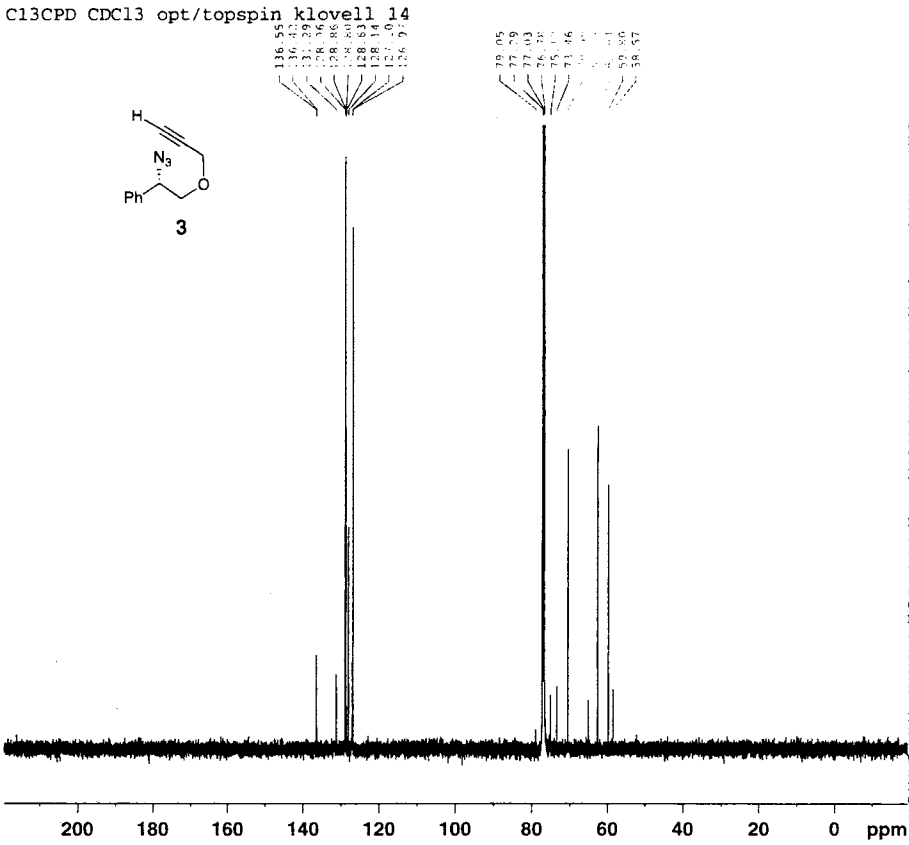
Intramolecular Azide-Alkyne [3+2] Cycloaddition: Versatile Route to New Heterocyclic Structural Scaffolds

*Rongti Li, Daniel J. Jansen, and Apurba Datta**

Department of Medicinal Chemistry, University of Kansas, 1251 Wescoe Hall Drive, Lawrence, KS 66045, USA

Copies of NMR Spectra of the New Compounds



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PROCNO                        1

F2 - Acquisition Parameters
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PULPROG                zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          768
DS                            4
SWH                30030.029 Hz
FIDRES             0.458222 Hz
AQ                 1.0912410 sec
RG                   14596.5
DW                    16.650 usec
DE                     6.00 usec
TE                    298.2 K
D1                 0.15000001 sec
d11                0.03000000 sec
DELTA              0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                      13C
P1                     11.00 usec
PL1                     2.20 dB
SFO1              125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     1.60 dB
PL12                   16.14 dB
PL13                   10.00 dB
SFO2              500.1320005 MHz

F2 - Processing parameters
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SF                125.7577890 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40
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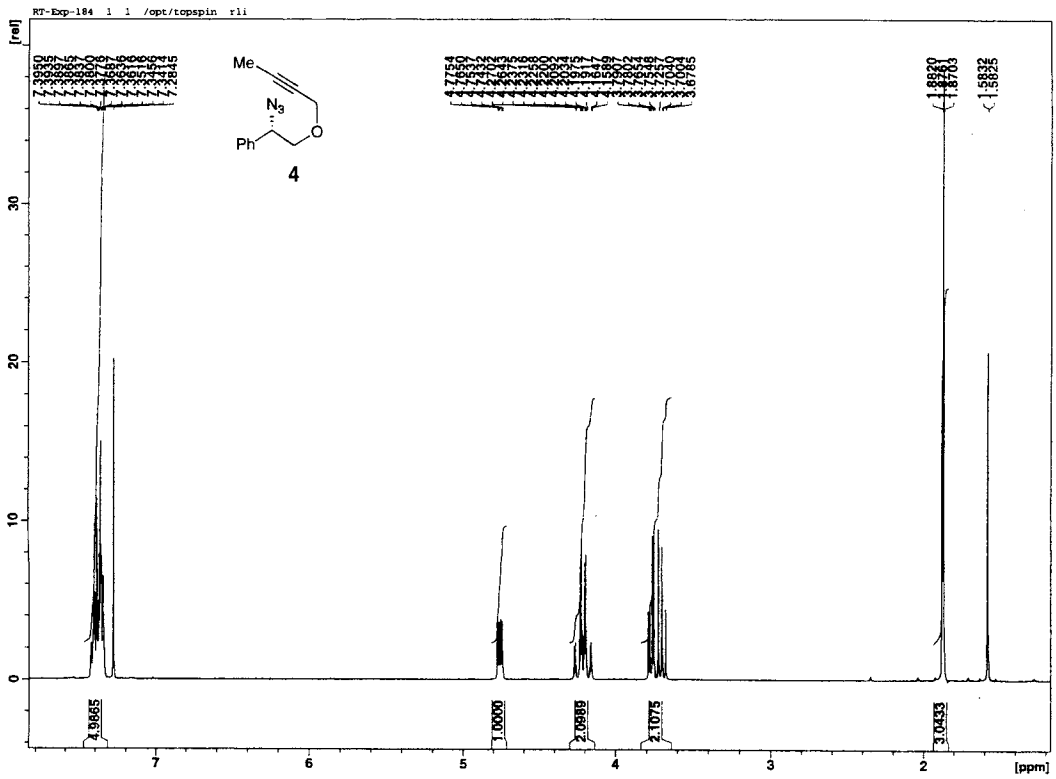
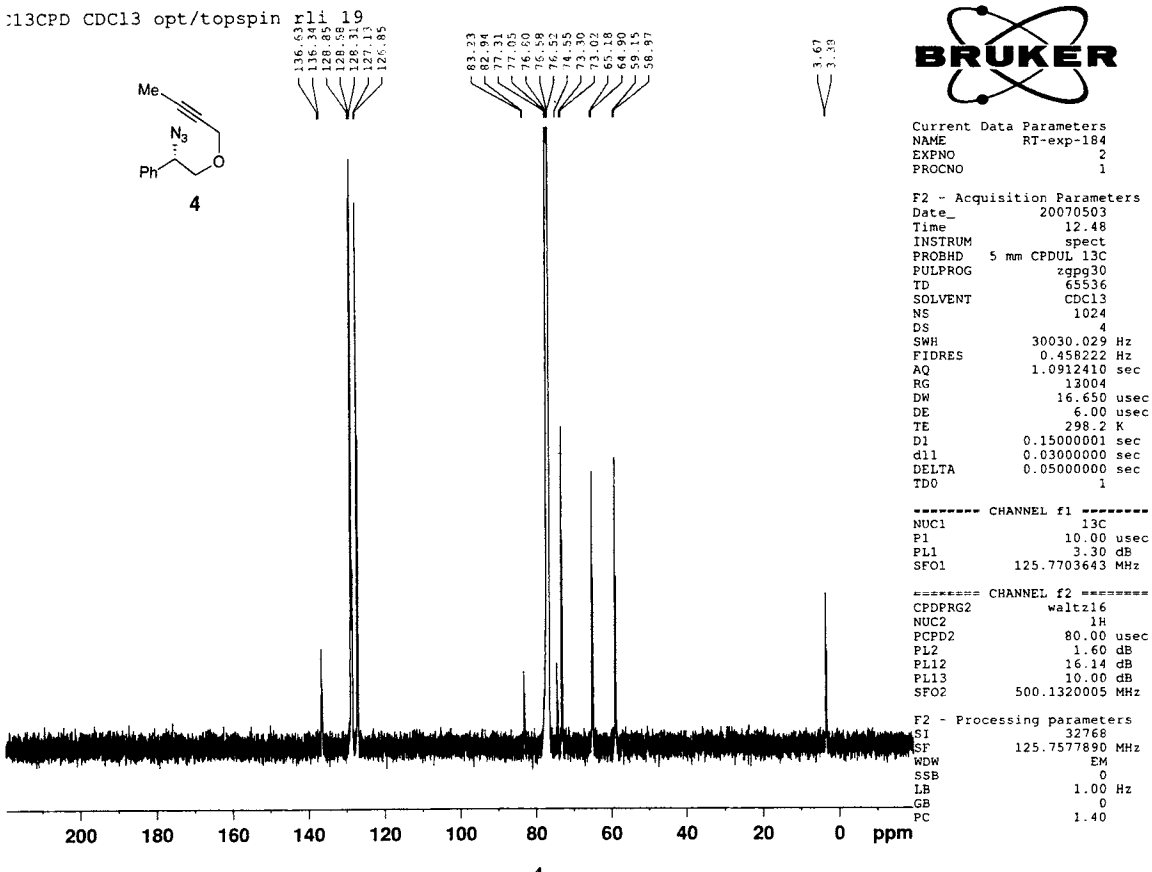




BRUKER

Current Data Parameters

NAME	RT-exp-184
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070503
Time	12.48
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	13004
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

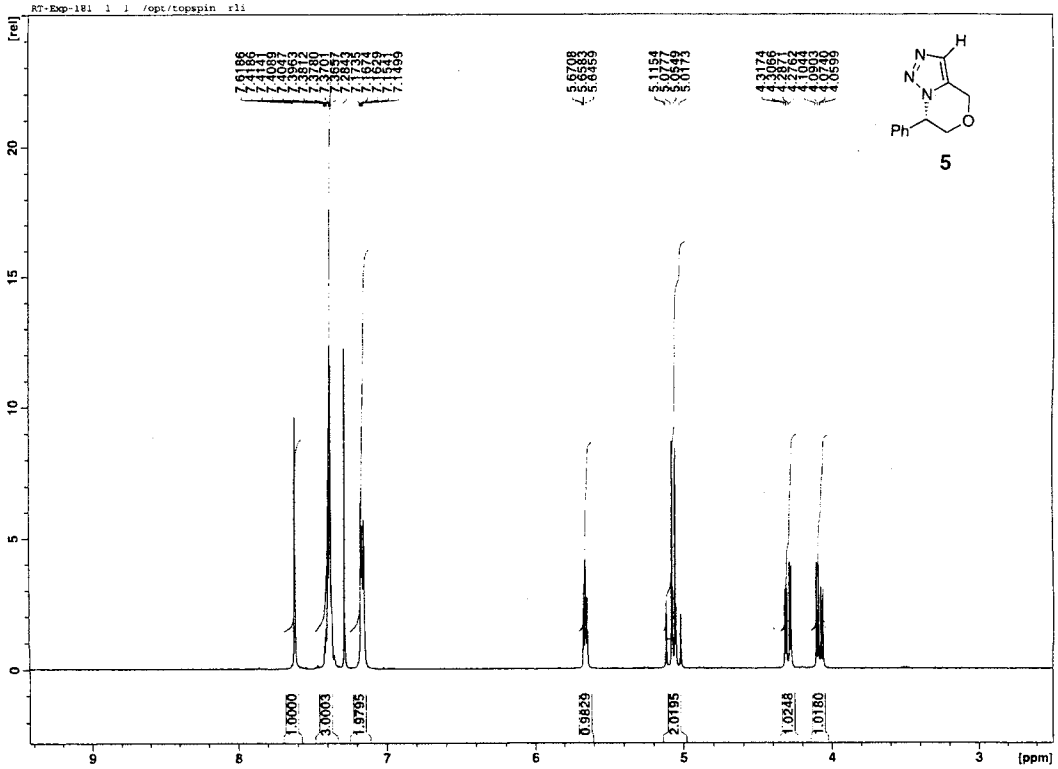
NUC1	13C
P1	10.00 usec
PL1	3.30 dB
SFO1	125.7703643 MHz

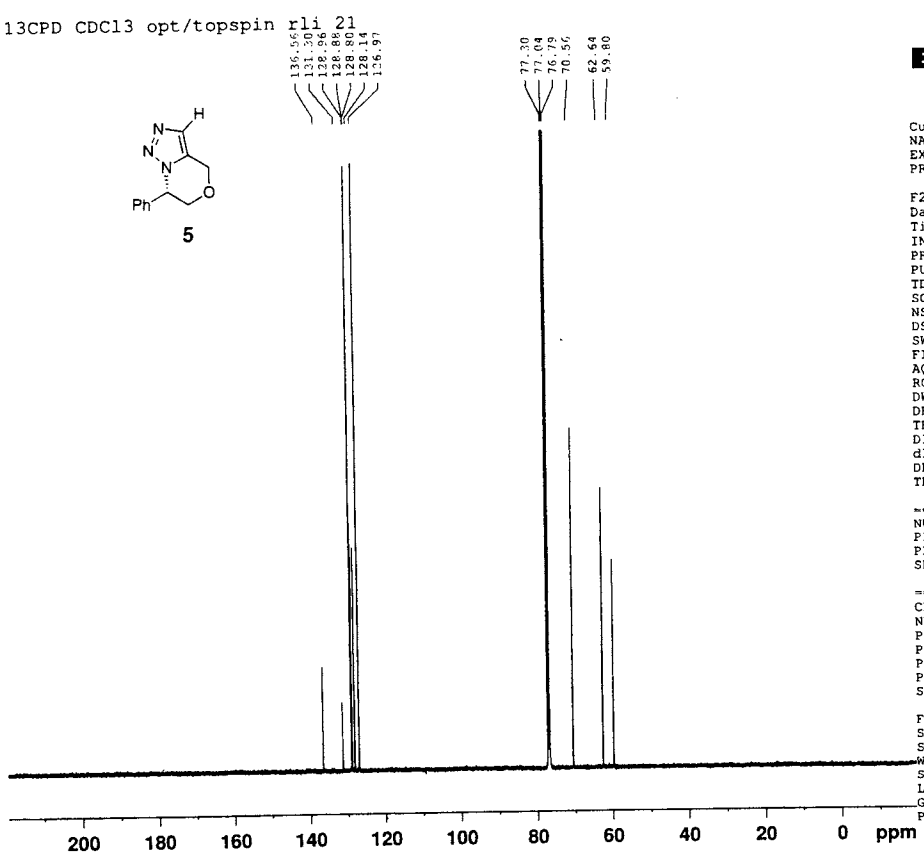
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





BRUKER

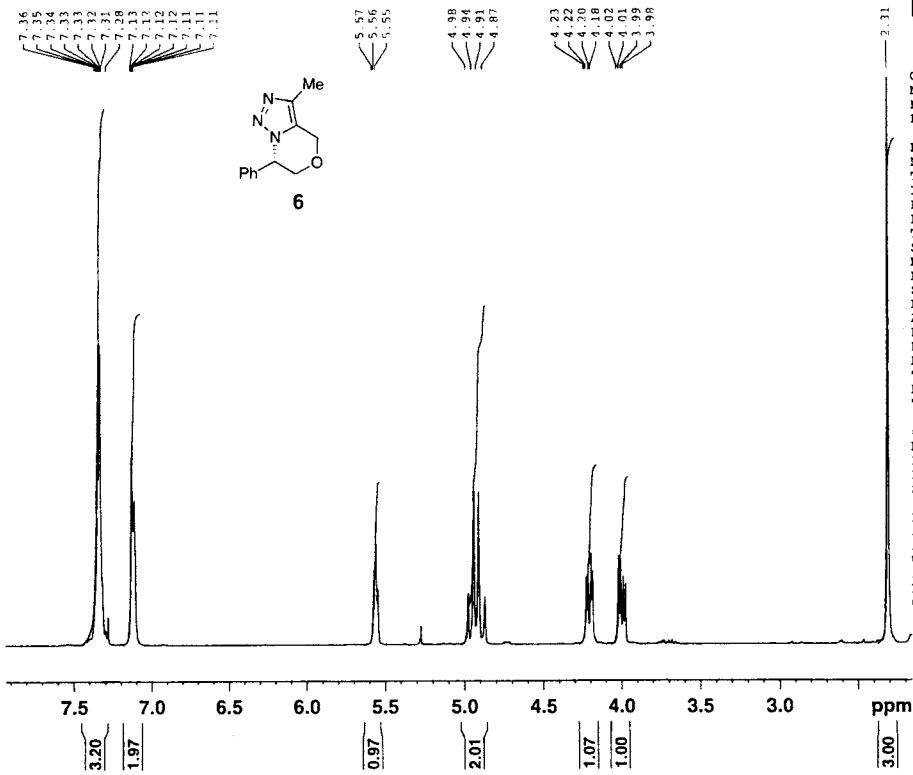
Current Data Parameters
NAME RT_exp_181
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070426
Time 19.53
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 768
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 11585.2
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.30 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



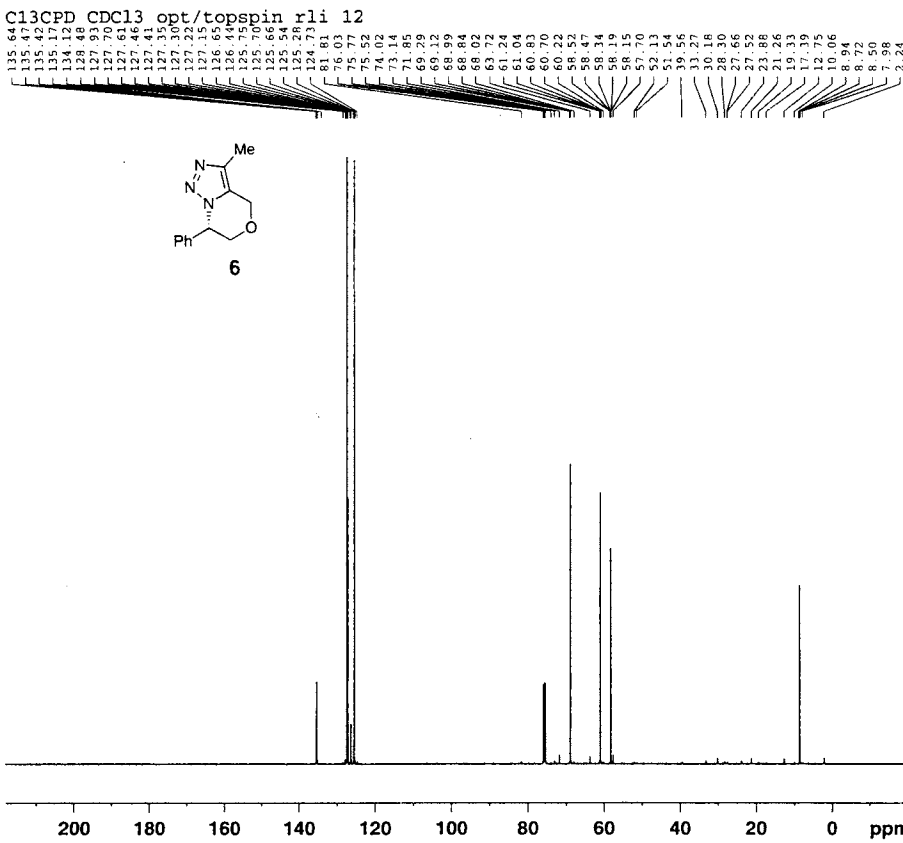
BRUKER

Current Data Parameters
NAME RT-Exp-187
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070507
Time 15.32
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 101.6
DW 60.400 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

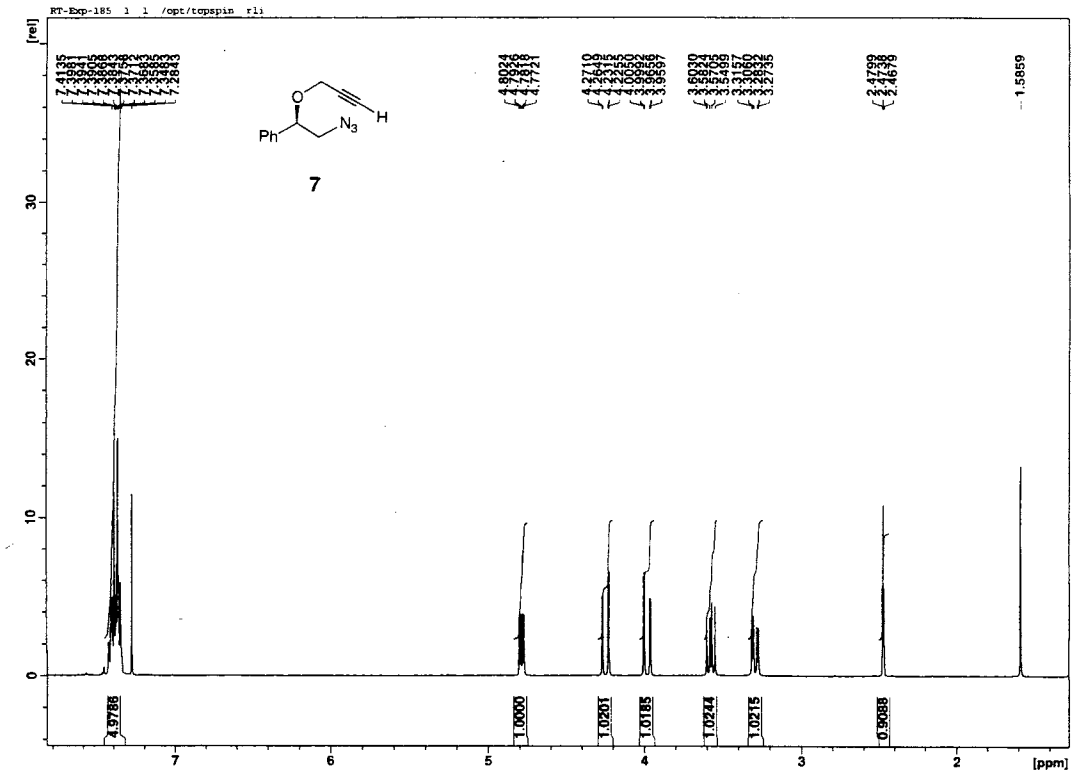
Current Data Parameters
NAME RT-exp-187
EXPNO 1
PROCNO 1

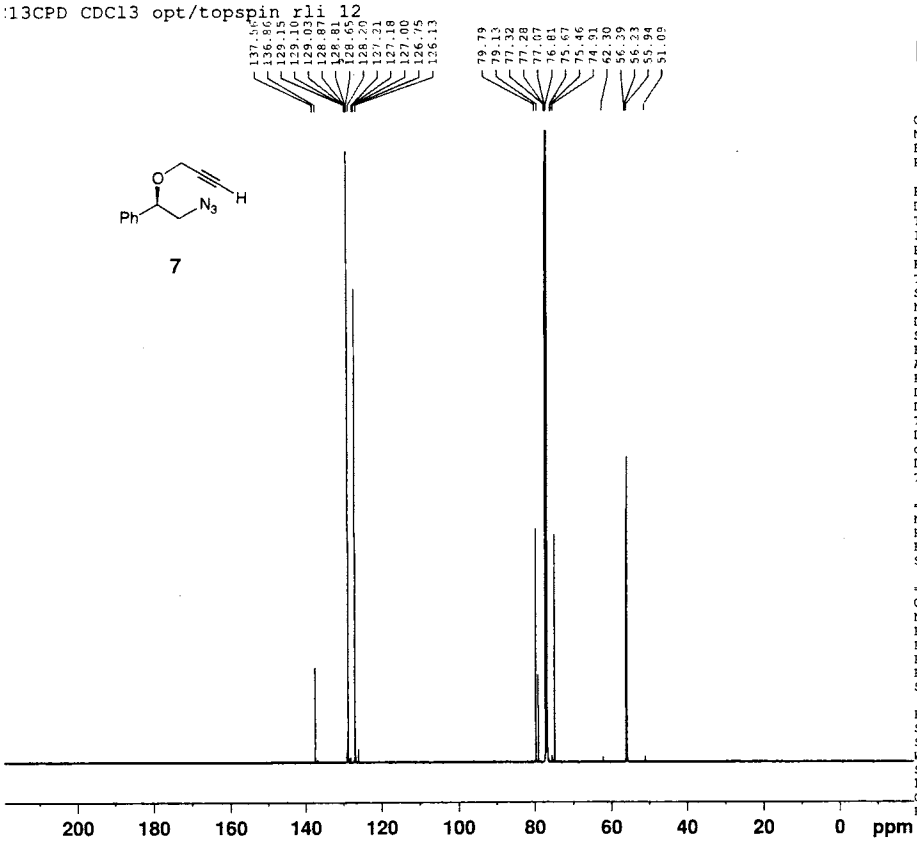
F2 - Acquisition Parameters
Date_ 20070507
Time 18.31
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 9195.2
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.30 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7579659 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





BRUKER

Current Data Parameters

NAME	RT-exp-185
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070502
Time	18.43
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1600
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	13004
DW	16.650 usec
DE	6.00 usec
TE	290.7 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

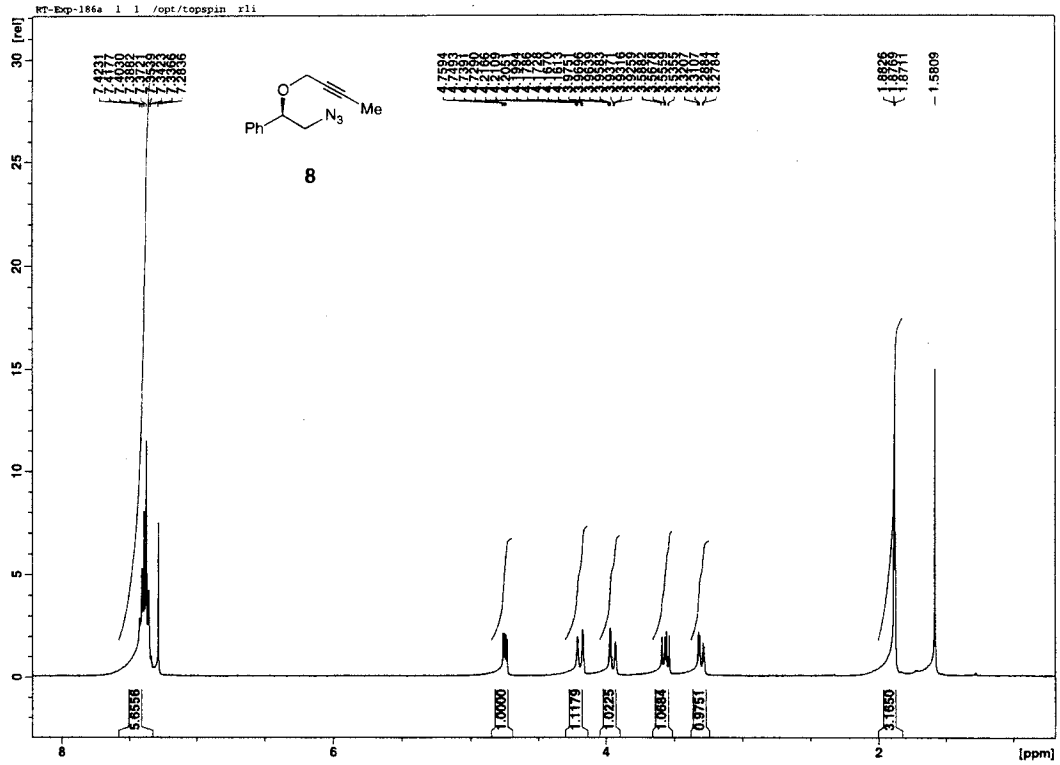
NUC1	13C
P1	10.00 usec
PL1	3.30 dB
SFO1	125.7703643 MHz

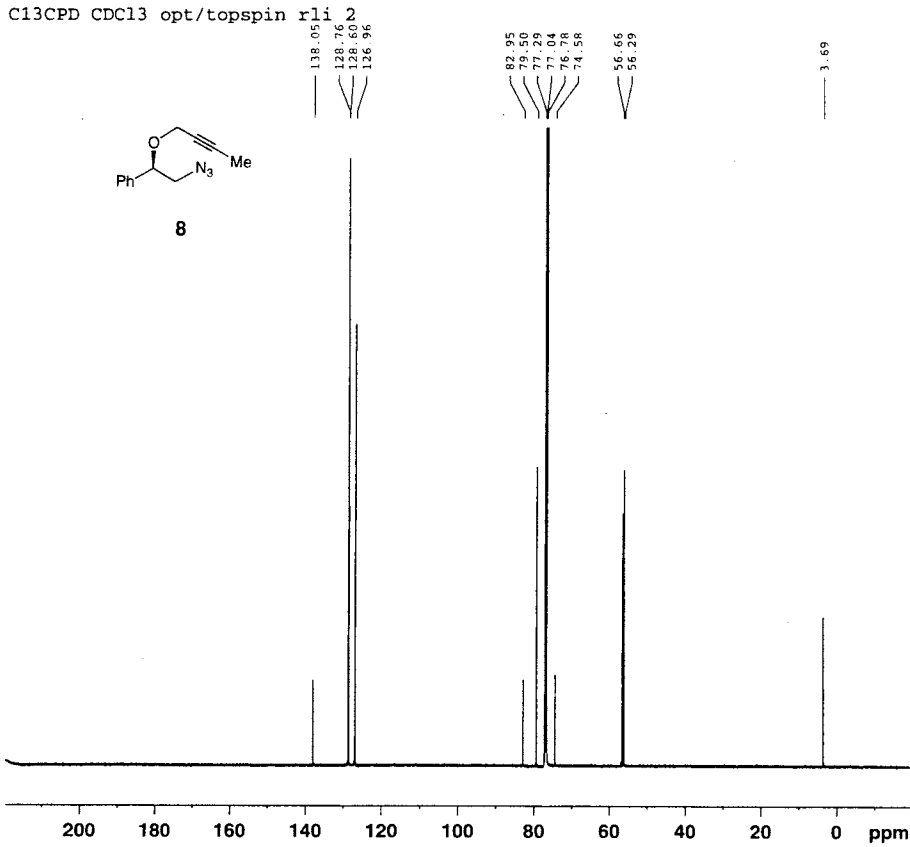
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





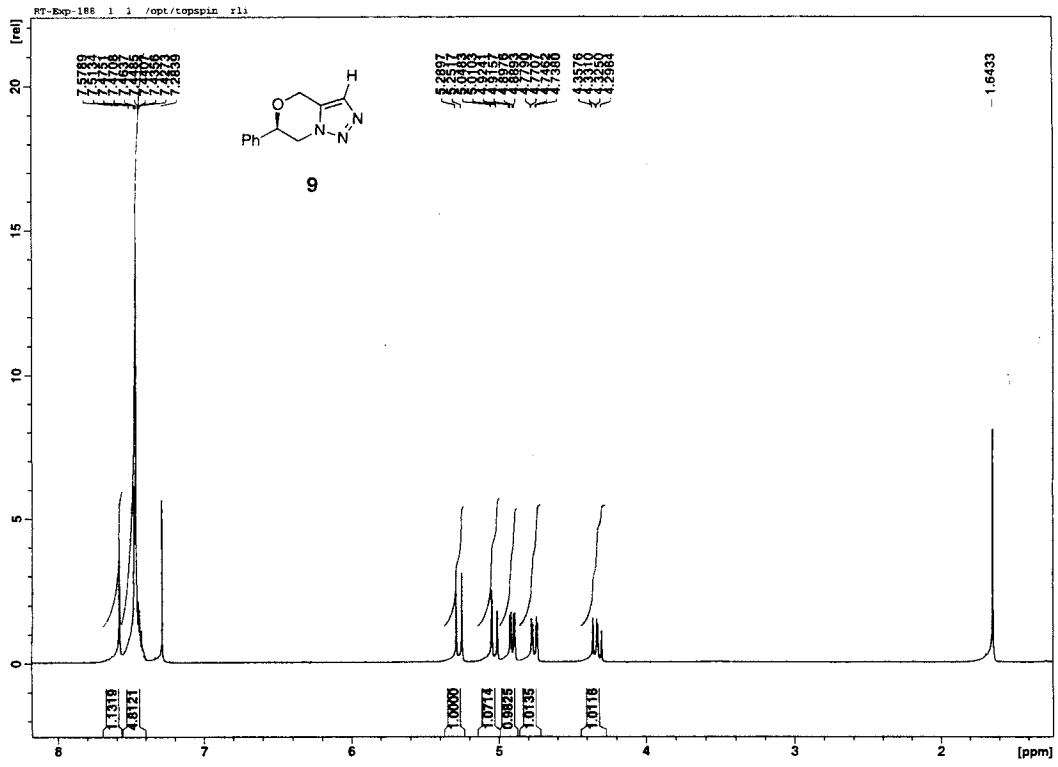
Current Data Parameters
NAME RT-exp-186
EXPNO 1
PROCNO 1

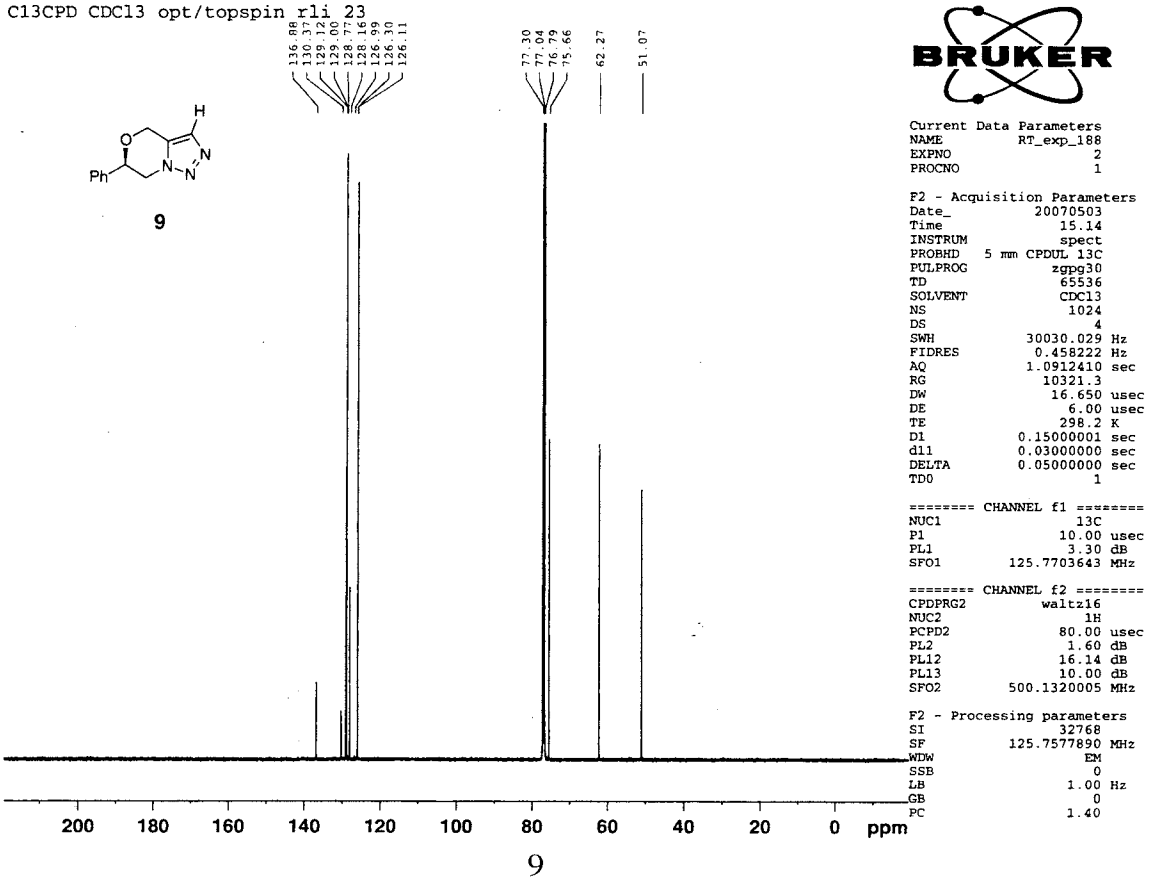
F2 - Acquisition Parameters
Date_ 20070504
Time 11.39
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.30 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters

NAME	RT_exp_188
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070503
Time	15.14
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	10321.3
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

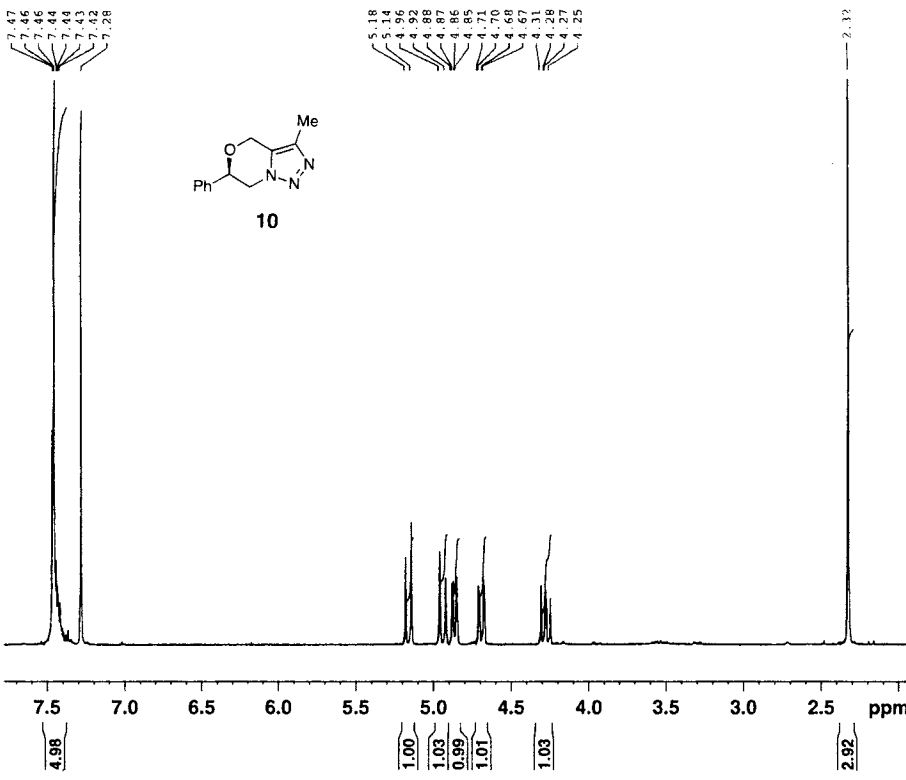
NUC1	13C
P1	10.00 usec
PL1	3.30 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

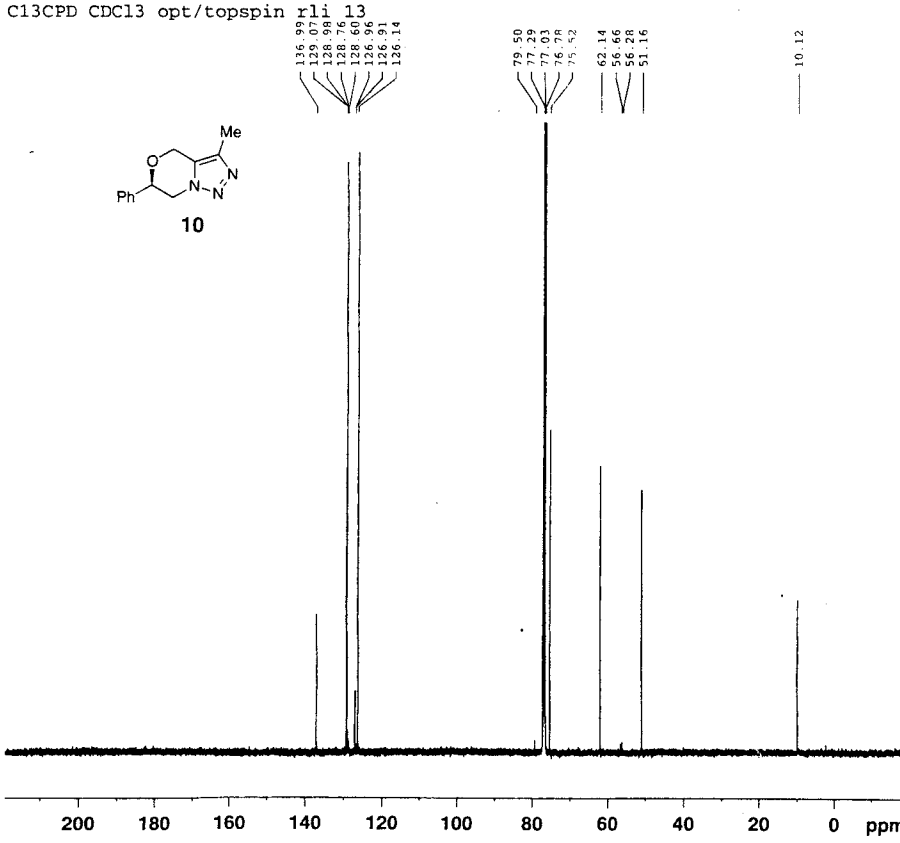
Current Data Parameters
NAME RT-Exp-189
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070507
Time 15.37
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 574.7
DW 60.400 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDCl3 opt/topspin rli 13



BRUKER

Current Data Parameters
NAME RT-exp-189
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070507
Time 18.58
INSTRUM spect
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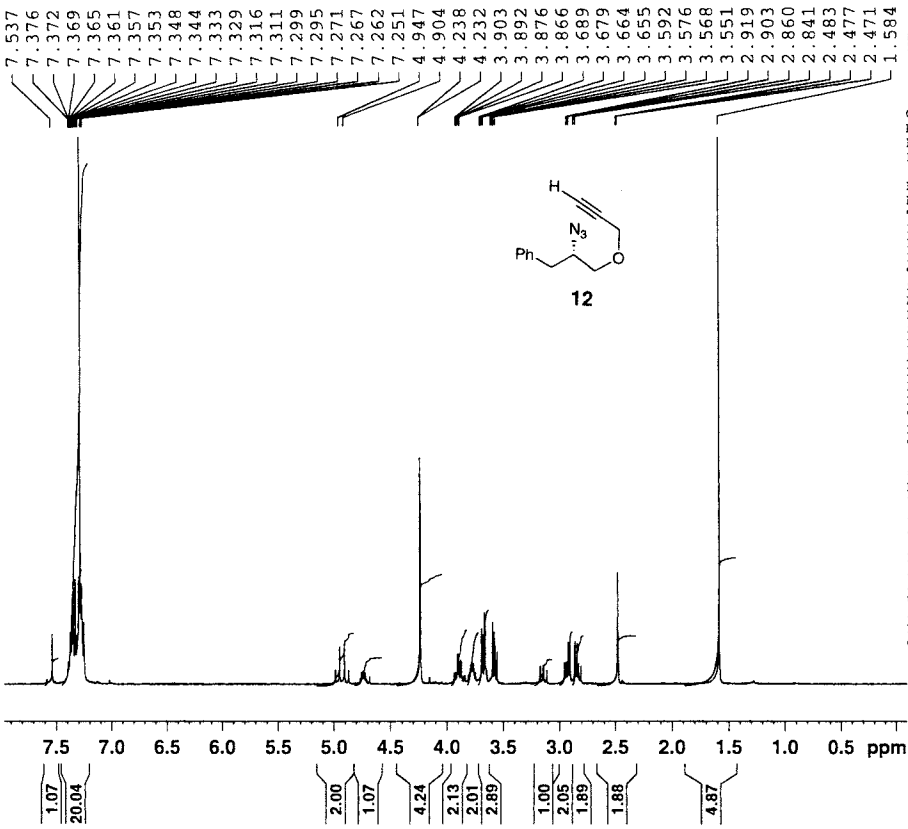
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 11585.2
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 3.30 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME KML-1-255
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 13.30
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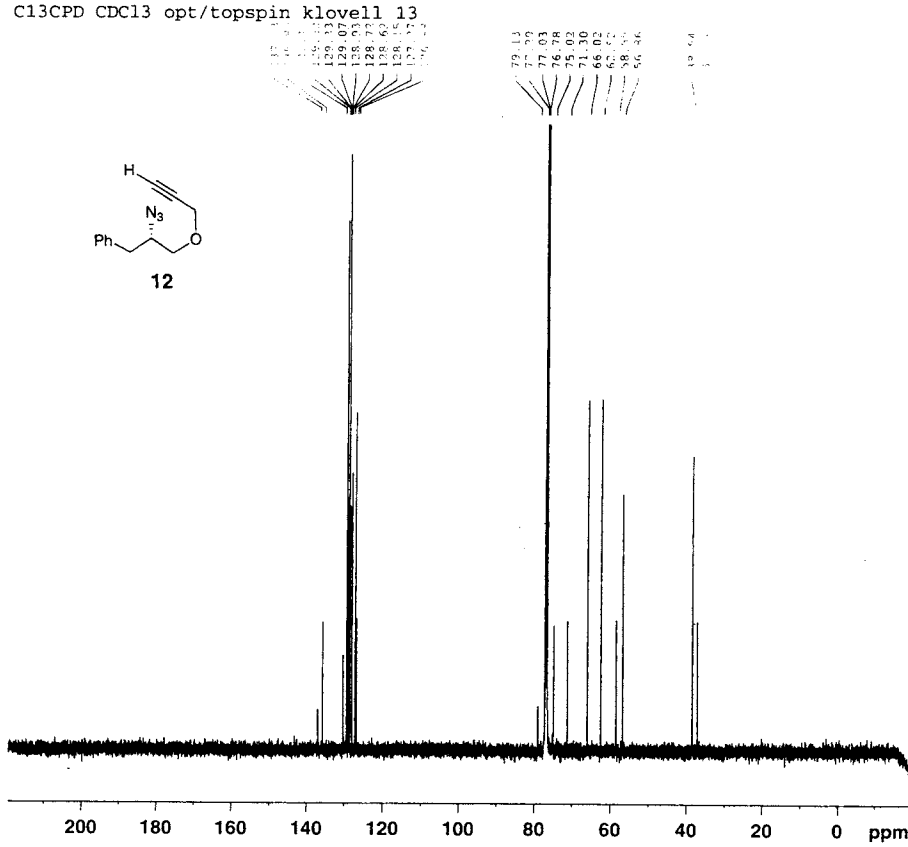
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDCl3 opt/topspin klovell 13



BRUKER

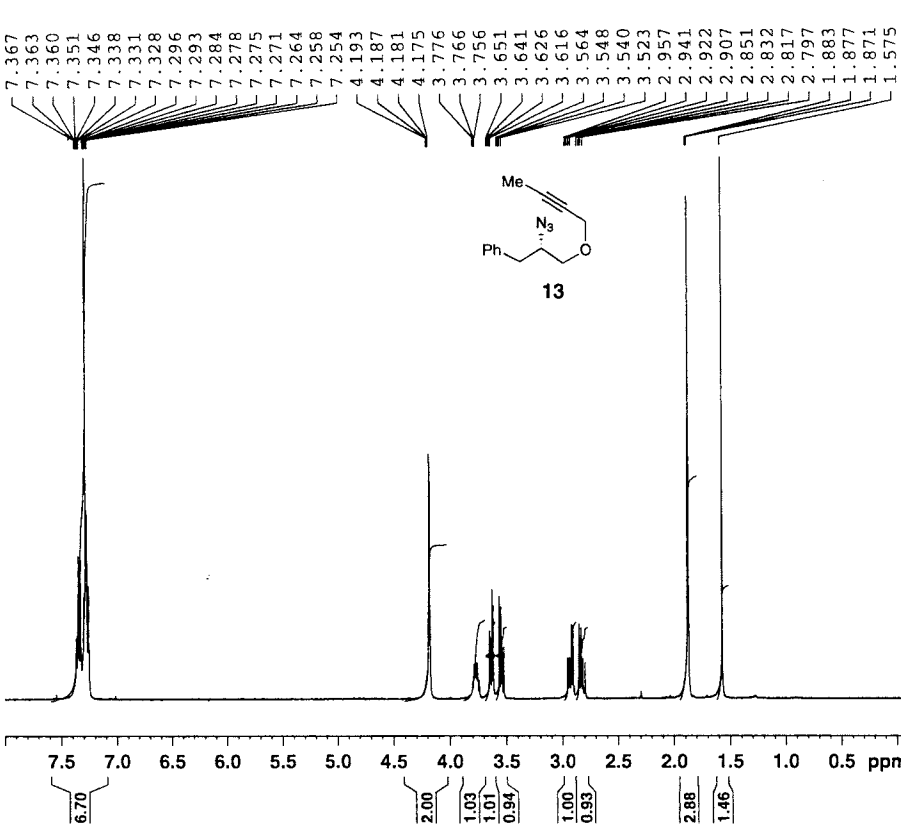
Current Data Parameters
NAME KML-1-255
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070904
Time 19.35
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 768
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 14596.5
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

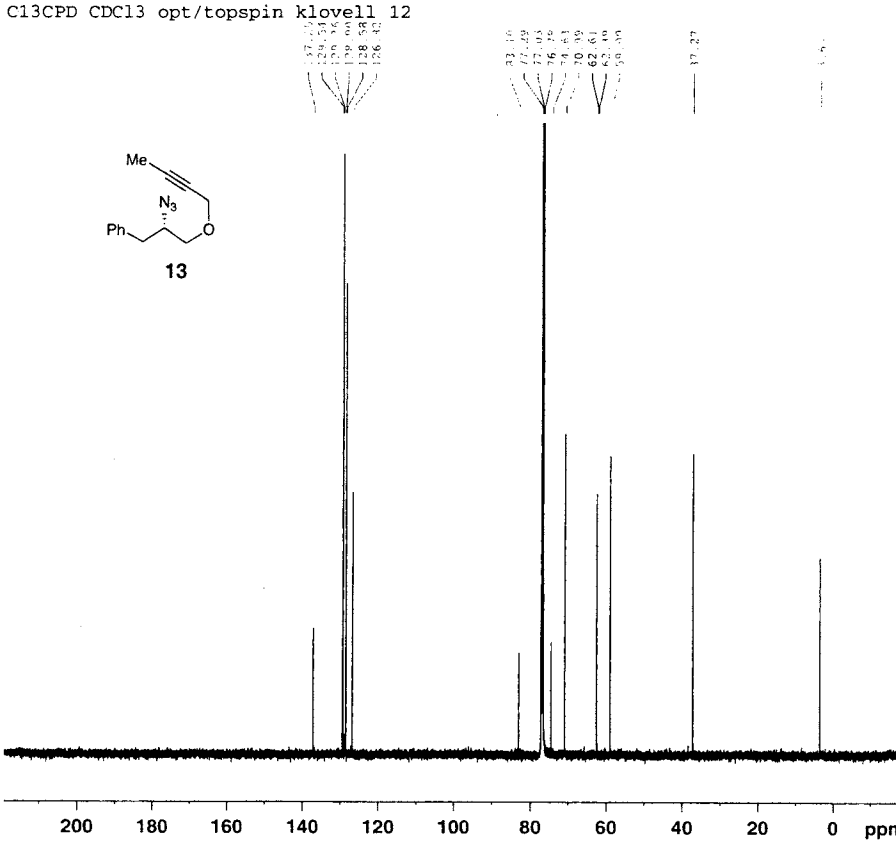
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



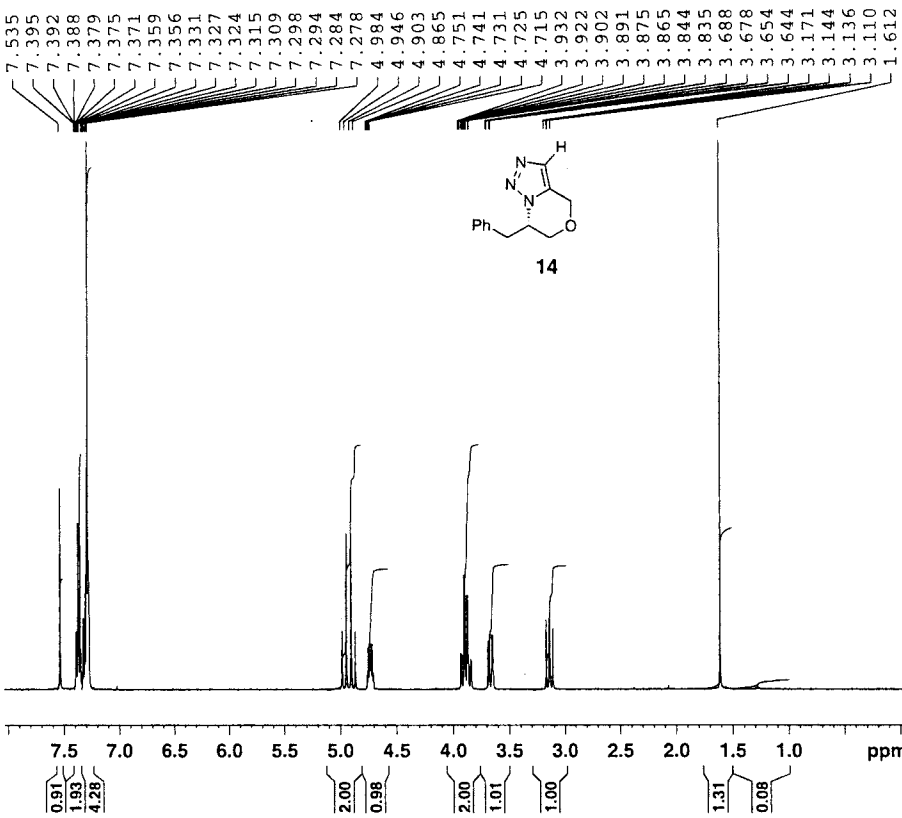
BRUKER

```
Current Data Parameters
NAME                  KML-1-253
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070901
Time                      13.34
INSTRUM                  drx400
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                        645.1
DW                       60.400 usec
DE                        6.00 usec
TE                       295.2 K
D1                    1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                       10.50 usec
PL1                      -5.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                           32768
SF                  400.1300000 MHz
WDW                             EM
SSB                              0
LB                            0.30 Hz
GB                               0
PC                            1.00
```



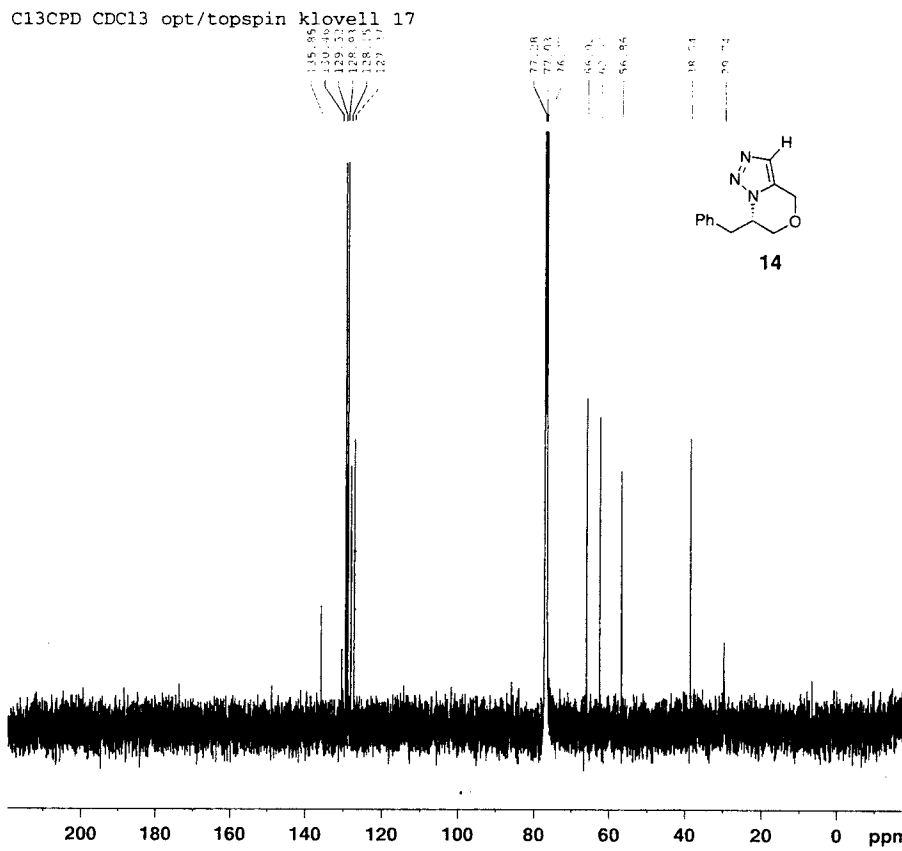
BRUKER

```
Current Data Parameters
NAME                  KML-1-253
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070904
Time                      19.13
INSTRUM                   spect
PROBHD    5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         768
DS                           4
SWH                  30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                        13004
DW                       16.650 usec
DE                        6.00 usec
TE                       298.2 K
D1                    0.15000001 sec
d11                   0.03000000 sec
DELTA                 0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       11.00 usec
PL1                       2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL2                       1.60 dB
PL12                     16.14 dB
PL13                     10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                           32768
SF                  125.7577890 MHz
WDW                             EM
SSB                              0
LB                            1.00 Hz
GB                               0
PC                            1.40
```



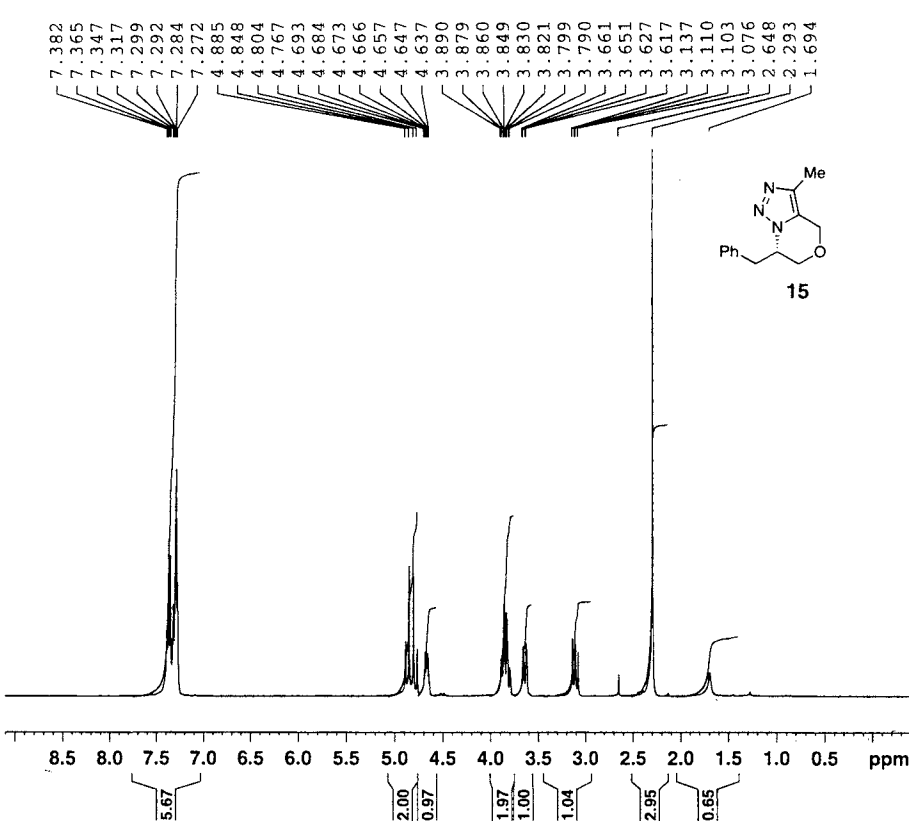
BRUKER

```
Current Data Parameters
NAME                  KML-1-263
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070902
Time                      15.25
INSTRUM                  drx400
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                 8278.146 Hz
FIDRES                0.126314 Hz
AQ                 3.9584243 sec
RG                         512
DW                    60.400 usec
DE                     6.00 usec
TE                     295.2 K
D1                 1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        1H
P1                     10.50 usec
PL1                    -5.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1300000 MHz
WDW                          EM
SSB                           0
LB                     0.30 Hz
GB                            0
PC                         1.00
```



BRUKER

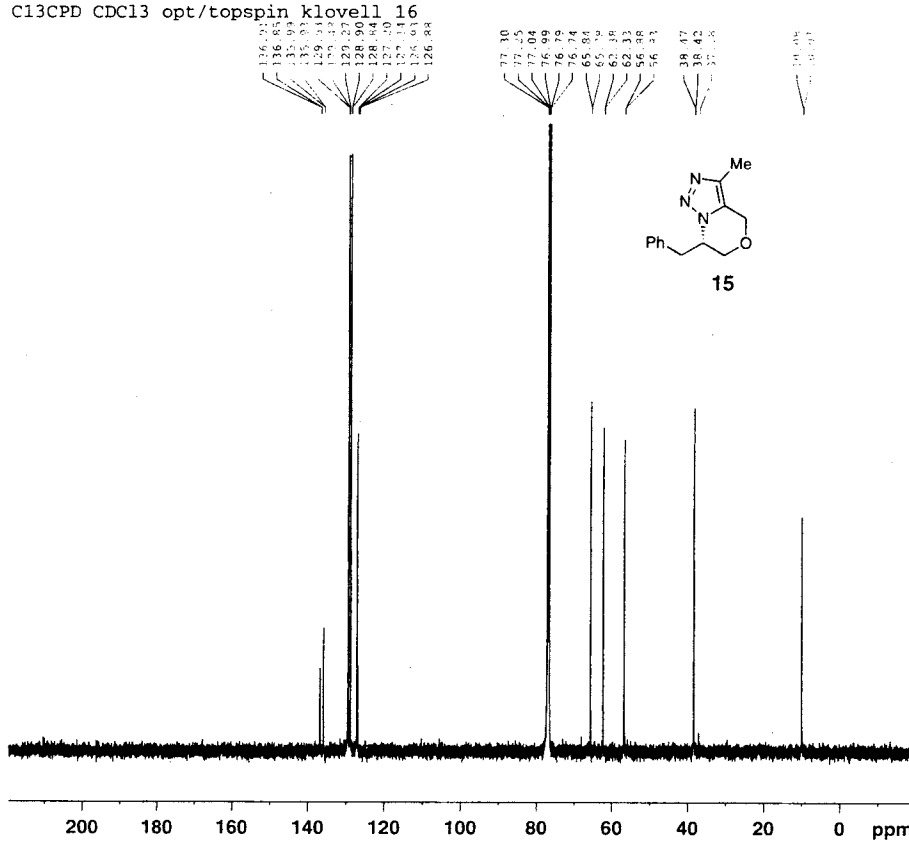
```
Current Data Parameters
NAME                  KML-1-263
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070904
Time                      21.03
INSTRUM                   spect
PROBHD    5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         768
DS                           4
SWH                30030.029 Hz
FIDRES                0.458222 Hz
AQ                 1.0912410 sec
RG                       13004
DW                    16.650 usec
DE                     6.00 usec
TE                     298.2 K
D1                 0.15000001 sec
d11                0.03000000 sec
DELTA              0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                       13C
P1                     11.00 usec
PL1                     2.20 dB
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                  80.00 usec
PL2                     1.60 dB
PL12                   16.14 dB
PL13                   10.00 dB
SFO2           500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF                 125.7577890 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                         1.40
```



BRUKER

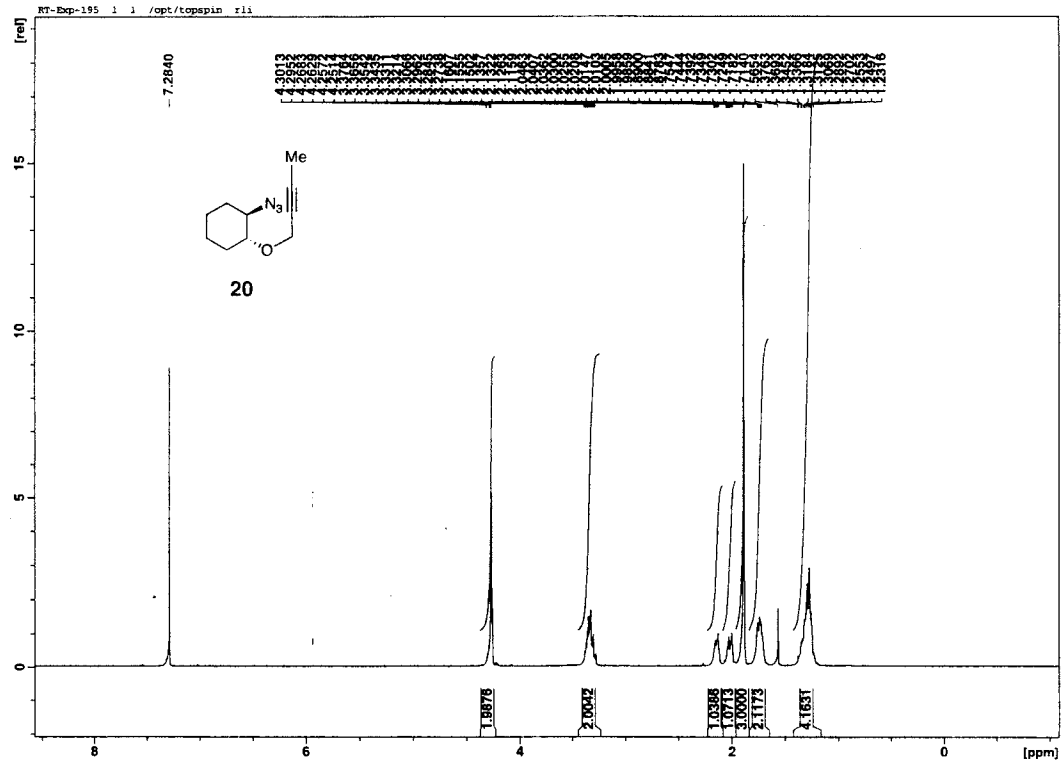
```
Current Data Parameters
NAME                  KML-1-261
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070904
Time                      10.45
INSTRUM                 drx400
PROBHD     5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          362
DW                        60.400 usec
DE                         6.00 usec
TE                        295.2 K
D1                  1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.50 usec
PL1                       -5.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                           32768
SF                  400.1300000 MHz
WDW                             EM
SSB                              0
LB                            0.30 Hz
GB                               0
PC                            1.00
```

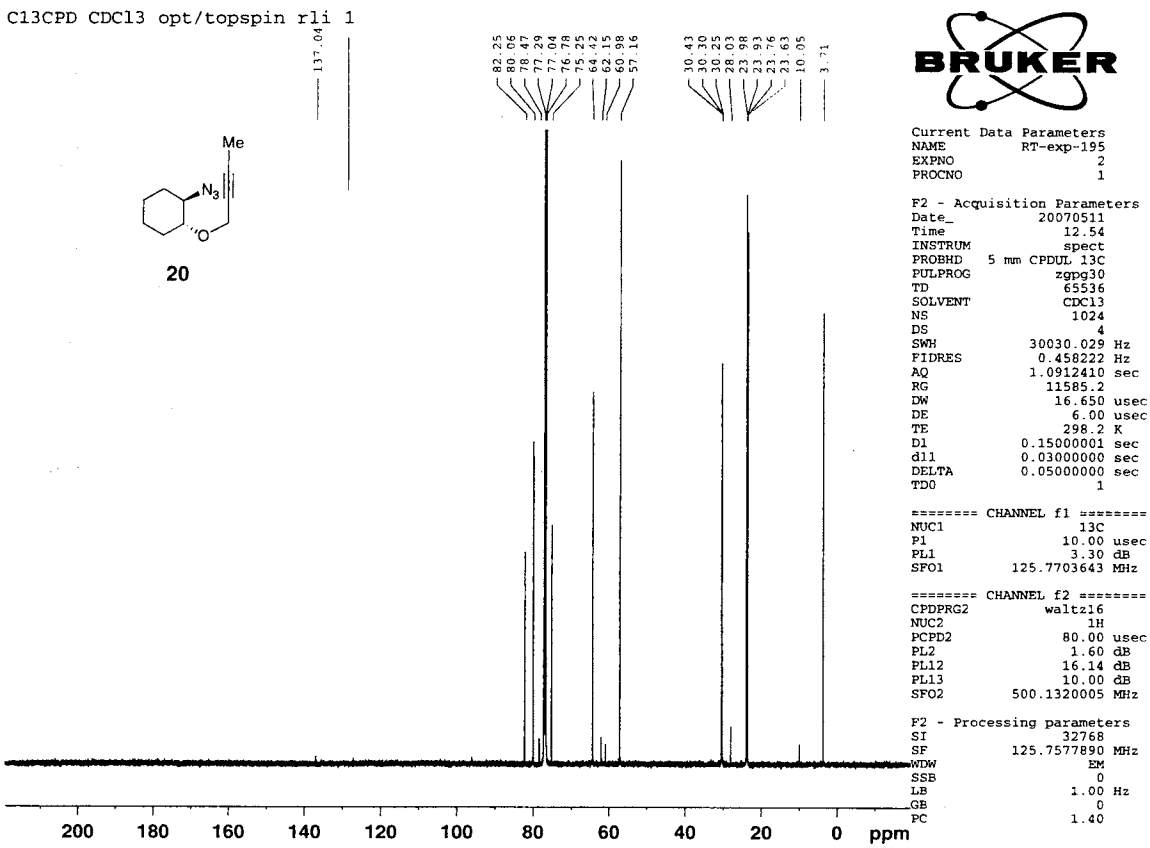
C13CPD CDCl3 opt/topspin klovell 16



BRUKER

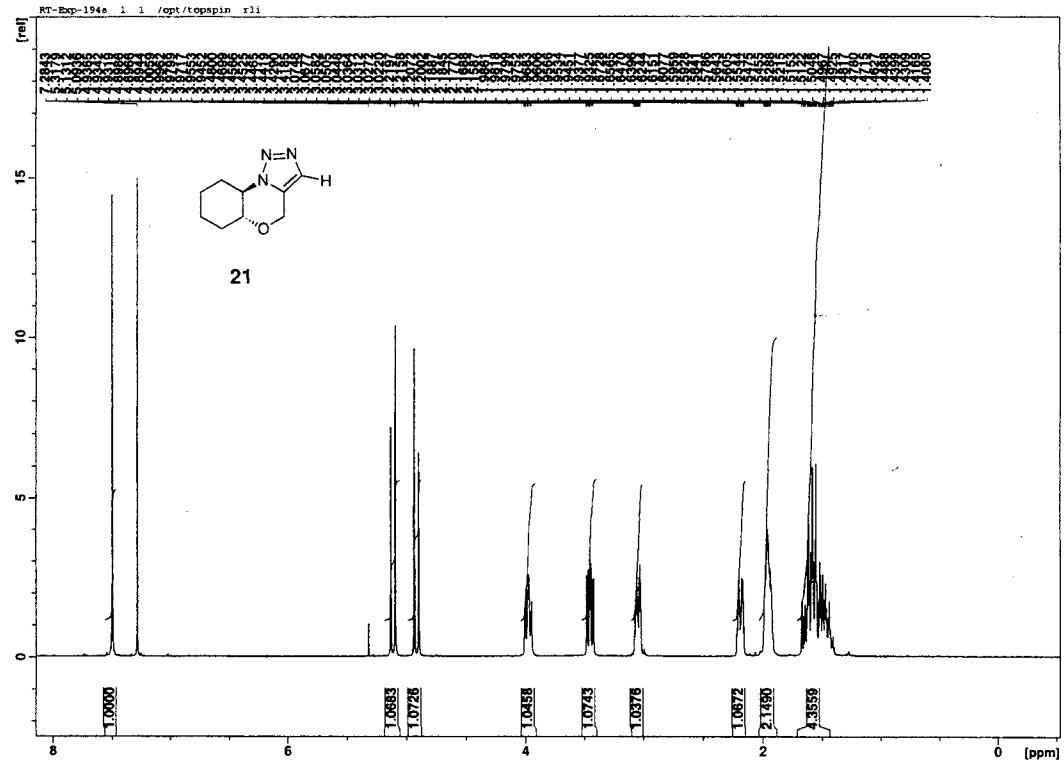
```
Current Data Parameters
NAME                  KML-1-261
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070904
Time                      20.41
INSTRUM                  spect
PROBHD     5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                           768
DS                             4
SWH                   30030.029 Hz
FIDRES                 0.458222 Hz
AQ                     1.0912410 sec
RG                        14596.5
DW                        16.650 usec
DE                         6.00 usec
TE                        298.2 K
D1                  0.15000001 sec
d11                 0.03000000 sec
DELTA               0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                        11.00 usec
PL1                        2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.60 dB
PL12                      16.14 dB
PL13                      10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                           32768
SF                  125.7577890 MHz
WDW                             EM
SSB                              0
LB                            1.00 Hz
GB                               0
PC                            1.40
```





BRUKER

```
Current Data Parameters
NAME          RT-exp-195
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070511
Time               12.54
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          30030.029 Hz
FIDRES         0.458222 Hz
AQ           1.0912410 sec
RG             11585.2
DW              16.650 usec
DE               6.00 usec
TE              298.2 K
D1          0.15000001 sec
d11         0.03000000 sec
DELTA       0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                3.30 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

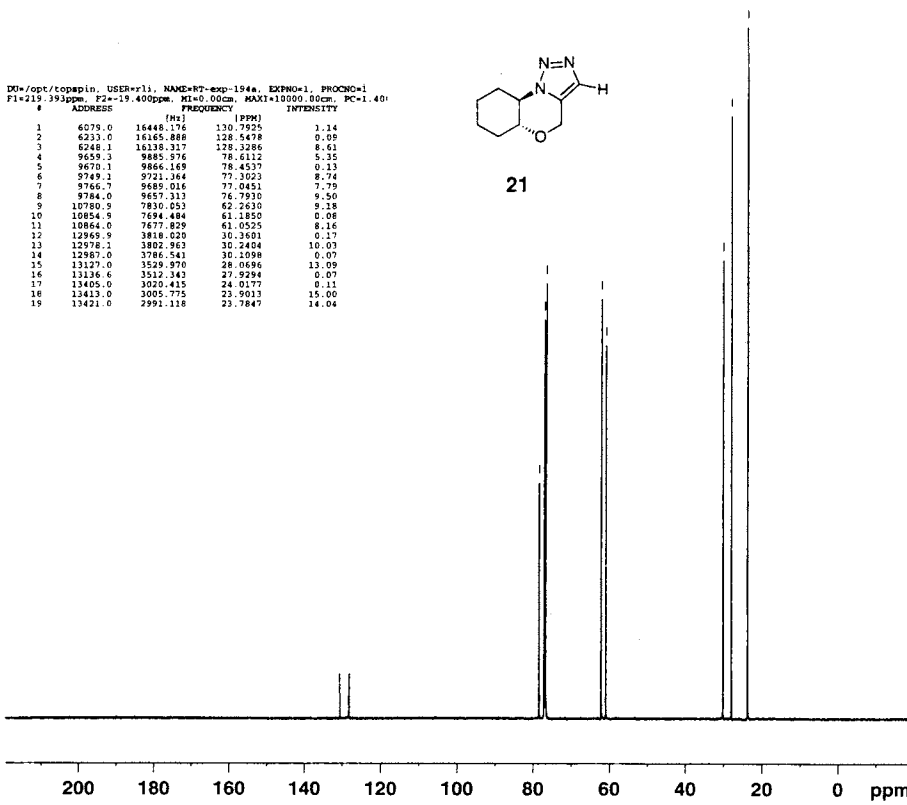


C13PPTI CDCl3 opt/topspin rli 8

DU=/opt/topspin, USER=rli, NAME=RT-exp-194a, EXPNO=1, PROCNO=1
F1=219.393ppm, F2=-19.400ppm, MI=0.00cm, MAXI=10000.00cm, PC=1.40

#	ADDRESS	FREQUENCY [Hz]	[PPM]	INTENSITY
1	6079.0	16448.176	130.7925	1.14
2	6233.0	16165.888	128.5478	0.09
3	6248.1	16138.317	128.3286	8.61
4	9659.3	9885.976	78.6112	5.35
5	9670.1	9866.169	78.4537	0.13
6	9749.1	9721.364	77.3023	8.74
7	9766.7	9689.016	77.0451	7.79
8	9784.0	9657.313	76.7930	9.50
9	10780.9	7830.053	62.2630	9.18
10	10854.9	7694.484	61.1850	0.08
11	10864.0	7677.829	61.0525	8.16
12	12969.9	3818.020	30.3601	0.17
13	12978.1	3802.963	30.2404	10.03
14	12987.0	3786.541	30.1098	0.07
15	13127.0	3529.970	28.0696	13.09
16	13136.6	3512.343	27.9294	0.07
17	13405.0	3020.415	24.0177	0.11
18	13413.0	3005.775	23.9013	15.00
19	13421.0	2991.118	23.7847	14.04

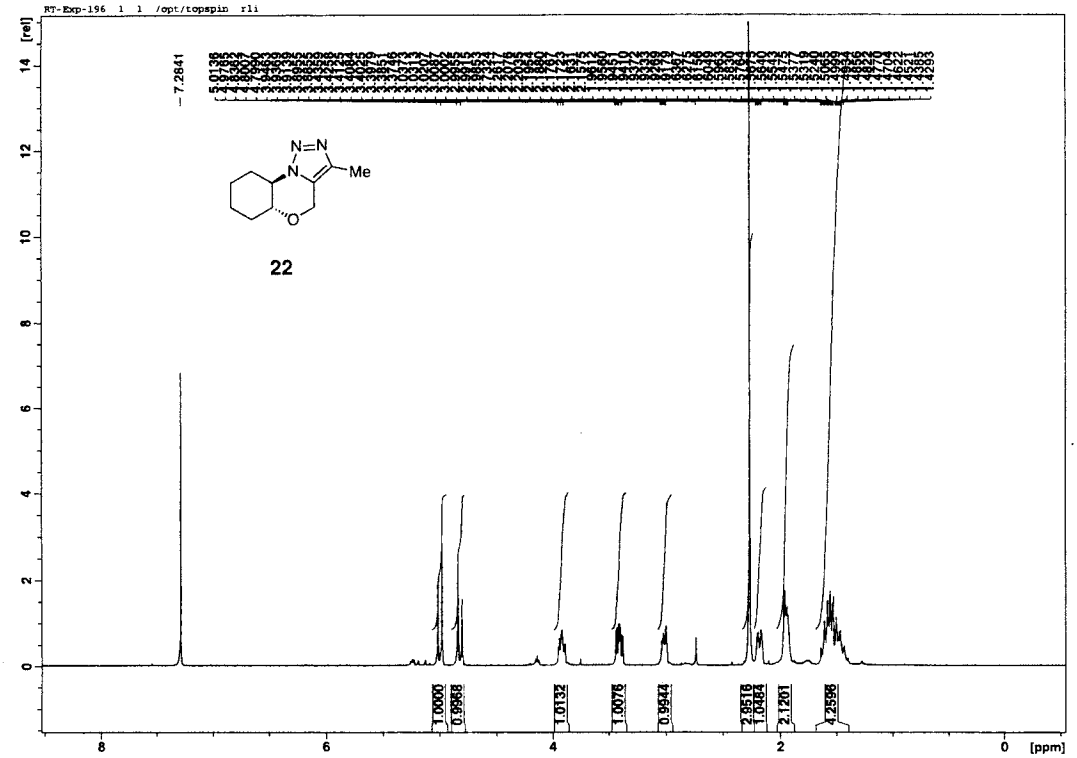
21

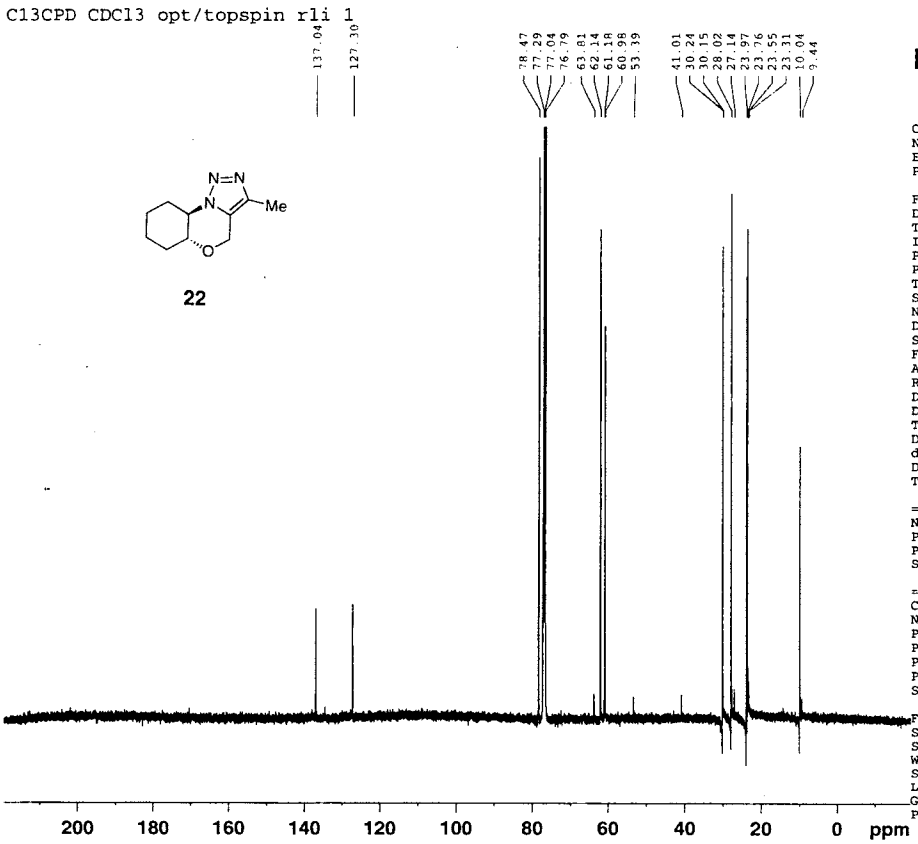


BRUKER

Current Data Parameters

NAME	RT-exp-194a	
EXPNO	1	
PROCNO	1	
F2 - Acquisition Parameters		
Date_	20070511	
Time	11.51	
INSTRUM	spect	
PROBHD	5 mm CPDUL 13C	
PULPROG	zgpg	
TD	32768	
SOLVENT	CDCl3	
NS	1069	
DS	4	
SWH	30030.029	Hz
FIDRES	0.916444	Hz
AQ	0.5456539	sec
RG	18390.4	
DW	16.650	usec
DE	6.00	usec
TE	298.2	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	10.00	usec
PL1	3.30	dB
SFO1	125.7703643	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	1.60	dB
PL12	16.14	dB
PL13	10.00	dB
SFO2	500.1320005	MHz
F2 - Processing parameters		
SI	16384	
SF	125.7577890	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	





BRUKER

Current Data Parameters

NAME	RT-exp-196
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070513
Time	16.47
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	13004
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

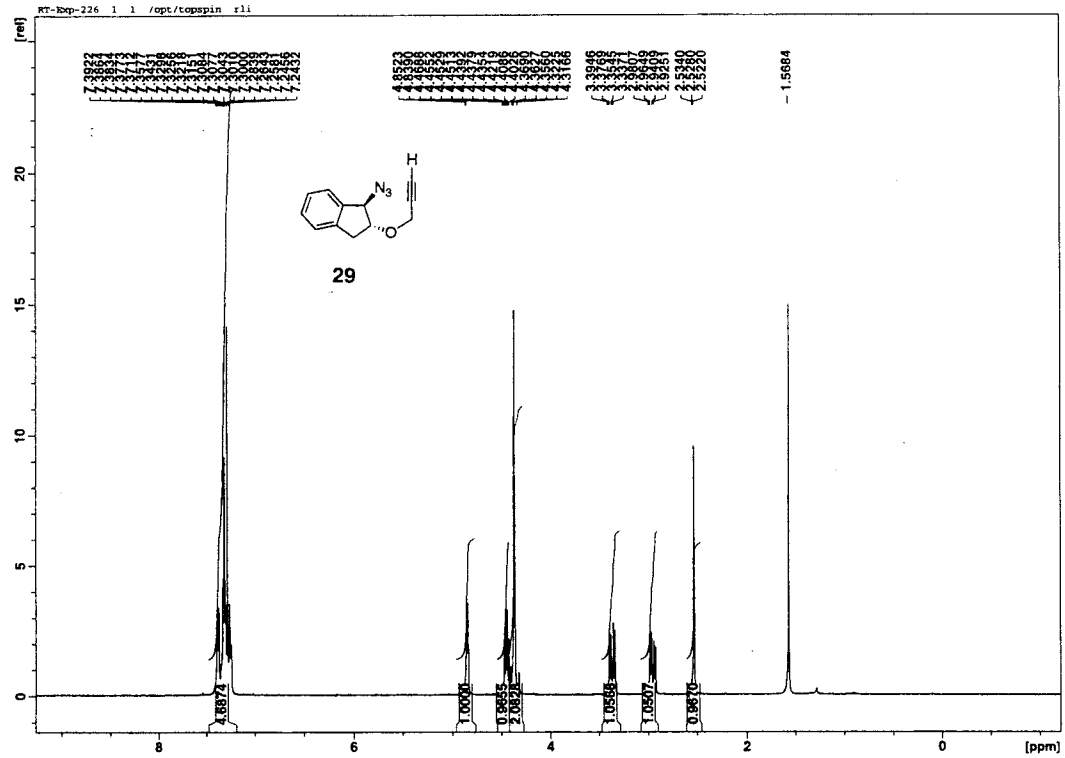
NUC1	13C
P1	10.00 usec
PL1	3.30 dB
SFO1	125.7703643 MHz

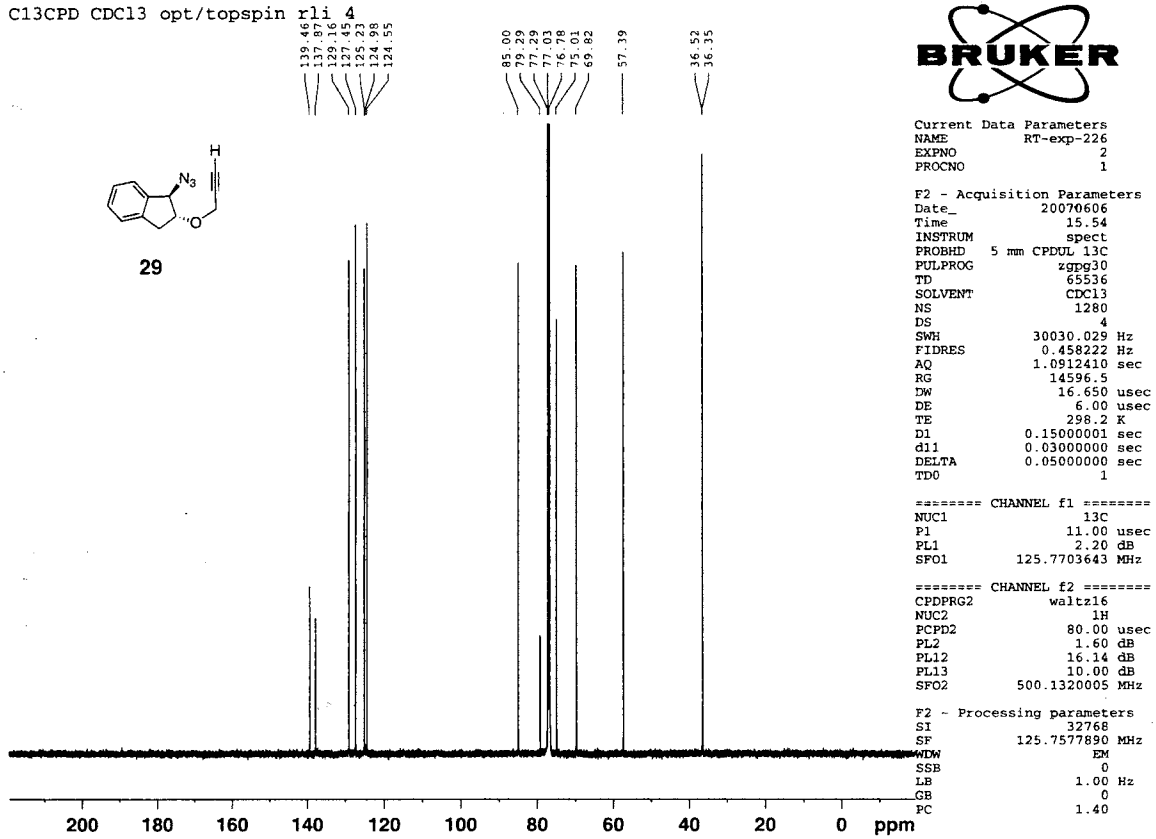
======== CHANNEL f2 ========

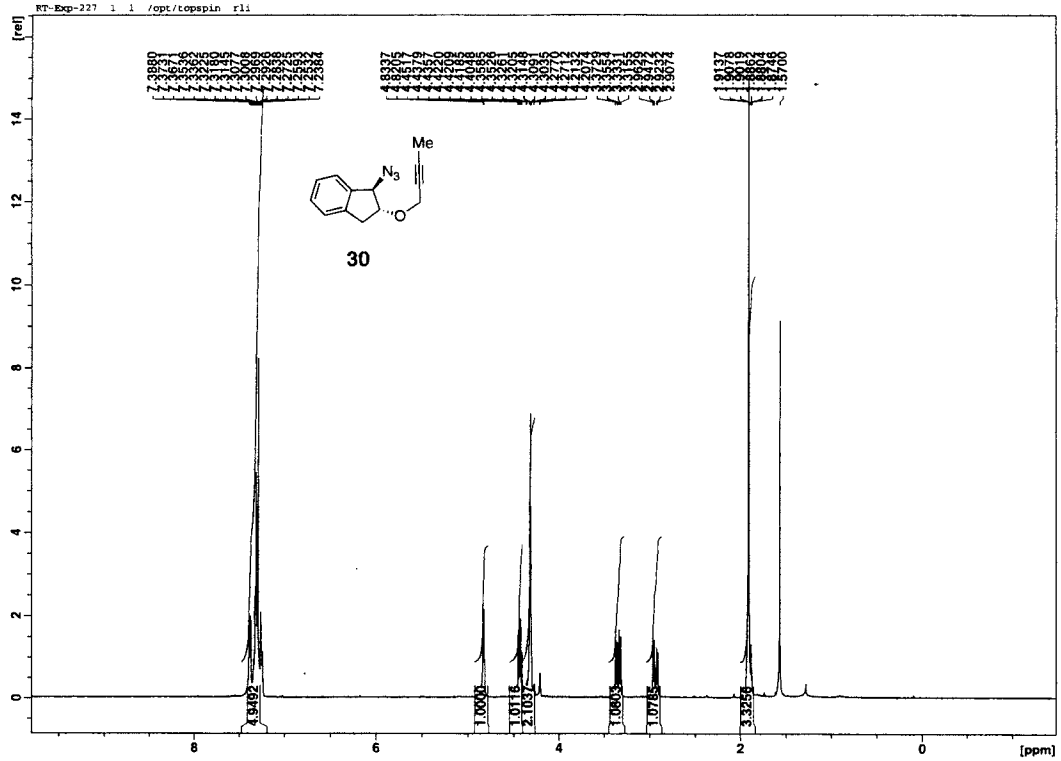
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

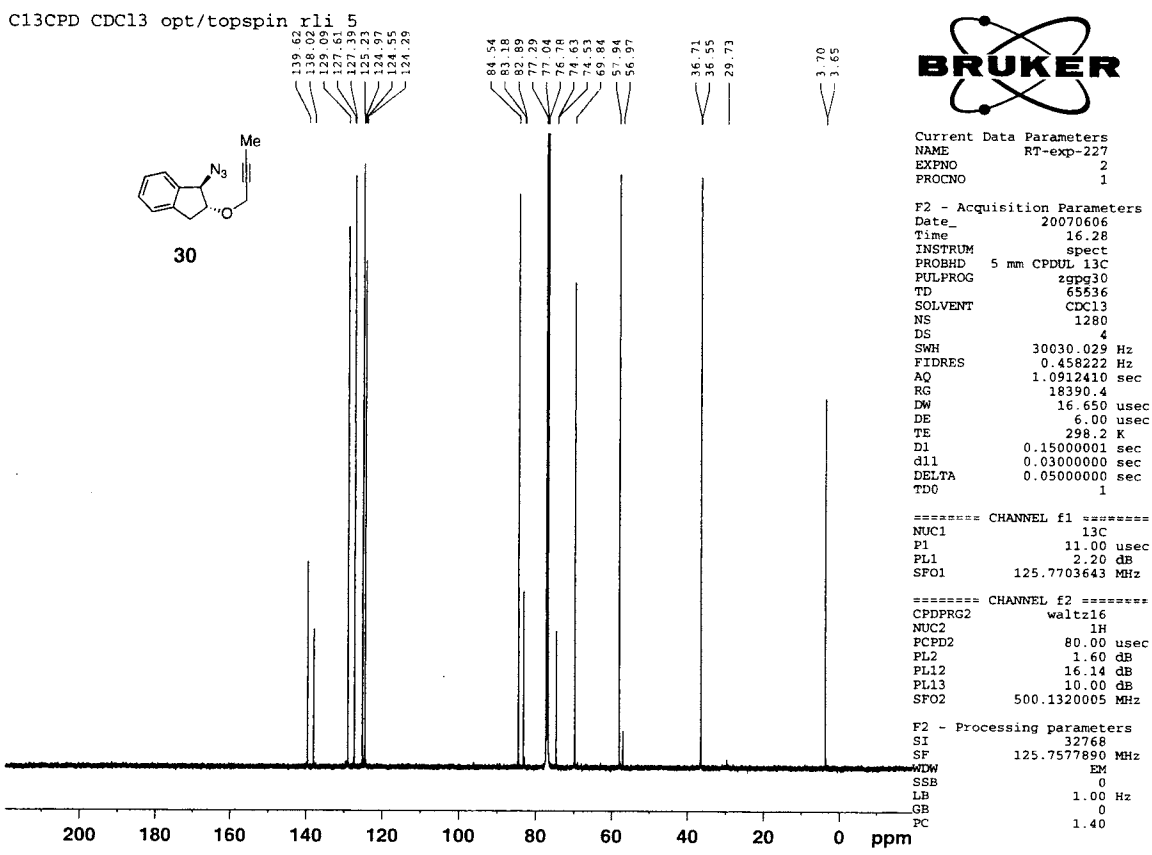
F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


RT-Exp-226 1 1 /opt/topspin rli
[rel]
[ppm]
29


C13CPD CDCl3 opt/topspin rli 4
29
ppm
Current Data Parameters
NAME RT-exp-226
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070606
Time 15.54
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1280
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 14596.5
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





BRUKER

Current Data Parameters

NAME	RT-exp-227
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070606
Time	16.28
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1280
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	18390.4
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

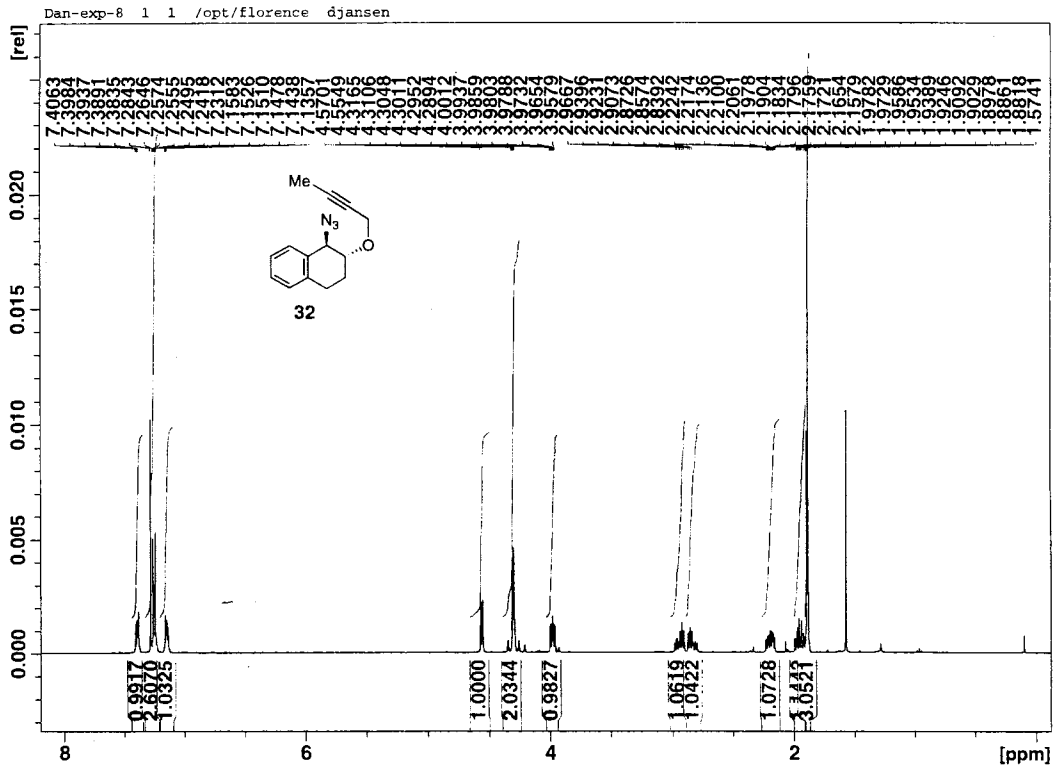
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

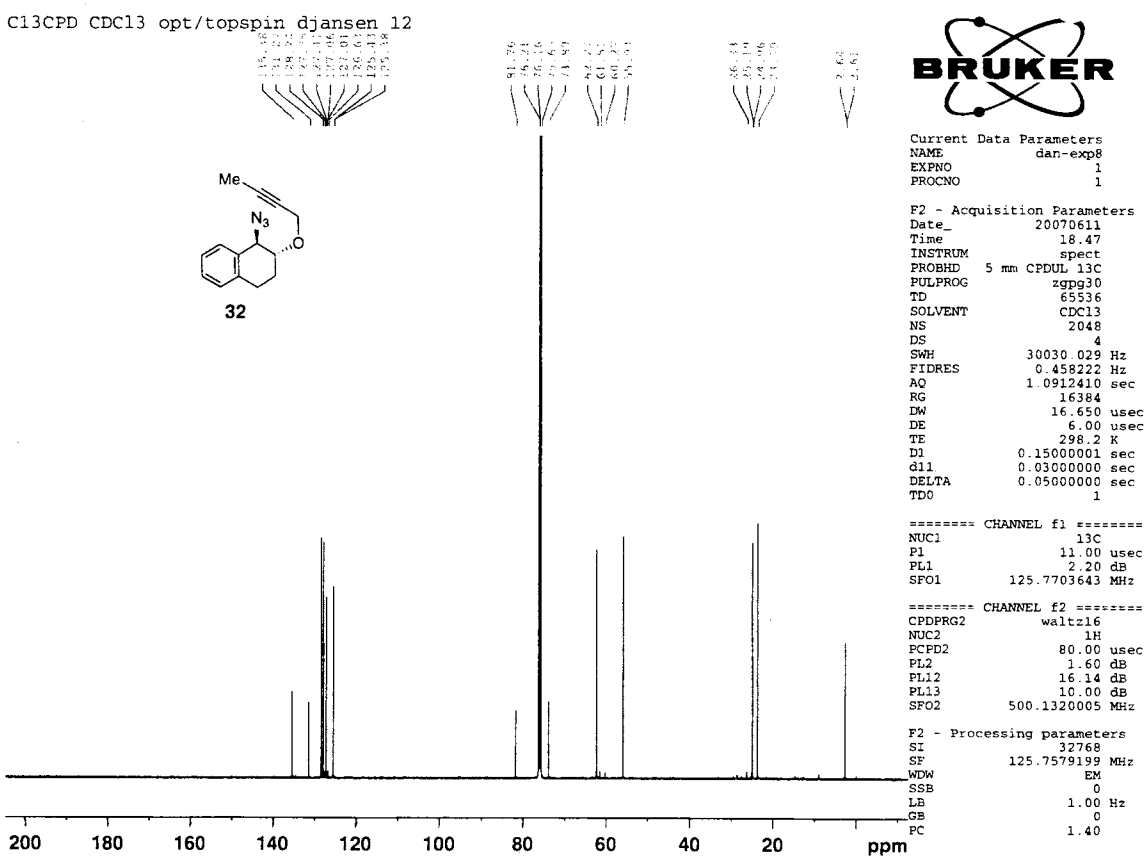
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





BRUKER

Current Data Parameters

NAME	dan-exp8
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070611
Time	18.47
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	16384
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

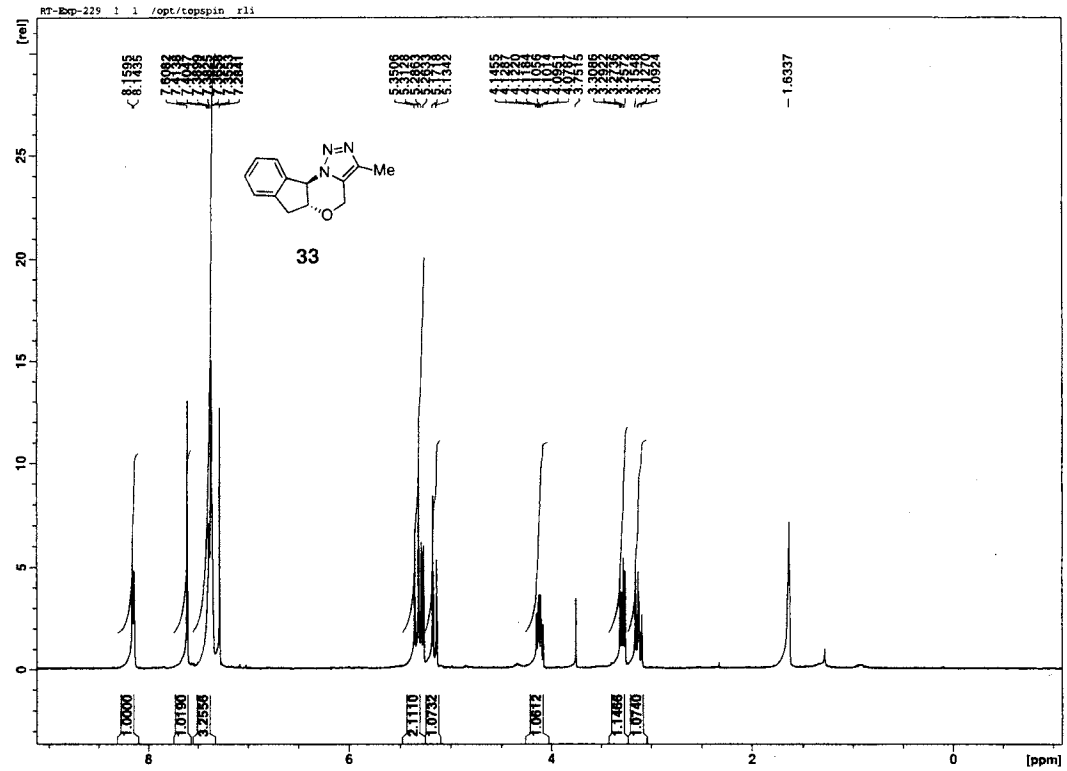
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

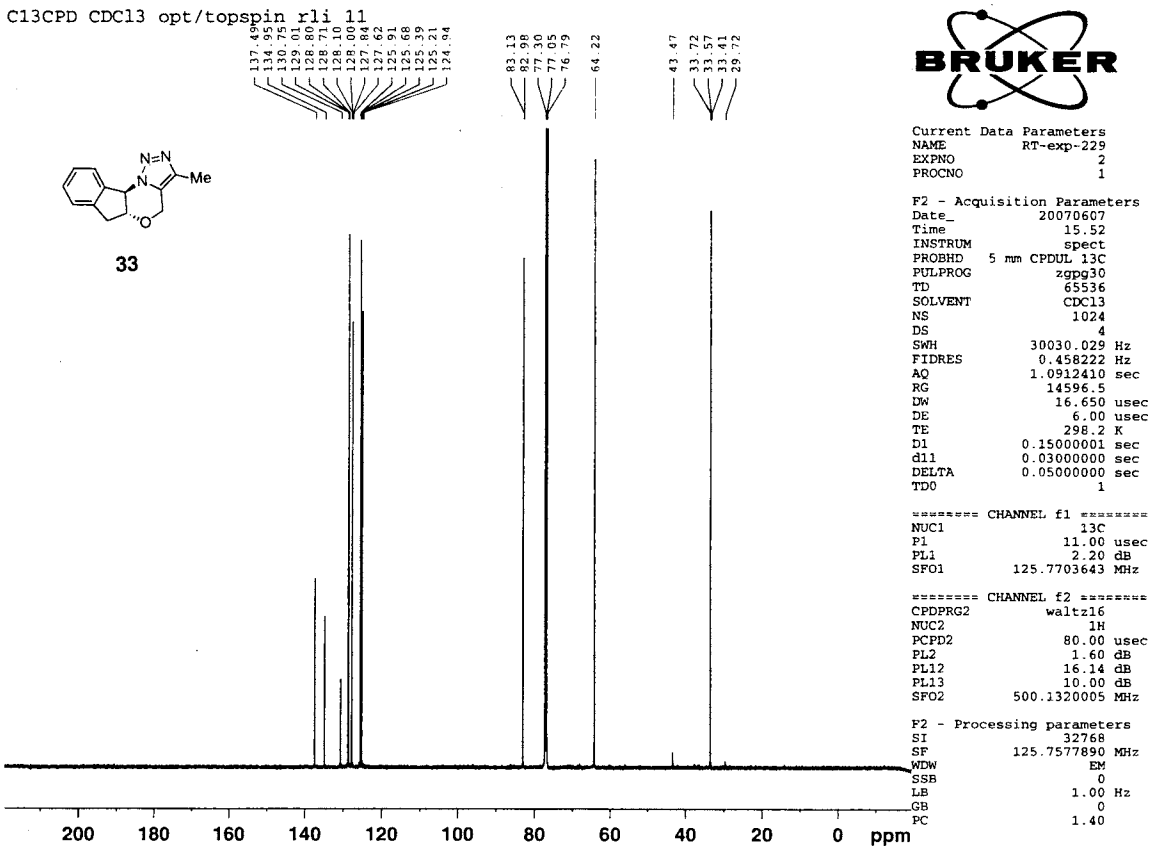
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7579199 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





BRUKER

Current Data Parameters

NAME	RT-exp-229
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070607
Time	15.52
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

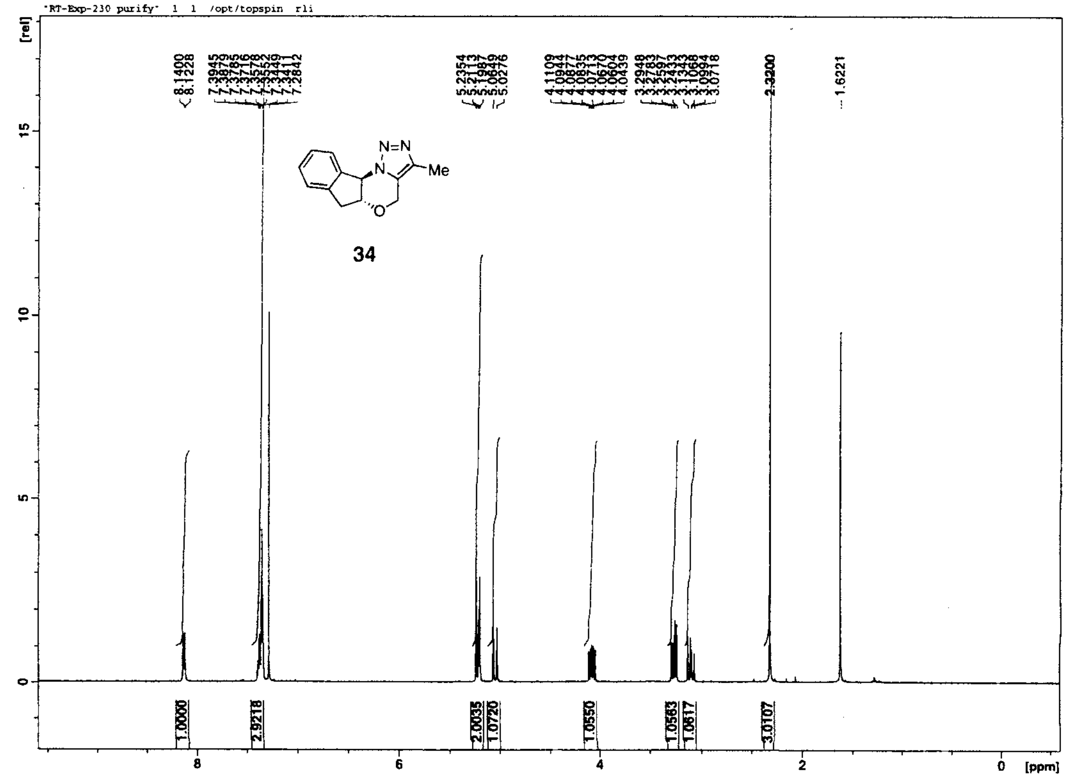
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

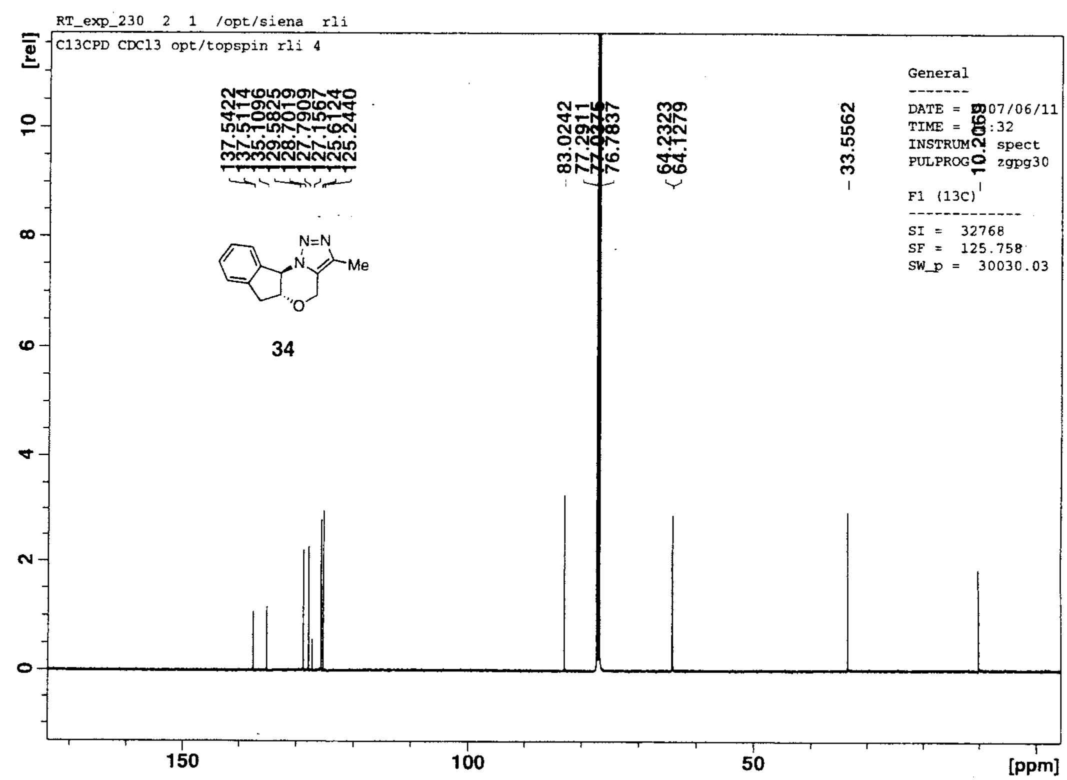
======== CHANNEL f2 ========

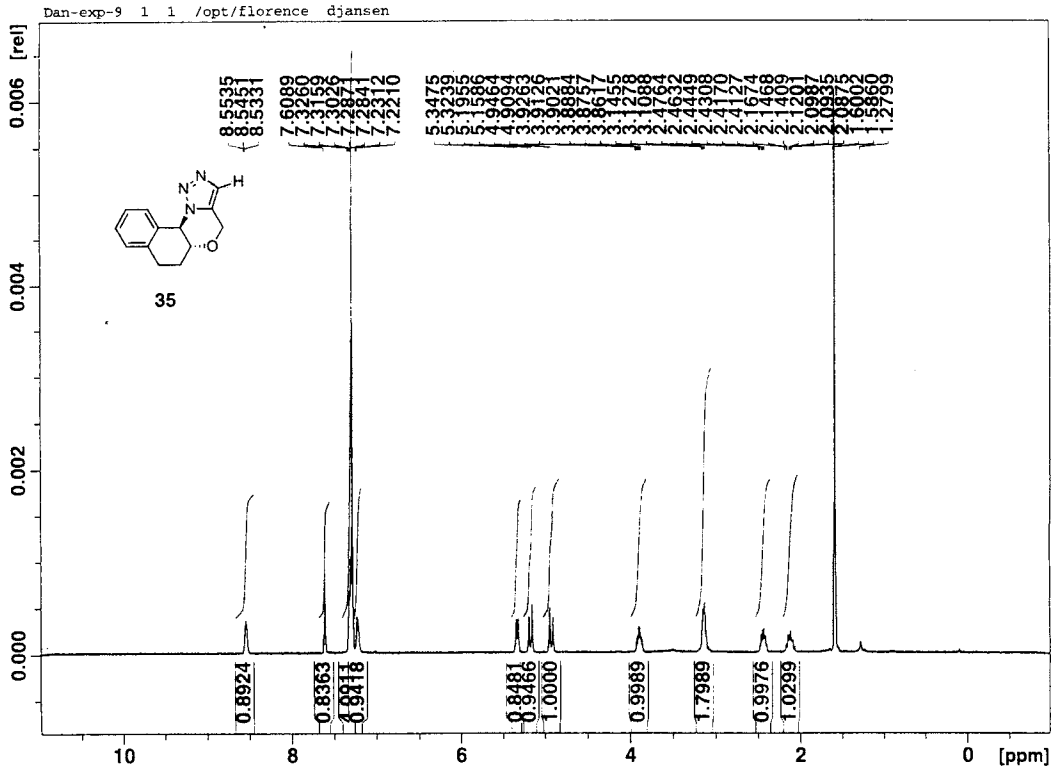
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

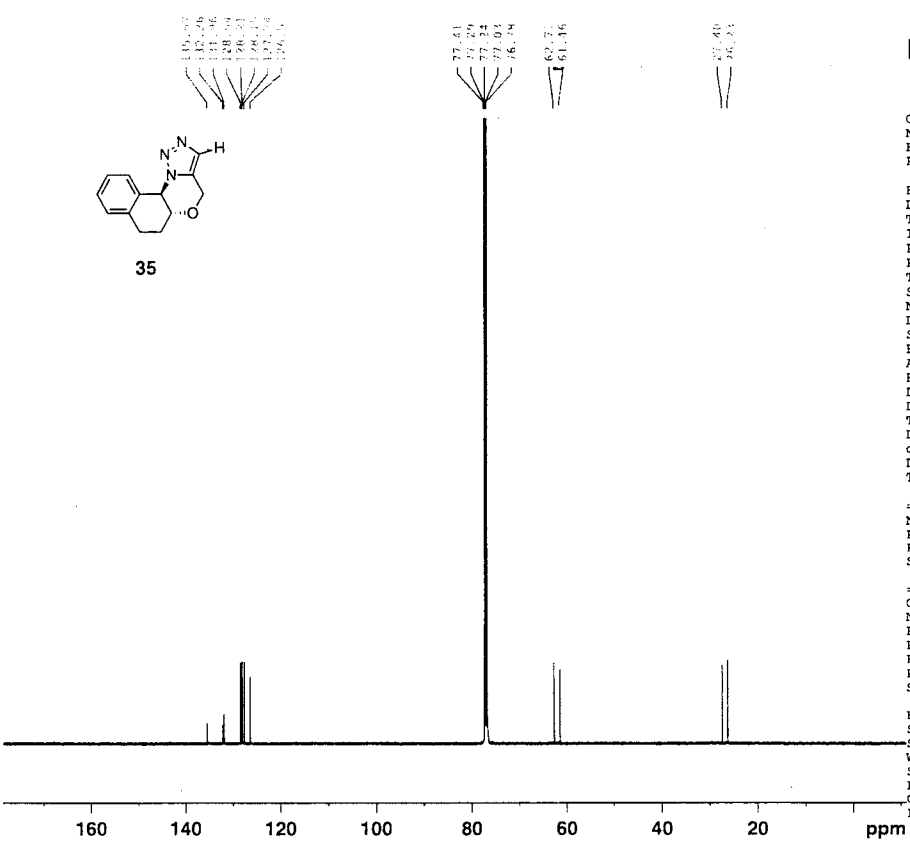
F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


"RT-Exp-230 purify" 1 1 /opt/topspin rli
34
Me
[ppm]


RT_exp_230 2 1 /opt/siena rli
C13CPD CDCl3 opt/topspin rli 4
34
Me
General
DATE = 2007/06/11
INSTRUM = spect
PULPROG = zgpg30
F1 (13C)
SI = 32768
SF = 125.758
SW_p = 30030.03
[ppm]





BRUKER

Current Data Parameters

NAME	dan-exp9
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070611
Time	19.37
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2048
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

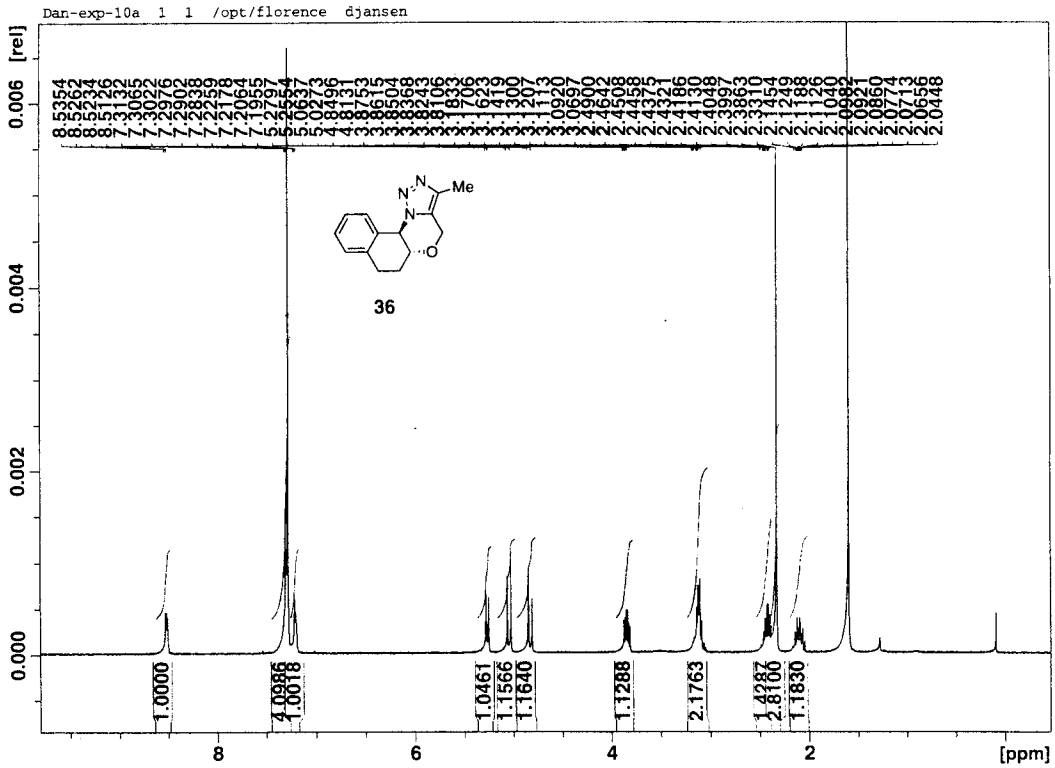
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

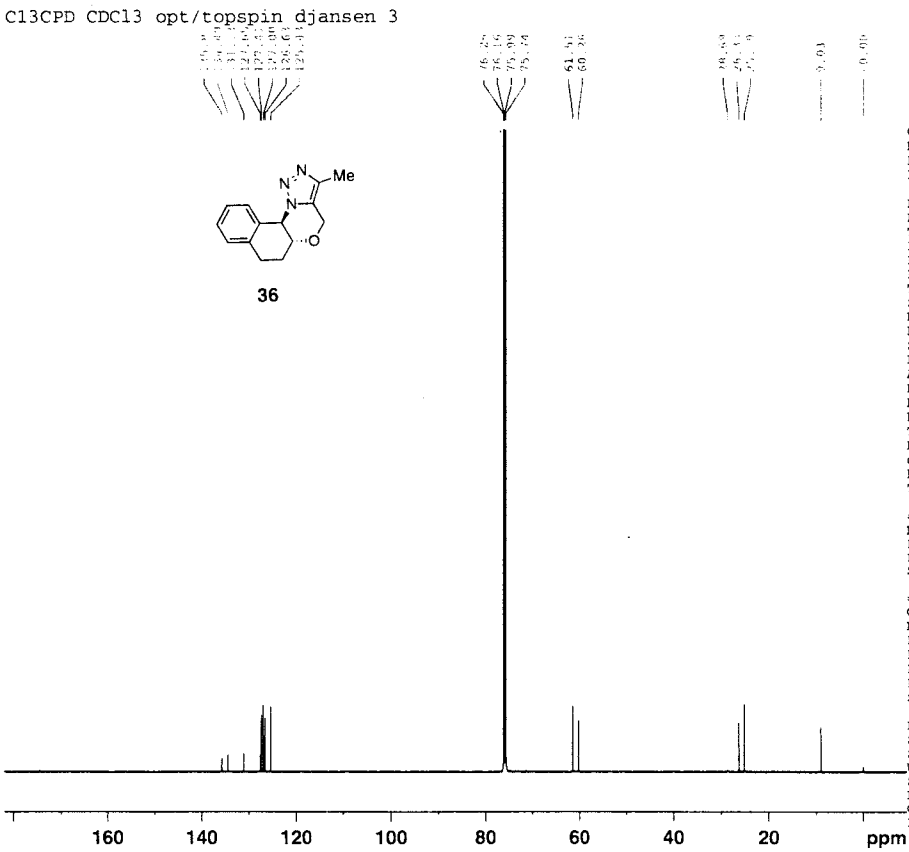
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

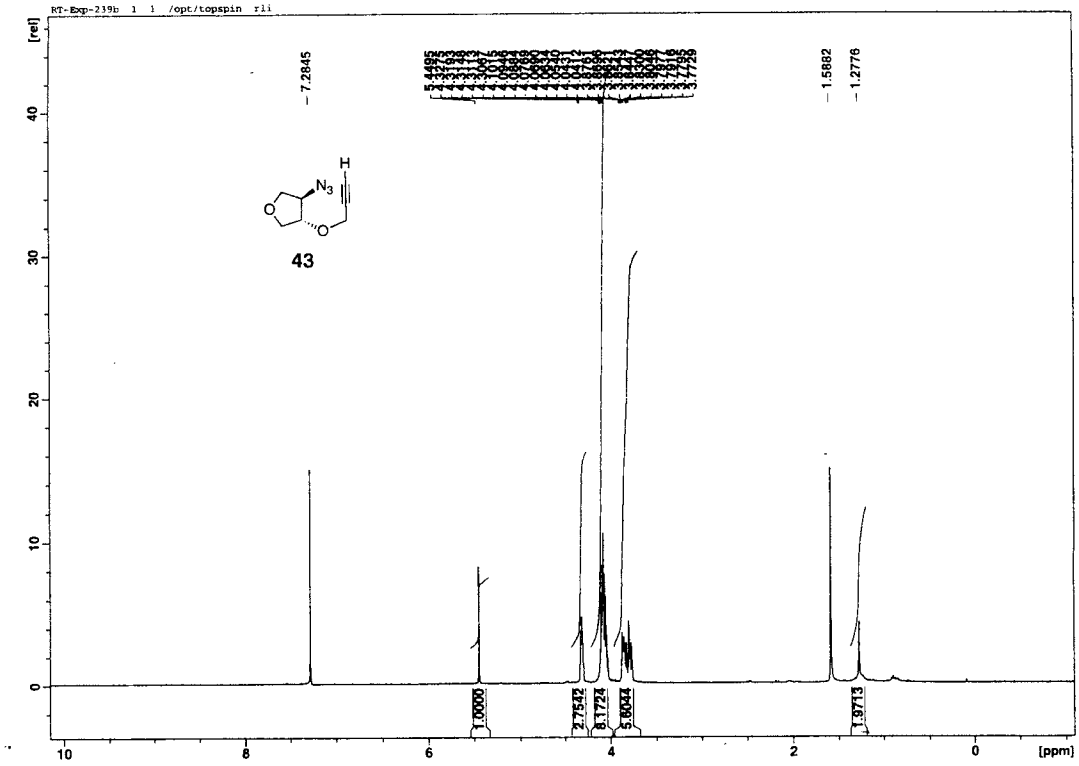
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



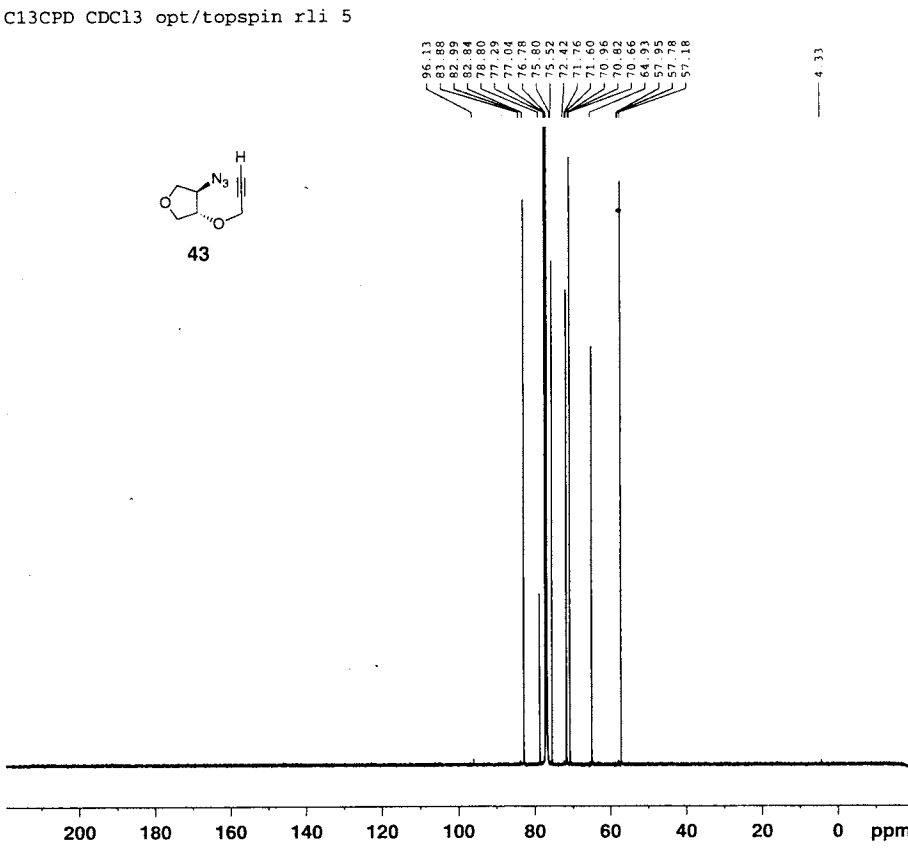


BRUKER

```
Current Data Parameters
NAME            DAN-exp-10
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20070613
Time                12.47
INSTRUM             spect
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH          30030.029 Hz
FIDRES         0.458222 Hz
AQ           1.0912410 sec
RG                 13004
DW              16.650 usec
DE               6.00 usec
TE              298.2 K
D1           0.15000001 sec
d11          0.03000000 sec
DELTA        0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1                2.20 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7579198 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



C13CPD CDCl3 opt/topspin rli 5



BRUKER

Current Data Parameters

NAME	RT-exp-239a
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070615
Time	17.18
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1600
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	13004
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

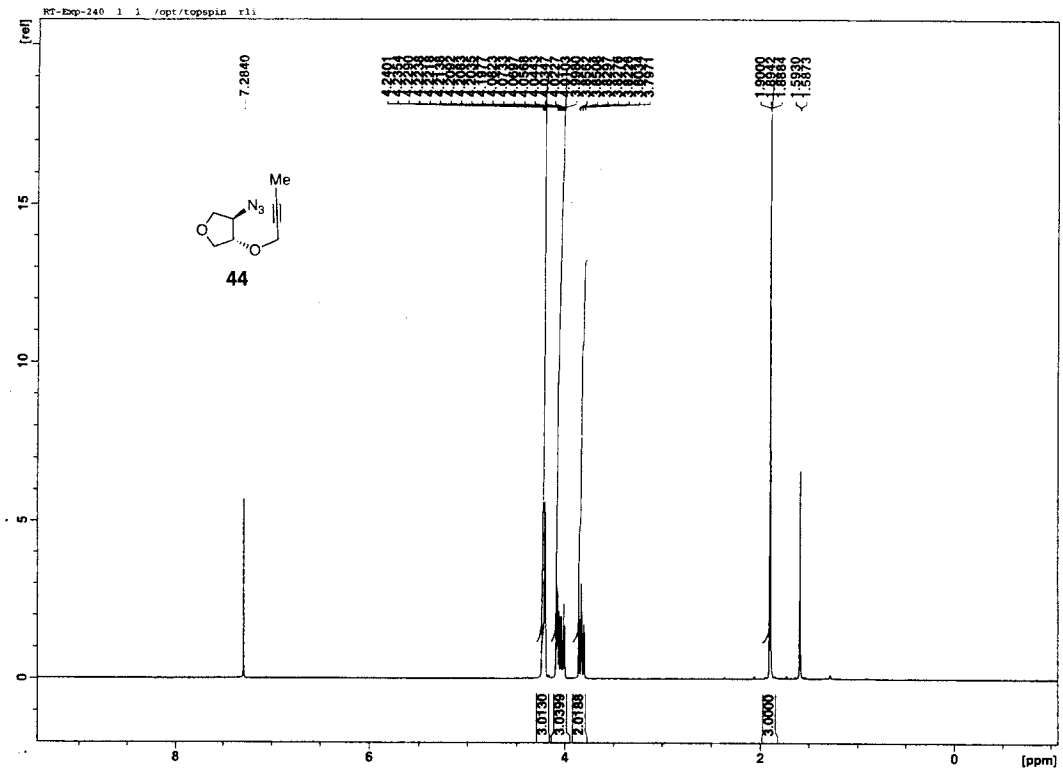
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

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

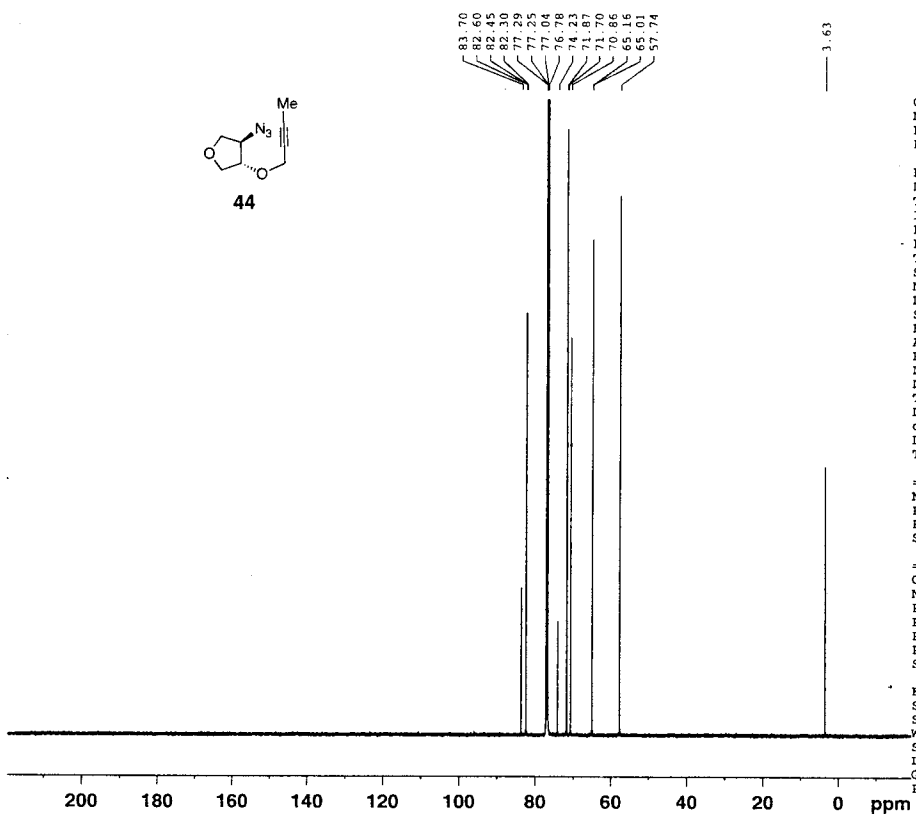
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



C13CPD CDCl3 opt/topspin rli 12



BRUKER

Current Data Parameters

NAME	RT-exp-240
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070615
Time	22.23
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

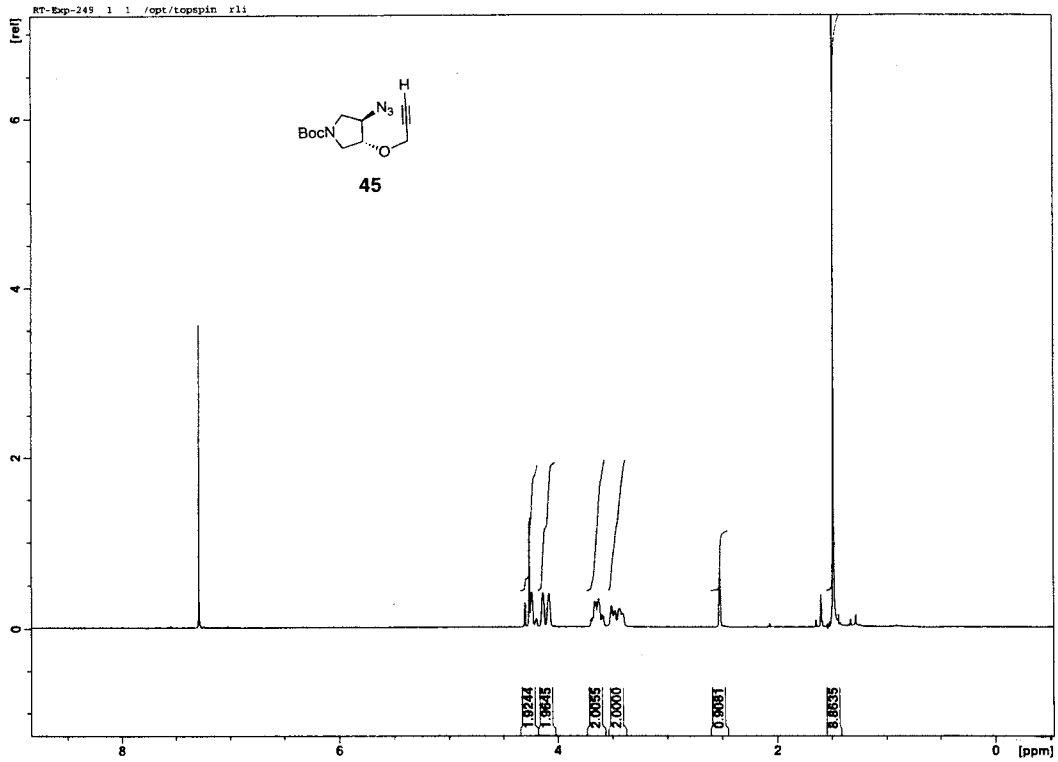
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

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

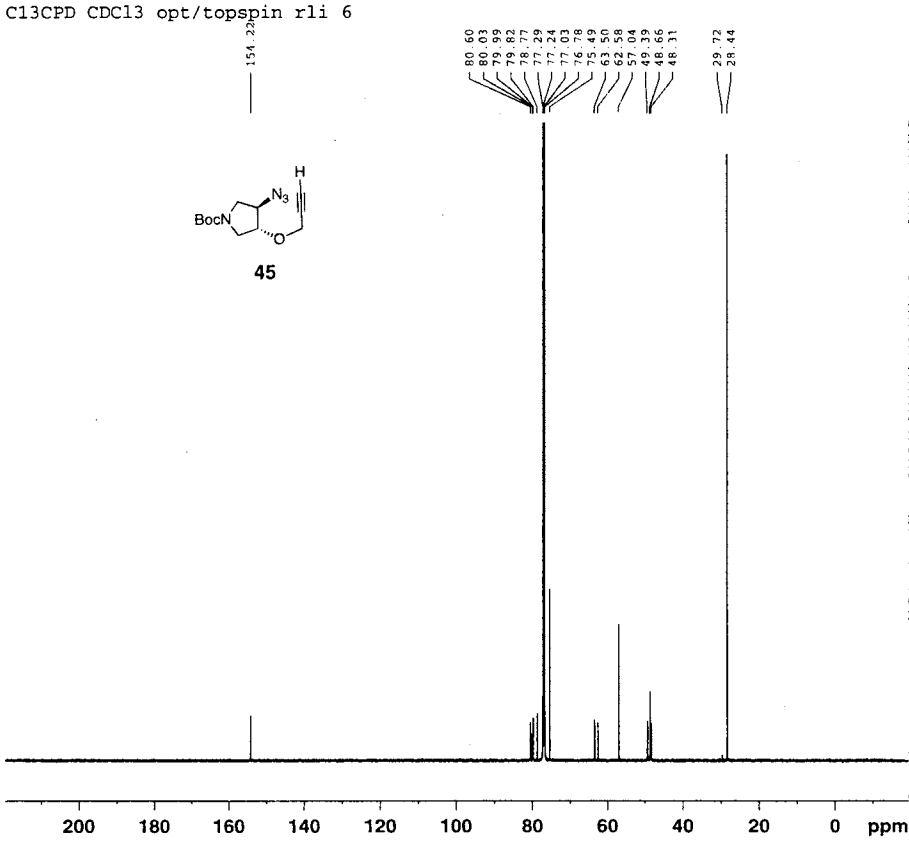
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



C13CPD CDC13 opt/topspin rli 6



BRUKER

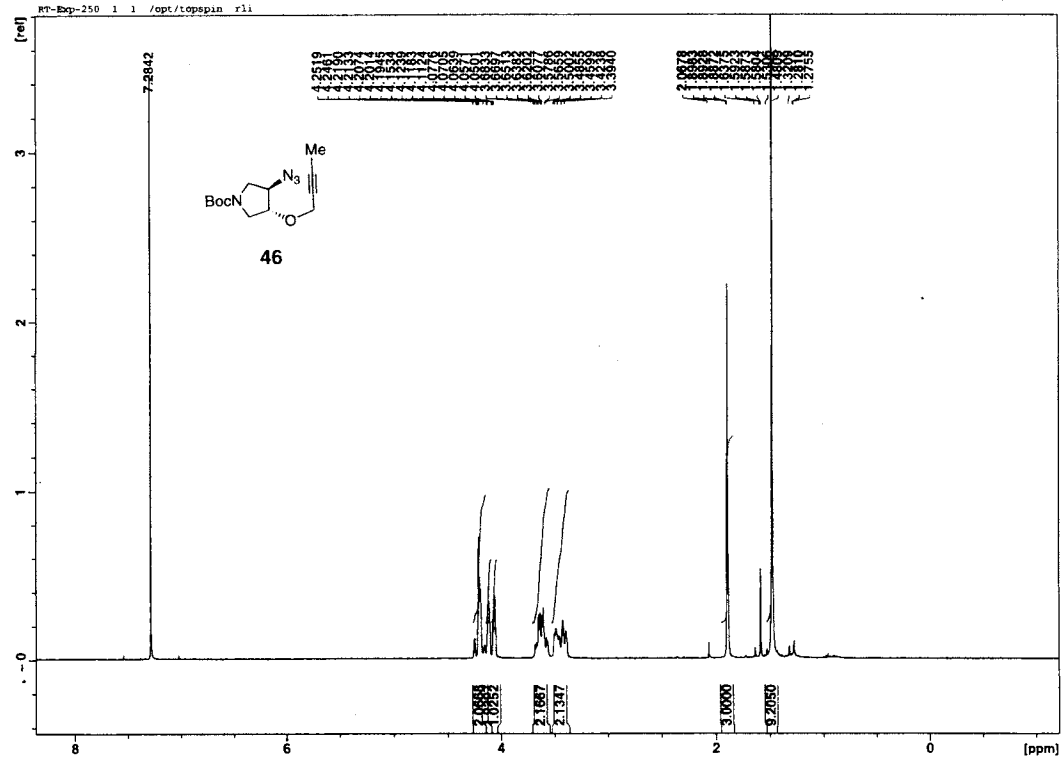
Current Data Parameters
NAME Rt-exp-244
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070627
Time 14.47
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1190
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

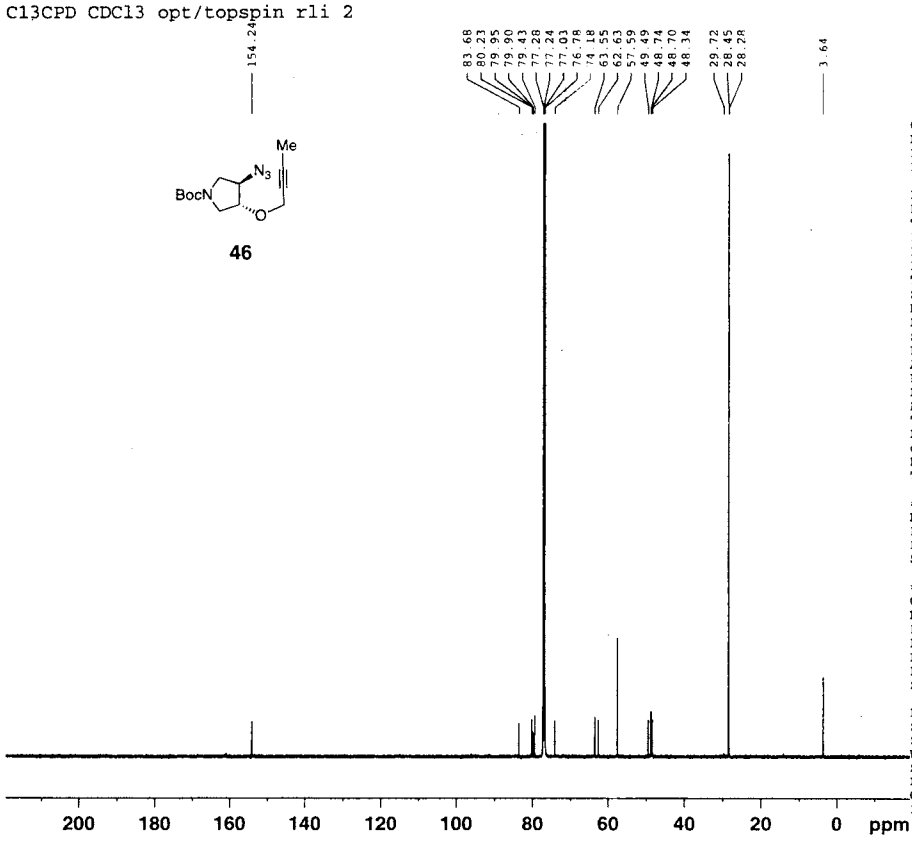
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

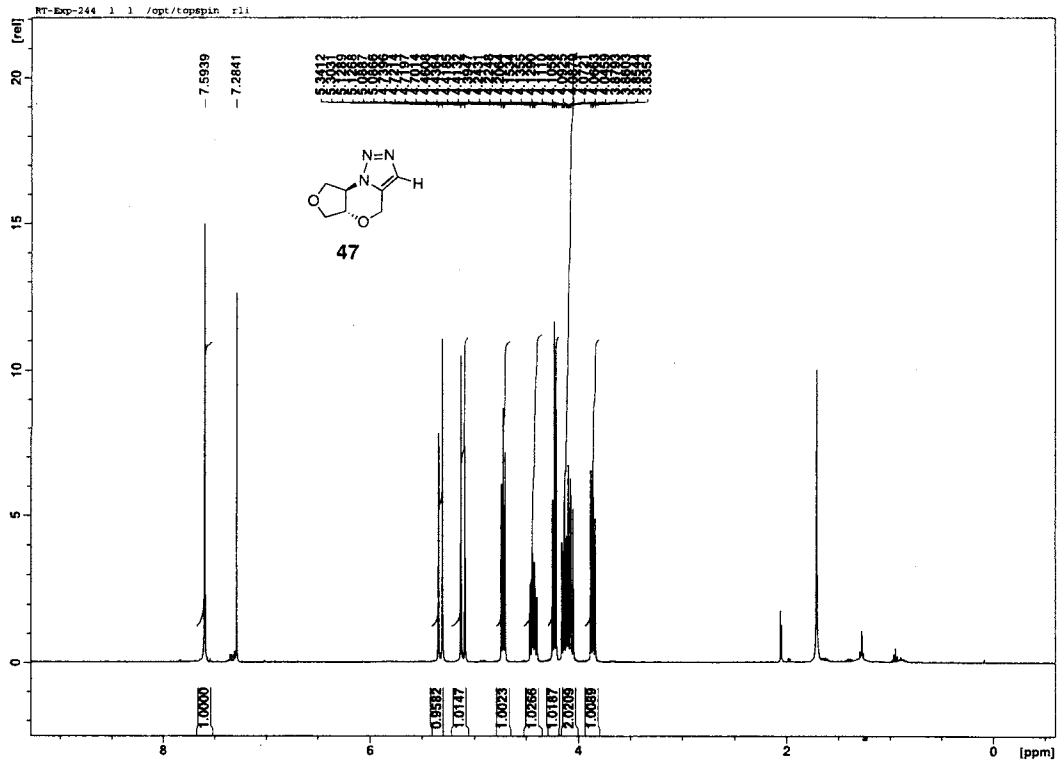


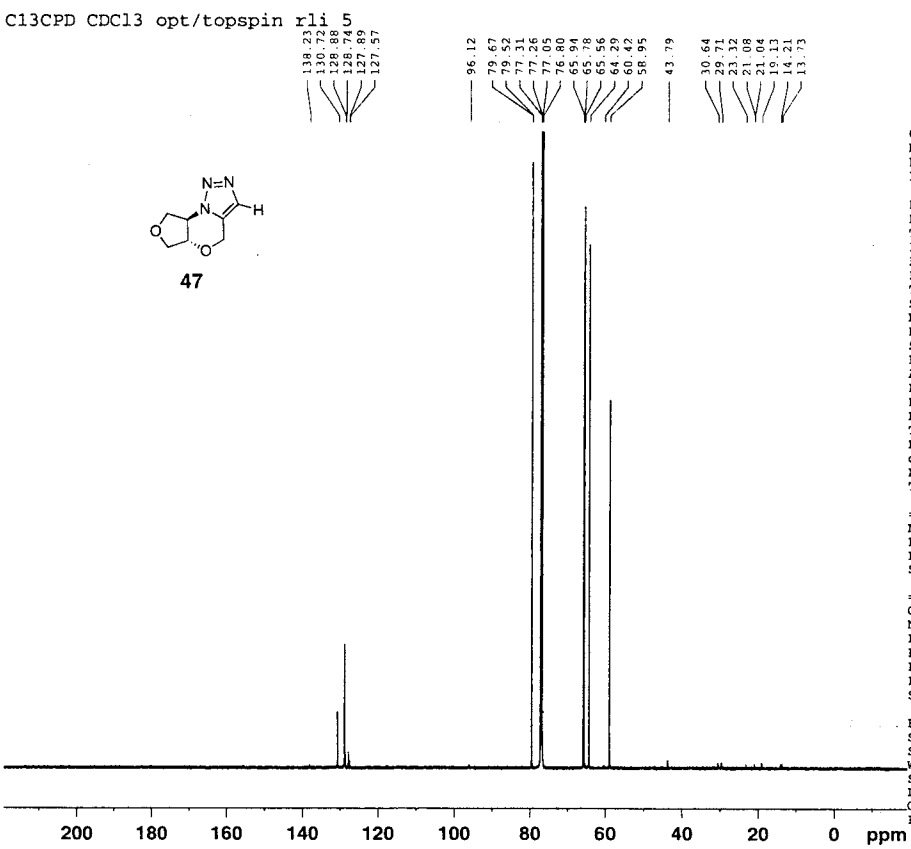
C13CPD CDCl3 opt/topspin rli 2



BRUKER

```
Current Data Parameters
NAME            RT-exp-250
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20070627
Time                 16.03
INSTRUM              spect
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           30030.029 Hz
FIDRES            0.458222 Hz
AQ                1.0912410 sec
RG                14596.5
DW                16.650 usec
DE                 6.00 usec
TE                298.2 K
D1              0.15000001 sec
d11             0.03000000 sec
DELTA           0.05000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  11.00 usec
PL1                  2.20 dB
SFO1          125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  1.60 dB
PL12                16.14 dB
PL13                10.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577890 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```





BRUKER

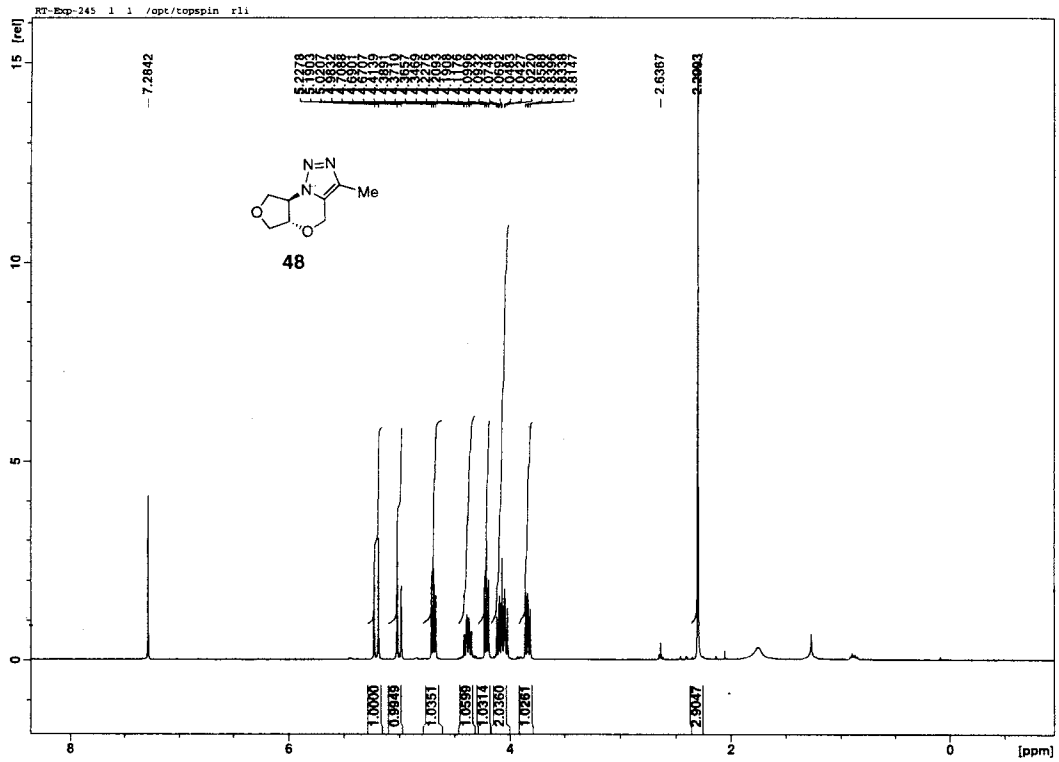
Current Data Parameters
NAME RT-EXP-244
EXPNO 1
PROCNO 1

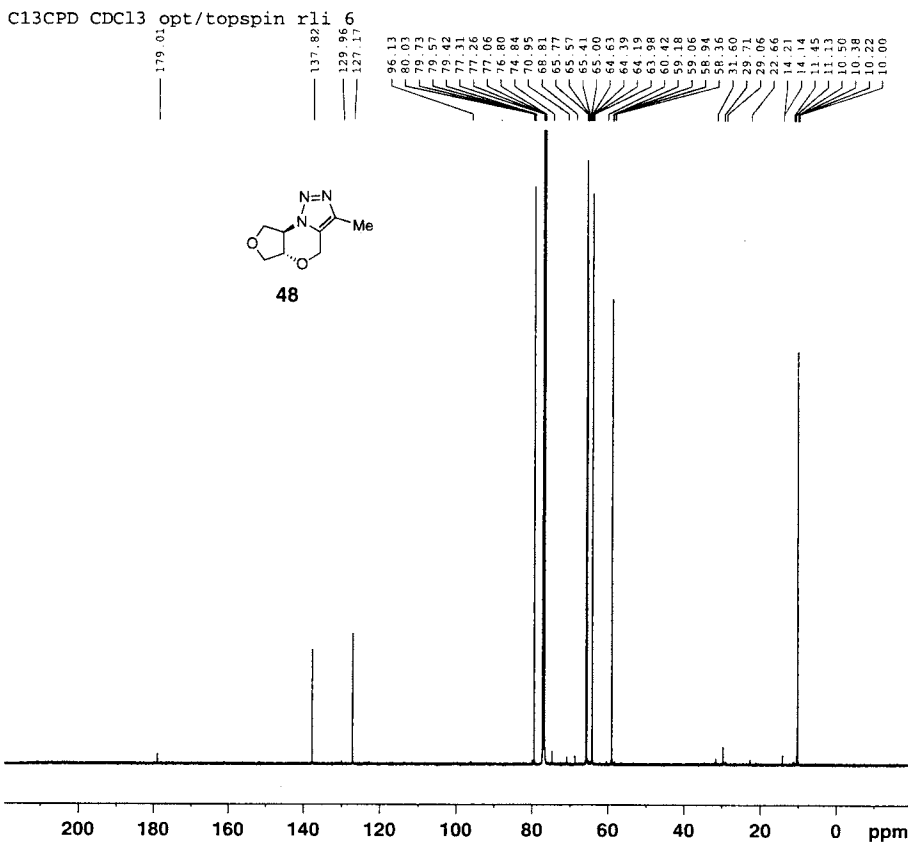
F2 - Acquisition Parameters
Date_ 20070621
Time 13.31
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 23170.5
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters

NAME	RT-EXP-245
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070621
Time	13.59
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	4096
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

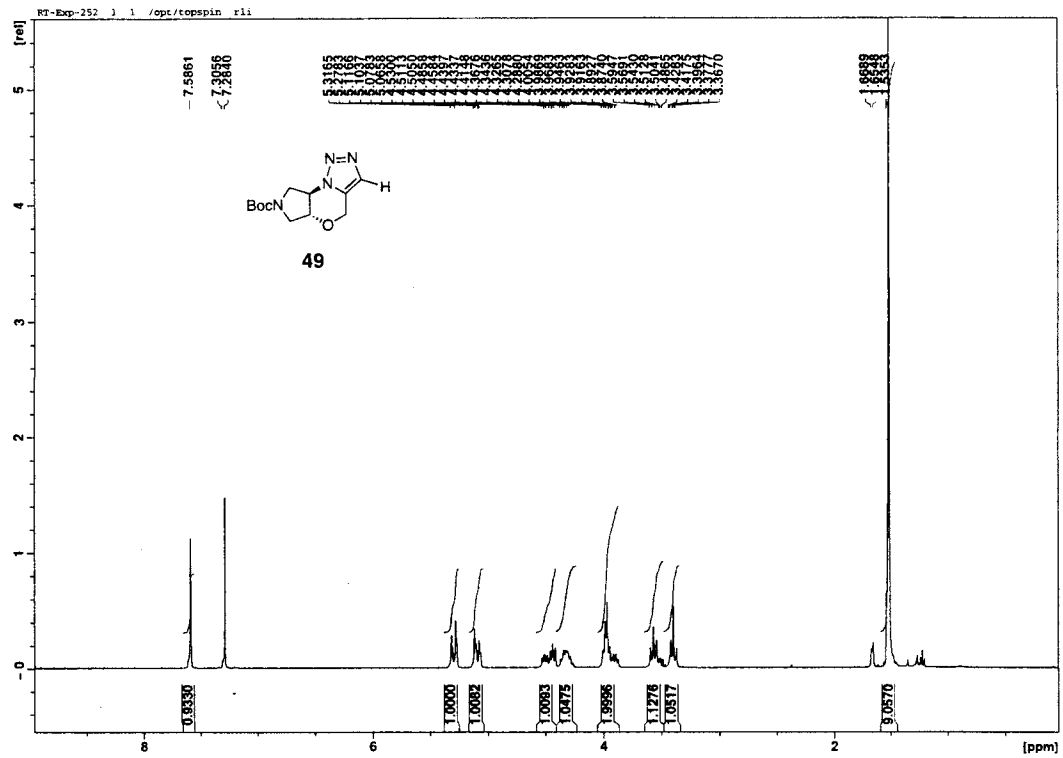
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

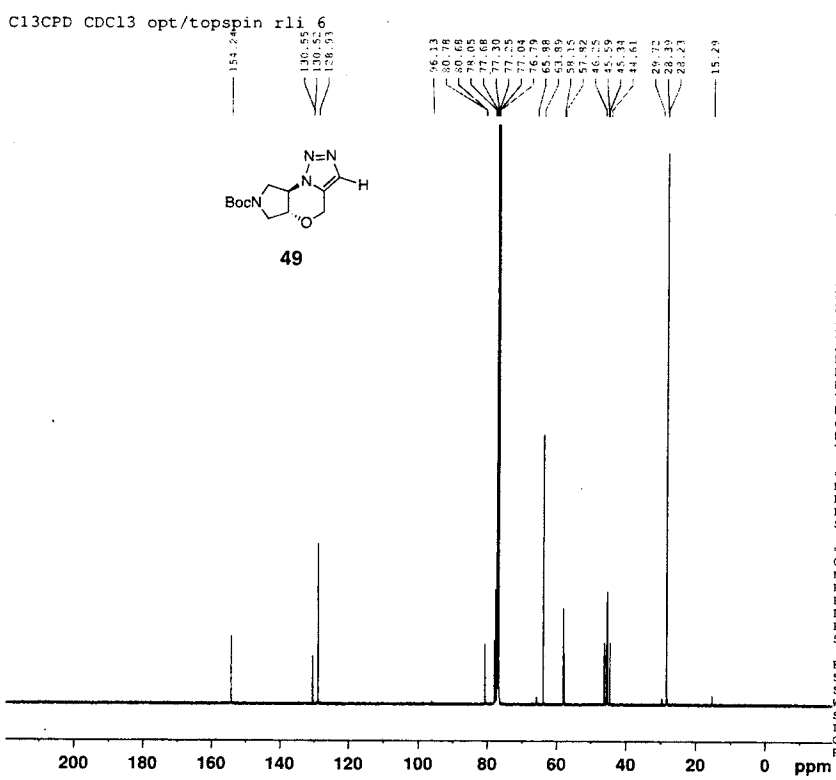
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

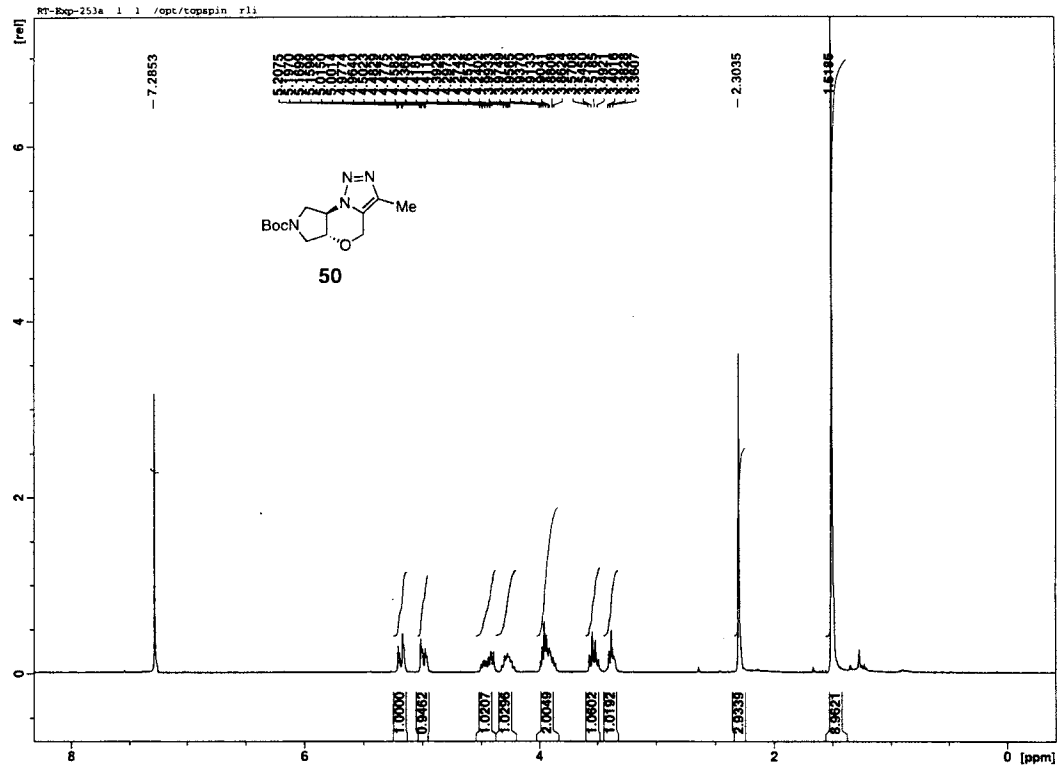
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

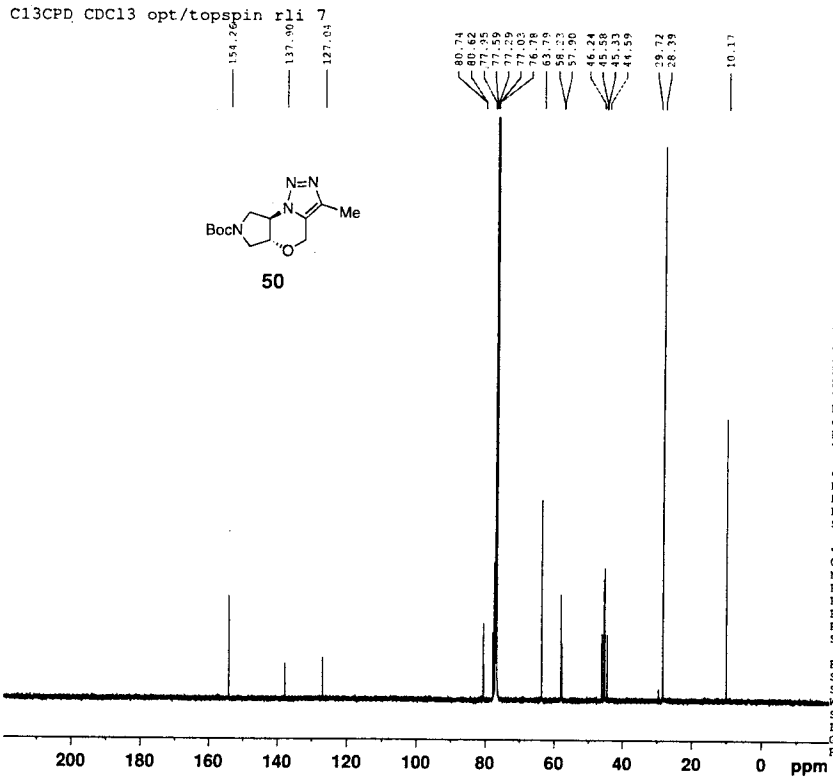




BRUKER

```
Current Data Parameters
NAME          RT-exp-252
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070628
Time               20.34
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1536
DS                    4
SWH           30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG              14596.5
DW               16.650 usec
DE                6.00 usec
TE               298.2 K
D1            0.15000001 sec
d11           0.03000000 sec
DELTA         0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                11.00 usec
PL1               2.20 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```





BRUKER

Current Data Parameters

NAME	RT-exp-253
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070628
Time	21.13
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1536
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

-------- CHANNEL f1 --------

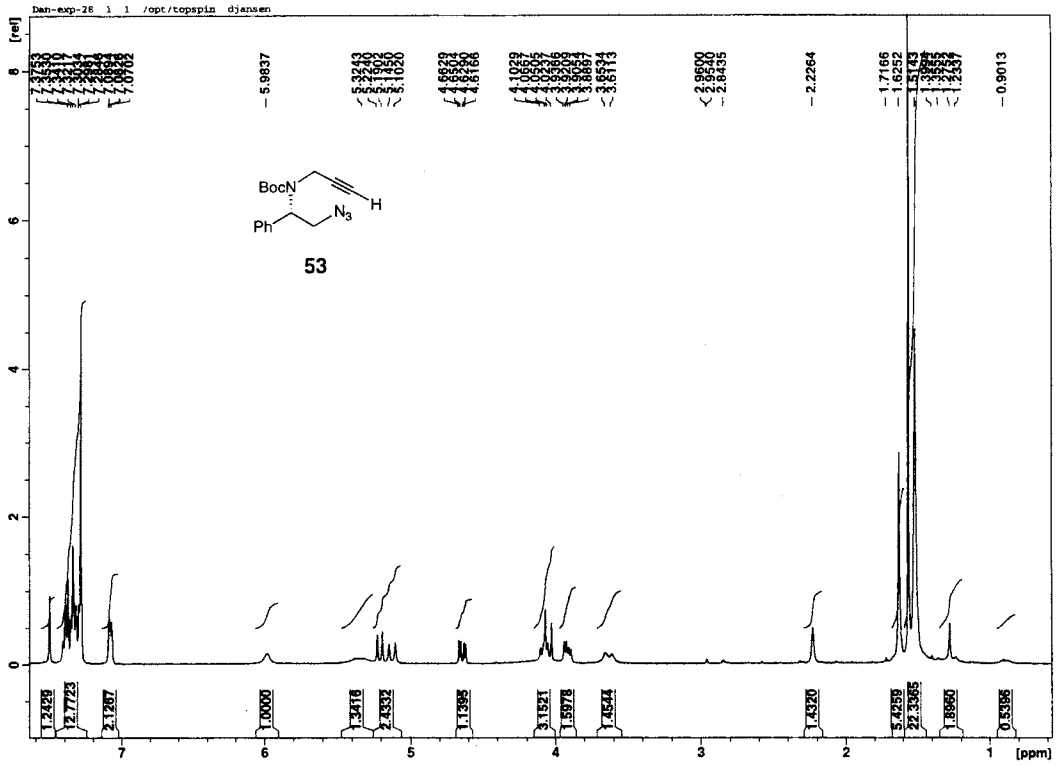
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

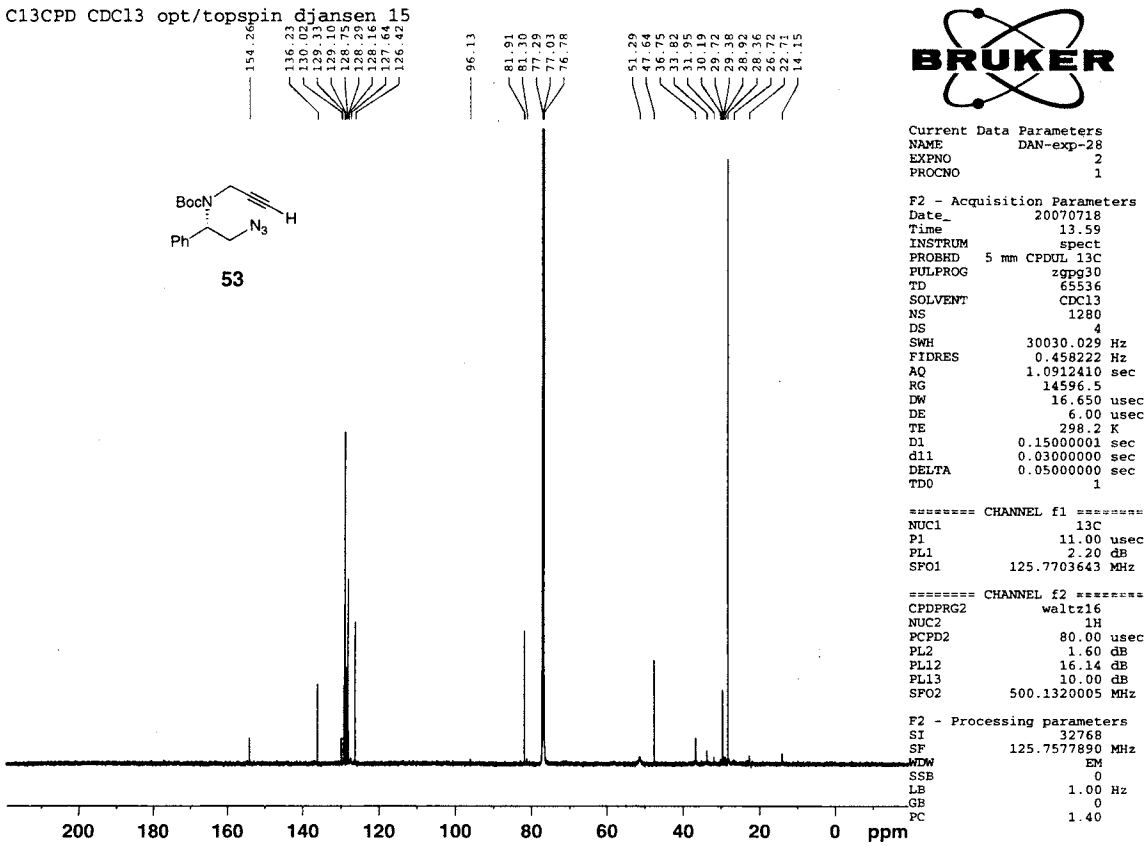
-------- CHANNEL f2 --------

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





BRUKER

Current Data Parameters

NAME	DAN-exp-28
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20070718
Time	13.59
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1280
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

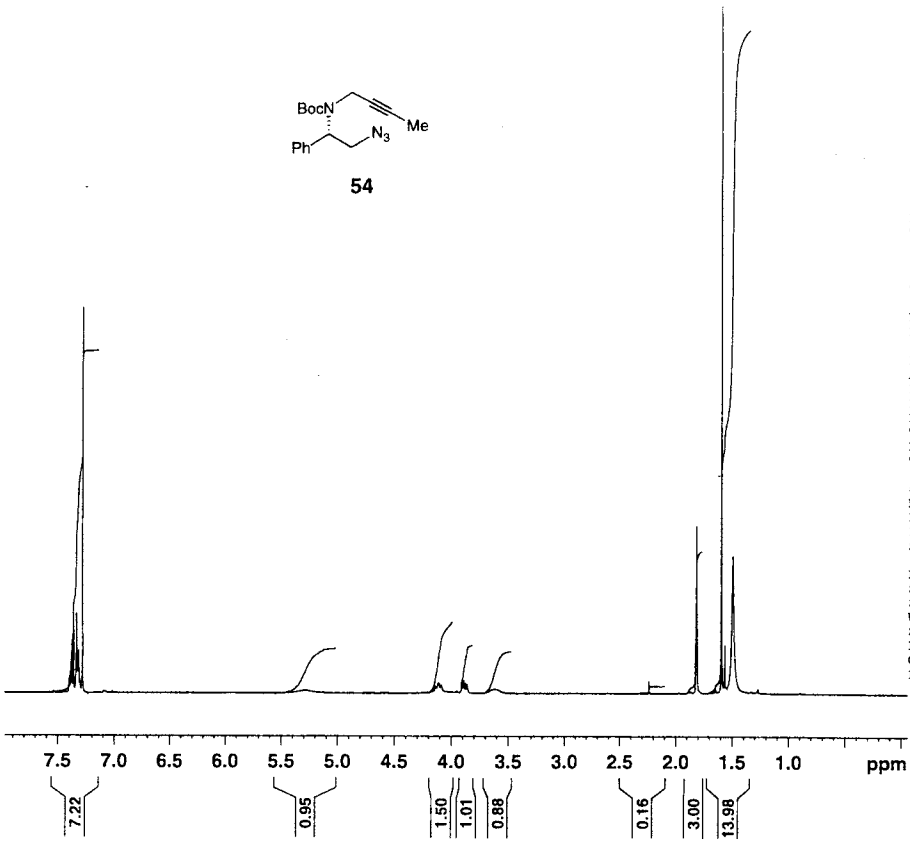
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

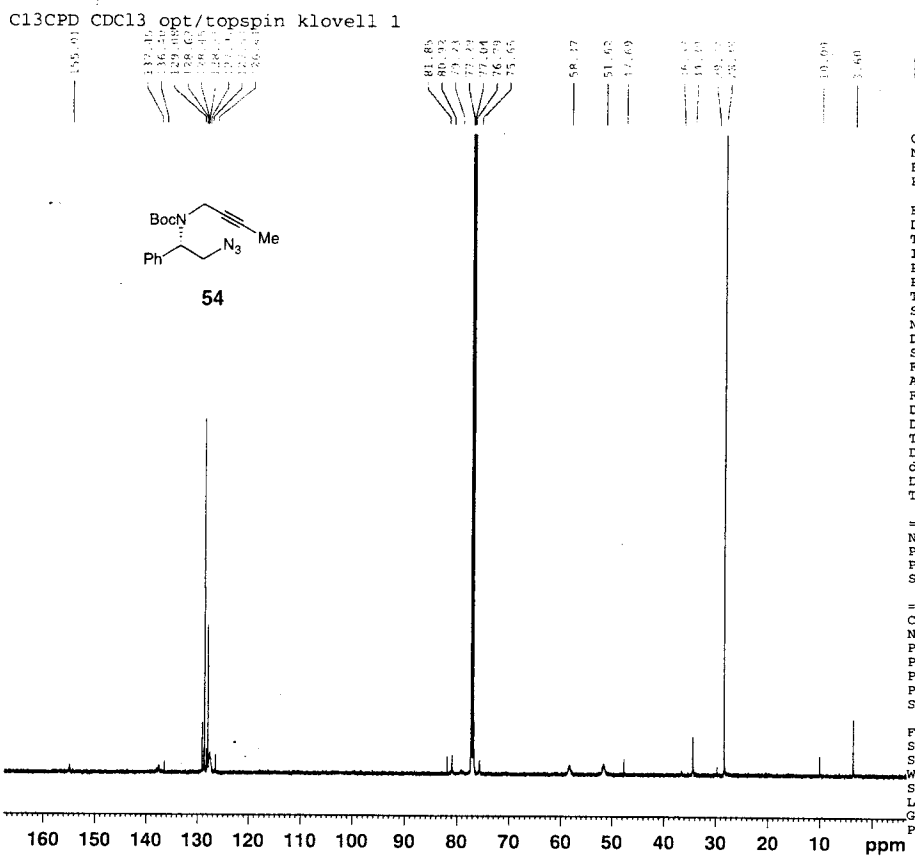
F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



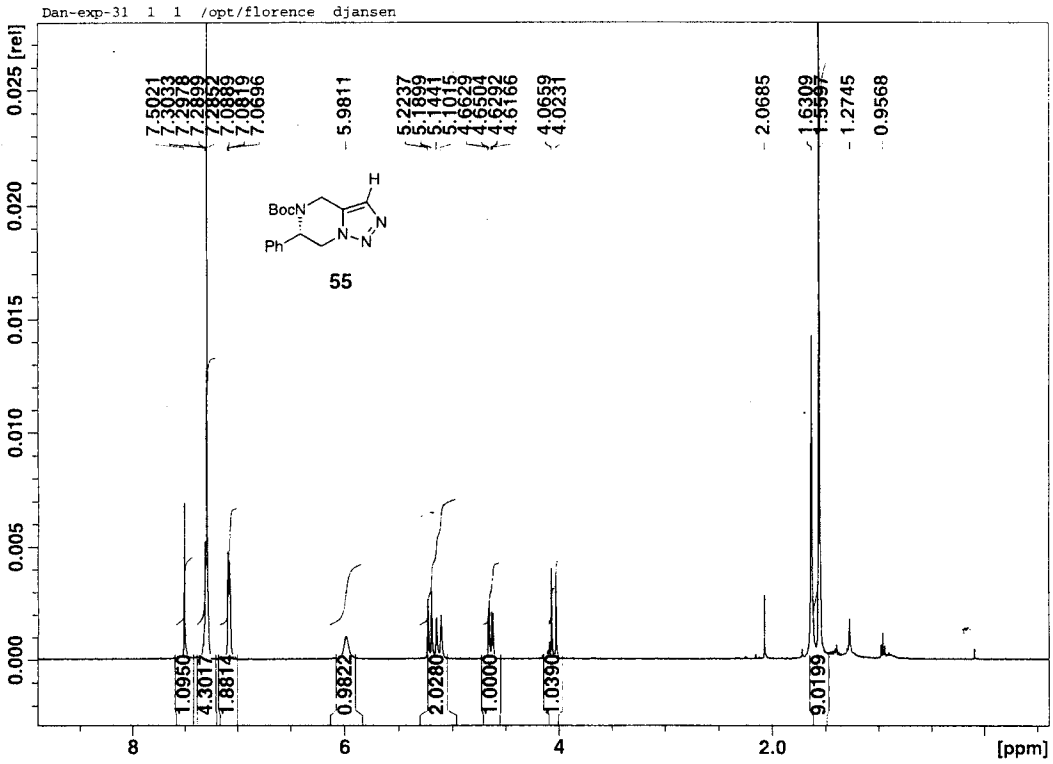
BRUKER

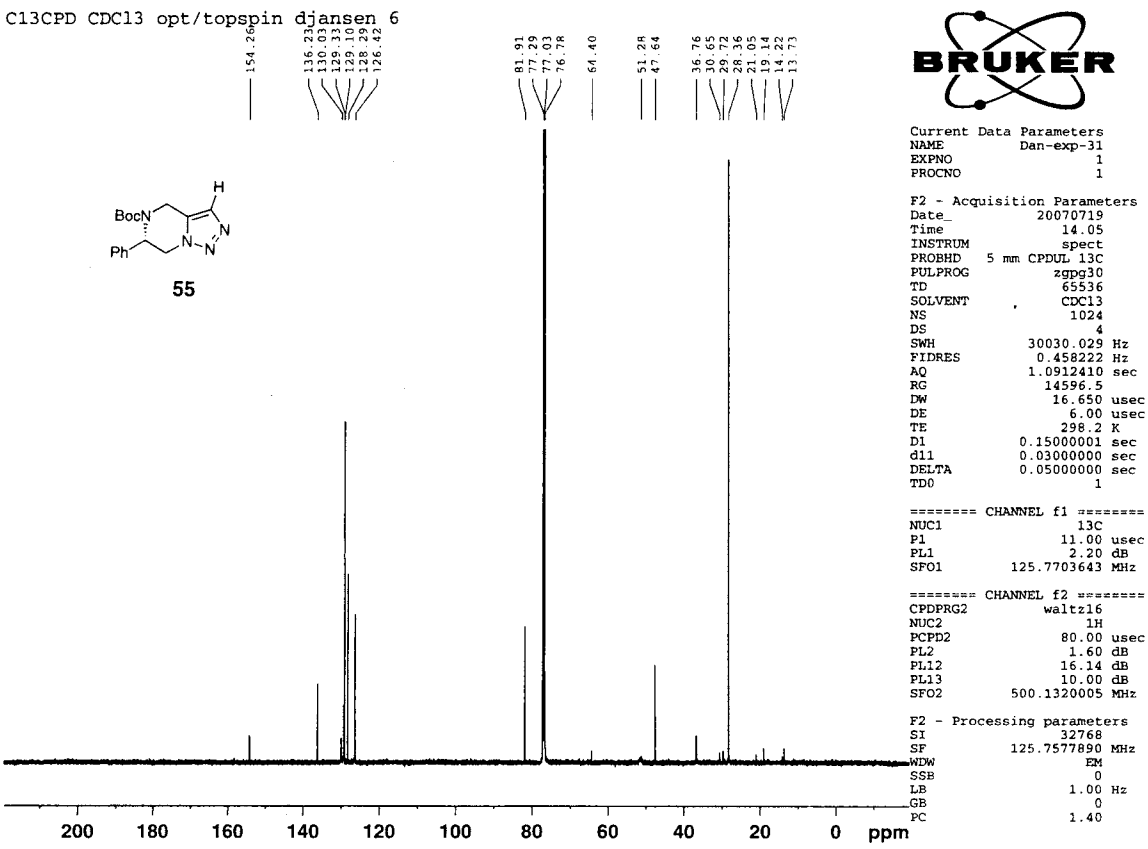
```
Current Data Parameters
NAME                  KML-1-275
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070910
Time                       8.57
INSTRUM                  drx400
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                           16
DS                            2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                       456.1
DW                    60.400 usec
DE                     6.00 usec
TE                     295.2 K
D1                1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                    10.50 usec
PL1                   -5.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF                400.1300000 MHz
WDW                          EM
SSB                           0
LB                     0.30 Hz
GB                            0
PC                         1.00
```



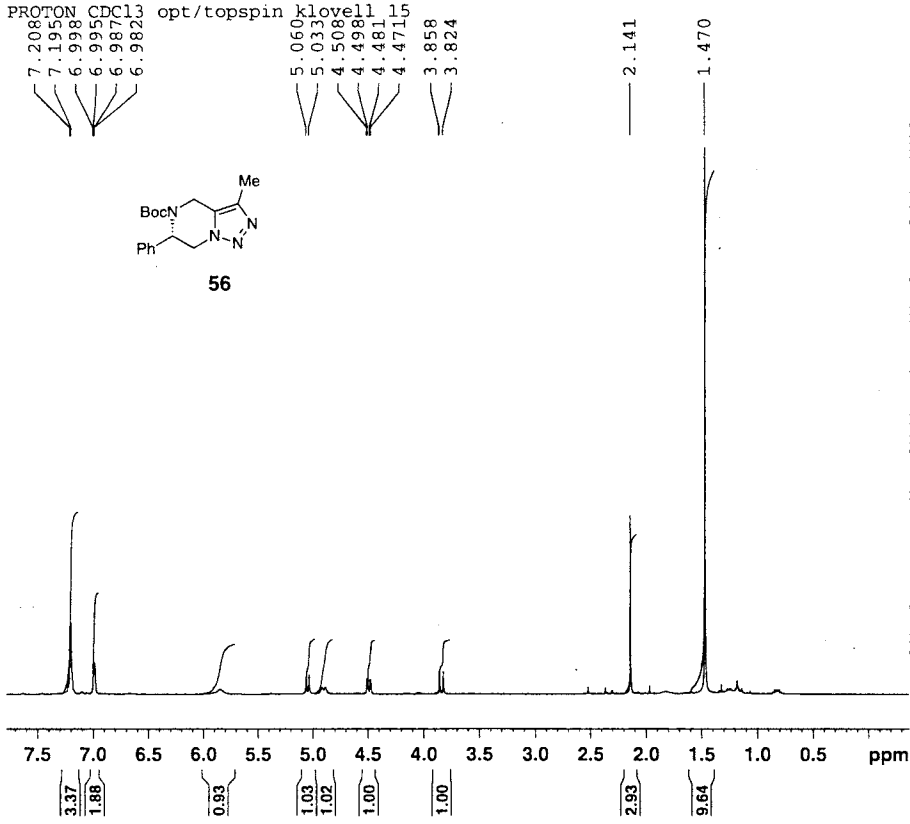
BRUKER

```
Current Data Parameters
NAME                  KML-1-275
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070912
Time                      14.34
INSTRUM                   spect
PROBHD    5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                           512
DS                             4
SWH                30030.029 Hz
FIDRES              0.458222 Hz
AQ                  1.0912410 sec
RG                     14596.5
DW                    16.650 usec
DE                     6.00 usec
TE                     298.2 K
D1                0.15000001 sec
d11               0.03000000 sec
DELTA             0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                    11.00 usec
PL1                    2.20 dB
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                         1H
PCPD2                 80.00 usec
PL2                    1.60 dB
PL12                  16.14 dB
PL13                  10.00 dB
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                        32768
SF                125.7577890 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                         1.40
```


Dan-exp-31 1 1 /opt/florence djansen
7.5021
7.3033
7.2978
7.2899
7.2852
7.0889
7.0819
7.0696
5.9811
5.2237
5.1899
5.1441
5.1015
4.6629
4.6504
4.6292
4.6166
4.0659
4.0231
2.0685
1.6309
1.5597
1.2745
0.9568
1.0950
4.3017
1.8814
0.9822
2.0280
1.0000
1.0390
9.0199
0.025 [rel]
0.020
0.015
0.010
0.005
0.000
8
6
4
2.0
[ppm]
BocN
Ph
H
N
55


C13CPD CDCl3 opt/topspin djansen 6
154.26
136.23
130.03
129.33
129.10
128.29
126.42
81.91
77.29
77.03
76.78
64.40
51.28
47.64
36.76
30.65
29.72
28.36
21.05
19.14
14.22
13.73
BocN
Ph
H
N
55
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME Dan-exp-31
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070719
Time 14.05
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 14596.5
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

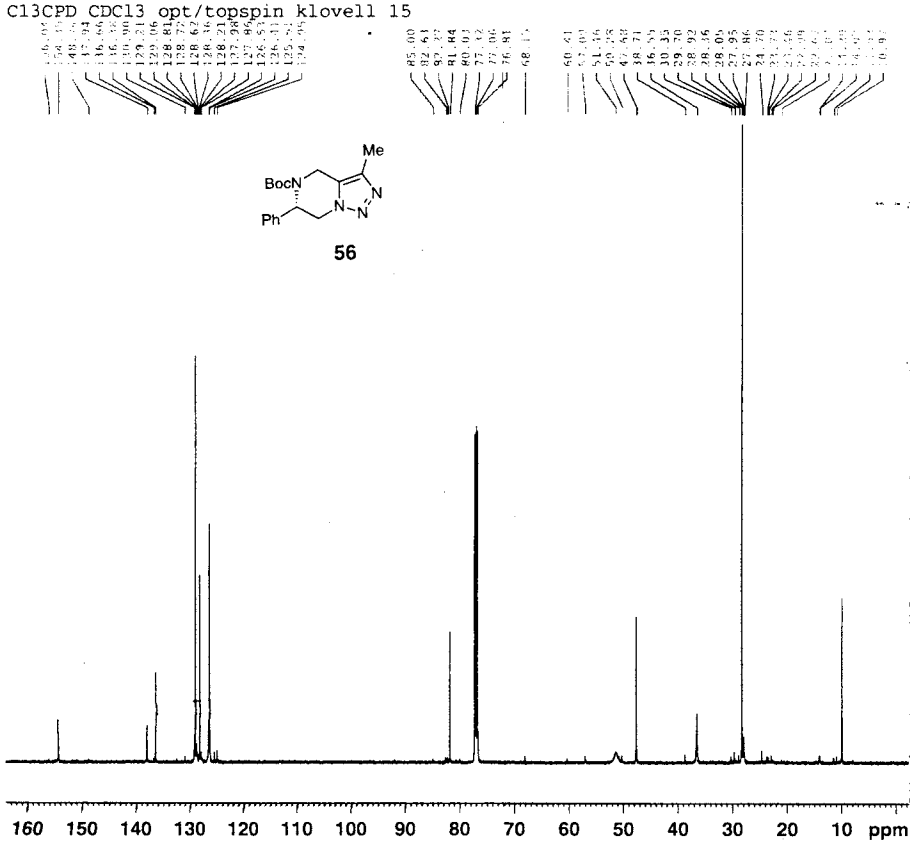
PROTON CDCl3 opt/topspin klovell 15



BRUKER

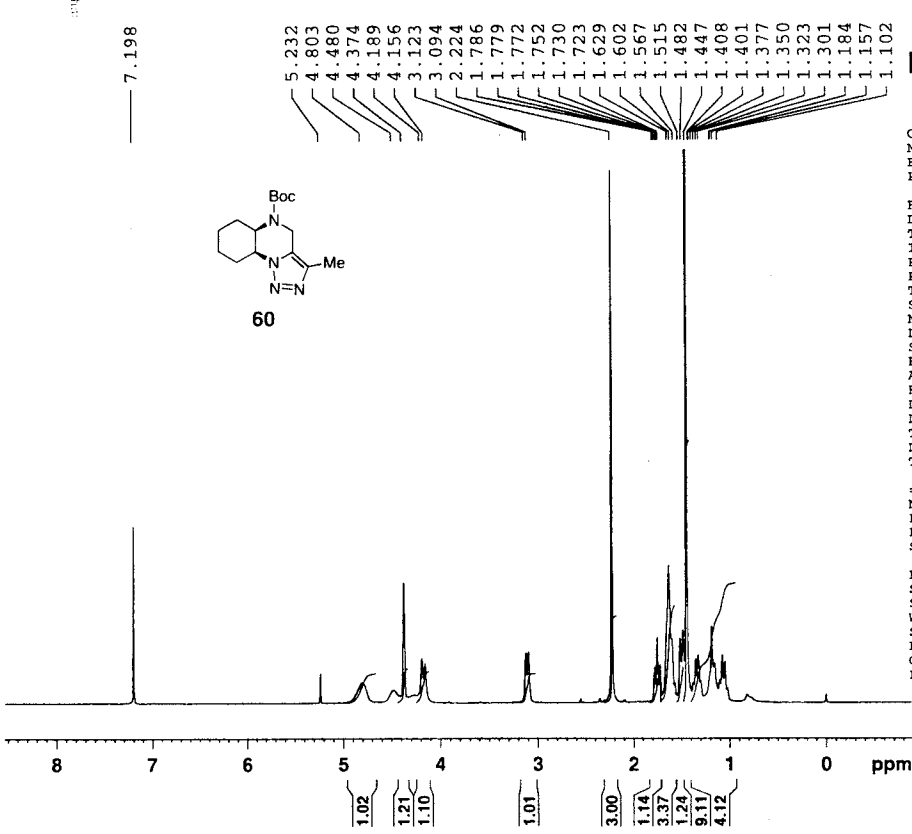
```
Current Data Parameters
NAME                  KML-1-277
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070912
Time                      19.31
INSTRUM                   spect
PROBHD     5 mm CPDUL 13C
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  10330.578 Hz
FIDRES               0.157632 Hz
AQ                   3.1720407 sec
RG                        90.5
DW                     48.400 usec
DE                      6.00 usec
TE                      298.2 K
D1                   0.15000001 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.00 usec
PL1                       1.60 dB
SFO1                500.1330885 MHz

F2 - Processing parameters
SI                       32768
SF                  500.1300421 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

C13CPD CDCl3 opt/topspin klovell 15



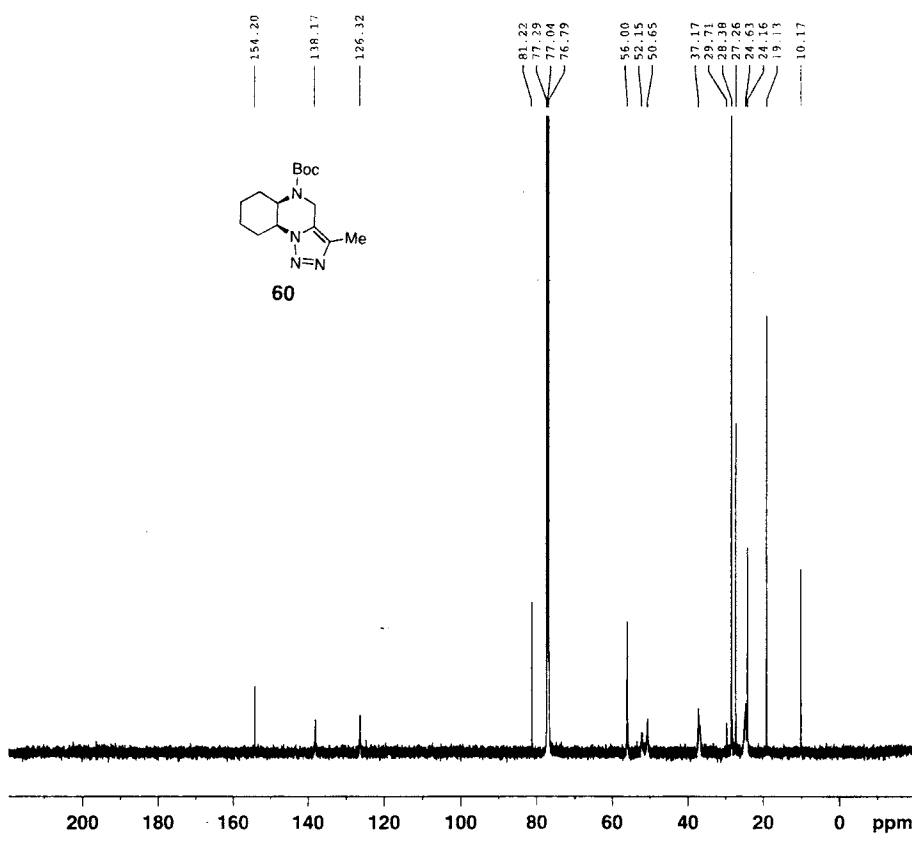
BRUKER

```
Current Data Parameters
NAME                  KML-1-277
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20070912
Time                      19.49
INSTRUM                   spect
PROBHD     5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         768
DS                           4
SWH                  30030.029 Hz
FIDRES               0.458222 Hz
AQ                   1.0912410 sec
RG                       13004
DW                     16.650 usec
DE                      6.00 usec
TE                      298.2 K
D1                   0.15000001 sec
d11                  0.03000000 sec
DELTA                0.05000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       11.00 usec
PL1                       2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       1.60 dB
PL12                     16.14 dB
PL13                     10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF                  125.7577890 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```



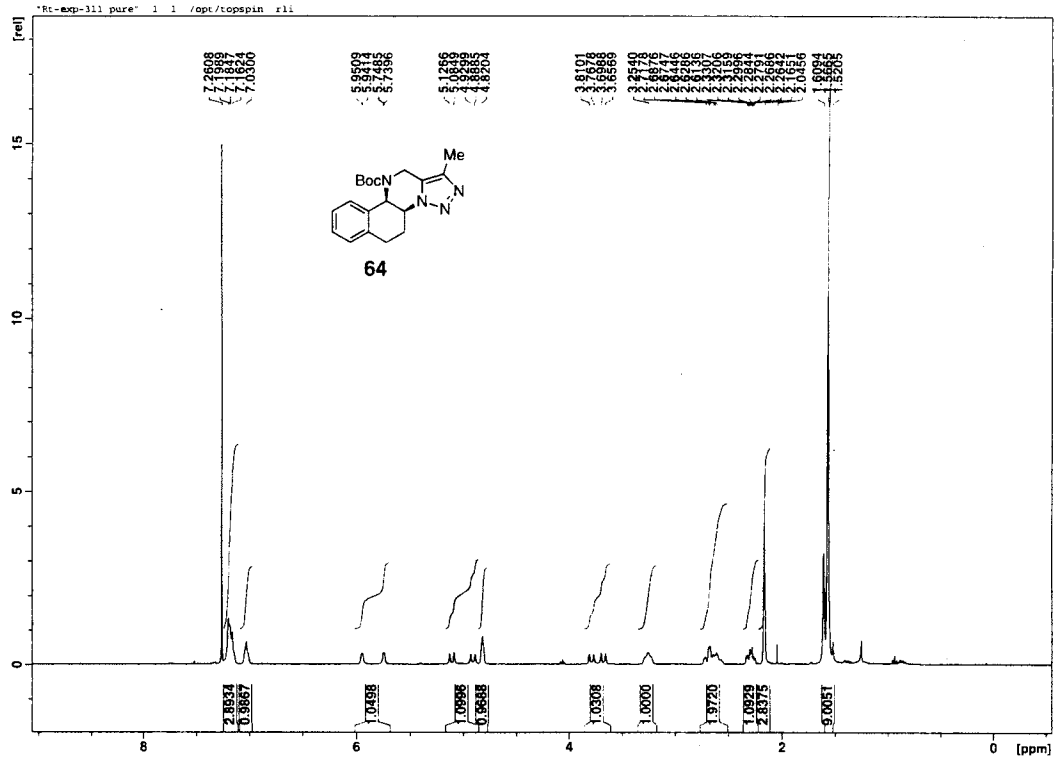
BRUKER

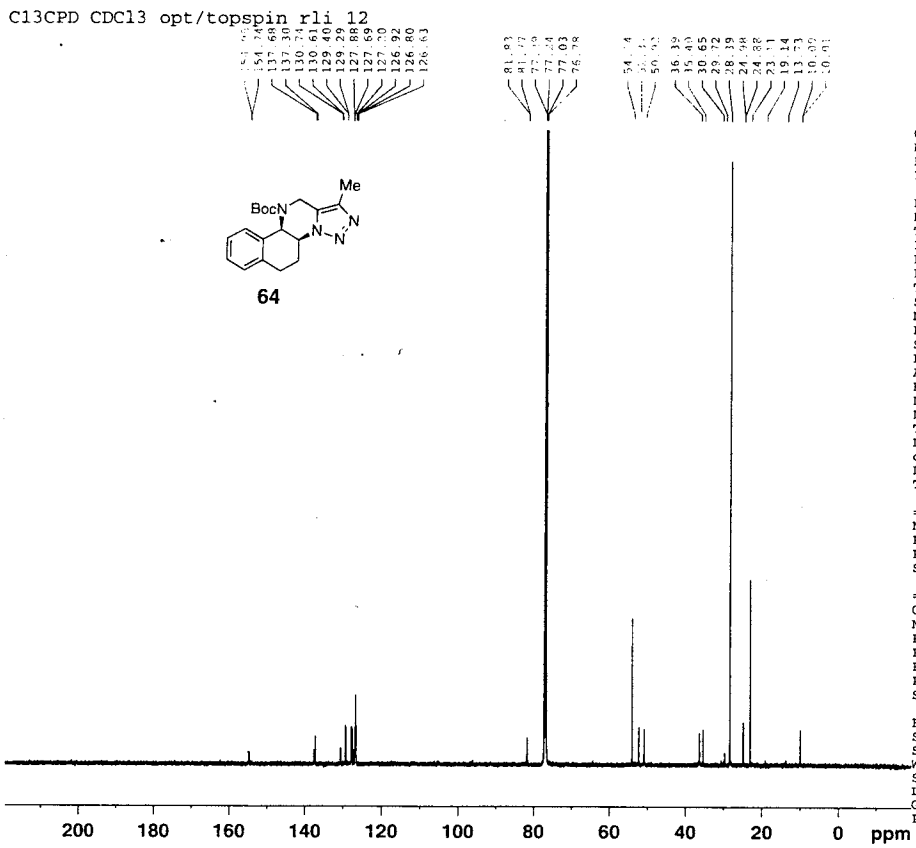
```
Current Data Parameters
NAME          Dan-exp-25
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20071001
Time              17.49
INSTRUM           spect
PROBHD   5 mm CPDUL 13C
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1720407 sec
RG                203.2
DW               48.400 usec
DE                6.00 usec
TE                298.2 K
D1            0.15000001 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                1.60 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                32768
SF           500.1300435 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



BRUKER

```
Current Data Parameters
NAME          Dan-exp-25
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20071001
Time              18.16
INSTRUM           spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1200
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG                16384
DW               16.650 usec
DE                6.00 usec
TE                298.2 K
D1            0.15000001 sec
d11           0.03000000 sec
DELTA         0.05000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1                2.20 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                32768
SF           125.7577890 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





Current Data Parameters

NAME	RT-exp-311
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070831
Time	19.38
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1800
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	14596.5
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

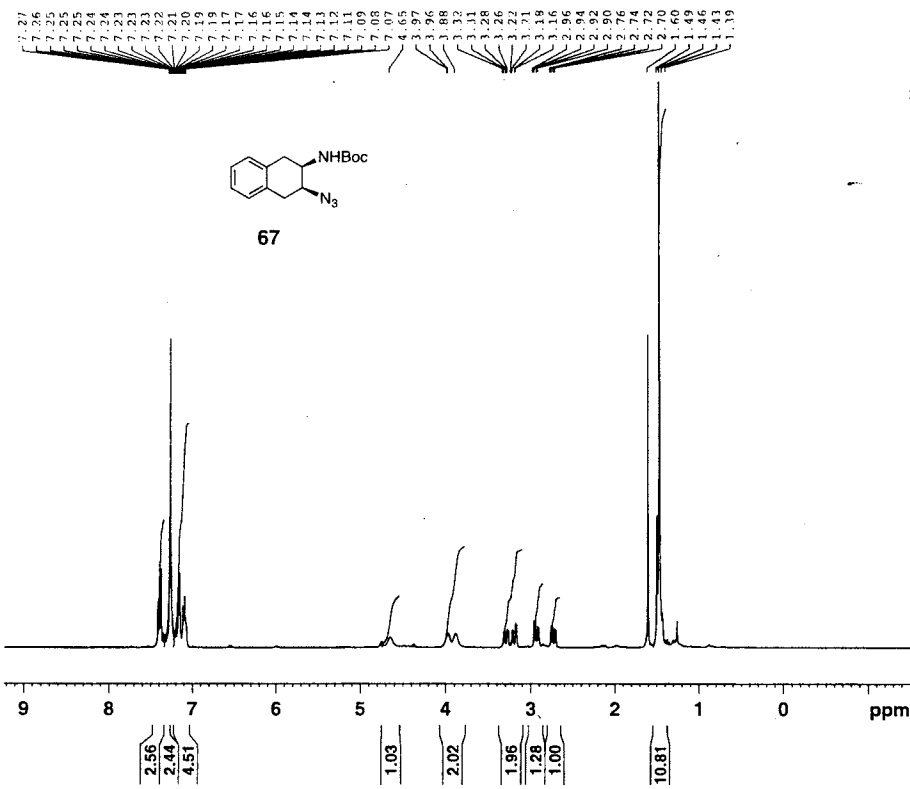
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

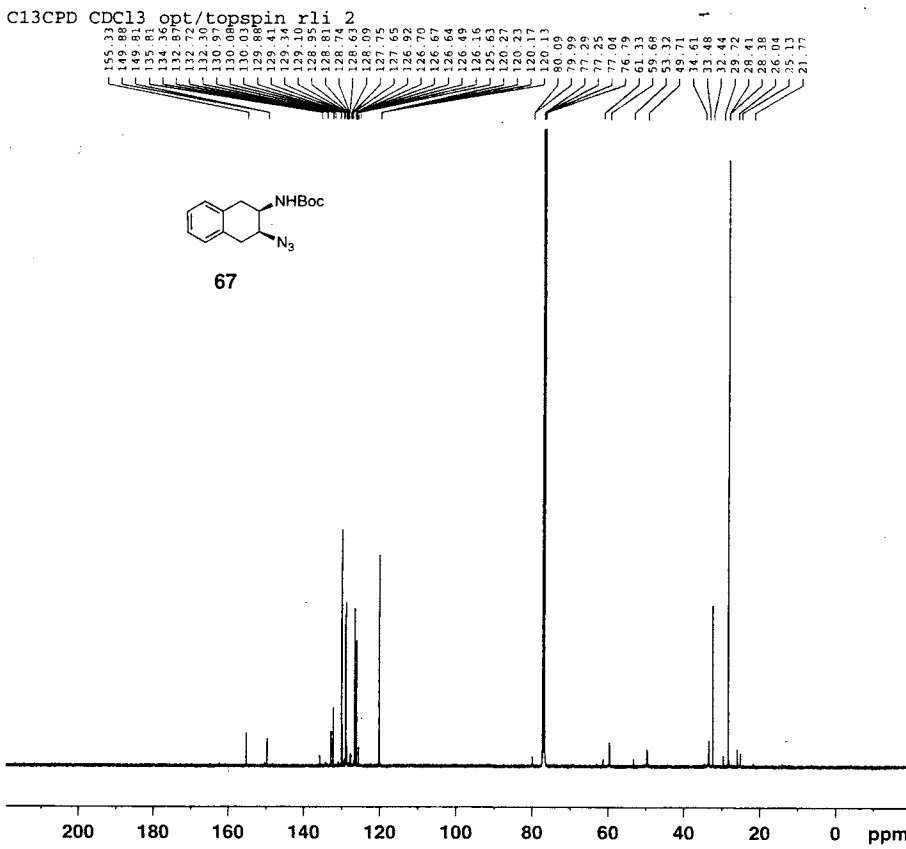


Current Data Parameters
NAME RT-Exp-288b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070726
Time 9.36
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 256
DW 60.400 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



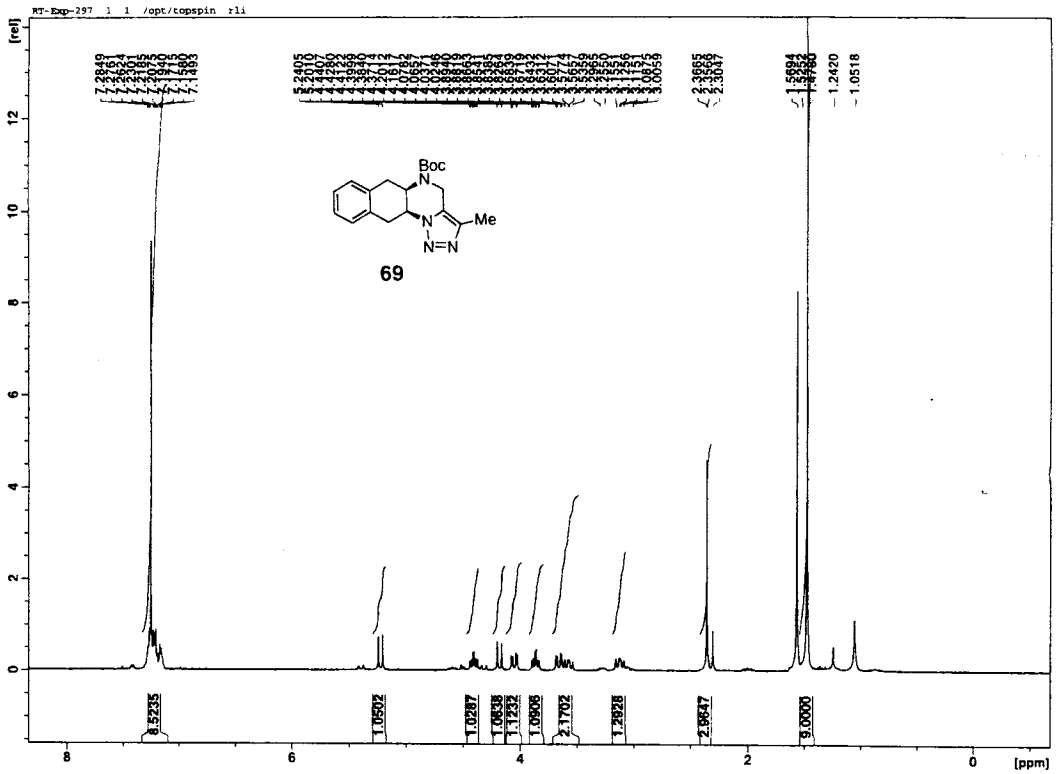
Current Data Parameters
NAME RT-exp-288
EXPNO 2
PROCNO 1

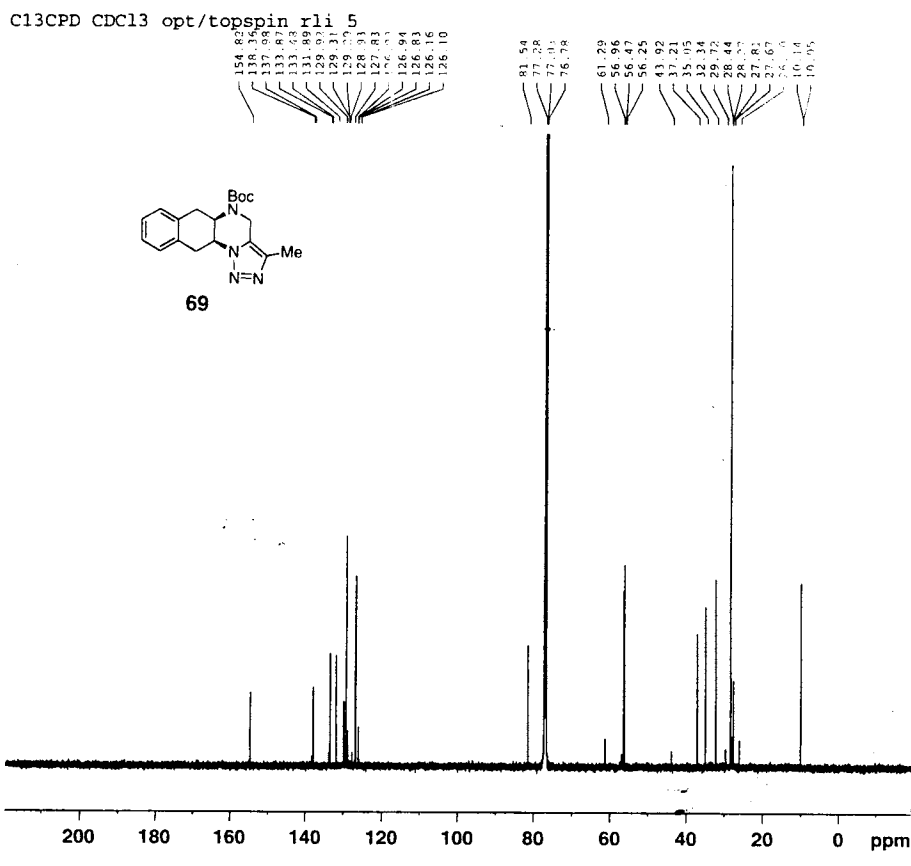
F2 - Acquisition Parameters
Date_ 20070726
Time 13.22
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

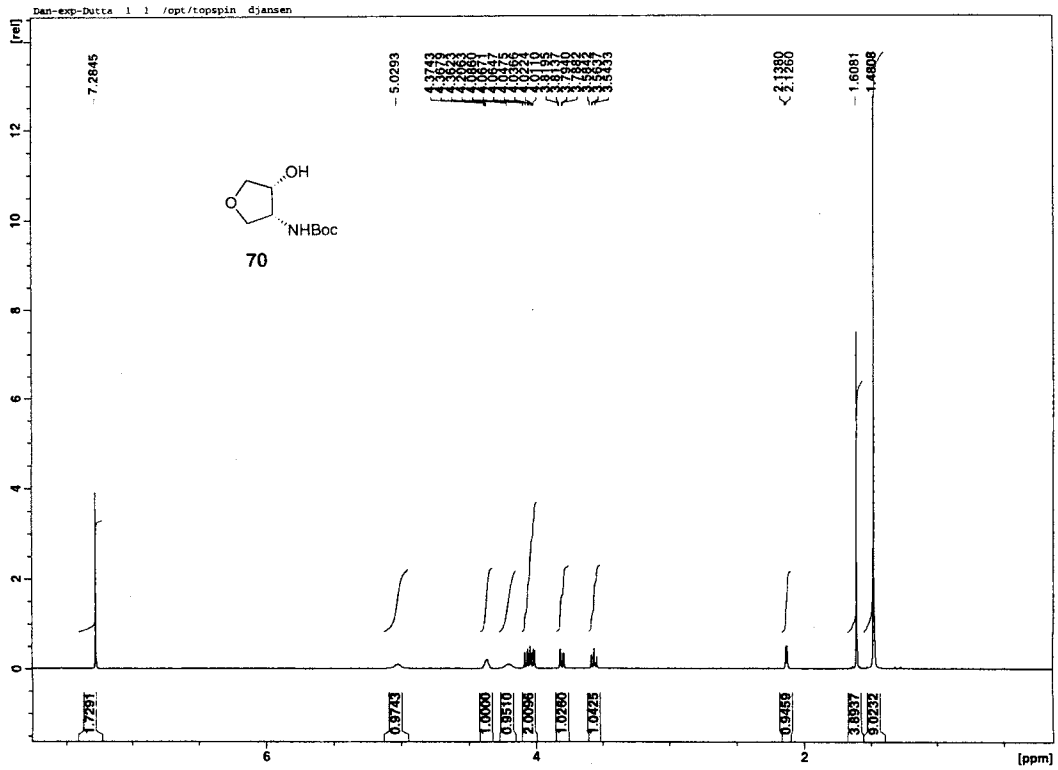
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



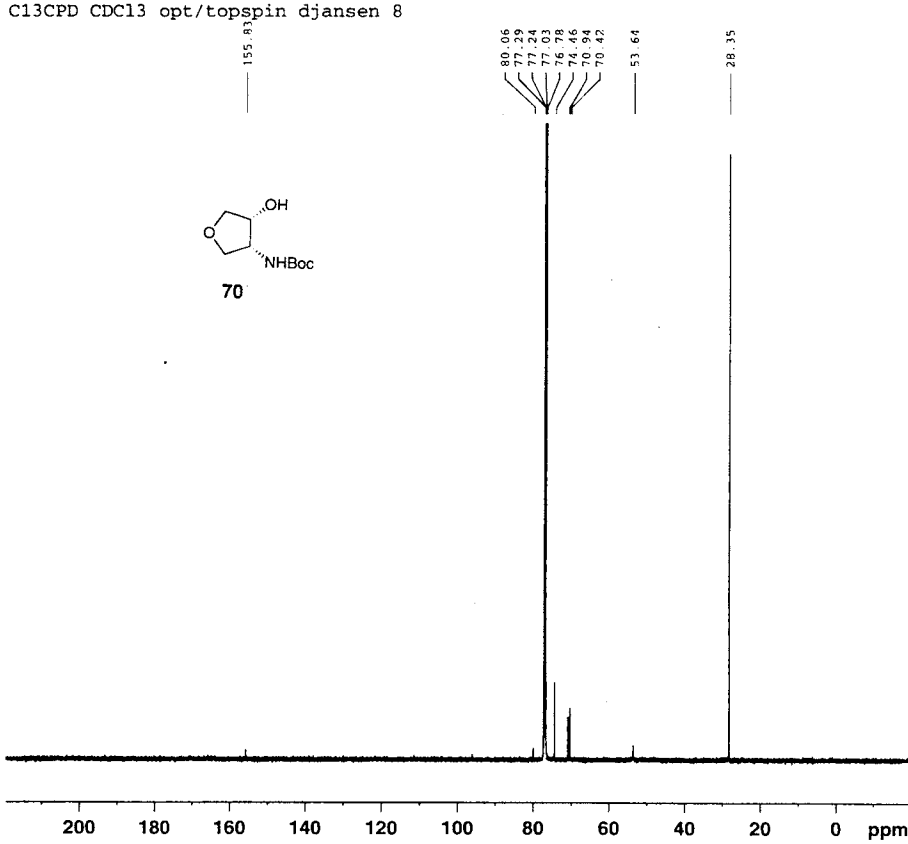


BRUKER

```
Current Data Parameters
NAME                 RT-exp-297
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20070817
Time                     17.04
INSTRUM                  spect
PROBHD     5 mm CPDUL 13C
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       2000
DS                          4
SWH                 30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                      13004
DW                     16.650 usec
DE                      6.00 usec
TE                     298.2 K
D1                 0.15000001 sec
d11                0.03000000 sec
DELTA              0.05000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       11.00 usec
PL1                       2.20 dB
SFO1               125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                       1.60 dB
PL12                     16.14 dB
PL13                     10.00 dB
SFO2               500.1320005 MHz

F2 - Processing parameters
SI                          32768
SF                 125.7577890 MHz
WDW                            EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

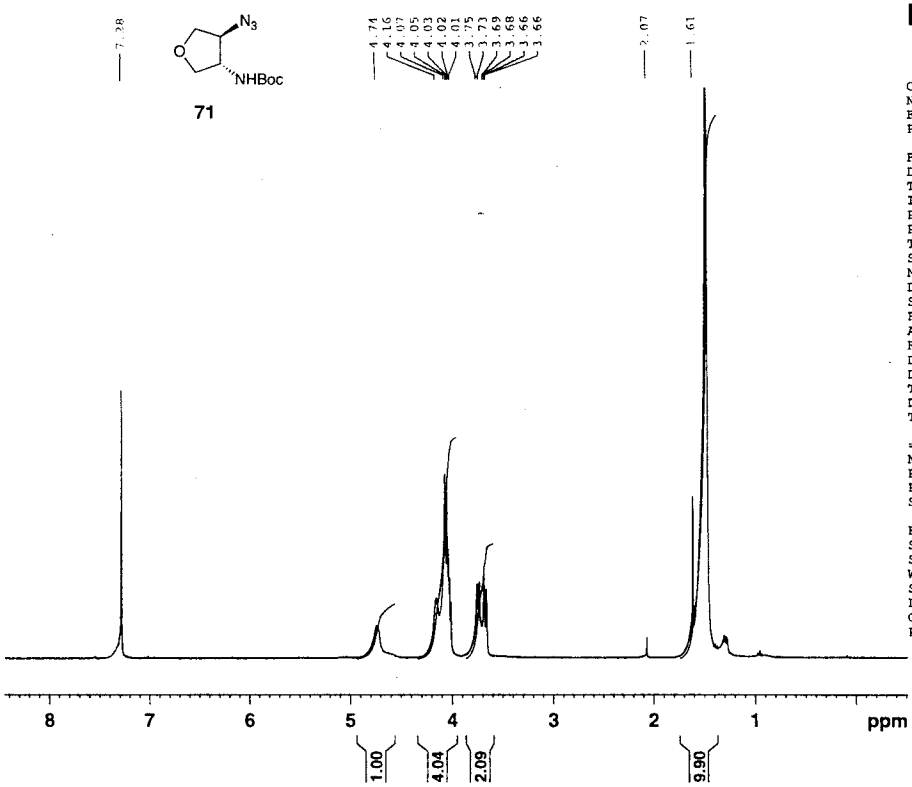


C13CPD CDCl3 opt/topspin djansen 8



BRUKER

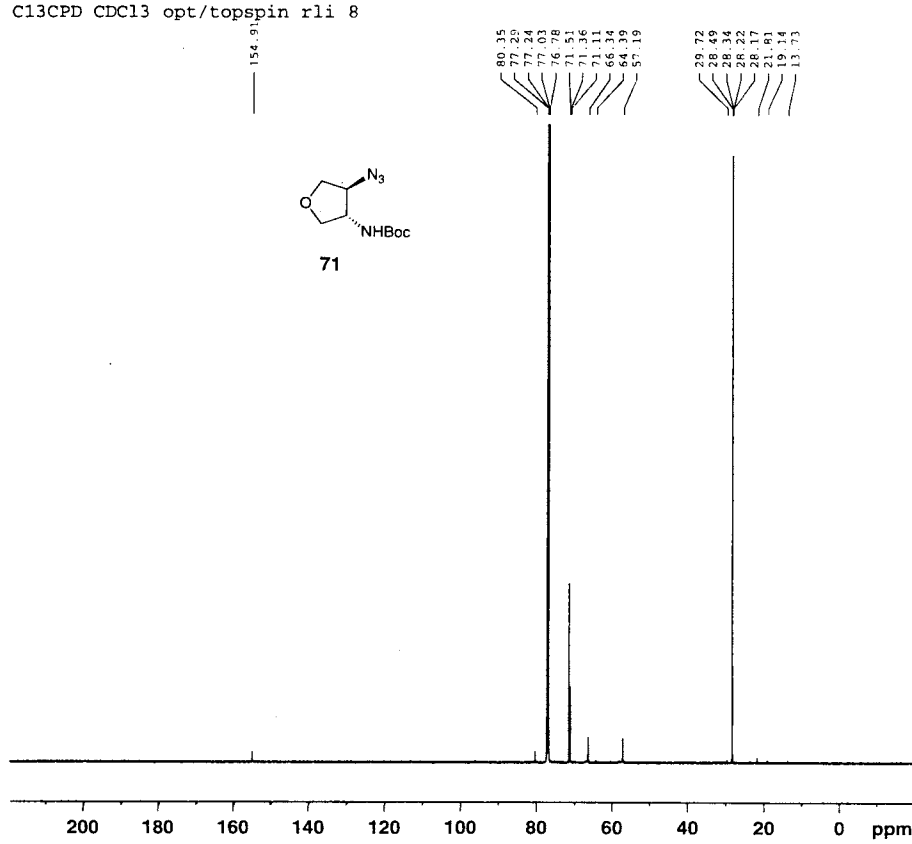
```
Current Data Parameters
NAME        Dan-exp-16-SM
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20070620
Time                15.00
INSTRUM             spect
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912410 sec
RG                  13004
DW                16.650 usec
DE                 6.00 usec
TE                298.2 K
D1            0.15000001 sec
d11           0.03000000 sec
DELTA         0.05000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.00 usec
PL1                 2.20 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 1.60 dB
PL12               16.14 dB
PL13               10.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF           125.7577890 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40
```



BRUKER

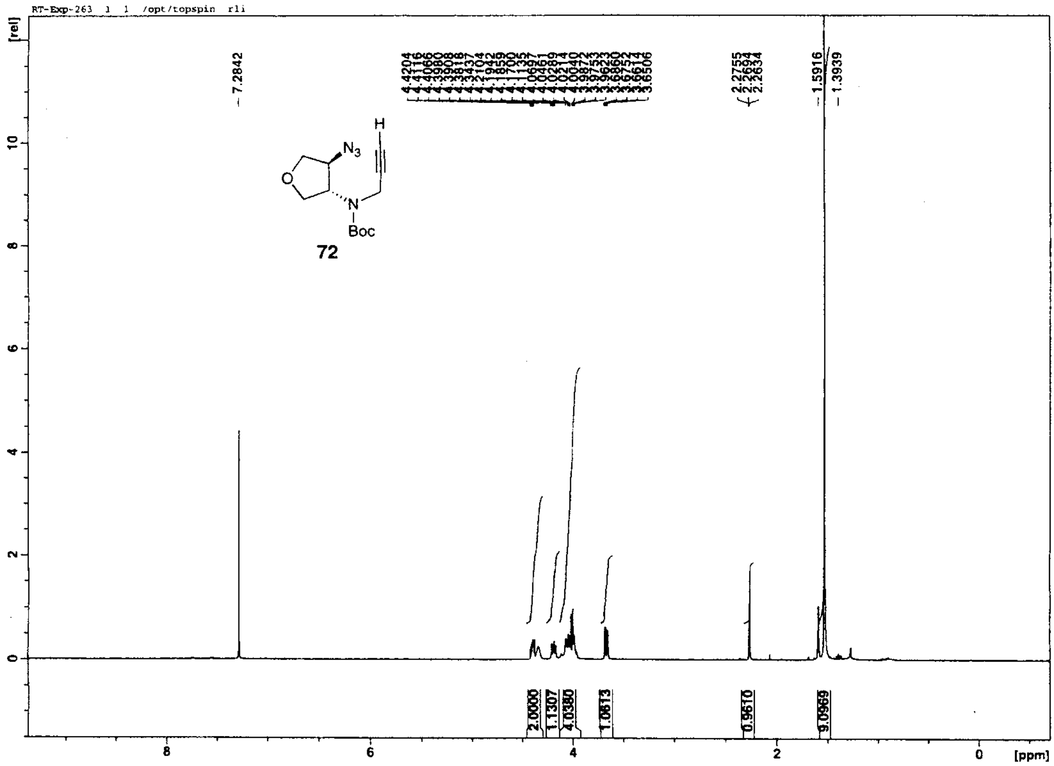
```
Current Data Parameters
NAME          RT-Exp-260
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070703
Time               15.56
INSTRUM          drx400
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG                322.5
DW             60.400 usec
DE              6.00 usec
TE              296.2 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1             10.50 usec
PL1            -5.00 dB
SFO1      400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB             0.30 Hz
GB                    0
PC                 1.00
```

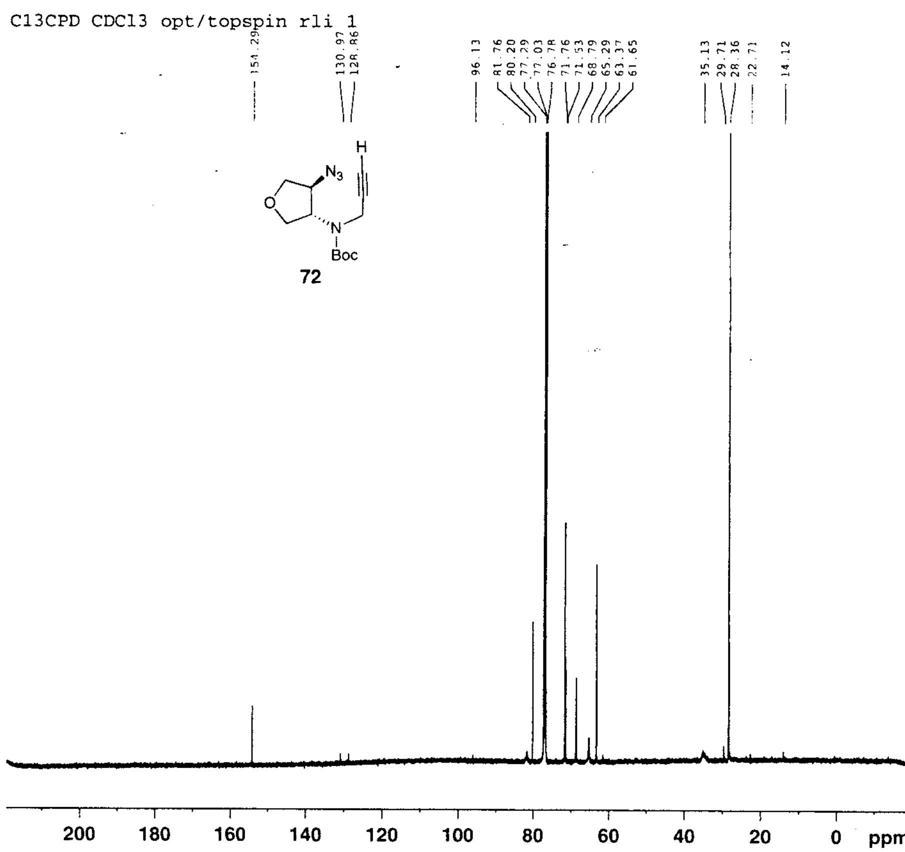
C13CPD CDCl3 opt/topspin rli 8



BRUKER

```
Current Data Parameters
NAME          RT-exp-260
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070703
Time               18.21
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG                13004
DW             16.650 usec
DE              6.00 usec
TE              298.2 K
D1          0.15000001 sec
d11         0.03000000 sec
DELTA       0.05000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1             11.00 usec
PL1             2.20 dB
SFO1      125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2          80.00 usec
PL2             1.60 dB
PL12           16.14 dB
PL13           10.00 dB
SFO2      500.1320005 MHz

F2 - Processing parameters
SI                32768
SF          125.7577890 MHz
WDW                  EM
SSB                   0
LB             1.00 Hz
GB                    0
PC                 1.40
```





BRUKER

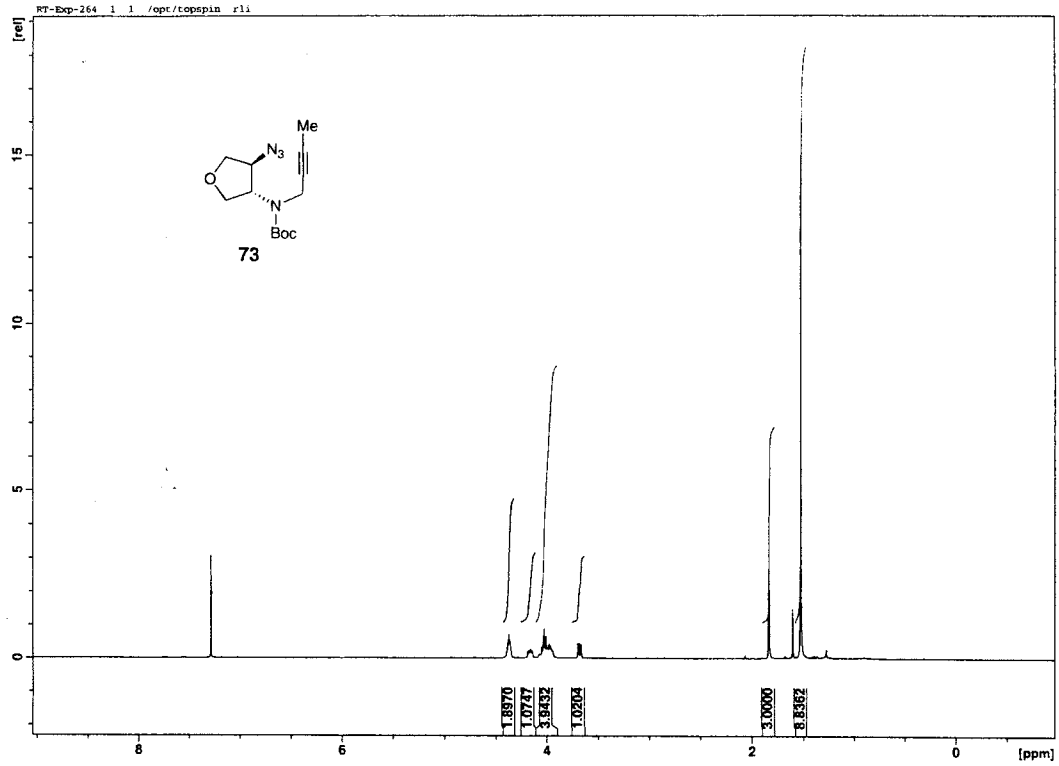
Current Data Parameters
NAME RT-exp-263
EXPNO 2
PROCNO 1

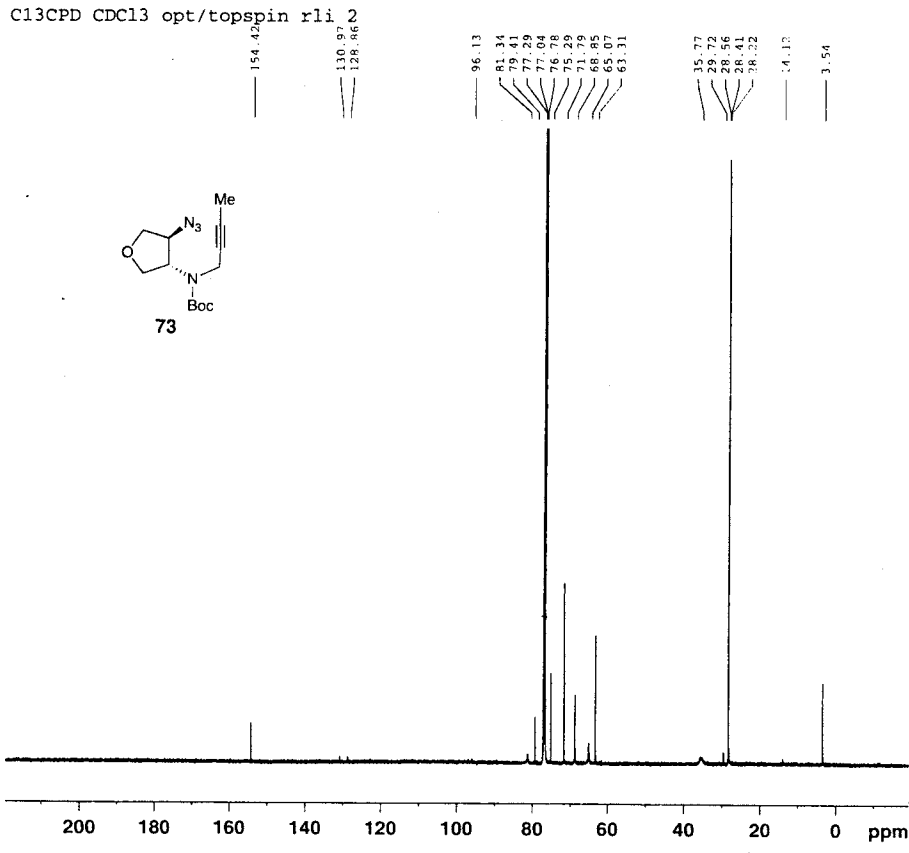
F2 - Acquisition Parameters
Date_ 20070709
Time 11.48
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

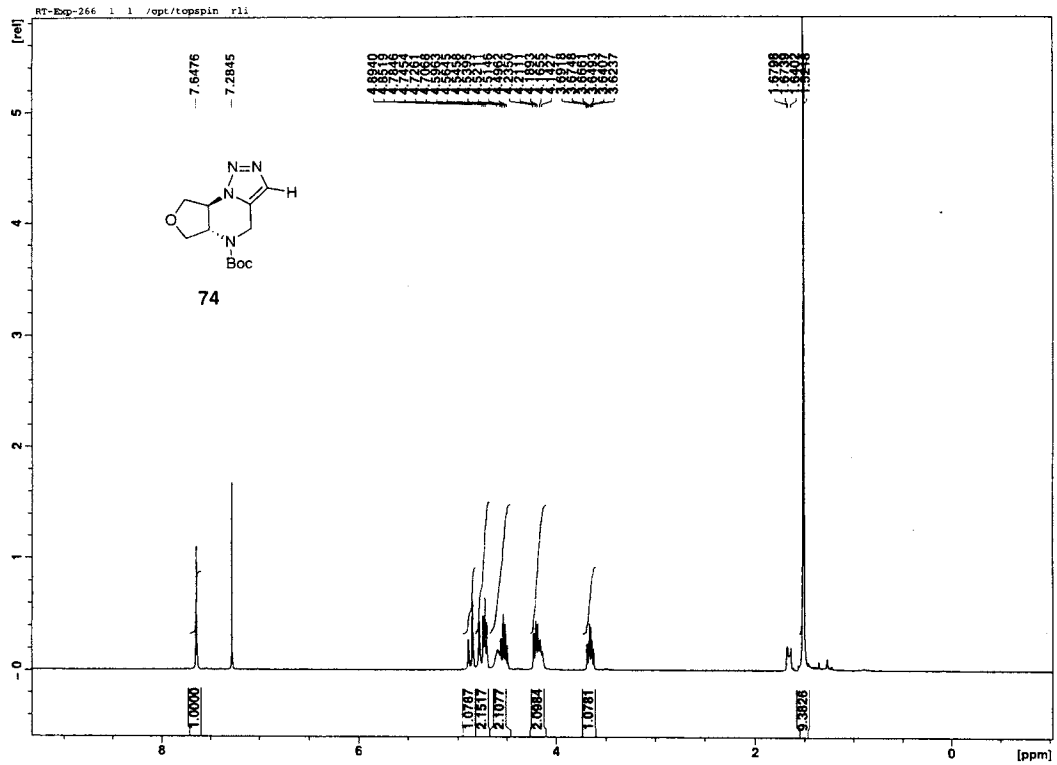
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

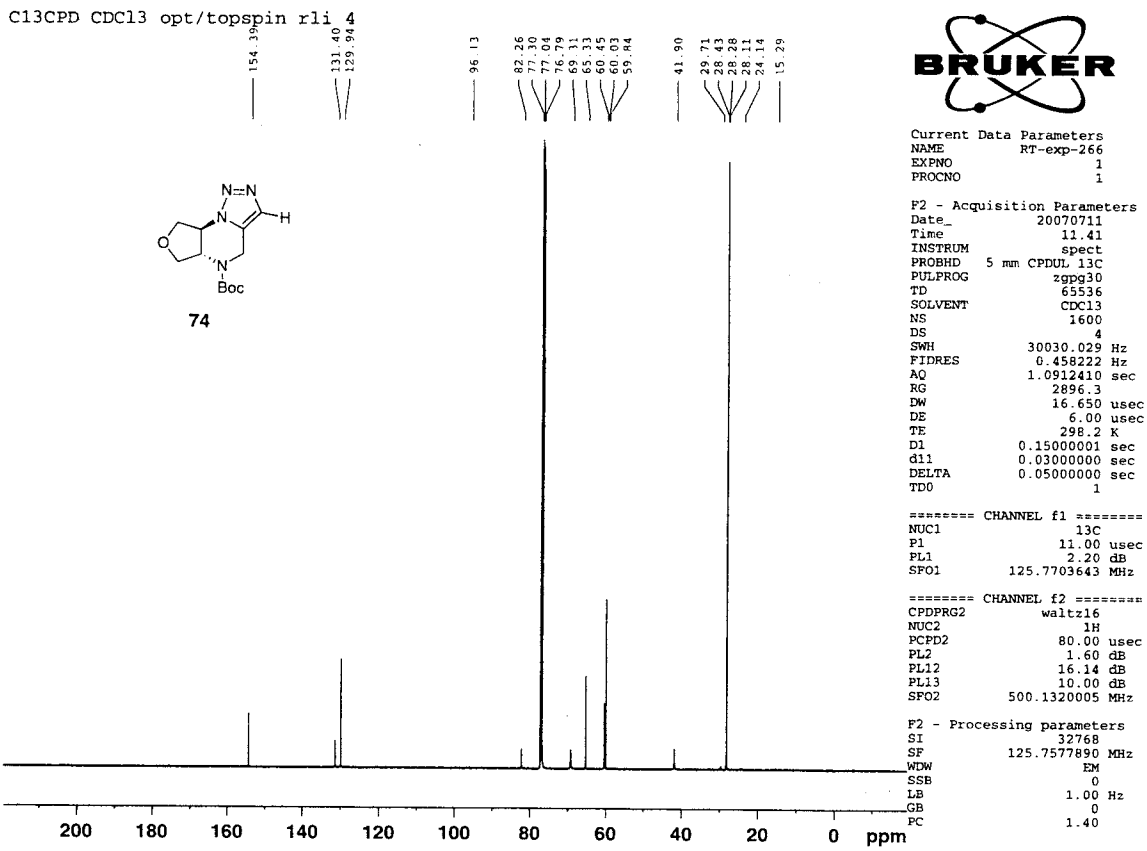




BRUKER

```
Current Data Parameters
NAME                  RT-exp-264
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20070709
Time                       12.15
INSTRUM                    spect
PROBHD     5 mm CPDUL 13C
PULPROG                 zgpg30
TD                         65536
SOLVENT                  CDCl3
NS                          1024
DS                             4
SWH                  30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                       9195.2
DW                        16.650 usec
DE                         6.00 usec
TE                        298.2 K
D1                    0.15000001 sec
d11                   0.03000000 sec
DELTA                 0.05000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                        11.00 usec
PL1                        2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.60 dB
PL12                      16.14 dB
PL13                      10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```





BRUKER

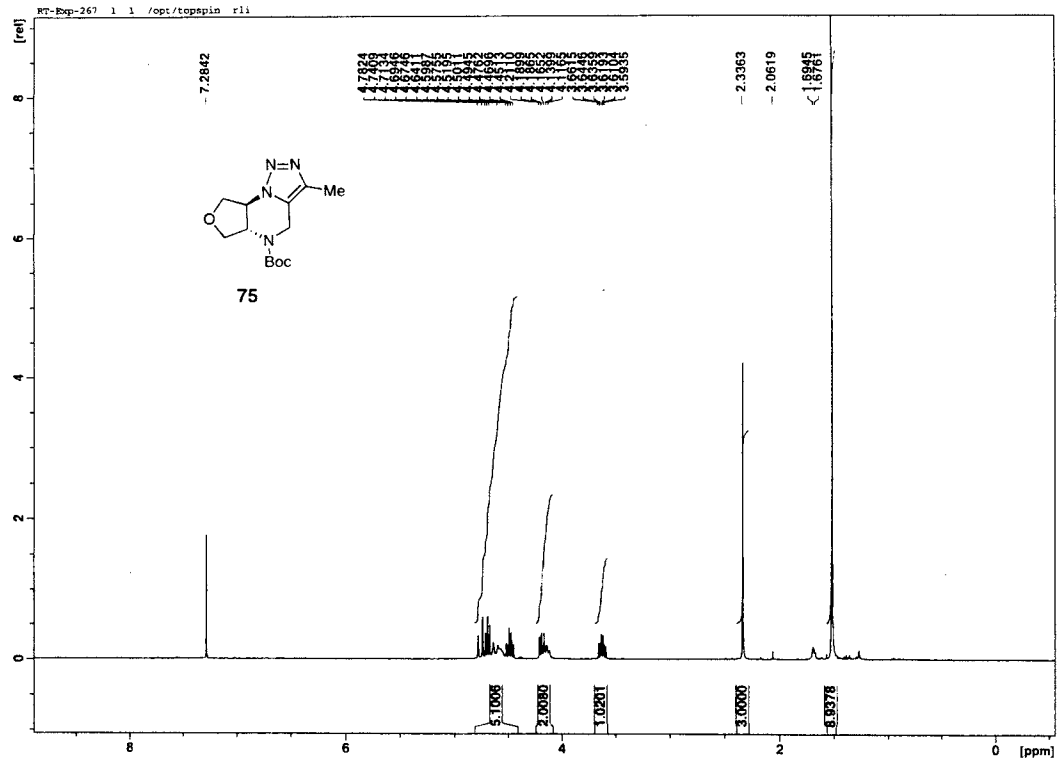
Current Data Parameters
NAME RT-exp-266
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070711
Time 11.41
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 2896.3
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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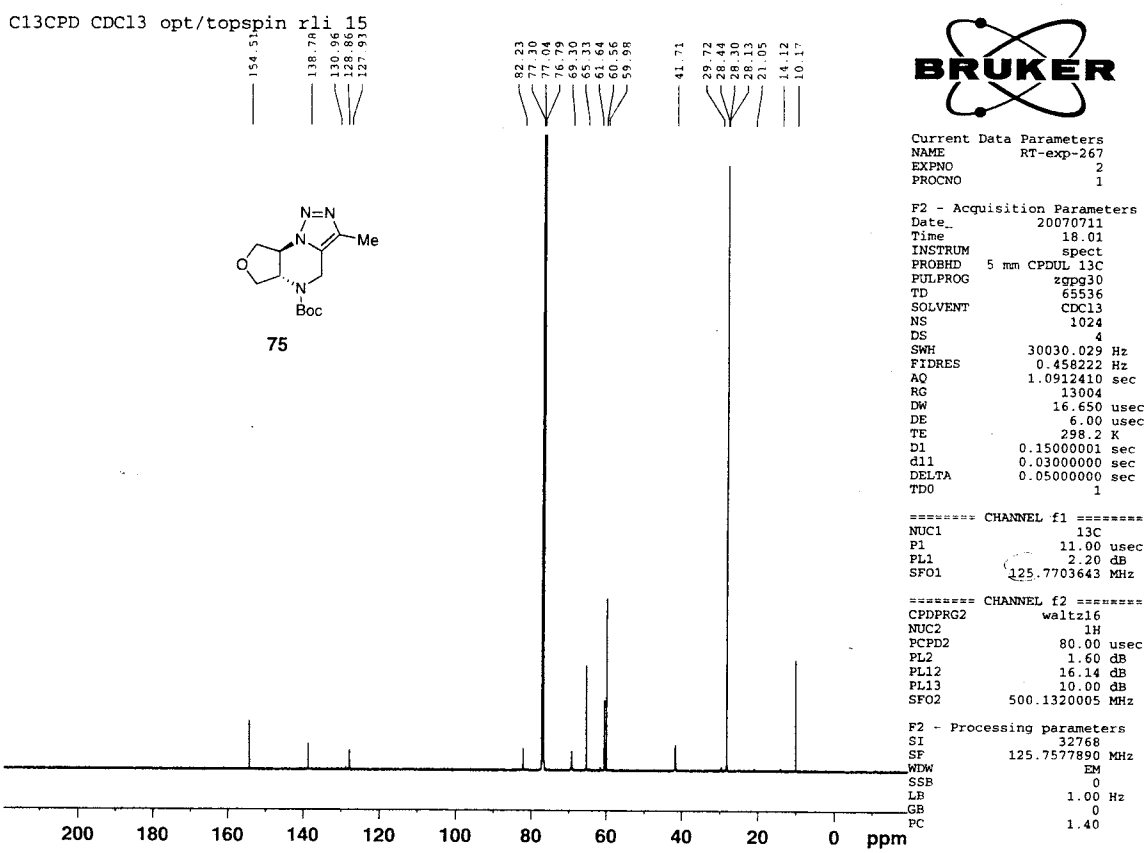

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BRUKER

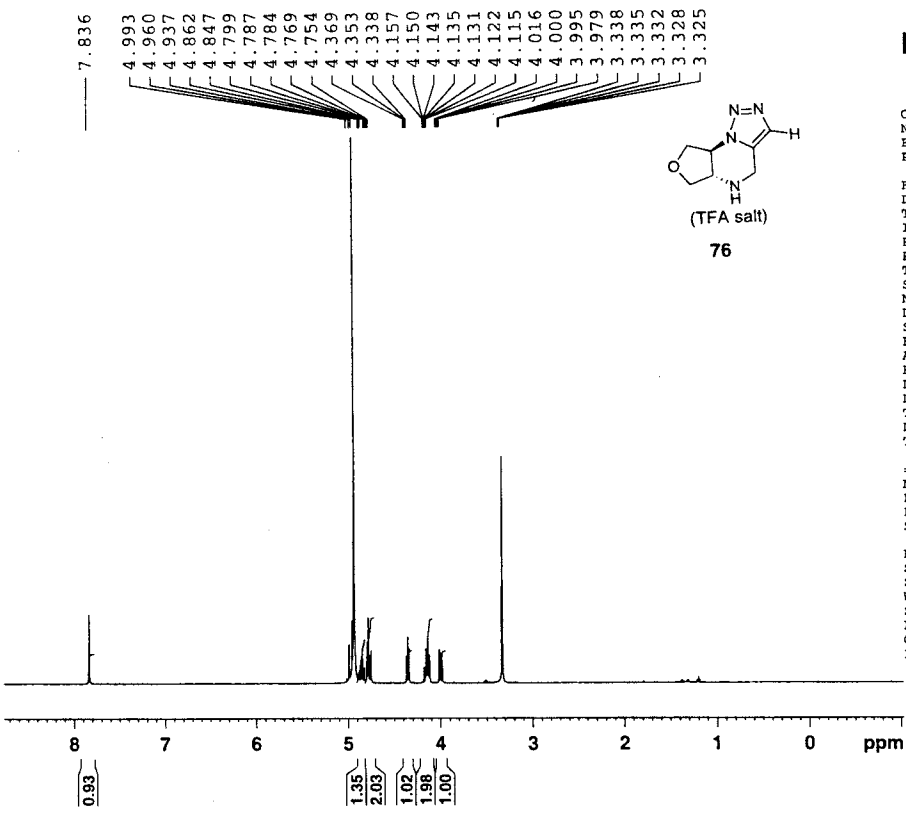
Current Data Parameters
NAME RT-exp-267
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070711
Time 18.01
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



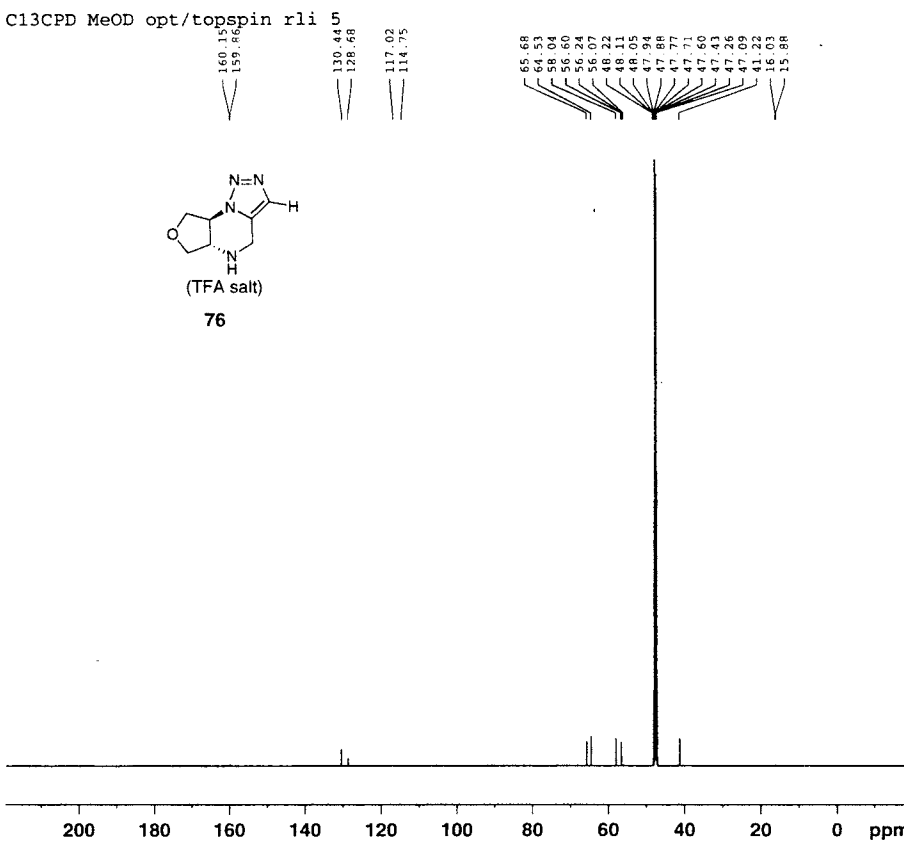
BRUKER

```
Current Data Parameters
NAME          RT-exp-278
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20070717
Time              15.44
INSTRUM           spect
PROBHD   5 mm CPDUL 13C
PULPROG            zg30
TD                65536
SOLVENT            MeOD
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1720407 sec
RG                  256
DW               48.400 usec
DE                6.00 usec
TE               298.2 K
D1            0.15000001 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                1.60 dB
SFO1         500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF          500.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



BRUKER

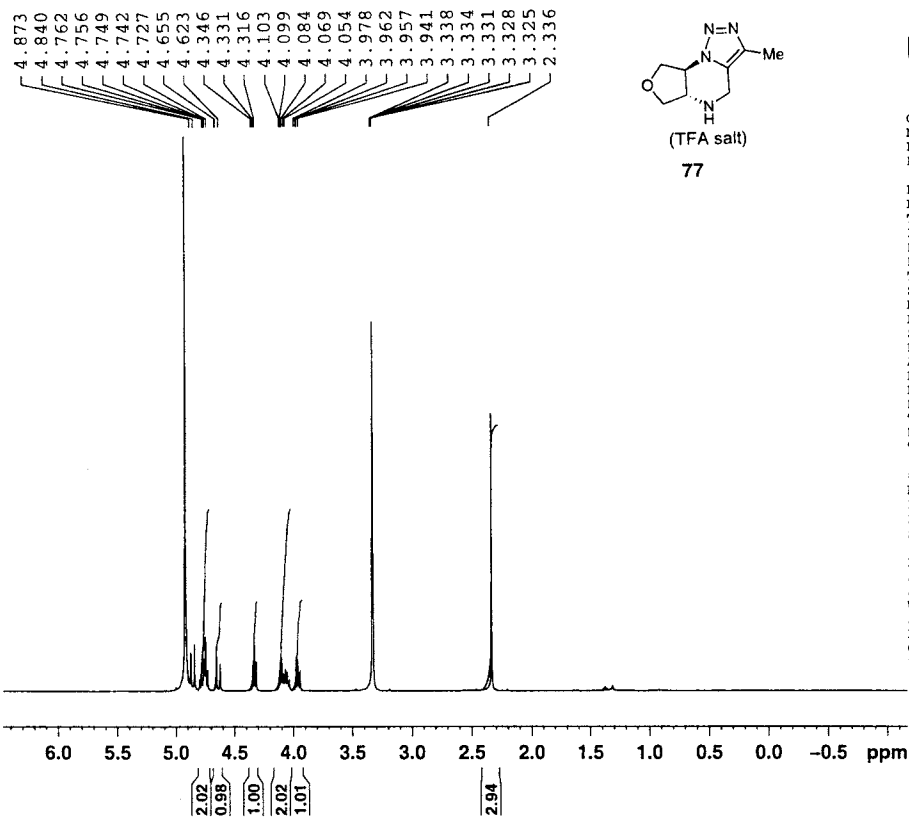
```
Current Data Parameters
NAME          RT-exp-278
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20070717
Time              16.07
INSTRUM           spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT            MeOD
NS                 1024
DS                    4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ            1.0912410 sec
RG              10321.3
DW               16.650 usec
DE                6.00 usec
TE               298.2 K
D1            0.15000001 sec
d11           0.03000000 sec
DELTA         0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1                2.20 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```



(TFA salt)

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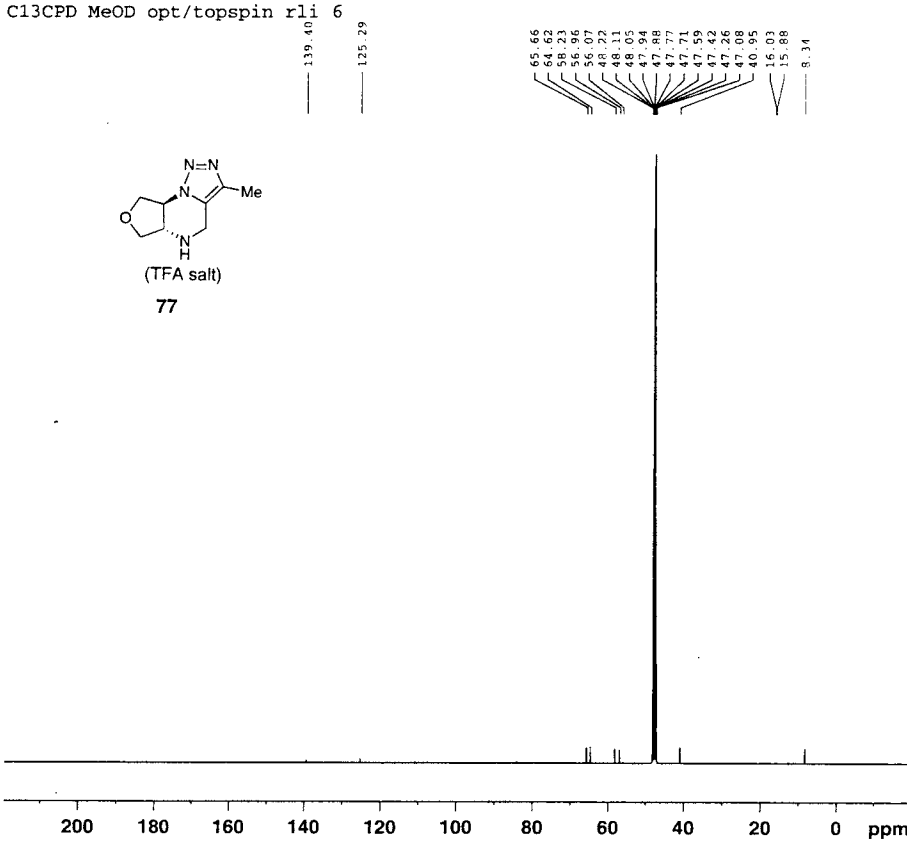
BRUKER

```
Current Data Parameters
NAME          RT-exp-279
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070717
Time               16.13
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1720407 sec
RG                   362
DW                48.400 usec
DE                 6.00 usec
TE                298.2 K
D1           0.15000001 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PL1                1.60 dB
SFO1        500.1330885 MHz

F2 - Processing parameters
SI                 32768
SF          500.1300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```



(TFA salt)

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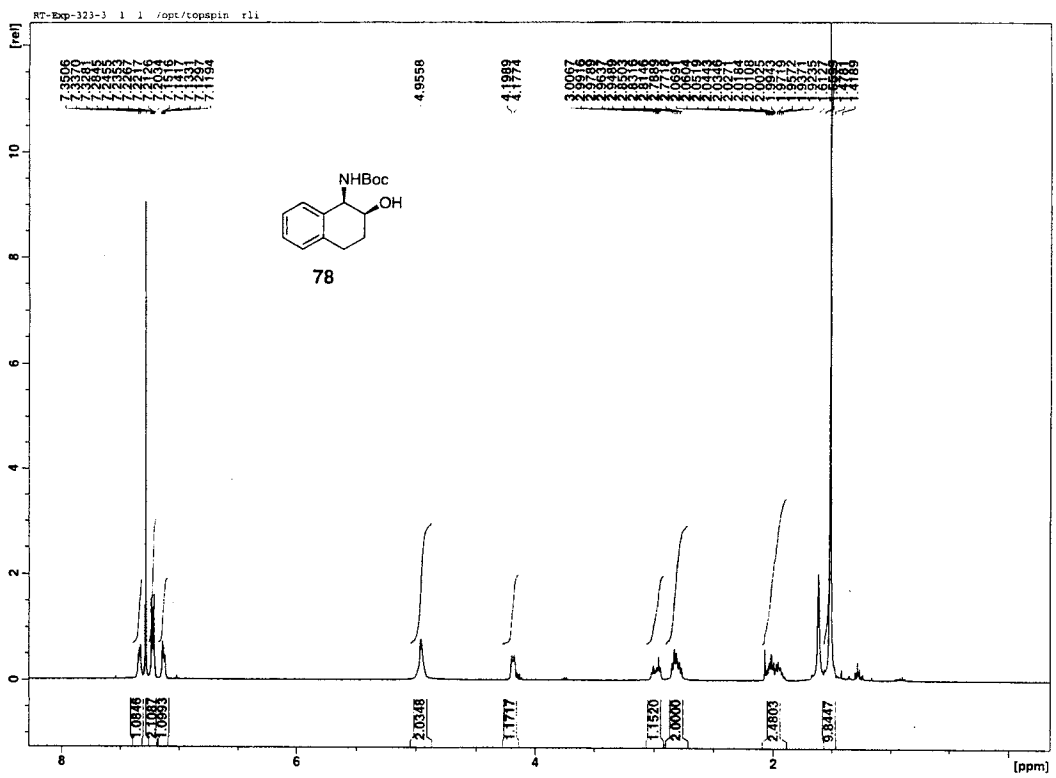
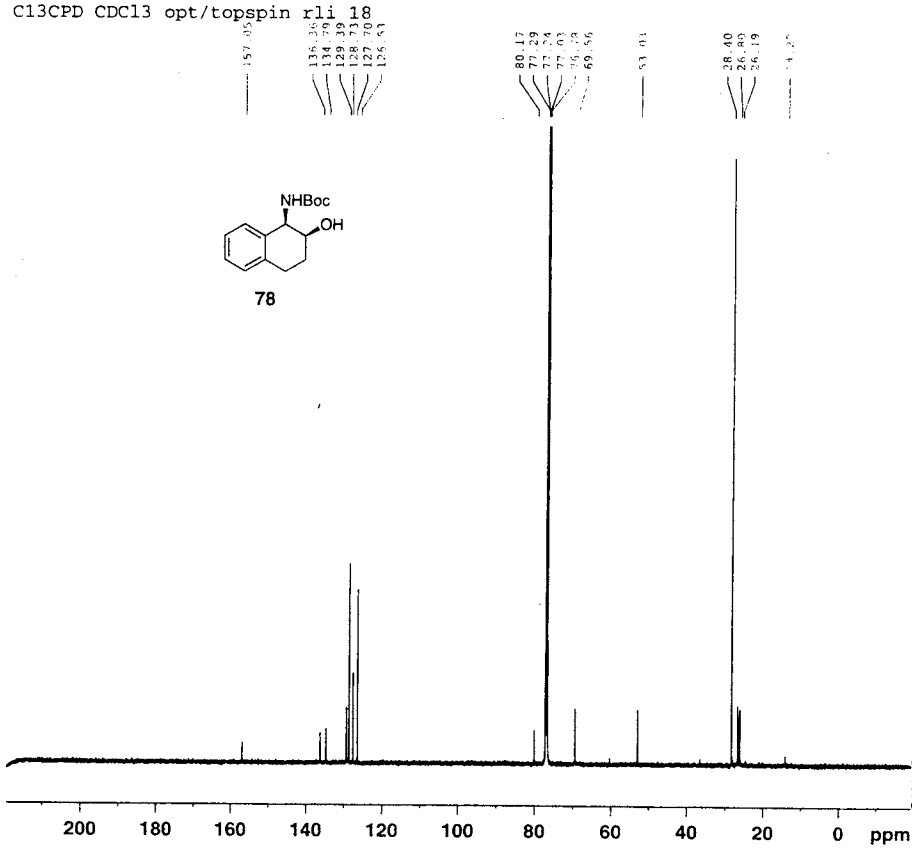
BRUKER

```
Current Data Parameters
NAME          RT-exp-279
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070717
Time               16.36
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT             MeOD
NS                  1024
DS                     4
SWH            30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912410 sec
RG                 13004
DW                16.650 usec
DE                 6.00 usec
TE                298.2 K
D1           0.15000001 sec
d11          0.03000000 sec
DELTA        0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1                2.20 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

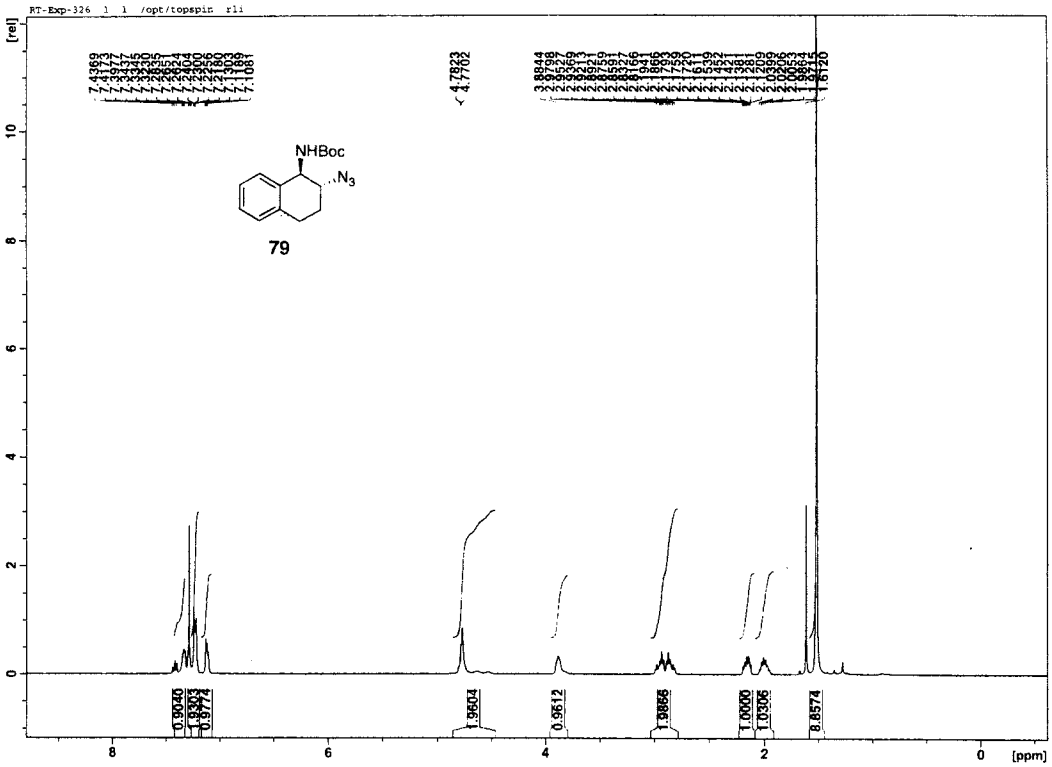


C13CPD CDCl3 opt/topspin rli 18

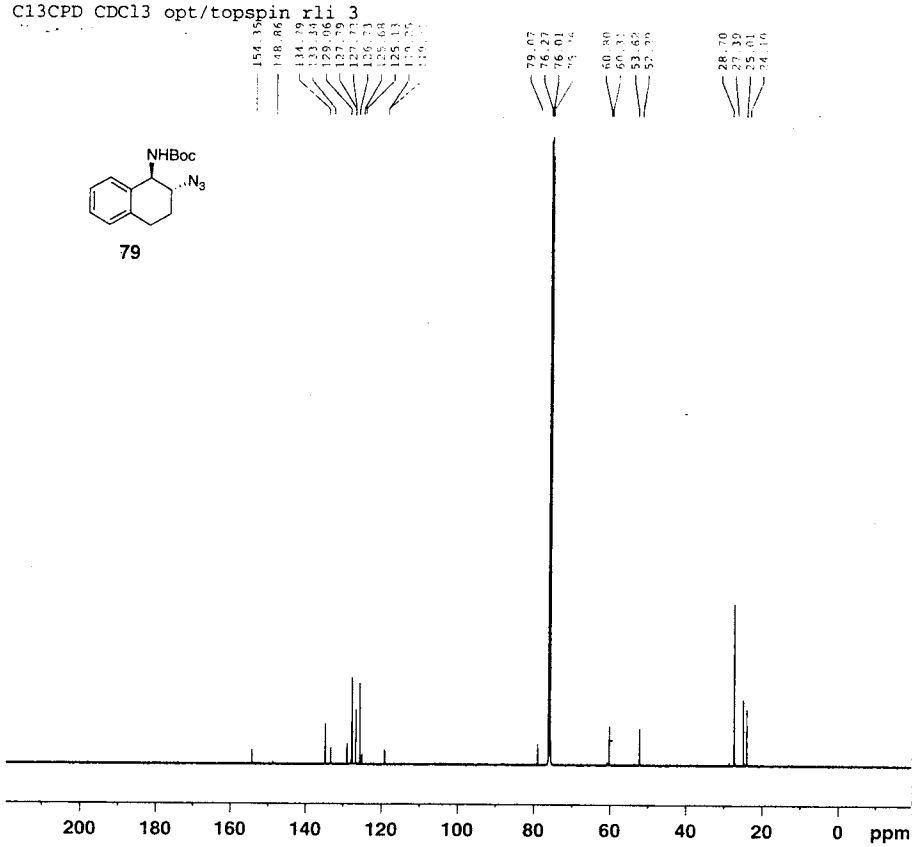


BRUKER

```
Current Data Parameters
NAME          RT-exp-323-3
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20070912
Time                   0.27
INSTRUM               spect
PROBHD    5 mm CPDUL 13C
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1280
DS                       4
SWH           30030.029 Hz
FIDRES         0.458222 Hz
AQ             1.0912410 sec
RG               14596.5
DW               16.650 usec
DE                6.00 usec
TE                298.2 K
D1            0.15000001 sec
d11           0.03000000 sec
DELTA         0.05000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                 11.00 usec
PL1                 2.20 dB
SFO1          125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 1.60 dB
PL12               16.14 dB
PL13               10.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF          125.7577890 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
```

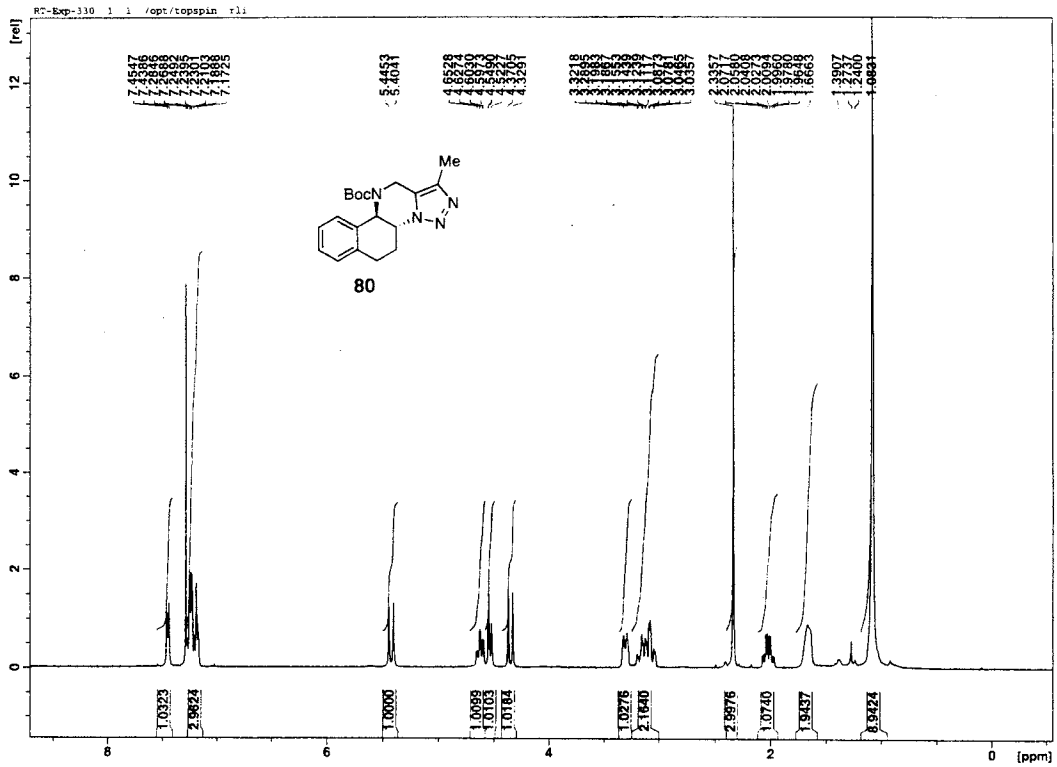


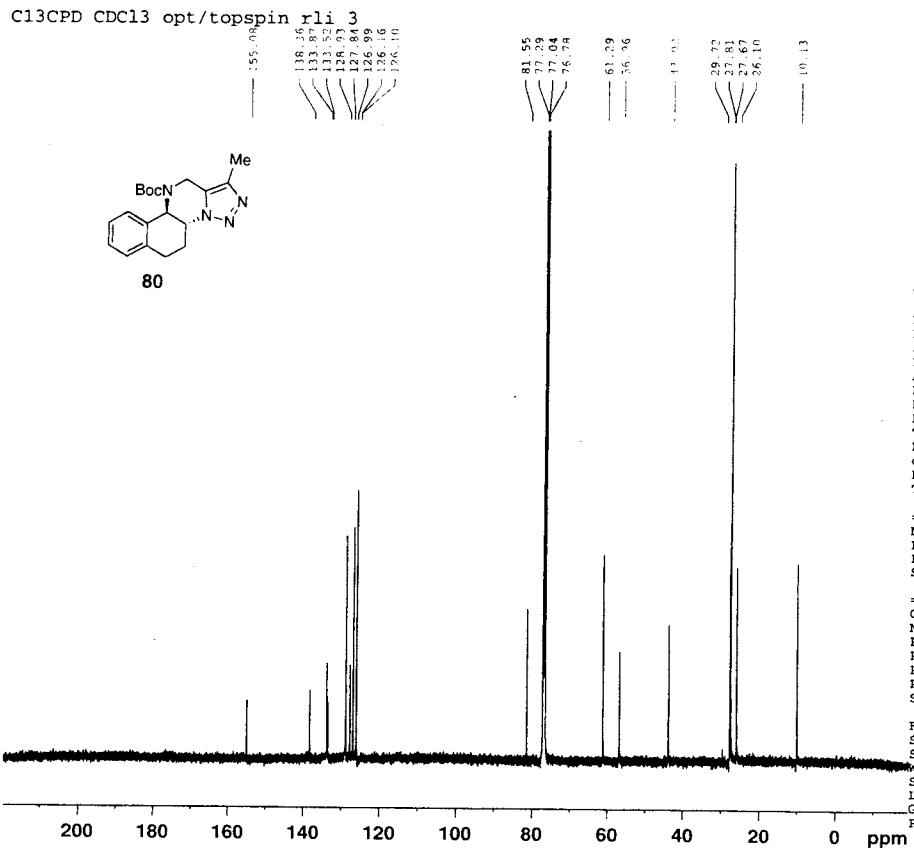
C13CPD CDCl3 opt/topspin rli 3



BRUKER

```
Current Data Parameters
NAME                  RT-exp-326
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20070912
Time                       15.44
INSTRUM                    spect
PROBHD     5 mm CPDUL 13C
PULPROG                 zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          1536
DS                             4
SWH                 30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                         13004
DW                        16.650 usec
DE                         6.00 usec
TE                        298.2 K
D1                    0.15000001 sec
d11                   0.03000000 sec
DELTA                 0.05000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                        11.00 usec
PL1                        2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.60 dB
PL12                      16.14 dB
PL13                      10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```





BRUKER

Current Data Parameters

NAME	RT-exp-330
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20070917
Time	10.46
INSTRUM	spect
PROBHD	5 mm CPDUL 13C
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	30030.029 Hz
FIDRES	0.458222 Hz
AQ	1.0912410 sec
RG	13004
DW	16.650 usec
DE	6.00 usec
TE	298.2 K
D1	0.15000001 sec
d11	0.03000000 sec
DELTA	0.05000000 sec
TD0	1

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

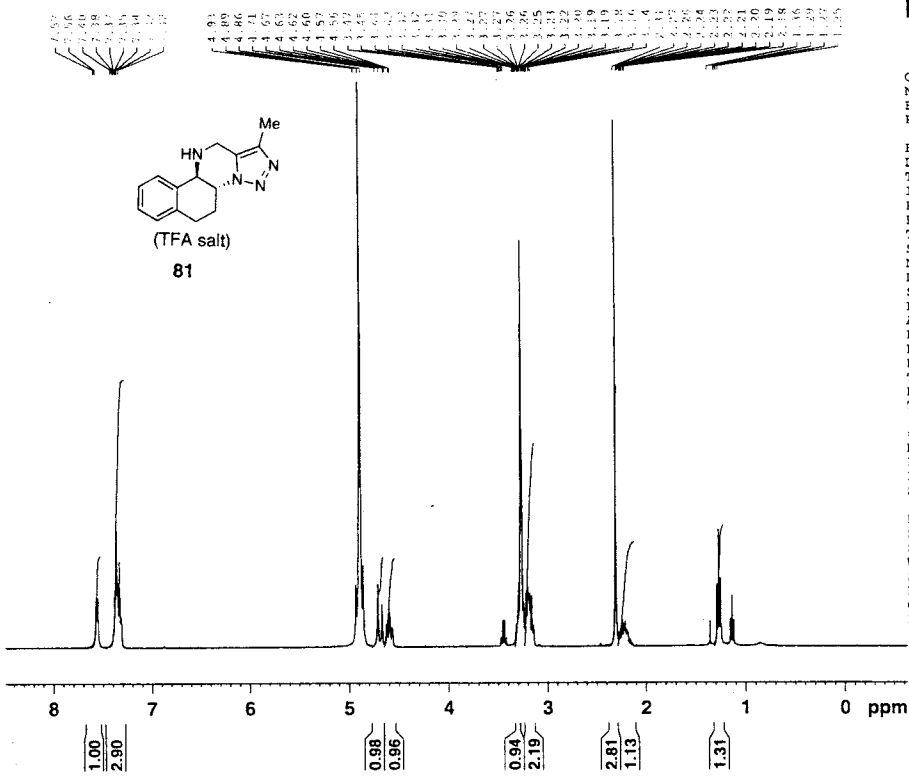
NUC1	13C
P1	11.00 usec
PL1	2.20 dB
SFO1	125.7703643 MHz

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.60 dB
PL12	16.14 dB
PL13	10.00 dB
SFO2	500.1320005 MHz

F2 - Processing parameters

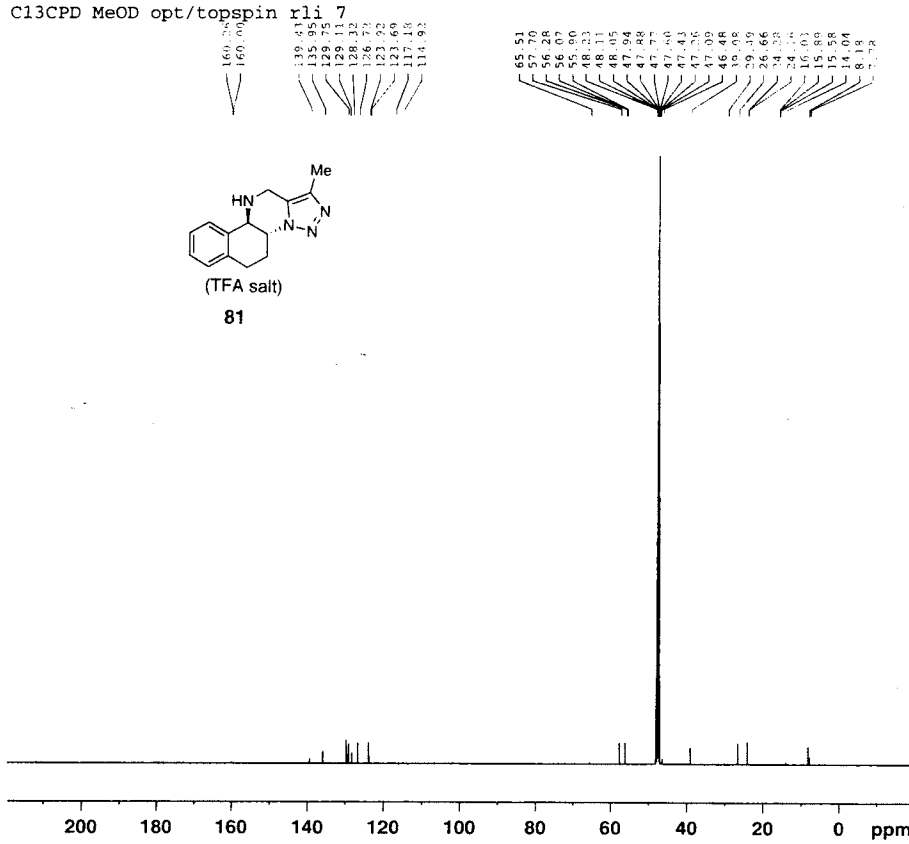
SI	32768
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

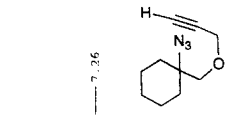
```
Current Data Parameters
NAME          RT-Exp-332a
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20070918
Time               16.35
INSTRUM           drx400
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT             MeOD
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ              3.9584243 sec
RG                   362
DW                60.400 usec
DE                 6.00 usec
TE                295.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.50 usec
PL1               -5.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1295170 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

C13CPD MeOD opt/topspin rli 7



BRUKER

```
Current Data Parameters
NAME          RT-exp-332
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20070919
Time               11.20
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG          zgpg30
TD                 65536
SOLVENT             MeOD
NS                  1500
DS                     4
SWH            30030.029 Hz
FIDRES          0.458222 Hz
AQ              1.0912410 sec
RG                 10321.3
DW                16.650 usec
DE                 6.00 usec
TE                298.2 K
D1           0.15000001 sec
d11          0.03000000 sec
DELTA        0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.00 usec
PL1                2.20 dB
SFO1        125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                1.60 dB
PL12              16.14 dB
PL13              10.00 dB
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



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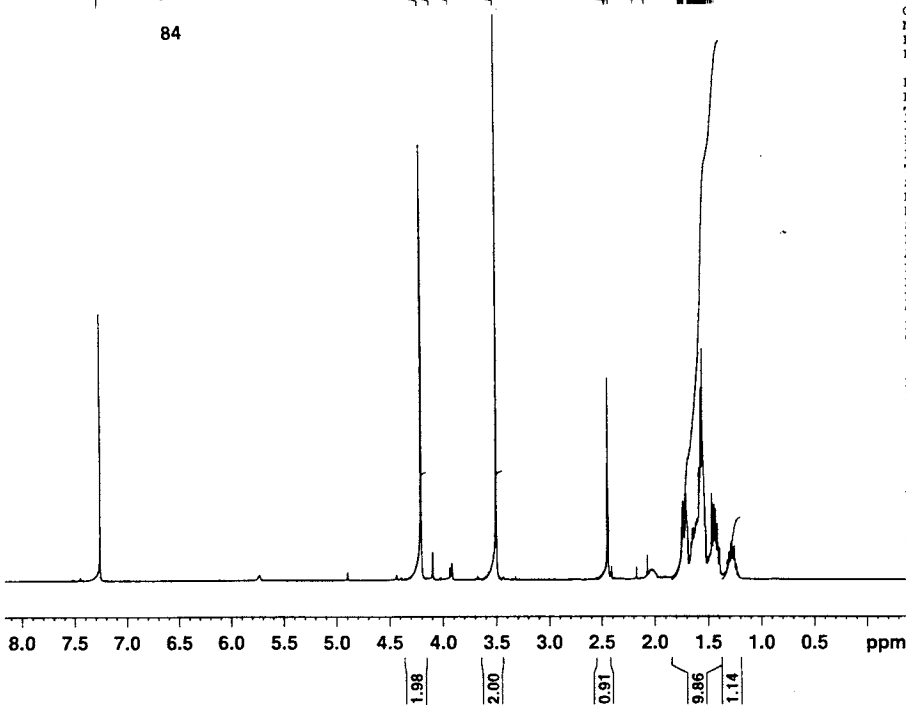
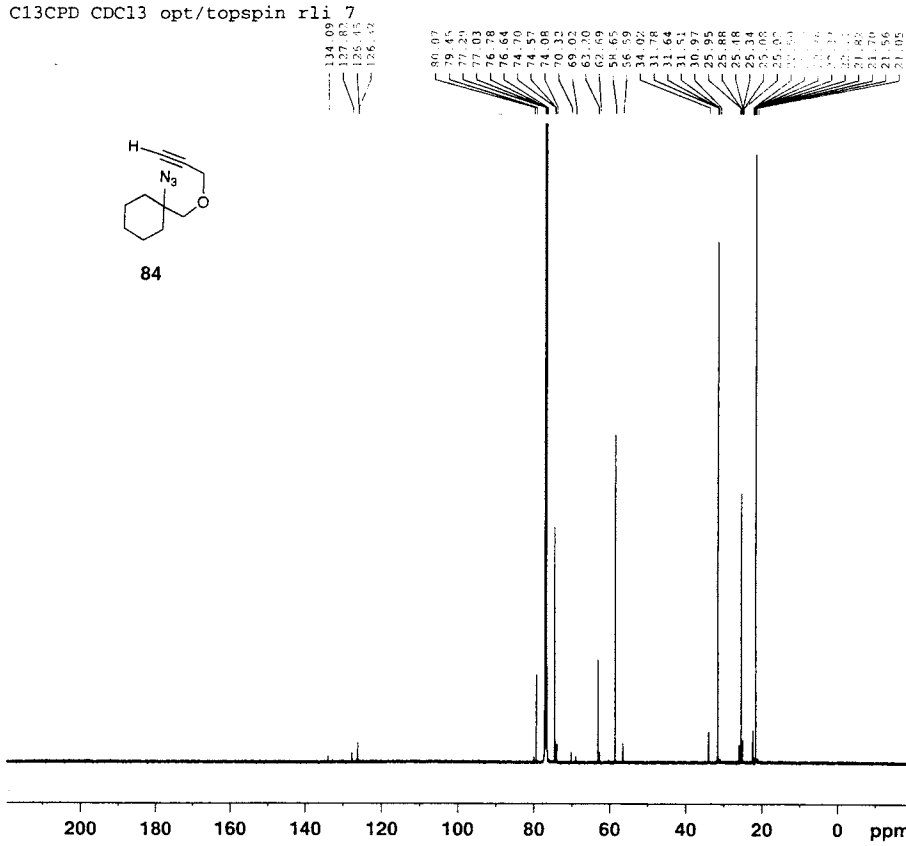


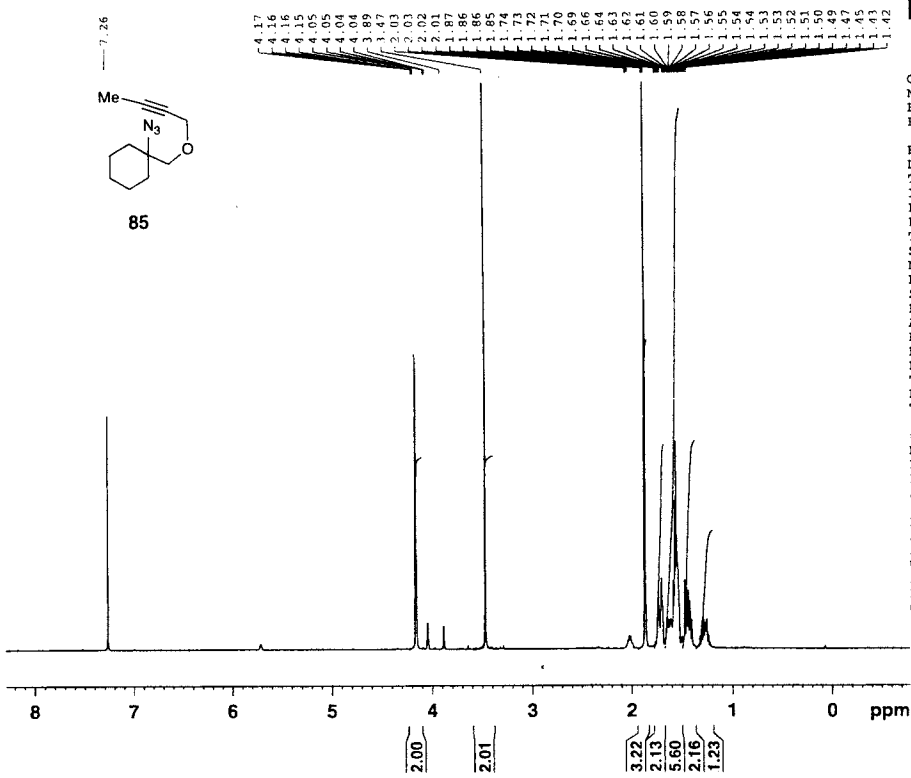

```
Current Data Parameters
NAME          RT-Exp-361
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20071204
Time               13.06
INSTRUM           drx400
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ            3.9584243 sec
RG                 362
DW             60.400 usec
DE              6.00 usec
TE              296.2 K
D1          1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1             10.50 usec
PL1             -5.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF         400.1300079 MHz
WDW                   EM
SSB                    0
LB              0.30 Hz
GB                     0
PC                  1.00
```

C13CPD CDCl3 opt/topspin rli 7

84




```
Current Data Parameters
NAME          RT-exp-361
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20071204
Time               16.08
INSTRUM            spect
PROBHD   5 mm CPDUL 13C
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH          30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG                14596.5
DW             16.650 usec
DE              6.00 usec
TE              300.0 K
D1          0.15000001 sec
d11         0.03000000 sec
DELTA       0.05000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1             11.00 usec
PL1             2.20 dB
SFO1       125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2          80.00 usec
PL2             1.60 dB
PL12           16.14 dB
PL13           10.00 dB
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF         125.7577890 MHz
WDW                   EM
SSB                    0
LB              1.00 Hz
GB                     0
PC                  1.40
```



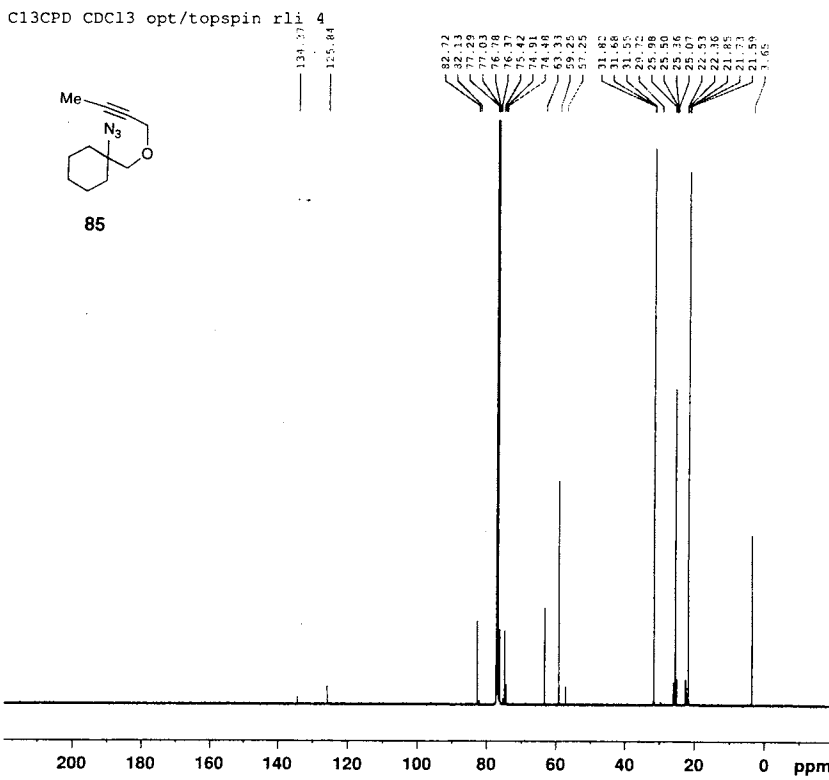
BRUKER

Current Data Parameters
NAME RT-Exp-363
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071206
Time 9.37
INSTRUM drx400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -5.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

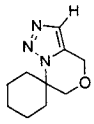
Current Data Parameters
NAME RT-exp-363
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071206
Time 12.11
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 13004
DW 16.650 usec
DE 6.00 usec
TE 300.0 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

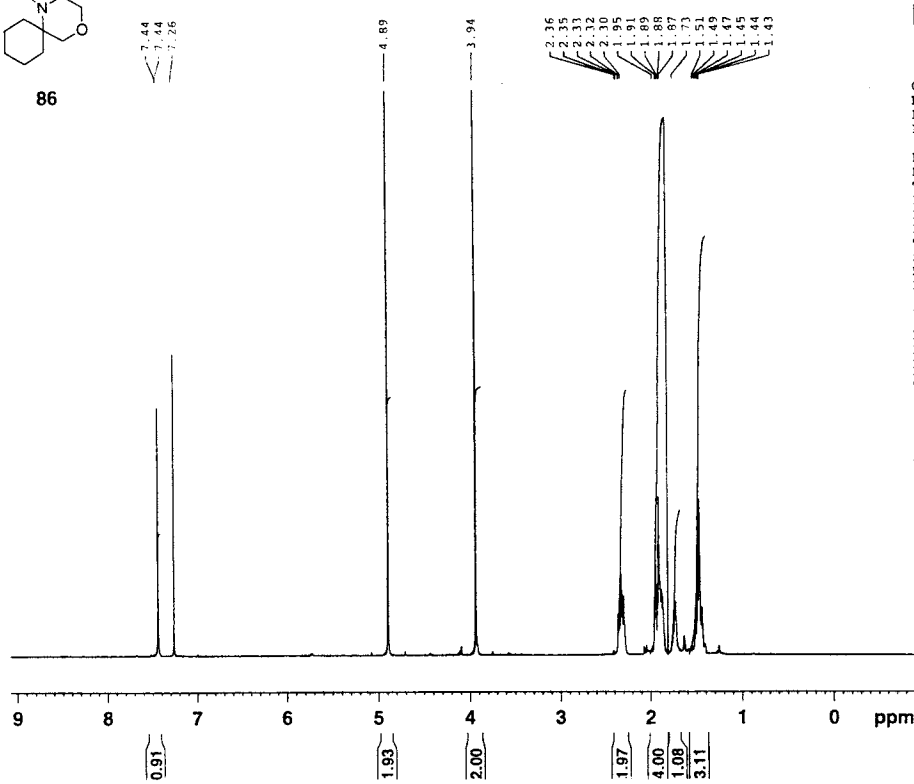
======== CHANNEL f1 ========
NUC1 13C
P1 11.00 usec
PL1 2.20 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.60 dB
PL12 16.14 dB
PL13 10.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



86

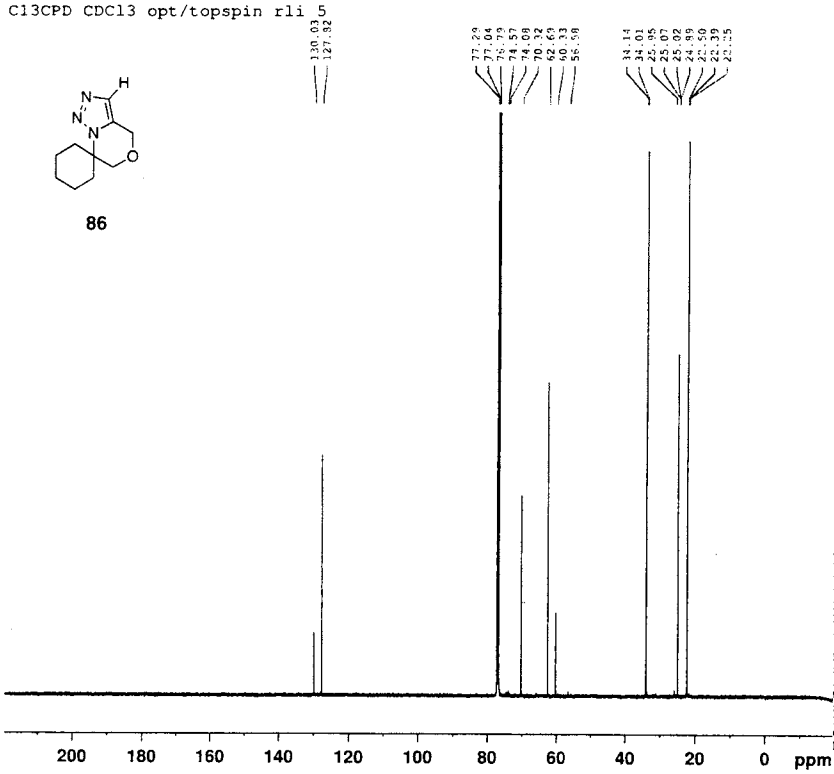


BRUKER

```
Current Data Parameters
NAME                  RT-Exp-364
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20071205
Time                      13.31
INSTRUM                  drx400
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   8278.146 Hz
FIDRES                0.126314 Hz
AQ                    3.9584243 sec
RG                         362
DW                      60.400 usec
DE                       6.00 usec
TE                      298.2 K
D1                 1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.50 usec
PL1                      -5.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300079 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```

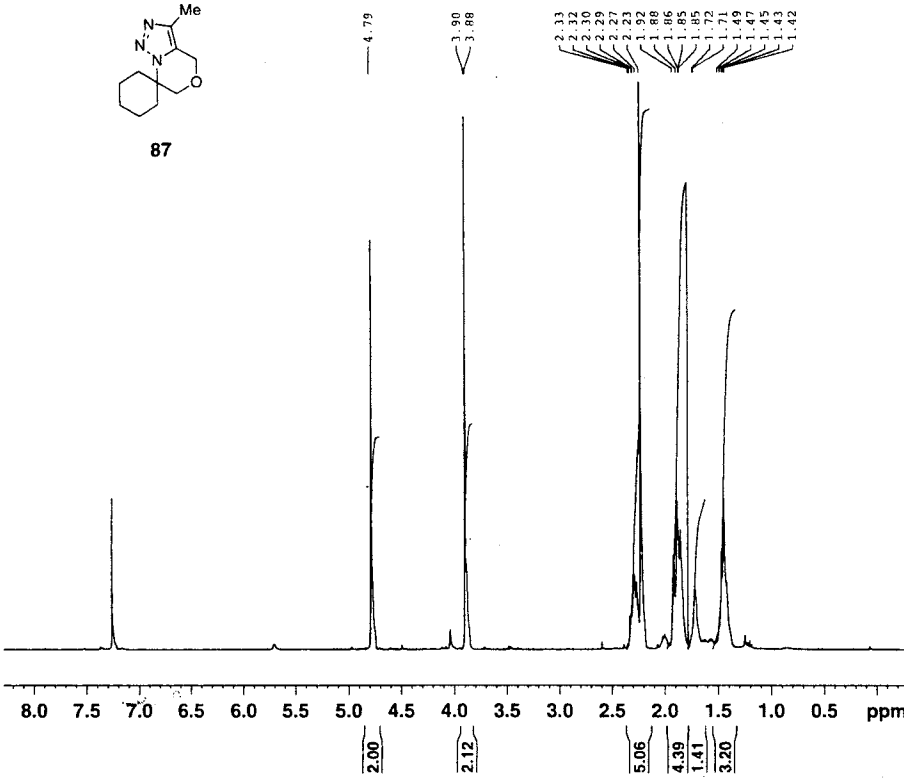
C13CPD CDCl3 opt/topspin rli 5

86



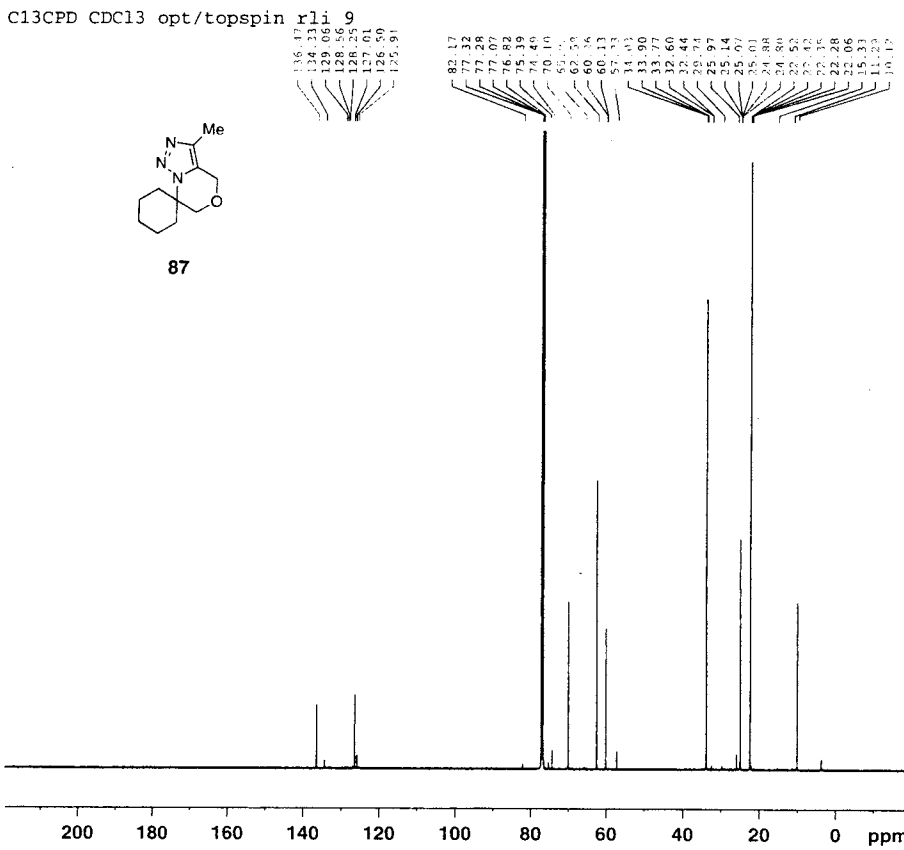
BRUKER

```
Current Data Parameters
NAME                  RT-exp-364
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20071206
Time                      12.28
INSTRUM                   spect
PROBHD    5 mm CPDUL 13C
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         504
DS                           4
SWH                  30030.029 Hz
FIDRES                0.458222 Hz
AQ                    1.0912410 sec
RG                        16384
DW                      16.650 usec
DE                       6.00 usec
TE                      300.0 K
D1                 0.15000001 sec
d11                0.03000000 sec
DELTA              0.05000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                       13C
P1                       11.00 usec
PL1                       2.20 dB
SFO1               125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      1.60 dB
PL12                    16.14 dB
PL13                    10.00 dB
SFO2               500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                 125.7577890 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```



BRUKER

```
Current Data Parameters
NAME                  RT-Exp-367
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20071207
Time                      13.24
INSTRUM                  drx400
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            2
SWH                    8278.146 Hz
FIDRES                 0.126314 Hz
AQ                     3.9584243 sec
RG                          362
DW                       60.400 usec
DE                        6.00 usec
TE                       296.2 K
D1                  1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         1H
P1                       10.50 usec
PL1                      -5.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300079 MHz
WDW                           EM
SSB                            0
LB                        0.30 Hz
GB                             0
PC                          1.00
```



BRUKER

```
Current Data Parameters
NAME                  RT-exp-367
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20071207
Time                      20.49
INSTRUM                   spect
PROBHD    5 mm CPDUL 13C
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                         1536
DS                            4
SWH                   30030.029 Hz
FIDRES                 0.458222 Hz
AQ                     1.0912410 sec
RG                       11585.2
DW                       16.650 usec
DE                        6.00 usec
TE                       300.0 K
D1                  0.15000001 sec
d11                 0.03000000 sec
DELTA               0.05000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                        13C
P1                       11.00 usec
PL1                       2.20 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                         1H
PCPD2                    80.00 usec
PL2                       1.60 dB
PL12                     16.14 dB
PL13                     10.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                          1.40
```