Supporting Information

Ag-Containing All Carbon 1,3-Dipoles: Generation and Formal Cycloaddition for Furo[3,2-*b*]-β/γ-lactams

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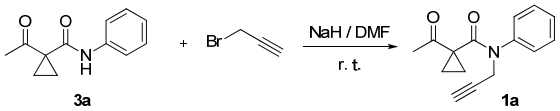
I. General Remarks:

All reagents were purchased from commercial sources and used without further treatment, unless otherwise indicated. ^{1}H NMR and ^{13}C NMR spectra were recorded at 25ºC on a 500 MHz and 125 MHz or 400 MHz and 100 MHz, respectively, and TMS as internal standard. IR spectra (KBr) were recorded on in the range of 400~4000 cm^{-1}. Melting points are uncorrected. All reactions were monitored by TLC with GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

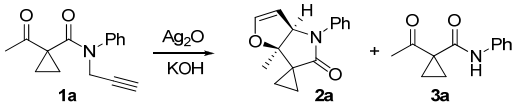
II. Typical Procedure:

(I) For 1 (1a as an example):



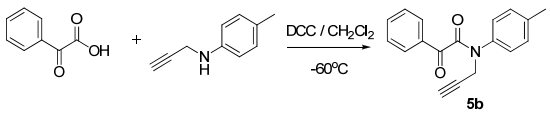
To the well stirred solution of anhydrous DMF (25 mL), cooling by ice-water, added 1-acetyl-*N*-phenylcyclopropanecarboxamide[1] (2.03 g, 0.01 mol), NaH[2] (70%) (0.41 g, 0.012 mol) and 3-bromoprop-1-yne (0.95 mL, 0.011 mol) The reaction mixture was stirred at room temperature for 24 h (monitored by TLC) before it was slowly poured into water (80 mL). Extracted with CH_2Cl_2 (8 mL×5), then the organic phase washed with water (20 mL×3), the solvent was removed under reduced pressure, and the residue was purified by a short flash silica gel column chromatography (eluent: diethyl ether/petroleum ether = 1/9), then the crude compound was recrystallized (diethyl ether/petroleum ether = 1/9) to gain **1a** (1.78g, 74%) as yellow crystal.

(II) For 2 (2a as an example):



The mixture of 1-acetyl-*N*-phenyl-*N*-(prop-2-ynyl)cyclopropanecarboxamide **1a** (0.24 g, 1.0 mmol), Ag_2O (0.116 g, 0.5 mmol) and KOH (0.112 g, 1.0 mmol) was well stirred for 24 h at room temperature in CH_3CN (4 mL), then to the mixture was added water (10 mL) and NH_4Cl (0.1g, 2.0 mmol), extracted with CH_2Cl_2 (6 mL×4). The solvent was removed under reduced pressure, and the residue was purified by a short flash silica gel column chromatography to give compound **2a** (0.18 g, 75%) as a yellow solid (eluent: diethyl ether/petroleum ether = 1/14) and **3a** (0.026 mg, 13%) (eluent: diethyl ether/petroleum ether = 1/9).

(III) For 5 (5b as an example):



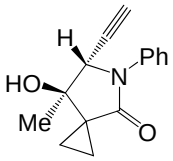
N,*N*'-methanediylidenedicyclohexanamine (DCC) (2.47 g, 0.012 mol) was added after the solution of 2-oxo-2-phenylacetic acid (1.50 g, 0.01 mol), 4-methyl-*N*-(prop-2-ynyl)aniline (1.45 g, 0.01 mol) in CH_2Cl_2 (30 mL) was stirred for 10 min at -60 ^{o}C. The mixture was stirred for further 4.0 h (monitored by TLC) before it was filtrated. The solvent was removed under reduced pressure, and the residue was purified by a short flash silica gel column chromatography to give compound **5b** (2.19 g, 79 %) as colorless oil (eluent: diethyl ether/petroleum ether = 1/5)

Reference:

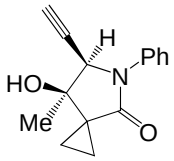
[1] The NMR data of **3**, please see *Angew. Chem. Int. Ed.* **2007**, *46*, 1726.

[2] Although there is no adverse reaction found in our experiment, the caution was also mentioned: the thermal runaway reaction involving sodium and DMF: G. DeWall, *Chem. Eng. News* **1982**, *60* (37), p.5 and p.43.

III. Analytical data of compounds **2**, **4** and **6**:



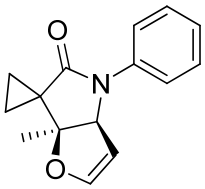
trans-**4a**



cis-**4a**

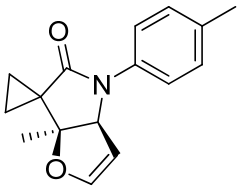
6-ethynyl-7-hydroxy-7-methyl-5-phenyl-5-azaspiro[2.4]heptan-4-one (*trans*-4a)

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.91-0.97 (m, 1H), 1.02-1.07 (m, 1H), 1.21-1.22 (m, 2H), 1.33 (s, 3H), 2.47 (s, 1H), 2.51 (s, 1H), 4.76 (s, 1H), 7.16-7.19 (m, 1H), 7.33-7.40 (m, 2H), 7.64-7.66 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 7.80, 14.10, 20.85, 33.99, 62.48, 74.96, 76.13, 79.16, 121.62, 125.21, 128.83, 133.20, 173.79.



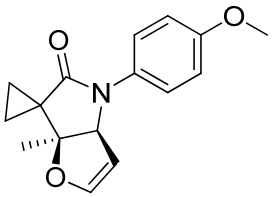
***cis*-6a'-methyl-4'-phenyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2a)**

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.10-1.13 (m, 1H), 1.17-1.25 (m, 2H), 1.33-1.38 (m, 4H), 4.98 (s, 1H), 5.19 (t, J = 2.5 Hz, 1H), 6.46 (d, J = 2.5 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 7.34-7.38 (m, 2H), 7.59-7.60 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 12.01, 13.43, 22.01, 32.19, 70.24, 86.70, 98.37, 120.91, 124.75, 128.94, 138.04, 150.03, 173.75; MS: calcd *m/z* 241.1, found 242.1 $[(M+1)]^+$; IR (KBr, neat): ν 3381, 3007, 2969, 2926, 1696, 1604, 1496, 1384, 1318, 1179, 1100, 1059, 974, 815cm^{-1}; Anal. Calcd for $C_{15}H_{15}NO_2$: C, 74.67; H, 6.27; N, 5.81. Found: C, 74.50; H, 6.14; N, 5.98.



***cis*-6a'-methyl-4'-*p*-tolyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2b)**

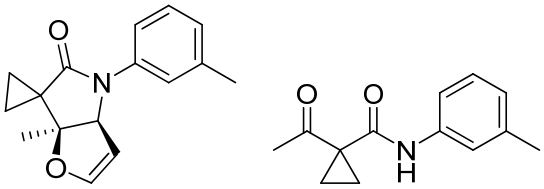
White solid; mp: 73-74°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.10-1.38 (m, 7H), 2.33 (s, 3H), 4.96 (d, J = 2.5 Hz, 1H), 5.18 (t, J = 2.5 Hz, 1H), 6.47 (d, J = 2.5 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.88, 13.28, 20.89, 22.04, 32.16, 70.43, 86.80, 99.51, 121.22, 129.53, 134.58, 135.54, 149.97, 173.58; IR (KBr, neat): ν 3098, 2972, 2924, 1694, 1612, 1514, 1384, 1317, 1094, 1056, 976, 815 cm^{-1}; Anal. Calcd for $C_{16}H_{17}NO_2$: C, 75.27; H, 6.71; N, 5.49. Found: C, 75.20; H, 6.90; N, 5.38.



***cis*-4'-(4-methoxyphenyl)-6a'-methyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2c)**

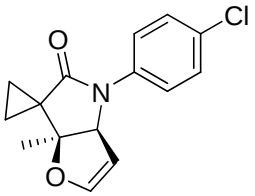
White crystal; mp: 111-114°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.09-1.12 (m, 1H), 1.15-1.23 (m, 2H), 1.31-1.34 (m, 4H), 3.80 (s, 3H), 4.90 (s, 1H), 5.14 (t, J = 2.5 Hz, 1H), 6.46 (d, J = 2.5 Hz, 1H), 6.90 (d, J = 9.0 Hz, 2H), 7.45 (d, J = 9.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.61, 13.00, 21.87, 31.88, 55.31, 70.69, 86.80, 99.42, 114.10, 123.24, 131.06, 149.83, 156.84, 173.35; IR (KBr, neat): ν 2965, 2931, 2840, 1689, 1606, 1515, 1446, 1380, 1253,

1170, 1135, 1028, 969, 830 cm^{-1}; Anal. Calcd for $C_{16}H_{17}NO_3$: C, 70.83; H, 6.32; N, 5.16. Found: C, 70.80; H, 6.43; N, 5.26.



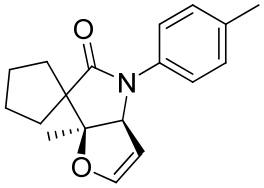
Mixture of ***cis*-6a'-methyl-4'-*m*-tolyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2d)** and **1-acetyl-*N*-*m*-tolylcyclopropanecarboxamide (3d)** (^{1}H NMR, ^{13}C NMR, Anal. Calcd. and IR database see SI of *Angew. Chem. Int. Ed.* **2007**, *46*, 1726.)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.12-1.26 (m, 3H), 1.33 (m, 4H), 2.19 (s, 3H), 4.71(s, 1H), 4.96 (s, 1H), 6.49 (s, 1H), 7.07-7.23 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.26, 12.68, 17.94, 21.94, 31.38, 72.03, 87.88, 99.81, 126.51, 126.65, 127.98, 131.05, 136.12, 149.76, 173.54.



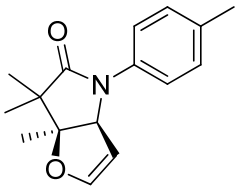
***cis*-4'-(4-chlorophenyl)-6a'-methyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2e)**

White crystal; mp: 89-91°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.13-1.15 (m, 1H), 1.19-1.24 (m, 2H), 1.33-1.35 (m, 4H), 4.95 (s, 1H), 5.17 (s, 1H), 6.47 (s, 1H), 7.32 (d, J = 9.0 Hz, 2H), 7.57 (d, J = 9.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 12.02, 13.43, 21.84, 32.02, 70.07, 86.53, 98.83, 121.78, 128.80, 129.64, 136.56, 150.16, 173.66; IR (KBr, neat): ν 3209, 2982, 2928, 1688, 1606, 1495, 1377, 1343, 1173, 1087, 1054, 972, 810 cm^{-1}; Anal. Calcd for $C_{15}H_{14}ClNO_2$: C, 65.34; H, 5.12; N, 5.08. Found: C, 65.47; H, 5.05; N, 5.00.



***cis*-6a'-methyl-4'-*p*-tolyl-3a',4'-dihydrospiro[cyclopentane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2f)**

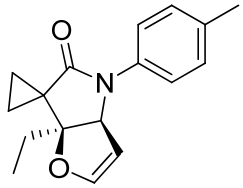
White solid; mp: 86-88°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.42 (s, 3H), 1.65-1.69 (m, 1H), 1.76-1.81 (m, 2H), 1.84-1.96 (m, 3H), 1.98-2.04 (m, 1H), 2.09-2.13 (m, 1H), 4.68 (d, J = 2.5 Hz, 1H), 5.13 (t, J = 2.5 Hz, 1H), 6.43 (d, J = 2.5 Hz, 1H), 7.16 (d, J = 8.5 Hz, 2H), 7.42 (d, J = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 18.64, 20.88, 25.95, 26.21, 30.79, 36.34, 57.93, 68.34, 91.17, 100.45, 109.73, 121.62, 129.40, 134.60, 135.38, 150.24, 177.37; MS: calcd *m/z* 283.1, found 284.1 $[(M+1)]^+$; IR (KBr, neat): ν 2956, 2925, 2868, 1898, 1688, 1608, 1514, 1384, 1367, 1294, 1266, 1138, 1057, 903, 838 cm^{-1}; Anal. Calcd for $C_{18}H_{21}NO_2$: C, 76.29; H, 7.47; N, 4.94. Found: C, 76.22; H,7.33; N, 4.88.



***cis*-6,6,6a-trimethyl-4-*p*-tolyl-6,6a-dihydro-3a*H*-furo[3,2-*b*]pyrrol-5(4*H*)-one (2g)**

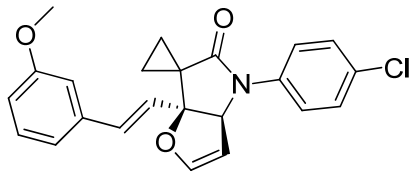
Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.22 (s, 3H), 1.32 (s, 3H), 1.38 (s, 3H), 2.32 (s, 3H), 4.71 (d, J = 2.5 Hz,

1H), 5.13 (t, *J* = 2.5 Hz, 1H), 6.44 (d, *J* = 2.5 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 17.93, 18.60, 20.86, 24.60, 47.49, 67.72, 91.21, 99.93, 121.80, 129.40, 134.76, 135.20, 150.37, 176.74; MS: calcd *m/z* 257.1, found 258.1 $[(M+1)]^+$; IR (KBr, neat): ν 2995, 2977, 2934, 1677, 1606, 1520, 1399, 1313, 1177, 1133, 1071, 897, 802 cm^{-1}; Anal. Calcd for $C_{16}H_{19}NO_2$: C, 74.68; H, 7.44; N, 5.44. Found: C, 74.40; H, 7.45; N, 5.53.



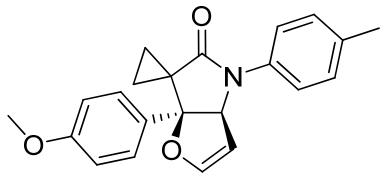
***cis*-6a'-ethyl-4'-*p*-tolyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2h)**

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.97 (t, *J* = 7.5 Hz, 3H), 1.09-1.32 (m, 4H), 1.60-1.72 (m, 2H), 2.33 (s, 3H), 5.11 (s, 1H),5.18 (s, 1H), 6.48 (d, *J* = 2.5 Hz, 1H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 6.76, 12.23, 12.48, 20.61, 28.58, 31.71, 67.95, 88.24, 99.88, 120.83, 129.28, 134.26, 135.57, 149.58, 173.60; IR (KBr, neat): ν 3008, 2967, 2923, 1697, 1615, 1558, 1514, 1388, 1311, 1177, 1056, 999, 814 cm^{-1}; Anal. Calcd for $C_{17}H_{19}NO_2$: C, 75.81; H, 7.11; N, 5.20. Found: C, 75.90; H, 7.10; N, 5.03.



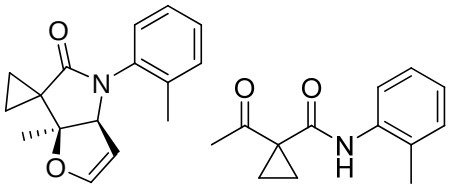
***cis*-(*E*)-4'-(4-chlorophenyl)-6a'-(3-methoxystyryl)-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2i)**

White solid; mp:140-141°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.11-1.15 (m, 1H), 1.20-1.24 (m, 1H), 1.30-1.34 (m, 1H), 1.37-1.41 (m, 1H), 3.82 (s, 3H), 5.17 (s, 1H), 5.23 (s, 1H), 6.09 (d, *J* = 15.5 Hz, 1H), 6.65 (d, *J* = 2.5 Hz, 1H), 6.69 (d, *J* = 15.5 Hz, 1H), 6.83-6.85 (m, 1H), 6.93 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 7.25-7.28 (m, 1H), 7.35 (d, *J* = 8.5 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.65, 15.10, 32.37, 55.26, 70.03, 88.64, 99.23, 112.10, 113.83, 119.28, 122.03, 126.82, 129.08, 129.74, 130.01, 136.61, 137.08, 150.75, 159.88, 173.49; IR (KBr, neat): ν 2921, 2852, 1691, 1593, 1494, 1417, 1377, 1290, 1237, 1173, 1086, 975, 826 cm^{-1}; Anal. Calcd for $C_{23}H_{20}ClNO_3$: C, 70.14; H, 5.12; N, 3.56. Found: C, 70.20; H, 5.08; N, 3.60.



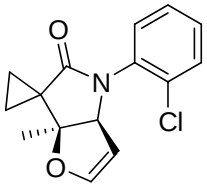
***cis*-6a'-(4-methoxyphenyl)-4'-*p*-tolyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2j)**

White solid; mp: 123-125°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.53-0.57 (m, 1H), 1.19-1.23 (m, 1H), 1.28-1.32 (m, 1H), 1.35-1.39 (m, 1H), 2.34 (s, 3H), 3.81 (s, 3H), 5.22 (t, *J* = 2.5 Hz, 1H), 5.28 (s, 1H), 6.64 (d, *J* = 2.5 Hz, 1H), 6.89-6.92 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.31-7.33 (m, 2H), 7.51 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 13.01, 15.62, 20.89, 34.66, 55.28, 73.03, 90.23, 100.03, 113.72, 121.20, 126.32, 129.57, 132.78, 134.71, 135.56, 149.88, 159.13, 173.38; MS: calcd *m/z* 347.2, found 348.2 $[(M+1)]^+$; IR (KBr, neat): ν 2923, 2850, 1739, 1694, 1647, 1538, 1514, 1368, 1170, 1058, 953, 792 cm^{-1}; Anal. Calcd for $C_{22}H_{21}NO_3$: C, 76.06; H, 6.09; N, 4.03. Found: C, 76.03; H, 5.96; N, 4.01.



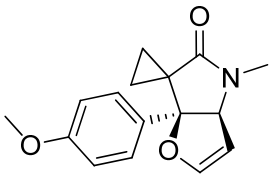
Mixture of ***cis*-6a'-methyl-4'-*o*-tolyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2k)** and **1-acetyl-*N*-*o*-tolylcyclopropanecarboxamide (3k)** (^{1}H NMR, ^{13}C NMR, Anal. Calcd. and IR database see SI of *Angew. Chem. Int. Ed.* **2007**, *46*, 1726.)

^{1}H NMR (500 MHz, $CDCl_3$): δ 1.14-1.25 (m, 3H), 1.32-1.38 (m, 4H), 2.21 (s, 3H), 4.73 (s, 1H), 4.97 (s, 1H), 6.51 (d, J = 2.5 Hz, 1H), 7.15 (t, J_1 = 6.5 Hz, J_2 = 2.5 Hz, 1H), 7.22-7.29 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): (mixture with **3k**) δ 11.20, 12.69, 15.22, 17.90, 20.14, 21.85, 25.10, 31.31, 63.56, 71.93, 87.83, 99.70, 103.87, 121.68, 124.18, 126.44, 126.59, 127.93, 130.20, 130.98, 135.98, 136.51, 149.72, 173.47.



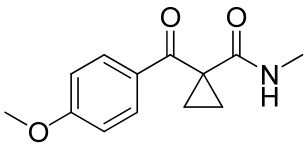
***cis*-4'-(2-chlorophenyl)-6a'-methyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2l)**

Colourless oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.13-1.35 (m, 7H), 4.88 (s, 1H), 4.92 (t, J = 2.5 Hz, 1H), 6.50 (d, J = 2.5 Hz, 1H), 7.23-7.31 (m, 3H), 7.45-7.47 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.40, 13.02, 21.78, 31.20, 70.81, 87.98, 99.50, 127.56, 129.20, 130.27, 130.75, 132.50, 134.78, 149.88, 174.33; IR (KBr, neat): ν 3007, 2971, 2925, 1704, 1610, 1481, 1343, 1184, 1058, 909, 817 cm^{-1}; Anal. Calcd for $C_{15}H_{14}ClNO_2$: C, 65.34; H, 5.12; N, 5.08. Found: C, 65.50; H, 5.17; N, 5.16.



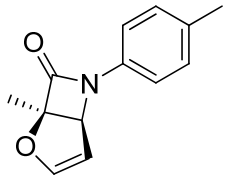
***cis*-6a'-(4-methoxyphenyl)-4'-methyl-3a',4'-dihydrospiro[cyclopropane-1,6'-furo[3,2-*b*]pyrrol]-5'(6a'*H*)-one (2m)**

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.40-0.46 (m, 1H), 1.06-1.12 (m, 1H), 1.13-1.18 (m, 1H), 1.20-1.22 (m, 1H), 2.93(s, 3H), 3.79 (s, 3H), 4.63 (s, 1H), 5.22 (s, 1H), 6.63 (d, J = 2.4 Hz, 1H), 6.87 (d, J = 8.8 Hz, 2H), 7.24 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): (mixture with **3k**) δ 11.69, 14.49, 14.64, 26.97, 28.03, 33.86, 34.77, 55.27, 55.51, 73.30, 91.17, 98.96, 113.67, 113.89, 126.22, 128.76, 131.53, 132.85, 149.97, 159.08, 163.91, 170.42, 173.93, 195.79.



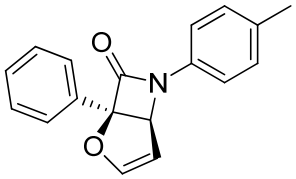
1-(4-methoxybenzoyl)-*N*-methylcyclopropanecarboxamide (3m)

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.28-1.31 (m, 2H), 1.55-1.57 (m, 2H), 2.72 (d, J = 4.4 Hz, 3H), 3.86 (s, 3H), 5.85 (s, 1H), 6.92 (d, J = 8.8 Hz, 2H), 7.96 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): (mixture with **2k**) δ 11.69, 14.49, 14.64, 26.97, 28.03, 33.86, 34.77, 55.27, 55.51, 73.30, 91.17, 98.96, 113.67, 113.89, 126.22, 128.76, 131.53, 132.85, 149.97, 159.08, 163.91, 170.42, 173.93, 195.79.



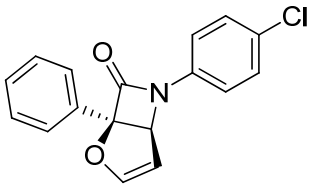
***cis*-1-methyl-6-*p*-tolyl-2-oxa-6-azabicyclo[3.2.0]hept-3-en-7-one (6a)**

Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.76 (s, 3H), 2.34 (s, 3H), 4.80 (s, 1H), 5.51 (s, 1H), 6.69 (s, 1H), 7.17 (d, J = 7.0 Hz, 2H), 7.30 (d, J = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 15.89, 20.88, 66.23, 94.55, 101.55, 116.85, 129.67, 134.11, 134.23, 153.88, 163.95; MS: calcd *m/z* 215.1, found 216.1 $[(M+1)]^+$; IR (KBr, neat): ν 3035, 2924, 2855, 2735, 2588, 1891, 1748, 1650, 1597, 1511, 1456, 1373, 1170, 1144, 1101, 1042, 986, 900, 837 cm^{-1}; Anal. Calcd for $C_{13}H_{13}NO_2$: C, 72.54; H, 6.09; N, 6.51. Found: C, 72.73; H, 6.23; N, 6.26.



***cis*-1-phenyl-6-*p*-tolyl-2-oxa-6-azabicyclo[3.2.0]hept-3-en-7-one (6b)**

White solid; mp: 104-106°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.32 (s, 3H), 5.04 (s, 1H), 5.60 (t, J = 2.5 Hz, 1H), 6.86 (d, J = 2.5 Hz, 1H), 7.16 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.40-7.42 (m, 2H), 7.57 (d, J = 7.0 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 20.91, 68.08, 97.51, 101.64, 117.04, 125.93, 128.79, 129.31, 129.74, 133.29, 134.11, 134.41, 154.46, 162.57; MS: calcd *m/z* 277.1, found 278.1 $[(M+1)]^+$; IR (KBr, neat): *v* 1733, 1599, 1515, 1451, 1384, 1340, 1156, 1044, 986, 841, 806 cm^{-1}; Anal. Calcd for $C_{18}H_{15}NO_2$: C, 77.96; H, 5.45; N, 5.05. Found: C, 77.99; H, 5.40; N, 5.12.

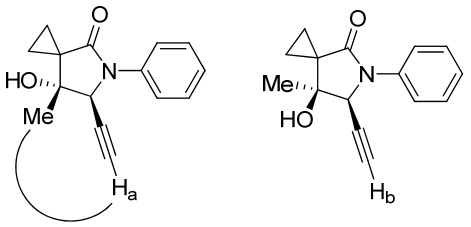


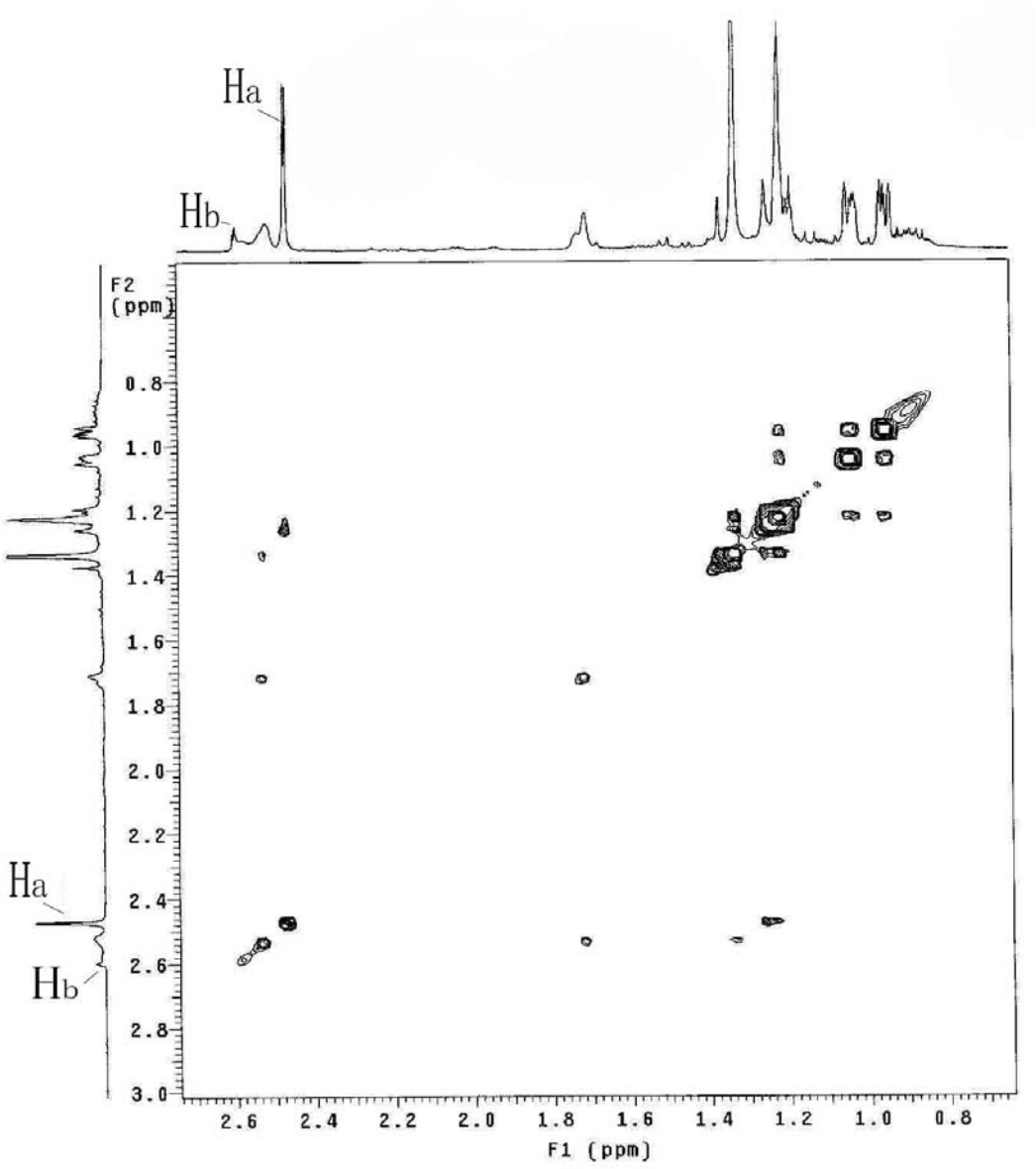
***cis*-6-(4-chlorophenyl)-1-phenyl-2-oxa-6-azabicyclo[3.2.0]hept-3-en-7-one (6c)**

White solid; mp: 130-132°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 5.07 (d, J = 2.5 Hz, 1H), 5.60 (t, J = 2.5 Hz, 1H), 6.89 (d, J = 2.5 Hz, 1H), 7.33 (d, J = 9.0 Hz, 2H), 7.38-7.44 (m, 5H), 7.55-7.57 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 68.30, 97.84, 101.22, 118.29, 125.94, 128.88, 129.38, 129.52, 129.77, 132.91, 135.01, 154.78, 162.75; IR (KBr, neat): *v* 1740, 1599, 1497, 1418, 1376, 1157, 1043, 822, 716 cm^{-1}; Anal. Calcd for $C_{17}H_{12}ClNO_2$: C, 68.58; H, 4.06; N, 4.70. Found: C, 68.50; H, 4.11; N, 4.62.

IV. ^{1}H-^{1}H COSY spectra copies of compound **4a**

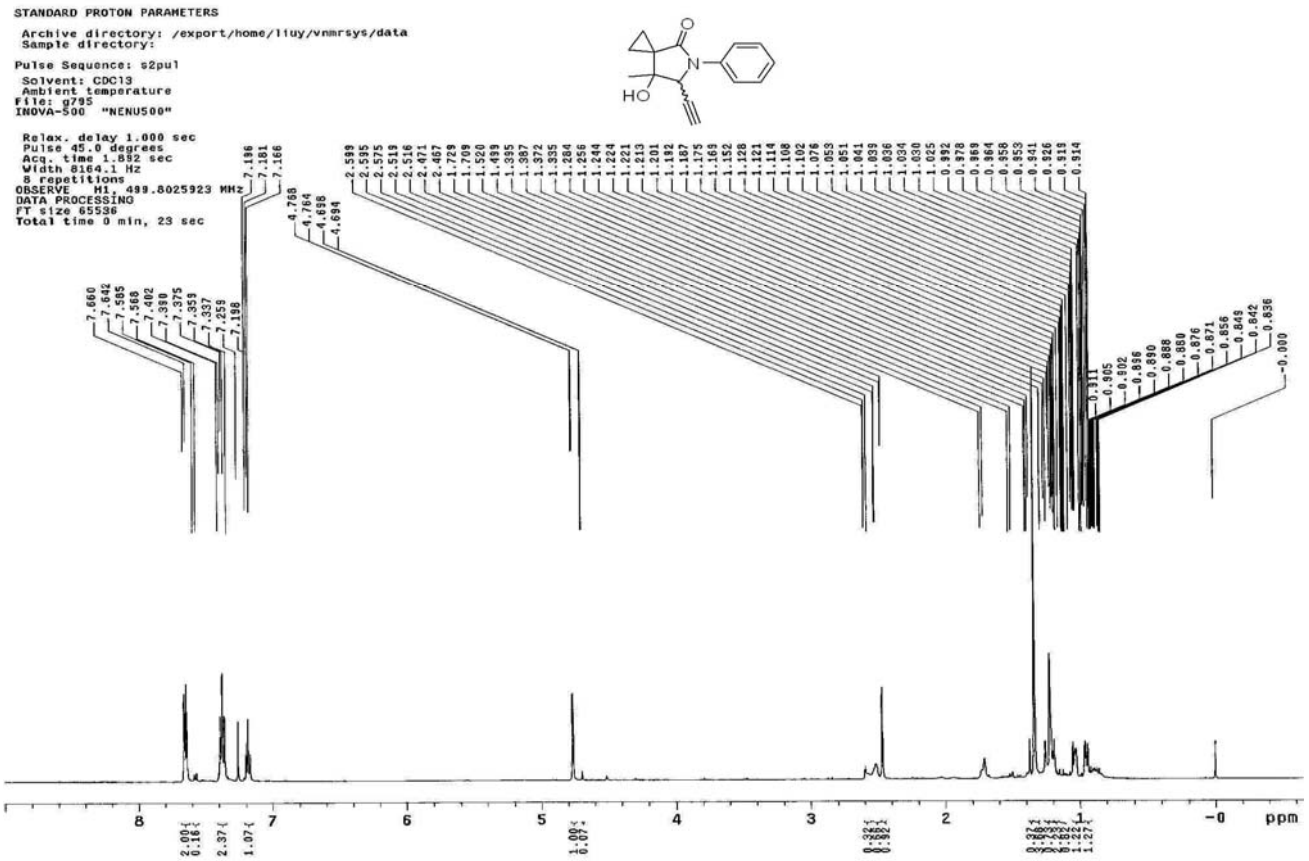
The relative stereochemistry of compound **4a** was determined by ^{1}H NMR NOE analysis as shown below.

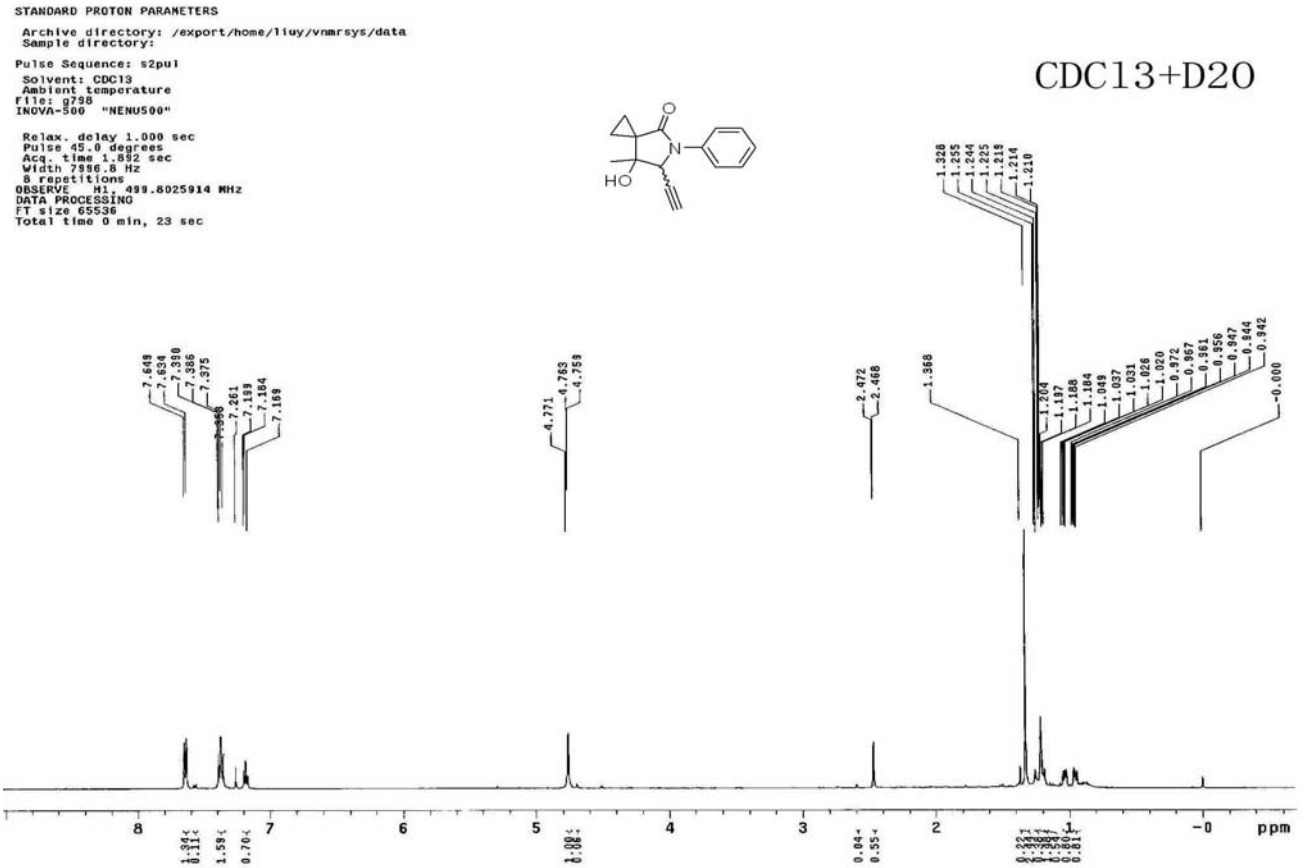


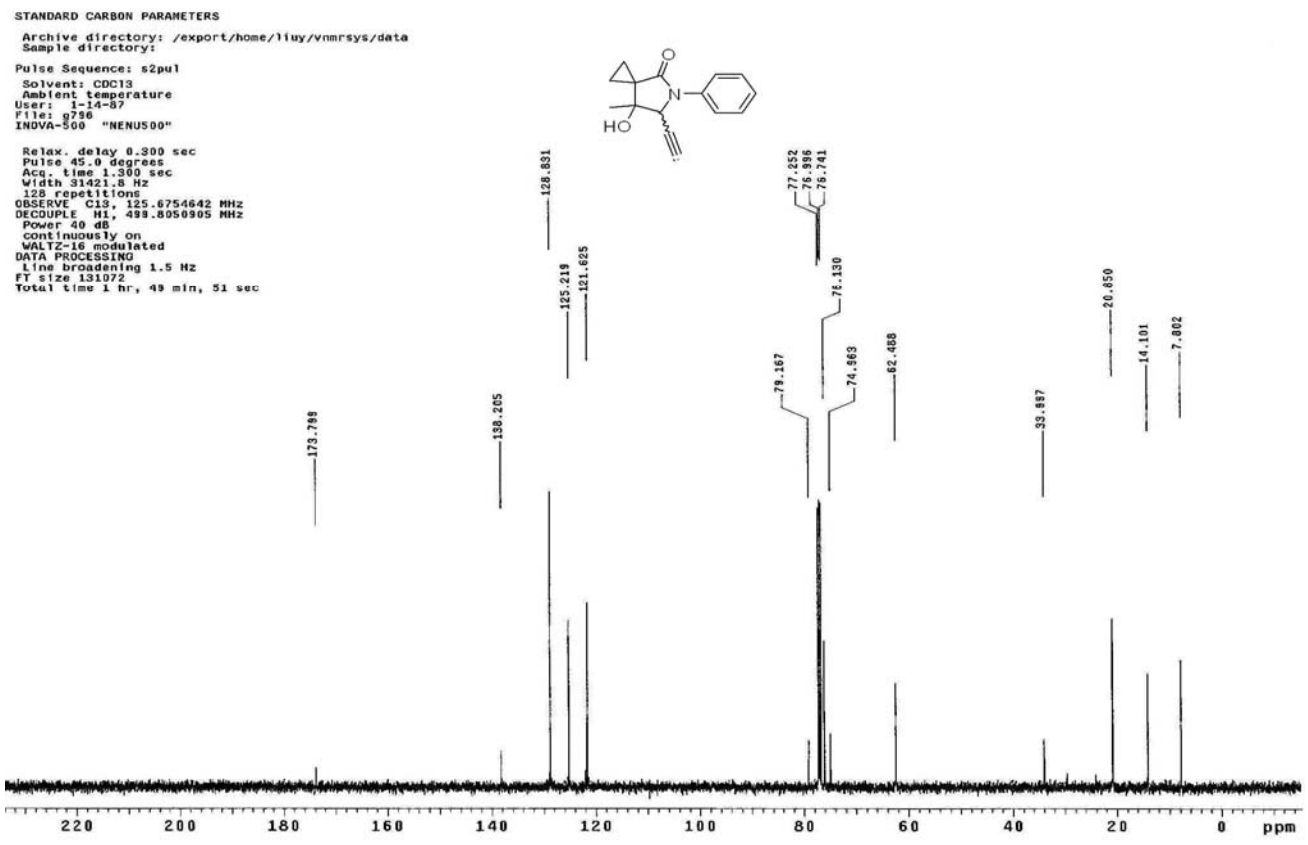


V. ^{1}H NMR and ^{13}C NMR spectra copies

Compound **4a**



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Sample directory:
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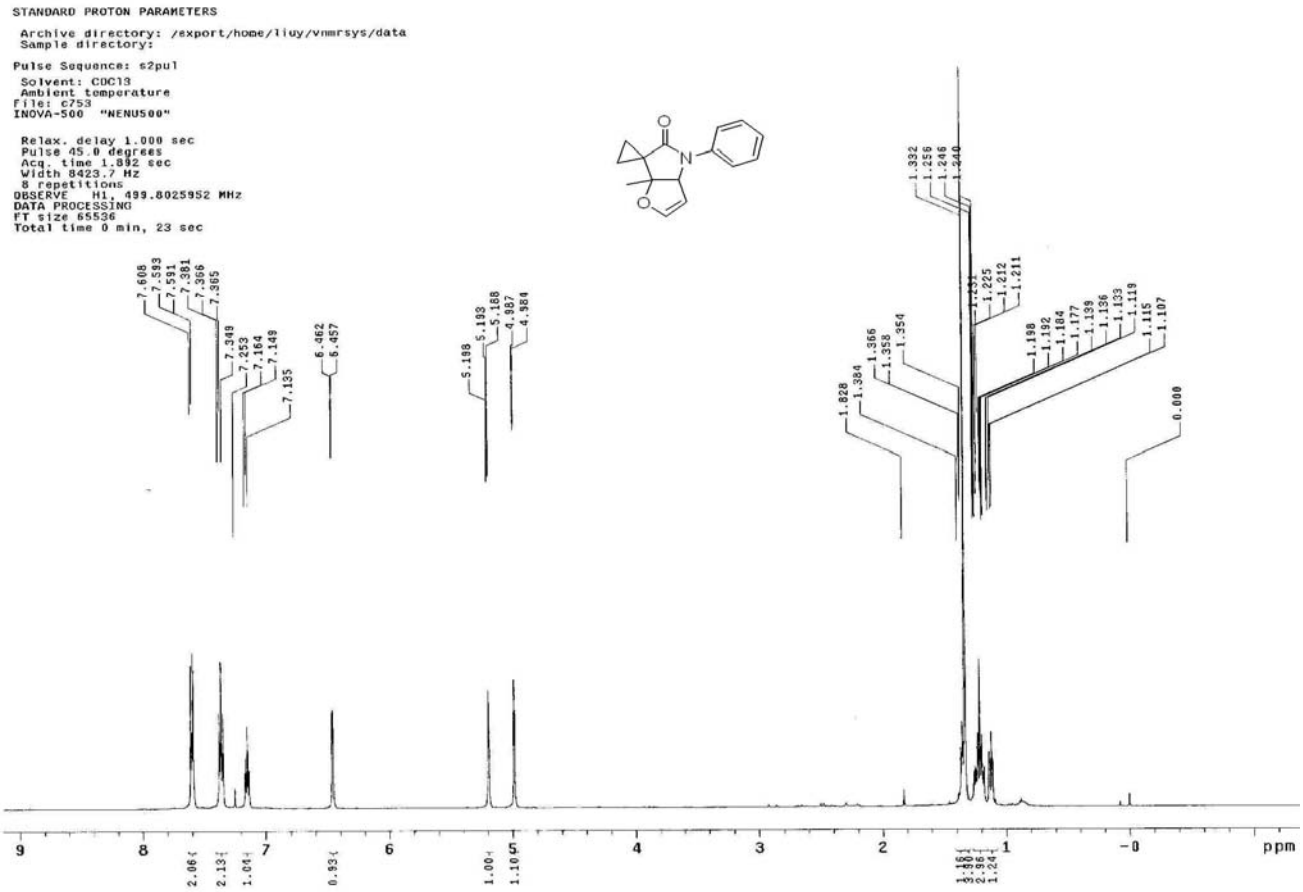
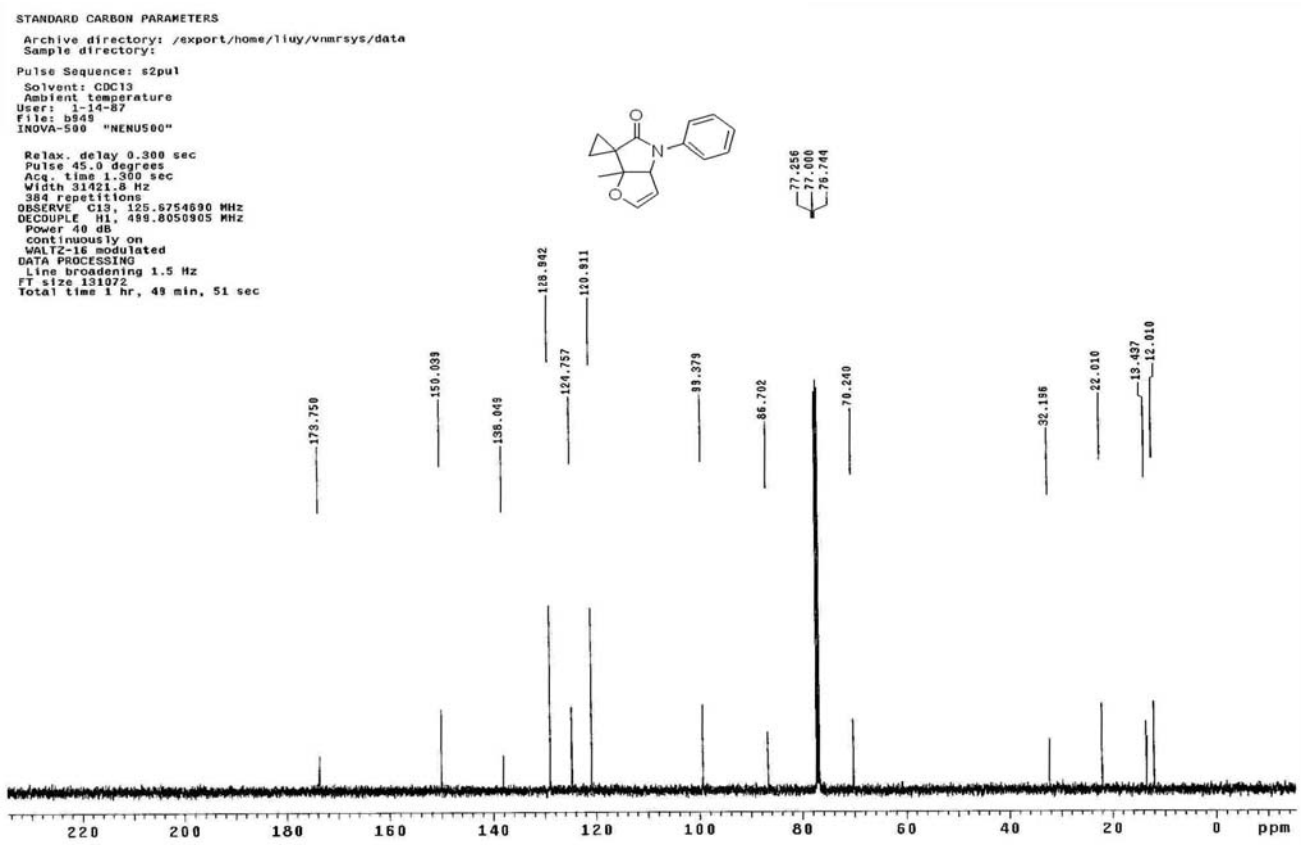
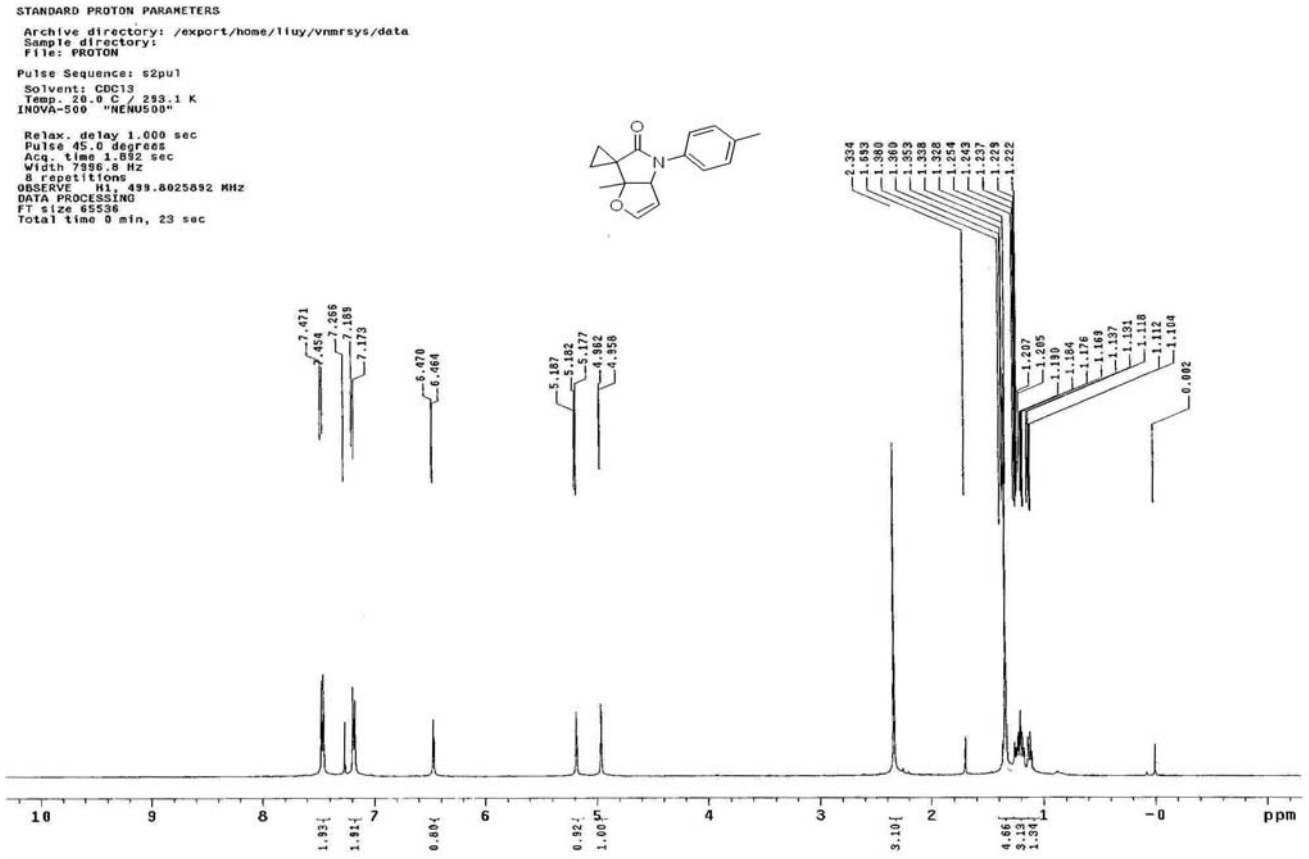
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: g796
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
O
N
HO
128.831
125.219
121.625
77.252
76.998
76.741
75.130
74.963
62.468
33.887
20.650
14.101
7.002
79.167
173.798
138.205
220
200
180
160
140
120
100
80
60
40
20
0
ppm

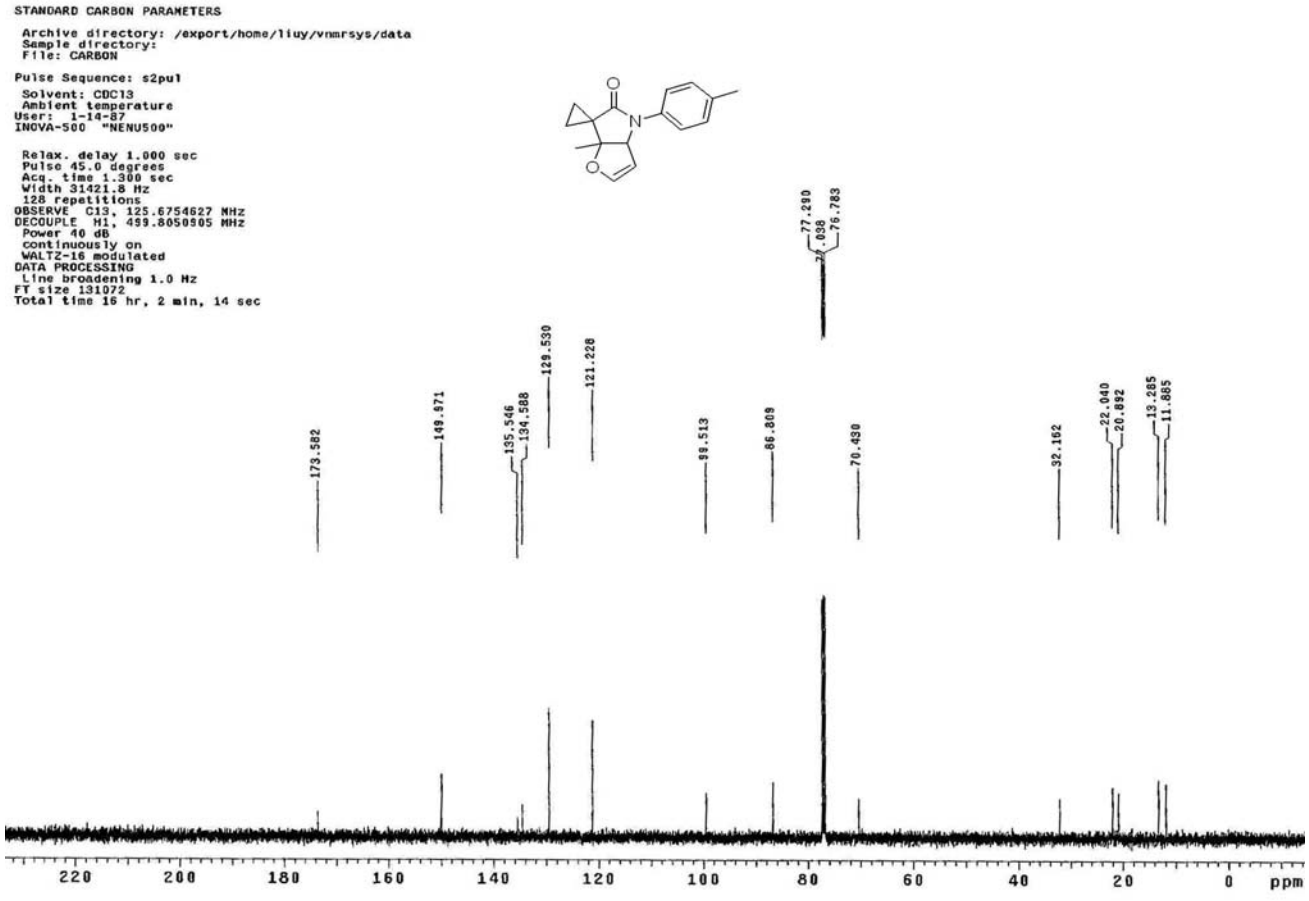
Compound **2a**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c753
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8423.7 Hz
8 repetitions
OBSERVE H1, 499.8025952 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

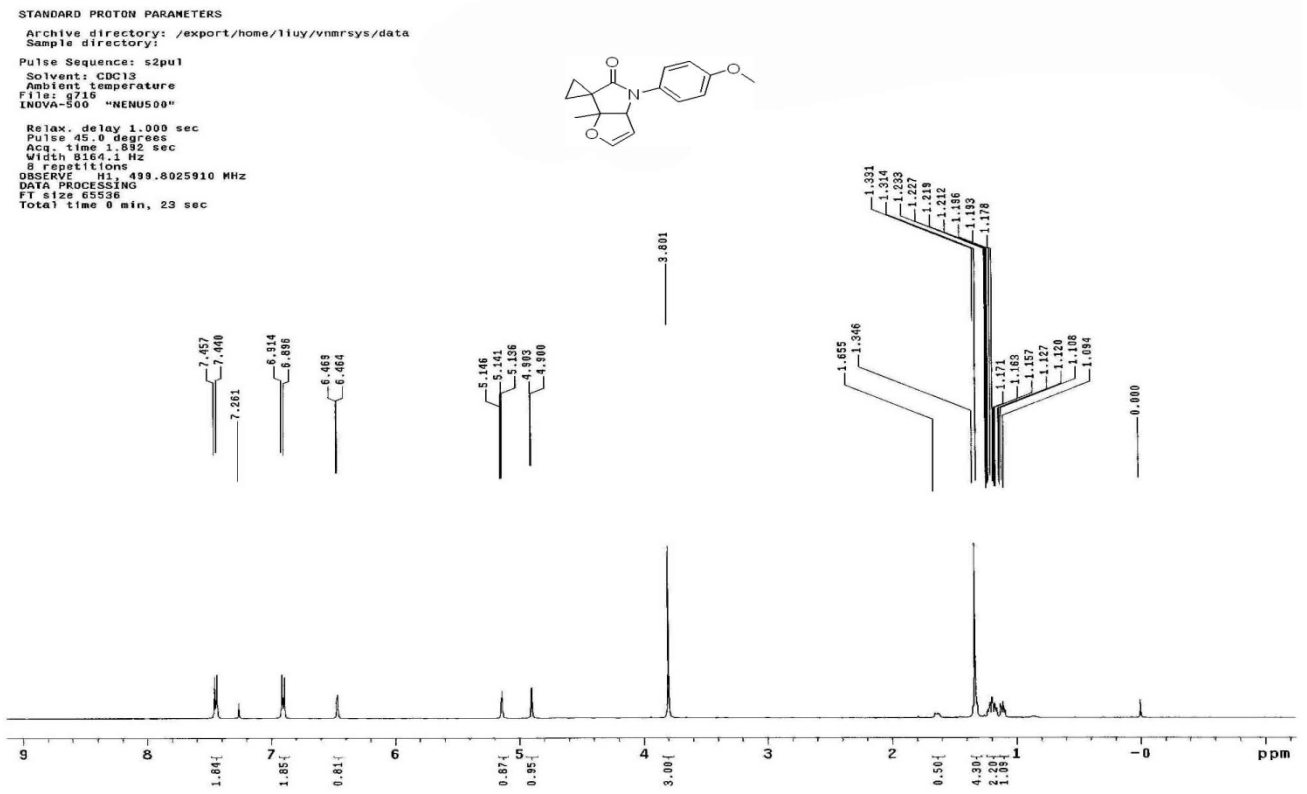

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: b949
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
384 repetitions
OBSERVE C13, 125.6754690 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
ppm

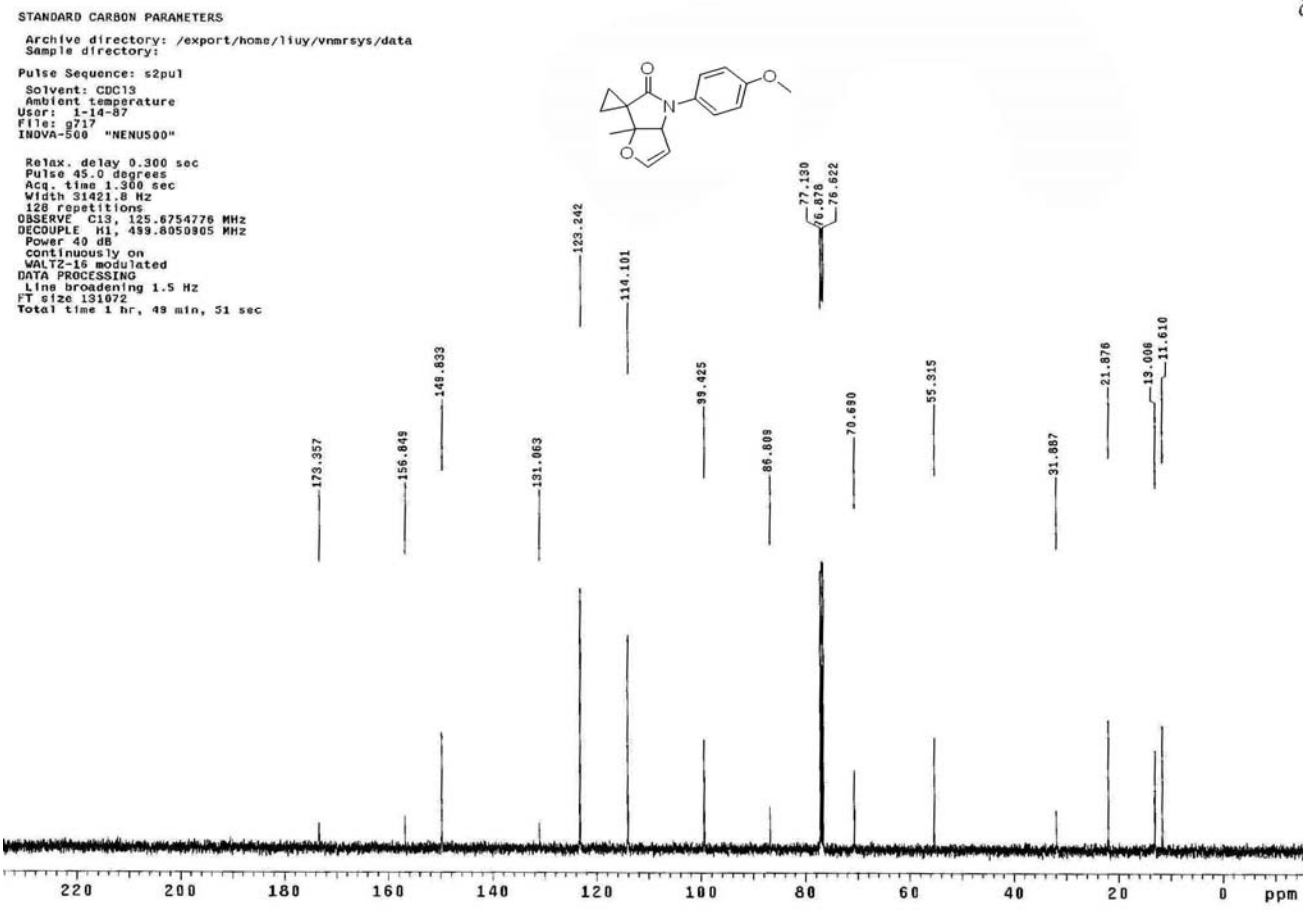
Compound **2b**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025892 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.471
7.454
7.266
7.189
7.173
6.470
6.464
5.187
5.182
5.177
4.962
4.958
2.334
1.653
1.380
1.360
1.353
1.338
1.328
1.254
1.243
1.237
1.229
1.222
1.207
1.205
1.190
1.184
1.176
1.169
1.137
1.131
1.118
1.112
1.104
0.002
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.93
1.91
0.80
0.92
1.00
3.10
4.66
3.19
1.34

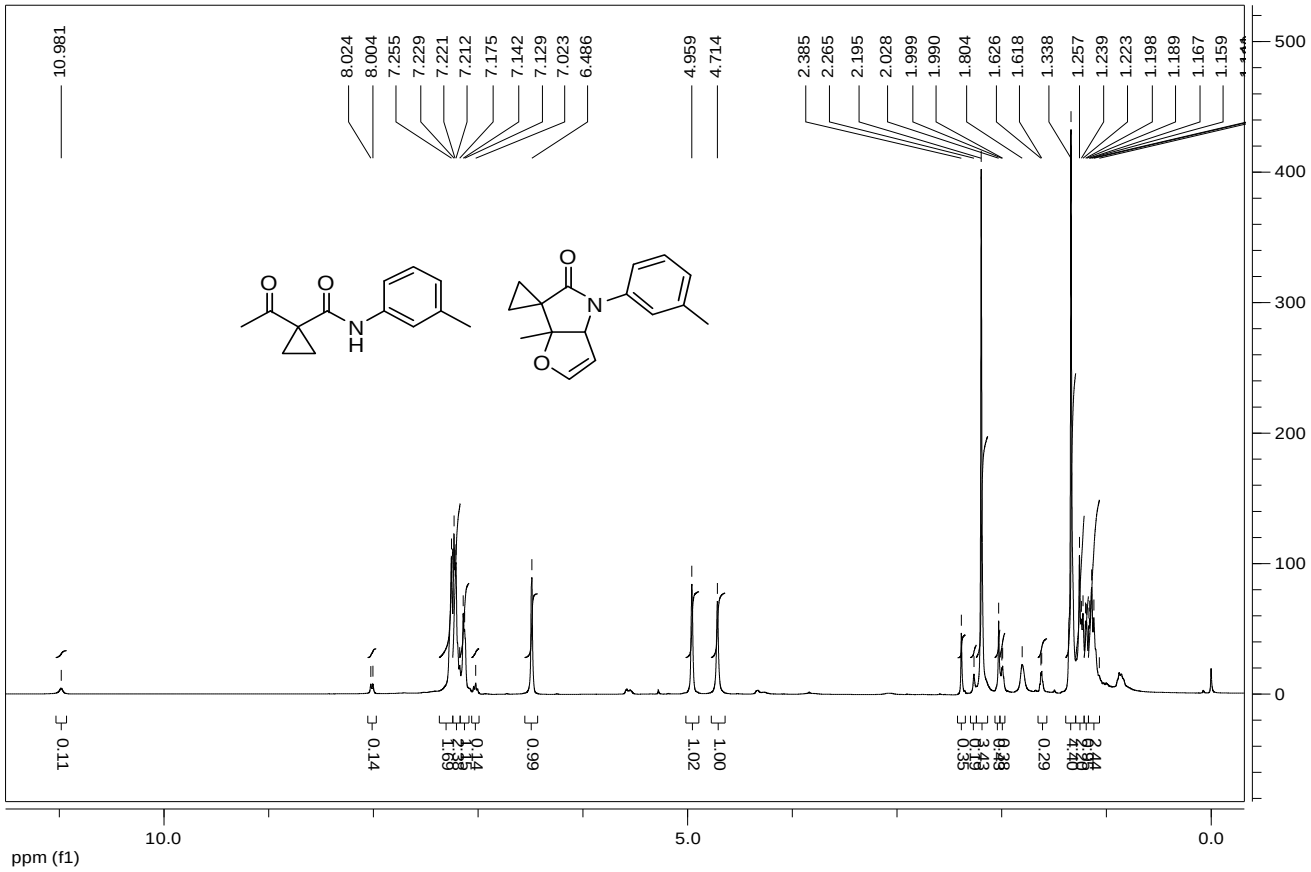

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754627 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 16 hr, 2 min, 14 sec
77.290
77.038
76.783
173.582
149.971
135.546
134.588
129.530
121.228
99.513
86.869
70.430
32.162
22.040
20.892
13.285
11.885
220
200
180
160
140
120
100
80
60
40
20
0
ppm

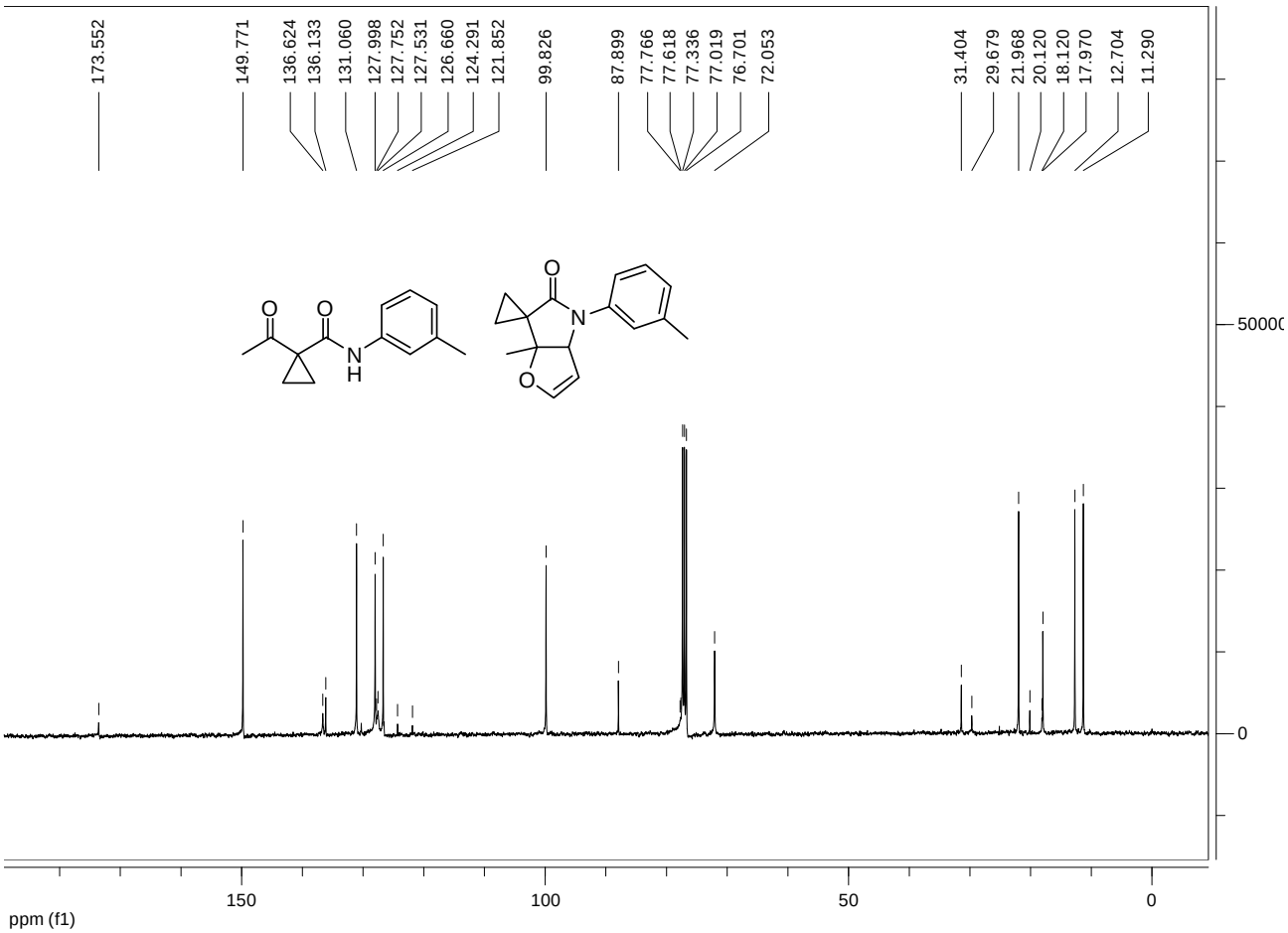
Compound **2c**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g716
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8164.1 Hz
8 repetitions
OBSERVE H1, 499.8025910 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.457
7.440
7.261
6.914
6.896
6.469
6.464
5.146
5.141
5.136
4.903
4.900
3.801
1.655
1.346
1.331
1.314
1.233
1.227
1.219
1.212
1.186
1.193
1.178
1.171
1.163
1.157
1.127
1.120
1.108
1.094
0.000
ppm

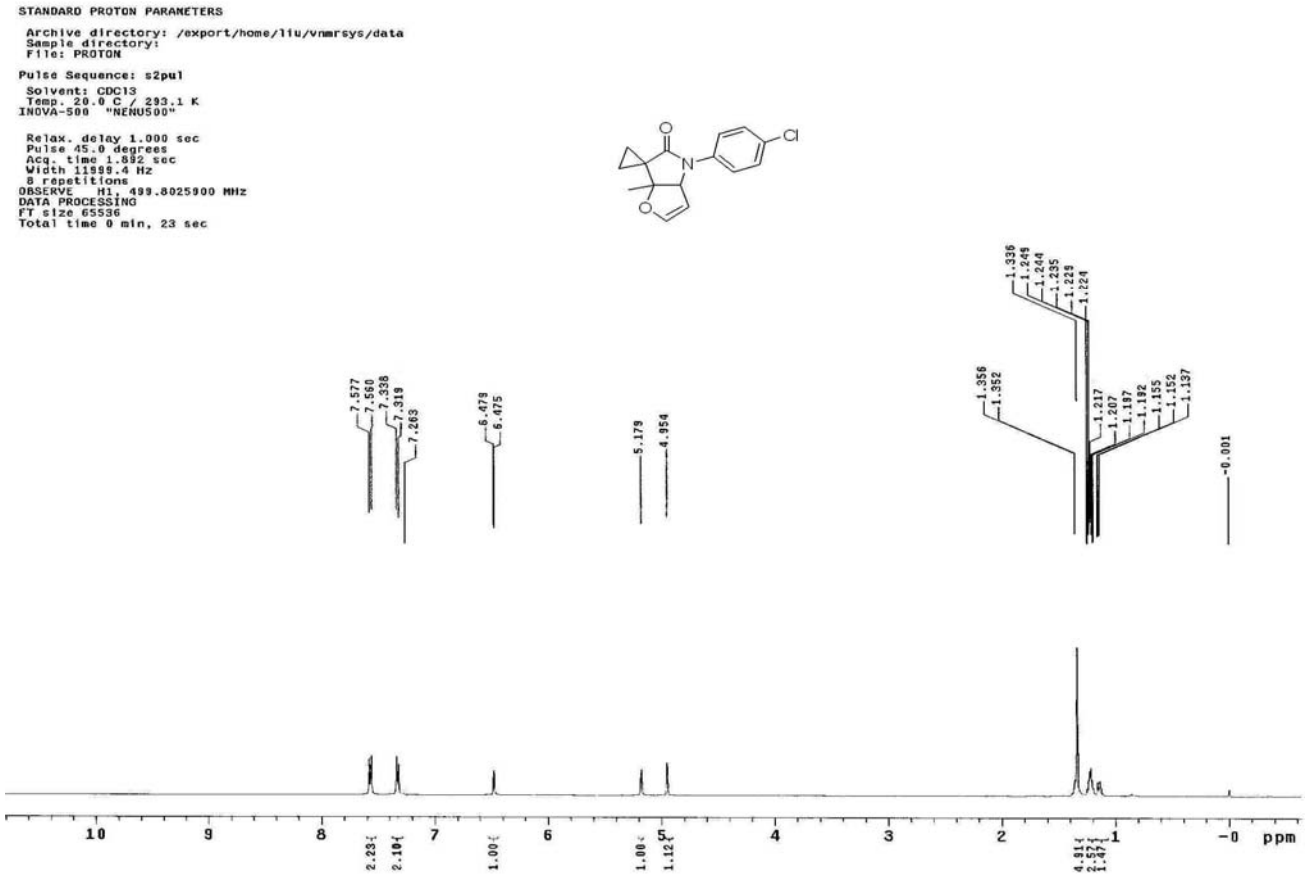

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: g717
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754776 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
173.357
156.849
148.833
131.063
123.242
114.101
99.425
86.809
77.130
76.878
76.622
70.680
55.315
31.887
21.876
19.006
11.610
ppm

Compound **2d**


10.981
8.024
8.004
7.255
7.229
7.221
7.212
7.175
7.142
7.129
7.023
6.486
4.959
4.714
2.385
2.265
2.195
2.028
1.999
1.990
1.804
1.626
1.618
1.338
1.257
1.239
1.223
1.198
1.189
1.167
1.159
0.11
0.14
0.96
1.02
1.00
0.29
10.0
5.0
0.0
ppm (f1)


173.552
149.771
136.624
136.133
131.060
127.998
127.752
127.531
126.660
124.291
121.852
99.826
87.899
77.766
77.618
77.336
77.019
76.701
72.053
31.404
29.679
21.968
20.120
18.120
17.970
12.704
11.290
150
100
50
0
ppm (f1)

Compound **2e**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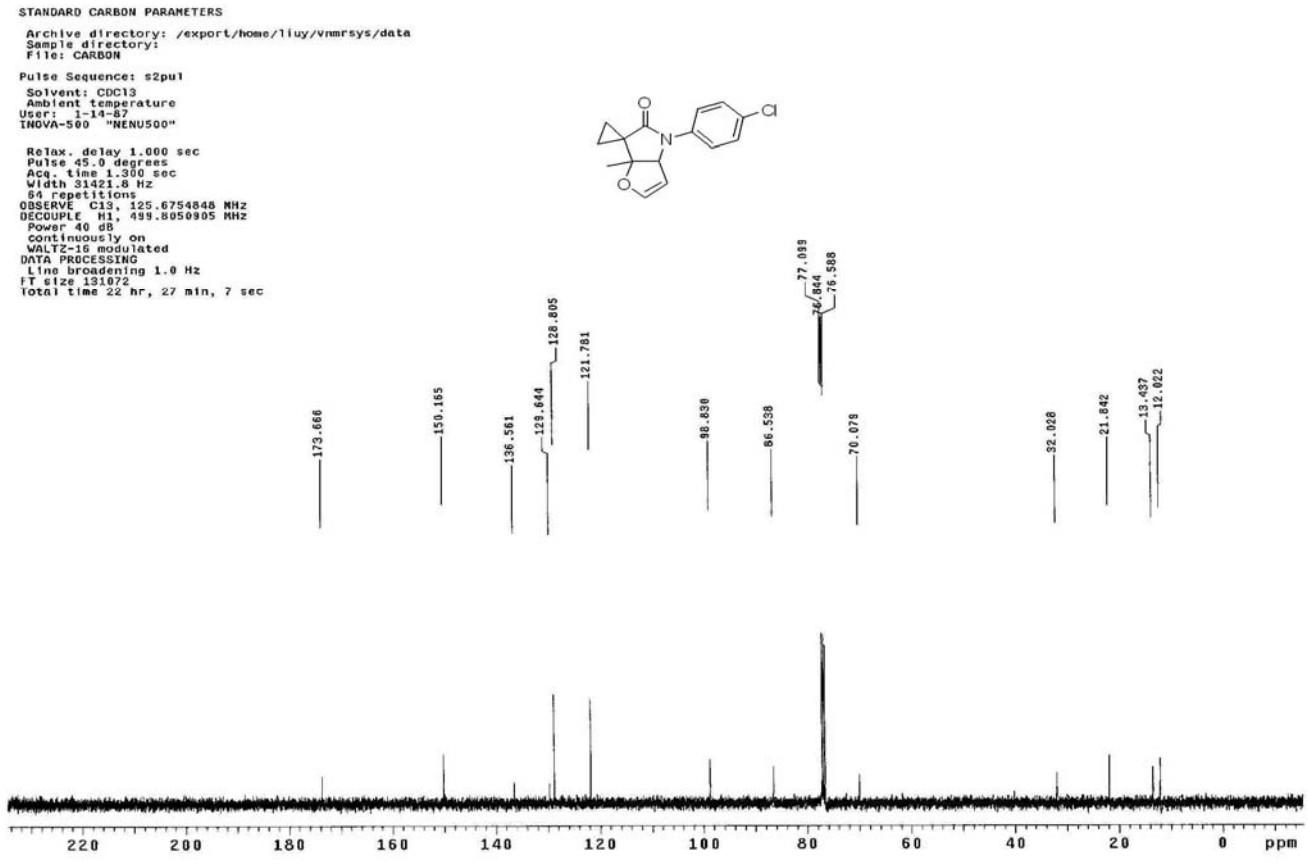
Archive directory: /export/home/liu/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 11998.4 Hz
8 repetitions
OBSERVE H1, 499.8025900 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
O
N
O
7.577
7.560
7.338
7.319
7.263
6.479
6.475
5.179
4.954
1.356
1.352
1.336
1.249
1.244
1.235
1.229
1.224
1.217
1.207
1.197
1.192
1.155
1.152
1.137
-0.001
10
9
8
7
6
5
4
3
2
1
-0
ppm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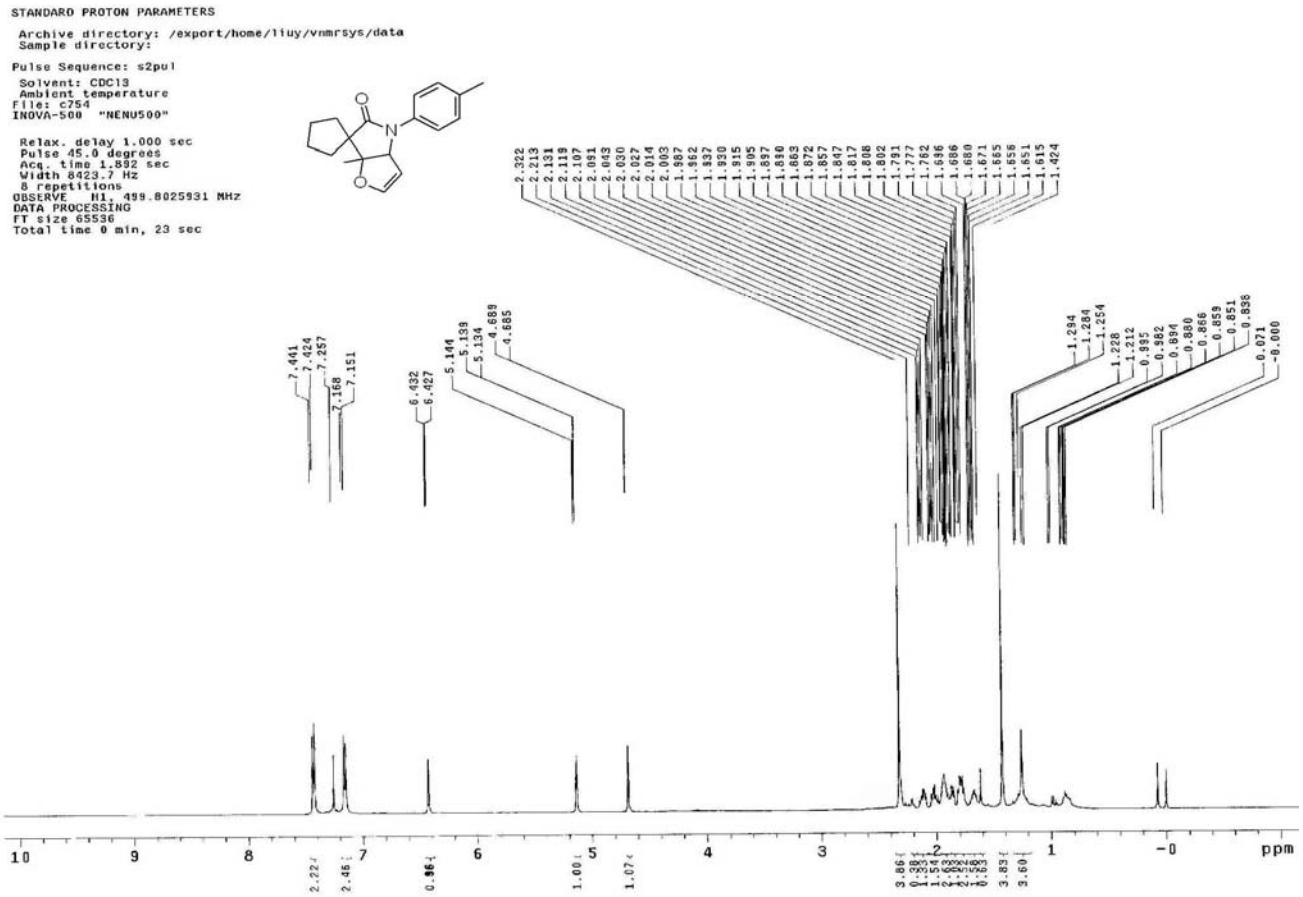
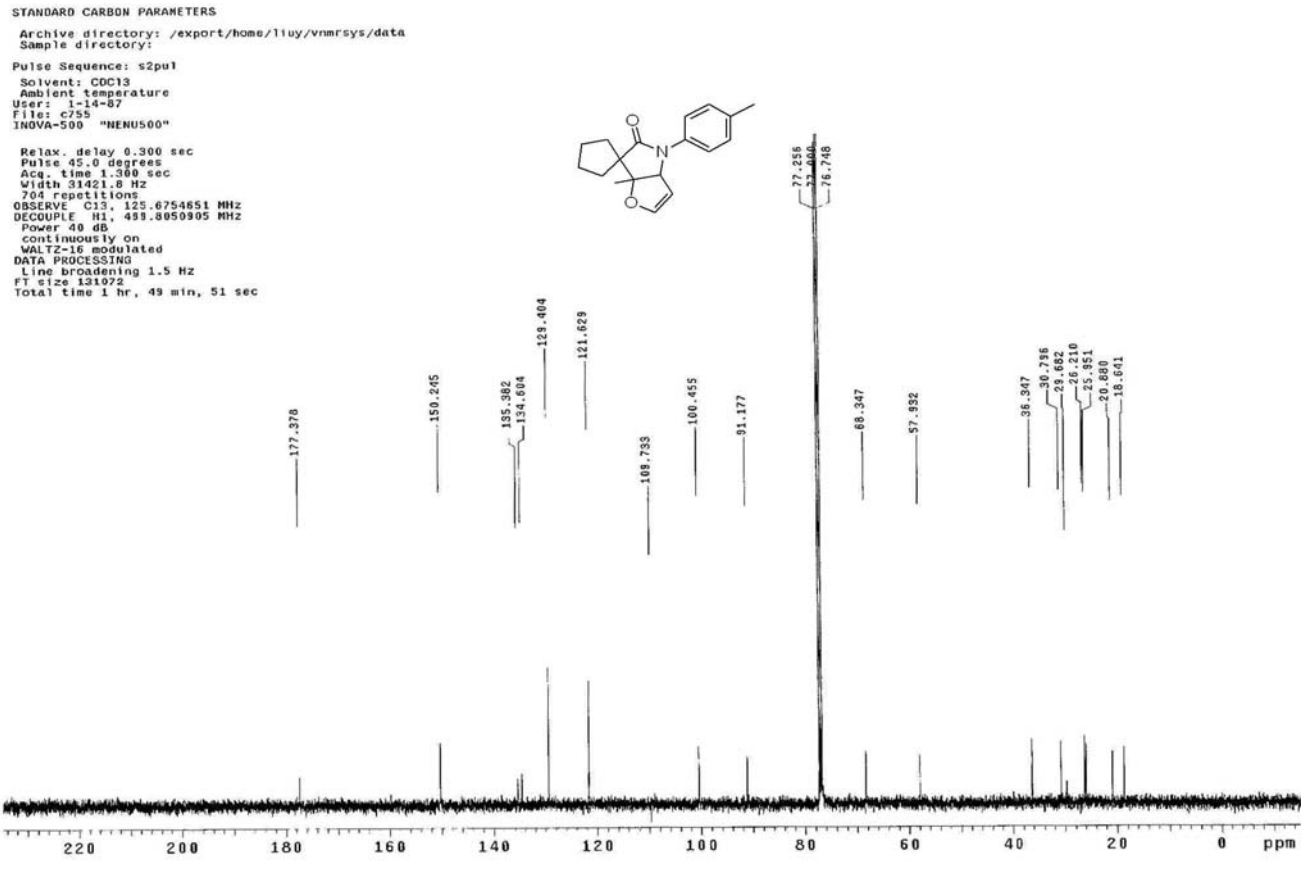
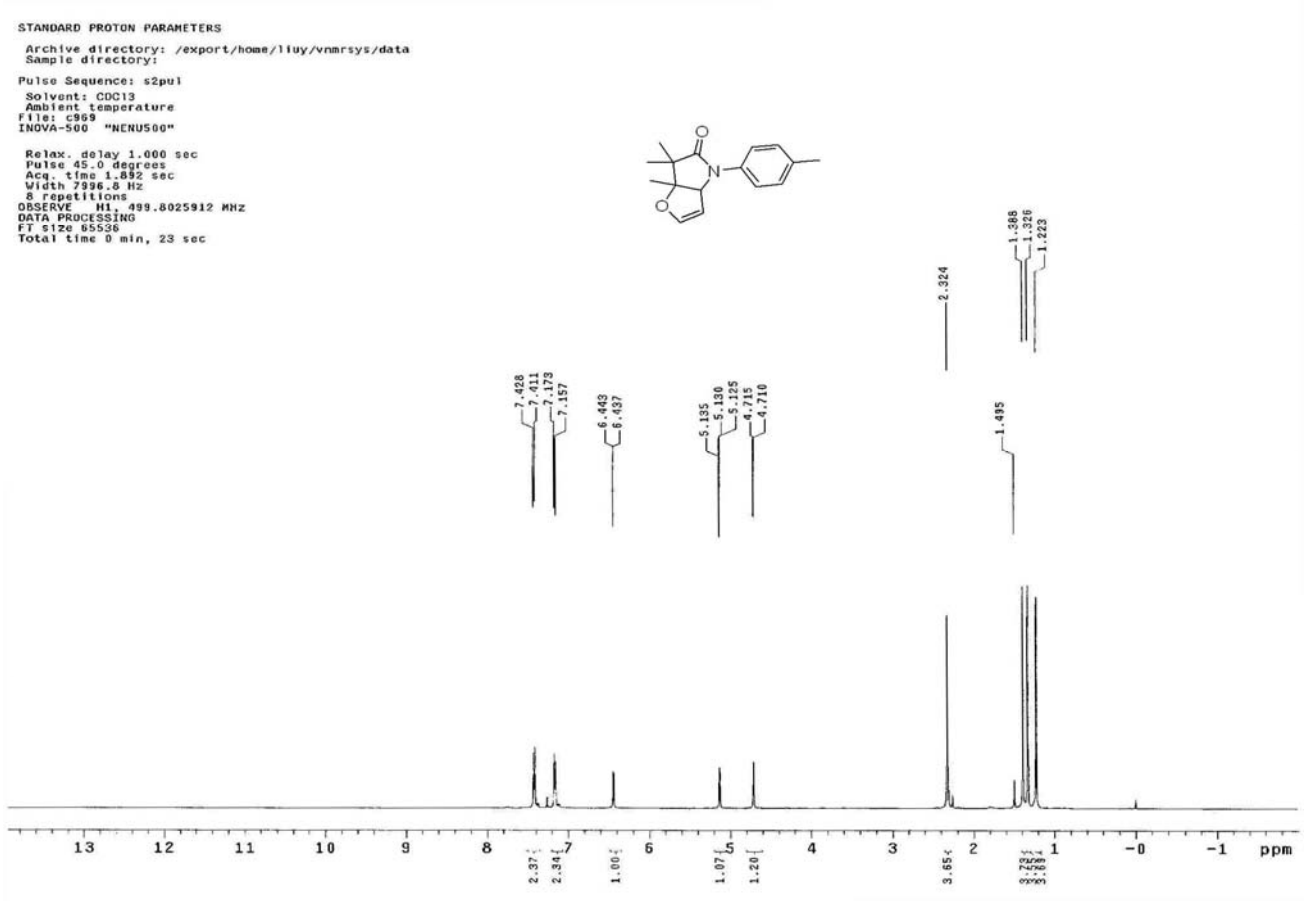
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754848 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 22 hr, 27 min, 7 sec
Cl
O
N
O
173.666
150.165
136.561
129.644
128.805
121.781
98.830
86.538
77.099
76.844
76.588
70.079
32.028
21.842
13.437
12.022
220
200
180
160
140
120
100
80
60
40
20
0
ppm

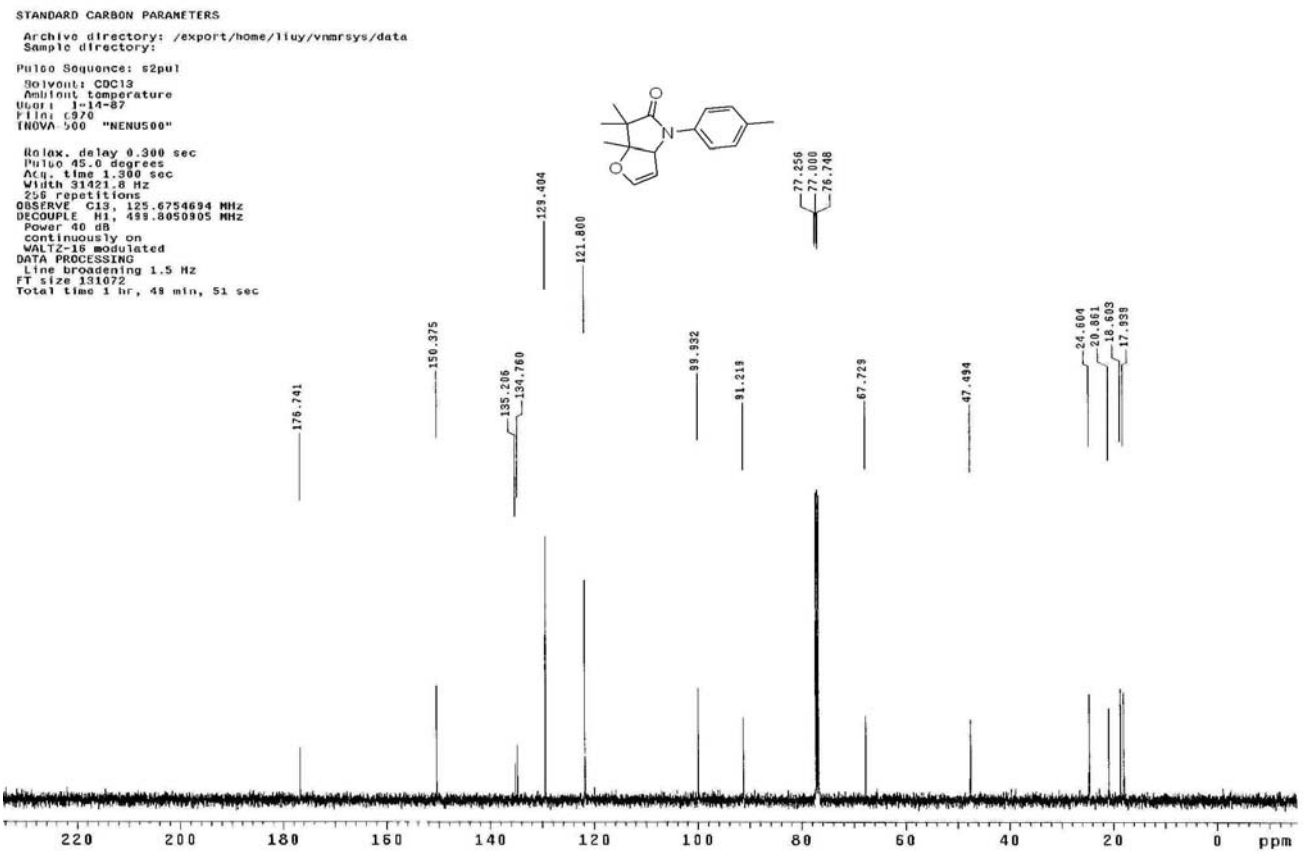
Compound **2f**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c754
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8423.7 Hz
8 repetitions
OBSERVE H1, 499.8025931 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

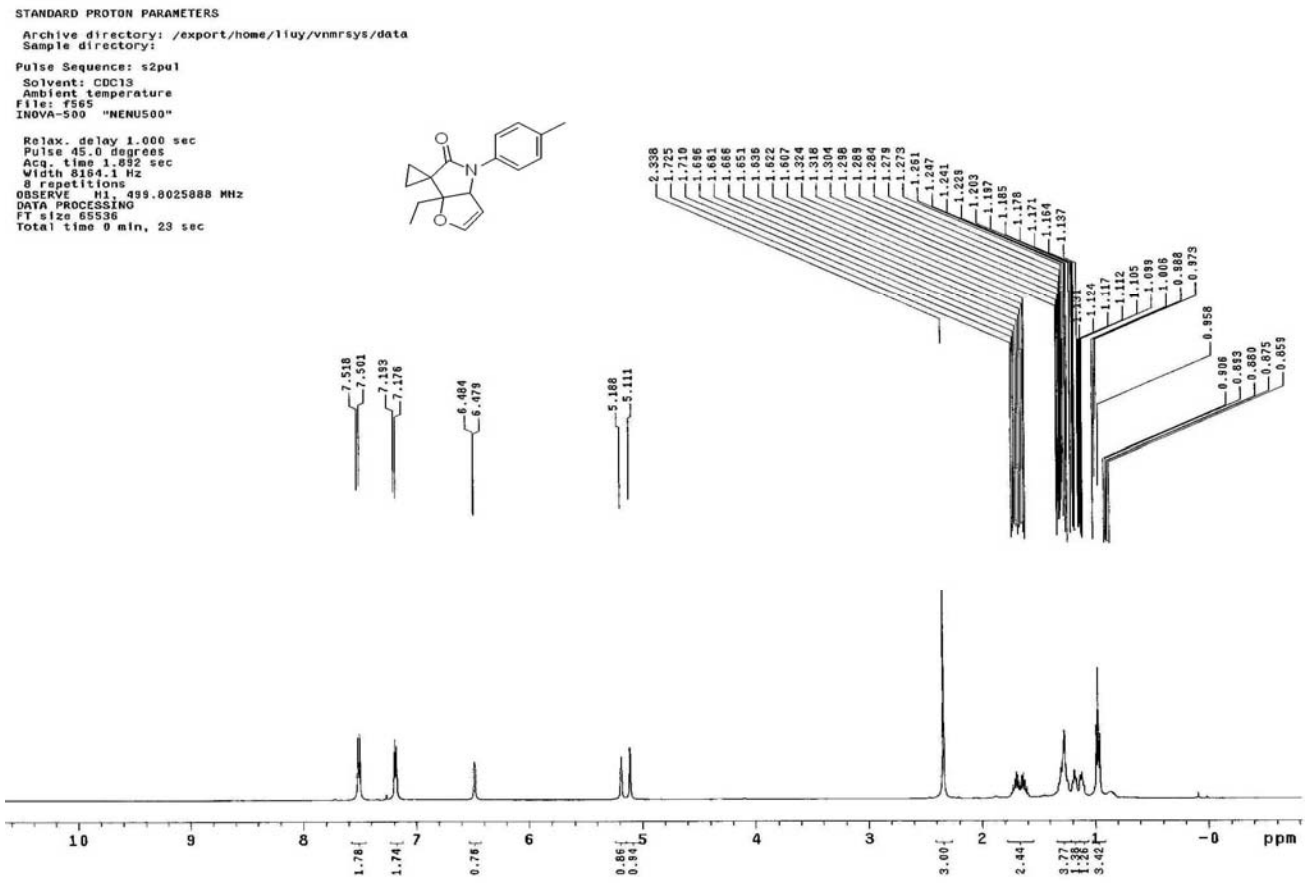

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c755
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
704 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
ppm

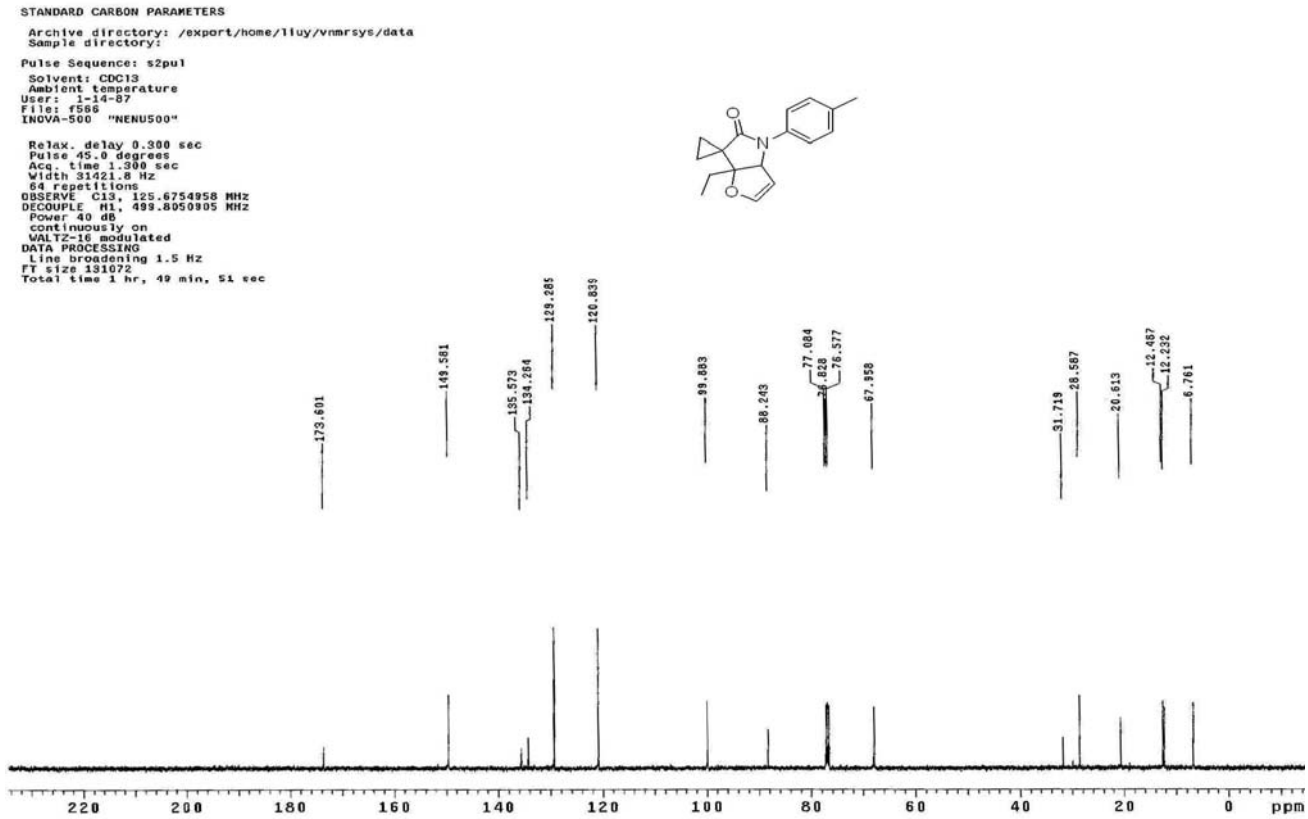
Compound **2g**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c969
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025912 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.428
7.411
7.173
7.157
6.443
6.437
5.135
5.130
5.125
4.715
4.710
2.324
1.495
1.388
1.326
1.223
ppm

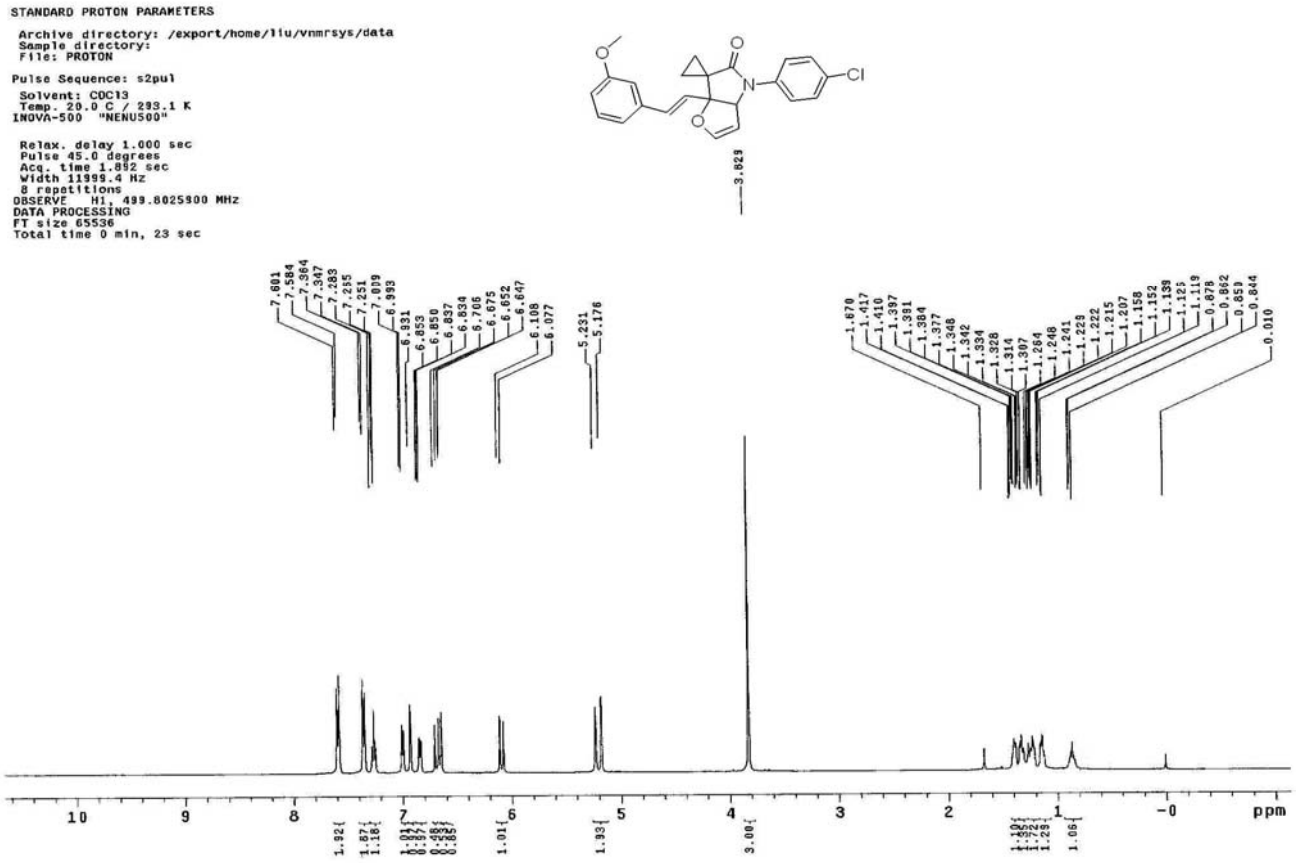

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: C970
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754694 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 48 min, 51 sec
176.741
150.375
135.206
134.760
129.404
121.800
99.932
91.218
77.256
77.000
76.748
67.729
47.494
24.604
20.861
18.603
17.939
ppm

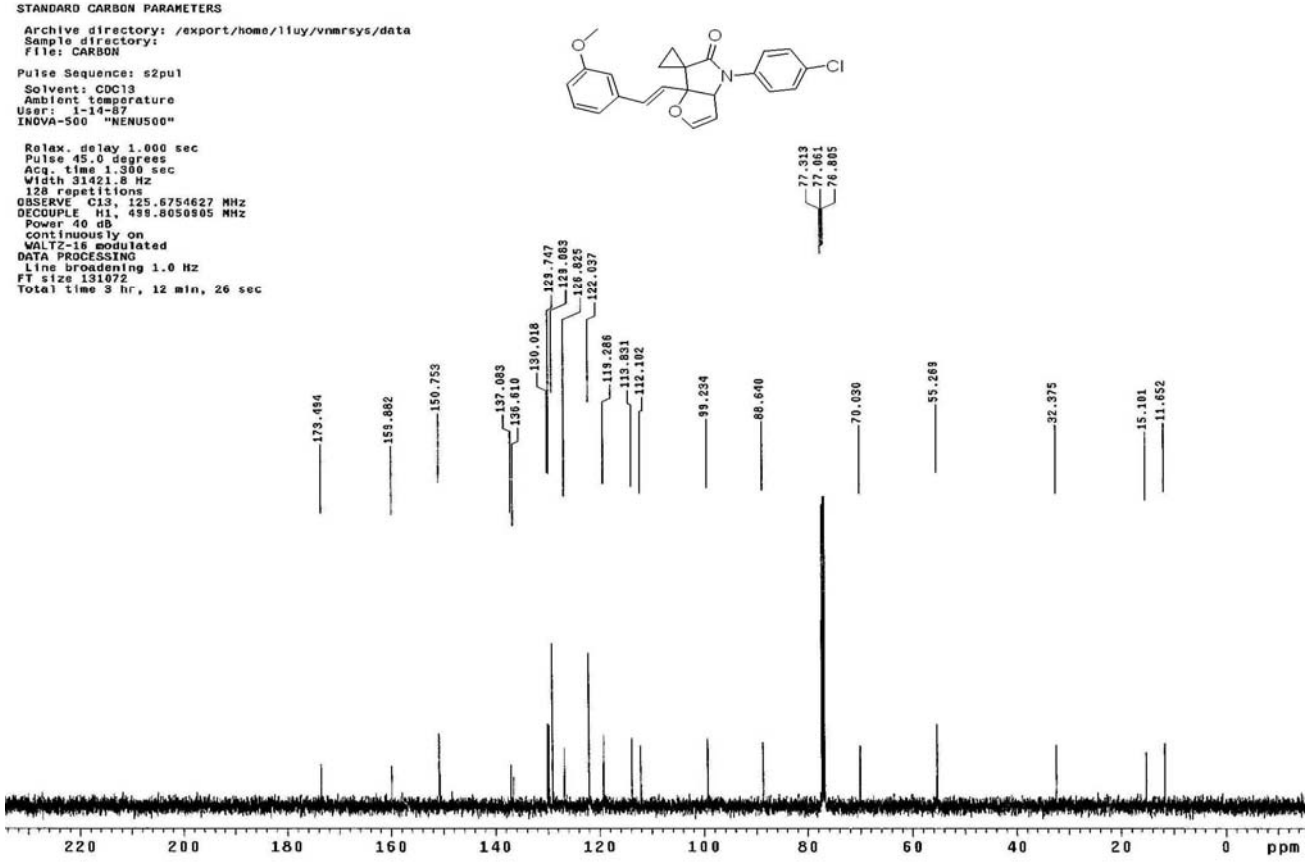
Compound **2h**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: f565
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8164.1 Hz
8 repetitions
OBSERVE H1, 499.8025888 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.518
7.501
7.193
7.176
6.484
6.479
5.188
5.111
2.338
1.725
1.710
1.696
1.681
1.666
1.651
1.636
1.622
1.607
1.324
1.318
1.304
1.298
1.289
1.284
1.279
1.273
1.261
1.247
1.241
1.228
1.203
1.197
1.185
1.178
1.171
1.164
1.137
1.124
1.117
1.112
1.105
1.099
1.088
0.958
0.906
0.893
0.880
0.875
0.859
10
9
8
7
6
5
4
3
2
1
-0
ppm
1.78
1.74
0.76
0.86
0.94
3.00
2.44
3.27
1.38
1.28
3.42

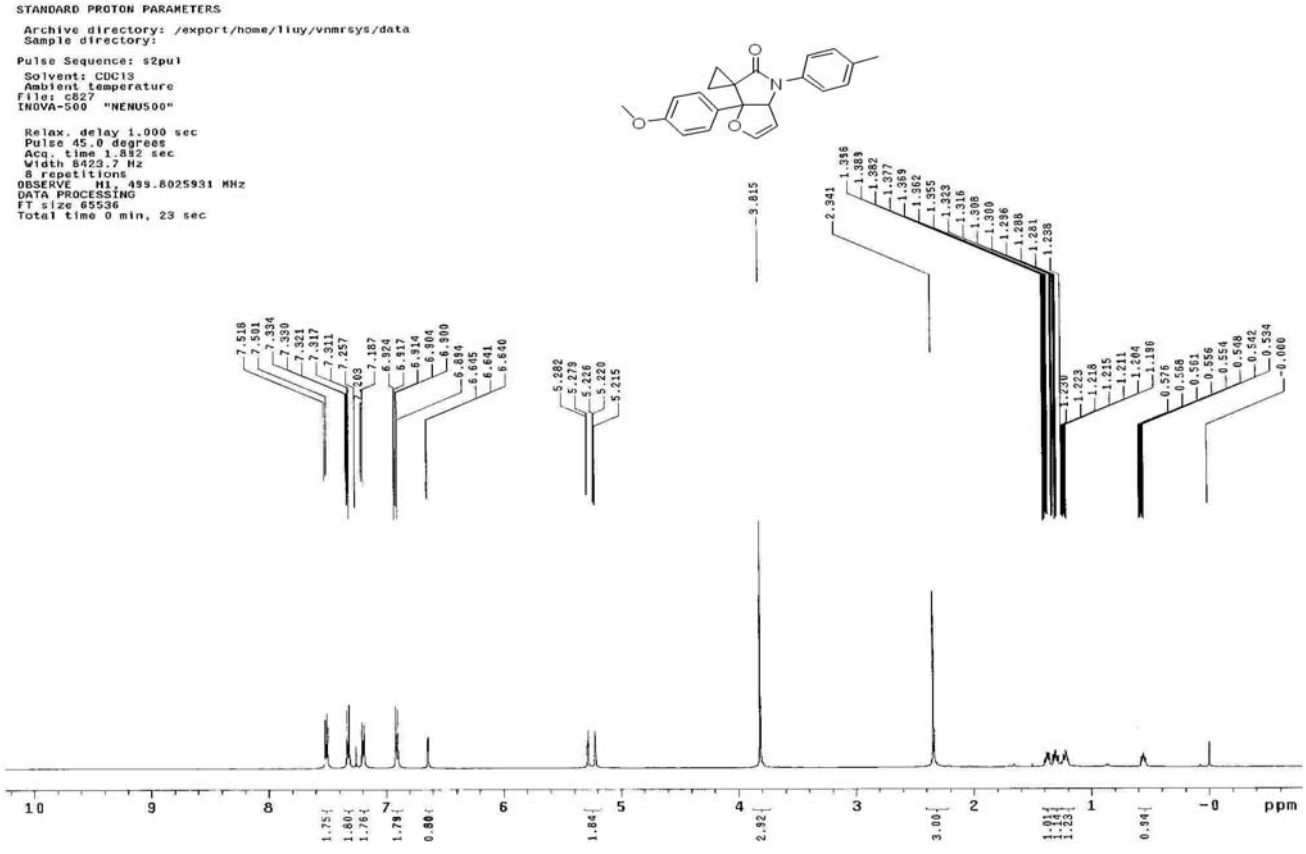

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: f586
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754958 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
173.601
149.581
135.573
134.264
129.285
120.639
99.883
88.243
77.084
76.828
76.577
67.858
31.719
28.587
20.613
12.467
12.232
6.761
220
200
180
160
140
120
100
80
60
40
20
0
ppm

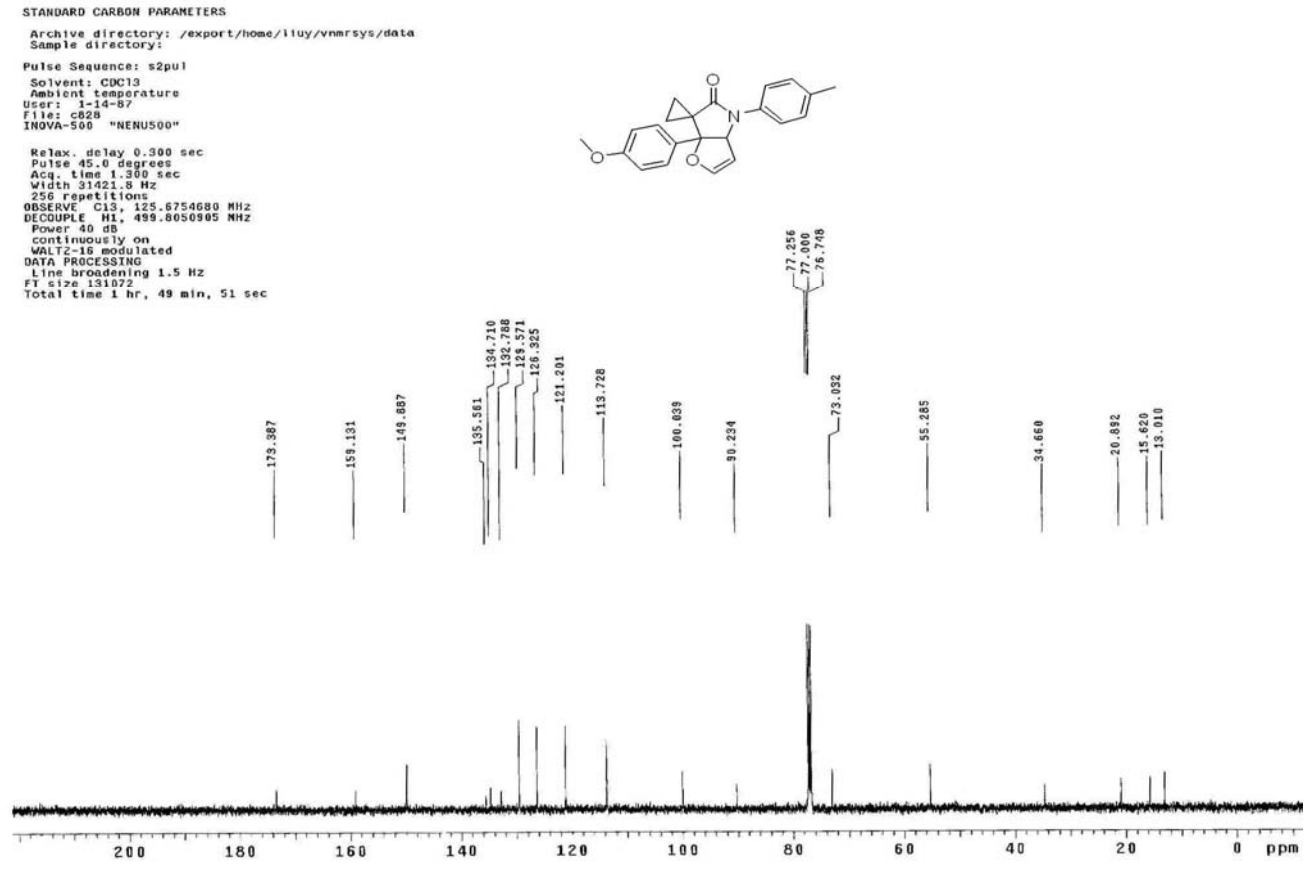
Compound **2i**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liu/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Solvent: CDCl3
Temp. 20.0 C / 293.1 K
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 11999.4 Hz
8 repetitions
OBSERVE H1, 499.8025800 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
ppm

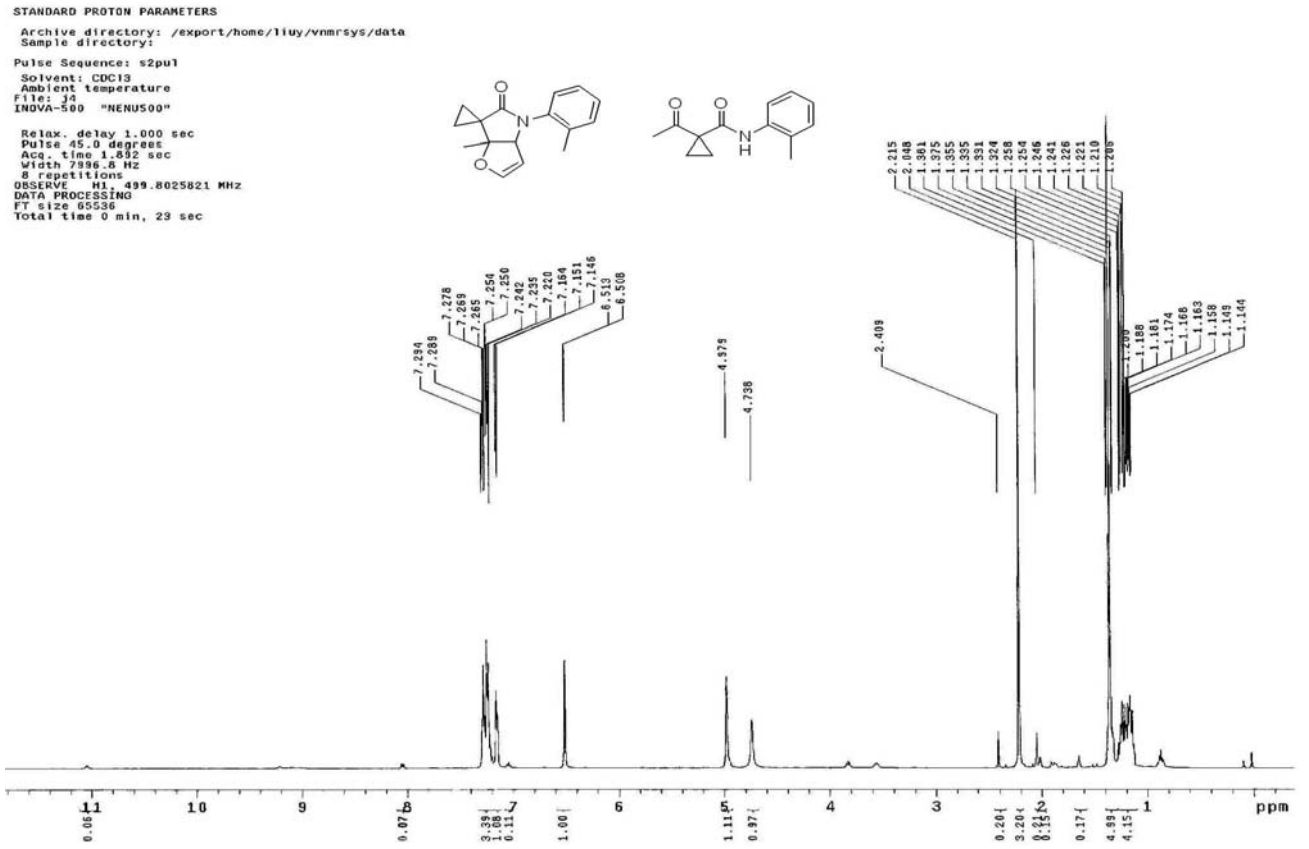

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754627 MHz
DECOUPLE H1, 499.8050505 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 3 hr, 12 min, 26 sec
Cl
ppm

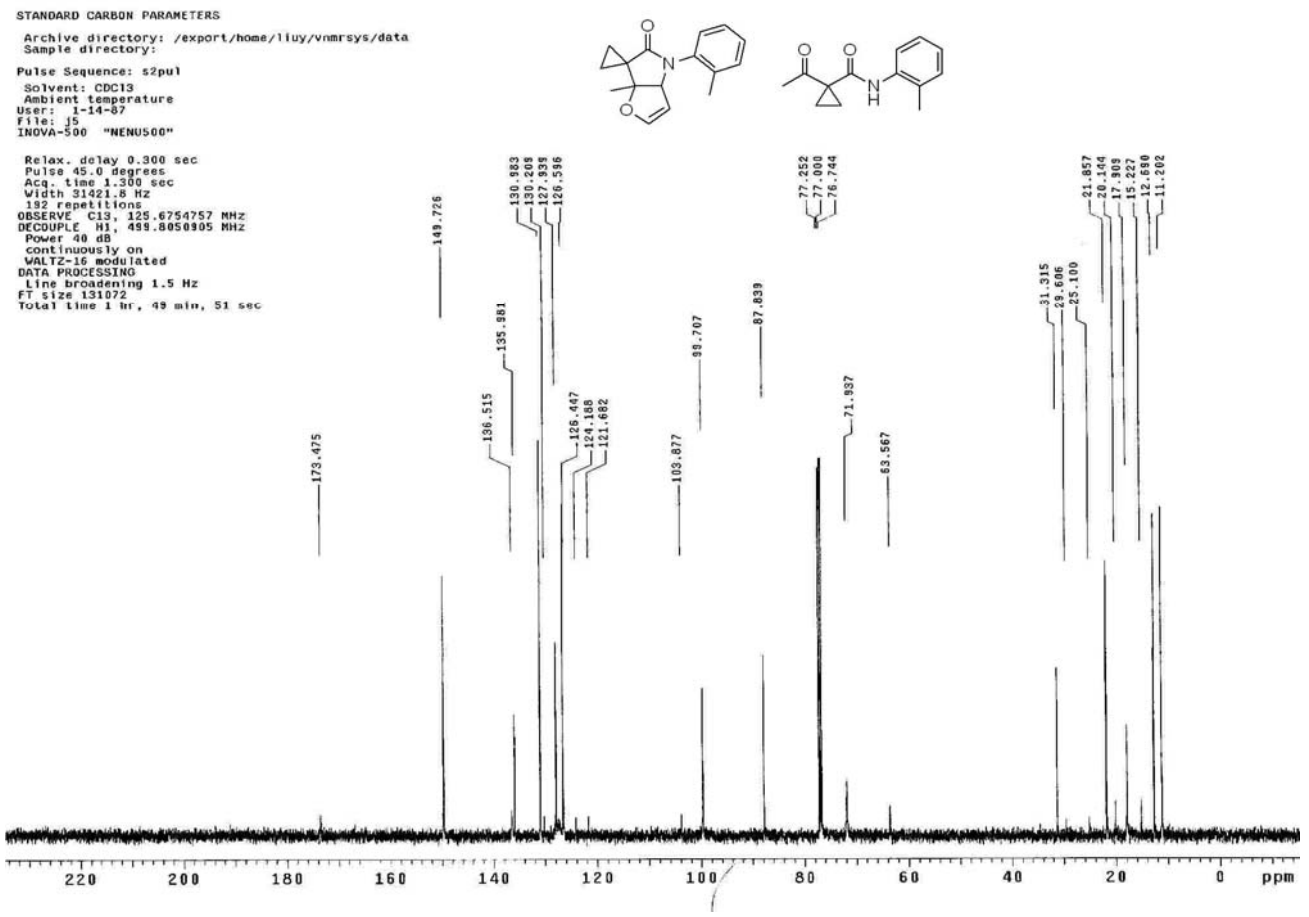
Compound **2j**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: c827
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 8423.7 Hz
8 repetitions
OBSERVE H1, 499.8025931 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

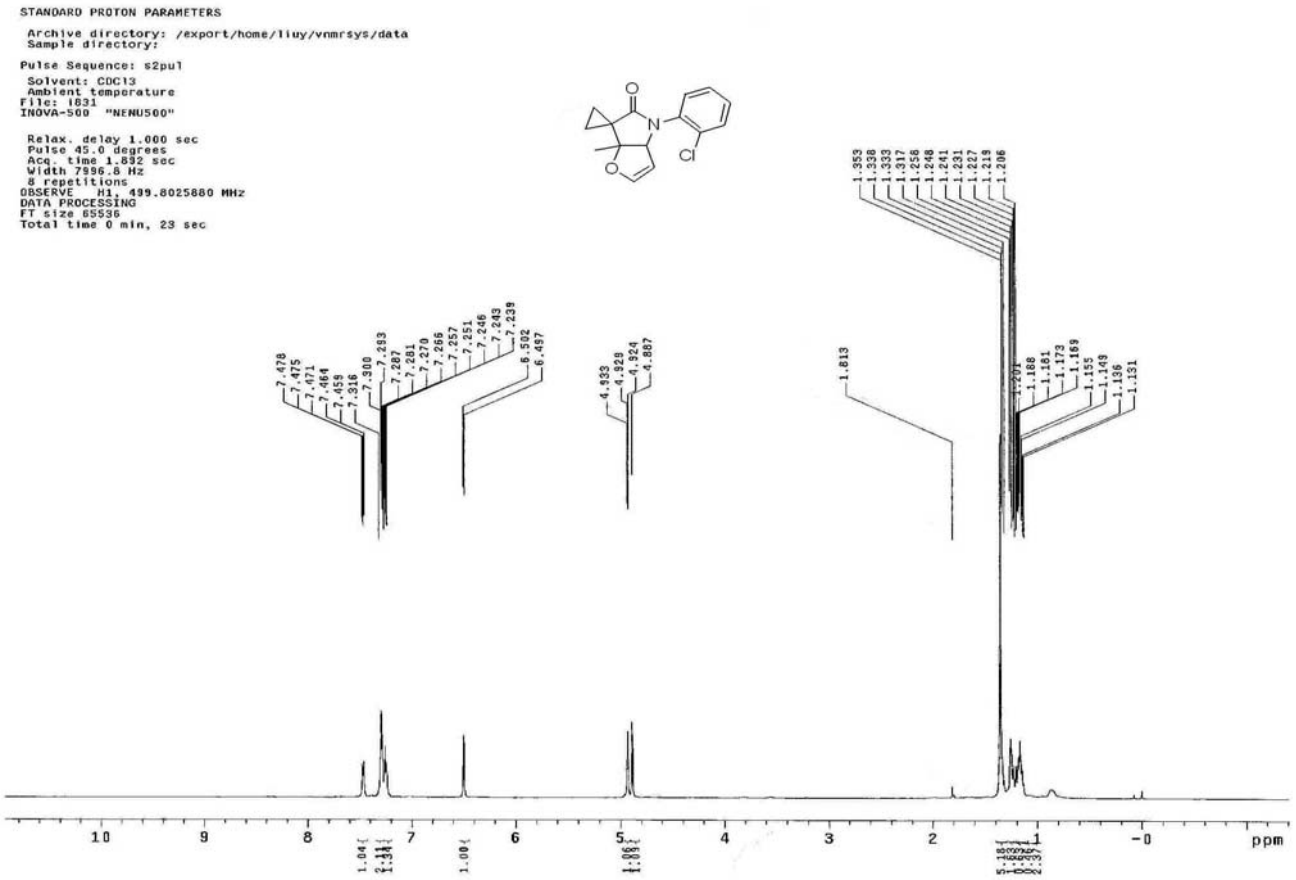

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: c828
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754680 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
ppm

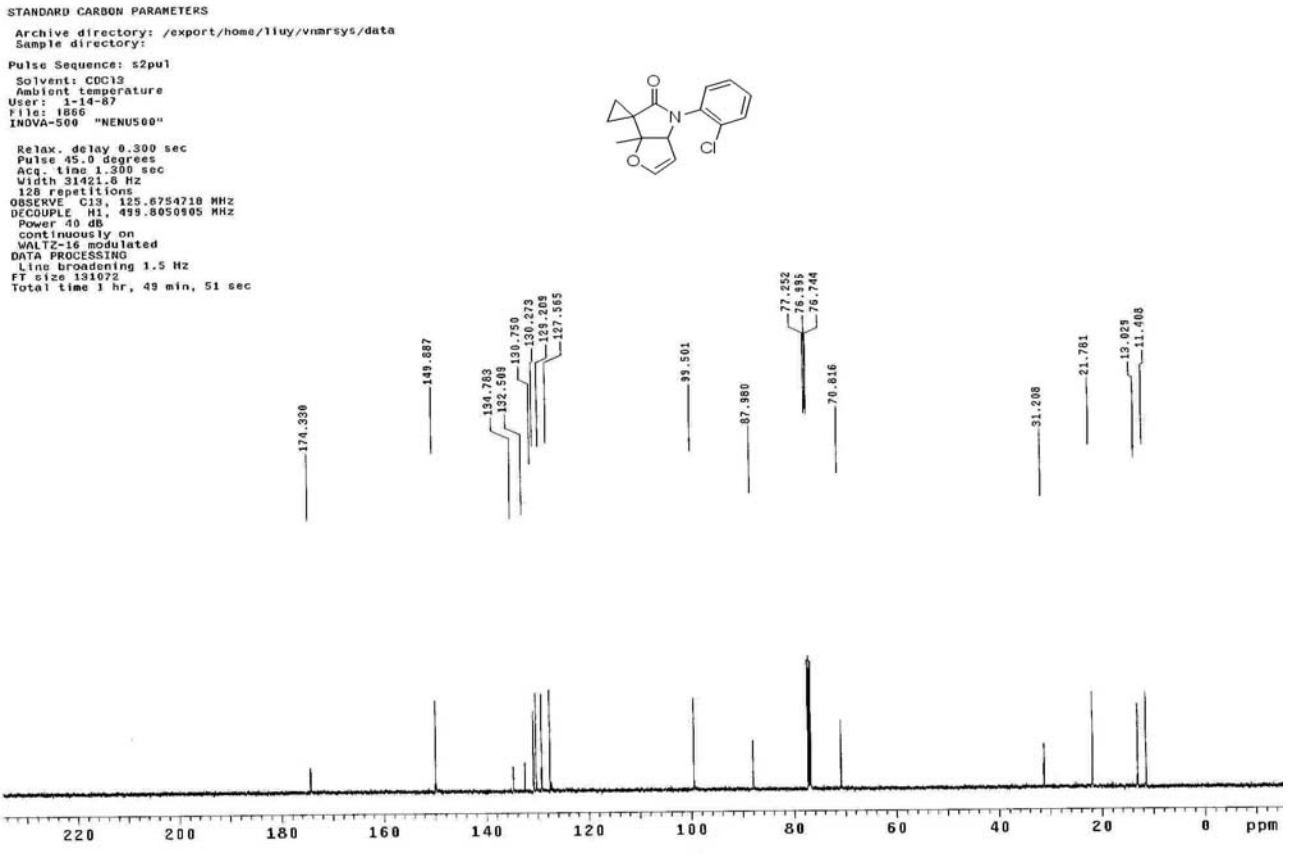
Compound **2k**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j4
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025821 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 29 sec
ppm

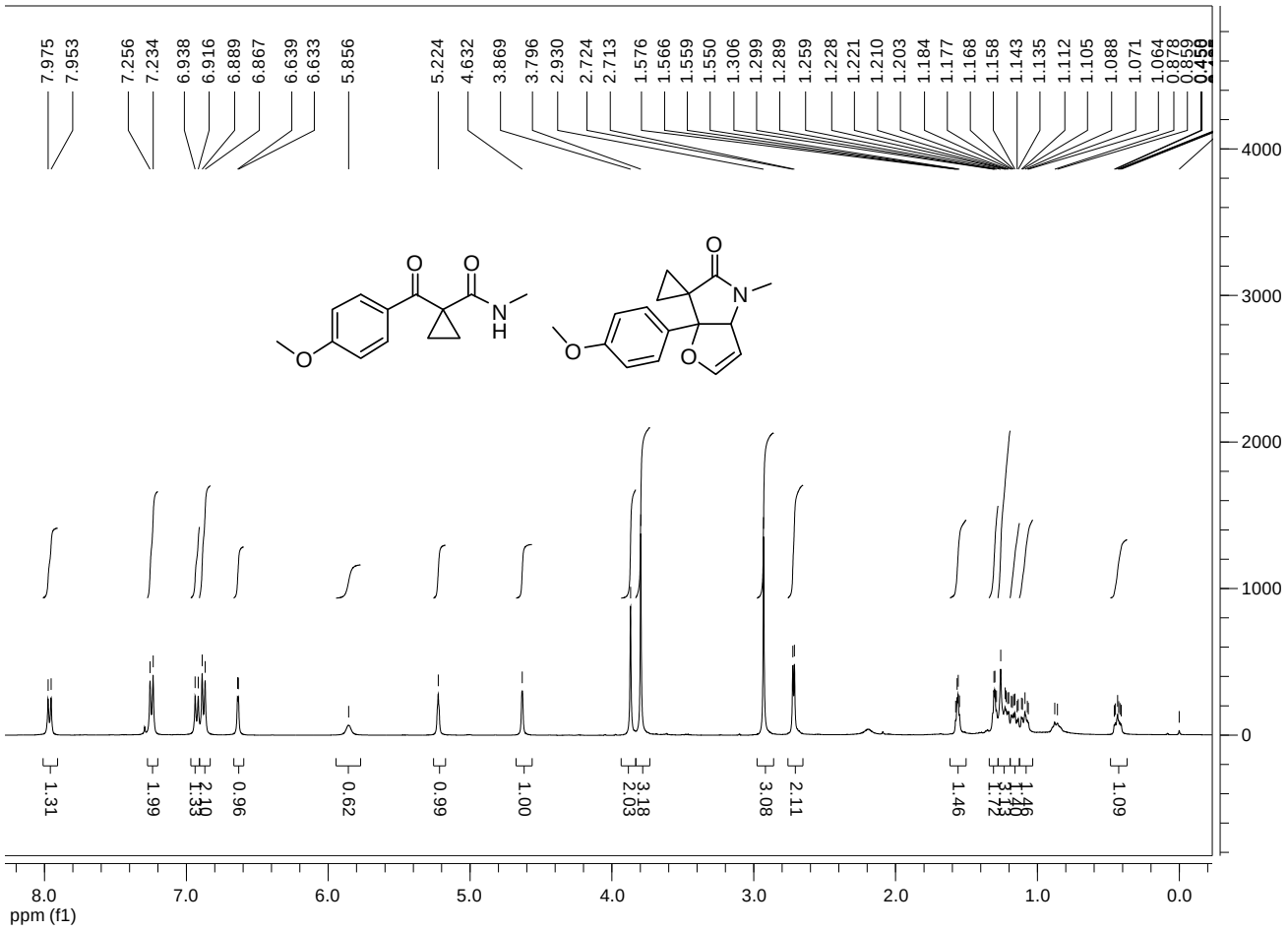

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: j5
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754757 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
ppm

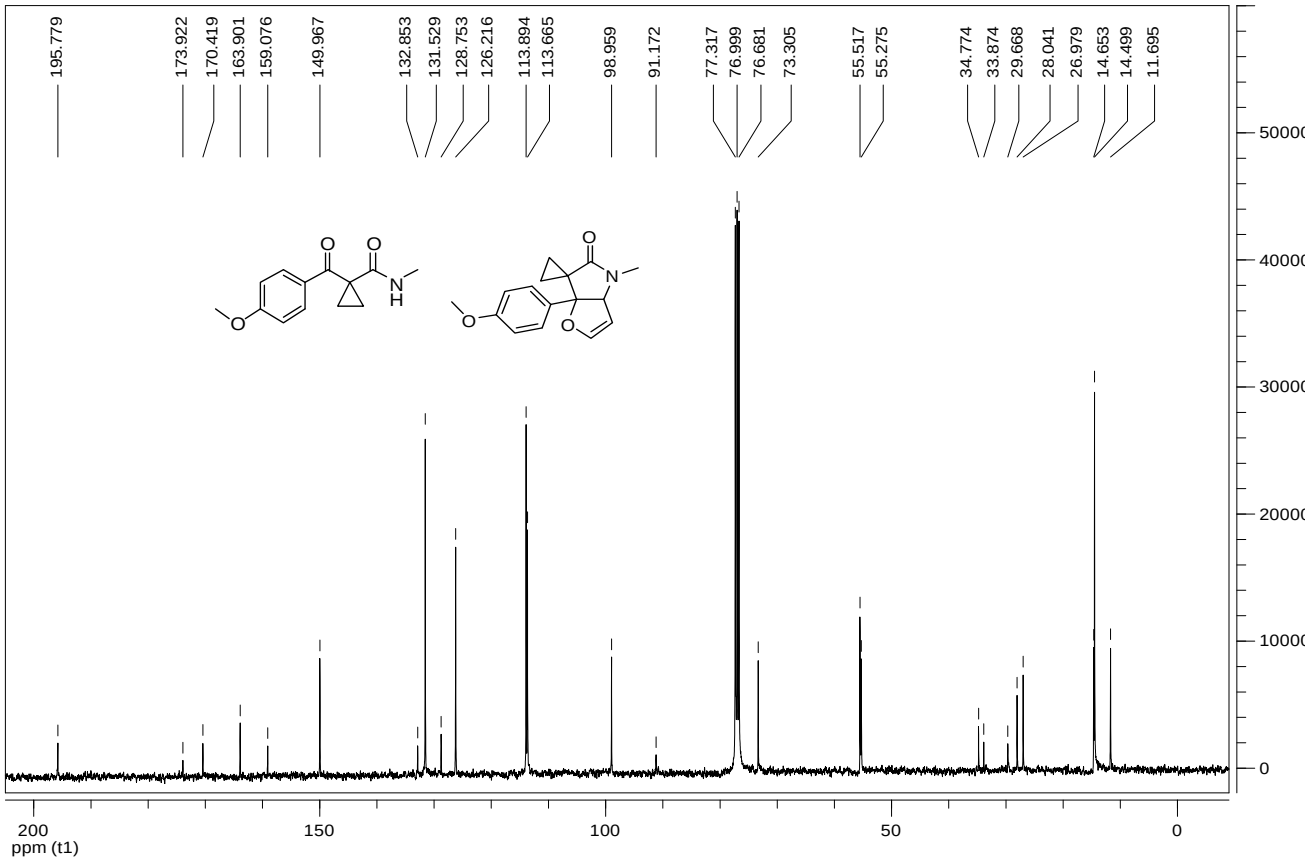
Compound **2l**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1831
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.832 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025880 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

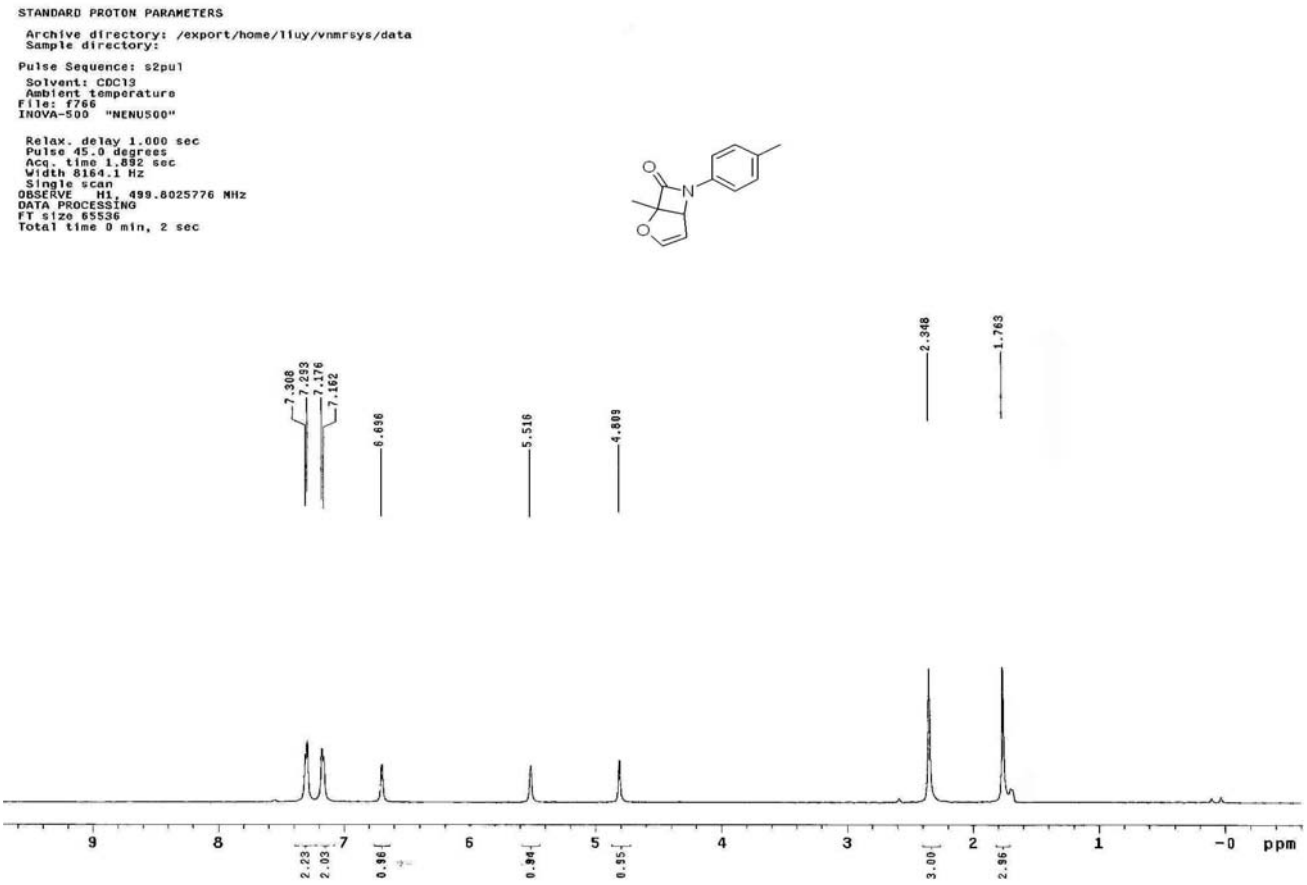

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 1866
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754718 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
ppm

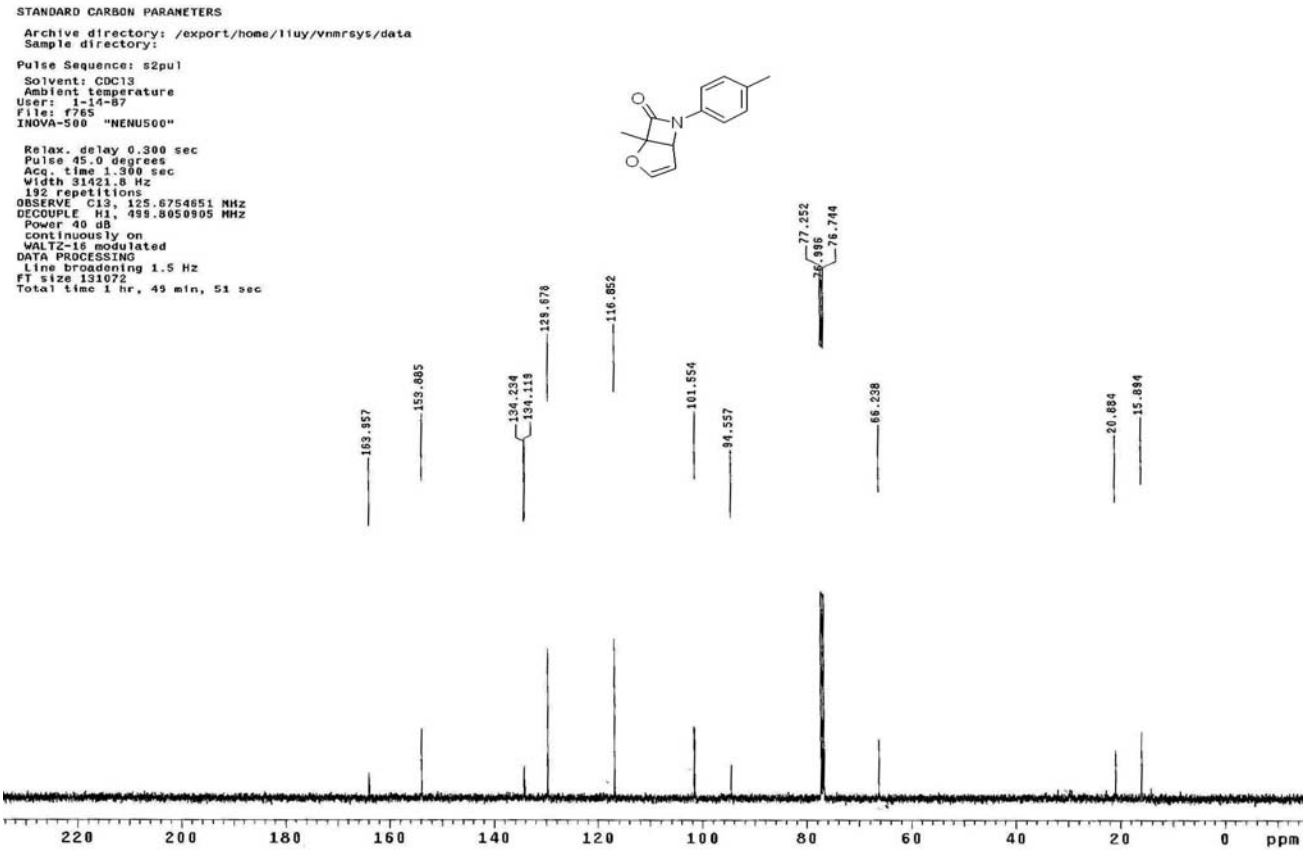
Compound **2m**


7.975
7.953
7.256
7.234
6.938
6.916
6.889
6.867
6.639
6.633
5.856
5.224
4.632
3.869
3.796
2.930
2.724
2.713
1.576
1.566
1.559
1.550
1.306
1.299
1.289
1.259
1.228
1.221
1.210
1.203
1.184
1.177
1.168
1.158
1.143
1.135
1.112
1.105
1.088
1.071
1.064
0.878
0.859
0.458
4000
3000
2000
1000
0
1.31
1.99
2.19
1.33
0.96
0.92
0.99
1.00
2.03
3.18
3.08
2.11
1.46
1.09
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)

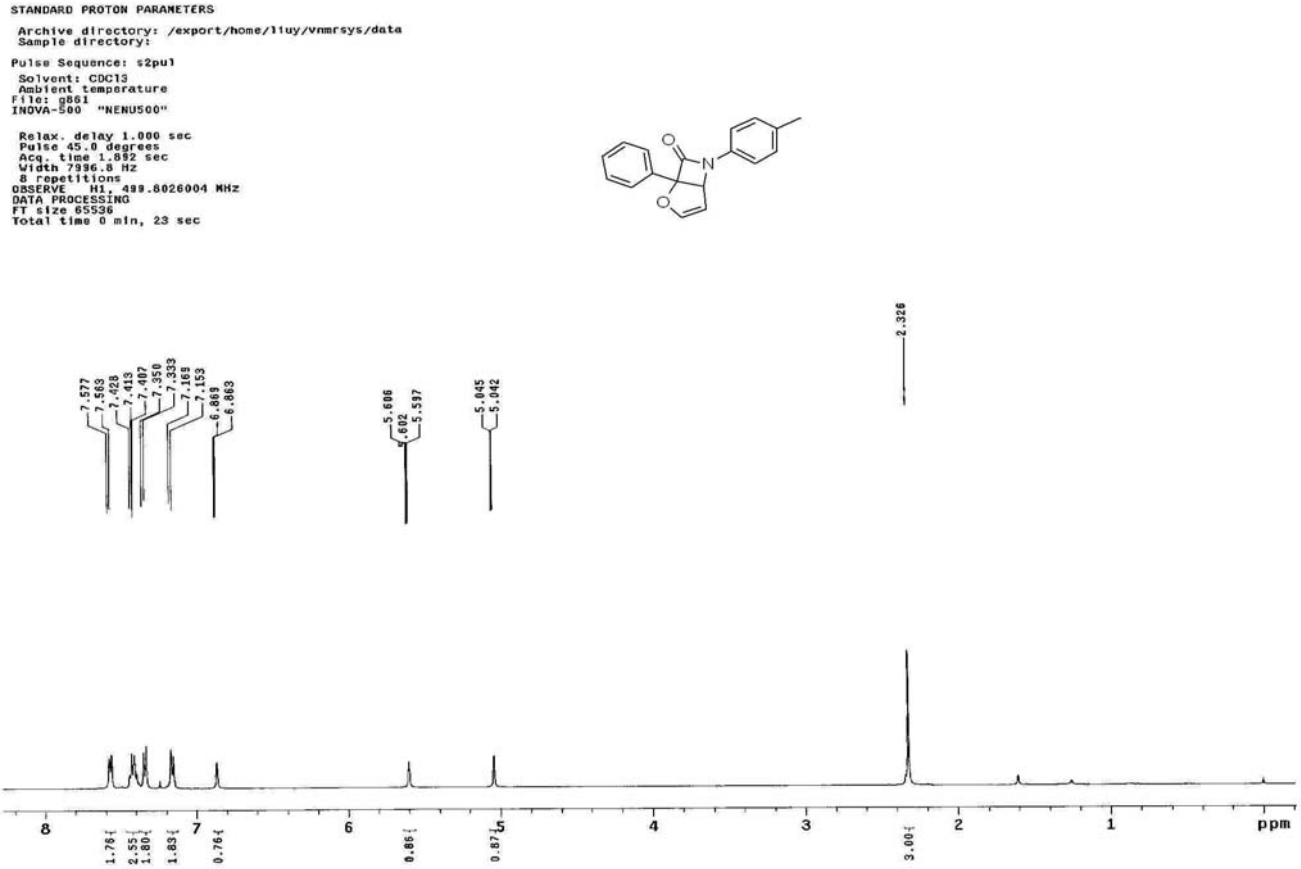

195.779
173.922
170.419
163.901
159.076
149.967
132.853
131.529
128.753
126.216
113.894
113.665
98.959
91.172
77.317
76.999
76.681
73.305
55.517
55.275
34.774
33.874
29.668
28.041
26.979
14.653
14.499
11.695
50000
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)

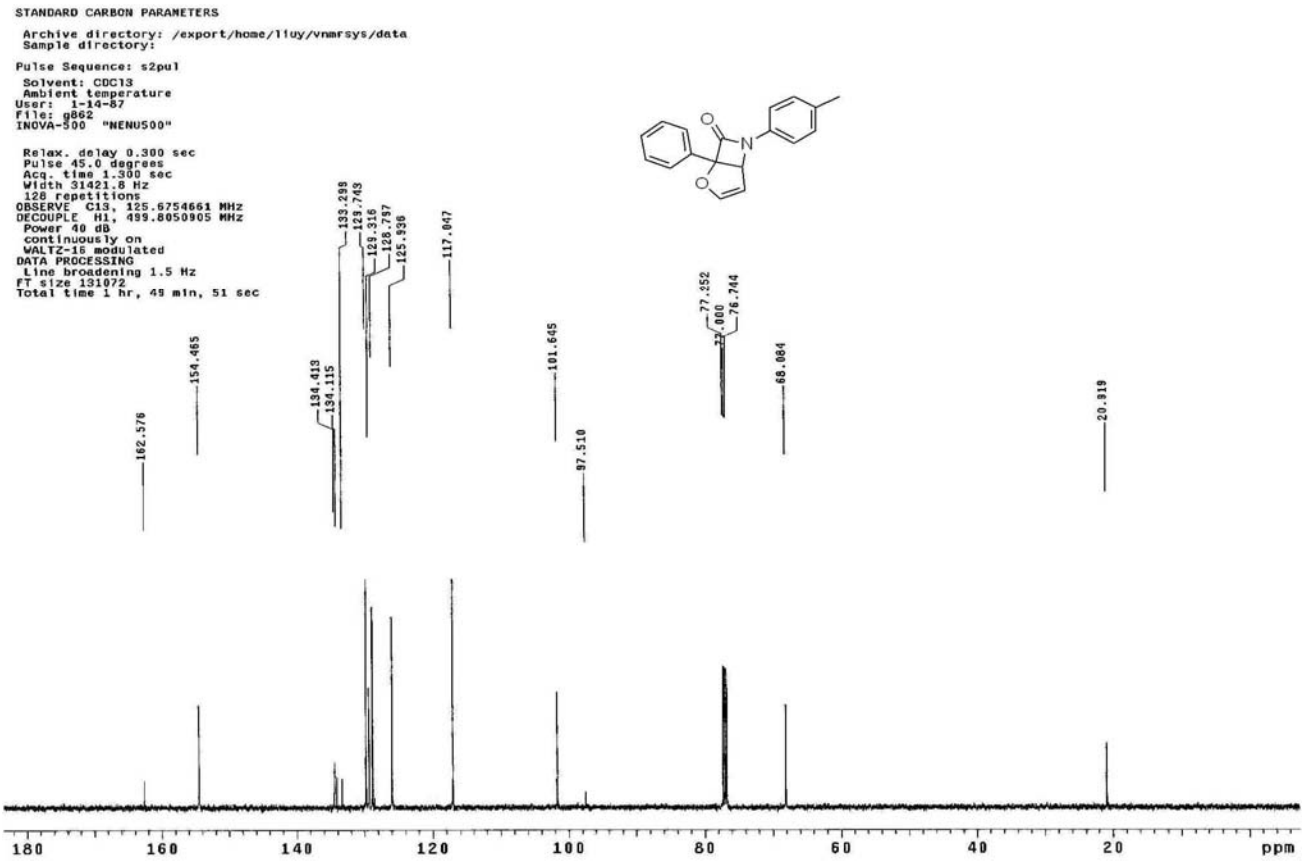
Compound **6a**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: f766
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8164.1 Hz
Single scan
OBSERVE H1, 499.8025776 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 2 sec
7.308
7.293
7.176
7.162
6.696
5.516
4.809
2.348
1.763
2.23
2.03
0.96
0.94
0.95
3.00
2.96
9
8
7
6
5
4
3
2
1
-0
ppm

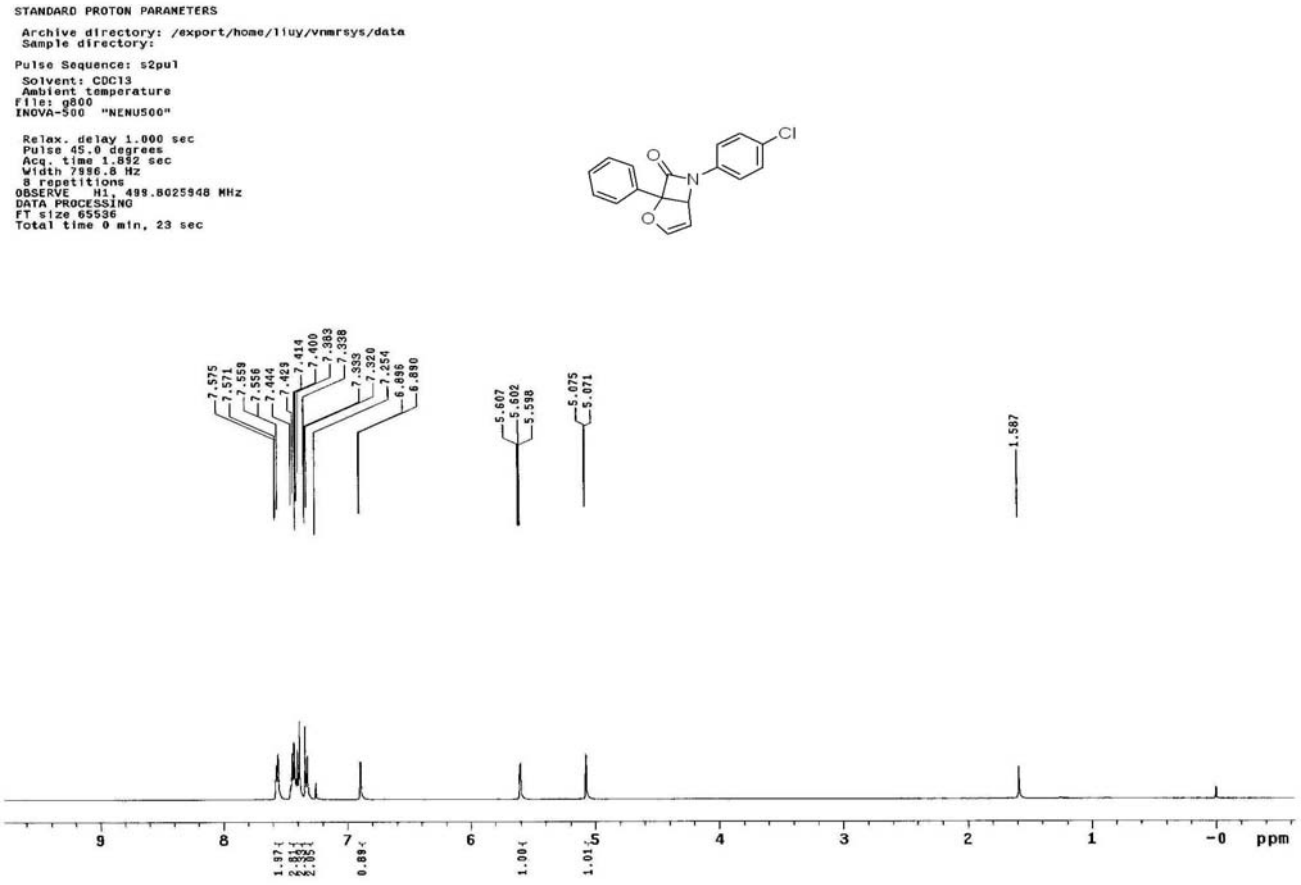

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: f765
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 45 min, 51 sec
77.252
77.000
76.744
129.678
116.852
163.857
153.885
134.234
134.119
101.554
94.557
66.238
20.884
15.884
220
200
180
160
140
120
100
80
60
40
20
0
ppm

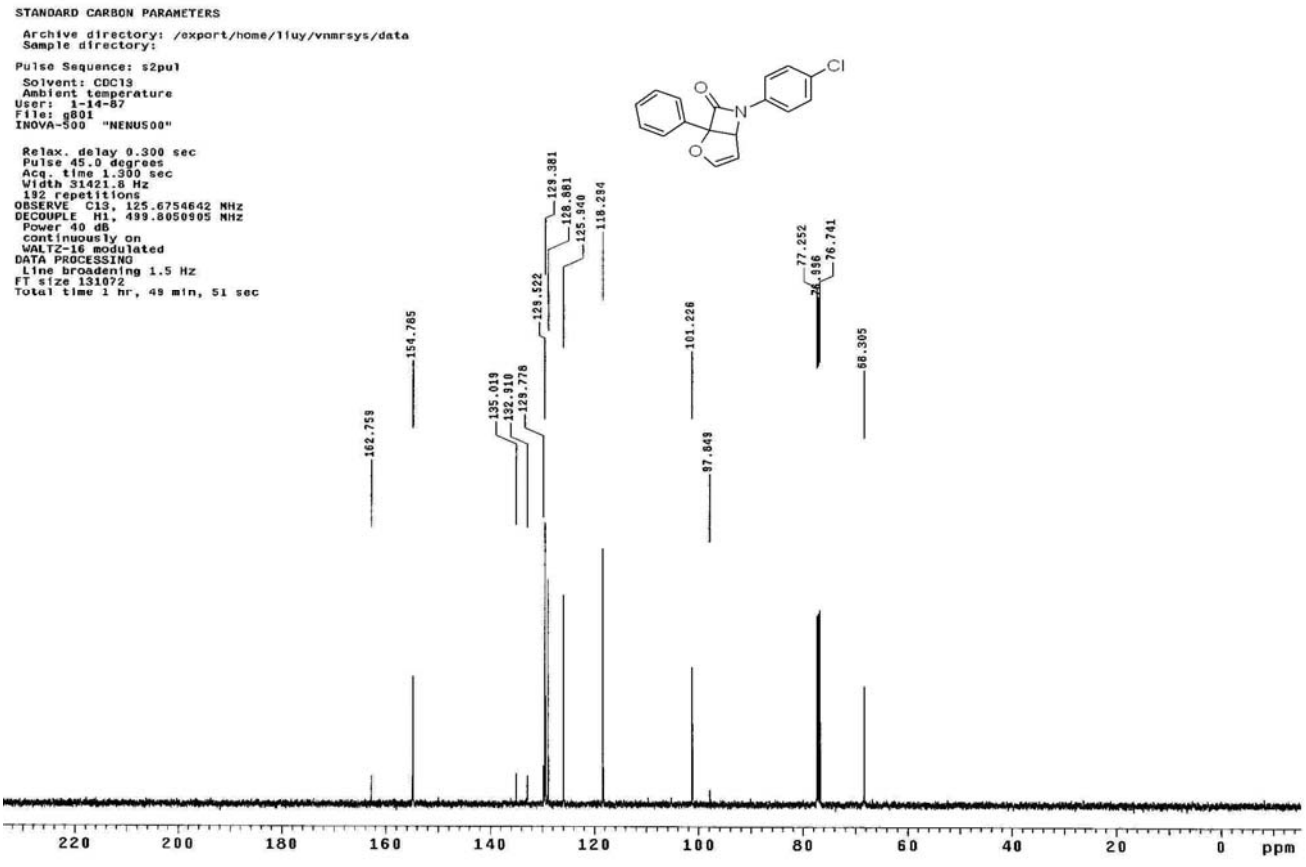
Compound **6b**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g861
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7936.8 Hz
8 repetitions
OBSERVE H1, 499.8026004 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.577
7.563
7.428
7.413
7.407
7.350
7.333
7.169
7.153
6.869
6.863
5.606
5.602
5.597
5.045
5.042
2.326
8
7
6
5
4
3
2
1
ppm
1.78
2.55
1.80
1.83
0.76
0.86
0.87
3.00


STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: g862
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
162.576
154.465
134.413
134.115
133.298
129.743
129.316
128.797
125.936
117.047
101.645
97.510
77.252
77.000
76.744
68.084
20.919
180
160
140
120
100
80
60
40
20
ppm

Compound **6c**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: g800
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7986.8 Hz
8 repetitions
OBSERVE H1, 499.8025948 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
Cl
O
N
O
7.575
7.571
7.558
7.556
7.444
7.423
7.414
7.400
7.383
7.338
7.333
7.320
7.254
6.896
6.890
5.607
5.602
5.598
5.075
5.071
1.587
9
8
7
6
5
4
3
2
1
-0
ppm
1.97
2.83
2.05
0.89
1.00
1.01


STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: g801
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
Cl
O
N
O
129.381
128.881
125.940
118.284
129.522
154.785
135.019
132.910
129.778
162.759
101.226
97.849
77.252
76.936
76.741
68.305
220
200
180
160
140
120
100
80
60
40
20
0
ppm