

Supporting Information

A Facile Synthesis of Isoxazolo[3,4-a]pyrrolizine and Isoxazolo[4,3-c]pyridine Derivatives via Intramolecular Nitrone Cycloaddition Reaction

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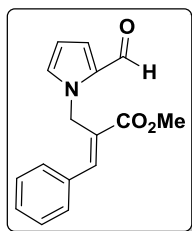
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EXPERIMENTAL SECTION

General Remarks: Melting points were recorded on a Superfit (India) capillary melting point apparatus and were uncorrected. IR spectra were recorded on a Bruker-FT-IR spectrometer using solid samples as KBr plates. For compounds (**3a**, **3h**, **3l**, **6a-l**, **11a**, **12a** and **13a-f**) spectra were recorded ^1H NMR (300 MHz and 400 MHz) and ^{13}C NMR (75 MHz and 100 MHz) in deuteriochloroform (CDCl_3) on a Bruker 300 MHz and 400 MHz spectrometer using tetramethylsilane (TMS, $\delta = 0$) as an internal standard at room temperature. Mass spectra were recorded on Agilent 1200 LC/MS-6110 mass spectrometer.

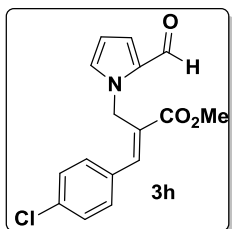
Typical experimental procedure for the synthesis of methyl (*E*)-2-((2-formyl-1*H*-pyrrol-1-yl)methyl)-3-phenylacrylate (**3a**)

A solution of pyrrole-2-carboxaldehyde (**2**) (0.48 g, 4 mmol) and potassium carbonate (1.12 g, 8 mmol) in acetonitrile solvent was stirred for 15 minutes at room temperature. To this solution, methyl 2-(acetoxymethyl)acrylate (**1a**) (1.44 g, 4.8 mmol) was added drop wise till the addition is complete. After the completion of reaction (checked with TLC), acetonitrile was evaporated. The crude mass was added EtOAc (15mL) and water (15 mL). This organic layer was extracted and washed with water (2×10 mL), and brine solution (2×10 mL). The organic layer was dried over anhydrous sodium sulphate. Removal of solvent led to the crude product which was purified through pad of silica gel (100-200 mesh) using ethylacetate and hexanes (1:9) solvent. The pure product was obtained as colourless solid (**3a**).



Yield (%): 96%; m.p.: 112-114 °C; IR (KBr): ν 2188, 1363, 1344 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.77 (s, 3H), 5.47 (s, 2H), 6.20 (t, 1H, $J = 2.7$ Hz), 6.95 – 7.36 (m, 7H), 8.07 (s, 1H), 9.58 (s, 1H); ^{13}C NMR (75 MHz, CDCl_3): δ 45.1, 52.4, 109.9, 124.7, 126.6, 128.8, 129.0, 129.1, 129.7, 131.8, 133.9, 145.1, 167.3, 179.5; MS (m/z): 269 $[\text{M}]^+$; Calculated for $\text{C}_{16}\text{H}_{15}\text{NO}_3$: C, 71.36; H, 5.61; N, 5.20. Found: C, 71.29; H, 5.55; N, 5.26.

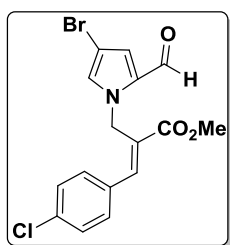
Methyl (*E*)-3-(4-chlorophenyl)-2-((2-formyl-1*H*-pyrrol-1-yl)methyl)acrylate (**3h**)



Yield (%): 87%; m.p.: 116-118 °C; IR (KBr): ν 2179, 1368, 1356 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 3.78 (s, 3H), 5.44 (s, 2H), 6.21 (dd, 1H, $J_1 = 2.4$ Hz, $J_2 = 3.6$ Hz), 6.91 (s, 1H), 6.96 (dd, 1H, $J_1 = 1.6$ Hz, $J_2 = 4$ Hz), 7.18 (d, 2H, $J = 8.8$ Hz), 7.33 (d, 2H, $J = 8.4$ Hz), 7.99 (s, 1H), 9.56 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 45.1, 52.6, 110.1, 125.0, 127.2, 129.2, 129.3, 130.5, 131.8, 132.4, 135.9, 143.8, 167.2, 179.7; DEPT 135 (100 MHz, CDCl_3): 45.3, 52.5, 110.0, 124.9, 129.0, 129.1, 130.4, 143.7, 179.5; MS (m/z): 303 $[\text{M}]^+$; Calculated for $\text{C}_{16}\text{H}_{14}\text{ClNO}_3$: C, 63.27; H, 4.65; N, 4.61; Found: 63.27; H, 4.65; N, 4.61.

Methyl (*E*)-2-((4-bromo-2-formyl-1*H*-pyrrol-1-yl)methyl)-3-(4-chlorophenyl)acrylate (**3l**)

To a stirred solution of methyl (*E*)-3-(4-chlorophenyl)-2-((2-formyl-1*H*-pyrrol-1-yl)methyl)acrylate **3h** (300 mg, 0.99 mmol) in THF (5 mL) at 0 °C was added *N*-bromosuccinimide (174 mg, 0.99 mmol) as a single portion. The reaction mixture was stirred for 1 h at 0 °C. After the completion of reaction (monitored by TLC), THF was evaporated *in vacuo*. The crude mass was added EtOAc (15 mL) and water (15 mL). This organic layer was extracted and washed with water (2×10 mL), and brine solution (2×10 mL). The organic layer was dried over anhydrous sodium sulphate. The organic layer was concentrated led to the crude product and was recrystallized from ethanol afforded the desired methyl (*E*)-2-((4-bromo-2-formyl-1*H*-pyrrol-1-yl)methyl)-3-(4-chlorophenyl)acrylate as a pale yellow solid.

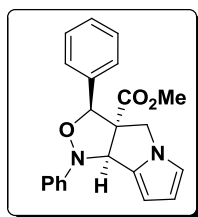


Yield (%): 82%; m.p.: 126-128 °C; IR (KBr): ν 2189, 1372, 1355 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 3.80 (s, 3H), 5.41 (s, 2H), 6.87 (s, 1H), 6.93 (d, 1H, $J = 1.6$ Hz), 7.17 (d, 2H, $J = 8.4$ Hz), 7.35 (d, 2H, $J = 8.8$ Hz), 8.01 (s, 1H); 9.49 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ 45.4, 52.7, 97.4, 125.5, 126.7, 128.6, 129.3, 130.5, 132.0, 132.2, 136.2, 144.4, 166.9, 179.2; DEPT 135 (100 MHz, CDCl_3): 45.2, 52.6, 125.4, 128.4, 129.2, 130.3, 144.2, 179.0; MS (m/z): 381

[M]⁺; Calculated for C₁₆H₁₃BrClNO₃: C, 50.22; H, 3.42; N, 3.66. Found: C, 50.25; H, 3.38; N, 3.72.

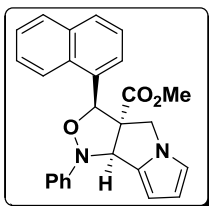
Typical experimental procedure for the synthesis of methyl 1,3-diphenyl-3,3a,4,8b-tetrahydro-1*H*-isoxazolo[3,4-*a*]pyrrolizine-3a-carboxylate (6a)

A mixture of (*Z*)-methyl 2-((2-formyl-1*H*-pyrrol-1-yl)methyl)-3-phenylacrylate (**3a**) (0.56 g, 2 mmol) and *N*-phenylhydroxylamine **4a** (0.33 g, 3 mmol) with 4 Å MS in ethanol (10 mL) was refluxed for 6 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (15 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layer was washed with brine (3 × 15 mL) and dried over anhydrous Na₂SO₄, the organic layer was concentrated and purified by column chromatography using ethyl acetate-hexane (1:9) to afford the pure methyl 1,3-diphenyl-3,3a,4,8b-tetrahydro-1*H*-isoxazolo[3,4-*a*]pyrrolizine-3a-carboxylate **6a**.



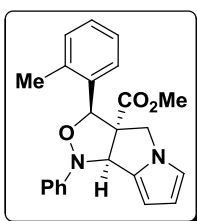
Yield (%): 80%; mp.: 164-166 °C; IR (KBr): ν 1732, 1582, 1353 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 3.74 – 3.79 (m, 4H), 4.12 (d, 1H, *J* = 11.7 Hz), 5.69 (s, 1H), 5.83 (s, 1H), 5.92 (d, 1H, *J* = 3 Hz), 6.23 - 7.36 (m, 12H); ¹³C NMR (75 MHz, CDCl₃): δ 49.5, 53.1, 72.1, 72.7, 84.5, 101.7, 114.0, 114.3, 115.0, 115.1, 118.5, 122.3, 126.8, 128.6, 128.7, 129.0, 129.2, 133.3, 134.6, 148.8, 172.1; MS (m/z): 360 [M]⁺; Calculated for C₂₂H₂₀N₂O₃: C, 73.32; H, 5.59; N, 7.77. Found: C, 73.30; H, 5.56; N, 7.81.

Methyl 3-(naphthalen-1-yl)-1-phenyl-3,3a,4,8b-tetrahydro-1*H*-isoxazolo[3,4-*a*]pyrrolizine-3a-carboxylate (6b)



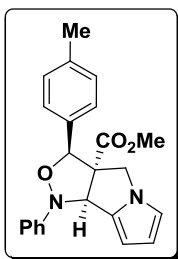
Yield (%): 75%; mp.: 165-167 °C; IR (KBr): ν 1735, 1588, 1343 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.55 (d, 1H, $J = 11.4$ Hz), 3.69 (s, 3H), 4.16 (d, 1H, $J = 11.7$ Hz), 5.95 (s, 1H), 5.99 (d, 1H, $J = 3$ Hz), 6.28 (dd, $J_1 = 11.7$ Hz, $J_2 = 14.7$ Hz, 2H), 6.58 (s, 1H), 7.03 – 7.91 (m, 13H); ^{13}C NMR (75 MHz, CDCl_3): δ 49.3, 53.1, 71.7, 74.2, 81.9, 101.7, 114.0, 114.3, 115.1, 122.5, 122.8, 125.4, 125.5, 125.8, 126.6, 129.0, 129.2, 130.5, 130.9, 132.9, 133.9, 133.6, 148.9, 172.2. MS (m/z): 410 $[\text{M}]^+$; Calculated for $\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}_3$: C, 76.08; H, 5.40; N, 6.82. Found: C, 76.06; H, 5.43; N, 6.85.

Methyl 1-phenyl-3-o-tolyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6c)



Yield (%): 80%; mp.: 161-163 °C; IR (KBr): ν 1715, 1597, 1345 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.21 (s, 3H), 3.66 – 3.72 (m, 4H), 4.26 (d, 1H, $J = 11.7$ Hz), 5.86 (s, 1H), 5.89 (d, 1H, $J = 3.3$ Hz), 5.95 (s, 1H), 6.25 – 7.36 (m, 11H); ^{13}C NMR (75 MHz, CDCl_3): δ 19.3, 49.1, 52.9, 71.2, 73.6, 82.5, 101.7, 113.9, 114.3, 115.1, 122.2, 126.1, 127.3, 128.5, 128.9, 130.7, 132.8, 133.0, 135.8, 148.8, 172.3; MS (m/z): 374 $[\text{M}]^+$; Calculated for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_3$: C, 73.78; H, 5.92; N, 7.48; Found: C, 73.72; H, 5.89; N, 7.52.

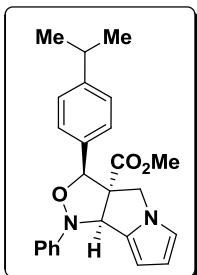
Methyl 1-phenyl-3-p-tolyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6d)



Yield (%): 81%; mp.: 164-166 °C; IR (KBr): ν 1734, 1584, 1338 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.36 (s, 3H), 3.73 (s, 3H), 3.79 (d, 1H, $J = 11.7$ Hz), 4.12 (d, 1H, $J = 11.4$ Hz), 5.65 (s, 1H), 5.83 (s, 1H), 5.91 (d, 1H, $J = 3$ Hz), 6.26 (t, 1H, $J = 3$ Hz), 6.45 (s, 1H), 7.08 – 7.36 (m, 9H); ^{13}C NMR (75 MHz, CDCl_3): δ 21.2, 49.5, 53.0, 72.1, 72.7, 84.6, 101.6, 114.0, 114.3, 115.0,

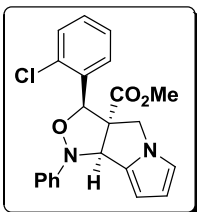
122.2, 126.7, 129.0, 129.3, 131.5, 133.3, 138.5, 148.9, 172.2; MS (m/z): 374 [M]⁺; Calculated for C₂₃H₂₂N₂O₃: C, 73.78; H, 5.92; N, 7.48; Found: C, 73.81; H, 5.96; N, 7.50.

Methyl 3-(4-isopropylphenyl)-1-phenyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6e)



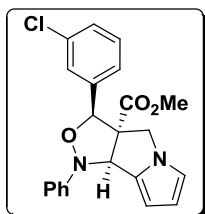
Yield (%): 77%; mp.: 169-171 °C; IR (KBr): ν 1739, 1594, 1323 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 1.26 (d, 6H, *J* = 6.9 Hz), 2.92 (sep, 1H, *J* = 11.4 Hz), 3.73 (s, 1H), 3.84 (d, 1H, *J* = 11.4 Hz), 4.12 (d, 1H, *J* = 11.4 Hz), 5.64 (s, 1H), 5.82 (s, 1H), 5.92 – 7.35 (m, 12 H); ¹³C NMR (75 MHz, CDCl₃): δ 23.8, 23.9, 33.9, 49.5, 53.0, 72.2, 72.7, 84.6, 101.6, 114.0, 114.3, 115.0, 122.2, 126.7, 126.8, 129.0, 131.8, 133.4, 149.0, 149.5, 172.2; MS (m/z): 402 [M]⁺; Calculated for C₂₅H₂₆N₂O₃: C, 74.60; H, 6.51; N, 6.96; Found: C, 74.64; H, 6.55; N, 6.99.

Methyl 3-(2-chlorophenyl)-1-phenyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6f)



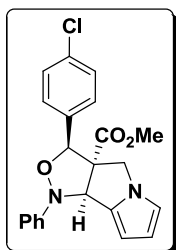
Yield (%): 76%; mp.: 170-172 °C; IR (KBr): ν 1739, 1529, 1363 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 3.63 – 3.66 (m, 4H), 4.43 (d, 1H, *J* = 11.4 Hz), 5.76 (s, 1H), 5.92 (s, 1H), 6.12 - 7.41 (m, 12H); ¹³C NMR (75 MHz, CDCl₃): δ 48.7, 53.0, 71.3, 74.2, 82.6, 101.8, 113.9, 114.4, 115.0, 122.4, 127.1, 128.6, 128.9, 129.5, 129.8, 132.6, 132.7, 133.2, 148.9, 171.7; MS (m/z): 394 [M]⁺; Calculated for C₂₂H₁₉ClN₂O₃: C, 66.92; H, 4.85; N, 7.09; Found: C, 66.88; H, 4.81; N, 7.14.

Methyl 3-(3-chlorophenyl)-1-phenyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6g)



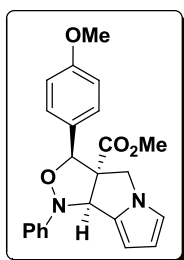
Yield (%): 86%; mp.: 161-163 °C; IR (KBr): ν 1724, 1588, 1353 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.69 – 3.73 (m, 4H), 4.11 (d, 1H, $J = 11.4$ Hz), 5.67 (s, 1H), 5.84 (s, 1H), 5.91 (d, 1H, $J = 3.3$ Hz), 6.26 (t, 1H, $J = 3$ Hz), 6.44 (t, 1H, $J = 3$ Hz), 7.00 – 7.36 (m, 9H); ^{13}C NMR (75 MHz, CDCl_3): δ 49.6, 53.2, 71.9, 72.6, 83.6, 101.9, 114.2, 114.3, 115.1, 122.5, 124.9, 127.0, 128.9, 129.0, 129.9, 133.0, 134.7, 136.8, 148.6, 171.9; MS (m/z): 394 $[\text{M}]^+$; Calculated for $\text{C}_{22}\text{H}_{19}\text{ClN}_2\text{O}_3$: C, 66.92; H, 4.85; N, 7.09; Found: C, 66.94; H, 4.82; N, 7.12.

Methyl 3-(4-chlorophenyl)-1-phenyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6h)



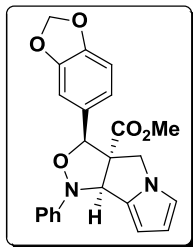
Yield (%): 78%; mp.: 163-165 °C; IR (KBr): ν 1736, 1584, 1352 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.66 – 3.72 (m, 4H), 4.08 (d, $J = 11.4$ Hz, 1H), 5.66 (s, 1H), 5.85 (s, 1H), 5.89 (d, $J = 3.3$ Hz, 1H), 6.25 (t, $J = 3$ Hz, 1H), 6.42 (t, $J = 0.9$ Hz, 1H), 7.00 – 7.35 (m, 9H); ^{13}C NMR (75 MHz, CDCl_3): δ 49.6, 53.1, 71.8, 72.5, 83.8, 101.9, 114.2, 114.3, 115.1, 122.5, 128.3, 128.8, 129.0, 133.1, 133.2, 134.6, 148.6, 171.9; MS (m/z): 394 $[\text{M}]^+$; Calculated for $\text{C}_{22}\text{H}_{19}\text{ClN}_2\text{O}_3$: C, 66.92; H, 4.85; N, 7.09; Found: C, 66.95; H, 4.82; N, 7.13.

Methyl 3-(2-methoxyphenyl)-1-phenyl-3,3a,4,8b-tetrahydro-1H-isoxazolo[3,4-a]pyrrolizine-3a-carboxylate (6i)



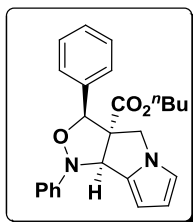
Yield (%) : 72%; mp.: 167-169 °C; IR (KBr): ν 2238, 1543, 1314 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.68 – 3.75 (m, 7H), 4.47 (d, 1H, $J = 11.7$ Hz), 5.66 (s, 1H), 5.89 (s, 1H), 5.92 (d, 1H, $J = 3.3$ Hz), 6.23 (t, 1H, $J = 3$ Hz), 6.44 (s, 1H), 6.86 – 7.48 (m, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 48.1, 52.7, 55.0, 71.9, 74.6, 82.1, 101.3, 109.9, 113.8, 114.5, 114.7, 120.9, 121.9, 123.6, 127.2, 128.9, 129.4, 133.0, 149.4, 155.6, 172.3; MS (m/z): 390 $[\text{M}]^+$; Calculated for $\text{C}_{23}\text{H}_{22}\text{N}_2\text{O}_4$: C, 70.75; H, 5.68; N, 7.17; Found: C, 70.72; H, 5.65; N, 7.21.

Methyl 3-(benzo[d][1,3]dioxol-4-yl)-1-phenyl-3,3a,4,8b-tetrahydro-1*H*-isoxazolo[3,4-*a*]pyrrolizine-3*a*-carboxylate (6j)



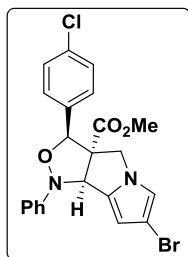
Yield (%): 76%; mp.: 164-166 °C; IR (KBr): ν 1735, 1588, 1343 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 3.72 – 3.84 (m, 4H), 4.11 (d, 1H, $J = 11.1$ Hz), 5.60 (s, 1H), 5.83 – 7.33 (m, 14H). ^{13}C NMR (75 MHz, CDCl_3): δ 49.5, 53.0, 71.9, 72.5, 84.4, 101.2, 101.7, 107.37, 108.4, 114.1, 114.3, 115.1, 120.5, 122.3, 128.2, 129.0, 133.2, 147.9, 148.8, 172.1; MS (m/z): 404. $[\text{M}]^+$; Calculated for $\text{C}_{23}\text{H}_{20}\text{N}_2\text{O}_5$: C, 68.31; H, 4.98; N, 6.93; Found: C, 68.29; H, 4.94; N, 6.97.

Butyl 1,3-diphenyl-3,3a,4,8b-tetrahydro-1*H*-isoxazolo[3,4-*a*]pyrrolizine-3*a*-carboxylate (6k)



Yield (%): 79%; mp.: 161-163 °C; IR (KBr): ν 1732, 1579, 1324 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 0.88 (t, 3H, $J = 7.2$ Hz), 1.18 – 1.25 (m, 2H), 1.45 – 1.50 (m, 2H), 3.73 (d, 1H, $J = 11.7$ Hz), 4.08 – 4.15 (m, 3H), 5.70 (s, 1H), 5.85 (s, 1H), 5.95 – 7.37 (m, 13H); ^{13}C NMR (75 MHz, CDCl_3): δ 13.6, 19.1, 30.3, 49.5, 66.1, 72.4, 73.0, 84.7, 101.5, 114.1, 114.2, 114.9, 122.3, 126.8, 128.6, 128.6, 129.0, 133.4, 134.7, 149.0, 171.7; MS (m/z): 402 $[\text{M}]^+$; Calculated for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_3$: C, 74.60; H, 6.51; N, 6.96; Found: C, 74.60; H, 6.51; N, 6.96.

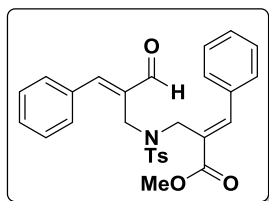
Methyl -7-bromo-3-(4-chlorophenyl)-1-phenyl-1,8b-dihydro-3*H*-isoxazolo[3,4-*a*]pyrrolizine-3*a*(4*H*)-carboxylate (6l)



Yield (%): 69%; mp.: 154-156 °C; IR (KBr): ν 1738, 1575, 1328 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 3.69 (d, 1H, $J = 11.6$ Hz), 3.75 (s, 3H), 4.06 (d, 1H, $J = 11.6$ Hz), 5.65 (s, 1H), 5.83 (s, 1H), 5.91 (t, 1H, $J = 0.08$ Hz), 6.46 (d, 1H, $J = 1.2$ Hz), 7.15 – 7.36 (m, 9H); ^{13}C NMR (100 MHz, CDCl_3): δ 49.8, 53.4, 72.1, 72.8, 83.8, 102.1, 114.4, 114.5, 115.3, 122.7, 125.1, 129.1, 129.2, 130.1, 134.9, 136.9, 148.7, 172.07; MS (m/z): 472 $[\text{M}]^+$; Calculated for $\text{C}_{22}\text{H}_{18}\text{BrClN}_2\text{O}_3$: C, 55.78; H, 3.83; N, 5.91; Found: C, 55.74; H, 3.76; N, 5.95.

Methyl (E)-2-(((N-((E)-2-formyl-3-phenylallyl)-4-methylphenyl)sulfonamido)methyl)-3-phenylacrylate (11a)

To a stirred solution of methyl (E)-2-(((N-((E)-2-(hydroxymethyl)-3-phenylallyl)-4-methylphenyl)sulfonamido)methyl)-3-phenylacrylate **10a** (2.0 g, 4 mmol) in dry DCE (10 mL) at room temperature was added activated MnO_2 (0.83 g, 10.18 mmol) and the reaction was continued at reflux temperature for 3 h. After completion of the reaction as monitored by TLC, the reaction mixture was diluted with DCE and filtered through Celite. The filtrate was evaporated to afford the crude product and further purification by column chromatography over silica gel (60-120 mesh) using EtOAc/hexanes as the eluent furnished (Z)-methyl 2-((N-((E)-2-formyl-3-phenylallyl)-4-methyl phenylsulfonamido)methyl)-3-phenylacrylate **11a** as Colourless solid.

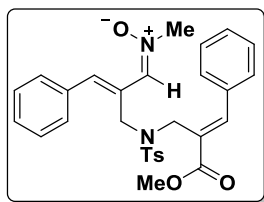


Yield (%): 72%; m.p.: 145-147 °C; IR (KBr): ν 2238, 1543, 1314 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.39 (s, 3H), 3.52 (s, 3H), 4.07 (s, 2H), 4.09 (s, 2H), 7.11 – 7.69 (m, 16H), 9.45 (s, 1H); ^{13}C NMR (75 MHz, CDCl_3): δ 21.5, 43.7, 45.6, 51.9, 128.1, 128.5, 128.8, 129.2, 129.5, 129.7, 130.5, 130.9, 133.2, 133.7, 134.5, 135.5, 141.9, 143.6, 153.8, 167.7, 194.3; MS (m/z) : 489 $[\text{M}]^+$; Calculated for $\text{C}_{28}\text{H}_{27}\text{NO}_5\text{S}$: C, 68.69; H, 5.56; N, 2.86; Found: C, 68.62; H, 5.51; N, 2.94.

Typical experimental procedure for the synthesis of (1Z,2E)-2-(((N-((E)-2-(methoxycarbonyl)-3-phenylallyl)-4-methylphenyl)sulfonamido)methyl)-N-methyl-3-phenylprop-2-en-1-imine oxide (12a)

A suspension of N-Methylhydroxylamine hydrochloride **4b** (0.38 g, 4.60 mmol), 4 Å MS and pyridine (0.44 g, 5.52 mmol) in EtOH (30 ml) was stirred at 0 °C for 1 h. A solution of aldehyde **11a** (1.5 g, 3.06 mmol) in EtOH (20 ml) was added, and the resulting mixture was

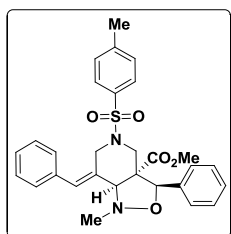
stirred for 12 h. at room temperature. After completion of the reaction as monitored by TLC, the solvent was evaporated under reduced pressure, the residue was chromatographed on a silicagel column with AcOEt as eluent to give (75%) of nitrone **12a**.



Yield (%): (75%); IR (KBr): ν 3060, 2950, 1415 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): δ 2.37 (s, 3H), 3.36 (s, 3H), 3.41 (s, 3H), 4.02 (d, 2H, $J = 1.6$ Hz), 4.09 (s, 1H), 7.04 – 7.59 (m, 17H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.6, 45.4, 47.4, 52.0, 54.6, 124.8, 126.9, 127.3, 127.6, 128.2, 128.3, 128.7, 129.7, 129.9, 130.5, 134.2, 134.7, 136.1, 137.9, 143.9, 144.7, 167.3; MS (m/z): 518 [M].⁺ Calculated for $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_5\text{S}$: C, 67.16; H, 5.83; N, 5.40; Found: C, 67.13; H, 5.78; N, 5.46.

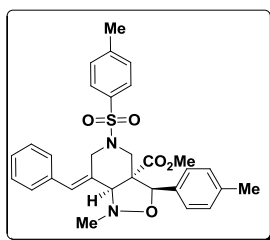
Typical experimental procedure for the synthesis of (*E*)-methyl 7-benzylidene-1-methyl-3-phenyl-5-tosyl octahydroisoxazolo[4,3-*c*]pyridine-3a-carboxylate (**13a**)

A mixture of (*Z*)-methyl 2-((*N*-((*E*)-2-formyl-3-phenylallyl)-4-methylphenylsulfonamido)methyl)-3-phenylacrylate **11a** (1 g, 2 mmol) *N*-methylhydroxyl amine hydrochloride **4b** (0.26 g, 3 mmol) and pyridine (0.24 g, 3 mmol) with 4Å MS in ethanol (10 mL) was refluxed for 6 h. After the completion of the reaction as indicated by TLC, the reaction mixture was concentrated and the resulting crude mass was diluted with water (15 mL) and extracted with ethyl acetate (3×15 mL). The combined organic layer was washed with brine (3×15 mL) and dried over anhydrous Na_2SO_4 , the organic layer was concentrated and purified by column chromatography on silica gel (60-120 mesh), using ethyl acetate-hexane (1:9) to afford the pure compound i.e., (*E*)-Methyl 7-benzylidene-1-methyl-3-phenyl-5-tosyl octahydroisoxazolo[4,3-*c*]pyridine-3a-carboxylate **13a**.



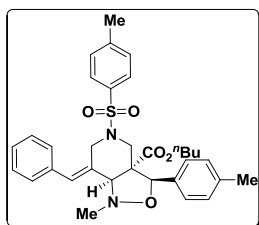
Yield (%): 83%; mp.: 170-172 °C; IR (KBr): ν 1735, 1588, 1343 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.43 (s, 3H), 2.65 (d, 1H, $J = 12.3$ Hz), 2.1 (s, 3H), 3.00 (d, 1H, $J = 12.3$ Hz), 3.62 (d, 1H, $J = 12$ Hz), 3.82 (s, 3H), 4.00 (s, 1H), 4.60 (d, 1H, $J = 12.6$ Hz), 5.44 (s, 1H), 6.66 (s, 1H), 7.23 – 7.42 (m, 14H); ^{13}C NMR (75 MHz, CDCl_3): δ 21.4, 44.1, 44.2, 45.9, 52.9, 60.7, 82.8, 126.2, 127.6, 127.9, 128.0, 128.3, 128.5, 128.6, 128.9, 129.6, 132.9, 133.2, 134.7, 135.1, 143.7, 170.8.; MS (m/z): 518 $[\text{M}]^+$; Calculated for $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_5\text{S}$: C, 67.16; H, 5.83; N, 5.40; Found: C, 67.13; H, 5.79; N, 5.45.

(E)-Methyl 7-benzylidene-1-methyl-3-p-tolyl-5-tosyloctahydroisoxazolo[4,3-c]pyridine-3a-carboxylate (13b)



Yield (%): 80%; mp.: 172-174 °C; IR (KBr): ν 1667, 1624, 1594 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 2.39 (s, 3H), 2.44 (s, 3H), 2.68 (d, 1H, $J = 12$ Hz), 2.81 (s, 3H), 3.02 (d, 1H, $J = 12.6$ Hz), 3.64 (d, 1H, $J = 11.7$ Hz), 3.80 (s, 3H), 4.01 (s, 1H), 4.59 (d, 1H, $J = 12.3$ Hz), 5.41 (s, 1H), 6.65 (s, 1H), 7.07 – 7.45 (m, 13H); ^{13}C NMR (75 MHz, CDCl_3): δ 21.2, 21.5, 44.1, 44.2, 45.6, 52.8, 60.8, 82.9, 126.1, 127.6, 127.8, 128.2, 128.4, 128.5, 128.9, 129.0, 129.6, 131.3, 133.0, 135.1, 138.3, 143.6, 170.4; MS (m/z): 532 $[\text{M}]^+$; Calculated for $\text{C}_{30}\text{H}_{32}\text{N}_2\text{O}_5\text{S}$: C, 67.65; H, 6.06; N, 5.26; Found: C, 67.61; H, 6.02; N, 5.30.

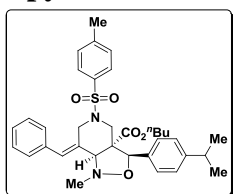
(E)-Butyl 7-benzylidene-1-methyl-3-p-tolyl-5-tosyloctahydroisoxazolo[4,3-c]pyridine-3a-carboxylate (13c)



Yield (%): 82%; mp.: 165-167 °C; IR (KBr): ν 1735, 1651 1614 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3): δ 0.92 (t, 3H, $J = 7.2$ Hz), 1.38 (q, 2H, $J = 7.5$ Hz), 1.63 – 1.68 (m, 2H), 2.39 (s, 3H), 2.43 (s, 3H), 2.66 (d, 1H, $J = 11.7$ Hz), 2.81 (s, 3H), 2.98 (t, 1H, $J = 12.3$ Hz), 3.65 (d, 1H, $J = 11.7$ Hz), 3.98 (s, 1H), 4.22 (t, 2H, $J = 6.3$ Hz), 4.57 (d, 1H, $J = 12.3$ Hz), 5.43 (s, 1H), 6.63 (s,

1H), 7.09 – 7.45 (m, 13H); ¹³C NMR (75 MHz, CDCl₃): δ 13.6, 19.0, 21.2, 21.5, 30.4, 44.0, 44.2, 45.7, 60.7, 65.8, 82.8, 126.1, 127.7, 127.8, 128.3, 128.5, 128.8, 128.9, 129.6, 131.6, 132.9, 135.1, 138.2, 143.6, 170.0; MS (m/z): 574 [M]⁺; Calculated for C₃₃H₃₈N₂O₅S: C, 68.96; H, 6.66; N, 4.87; Found: C, 68.93; H, 6.69; N, 4.90.

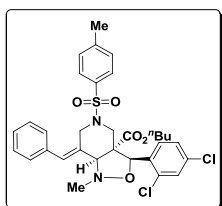
(E)-Butyl 7-benzylidene-3-(4-isopropylphenyl)-1-methyl-5-tosylocta hydroisoxazolo[4,3-c]pyridine-3a-carboxylate (13d)



Yield (%): 84%; mp.: 162-164 °C; IR (KBr): ν 1667, 1624, 1594 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 0.91 (t, 3H, J = 7.2 Hz), 1.28 – 1.43 (m, 8H), 1.63 – 1.68 (m, 2H), 2.43 (s, 3H), 2.66 (t, 1H, J = 12 Hz), 2.80 (s, 3H), 2.90 – 3.00 (m, 2H), 3.67 (d, 1H, J = 11.7Hz), 3.98 (s, 1H), 4.23 (t, 2H, J = 6.6 Hz), 4.58 (d, 1H, J = 12.6 Hz), 5.43 (s, 1H), 6.64 (s, 1H), 7.14 – 7.44 (m, 13H).

¹³C NMR (75 MHz, CDCl₃): δ 13.6, 19.0, 21.5, 23.9, 24.0, 30.4, 33.9, 44.1, 45.9, 60.7, 65.8, 82.8, 126.3, 127.6, 127.8, 128.3, 128.5, 128.8, 129.6, 131.9, 132.9, 135.2, 143.6, 149.2, 170.1; MS (m/z): 602 [M]⁺; Calculated for C₃₅H₄₂N₂O₅S: C, 69.74; H, 7.02; N, 4.65; Found: C, 69.72; H, 7.05; N, 4.67.

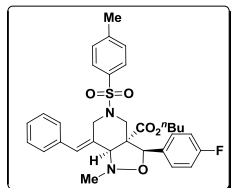
(E)-Butyl 7-benzylidene-3-(2,4-dichlorophenyl)-1-methyl-5-tosyloctahydroisoxazolo[4,3-c]pyridine-3a-carboxylate (13e)



Yield (%): 86%; mp.: 167-169 °C; IR (KBr): ν 1668, 1624, 1593 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 0.91 (t, 3H, J = 7.5 Hz), 1.35 – 1.42 (m, 2H), 1.61 – 1.68 (m, 2H), 2.43 (s, 3H), 2.65 (d, 2H, J = 11.2 Hz), 2.78 (s, 3H), 2.96 (d, 2H, J = 12.3 Hz), 3.64 (d, 1H, J = 11.4 Hz), 3.98 (s, 1H), 4.07 – 4.31 (m, 2H), 4.52 (d, 1H, J = 12.3 Hz), 5.77 (s, 1H), 6.65 (s, 1H), 7.17 – 7.48 (m, 12H); ¹³C NMR (75 MHz, CDCl₃): δ 13.6, 19.0, 21.5, 30.2, 43.7, 44.1, 45.5, 59.6, 66.1, 77.9, 79.7, 126.8, 127.6, 127.7, 127.9, 128.5, 128.8, 129.4, 129.5, 129.6, 132.1, 132.8, 133.2, 133.6,

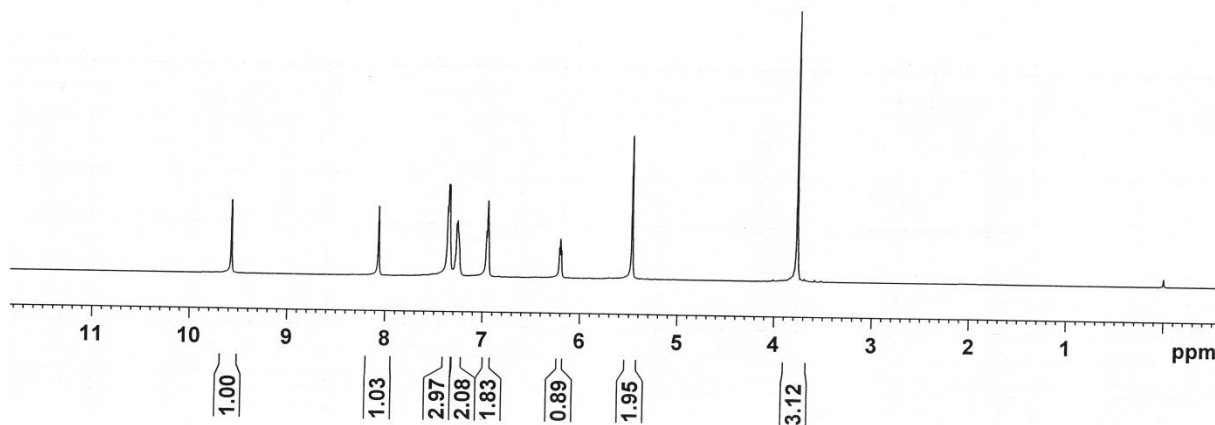
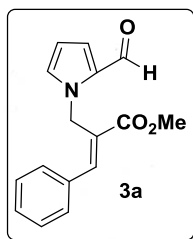
134.8, 134.9, 143.7, 169.6; MS (m/z): 628 [M]⁺; Calculated for C₃₂H₃₄Cl₂N₂O₅S: C, 61.05; H, 5.44; N, 4.45; Found: C, 61.03; H, 5.47; N, 4.48.

(E)-Butyl 7-benzylidene-3-(4-fluorophenyl)-1-methyl-5-tosyl octahydroisoxazolo[4,3-c]pyridine-3a-carboxylate (13f)



Yield (%): 84%; mp.: 165-167 °C; IR (KBr): ν 1741, 1646, 1615 cm⁻¹; ¹H NMR (300 MHz, CDCl₃): δ 0.92 (t, 3H, *J* = 7.2 Hz), 1.35 – 1.45 (m, 2H), 1.59 – 1.71 (m, 2H), 2.42 (s, 3H), 2.59 (d, 1H, *J* = 11.7 Hz), 2.79 (s, 3H), 2.97 (d, 2H, *J* = 11.4 Hz), 3.58 (d, 1H, *J* = 11.7 Hz), 3.95 (s, 1H), 4.23 (t, 2H, *J* = 6.6 Hz), 4.58 (d, 1H, *J* = 12.6 Hz), 5.42 (s, 1H), 6.65 (s, 1H), 7.02 – 7.48 (m, 13H); ¹³C NMR (75 MHz, CDCl₃): δ 13.6, 19.0, 21.5, 30.4, 44.0, 44.1, 46.0, 60.4, 65.9, 82.0, 115.1, 115.3, 127.6, 127.8, 127.9, 128.0, 128.1, 128.5, 128.8, 129.6, 130.8, 130.8, 132.9, 133.3, 135.1, 143.7, 161.0, 164.3, 170.1. MS (m/z): 578 [M]⁺; Calculated for C₃₂H₃₅FN₂O₅S: C, 66.42; H, 6.10; N, 4.84. Found: C, 66.45; H, 6.14; N, 4.87.

9.577
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 7.271
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 6.949
 6.213
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 3.767



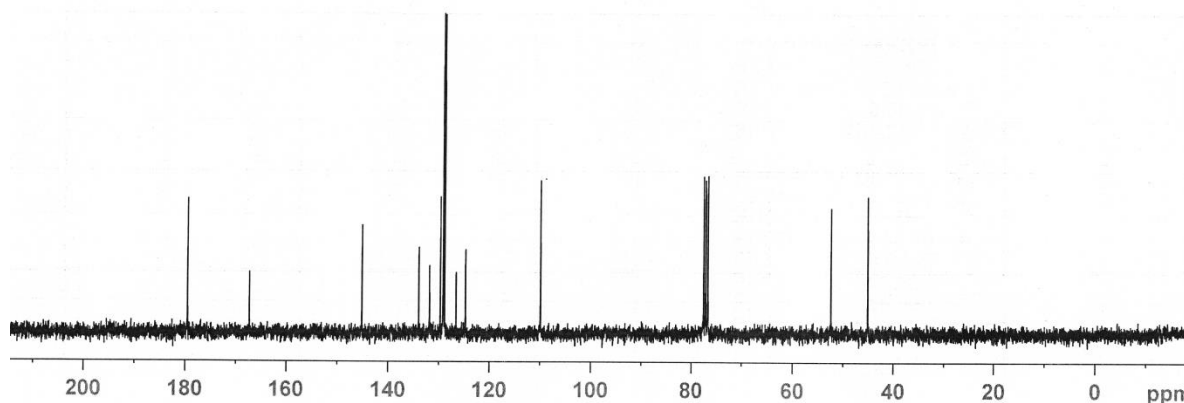
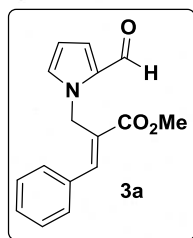
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 TE 300.0 K
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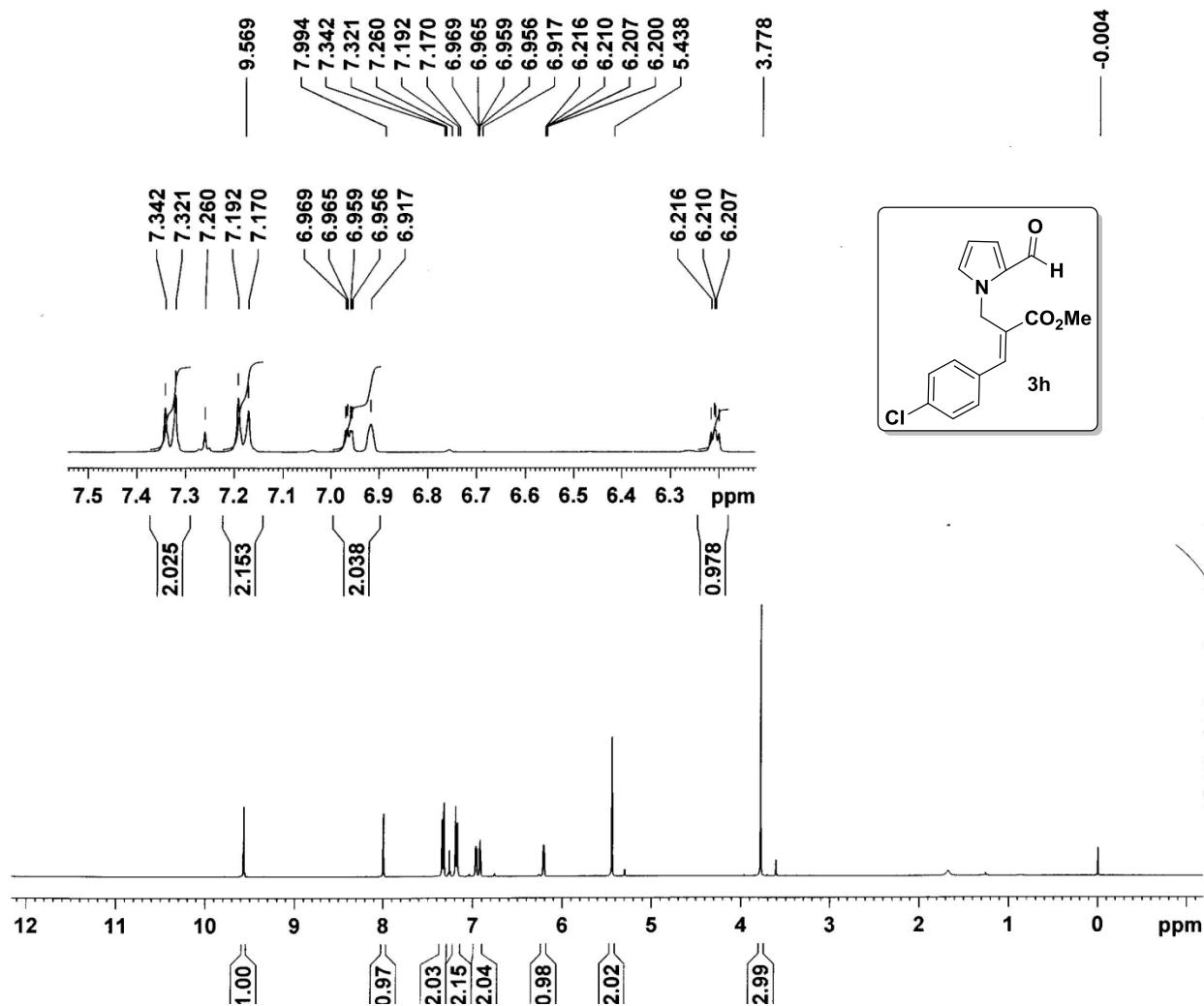
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PROTON CDC13 {D:\MB} KOPAL 1



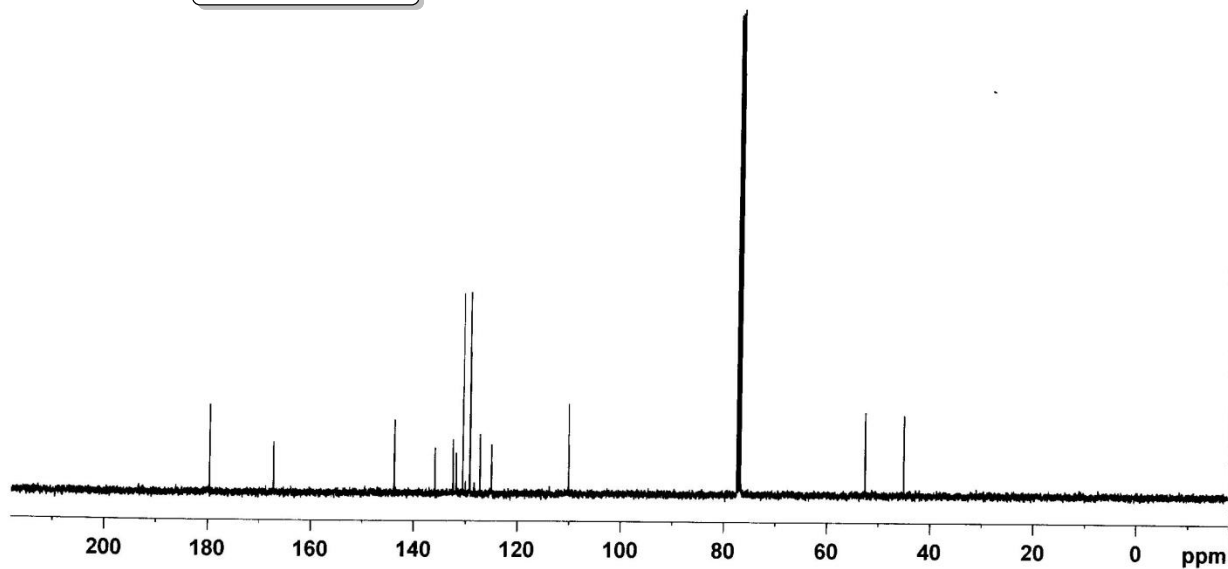
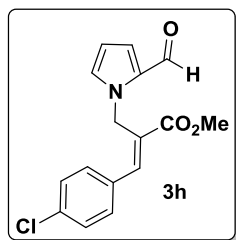
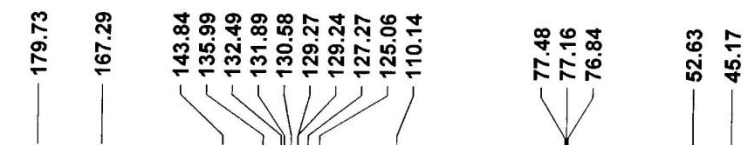
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TD0 1

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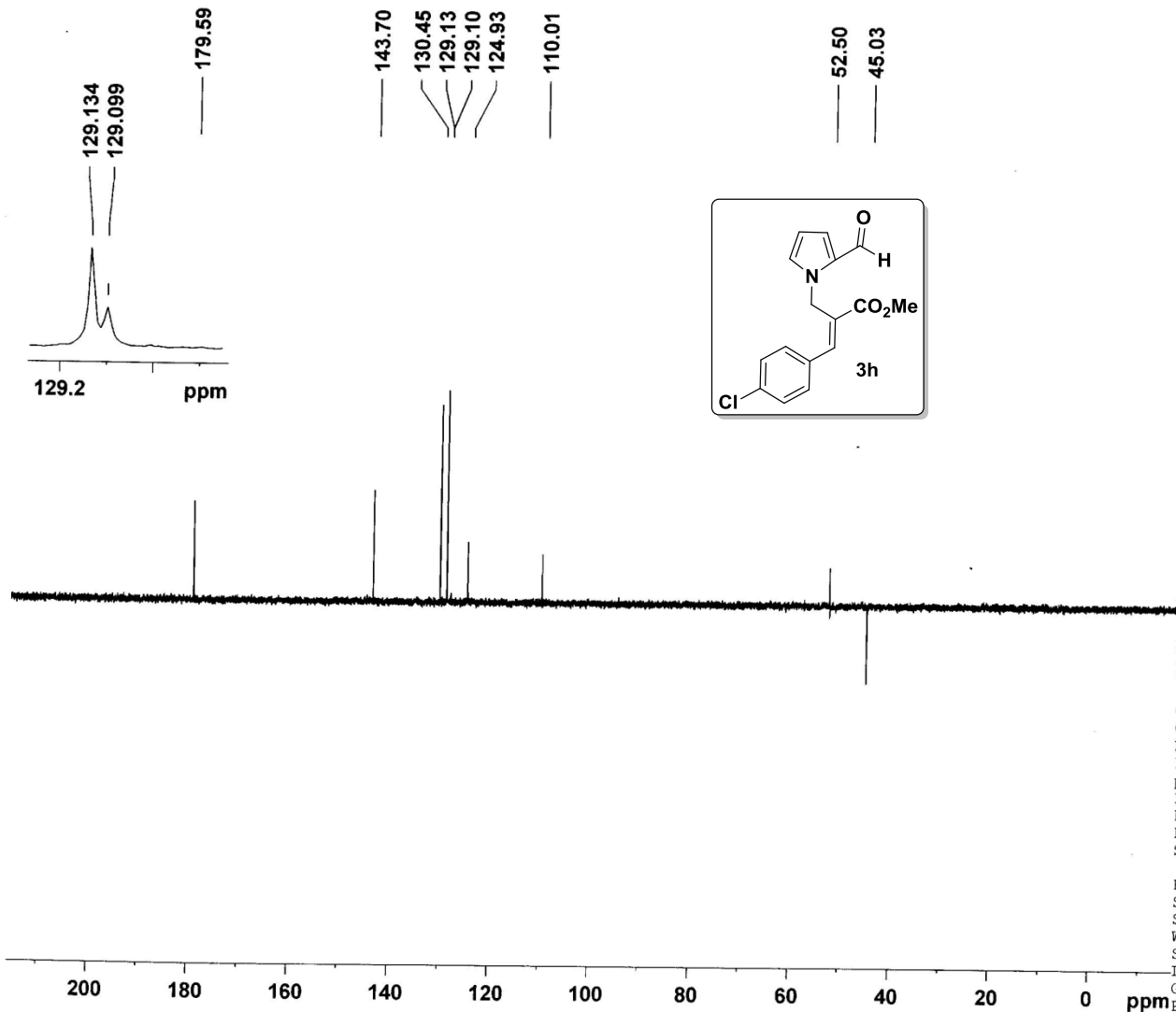
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PL2 -3.00 dB
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F2 - Processing parameters
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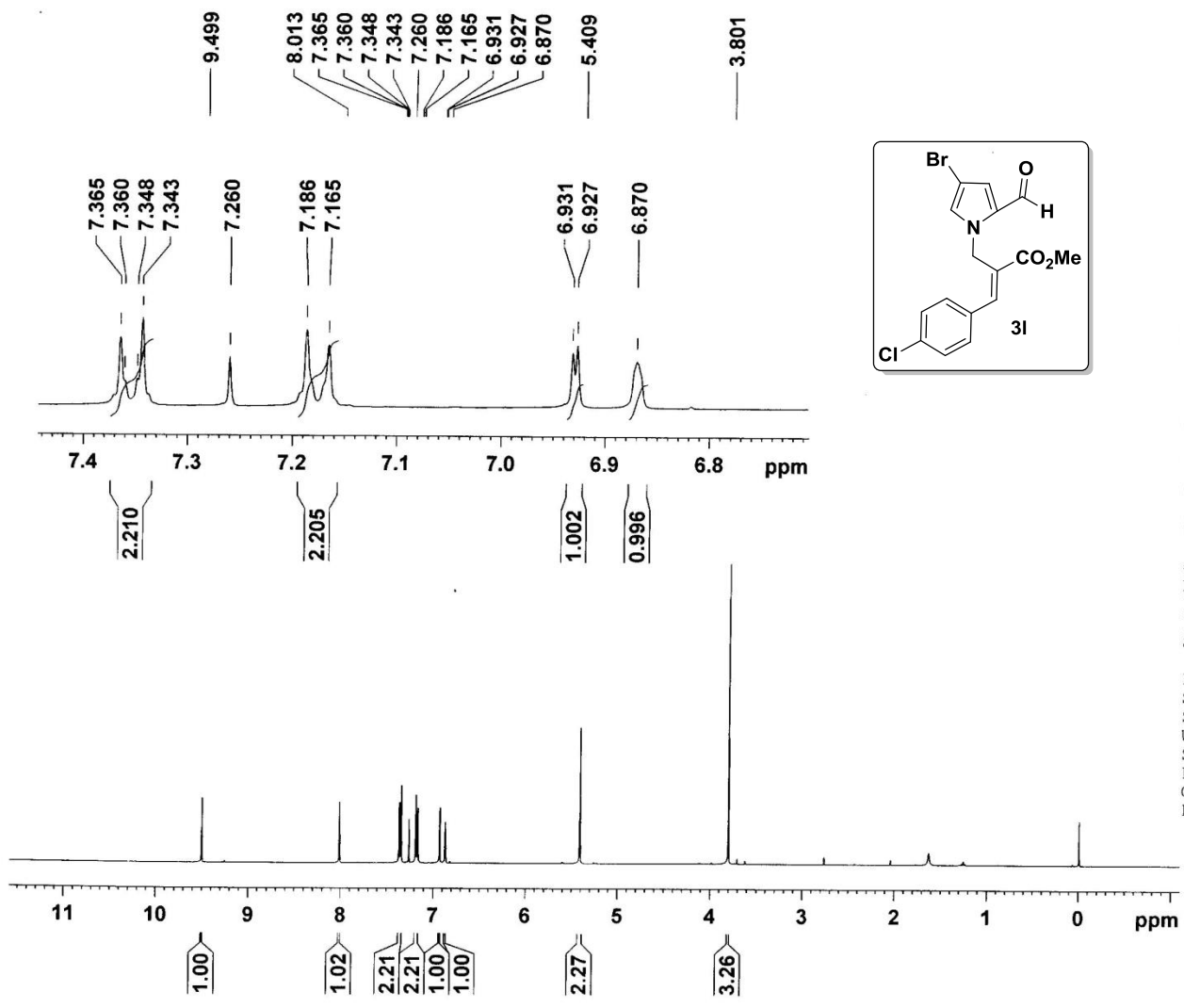
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PROTON CDC13 {D:\MB} KOPAL 1



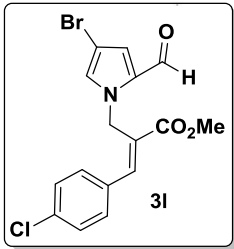
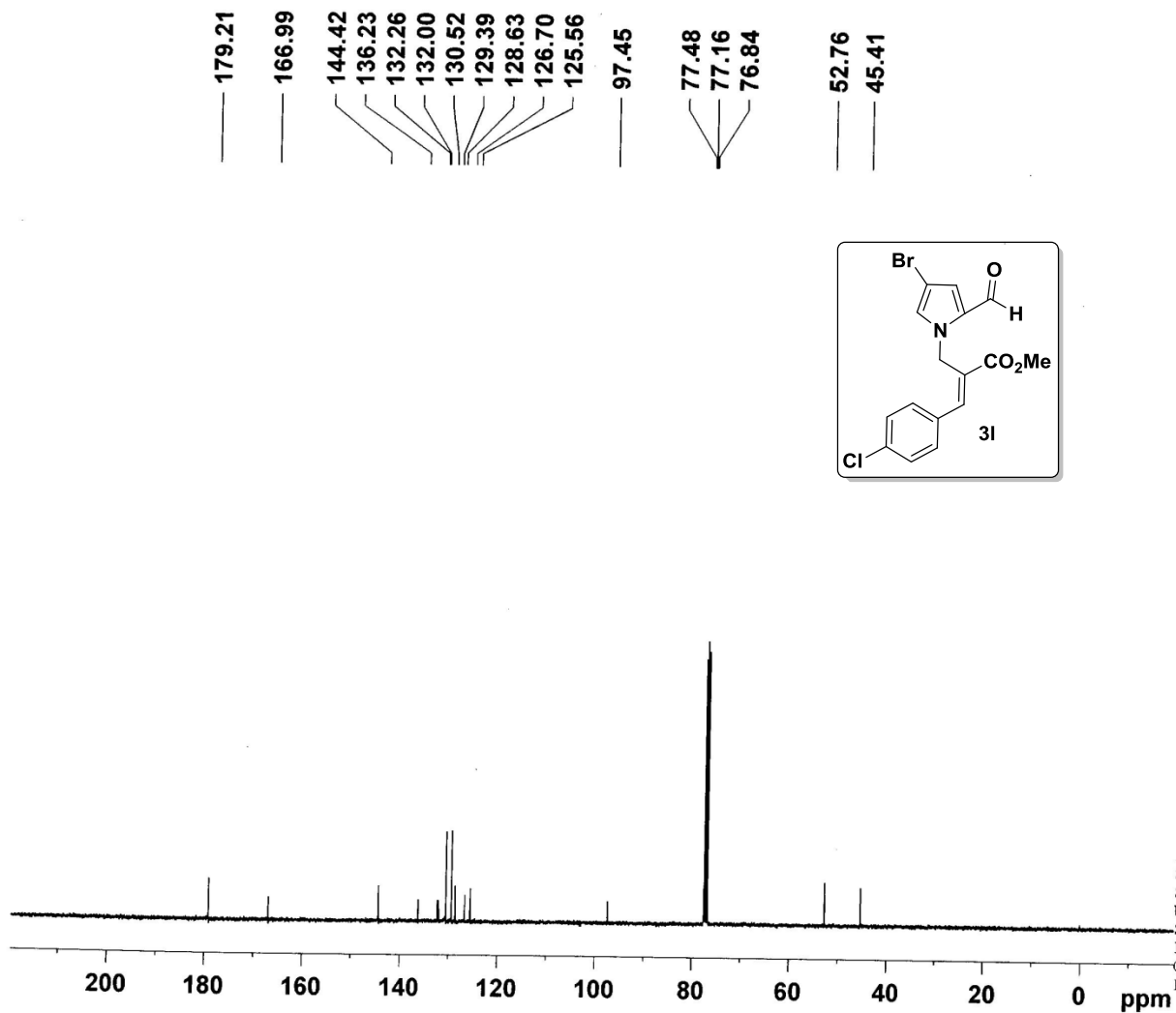
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PROCNO 1

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DE 6.00 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

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PC 1.00

C13CPD CDC13 {D:\MB} KOPAL 1



Current Data Parameters
NAME VA-JS-BR-6
EXPNO 2
PROCNO 1

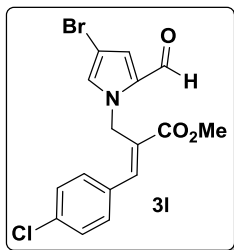
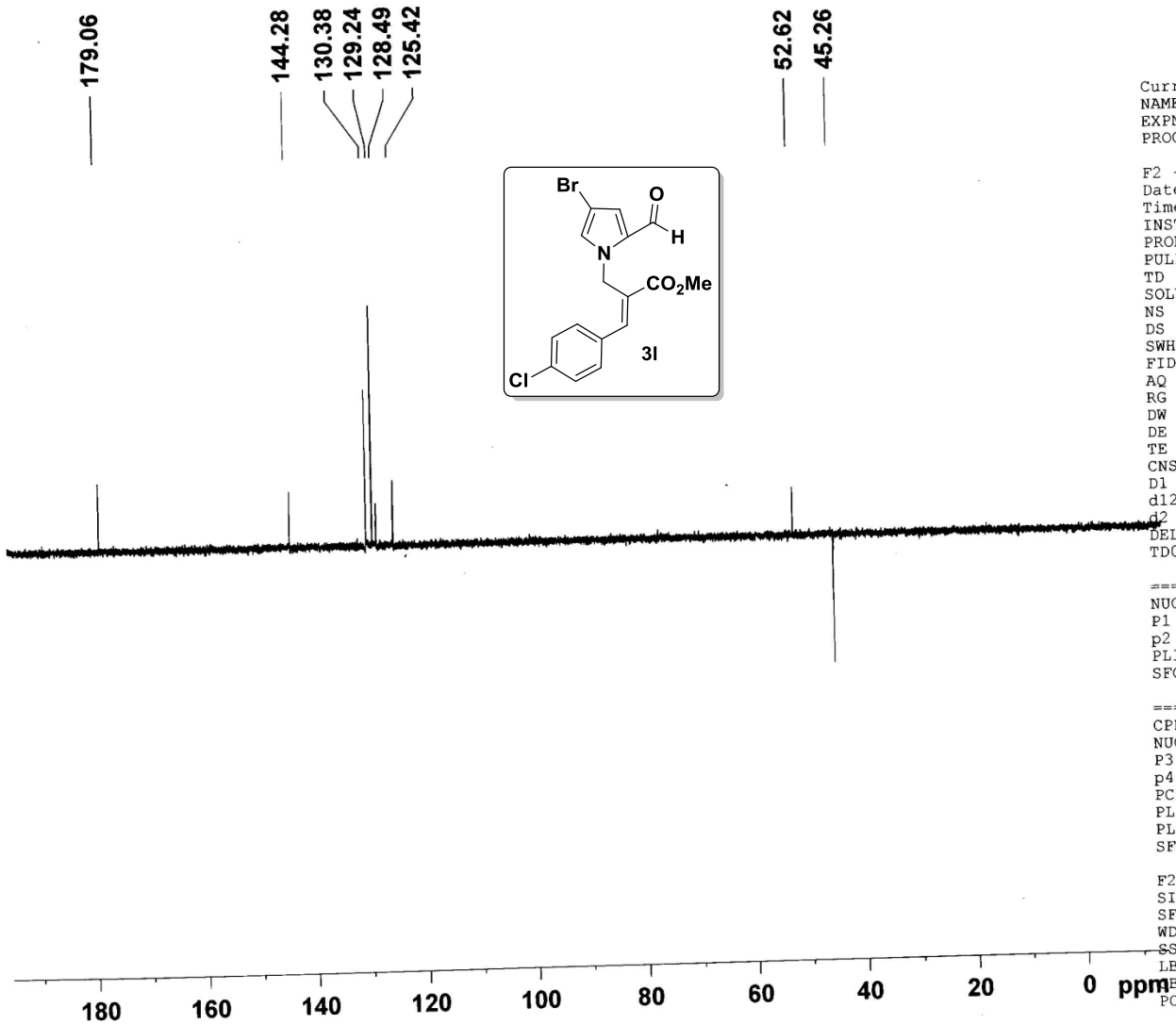
F2 - Acquisition Parameters
Date_ 20150703
Time 11.39
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 50.8
DW 20.800 usec
DE 6.00 usec
TE 297.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400,1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127545 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB ^
PC 1.

C13DEPT135 CDCl3 {D:\MB} KOPAL 1



Current Data Parameters
NAME VA-JS-BR-6
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150703
Time 13.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 109
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.1 K
CNST2 145.000000
D1 2.00000000 sec
d12 0.00002000 sec
d2 0.00344828 sec
DELTA 0.00001165 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
p2 18.30 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 11.42 usec
p4 22.84 usec
PCPD2 90.00 usec
PL12 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
PC 1.40



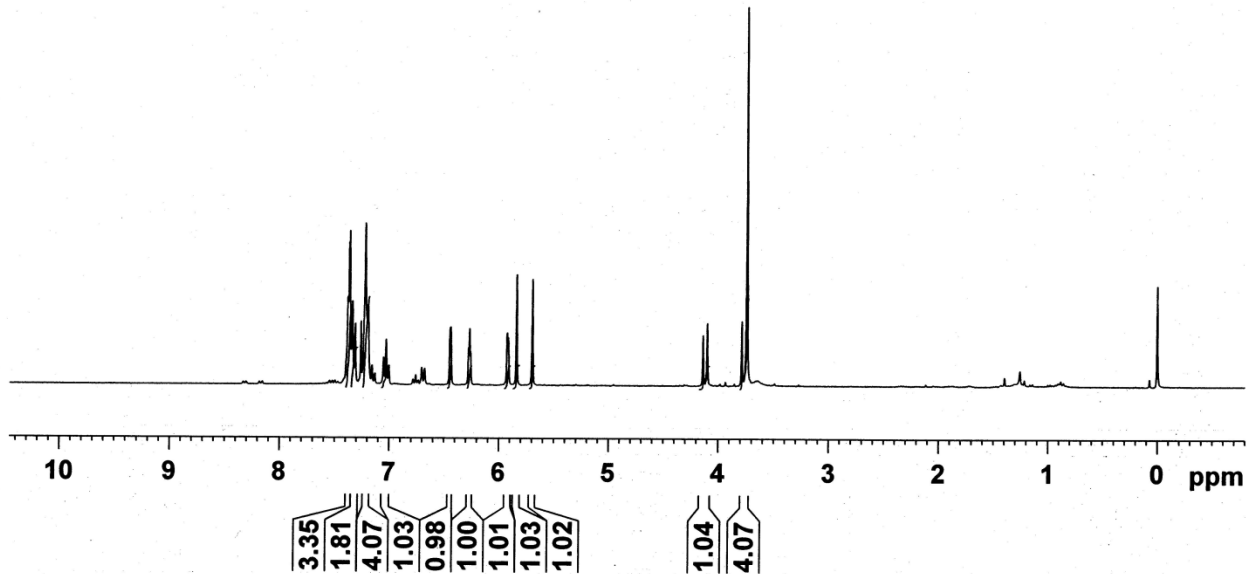
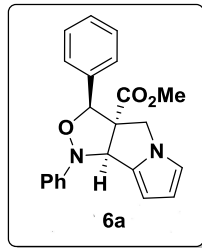
Current Data Parameters
NAME JSI-284
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20101123
Time 15.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

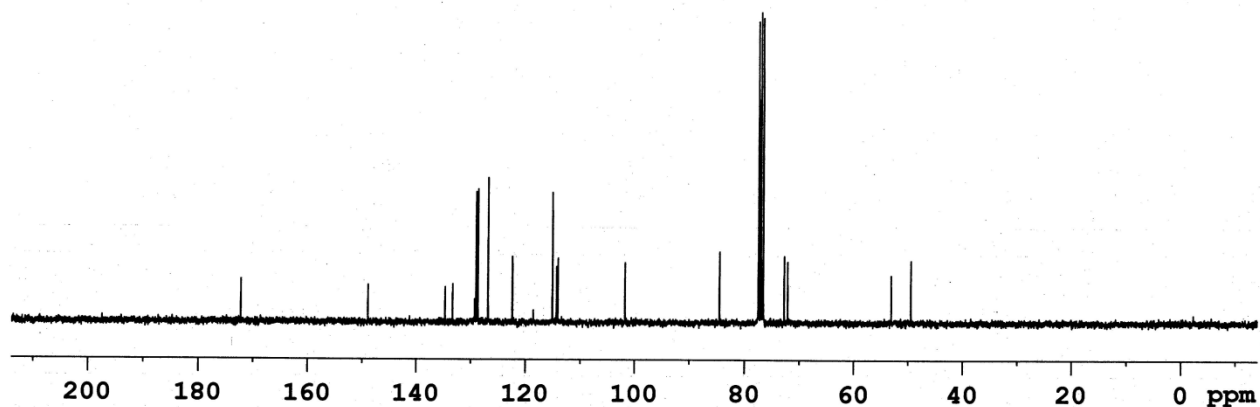
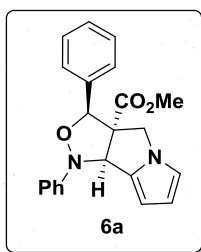
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.381
7.367
7.361
7.337
7.311
7.258
7.219
7.195
7.158
7.131
7.051
7.027
7.003
6.441
6.437
6.276
6.266
6.256
6.224
6.215
5.922
5.912
5.836
5.694
4.136
4.097
3.785
3.738



172.19
 148.89
 134.68
 133.30
 129.29
 129.04
 128.74
 128.67
 126.83
 122.38
 118.56
 115.12
 115.08
 114.35
 114.07
 101.75
 84.56
 77.48
 77.06
 76.63
 72.78
 72.16
 53.13
 49.53



Current Data Parameters
 NAME JSI-284
 EXPNO 3
 PROCNO 1

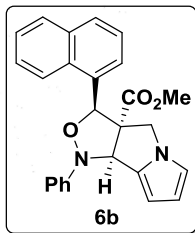
F2 - Acquisition Parameters
 Date_ 20101125
 Time 12.12
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999999 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

7.869
7.841
7.815
7.525
7.505
7.483
7.458
7.428
7.401
7.381
7.354
7.328
7.302
7.275
7.245
7.074
7.050
7.026
6.578
6.326
6.287
6.277
6.267
5.999
5.989
5.949
4.183
4.144
3.691
3.567
3.529

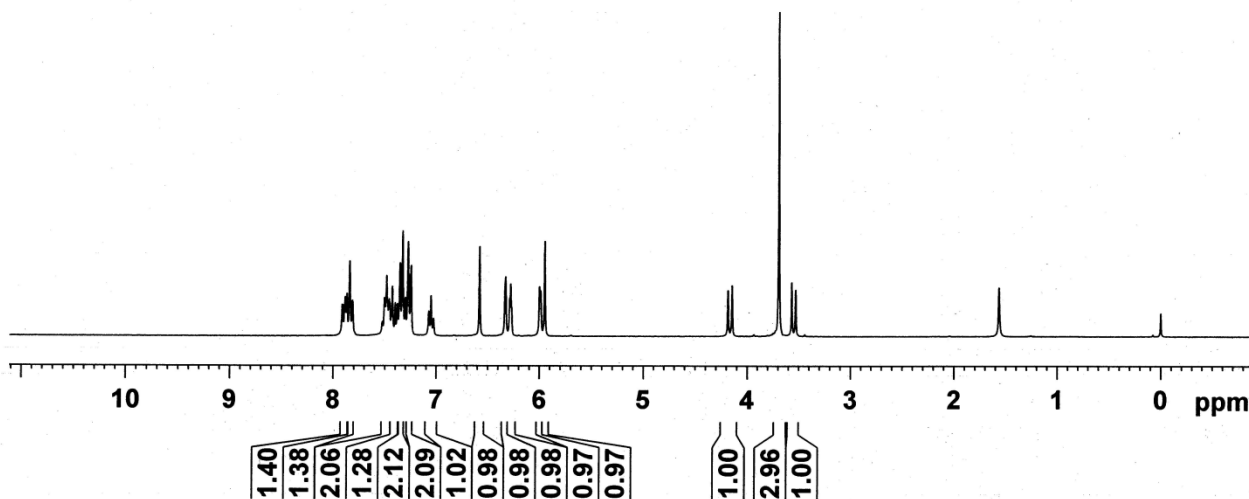


Current Data Parameters
NAME JS-II-13
EXPNO 1
PROCNO 1

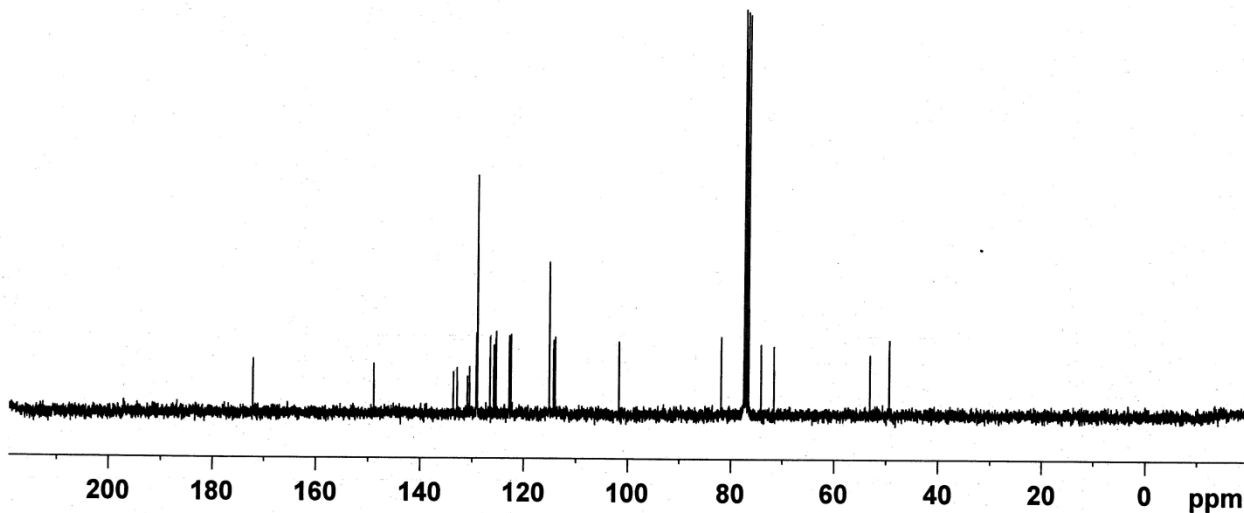
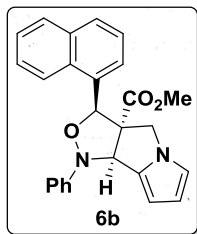
F2 - Acquisition Parameters
Date_ 20121107
Time 1.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 10
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



172.27
148.96
133.69
132.96
130.98
130.56
129.24
129.07
126.60
125.88
125.48
125.42
122.88
122.50
115.16
114.34
114.00
101.71
81.91
77.48
77.05
76.63
74.21
71.70
53.13
49.39



Current Data Parameters
NAME JS-II-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121107
Time 1.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3251
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

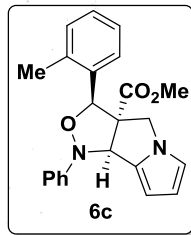
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.366
7.338
7.313
7.277
7.261
7.218
7.190
7.157
7.133
7.054
7.030
7.005
6.420
6.416
6.269
6.259
6.249
5.956
5.895
5.884
5.865
4.287
4.248
3.715
3.675
3.663
2.212

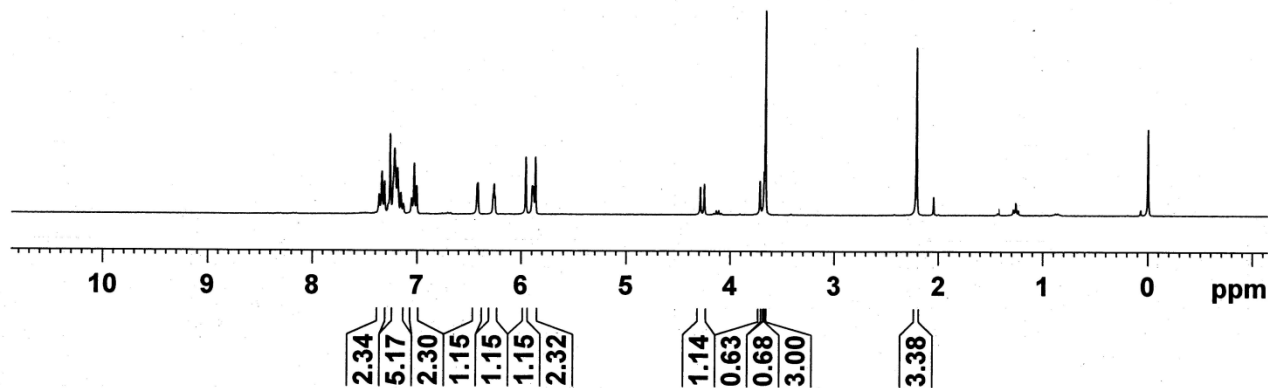


Current Data Parameters
NAME J.S.II-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101221
Time 12.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 406.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

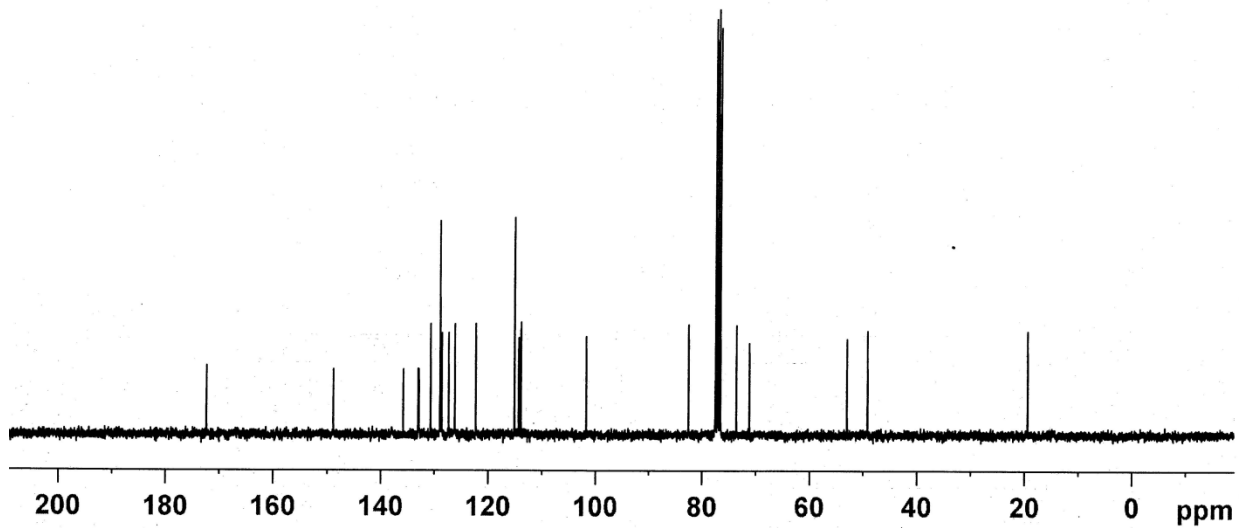
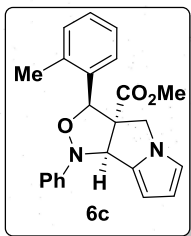
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



172.37
148.85
135.83
133.06
132.89
130.72
128.96
128.61
127.34
126.21
122.29
115.12
114.34
113.93
101.74
82.53
77.49
77.07
76.64
73.63
71.22
53.02
49.17

19.41



Current Data Parameters
NAME JS-II-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101221
Time 15.57
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 208
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



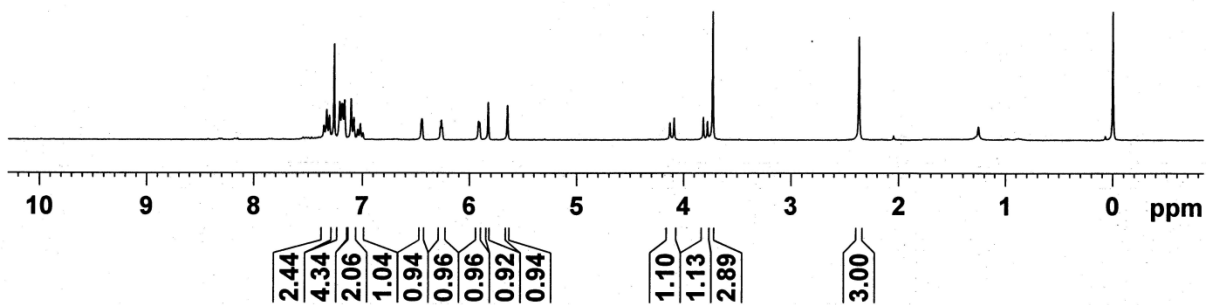
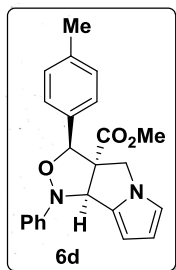
Current Data Parameters
NAME J.S.II-2
EXPNO 1
PROCNO 1

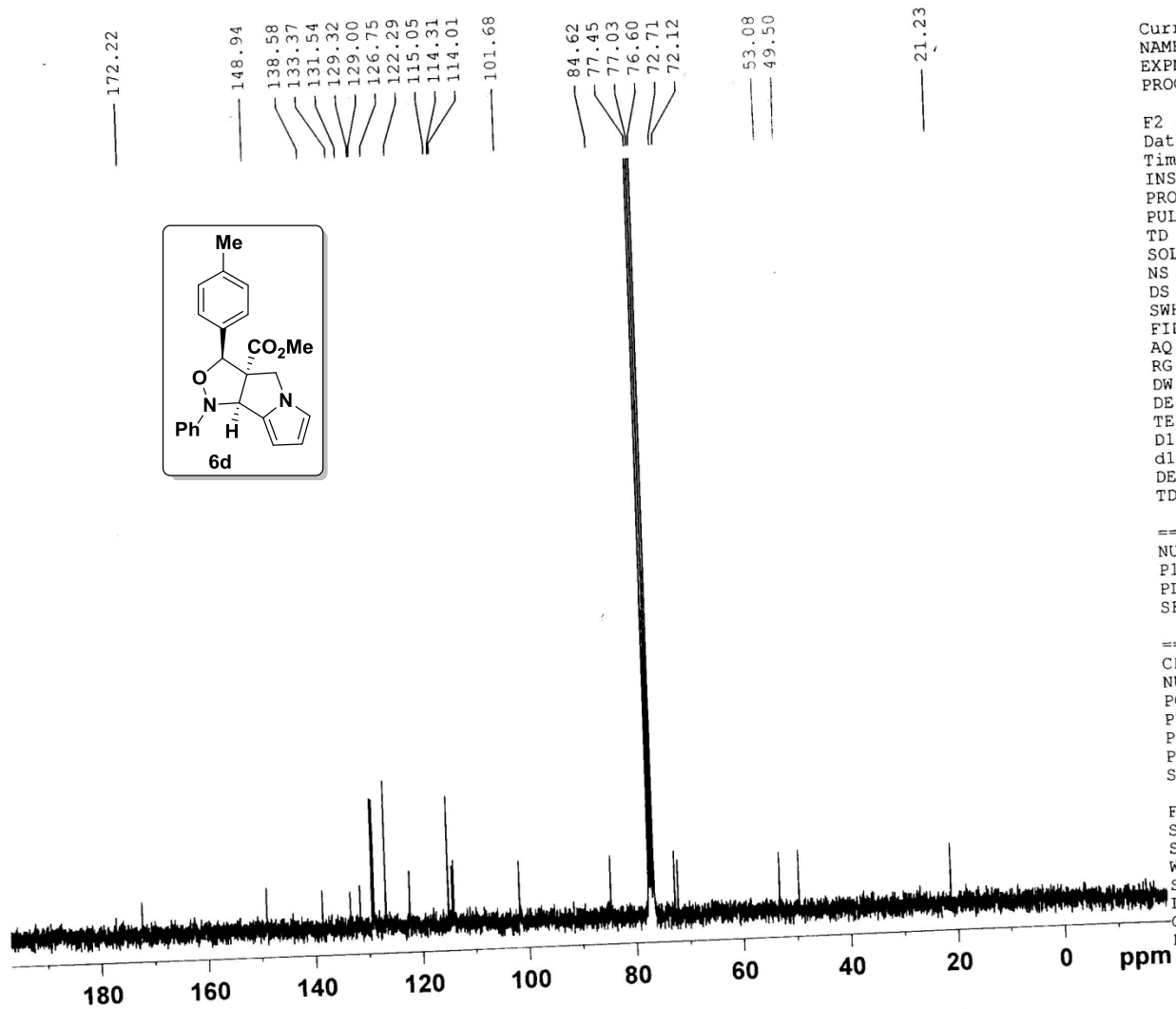
F2 - Acquisition Parameters
Date 20101221
Time 12.56
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 512
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.358
7.330
7.305
7.211
7.187
7.167
7.106
7.079
6.445
6.274
6.264
6.255
5.917
5.907
5.827
5.648
4.128
4.090
3.816
3.777
3.729
2.369





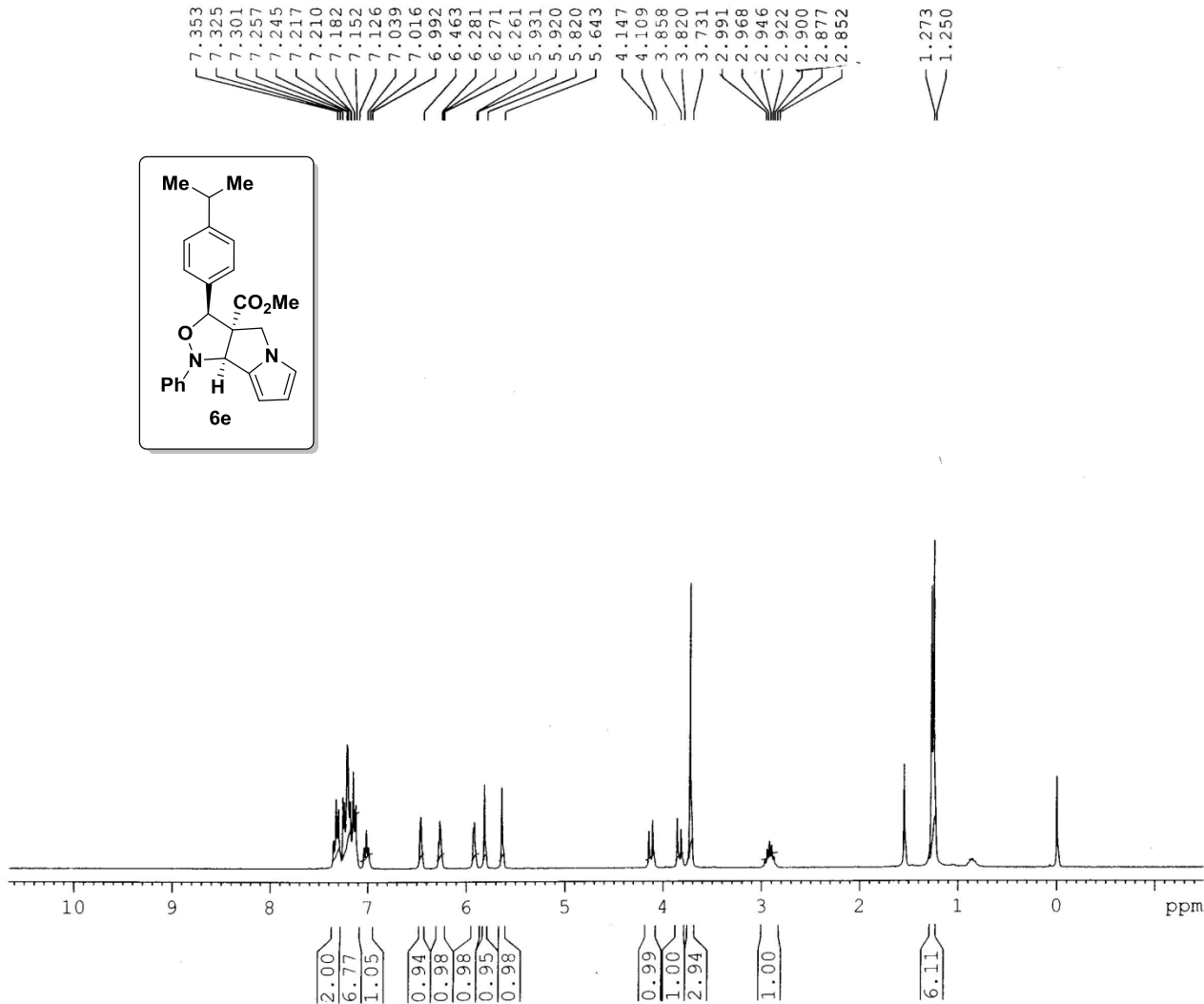
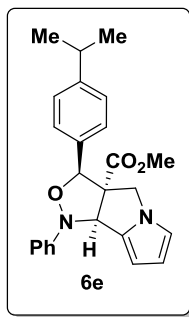
Current Data Parameters
NAME JS-II-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101222
Time_ 10.24
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

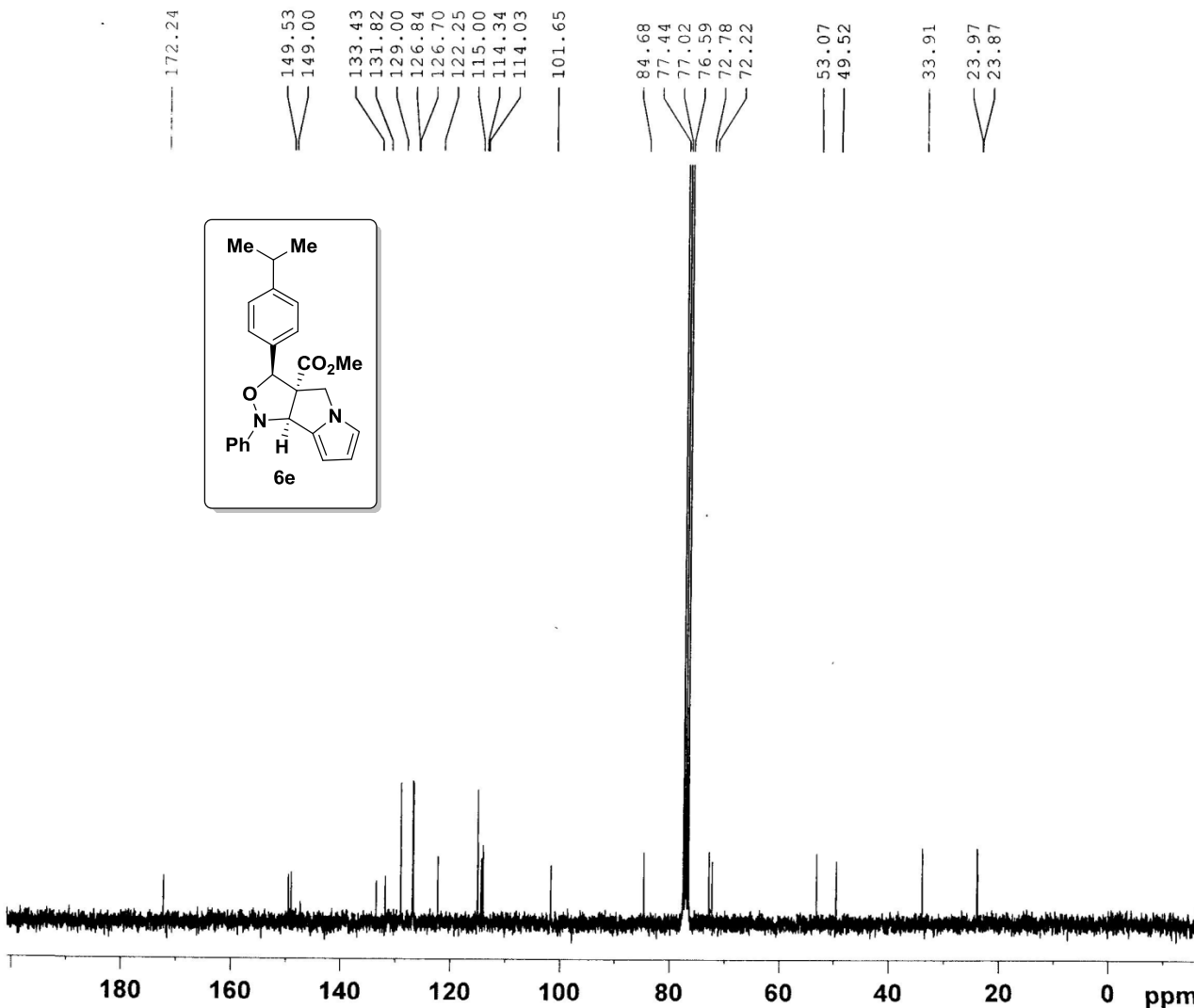


Current Data Parameters
NAME J.S.II-7
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101221
Time 20.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 287.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME J.S.II-7
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101221
Time 20.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 402
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

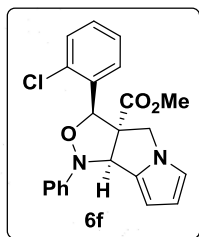
=====
CHANNEL f1
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.415
7.390
7.345
7.321
7.252
7.217
7.062
7.039
6.393
6.250
6.123
5.922
5.760
4.447
4.408
3.667
3.646
3.636

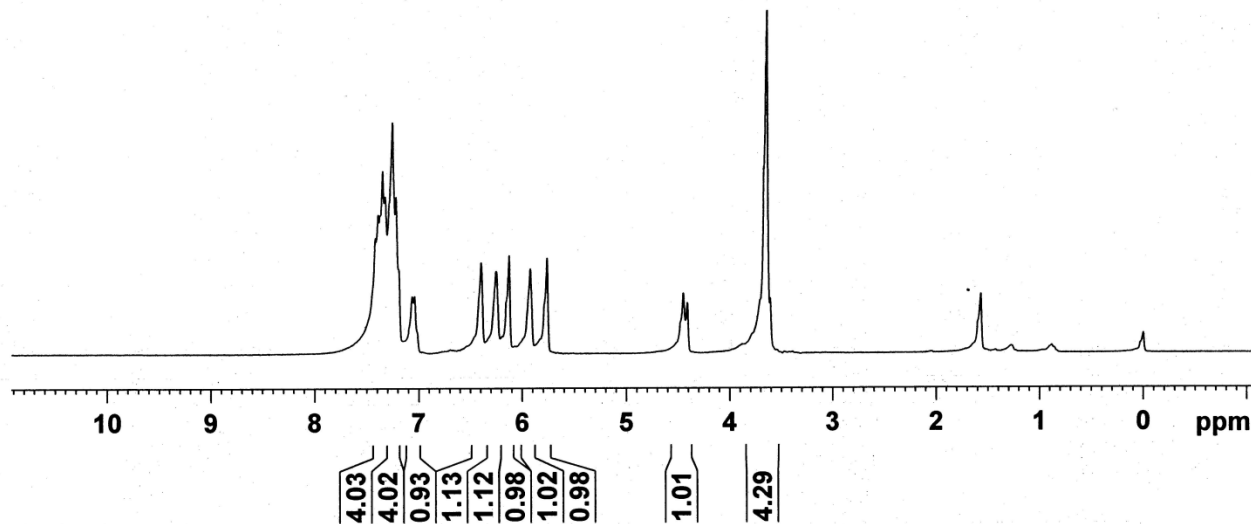


Current Data Parameters
NAME JS-II-9-2-C1
EXPNO 1
PROCNO 1

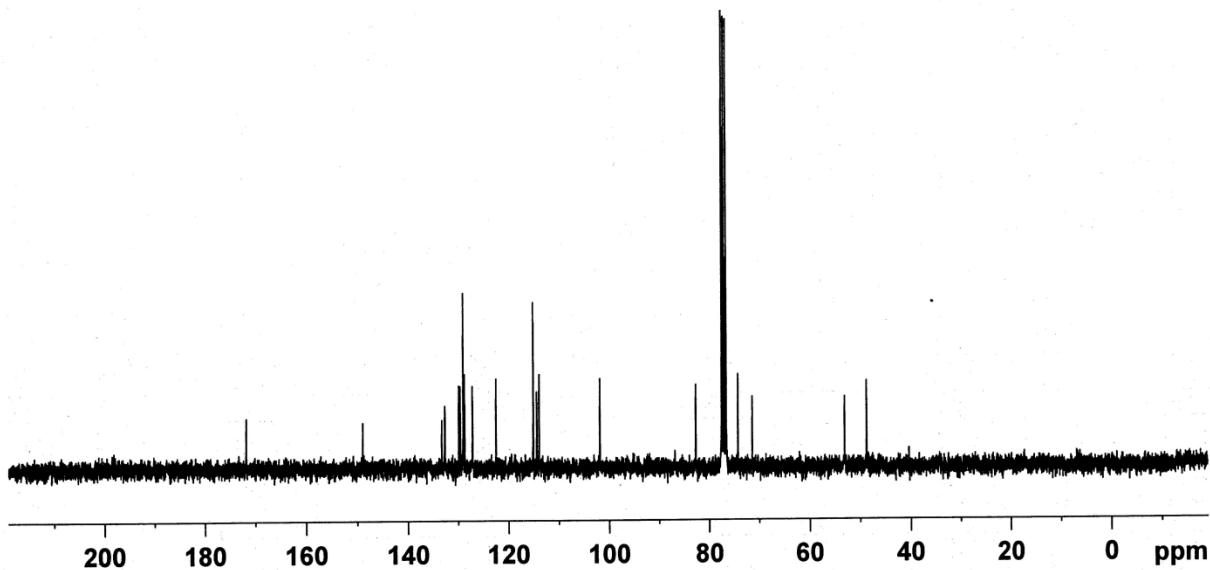
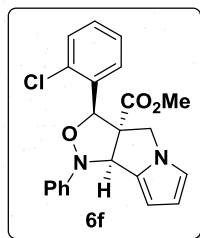
F2 - Acquisition Parameters
Date_ 20101228
Time 21.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



171.78
148.90
133.28
132.66
132.61
129.85
129.57
128.97
128.69
127.13
122.43
115.08
114.41
113.92
101.81
82.67
77.47
77.05
76.62
74.25
71.39
53.08
48.74



Current Data Parameters
NAME JS-II-9-2-C1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101228
Time 22.00
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 151
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



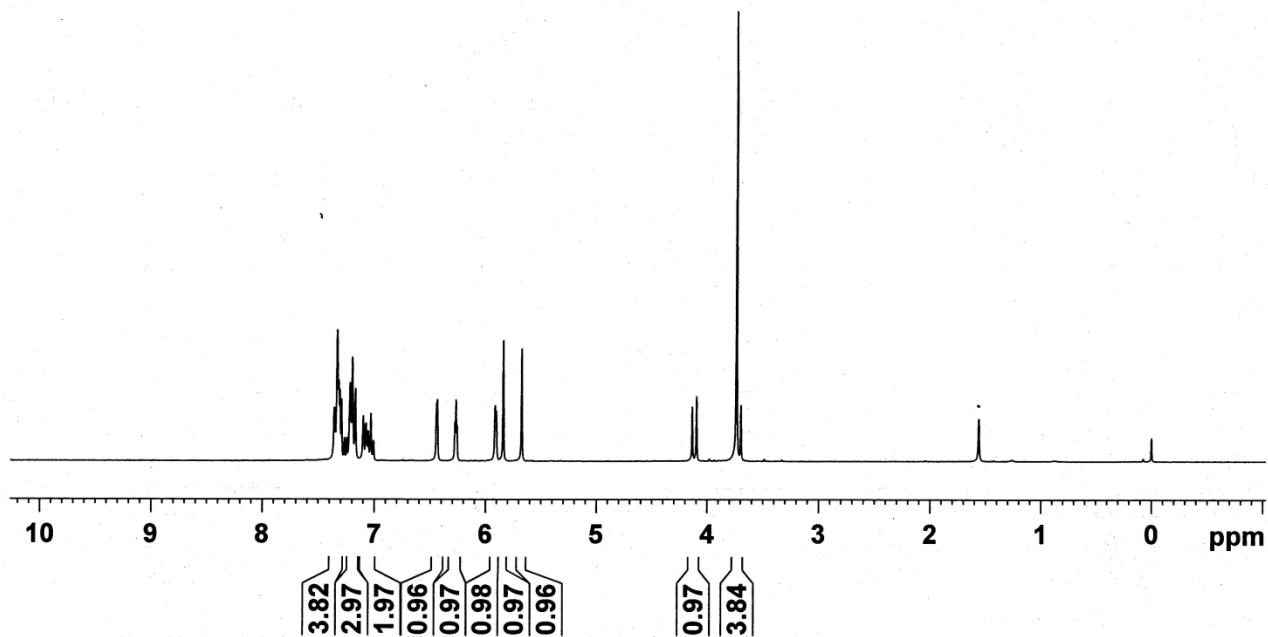
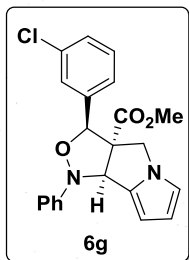
Current Data Parameters
NAME JS-II-83-C1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101228
Time_ 21.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

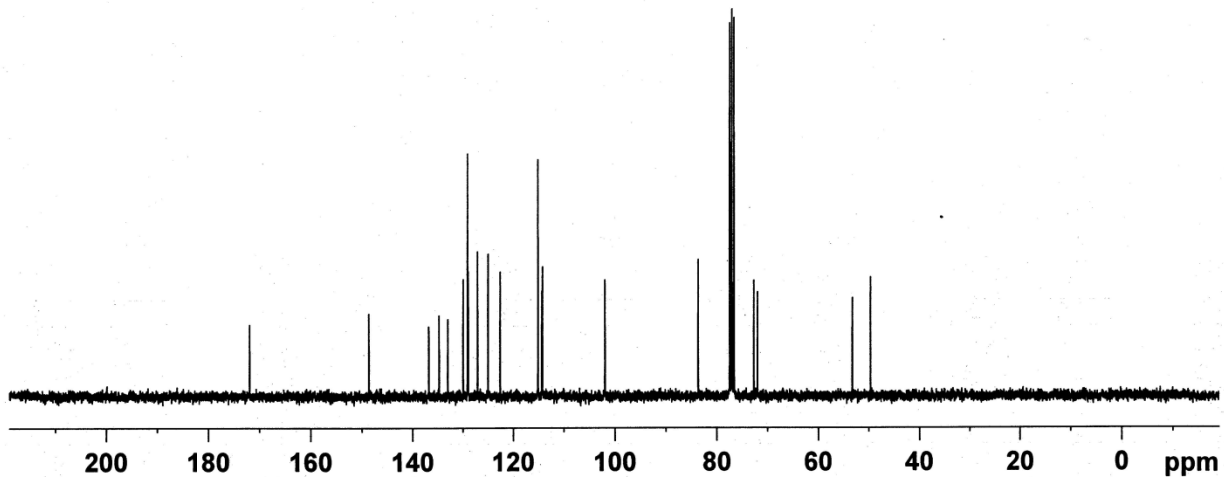
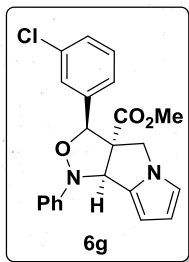
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.310
7.295
7.269
7.247
7.220
7.199
7.171
7.100
7.076
7.059
7.056
7.033
7.010
7.008
6.446
6.441
6.437
6.278
6.268
6.258
5.914
5.903
5.840
5.673
4.134
4.096
3.737
3.697



171.93
148.62
136.83
134.77
133.02
129.95
129.07
128.95
127.09
124.98
122.58
115.14
114.38
114.24
101.96
83.65
77.47
77.05
76.63
72.69
71.97
53.23
49.66



Current Data Parameters
NAME JS-II-83-C1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101228
Time_ 21.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 207
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

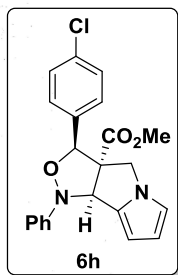
===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.355
7.327
7.303
7.242
7.195
7.169
7.150
7.122
7.052
7.027
7.003
6.428
6.425
6.421
6.266
6.256
6.245
5.900
5.889
5.854
5.664
4.100
4.062
3.721
3.704
3.665

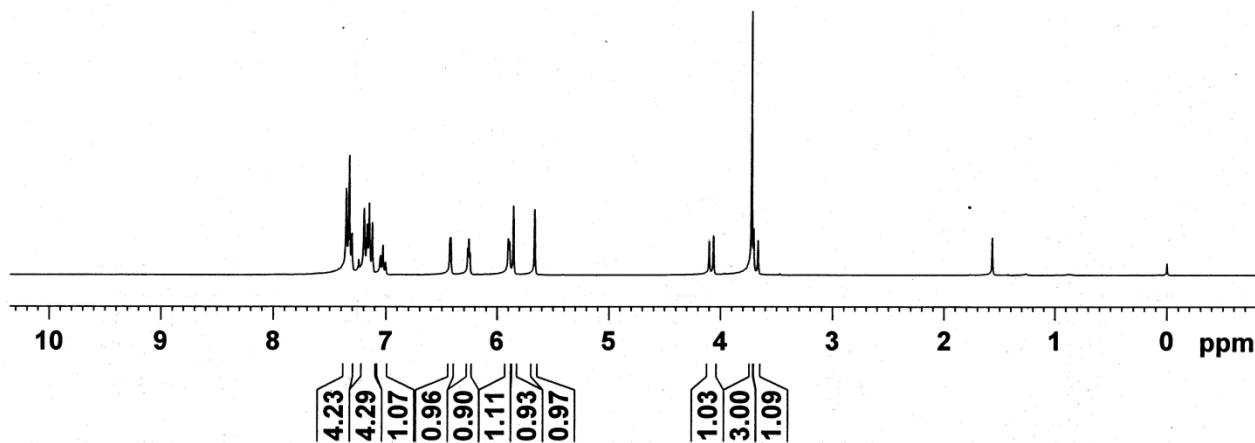


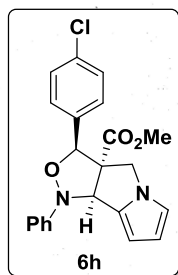
Current Data Parameters
NAME JSI-II-10
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101229
Time 15.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 90.5
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300114 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





171.99
 148.63
 134.69
 133.28
 133.13
 129.06
 128.89
 128.32
 122.56
 115.15
 114.35
 114.20
 101.93
 83.81
 77.49
 77.07
 76.64
 72.53
 71.88
 53.19
 49.65



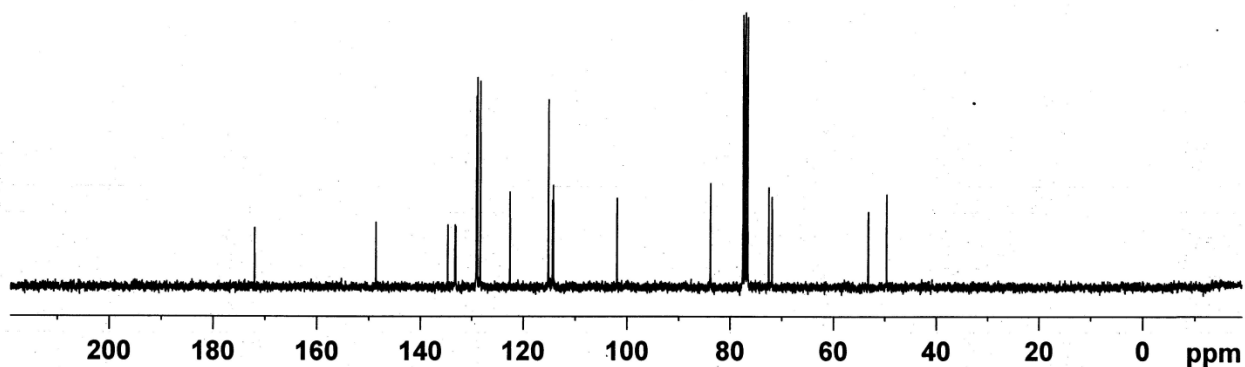
Current Data Parameters
 NAME JSI-II-10
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101229
 Time 15.10
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 150
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 362
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TD0 1

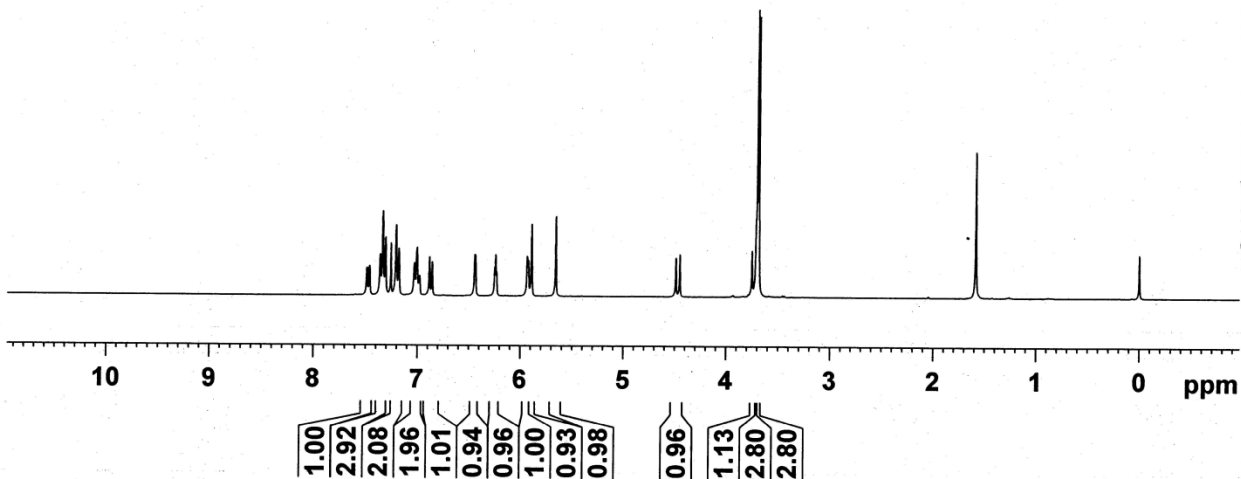
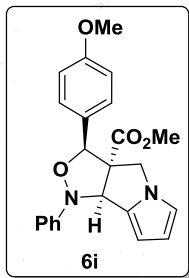
===== CHANNEL f1 =====
 NUC1 13C
 P1 7.40 usec
 PL1 -2.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



7.487
7.462
7.360
7.334
7.308
7.255
7.206
7.180
7.029
7.004
6.985
6.979
6.884
6.857
6.442
6.249
6.239
6.230
5.933
5.922
5.890
5.657
4.489
4.450
3.751
3.711
3.700
3.687



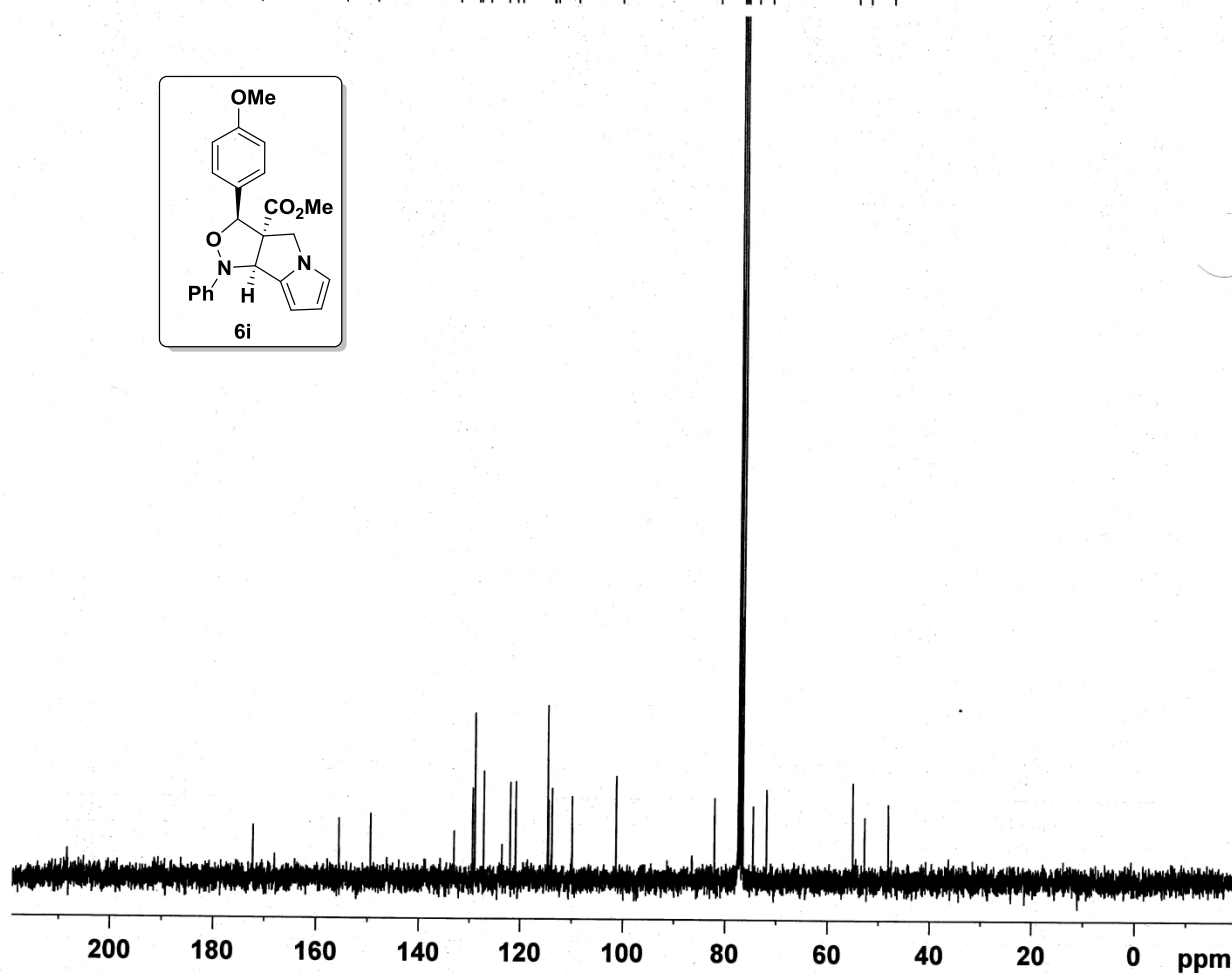
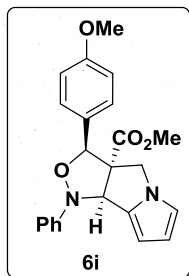
Current Data Parameters
NAME JS-II-12
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121107
Time_ 0.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

172.31
155.62
149.46
133.08
129.42
128.96
127.20
123.63
121.99
120.92
114.71
114.53
113.87
109.95
101.35
82.11
77.46
77.03
76.61
74.60
71.95
55.09
52.76
48.12



Current Data Parameters
NAME JS-II-12
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121107
Time_ 0.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 100
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2298.8
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



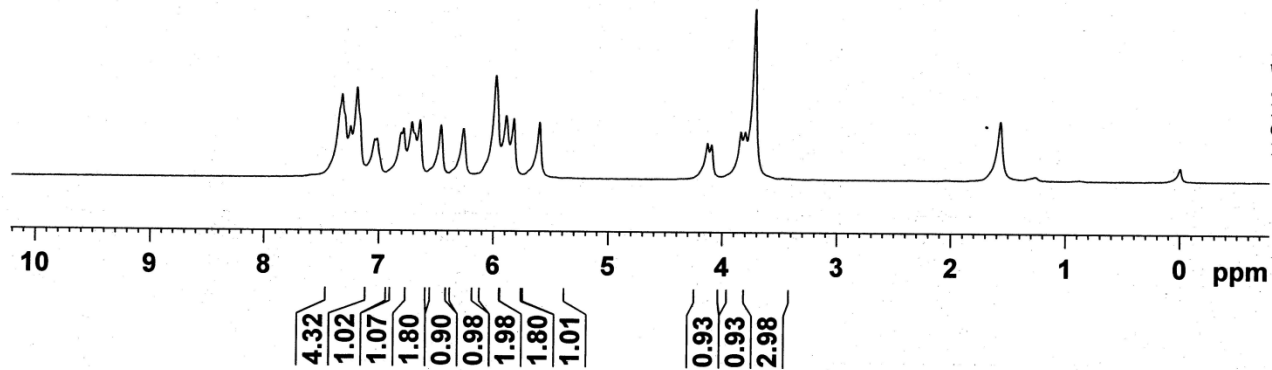
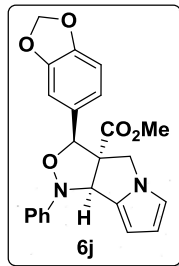
Current Data Parameters
NAME JS-II-11
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121107
Time_ 10.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 12
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

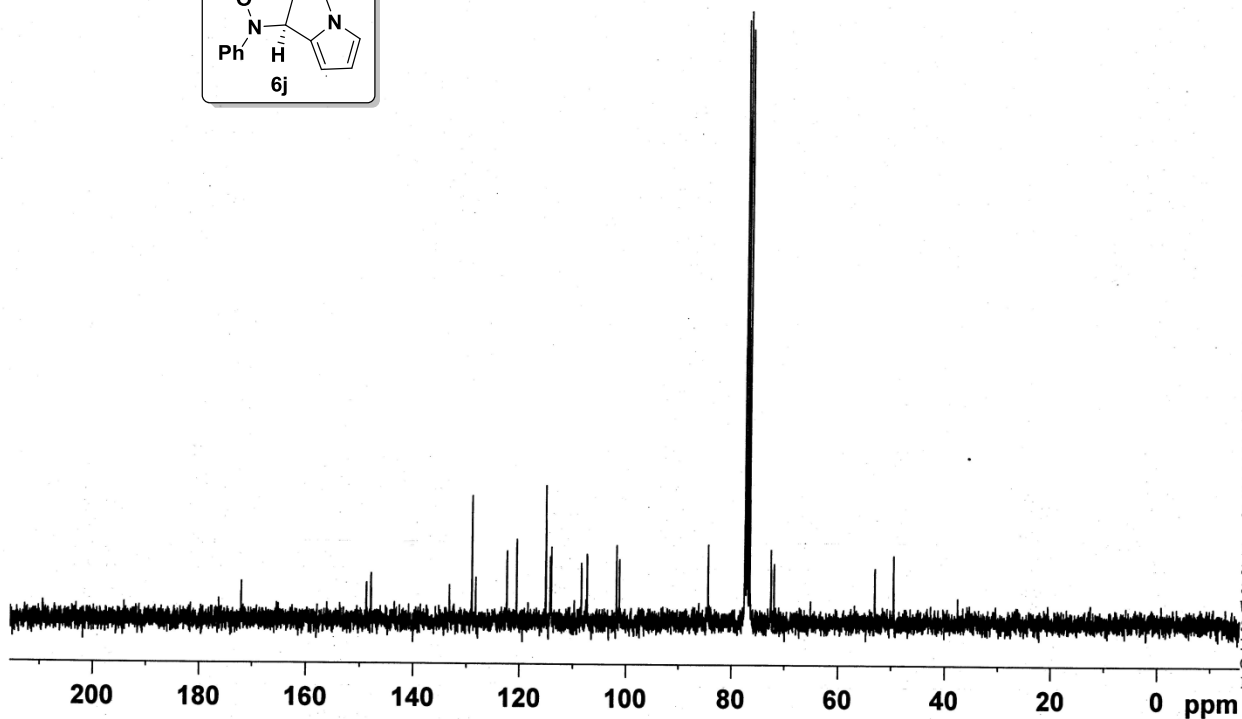
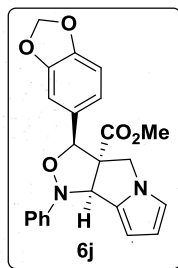
===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.327
7.253
7.196
7.040
7.022
6.811
6.789
6.717
6.647
6.461
6.265
5.981
5.891
5.826
5.602
4.131
4.094
3.841
3.803
3.718



172.15
148.80
147.95
133.24
129.00
128.28
122.39
120.56
115.12
114.31
114.10
108.41
107.37
101.79
101.25
84.41
77.45
77.03
76.60
72.55
71.98
53.08
49.58



Current Data Parameters
NAME JS-II-11
EXPNO 3
PROCNO 1

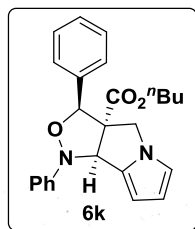
F2 - Acquisition Parameters
Date 20121107
Time 10.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 223
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 912.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

7.377
7.371
7.364
7.355
7.329
7.325
7.300
7.253
7.223
7.220
7.212
7.198
7.017
6.440
6.436
6.432
6.289
6.279
5.969
5.958
5.854
5.708
4.155
4.131
4.116
4.109
4.087
3.753
3.714
1.507
1.485
1.458
1.257
1.233
1.208
1.183
0.888
0.864
0.840

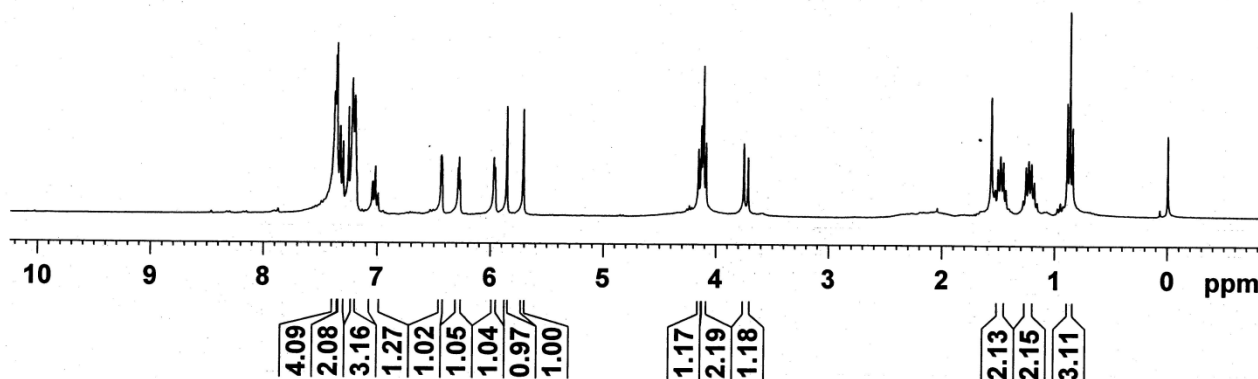


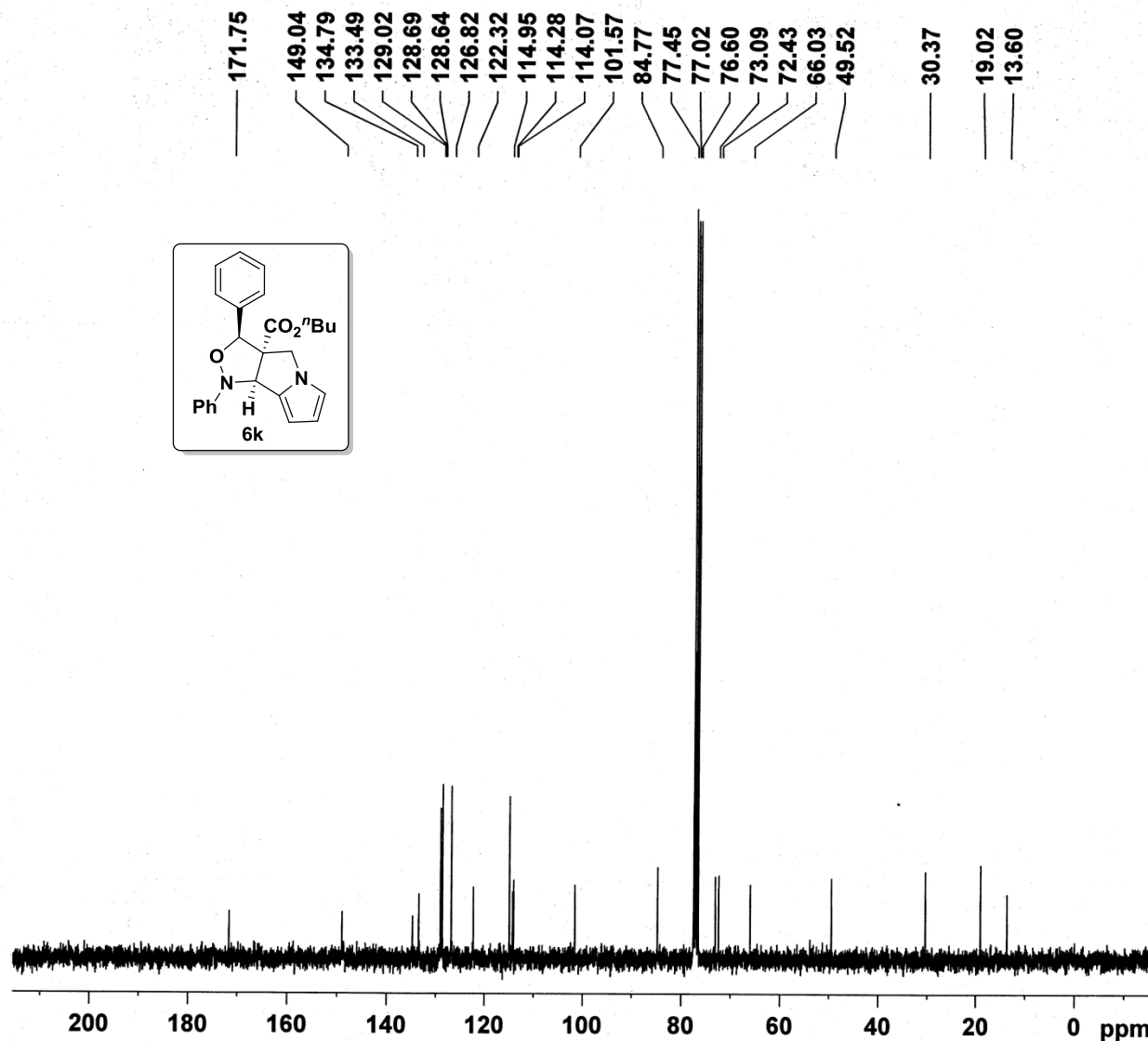
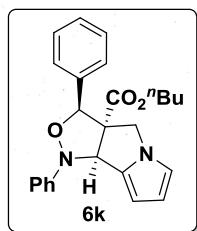
Current Data Parameters
NAME JS-IV-82
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20130327
Time 18.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.130084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME JS-IV-82
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130327
Time 18.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 201
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1448.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

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

NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

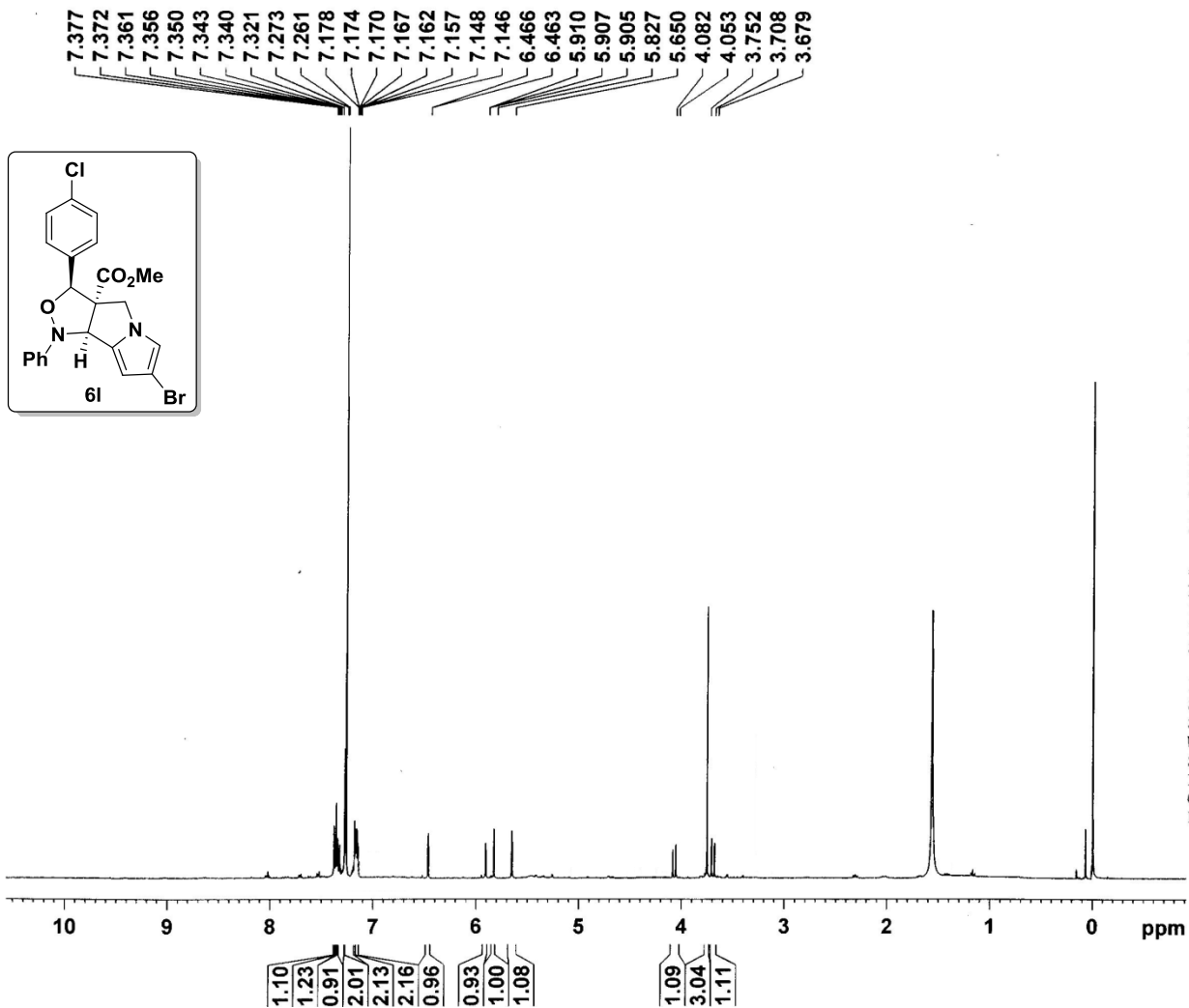
===== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters

SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\MB} KOPAL 1



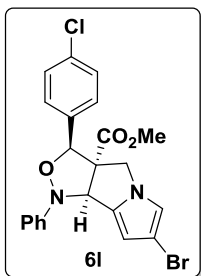
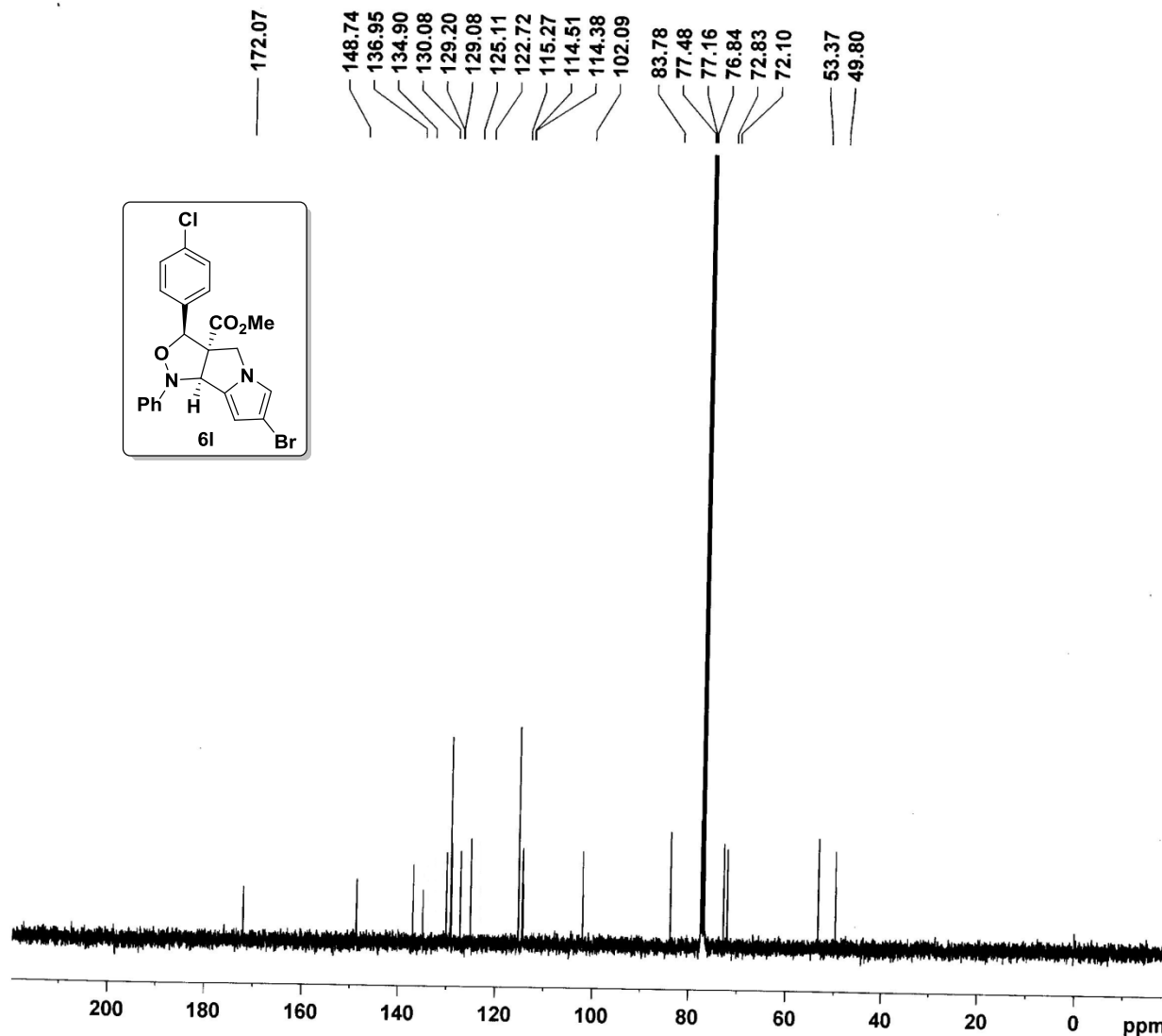
Current Data Parameters
NAME VA-JS-08-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150706
Time 11.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

C13CPD CDC13 {D:\MB} KOPAL 1



Current Data Parameters
NAME VA-JS-08-1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150707
Time_ 14.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME JSNA-01
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20121208
Time 18.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 143.7
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

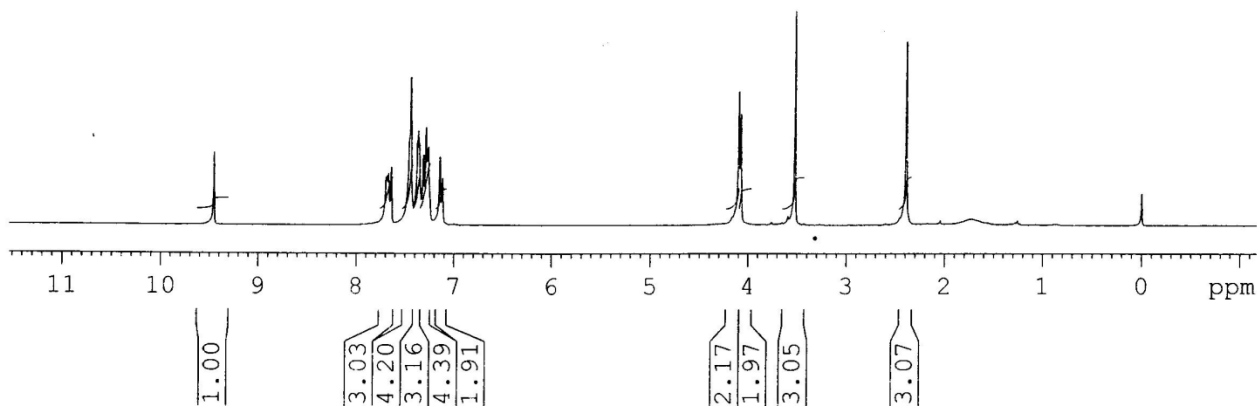
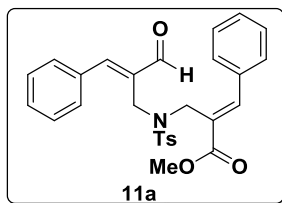
==== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

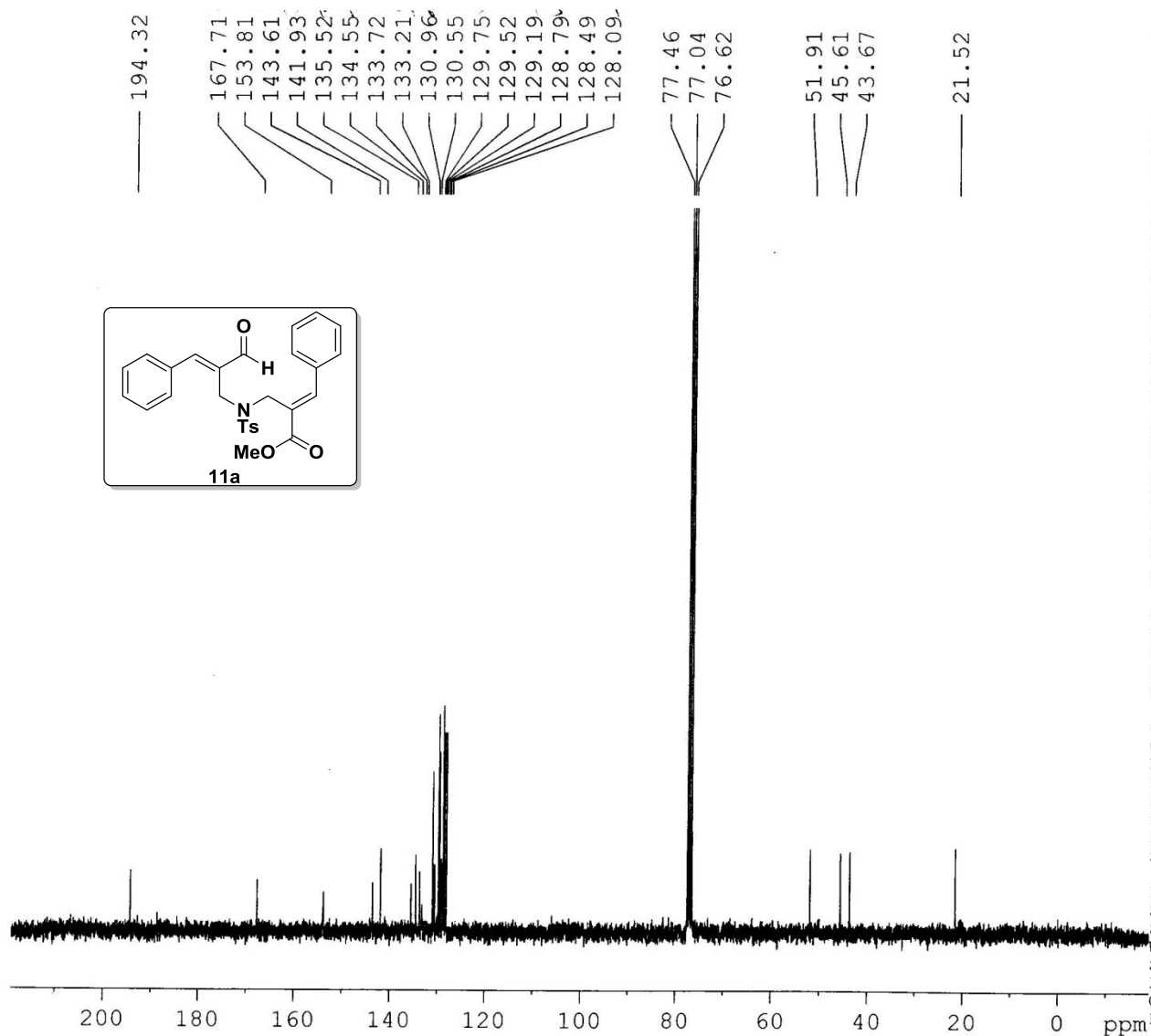
F2 - Processing parameters
SI 32768
SF 300.1300058 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.452
7.695
7.684
7.671
7.641
7.452
7.441
7.375
7.366
7.355
7.314
7.287
7.275
7.263
7.144
7.118

4.095
4.074
3.519

2.390





Current Data Parameters
NAME JSNA-01
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20121208
Time 18.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 182
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 512
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

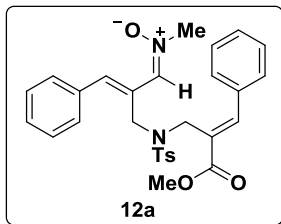
=====
CHANNEL f1
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PROTON CDC13 {D:\MB} KOPAL 1

7.595
7.586
7.565
7.500
7.480
7.355
7.347
7.341
7.324
7.321
7.315
7.304
7.298
7.230
7.213
7.197
7.192
7.183
7.175
7.167
7.149
7.101
7.083
7.056
7.037
4.097
4.021
4.017
3.411
3.364
2.372

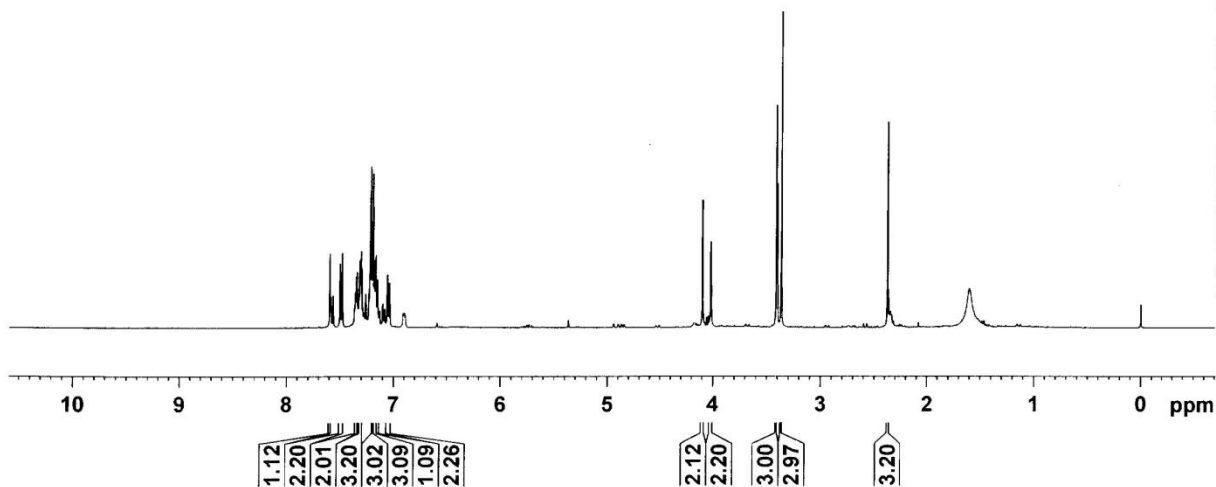


Current Data Parameters
NAME VA-JS-RSC-22
EXPNO 3
PROCNO 1

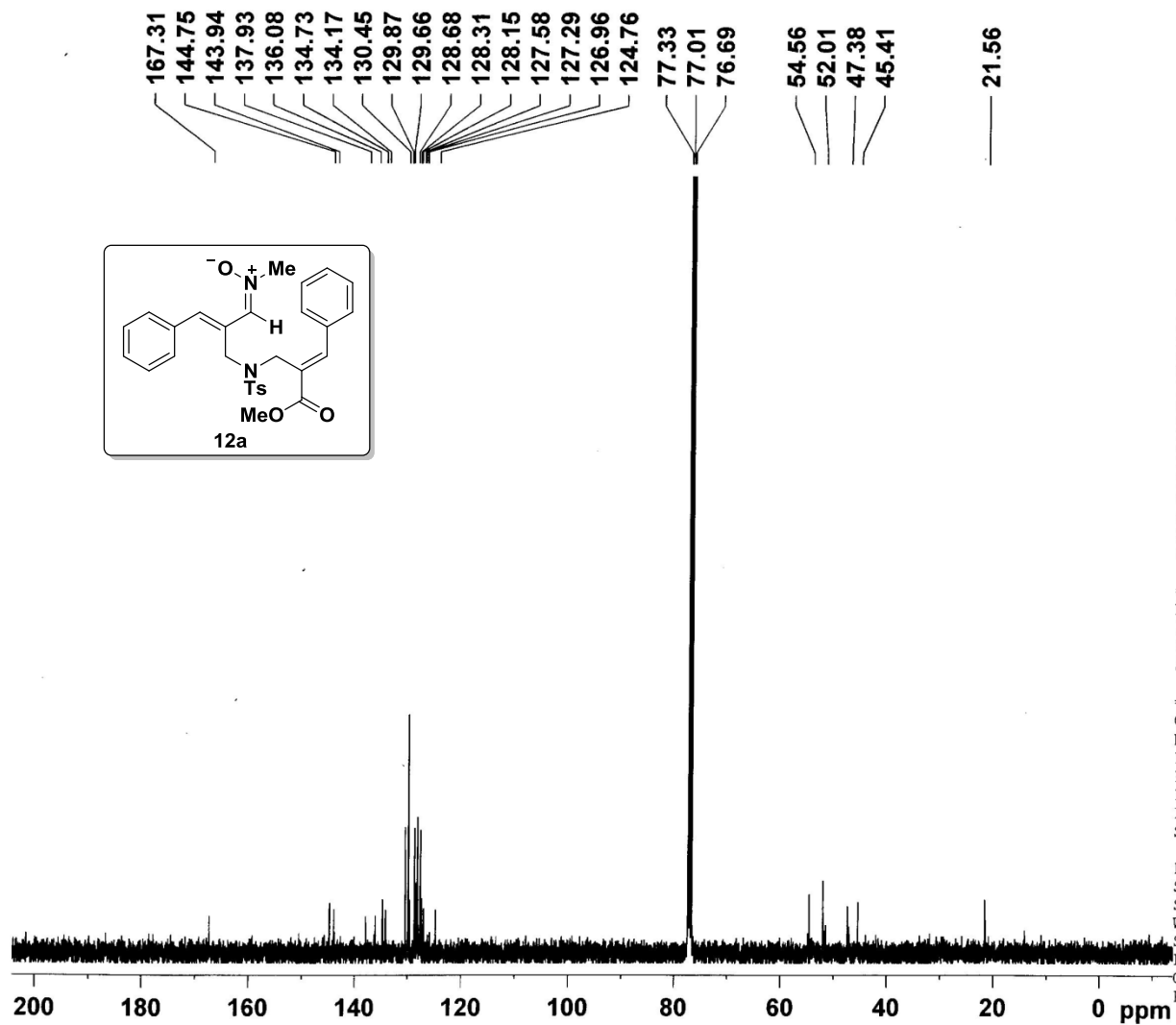
F2 - Acquisition Parameters
Date_ 20150720
Time_ 14.20
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300323 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



C13CPD CDC13 {D:\MB} KOPAL 1



Current Data Parameters
NAME VA-JS-RSC-22
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150720
Time_ 14.27
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB
GB
PC



Current Data Parameters
NAME JS-IV-48
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

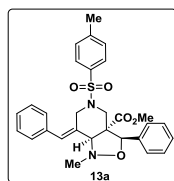
Date_ 20121216
Time_ 23.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

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

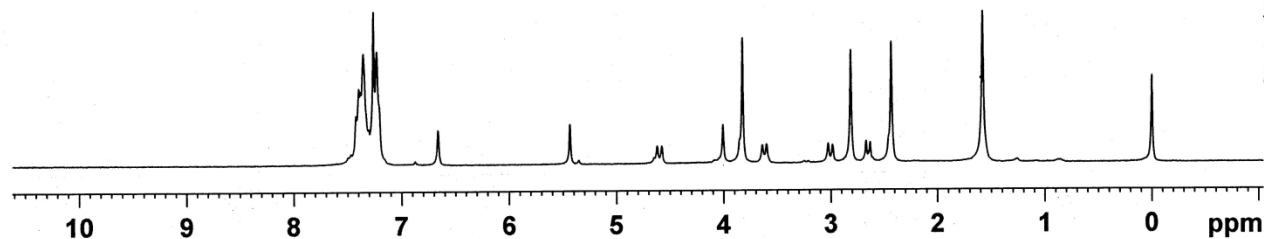
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
SF 300.1300063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.423
7.398
7.381
7.357
7.305
7.262
7.231
6.662
5.437
4.621
4.579
4.006
3.824
3.642
3.602
3.027
2.986
2.813
2.670
2.629
2.430



2.13
6.01
6.28
1.04
1.00
1.02
1.12
3.03
1.19
1.07
3.07
1.16
3.06



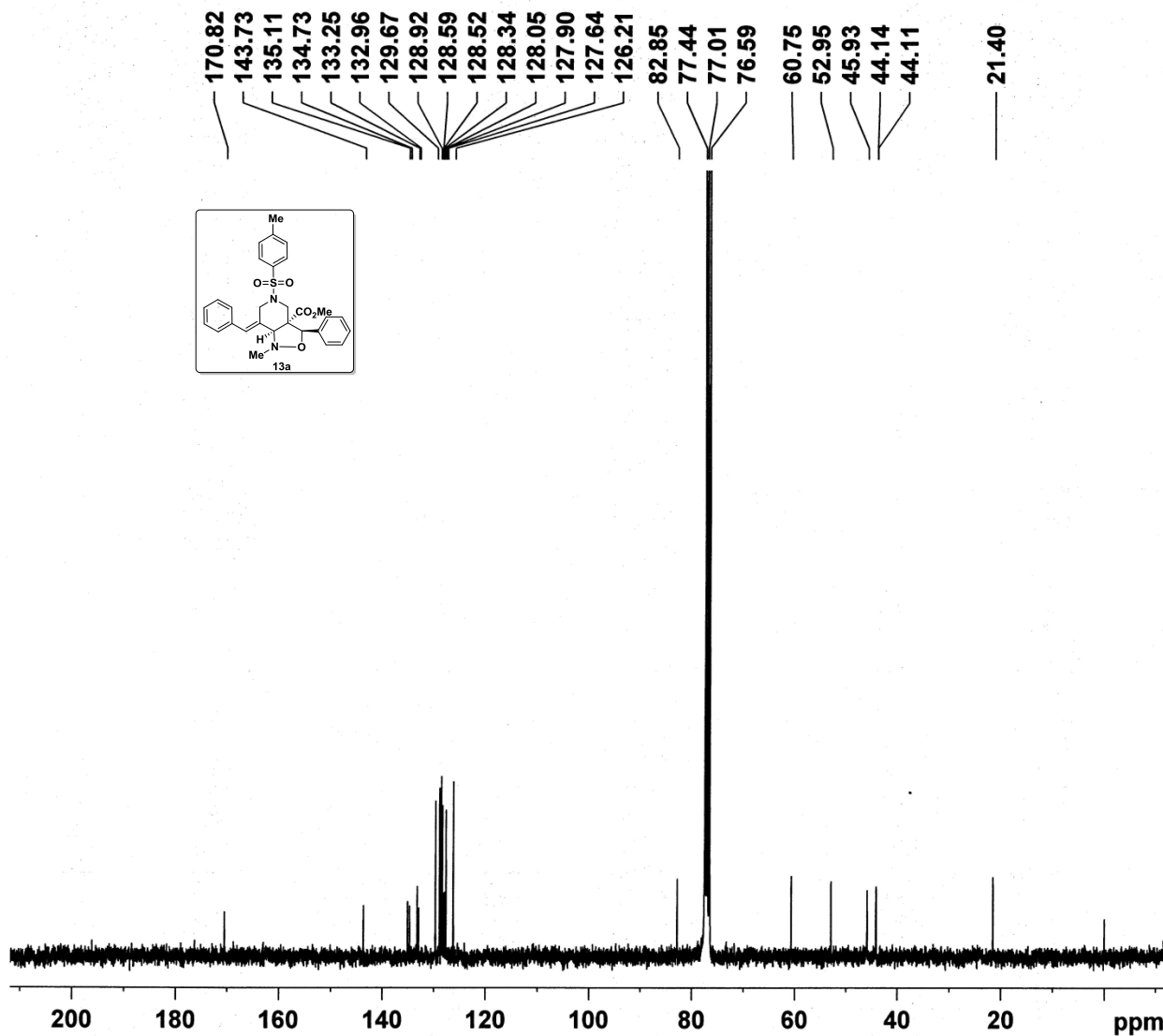
Current Data Parameters
NAME JS-IV-48
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121217
Time_ 8.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

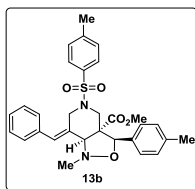
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.451
7.424
7.401
7.378
7.353
7.323
7.298
7.271
7.261
7.245
7.224
7.200
7.168
7.141
7.120
7.101
7.075
6.645
5.410
4.655
4.616
4.575
4.010
3.802
3.669
3.630
3.044
3.002
2.812
2.704
2.664
2.435
2.392

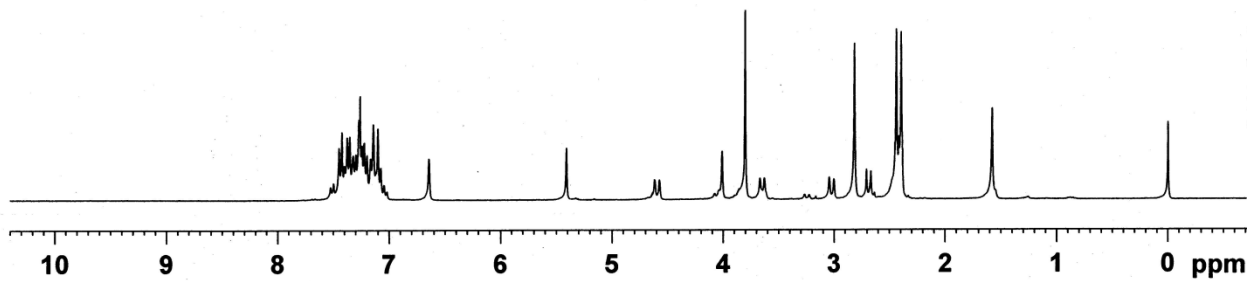


Current Data Parameters
NAME JS-IV-64
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130212
Time_ 22.38
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 203.2
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.14
2.34
1.16
1.01
1.24
1.02
2.03
2.24
1.23
1.12
1.02
1.06
0.98
3.00
1.10
1.06
3.08
1.13
3.13
3.13



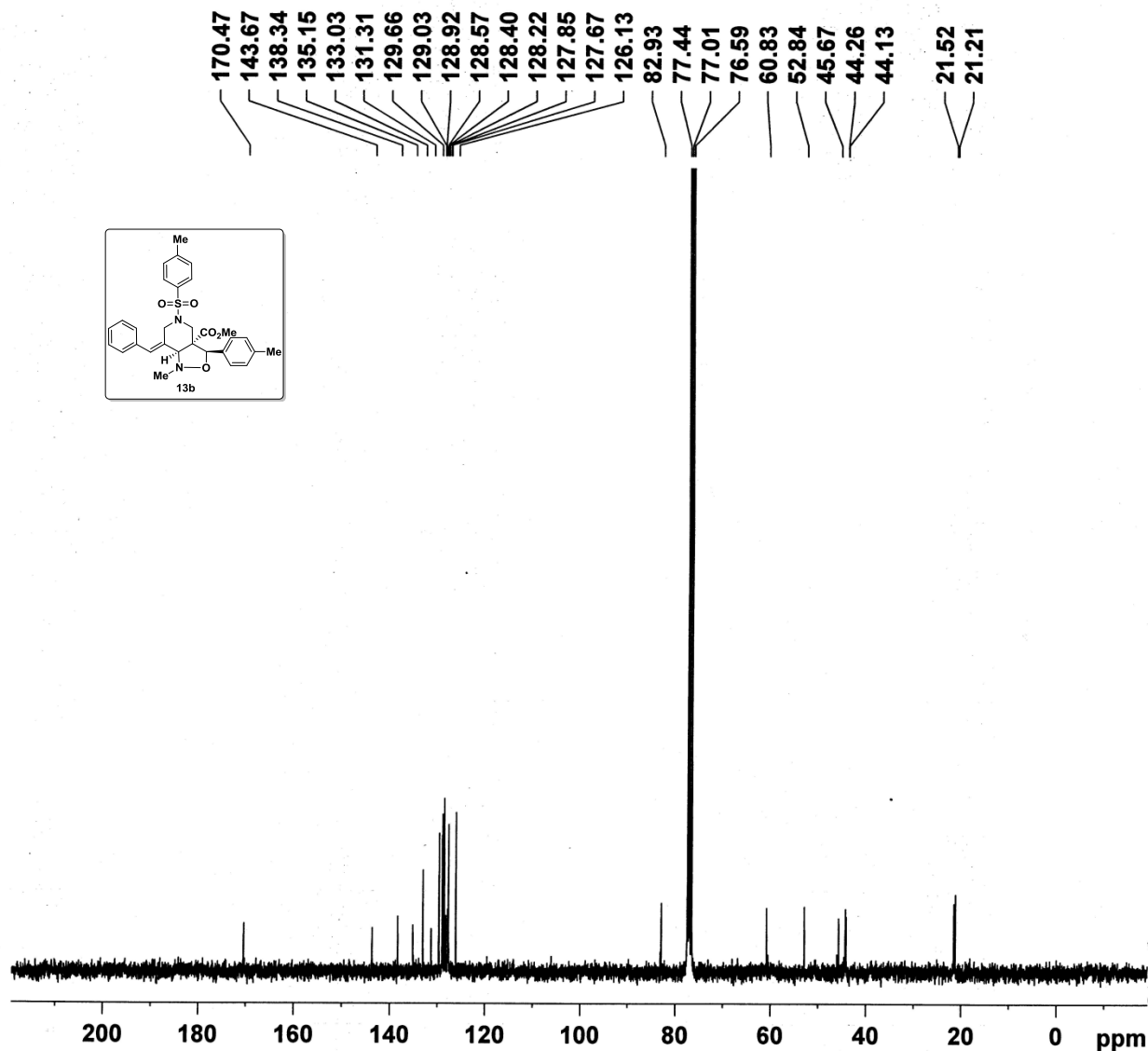
Current Data Parameters
NAME JS-IV-64
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130212
Time 23.34
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 851
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1290.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

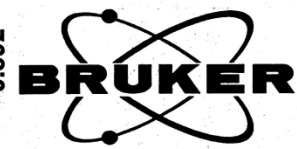
=====
CHANNEL f1
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

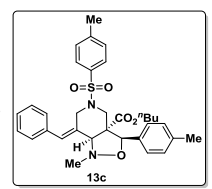


7.452
7.425
7.400
7.376
7.353
7.320
7.296
7.263
7.241
7.221
7.196
7.167
7.140
7.124
7.098
6.635
5.431
4.556
4.244
4.223
4.201
3.988
3.626
3.003
2.962
2.806
2.687
2.648
2.433
2.393
1.681
1.658
1.634
1.415
1.391
1.366
0.940
0.916
0.892



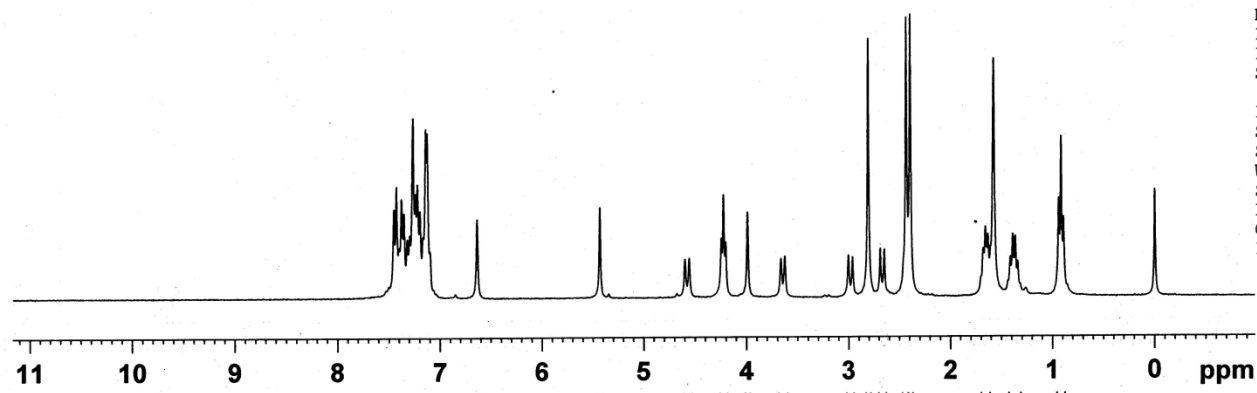
Current Data Parameters
NAME JSBHNTS-13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130514
Time 20.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1



===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.10
2.10
1.82
3.11
4.04
0.85
0.89
0.89
1.89
0.90
0.97
0.89
2.59
0.99
2.99
3.00
2.15
2.12
3.00



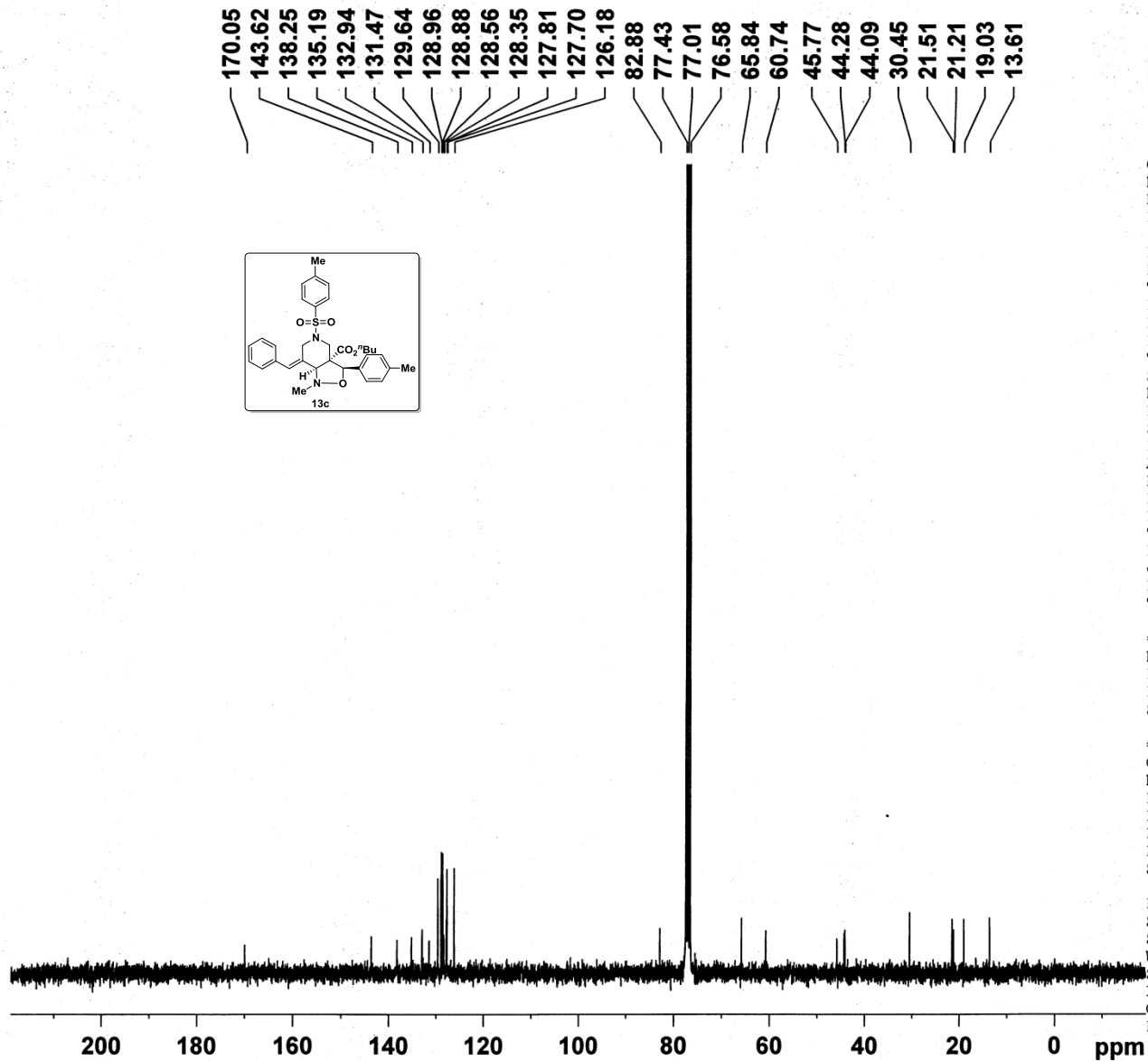
Current Data Parameters
NAME JSBHNTS-13
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130514
Time 20.10
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 681
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

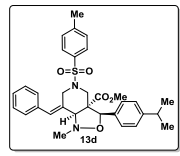
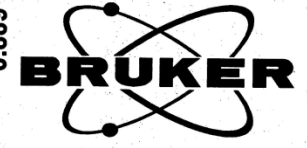
==== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



7.439
7.412
7.378
7.354
7.320
7.298
7.260
7.221
7.192
7.167
7.141
6.641
5.427
4.601
4.559
4.252
4.230
4.208
3.978
3.693
3.654
3.001
2.959
2.948
2.801
2.685
2.645
2.430
1.684
1.660
1.637
1.409
1.385
1.360
1.307
1.284
0.938
0.914
0.889

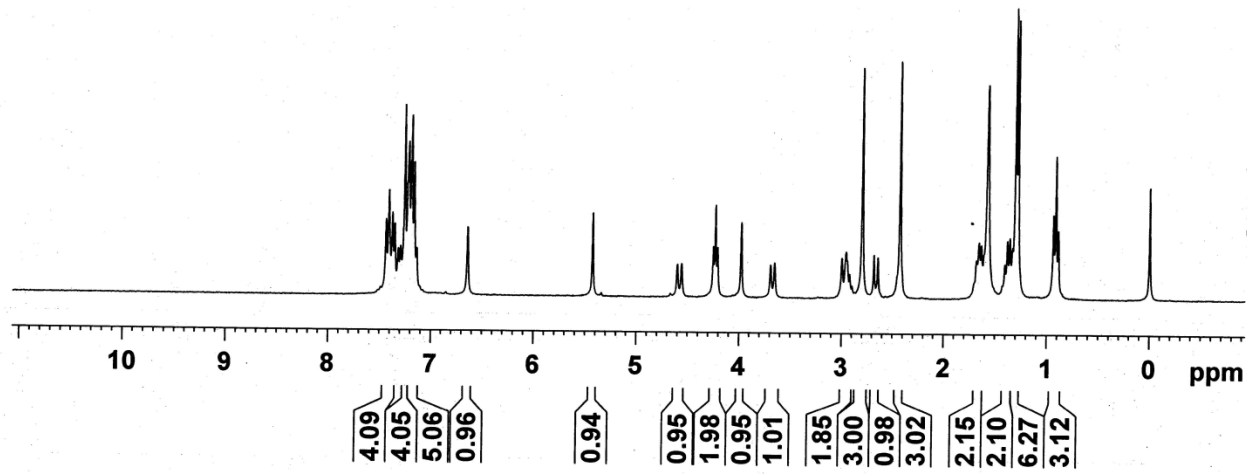


Current Data Parameters
NAME JSBHNTS-21
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130518
Time_ 17.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 203.2
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



10 9 8 7 6 5 4 3 2 1 0 ppm



Current Data Parameters
NAME JSBHNTS-21
EXPNO 2
PROCNO 1

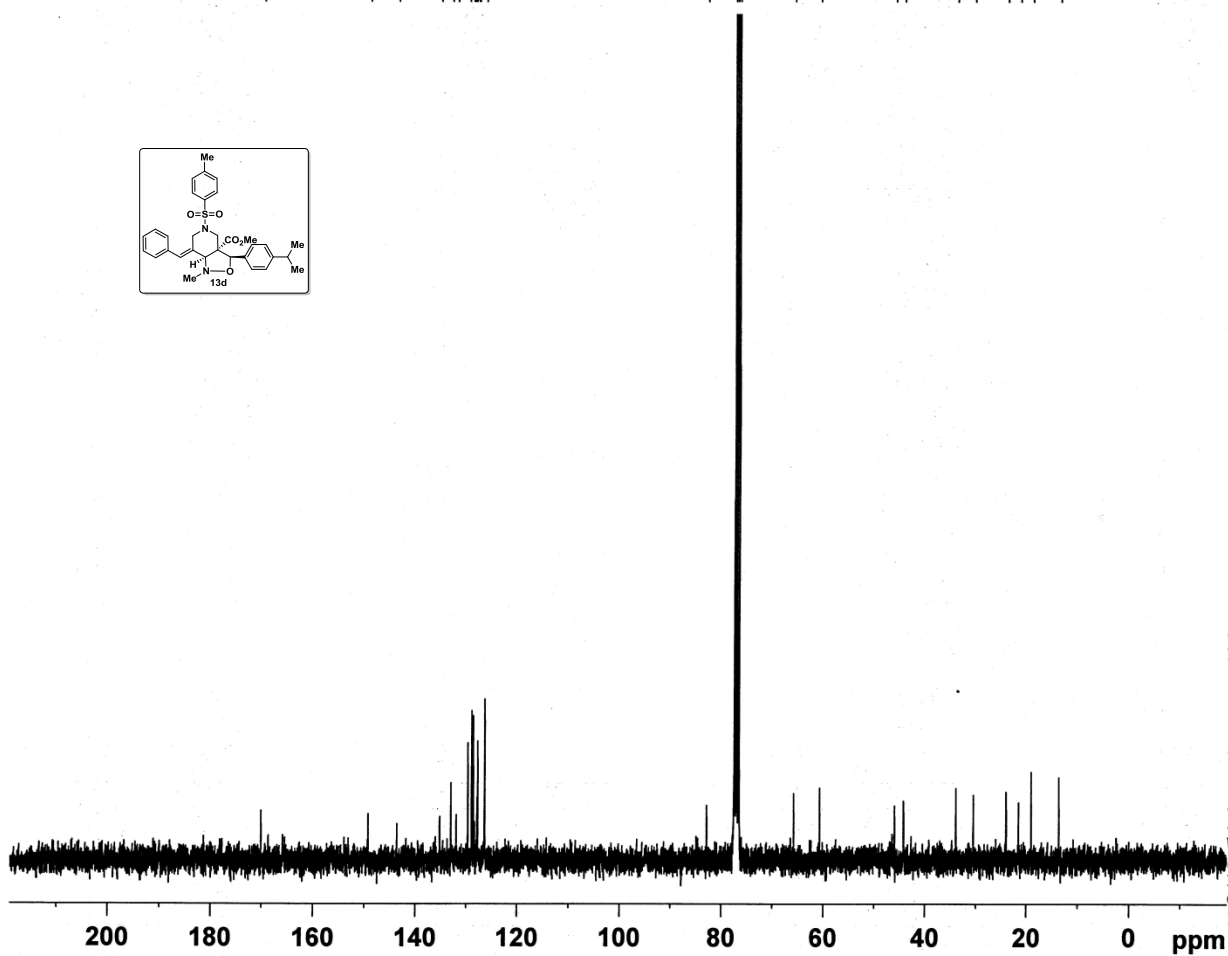
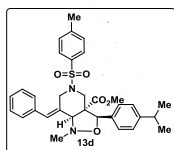
F2 - Acquisition Parameters
Date_ 20130518
Time_ 17.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 667
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2580.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

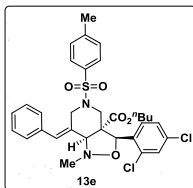
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170.13
149.22
143.61
135.20
132.98
131.92
129.63
128.89
128.56
128.34
127.82
127.68
126.31
82.85
77.43
77.00
76.58
65.83
60.72
45.93
44.19
33.90
30.46
24.00
23.95
21.51
19.04
13.62



7.484
7.455
7.428
7.402
7.395
7.371
7.346
7.322
7.299
7.261
7.243
7.194
7.170
6.652
5.773
4.543
4.502
4.289
4.275
4.253
4.147
4.125
4.111
4.103
4.089
3.989
3.657
3.619
2.986
2.945
2.778
2.674
2.635
2.438
2.410
1.688
1.665
1.638
1.616
1.560
1.423
1.398
1.373
1.347
0.937
0.912
0.888

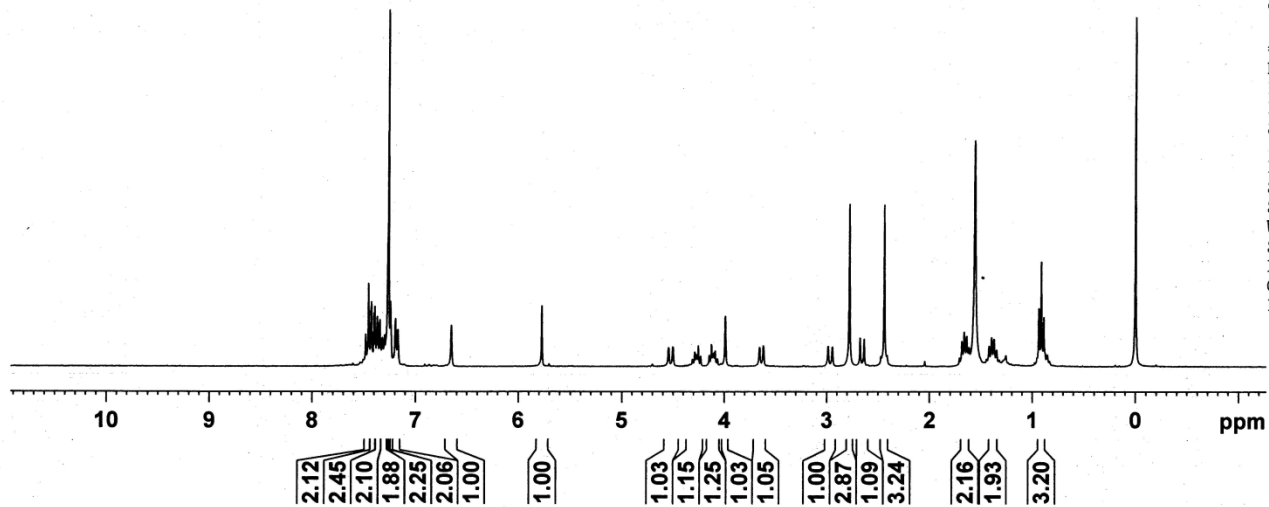


Current Data Parameters
NAME JSBHNTS-28
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131120
Time 0.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 50
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 13.15 use
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





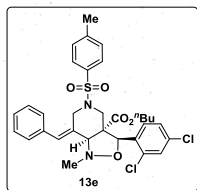
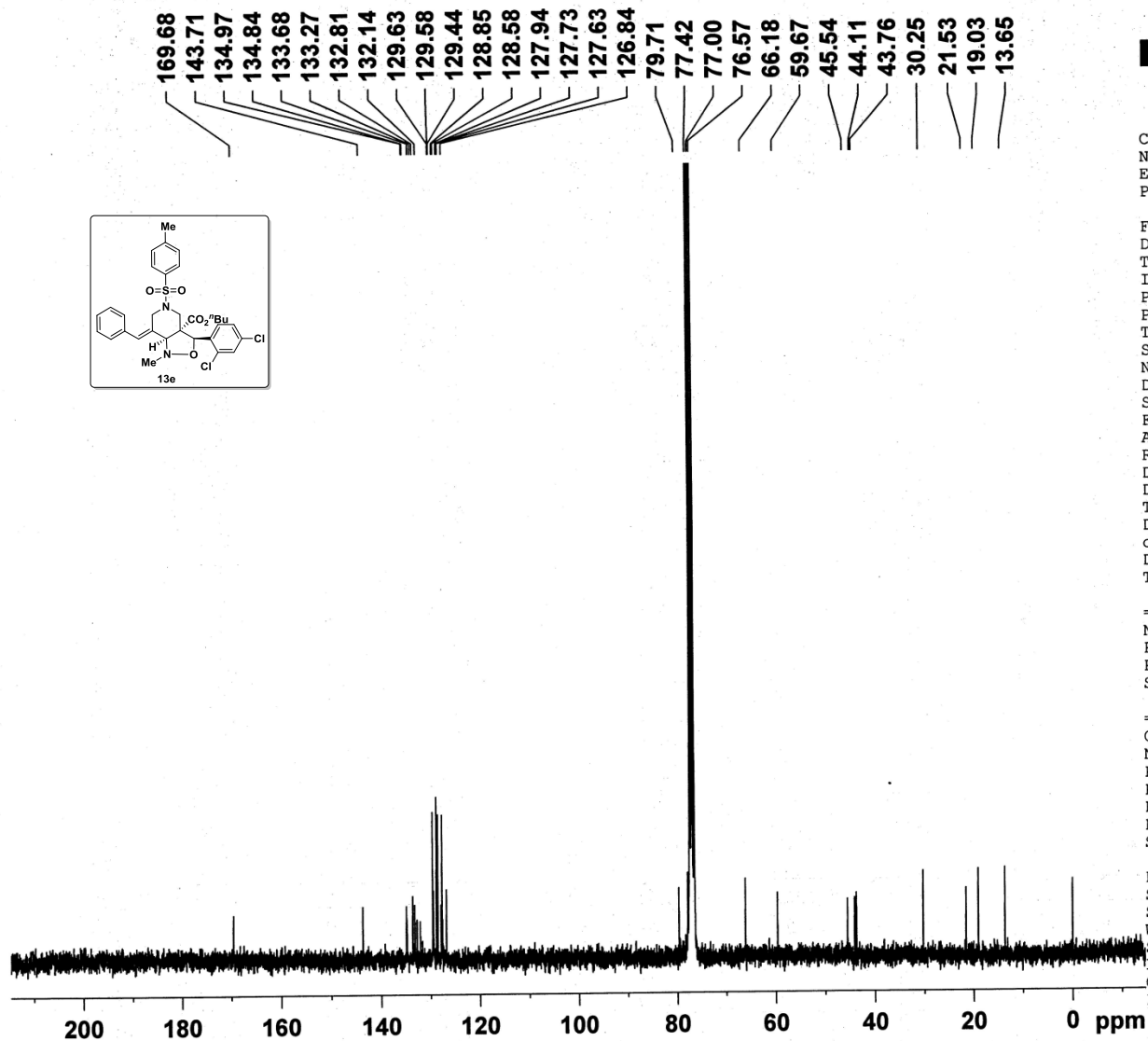
Current Data Parameters
NAME JSBHNTS-28
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131120
Time_ 8.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 7072
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1290.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

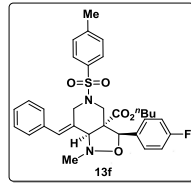


7.480
7.433
7.405
7.380
7.355
7.324
7.300
7.259
7.233
7.222
7.194
7.078
7.050
7.021
6.654
5.426
4.610
4.568
4.259
4.237
4.215
3.955
3.600
3.561
2.994
2.952
2.792
2.612
2.573
2.425
1.715
1.694
1.671
1.644
1.622
1.599
1.452
1.428
1.403
1.378
1.354
0.948



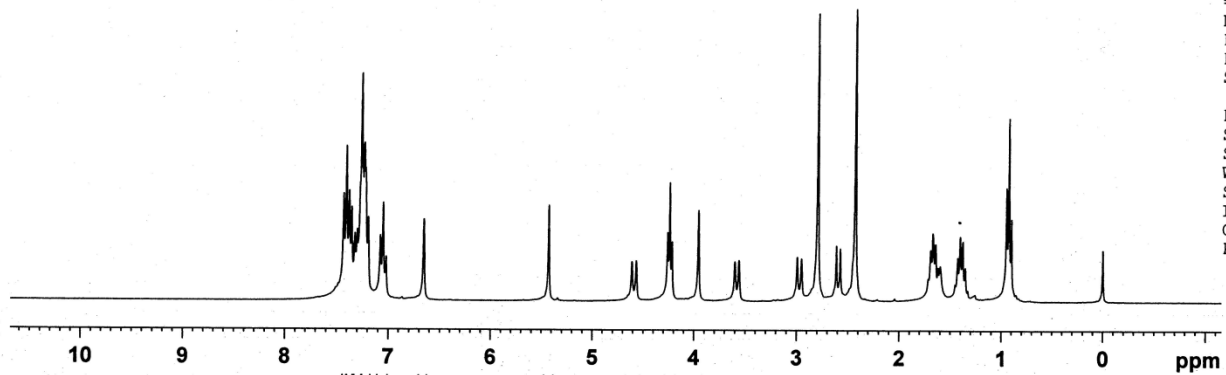
Current Data Parameters
 NAME JSBHNTS-44
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131120
 Time_ 8.32
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 90.5
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1



==== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



1.97
2.17
3.35
3.98
2.11
1.00
0.99
1.09
2.05
0.99
1.08
1.16
3.00
1.20
3.11
2.06
2.15
3.19



Current Data Parameters
NAME JSBHNTS-44
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131120
Time_ 9.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 784
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 912.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

