

## SUPPORTING INFORMATION

### Synthesis of Isoquinolines and Pyridines by the Palladium/ Copper-Catalyzed Coupling and Cyclization of Terminal Acetylenes and Unsaturated Imines: The Total Synthesis of Decumbenine B

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#### Aldehydes Prepared

**2-(2-Cyclohex-1-enylethynyl)benzaldehyde (6).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and 1-ethynylcyclohexene (1.27 g, 12.0 mmol) for 3 h. Column chromatography using 25:1 hexanes/EtOAc afforded 2.00 g (95%) of the compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.57-1.72 (m, 4H), 2.11-2.18 (m, 2H), 2.20-2.25 (m, 2H), 6.27 (dd, *J* = 1.8, 1.8, 6.0, 6.0 Hz, 1H), 7.33-7.39 (m, 1H), 7.49-7.51 (m, 2H), 7.87 (dt, *J* = 1.2, 7.8 Hz, 1H), 10.52 (d, *J* = 0.9 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 21.5, 22.3, 25.9, 29.0, 82.5, 98.6, 120.4, 127.1, 127.7, 128.1, 133.1, 133.8, 135.7, 136.9, 192.0.

**2-(2-Cyclohexylethynyl)benzaldehyde (7).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and cyclohexyl acetylene (1.29 g, 12.0 mmol) for 2 h. Column chromatography using 25:1 hexanes/EtOAc afforded 2.01 g (95%) of the compound as a yellow oil: <sup>1</sup>H NMR

(CDCl<sub>3</sub>) δ 1.34-1.45 (m, 3H), 1.52-1.63 (m, 3H), 1.71-1.78 (m, 2H), 1.87-1.92 (m, 2H), 2.68 (dd, *J* = 3.6, 3.6, 12.6, 12.6 Hz, 1H), 7.34-7.39 (m, 1H), 7.48-7.54 (m, 2H), 7.88 (d, *J* = 8.1 Hz, 1H), 10.56 (d, *J* = 0.6 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 24.9, 25.9, 29.9, 32.5, 76.3, 102.2, 126.9, 127.9, 128.1, 133.3, 133.7, 136.0, 192.3.

**2-[4-(Tetrahydropyran-2-yloxy)but-1-ynyl]benzaldehyde (8).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and 2-(3-butynyloxy)tetrahydro-2*H*-pyran (1.85 g, 12.0 mmol) for 2 h. Column chromatography using 10:1 hexanes/EtOAc afforded 2.56 g (99%) of the compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.48-1.66 (m, 4H), 1.67-1.89 (m, 2H), 2.78 (t, *J* = 6.9 Hz, 2H), 3.49-3.56 (m, 1H), 3.57 (m, 1H), 3.57 (m, 1H), 3.85-3.98 (m, 2H), 3.45-3.41 (m, 1H), 7.49-7.51 (m, 2H), 7.87 (ddd, *J* = 0.6, 0.6, 7.2 Hz, 1H), 10.54 (d, *J* = 0.9 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 19.5, 21.2, 25.5, 30.6, 62.3, 65.5, 77.2, 94.9, 98.9, 127.0, 127.6, 128.2, 133.3, 133.8, 136.2, 192.2.

**2-(3-Hydroxyprop-1-ynyl)benzaldehyde (9).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and propargyl alcohol (0.67 g, 12.0 mmol) for 6 h. Column chromatography using 1:1 hexanes/EtOAc afforded 1.43 g (89%) of the compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 3.68 (br s, 1H), 4.51 (s, 2H), 7.34 (ddd, *J* = 0.6, 3.9, 3.9, 8.7 Hz, 1H), 7.45 (ddd, *J* = 1.2, 1.2, 5.1 Hz, 2H), 7.80 (ddd, *J* = 0.9, 0.9, 7.8 Hz, 1H), 10.41 (d, *J* = 0.6 Hz, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 51.3, 81.0, 94.9, 126.2, 127.5, 128.8, 133.5, 133.9, 135.9, 192.1.

**2-(3-Hydroxy-3-methylbut-1-ynyl)benzaldehyde (10).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and 2-methyl-3-butyn-2-ol (1.01 g, 12.0 mmol) for 2

h. Column chromatography using 3:1 hexanes/EtOAc afforded 1.80 g (96%) of the compound as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.64 (s, 6H), 2.73 (br s, 1H), 7.36-7.42 (m, 1H), 7.48-7.51 (m, 2H), 7.86 (ddd,  $J = 0.9, 0.9, 6.9$  Hz, 1H), 10.46 (d,  $J = 0.6$  Hz, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  31.4, 65.7, 77.8, 101.2, 126.4, 127.4, 128.7, 133.4, 133.8, 135.9, 191.9.

**2-(2-Triisopropylsilyl ethynyl)benzaldehyde (11).** The aldehyde was prepared by the method used to prepare 2-(2-phenylethynyl)benzaldehyde, but employing 2-bromobenzaldehyde (1.85 g, 10.0 mmol) and (triisopropylsilyl)acetylene (2.19 g, 12.0 mmol) for 2 h. Column chromatography using 35:1 hexanes/EtOAc afforded 2.65 g (92%) of the compound as a colorless oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.15 (s, 21H), 7.44 (dd,  $J = 0.6, 0.6, 7.8, 7.8$  Hz, 1H), 7.52-7.62 (m, 2H), 7.92 (ddd,  $J = 0.6, 0.6, 7.8$  Hz, 1H), 10.62 (d,  $J = 0.9$  Hz, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  11.3, 18.7, 99.2, 102.1, 126.9, 127.2, 128.8, 133.7, 134.0, 136.3, 191.8.

### Imines Prepared

***N*-(2-Phenylethynylbenzylidene)-*tert*-butylamine (3).** The imine was prepared by the method used to prepare imine **1**, but employing 2-(2-phenyl-ethynyl)benzaldehyde (0.80 g, 3.88 mmol). Removal of the solvent afforded 1.00 g (97%) of the imine **3** as a yellow oil, which solidified upon cooling: mp 52-53 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.34 (s, 9H), 7.28-7.35 (m, 5H), 7.49-7.54 (m, 3H), 8.07-8.10 (m, 1H), 8.94 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  30.0, 58.0, 86.9, 95.1, 123.3, 124.1, 126.2, 128.7, 128.7, 128.8, 129.9, 131.6, 132.4, 138.0, 154.2; IR ( $\text{CHCl}_3$ ,  $\text{cm}^{-1}$ ) 3060, 2214, 1637; HRMS Calcd for  $\text{C}_{19}\text{H}_{19}\text{N}$ : 261.1518. Found: 261.1518.

***N*-(2-Cyclohex-1-enylethynylbenzylidene)-*tert*-butylamine (12).** The imine was prepared by the method used to prepare imine **1**, but employing

2-(2-cyclohex-1-enylethynyl)benzaldehyde (1.05 g, 5 mmol). Removal of the solvent afforded 1.28 g (96%) of the imine **12** as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.32 (s, 9H), 1.59-1.74 (m, 4H), 2.13-2.20 (m, 2H), 2.22-2.27 (m, 2H), 6.23 (dd,  $J$  = 1.8, 1.8, 6.0, 6.0 Hz, 1H), 7.29-7.33 (m, 2H), 7.39-7.45 (m, 1H), 7.98-8.05 (m, 1H), 8.82 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  21.6, 22.4, 25.9, 29.3, 29.9, 57.8, 84.2, 97.0, 120.8, 124.5, 125.9, 128.2, 129.7, 132.1, 135.6, 137.6, 154.6; IR (neat,  $\text{cm}^{-1}$ ) 3062, 2200, 1637; HRMS Calcd for  $\text{C}_{19}\text{H}_{23}\text{N}$ : 265.1830. Found: 265.1831.

**N-(2-Cyclohexylethynylbenzylidene)-*tert*-butylamine (13).** The imine was prepared by the method used to prepare imine **1**, but employing 2-(2-cyclohexyl-ethynyl)benzaldehyde (0.85 g, 4 mmol). Removal of the solvent afforded 1.01 g (95%) of the imine **13** as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.31 (s, 9H), 1.35-1.45 (m, 3H), 1.50-1.63 (m, 3H), 1.73-1.81 (m, 2H), 1.85-1.92 (m, 2H), 2.68 (dd,  $J$  = 3.6, 3.6, 12.3, 12.3 Hz, 1H), 7.26-7.31 (m, 2H), 7.37-7.43 (m, 1H), 7.98-8.03 (m, 1H), 8.83 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  24.8, 26.0, 29.8, 29.9, 32.7, 57.8, 78.0, 100.2, 124.9, 125.8, 127.9, 129.7, 132.2, 137.8, 154.8; IR (neat,  $\text{cm}^{-1}$ ) 3062, 2224, 1683; HRMS Calcd for  $\text{C}_{19}\text{H}_{25}\text{N}$ : 267.1987. Found: 267.1987.

**N-[4-(Tetrahydropyran-2-yloxy)but-1-ynylbenzylidene]-*tert*-butylamine (14).** The imine was prepared by the method used to prepare imine **1**, but employing 2-[4-(tetrahydropyran-2-yloxy)but-1-ynyl]benzaldehyde (0.78 g, 3 mmol). Removal of the solvent afforded 0.88 g (94%) of the imine **14** as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.30 (s, 9H), 1.48-1.65 (m, 4H), 1.68-1.89 (m, 2H), 2.78 (t,  $J$  = 7.2 Hz, 2H), 3.48-3.56 (m, 1H), 3.67 (m, 1H), 3.86-3.97 (m, 2H), 4.68 (t,  $J$  = 3.0 Hz, 1H), 7.26-7.31 (m, 2H), 7.37-7.42 (m, 1H), 7.97-8.03 (m, 1H), 8.78 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  19.5, 21.2, 25.5, 29.8, 30.7, 57.7, 62.3, 65.9, 78.8, 92.7, 98.9, 124.4, 125.9, 128.1, 129.7, 132.4, 137.8, 154.5; IR (neat,  $\text{cm}^{-1}$ ) 3063, 2229, 1637; HRMS Calcd for  $\text{C}_{20}\text{H}_{27}\text{NO}_2$ : 313.2040. Found: 313.2042.

**N-[2-(3-Hydroxyprop-1-ynyl)benzylidene]-*tert*-butylamine (15).** The imine was prepared by the method used to prepare imine **1**, but employing 2-(3-hydroxyprop-1-ynyl)benzaldehyde (1.00 g, 6.25 mmol). Removal of the solvent afforded 1.30 g (96%) of the imine **15** as a tan solid: mp 50-51 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.30 (s, 9H), 4.04 (br s, 1H), 4.45 (s, 2H), 7.23-7.38 (m, 3H), 7.99 (dd, *J* = 1.8, 7.5 Hz, 1H), 8.01 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 29.8, 51.0, 58.1, 82.3, 93.6, 123.6, 126.1, 128.7, 129.9, 132.6, 137.6, 155.1; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3332, 3066, 2969, 1637; HRMS Calcd for C<sub>14</sub>H<sub>17</sub>NO: 215.1310. Found: 215.1310.

**N-[2-(3-Hydroxy-3-methylbut-1-ynyl)benzylidene]-*tert*-butylamine (16).** The imine was prepared by the method used to prepare imine **1**, but employing 2-(3-hydroxy-3-methylbut-1-ynyl)benzaldehyde (0.75 g, 4 mmol). Removal of the solvent afforded 0.94 g (97%) of the imine **16** as a viscous yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.31 (s, 9H), 1.64 (s, 6H), 2.47 (br s, 1H), 7.27-7.36 (m, 2H), 7.38-7.43 (m, 1H), 8.01-8.04 (m, 1H), 8.77 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 29.8, 31.6, 58.0, 65.7, 79.5, 99.5, 123.4, 126.0, 128.7, 129.7, 132.3, 137.9, 154.3; IR (neat, cm<sup>-1</sup>) 3359, 3063, 2222, 1637; HRMS Calcd for C<sub>16</sub>H<sub>21</sub>NO: 243.1619. Found: 243.1623.

**N-[2-(Triisopropylsilylethynyl)benzylidene]-*tert*-butylamine (17).** The imine was prepared by the method used to prepare imine **1**, but employing 2-(triisopropylsilylethynyl)benzaldehyde (0.57 g, 2 mmol). Removal of the solvent afforded 0.66 g (97%) of the imine **17** as a colorless oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.15 (s, 21H), 1.31 (s, 9H), 7.29-7.38 (m, 2H), 7.49-7.52 (m, 1H), 8.02-8.08 (m, 1H), 8.88 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 11.37, 18.8, 29.9, 57.8, 96.5, 104.2, 124.2, 125.9, 128.7, 129.6, 133.1, 138.2, 154.3; IR (neat, cm<sup>-1</sup>) 3064, 2153, 1702, 1637; HRMS Calcd for C<sub>22</sub>H<sub>35</sub>NSi: 341.2540. Found: 341.2539.

**N-(6-Bromobenzo[1,3]dioxol-5-ylmethylene)-*tert*-butylamine (25).** The imine was prepared by the method used to prepare imine **1**, but employing 2-bromopiperonal (2.00 g, 8.73 mmol). Removal of the solvent afforded 2.27 g (92%) of the imine **25** as a white solid: mp 73–74 °C; <sup>1</sup>H NMR ( $\text{CDCl}_3$ ) δ 1.29 (s, 9H), 5.99 (s, 2H), 6.98 (s, 1H), 7.52 (s, 1H), 8.50 (s, 1H); <sup>13</sup>C NMR ( $\text{CDCl}_3$ ) δ 29.8, 57.8, 102.1, 107.8, 112.5, 117.2, 129.5, 147.9, 150.1, 154.2; IR ( $\text{CHCl}_3$ ,  $\text{cm}^{-1}$ ) 3077, 2963, 1627; HRMS Calcd for  $\text{C}_{12}\text{H}_{14}\text{BrNO}_2$ : 283.0208. Found: 283.0205.

**N-(2-Bromopyridin-3-ylmethylene)-*tert*-butylamine (28).** The imine was prepared by the method used to prepare imine **1**, but employing 2-bromo-3-formylpyridine (0.51 g, 2.74 mmol). Removal of the solvent afforded 0.62 g (94%) of the imine **28** as a yellow oil: <sup>1</sup>H NMR ( $\text{CDCl}_3$ ) δ 1.28 (s, 9H), 7.27 (dd,  $J = 4.8, 7.8$  Hz, 1H), 8.25 (dd,  $J = 1.8, 7.5$  Hz, 1H), 8.34 (dd,  $J = 0.9, 4.5$  Hz, 1H), 8.48 (s, 1H); <sup>13</sup>C NMR ( $\text{CDCl}_3$ ) δ 29.6, 58.5, 123.2, 132.9, 136.9, 144.0, 151.1, 153.2; IR (neat,  $\text{cm}^{-1}$ ) 3043, 2968, 1633, 1576; HRMS Calcd for  $\text{C}_{10}\text{H}_{13}\text{BrN}_2$ : 240.0262. Found: 240.0262.

**N-(2-Bromocyclopent-1-enylmethylene)-*tert*-butylamine (31).** The imine was prepared by the method used to prepare imine **1**, but employing 2-bromocyclopentene-1-carboxaldehyde (0.75 g, 4.31 mmol). Removal of the solvent afforded 0.89 g (90%) of the imine **31** as a dark yellow oil: <sup>1</sup>H NMR ( $\text{CDCl}_3$ ) δ 1.22 (s, 9H), 1.97 (quintet,  $J = 7.5$  Hz, 2H), 2.59 (tt,  $J = 2.1, 7.5$  Hz, 2H), 2.79 (tt,  $J = 2.4, 7.5$  Hz, 2H), 8.18 (s, 1H); <sup>13</sup>C NMR ( $\text{CDCl}_3$ ) δ 21.6, 29.8, 31.1, 41.6, 57.7, 127.9, 139.1, 151.8; IR (neat,  $\text{cm}^{-1}$ ) 2965, 1630; HRMS Calcd for  $\text{C}_{10}\text{H}_{16}\text{BrN}$ : 229.0466. Found: 229.0460.

**N-(1-Bromo-3,4-dihydroronaphthalen-2-ylmethylene)-*tert*-butylamine (34).** The imine was prepared by the method used to prepare imine **1**, but employing 1-bromo-3,4-dihydroronaphthalene-2-carboxaldehyde (0.77 g, 3.26 mmol). Removal of the solvent afforded

0.85 g (89%) of the imine **34** as a viscous yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.31 (s, 9H), 2.81-2.83 (m, 4H), 7.16 (dd,  $J$  = 1.8, 6.9 Hz, 1H), 7.22-7.31 (m, 2H), 7.79 (dd,  $J$  = 1.8, 7.2 Hz, 1H), 8.61 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  25.3, 27.7, 30.0, 58.1, 126.8, 127.3, 127.6, 128.6, 129.1, 134.2, 135.9, 138.3, 157.0; IR (neat,  $\text{cm}^{-1}$ ) 3063, 2965, 1612; HRMS Calcd for  $\text{C}_{15}\text{H}_{18}\text{BrN}$ : 291.0623. Found: 290.0548 (M-H).

**N-[(Z)-3-Iodo-3-phenylallylidene]-*tert*-butylamine (36).** The imine was prepared by the method used to prepare imine **1**, but employing Z-3-iodo-3-phenyl-2-propenal (0.60 g, 2.33 mmol). Removal of the solvent afforded 0.64 g (87%) of the imine **36** as a yellow solid: mp 81-83 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.29 (s, 9H), 6.77 (d,  $J$  = 7.8 Hz, 1H), 7.32-7.35 (m, 3H), 7.56-7.60 (m, 2H), 8.15 (d,  $J$  = 7.5 Hz, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  29.7, 58.4, 113.6, 128.5, 128.8, 129.6, 134.9, 142.0, 161.4; IR ( $\text{CHCl}_3$ ,  $\text{cm}^{-1}$ ) 3078, 2967, 1614; HRMS Calcd for  $\text{C}_{13}\text{H}_{16}\text{IN}$ : 313.0328. Found: 313.0332.

### Isoquinolines Prepared by the Copper-Catalyzed Cyclization of Iminoalkynes

**3-(Cyclohex-1-enyl)isoquinoline (4).** The reaction mixture was chromatographed using 15:1 hexanes/EtOAc to afford 42 mg (81%) of the indicated compound as a yellow solid: mp 114-115 °C (hexanes/EtOAc);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.67-1.75 (m, 2H), 1.81-1.89 (m, 2H), 2.29-2.36 (m, 2H), 2.54-2.60 (m, 2H), 7.02 (tt,  $J$  = 2.4, 3.6 Hz, 1H), 7.48 (dt,  $J$  = 0.6, 14.4 Hz, 1H), 7.57 (s, 1H), 7.63 (dd,  $J$  = 1.2, 6.9 Hz, 1H), 7.74 (d,  $J$  = 8.1 Hz, 1H), 7.89 (d,  $J$  = 8.1 Hz, 1H), 9.18 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  22.3, 23.1, 26.1, 26.2, 114.2, 126.4, 126.8, 127.6, 128.4, 130.3, 135.7, 136.7, 151.7, 152.5 (one  $\text{sp}^2$  carbon missing due to overlap); IR ( $\text{CHCl}_3$ ,  $\text{cm}^{-1}$ ) 3060, 2919, 1621, 1574; MS  $m/z$  (rel intensity) 209 (100,  $\text{M}^+$ ), 208 (89), 194 (42), 180 (51). Anal. Calcd for  $\text{C}_{15}\text{H}_{15}\text{N}$ : C, 86.09; H, 7.23; N, 6.69. Found: C, 86.03; H, 7.30; N, 6.73.

**3-Cyclohexylisoquinoline (5).** The reaction mixture was chromatographed using 15:1 hexanes/EtOAc to afford 49 mg (93%) of the indicated compound as a yellow oil, which solidified upon cooling: mp 40-41 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.25-1.67 (m, 6H), 1.89 (dt, *J* = 2.7, 12.6 Hz, 2H), 2.06 (dd, *J* = 1.5, 12.9 Hz, 2H), 2.84 (tt, *J* = 3.3, 11.7 Hz, 1H), 7.45 (s, 1H), 7.50 (ddd, *J* = 1.2, 6.9, 8.1 Hz, 1H), 7.62 (dt, *J* = 1.2, 6.9 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 9.19 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 26.3, 26.8, 33.2, 46.2, 116.2, 126.3, 126.4, 127.3, 127.5, 130.2, 136.7, 151.9, 160.2; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3055, 2926, 1628, 1585; HRMS Calcd for C<sub>15</sub>H<sub>17</sub>N: 211.1356. Found: 211.1361.

**3-[2-(Tetrahydropyran-2-yloxy)ethyl]isoquinoline (18).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 53 mg (83%) of the indicated compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.40-1.60 (m, 4H), 1.61-1.82 (m, 2H), 3.23 (t, *J* = 7.2 Hz, 2H), 3.42-3.48 (m, 1H), 3.76 (ddd, *J* = 3.3, 8.1, 11.7 Hz, 1H), 3.87 (ddd, *J* = 6.9, 9.6, 16.5 Hz, 1H), 4.18 (ddd, *J* = 6.9, 9.6, 16.8 Hz, 1H), 4.62 (m, 1H), 7.52 (ddd, *J* = 1.2, 6.9, 9.3 Hz, 1H), 7.55 (s, 1H), 7.63 (ddd, *J* = 1.2, 6.6, 9.3 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 9.19 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 19.6, 25.5, 30.7, 38.5, 62.3, 67.0, 98.9, 119.2, 126.2, 126.6, 127.3, 127.6, 130.3, 136.5, 152.1, 152.6; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3054, 2942, 1629, 1588; HRMS Calcd for C<sub>16</sub>H<sub>19</sub>NO<sub>2</sub>: 257.1416. Found: 257.1415.

### Isoquinolines and Pyridines Prepared by the Palladium/Copper-Catalyzed Coupling and Cyclization of Terminal Alkynes

**3-(Cyclohex-1-enyl)isoquinoline (4).** The reaction mixture was chromatographed using 15:1 hexanes/EtOAc to afford 85 mg (81%) of the indicated compound, whose spectral data were identical with that reported above.

**3-Cyclohexylisoquinoline (5).** The reaction mixture was chromatographed using 15:1 hexanes/EtOAc to afford 93 mg (88%) of the indicated compound, whose spectral data were identical with that reported above.

**3-[2-(Tetrahydropyran-2-yloxy)ethyl]isoquinoline (18).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 122 mg (95%) of the indicated compound, whose spectral data were identical with that reported above.

**3-(Diethoxymethyl)isoquinoline (22).** The reaction mixture was chromatographed using 4:1 hexanes/EtOAc to afford 97 mg (84%) of the indicated compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.25 (dt, *J* = 0.6, 13.5 Hz, 6H), 3.67 (dddd, *J* = 0.6, 7.2, 7.8, 16.5 Hz, 4H), 5.67 (s, 1H), 7.54 (dddd, *J* = 1.2, 1.2, 8.1, 8.1 Hz, 1H), 7.64 (dddd, *J* = 1.2, 1.2, 6.9, 6.9 Hz, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.90-7.93 (m, 2H), 9.23 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 15.3, 62.0, 102.4, 117.7, 127.2, 127.46, 127.51, 128.4, 130.5, 136.2, 151.5, 152.2; IR (neat, cm<sup>-1</sup>) 3056, 2975, 1629, 1587; HRMS Calcd for C<sub>14</sub>H<sub>17</sub>NO<sub>2</sub>: 231.1259. Found: 232.1338 (M+H).

**4-(3-Isoquinoliny)butanenitrile (23).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 85 mg (87%) of the indicated compound as an off-white solid: mp 104-105 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.18 (pentet, *J* = 7.2 Hz, 2H), 2.36 (t, *J* = 7.8 Hz, 2H), 3.04 (t, *J* = 7.2 Hz, 2H), 7.48 (s, 1H), 7.53 (ddd, *J* = 1.2, 6.9, 9.3 Hz, 1H), 7.64 (ddd, *J* = 1.2, 6.9, 9.3 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 9.17 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 16.6, 25.3, 36.4, 118.9, 119.7, 126.2, 126.9, 127.4, 127.6, 130.7, 136.4, 152.6, 152.8; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3054, 2946, 1627, 1586; HRMS Calcd for C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>: 196.1000. Found: 196.1001.

**3-[3-(3-Isoquinoliny)propyl]isoquinoline (24).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 42 mg (56%) of the indicated compound

as a yellow solid: mp 116-117 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.37 (pentet, *J* = 8.1 Hz, 2H), 3.05 (t, *J* = 8.4 Hz, 4H), 7.48 (s, 2H), 7.51 (ddd, *J* = 1.2, 6.9, 9.3 Hz, 2H), 7.62 (ddd, *J* = 1.2, 6.9, 9.6 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.91 (d, *J* = 8.4 Hz, 2H), 9.19 (br s, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 30.1, 37.8, 118.3, 126.2, 126.4, 127.2, 127.5, 130.3, 136.6, 152.2, 155.3; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3054, 2946, 1627, 1586; HRMS Calcd for C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>: 298.1470. Found: 298.1469.

**7-Cyclohexyl-1,3-dioxolo[4,5-*g*]isoquinoline (26).** The reaction mixture was chromatographed using 2:1 hexanes/EtOAc to afford 97 mg (76%) of the indicated compound as a yellow solid: mp 93-94 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.20-1.61 (m, 5H), 1.71-1.77 (m, 1H), 1.85 (dt, *J* = 3.0, 12.3 Hz, 2H), 1.97-2.02 (m, 2H), 2.74 (tt, *J* = 3.3, 8.1 Hz, 1H), 6.01 (s, 2H), 6.95 (s, 1H), 7.09 (s, 1H), 7.25 (s, 1H), 8.89 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 26.3, 26.8, 33.3, 46.0, 101.4, 102.3, 103.0, 116.1, 124.3, 135.1, 147.7, 149.7, 150.8, 159.3; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3029, 2923, 1601, 1584, 1482, 1453; HRMS Calcd for C<sub>16</sub>H<sub>17</sub>NO<sub>2</sub>: 255.1259. Found: 255.1254.

**7-[2-(Tetrahydropyran-2-yloxy)ethyl]-1,3-dioxolo[4,5-*g*]isoquinoline (27).** The reaction mixture was chromatographed using 1:2 hexanes/EtOAc to afford 122 mg (81%) of the indicated compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 1.38-1.79 (m, 6H), 3.12 (t, *J* = 6.9 Hz, 2H), 3.38-3.45 (m, 1H), 3.69-3.84 (m, 2H), 4.06-4.15 (m, 1H), 4.57-4.59 (m, 1H), 6.01 (s, 2H), 6.94 (s, 1H), 7.08 (s, 1H), 7.34 (s, 1H), 8.87 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 19.6, 25.5, 30.7, 38.3, 62.3, 67.1, 98.9, 101.5, 102.2, 103.0, 119.0, 124.4, 134.9, 147.9, 149.8, 150.9, 151.7; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3051, 2942, 1604, 1481, 1456; HRMS Calcd for C<sub>17</sub>H<sub>19</sub>NO<sub>4</sub>: 301.1314. Found: 301.1313.

**7-Phenyl-1,6-naphthyridine (29).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 88 mg (85%) of the indicated compound as a yellow solid: mp 135-136 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.39-7.45 (m, 2H), 7.48-7.53 (m, 2H), 8.13-8.17 (m, 2H), 8.23 (d, *J* = 8.1 Hz, 1H), 8.31 (s, 1H), 9.04 (br s, 1H), 9.30 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 117.9, 122.3, 122.7, 127.3, 129.0, 129.2, 135.6, 138.9, 151.4, 152.7, 155.1, 155.2; IR (CDCl<sub>3</sub>, cm<sup>-1</sup>) 3048, 1618, 1594, 1558; HRMS Calcd for C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>: 206.0844. Found: (CDCl<sub>3</sub>, cm<sup>-1</sup>) 3048, 1618, 1594, 1558; HRMS Calcd for C<sub>14</sub>H<sub>10</sub>N<sub>2</sub>: 206.0844. Found: 206.0840.

**7-*n*-Butyl-1,6-naphthyridine (30).** The reaction mixture was chromatographed using 1:1 hexanes/EtOAc to afford 67 mg (72%) of the indicated compound as a yellow oil: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 0.91 (t, *J* = 7.5 Hz, 3H), 1.38 (sextet, *J* = 7.5 Hz, 2H), 1.77 (quintet, *J* = 7.5 Hz, 2H), 2.95 (t, *J* = 7.5 Hz, 2H), 7.39 (dd, *J* = 4.2, 8.4 Hz, 1H), 7.69 (s, 1H), 8.19 (dd, *J* = 0.9, 8.4 Hz, 1H), 8.99 (d, *J* = 2.7 Hz, 1H), 9.16 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 14.0, 22.5, 31.9, 38.0, 119.6, 121.7, 121.9, 135.6, 151.1, 152.4, 154.8, 160.4; IR (neat, cm<sup>-1</sup>) 3051, 2942, 1604, 1481, 1456; HRMS Calcd for C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>: 186.1157. Found: 186.1159.

**6,7-Dihydro-5*H*[2]-3-phenylpyrindine (32).** The reaction mixture was chromatographed using 7:1 hexanes/EtOAc to afford 68 mg (69%) of the indicated compound with <sup>1</sup>H spectral properties identical to those previously reported<sup>1</sup>: mp 49-50 °C (hexanes/EtOAc); <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.13 (quintet, *J* = 7.5 Hz, 2H), 2.95 (t, *J* = 7.2 Hz, 4H); 7.35-7.41 (m, 1H), 7.42-7.48 (m, 2H), 7.59 (d, *J* = 0.3 Hz, 1H), 7.94-7.98 (m, 2H), 8.54 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 25.2, 30.1, 32.8, 116.9, 127.0, 128.5, 128.7, 138.8, 140.1, 145.5, 154.7, 155.5; IR (CHCl<sub>3</sub>, cm<sup>-1</sup>) 3067, 2950, 1611, 1556; HRMS Calcd for C<sub>14</sub>H<sub>13</sub>N: 195.1048. Found: 194.0965 (M-H).

**6,7-Dihydro-5H[2]-3-(cyclohex-1-enyl)pyrindine (33).** The reaction mixture was chromatographed using 7:1 hexanes/EtOAc to afford 55 mg (55%) of the indicated compound as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  1.62-1.69 (m, 2H), 1.74-1.81 (m, 2H), 2.07 (quintet,  $J = 7.5$  Hz, 2H), 2.22-2.25 (m, 2H), 2.47-2.49 (m, 2H), 2.88 (q,  $J = 6.9$  Hz, 4H), 6.56-6.59 (m, 1H), 7.24 (s, 1H), 8.38 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  22.3, 23.0, 25.2, 26.0, 26.4, 30.1, 32.8, 115.2, 127.5, 136.9, 137.9, 144.5, 154.1, 157.2; IR ( $\text{CHCl}_3$ ,  $\text{cm}^{-1}$ ) 3059, 2854, 1602, 1554, 1477; HRMS Calcd for  $\text{C}_{14}\text{H}_{17}\text{N}$ : 199.1361. Found: 199.1361.

**2-n-Butyl-5,6-dihydrobenzo[f]isoquinoline (35).** The reaction mixture was chromatographed using 4:1 hexanes/EtOAc to afford 55 mg (46%) of the indicated compound as a yellow oil:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  0.96 (t,  $J = 7.5$  Hz, 3H), 1.42 (sextet,  $J = 7.5$  Hz, 2H), 1.75 (quintet,  $J = 7.8$  Hz, 2H), 2.80-2.92 (m, 6H), 7.24-7.36 (m, 3H), 7.44 (s, 1H), 7.75-7.82 (m, 1H), 8.39 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  14.1, 22.6, 25.1, 28.7, 32.4, 38.2, 116.5, 124.2, 127.2, 128.6, 129.0, 129.3, 132.3, 138.4, 142.0, 148.5, 161.3; IR (neat,  $\text{cm}^{-1}$ ) 3061, 2933, 1603, 1544, 1483; HRMS Calcd for  $\text{C}_{17}\text{H}_{19}\text{N}$ : 237.1517. Found: 237.1508.

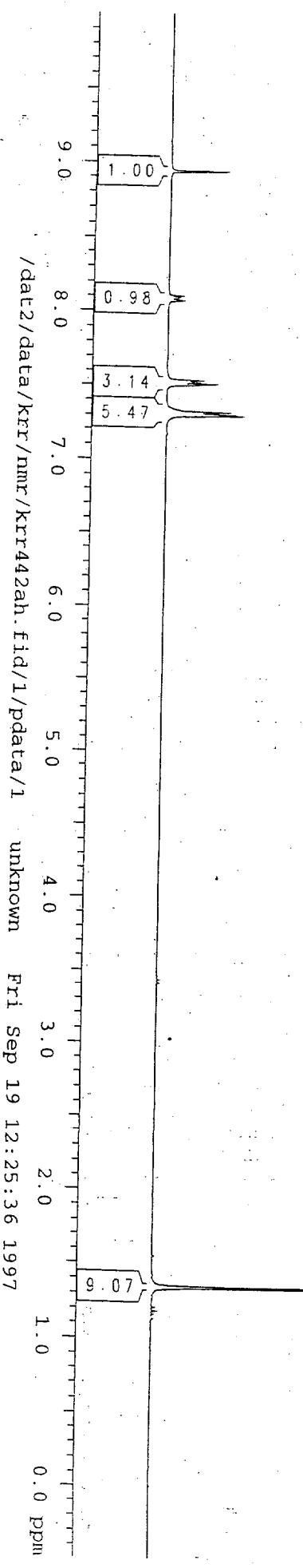
**2,4-Diphenylpyridine (37).** The reaction mixture was chromatographed using 15:1 hexanes/EtOAc to afford 66 mg (57%) of the indicated compound as a yellow oil with spectral properties identical to those previously reported.<sup>2</sup>

**$^1\text{H}$  and  $^{13}\text{C}$  Spectra for Compounds 3, 12-17, 18, 23-25, 27-29, 32 and 35 follow.**

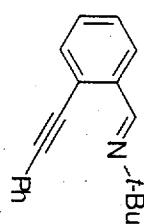
## References

1. Battaglia, L. P.; Delledonne, D.; Nardelli, M.; Predieri, G.; Chiusoli, G. P.; Costa, M.; Pelizzi, C. *J. Organomet. Chem.* **1989**, 363, 209.

2. (a) Katritzky, A. R.; Mazurkiewicz, R.; Stevens, C. V.; Gordeev, M. F. *J. Org. Chem.* **1994**, 59, 2740. (b) Katritzky, A. R.; Chapman, A. V.; Cook, M. J.; Millet, G. H. *J. Chem. Soc., Perkin Trans. 1* **1980**, 2743.



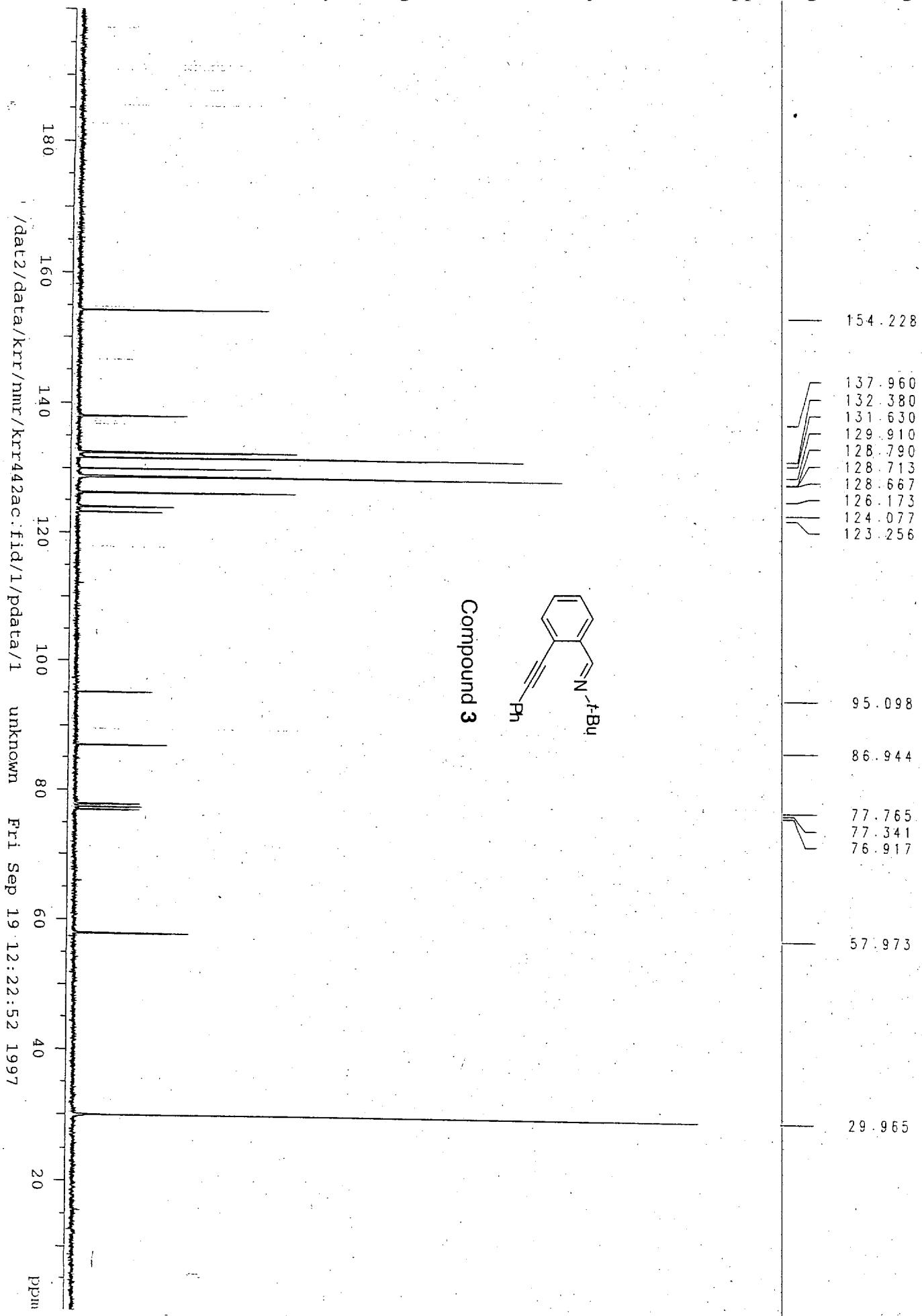
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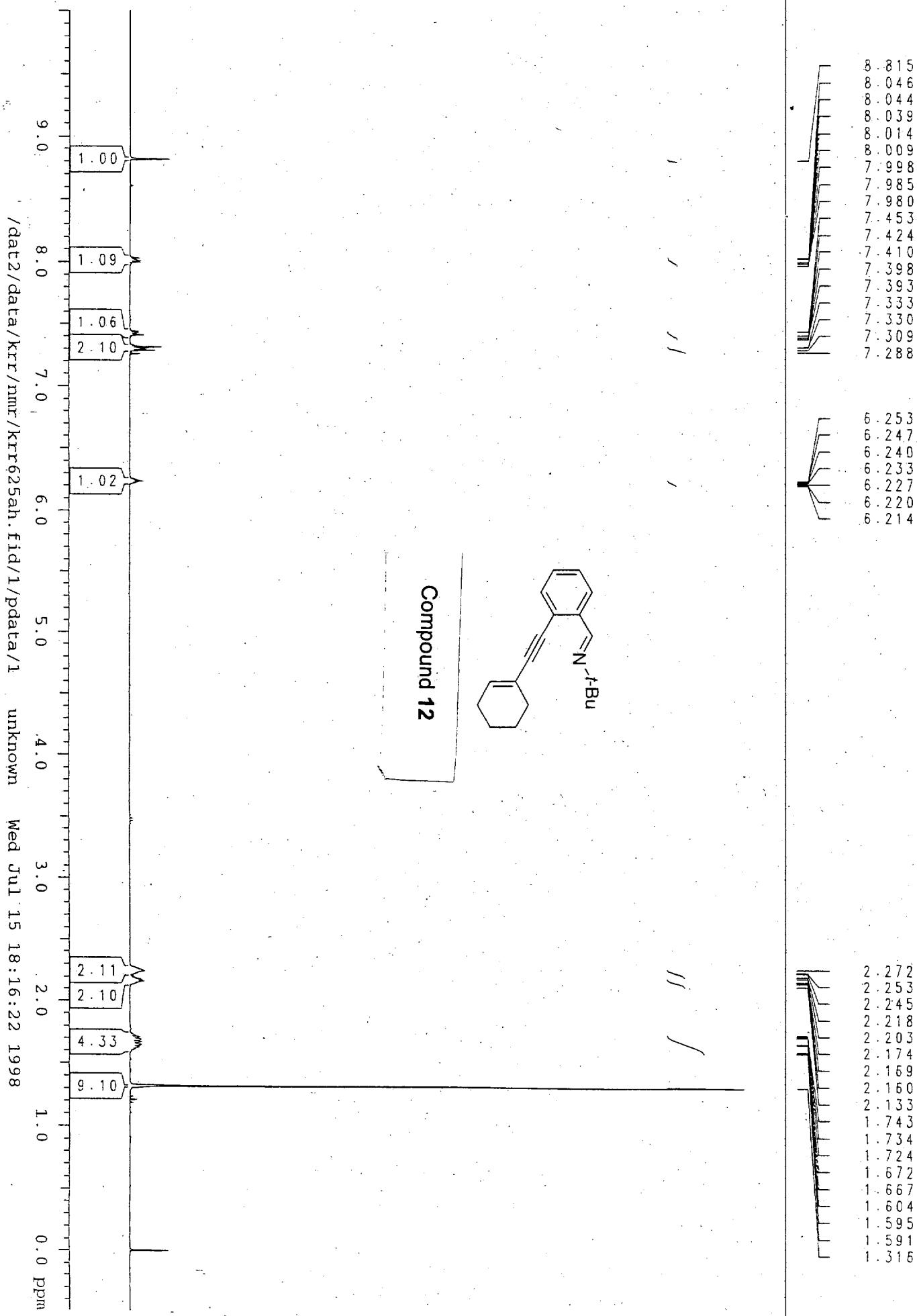


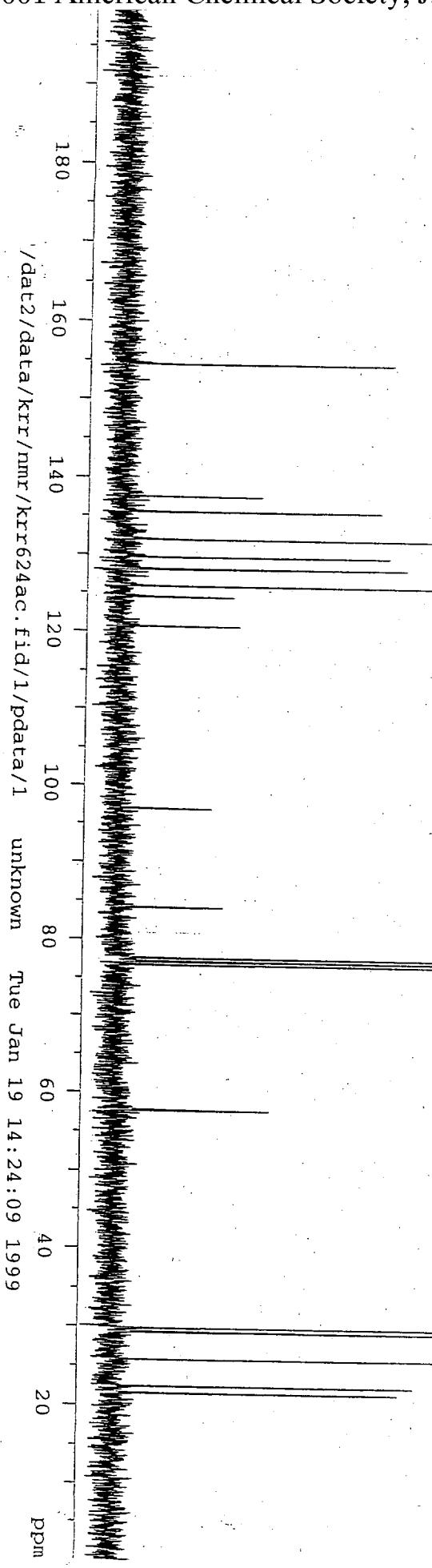
Compound 3

The figure shows a <sup>13</sup>C NMR spectrum with the x-axis ranging from 8.0 to 7.0 ppm. Peak labels are listed on the right side of the spectrum, corresponding to the chemical shifts: 8.937, 8.103, 8.095, 8.091, 8.089, 8.086, 8.079, 8.072, 7.536, 7.531, 7.529, 7.523, 7.520, 7.509, 7.503, 7.493, 7.346, 7.340, 7.337, 7.324, 7.316, 7.312, 7.307, 7.301, 7.296, 7.286, 7.278.

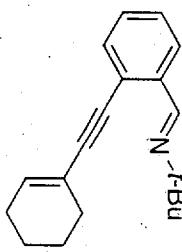
1.340



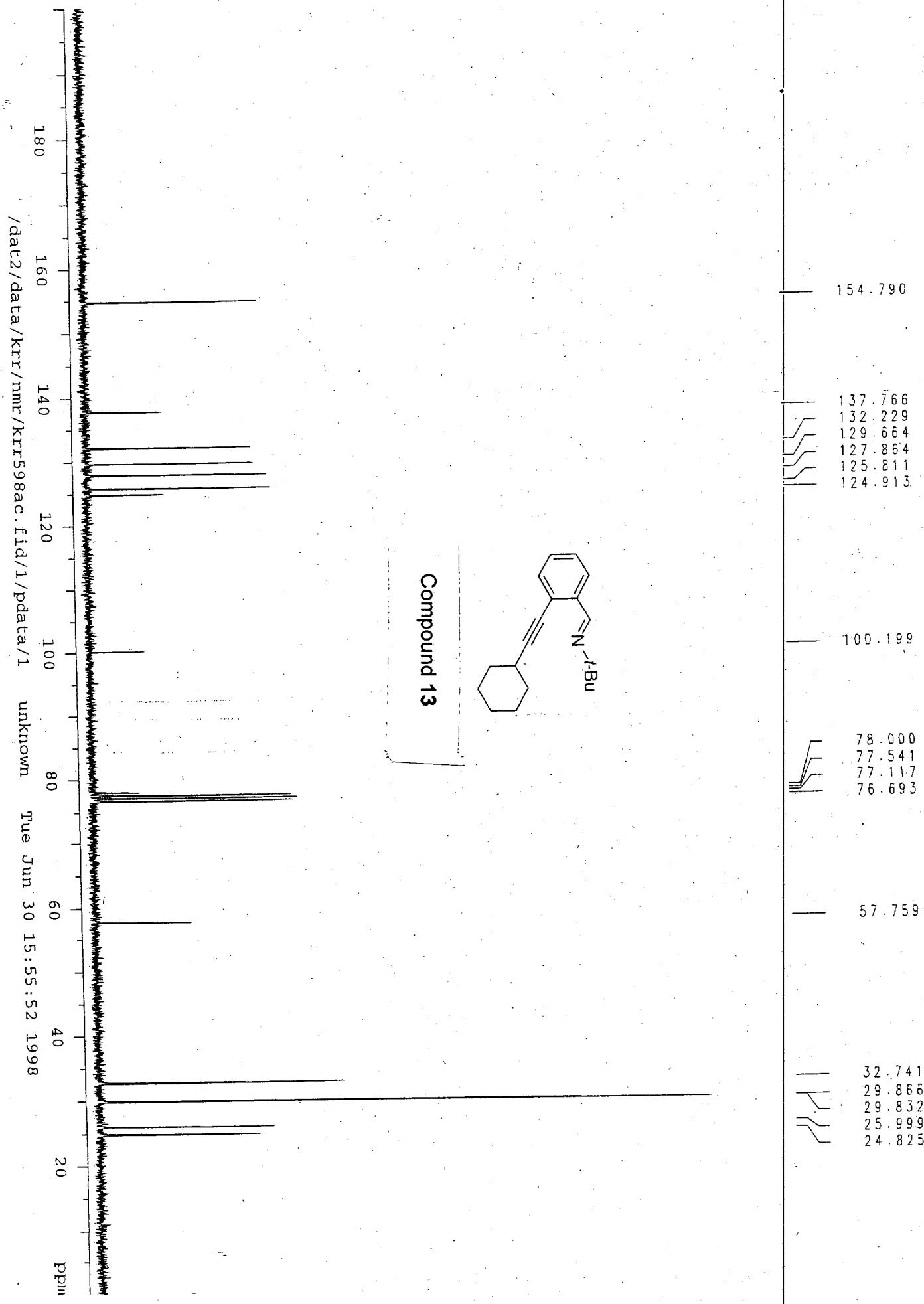


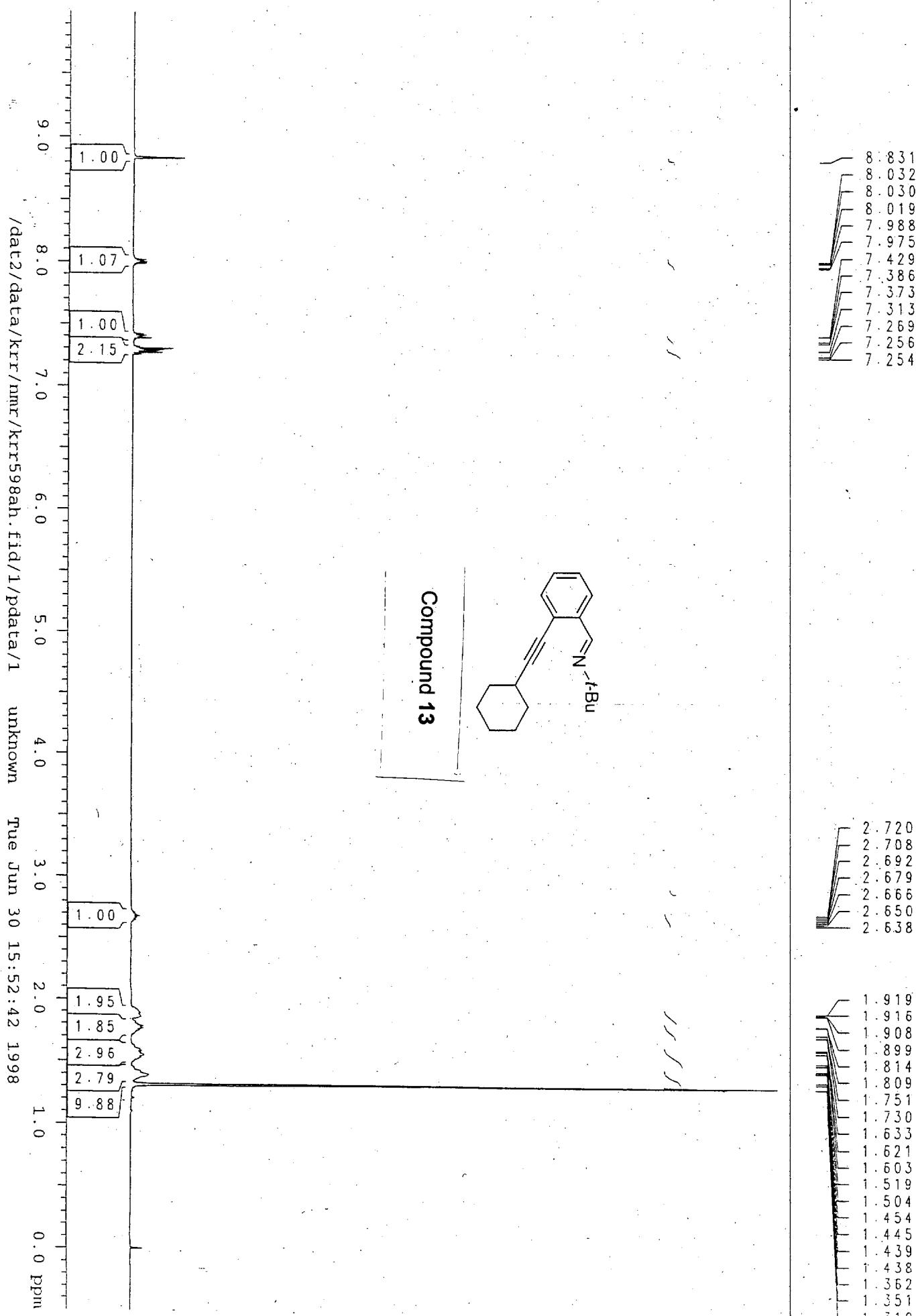


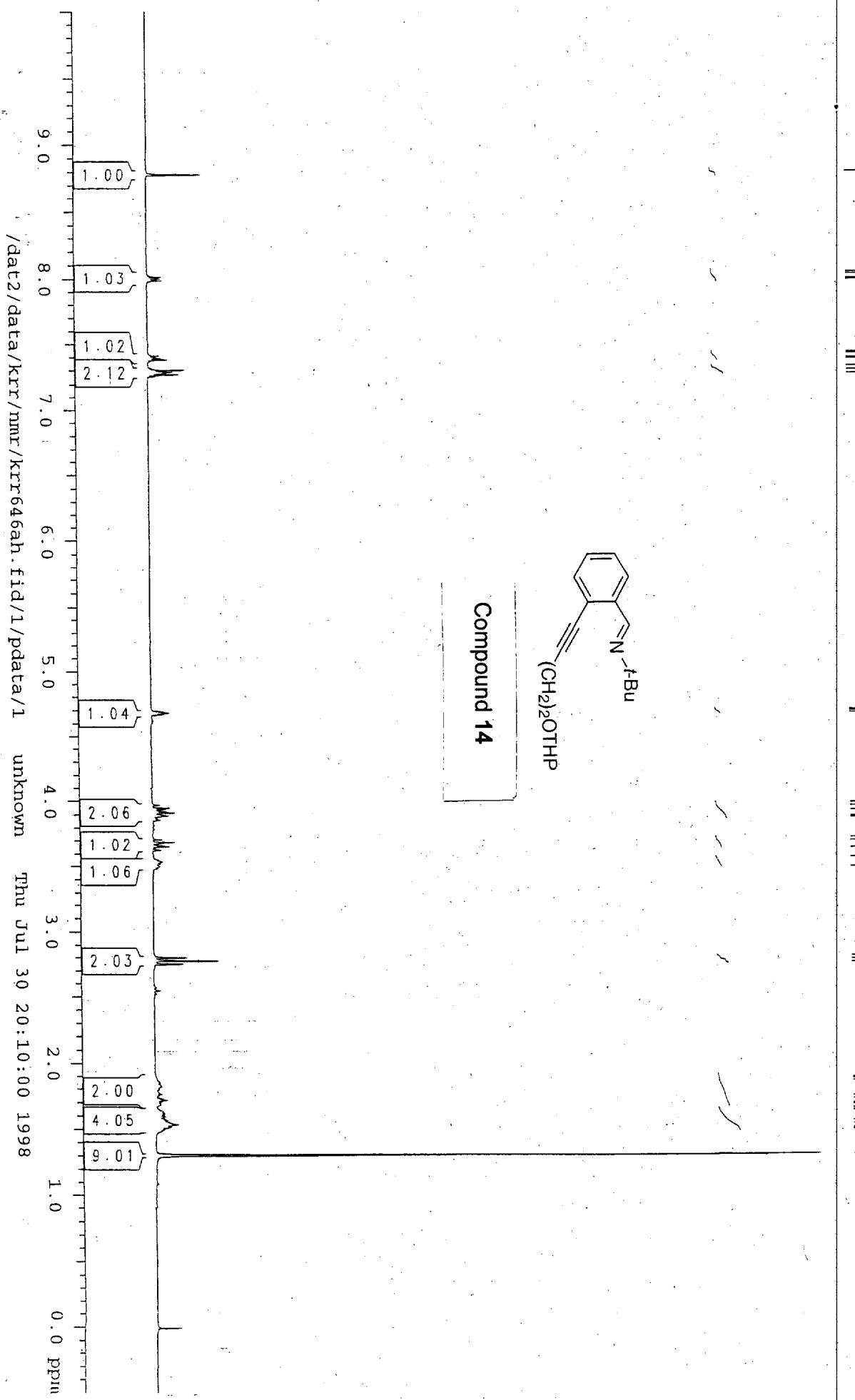
Compound 12



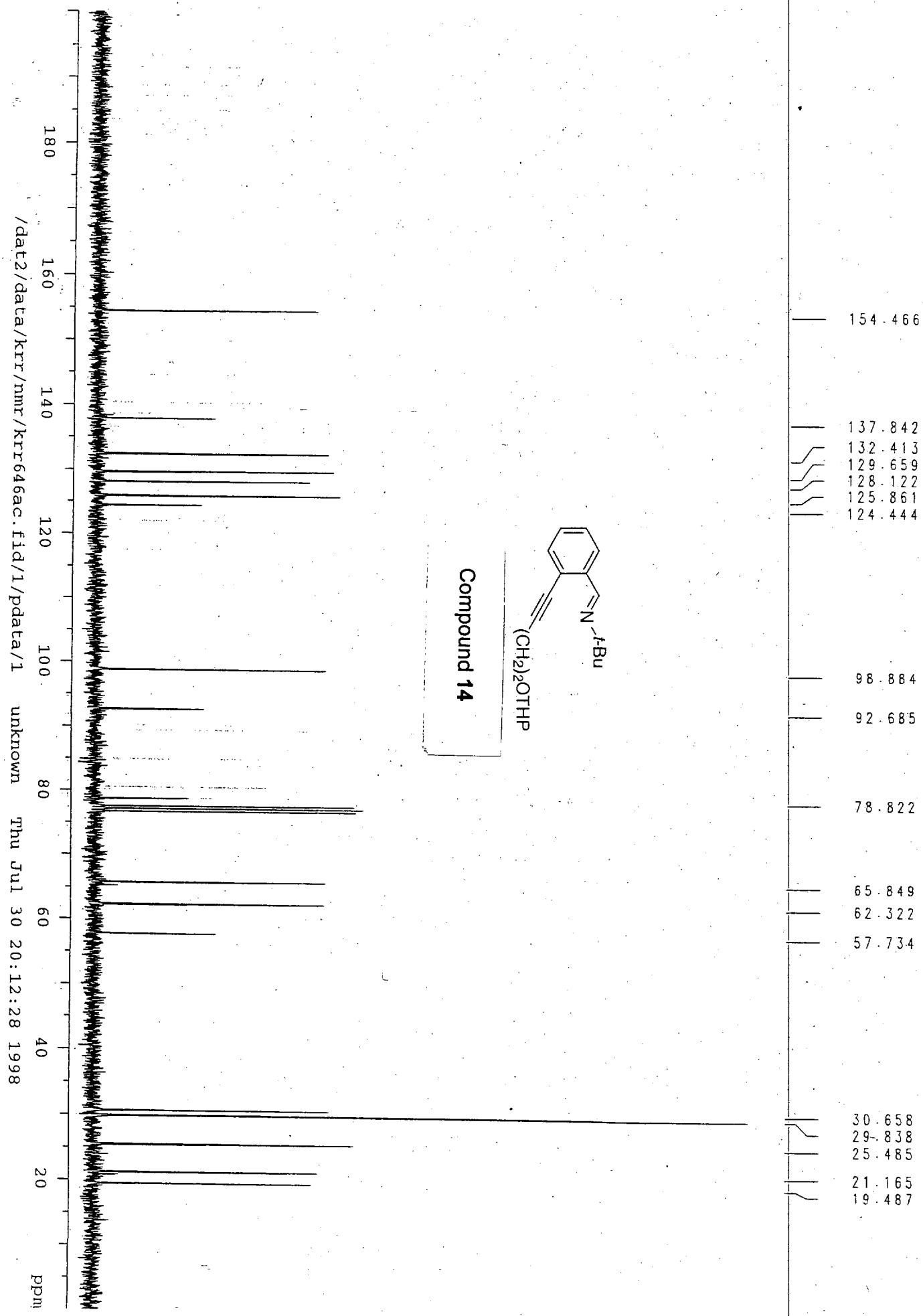
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797.00	797.00	797.00
800.00	800.00	800.00
803.00	803.00	803.00
806.00	806.00	806.00
809.00	809.00	809.00
812.00	812.00	812.00
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818.00	818.00	818.00
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824.00	824.00	824.00
827.00	827.00	827.00
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839.00	839.00	839.00
842.00	842.00	842.00
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848.00	848.00	848.00
851.00	851.00	851.00
854.00	854.00	854.00
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902.00	902.00	902.00
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908.00	908.00	908.00
911.00	911.00	911.00
914.00	914.00	914.00
917.00	917.00	917.00
920.00	920.00	920.00
923.00	923.00	923.00
926.00	926.00	926.00
929.00	929.00	929.00
932.00	932.00	932.00
935.00	935.00	935.00
938.00	938.00	938.00
941.00	941.00	941.00
944.00	944.00	944.00
947.00	947.00	947.00
950.00	950.00	950.00
953.00	953.00	953.00
956.00	956.00	956.00
959.00	959.00	959.00
962.00	962.00	962.00
965.00	965.00	965.00
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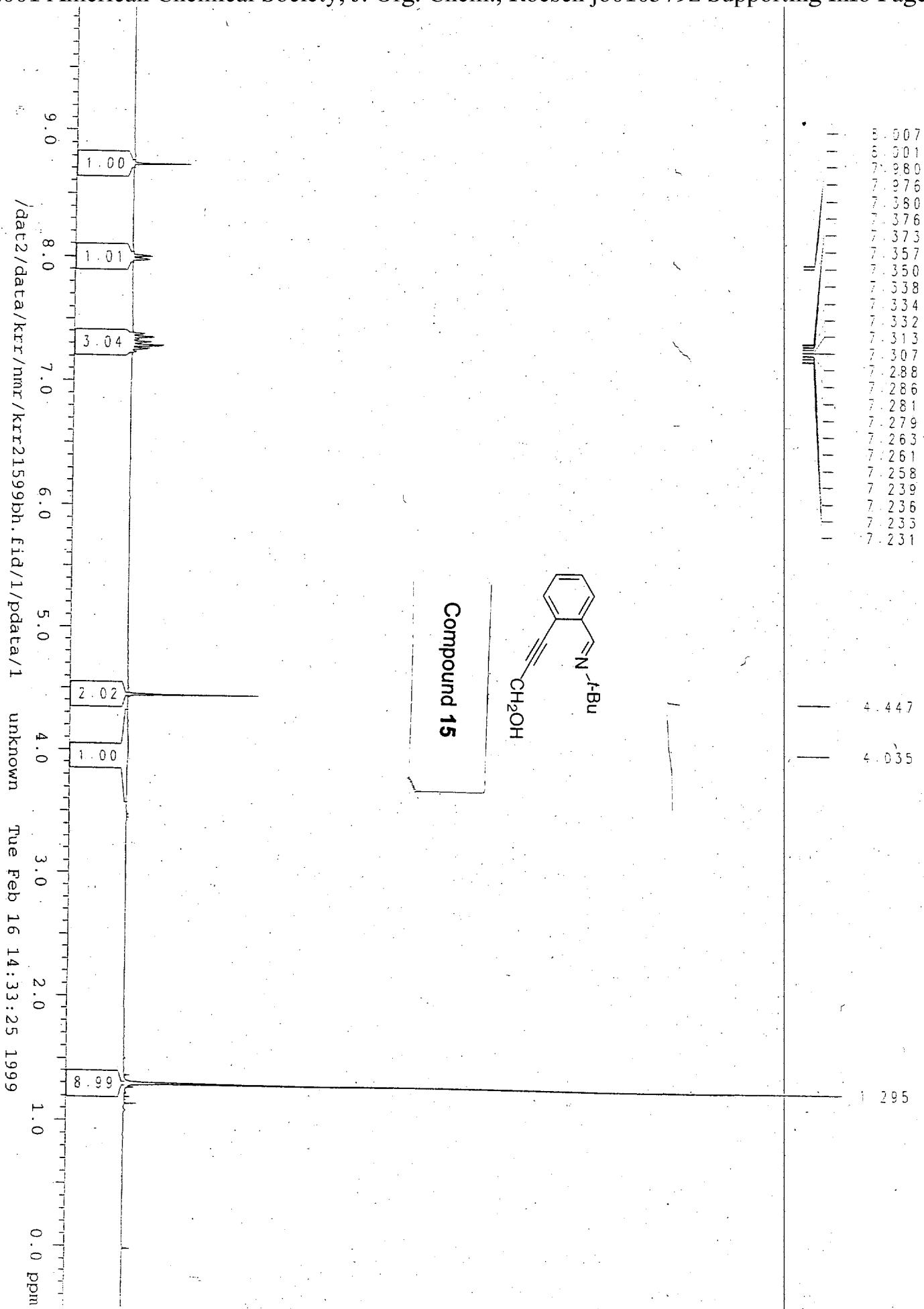


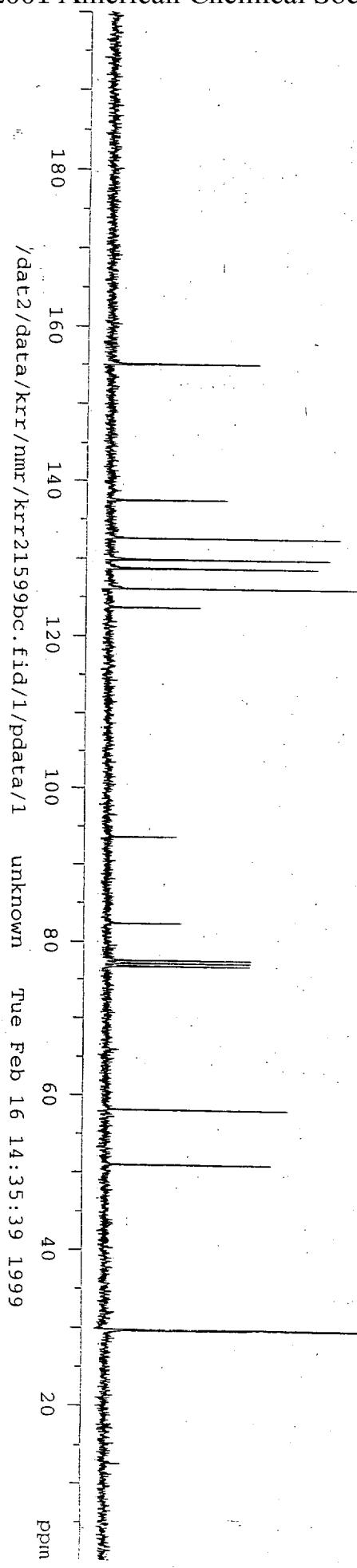




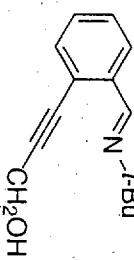
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4.681
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3.859
3.706
3.682
3.626
3.559
3.479
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1.876
1.857
1.740
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1.484
1.301





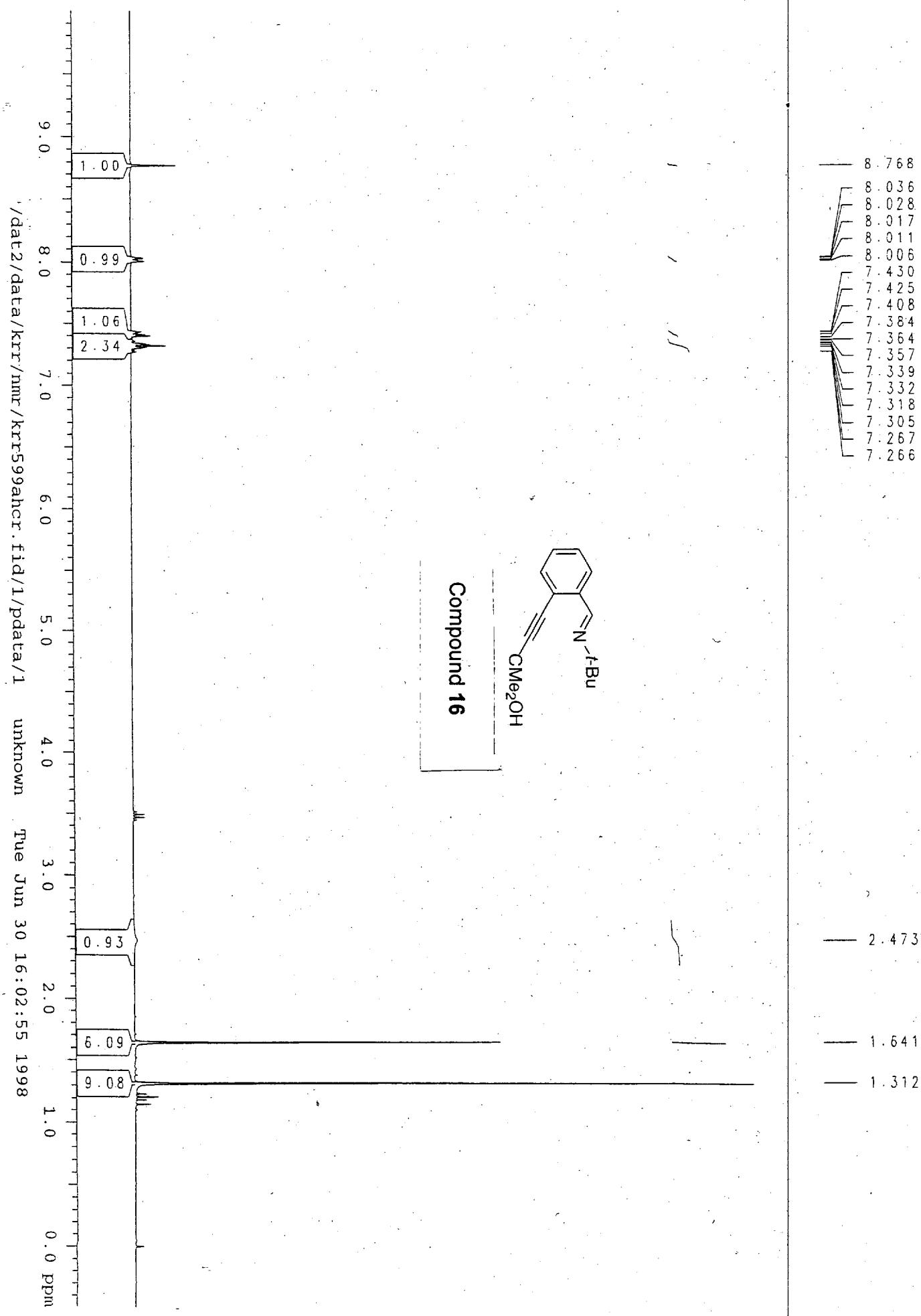


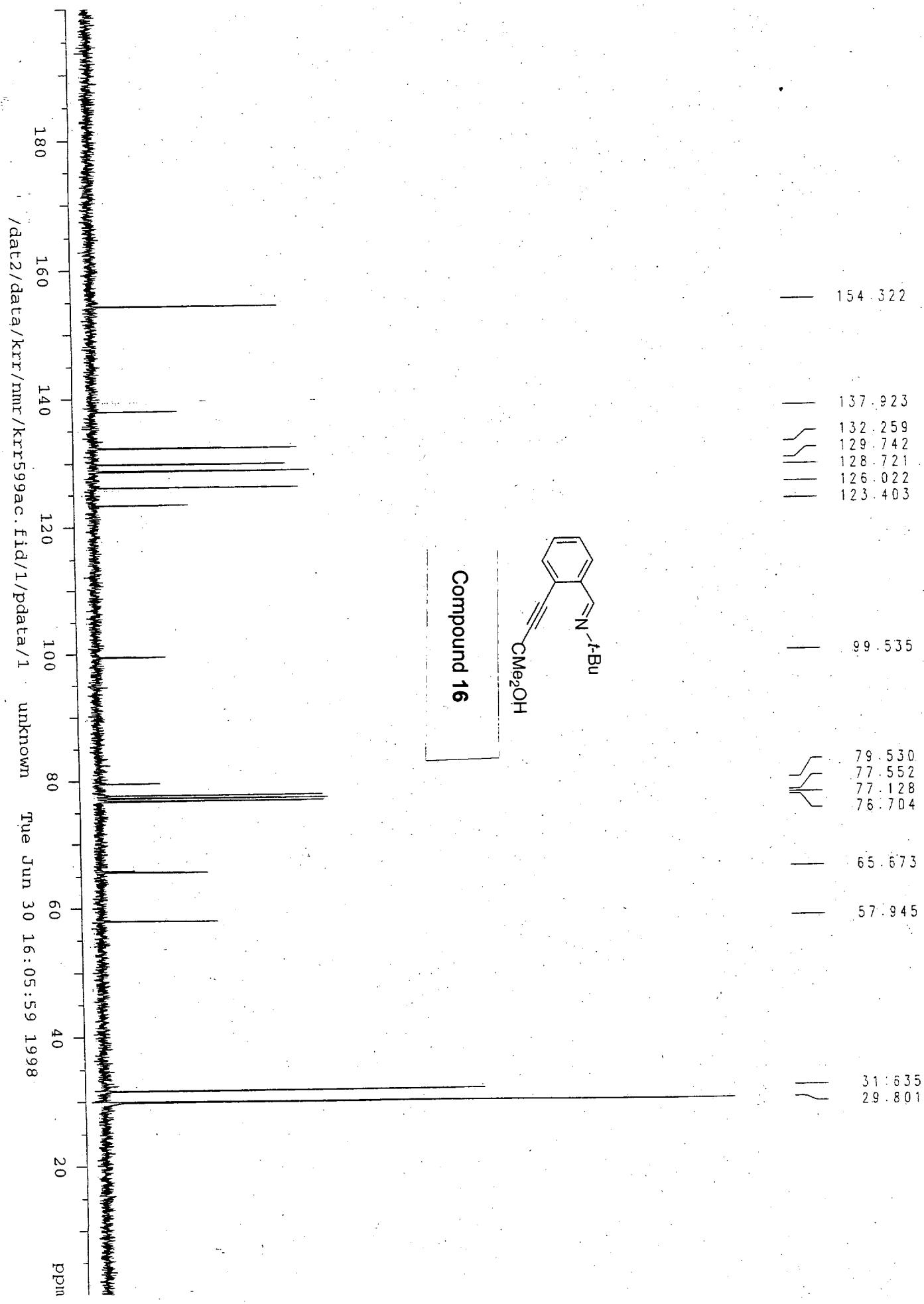
Compound 15

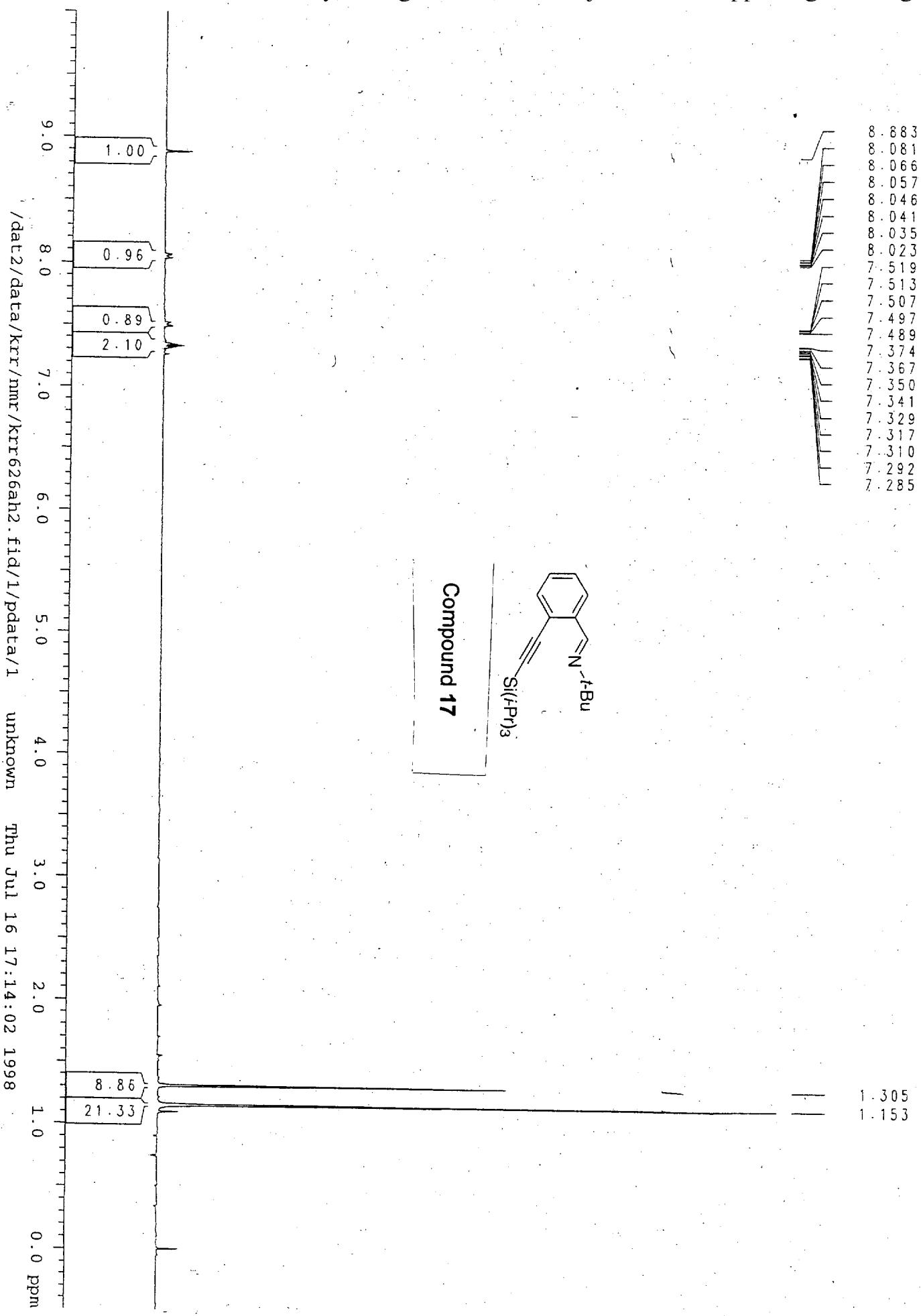


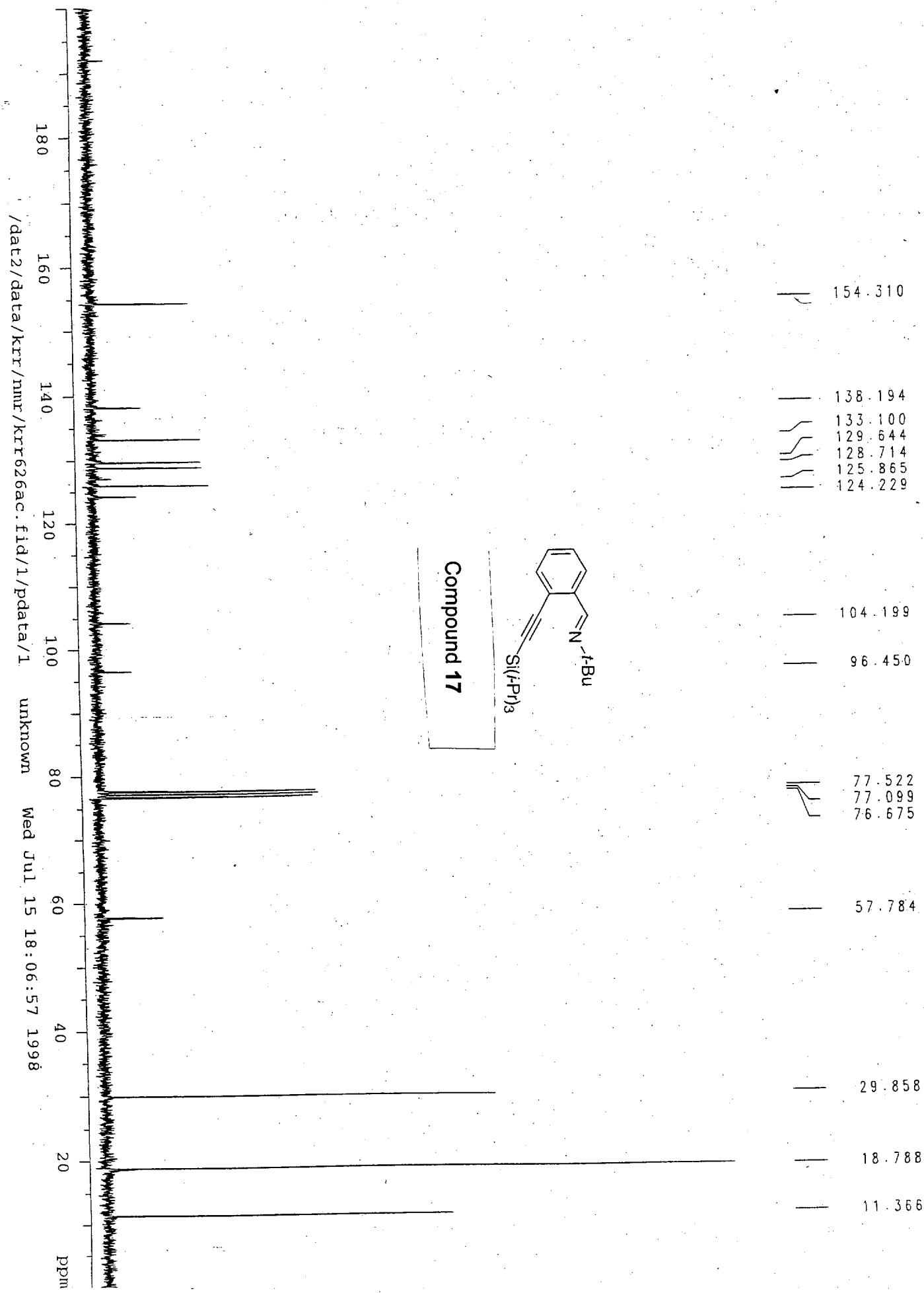
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8.2300
3.617
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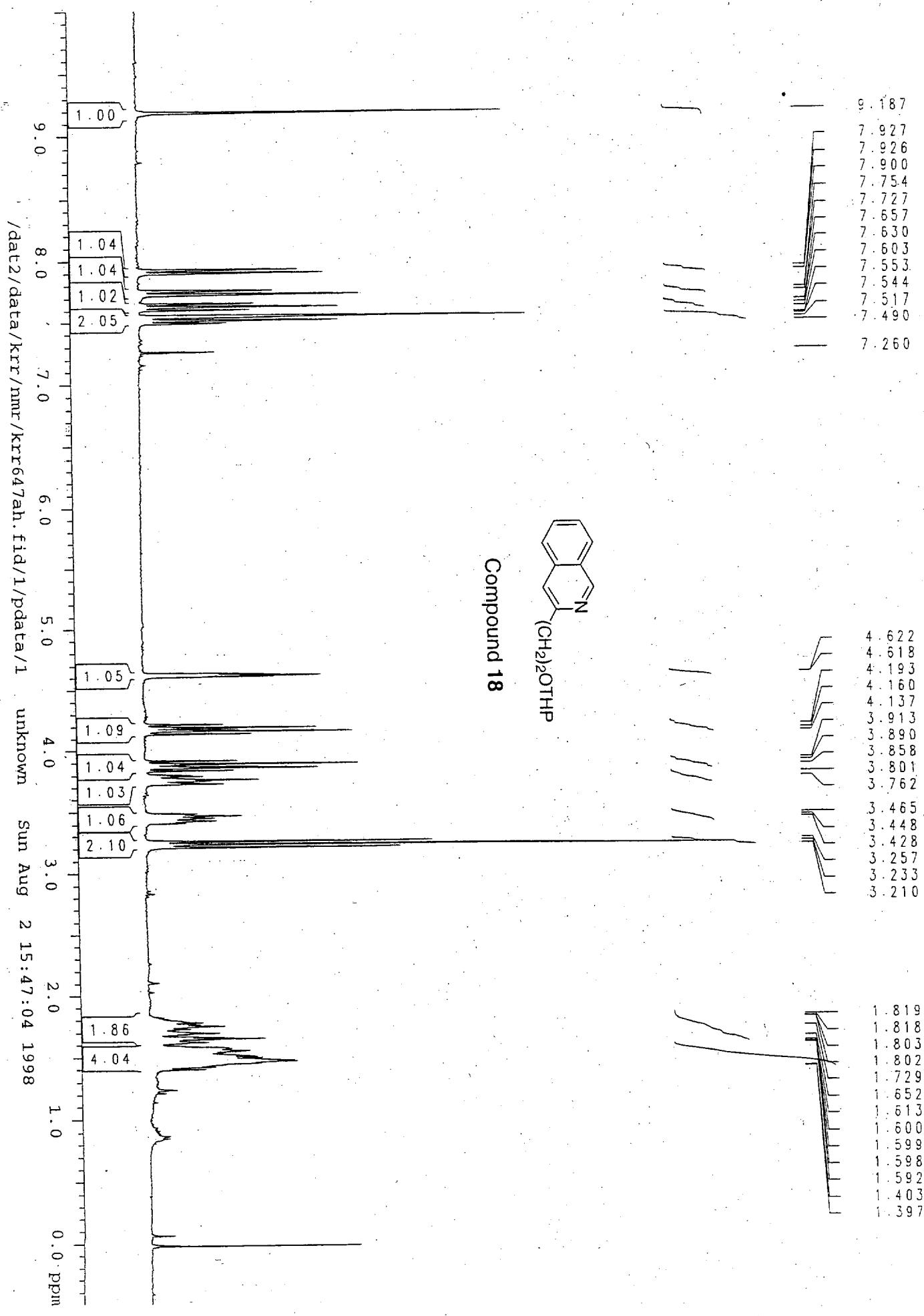
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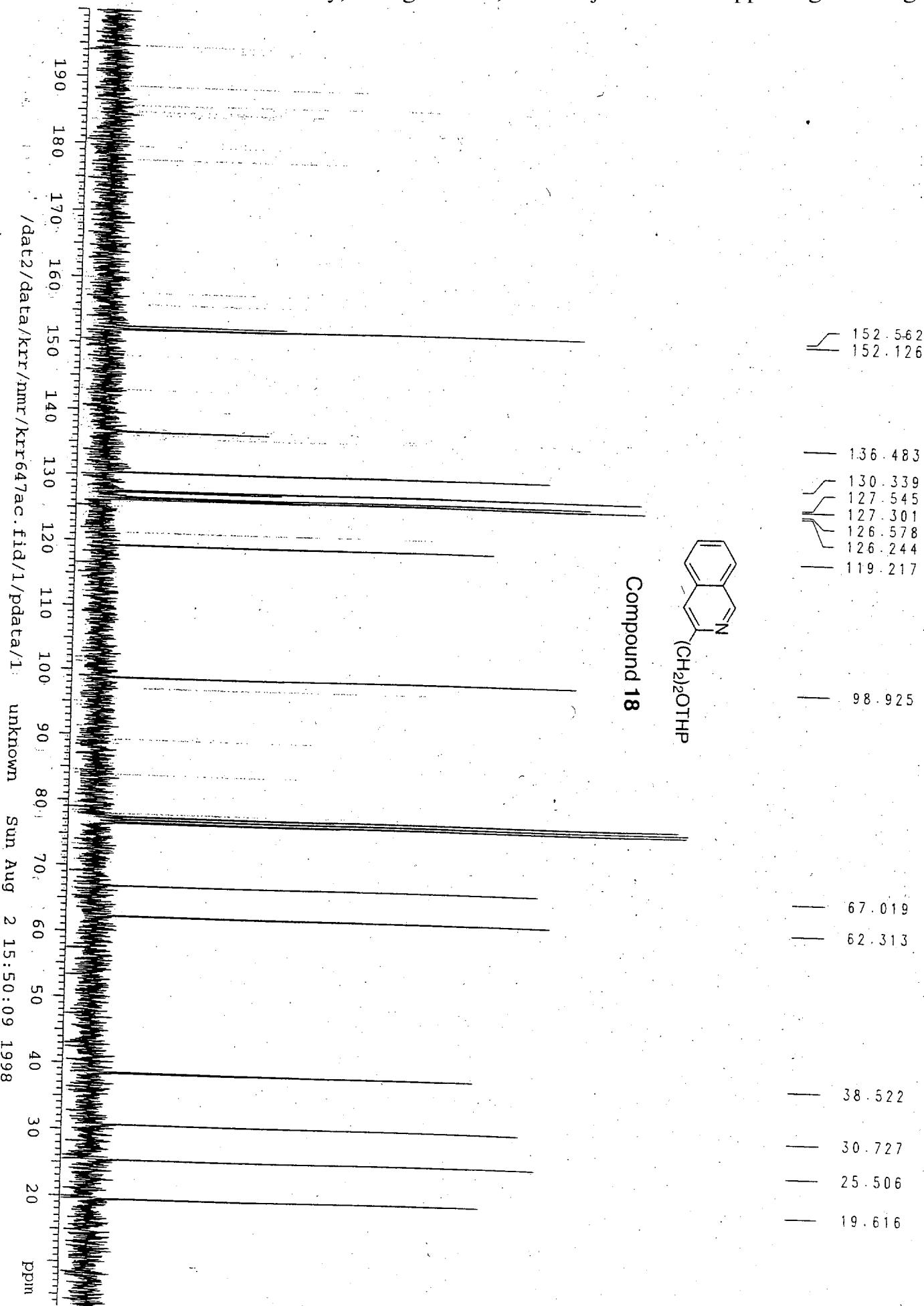


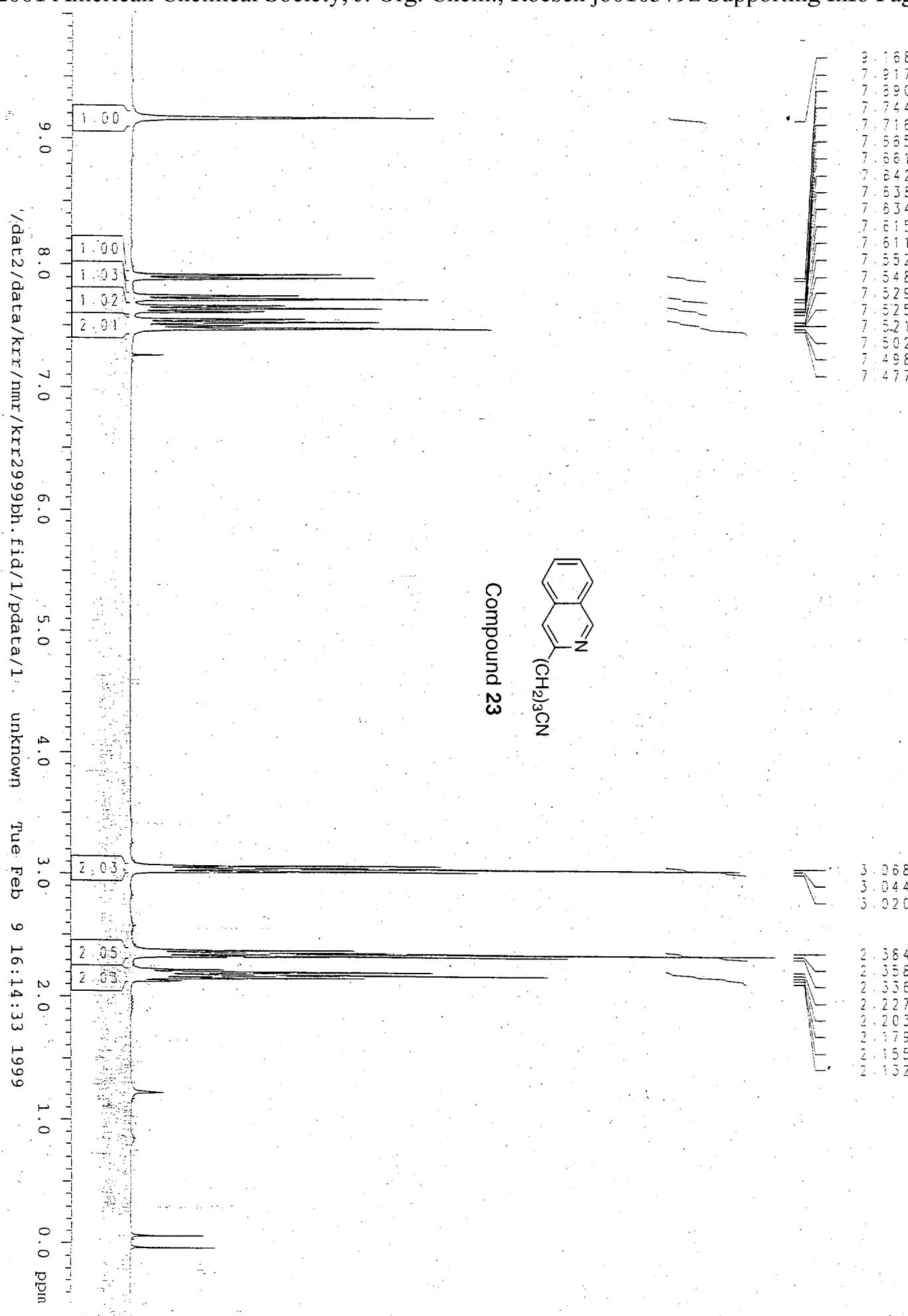


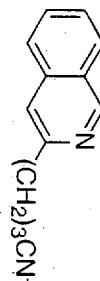
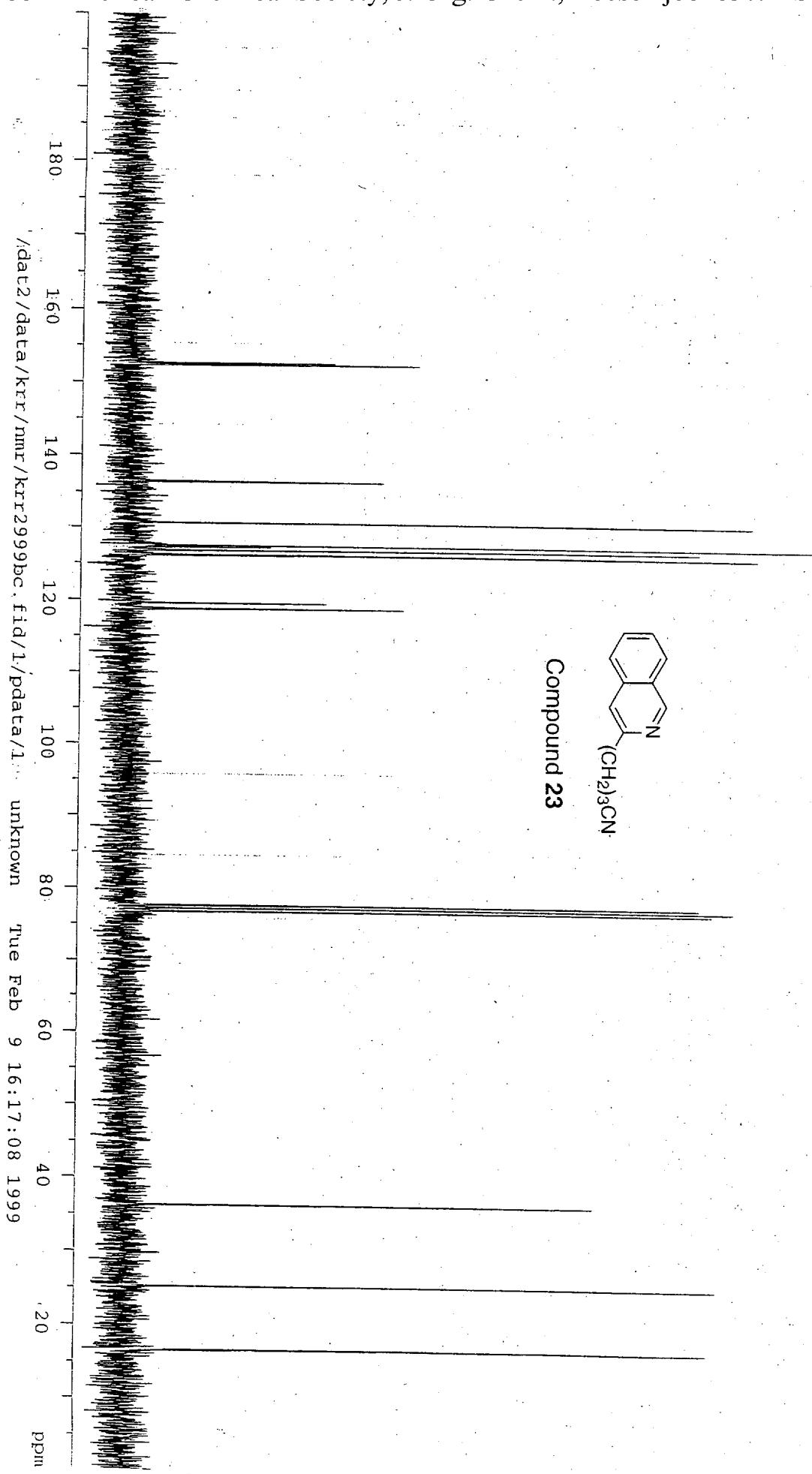




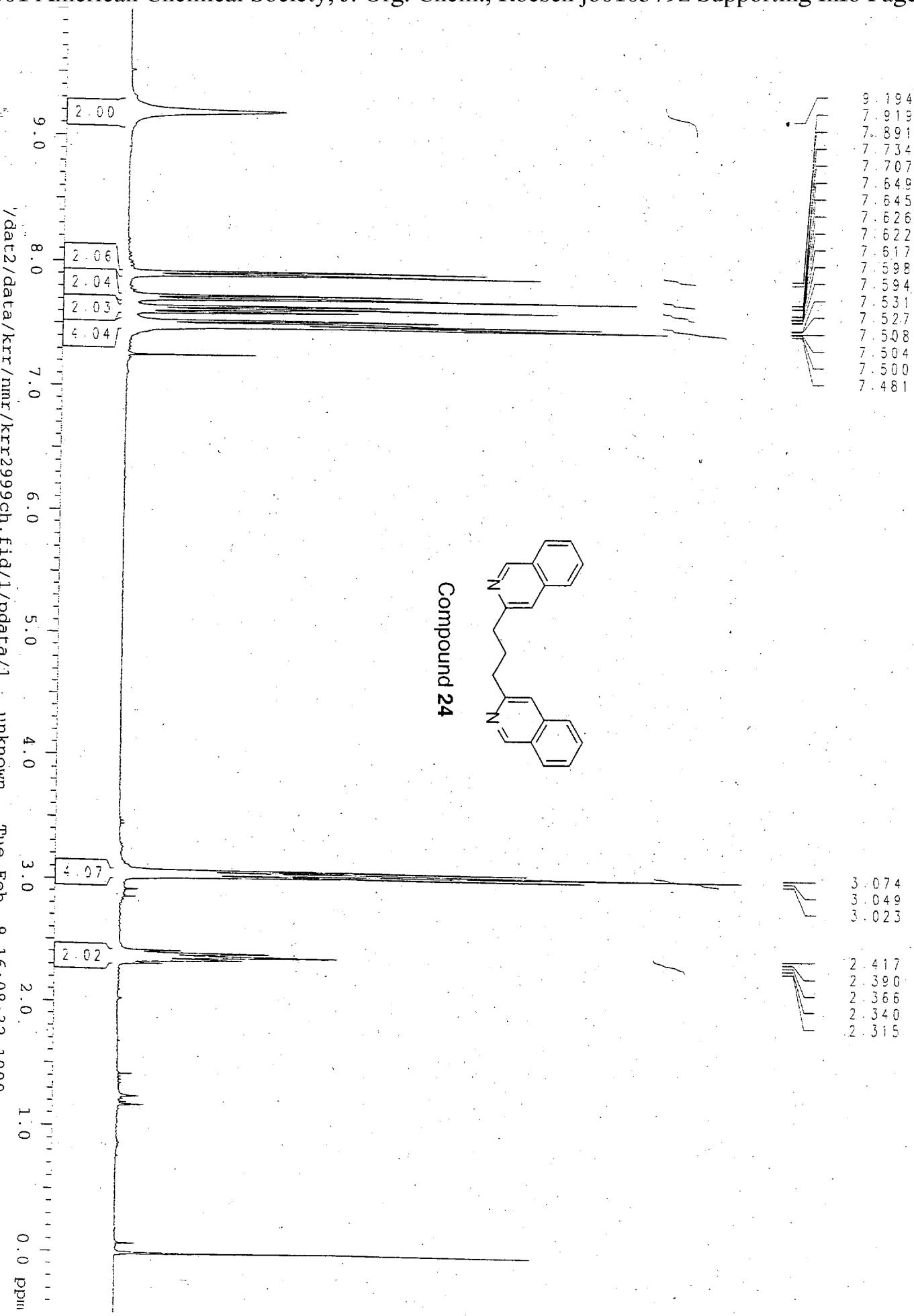


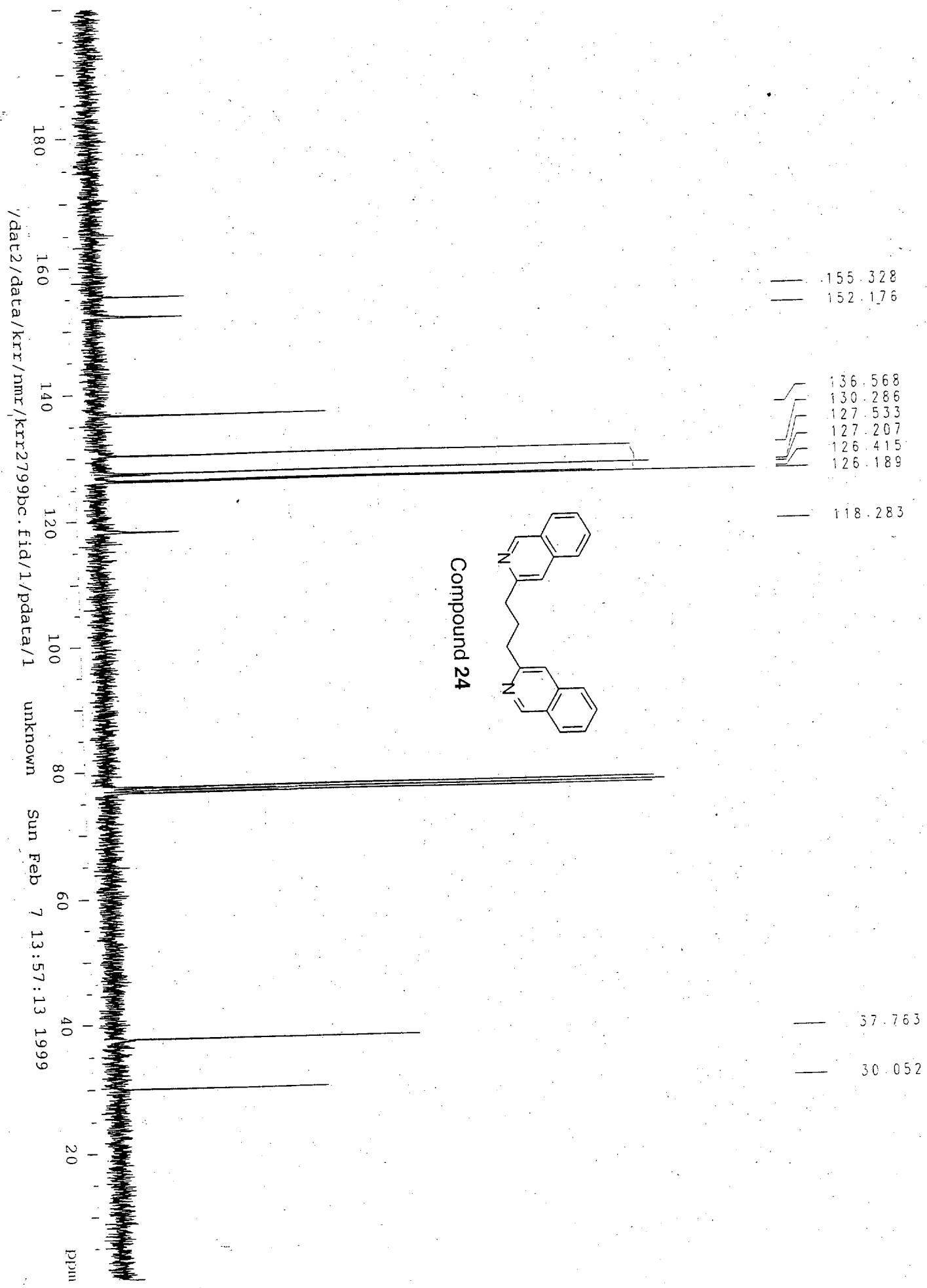


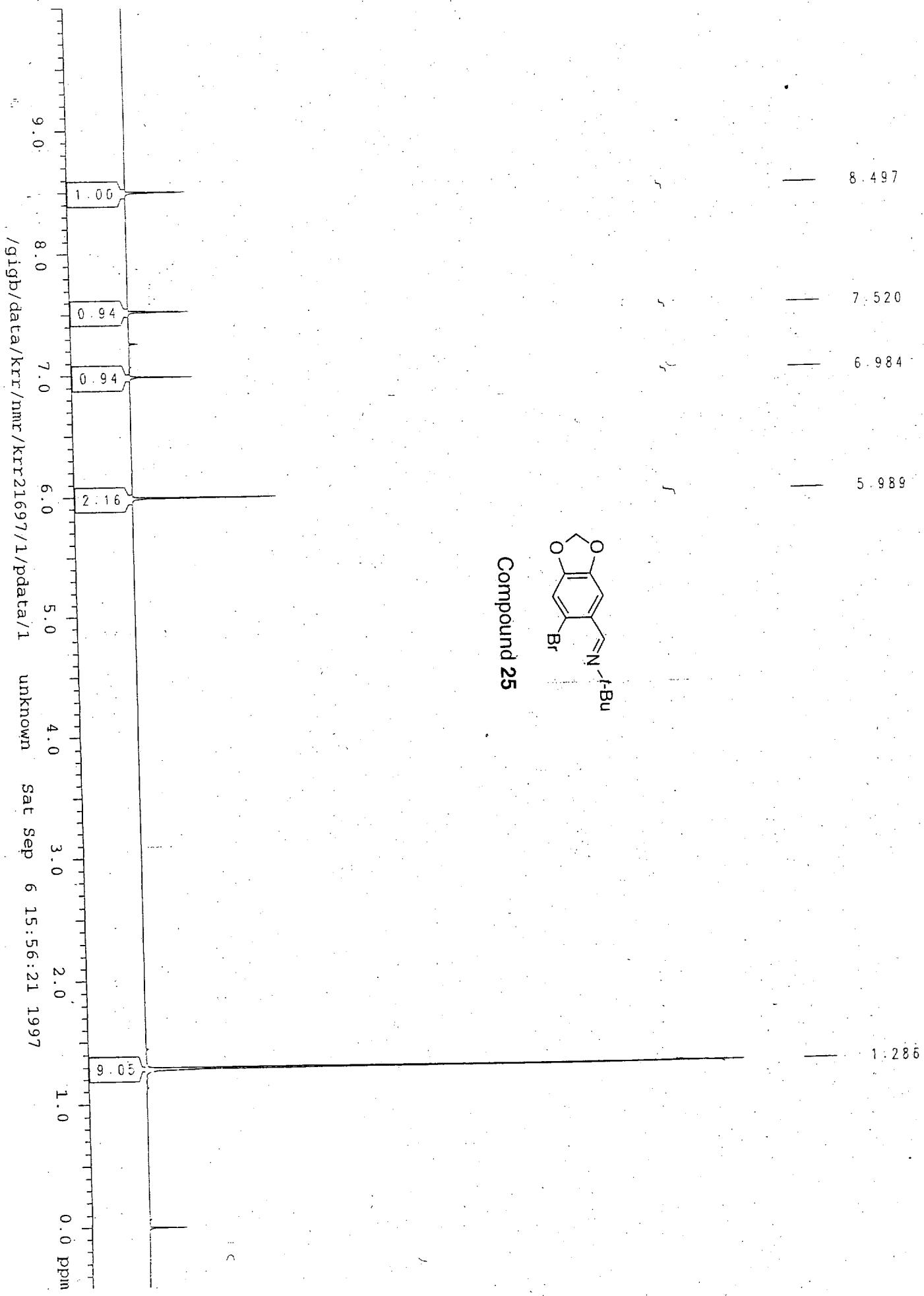


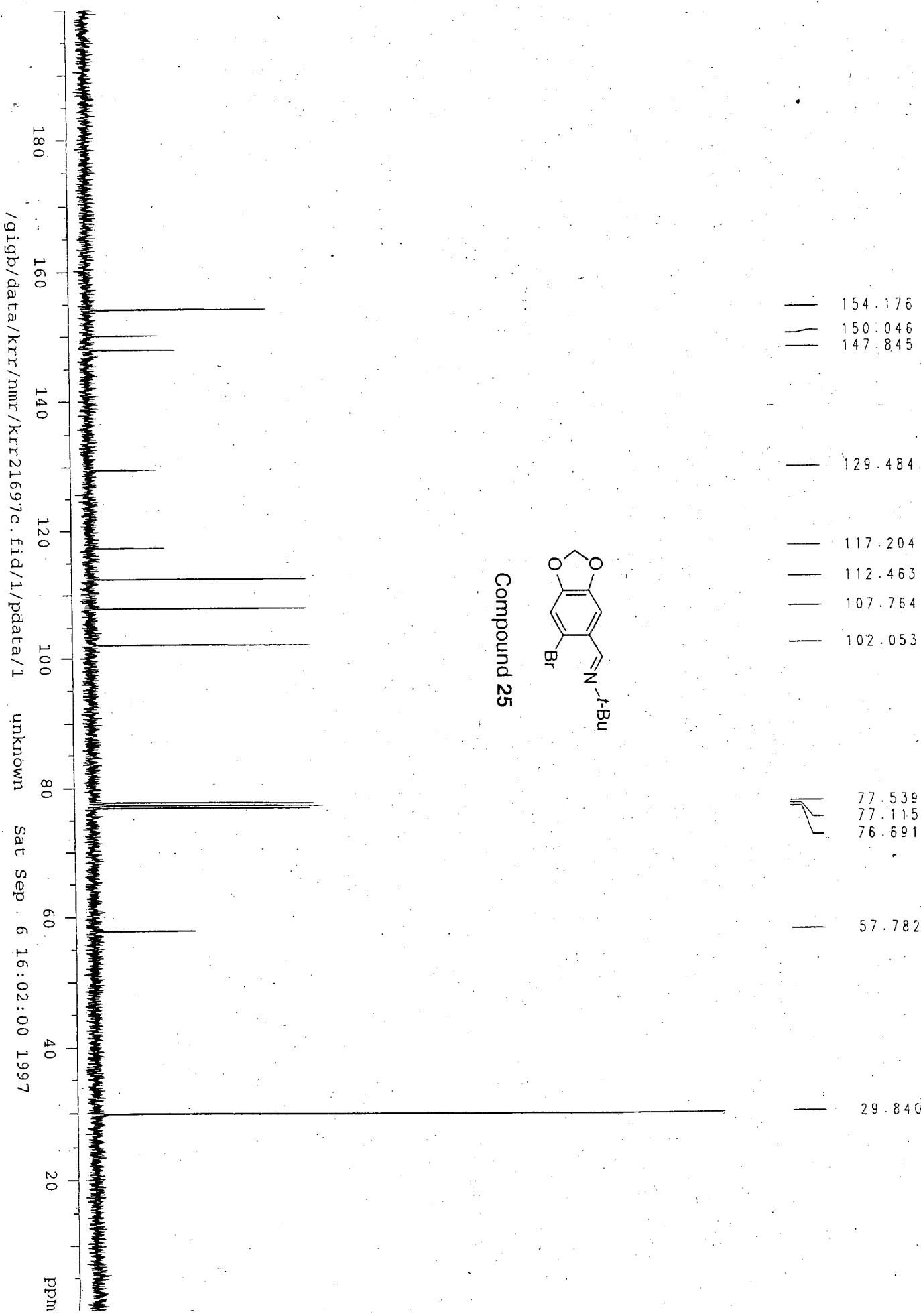


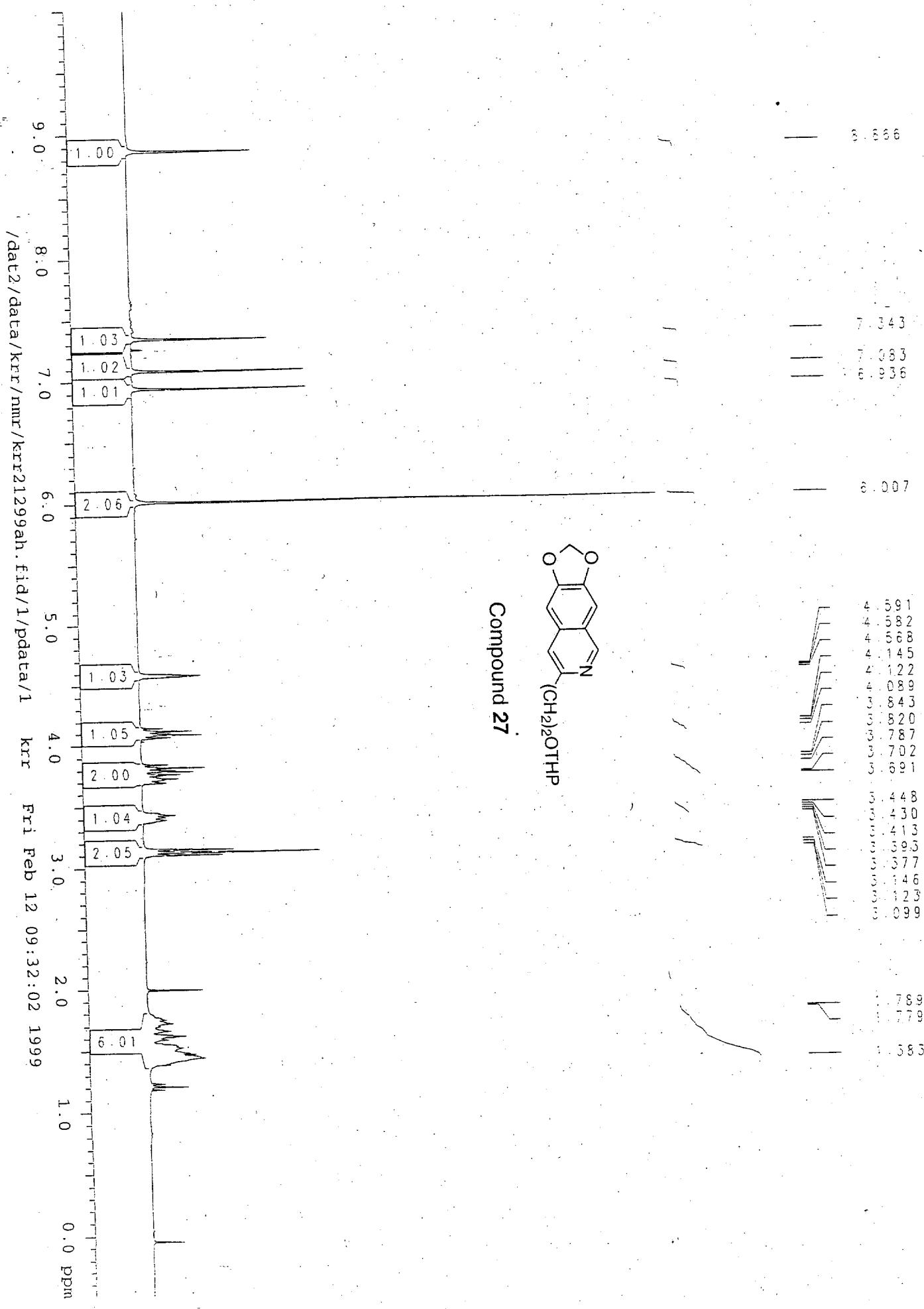
Compound 23

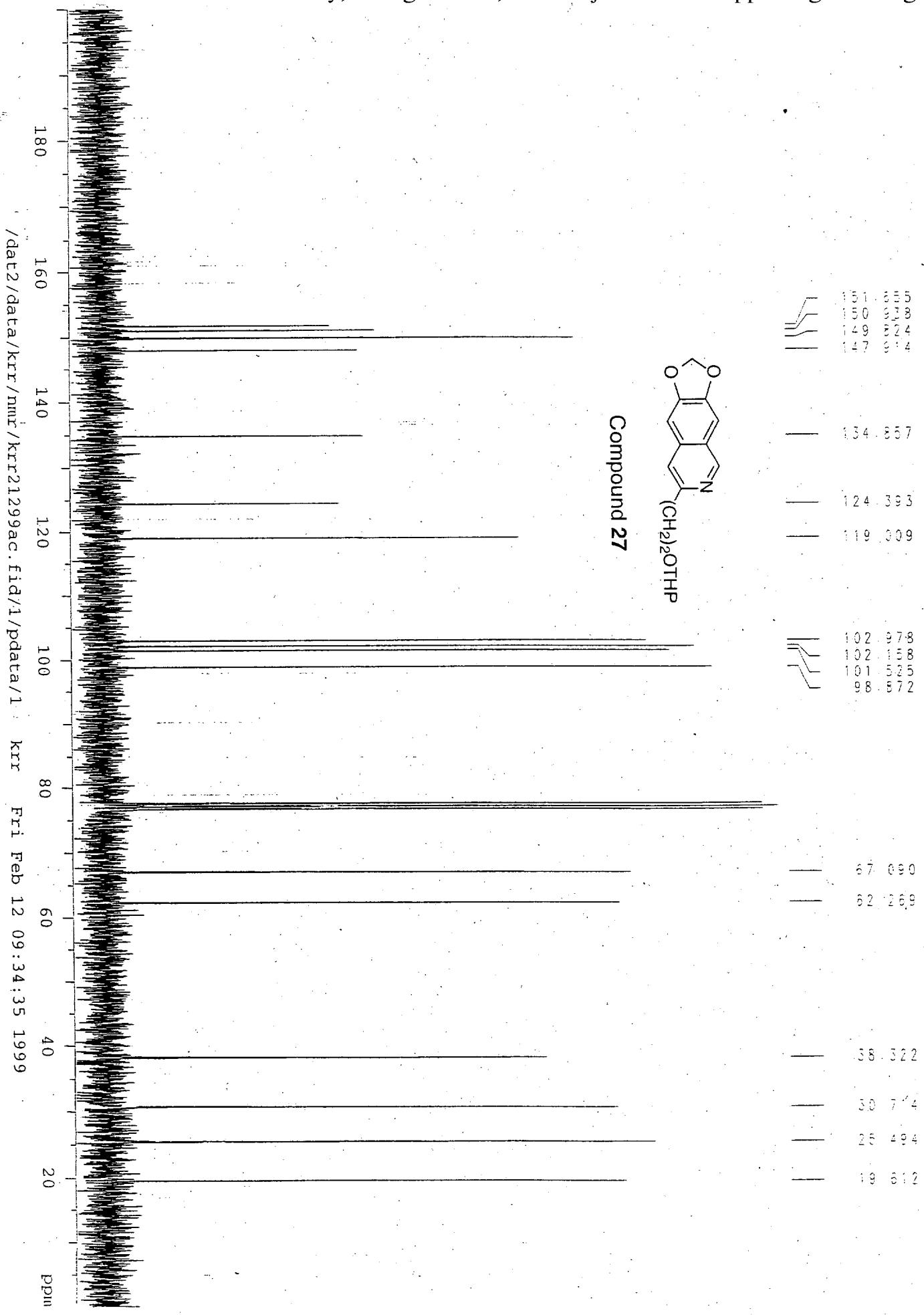


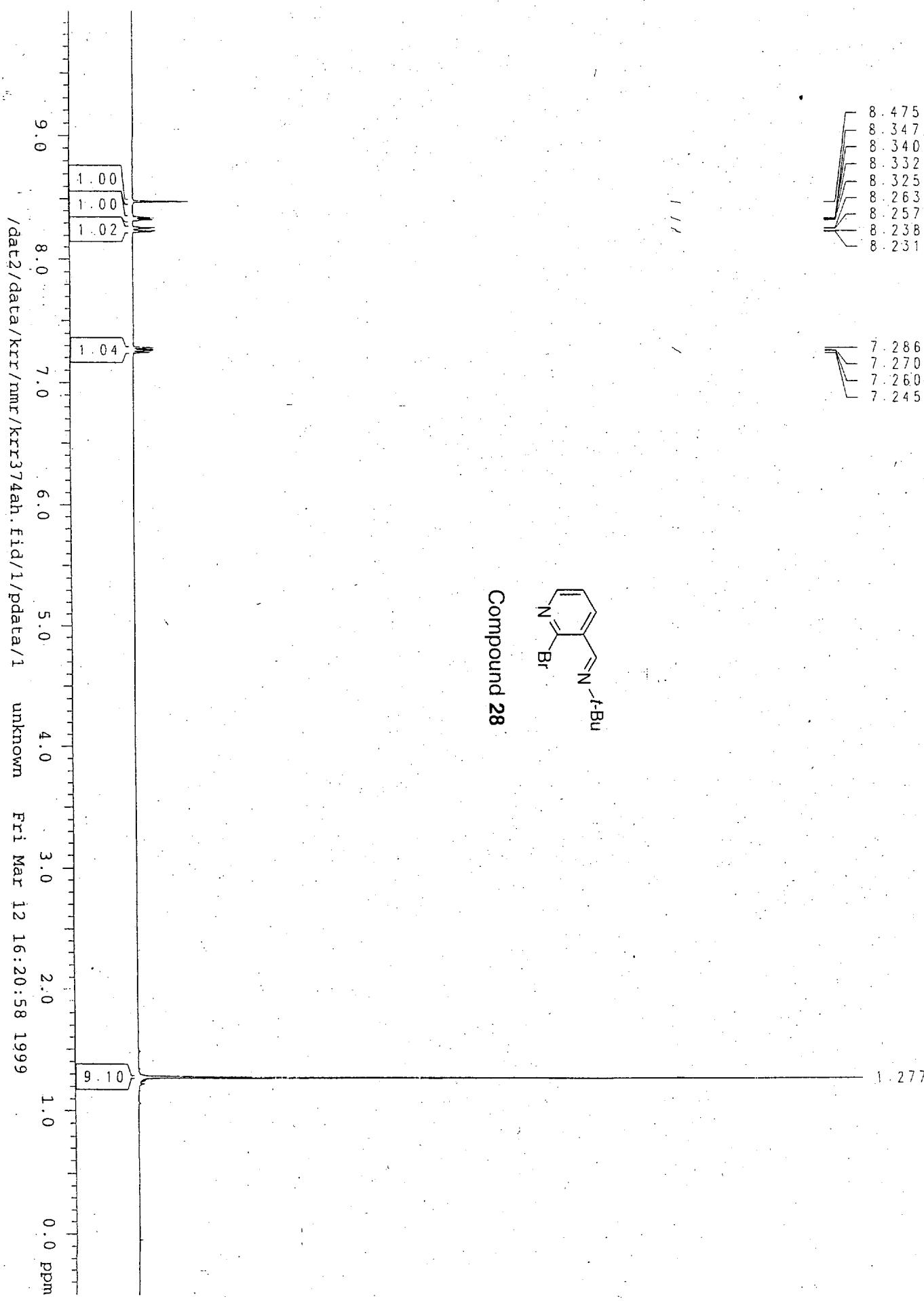


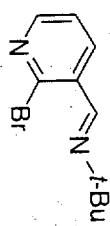
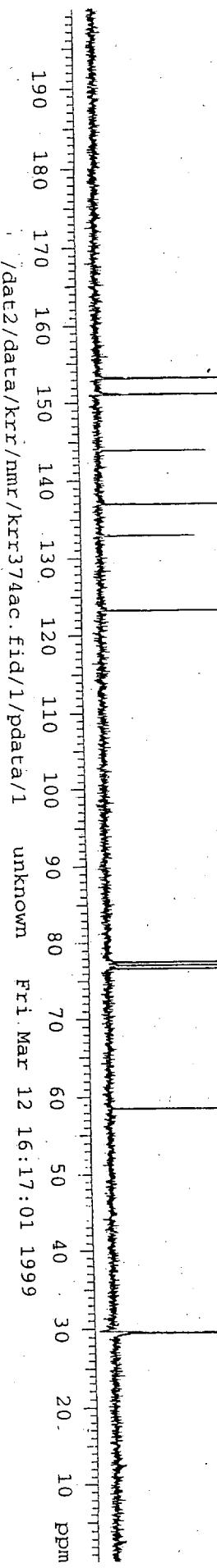












Compound 28

153.176  
151.122  
143.947  
136.889  
132.885  
123.223

58.487  
29.610

