

## Electronic Supplementary Information (ESI)

# Direct N-Alkylation of Amino-azoles with Alcohols Catalyzed by an Iridium Complex/Base System

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### General Experimental Details

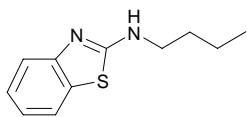
Infrared spectra were recorded on a Nicolet iS10 FT-IR spectrometer. High-resolution mass spectra (HRMS) were obtained on a HPLC-Q-ToF MS(Micro) spectrometer and are reported as m/z (relative intensity). Accurate masses are reported for the molecular ion  $[M+H]^+$ . Melting points were measured on a X-6 micro-melting apparatus (Beijing Tech Instrument Co., Ltd). Proton nuclear magnetic resonance ( $^1\text{H}$  NMR) spectra were recorded at 500 MHz using a Bruker Avance 500 spectrometer. Chemical shifts are reported in delta ( $\delta$ ) units, parts per million (ppm) downfield from trimethylsilane or ppm relative to the center of the singlet at 7.26 ppm for  $\text{CDCl}_3$  and 2.50 ppm for  $\text{DMSO-d}_6$ . Coupling constants J values are reported in Hertz (Hz), and the splitting patterns were designated as follows: s, singlet; d, doublet; t, triplet; m, multiplet; b, broad. Carbon-13 nuclear magnetic resonance ( $^{13}\text{C}$  NMR) spectra were recorded at 125 MHz using a Bruker Avance 500 spectrometer. Chemical shifts are reported in delta ( $\delta$ ) units, ppm relative to the center of the triplet at 77.0 ppm for  $\text{CDCl}_3$  and 39.5 ppm for  $\text{DMSO-d}_6$ .  $^{13}\text{C}$  NMR spectra were routinely run with broadband decoupling.

$[\text{Cp}^*\text{IrCl}_2]_2$  ( $\text{Cp}^*$  = pentamethylcyclopentadienyl) and  $[\text{Ir}(\text{cod})\text{Cl}]_2$  (cod = 1,5-cyclooctadiene) were prepared according to literature methods.<sup>1,2</sup> Commercially unavailable amino-azoles were synthesized according to the previously reported procedures.<sup>3,4</sup> Reactions tubes were purchased from Beijing Synthware Glass Inc. All reactions were run under an atmosphere of nitrogen, unless otherwise indicated. Analytical thin-layer chromatography (TLC) was carried out using 0.2-mm commercial silica gel plates.

### General Procedure for direct N-alkylation of amino-azoles with alcohols catalyzed by an iridium complex/base system

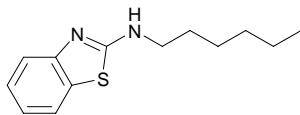
To an oven-dried, nitrogen purged 20 ml Schlenk tube were added amino-azole (1mmol),  $[\text{Cp}^*\text{IrCl}_2]_2$  (0.002 mmol, 0.2 mol%), base (0.2 mmol, 20 mol%) and alcohol (5 mmol, 500 mol%). The resulting mixture was heated at 150 °C for 12h, followed by the mixture of the reaction was allowed to cool to ambient temperature. The mixture of the reaction was concentrated in *vacuo* and purified by flash column chromatography with hexane/ethyl acetate to afford the corresponding product.

**N-butylbenzo[d]thiazol-2-amine (3aa)<sup>5</sup>**



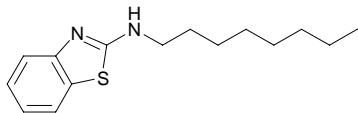
mp 69.6-70.6 °C (lit.<sup>5</sup> mp 68 °C); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 7.9 Hz, 1H, ArH), 7.52 (d, *J* = 8.1 Hz, 1H, ArH), 7.29 (t, *J* = 7.6 Hz, 1H, ArH), 7.07 (t, *J* = 7.6 Hz, 1H, ArH), 5.49 (br s, 1H, NH), 3.42 (t, *J* = 7.1 Hz, 2H, CH<sub>2</sub>N), 1.68 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.45 (sext, *J* = 7.4 Hz, 2H, CH<sub>2</sub>), 0.97 (t, *J* = 7.4 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.0, 152.4, 130.2, 125.9, 121.2, 120.7, 118.5, 45.4, 31.6, 20.0, 13.7.

**N-hexylbenzo[d]thiazol-2-amine (3ab)<sup>6</sup>**



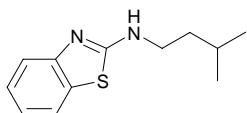
mp 58.5-59.4 °C (lit.<sup>6</sup> mp 53.2-55.4 °C); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 7.9 Hz, 1H, ArH), 7.53 (d, *J* = 8.1 Hz, 1H, ArH), 7.29 (t, *J* = 7.7 Hz, 1H, ArH), 7.10 (t, *J* = 7.5 Hz, 1H, ArH), 5.39 (br s, 1H, NH), 3.41 (t, *J* = 7.1Hz, 2H, CH<sub>2</sub>N), 1.68 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.41 (quint, *J* = 7.2 Hz, 2H, CH<sub>2</sub>), 1.34-1.30 (m, 4H, 2xCH<sub>2</sub>), 0.90 (t, *J* = 7.1Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.0, 152.5, 130.2, 125.8, 121.2, 120.7, 118.5, 45.7, 31.4, 29.5, 26.5, 22.5, 13.9.

**N-octylbenzo[d]thiazol-2-amine (3ac)**



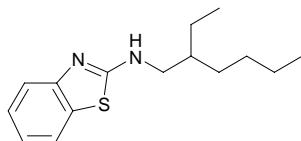
mp 43.0-44.3 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 7.7 Hz, 1H, ArH), 7.50 (d, *J* = 8.1 Hz, 1H, ArH) 7.28 (t, *J* = 7.8 Hz, 1H, ArH), 7.06 (t, *J* = 7.6 Hz, 1H, ArH), 6.29 (br s, 1H, NH), 3.38 (t, *J* = 7.1 Hz, 2H, CH<sub>2</sub>N), 1.67 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.38 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.33-1.23 (m, 8H, 4xCH<sub>2</sub>), 0.87 (t, *J* = 7.0 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.0, 152.5, 130.2, 125.8, 121.2, 120.7, 118.5, 45.7, 31.4, 29.5, 29.2, 29.1, 26.8, 22.6, 14.0; FTIR (net, cm<sup>-1</sup>) 3196, 2915, 1606, 1557, 1468, 1125; HRMS-EI (70 eV) m/z calcd for C15H23N2S [M+H]<sup>+</sup> 263.1582, found 263.1585.

**N-isopentylbenzo[d]thiazol-2-amine (3ad)**



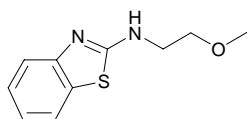
mp 76.8-77.7 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 8.0 Hz, 1H, ArH), 7.53 (d, *J* = 8.0 Hz, 1H, ArH), 7.29 (t, *J* = 7.7 Hz, 1H, ArH), 7.07 (t, *J* = 7.6 Hz, 1H, ArH), 5.45 (brs, 1H, NH), 3.43 (t, *J* = 7.4 Hz, 2H, CH<sub>2</sub>N), 1.72 (m, 1H, CH), 1.58 (quart, *J* = 7.2 Hz, 2H, CH<sub>2</sub>), 0.96 (d, *J* = 6.6 Hz, 6H, 2xCH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.0, 152.5, 130.2, 125.8, 121.2, 120.7, 118.5, 44.0, 38.4, 25.7, 22.4; FTIR (net, cm<sup>-1</sup>) 3194, 2954, 1609, 1557, 1446, 1125; HRMS-EI (70 eV) m/z calcd for C<sub>12</sub>H<sub>17</sub>N<sub>2</sub>S [M+H]<sup>+</sup> 221.1112, found 221.1107.

***N*-(2-ethylhexyl)benzo[d]thiazol-2-amine (3ae)**



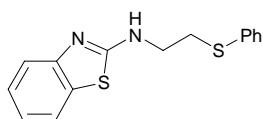
mp 80.2-81.2 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.58 (d, *J* = 7.8 Hz, 1H, ArH), 7.51 (d, *J* = 8.2 Hz, 1H, ArH), 7.29 (t, *J* = 7.3 Hz, 1H, ArH), 7.07 (t, *J* = 7.1 Hz, 1H, ArH) 5.50 (br s, 1H, NH), 3.32 (d, *J* = 6.2 Hz, 2H, CH<sub>2</sub>N), 1.61 (sept, *J* = 6.1 Hz, 1H, CH), 1.41 (quint, *J* = 7.2 Hz, 2H, CH<sub>2</sub>), 1.37-1.26 (m, 6H, 3xCH<sub>2</sub>), 0.94-0.90 (m, 6H, 2xCH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.3, 152.5, 130.3, 125.9, 121.2, 120.7, 118.6, 48.9, 39.5, 30.9, 28.8, 24.2, 22.9, 14.0, 10.9; FTIR (net, cm<sup>-1</sup>) 3196, 2950, 1623, 1575, 1467, 1124; HRMS-EI (70 eV) m/z calcd for C<sub>15</sub>H<sub>23</sub>N<sub>2</sub>S [M+H]<sup>+</sup> 263.1582, found 263.1583.

***N*-(2-methoxyethyl)benzo[d]thiazol-2-amine (3af)**



Oil; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.56-7.54 (m, 2H, ArH), 7.28 (t, *J* = 8.1 Hz, 1H, ArH), 7.07 (t, *J* = 7.6 Hz, 1H, ArH), 6.13 (br s, 1H, NH), 3.65-3.60 (m, 4H, CH<sub>2</sub>N, CH<sub>2</sub>O), 3.37 (d, *J* = 3.8 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 167.2, 152.4, 130.4, 125.8, 121.5, 120.7, 118.8, 70.7, 58.7, 44.7; FTIR (net, cm<sup>-1</sup>) 3218, 2921, 1681, 1597, 1443, 1119; HRMS-EI (70 eV) m/z calcd for C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>OS [M+H]<sup>+</sup> 209.0749, found 209.0751.

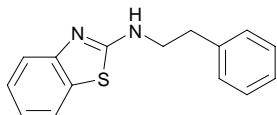
***N*-(2-(phenylthio)ethyl)benzo[d]thiazol-2-amine (3ag)**



mp 147.5-148.7 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.57 (d, *J* = 7.7 Hz, 1H, ArH), 7.54 (d, *J* = 8.1 Hz, 1H, ArH), 7.42 (d, *J* = 7.6 Hz, 2H, ArH), 7.32-7.28 (m, 3H, ArH), 7.23 (t, *J* = 7.4 Hz, 1H, ArH), 7.09 (t, *J* = 7.6 Hz, 1H, ArH), 5.61 (br s, 1H, NH), 3.67 (t, *J* = 6.4 Hz, 2H, CH<sub>2</sub>N), 3.24 (t, *J* = 6.4 Hz, 2H, CH<sub>2</sub>S); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 166.7, 152.3, 134.5, 130.5, 130.2, 129.1, 126.8, 126.0, 121.8,

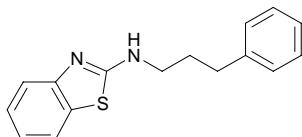
120.8, 119.0, 43.9, 33.6; FTIR (net,  $\text{cm}^{-1}$ ) 3188, 2903, 1614, 1574, 1436; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{15}\text{H}_{15}\text{N}_2\text{S}_2$  [ $\text{M}+\text{H}]^+$  287.0677, found 287.0679.

**N-phenethylbenzo[d]thiazol-2-amine (3ah)**



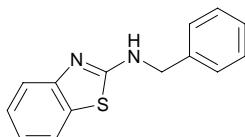
mp 143.6-144.4 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) δ 7.59 (d,  $J = 7.9$  Hz, 1H, ArH), 7.53 (d,  $J = 8.1$  Hz, 1H, ArH), 7.34-7.28 (m, 3H, ArH), 7.27-7.23 (m, 4H, ArH), 7.09 (t,  $J = 7.6$  Hz, 1H, ArH), 5.42 (br s, 1H, NH), 3.70 (t,  $J = 6.9$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 3.01 (t,  $J = 6.9$  Hz, 2H,  $\text{CH}_2\text{Ph}$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) δ 167.4, 152.4, 138.3, 130.3, 128.8, 128.7, 126.7, 126.0, 121.5, 120.8, 118.8, 46.6, 35.5; FTIR (net,  $\text{cm}^{-1}$ ) 3199, 2910, 1620, 1573, 1446, 1186; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{15}\text{H}_{15}\text{N}_2\text{S}$  [ $\text{M}+\text{H}]^+$  255.0956, found 255.0959.

**N-(3-phenylpropyl)benzo[d]thiazol-2-amine (3ai)<sup>7</sup>**



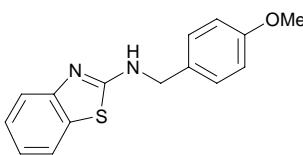
mp 101.2-102.0 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) δ 7.58 (d,  $J = 7.9$  Hz, 1H, ArH), 7.53 (d,  $J = 8.0$  Hz, 1H, ArH), 7.31-7.28 (m, 3H, ArH), 7.23-7.19 (m, 3H, ArH), 7.09 (t,  $J = 7.6$  Hz, 1H, ArH), 5.54 (br s, 1H, NH), 3.45 (t,  $J = 7.0$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 2.75 (t,  $J = 7.6$  Hz, 2H,  $\text{CH}_2\text{Ph}$ ), 2.04 (quint,  $J = 7.3$  Hz, 2H,  $\text{CH}_2$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) δ 167.9, 152.3, 141.0, 130.2, 128.5, 128.3, 126.1, 125.9, 121.3, 120.8, 118.6, 45.1, 33.0, 31.0.

**N-benzylbenzo[d]thiazol-2-amine (3aj)<sup>8</sup>**



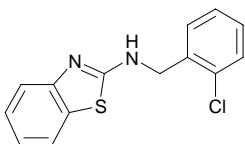
$^1\text{H}$  NMR (500 MHz,  $\text{DMSO-d}_6$ ) δ 8.50 (t,  $J = 5.6$  Hz, 1H, NH), 7.67 (d,  $J = 7.8$  Hz, 1H, ArH), 7.39-7.33 (m, 5H, ArH), 7.26 (t,  $J = 7.1$  Hz, 1H, ArH), 7.22 (t,  $J = 7.7$  Hz, 1H, ArH), 7.02 (t,  $J = 7.5$  Hz, 1H, ArH), 4.60 (br s, 2H,  $\text{CH}_2\text{N}$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{DMSO-d}_6$ ) δ 166.2, 152.4, 138.9, 130.4, 128.3, 127.3, 127.0, 125.5, 120.95, 120.89, 118.1, 47.2.

**N-(4-methoxybenzyl)benzo[d]thiazol-2-amine (3ak)<sup>8</sup>**



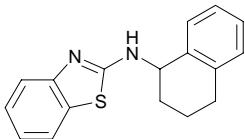
<sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ 8.42 (t, *J* = 5.6 Hz, 1H, NH), 7.66 (d, *J* = 7.5 Hz, 1H, ArH), 7.38 (d, *J* = 8.0 Hz, 1H, ArH), 7.31 (d, *J* = 8.5 Hz, 2H, ArH), 7.21 (t, *J* = 7.6 Hz, 1H, ArH), 7.01 (t, *J* = 7.5 Hz, 1H, ArH), 6.90 (d, *J* = 8.5, 2H, ArH), 4.51 (d, *J* = 5.7 Hz, 2H, CH<sub>2</sub>N), 3.73 (s, 3H, OCH<sub>3</sub>); <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>) δ 166.1, 158.4, 152.5, 130.7, 130.4, 128.8, 125.5, 120.9, 118.0, 113.7, 55.0, 46.7.

***N*-(2-chlorobenzyl)benzo[d]thiazol-2-amine (3al)<sup>8</sup>**



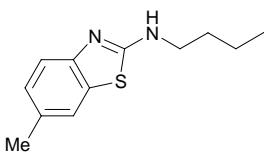
<sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>) δ 8.54 (br s, 1H, NH), 7.69 (d, *J* = 7.8 Hz, 1H, ArH), 7.48 (d, *J* = 6.7 Hz, 2H, ArH), 7.40 (d, *J* = 8.0 Hz, 1H, ArH), 7.35-7.30 (m, 2H, ArH), 7.22 (t, *J* = 7.6 Hz, 1H, ArH), 7.04 (t, *J* = 7.6 Hz, 1H, ArH), 4.68 (br s, 2H, CH<sub>2</sub>N); <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>) δ 166.0, 152.3, 135.9, 132.3, 130.5, 129.3, 129.1, 128.9, 127.2, 125.6, 121.1, 121.0, 118.2, 45.0.

***N*-(1,2,3,4-tetrahydronaphthalen-1-yl)benzo[d]thiazol-2-amine (3am)**



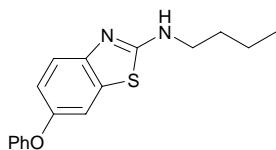
mp 131.7-132.3 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.56 (d, *J* = 7.5, 1H, ArH), 7.42 (d, *J* = 7.8 Hz, 1H, ArH), 7.37 (d, *J* = 8.0 Hz, 1H, ArH), 7.24 (t, *J* = 7.6 Hz, 1H, ArH), 7.20-7.13 (m, 2H, ArH), 7.10 (d, *J* = 7.5 Hz, 1H, ArH), 7.06 (t, *J* = 7.6 Hz, 1H, ArH), 6.04 (br s, 1H, NH), 5.01 (t, *J* = 5.5 Hz, 1H, CHN), 2.85-2.73 (m, 2H, CH<sub>2</sub>), 2.19-2.13 (m, 1H, CH), 2.07-2.01 (m, 1H, CH), 1.94-1.81 (m, 2H, CH<sub>2</sub>); <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 166.6, 152.4, 137.5, 136.1, 130.2, 129.2, 128.9, 127.6, 126.3, 125.9, 121.5, 120.7, 118.8, 53.9, 29.9, 29.1, 19.9; FTIR (net, cm<sup>-1</sup>) 3213, 2937, 1722, 1567, 1447, 1155; HRMS-EI (70 eV) m/z calcd for C<sub>17</sub>H<sub>17</sub>N<sub>2</sub>S [M+H]<sup>+</sup> 281.1112, found 281.1113.

***N*-butyl-6-methylbenzo[d]thiazol-2-amine (3ba)<sup>9</sup>**



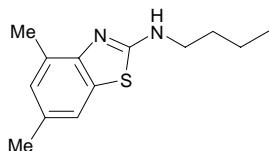
mp 90.7-91.7 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.41 (d,  $J = 8.2$  Hz, 1H, ArH), 7.38 (s, 1H, ArH), 7.09 (d,  $J = 8.2$  Hz, 2H, ArH), 5.47 (br s, 1H, NH), 3.39 (t,  $J = 7.0$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 2.39 (s, 3H,  $\text{CH}_3\text{Ar}$ ), 1.66 (quint,  $J = 7.3$  Hz, 2H), 1.43 (sext,  $J = 7.5$  Hz, 2H), 0.96 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  167.4, 150.2, 130.9, 130.3, 127.0, 120.8, 118.1, 45.4, 31.6, 21.1, 20.0, 13.7.

### **N-butyl-6-phenoxybenzo[d]thiazol-2-amine (3ca)**



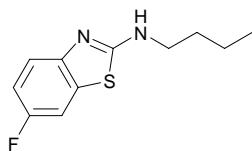
mp 116.0-116.7 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48 (d,  $J = 8.8$  Hz, 1H, ArH), 7.31 (t,  $J = 8.0$  Hz, 2H, ArH), 7.25 (s, 1H, ArH), 7.06 (t,  $J = 7.4$  Hz, 1H, ArH), 7.00 (dd,  $J = 8.3$  Hz and 2.5 Hz, 1H, ArH), 6.98 (d,  $J = 7.9$  Hz, 1H, ArH), 5.23 (br s, 1H, NH), 3.41 (t,  $J = 7.1$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.67 (quint,  $J = 7.4$  Hz, 2H,  $\text{CH}_2$ ), 1.45 (sext,  $J = 7.4$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  167.2, 158.3, 151.4, 148.9, 131.3, 129.6, 122.6, 119.2, 118.3, 117.9, 112.0, 45.3, 31.6, 20.0, 13.7; FTIR (net,  $\text{cm}^{-1}$ ) 3165, 2956, 1611, 1593, 1455, 1149. HRMS-EI (70 eV) m/z calcd for  $\text{C}_{17}\text{H}_{19}\text{N}_2\text{OS}$  [M+H]<sup>+</sup> 299.1218, found 299.1223.

### **N-butyl-4,6-dimethylbenzo[d]thiazol-2-amine (3da)**



mp 46.0-47.2 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.24 (s, 1H, ArH), 6.93 (s, 1H, ArH), 5.29 (br s, 1H, NH), 3.34 (quart,  $J = 5.8$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 2.51 (s, 3H,  $\text{CH}_3\text{Ar}$ ), 2.35 (s, 3H,  $\text{CH}_3\text{Ar}$ ), 1.65 (quint,  $J = 5.8$  Hz, 2H,  $\text{CH}_2$ ), 1.44 (sext,  $J = 7.4$  Hz, 2H,  $\text{CH}_2$ ), 0.96 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  166.7, 149.2, 130.8, 130.1, 128.0, 127.9, 118.3, 45.6, 31.6, 21.1, 19.9, 18.3, 13.7; FTIR (net,  $\text{cm}^{-1}$ ) 3242, 2959, 1606, 1557, 1447, 1145; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{13}\text{H}_{19}\text{N}_2\text{S}$  [M+H]<sup>+</sup> 235.1269, found 235.1271.

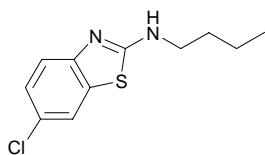
### **N-butyl-6-fluorobenzo[d]thiazol-2-amine (3ea)**



mp 95.8-96.6 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.43 (dd,  $J = 8.7$  Hz and 4.8 Hz, 1H, ArH), 7.29 (dd,  $J = 8.2$  Hz and 2.5 Hz, 1H, ArH), 7.00 (td,  $J = 8.9$  Hz and 2.6 Hz, 1H, ArH), 5.40 (br s, 1H, NH), 3.40 (t,

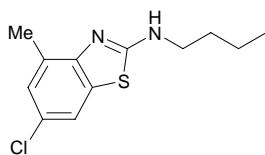
$J = 7.1$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.67 (quint,  $J = 7.3$  Hz, 2H,  $\text{CH}_2$ ), 1.44 (sext,  $J = 7.5$  Hz, 2H,  $\text{CH}_2$ ), 0.96 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  167.4, 158.1 (d,  $J_{\text{C}-\text{F}} = 238.3$  Hz), 148.9, 131.0 (d,  $J_{\text{C}-\text{F}} = 10.7$  Hz), 118.9, 113.5 (d,  $J_{\text{C}-\text{F}} = 23.6$  Hz), 107.5 (d,  $J_{\text{C}-\text{F}} = 26.2$ ), 45.4, 31.6, 20.0, 13.7; FTIR (net,  $\text{cm}^{-1}$ ) 3214, 2972, 1621, 1569, 1461, 1137; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{11}\text{H}_{14}\text{N}_2\text{FS} [\text{M}+\text{H}]^+$  225.0862, found 225.0863

**N-butyl-6-chlorobenzo[d]thiazol-2-amine (3fa)<sup>10</sup>**



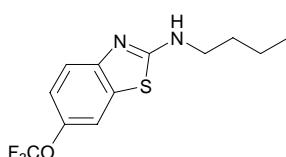
mp 109.5-110.6 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.54 (d,  $J = 2.1$  Hz, 1H, ArH), 7.41 (d,  $J = 8.7$  Hz, 1H, ArH), 7.24 (dd,  $J = 8.7$  Hz and 2.4 Hz, 1H, ArH), 5.44 (br s, 1H, NH), 3.41 (t,  $J = 7.1$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.67 (quint,  $J = 7.3$  Hz, 2H,  $\text{CH}_2$ ), 1.44 (sext,  $J = 7.5$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.3$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  168.0, 151.1, 131.5, 126.4, 126.3, 120.4, 119.2, 45.4, 31.5, 20.0, 13.7.

**N-butyl-6-chloro-4-methylbenzo[d]thiazol-2-amine (3ga)**



mp 70.1-71.4 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.40 (s, 1H, ArH), 7.08 (s, 1H, ArH), 5.32 (br s, 1H, NH), 3.36 (quart,  $J = 6.1$  Hz,  $\text{CH}_2\text{N}$ ), 2.51 (s, 3H,  $\text{CH}_3\text{Ar}$ ), 1.66 (quint,  $J = 7.3$  Hz, 2H,  $\text{CH}_2$ ), 1.44 (sext,  $J = 7.4$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  167.2, 150.1, 131.0, 129.6, 126.9, 126.0, 117.8, 45.5, 31.6, 19.9, 18.2, 13.6; FTIR (net,  $\text{cm}^{-1}$ ) 3219, 2958, 1600, 1553, 1435, 1138; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{12}\text{H}_{16}\text{N}_2\text{SCl} [\text{M}+\text{H}]^+$  255.0723, found 255.0722.

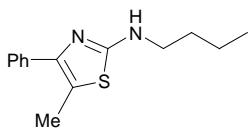
**N-butyl-6-(trifluoromethoxy)benzo[d]thiazol-2-amine (3ha)**



mp 76.4-77.4 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.48-7.45 (m, 2H, ArH), 7.15 (d,  $J = 8.7$  Hz, 1H, ArH), 5.47 (br s, 1H, NH), 3.42 (t,  $J = 7.0$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.68 (quint,  $J = 7.3$  Hz, 2H,  $\text{CH}_2$ ), 1.45 (sext,  $J = 7.5$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ )  $\delta$  168.2, 151.3, 143.5, 131.0, 120.6 (q,  $J_{\text{C}-\text{F}} = 254.8$  Hz), 119.6, 118.9, 114.0, 45.4, 31.6, 20.0, 13.7; FTIR (net,  $\text{cm}^{-1}$ ) 3223,

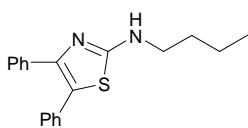
3094, 1619, 1574, 1455, 1143; HRMS-EI (70 eV) m/z calcd for  $C_{12}H_{14}N_2OF_3S$  [M+H]<sup>+</sup> 291.0779, found 291.0775.

**N-butyl-5-methyl-4-phenylthiazol-2-amine (3ia)<sup>11</sup>**



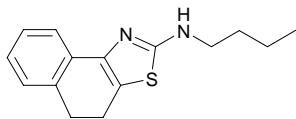
mp 55.4-56.8 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.57 (d, *J* = 7.8 Hz, 2H, ArH), 7.38 (t, *J* = 7.7 Hz, 2H, ArH), 7.28 (t, *J* = 7.4 Hz, 1H, ArH), 5.26 (br s, 1H, NH), 3.20 (quart, *J* = 6.0 Hz, 2H, CH<sub>2</sub>N), 3.40 (s, 3H, CH<sub>3</sub>), 1.59 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.39 (sext, *J* = 7.4 Hz, 2H, CH<sub>2</sub>), 0.94 (t, *J* = 7.4 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 166.2, 146.3, 135.4, 128.4, 128.2, 127.1, 115.3, 45.9, 31.6, 20.0, 13.7, 12.4.

**N-butyl-4,5-diphenylthiazol-2-amine (3ja)<sup>11</sup>**



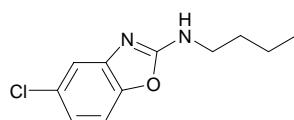
mp 116.2-117.0 (lit.<sup>12</sup> mp 117-118 °C); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.47 (dd, *J* = 7.9 Hz and 2.2 Hz, 2H, ArH), 7.27-7.17 (m, 8H, ArH), 6.15 (br s 1H, NH), 3.14 (quart, *J* = 6.2 Hz, 2H, CH<sub>2</sub>N), 1.51 (quint, *J* = 7.4 Hz, 2H, CH<sub>2</sub>), 1.33 (sext, *J* = 7.4 Hz, 2H, CH<sub>2</sub>), 0.90 (t, *J* = 7.3 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.0, 146.1, 135.6, 133.0, 129.2, 129.0, 128.4, 128.1, 127.4, 126.8, 119.9, 46.0, 31.3, 20.0, 13.7.

**N-butyl-4,5-dihydronaphtho[1,2-d]thiazol-2-amine (3ka)**



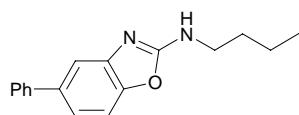
mp 89.8-90.6 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.70 (d, *J* = 7.6 Hz, 1H, ArH), 7.23 (t, *J* = 7.3 Hz, 1H, ArH), 7.17-7.11 (m, 3H, ArH), 5.1 (br s, 1H, NH), 3.27 (quart, *J* = 6.5 Hz, 2H, CH<sub>2</sub>N), 3.02 (t, *J* = 7.8 Hz, 2H, CH<sub>2</sub>), 2.85 (t, *J* = 7.8 Hz, 2H, CH<sub>2</sub>), 1.65 (quint, *J* = 7.3 Hz, 2H, CH<sub>2</sub>), 1.43 (sext, *J* = 7.5 Hz, 2H, CH<sub>2</sub>), 0.96 (t, *J* = 7.3 Hz, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 168.3, 145.4, 134.4, 131.8, 127.5, 126.8, 126.5, 122.7, 117.7, 45.8, 31.5, 29.2, 21.8, 20.0, 13.7; FTIR (net, cm<sup>-1</sup>) 3201, 2958, 1600, 1553, 1435, 1138; HRMS-EI (70 eV) m/z calcd for  $C_{15}H_{19}N_2S$  [M+H]<sup>+</sup> 259.1269, found 259.1274.

**N-butyl-5-chlorobenzo[d]oxazol-2-amine (3la)<sup>12</sup>**



mp 109.5-110.6 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) δ 7.31 (s, 1H, ArH), 7.13 (d,  $J = 8.3$  Hz, 1H, ArH), 6.98 (d,  $J = 8.1$  Hz, 1H, ArH), 5.18 (br s, 1H, NH), 3.48 (quart,  $J = 6.4$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.67 (quint,  $J = 7.2$  Hz, 2H,  $\text{CH}_2$ ), 1.44 (sext,  $J = 7.5$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) δ 163.2, 147.1, 144.4, 129.2, 120.4, 116.2, 109.1, 42.8, 31.8, 19.9, 13.7.

### N-butyl-5-phenylbenzo[d]oxazol-2-amine (3ma)

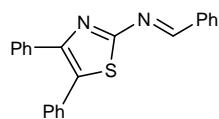


mp 132.3-133.6 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) δ 7.59-7.58 (m, 3H, ArH), 7.43 (t,  $J = 7.7$  Hz, 2H, ArH), 7.33 (t,  $J = 7.4$ , 1H, ArH), 7.29-7.26 (m, 2H, ArH), 5.10 (br s, 1H, NH), 3.51 (t,  $J = 6.6$  Hz, 2H,  $\text{CH}_2\text{N}$ ), 1.68 (quint,  $J = 7.4$  Hz, 2H,  $\text{CH}_2$ ), 1.45 (sext,  $J = 7.5$  Hz, 2H,  $\text{CH}_2$ ), 0.97 (t,  $J = 7.4$  Hz, 3H,  $\text{CH}_3$ );  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) δ 162.7, 148.1, 143.6, 141.6, 137.7, 128.7, 127.3, 126.9, 120.1, 114.8, 108.6, 42.9, 31.8, 19.9, 13.7; FTIR (net,  $\text{cm}^{-1}$ ) 3157, 2953, 1690, 1592, 1467, 1181; HRMS-EI (70 eV) m/z calcd for  $\text{C}_{17}\text{H}_{19}\text{N}_2\text{O}$  [ $\text{M}+\text{H}]^+$  267.1497, found 267.1499.

### Procedure for the condensation of 4,5-diphenylthiazol-2-amine with benzaldehyde

To an oven-dried, nitrogen purged 20 ml Schlenk tube were added 4,5-diphenylthiazol-2-amine (1 mmol), base (0.2 mmol, 20 mol%) and benzaldehyde (5 mmol, 500 mol%). The resulting mixture was heated at 150 °C for 12h, followed by the mixture of the reaction was allowed to cool to ambient temperature. The mixture of the reaction was concentrated in *vacuo* and purified by flash column chromatography with hexane/ethyl acetate to afford the corresponding product.

### (E)-N-benzylidene-4,5-diphenylthiazol-2-amine<sup>13</sup>

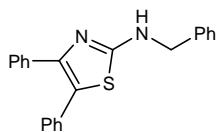


mp 109.4-110.2 °C;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) δ 9.09 (s, 1H,  $\text{CH}=\text{N}$ ), 8.01 (d,  $J = 7.1$  Hz, 2H, ArH), 7.58-7.56 (m, 2H, ArH), 7.54 (d,  $J = 7.1$  Hz, 1H, ArH), 7.50 (t,  $J = 7.3$  Hz, 2H, ArH), 7.39-7.37 (m, 2H, ArH), 7.34-7.32 (m, 3H, ArH), 7.30-7.29 (m, 3H, ArH);  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) δ 169.8, 163.1, 148.5, 135.1, 134.8, 132.6, 132.2, 132.1, 129.9, 129.6, 129.2, 128.9, 128.7, 128.24, 128.17, 127.9.

### Procedure for the reaction of (E)-N-benzylidene-4,5-diphenylthiazol-2-amine with benzyl alcohol

To an oven-dried, nitrogen purged 20 ml Schlenk tube were added (*E*)-N-benzylidene-4,5-diphenylthiazol-2-amine (1mmol), [Cp\*IrCl<sub>2</sub>]<sub>2</sub> (0.002 mmol, 0.2 mol%), NaOH (0.2 mmol, 20 mol%) and benzyl alcohol (5 mmol, 500 mol%). The resulting mixture was heated at 150 °C for 12h, followed by the mixture of the reaction was allowed to cool to ambient temperature. The mixture of the reaction was concentrated in *vacuo* and purified by flash column chromatography with hexane/ethyl acetate to afford the corresponding product. The yield of N-benzyl-4,5-diphenylthiazol-2-amine is isolated yield, and the yield of benzaldehyde is determined by the <sup>1</sup>H NMR integration.

**N-benzyl-4,5-diphenylthiazol-2-amine<sup>11</sup>**

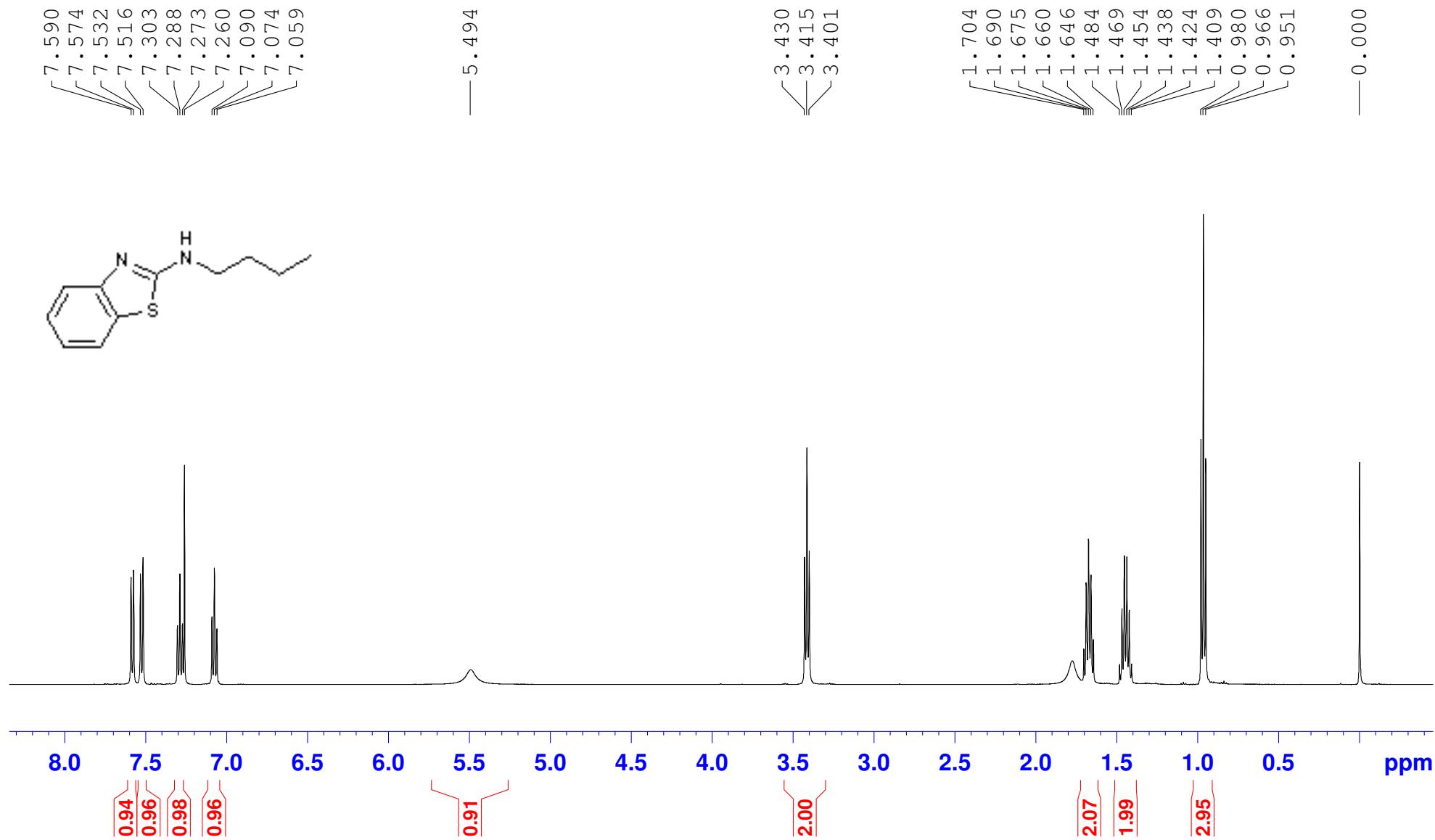
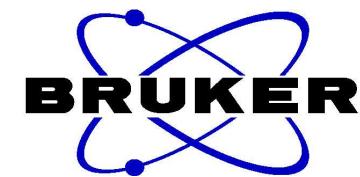


mp 142.1-143.2 °C; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.48-7.47 (m, 2H, ArH), 7.38-7.33 (m, 4H, ArH), 7.31-7.28 (m, 1H, ArH), 7.25-7.19 (m, 8H, ArH), 6.13 (br s, 1H, NH), 4.42 (s, 2H, CH<sub>2</sub>); <sup>13</sup>C NMR (125MHz, CDCl<sub>3</sub>) δ 167.3, 146.0, 137.7, 135.5, 132.8, 129.3, 129.0, 128.7, 128.5, 128.1, 127.7, 127.6, 127.5, 127.0, 120.8, 49.8

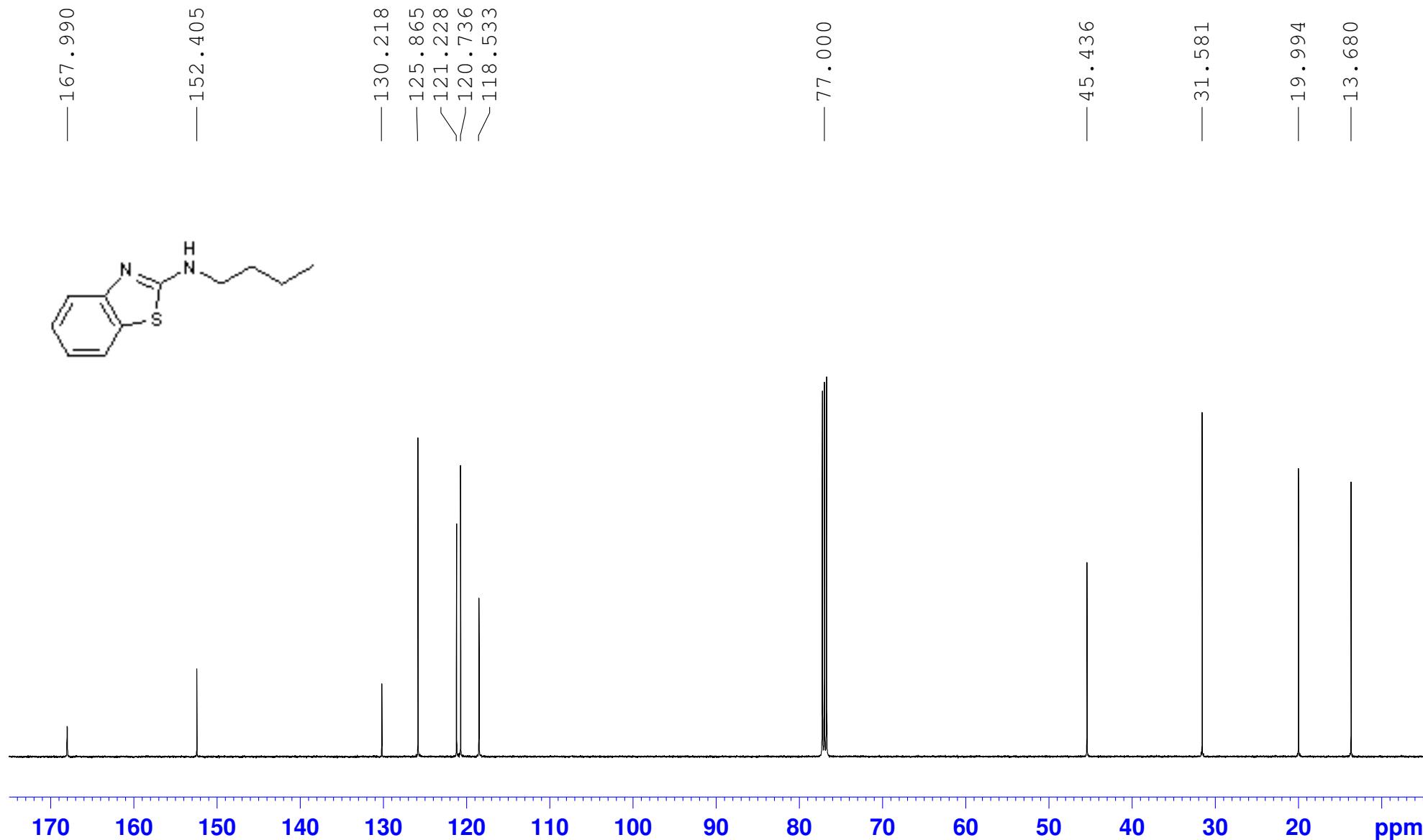
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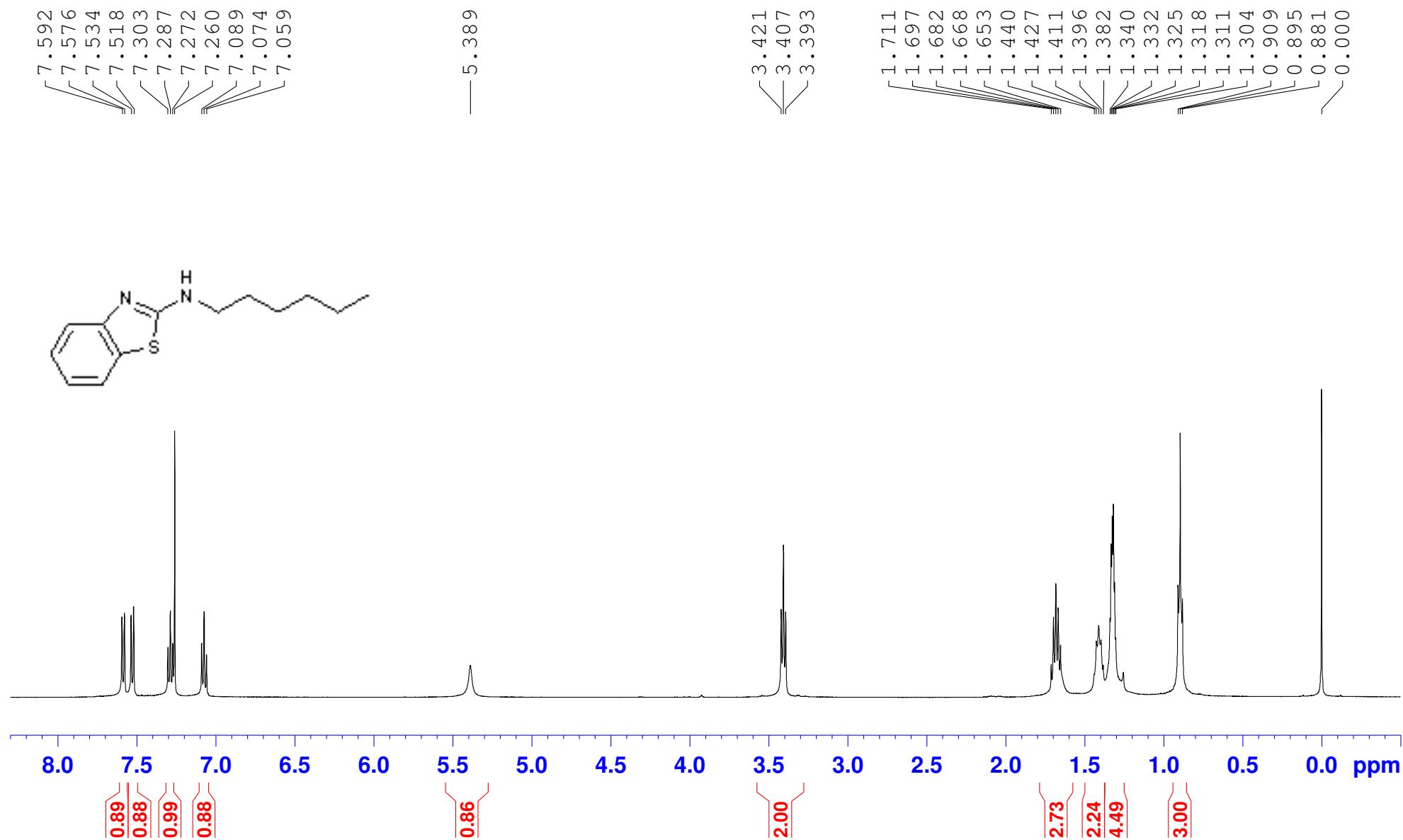
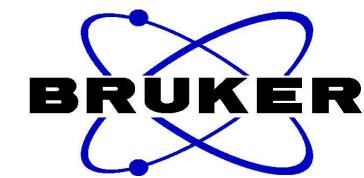
N-butylbenzo[d]thiazol-2-amine  
Proton CDCl<sub>3</sub>



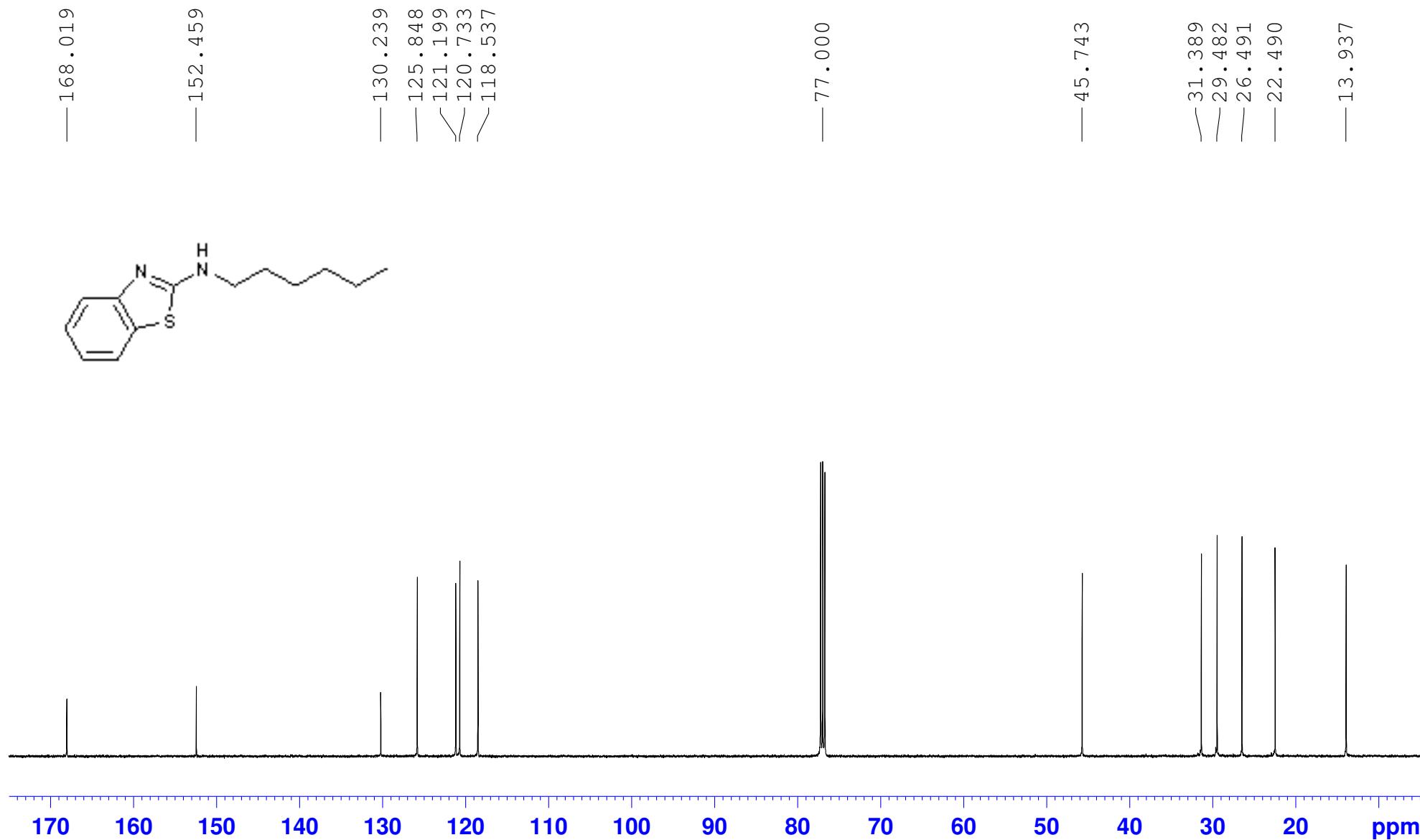
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C13CPD CDCl<sub>3</sub>



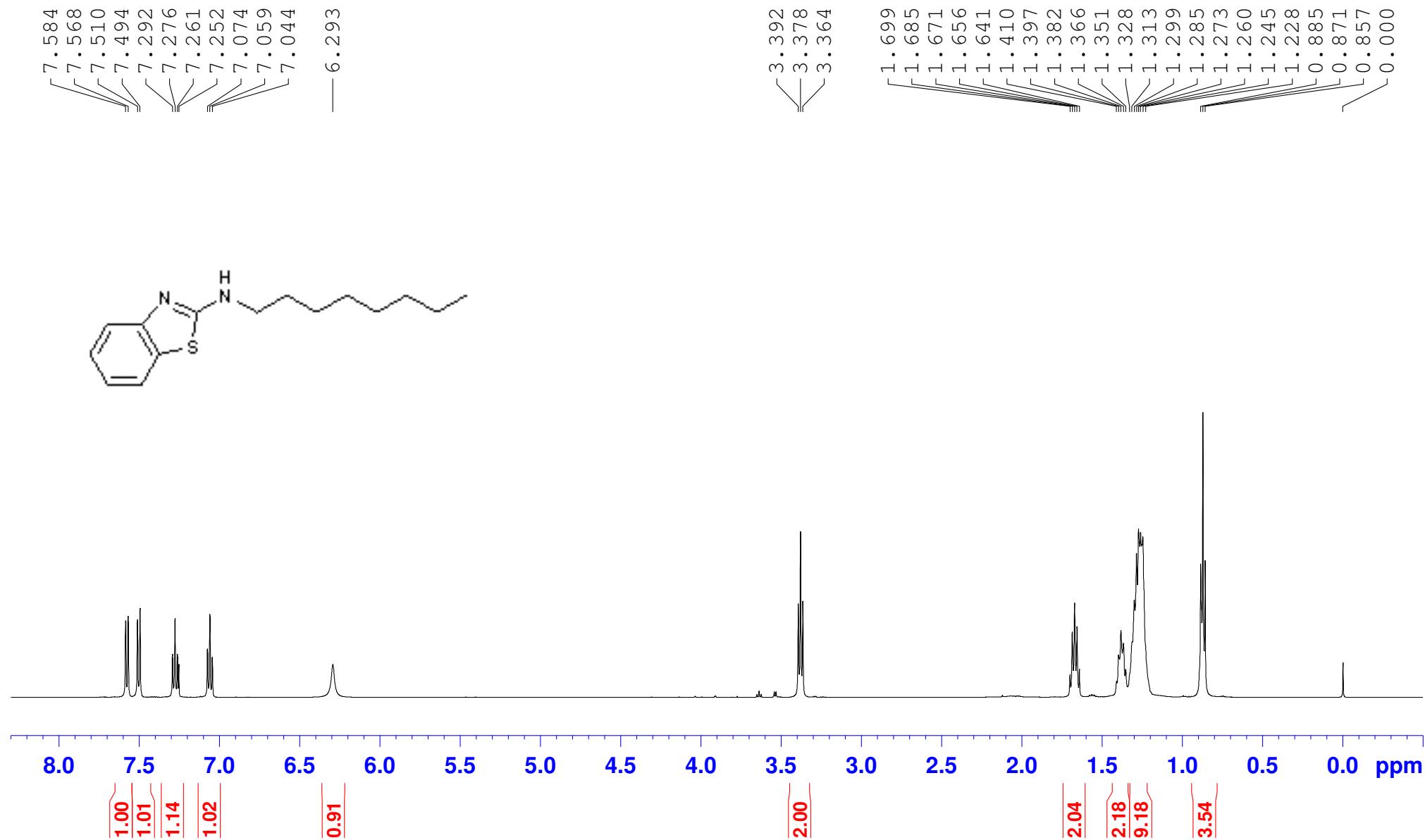
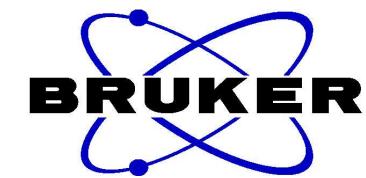
N-hexylbenzo[d]thiazol-2-amine  
Proton CDCl<sub>3</sub>



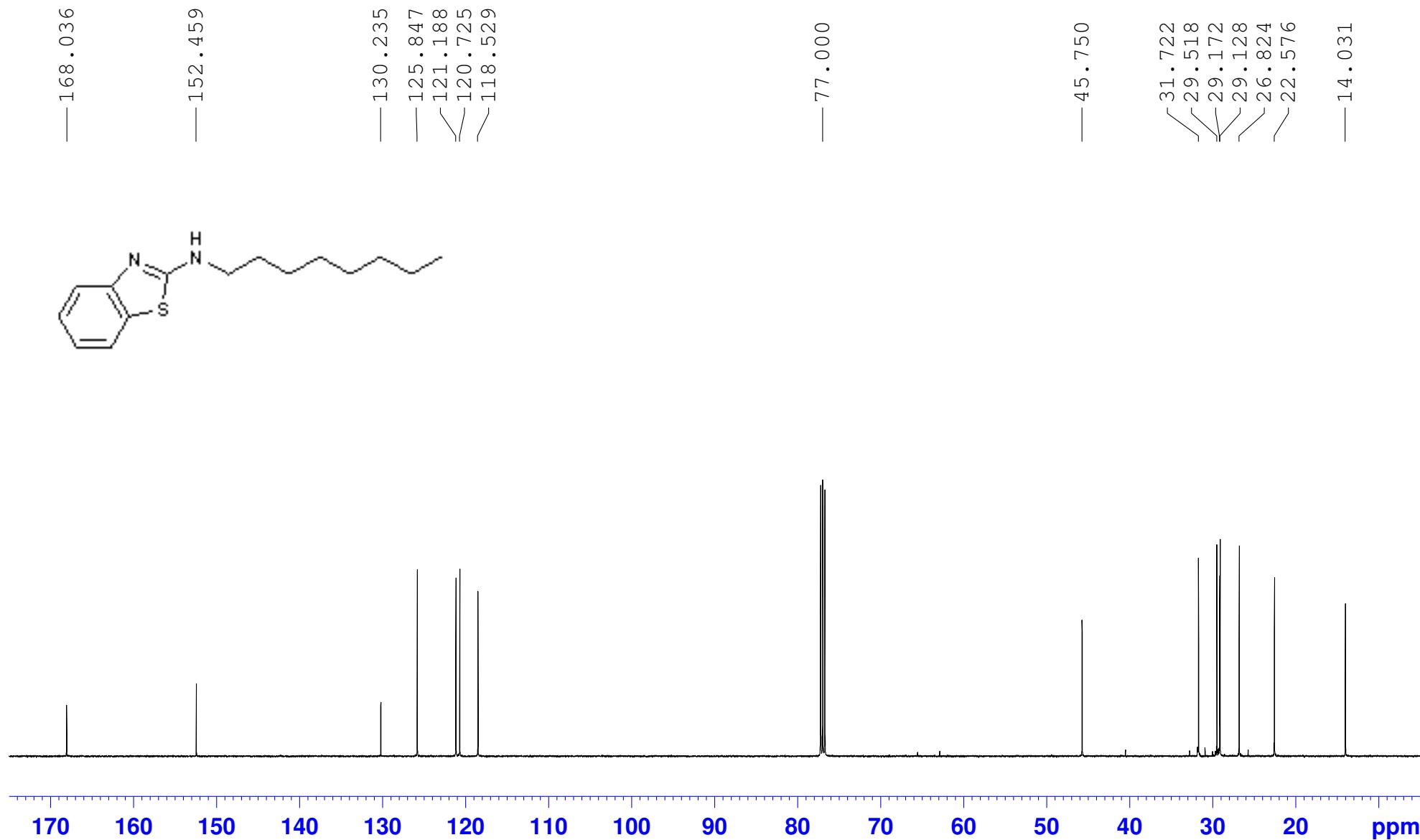
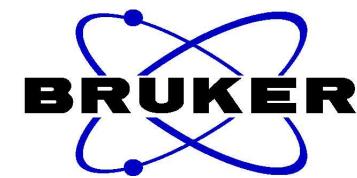
N-hexylbenzo[d]thiazol-2-amine  
C13CPD CDCl<sub>3</sub>



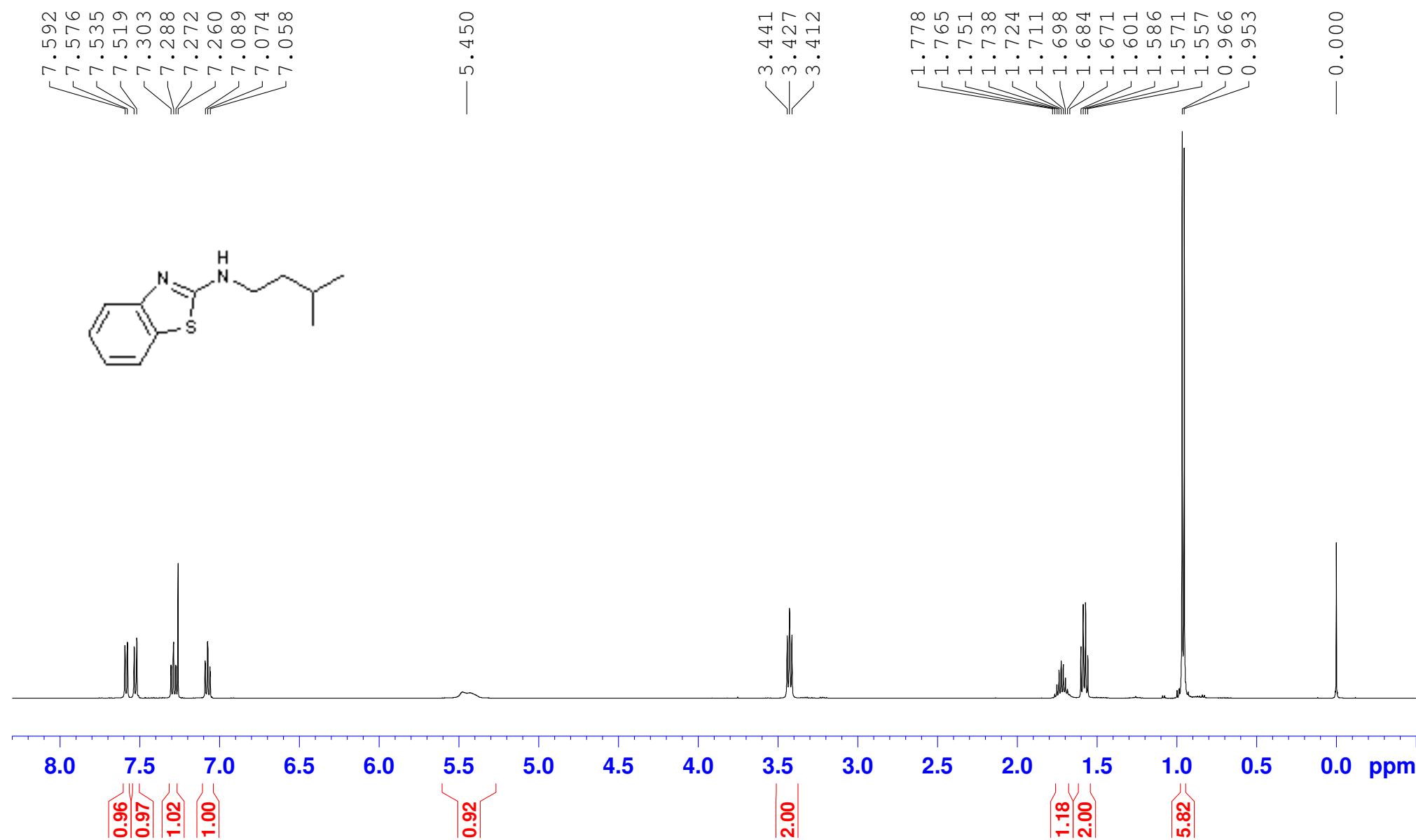
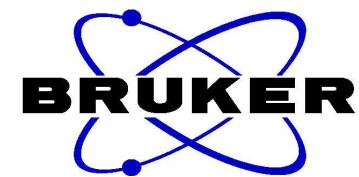
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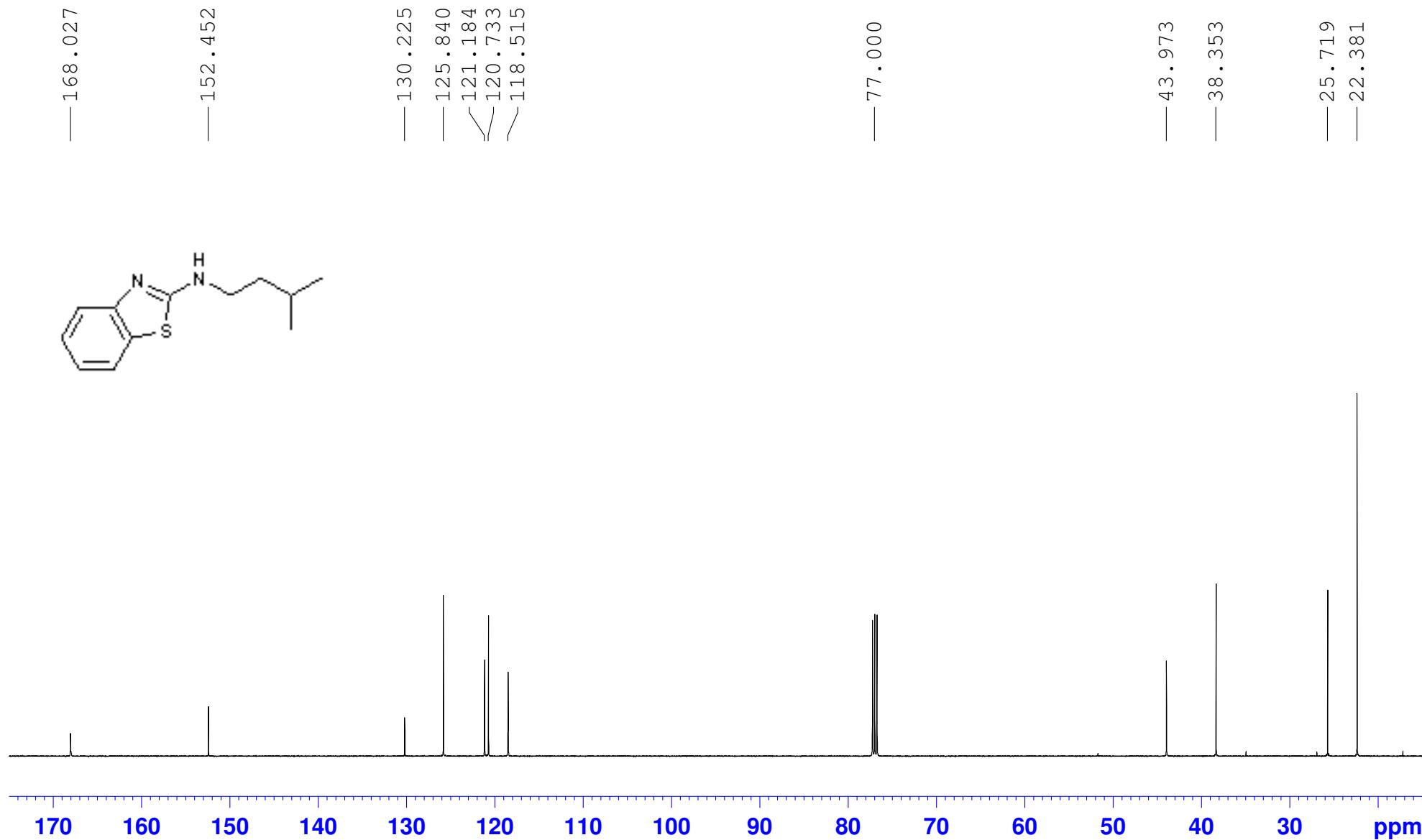
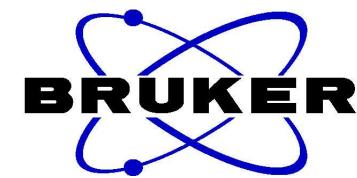
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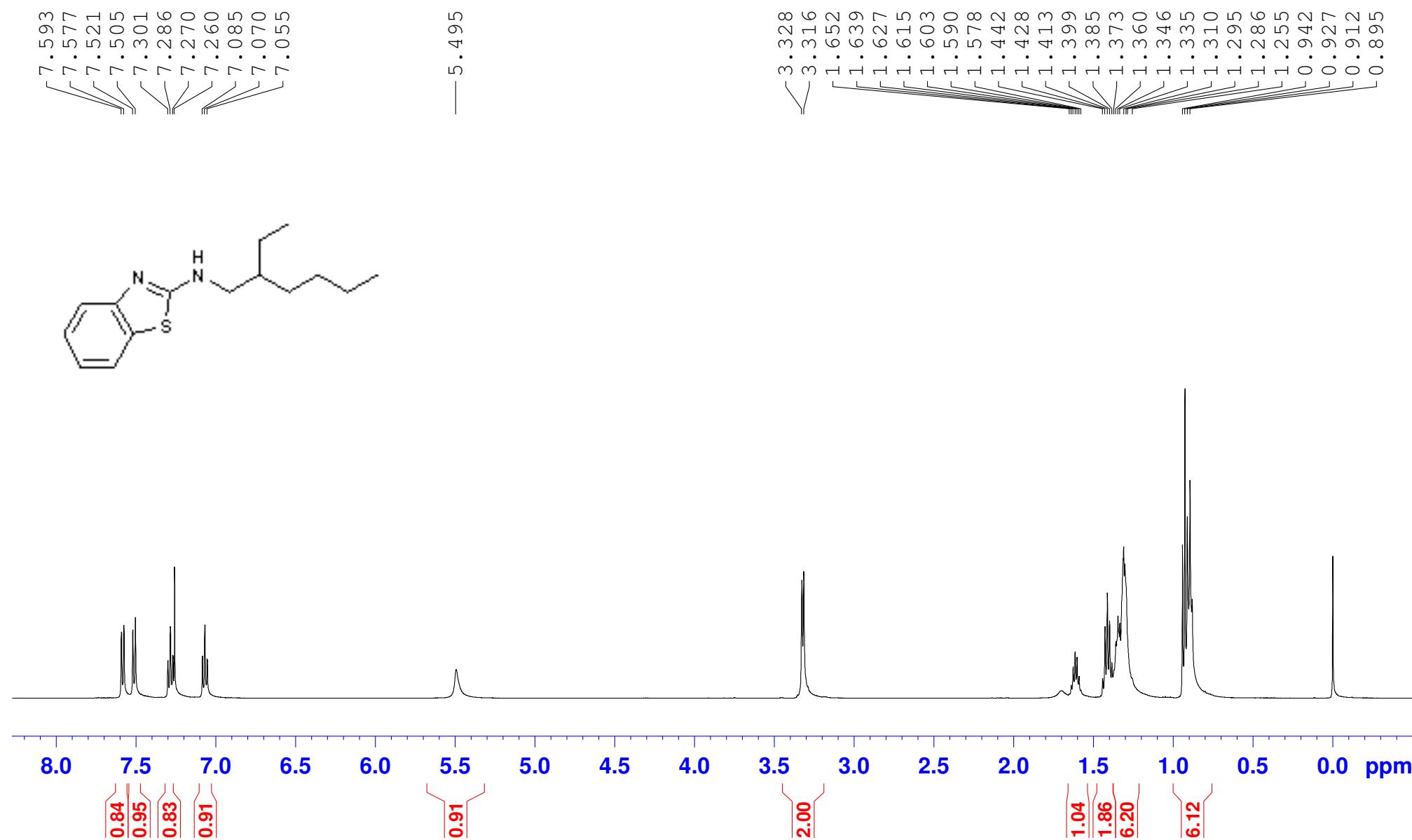
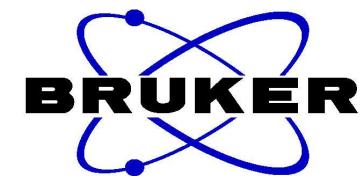
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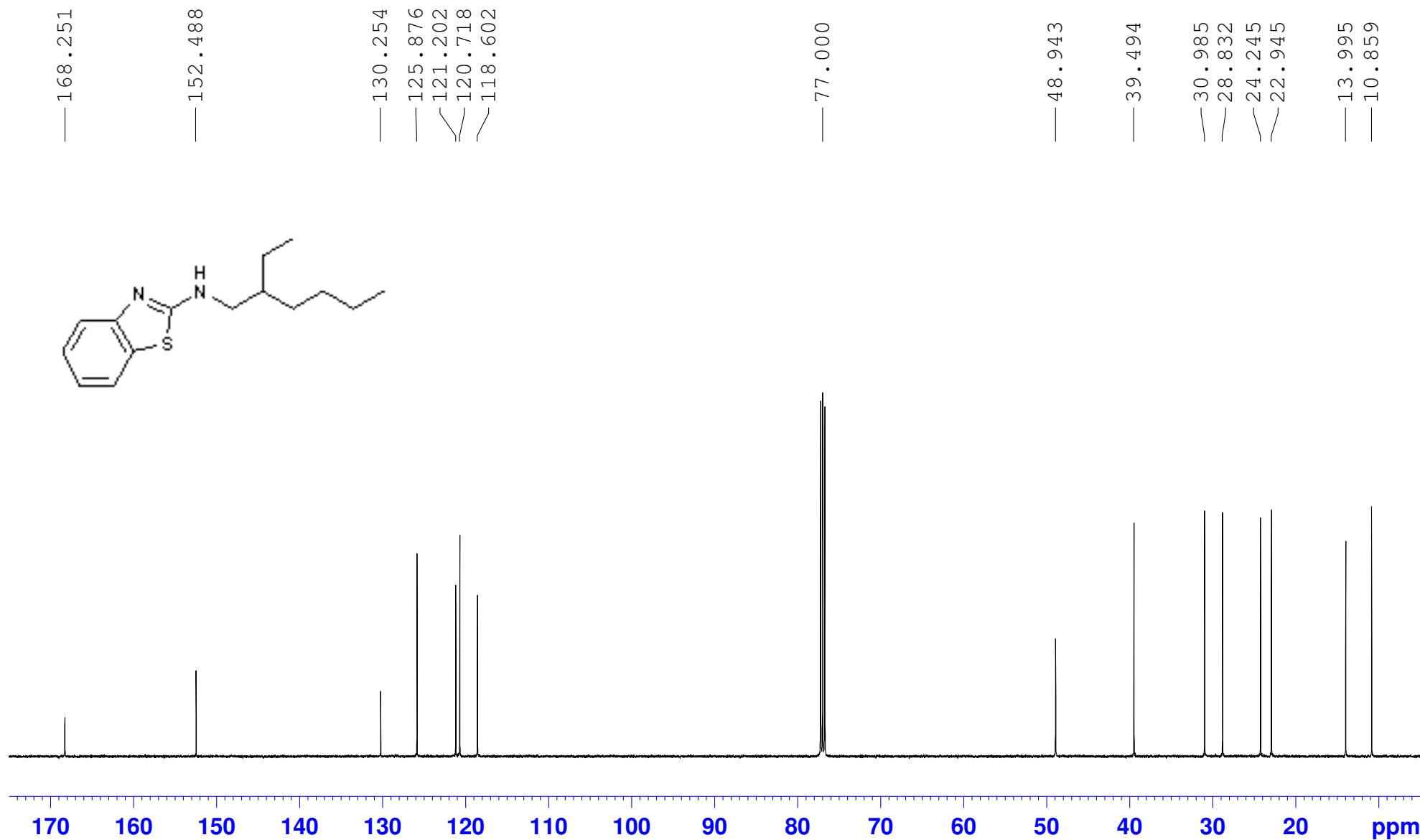
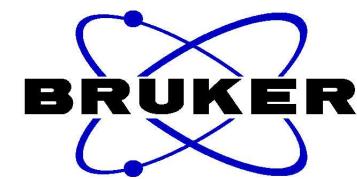
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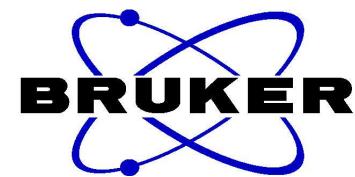
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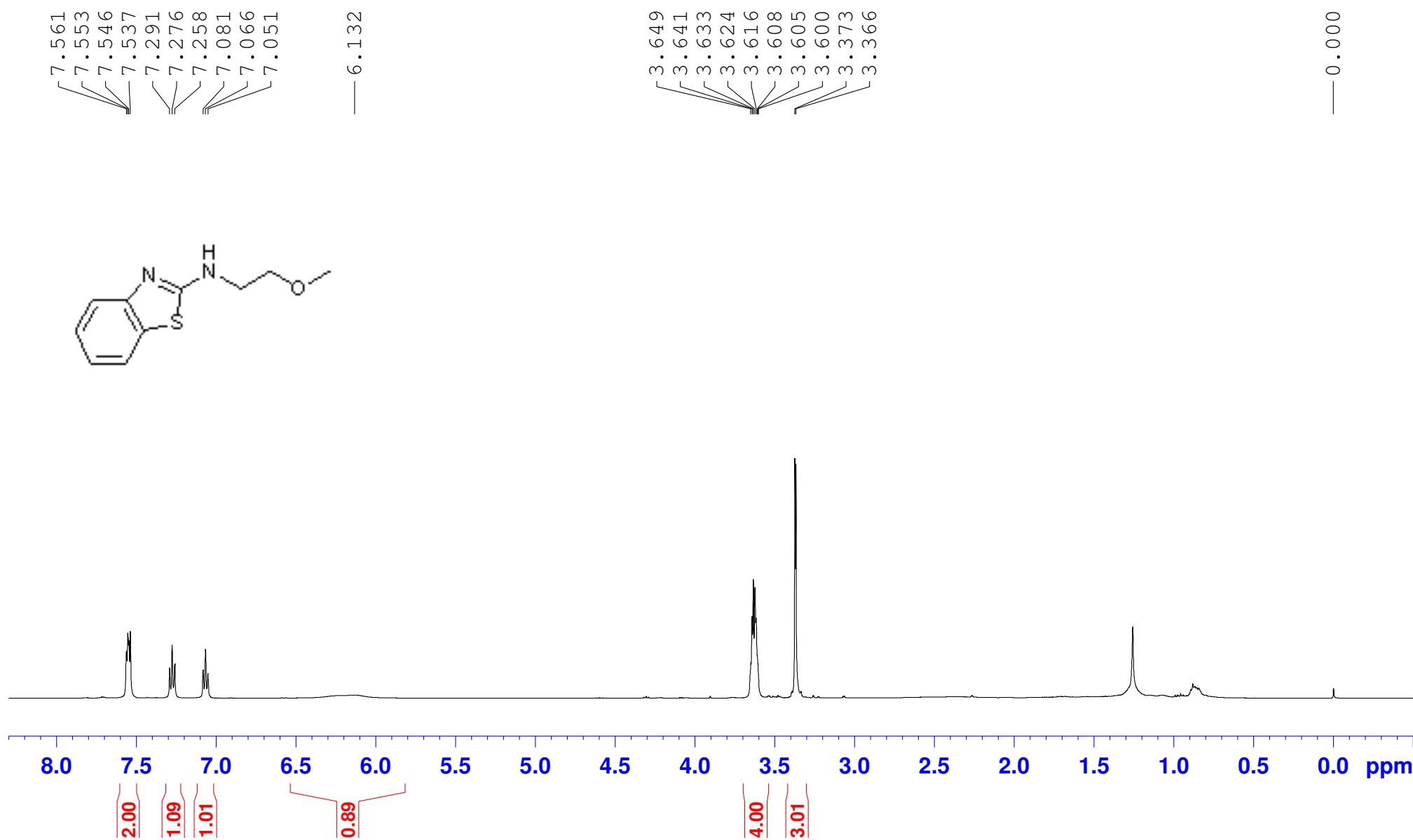
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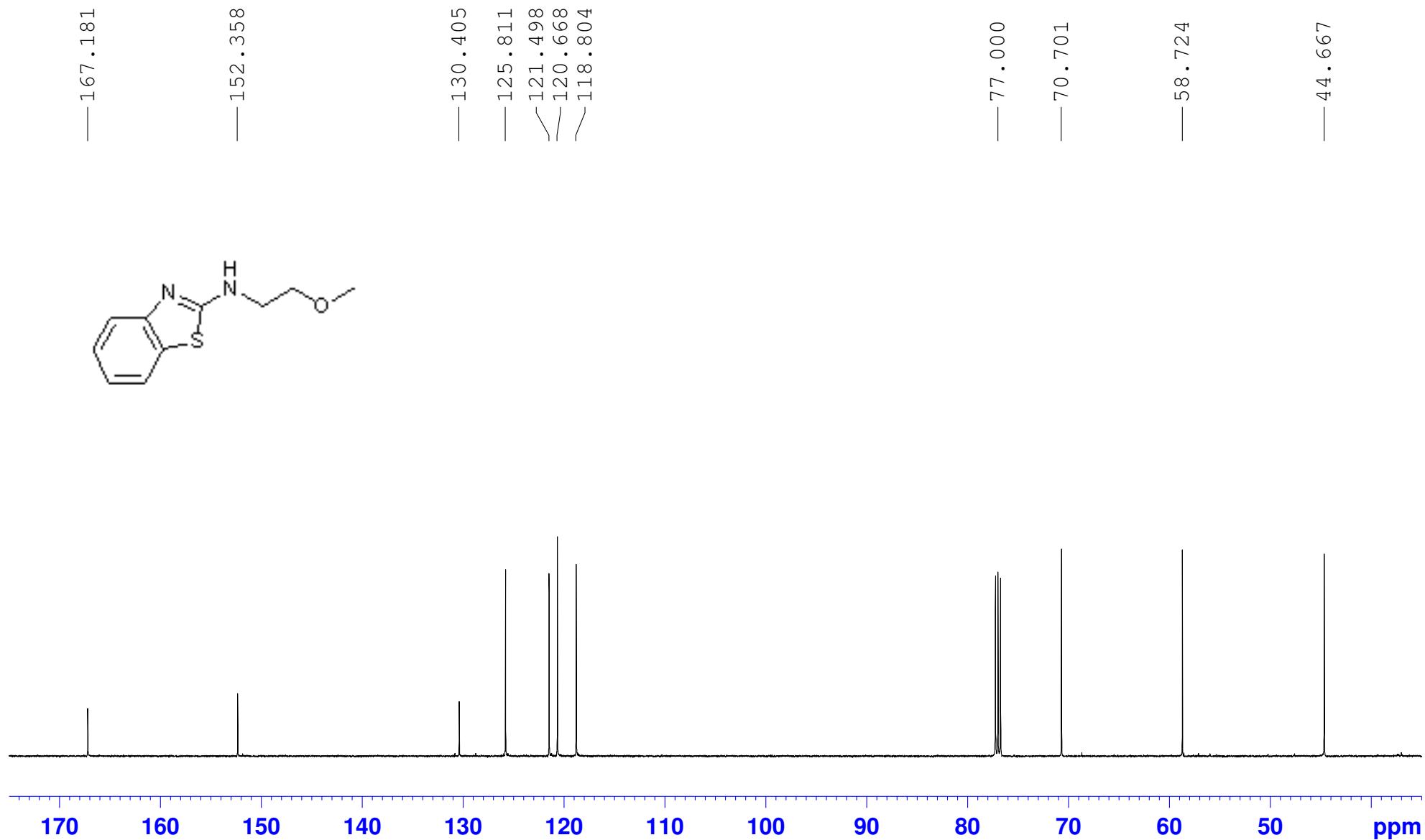
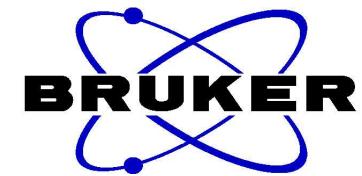
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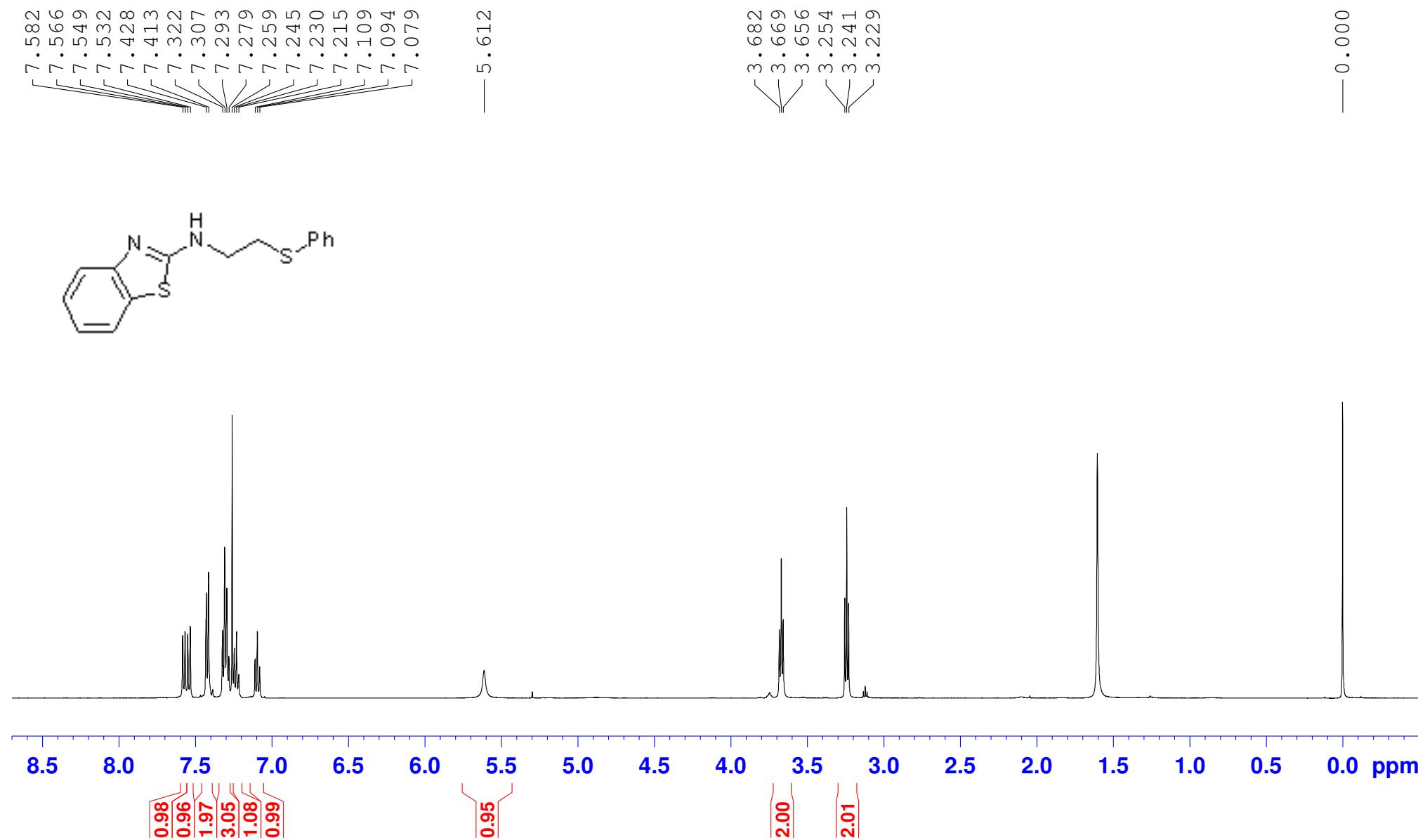
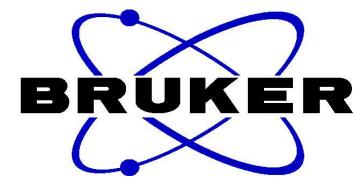
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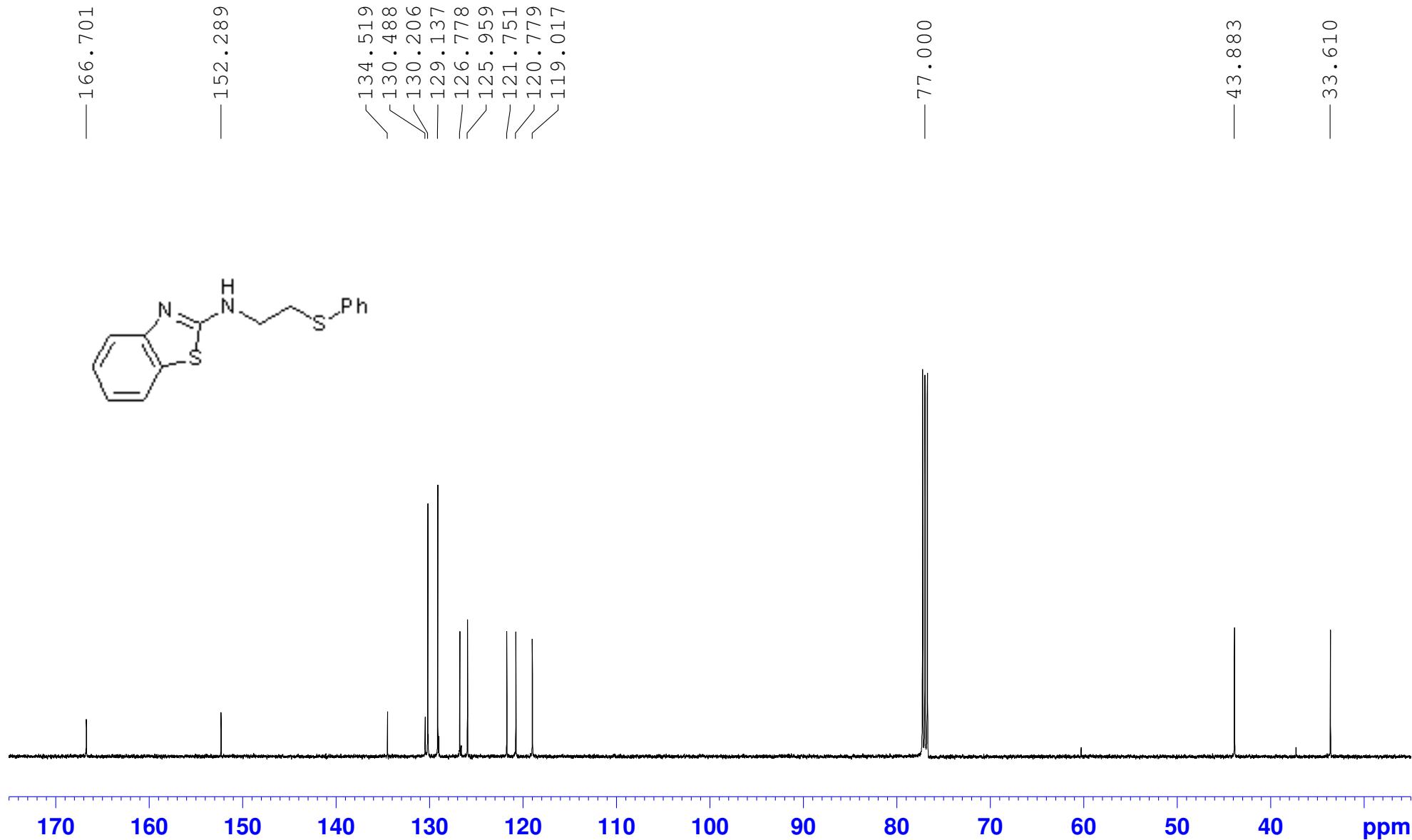
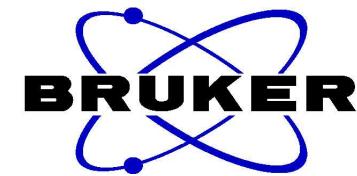
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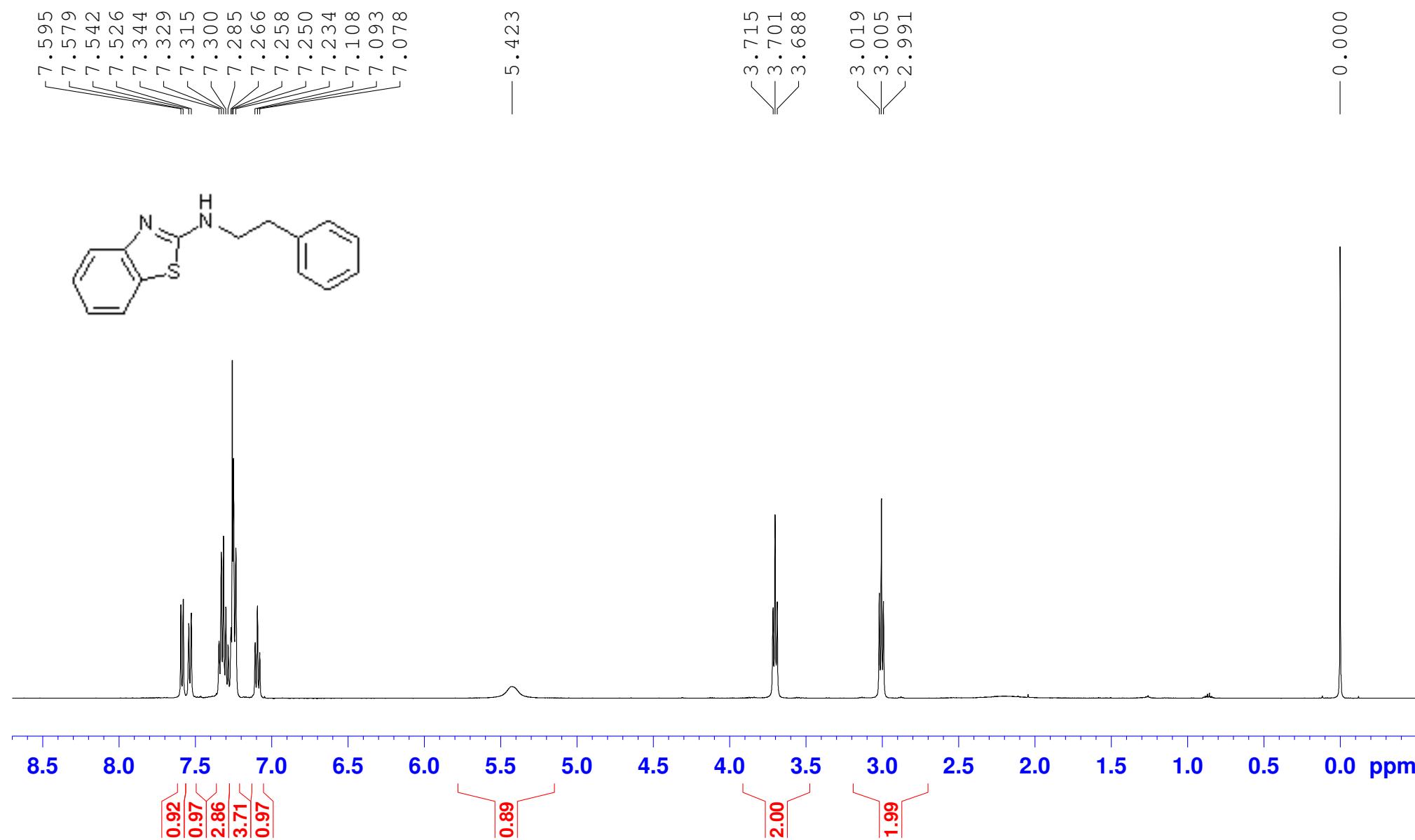
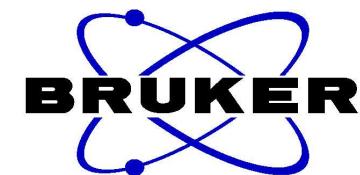
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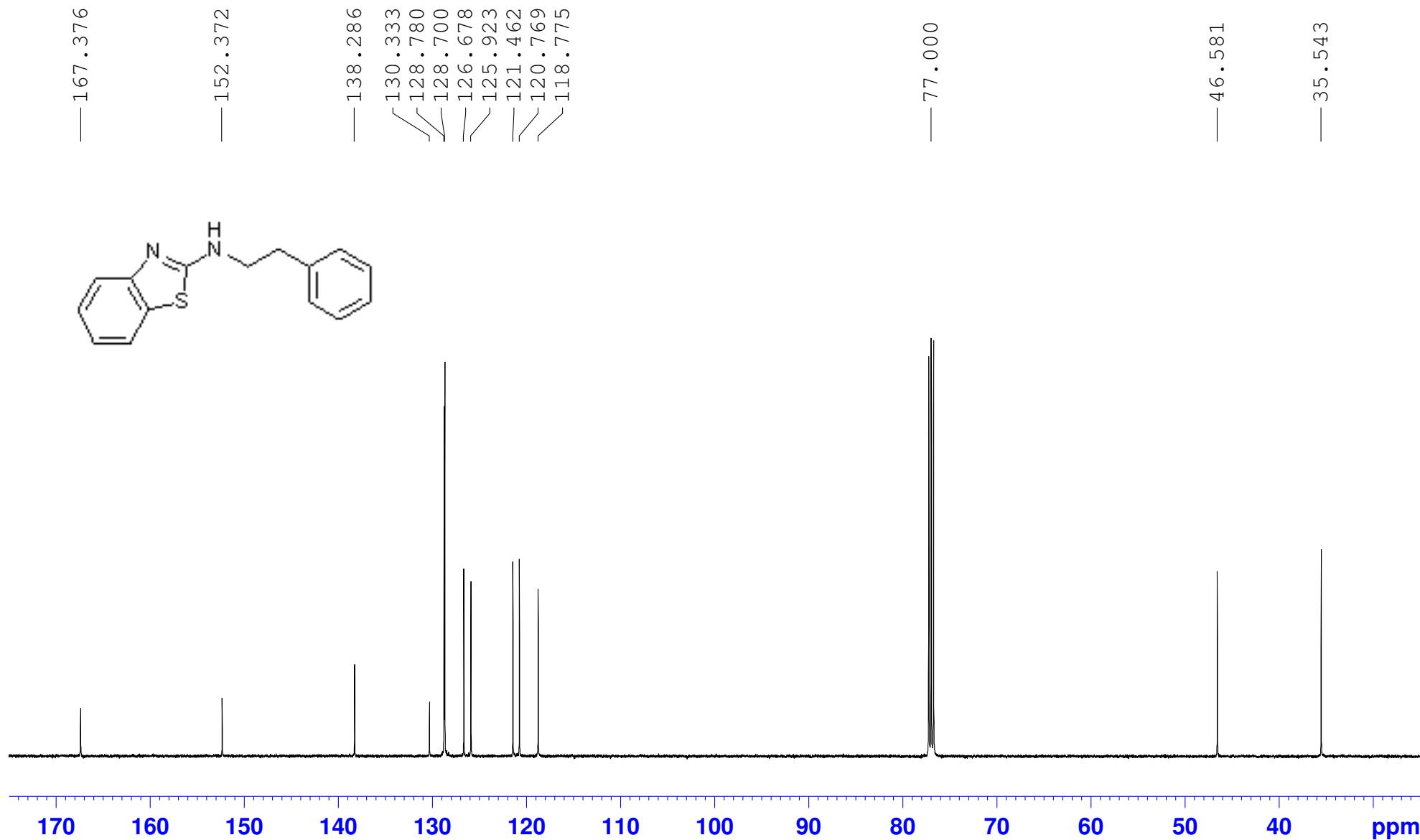
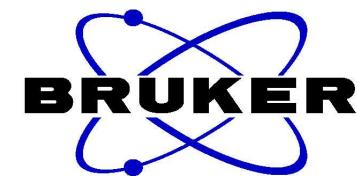
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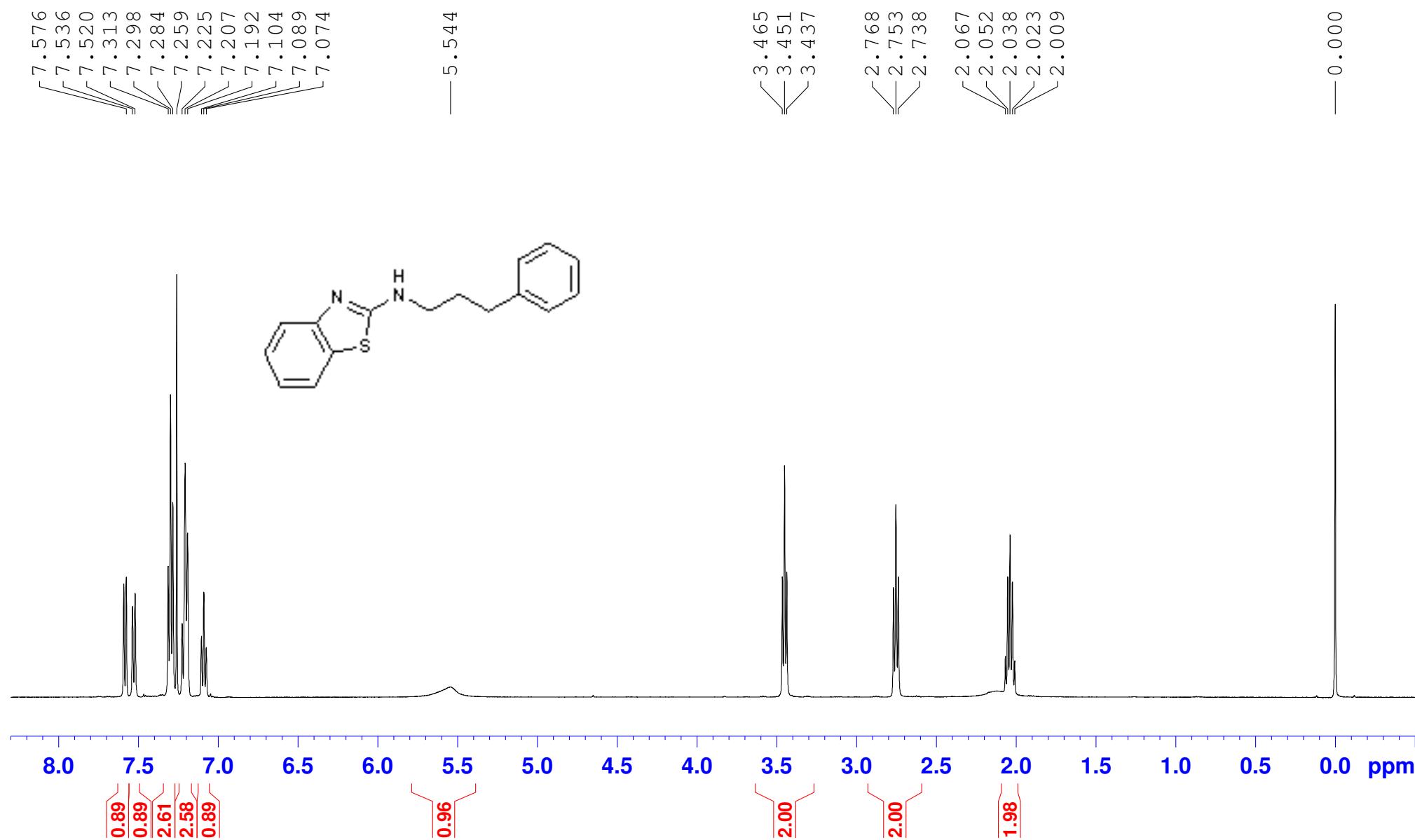
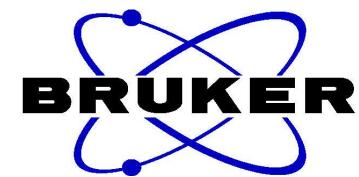
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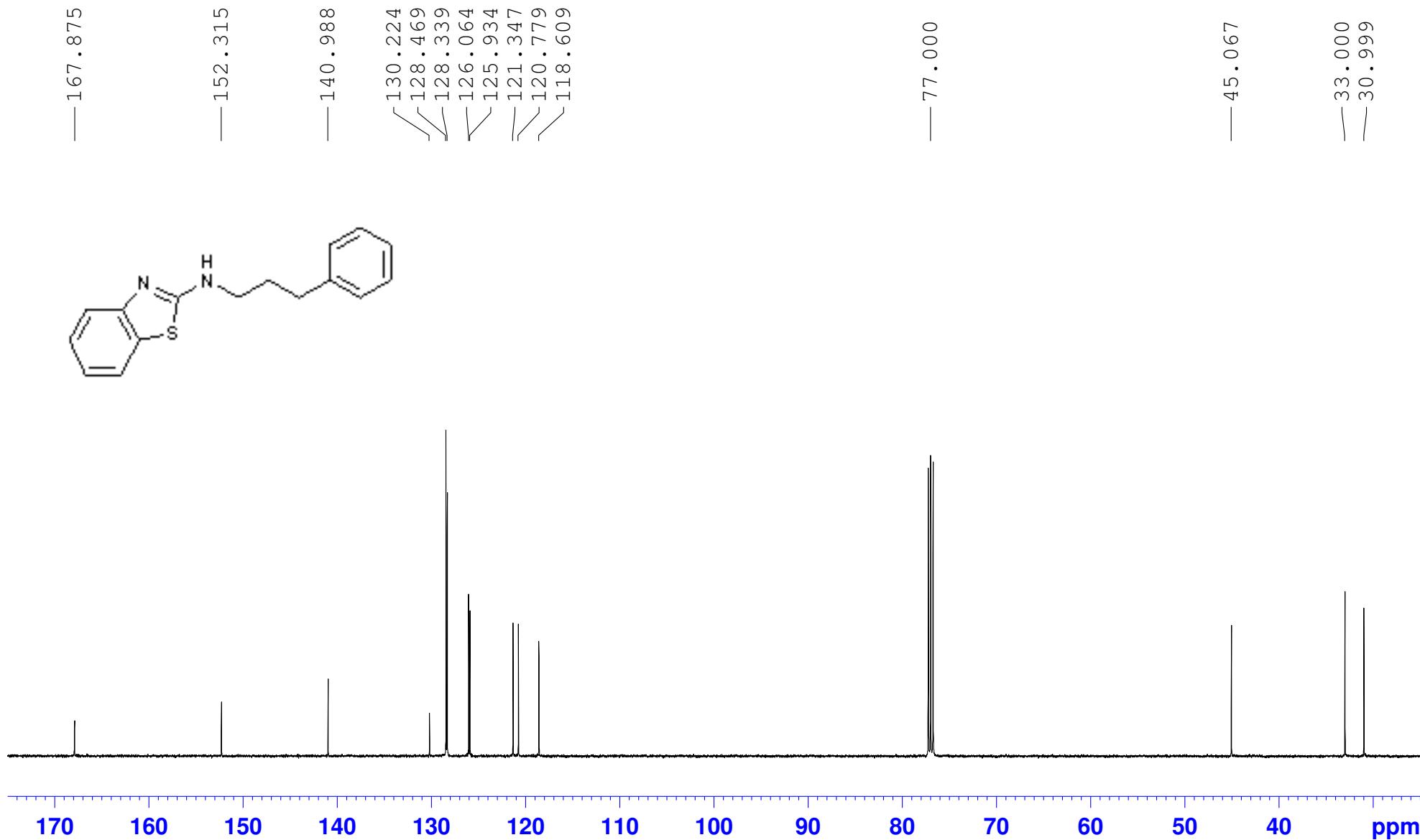
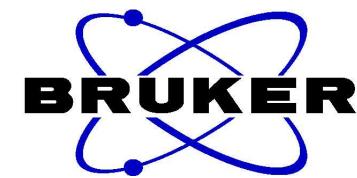
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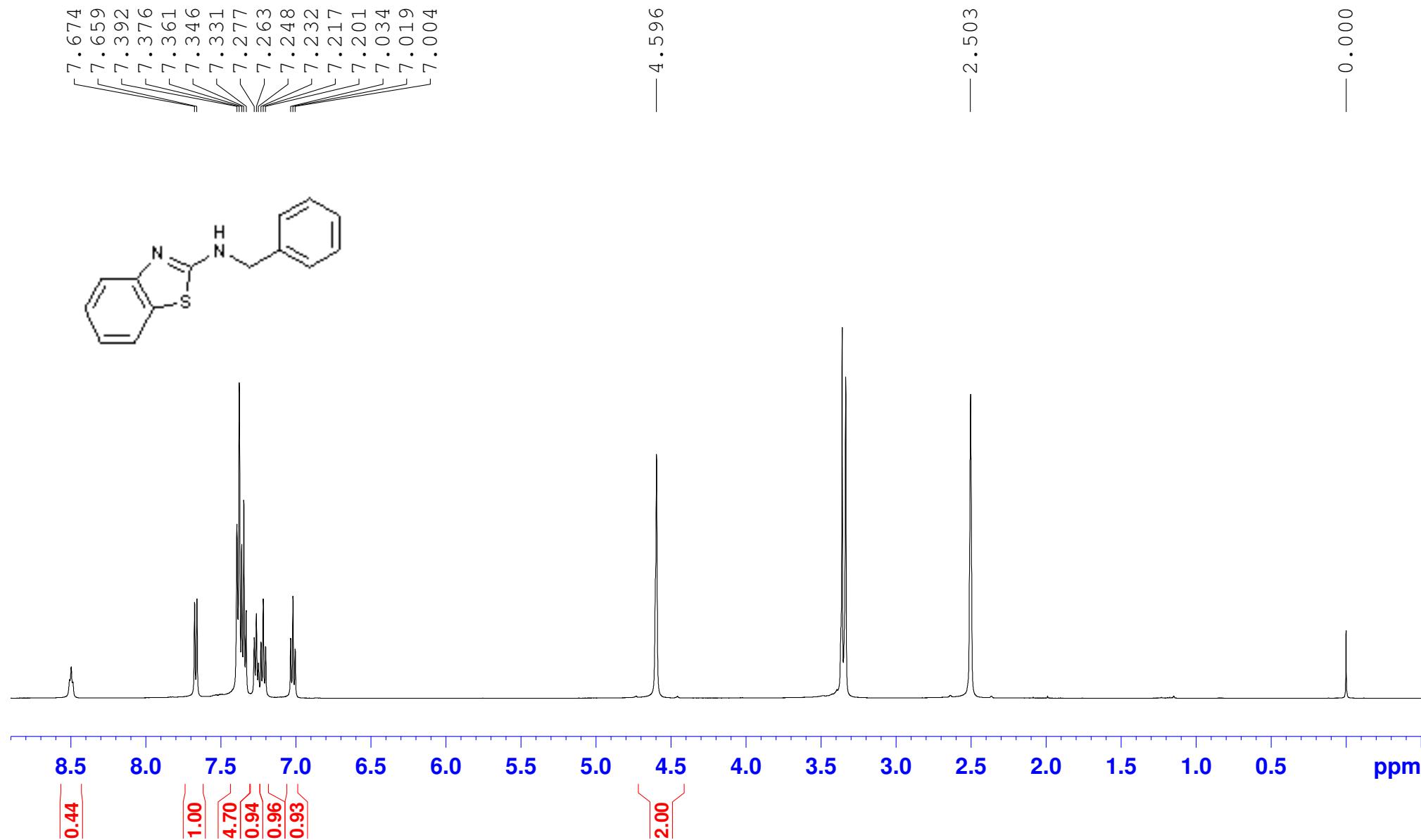
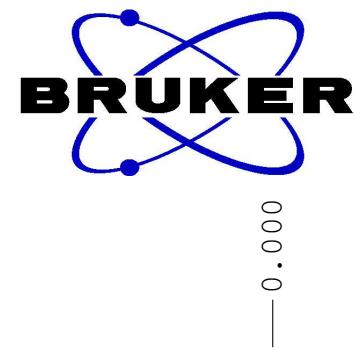
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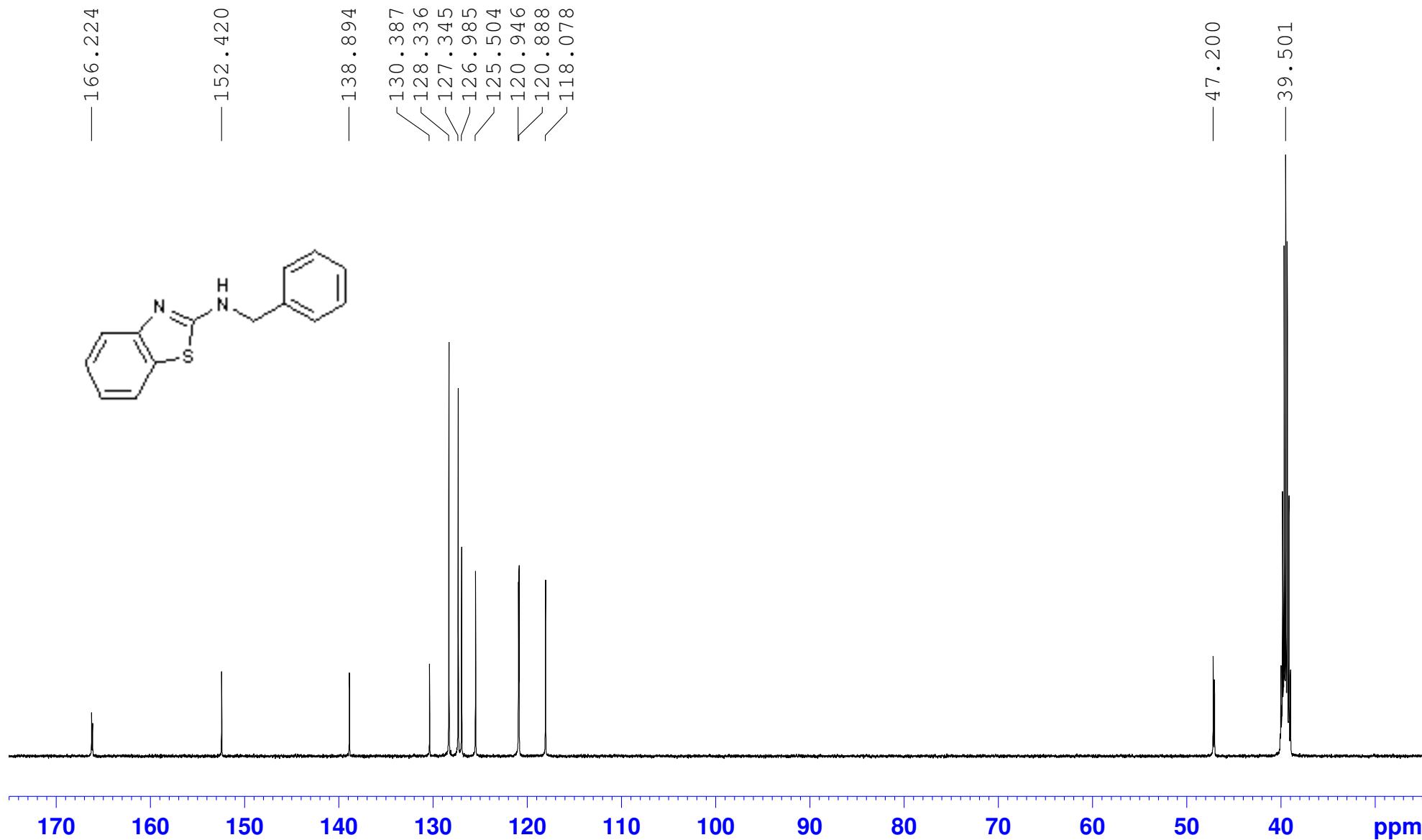
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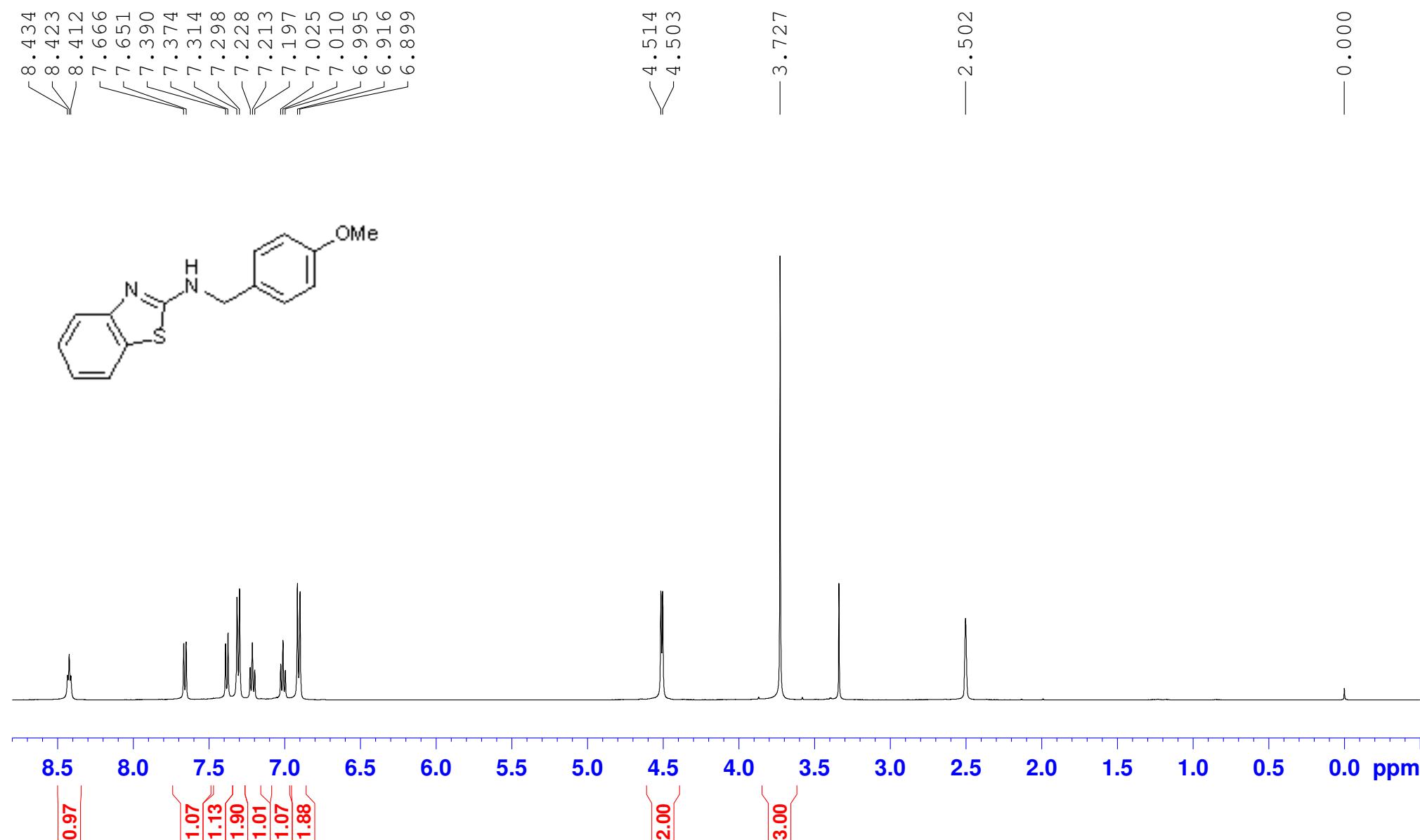
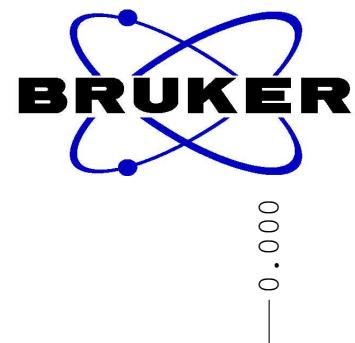
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Proton DMSO-d6



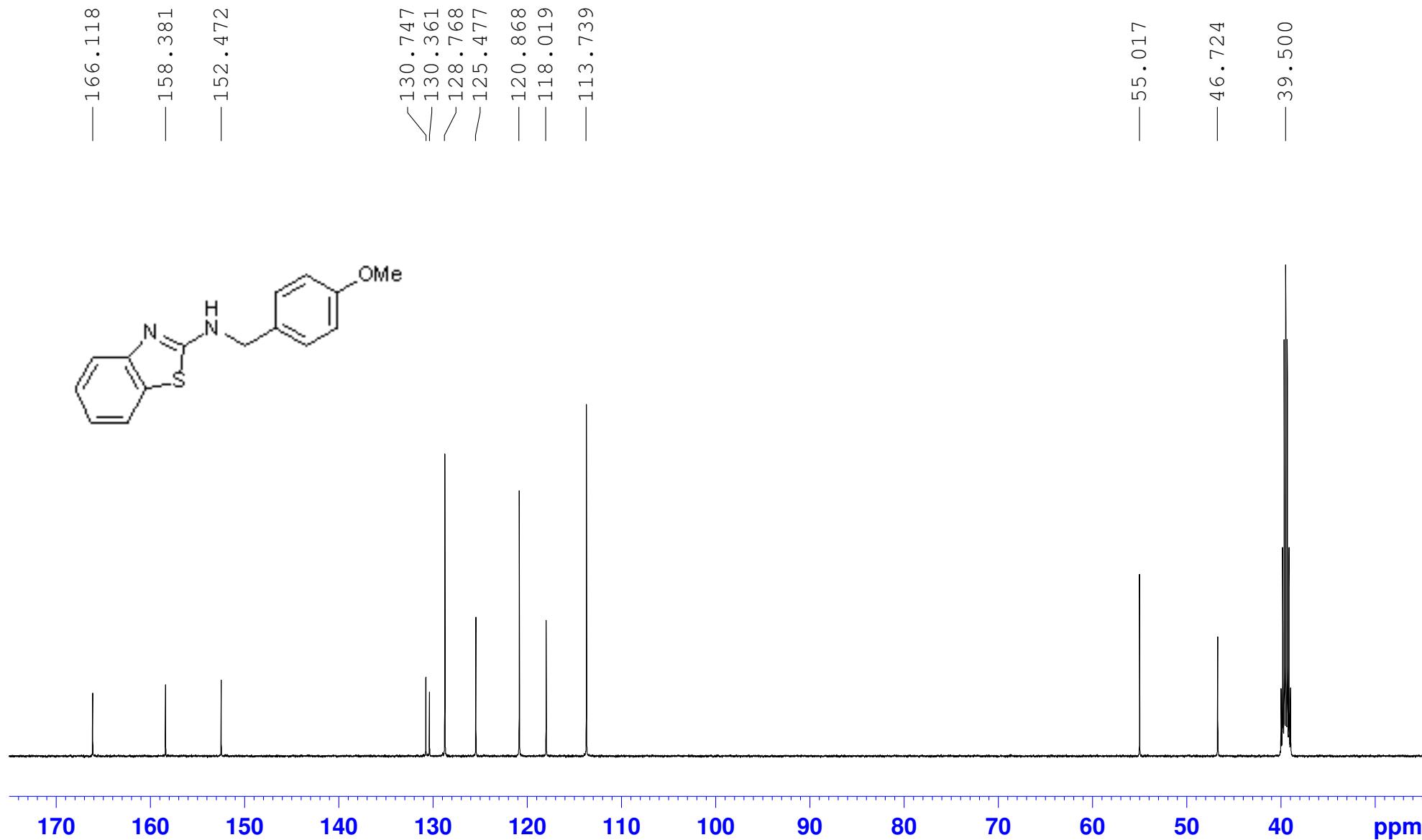
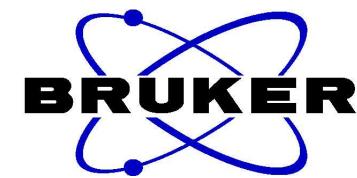
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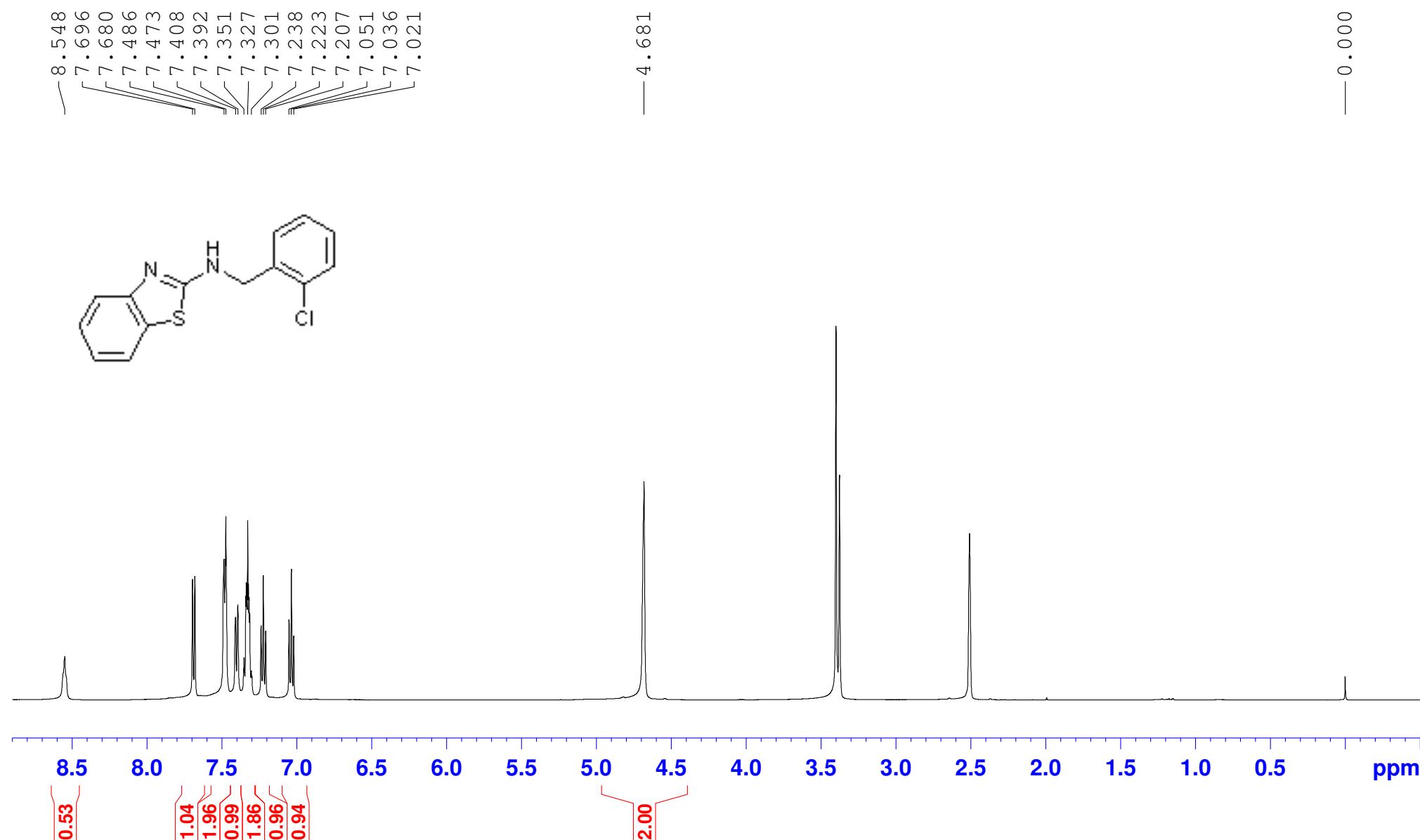
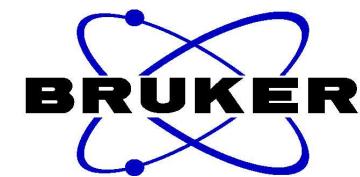
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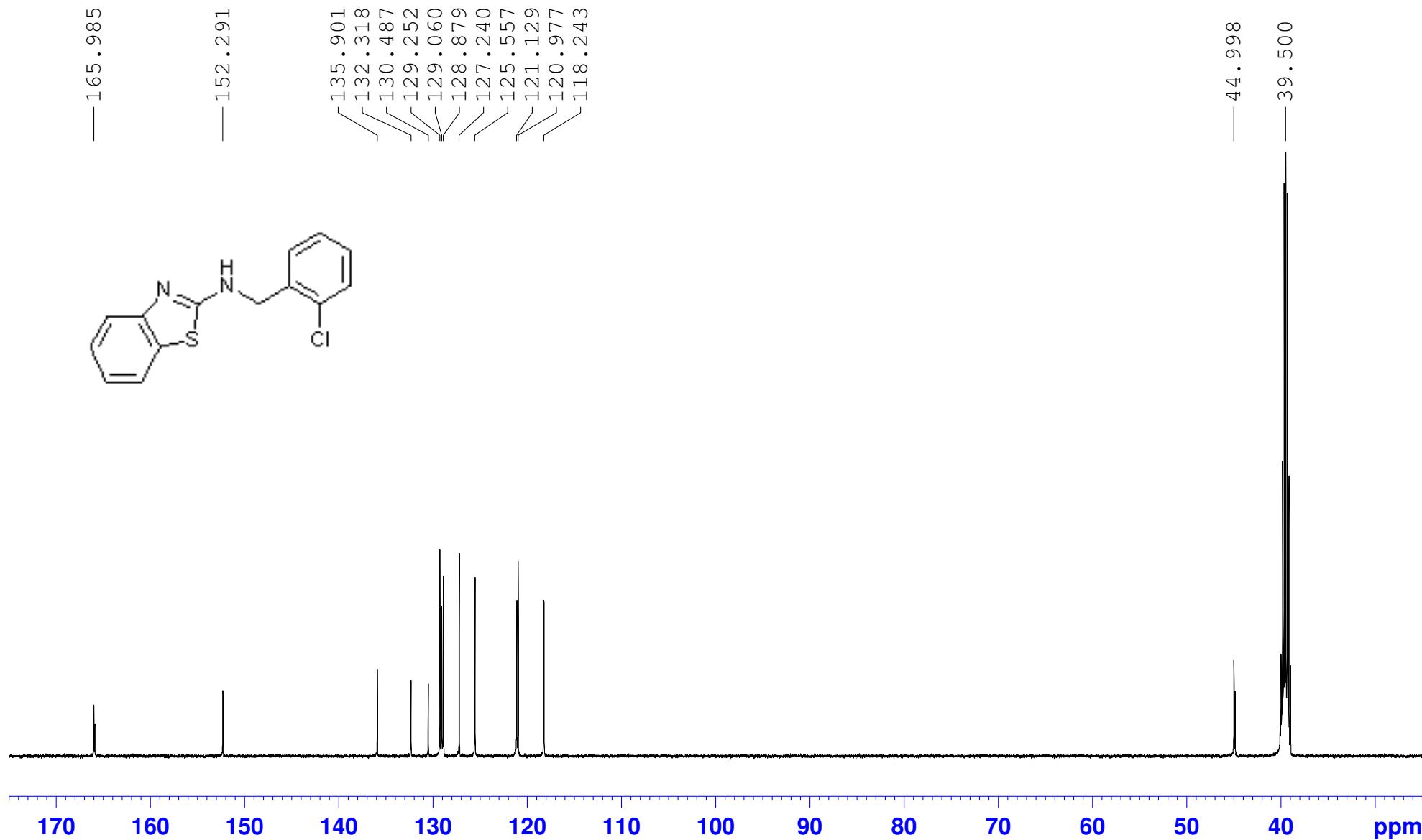
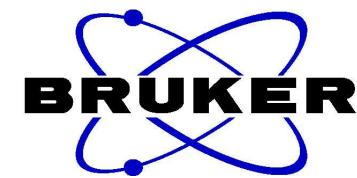
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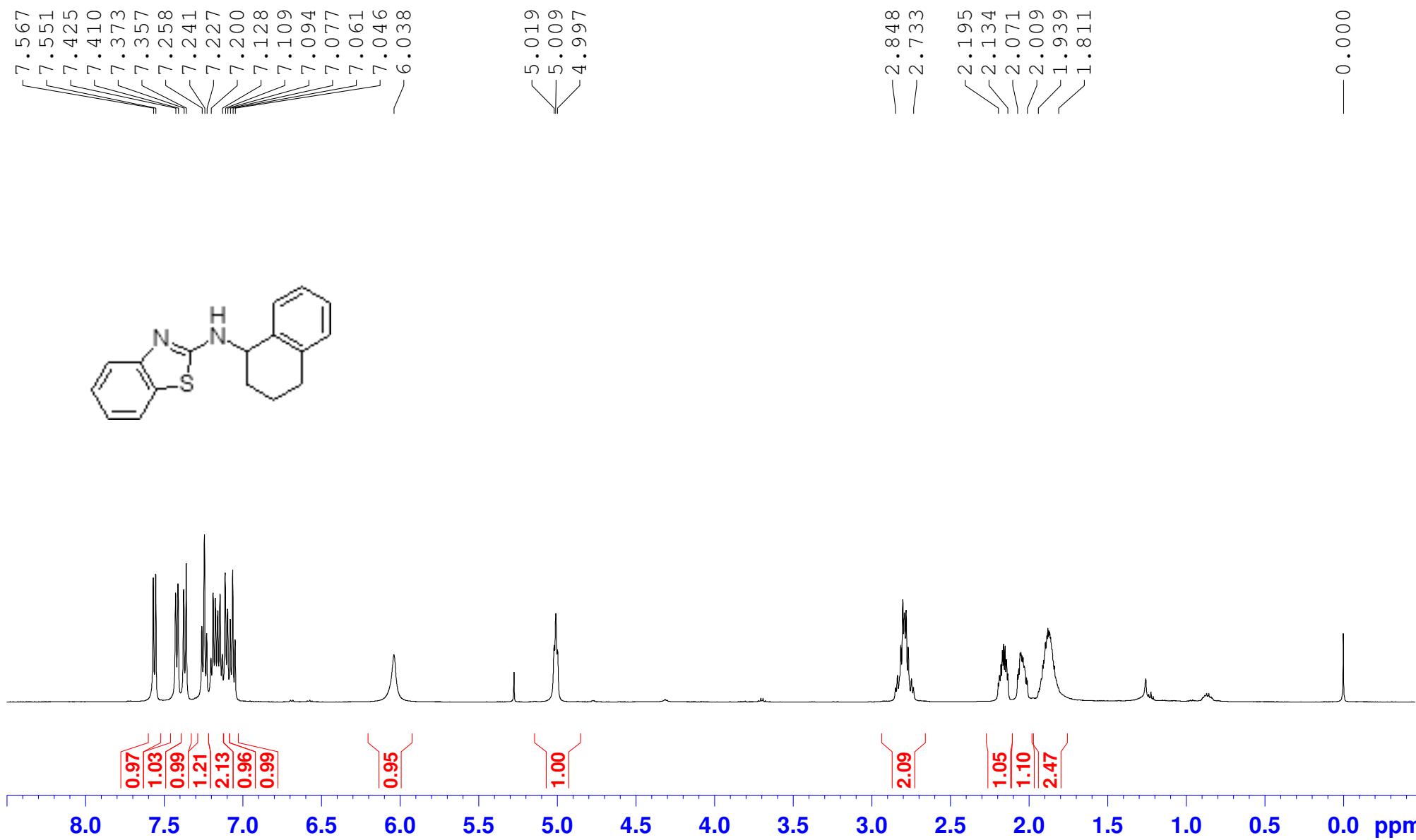
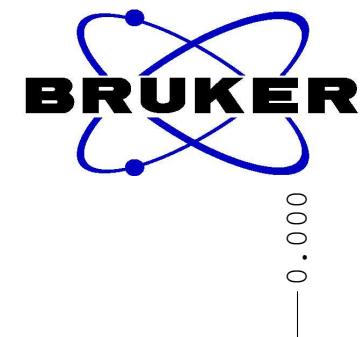
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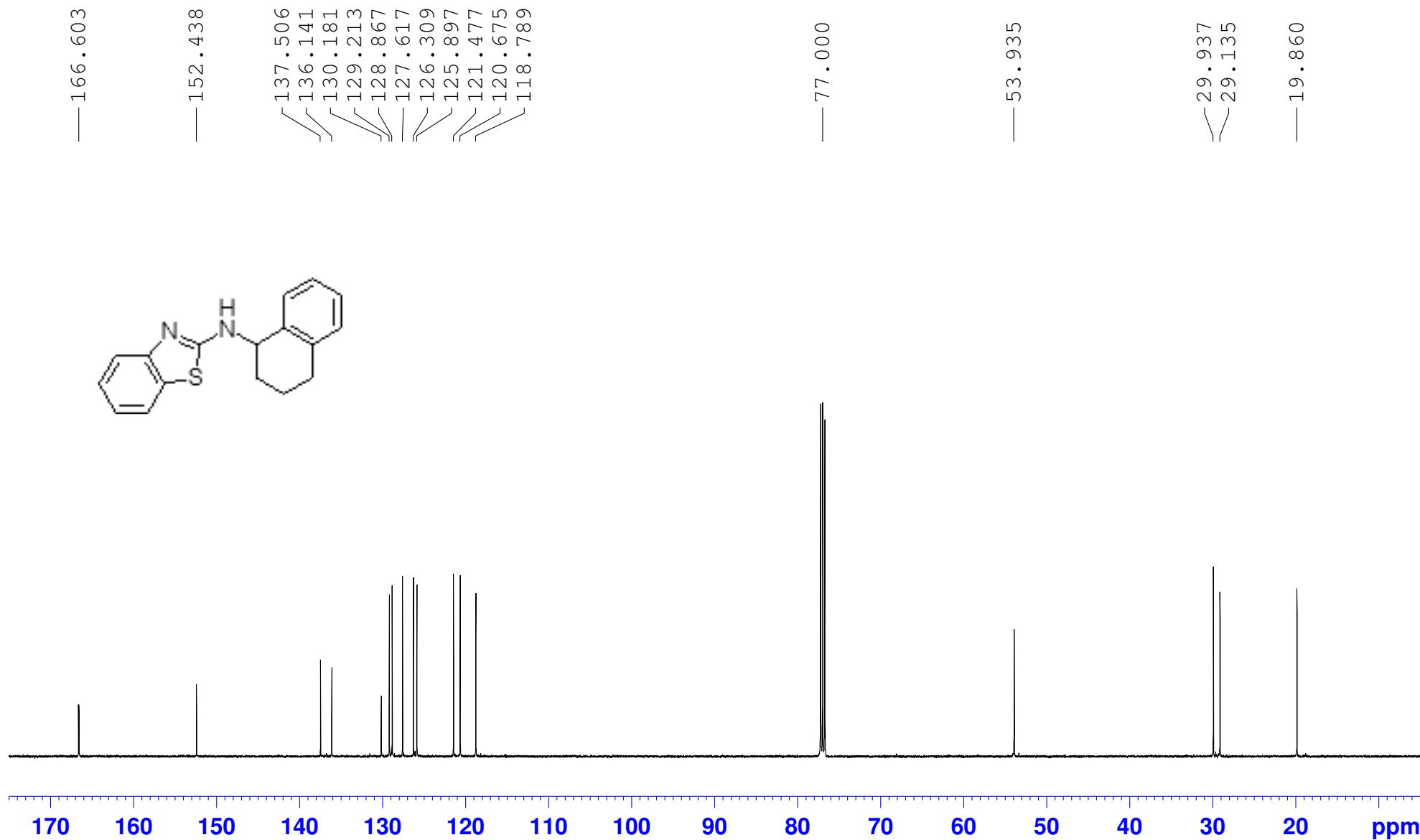
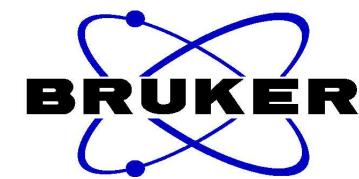
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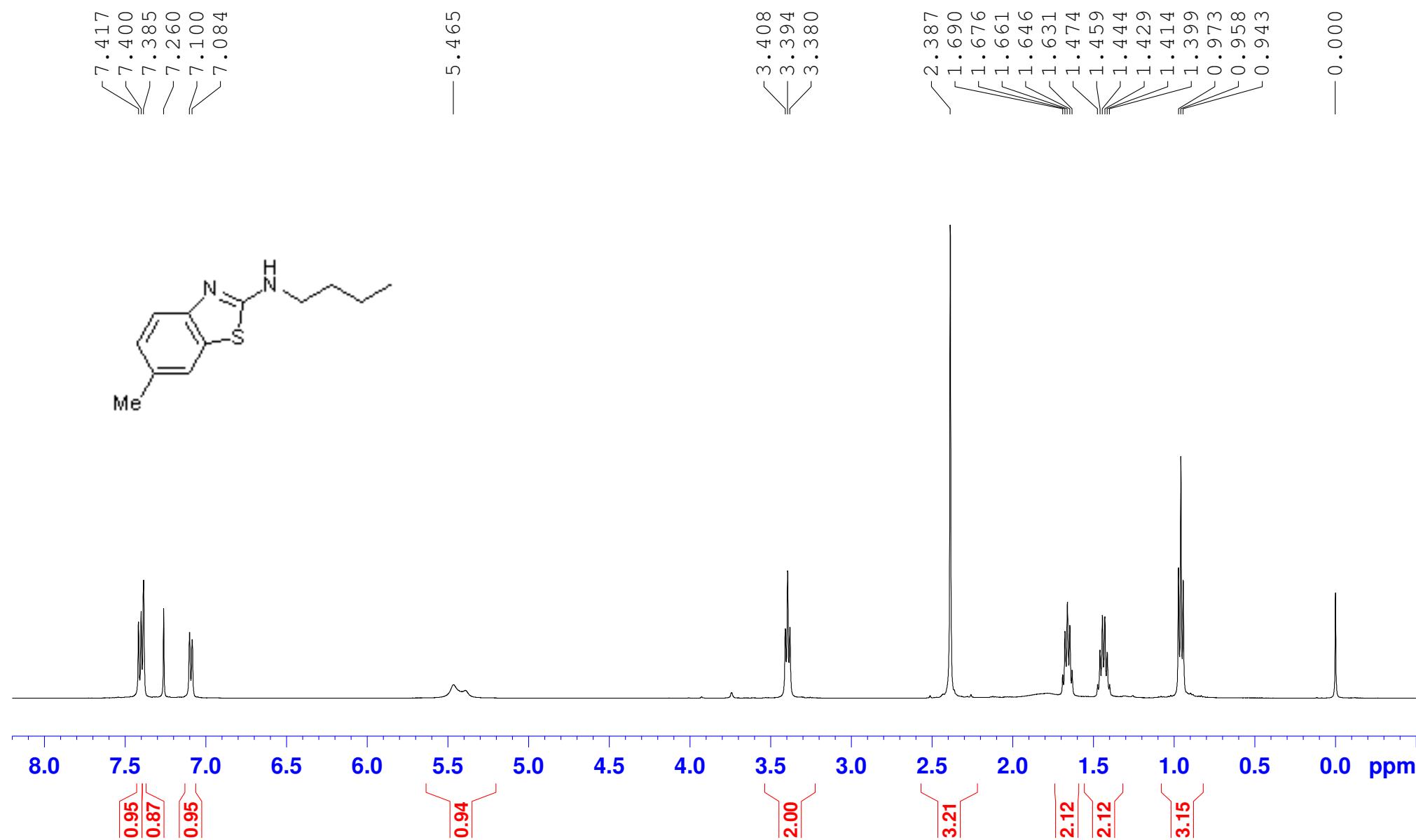
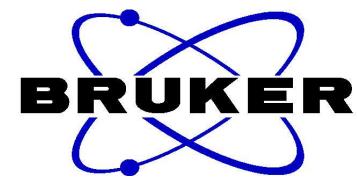
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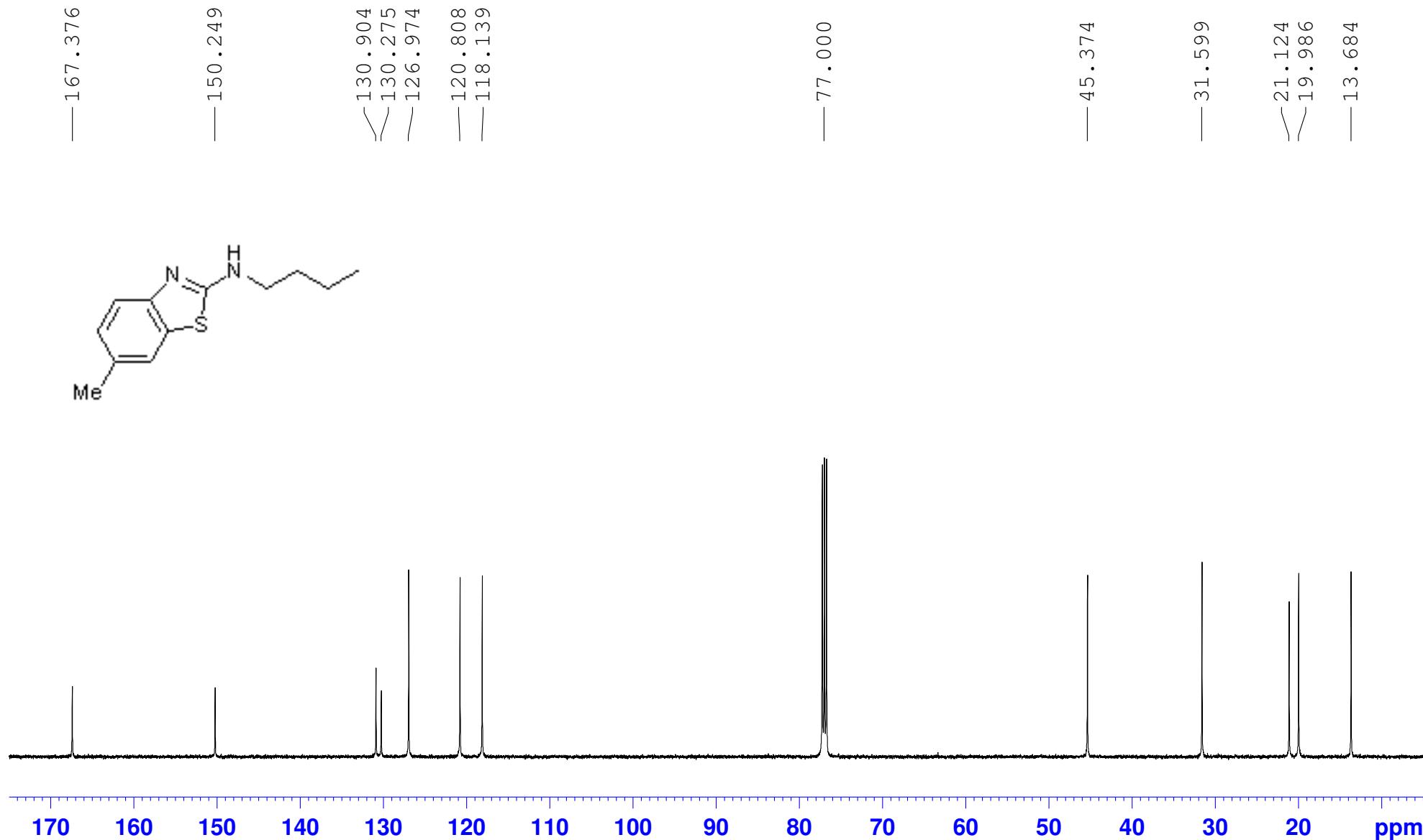
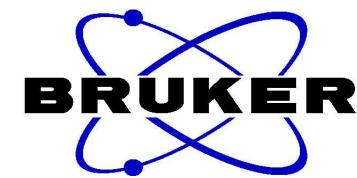
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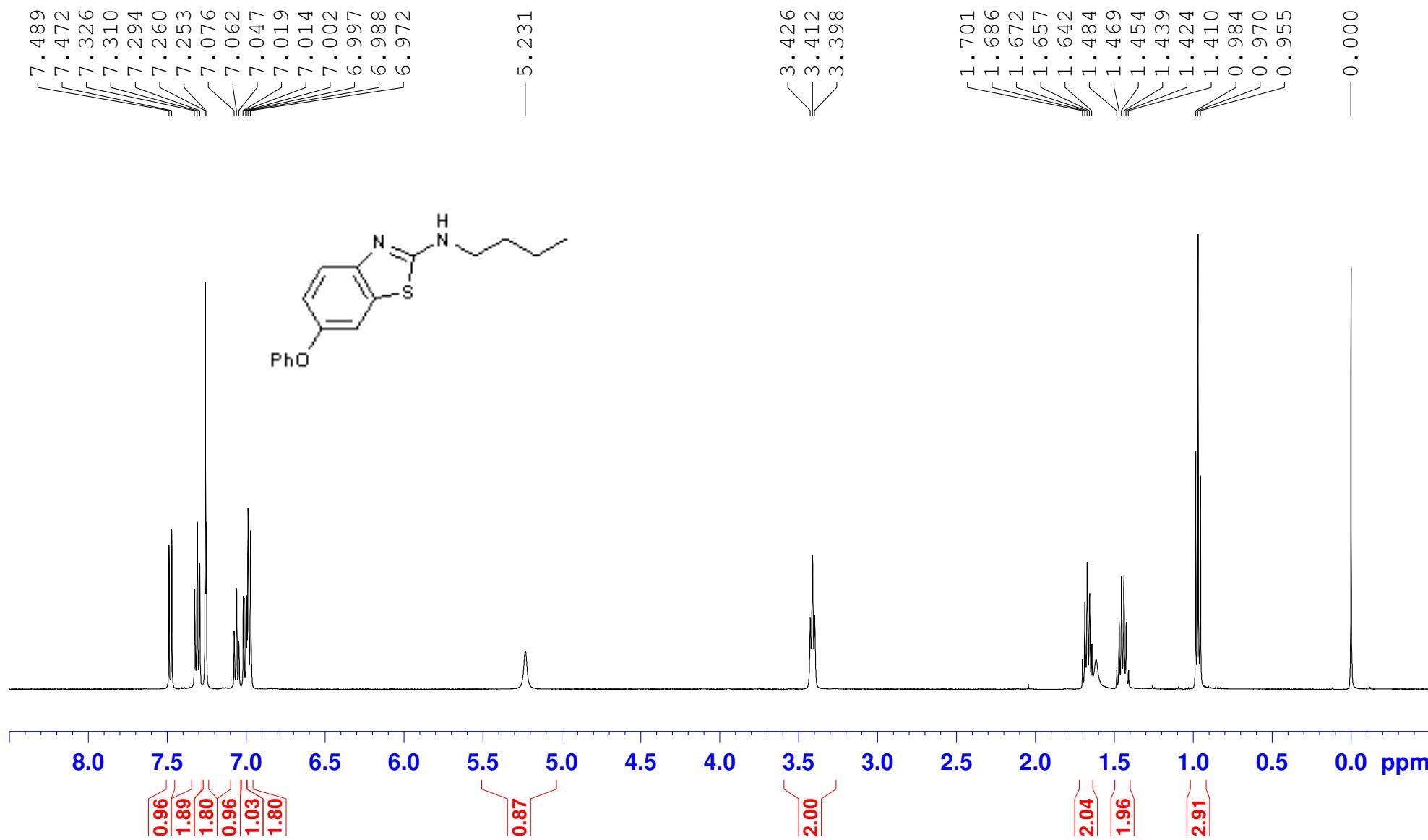
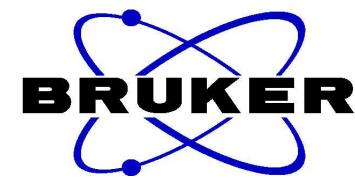
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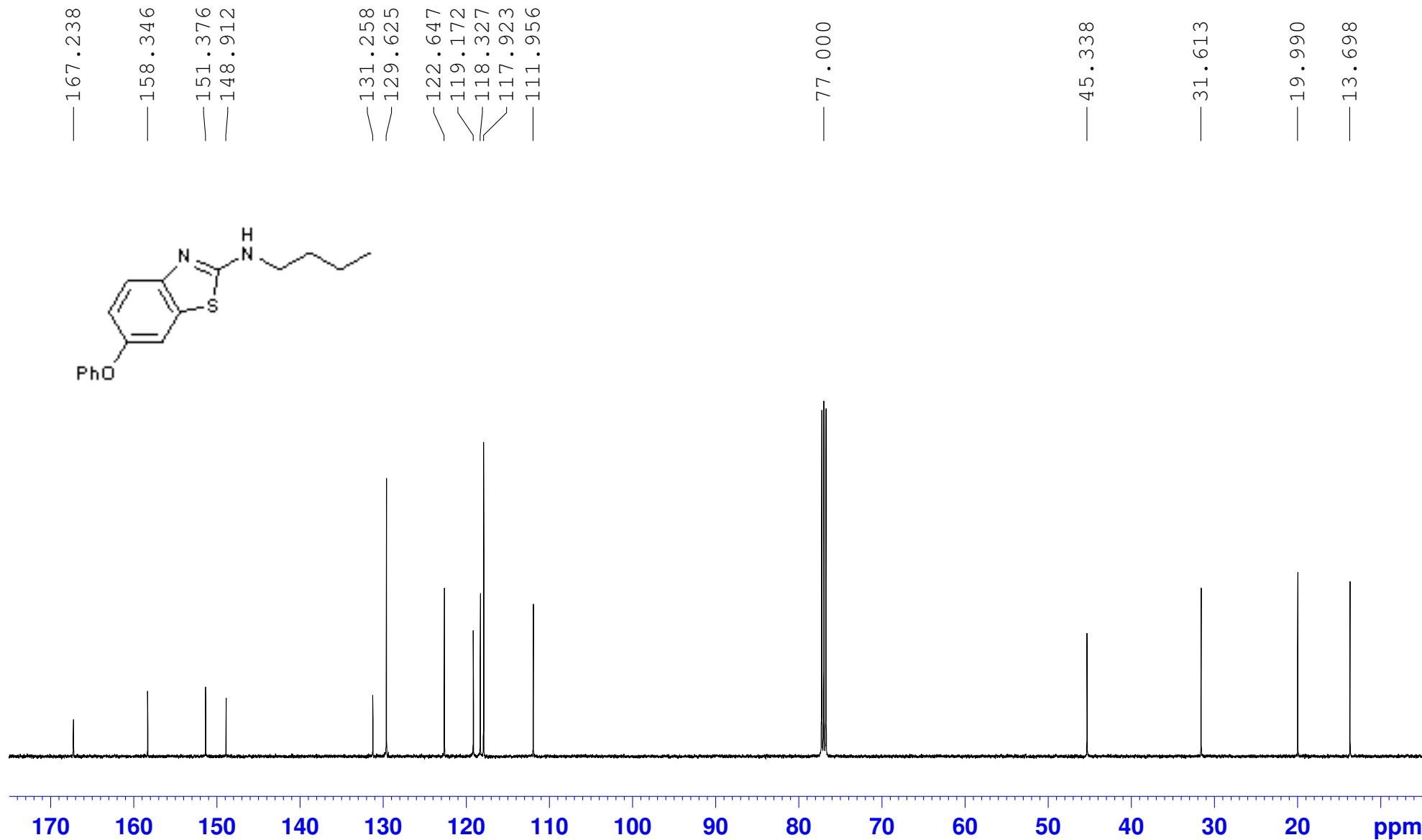
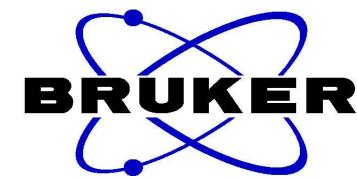
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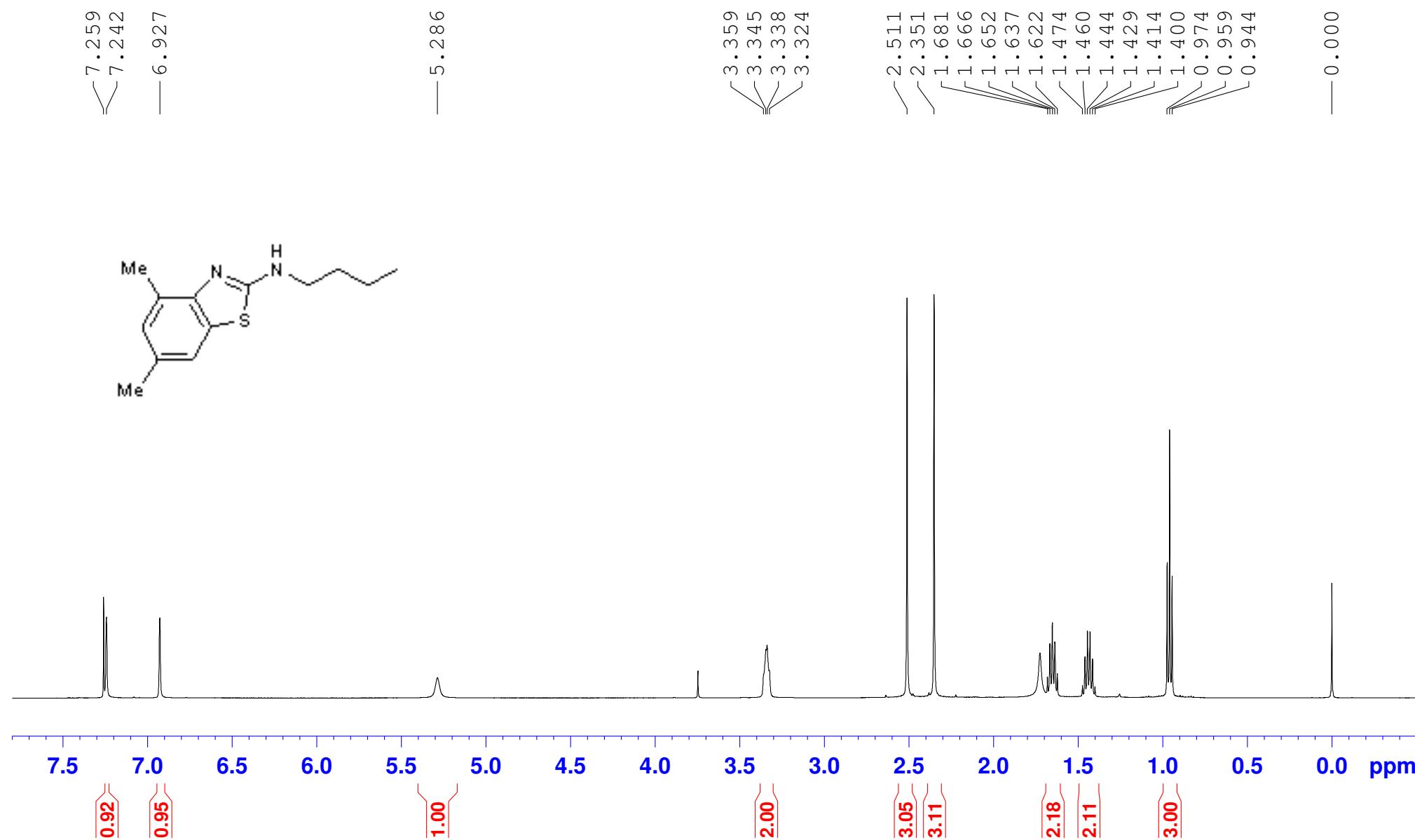
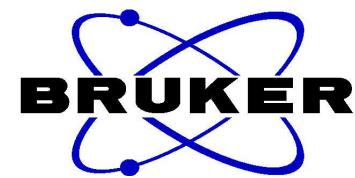
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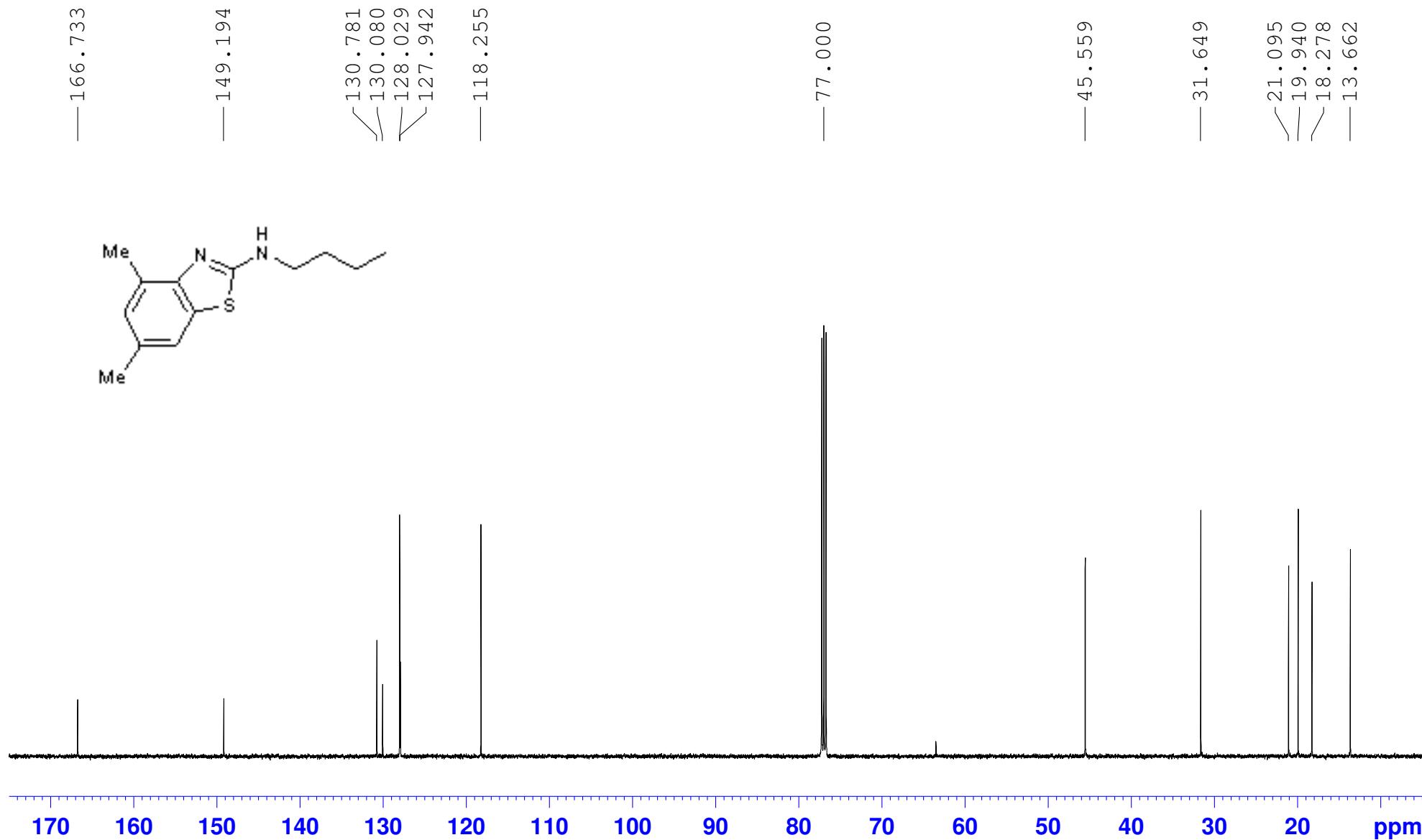
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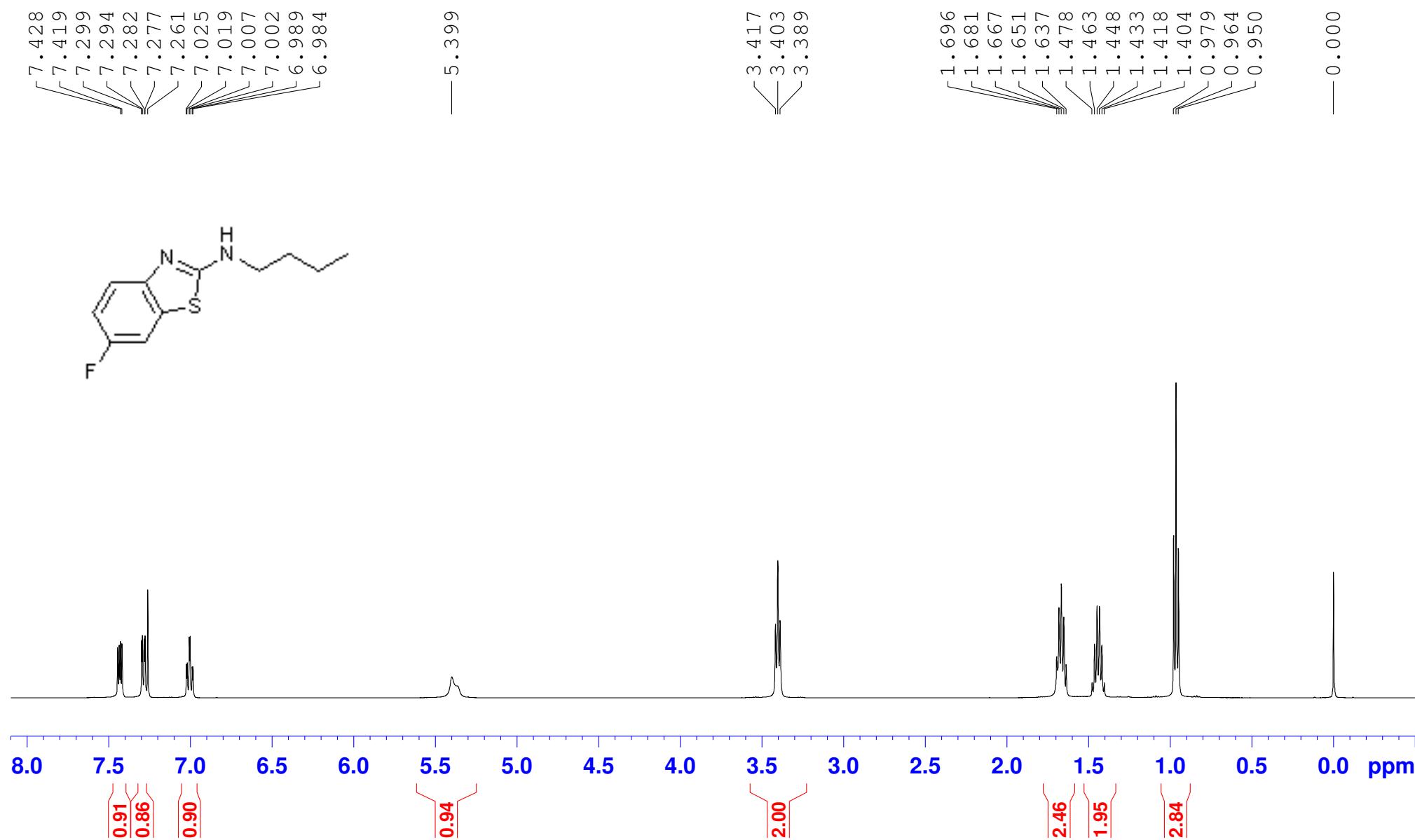
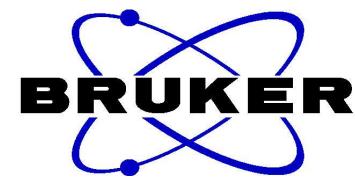
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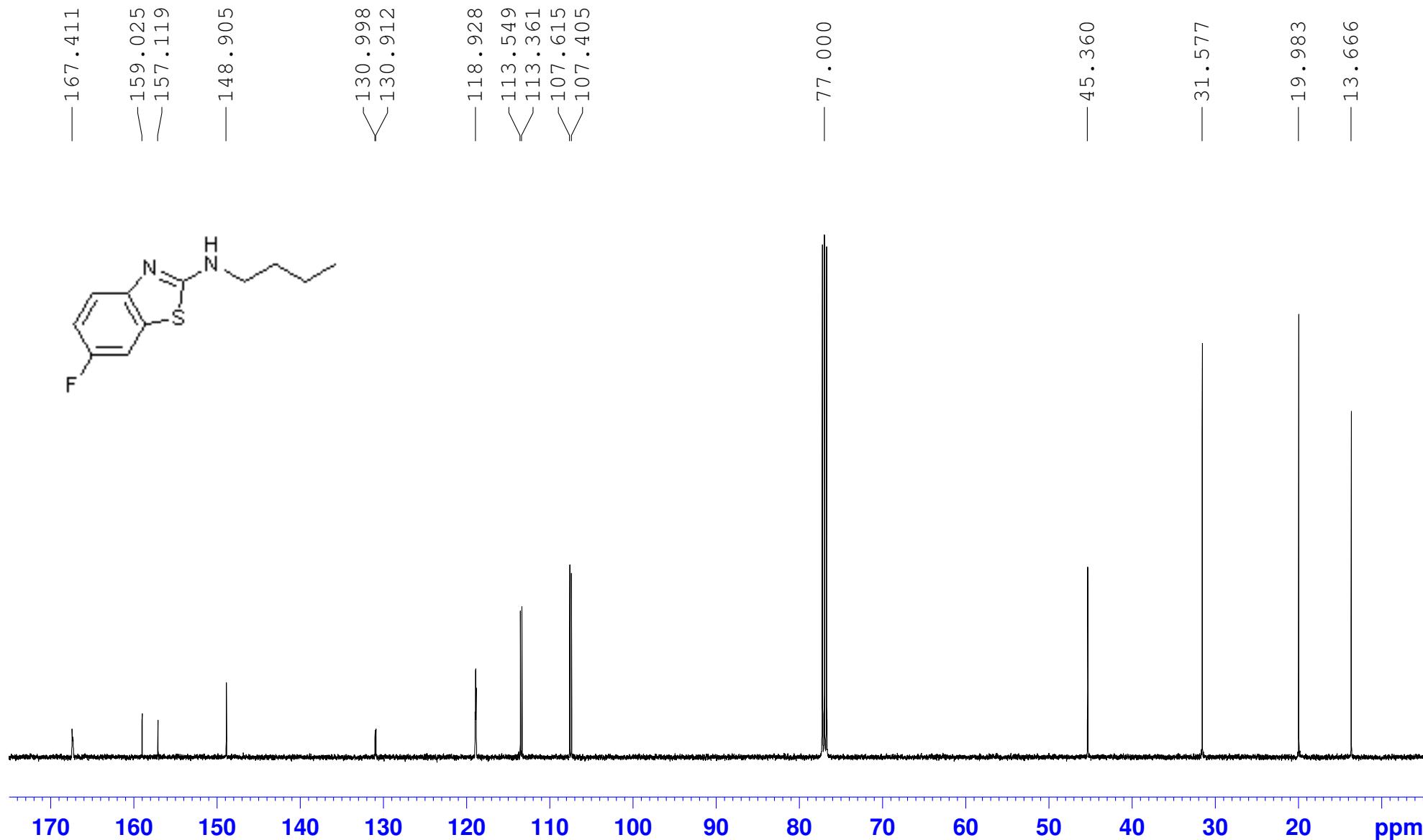
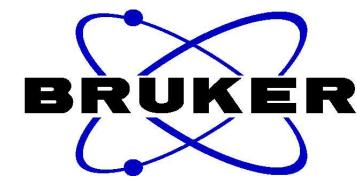
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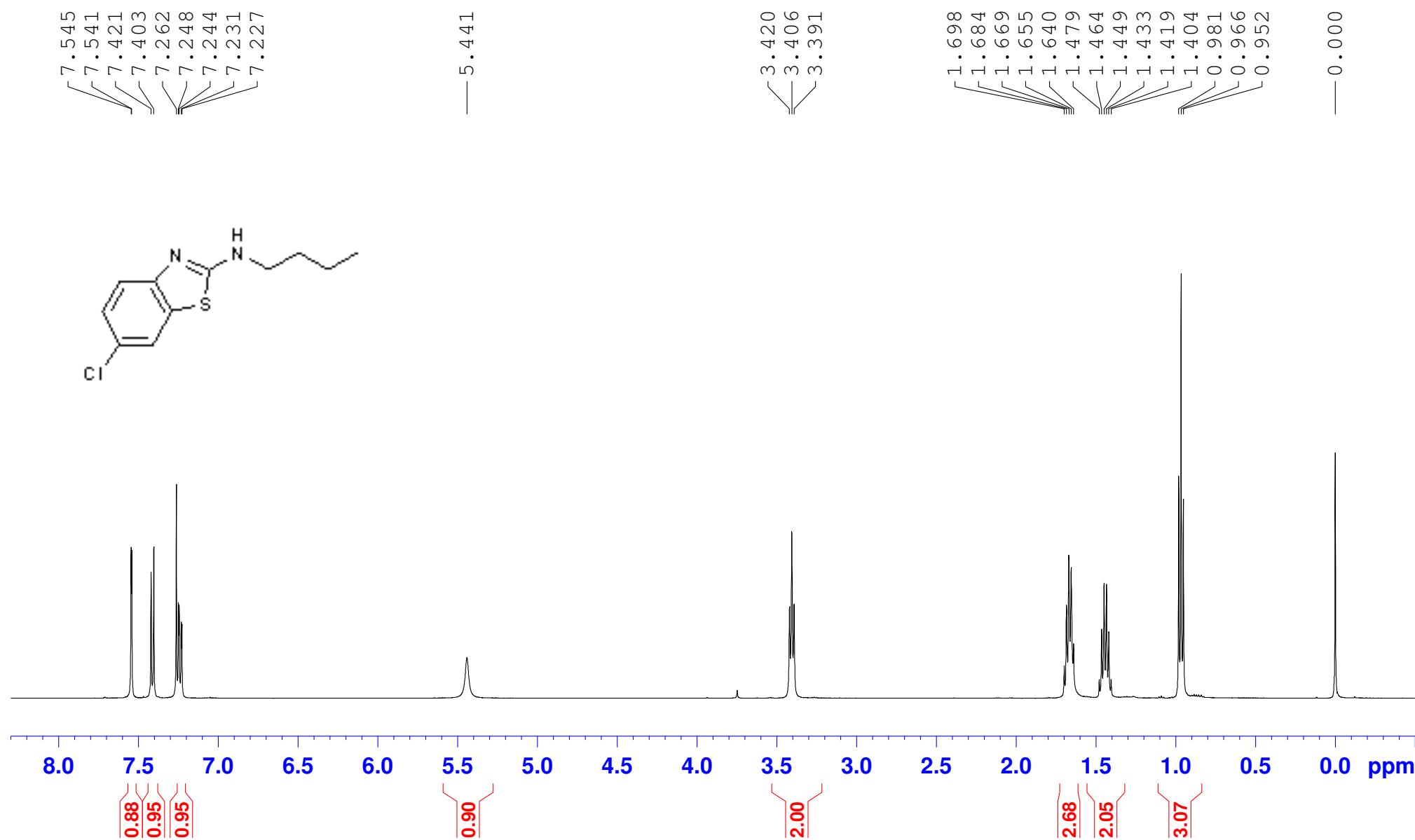
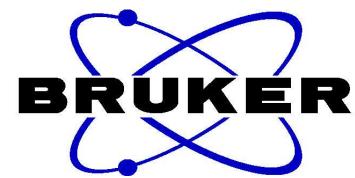
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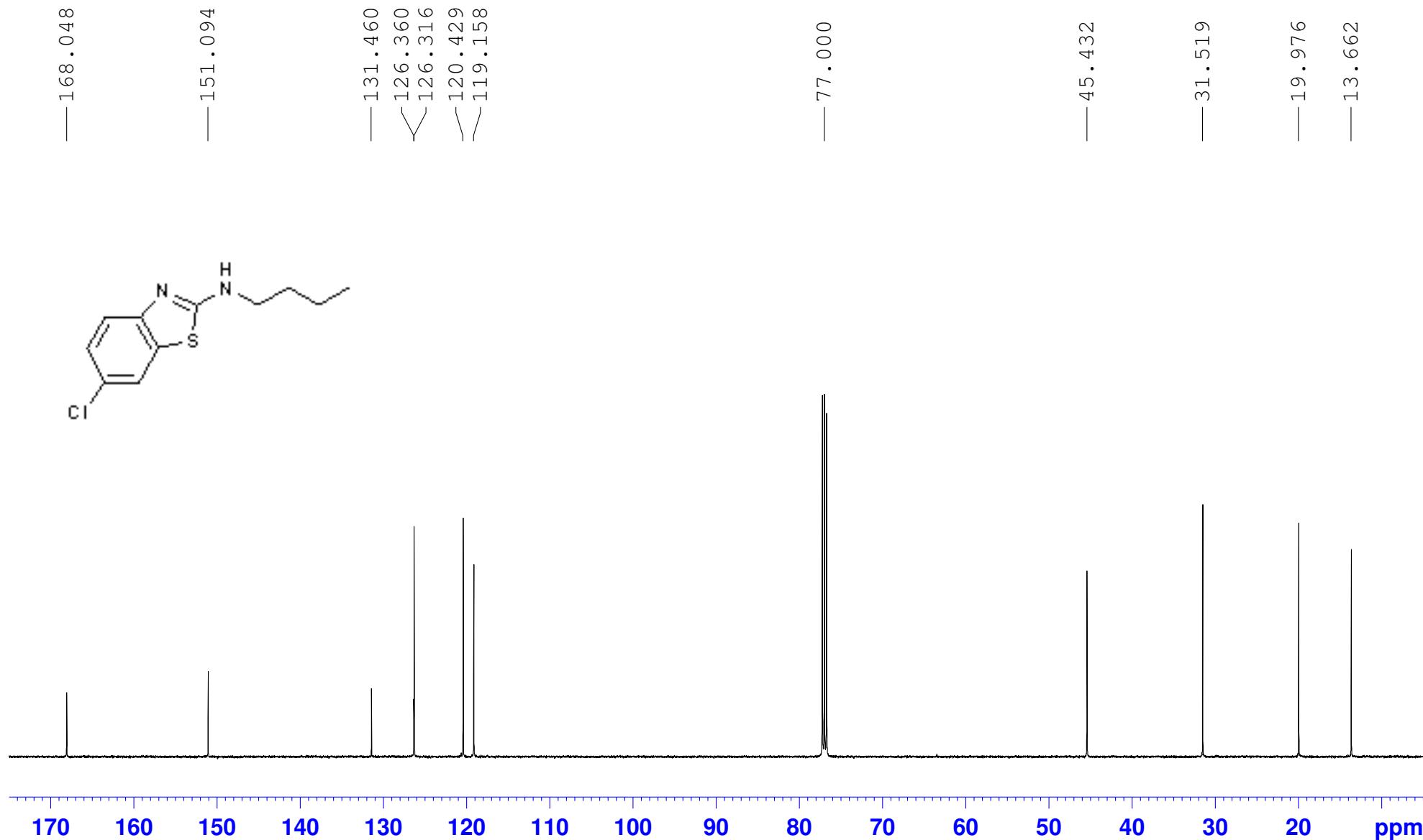
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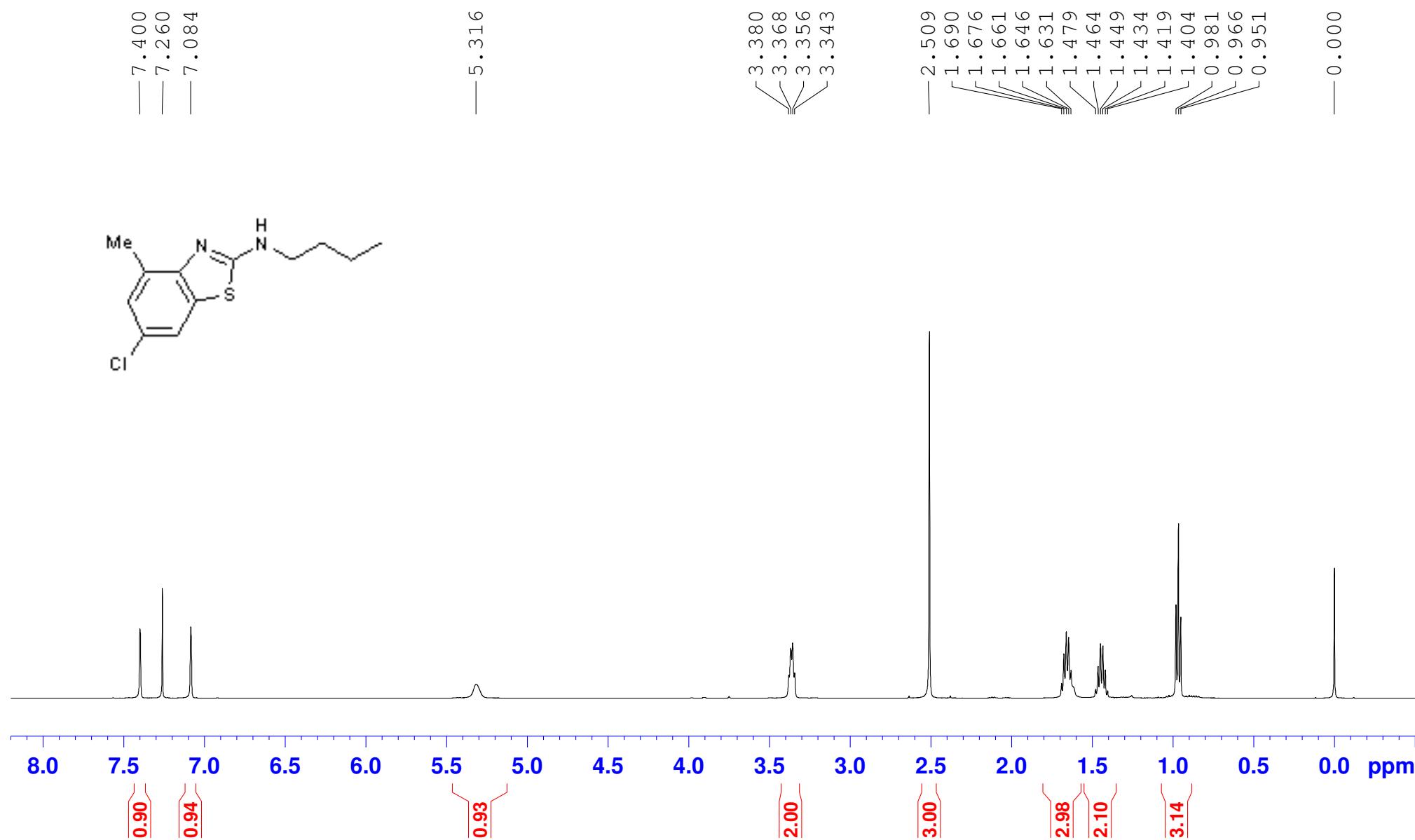
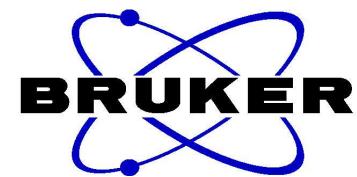
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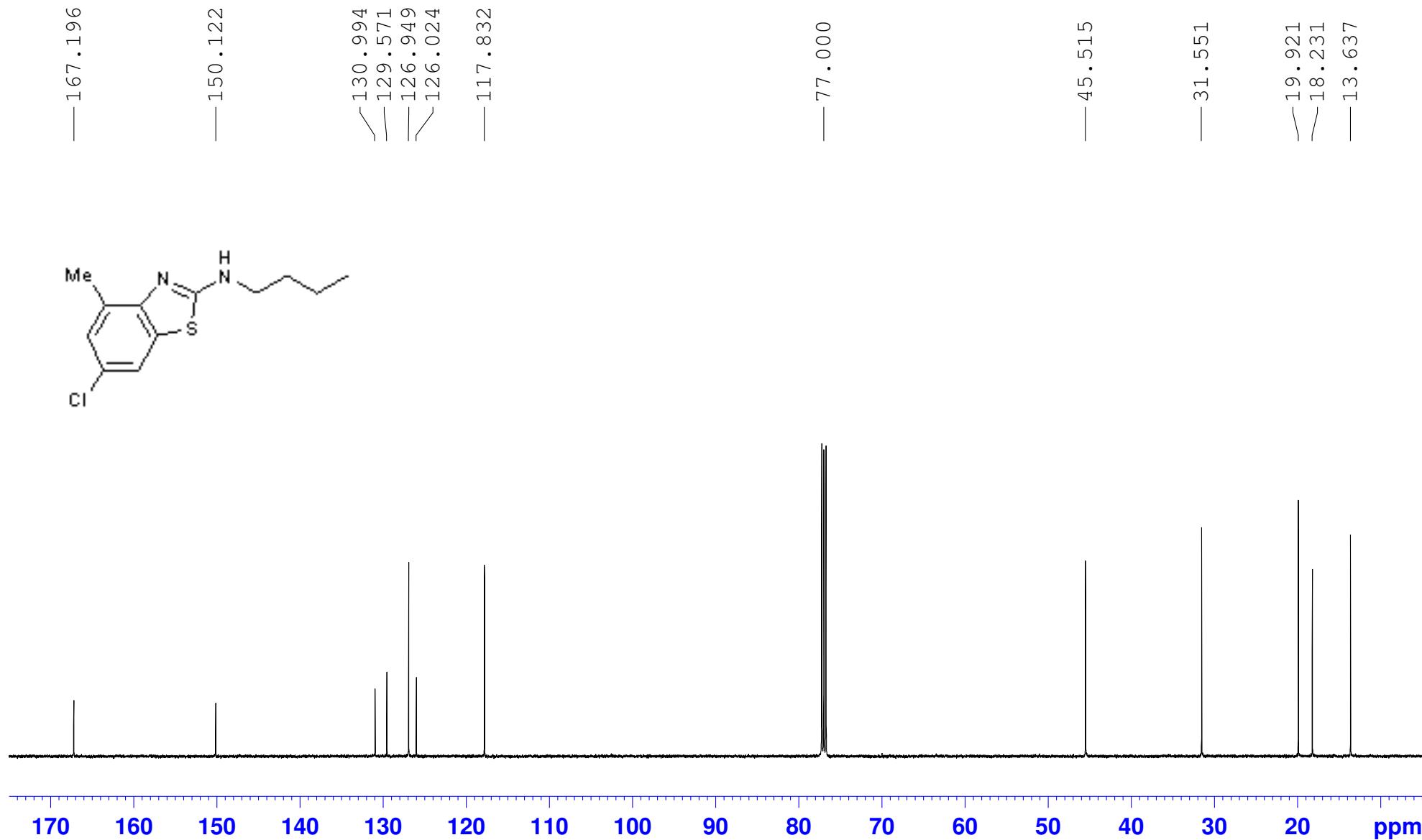
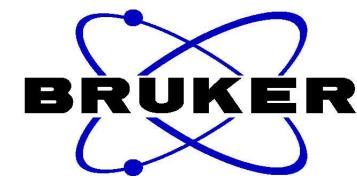
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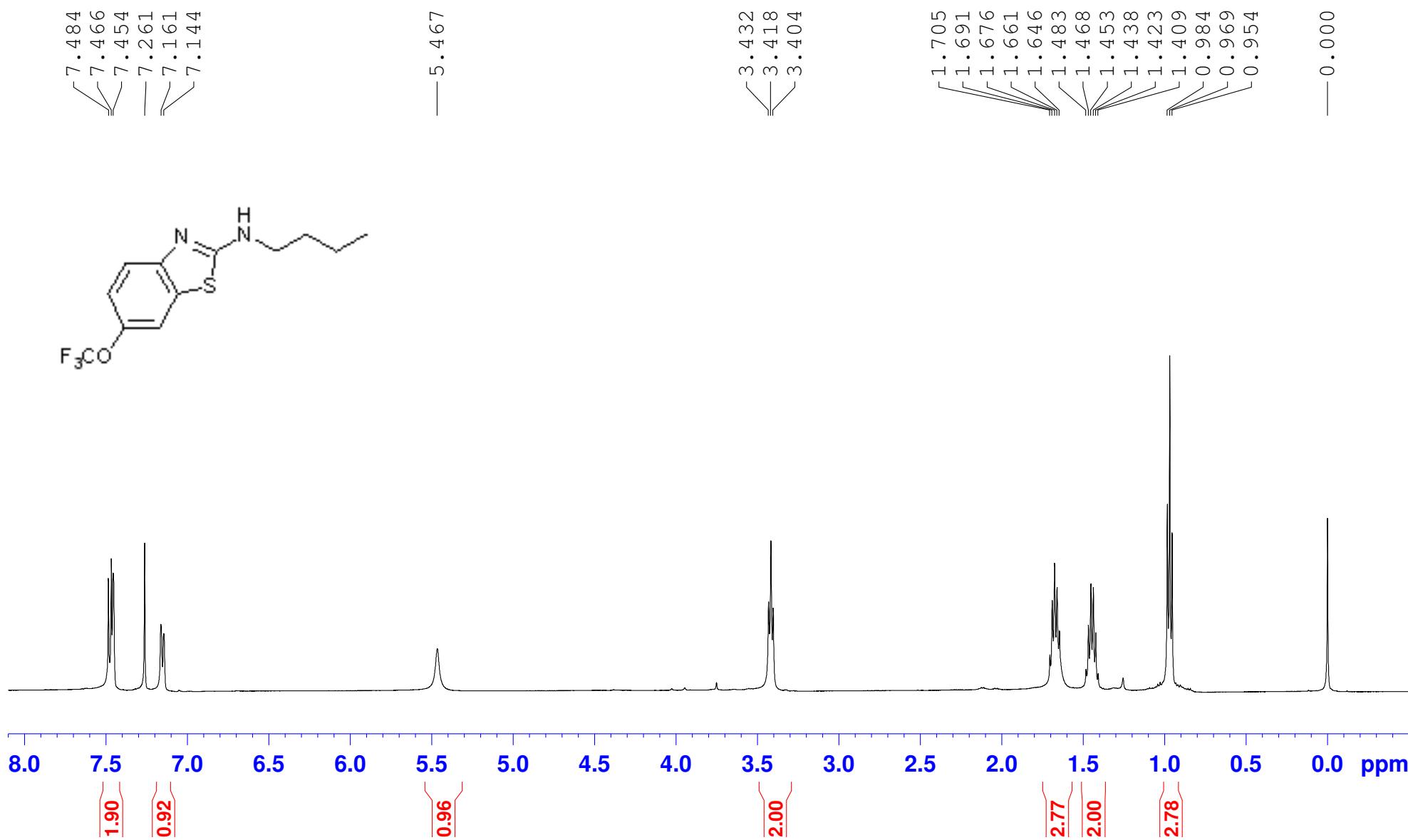
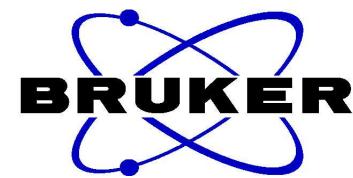
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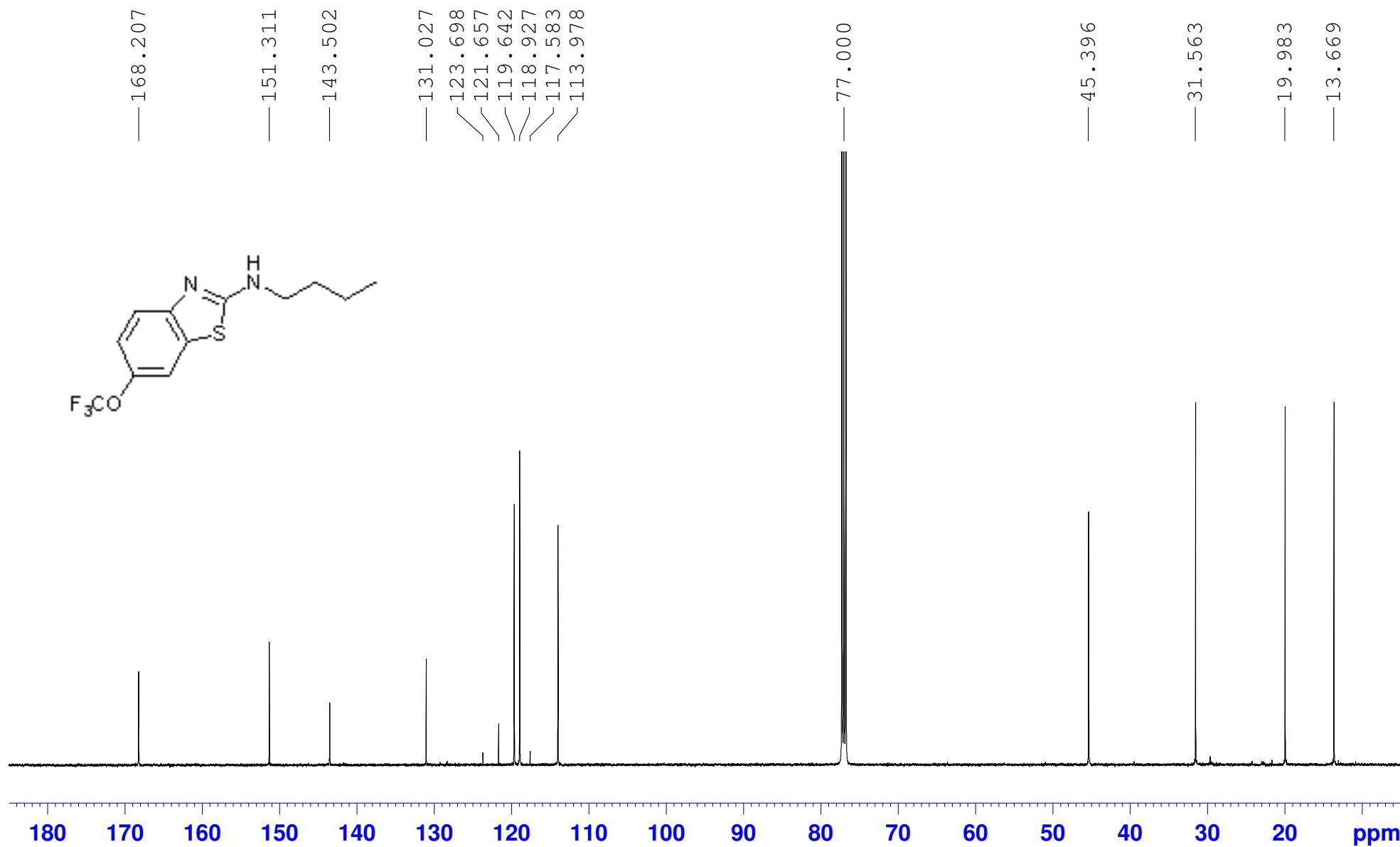
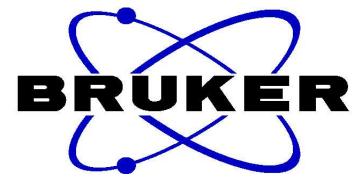
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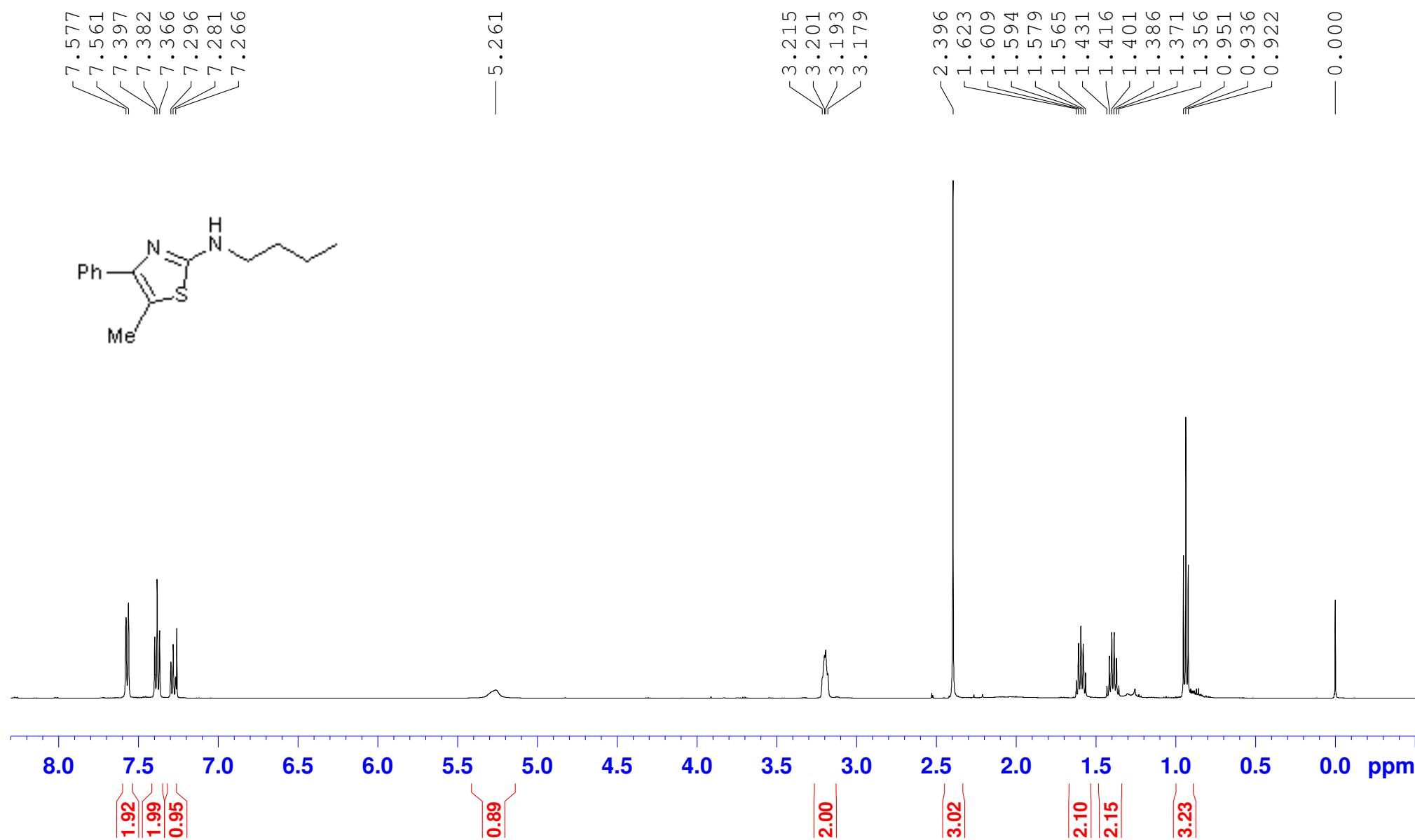
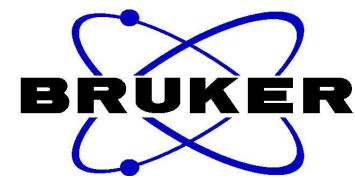
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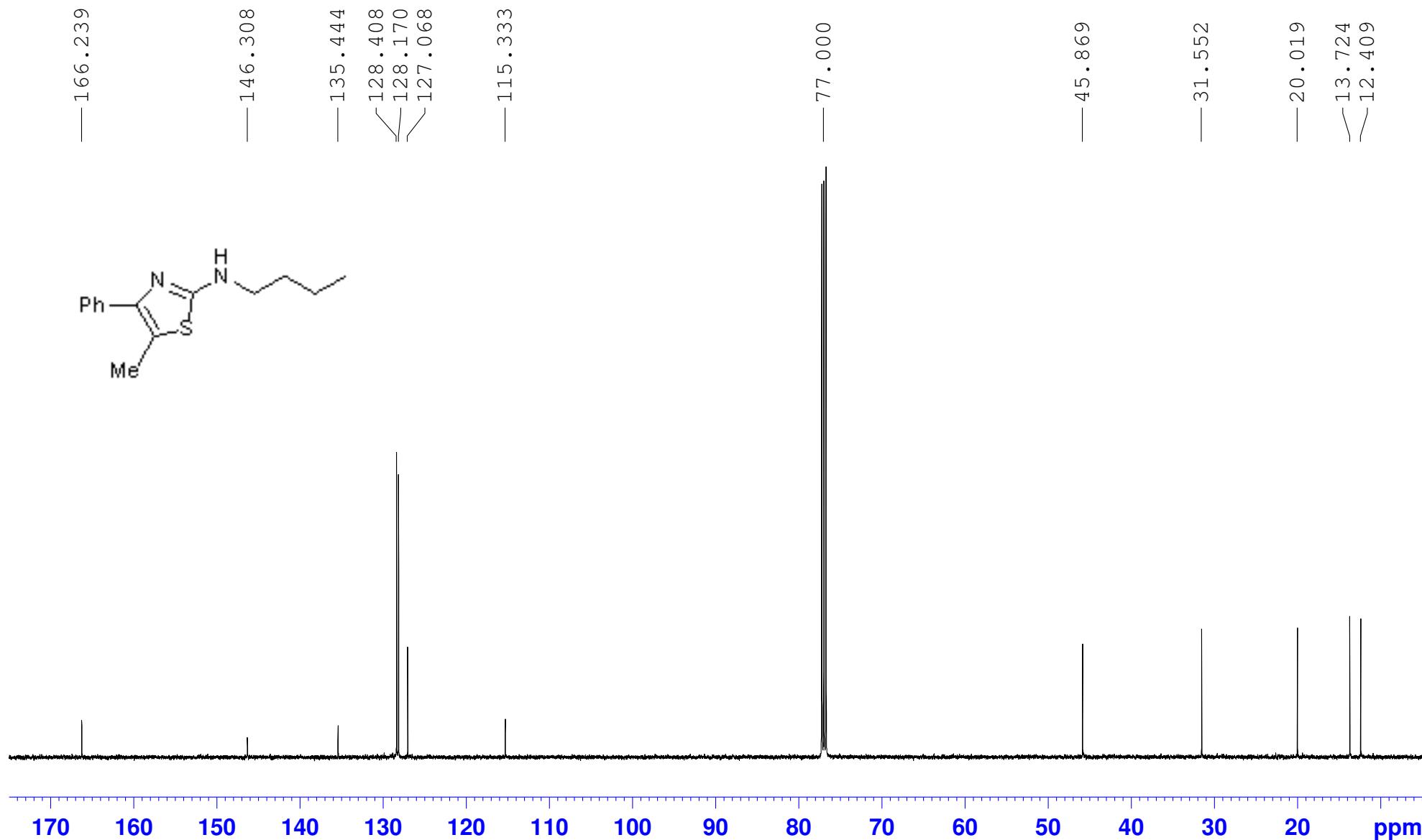
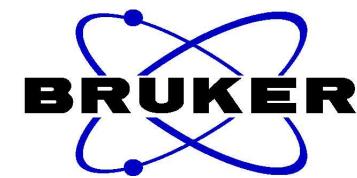
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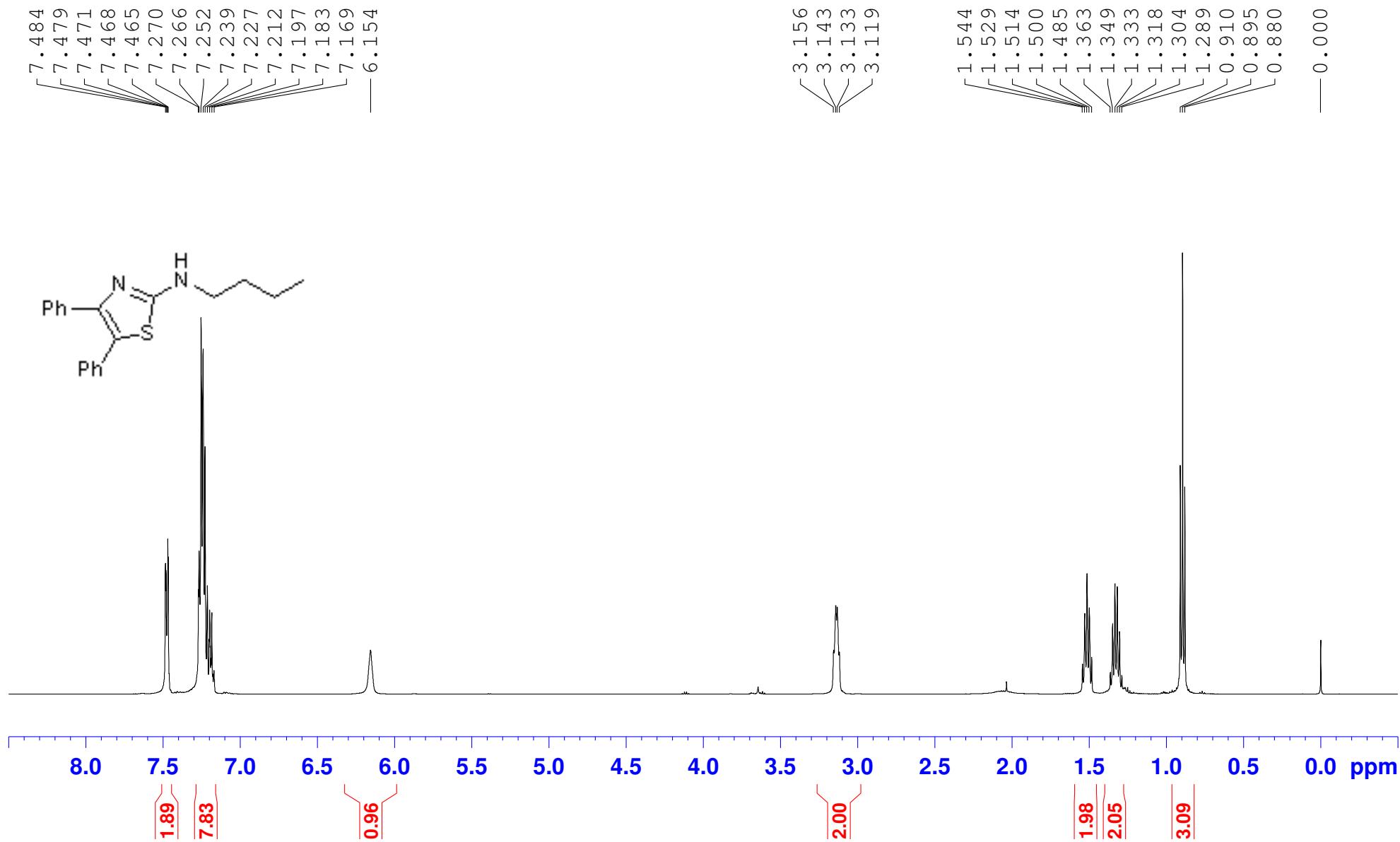
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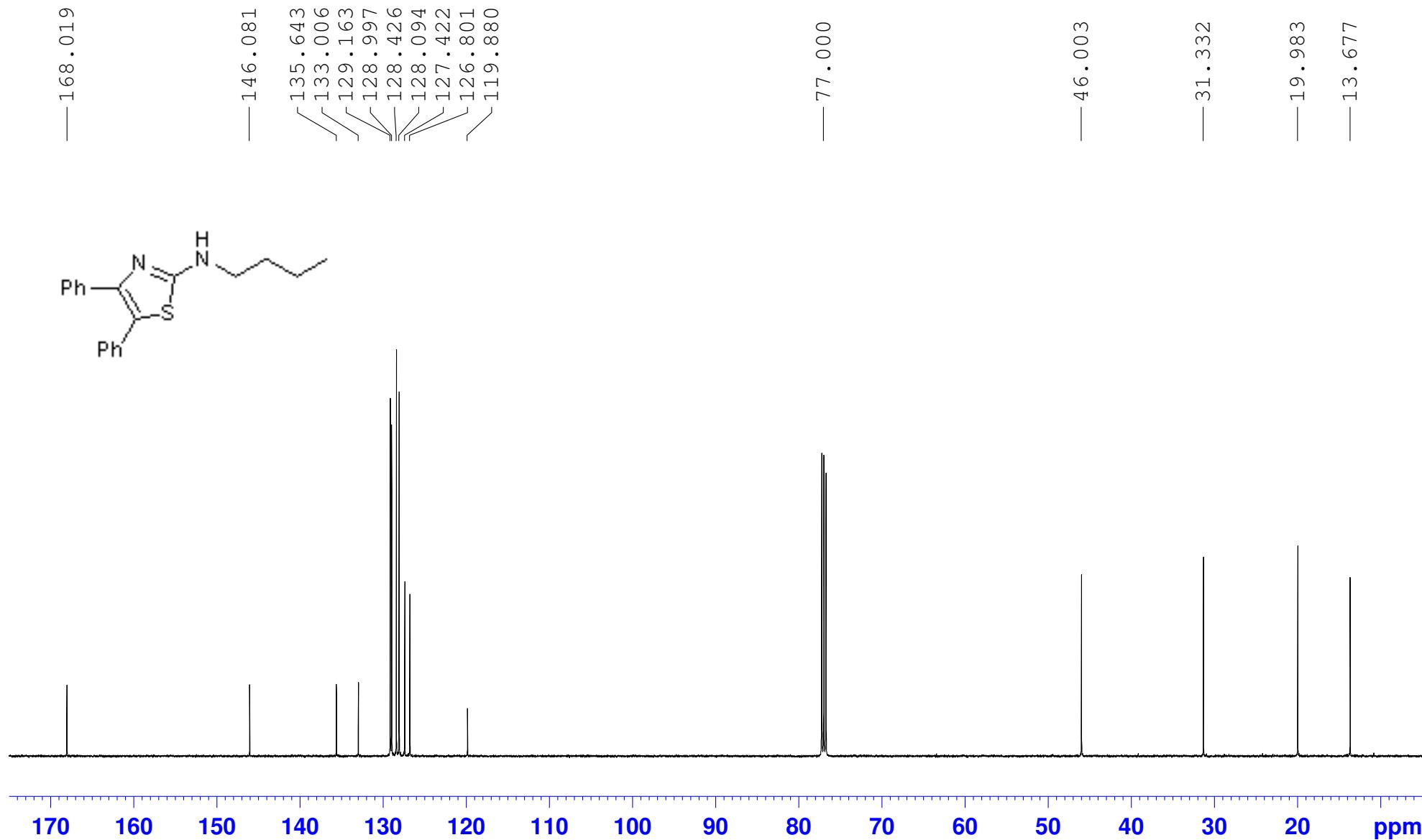
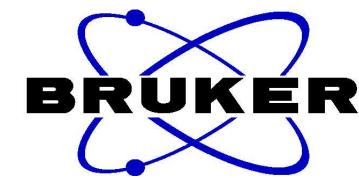
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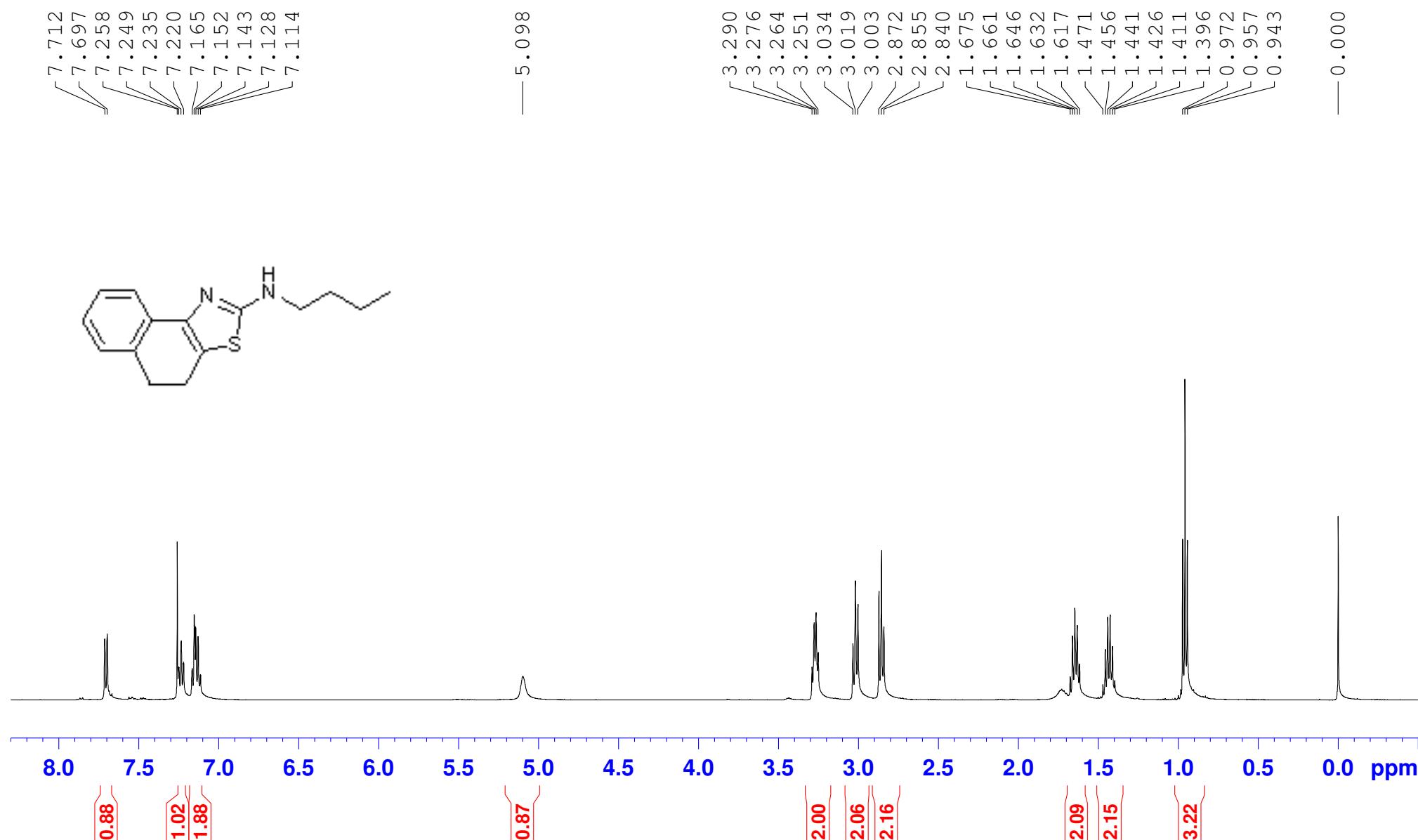
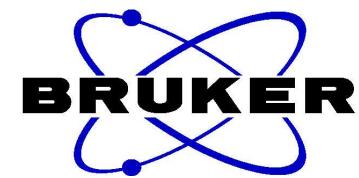
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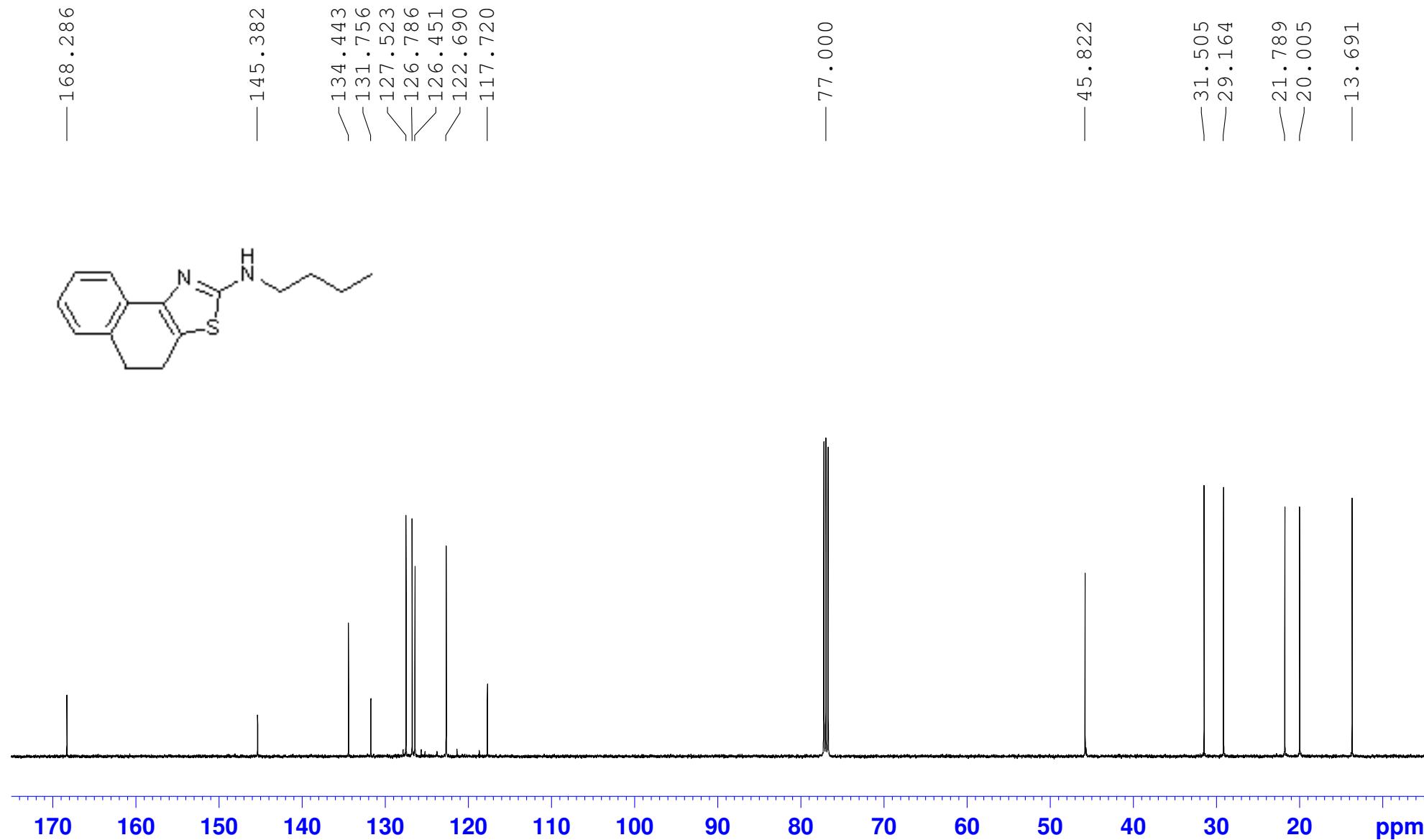
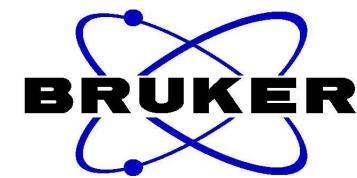
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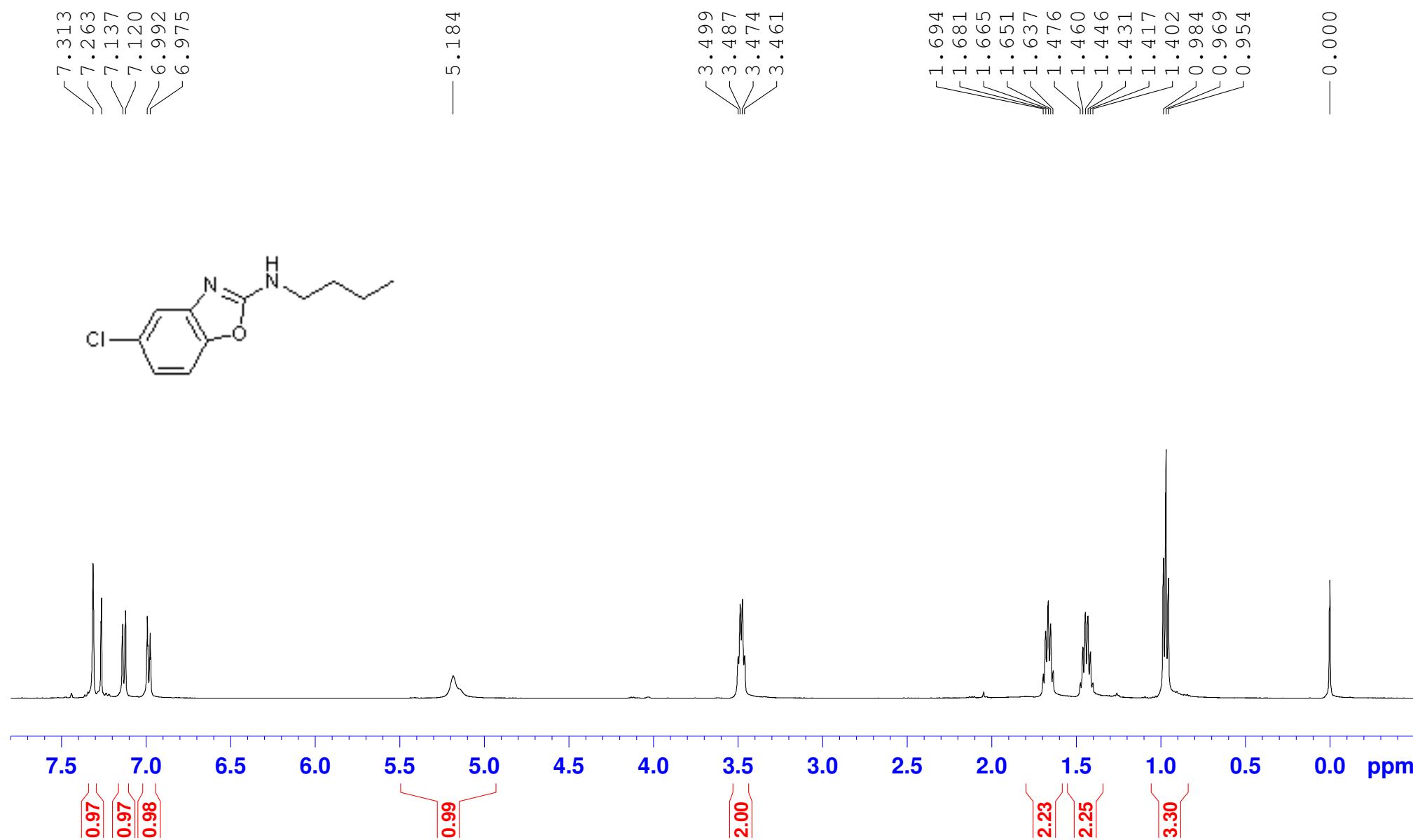
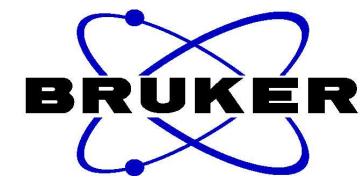
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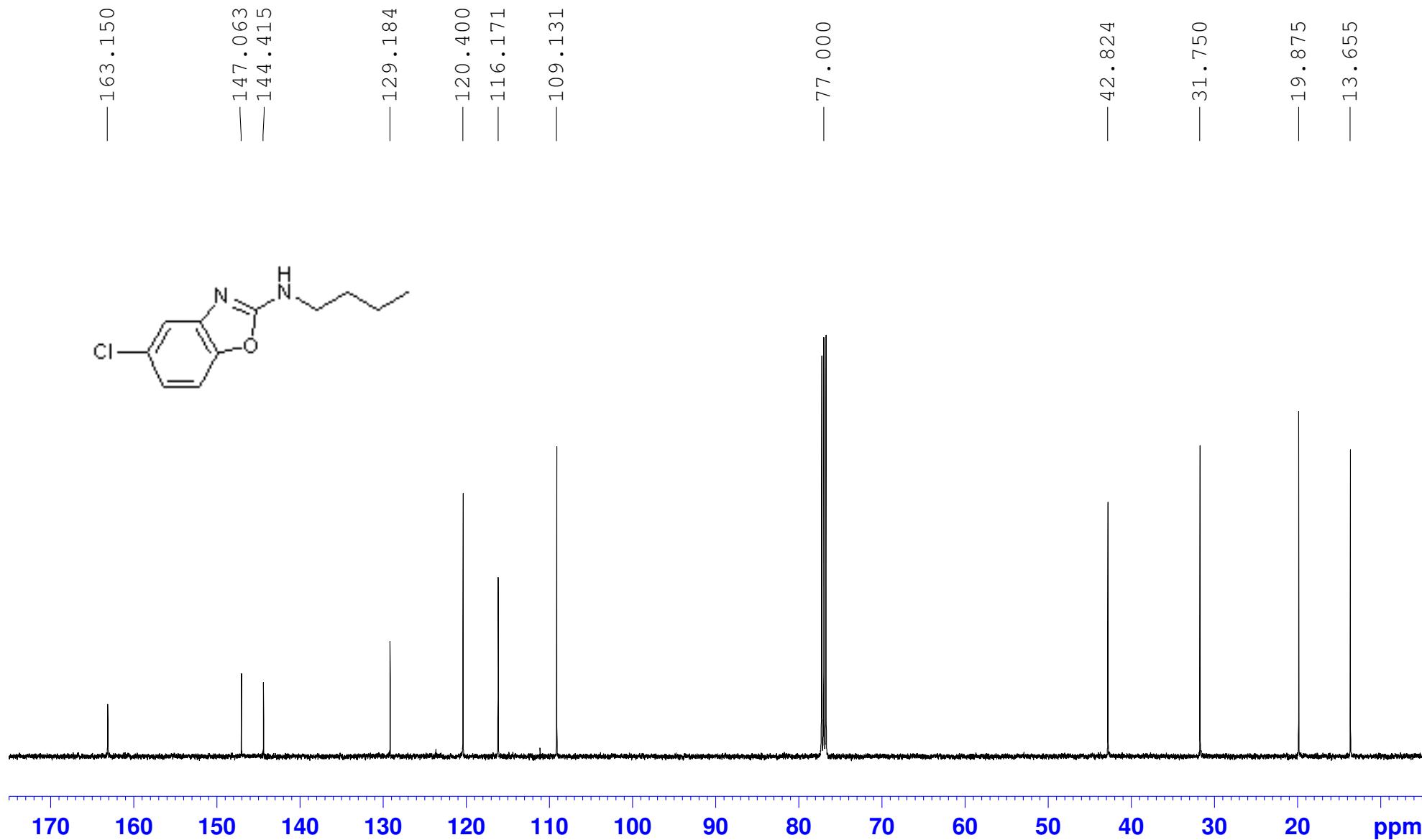
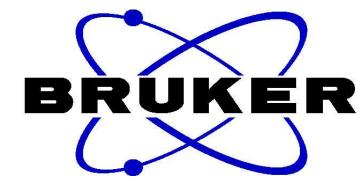
N-butyl-4,5-dihydronaphtho[1,2-d]thiazol-2-amine  
C13CPD CDCl<sub>3</sub>



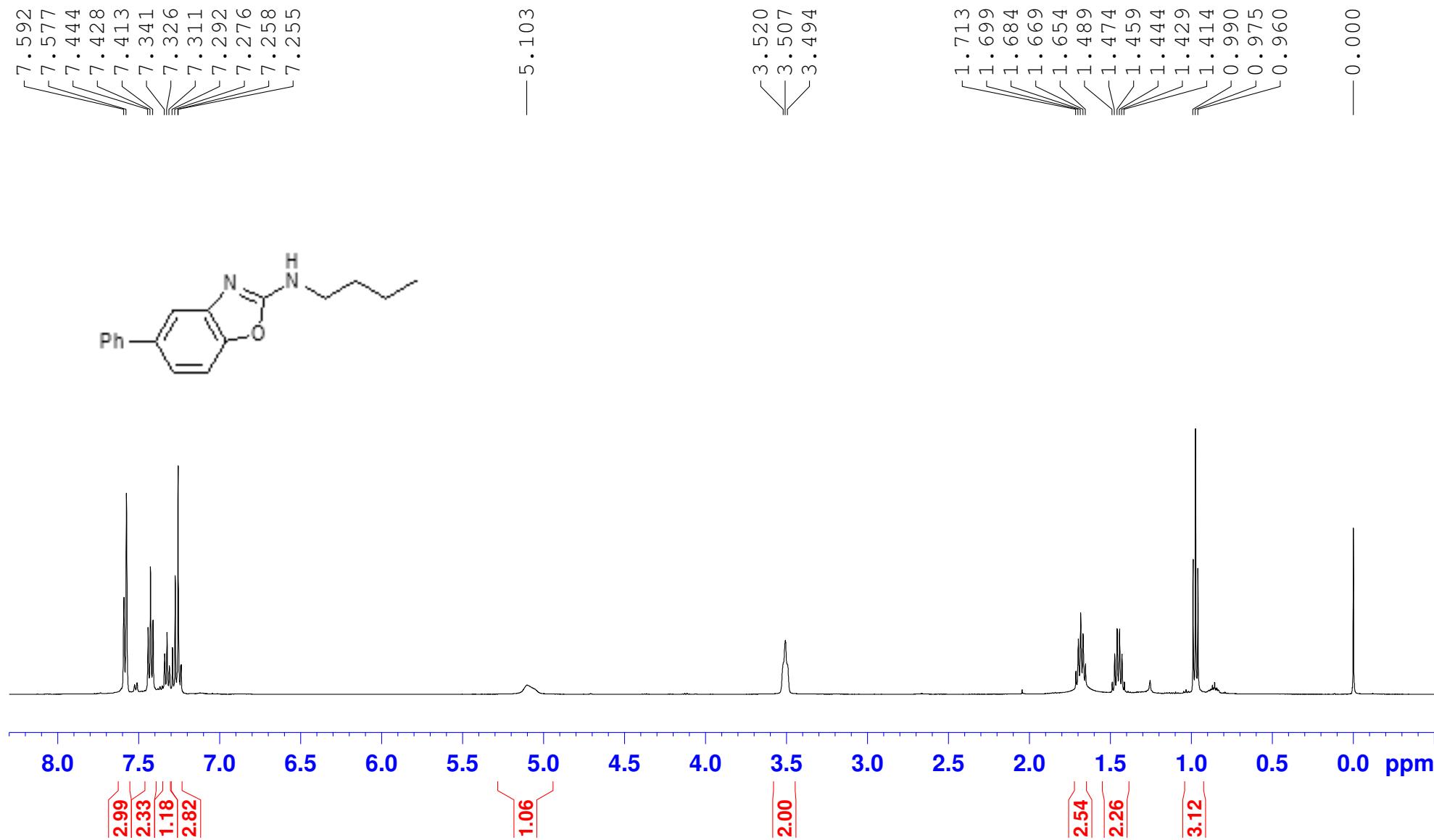
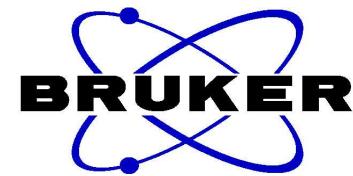
N-butyl-5-chlorobenzo [d] oxazol-2-amine  
Proton CDCl<sub>3</sub>



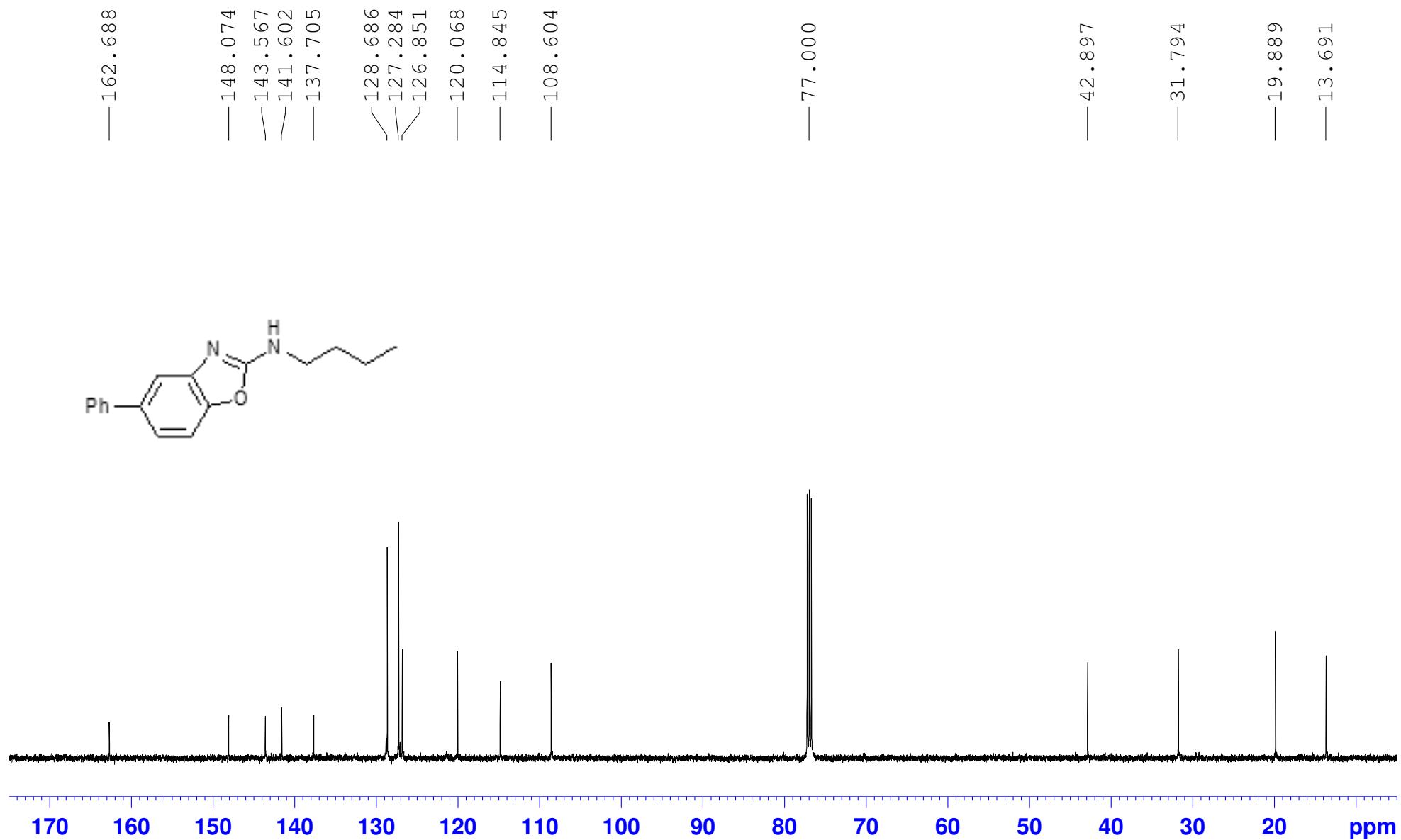
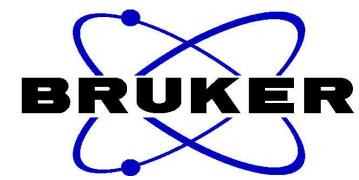
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C13CPD CDCl<sub>3</sub>



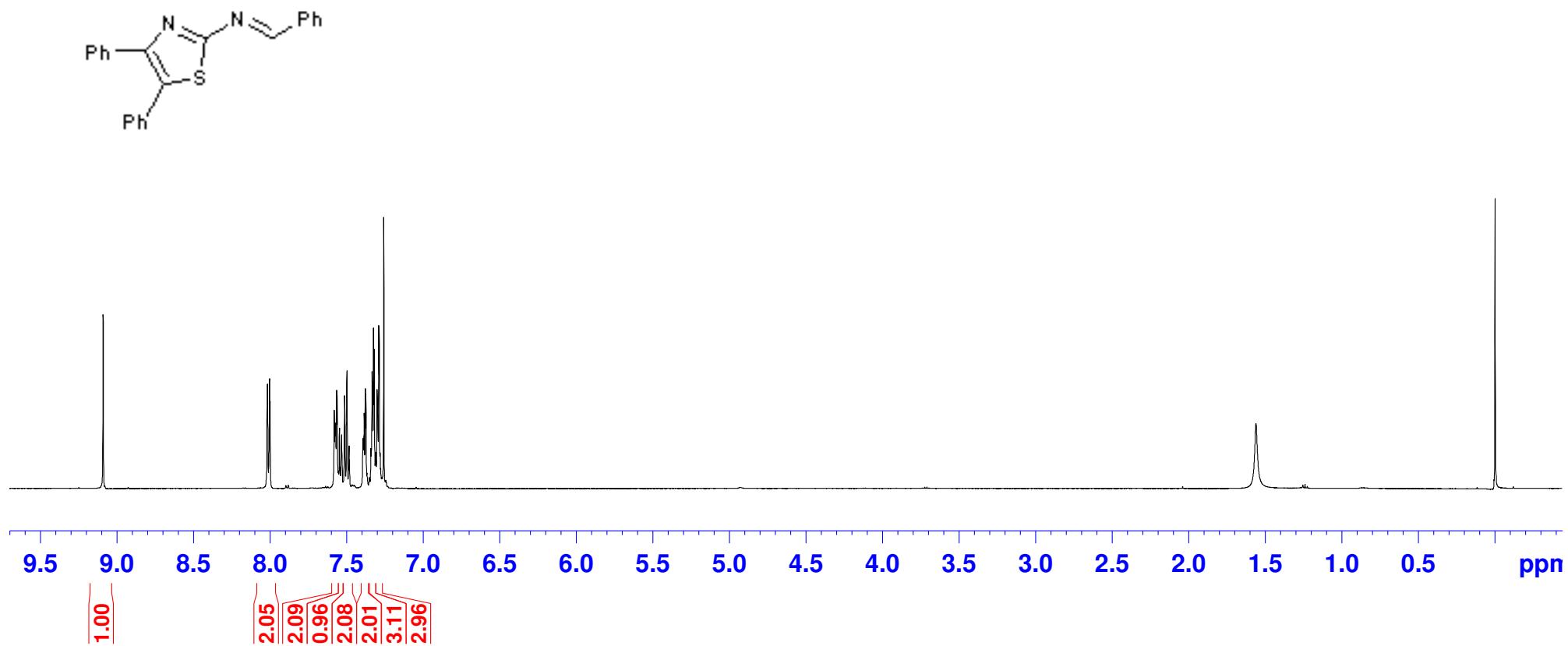
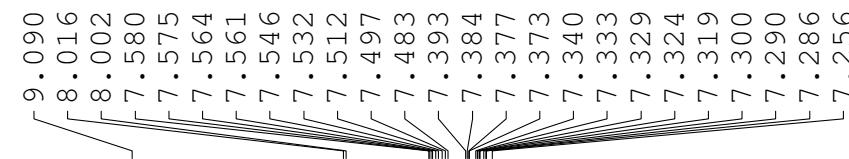
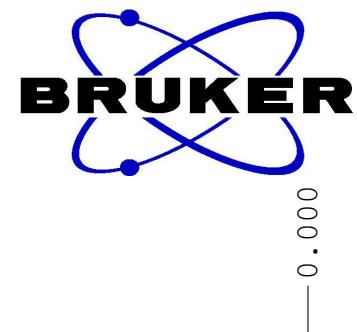
N-butyl-5-phenylbenzo[d]oxazol-2-amine  
Proton CDCl<sub>3</sub>



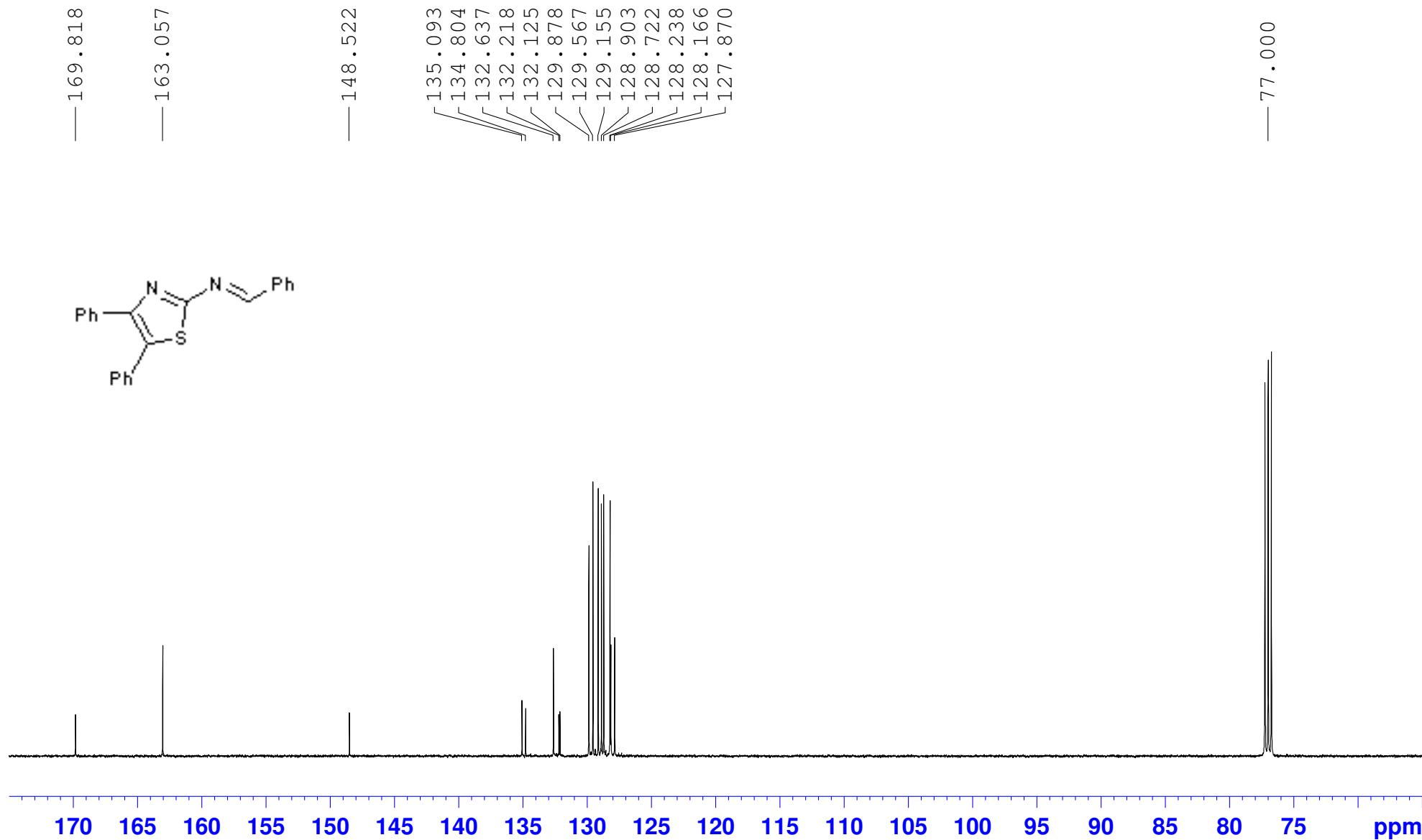
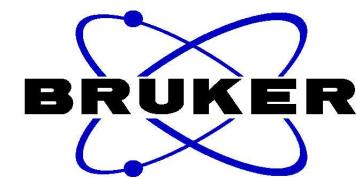
N-butyl-5-phenylbenzo[d]oxazol-2-amine  
C13CPD CDCl<sub>3</sub>



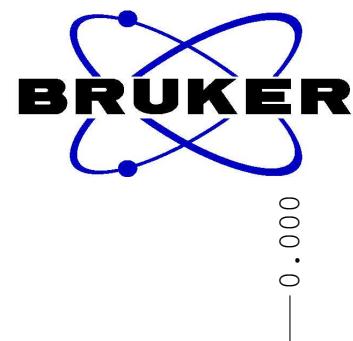
(E)-N-benzylidene-4,5-diphenylthiazol-2-amine  
Proton CDCl<sub>3</sub>



(E)-N-benzylidene-4,5-diphenylthiazol-2-amine  
C13CPD CDCl<sub>3</sub>



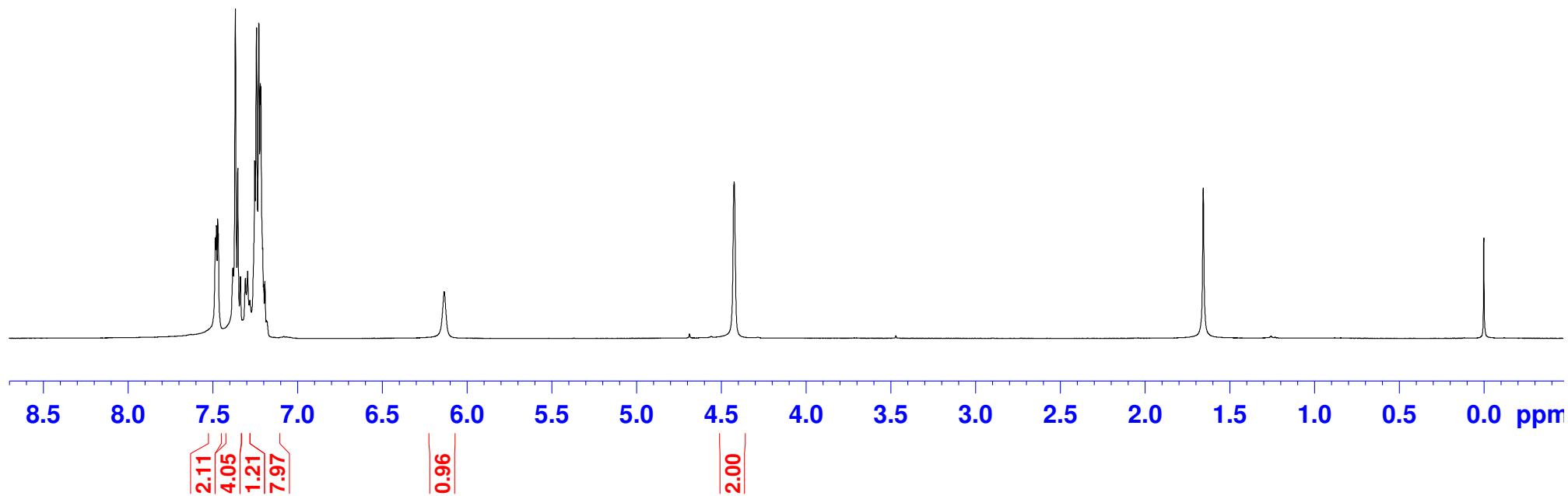
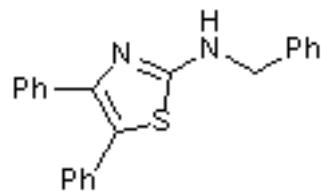
N-benzyl-4,5-diphenylthiazol-2-amine  
Proton CDCl<sub>3</sub>



7.484  
7.476  
7.468  
7.465  
7.379  
7.364  
7.350  
7.335  
7.306  
7.292  
7.279  
7.250  
7.239  
7.226  
7.218  
7.214  
7.190  
6.134

— 4.424

— 0.000



N-benzyl-4,5-diphenylthiazol-2-amine  
C13CPD CDCl<sub>3</sub>

