

Electronic Supplementary Information (ESI)

Regioselective *N*-alkylation of 2-aminobenzothiazoles with benzylic alcohols

Feng Li,* Haixia Shan, Qikai Kang and Lin Chen

School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China

General Experimental Details.

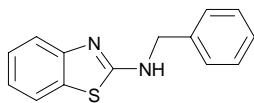
Infrared spectra were recorded on a Nicolet iS10 FT-IR spectrometer. High-resolution mass spectra (HRMS) were obtained on a HPLC-Q-ToF MS(Micro) spectrometer and are reported as *m/z* (relative intensity). Accurate masses are reported for the molecular ion $[M+H]^+$, $[M-H]^+$ or a suitable fragment ion. Melting points were measured on a X-6 micro-melting apparatus (Beijing Tech Instrument Co., Ltd). Proton nuclear magnetic resonance (^1H NMR) spectra were recorded at 500 MHz using a Bruker Avance 500 spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane or ppm relative to the center of the singlet at 7.26 ppm for CDCl_3 and 2.50 ppm for 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; q, quartet; m, multiplet; b, broad. Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded at 125 MHz using a Bruker Avance 500 spectrometer. Chemical shifts are reported in delta (δ) units, ppm relative to the center of the triplet at 77.0 ppm for CDCl_3 and 39.5 ppm for DMSO-d_6 . ^{13}C NMR spectra were routinely run with broadband decoupling.

All reactions were run under an atmosphere of nitrogen, unless otherwise indicated. Anhydrous solvents were transferred *via* oven-dried syringe. Reaction tubes were oven-dried and cooled under a stream of nitrogen. Reaction tubes were purchased from Beijing Synthware Glass Inc. Commercially unavailable 2-aminobenzothiazoles were readily prepared according to the previously reported procedures.¹ *p*-Xylene was distilled from calcium hydride. Analytical thin-layer chromatography (TLC) was carried out using 0.2-mm commercial silica gel plates.

General Procedure for the regioselective *N*-alkylation of 2-aminobenzothiazoles with alcohols.

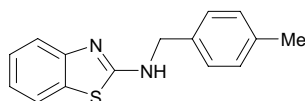
To an oven-dried, nitrogen purged 20 ml Schlenk tube were added 2-aminobenzothiazole (1mmol), copper salt (0.01 mmol, 1 mol%), base (0.2 mmol, 20 mol%), alcohol (1.2 mmol, 120 mol%) and *p*-xylene (1 ml). The mixture was then heated at 130 °C for 12h, at which point the reaction mixture was allowed to cool to ambient temperature. The reaction mixture was concentrated in *vacuo* and purified by flash column chromatography with hexane/ethyl acetate to afford the corresponding product.

N-benzylbenzo[d]thiazol-2-amine (1c)²



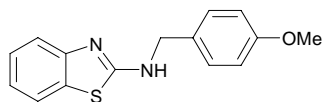
mp 164.4-165.2 °C (lit.² mp 164-168 °C); ¹H NMR (500 MHz, DMSO-d₆) δ 8.51 (t, *J* = 5.5 Hz, 1H, NH), 7.67 (d, *J* = 7.8 Hz, 1H, ArH), 7.39-7.33 (m, 5H, ArH), 7.26 (t, *J* = 7.1 Hz, 1H, ArH), 7.22 (t, *J* = 7.7 Hz, 1H, ArH), 7.02 (t, *J* = 7.5 Hz, 1H, ArH), 4.60 (s, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.2, 152.4, 138.9, 130.4, 128.3, 127.3, 127.0, 125.5, 121.0, 120.9, 118.1, 47.2.

N-(4-methylbenzyl)benzo[d]thiazol-2-amine (2c)³



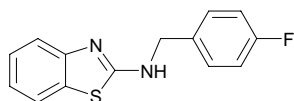
mp 188.9-189.4 °C (lit.³ mp 186-188 °C); ¹H NMR (500 MHz, CDCl₃) δ 7.56 (d, *J* = 7.9 Hz, 1H, ArH), 7.43 (d, *J* = 8.1 Hz, 1H, ArH), 7.29-7.25 (m, 3H, ArH), 7.16 (d, *J* = 7.8 Hz, 2H, ArH), 7.07 (t, *J* = 7.5 Hz, 1H, ArH), 6.38 (br s, 1H, NH), 4.58 (s, 2H, CH₂N), 2.34 (s, 3H, CH₃); ¹³C NMR (125 MHz, CDCl₃) δ 167.4, 152.2, 137.7, 134.4, 130.5, 129.5, 127.7, 126.0, 121.6, 120.8, 118.9, 49.2, 21.1.

N-(4-methoxybenzyl)benzo[d]thiazol-2-amine (3c)⁴



mp 173.5-174.0 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.58 (d, *J* = 7.8 Hz, 1H, ArH), 7.52 (d, *J* = 8.1 Hz, 1H, ArH), 7.33-7.28 (m, 3H, ArH), 7.09 (t, *J* = 7.6 Hz, 1H, ArH), 6.90-6.88 (m, 2H, ArH), 5.86 (br s, 1H, NH), 4.57 (s, 2H, CH₂N), 3.81 (s, 3H, OCH₃); ¹³C NMR (125 MHz, CDCl₃) δ 167.4, 159.3, 152.1, 130.4, 129.4, 129.1, 126.0, 121.6, 120.8, 118.8, 114.2, 55.3, 48.9.

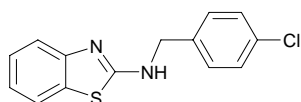
N-(4-fluorobenzyl)benzo[d]thiazol-2-amine (4c)⁴



mp 148.0-149.2 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.58 (d, *J* = 7.8 Hz, 1H, ArH), 7.44 (d, *J* = 8.0 Hz,

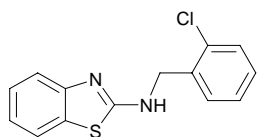
1H, ArH), 7.37 (t, $J = 6.8$ Hz, 2H, ArH), 7.28 (t, $J = 7.8$ Hz, 1H, ArH), 7.10 (t, $J = 7.6$ Hz, 1H, ArH), 7.04 (t, $J = 8.6$ Hz, 2H, ArH), 6.43 (br s, 1H, NH), 4.60 (s, 2H, CH₂N); ¹³C NMR (125 MHz, CDCl₃) δ 167.7, 162.4 (d, $J_{C-F} = 243.8$ Hz), 152.0, 133.2 (d, $J_{C-F} = 3.8$ Hz), 130.2, 129.3 (d, $J_{C-F} = 8.1$ Hz), 126.0, 121.7, 120.8, 118.7, 115.6 (d, $J_{C-F} = 20.8$ Hz), 48.6.

N-(4-chlorobenzyl)benzo[d]thiazol-2-amine (5c)²



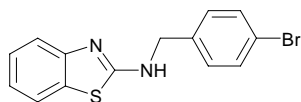
mp 188.2-188.8 °C (lit.² mp 175-180 °C); ¹H NMR (500 MHz, DMSO-d₆) δ 8.53 (t, $J = 5.7$ Hz, 1H, NH), 7.67 (d, $J = 7.6$ Hz, 1H, ArH), 7.42-7.37 (m, 5H, ArH), 7.22 (t, $J = 7.6$ Hz, 1H, ArH), 7.03 (t, $J = 7.6$ Hz, 1H, ArH), 4.59 (d, $J = 3.8$ Hz, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.0, 152.3, 138.0, 131.5, 130.4, 129.2, 128.3, 125.5, 121.0, 118.1, 46.3.

N-(2-chlorobenzyl)benzo[d]thiazol-2-amine (6c)



mp 134.7-135.2 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.54 (t, $J = 5.4$ Hz, 1H, NH), 7.69 (d, $J = 7.8$ Hz, 1H, ArH), 7.48 (dd, $J = 6.6$ Hz and 2.1 Hz, 2H, ArH), 7.40 (d, $J = 7.9$ Hz, 1H, ArH), 7.35-7.30 (m, 2H, ArH), 7.22 (t, $J = 7.7$ Hz, 1H, ArH), 7.04 (t, $J = 7.6$ Hz, 1H, ArH), 4.68 (s, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.0, 152.3, 135.9, 132.3, 130.5, 129.3, 129.1, 128.9, 127.3, 125.6, 121.1, 121.30, 118.2, 45.0; FTIR (net, cm⁻¹) 3198, 3050, 1631, 1591, 1443, 1285; HRMS-EI (70 eV) m/z calcd for C₁₄H₁₂N₂SCl [M+H]⁺ 275.0410, found 275.0411.

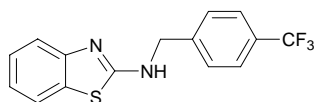
N-(4-bromobenzyl)benzo[d]thiazol-2-amine (7c)⁵



mp 195.1-195.6 °C (lit.⁵ mp 197-200 °C); ¹H NMR (500 MHz, DMSO-d₆) δ 8.54 (s, 1H, NH), 7.67 (d, $J = 7.9$ Hz, 1H, ArH), 7.54 (d, $J = 8.5$ Hz, 2H, ArH), 7.39-7.33 (m, 3H, ArH), 7.22 (t, $J = 7.6$ Hz, 1H, ArH), 7.03 (t, $J = 7.6$ Hz, 1H, ArH), 4.57 (s, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.0,

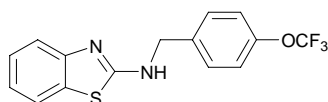
152.3, 138.4, 131.2, 130.4, 129.5, 125.5, 121.0, 120.9, 120.0, 118.1, 46.3; HRMS-EI (70 eV) m/z calcd for $C_{14}H_{12}N_2SBr$ $[M+H]^+$ 318.9905, found 318.9905.

N-(4-(trifluoromethyl)benzyl)benzo[d]thiazol-2-amine (8c)



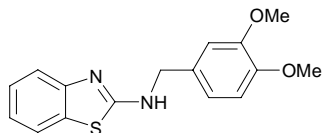
mp 164.2-164.8 °C; 1H NMR (500 MHz, DMSO- d_6) δ 8.63 (t, J = 5.9 Hz, 1H, NH), 7.72 (d, J = 8.2 Hz, 2H, ArH), 7.69 (dd, J = 7.9 Hz, 1H, ArH), 7.60 (d, J = 8.0 Hz, 2H, ArH), 7.38 (d, J = 8.0 Hz, 1H, ArH), 7.22 (t, J = 7.8 Hz, 1H, ArH), 7.03 (t, J = 7.7 Hz, 1H, ArH), 4.70 (d, J = 5.7 Hz, 2H, CH_2N); ^{13}C NMR (125 MHz, DMSO- d_6) δ 166.6, 152.8, 144.5, 130.9, 128.4, 128.1 (q, J_{C-F} = 31.6 Hz), 126.0, 125.7 (q, J_{C-F} = 3.6 Hz), 124.8 (q, J_{C-F} = 270.0 Hz), 121.6, 121.5, 118.7, 47.1; FTIR (net, cm^{-1}) 3139, 3089, 1606, 1558, 1448, 1267; HRMS-EI (70 eV) m/z calcd for $C_{15}H_{12}N_2F_3S$ $[M+H]^+$ 309.0673, found 309.0678.

N-(4-(trifluoromethoxy)benzyl)benzo[d]thiazol-2-amine (9c)



mp 149.8-150.7 °C; 1H NMR (500 MHz, DMSO- d_6) δ 8.55 (t, J = 5.8 Hz, 1H, NH), 7.68 (d, J = 7.4 Hz, 1H, ArH), 7.50 (d, J = 8.5 Hz, 2H, ArH), 7.39-7.34 (m, 3H, ArH), 7.22 (t, J = 7.7 Hz, 1H, ArH), 7.03 (t, J = 7.6 Hz, 1H, ArH), 4.63 (d, J = 5.9 Hz, 2H, CH_2N); ^{13}C NMR (125 MHz, DMSO- d_6) δ 166.1, 152.4, 147.3, 138.6, 130.4, 129.2, 125.5, 121.1, 120.99, 120.95, 120.1 (q, J_{C-F} = 254.6 Hz), 118.2, 46.4; FTIR (net, cm^{-1}) 3180, 3086, 1614, 1576, 1449, 1210; HRMS-EI (70 eV) m/z calcd for $C_{15}H_{12}N_2OSF_3$ $[M+H]^+$ 325.0622, found 325.0615.

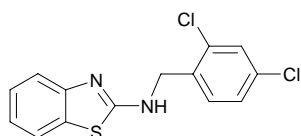
N-(3,4-dimethoxybenzyl)benzo[d]thiazol-2-amine (10c)



mp 145.8-146.6 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, J = 7.7 Hz, 1H, ArH), 7.45 (d, J = 8.1 Hz, 1H, ArH), 7.27 (t, J = 6.6 Hz, 1H, ArH), 7.08 (t, J = 7.4 Hz, 1H, ArH), 6.93 (t, J = 6.8 Hz, 2H, ArH),

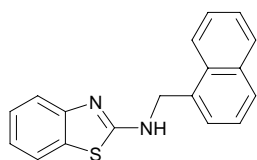
6.83 (d, $J = 7.9$ Hz, 1H, ArH), 6.43 (br s, 1H, NH), 4.55 (s, 2H, CH₂N), 3.87 (s, 3H, OCH₃), 3.82 (s, 3H, OCH₃); ¹³C NMR (125 MHz, CDCl₃) δ 167.9, 152.0, 149.2, 148.6, 130.1, 129.9, 125.9, 121.4, 120.7, 120.0, 118.6, 111.2, 110.8, 55.8, 55.7, 49.3; FTIR (net, cm⁻¹) 3184, 3085, 1598, 1549, 1444, 1260; HRMS-EI (70 eV) m/z calcd for C₁₆H₁₇N₂O₂S [M+H]⁺ 301.1011, found 301.1011.

N-(2,4-dichlorobenzyl)benzo[d]thiazol-2-amine (11c)



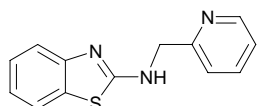
mp 144.8-145.2 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.57 (d, $J = 7.9$ Hz, 1H, ArH), 7.48 (d, $J = 8.0$ Hz, 1H, ArH), 7.44 (d, $J = 8.3$ Hz, 1H, ArH), 7.41 (d, $J = 2.2$ Hz, 1H, ArH), 7.28 (t, $J = 7.7$ Hz, 1H, ArH), 7.21 (dd, $J = 8.3$ Hz and 2.1 Hz, 1H, ArH), 7.09 (t, $J = 7.6$ Hz, 1H, ArH), 6.27 (br s, 1H, NH), 4.70 (s, 2H, CH₂N); ¹³C NMR (125 MHz, CDCl₃) δ 167.5, 152.0, 134.2, 134.1, 133.7, 130.3, 130.2, 129.5, 127.4, 126.1, 121.8, 120.9, 118.9, 46.5; FTIR (net, cm⁻¹) 3178, 3083, 1606, 1585, 1445, 1221; HRMS-EI (70 eV) m/z calcd for C₁₁H₁₅N₂S₂Cl₂ [M+H]⁺ 309.0054, found 309.0050.

N-(naphthalen-1-ylmethyl)benzo[d]thiazol-2-amine (12c)



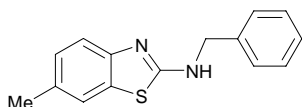
mp 150.1-150.8 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.55 (t, $J = 5.3$ Hz, 1H, NH), 8.13 (d, $J = 8.1$ Hz, 1H, ArH), 7.98 (d, $J = 7.8$ Hz, 1H, ArH), 7.88 (d, $J = 8.2$ Hz, 1H, ArH), 7.68 (d, $J = 7.9$ Hz, 1H, ArH), 7.60-7.54 (m, 3H, ArH), 7.49 (t, $J = 7.6$ Hz, 1H, ArH), 7.41 (d, $J = 8.0$, 1H, ArH), 7.23 (t, $J = 7.7$ Hz, 1H, ArH), 7.03 (t, $J = 7.6$ Hz, 1H, ArH), 5.07 (d, $J = 5.4$ Hz, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.5, 152.9, 134.5, 133.8, 131.5, 131.0, 129.0, 128.3, 126.8, 126.4, 126.1, 126.0, 125.9, 124.0, 121.5, 121.4, 118.6, 45.9; FTIR (net, cm⁻¹) 3139, 3045, 1608, 1557, 1448, 1275; HRMS-EI (70 eV) m/z calcd for C₁₈H₁₅N₂S [M+H]⁺ 291.0956, found 291.0953.

N-(pyridin-2-ylmethyl)benzo[d]thiazol-2-amine (13c)



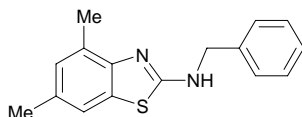
mp 156.9-157.5 °C; ¹H NMR (500 MHz, DMSO-d₆ at 353k) δ 8.54 (s, 1H, NH), 8.33 (brs, 1H, ArH), 7.74 (t, *J* = 7.6 Hz, 1H, ArH), 7.64 (d, *J* = 7.8 Hz, 1H, ArH), 7.42 (d, *J* = 7.5 Hz, 1H, ArH), 7.37 (d, *J* = 7.9 Hz, 1H, ArH), 7.25 (t, *J* = 5.5 Hz, 1H, ArH), 7.20 (t, *J* = 7.6 Hz, 1H, ArH), 7.00 (t, *J* = 7.6 Hz, 1H, ArH), 4.69 (s, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆ at 353k) δ 160.0, 157.8, 152.1, 148.4, 136.2, 130.2, 125.0, 121.8, 121.0, 120.6, 120.4, 117.8, 48.9; FTIR (net, cm⁻¹) 3241, 3036, 1596, 1567, 1455, 1251; HRMS-EI (70 eV) *m/z* calcd for C₁₃H₁₂N₃S [M+H]⁺ 242.0752, found 242.0751.

N-benzyl-6-methylbenzo[d]thiazol-2-amine (14c)⁶



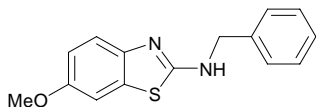
mp 179.7-180.2 °C (lit.⁶ mp 176-178 °C); ¹H NMR (500 MHz, DMSO-d₆) δ 8.39 (t, *J* = 5.7 Hz, 1H, NH), 7.46 (s, 1H, ArH), 7.39-7.33 (m, 4H, ArH), 7.28-7.24 (m, 2H, ArH), 7.02 (d, *J* = 8.0 Hz, 1H, ArH), 4.58 (s, 2H, CH₂N), 2.31 (s, 3H, CH₃); ¹³C NMR (125 MHz, DMSO-d₆) δ 165.4, 150.3, 139.0, 130.5, 130.1, 128.3, 127.4, 127.0, 126.5, 120.9, 117.8, 47.1, 20.7.

N-benzyl-4,6-dimethylbenzo[d]thiazol-2-amine (15c)



mp 115.0-115.8 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.37 (t, *J* = 5.7 Hz, 1H, NH), 7.40 (d, *J* = 7.5 Hz, 2H, ArH), 7.34 (t, *J* = 7.5 Hz, 2H, ArH), 7.26 (t, *J* = 6.6 Hz, 2H, ArH), 6.87 (s, 1H, ArH), 4.56 (d, *J* = 5.8 Hz, 2H, CH₂N), 2.39 (s, 3H, CH₃), 2.27 (s, 3H, CH₃); ¹³C NMR (125 MHz, DMSO-d₆) δ 164.9, 149.2, 139.1, 129.9, 129.8, 128.3, 127.6, 127.4, 127.0, 126.8, 118.2, 47.4, 20.7, 18.0; FTIR (net, cm⁻¹) 3222, 3029, 1594, 1561, 1451, 1274; HRMS-EI (70 eV) *m/z* calcd for C₁₆H₁₇N₂S [M+H]⁺ 269.1112, found 269.1111.

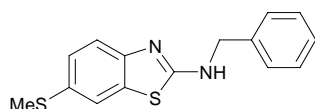
N-benzyl-6-methoxybenzo[d]thiazol-2-amine (16c)



mp 133.4-134.7 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.28 (t, *J* = 5.8 Hz, 1H, NH), 7.38-7.24 (m, 7H,

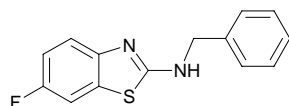
ArH), 6.82 (dd, $J = 8.7$ Hz and 2.6 Hz, 1H, ArH), 4.56 (d, $J = 5.7$ Hz, 2H, CH₂N), 3.73 (s, 3H, OCH₃); ¹³C NMR (125 MHz, DMSO-d₆) δ 164.6, 154.4, 146.5, 139.1, 131.4, 128.3, 127.3, 126.9, 118.4, 112.9, 105.6, 55.5, 47.2; FTIR (net, cm⁻¹) 3171, 3092, 1606, 1557, 1445, 1261; HRMS-EI (70 eV) m/z calcd for C₁₅H₁₅N₂OS [M+H]⁺ 271.0905, found 271.0909.

N-benzyl-6-(methylthio)benzo[d]thiazol-2-amine (17c)



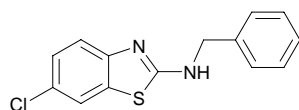
mp 176.8-177.2 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.51 (t, $J = 5.6$ Hz, 1H, NH), 7.66 (d, $J = 1.3$ Hz, 1H, ArH), 7.38-7.31 (m, 5H, ArH), 7.27 (t, $J = 7.0$ Hz, 1H, ArH), 7.16 (dd, $J = 8.3$ Hz and 1.6 Hz, 1H, ArH), 4.58 (d, $J = 5.6$ Hz, 2H, CH₂N), 2.46 (s, 3H, SCH₃); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.0, 150.6, 138.8, 131.6, 129.3, 128.3, 127.4, 127.0, 125.6, 119.9, 118.3, 47.2, 16.6; FTIR (net, cm⁻¹) 3174, 3088, 1603, 1567, 1445, 1260; HRMS-EI (70 eV) m/z calcd for C₁₅H₁₅N₂S [M+H]⁺ 287.0677, found 287.0686.

N-benzyl-6-fluorobenzo[d]thiazol-2-amine (18c)²



mp 191.1-192.0 °C (lit.² mp 180-184 °C); ¹H NMR (500 MHz, DMSO-d₆) δ 8.49 (t, $J = 5.9$ Hz, 1H, NH), 7.61 (dd, $J = 8.7$ Hz and 2.8 Hz, 1H, ArH), 7.38-7.33 (m, 5H, ArH), 7.27 (t, $J = 6.9$ Hz, 1H, ArH), 7.05 (dd, $J = 9.1$ Hz and 2.7 Hz, 1H, ArH), 4.58 (s, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.0 (d, $J_{C-F} = 13.8$ Hz), 157.2 (d, $J_{C-F} = 233.8$ Hz), 149.1, 138.8, 131.4 (d, $J_{C-F} = 10.8$ Hz), 128.4, 127.4, 127.0, 118.5 (d, $J_{C-F} = 8.6$ Hz), 112.8 (d, $J_{C-F} = 23.5$ Hz), 107.8 (d, $J_{C-F} = 27.1$ Hz), 47.1; HRMS-EI (70 eV) m/z calcd for C₁₄H₁₂N₂SF [M+H]⁺ 259.0705, found 259.0706.

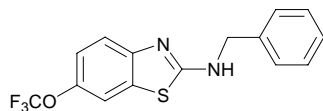
N-benzyl-6-chlorobenzo[d]thiazol-2-amine (19c)



mp 194.7-195.1 °C; ¹H NMR (500 MHz, DMSO-d₆) δ 8.62 (s, 1H, NH), 7.80 (s, 1H, ArH), 7.37-7.22 (m, 7H, ArH), 4.59 (d, $J = 4.3$ Hz, 2H, CH₂N); ¹³C NMR (125 MHz, DMSO-d₆) δ 166.8, 151.4, 138.7,

132.1, 128.4, 127.4, 127.0, 125.6, 124.7, 120.6, 118.9, 47.2; FTIR (net, cm^{-1}) 3183, 3086, 1616, 1573, 1447, 1263; HRMS-EI (70 eV) m/z calcd for $\text{C}_{14}\text{H}_{12}\text{N}_2\text{SCI}$ $[\text{M}+\text{H}]^+$ 275.0410, found 275.0407.

N-benzyl-6-(trifluoromethoxy)benzo[d]thiazol-2-amine (20c)



mp 176.2-177.1 °C; ^1H NMR (500 MHz, DMSO-d_6) δ 8.67 (t, $J = 5.4$ Hz, 1H, NH), 7.81 (s, 1H, ArH), 7.43 (d, $J = 8.6$ Hz, 1H, ArH), 7.38-7.34 (m, 4H, ArH), 7.27 (t, $J = 6.8$ Hz, 1H, ArH), 7.20 (d, $J = 8.4$ Hz, 1H, ArH), 4.61 (d, $J = 4.9$ Hz, 2H, CH_2N); ^{13}C NMR (125 MHz, DMSO-d_6) δ 167.4, 151.6, 142.2, 138.6, 131.5, 128.3, 127.3, 127.0, 120.2 (q, $J_{\text{C-F}} = 254.0$ Hz), 119.0, 118.3, 114.4, 47.2; FTIR (net, cm^{-1}) 3195, 3094, 1620, 1587, 1461, 1250; HRMS-EI (70 eV) m/z calcd for $\text{C}_{15}\text{H}_{12}\text{N}_2\text{OF}_3\text{S}$ $[\text{M}+\text{H}]^+$ 325.0622, found 325.0630.

References

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N-benzylbenzo[d]thiazol-2-amine
PROTON DMSO-d6

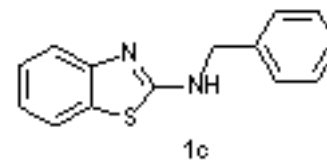
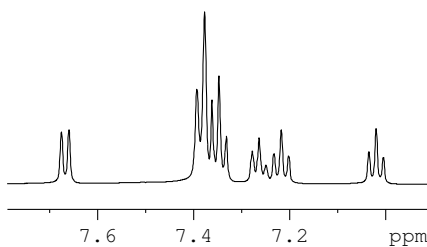


8.508
8.497
8.486
7.674
7.659
7.392
7.376
7.361
7.346
7.331
7.277
7.263
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7.034
7.019
7.004

4.602
4.596

2.503

0.000

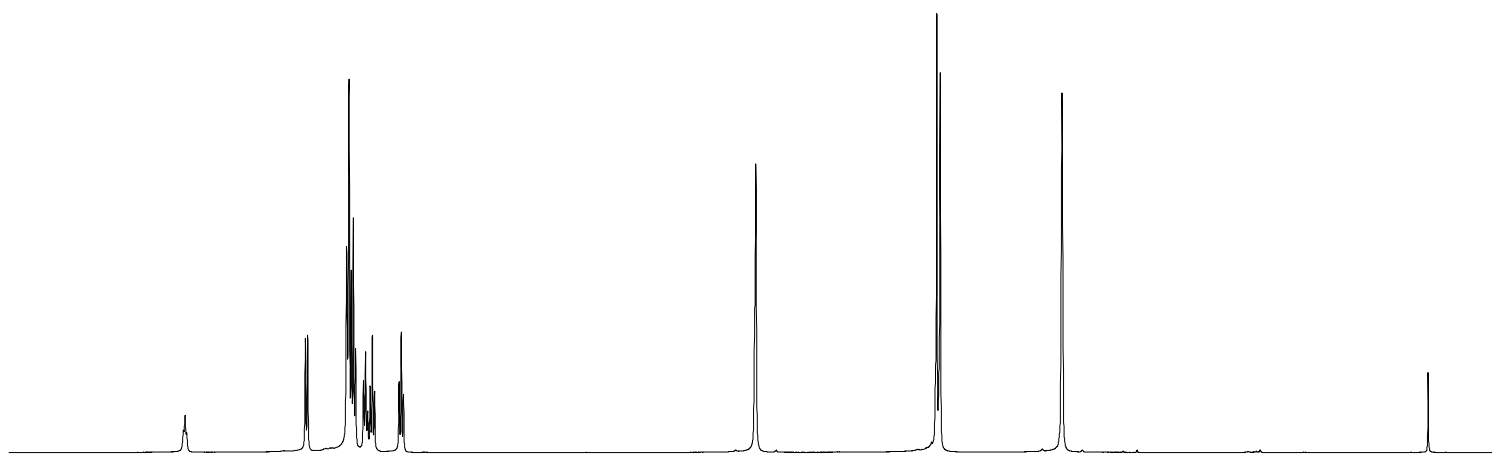


Current Data Parameters
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EXPNO 125
PROCNO 1

F2 - Acquisition Parameters
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PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



9

8

6

5

4

3

2

1

ppm

0.44

1.02

4.49

0.89

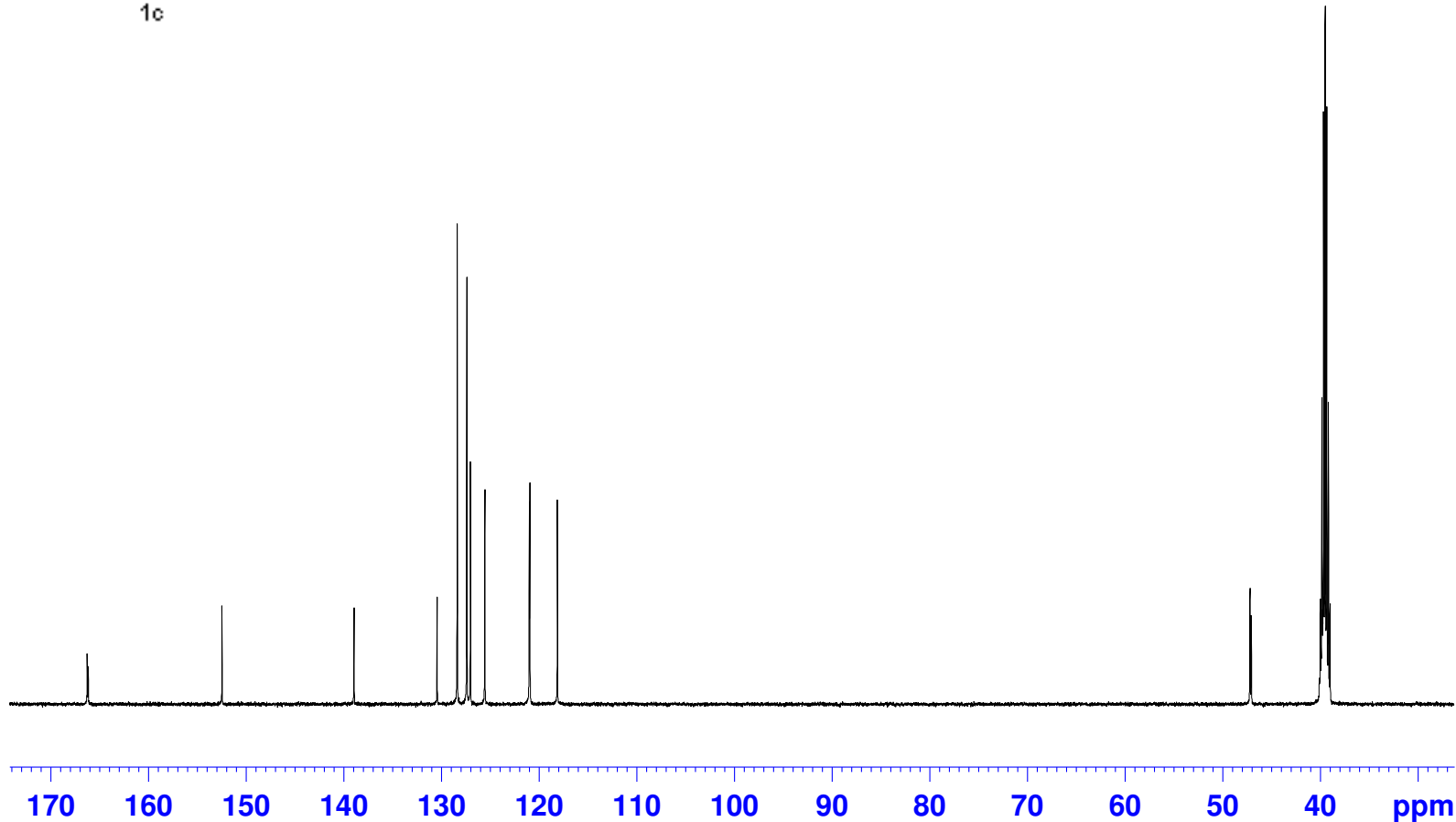
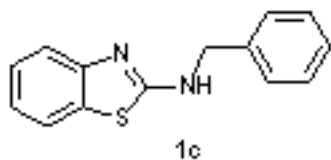
0.92

0.93

2.00

N-benzylbenzo[d]thiazol-2-amine
C13CPD DMSO-d6

166.24
152.42
138.90
130.39
128.34
127.35
126.99
125.51
120.95
120.89
118.08



Current Data Parameters
NAME Lifeng-1H
EXPNO 126
PROCNO 1

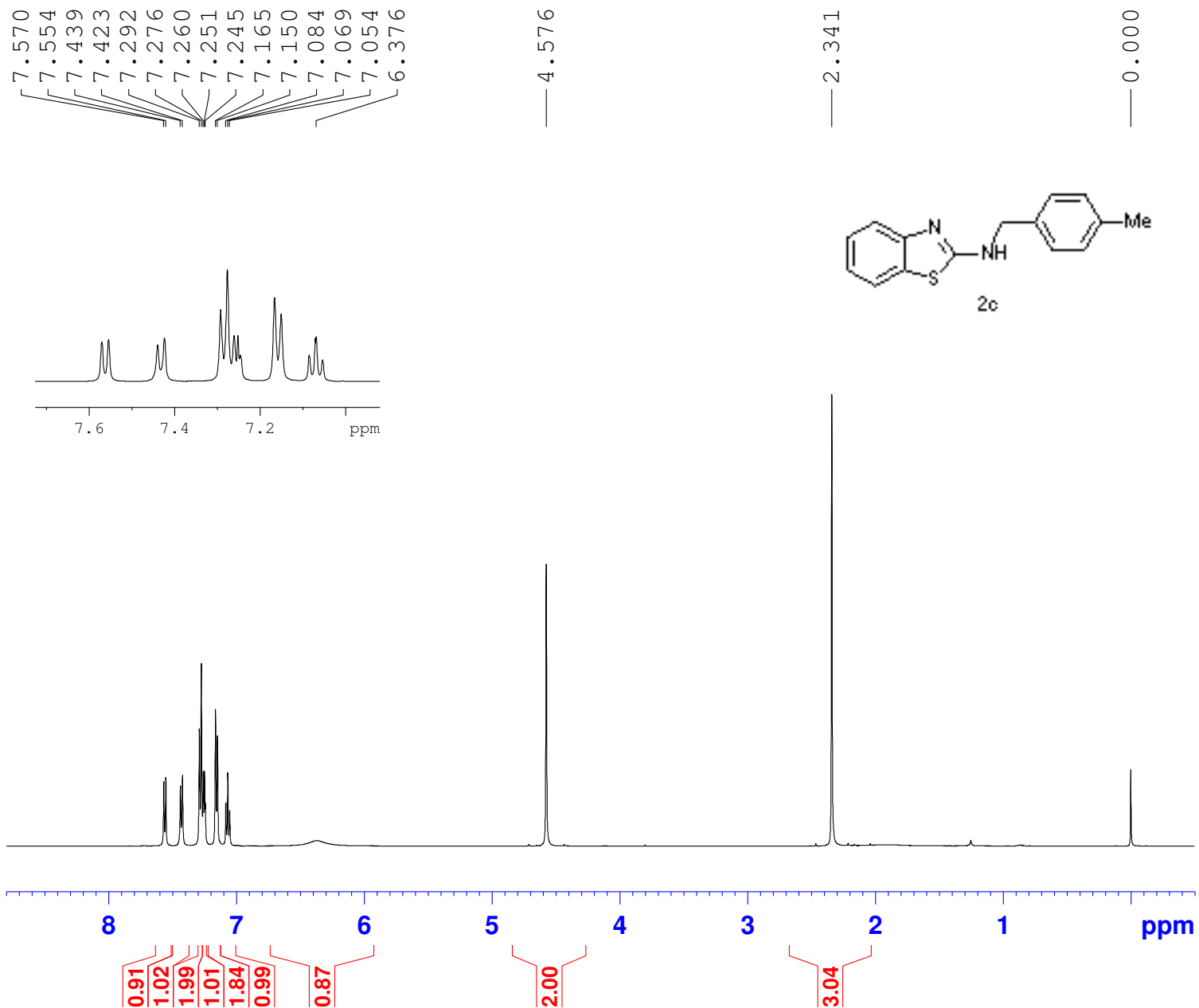
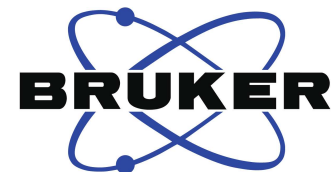
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Time 4.40
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-methylbenzyl)benzo[d]thiazol-2-amine
PROTON CDC13



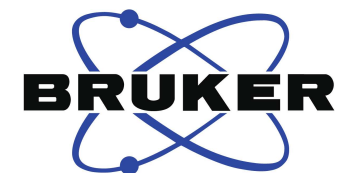
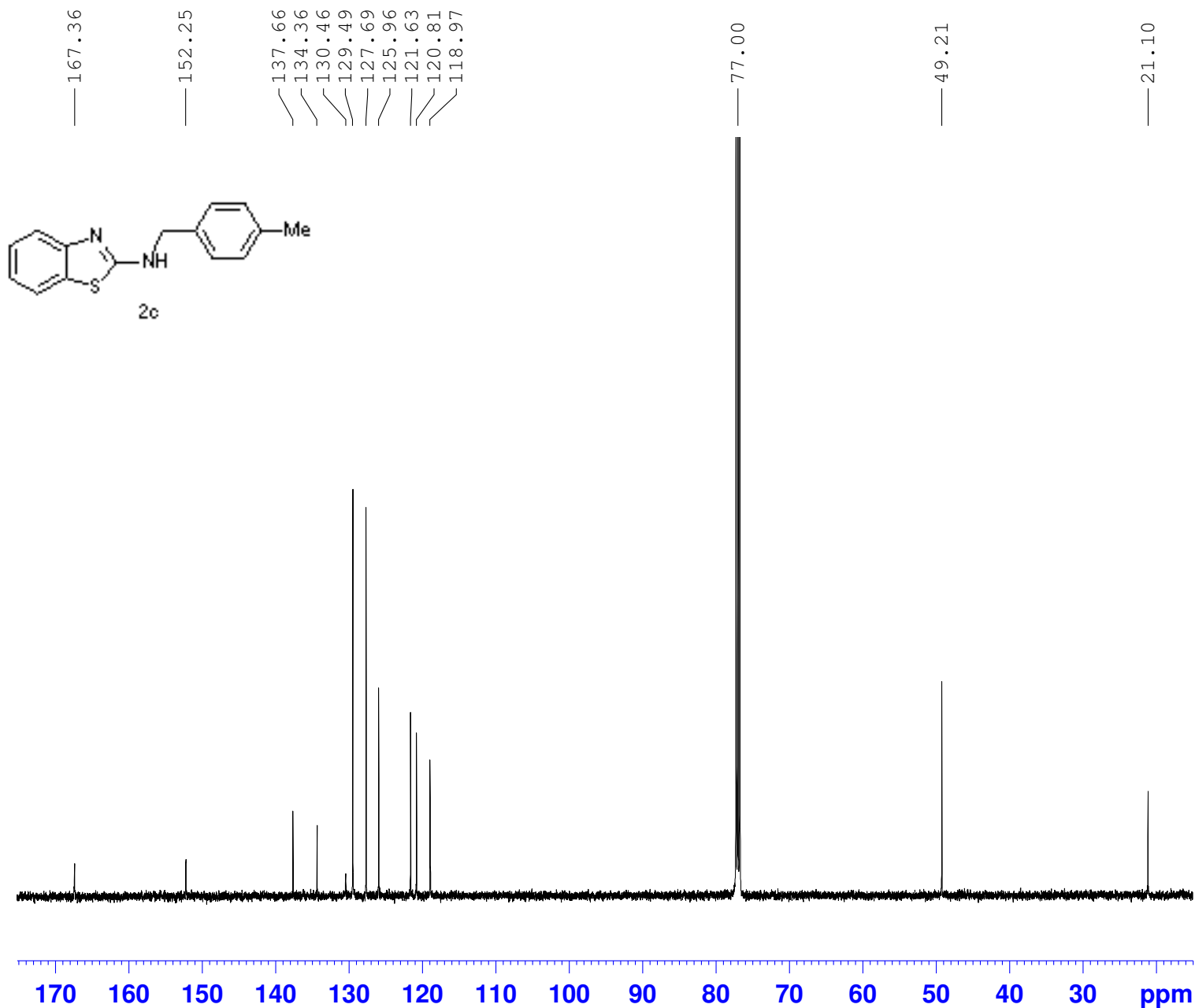
Current Data Parameters
NAME Lifeng-1H
EXPNO 99
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time 1.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 101
DW 48.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(4-methylbenzyl)benzo[d]thiazol-2-amine
C13CPD CDC13



Current Data Parameters
NAME Lifeng-1H
EXPNO 100
PROCNO 1

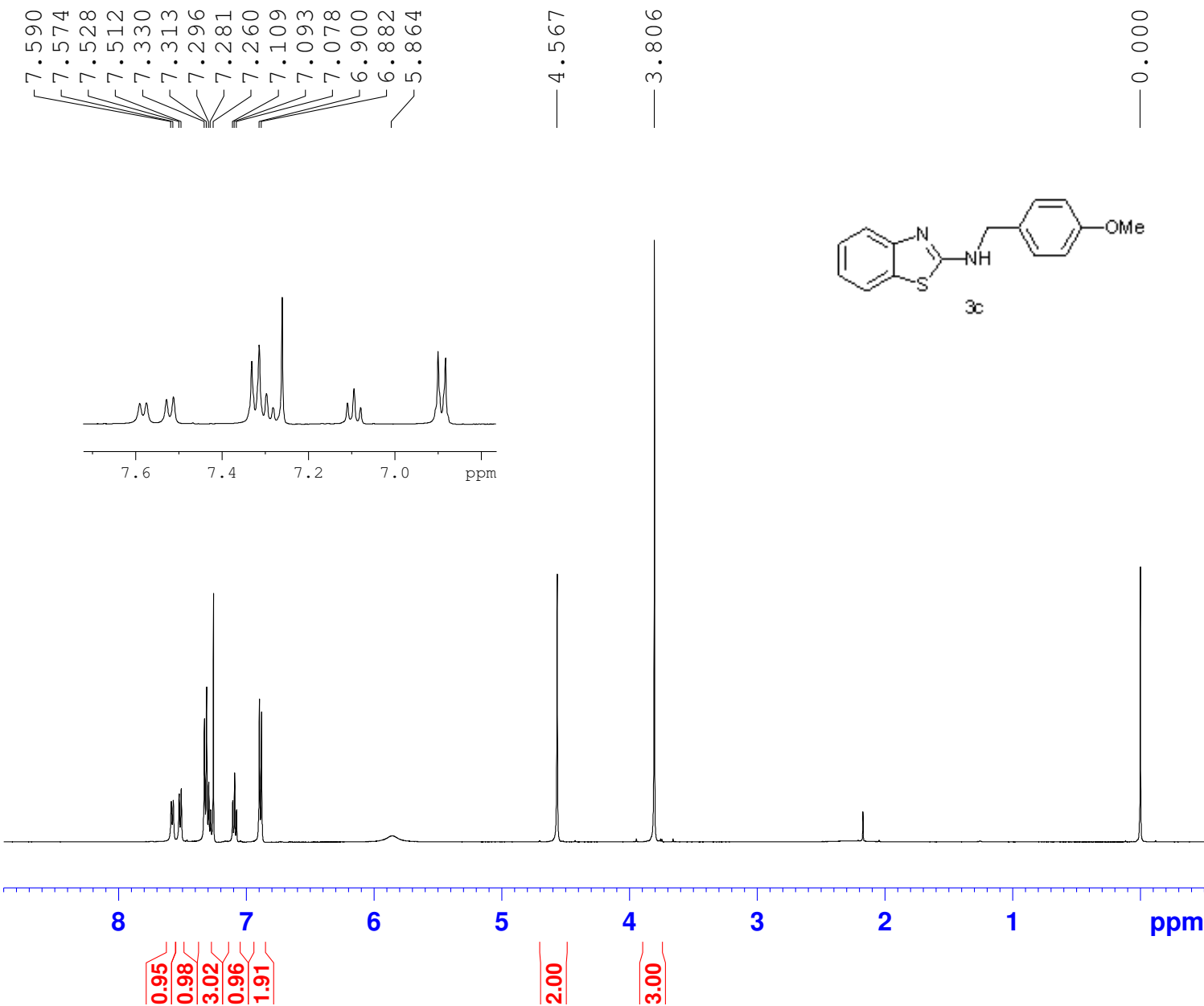
F2 - Acquisition Parameters
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Time 3.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7326440 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

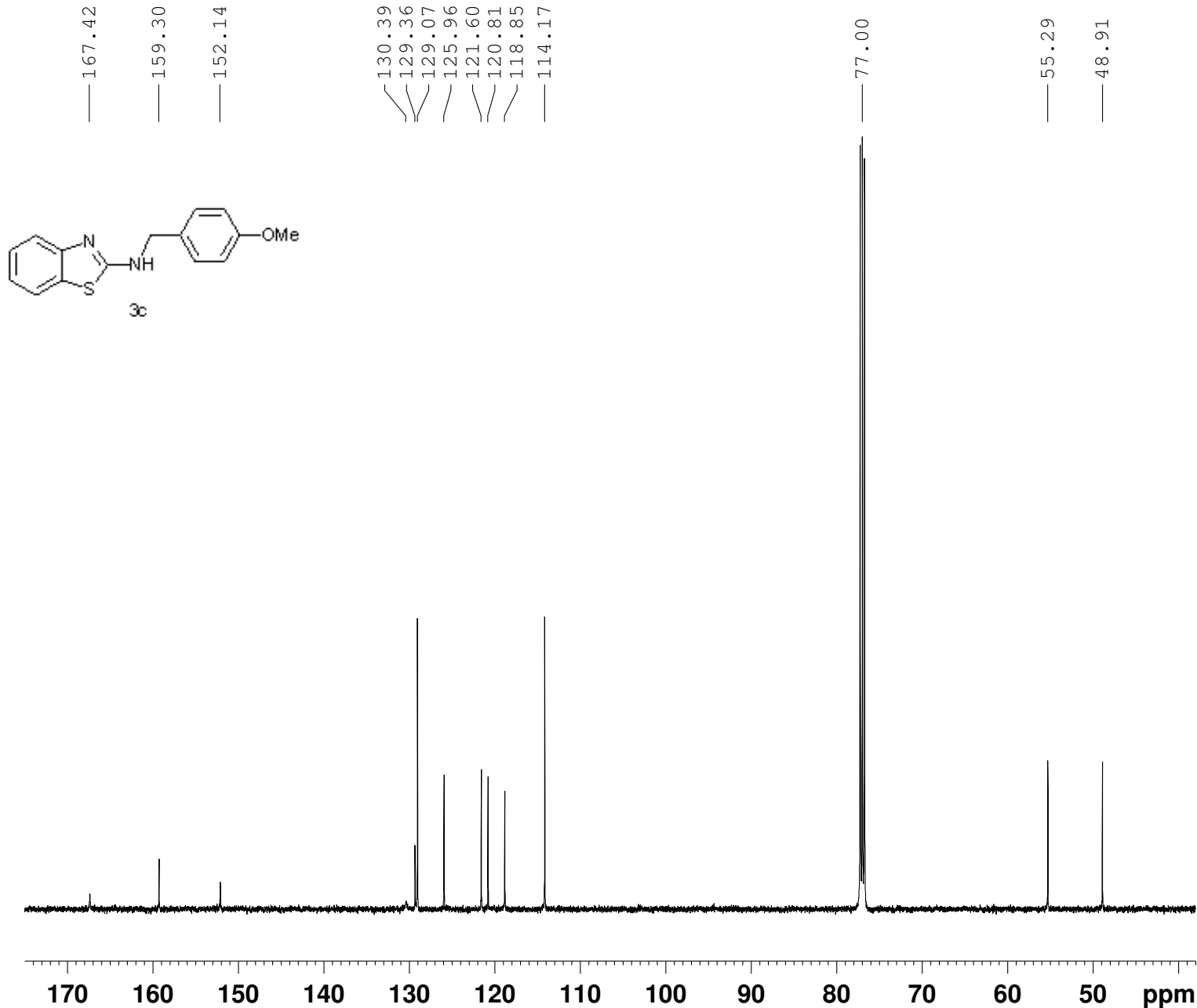
N-(4-methoxybenzyl)benzo[d]thiazol-2-amine
PROTON CDCL₃



NAME 600-700
EXPNO 100
PROCNO 1
Date_ 20110302
Time 13.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
SI 32768
SF 500.0300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(4-methoxybenzo[d]thiazol-2-amine)
C13CPD CDC13



Current Data Parameters
NAME Lifeng-13C
EXPNO 660
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110301
Time 13.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PLW1 125.86000061 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 16.96400070 W
PLW12 0.35054001 W
PLW13 0.22434001 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

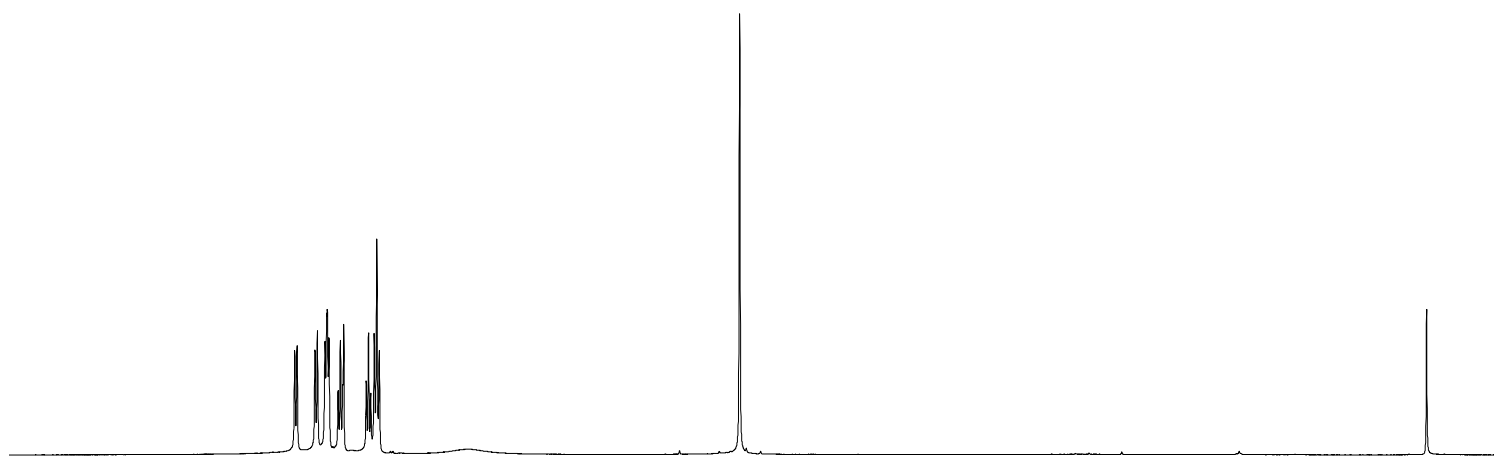
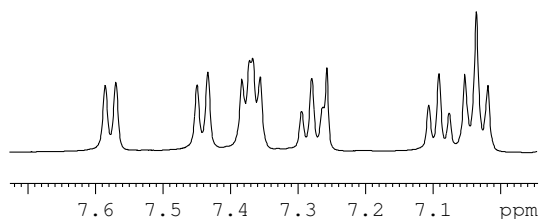
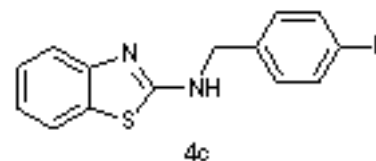
N-(4-fluorobenzyl)benzo[d]thiazol-2-amine
PROTON CDC13



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7.433
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7.371
7.366
7.355
7.294
7.279
7.263
7.256
7.106
7.090
7.075
7.052
7.035
7.018
6.435

4.603

0.000



9 8 7 6 5 4 3 2 1 ppm

1.00
1.09
1.92
1.41
1.03
1.77
0.87

2.00

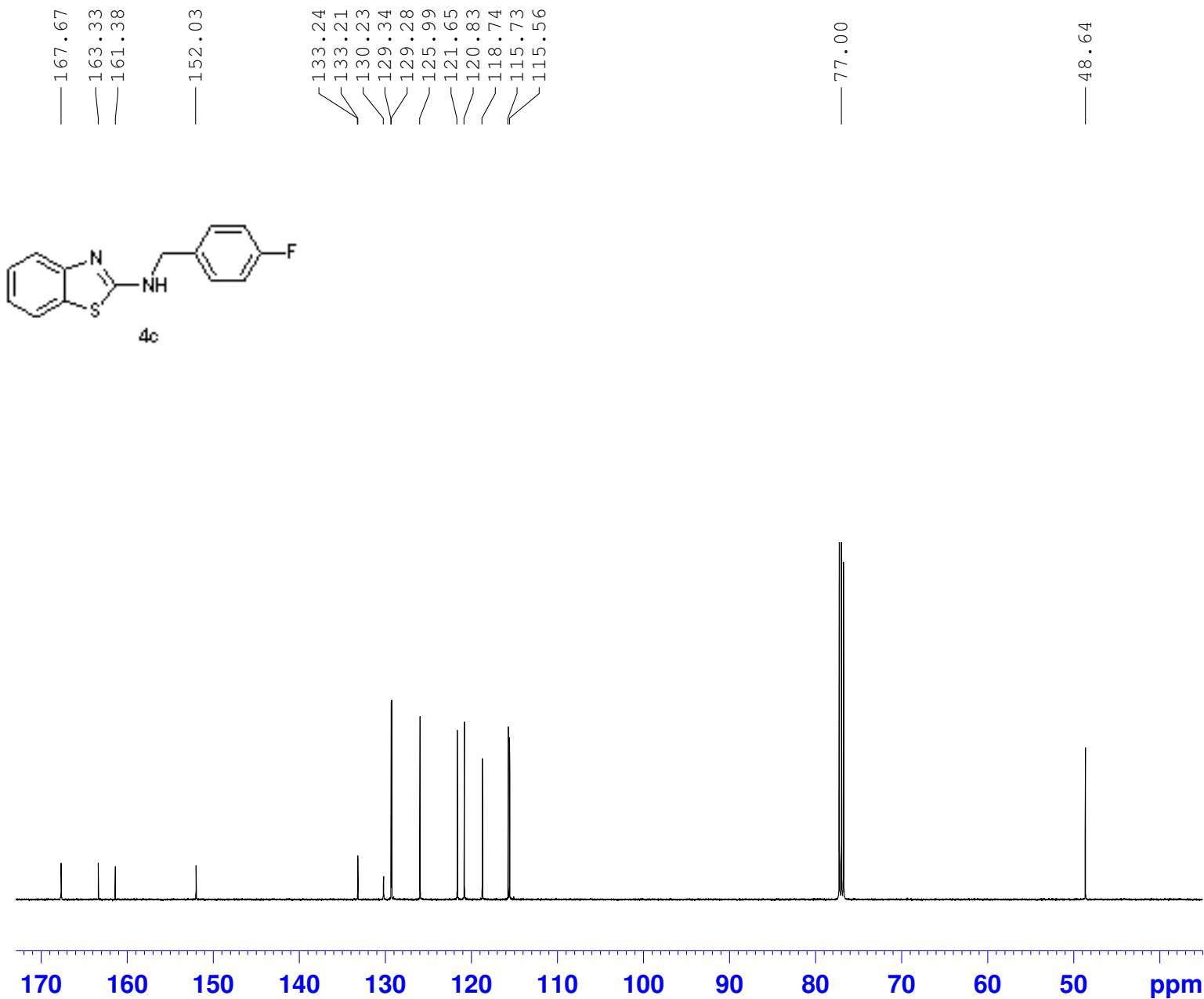
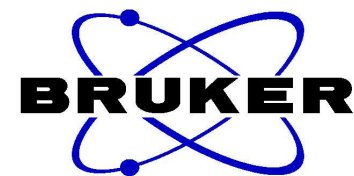
Current Data Parameters
NAME Lifeng-1H
EXPNO 584
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101121
Time 0.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

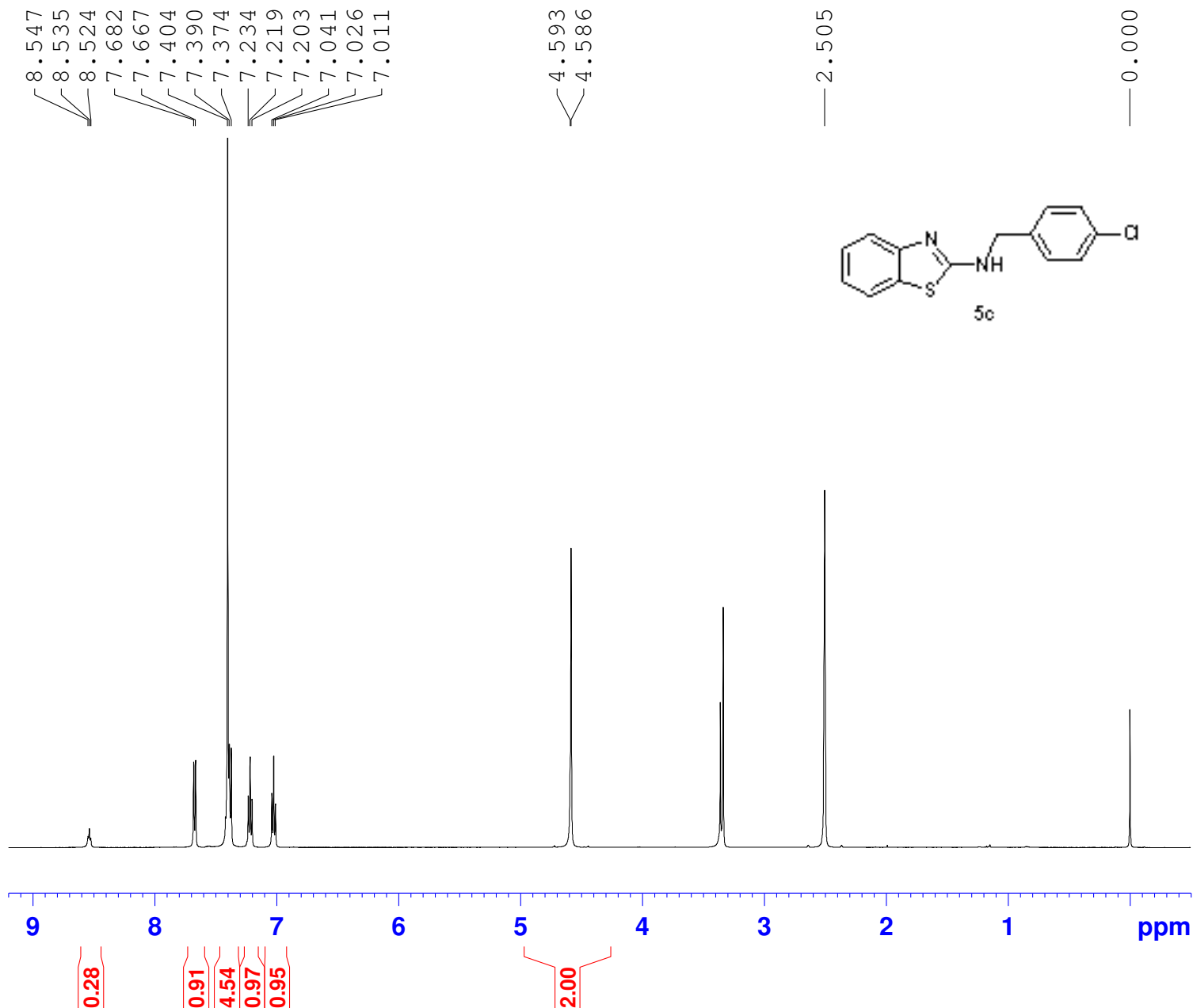
N-(4-fluorobenzyl)benzo[d]thiazol-2-amine
C13CPD CDC13



NAME 3
EXPNO 610
PROCNO 1
Date_ 20101229
Time 20.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1868
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
SI 32768
SF 125.7320527 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-chlorobenzyl)benzo[d]thiazol-2-amine
PROTON DMSO-d₆



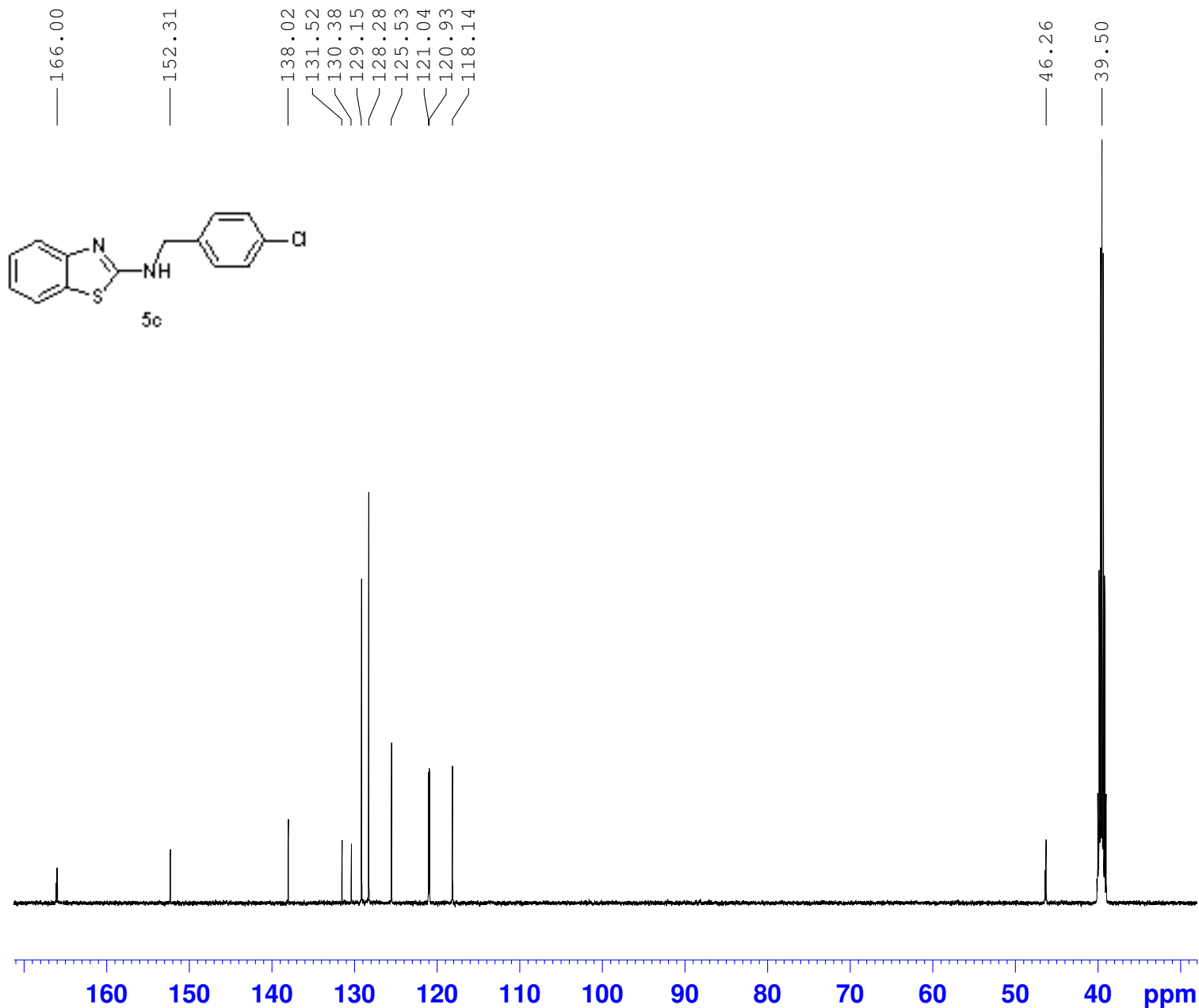
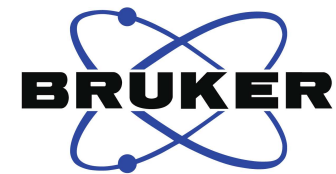
Current Data Parameters
NAME Lifeng-1H
EXPNO 101
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time 4.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0323755 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(4-chlorobenzyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6

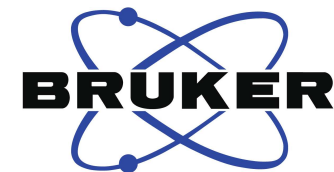
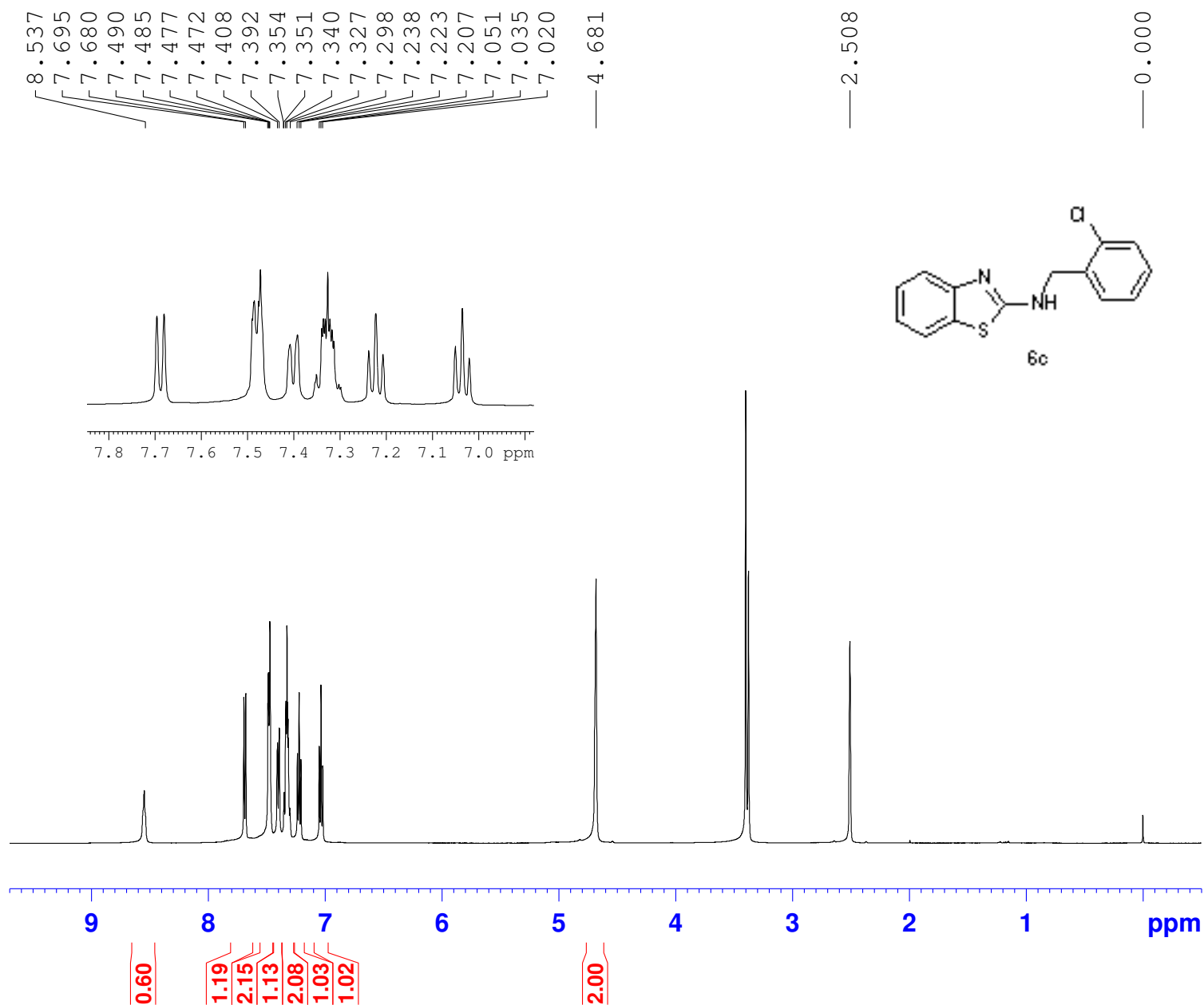


Current Data Parameters
NAME Lifeng-1H
EXPNO 102
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
NUC1 13C
P1 9.60 usec
PLW1 -1.00000000 W
SFO1 125.7452168 MHz
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 -1.00000000 W
PLW12 -1.00000000 W
PLW13 -1.00000000 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(2-chlorobenzyl)benzo[d]thiazol-2-amine
PROTON DMSO-d6



Current Data Parameters
NAME Lifeng-1H
EXPNO 107
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time 16.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
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RG 50.8
DW 48.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1

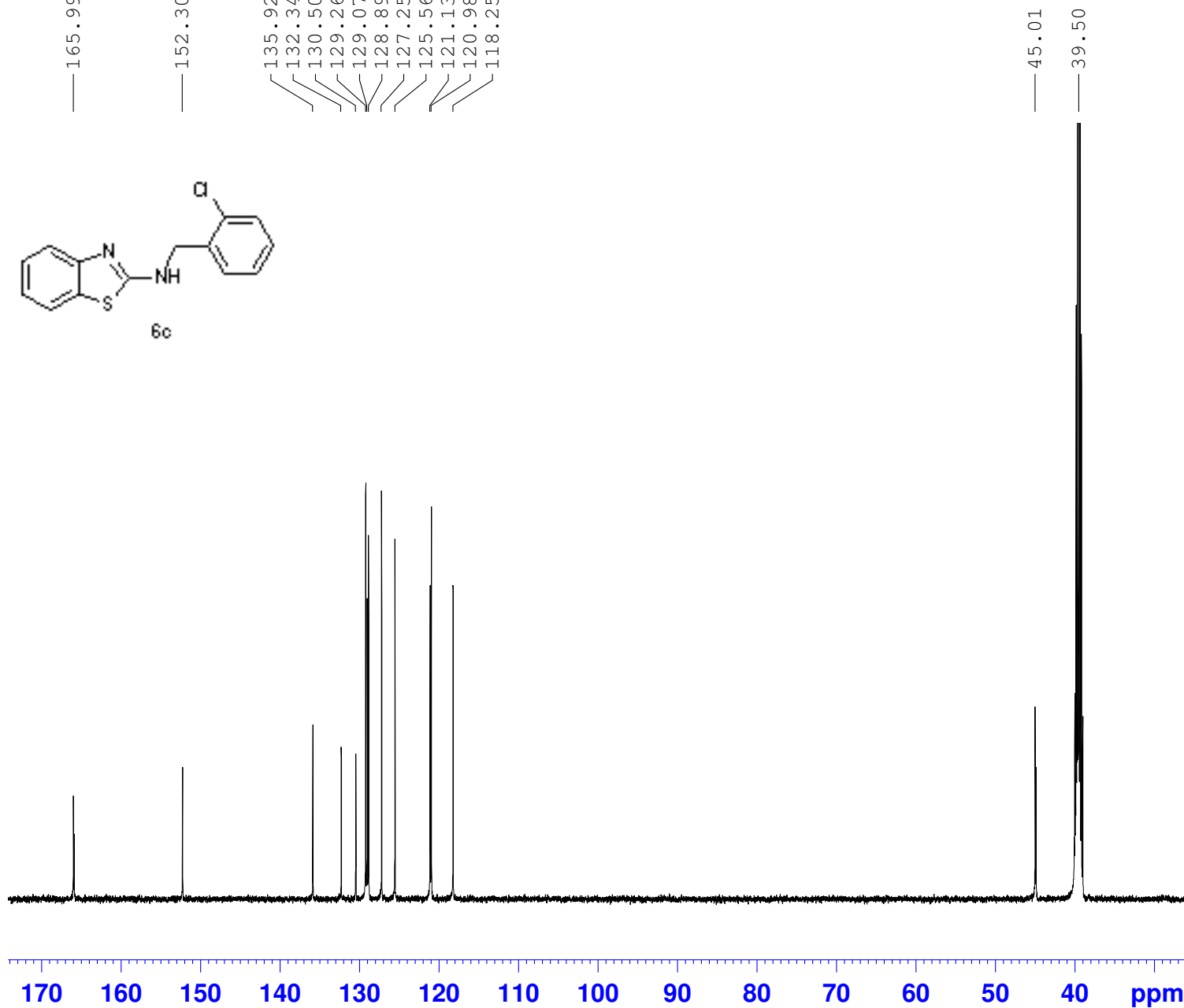
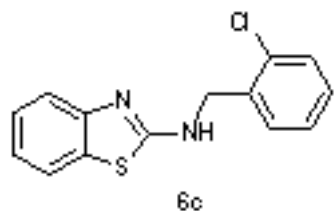
===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0299986 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(2-chlorobenzyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



165.99
152.30
135.92
132.34
130.50
129.26
129.07
128.89
127.25
125.56
121.13
120.98
118.25



Current Data Parameters
NAME Lifeng-1H
EXPNO 109
PROCNO 1

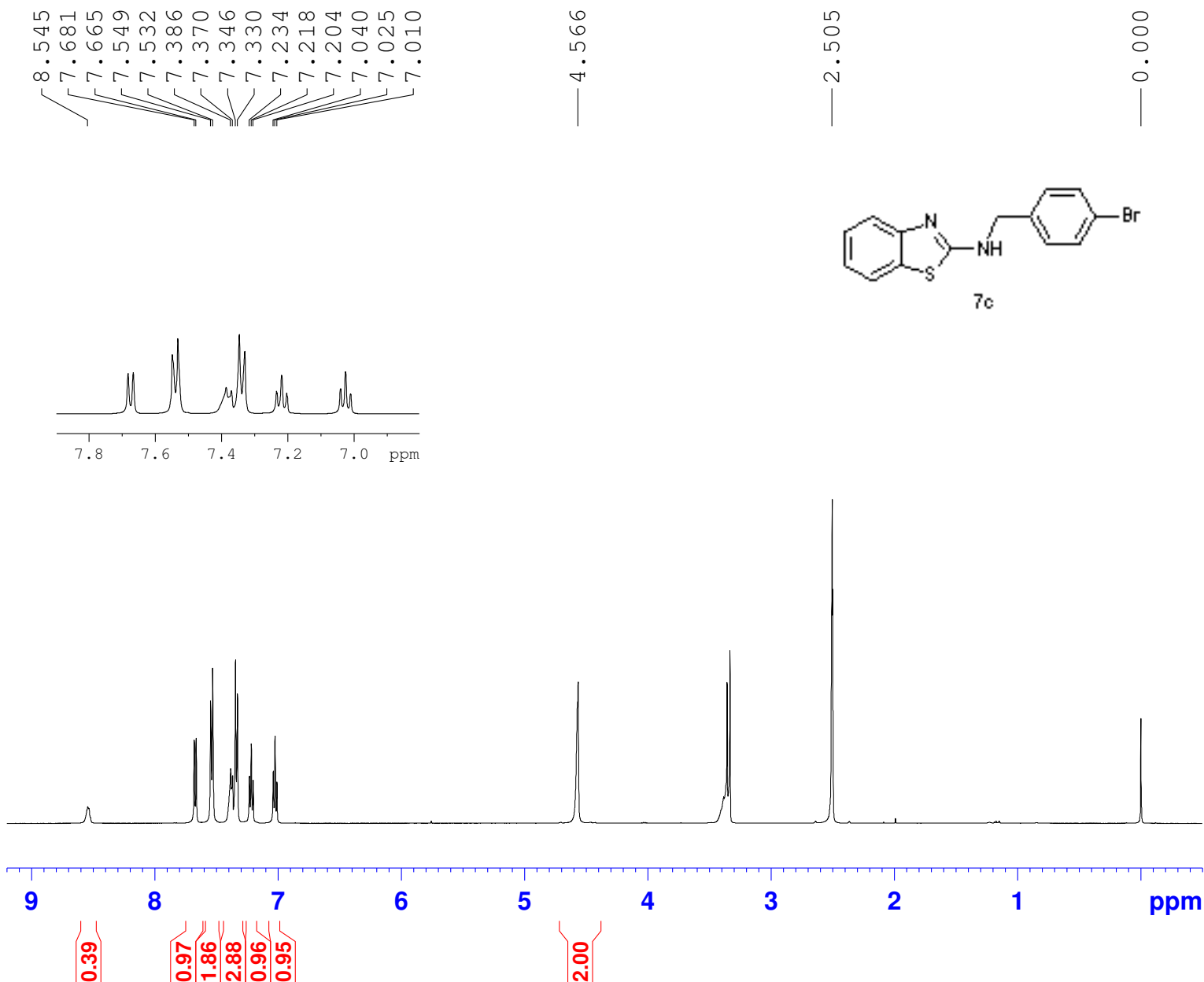
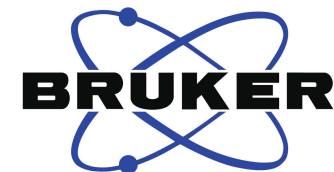
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Date_ 20100708
Time 17.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327039 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-bromobenzyl)benzo[d]thiazol-2-amine
PROTON DMSO-d₆



Current Data Parameters
NAME Lifeng-1H
EXPNO 103
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100708
Time 5.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

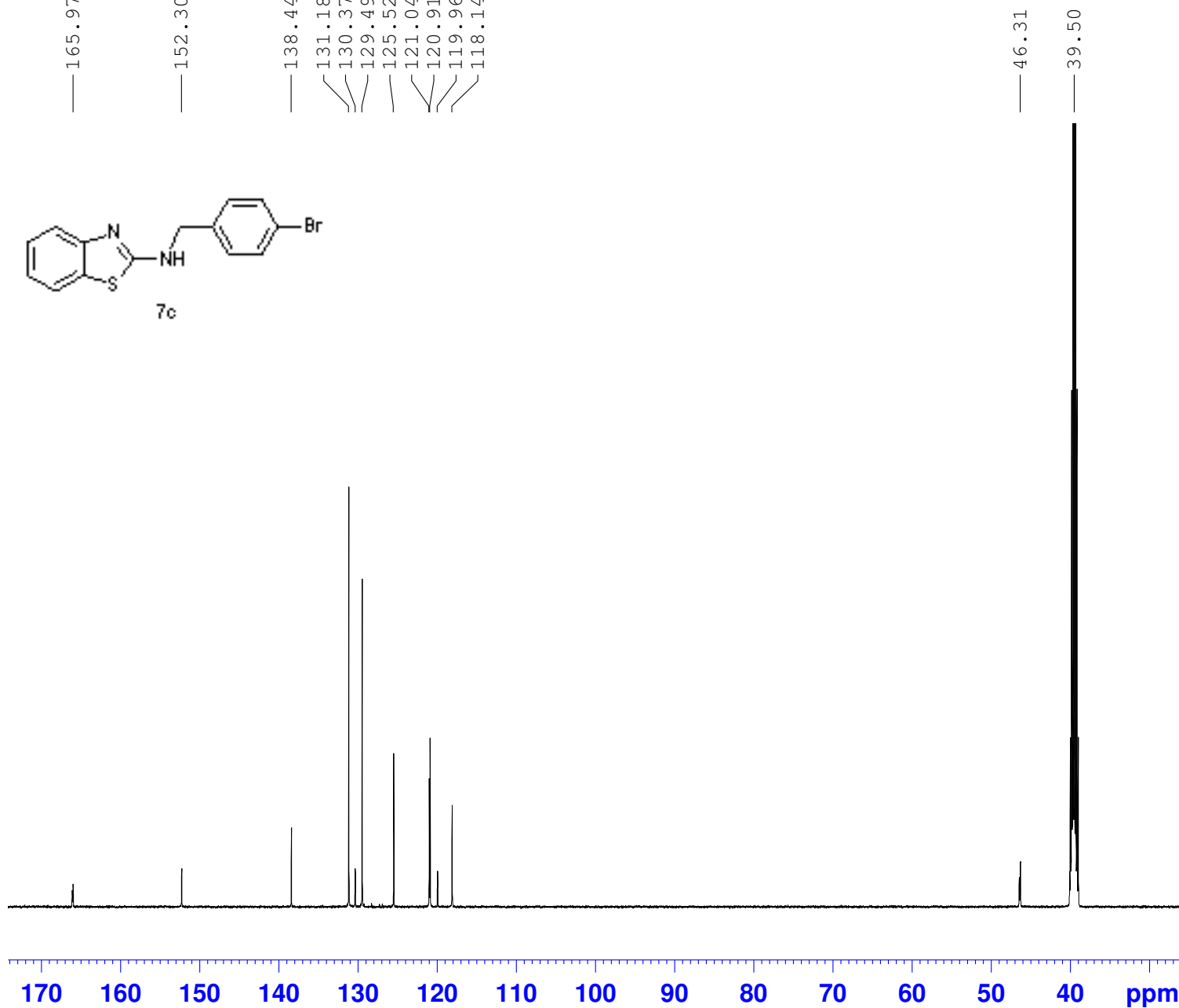
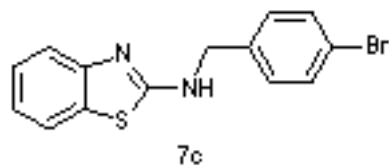
==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SF01 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300006 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(4-bromobenzyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



165.97
152.30
138.44
131.18
130.37
129.49
125.52
121.04
120.91
119.96
118.14



Current Data Parameters
NAME Lifeng-1H
EXPNO 104
PROCNO 1

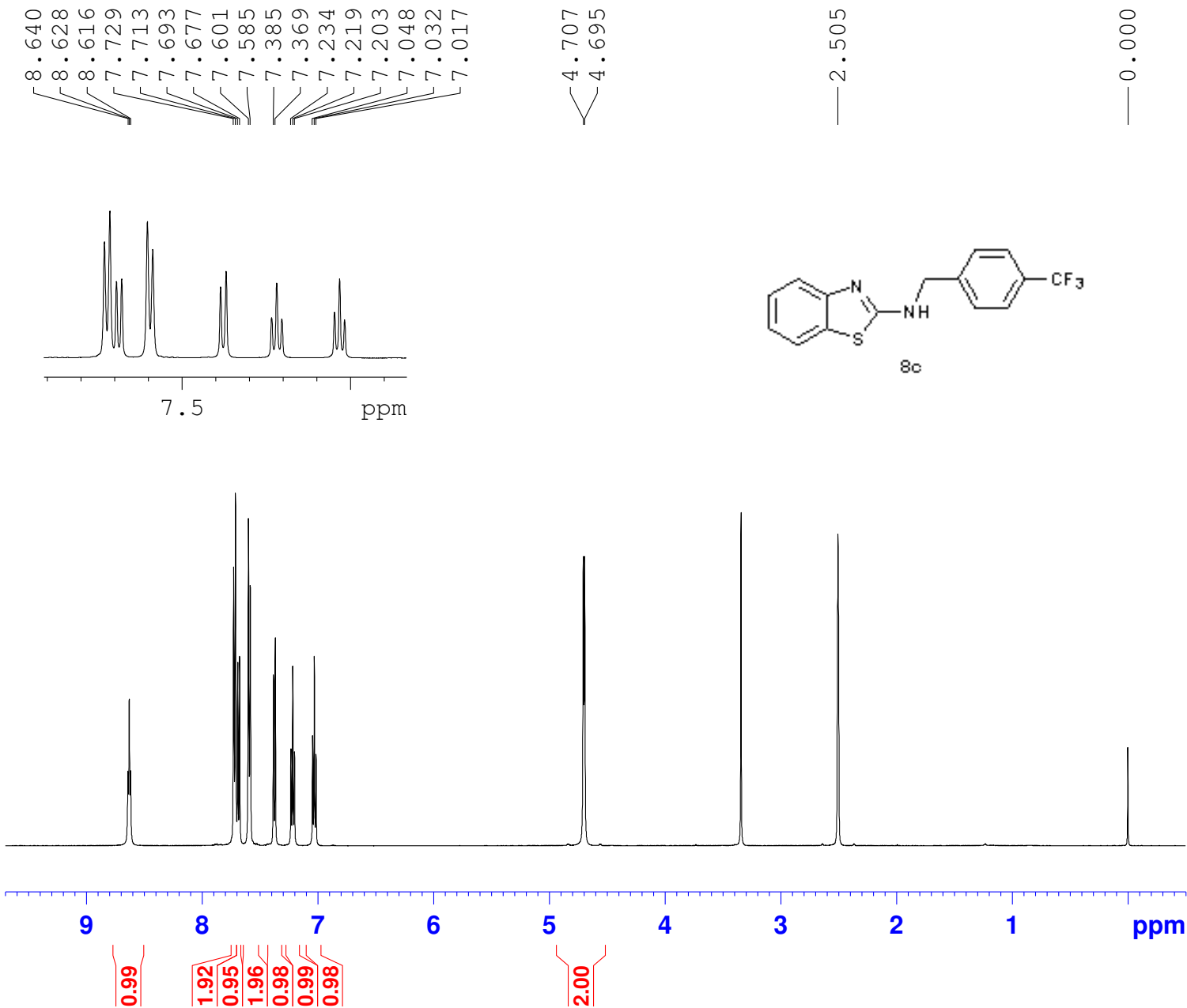
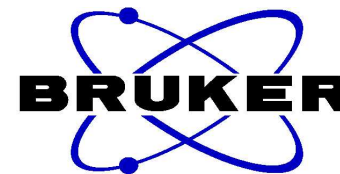
F2 - Acquisition Parameters
Date_ 20100708
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 6144
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327104 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

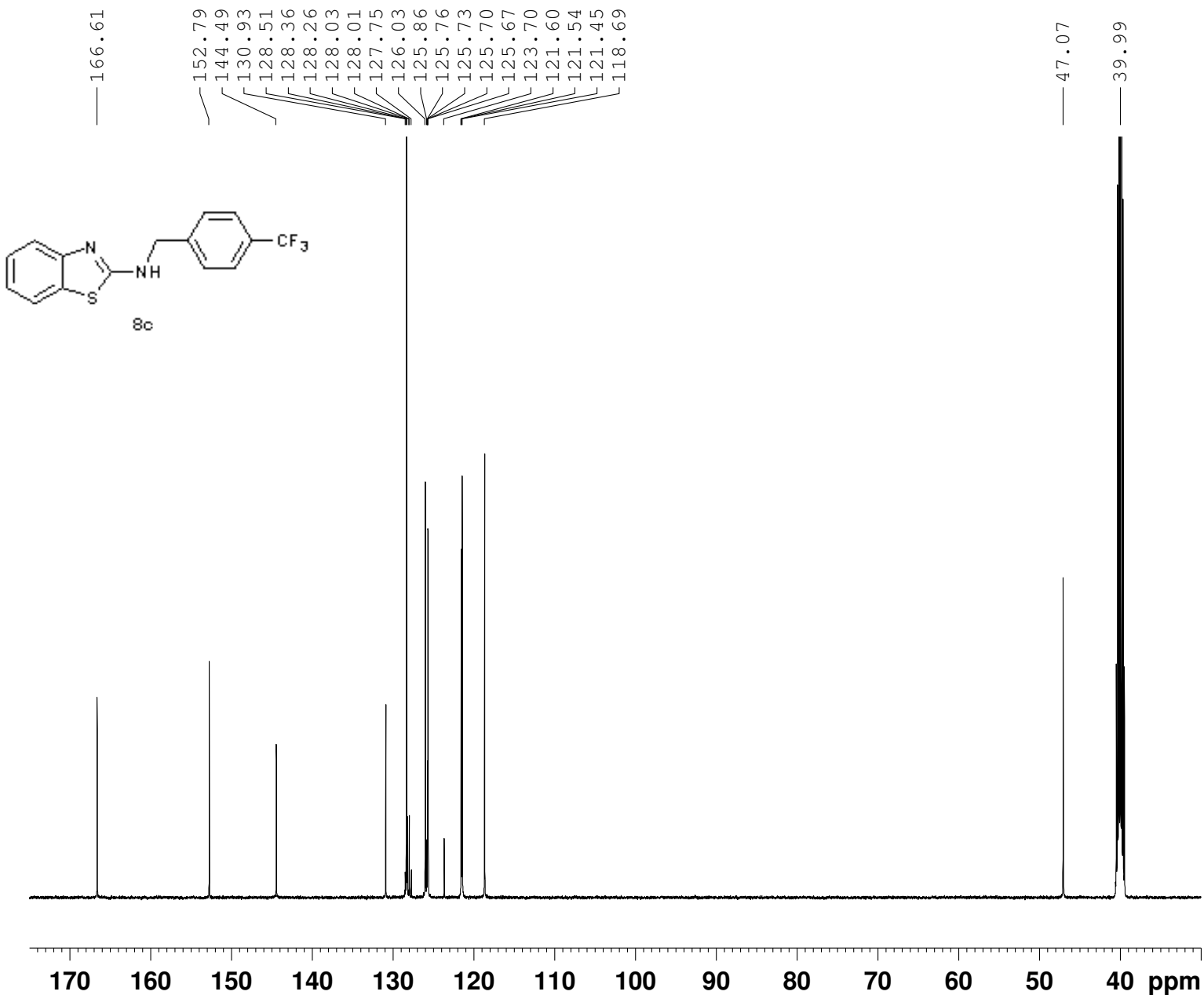
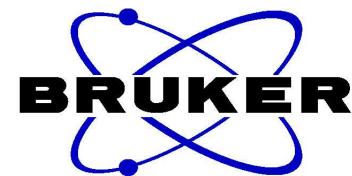
N-(4-(trifluoromethyl)benyl)benzo[d]thiazol-2-amine
PROTON DMSO-d₆



NAME Shx-1
EXPNO 570
PROCNO 1
Date_ 20101121
Time 1.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz
SI 32768
SF 500.0300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-(4-(trifluoromethyl)benzyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6

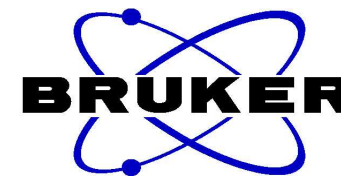


NAME Shx-1
EXPNO 577
PROCNO 1
Date_ 20101122
Time 4.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4287
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz
SI 32768
SF 125.7326450 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(4-trifluoromethoxybenzyl)benzo[d]thiazol-2-amine
PROTON DMSO-d6

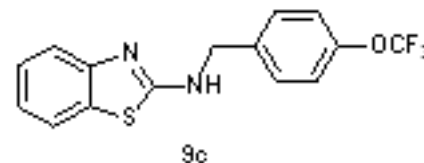


8.555
8.543
7.686
7.671
7.512
7.495
7.393
7.377
7.360
7.343
7.235
7.219
7.204
7.043
7.028
7.013

4.634
4.622

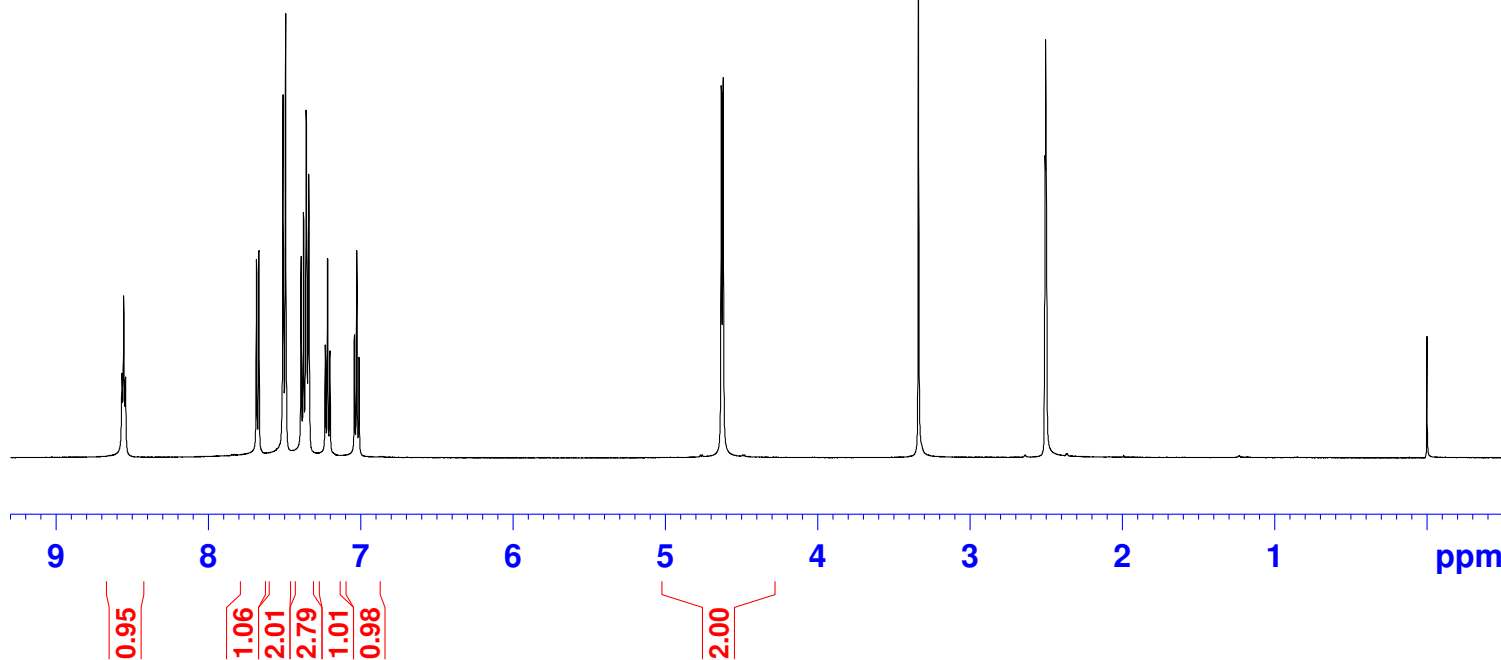
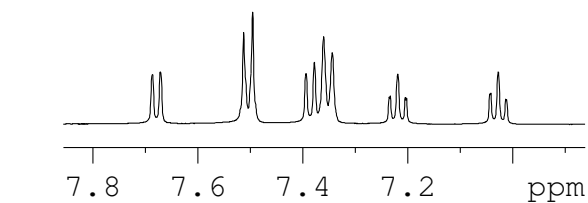
2.504

0.000

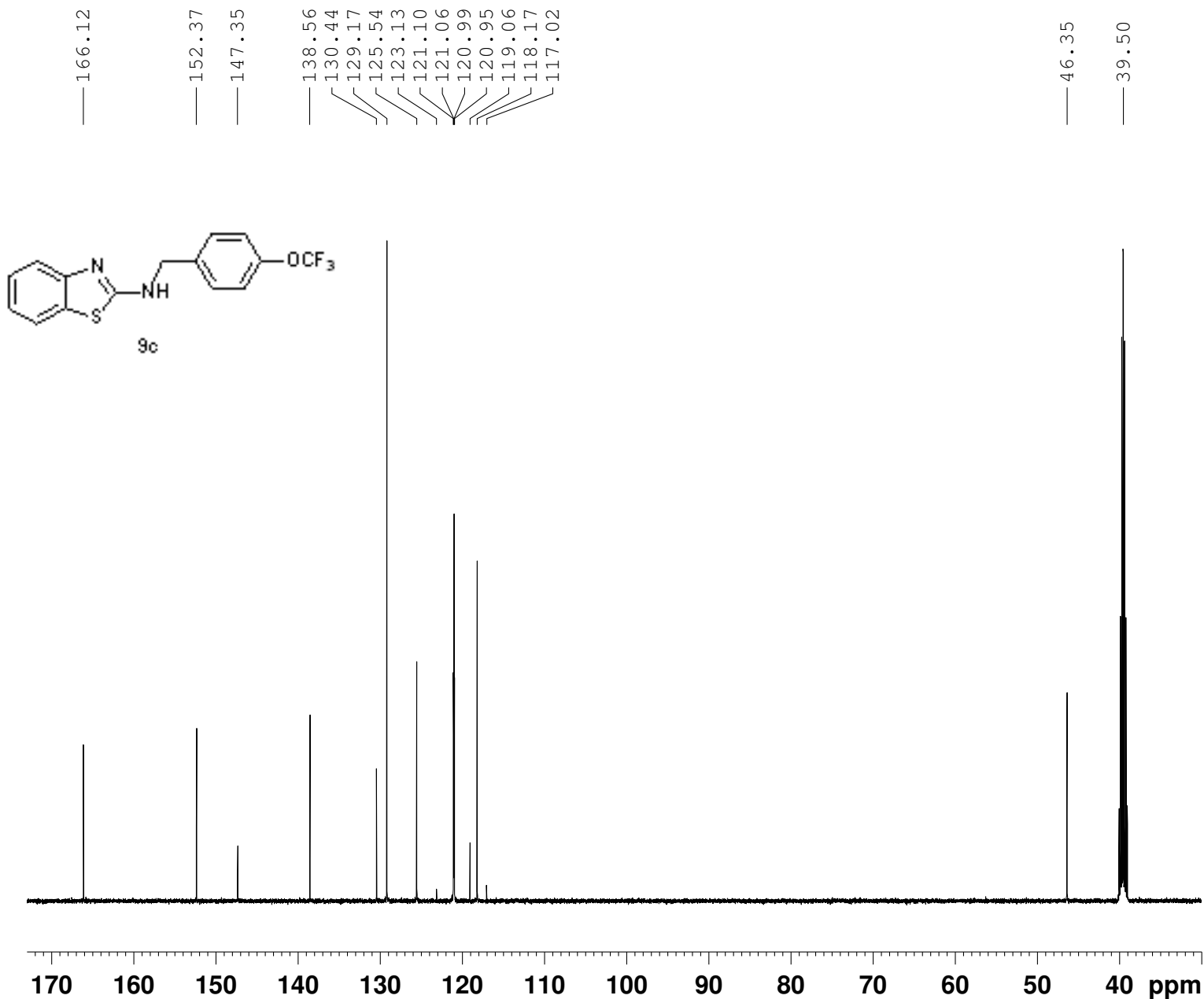
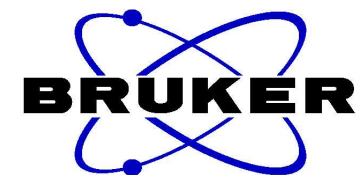


NAME Shx-1
EXPNO 580
PROCNO 1
Date_ 20101122
Time 5.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz
SI 32768
SF 500.0300008 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



N-(4-trifluoromethoxybenzyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



NAME Shx-1
EXPNO 572
PROCNO 1
Date_ 20101121
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz
SI 32768
SF 125.7327054 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

N-(3,4-dimethoxybenzyl)benzo[d]thiazol-2-amine
PROTON CDCl₃

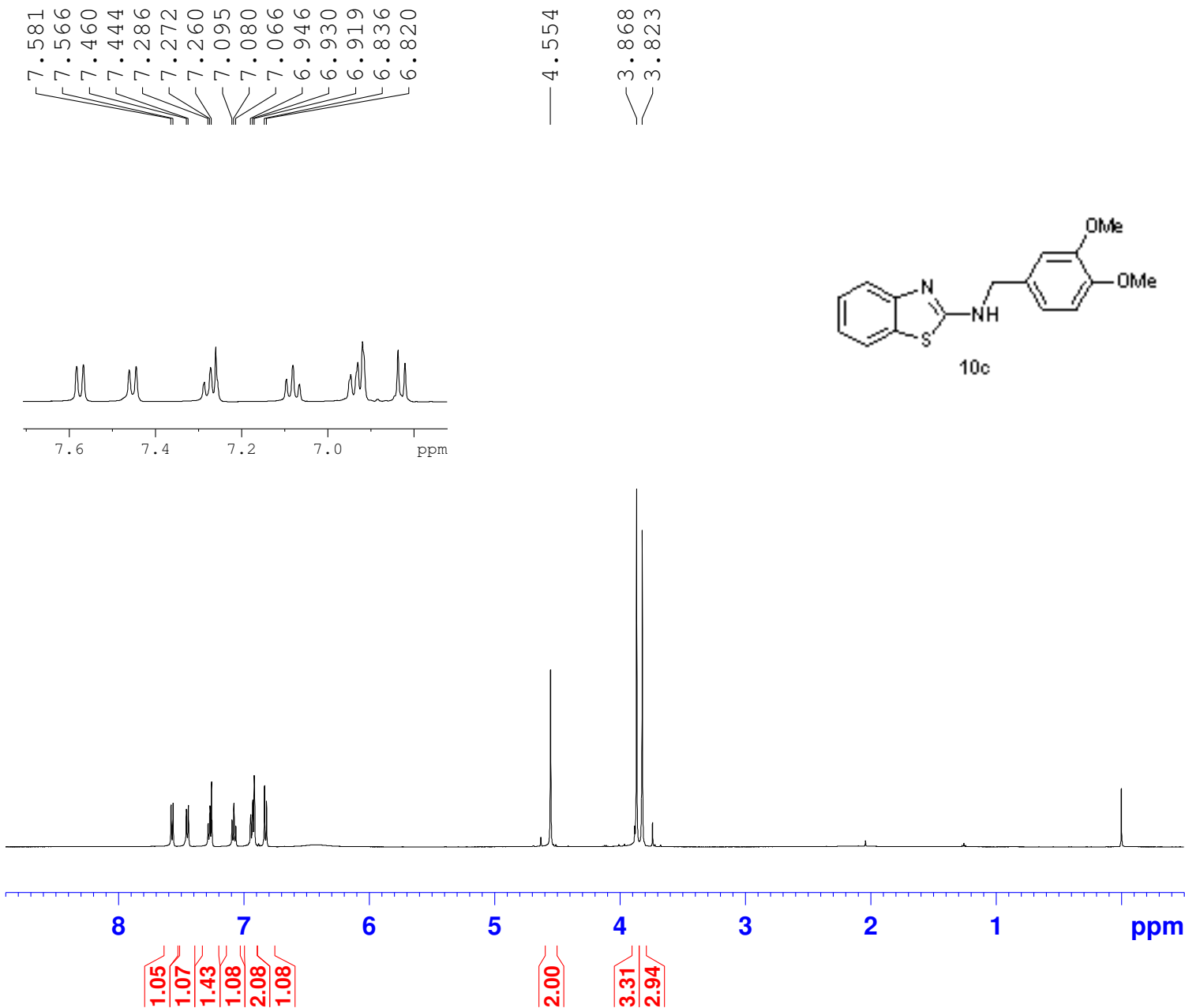
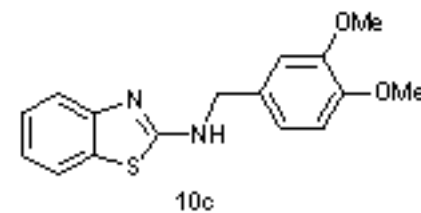


Current Data Parameters
NAME Lifeng-1H
EXPNO 115
PROCNO 1

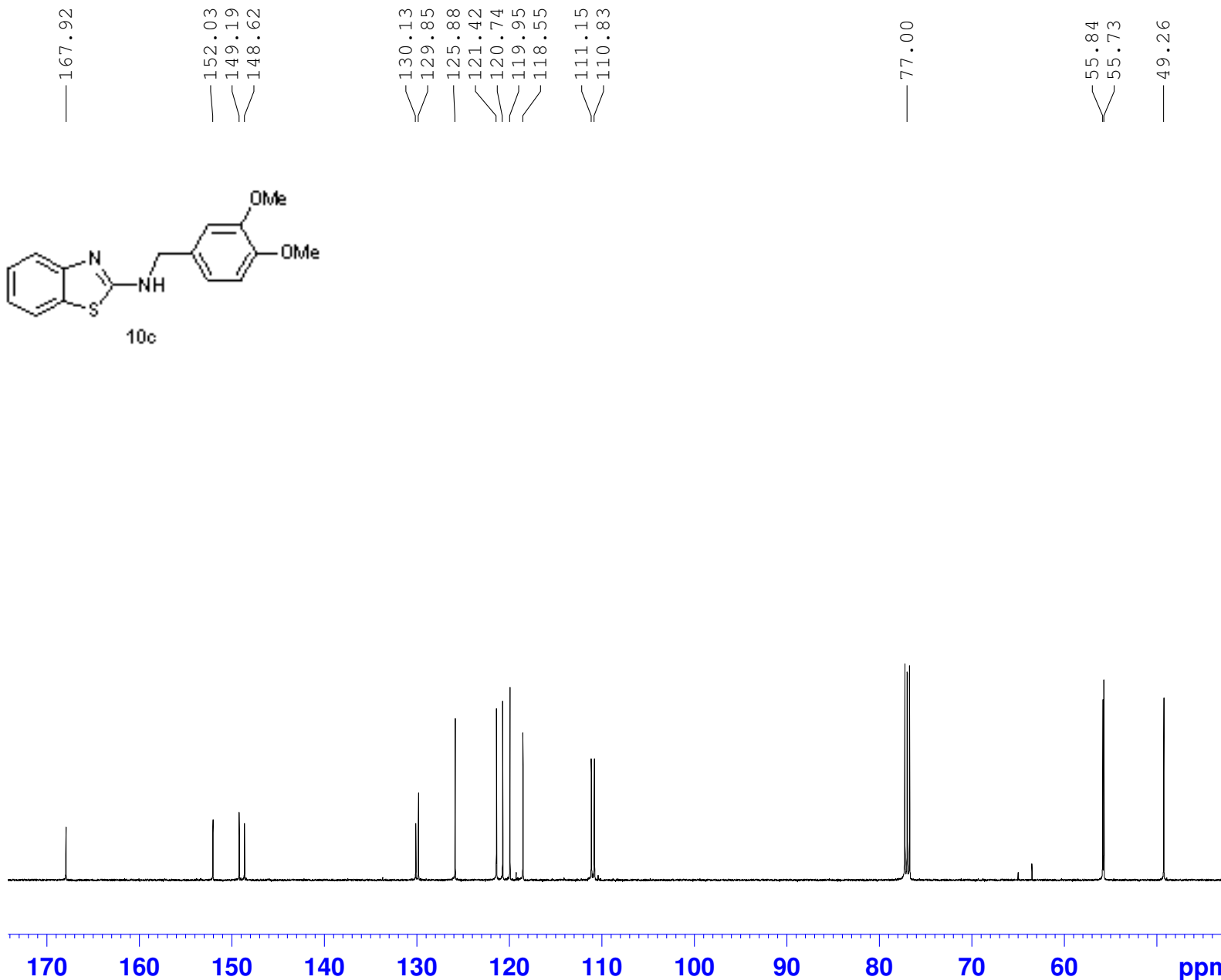
F2 - Acquisition Parameters
Date_ 20100808
Time 0.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 36
DW 48.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



N-(3,4-dimethoxybenzyl)benzo[d]thiazol-2-amine
C13CPD CDC13



Current Data Parameters
NAME Lifeng-1H
EXPNO 116
PROCNO 1

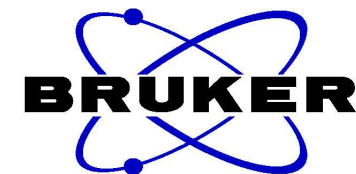
F2 - Acquisition Parameters
Date_ 20100808
Time 16.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

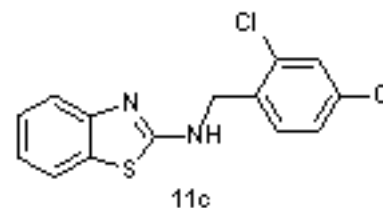
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7326564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(2,4-dichlorobenzyl)benzo[d]thiazol-2-amine
PROTON CDC13

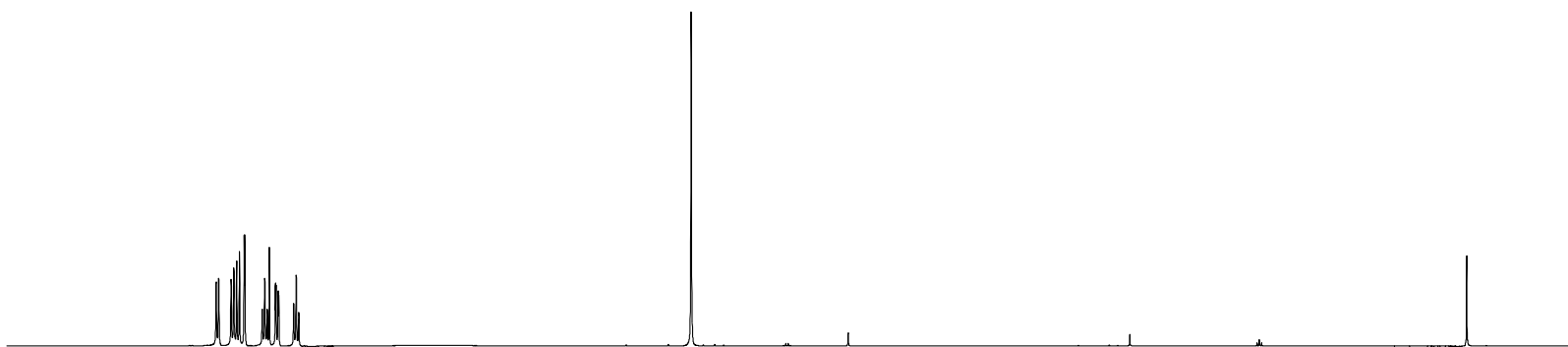
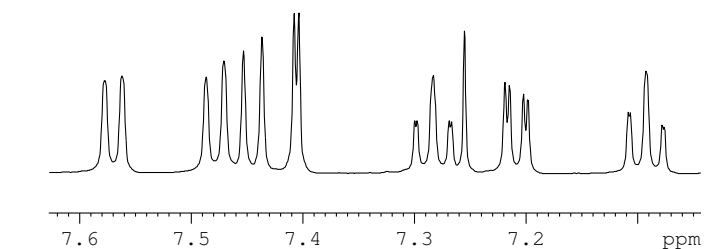


7.471
7.453
7.436
7.408
7.403
7.298
7.283
7.268
7.255
7.219
7.215
7.202
7.198
7.107
7.093
7.077
6.272
— 4.699
— 0.000



NAME Shx-1
EXPNO 131
PROCNO 1
Date_ 20100804
Time 1.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz
SI 32768
SF 500.0300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

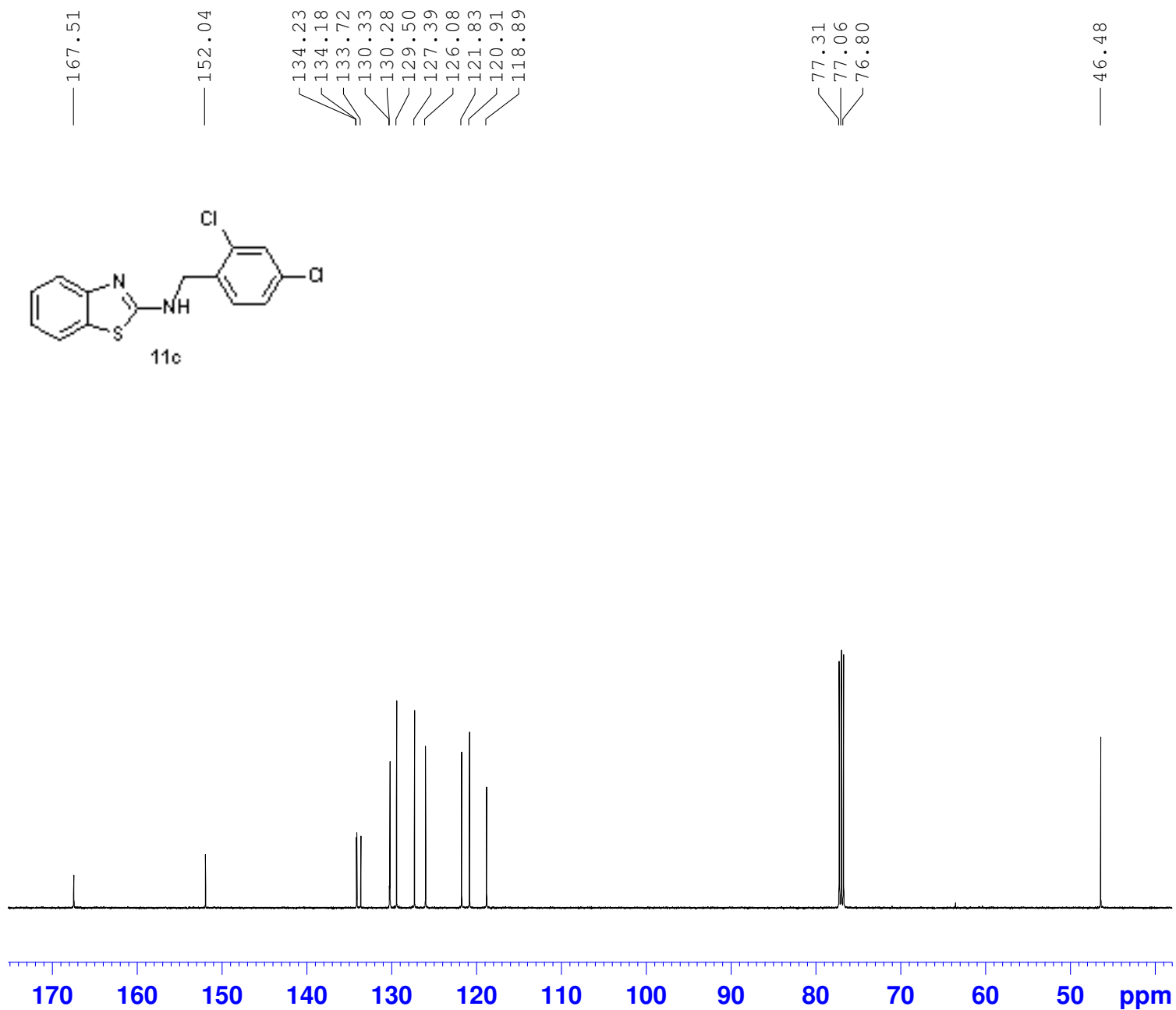
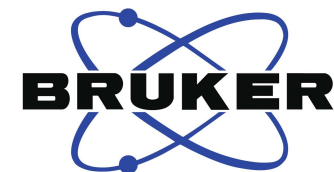


0.98
1.01
0.97
0.89
1.01
0.93
0.97

2.00

8 7 6 5 4 3 2 1 0 ppm

N-(2,4-dichlorobenzyl)benzo[d]thiazol-2-amine
C13CPD CDC13



Current Data Parameters
NAME Lifeng-1H
EXPNO 161
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100808
Time 15.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

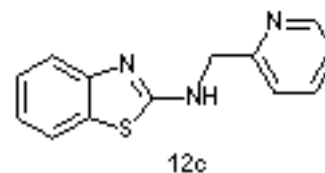
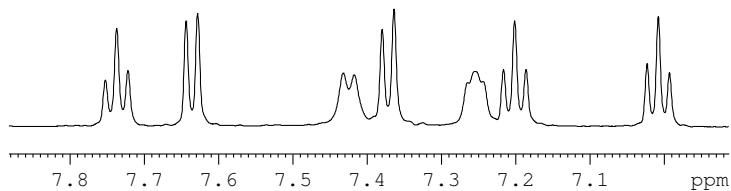
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7326512 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-(pyridin-2-ylmethyl)benzo[d]thiazol-2-amine
PROTON DMSO-d₆, at 353 K

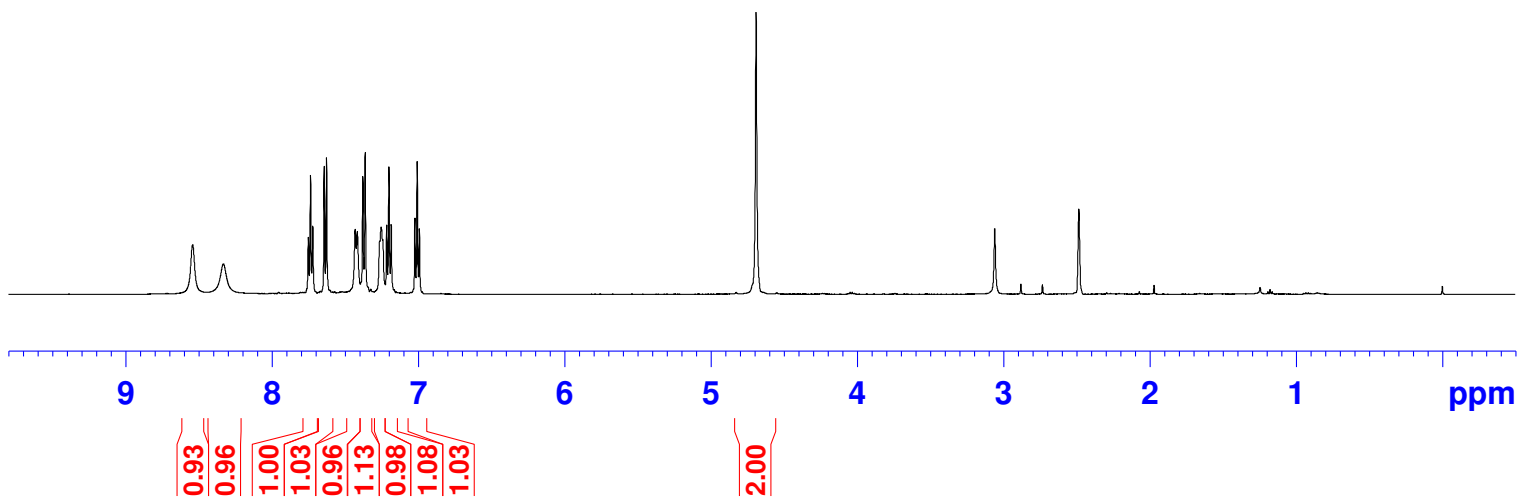


8.540
8.330
7.752
7.737
7.722
7.644
7.628
7.432
7.417
7.380
7.364
7.265
7.254
7.243
7.216
7.201
7.186
7.024
7.008
6.993
— 4.691
— 2.485
— 0.000

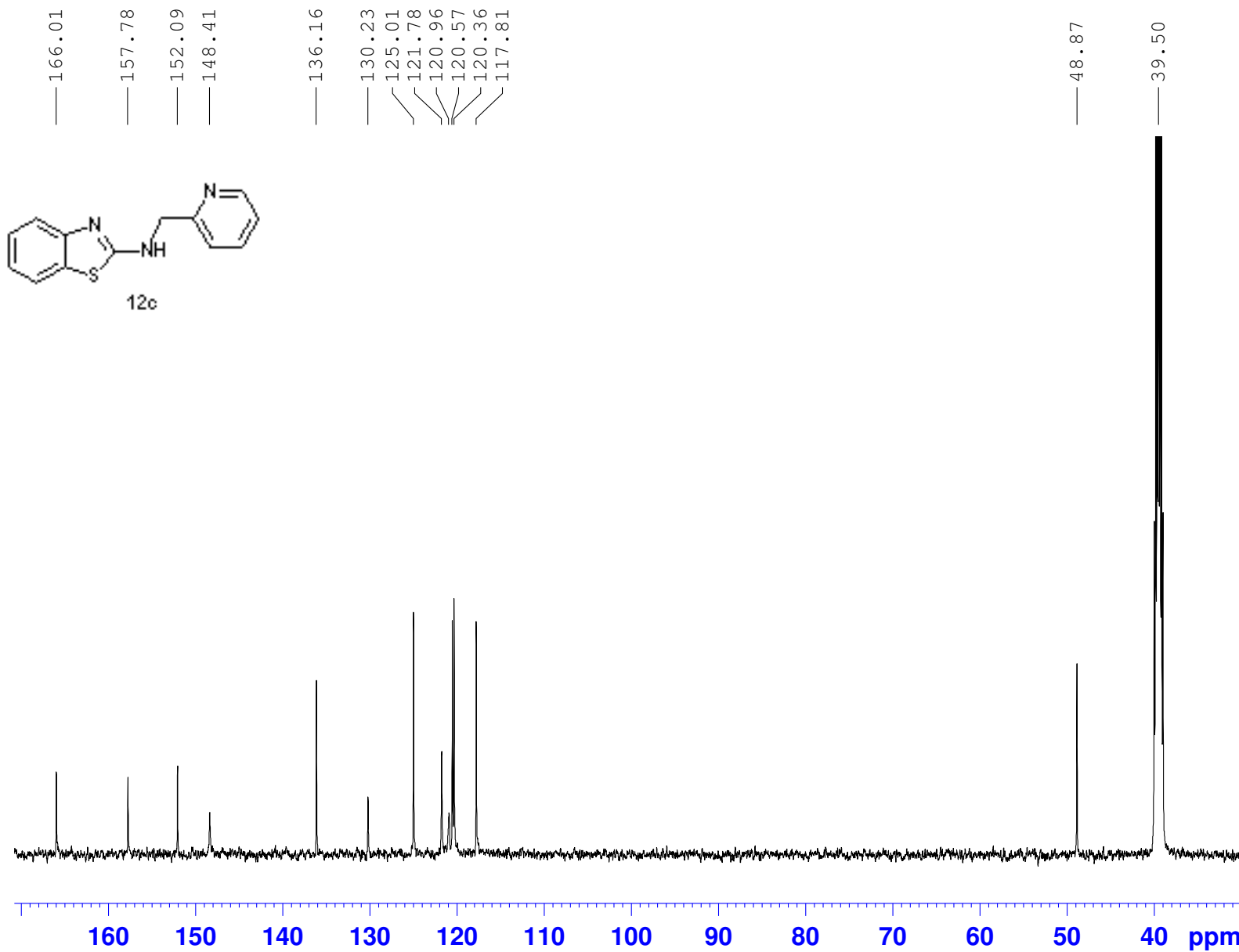
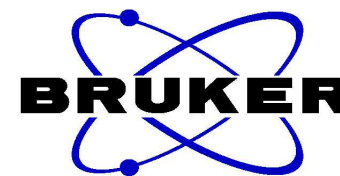


```
NAME          test
EXPNO         3
PROCNO       1
Date_        20110104
Time         17.10
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      DMSO
NS           8
DS           2
SWH          8000.000 Hz
FIDRES       0.122070 Hz
AQ           4.0960498 sec
RG           90.5
DW           62.500 usec
DE           9.46 usec
TE           353.0 K
D1           1.00000000 sec
```

```
===== CHANNEL f1 =====
NUC1          1H
P1            11.50 usec
SI            32768
SF            500.0300109 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
```



N-(pyridin-2-ylmethyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6 at 353 K



N-(naphthalen-1-ylmethyl)benzo[d]thiazol-2-amine
PROTON DMSO-d6

8.549
8.538
8.143
8.127
7.984
7.968
7.893
7.877
7.685
7.669
7.602
7.589
7.575
7.563
7.557
7.543
7.508
7.492
7.477
7.422
7.406
7.243
7.228
7.212
7.044
7.029
7.014
5.075
5.064

2.502

0.000



Current Data Parameters
NAME Lifeng-1H
EXPNO 582
PROCNO 1

F2 - Acquisition Parameters

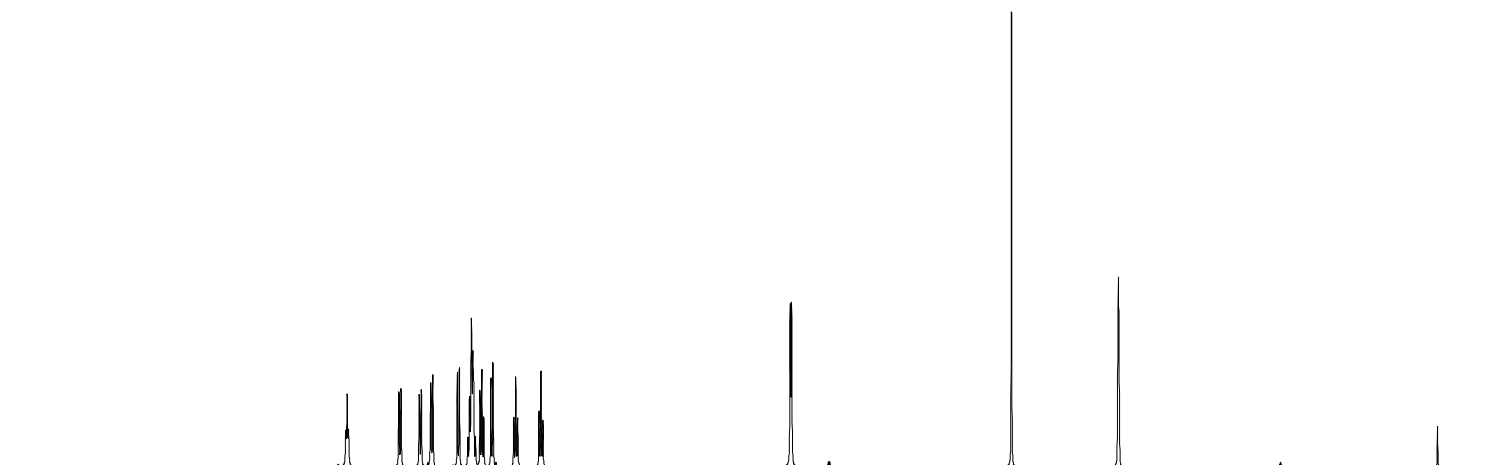
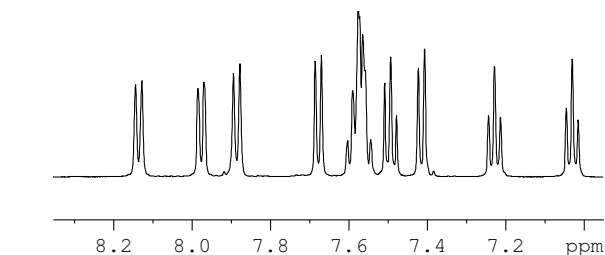
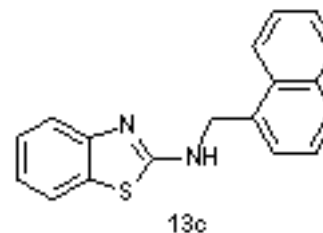
Date_ 20101122
Time 5.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====

NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters

SI 32768
SF 500.0300018 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

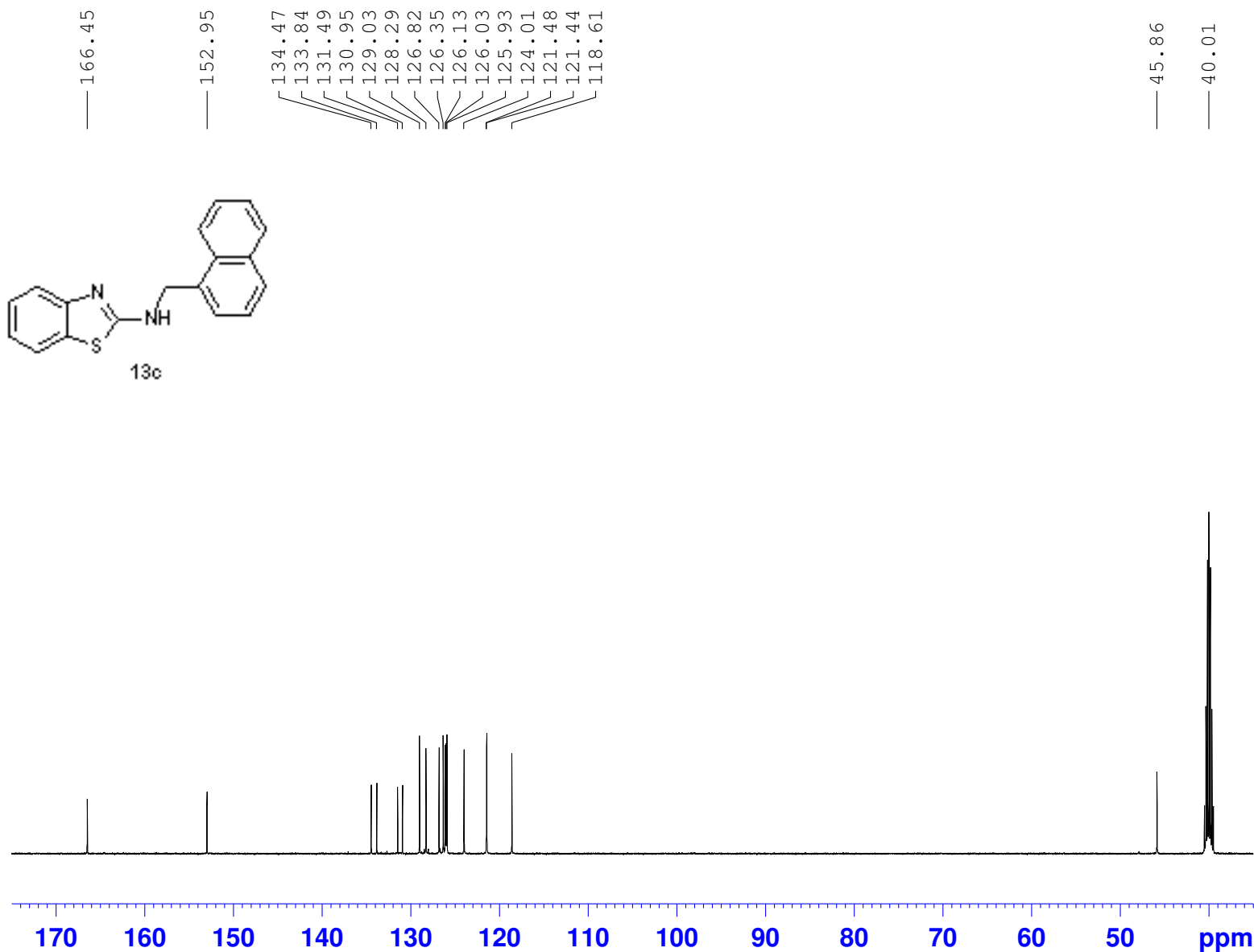


11 10 9 8 7 6 5 4 3 2 1 ppm

1.00
1.02
1.01
1.14
1.05
3.07
1.09
1.04
1.06
1.05

2.07

N-(naphthalen-1-ylmethyl)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



Current Data Parameters
NAME Lifeng-1H
EXPNO 576
PROCNO 1

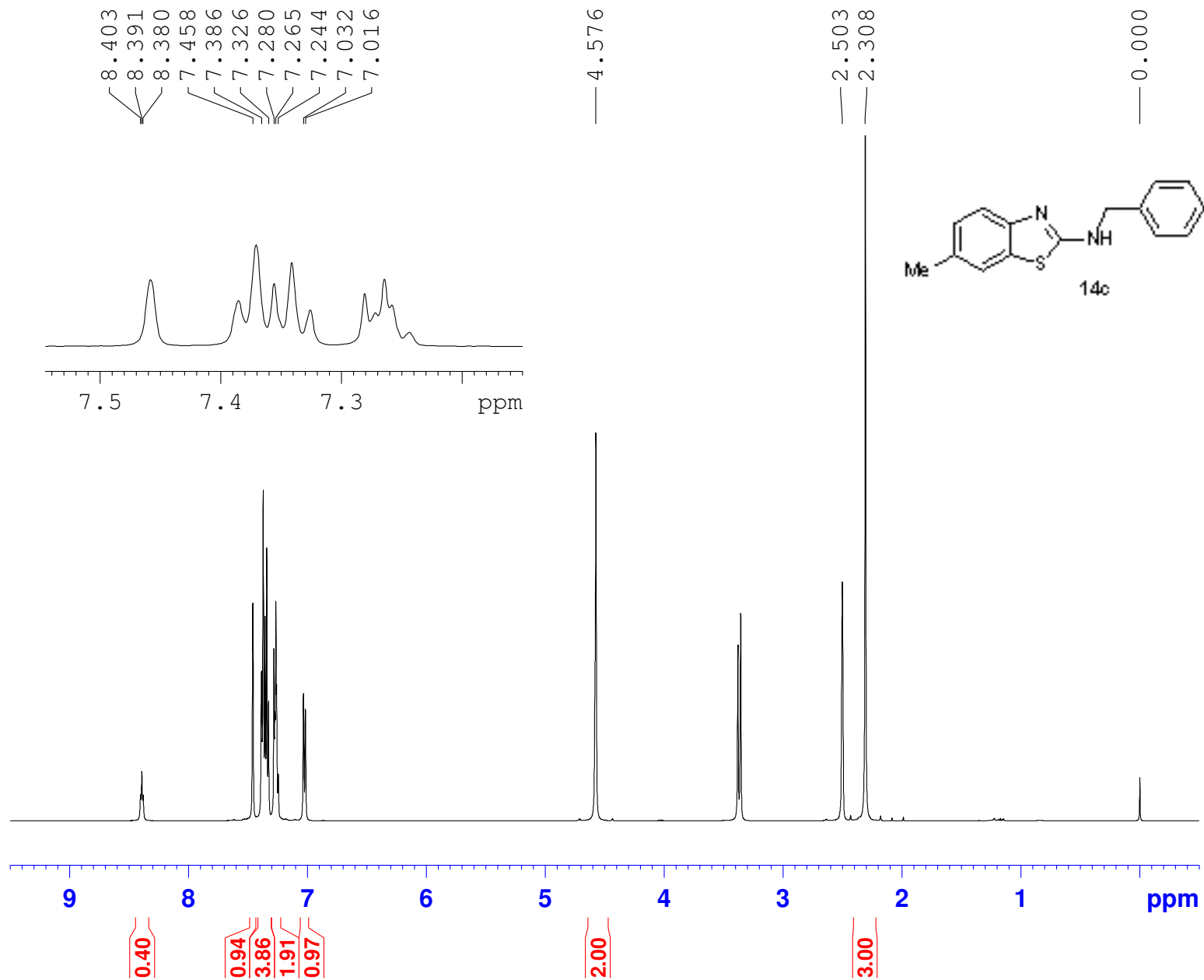
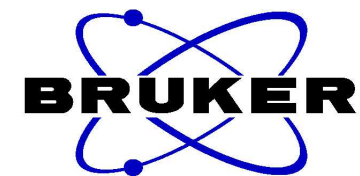
F2 - Acquisition Parameters
Date_ 20101122
Time 0.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 833
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7326450 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

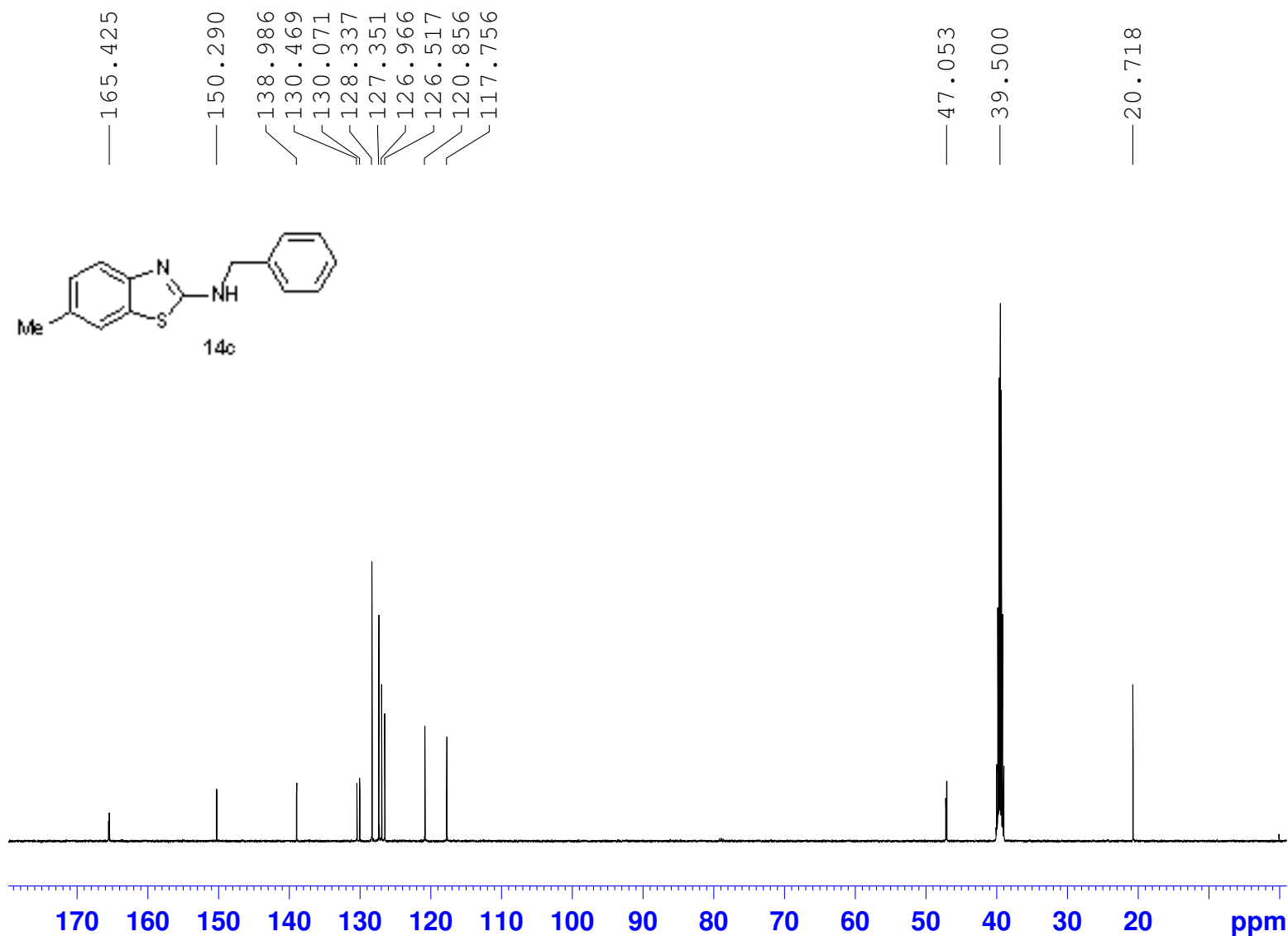
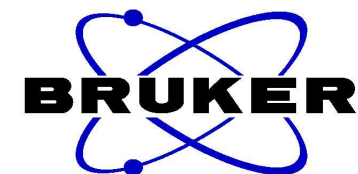
N-benzyl-6-methylbenzo[d]thiazol-2-amine
PROTON DMSO-d6



NAME Shx-1
EXPNO 111
PROCNO 1
Date_ 20100711
Time 15.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 50.8
DW 48.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz
SI 32768
SF 500.0300013 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

N-benzyl-6-methylbenzo[d]thiazol-2-amine
C13CPD DMSO-d6

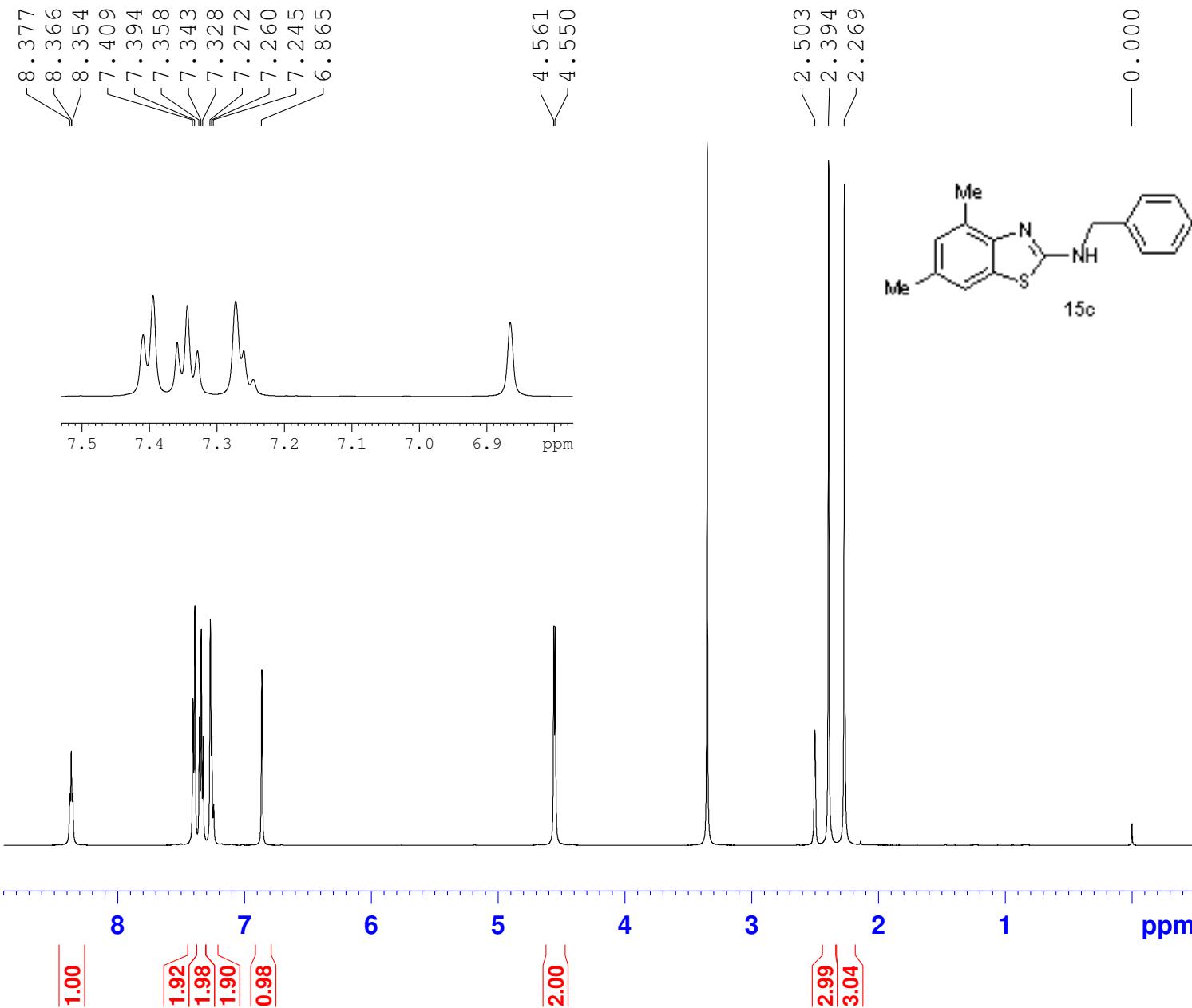
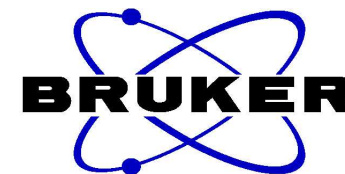


NAME Shx-1
EXPNO 112
PROCNO 1
Date_ 20100711
Time 16.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz
SI 32768
SF 125.7327058 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

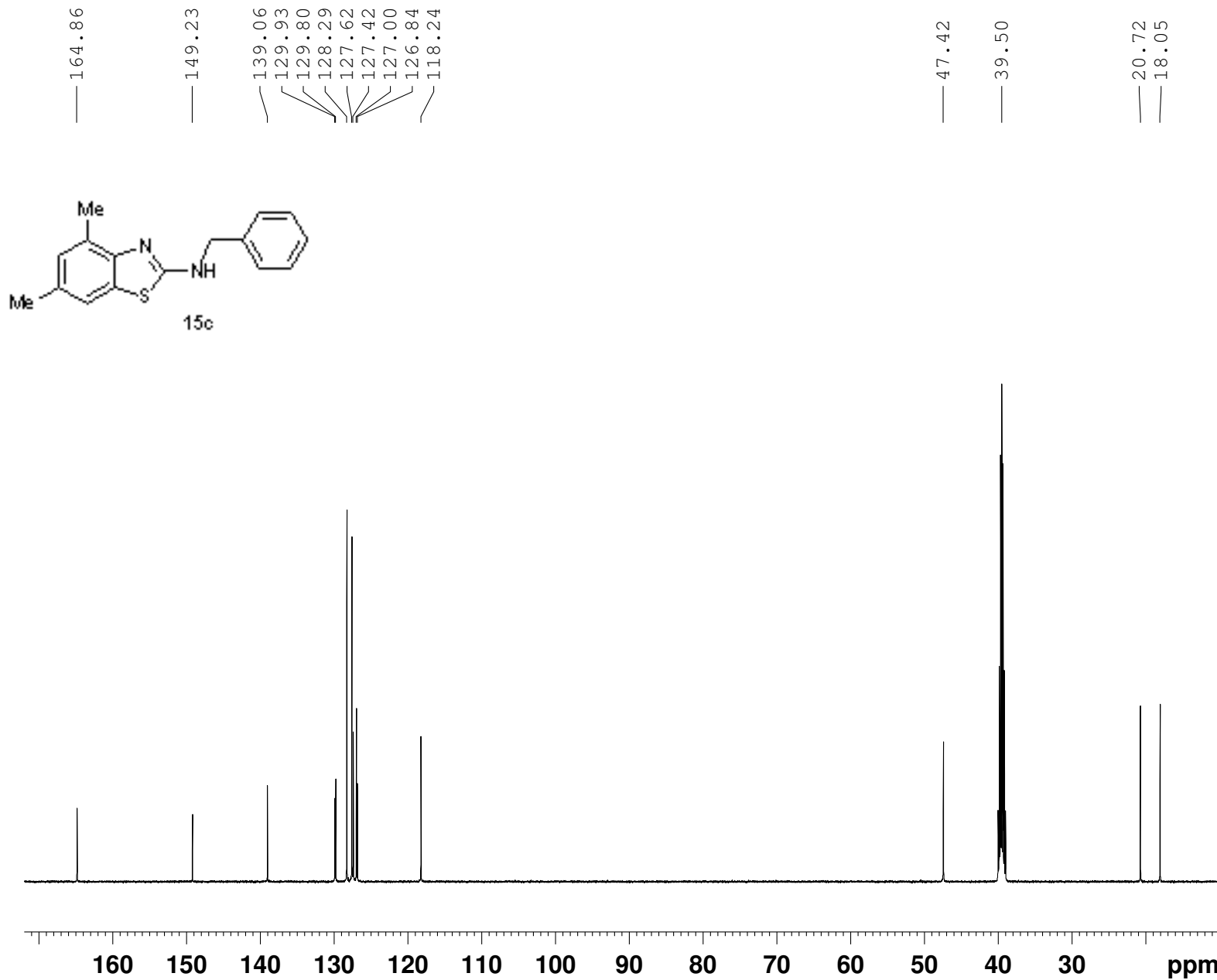
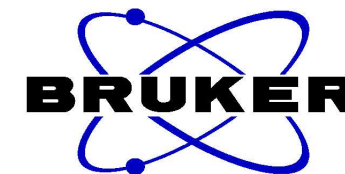
N-benzyl-4,6-dimethylbenzo[d]thiazol-2-amine
PROTON DMSO-d6



NAME 600-700
EXPNO 638
PROCNO 1
Date_ 20110120
Time 11.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
SI 65536
SF 500.0300023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

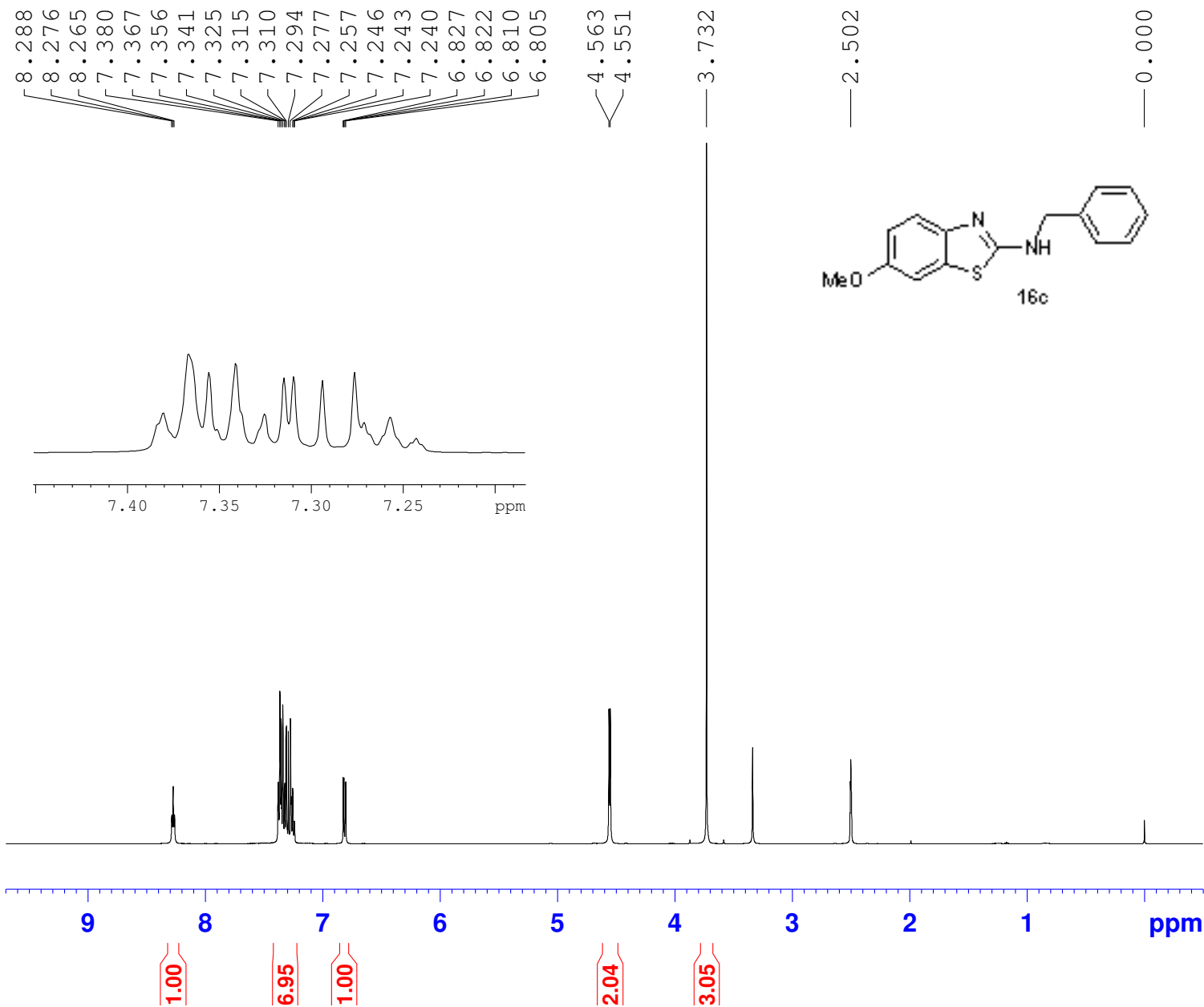
N-benzyl-4,6-dimethylbenzo[d]thiazol-2-amine
C13CPD DMSO-d6



NAME 600-700
EXPNO 641
PROCNO 1
Date_ 20110120
Time 13.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1228
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.0000000 sec
D11 0.0300000 sec

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
SI 32768
SF 125.7327058 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

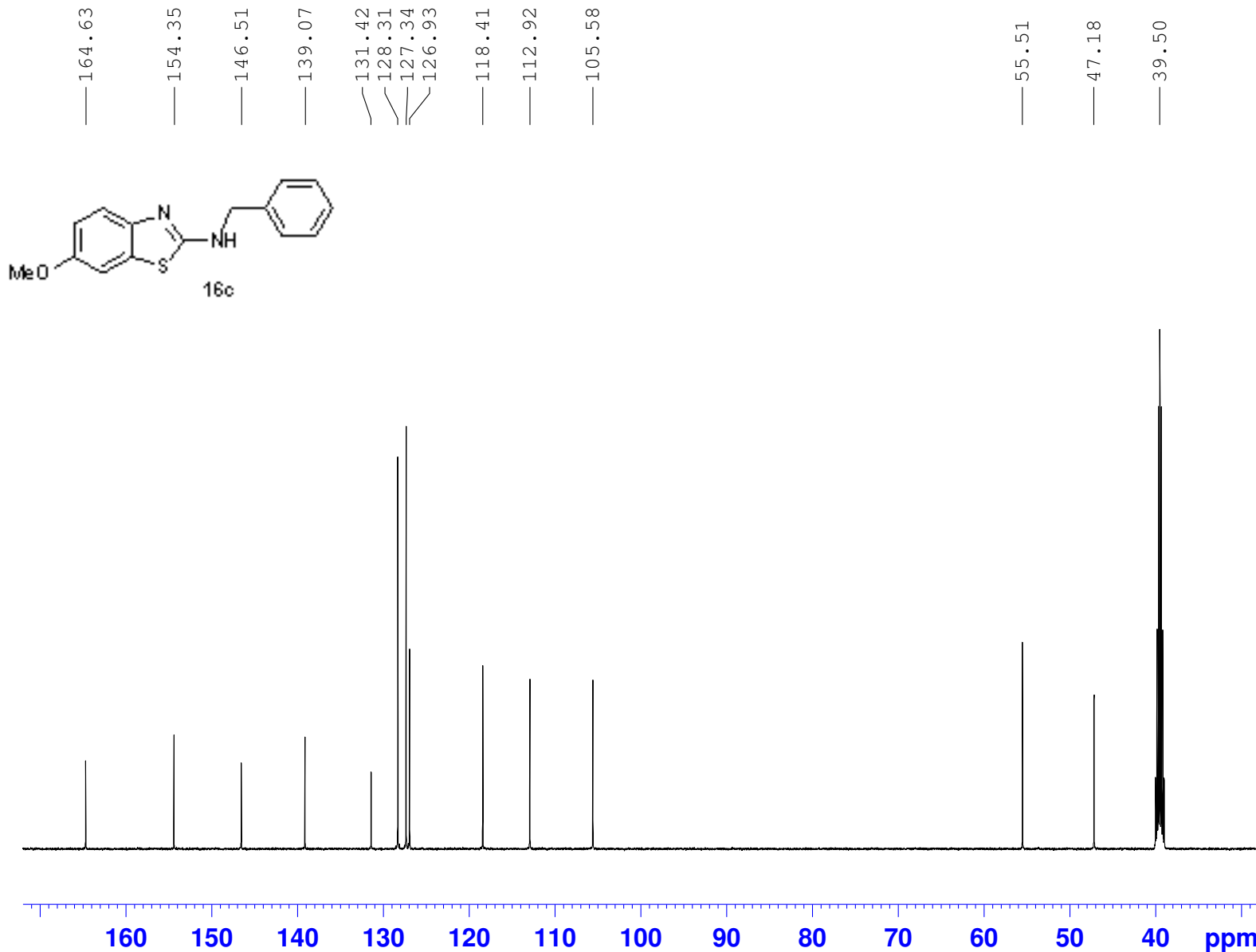
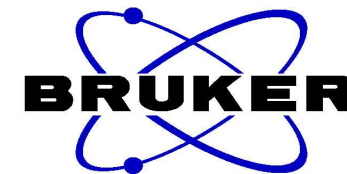
N-benzyl-6-methoxybenzo[d]thiazol-2-amine
PROTON DMSO-d6



```
NAME 3
EXPNO 608
PROCNO 1
Date_ 20101230
Time 1.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
```

```
===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
SI 32768
SF 500.0300017 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
```

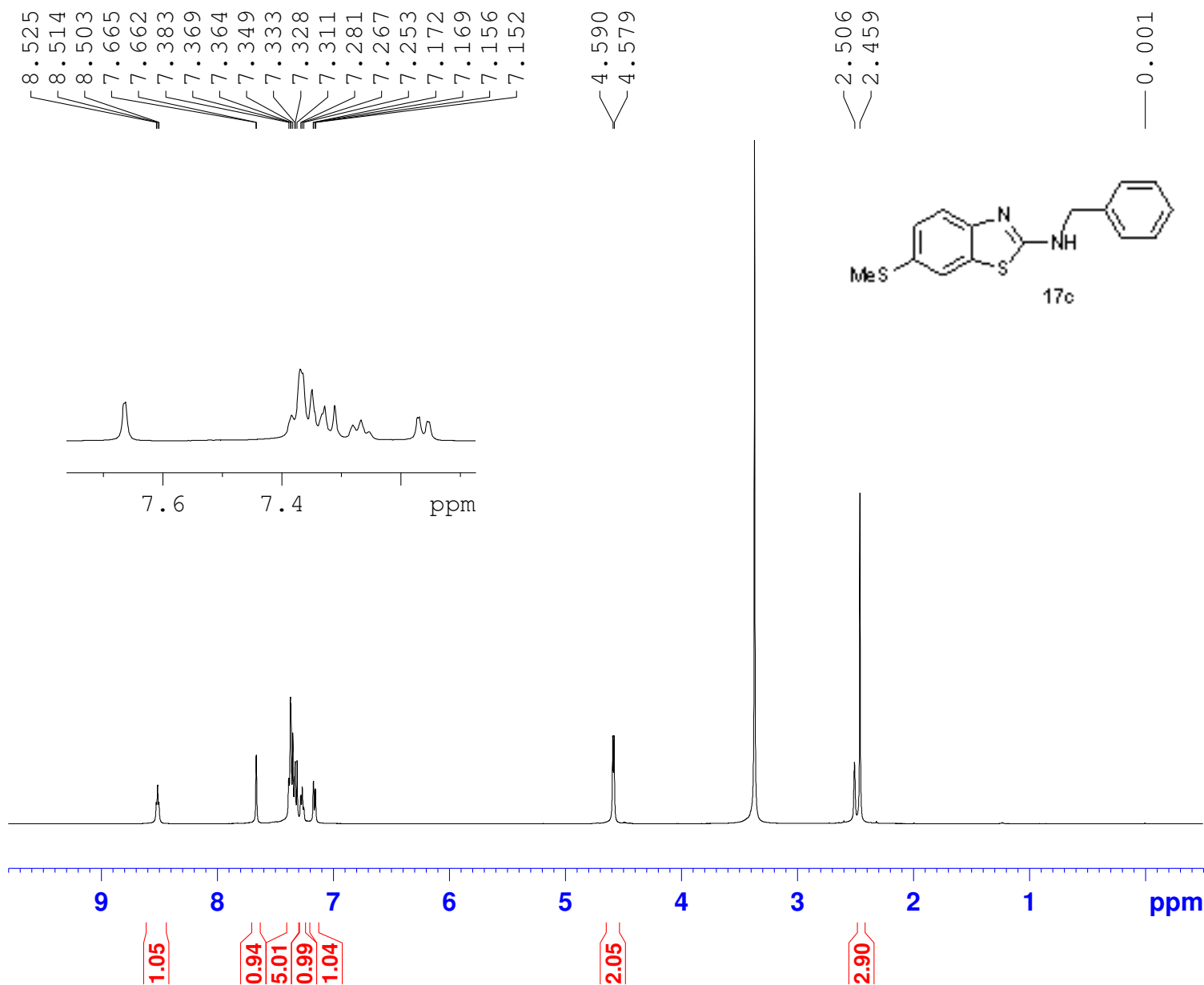

N-benzyl-6--methoxybenzo[d]thiazol-2-amine
C13CPD DMSO-d6



```
NAME 3
EXPNO 609
PROCNO 1
Date_ 20101230
Time 4.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 745
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.0000000 sec
D11 0.0300000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
SI 32768
SF 125.7327077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

N-benzyl-6-(methylthio)benzo[d]thiazol-2-amine
PROTON DMSO-d6



Current Data Parameters
NAME Lifeng-1H
EXPNO 583
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101130
Time 5.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 293.3 K
D1 1.0000000 sec
TD0 1

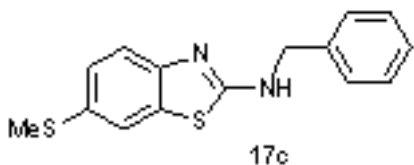
==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

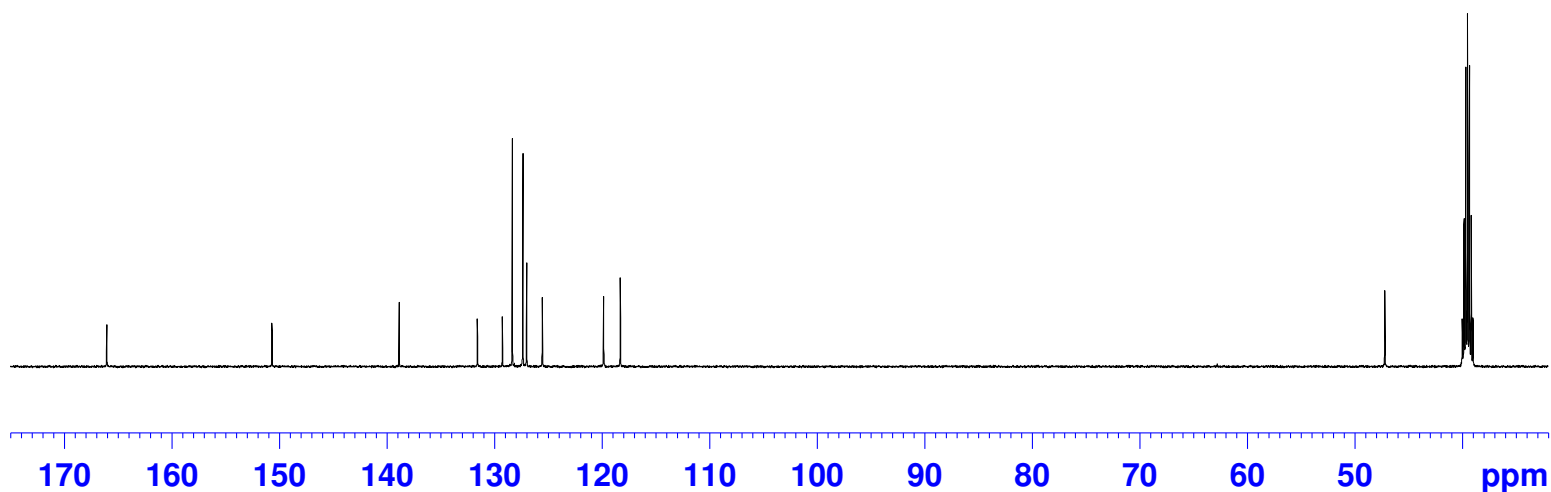
N-benzyl-6-(methylthio)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



166.03
150.64
138.81
131.59
129.27
128.34
127.37
127.01
125.56
119.86
118.30



47.22
39.50



Current Data Parameters
NAME Lifeng-1H
EXPNO 575
PROCNO 1

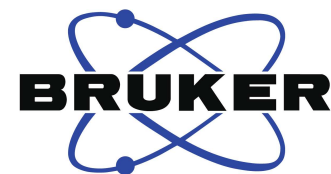
F2 - Acquisition Parameters
Date_ 20101121
Time 23.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 600
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz

F2 - Processing parameters
SI 32768
SF 125.7327077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-benzyl-6-fluorobenzo[d]thiazol-2-amine
PROTON DMSO-d6



8.500
8.489
8.477
7.617
7.612
7.600
7.595
7.384
7.371
7.368
7.363
7.349
7.333
7.280
7.266
7.252
7.072
7.067
7.054
7.048
7.036
7.030
— 4.579

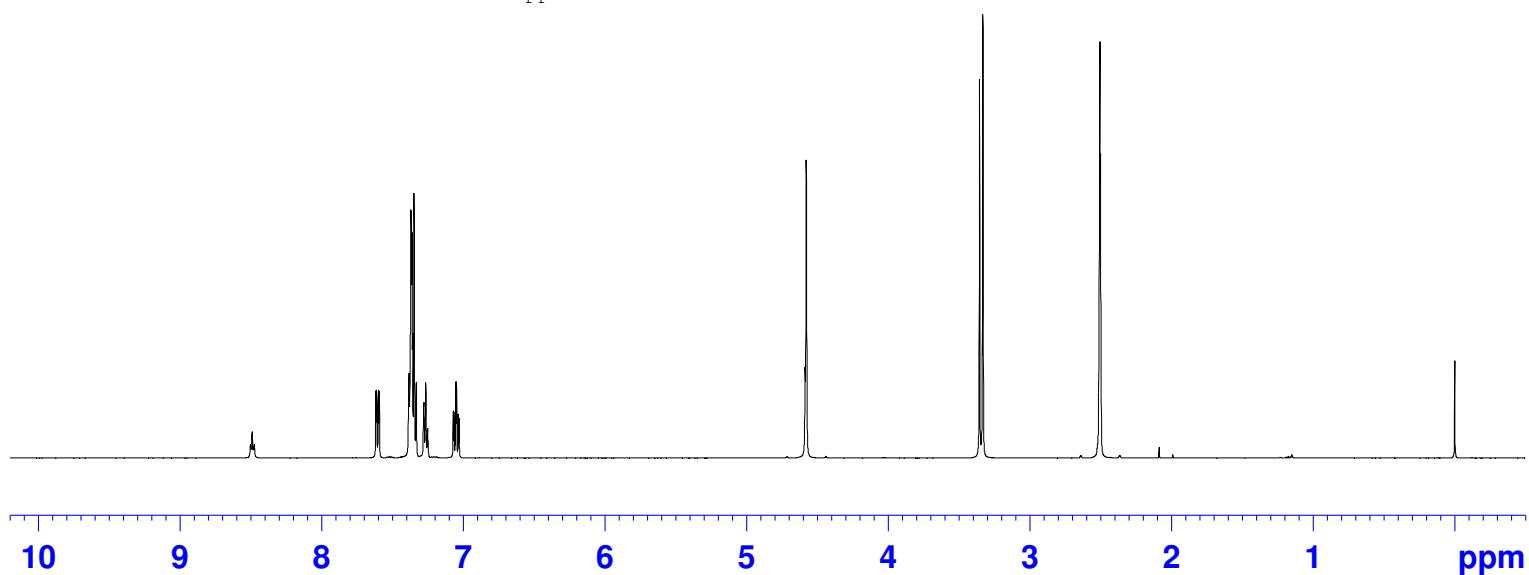
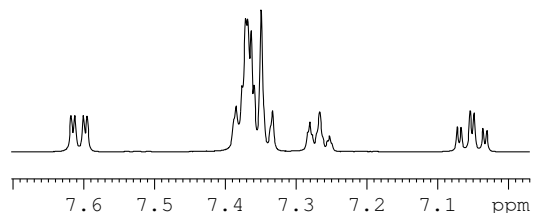
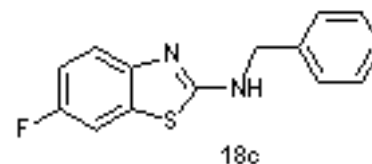
— 2.505
— 0.000

Current Data Parameters
NAME Lifeng-1H
EXPNO 196
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100904
Time 3.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 4
DW 48.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

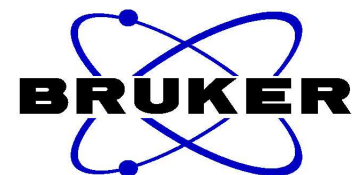
F2 - Processing parameters
SI 32768
SF 500.0300004 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



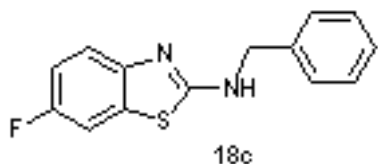
0.33
0.92
4.73
0.92
0.97

2.00

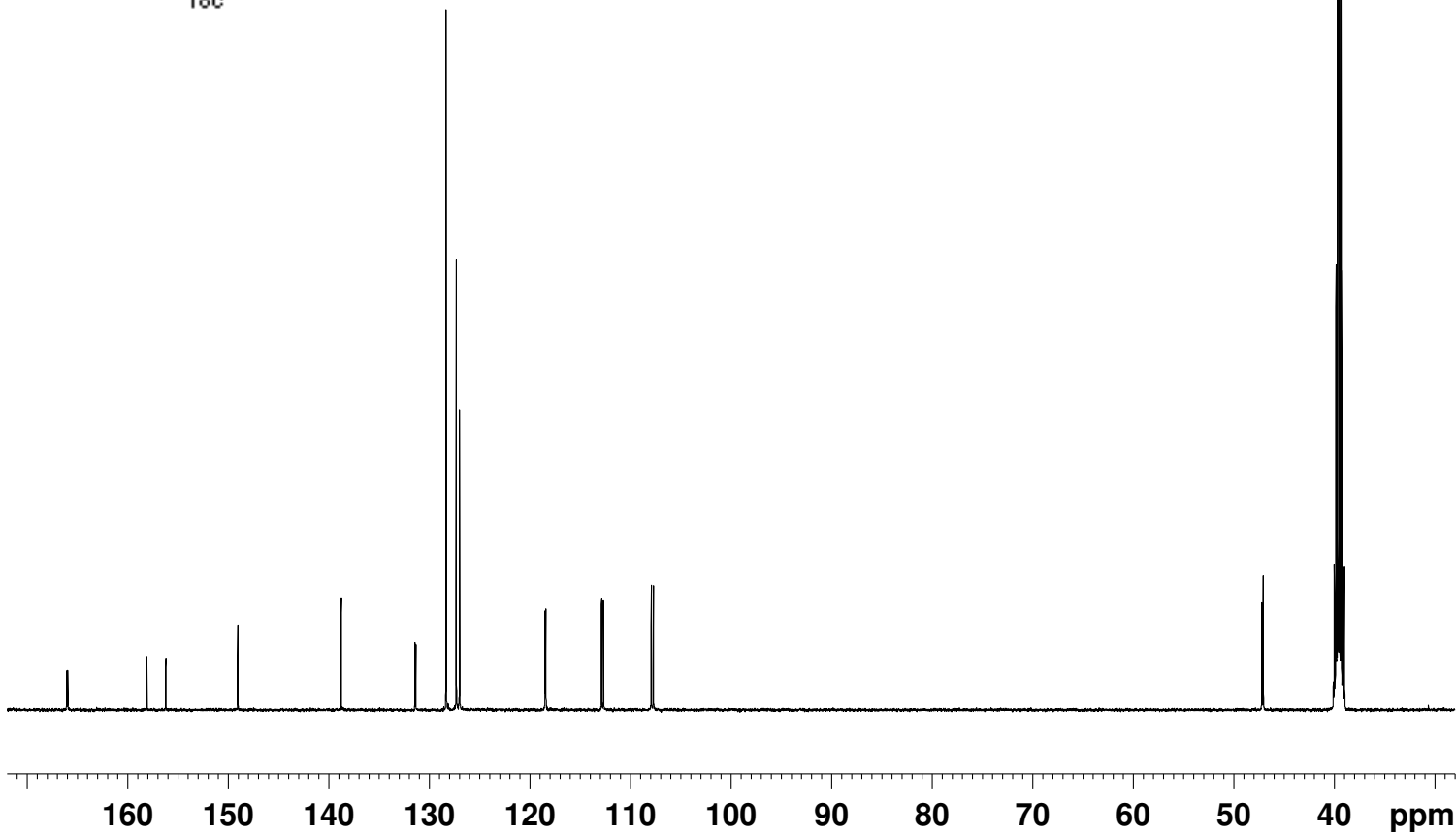
N-benzyl-6-fluorobenzo[d]thiazol-2-amine
C13CPD DMSO-d6



166.10
165.99
158.13
156.26
149.09
138.79
131.46
131.37
128.35
127.36
127.02
118.51
118.45
112.90
112.71
107.95
107.74



47.21
47.08
39.50

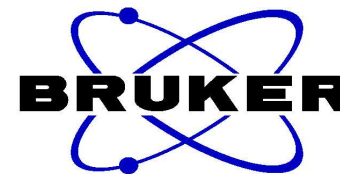


NAME Shx-1
EXPNO 206
PROCNO 1
Date_ 20100905
Time 17.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz
SI 32768
SF 125.7327068 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

N-benzyl-6-chlorobenzo[d]thiazol-2-amine
PROTON DMSO-d6

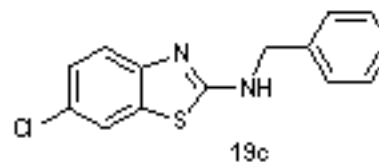
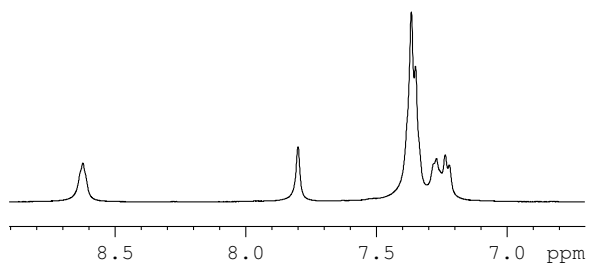


8.623
7.803
7.368
7.351
7.283
7.271
7.238
7.222

4.596
4.588

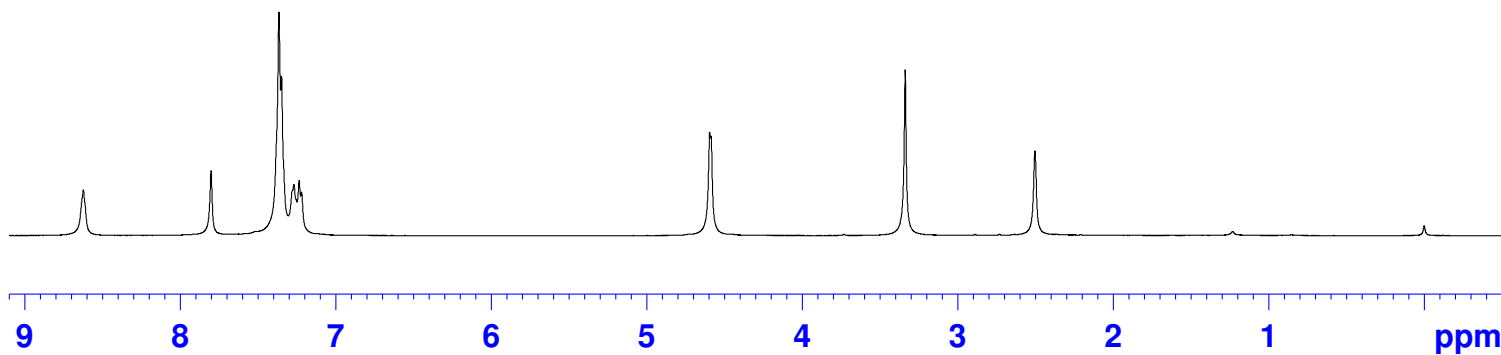
2.504

0.000



```
NAME          3
EXPNO         606
PROCNO        1
Date_         20101230
Time          3.59
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            64
DW            48.400 usec
DE            6.50 usec
TE            295.6 K
D1            1.00000000 sec
```

```
===== CHANNEL f1 =====
NUC1           1H
P1             11.50 usec
SI             32768
SF             500.0300012 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
```



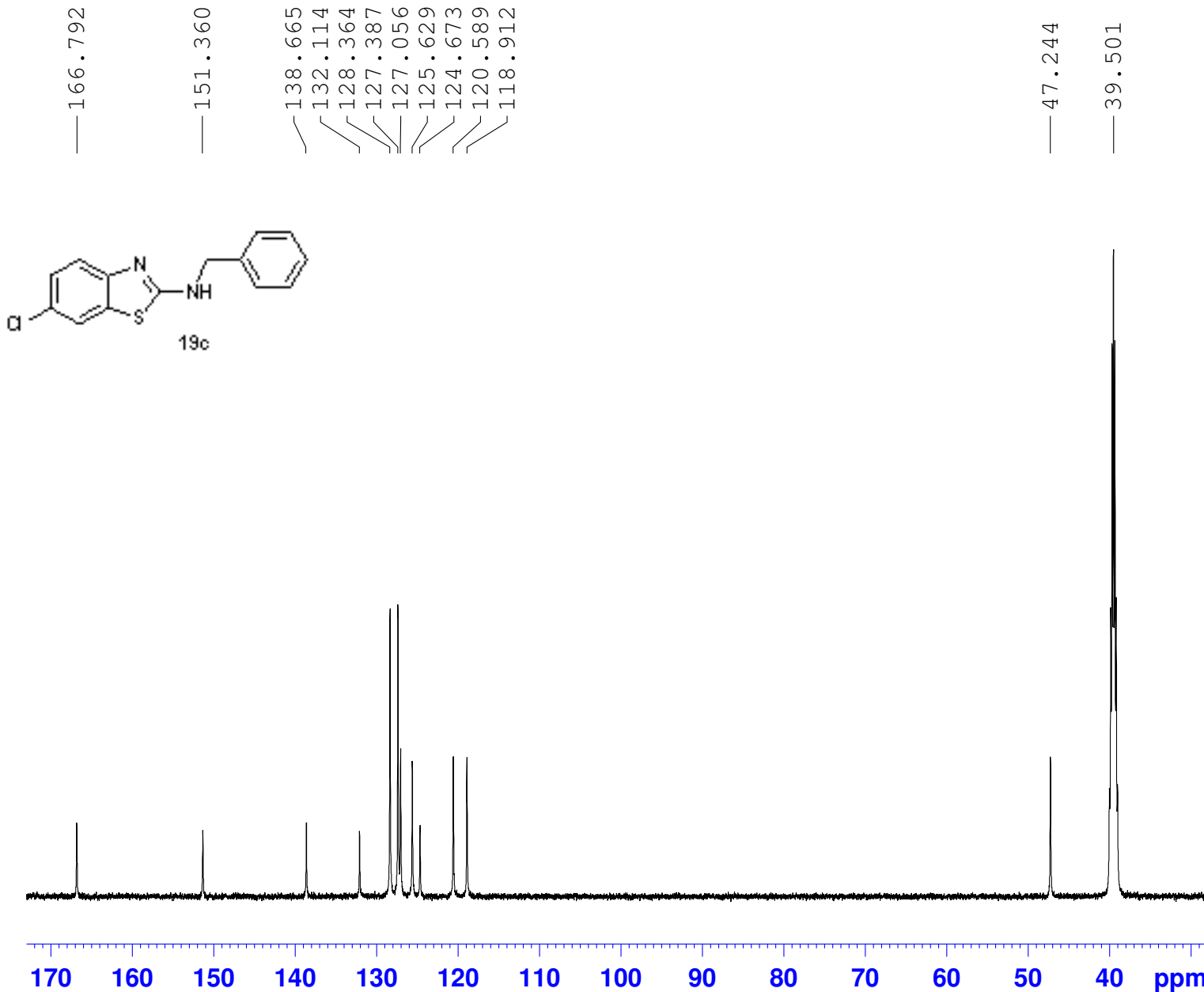
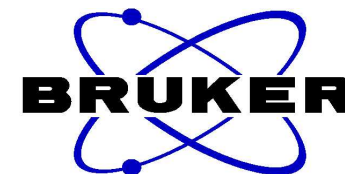
0.95

0.86

6.90

2.00

N-benzyl-6-chlorobenzo[d]thiazol-2-amine
C13CPD DMSO-d6



```
NAME 3
EXPNO 607
PROCNO 1
Date_ 20101230
Time 6.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1075
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
```

```
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
SI 32768
SF 125.7327076 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
```

N-benzyl-6-(trifluoromethoxy)benzo[d]thiazol-2-amine
PROTON DMSO-d₆

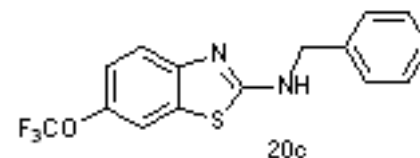


8.680
8.670
8.659
7.806
7.437
7.420
7.386
7.370
7.352
7.337
7.285
7.272
7.258
7.204
7.187

4.610
4.601

2.504

0.000

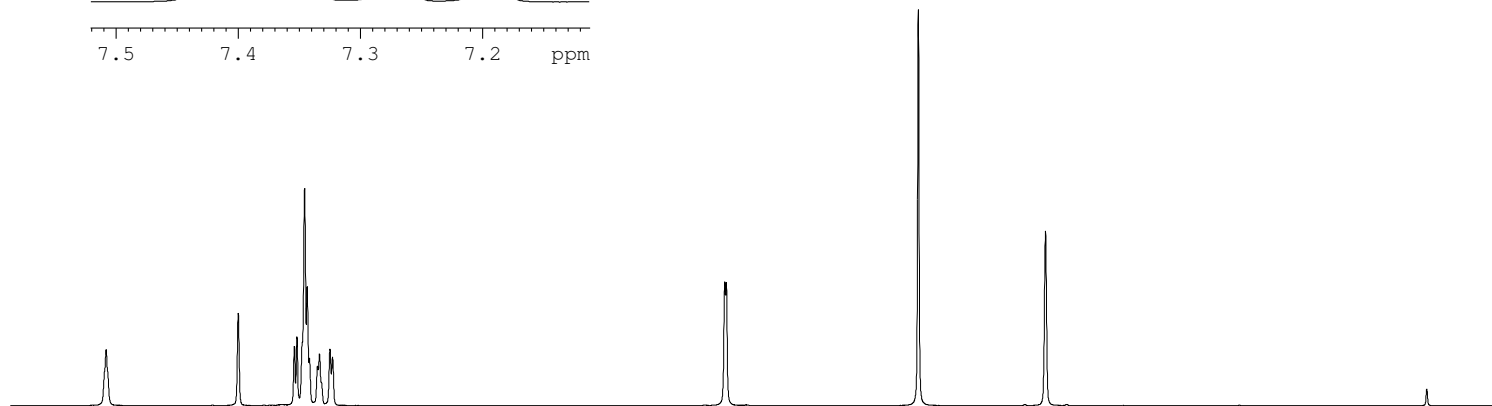
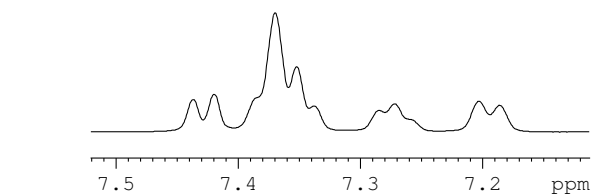


Current Data Parameters
NAME Lifeng-1H
EXPNO 578
PROCNO 1

F2 - Acquisition Parameters
Date_ 20101122
Time 5.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.171923 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.50 usec
PL1 1.10 dB
PL1W 16.96364784 W
SFO1 500.0330879 MHz

F2 - Processing parameters
SI 32768
SF 500.0300007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

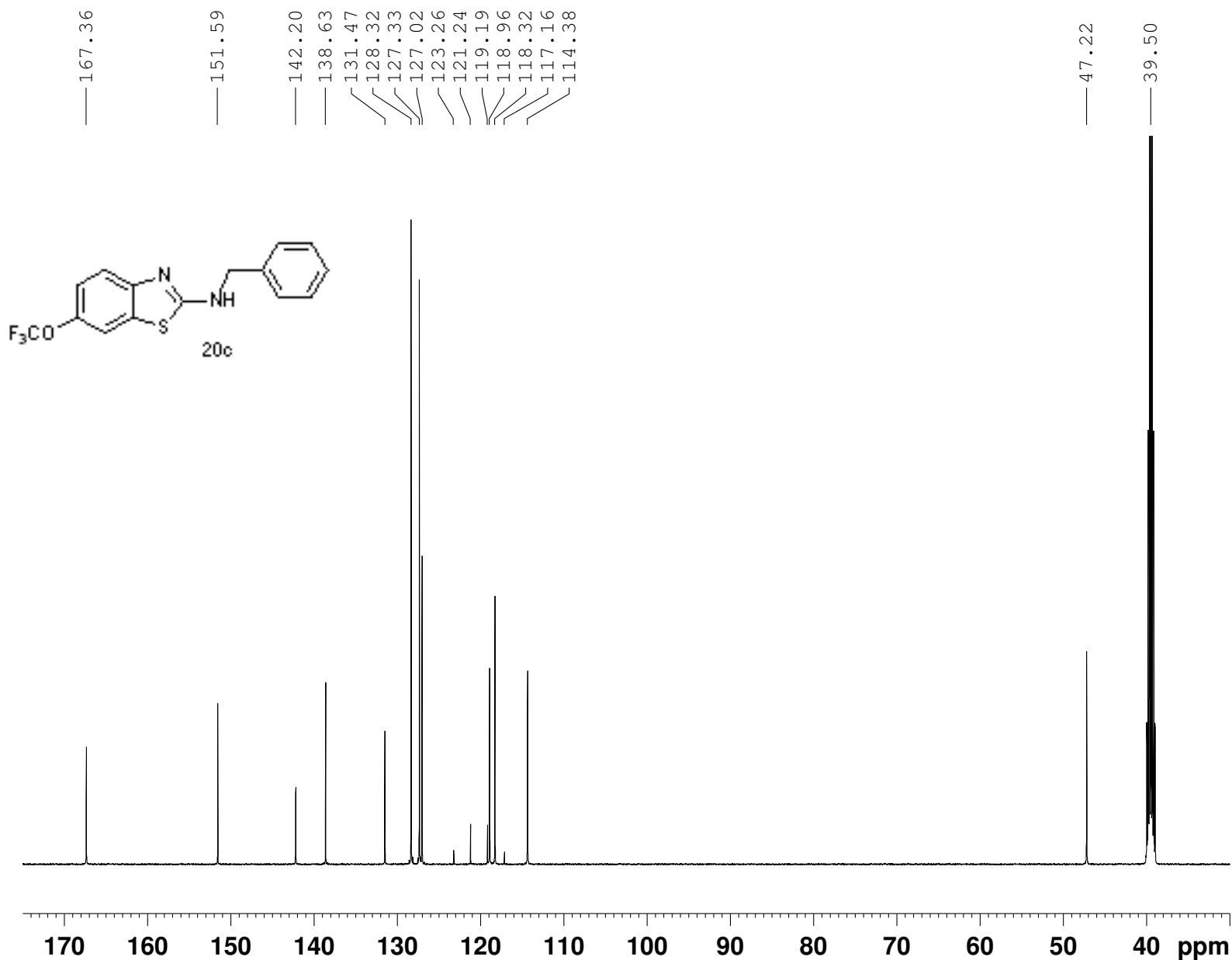
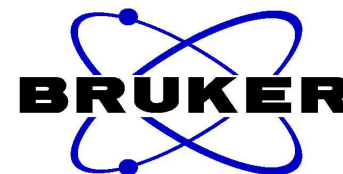


1.02
0.92
1.01
3.92
0.98
1.02

2.00

9 8 7 6 5 4 3 2 1 ppm

N-benzyl-6-(trifluoromethoxy)benzo[d]thiazol-2-amine
C13CPD DMSO-d6



NAME Shx-1
EXPNO 579
PROCNO 1
Date_ 20101205
Time 15.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10240
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.00 dB
PL1W 125.85865021 W
SFO1 125.7452168 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.10 dB
PL12 17.95 dB
PL13 17.95 dB
PL2W 16.96364784 W
PL12W 0.35036376 W
PL13W 0.35036376 W
SFO2 500.0320001 MHz
SI 32768
SF 125.7327113 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40