Supporting information for

Recyclable CuO-Catalyzed Synthesis of 4(3*H*)-Quinazolinones

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Contents:

General Remarks

All glassware used was dried in electric oven at 120 ^{o}C. All chemicals were purchased from Sigma-Aldrich, Alfa Aesar, Shanghai Aladdin Reagent Co., Ltd, and Chengdu Changzheng Chemical Co. and used as received.

All compounds were characterized by ^{1}H NMR, ^{13}C NMR, ESI-MS and IR spectroscopy. Copies of the ^{1}H and ^{13}C spectra can be found at the end of the Supporting Information. Nuclear Magnetic Resonance spectra were recorded on a Bruker Advance 300MHz or 400 MHz instrument. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) or DMSO (2.50 ppm) in the deuterated solvent, unless otherwise stated. All ^{13}C NMR spectra are reported in ppm relative to deuteron-chloroform (77.23 ppm) or DMSO-d_6 (δ = 39.60 ppm), unless otherwise stated, and all were obtained with ^{1}H decoupling. All IR spectra were taken on a Bruker Tensor-27 infrared spectrometer with an OPUS workstation. Electron-spraying ionization Mass Spectra are recorded on an Agilent 1200 series LC/MS DVL instrument. Melting points were determined on an Electrothermal melting-point apparatus. The purities of all the synthesized compounds were checked by thin-layer chromatography (TLC) using different organic solvents.

Experimental Section

Typical procedure for the synthesis of 4(3*H*)-quinazolinones

A mixture of anthranilamide (1.0 mmol), benzaldehyde (1.0 mmol) and CuO (0.03 mmol) in DMA (3 ml) was stirred under air in an oil bath at 120 ^{o}C for 24 hours. And then the reaction mixture was cooled to room temperature and the upper clear solution was carefully removed by a pipette. DMA (3 mL) was added to the vial, and the vial was shaken and then kept in stillness for a moment, and then the upper clear solution was removed by a pipette again. DMA (3 mL) was added to the vial again and the upper clear solution was removed again (Note: The black solid CuO in the bottom of the vial may be used as the recycling catalyst for the following synthesis of 4(3H)-quinazolinone once other reagents were added). The combined solution was condensed in vacuum to remove the solvent DMA, which was used as the solvent for the next reaction. The residual was purified by column chromatography on silica gel (gradient eluent with a mixed solution of petroleum ether and ethyl acetate) to give the pure 4(3H)-quinazolinone.

Typical procedure for the synthesis of 4(3*H*)-quinazolinones with the recycling catalyst CuO

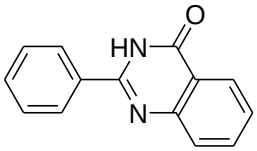
During the workup operation of the typical procedure for the synthesis of 4(3H)-quinazolinones, the black powder CuO in the bottom of the vial was suitable for the recycling catalyst of the synthesis of 4(3H)-quinazolinone. To the vial was added anthranilamide (1.0 mmol), benzaldehyde (1.0 mmol), DMA (3 mL). The vial was stirred under air in an oil bath at 120 ^{o}C for 24 hours. After similar workup, the reaction of the first recycling of the catalyst CuO was complete. And the next time recycling reaction may be continued with the black powder CuO in the bottom of the vial.

Scale-up procedure for the synthesis of 2-phenyl-4(3*H*)-quinazolinone

A mixture of anthranilamide (20 mmol), benzaldehyde (20 mmol) and CuO (0. 6 mmol) in DMA (60 ml) was stirred under air in an oil bath at 120 ^{o}C for 24 hours. And then the reaction mixture was cooled to room temperature and filtrated to remove CuO. The filtrate was condensed in vacuum to remove the solvent DMA, which may be used for next reaction. The resulting residual was recrystallized from ethanol to give white solid 2-phenyl-4(3H)-quinazolinone **3a**.

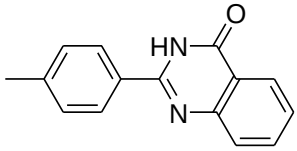
Analytical Data for Compounds 3a-3o

2-phenyl-4(3*H*)-quinazolinone (3a)



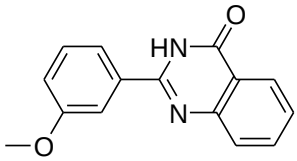
White solid. Mp 239-241 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 11.12 (s, 1H), 8.33 (d, *J* = 7.52 Hz, 1H), 8.20-8.22 (m, 2H) 7.78-7.85 (m, 2H), 7.59 (t, *J* = 2.78 Hz, 3H) 7.51(t, *J* = 3.19 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$), δ (ppm): 163.6, 151.6, 149.5, 134.8, 132.8, 131.6, 129.0, 128.0, 127.3, 126.8, 126.5, 120.8. ESI-MS (negative mode), m/z = 221 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2924, 1730, 1664, 1601, 1451, 1375, 1212, 1045, 942, 752, 694. Anal. calcd. (%) for C14H10N2O: C, 75.66; H, 4.54; N, 12.60. Found: C, 75.32; H, 4.41; N, 12.53.

2-(4-Methylphenyl)-4(3*H*)-quinazolinone (3b)



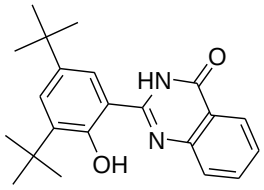
White solid. Mp 240-241 °C. ^{1}H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.46 (s, 1H), 8.14 (d, *J* = 7.95Hz, 1H), 8.09 (d, *J* = 8.21Hz, 2H), 7.83 (t, *J* = 6.87Hz, 1H), 7.72 (d, *J* = 7.68Hz, 1H), 7.51 (t, *J* = 7.02Hz, 1H), 7.35 (d, *J* = 8.07Hz, 2H), 2.39. ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 167.4, 157.4, 154.0, 146.6, 139.7, 135.1, 134.4, 132.8, 132.6, 131.6, 131.0, 126.1, 26.2. ESI-MS (negative mode), m/z = 235 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2921, 1657, 1599, 1445, 1300, 1149, 939, 765, 686. Anal. calcd. (%) for C15H12N2O: C, 76.25; H, 5.12; N, 11.86. Found: C, 76.12; H, 5.03; N, 11.69.

2-(3-methoxyphenyl)-4(3*H*)-quinazolinone (3c)



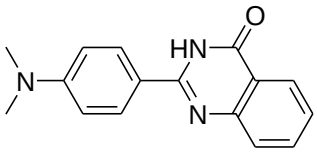
White solid. Mp 202-204 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 10.75 (s, 1H), 8.31 (d, *J* = 8.16 Hz, 1H), 7.81-7.84 (m, 2H), 7.69-7.73 (m, 2H), 7.46-7.53 (m, 2H), 7.15 (d, *J* = 1.71 Hz, 1H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 162.7, 159.8, 152.5, 135.0, 134.4, 130.2, 127.1, 126.3, 121.4, 120.5, 118.0, 113.0, 55.8. ESI-MS (negative mode), m/z = 251 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2987, 1786, 1679, 1584, 1375, 1218, 1043, 758, 669. Anal. calcd. (%) for C15H12N2O2: C, 71.42; H, 4.79; N, 11.10. Found: C, 71.25; H, 4.86; N, 11.18.

2-(3,5-ditertbutyl-2-hydroxyphenyl)-4(3*H*)-quinazolinone (3d)



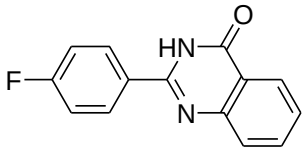
White solid. Mp 287-288 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 14.37 (s, 1H), 10.54 (s, 1H), 8.32 (d, *J* = 7.95Hz, 1H), 7.74-7.83 (m, 2H), 7.47-7.59 (m, 2H) 7.46-7.51 (m, 1H), 1.49 (s, 9H), 1.39 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 162.1, 158.2 155.4, 145.9, 140.1, 137.0, 135.5, 128.2, 127.3, 126.5, 126.1, 122.4, 121.0, 112.4, 35.3, 34.9, 31.8, 29.8. ESI-MS (negative mode), m/z = 349 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2965, 1676, 1610, 1563, 1456, 1217, 1047, 769, 667. Anal. calcd. (%) for C22H26N2O2: C, 75.40; H, 7.48; N, 7.99. Found: C, 75.22; H, 7.59; N, 7.82.

2-(4-(dimethylamino)phenyl)-4(3*H*)-quinazolinone (3e)



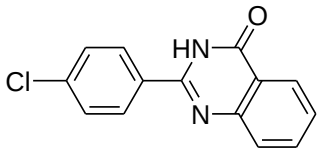
White solid. Mp 247-248 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 9.83 (s, 1H), 8.27 (d, *J* = 7.78Hz, 1H), 8.04 (d, *J* = 8.92Hz, 2H), 7.85 (d, *J* = 8.21Hz, 1H), 7.76 (dt, *J* = 7.01Hz, 1.42Hz, 1H), 7.43 (t, *J* = 6.93Hz, 1H), 6.79 (d, *J* = 9.05Hz, 2H), 3.03 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$), δ (ppm): 163.2, 152.5, 151.6, 150.0, 134.6, 129.5, 128.4, 127.4, 126.3 125.6, 112.0, 111.7, 40.1. ESI-MS (negative mode), m/z = 264 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 3018, 1731, 1665, 1592, 1533, 1372, 1215, 1046, 939, 750, 667. Anal. calcd. (%) for C16H15N3O: C, 72.43; H, 5.70; N, 15.84. Found: C, 72.51; H, 5.63; N, 15.72.

2-(4-fluorophenyl)-4(3*H*)-quinazolinone (3f)



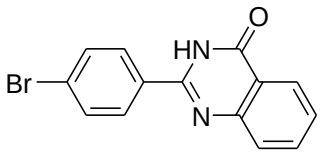
White solid. Mp 288-289 °C. ^{1}H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.57 (s, 1H), 8.23-8.27 (m, 2H), 8.15 (d, *J* = 7.92 Hz, 1H), 7.84 (t, *J* = 6.84 Hz, 1H), 7.74 (d, *J* = 8.08 Hz, 1H), 7.53 (t, *J* = 7.03 Hz, 1H), 7.39 (t, *J* = 8.85 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 167.4, 156.6, 153.8, 139.8, 135.6, 134.4, 132.6, 131.8, 131.0, 126.1, 120.9, 120.7. ESI-MS (negative mode), m/z = 239 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2920, 1660, 1603, 1483, 1346, 1232, 1149, 1076, 939, 763, 684. Anal. calcd. (%) for C14H9FN2O: C, 69.99; H, 3.78; N, 11.66. Found: C, 69.87; H, 3.89; N, 11.48.

2-(4-chlorophenyl)-4(3*H*)-quinazolinone (3g)



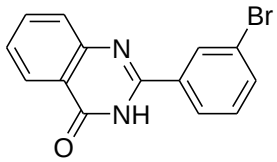
White solid. Mp 298-299 °C. ^{1}H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.61 (s, 1H), 8.20 (d, J = 8.55Hz, 2H), 8.15 (d, J = 7.92Hz, 1H), 7.85 (t, J = 7.10Hz, 1H), 7.74 (d, J = 8.16Hz, 1H), 7.63 (d, J = 8.55Hz, 2H), 7.53 (t, J = 7.37Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 162.6, 151.8, 148.9, 136.7, 135.1, 132.0 130.0, 129.1, 127.9, 127.2, 126.3, 121.4. ESI-MS (negative mode), m/z = 255 [M–H]$^{-}$. IR (KBr), ν (cm^{-1}): 2922, 1671, 1598, 1476, 1344, 1280, 1121, 1093, 982, 760, 683. Anal. calcd. (%) for C14H9ClN2O: C, 65.51; H, 3.53; N, 10.91. Found: C, 65.63; H, 3.64; N, 10.78.

2-(4-bromophenyl)-4(3*H*)-quinazolinone (3h)



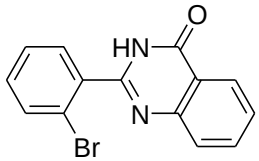
White solid. Mp 298-300 °C. ^{1}H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.60 (s, 1H), 8.14 (t, J = 7.41Hz, 3H), 7.85 (t, J = 7.02Hz, 1H), 7.76 (t, J = 7.56Hz, 3H), 7.54 (t, J = 7.56Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 162.6, 151.9, 148.9, 135.1, 132.3, 132.0, 130.2, 127.9, 127.2, 126.3, 125.7, 121.4. ESI-MS (negative mode), m/z = 299 [M (^{79}Br) –H]$^{-}$, 301 [M (^{81}Br) –H]$^{-}$. IR (KBr), ν (cm^{-1}): 2986, 1732, 1375, 1216, 1047, 756, 668. Anal. calcd. (%) for C14H9BrN2O: C, 55.84; H, 3.01; N, 9.30. Found: C, 55.92; H, 3.16; N, 9.23.

2-(3-bromophenyl)-4(3*H*)-quinazolinone (3i)



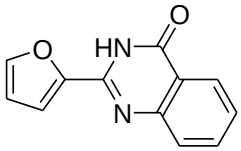
White solid. Mp 271-272 °C. ^{1}H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.62 (s, 1H), 8.38 (s, 1H), 8.10-8.20 (m, 2H), 7.78-7.88 (m, 2H), 7.66-7.75 (m, 1H), 7.57-7.45 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 162.5, 151.3, 135.4, 135.2, 134.5, 131.2, 131.2, 130.8, 128.1, 127.4, 127.3, 126.3, 122.4, 121.6. ESI-MS (negative mode), m/z = 299 [M (^{79}Br) –H]$^{-}$, 301 [M (^{81}Br) –H]$^{-}$. IR (KBr), ν (cm^{-1}): 2923, 1678, 1607, 1471, 1309, 1152, 952, 794, 677. Anal. calcd. (%) for C14H9BrN2O: C, 55.84; H, 3.01; N, 9.30. Found: C, 55.90; H, 3.21; N, 9.22.

2-(2-bromophenyl)-4(3*H*)-quinazolinone (3j)



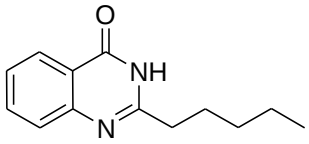
White solid. Mp 159-160 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 9.54 (s, 1H), 8.32 (d, *J* = 7.87 Hz, 1H), 7.83 (d, *J* = 2.23Hz, 2H), 7.71-7.77 (m, 2H), 7.48-7.57 (m, 2H), 7.41 (dt, *J* = 7.87Hz, 1.08Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$), δ (ppm): 162.2, 151.9, 148.8, 134.8, 133.7, 132.0, 131.2, 127.97, 127.94, 127.3, 126.4, 121.0, 120.8. ESI-MS (negative mode), m/z = 299 [M (^{79}Br) –H]$^{-}$, 301 [M (^{81}Br) –H]$^{-}$. IR (KBr), ν (cm^{-1}): 3015, 1673, 1606, 1472, 1304, 1216, 1145, 1046, 945,755, 666. Anal. calcd. (%) for C14H9BrN2O: C, 55.84; H, 3.01; N, 9.30. Found: C, 55.97; H, 3.25; N, 9.17.

2-furyl-4(3*H*)-quinazolinone (3k)



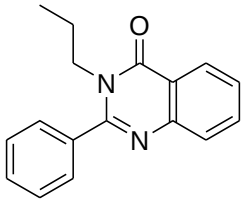
White solid. Mp 208-210 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 10.85 (s, 1H), 8.30 (d, *J* = 7.75Hz, 1H), 7.77 (d, *J* = 5.36Hz, 2H), 7.66 (s, 1H), 7.45-7.50 (m, 2H), 6.65-6.67 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$), δ (ppm): 162.8, 149.2, 146.2, 145.5, 143.5, 134.9, 127.7, 126.6, 120.9, 114.0, 112.8, 14.1. ESI-MS (negative mode), m/z = 211 [M–H]$^{-}$. IR ($CHCl_3$), ν (cm^{-1}): 2986, 1667, 1603, 1552, 1502, 1459, 1344, 1315, 1242, 1217, 1173, 1030, 965, 750, 666. Anal. calcd. (%) for C12H8N2O2: C, 67.92; H, 3.80; N, 13.20. Found: C, 67.99; H, 3.96; N, 13.12.

2-pentylquinazolin-4(3H)-one (3l)



White solid, Mp. 152-154 °C. **1**H NMR (300 MHz, DMSO-d_6), δ (ppm): 12.15 (s, 1H), 8.07 (d, *J* = 7.89 Hz, 1H), 7.72-7.78 (m, 1H), 7.58 (d, *J* = 8.10 Hz, 1H), 7.41-7.46 (m, 1H), 2.49-2.60 (m, 2H.), 1.67-1.72 (m, 2H), 1.29 (d, *J* = 7.14 Hz, 4H), 0.85 (d, *J* = 6.66 Hz, 3H). ^{13}C NMR (75 MHz, DMSO-d_6), δ (ppm): 162.0, 157.7, 149.0, 134.4, 126.8, 126.0, 125.8, 120.8. IR (KBr), ν (cm^{-1}): 3846, 3696, 3121, 2925, 1845, 1675, 1614, 1564, 1470, 1380, 1324, 1254, 1027, 976, 737, 647. Anal. calcd. (%) for C13H16N2O: C, 72.19; H, 7.46; N, 12.95. Found: C, 72.12; H, 7.58; N, 12.82.

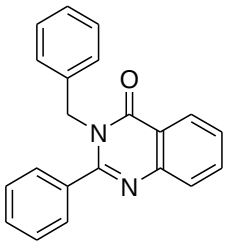
2-phenyl-3-propyl-4(3*H*)-quinazolinone (3m)



White solid. Mp 98-100 °C. ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm): 8.19-8.22 (m, 1H), 7.83 (t, *J* = 7.60Hz, 1H), 7.62-7.68 (m, 3H), 7.55-7.58 (m, 4H), 3.84 (t, *J* = 7.60Hz, 2H), 1.49-1.54 (m, 2H), 0.63-0.67 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 161.6, 156.5, 147.3, 135.9, 134.8,

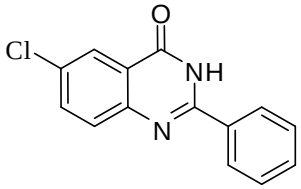
130.0, 129.7, 128.9, 128.8, 128.4, 127.6, 127.4, 126.6, 120.9, 47.1, 21.7, 11.4. ESI-MS (negative mode), m/z = 263 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 2983, 1677, 1604, 1461, 1360, 1249, 1073, 770, 697. Anal. calcd. (%) for C17H16N2O: C, 77.25; H, 6.10; N, 10.60. Found: C, 77.45; H, 6.32; N, 10.46.

3-benzyl-2-phenyl-4(3*H*)-quinazolinone (3n)

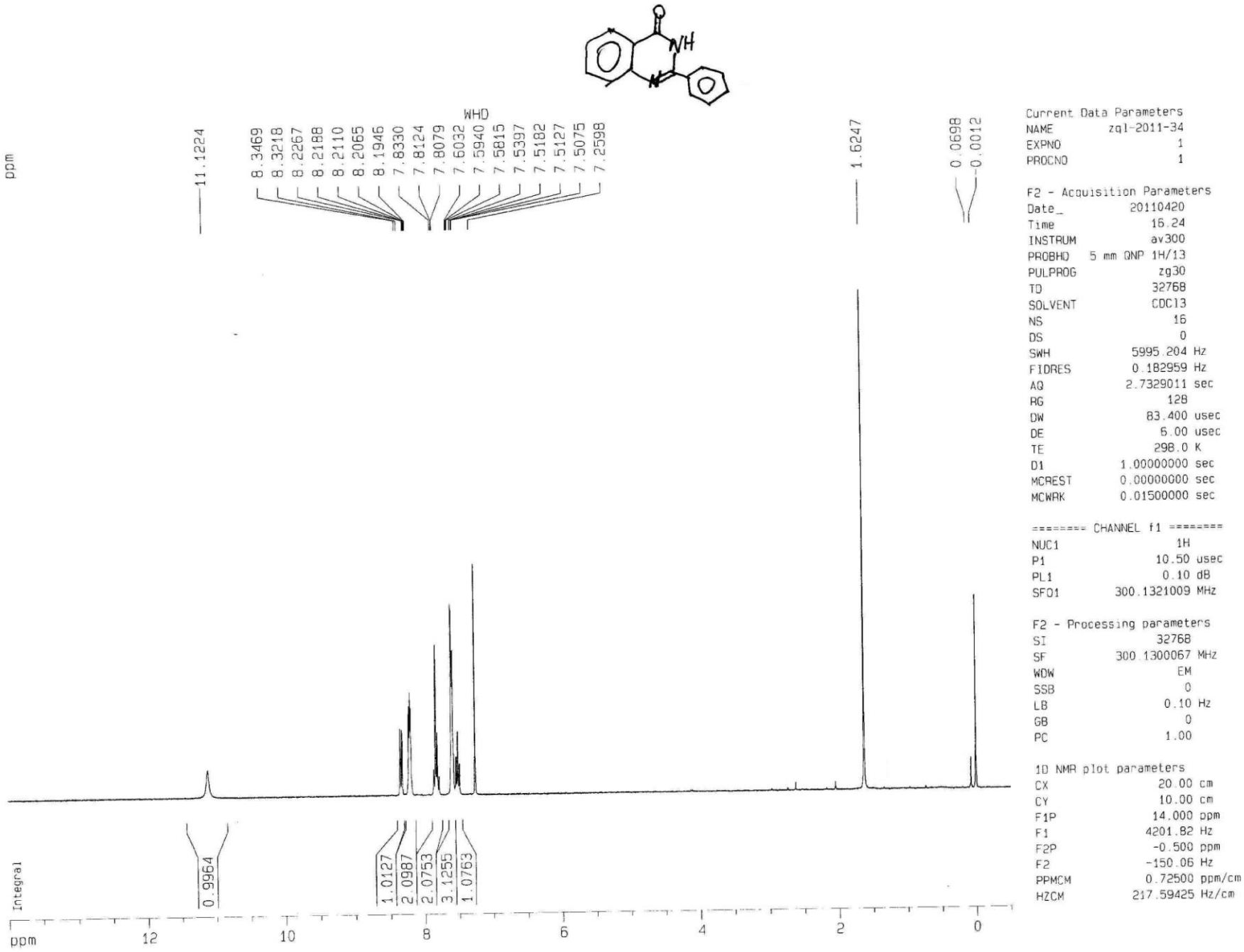


White solid. Mp 148-150 °C. ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm): 8.21-8.23 (m, 1H), 7.88 (t, *J* = 7.60 Hz, 1H), 7.72 (d, *J* = 8.00 Hz, 1H), 7.58-7.62 (m, 1H), 7.40-7.50 (m, 5H), 7.22 (d, *J* = 6.00 Hz, 3H), 6.92 (d, *J* = 6.80 Hz, 2H), 5.19 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6), δ (ppm): 161.8, 156.6, 147.4, 137.1, 135.6, 135.2, 130.1, 128.8, 128.6, 128.4, 127.8, 127.6, 127.5, 126.8, 126.7, 120.8, 48.6. ESI-MS (negative mode), m/z = 311 $[M–H]^-$. IR (KBr), ν (cm^{-1}): 3033, 1674, 1584, 1352, 1244, 949, 771, 698. Anal. calcd. (%) for C21H16N2O: C, 80.75; H, 5.16; N, 8.97. Found: C, 80.87; H, 5.28; N, 8.82.

6-chloro-2-phenylquinazolin-4(3H)-one (3o)



White solid, Mp. 282-284 °C. ^{1}H NMR (300 MHz, $CDCl_3$), δ (ppm): 12.75 (br, 1H), 8.17 (d, J = 6.9 Hz, 2H), 8.09 (d, J = 2.1 Hz, 1H), 7.87 (dd, J1 = 8.7 Hz, J2 = 2.1 Hz, 1H), 7.77 (d, J = 87 Hz, 1H), 7.53-7.63 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm): 161.4, 152.9, 147.4, 134.7, 130.8, 129.7, 128.6, 127.8, 124.9, 122.2. IR (KBr), ν (cm^{-1}): 3724, 3565, 2983, 2351, 1681, 1605, 1577, 1482, 1305, 1158, 1122, 946, 888, 847, 770, 667. Anal. calcd. (%) for C14H9ClN2O: C, 65.51; H, 3.53; N, 10.91. Found: C, 65.57; H, 3.59; N, 10.42.



Current Data Parameters

NAME	zq1-2011-34
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20110420
Time	16.24
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	298.0 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

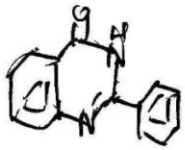
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

F2 - Processing parameters

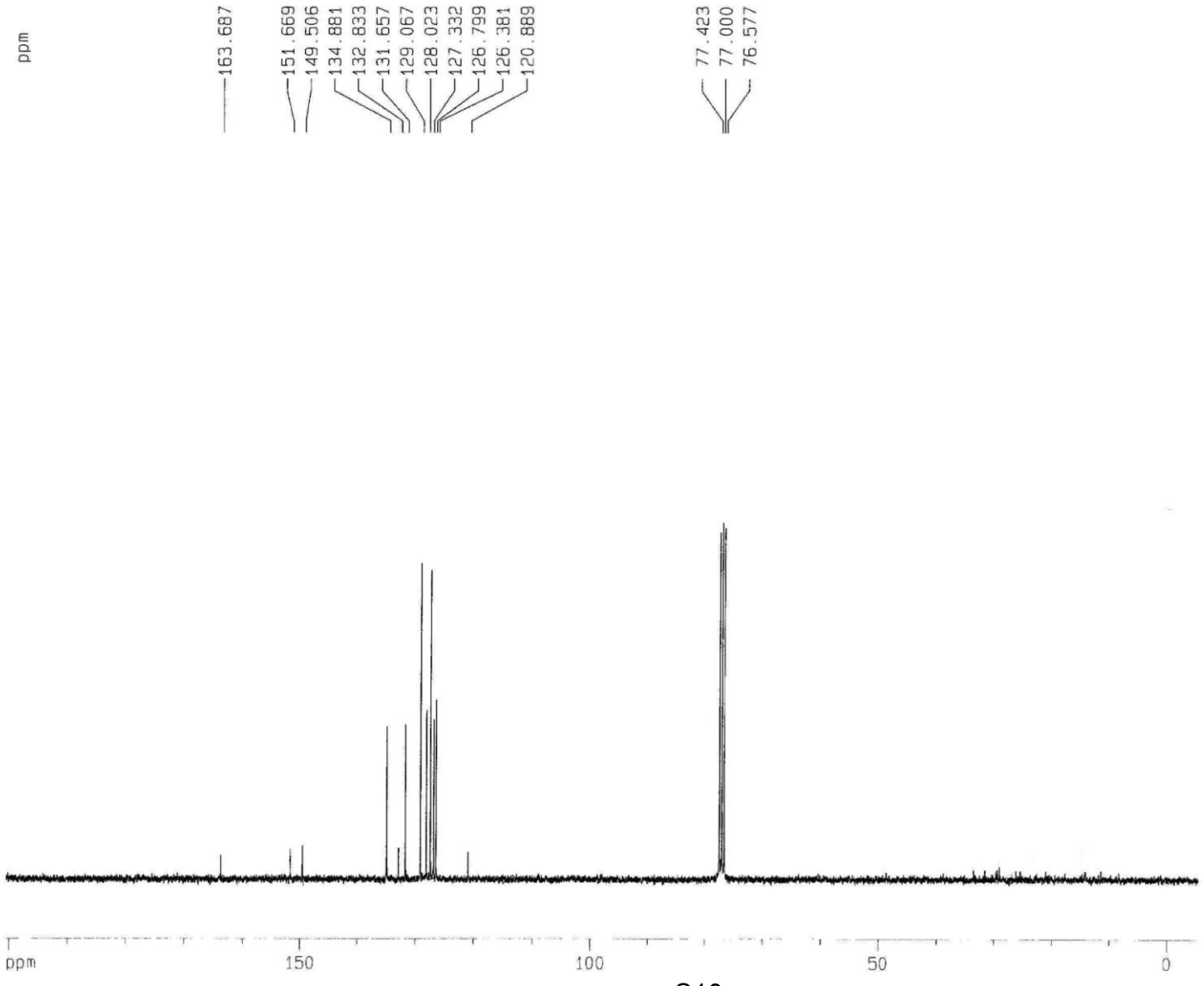
SI	32768
SF	300.1300067 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	14.000 ppm
F1	4201.82 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.72500 ppm/cm
HZCM	217.59425 Hz/cm



ZD-1




```
Current Data Parameters
NAME        zql-2011-176
EXPNO                 2
PROCNO                1

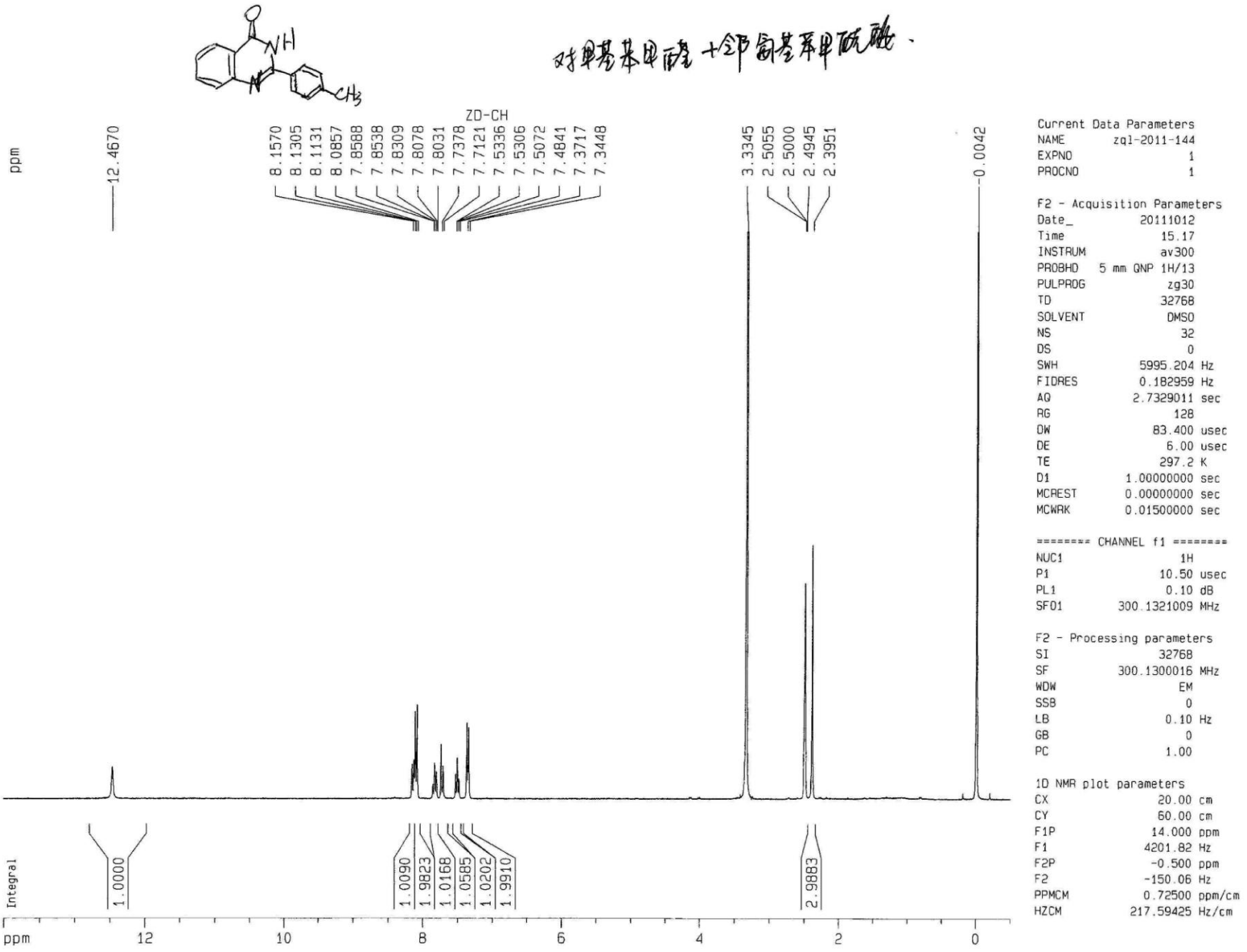
F2 - Acquisition Parameters
Date_          20111116
Time              14.27
INSTRUM           av300
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg
TD               65536
SOLVENT          CDCl3
NS                2391
DS                   4
SWH          22675.736 Hz
FIDRES        0.346004 Hz
AQ            1.4451188 sec
RG                8192
DW              22.050 usec
DE               6.00 usec
TE              296.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1               10.50 usec
PL1              -0.81 dB
SFO1         75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2               0.10 dB
PL12             17.74 dB
PL13             17.74 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI               65536
SF          75.4677497 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40

1D NMR plot parameters
CX              20.00 cm
CY               6.00 cm
F1P            200.500 ppm
F1           15131.28 Hz
F2P             -5.500 ppm
F2            -415.07 Hz
PPMCM        10.30000 ppm/cm
HZCM        777.31787 Hz/cm
```



Current Data Parameters

NAME	zql-2011-144
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20111012
Time	15.17
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	297.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

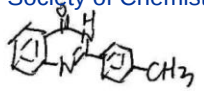
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

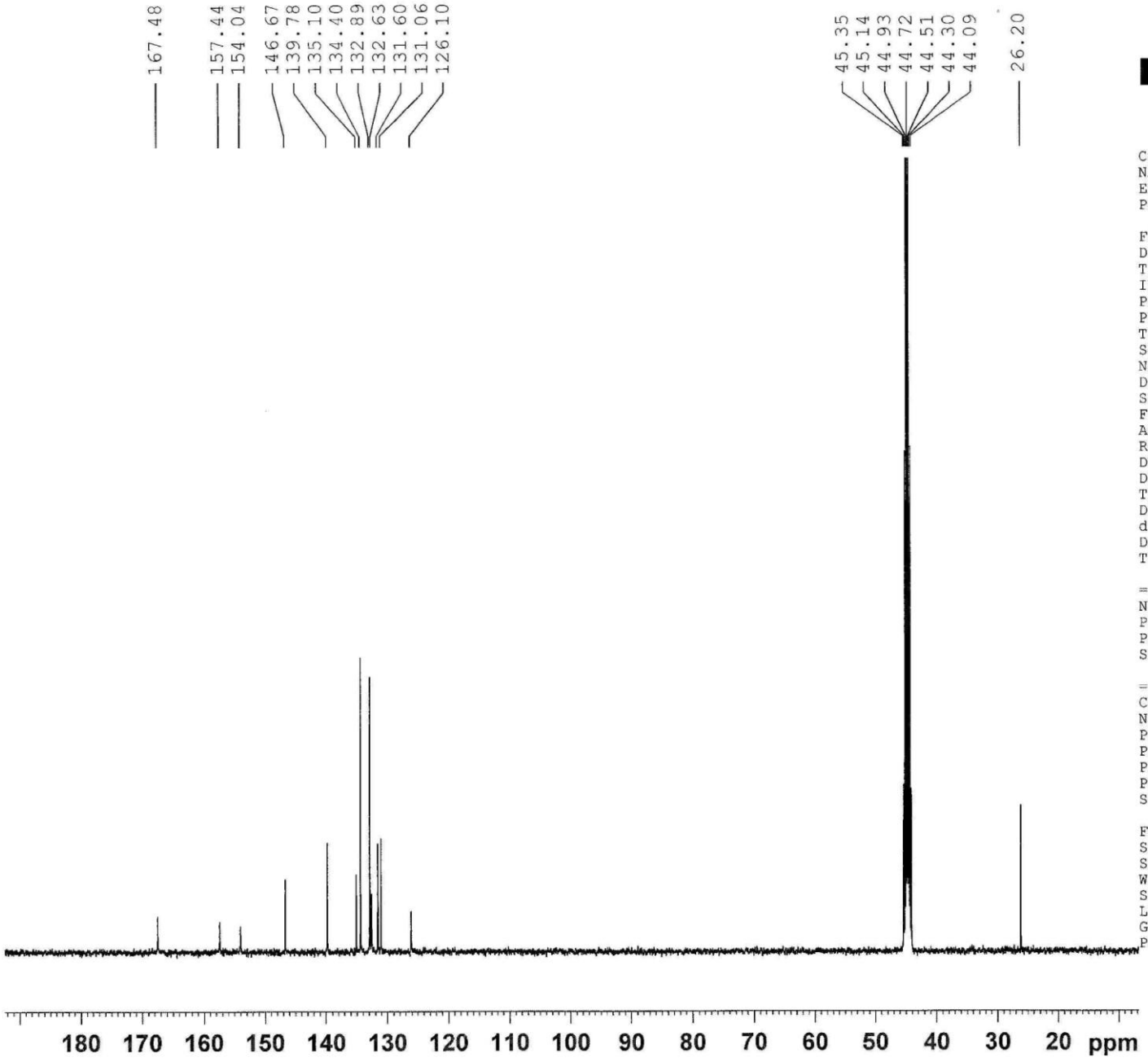
F2 - Processing parameters

SI	32768
SF	300.1300016 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	60.00 cm
F1P	14.000 ppm
F1	4201.82 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.72500 ppm/cm
HZCM	217.59425 Hz/cm





BRUKER

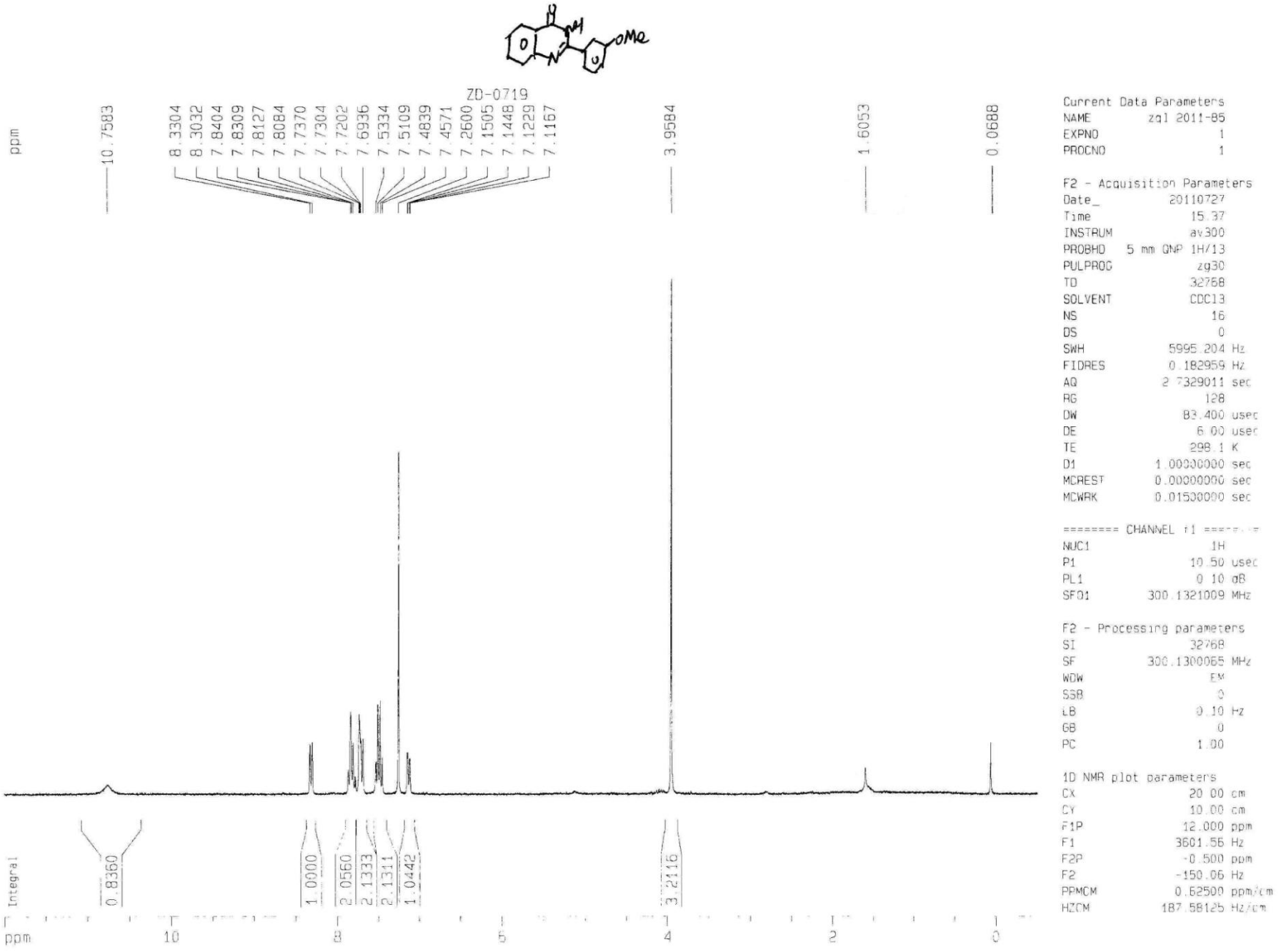
```
Current Data Parameters
NAME      2011-11-30 zandan-ZD-9
EXPNO                          2
PROCNO                         1

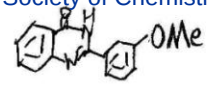
F2 - Acquisition Parameters
Date_              20111130
Time                  15.34
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     580
DS                       0
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                    90.5
DW                  20.800 usec
DE                   6.50 usec
TE                  300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

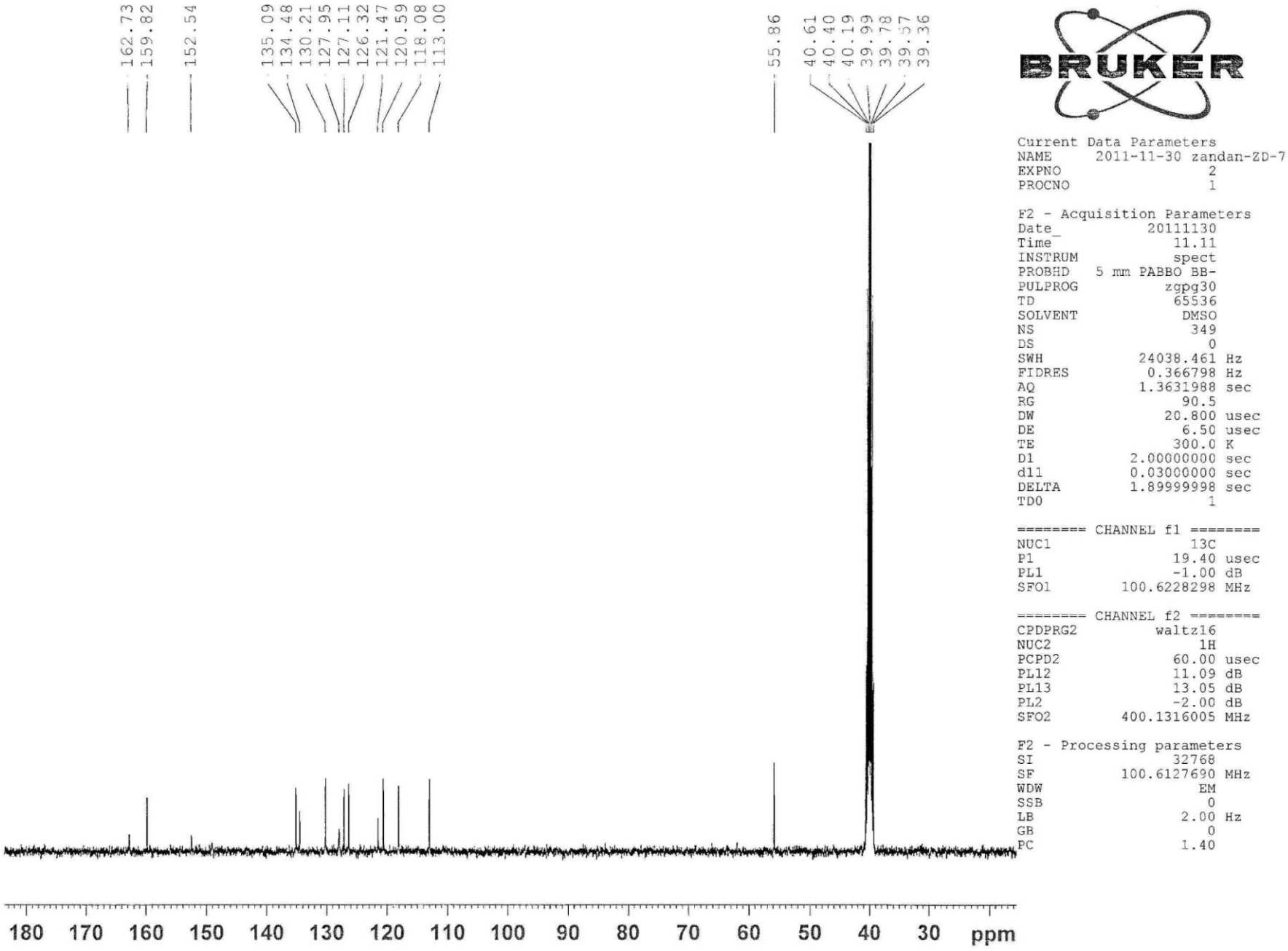
======== CHANNEL f1 ========
NUC1                   13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127690 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.40
```







BRUKER

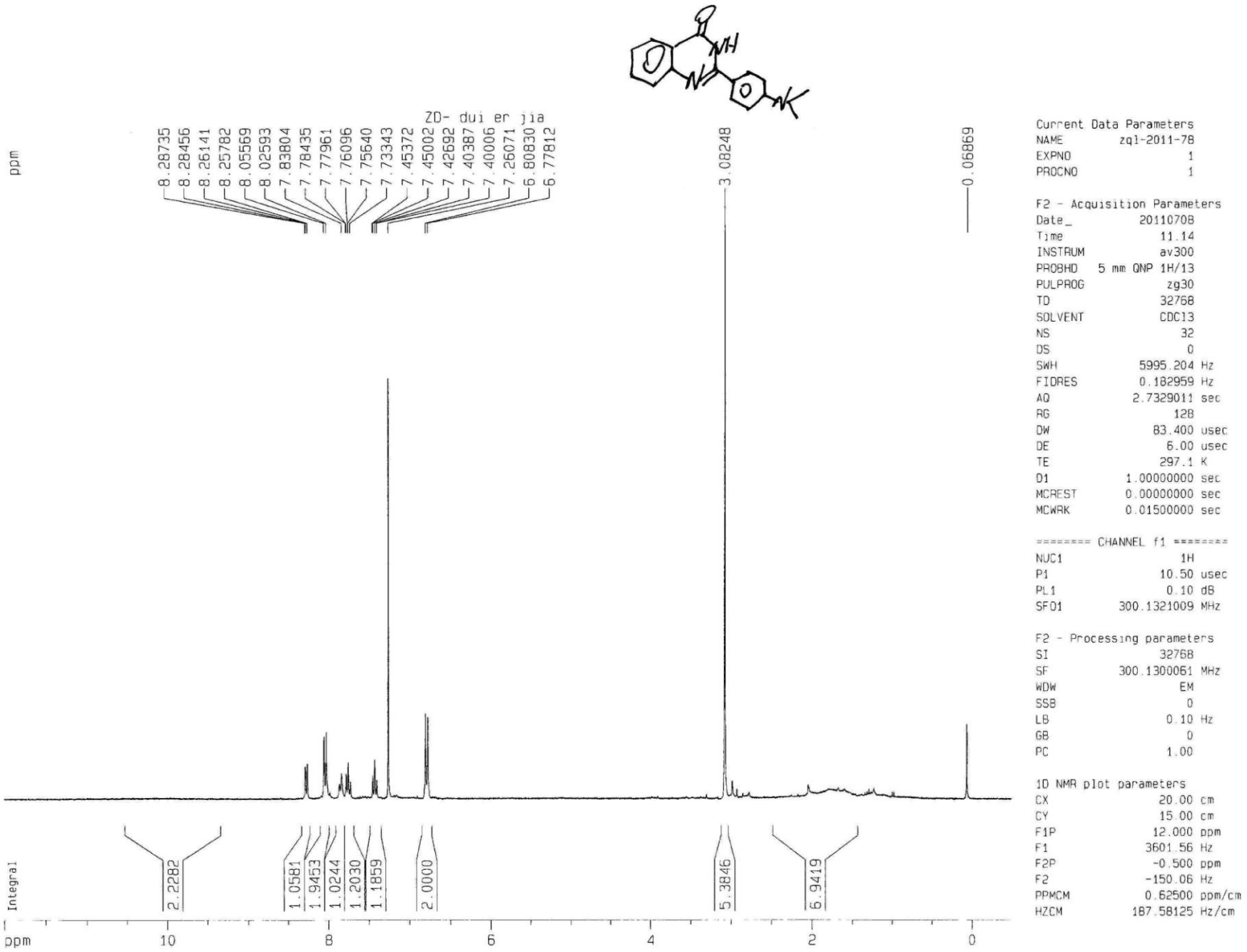
```
Current Data Parameters
NAME      2011-11-30 zandan-ZD-7
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20111130
Time                       11.11
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                      DMSO
NS                            349
DS                              0
SWH                     24038.461 Hz
FIDRES                   0.366798 Hz
AQ                       1.3631988 sec
RG                            90.5
DW                          20.800 usec
DE                           6.50 usec
TE                          300.0 K
D1                      2.00000000 sec
d11                     0.03000000 sec
DELTA                   1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                          19.40 usec
PL1                         -1.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                       60.00 usec
PL12                        11.09 dB
PL13                        13.05 dB
PL2                         -2.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                            32768
SF                  100.6127690 MHz
WDW                              EM
SSB                               0
LB                             2.00 Hz
GB                                0
PC                             1.40
```



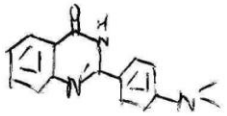
Current Data Parameters
NAME zql-2011-78
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110708
Time 11.14
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

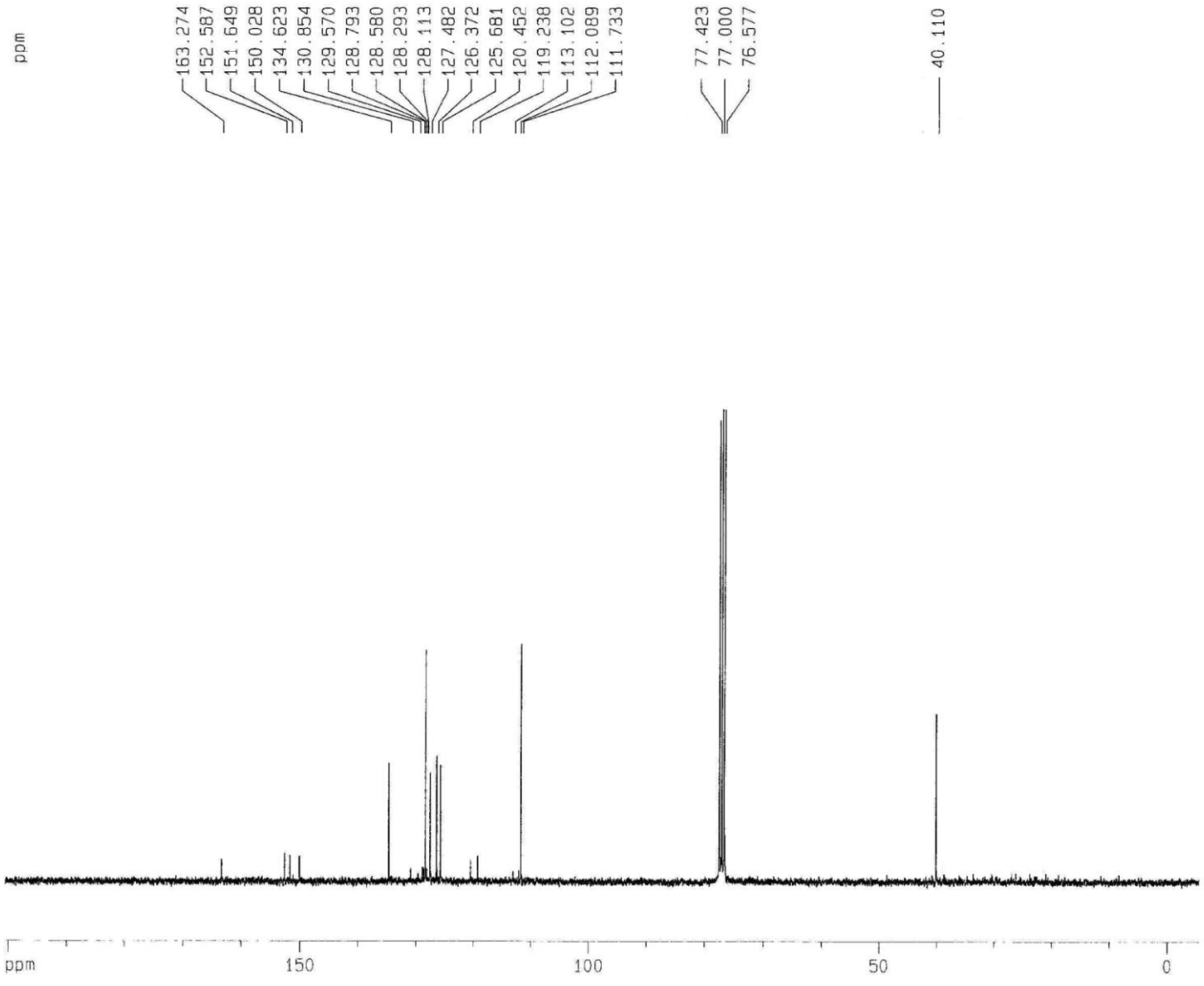
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz

F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm



ZD-3



Current Data Parameters

NAME	zql-2011-178
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20111115
Time	22.11
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	4096
DS	4
SWH	22675.736 Hz
FIDRES	0.346004 Hz
AQ	1.4451188 sec
RG	8192
DW	22.050 usec
DE	6.00 usec
TE	297.7 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

NUC1	13C
P1	10.50 usec
PL1	-0.81 dB
SF01	75.4760505 MHz

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

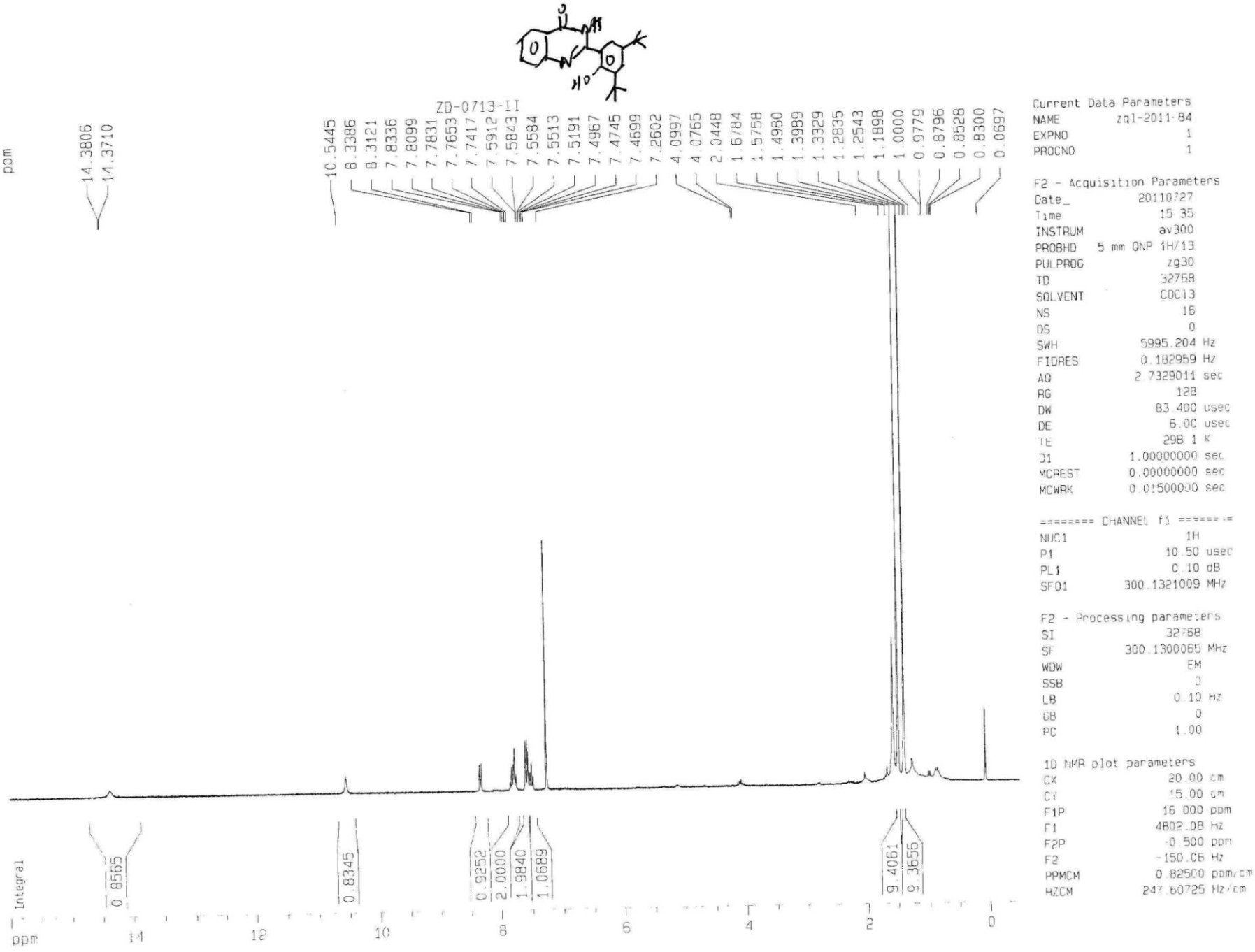
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.10 dB
PL12	17.74 dB
PL13	17.74 dB
SF02	300.1312005 MHz

F2 - Processing parameters

SI	65536
SF	75.4677494 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
CY	8.00 cm
F1P	200.500 ppm
F1	15131.28 Hz
F2P	-5.500 ppm
F2	-415.07 Hz
PPMCM	10.30000 ppm/cm
HZCM	777.31787 Hz/cm



Current Data Parameters

NAME	zq1-2011-84
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20110727
Time	15 35
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	298.1 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

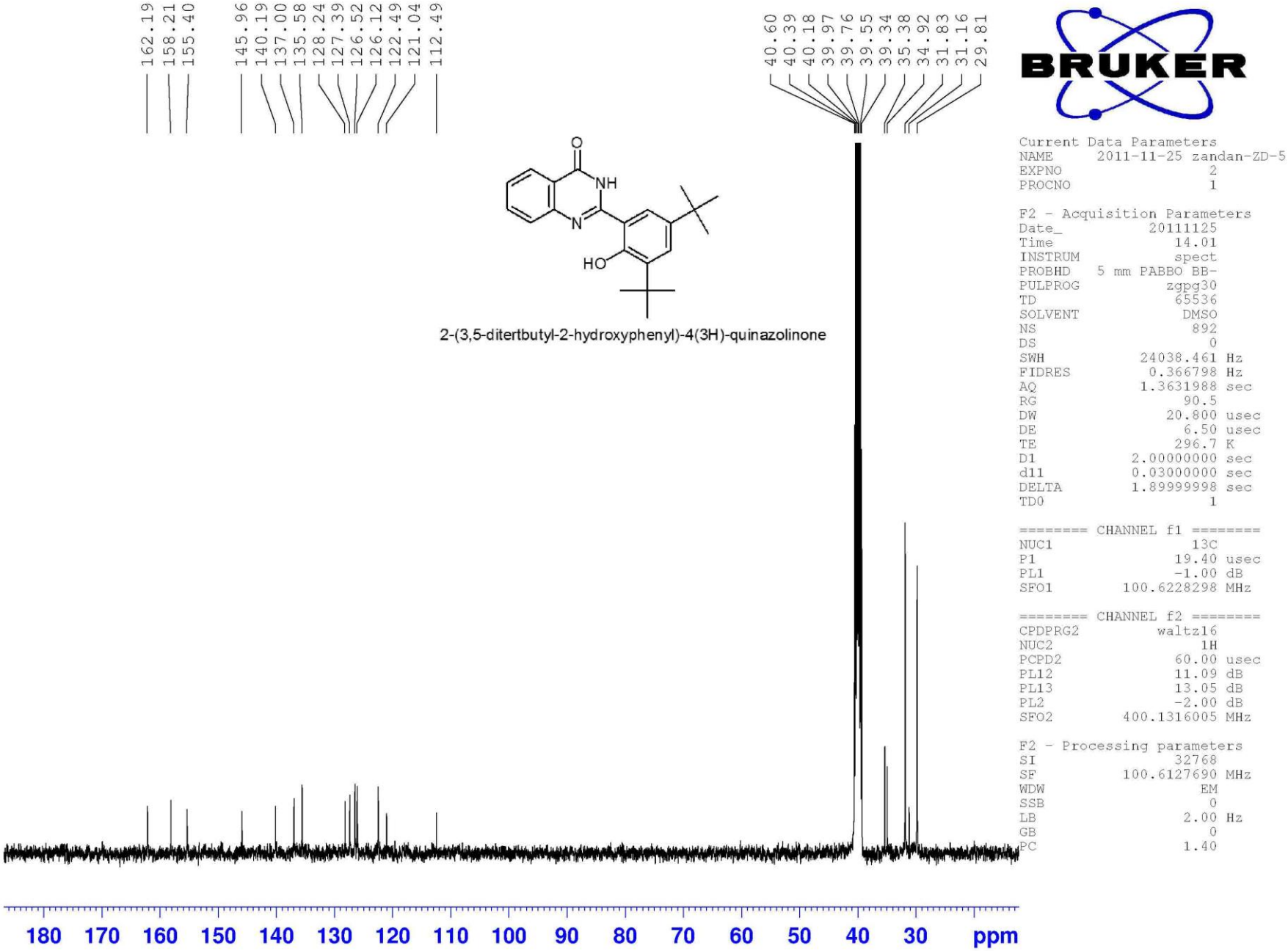
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

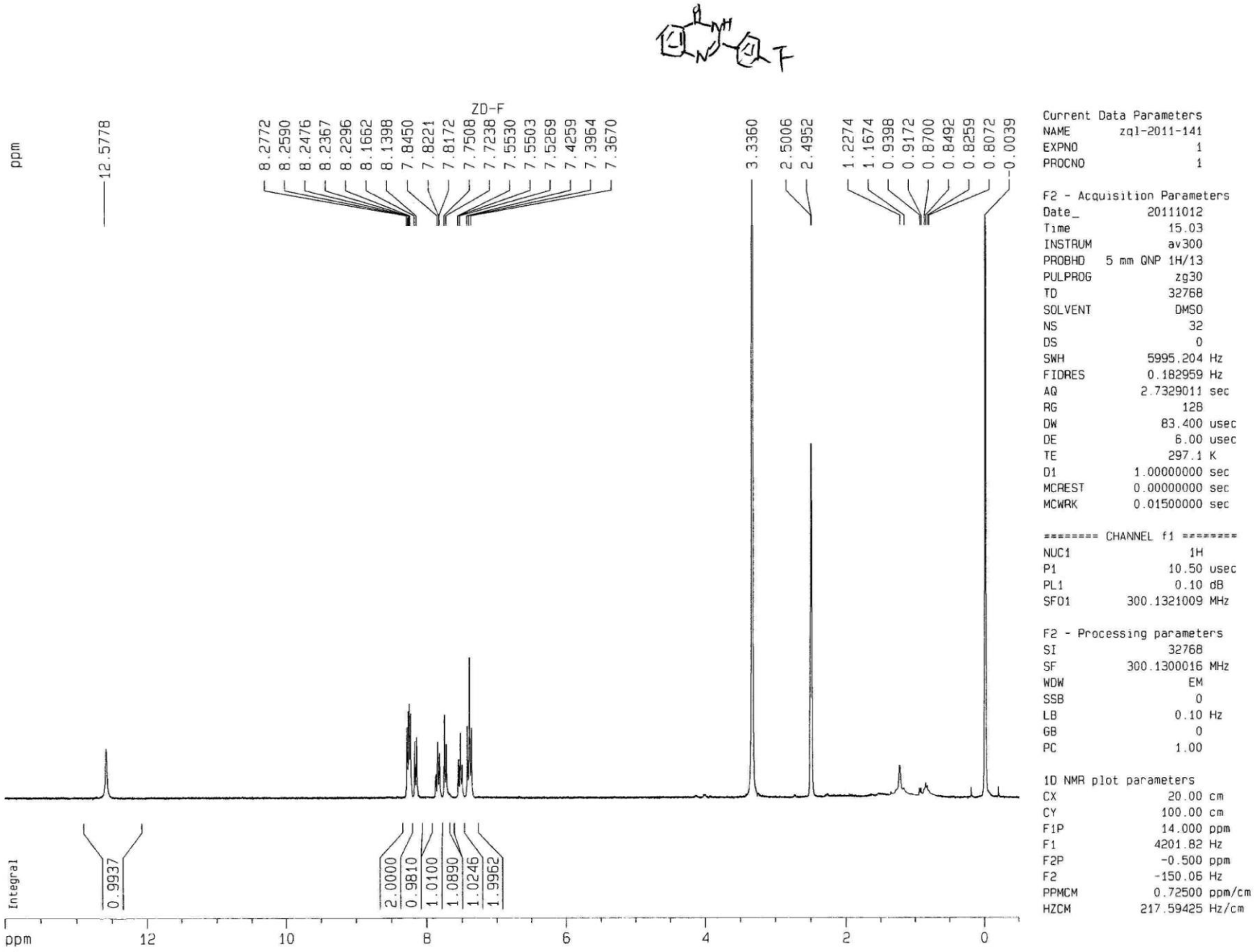
F2 - Processing parameters

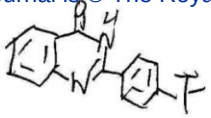
SI	32768
SF	300.1300065 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

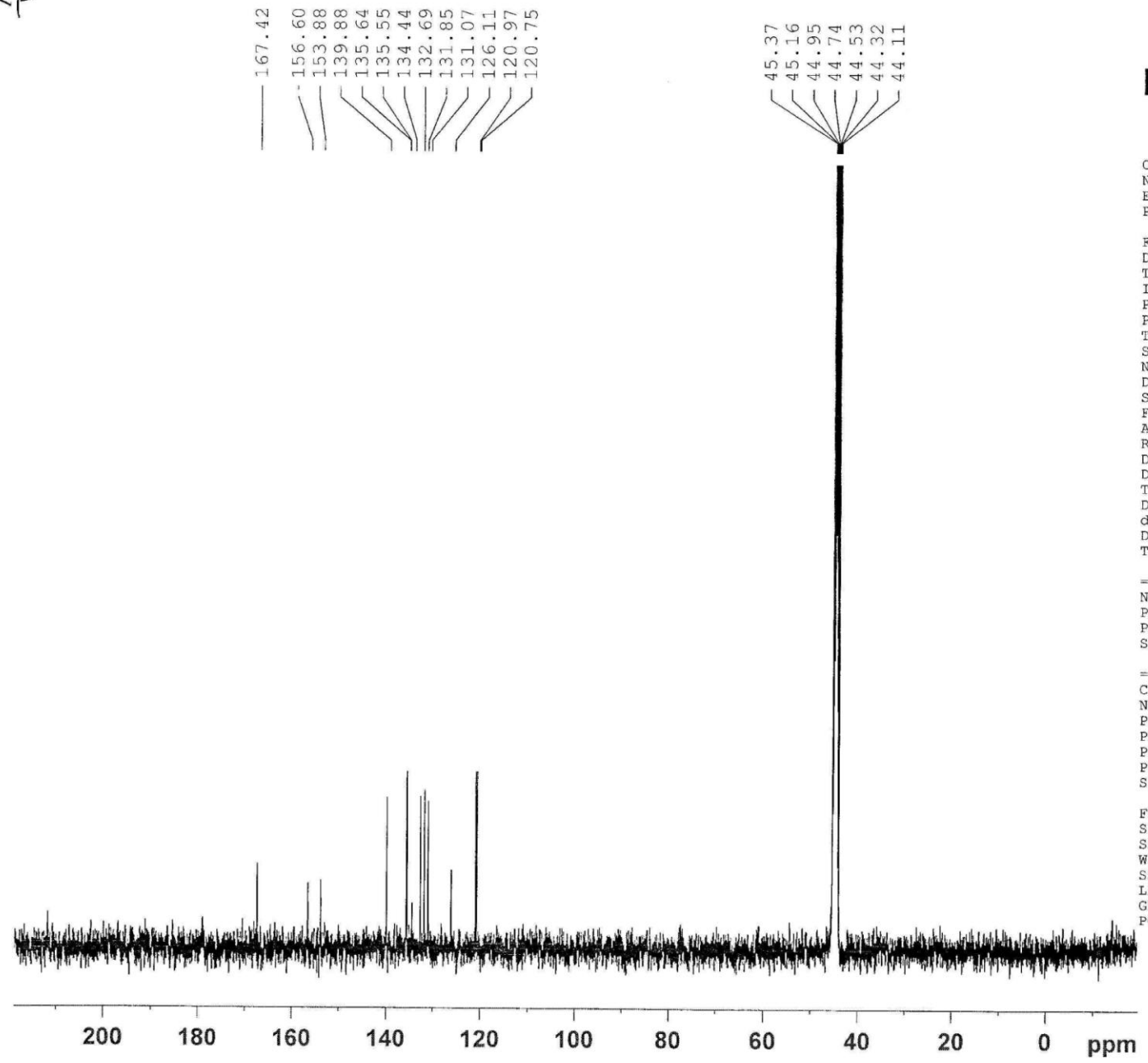
1D NMR plot parameters

CX	20.00 cm
CY	15.00 cm
F1P	16.000 ppm
F1	4802.08 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.82500 ppm/cm
HZCM	247.60725 Hz/cm









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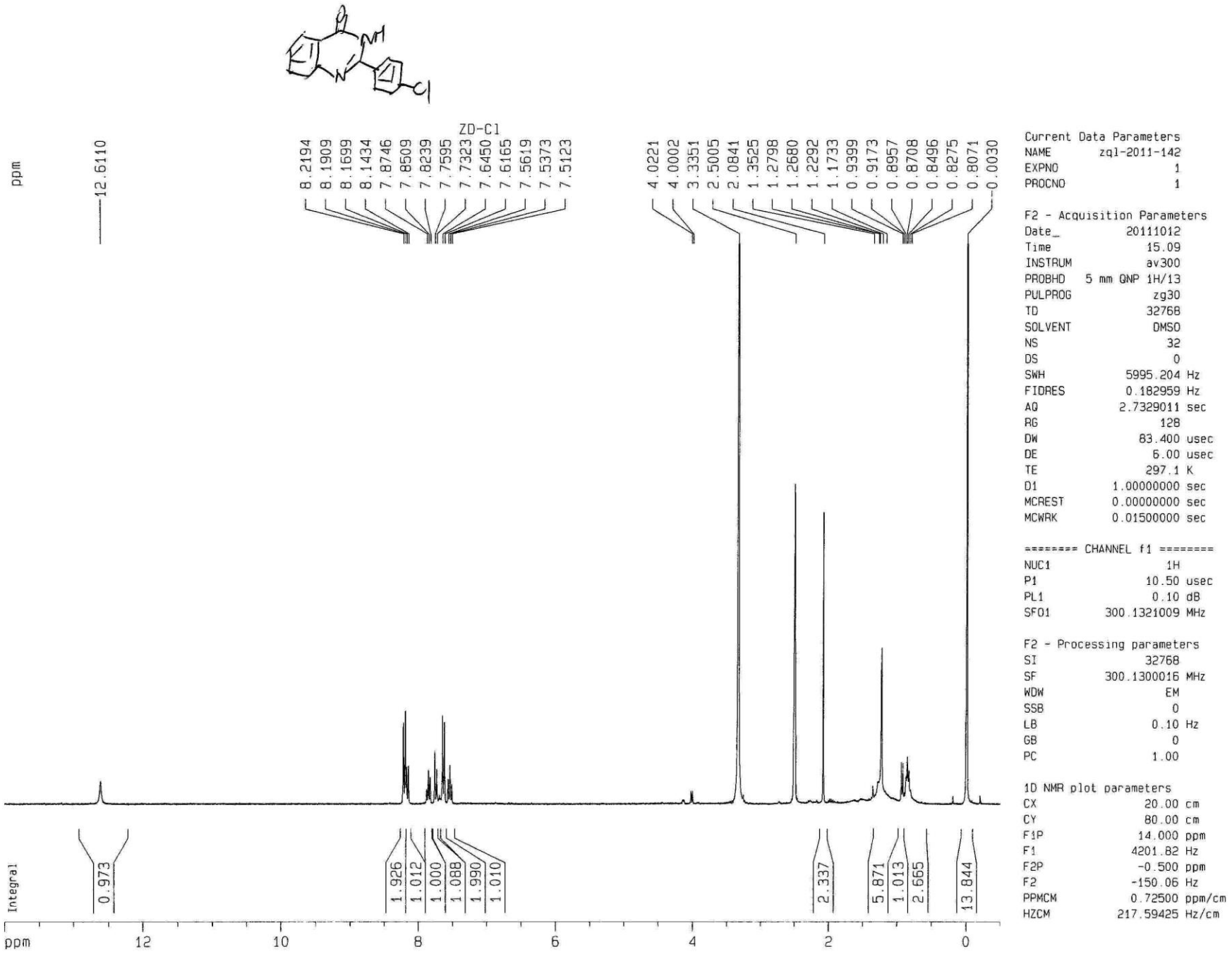
```
Current Data Parameters
NAME      2011-11-30 zandan-ZD-11
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20111130
Time              12.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  872
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 90.5
DW                20.800 usec
DE                 6.50 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                19.40 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```



Current Data Parameters

NAME	zql-2011-142
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20111012
Time	15.09
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	297.1 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

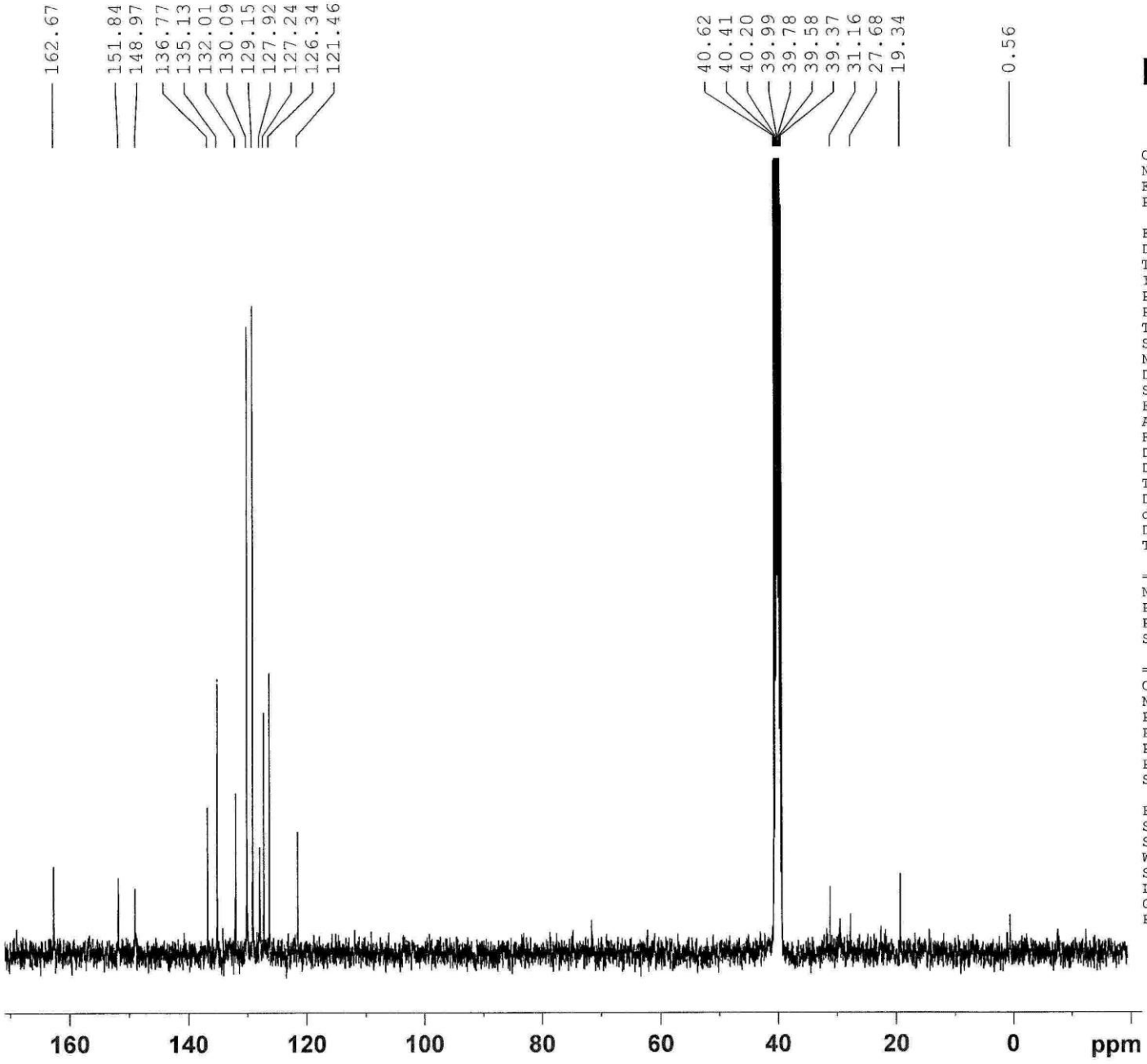
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

F2 - Processing parameters

SI	32768
SF	300.1300016 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	80.00 cm
F1P	14.000 ppm
F1	4201.82 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.72500 ppm/cm
HZCM	217.59425 Hz/cm




```
Current Data Parameters
NAME      2011-11-30 zandan-ZD-10
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20111130
Time              14.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD              65536
SOLVENT          DMSO
NS                 684
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                90.5
DW              20.800 usec
DE               6.50 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                19.40 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            60.00 usec
PL12             11.09 dB
PL13             13.05 dB
PL2              -2.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                  0
LB                2.00 Hz
GB                   0
PC                1.40
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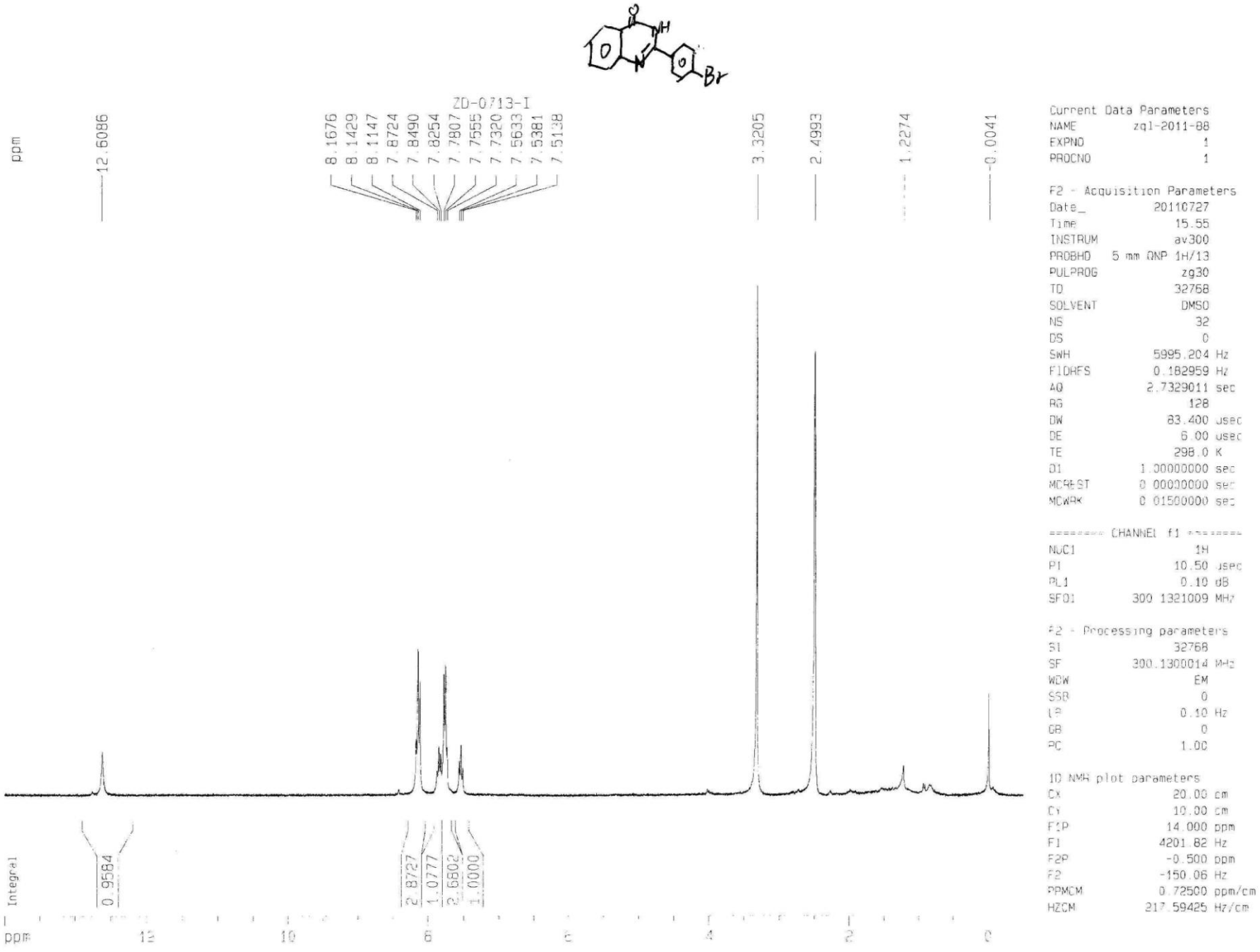


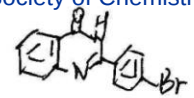
Current Data Parameters
NAME zql-2011-88
EXPNO 1
PROCNO 1

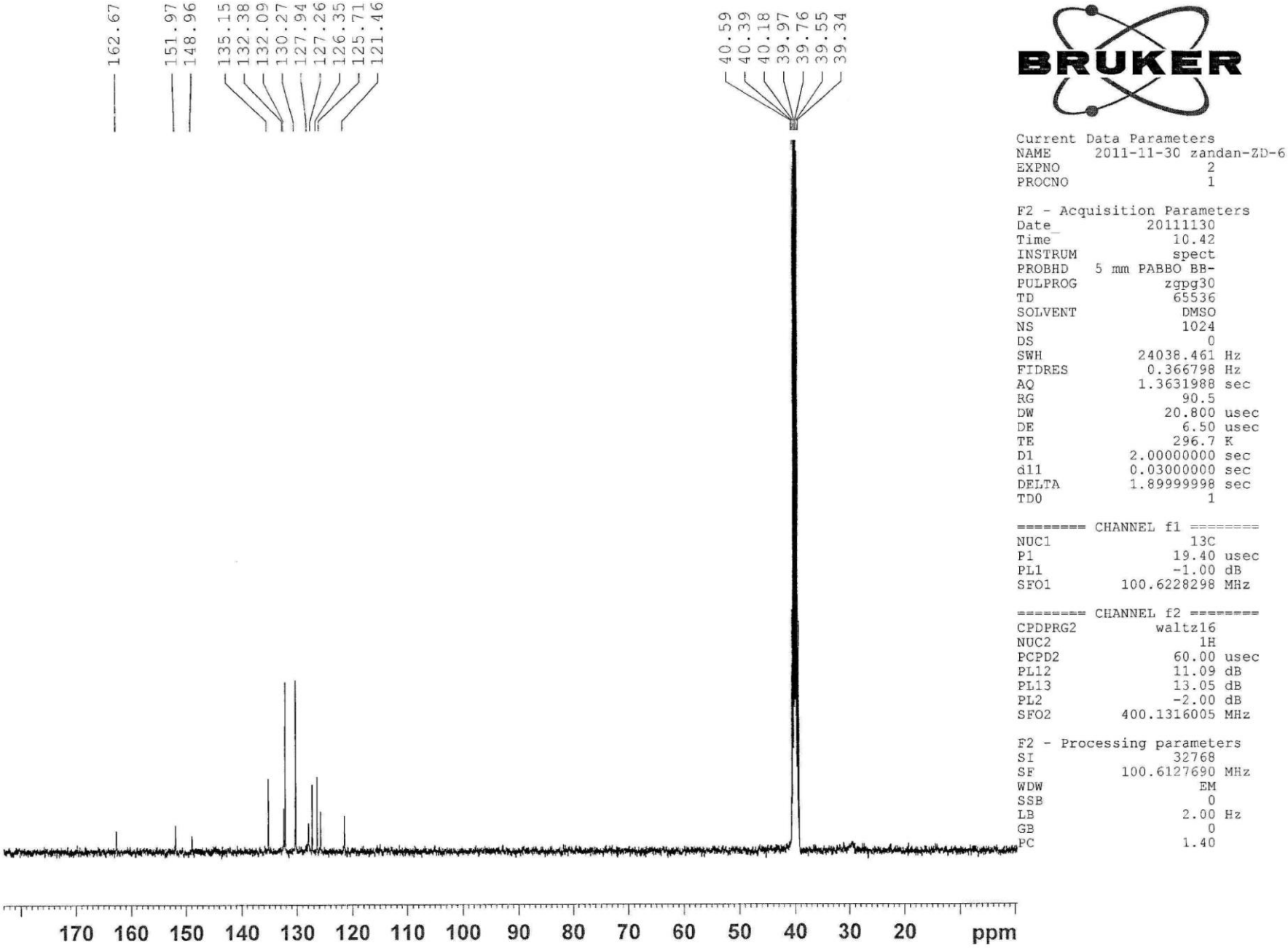
F2 - Acquisition Parameters
Date_ 20110727
Time 15.55
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz

F2 - Processing parameters
SI 32768
SF 300.1300014 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 14.000 ppm
F1 4201.82 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.72500 ppm/cm
HZCM 217.59425 Hz/cm





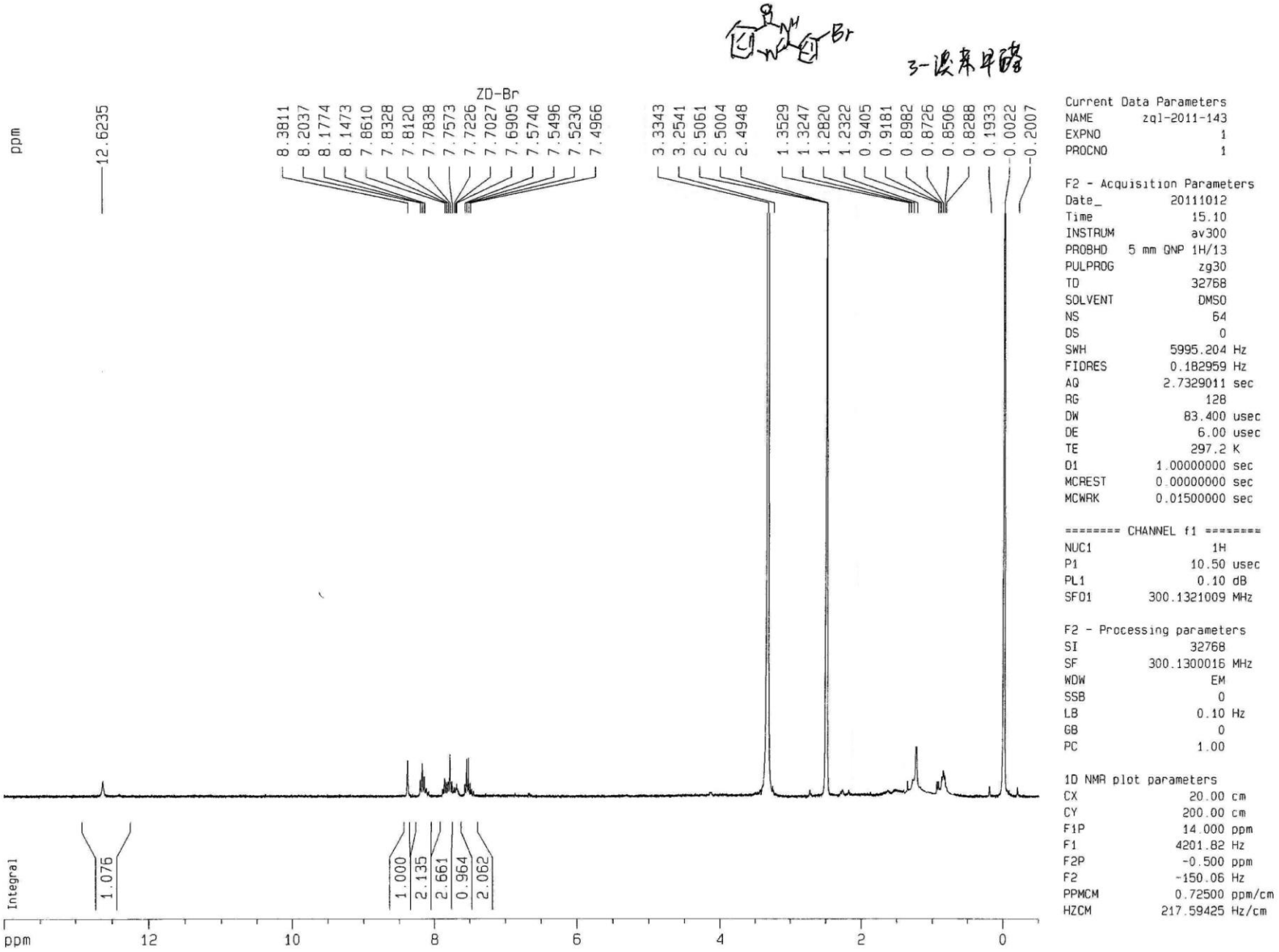

```
Current Data Parameters
NAME      2011-11-30 zandan-ZD-6
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20111130
Time                       10.42
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                     DMSO
NS                          1024
DS                             0
SWH                    24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                          90.5
DW                        20.800 usec
DE                         6.50 usec
TE                        296.7 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                        19.40 usec
PL1                       -1.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     60.00 usec
PL12                      11.09 dB
PL13                      13.05 dB
PL2                       -2.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                           32768
SF                  100.6127690 MHz
WDW                             EM
SSB                              0
LB                        2.00 Hz
GB                               0
PC                             1.40
```



Current Data Parameters

NAME	zql-2011-143
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20111012
Time	15.10
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	64
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	297.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

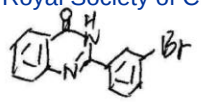
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

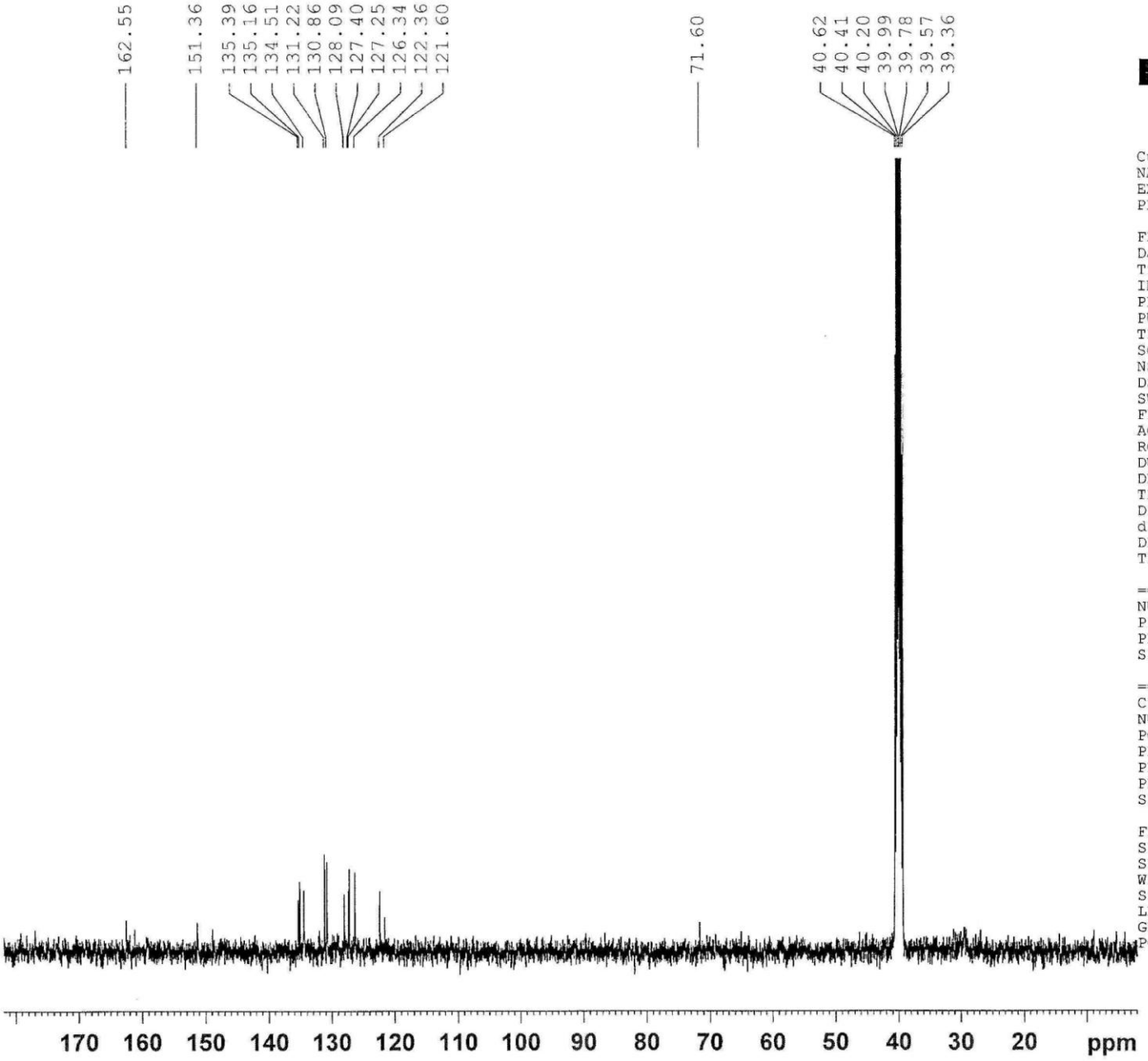
F2 - Processing parameters

SI	32768
SF	300.1300016 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	200.00 cm
F1P	14.000 ppm
F1	4201.82 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.72500 ppm/cm
HZCM	217.59425 Hz/cm





BRUKER

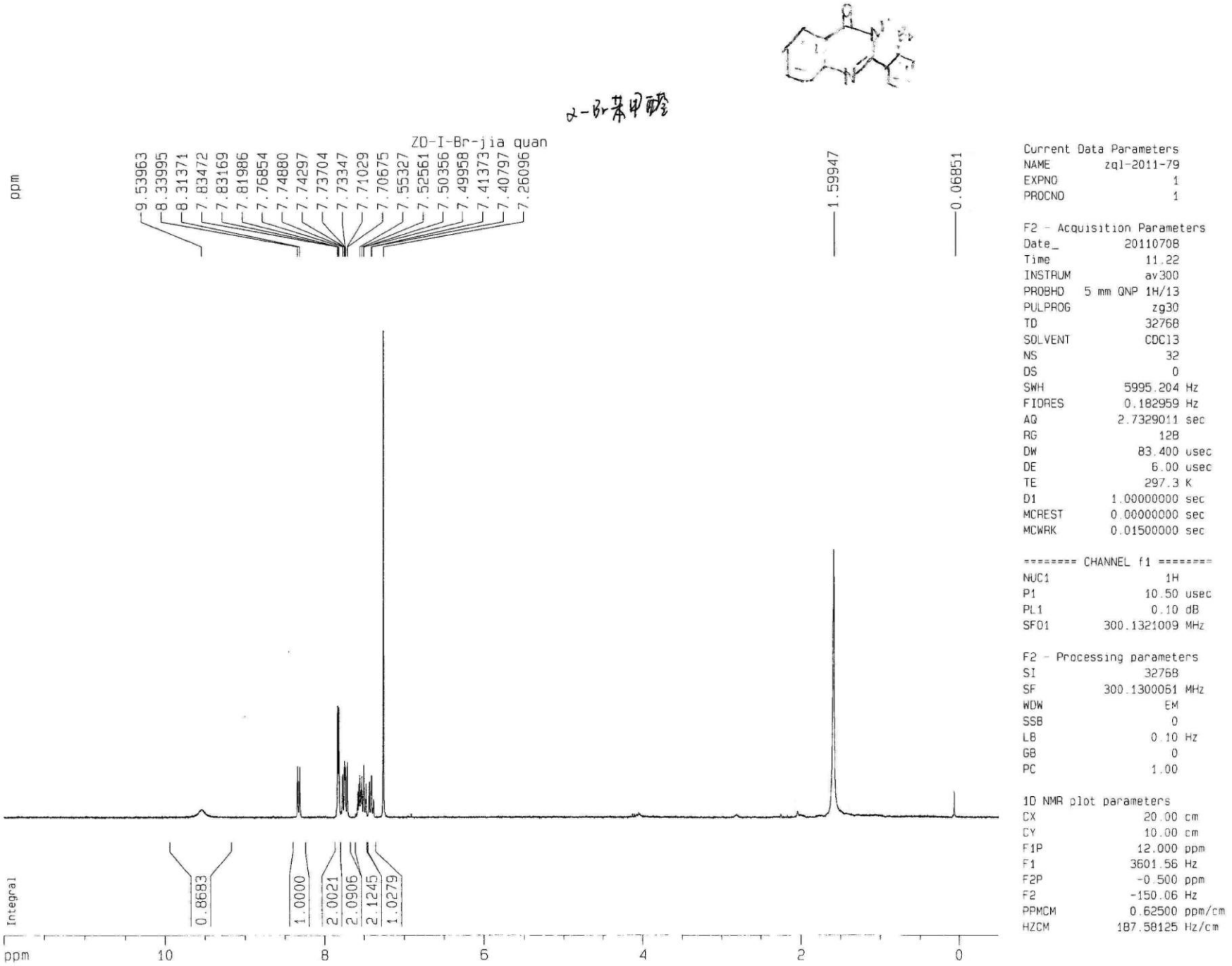
```
Current Data Parameters
NAME      2011-11-25 zandan-ZD-8
EXPNO                  2
PROCNO                 1

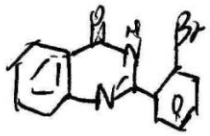
F2 - Acquisition Parameters
Date_           20111125
Time               10.31
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                   512
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                90.5
DW              20.800 usec
DE               6.50 usec
TE              296.8 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                19.40 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

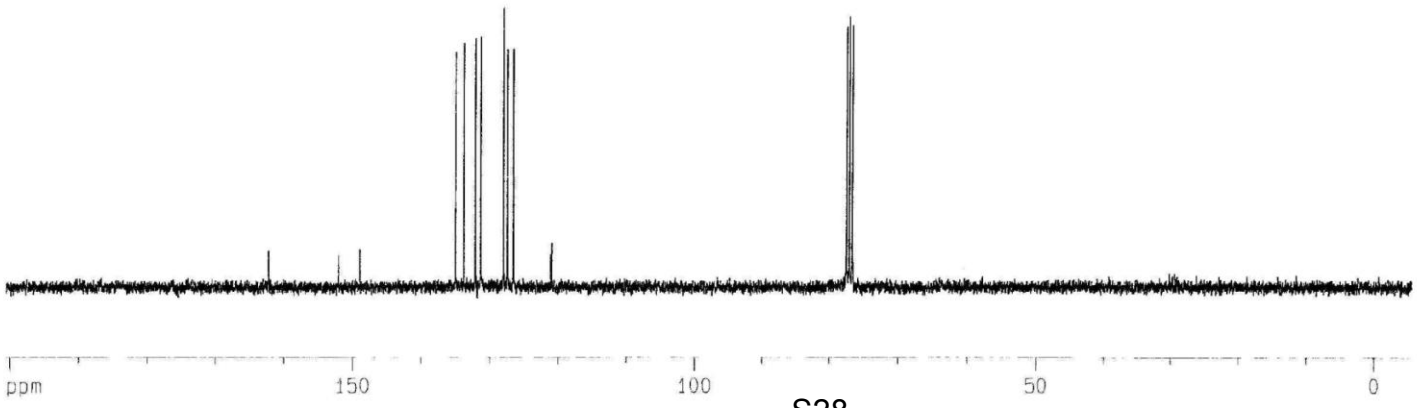

2-Br苯甲醛
ZD-I-Br-jia quan
ppm
9.53963
8.33995
8.31371
7.83472
7.83169
7.81986
7.76854
7.74880
7.74297
7.73704
7.73347
7.71029
7.70675
7.55327
7.52561
7.50356
7.49958
7.41373
7.40797
7.26096
1.59947
0.06851
Integral
0.8683
1.0000
2.0021
2.0906
2.1245
1.0279
ppm
10
8
6
4
2
0
Current Data Parameters
NAME zql-2011-79
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110708
Time 11.22
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 297.3 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz
F2 - Processing parameters
SI 32768
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 12.000 ppm
F1 3601.56 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.62500 ppm/cm
HZCM 187.58125 Hz/cm



ZD-2

ppm

162.239
151.997
148.884
134.896
133.729
132.019
131.262
127.974
127.948
127.377
126.487
121.073
120.889
77.424
77.000
76.577




```
Current Data Parameters
NAME        zql-2011-177
EXPNO                  2
PROCNO                 1

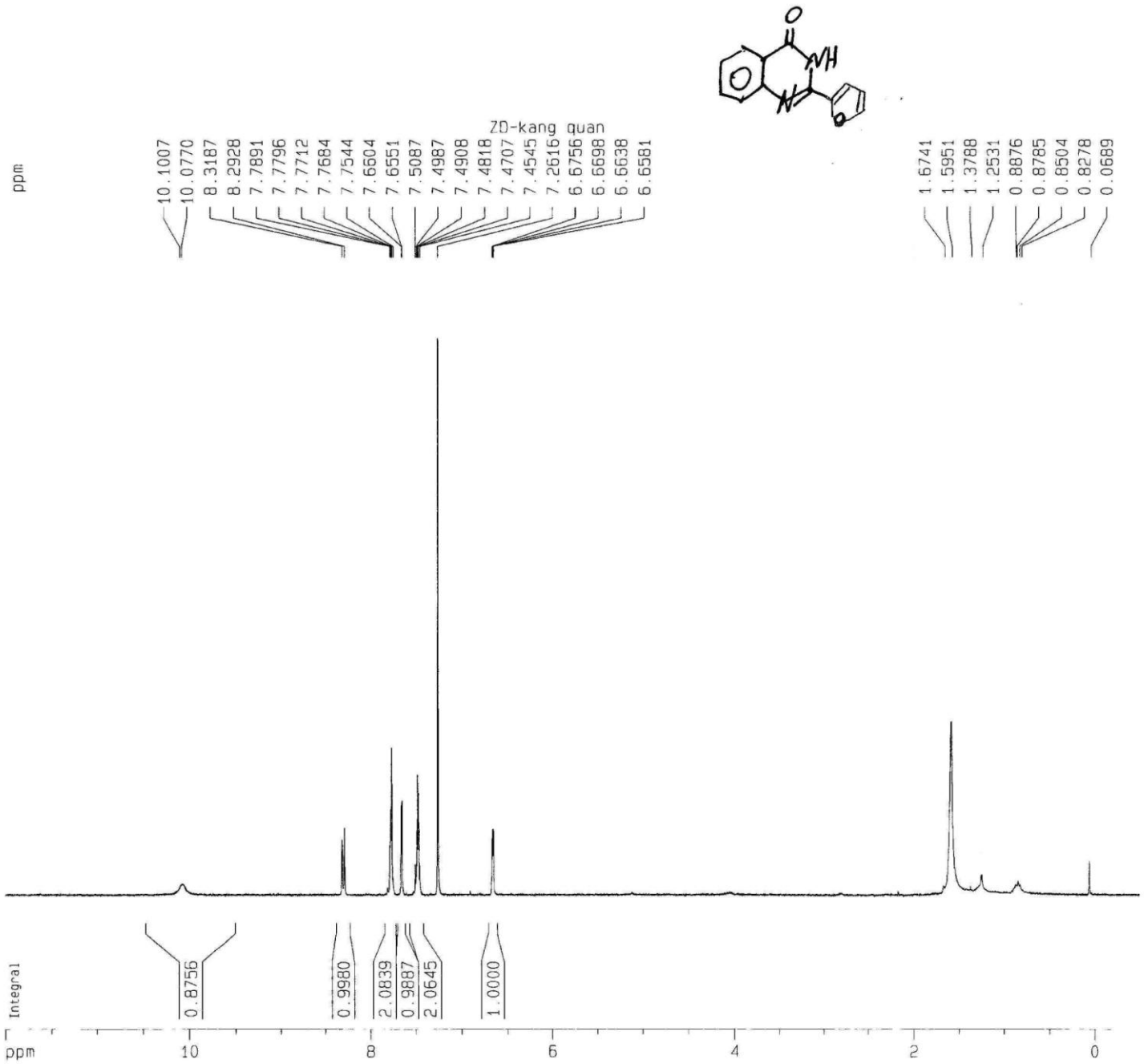
F2 - Acquisition Parameters
Date_           20111121
Time                9.34
INSTRUM            av300
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           22675.736 Hz
FIDRES         0.346004 Hz
AQ             1.4451188 sec
RG                  8192
DW                22.050 usec
DE                 6.00 usec
TE                295.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.50 usec
PL1                -0.81 dB
SFO1          75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.10 dB
PL12               17.74 dB
PL13               17.74 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 65536
SF            75.4677516 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                  4.00 cm
F1P               200.500 ppm
F1                15131.28 Hz
F2P                -5.500 ppm
F2                 -415.07 Hz
PPMCM             10.30000 ppm/cm
HZCM             777.31787 Hz/cm
```



Current Data Parameters

NAME	zql-2011-80
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20110708
Time	11.27
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	297.2 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

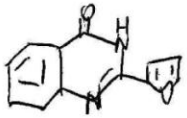
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SFO1	300.1321009 MHz

F2 - Processing parameters

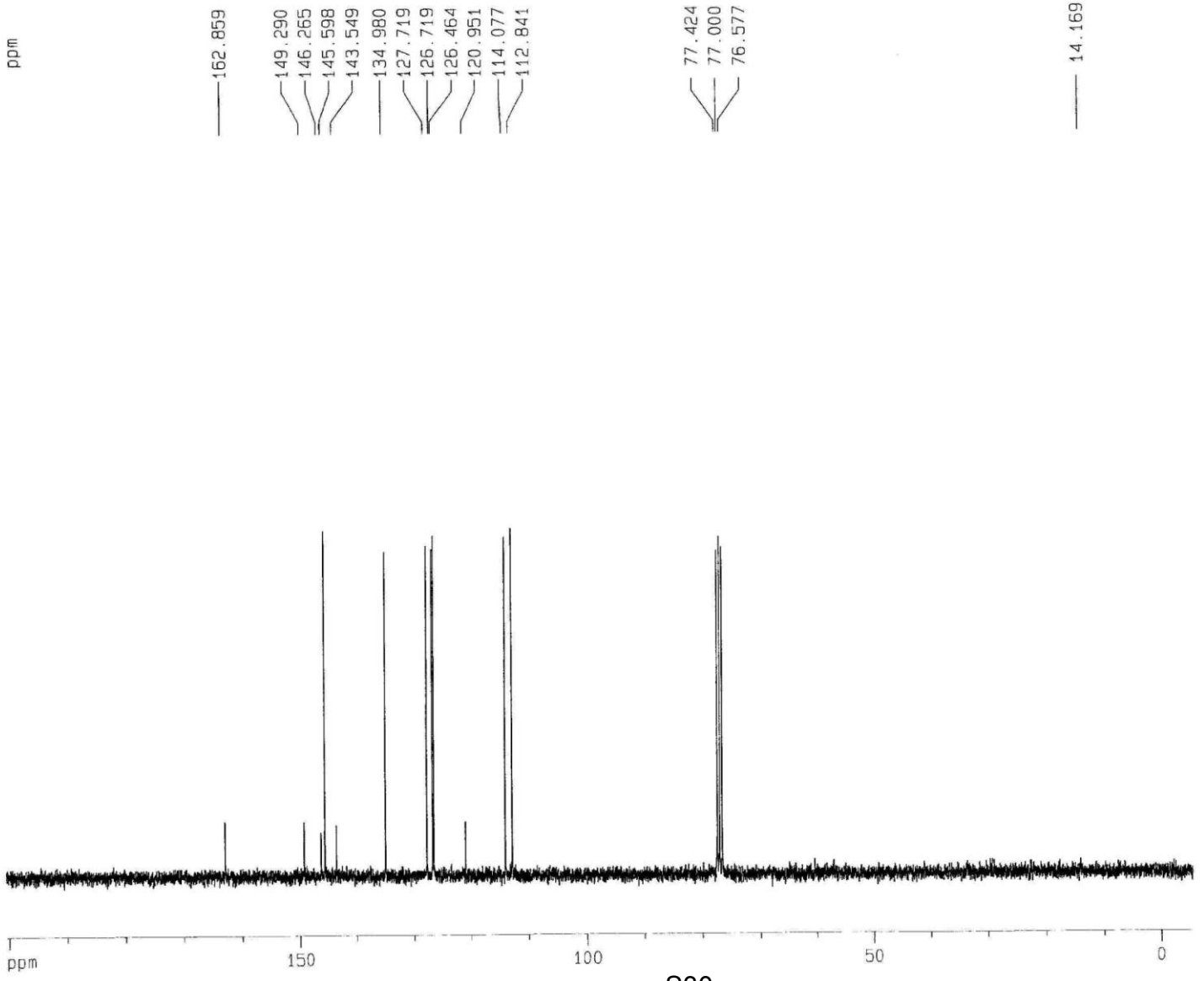
SI	32768
SF	300.1300061 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	10.00 cm
F1P	12.000 ppm
F1	3601.56 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.62500 ppm/cm
HZCM	187.58125 Hz/cm



ZD-4




```
Current Data Parameters
NAME        zql-2011-179
EXPNO                  2
PROCNO                 1

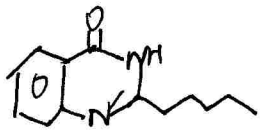
F2 - Acquisition Parameters
Date_           20111115
Time               16.34
INSTRUM            av300
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg
TD                 65536
SOLVENT             CDCl3
NS                   512
DS                     4
SWH          22675.736 Hz
FIDRES        0.346004 Hz
AQ            1.4451188 sec
RG                  8192
DW               22.050 usec
DE                6.00 usec
TE               294.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

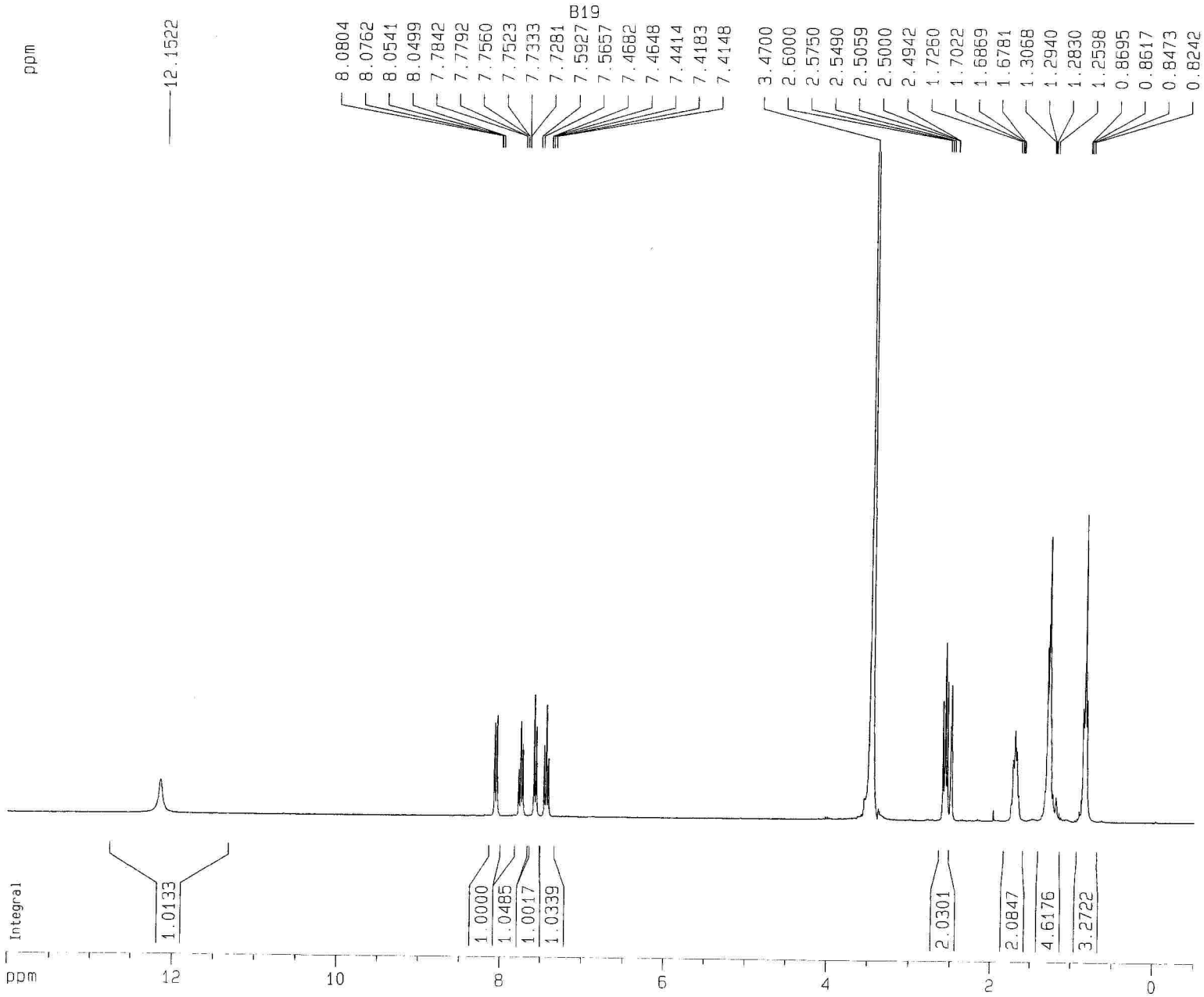
======== CHANNEL f1 ========
NUC1                 13C
P1                10.50 usec
PL1               -0.81 dB
SF01         75.4760505 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.10 dB
PL12              17.74 dB
PL13              17.74 dB
SF02        300.1312005 MHz

F2 - Processing parameters
SI                 65536
SF          75.4677517 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                20.00 cm
CY                 6.00 cm
F1P              200.500 ppm
F1             15131.28 Hz
F2P               -5.500 ppm
F2              -415.07 Hz
PPMCM           10.30000 ppm/cm
HZCM           777.31787 Hz/cm
```





Current Data Parameters

NAME	zgl-2012-149
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120821
Time	11.30
INSTRUM	av300
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	16
DS	0
SWH	5995.204 Hz
FIDRES	0.182959 Hz
AQ	2.7329011 sec
RG	128
DW	83.400 usec
DE	6.00 usec
TE	297.7 K
D1	1.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

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

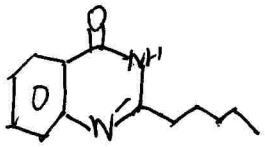
NUC1	1H
P1	10.50 usec
PL1	0.10 dB
SF01	300.1321009 MHz

F2 - Processing parameters

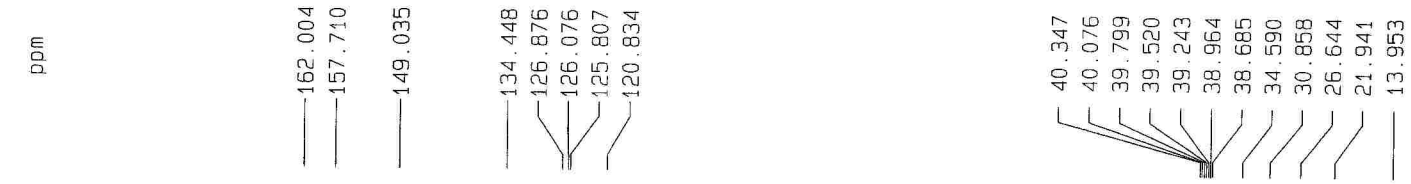
SI	32768
SF	300.1300018 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	1.00

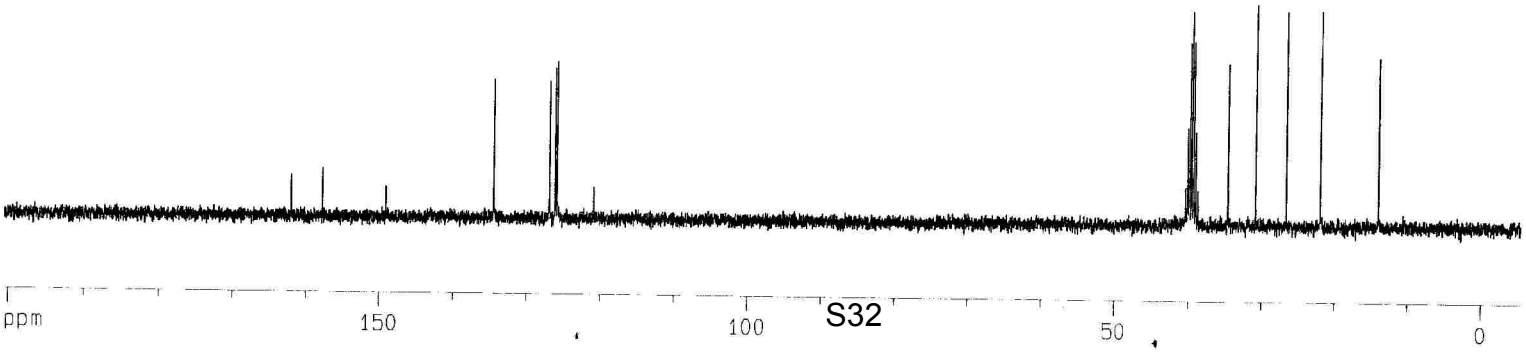
1D NMR plot parameters

CX	20.00 cm
CY	120.00 cm
F1P	14.000 ppm
F1	4201.82 Hz
F2P	-0.500 ppm
F2	-150.06 Hz
PPMCM	0.72500 ppm/cm
HZCM	217.59425 Hz/cm



B19






```
Current Data Parameters
NAME                  zgl-2012-149
EXPNO                            2
PROCNO                           1

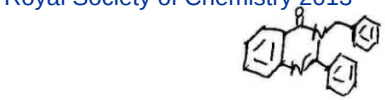
F2 - Acquisition Parameters
Date_                     20120821
Time                         11.36
INSTRUM                      av300
PROBHD    5 mm QNP 1H/13
PULPROG                       zgpg
TD                           65536
SOLVENT                       DMSO
NS                             126
DS                               4
SWH                    22675.736 Hz
FIDRES                  0.346004 Hz
AQ                     1.4451188 sec
RG                            8192
DW                       22.050 usec
DE                        6.00 usec
TE                         298.1 K
D1                    2.00000000 sec
d11                   0.03000000 sec
DELTA                 1.89999998 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

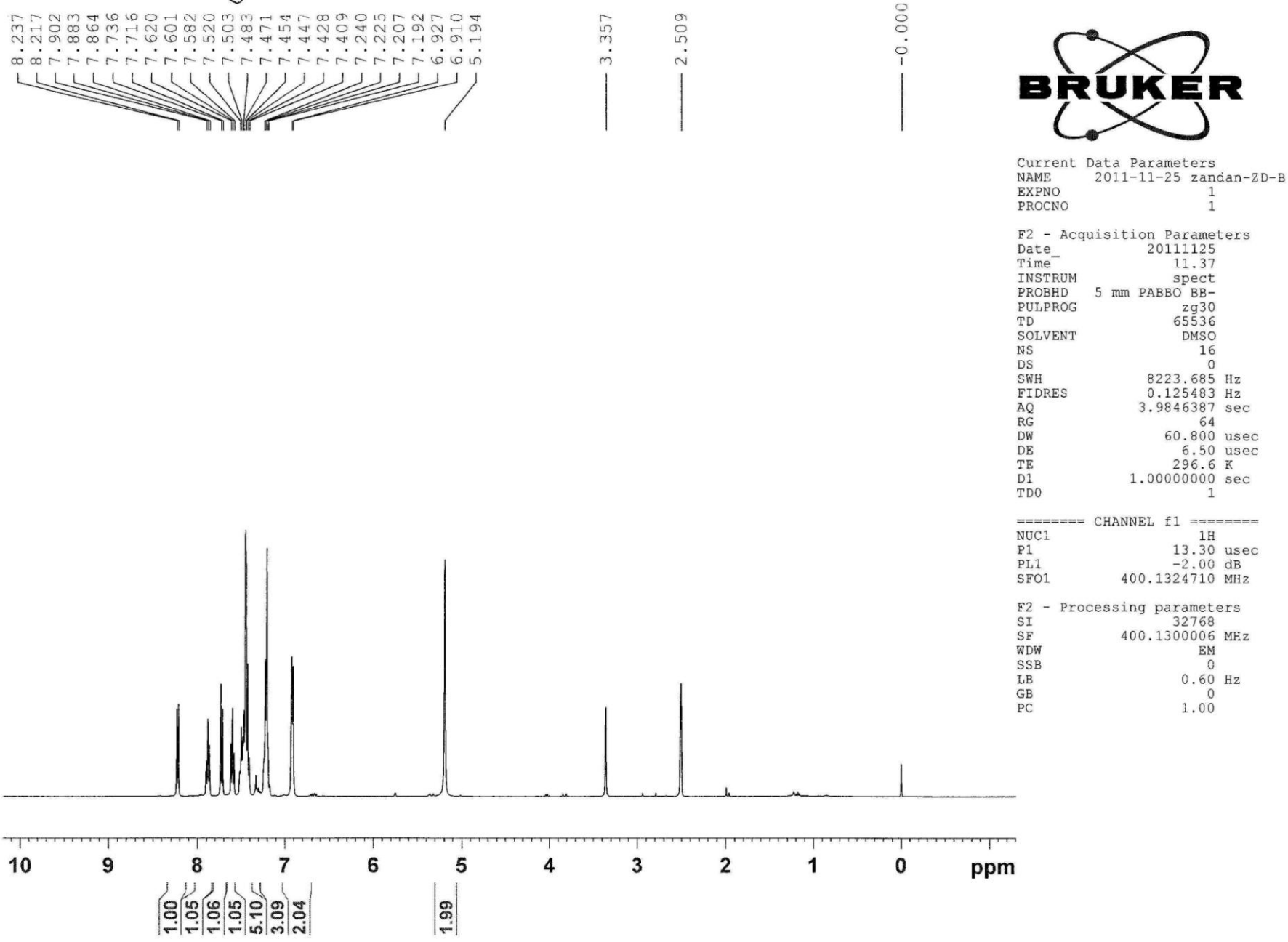
======== CHANNEL f1 ========
NUC1                          13C
P1                       10.50 usec
PL1                       -0.81 dB
SFO1                  75.4775598 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                          1H
PCPD2                    80.00 usec
PL2                       0.10 dB
PL12                     17.74 dB
PL13                     17.74 dB
SFO2                 300.1312005 MHz

F2 - Processing parameters
SI                           65536
SF                    75.4677732 MHz
WDW                             EM
SSB                              0
LB                        1.00 Hz
GB                               0
PC                            1.40

1D NMR plot parameters
CX                       20.00 cm
CY                        3.00 cm
F1P                     200.500 ppm
F1                     15131.29 Hz
F2P                      -5.500 ppm
F2                      -415.07 Hz
PPMCM                  10.30000 ppm/cm
HZCM                 777.31812 Hz/cm
```



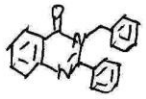


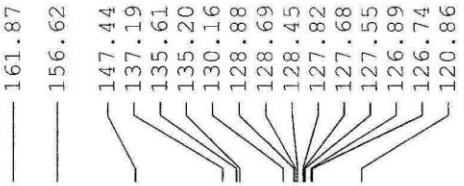
Current Data Parameters
NAME 2011-11-25 zandan-ZD-B
EXPNO 1
PROCNO 1

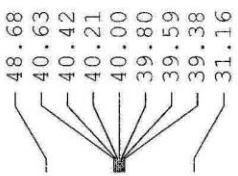
F2 - Acquisition Parameters
Date_ 20111125
Time 11.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300006 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00







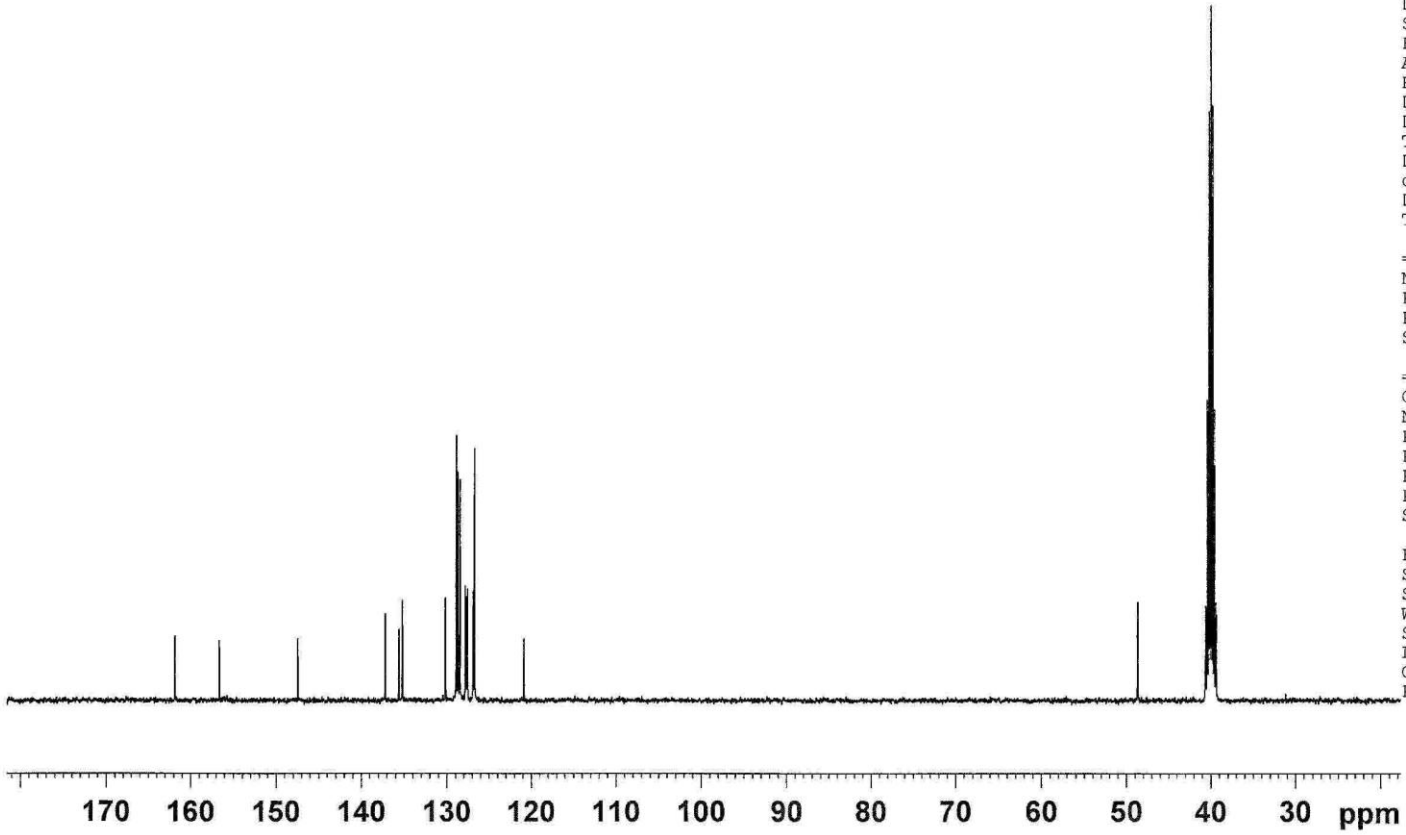

```
Current Data Parameters
NAME      2011-11-25 zandan-ZD-B
EXPNO                         2
PROCNO                        1

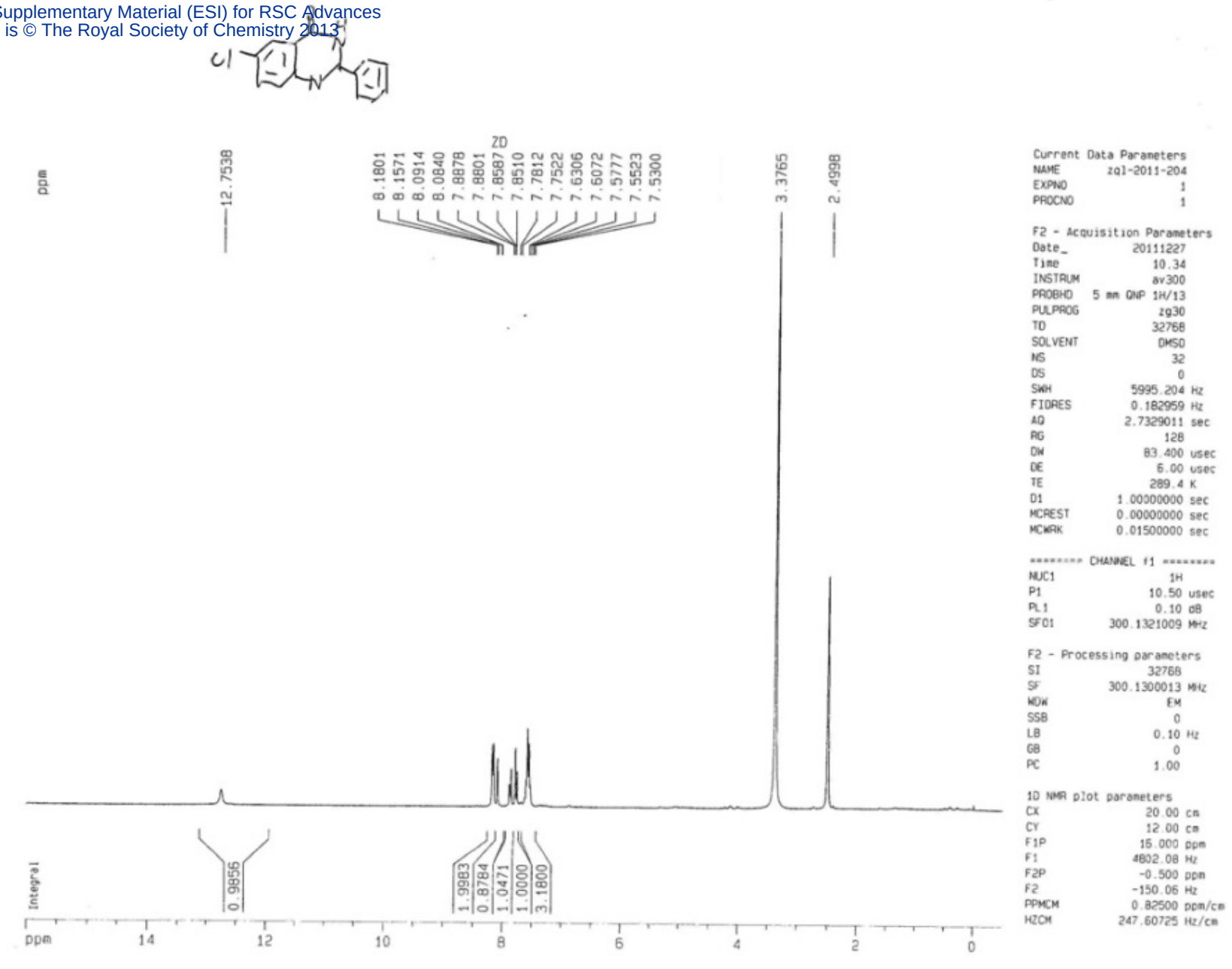
F2 - Acquisition Parameters
Date_              20111125
Time                  11.54
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      293
DS                        0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    90.5
DW                  20.800 usec
DE                   6.50 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    19.40 usec
PL1                   -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF            100.6127690 MHz
WDW                       EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.40
```





Current Data Parameters
NAME zql-2011-204
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111227
Time 10.34
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 128
DW 83.400 usec
DE 6.00 usec
TE 289.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.10 dB
SFO1 300.1321009 MHz

F2 - Processing parameters
SI 32768
SF 300.1300013 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 16.000 ppm
F1 4802.08 Hz
F2P -0.500 ppm
F2 -150.06 Hz
PPMCM 0.82500 ppm/cm
HZCM 247.60725 Hz/cm