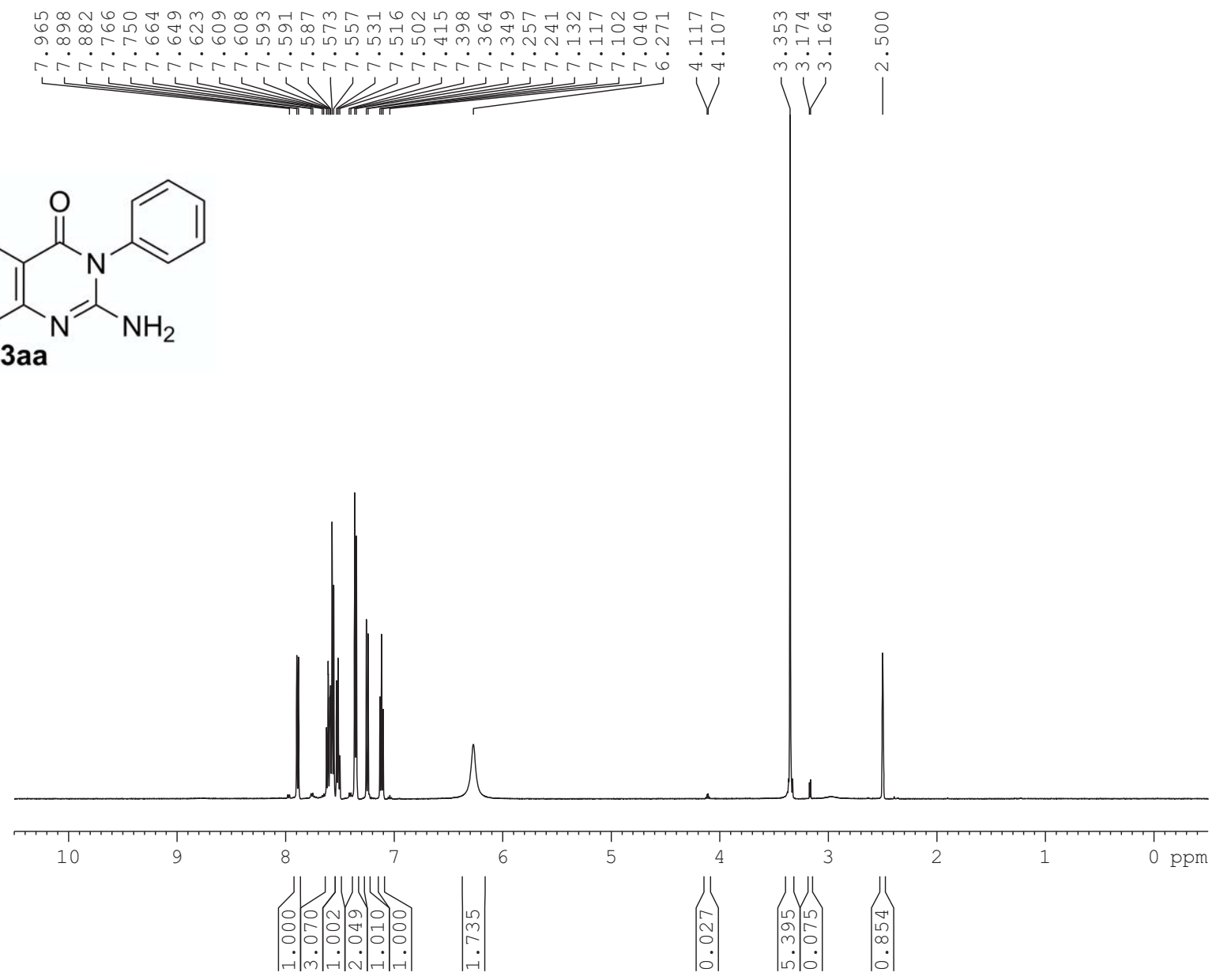
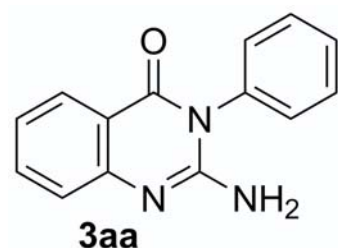


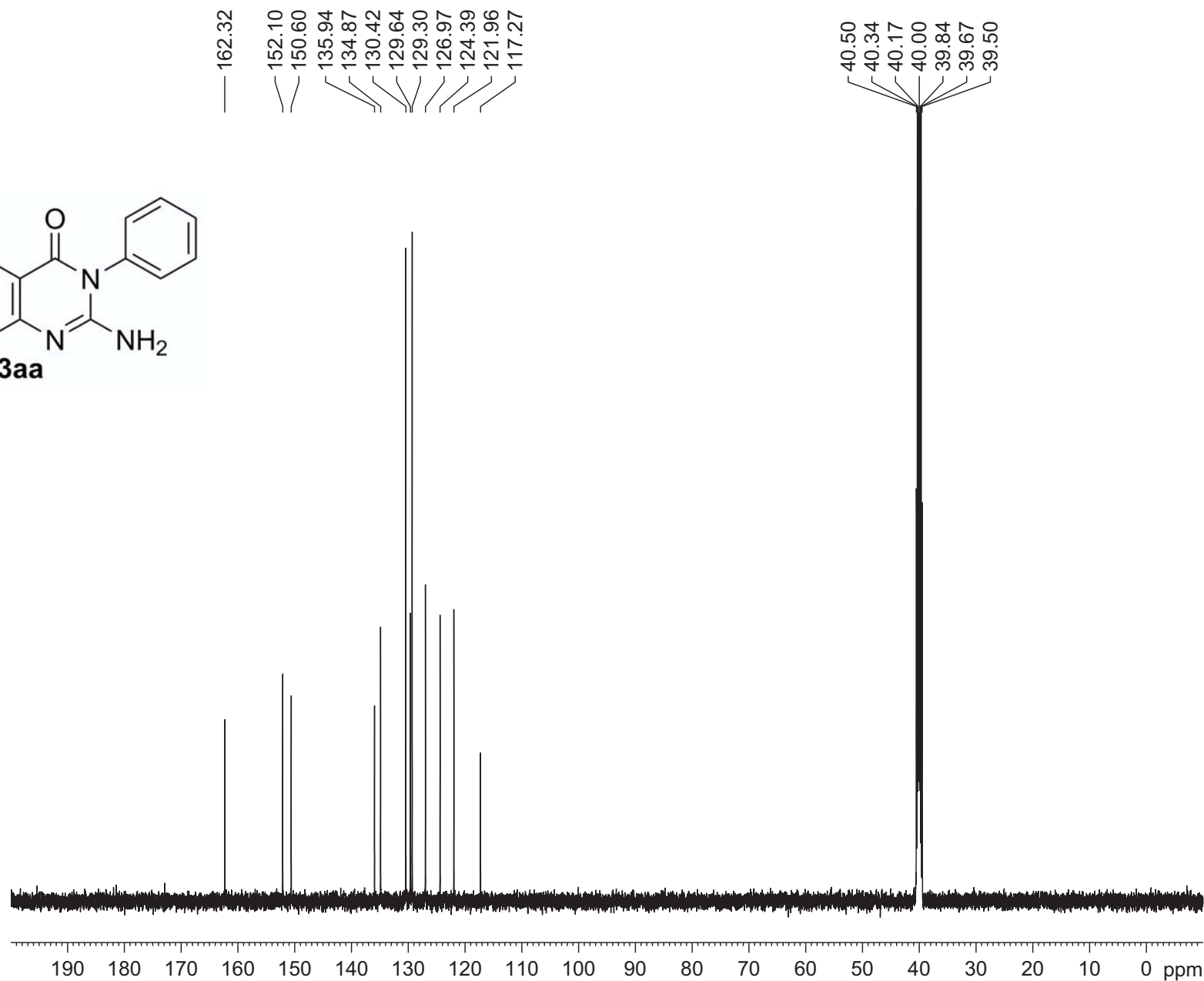
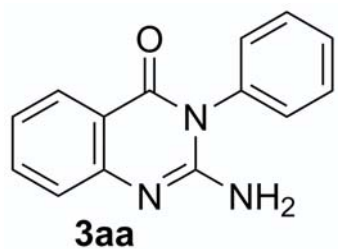


Current Data Parameters
NAME RK178
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120428
Time 14.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



```

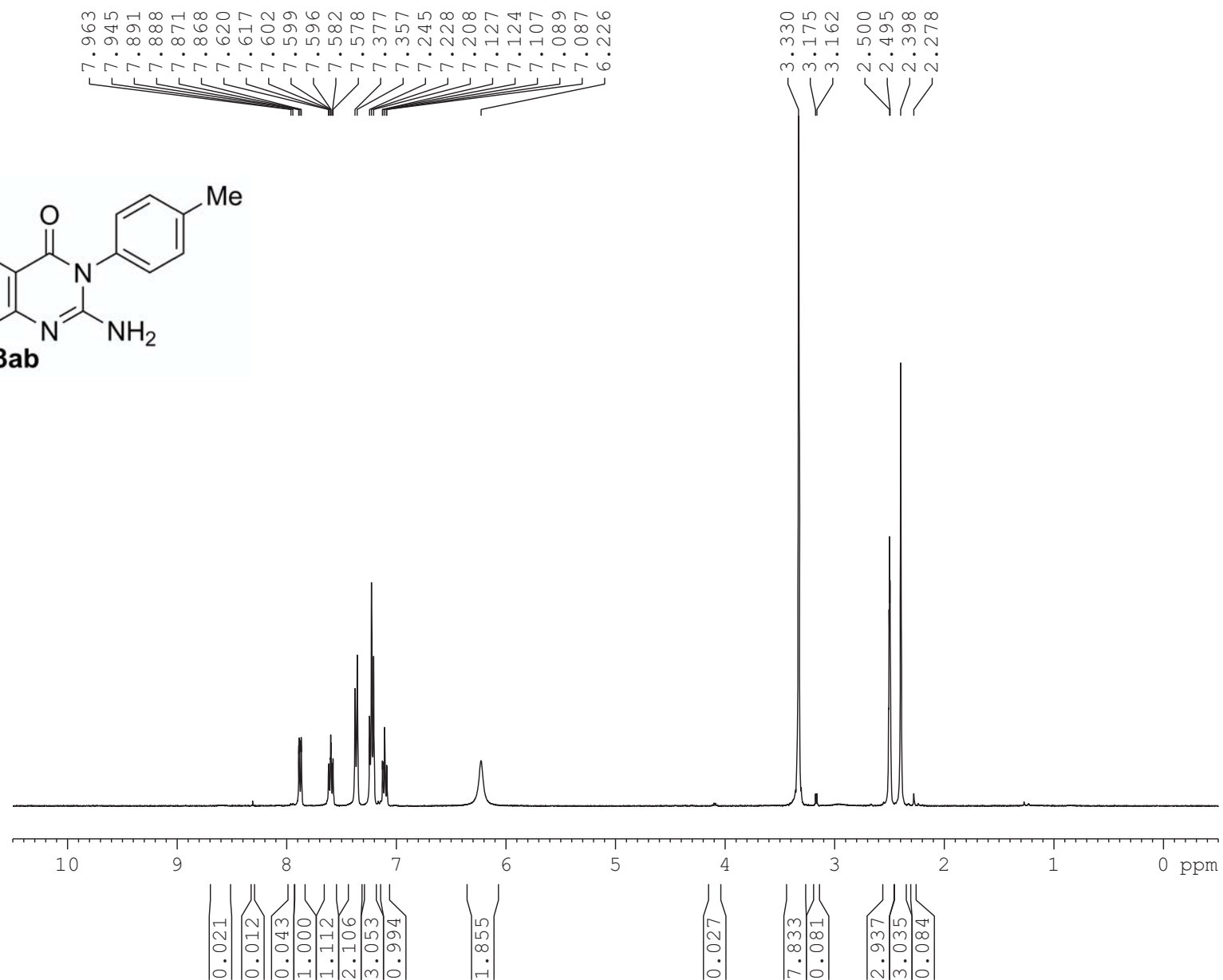
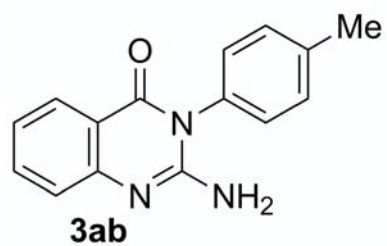
NAME      RK178
EXPNO     2
PROCNO    1
Date_     20120428
Time      14.17
INSTRUM    spect
PROBHD    5 mm PABBO BB-
PULPROG    zgpg30
TD        65536
SOLVENT    DMSO
NS         500
DS         0
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0912410 sec
RG         4597.6
DW         16.650 usec
DE         6.50 usec
TE         296.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         10.50 usec
PL1        7.00 dB
SFO1       125.7709931 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       90.00 usec
PL2         -0.60 dB
PL12        15.00 dB
PL13        18.00 dB
SFO2        500.1320005 MHz
SI          65536
SF          125.7577890 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.00
  
```



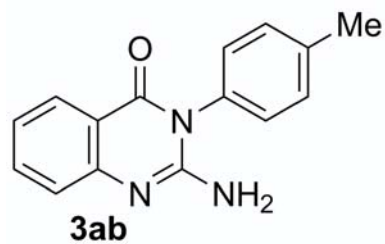
```

NAME      RK143
EXPNO     1
PROCNO    1
Date_     20120307
Time      20.37
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD        32768
SOLVENT   DMSO
NS        12
DS        0
SWH       7246.377 Hz
FIDRES    0.221142 Hz
AQ        2.2611110 sec
RG        228.1
DW        69.000 usec
DE        6.50 usec
TE        298.5 K
D1        2.00000000 sec
TD0       1
  
```

```

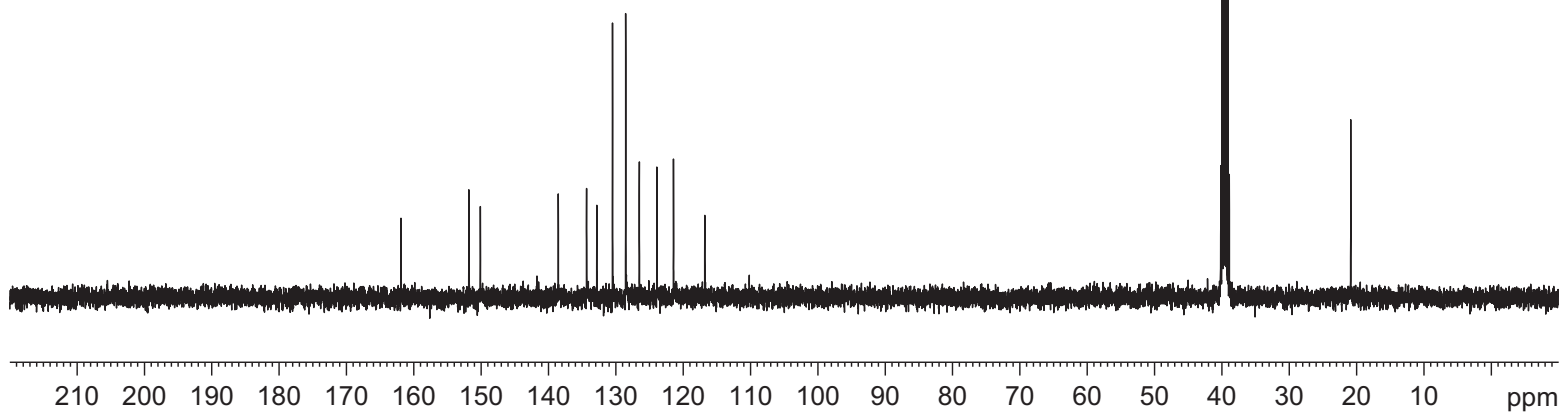
===== CHANNEL f1 =====
NUC1      1H
P1        11.70 usec
PL1       4.00 dB
SFO1      400.1324008 MHz
SI        16384
SF        400.1300022 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

2-amino-3-p-tolyl



161.878
151.801
150.095
138.518
134.322
132.806
130.468
128.513
126.488
123.884
121.413
116.766

40.132
39.926
39.717
39.508
39.300
39.091
38.883
20.845



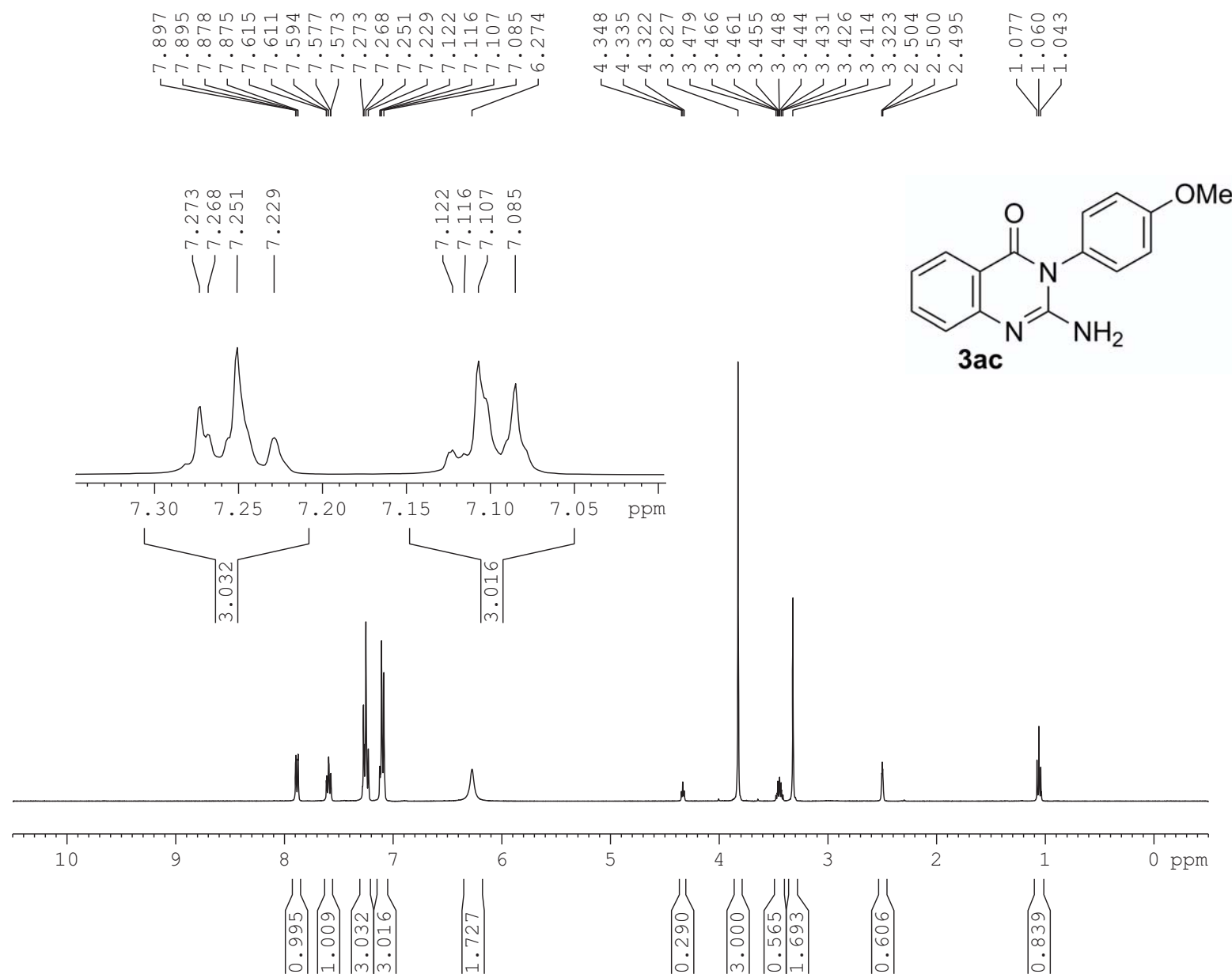
Current Data Parameters
NAME 20120306
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120306
Time 20.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 56
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128169 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

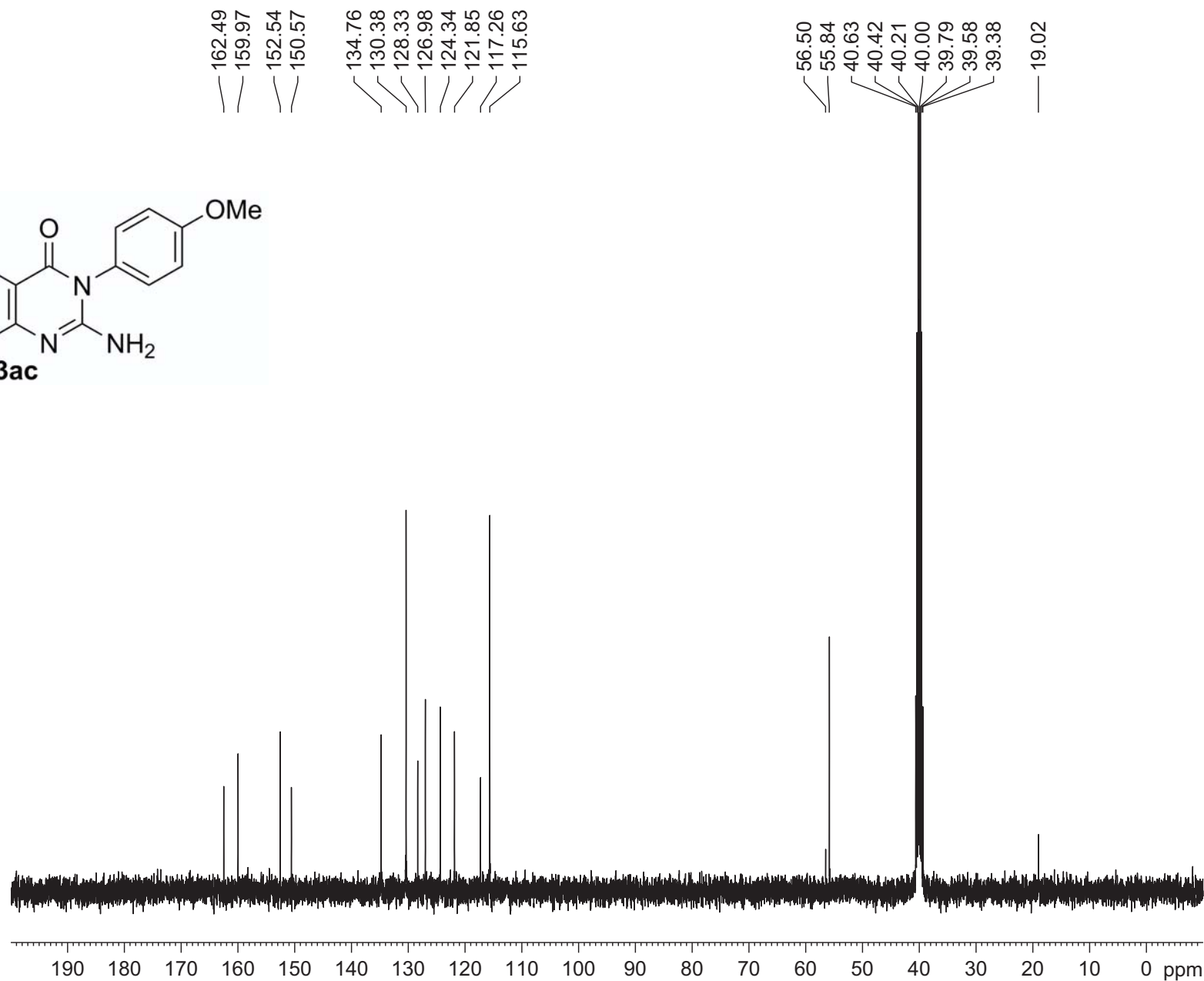
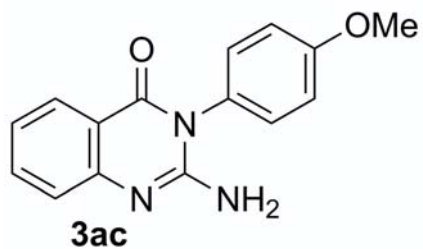


Current Data Parameters
 NAME RK157
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120331
 Time 10.41
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 90.5
 DW 69.000 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300022 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



```

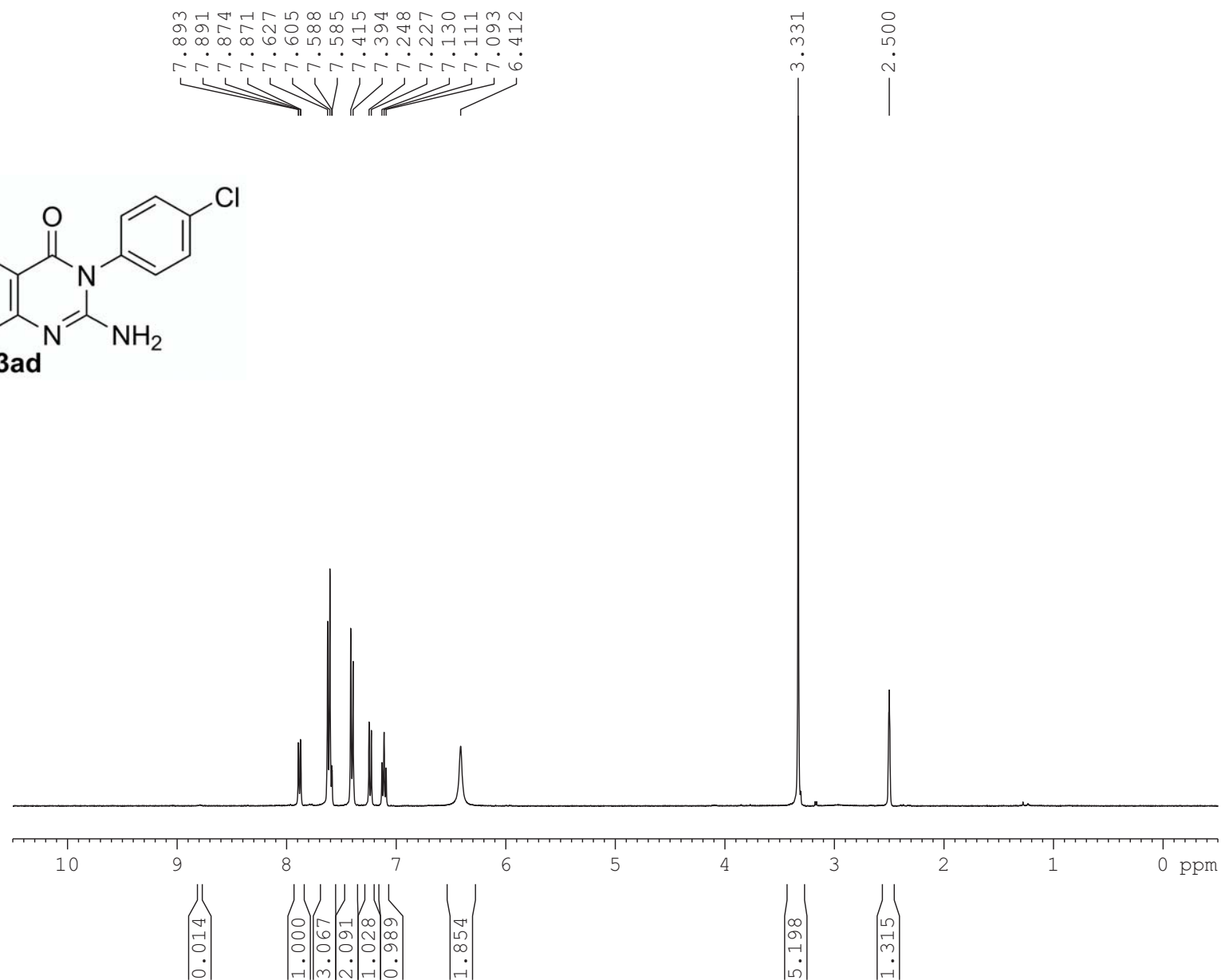
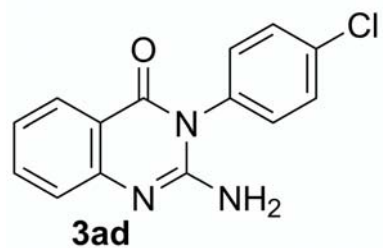
NAME      RK157
EXPNO     5
PROCNO    1
Date_     20120331
Time      10.44
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        32768
SOLVENT   DMSO
NS        64
DS        0
SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ        0.6816452 sec
RG        2896.3
DW        20.800 usec
DE        6.50 usec
TE        299.4 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        8.90 usec
PL1       7.00 dB
SFO1     100.6233325 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       3.80 dB
PL12      21.60 dB
PL13      24.60 dB
SFO2     400.1316005 MHz
SI        32768
SF       100.6127690 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```

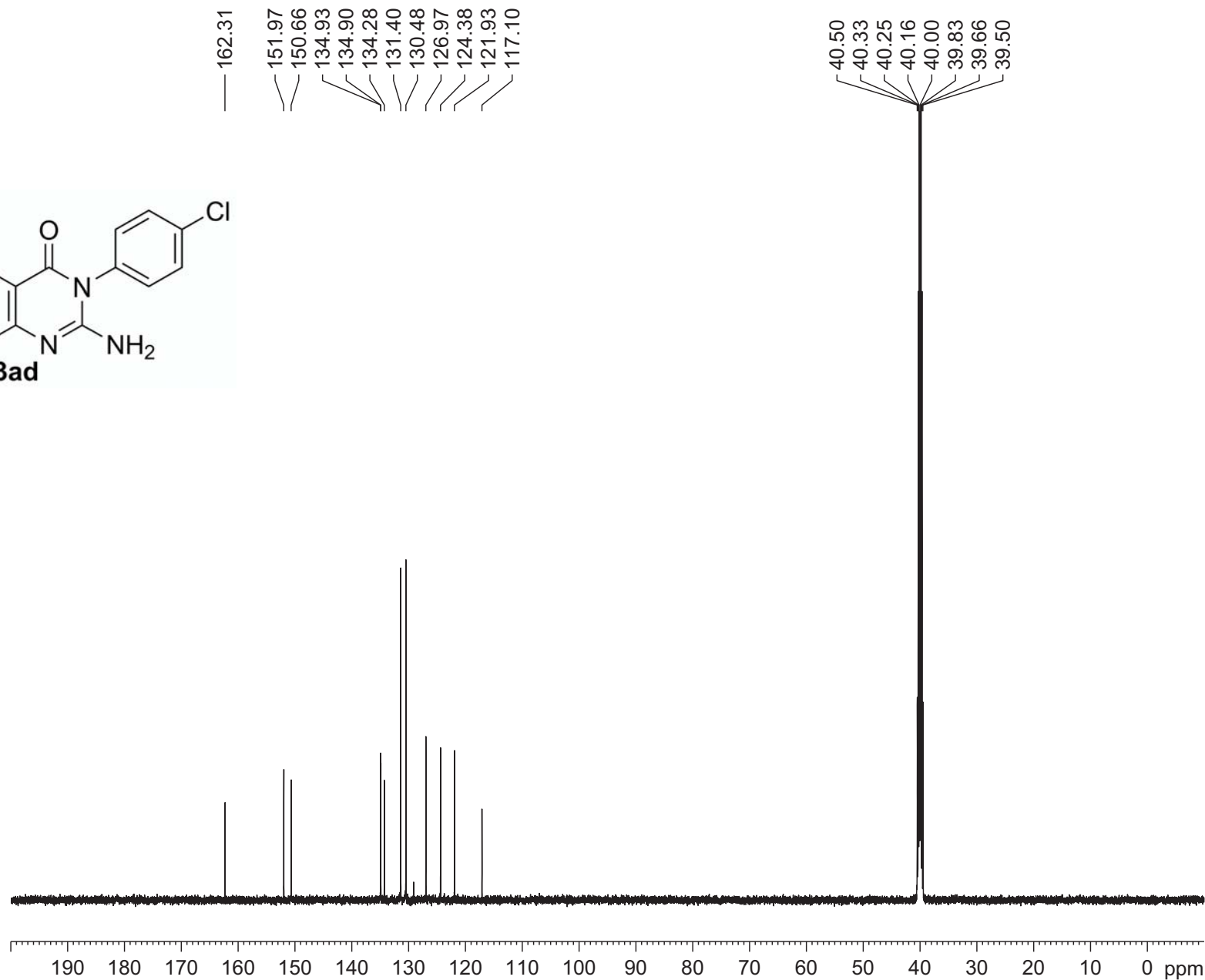
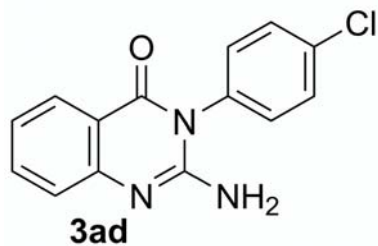


Current Data Parameters
 NAME RK192
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120516
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 228.1
 DW 69.000 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300017 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



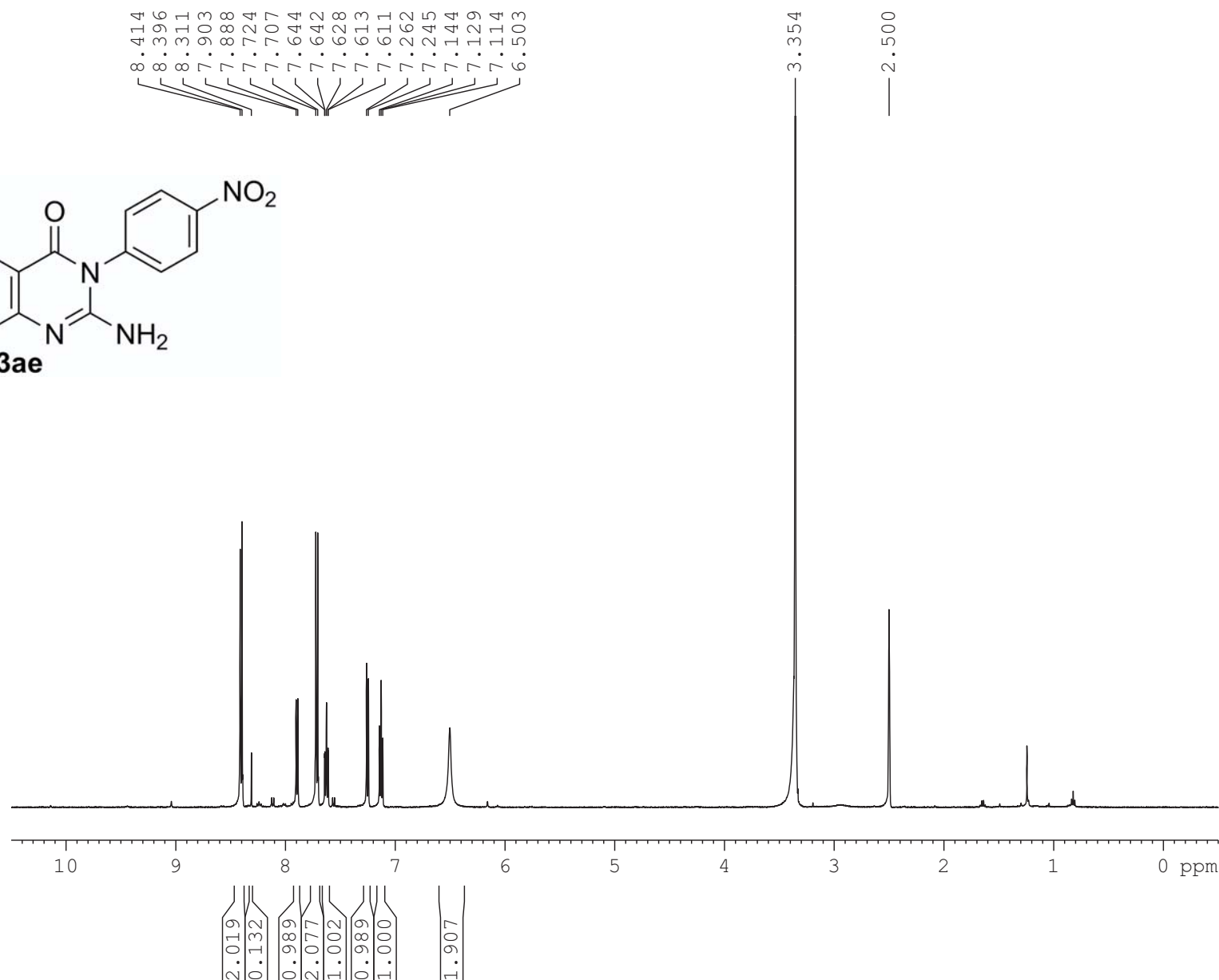
Current Data Parameters
NAME RK192
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120526
Time 14.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 4096
DW 16.650 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 125.7709931 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

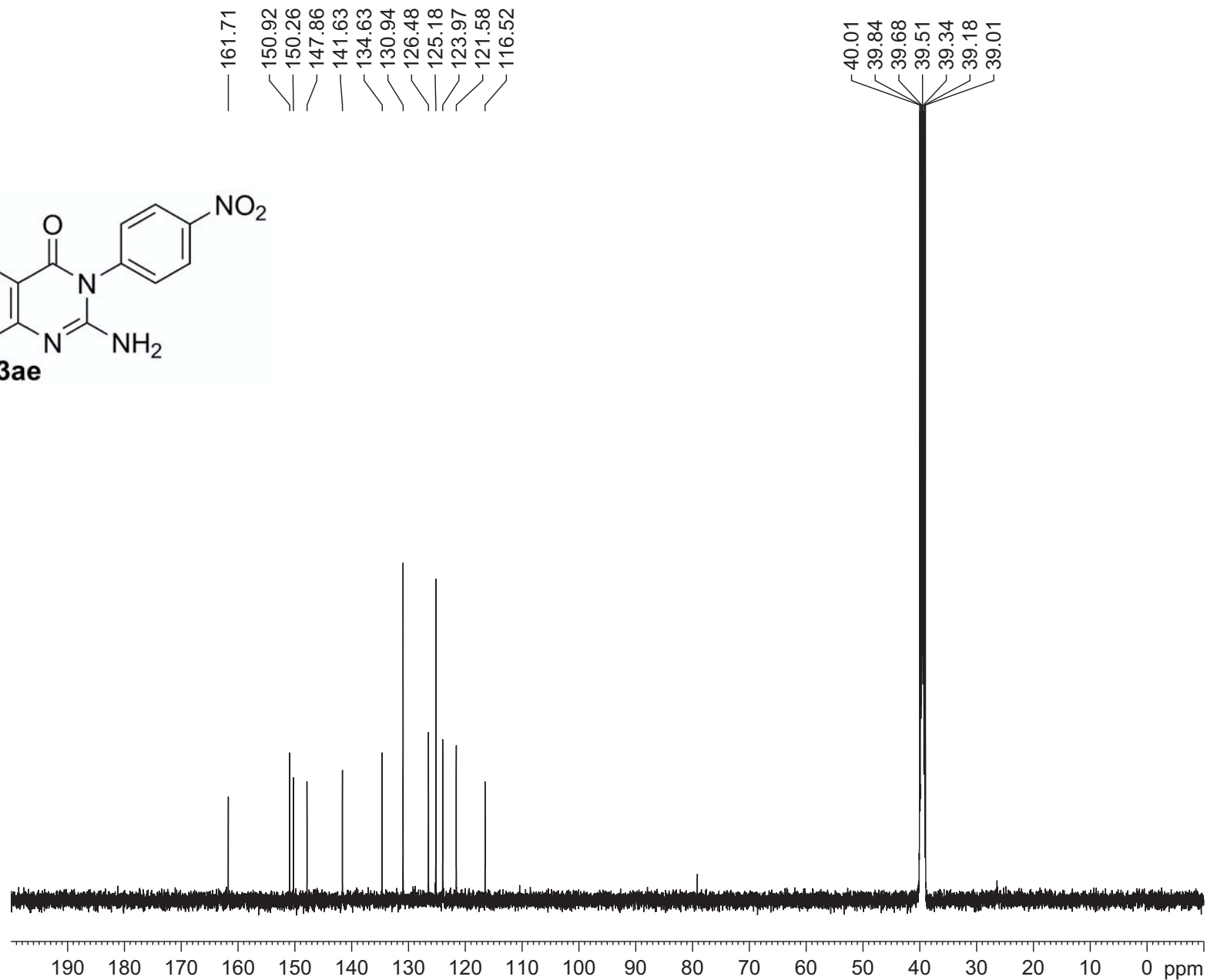


Current Data Parameters
 NAME RM092-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120922
 Time 12.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 294.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300041 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



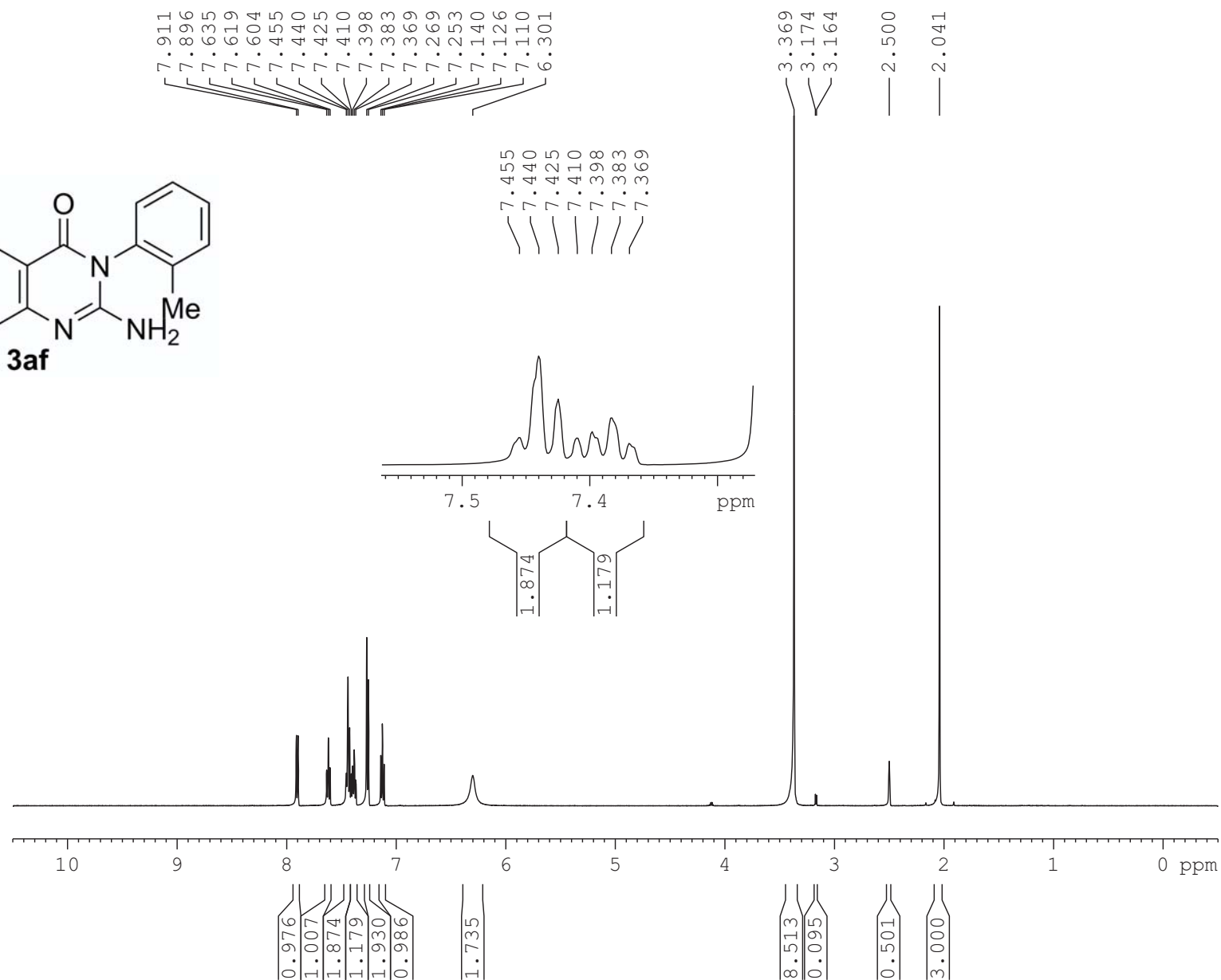
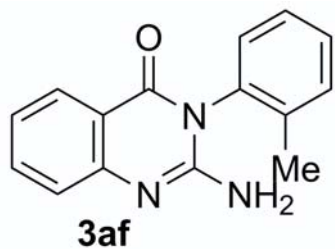
Current Data Parameters
 NAME RM092-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120922
 Time 13.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 4597.6
 DW 16.650 usec
 DE 6.50 usec
 TE 296.3 K
 D1 4.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578498 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

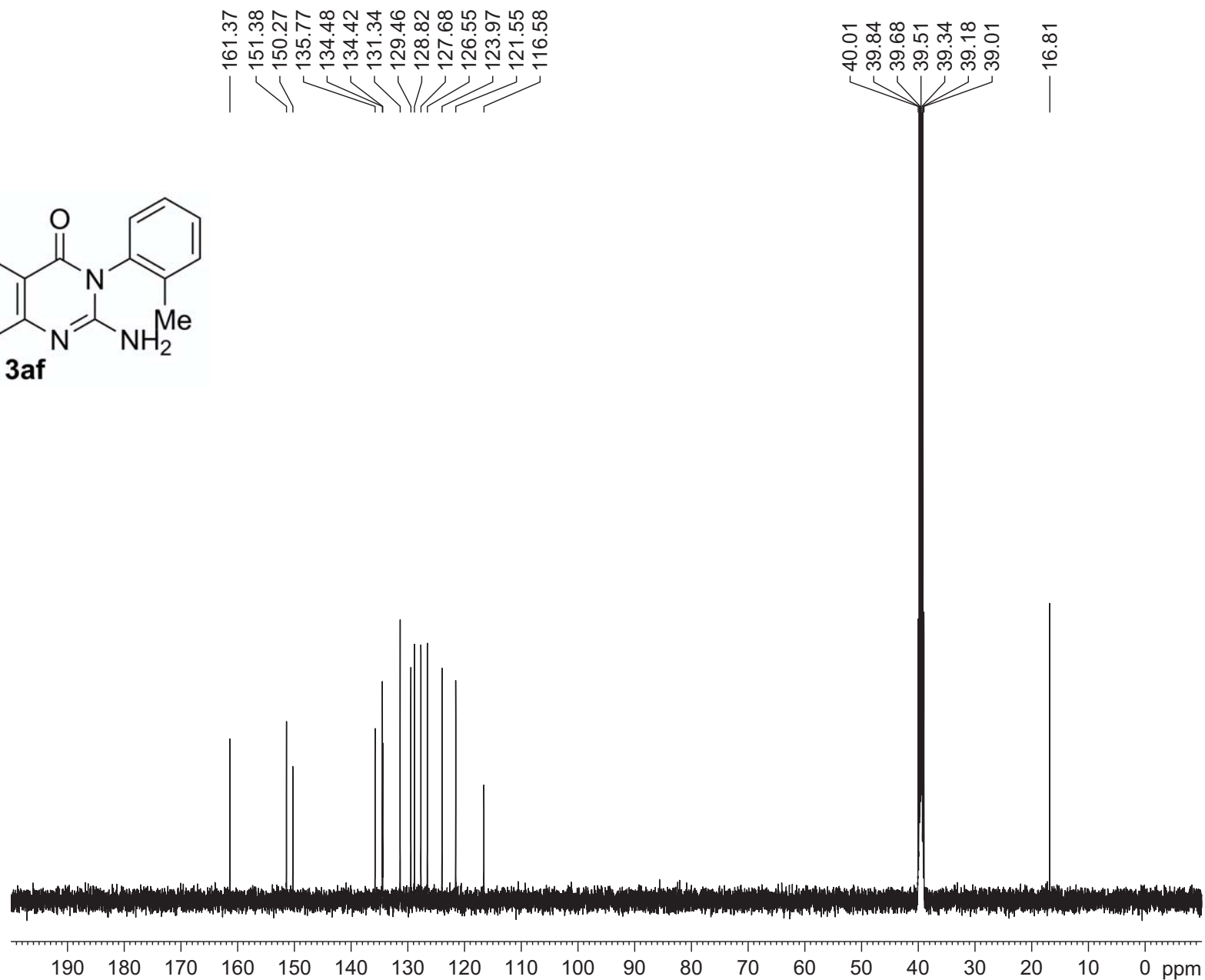
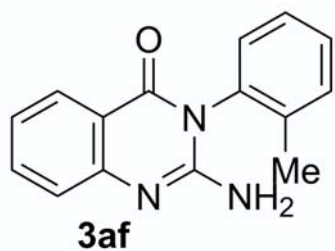


Current Data Parameters
 NAME RM187-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130119
 Time 9.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 114
 DW 55.200 usec
 DE 6.50 usec
 TE 294.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME RM187-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130119
Time 9.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 148
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

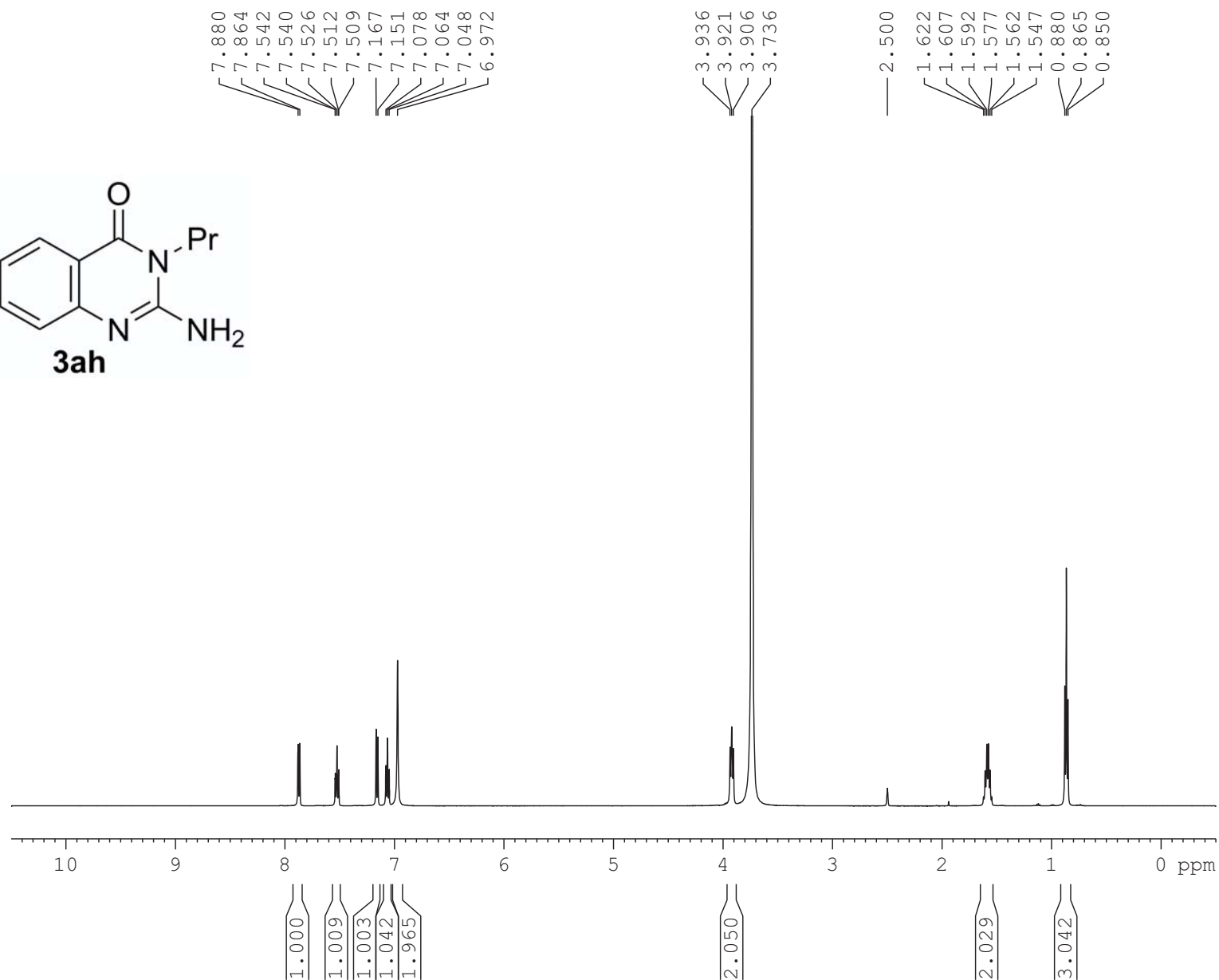
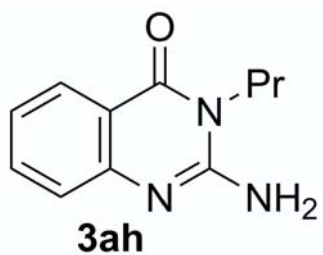
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

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

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 65536
SF 125.7578479 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

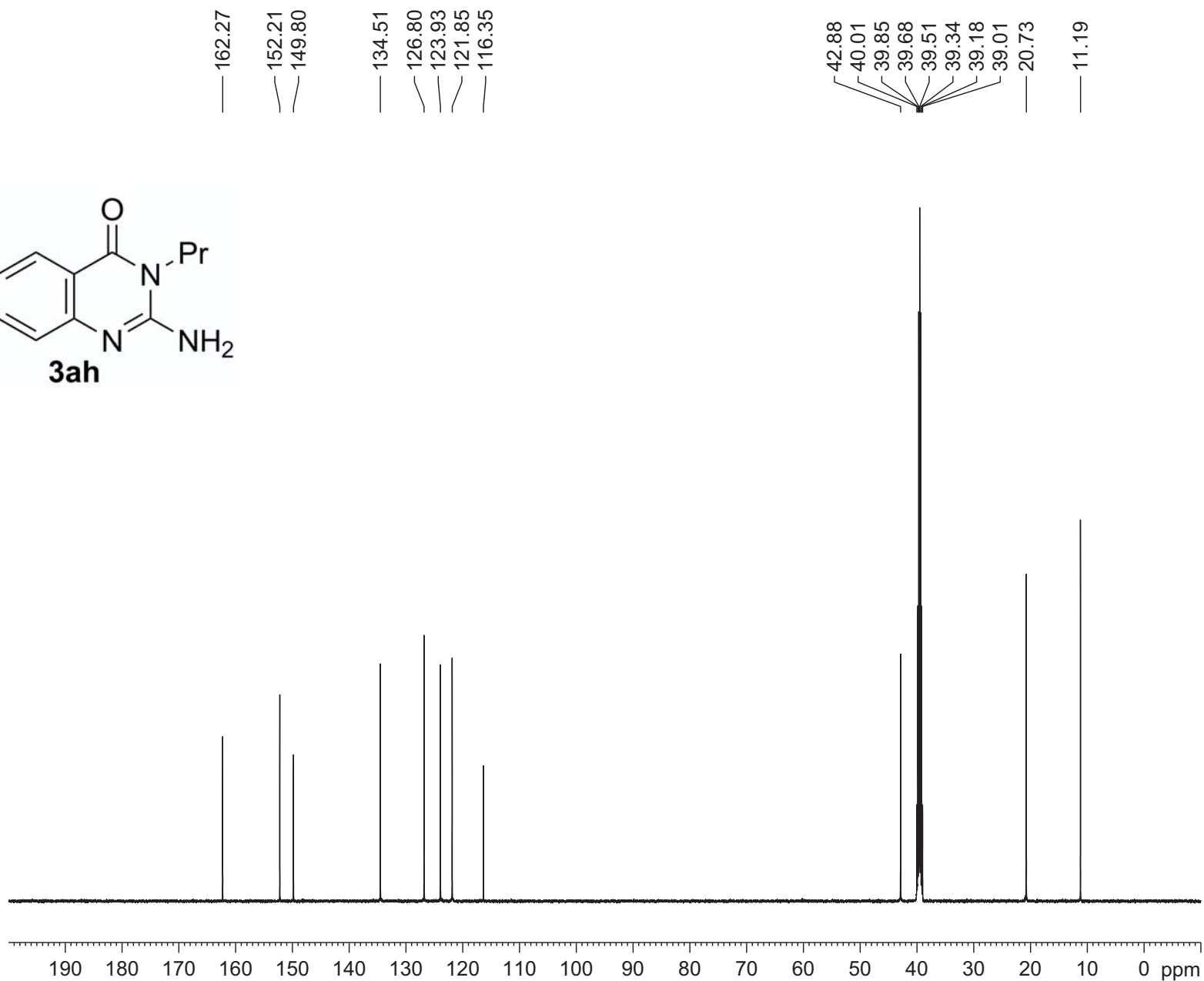
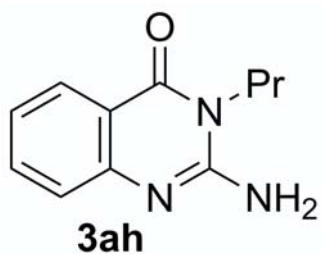


Current Data Parameters
 NAME RM190-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130208
 Time 11.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 22.6
 DW 55.200 usec
 DE 6.50 usec
 TE 295.9 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300058 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM190-1
 EXPNO 3
 PROCNO 1

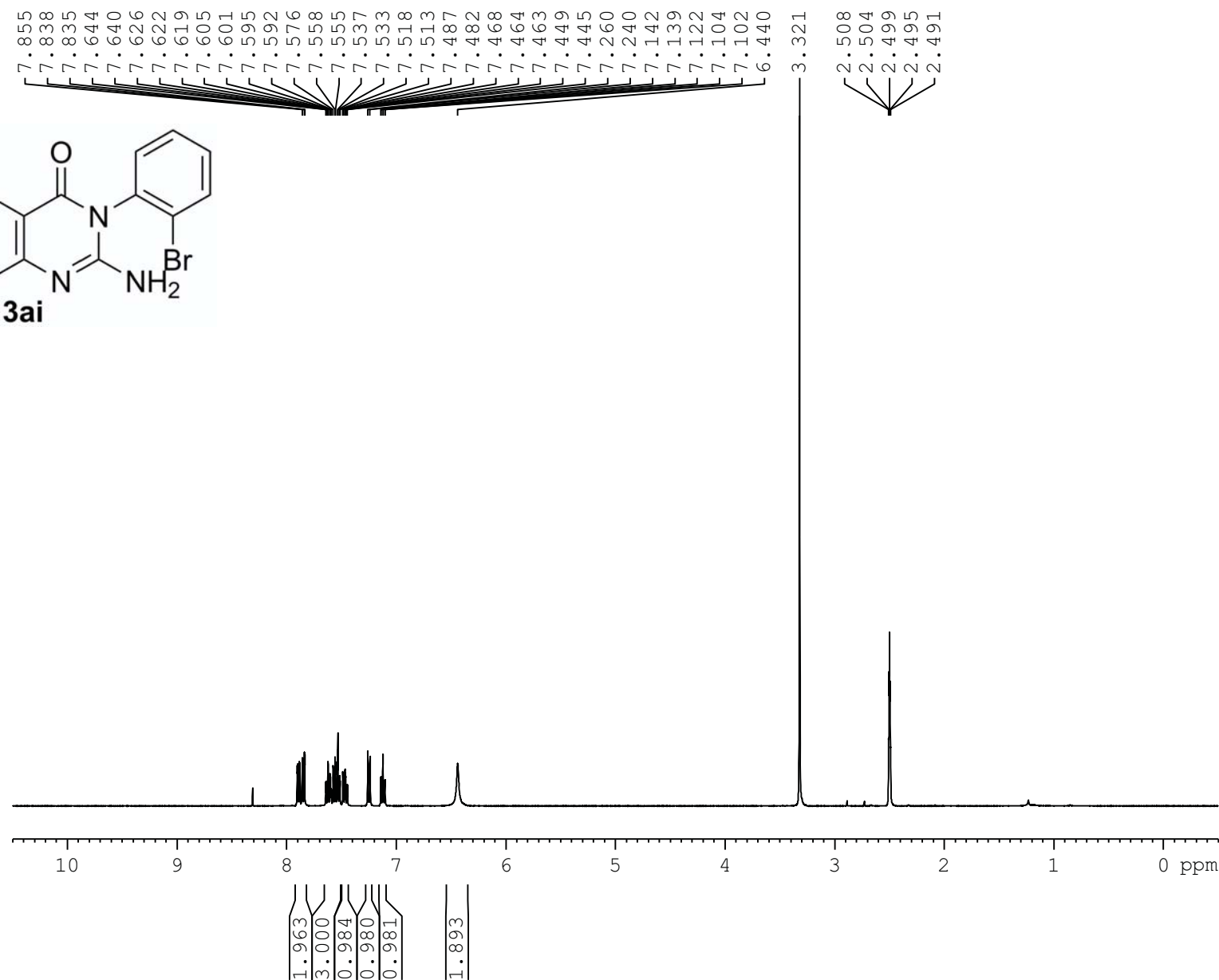
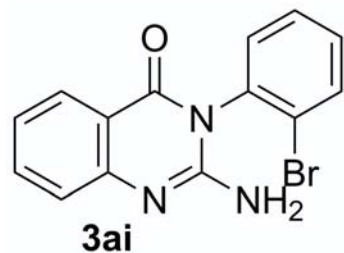
F2 - Acquisition Parameters
 Date_ 20130208
 Time 13.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 1024
 DW 16.650 usec
 DE 6.50 usec
 TE 297.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578027 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H



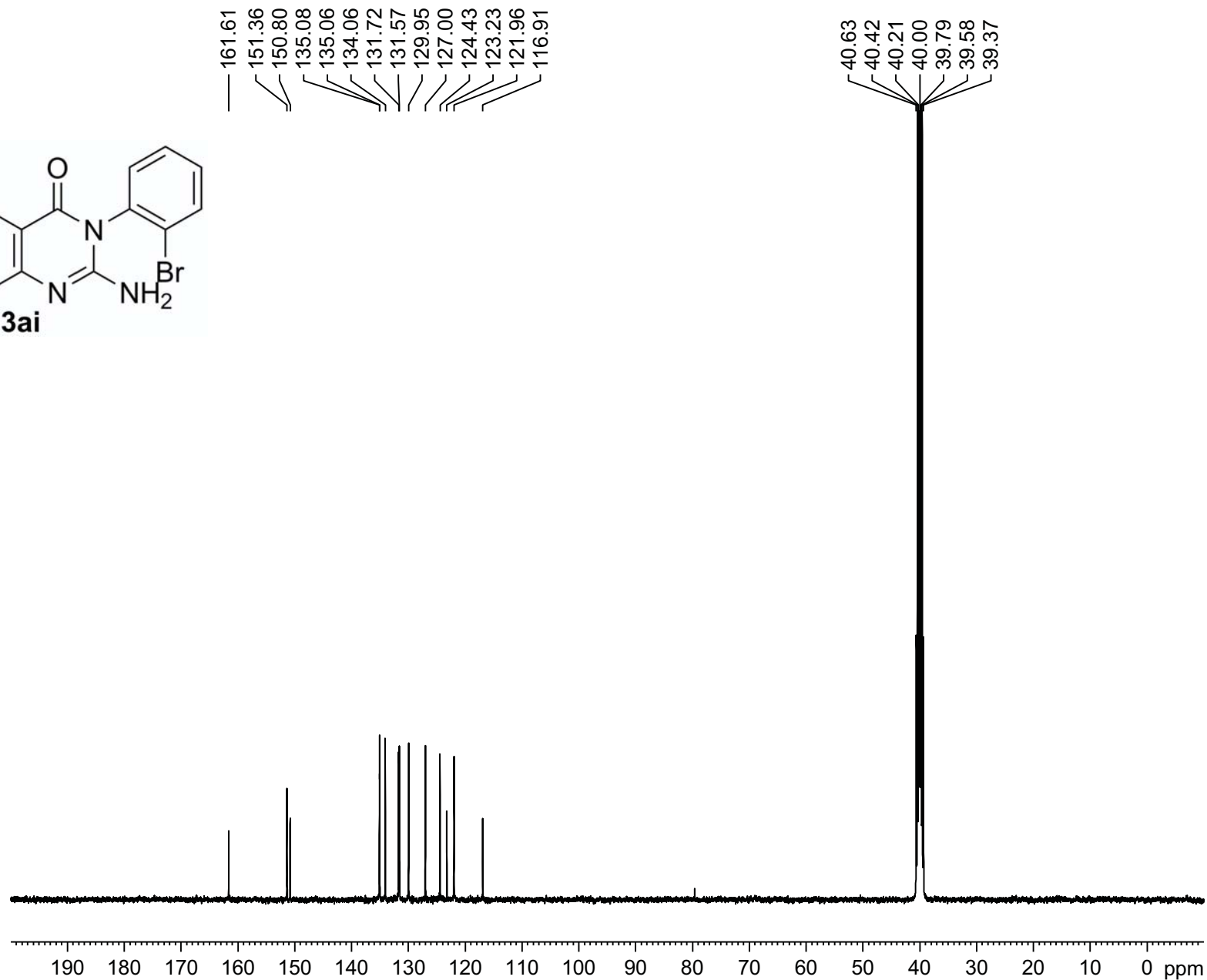
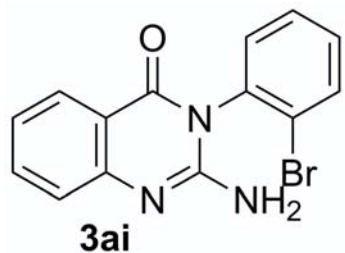
Current Data Parameters
 NAME RX134
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140801
 Time 10.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 198.09
 DW 69.333 usec
 DE 10.52 usec
 TE 298.7 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 ¹H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300032 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C



Current Data Parameters

NAME RX134
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140802
Time 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2867
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

SFO1 100.6233319 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 46.00000000 W

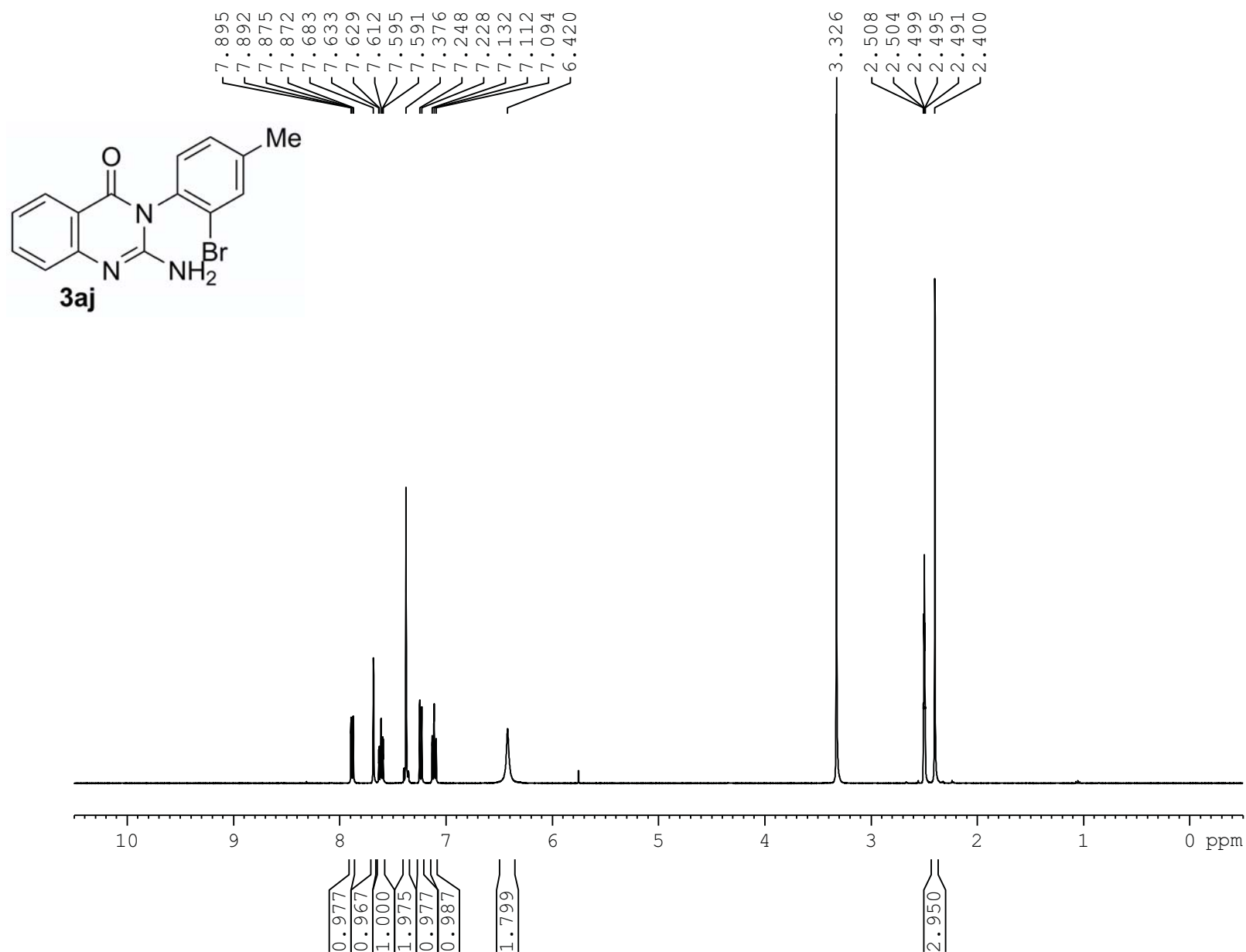
===== CHANNEL f2 =====

SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters

SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

¹H



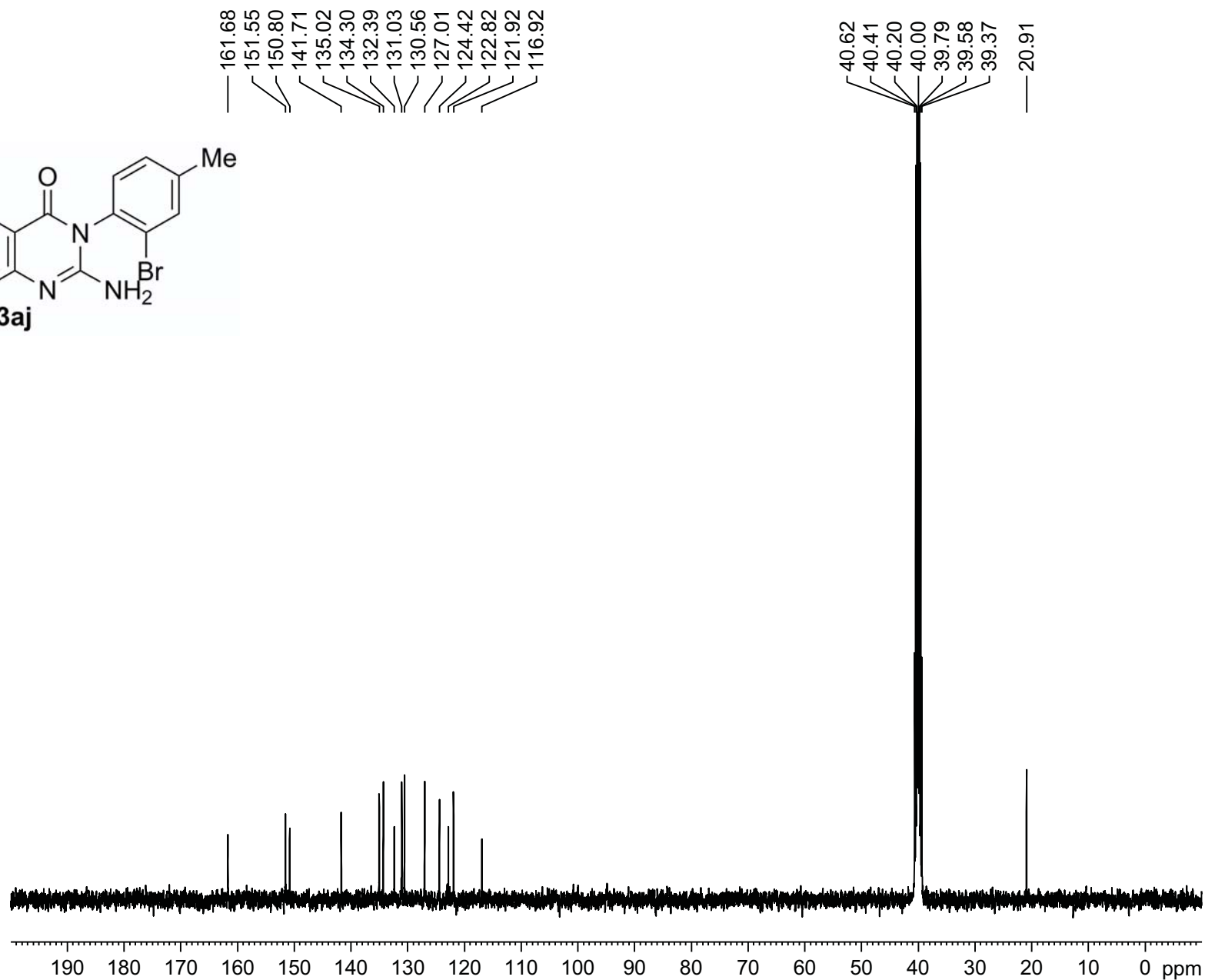
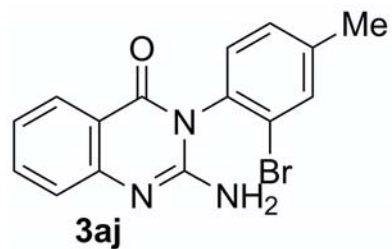
Current Data Parameters
 NAME RX159 recrystall
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141016
 Time 20.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 198.09
 DW 69.333 usec
 DE 10.52 usec
 TE 298.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 ¹H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300034 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C



Current Data Parameters
NAME RX159 recrystall
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141017
Time 13.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 200
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127701 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

a16584

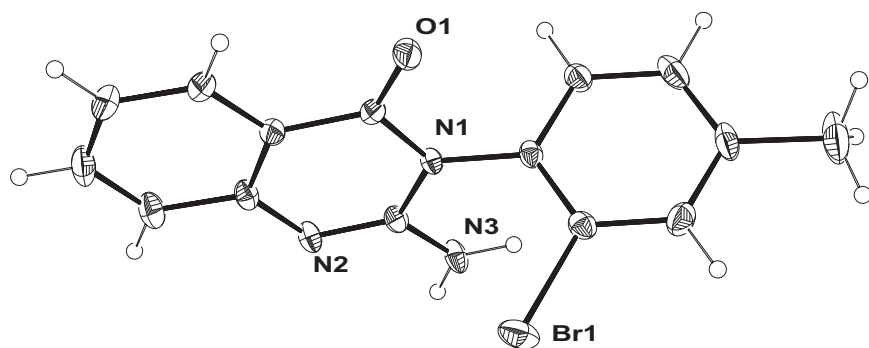
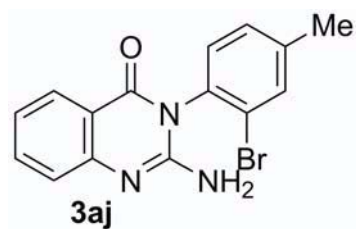


Table 1. Crystal data and structure refinement for a16584.

Identification code	a16584	
Empirical formula	C15 H12 Br N3 O	
Formula weight	330.19	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.7721(7) Å	$\alpha = 90^\circ$.
	b = 9.4199(6) Å	$\beta = 107.313(4)^\circ$.
	c = 14.3014(8) Å	$\gamma = 90^\circ$.
Volume	1385.44(15) Å ³	
Z	4	
Density (calculated)	1.583 Mg/m ³	
Absorption coefficient	2.965 mm ⁻¹	
F(000)	664	
Crystal size	0.29 x 0.27 x 0.03 mm ³	
Theta range for data collection	2.63 to 25.04°	
Index ranges	-12 ≤ h ≤ 12, -11 ≤ k ≤ 9, -17 ≤ l ≤ 16	
Reflections collected	9360	
Independent reflections	2442 [R(int) = 0.0423]	
Completeness to theta = 25.04°	99.7 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9163 and 0.4801	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2442 / 0 / 181	
Goodness-of-fit on F ²	1.022	
Final R indices [I > 2sigma(I)]	R1 = 0.0429, wR2 = 0.1144	
R indices (all data)	R1 = 0.0634, wR2 = 0.1255	
Largest diff. peak and hole	1.261 and -0.455 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for a16584. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9054(4)	8642(4)	7427(3)	27(1)
C(2)	9137(4)	8883(5)	6495(3)	38(1)
C(3)	8192(4)	8352(5)	5686(3)	38(1)
C(4)	8333(6)	8572(7)	4667(3)	68(2)
C(5)	7156(4)	7642(5)	5833(3)	40(1)
C(6)	7056(4)	7403(4)	6753(3)	30(1)
C(7)	8018(4)	7895(4)	7566(3)	23(1)
C(8)	7142(3)	8517(4)	8888(3)	24(1)
C(9)	7238(4)	8301(4)	9911(3)	26(1)
C(10)	6505(4)	9130(5)	10359(3)	35(1)
C(11)	6548(4)	8895(6)	11312(3)	44(1)
C(12)	7363(5)	7849(5)	11839(3)	43(1)
C(13)	8115(4)	7050(5)	11426(3)	37(1)
C(14)	8072(4)	7245(4)	10446(3)	26(1)
C(15)	8715(3)	6576(4)	9115(3)	23(1)
N(1)	7937(3)	7622(3)	8532(2)	21(1)
N(2)	8811(3)	6387(3)	10037(2)	28(1)
N(3)	9398(3)	5761(3)	8684(2)	31(1)
O(1)	6437(3)	9392(3)	8346(2)	34(1)
Br(1)	10353(1)	9382(1)	8511(1)	44(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for a16584.

C(1)-C(2)	1.381(6)
C(1)-C(7)	1.382(5)
C(1)-Br(1)	1.887(4)
C(2)-C(3)	1.387(6)
C(2)-H(2)	0.9500
C(3)-C(5)	1.369(6)
C(3)-C(4)	1.524(6)
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.369(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.387(5)
C(6)-H(6)	0.9500
C(7)-N(1)	1.433(5)
C(8)-O(1)	1.228(4)
C(8)-N(1)	1.401(5)
C(8)-C(9)	1.450(5)
C(9)-C(10)	1.394(6)
C(9)-C(14)	1.405(5)
C(10)-C(11)	1.368(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.384(7)
C(11)-H(11)	0.9500
C(12)-C(13)	1.363(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.400(6)
C(13)-H(13)	0.9500
C(14)-N(2)	1.380(5)
C(15)-N(2)	1.304(5)
C(15)-N(3)	1.334(5)
C(15)-N(1)	1.397(4)
N(3)-H(3A)	0.8800
N(3)-H(3B)	0.8800

C(2)-C(1)-C(7)	120.7(4)
C(2)-C(1)-Br(1)	119.1(3)
C(7)-C(1)-Br(1)	120.2(3)
C(1)-C(2)-C(3)	120.2(4)
C(1)-C(2)-H(2)	119.9
C(3)-C(2)-H(2)	119.9
C(5)-C(3)-C(2)	118.5(4)
C(5)-C(3)-C(4)	122.1(4)
C(2)-C(3)-C(4)	119.4(5)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-C(6)	121.9(4)
C(3)-C(5)-H(5)	119.1
C(6)-C(5)-H(5)	119.1
C(5)-C(6)-C(7)	119.9(4)
C(5)-C(6)-H(6)	120.1
C(7)-C(6)-H(6)	120.1
C(1)-C(7)-C(6)	118.8(4)
C(1)-C(7)-N(1)	120.9(3)
C(6)-C(7)-N(1)	120.3(4)
O(1)-C(8)-N(1)	120.3(3)
O(1)-C(8)-C(9)	125.2(4)
N(1)-C(8)-C(9)	114.5(3)
C(10)-C(9)-C(14)	120.3(4)
C(10)-C(9)-C(8)	120.3(4)
C(14)-C(9)-C(8)	119.4(4)
C(11)-C(10)-C(9)	120.7(4)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(10)-C(11)-C(12)	119.0(4)
C(10)-C(11)-H(11)	120.5

C(12)-C(11)-H(11)	120.5
C(13)-C(12)-C(11)	121.3(4)
C(13)-C(12)-H(12)	119.3
C(11)-C(12)-H(12)	119.3
C(12)-C(13)-C(14)	121.0(4)
C(12)-C(13)-H(13)	119.5
C(14)-C(13)-H(13)	119.5
N(2)-C(14)-C(13)	119.8(4)
N(2)-C(14)-C(9)	122.7(3)
C(13)-C(14)-C(9)	117.6(4)
N(2)-C(15)-N(3)	120.0(3)
N(2)-C(15)-N(1)	123.5(3)
N(3)-C(15)-N(1)	116.5(3)
C(15)-N(1)-C(8)	122.0(3)
C(15)-N(1)-C(7)	120.2(3)
C(8)-N(1)-C(7)	117.5(3)
C(15)-N(2)-C(14)	117.8(3)
C(15)-N(3)-H(3A)	120.0
C(15)-N(3)-H(3B)	120.0
H(3A)-N(3)-H(3B)	120.0

Symmetry transformations used to generate equivalent atoms:

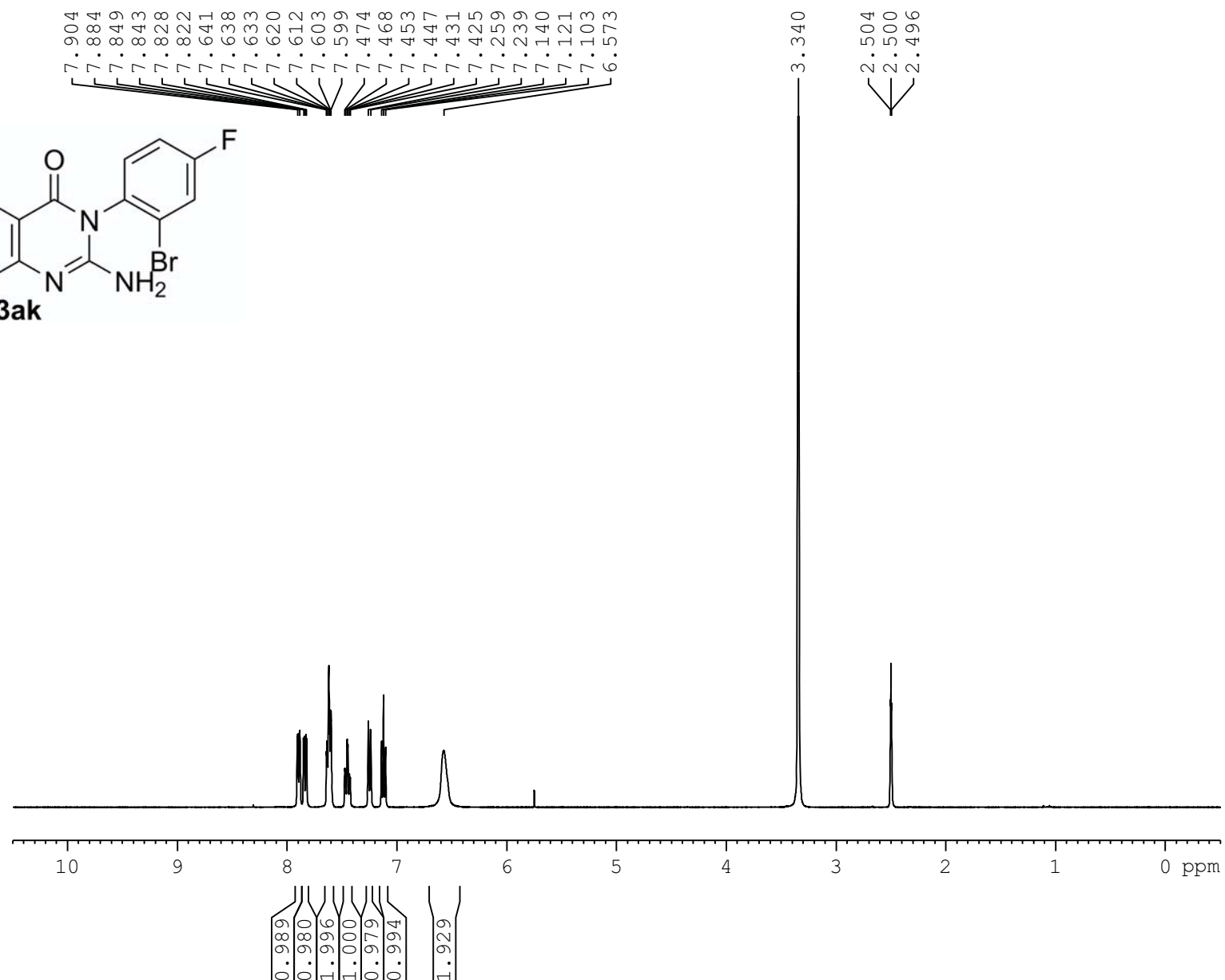
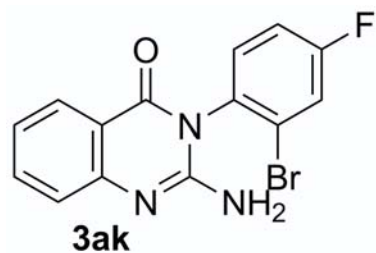
Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for a16584. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(2)	26(2)	25(2)	2(2)	5(2)	5(2)
C(2)	35(2)	43(3)	39(3)	16(2)	19(2)	6(2)
C(3)	51(3)	45(3)	20(2)	9(2)	12(2)	17(2)
C(4)	94(4)	87(5)	31(3)	14(3)	32(3)	26(4)
C(5)	47(3)	46(3)	21(2)	-6(2)	-1(2)	11(2)
C(6)	30(2)	32(2)	24(2)	-2(2)	5(2)	2(2)
C(7)	27(2)	23(2)	19(2)	4(2)	7(2)	6(2)
C(8)	22(2)	27(2)	25(2)	1(2)	9(2)	1(2)
C(9)	25(2)	32(2)	22(2)	-1(2)	7(2)	-4(2)
C(10)	28(2)	50(3)	31(2)	1(2)	13(2)	7(2)
C(11)	39(3)	63(3)	36(3)	-7(2)	22(2)	0(2)
C(12)	59(3)	52(3)	23(2)	-2(2)	19(2)	-8(3)
C(13)	50(3)	36(3)	23(2)	5(2)	11(2)	-2(2)
C(14)	35(2)	23(2)	20(2)	-1(2)	7(2)	-7(2)
C(15)	28(2)	20(2)	20(2)	1(2)	5(2)	1(2)
N(1)	25(2)	21(2)	17(2)	2(1)	6(1)	1(1)
N(2)	38(2)	25(2)	19(2)	2(2)	6(1)	2(2)
N(3)	45(2)	27(2)	19(2)	7(1)	7(2)	11(2)
O(1)	35(2)	42(2)	28(2)	9(1)	11(1)	14(1)
Br(1)	33(1)	43(1)	44(1)	4(1)	-5(1)	-10(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for a16584.

	x	y	z	U(eq)
H(2)	9845	9413	6408	45
H(4A)	9128	9111	4718	102
H(4B)	7580	9098	4262	102
H(4C)	8382	7647	4366	102
H(5)	6488	7305	5282	48
H(6)	6330	6901	6833	35
H(10)	5970	9866	9998	42
H(11)	6025	9442	11608	53
H(12)	7398	7684	12502	52
H(13)	8678	6351	11808	44
H(3A)	9913	5096	9023	37
H(3B)	9334	5888	8062	37

¹H



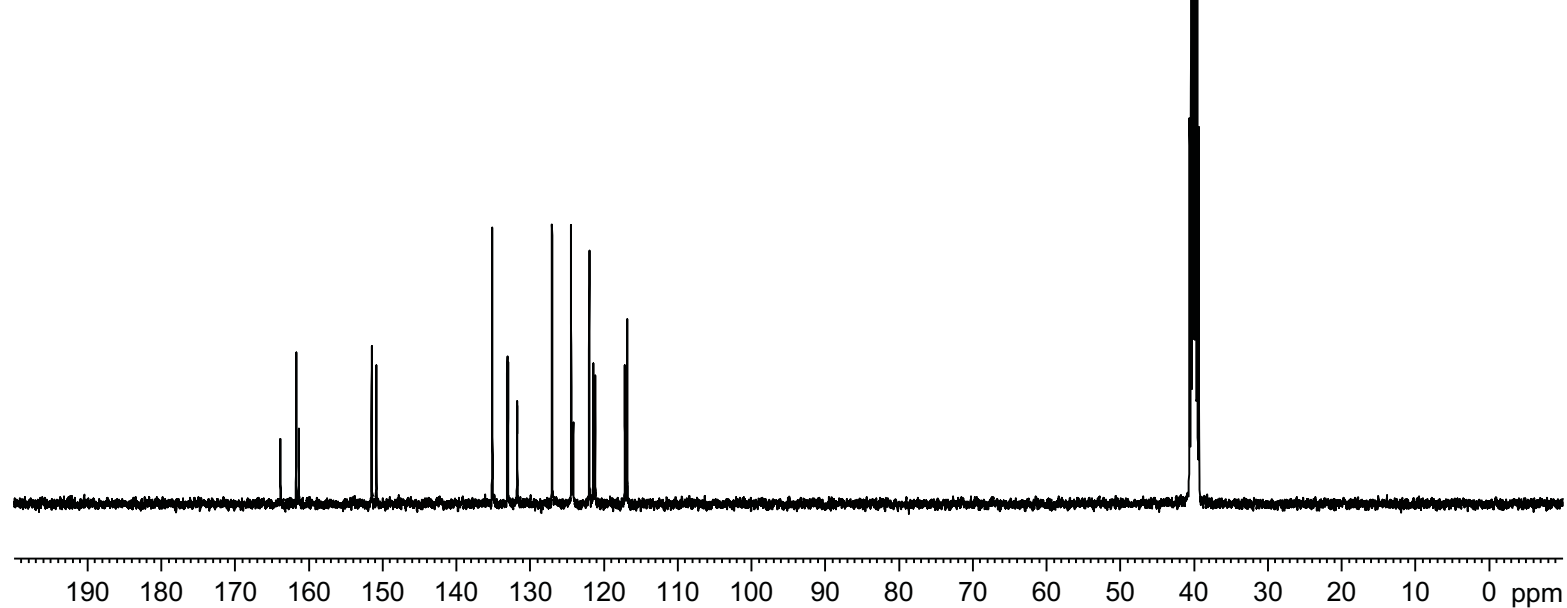
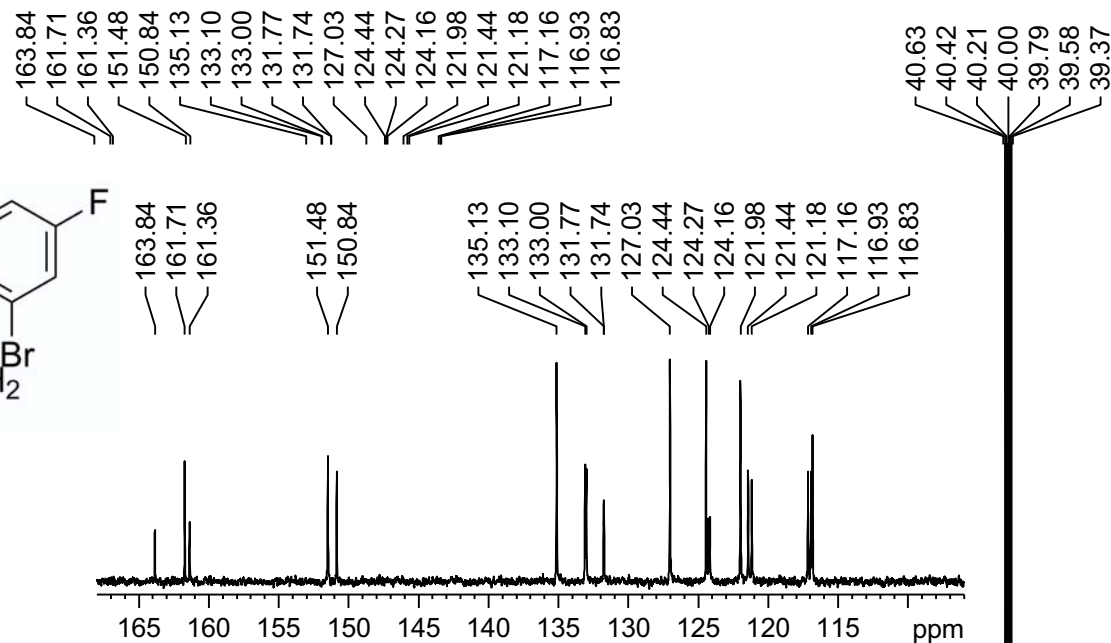
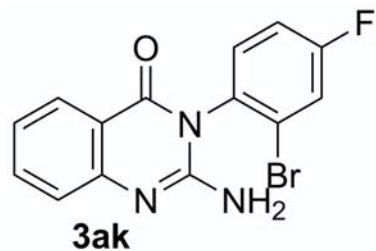
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 PROCNO 1

F2 - Acquisition Parameters
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 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 99.72
 DW 69.333 usec
 DE 10.52 usec
 TE 298.5 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 ¹H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300032 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

13C



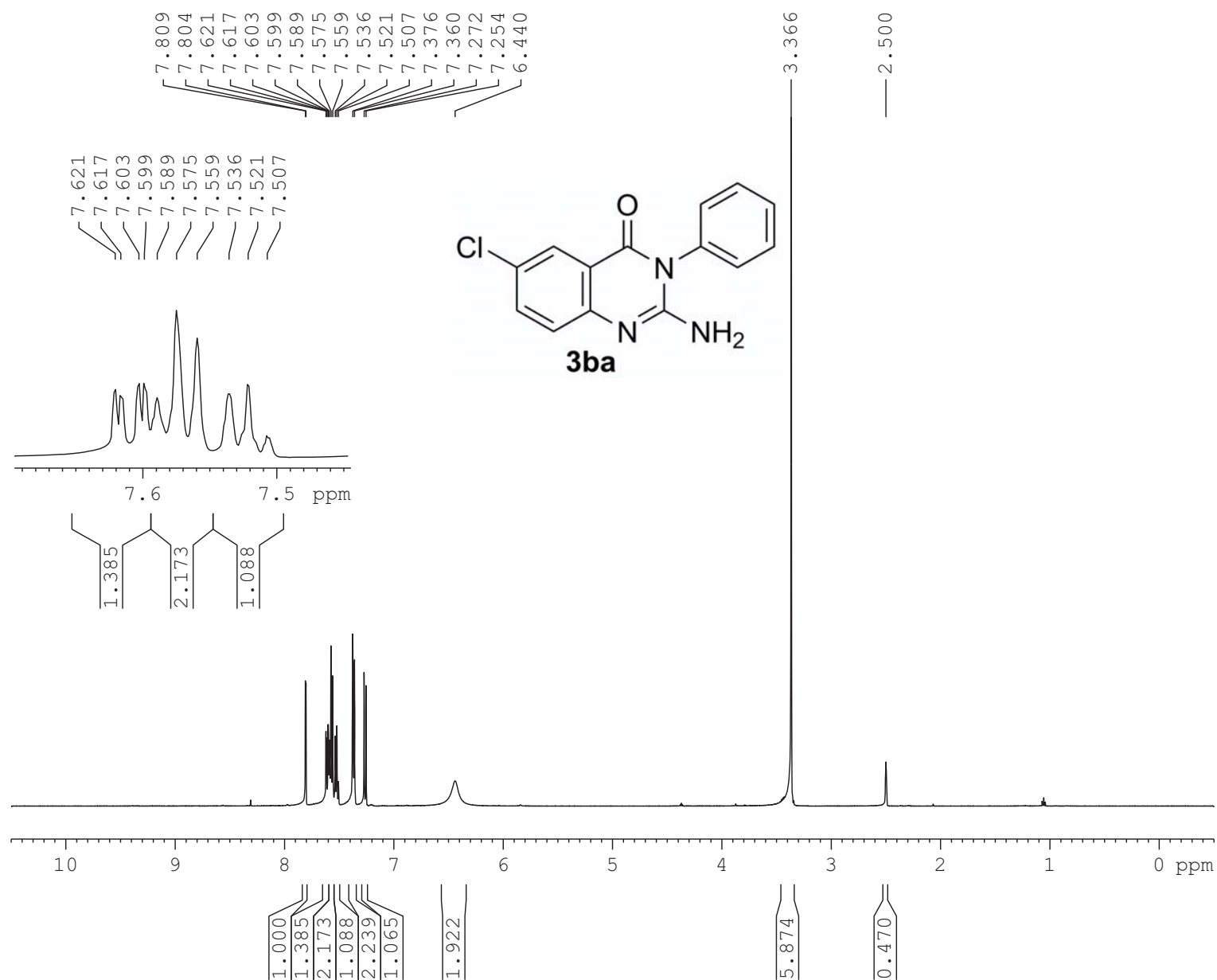
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NAME RX167 recrystall
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
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Time 13.17
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PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1609
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127692 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

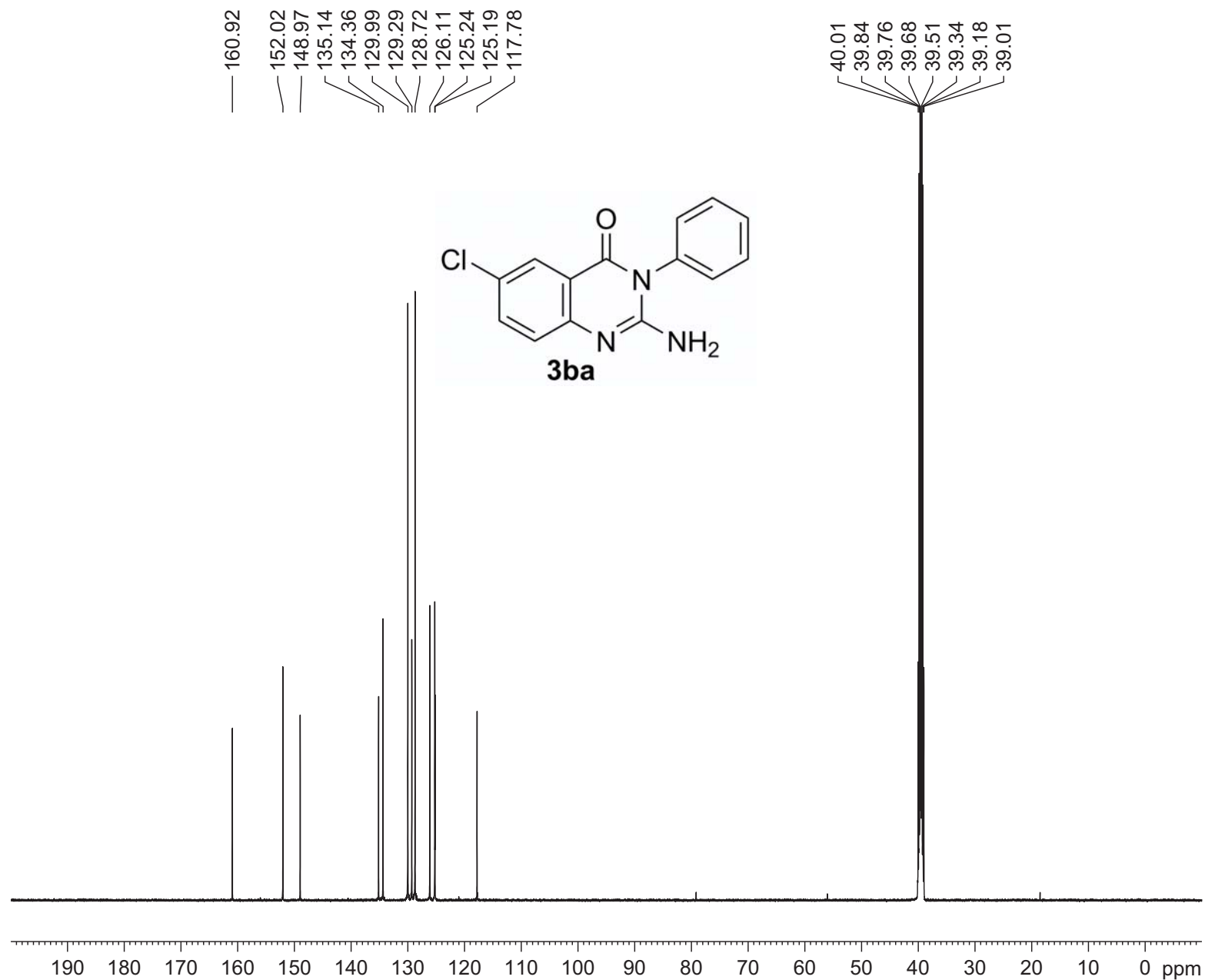


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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130322
 Time 22.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 90.5
 DW 55.200 usec
 DE 6.50 usec
 TE 296.9 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300054 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



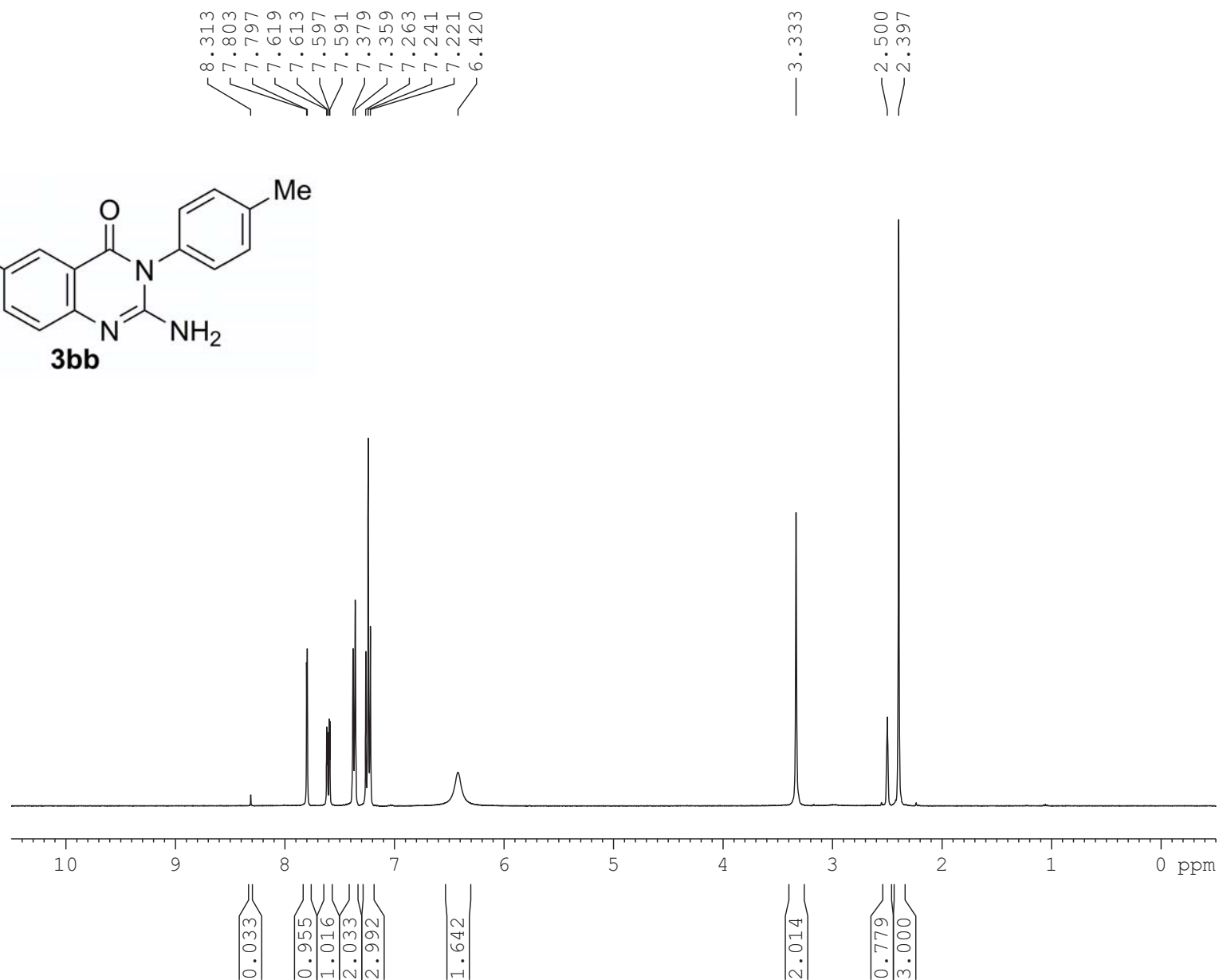
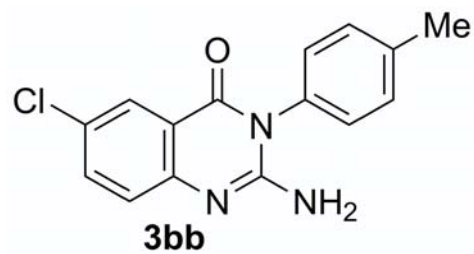
Current Data Parameters
 NAME RV004athree
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130323
 Time 9.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 12791
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 2896.3
 DW 16.650 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578513 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

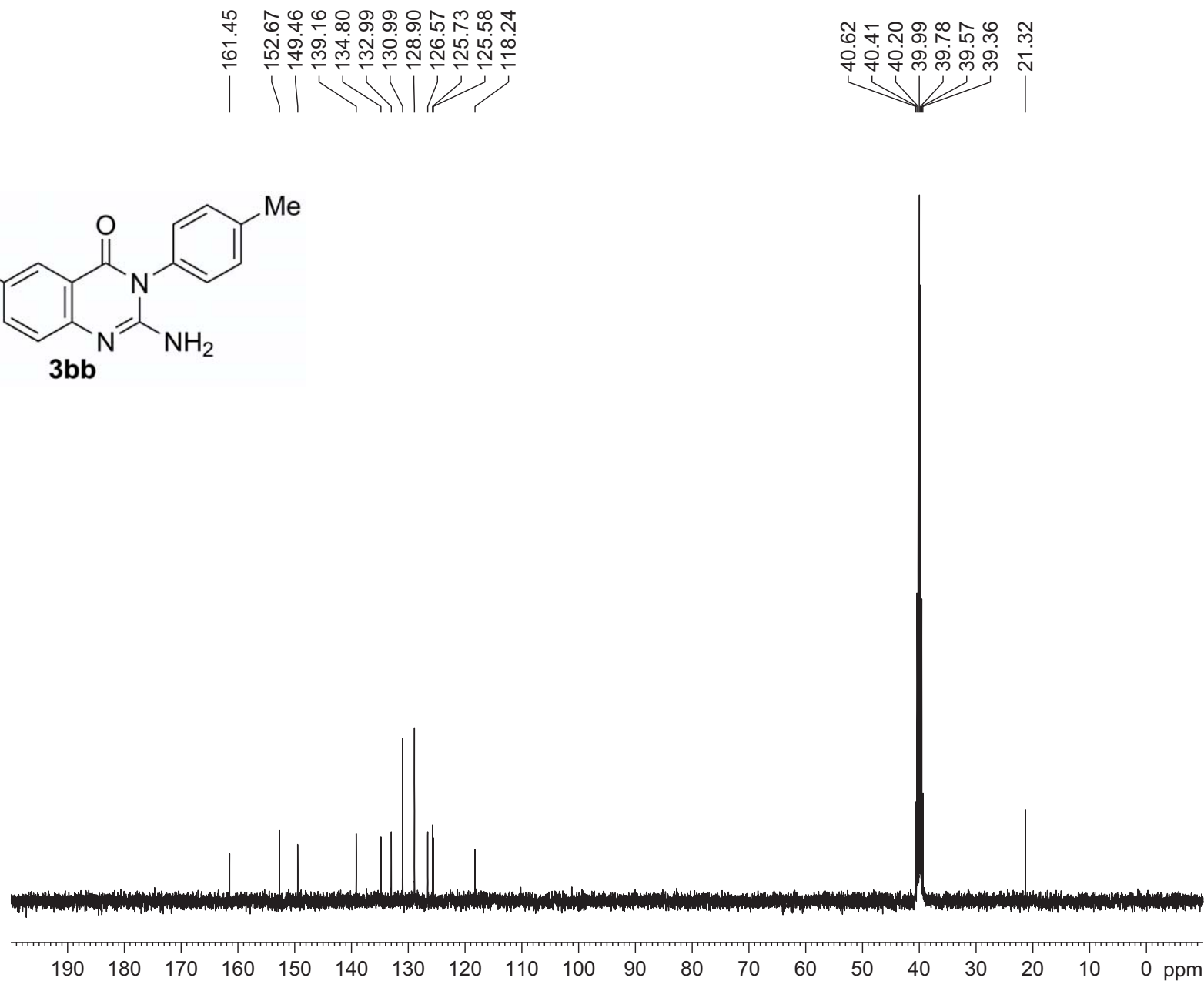


Current Data Parameters
 NAME RK163
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
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 Time 20.11
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 114
 DW 69.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300017 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME RK163
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120409
Time 20.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 61
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

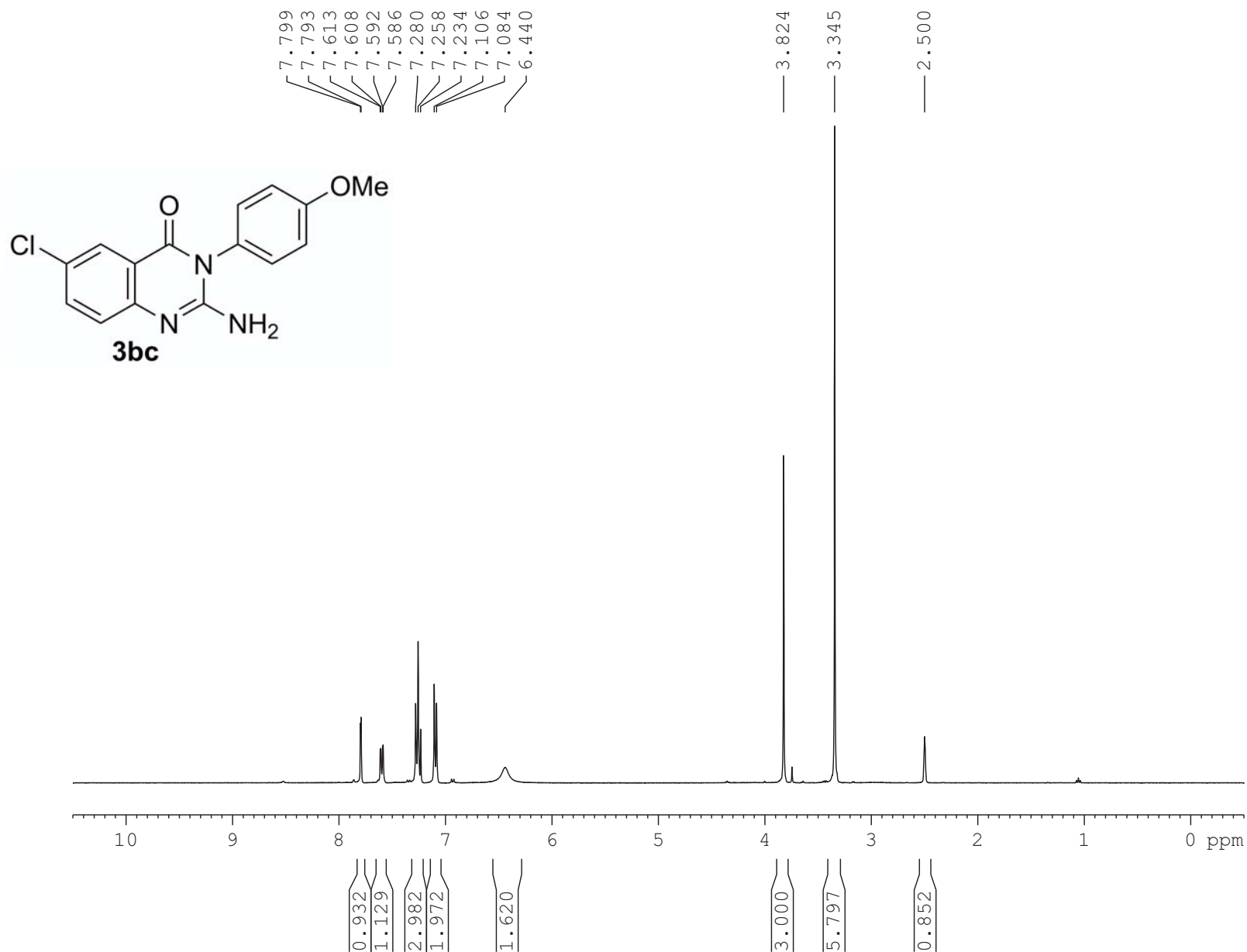
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

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

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

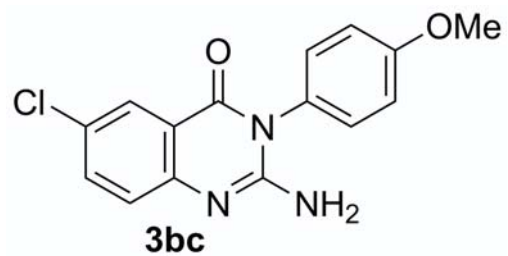


Current Data Parameters
 NAME RK159
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120409
 Time 15.39
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 90.5
 DW 69.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 TD0 1

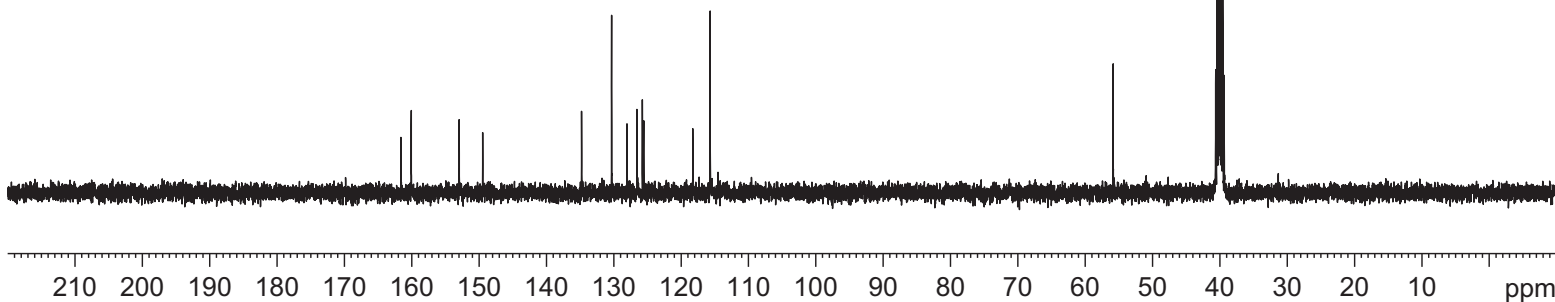
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 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300022 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



161.582
160.060
152.938
149.449
134.764
130.308
128.011
126.544
125.738
125.532
118.251
115.679

55.850
40.619
40.410
40.201
39.992
39.784
39.575
39.367



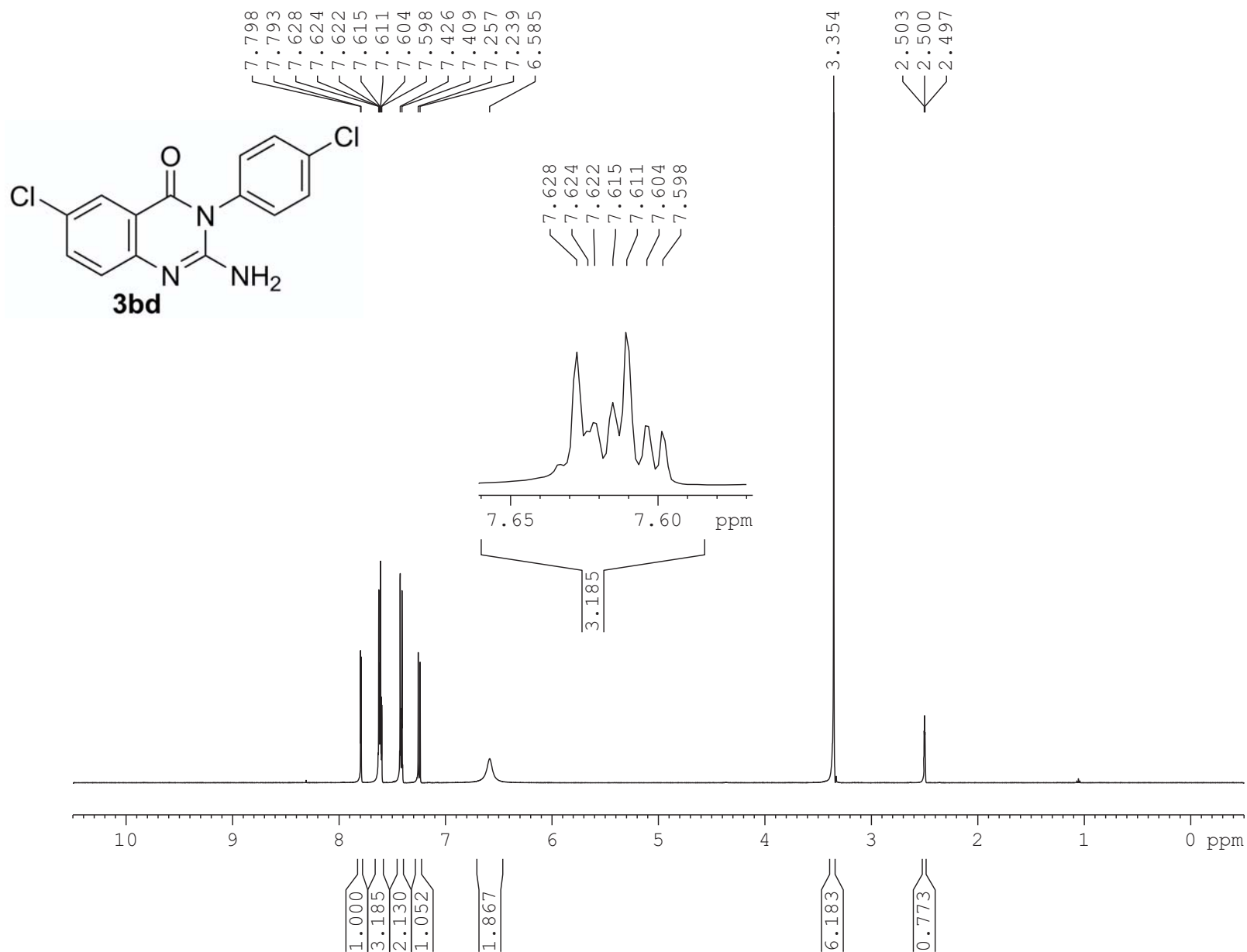
Current Data Parameters
NAME RK159
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
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Time 11.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 80
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz

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

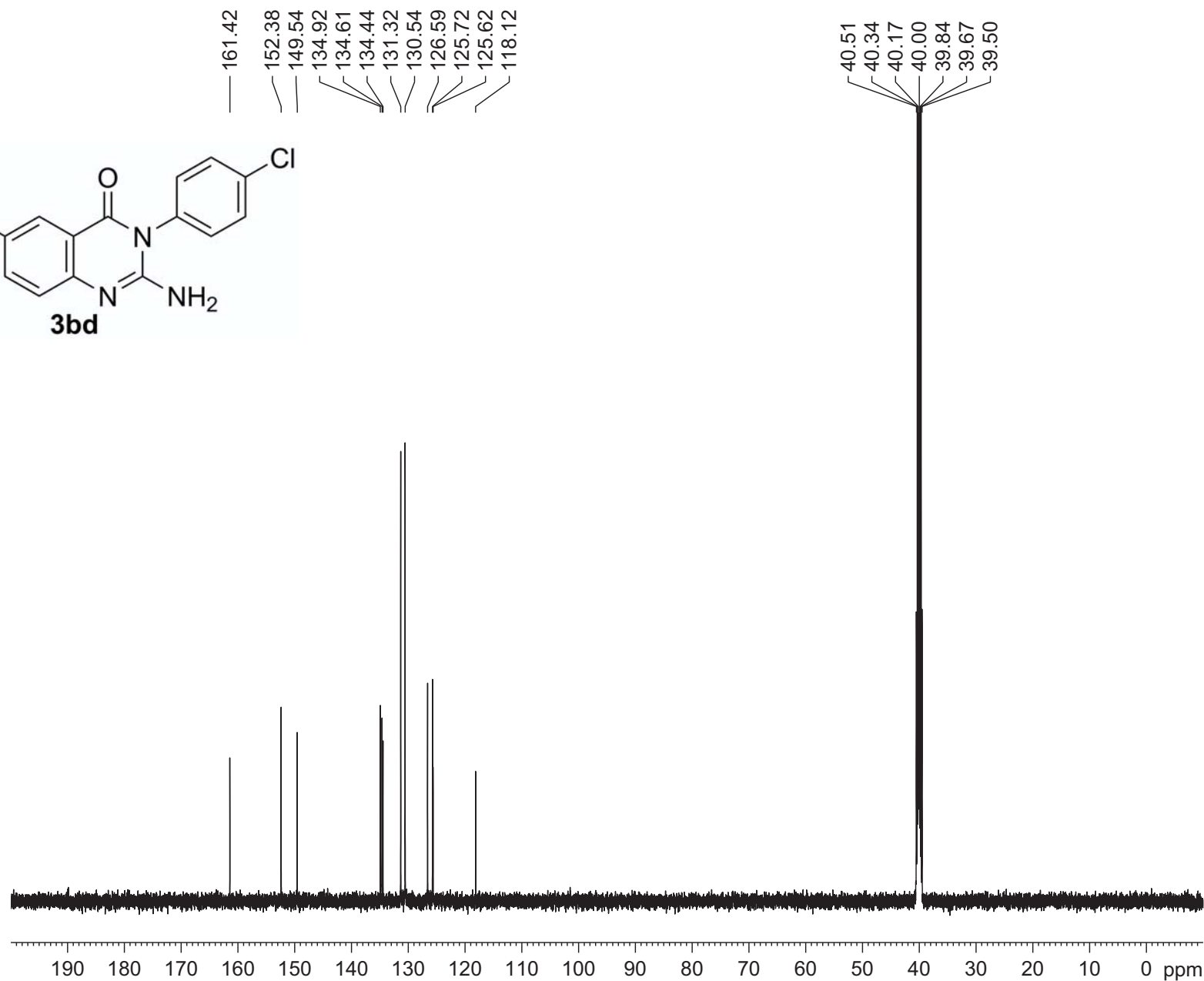
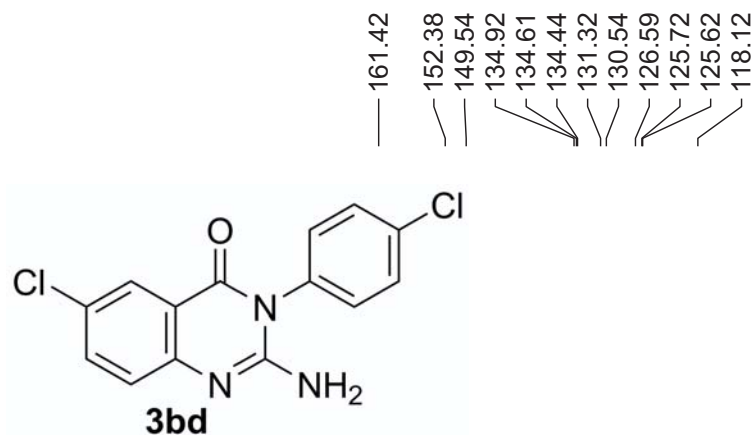


Current Data Parameters
NAME RK196three
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 161.3
DW 55.200 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



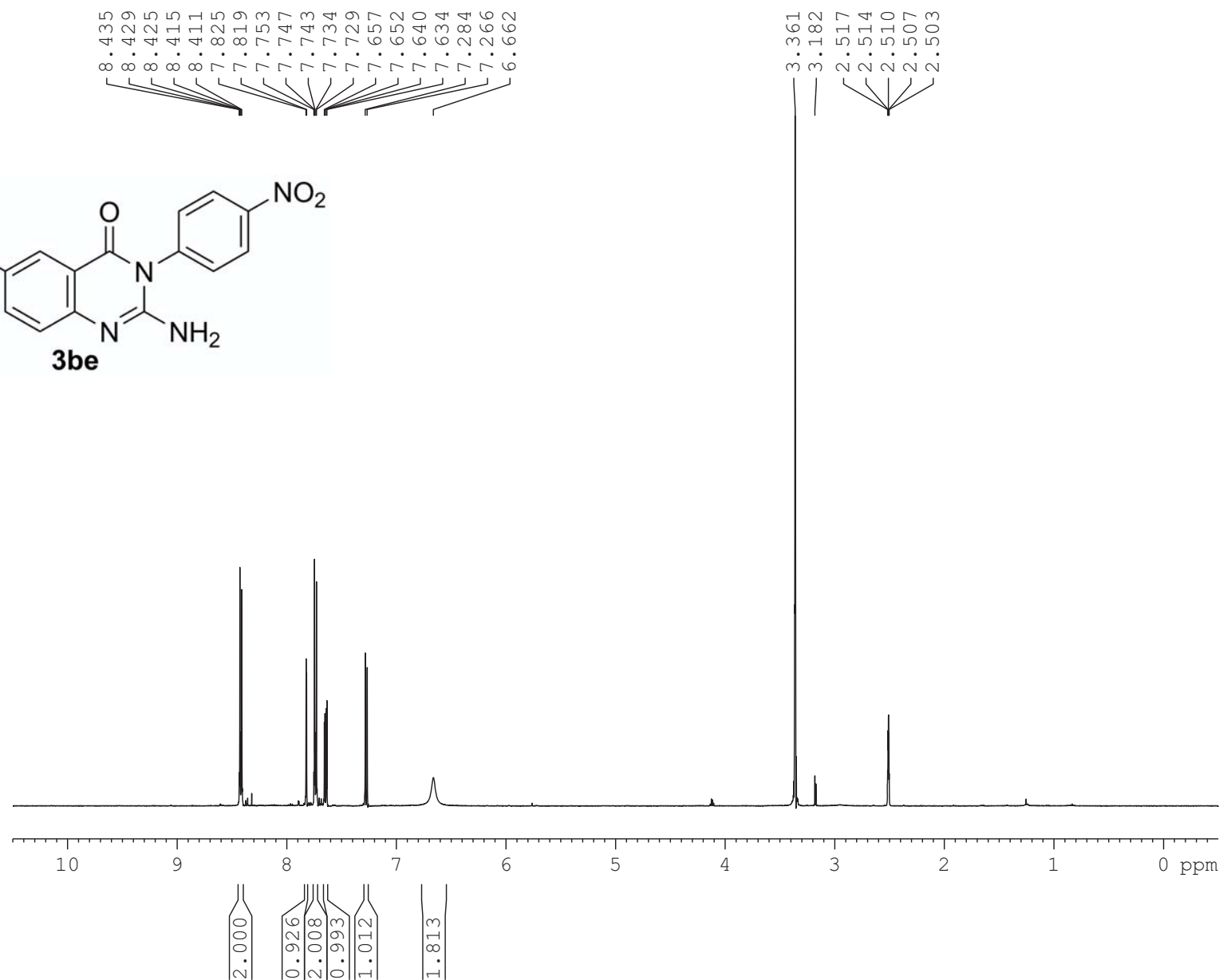
Current Data Parameters
 NAME RK196three
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130330
 Time 11.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 289
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 4096
 DW 16.650 usec
 DE 6.50 usec
 TE 297.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

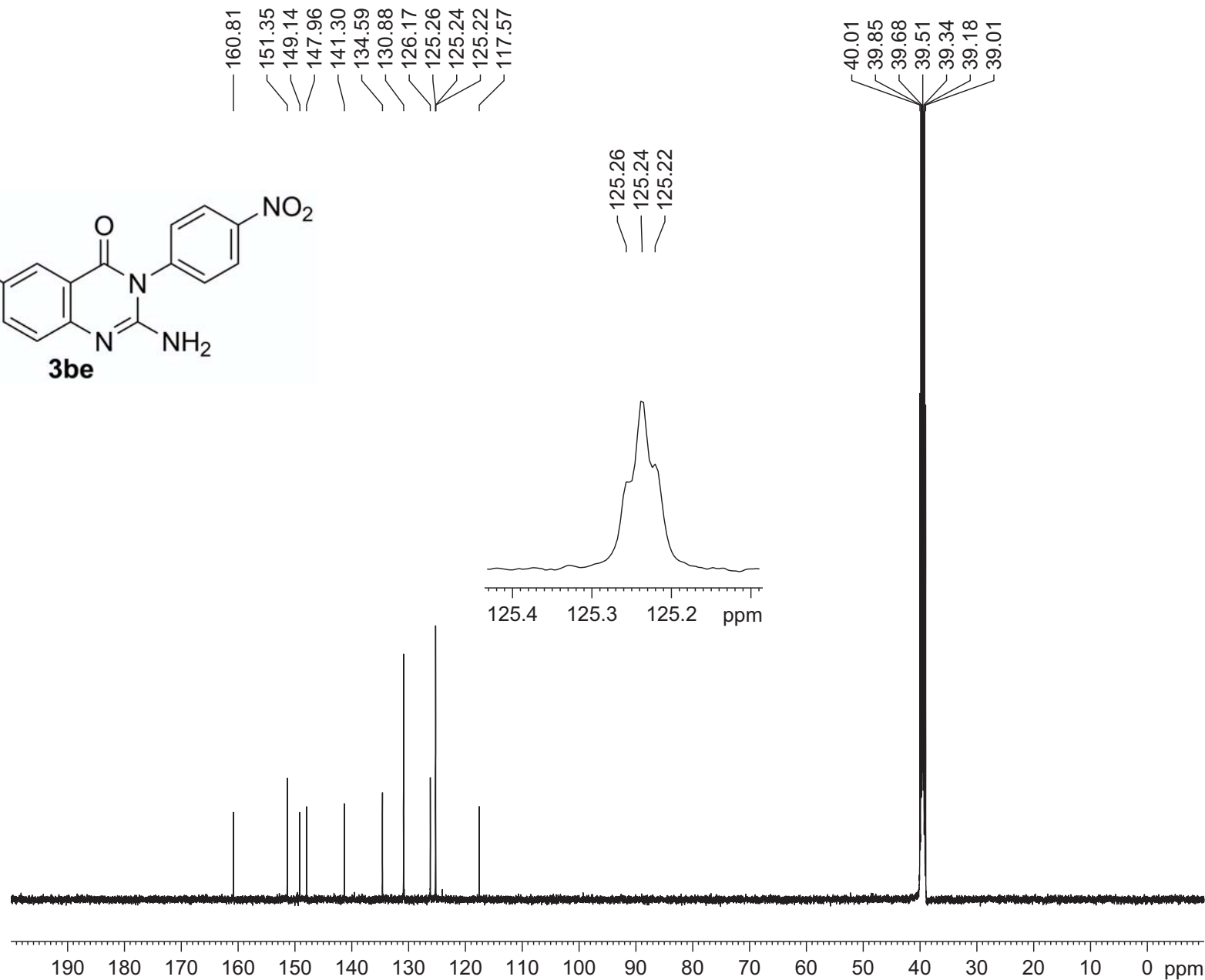


Current Data Parameters
 NAME RM093-1
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121006
 Time 9.18
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 295.2 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300000 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM093-1
 EXPNO 2
 PROCNO 1

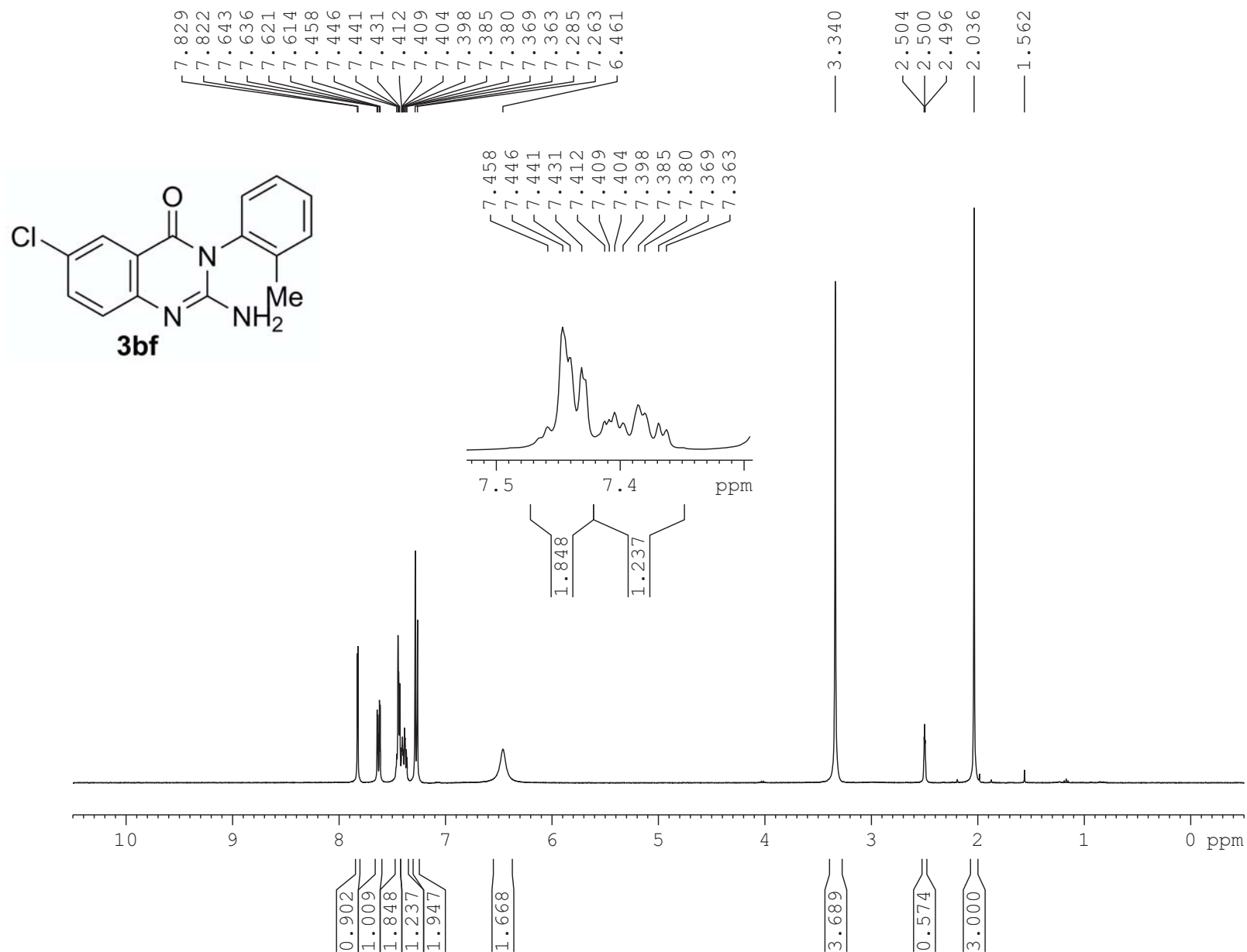
F2 - Acquisition Parameters
 Date_ 20121006
 Time 12.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1612
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 2896.3
 DW 16.650 usec
 DE 6.50 usec
 TE 297.1 K
 D1 4.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578504 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

recrystallized



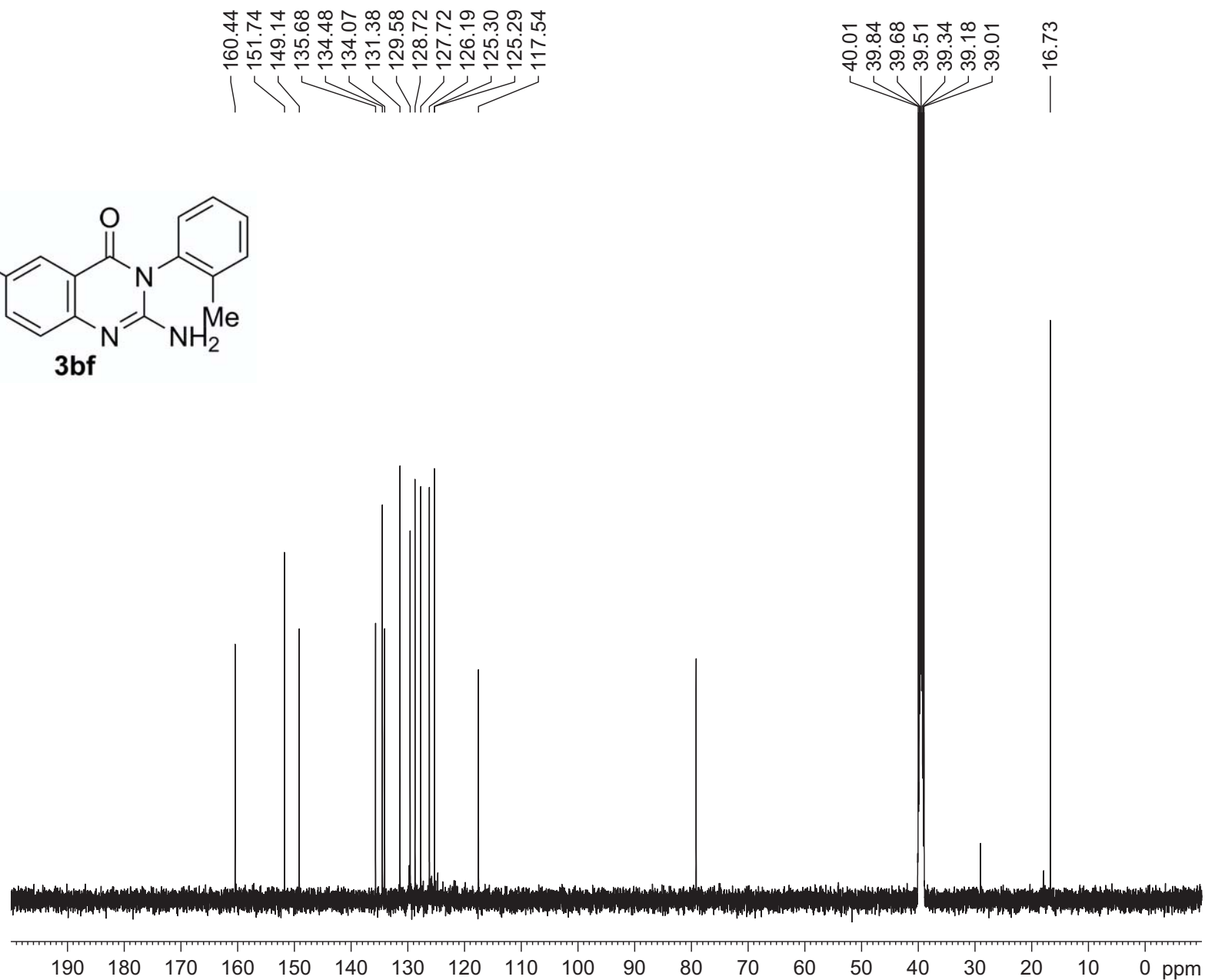
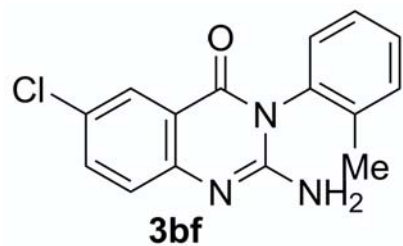
Current Data Parameters
NAME RM020
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130125
Time 20.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 161.3
DW 69.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

NaOH extracted



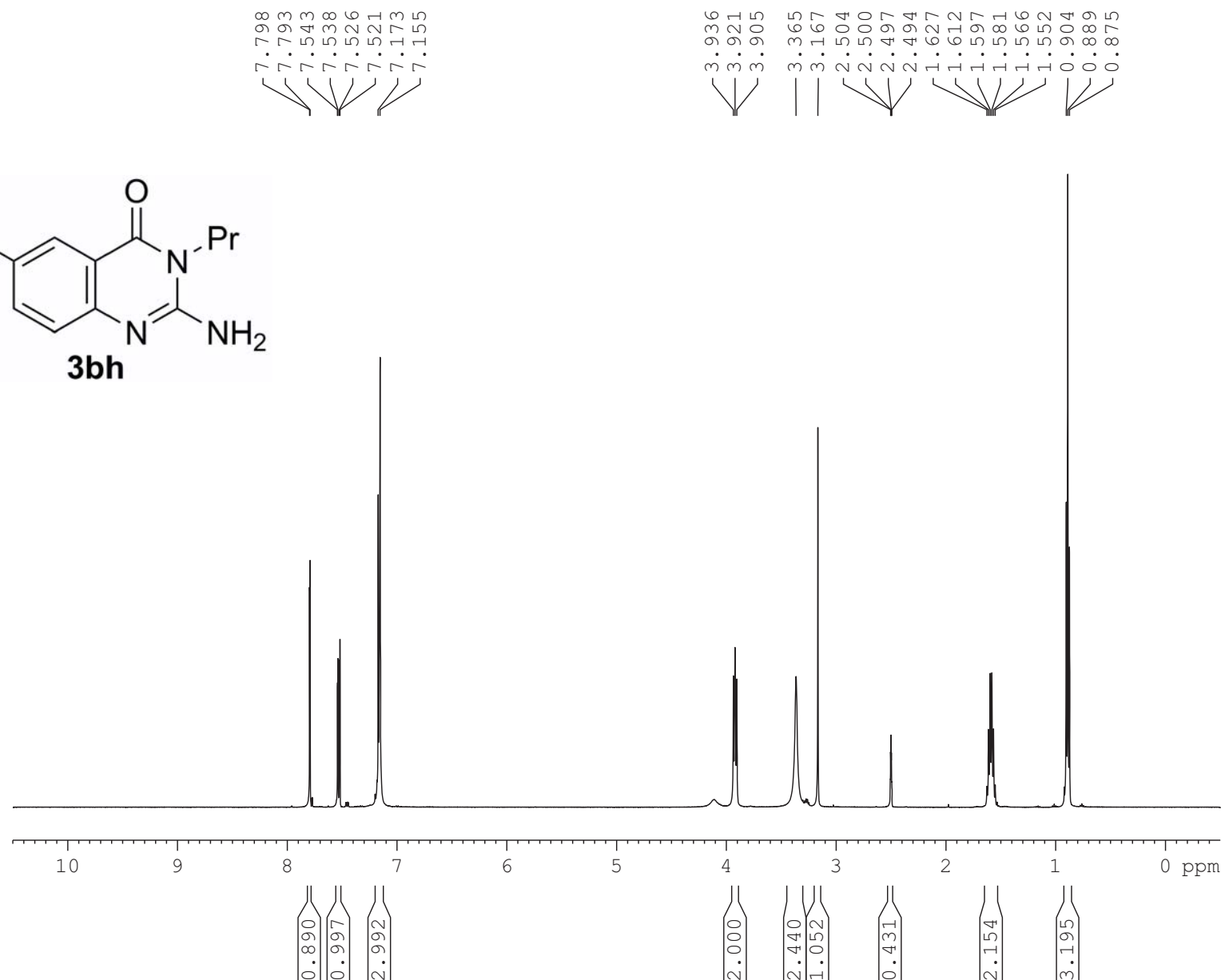
Current Data Parameters
 NAME RM020
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121230
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 2896.3
 DW 16.650 usec
 DE 6.50 usec
 TE 297.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578499 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

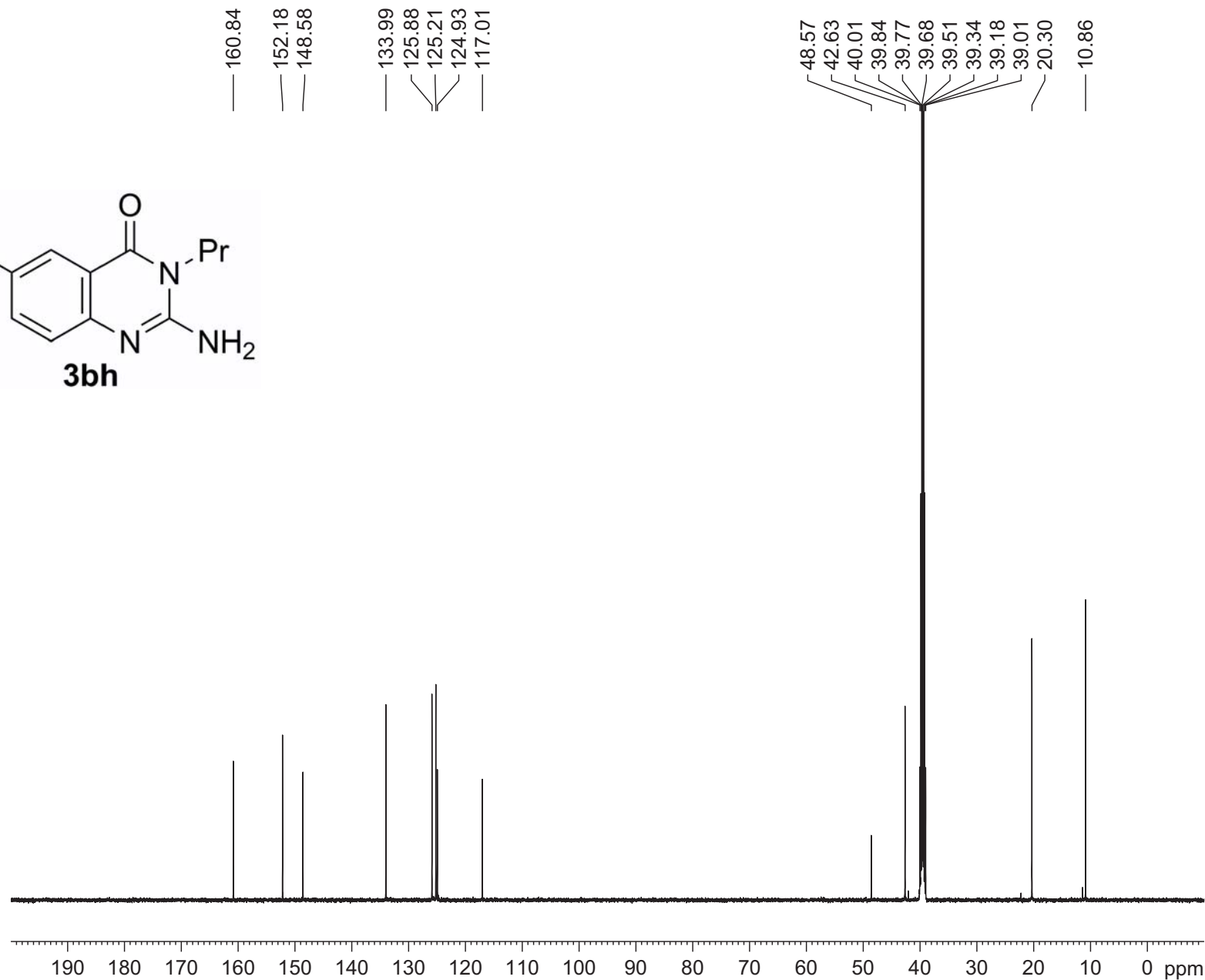


Current Data Parameters
 NAME RM192three
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130309
 Time 9.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 90.5
 DW 55.200 usec
 DE 6.50 usec
 TE 295.7 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



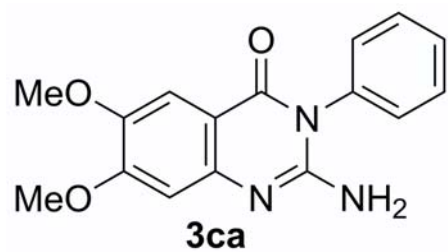
Current Data Parameters
 NAME RM192three
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130309
 Time 11.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 2896.3
 DW 16.650 usec
 DE 6.50 usec
 TE 297.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578499 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

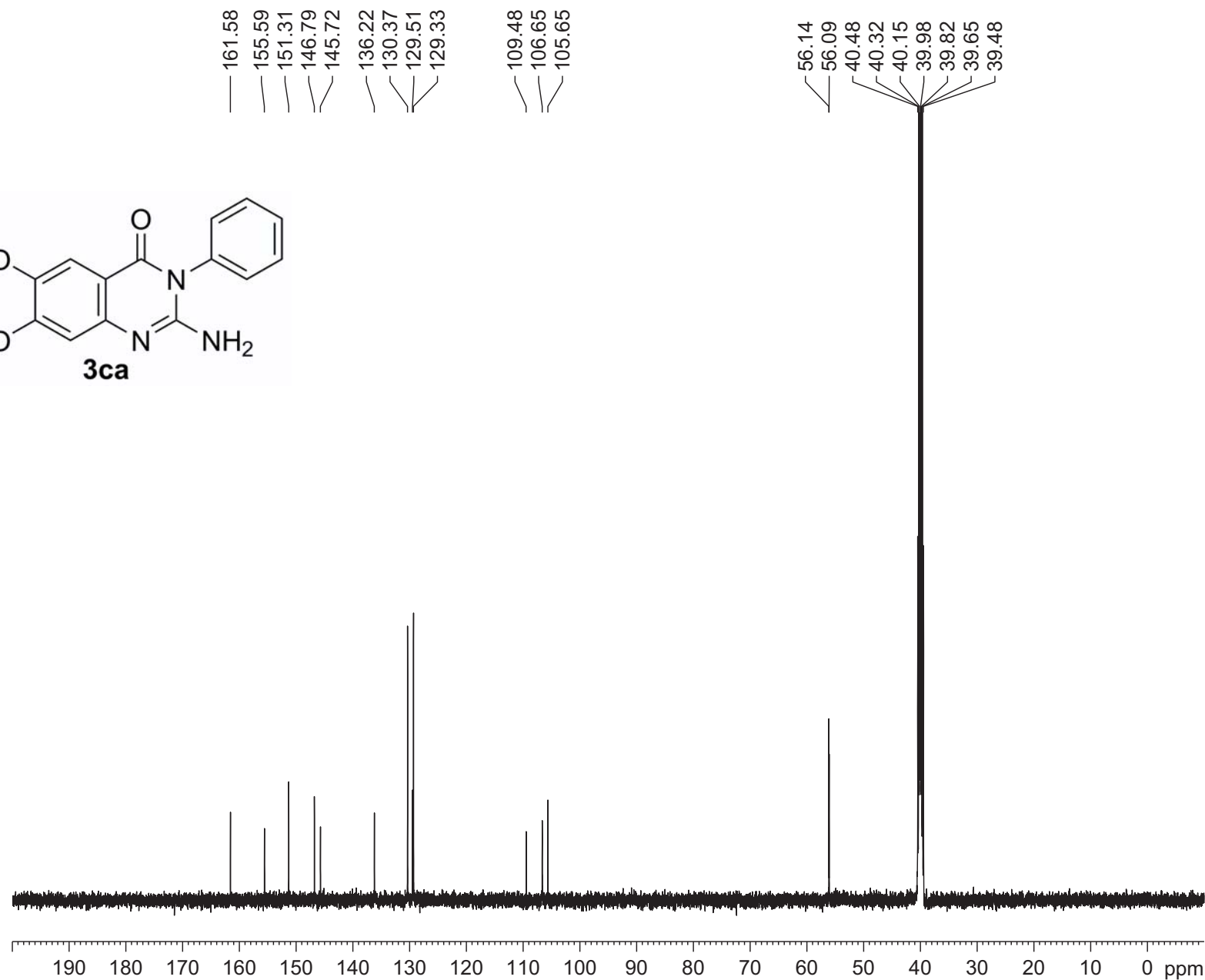
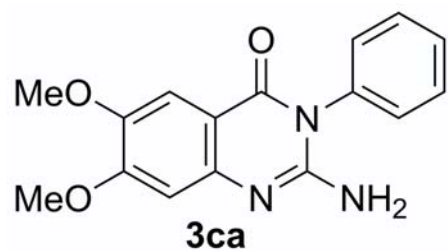


Current Data Parameters
 NAME RK186
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120512
 Time 14.26
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 161.3
 DW 55.200 usec
 DE 6.50 usec
 TE 295.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300043 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



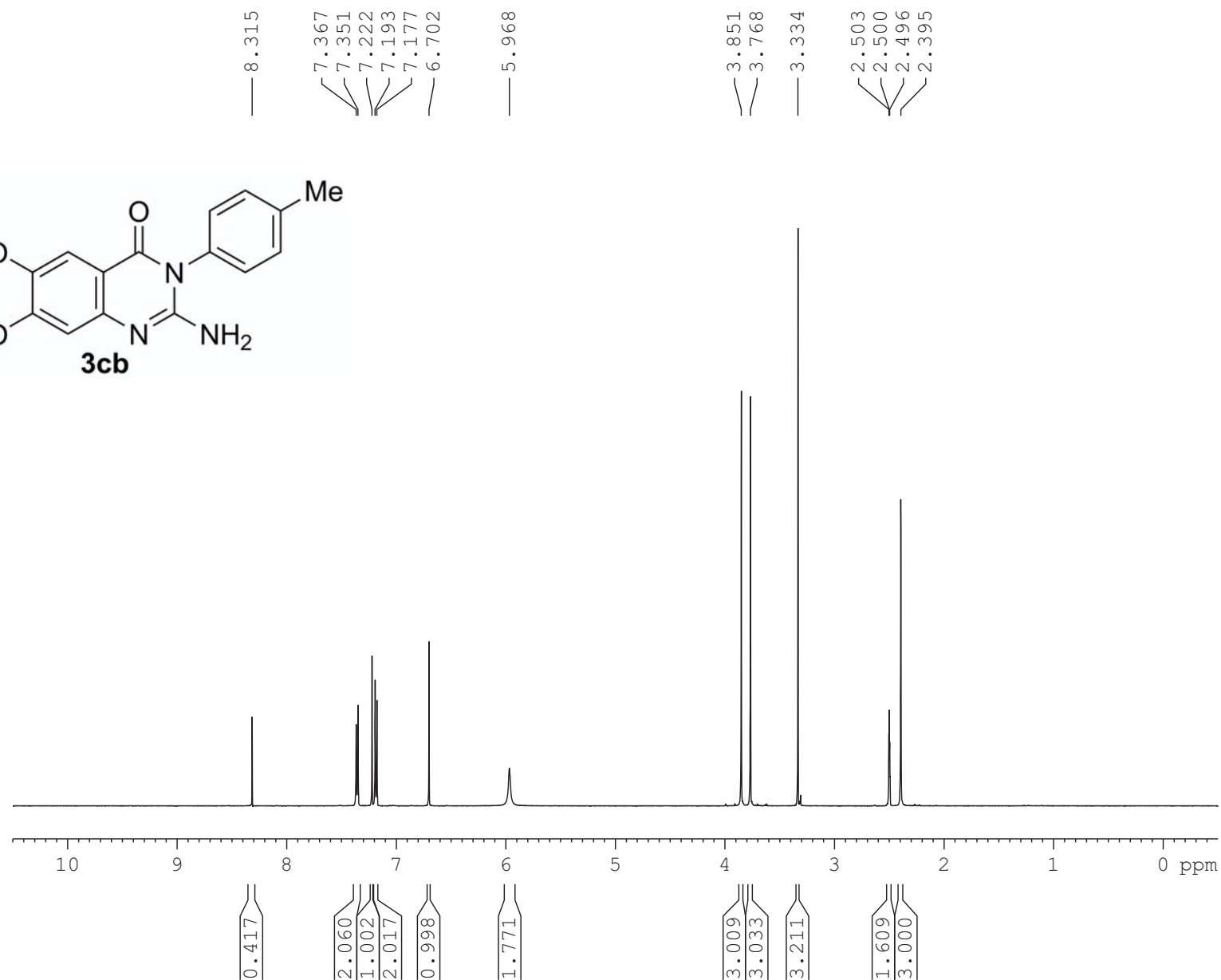
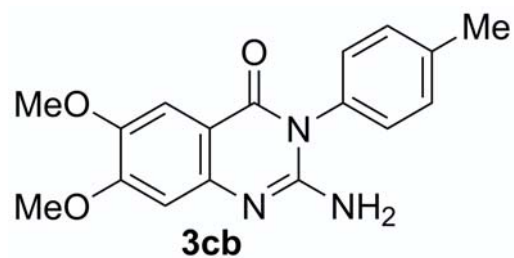
Current Data Parameters
 NAME RK186
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120512
 Time 14.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 500
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 4096
 DW 16.650 usec
 DE 6.50 usec
 TE 296.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

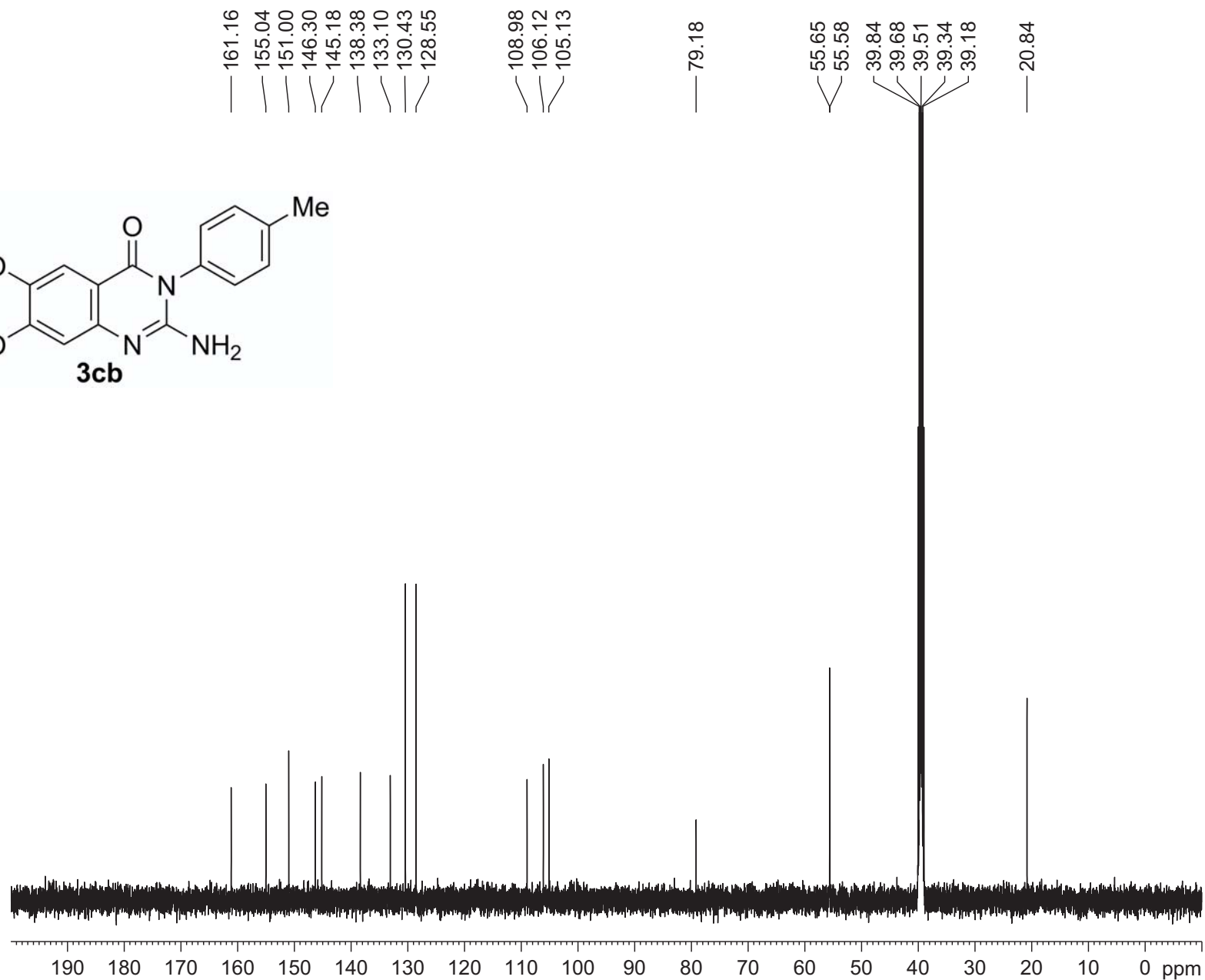
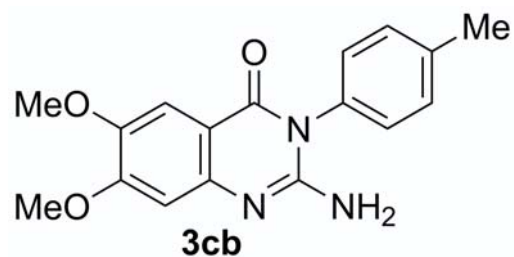
===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00



NAME RK170-1
 EXPNO 1
 PROCNO 1
 Date_ 20120415
 Time 14.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088988 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 295.6 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0.00 dB
 SFO1 500.1330008 MHz
 SI 16384
 SF 500.1300043 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



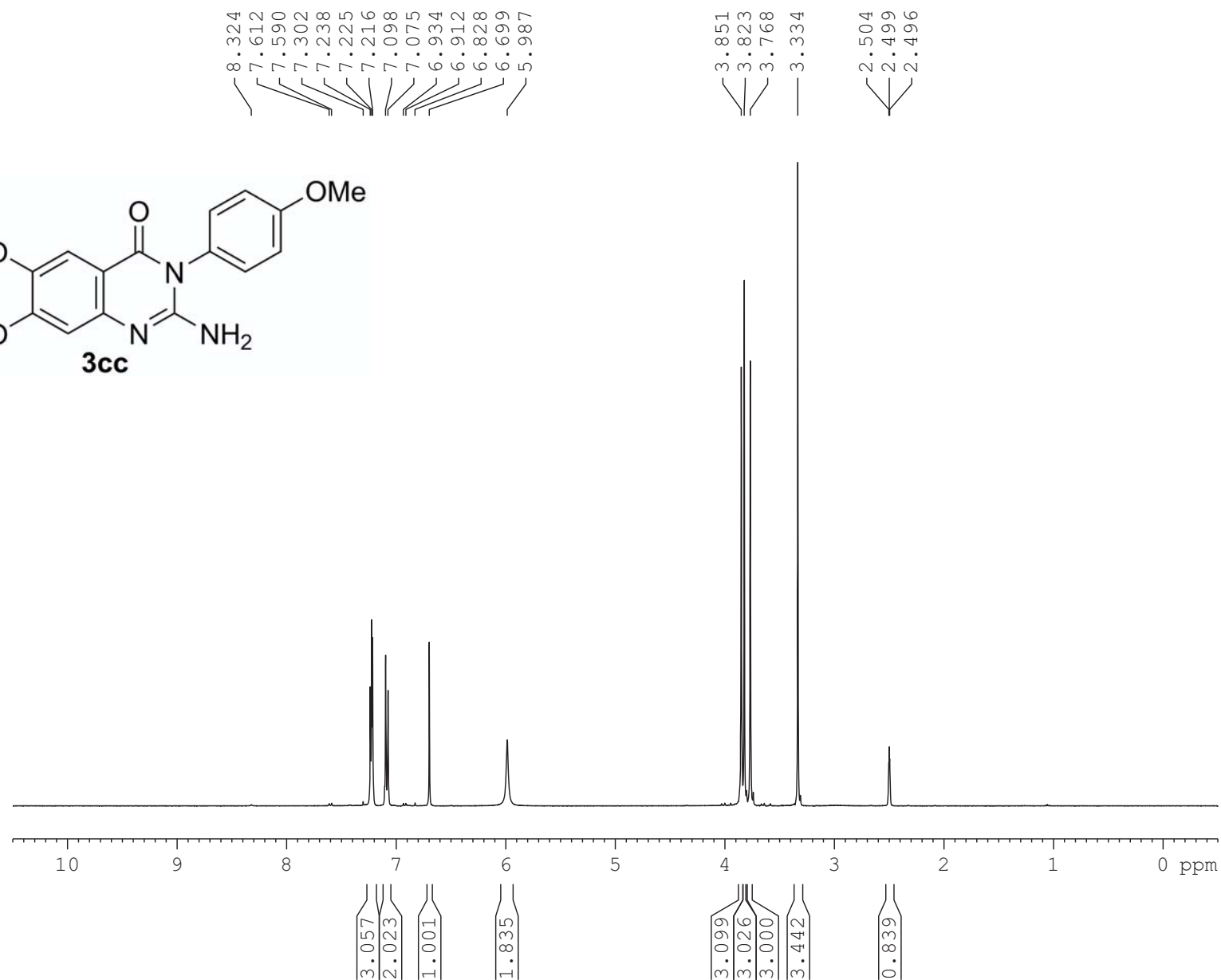
Current Data Parameters
 NAME RK170-1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120415
 Time 14.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 176
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 6502
 DW 16.650 usec
 DE 6.50 usec
 TE 296.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578484 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

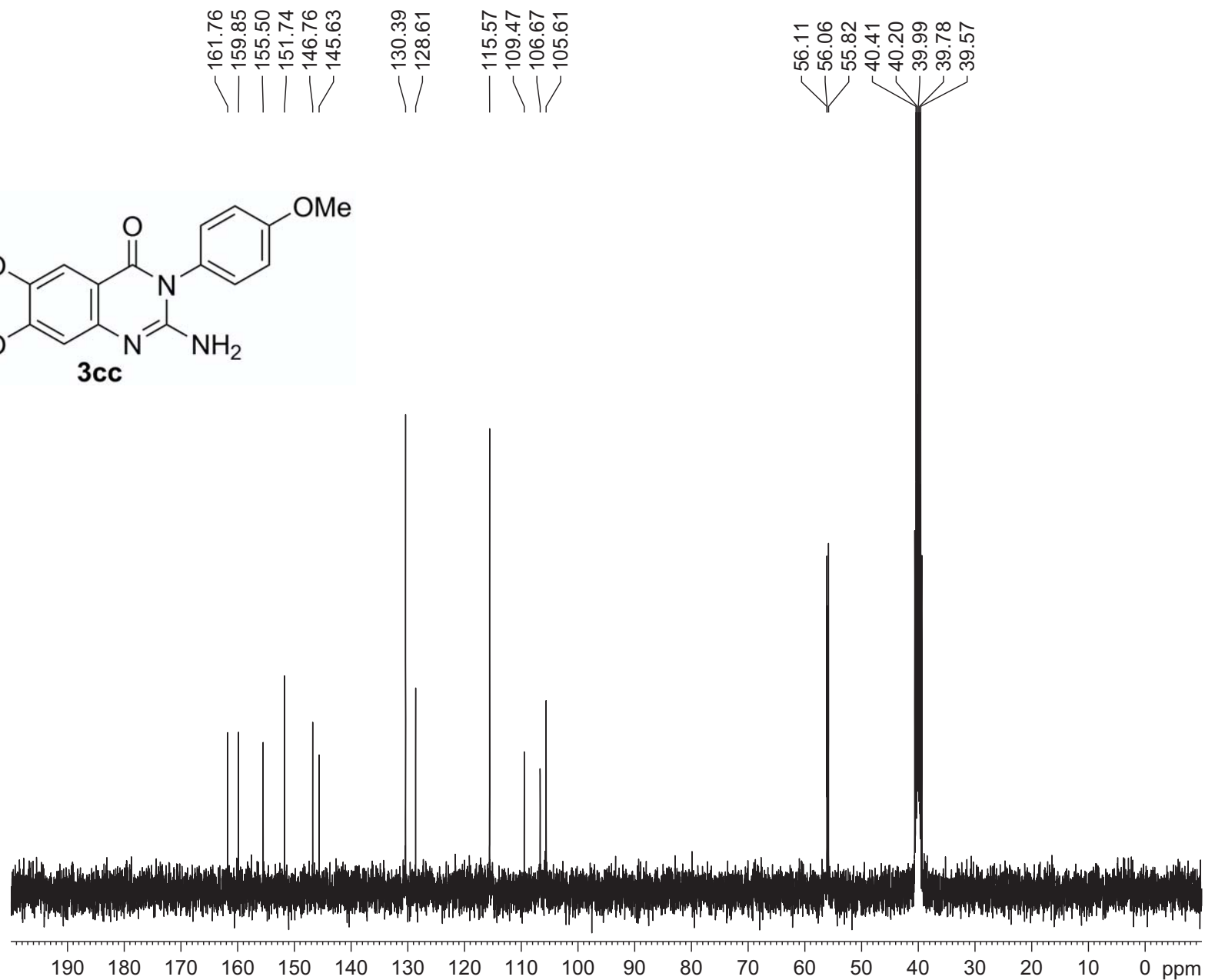


Current Data Parameters
 NAME RK176
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120425
 Time 11.07
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 90.5
 DW 69.000 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300022 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



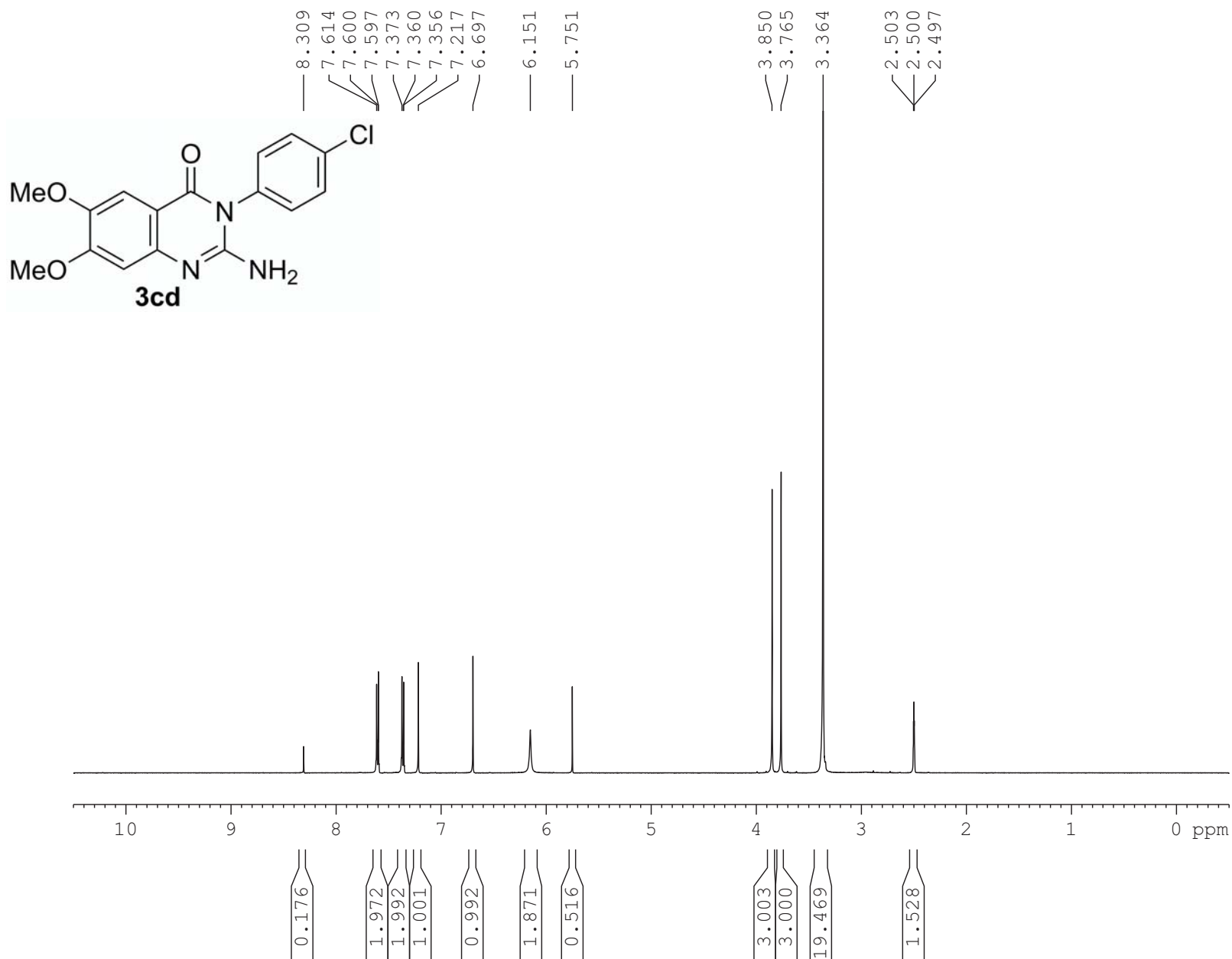
Current Data Parameters
 NAME RK176
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120425
 Time 11.10
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 100
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 2896.3
 DW 20.800 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.90 usec
 PL1 7.00 dB
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 3.80 dB
 PL12 21.60 dB
 PL13 24.60 dB
 SFO2 400.1316005 MHz

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

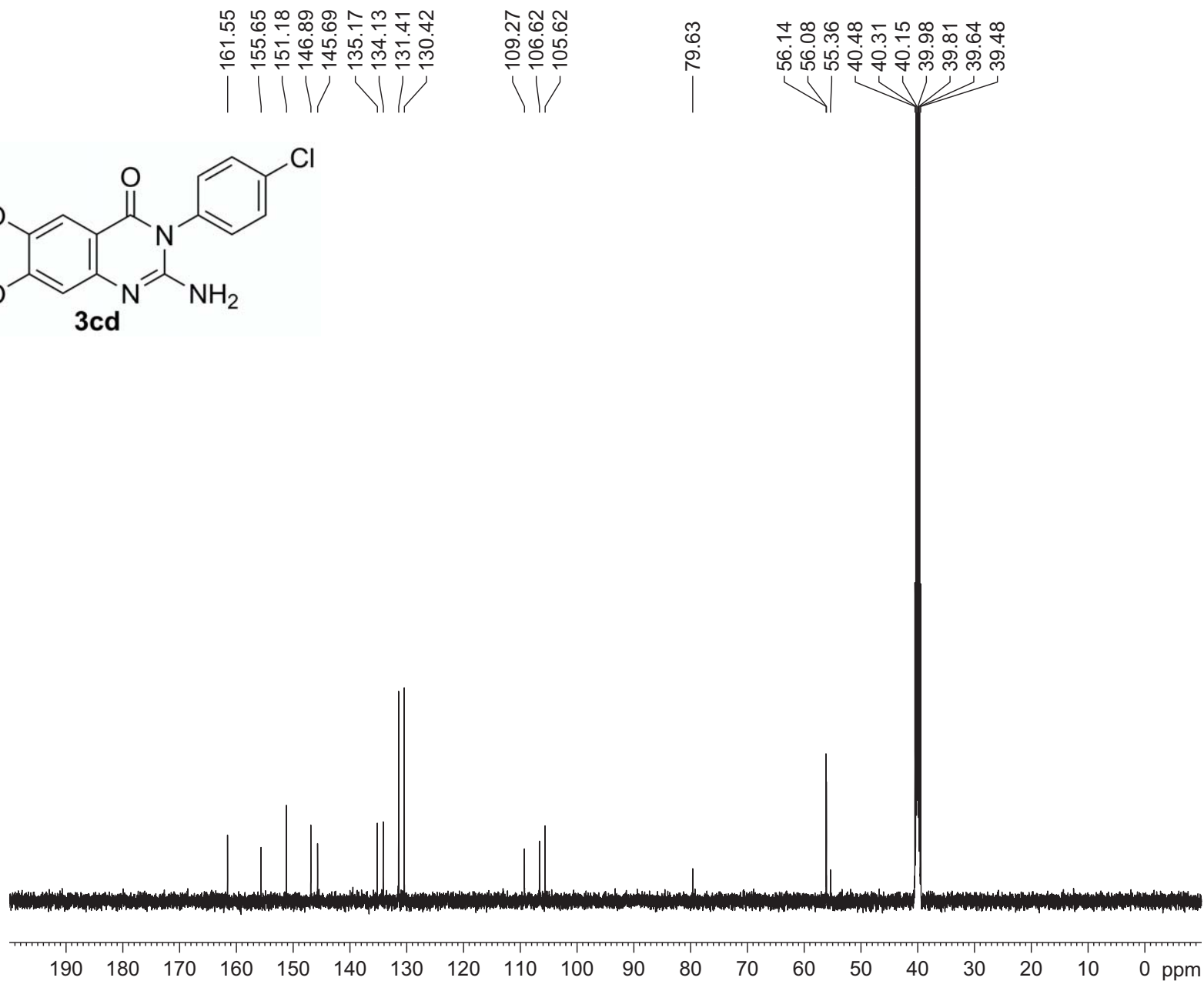
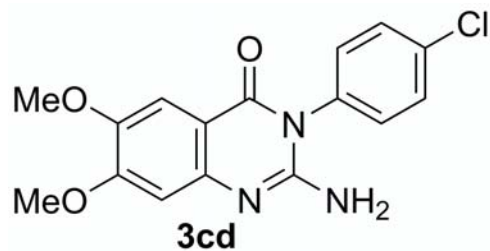


Current Data Parameters
 NAME RK198
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120602
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 161.3
 DW 55.200 usec
 DE 6.50 usec
 TE 295.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0 dB
 SFO1 500.1330008 MHz

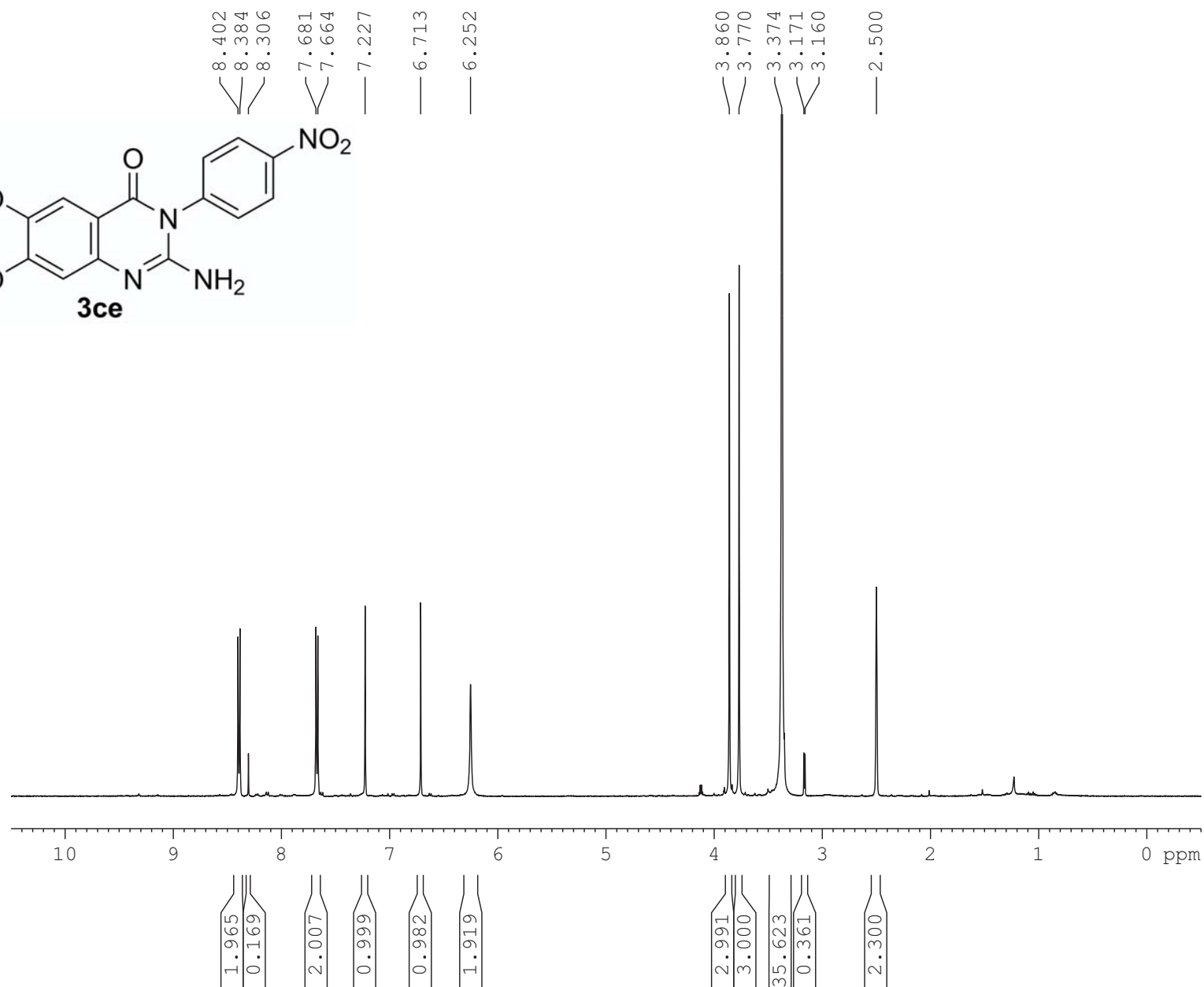
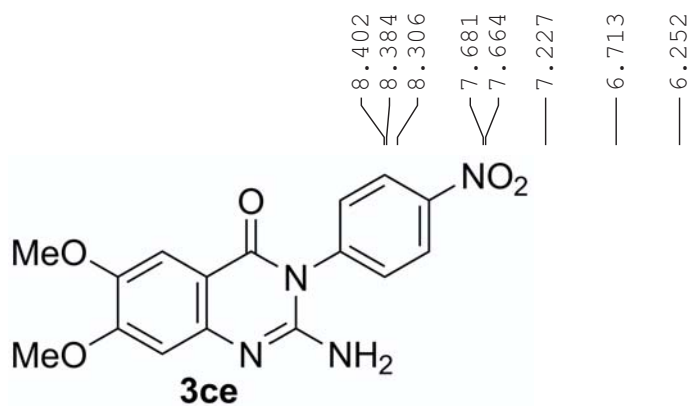
F2 - Processing parameters
 SI 16384
 SF 500.1300043 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



NAME RK198
 EXPNO 2
 PROCNO 1
 Date_ 20120602
 Time 14.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 350
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 4096
 DW 16.650 usec
 DE 6.50 usec
 TE 296.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz
 SI 65536
 SF 125.7577890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

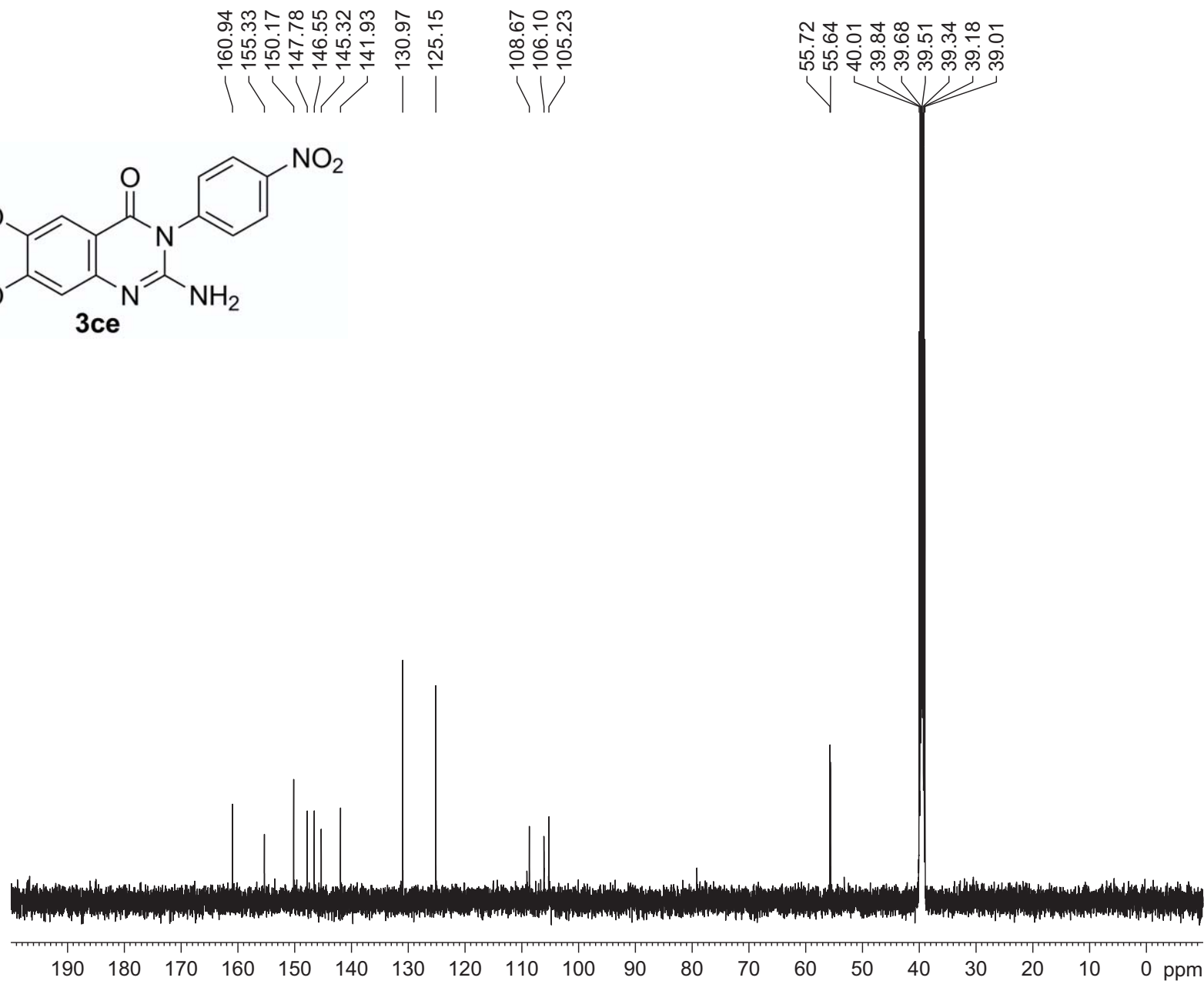
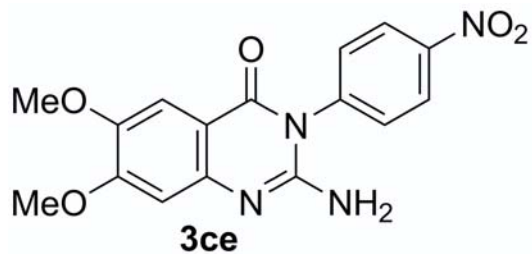


Current Data Parameters
 NAME RM031-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120714
 Time 10.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 294.6 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300040 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM031-2
 EXPNO 2
 PROCNO 1

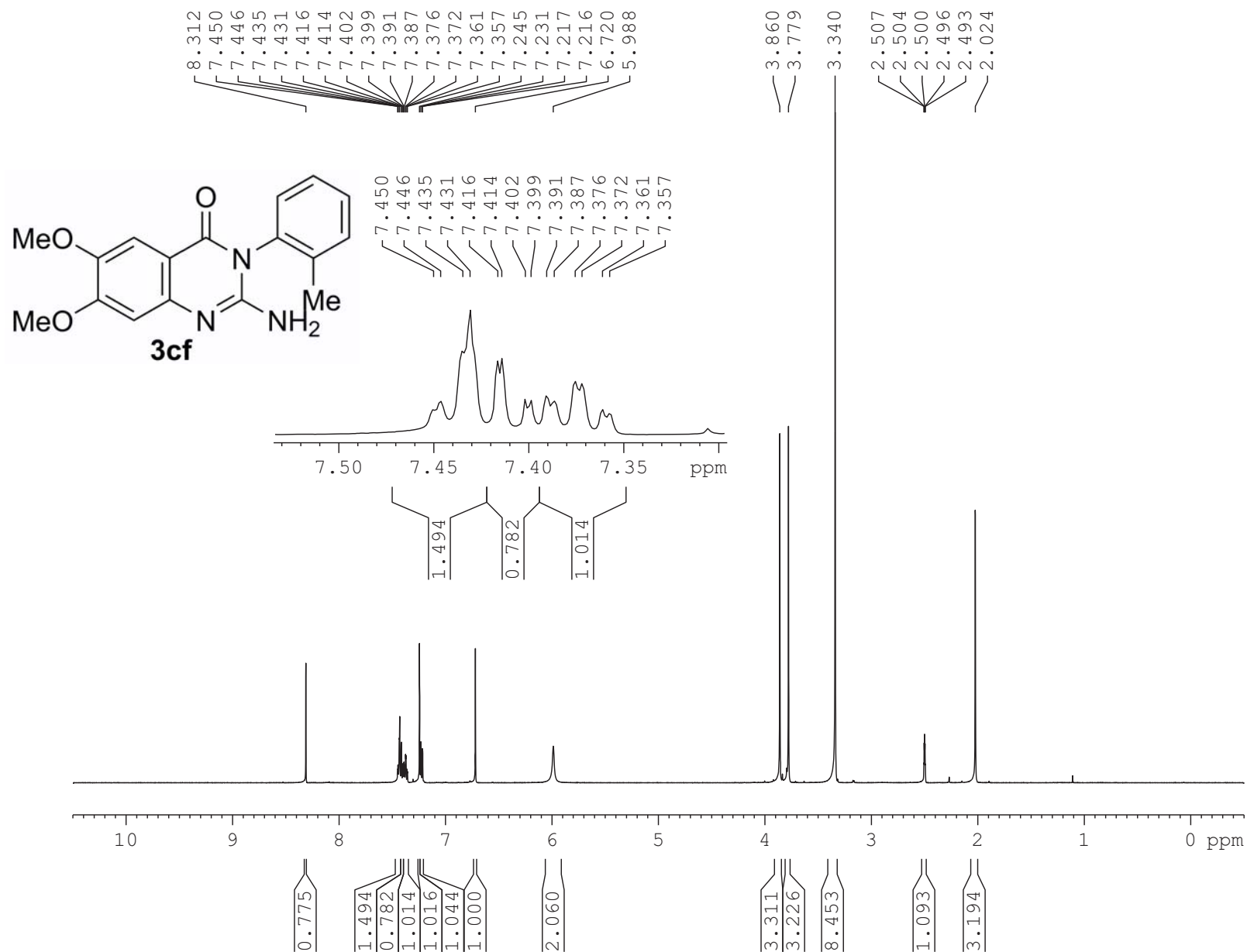
F2 - Acquisition Parameters
 Date_ 20120714
 Time 10.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 350
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 4096
 DW 16.650 usec
 DE 6.50 usec
 TE 296.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578467 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

NaOH extracted



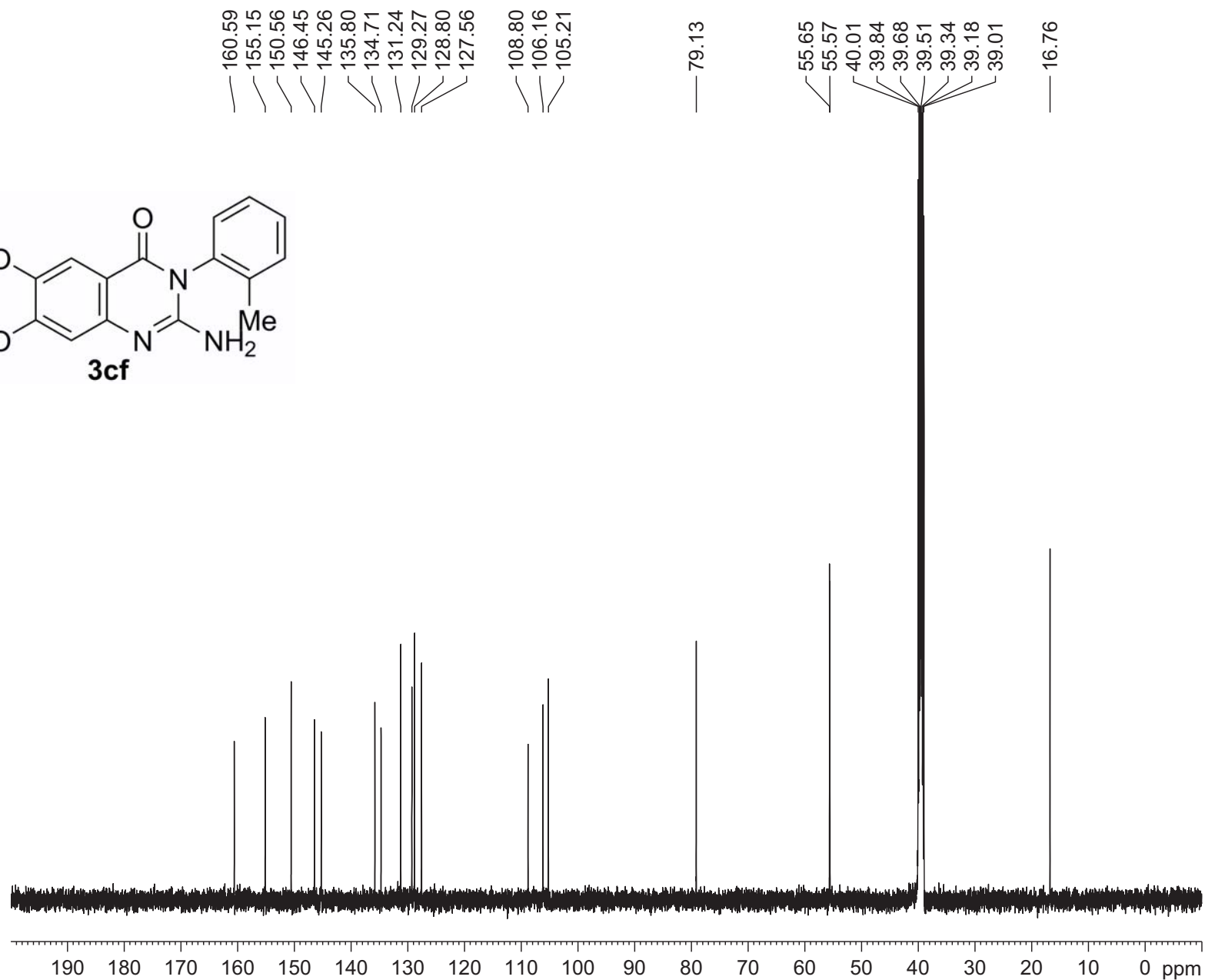
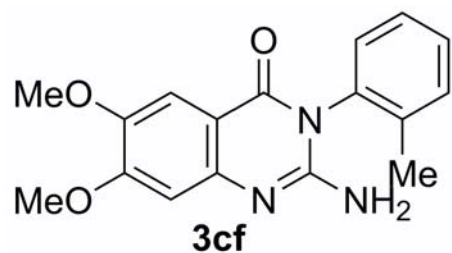
Current Data Parameters
 NAME RM017
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121230
 Time 12.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 296.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300051 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

NaOH extracted



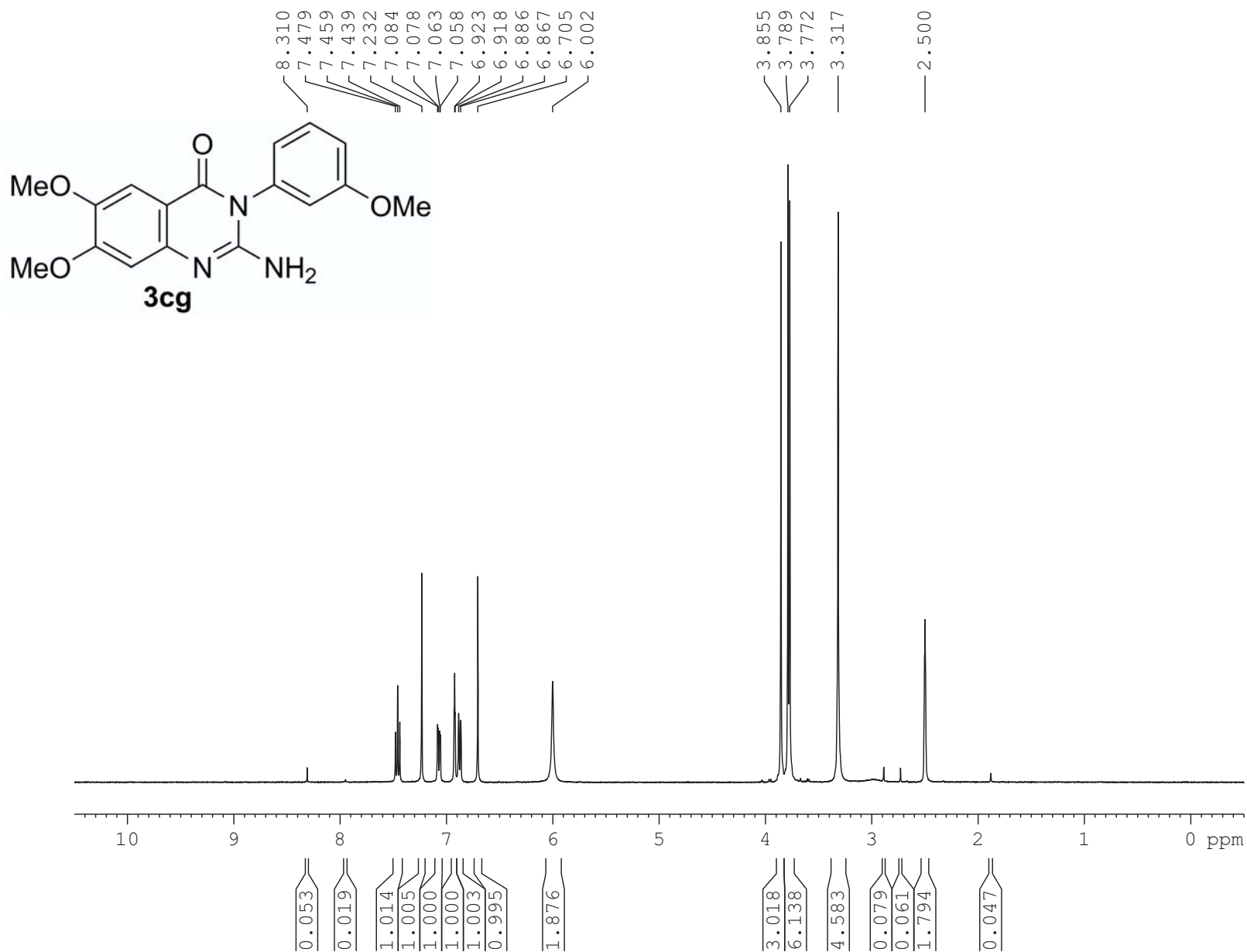
Current Data Parameters
NAME RM017
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121230
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 4096
DW 16.650 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7578531 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

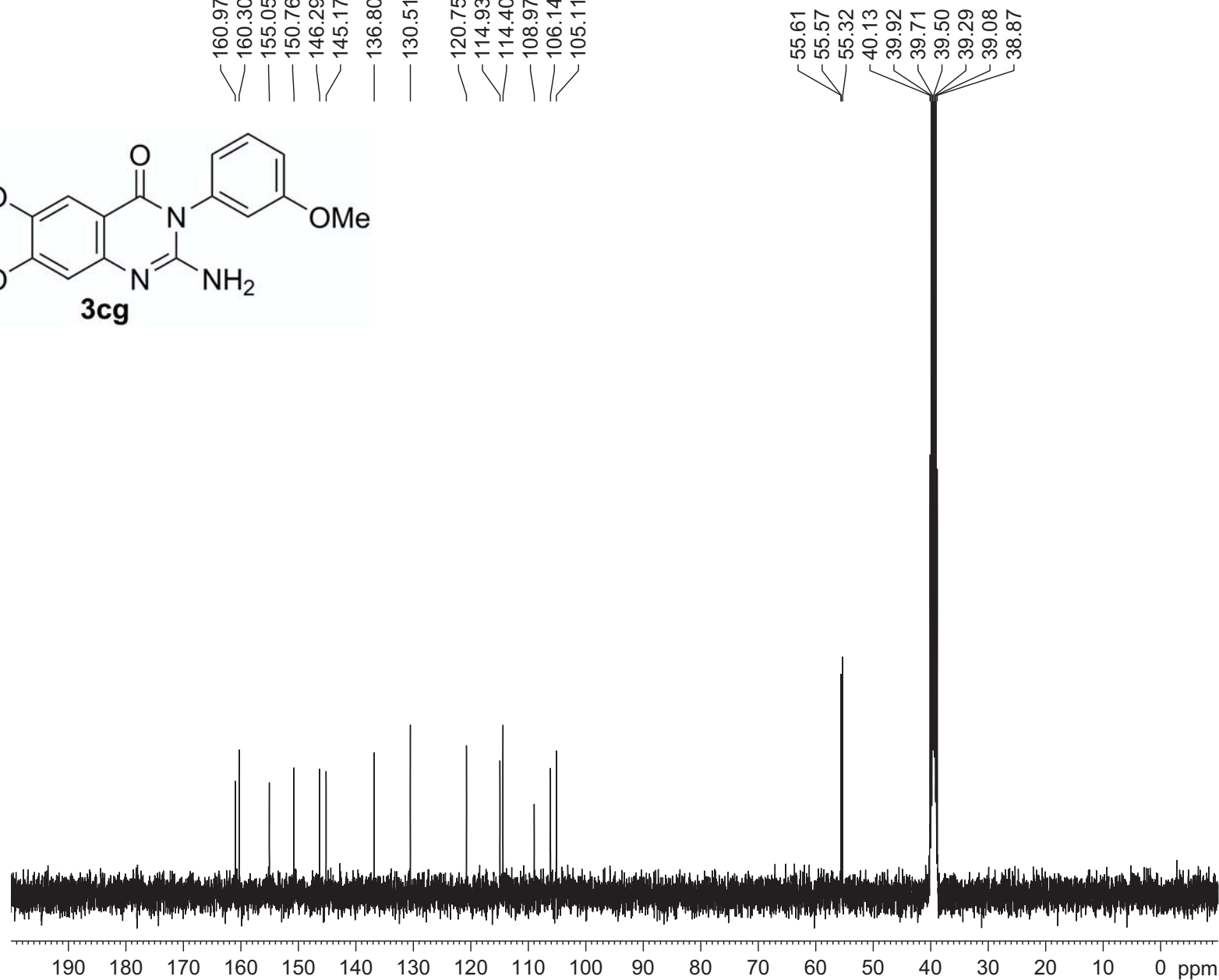
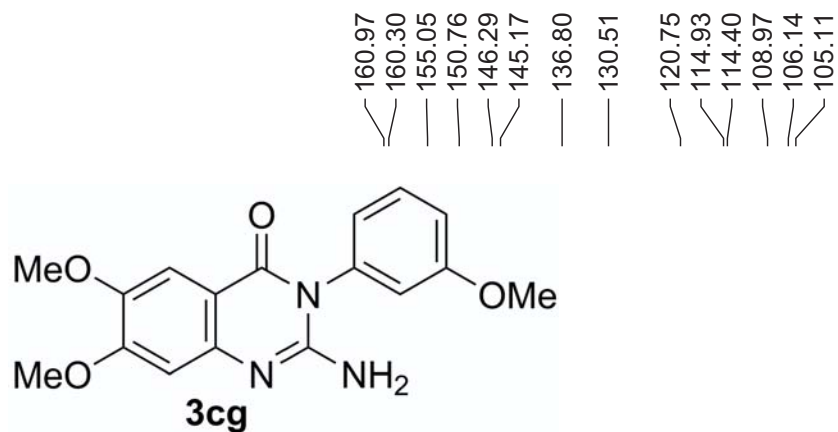


Current Data Parameters
 NAME RM200three
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130322
 Time 8.48
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 181
 DW 69.000 usec
 DE 6.50 usec
 TE 299.7 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.90 usec
 PL1 3.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300031 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM200three
 EXPNO 3
 PROCNO 1

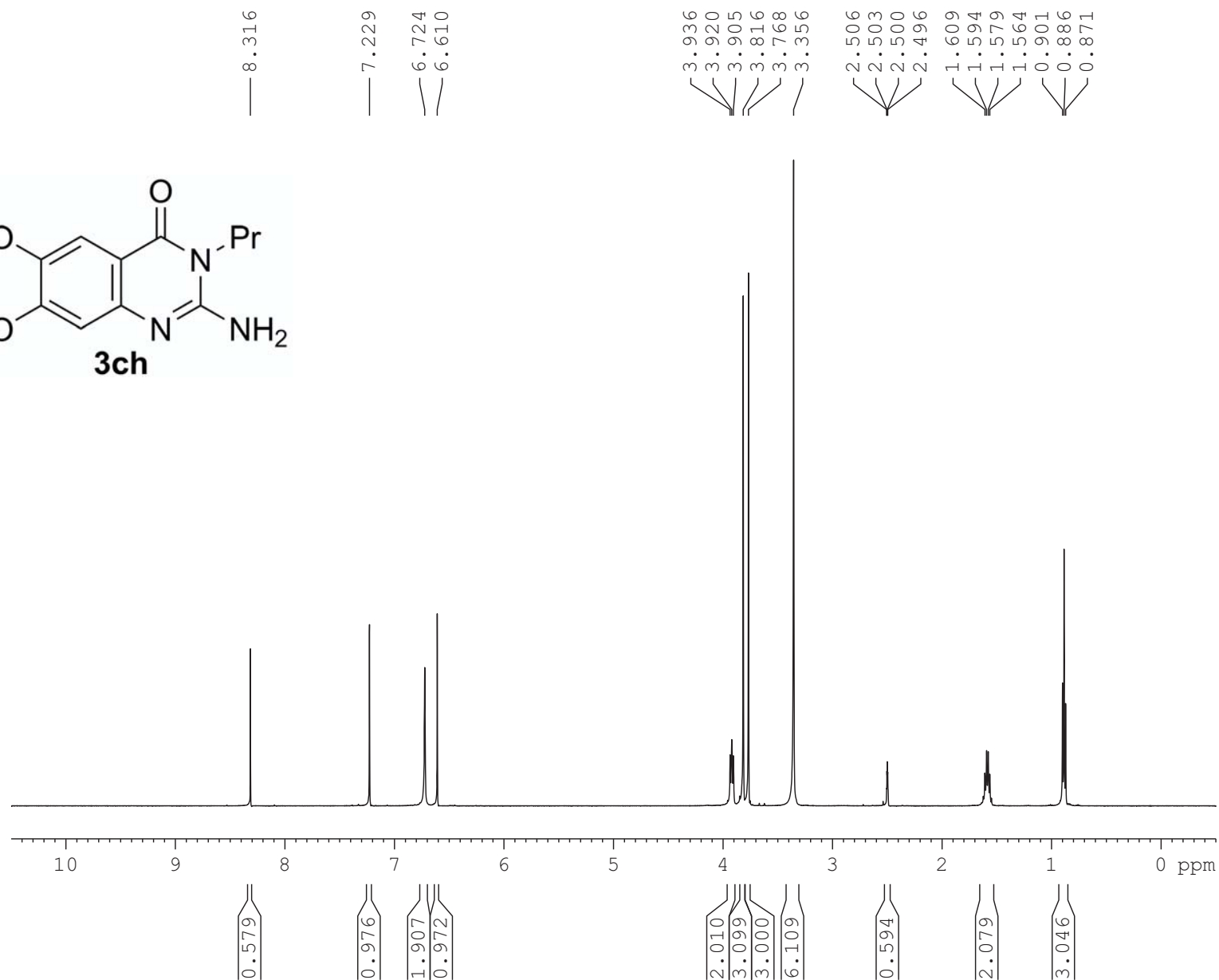
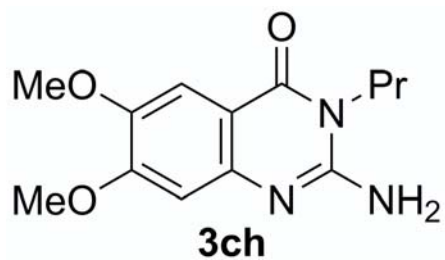
F2 - Acquisition Parameters
 Date_ 20130322
 Time 9.02
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 261
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 4597.6
 DW 20.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.40 usec
 PL1 7.00 dB
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 3.00 dB
 PL12 20.70 dB
 PL13 23.70 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128209 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

NaOH extracted



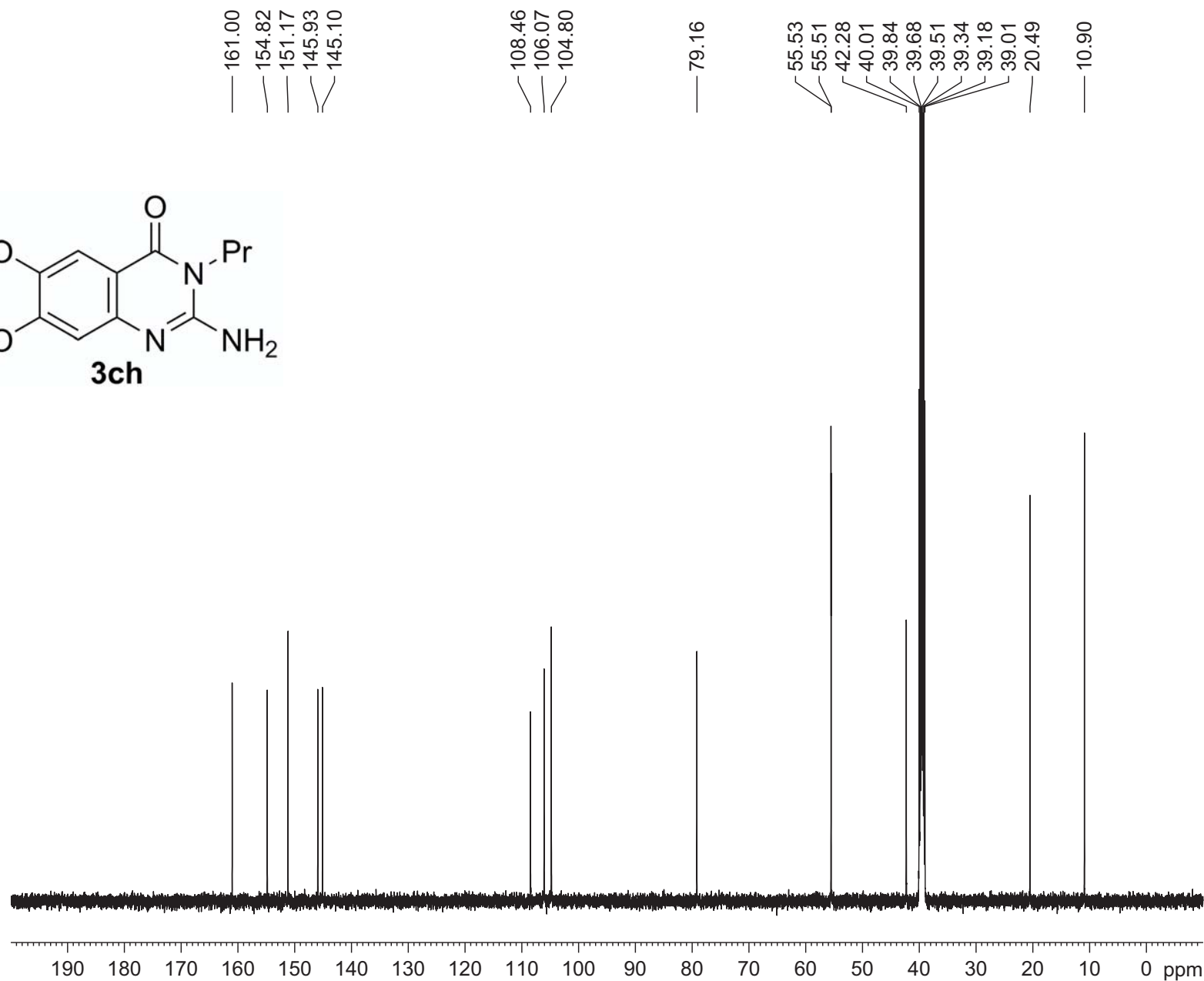
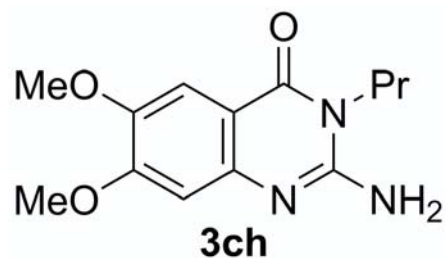
Current Data Parameters
NAME RM036
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121230
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 114
DW 55.200 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300053 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

NaOH extracted



Current Data Parameters
NAME RM036
EXPNO 2
PROCNO 1

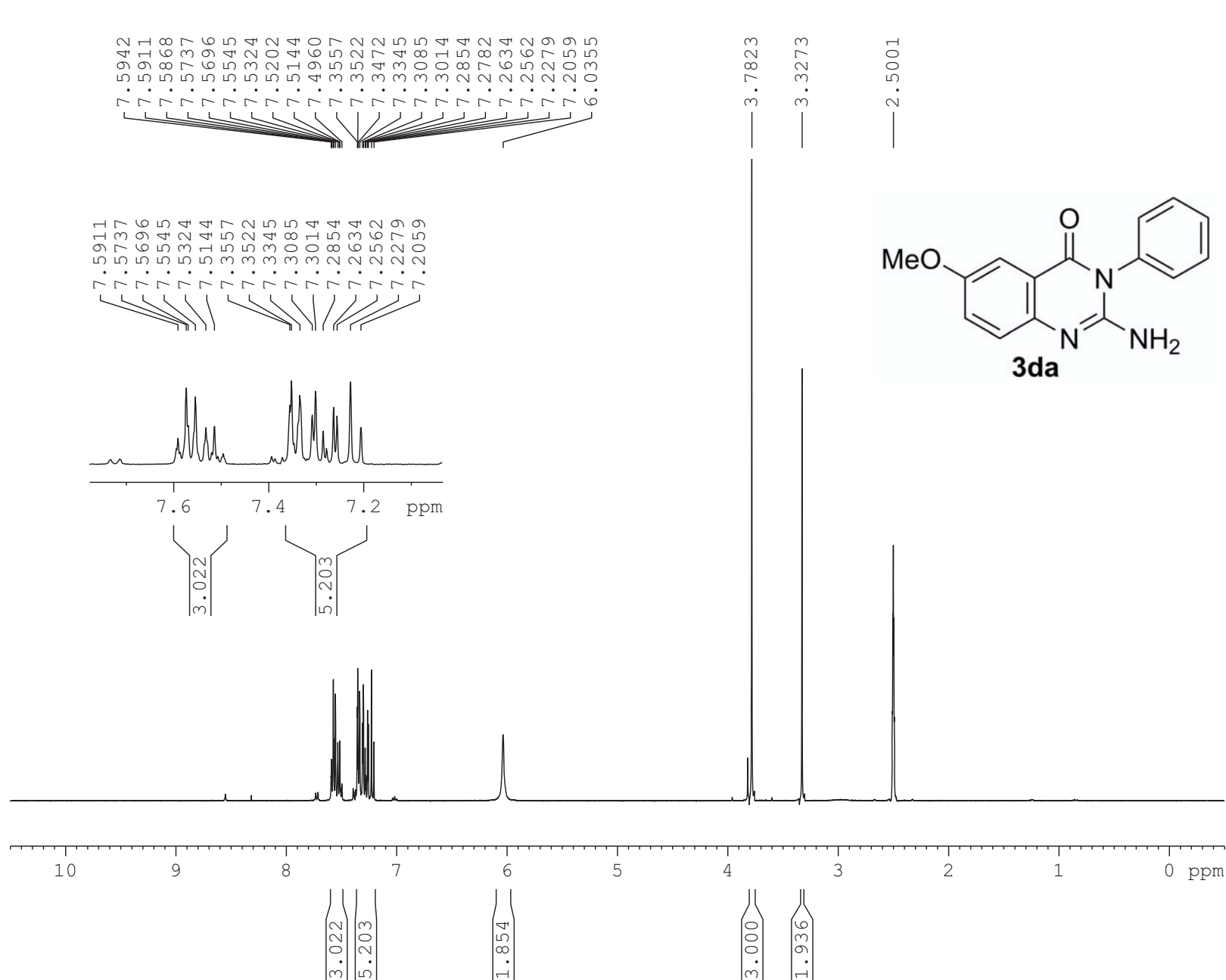
F2 - Acquisition Parameters
Date_ 20121230
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7578513 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

H of



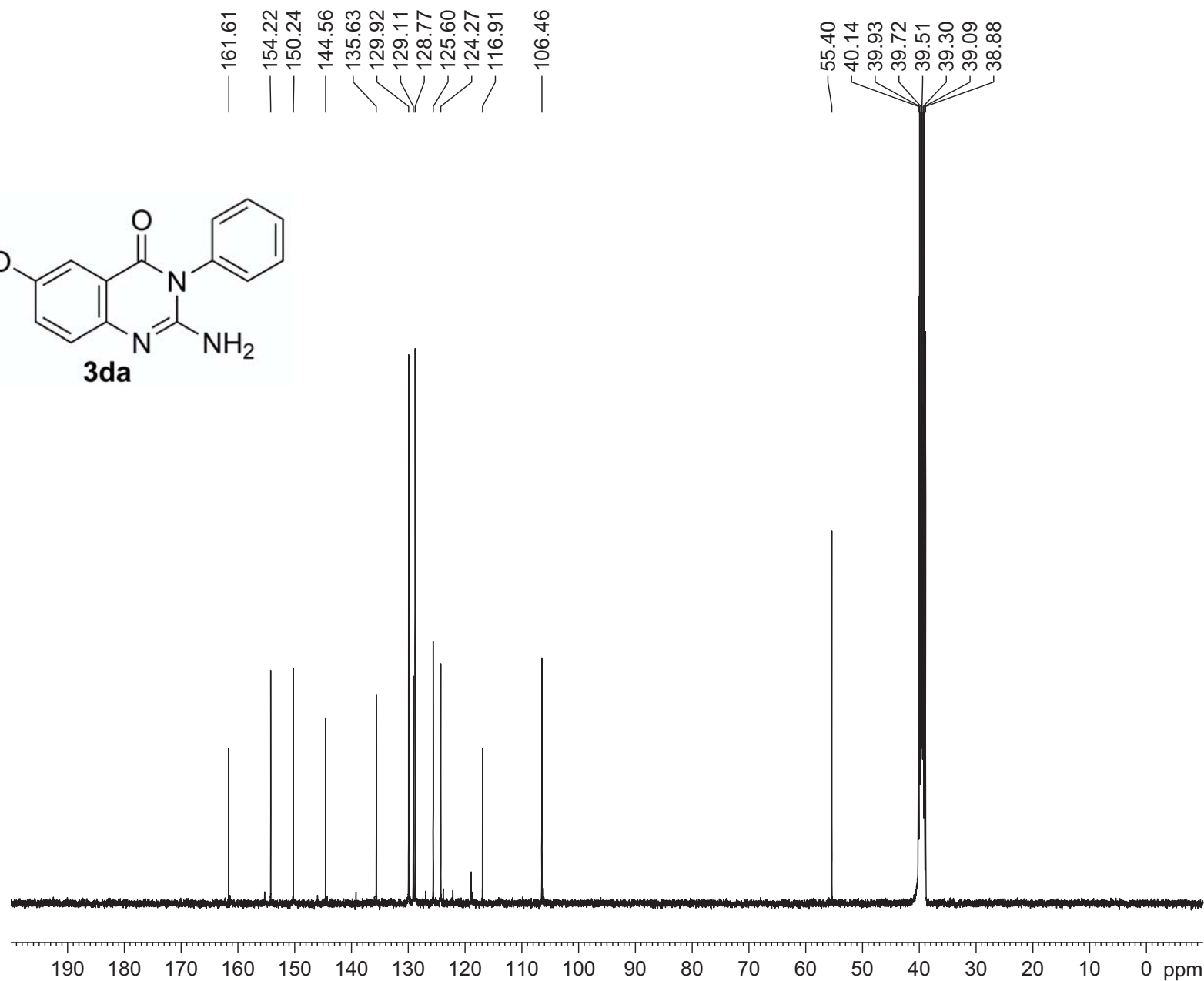
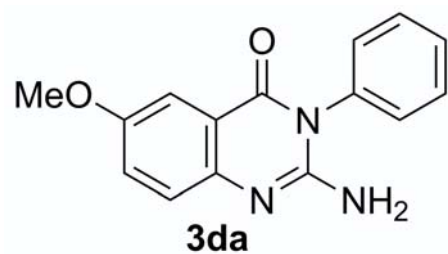
Current Data Parameters
 NAME TO012
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160910
 Time 16.12
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 362
 DW 69.000 usec
 DE 6.50 usec
 TE 296.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.40 usec
 PL1 1.80 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300026 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

13C of 3



Current Data Parameters
NAME TO012
EXPNO 11
PROCNO 1

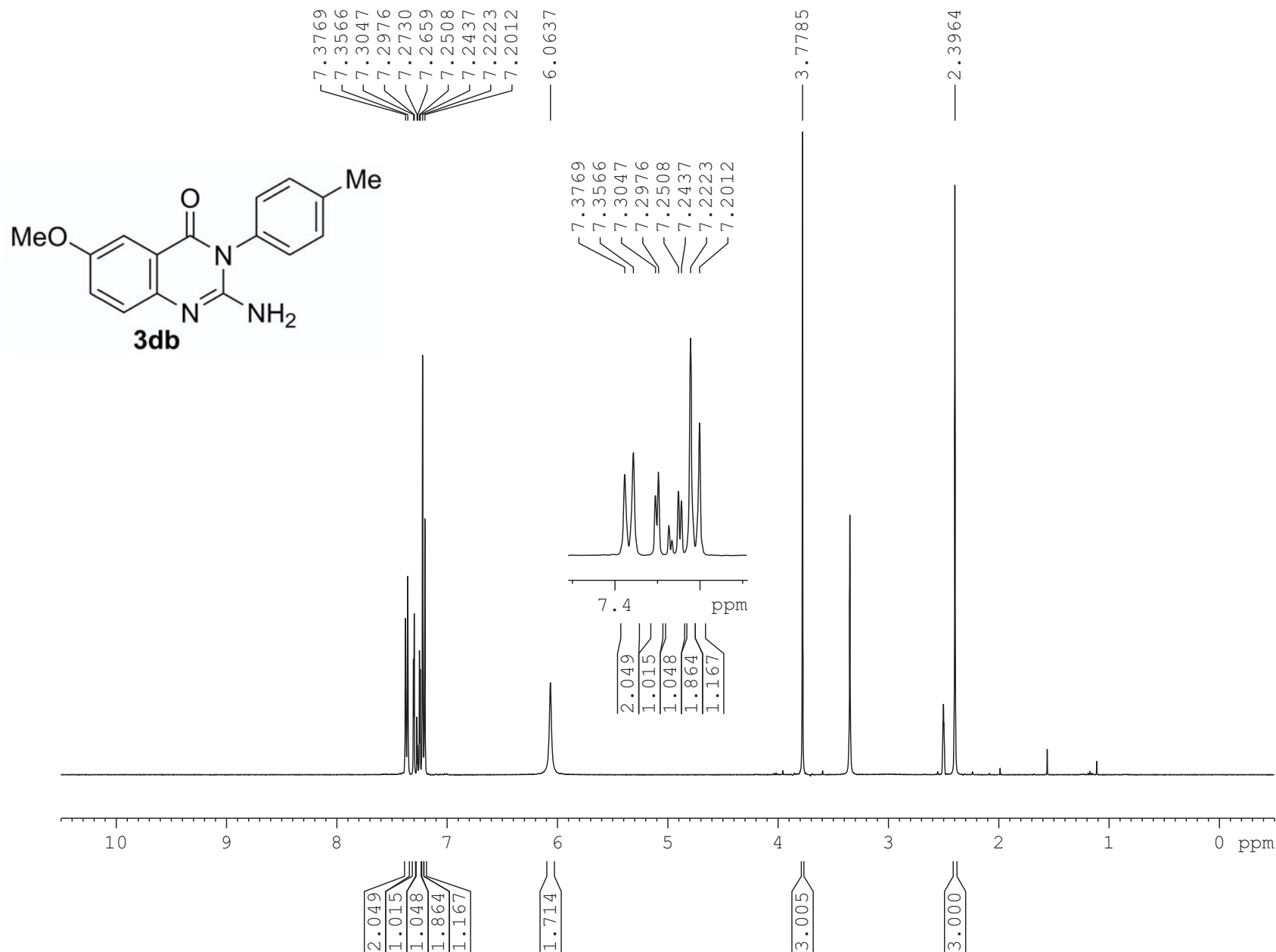
F2 - Acquisition Parameters
Date_ 20161006
Time 7.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 11700
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 297.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128177 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1 H



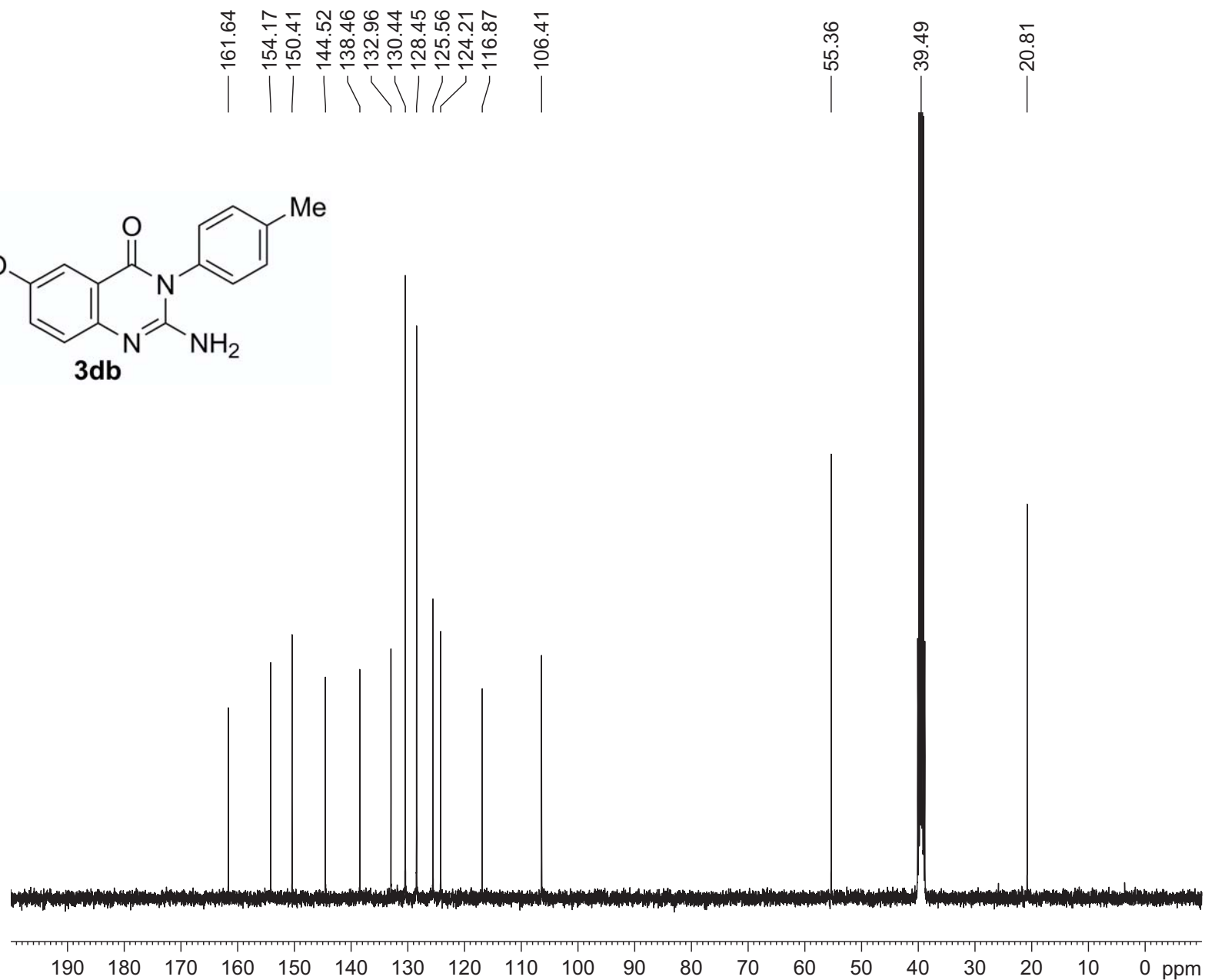
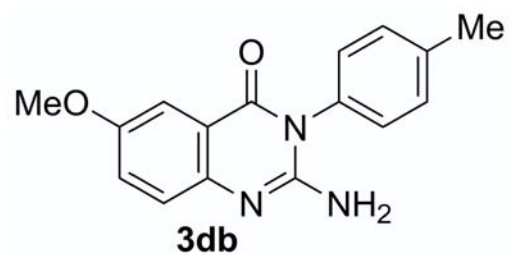
Current Data Parameters
NAME SI055-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141224
Time 7.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300029 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C



Current Data Parameters
NAME SI055-3
EXPNO 3
PROCNO 1

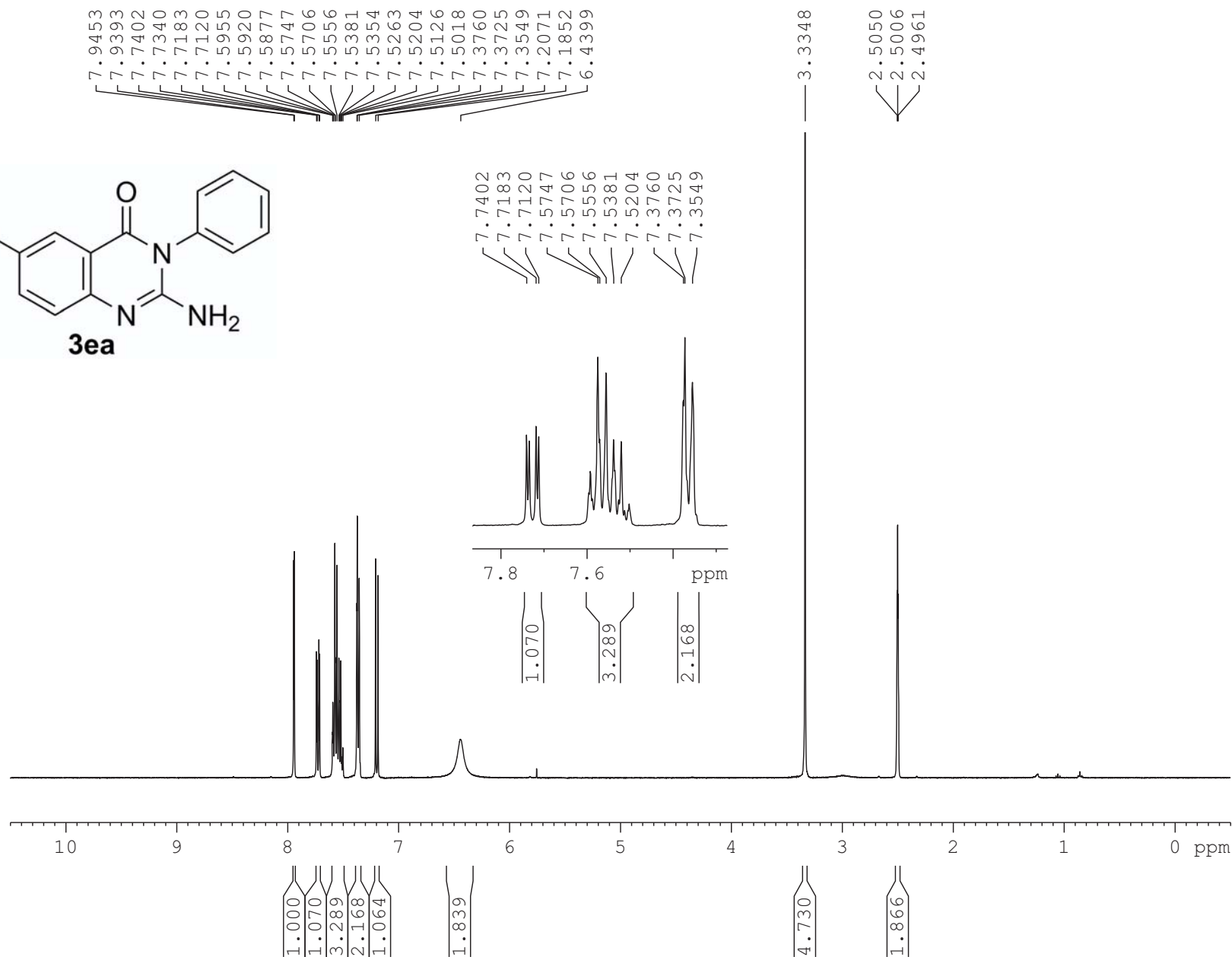
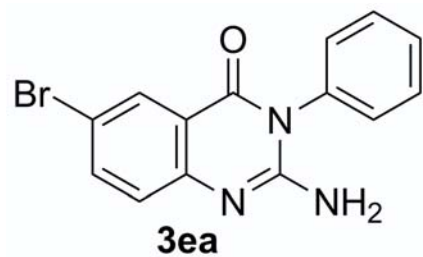
F2 - Acquisition Parameters
Date_ 20141224
Time 8.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 701
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128195 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

H of



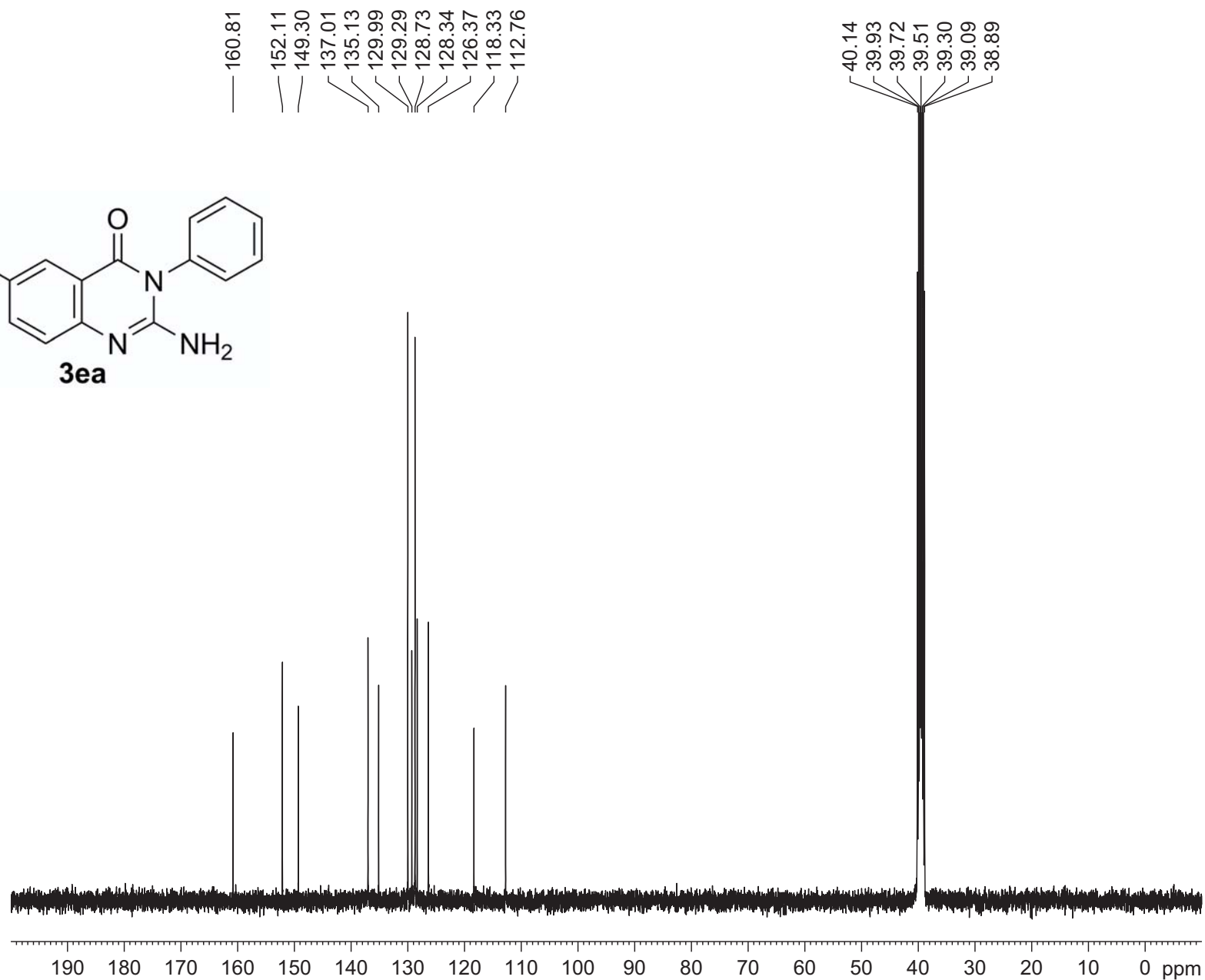
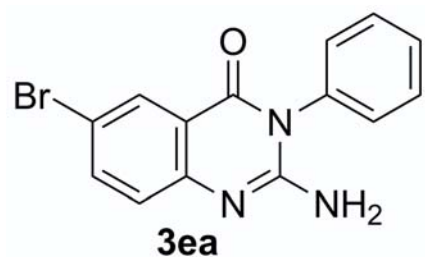
Current Data Parameters
NAME TO027
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161110
Time 23.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.40 usec
PL1 1.80 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of 3



Current Data Parameters

NAME TO027
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

Date_ 20161110
Time 23.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 ¹³C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

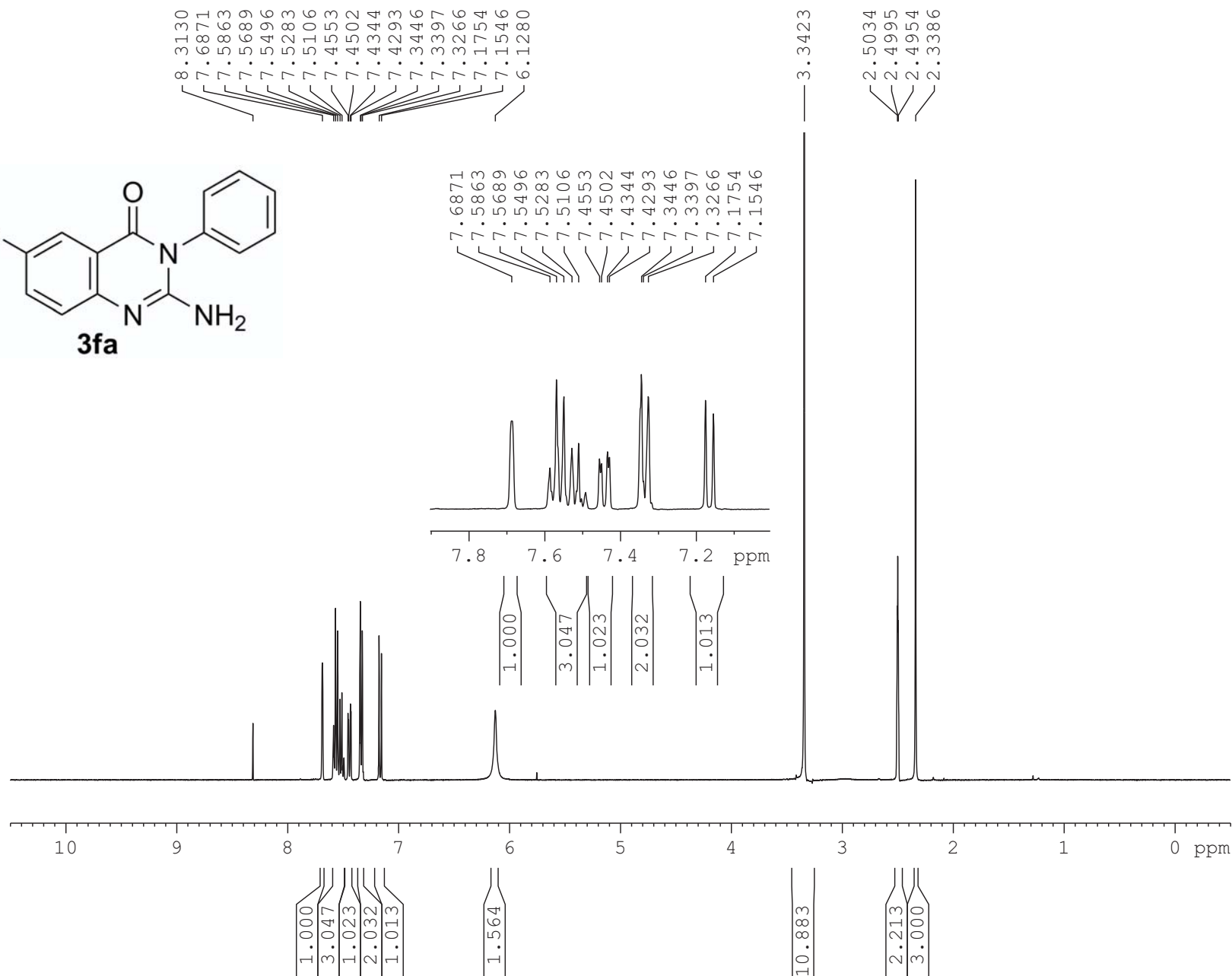
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

-3-s



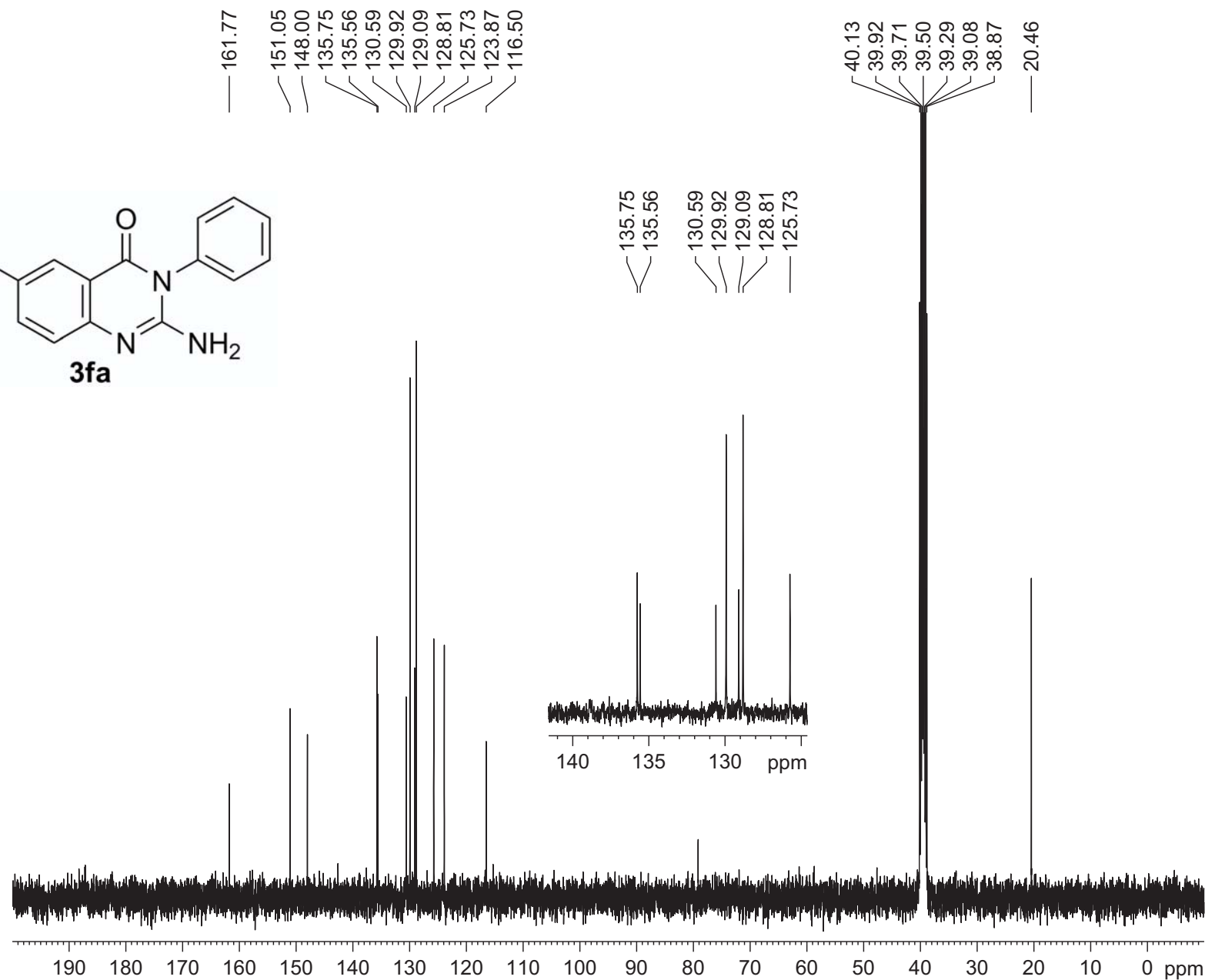
Current Data Parameters
NAME SG081
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141207
Time 3.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

1H -3-sit



Current Data Parameters

NAME SG081
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141207
Time 3.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 406
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 11585.2
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

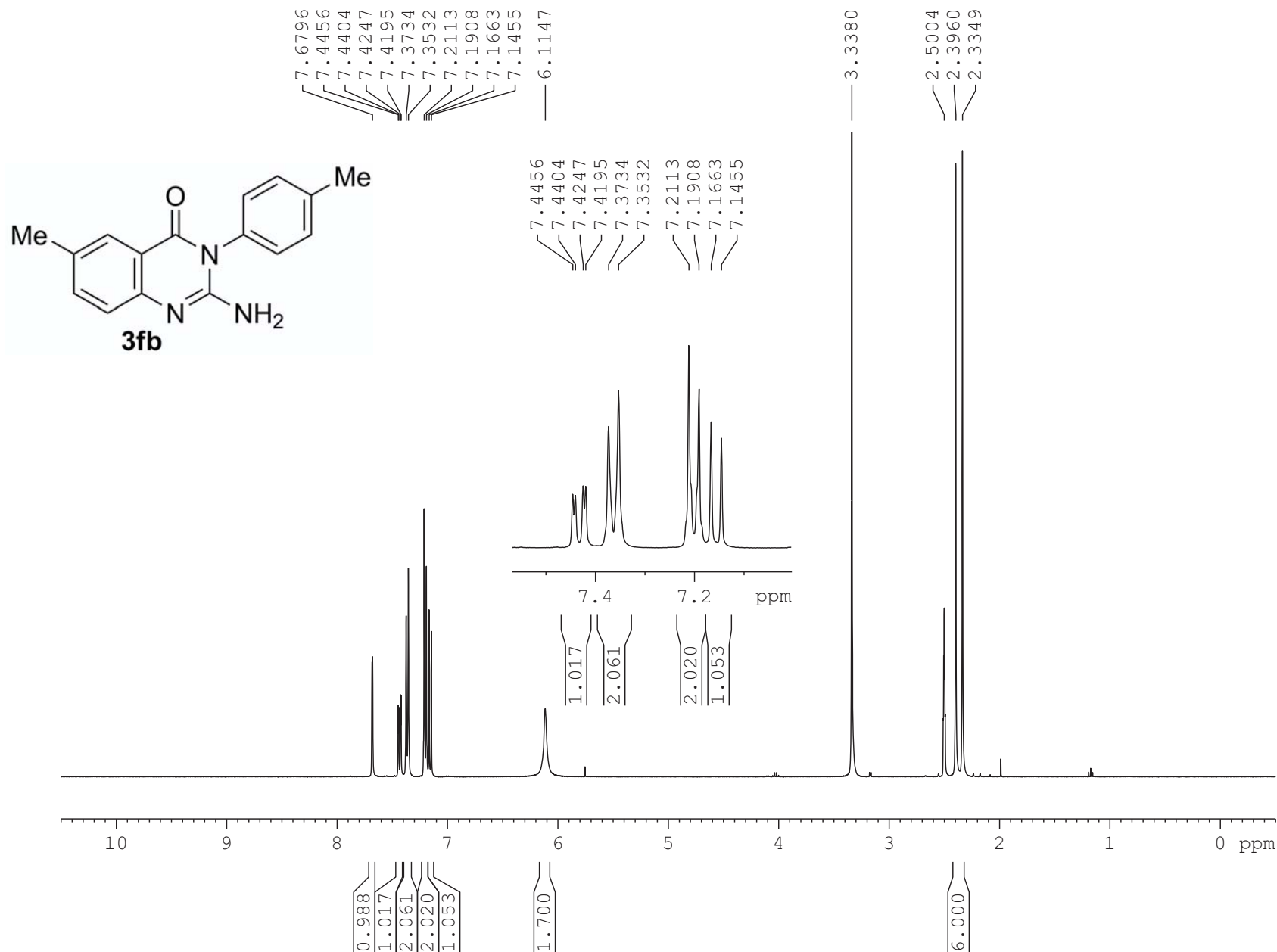
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128178 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H



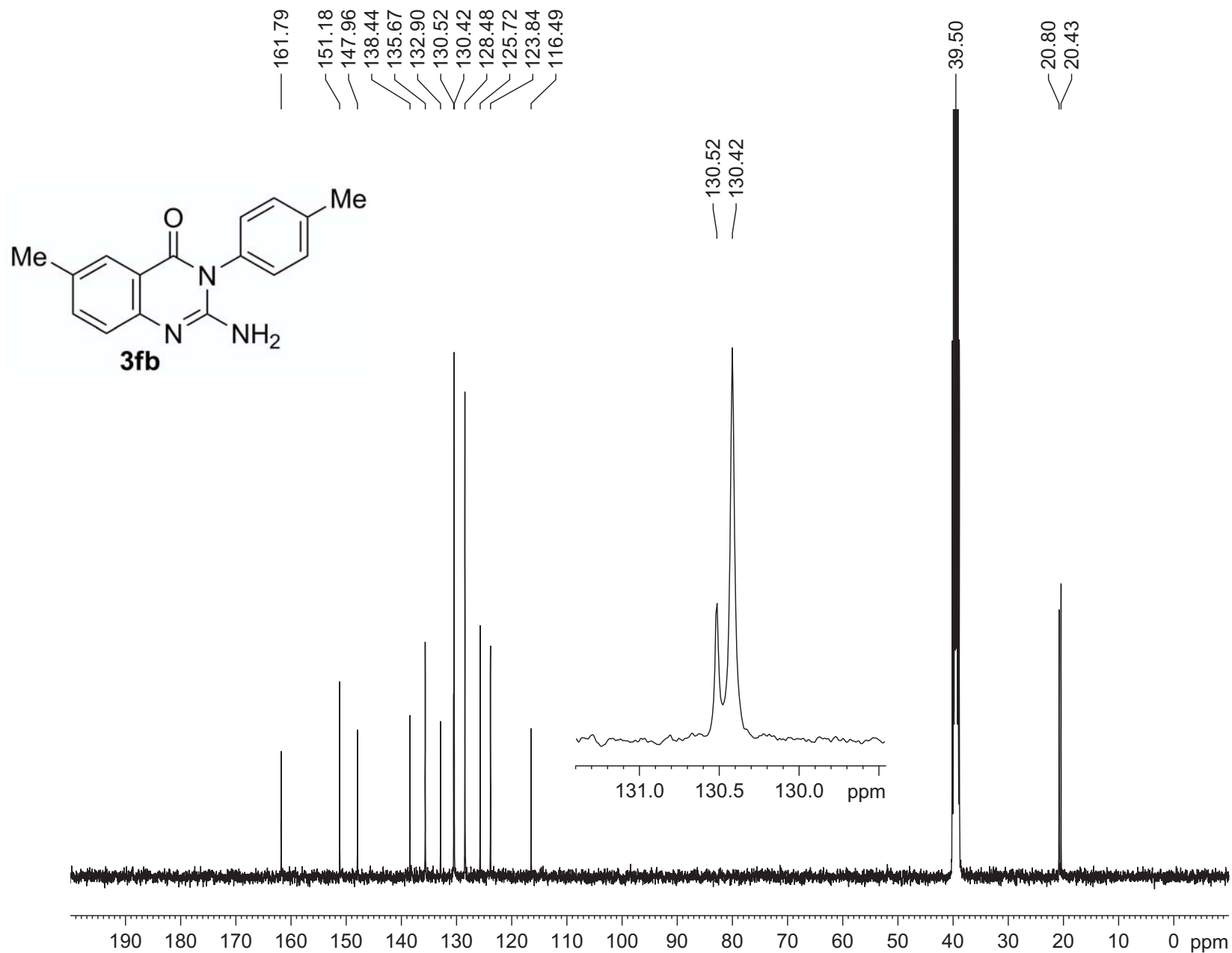
Current Data Parameters
NAME SI052-3
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141220
Time 1.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300023 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C



Current Data Parameters

NAME SI052-3
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141220
Time 3.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

SFO1 100.6233319 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 46.00000000 W

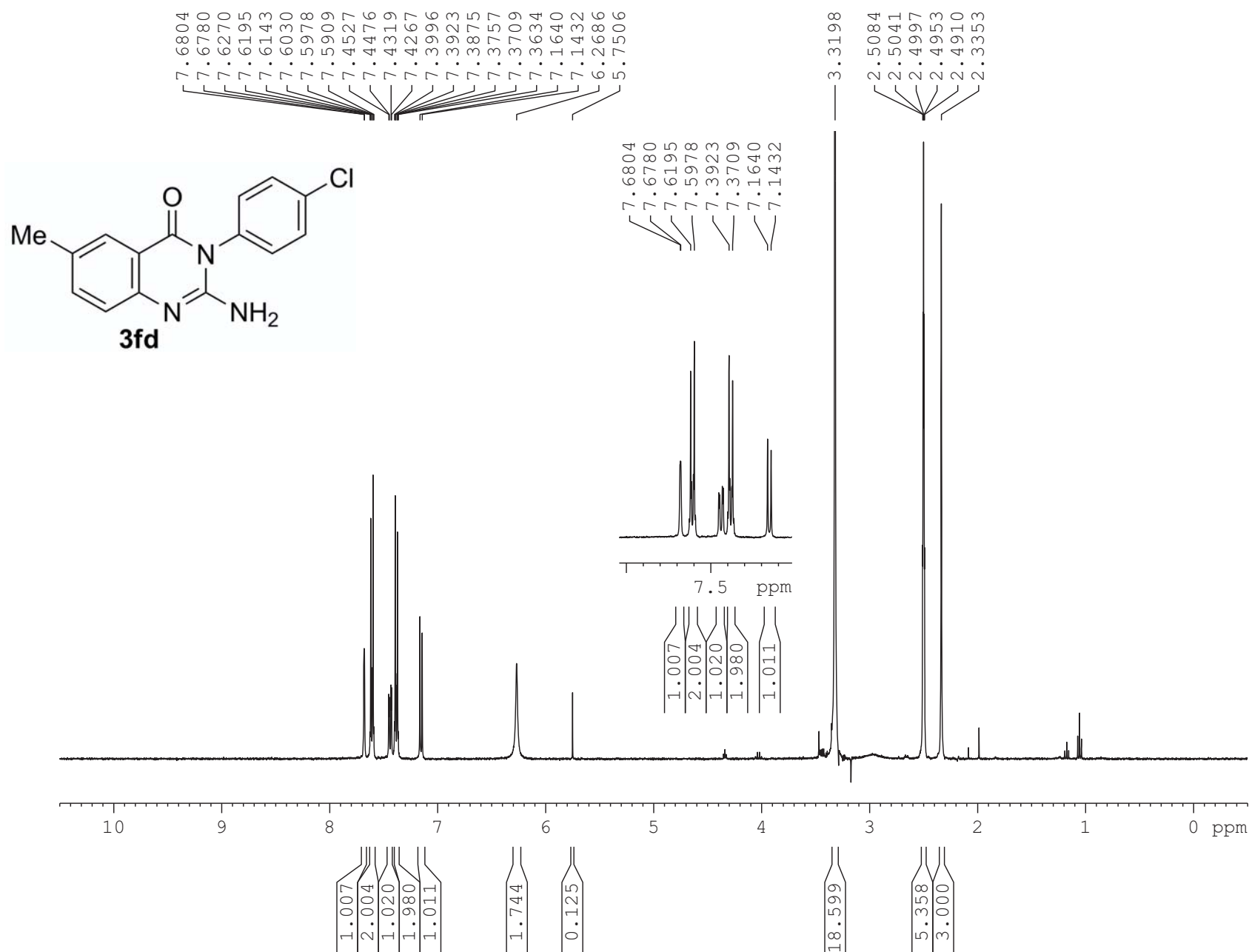
===== CHANNEL f2 =====

SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters

SI 32768
SF 100.6128199 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

-3-s



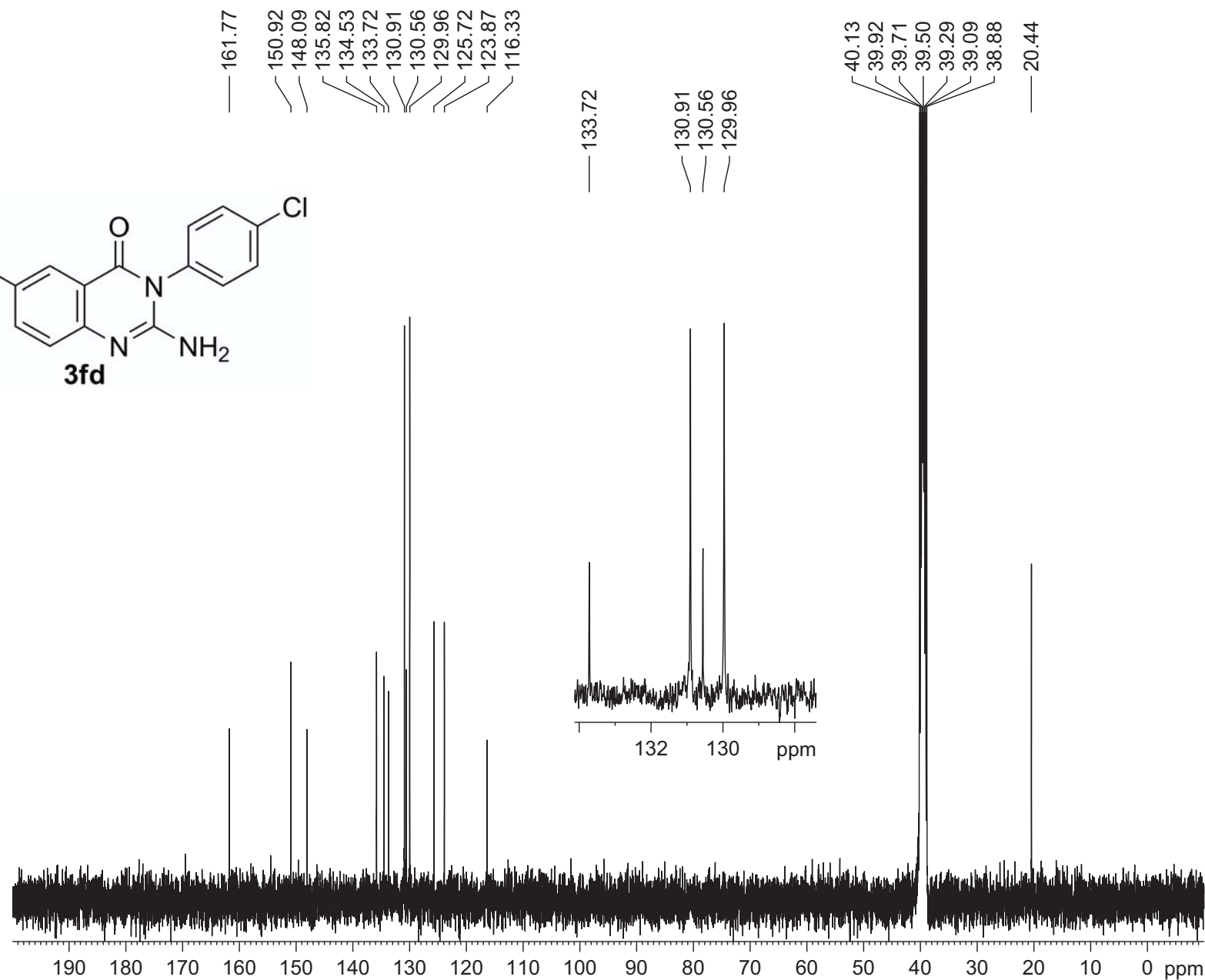
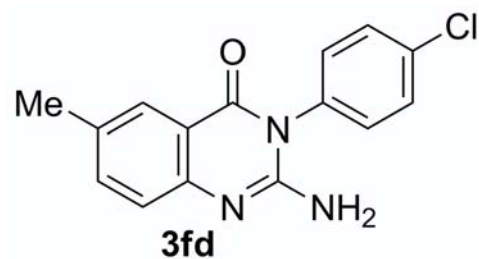
Current Data Parameters
NAME SG079
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141204
Time 14.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 322.5
DW 69.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

1H -3-sit



Current Data Parameters
NAME SG079
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141207
Time 0.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 11585.2
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

or 13



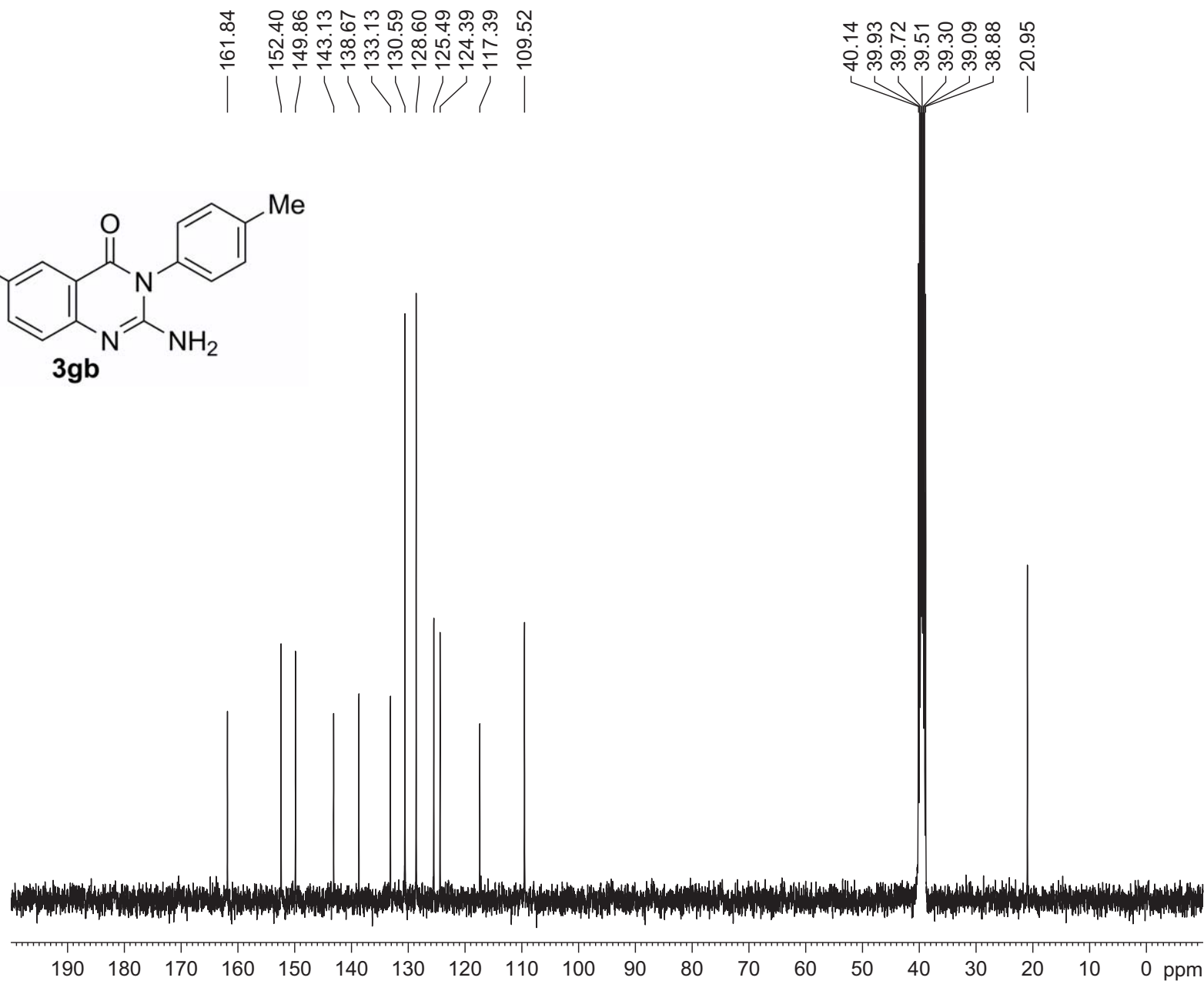
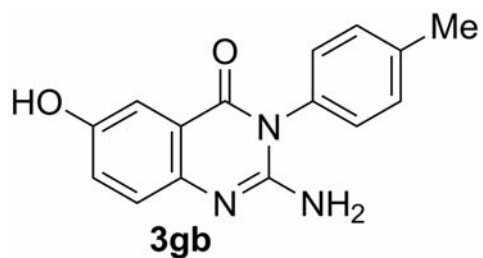
Current Data Parameters
 NAME SG083
 EXPNO 105
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141220
 Time 23.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 38.89
 DW 69.333 usec
 DE 10.52 usec
 TE 297.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 1H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

for 13c



Current Data Parameters

NAME SG083
EXPNO 107
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141220
Time 23.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 400
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

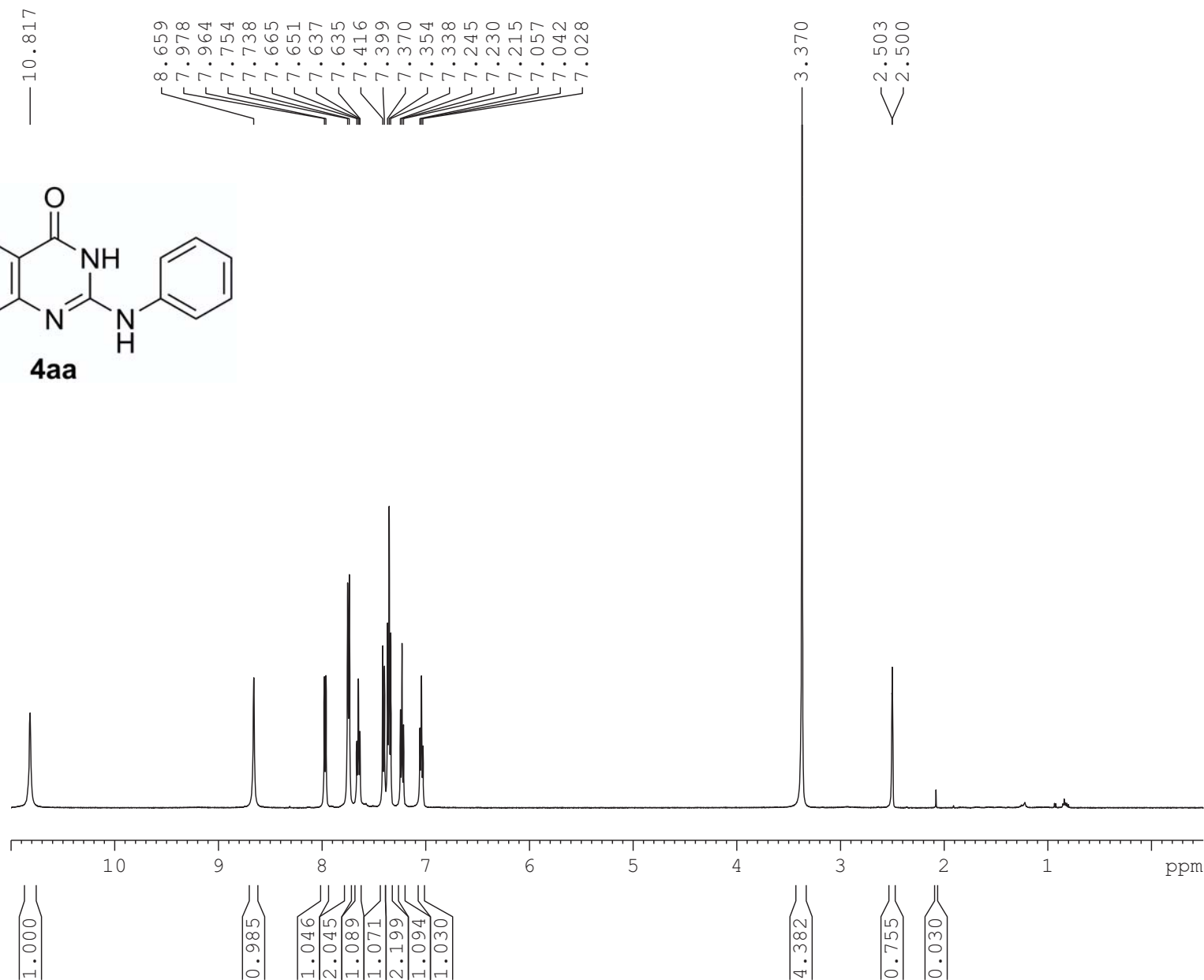
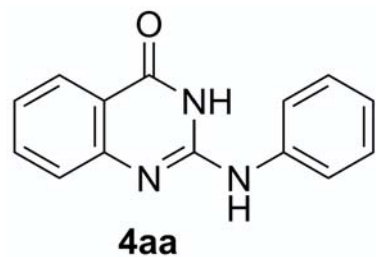
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

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

SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

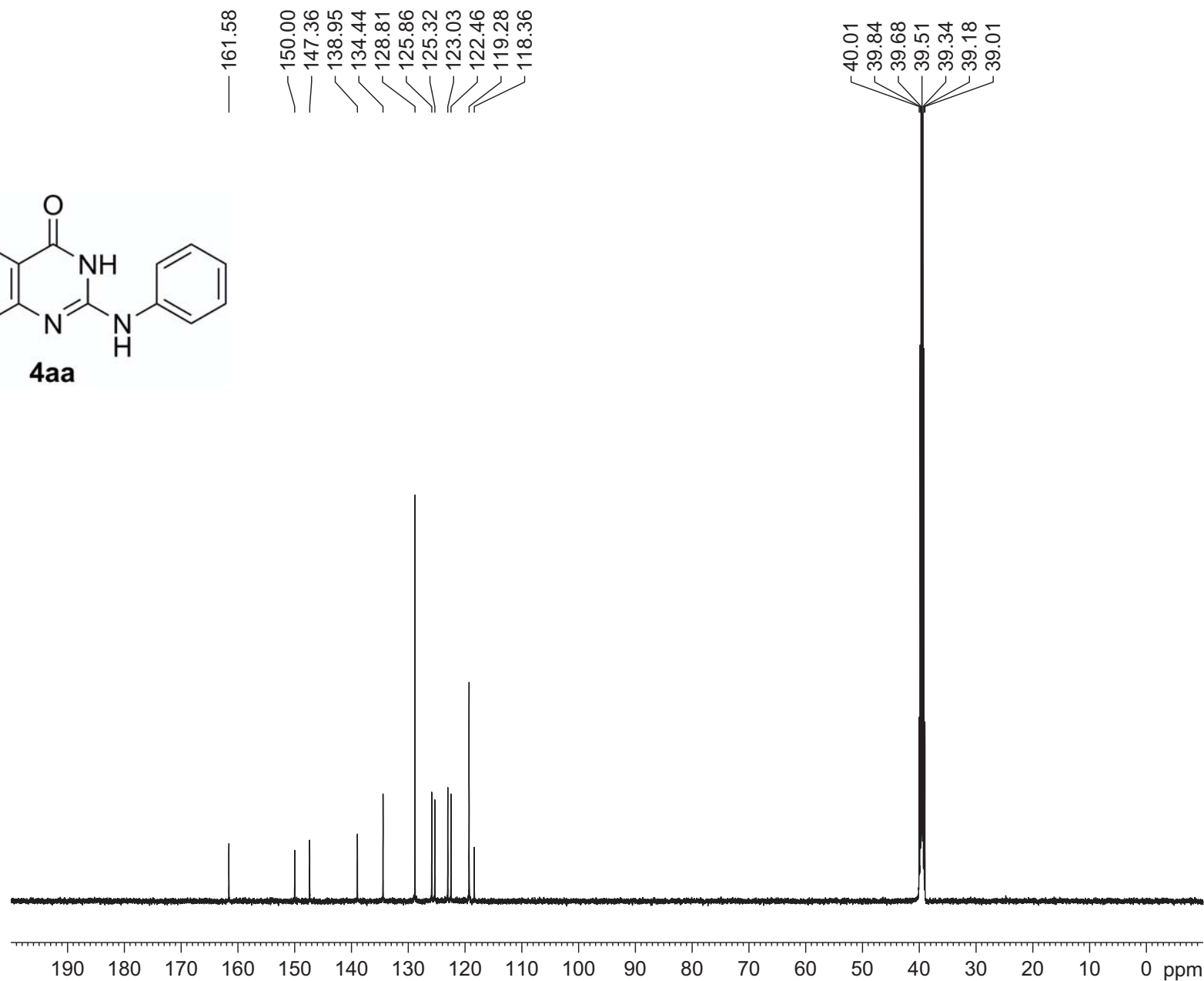
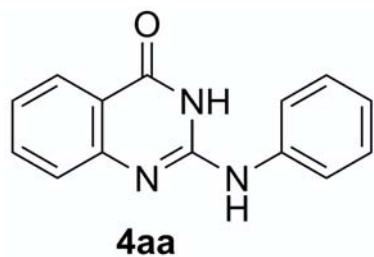
F2 - Processing parameters

SI 32768
SF 100.6128016 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



NAME RN050
 EXPNO 1
 PROCNO 1
 Date_ 20130202
 Time 14.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8088988 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 294.7 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz
 SI 16384
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME RN050
EXPNO 3
PROCNO 1

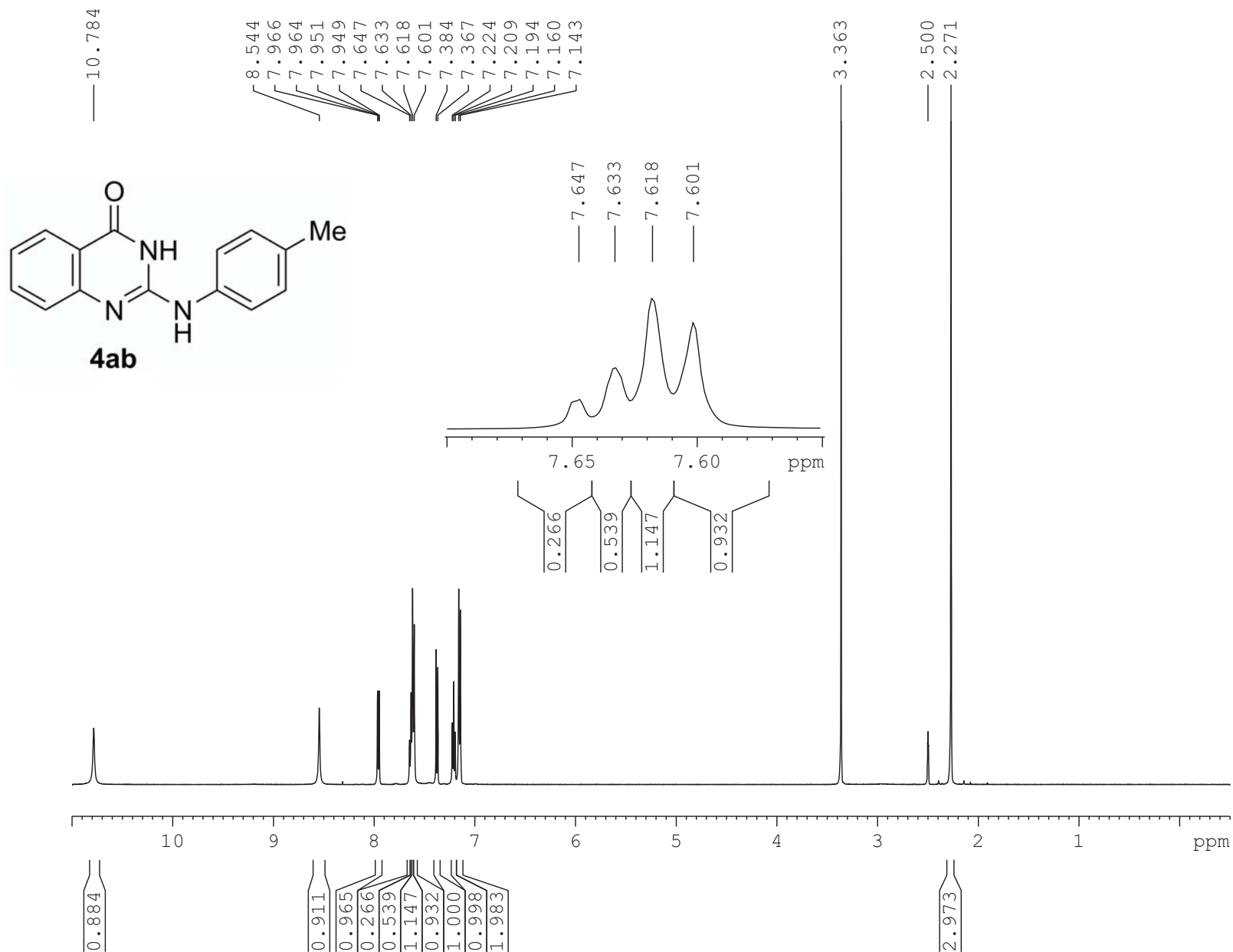
F2 - Acquisition Parameters
Date_ 20130202
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 4096
DW 16.650 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7578507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

recrystallized



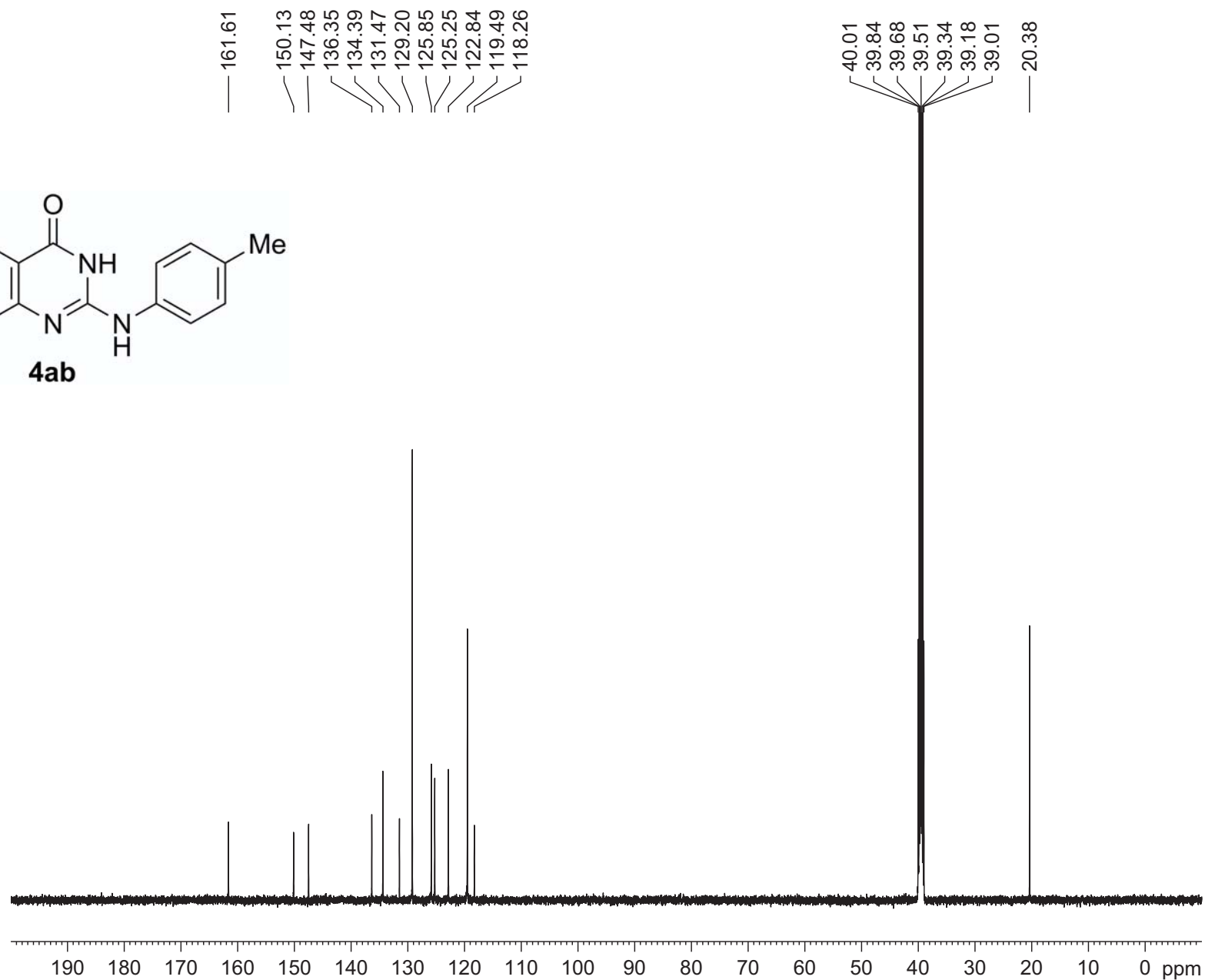
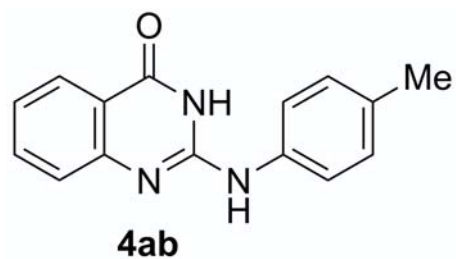
Current Data Parameters
NAME RM115
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20121020
Time 10.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 9057.971 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 294.5 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300053 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

recrystallized



Current Data Parameters

NAME RM115
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121020
Time 10.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 294.8 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

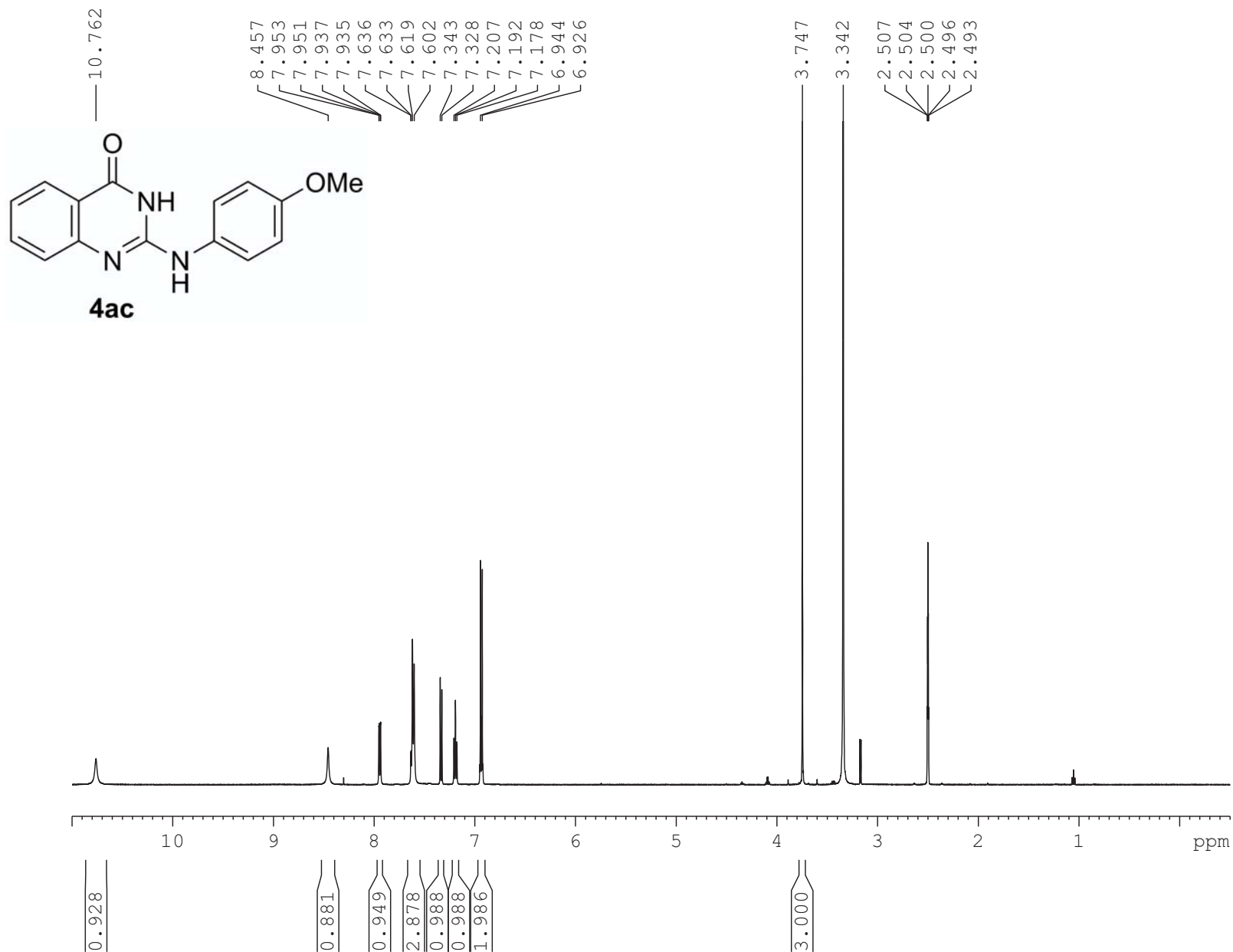
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 65536
SF 125.7578507 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of SC 60 recrystallized



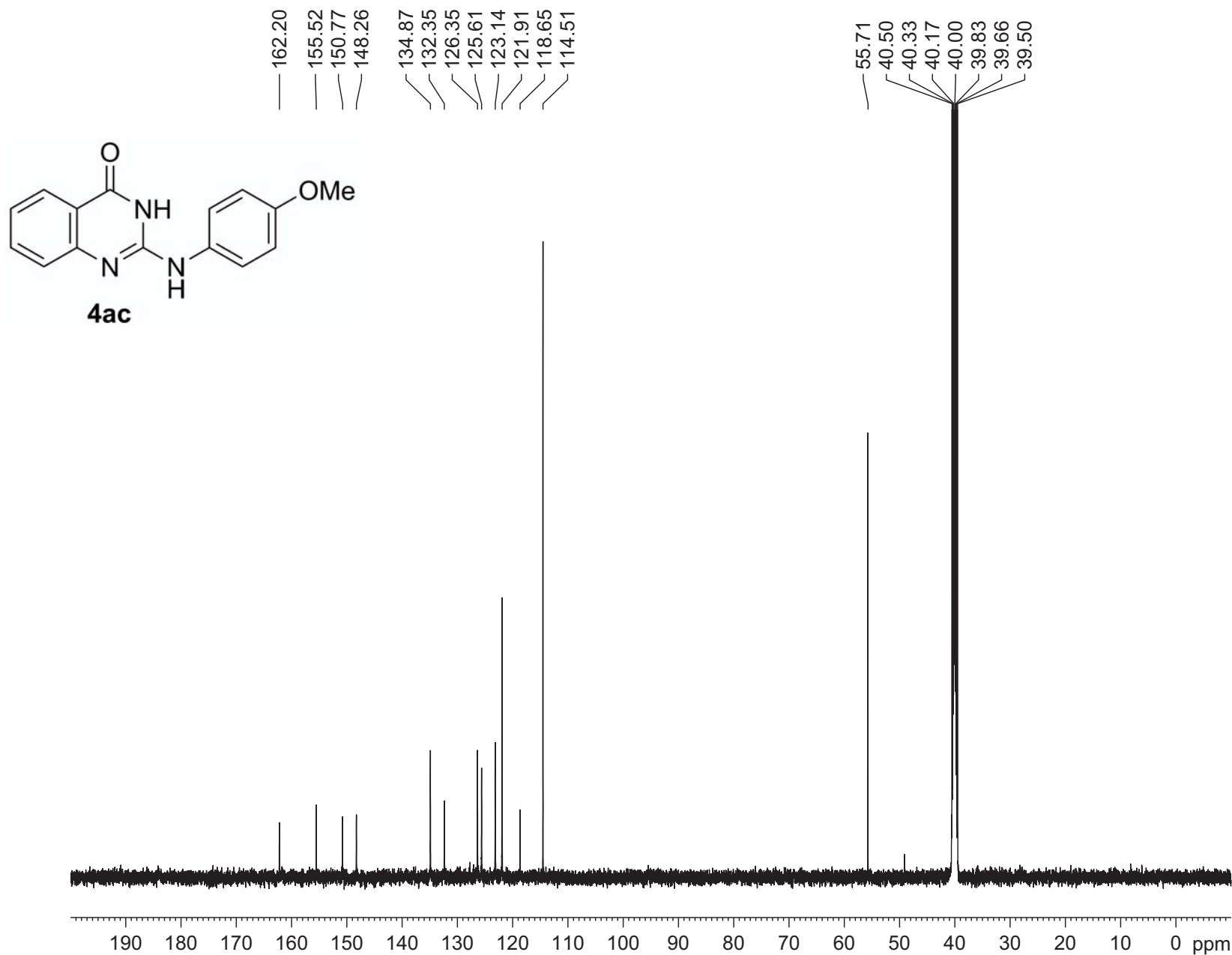
Current Data Parameters
 NAME TCC-20140603
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140605
 Time 17.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of SC 60 recrystallized



Current Data Parameters
 NAME TCC-20140603
 EXPNO 13
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140605
 Time 16.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2033
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577880 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

4ad

Chemical structure of 4ad: O=C1NC(=N2C=CC(=O)N2)C(=N1)C3=CC=C(C=C3)Cl

¹H NMR spectrum (CDCl₃) showing peaks from 0 to 11 ppm. The x-axis is labeled ppm.

Peak list (ppm): 8.849, 7.997, 7.995, 7.981, 7.979, 7.797, 7.780, 7.671, 7.668, 7.657, 7.654, 7.652, 7.641, 7.637, 7.419, 7.399, 7.395, 7.385, 7.381, 7.258, 7.256, 7.242, 7.228, 7.226, 3.366, 2.517, 2.513, 2.510, 2.506, 2.503, 1.080, 1.066, 1.052, 10.911.

Integration values (from left to right): 0.972, 0.962, 1.000, 2.053, 1.075, 3.080, 1.078, 0.540, 0.381, 0.138.

```

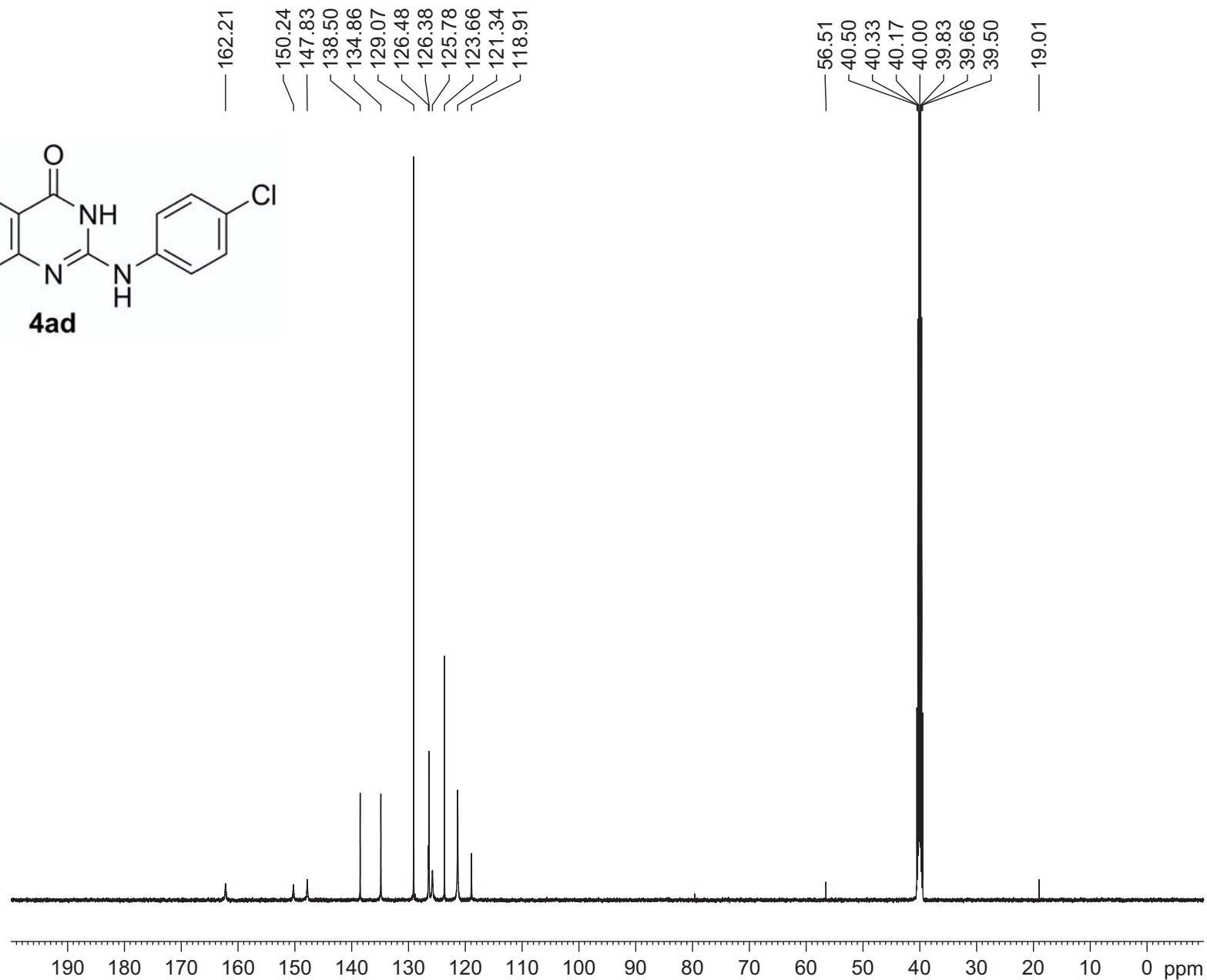
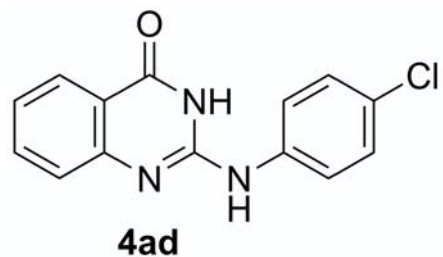
F2 - Acquisition Parameters
Date_          20140424
Time           17.58
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       DMSO
NS            16
DS            0
SWH          9057.971 Hz
FIDRES       0.276427 Hz
AQ           1.8087935 sec
RG           114
DW           55.200 usec
DE           6.50 usec
TE           300.0 K
D1           2.00000000 sec
TD0          1

```

```
===== CHANNEL f1 =====
NUC1      1H
P1         13.20 usec
PL1        -0.60 dB
SFO1      500.1330008 MHz
```

```
F2 - Processing parameters
SI      32768
SF      500.1300000 MHz
WDW      EM
SSB      0
LB      0 Hz
GB      0
PC      1.00
```

¹³C of RX84

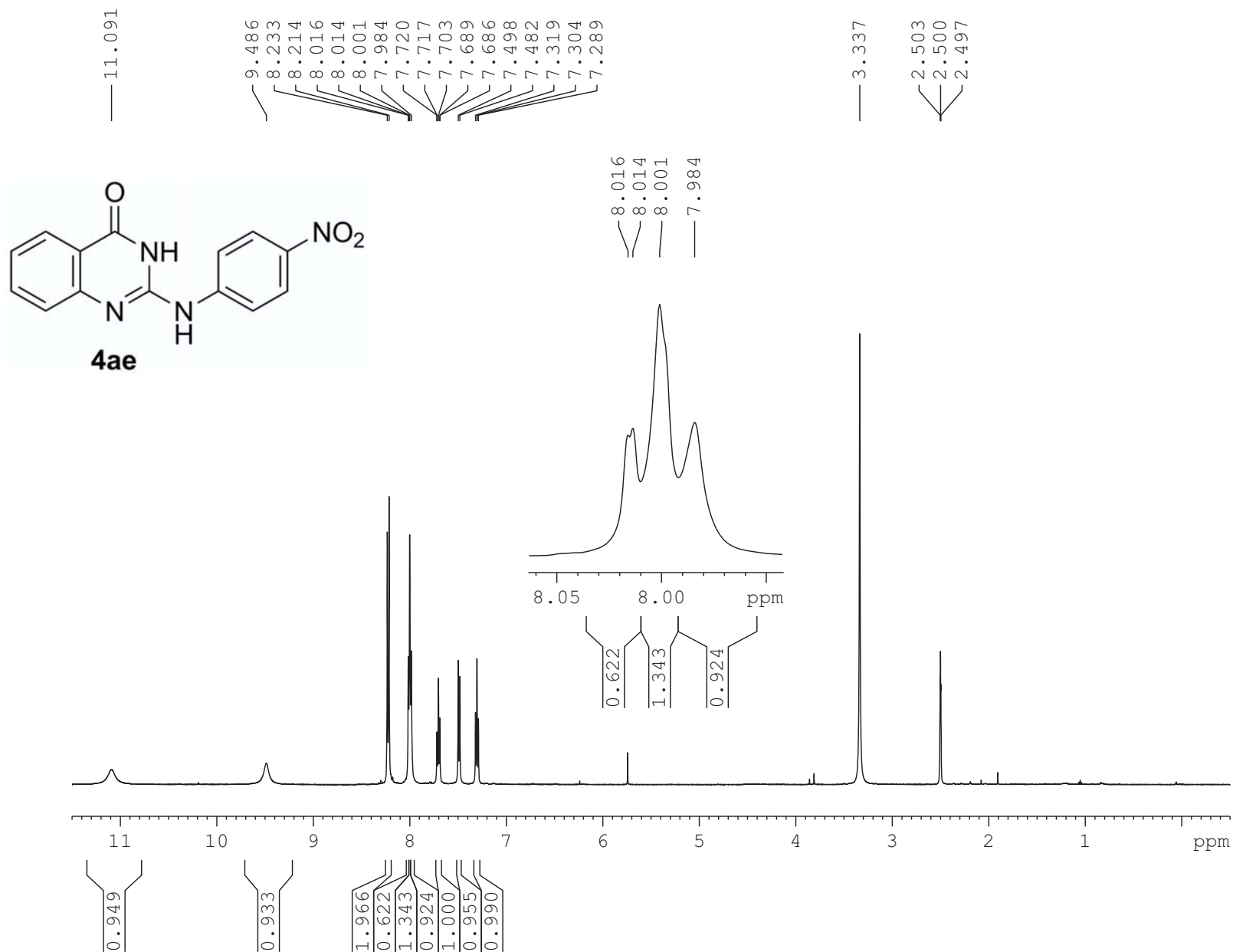


NAME TCC-20140424
 EXPNO 2
 PROCNO 1
 Date_ 20140424
 Time 18.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2350
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0814105 sec
 RG 5792.6
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz
 SI 65536
 SF 125.7577899 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of RX100



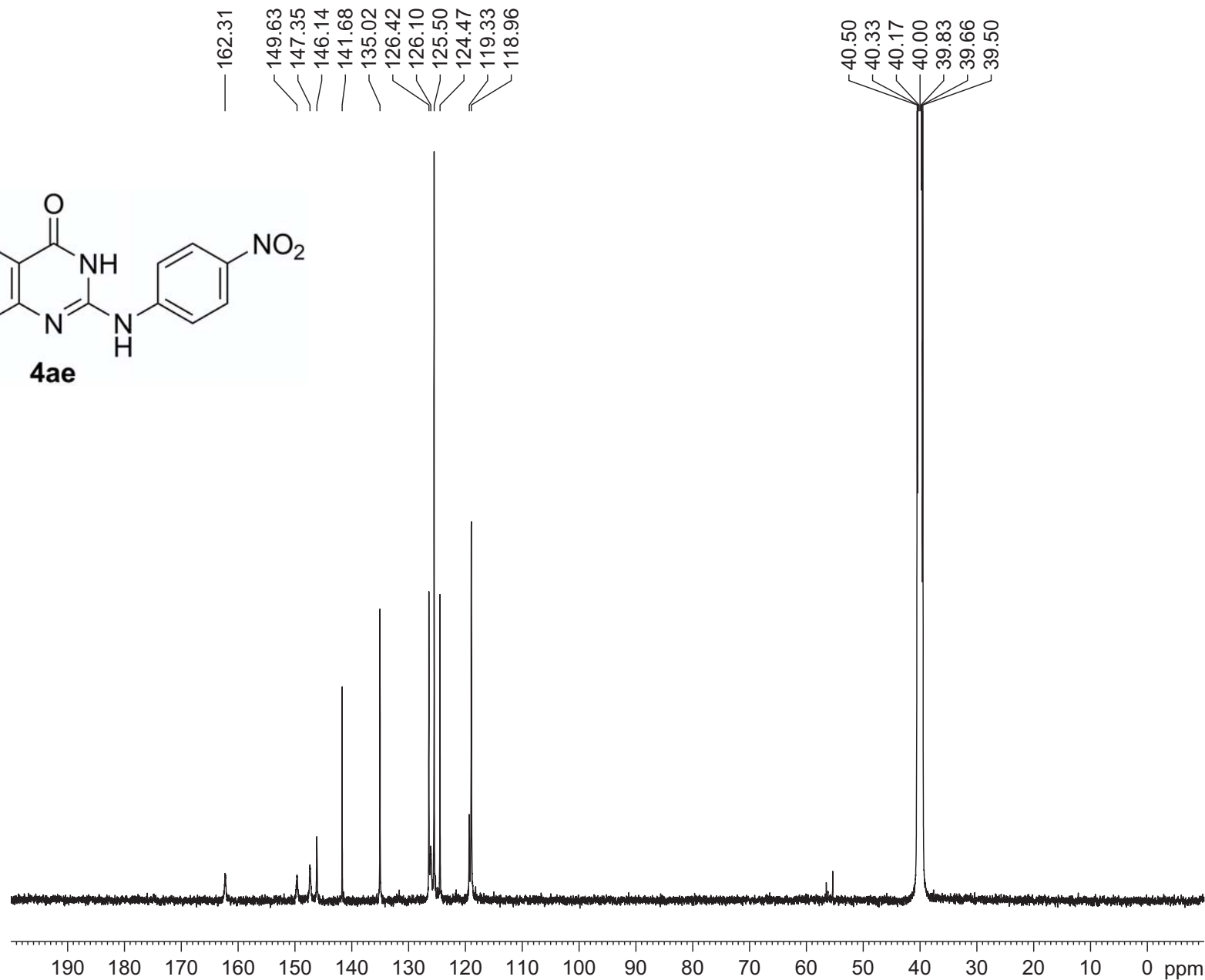
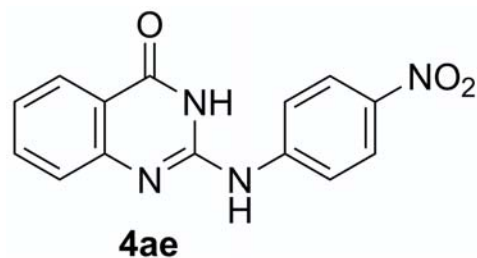
Current Data Parameters
 NAME TCC-20140424
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140428
 Time 18.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 161.3
 DW 55.200 usec
 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX100



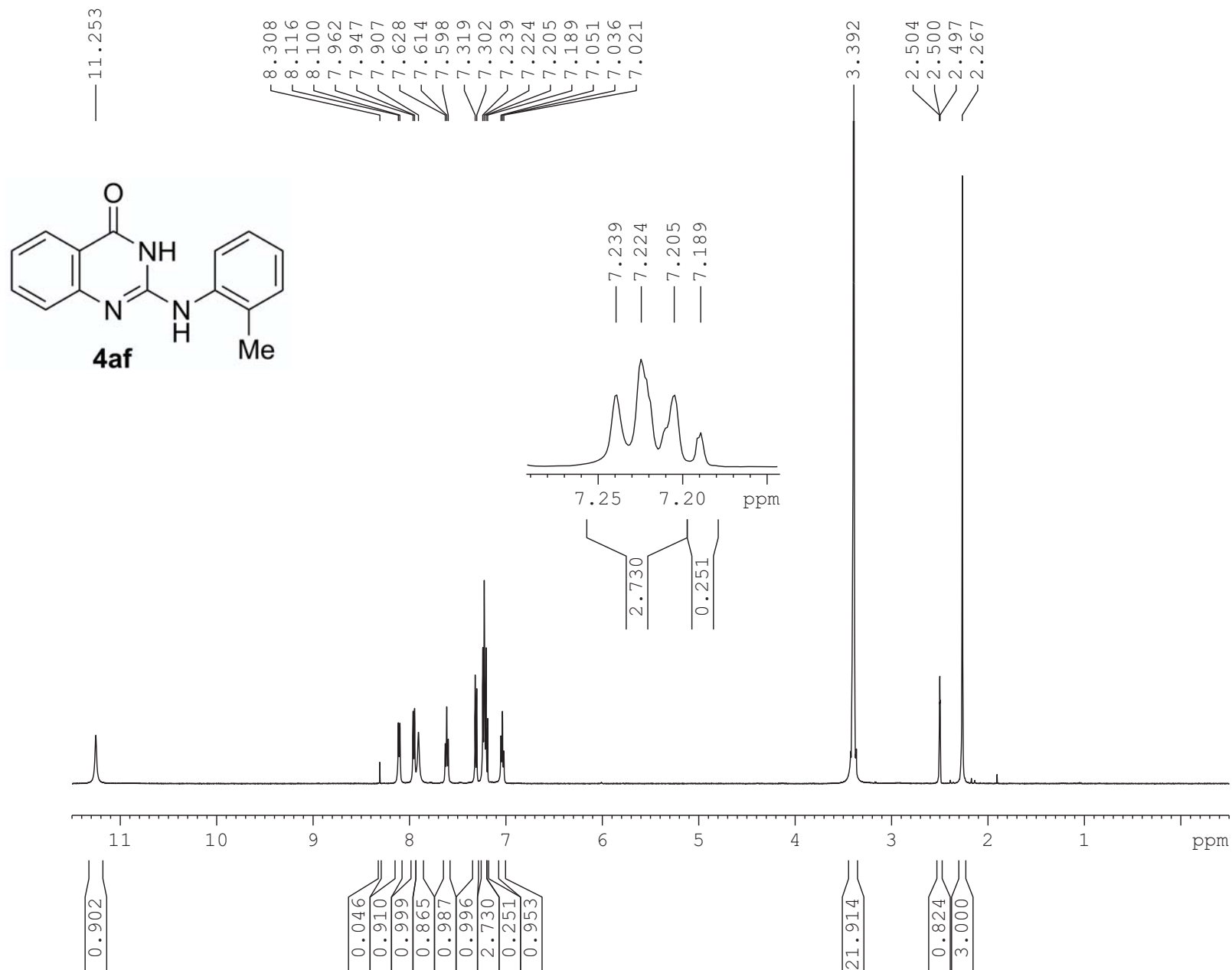
Current Data Parameters
 NAME TCC-20140424
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140429
 Time 3.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 17363
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577903 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

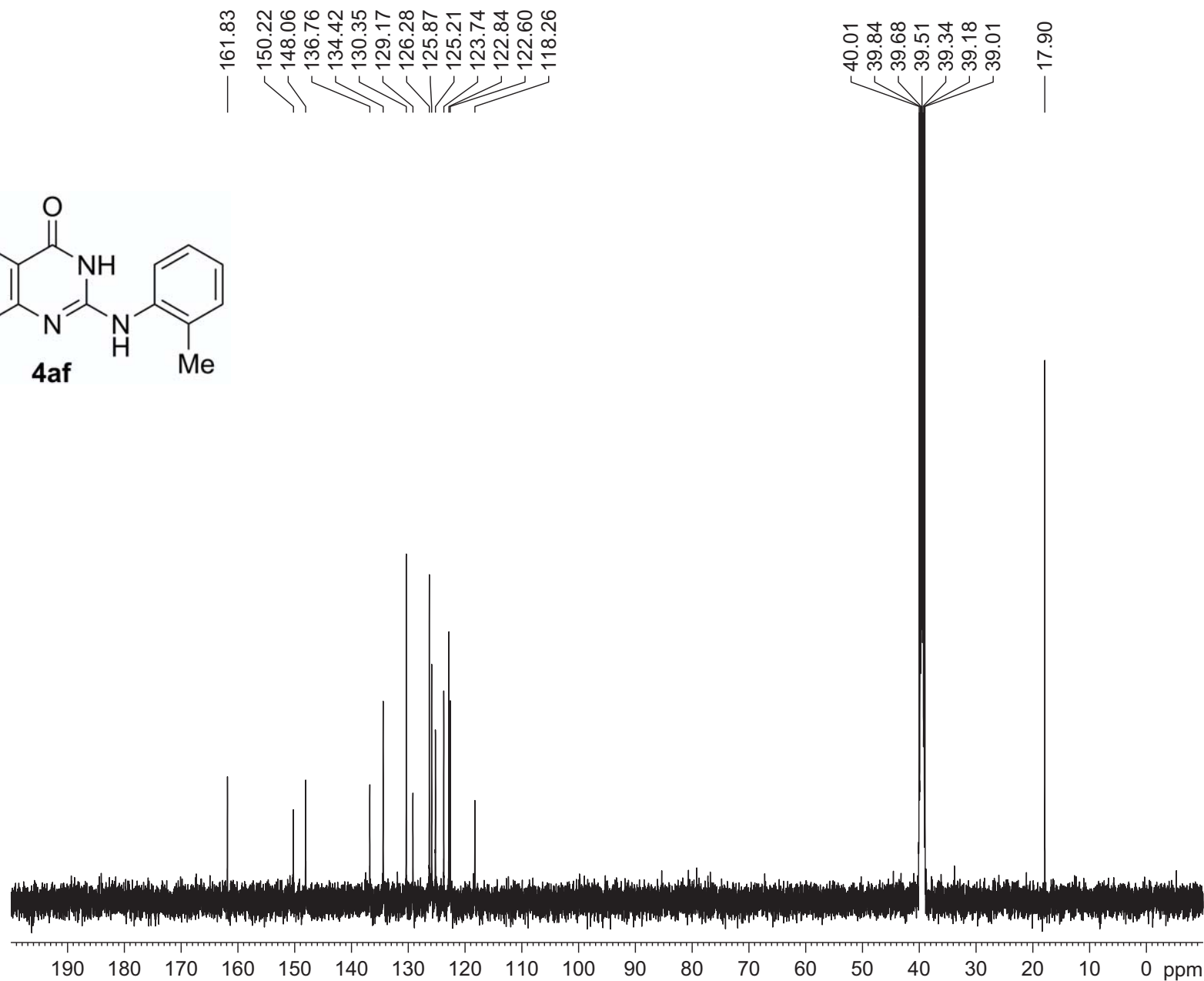
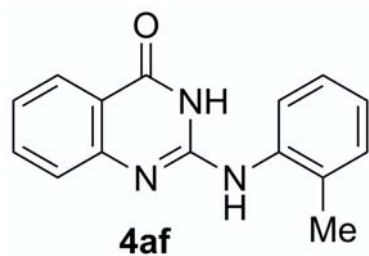


Current Data Parameters
 NAME RM187-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130119
 Time 10.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 293.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM187-2
 EXPNO 2
 PROCNO 1

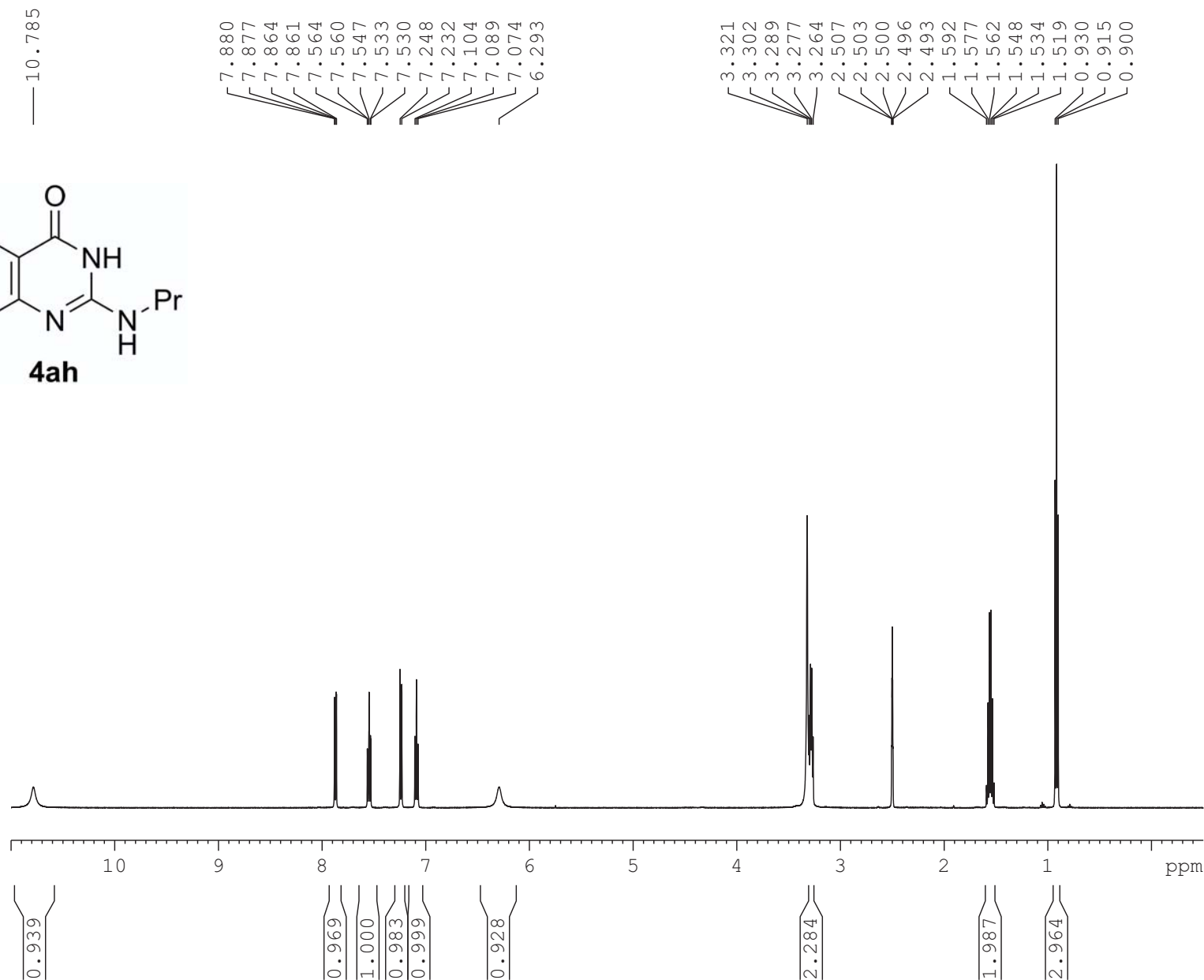
F2 - Acquisition Parameters
 Date_ 20130119
 Time 10.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 500
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 2896.3
 DW 16.650 usec
 DE 6.50 usec
 TE 295.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578459 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of RX 105 recrystallized



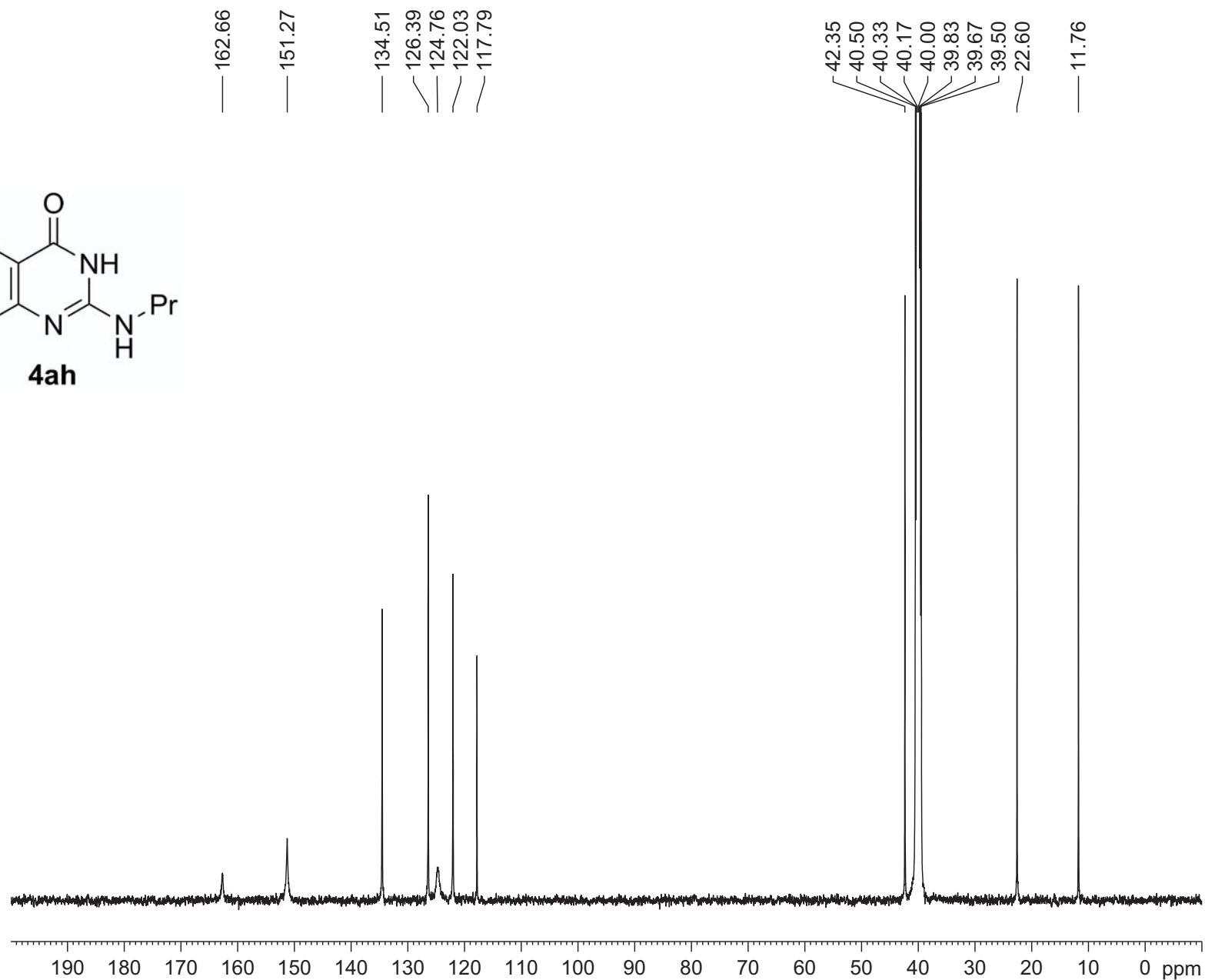
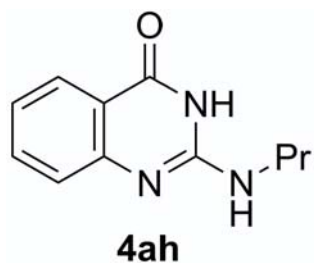
Current Data Parameters
 NAME TCC-20140603
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140605
 Time 12.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX 105 recrystallized



Current Data Parameters
 NAME TCC-20140604
 EXPNO 8
 PROCNO 1

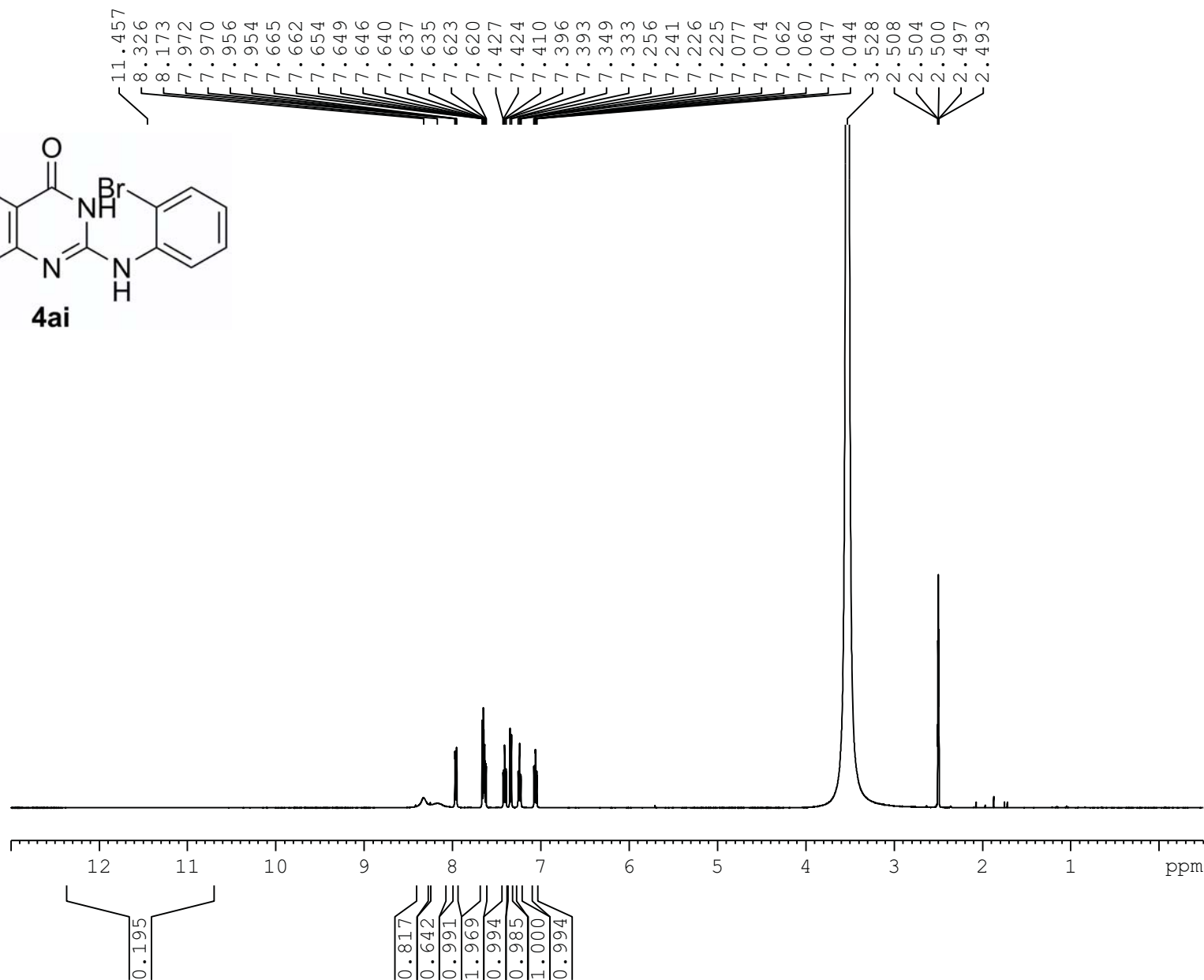
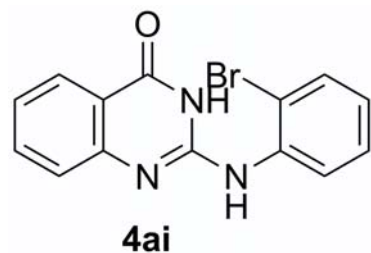
F2 - Acquisition Parameters
 Date_ 20140604
 Time 19.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 6995
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 5792.6
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577906 MHz
 WDW EM
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.00

1H of rx121



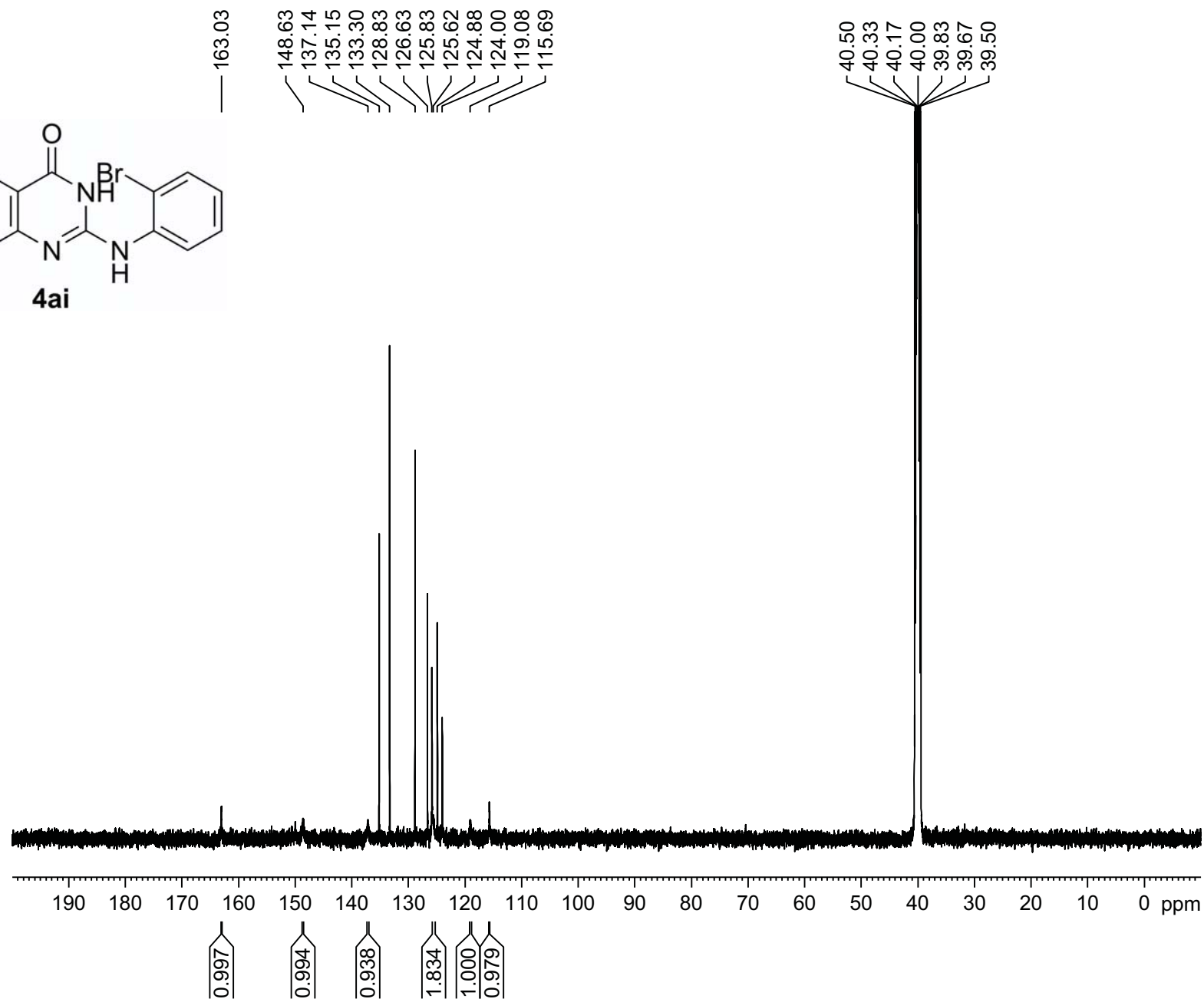
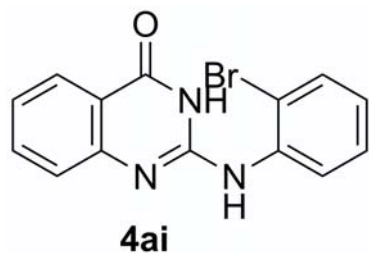
Current Data Parameters
 NAME 2014050115
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140717
 Time 15.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 35.9
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

13C of rx121



Current Data Parameters
NAME 2014050115
EXPNO 5
PROCNO 1

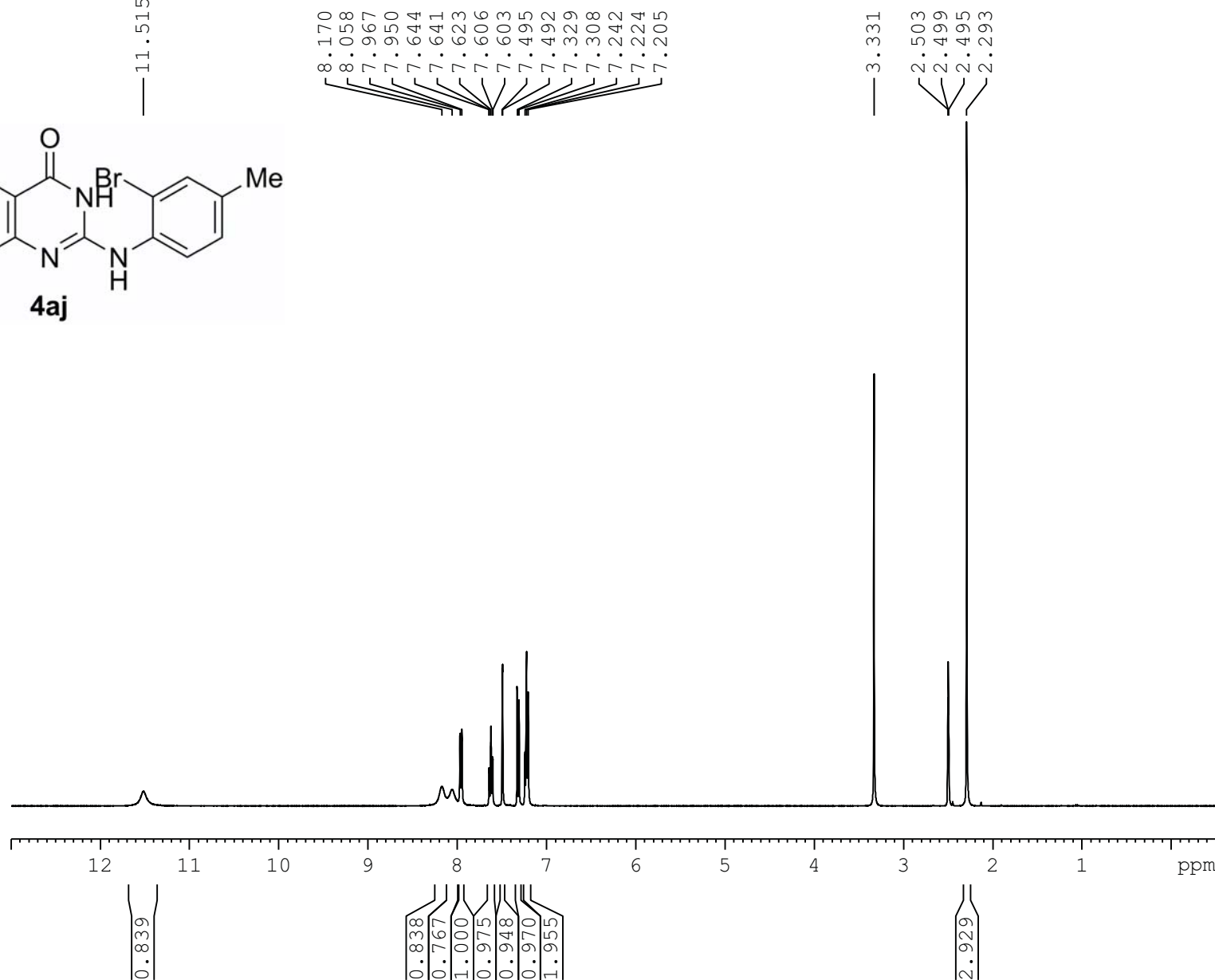
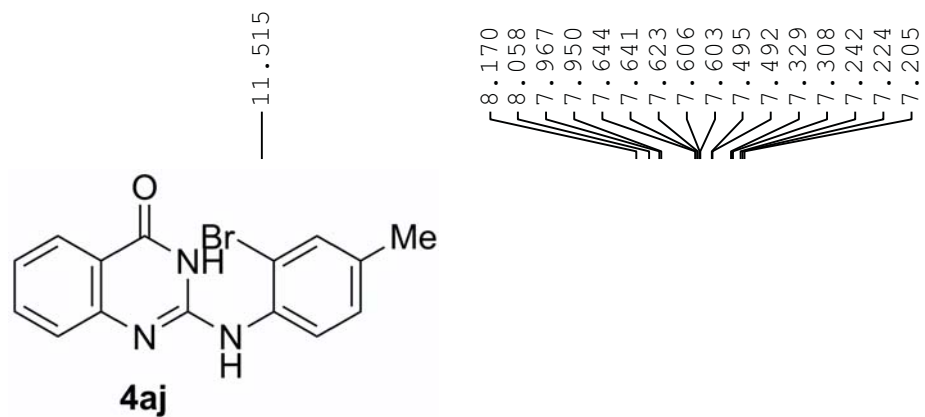
F2 - Acquisition Parameters
Date_ 20140717
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 21883
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577621 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H



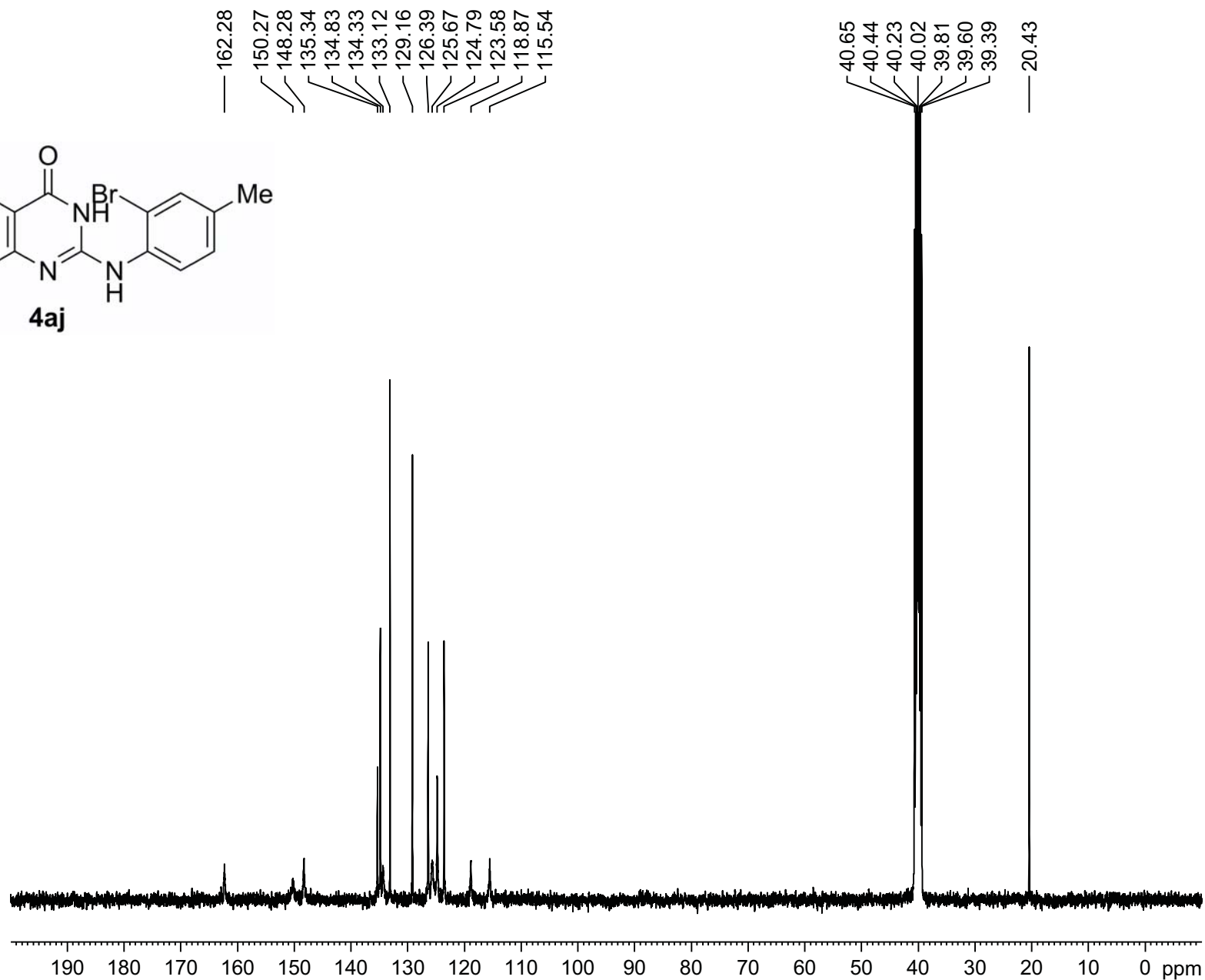
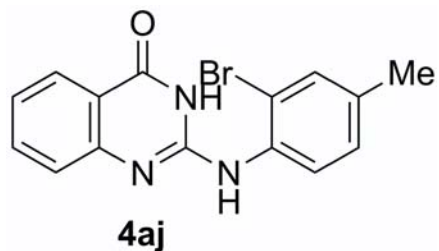
Current Data Parameters
 NAME RX160 recrystall
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141017
 Time 12.57
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 158.74
 DW 69.333 usec
 DE 10.52 usec
 TE 297.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324008 MHz
 NUC1 ¹H
 P1 12.80 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 16384
 SF 400.1300034 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C



Current Data Parameters
NAME RX160 recrystall
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141020
Time 17.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2839
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

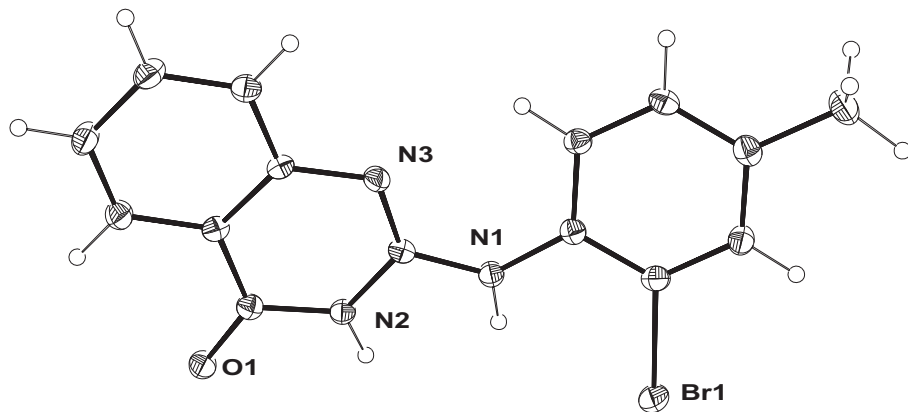
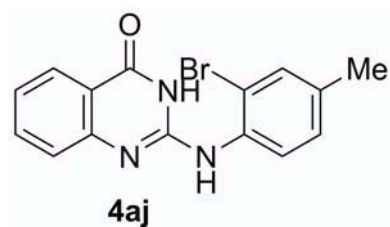


Table 1. Crystal data and structure refinement for ch16585.

Identification code	ch16585	
Empirical formula	C15 H12 Br N3 O	
Formula weight	330.19	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.4056(2) Å	$\alpha = 90^\circ$.
	b = 22.7204(7) Å	$\beta = 100.885(2)^\circ$.
	c = 9.3434(3) Å	$\gamma = 90^\circ$.
Volume	1335.35(7) Å ³	
Z	4	
Density (calculated)	1.642 Mg/m ³	
Absorption coefficient	3.077 mm ⁻¹	
F(000)	664	
Crystal size	0.71 x 0.37 x 0.32 mm ³	
Theta range for data collection	1.79 to 25.07°	
Index ranges	-7 ≤ h ≤ 7, -27 ≤ k ≤ 25, -10 ≤ l ≤ 11	
Reflections collected	6954	
Independent reflections	2348 [R(int) = 0.0226]	
Completeness to theta = 25.07°	99.2 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.4393 and 0.2187	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2348 / 0 / 181	
Goodness-of-fit on F ²	1.201	
Final R indices [I > 2σ(I)]	R1 = 0.0258, wR2 = 0.0762	
R indices (all data)	R1 = 0.0332, wR2 = 0.0914	
Largest diff. peak and hole	0.388 and -0.550 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for ch16585. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8042(4)	747(1)	12749(3)	28(1)
C(2)	10012(4)	968(1)	13386(3)	32(1)
C(3)	10934(4)	1419(1)	12723(3)	30(1)
C(4)	13066(4)	1666(1)	13437(3)	41(1)
C(5)	9830(4)	1632(1)	11404(3)	28(1)
C(6)	7866(4)	1408(1)	10755(3)	25(1)
C(7)	6919(4)	958(1)	11427(3)	23(1)
C(8)	3383(4)	903(1)	9731(3)	23(1)
C(9)	-193(4)	659(1)	8514(3)	25(1)
C(10)	-92(4)	1191(1)	7675(3)	24(1)
C(11)	-1853(4)	1376(1)	6634(3)	30(1)
C(12)	-1738(4)	1886(1)	5870(3)	35(1)
C(13)	122(4)	2225(1)	6139(3)	35(1)
C(14)	1840(4)	2053(1)	7162(3)	32(1)
C(15)	1779(4)	1530(1)	7957(3)	24(1)
N(1)	4947(3)	701(1)	10833(2)	26(1)
N(2)	1630(3)	539(1)	9504(2)	25(1)
N(3)	3547(3)	1382(1)	9007(2)	26(1)
O(1)	-1747(3)	327(1)	8408(2)	32(1)
Br(1)	6839(1)	142(1)	13753(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for ch16585.

C(1)-C(2)	1.384(4)
C(1)-C(7)	1.392(3)
C(1)-Br(1)	1.907(3)
C(2)-C(3)	1.386(4)
C(2)-H(2)	0.9500
C(3)-C(5)	1.387(4)
C(3)-C(4)	1.510(4)
C(4)-H(4A)	0.9859
C(4)-H(4B)	0.9451
C(4)-H(4C)	1.0540
C(5)-C(6)	1.386(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.396(3)
C(6)-H(6)	0.9500
C(7)-N(1)	1.407(3)
C(8)-N(3)	1.295(3)
C(8)-N(1)	1.373(3)
C(8)-N(2)	1.379(3)
C(9)-O(1)	1.238(3)
C(9)-N(2)	1.373(3)
C(9)-C(10)	1.450(3)
C(10)-C(15)	1.406(3)
C(10)-C(11)	1.408(4)
C(11)-C(12)	1.370(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.400(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.371(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.405(4)
C(14)-H(14)	0.9500
C(15)-N(3)	1.393(3)
N(1)-H(1)	0.8800
N(2)-H(2A)	0.8800

C(2)-C(1)-C(7)	122.2(2)
C(2)-C(1)-Br(1)	118.1(2)
C(7)-C(1)-Br(1)	119.73(19)
C(1)-C(2)-C(3)	120.4(2)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(2)-C(3)-C(5)	117.8(2)
C(2)-C(3)-C(4)	120.2(3)
C(5)-C(3)-C(4)	122.0(3)
C(3)-C(4)-H(4A)	110.4
C(3)-C(4)-H(4B)	111.5
H(4A)-C(4)-H(4B)	100.8
C(3)-C(4)-H(4C)	115.3
H(4A)-C(4)-H(4C)	109.7
H(4B)-C(4)-H(4C)	108.1
C(6)-C(5)-C(3)	122.0(2)
C(6)-C(5)-H(5)	119.0
C(3)-C(5)-H(5)	119.0
C(5)-C(6)-C(7)	120.4(2)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(1)-C(7)-C(6)	117.1(2)
C(1)-C(7)-N(1)	118.8(2)
C(6)-C(7)-N(1)	124.0(2)
N(3)-C(8)-N(1)	123.6(2)
N(3)-C(8)-N(2)	124.6(2)
N(1)-C(8)-N(2)	111.9(2)
O(1)-C(9)-N(2)	120.2(2)
O(1)-C(9)-C(10)	125.6(2)
N(2)-C(9)-C(10)	114.2(2)
C(15)-C(10)-C(11)	120.6(2)
C(15)-C(10)-C(9)	118.6(2)
C(11)-C(10)-C(9)	120.7(2)
C(12)-C(11)-C(10)	119.9(2)
C(12)-C(11)-H(11)	120.1

C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	119.9(2)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	120.8(3)
C(14)-C(13)-H(13)	119.6
C(12)-C(13)-H(13)	119.6
C(13)-C(14)-C(15)	120.7(2)
C(13)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
N(3)-C(15)-C(14)	118.5(2)
N(3)-C(15)-C(10)	123.4(2)
C(14)-C(15)-C(10)	118.1(2)
C(8)-N(1)-C(7)	129.1(2)
C(8)-N(1)-H(1)	115.5
C(7)-N(1)-H(1)	115.5
C(9)-N(2)-C(8)	123.3(2)
C(9)-N(2)-H(2A)	118.3
C(8)-N(2)-H(2A)	118.3
C(8)-N(3)-C(15)	115.8(2)

Symmetry transformations used to generate equivalent atoms:

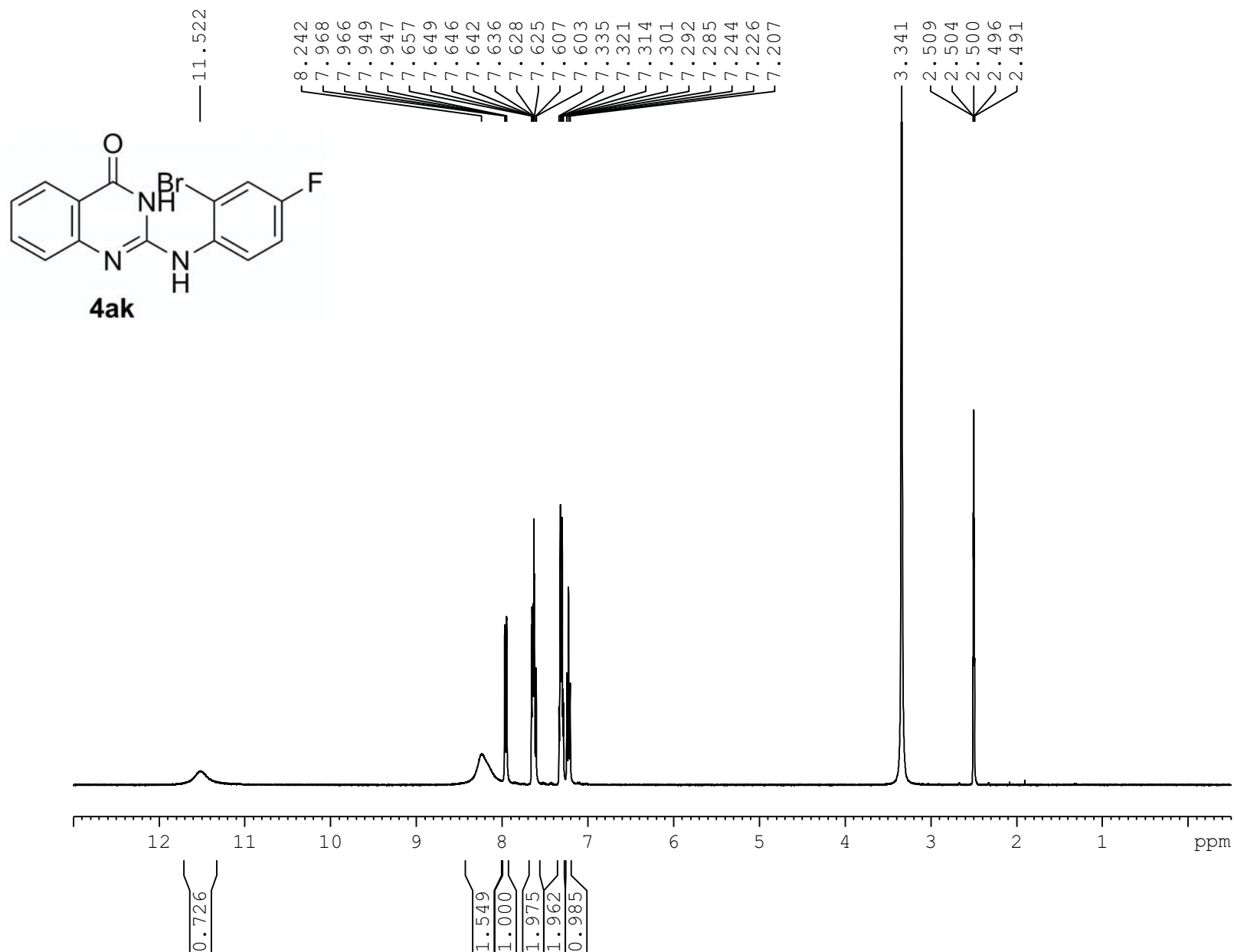
Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ch16585. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	29(1)	28(1)	28(1)	3(1)	9(1)	0(1)
C(2)	28(1)	40(2)	26(1)	1(1)	2(1)	2(1)
C(3)	26(1)	34(2)	31(2)	-7(1)	7(1)	1(1)
C(4)	26(1)	53(2)	43(2)	-6(1)	5(1)	-7(1)
C(5)	26(1)	27(1)	32(1)	-2(1)	11(1)	-2(1)
C(6)	25(1)	25(1)	27(1)	2(1)	8(1)	3(1)
C(7)	23(1)	23(1)	25(1)	-2(1)	6(1)	3(1)
C(8)	24(1)	21(1)	25(1)	-2(1)	7(1)	-2(1)
C(9)	27(1)	25(1)	24(1)	-2(1)	6(1)	-1(1)
C(10)	29(1)	22(1)	22(1)	-2(1)	6(1)	-2(1)
C(11)	29(1)	30(1)	30(1)	-1(1)	2(1)	-5(1)
C(12)	37(2)	33(1)	31(2)	6(1)	-4(1)	1(1)
C(13)	42(2)	31(1)	29(2)	7(1)	4(1)	0(1)
C(14)	32(1)	28(1)	34(2)	6(1)	5(1)	-6(1)
C(15)	28(1)	25(1)	20(1)	2(1)	6(1)	0(1)
N(1)	25(1)	24(1)	29(1)	5(1)	2(1)	-2(1)
N(2)	26(1)	21(1)	27(1)	3(1)	3(1)	-3(1)
N(3)	23(1)	25(1)	30(1)	3(1)	4(1)	-3(1)
O(1)	31(1)	28(1)	34(1)	4(1)	0(1)	-10(1)
Br(1)	39(1)	42(1)	36(1)	16(1)	3(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for ch16585.

	x	y	z	U(eq)
H(2)	10738	809	14284	38
H(4A)	12958	2093	13592	49
H(4B)	14047	1657	12798	49
H(4C)	13780	1461	14420	49
H(5)	10438	1940	10932	33
H(6)	7159	1562	9846	30
H(11)	-3118	1148	6462	36
H(12)	-2918	2009	5158	42
H(13)	193	2578	5607	41
H(14)	3085	2289	7335	38
H(1)	4678	364	11222	31
H(2A)	1682	213	10019	30

¹H



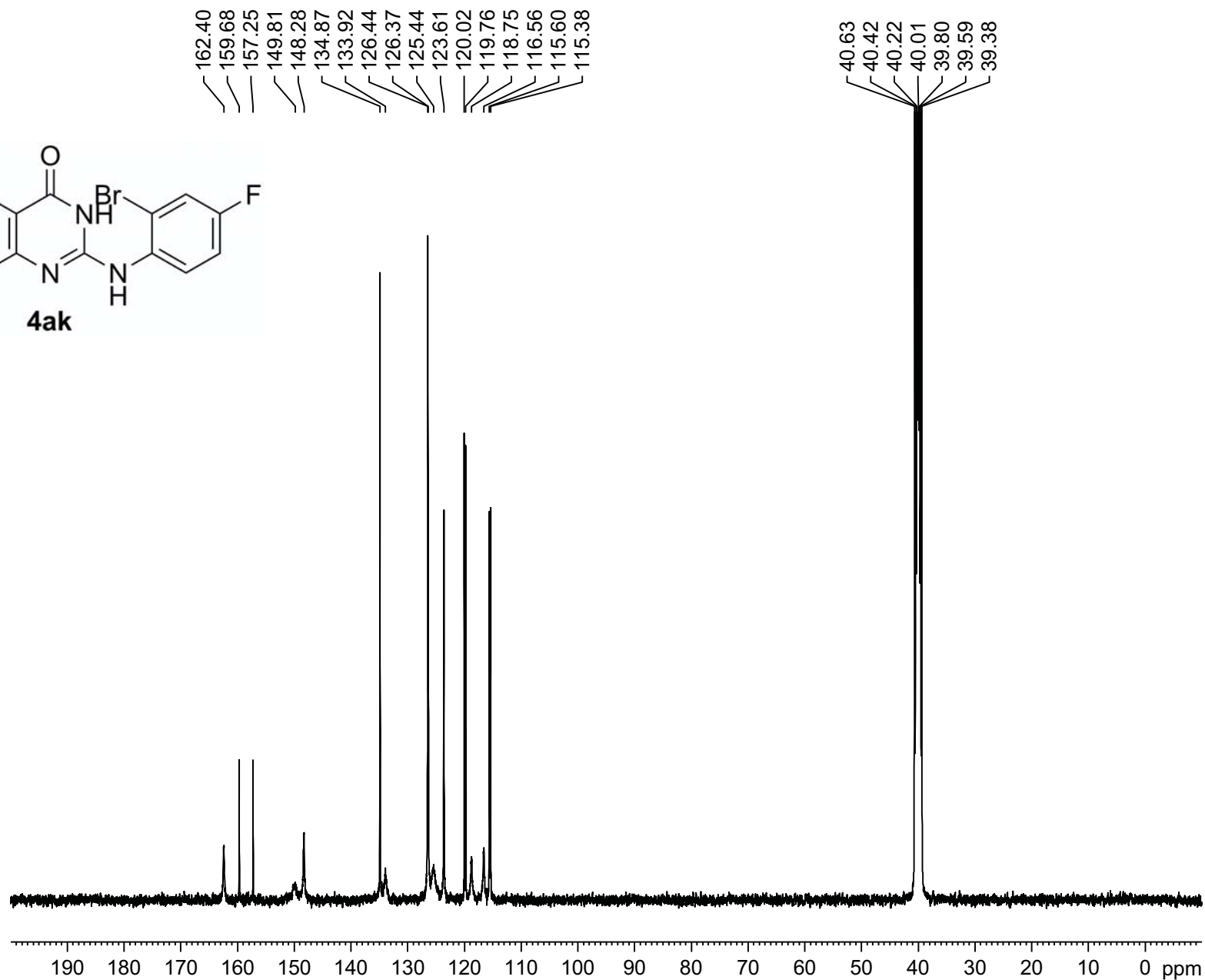
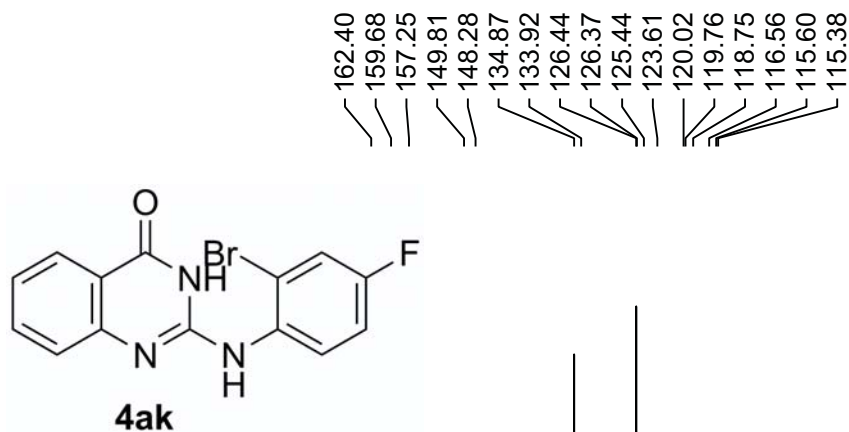
Current Data Parameters
NAME RX168 recrystall
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141027
Time 20.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 113.31
DW 69.333 usec
DE 10.52 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 ¹H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C



Current Data Parameters
NAME RX168 recrystall
EXPNO 8
PROCNO 1

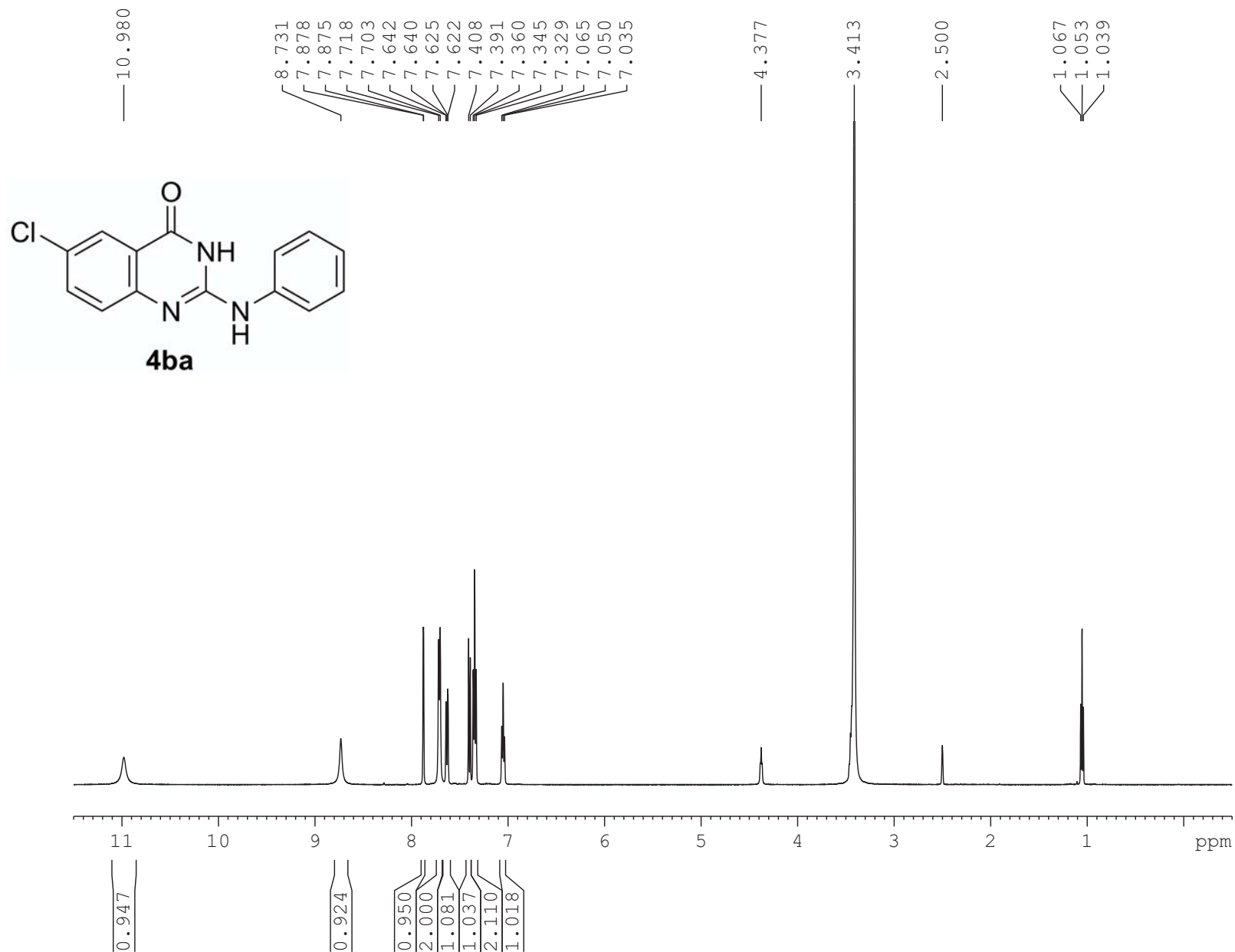
F2 - Acquisition Parameters
Date_ 20141029
Time 22.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 13254
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 ¹³C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 ¹H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

¹H of RX91 recrystallized



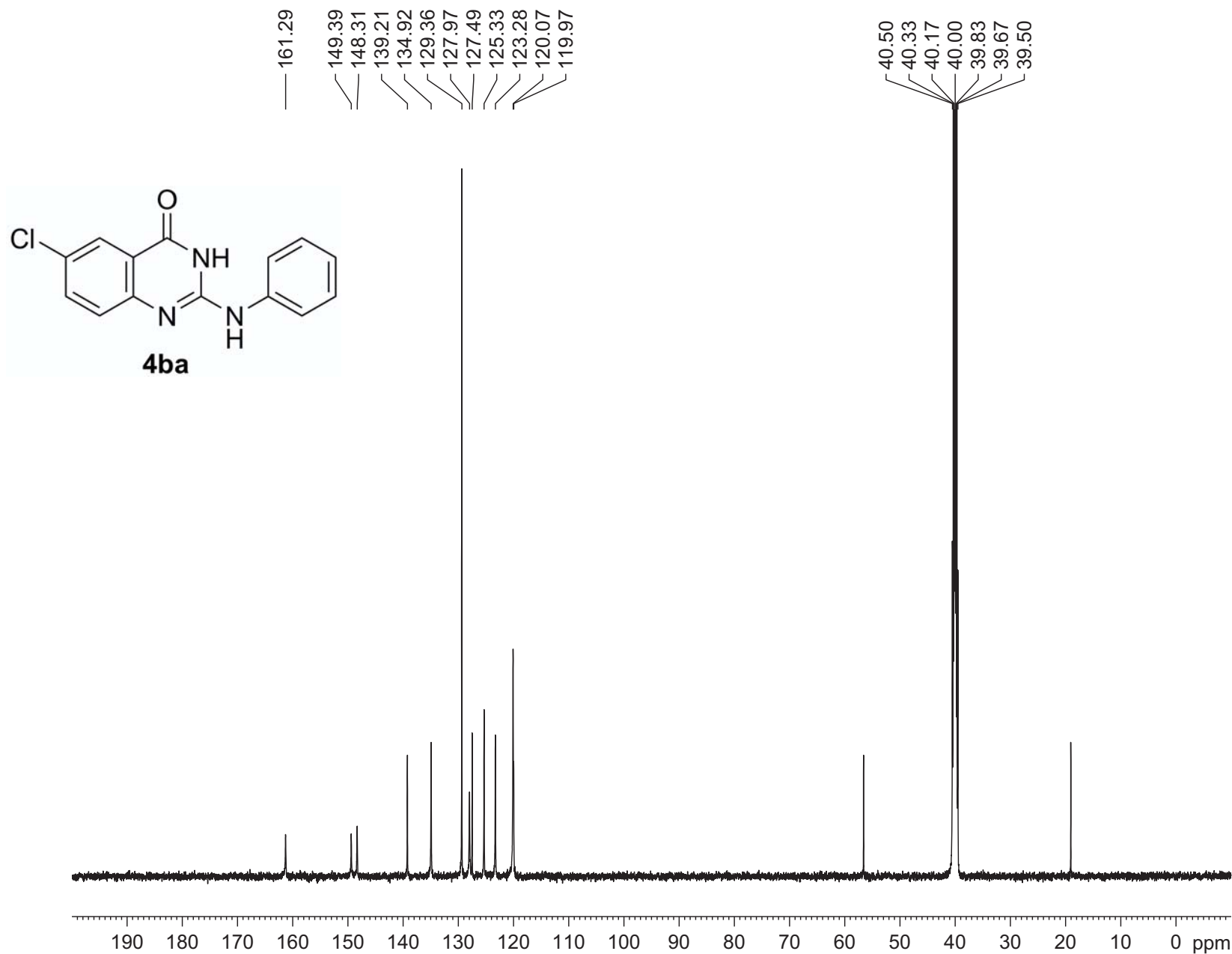
Current Data Parameters
 NAME TCC-20140424
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140502
 Time 16.34
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 71.8
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX91 recrystallized



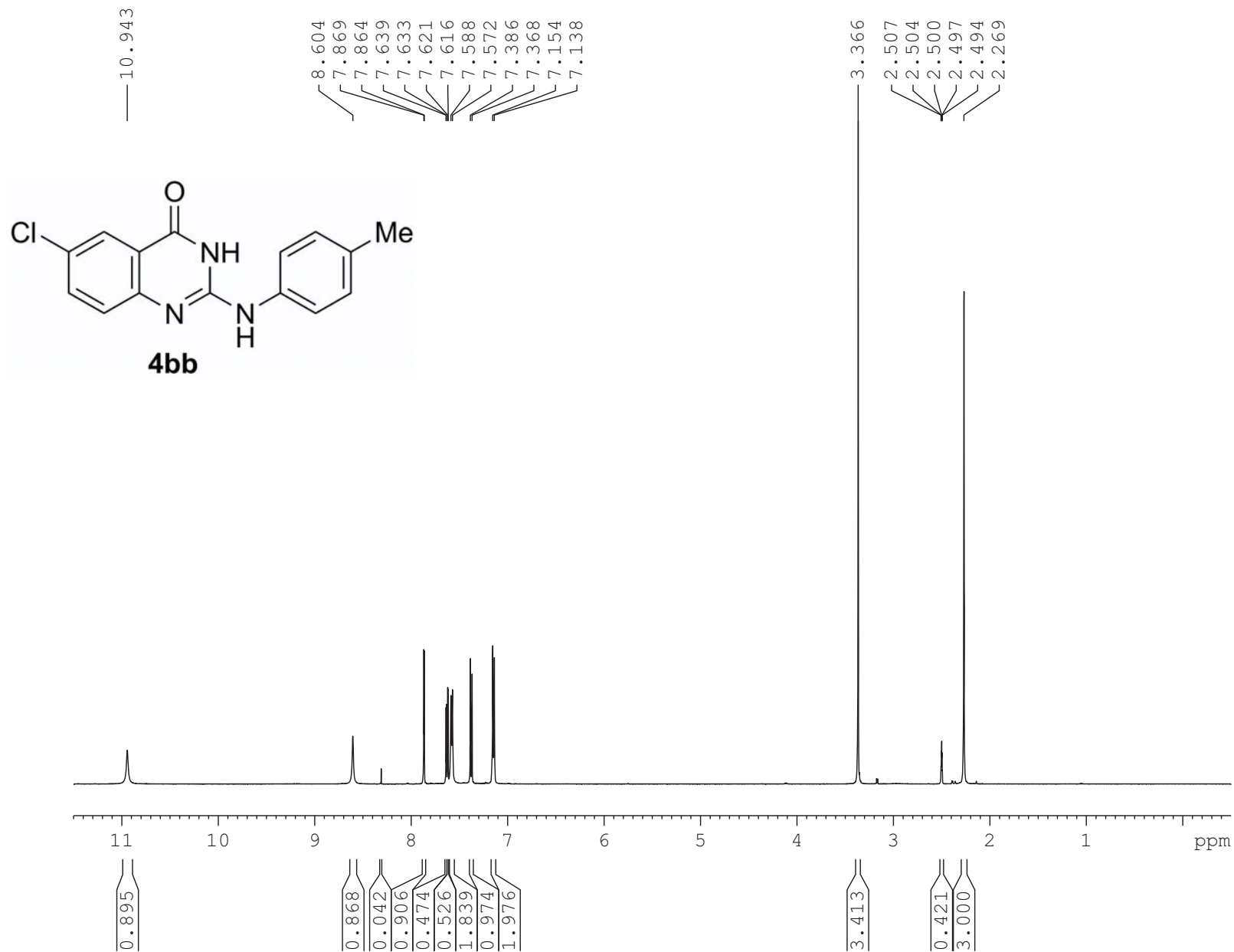
Current Data Parameters
NAME TCC-20140424
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140502
Time 15.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1509
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577805 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

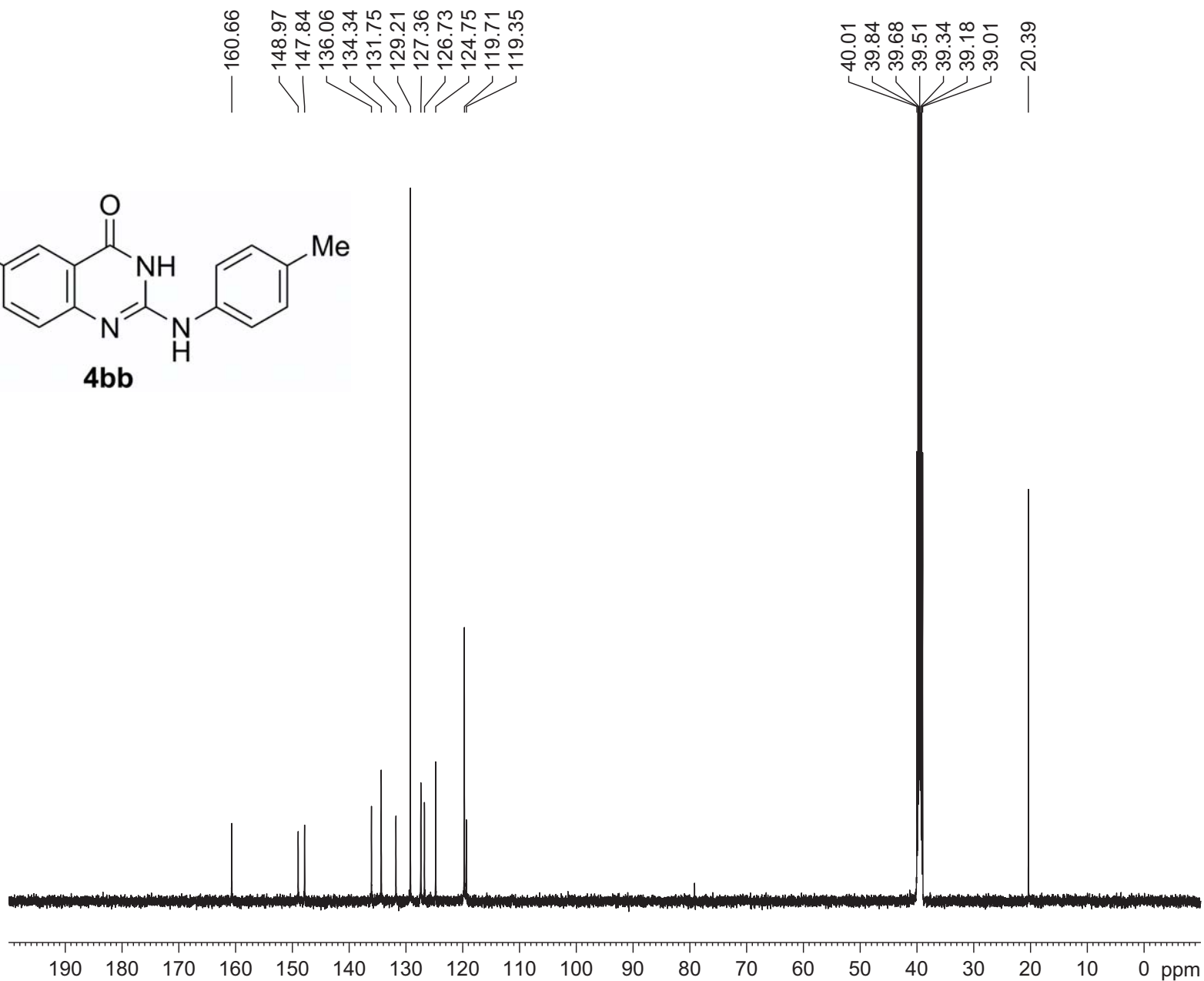
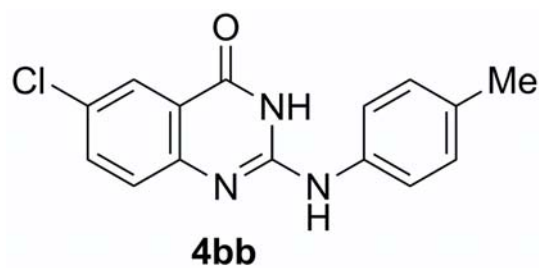


Current Data Parameters
 NAME RM116
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20121020
 Time 14.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 294.5 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME RM116
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20121020
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 667
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 295.4 K
D1 4.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

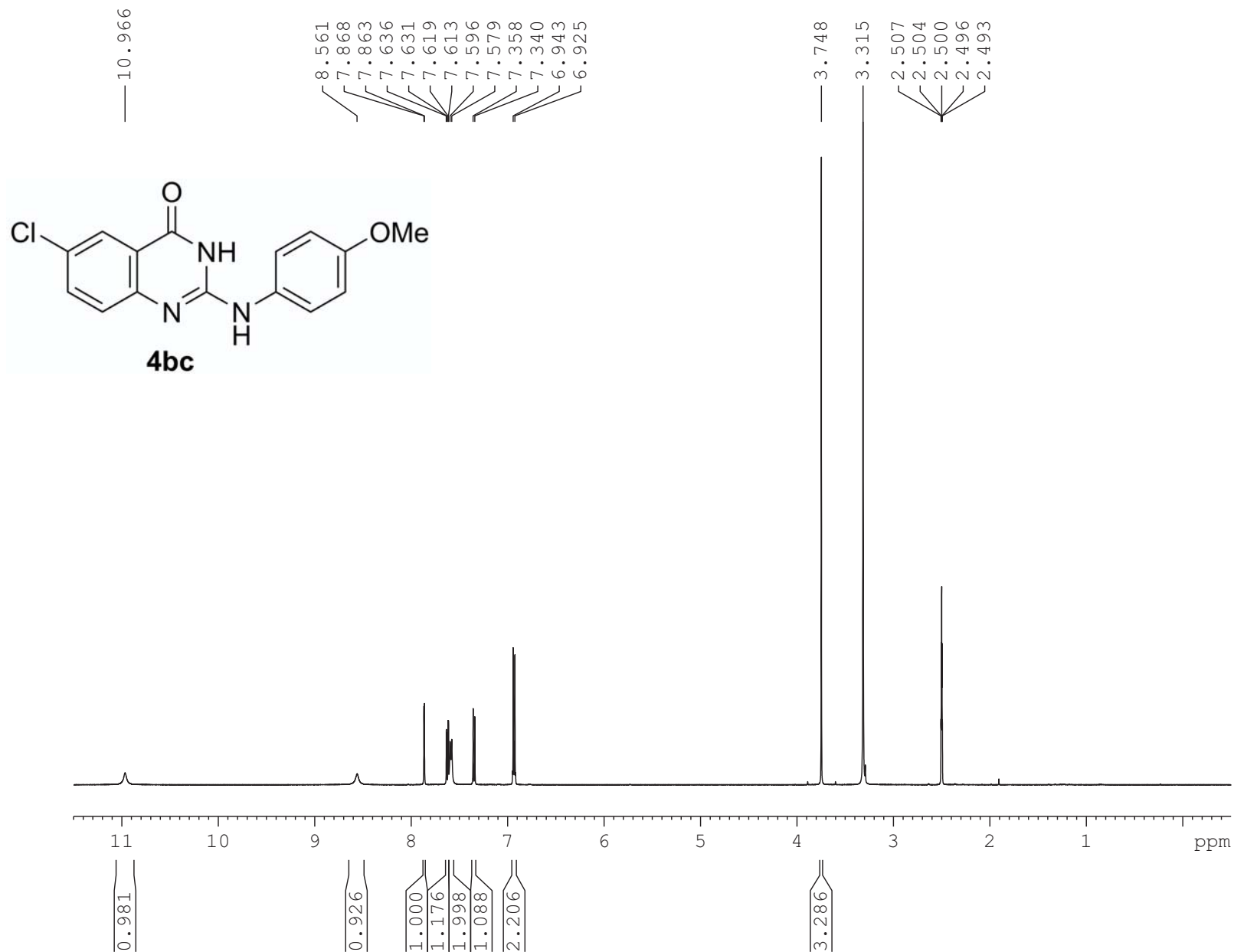
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 65536
SF 125.7578500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of RK-159-2



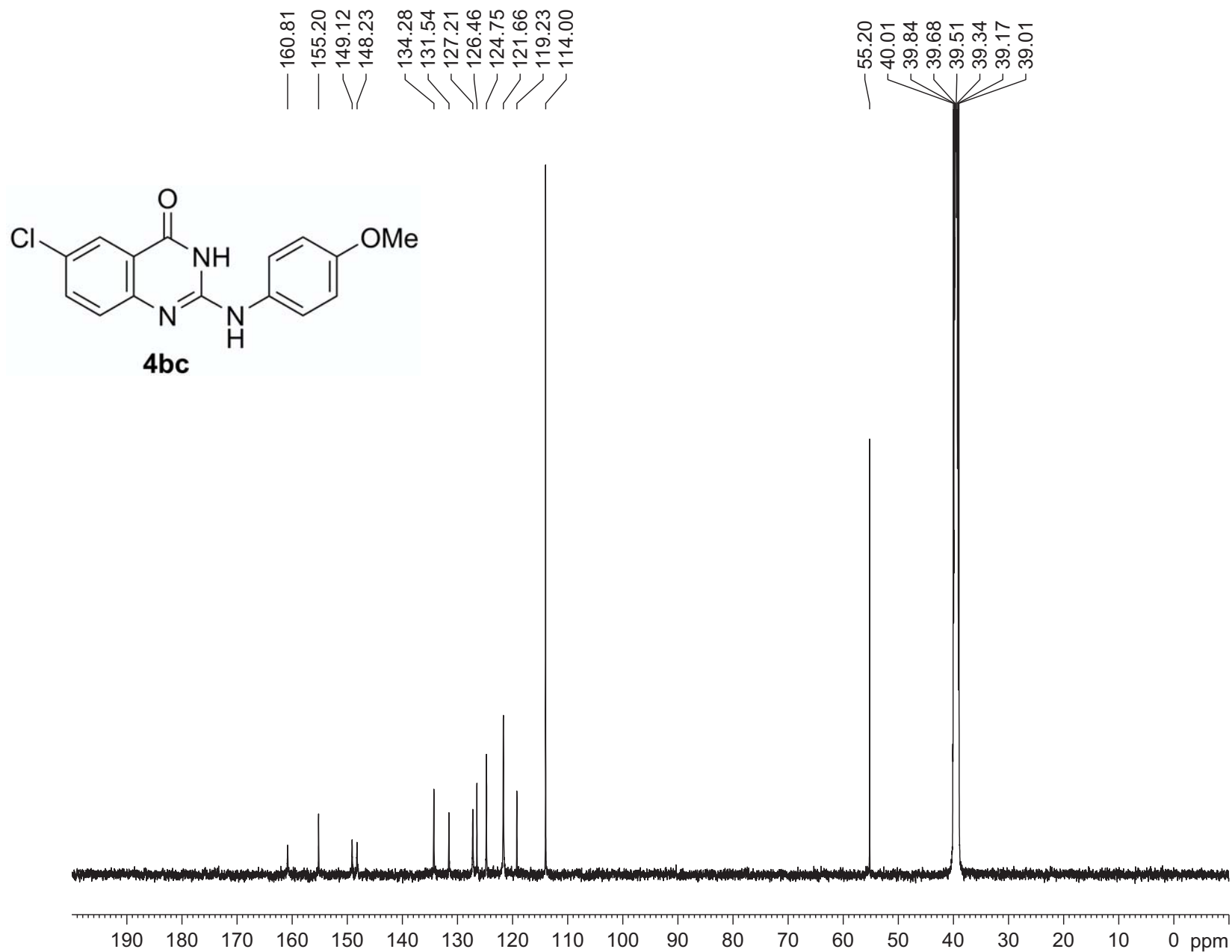
Current Data Parameters
 NAME 2013120115
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131211
 Time 1.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 256
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RK-159-2



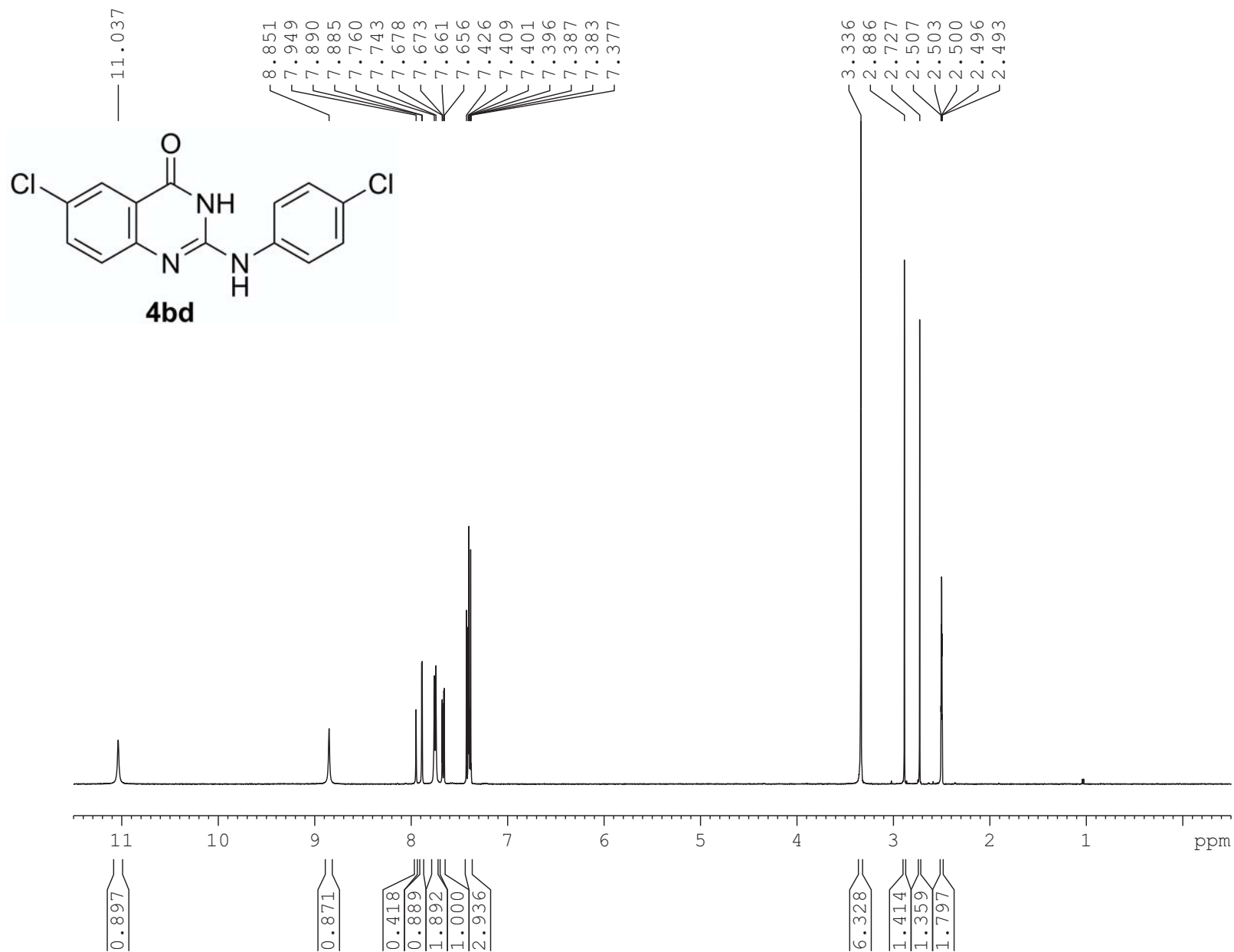
Current Data Parameters
 NAME 2013120115
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131210
 Time 18.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 11556
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578533 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME	RM161two
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

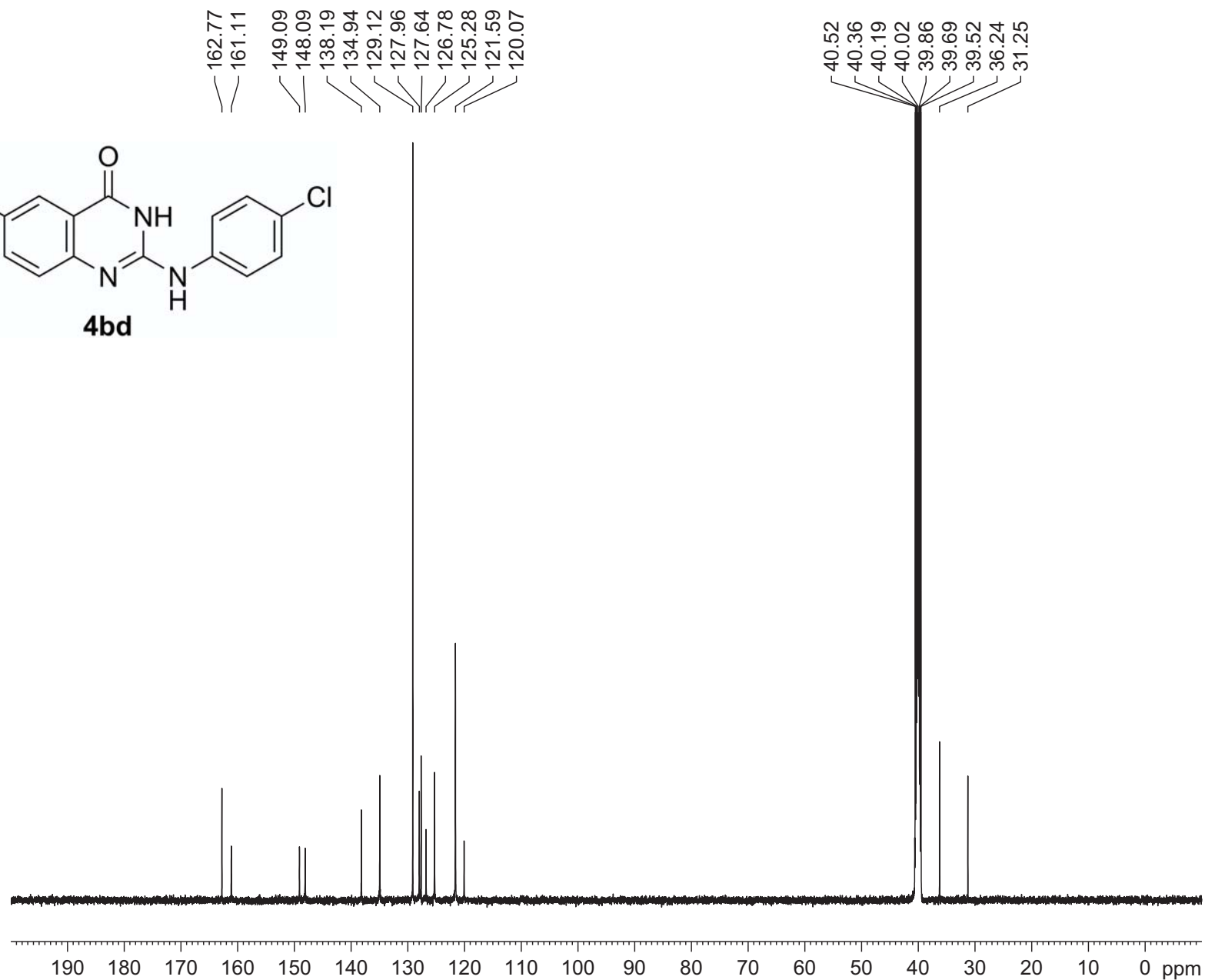
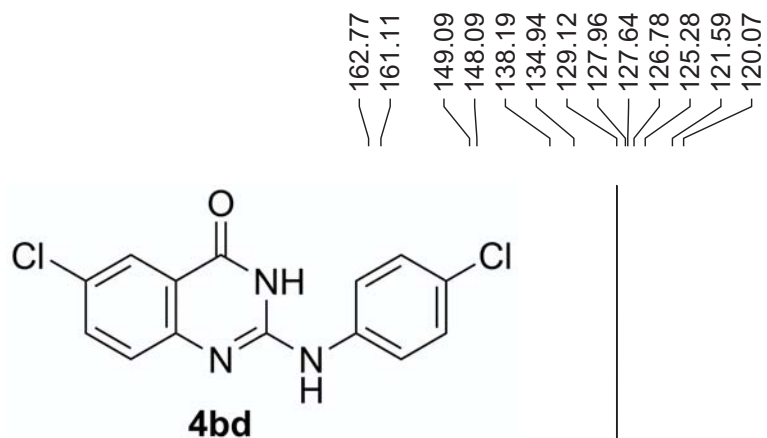
Date_	20130228
Time	20.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	12
DS	0
SWH	9057.971 Hz
FIDRES	0.276427 Hz
AQ	1.8087935 sec
RG	256
DW	55.200 usec
DE	6.50 usec
TE	296.5 K
D1	2.00000000 sec
TD0	1

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

NUC1	1H
P1	13.20 usec
PL1	-0.60 dB
SFO1	500.1330008 MHz

F2 - Processing parameters

SI	16384
SF	500.1300053 MHz
WDW	EM
SSB	0
LB	0 Hz
GB	0
PC	1.00



Current Data Parameters
NAME RM161two
EXPNO 3
PROCNO 1

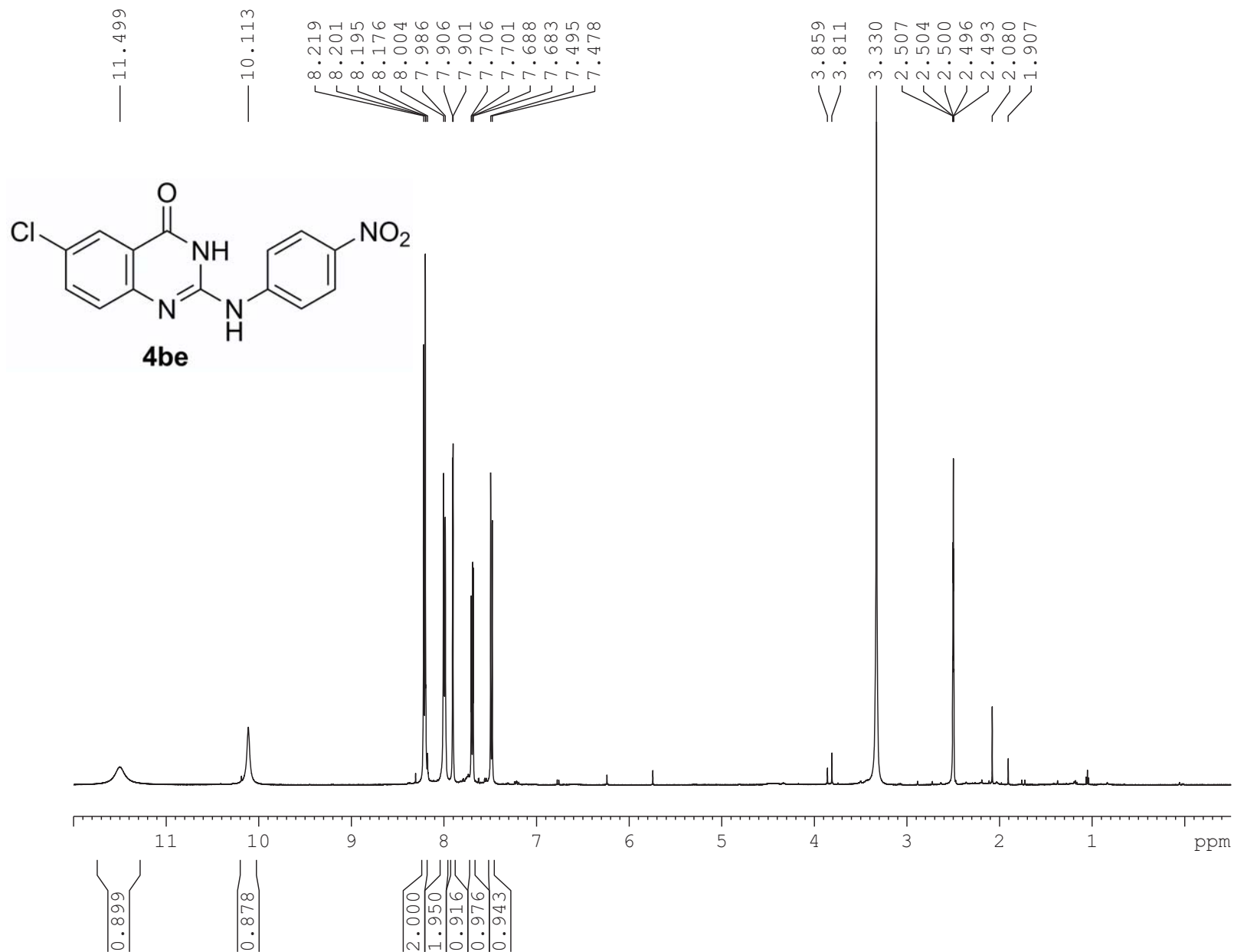
F2 - Acquisition Parameters
Date_ 20130301
Time 5.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10000
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 5792.6
DW 16.650 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of RX101 recrystallized



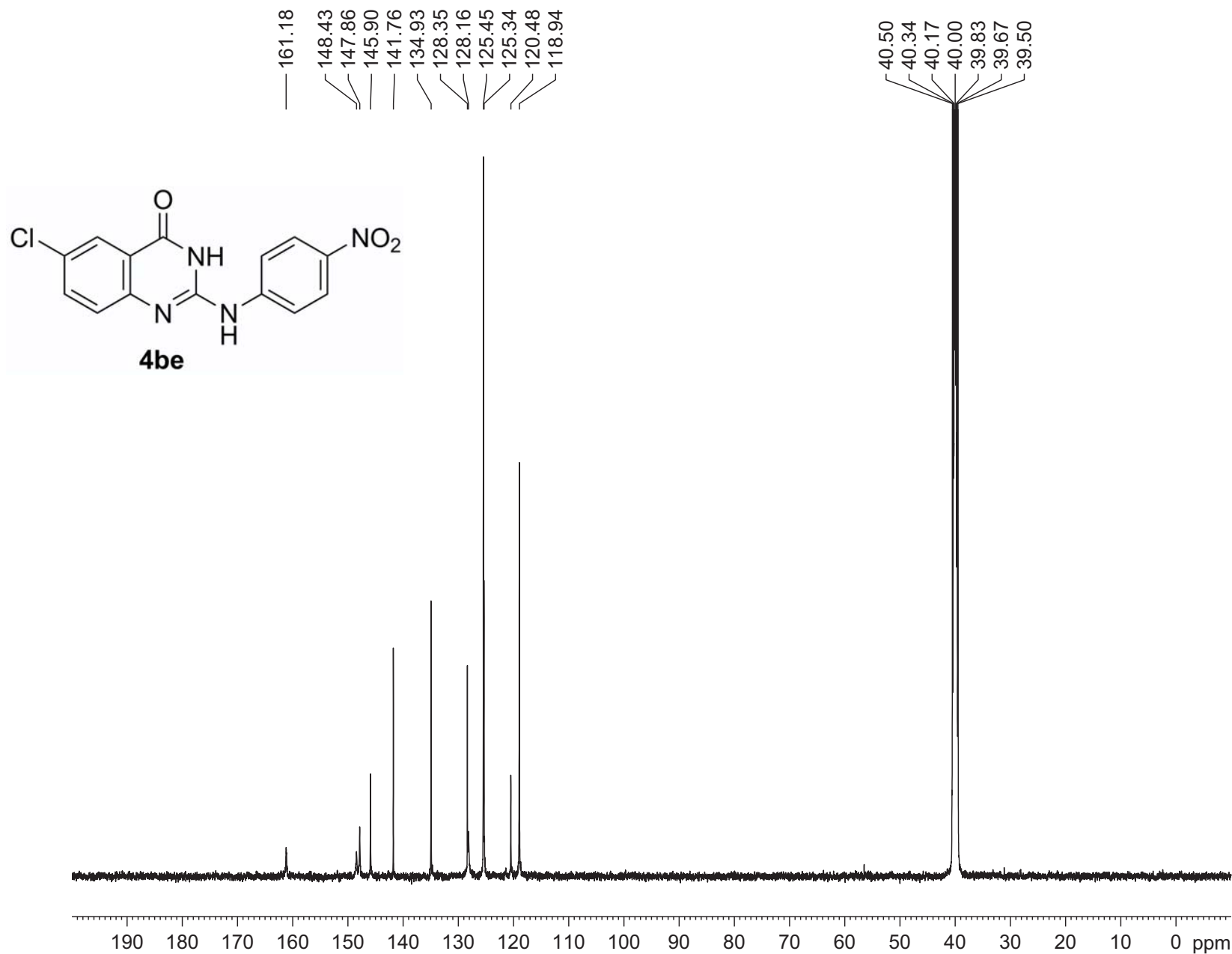
Current Data Parameters
 NAME TCC-20140424
 EXPNO 14
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140429
 Time 17.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX101 recrystallized



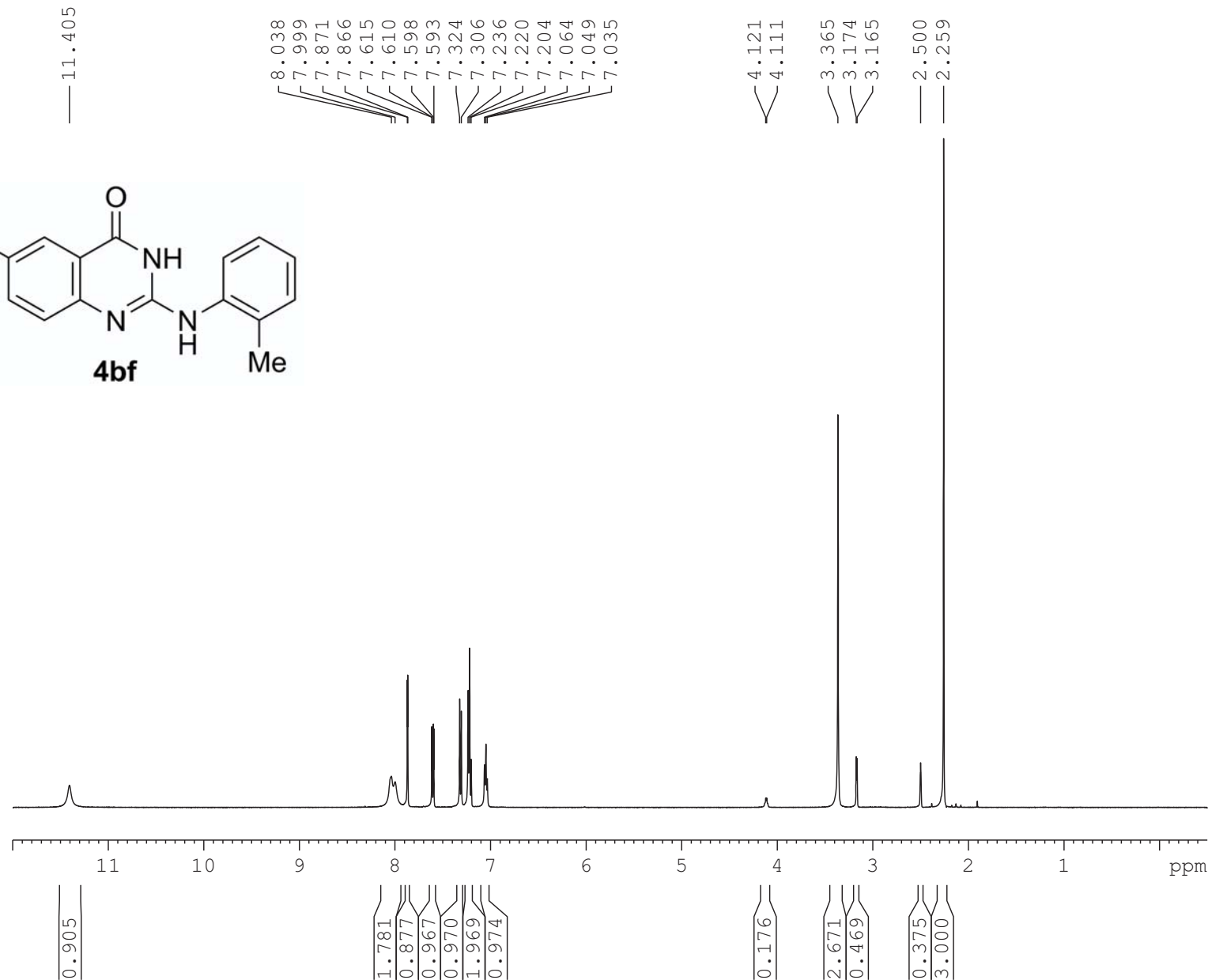
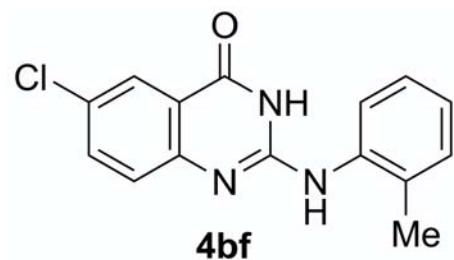
Current Data Parameters
NAME TCC-20140424
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140429
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 6400
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577899 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

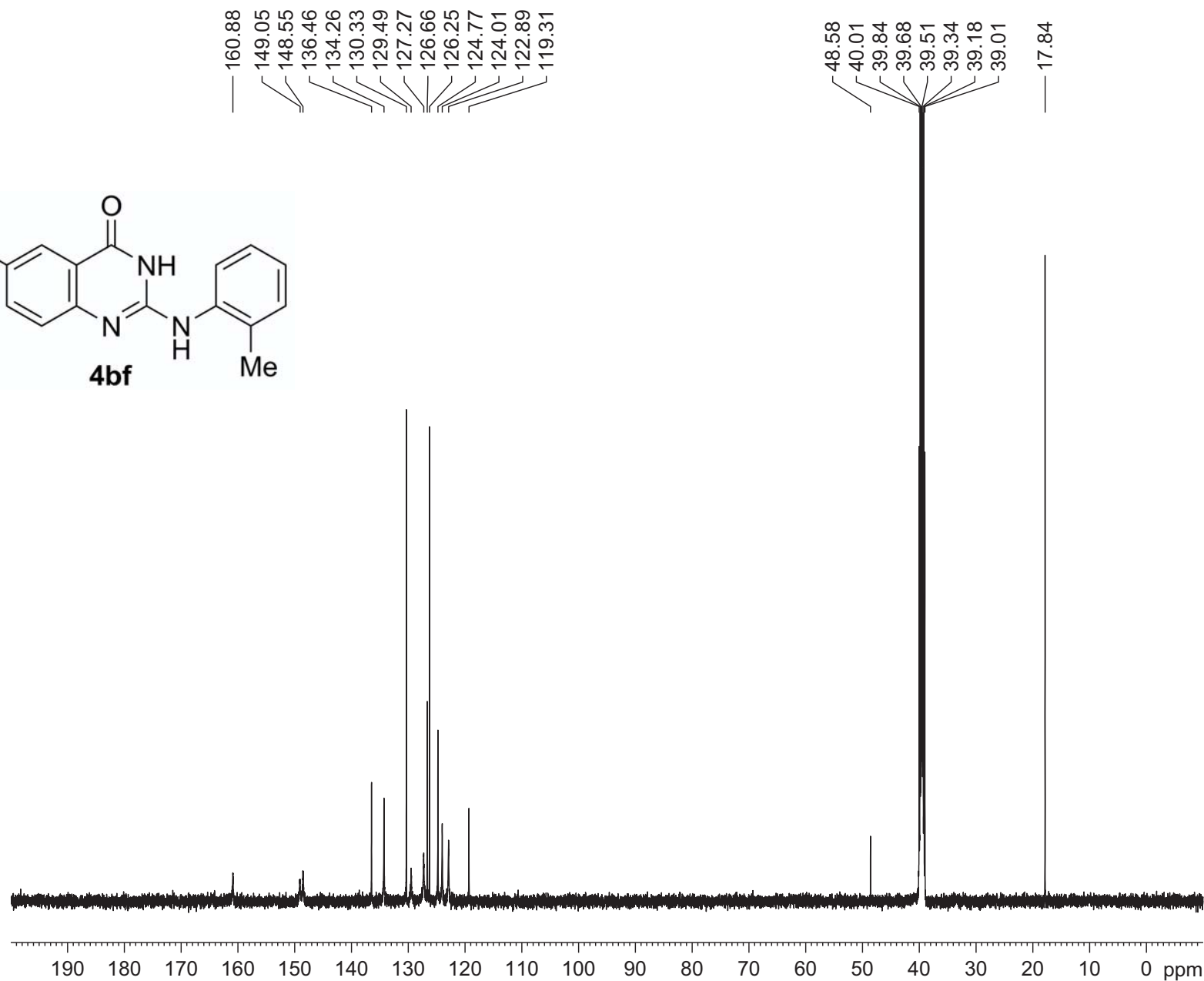
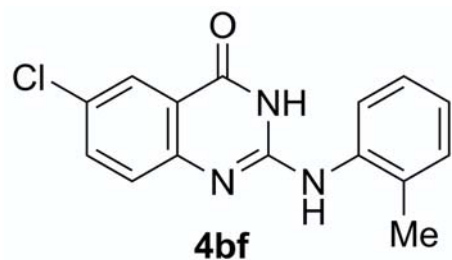


Current Data Parameters
 NAME RM188-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130119
 Time 11.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 293.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300049 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters

NAME RM188-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20130119
Time 12.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 951
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 2896.3
DW 16.650 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709931 MHz

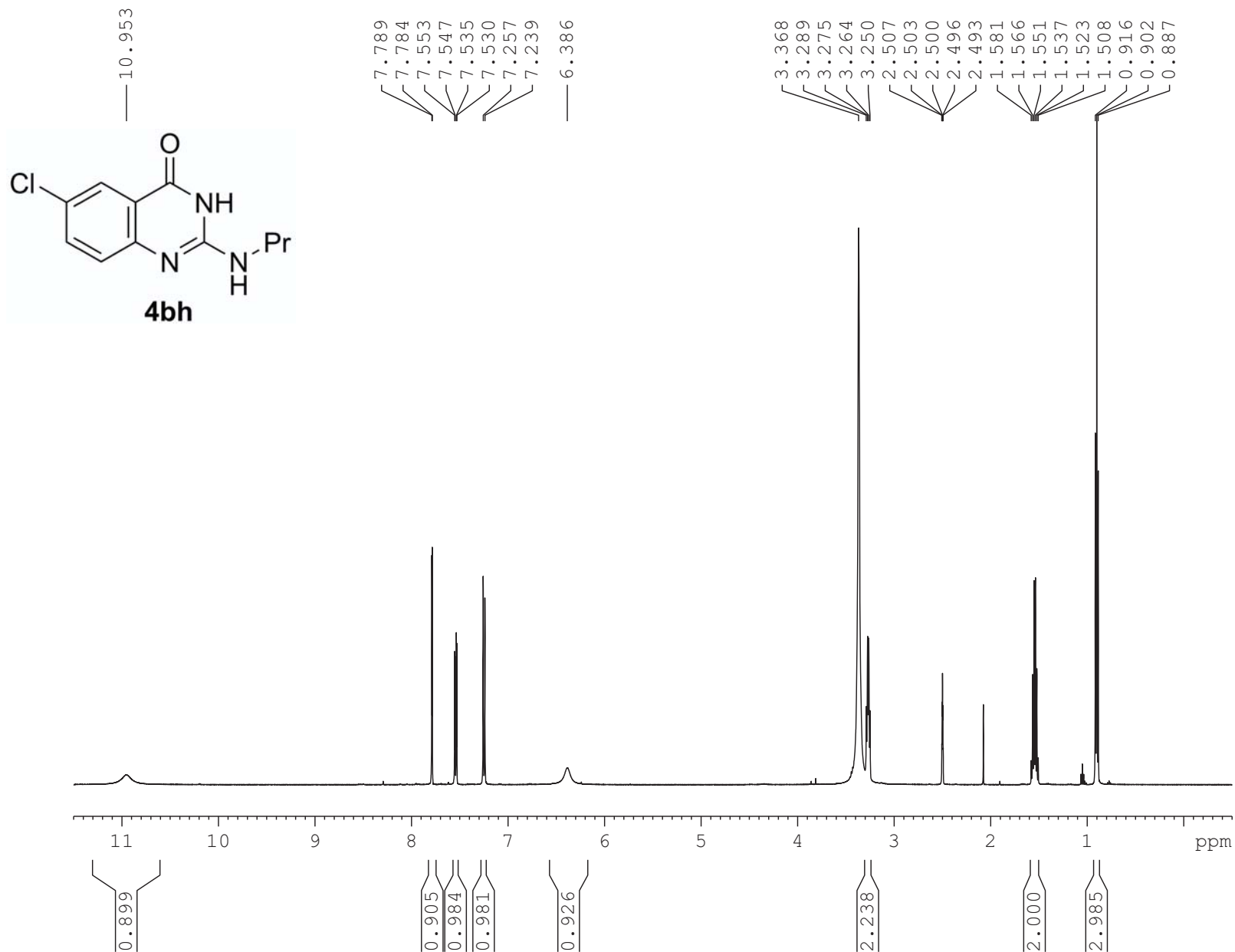
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters

SI 65536
SF 125.7578500 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of RX 106 recrystallized



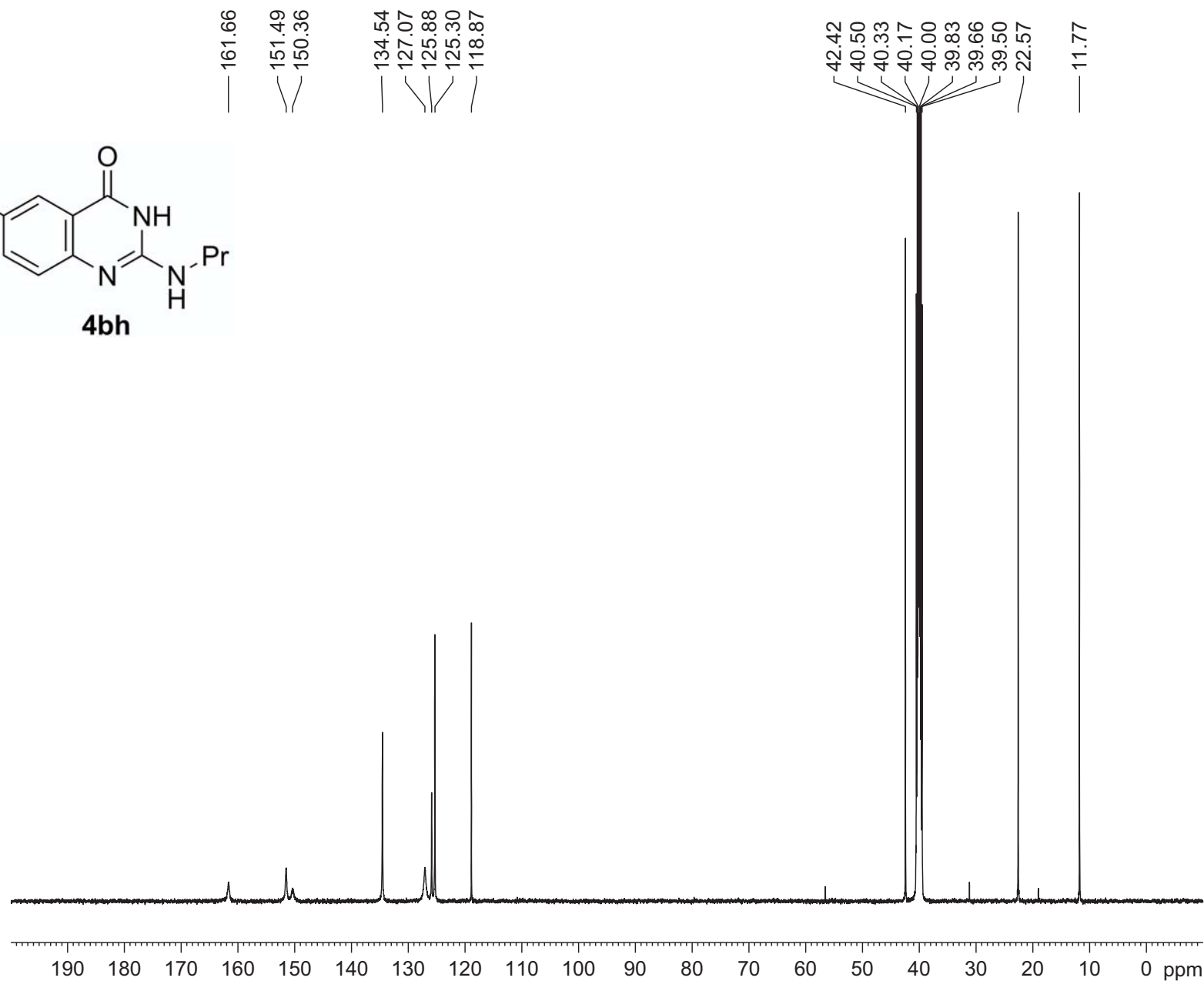
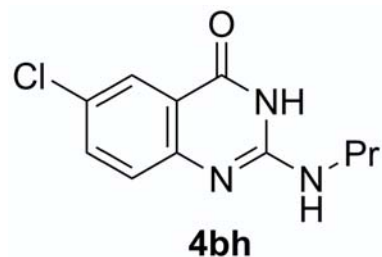
Current Data Parameters
 NAME TCC-20140603
 EXPNO 27
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140612
 Time 15.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 71.8
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX 106 recrystallized



Current Data Parameters
 NAME TCC-20140603
 EXPNO 28
 PROCNO 1

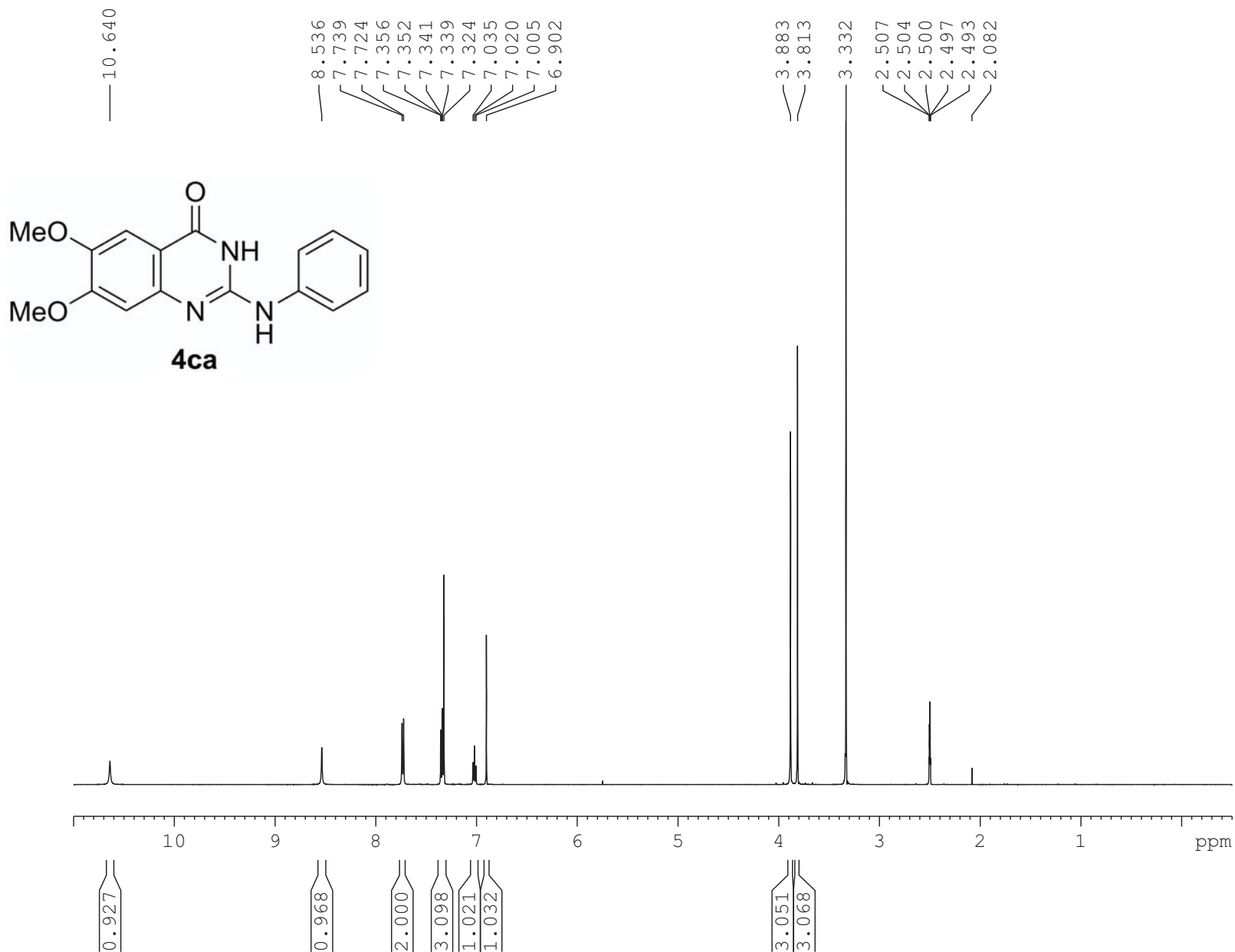
F2 - Acquisition Parameters
 Date_ 20140612
 Time 15.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 11629
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577852 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

¹H of RX92 recrystallized



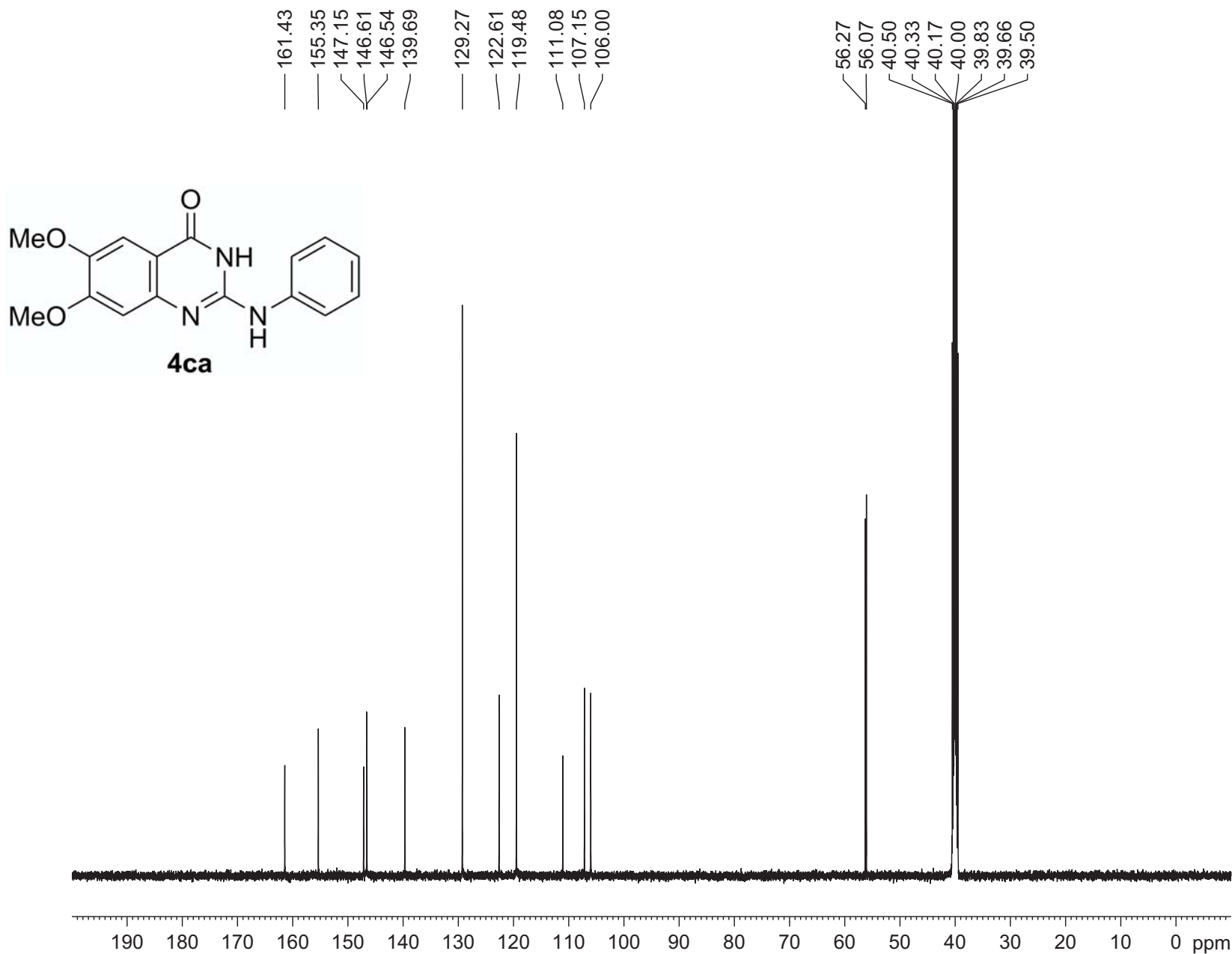
Current Data Parameters
 NAME TCC-20140424
 EXPNO 17
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140502
 Time 12.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 161.3
 DW 55.200 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

¹³C of RX92 recrystallized



Current Data Parameters
 NAME TCC-20140424
 EXPNO 18
 PROCNO 1

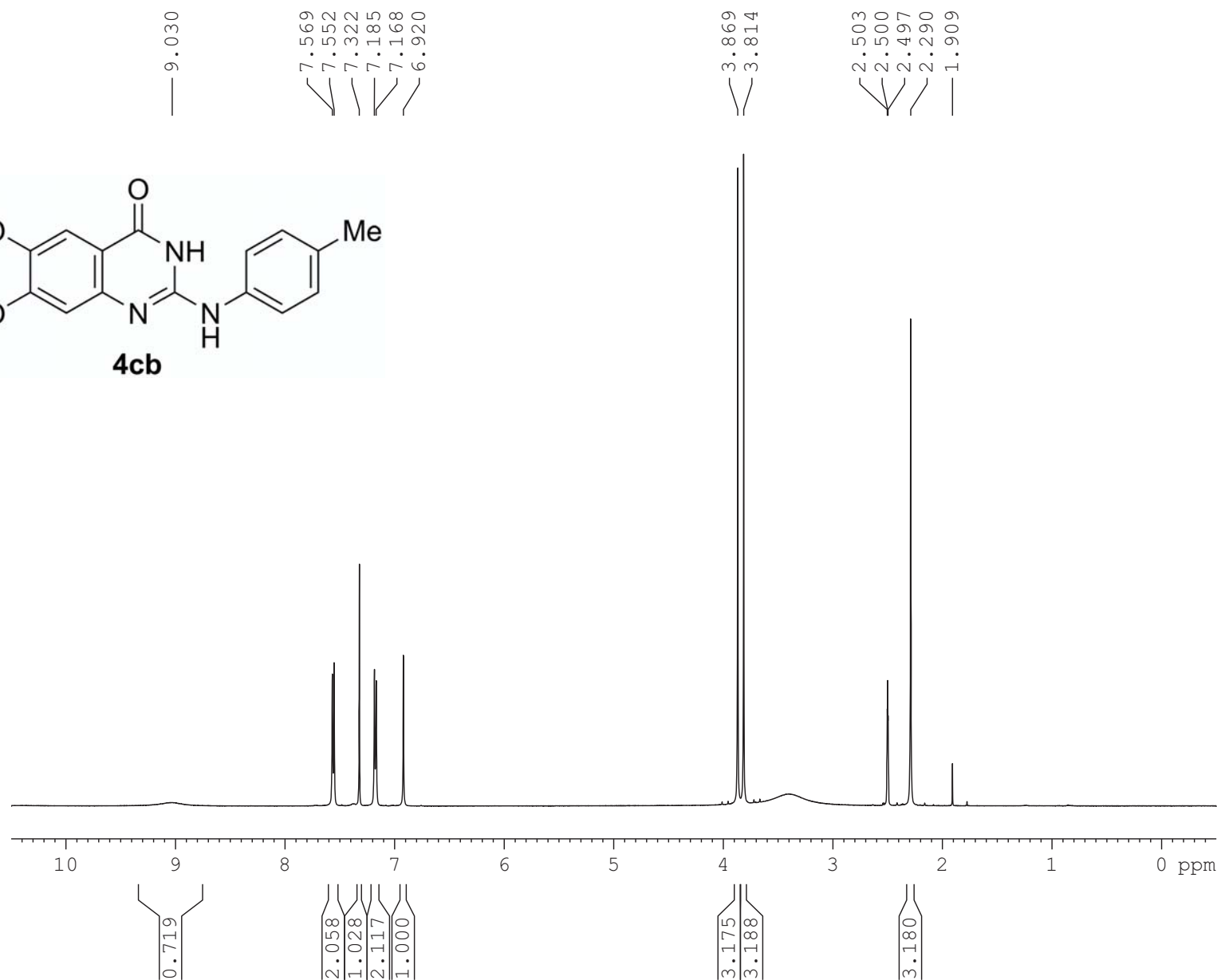
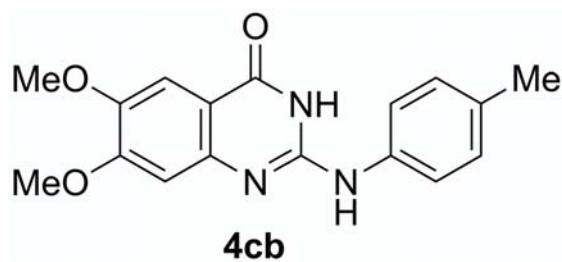
F2 - Acquisition Parameters
 Date_ 20140502
 Time 11.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2310
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577894 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of RM167d



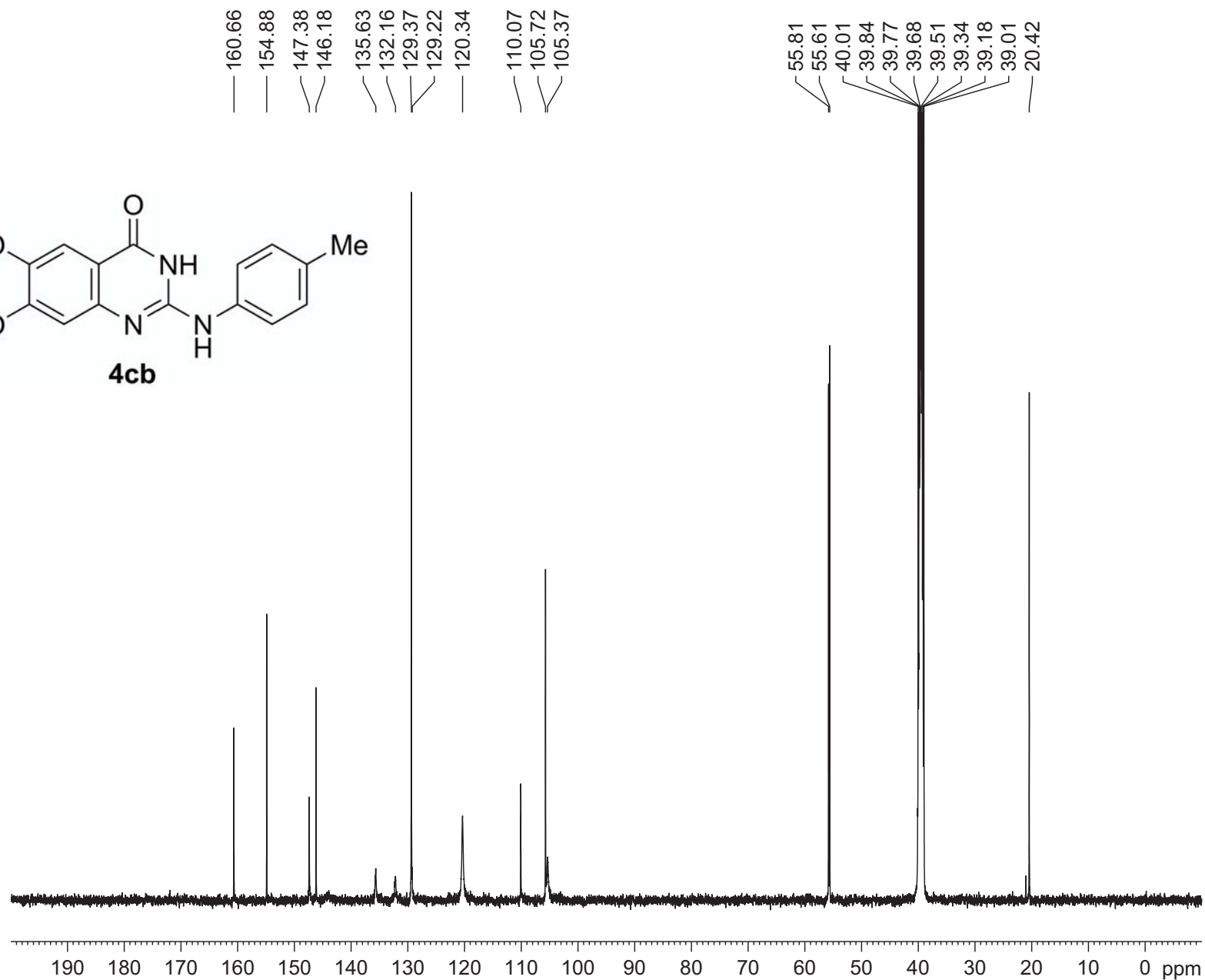
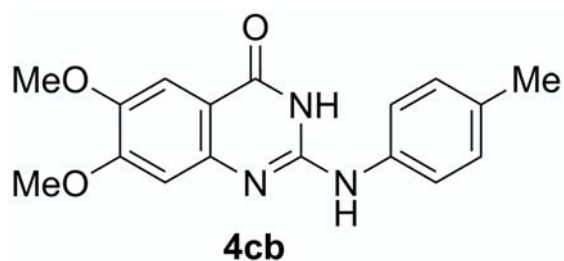
Current Data Parameters
NAME 2013120115
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20131210
Time 10.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of RM167d



Current Data Parameters
 NAME 2013120115
 EXPNO 2
 PROCNO 1

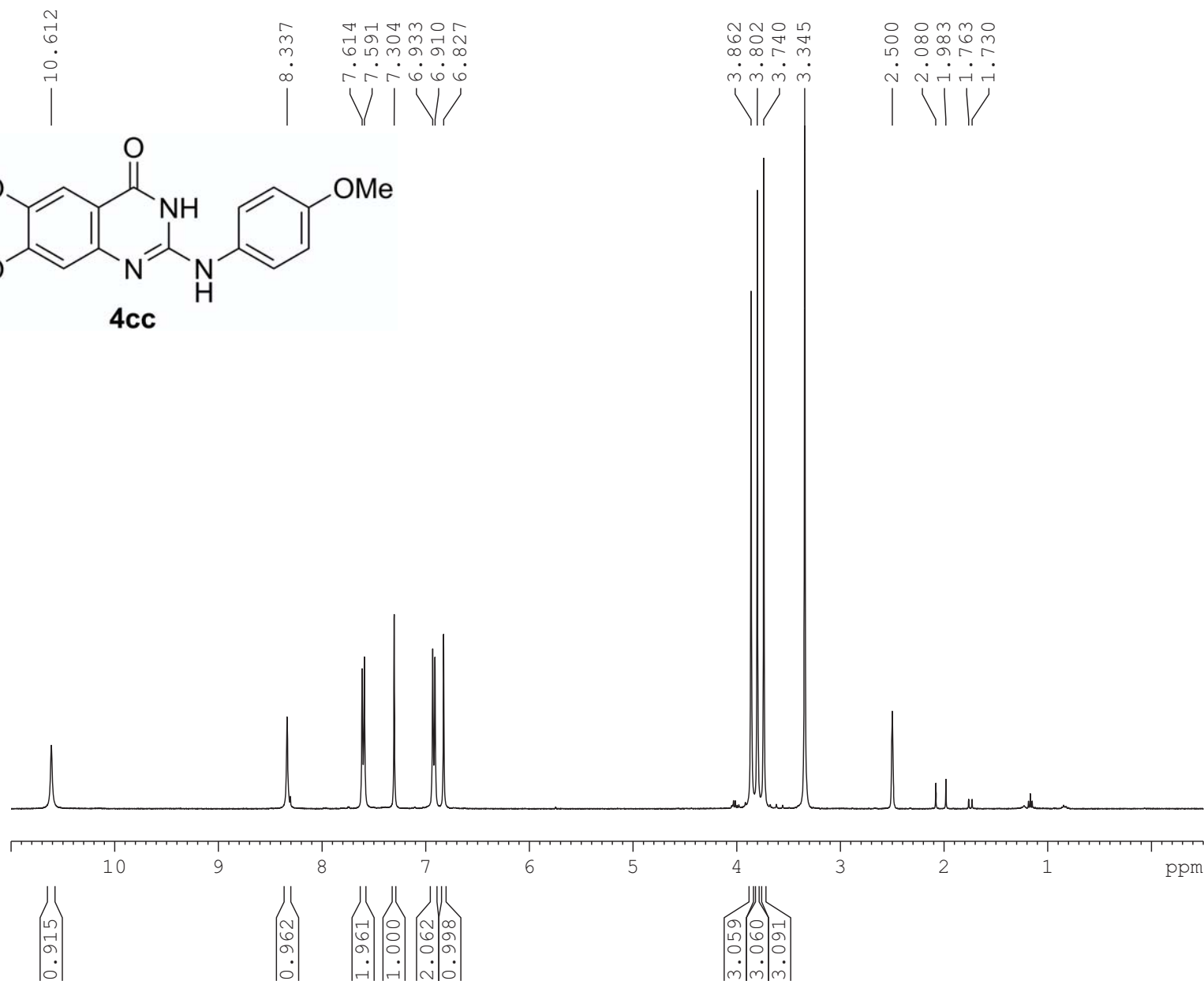
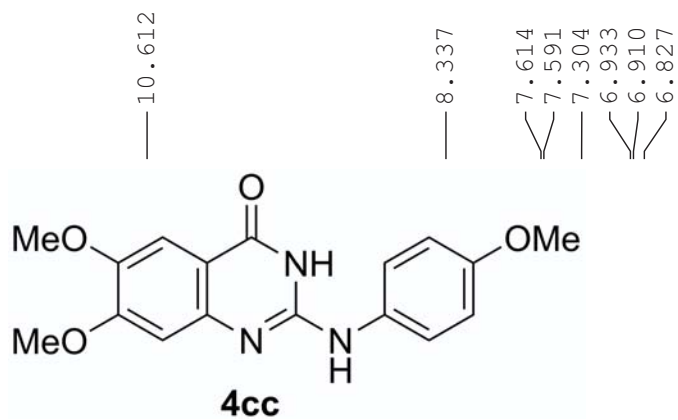
F2 - Acquisition Parameters
 Date_ 20131210
 Time 10.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 6260
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 5792.6
 DW 16.500 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578520 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

1H after adding



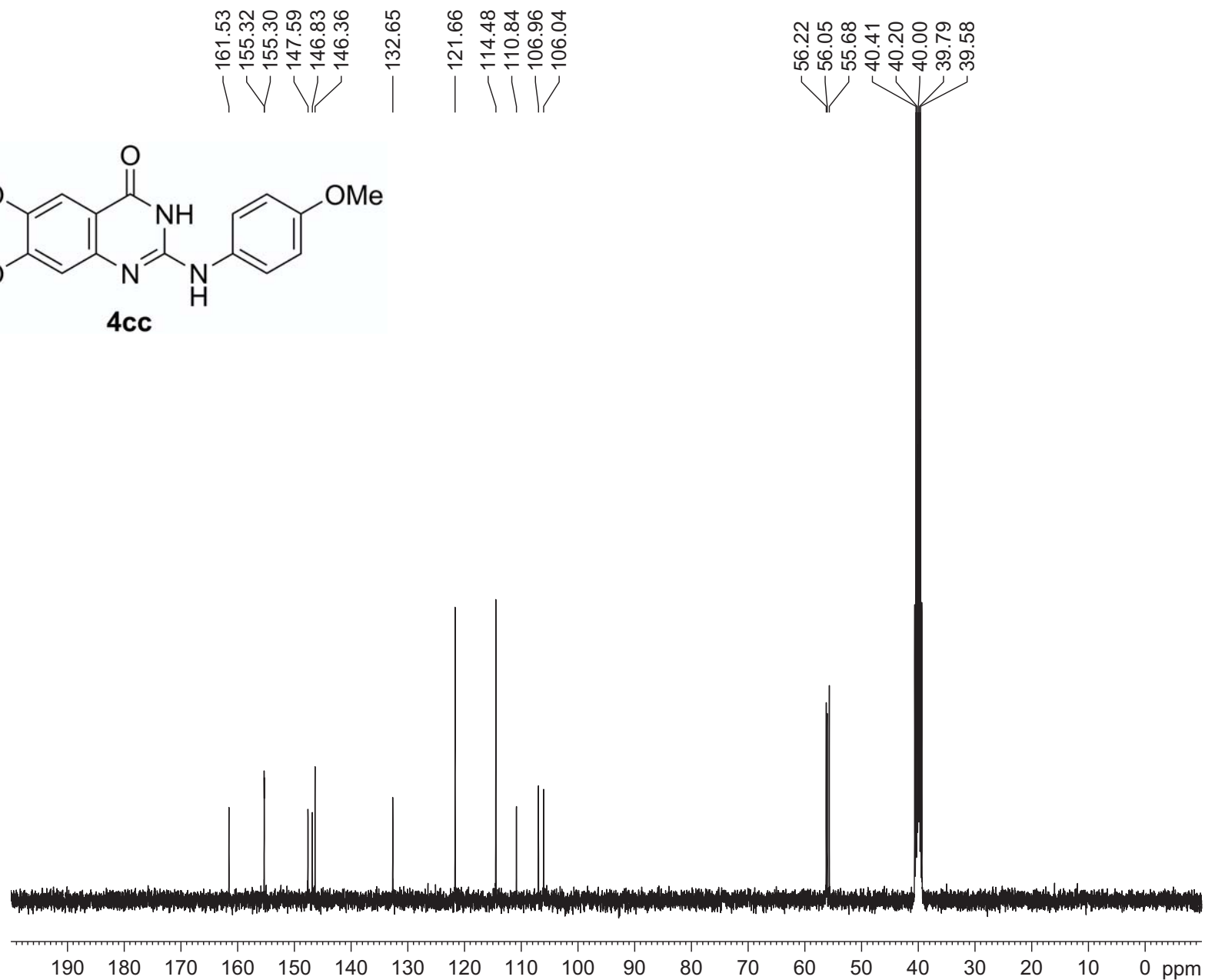
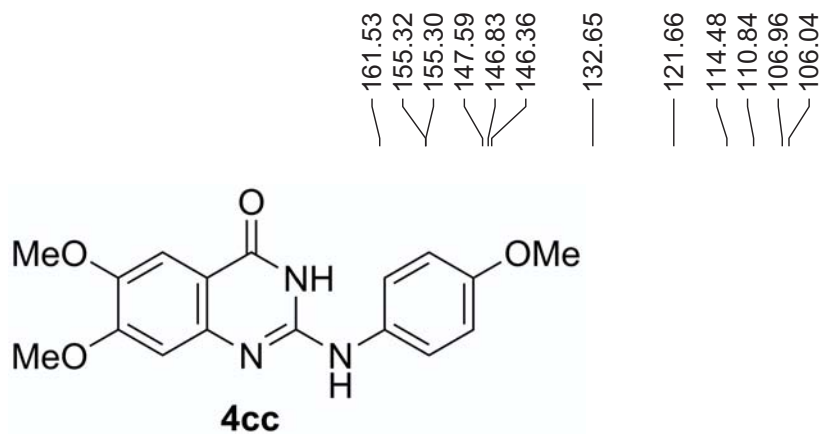
Current Data Parameters
NAME RX85 recrystallized
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140422
Time 9.35
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C after adding



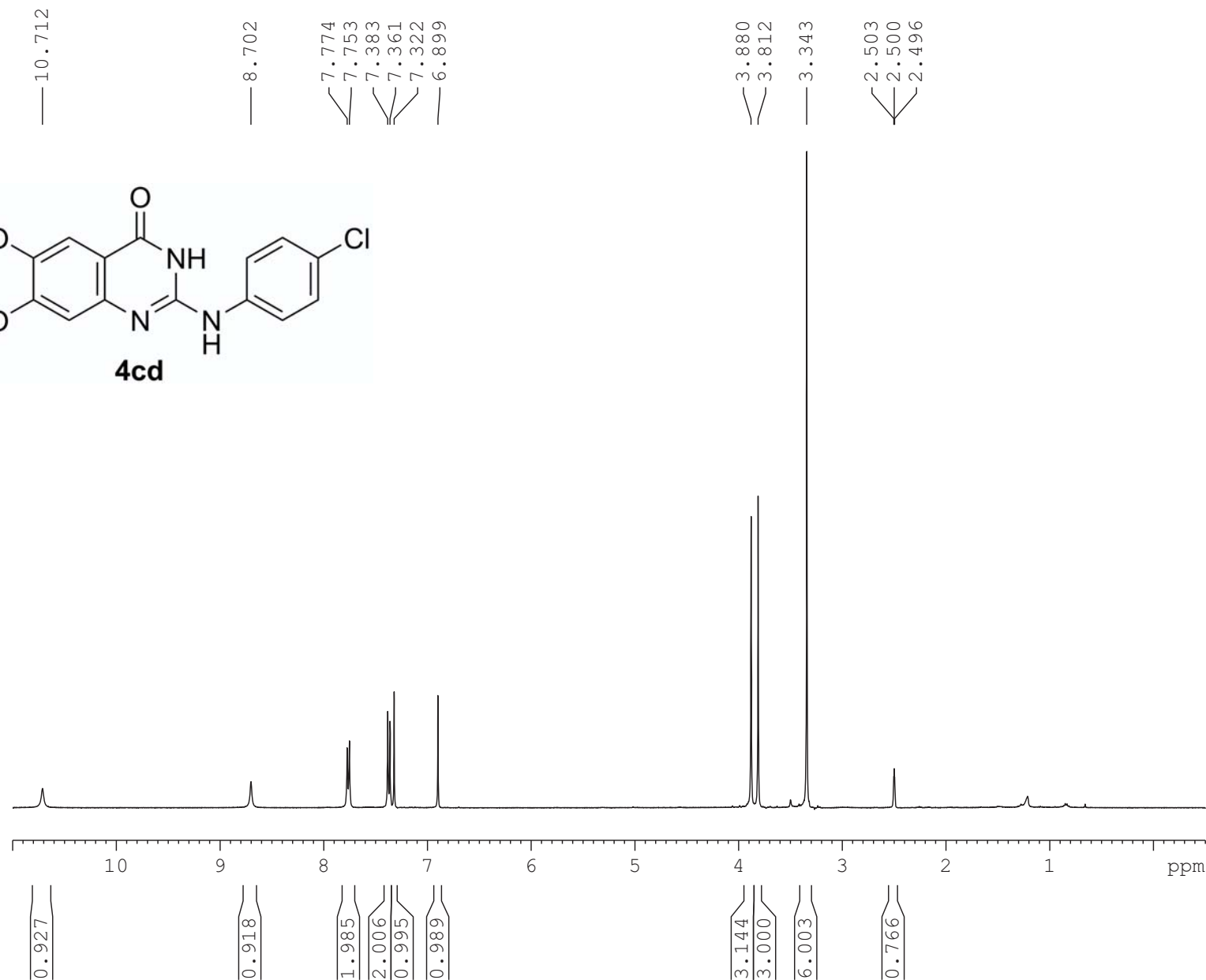
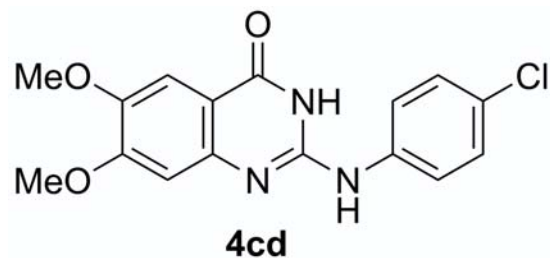
Current Data Parameters
NAME RX85 recrystallized
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140422
Time 12.26
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 5.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127677 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

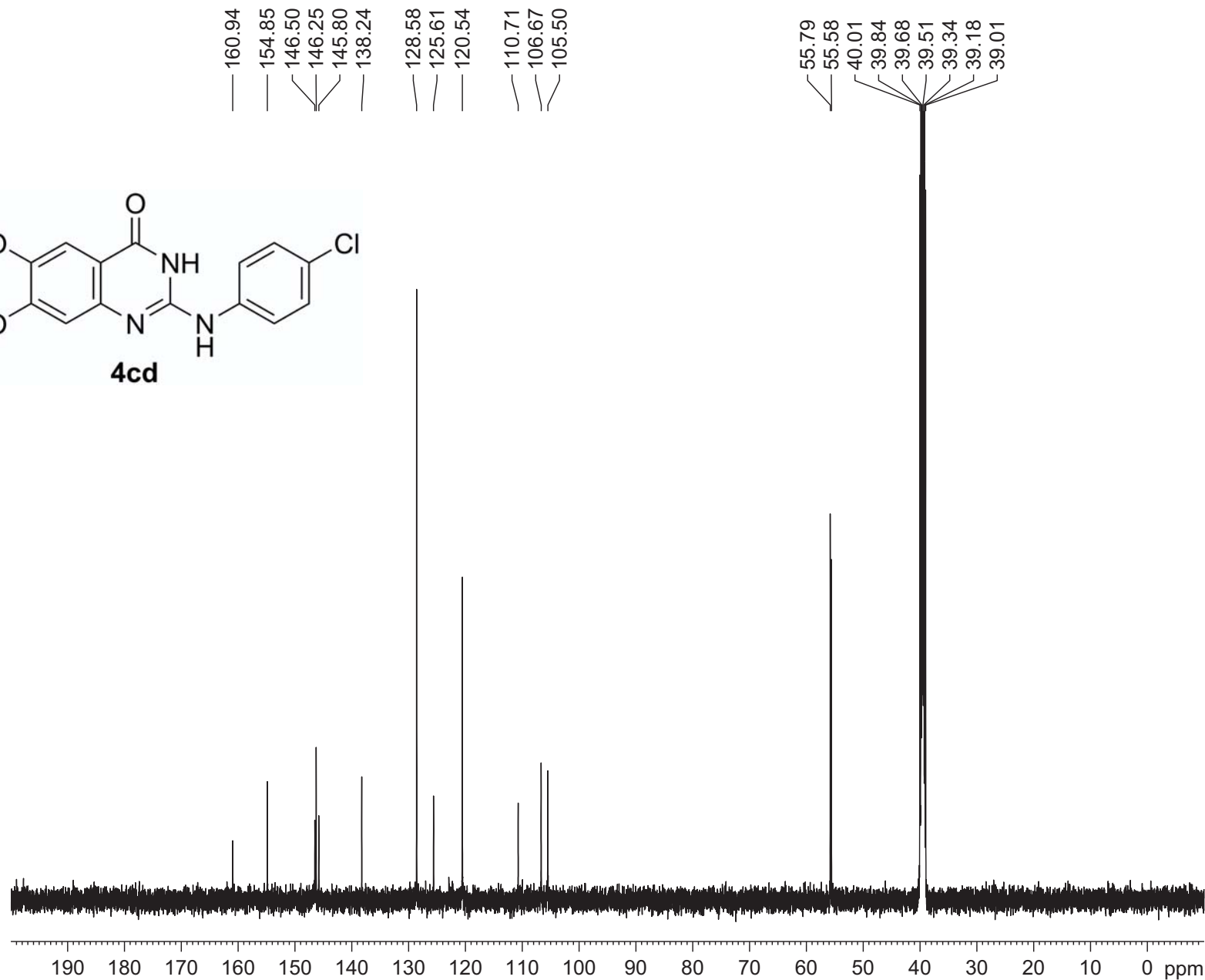
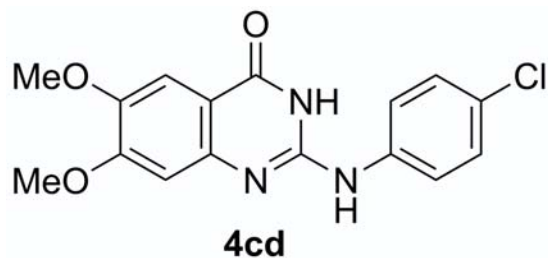


Current Data Parameters
 NAME RM080
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120911
 Time 15.38
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 161.3
 DW 69.000 usec
 DE 6.50 usec
 TE 298.9 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 11.70 usec
 PL1 4.00 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300016 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME RM080
 EXPNO 2
 PROCNO 1

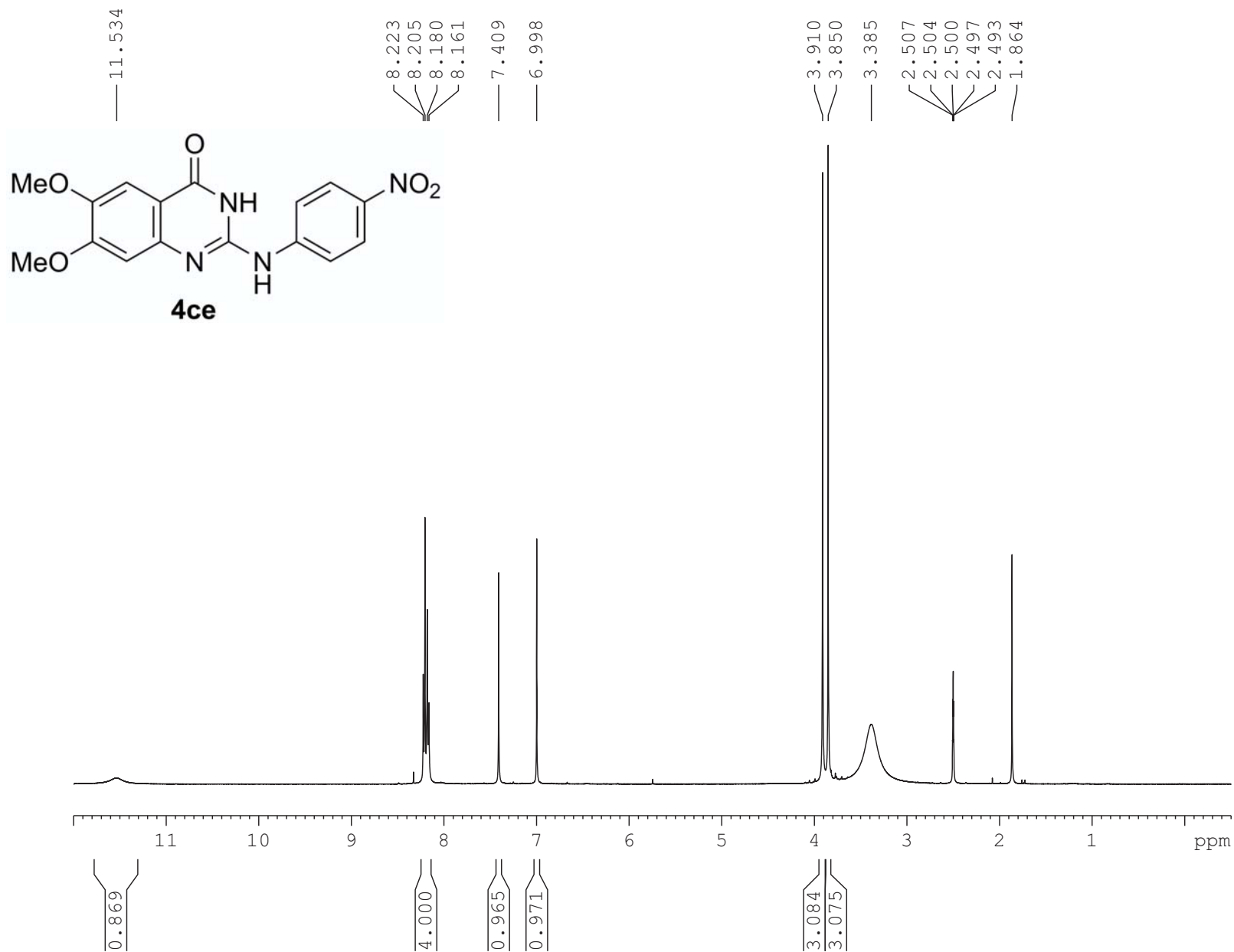
F2 - Acquisition Parameters
 Date_ 20120912
 Time 21.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 450
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0911744 sec
 RG 4096
 DW 16.650 usec
 DE 6.50 usec
 TE 295.9 K
 D1 4.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.50 usec
 PL1 7.00 dB
 SFO1 125.7709931 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.00 dB
 PL13 18.00 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7578495 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of RX102 recrystallized



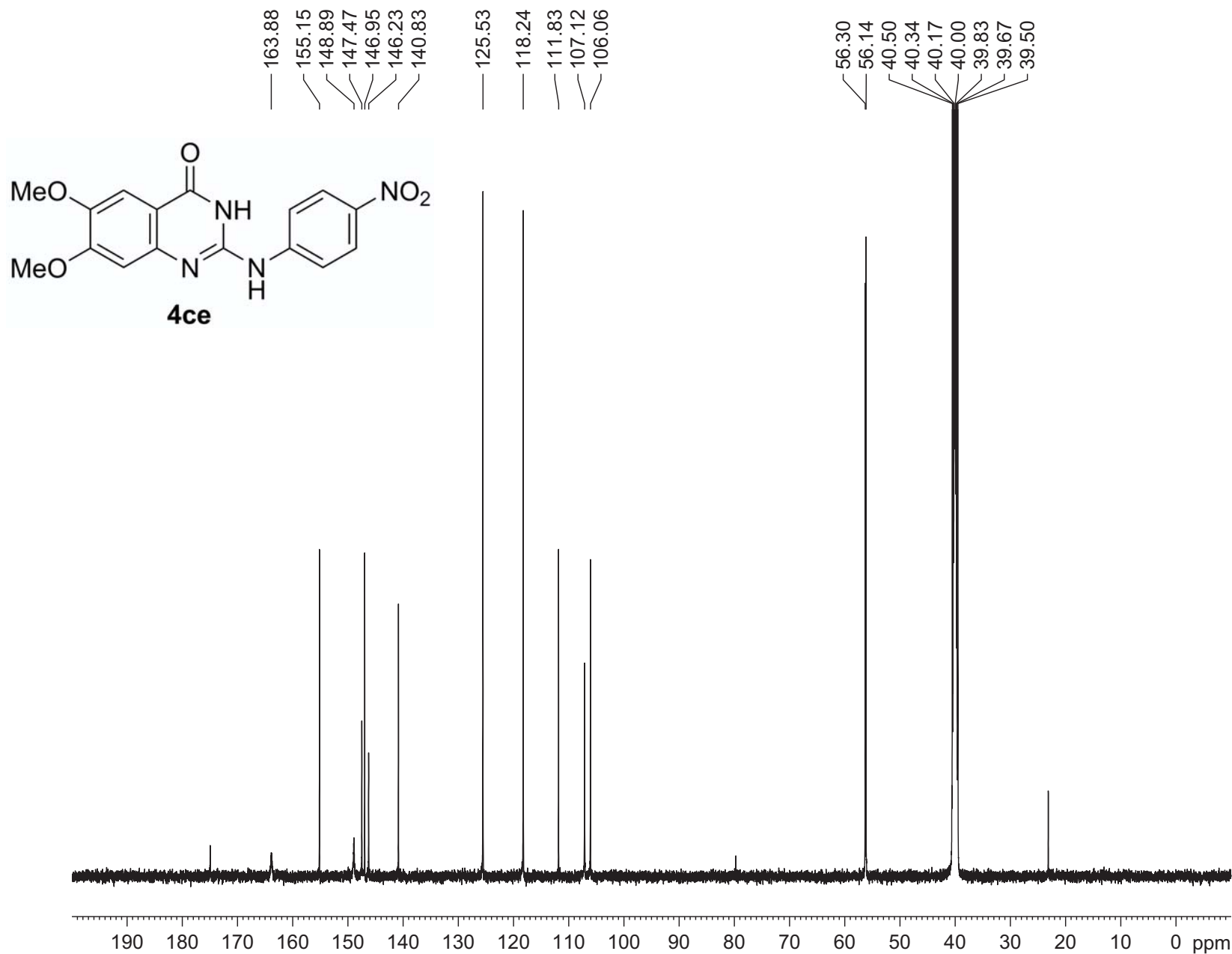
Current Data Parameters
 NAME TCC-20140424
 EXPNO 23
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140505
 Time 16.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.276427 Hz
 AQ 1.8087935 sec
 RG 128
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of RX102 recrystallized



Current Data Parameters
NAME TCC-20140424
EXPNO 24
PROCNO 1

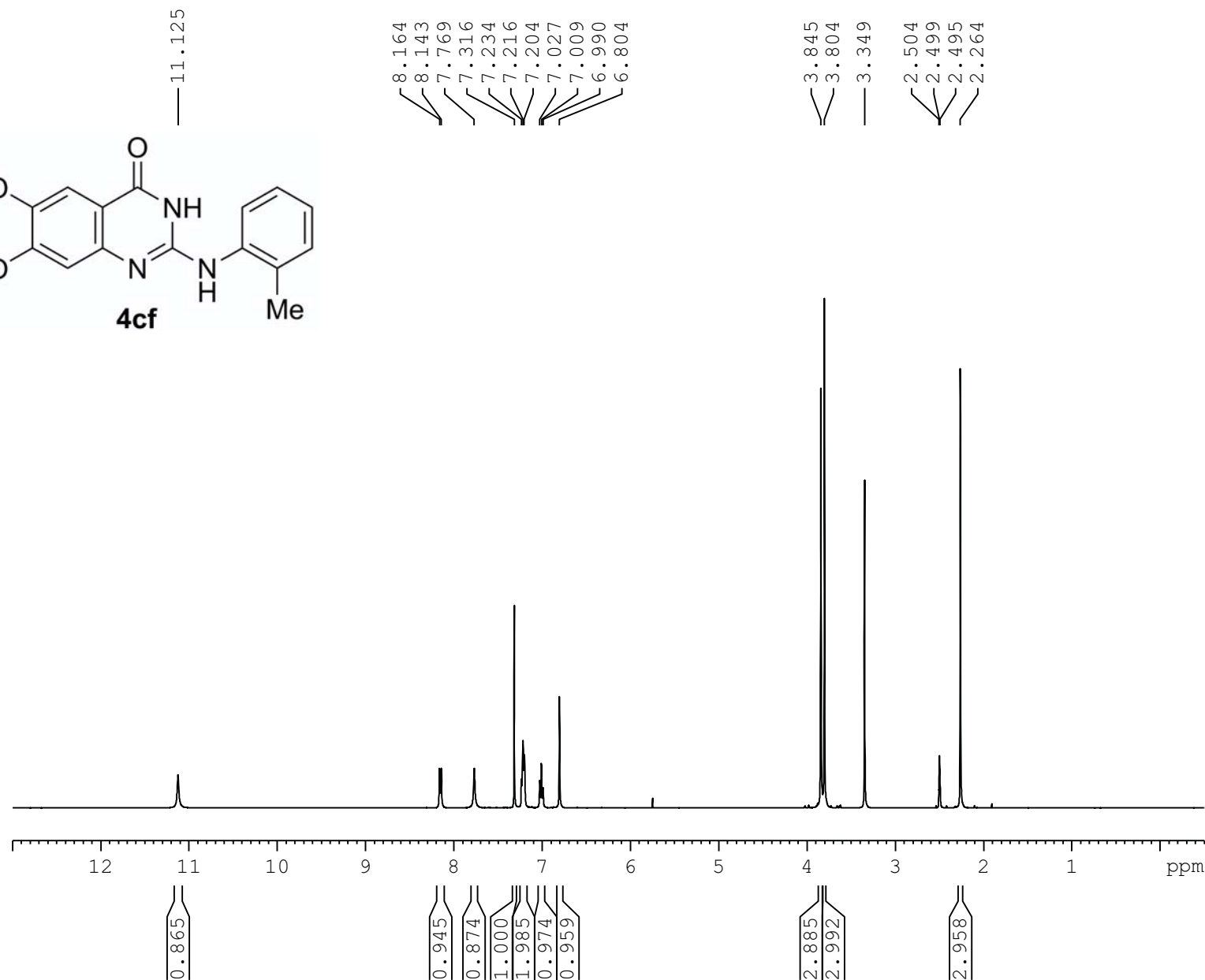
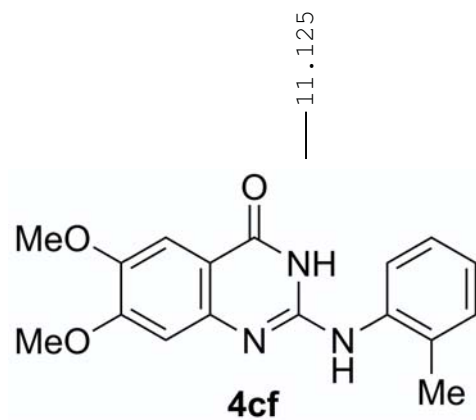
F2 - Acquisition Parameters
Date_ 20140505
Time 9.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 7835
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577852 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H



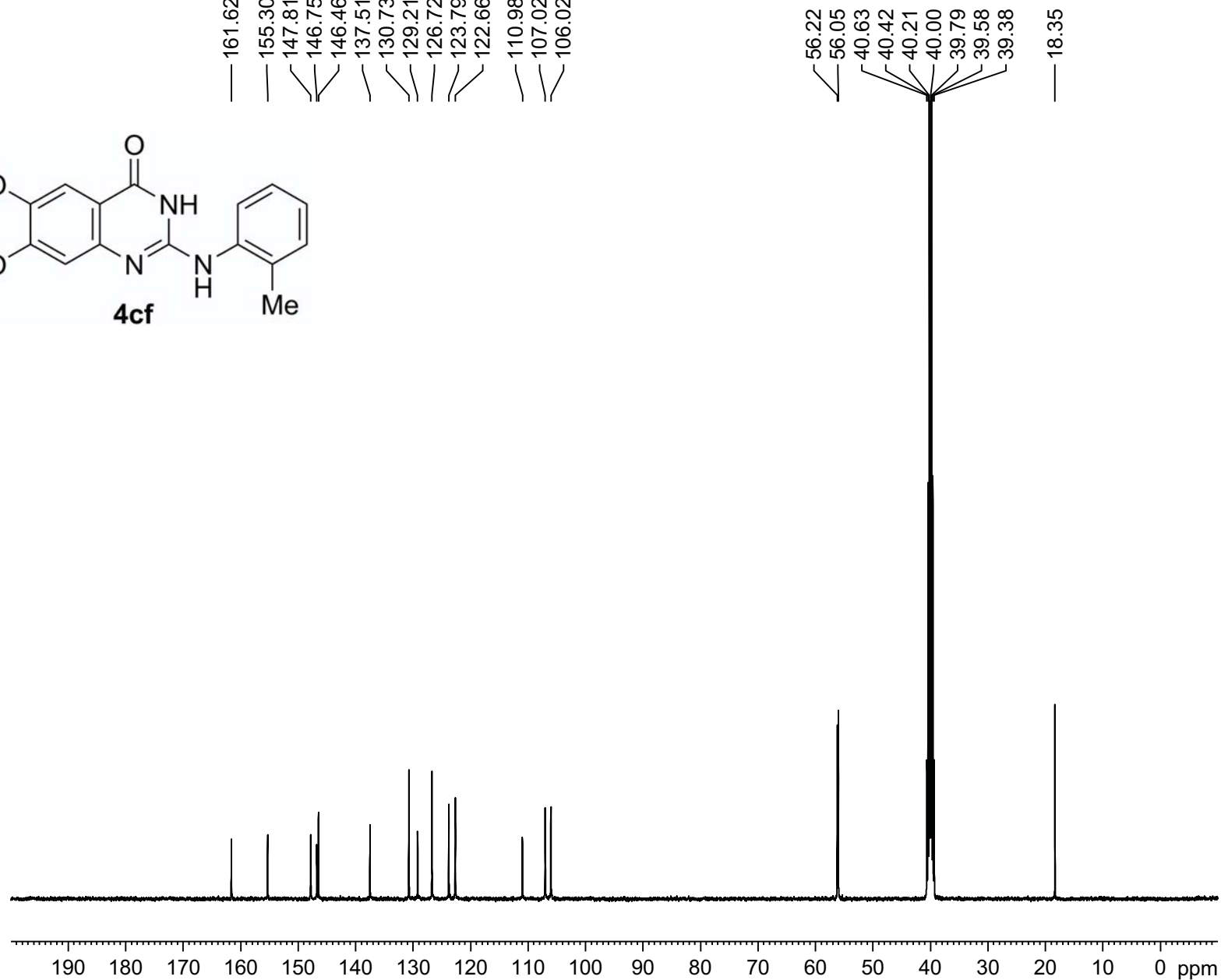
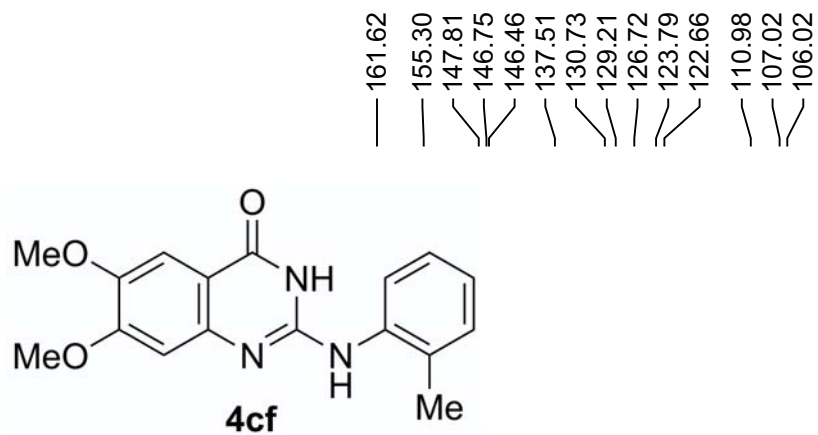
Current Data Parameters
NAME RX184 recrystall
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141201
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C



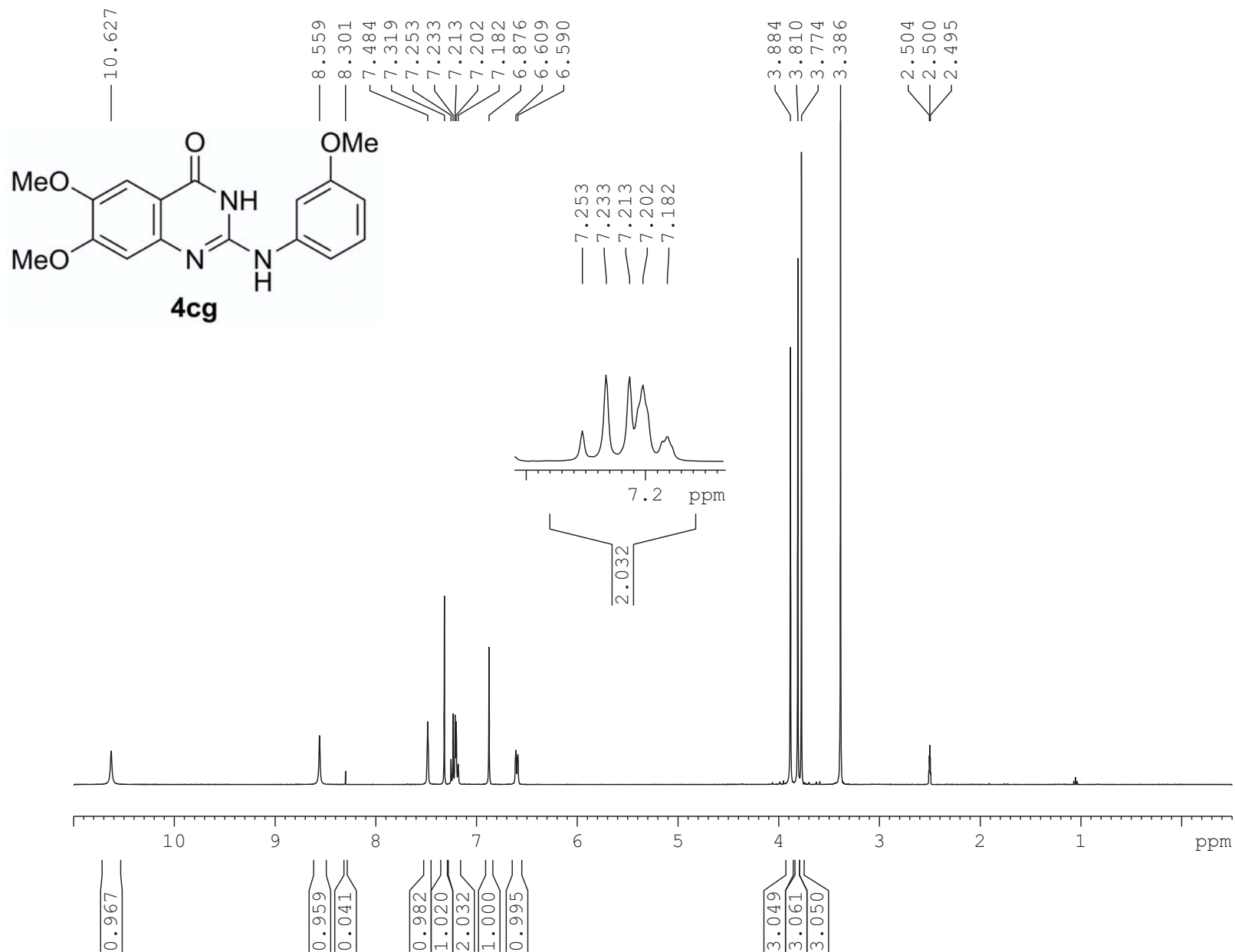
Current Data Parameters
 NAME RX184 recrystall
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141201
 Time 17.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 1913
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 299.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6233319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 15.00000000 W
 PLW12 0.34252000 W
 PLW13 0.27744001 W

F2 - Processing parameters
 SI 32768
 SF 100.6127692 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

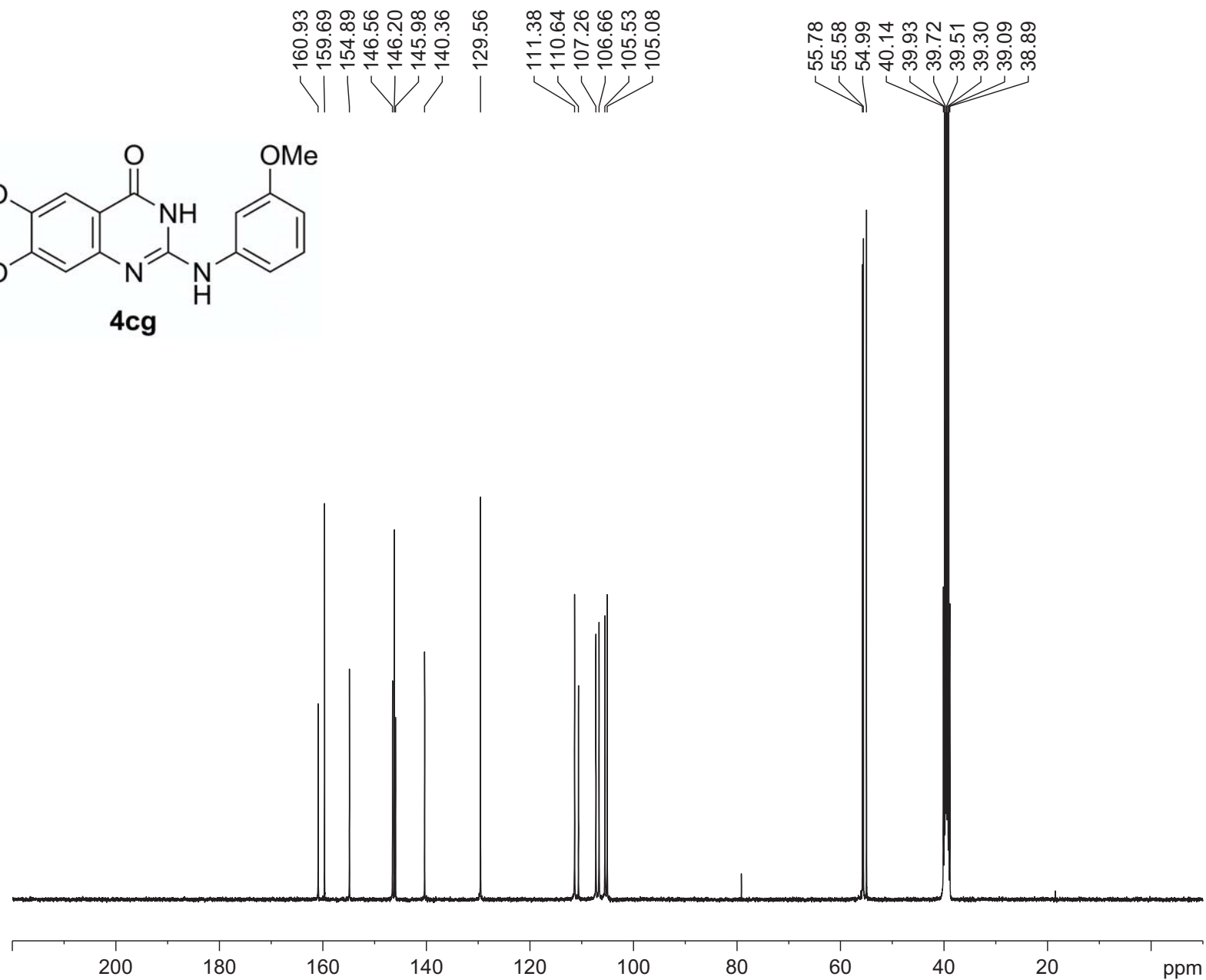


Current Data Parameters
 NAME SC158
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140724
 Time 11.11
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 64
 DW 69.000 usec
 DE 6.50 usec
 TE 297.8 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300035 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

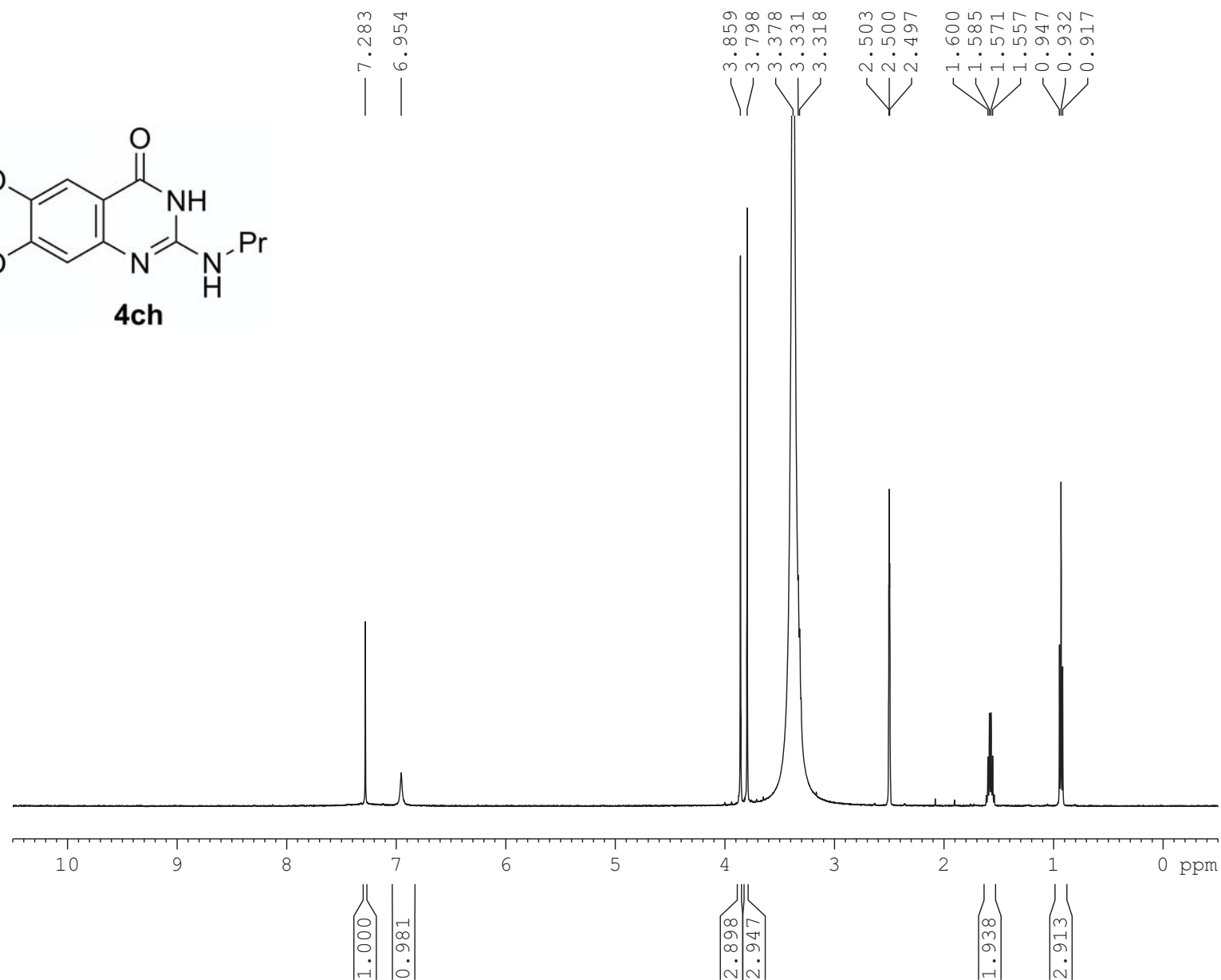
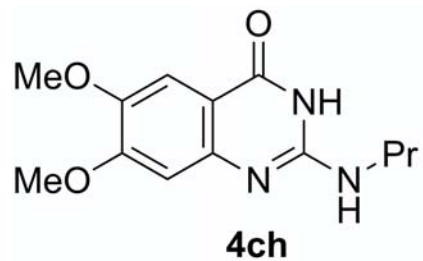


NAME SC158
 EXPNO 2
 PROCNO 1
 Date_ 20140721
 Time 9.35
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 14672
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6816452 sec
 RG 2048
 DW 20.800 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.70 dB
 SFO1 100.623325 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -5.85 dB
 PL12 9.10 dB
 PL13 12.10 dB
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6128154 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of RX 107 recrystallized



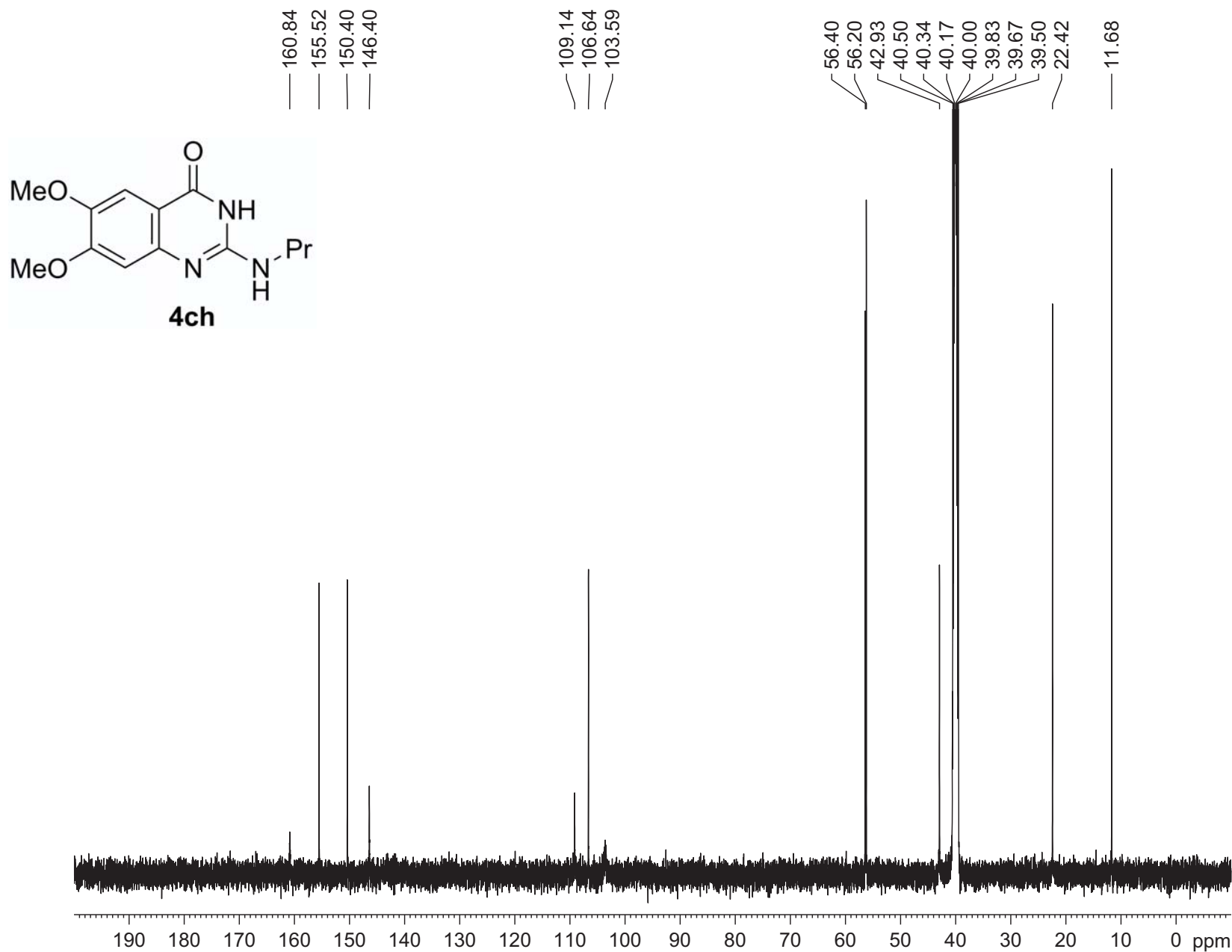
Current Data Parameters
NAME TCC-20140603
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140616
Time 10.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 71.8
DW 55.200 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of RX 107 recrystallized



Current Data Parameters
NAME TCC-20140603
EXPNO 25
PROCNO 1

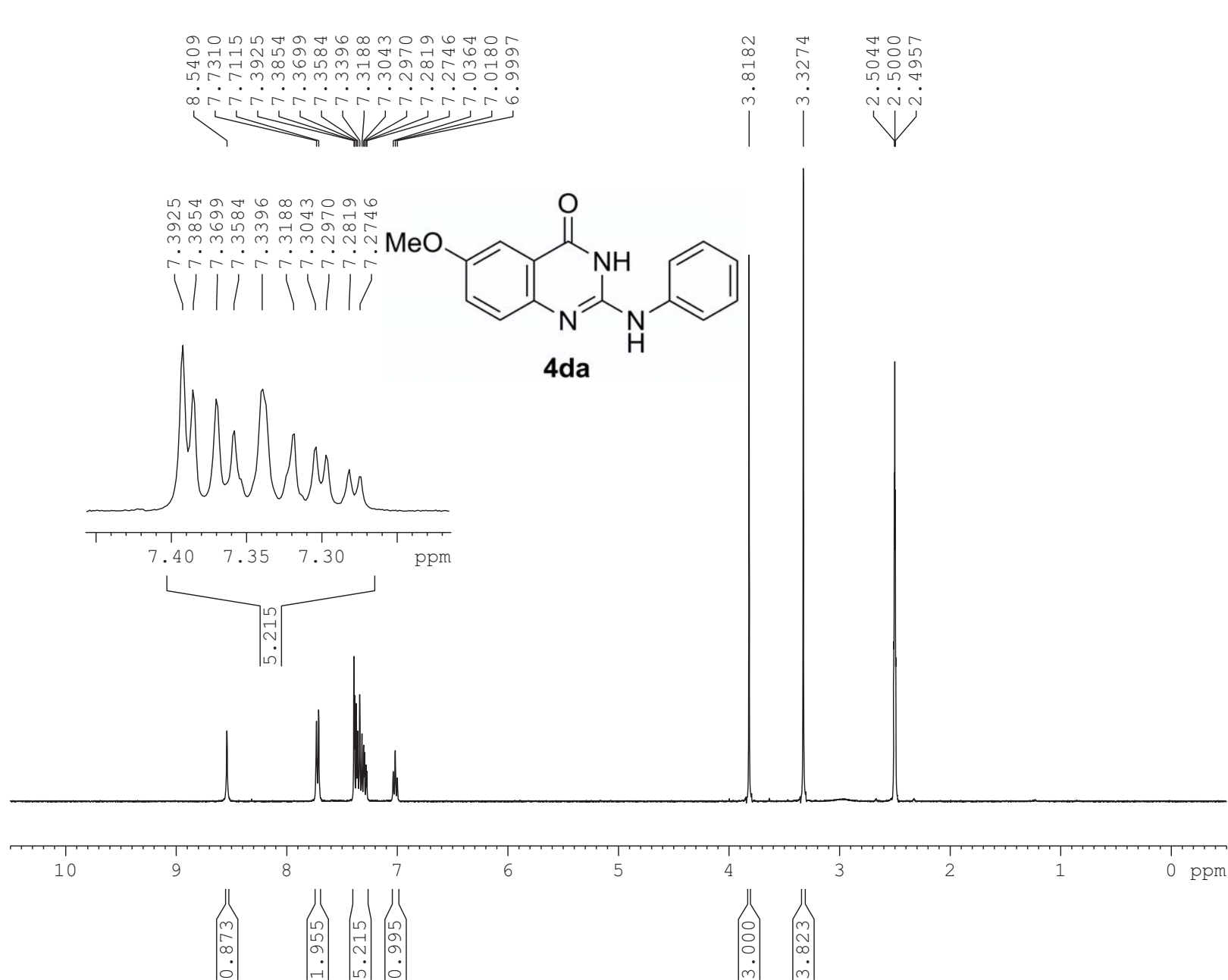
F2 - Acquisition Parameters
Date_ 20140616
Time 10.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5205
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577838 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

H of



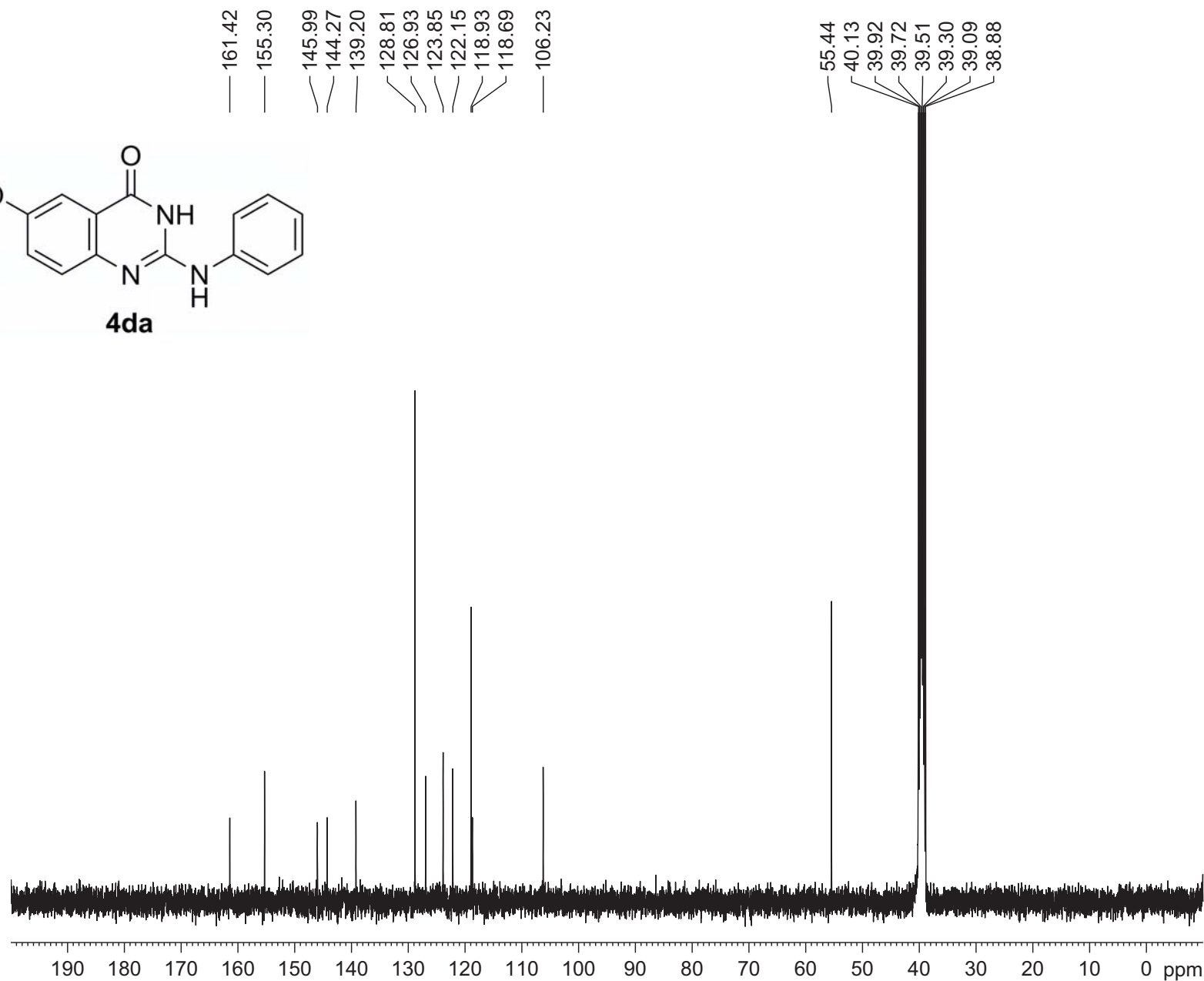
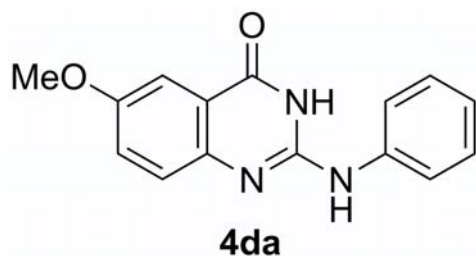
Current Data Parameters
 NAME TO012
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160910
 Time 16.22
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 456.1
 DW 69.000 usec
 DE 6.50 usec
 TE 296.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.40 usec
 PL1 1.80 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300026 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

13C of 2



Current Data Parameters

NAME TO012
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters

Date_ 20161118
Time 23.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

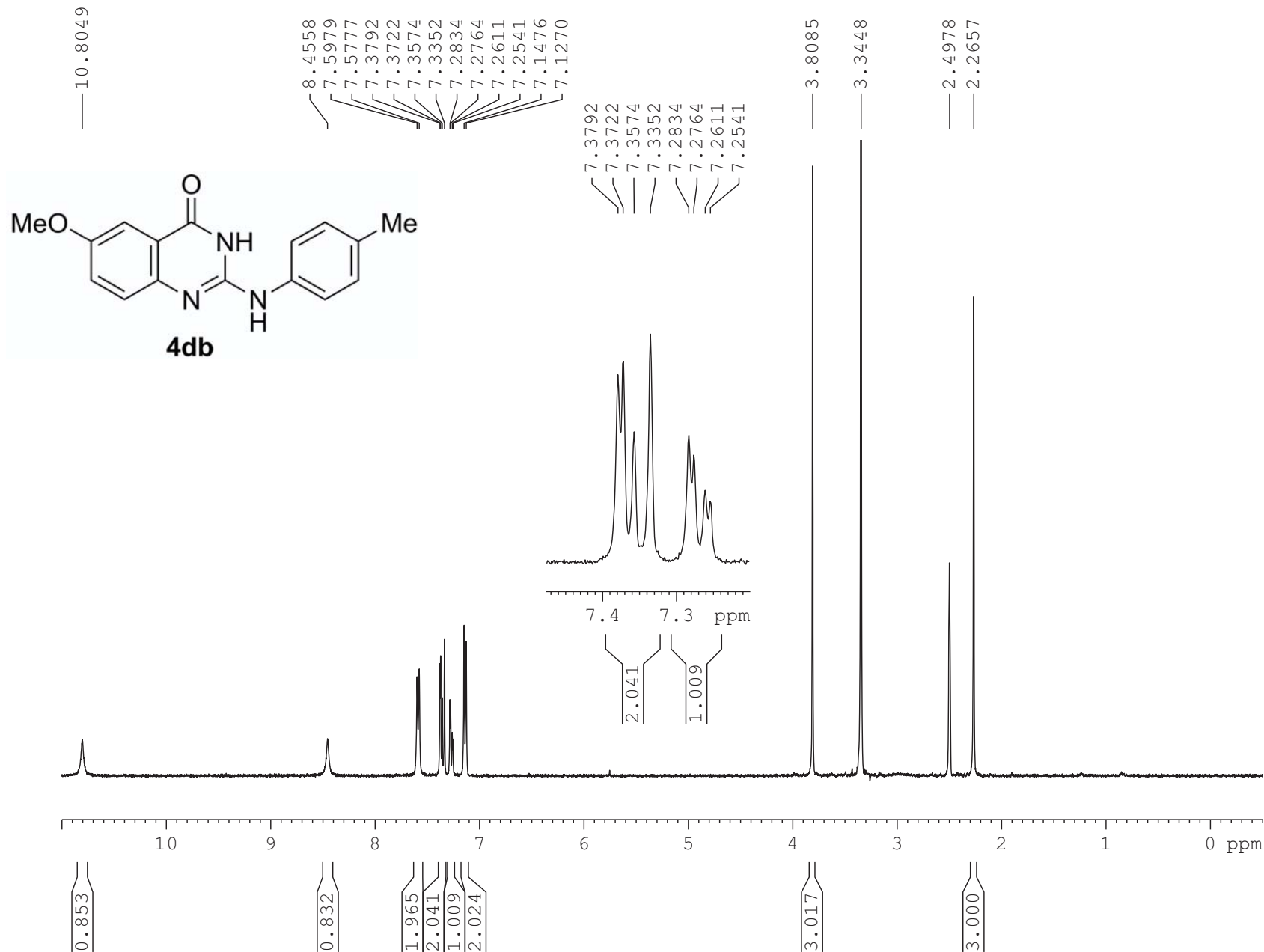
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128162 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1 H



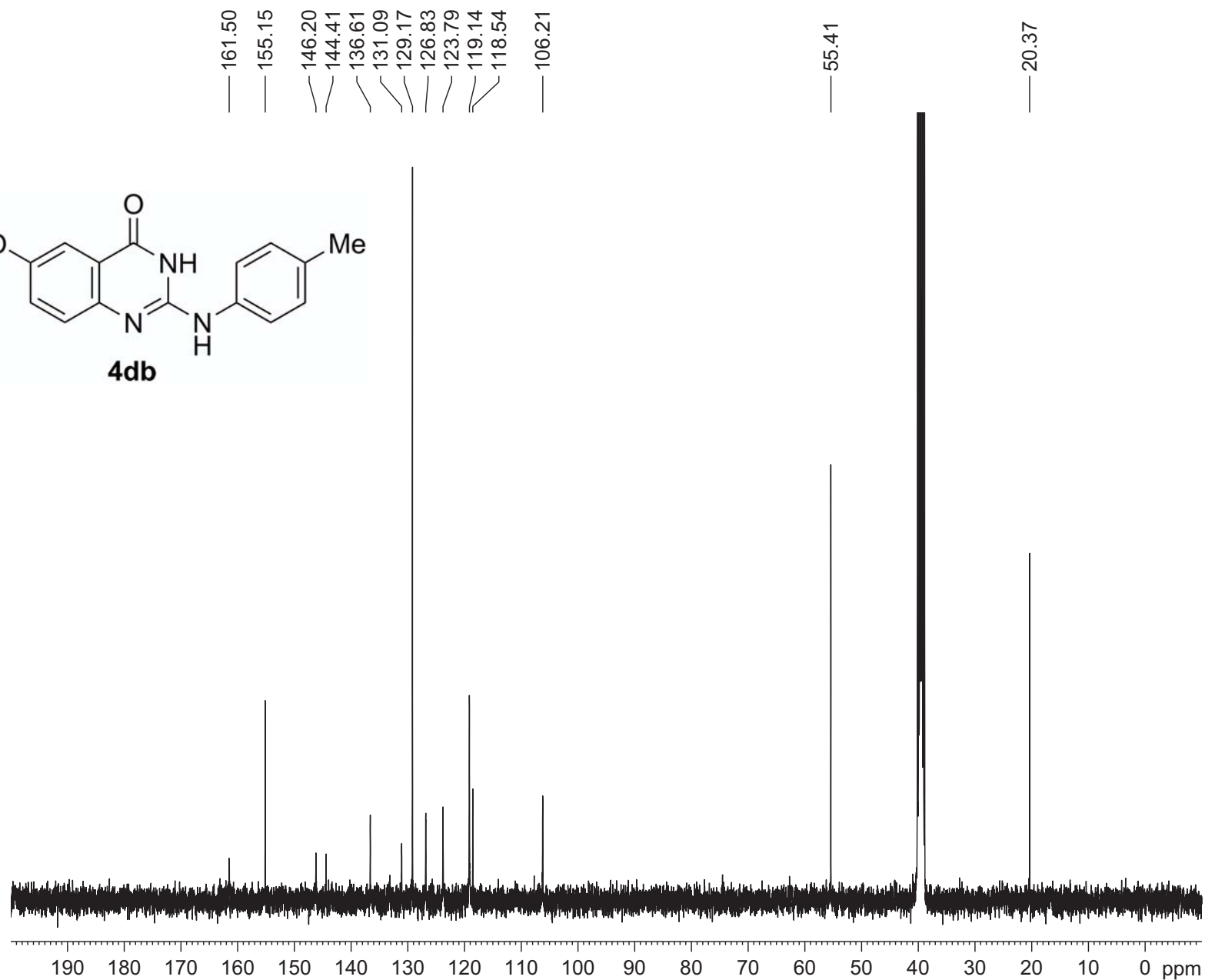
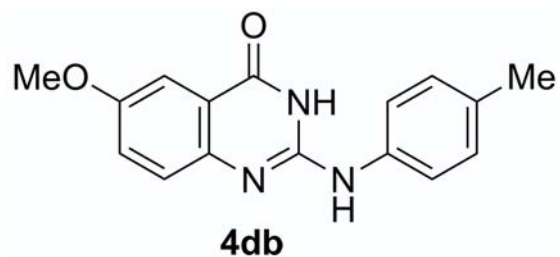
Current Data Parameters
NAME SI055-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141221
Time 11.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300038 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C



Current Data Parameters

NAME SI055-2
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141221
Time 11.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 ¹³C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

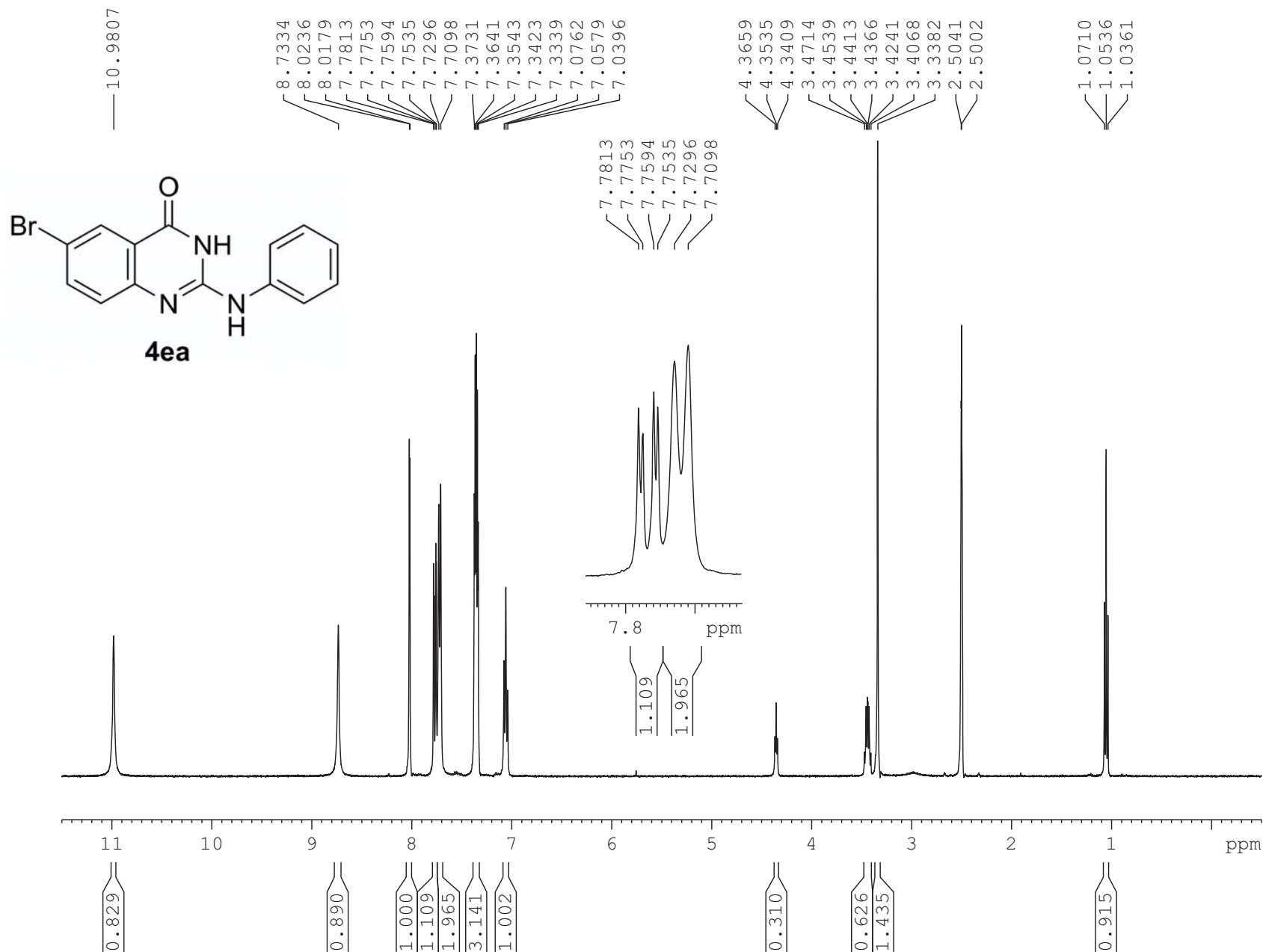
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128179 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

H of



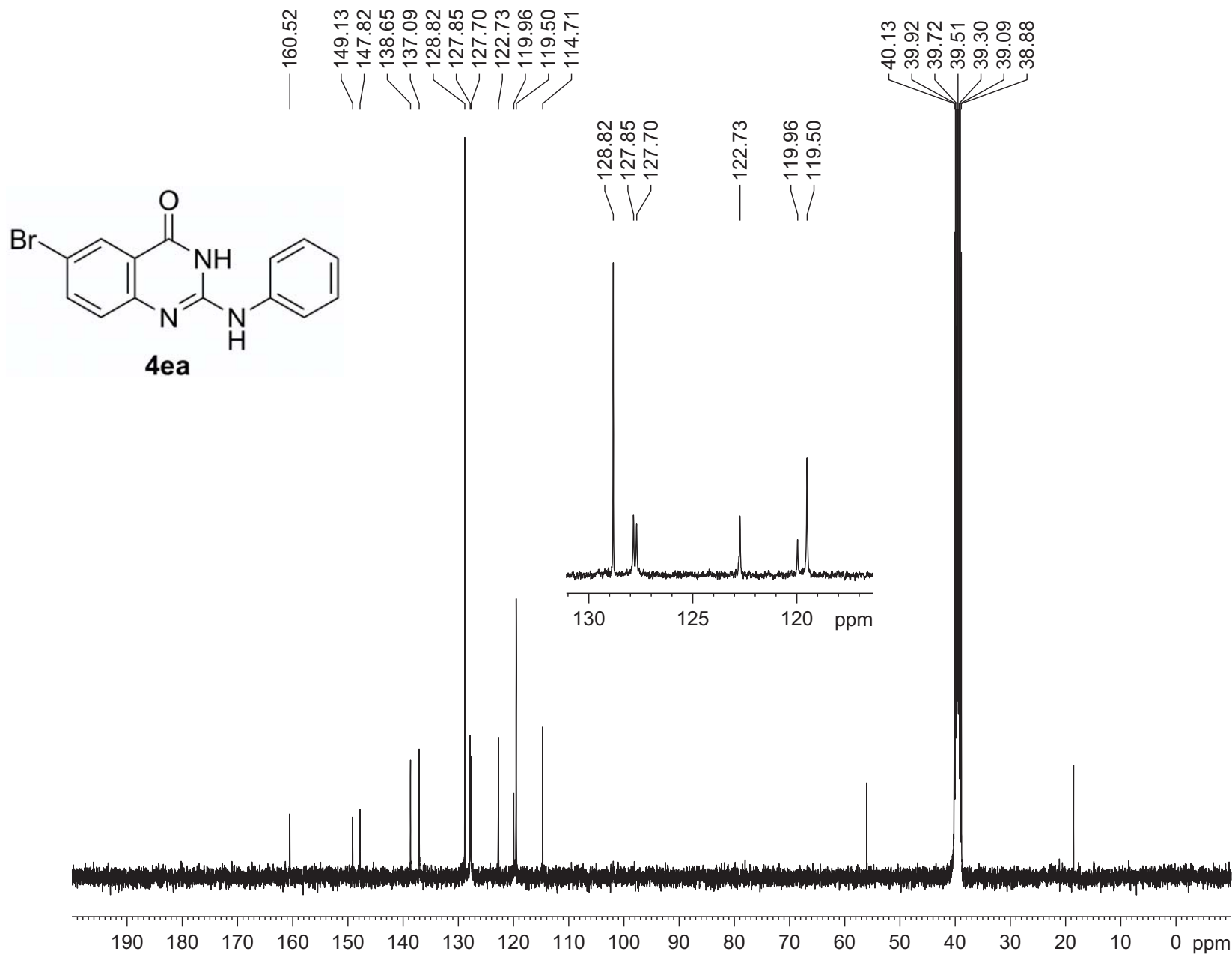
Current Data Parameters
 NAME TO031
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161207
 Time 21.56
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 228.1
 DW 69.000 usec
 DE 6.50 usec
 TE 296.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.40 usec
 PL1 1.80 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300026 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of 2



Current Data Parameters

NAME TO031
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

Date_ 20161208
Time 0.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 2000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 ¹³C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

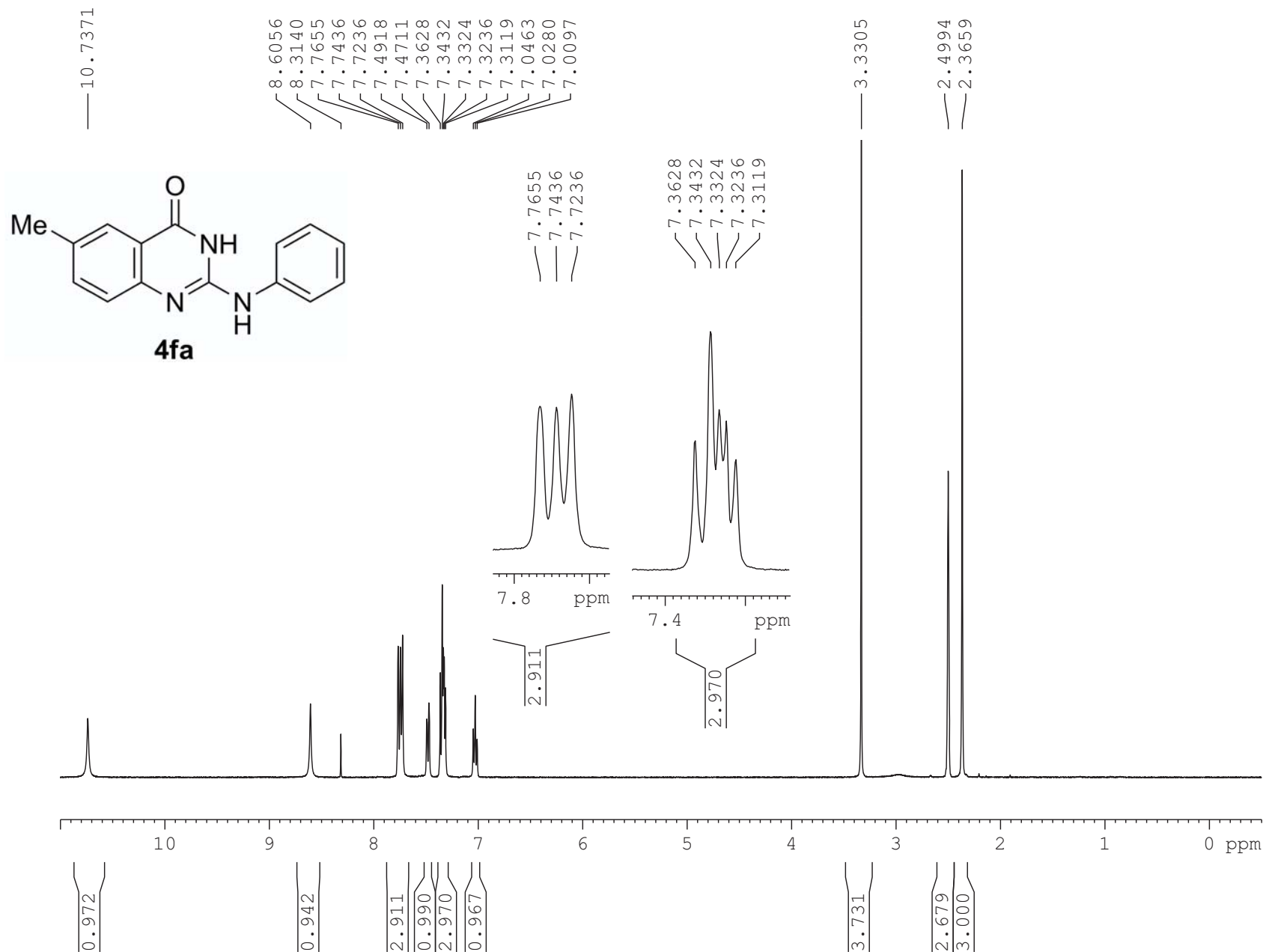
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128184 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

-2-s



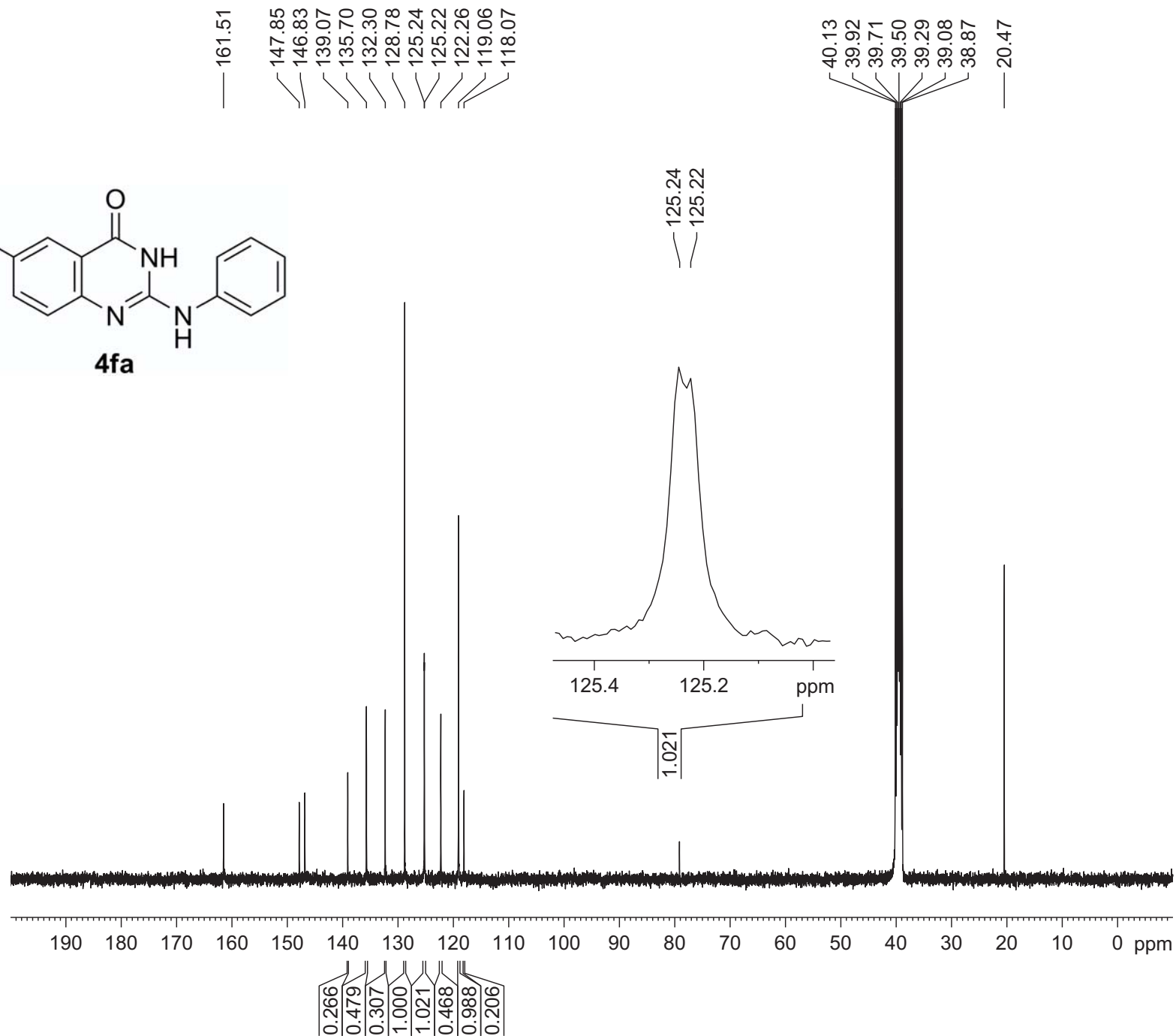
Current Data Parameters
NAME SG081
EXPNO 9
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141209
Time 2.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

1H -2-sit



Current Data Parameters

NAME SG081
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141209
Time 2.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 6616
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 11585.2
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

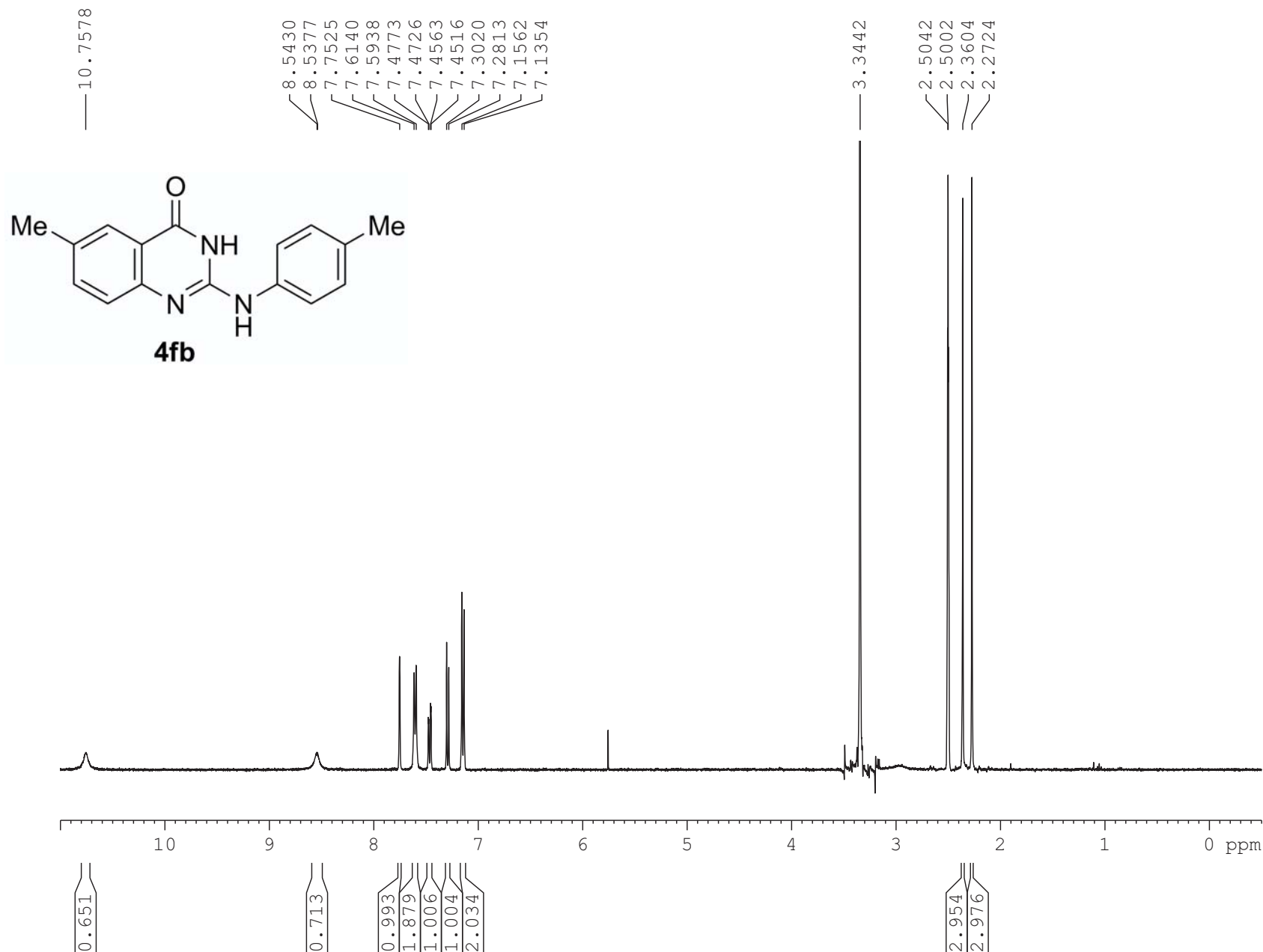
===== CHANNEL f2 =====

CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6128194 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of



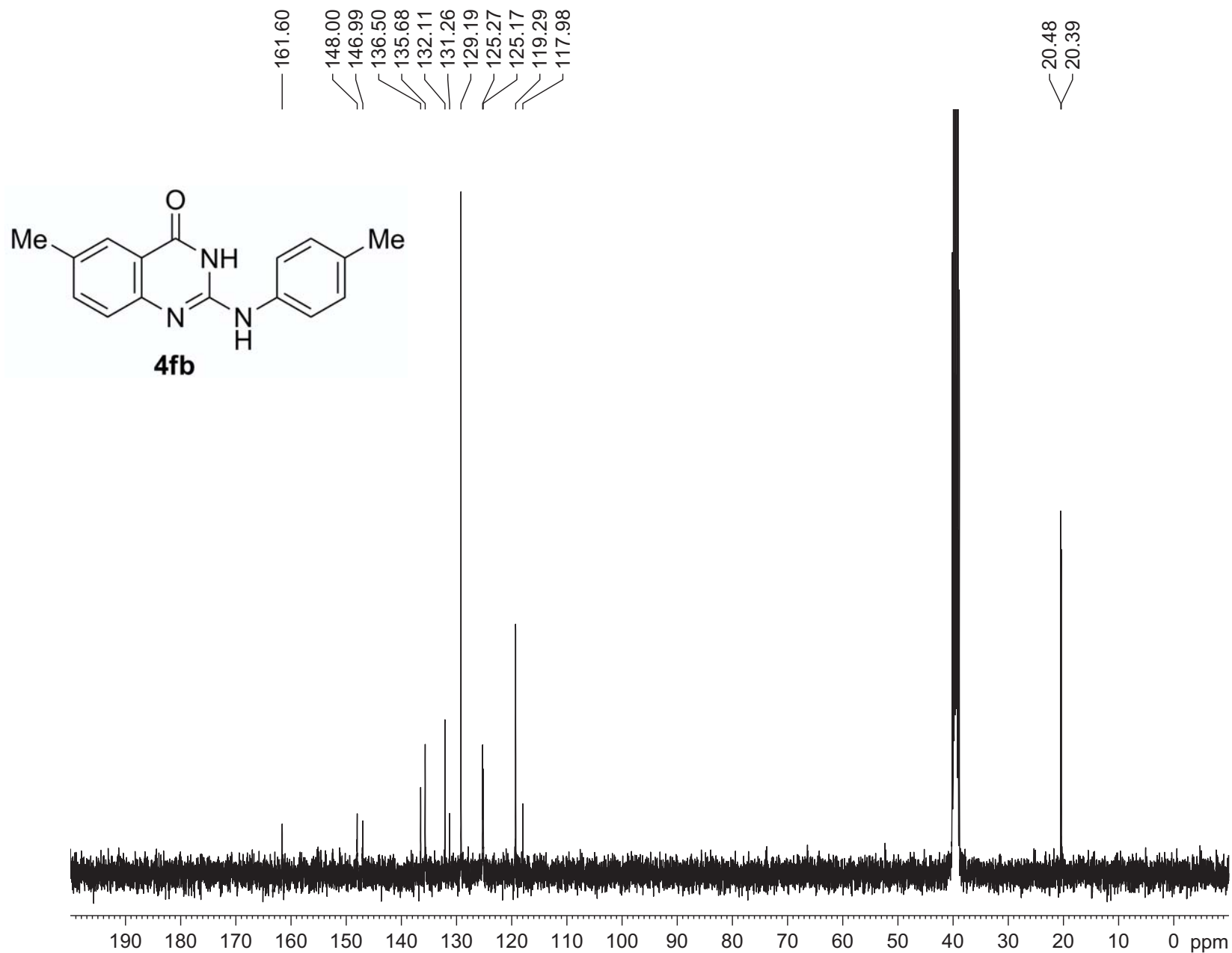
Current Data Parameters
 NAME SI062-2
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150205
 Time 11.37
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 12
 DS 0
 SWH 7246.377 Hz
 FIDRES 0.221142 Hz
 AQ 2.2609921 sec
 RG 362
 DW 69.000 usec
 DE 6.50 usec
 TE 295.6 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.00 usec
 PL1 -5.85 dB
 SFO1 400.1324008 MHz

F2 - Processing parameters
 SI 16384
 SF 400.1300030 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C



Current Data Parameters
 NAME SI062-2
 EXPNO 4
 PROCNO 1

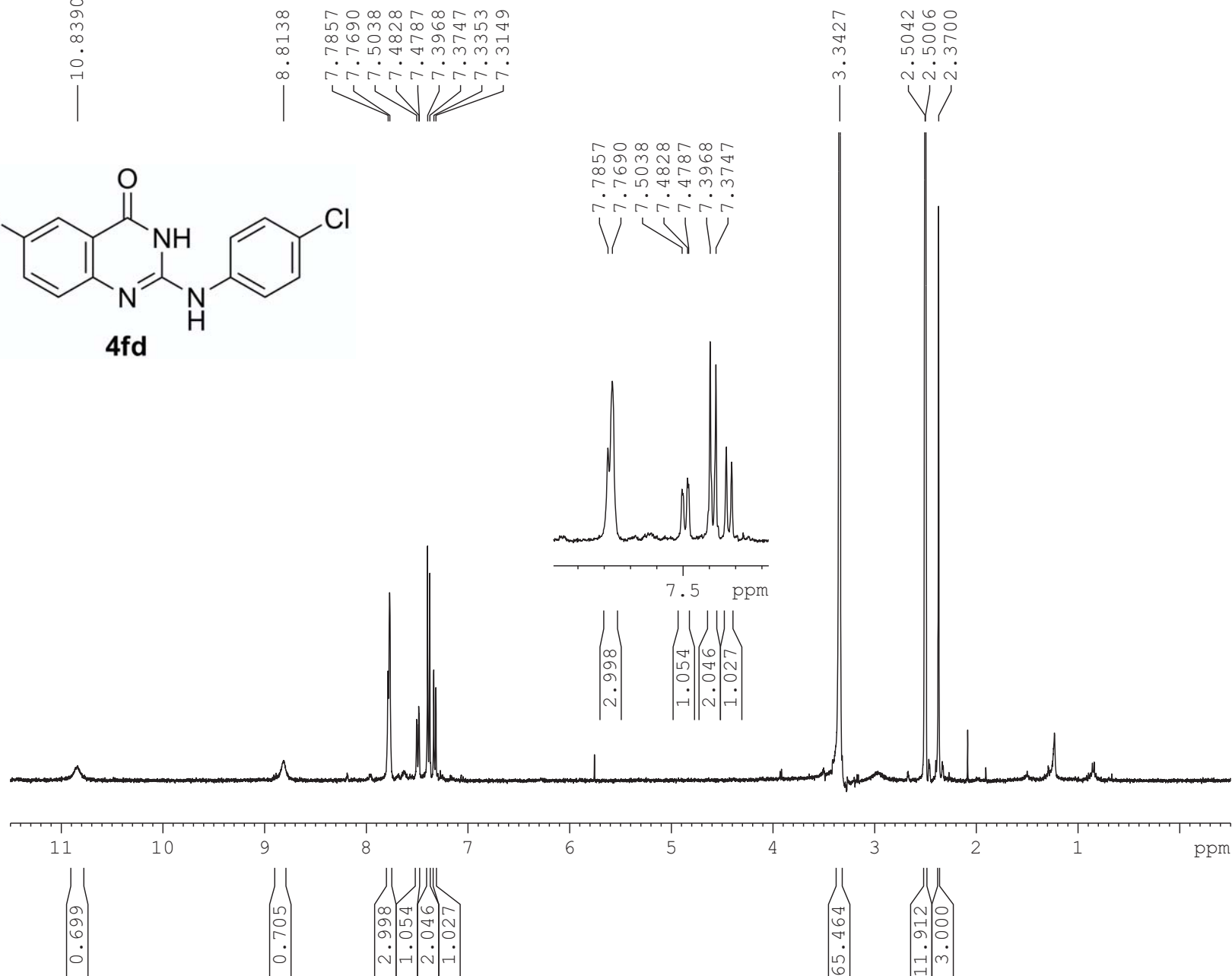
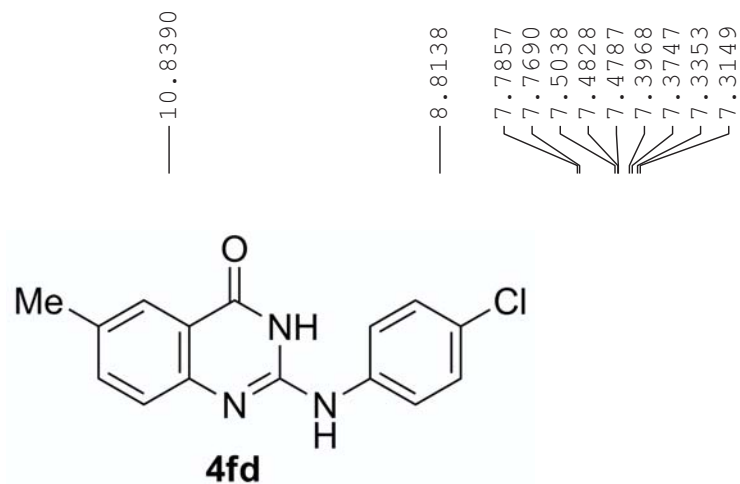
F2 - Acquisition Parameters
 Date_ 20150207
 Time 9.05
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 761
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 8192
 DW 20.800 usec
 DE 6.50 usec
 TE 296.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 10.00 usec
 PL1 6.70 dB
 SFO1 100.6233325 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 90.00 usec
 PL2 -5.85 dB
 PL12 9.10 dB
 PL13 12.10 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128171 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

-2-s



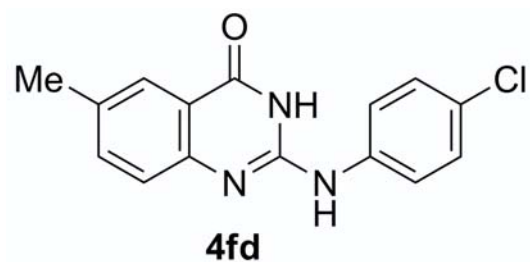
Current Data Parameters
NAME SG080
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141207
Time 1.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

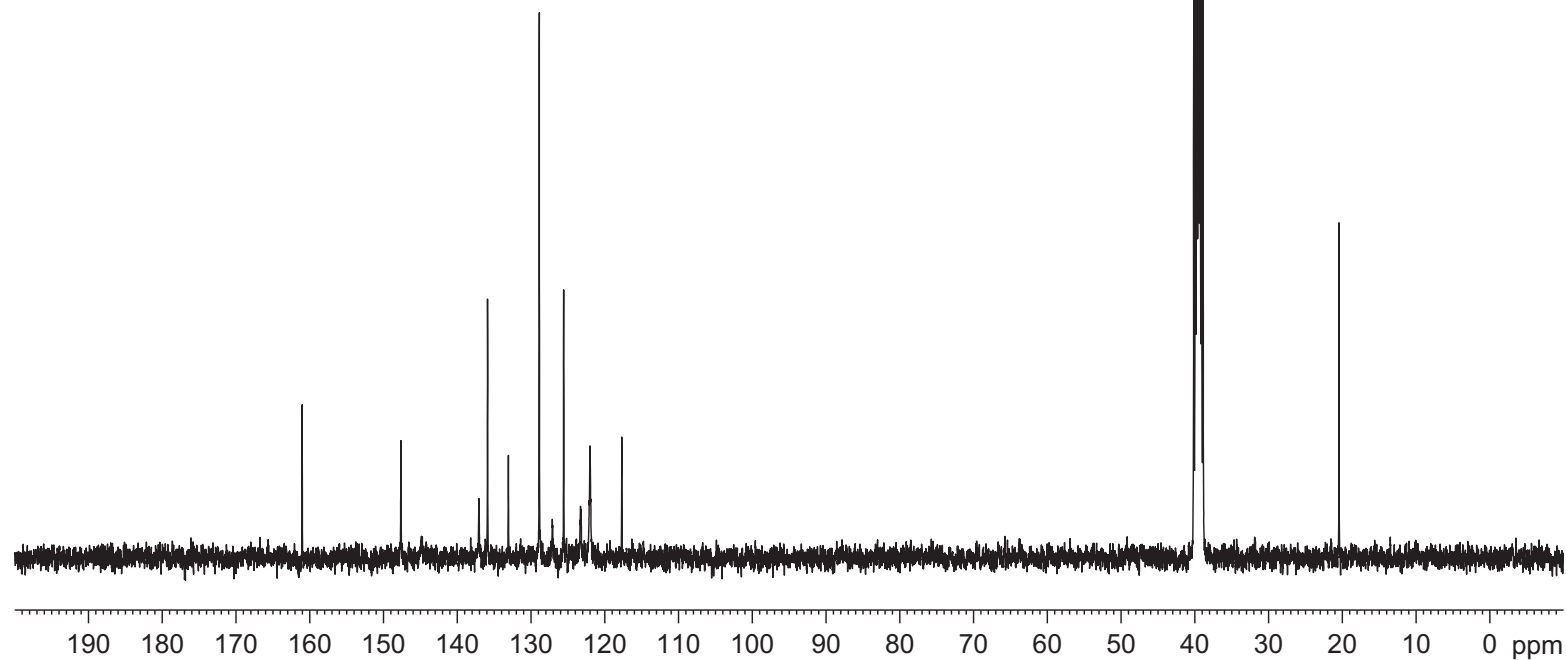
F2 - Processing parameters
SI 16384
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

3-



161.02
147.63
144.89
137.06
135.89
133.06
128.87
127.11
125.56
123.28
121.99
117.68

20.44



Current Data Parameters

NAME SG080
EXPNO 112
PROCNO 1

F2 - Acquisition Parameters

Date_ 20160729
Time 18.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 299
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

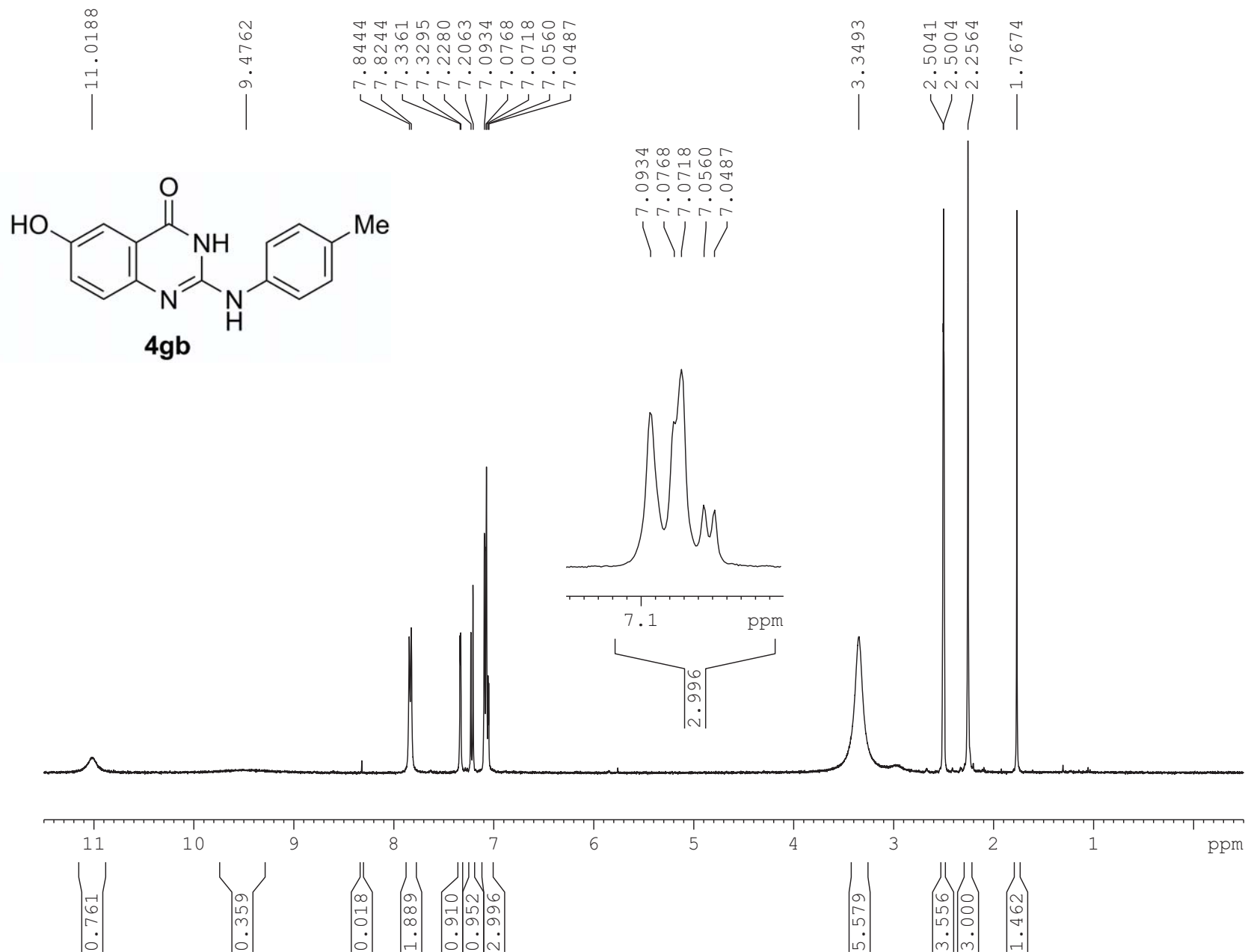
===== CHANNEL f2 =====

SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters

SI 32768
SF 100.6128189 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

¹H



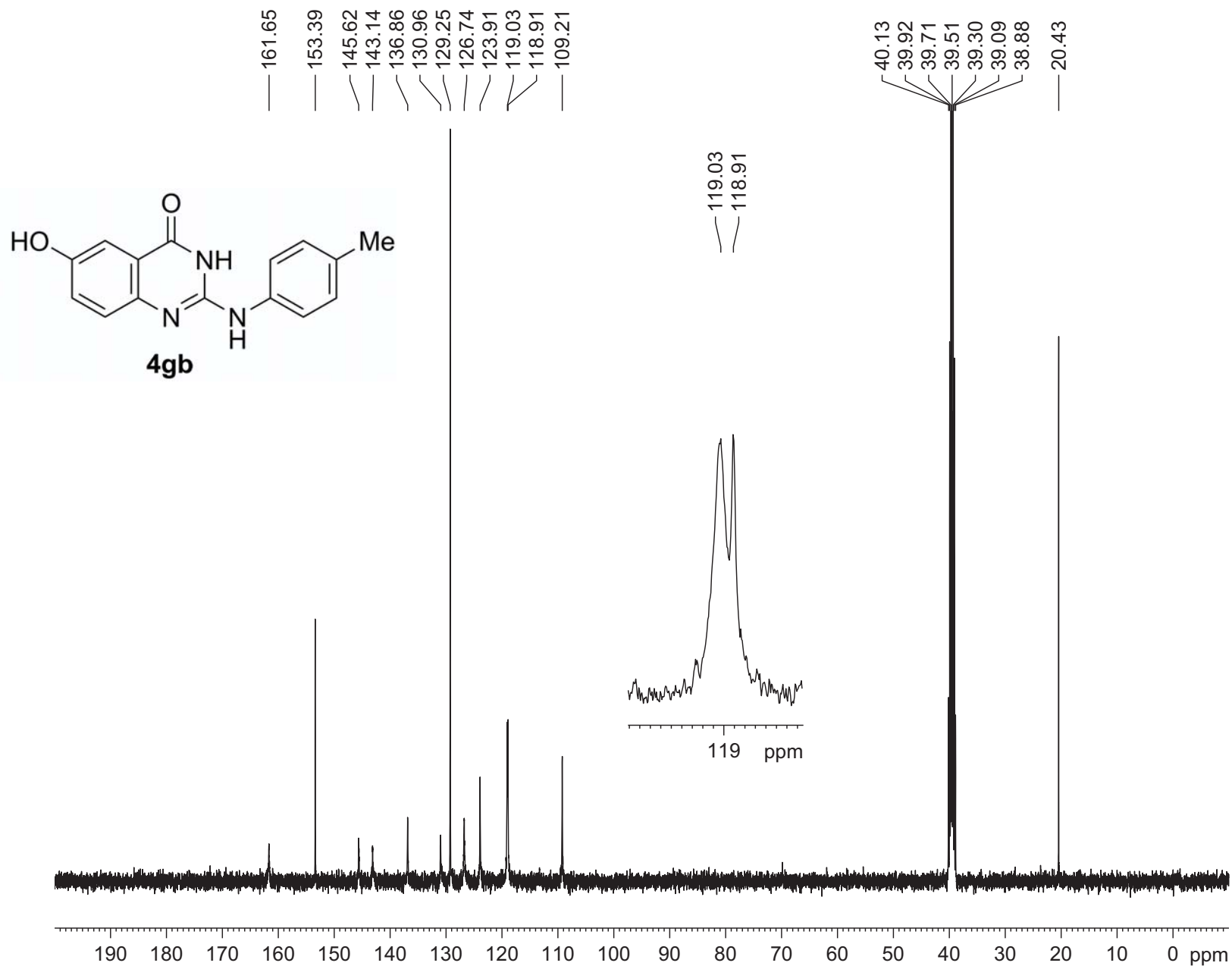
Current Data Parameters
NAME SG089
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141219
Time 20.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 322.5
DW 69.000 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C



Current Data Parameters

NAME SG089
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters

Date_ 20141226
Time 8.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 135
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4096
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

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

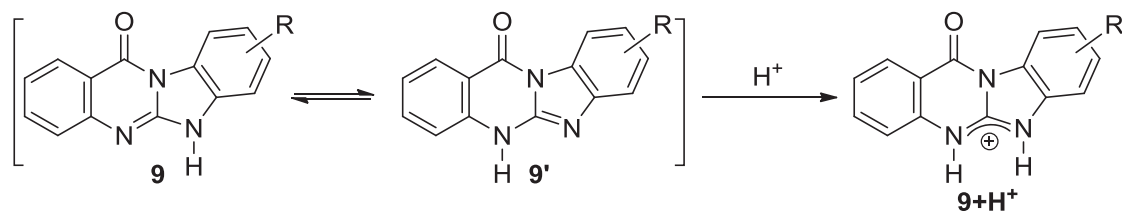
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

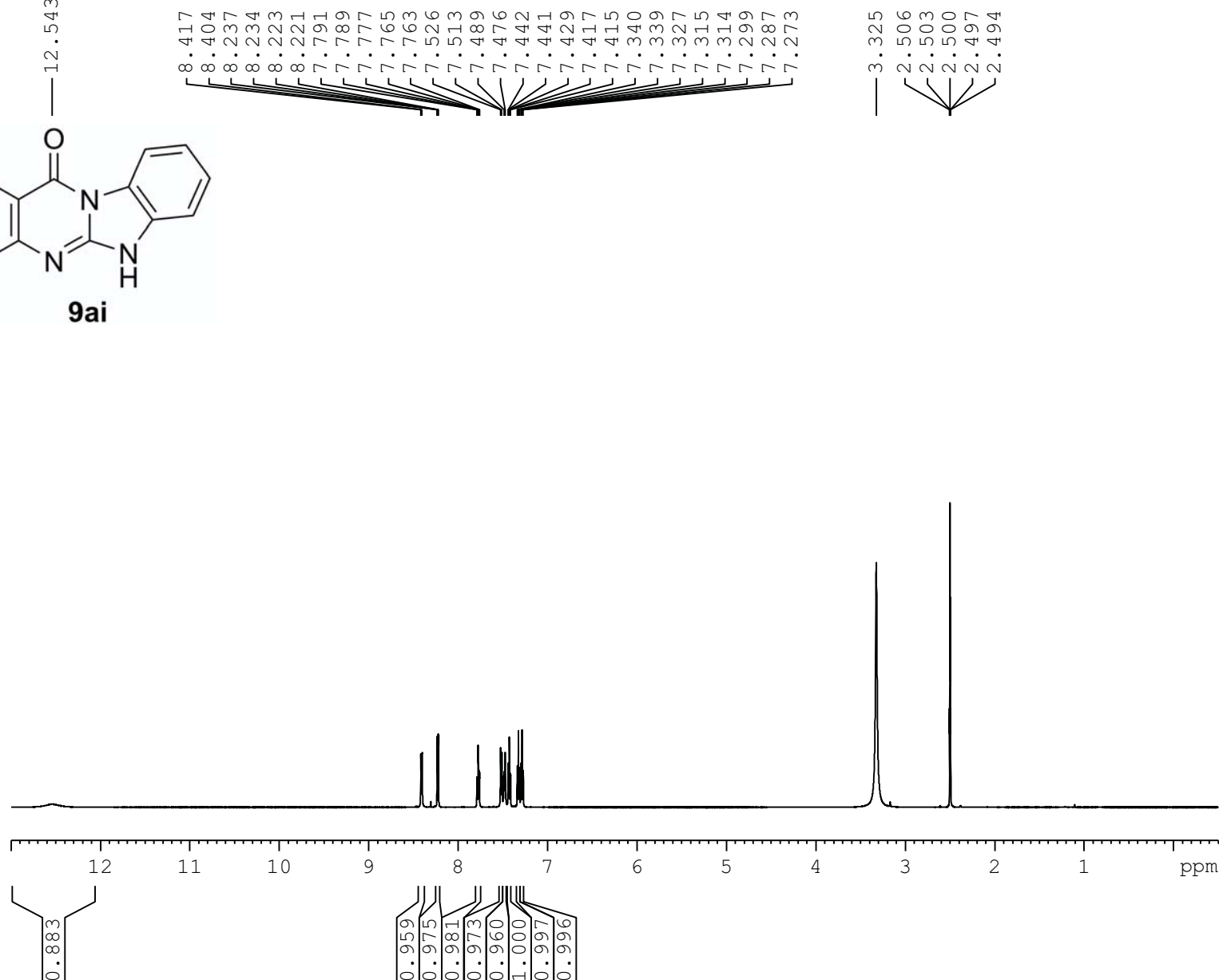
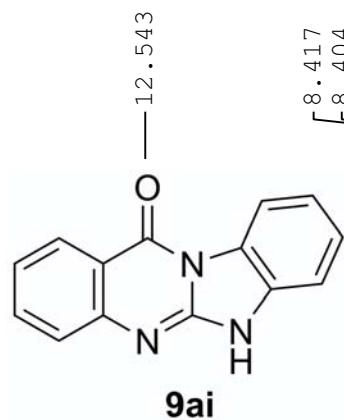
SI 32768
SF 100.6128081 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

*** notes for the NMR spectra of benzimidazo[2,1-*b*]quinazolin-12-ones (**9**)

During structural characterization of benzimidazo[2,1-*b*]quinazolin-12-ones (**9**) with NMR spectroscopy, we observed obscure ^{13}C NMR spectra with indistinct and broad peaks as well as obvious missing peaks, particularly for the quaternary carbons. We rationalized that the nitrogen-bonded protons of benzimidazo[2,1-*b*]quinazolin-12-ones (**9**) can rapidly hopping among the basic nitrogens inter- and intra-molecularly in solution. The dynamic process involves at least the equilibrium between two non-equivalent structures (**9** and **9'**) and the transient states in between, which caused significant peak broadening due to non-equivalent environments for the carbons nearby the basic nitrogens. Although the missing or broad peaks can be verified by raising the NMR experiment temperature to accelerate the proton transfer process, the temperature-variable NMR experiments are somehow troublesome and less practical for general structural identification. Therefore, for NMR spectroscopic characterization purpose, an additional set of ^1H & ^{13}C NMR spectra for benzimidazo[2,1-*b*]quinazolin-12-ones (**9**) were acquired with the addition of one drop of TFA, which was intended to saturate the basic nitrogen sites with additional proton source to prevent the proton transfer. As a result, the carbon skeletons of benzimidazo[2,1-*b*]quinazolin-12-ones (**9**) were confirmed unambiguously by both unprotonated and protonated ^{13}C NMR spectra.



1H of RX127



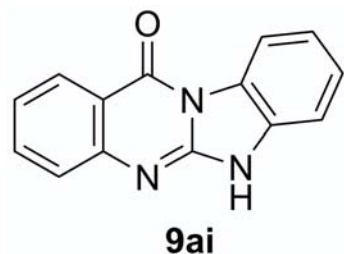
Current Data Parameters
NAME RX127-NMR600
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140718
Time 13.38
INSTRUM spect
PROBHD 5 mm PATBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 0
SWH 10822.511 Hz
FIDRES 0.165138 Hz
AQ 3.0277631 sec
RG 250.57
DW 46.200 usec
DE 12.09 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1736010 MHz
NUC1 1H
P1 12.05 usec
PLW1 30.00000000 W

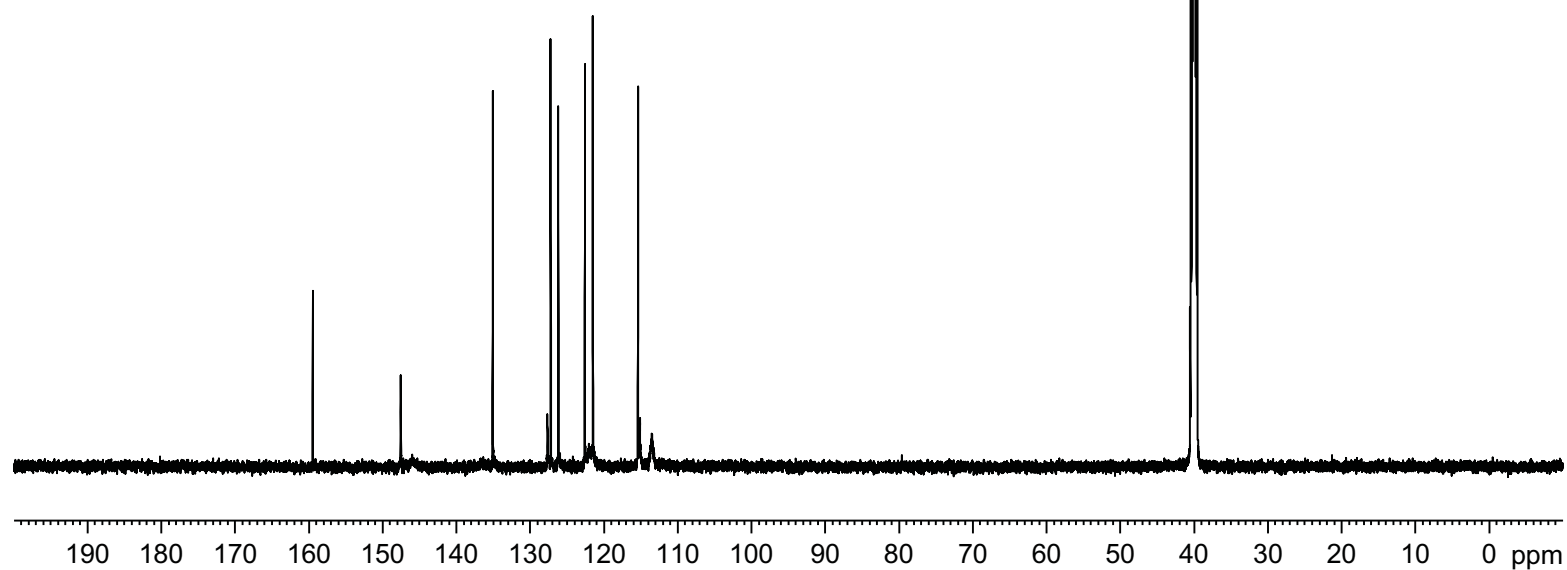
F2 - Processing parameters
SI 32768
SF 600.1700045 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of RX127



159.47
147.54
146.01
135.08
127.65
127.22
126.17
122.59
122.07
121.50
115.38
115.10
113.50

40.41
40.28
40.14
40.00
39.86
39.72
39.58



Current Data Parameters
NAME RX127-NMR600
EXPNO 5
PROCNO 1

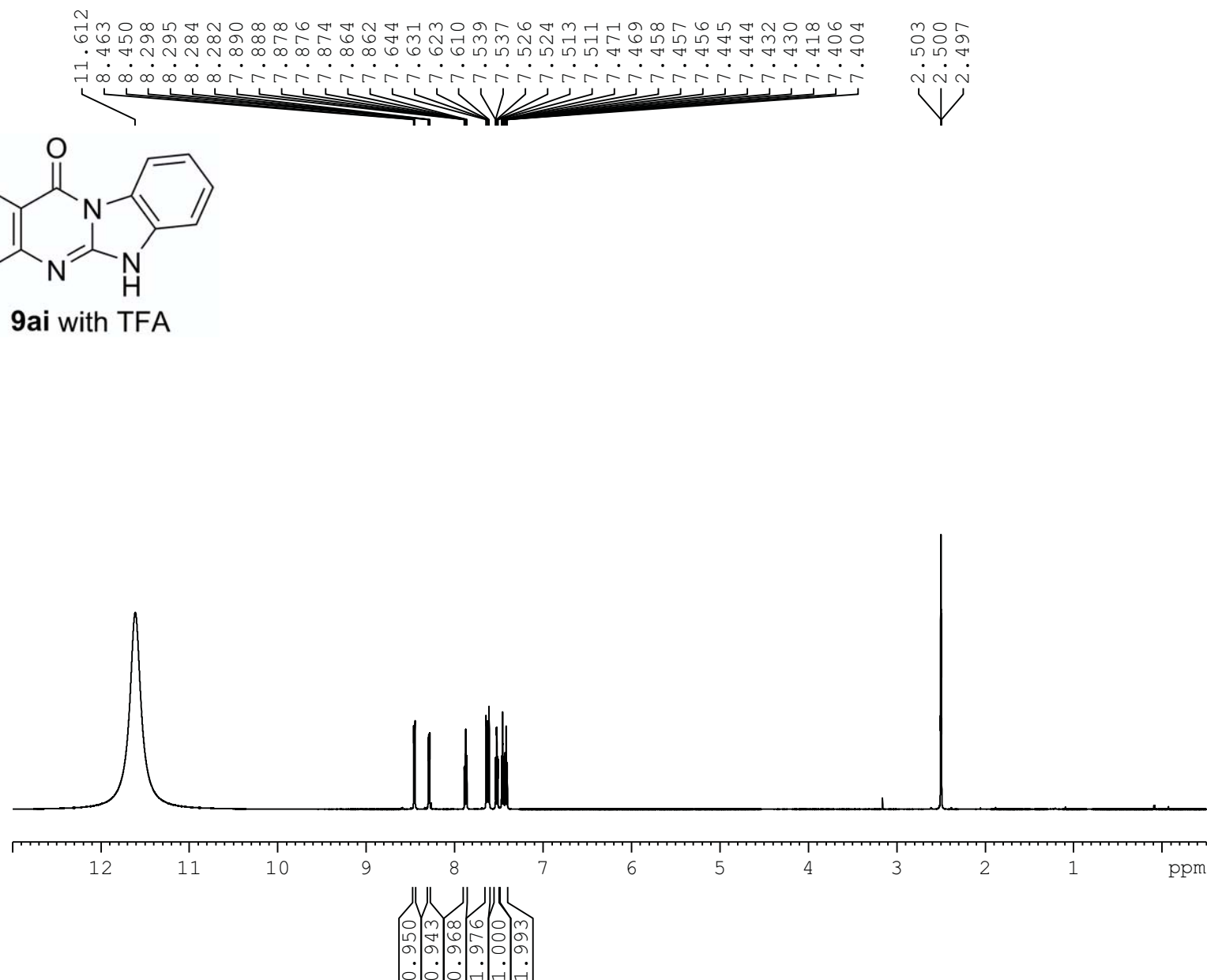
F2 - Acquisition Parameters
Date_ 20140718
Time 5.35
INSTRUM spect
PROBHD 5 mm PATBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15000
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 200.5
DW 13.867 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 150.9287115 MHz
NUC1 ¹³C
P1 10.80 usec
PLW1 50.00000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 ¹H
CPDPRG2 waltz64
PCPD2 70.00 usec
PLW2 30.00000000 W
PLW12 1.03470004 W
PLW13 0.50700003 W

F2 - Processing parameters
SI 32768
SF 150.9128699 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of RX127-TFA



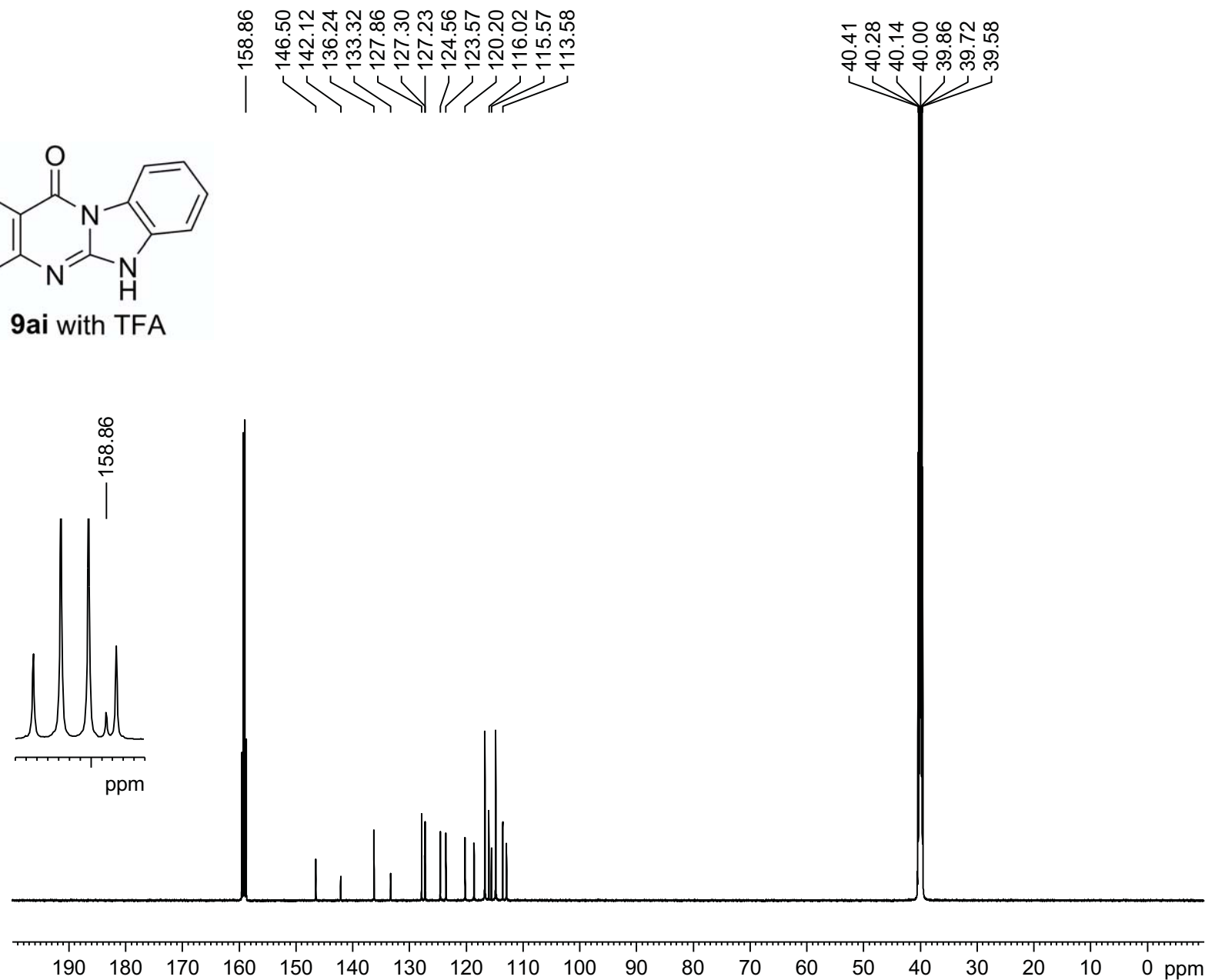
Current Data Parameters
NAME 2014080119
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140820
Time 18.16
INSTRUM spect
PROBHD 5 mm PATBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 128
DS 0
SWH 10822.511 Hz
FIDRES 0.165138 Hz
AQ 3.0277631 sec
RG 123.59
DW 46.200 usec
DE 12.09 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1736010 MHz
NUC1 1H
P1 12.05 usec
PLW1 30.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1700047 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of RX127-TFA



Current Data Parameters
 NAME 2014080119
 EXPNO 2
 PROCNO 1

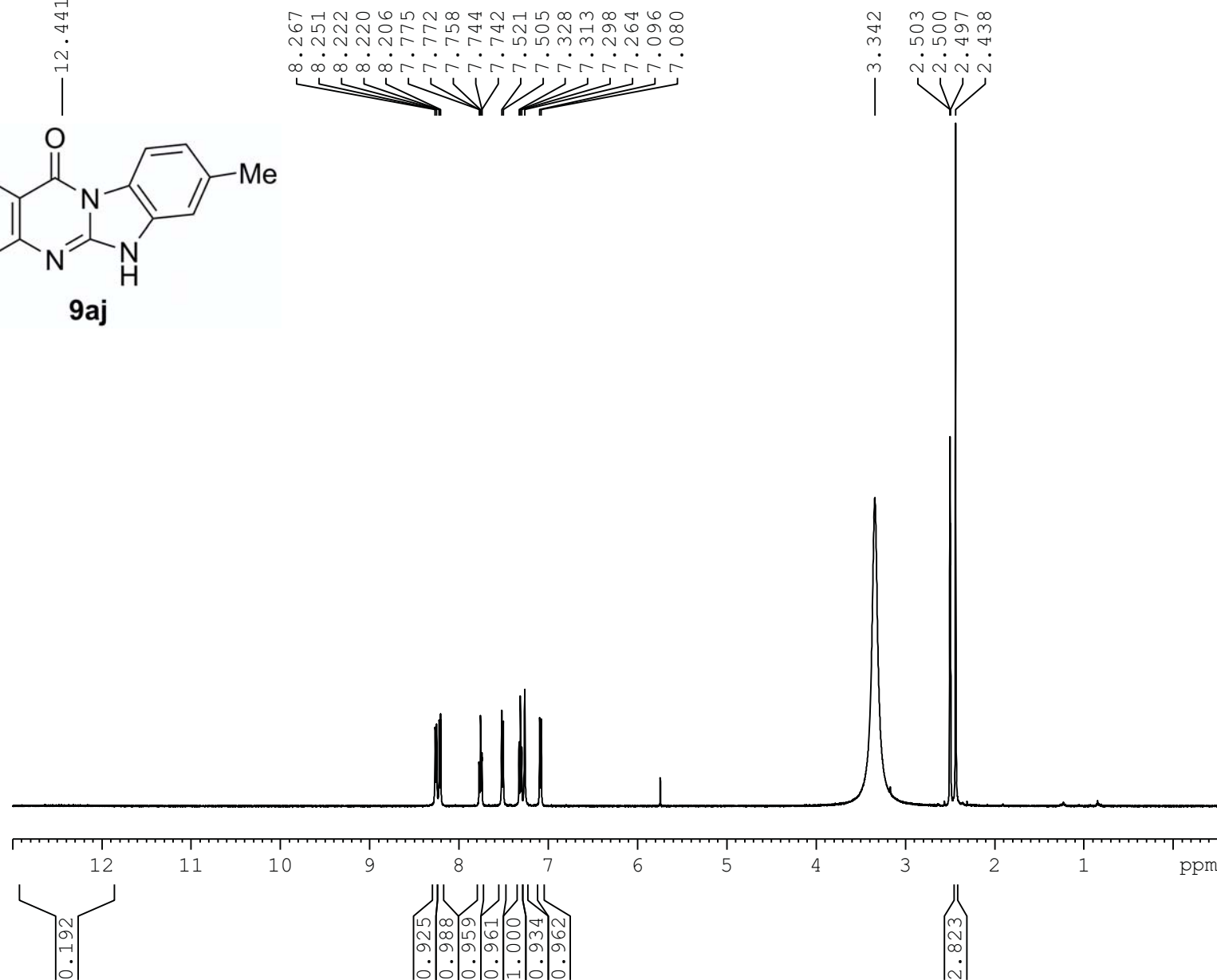
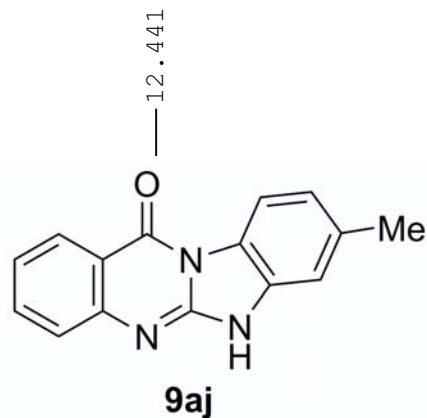
F2 - Acquisition Parameters
 Date_ 20140821
 Time 19.10
 INSTRUM spect
 PROBHD 5 mm PATBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 30000
 DS 0
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 2050
 DW 13.867 usec
 DE 6.50 usec
 TE 300.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9287115 MHz
 NUC1 ¹³C
 P1 10.80 usec
 PLW1 50.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 ¹H
 CPDPRG[2] waltz64
 PCPD2 70.00 usec
 PLW2 30.00000000 W
 PLW12 1.03470004 W
 PLW13 0.50700003 W

F2 - Processing parameters
 SI 32768
 SF 150.9128226 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

1H of re 173



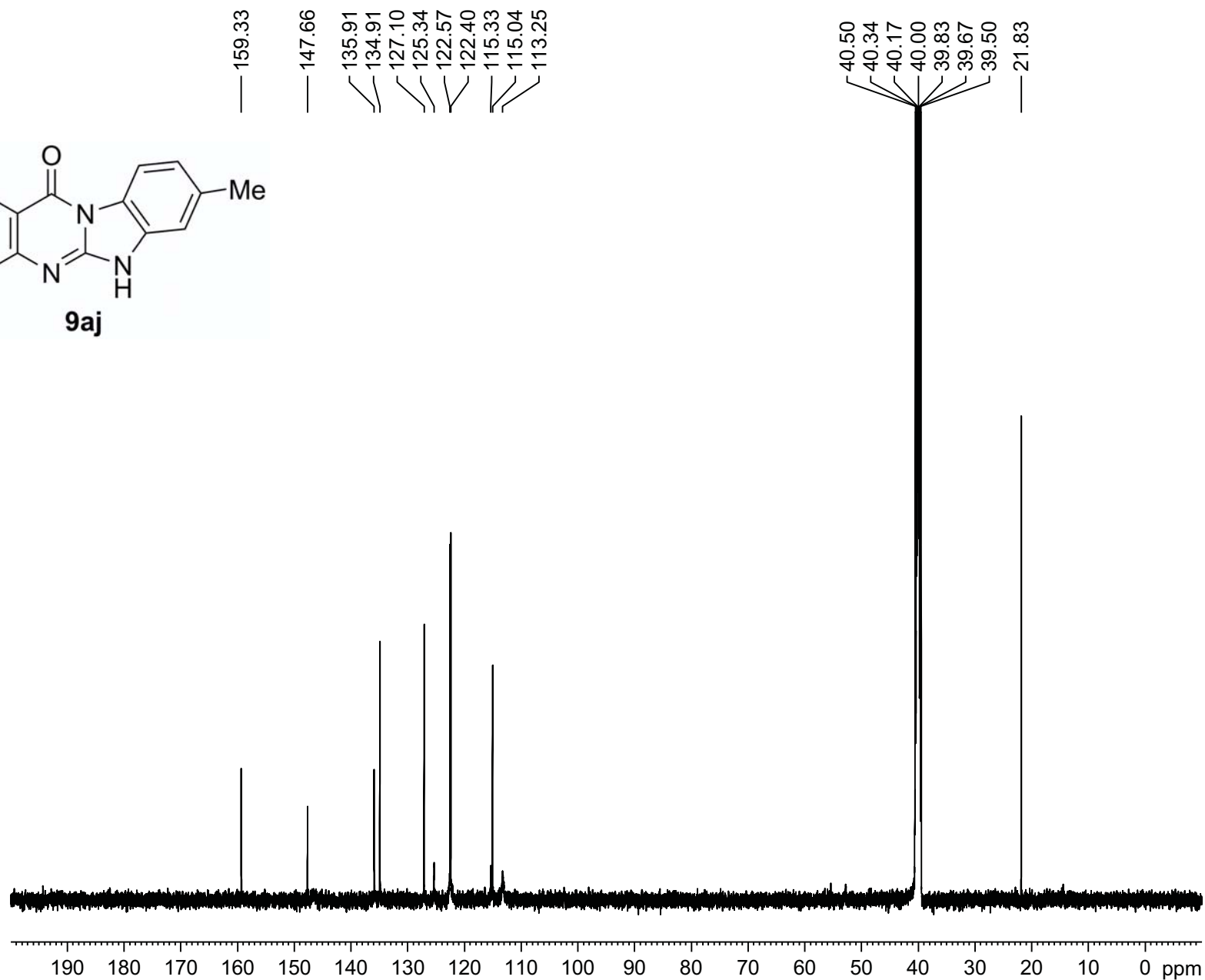
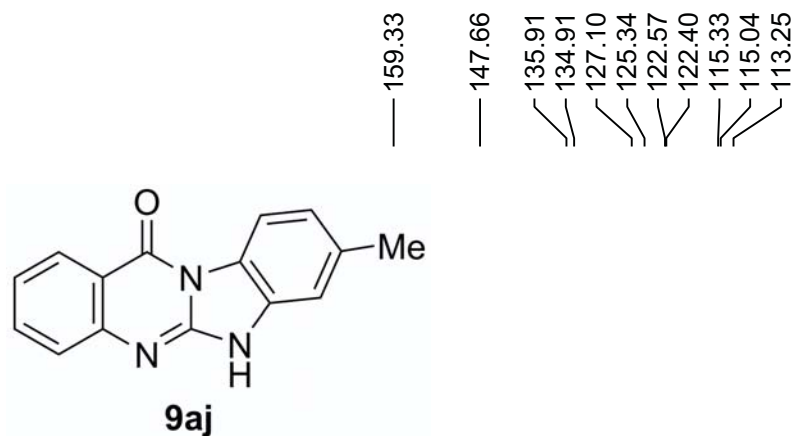
Current Data Parameters
NAME TCC-2014110118
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141112
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 181
DW 55.200 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of re 173



Current Data Parameters
 NAME TCC-2014110118
 EXPNO 5
 PROCNO 1

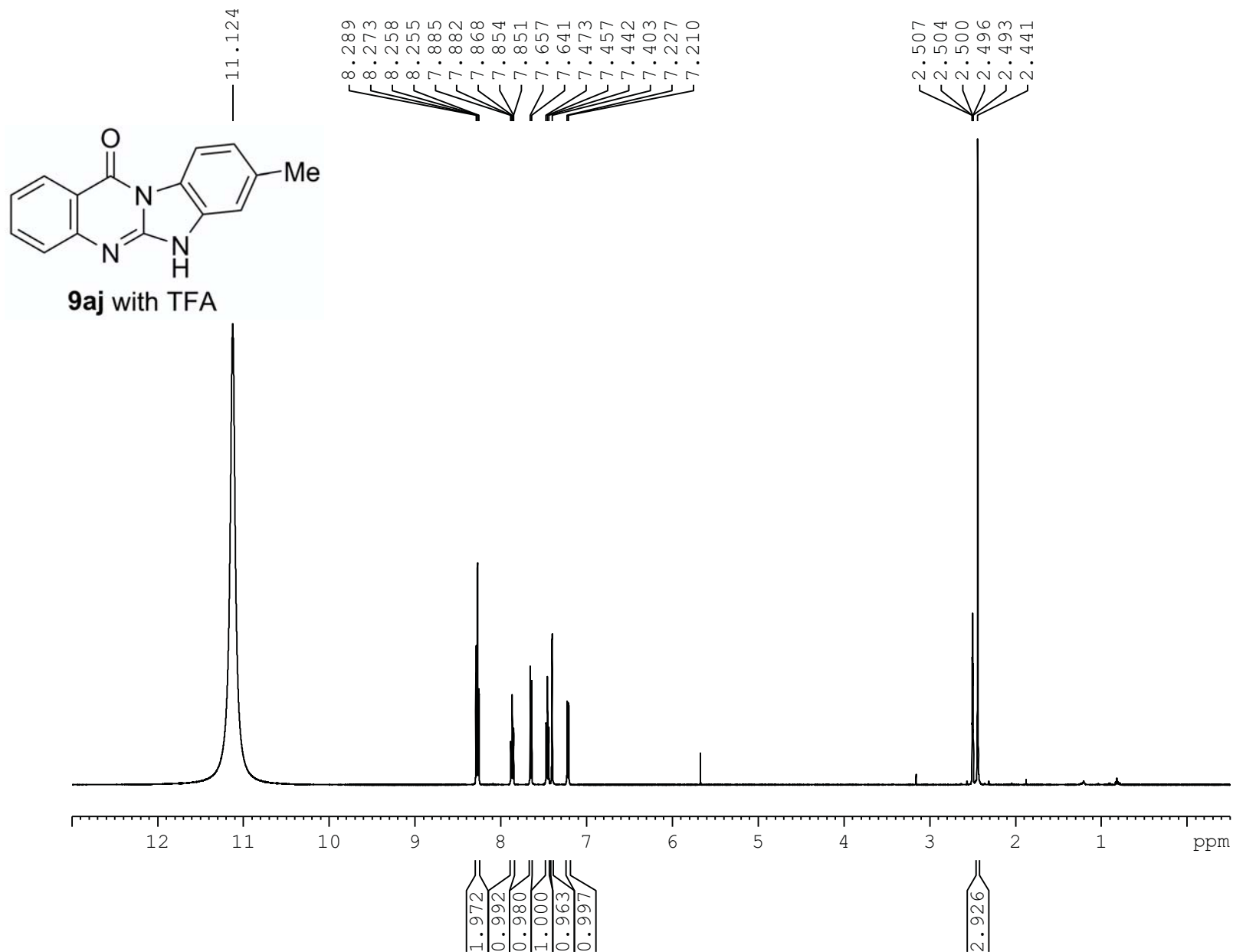
F2 - Acquisition Parameters
 Date_ 20141112
 Time 10.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 6076
 DS 0
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0813440 sec
 RG 8192
 DW 16.500 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.00 usec
 PL1 6.50 dB
 SFO1 125.7709936 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -0.60 dB
 PL12 15.20 dB
 PL13 18.20 dB
 SFO2 500.1320005 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577884 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

¹H of re 173+TFA



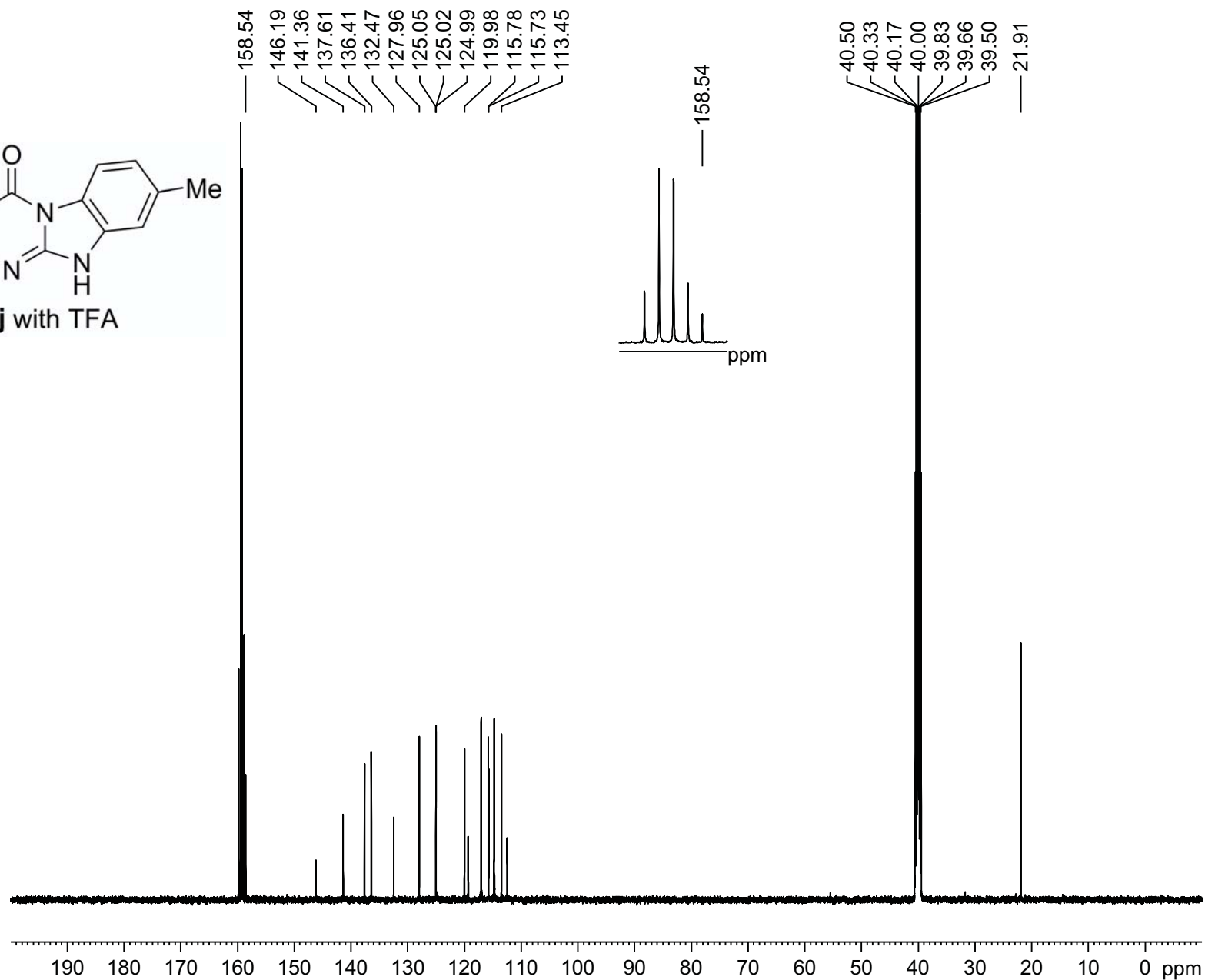
Current Data Parameters
 NAME TCC-2014110118
 EXPNO 12
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141114
 Time 15.22
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 71.8
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 65536
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of re 173+TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 13
PROCNO 1

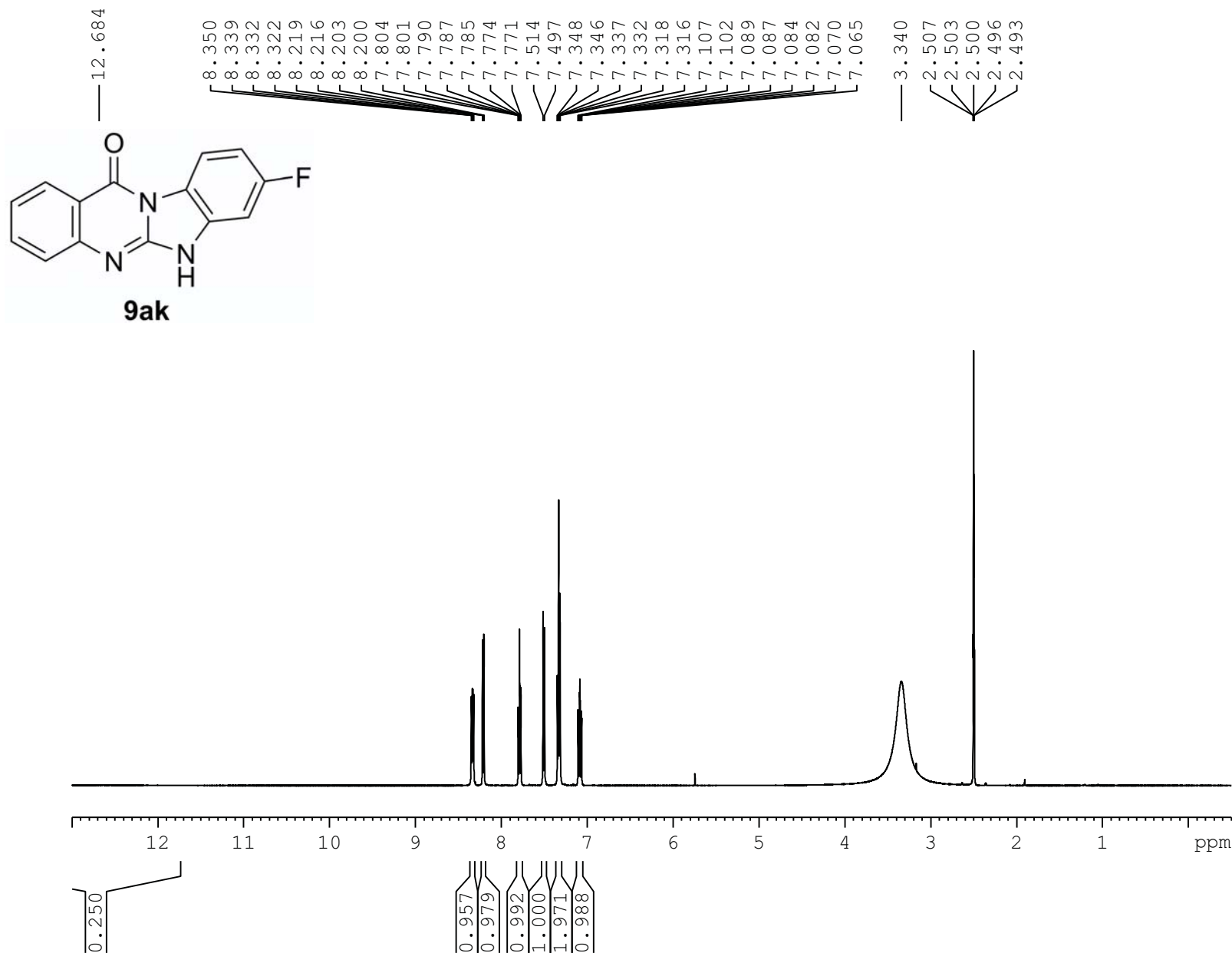
F2 - Acquisition Parameters
Date_ 20141114
Time 14.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3746
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577358 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00

1H of re 171



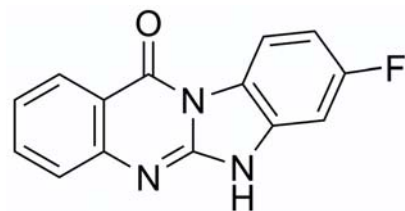
Current Data Parameters
 NAME TCC-2014110118
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141124
 Time 11.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 64
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300050 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

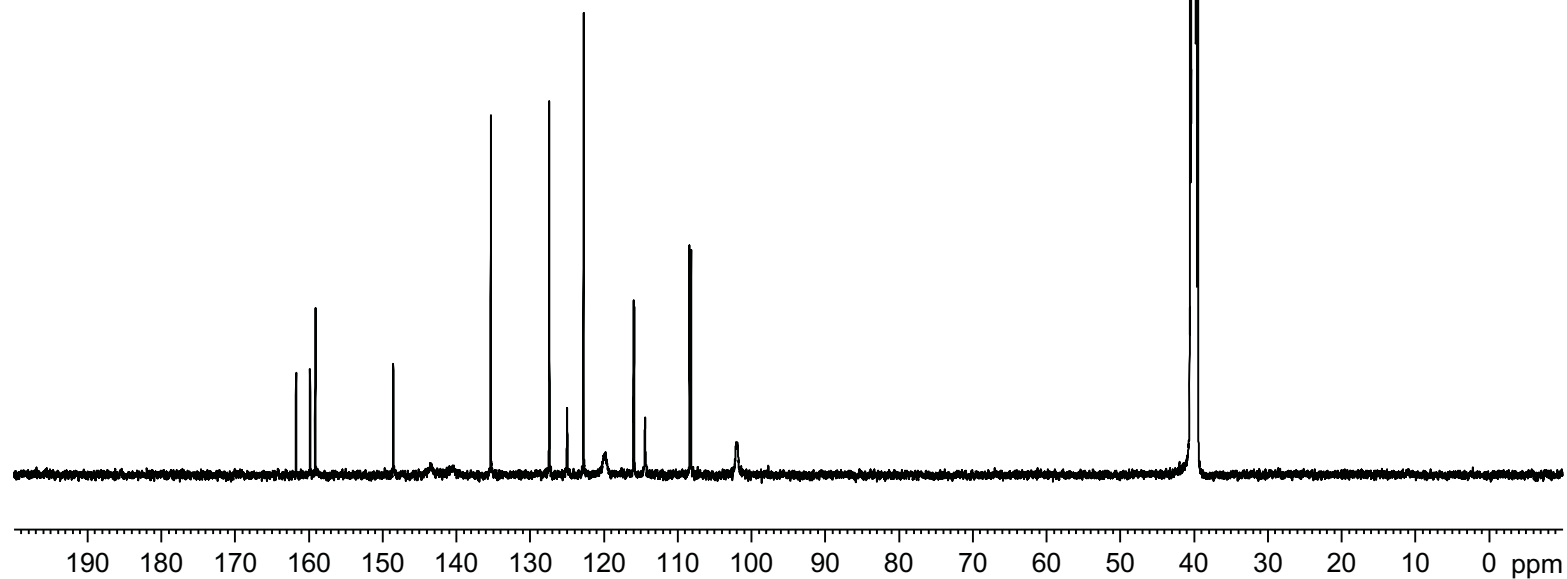
¹³C of re 171



9ak

161.73
159.83
159.12
148.56
143.54
140.51
135.35
127.40
124.98
122.76
119.78
115.99
115.90
114.42
108.39
108.19
102.07
101.88

40.50
40.33
40.17
40.00
39.83
39.66
39.50



Current Data Parameters
NAME TCC-2014110118
EXPNO 22
PROCNO 1

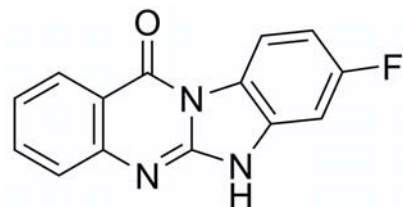
F2 - Acquisition Parameters
Date_ 20141124
Time 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 20600
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

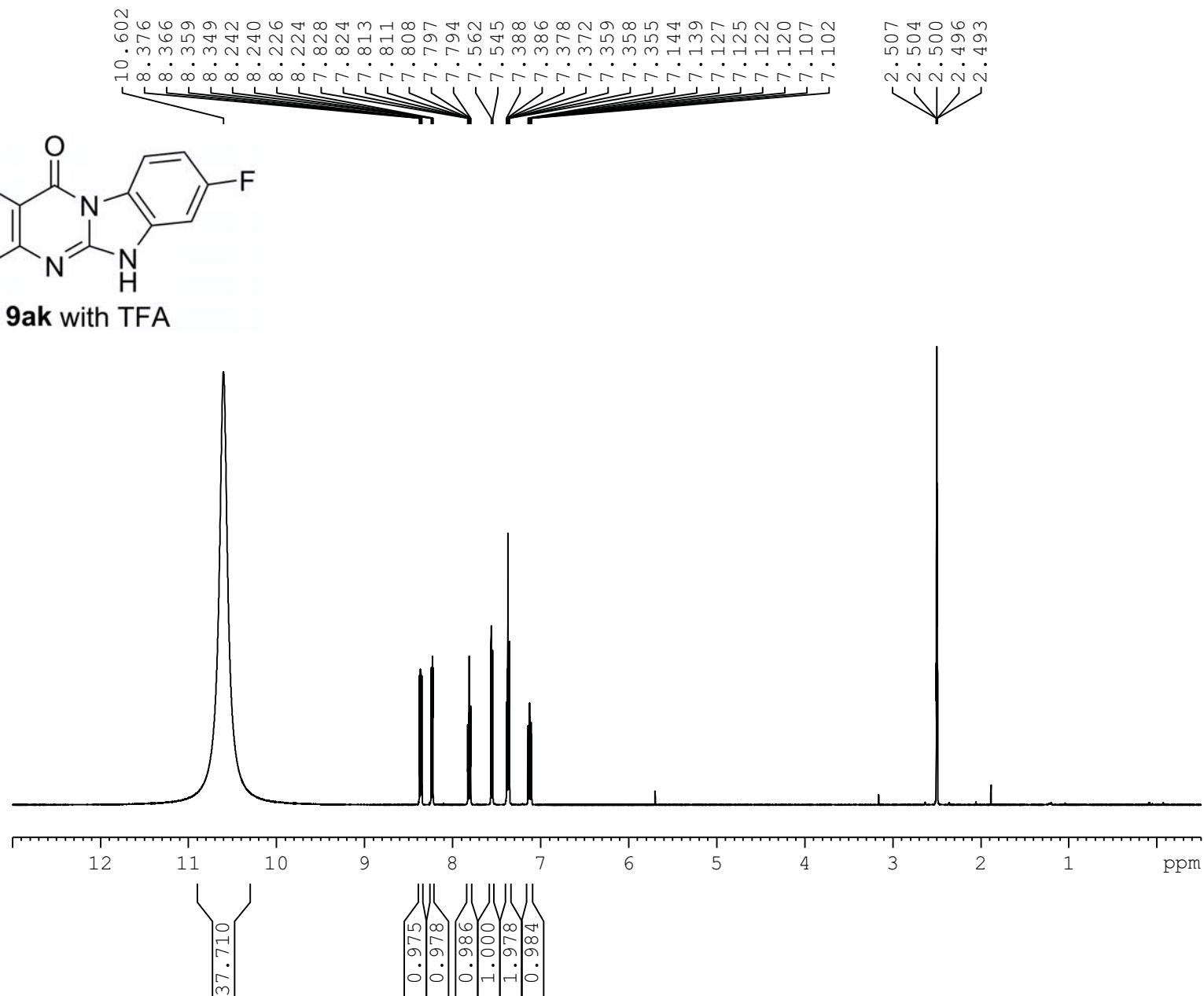
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577894 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1H of re 171+TFA



9ak with TFA



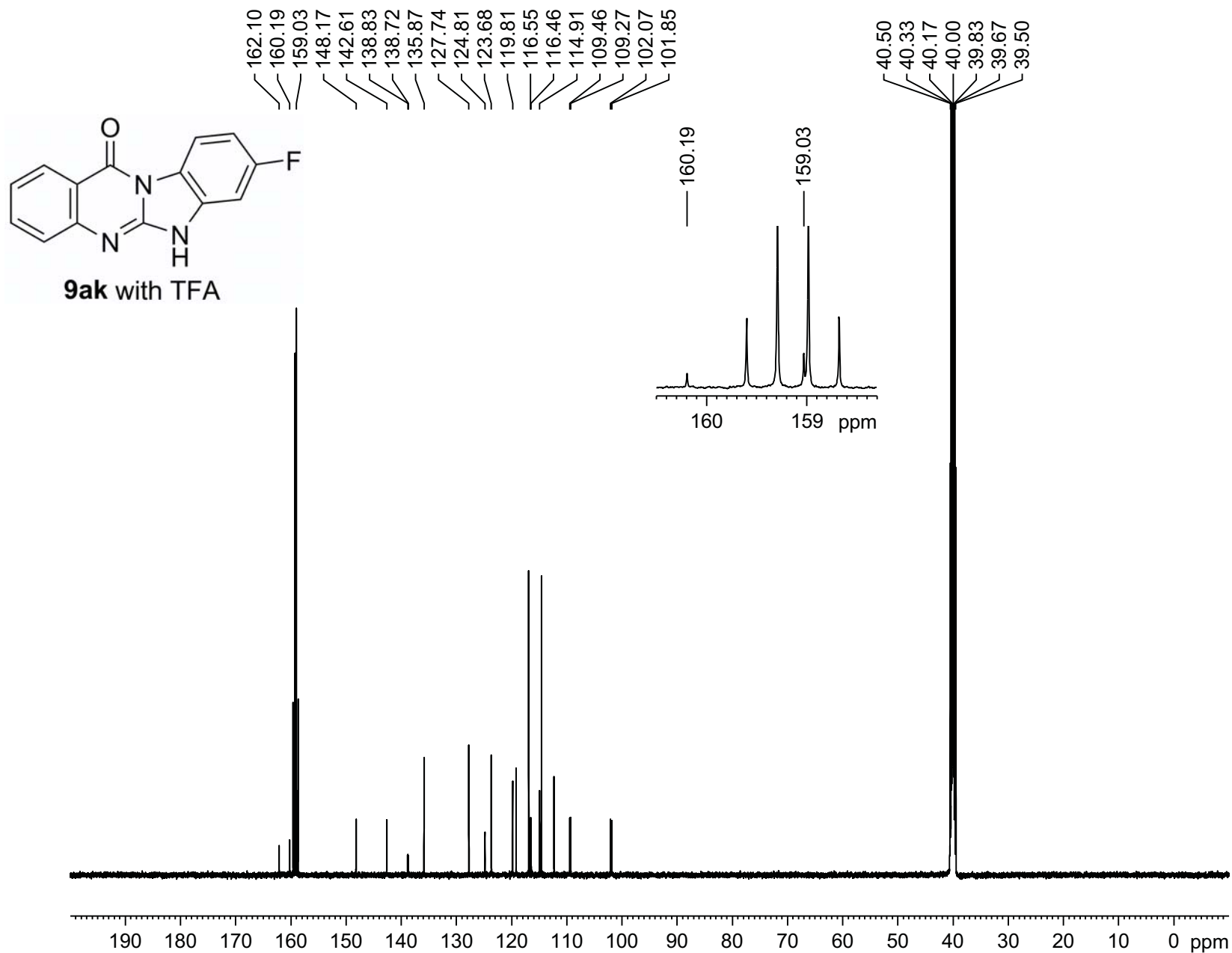
Current Data Parameters
NAME TCC-2014110118
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141125
Time 16.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 32768
SF 500.1300050 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of re 171+TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 25
PROCNO 1

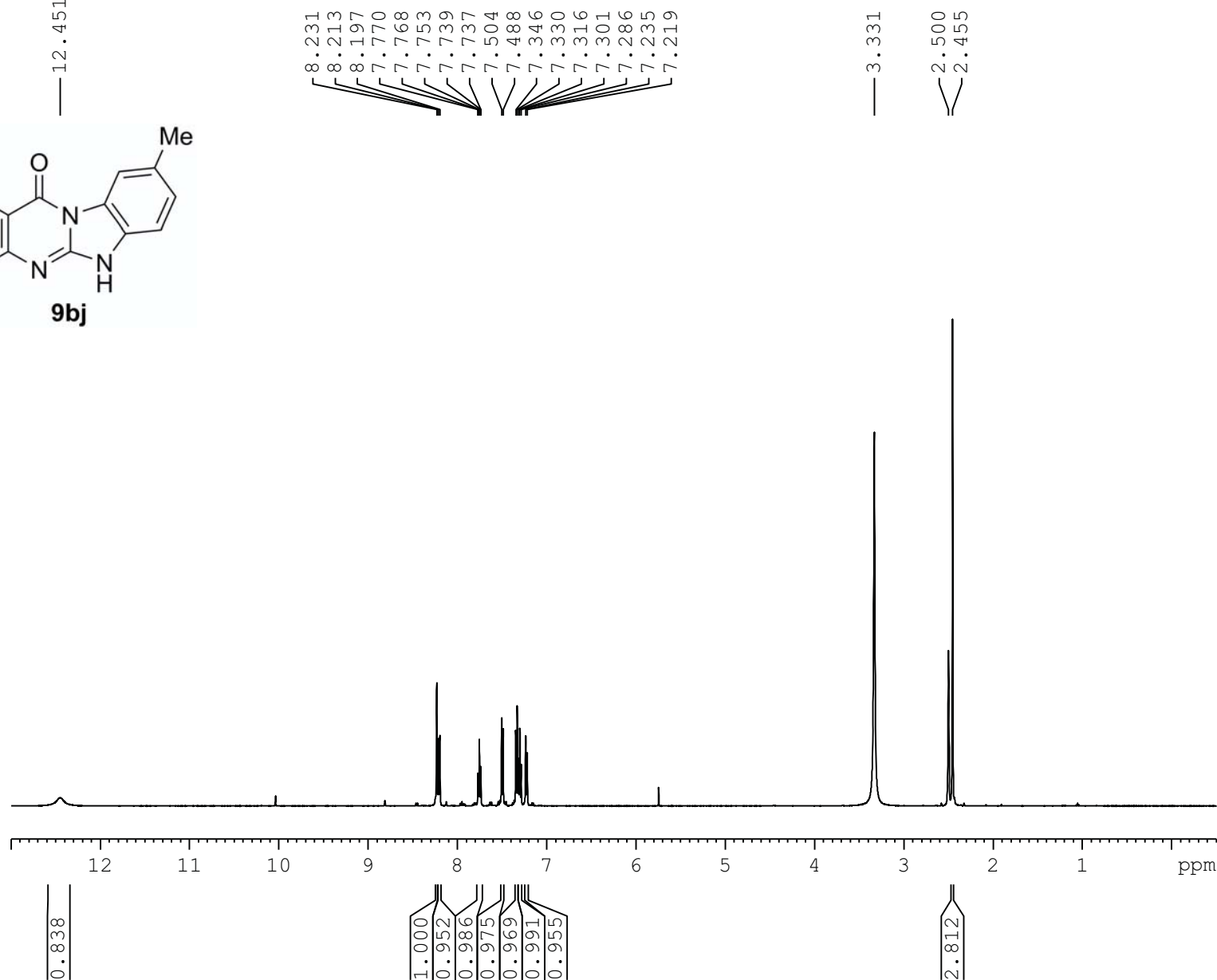
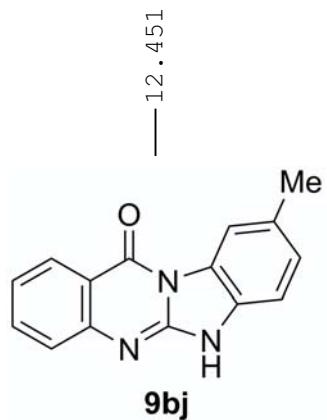
F2 - Acquisition Parameters
Date_ 20141125
Time 10.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 4632
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577538 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H of re 174



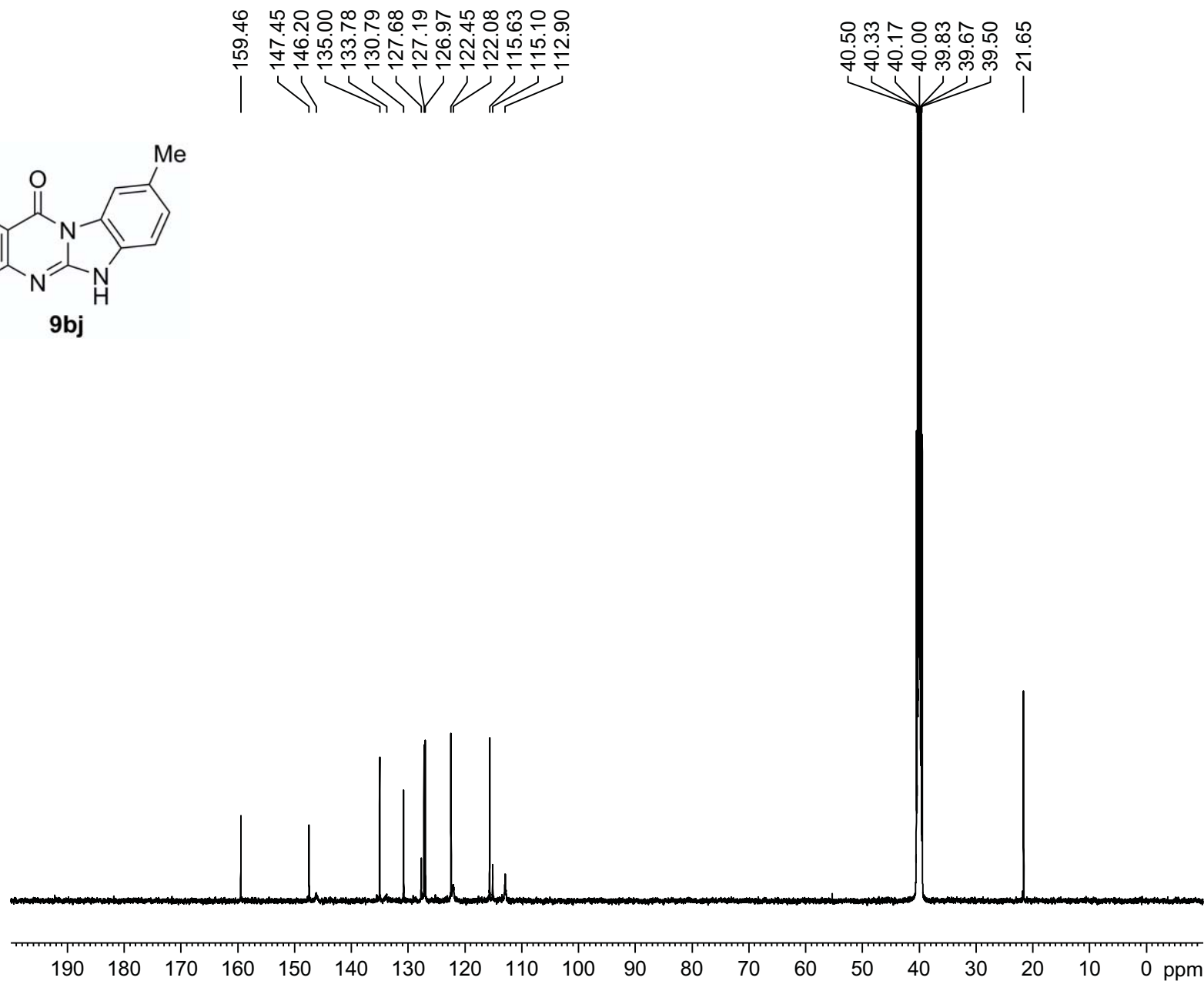
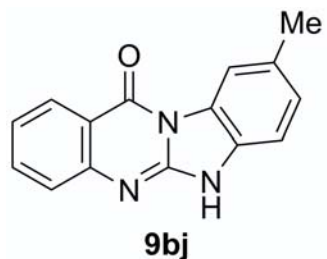
Current Data Parameters
 NAME TCC-2014110118
 EXPNO 9
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141113
 Time 19.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 0
 SWH 9057.971 Hz
 FIDRES 0.138214 Hz
 AQ 3.6175871 sec
 RG 181
 DW 55.200 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.20 usec
 PL1 -0.60 dB
 SFO1 500.1330008 MHz

F2 - Processing parameters
 SI 16384
 SF 500.1300048 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

¹³C of re 174



Current Data Parameters
NAME TCC-2014110118
EXPNO 10
PROCNO 1

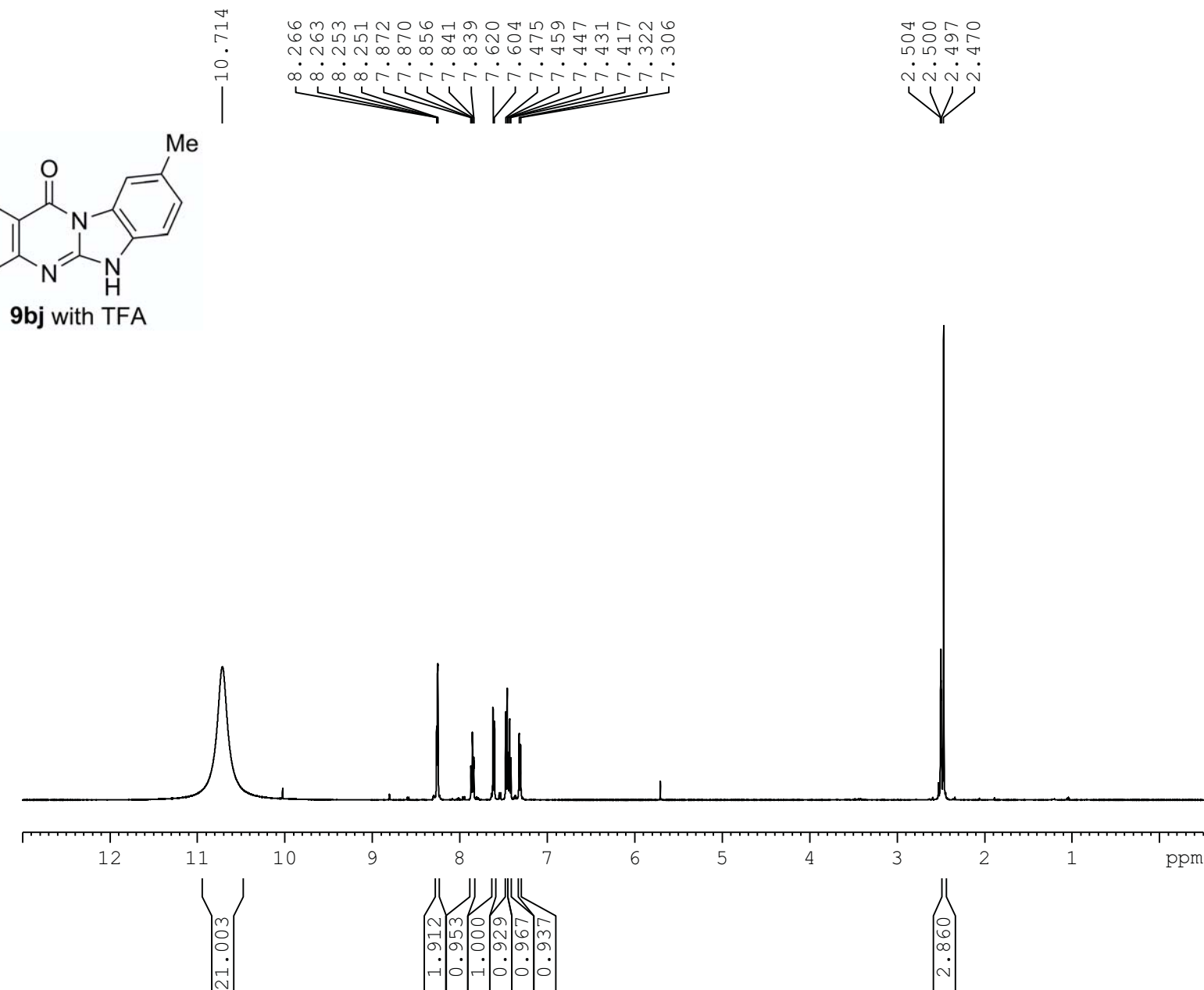
F2 - Acquisition Parameters
Date_ 20141113
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5157
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577899 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

¹H of re 174+TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141117
Time 11.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 128
DW 55.200 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

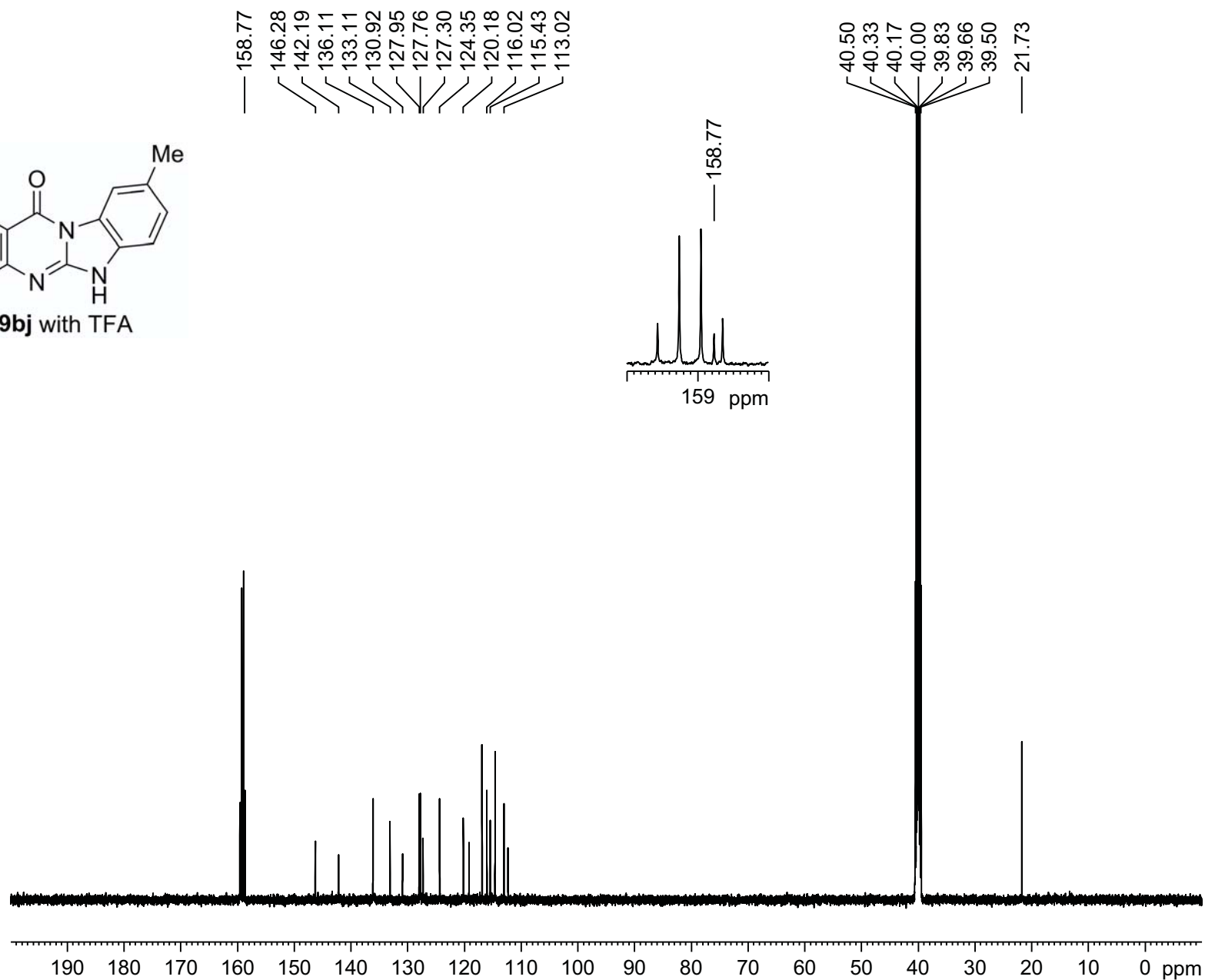
===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 32768
SF 500.1300047 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of re 174+TFA



9bj with TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 19
PROCNO 1

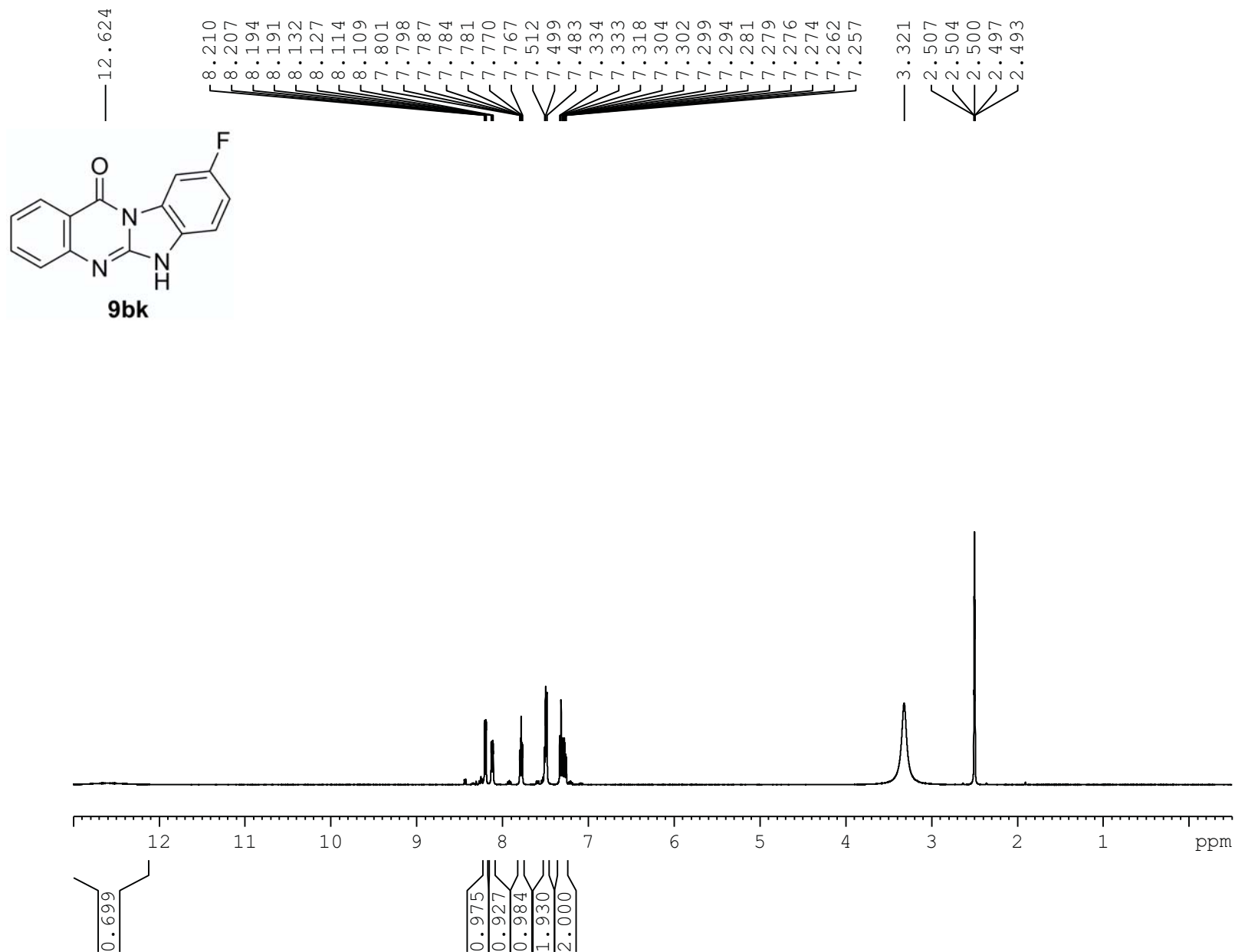
F2 - Acquisition Parameters
Date_ 20141117
Time 11.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 5792.6
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577607 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1H of re 172



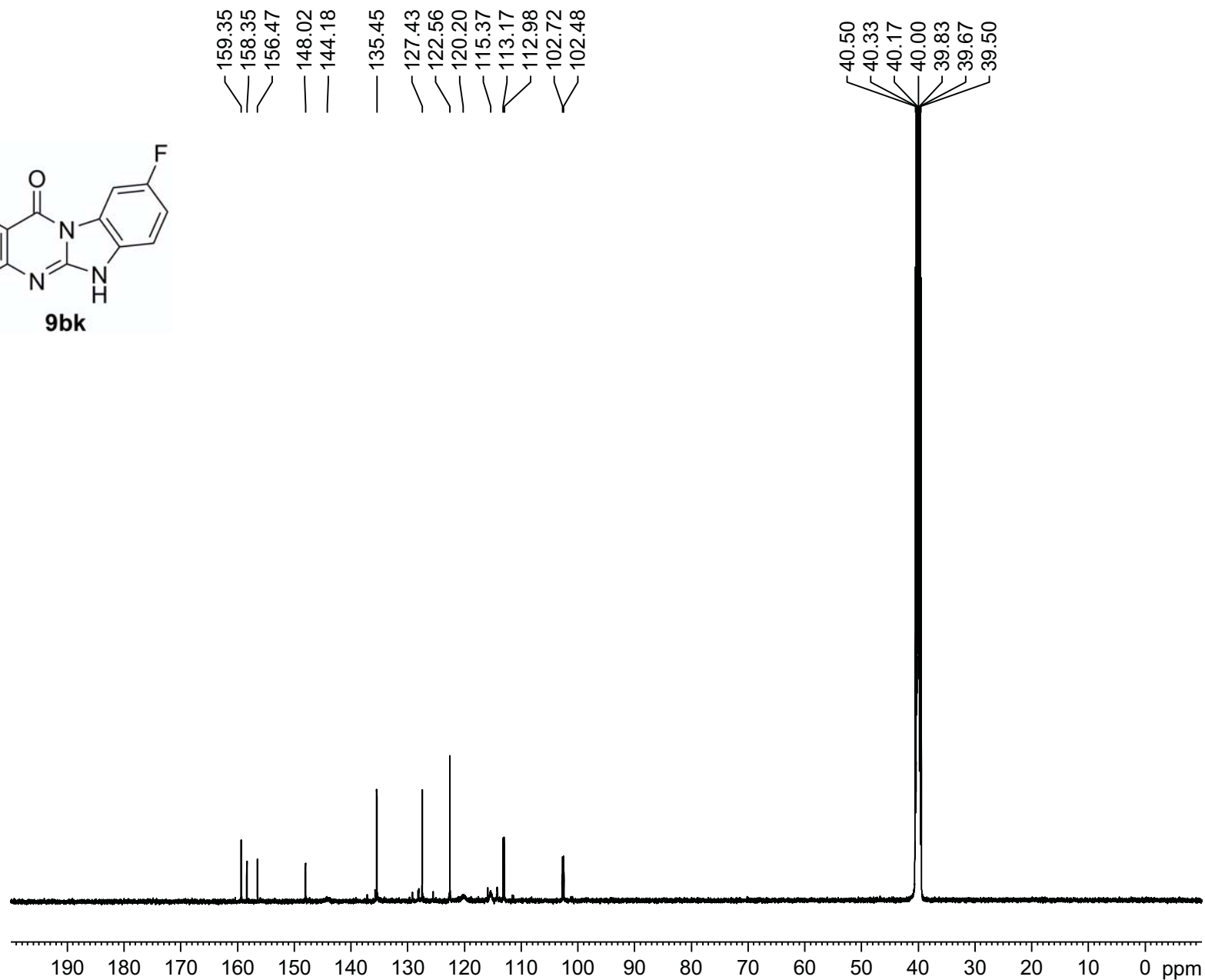
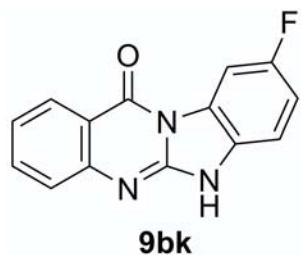
Current Data Parameters
NAME TCC-2014110118
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141112
Time 8.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 256
DW 55.200 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 65536
SF 500.1300049 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

¹³C of re 172



Current Data Parameters
NAME TCC-2014110118
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141111
Time 14.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 20000
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

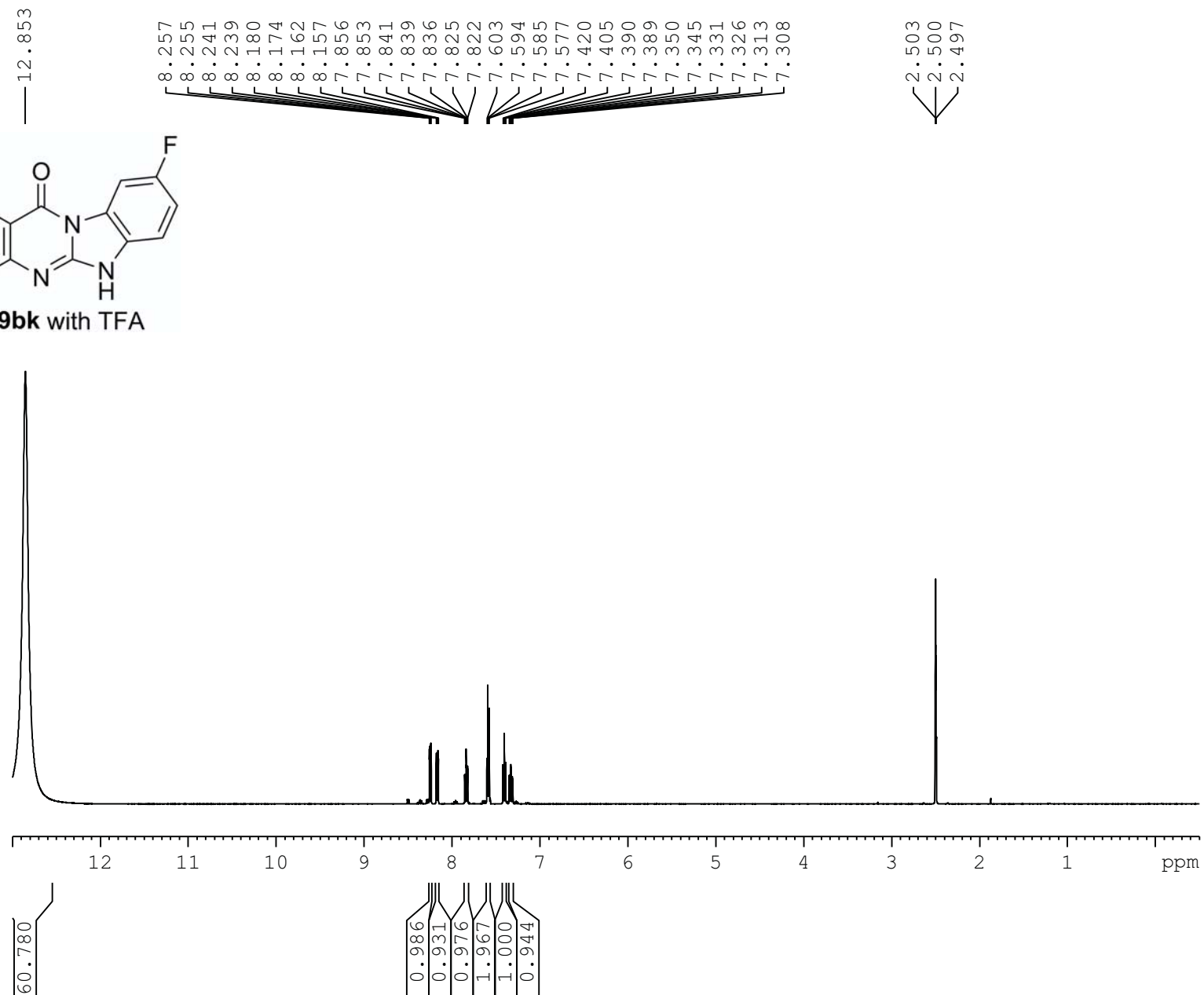
===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577908 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

¹H of re 172+TFA



9bk with TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 15
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141114
Time 17.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 9057.971 Hz
FIDRES 0.138214 Hz
AQ 3.6175871 sec
RG 114
DW 55.200 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

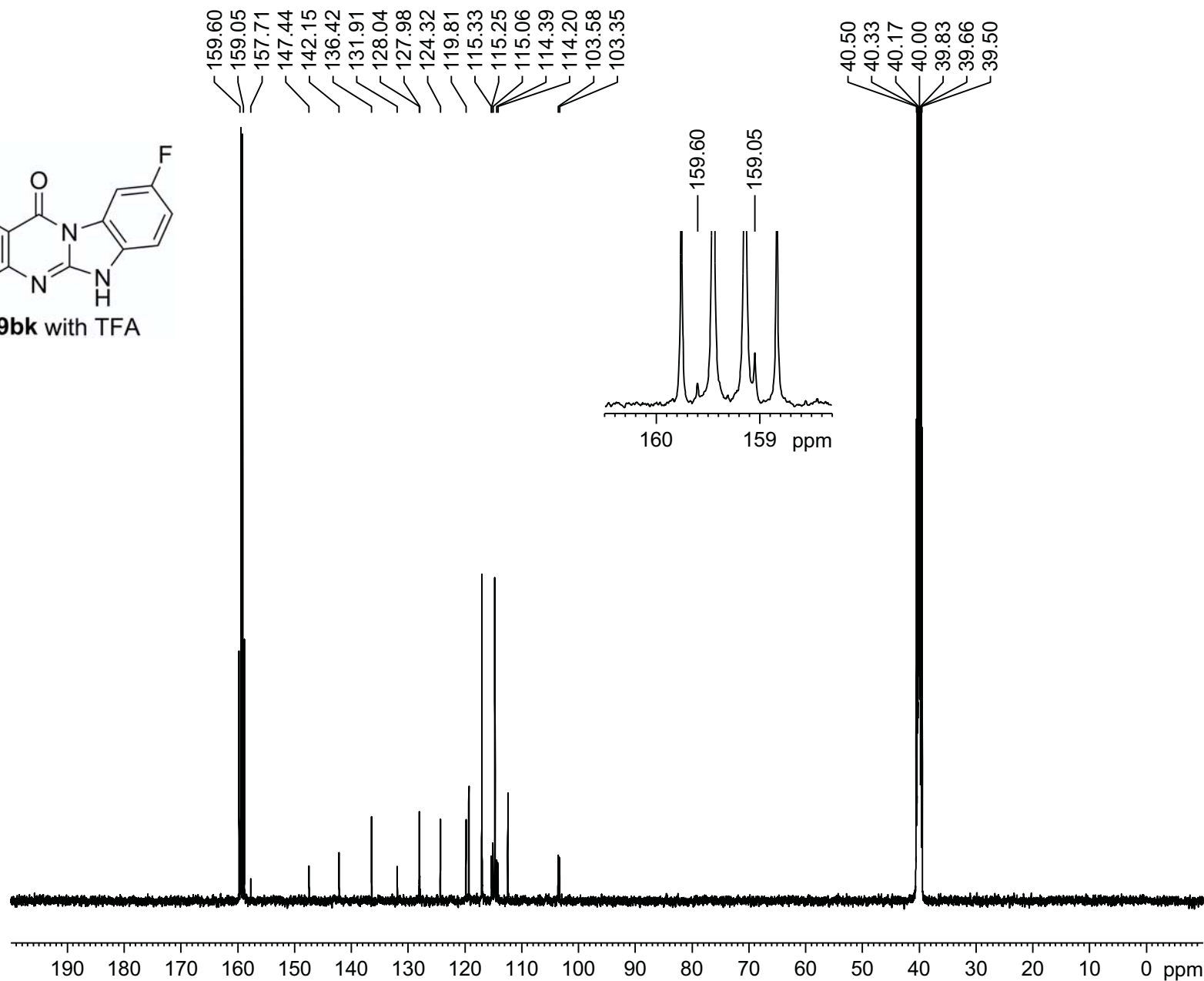
===== CHANNEL f1 =====
NUC1 1H
P1 13.20 usec
PL1 -0.60 dB
SFO1 500.1330008 MHz

F2 - Processing parameters
SI 16384
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

¹³C of re 172+TFA



9bk with TFA



Current Data Parameters
NAME TCC-2014110118
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141114
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1487
DS 0
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 8192
DW 16.500 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ¹³C
P1 10.00 usec
PL1 6.50 dB
SFO1 125.7709936 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.20 dB
PL13 18.20 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 65536
SF 125.7577335 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00