Supplementary information

One-pot build-up procedure for the synthesis of variously substituted purine derivatives
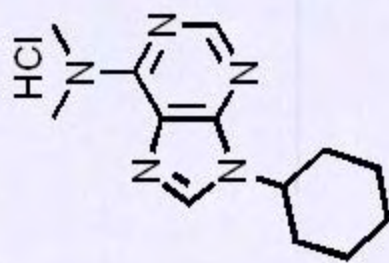
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Table 1, Entry 3

Dejmek_MD327
1H NMR in DMSO
1-11-11 DR
****

NAME   Dejmek_MD32
EXPNO   1
PROCNO   1
Date_   20111101
Time   12.17
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 =
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 N
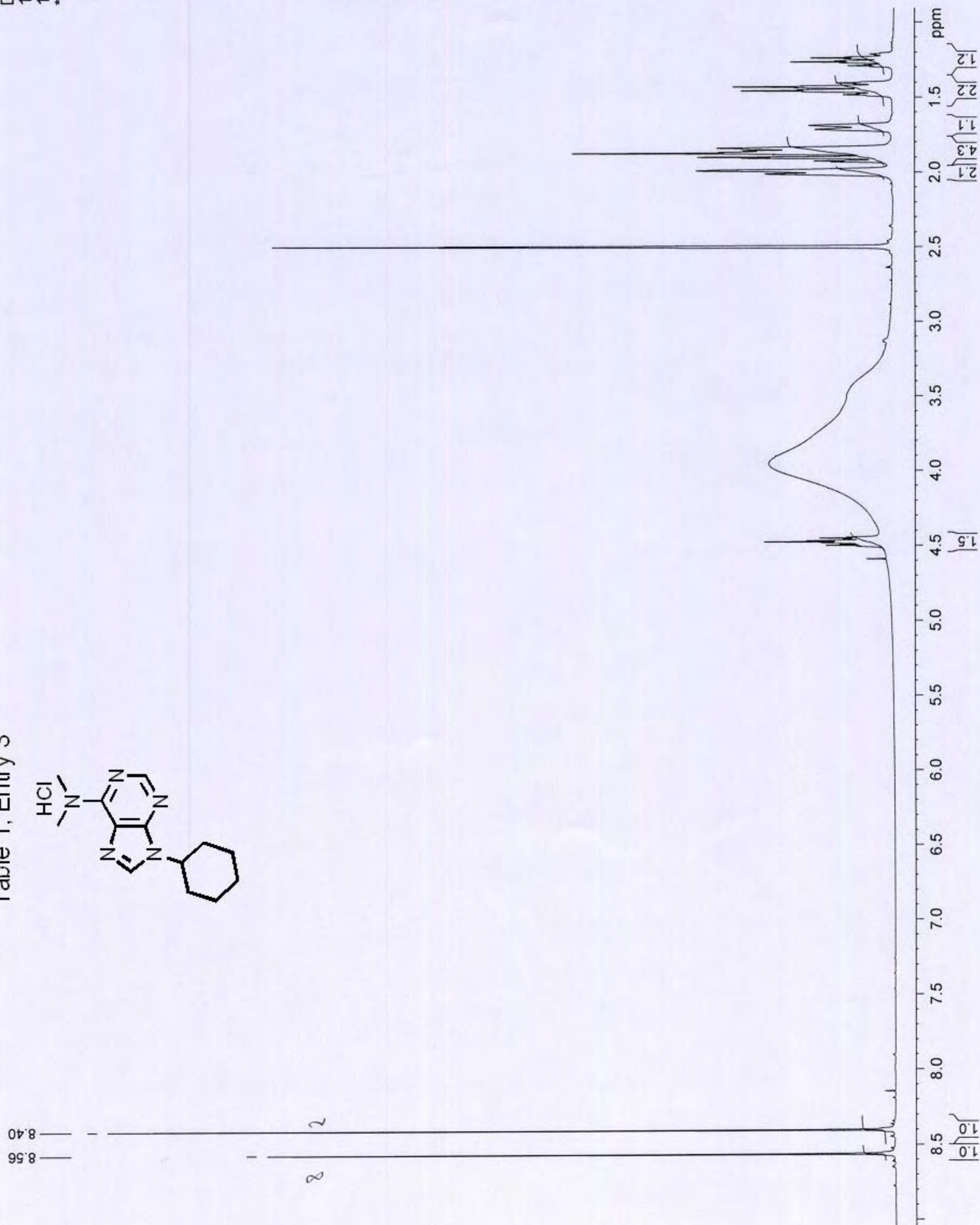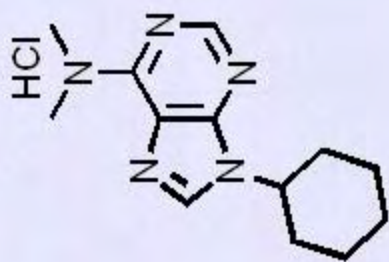SI   131072
SF   499.9499978 MI-
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

8.40
8.56

Dejmek_MD327
APT in DMSO
1-11-11 DR
****

NAME   Dejmek_MD327
EXPNO   2
PROCNO   1
Date_   20111101
Time   13.24
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1279
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125590 MHz
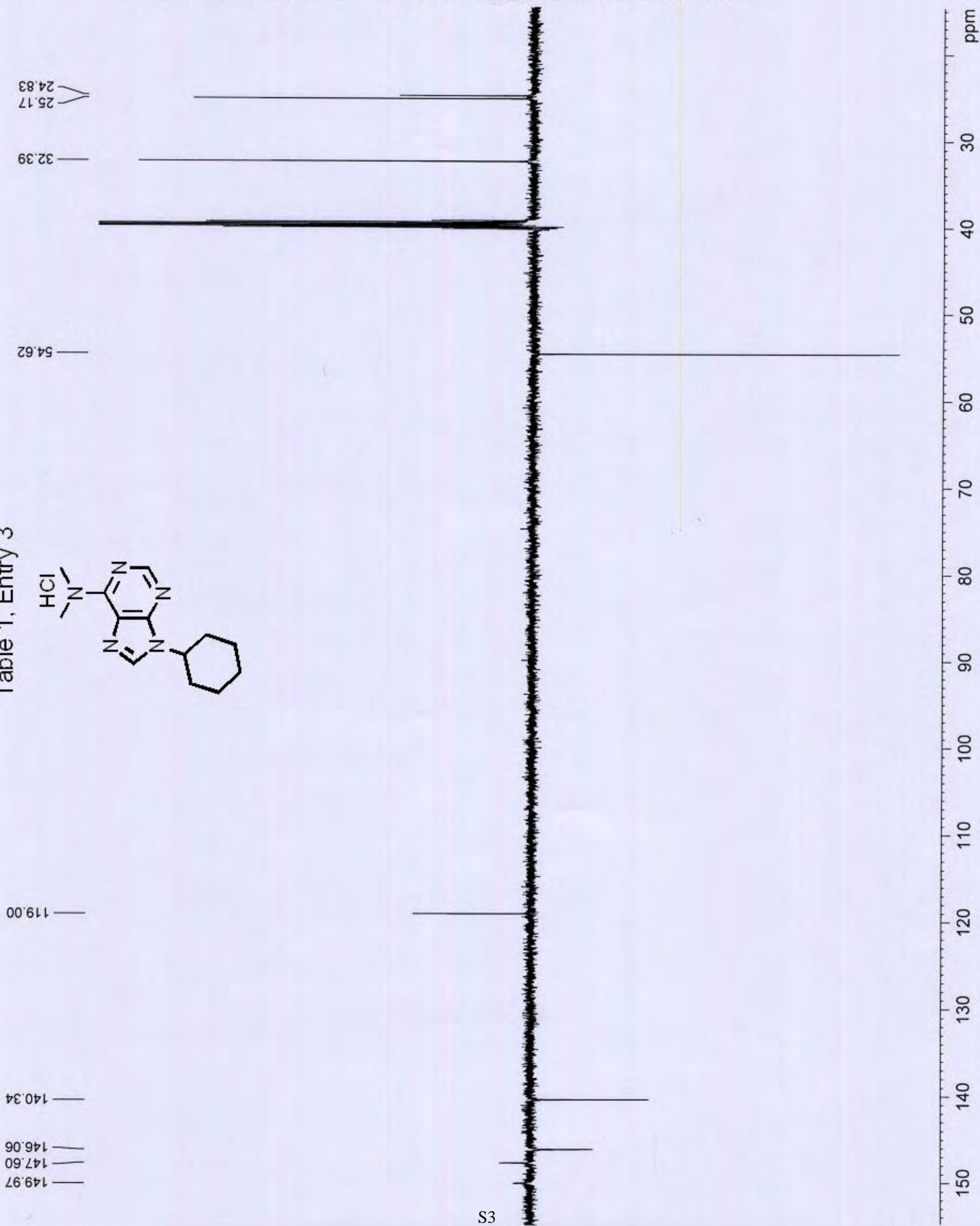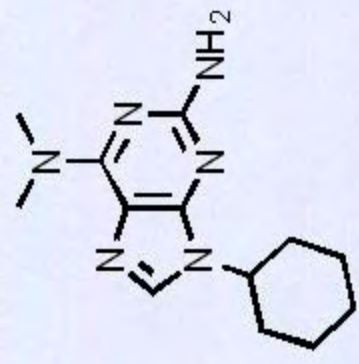WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

24.83
25.17

32.39

54.62

Table 1, Entry 3

119.00

140.34

146.06
147.60

149.97

ppm

30
40
50
60
70
80
90
100
110
120
130
140
150

S3

Table 1, Entry 11

Dejmek_MD328
1H-NMR in DMSO
8.9.2011 DR
****

NAME   Dejmek_MD328
EXPNO   1
PROCNO   1
Date_   20110908
Time_   9.51
INSTRUM   spect
PROBHD   5 mm CPTCI 1H-
PULPROG   zg30
TD   72114
SOLVENT   DMSO
NS   32
DS   0
SWH   9014.423 Hz
FIDRES   0.125002 Hz
AQ   3.9999733 sec
RG   9
DW   55.467 usec
DE   20.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   1H
P1   10.00 usec
PL1   8.10 dB
PL1W   5.29101372 W
SFO1   600.1330006 MHz
SI   131072
SF   600.1300065 MHz
WDW   no
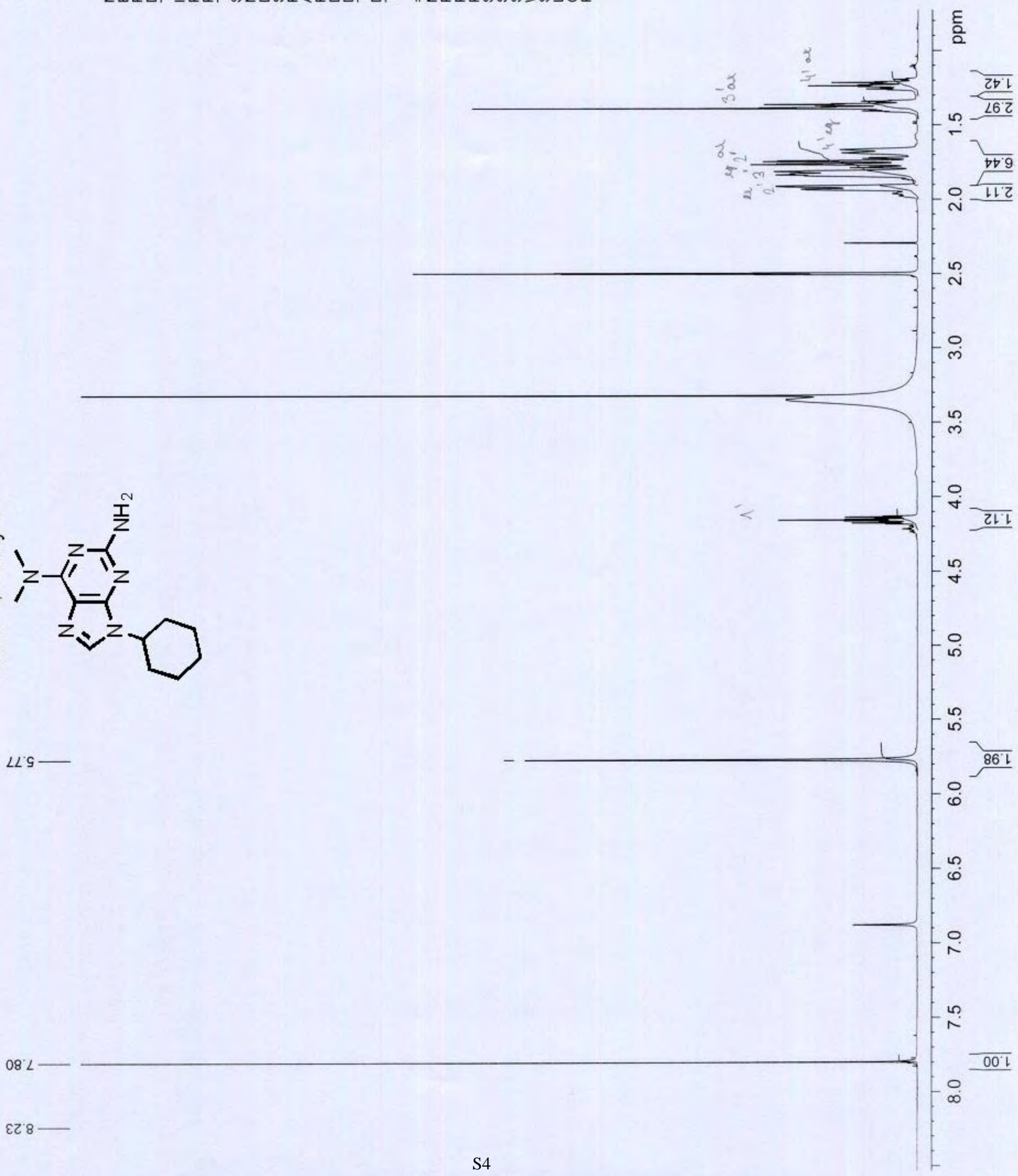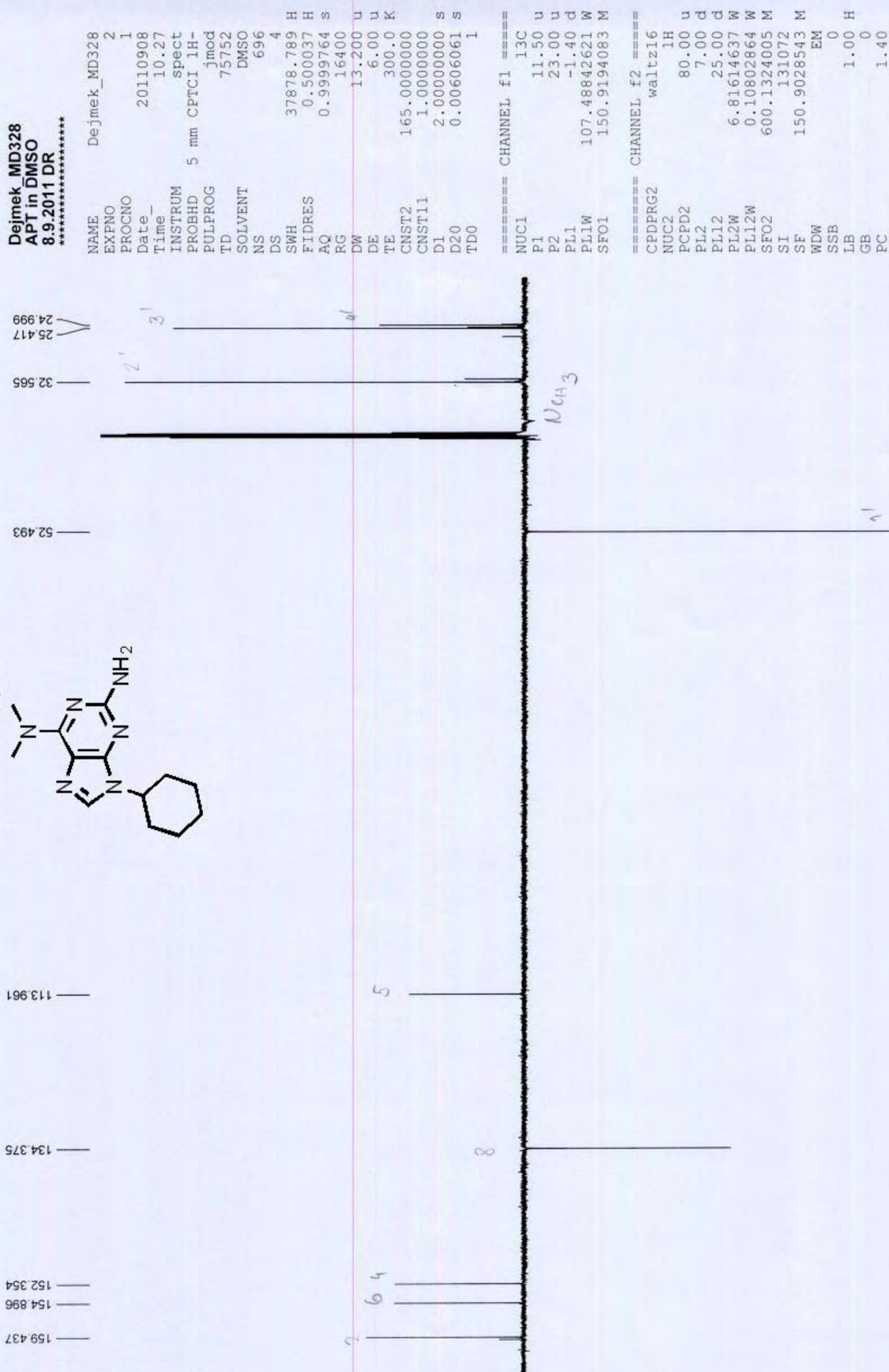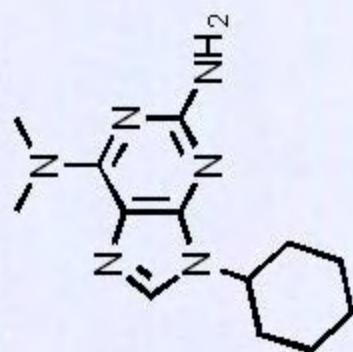SSB   0
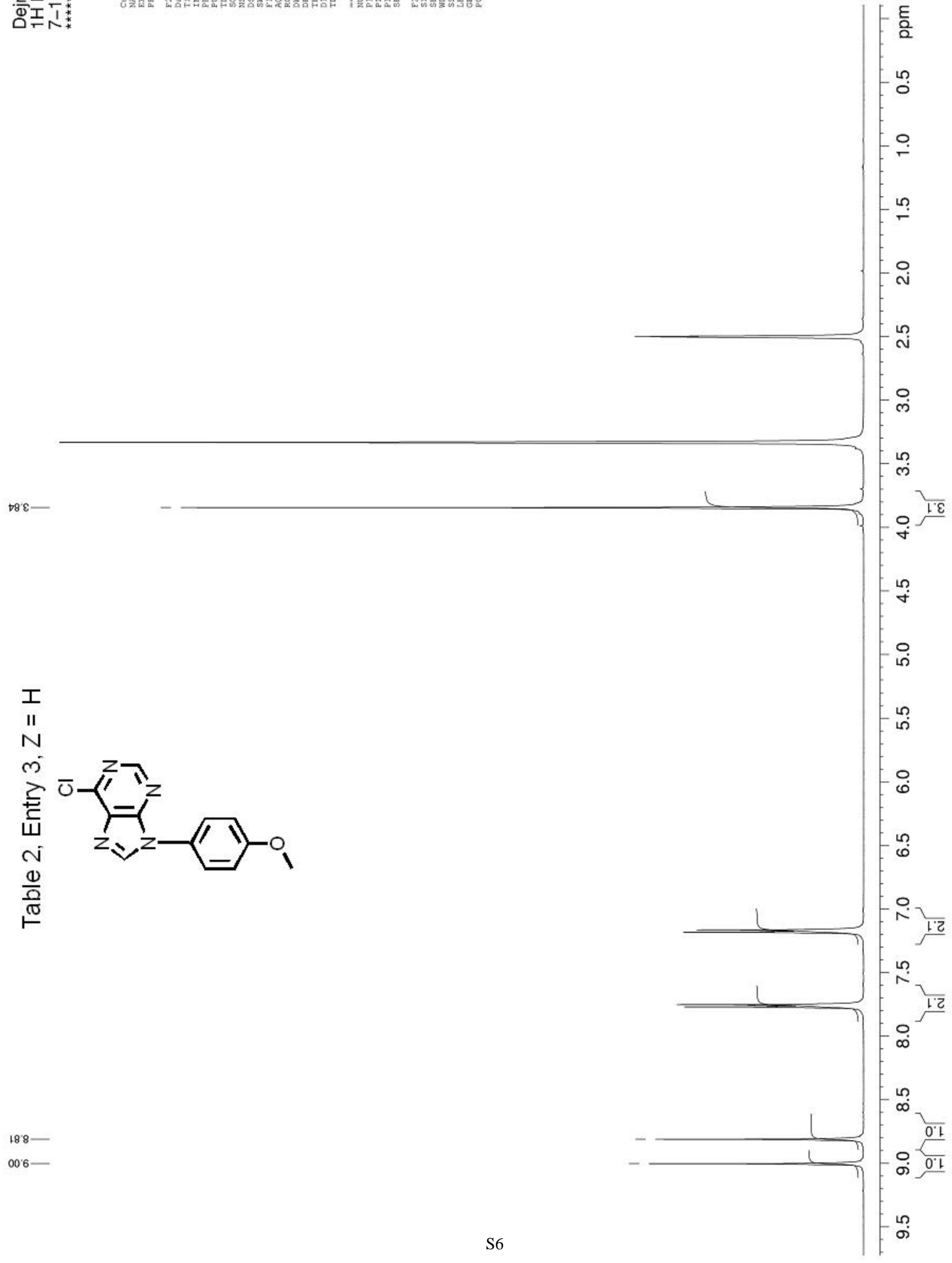LB   0.00 Hz
GB   0
PC   0.50

8.23
7.80
5.77

ppm 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 ppm

1.00   1.98   1.12   2.11 6.44 2.97 1.42

Dejmek_MD328
APT in DMSO
8.9.2011 DR
****

NAME	Dejmek_MD328
EXPNO	2
PROCNO	1
Date_	20110908
Time	10.27
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	jmod
TD	75752
SOLVENT	DMSO
NS	696
DS	4
SWH	37878.789 H
FIDRES	0.500037 H
AQ	0.9999764 s
RG	16400
DW	13.200 u
DE	6.00 u
TE	300.0 K
CNST2	165.0000000
CNST11	1.0000000
D1	2.00000000 s
D20	0.00606061 s
TD0	1
========	CHANNEL f1 ========
NUC1	13C
P1	11.50 u
P2	23.00 u
PL1	-1.40 d
PL1W	107.48842621 W
SFO1	150.9194083 M
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 u
PL2	7.00 d
PL12	25.00 d
PL2W	6.81614637 W
PL12W	0.10802864 W
SFO2	600.1324005 M
SI	131072
SF	150.9028543 M
WDW	EM
SSB	0
LB	1.00 H
GB	0
PC	1.40

Table 1, Entry 11

Dejmek_MD381
1H NMR in DMSO
7-12-11 DR

Table 2, Entry 3, Z = H

Dejmek_MD381
APT in DMSO
7-12-11 DR
****

NAME   Dejmek_MD381
EXPNO   2
PROCNO   1
Date_   20111207
Time   14.48
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   376
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125630 MHz
WDW   EM
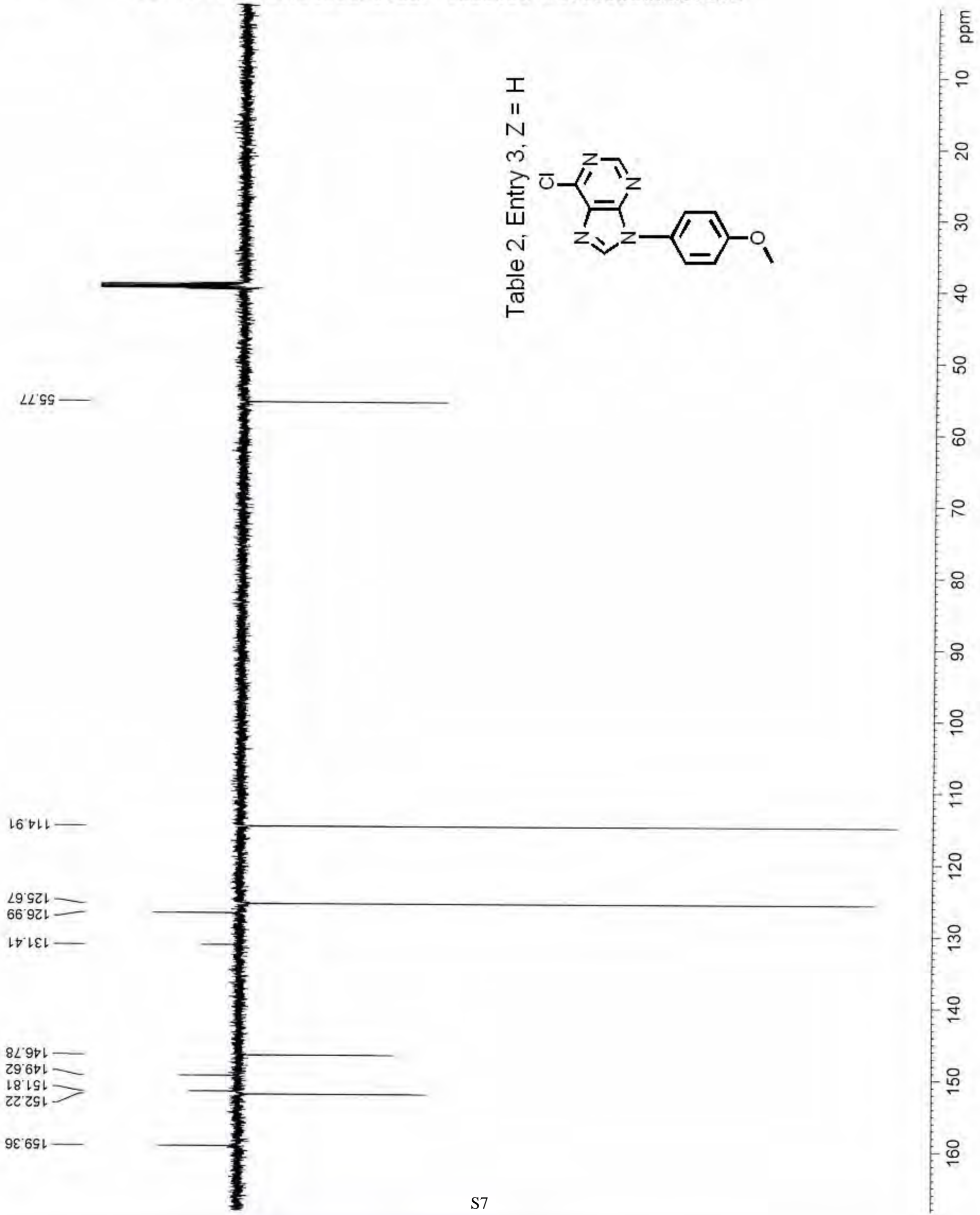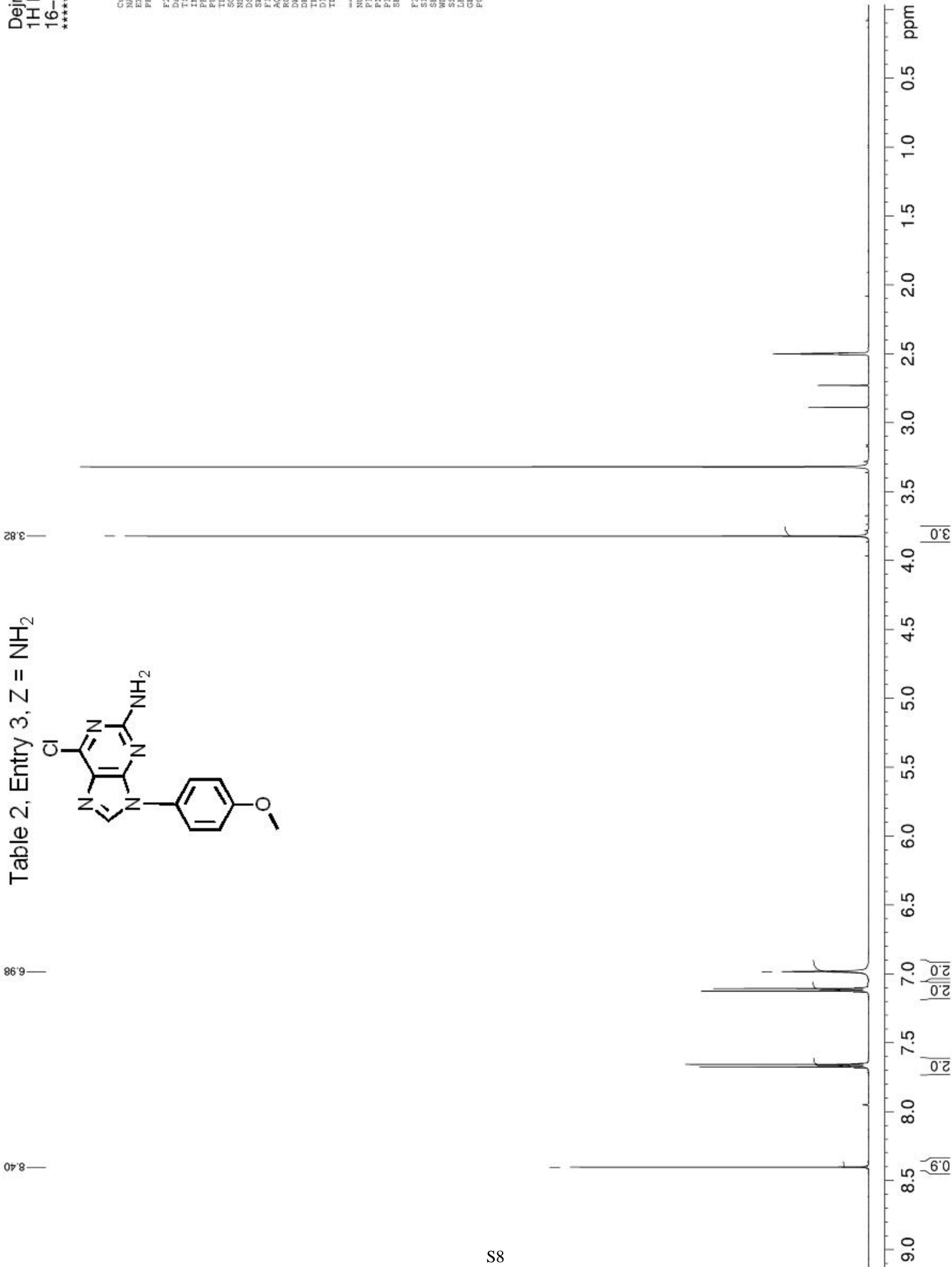SSB   0
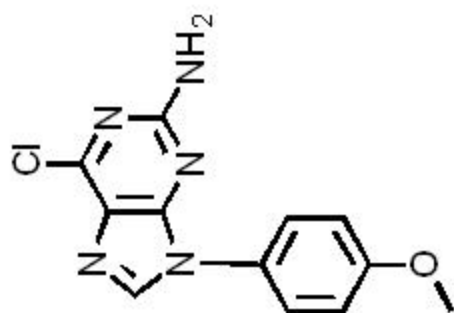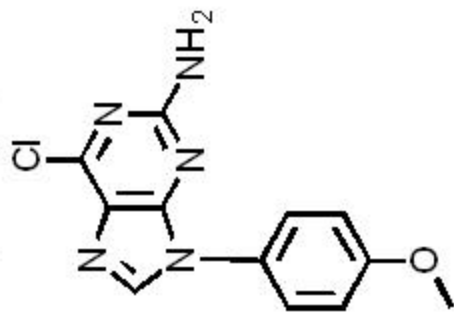LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 3, Z = H

55.77

114.91

125.67
126.99

131.41

146.78
149.62
151.81
152.22

159.36

ppm
10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160

S7

Dejmek_MD364
1H NMR in DMSO
16–11–11 DR
****

Current Data Parameters
NAME   Dejmek_MD364
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20111116
Time   13.41
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz

F2 - Processing parameters
SI   131072
SF   499.9499979 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 3, Z = NH$_2$

3.82

6.98

8.40

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

3.0   2.0 2.0   2.0   0.9

S8

Dejmek_MD364
APT in DMSO
16–11–11 DR
****
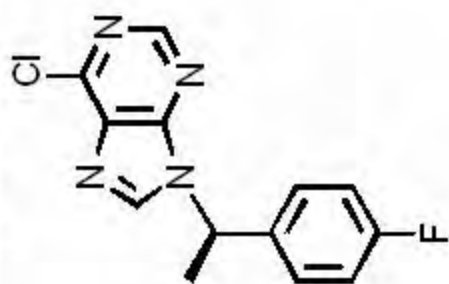
Current Data Parameters
NAME   Dejmek_MD364
EXPNO   2
PROCNO   1

F2 – Acquisition Parameters
Date_   20111116
Time   14.00
INSTRUM   spect
PROBHD   5 mm TXI 1H–13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1261
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.0000000 sec
D20   0.00606061 sec
TD0   1

===== CHANNEL f1 =====
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz

F2 – Processing parameters
SI   131072
SF   125.7125639 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 3, Z = NH$_2$

55.73

114.75

123.69
125.57
127.58

142.45

149.98

154.02

158.94
160.34

ppm

10   20   30   40   50   60   70   80   90   100   110   120   130   140   150   160

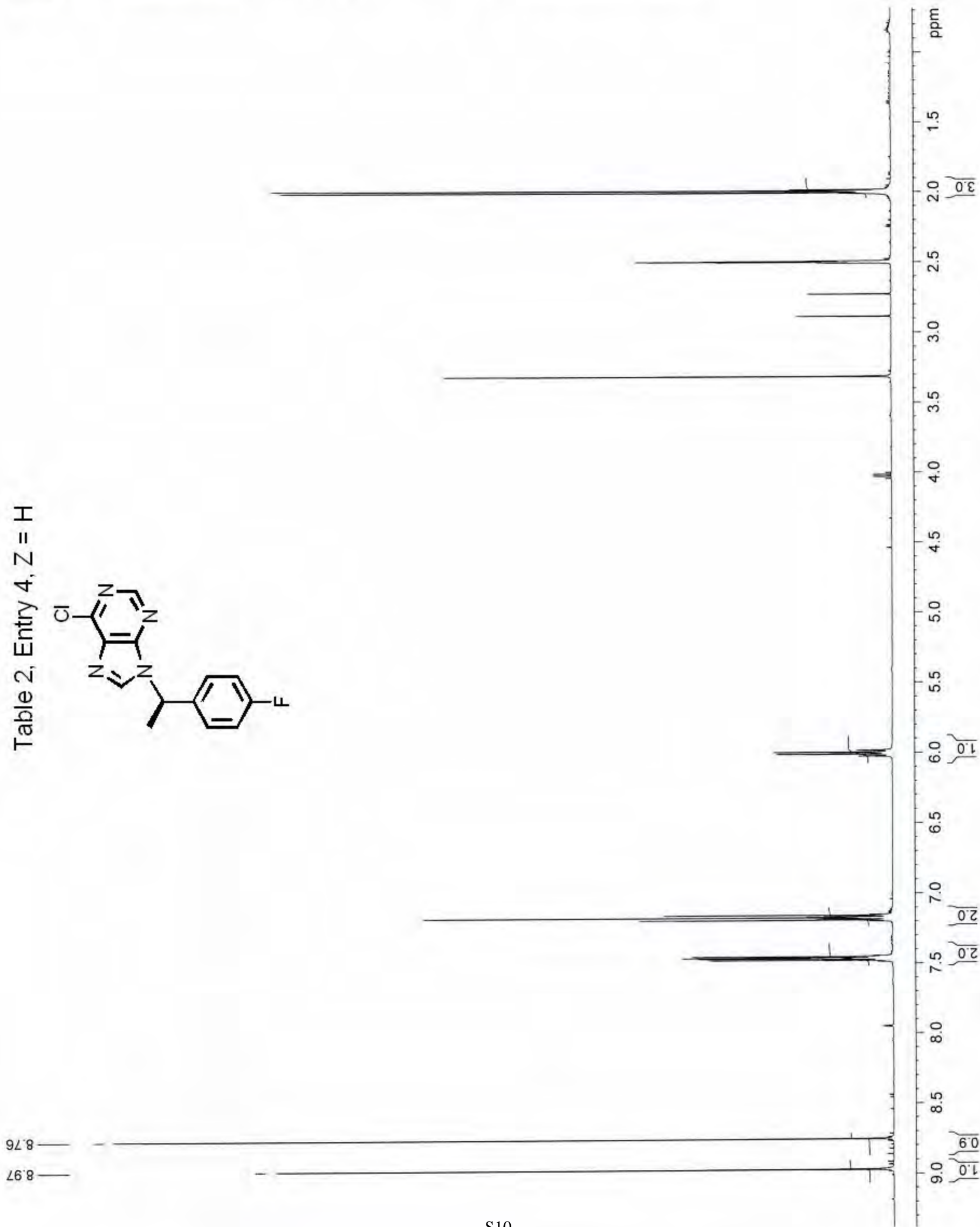S9

Dejmek_MD342
1H NMR in DMSO
12-10-11 DR
****

NAME   Dejmek_MD34
EXPNO   1
PROCNO   1
Date_   20111012
Time   17.10
INSTRUM   spect
PROBHD   5 mm TXI 1H
PULPROG
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023700 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.1 K
D1   1.00000000 sec
TD0   1

===== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500007 MH
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 4, Z = H

8.76
8.97
ppm

S10

Dejmek_MD342
APT in DMSO
12-10-11 DR
****

NAME   Dejmek_MD342
EXPNO   2
PROCNO   1
Date_   20111012
Time   17.51
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   768
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.72263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125663 MHz
WDW   EM
SSB   0
LB   1.00 Hz
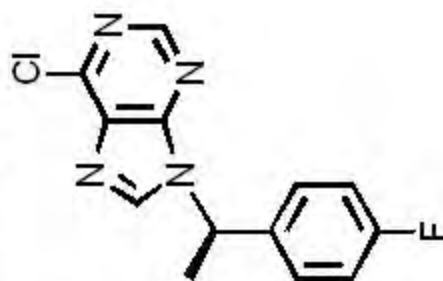GB   0
PC   1.00

20.42

54.00

115.61
115.78
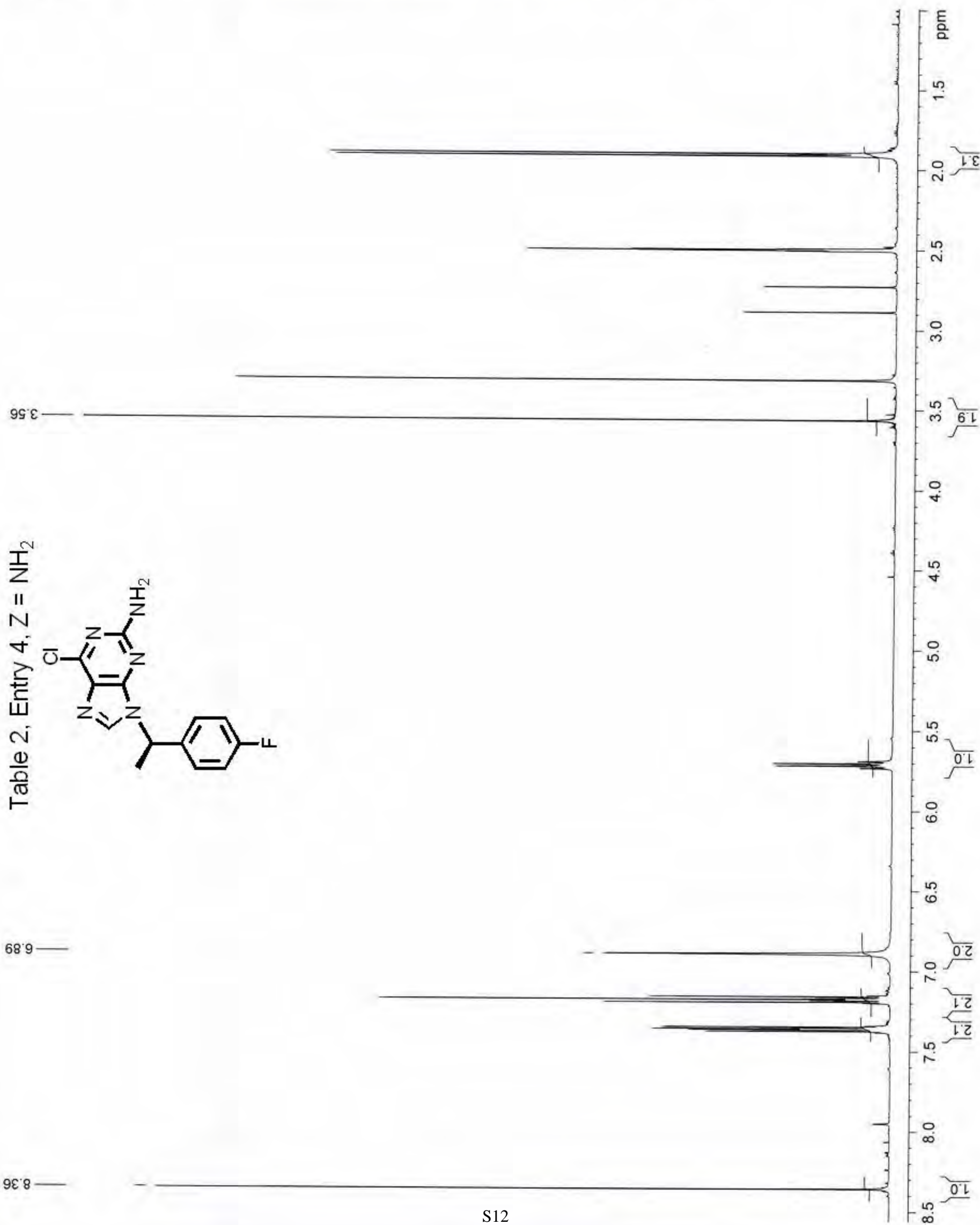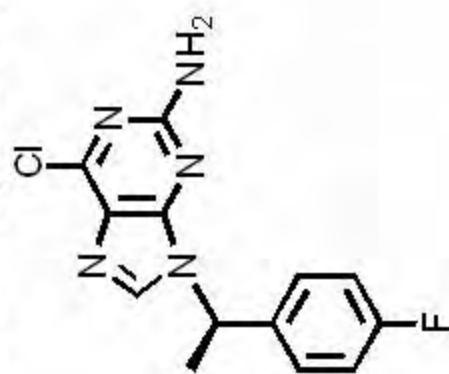
128.74
128.80
131.29

136.98
137.00

146.07

149.35

151.65

160.83
162.78

Table 2, Entry 4, Z = H

S11

Dejmek_MD341
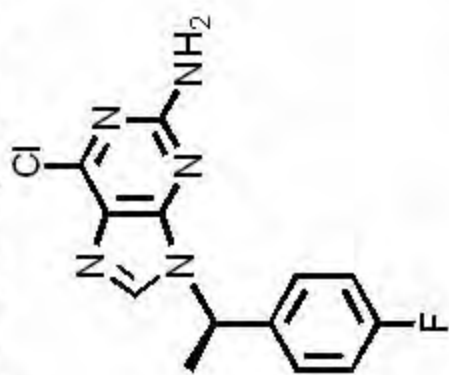1H NMR in DMSO
12-10-11 DR
****

NAME   Dejmek_MD341
EXPNO   1
PROCNO   1
Date_   20111012
Time   15.24
INSTRUM   spect
PROBHD   5 mm TXI 1H
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.1 K
D1   1.00000000 sec
TD0   1

====== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500006 MH
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 4, Z = NH₂

8.36 —
6.89 —
3.55 —

ppm

1.1 3.1 1.9 1.0 2.0 2.1 2.1 1.0

Dejmek_MD341
APT in DMSO
12-10-11 DR
****

NAME   Dejmek_MD341
EXPNO   2
PROCNO   1
Date_   20111012
Time   15.44
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1196
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.1 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125657 MHz
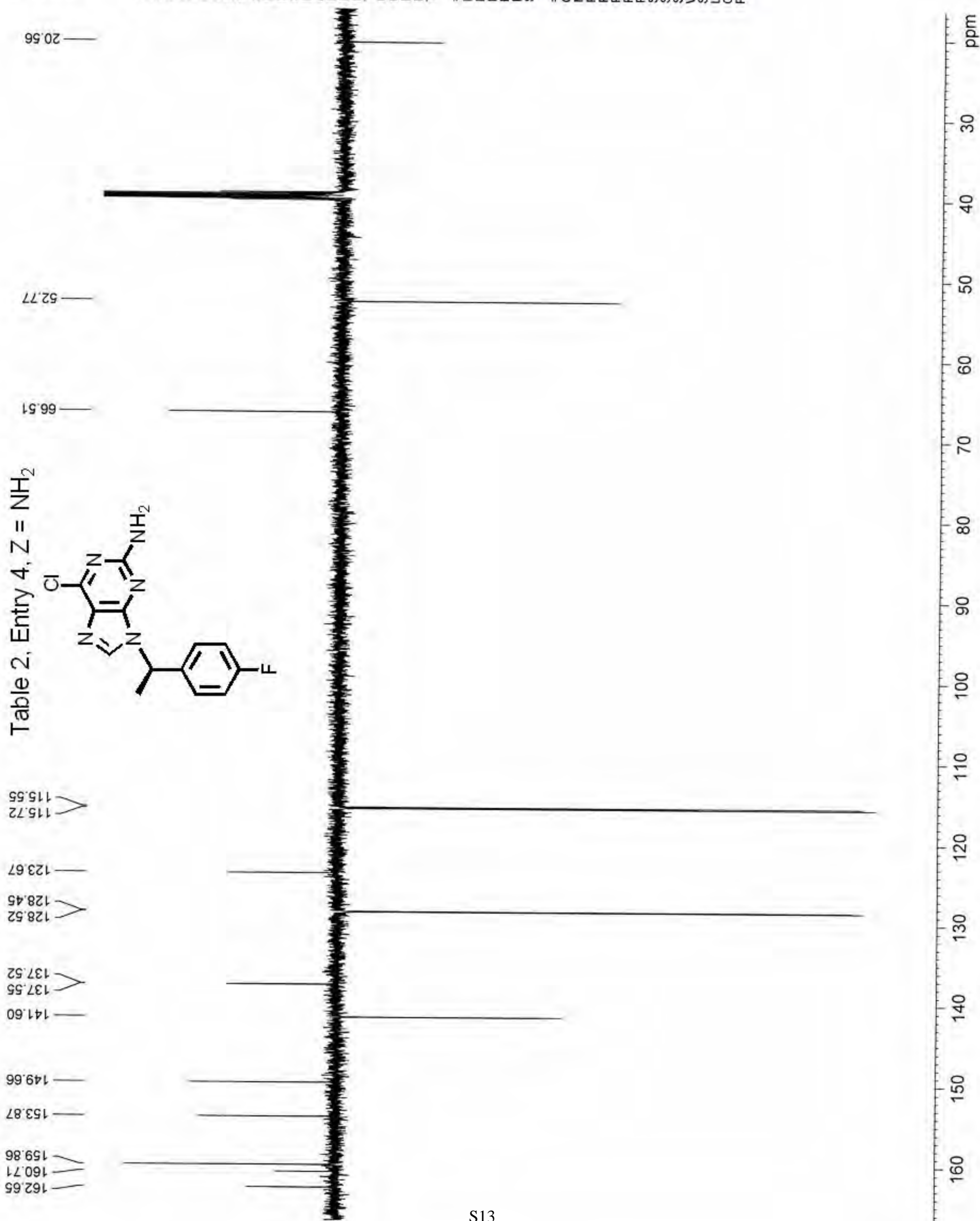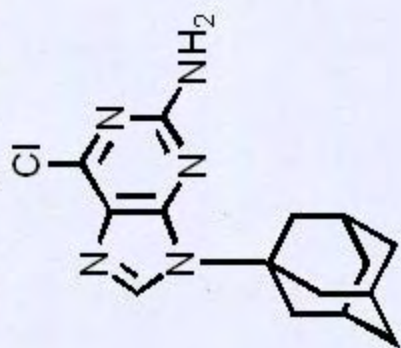WDW   EM
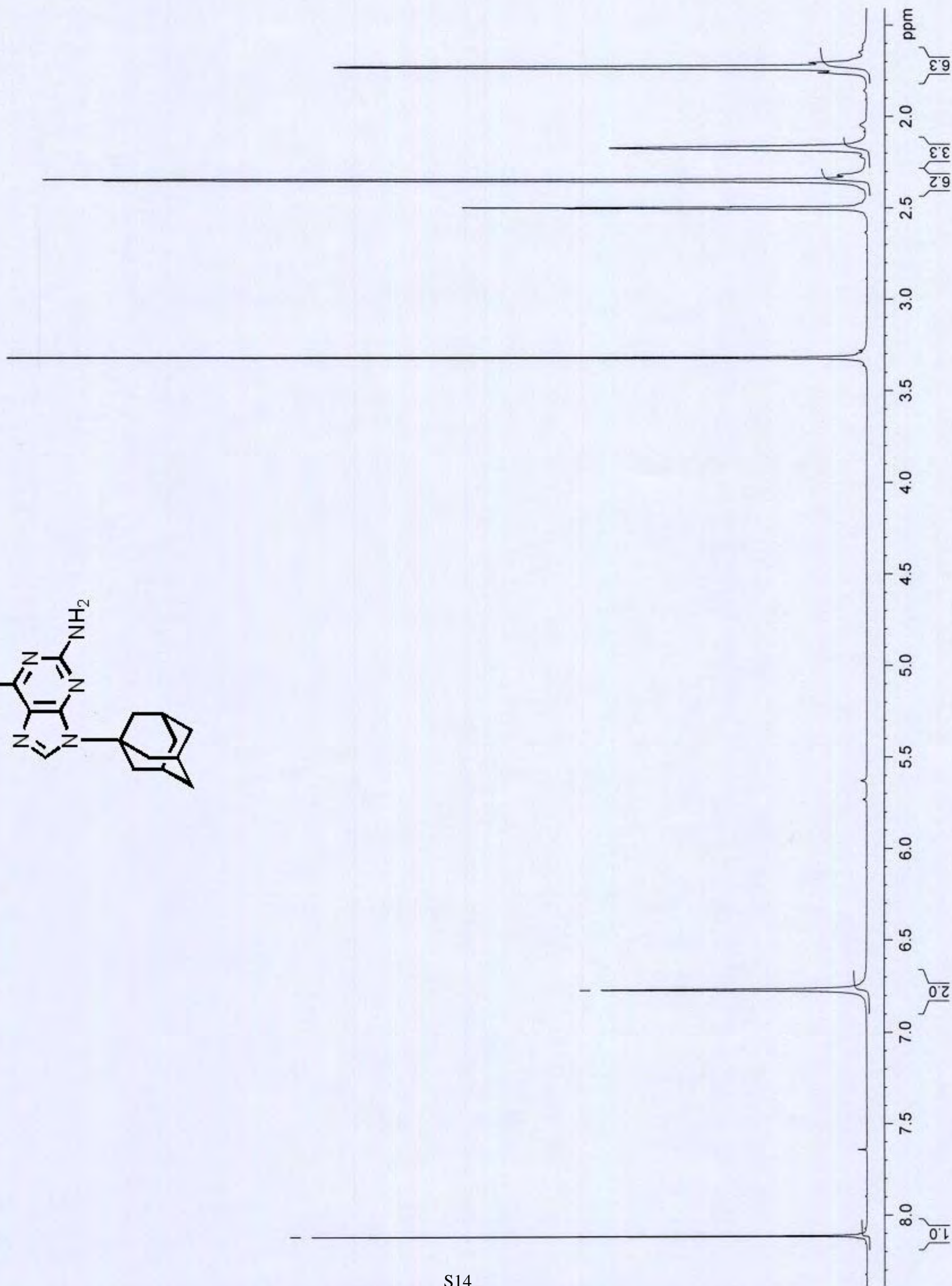SSB   0
LB   1.00 Hz
GB   0
PC   1.00

20.56

52.77

66.51

Table 2, Entry 4, Z = NH$_2$

115.55
115.72

123.67

128.45
128.52

137.52
137.55

141.60

149.66

153.87

159.86
160.71
162.65

ppm

S13

Dejmek_MD330
1H NMR in DMSO
7-9-11 DR
****

NAME   Dejmek_MD33
EXPNO   1
PROCNO   1
Date_   20110907
Time   15.13
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 H:
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
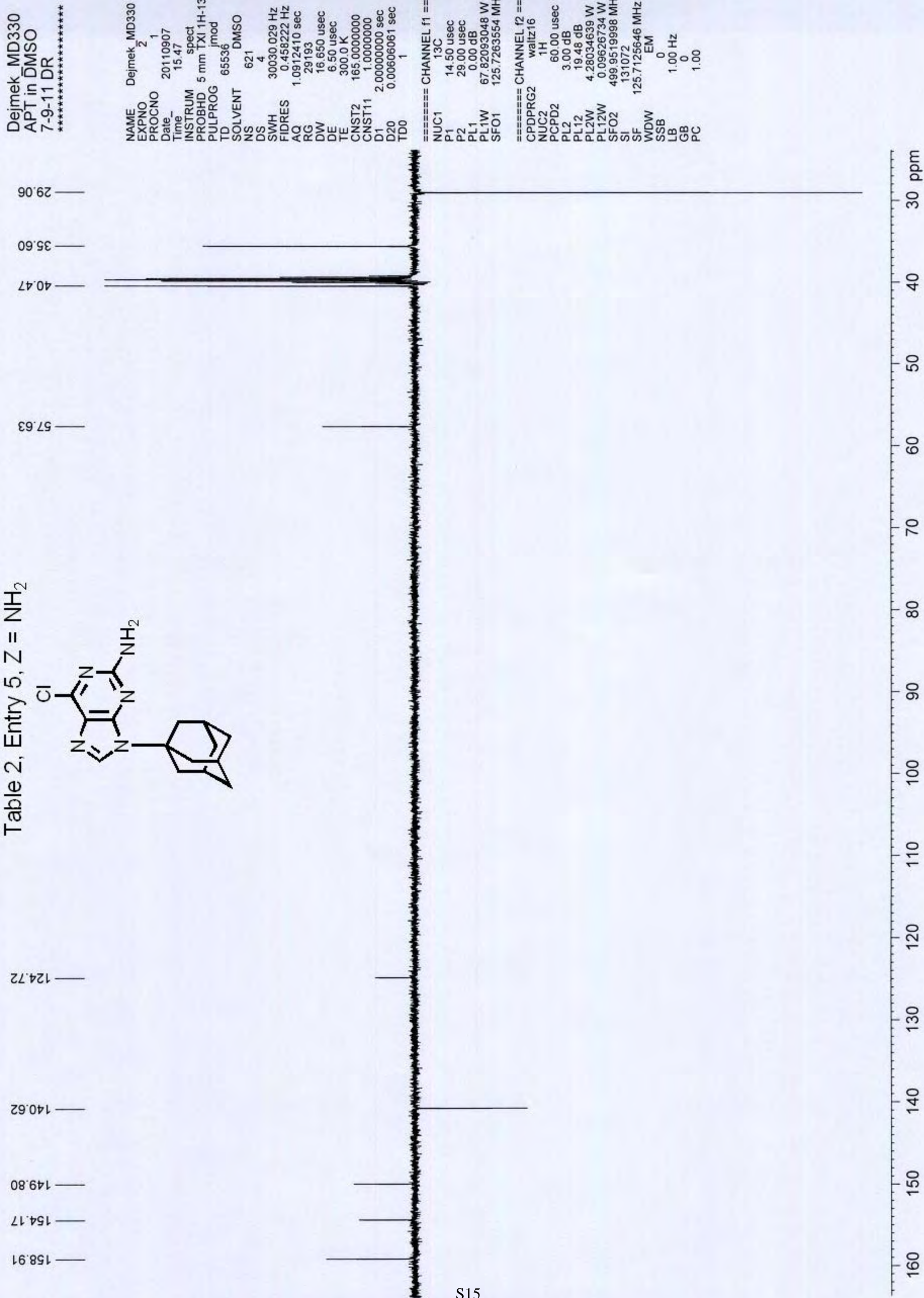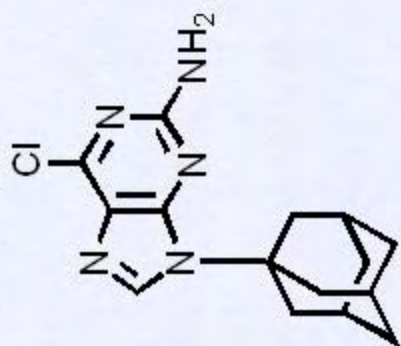SF   499.9499988 MI-
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 5, Z = NH₂

8.11 —

6.77 —

Dejmek_MD330
APT in DMSO
7-9-11 DR
****

NAME   Dejmek_MD330
EXPNO   2
PROCNO   1
Date_   20110907
Time   15.47
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   621
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

====== CHANNEL f1 ======
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

====== CHANNEL f2 ======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125646 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 5, Z = NH$_2$

29.06
35.60
40.47
57.63
124.72
140.62
149.80
154.17
158.91

ppm 30 40 50 60 70 80 90 100 110 120 130 140 150 160

S15

Dejmek_MD336
1H NMR in DMSO
16-9-11 DR
****

NAME   Dejmek_MD33
EXPNO   1
PROCNO   1
Date_   20110916
Time   10.32
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 H:
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
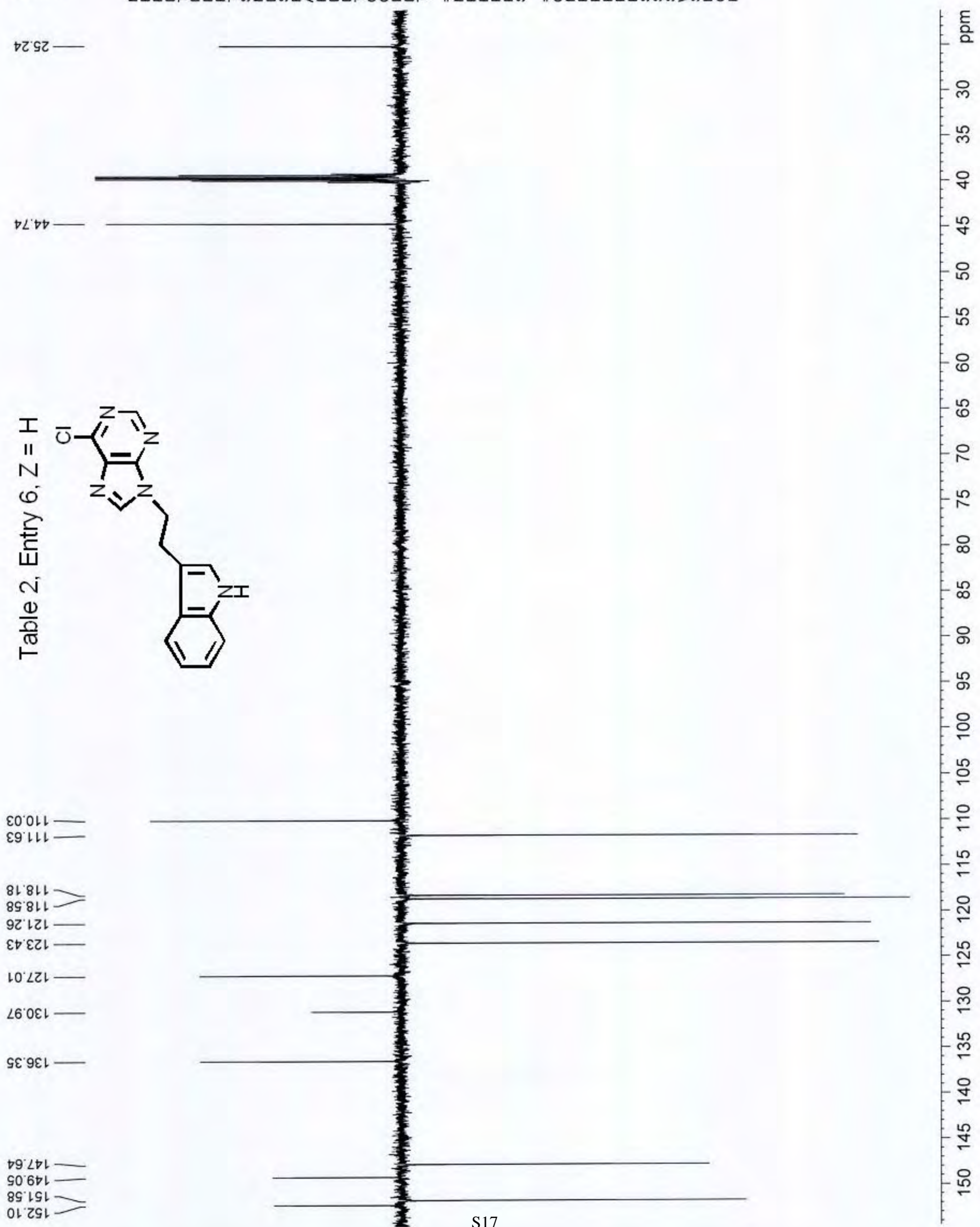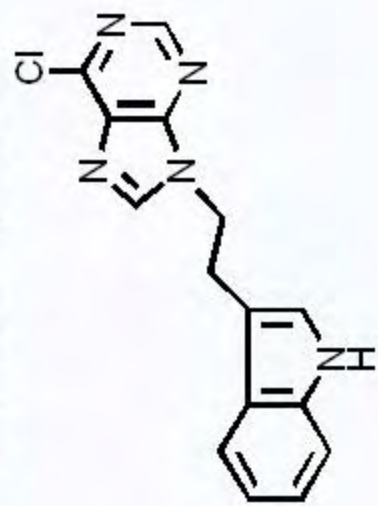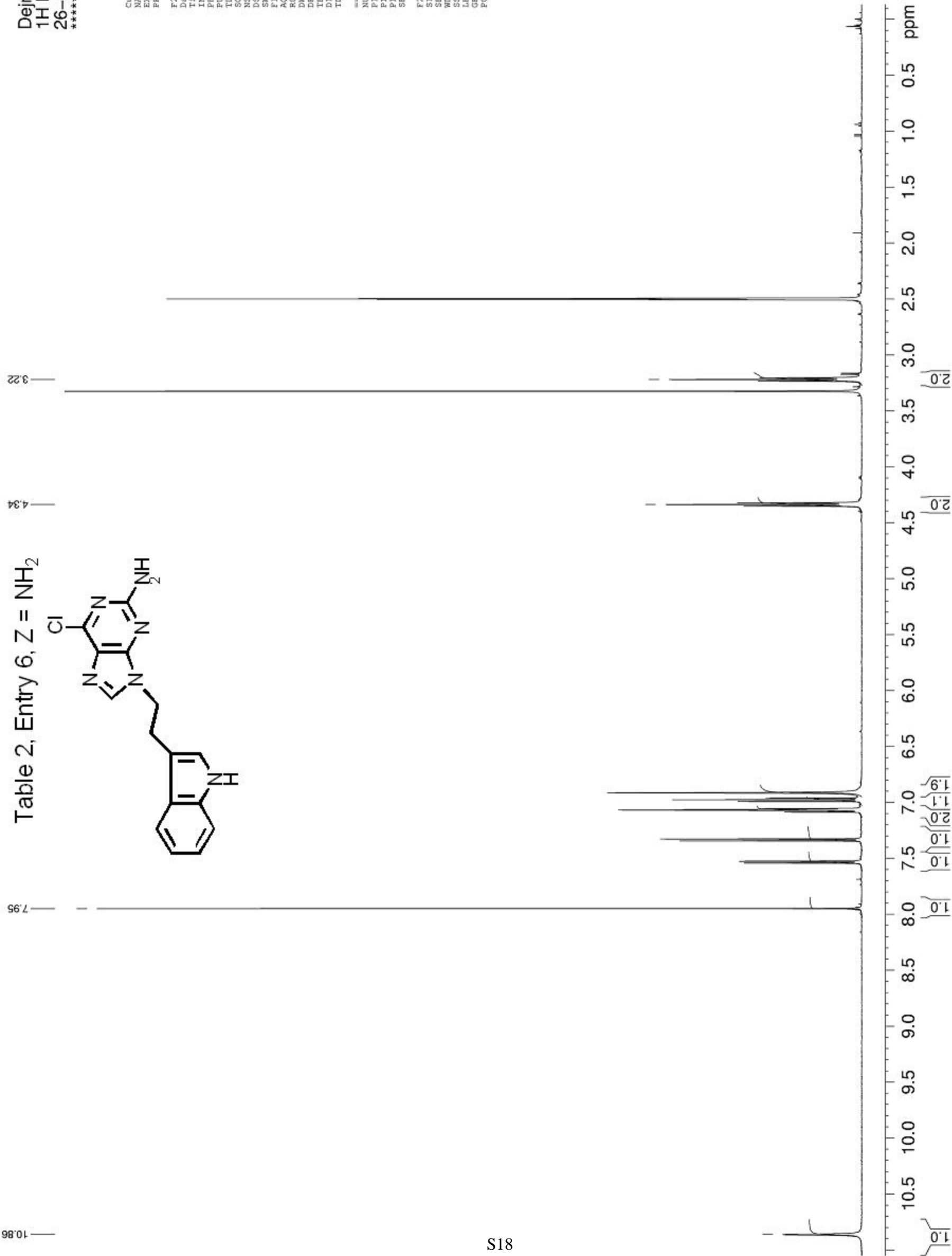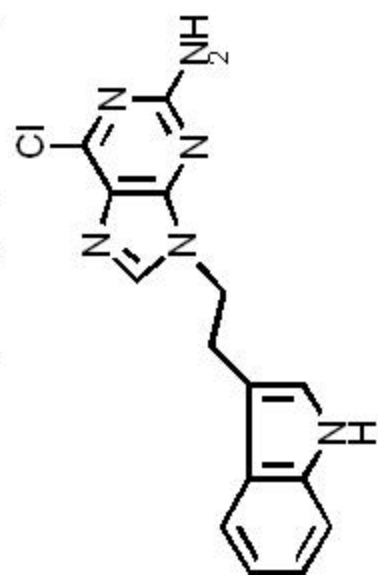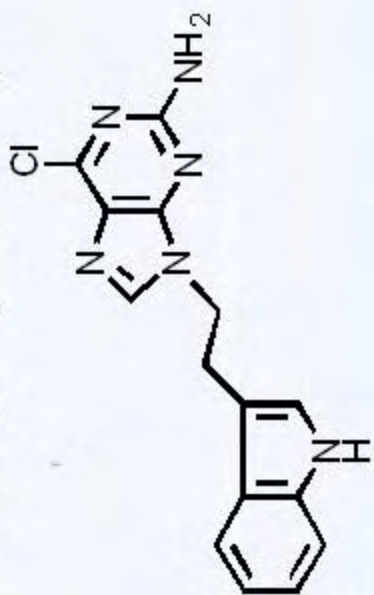DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======= CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 V
SFO1   499.9534997 N
SI   131072
SF   499.9500005 MI
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 6, Z = H

10.86 —

8.79 —
8.54 —

4.58 —

ppm
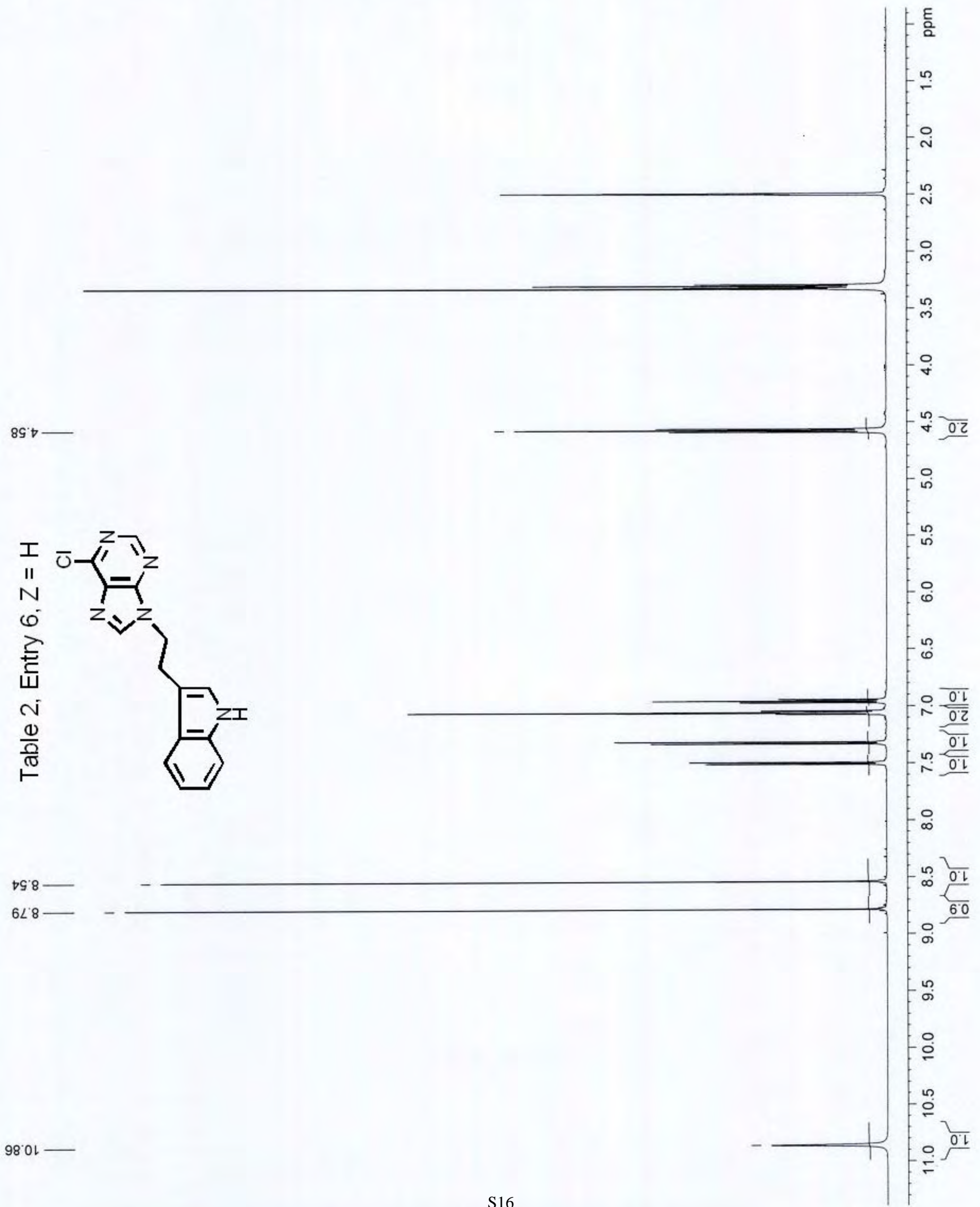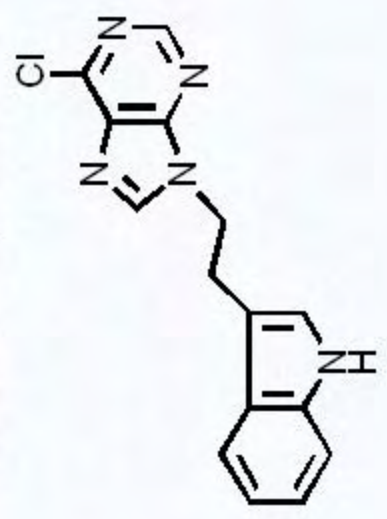
Dejmek_MD336
APT in DMSO
16-9-11 DR
****

NAME   Dejmek_MD336
EXPNO   2
PROCNO   1
Date_   20110916
Time   11.08
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   687
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125654 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 6, Z = H

25.24

44.74

110.03
111.63

118.18
118.58
121.26
123.43

127.01

130.97

136.35

147.64
149.05
151.58
152.10

ppm

150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30

S17

Dejmek_MD332
1H NMR in DMSO
26–9–11 DR
****

Table 2, Entry 6, Z = NH₂

10.86

7.95

4.34

3.22

Dejmek_MD332
APT in DMSO
26-9-11 DR
****

NAME   Dejmek_MD332
EXPNO   2
PROCNO   1
Date_   20110926
Time   16.26
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   493
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1W   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125655 MHz
WDW   EM
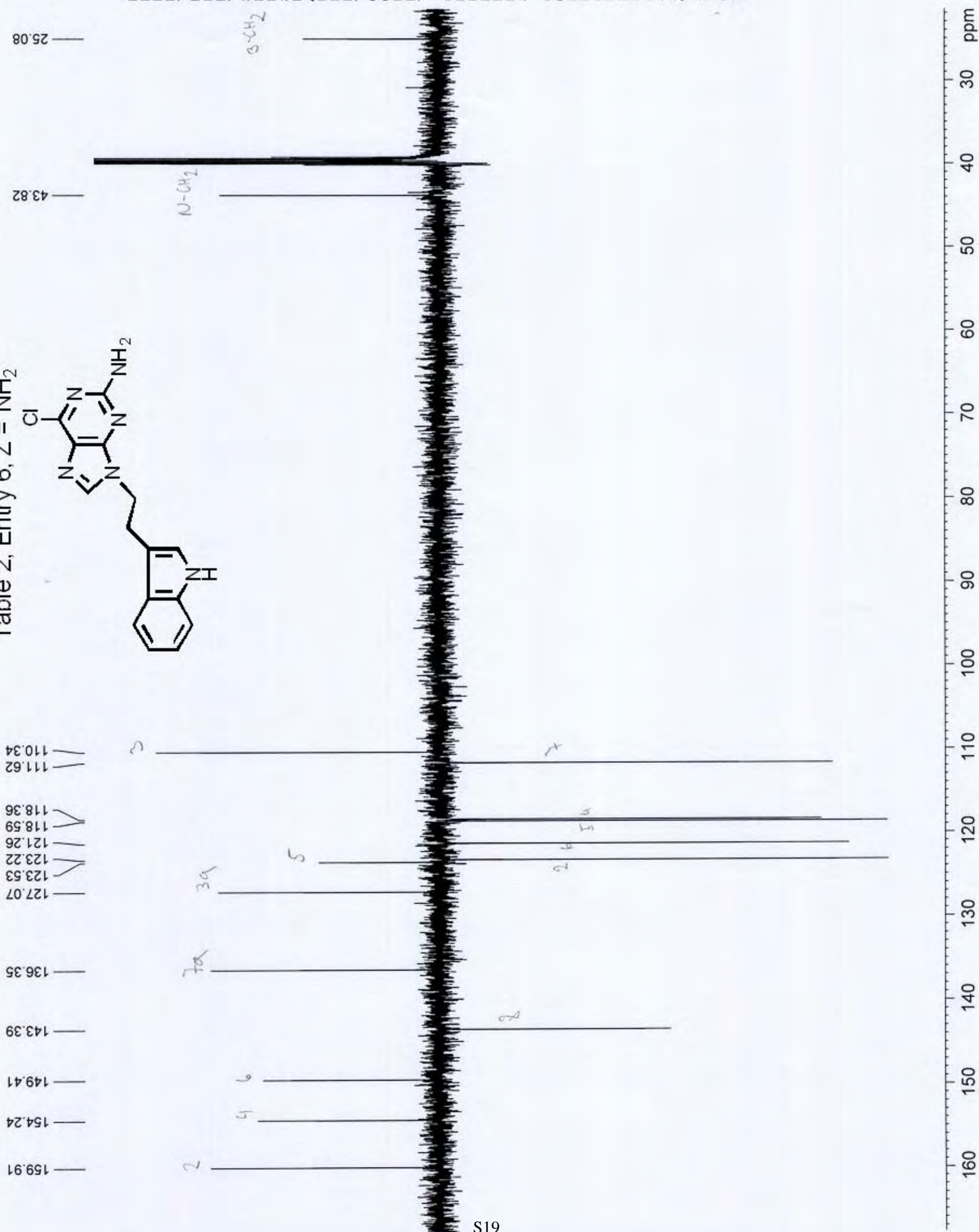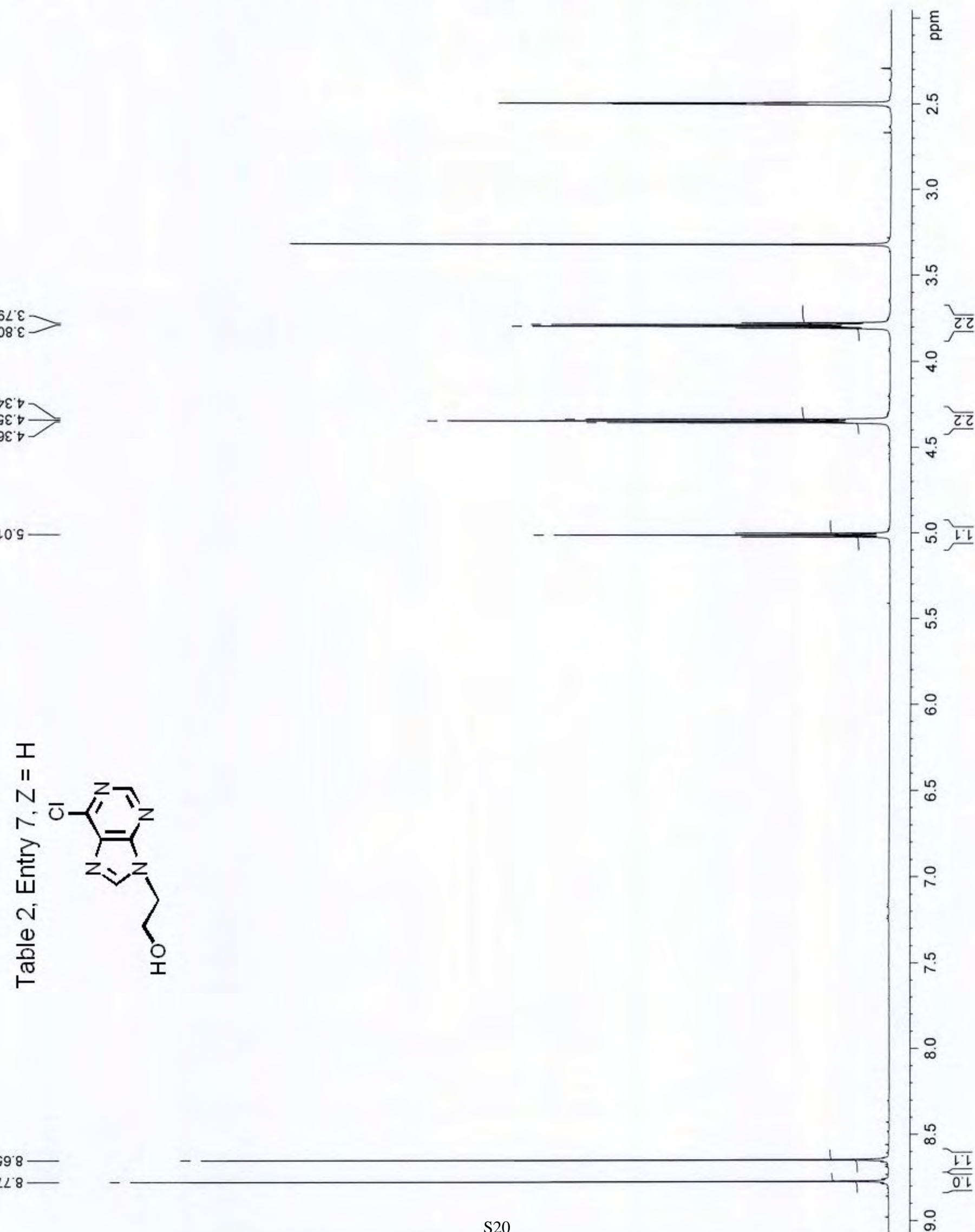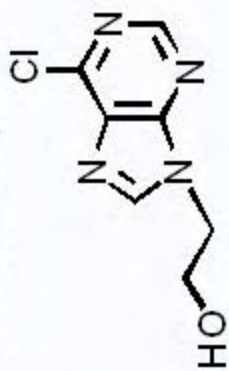SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 6, Z = NH₂

25.08
43.82
110.34
111.62
118.36
118.59
121.26
123.22
123.53
127.07
136.35
143.39
149.41
154.24
159.91

ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
160

S19

Table 2, Entry 7, Z = H

Dejmek_MD337
1H NMR in DMSO
16-9-11 DR
****

8.65
8.77

5.01

4.34
4.35
4.36

3.79
3.80

2.2
2.2
1.1
1.1
1.0

ppm
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0

Dejmek_MD337
APT in DMSO
16-9-11 DR
****

NAME   Dejmek_MD337
EXPNO   2
PROCNO   1
Date_   20110916
Time   9.27
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1450
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125653 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 7, Z = H

46.77
59.04
131.03
148.15
148.97
151.51
152.28

ppm
45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155

S21
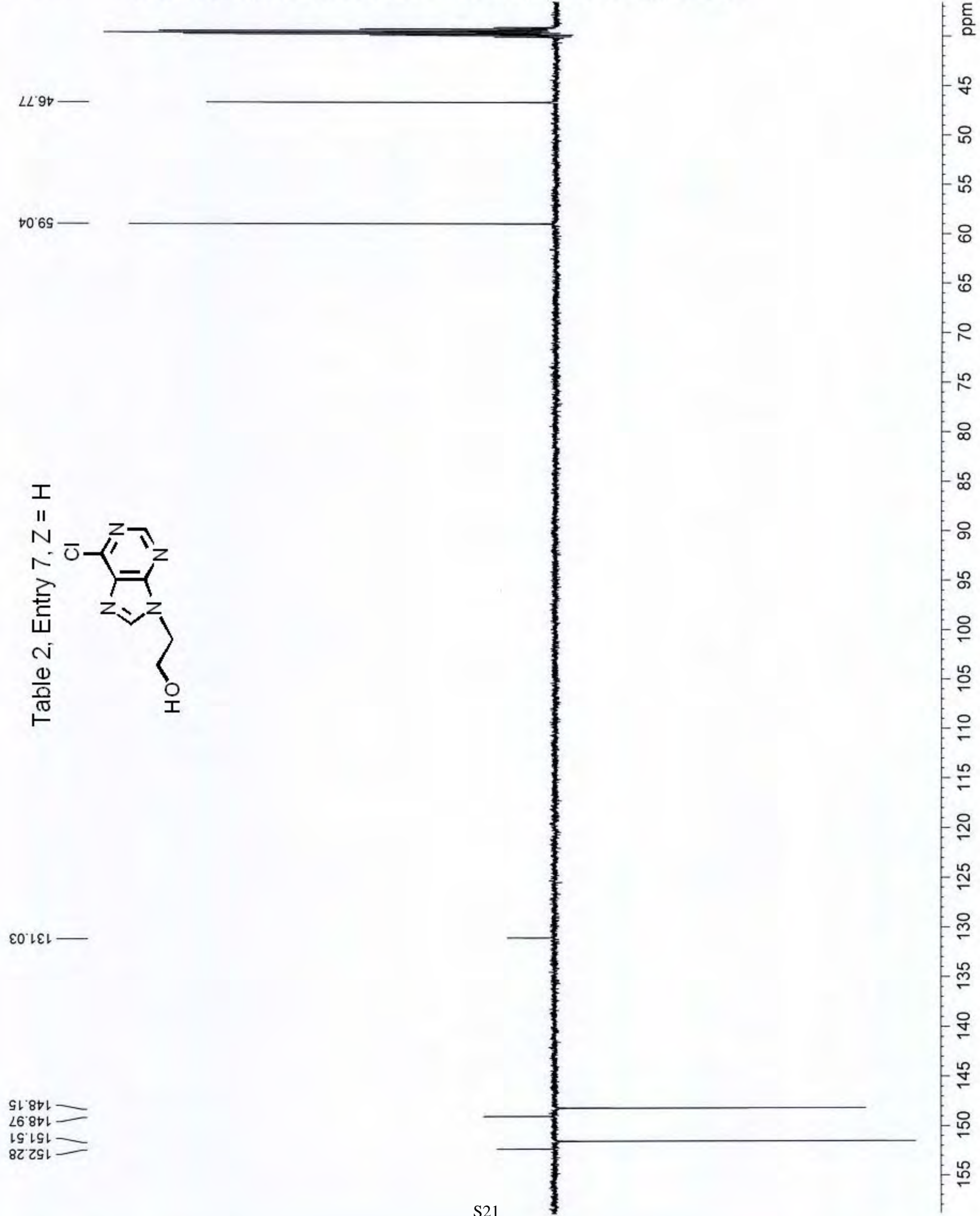
Dejmek_MD335
1H NMR in DMSO
26-9-11 DR
****
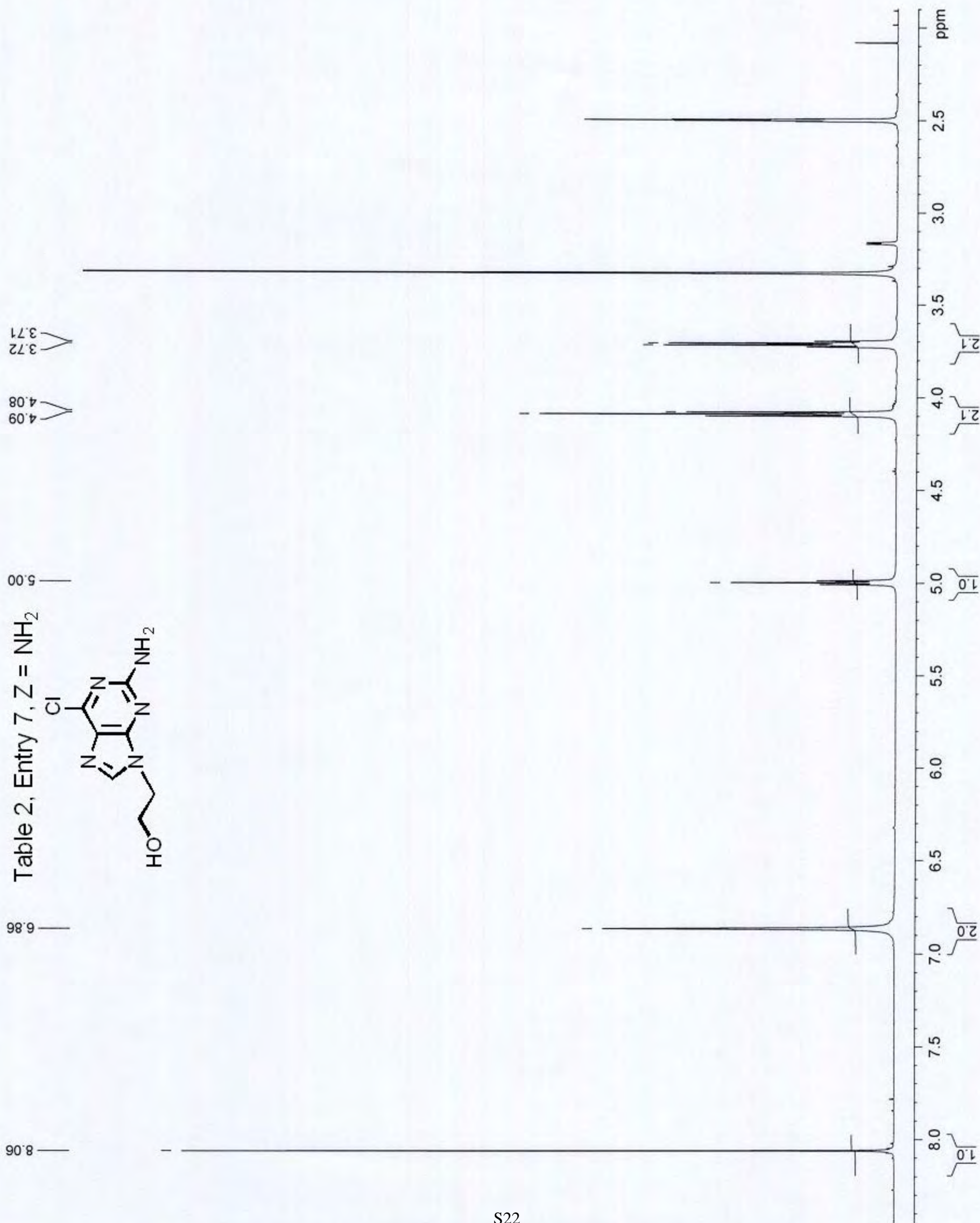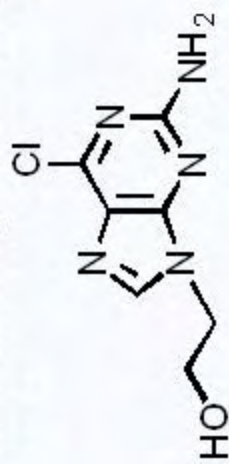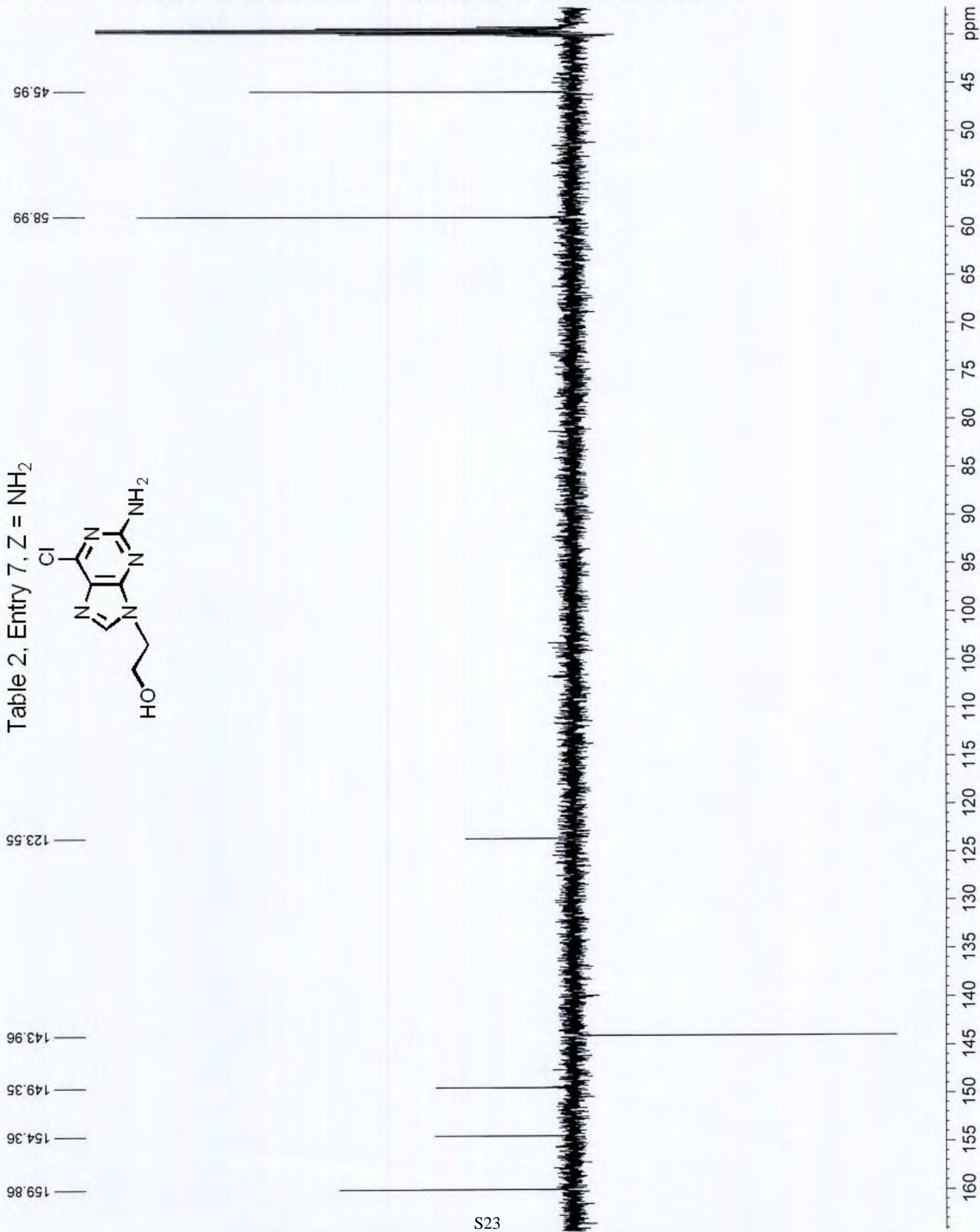
NAME   Dejmek_MD335
EXPNO   1
PROCNO   1
Date_   20110926
Time   15.13
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

===== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500007 MI-
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 7, Z = NH$_2$

Dejmek_MD335
APT in DMSO
26-9-11 DR
****

Table 2, Entry 7, Z = NH₂

NAME   Dejmek_MD335
EXPNO   2
PROCNO   1
Date_   20110926
Time   15.27
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   267
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125638 MHz
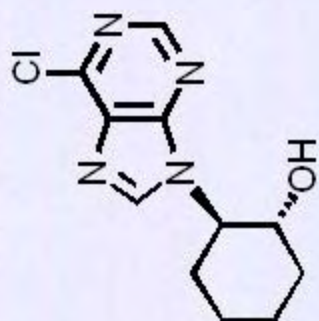WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

45.95
58.99
123.55
143.96
149.35
154.36
159.86

ppm
45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155 160

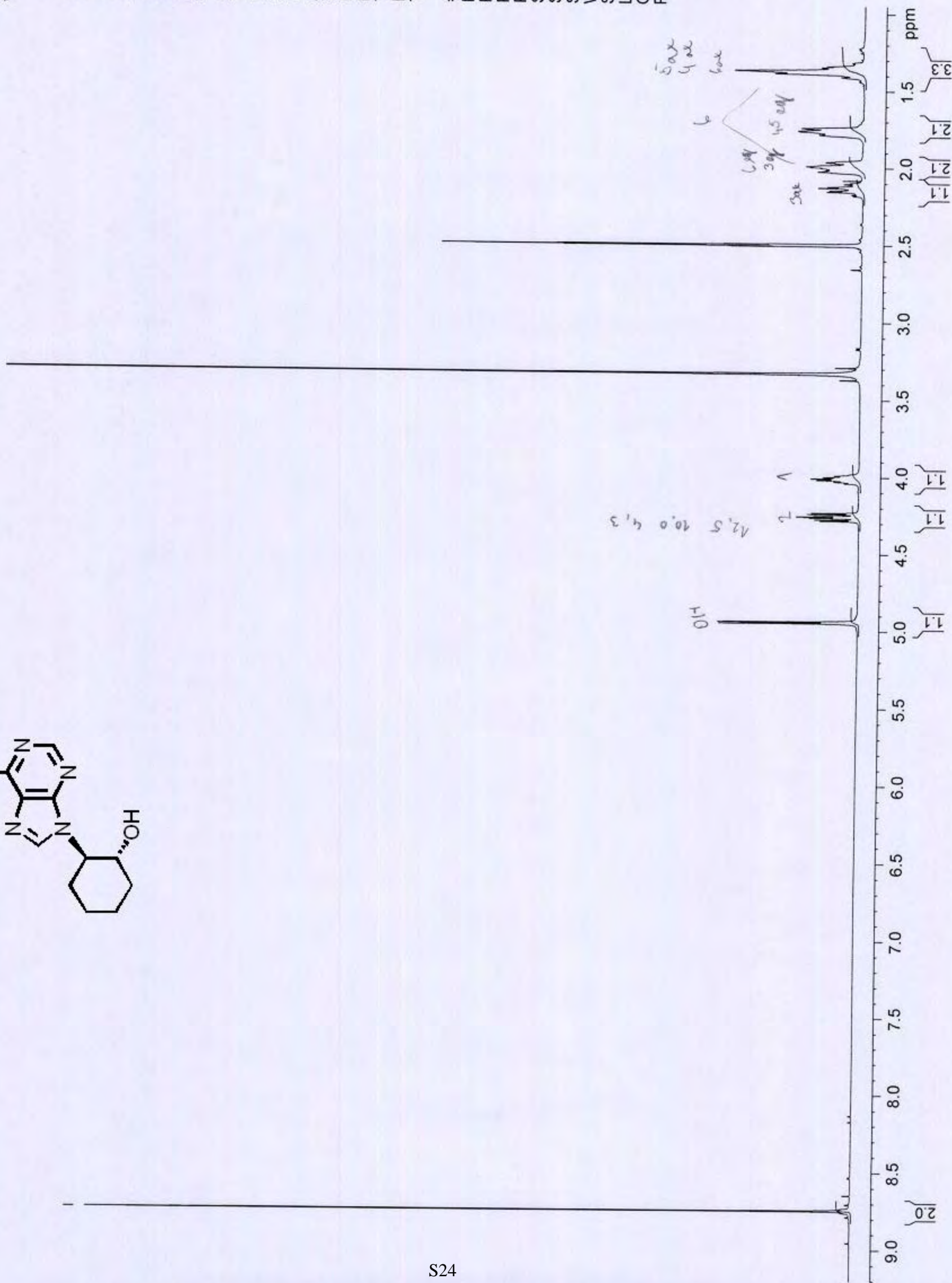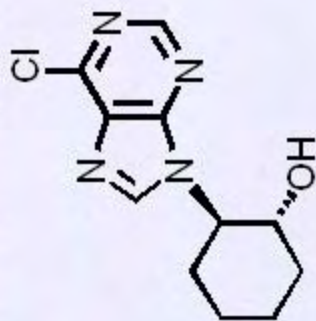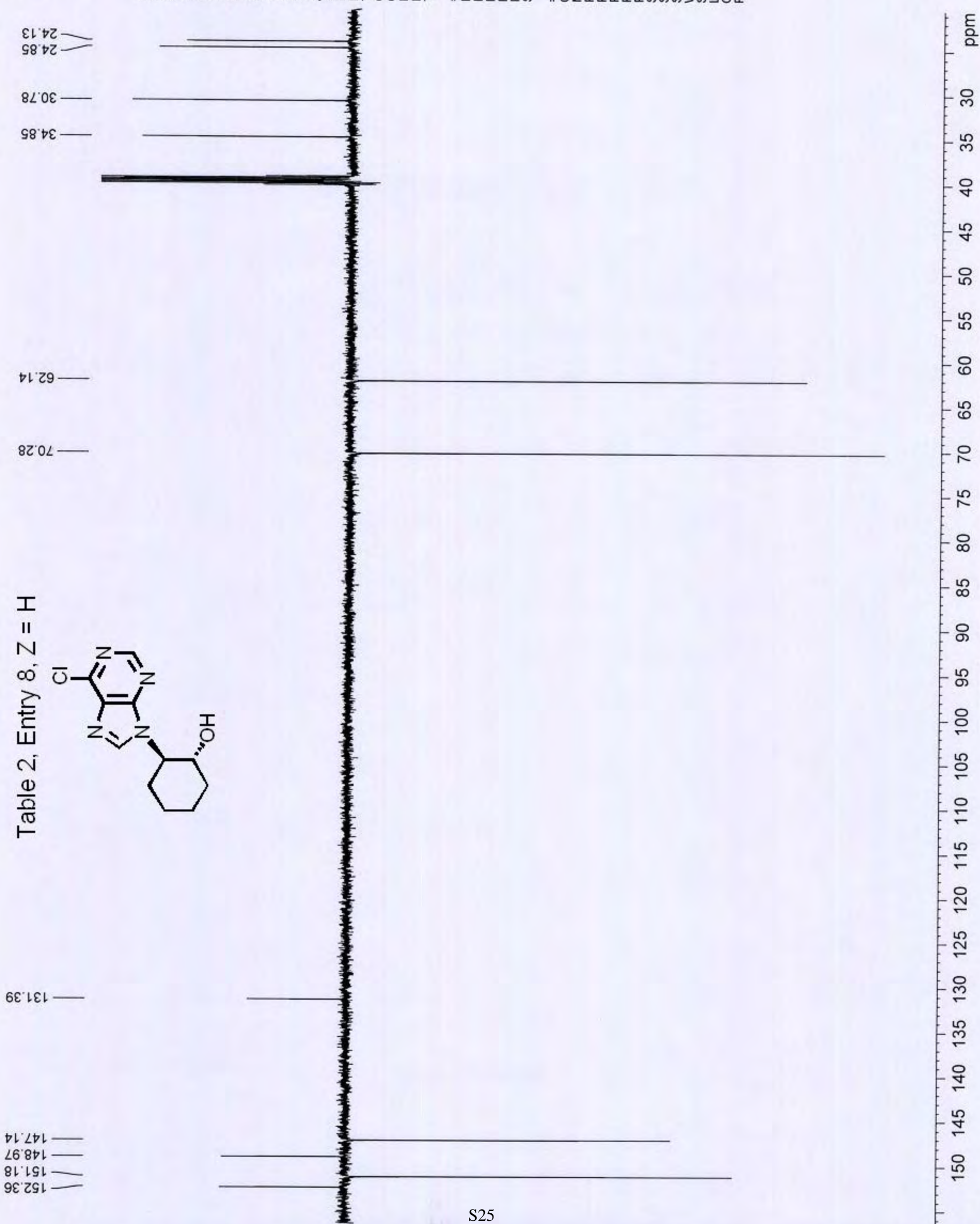Table 2, Entry 8, Z = H

Dejmek_MD331
1H NMR in DMSO
7-12-11 DR
****

NAME   Dejmek_MD331
EXPNO   1
PROCNO   1
Date_   20111207
Time   15.34
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 =====
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz
SI   131072
SF   499.9499978 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00
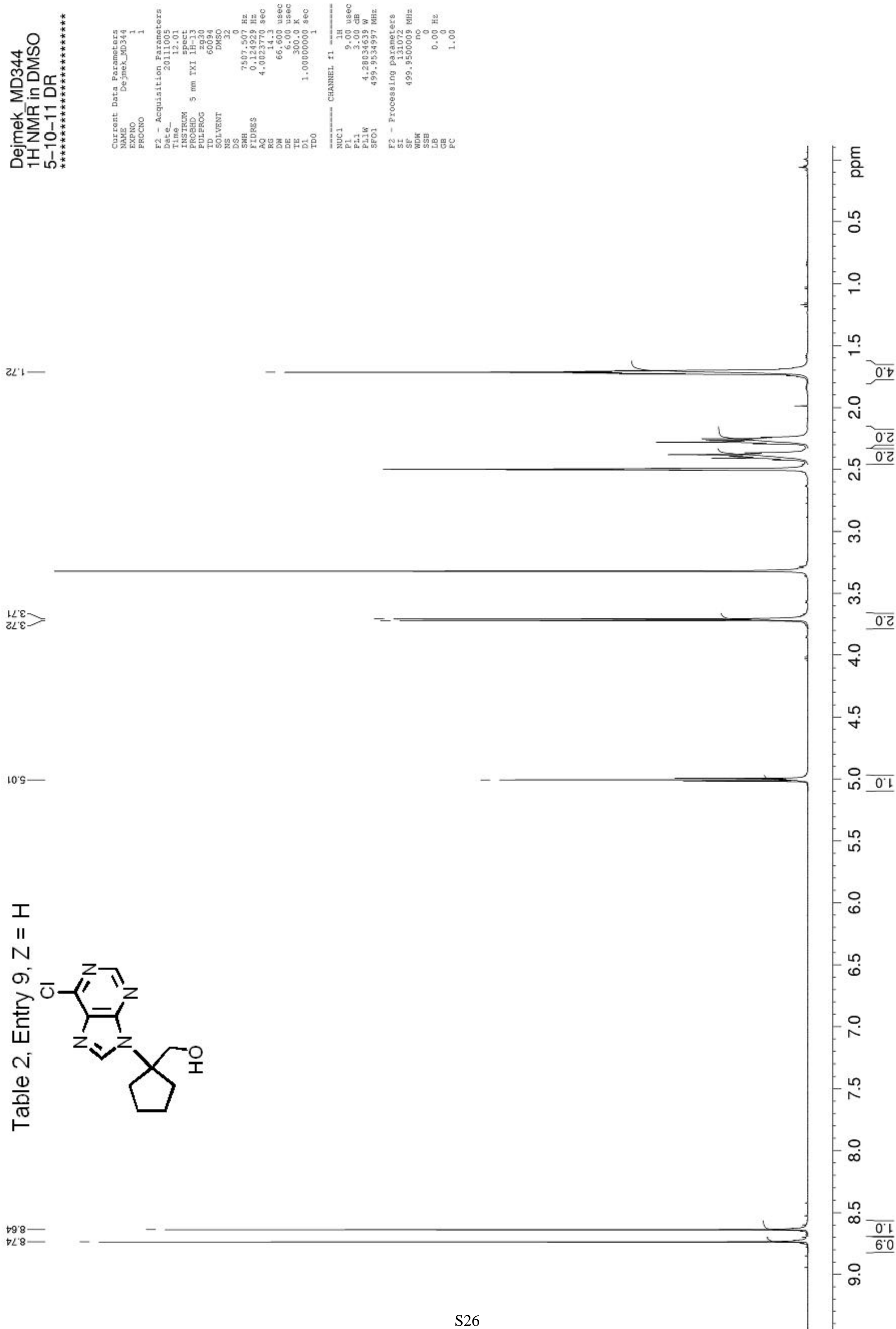
Table 2, Entry 8, Z = H

Dejmek_MD344
1H NMR in DMSO
5-10-11 DR

Table 2, Entry 9, Z = H

Dejmek_MD344
APT in DMSO
5-10-11 DR
****

NAME   Dejmek_MD344
EXPNO   2
PROCNO   1
Date_   20111005
Time_   12.15
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   252
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 =======
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125654 MHz
WDW   EM
SSB   0
LB   1.00 Hz
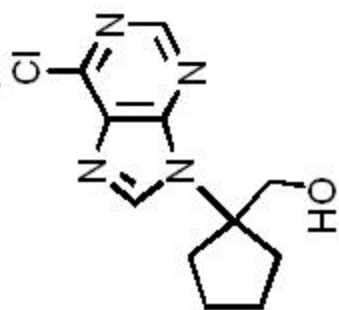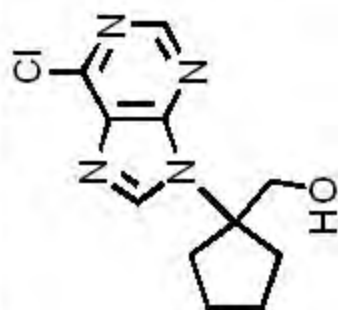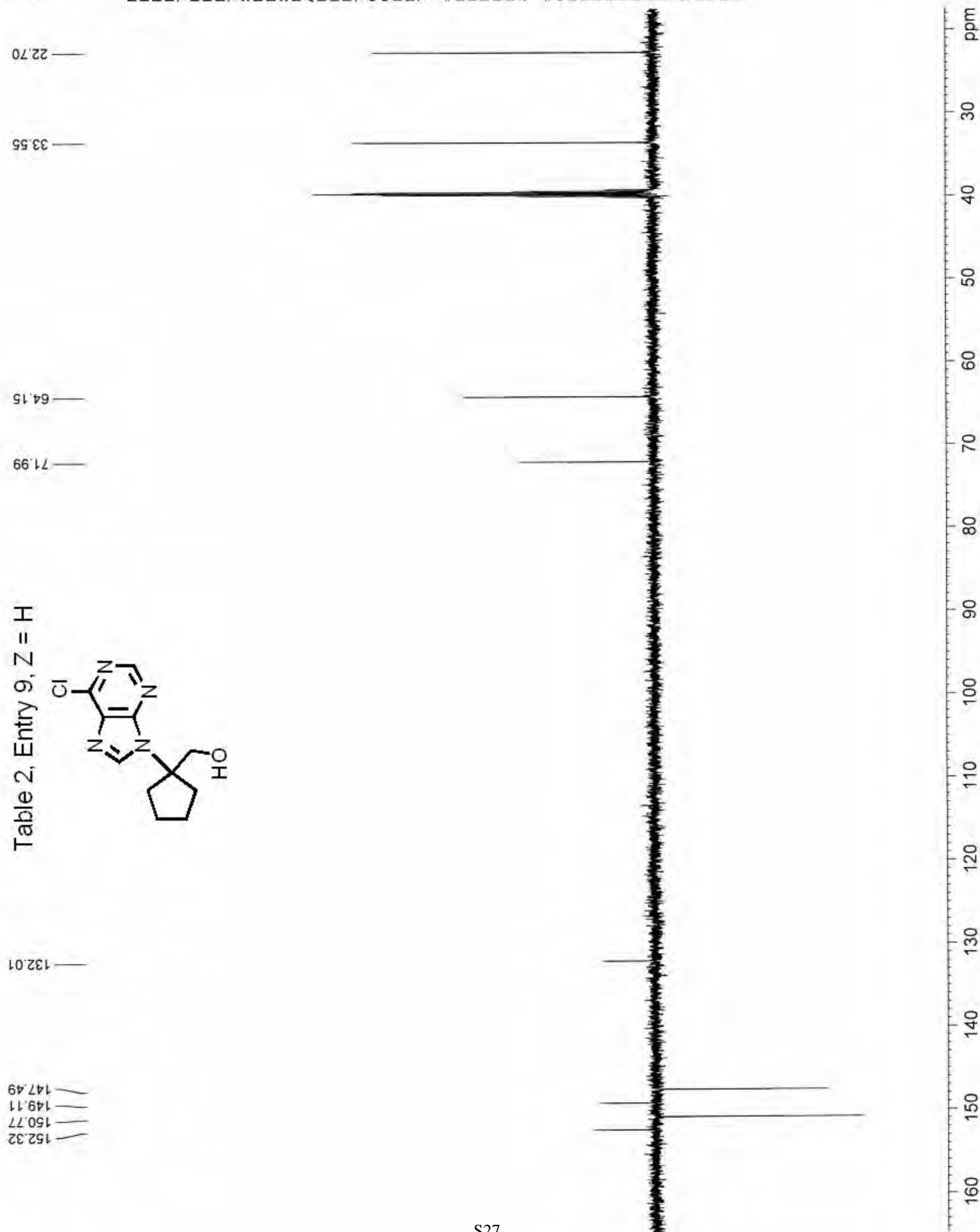GB   0
PC   1.00

Table 2, Entry 9, Z = H

22.70

33.55

64.15

71.99

132.01

147.49
149.11
150.77
152.32

ppm 30 40 50 60 70 80 90 100 110 120 130 140 150 160

Table 2, Entry 9, Z = NH₂

Dejmek MD343
APT in DMSO
5-10-11 DR
****

22.64 ——

33.35 ——

63.73 ——

70.99 ——

Table 2, Entry 9, Z = NH$_2$

124.57 ——

143.20 ——

149.44 ——

154.38 ——

159.13 ——

ppm scale: 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 ppm

Dejmek_MD339
1H NMR in DMSO
5-10-11 DR
****

Current Data Parameters
NAME   Dejmek_MD339
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20111005
Time   14.20
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 MHz

F2 - Processing parameters
SI   131072
SF   499.9500008 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
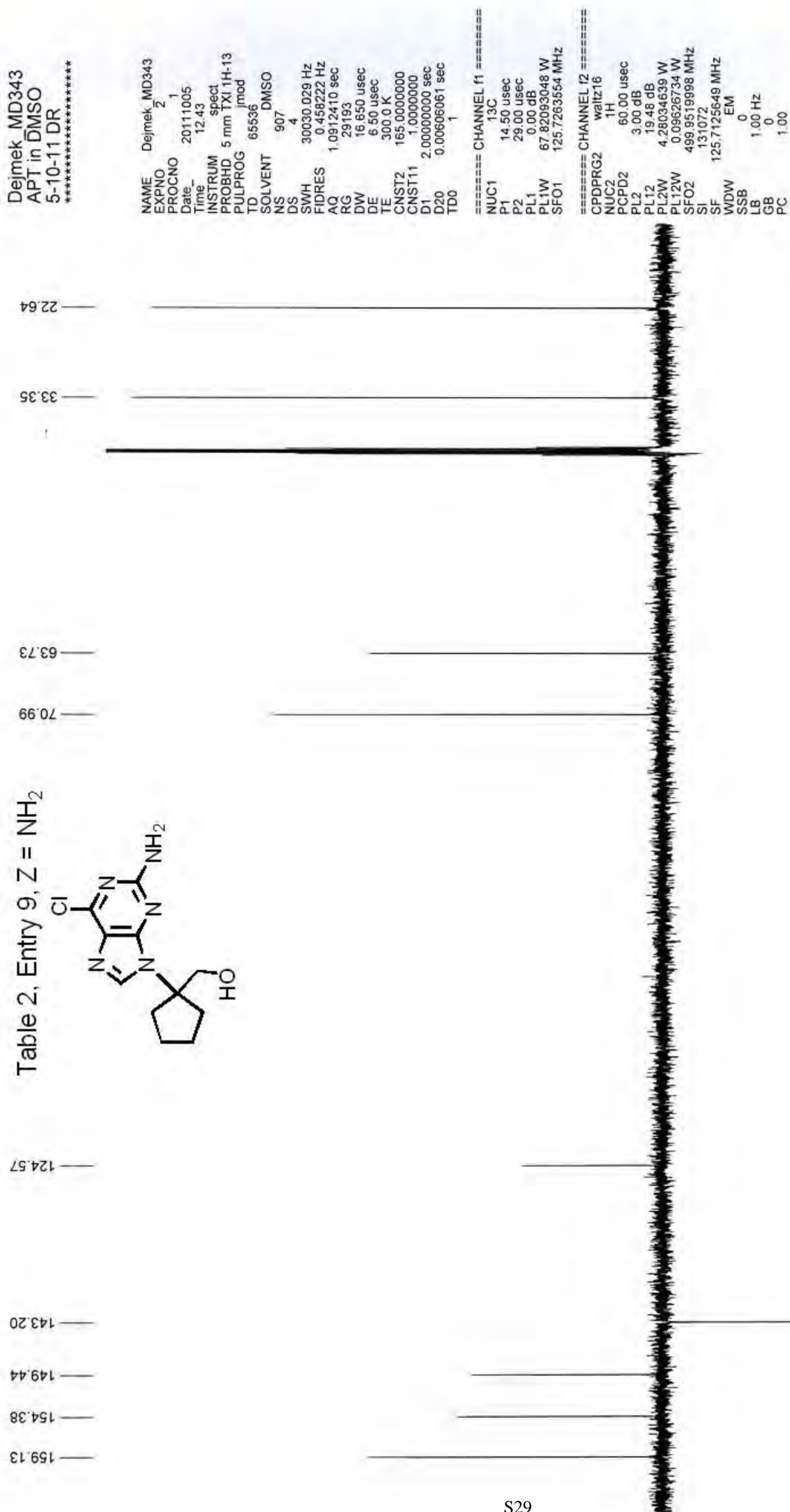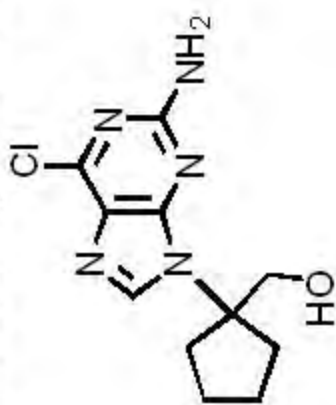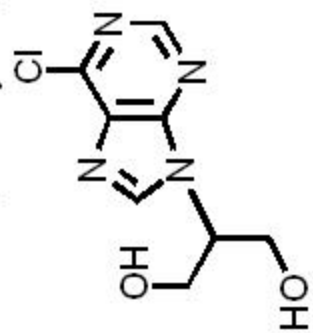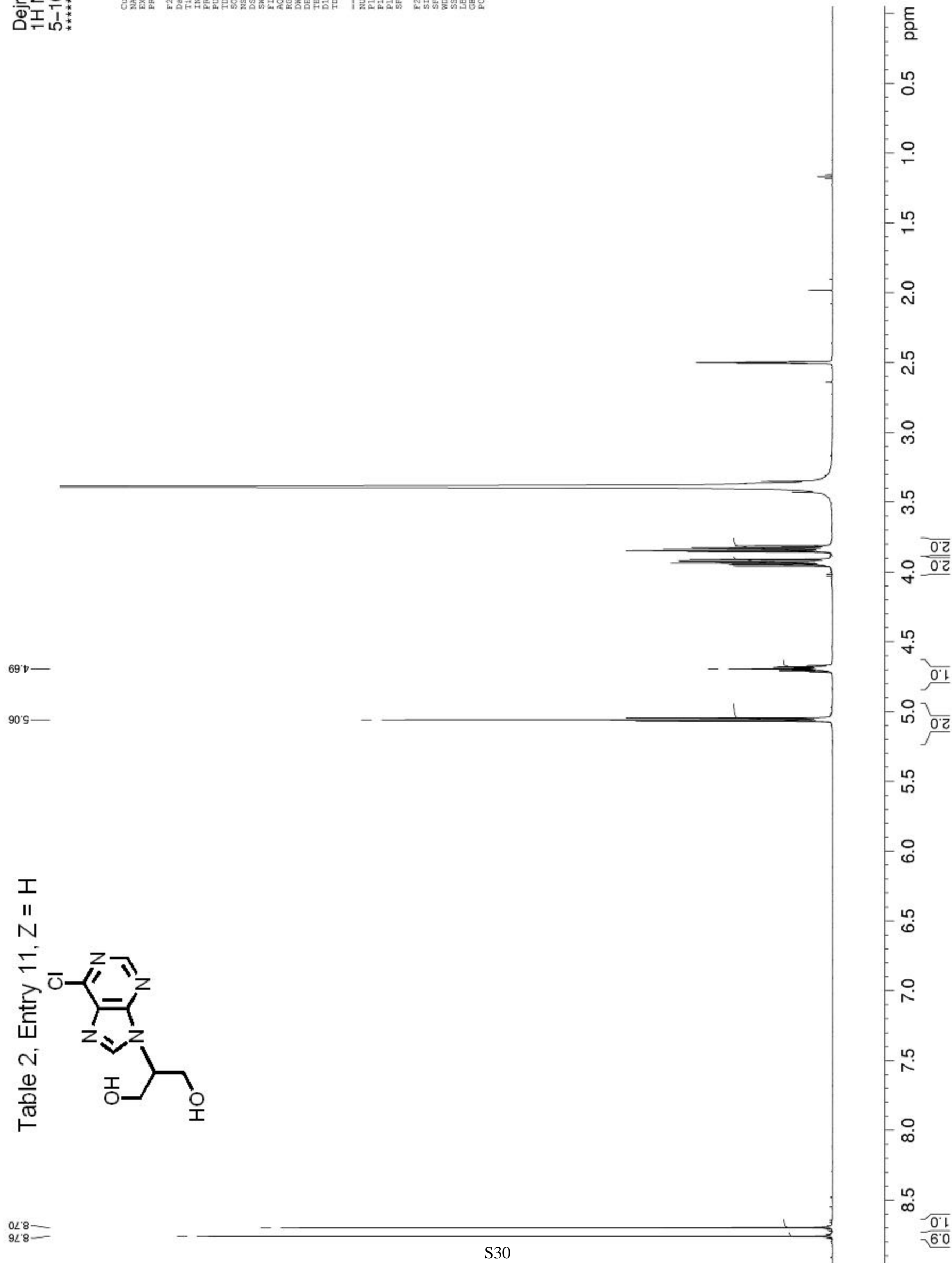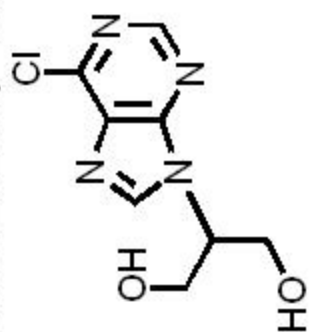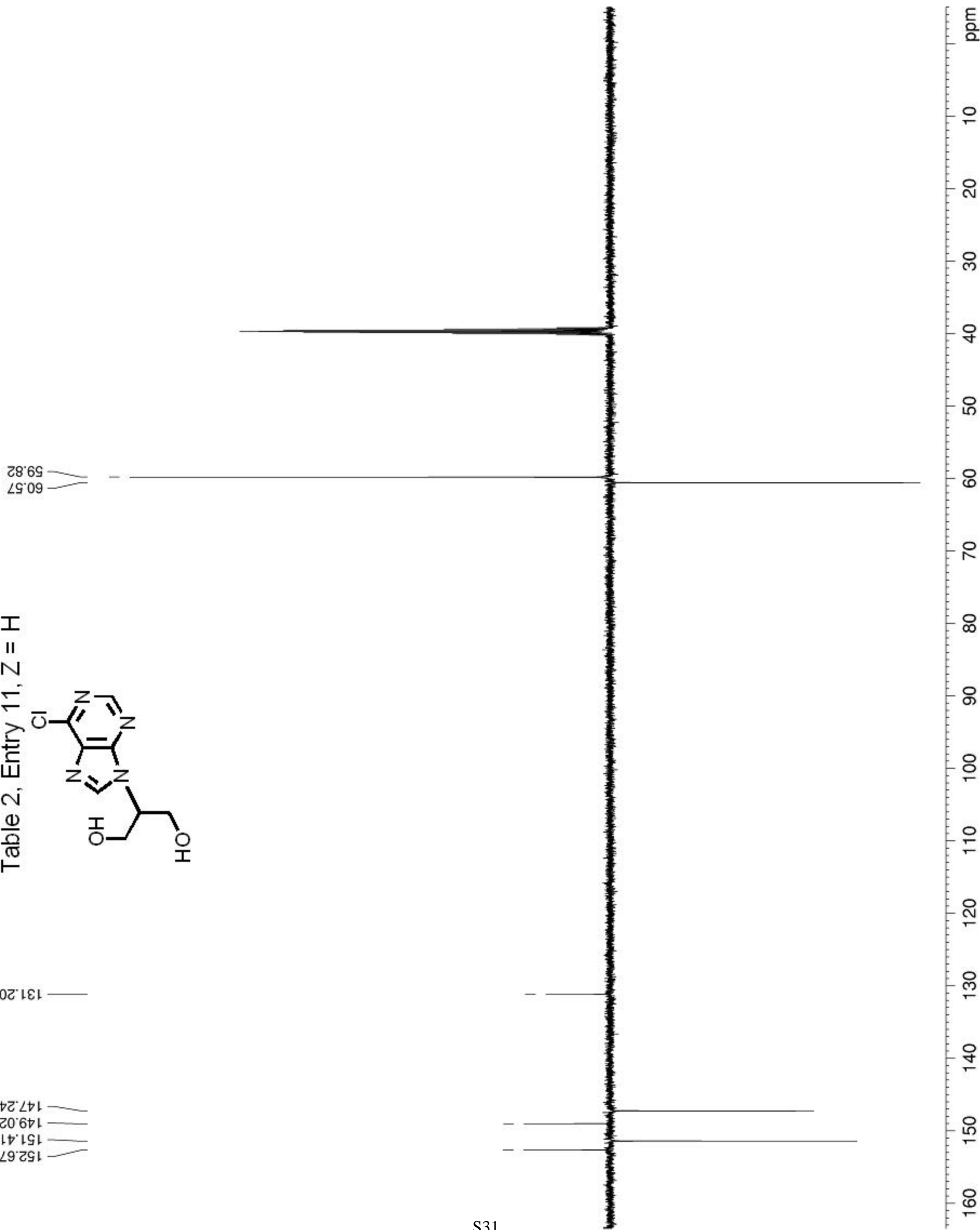PC   1.00

Table 2, Entry 11, Z = H

S30

Dejmek_MD339
APT in DMSO
5–10–11 DR
****

Current Data Parameters
NAME   Dejmek_MD339
EXPNO   2
PROCNO   1

F2 – Acquisition Parameters
Date_   20111005
Time   15.08
INSTRUM   spect
PROBHD   5 mm TXI 1H–13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   4
DS   928
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

===== CHANNEL f1 =====
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz

F2 – Processing parameters
SI   131072
SF   125.7125562 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 11, Z = H

59.82
60.57

131.20

147.24
149.02
151.41
152.67

160   150   140   130   120   110   100   90   80   70   60   50   40   30   20   10   ppm

Dejmek_MD340
1H NMR in DMSO
30-9-11 DR
****

NAME   Dejmek_MD34
EXPNO   1
PROCNO   1
Date_   20110930
Time   13.05
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 H:
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500006 MF
WDW   no
SSB   0
LB   0.00 Hz
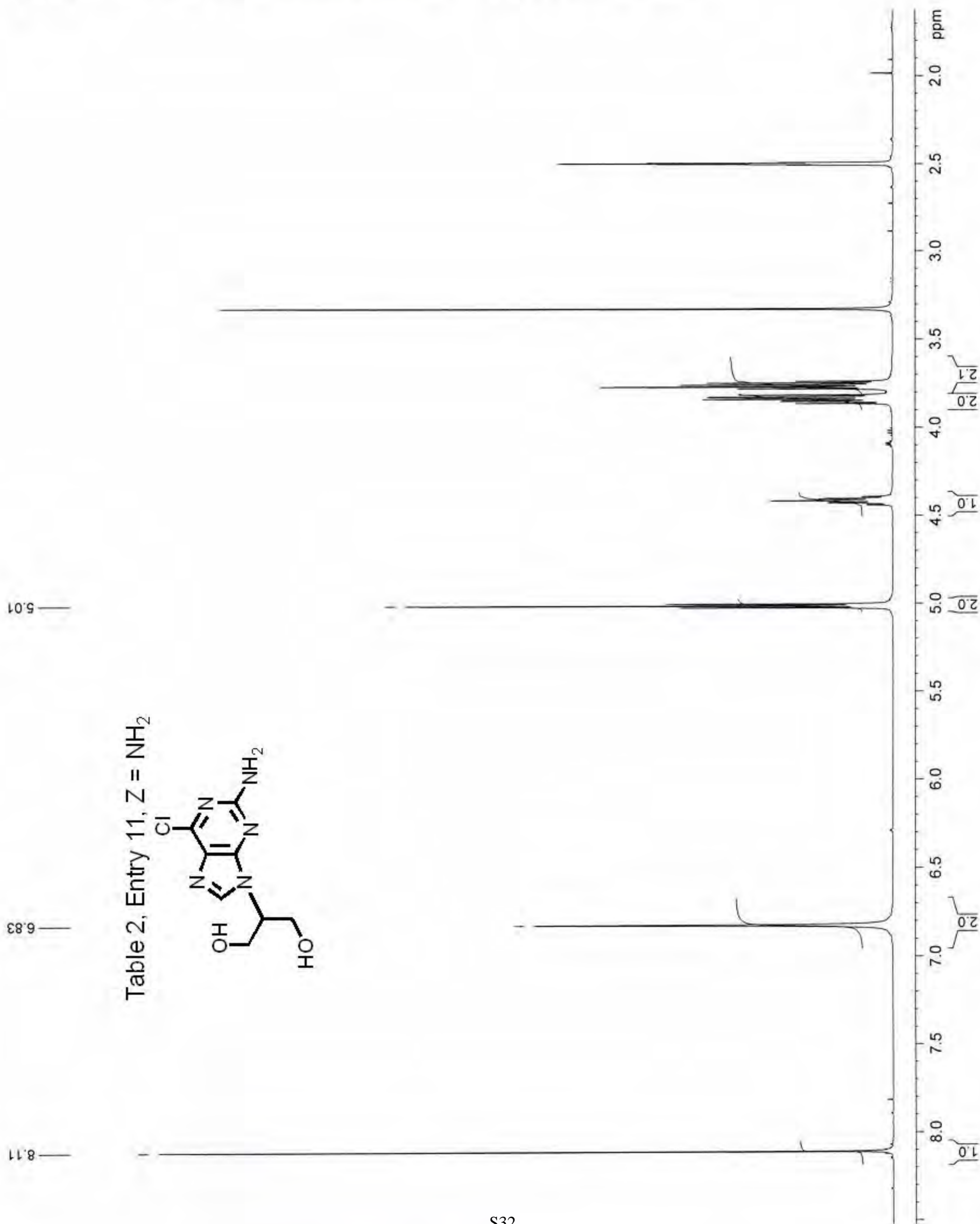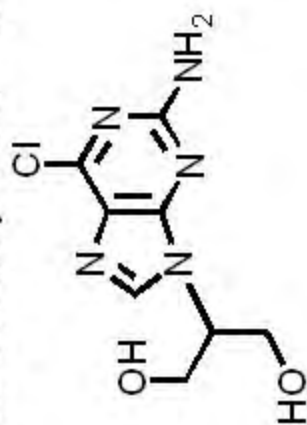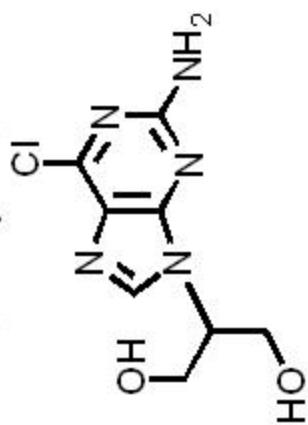GB   0
PC   1.00

Table 2, Entry 11, Z = NH₂

Dejmek_MD340
APT in DMSO
30–9–11 DR
****

Current Data Parameters
NAME   Dejmek_MD340
EXPNO   2
PROCNO   1

F2 – Acquisition Parameters
Date_   20110930
Time   13.50
INSTRUM   spect
PROBHD   5 mm TXI 1H–13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   869
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

====== CHANNEL f1 ======
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

====== CHANNEL f2 ======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz

F2 – Processing parameters
SI   131072
SF   125.7125639 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 2, Entry 11, Z = NH₂

59.21
59.74

123.65

142.85

149.28

154.64

159.66

ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160

S33

Table 2, Entry 13, Z = H

Dejmek_MD346
1H-NMR in DMSO
30.9.2011 DR
****

NAME   Dejmek_MD346
EXPNO   1
PROCNO   1
Date_   20110930
Time   10.07
INSTRUM   spect
PROBHD   5 mm CPTCI 1H-
PULPROG   zg30
TD   72114
SOLVENT   DMSO
NS   32
DS   0
SWH   9014.423 Hz
FIDRES   0.125002 Hz
AQ   3.9999733 sec
RG   9
DW   55.467 usec
DE   20.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   8.10 dB
PL1W   5.29101372 W
SFO1   600.1330006 MHz
SI   131072
SF   600.1300066 MHz
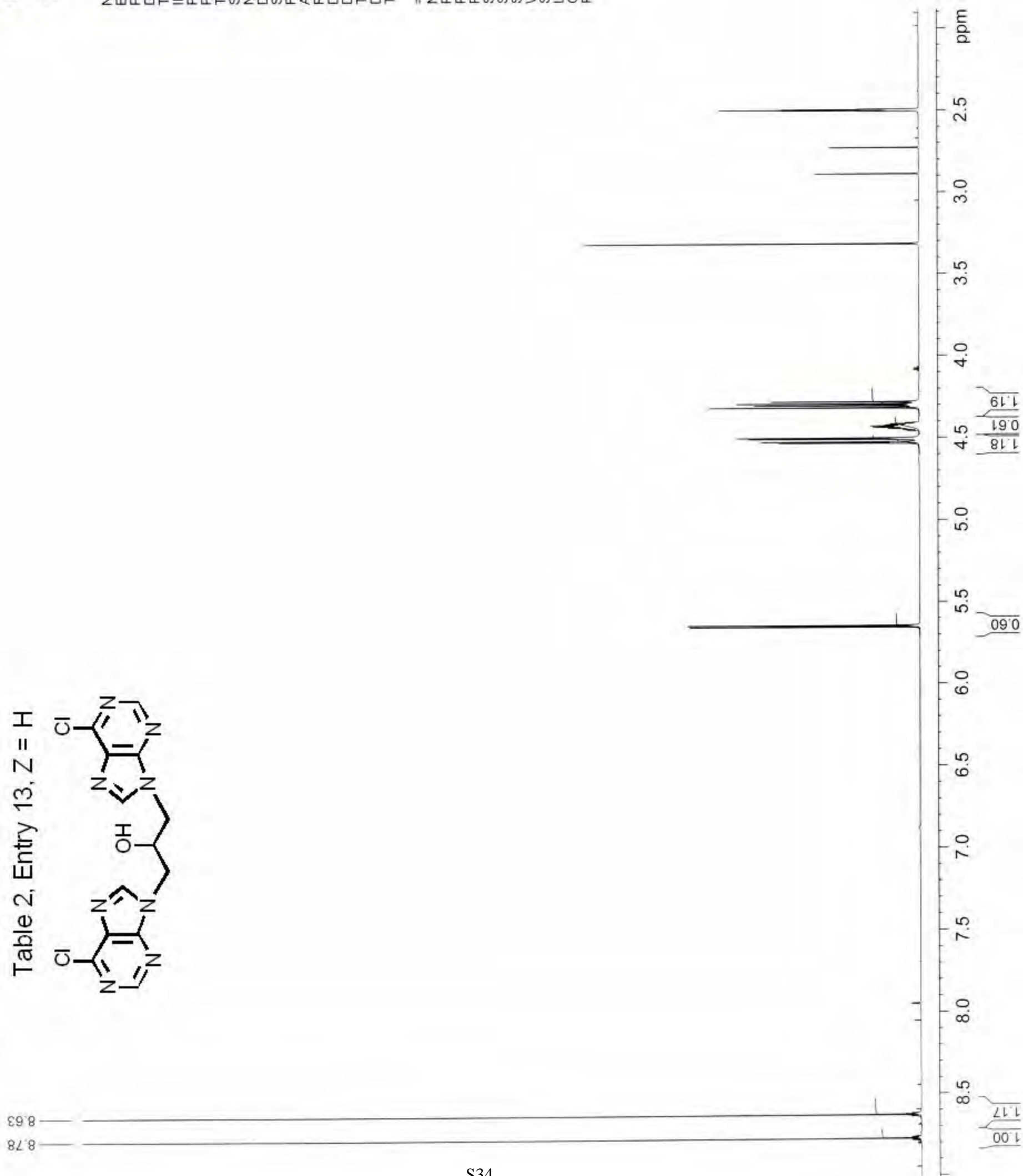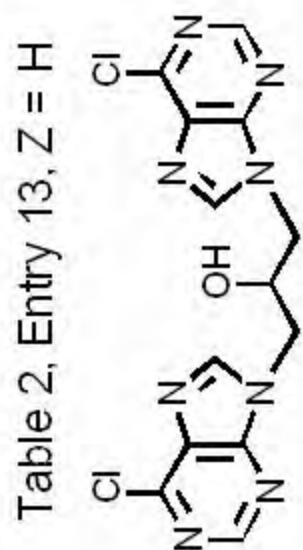WDW   no
SSB   0
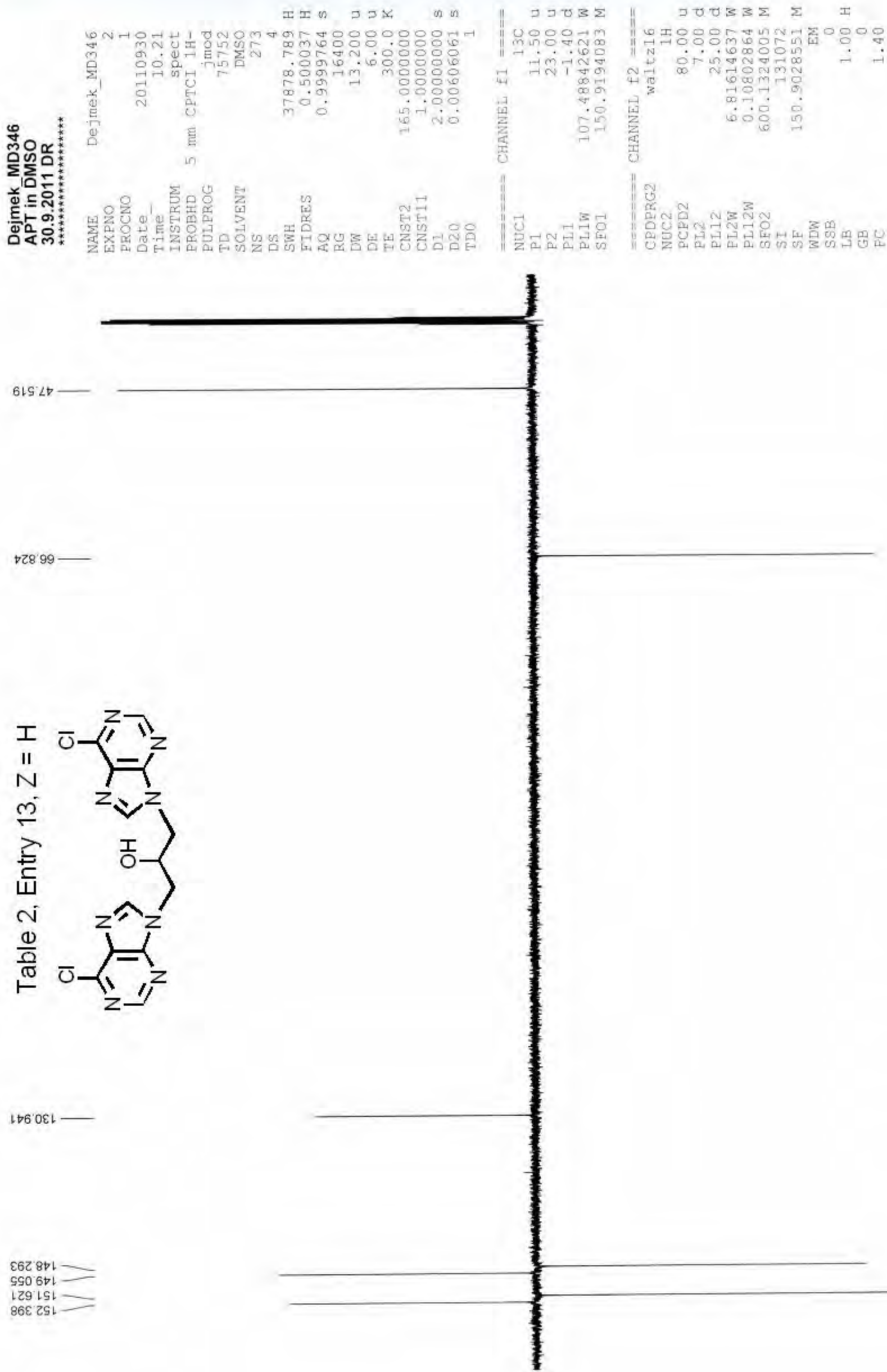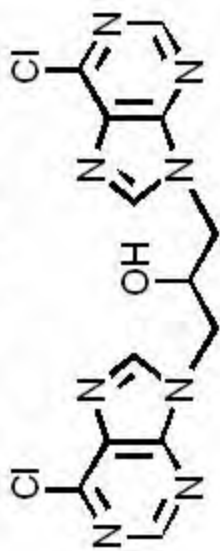LB   0.00 Hz
GB   0
PC   0.50

S34

Dejmek_MD346
APT in DMSO
30.9.2011 DR
****

NAME	Dejmek_MD346
EXPNO	2
PROCNO	1
Date_	20110930
Time	10.21
INSTRUM	spect
PROBHD	5 mm CPTCI 1H-
PULPROG	jmod
TD	75752
SOLVENT	DMSO
NS	273
DS	4
SWH	37878.789 H
FIDRES	0.500037 H
AQ	0.9999764 s
RG	16400
DW	13.200 u
DE	6.00 u
TE	300.0 K
CNST2	165.0000000
CNST11	1.0000000
D1	2.00000000 s
D20	0.00606061 s
TD0	1

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

NUC1	13C
P1	11.50 u
P2	23.00 u
PL1	-1.40 d
PL1W	107.48842621 W
SFO1	150.9194083 M

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 u
PL2	7.00 d
PL12	25.00 d
PL2W	6.81614637 W
PL12W	0.10802864 W
SFO2	600.1324005 M
SI	131072
SF	150.9028551 M
WDW	EM
SSB	0
LB	1.00 H
GB	0
FC	1.40

Table 2, Entry 13, Z = H

47.519

66.824

130.941

148.293
149.055
151.621
152.398

ppm
45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125 130 135 140 145 150 155

Dejmek_MD345
1H-NMR in DMSO
30.9.2011 DR
****

NAME   Dejmek_MD345
EXPNO   1
PROCNO   1
Date_   20110930
Time   9.16
INSTRUM   spect
PROBHD 5 mm CPTCI 1H-
PULPROG   zg30
TD   72114
SOLVENT   DMSO
NS   32
DS   0
SWH   9014.423 Hz
FIDRES   0.125002 Hz
AQ   3.9999733 sec
RG   9
DW   55.467 usec
DE   20.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   10.00 usec
PL1   8.10 dB
PL1W   5.29101372 W
SFO1   600.1330006 MHz
SI   131072
SF   600.1300065 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   0.50

Table 2, Entry 13, Z = NH$_2$

5.59
5.60

6.88

8.06

2.5   3.0   3.5   4.0   4.5   5.0   5.5   6.0   6.5   7.0   7.5   8.0   ppm

1.05   1.02   0.52   0.49   2.04   1.00

Dejmek_MD345
APT in DMSO
30.9.2011 DR
****
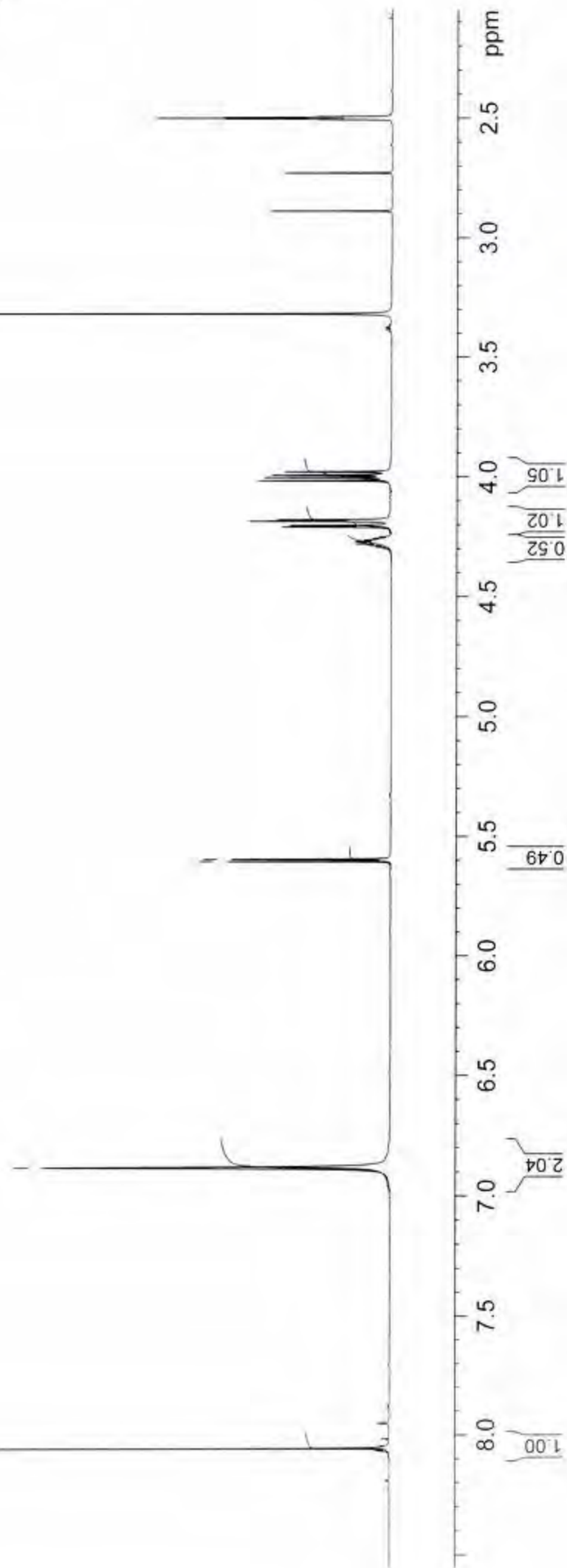
NAME   Dejmek_MD345
EXPNO   2
PROCNO   1
Date_   20110930
Time   9.40
INSTRUM   spect
PROBHD   5 mm CPTCI 1H-
PULPROG   Jmod
TD   75752
SOLVENT   DMSO
NS   459
DS   4
SWH   37878.789 H
FIDRES   0.500037 H
AQ   0.9999764 s
RG   16400
DW   13.200 u
DE   6.00 u
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 s
D20   0.00606061 s
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   11.50 u
P2   23.00 u
PL1   -1.40 d
PL1W   107.48842621 W
SFO1   150.9194083 M

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 u
PL2   7.00 d
PL12   25.00 d
PL2W   6.81614637 W
PL12W   0.10802864 W
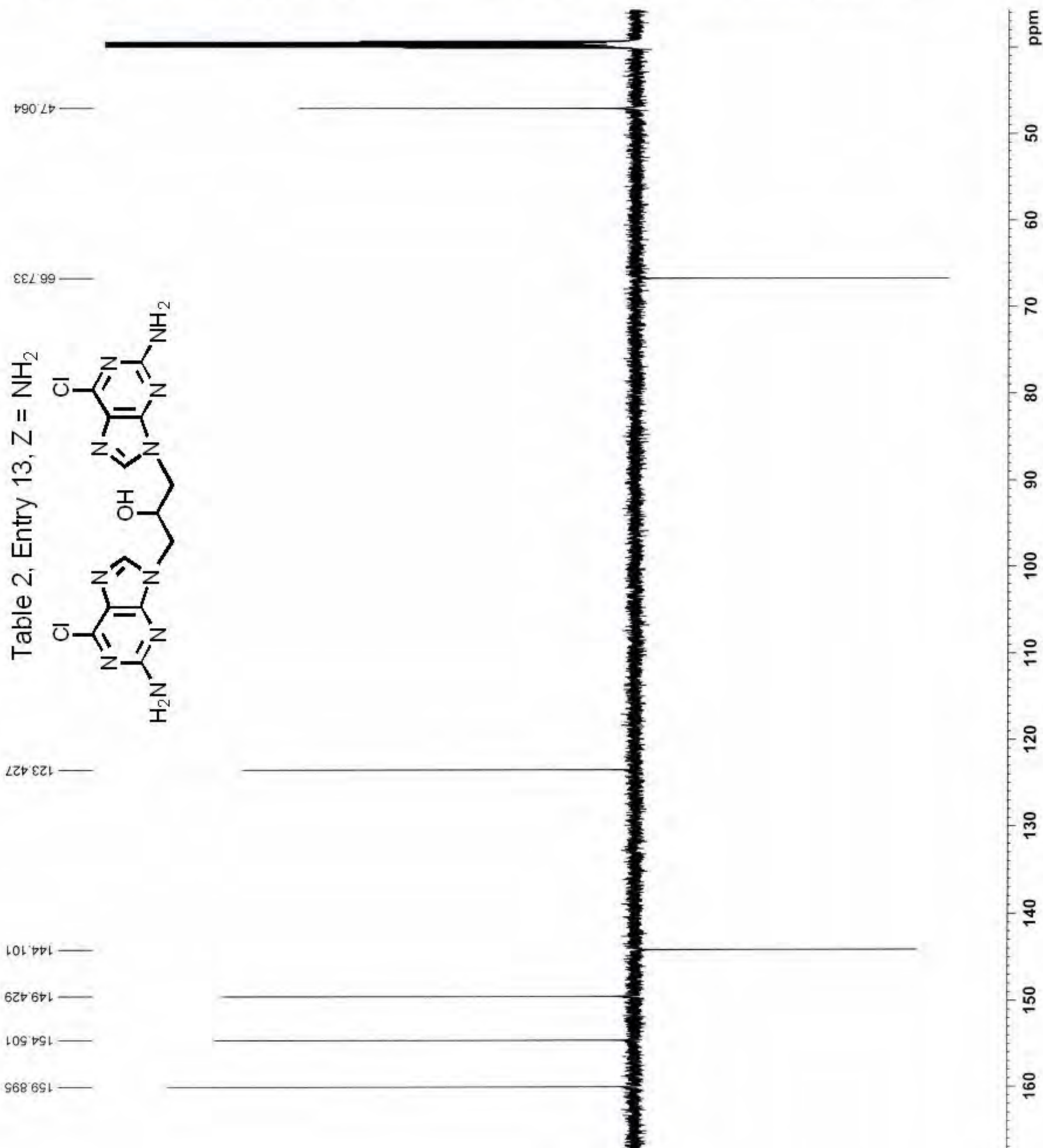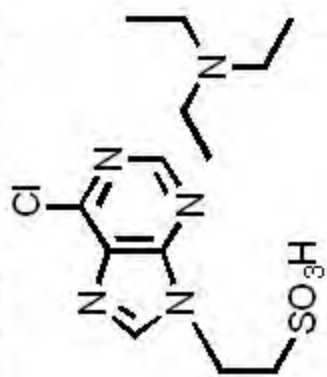SFO2   600.1324005 M
SI   131072
SF   150.9028542 M
WDW   EM
SSB   0
LB   1.00 H
GB   0
PC   1.40

Table 2, Entry 13, Z = NH$_2$

47.064
66.733
123.427
144.101
149.429
154.501
159.895

ppm
50
60
70
80
90
100
110
120
130
140
150
160

Dejmek_MD348
1H NMR in DMSO
7-11-11 DR
****

NAME   Dejmek_MD34
EXPNO   1
PROCNO   1
Date_   20111107
Time   10.00
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

===== CHANNEL f1 =
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 N
SI   131072
SF   499.9499978 MI-
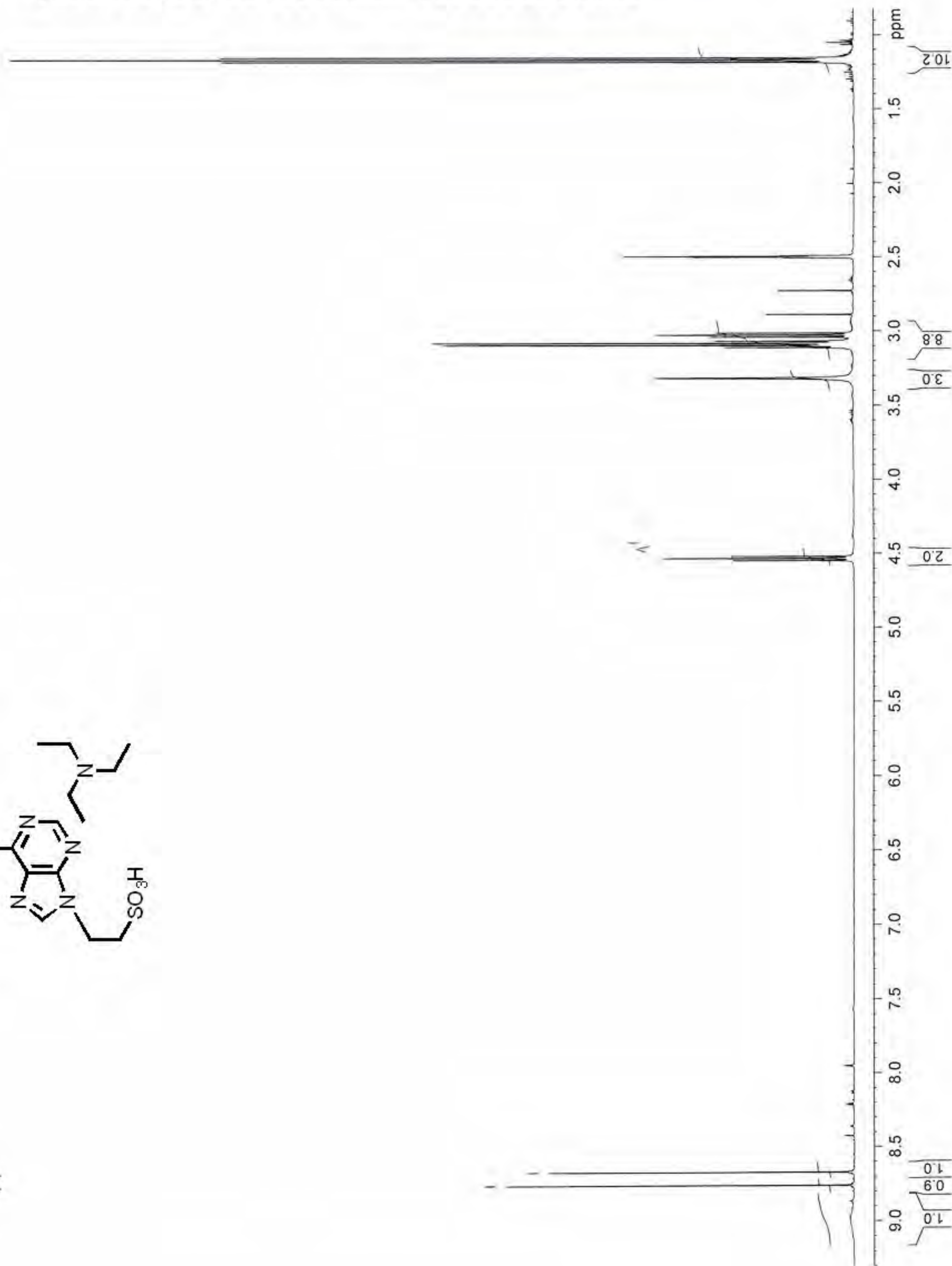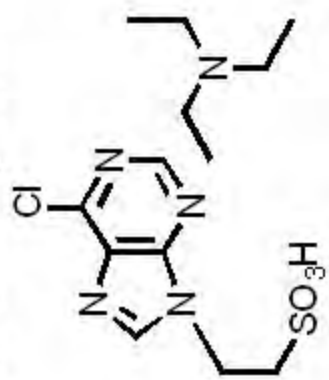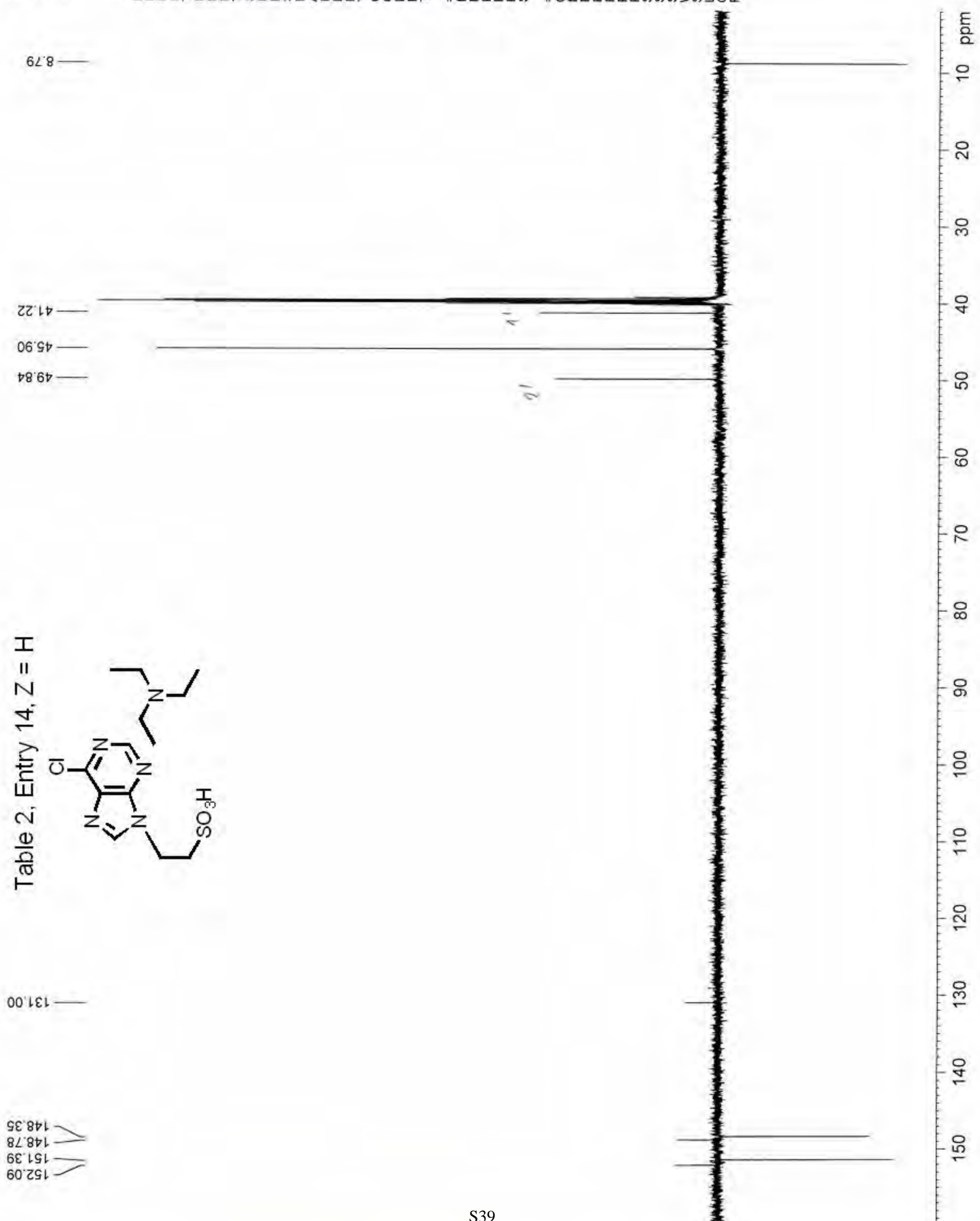WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 14, Z = H

8.67
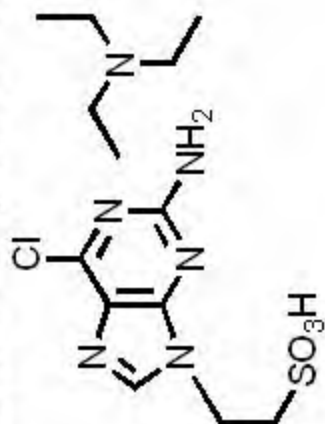8.76

S38

Dejmek_MD348
APT in DMSO
7-11-11 DR
****

NAME   Dejmek_MD348
EXPNO   2
PROCNO   1
Date_   20111107
Time   11.03
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1202
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125648 MHz
WDW   EM
SSB   0
LB   1.00 Hz
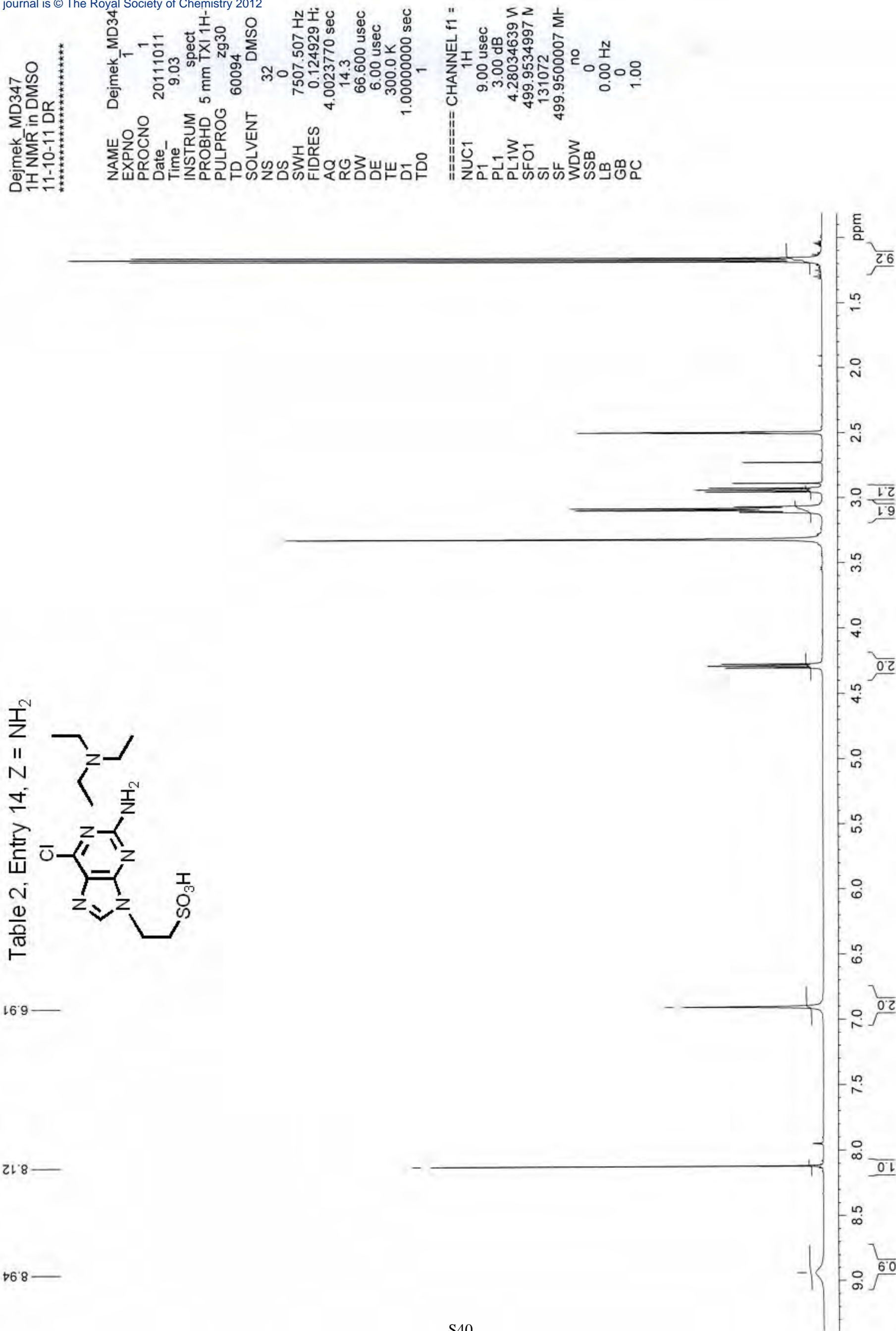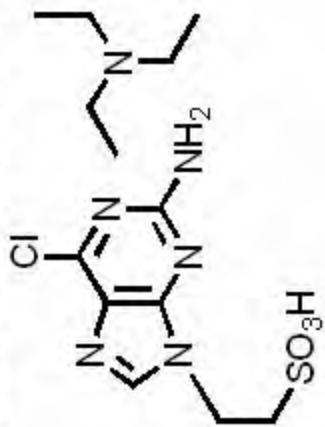GB   0
PC   1.00

Table 2, Entry 14, Z = H

8.79

41.22

45.90

49.84

131.00

148.35
148.78
151.39
152.09

S39

Dejmek_MD347
1H NMR in DMSO
11-10-11 DR
****

NAME   Dejmek_MD34
EXPNO   1
PROCNO   1
Date_   20111011
Time   9.03
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 H:
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500007 MF
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 14, Z = NH$_2$

8.94 ——

8.12 ——

6.91 ——

S40

Dejmek_MD347
APT in DMSO
11-10-11 DR
****

NAME   Dejmek_MD347
EXPNO   2
PROCNO   1
Date_   20111011
Time_   9.30
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1066
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.0060606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
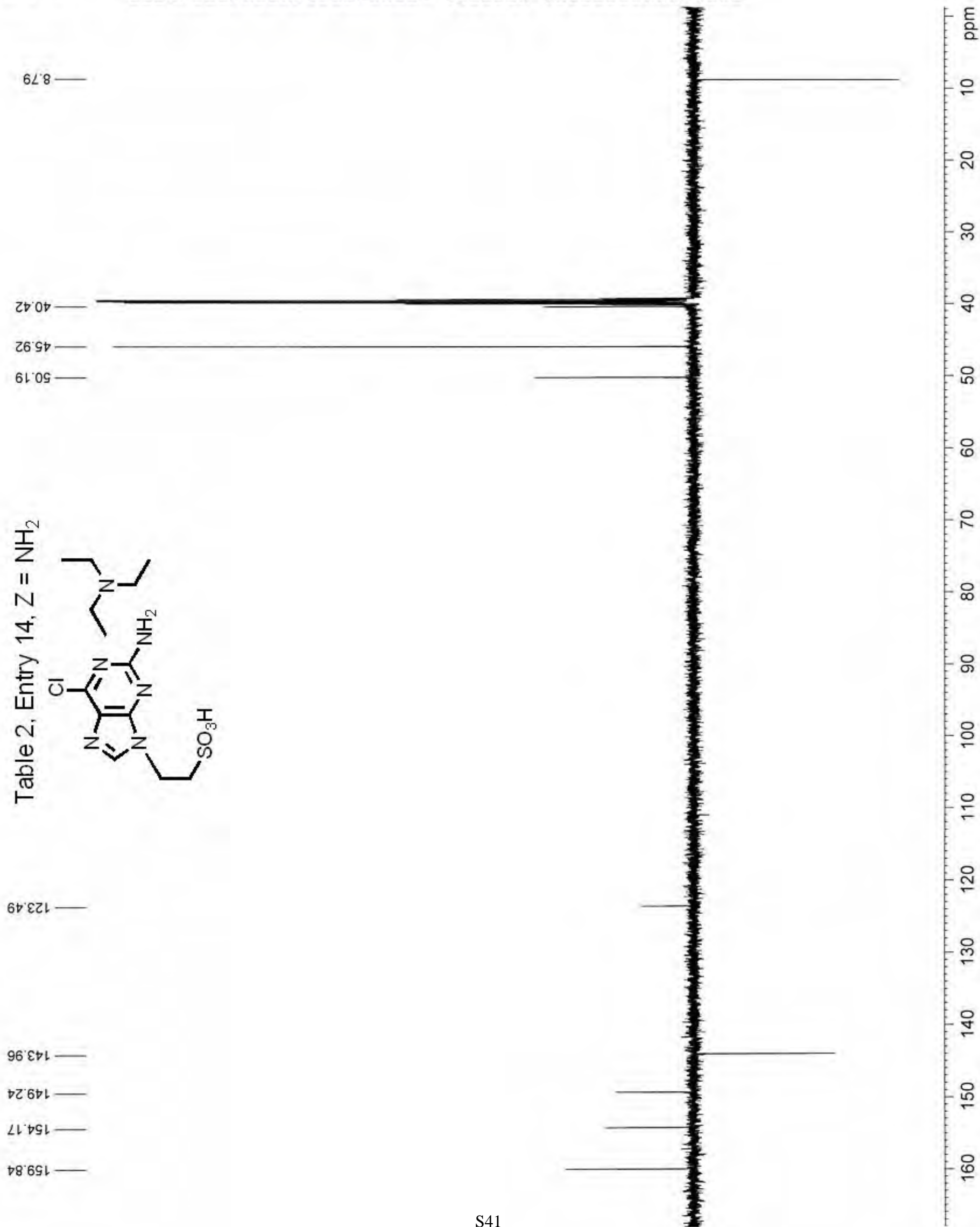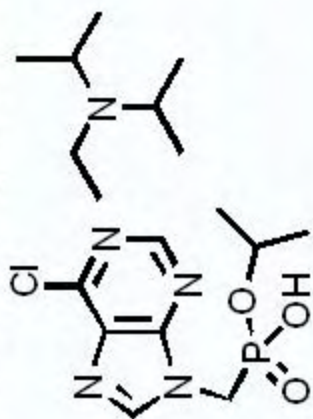SF   125.7125653 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

8.79

40.42

45.92

50.19

Table 2, Entry 14, Z = NH$_2$

123.49

143.96

149.24

154.17

159.84

ppm

10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160
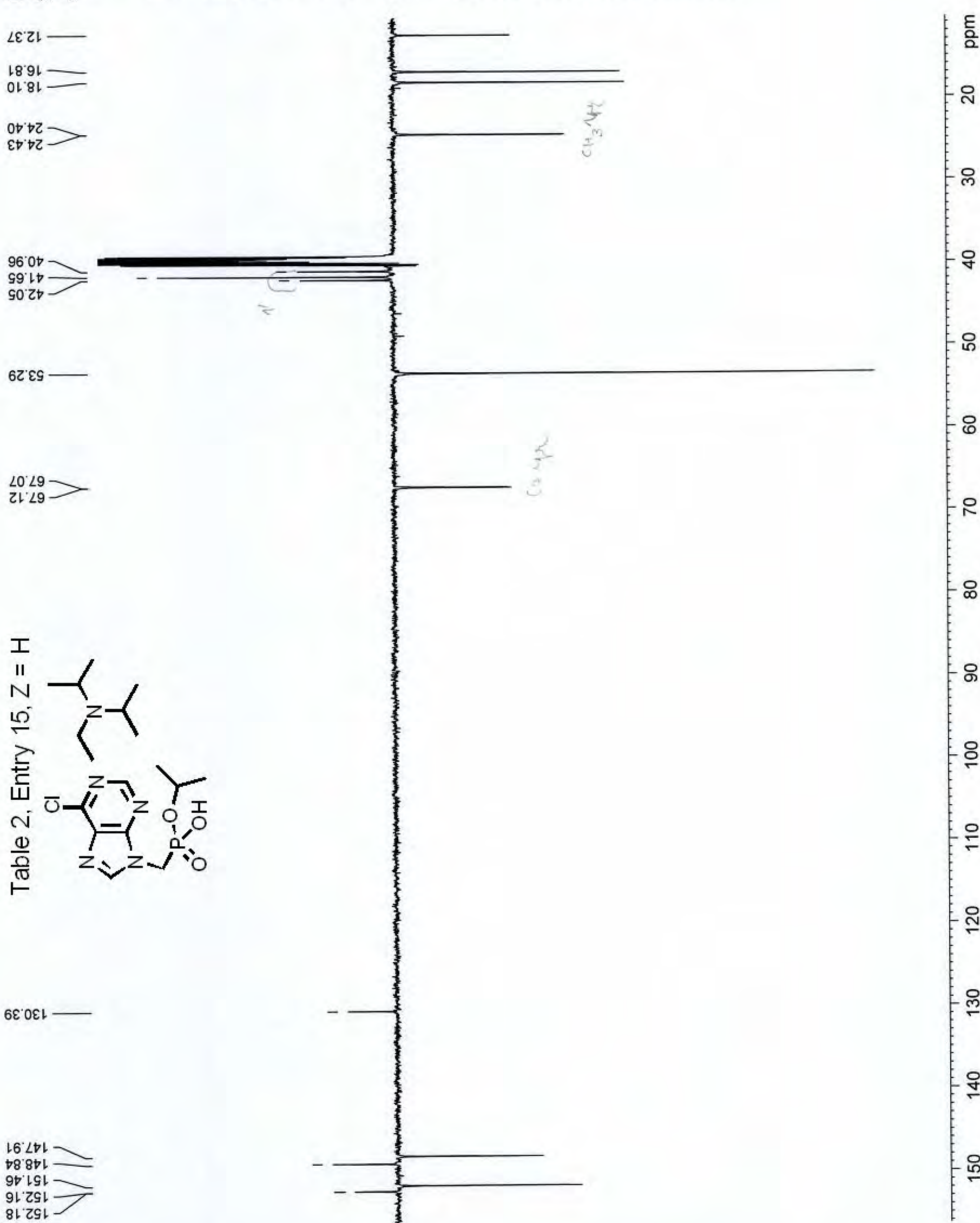

S41

Dejmek_MD338
1H NMR in DMSO
15-9-11 DR
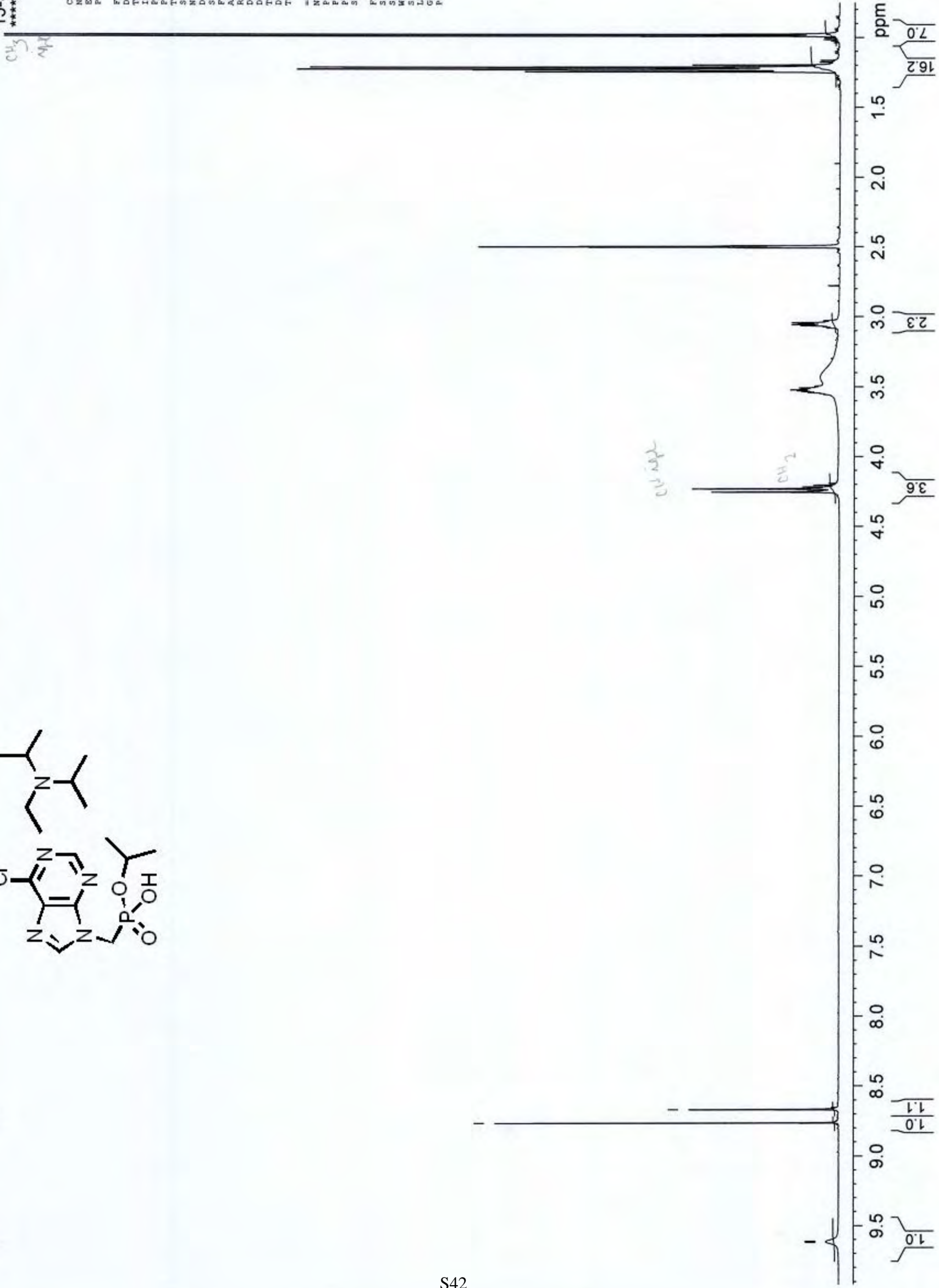
Table 2, Entry 15, Z = H
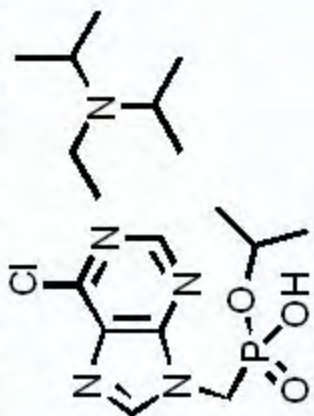
Dejmek_MD338
APT in DMSO
15-9-11 DR

Table 2, Entry 15, Z = H

ppm

Dejmek_MD333
1H NMR in DMSO
26-9-11 DR
****

NAME   Dejmek_MD33
EXPNO   1
PROCNO   1
Date_   20110926
Time   8.58
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

====== CHANNEL f1 =
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 N
SI   131072
SF   499.9500008 MH
WDW   no
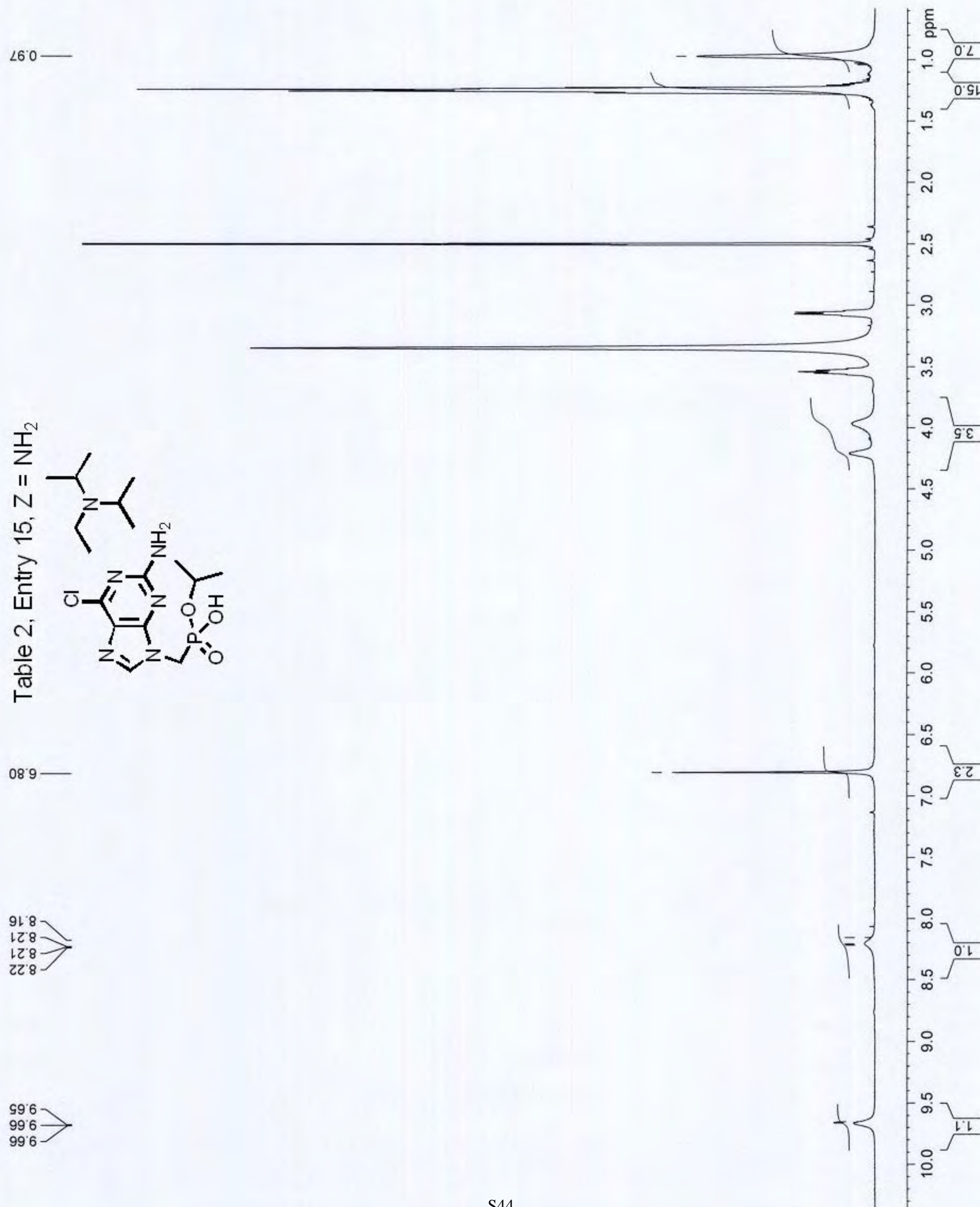SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 15, Z = NH$_2$

0.97 —

6.80 —

8.16
8.21
8.21
8.22

9.65
9.66
9.66

S44

Dejmek_MD333
APT in DMSO
26-9-11 DR
****

Table 2, Entry 15, Z = NH$_2$
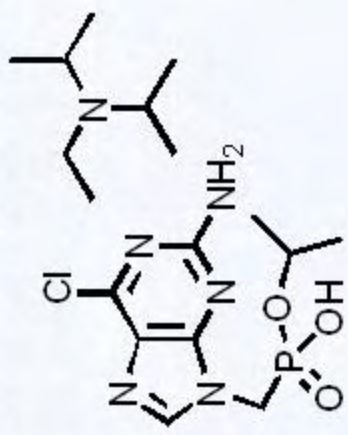
NAME   Dejmek_MD333
EXPNO   2
PROCNO   1
Date_   20110926
Time_   10.17
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   4257
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 =========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 =========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125647 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

12.32
16.84
18.10
24.44
41.61
53.29
122.97
149.07
154.43
154.46
159.78
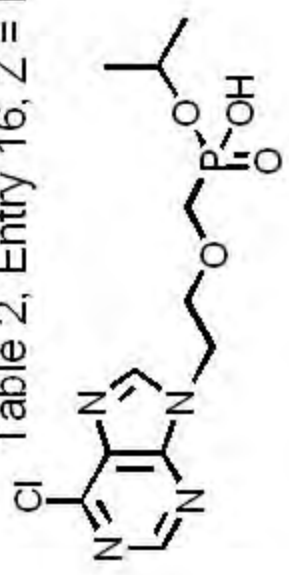
Dejmek_MD395
1H NMR in DMSO
15-12-11 DR

Table 2, Entry 16, Z = H
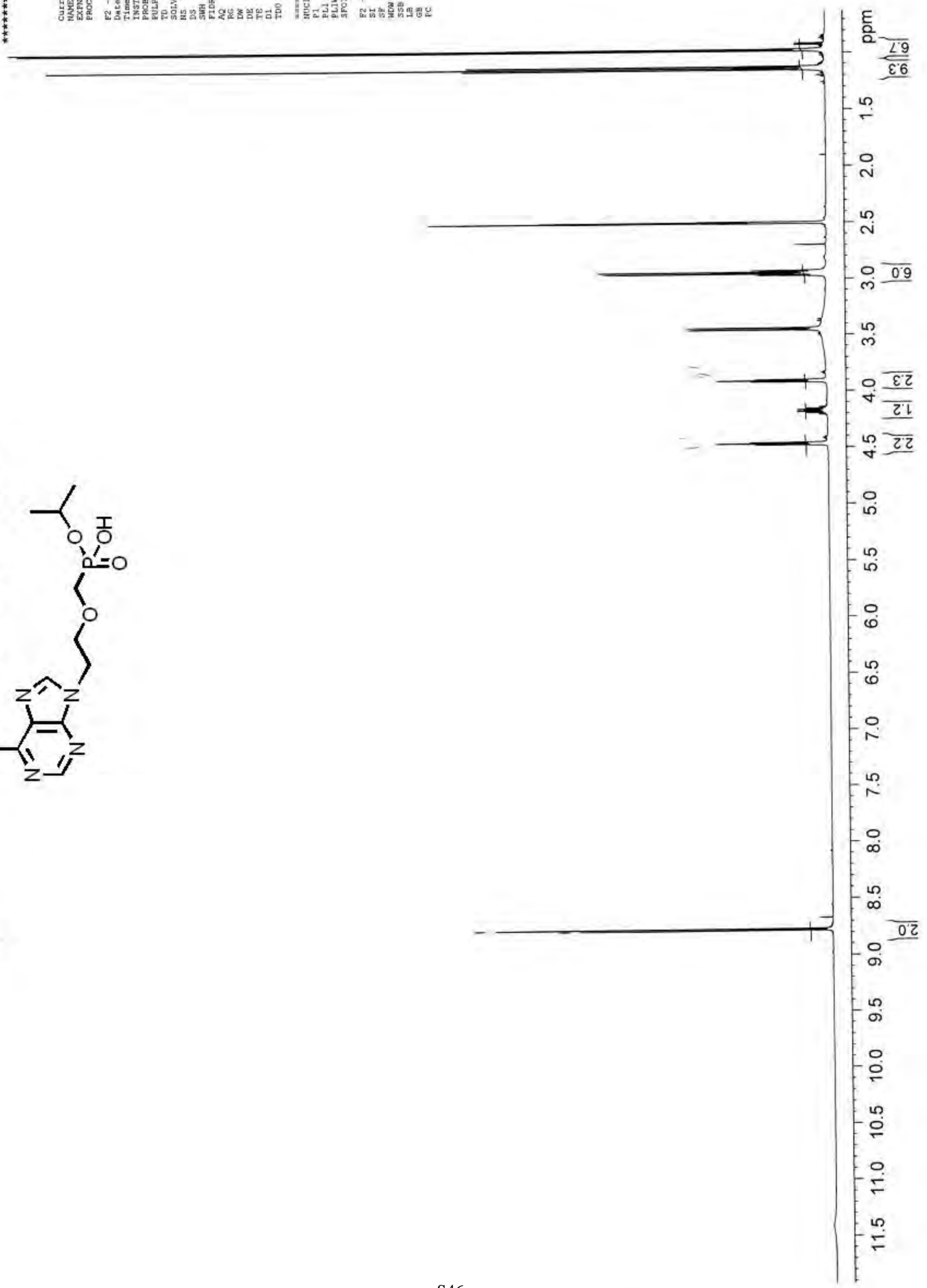
Dejmek_MD395
APT in DMSO
15-12-11 DR
****

8.51

24.33
24.36

43.67
45.16

66.72
68.01
69.38
69.46

Table 2, Entry 16, Z = H

130.86

148.17
148.98
151.53
152.14

ppm

S47

Dejmek_MD396
1H NMR in DMSO
16-12-11 DR
****

NAME   Dejmek_MD396
EXPNO   1
PROCNO   1
Date_   20111216
Time   9.04
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ======
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz
SI   131072
SF   499.9499979 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 2, Entry 16, Z = NH₂

6.88

8.16

ppm 6.0 / 9.4 (1.0)
9.0 (2.5)
6.0 (3.0)
3.4 (4.0)
2.0 (7.0)
1.0 (8.0)
0.7 (11.5)
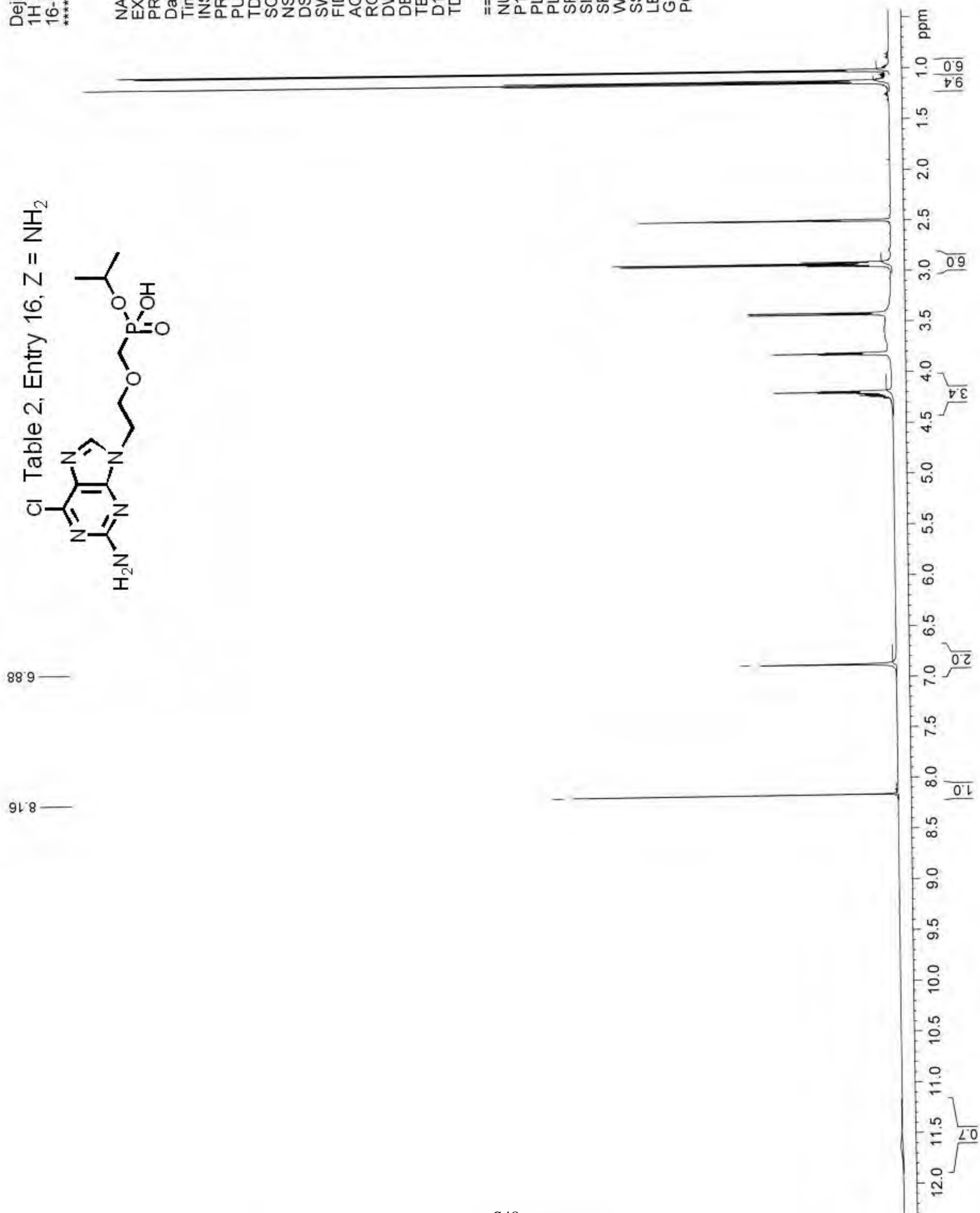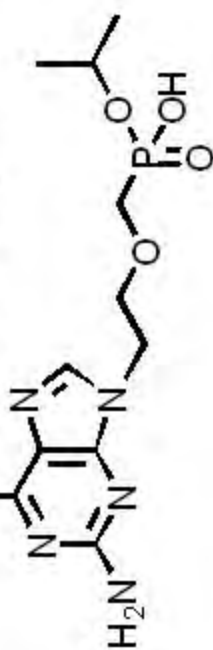
Dejmek_MD396
APT in DMSO
16-12-11 DR
****

NAME   Dejmek_MD396
EXPNO   2
PROCNO   1
Date_   20111216
Time   9.25
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   389
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 =======
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125635 MHz
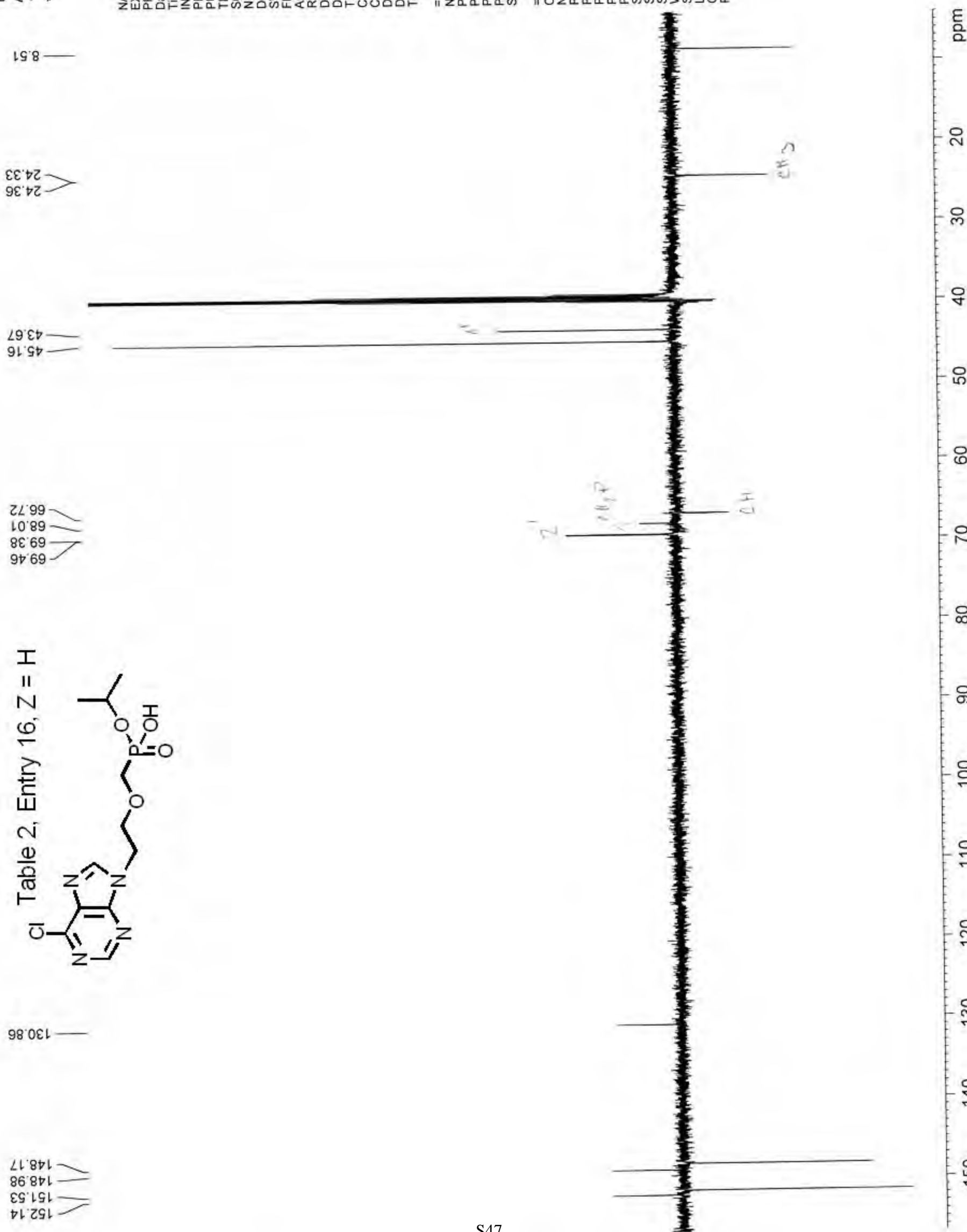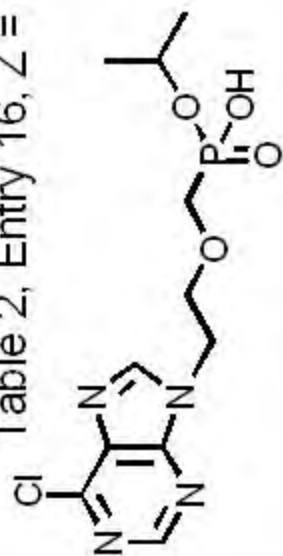WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

8.48

24.44
24.46

42.92
45.11

66.70
66.75
66.96
68.20
69.50
69.58

Table 2, Entry 16, Z = NH₂

123.39

143.85

149.34

154.27

159.89

ppm

Dejmek_MD379
1H NMR in DMSO
25-11-11 DR

Table 3, Entry 1

Current Data Parameters
NAME   Dejmek_MD379
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20111125
Time   16:15
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz

F2 - Processing parameters
SI   131072
SF   499.9499979 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

7.15 ——

7.99 ——
8.18 ——

10.84 ——
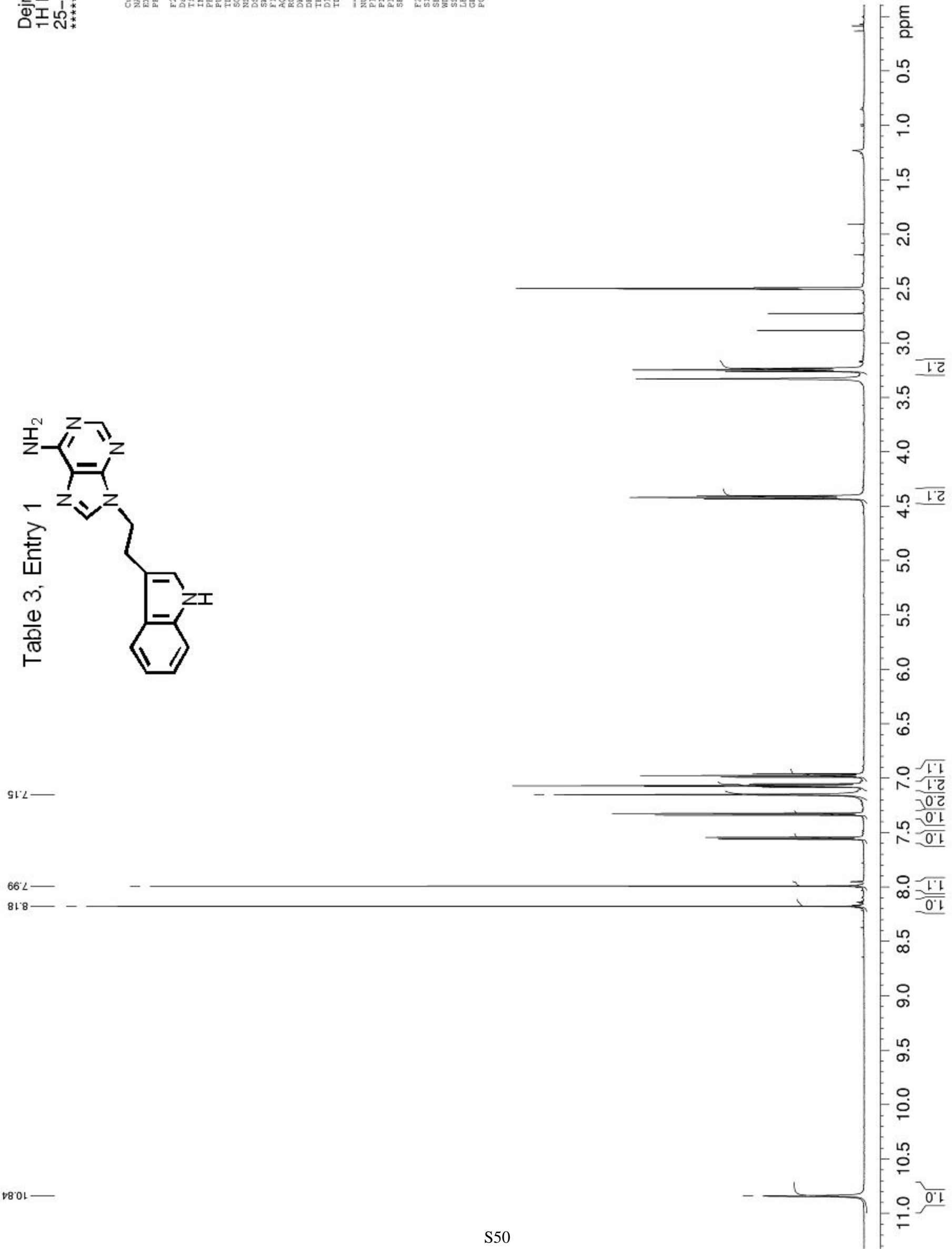
Dejmek_MD379
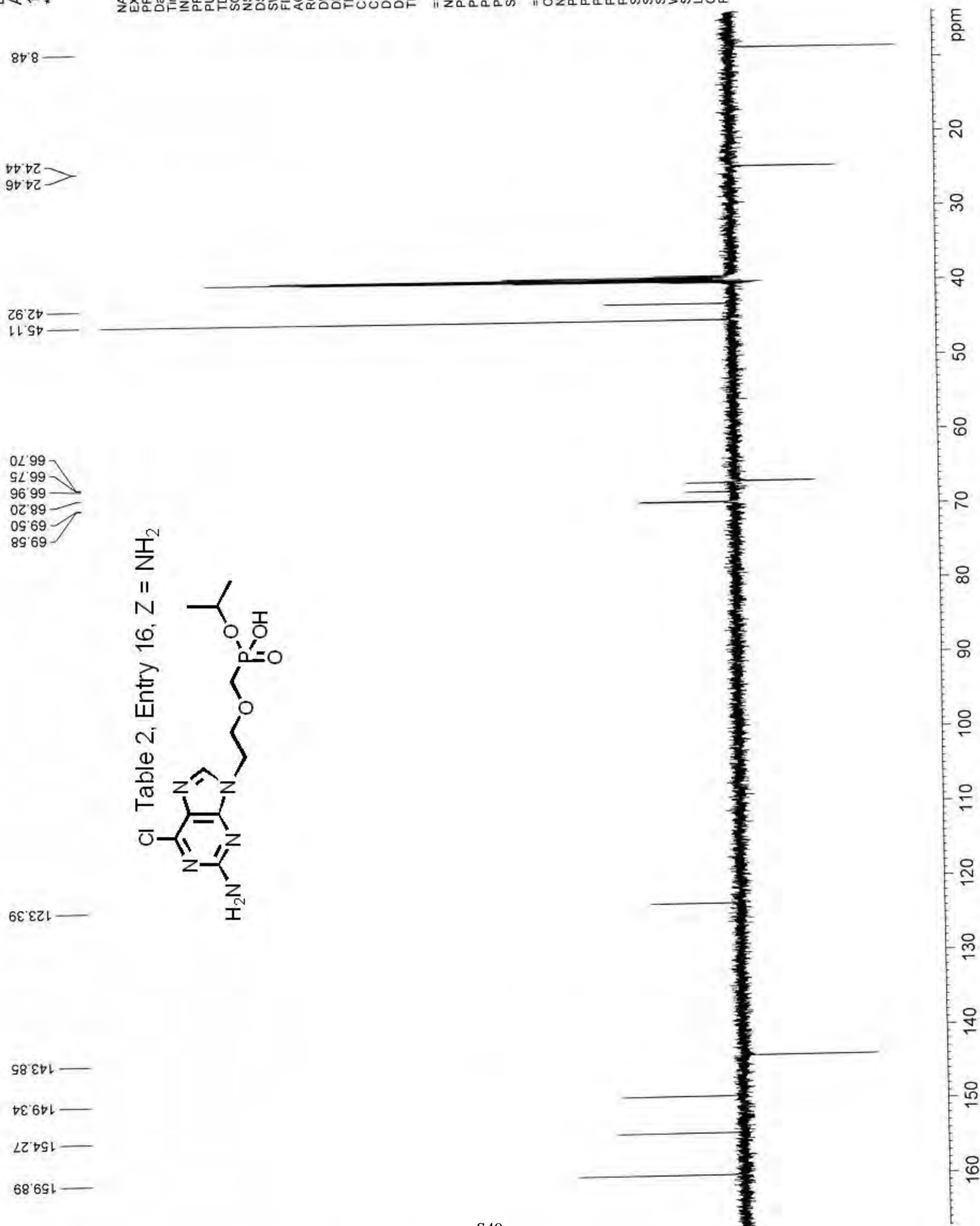APT in DMSO
25-11-11 DR
****

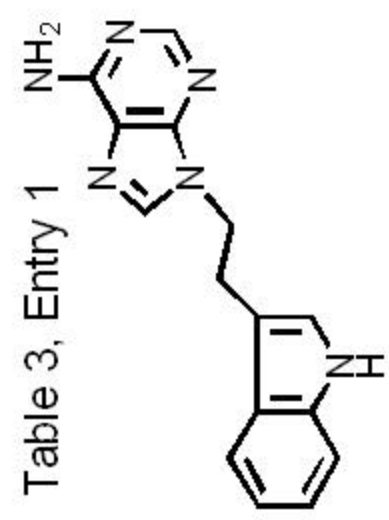NAME   Dejmek_MD379
EXPNO   2
PROCNO   1
Date_   20111125
Time_   16.32
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   312
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   1.00000000 sec
D20   2.00000000 sec
TD0   0.00606061 sec
                 1

====== CHANNEL f1 ======
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

====== CHANNEL f2 ======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125642 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

25.63

43.80

Table 3, Entry 1

110.54
111.60

118.36
118.56
118.94
121.22
123.20

127.14

136.36

140.96

149.70

152.54

156.10

ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
160
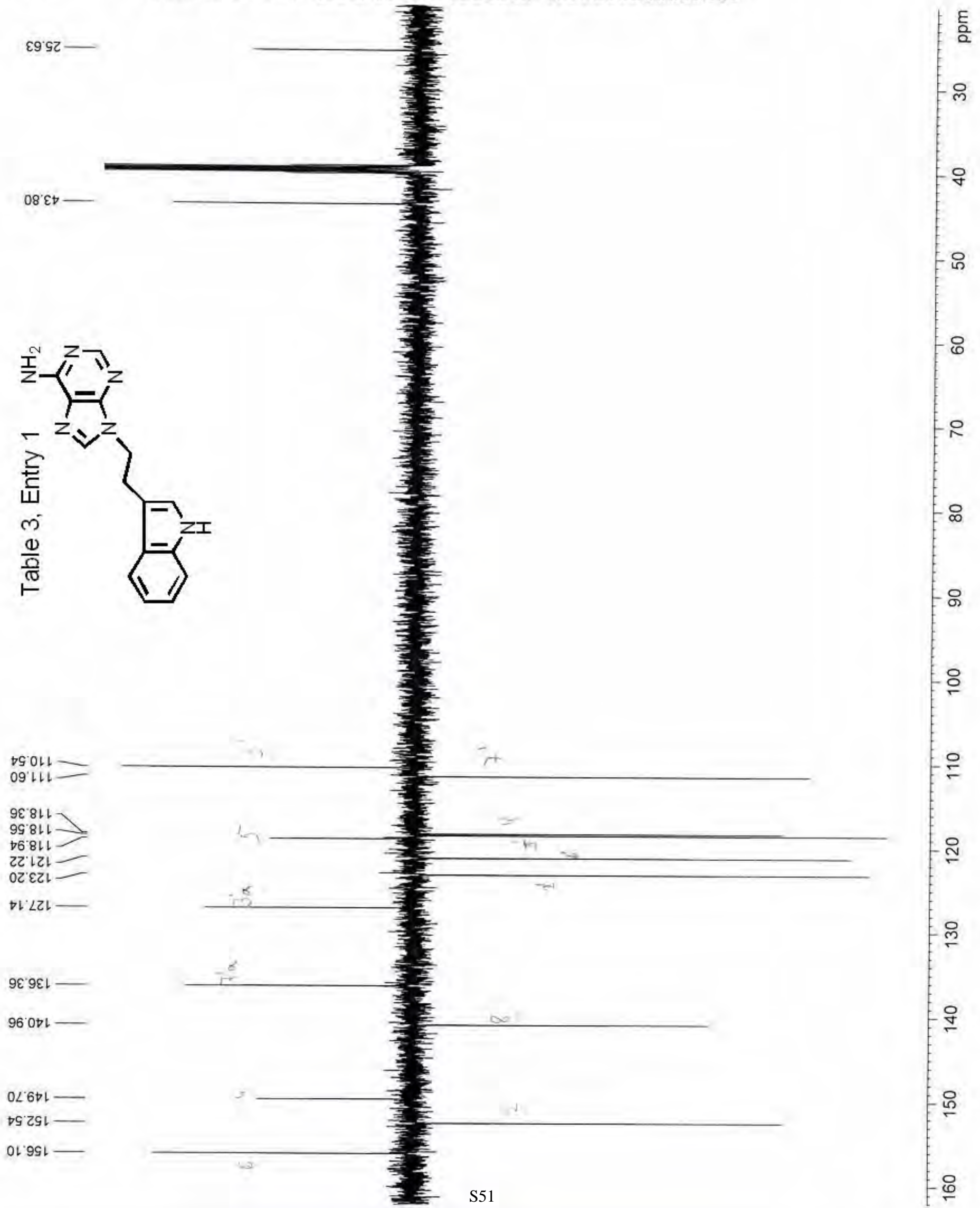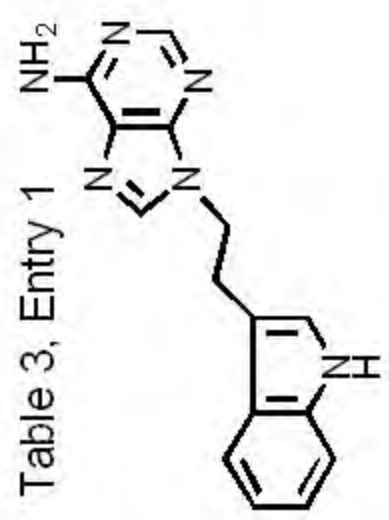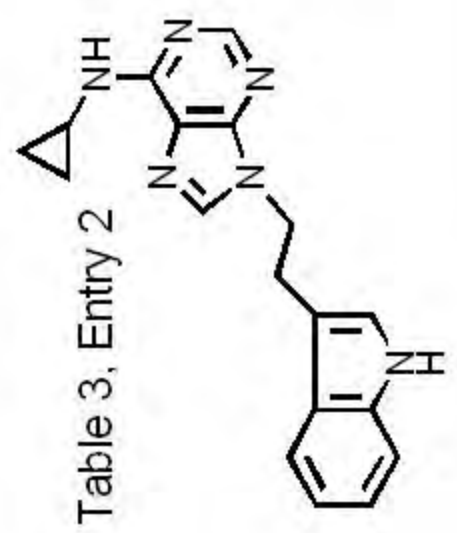
Dejmek_MD378
1H NMR in DMSO
6-12-11 DR
****

NAME   Dejmek_MD378
EXPNO   1
PROCNO   1
Date_   20111206
Time   15.25
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

===== CHANNEL f1 =====
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1 499.9534997 MHz
SI   131072
SF   499.9499979 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 3, Entry 2

7.79
7.80
8.00
8.28

10.84

Dejmek_MD378
APT in DMSO
6-12-11 DR
****

NAME   Dejmek_MD378
EXPNO   2
PROCNO   1
Date_   20111206
Time   15.41
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1271
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125645 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

25.64

43.77

Table 3, Entry 2

110.52
111.60
118.36
118.56
119.29
121.23
123.20
127.14
136.36
140.78
152.45
155.67

ppm
30
40
50
60
70
80
90
100
110
120
130
140
150

Dejmek_MD380
1H–NMR in DMSO
2.12.2011 DR
****

Current Data Parameters
NAME   Dejmek_MD380
EXPNO   1
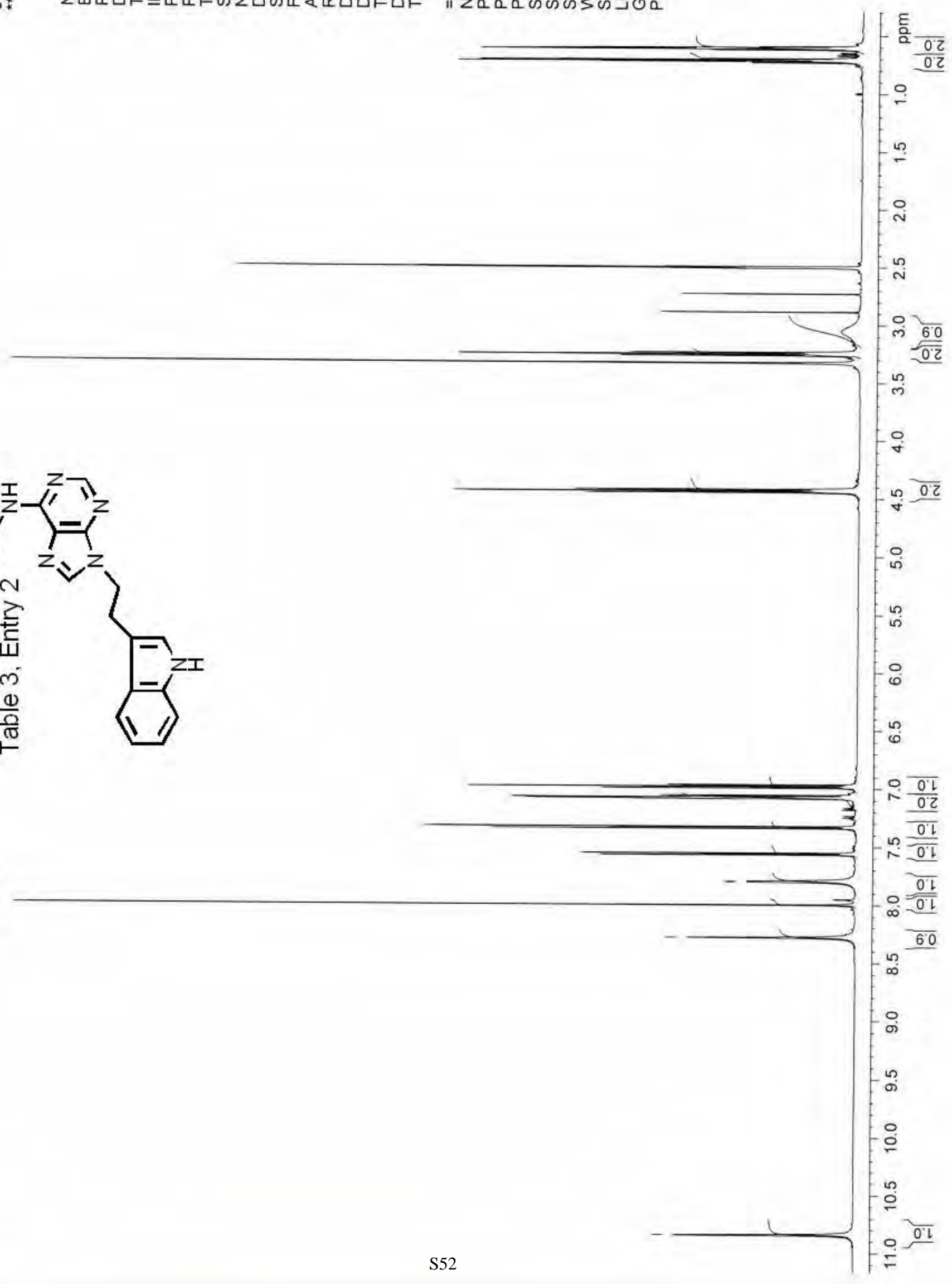PROCNO   1

F2 - Acquisition Parameters
Date_   20111202
Time   8.28
INSTRUM   spect
PROBHD   5 mm BBI 1H/D-
PULPROG   zg30
TD   72114
SOLVENT   DMSO
NS   32
DS   0
SWH   9014.423 Hz
FIDRES   0.125002 Hz
AQ   3.9999733 sec
RG   9
DW   55.467 usec
DE   20.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   11.95 usec
PL1   2.33 dB
PL1W   19.97739792 W
SFO1   600.1342009 MHz

F2 - Processing parameters
SI   131072
SF   600.1300067 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   0.50

Table 3, Entry 3

10.84 ——

8.30 ——
8.06 ——

4.19 ——
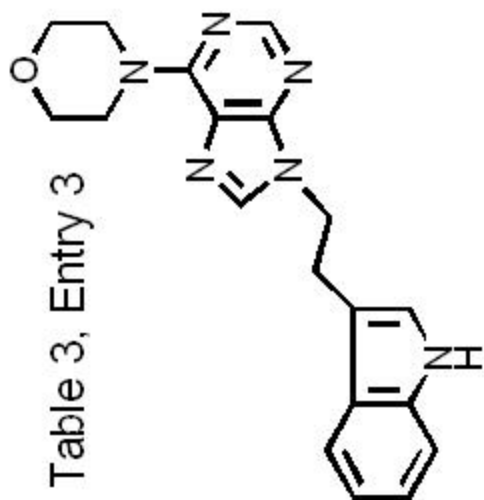
Dejmek_MD380
APT in DMSO
2.12.2011 DR
****

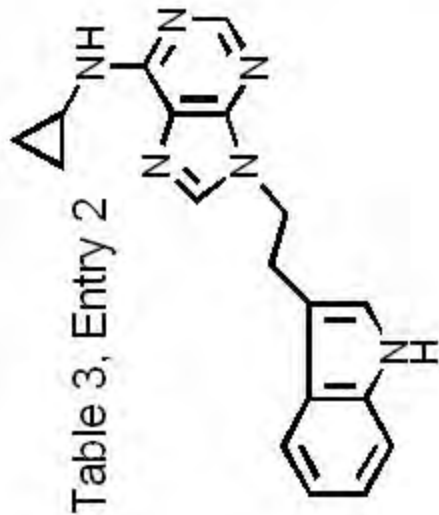NAME   Dejmek_MD380
EXPNO   2
PROCNO   1
Date_   20111202
Time_   9.05
INSTRUM   spect
PROBHD   5 mm BBI 1H/D-
PULPROG   jmod
TD   75752
SOLVENT   DMSO
NS   1450
DS   4
SWH   37878.789 H
FIDRES   0.500037 H
AQ   0.9999764 s
RG   16400
DW   13.200 u
DE   6.00 u
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 s
D20   0.00606061 s
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   13.25 u
P2   26.50 u
PL1   -2.10 d
PL1W   126.28787994 W
SFO1   150.9194083 M

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 u
PL2   2.33 d
PL12   18.84 d
PL12   19.97739792 W
PL2W   0.44620958 W
PL12W   600.1324005 M
SFO2   131072
SI   150.9028607 M
SF   EM
WDW   0
SSB   1.00 H
LB   0
GB   1.40
PC

Table 3, Entry 3

25.479
43.801
66.322
110.409
111.570
118.305
118.527
119.312
121.197
123.209
127.106
136.348
140.292
150.821
151.854
153.387
155.413

20 30 40 50 60 70 80 90 100 110 120 130 140 150 ppm

Dejmek_MD382
1H–NMR in DMSO
19.12.2011 DR

Table 3, Entry 4

S56

Dejmek_MD382
APT in DMSO
19.12.2011 DR
****

NAME   Dejmek_MD382
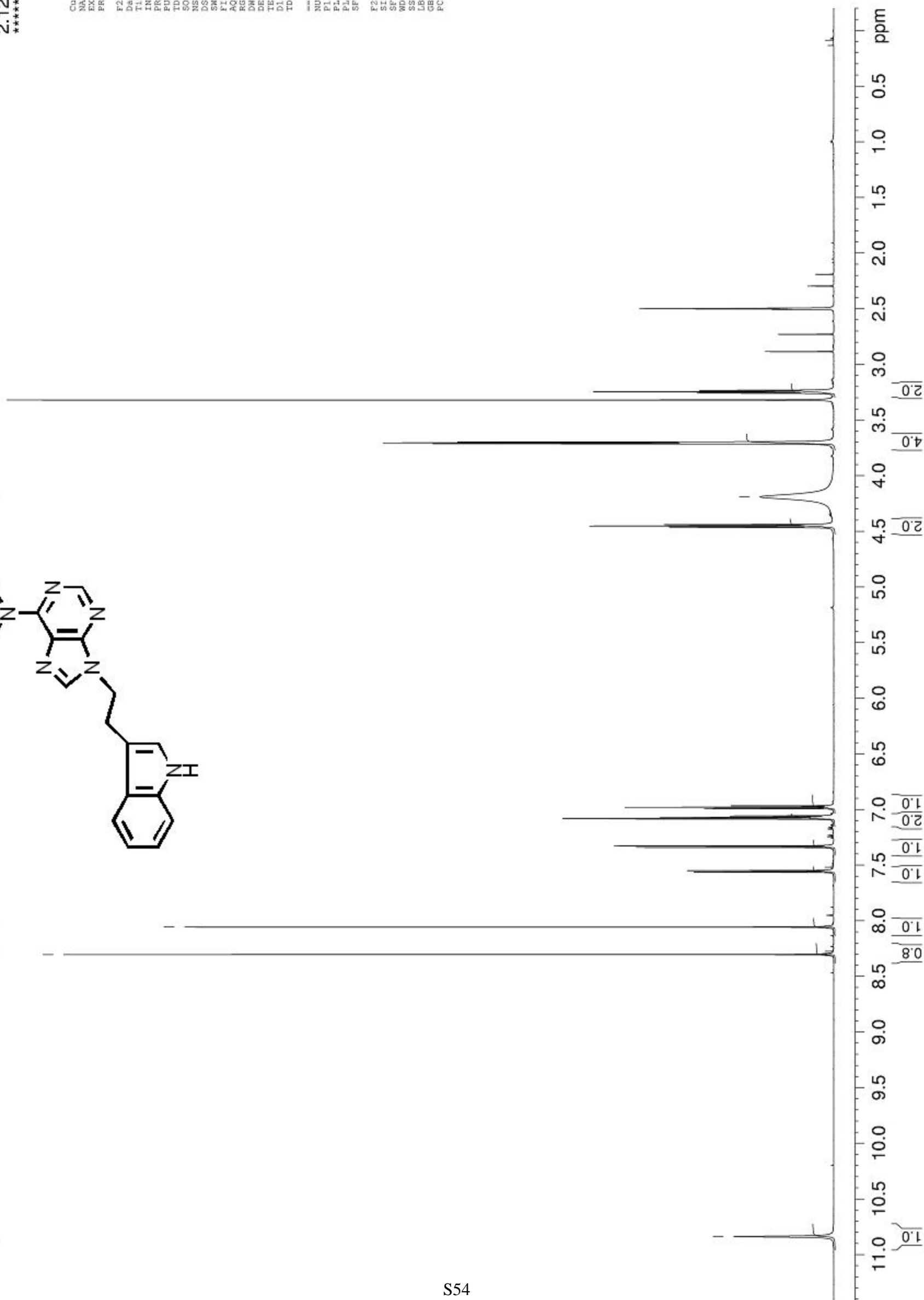EXPNO   2
PROCNO   1
Date_   20111219
Time   15.49
INSTRUM   spect
PROBHD   5 mm BBI 1H/D-
PULPROG   jmod
TD   75752
SOLVENT   DMSO
NS   1461
DS   4
SWH   37878.789 H
FIDRES   0.500037 H
AQ   0.9999764 s
RG   16400
DW   13.200 u
DE   6.00 u
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 s
D20   0.00606061 s
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   13.25 u
P2   26.50 u
PL1   -2.10 d
PL1W   126.28787994 W
SFO1   150.9194083 M

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 u
PL2   2.33 d
PL12   18.84 d
PL12W   19.97739792 W
PL2W   0.44620958 W
PL12W   600.1324005 M
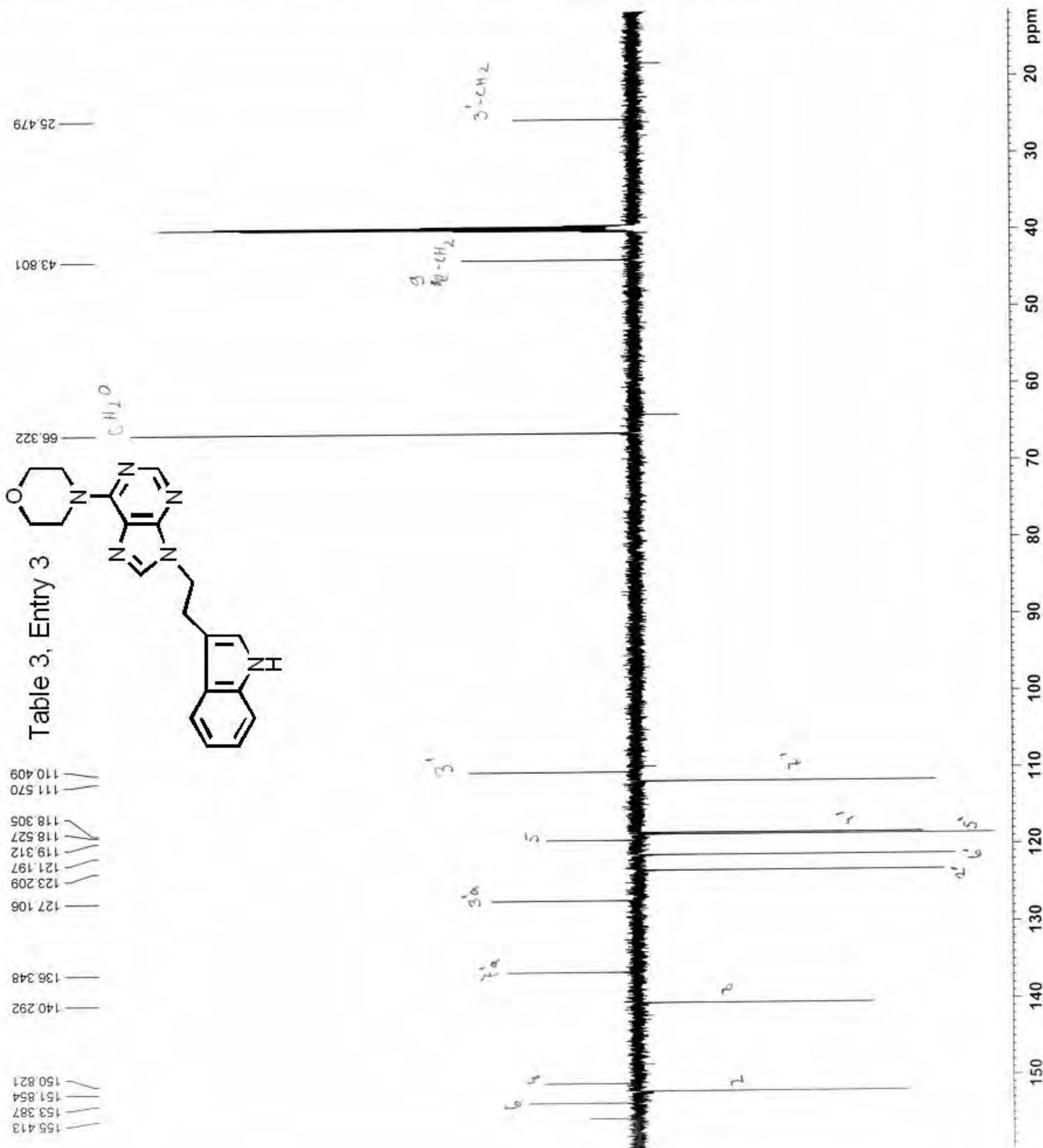SFO2   131072
SI   150.9028619 M
SF
WDW   EM
SSB   0
LB   1.00 H
GB   0
PC   1.40

25.578

44.246

63.892

110.109
111.589

118.229
118.551
121.212
123.313

127.007

135.109
136.338

143.133
144.208
144.907

155.405

175.872

Table 3, Entry 4

ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180

S57

Dejmek_MD394
1H NMR in DMSO
25-11-11 DR

Table 3, Entry 5

10.84

8.55

8.23

4.09

ppm

Dejmek_MD394
APT in DMSO
25-11-11 DR
****

NAME   Dejmek_MD394
EXPNO   2
PROCNO   1
Date_   20111125
Time   10.03
INSTRUM   spect
PROBHD 5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   737
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 =======
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125648 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 3, Entry 5

25.47

44.27

53.98

110.27
111.61
118.27
118.58
120.74
121.24
123.29
127.08
136.35
143.94
151.55
152.22
160.36

ppm
30
40
50
60
70
80
90
100
110
120
130
140
150
160

S59

Dejmek_MD350
1H NMR in DMSO
6–10–11 DR
****
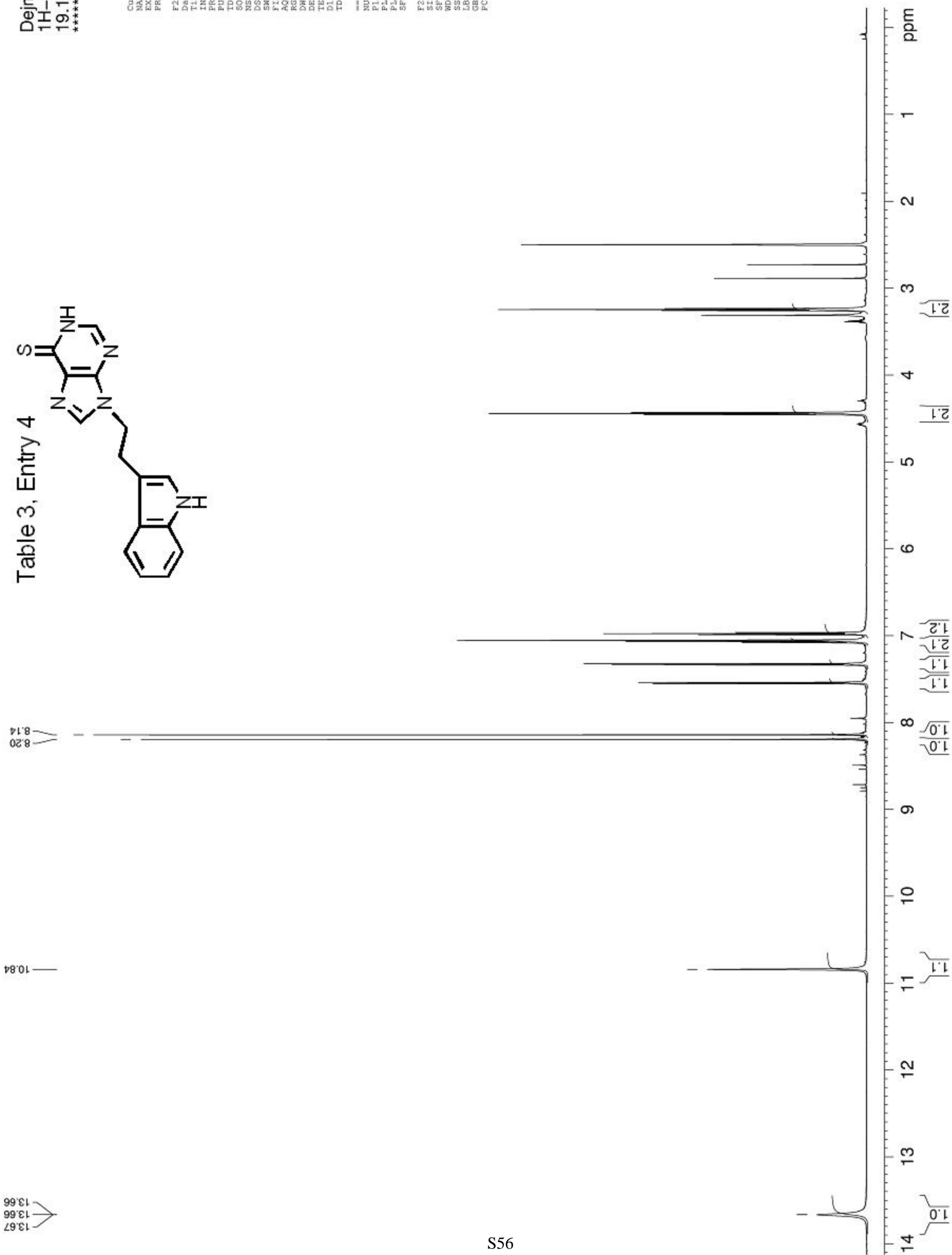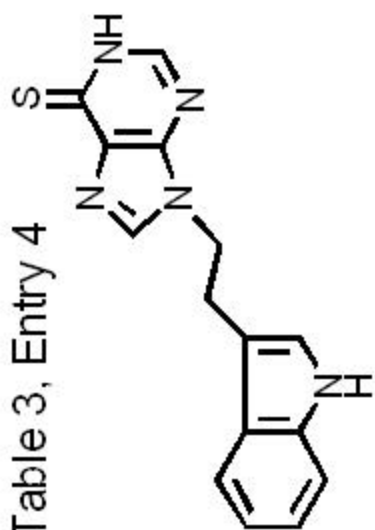
Current Data Parameters
NAME   Dejmek_MD350
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20111006
Time   9.43
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   9.00 usec
PL1   3.00 dB
PL1W   4.28034639 W
SFO1   499.9534997 MHz

F2 - Processing parameters
SI   131072
SF   499.9500006 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 3, Entry 6

12.67 ——

10.92 ——

8.47 ——

8.18 ——

Dejmek_MD350
APT in DMSO
6-10-11 DR
****

Table 3, Entry 6

NAME   Dejmek_MD350
EXPNO   2
PROCNO   1
Date_   20111006
Time_   9.47
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   922
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======= CHANNEL f1 ========
NUC1   13C
P1   14.50 usec
P2   29.00 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======= CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   3.00 dB
PL12   19.48 dB
PL2W   4.28034639 W
PL12W   0.09626734 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125644 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

25.54 ——

44.97 ——

109.91 ——
111.67 ——

118.18 ——
118.61 ——
121.28 ——
123.45 ——

127.04 ——

136.37 ——

140.21 ——

146.93 ——
148.01 ——

155.59 ——

ppm
30
40
50
60
70
80
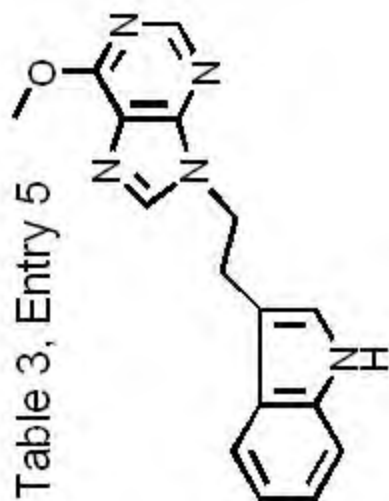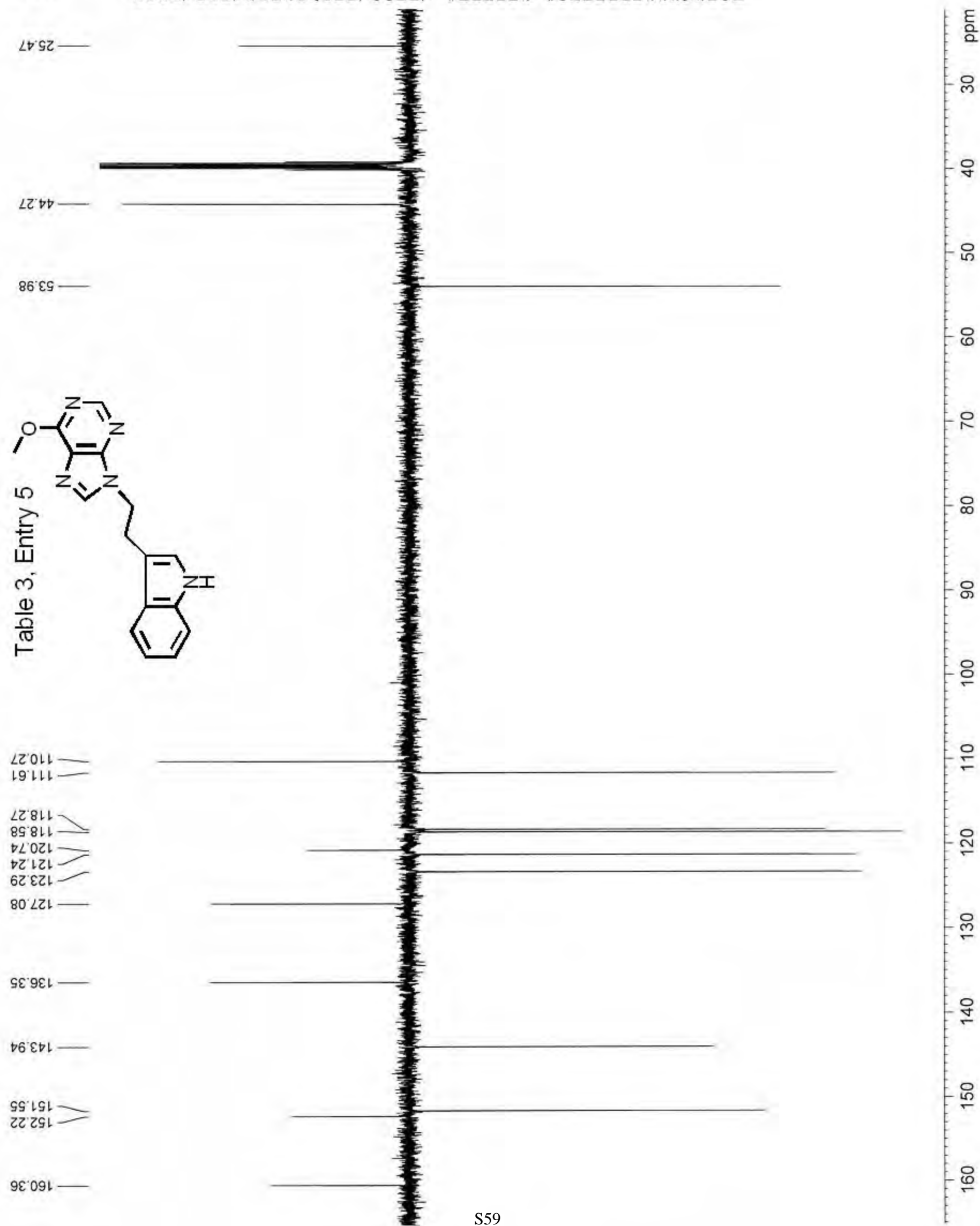90
100
110
120
130
140
150
160

Dejmek_MD390
1H NMR in DMSO
6-12-11 DR
****

Current Data Parameters
NAME   Dejmek_MD390
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20111206
Time   13.30
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz

F2 - Processing parameters
SI   131072
SF   499.9499977 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 3, Entry 7

3.18

4.25

7.56

10.84

2.0

1.9

1.9

1.9

1.1
2.0

1.0

2.0

0.1

11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

S62

Dejmek_MD390
APT in DMSO
6-12-11 DR
****

Table 3, Entry 7

NAME   Dejmek_MD390
EXPNO   2
PROCNO   1
Date_   20111206
Time   13.49
INSTRUM   spect
PROBHD 5 mm TXI1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   355
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

===== CHANNEL f1 =======
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

===== CHANNEL f2 =======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125634 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

25.59
43.15
110.82
111.58
113.42
118.48
118.56
121.22
123.05
127.18
136.36
137.64
151.94
156.26
160.41

ppm 30 40 50 60 70 80 90 100 110 120 130 140 150 160

S63

Dejmek_MD389
1H NMR in DMSO
25-11-11 DR
****
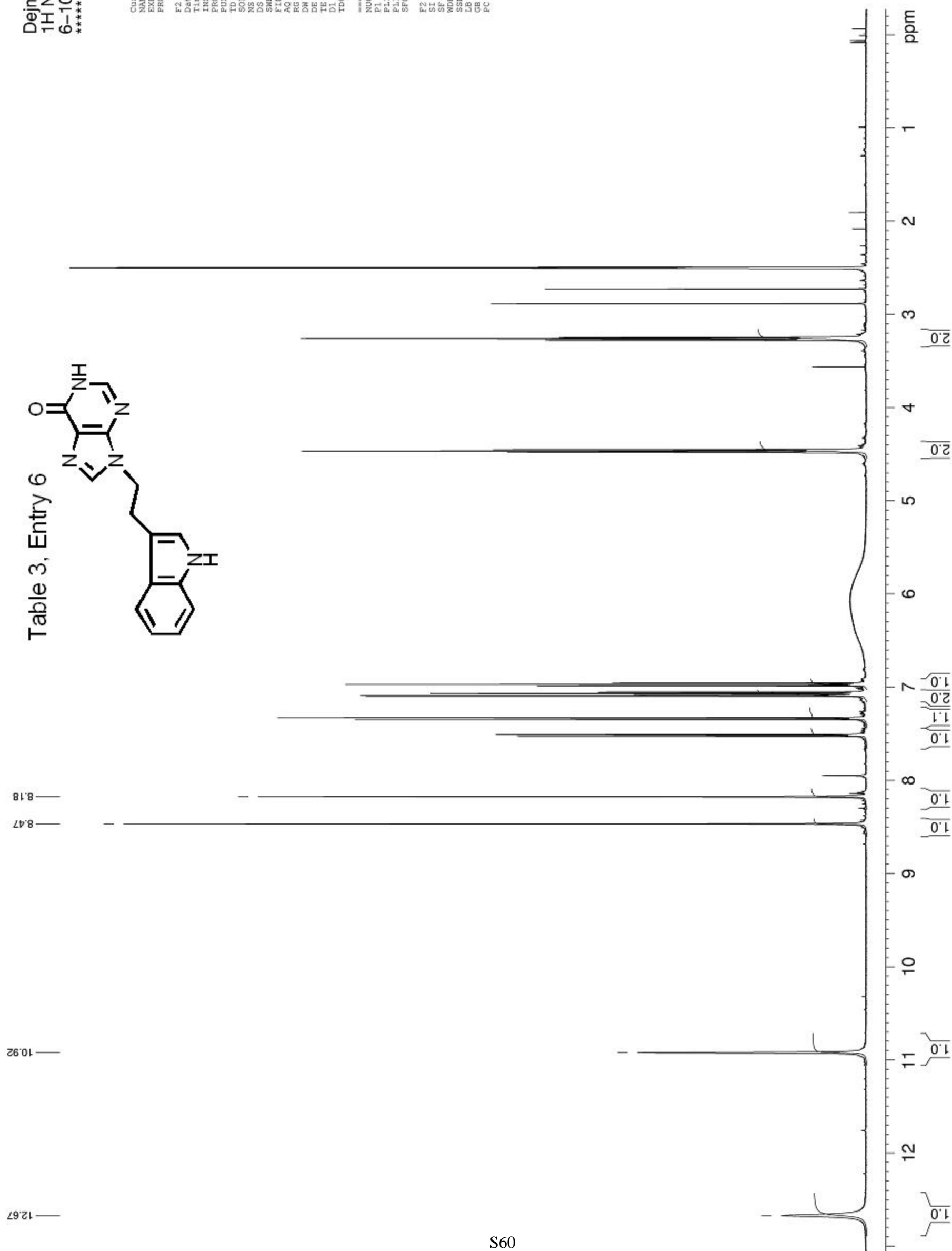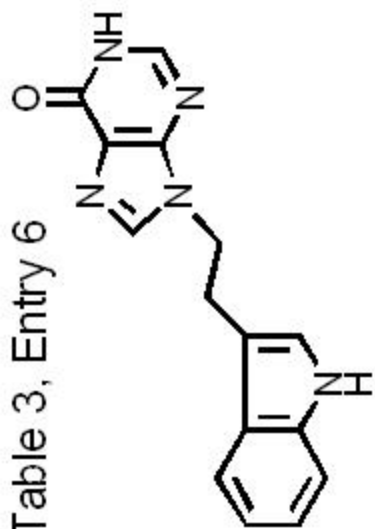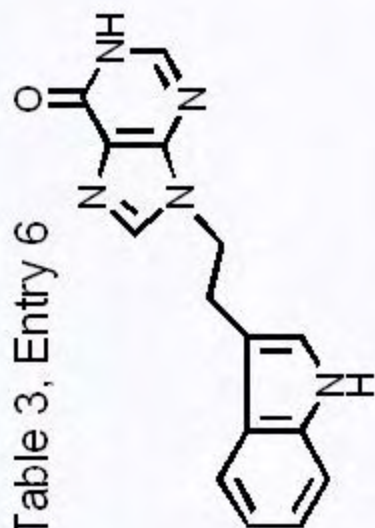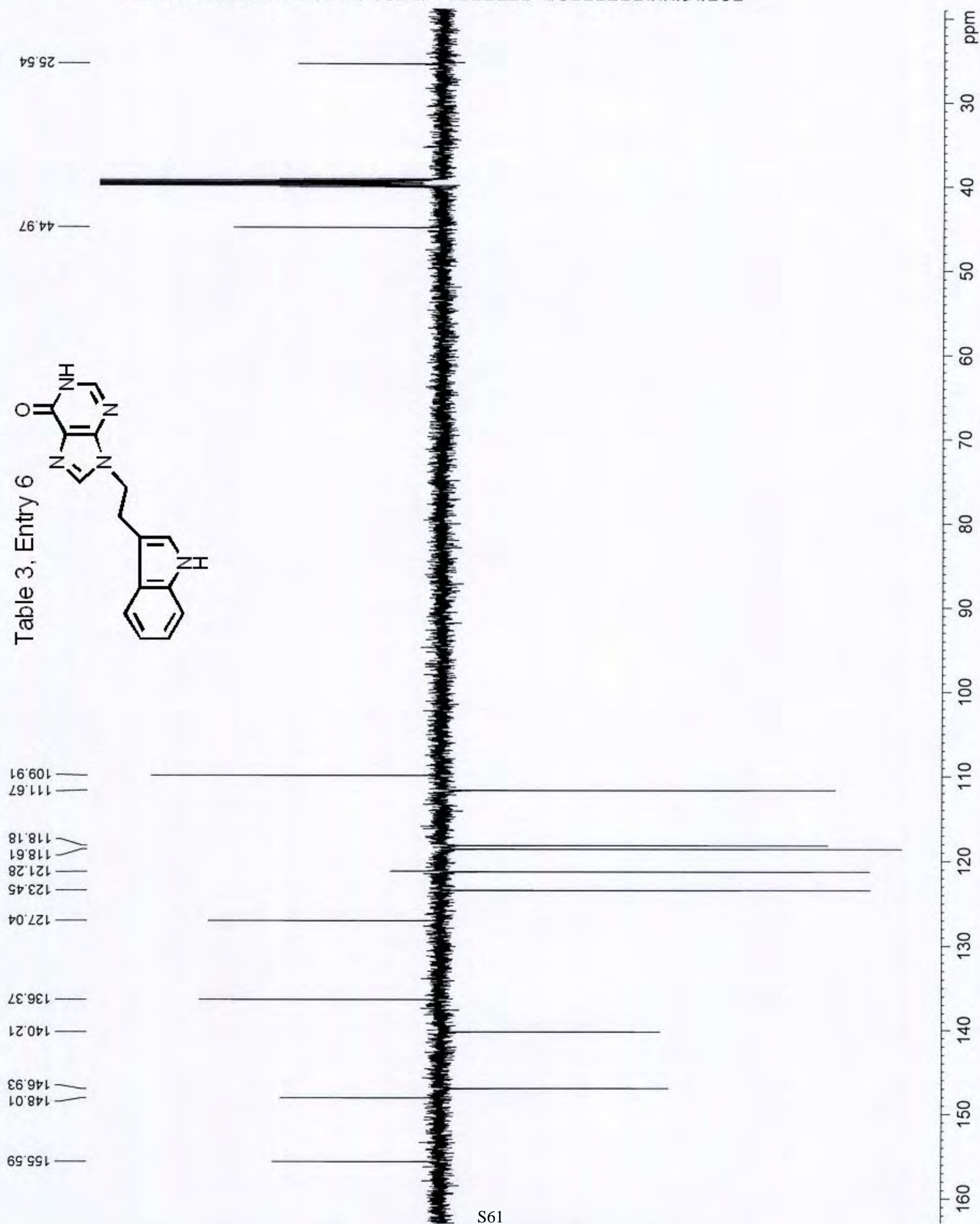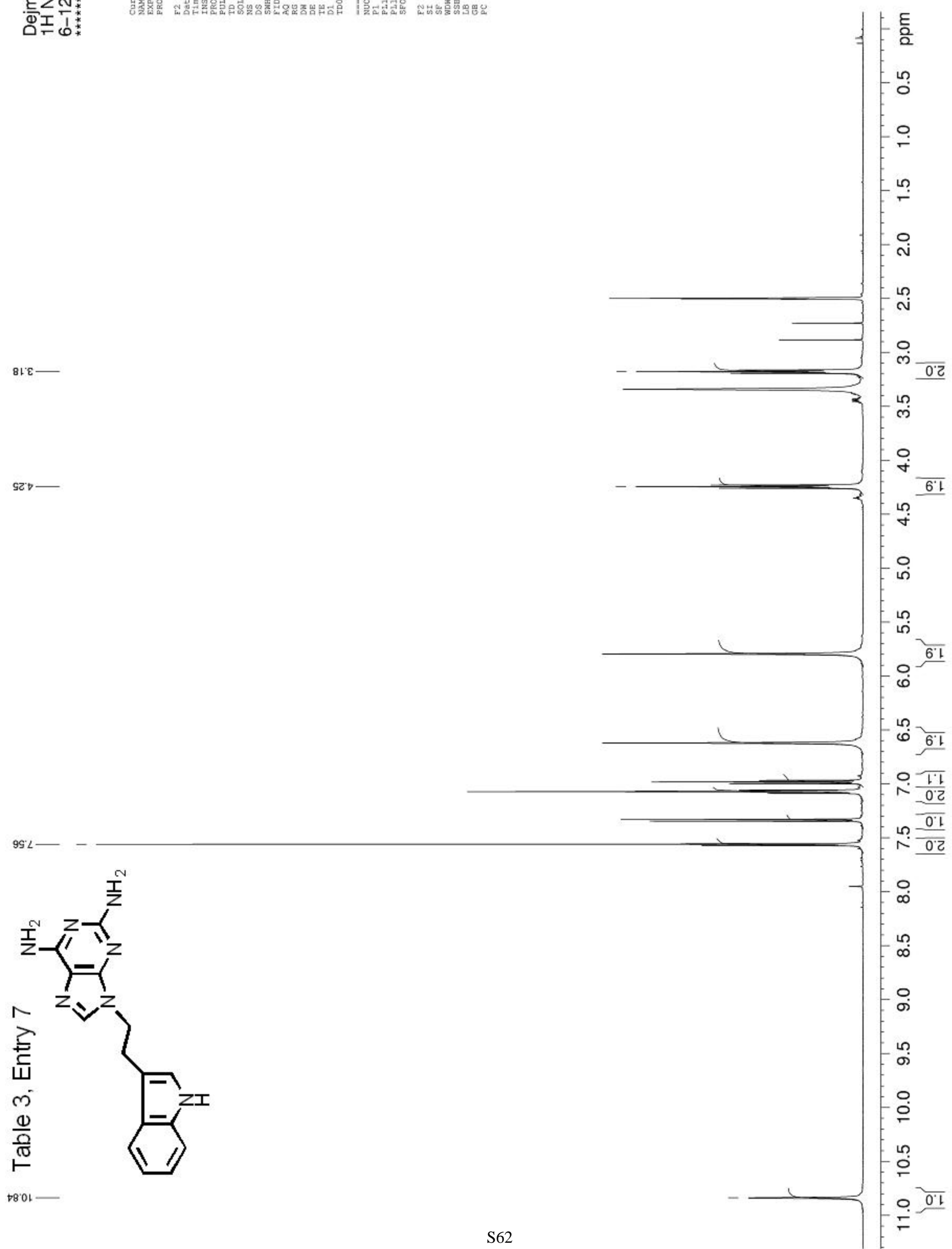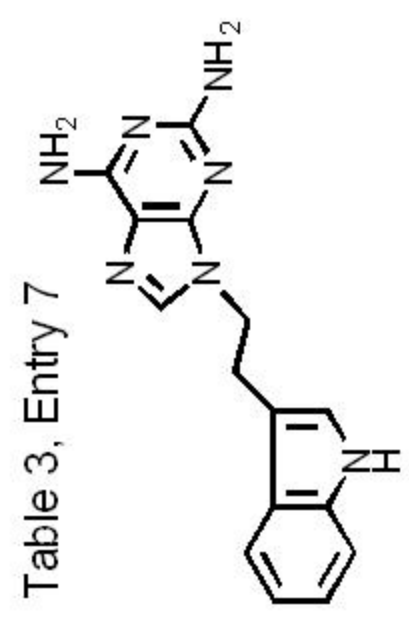
NAME   Dejmek_MD38
EXPNO   1
PROCNO   1
Date_   20111125
Time   10.27
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

===== CHANNEL f1 =
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 M
SI   131072
SF   499.9499978 MH
WDW   no
SSB   0
LB   0.00 Hz
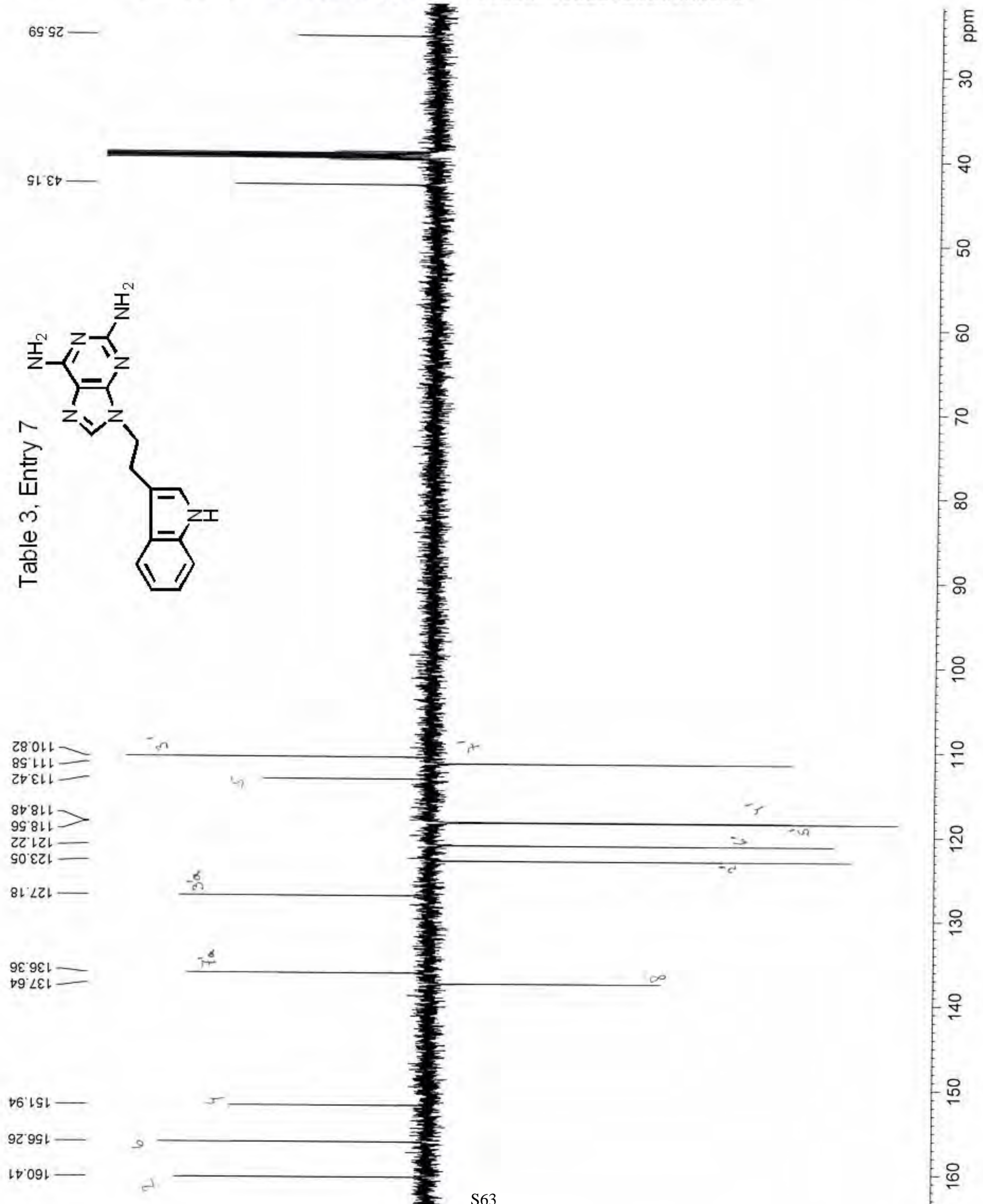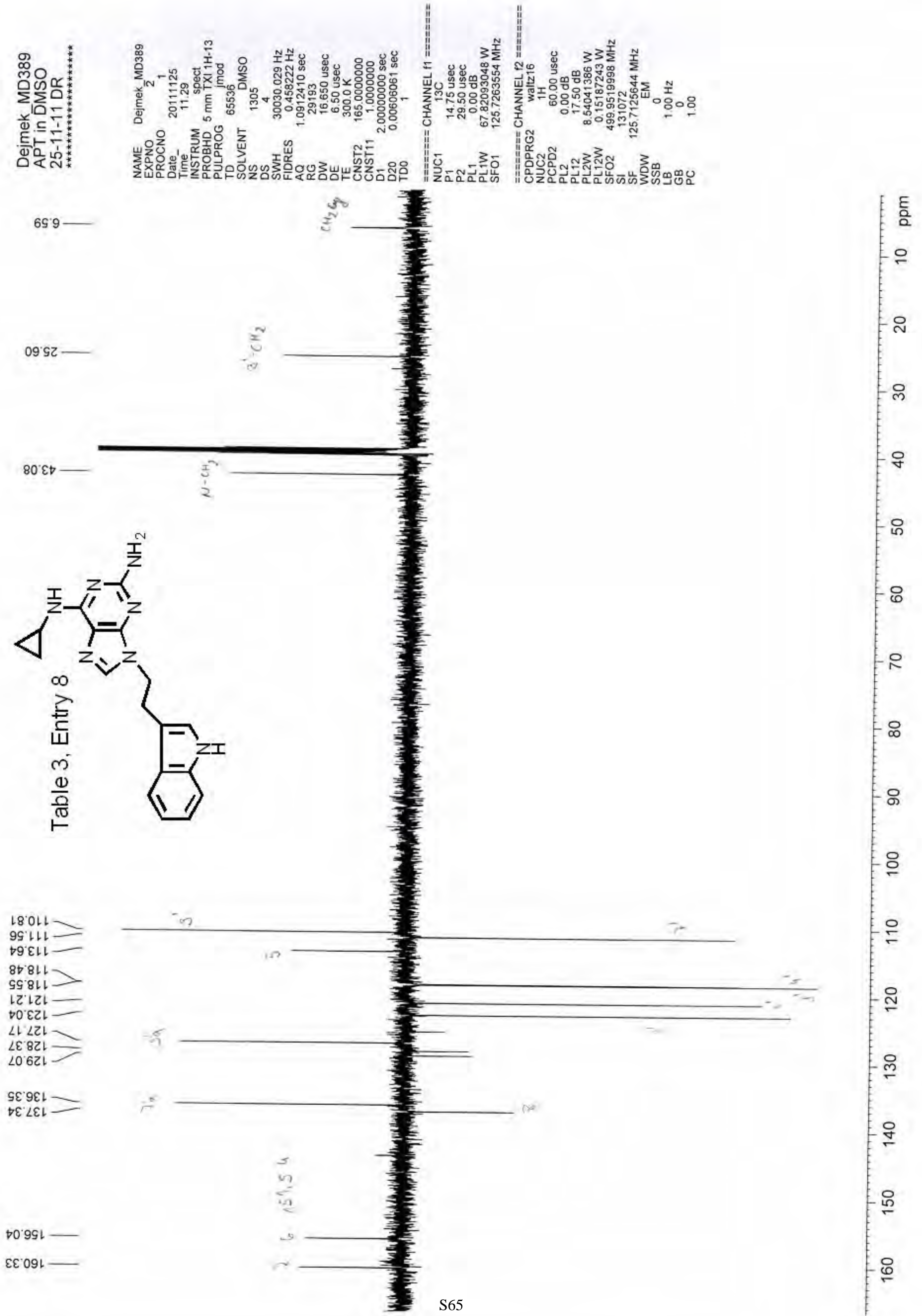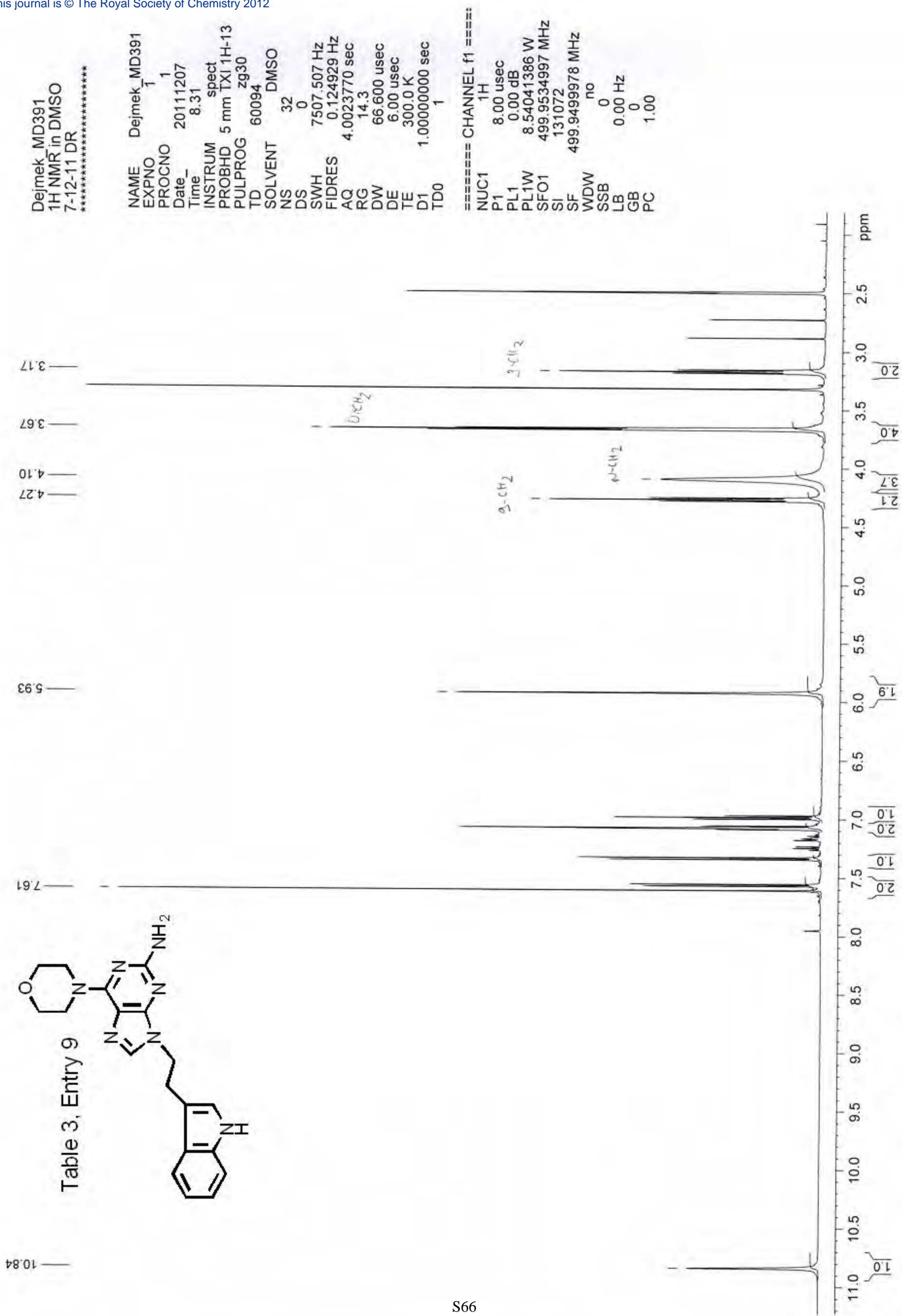GB   0
PC   1.00

Table 3, Entry 8

10.83 ———

7.55 ———

5.84 ———

4.25 ———

Dejmek_MD389
APT in DMSO
25-11-11 DR
****

Table 3, Entry 8

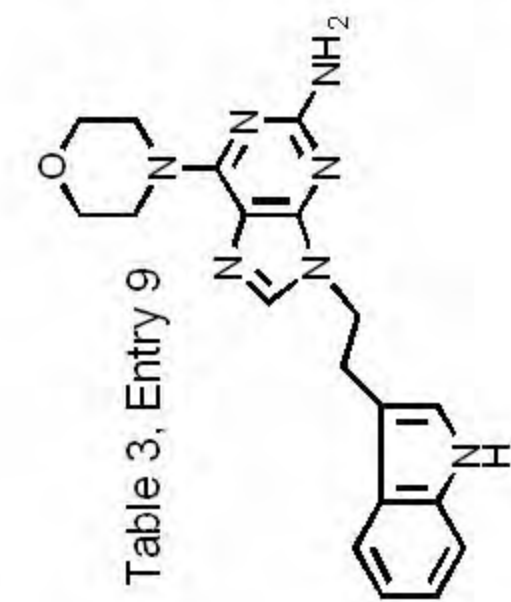NAME   Dejmek_MD389
EXPNO   2
PROCNO   1
Date_   20111125
Time   11.29
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1305
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1W   0.00 dB
SFO1   67.82093048 W
              125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125644 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

6.59

25.60

43.08

110.81
111.56
113.64
118.48
118.55
121.21
123.04
127.17
128.37
129.07
136.35
137.34
156.04
160.33

CH₂ 6g

3'-CH₂

N-CH₂

ppm 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160

Dejmek_MD391
1H NMR in DMSO
7-12-11 DR
****

NAME   Dejmek_MD391
EXPNO   1
PROCNO   1
Date_   20111207
Time   8.31
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======= CHANNEL f1 =======
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 MHz
SI   131072
SF   499.9499978 MHz
WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 3, Entry 9

Dejmek_MD391
APT in DMSO
7-12-11 DR
****

NAME   Dejmek_MD391
EXPNO   2
PROCNO   1
Date_   20111207
Time   9.39
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   1289
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
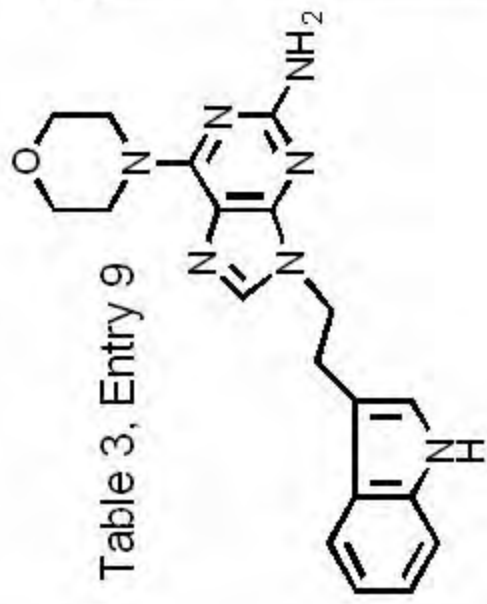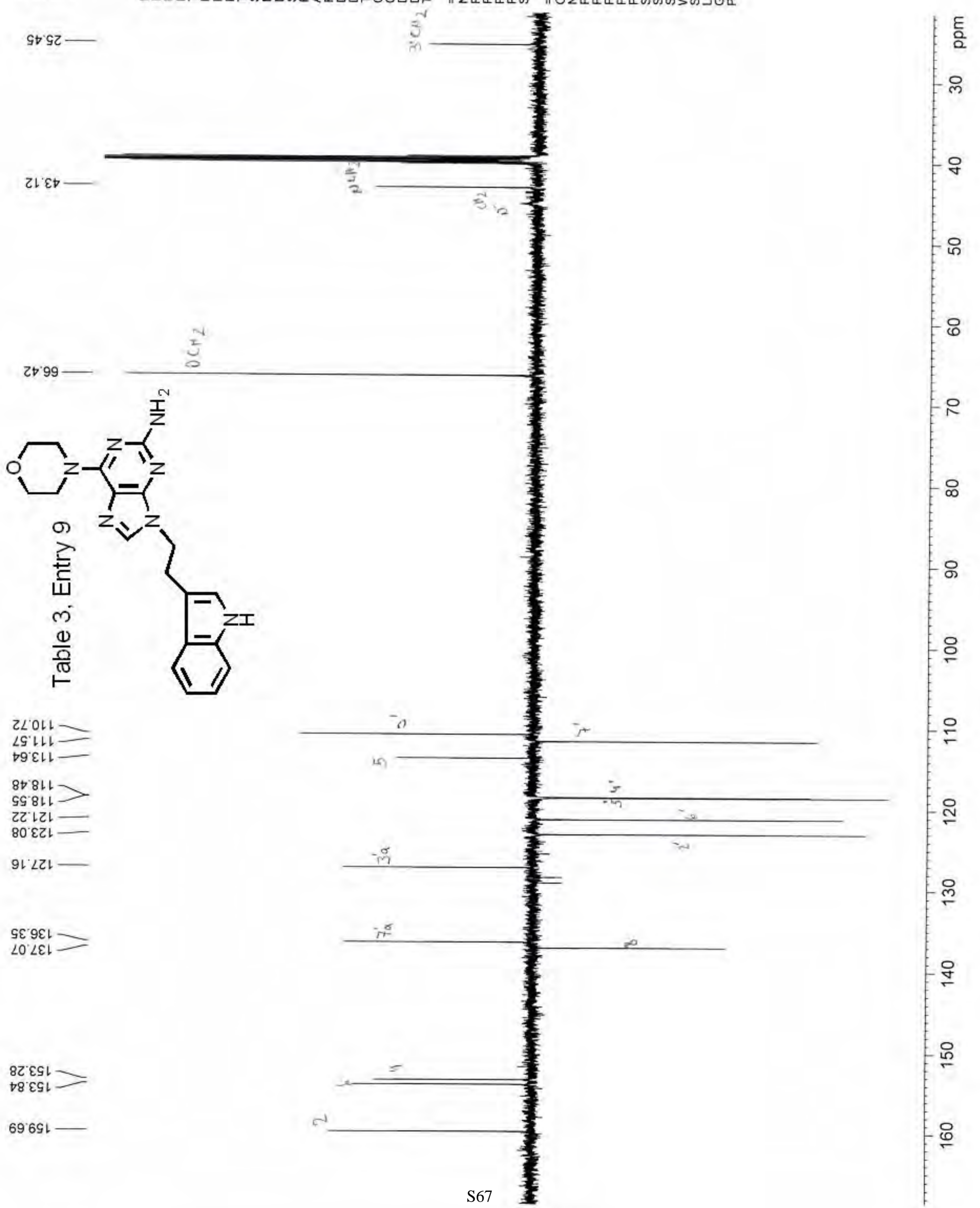TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125646 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

Table 3, Entry 9

25.45
43.12
66.42
110.72
111.57
113.64
118.48
118.55
121.22
123.08
127.16
136.35
137.07
153.28
153.84
159.69

ppm: 30 40 50 60 70 80 90 100 110 120 130 140 150 160

S67

Dejmek_MD392
1H-NMR in DMSO
2.12.2011 DR
****

NAME   Dejmek_MD392
EXPNO   1
PROCNO   1
Date_   20111202
Time   11.22
INSTRUM   spect
PROBHD   5 mm BBI 1H/D-
PULPROG   zg30
TD   72114
SOLVENT   DMSO
NS   32
DS   0
SWH   9014.423 Hz
FIDRES   0.125002 Hz
AQ   3.9999733 sec
RG   9
DW   55.467 usec
DE   20.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

======== CHANNEL f1 ========
NUC1   1H
P1   11.95 usec
PL1   2.33 dB
PL1W   19.97739792 W
SFO1   600.1342009 MHz
SI   131072
SF   600.1300067 MHz
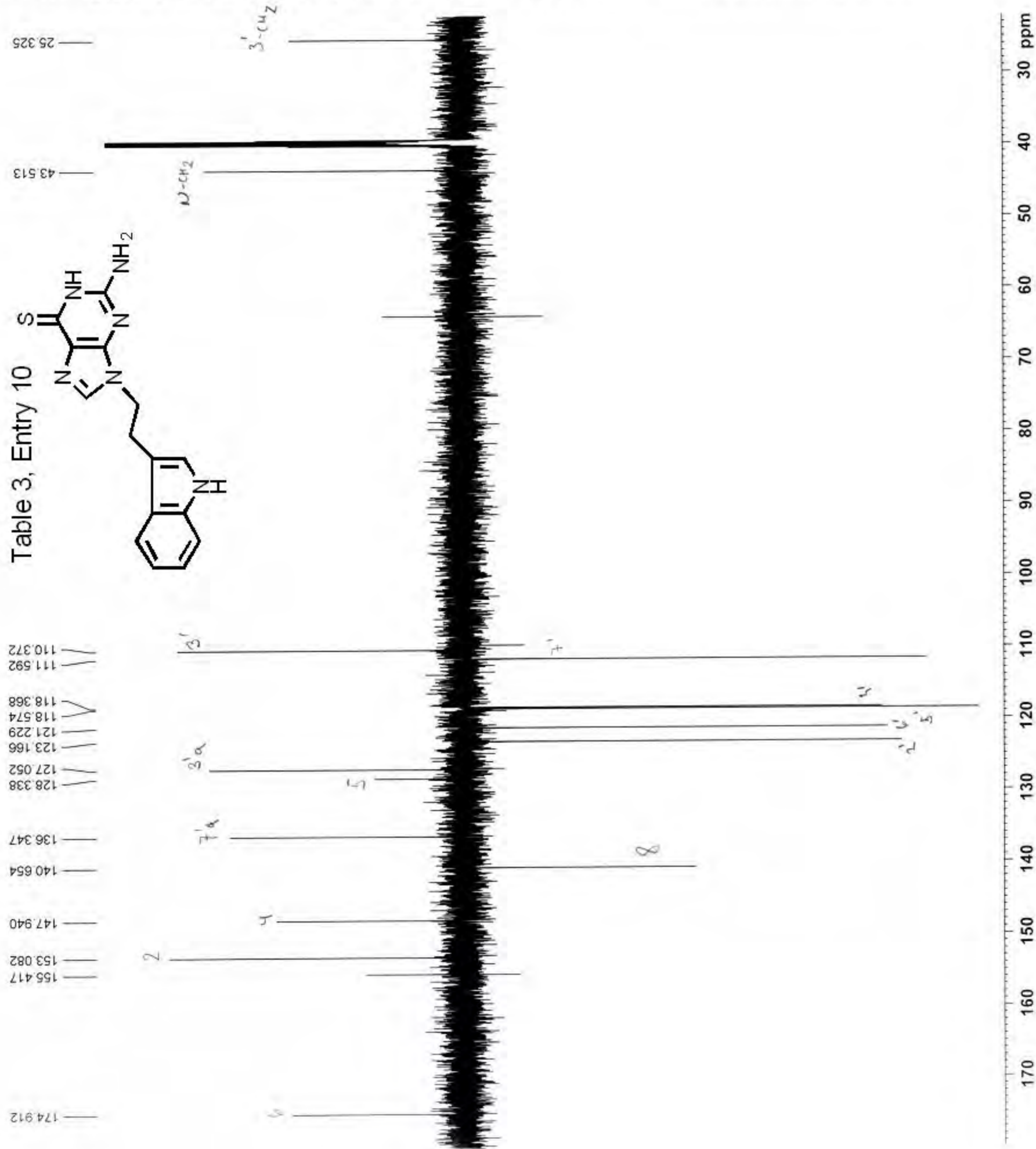WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   0.50

Table 3, Entry 10

7.74

10.85

11.86

2.54
2.07
1.95
1.22
2.29
1.13
1.14
1.00
1.12
1.00

ppm
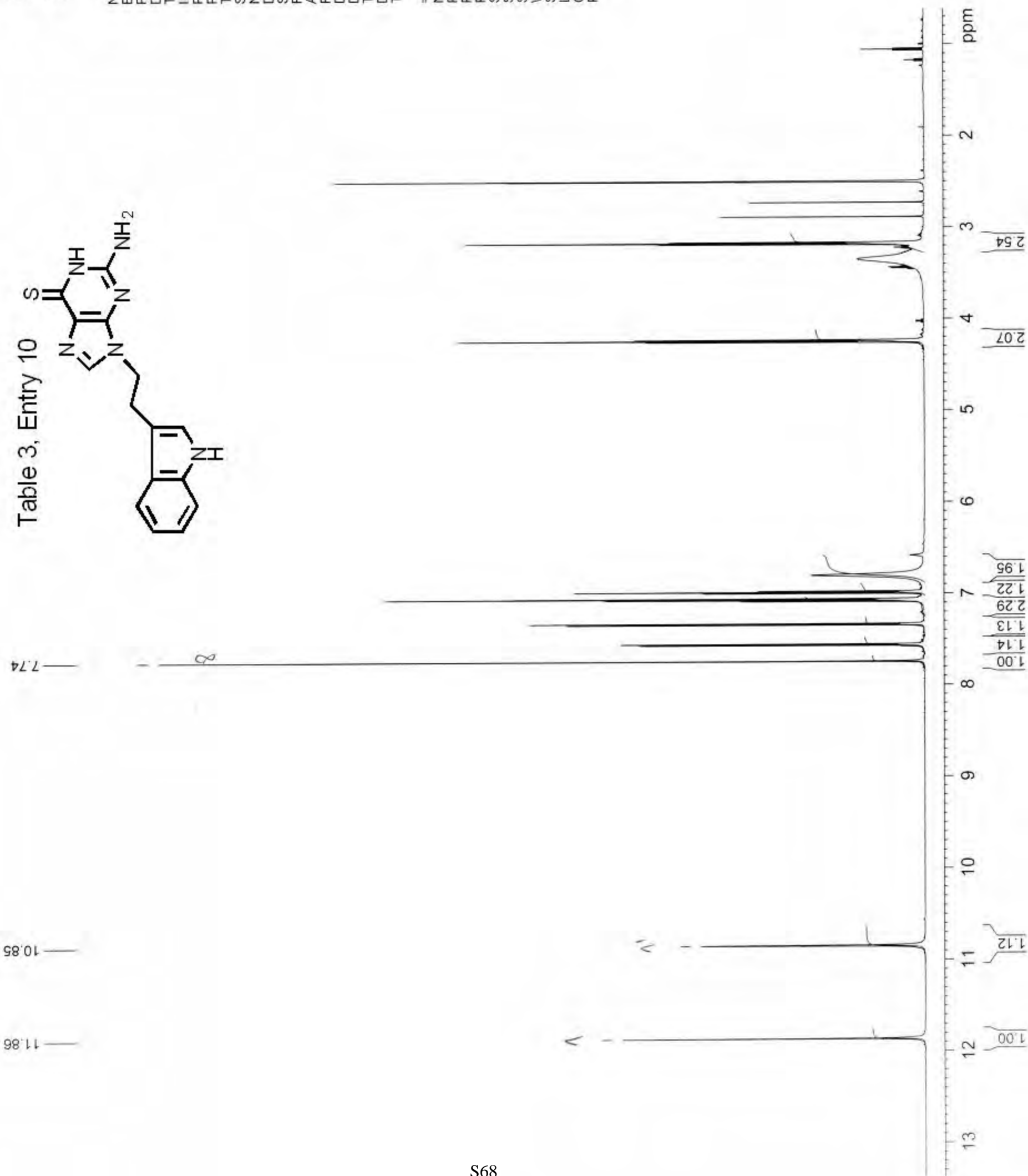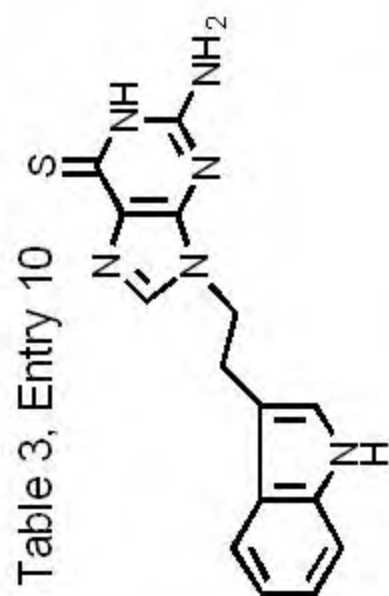
Dejmek MD392
APT in DMSO
2.12.2011 DR
****

NAME	Dejmek_MD392
EXPNO	2
PROCNO	1
Date_	20111202
Time	12.22
INSTRUM	spect
PROBHD	5 mm BBI 1H/D-
PULPROG	jmod
TD	75752
SOLVENT	DMSO
NS	1186
DS	4
SWH	37878.789 H
FIDRES	0.500037 H
AQ	0.9999764 s
RG	16400
DW	13.200 u
DE	6.00 u
TE	300.0 K
CNST2	165.0000000
CNST11	1.0000000
D1	1.00000000 s
D20	2.00000000 s
TD0	0.0060606i 1

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

NUC1	13C
P1	13.25 u
P2	26.50 u
PL1	-2.10 d
PL1W	126.28787994 W
SFO1	150.9194083 M

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

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 u
PL2	2.33 d
PL12	18.84 d
PL2W	19.97739792 W
PL12W	0.44620958 W
SFO2	600.1324005 M
SI	131072
SF	150.9028595 M
WDW	EM
SSB	0
LB	1.00 H
GB	0
PC	1.40

Table 3, Entry 10

25.325

43.513

110.372
111.592

118.368
118.574
121.229
123.166

127.052
128.338

136.347

140.654

147.940

153.082
155.417

174.912

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

Dejmek_MD393
1H NMR in DMSO
25-11-11 DR
****

NAME   Dejmek_MD39
EXPNO   1
PROCNO   1
Date_   20111125
Time   8.17
INSTRUM   spect
PROBHD   5 mm TXI 1H-
PULPROG   zg30
TD   60094
SOLVENT   DMSO
NS   32
DS   0
SWH   7507.507 Hz
FIDRES   0.124929 Hz
AQ   4.0023770 sec
RG   14.3
DW   66.600 usec
DE   6.00 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

====== CHANNEL f1 =
NUC1   1H
P1   8.00 usec
PL1   0.00 dB
PL1W   8.54041386 W
SFO1   499.9534997 N
SI   131072
SF   499.9499979 MH
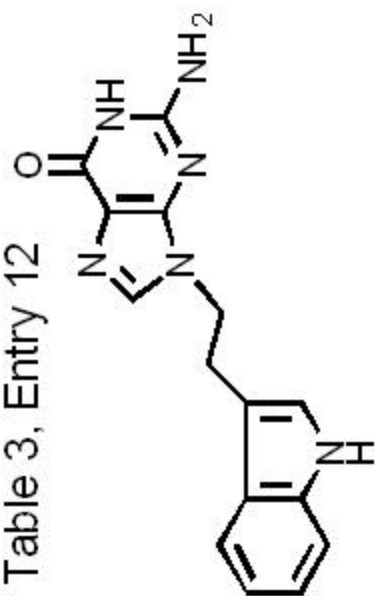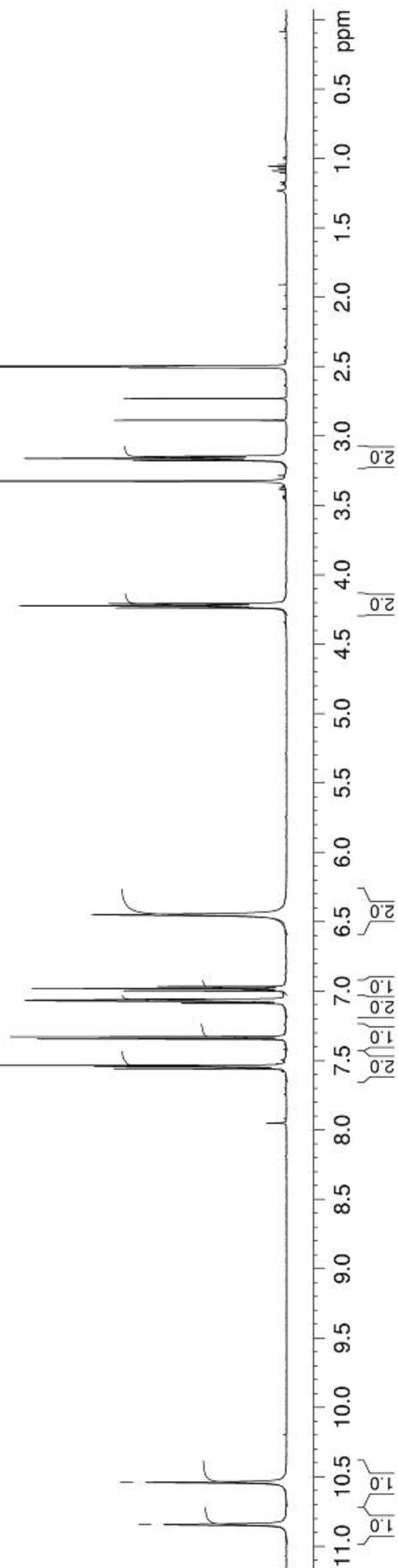WDW   no
SSB   0
LB   0.00 Hz
GB   0
PC   1.00

Table 3, Entry 11

3.95

6.42

7.69

10.84

ppm
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0
8.5
9.0
9.5
10.0
10.5
11.0

2.0
3.0
2.0
2.0
1.1
2.0
6.0
4.0
1.0
1.0
1.0
1.0

Dejmek_MD393
APT in DMSO
25-11-11 DR
****

Table 3, Entry 11

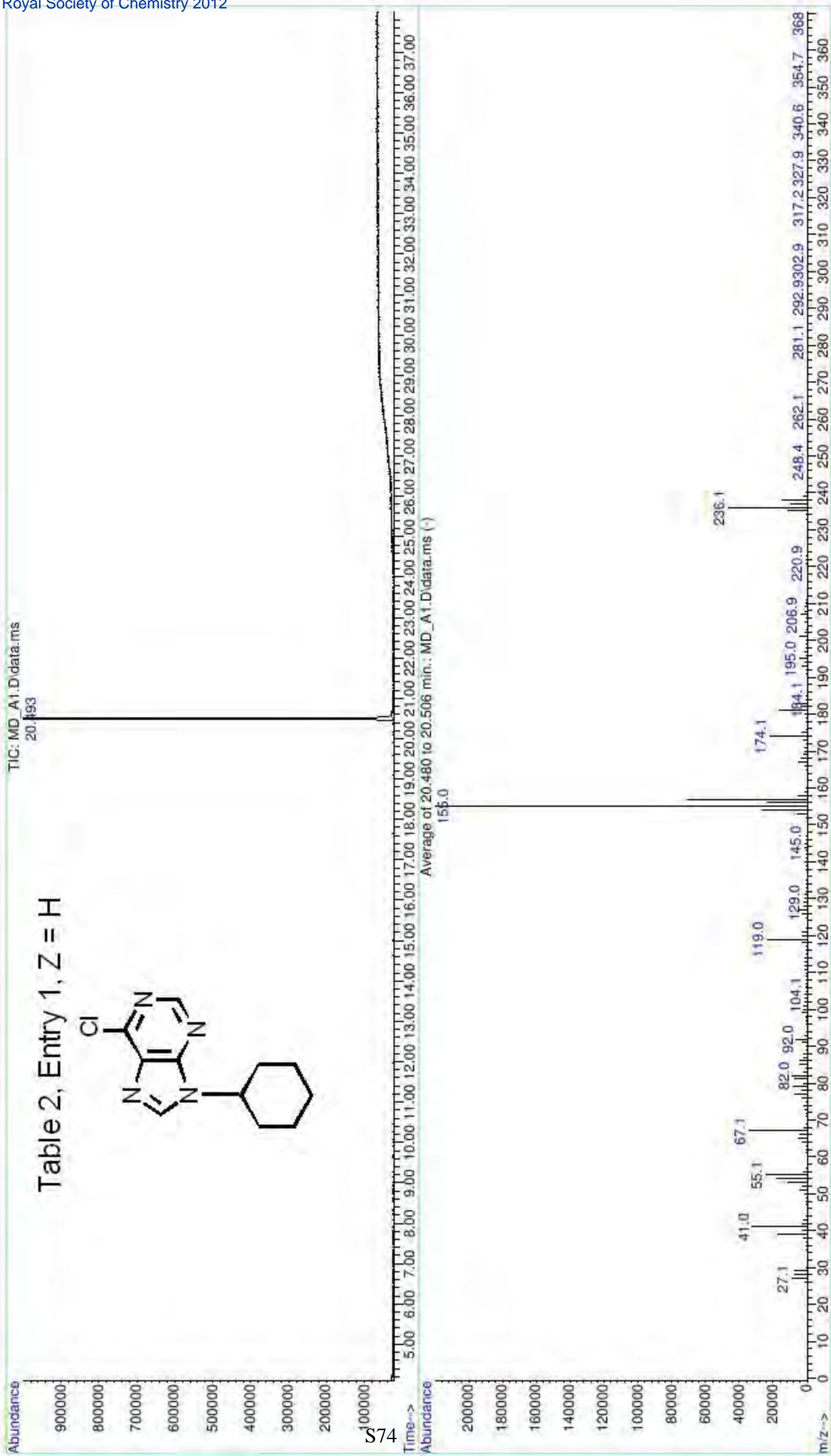NAME   Dejmek_MD393
EXPNO   2
PROCNO   1
Date_   20111125
Time   8.52
INSTRUM   spect
PROBHD   5 mm TXI 1H-13
PULPROG   jmod
TD   65536
SOLVENT   DMSO
NS   655
DS   4
SWH   30030.029 Hz
FIDRES   0.458222 Hz
AQ   1.0912410 sec
RG   29193
DW   16.650 usec
DE   6.50 usec
TE   300.0 K
CNST2   165.0000000
CNST11   1.0000000
D1   2.00000000 sec
D20   0.00606061 sec
TD0   1

====== CHANNEL f1 ======
NUC1   13C
P1   14.75 usec
P2   29.50 usec
PL1   0.00 dB
PL1W   67.82093048 W
SFO1   125.7263554 MHz

====== CHANNEL f2 ======
CPDPRG2   waltz16
NUC2   1H
PCPD2   60.00 usec
PL2   0.00 dB
PL12   17.50 dB
PL2W   8.54041386 W
PL12W   0.15187243 W
SFO2   499.9519998 MHz
SI   131072
SF   125.7125646 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.00

25.38

43.45

53.24

110.59
111.58
113.97

118.42
118.57
121.23
123.10
125.48
127.13
128.37
129.06

136.34

139.92

154.30

159.92
160.77

S71

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

Table 3, Entry 12

10.54

10.84

Dejmek_MD357
APT in DMSO
5-10-11 DR
****

Table 3, Entry 12

25.63

43.45

110.59
111.59

116.76
118.42
118.58
121.23
123.10

127.13

136.34
137.58

151.30

153.65

156.99

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

S73

File   : D:\Data\MD_A1.D
Operator : Dejmek
Acquired : 1 Mar 2012 16:42   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument: 6890N + 5975B
Sample Name: MD_A1
Misc Info :
Vial Number: 1

Abundance

TIC: MD_A1.D\data.ms

20.493

900000
800000
700000
600000
500000
400000
300000
200000
100000

Time--> 5.00 6.00 7.00 8.00 9.00 10.00 11.00 12.00 13.00 14.00 15.00 16.00 17.00 18.00 19.00 20.00 21.00 22.00 23.00 24.00 25.00 26.00 27.00 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00 37.00

Table 2, Entry 1, Z = H

S74

Abundance

Average of 20.480 to 20.506 min.: MD_A1.D\data.ms (-)

155.0

200000
180000
160000
140000
120000
100000
80000
60000
40000
20000

27.1 41.0 55.1 67.1 82.0 92.0 104.1 119.0 129.0 145.0 174.1 184.1 195.0 206.9 220.9 236.1 248.4 262.1 281.1 292.9 302.9 317.2 327.9 340.6 354.7 368

m/z--> 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360

File   :D:\Data\MD_A2.D
Operator   : Dejmek
Acquired   : 1 Mar 2012 19:47   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_A2
Misc Info :
Vial Number: 1

Table 2, Entry 2, Z = H

TIC: MD_A2.D\data.ms

Average of 20.307 to 20.324 min.: MD_A2.D\data.ms (-)

S75
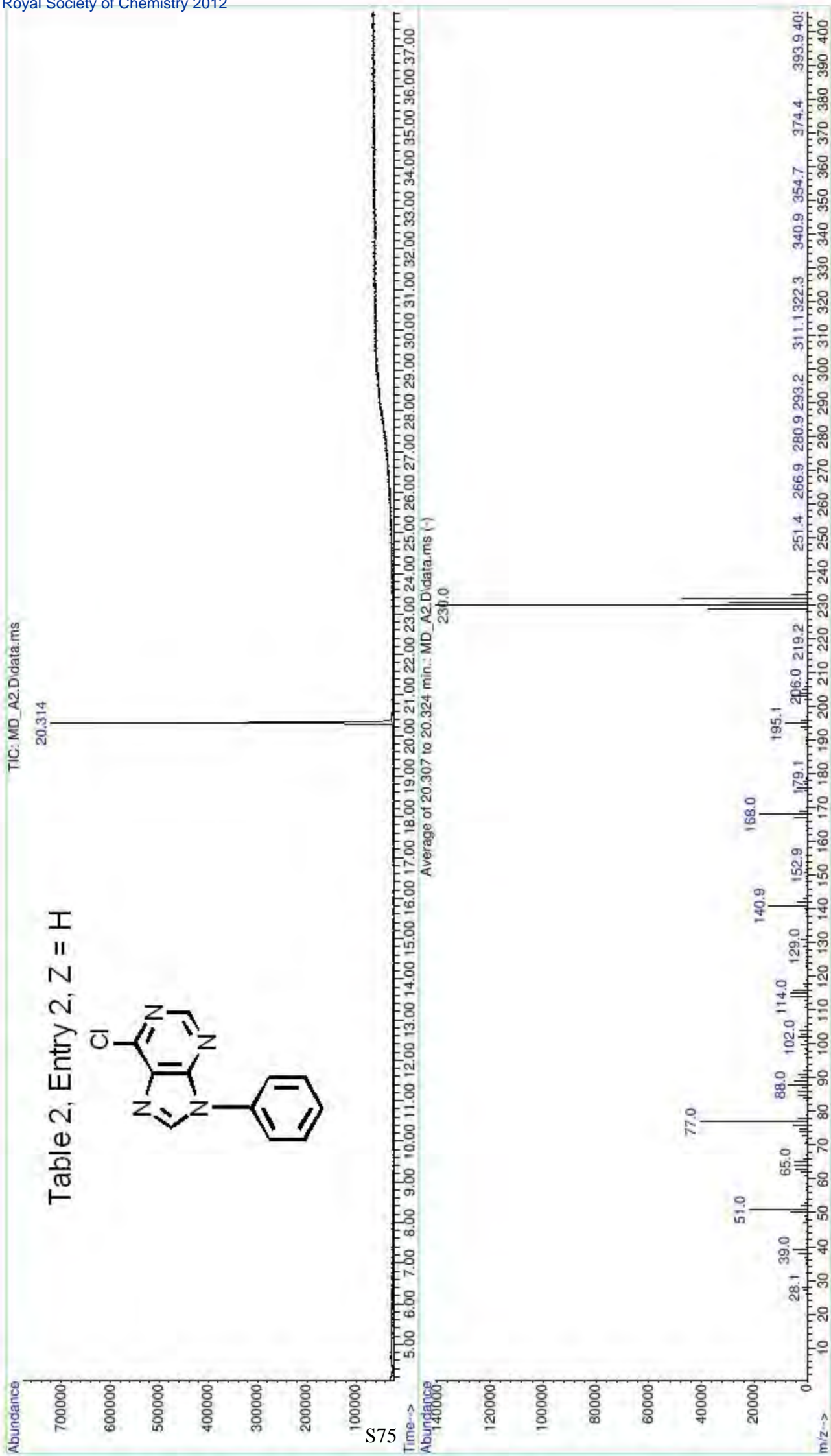
File   :D:\Data\MD_A5.D
Operator : Dejmek
Acquired : 1 Mar 2012 21:17 using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_A5
Misc Info :
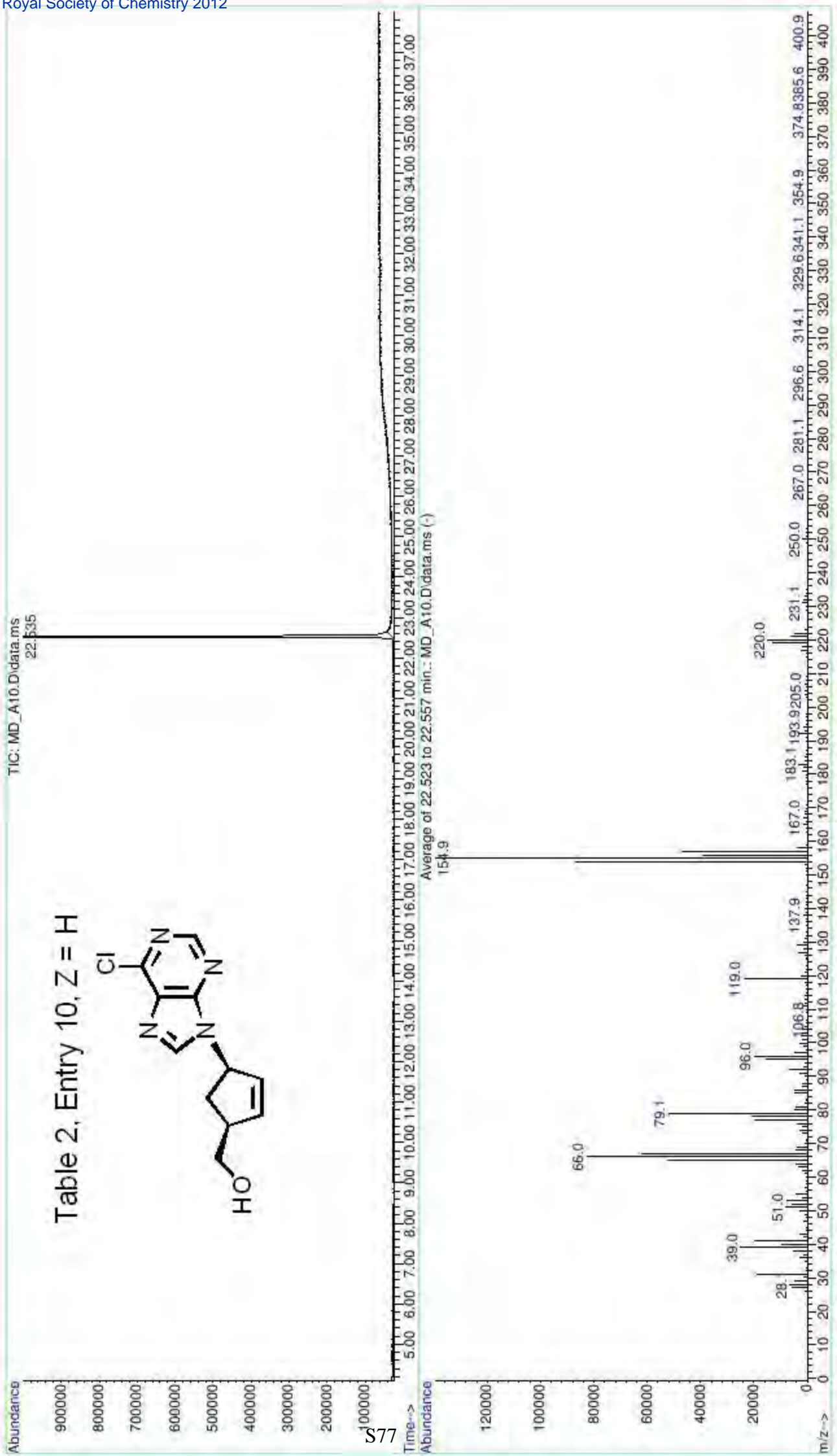Vial Number: 3

TIC: MD_A5.D\data.ms

Table 2, Entry 5, Z = H

Average of 24.937 to 24.955 min.: MD_A5.D\data.ms
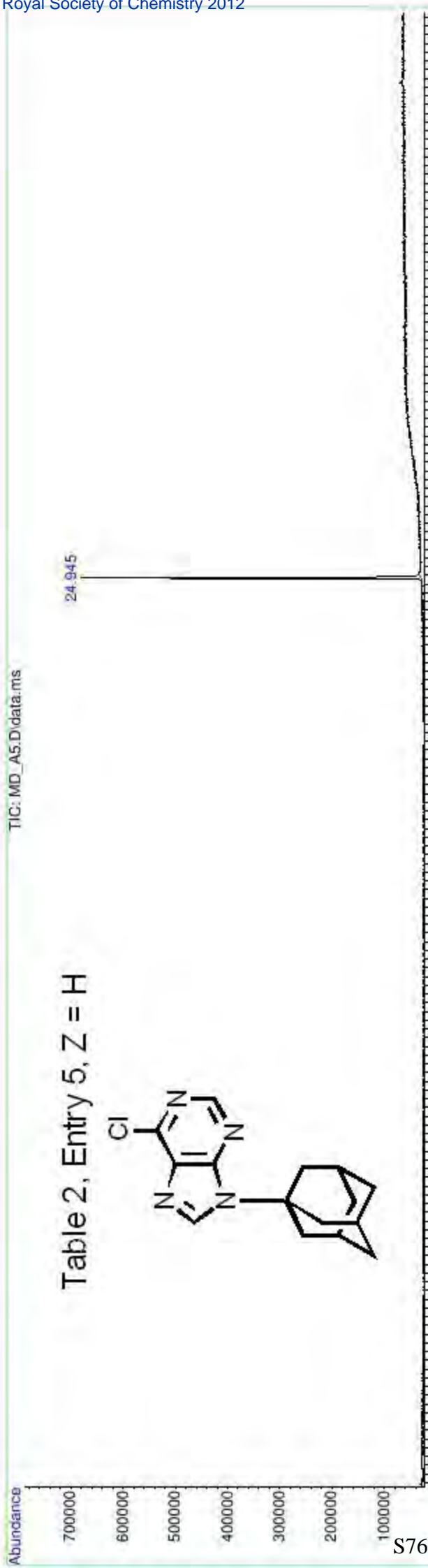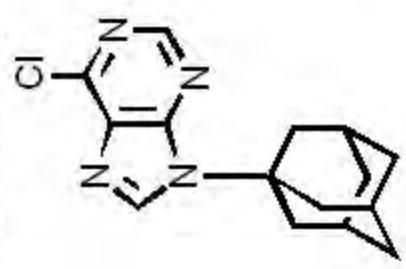
S76
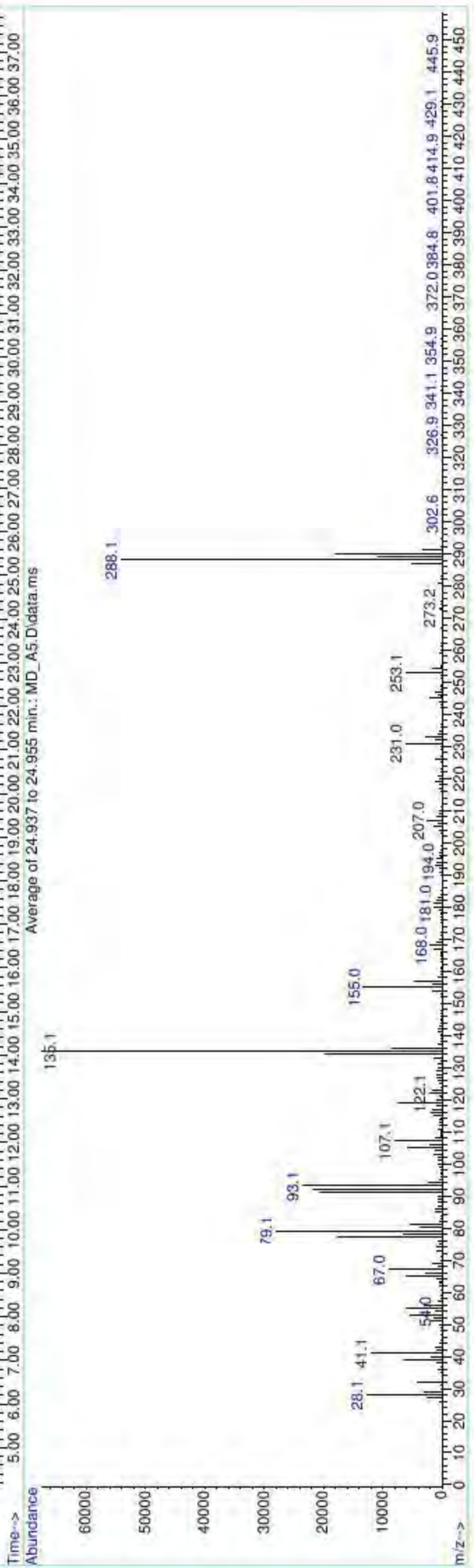
File   :D:\Data\MD_A10.D
Operator : Dejmek
Acquired : 1 Mar 2012 22:46   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_A10
Misc Info :
Vial Number: 5

Table 2, Entry 10, Z = H

TIC: MD_A10.D\data.ms

Average of 22.523 to 22.557 min.: MD_A10.D\data.ms (-)

S77

File   :D:\Data\MS_PA9_cr.D
Operator : Sala
Acquired : 7 Mar 2012 14:37   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument: 6890N + 5975B
Sample Name: MS_PA9_cr
Misc Info :
Vial Number: 1

TIC: MS_PA9_cr.D\data.ms

Table 2, Entry 12, Z = H

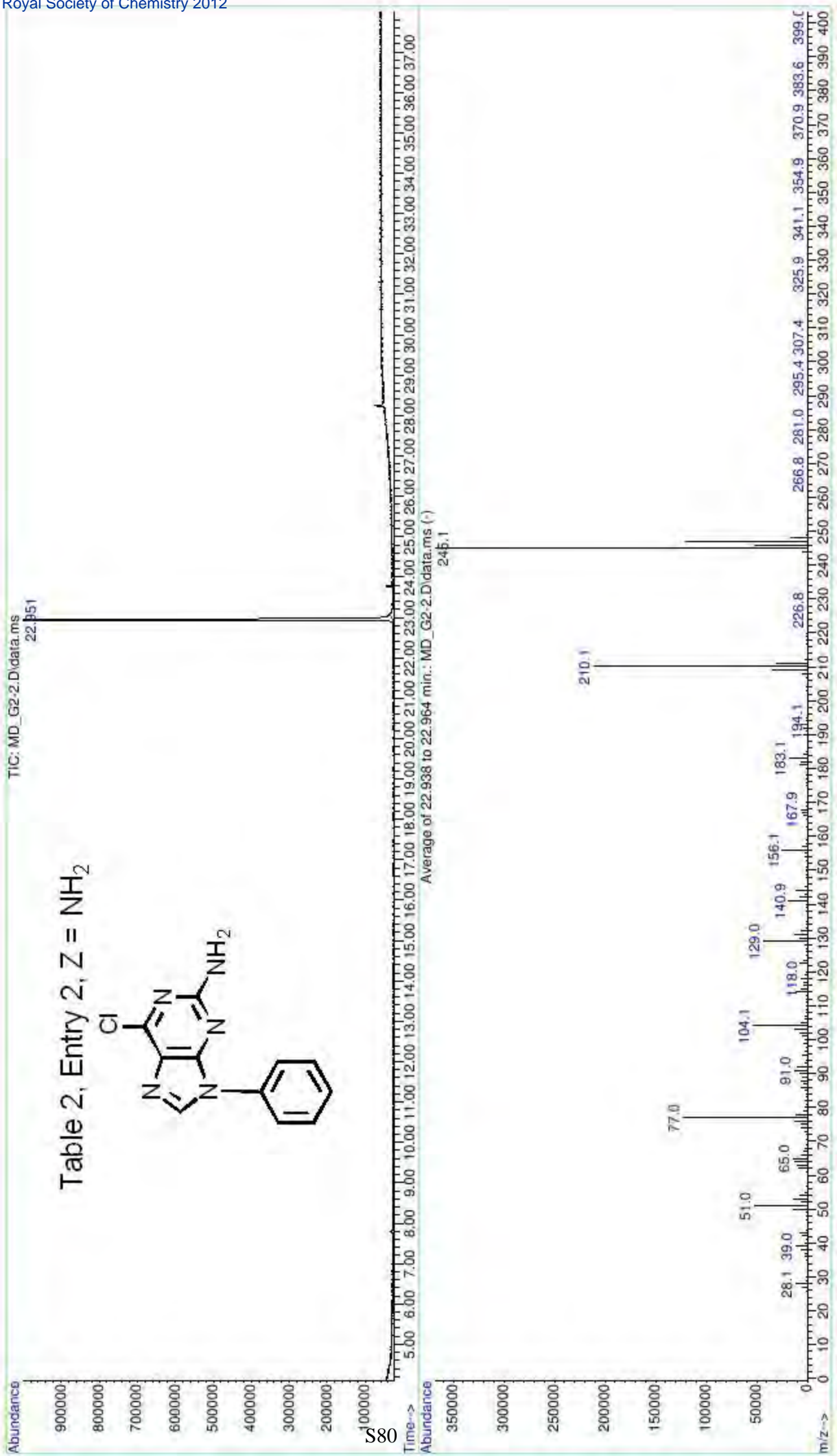Average of 20.835 to 20.869 min.: MS_PA9_cr.D\data.ms (-)

S78
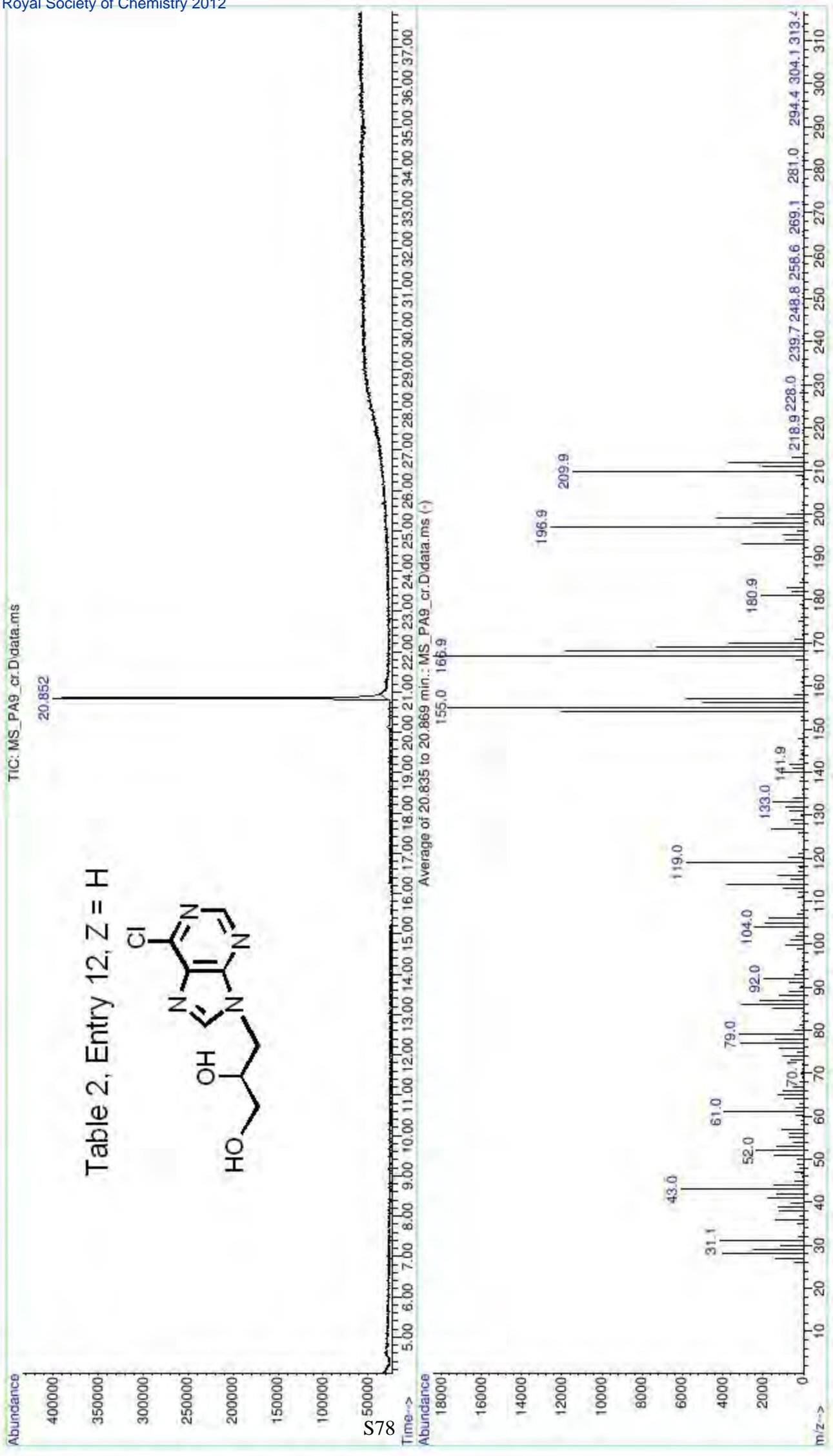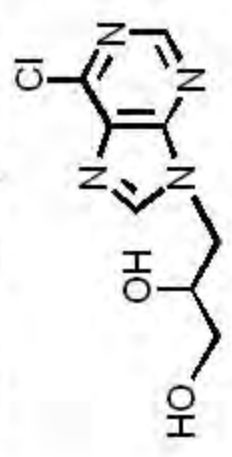
File   :D:\Data\MD_G1.D
Operator   : Dejmek
Acquired   : 1 Mar 2012 17:26   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_G1
Misc Info :
Vial Number: 2

TIC: MD_G1.D\data.ms

23.034

Time-->

Average of 23.025 to 23.051 min.: MD_G1.D\data.ms (-)

169.0

251.1

133.9

28.1 41.0 55.0 67.0 79.0 92.0 107.0 119.1 146.0 158.1 181.9 196.0 216.1 236.0 266.8 283.1 304.6 315.8 326.6 341.1 355.1 366.3 379.6

m/z-->

Table 2, Entry 1, Z = NH$_2$

S79

TIC: MD_G2-2.D\data.ms

22.951

Average of 22.938 to 22.964 min.: MD_G2-2.D\data.ms (-)

245.1

Table 2, Entry 2, Z = NH₂

S80

File   :D:\Data\MD_A8.D
Operator   : Dejmek
Acquired   : 1 Mar 2012 22:01   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_A8
Misc Info   :
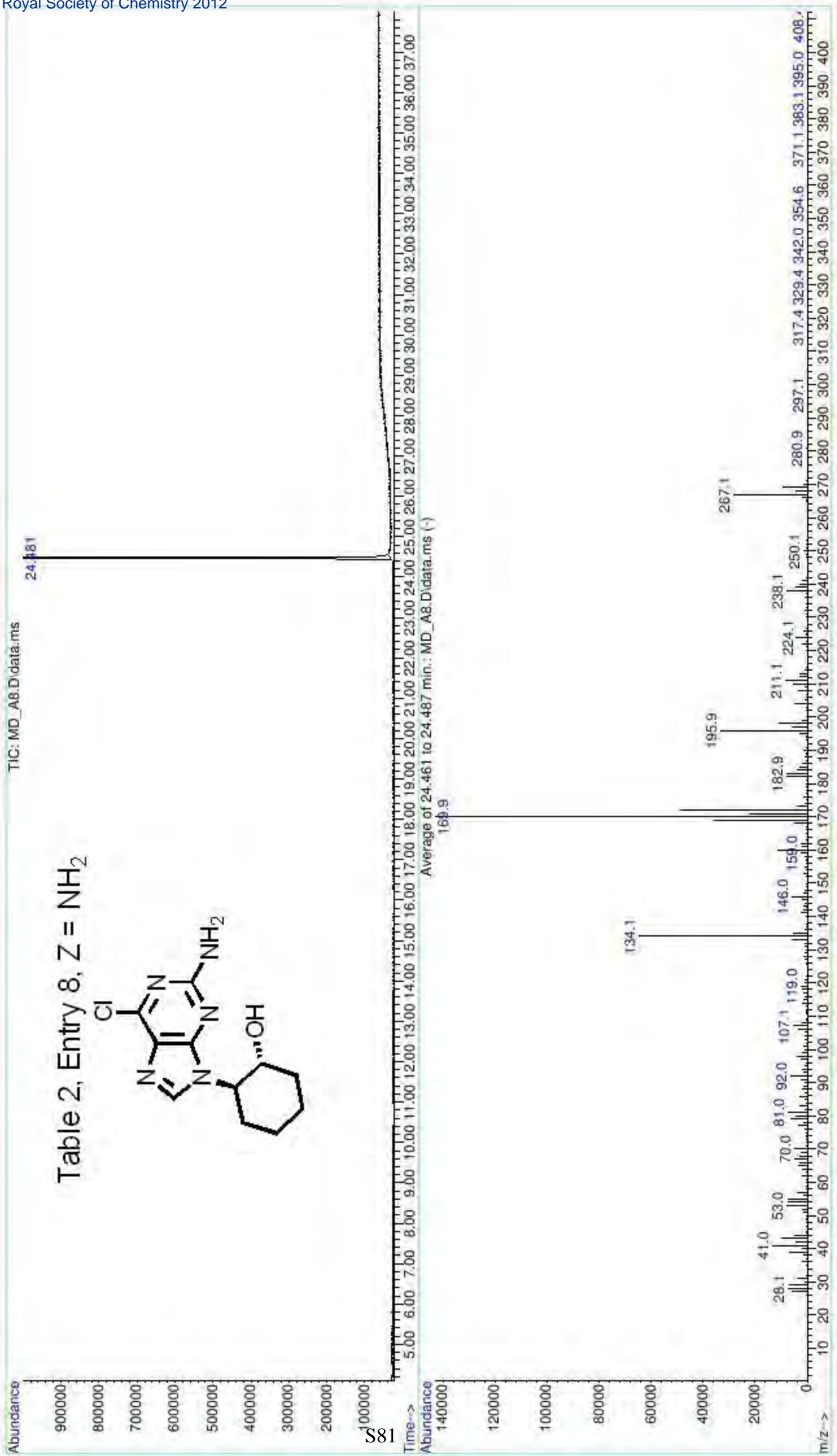Vial Number: 4

Table 2, Entry 8, Z = NH$_2$

TIC: MD_A8.D\data.ms

Average of 24.461 to 24.487 min.: MD_A8.D\data.ms (-)

S81

File   :D:\Data\MD_G10.D
Operator   : Dejmek
Acquired   : 1 Mar 2012 18:11   using AcqMethod AS_M-VYSOKE_C-VYSOKE.M
Instrument : 6890N + 5975B
Sample Name: MD_G10
Misc Info   :
Vial Number: 3

TIC: MD_G10.D\data.ms

24.738

Table 2, Entry 10, Z = NH$_2$

Average of 24.721 to 24.747 min.: MD_G10.D\data.ms (-)

169.0

133.9

145.1 156.9

183.0

197.1 210.0 221.8

234.9 246.9

265.1

281.0 294.9 312.8 325.1 341.1 355.1 370.1 382.4

28. 41.0 53.0 67.0 79.0 96.0 107.1 119.0

S82

Table 2, Entry 12, Z = NH$_2$

TIC: MD_G12-2.D\data.ms

Average of 23.276 to 23.371 min.: MD_G12-2.D\data.ms (-)

S83
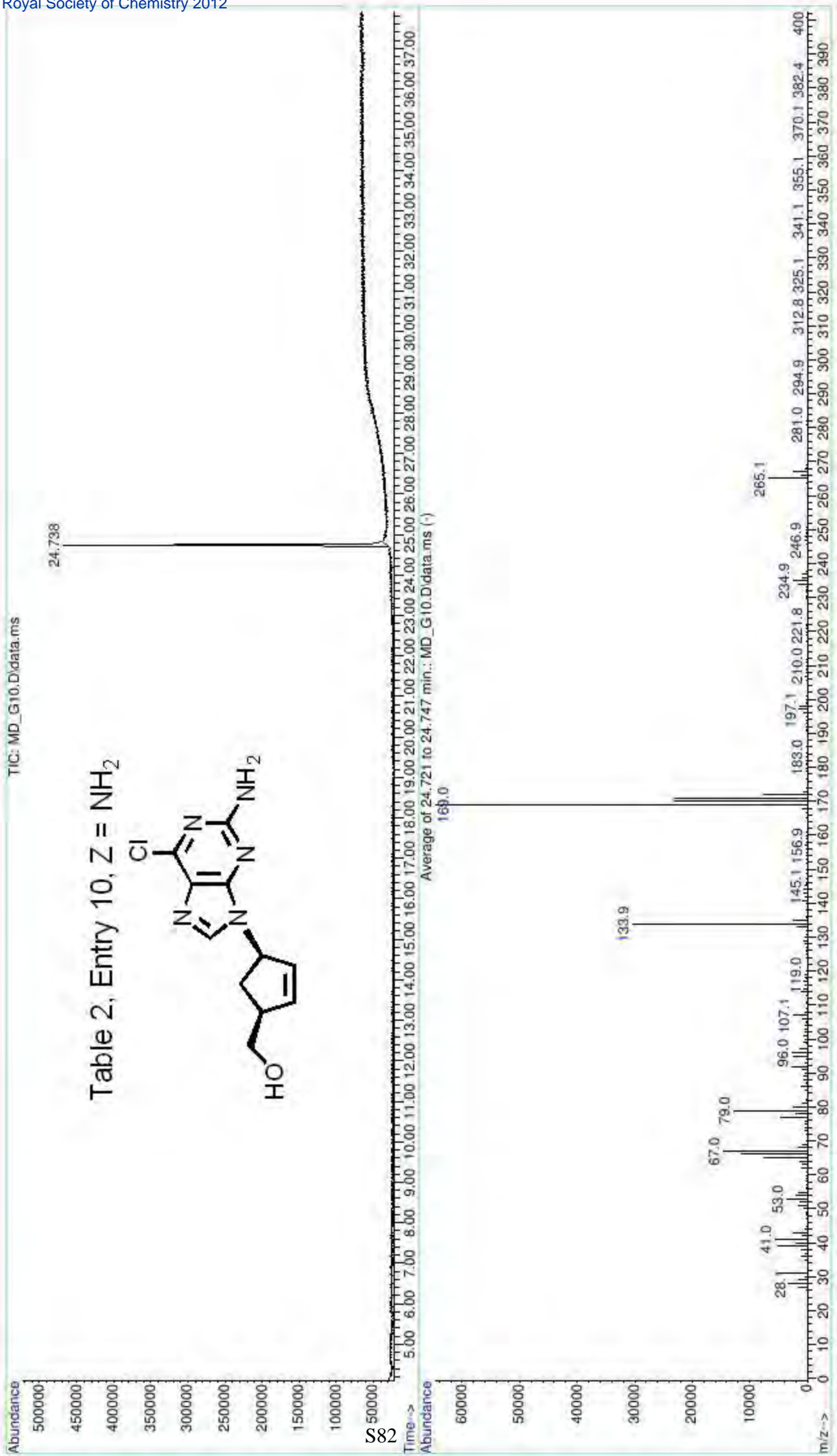
File   :D:\Data\MD_S1-2.D
Operator : Dejmek
Acquired : 2 Mar 2012 00:59   using AcqMethod AS_M-VYSOKE_C-NIZKE.M
Instrument : 6890N + 5975B
Sample Name: MD_S1-2
Misc Info :
Vial Number: 8

Scheme 1

TIC: MD_S1-2.D\data.ms

26.097

Average of 26.080 to 26.106 min.: MD_S1-2.D\data.ms

175.1
189.1
286.1
162.1
150.1
134.0
120.0
108.1
93.0
79.0
67.0
53.0
41.1
28.1
207.0
221.1
241.1
256.1
271.1
308.9
326.9
340.9
355.0
366.7
379.1
401.1
415.3
429

S84