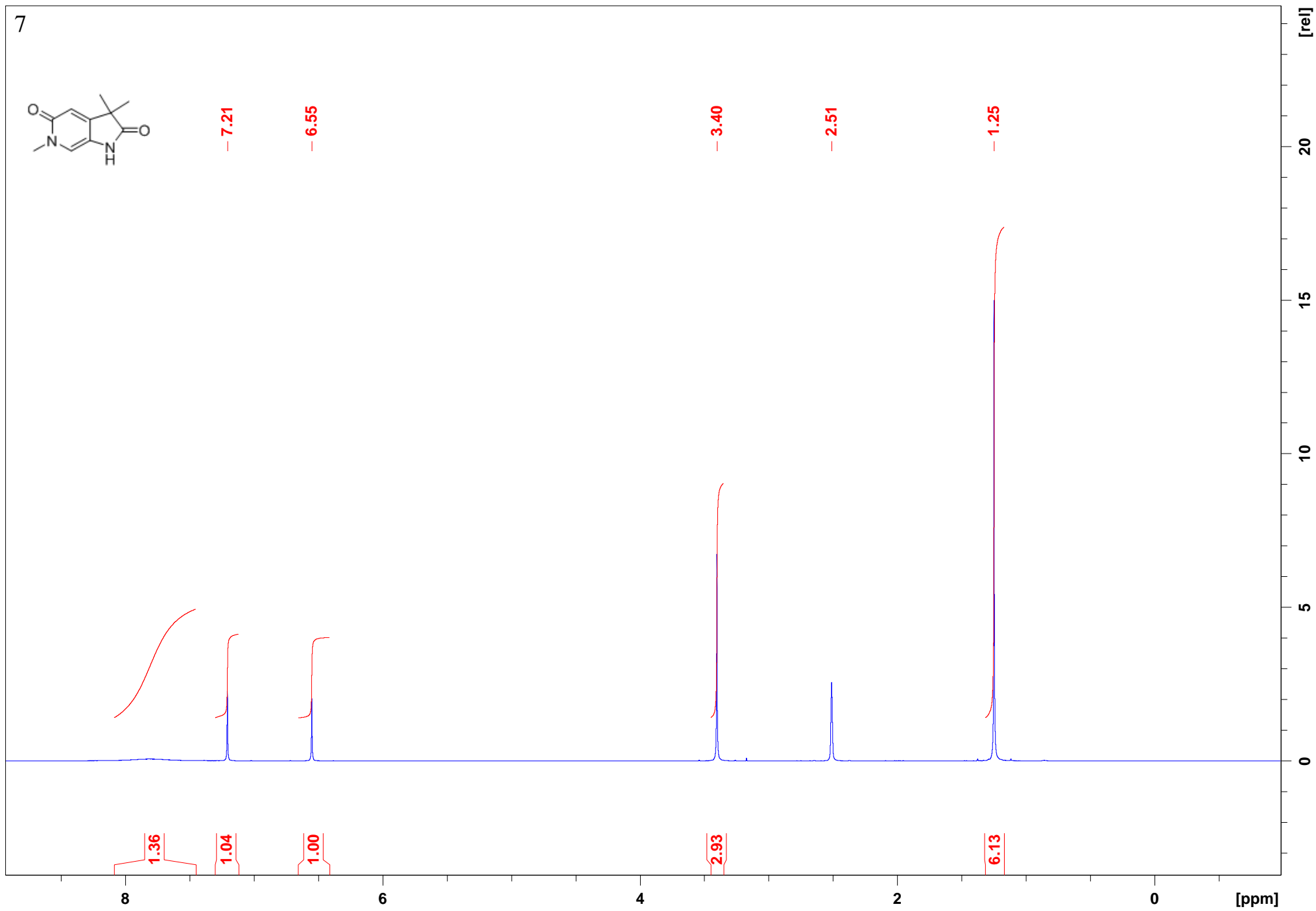


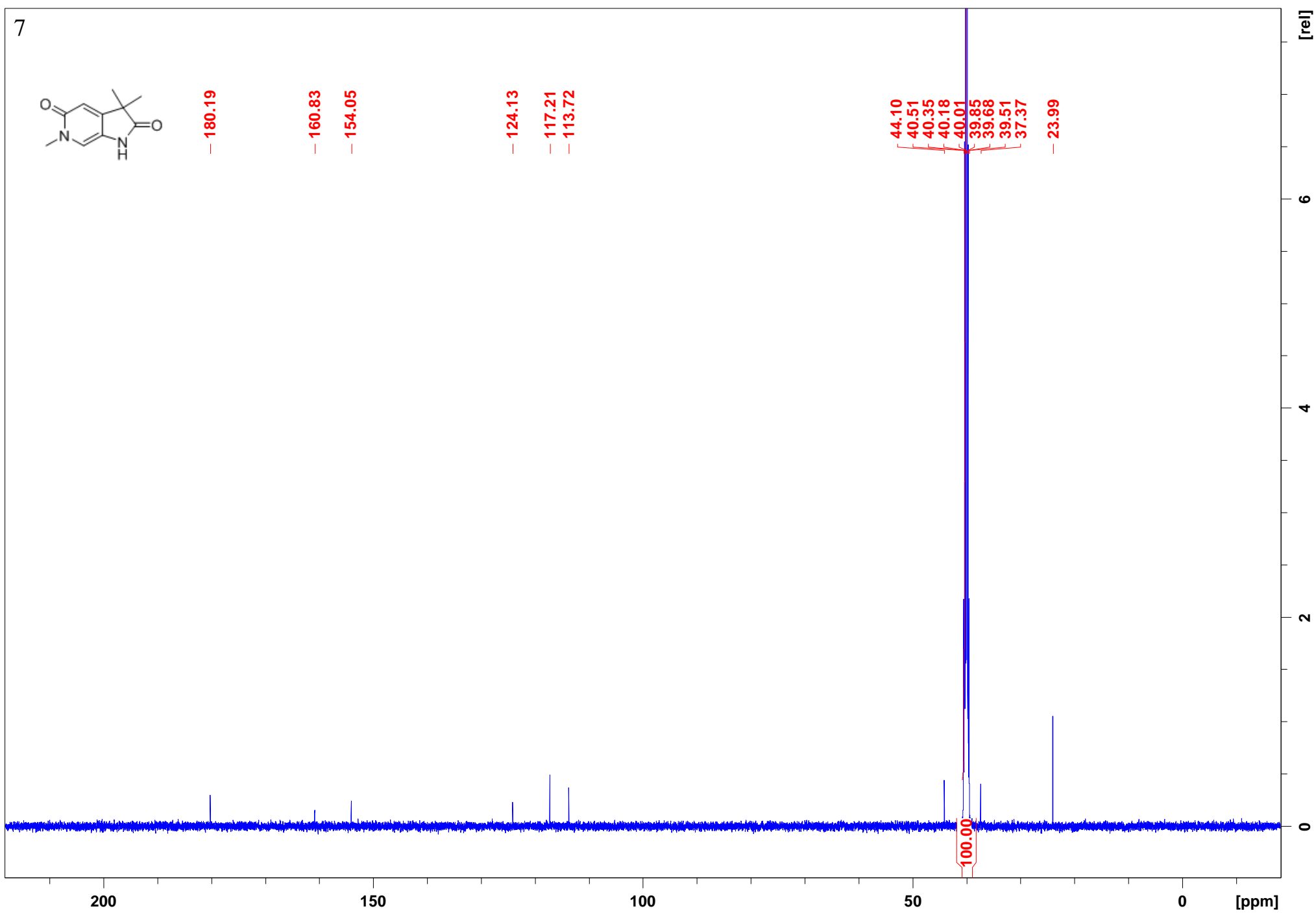
Supplementary Information

For

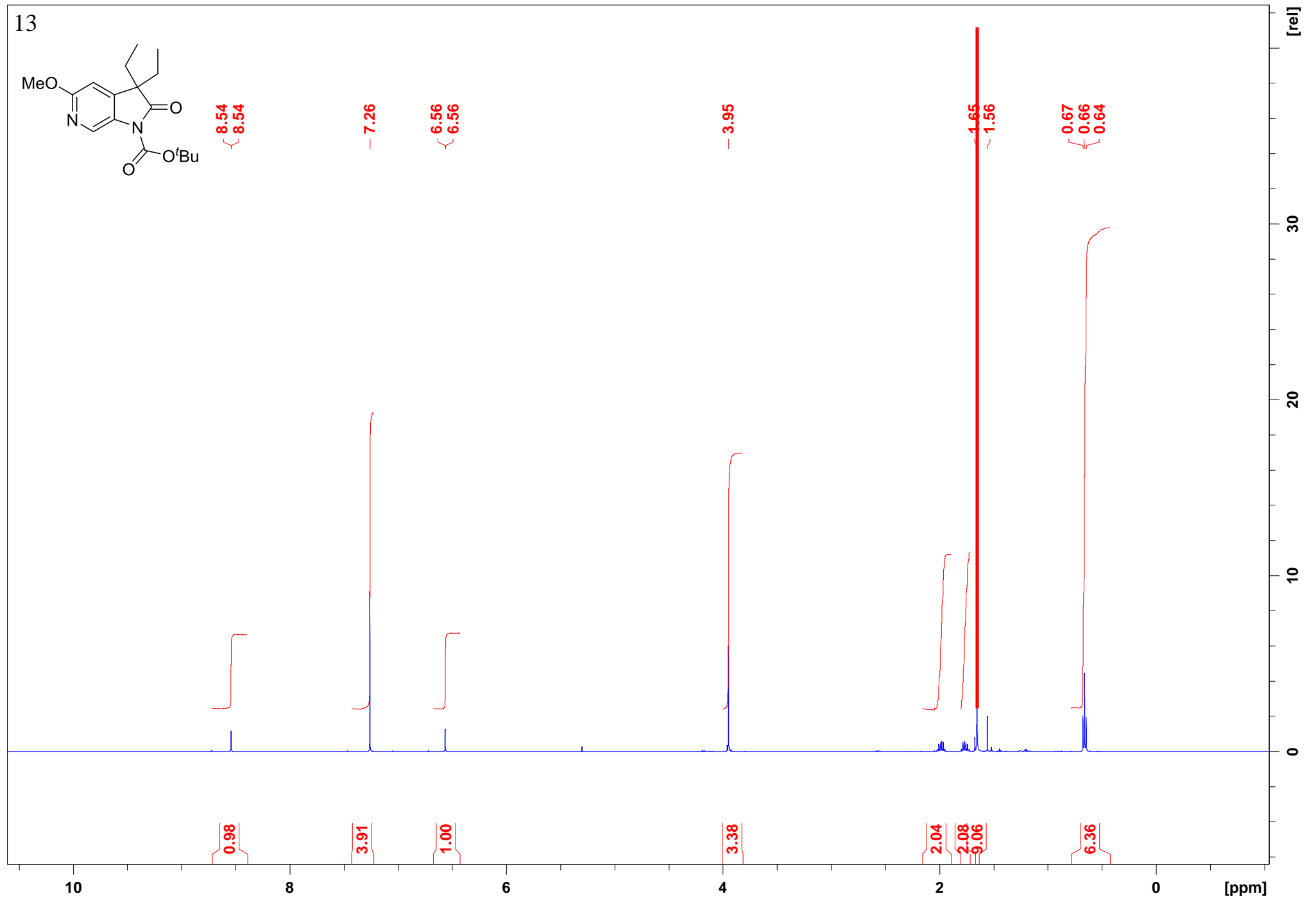
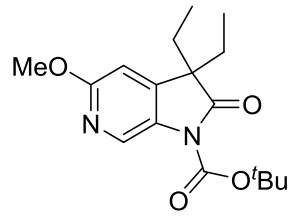
Identification of a Novel Ligand for the ATAD2 Bromodomain with Selectivity Over BRD4 Through a Fragment Growing Approach.

Duncan C. Miller, Mathew P. Martin, Santosh Adhikari, Alfie Brennan, Jane a. Endicott, Bernard T. Golding, Ian R. Hardcastle, Amy Heptinstall, Stephen Hobson, Claire Jennings, Lauren Molyneux, Yvonne Ng, Stephen R. Wedge, Martin E. M. Noble, Celine Cano

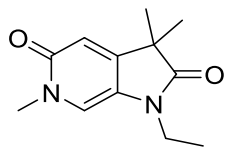




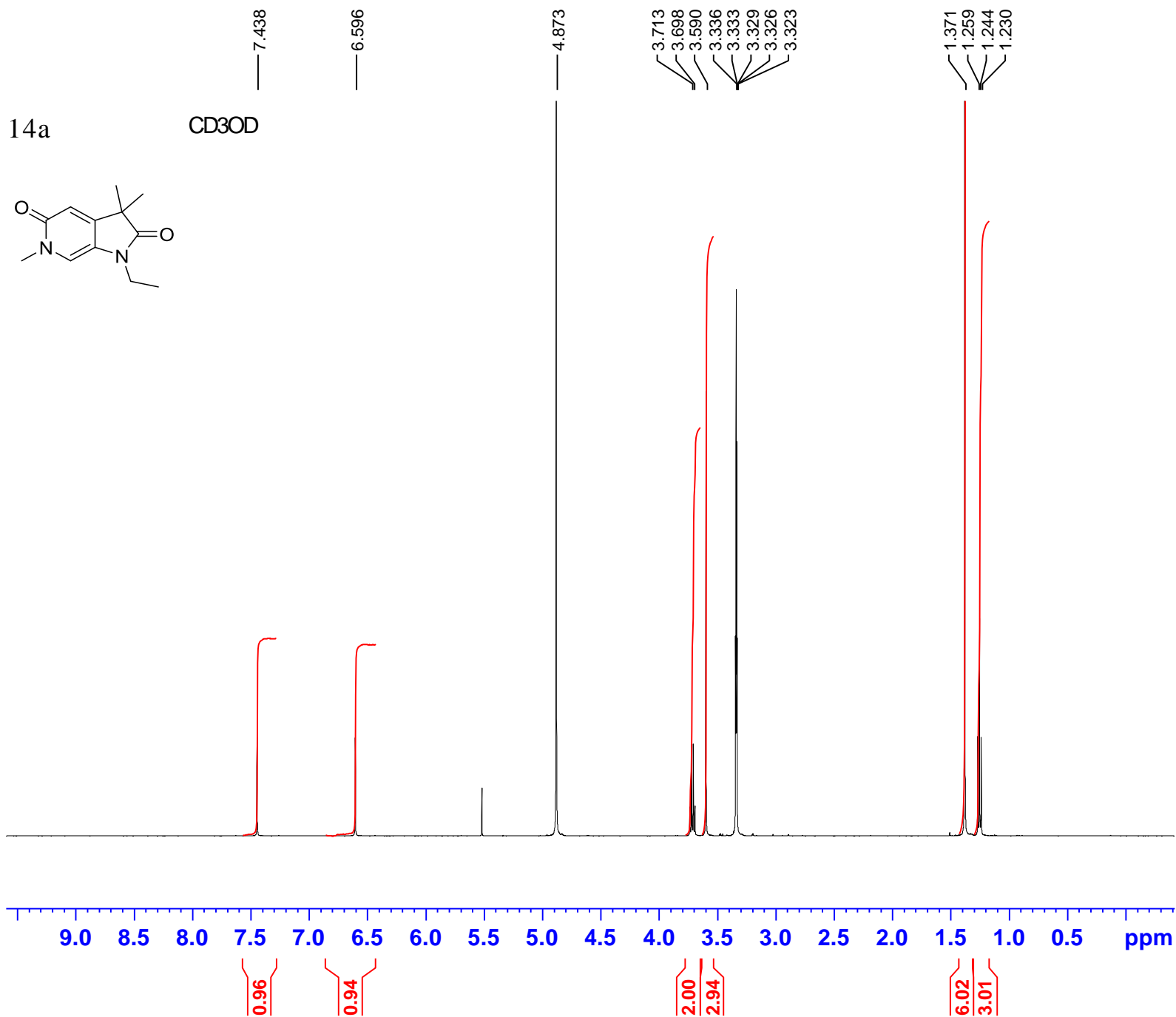
13



14a



CD3OD



Current Data
 Name DCM-494-29-A CD3OD
 EXPNO 10
 PROCNO 1

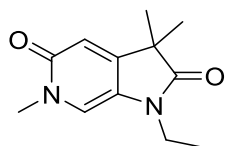
F2 - Acquisition
 Parameters 20140910
 Time 13.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 575
 DW 48.400 usec
 DE 11.99 usec
 TE 297.9 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

F2 - Processing parameters SI
 65536
 SF 500.2999951 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

14a

CD3OD



178.79

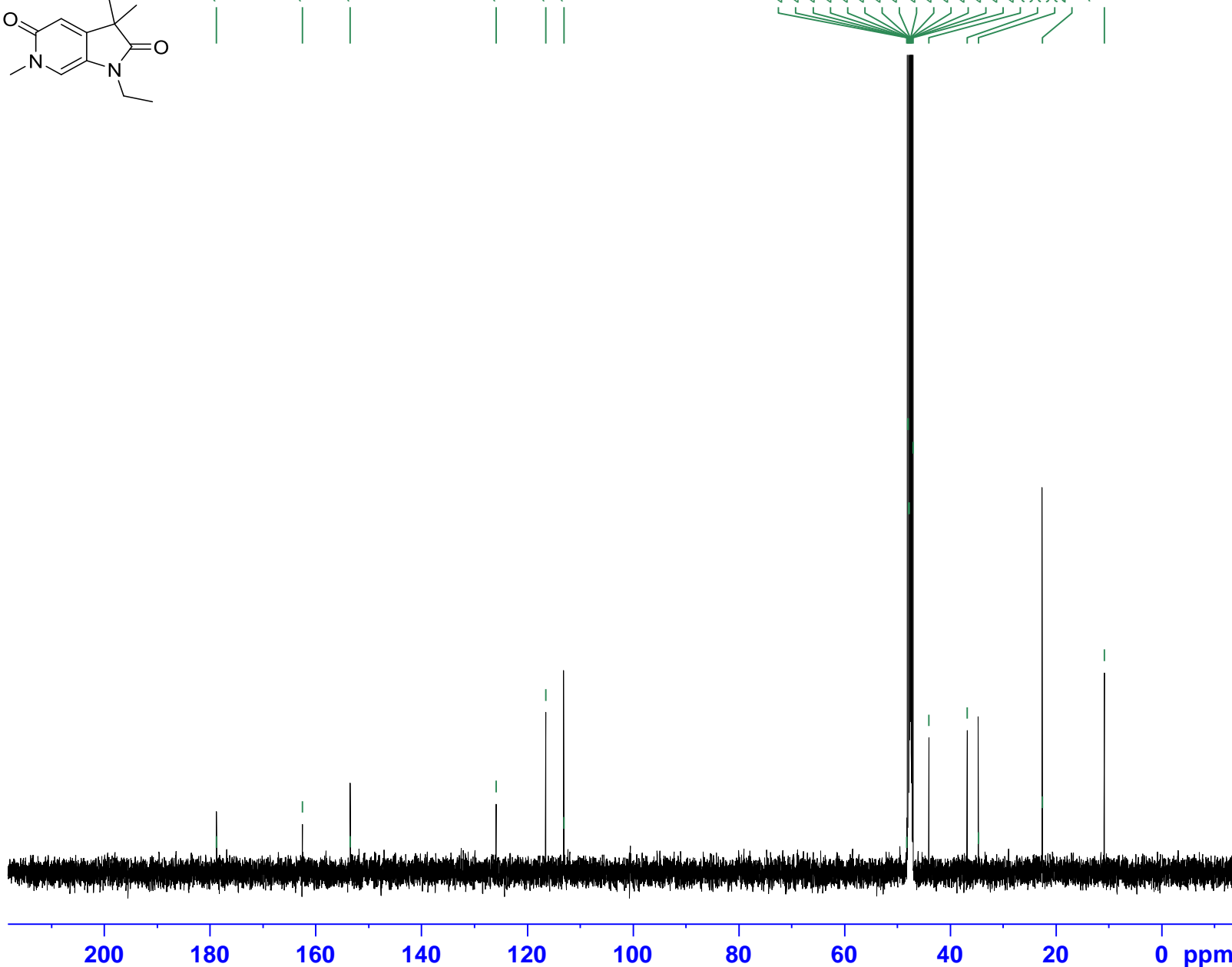
162.56

153.50

125.90

116.53

113.12

48.22
48.10
48.05
47.93
47.88
47.76
47.71
47.59
47.54
47.50
47.42
47.33
47.25
47.08
44.06
36.82
34.72
22.62
10.88

Current Data Parameters
 NAME DCM-494-29-A CD3OD
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20140911
 Time 3.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.6 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

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

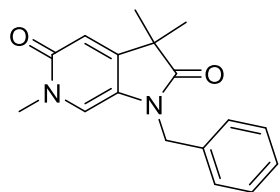
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

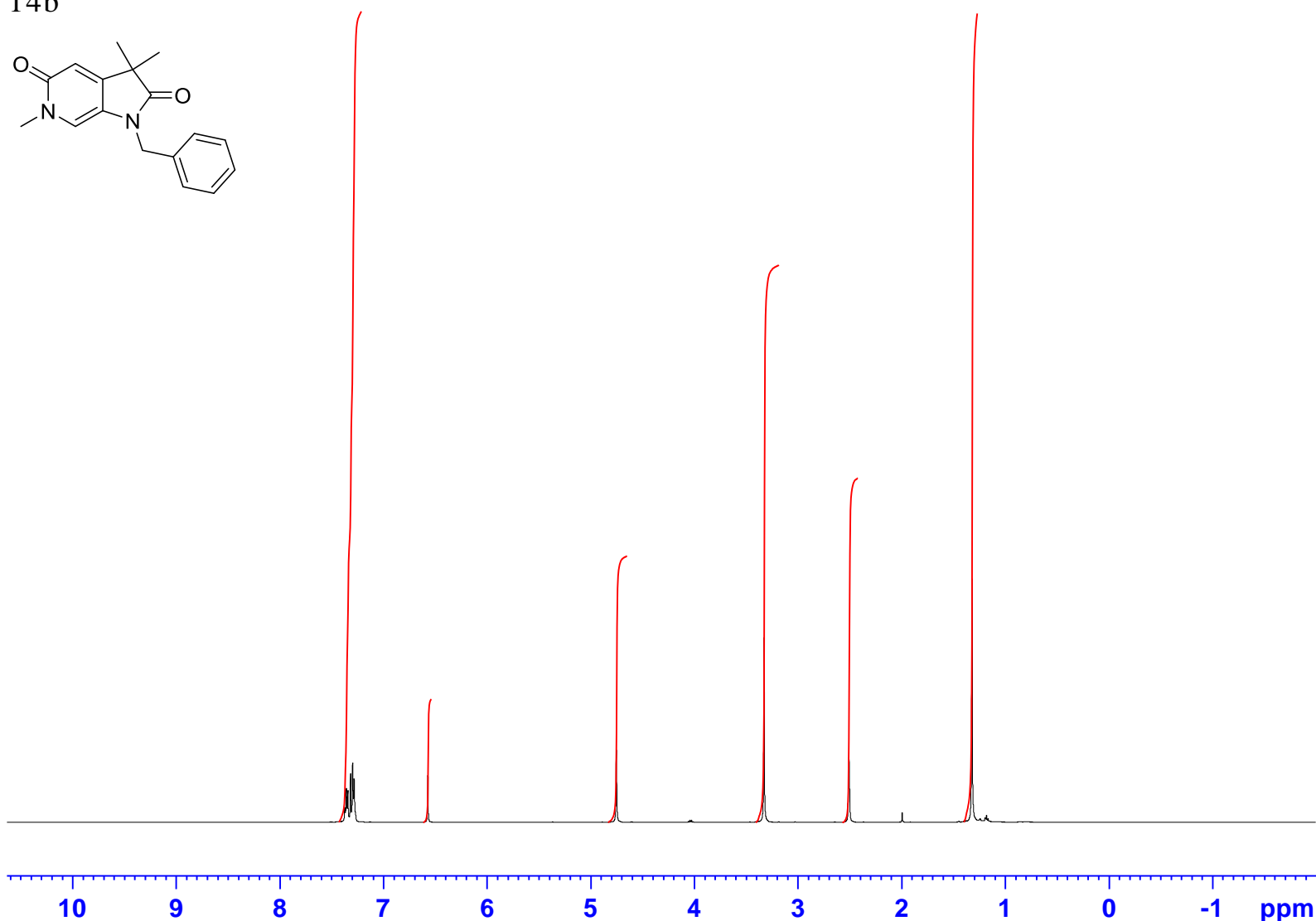
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.7565400 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 VDV EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

14b



7.358
7.344
7.318
7.299
7.285
6.573
4.753
3.328
2.508
1.322



6.09
0.93
2.00
4.19
2.59
6.09



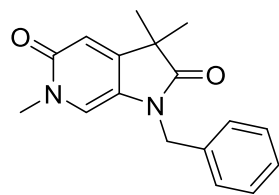
Current Data
NAME SA-473-192
EXPNO 20
PROCNO 1

F2 - Acquisition
Date_ 20141128
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 406
DW 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

14b



178.26

161.19

152.16

136.35

129.18

127.95

127.56

124.32

117.17

114.19

43.87

43.25

40.52

40.35

40.18

40.01

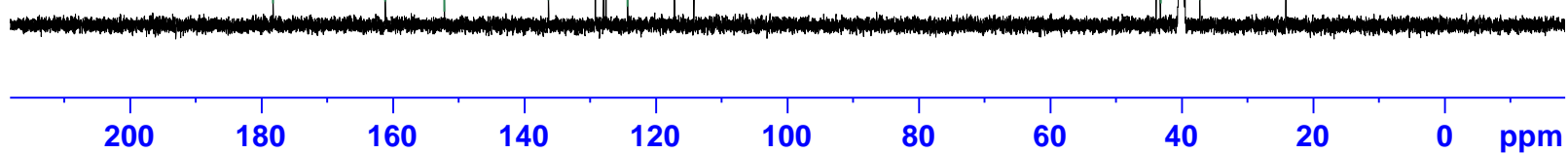
39.85

39.68

39.51

37.27

24.15



Current Data Parameters
 NAME SA-473-192
 EXPNO 21
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141128
 Time 10.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 256
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

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

SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

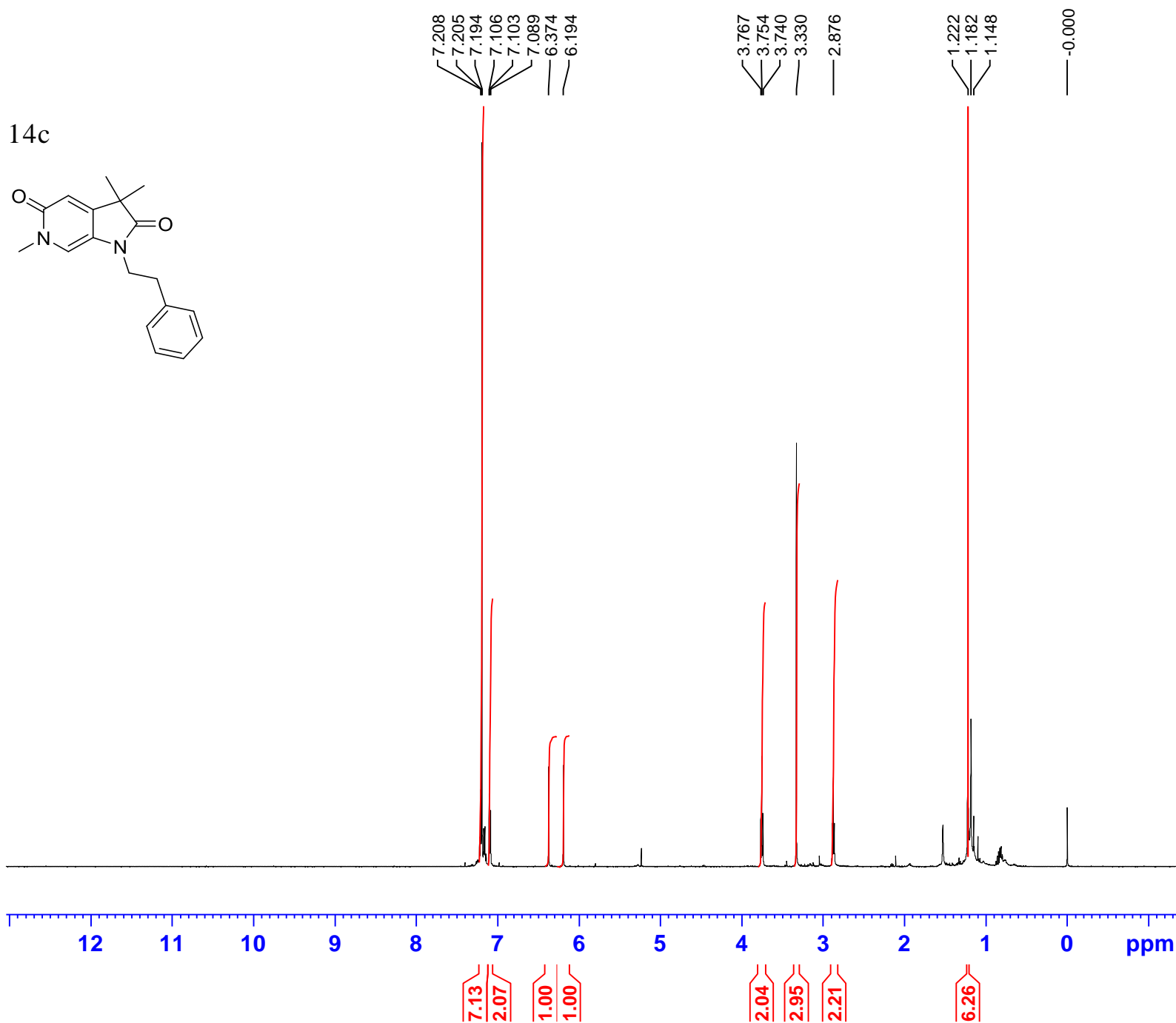
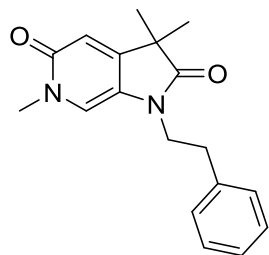
===== CHANNEL f2 =====

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing

Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 G 0
 B 1.40
 P
 C

14c



Current Data

NAME SA-473-196
EXPNO 30
PROCNO 1

F2 - Acquisition

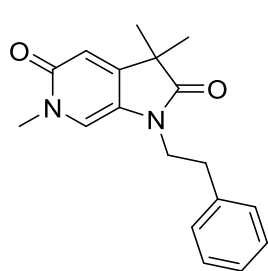
Data 20141215
Time 14.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DW 48.400 usec
DE 11.99 usec
TE 290.9 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

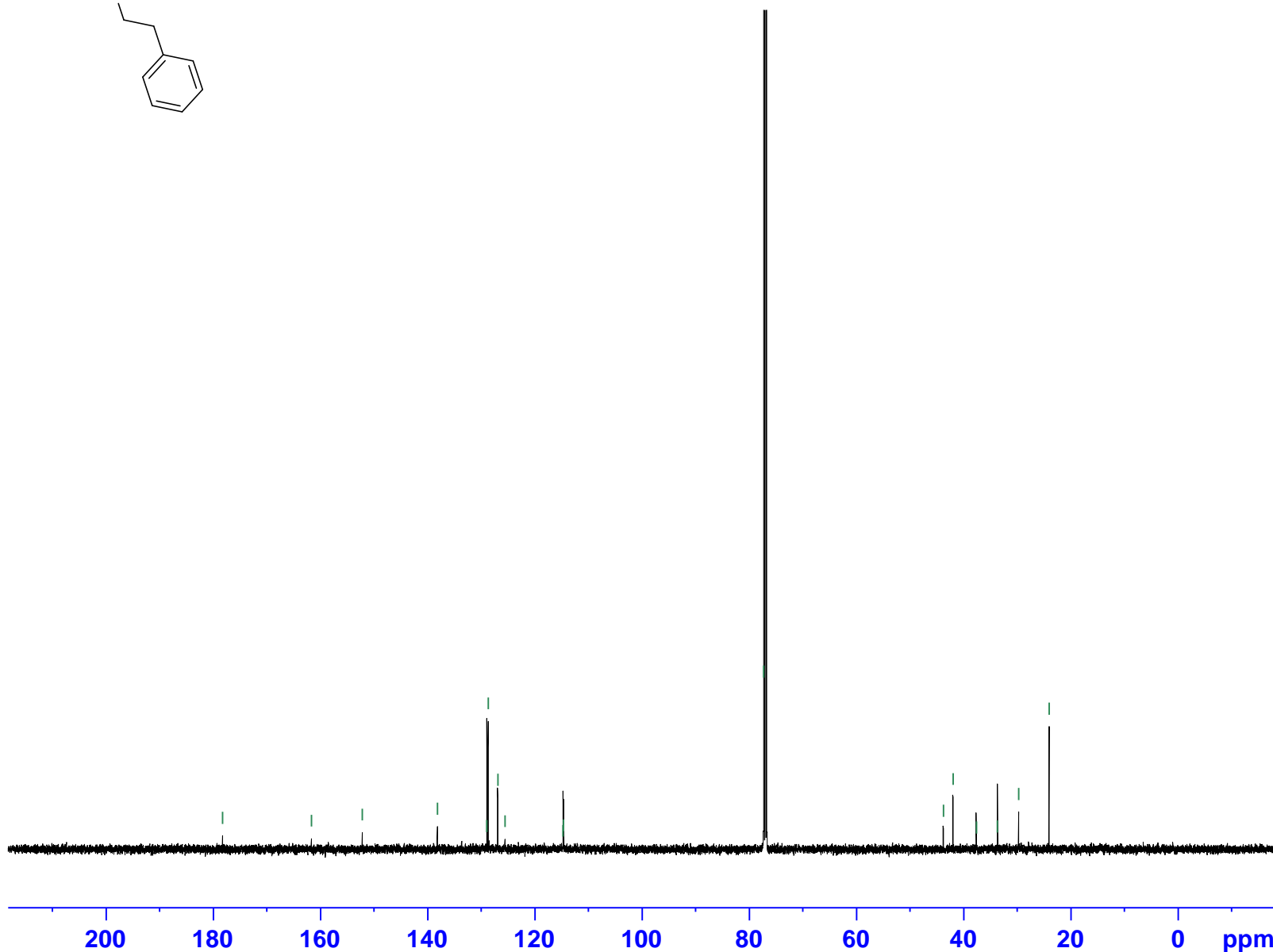
F2 - Processing parameters SI

65536
SF 500.3000446 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

14c



178.28
 161.69
 152.21
 138.19
 128.95
 128.72
 126.92
 125.58
 114.72
 114.62
 77.28
 77.02
 76.77
 43.80
 41.99
 37.65
 33.68
 29.72
 24.04



Current Data Parameters
 NAME SA-473-196
 EXPNO 31
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141217
 Time 21.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 26782
 SOLVENT CDCl3
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 1.111265 Hz
 AQ 0.4499376 sec
 RG 575
 DW 16.800 usec
 DE 7.72 usec
 TE 296.1 K
 D1 5.0000000 sec
 D11 0.0300000 sec
 TD0 1

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

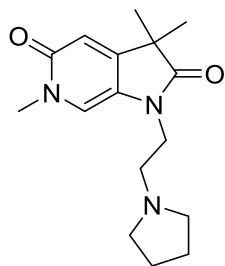
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

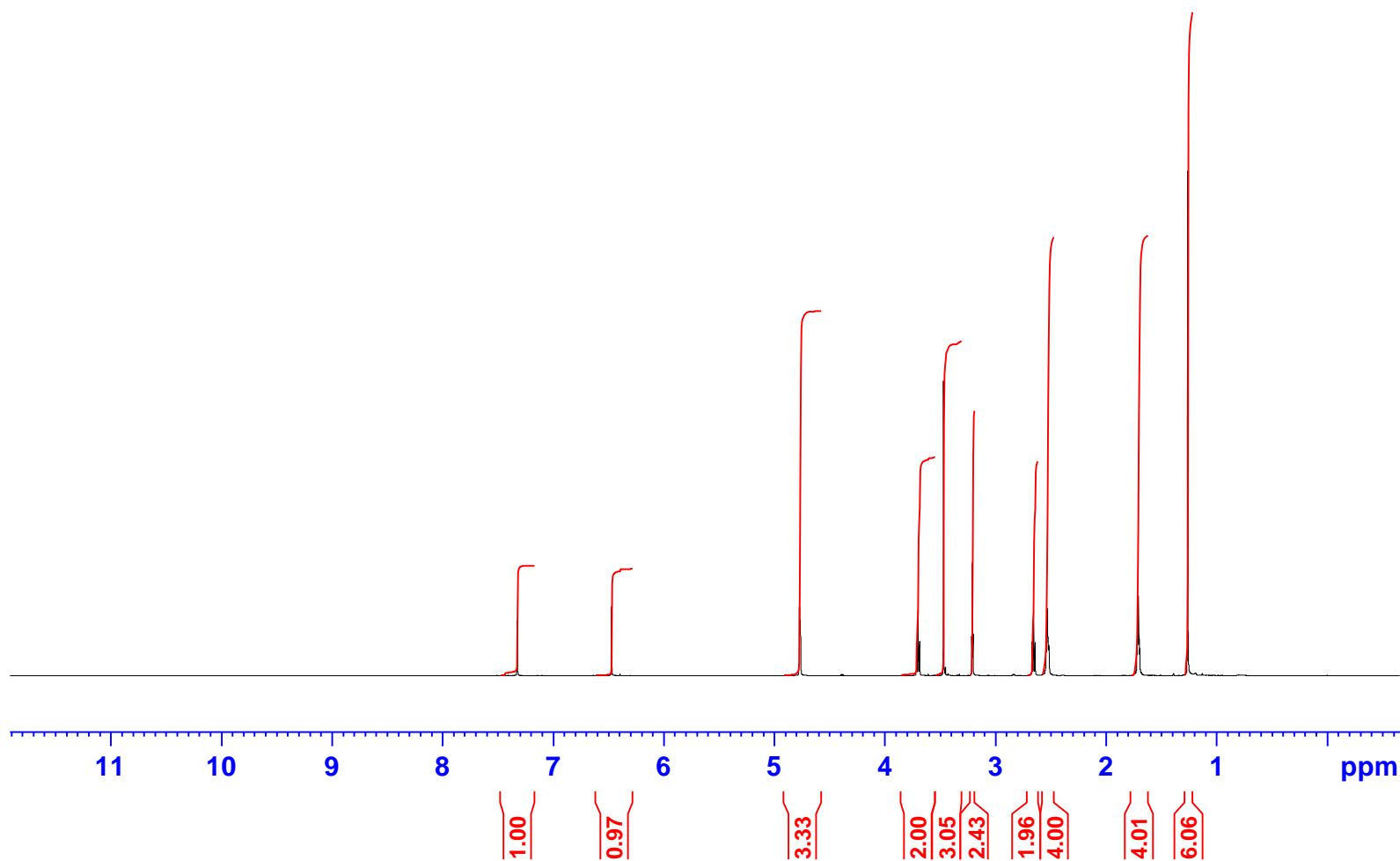
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

14d



7.326
6.473
4.774
3.701
3.687
3.471
3.216
3.212
3.209
3.206
3.203
2.670
2.656
2.531
1.716
1.709
1.701
1.262



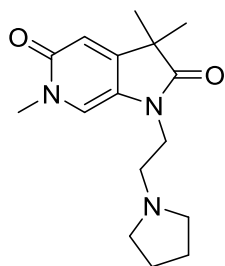
Current Data Parameters
NAME SA-500-16-2nd
EXPNO purification 11
PROCNO 1

F2 - Acquisition
Parameters 20150116
Time 1.57
INSTRUM spect
PROBHD 5 mmPABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 362
DV 48.400 usec
DE 11.99 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing
Parameters 65536
SF 500.3000602 MHz
VDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

14d



179.19

162.53

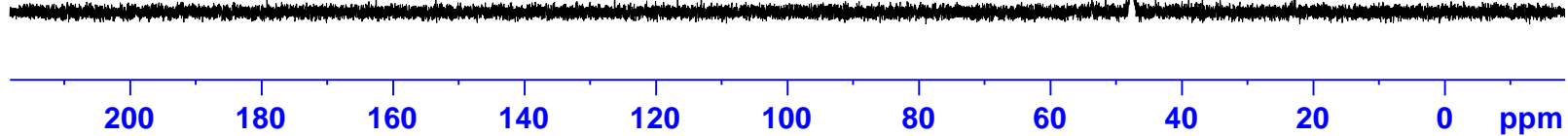
153.47

126.24

116.64

113.06

53.67
51.58
48.11
47.94
47.77
47.60
47.43
47.25
47.08
44.05
38.95
36.85
22.92
22.72



Current Data Parameters
NAME SA-500-16-2nd_purification
EXPNO 10
PROCNO 1

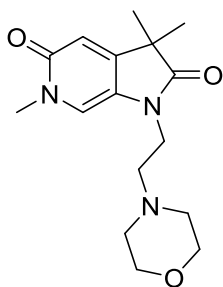
F2 - Acquisition Parameters
Date_ 20150116
Time 1.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 256
DS 2
SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 456
DW 16.800 usec
DE 7.68 usec
TE 296.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131151 MHz
NUC 13C
1P1 9.75 usec
PLW1 82.38999939 W

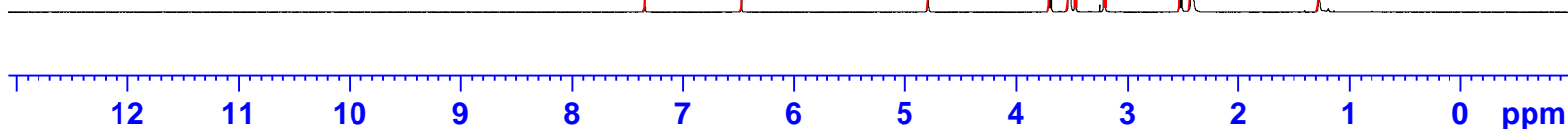
===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

F2 - Processing
Parameters 65536
SF 125.8005350 MHz
WD EM
W 0
SSB 1.00 Hz
LB 0
GB 1.40
PC

14e



7.345
6.478
4.793
3.700
3.688
3.525
3.516
3.507
3.469
3.216
3.212
3.209
3.206
3.203
2.534
2.522
2.509
2.417
1.273



1.04
1.00
3.11
2.10
4.11
3.20
5.60
2.14
3.91
6.46



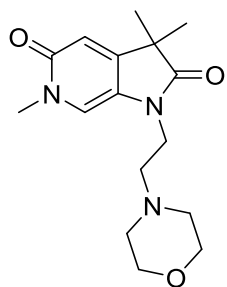
Current Data
NAME SA-500-14
EXPNO 30
PROCNO 1

F2 - Acquisition
Date_ 20150115
Time 15.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 512
DW 48.400 usec
DE 11.99 usec
TE 293.7 K
D1 1.00000000 sec
TDO 1

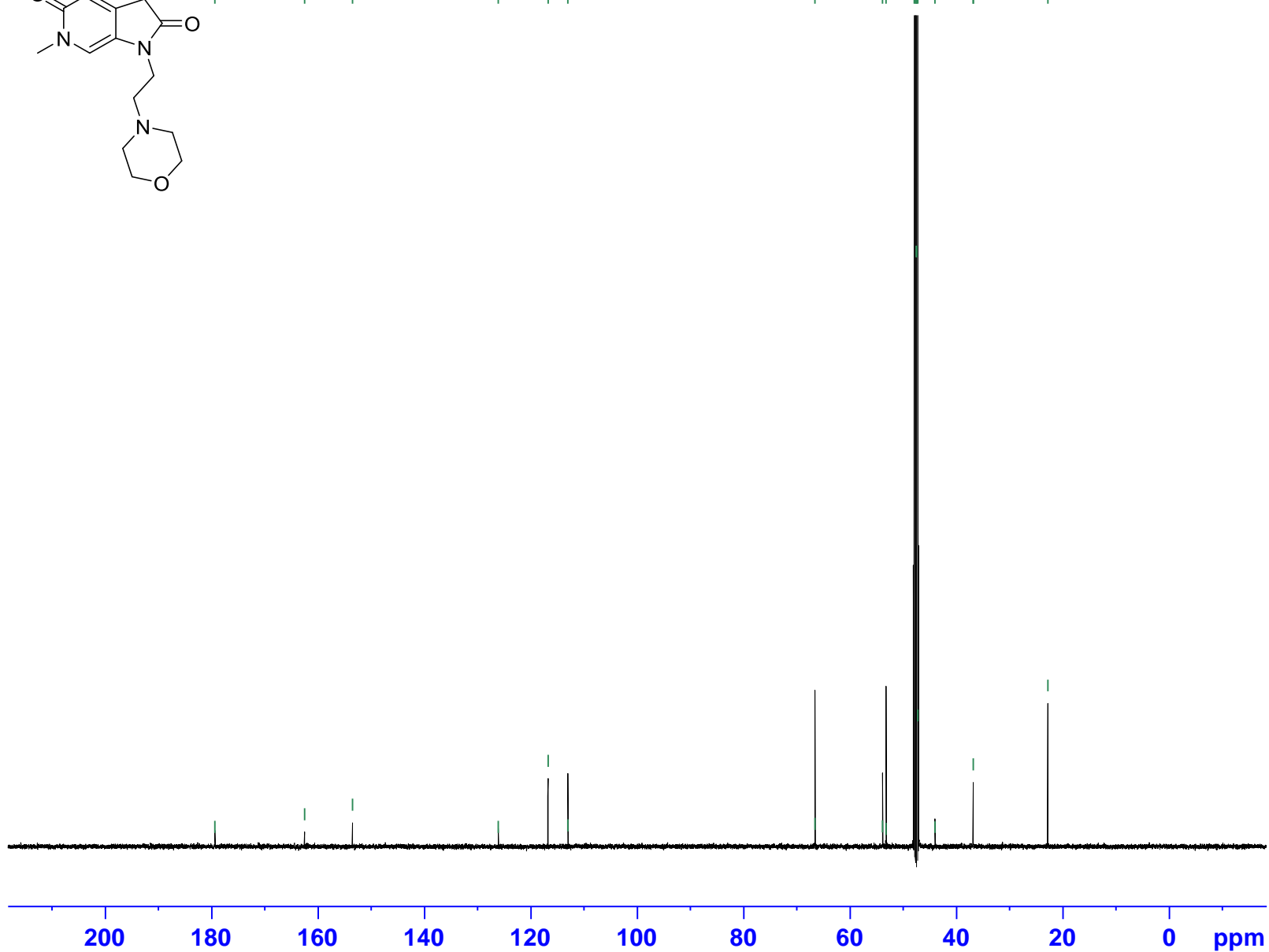
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000602 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

14e



179.35
162.52
153.50
126.12
116.77
113.01
66.58
53.88
53.24
47.93
47.76
47.59
47.42
47.25
44.04
36.86
36.82
22.82



Current Data Parameters
NAME SA-500-14
EXPNO 35
PROCNO 1

F2 - Acquisition
Parameters Date_ 20150116
Time 1.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 26782
SOLVENT MeOD
NS 2048
DS 2
SMH 29761.904 Hz
FIDRES 1.111265 Hz
AQ 0.4499376 sec
RG 456
DW 16.800 usec
DE 7.72 usec
TE 296.6 K
D1 5.0000000 sec
D11 0.03000000 sec
TD0 1

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

SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

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

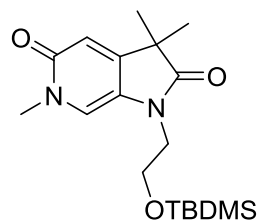
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

F2 - Processing

Parameters 65536
SF 125.8005350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

":\Old Server\SA\nmr"

14f



7.49

6.56

3.42

3.36

2.55

2.55

2.55

1.30

0.83

0.82

-0.00

1.00

0.97

1.99

2.02

2.98

6.29

9.00

5.91

8

6

4

2

0

[ppm]

[rel]

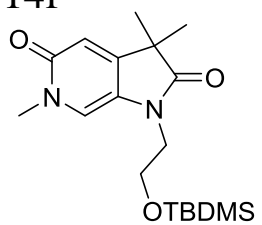
15

10

5

0

14f



— 178.14

— 161.12

— 152.23

— 125.14

— 117.61

— 113.67

60.01

43.69

42.56

40.52

40.35

40.27

40.18

40.02

39.85

39.68

39.51

37.23

26.05

24.16

— 18.21

— -5.09

100.00

200

150

100

50

0

[ppm]

[rel]

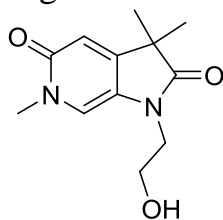
6

4

2

0

14g



7.441
6.520
4.826
3.605
3.598
3.586
3.575
3.392
3.324
2.516
2.512
2.508
2.505
2.501
1.263



Current Data
NAME SA-473-216
EXPNO 20
PROCNO 1

F2 - Acquisition
Date_ Time 20141211 14.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 575
DW 48.400 usec
DE 11.99 usec
TE 297.7 K
D1 1.00000000 sec
TDO 1

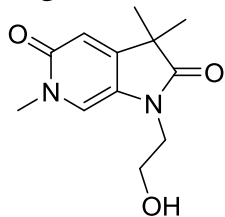
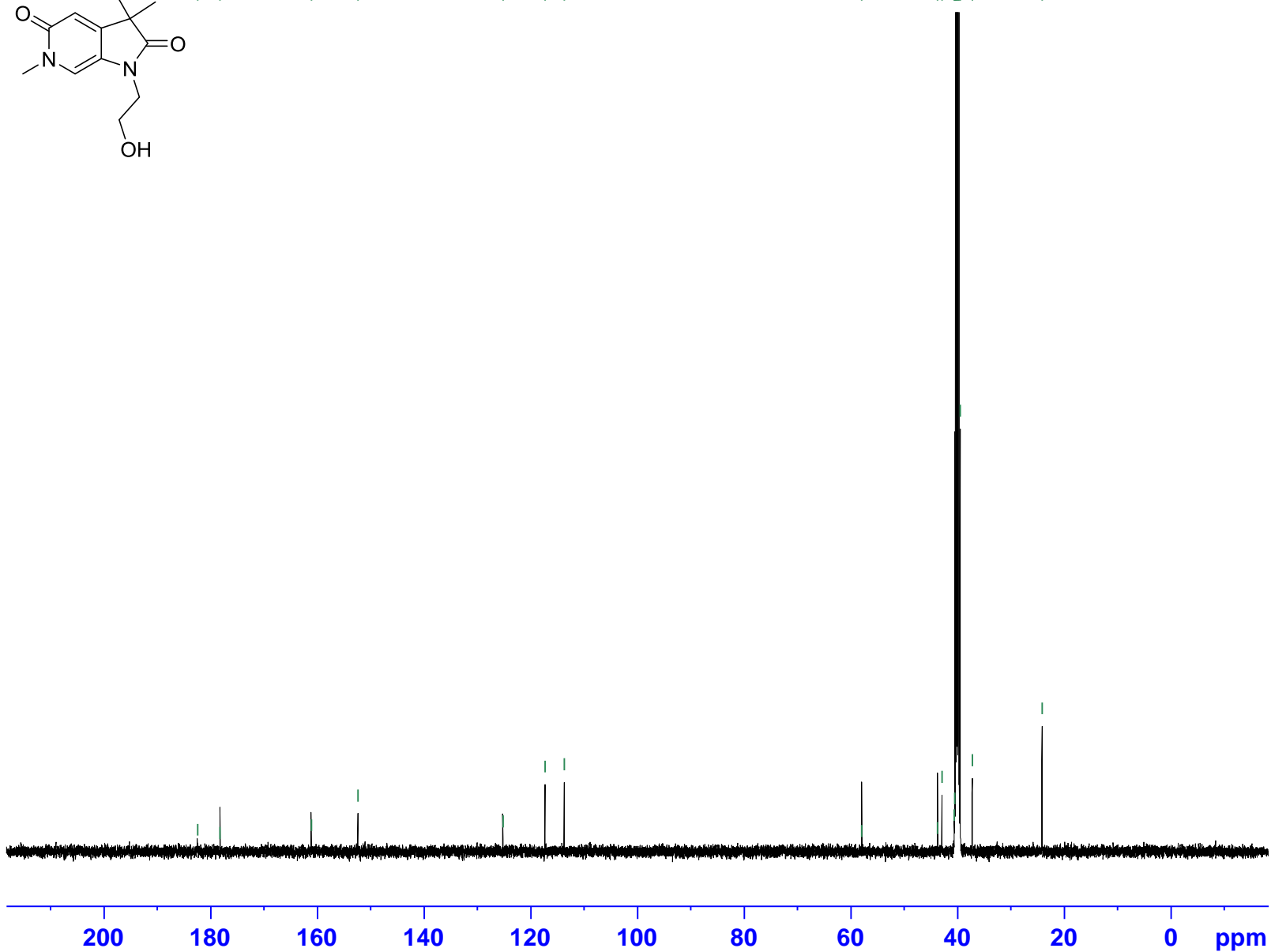
===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.00 0.98 0.99 4.06 2.97 1.21 4.87 6.20

14g

182.47
178.23161.15
152.41125.22
117.30
113.7057.98
43.74
42.92
40.61
40.51
40.44
40.35
40.27
40.18
40.01
39.85
39.68
39.51
37.25
24.17

Current Data Parameters
 NAME SA-473-216
 EXPNO 25
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141212
 Time 0.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1024
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

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

SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

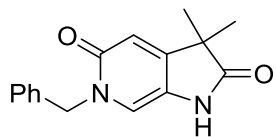
===== CHANNEL f2 =====

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing

Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

15c

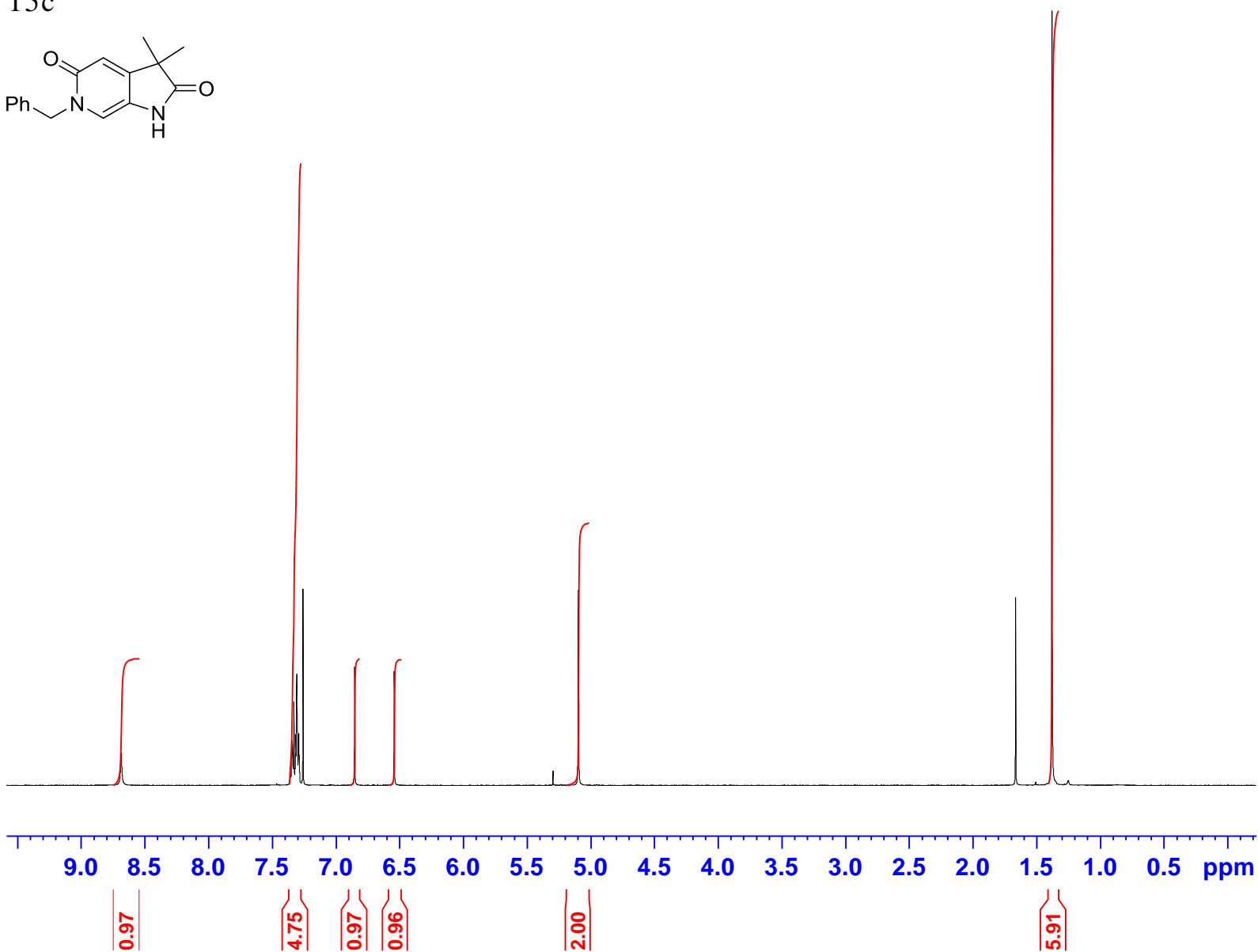


7.357
7.356
7.333
7.327
7.285
6.880
6.879
6.569

5.122

1.690

1.405



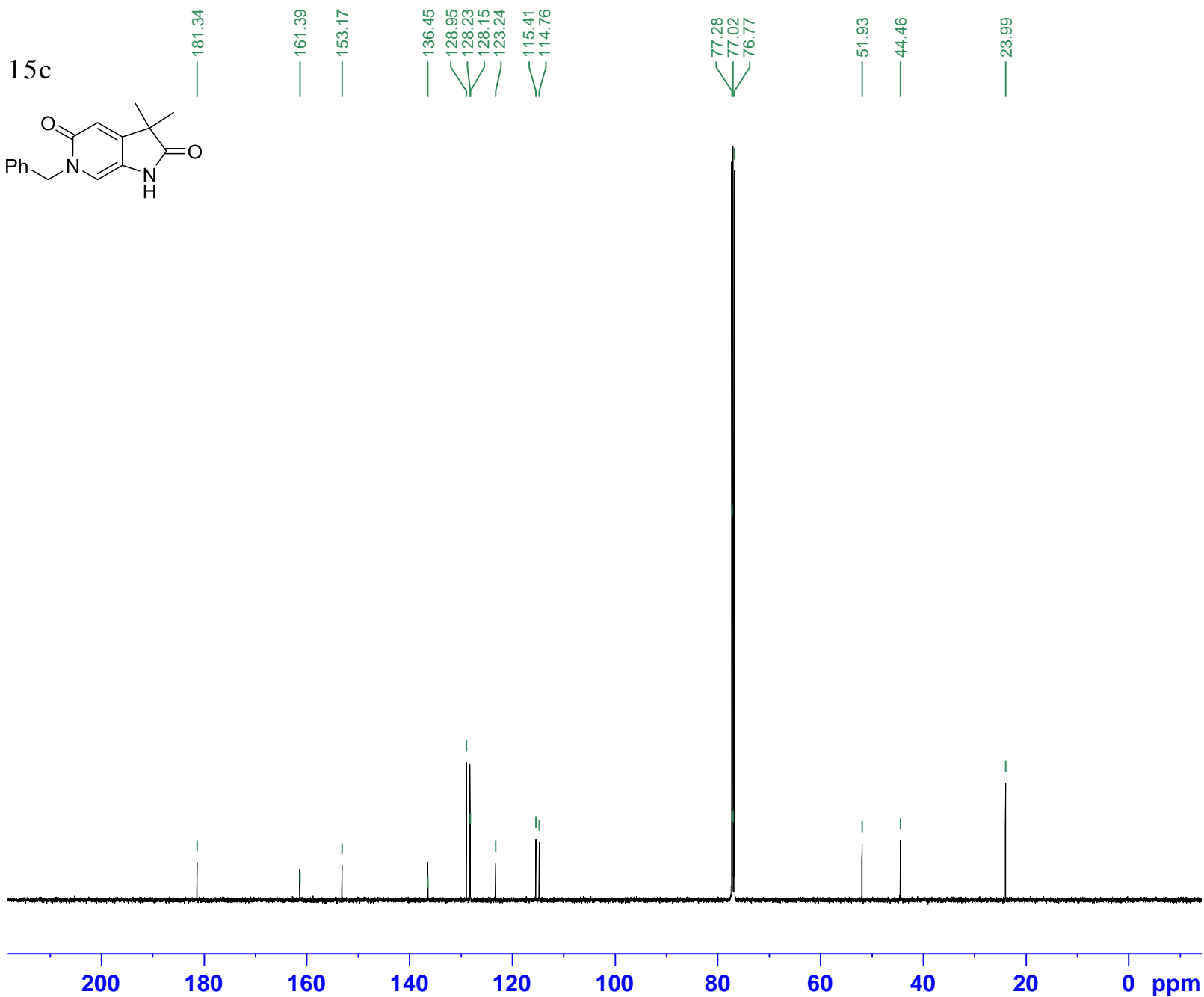
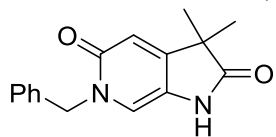
Current Data Parameters
NAME DCM-494-73-B CDCL3 CONC
EXPNO 11
PROCNO 1

F2 - Acquisition
Parameters 20141029
Time 8.32
INSTRUM spect
PROBHD 5 mmPABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 456
DV 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing
Parameters 65536
S 500.3000125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

15c



Current Data Parameters
 NAME DCM-494-73-B CDCL3 CONC
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141029
 Time 4.42
 INSTRUM spect
 PROBHD 5 mmPABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVEN CDCl3
 TNS 2048
 DS 2
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DW 16.800 usec
 DE 7.68 usec
 TE 298.1 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.3899939 W

==== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing parameters
 S1 65536
 SF 125.8005350 MHz
 VDW EM
 SSB 0
 LB 1.00 Hz
 CB 0
 PC 1.40

7.294
7.279
7.259
7.194
7.191
7.178
6.600
6.517

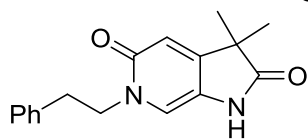
4.094
4.079

3.041

1.598
1.391

15d

CDCl₃



Current Data
NAME DCM-494-80-A CDCl₃
EXPNO 10
PROCNO 1

F2 - Acquisition
Data parameters 20141030
Time 14.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DW 48.400 usec
DE 11.99 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000127 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

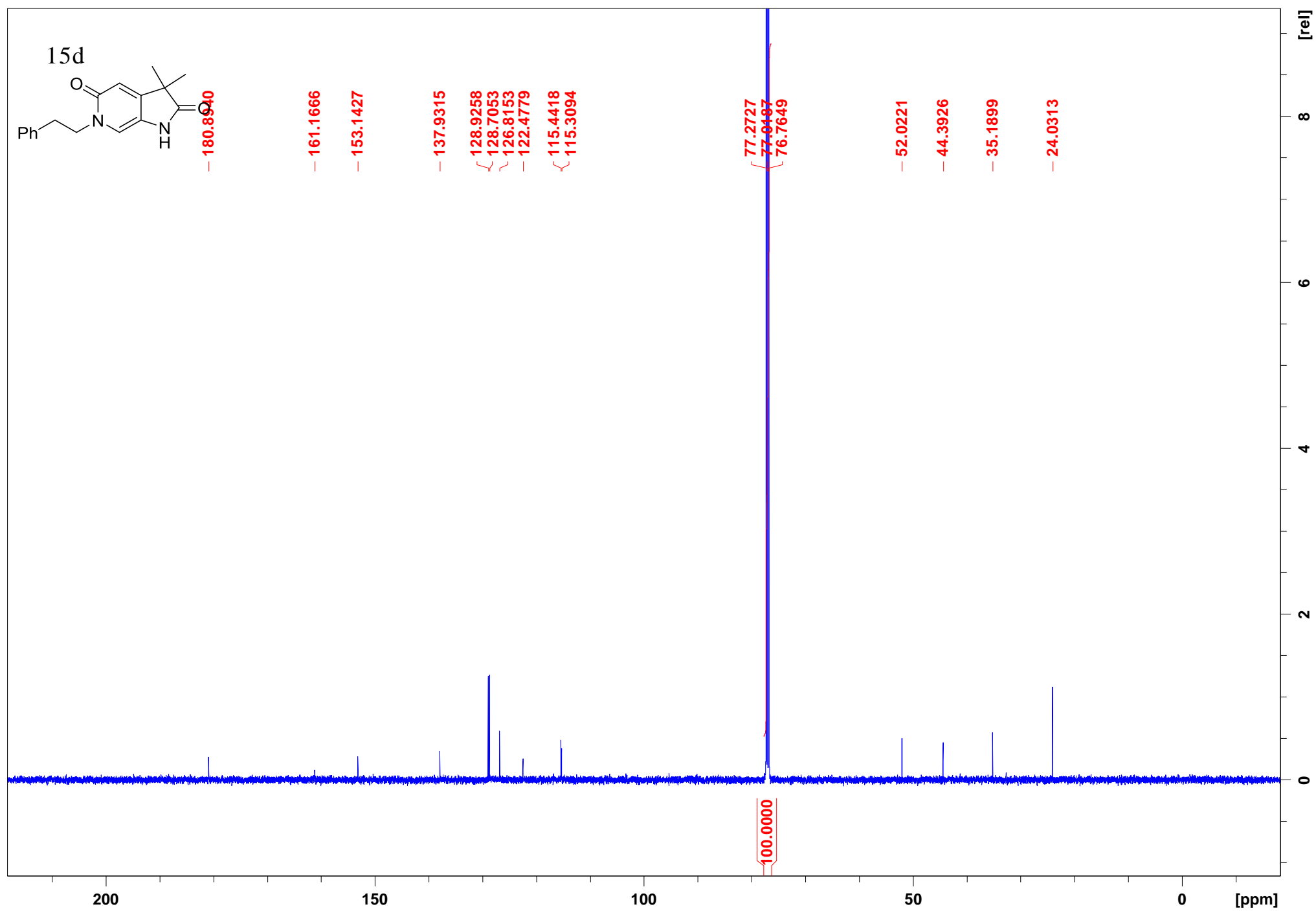
10 9 8 7 6 5 4 3 2 1 ppm

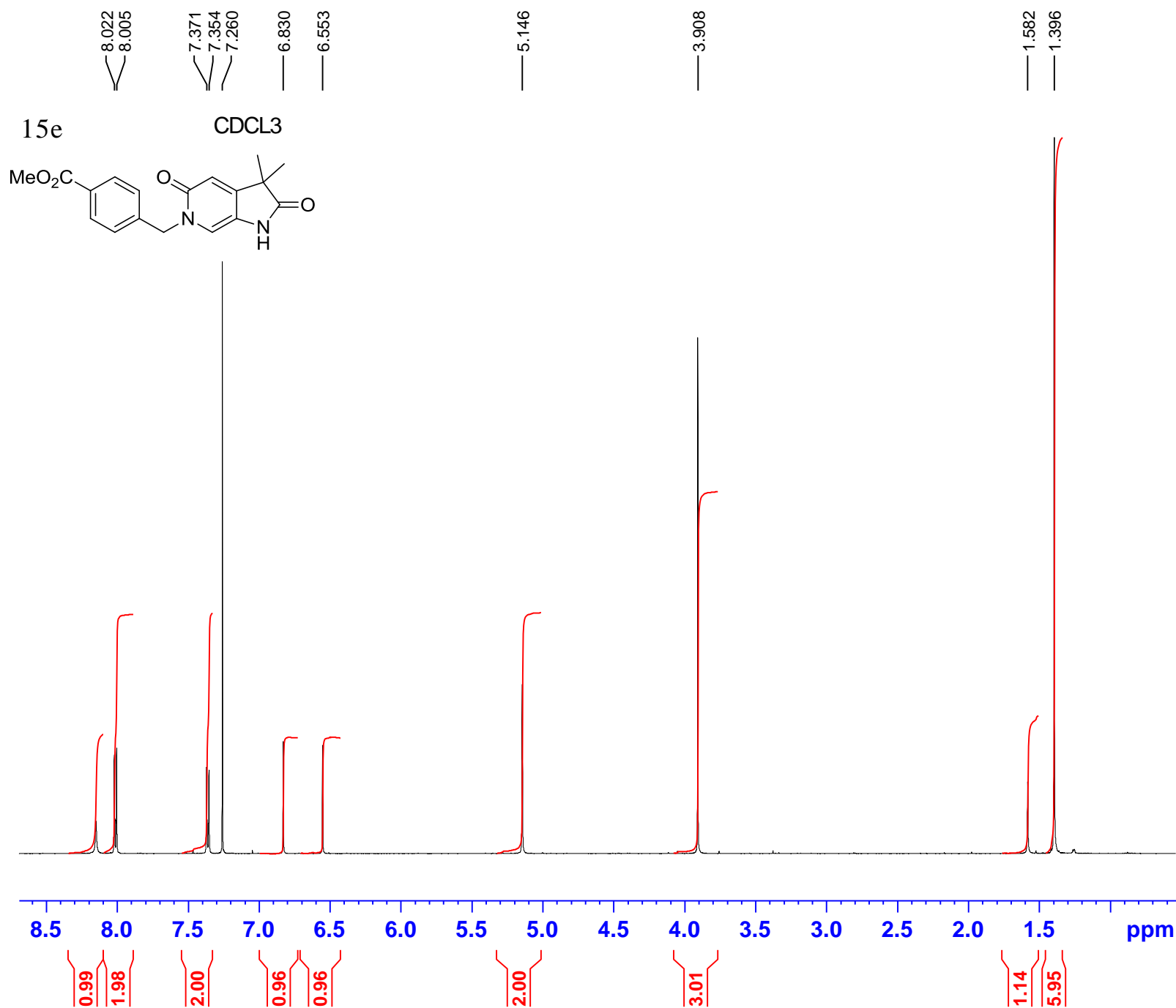
0.97
2.03
1.12
2.03
1.00
1.00

2.03

2.01

1.64
6.09



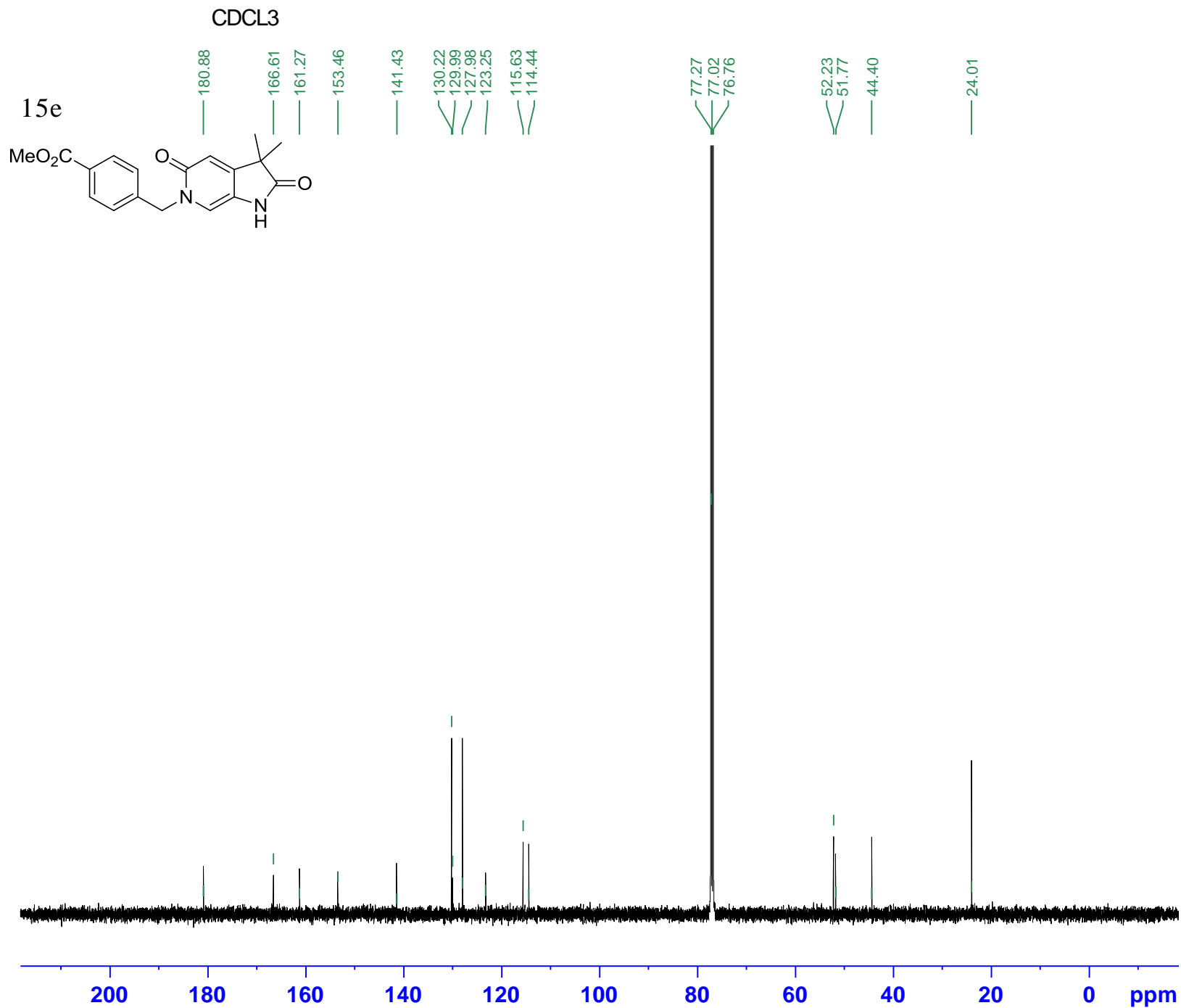


Current Data Parameters
NAME DCM-494-115-A_CDCl3_CONC
EXPNO 10
PROCNO 1

F2 - Acquisition
Date_ 20141209
Time 16.21
INSTRUM spect
PROBHD 5 mmPABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DV 48.400 usec
DE 11.99 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing
Parameters 65536
SF 500.3000124 MHz
VDM EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME DCM-494-115-A CDCL₃ CONC
EXPNO 12
PROCNO 1

F2 - Acquisition
Parameters 20141209
Time 23.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg3
TD 0
SOLVENT 6553
NS 6
DS CDC13
SMH 2048
FIDRES 2
AQ 29761.904 Hz
RG 0.454131 Hz
DW 1.1010048 sec
DE 575
TE 16.800 usec
D1 7.68 usec
D11 298.0 K
TD0 2.00000000 sec
0.03000000 sec

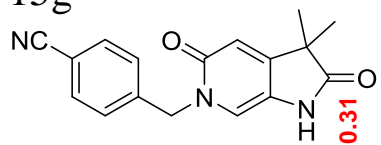
==== CHANNEL f1 =====
SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

==== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

F2 - Processing
Parameters 65536
SF 125.8005350 MHz
VDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

10 1

15g



-10.31

7.86
7.84
7.49
7.47
7.28

-6.60

-5.17

-3.40

2.55
2.54
2.54
2.53

-1.29

0.99

1.97
2.01
0.96

0.97

2.00

6.08

15.12

6.26

12

10

8

6

4

2

0

[ppm]

[rel]

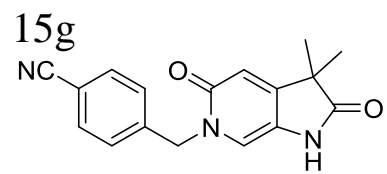
80

60

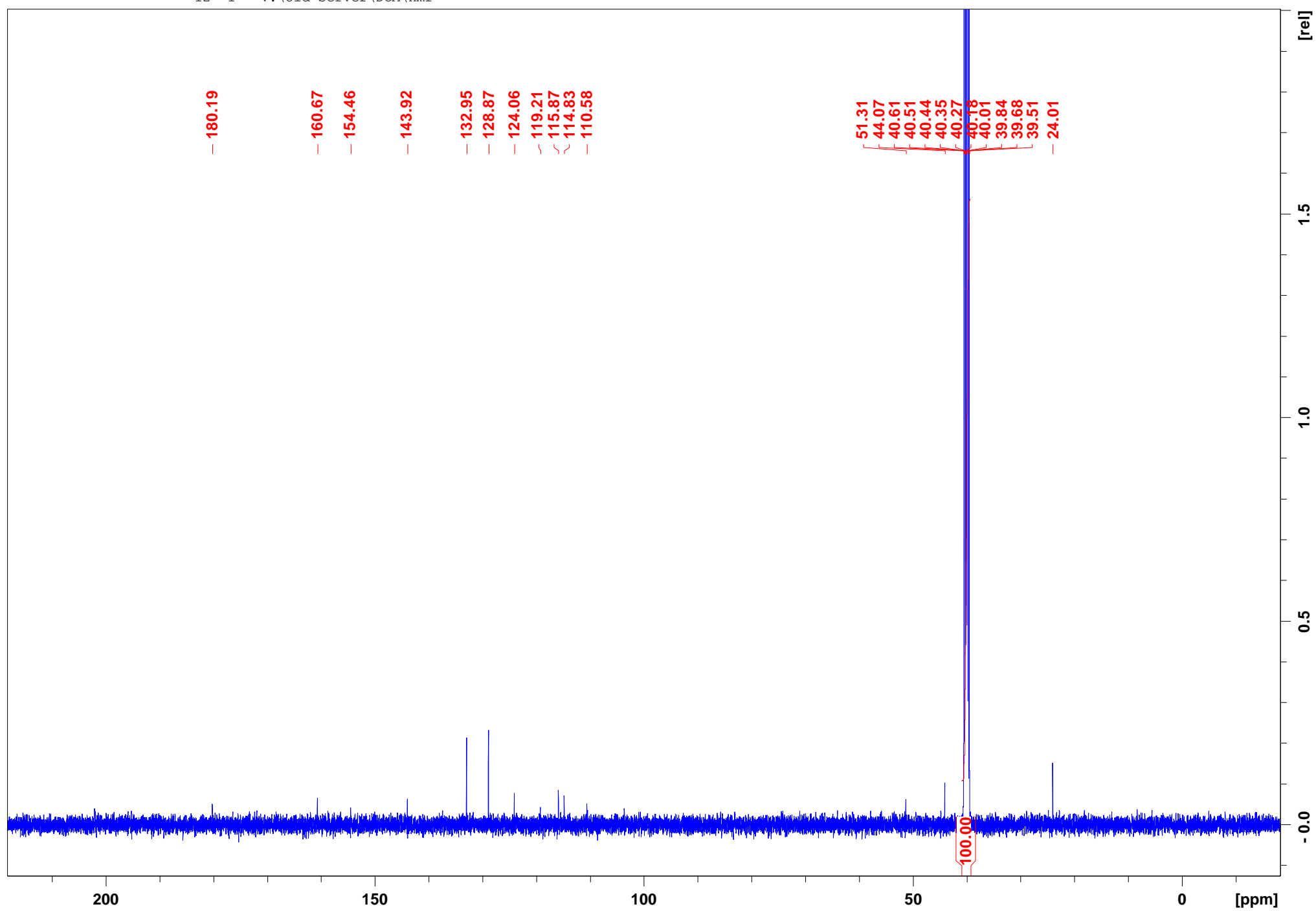
40

20

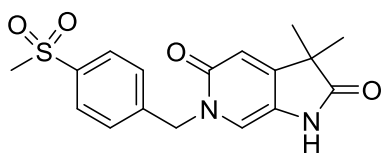
0



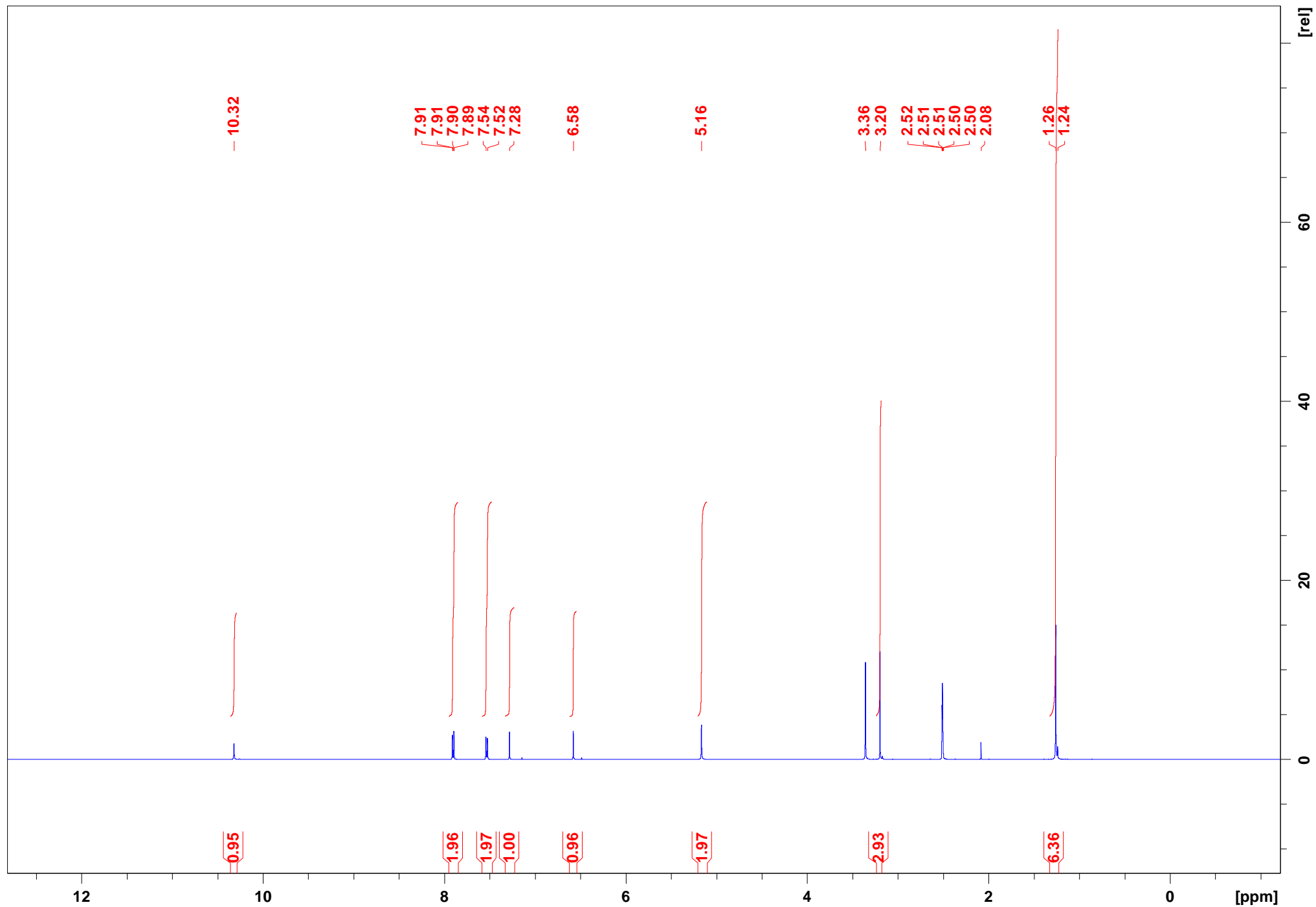
12 1 "V:\Old Server\DCM\nmr"



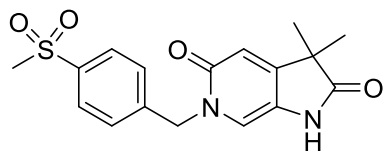
15i



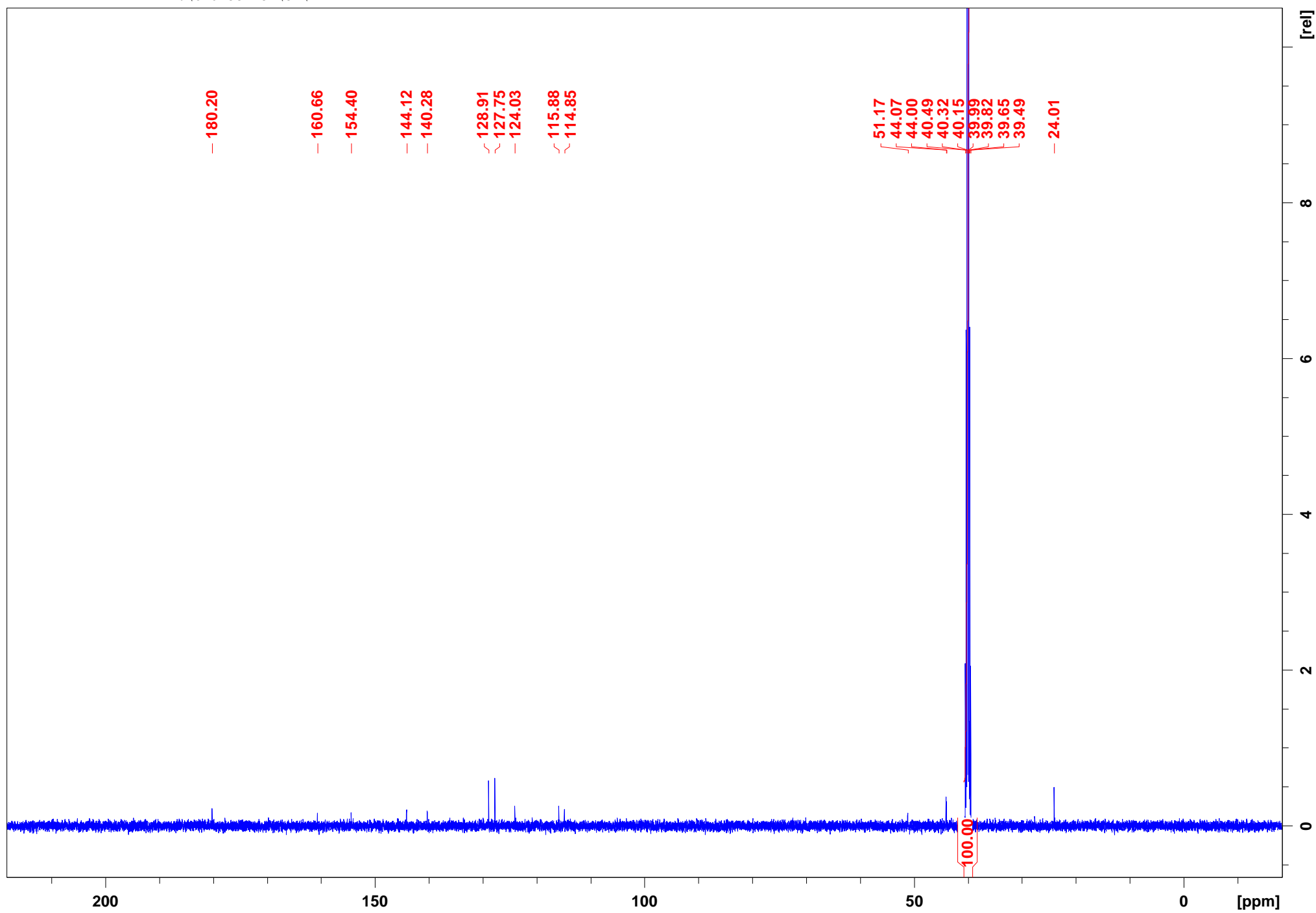
20 1 "V:\Old Server\SA\nmr"



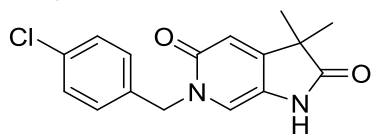
15i



"V:\Old Server\SA\nmr"



15j

7.318
7.2446.506
6.5065.064
4.8053.215
3.212
3.209
3.205
3.202
3.019

1.261

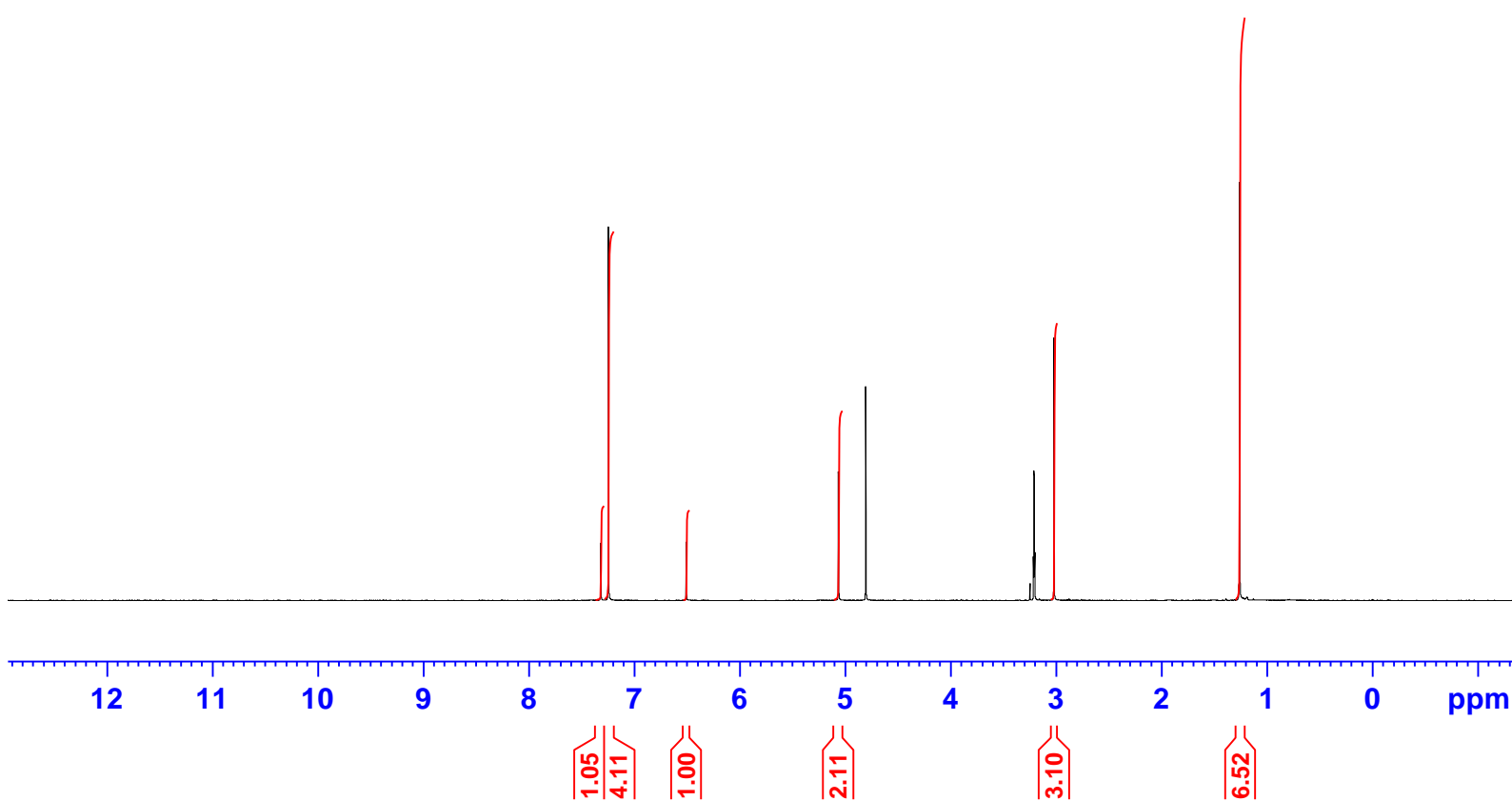


Current Data
 NAME SA-500-42
 EXPNO 10
 PROCNO 1

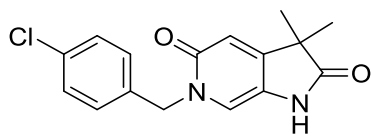
F2 - Acquisition
 Parameters 20150122
 Time 17.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 456
 DW 48.400 usec
 DE 11.99 usec
 TE 292.6 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

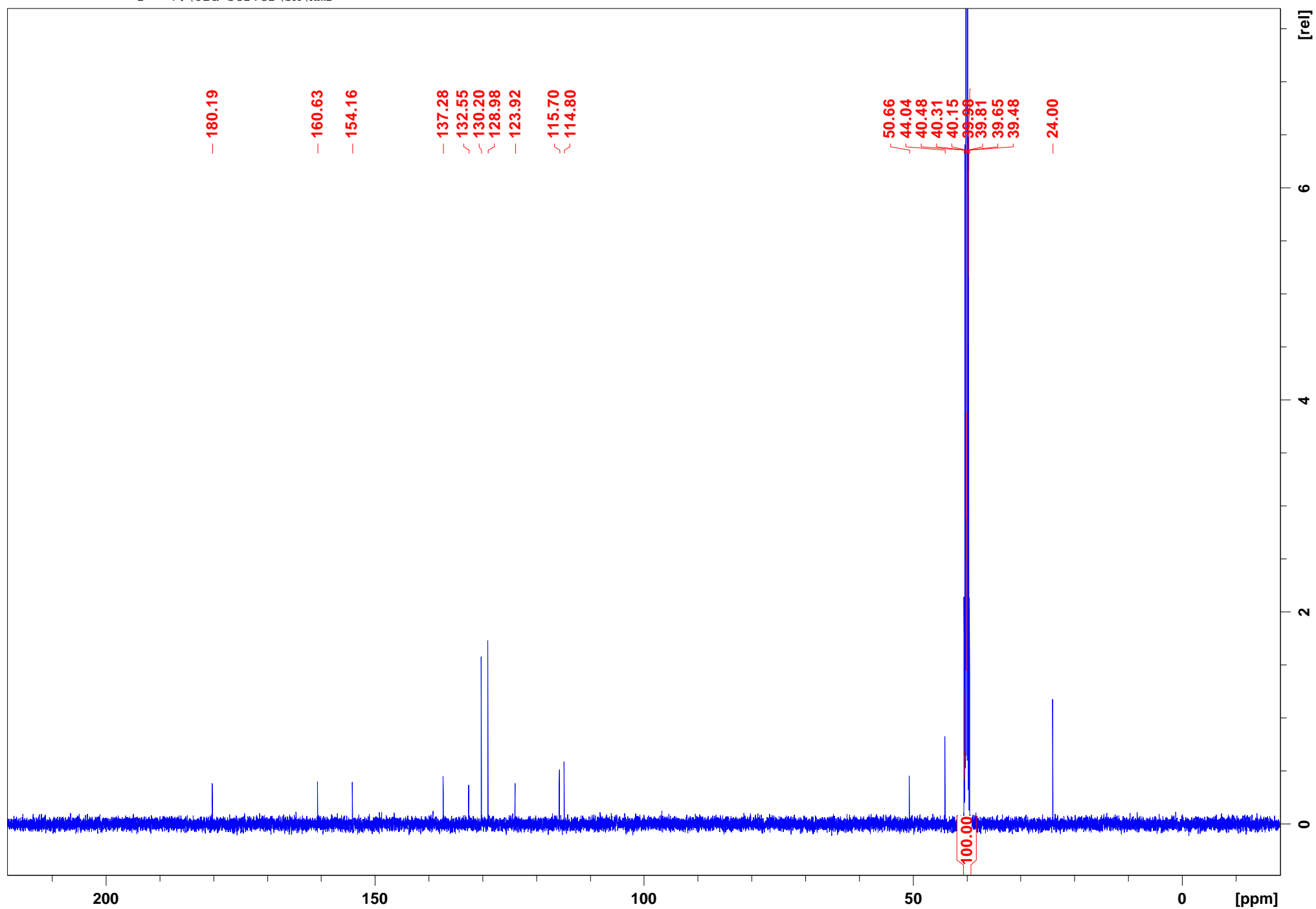
F2 - Processing parameters SI
 65536
 SF 500.3000605 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



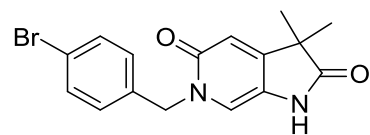
15j



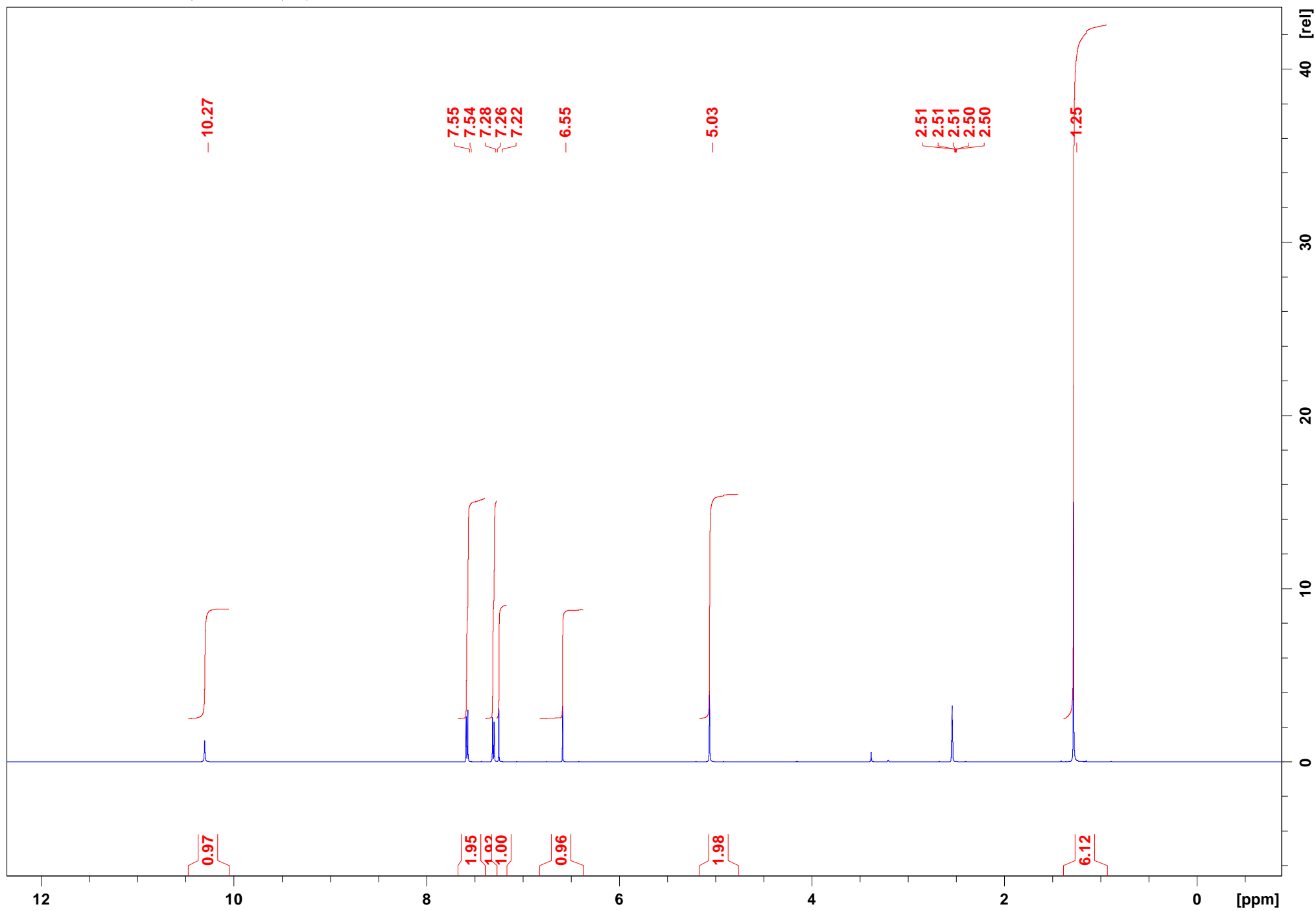
1 "V:\Old Server\SA\nmr"



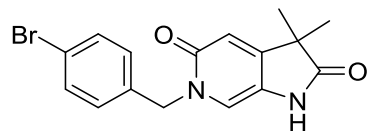
15k



10 1 "V:\Old Server\SA\nmr"

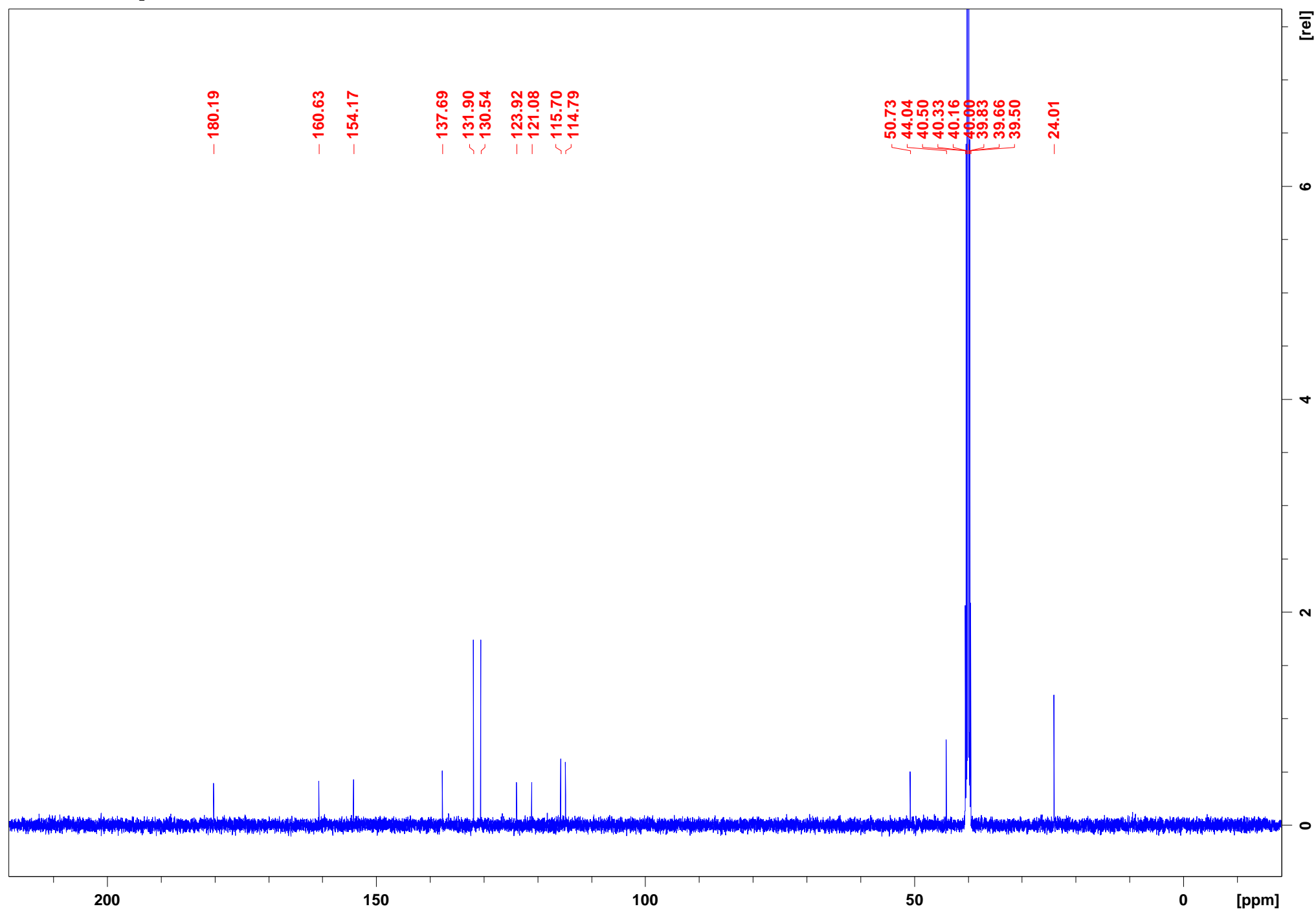


15k

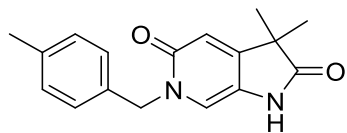


"V:\Old Server\SA\nmr"

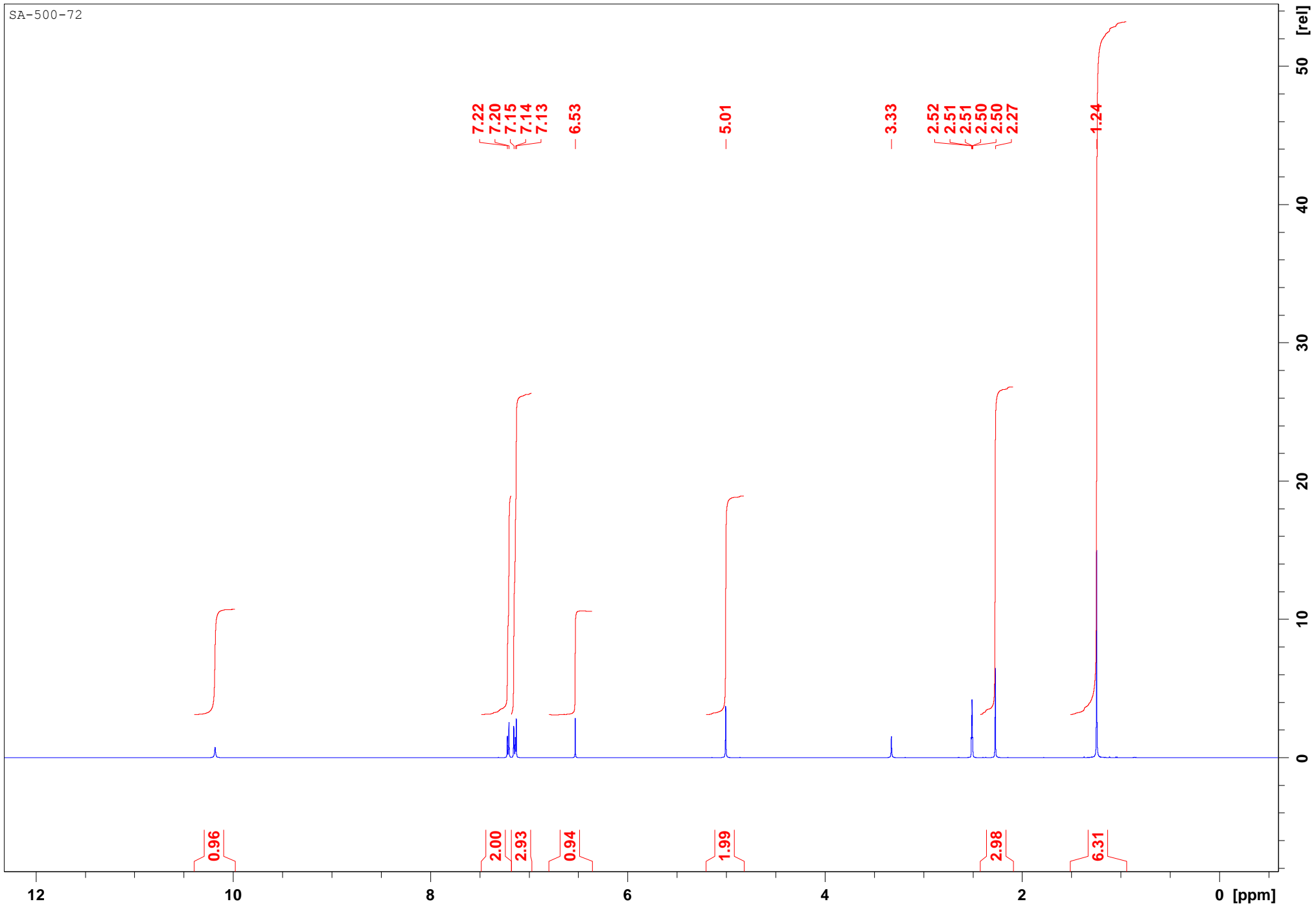
1



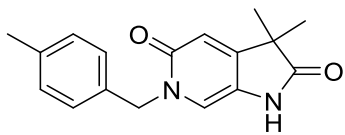
151



SA-500-72 10 1 "v:\Old Server\SA\nmr"

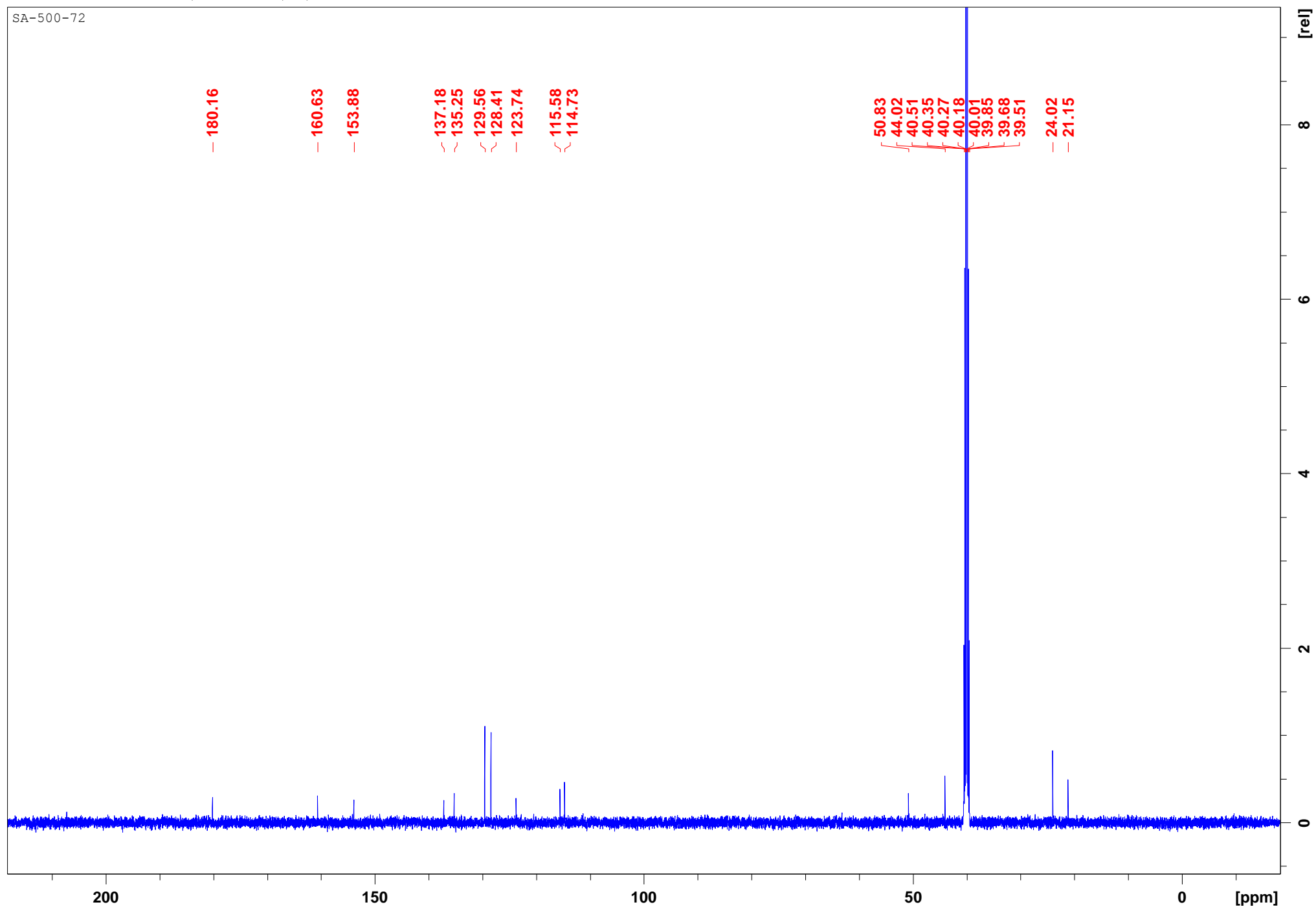


151

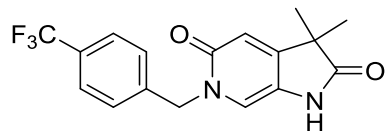


SA-500-72 11 1 "v:\Old Server\SA\nmr"

SA-500-72

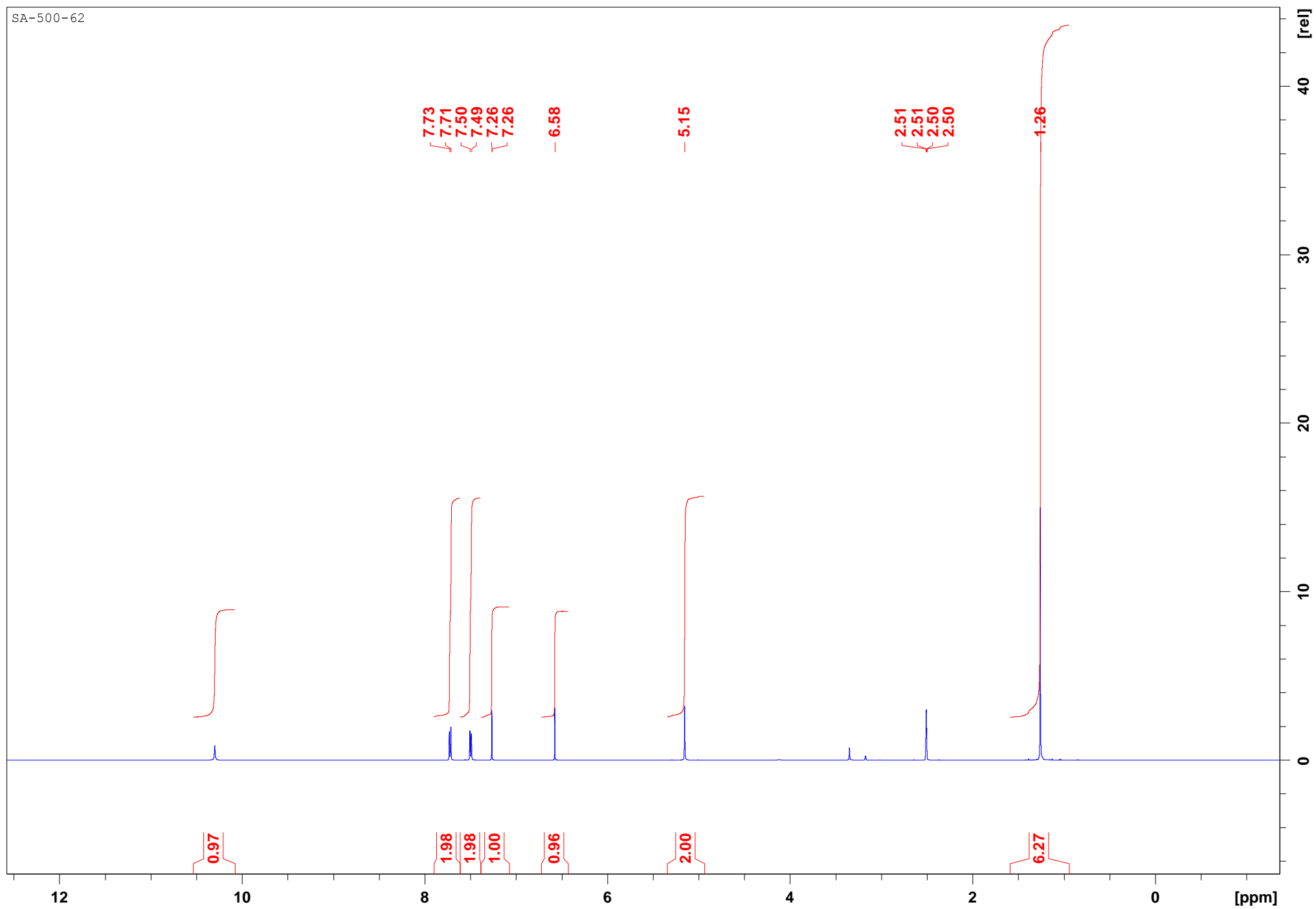


15m

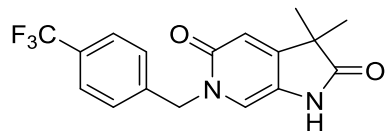


SA-500-62 10 1 "V:\Old Server\SA\nmr"

SA-500-62

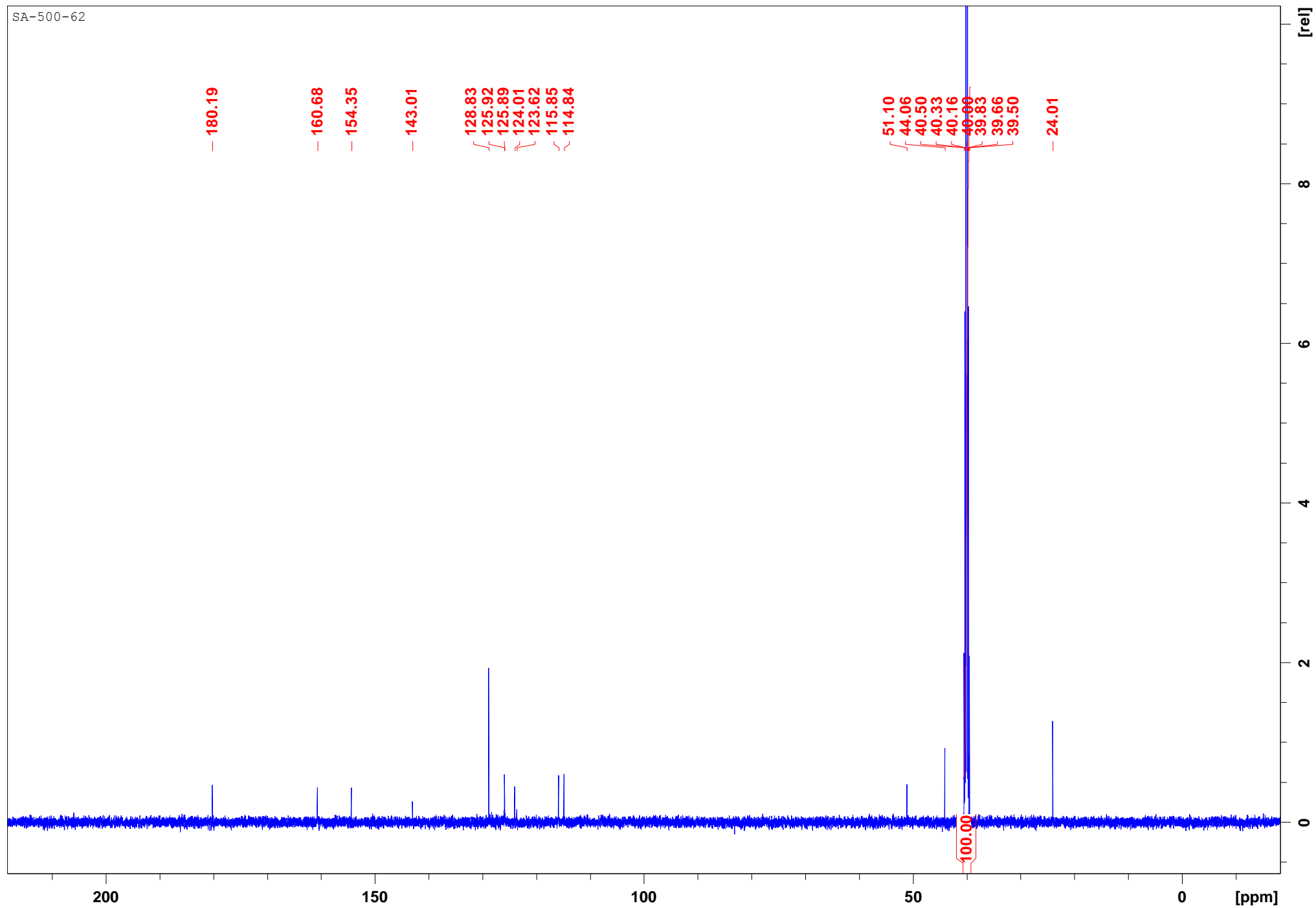


15m

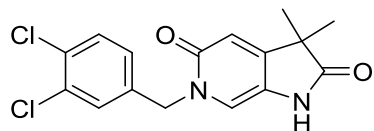


SA-500-62 11 1 "v:\Old Server\SA\nmr"

SA-500-62

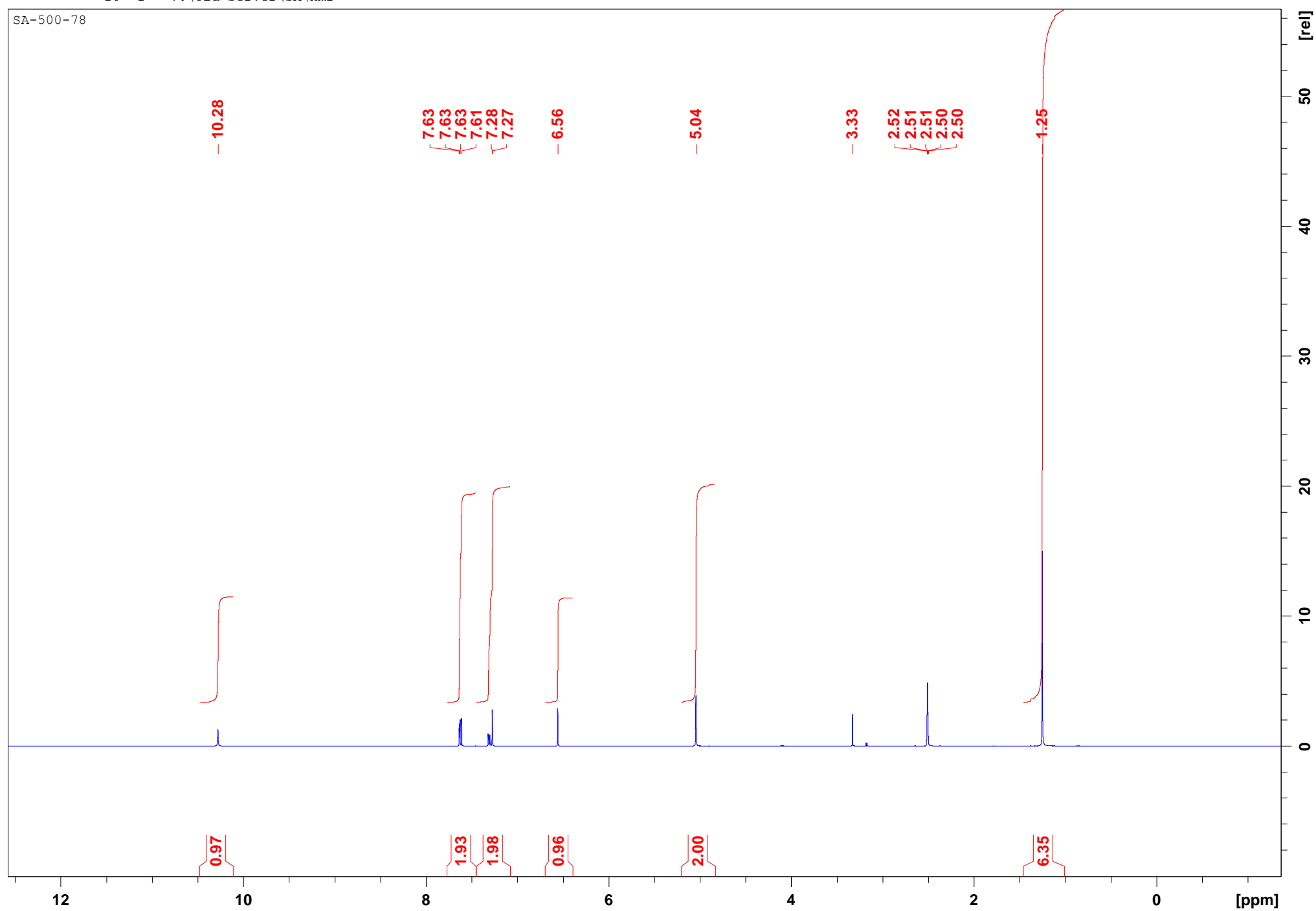


15n

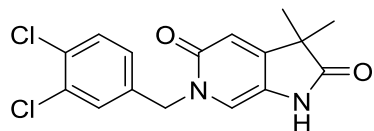


SA-500-78 10 1 "V:\Old Server\SA\nmr"

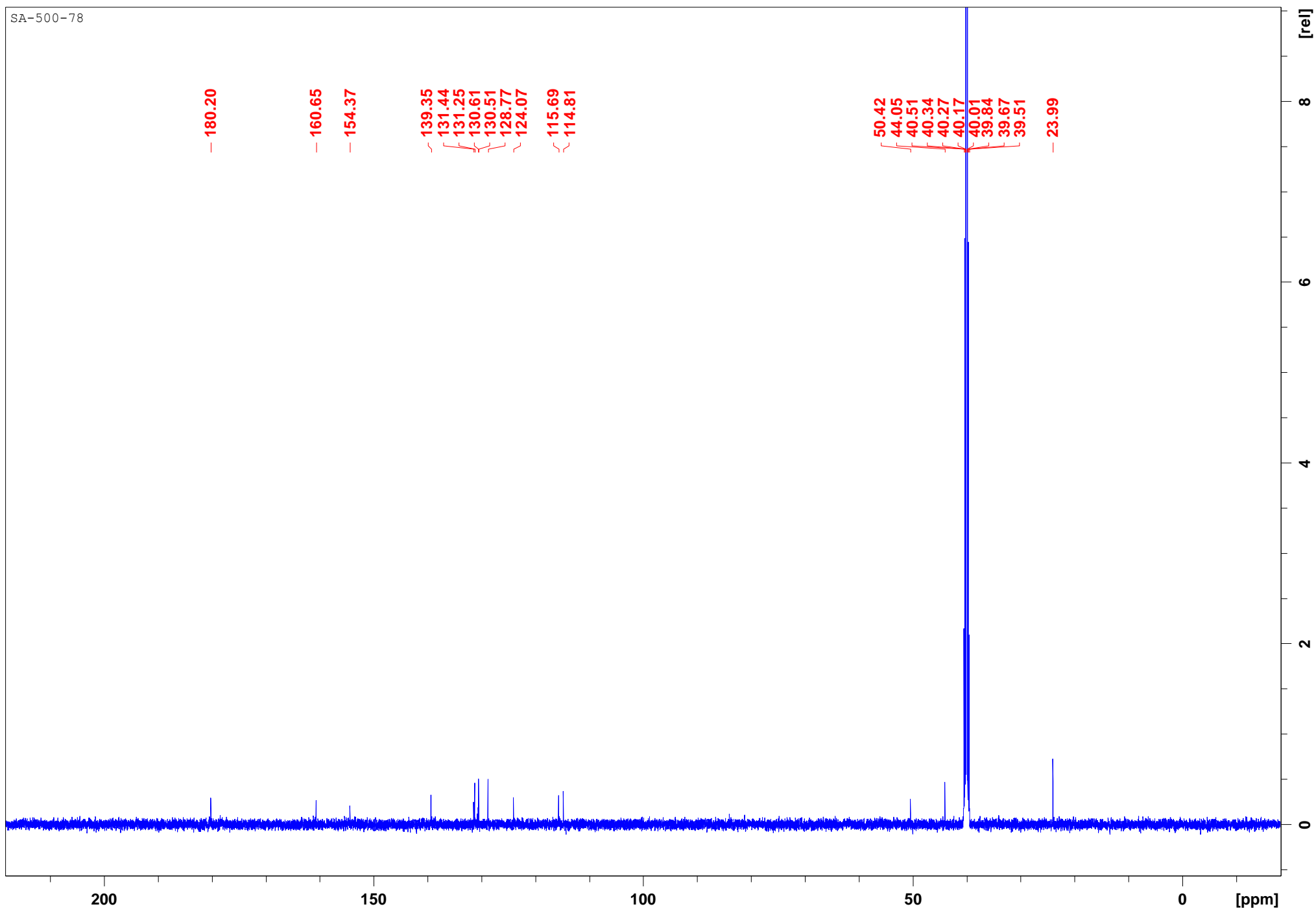
SA-500-78



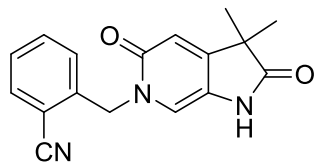
15n



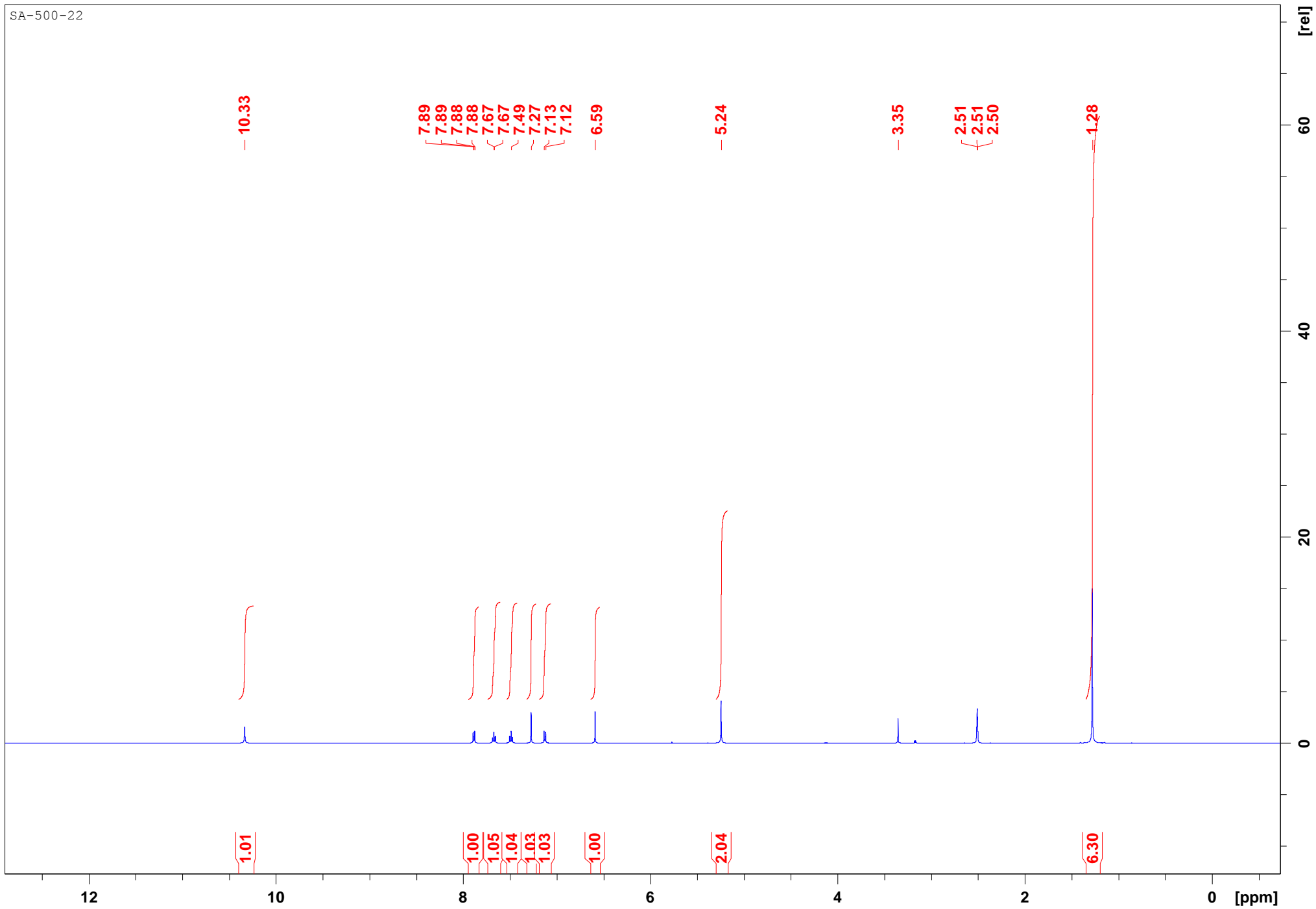
SA-500-78 11 1 "V:\Old Server\SA\nmr"



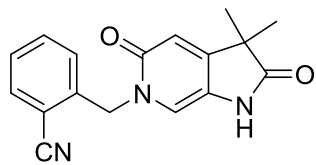
15o



SA-500-22 10 1 "v:\Old Server\SA\nmr"

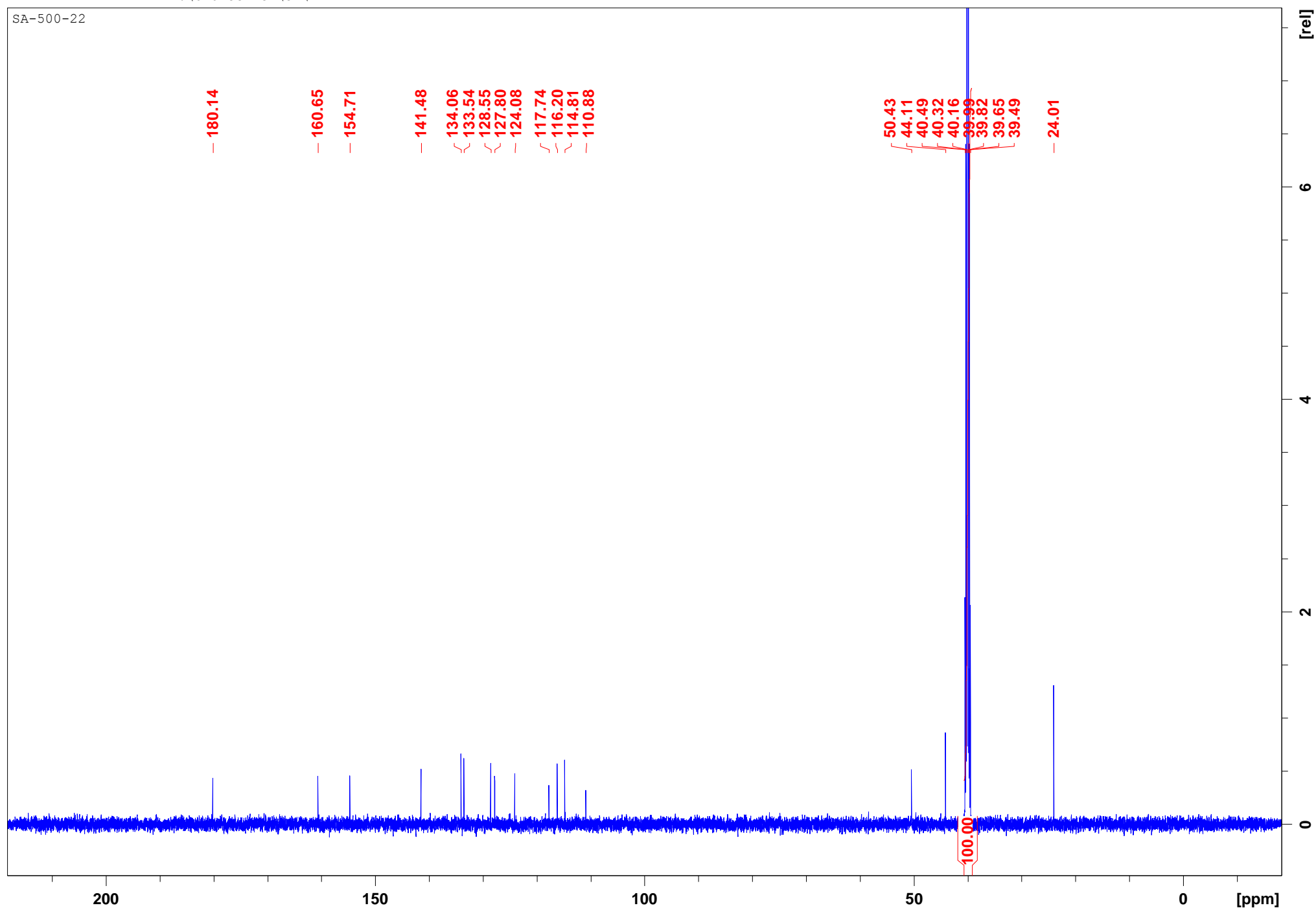


15o

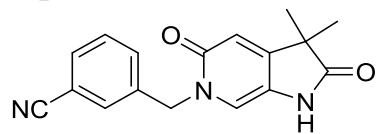


SA-500-22 11 1 "v:\Old Server\SA\nmr"

SA-500-22

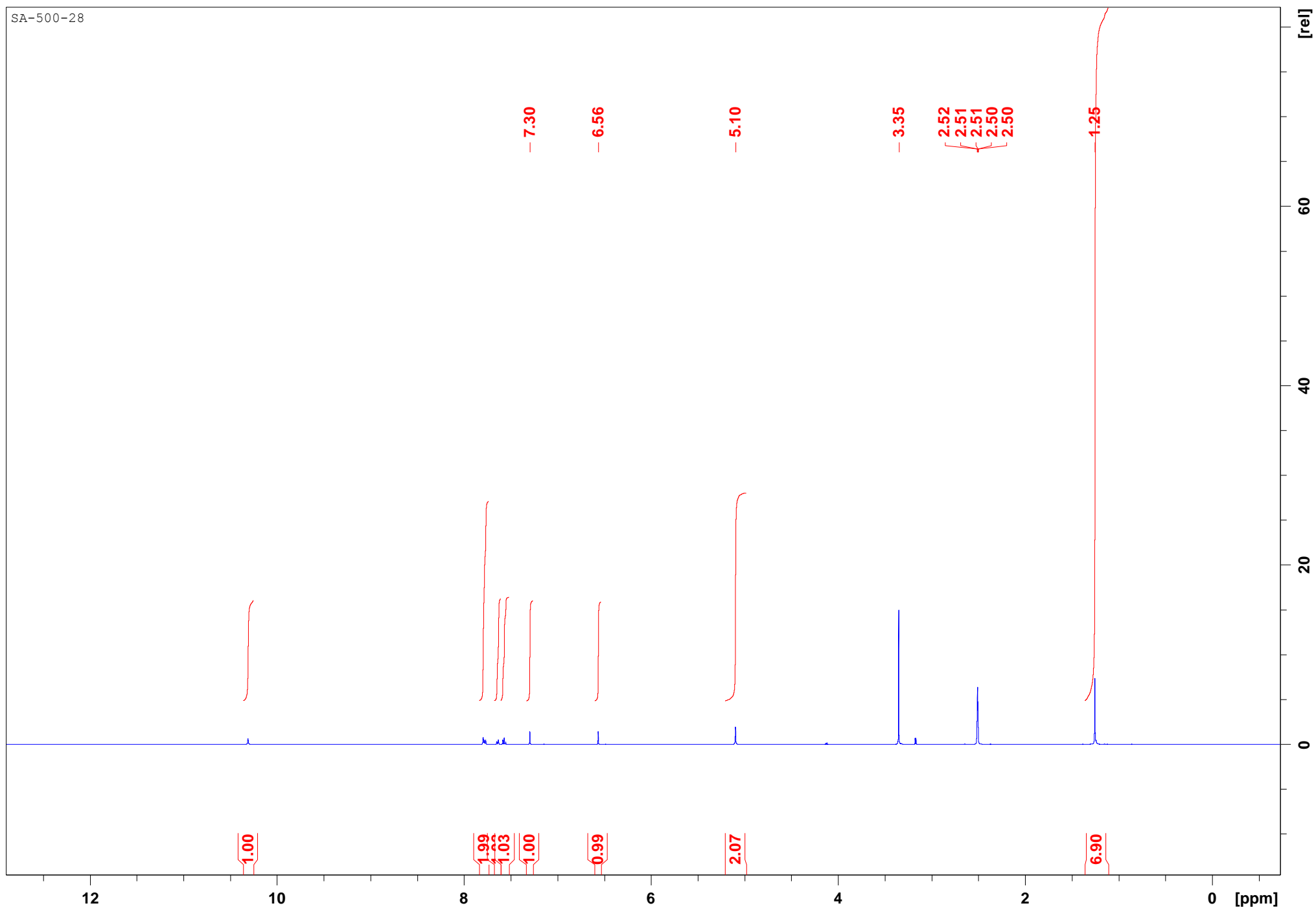


15p

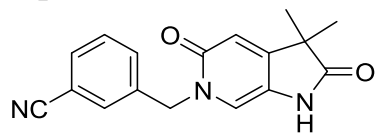


SA-500-28 10 1 "V:\Old Server\SA\nmr"

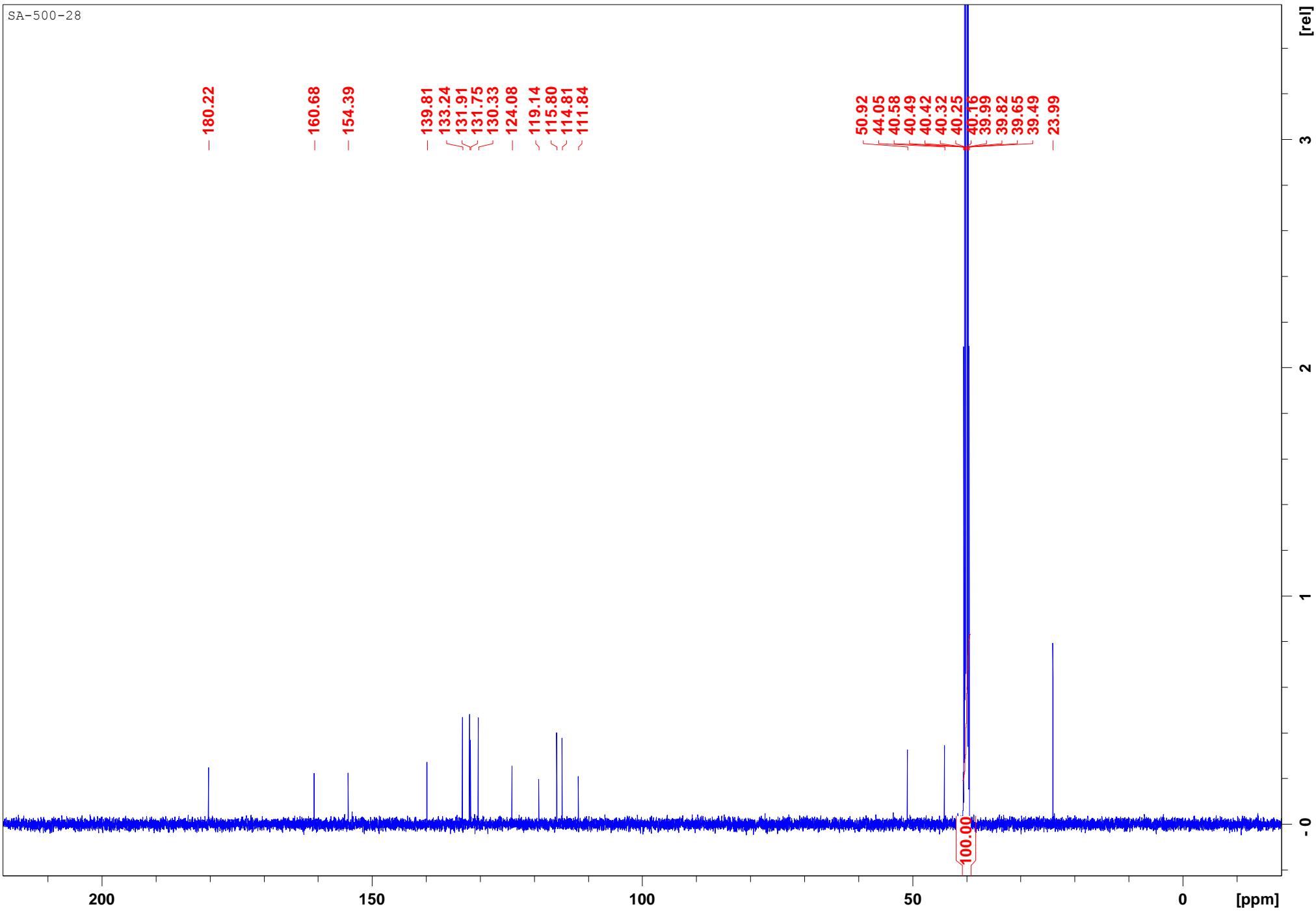
SA-500-28



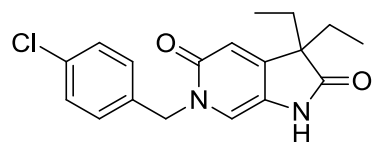
15p



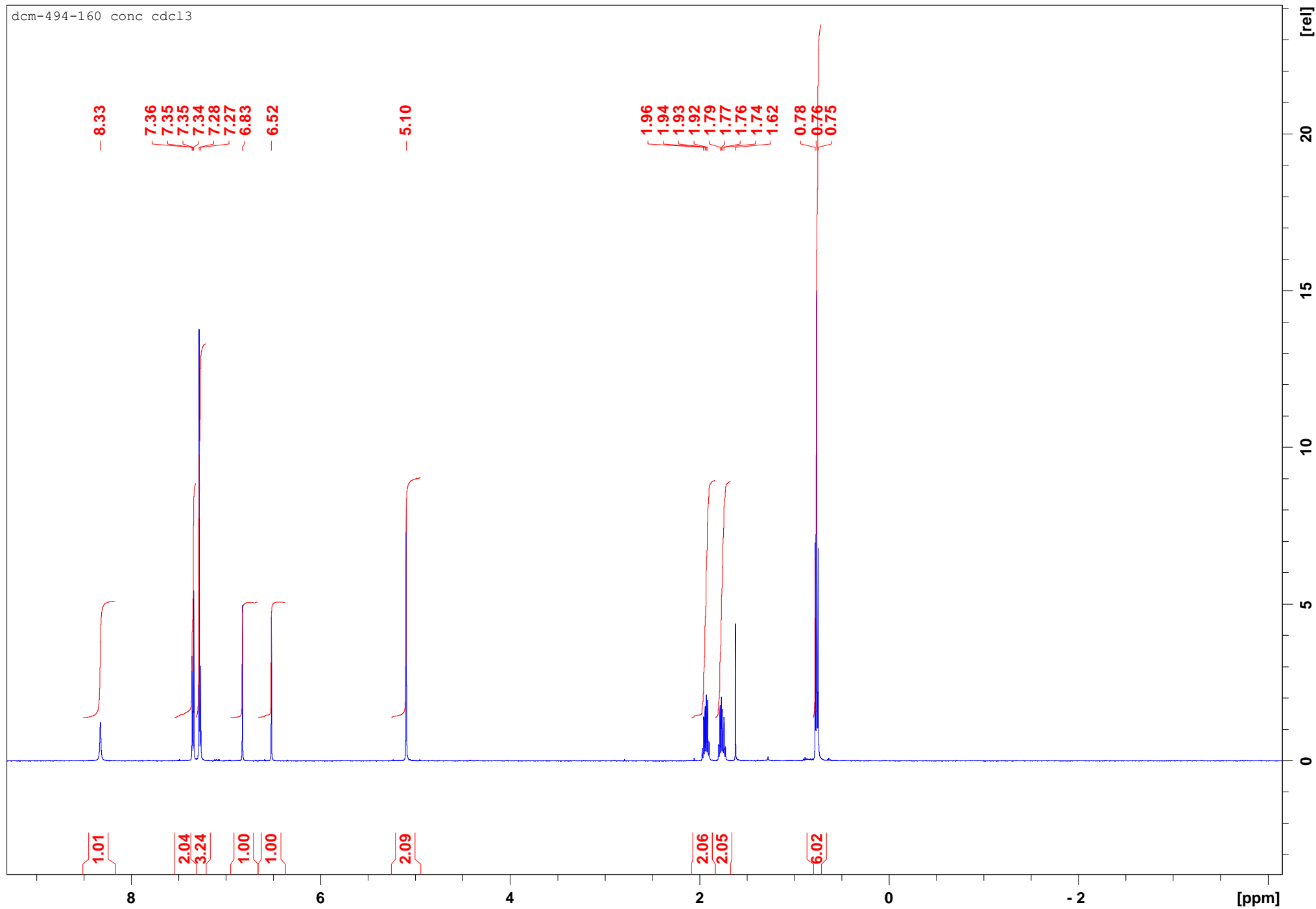
SA-500-28 15 1 "V:\Old Server\SA\nmr"



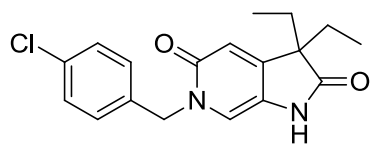
16a



"dcm-494-160 conc cdcl3" 10 1 X:\data\DCM\nmr

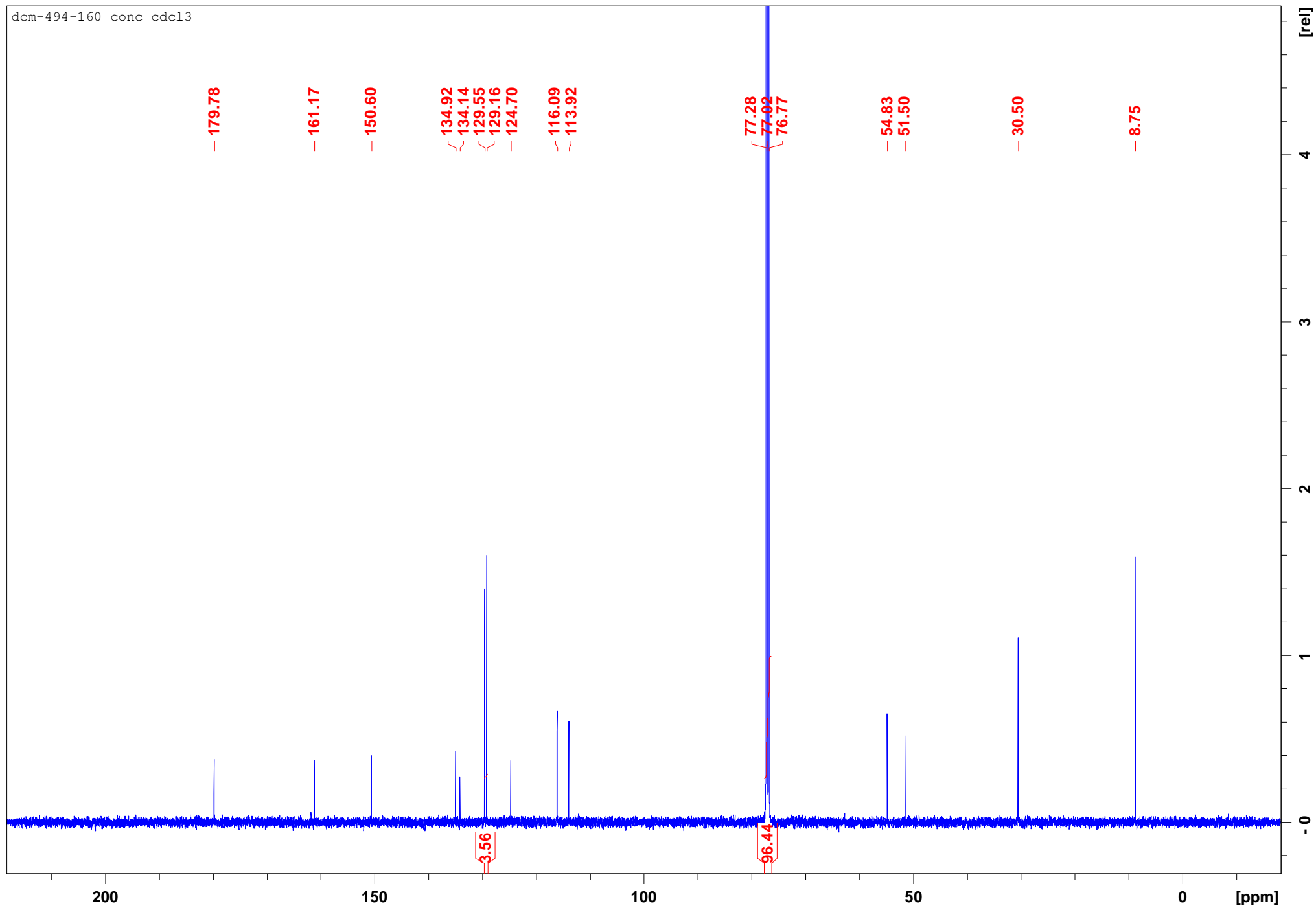


16a

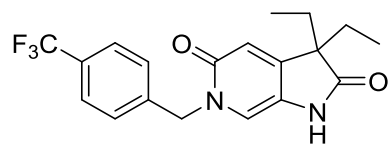


"dcm-494-160 conc cdcl3" 13 1 X:\data\DCM\nmr

dcm-494-160 conc cdcl3

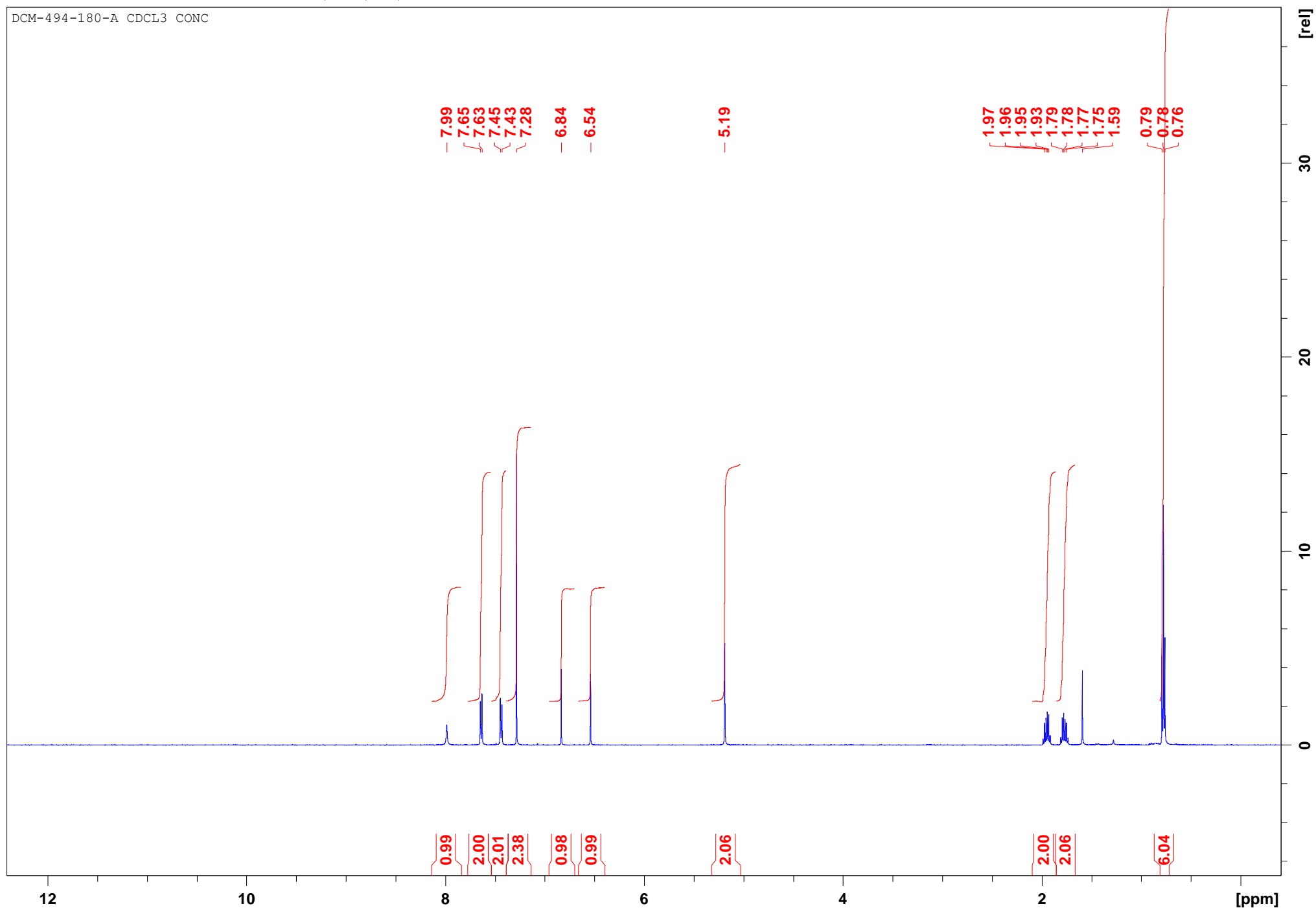


16b

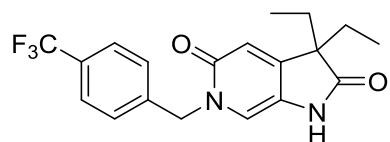


"DCM-494-180-A CDCL3 CONC" 10 1 X:\data\DCM\nmr

DCM-494-180-A CDCL3 CONC

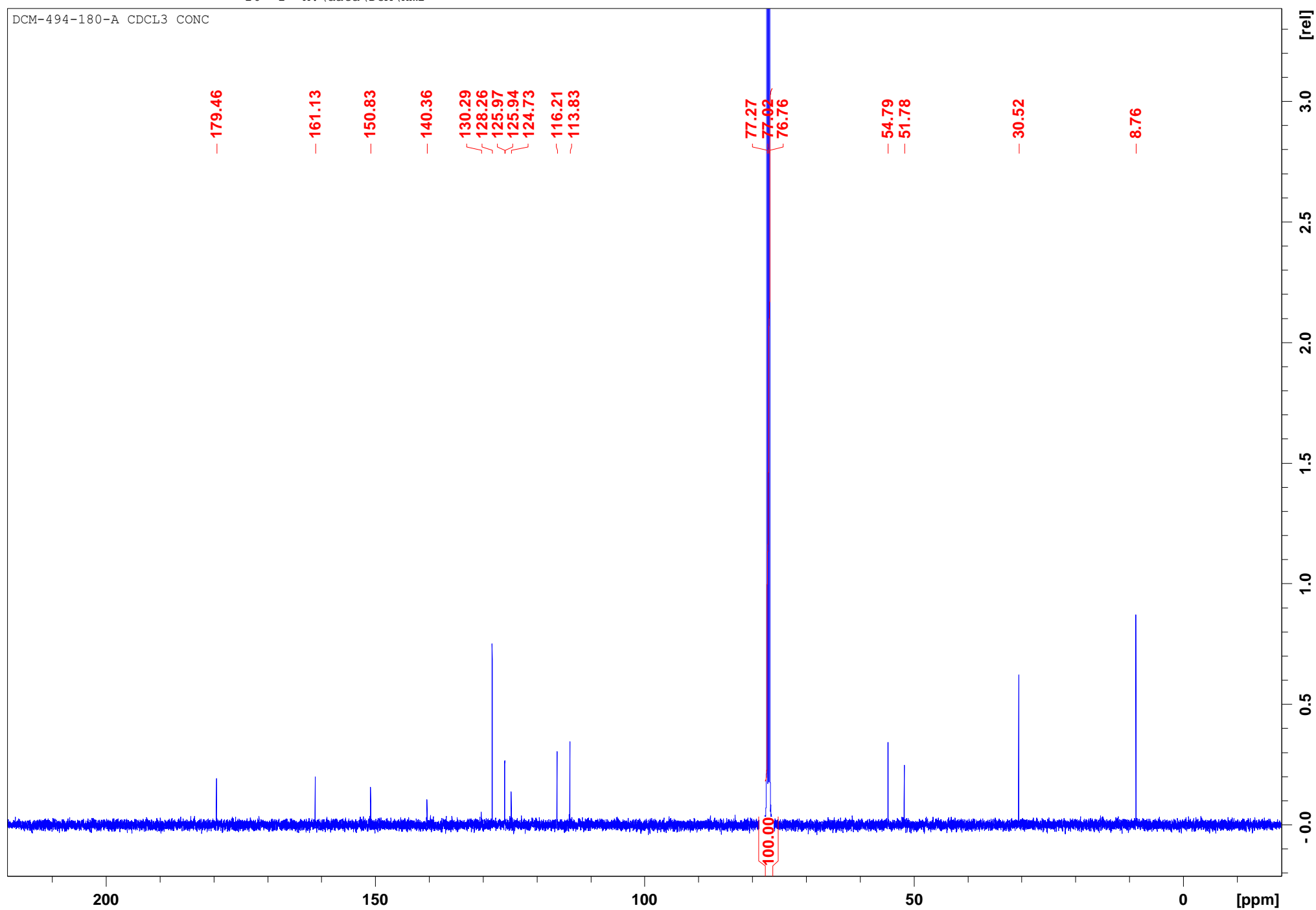


16b

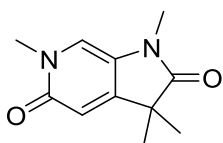


"DCM-494-180-A CDCL3 CONC" 16 1 X:\data\DCM\nmr

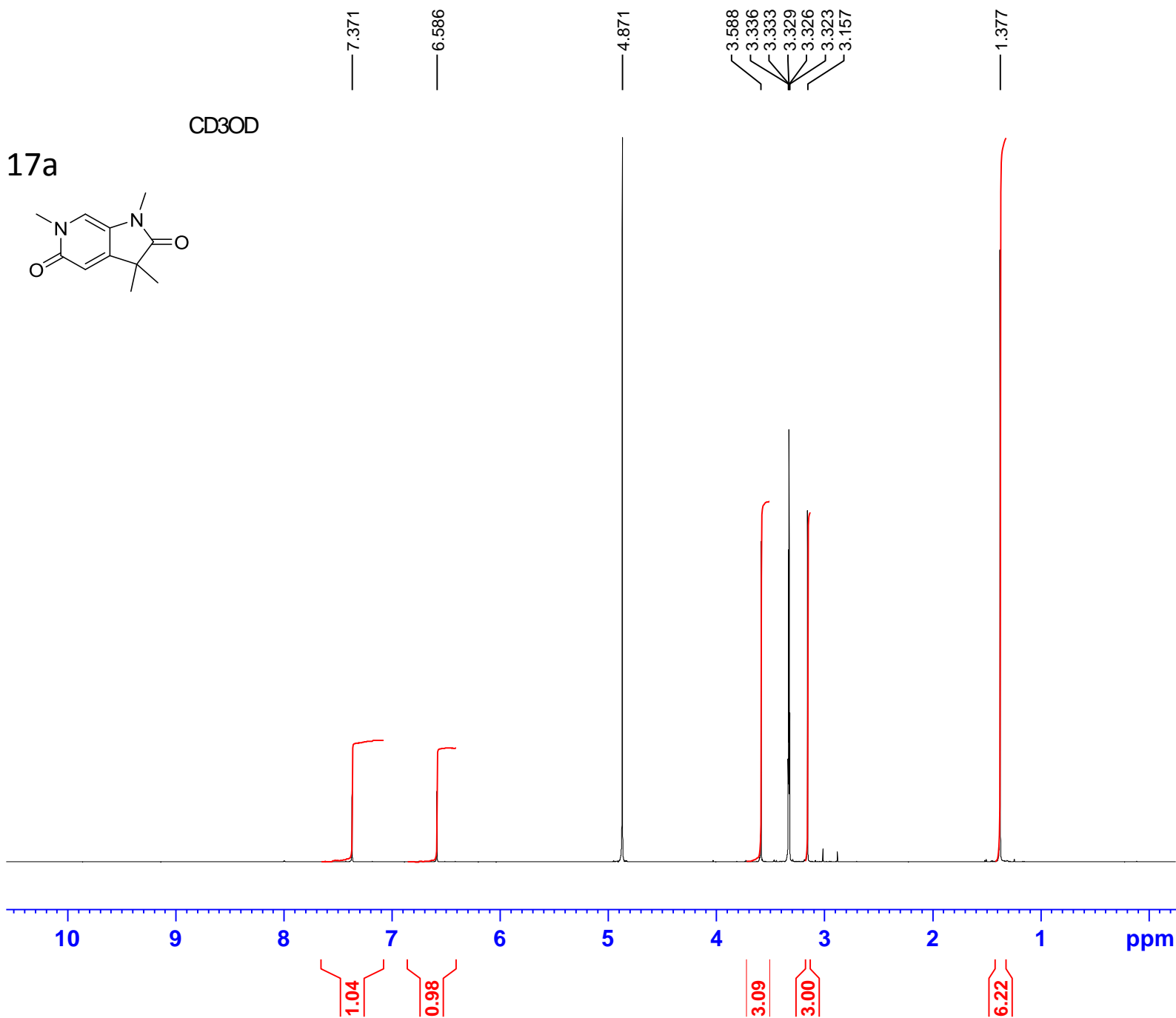
DCM-494-180-A CDCL3 CONC



17a



CD3OD

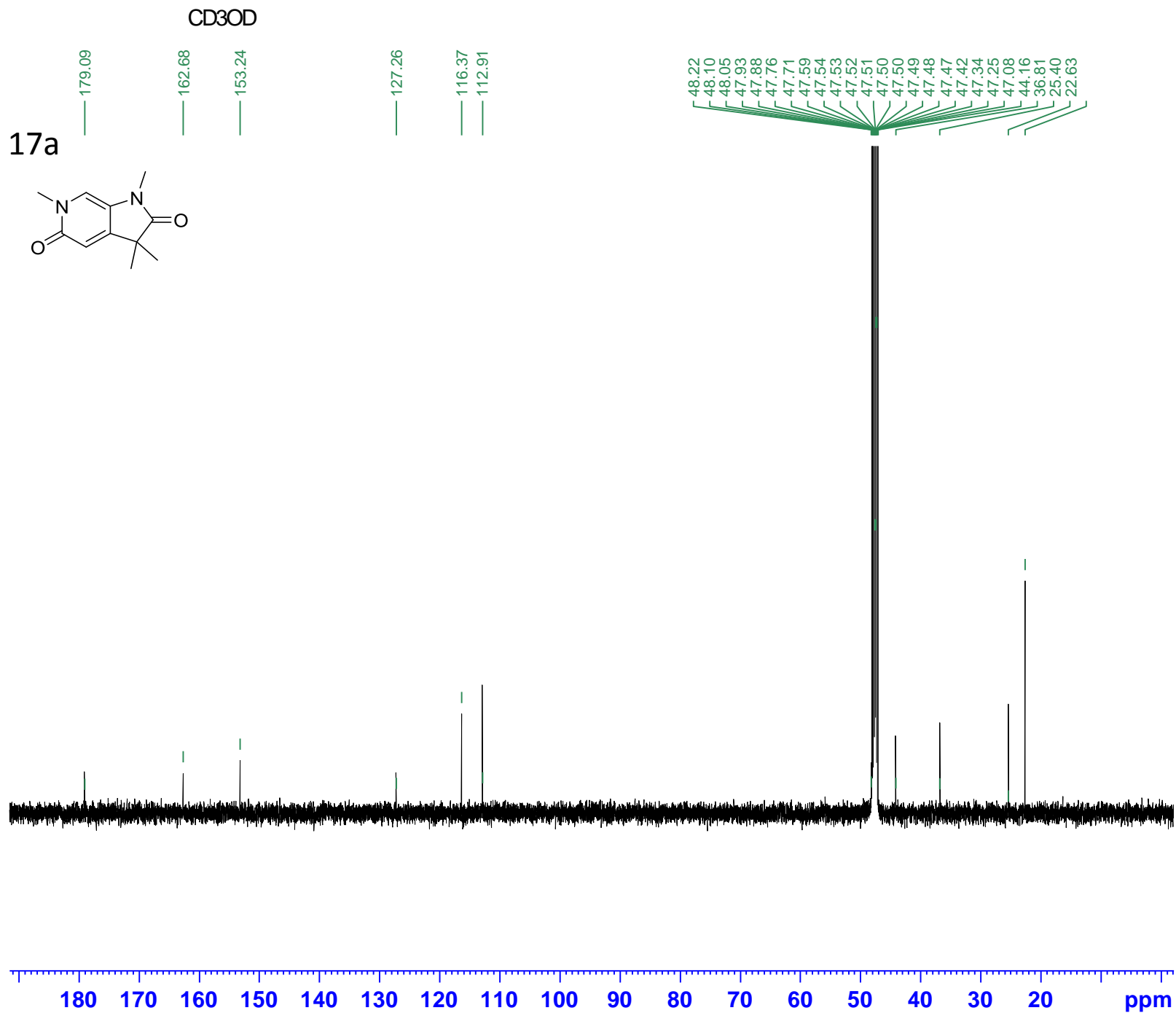


Current Data
 NAME DCM-494-23-A CD3OD
 EXPNO 10
 PROCNO 1

F2 - Acquisition
 Parameters 20140908
 Time 13.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 575
 DW 48.400 usec
 DE 11.99 usec
 TE 297.9 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

F2 - Processing parameters SI
 65536
 SF 500.3000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME DCM-494-23-A CD3OD
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20140909
 Time 2.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

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

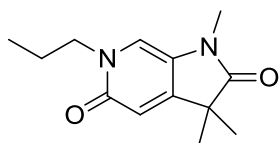
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

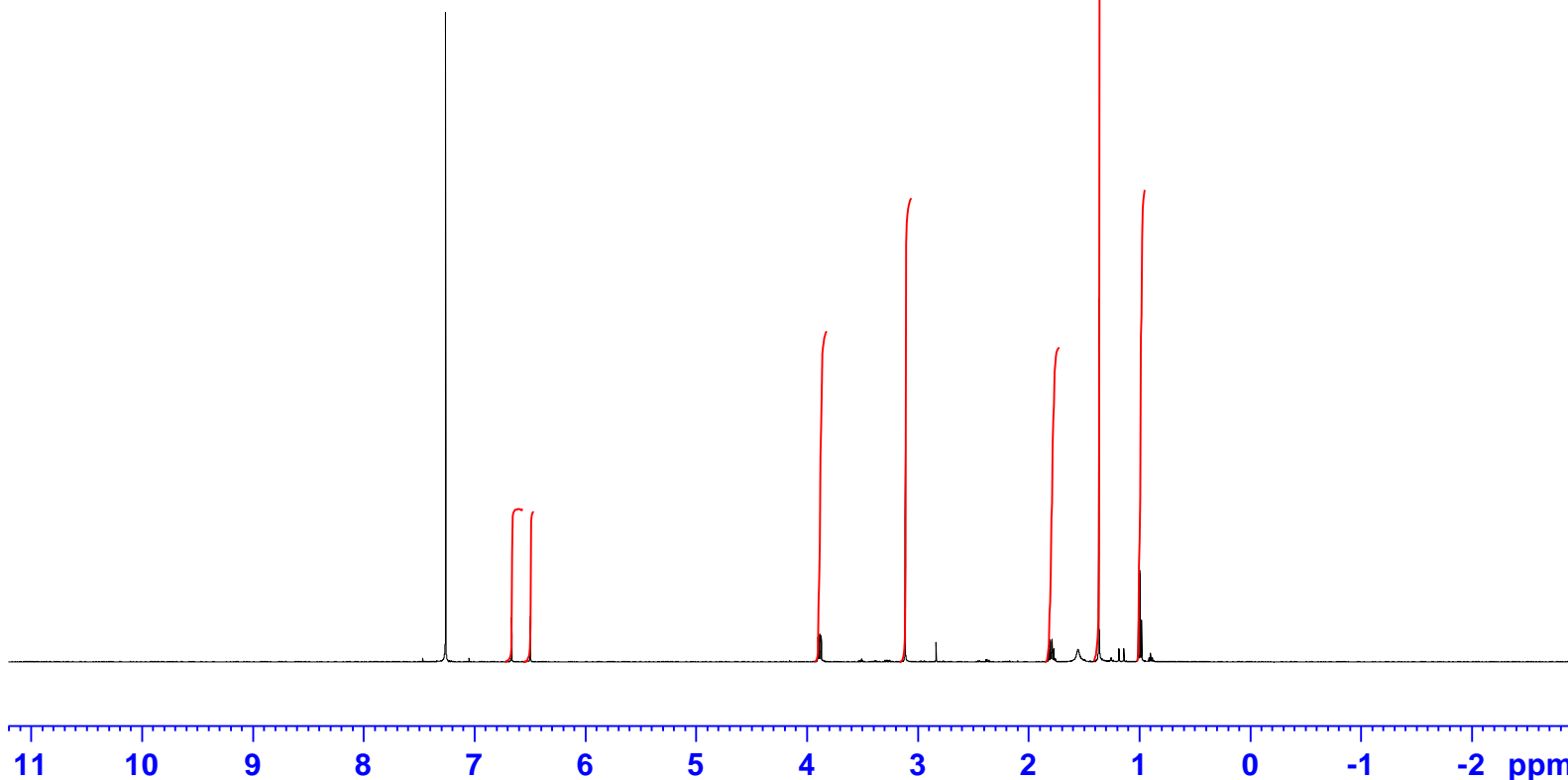
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17b

CDCl₃

7.260
6.665
6.497
6.496
3.900
3.885
3.870
3.113
1.365
1.010
0.995
0.980



11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm

1.00
0.98
2.16
3.04
2.06
6.33
3.10



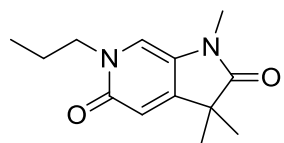
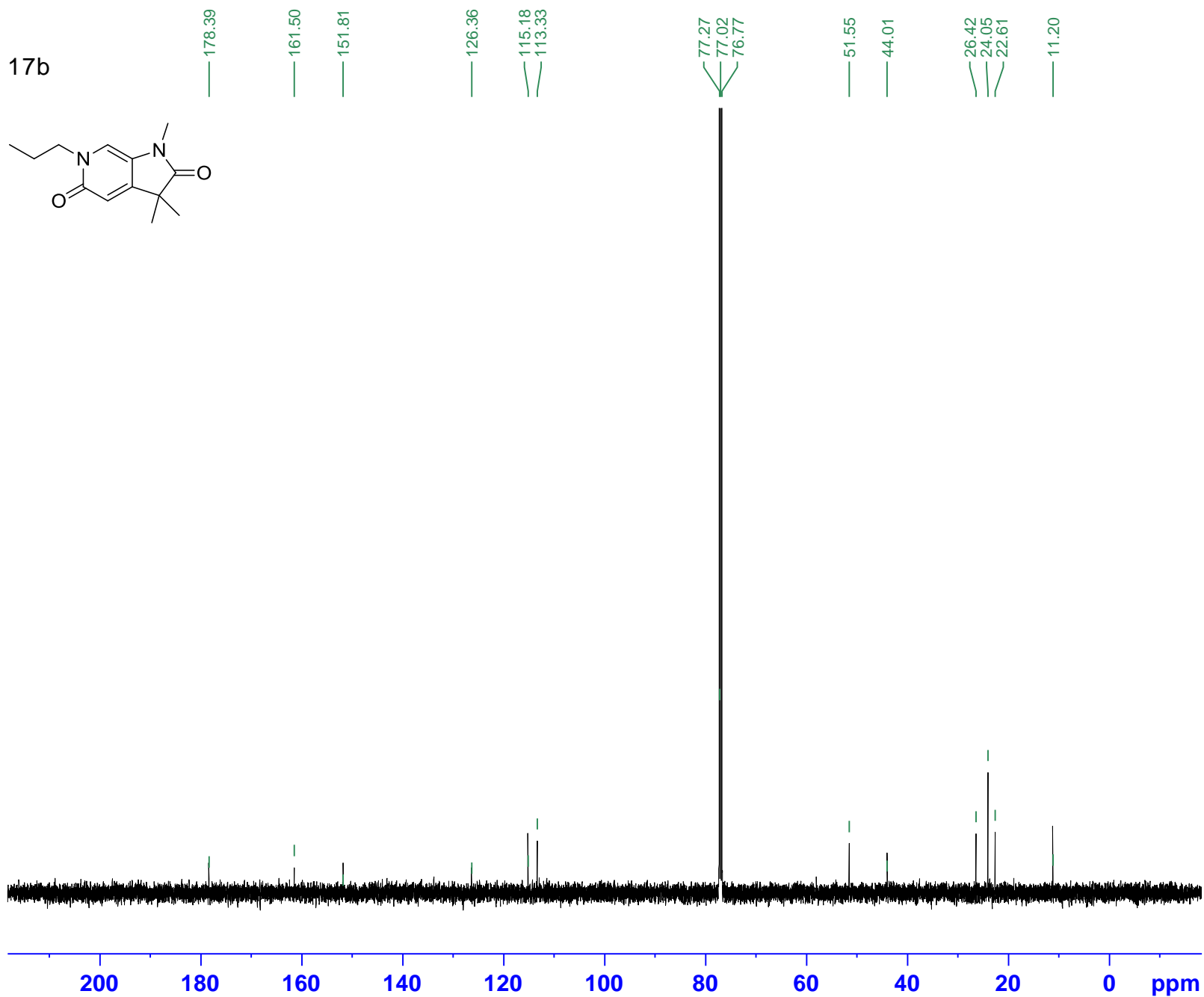
Current Data
NAME DCM-494-115-A CDCl₃
EXPNO 10
PROCNO 1

F2 - Acquisition
Date_ 20141126
Time 9.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 812
DW 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17b

CDCL₃

Current Data Parameters
 NAME DCM-494-114-A CDCL₃
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141209
 Time 12.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 256
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

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

SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

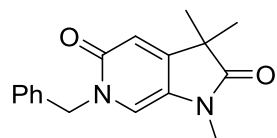
===== CHANNEL f2 =====

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



17c

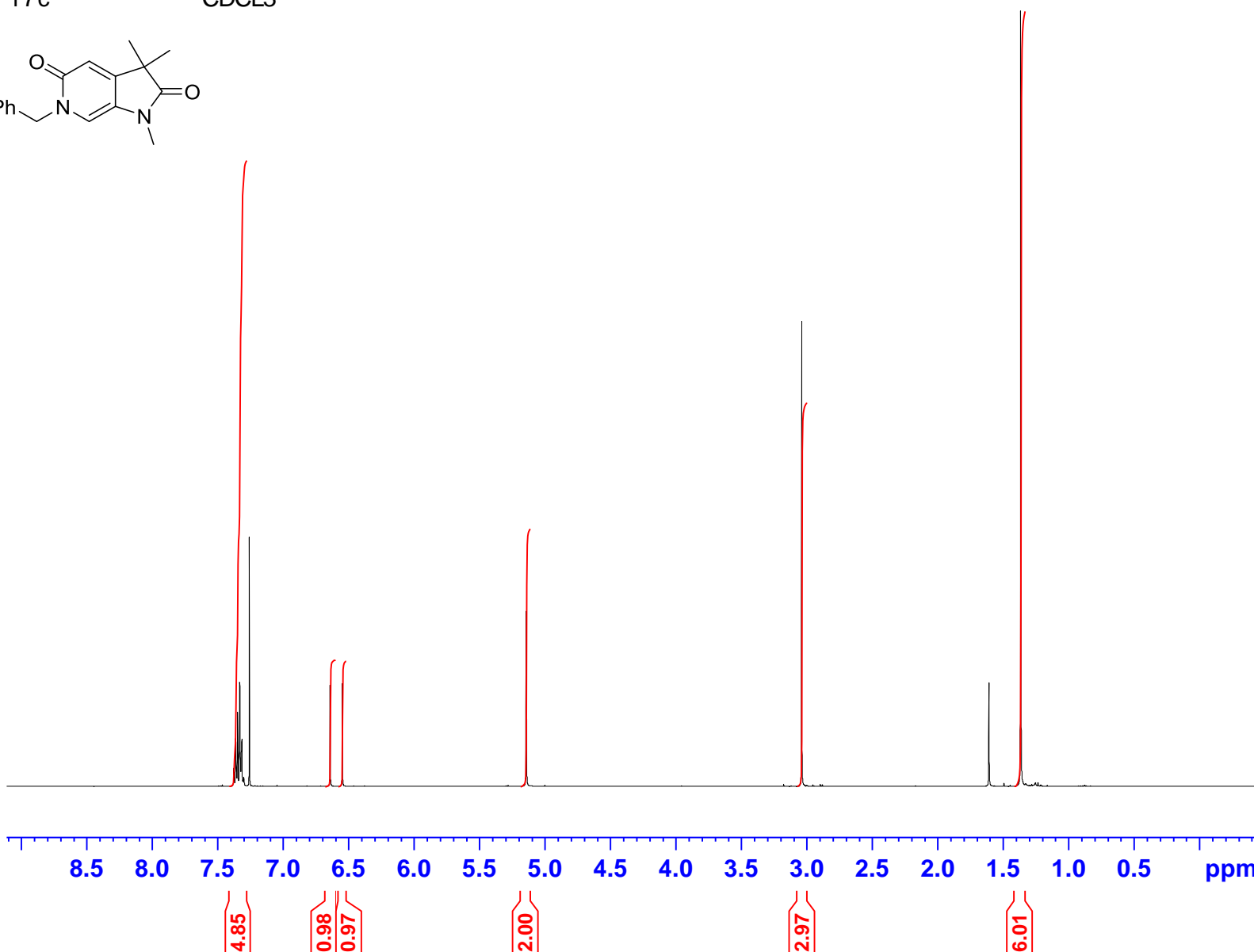
CDCl₃7.375
7.358
7.2856.668
6.575

5.169

3.065

1.634

1.391



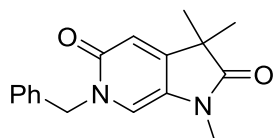
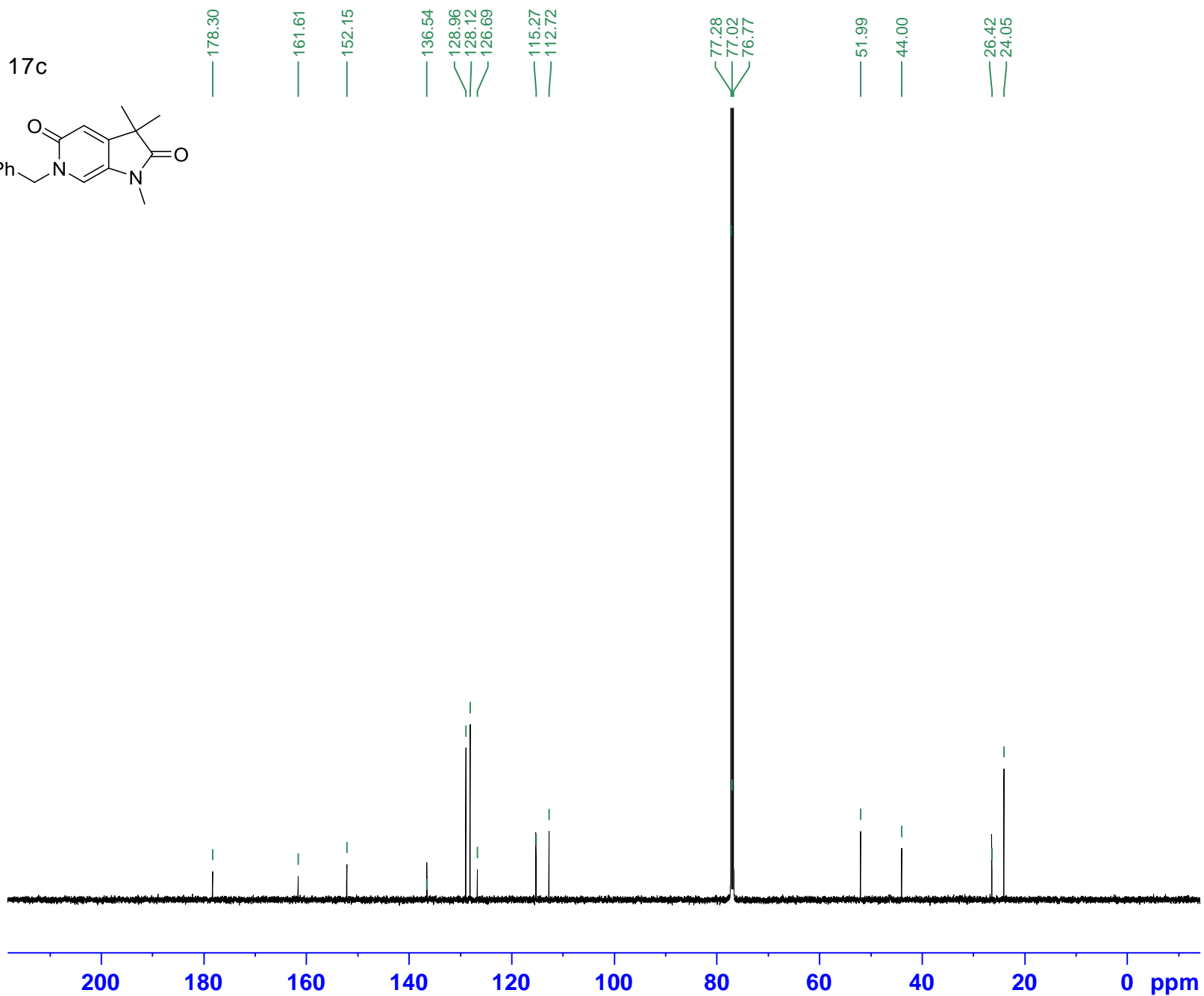
Current Data Parameters
NAME DCM-494-75-A CDCl₃ CONC
EXPNO 11
PROCNO 1

F2 - Acquisition
Parameters 20141029
Time 8.38
INSTRUM spect
PROBHD 5 mmPABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 575
DV 48.400 usec
DE 11.99 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing
Parameters 65536
S 500.3000125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17c

CDCL₃

Current Data Parameters
 NAME DCM-494-75-A CDCL₃ CONC
 EXPNO 10
 PROCNO 1

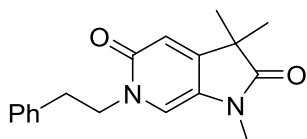
F2 - Acquisition Parameters
 Date_Time 20141029
 Time 6.35
 INSTRUM spect
 PROBHD 5 mmPABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVEN CDCL₃
 TNS 2048
 DS 2
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.3899939 W

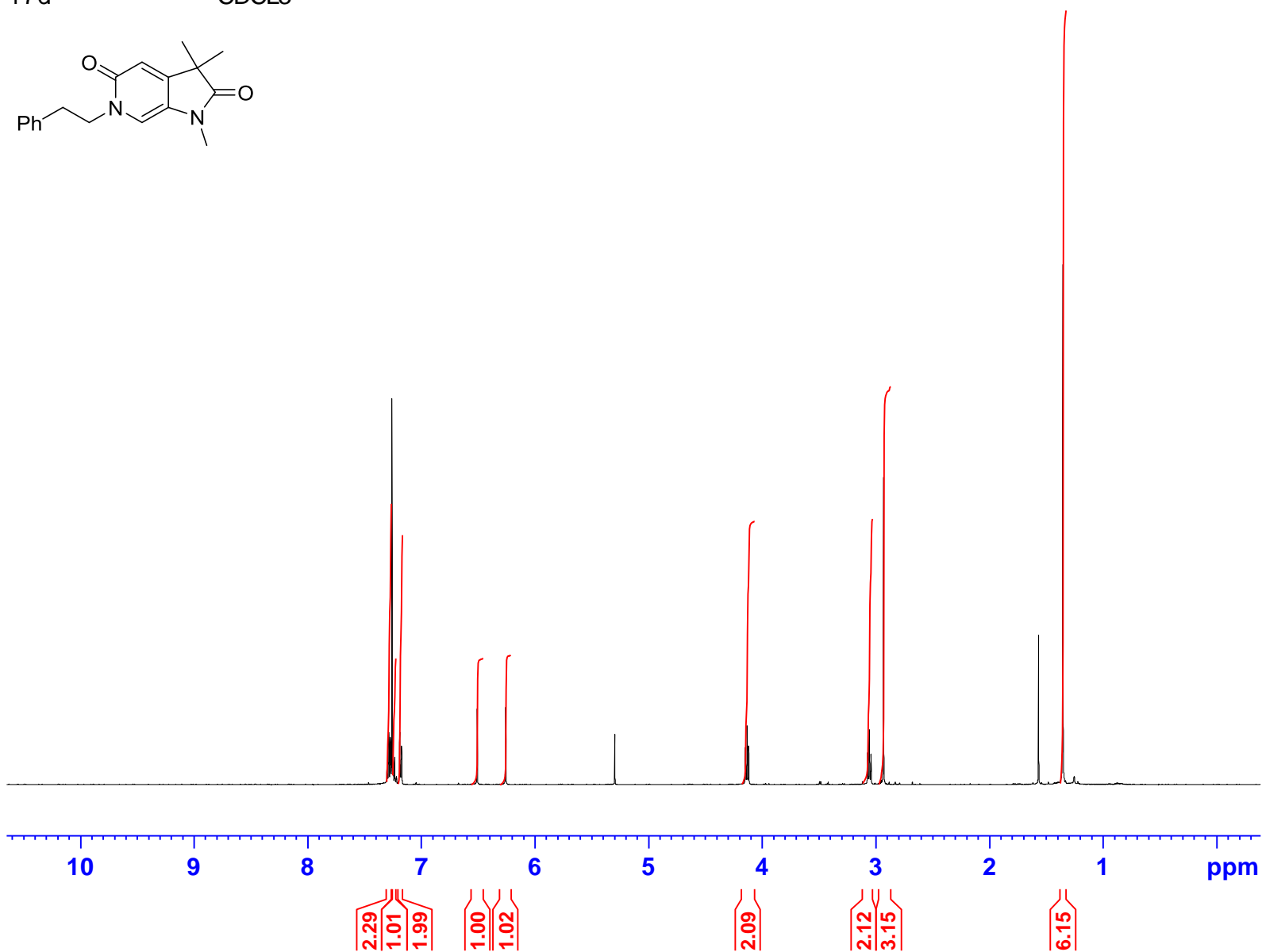
===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing parameters
 S1 65536
 SF 125.8005350 MHz
 VDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17d

CDCL₃

7.288
7.273
7.259
7.192
7.189
7.176
— 6.509
— 6.258
— 5.298
4.148
4.134
4.119
3.057
2.933
1.568
1.354



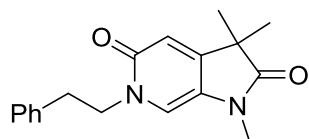
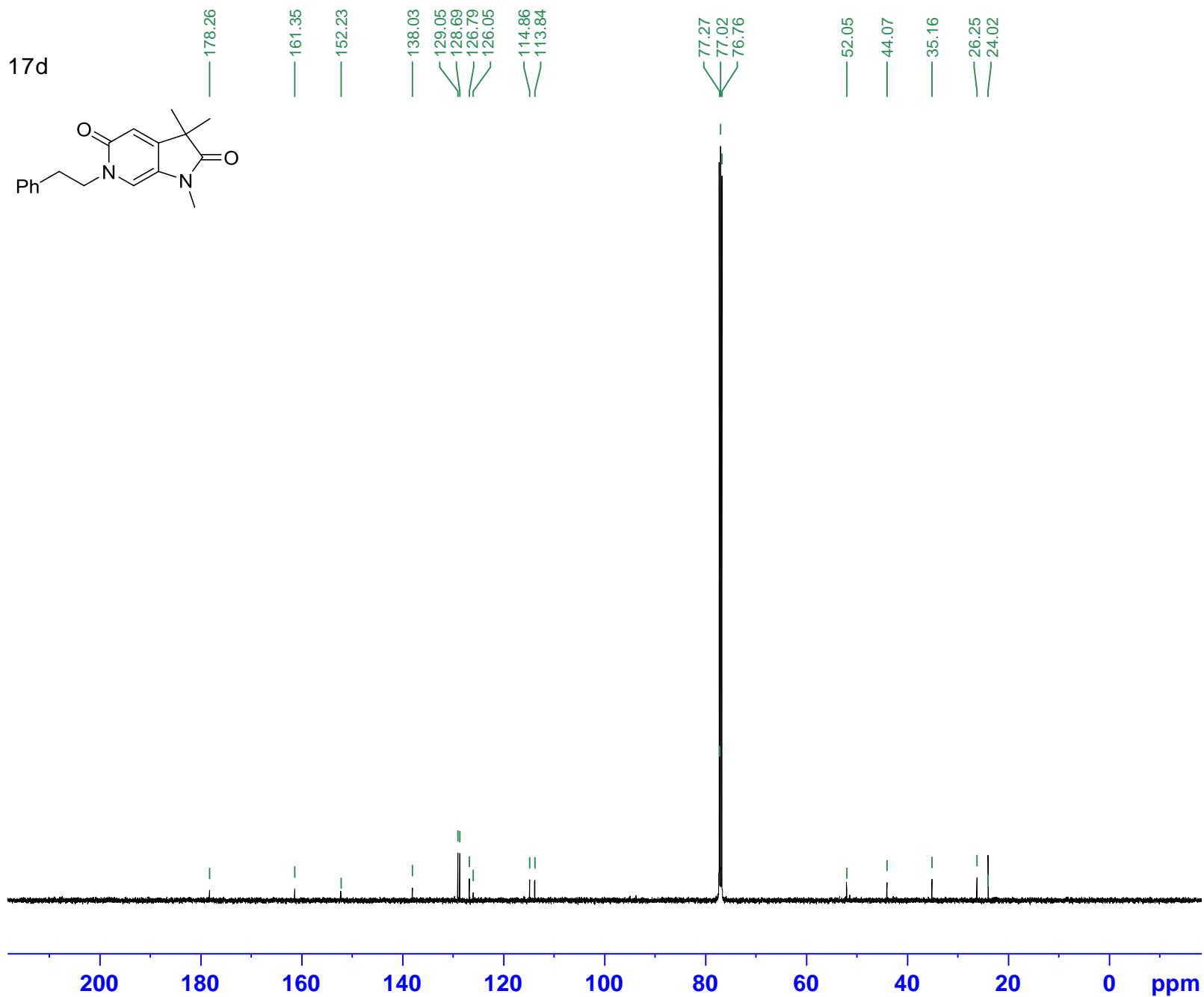
Current Data
NAME DCM-494-103-A CDCL₃
EXPNO 10
PROCNO 1

F2 - Acquisition
Date_ 20141119
Time 16.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DW 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17d

CDCL₃

Current Data Parameters
 NAME DCM-494-103-A CDCL₃
 EXPNO 14
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141121
 Time 1.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCL₃
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.5 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

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

SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

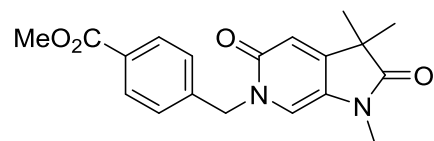
===== CHANNEL f2 =====

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

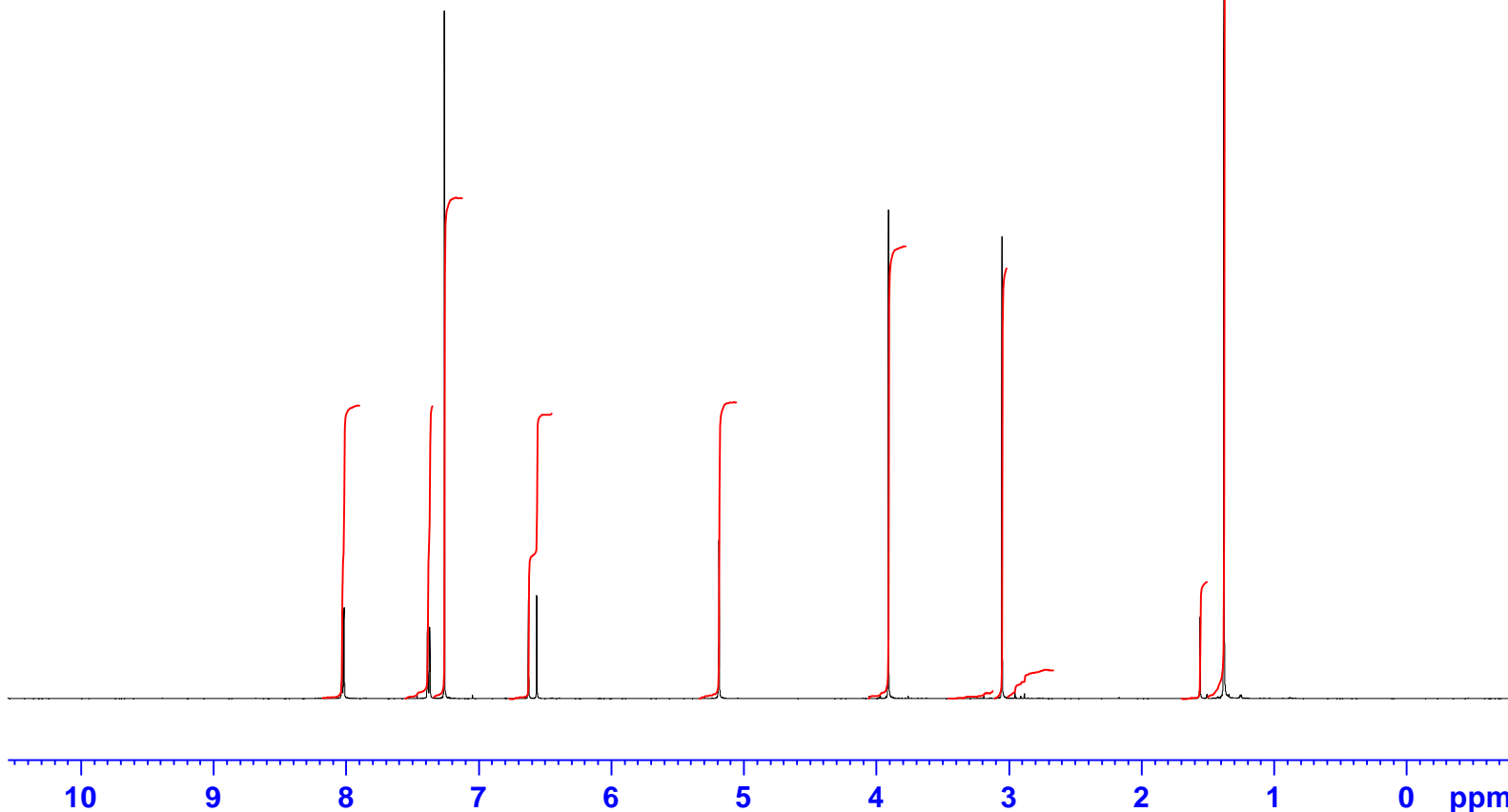
F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



17e

CDCl₃

8.034
8.017
7.387
7.370
7.259
6.625
6.563
5.188
3.910
3.053
1.559
1.378



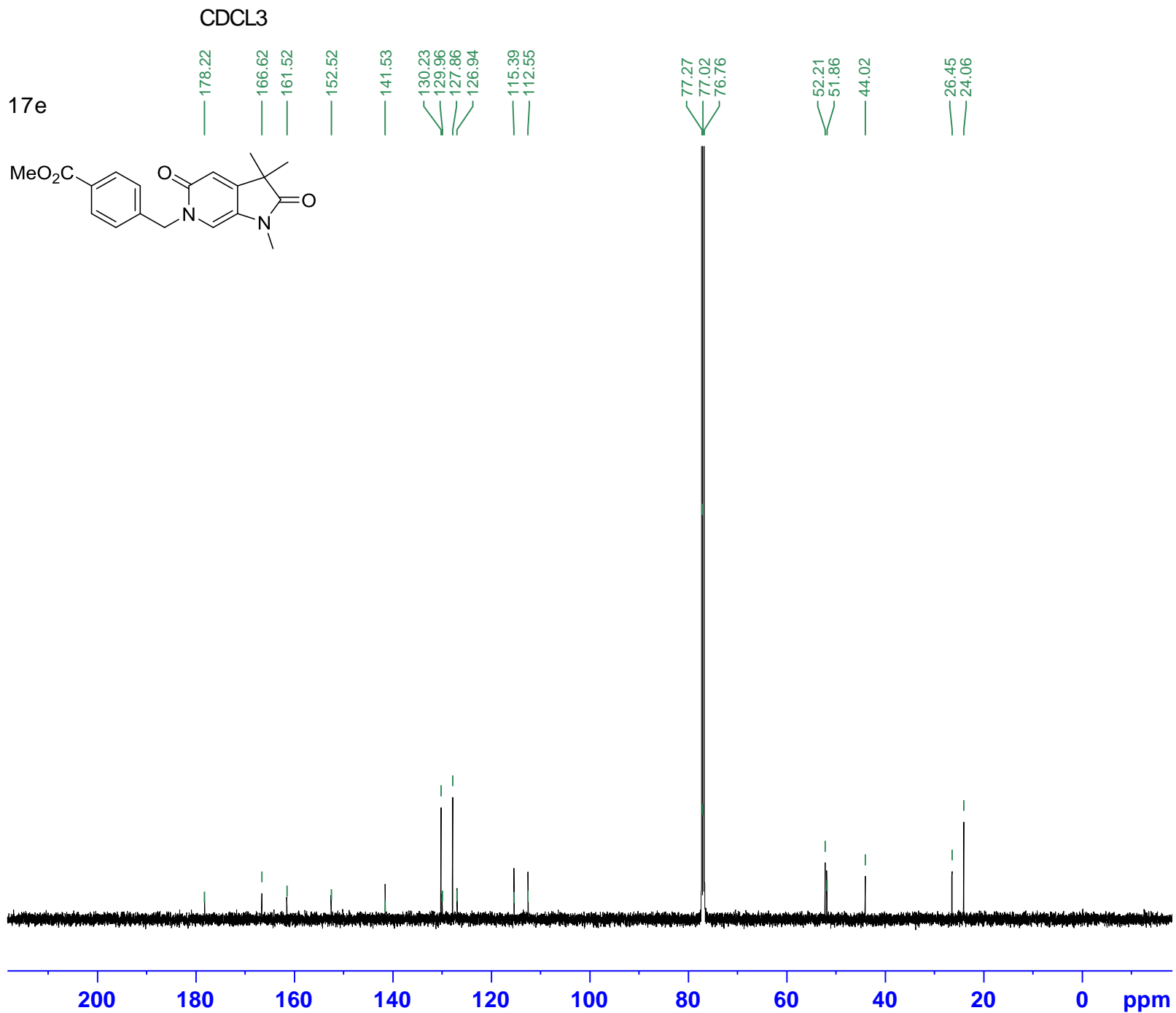
1.98
1.98
3.37
1.92
2.00
3.05
0.05
2.91
0.19
0.82
6.29

Current Data
NAME DCM-494-117-A CDCl₃
EXPNO 10
PROCNO 1

F2 - Acquisition
Data parameters 20141204
Time 9.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 724
DW 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000125 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME DCM-494-117-A CDCL₃
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141204
 Time 19.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

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

SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

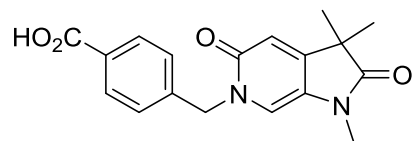
===== CHANNEL f2 =====

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

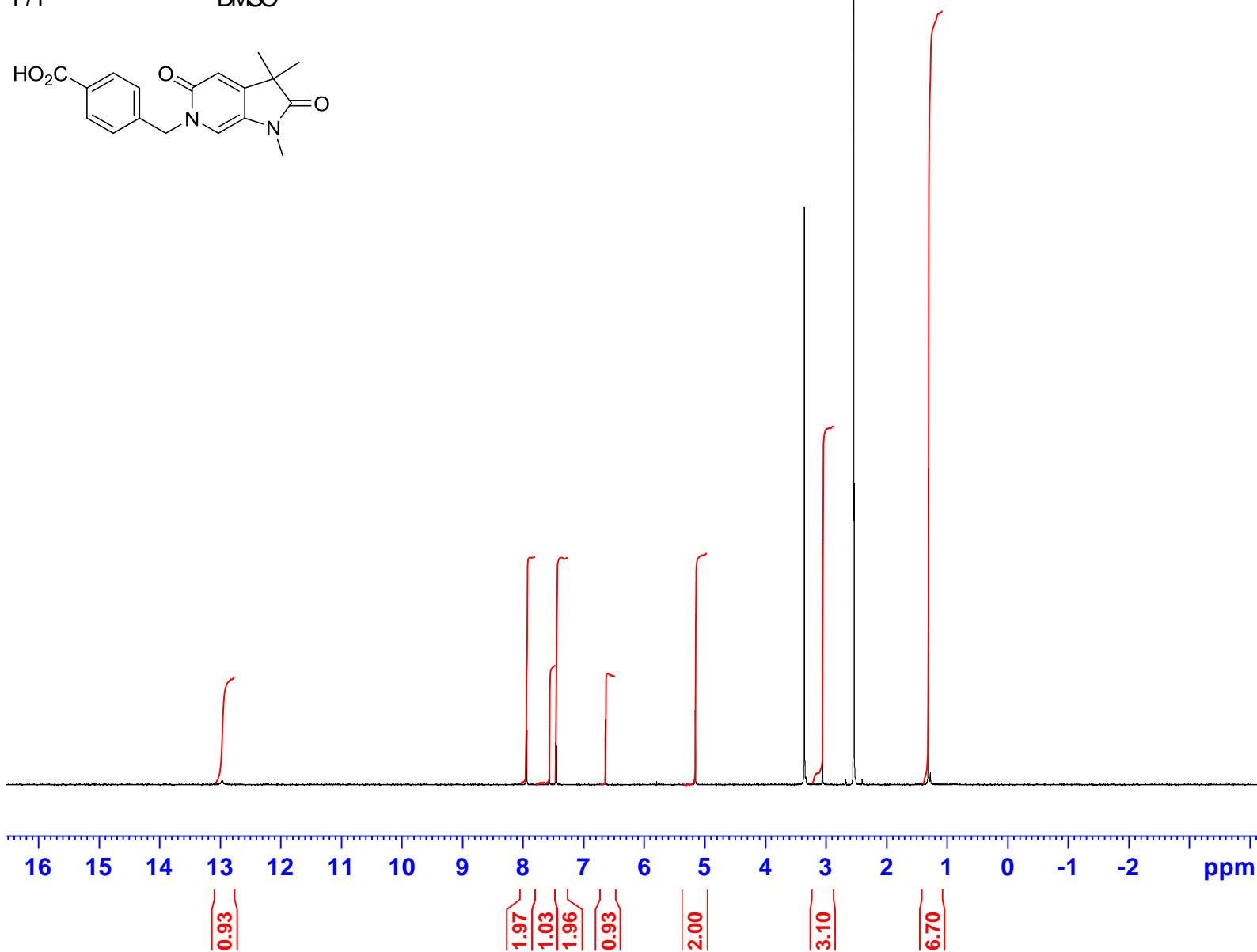
F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17f

DMSO



7.953
7.936
7.565
7.463
7.446
6.641
— 5.156
3.354
3.055
2.547
2.543
2.540
2.536
2.532
1.309



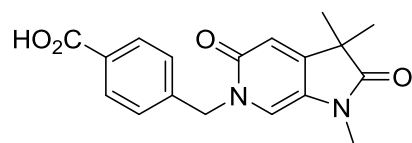
Current Data
NAME DCM-494-119-A DMSO
EXPNO 10
PROCNO 1

F2 - Acquisition
Date_ 20141208
Time 16.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 812
DW 48.400 usec
DE 11.99 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.2999843 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17f



DMSO

177.92

167.55

160.94

152.70

142.91

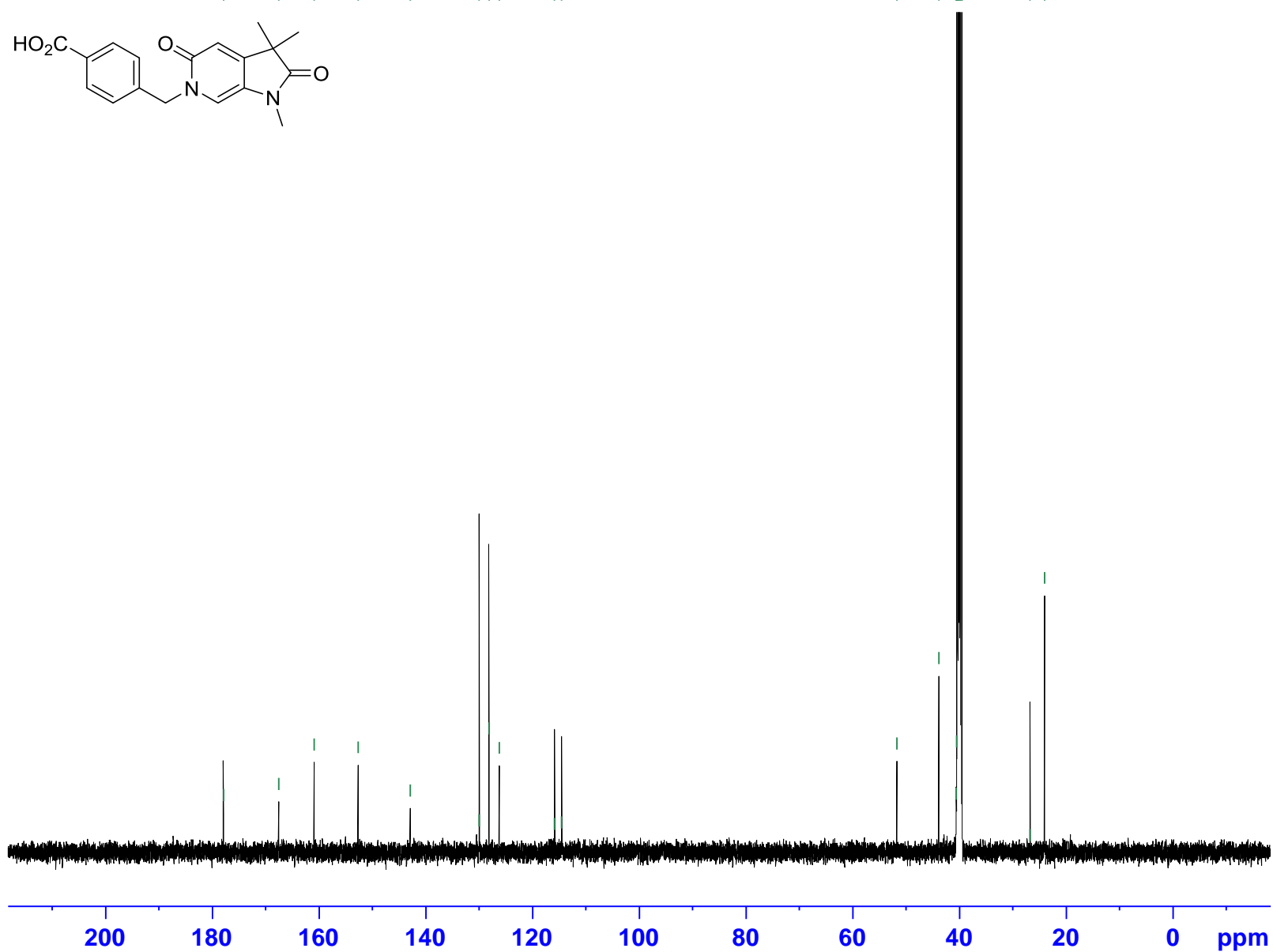
129.99

128.16

126.23

115.86

114.55

 51.71
 43.88
 40.60
 40.51
 40.43
 40.34
 40.27
 40.18
 40.01
 39.84
 39.68
 39.51
 26.77
 24.04


Current Data Parameters
 NAME DCM-494-119-A DMSO
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20141209
 Time 5.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 2
 S/MH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

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

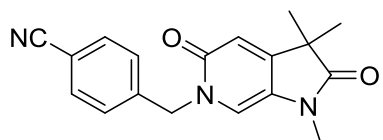
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

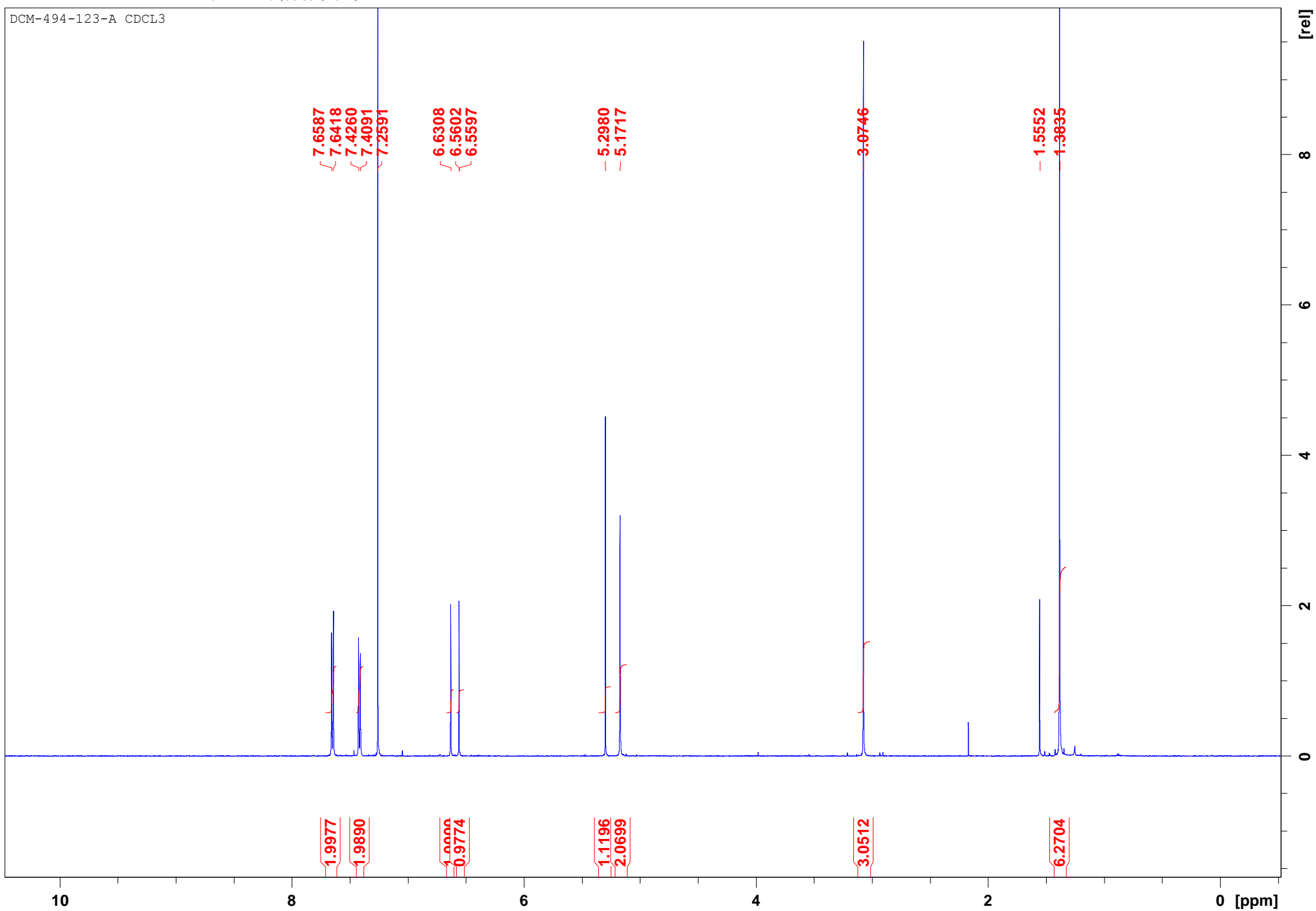
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

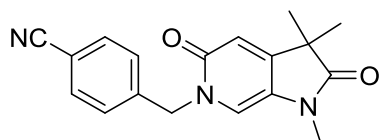
17g



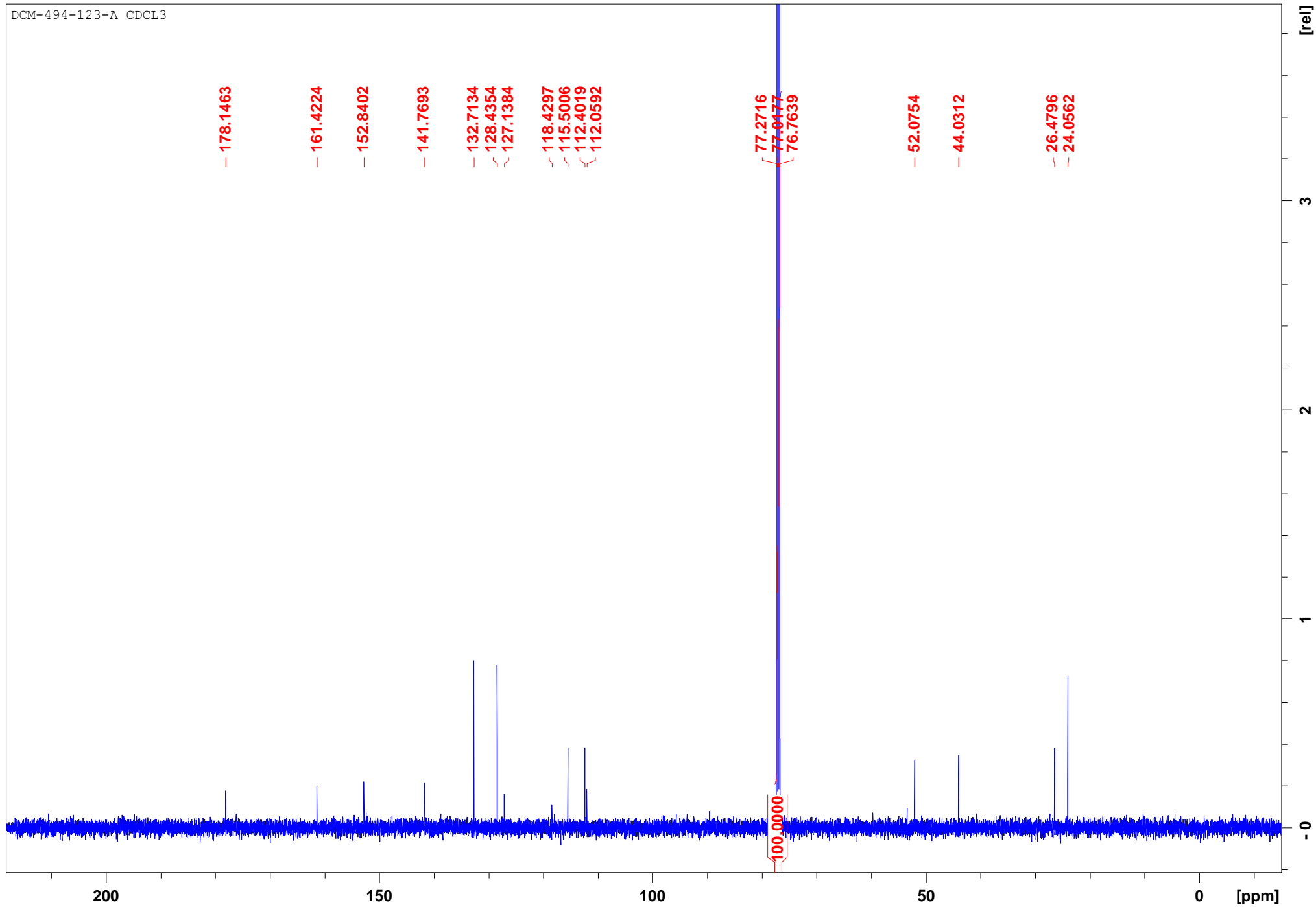
"DCM-494-123-A CDCL3" 10 1 z:\data\DCM\nmr



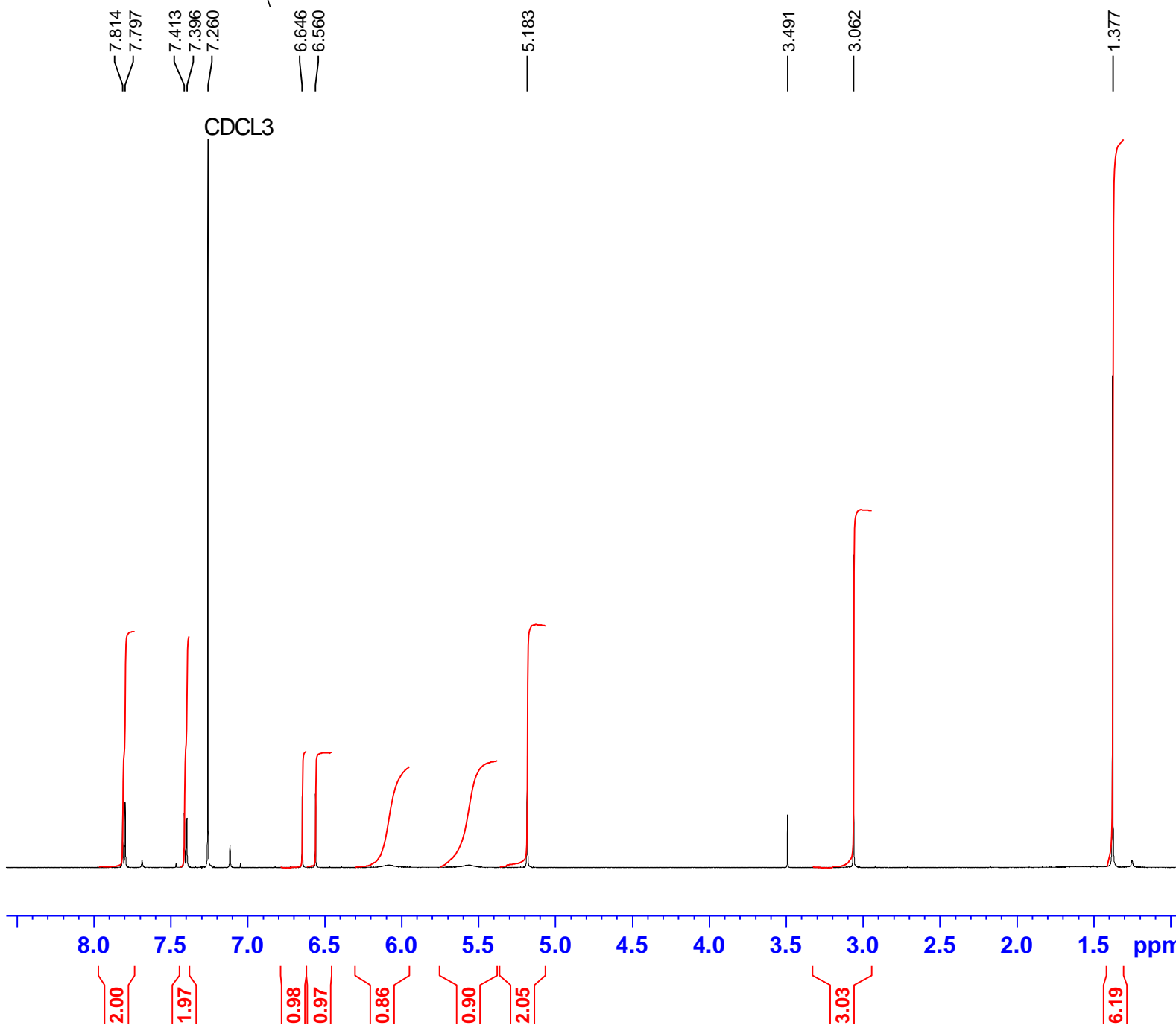
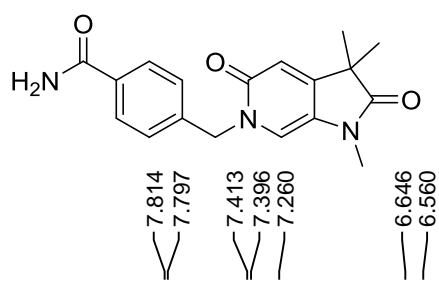
17g



"DCM-494-123-A CDCL3" 11 1 z:\data\DCM\nmr



17h



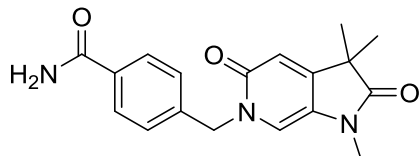
Current Data
 NAME DCM-494-147-B CDCL3
 EXPNO 10
 PROCNO 1

F2 - Acquisition
 Parameters 20150129
 Time 14.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 724
 DW 48.400 usec
 DE 11.99 usec
 TE 293.5 K
 D1 1.00000000 sec
 TD0 1

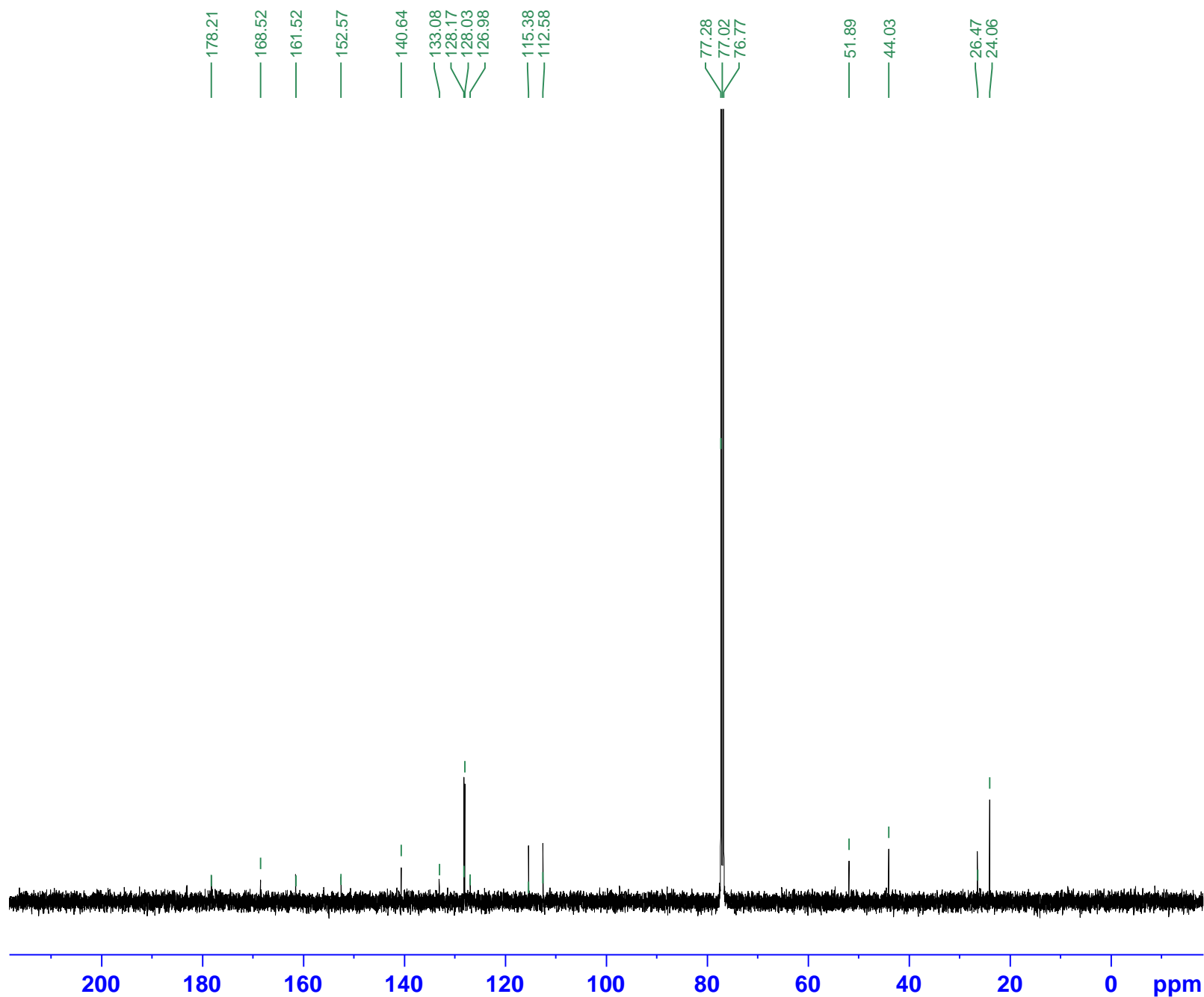
===== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

F2 - Processing parameters SI
 65536
 SF 500.3000124 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

17h



DCM-494-147-B CDCL3



Current Data Parameters
 NAME DCM-494-147-B CDCL3
 EXPNO 11
 PROCNO 1

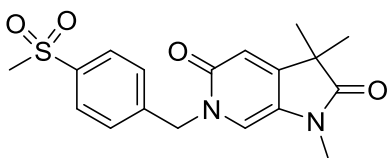
F2 - Acquisition
 Parameters Date_ 20150129
 Time 20.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 812
 DW 16.800 usec
 DE 7.68 usec
 TE 296.2 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

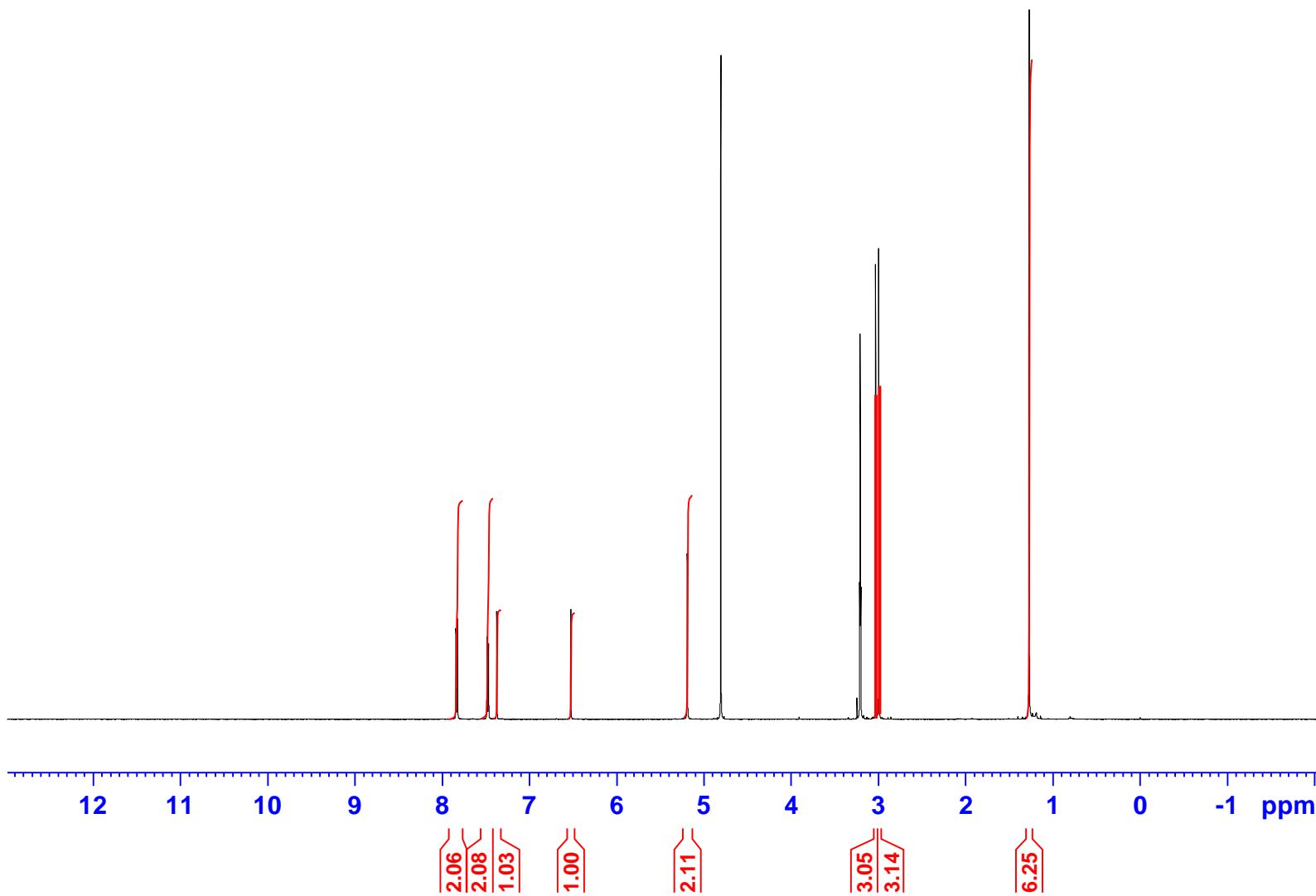
F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17i



SA-500-34

7.842
7.825
7.486
7.469
7.374
6.526
5.191
4.807
3.215
3.212
3.209
3.205
3.202
3.032
2.996
1.273



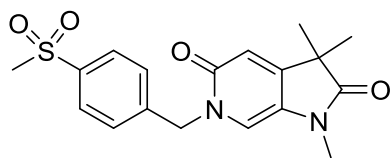
Current Data
NAME SA-500-34
EXPNO 10
PROCNO 1

F2 - Acquisition
Date_ 20150122
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 456
DW 48.400 usec
DE 11.99 usec
TE 292.3 K
D1 1.0000000 sec
TDO 1

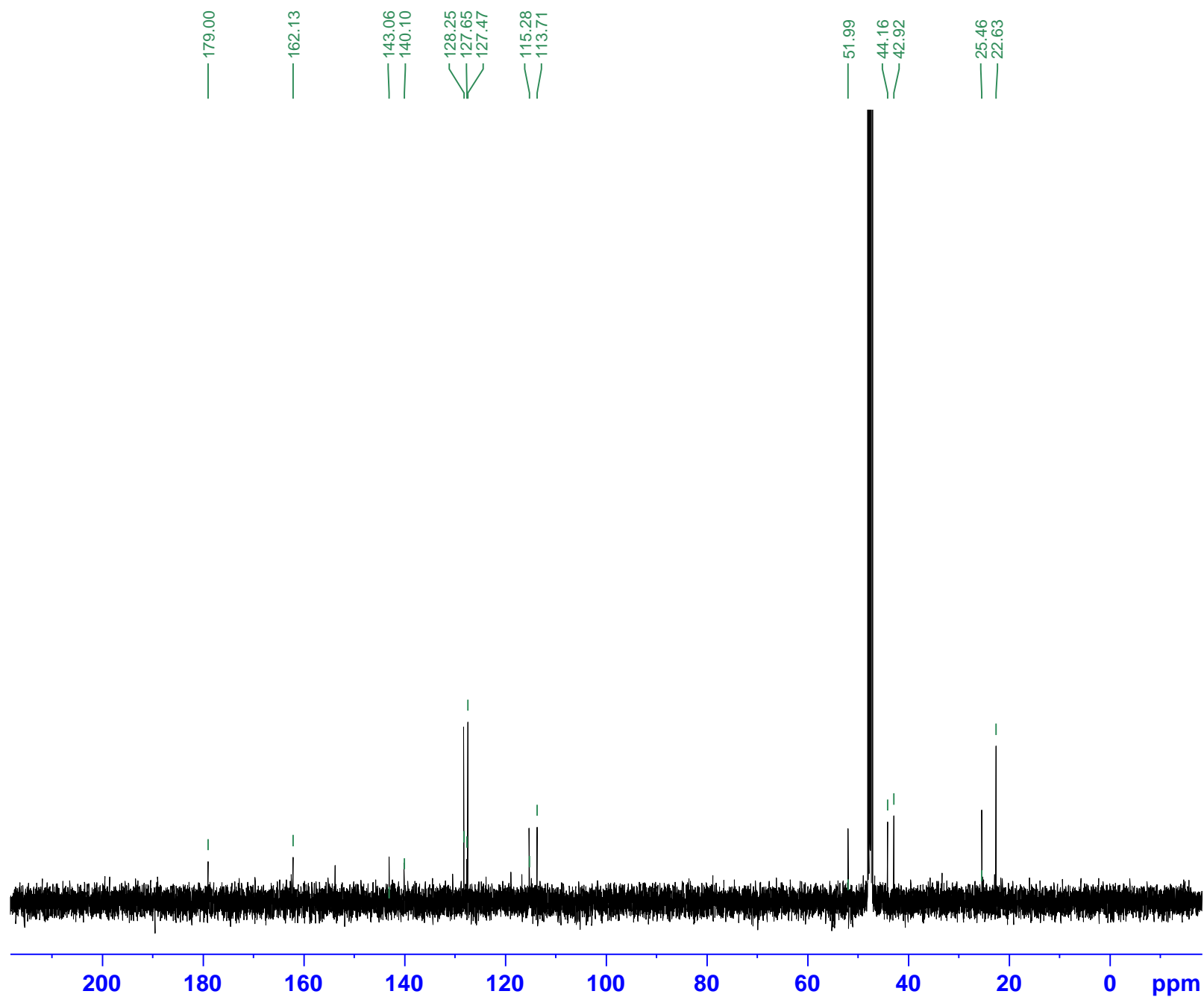
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.300603 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17i



SA-500-34



Current Data Parameters
NAME SA-500-34
EXPNO 11
PROCNO 1

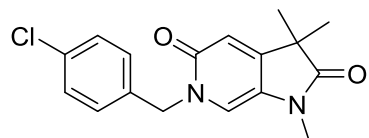
F2 - Acquisition
Parameters Date_ 20150122
Time 16.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 256
DS 2
SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 812
DV 16.800 usec
DE 7.68 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

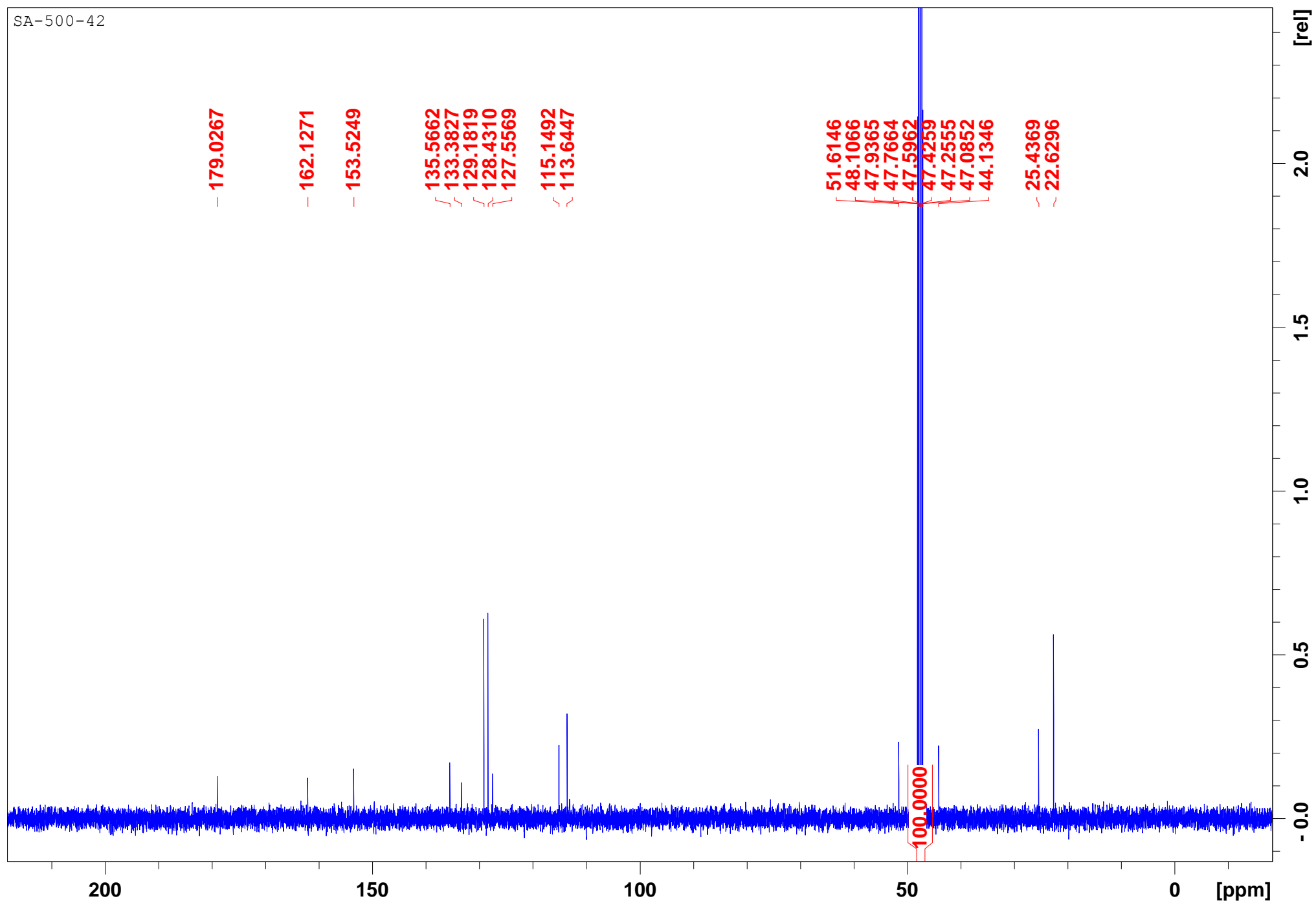
F2 - Processing
Parameters 65536
SF 125.8005350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

17j

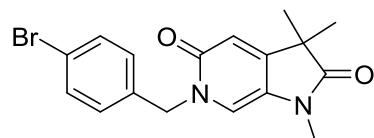


SA-500-42 11 1 z:\data\SA\nmr

SA-500-42



17k



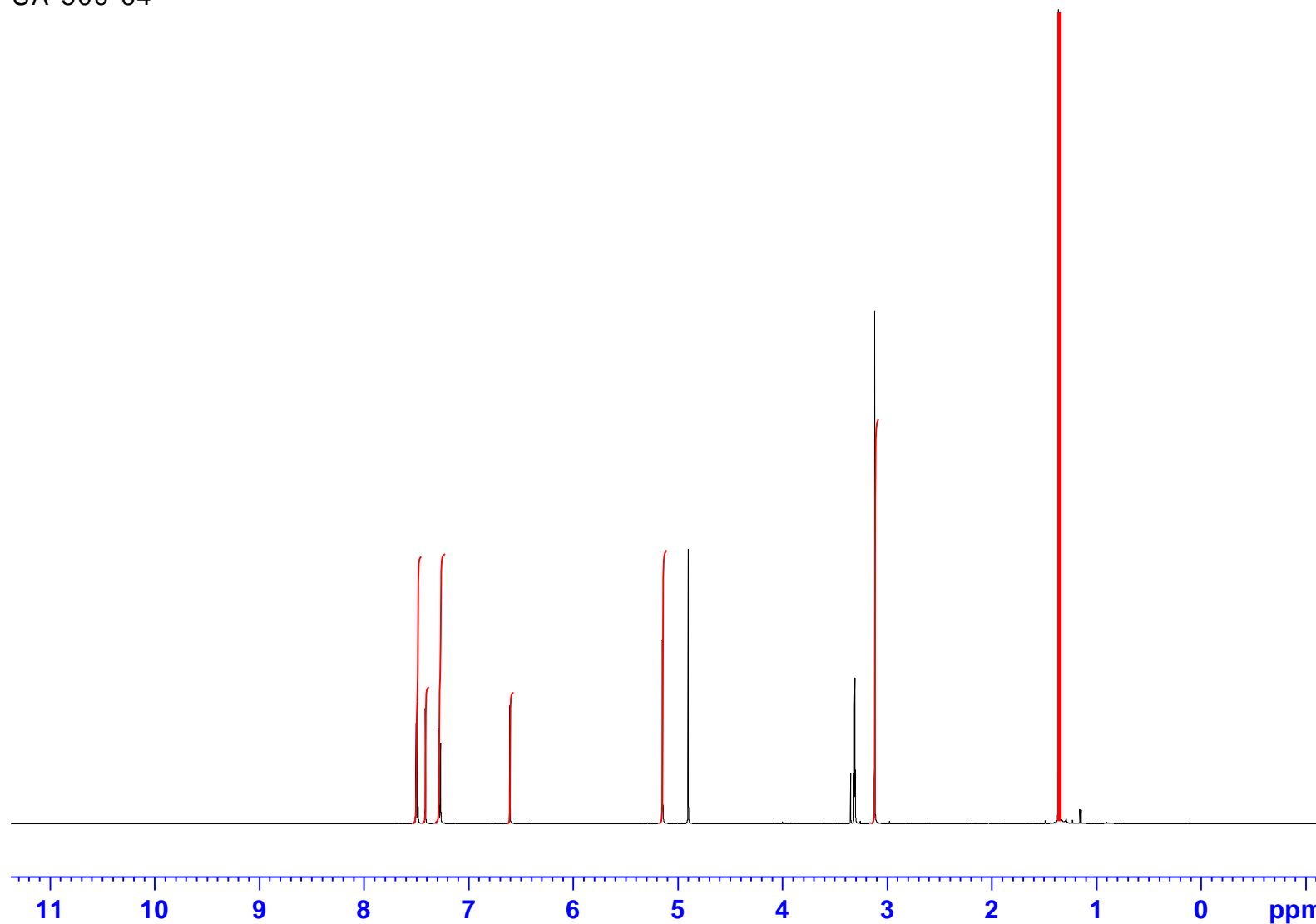
7.503
7.486
7.415
7.286
7.269
6.607

5.148
4.902

3.313
3.310
3.307
3.119

1.361

SA-500-64



2.03
1.04
2.06
1.00

2.08

3.09

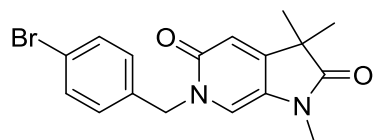
6.20

Current Data
NAME SA-500-64
EXPNO 10
PROCNO 1
F2 - Acquisition
Date_ Time 20150213 13.49
INSTRUM spect
PROBHD 5 mmPABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 406
DW 48.400 usec
DE 11.99 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1

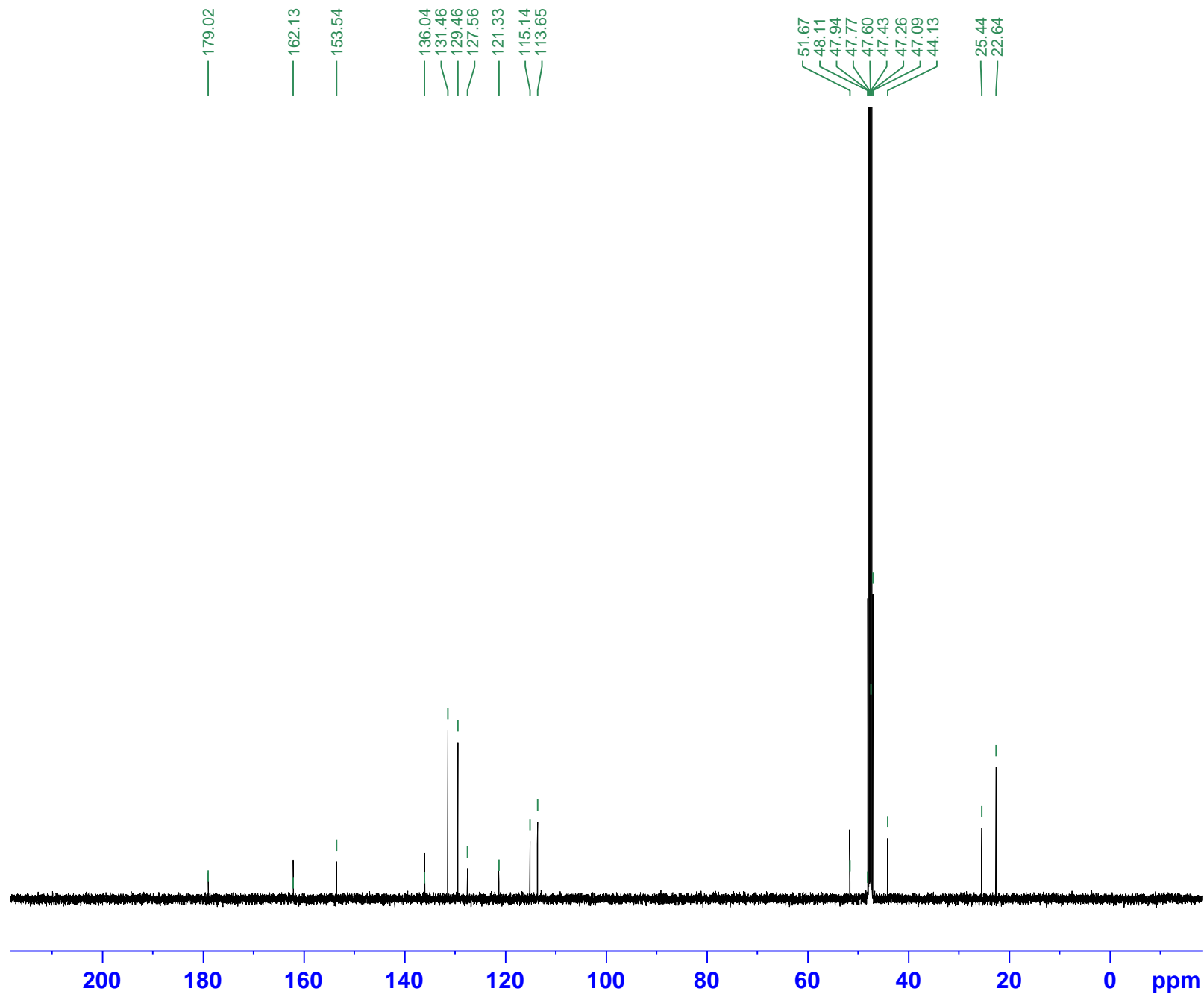
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
SF 500.3000098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17k



SA-500-64



Current Data Parameters
 NAME SA-500-64
 EXPNO 11
 PROCNO 1

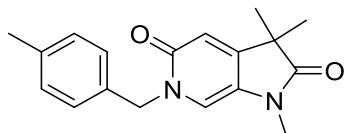
F2 - Acquisition
 Parameters Date_ 20150213
 Time 14.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 256
 DS 2
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DV 16.800 usec
 DE 7.68 usec
 TE 296.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

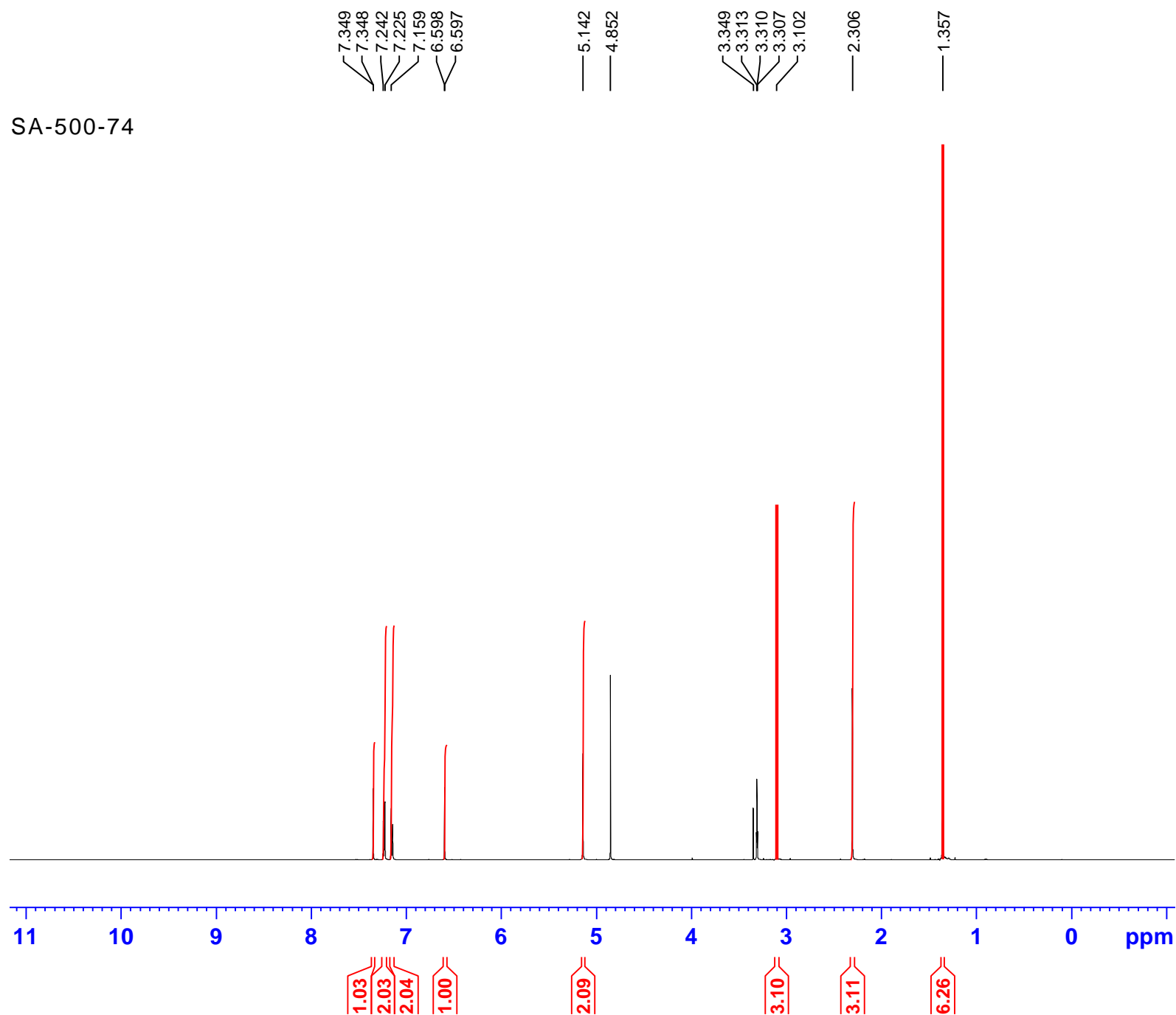
===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

171



SA-500-74



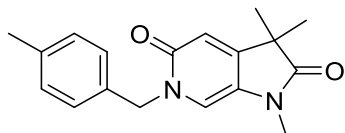
Current Data
 Name SA-500-74
 EXPNO 10
 PROCNO 1

F2 - Acquisition
 Parameters 20150218
 Time 14.51
 INSTRUM spect
 PROBHD 5 mmPABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 406
 DW 48.400 usec
 DE 11.99 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

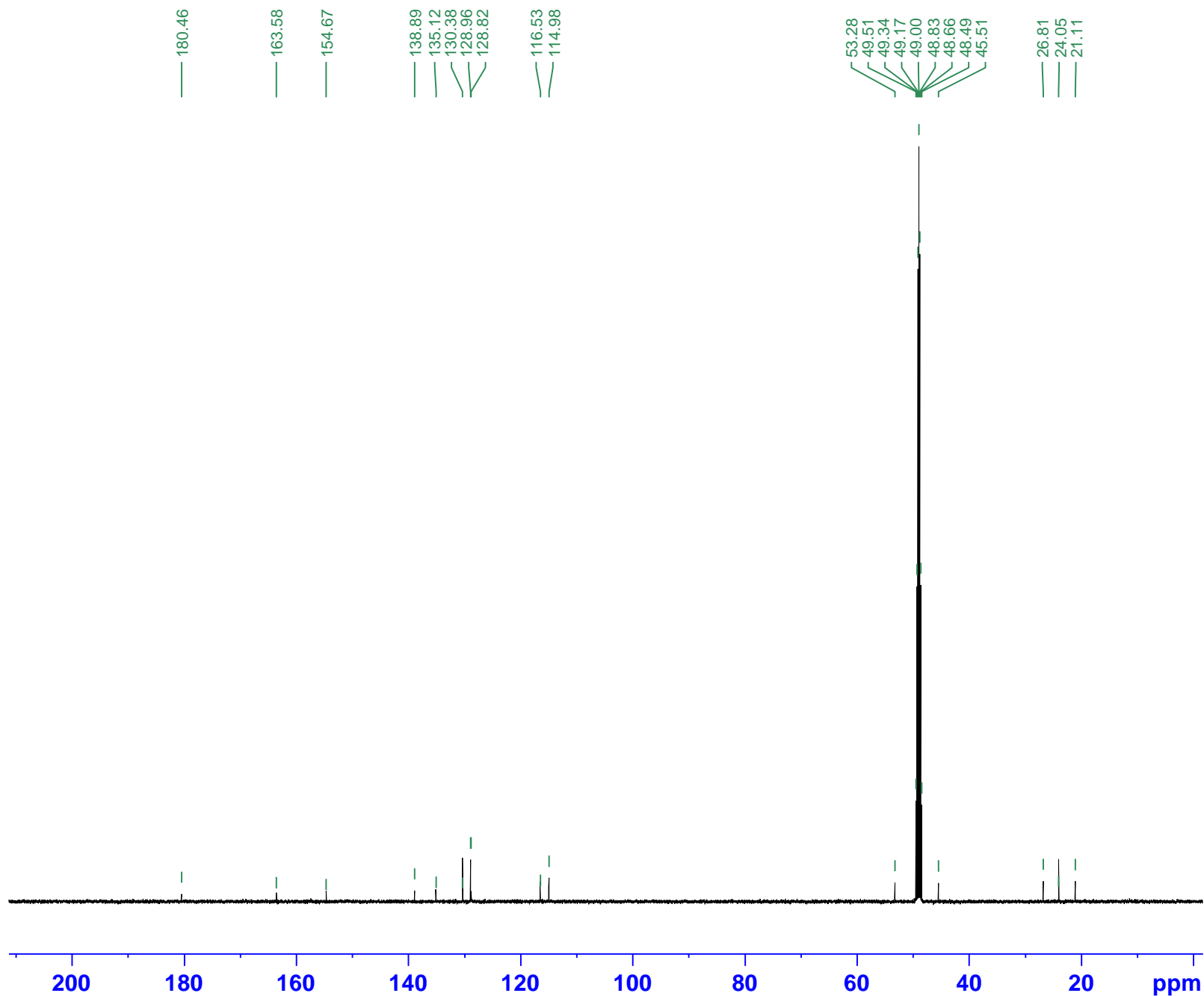
===== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

F2 - Processing parameters SI
 65536
 SF 500.3000097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

171



SA-500-74



Current Data Parameters
 NAME SA-500-74
 EXPNO 11
 PROCNO 1

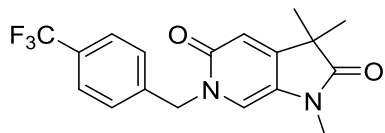
F2 - Acquisition
 Parameters Date_ 20150218
 Time 17.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 256
 DS 2
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DV 16.800 usec
 DE 7.68 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

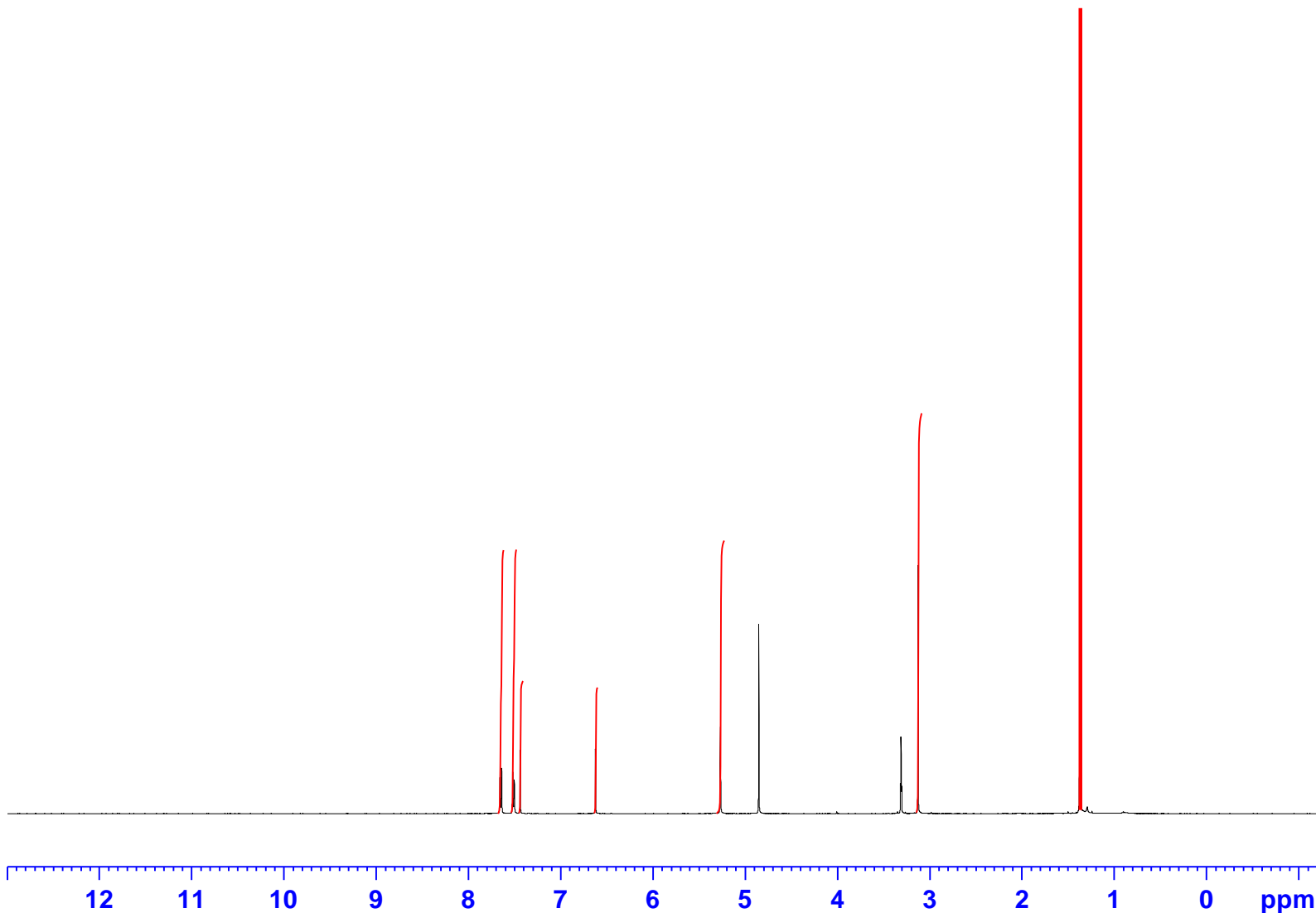
F2 - Processing
 Parameters 65536
 SF 125.8003589 MHz
 WDV EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17m



SA-500-68

7.657
7.641
7.519
7.503
7.439
6.622
5.268
4.852
3.316
3.313
3.310
3.307
3.126
1.372



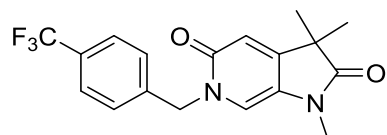
Current Data
NAME SA-500-68
EXPNO 10
PROCNO 1

F2 - Acquisition
Data 20150216
Time 16.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 406
DW 48.400 usec
DE 11.99 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

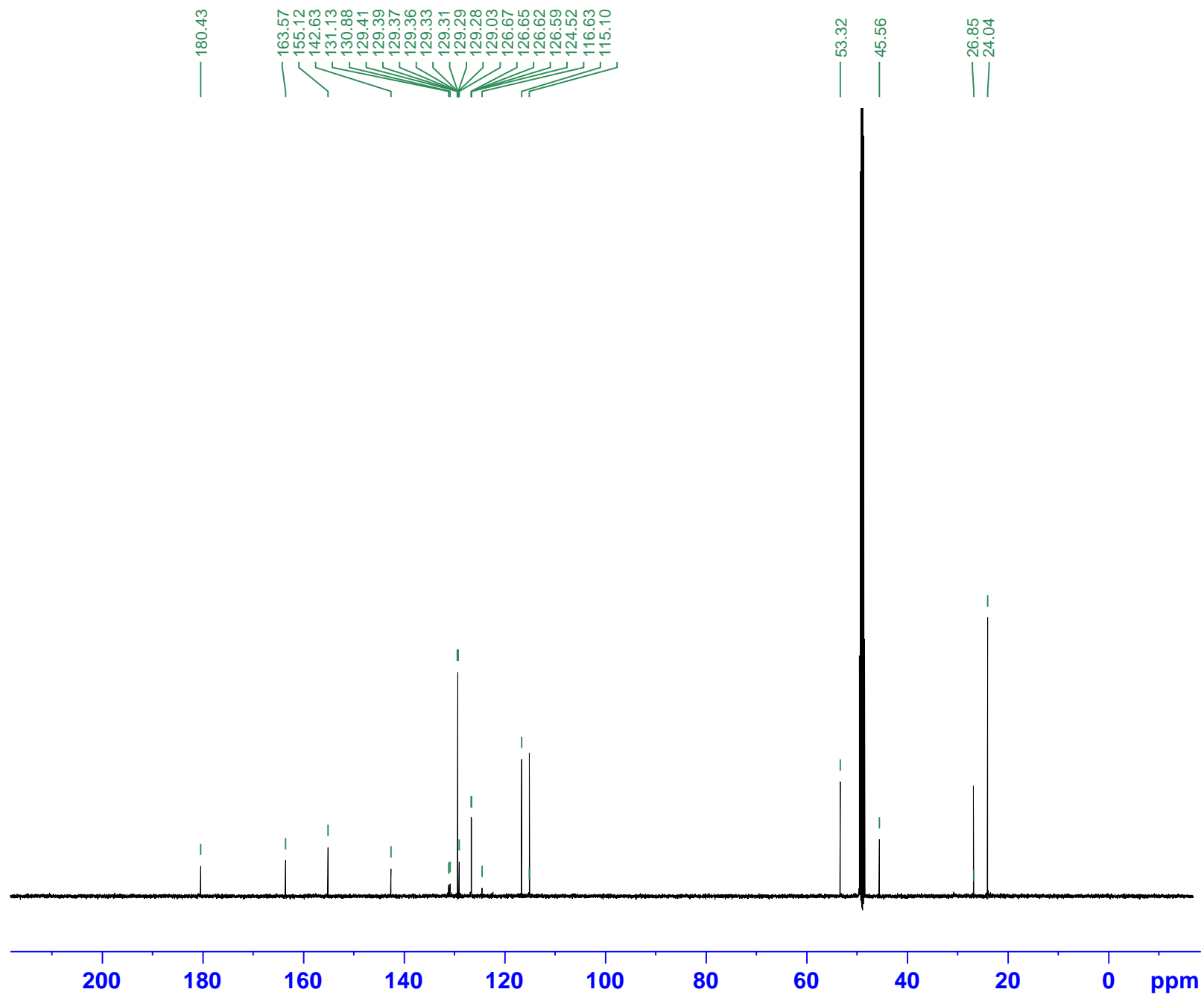
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17m



SA-500-68



Current Data Parameters
 NAME SA-500-68
 EXPNO 15
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20150216
 Time 22.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 26782
 SOLVENT MeOD
 NS 2048
 DS 2
 SMH 29761.904 Hz
 FIDRES 1.111265 Hz
 AQ 0.4499376 sec
 RG 456
 DV 16.800 usec
 DE 7.72 usec
 TE 298.0 K
 D1 5.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

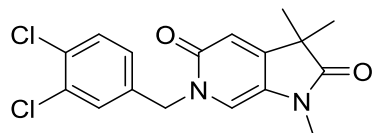
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

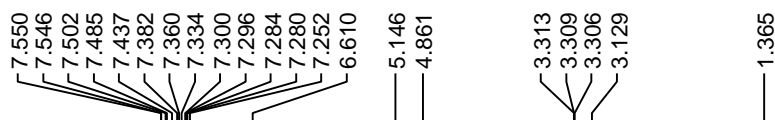
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17n



SA-500-100

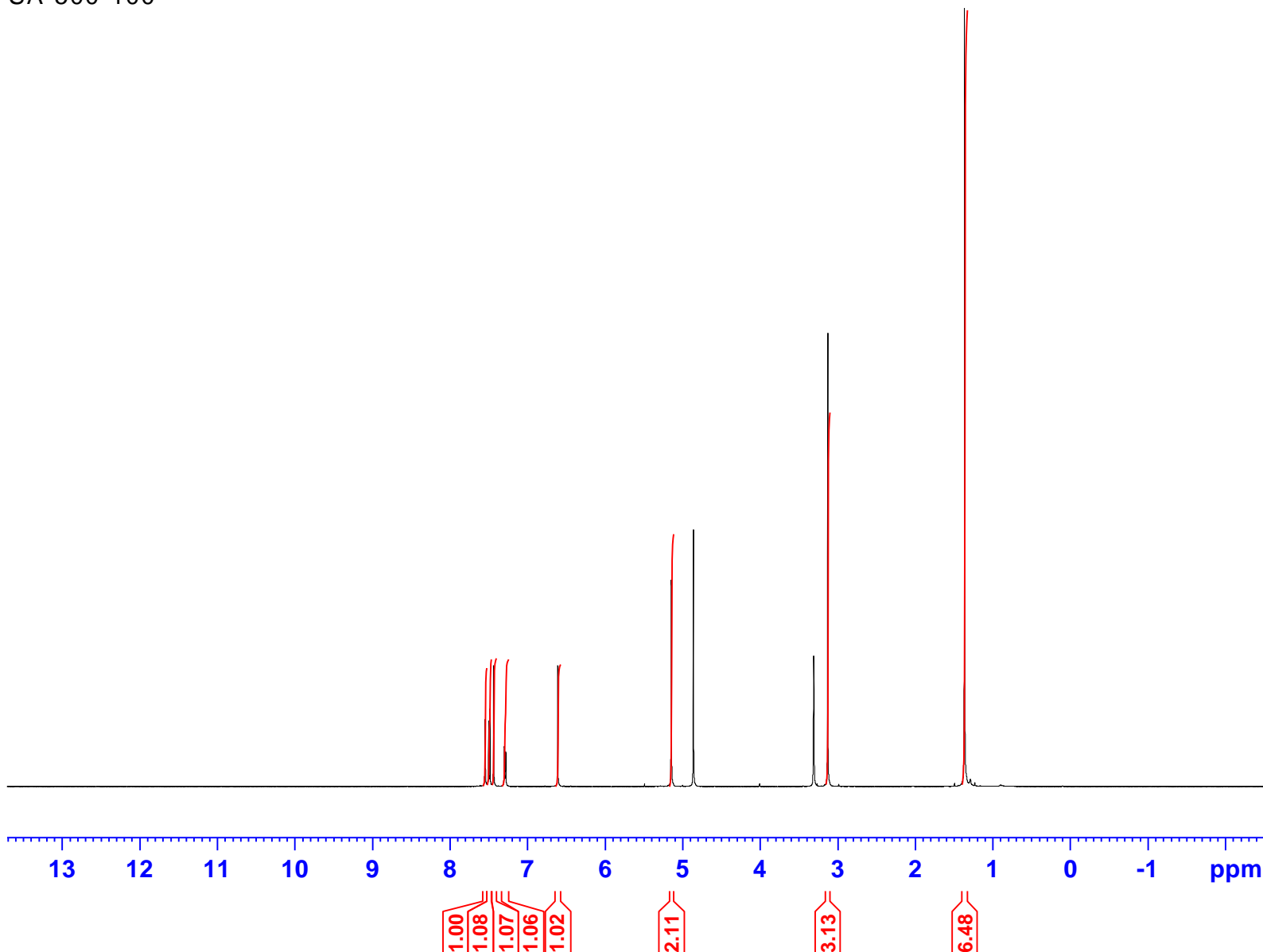


Current Data
NAME SA-500-100-DRIED
EXPNO 10
PROCNO 1

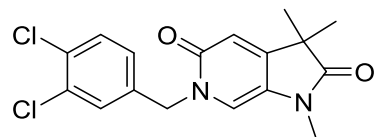
F2 - Acquisition
Date_ 20150317
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 456
DW 48.400 usec
DE 11.99 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

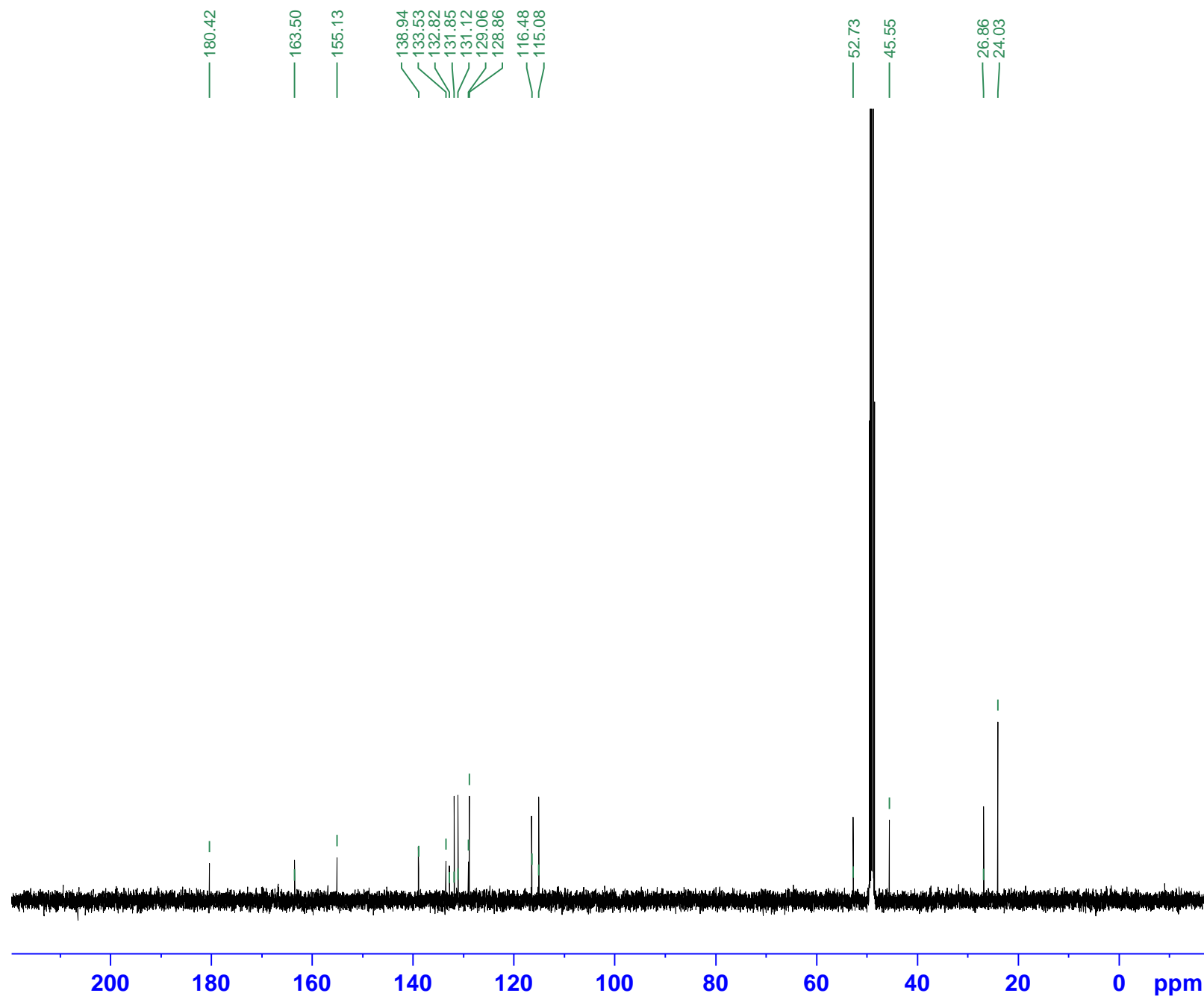
F2 - Processing parameters SI
65536
SF 500.3000099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



17n



SA-500-100



Current Data Parameters
NAME SA-500-100-DRIED
EXPNO 11
PROCNO 1

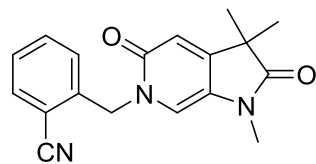
F2 - Acquisition
Parameters Date_ 20150317
Time 23.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 256
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 575
DW 16.800 usec
DE 7.68 usec
TE 297.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

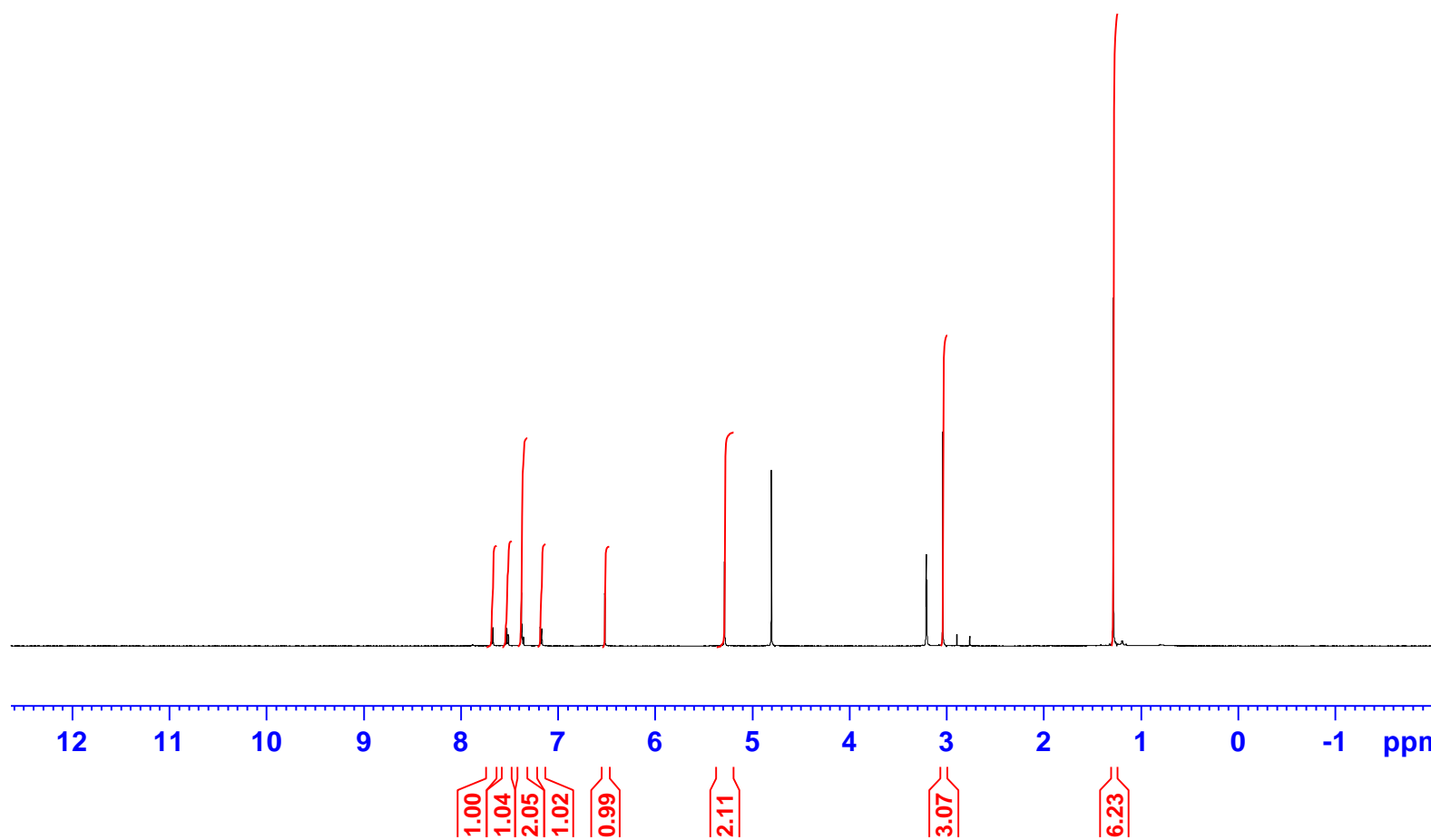
F2 - Processing
Parameters 65536
SF 125.8003589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

17o



SA-500-26

7.378 6.519 5.287 4.805 3.215 3.211 3.208 3.205 3.202 3.039 1.285



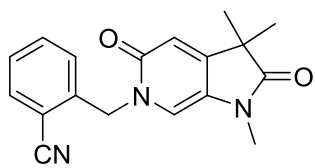
Current Data
 Name SA-500-26
 EXPNO 10
 PROCNO 1

F2 - Acquisition
 Parameters 20150122
 Time 15.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 406
 DW 48.400 usec
 DE 11.99 usec
 TE 292.3 K
 D1 1.0000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.3360044 W

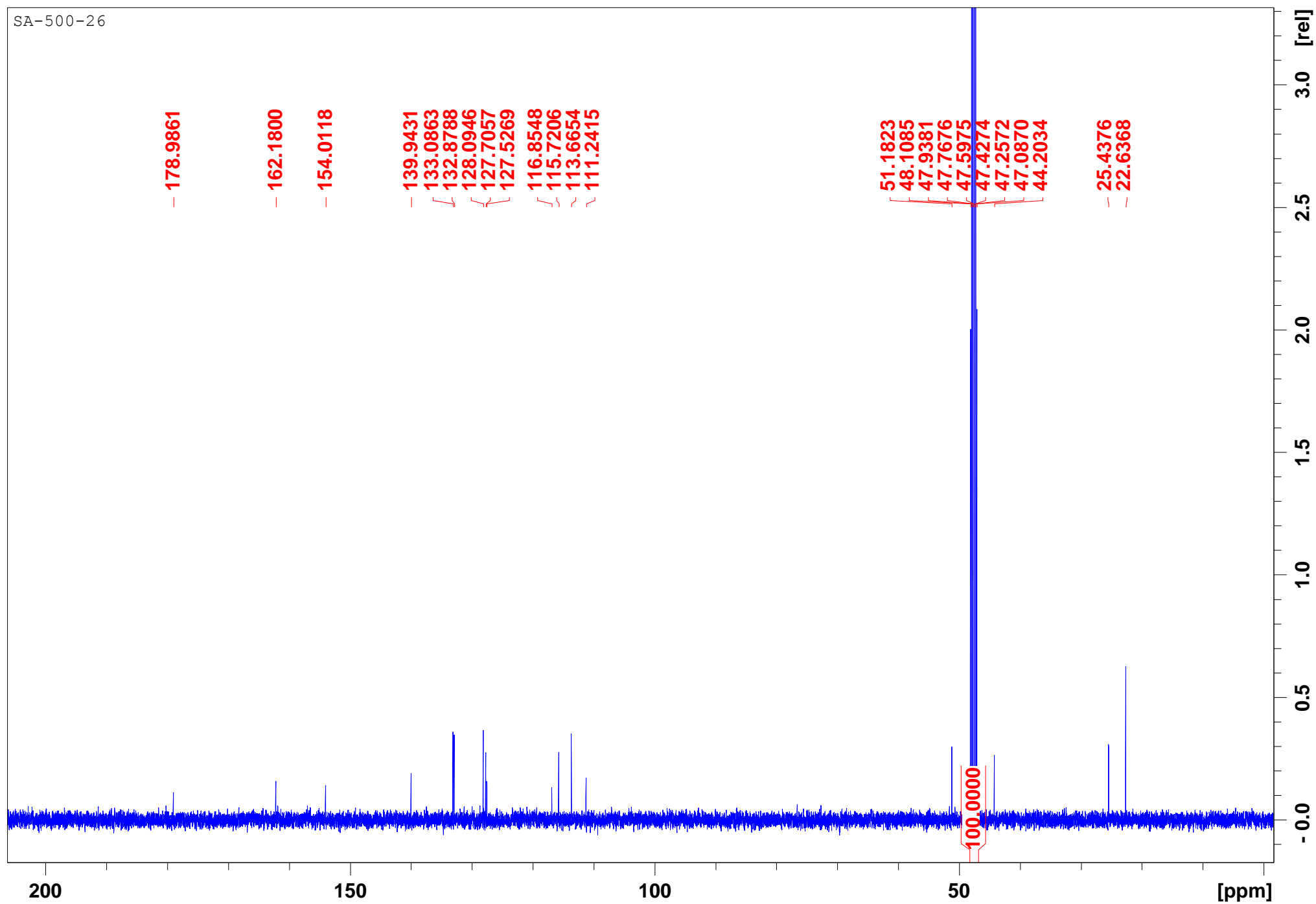
F2 - Processing parameters SI
 65536
 SF 500.3000605 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

17o

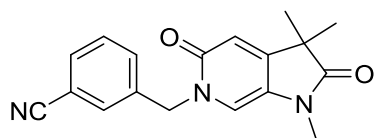


SA-500-26 11 1 z:\data\SA\nmr

SA-500-26

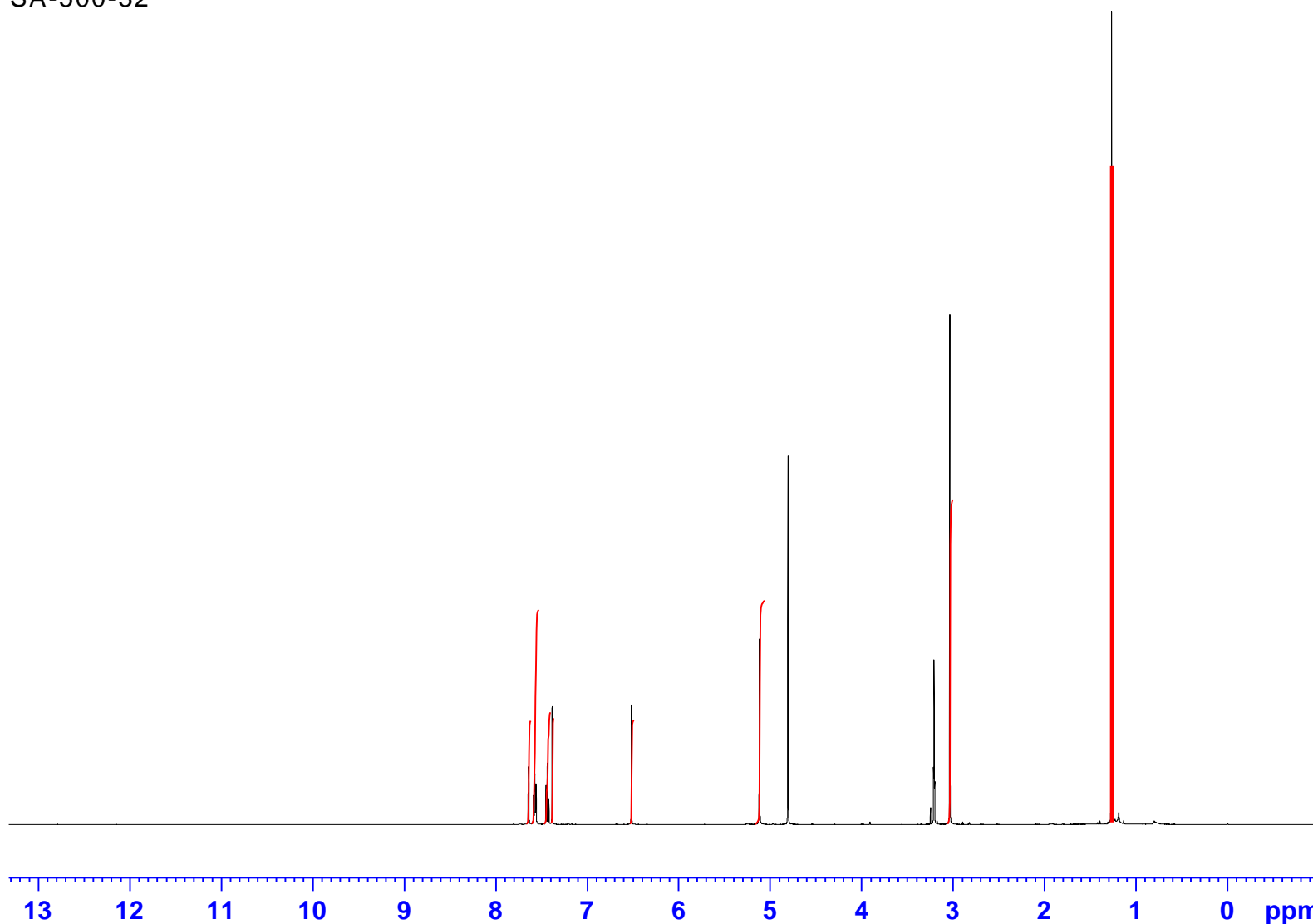


17p



7.641
7.435
7.383
6.517
5.116
4.806
3.215
3.211
3.208
3.205
3.201
3.036
1.266

SA-500-32



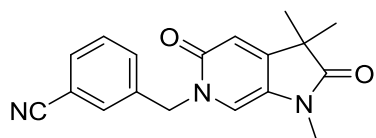
Current Data
NAME SA-500-32
EXPNO 10
PROCNO 1

F2 - Acquisition
Data parameters 20150122
Time 15.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 362
DW 48.400 usec
DE 11.99 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1

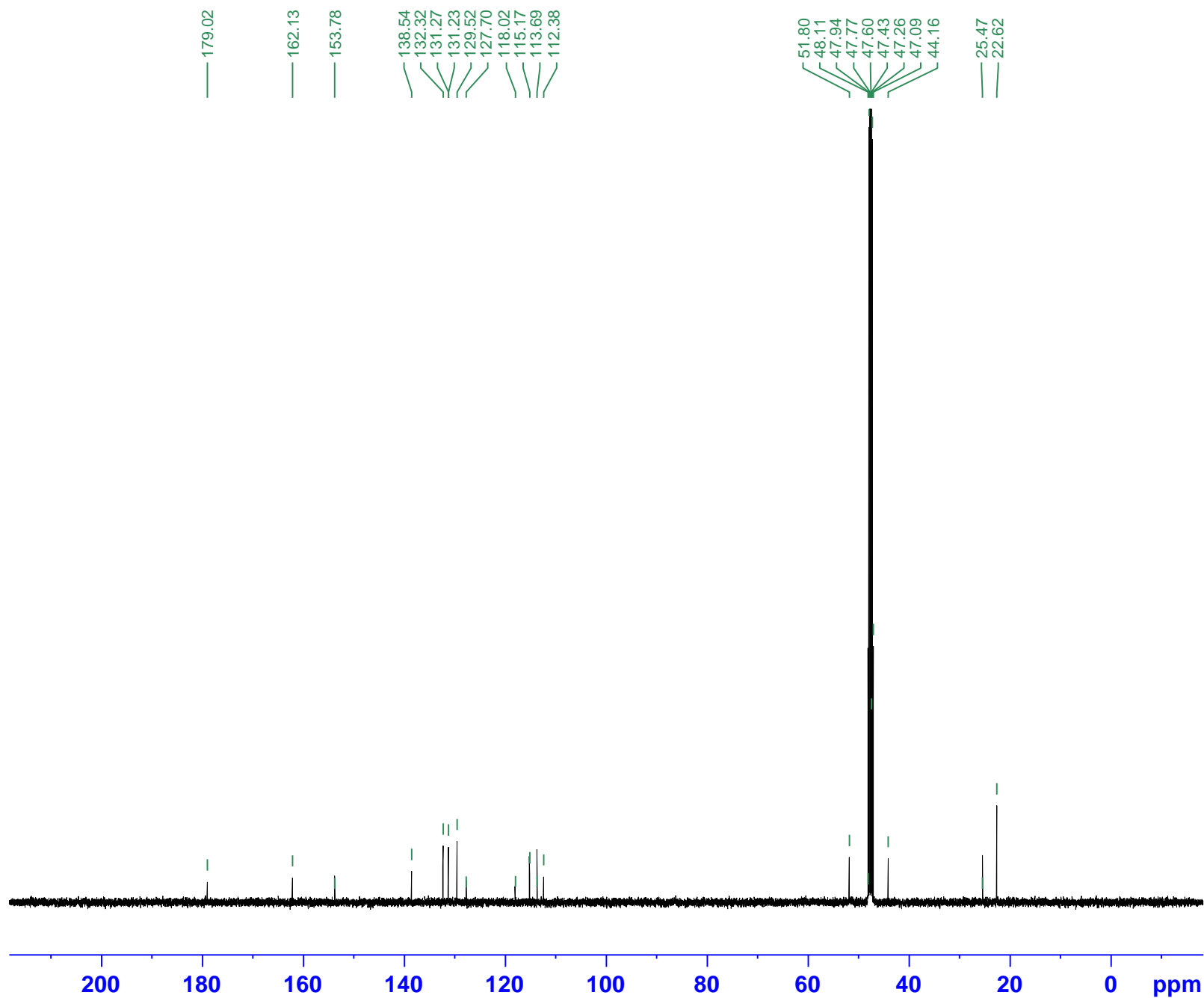
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.300606 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17p



SA-500-32



Current Data Parameters
 NAME SA-500-32
 EXPNO 11
 PROCNO 1

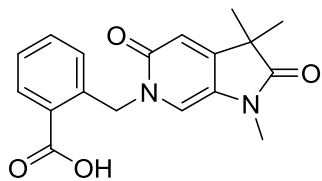
F2 - Acquisition
 Parameters Date_ 20150122
 Time 15.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 256
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 294.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

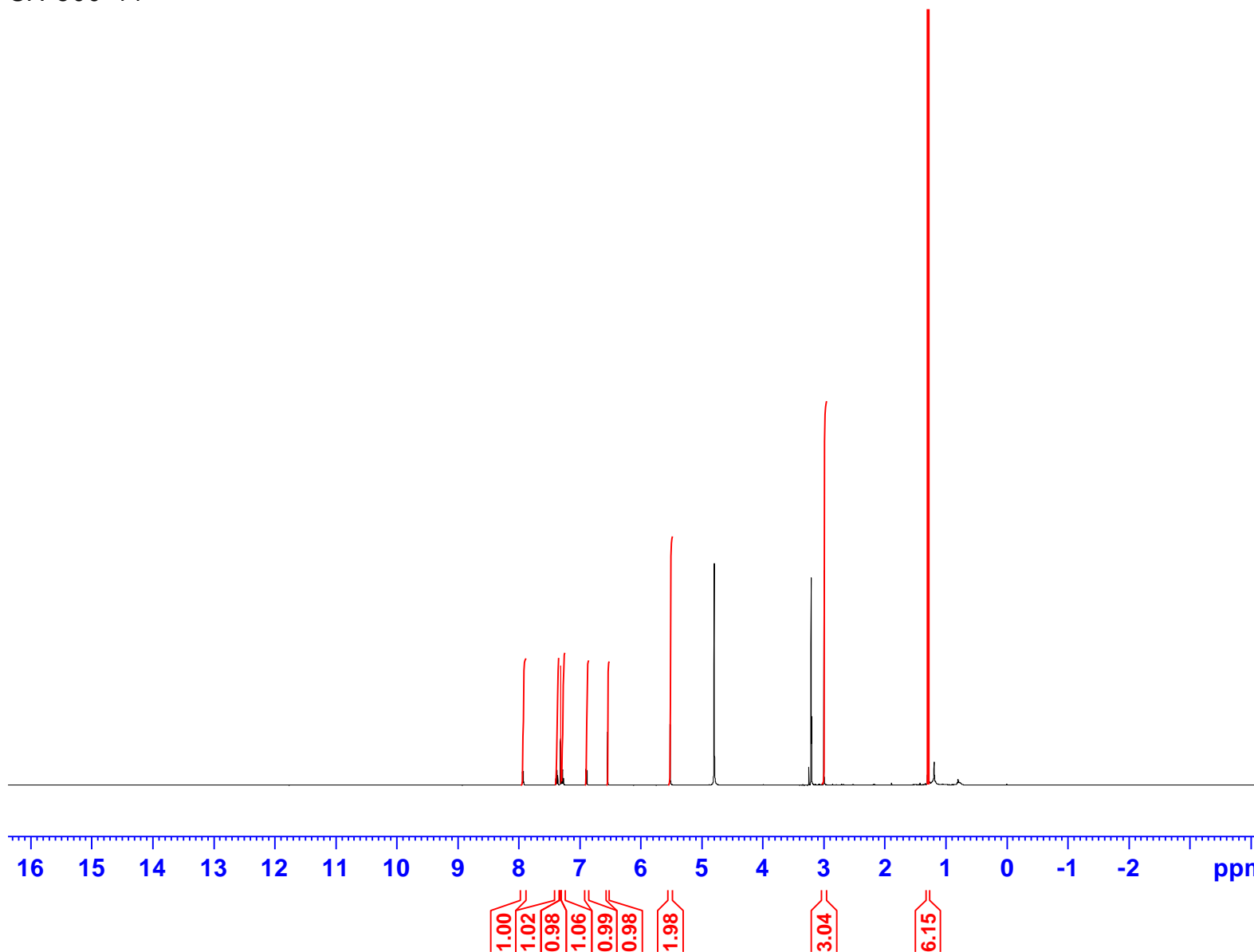
F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

17q



7.942
7.940
7.927
7.925
7.394
7.392
7.379
7.377
7.364
7.361
7.318
7.298
7.282
7.269
6.900
6.884
6.545
5.520
4.798
3.215
3.212
3.209
3.205
3.202
2.998
1.296

SA-500-44



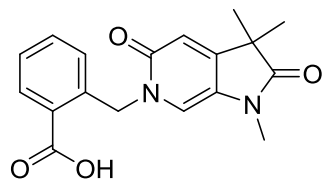
Current Data
NAME SA-500-44
EXPNO 10
PROCNO 1

F2 - Acquisition
Data Parameters 20150128
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 456
DW 48.400 usec
DE 11.99 usec
TE 293.7 K
D1 1.00000000 sec
TDO 1

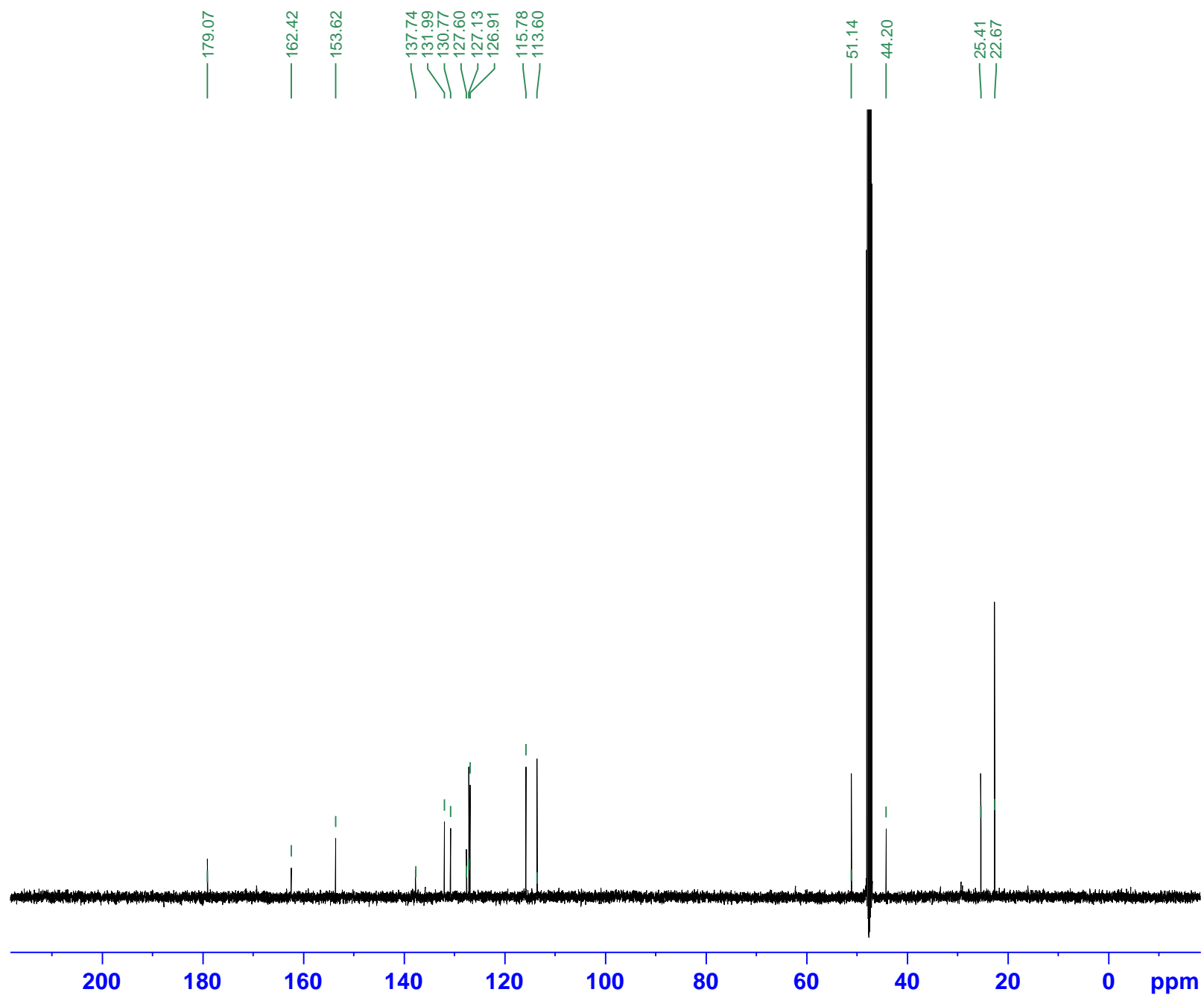
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000603 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

17q



SA-500-44



Current Data Parameters
 NAME SA-500-44
 EXPNO 12
 PROCNO 1

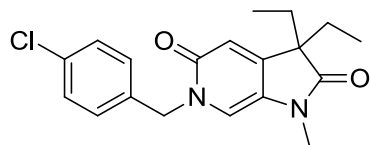
F2 - Acquisition
 Parameters Date_ 20150128
 Time 21.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 26782
 SOLVENT MeOD
 NS 2048
 DS 2
 SMH 29761.904 Hz
 FIDRES 1.111265 Hz
 AQ 0.4499376 sec
 RG 724
 DV 16.800 usec
 DE 7.72 usec
 TE 296.4 K
 D1 5.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

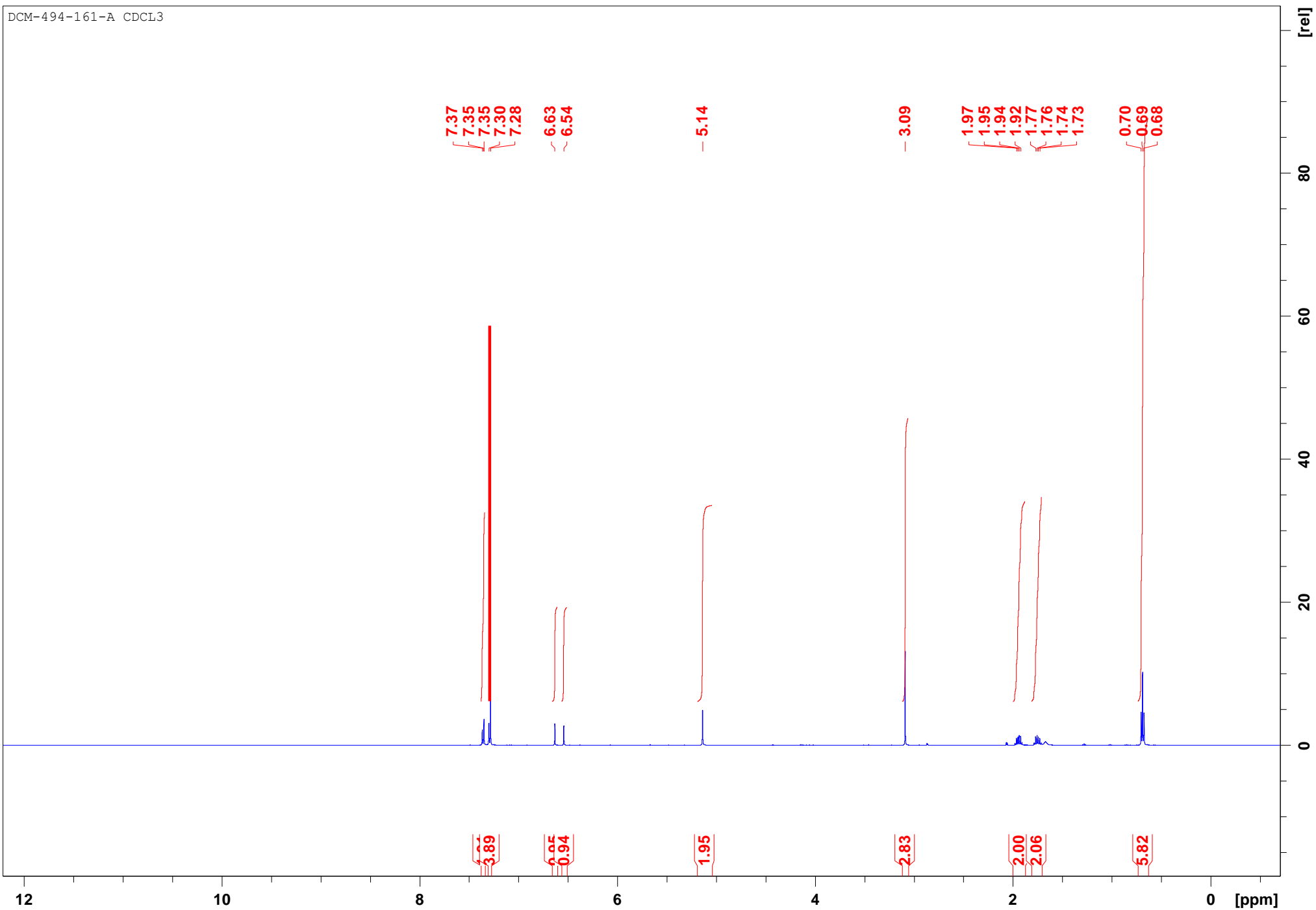
F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

18a

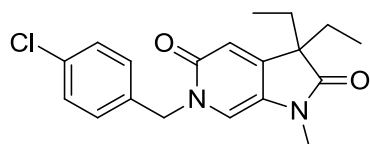


"dcm-494-161-a cdcl3" 10 1 "X:\Old Server\DCM\nmr"

DCM-494-161-A CDCL3

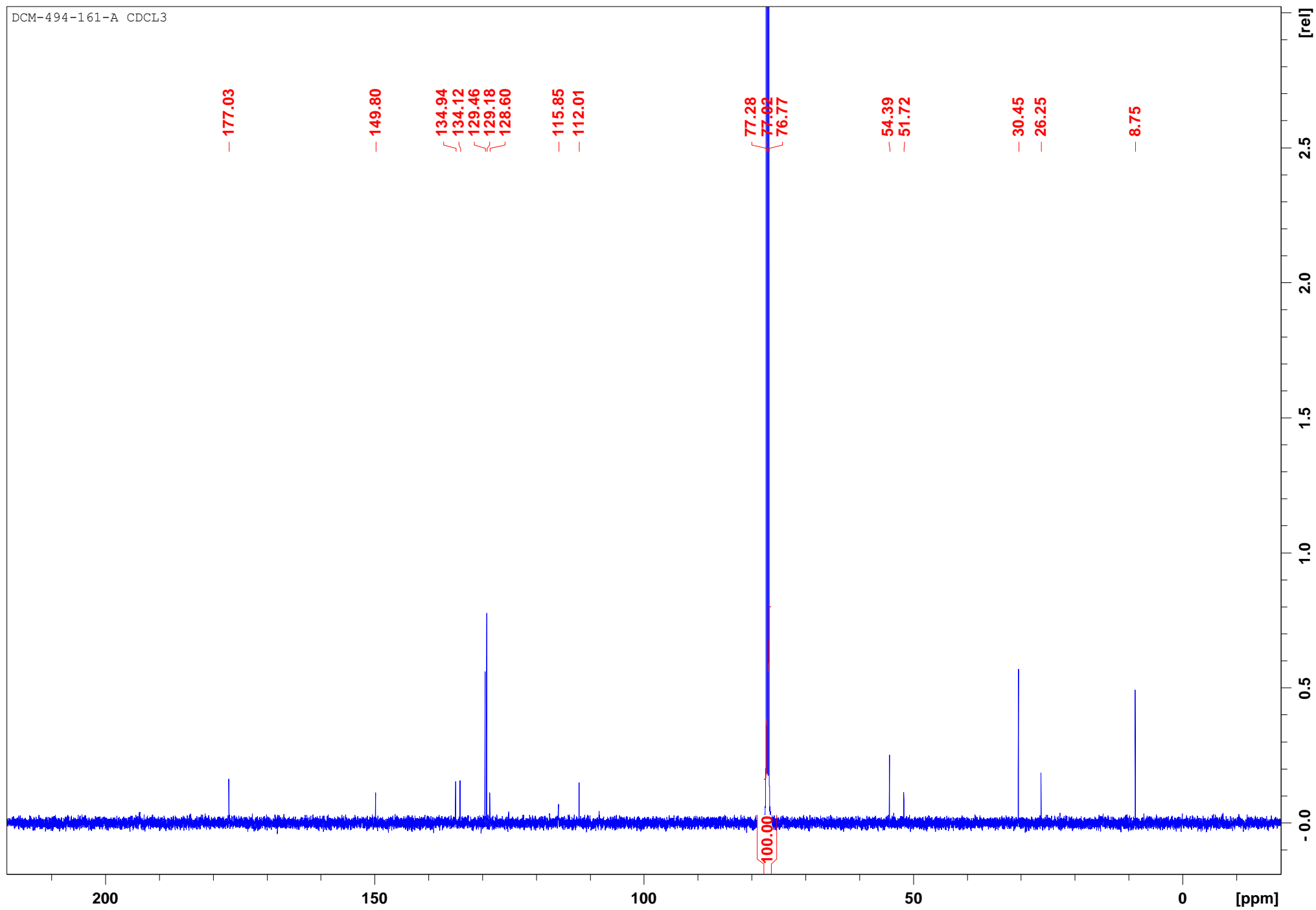


18a

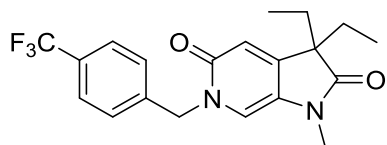


"dcm-494-161-a cdcl3" 13 1 "X:\Old Server\DCM\nmr"

DCM-494-161-A CDCL3

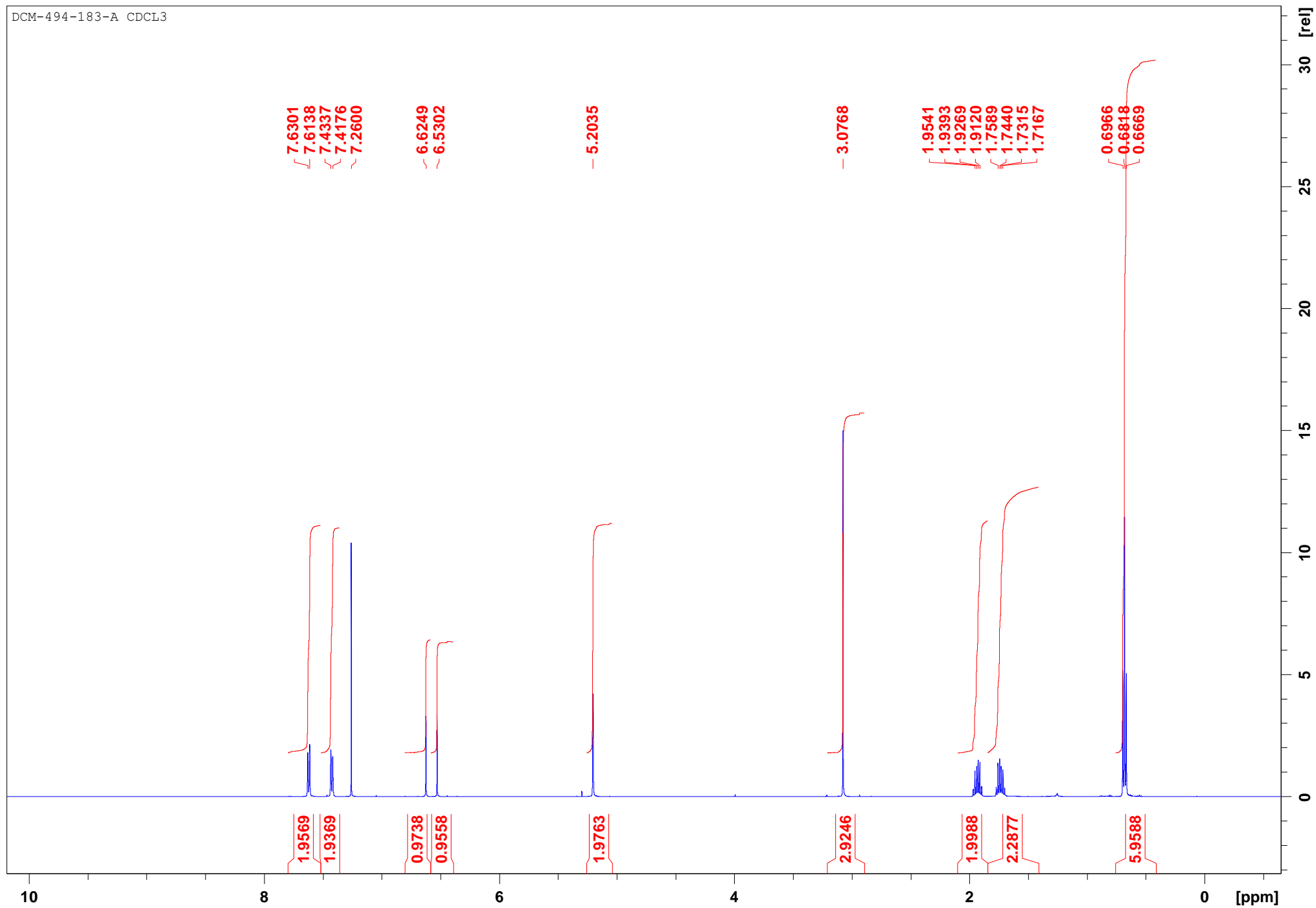


18b

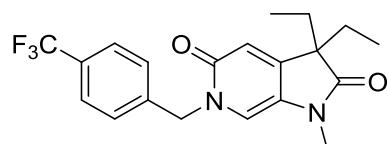


"DCM-494-183-A CDCL3" 10 1 Z:\data\DCM\nmr

DCM-494-183-A CDCL3

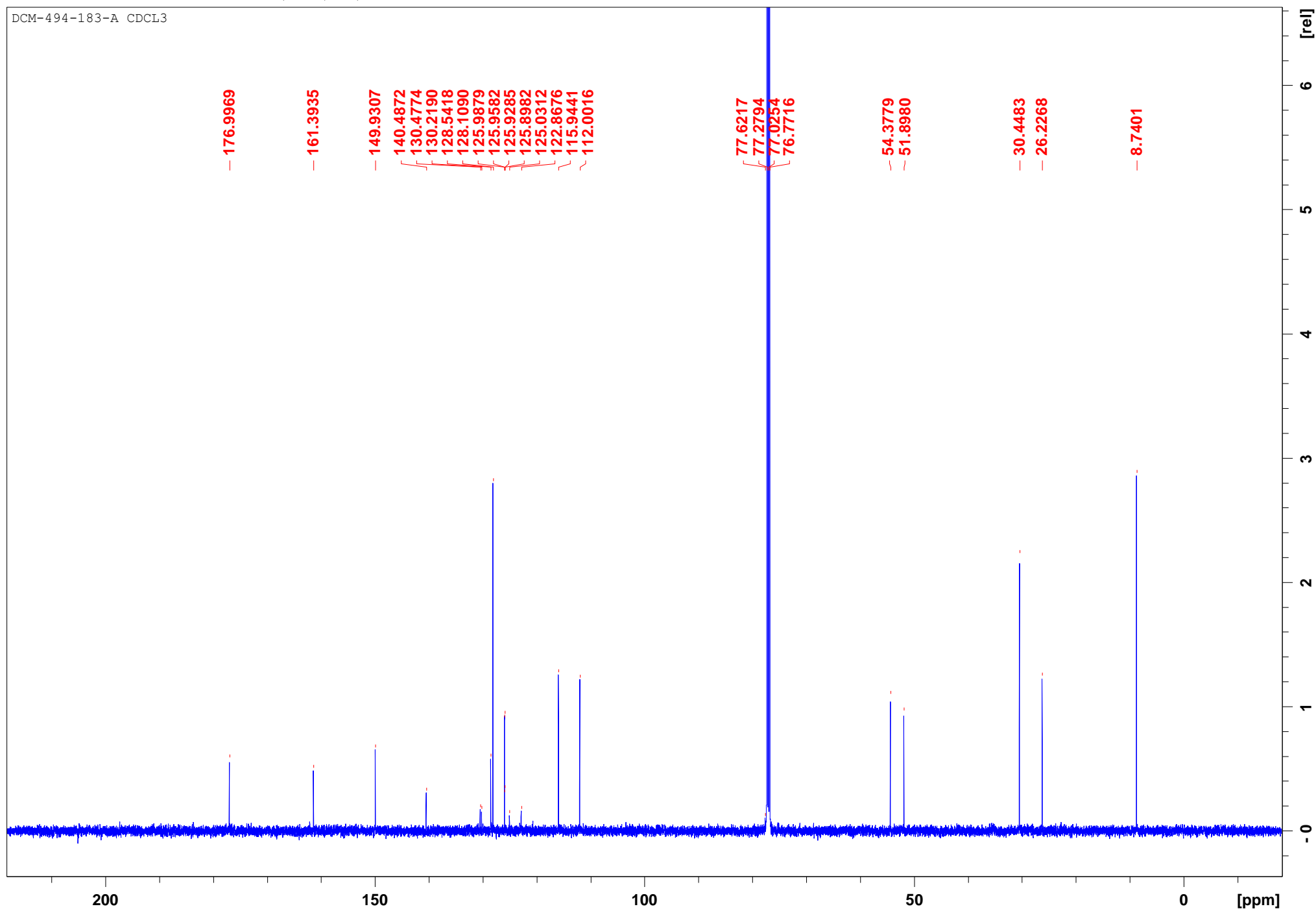


18b

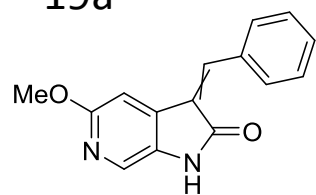


"DCM-494-183-A CDCL3" 11 1 Z:\data\DCM\nmr

DCM-494-183-A CDCL3

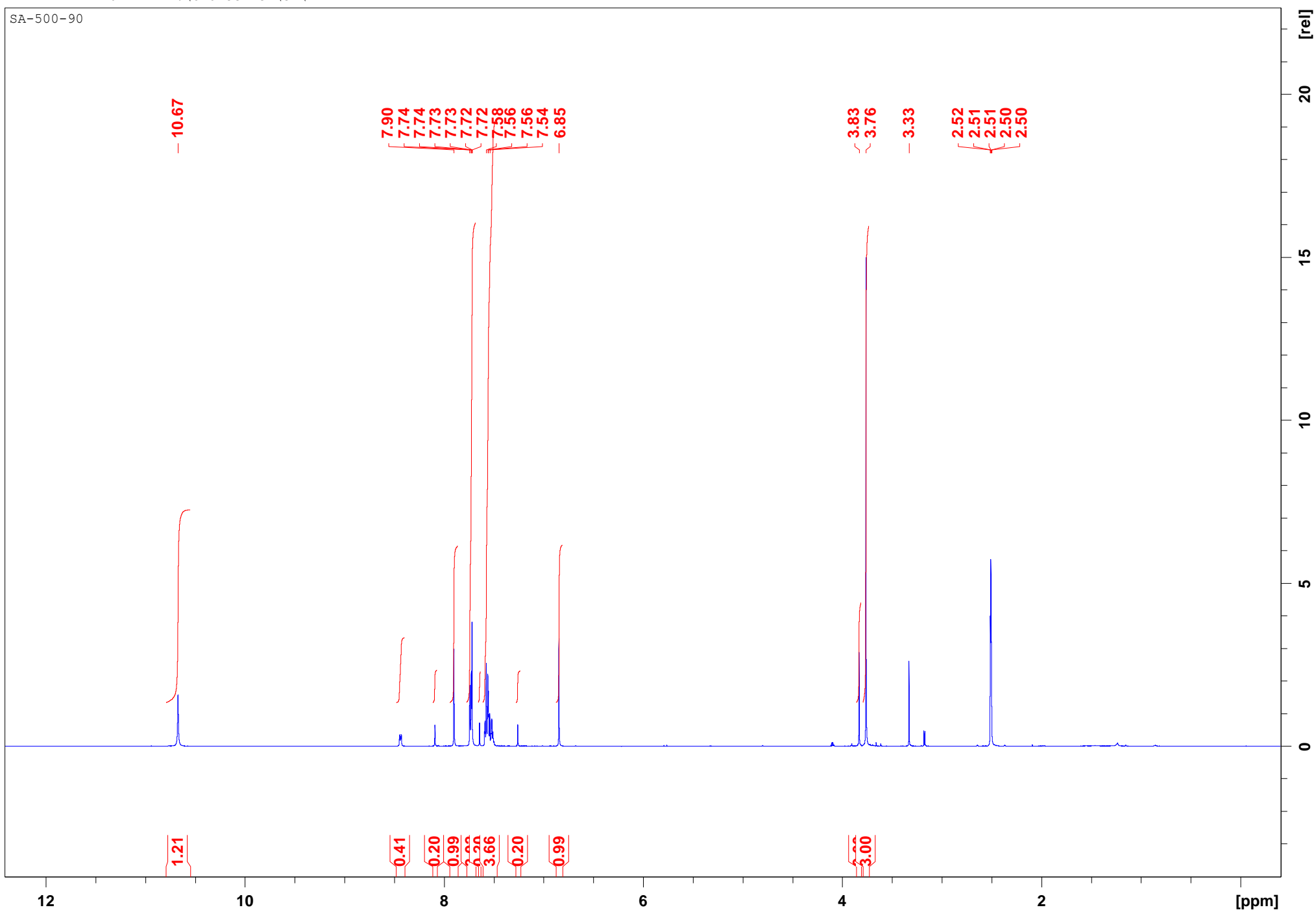


19a

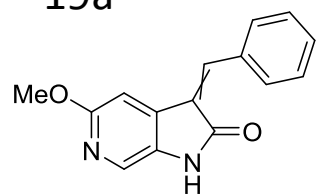


SA-500-90 10 1 "X:\Old Server\SA\nmr"

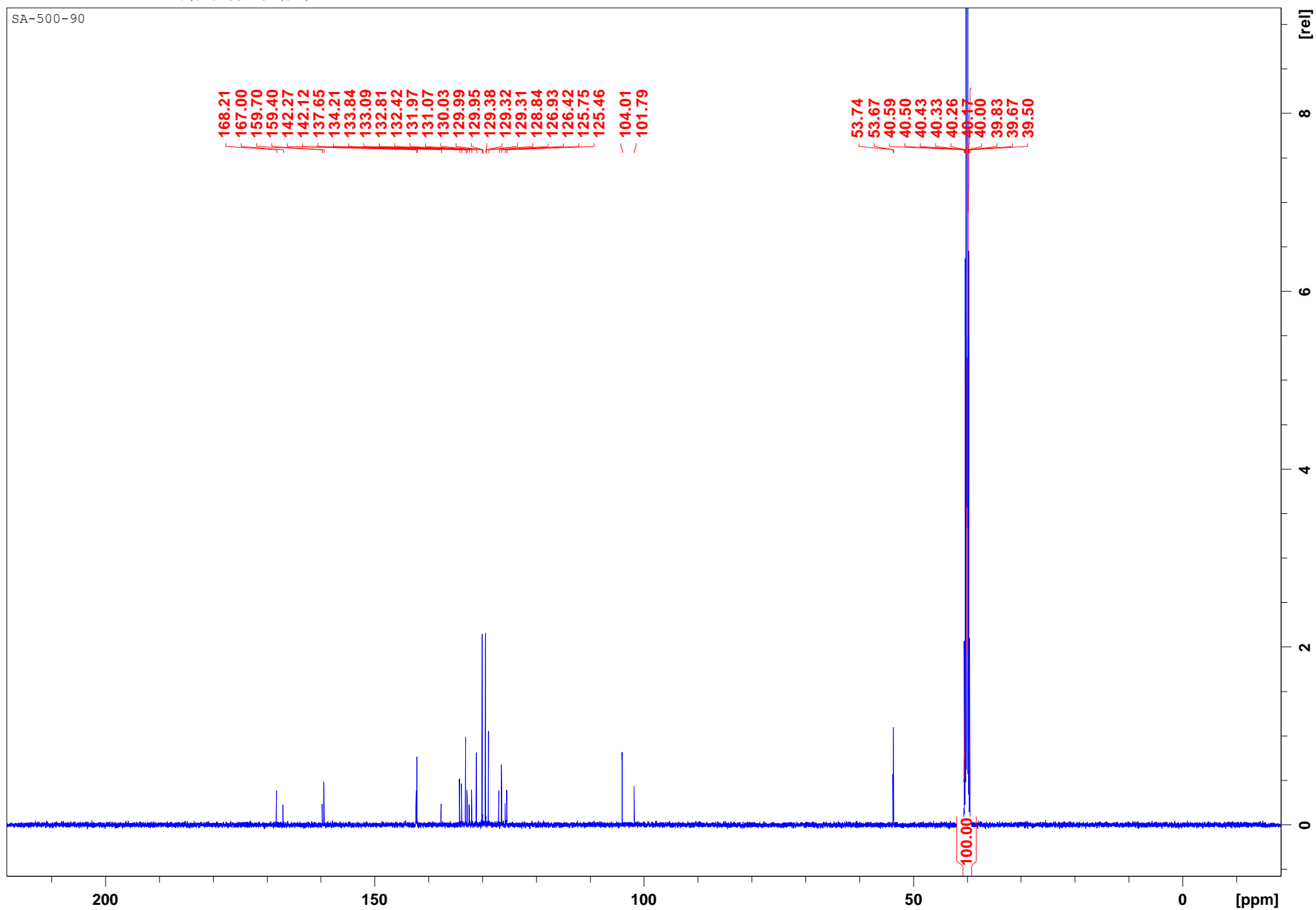
SA-500-90



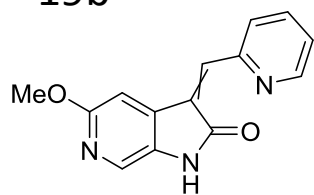
19a



SA-500-90 13 1 "X:\Old Server\SA\nmr"

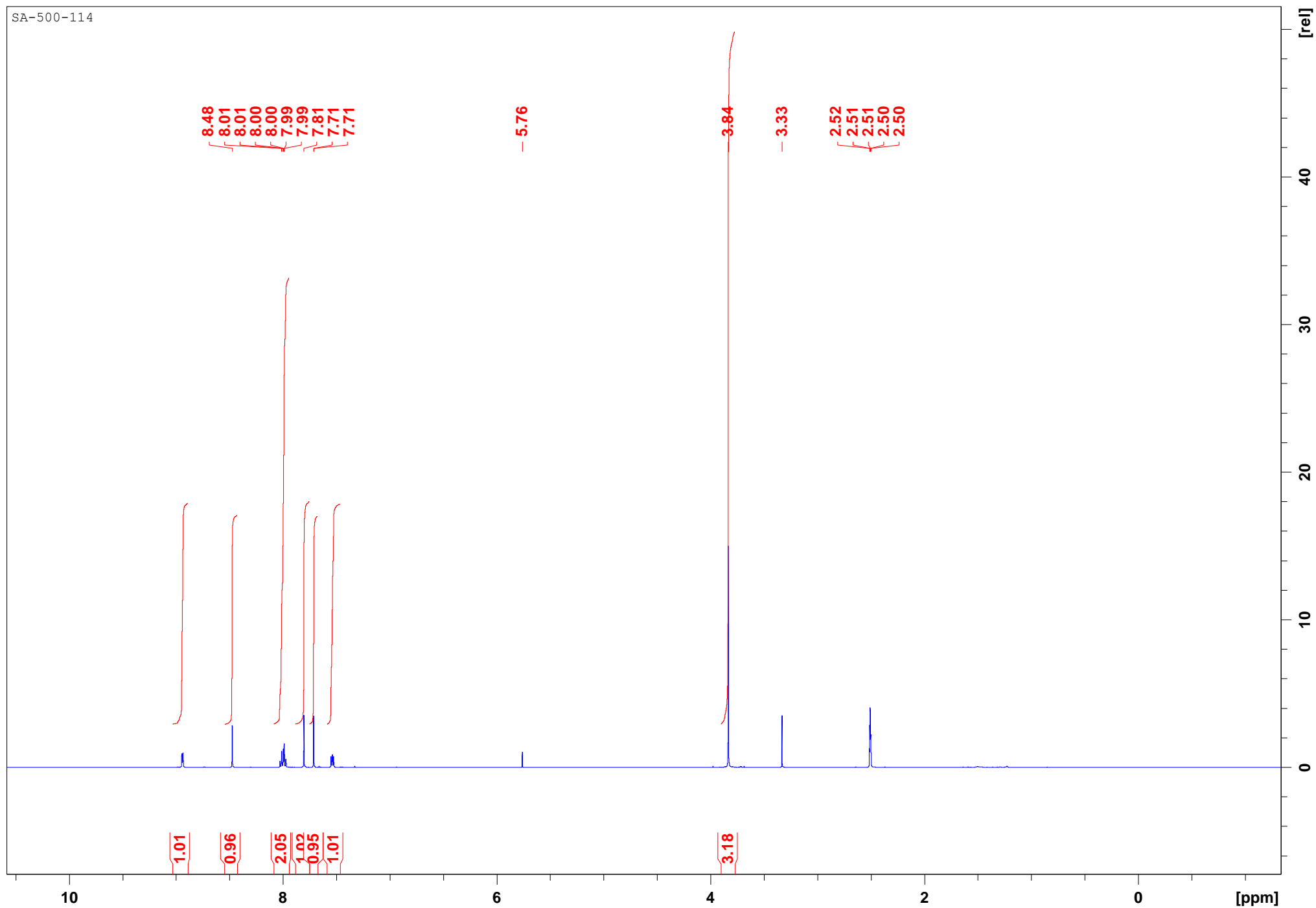


19b

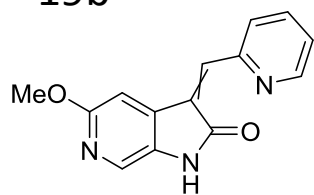


SA-500-114 10 1 "X:\Old Server\SA\nmr"

SA-500-114

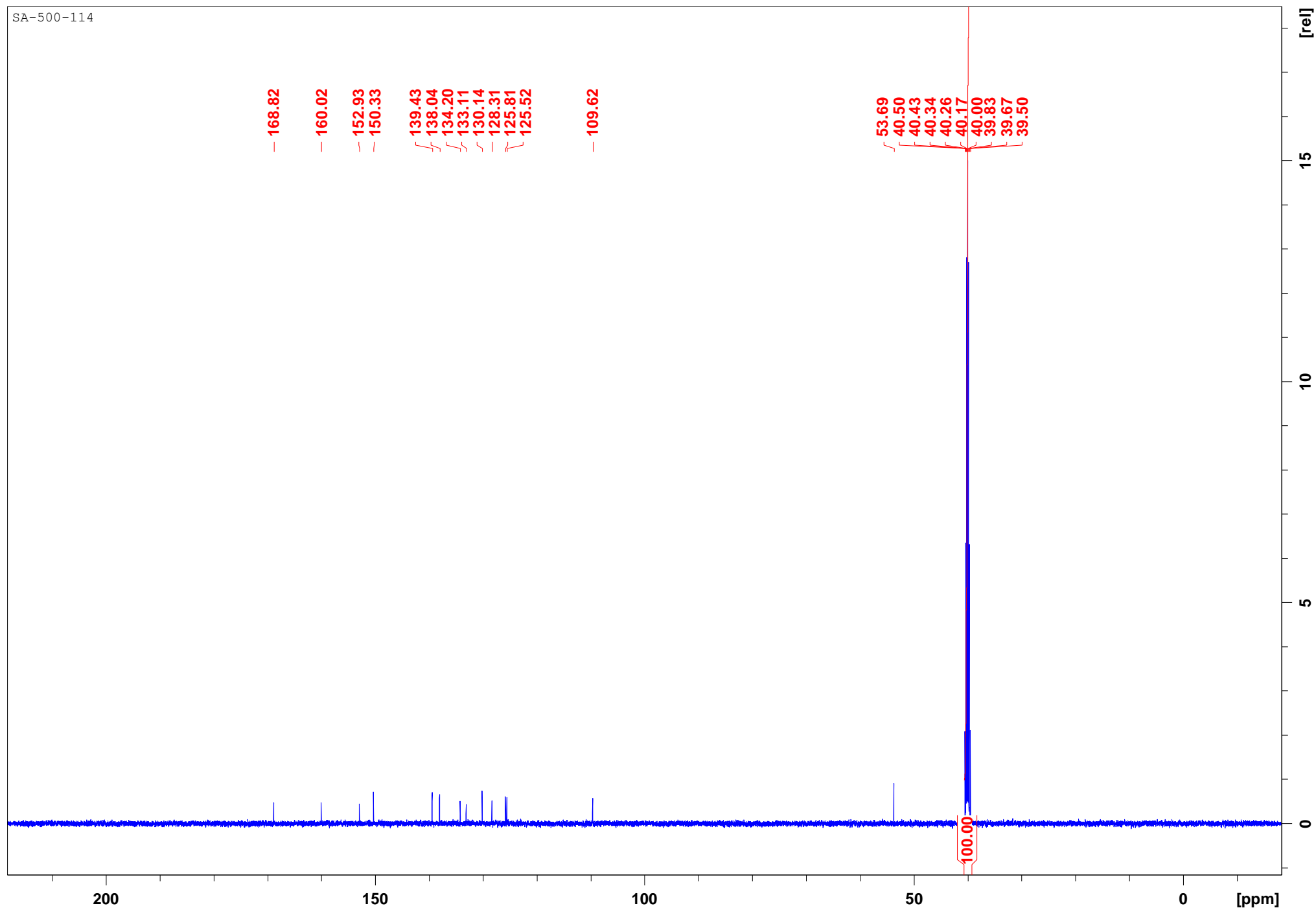


19b

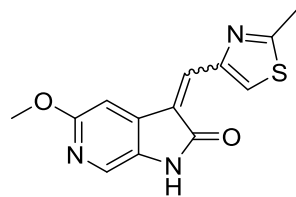


SA-500-114 11 1 "X:\Old Server\SA\nmr"

SA-500-114

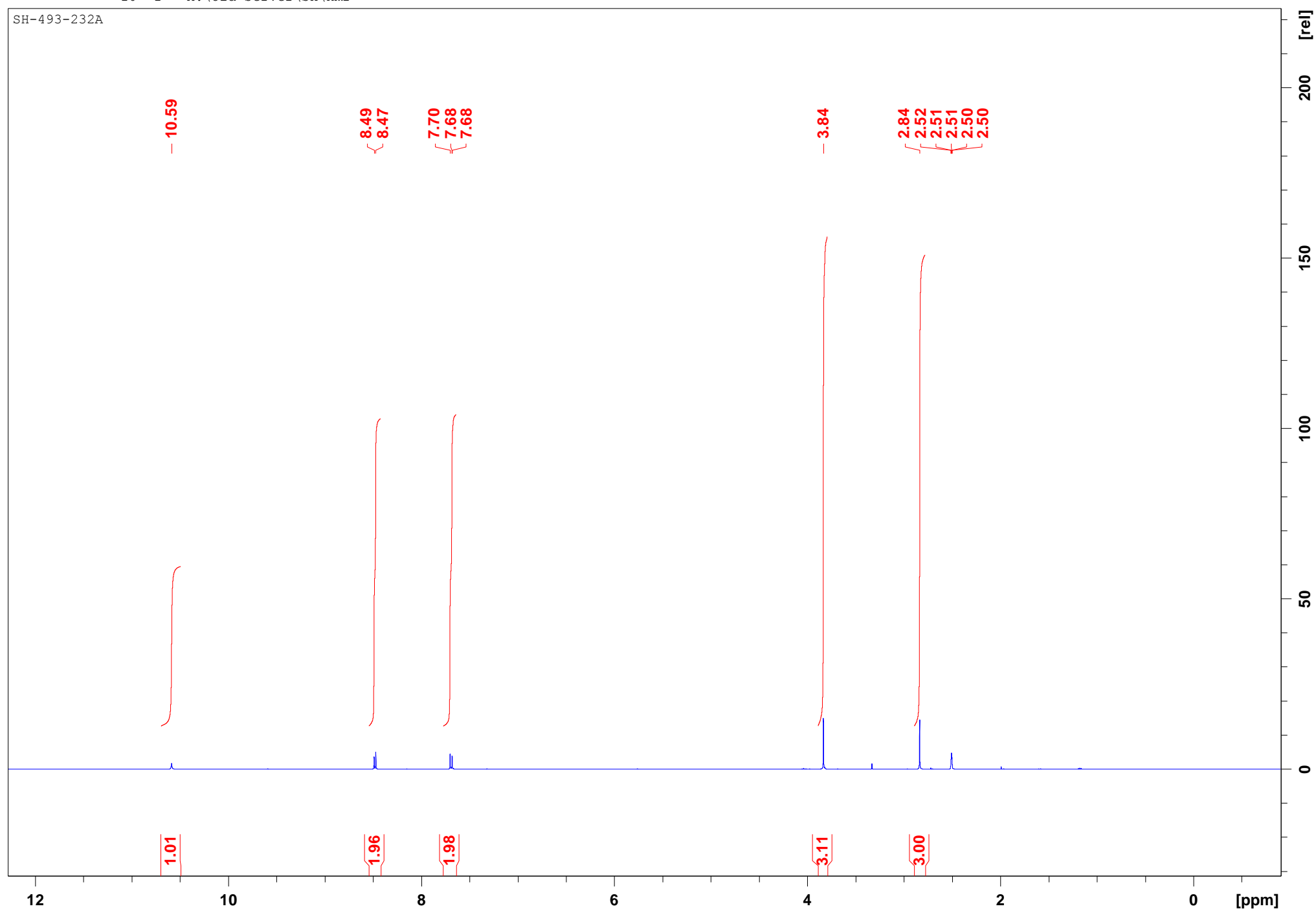


19c

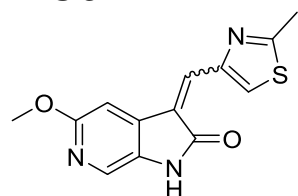


SH-493-232A 10 1 "X:\Old Server\SH\nmr"

SH-493-232A

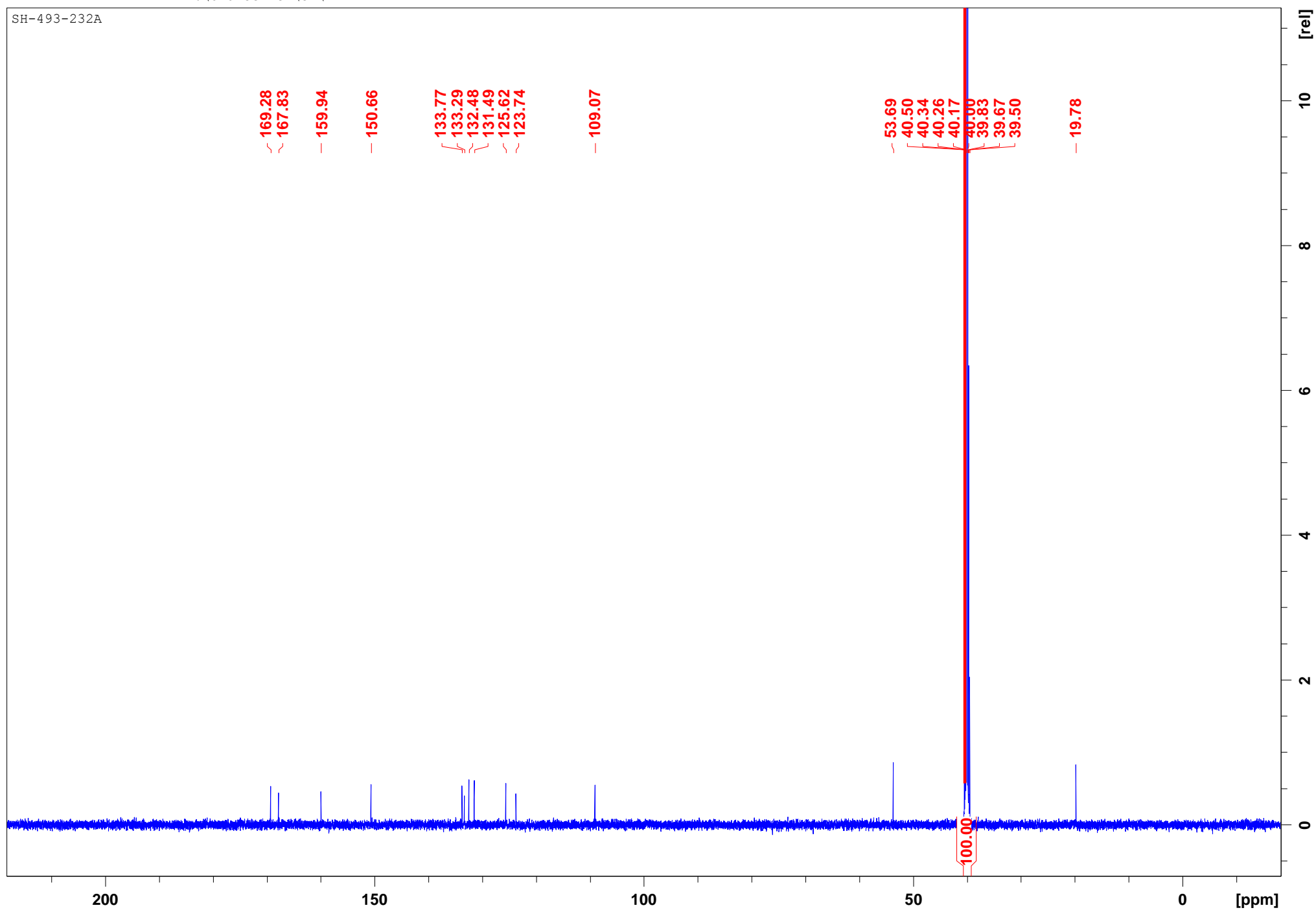


19c

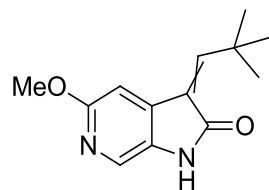


SH-493-232A 11 1 "X:\Old Server\SH\nmr"

SH-493-232A

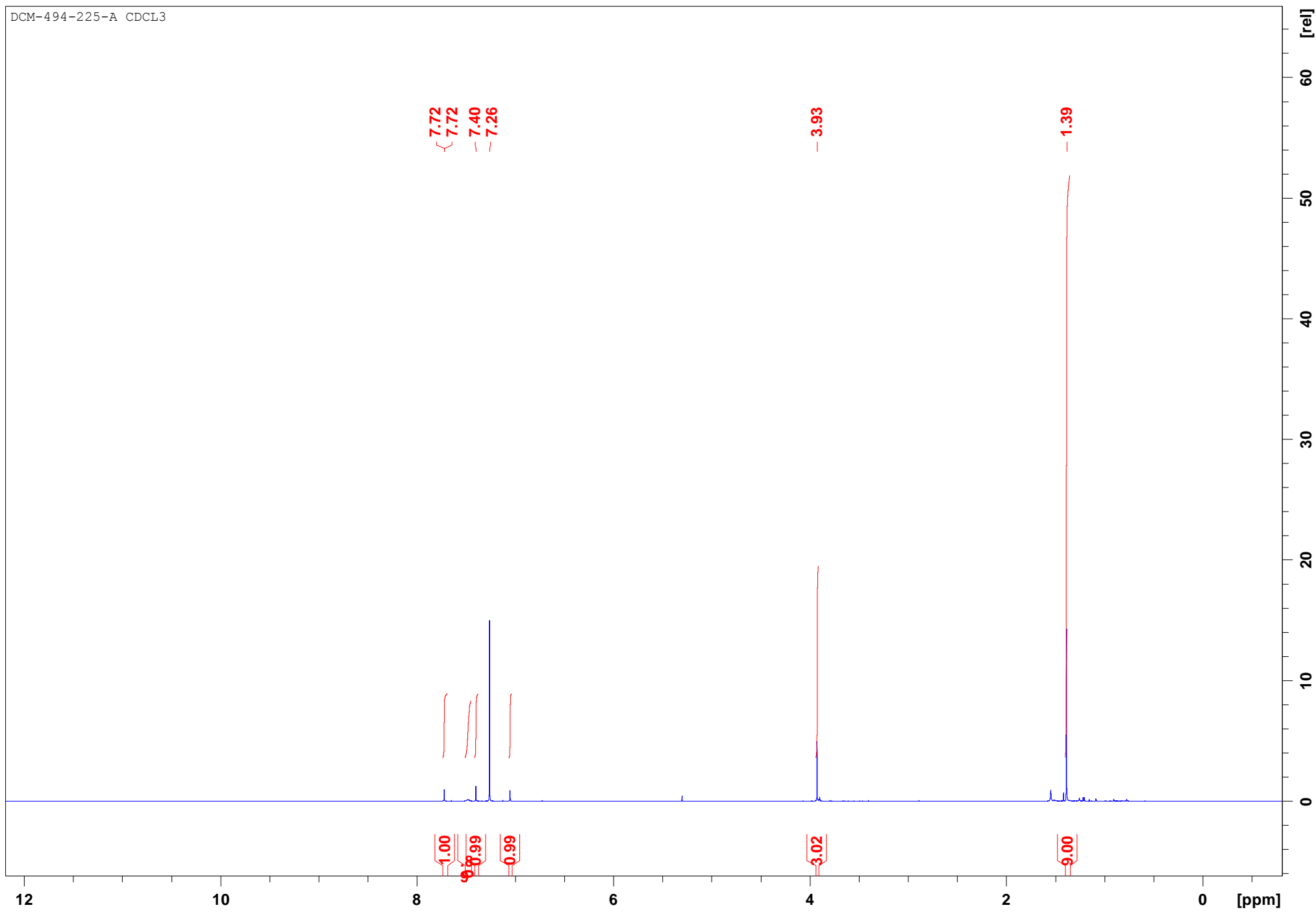


19d

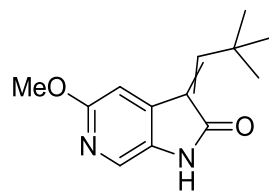


"DCM-494-225-A CDCL3" 10 1 X:\data\DCM\nmr

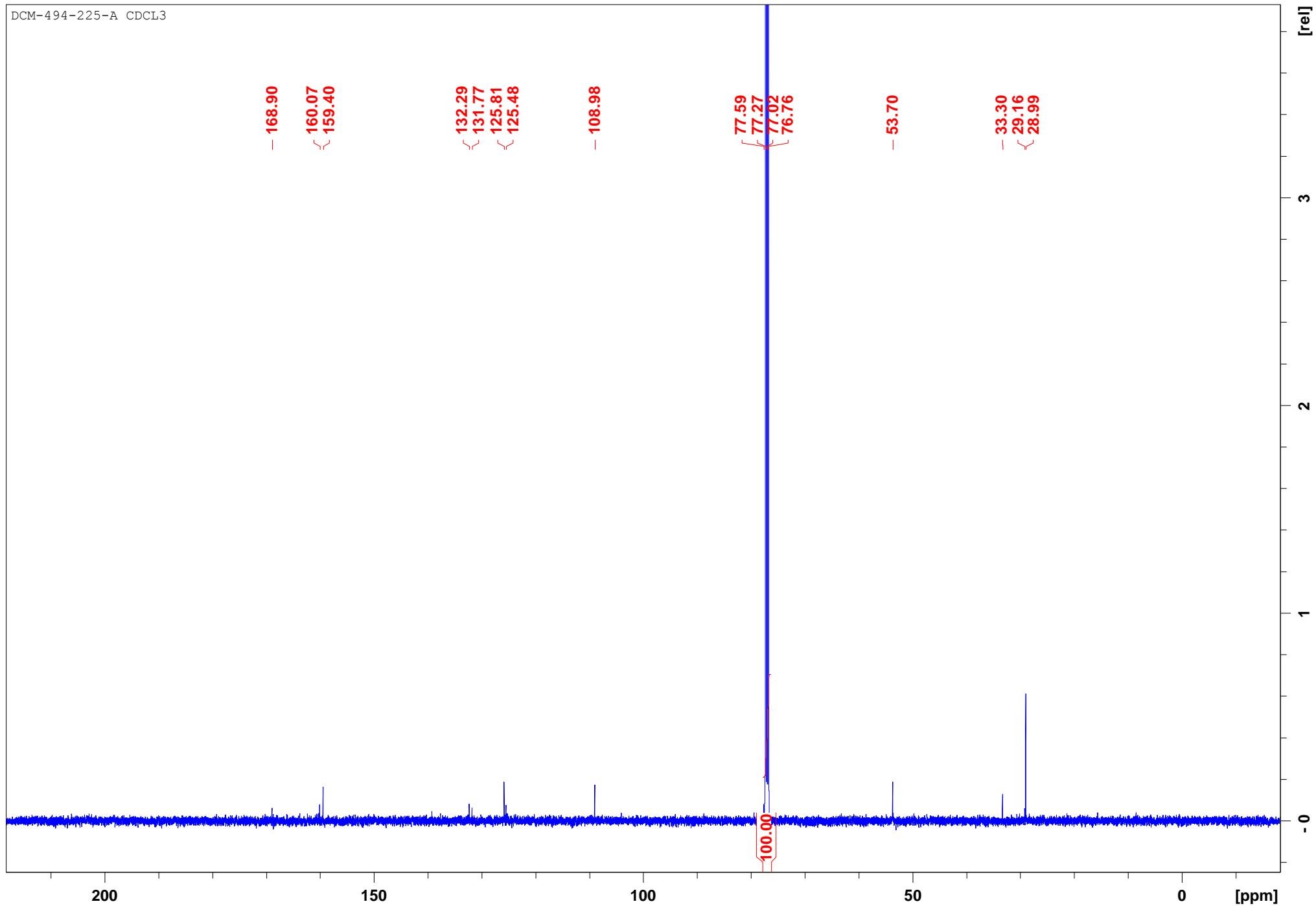
DCM-494-225-A CDCL3



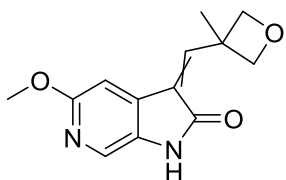
19d



"DCM-494-225-A CDCL3" 11 1 X:\data\DCM\nmr

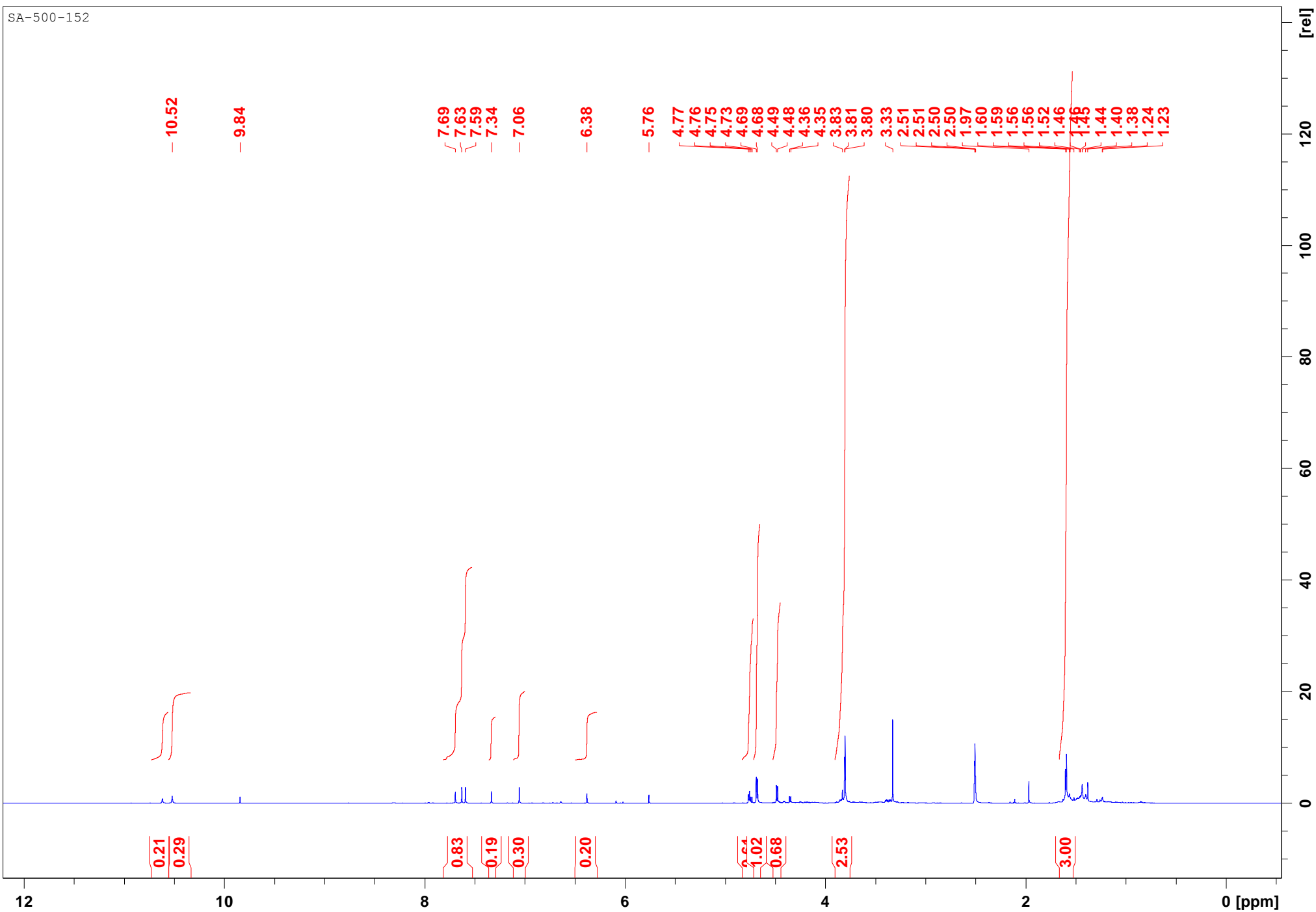


19e

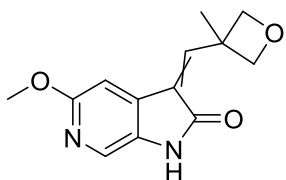


SA-500-152 10 1 "X:\Old Server\SA\nmr"

SA-500-152

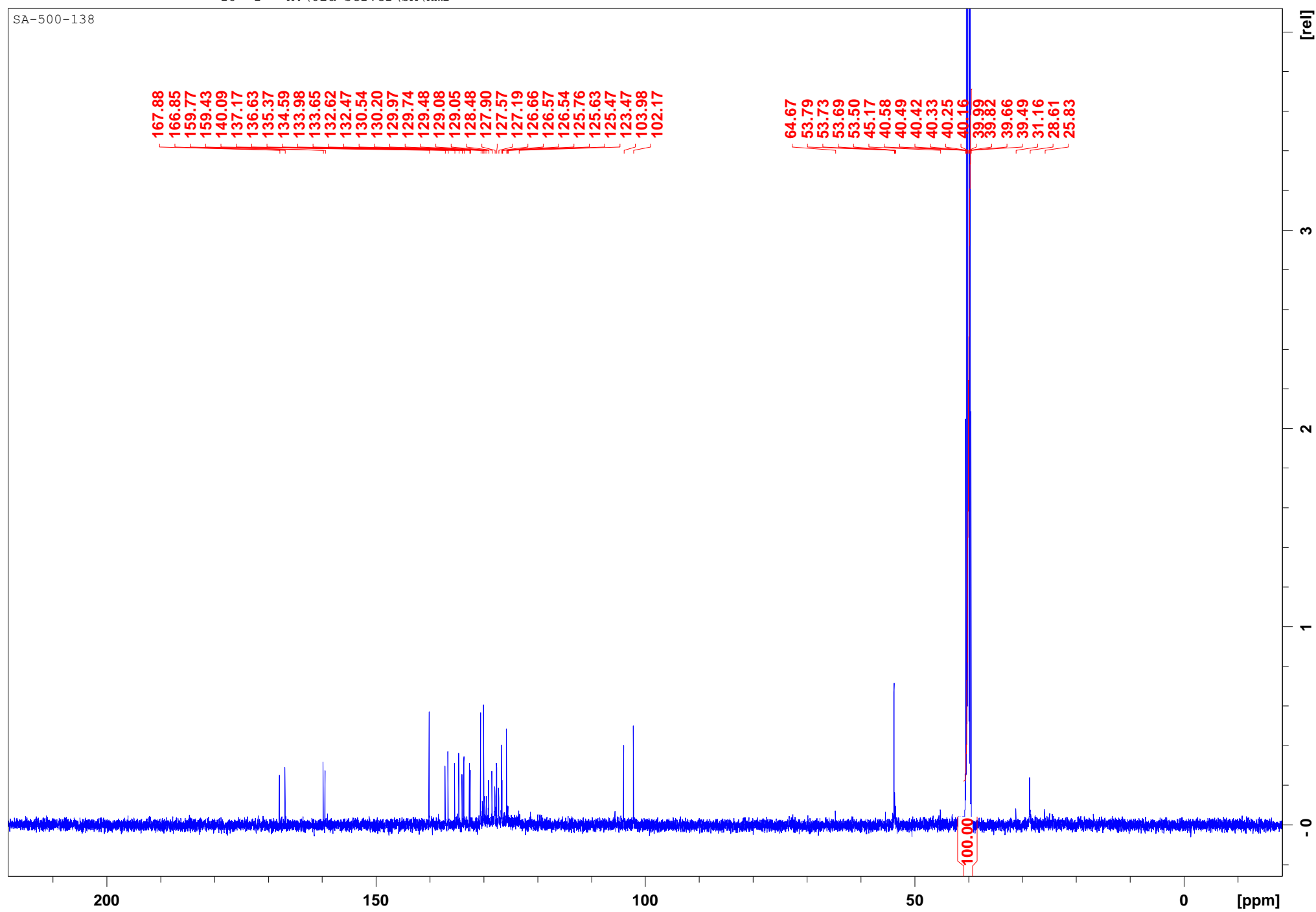


19e

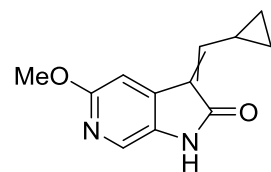


SA-500-138-CONCENTRATED 15 1 "X:\Old Server\SA\nmr"

SA-500-138

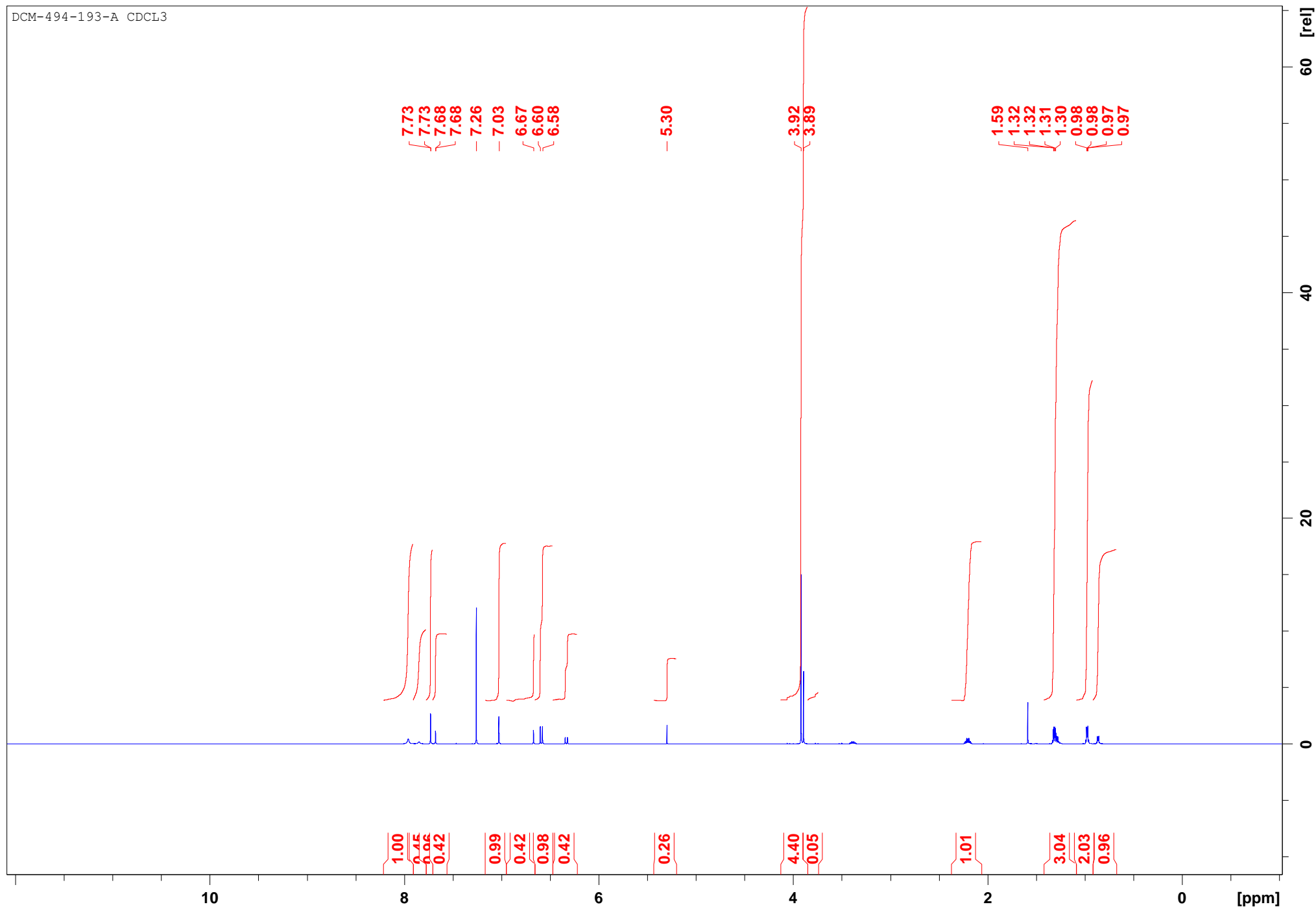


19f

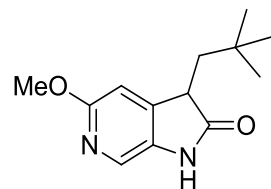


"DCM-494-193-A CDCL3" 10 1 "X:\Old Server\DCM\nmr"

DCM-494-193-A CDCL3

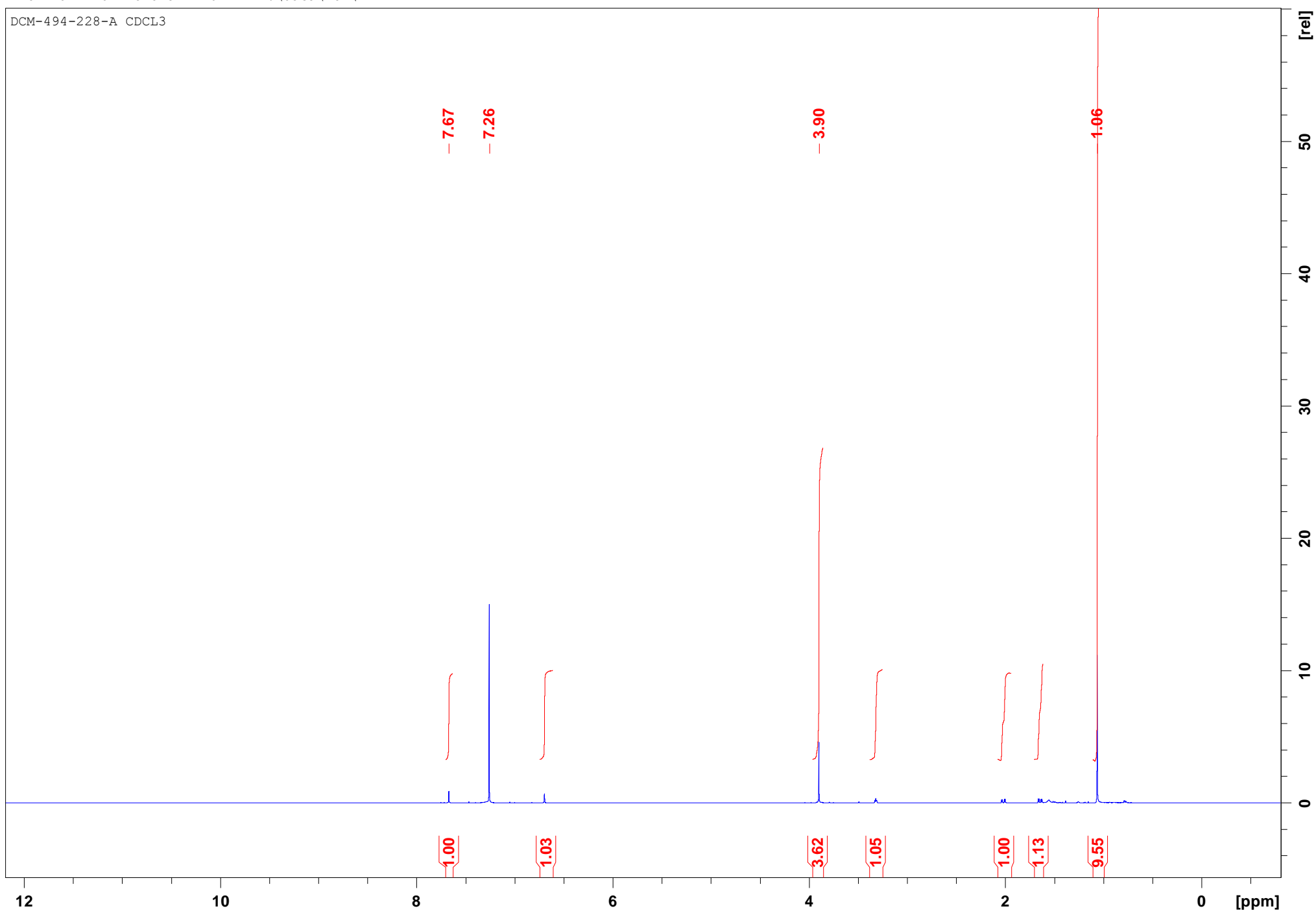


20d

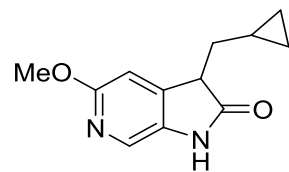


"DCM-494-228-A CDCL3" 10 1 X:\data\DCM\nmr

DCM-494-228-A CDCL3

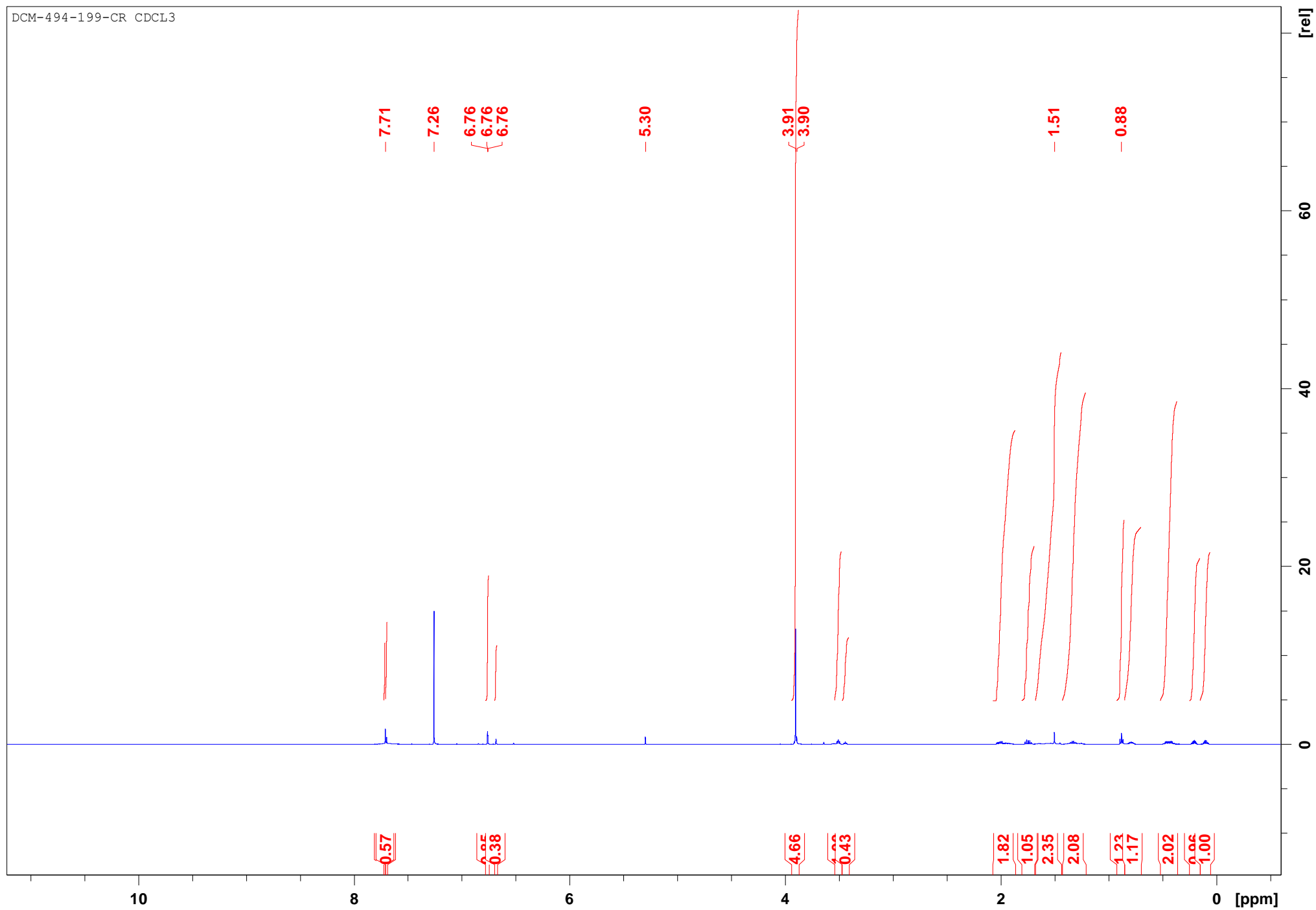


20f

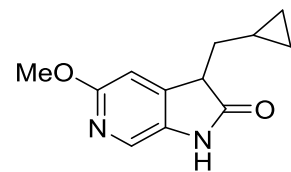


"DCM-494-199-CR CDCL3" 10 1 "X:\Old Server\DCM\nmr"

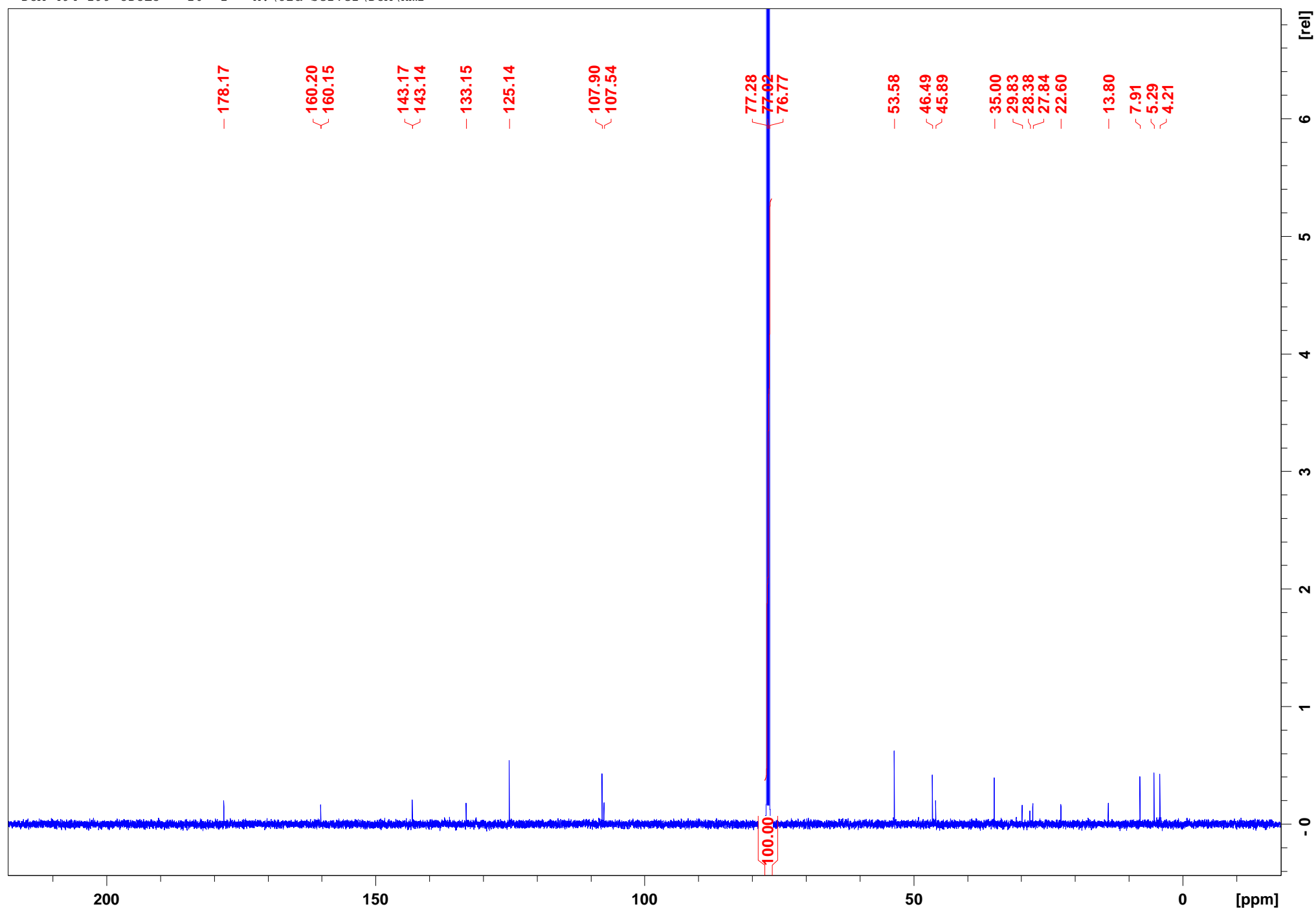
DCM-494-199-CR CDCL3



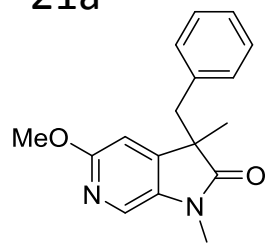
20f



"DCM-494-199 CDCL3" 10 1 "X:\Old Server\DCM\nmr"

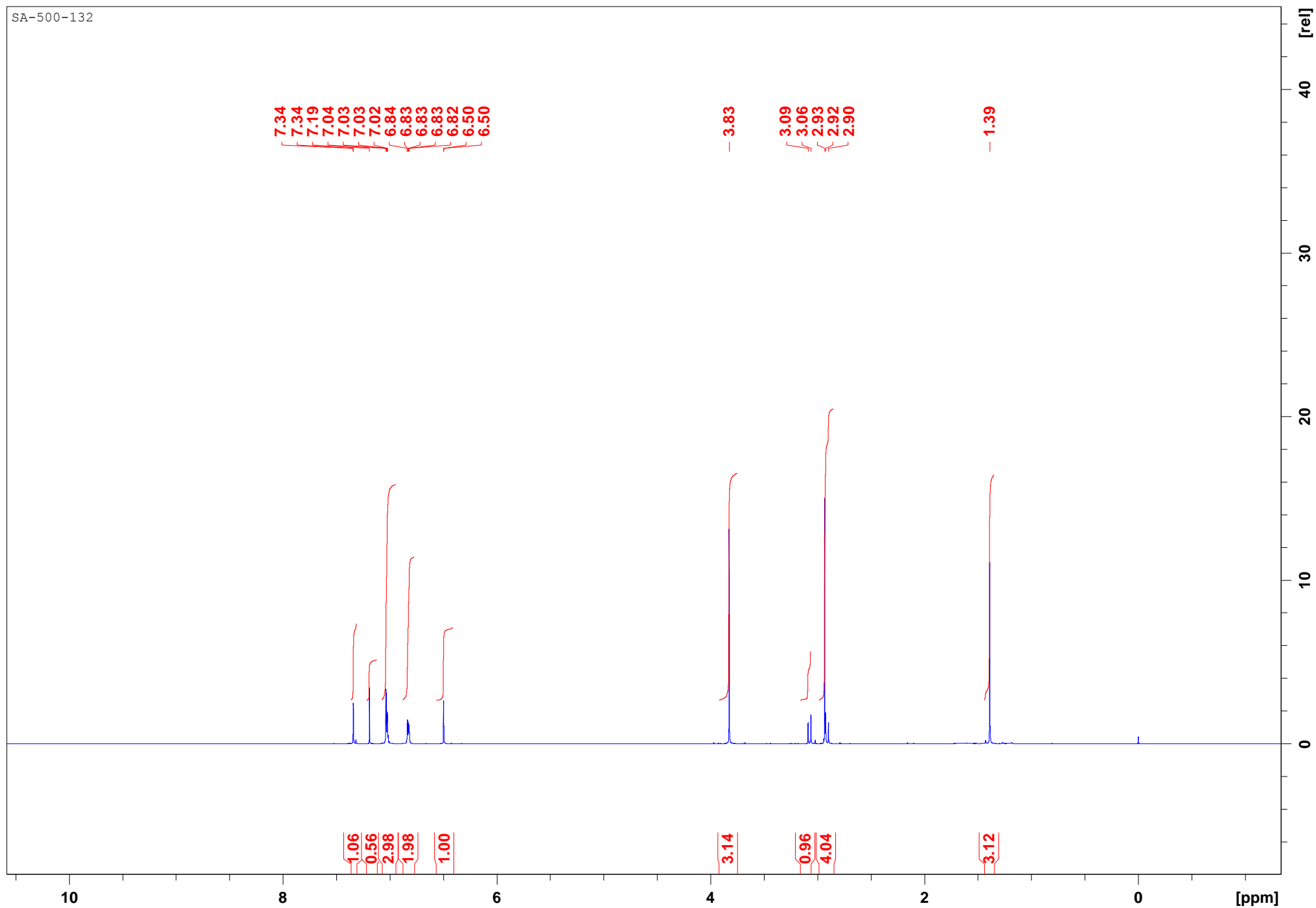


21a

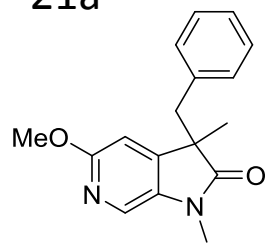


SA-500-132 10 1 "X:\Old Server\SA\nmr"

SA-500-132

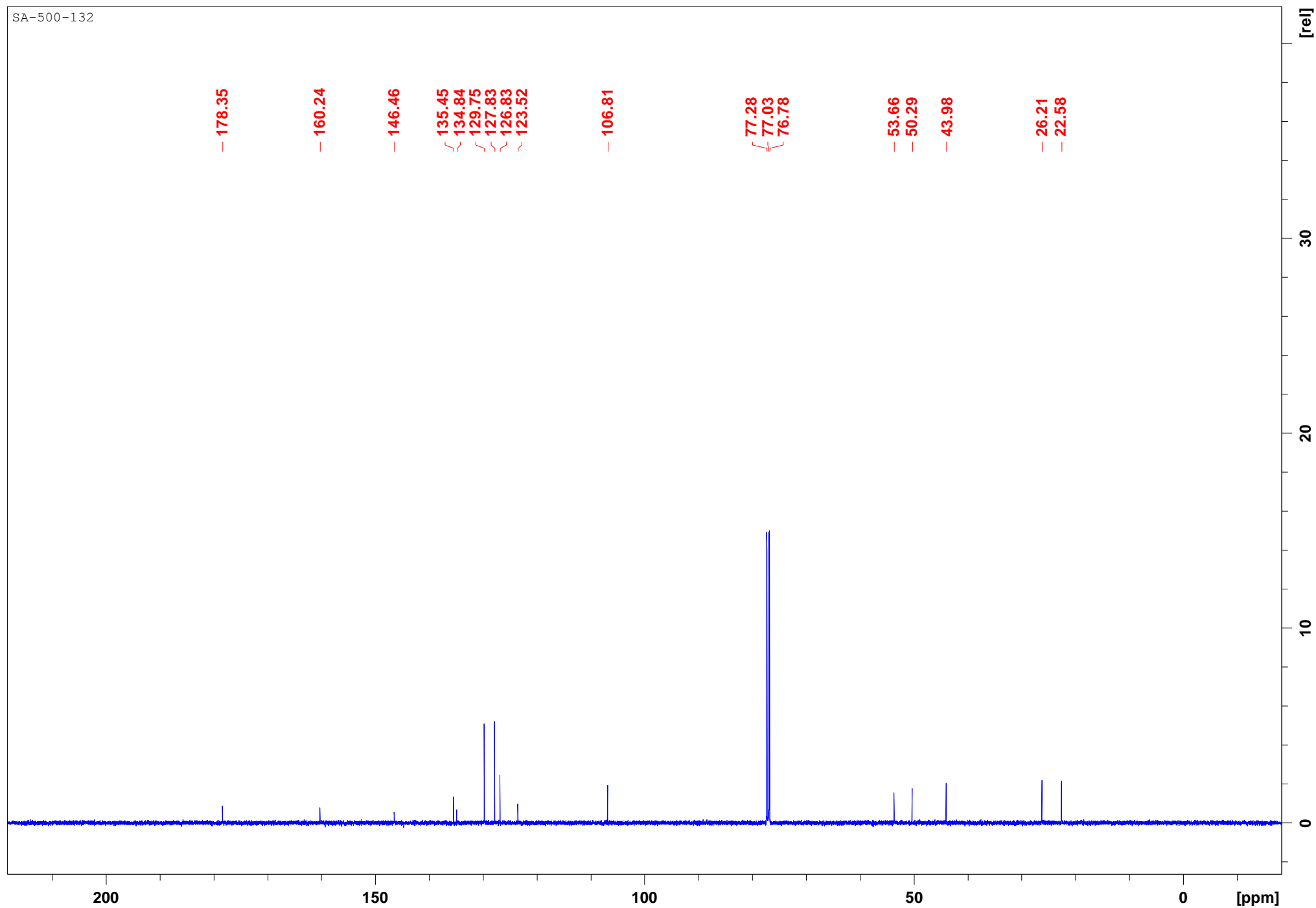


21a

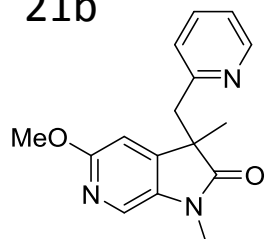


SA-500-132 11 1 "X:\Old Server\SA\nmr"

SA-500-132

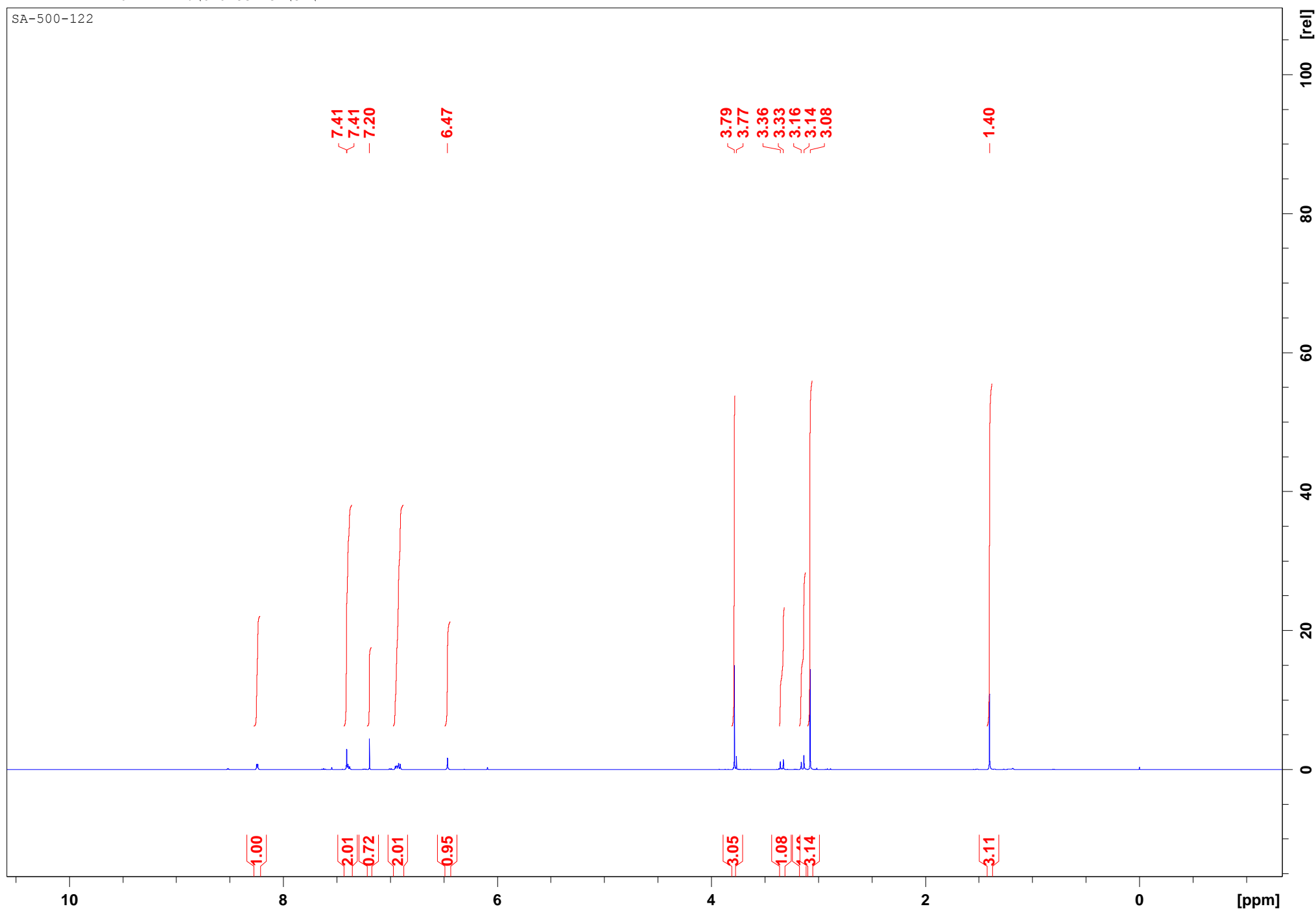


21b

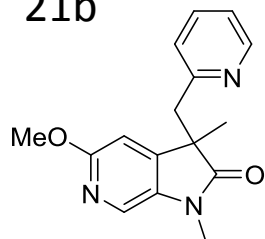


SA-500-122 10 1 "X:\Old Server\SA\nmr"

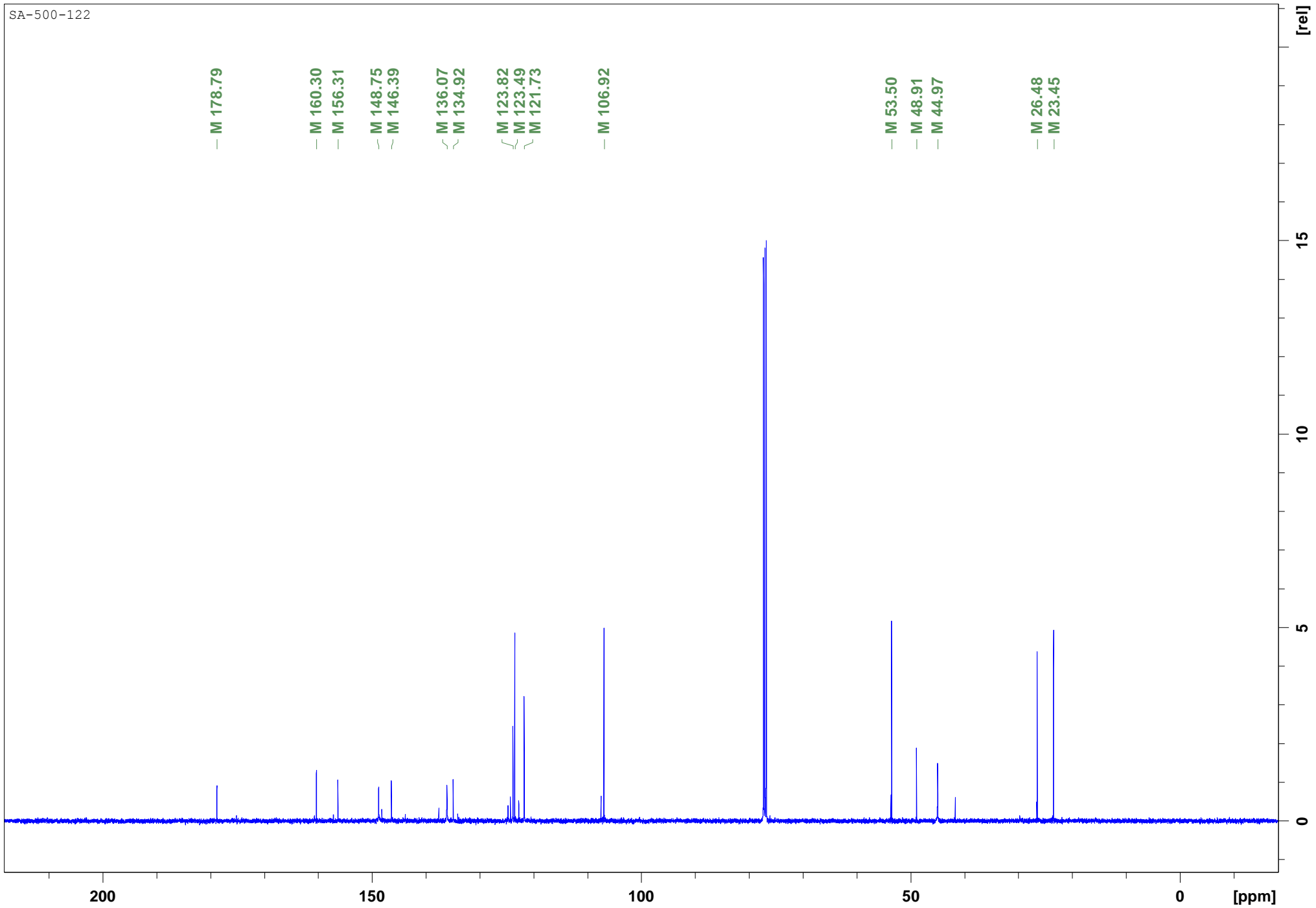
SA-500-122



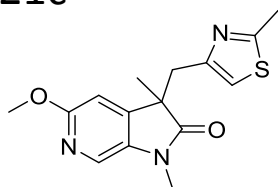
21b



SA-500-122 24 1 "X:\Old Server\SA\nmr"

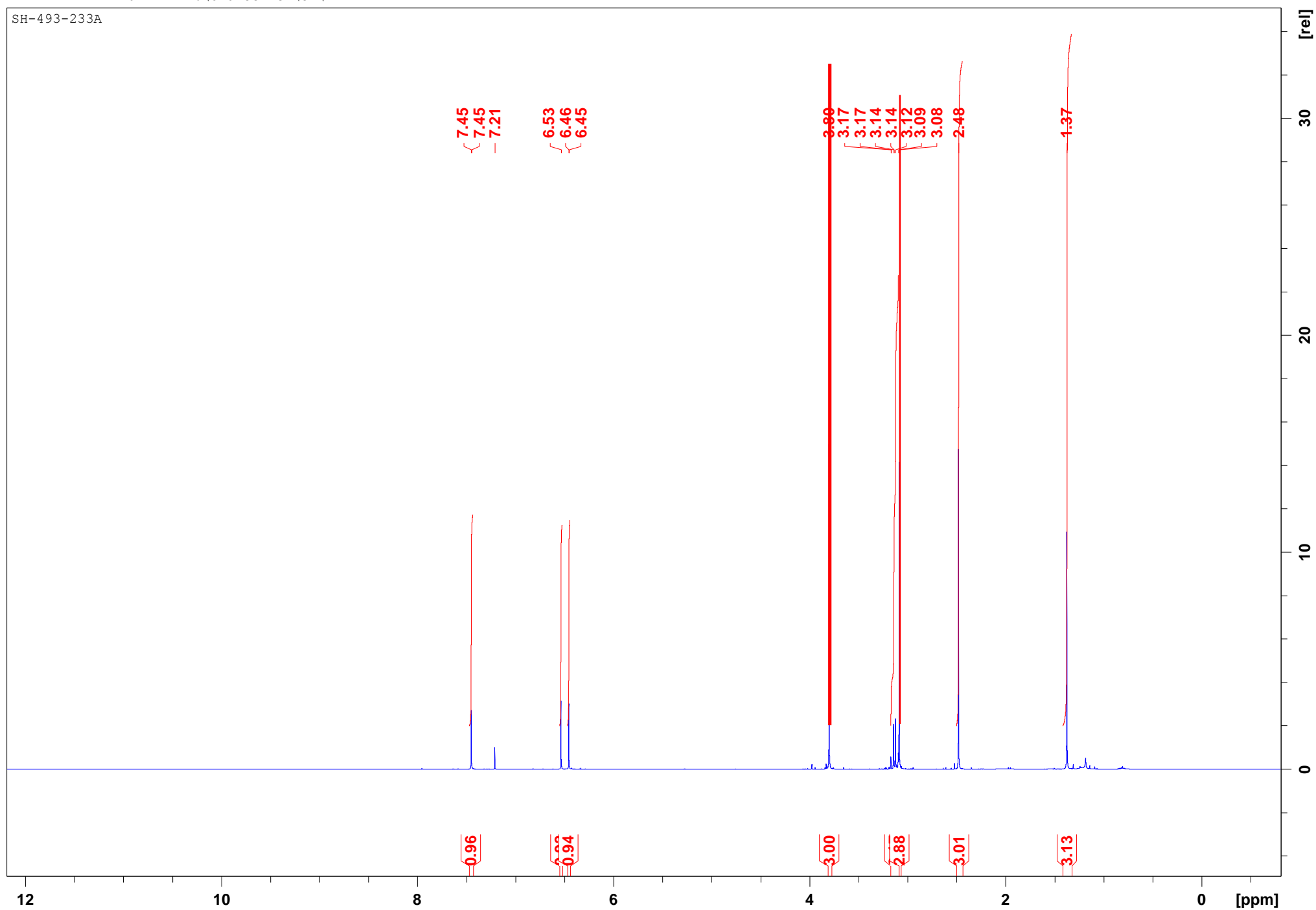


21c

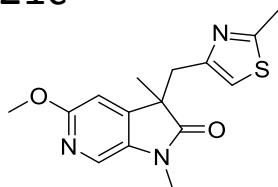


SH-493-233A 10 1 "X:\Old Server\SH\nmr"

SH-493-233A

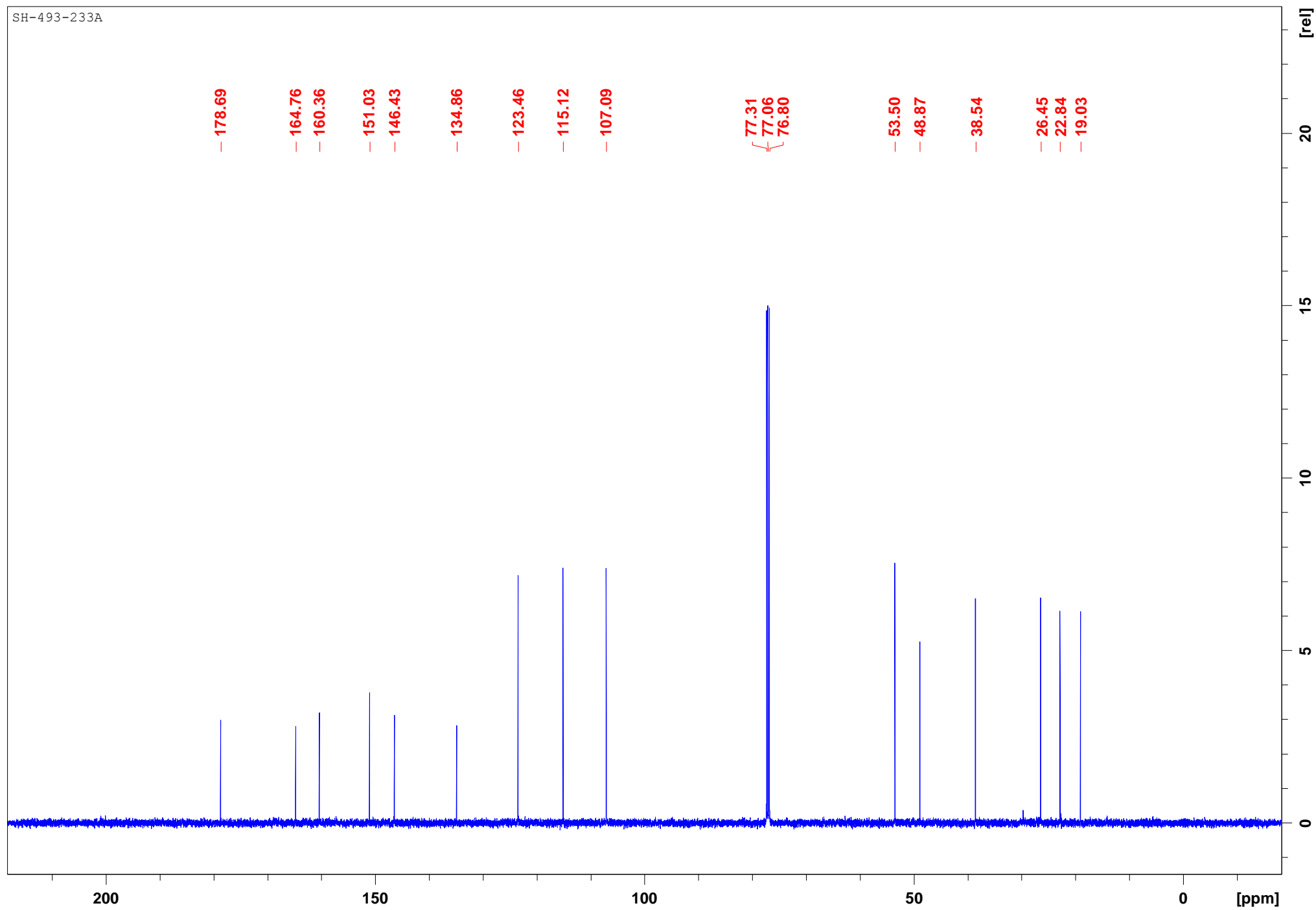


21c

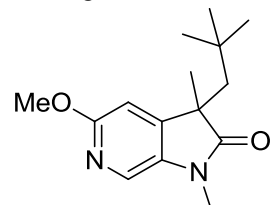


SH-493-233A 11 1 "X:\Old Server\SH\nmr"

SH-493-233A

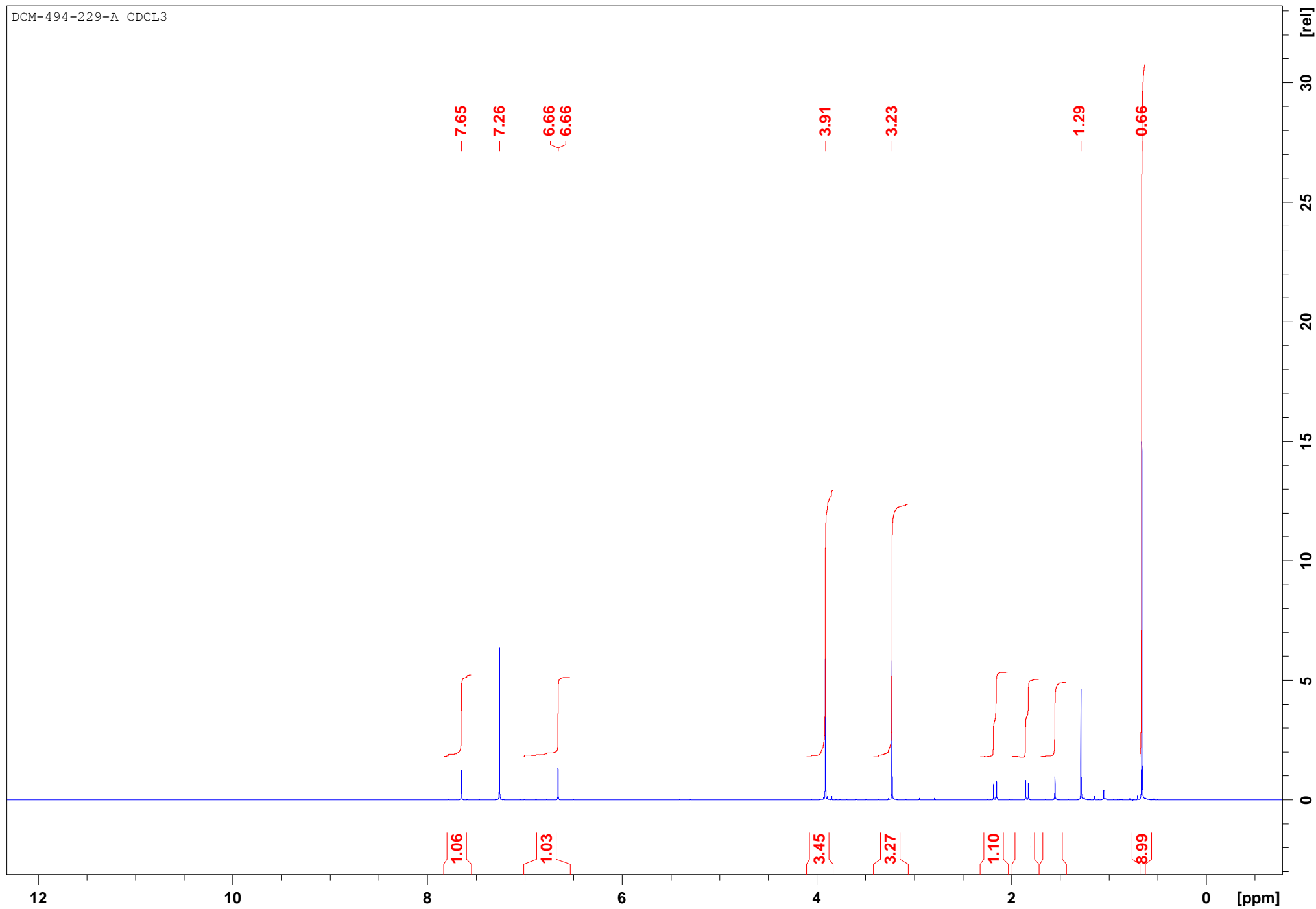


21d

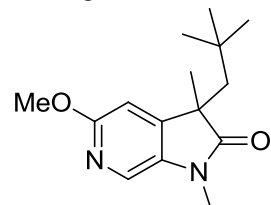


"DCM-494-229-A CDCL3" 10 1 X:\data\DCM\nmr

DCM-494-229-A CDCL3

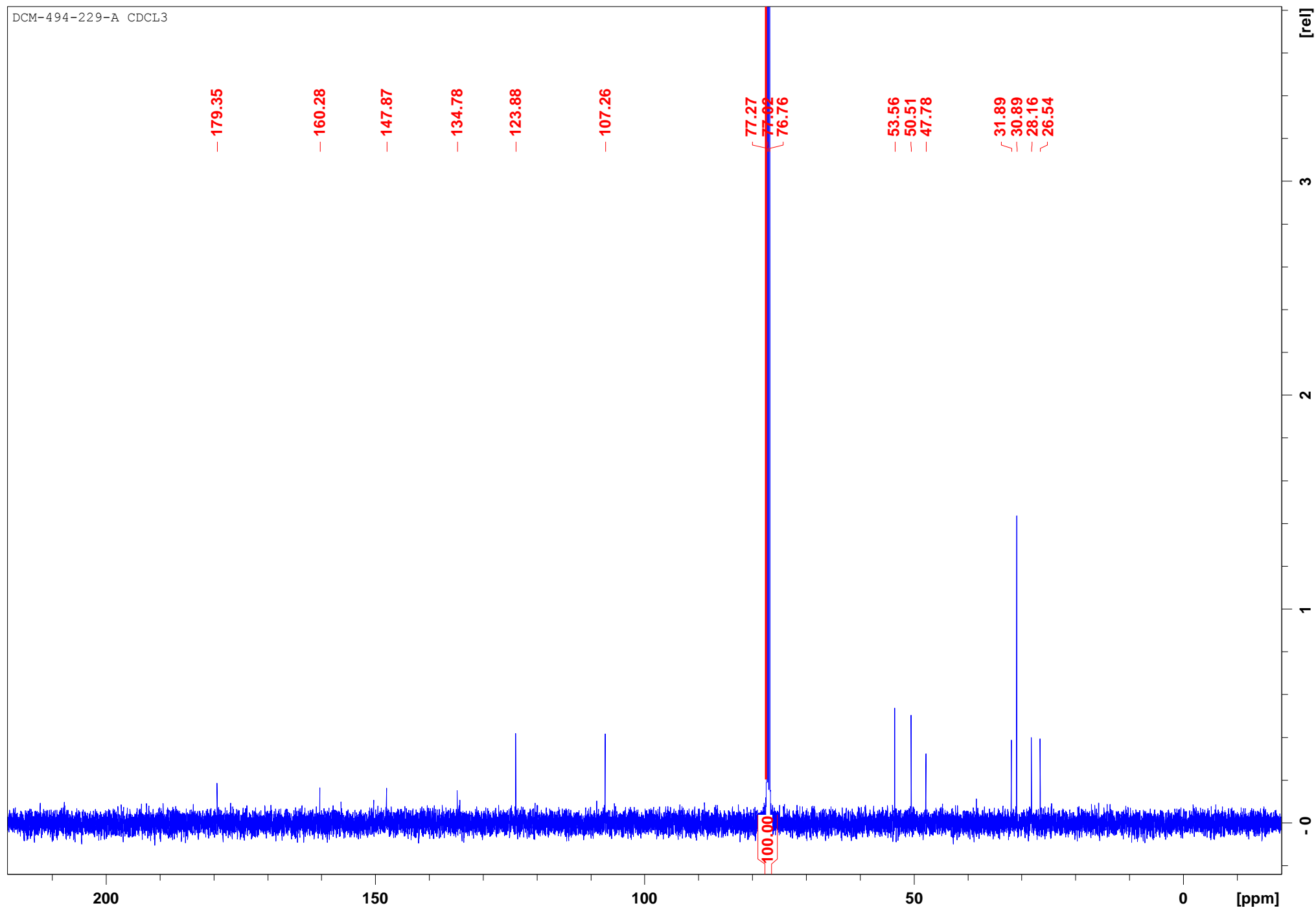


21d

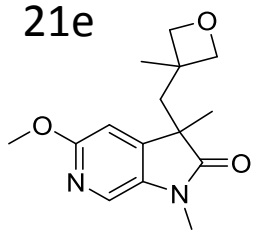


"DCM-494-229-A CDCL3" 12 1 X:\data\DCM\nmr

DCM-494-229-A CDCL3

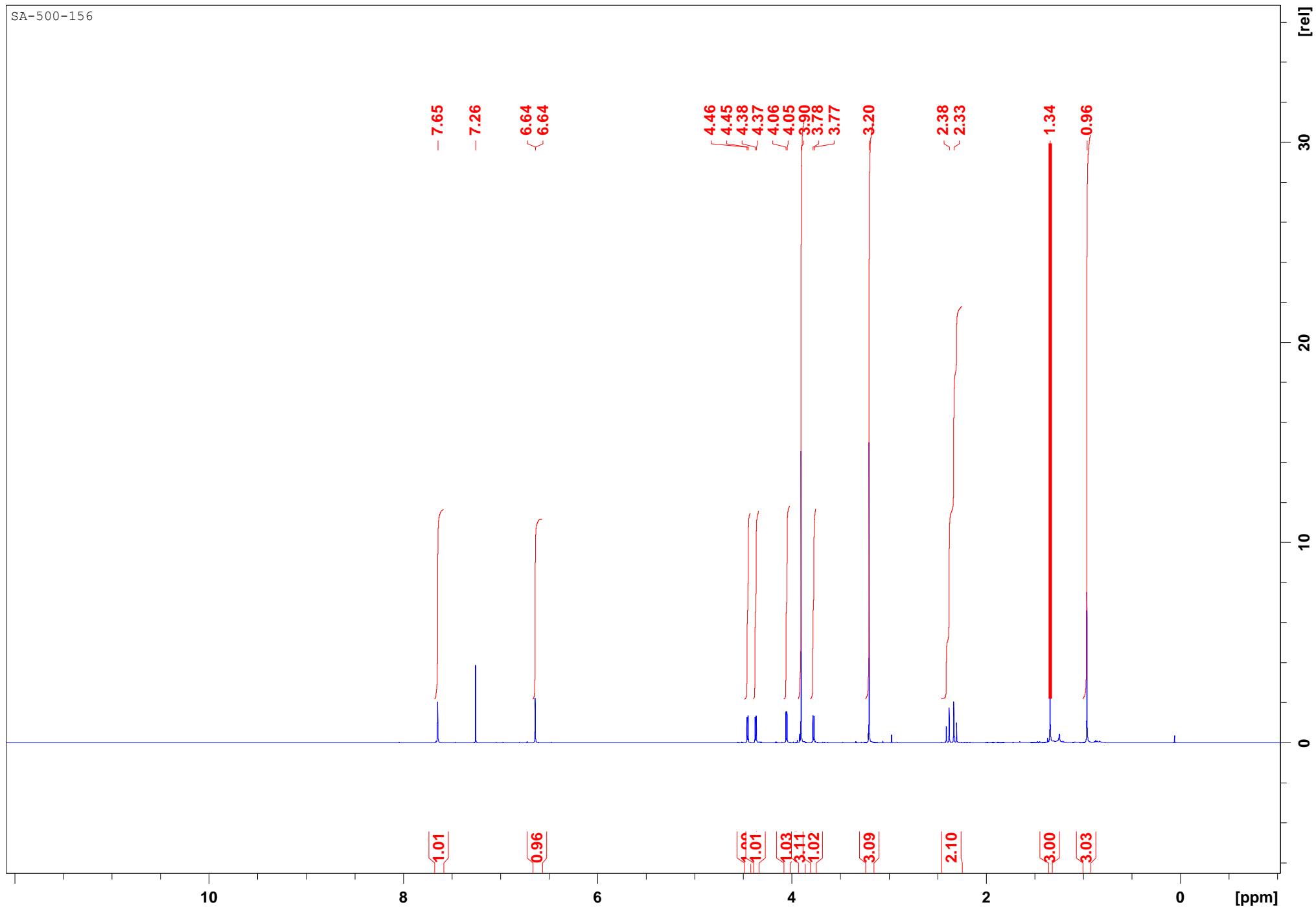


21e

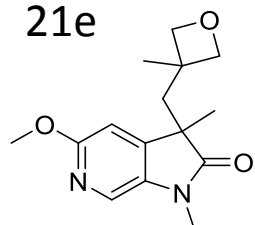


SA-500-156 10 1 "X:\Old Server\SA\nmr"

SA-500-156

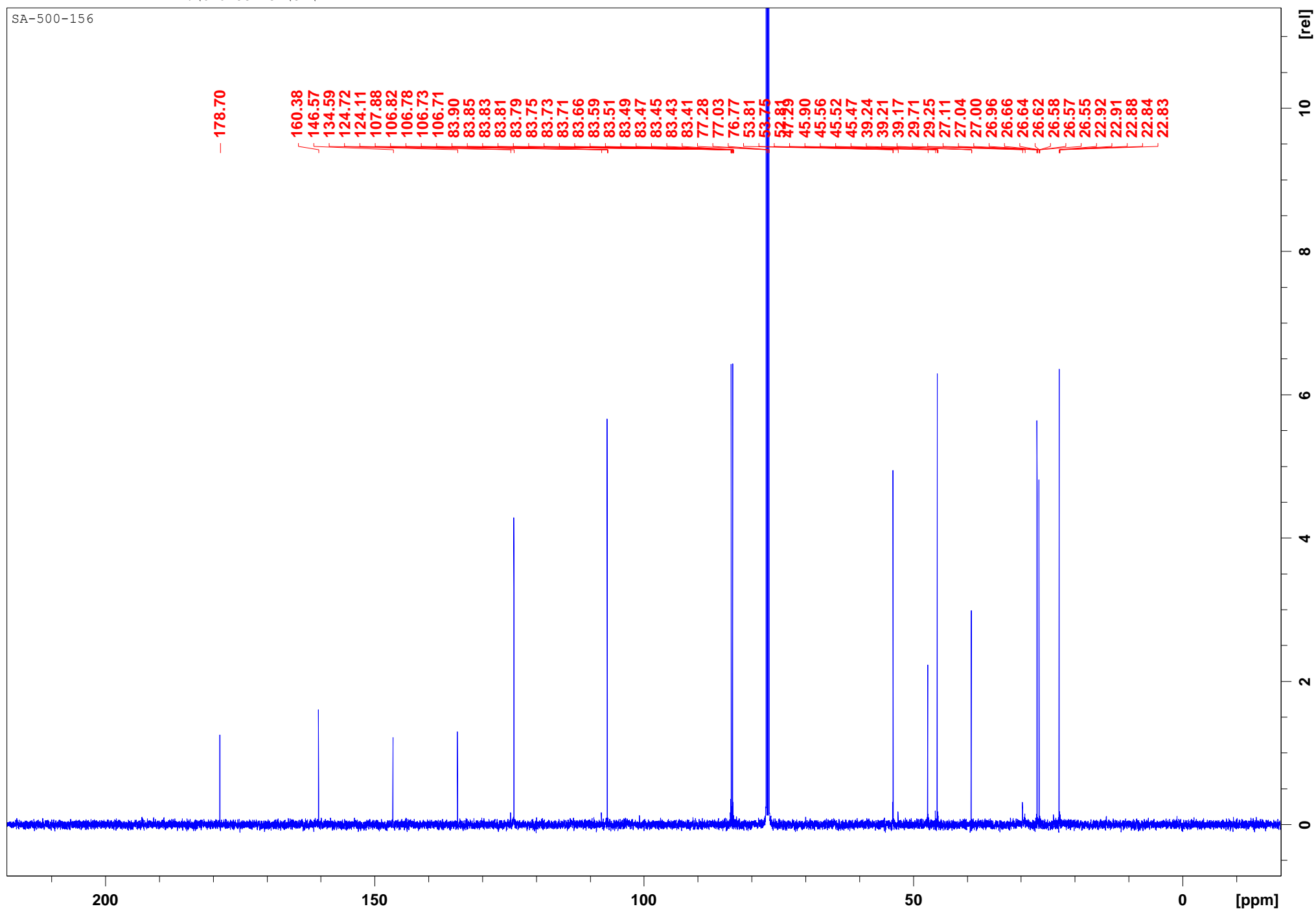


21e

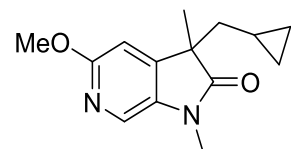


SA-500-156 11 1 "X:\Old Server\SA\nmr"

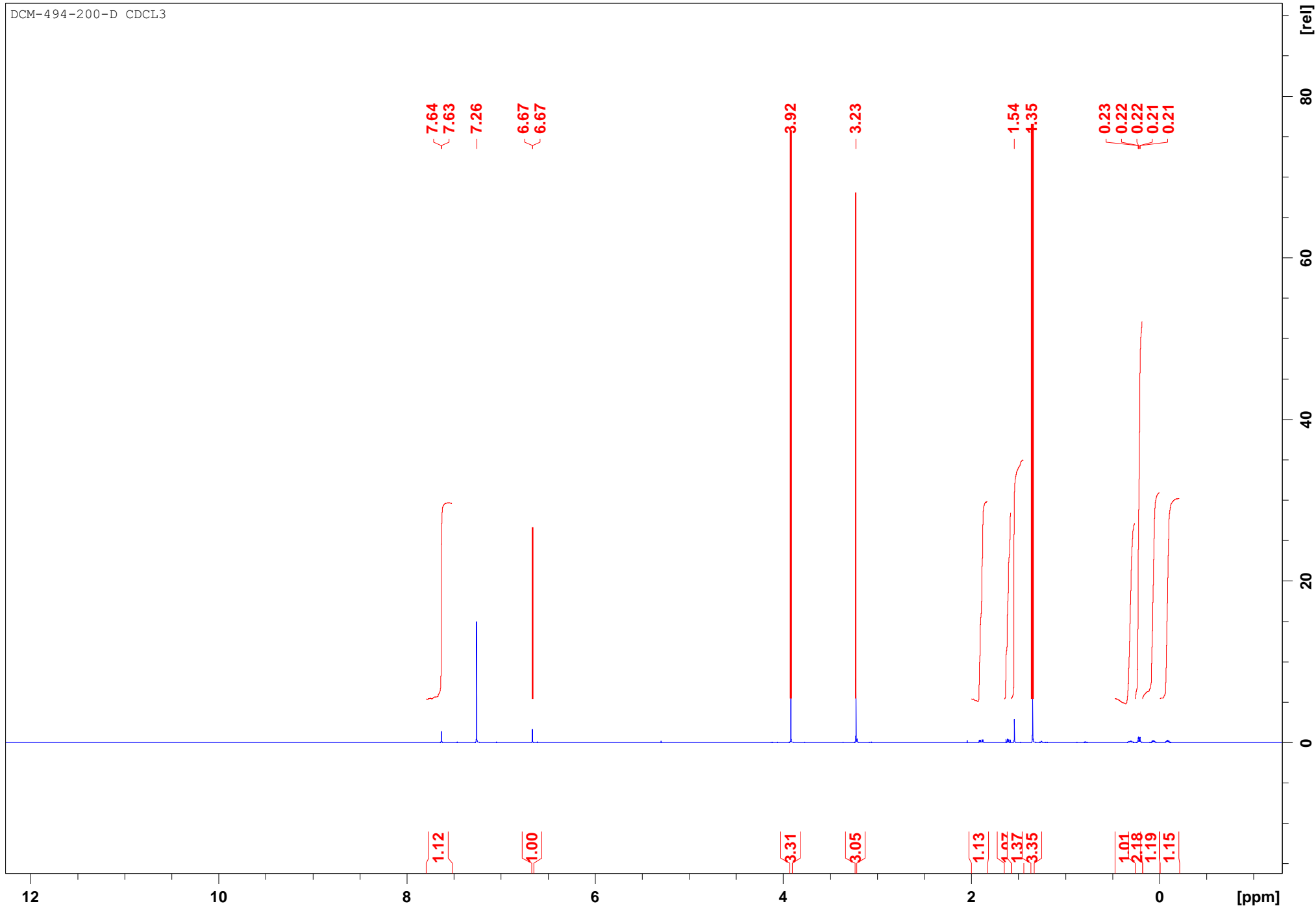
SA-500-156



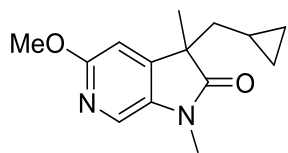
21f



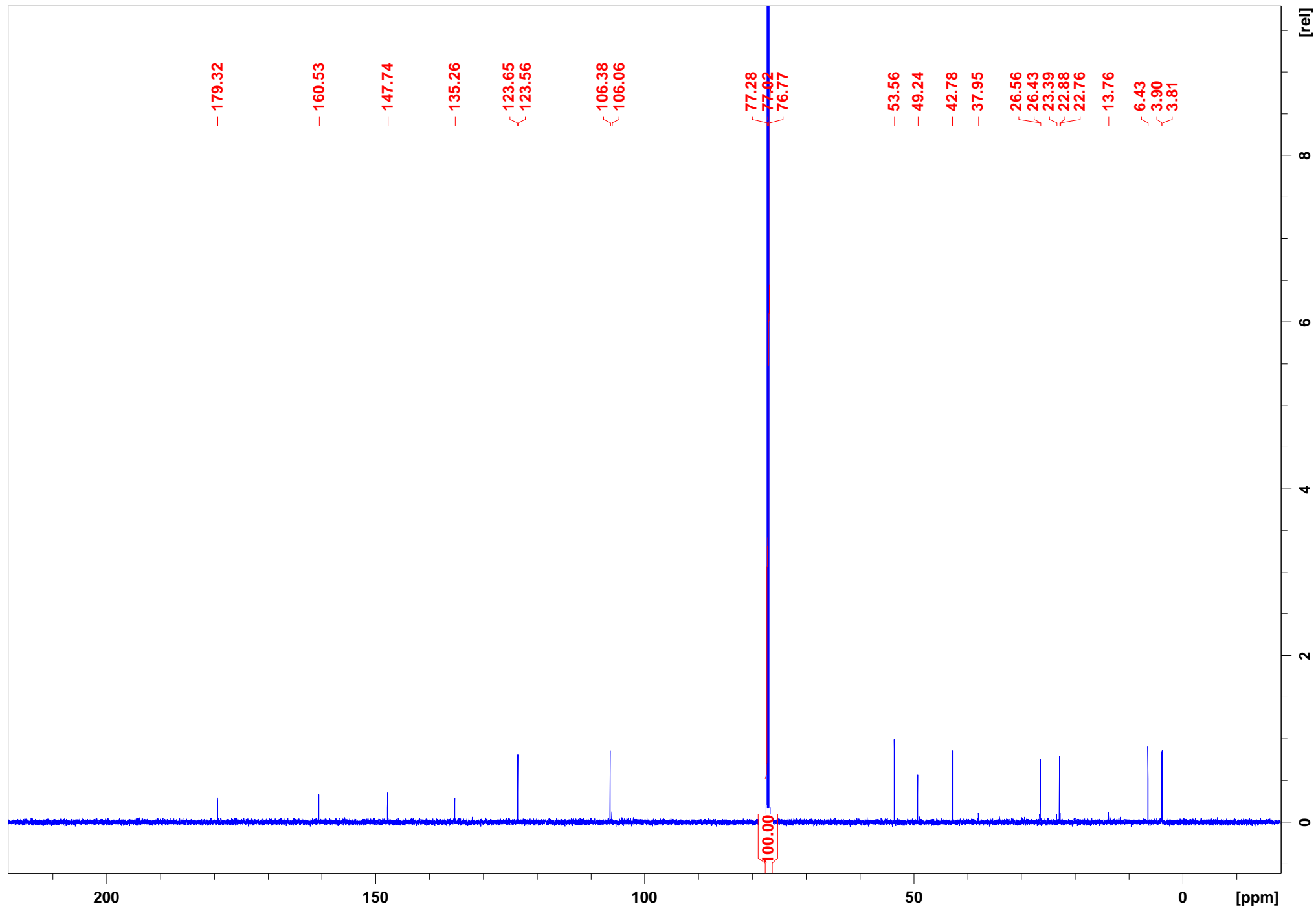
"DCM-494-200-D CDCL3" 10 1 "X:\Old Server\DCM\nmr"



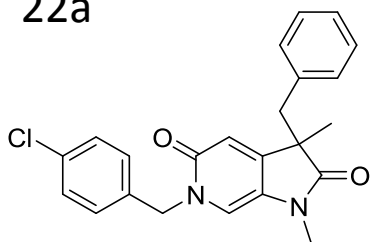
21f



"DCM-494-200-A CDCl3" 20 1 "X:\Old Server\DCM\nmr"



22a



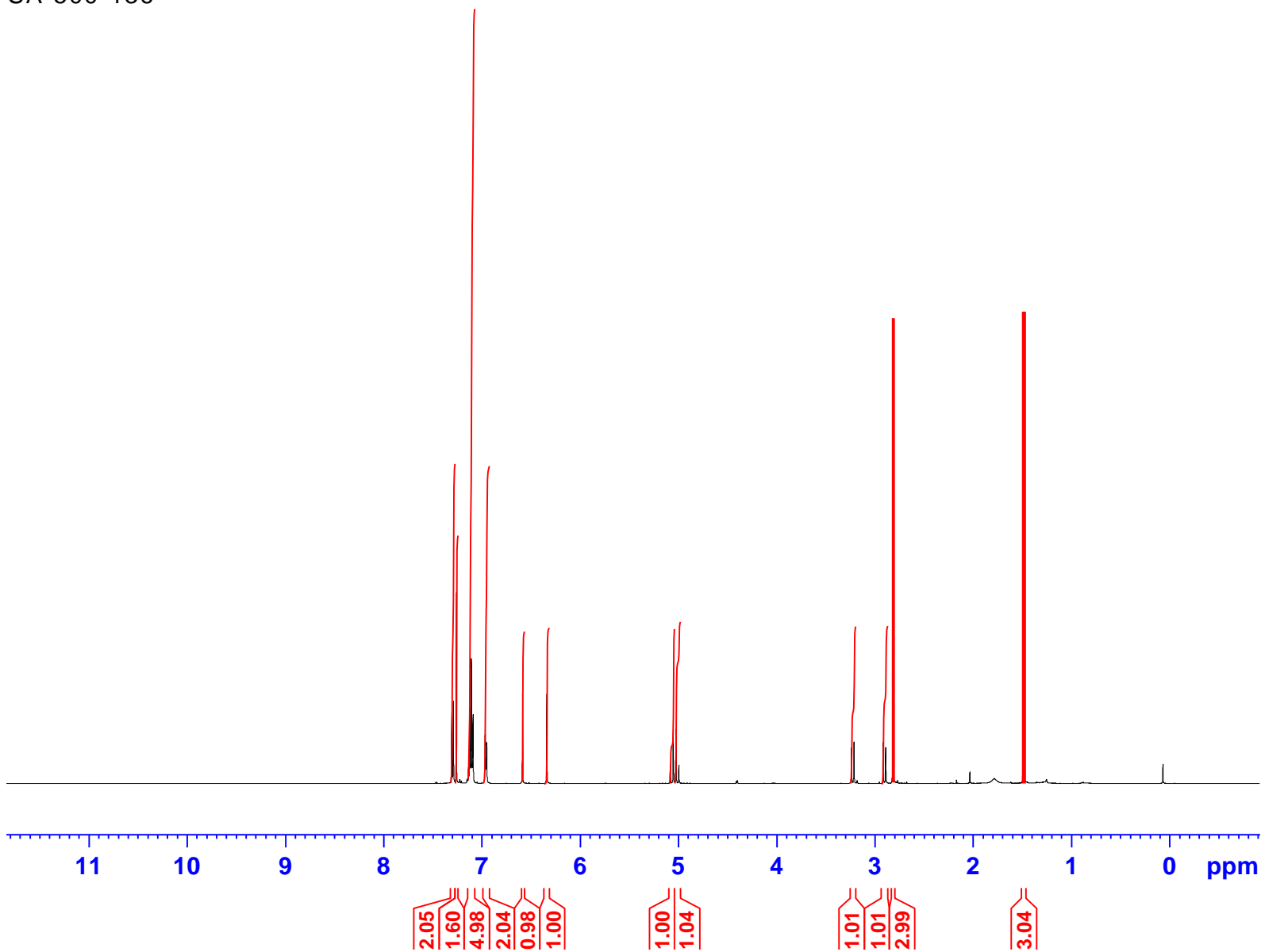
SA-500-136

7.307
7.291
7.260
7.123
7.107
7.090
6.969
6.966
6.954
6.951
6.587
6.340

5.053
5.025

3.239
3.213
2.916
2.890
2.818

1.488



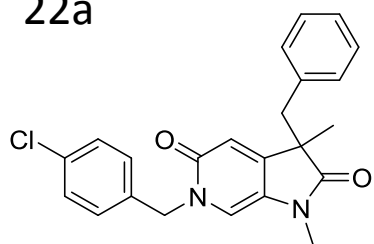
Current Data
Name SA-500-136-DRIED
EXPNO 10
PROCNO 1

F2 - Acquisition
Data 20150317
Time 17.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 512
DW 48.400 usec
DE 11.99 usec
TE 296.9 K
D1 1.0000000 sec
TD0 1

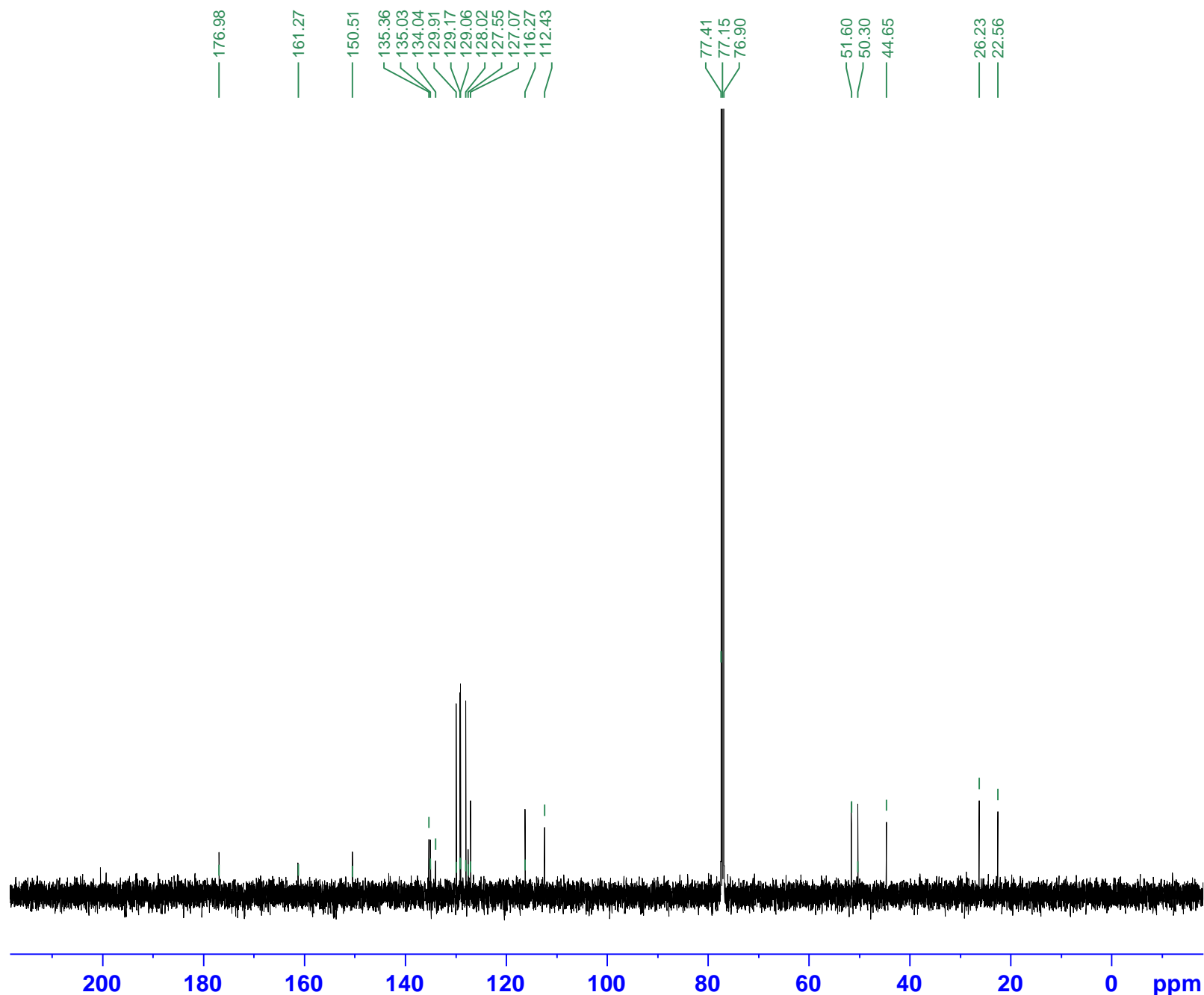
==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

F2 - Processing parameters SI
65536
SF 500.3000120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

22a



SA-500-136



Current Data Parameters
 NAME SA-500-136-DRIED
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20150318
 Time 1.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 297.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

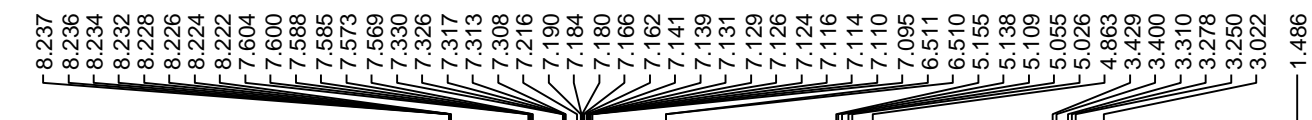
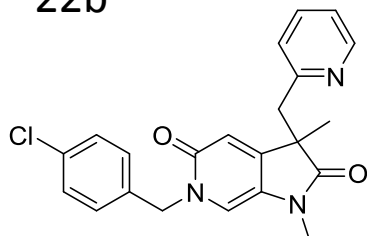
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

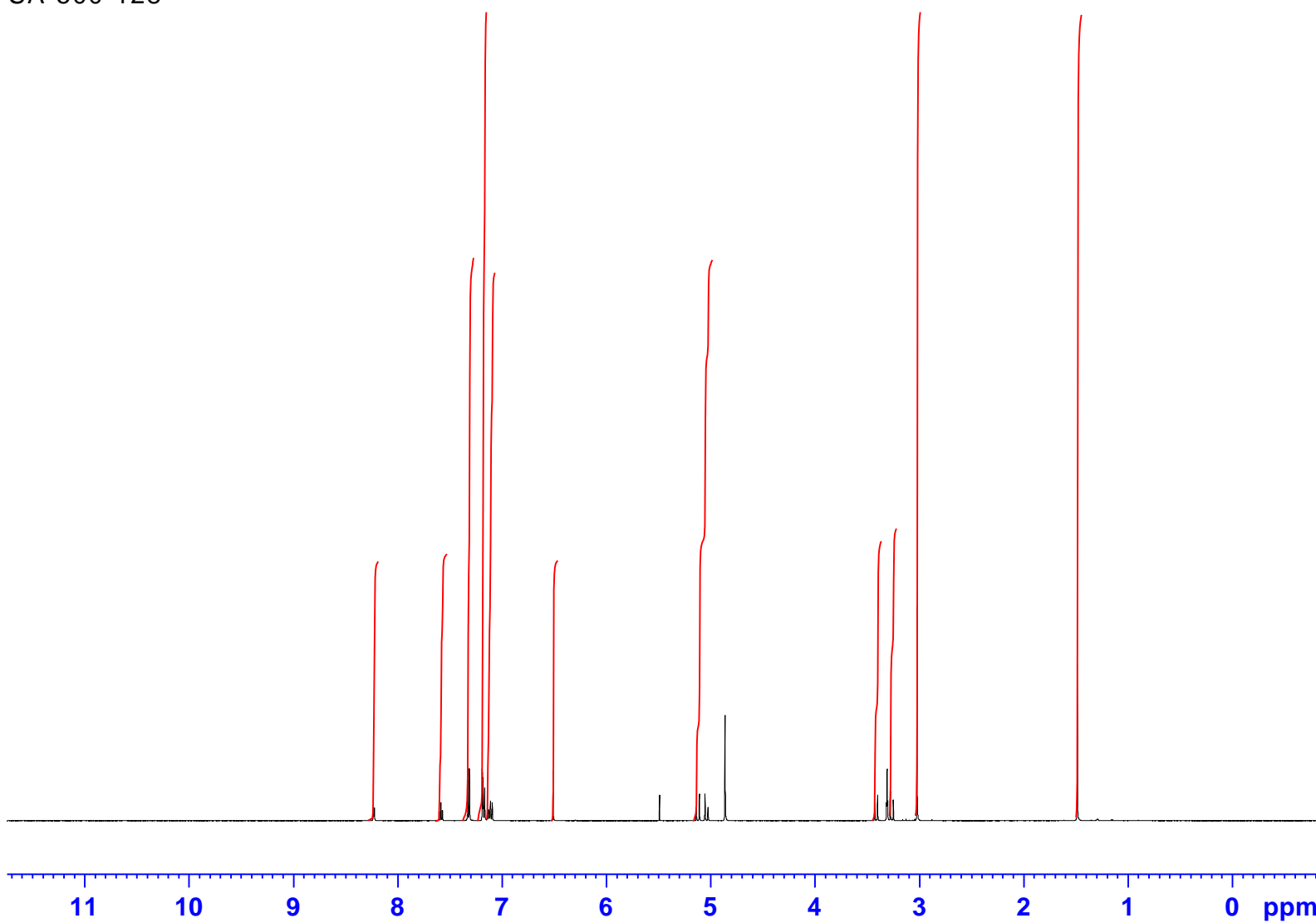
SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005190 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.20

22b



SA-500-128



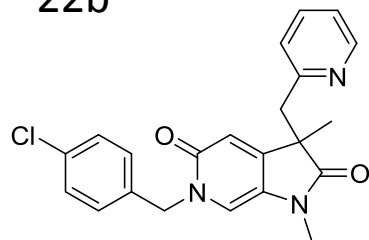
Current Data
 Name SA-500-128
 EXPNO 10
 PROCNO 1

F2 - Acquisition
 Date 20150312
 Time 19.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 0
 SMH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1719425 sec
 RG 406
 DW 48.400 usec
 DE 11.99 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 500.3030896 MHz
 NUC1 1H
 P1 16.25 usec
 PLW1 18.33600044 W

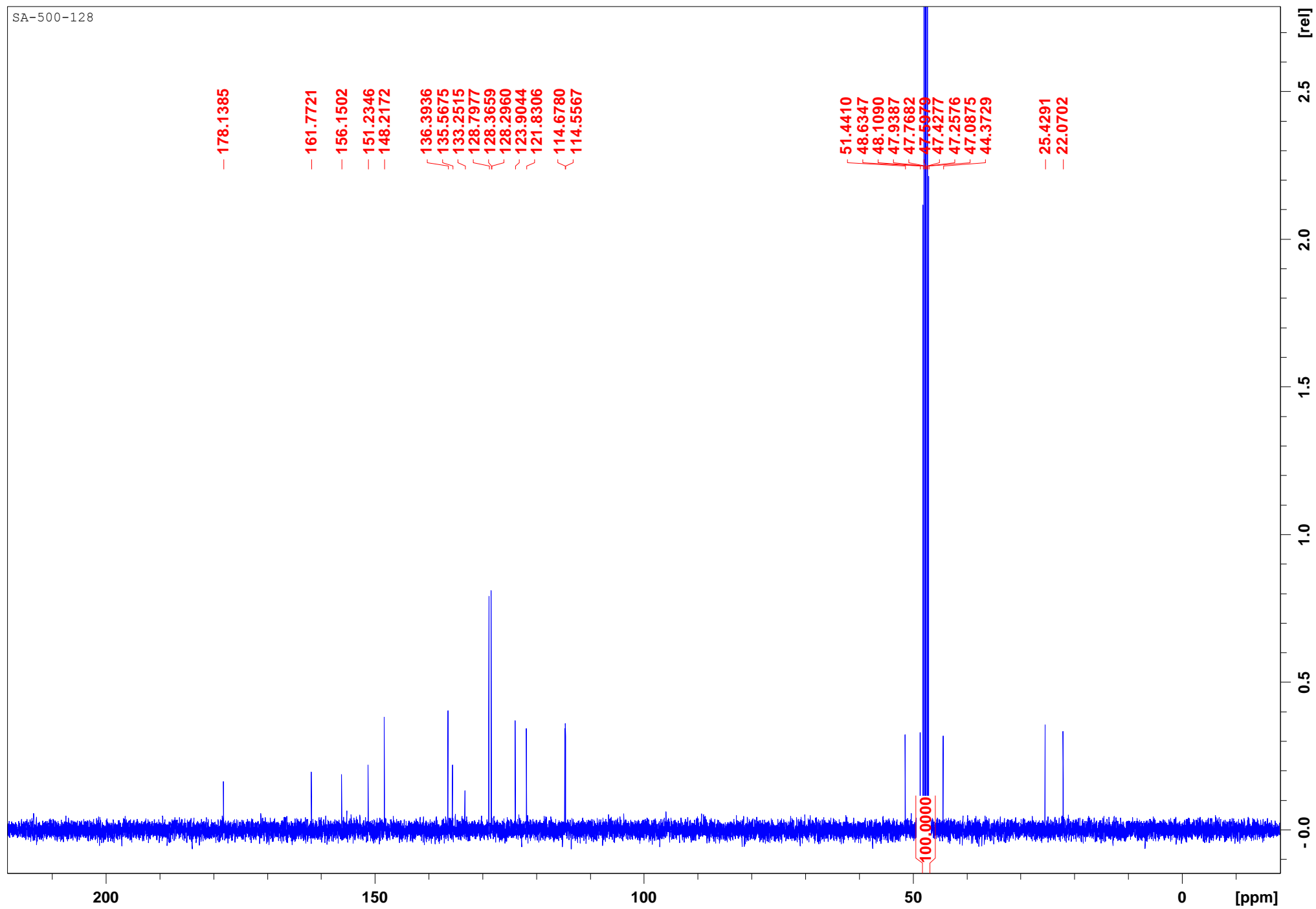
F2 - Processing parameters SI
 65536
 SF 500.300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

22b

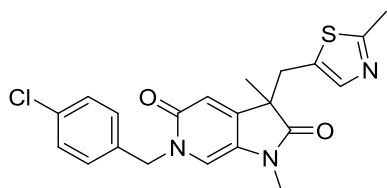


SA-500-128 11 1 Z:\data\SA\nmr

SA-500-128



22c



7.244
7.227
7.111
7.095
6.606
6.421
6.360

5.024
4.993
4.984
4.954

3.220
3.192
3.066
3.037
2.925
2.467

1.391

SH-493-239A -
diluted

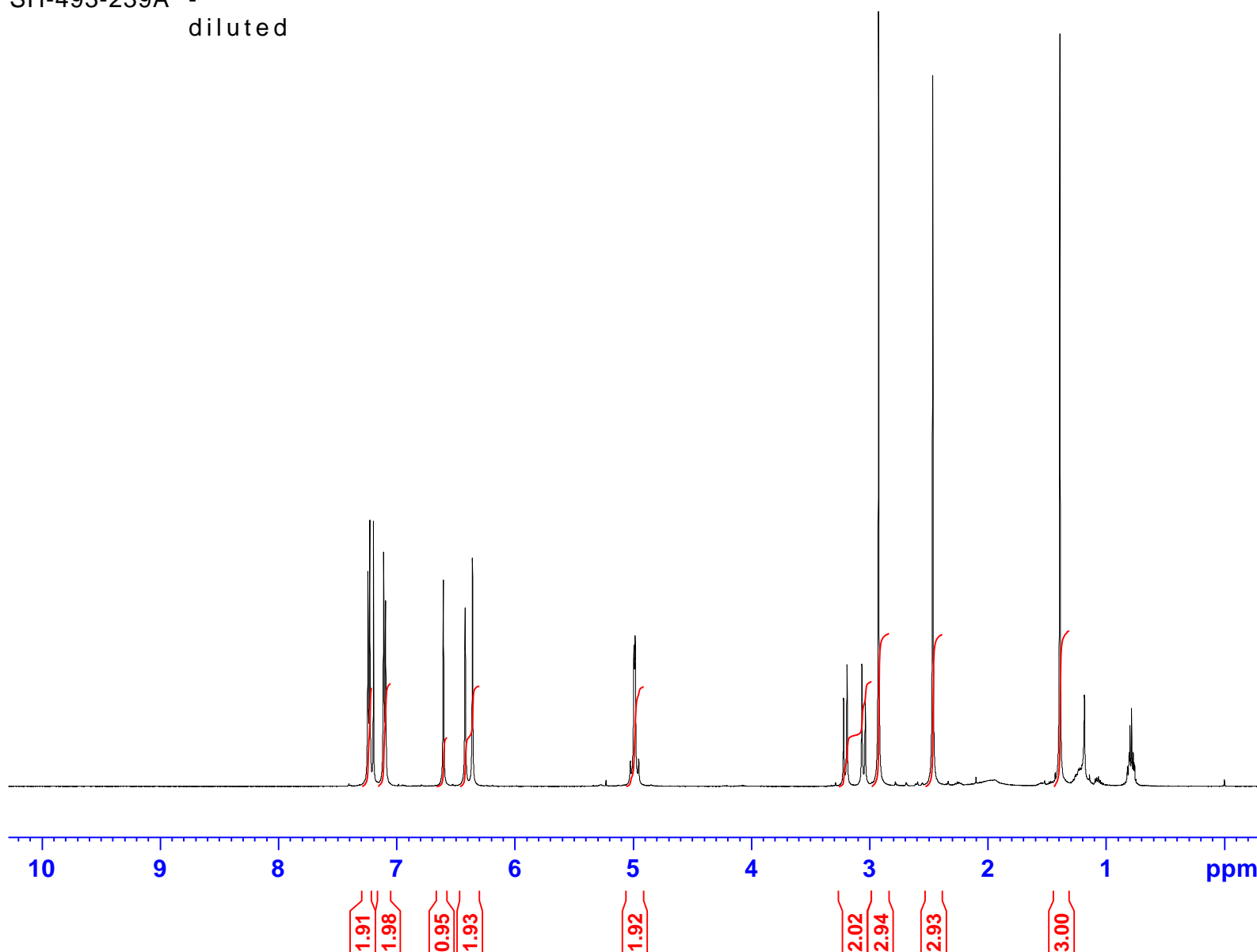


Current Data
NAME SH-493-239A
EXPNO 16
PROCNO 1

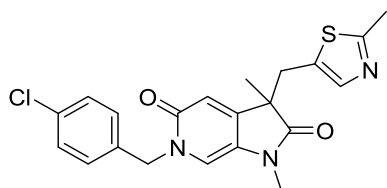
F2 - Acquisition
Data 20150410
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 322
DW 48.400 usec
DE 11.99 usec
TE 297.0 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

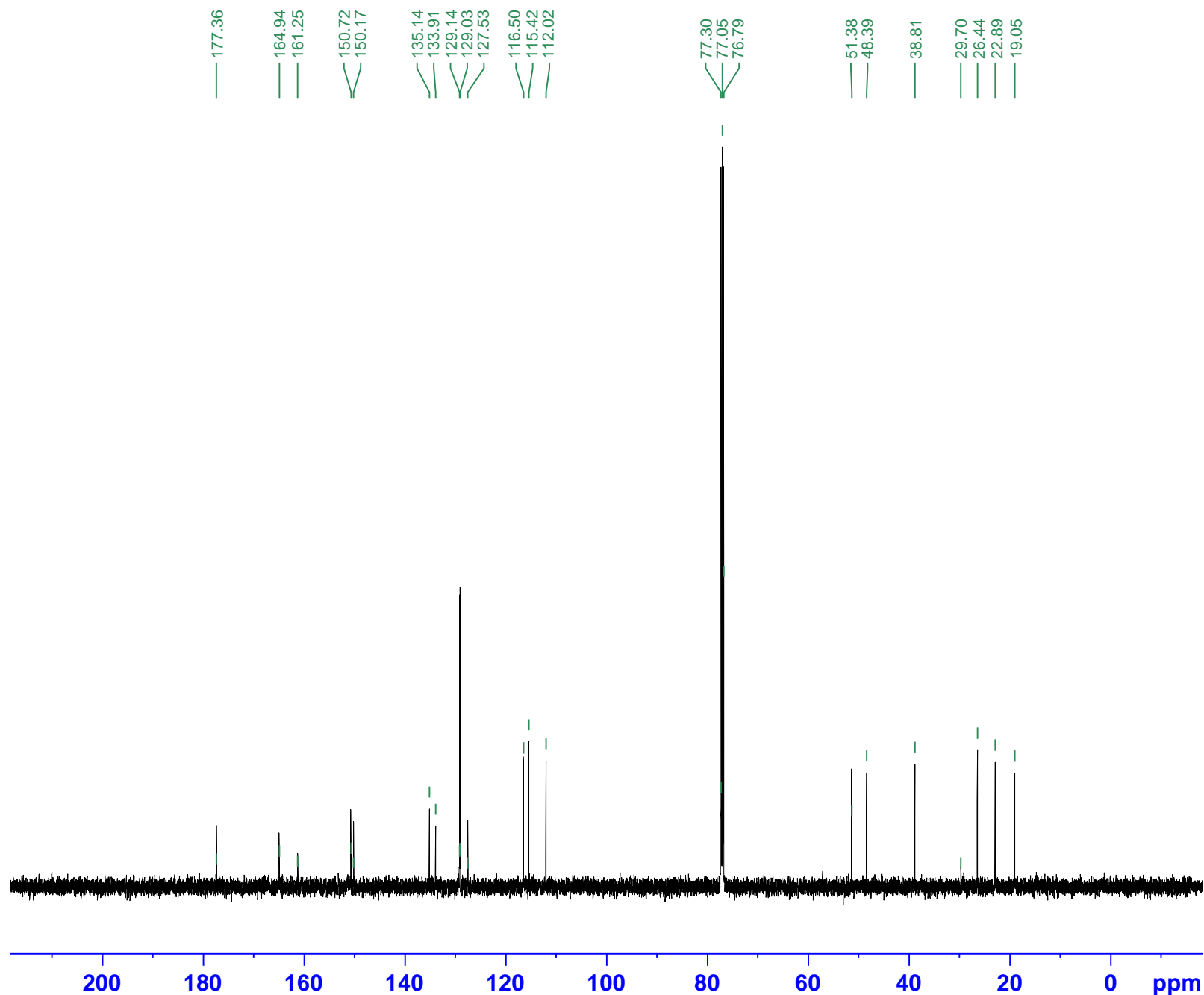
F2 - Processing parameters SI
65536
SF 500.3000438 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



22c



SH-493-239A



Current Data Parameters
 NAME SH-493-239A
 EXPNO 11
 PROCNO 1

F2 - Acquisition
 Parameters Date_ 20150410
 Time 8.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 2
 SMH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DV 16.800 usec
 DE 7.68 usec
 TE 298.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

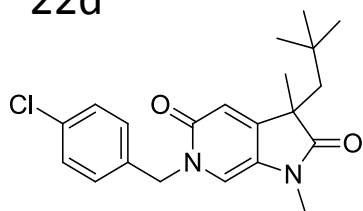
SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

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

SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

22d



DCM-494-231-A CDCL3

7.336
7.320
7.260
7.251
6.634
6.562

3.065

1.301

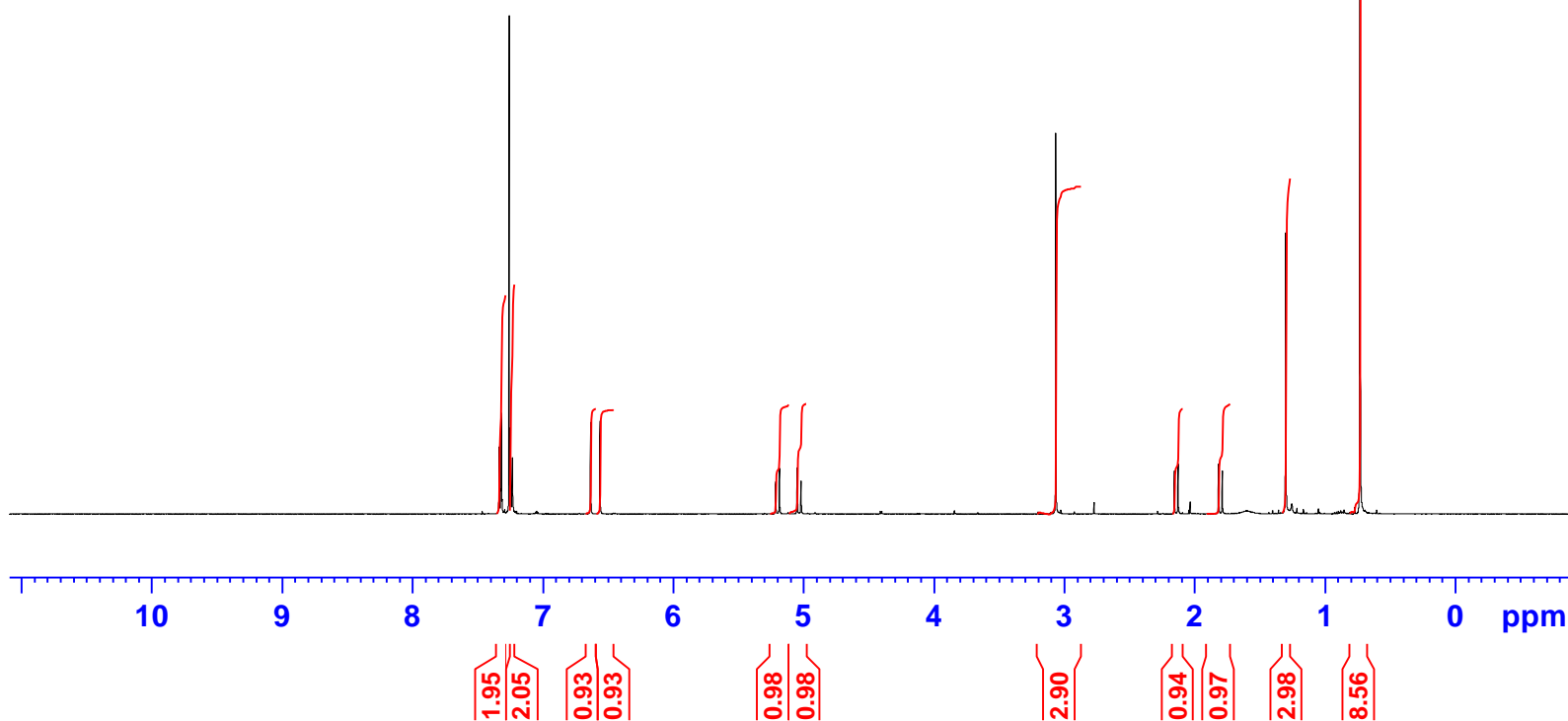
0.731



Current Data
NAME DCM-494-231-A CDCL3
EXPNO 10
PROCNO 1

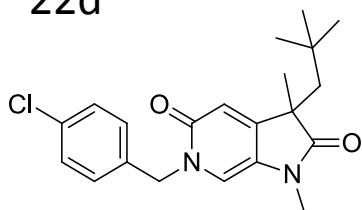
F2 - Acquisition
Date_ 20150506
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCL3
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DW 48.400 usec
DE 11.99 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W

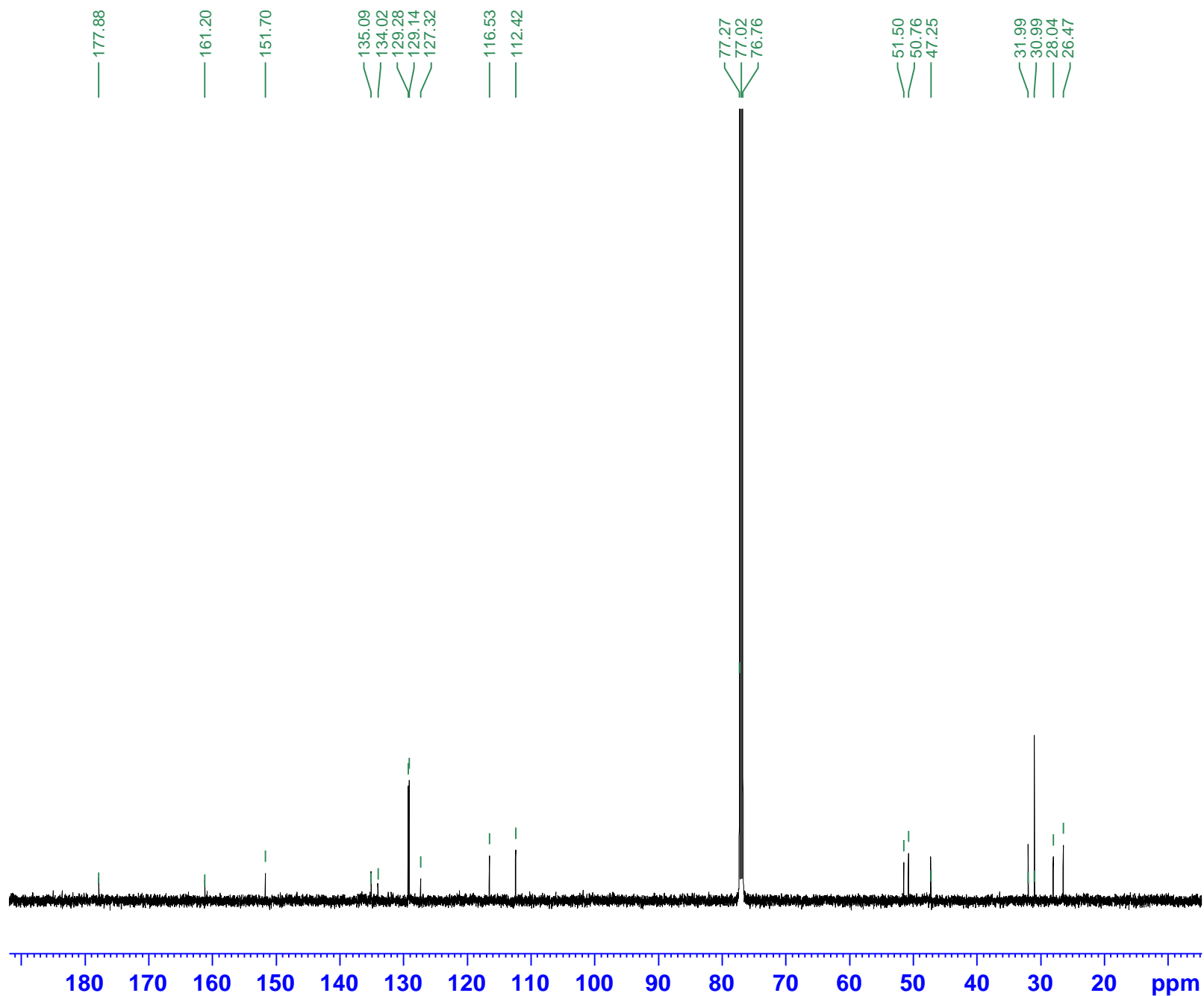


F2 - Processing parameters SI
65536
SF 500.3000118 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

22d



DCM-494-231-A CDCL3



Current Data Parameters
 NAME DCM-494-231-A_CDCL3
 EXPNO 12
 PROCNO 1

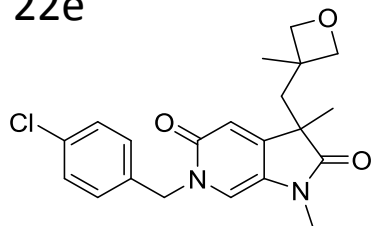
F2 - Acquisition
 Parameters Date_ 20150506
 Time 20.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCL3
 NS 2048
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 456
 DW 16.800 usec
 DE 7.68 usec
 TE 297.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

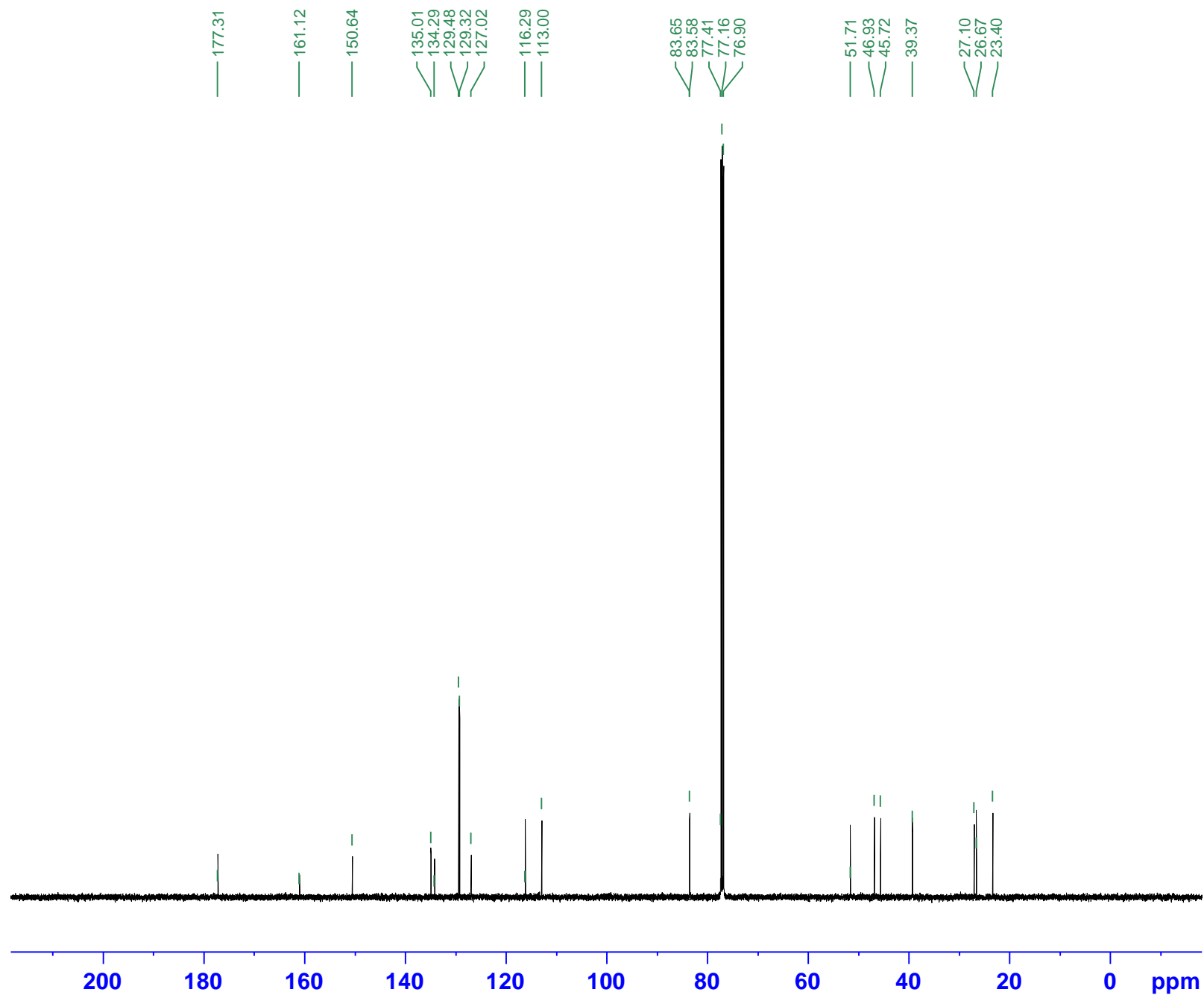
==== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

F2 - Processing
 Parameters 65536
 SF 125.8005350 MHz
 WDV EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

22e



SA-500-160



Current Data Parameters
 NAME SA-500-160
 EXPNO 11
 PROCNO 1

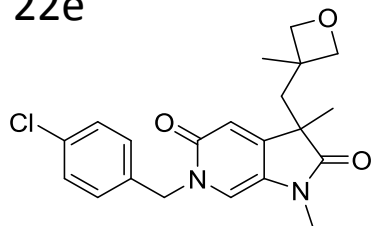
F2 - Acquisition
 Parameters Date_ 20150402
 Time 12.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 2
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DW 16.800 usec
 DE 7.68 usec
 TE 297.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 125.8131151 MHz
 NUC1 13C
 P1 9.75 usec
 PLW1 82.38999939 W

===== CHANNEL f2 =====
 SFO2 500.3020012 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 18.33600044 W
 PLW12 0.75654000 W
 PLW13 0.48418999 W

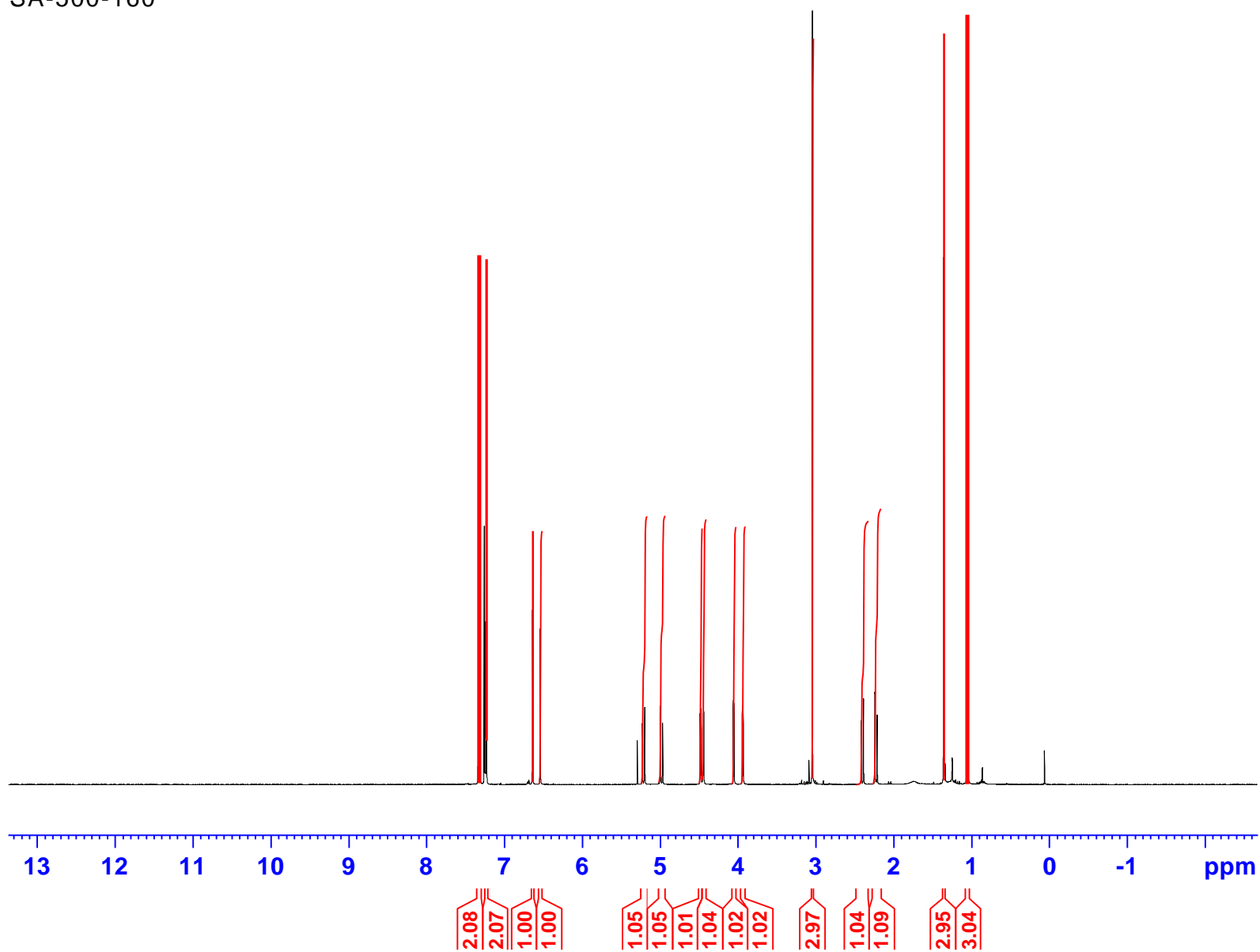
F2 - Processing
 Parameters 65536
 SF 125.8005190 MHz
 WDV EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

22e



SA-500-160

7.338
7.325
7.321
7.260
7.248
7.230
6.640
6.541
5.228
5.199
4.999
4.969
4.487
4.476
4.452
4.440
4.062
4.051
3.945
3.933
3.046
2.418
2.389
2.242
2.213
1.358
1.058

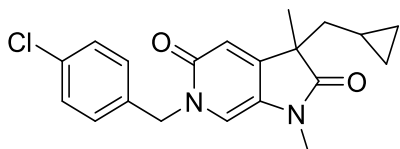


Current Data
NAME SA-500-160
EXPNO 10
PROCNO 1

F2 - Acquisition
Data Parameters 20150402
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SMH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 322
DW 48.400 usec
DE 11.99 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1
SFO1 =====
NUC1 500.3030896 MHz
P1 1H
PLW1 16.25 usec
18.33600044 W
F2 Processing parameters
- S1 65536
SF 500.3000122 MHz
VDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

22f



7.340
7.327
7.323
7.279
7.260

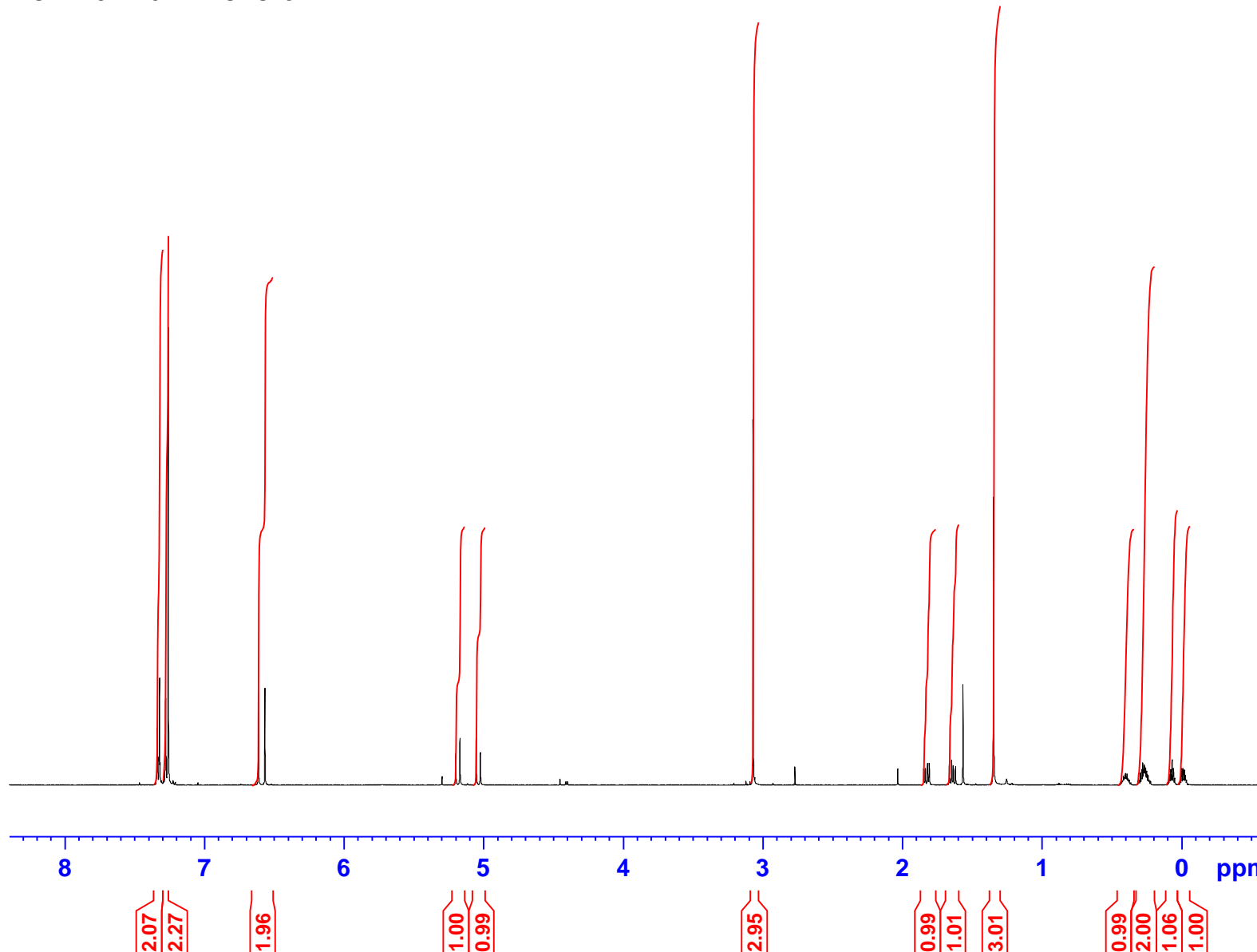
6.614
6.567

5.200
5.170
5.053
5.024

3.070

1.647
1.567
1.347

0.068

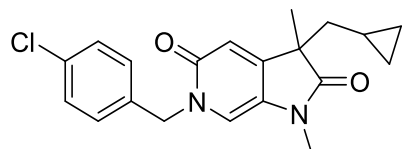
DCM-494-202-A CDCL₃

Current Data
NAME DCM-494-202-A CDCL₃
EXPNO 10
PROCNO 1

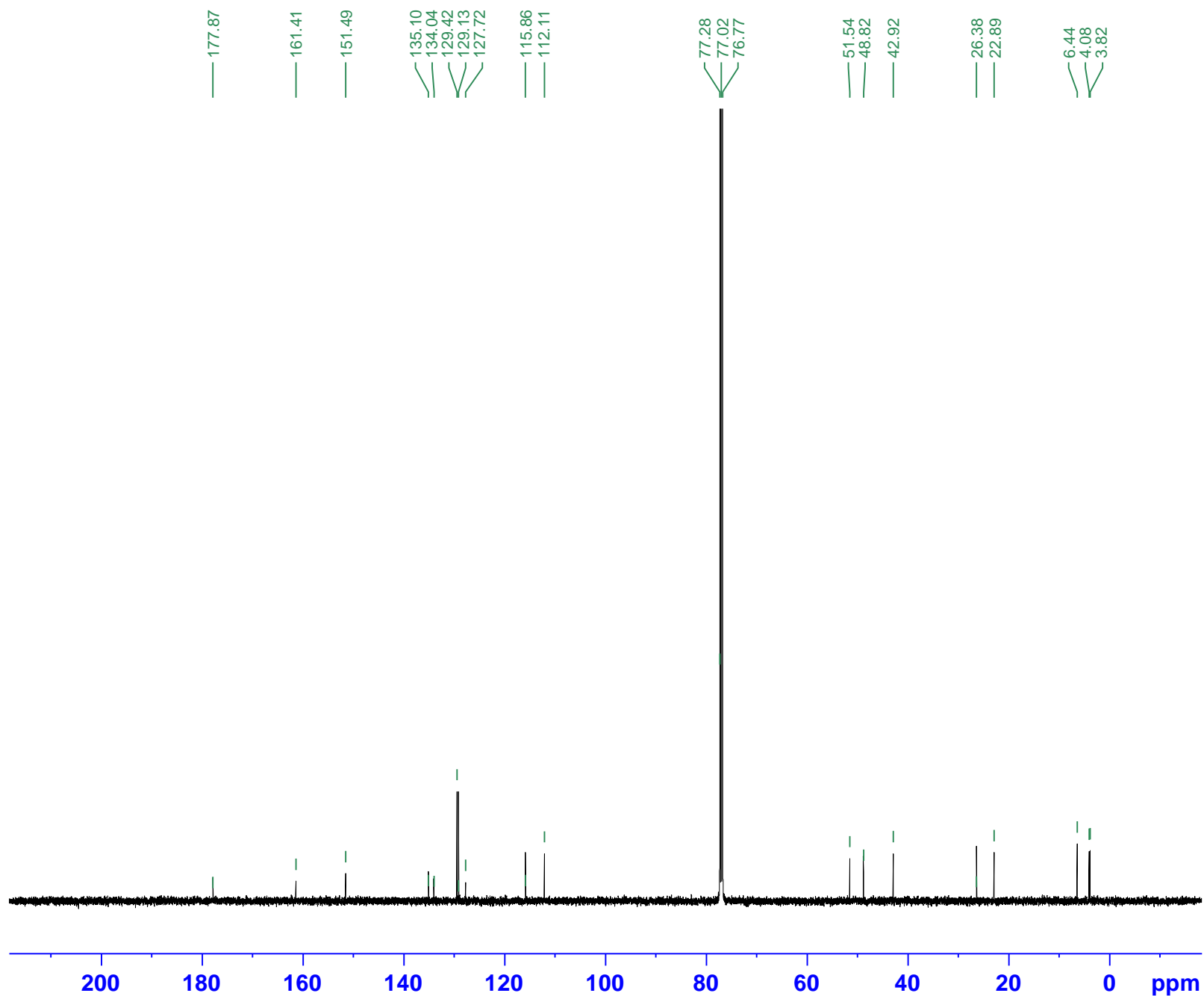
F2 - Acquisition
Date_ 20150317
Time 17.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCL₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 645
DW 48.400 usec
DE 11.99 usec
TE 297.0 K
D1 1.00000000 Sec
TD0 1

==== CHANNEL f1
SFO1 500.3030896 MHz
NUC1 1H
P1 16.25 usec
PLW1 18.33600044 W
F2 Processing parameters
- SI 65536
SF 500.3000120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

22f



DCM-494-202-A CDCL3



Current Data Parameters
NAME DCM-494-202-A CDCL3
EXPNO 11
PROCNO 1

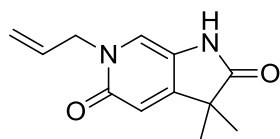
F2 - Acquisition
Parameters Date_ 20150318
Time 5.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCL3
NS 3096
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 456
DW 16.800 usec
DE 7.68 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

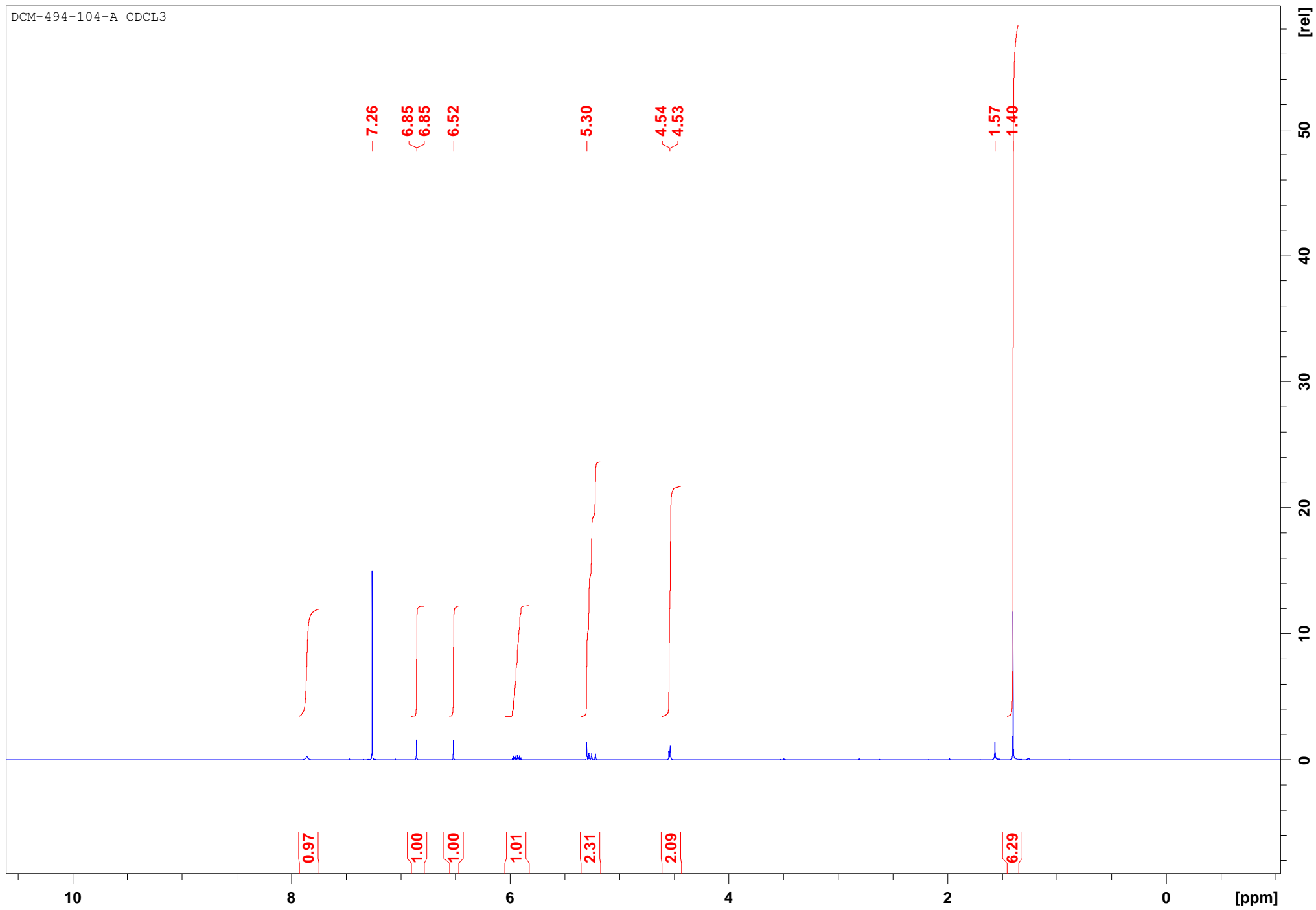
===== CHANNEL f2 =====
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.48418999 W

F2 - Processing
Parameters 65536
SF 125.8005350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

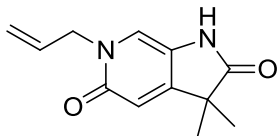
23



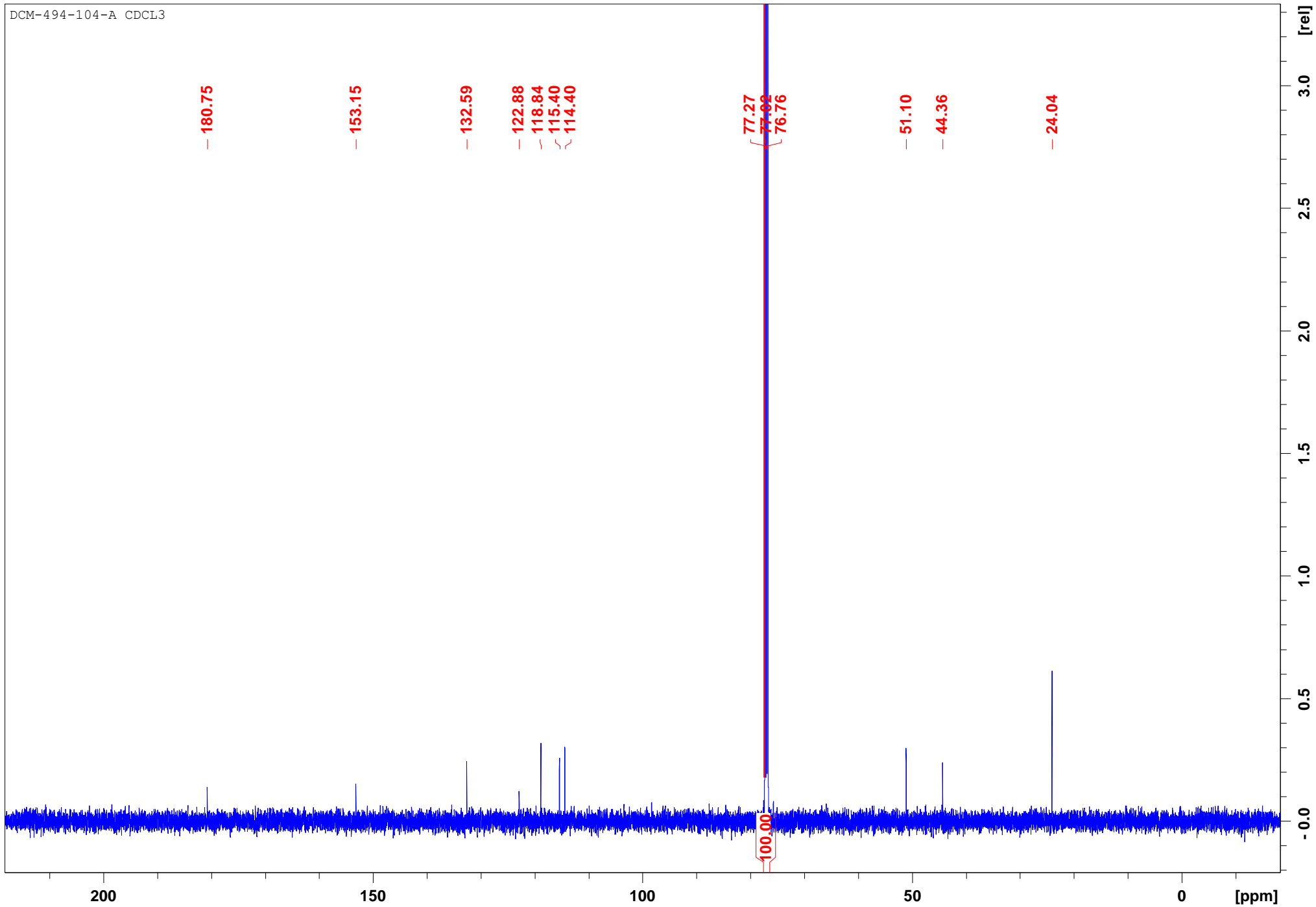
"DCM-494-104-A CDCL3" 10 1 "V:\Old Server\DCM\nmr"



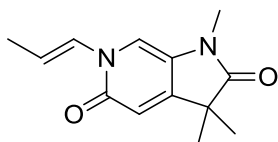
23



"DCM-494-104-A CDCL3" 14 1 "V:\Old Server\DCM\nmr"

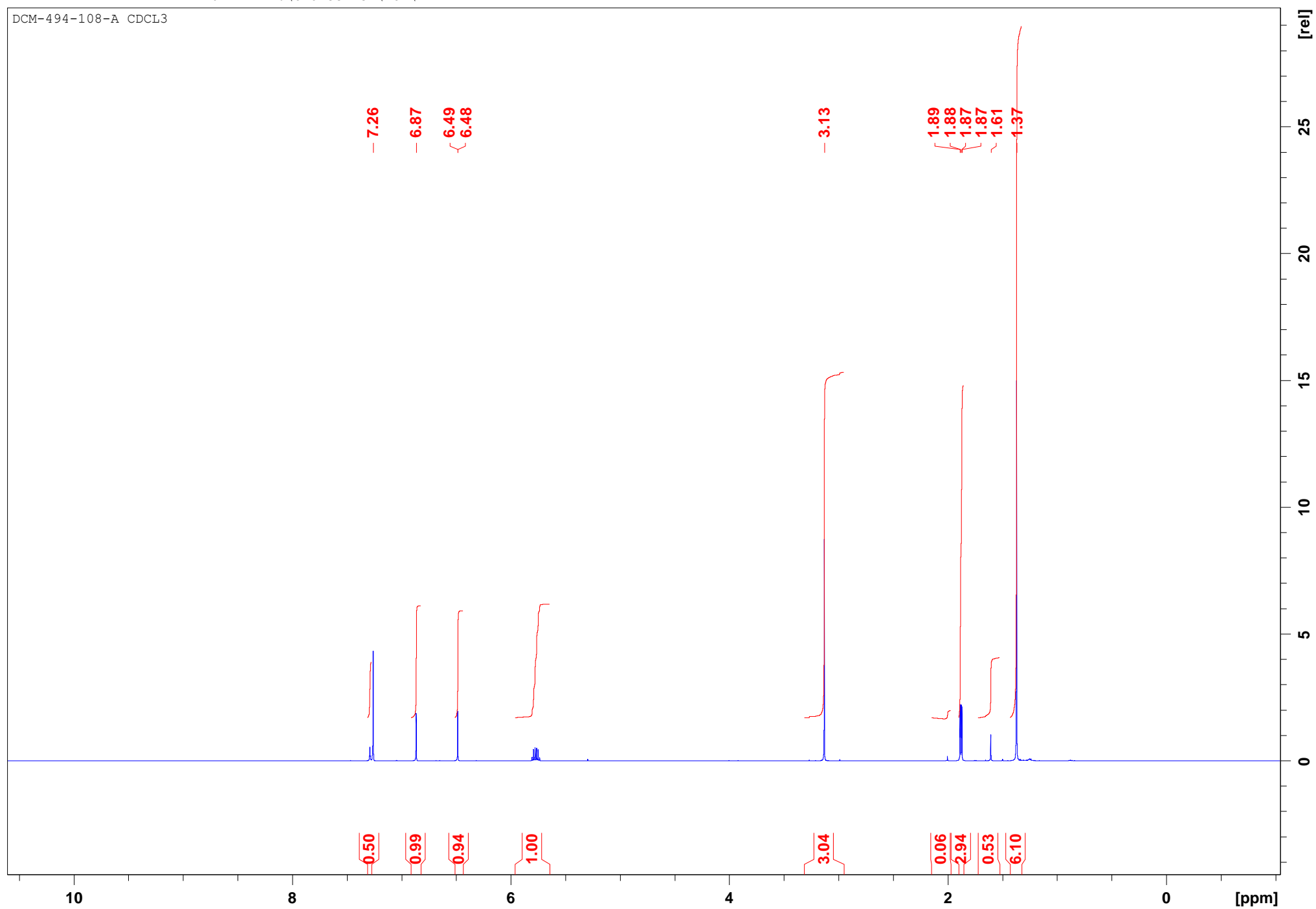


24

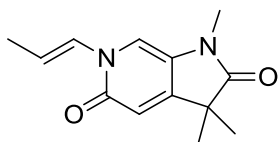


"DCM-494-108-A CDCL3" 10 1 "V:\Old Server\DCM\nmr"

DCM-494-108-A CDCL3

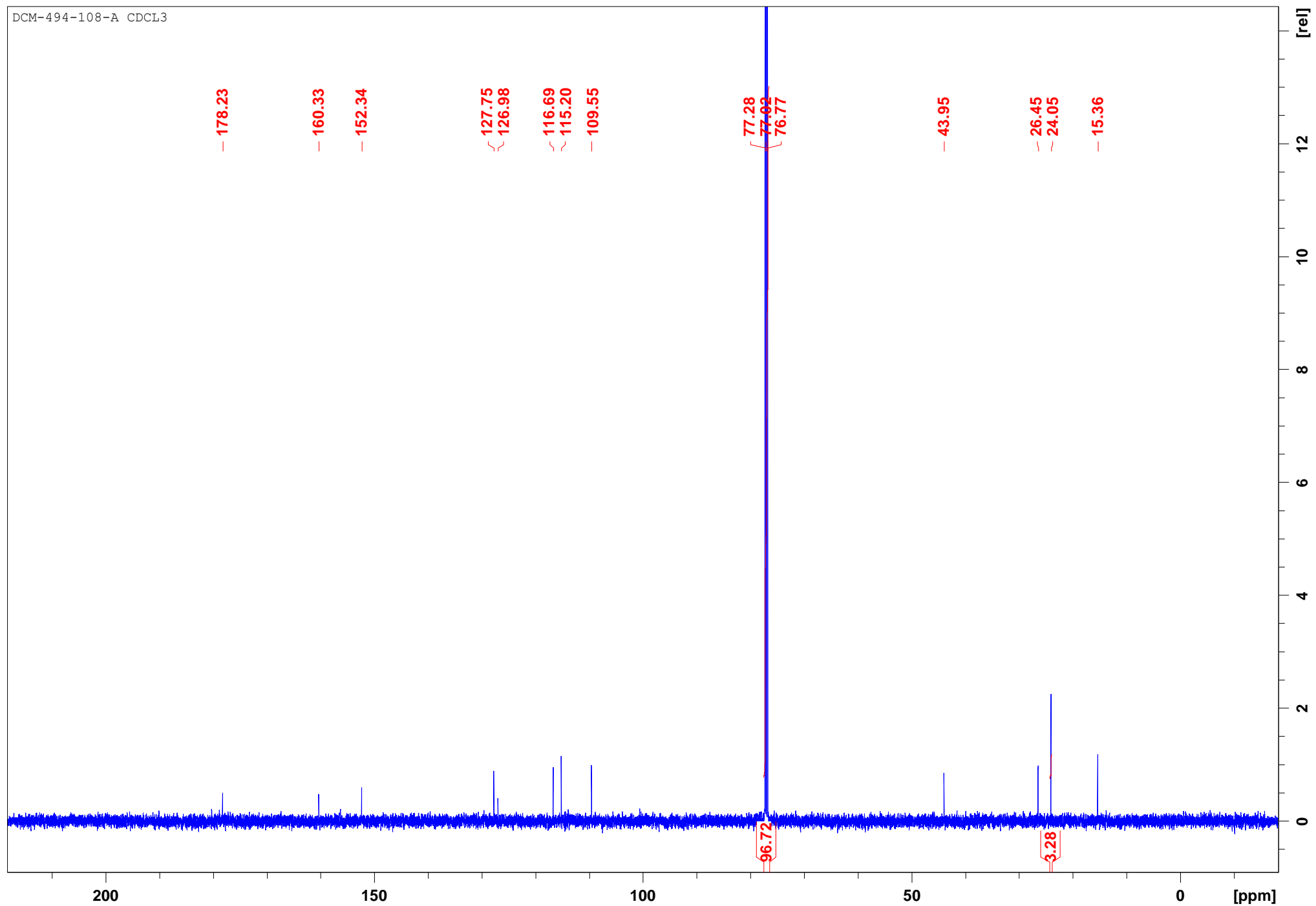


24

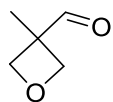


"DCM-494-108-A CDCL3" 11 1 "V:\Old Server\DCM\nmr"

DCM-494-108-A CDCL3

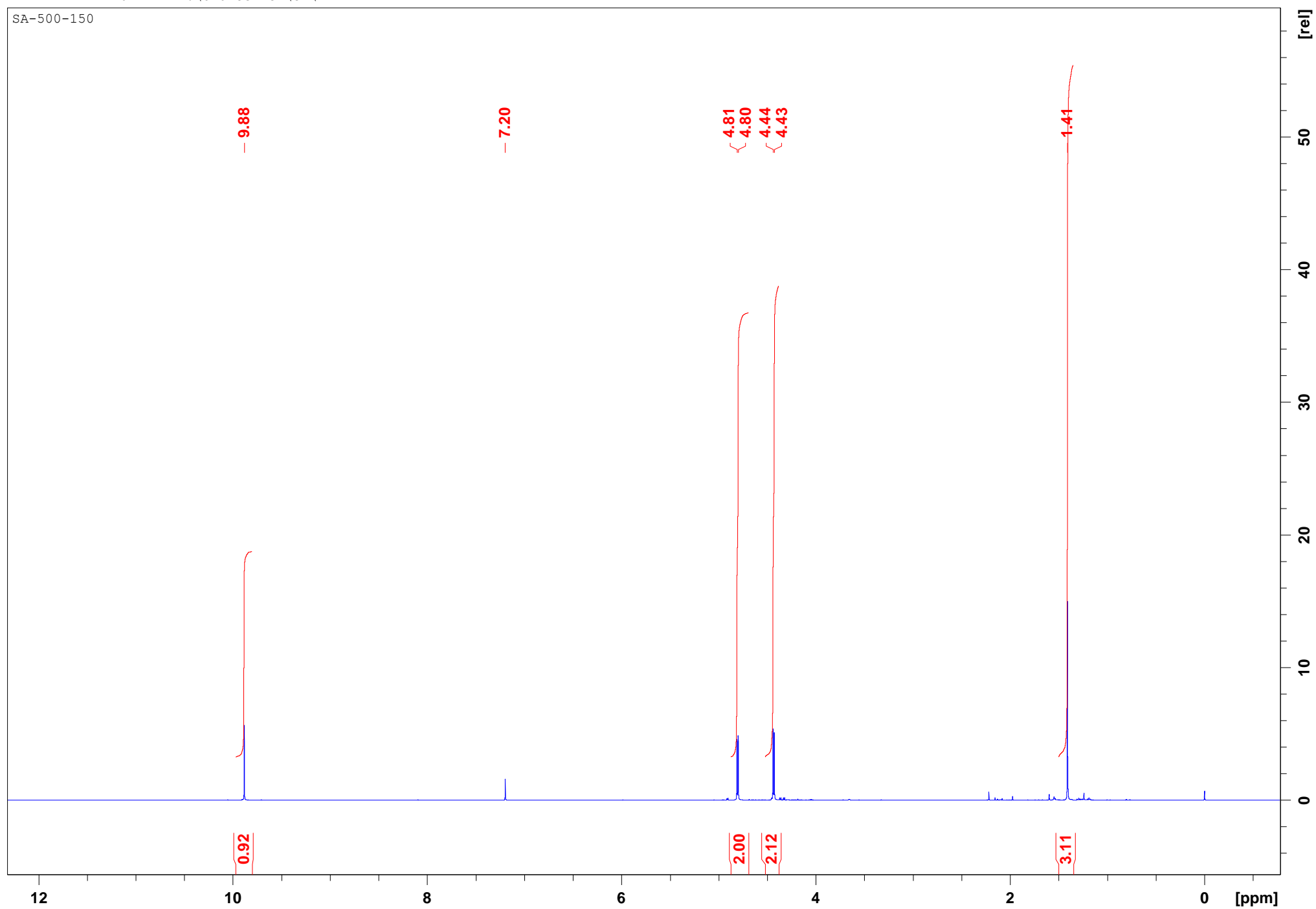


26

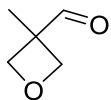


SA-500-150 10 1 "X:\Old Server\SA\nmr"

SA-500-150



26



SA-500-150 11 1 "X:\Old Server\SA\nmr"

SA-500-150

