

HEBA-4A
 PROTON_BSU CDC13 {C:\data} nmr 18

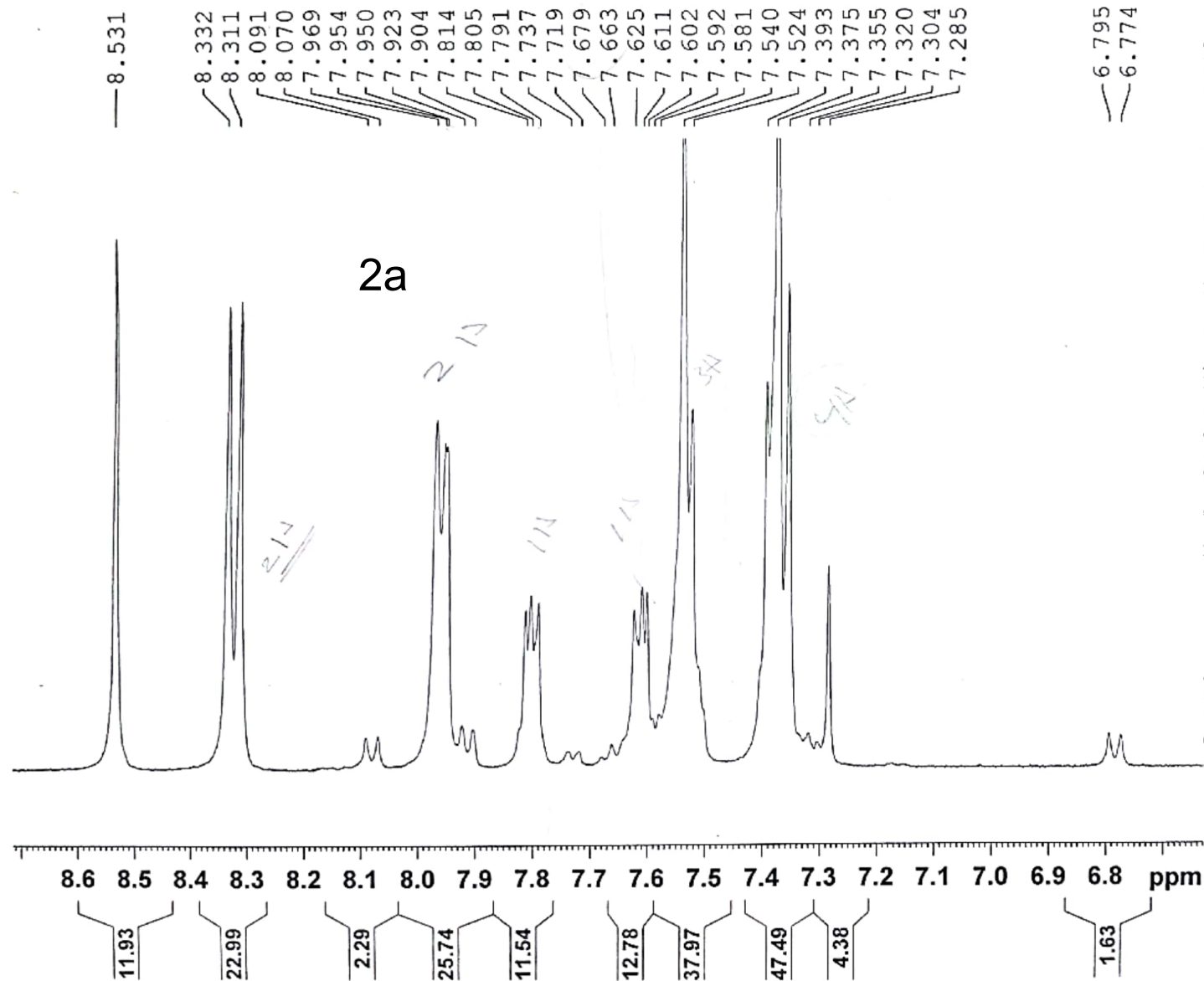


Current Data Parameters
 NAME Mar17-2015-nmr
 EXPNO 450
 PROCNO 1

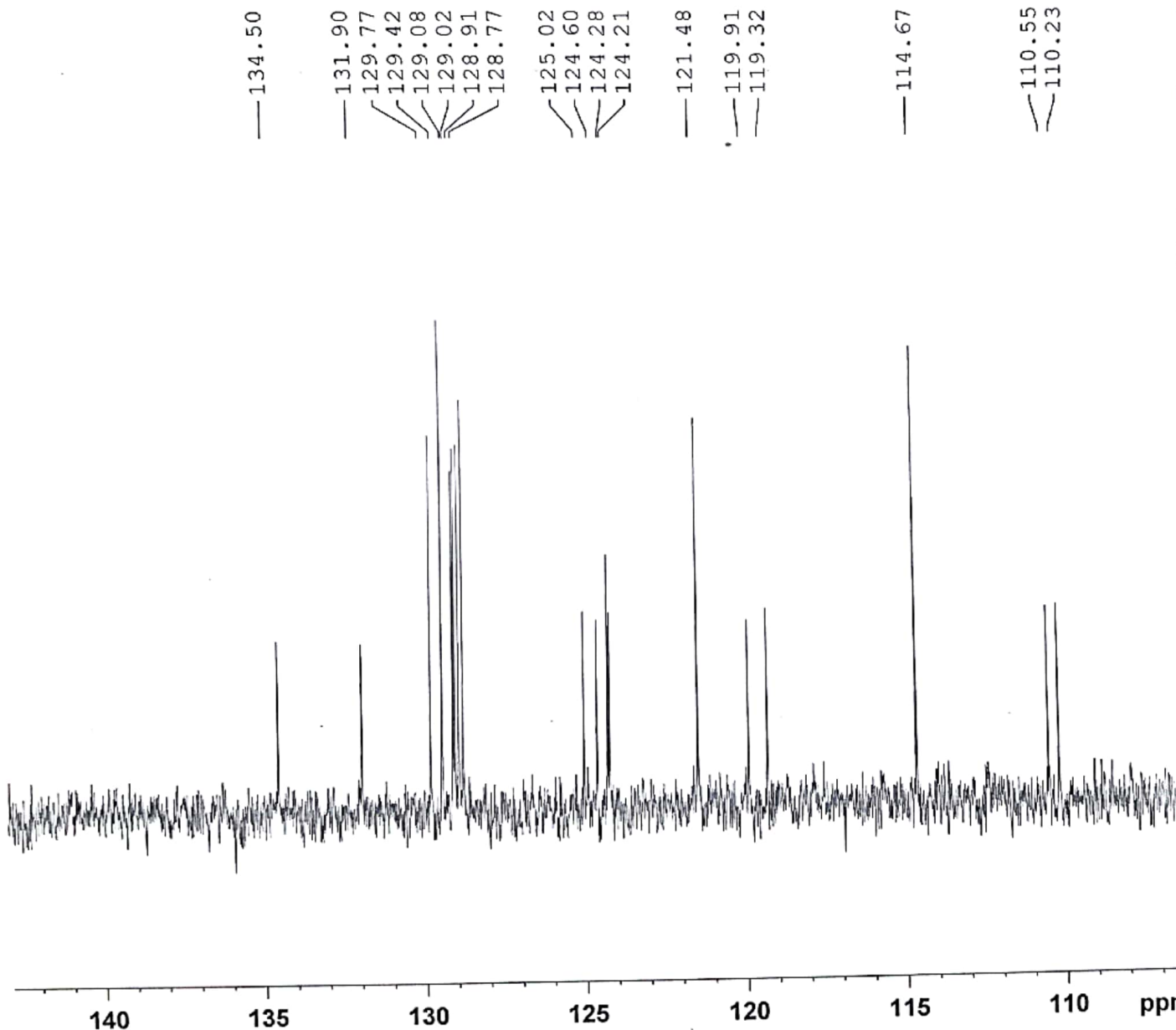
F2 - Acquisition Parameters
 Date_ 20150317
 Time_ 12.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-4A
 DEPTQ-BSU CDC13 {C:\data} nmr 21



Current Data Parameters
 NAME Mar31-2015-nmr
 EXPNO 370
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150401
 Time_ 9.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptqgpgp
 TD 65536
 SOLVENT CDC13
 NS 2460
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 294.5 K
 CNST2 145.0000000
 CNST12 1.5000000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SPNAM[5] Crp60comp.4
 SPOALS 0.500
 SPOFFS5 0 Hz
 SPWS 10.08399963 W

----- CHANNEL f2 -----
 SFO2 400.1312797 MHz
 NUC2 1H
 CPDPRG[2] waltr16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GP21 31.00 %
 GP22 31.00 %
 GP23 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LE 1.00 Hz
 GB 0
 PC 1.40

HEBA-4B
 PROTON_BSU CDC13 {C:\data} nmr 20

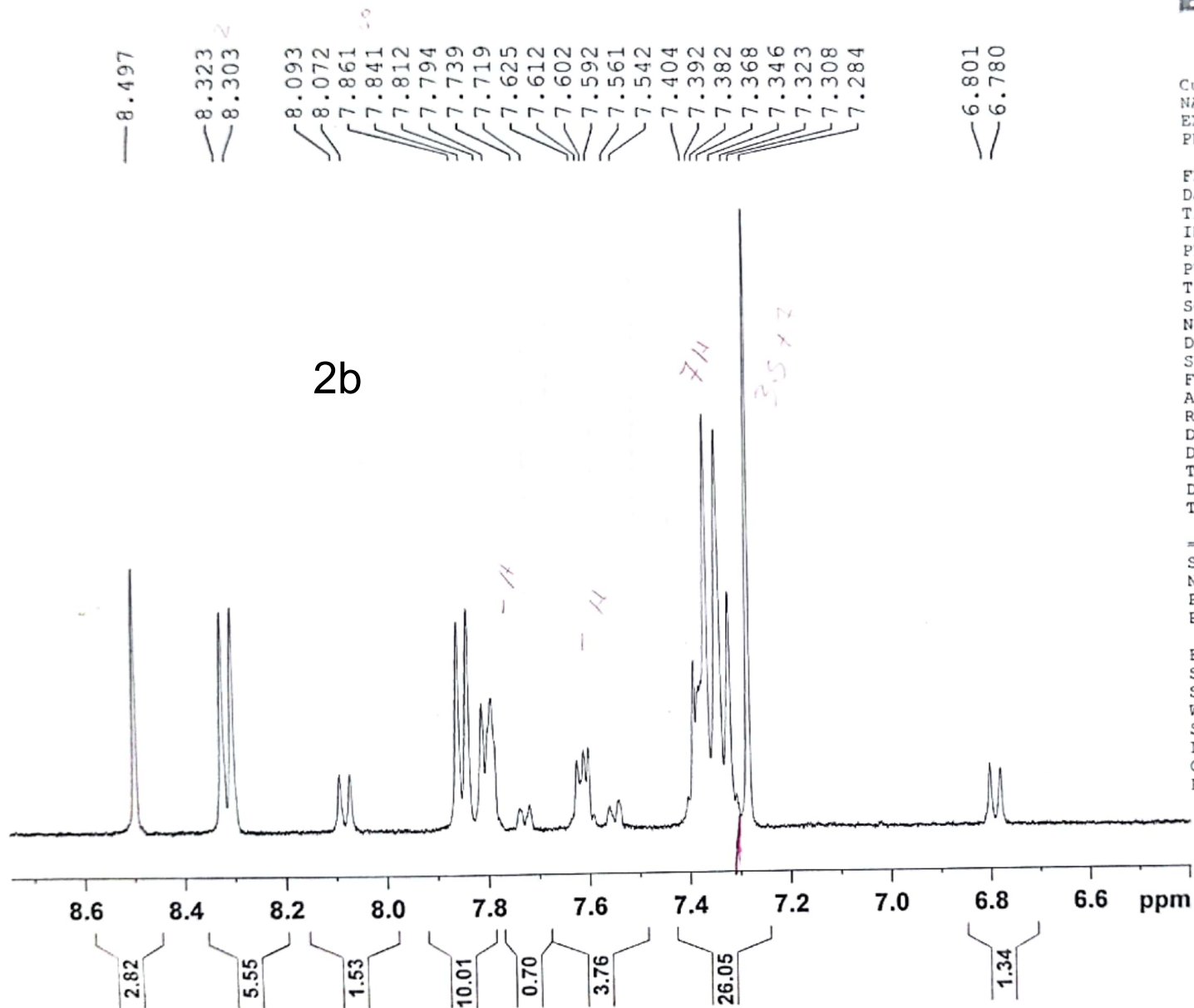


Current Data Parameters
 NAME Mar17-2015-nmr
 EXPNO 470
 PROCNO 1

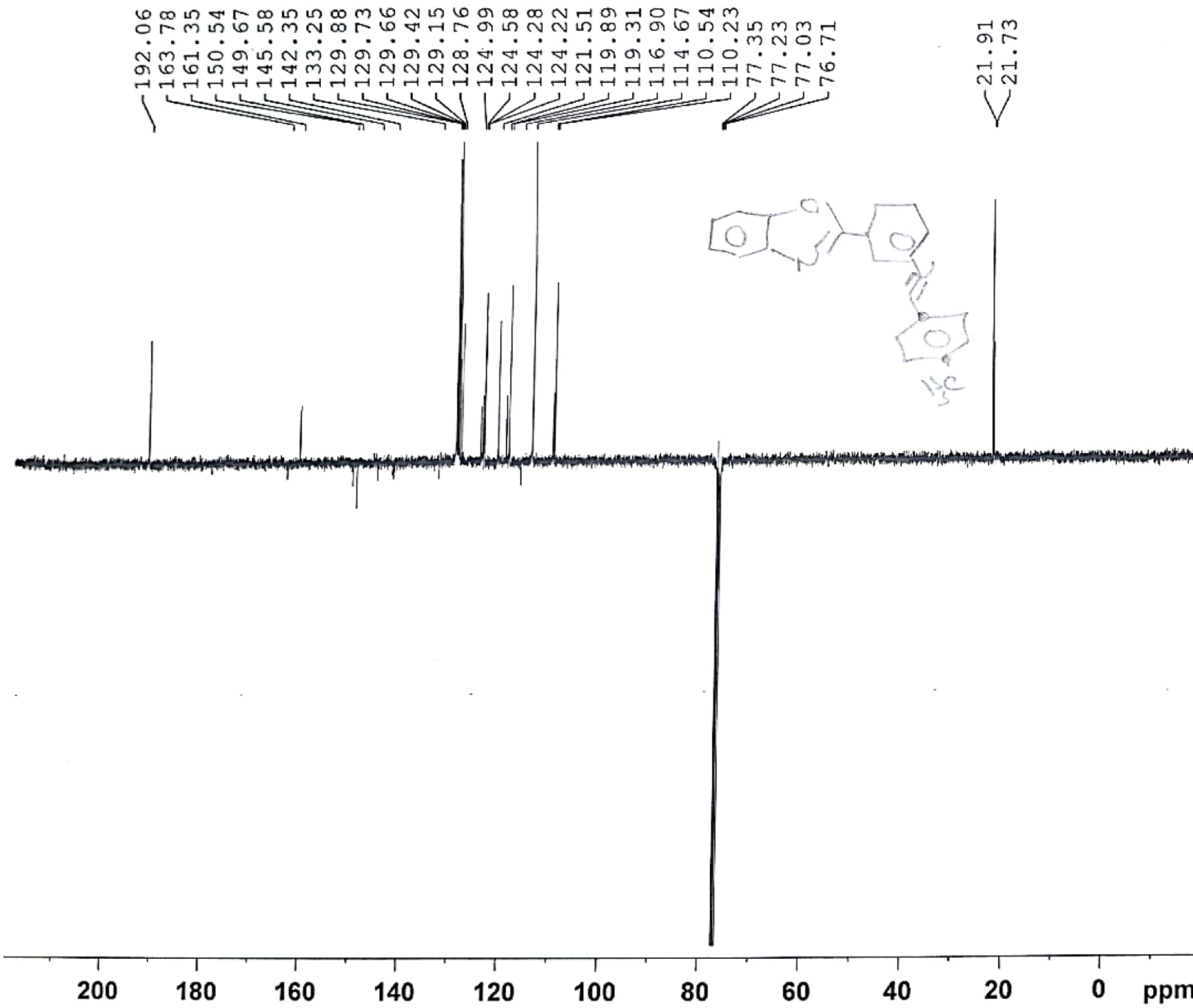
F2 - Acquisition Parameters
 Date_ 20150317
 Time 13.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 DL 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-4B
 DEPTQ-BSU CDC13 {C:\data} nmr 19



192.06
 163.78
 161.35
 150.54
 149.67
 145.58
 142.35
 133.25
 129.88
 129.73
 129.66
 129.42
 129.15
 128.76
 124.99
 124.58
 124.28
 124.22
 121.51
 119.89
 119.31
 116.90
 114.67
 110.54
 110.23
 77.35
 77.23
 77.03
 76.71

21.91
 21.73

Current Data Parameters
 NAME Apr30-2015-nmr
 EXPNO 390
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150502
 Time 9.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptgpgp
 TD 65536
 SOLVENT CDC13
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 295.2 K
 CNST2 145.000000
 CNST12 1.500000
 D1 2.0000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 TDD 1

==== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SPNAM[5] Crp60comp.4
 SFOALS 0.500
 SPOFFS5 0 Hz
 SPW5 10.08399963 W

==== CHANNEL f2 =====
 SFO2 400.1312797 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 F0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 31.00 t
 GPZ2 31.00 t
 GPZ3 31.00 t
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

HEBA-4C

PROTON_BSU CDC13 {C:\data} nmr 5



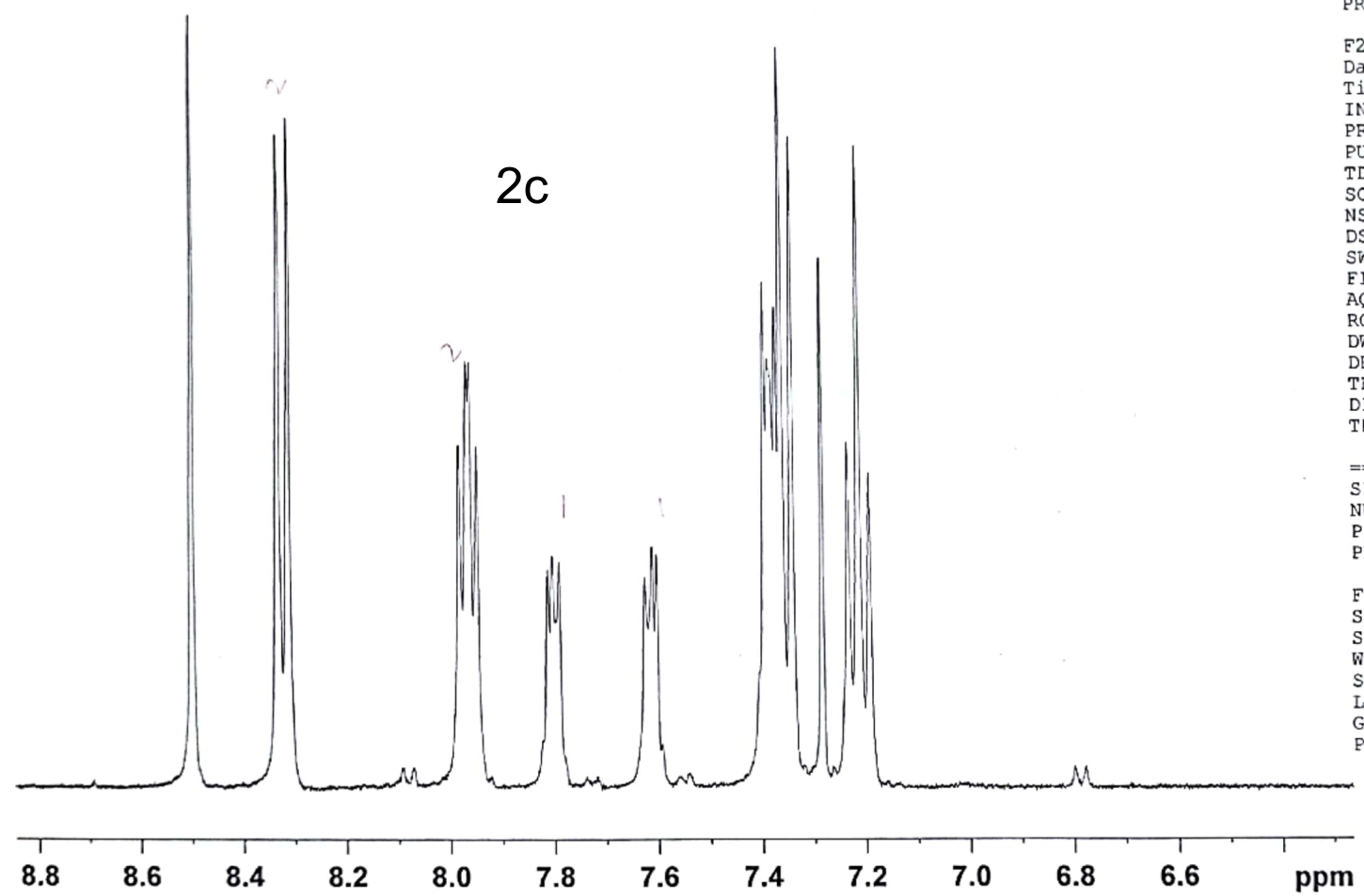
8.496
8.330
8.309
7.981
7.967
7.961
7.947
7.812
7.804
7.790
7.626
7.612
7.603
7.396
7.387
7.373
7.363
7.342
7.284
7.234
7.213
7.192
6.799
6.777

Current Data Parameters
NAME Mar05-2015-nmr
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150305
Time_ 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



49.31
96.54
97.96
47.78
49.01
187.89
11.55
123.65

HEBA-4C
 DEPTQ-BSU CDC13 {C:\data} nmr 18



Current Data Parameters
 NAME Marl5-2015-nmr
 EXPNO 300
 PROCNO 1

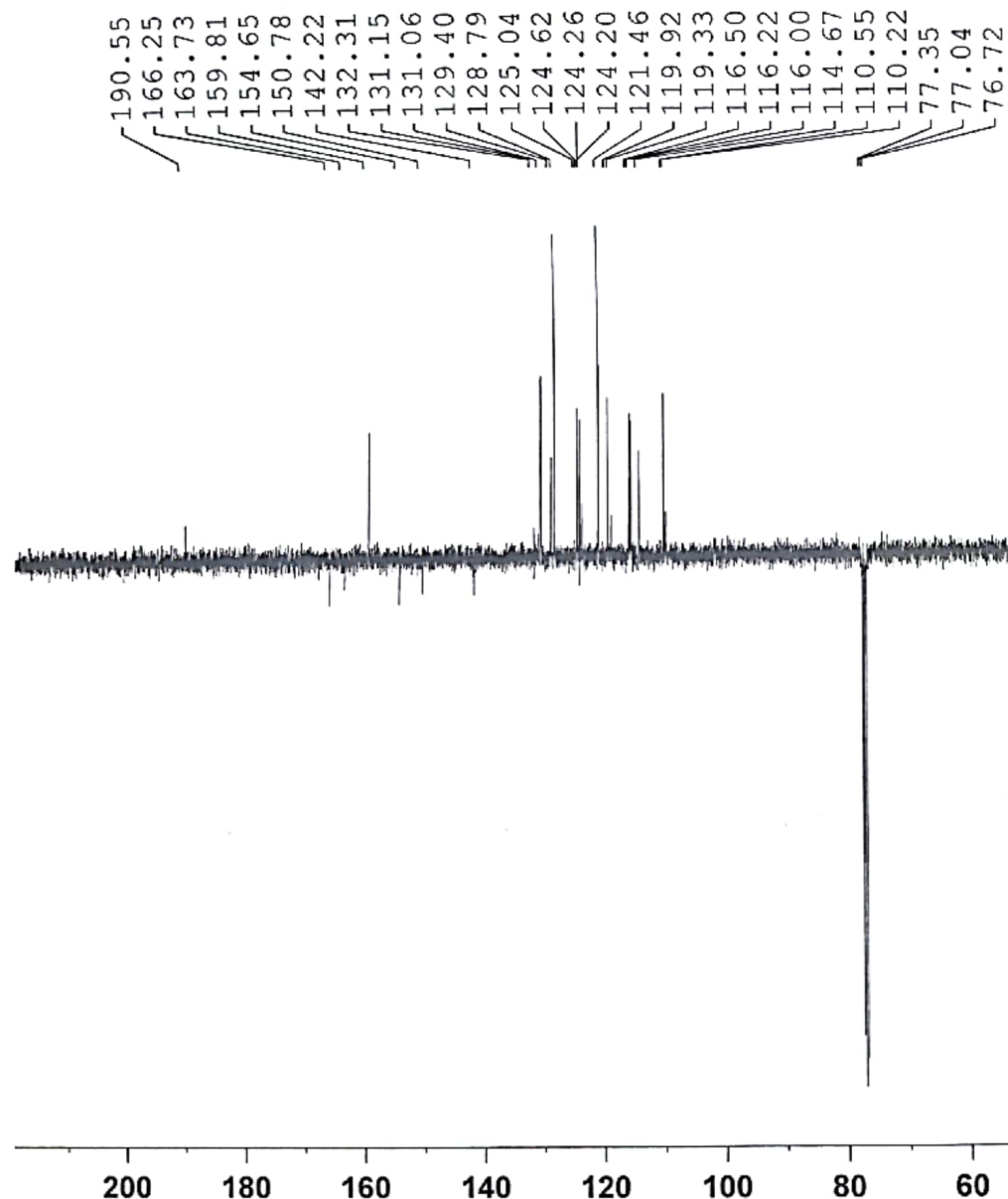
F2 - Acquisition Parameters
 Date 20150316
 Time 9.17
 INSTRUM spect
 PROBHD 5 mm PARBO BB/
 PULPROG deptqqqsp
 TD 65536
 SOLVENT CDC13
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 294.3 K
 CNST2 145.000000
 CNST12 1.500000
 D1 2.0000000 sec
 D2 0.0034828 sec
 D12 0.0000200 sec
 D16 0.0002000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SPNAM[5] Crp60comp.4
 SPOALS 0.500
 SPOFFS5 0 Hz
 SPW5 10.08399963 W

===== CHANNEL f2 =====
 SFO2 400.1312797 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 31.00 %
 GPZ2 31.00 %
 GPZ3 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 S1 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



HEBA-4G
 PROTON_BSU CDC13 (C:\data) nmr 3



Current Data Parameters
 NAME May03-2015-nmr
 EXPNO 270
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150503
 Time_ 12.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.089465 sec
 RG 81.84
 DW 62.400 usec
 DE 6.50 usec
 TE 294.0 K
 D1 1.00000000 sec
 TD0 1

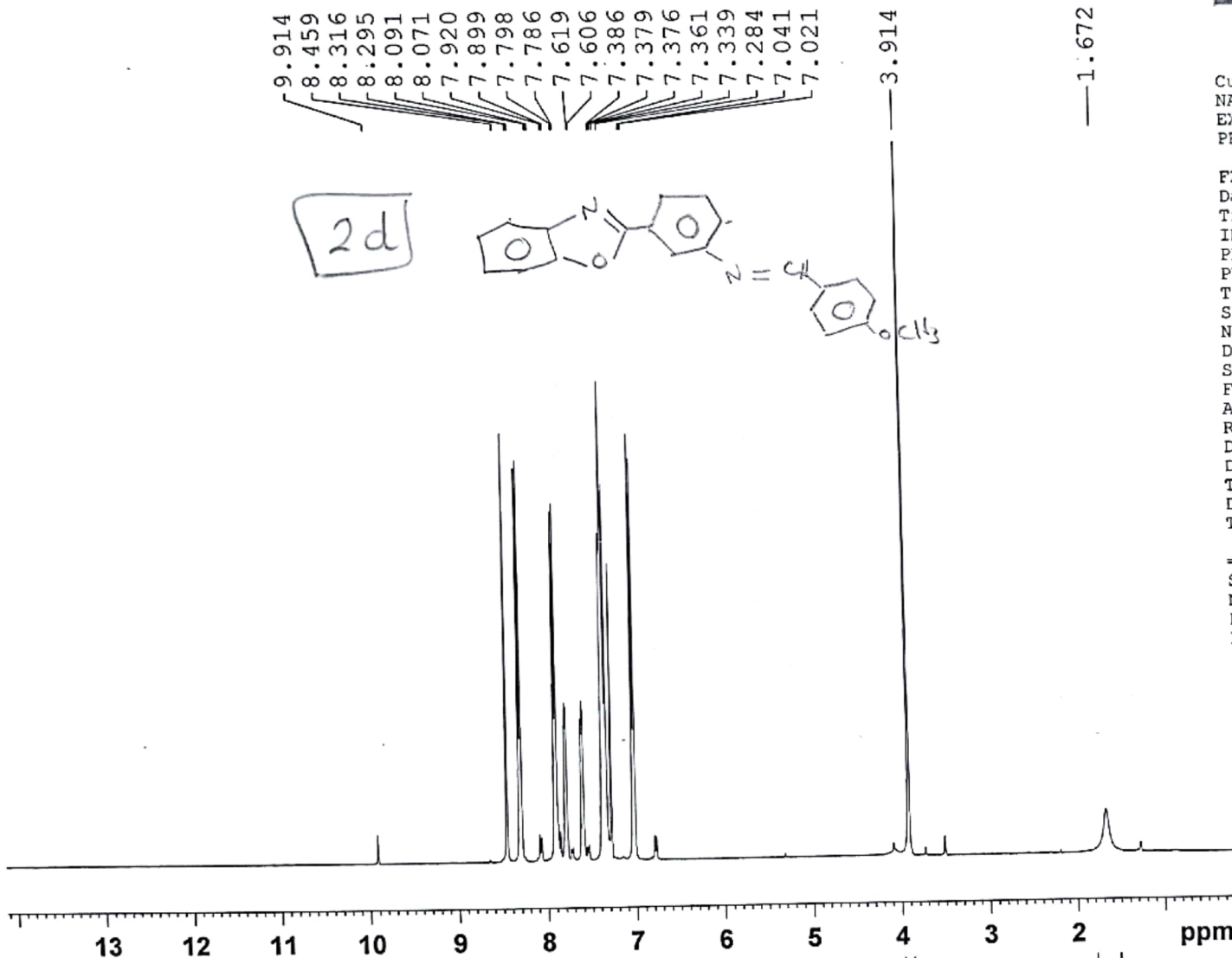
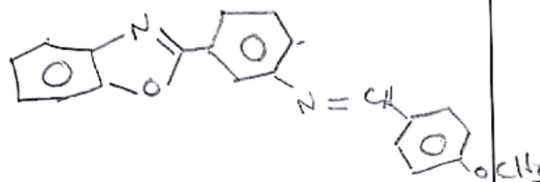
===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

9.914
 8.459
 8.316
 8.295
 8.091
 8.071
 7.920
 7.899
 7.798
 7.786
 7.619
 7.606
 7.386
 7.379
 7.376
 7.361
 7.339
 7.284
 7.041
 7.021

— 1.672

2d



1.00
 2.00
 0.15
 2.10
 1.00
 1.03
 4.05
 0.72
 2.13
 0.13

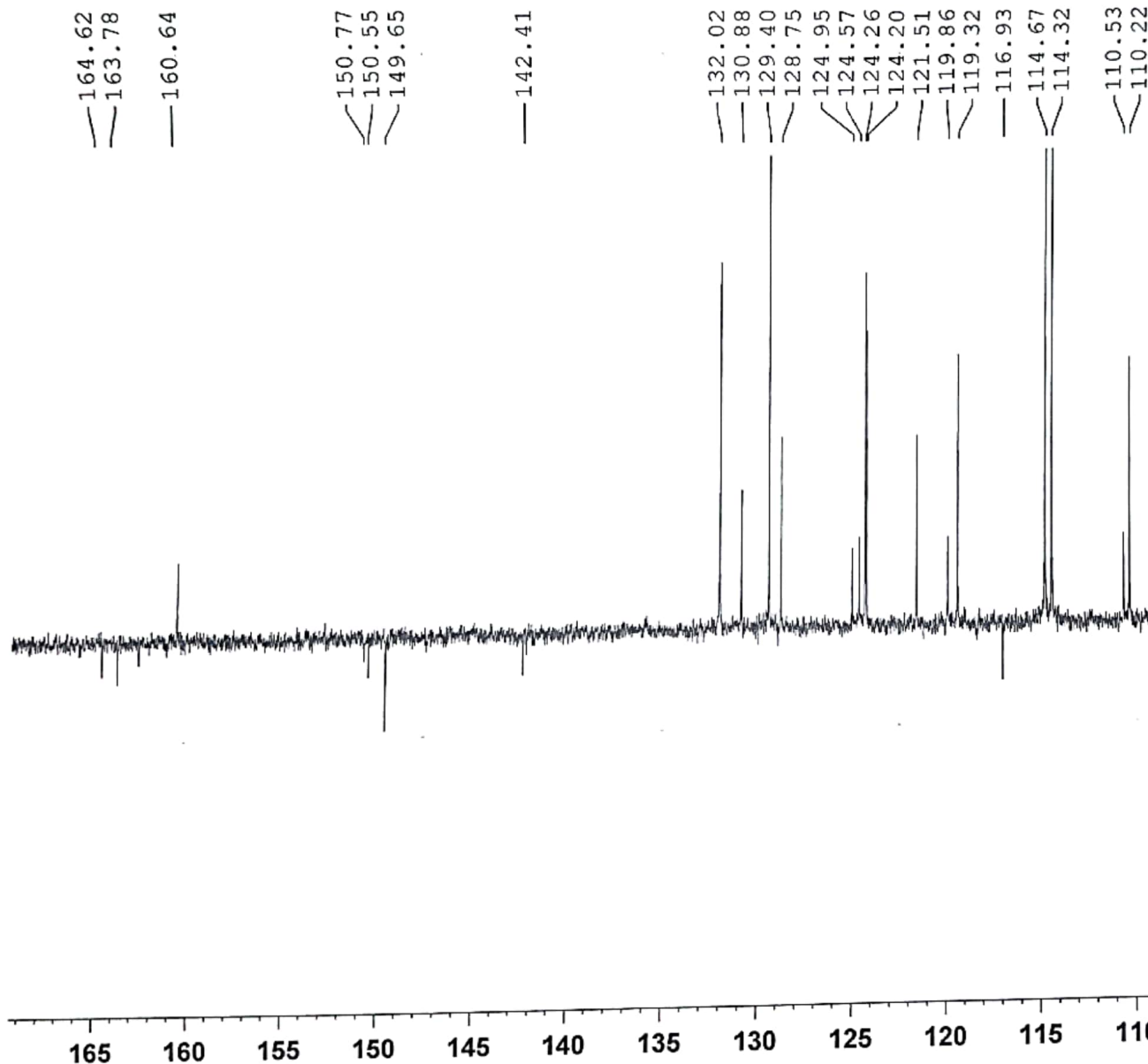
2 2 1 1 2

CDCl₃

3.21

0.79

HEBA-4G
DEPTQ-BSU CDC13 {C:\data} nmr 5



Current Data Parameters
NAME Jun11-2015-nmr
EXPNO 400
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150613
Time_ 18.30
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG deptqqqpp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0002000 sec
D16 0.0002000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFXAM[5] Crp60comp.4
SFOAL5 0.500
SFOFSS 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG2 waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-4D
PROTON_BSU CDCl3 {C:\data} nmr 24

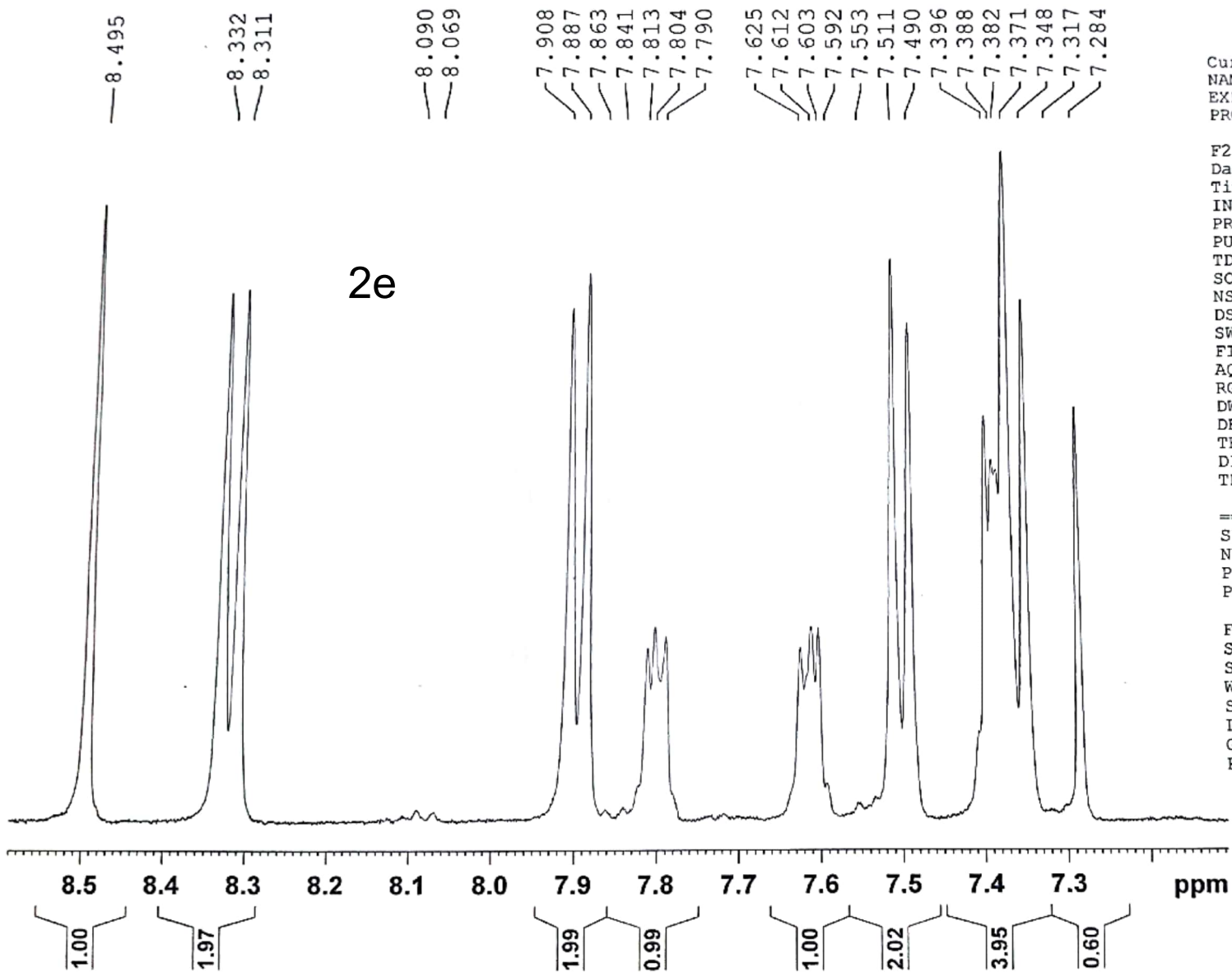


Current Data Parameters
NAME Mar05-2015-nmr
EXPNO 230
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150305
Time 12.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-1-MCL
PROTON_BSU CDC13 {C:\data} nmr 18

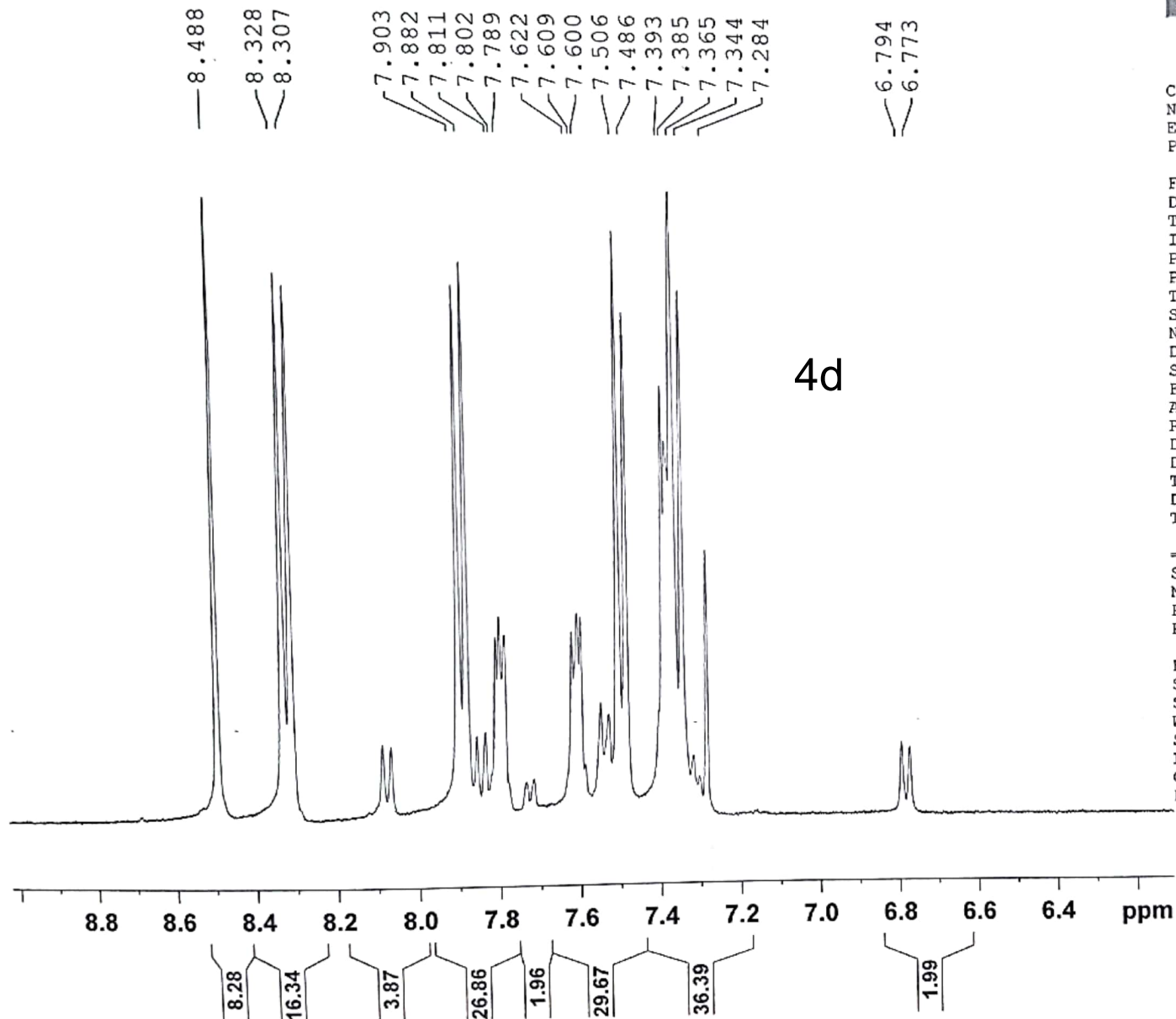


Current Data Parameters
NAME Mar05-2015-nmr
EXPNO 170
PROCNO 1

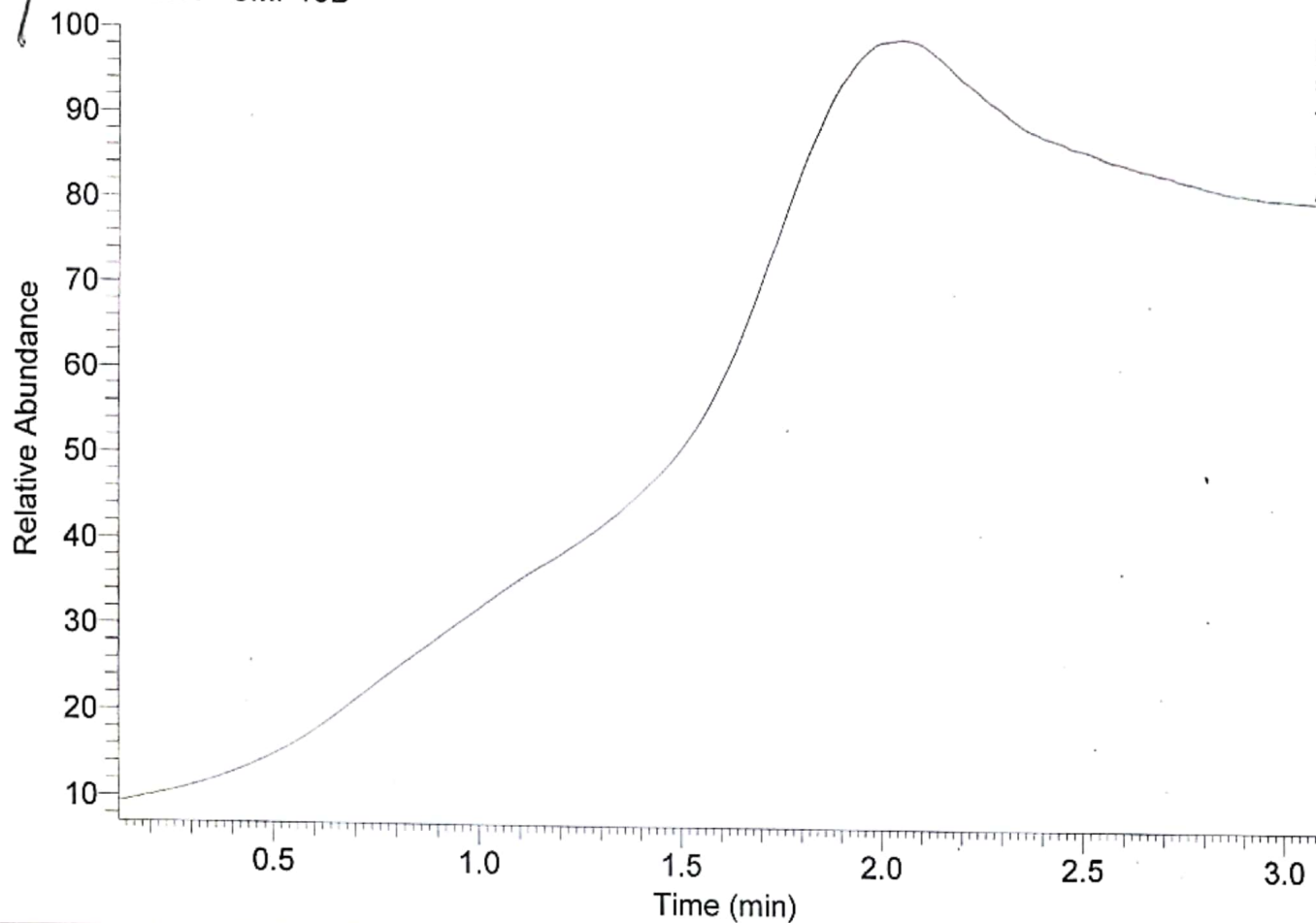
F2 - Acquisition Parameters
Date_ 20150305
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

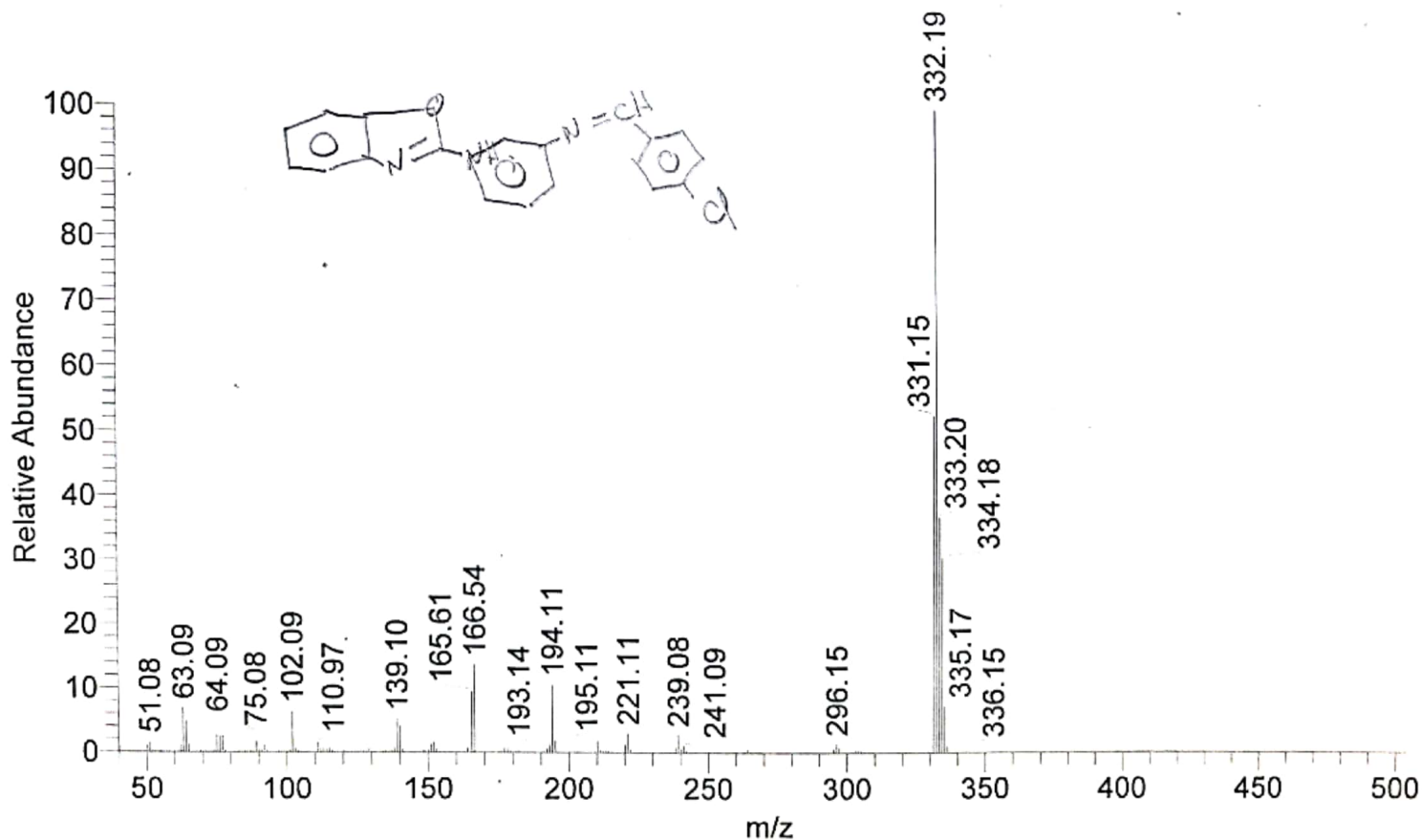


RT: 0.12 - 3.10 SM: 15B



NL:
5.08E8
TIC MS
HEBA-
ATEF-4D

HEBA-ATEF-4D #121 RT: 2.04 AV: 1 NL: 1.41E8
T: {0,0} + c EI Full ms [40.00-1000.00]



A-ATEF-4D#121 RT: 2.04

{0,0} + c EI Full ms [40.00-1000.00]

z= 40.00-504.01

m/z	Intensity	Relative
40.17	1209924.4	0.86
50.07	1350006.5	0.96
51.08	2157045.8	1.53
62.09	1369074.9	0.97
63.09	9699247.0	6.89
64.09	6923080.0	4.92
65.10	1597905.0	1.13
75.08	3756161.3	2.67
76.09	3364332.8	2.39
77.10	3453805.3	2.45
89.10	2427412.0	1.72
92.08	1579385.0	1.12
102.09	8836083.0	6.28
110.97	2194348.5	1.56
113.08	1067448.5	0.76
139.10	7146959.5	5.08
140.10	5721987.5	4.06
151.19	1773000.5	1.26
152.12	2257774.8	1.60
165.61	13383663.0	9.51
166.54	19211098.0	13.64
177.10	1048933.5	0.75
178.11	1015557.2	0.72
193.14	1456183.3	1.03
194.11	14918124.0	10.60
195.11	2620085.0	1.86
210.11	2420634.5	1.72
220.11	1670932.1	1.19
221.11	4170292.3	2.96
238.12	1294302.4	0.92
239.08	3818686.0	2.71
241.09	1428294.4	1.01
296.15	1951939.8	1.39
297.17	1048052.9	0.74
331.15	74490352.0	52.91
332.19	140794816.0	100.00
333.20	52392040.0	37.21
334.18	43396020.0	30.82
335.17	10219559.0	7.26
336.15	1362400.9	0.97

HEBA-4E
 PROTON_BSU CDC13 {C:\data} nmr 3

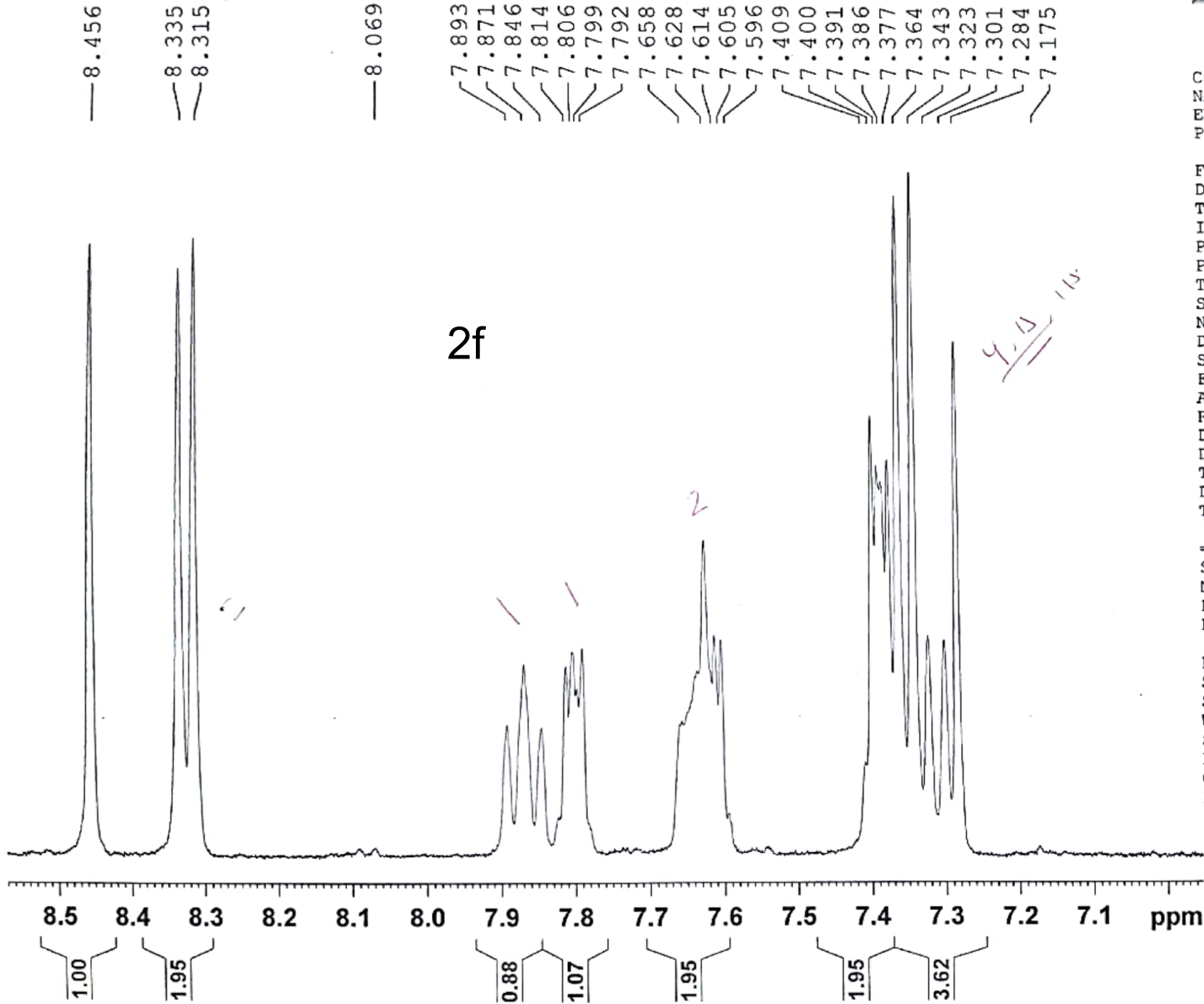


Current Data Parameters
 NAME Mar05-2015-nmr
 EXPNO 260
 PROCNO 1

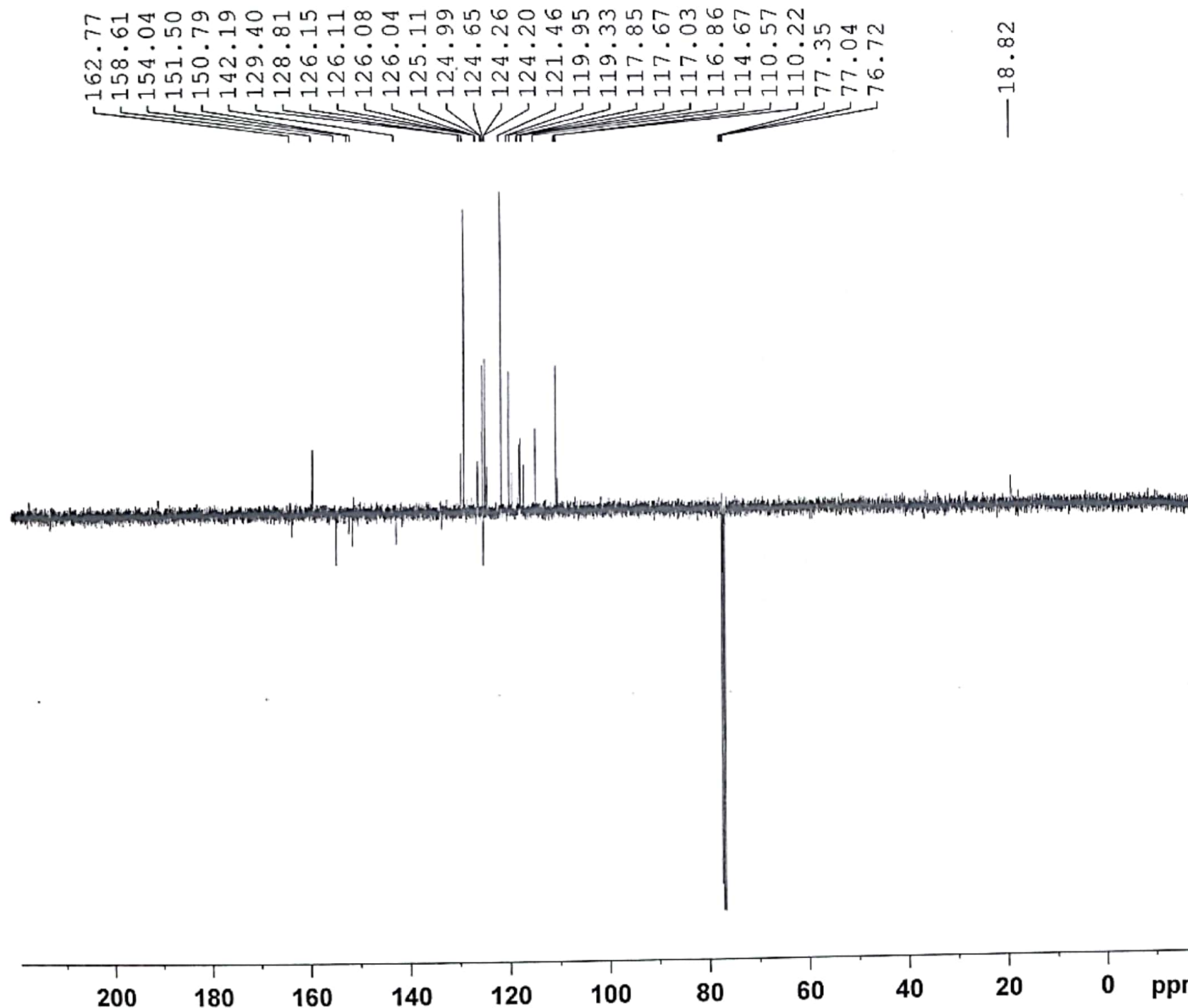
F2 - Acquisition Parameters
 Date_ 20150305
 Time_ 12.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.8 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-4E
 DEPTQ-BSU CDCl3 {C:\data} nmr 19



162.77
 158.61
 154.04
 151.50
 150.79
 142.19
 129.40
 128.81
 126.15
 126.11
 126.08
 126.04
 125.11
 124.99
 124.65
 124.26
 124.20
 121.46
 119.95
 119.33
 117.85
 117.67
 117.03
 116.86
 114.67
 110.57
 110.22
 77.35
 77.04
 76.72

—18.82

Current Data Parameters
 NAME Mar15-2015-nmr
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150316
 Time 10.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptqppsp
 TD 65536
 SOLVENT CDCl3
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 294.3 K
 CNST2 145.000000
 CNST12 1.500000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SPNAM[5] Crp60comp.4
 SPOALS 0.500
 SPOFFS5 0 Hz
 SPW5 10.08399963 W

==== CHANNEL f2 =====
 SFO2 400.1312797 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

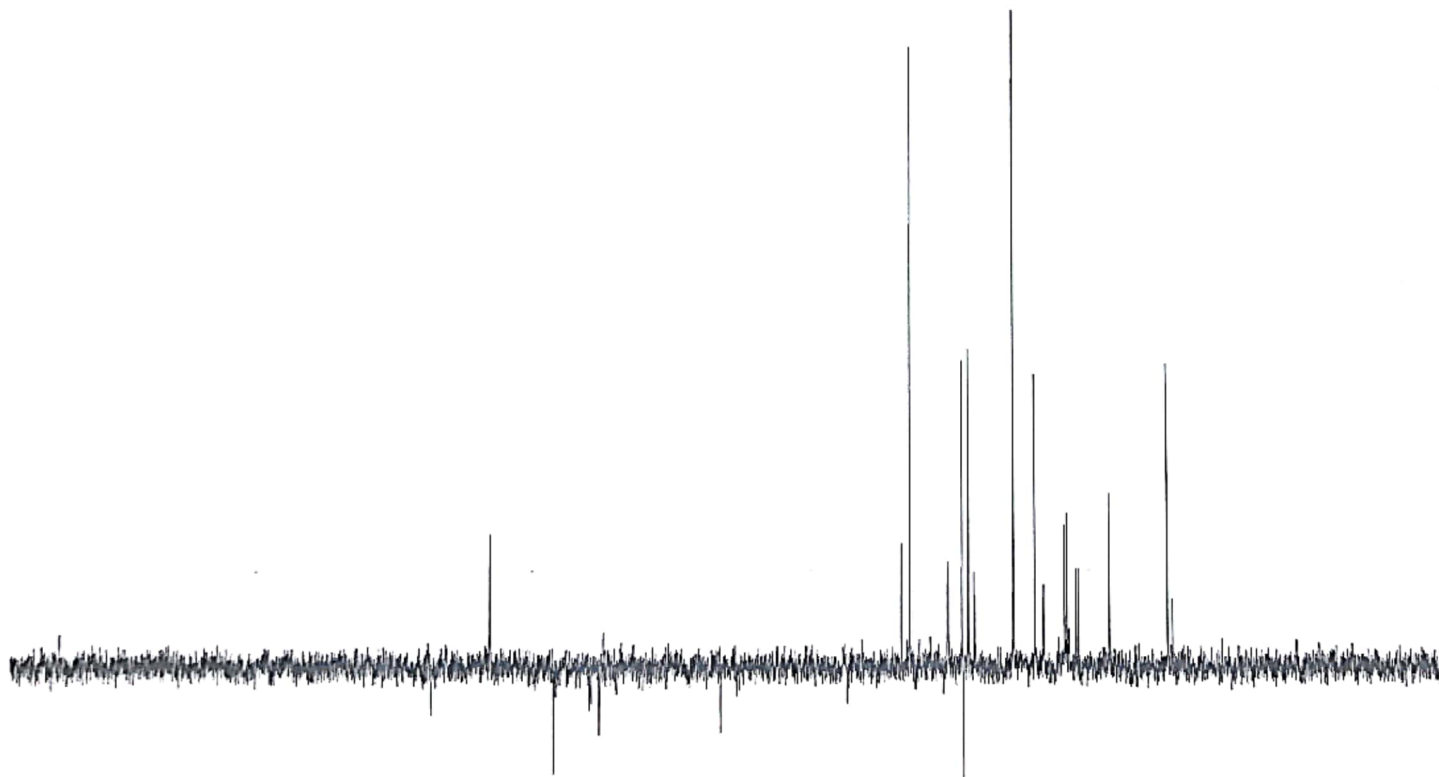
==== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GENAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 31.00 %
 GPZ2 31.00 %
 GPZ3 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127890 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

HEBA-4E
DEPTQ-BSU CDC13 {C:\data} nmr 19



— 162.77
— 158.61
— 154.04
— 151.50
— 150.79
142.19
129.40
128.81
126.15
126.11
126.08
126.04
125.11
124.99
124.65
124.26
124.20
121.46
119.95
119.33
117.85
117.67
117.03
116.86
114.67
110.57
110.22



Current Data Parameters
NAME Mar15-2015-nmr
EXPNO 310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150316
Time_ 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqppp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
CNST2 145.000000
CNST12 1.500000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLWD 0 W
PLW1 66.00000000 W
SFNAM[5] Crp60ccomp.4
SFOALS 0.500
SPOFFS5 0 Hz
SFWS 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GFNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-4F
PROTON_BSU CDC13 {C:\data} nmr 4



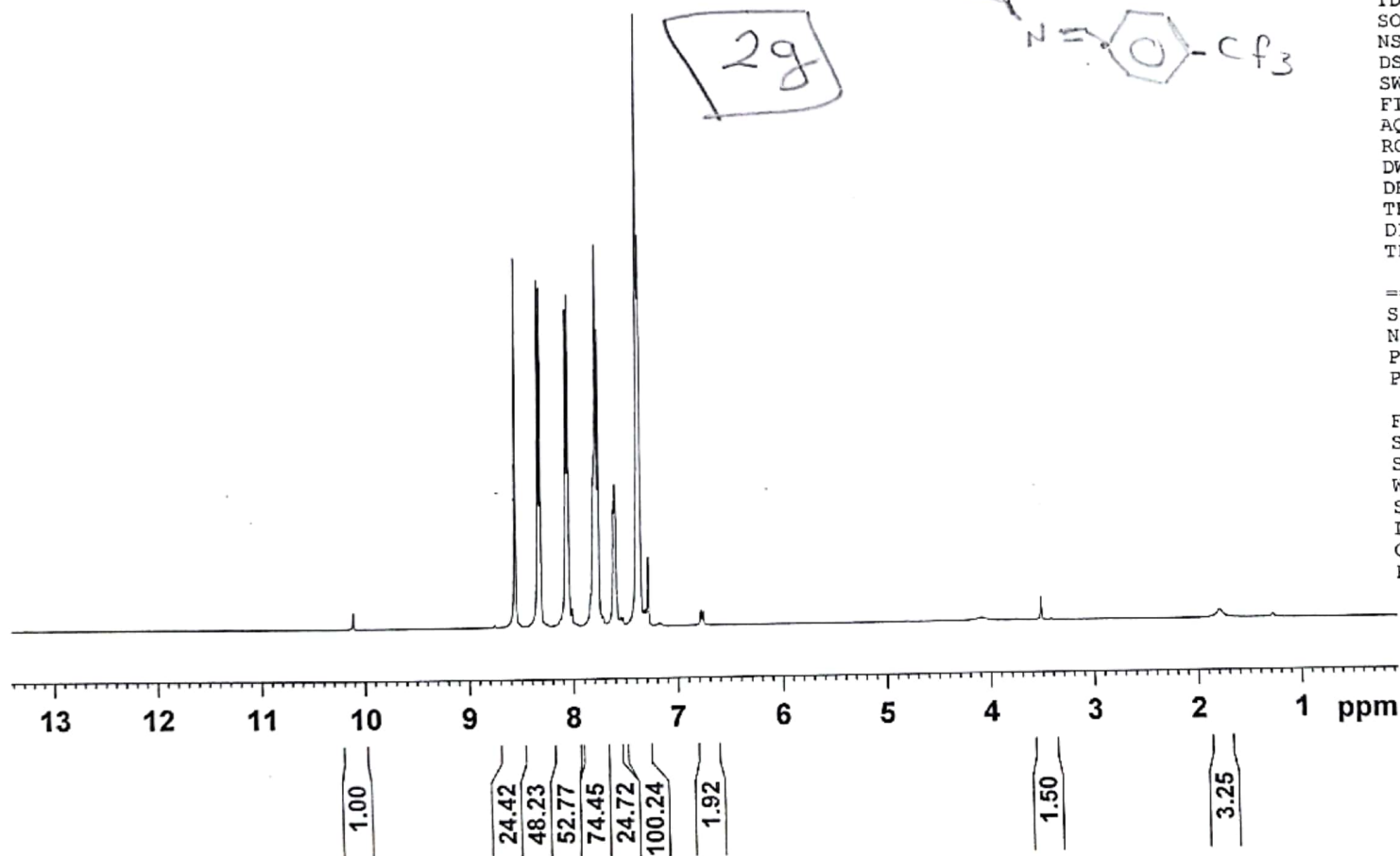
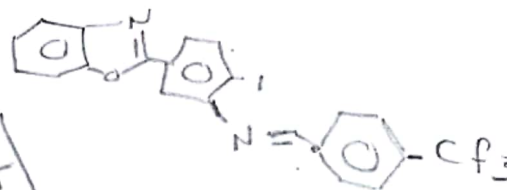
Current Data Parameters
NAME Mar05-2015-nmr
EXPNO 270
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150305
Time_ 12.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.9 K
D1 1.0000000 sec
TD0 1

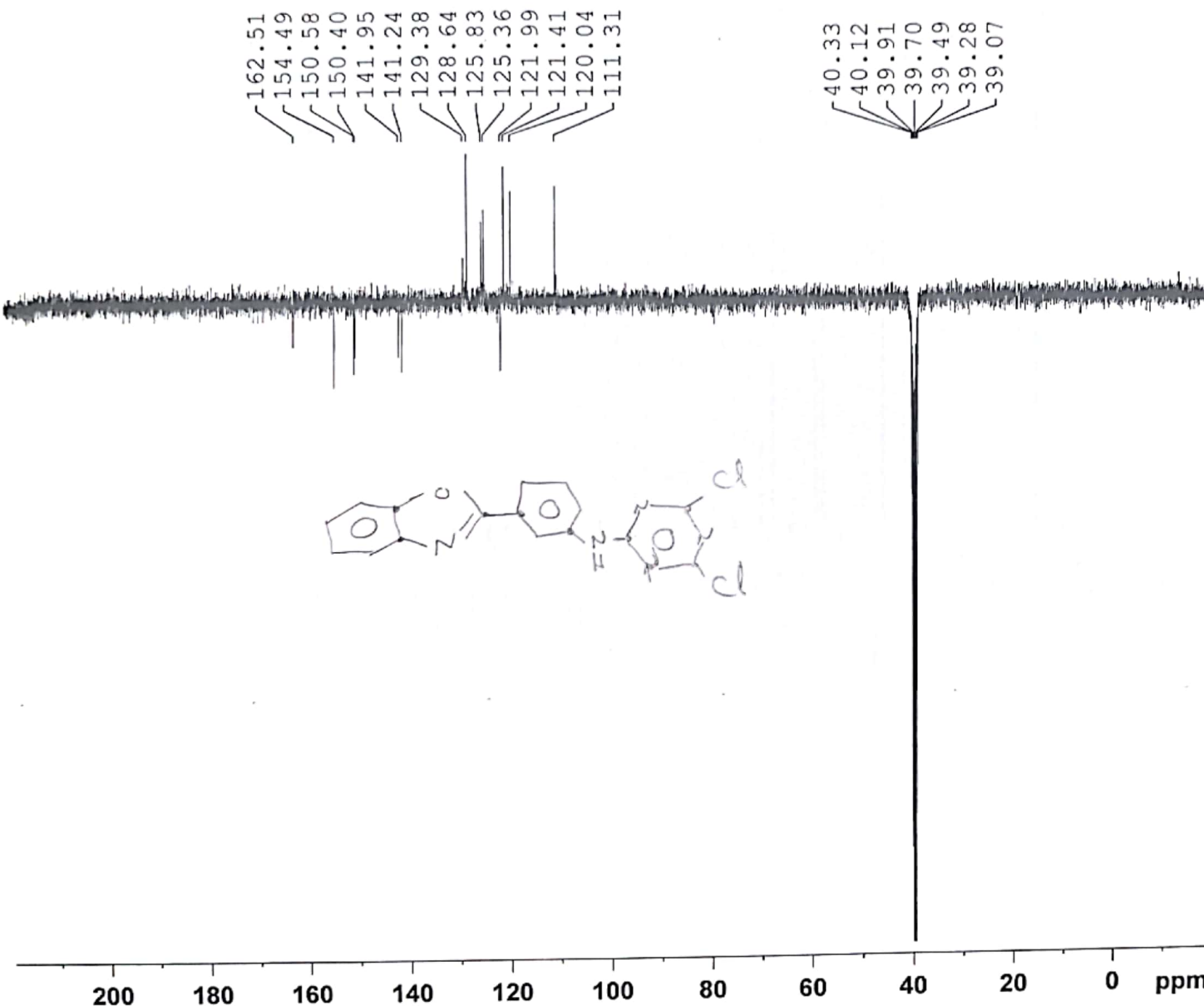
==== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

10.113
8.557
8.336
8.316
8.069
8.049
8.012
7.835
7.810
7.801
7.780
7.760
7.738
7.714
7.616
7.603
7.595
7.549
7.528
7.383
7.364
7.327
7.311
7.284
6.784
6.763
3.513
1.787



HEBA-M11
DEPTQ-BSU DMSO (C:\data) nmr 20



Current Data Parameters
NAME Apr19-2015-nmr
EXPNO 520
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150420
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqqpp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
LW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

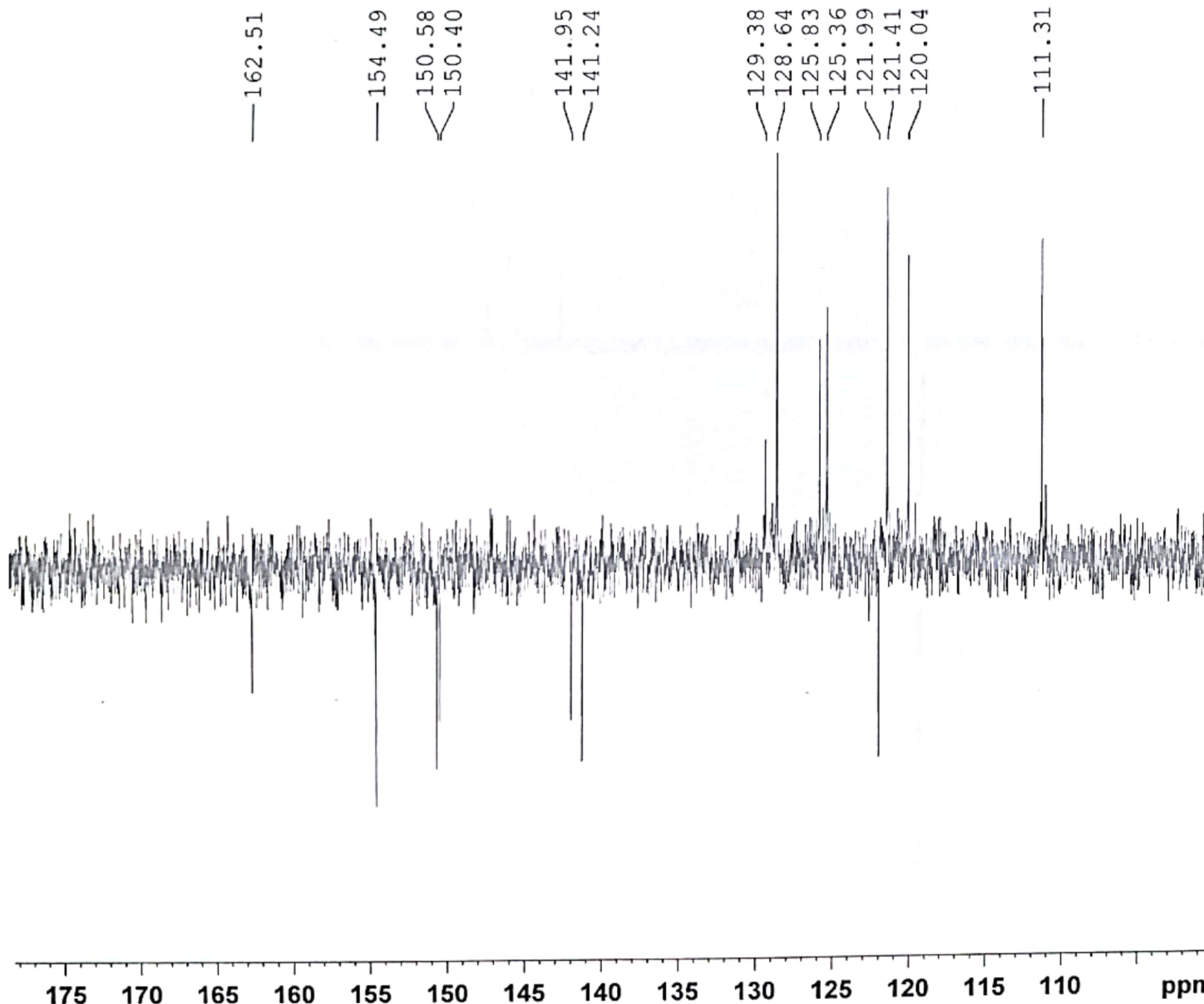
----- CHANNEL f1 -----
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFNAM[5] Crp60comp.4
SFOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

----- CHANNEL f2 -----
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 31.00 %
GP22 31.00 %
GP23 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-M11
DEPTQ-BSU DMSO {C:\data} nmr 20



Current Data Parameters
NAME Apr19-2015-nmr
EXPNO 520
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150420
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60ccmp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

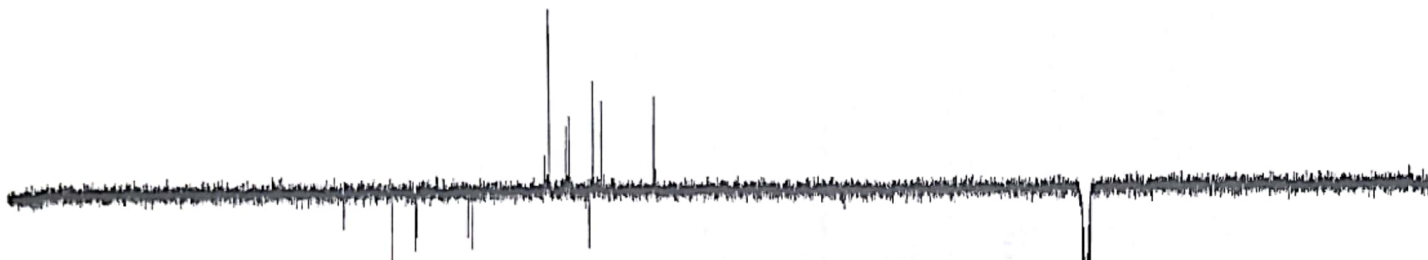
HEBA-M11
DEPTQ-BSU DMSO {C:\data} nmr 20

another
copy



162.51
154.49
150.58
150.40
141.95
141.24
129.38
128.64
125.83
125.36
121.99
121.41
120.04
111.31

40.33
40.12
39.91
39.70
39.49
39.28
39.07



Current Data Parameters
NAME Apr19-2015-nmr
EXPNO 520
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150420
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.000000
CNST12 1.500000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GFZ1 31.00 %
GFZ2 31.00 %
GFZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

HEBA-M11
DEPTQ-BSU DMSO {C:\data} nmr 20



Current Data Parameters
NAME Apr19-2015-nmr
EXPNO 520
PROCNO 1

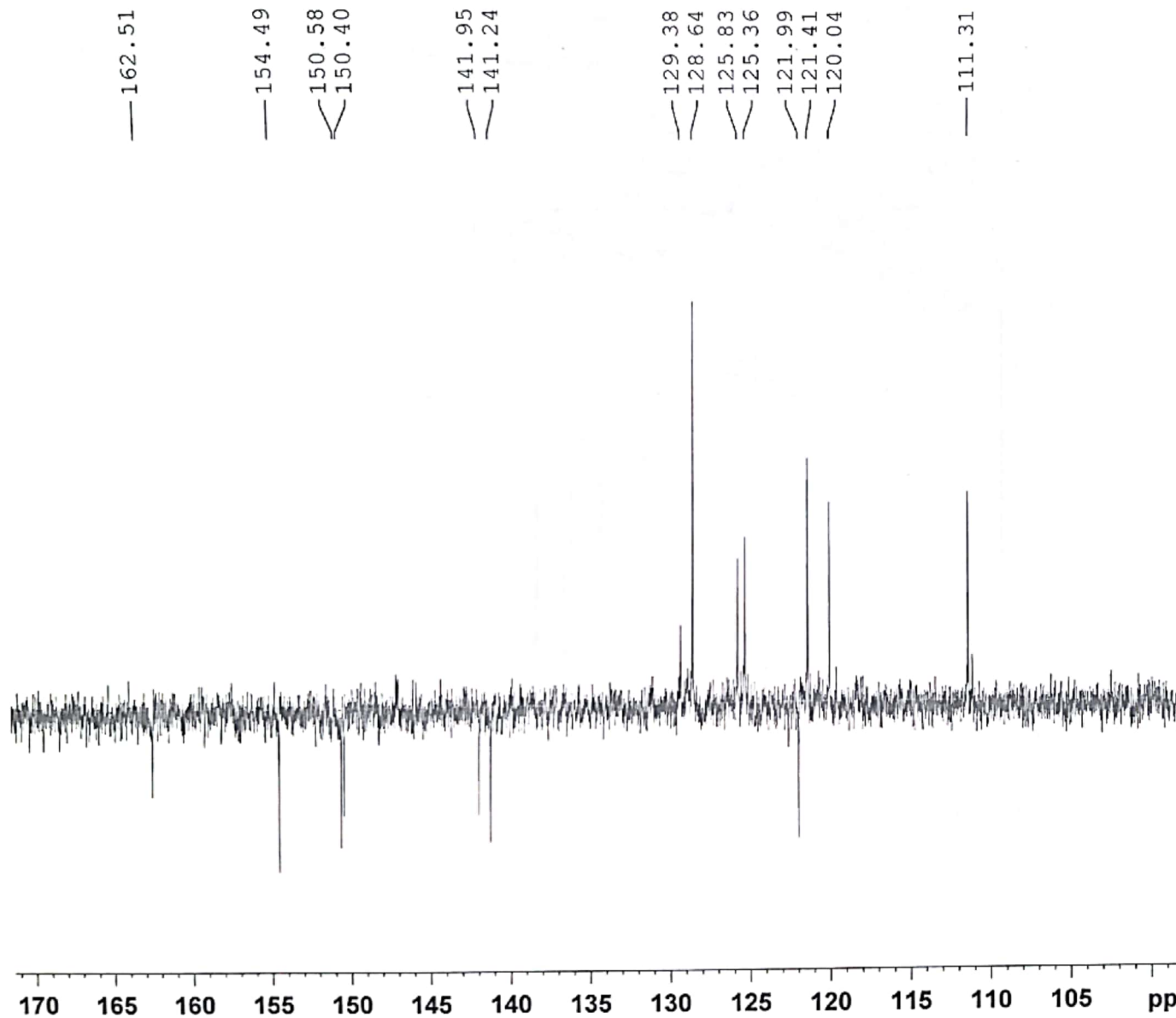
F2 - Acquisition Parameters
Date_ 20150420
Time 9.11
INSTRUM spect
PROBHD 5 mm PABSO BB/
PULPROG deptqqsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.000000
CNST12 1.500000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

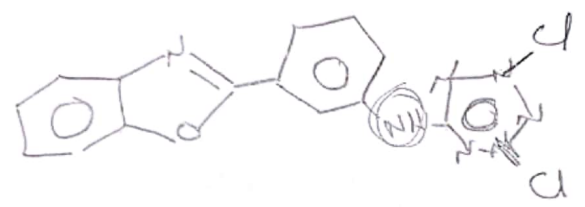
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-11
PROTON_B9

11.507
10.900
10.785
10.772
8.400
8.387
8.286
8.250
8.216
8.198
8.176
8.076
8.064
8.037
8.027
8.024
8.016
7.991
7.879
7.863
7.857
7.784
7.726
7.534
7.410
7.402
7.138
7.114
6.993

*Cryst (11 new)
25 Start (16)*



3

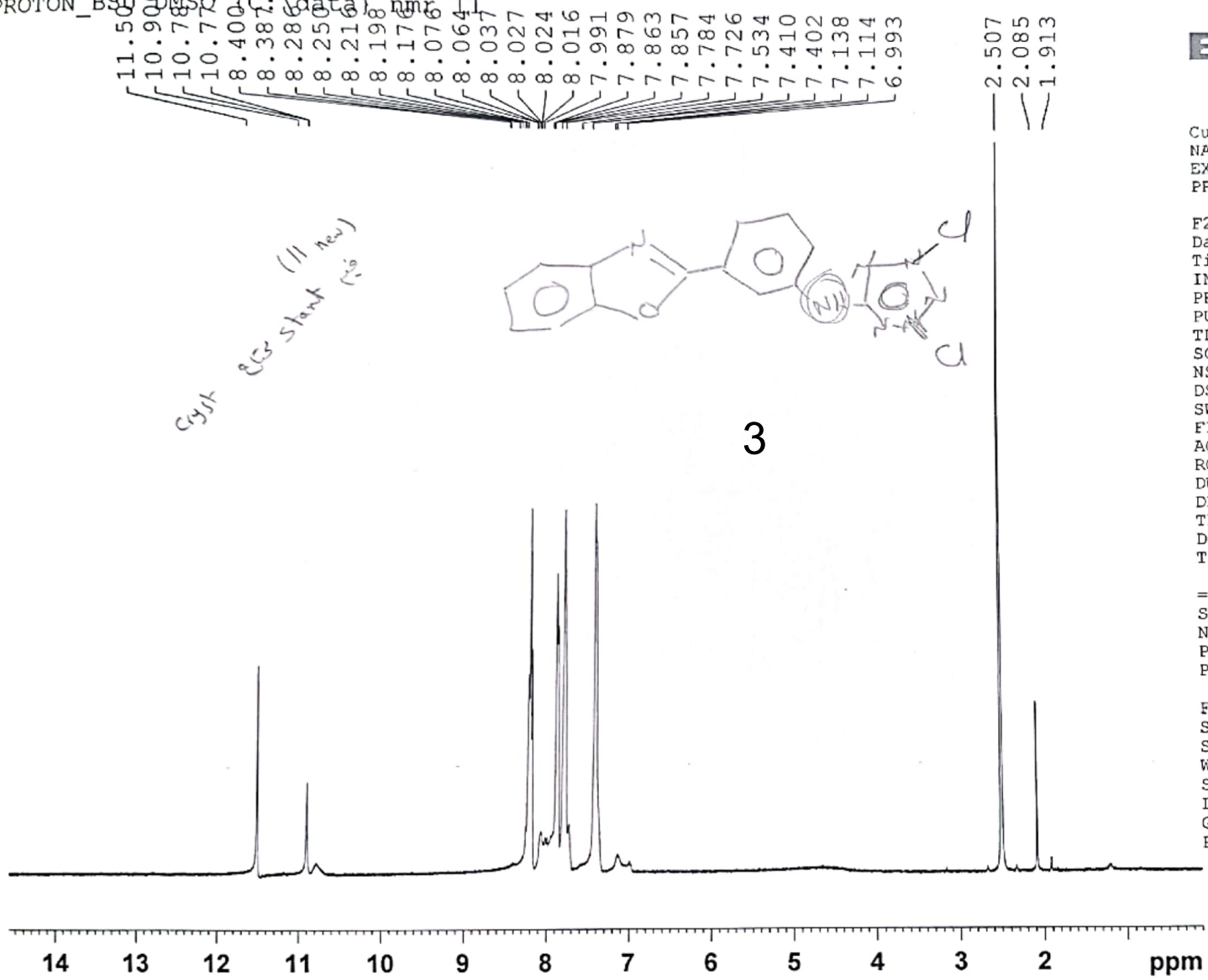


Current Data Parameters
NAME Apr26-2015-nmr
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date 20150426
Time 12.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



1.00 0.60 4.52 1.44 3.90 4.90 5.18 0.65 0.42 4.30 0.50

HEBA-11
PROTON_BSU DMSO {C:\data} nmr 11

8.400
8.387
8.286
8.250
8.216
8.198
8.176
8.076
8.064
8.037
8.027
8.024
8.016
7.991
7.879
7.863
7.857
7.784
7.726

— 7.534

< 7.410
< 7.402

< 7.138
< 7.114

— 6.993

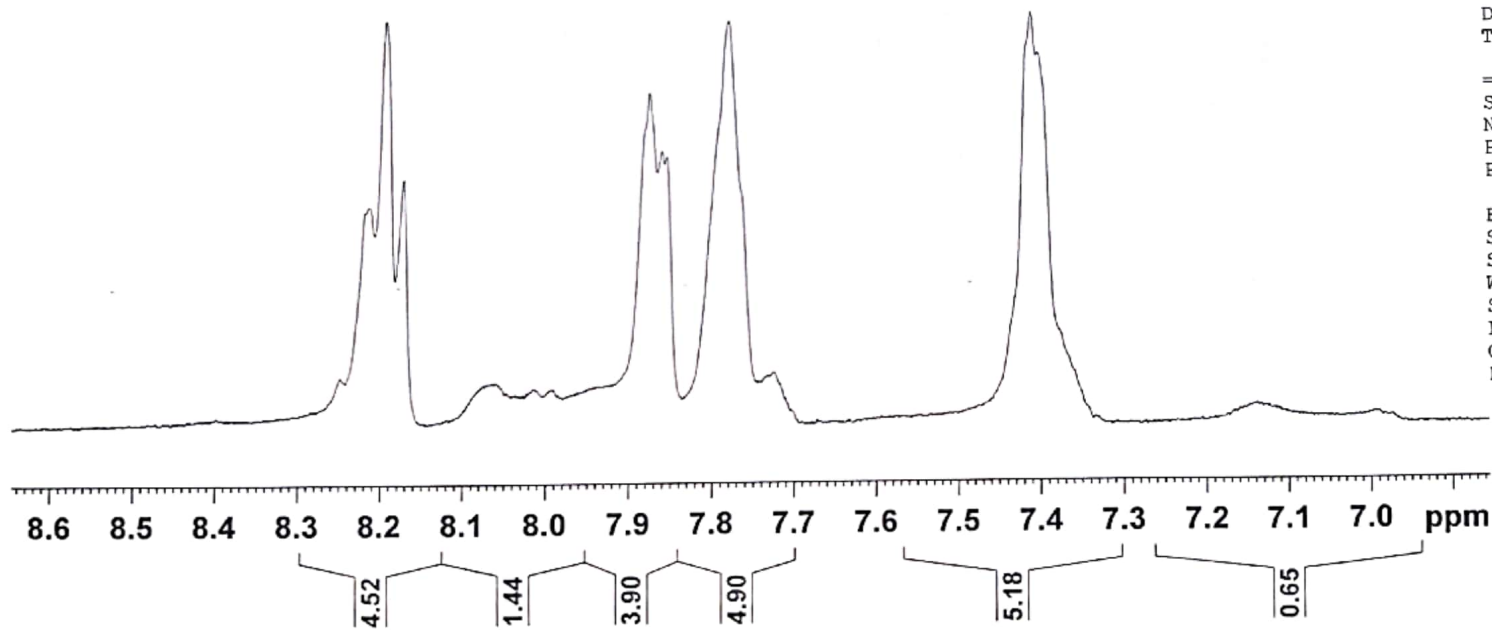


Current Data Parameters
NAME Apr26-2015-nmr
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date 20150426
Time 12.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-12A
PROTON_BSU CDC13 {C:\data} nmr 13



Current Data Parameters
NAME May14-2015-nmr
EXPNO 160
PROCNO 1

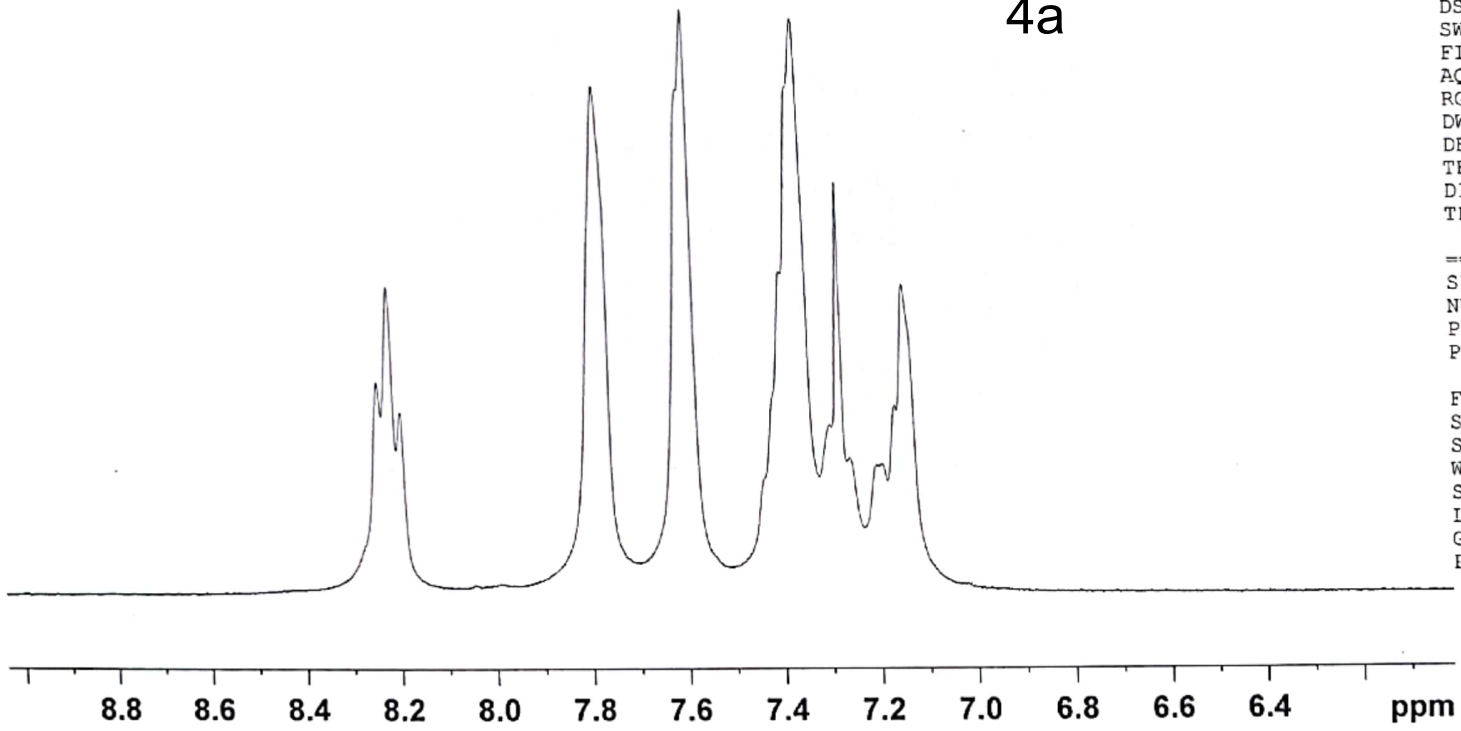
F2 - Acquisition Parameters
Date 20150514
Time 11.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

8.247
8.223
8.197
7.790
7.600
7.405
7.368
7.301
7.284
7.263
7.205
7.200
7.194
7.167
7.147

4a



1.00
1.53
1.74
2.19
0.83
1.22

HEBA-12A
 DEPTQ-BSU DMSO (C:\data) nmr 18



Current Data Parameters
 NAME Jul21-2015-nmr
 EXPMO 250
 PROCNO 1

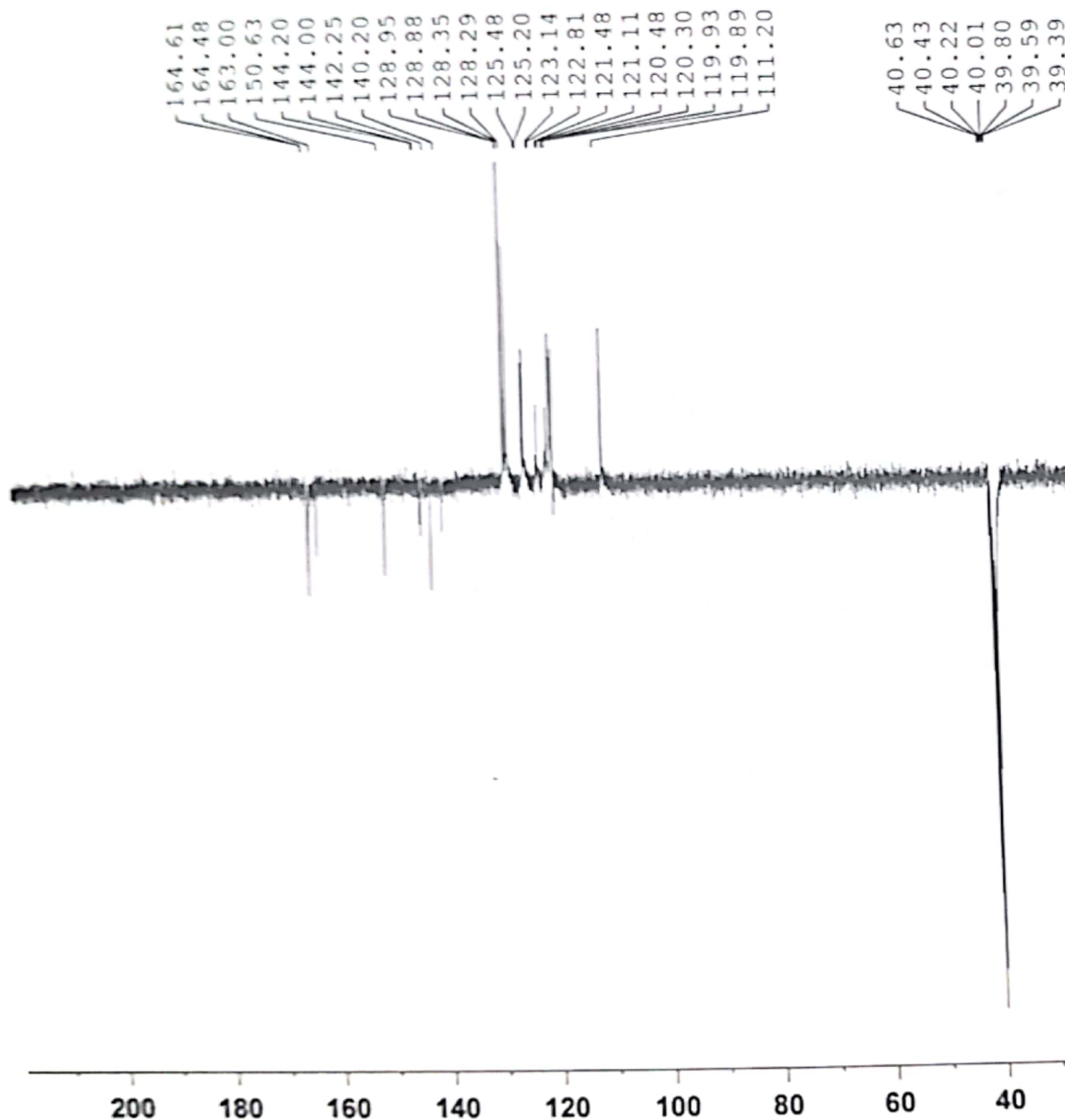
F2 - Acquisition Parameters
 Date_ 20150722
 Time_ 0.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG deptqppp
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 300.8 K
 CNST2 145.000000
 CNST12 1.500000
 D1 2.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 C16 0.00020000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SFO1(5) Crp60comp.4
 SFO1(5) 0.500
 SFOFF5 0 Hz
 SPW5 10.08399963 W

----- CHANNEL f2 -----
 SFO2 400.1312797 MHz
 NUC2 1H
 CPOPRG2 waltz16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 P4 90.00 usec
 PCPD2 16.00000000 W
 PLW2 0.21779999 W

----- GRADIENT CHANNEL -----
 GPNAM[1] SMO210.100
 GPNAM[2] SMO210.100
 GPNAM[3] SMO210.100
 GP21 31.00 A
 GP22 31.00 A
 GP23 31.00 A
 P16 1000.00 usec

F2 - Processing parameters
 SI 32.68
 SF 100.6127690 MHz
 EQU EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



HEBA-12A
DEPTQ-BSU DMSO {C:\data} nmr 18



Current Data Parameters
NAME Jul21-2015-nmr
EXPNO 250
PROCNO 1

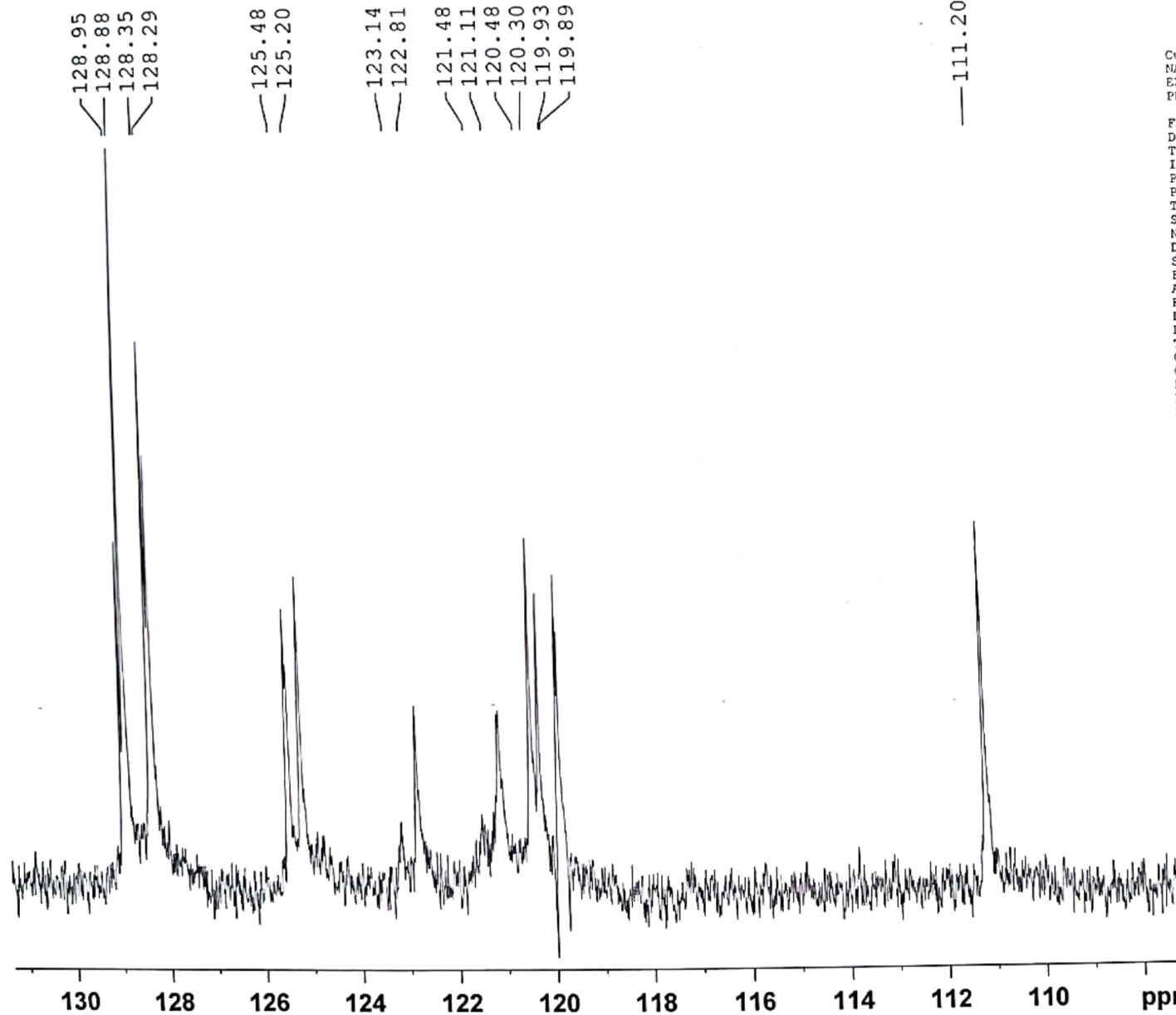
F2 - Acquisition Parameters
Date_ 20150722
Time 0.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 300.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-12A
DEPTQ-BSU DMSO {C:\data} nmr 18



164.61
164.48
163.00

150.63

144.20
144.00

142.25

140.20

Current Data Parameters
NAME Jul21-2015-nmr
EXPNO 250
PROCNO 1

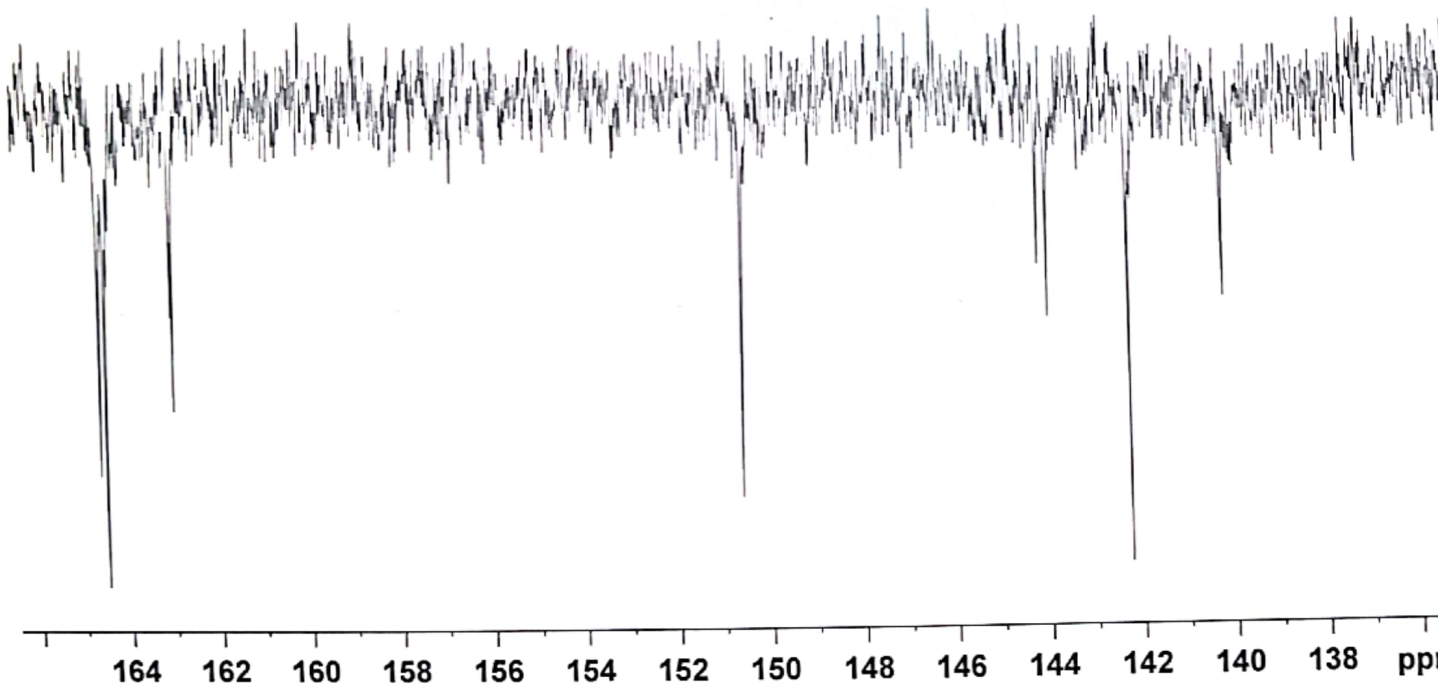
F2 - Acquisition Parameters
Date 20150722
Time 0.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 300.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344829 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

==== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-12B
 PROTON_BSU CDC13 {C:\data} nmr 20

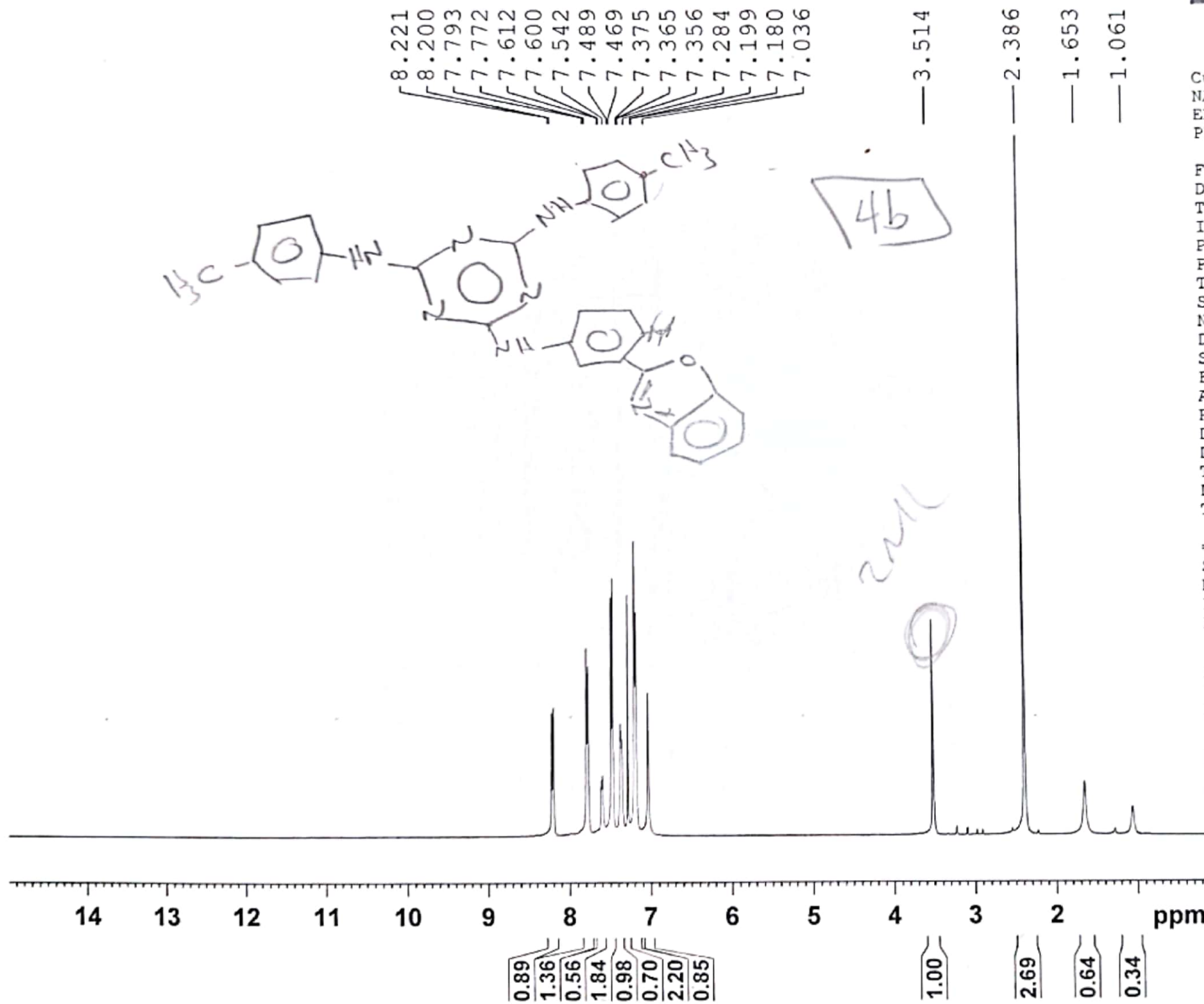


Current Data Parameters
 NAME May19-2015-nmr
 EXPNO 410
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150519
 Time_ 13.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-12B
 PROTON_BSU CDC13 {C:\data} nmr 20

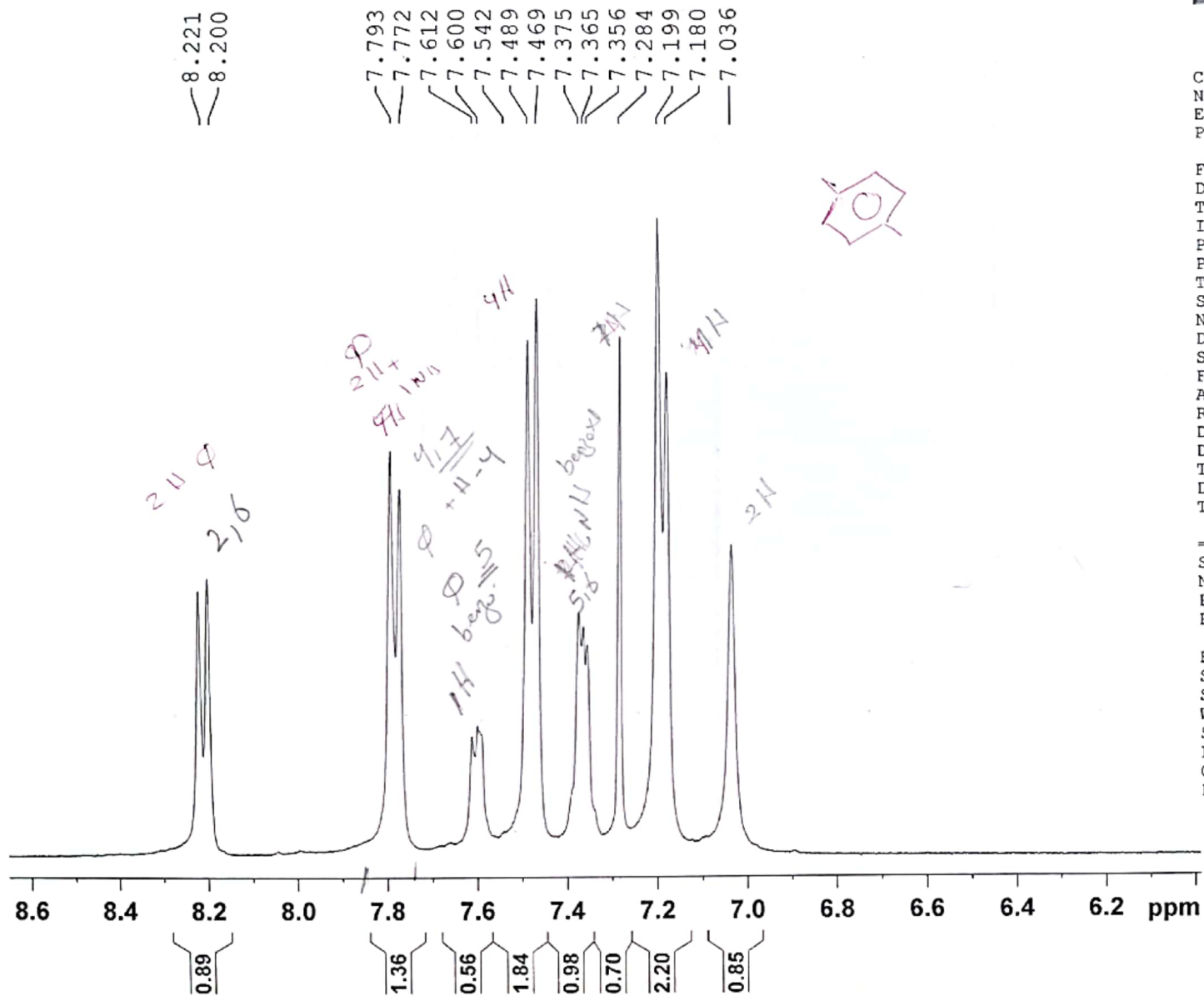


Current Data Parameters
 NAME May19-2015-nmr
 EXPNO 410
 PROCNO 1

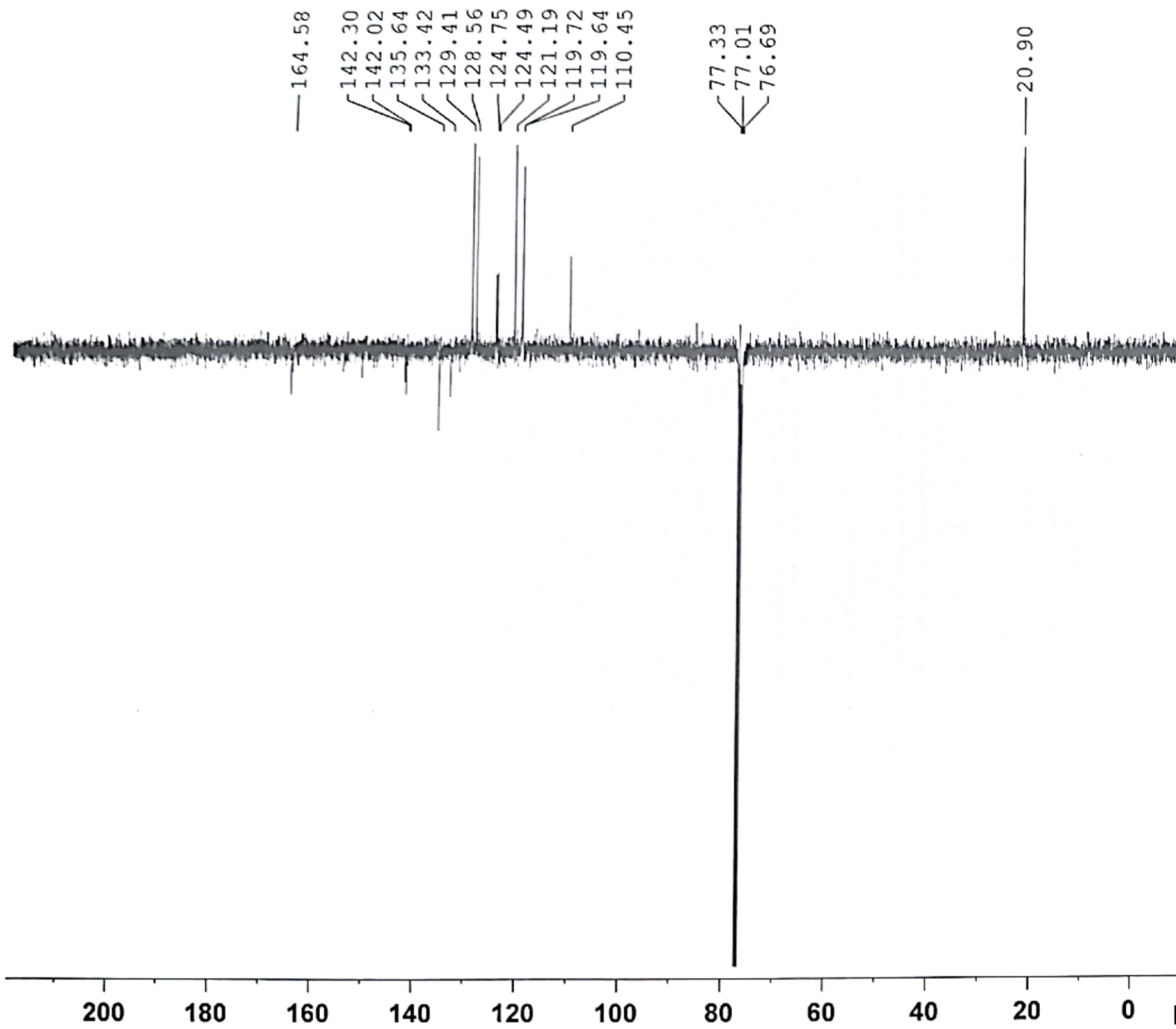
F2 - Acquisition Parameters
 Date_ 20150519
 Time_ 13.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 295.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-12B
DEPTQ-BSU CDC13 {C:\data} nmr 20



164.58
142.30
142.02
135.64
133.42
129.41
128.56
124.75
124.49
121.19
119.72
119.64
110.45

77.33
77.01
76.69

20.90

Current Data Parameters
NAME Jun28-2015-nmr
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150629
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00002000 sec
TDO 1

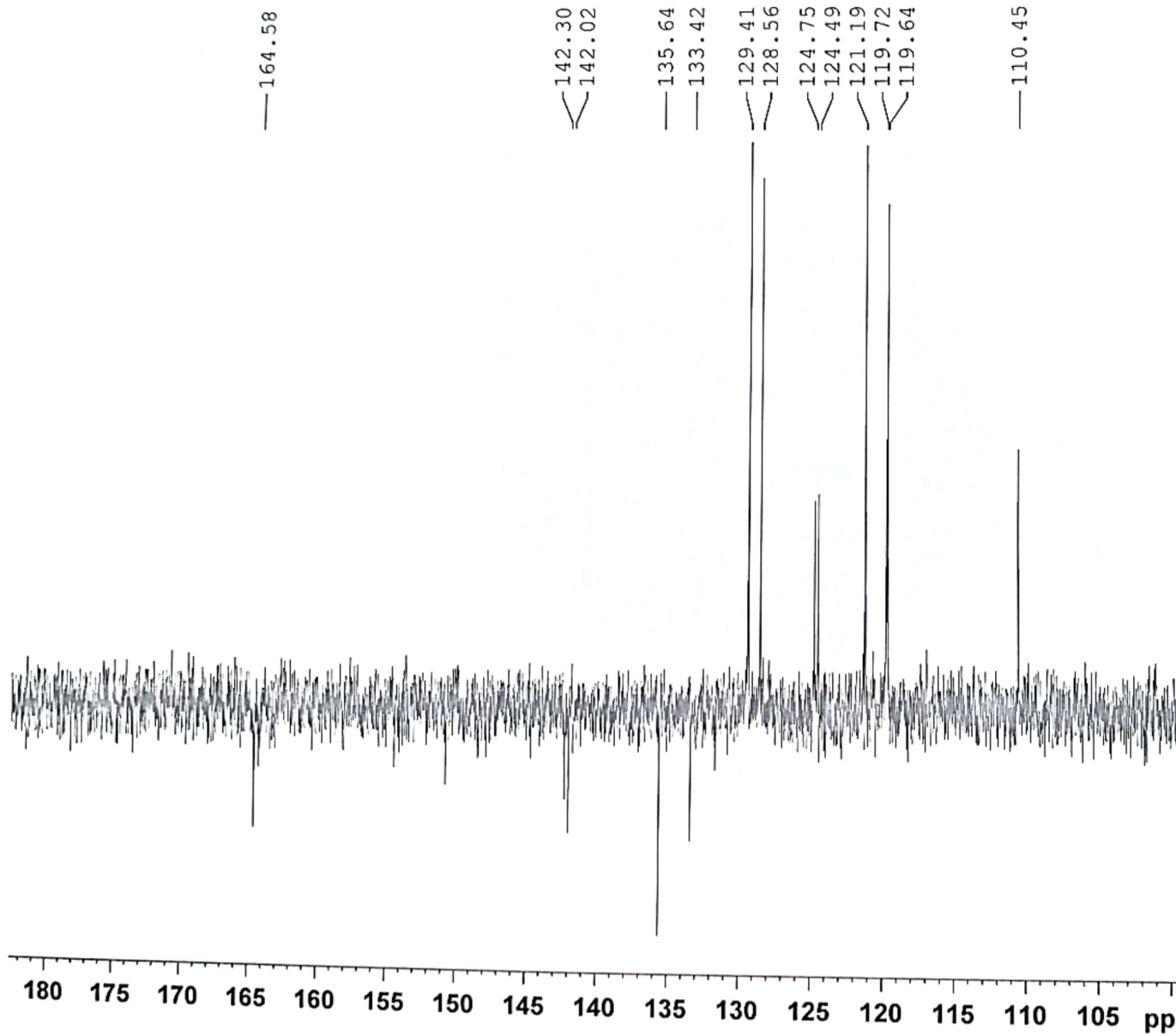
===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFOAL5 Crp60comp.4
SFOALS 0.500
SFOFFS5 0 Hz
SFO5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG2 waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-12B
DEPTQ-BSU CDC13 (C:\data) nmr 20



Current Data Parameters
NAME Jun28-2015-nmr
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150629
Time_ 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptgpgsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.000000
CNST12 1.500000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

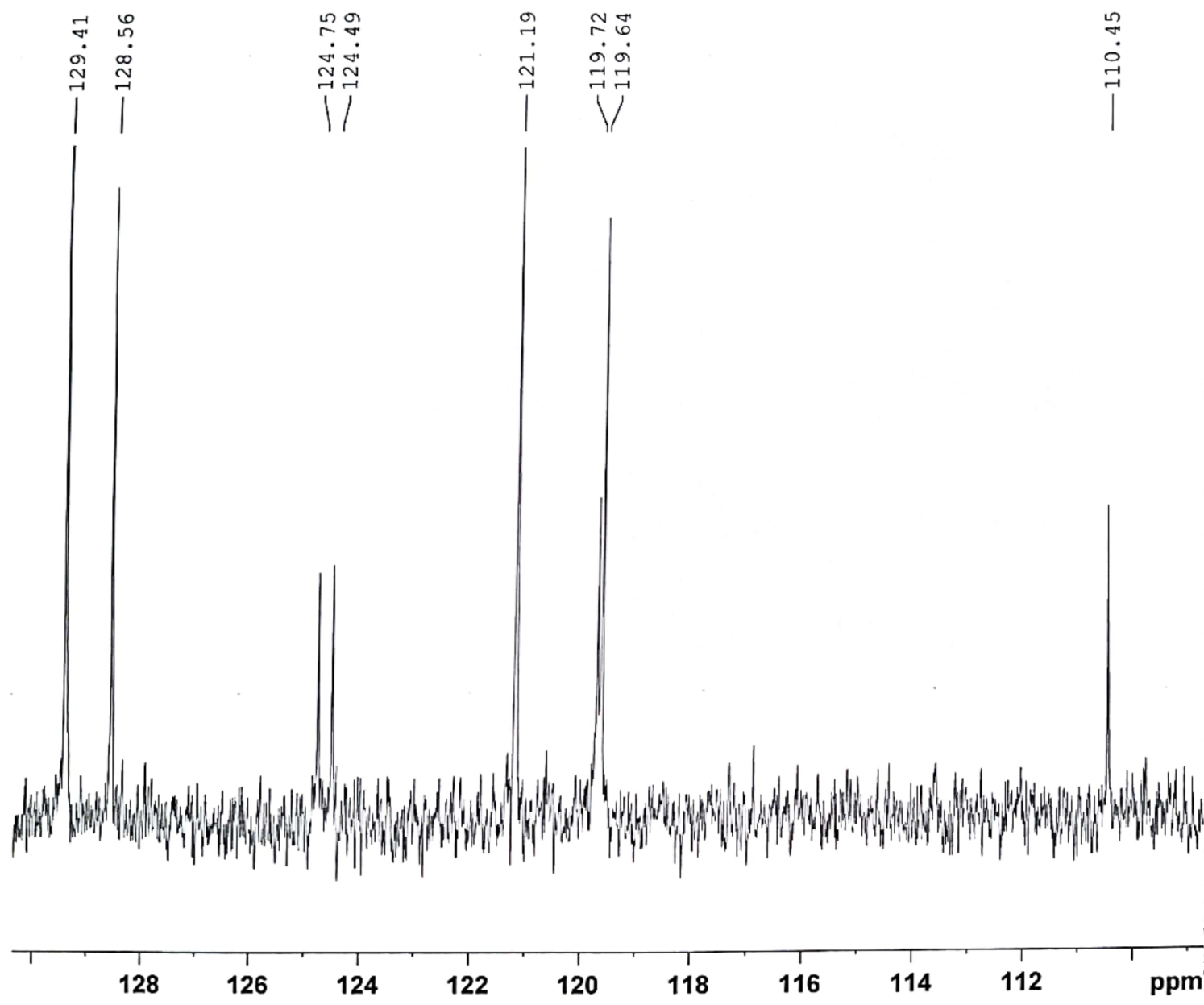
===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG2 waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-12B
DEPTQ-BSU CDC13 {C:\data} nmr 20



Current Data Parameters
NAME Jun28-2015-nmr
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150629
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

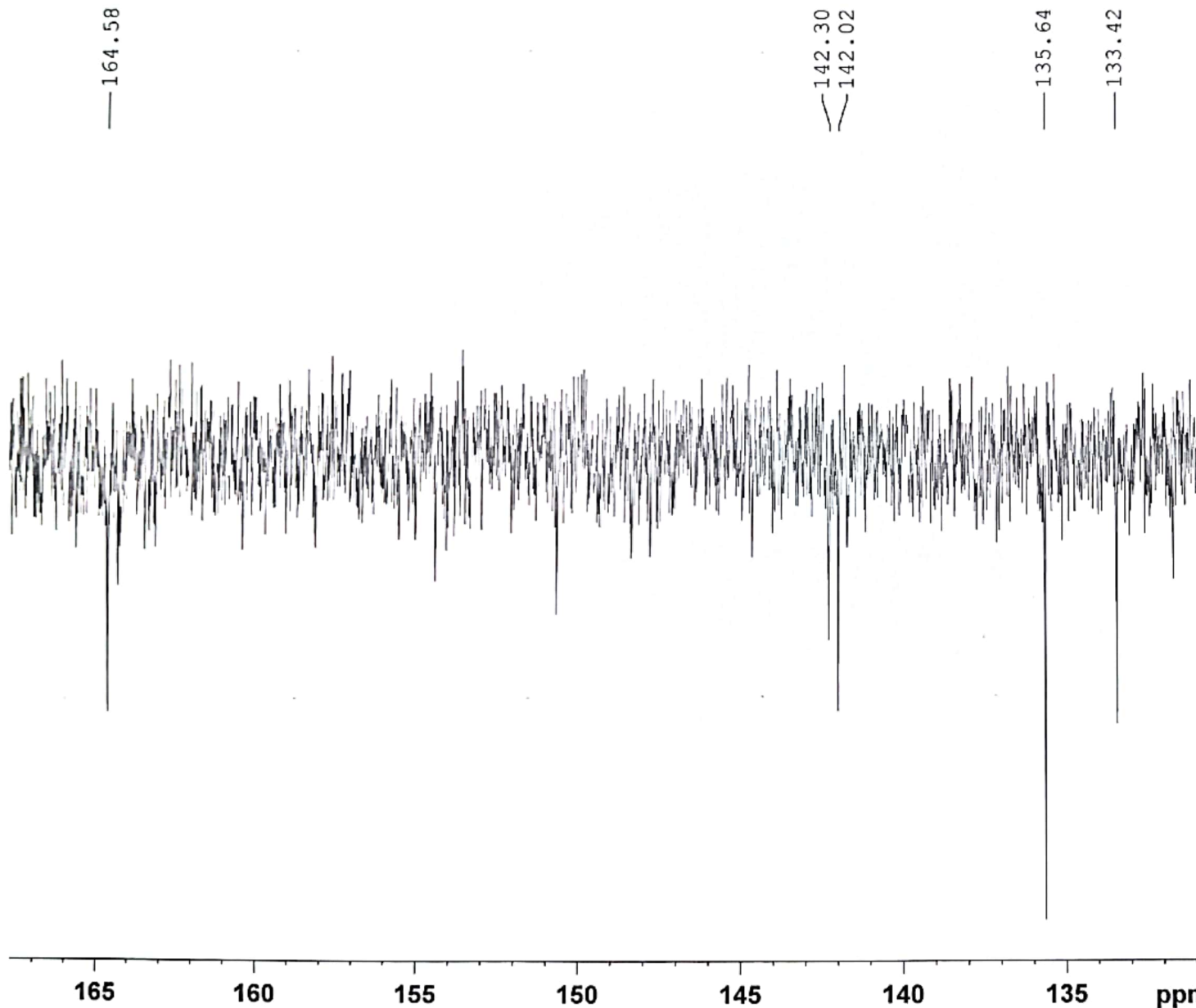
===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-12B
DEPTQ-BSU CDC13 {C:\data} nmr 20



Current Data Parameters
NAME Jun28-2015-nmr
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150629
Time 8.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpap
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60ccmp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SF02 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-M12D
PROTON_BSU DMSO {C:\data} nmr 20



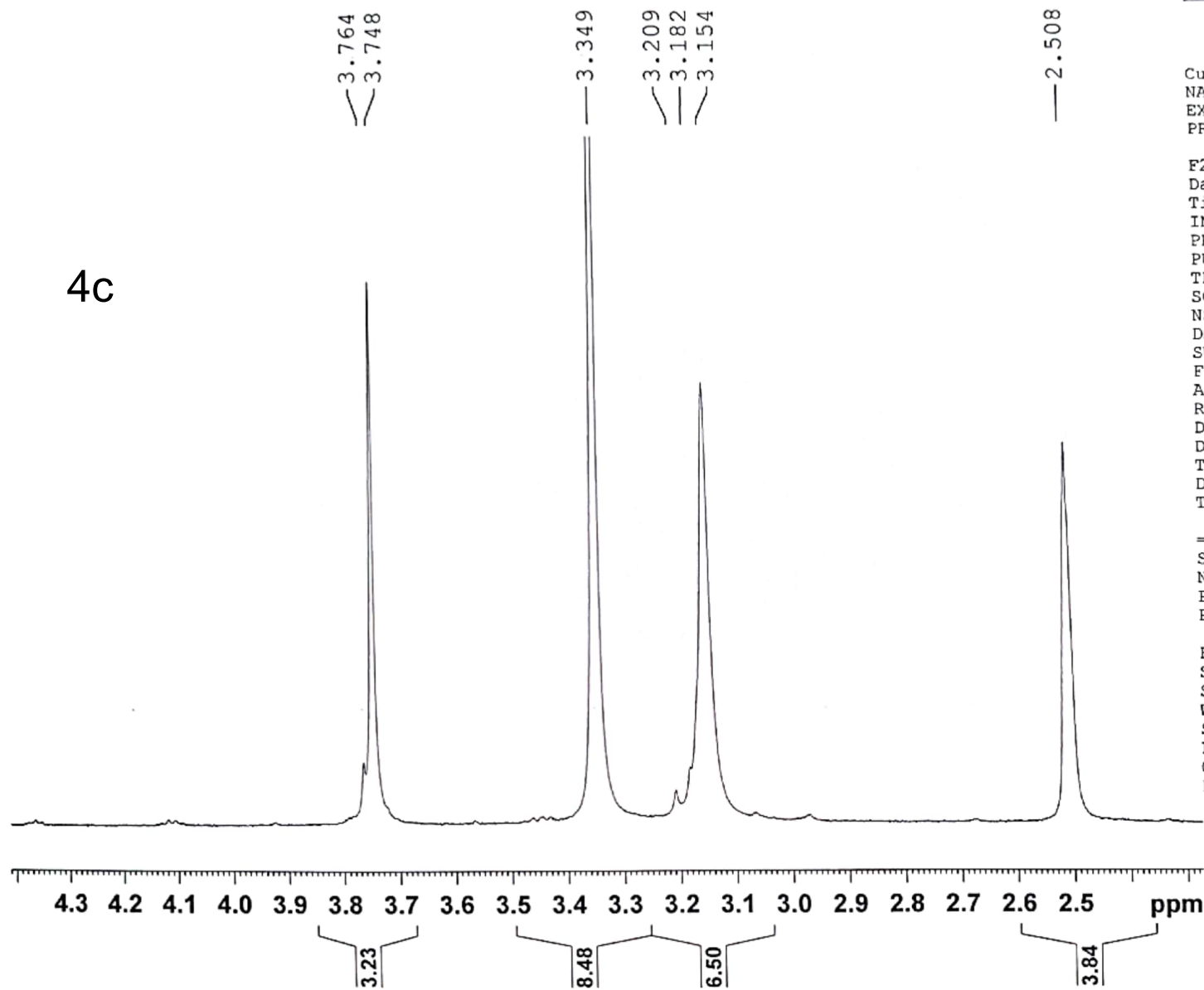
Current Data Parameters
NAME Jun16-2015-nmr
EXPNO 120
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150616
Time_ 10.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

4c



HEBA-M12D
 PROTON_BSU DMSO (C:\data) nmr 20

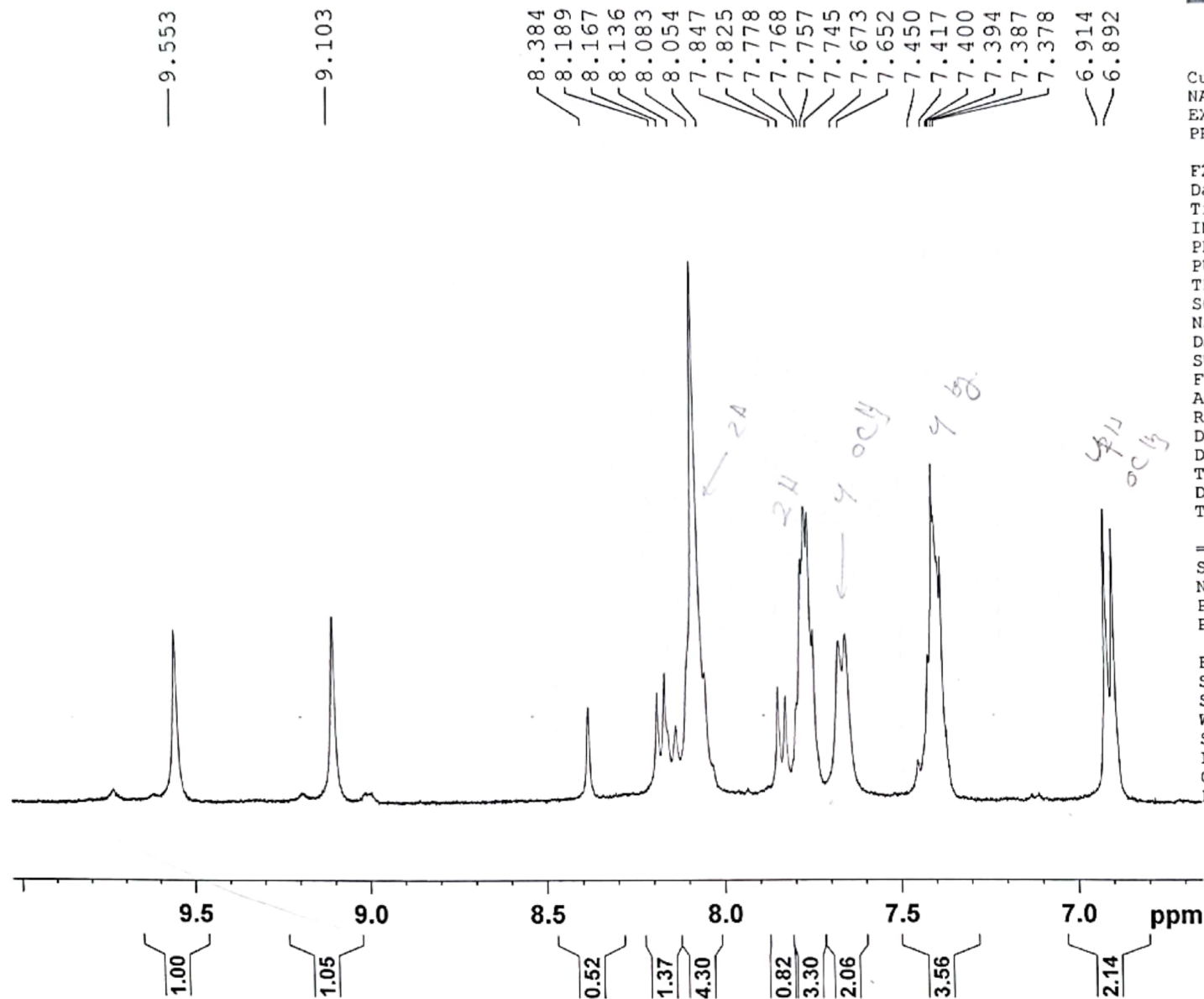


Current Data Parameters
 NAME Jun16-2015-nmr
 EXPNO 120
 PROCNO 1

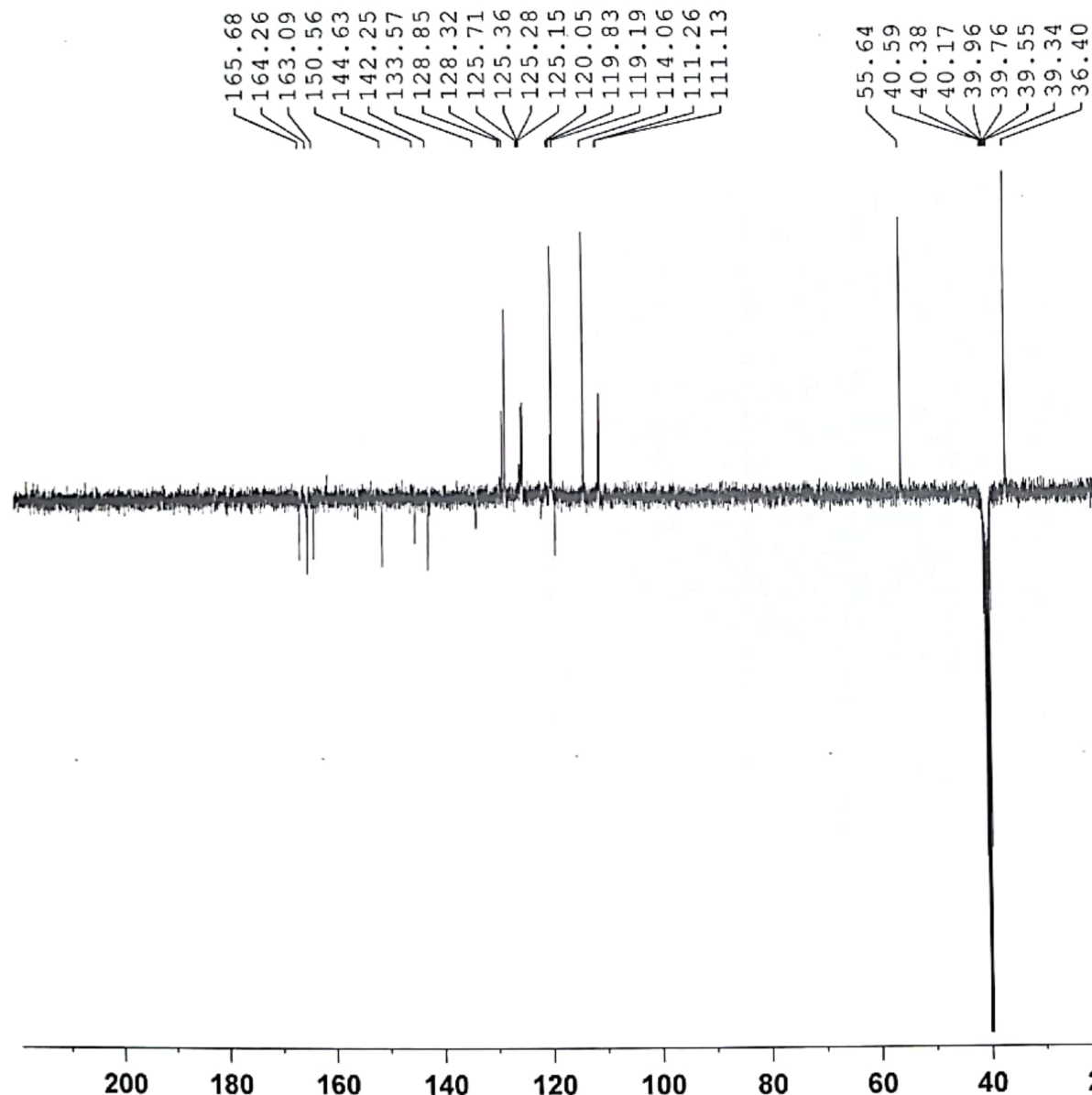
F2 - Acquisition Parameters
 Date_ 20150616
 Time_ 10.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 296.9 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-M12D
 DEPTQ-BSU DMSO {C:\data} nmr 19



Current Data Parameters
 NAME Jun17-2015-nmr
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150617
 Time_ 20.41
 INSTRUM spect
 PROBHD 5 mm PARBO BB/
 PULPROG deptqgppsp
 TD 65536
 SOLVENT DMSO
 NS 4000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 205.44
 DW 20.800 usec
 DE 6.50 usec
 TE 296.9 K
 CNST2 145.0000000
 CNST12 1.5000000
 D1 2.0000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 TDO 1

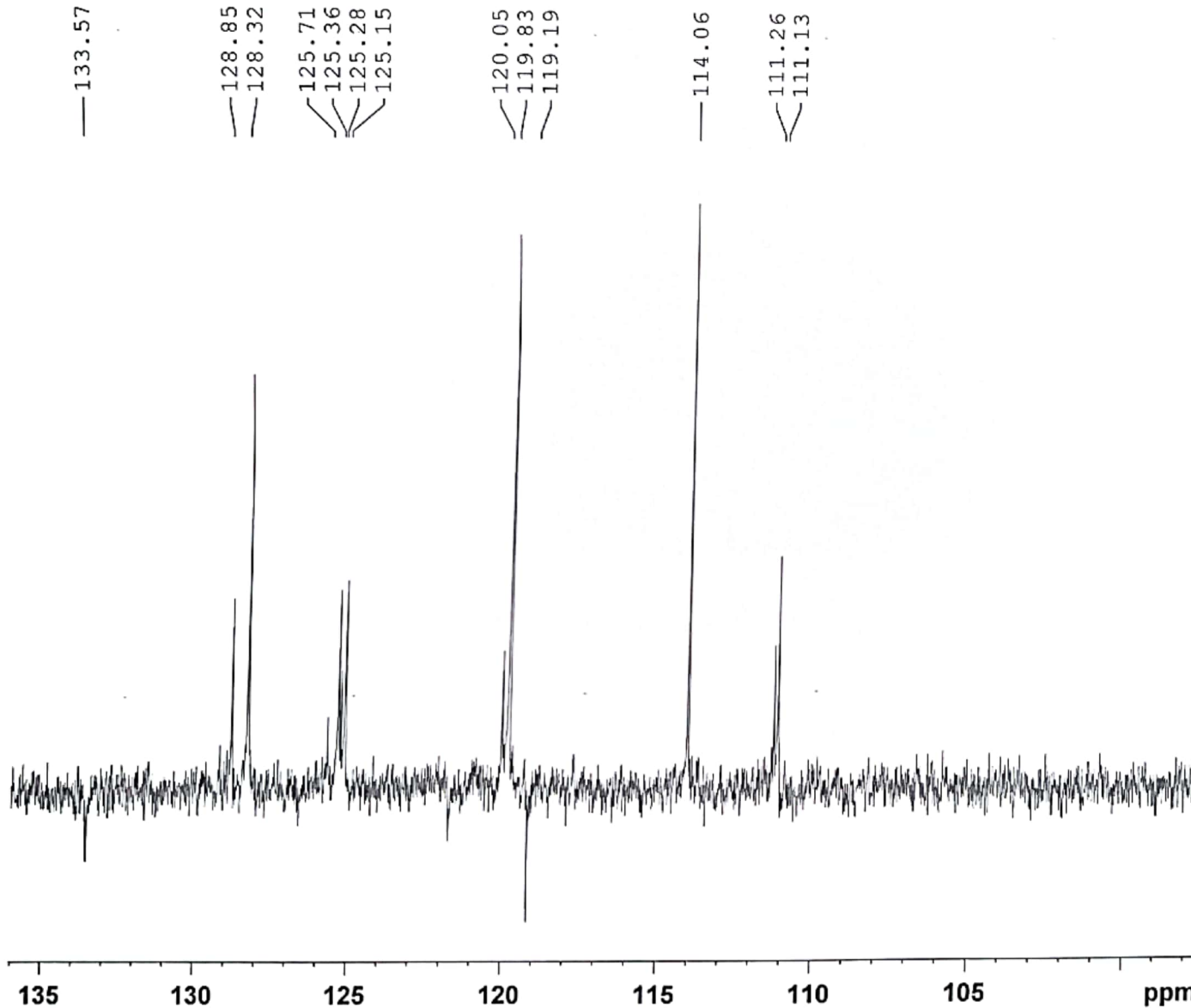
===== CHANNEL f1 =====
 SFO1 100.6228303 MHz
 NUC1 13C
 P1 10.00 usec
 P13 2000.00 usec
 PLW0 0 W
 PLW1 66.00000000 W
 SPNAM[5] Crp60comp.4
 SPCAL5 0.500
 SPOFFS5 0 Hz
 SPW5 10.08399963 W

===== CHANNEL f2 =====
 SFO2 400.1312797 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 P0 15.75 usec
 P3 10.50 usec
 P4 21.00 usec
 PCPD2 90.00 usec
 PLW2 16.00000000 W
 PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 31.00 %
 GPZ2 31.00 %
 GPZ3 31.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 FC 1.40

HEBA-M12D
DEPTQ-BSU DMSO {C:\data} nmr 19



Current Data Parameters
NAME Jun17-2015-nmr
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150617
Time 20.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptgggsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344825 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SFOFF5 0 Hz
SPW5 10.08399963 W

==== CHANNEL f2 =====
SFC2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-M12D
DEPTQ-BSU DMSO {C:\data} nmr 19



Current Data Parameters
NAME Jun17-2015-nmr
EXPNO 20
PROCNO 1

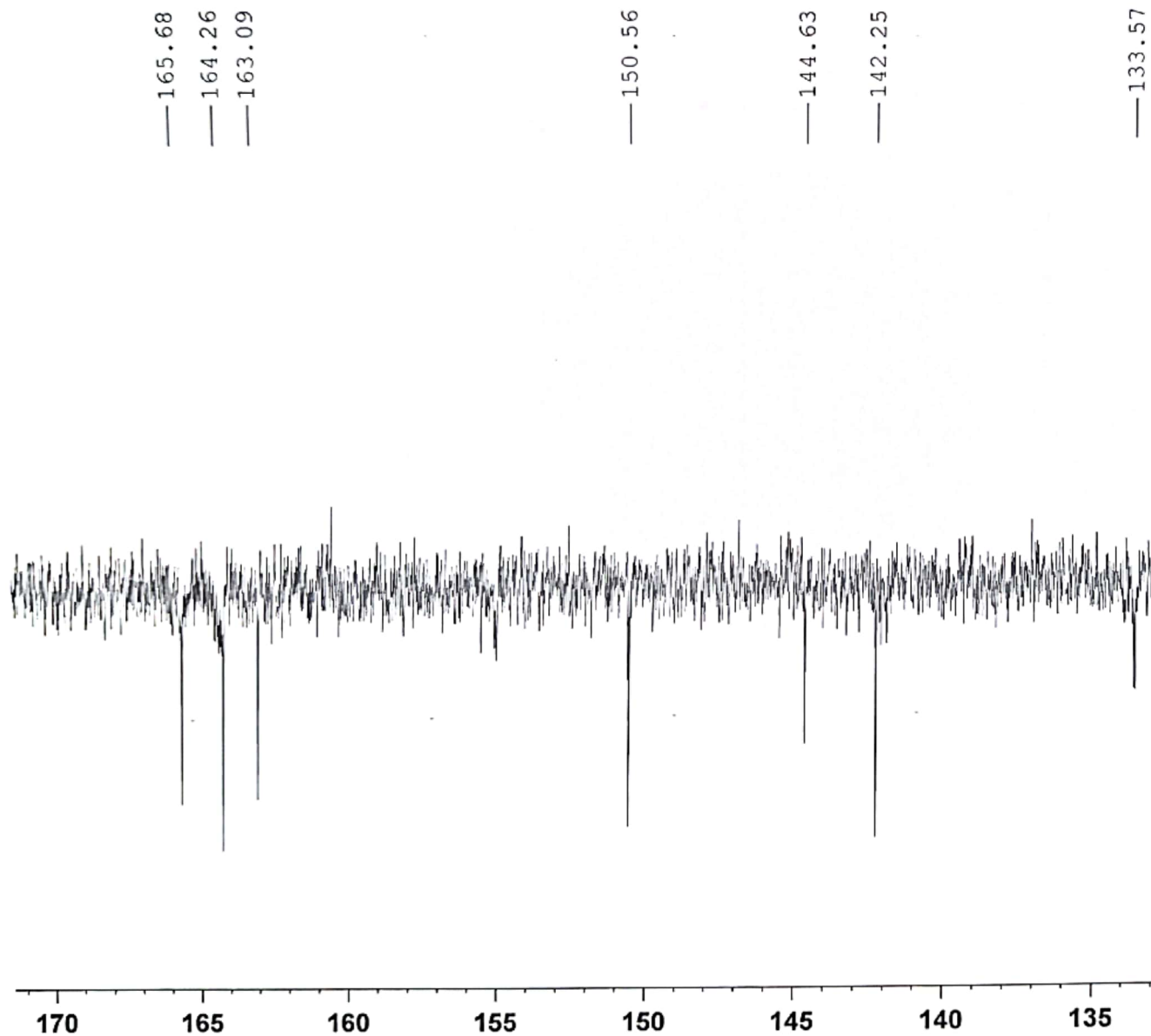
F2 - Acquisition Parameters
Date_ 20150617
Time 20.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOALS 0.500
SFOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GFNAM[3] SMSQ10.100
GPZ1 31.00 A
GPZ2 31.00 A
GPZ3 31.00 A
P16 1000.00 usec

F2 - Processing parameters
S1 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-12C
 PROTON_BSU DMSO (C:\data) nmr 19

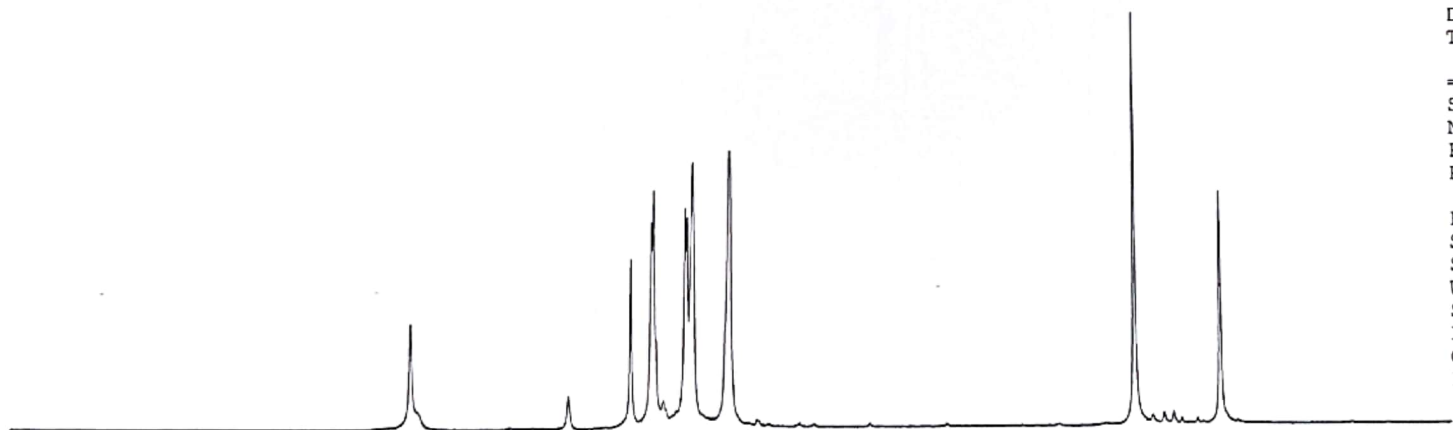
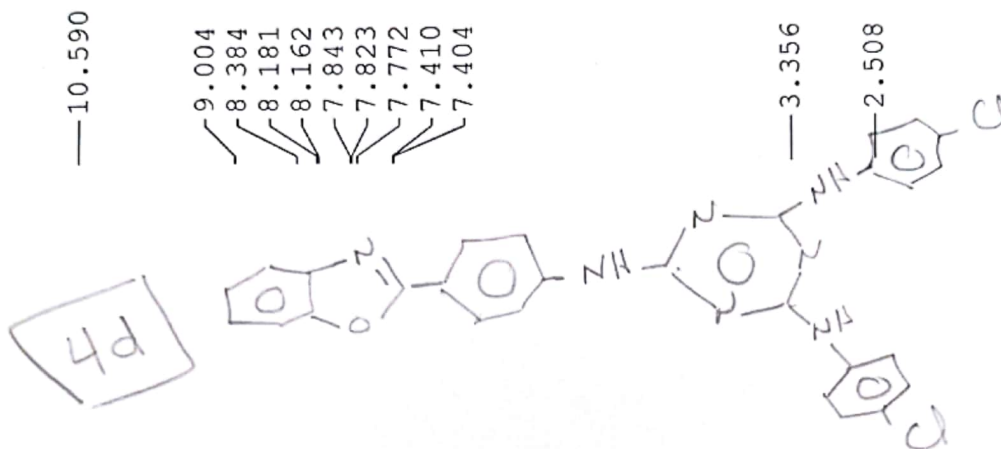


Current Data Parameters
 NAME Jun16-2015-nmr
 EXPNO 110
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150616
 Time_ 10.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



14 13 12 11 10 9 8 7 6 5 4 3 2 ppm

1.00
 0.22
 0.90
 2.58
 4.00
 2.88
 2.01
 1.31

HEBA-12C
 PROTON_BSU DMSO (C:\data) nmr 19

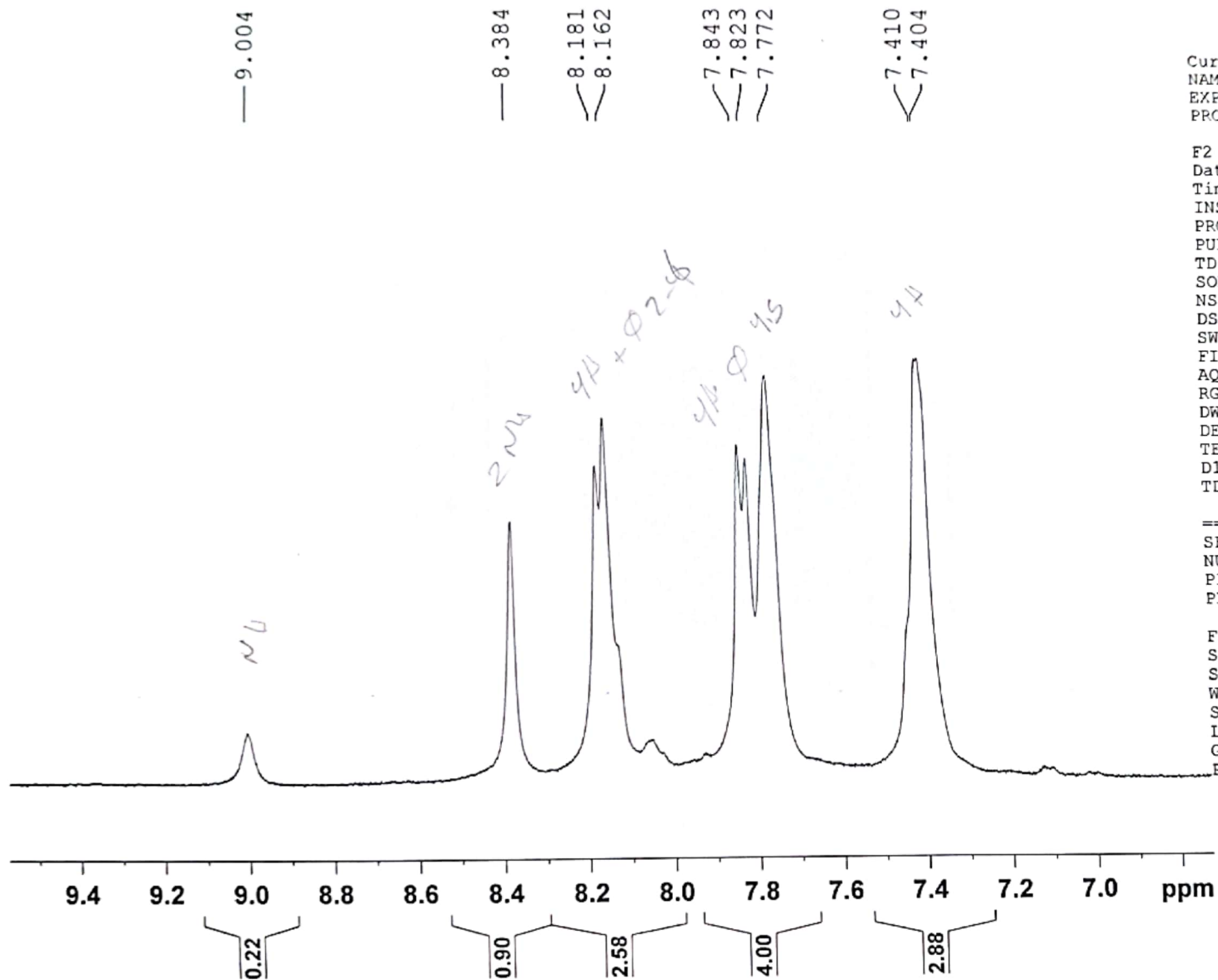


Current Data Parameters
 NAME Jun16-2015-nmr
 EXPNO 110
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150616
 Time_ 10.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 296.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-12C
PROTON_BSU DMSO (C:\data) nmr 19

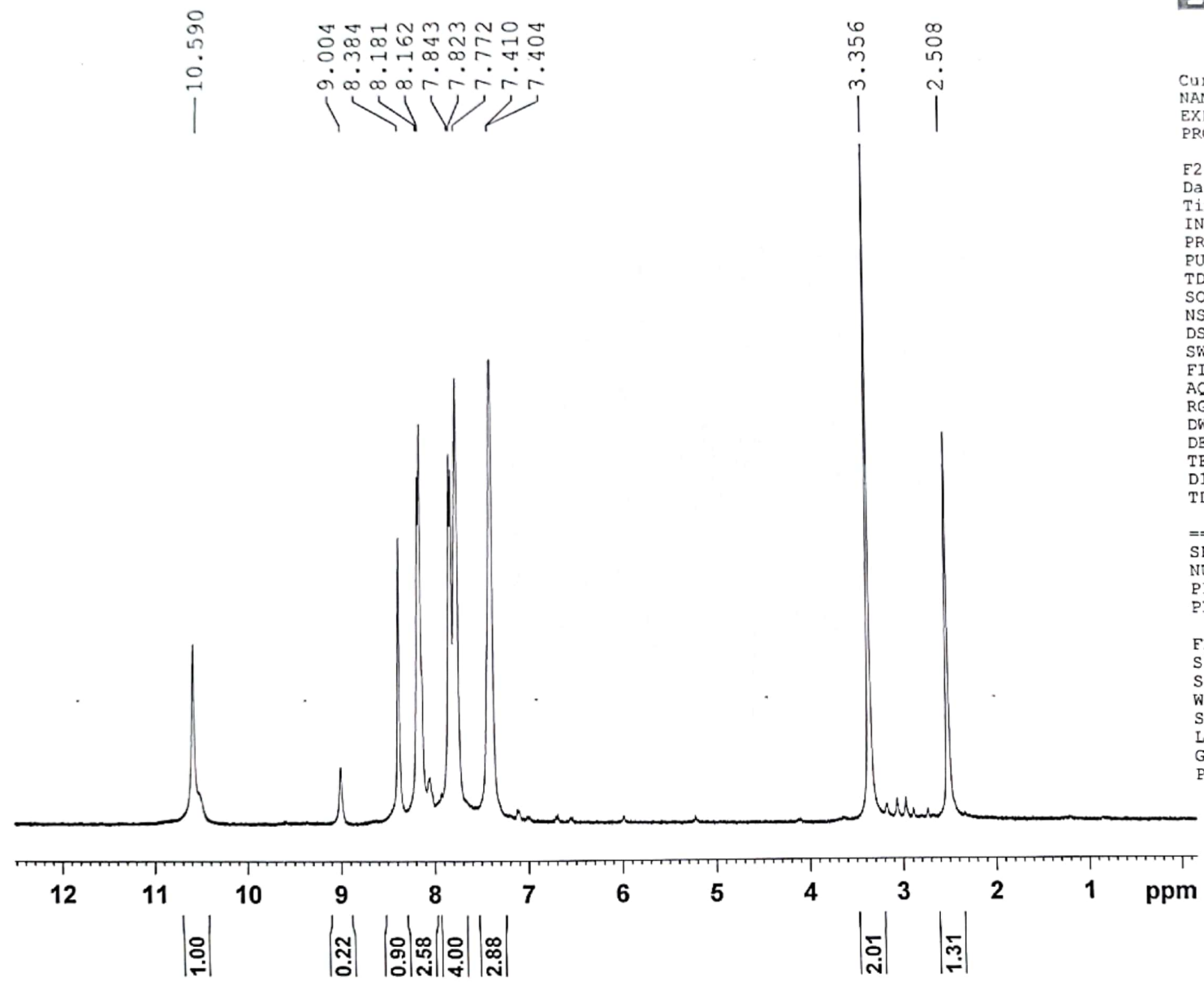


Current Data Parameters
NAME Jun16-2015-nmr
EXPNO 110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150616
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-12C
PROTON_BSU DMSO {C:\data} nmr 19

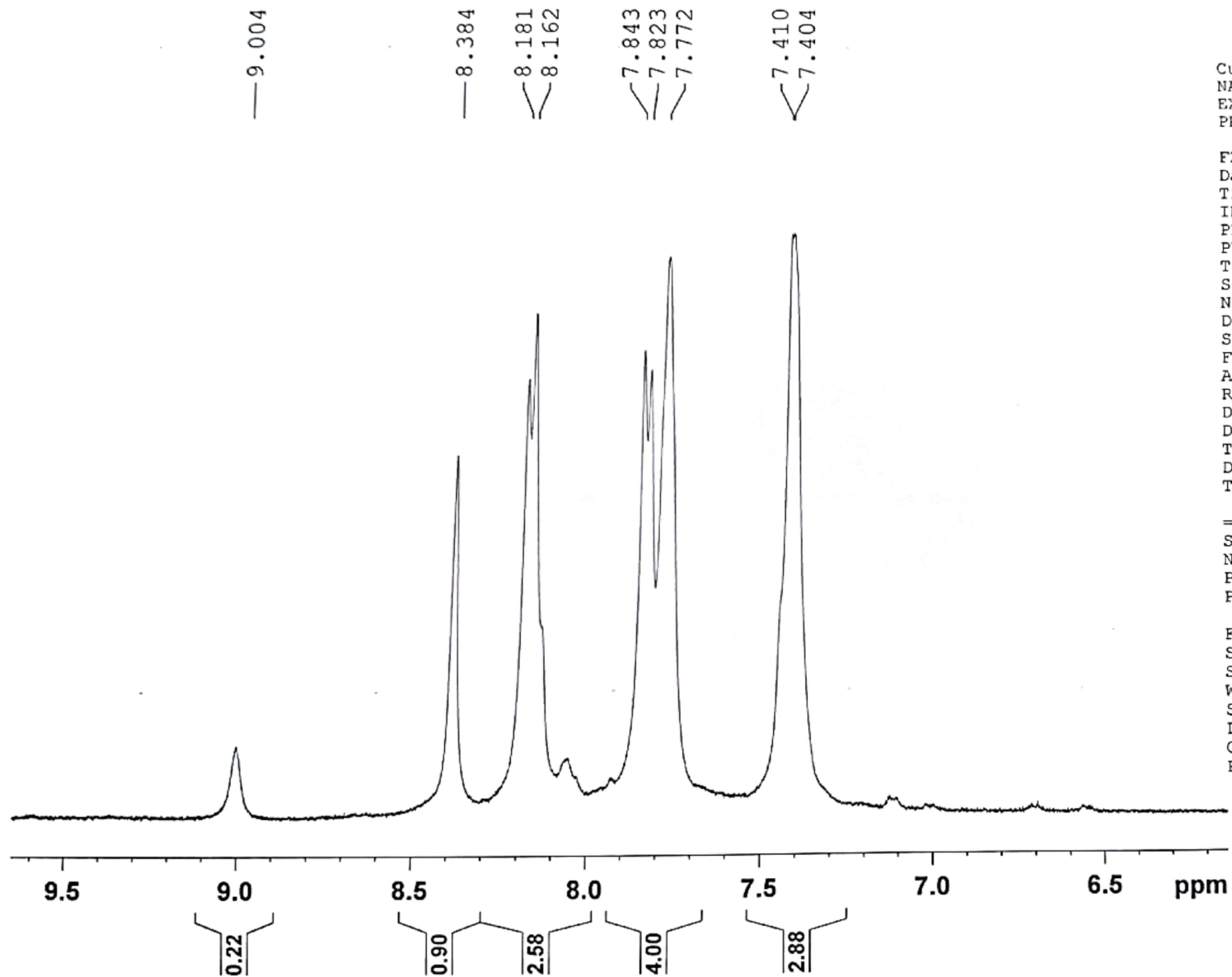


Current Data Parameters
NAME Jun16-2015-nmr
EXPNO 110
PROCNO 1

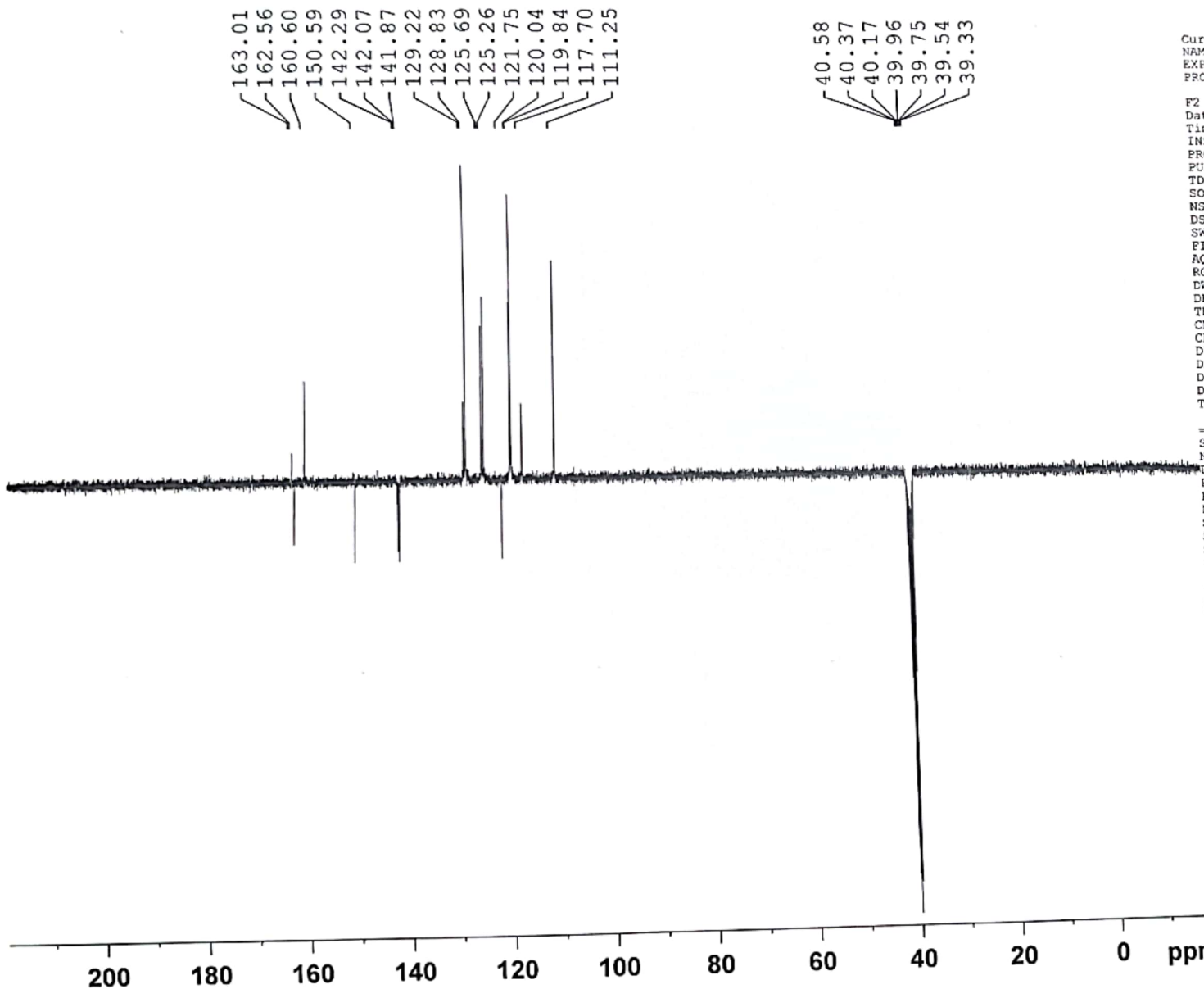
F2 - Acquisition Parameters
Date_ 20150616
Time 10.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-12C
DEPTQ-BSU DMSO {C:\data} nmr 20



163.01
162.56
160.60
150.59
142.29
142.07
141.87
129.22
128.83
125.69
125.26
121.75
120.04
119.84
117.70
111.25

40.58
40.37
40.17
39.96
39.75
39.54
39.33

Current Data Parameters
NAME Jun17-2015-nmr
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150618
Time_ 0.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqppsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.000000
CNST12 1.500000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOALS 0.500
SFOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CFDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-12C
DEPTQ-BSU DMSO (C:\data) nmr 20



Current Data Parameters
NAME Jun17-2015-nmr
EXFNO 30
PROCNO 1

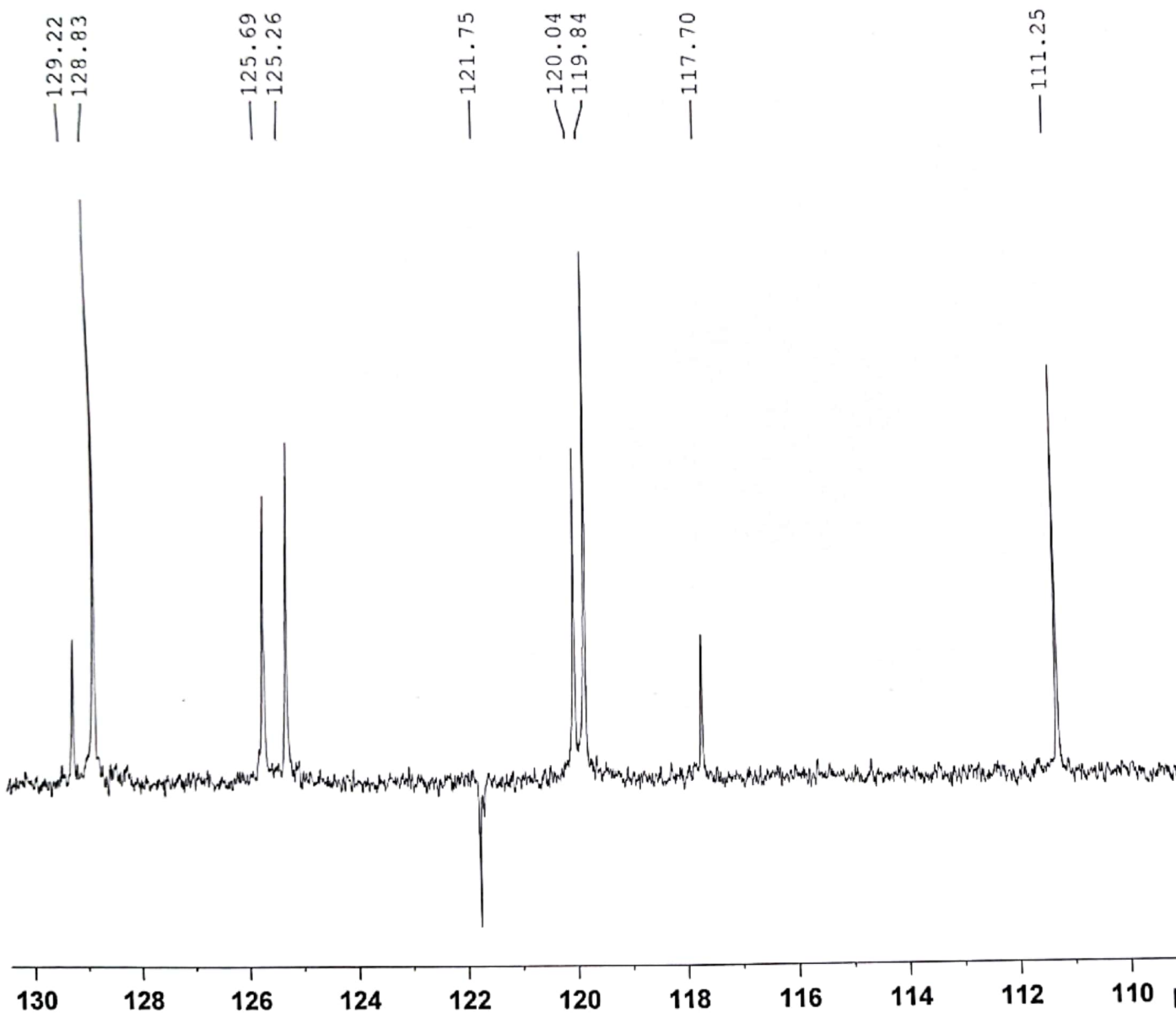
F2 - Acquisition Parameters
Date_ 20150618
Time 0.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqqpp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24039.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
F16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-12C
DEPTQ-BSU DMSO {C:\data} nmr 20



Current Data Parameters
NAME Jun17-2015-nmr
EXPNO 30
PROCNO 1

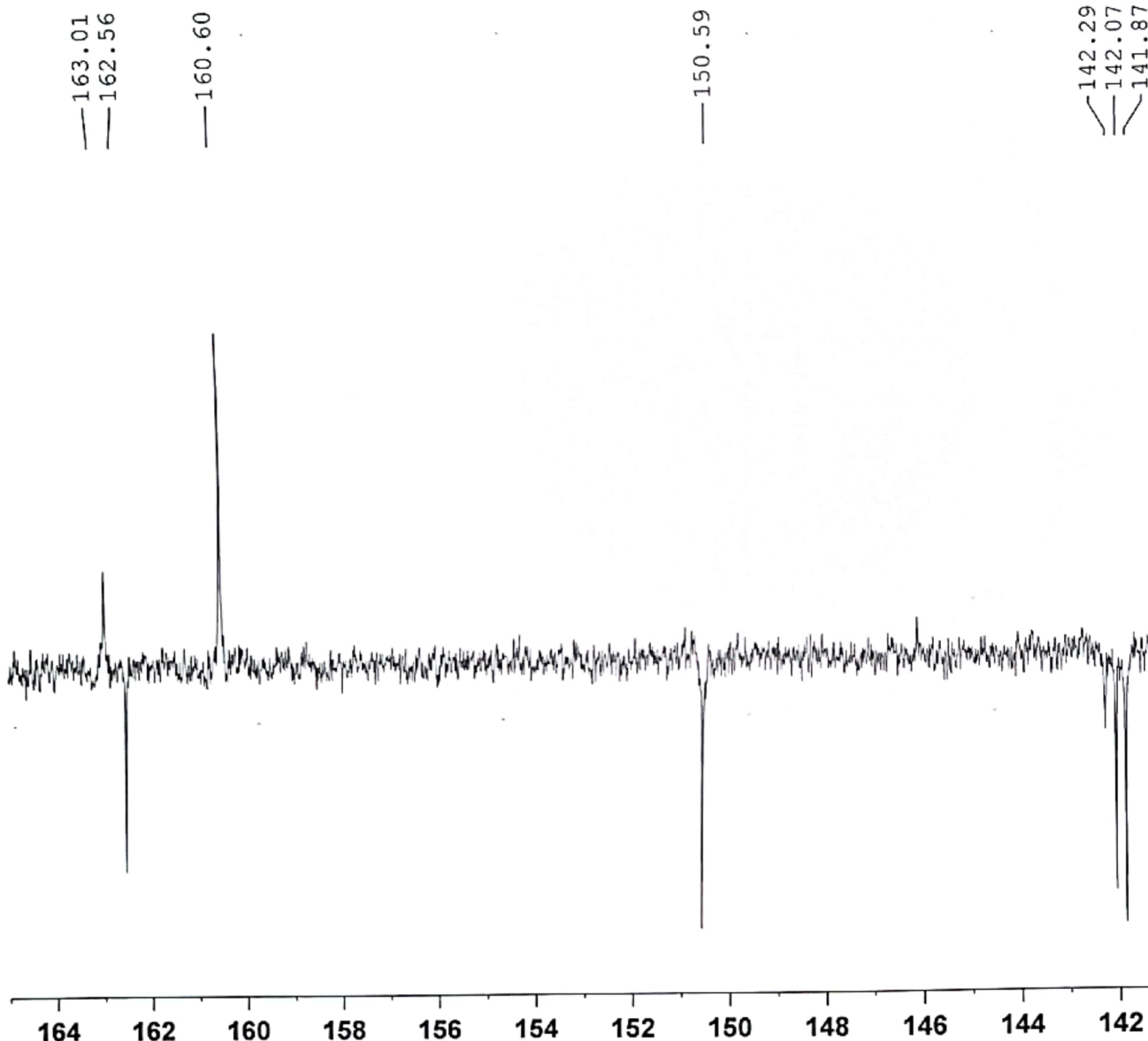
F2 - Acquisition Parameters
Date_ 20150618
Time_ 0.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-M-CLCL
 PROTON_BSU CDC13 {C:\data} nmr 9

M13a

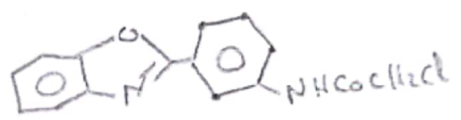


8.429
8.389
8.299
8.278
7.835
7.793
7.773
7.617
7.603
7.595
7.392
7.384
7.378
7.369
7.284

2+
clac.d

1.684
1.623
1.548
1.273

5a

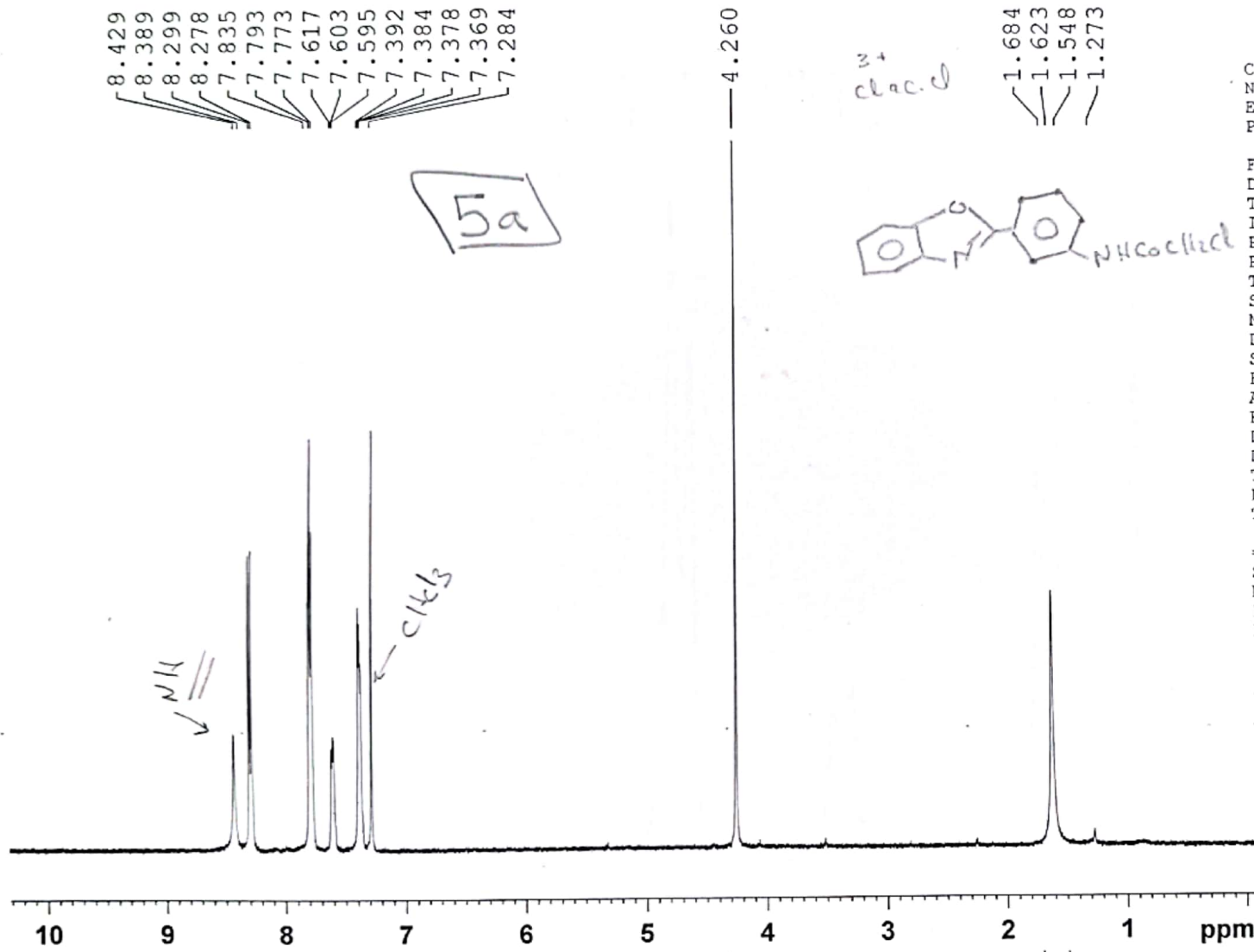


Current Data Parameters
 NAME Mar15-2015-nmr
 EXPNO 200
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150315
 Time_ 12.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



1.00
2.14
3.22
1.10
2.16
1.11

1 2 3 1 2

HEBA-M-CLCL
 PROTON_BSU CDC13 {C:\data} nmr 9

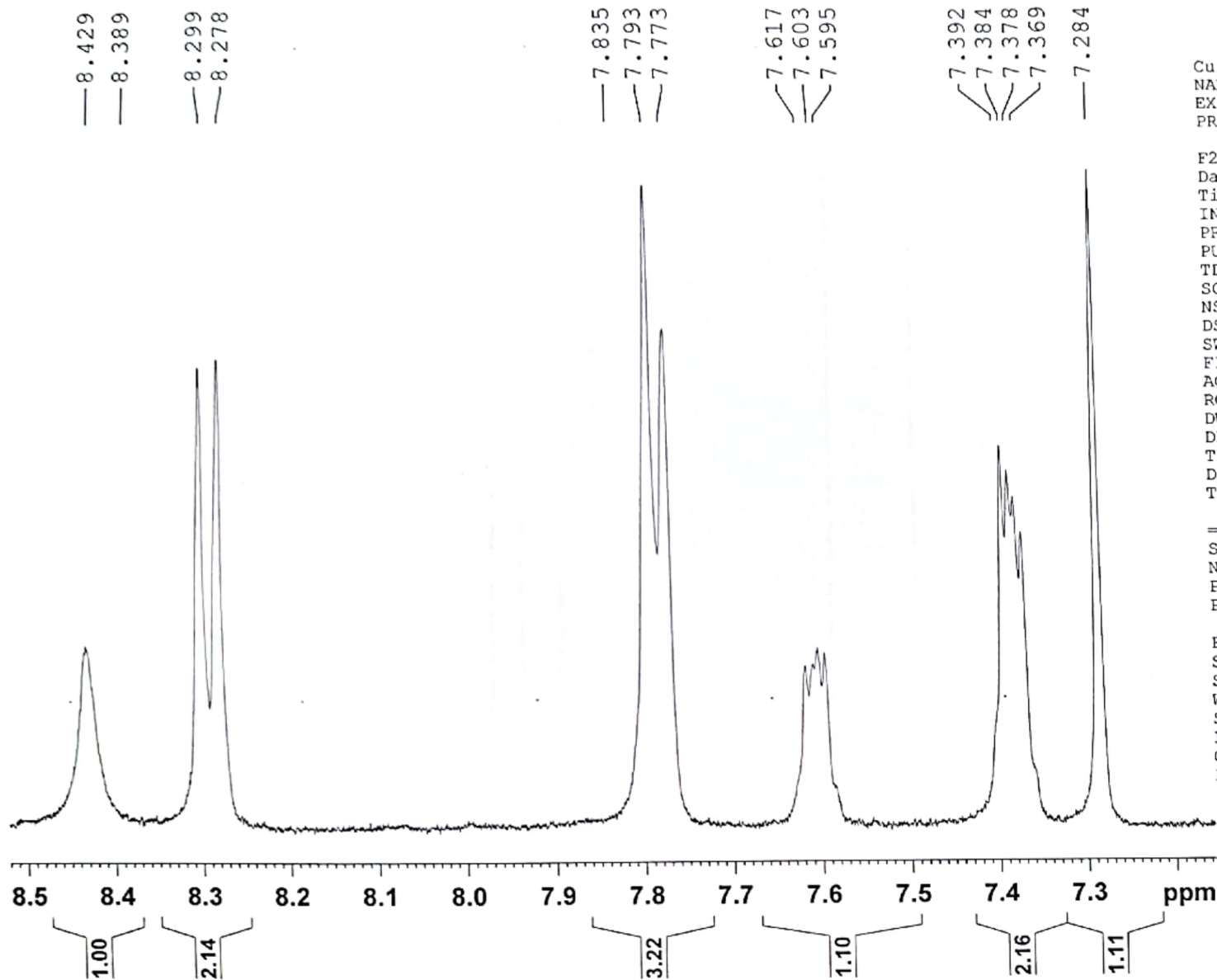


Current Data Parameters
 NAME Mar15-2015-nmr
 EXPNO 200
 PROCNO 1

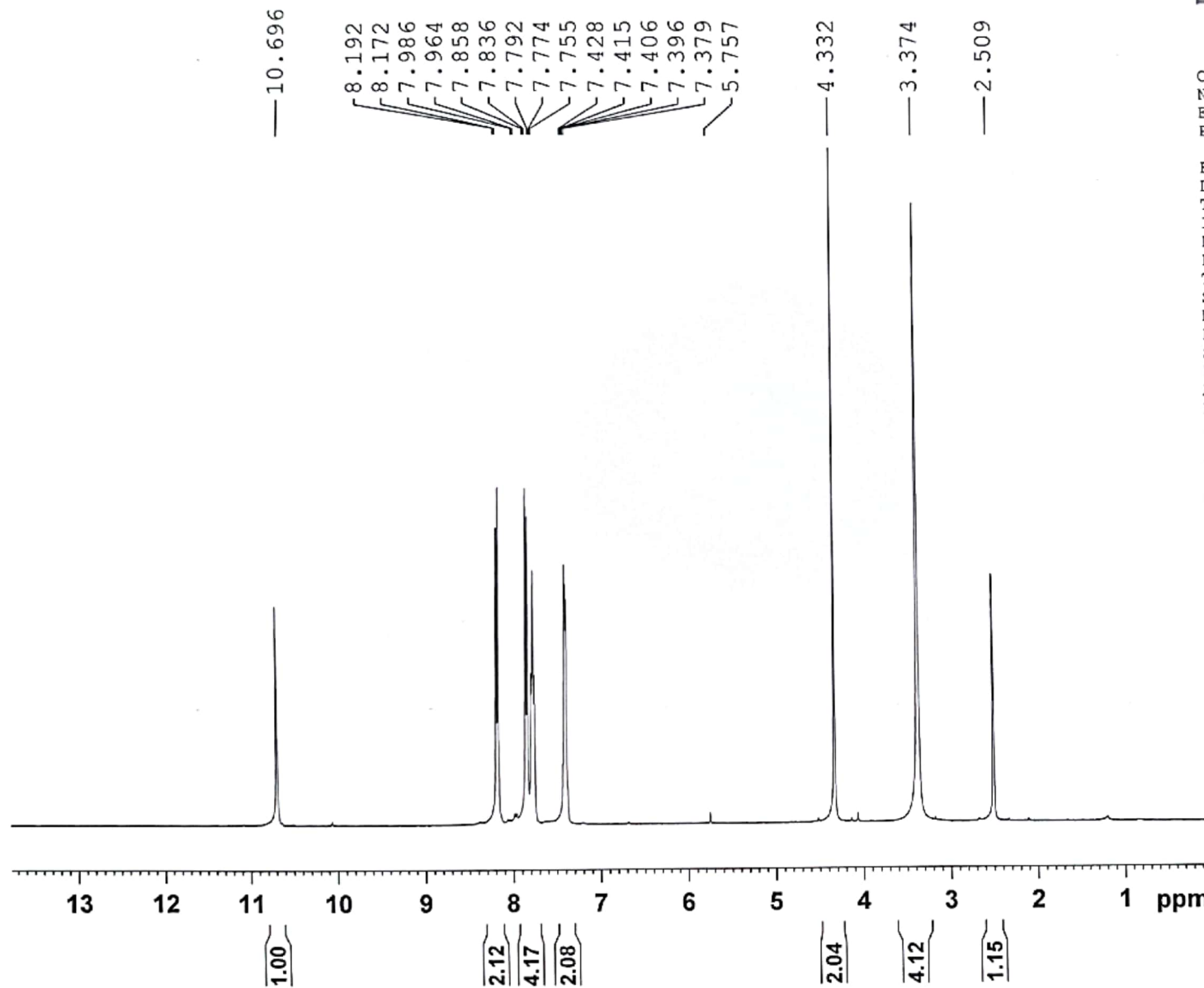
F2 - Acquisition Parameters
 Date_ 20150315
 Time_ 12.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-13A
 PROTON_BSU DMSO {C:\data} nmr 9



Current Data Parameters
 NAME Jul15-2015-nmr
 EXPNO 250
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150718
 Time 11.37
 INSTRUM spect
 PROBHD 5 mm FABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

HEBA-13A
PROTON_BSU DMSO {C:\data} nmr 9



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 250
PROCNO 1

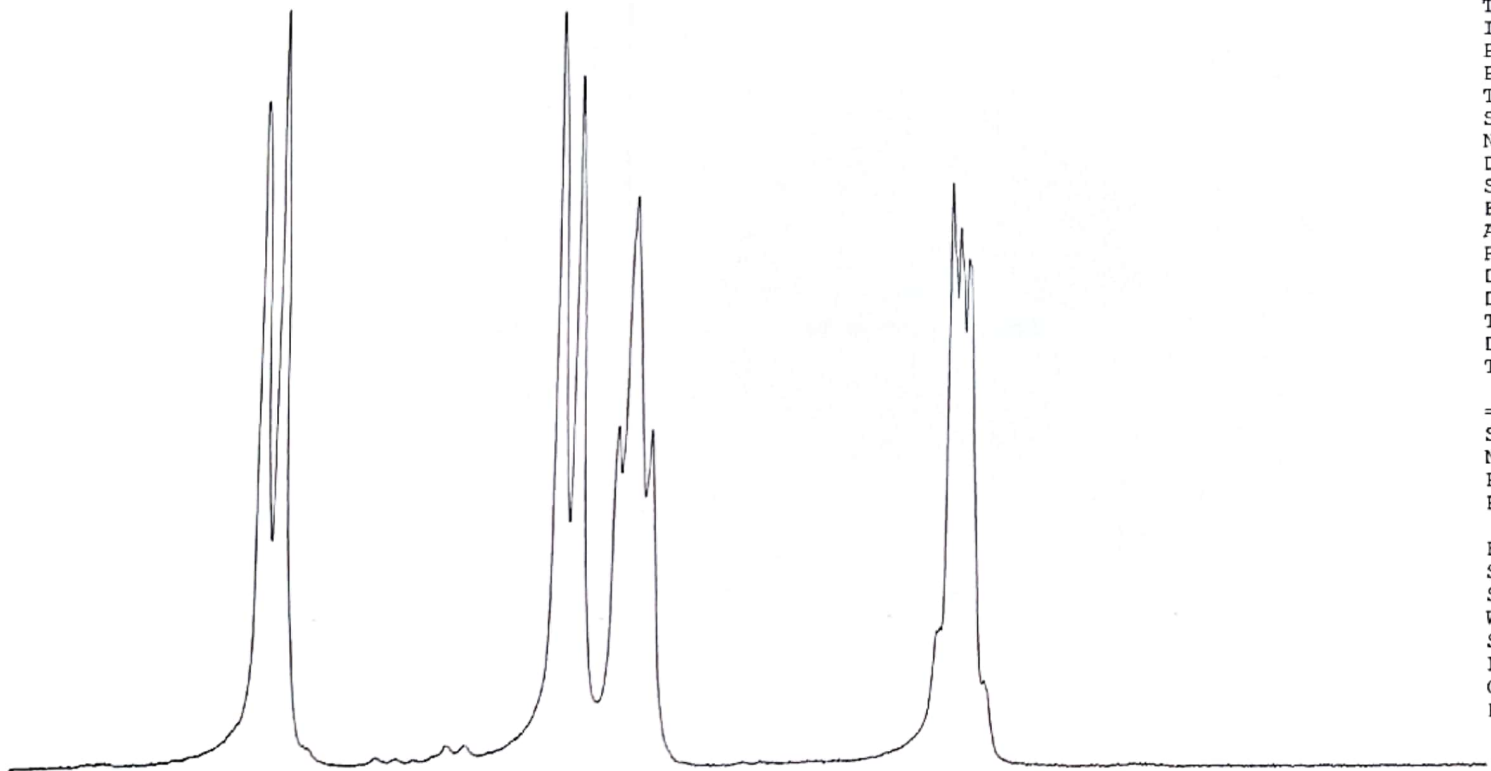
F2 - Acquisition Parameters

Date_ 20150718
Time 11.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

8.192
8.172
7.986
7.964
7.858
7.836
7.792
7.774
7.755
7.428
7.415
7.406
7.396
7.379



8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 ppm

2.12
4.17
2.08

HEBA-13A
DEPTQ-BSU DMSO {C:\data} nmr 9



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 251
PROCNO 1

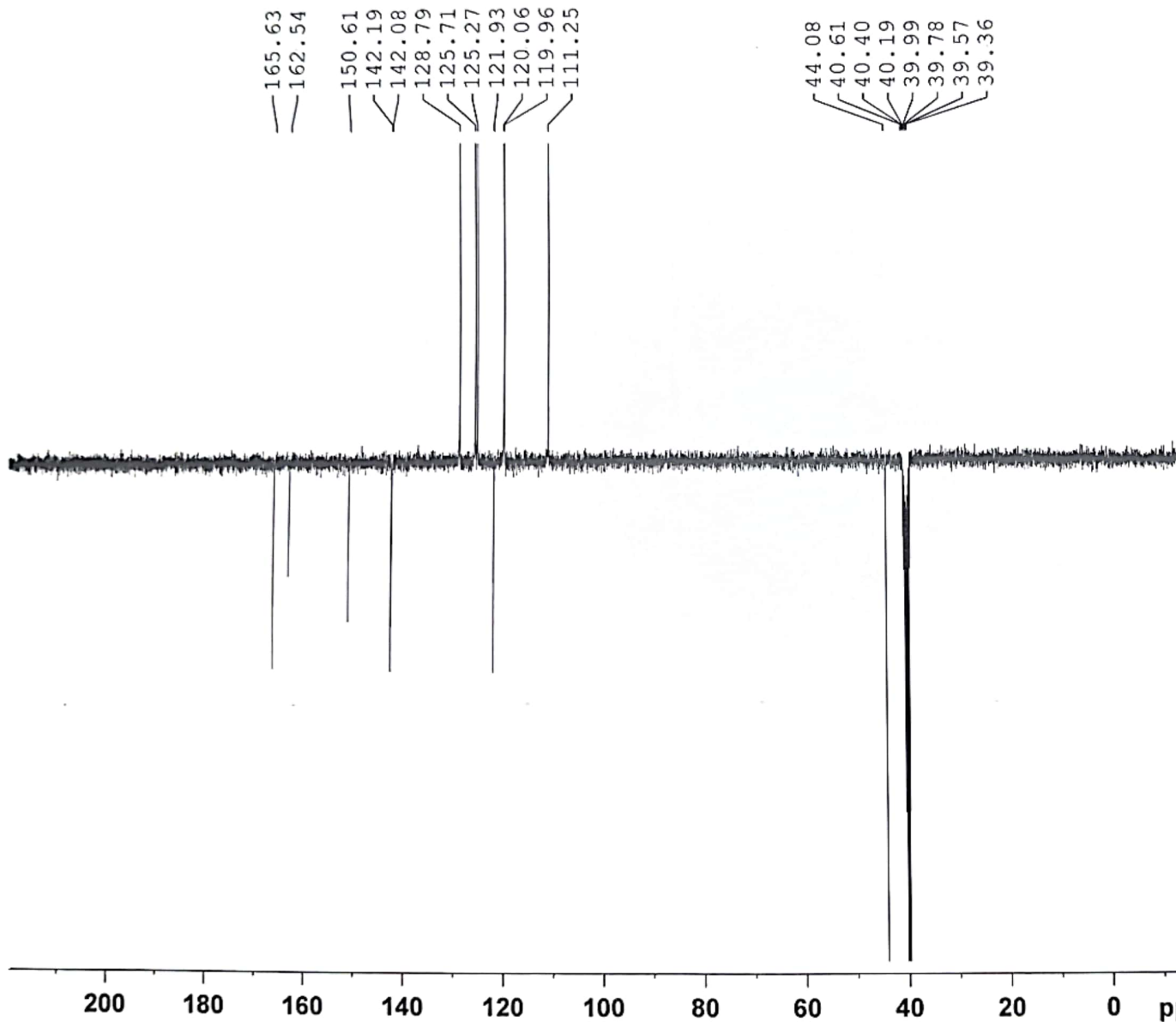
F2 - Acquisition Parameters
Date_ 20150718
Time_ 15.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

----- CHANNEL f1 -----
SF01 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFPAM[5] Crp60comp.4
SFOALS 0.500
SFOFFS5 0 Hz
SFW5 10.08399963 W

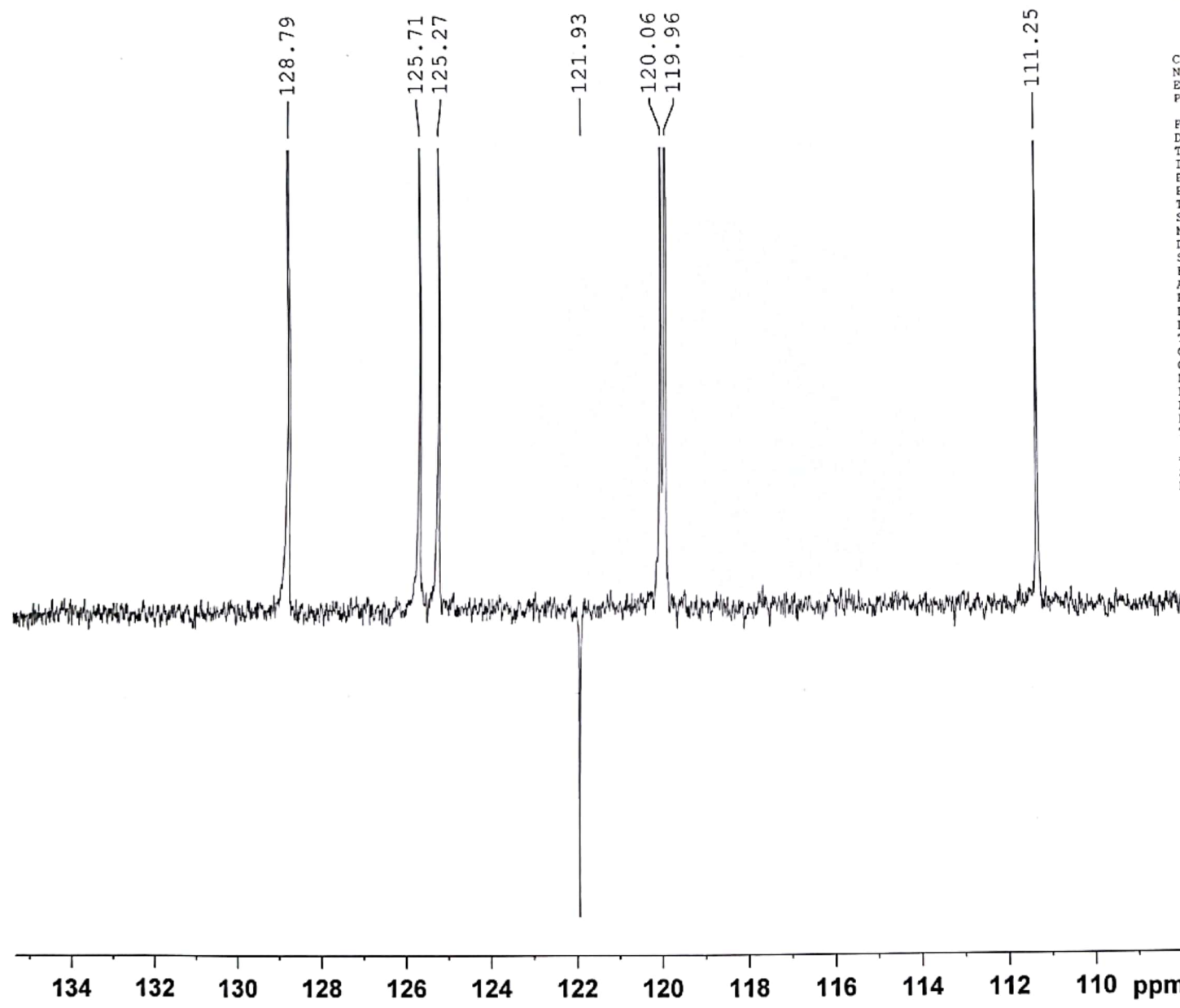
----- CHANNEL f2 -----
SF02 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-13A
DEPTQ-BSU DMSO {C:\data} nmr 9



Current Data Parameters
NAME Jul15-2015-nmr
EXRNO 251
PROCNO 1

F2 - Acquisition Parameters
Date 20150718
Time 15.26
INSTRUM spect
PROSHD 5 mm PABBO BB/
PULPROG deptqgpgp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13C-13A
DEPTQ-BSU DMSO {C:\data} nmr 9



Current Data Parameters
NAME Jul15-2015-nmr
EXFNO 251
PROCNO 1

F2 - Acquisition Parameters

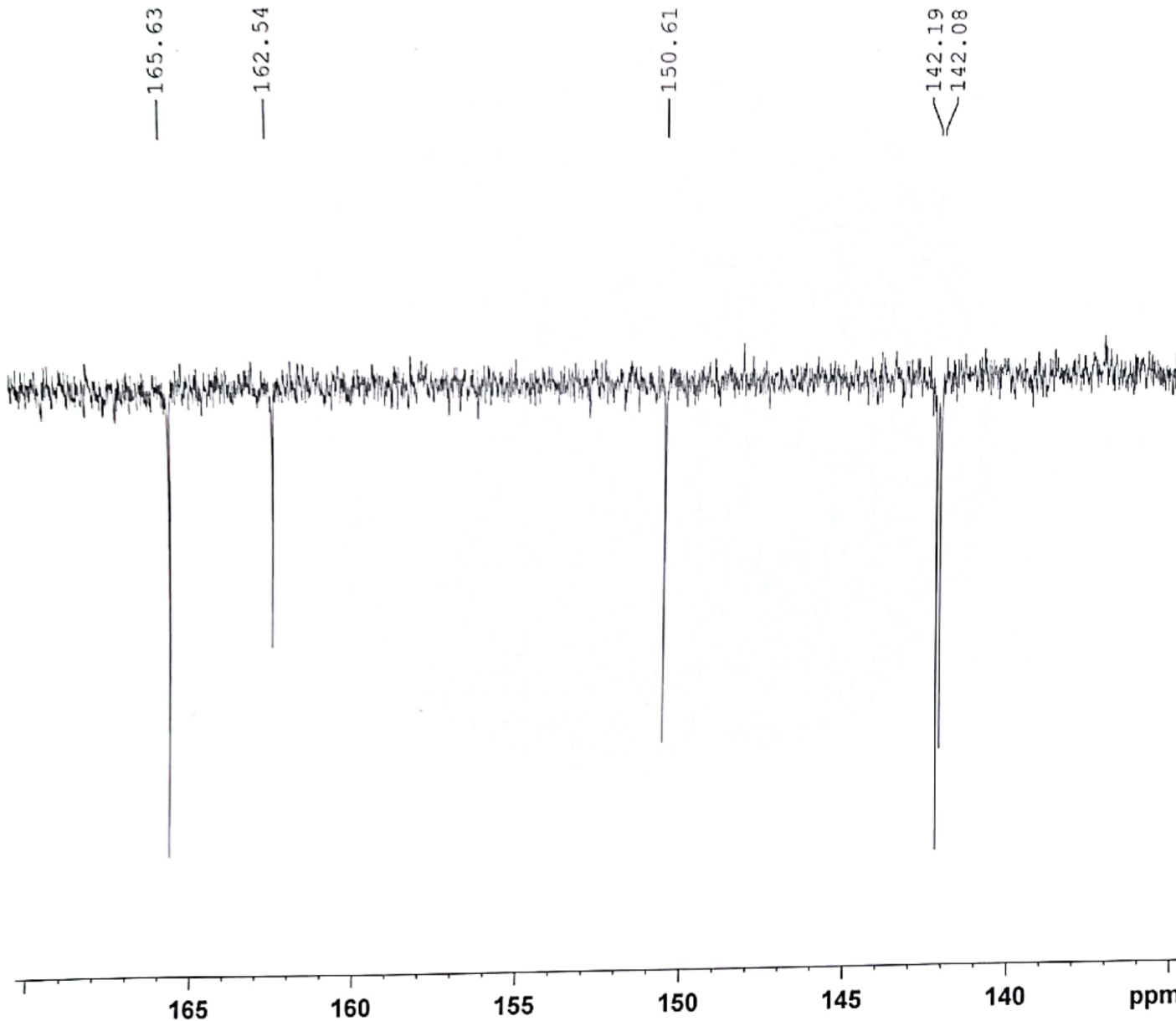
Date 20150718
Time 15.26
INSTRUM spect
PROBHD 5 mm F4BBO BB/
PULPROG deptqppsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFESS 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SF02 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-13C
PROTON_BSU DMSO {C:\data} nmr 22

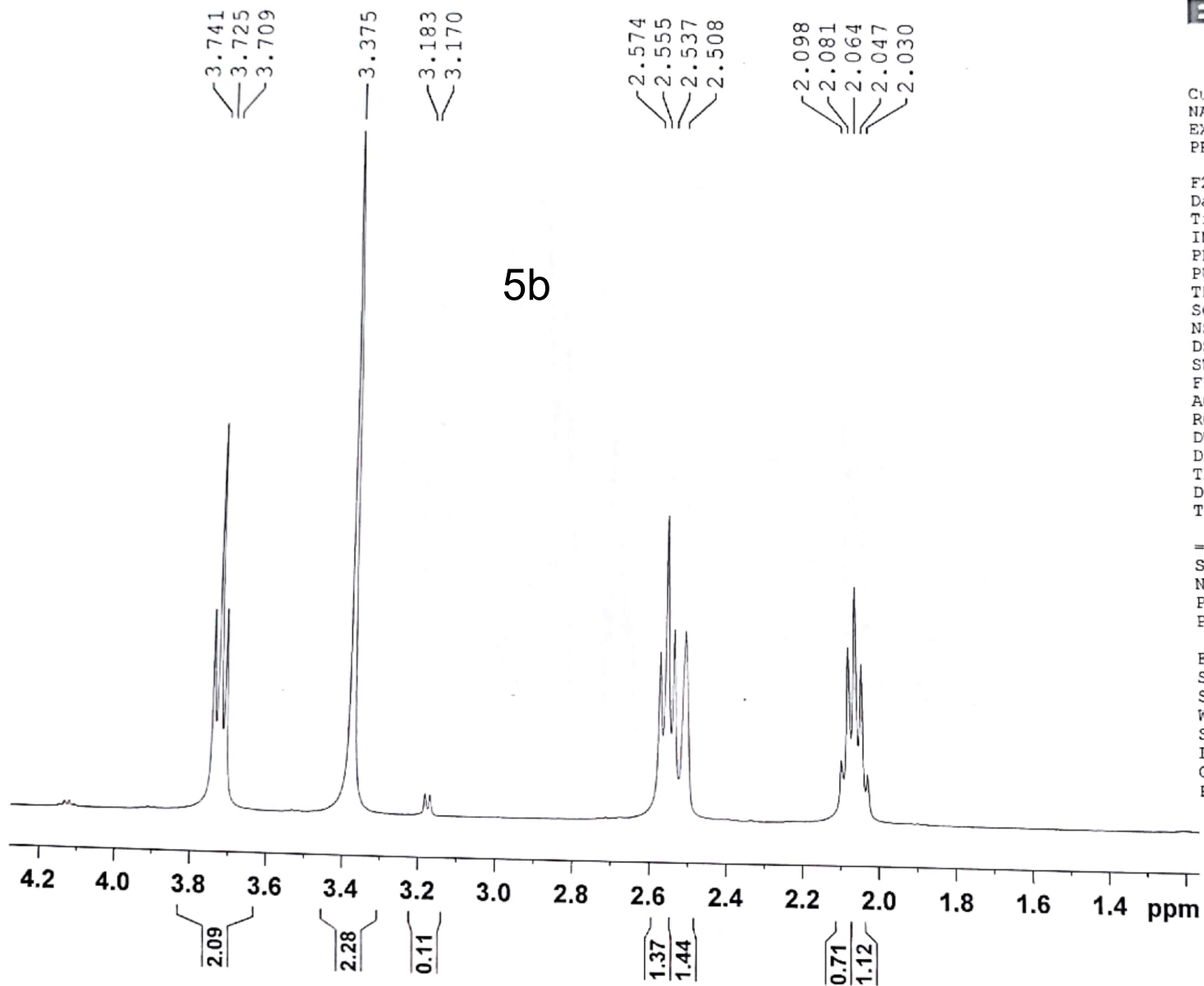


Current Data Parameters
NAME Apr28-2015-nmr
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150428
Time_ 12.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 81.84
DW 62.400 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-13C
PROTON_BSU DMSO {C:\data} nmr 22

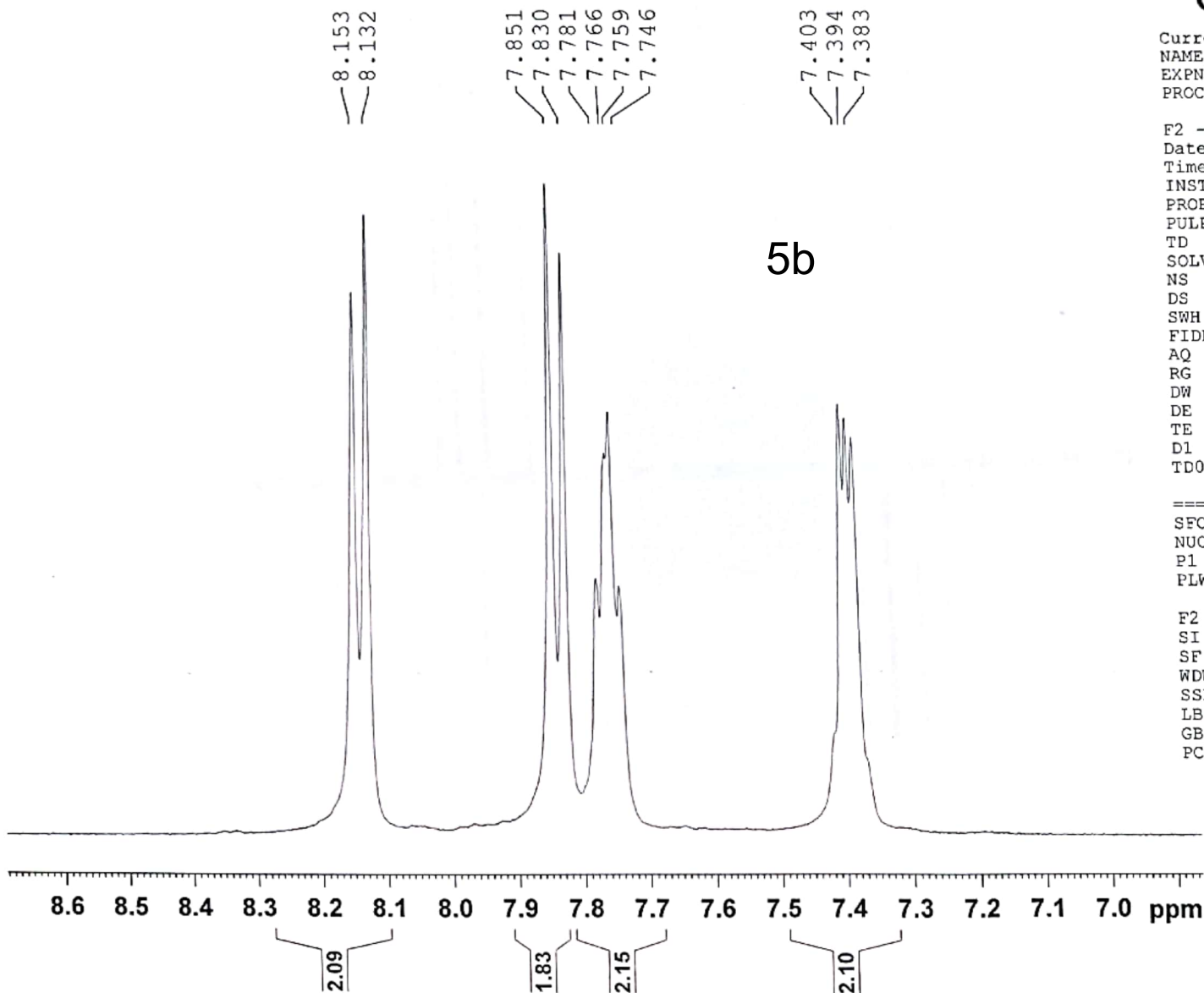


Current Data Parameters
NAME Apr28-2015-nmr
EXPNO 290
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150428
Time_ 12.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 81.84
DW 62.400 usec
DE 6.50 usec
TE 294.1 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-13C
DEPTQ-BSU DMSO {C:\data} nmr 2



Current Data Parameters
NAME May04-2015-nmr
EXPNO 50
PROCNO 1

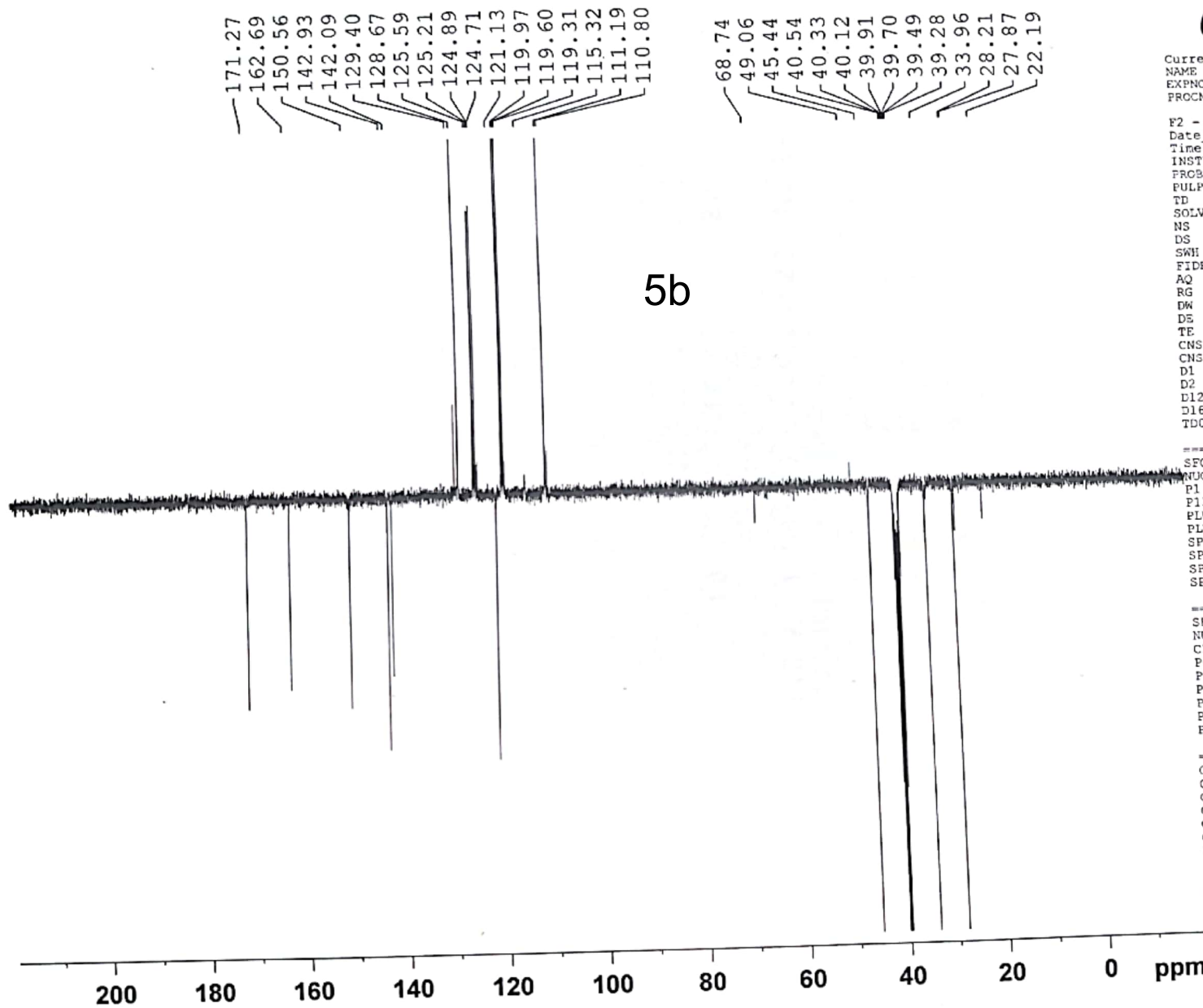
F2 - Acquisition Parameters
Date_ 20150505
Time 8.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 3685
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00020000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[S] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

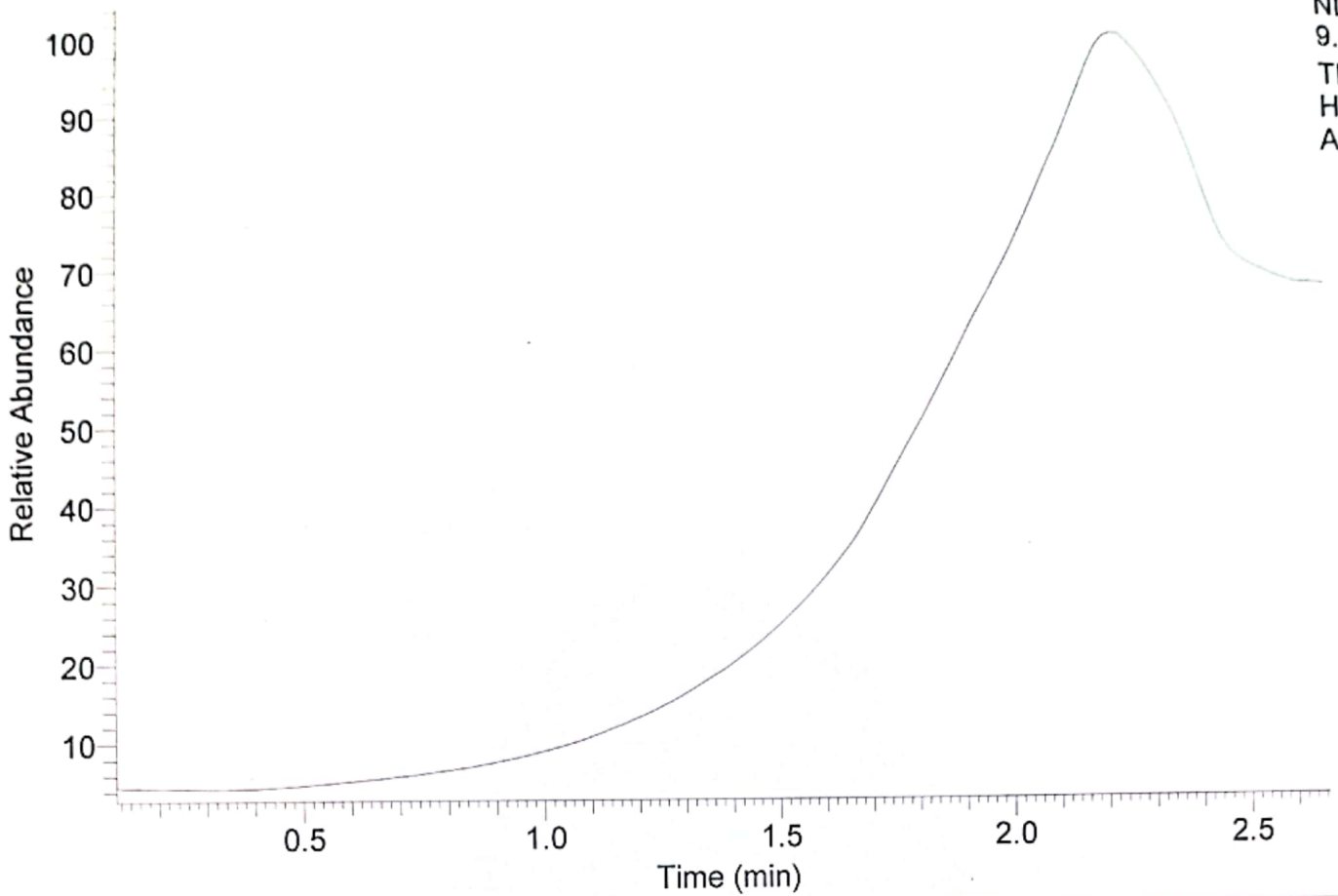
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB C
PC 1.40



171.27
162.69
150.56
142.93
142.09
129.40
128.67
125.59
125.21
124.89
124.71
121.13
119.97
119.60
119.31
115.32
111.19
110.80

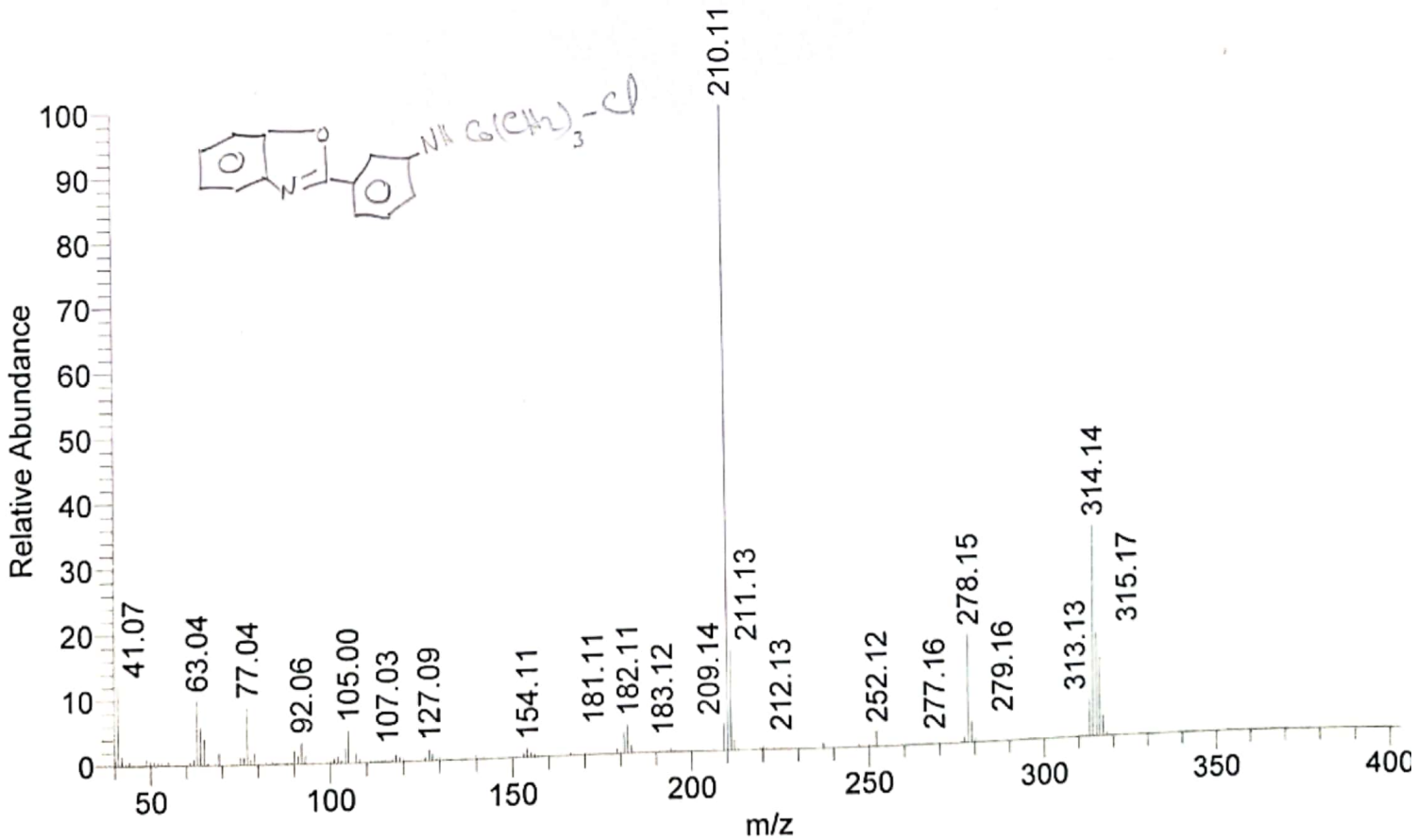
68.74
49.06
45.44
40.54
40.33
40.12
39.91
39.70
39.49
39.28
33.96
28.21
27.87
22.19

RT: 0.11 - 2.66 SM: 15B



NL: 9.13E7
TIC MS
HEBA-ATEF-13C

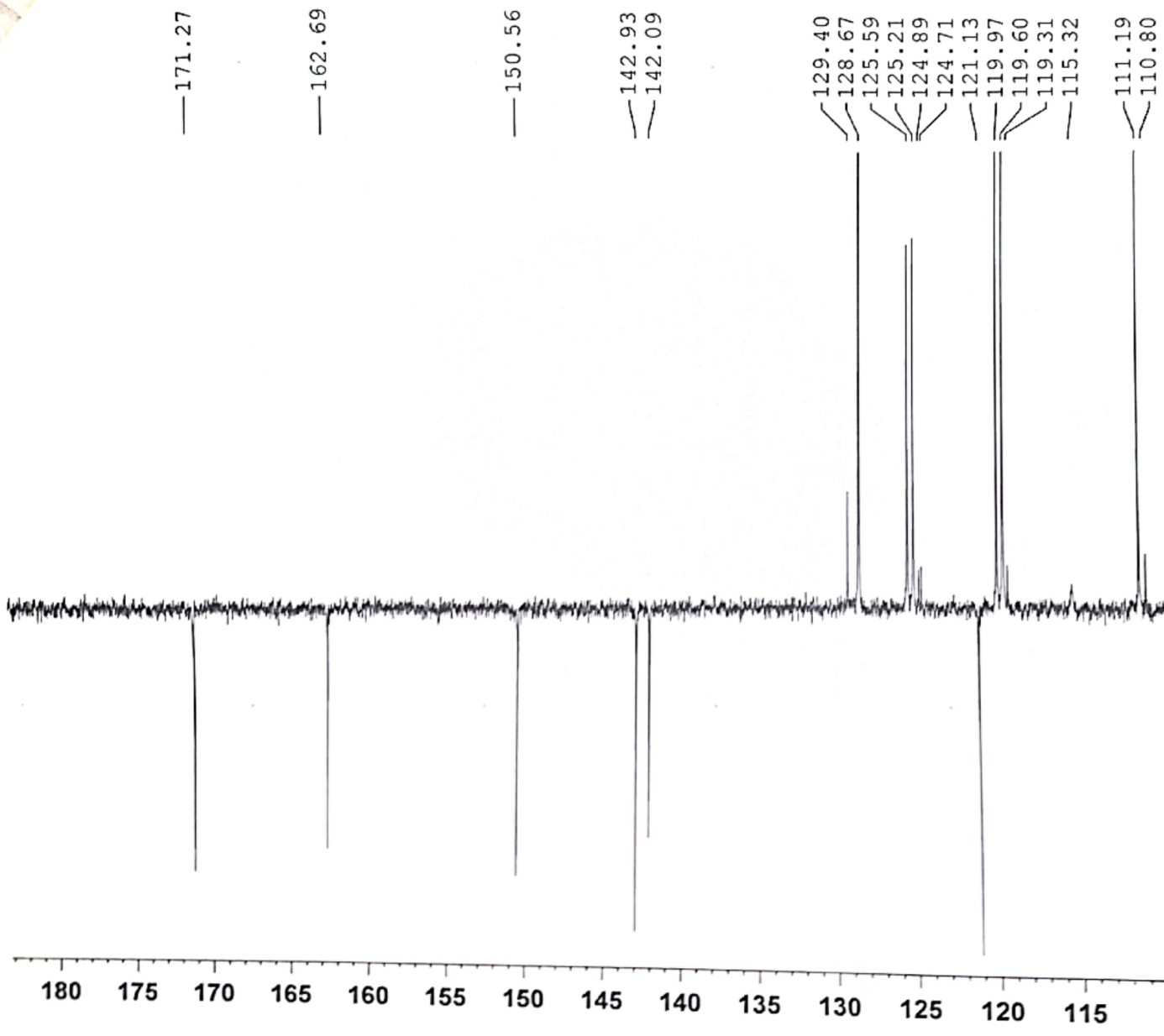
HEBA-ATEF-13C #132 RT: 2.23 AV: 1 SB: 20 2.09-2.24 , 2.11-2.26 NL: 2.45E6
T: {0,0} + c EI Full ms [40.00-1000.00]



HEBA-ATEF-13C#132 RT: 2.23
SB: 20 2.09-2.24 , 2.11-2.26
T: (0,0) + c EI Full ms [40.00-1000.00]
m/z= 40.00-403.24

m/z	Intensity	Relative
40.17	18571.0	0.76
41.07	301330.9	12.30
42.07	33646.5	1.37
49.00	23966.5	0.98
55.05	17728.1	0.72
62.04	22549.1	0.92
63.04	244655.2	9.98
64.05	139625.3	5.70
65.06	97373.1	3.97
69.16	44389.5	1.81
75.05	27301.7	1.11
76.08	26919.3	1.10
77.04	216119.4	8.82
78.07	18742.4	0.76
79.05	41918.7	1.71
90.08	49673.5	2.03
91.07	30724.9	1.25
92.06	79311.6	3.24
93.07	28873.0	1.18
102.06	21160.5	0.86
104.13	54559.9	2.23
105.00	119958.8	4.89
107.03	33946.4	1.39
118.10	24660.4	1.01
119.03	18112.8	0.74
127.09	42324.6	1.73
128.08	24754.0	1.01
154.11	30984.5	1.26
181.11	80646.1	3.29
182.11	107035.9	4.37
183.12	29606.4	1.21
209.14	104506.1	4.26
210.11	2450818.0	100.00
211.13	383757.4	15.66
212.13	38601.8	1.58
252.12	59193.8	2.42
277.16	23491.0	0.96
278.15	419941.8	17.13
279.16	80647.8	3.29
313.13	147587.3	6.02
314.14	818728.8	33.41
315.17	404981.1	16.52
316.15	307235.3	12.54
317.15	80292.7	3.28

13C
1Q-BSU DMSO {C:\data} nmr 2



Current Data Parameters
NAME May04-2015-nmr
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150505
Time_ 8.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 3685
DS 4
SWH 24038.461 Hz
FIDRES 0.366799 Hz
AQ 1.3631488 sec
RG 205.44
LW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFOFF5 0 Hz
SFOFF5 10.08399963 W

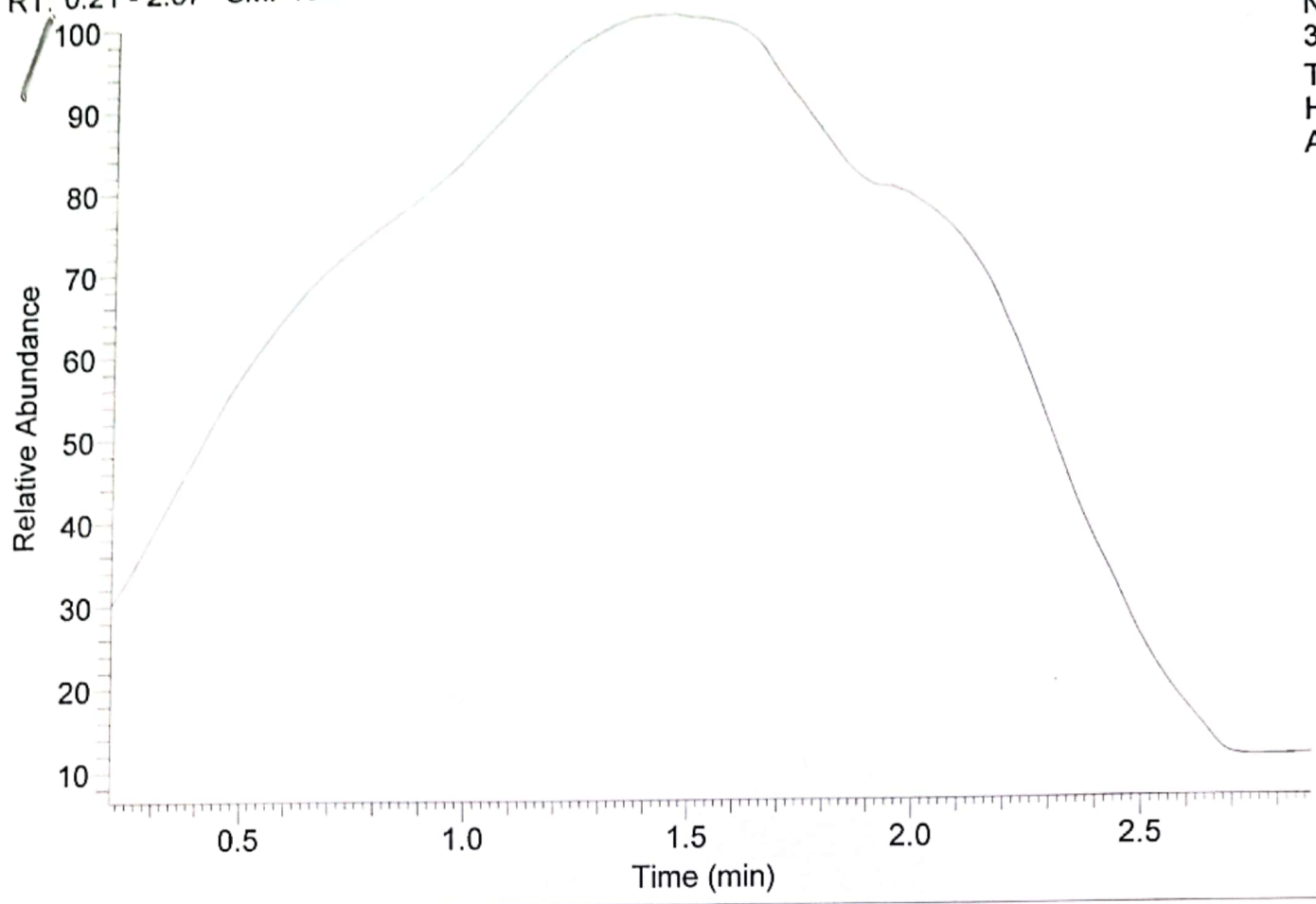
----- CHANNEL f2 -----
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG2 waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GF21 31.00 %
GF22 31.00 %
GF23 31.00 %
F16 1000.00 usec

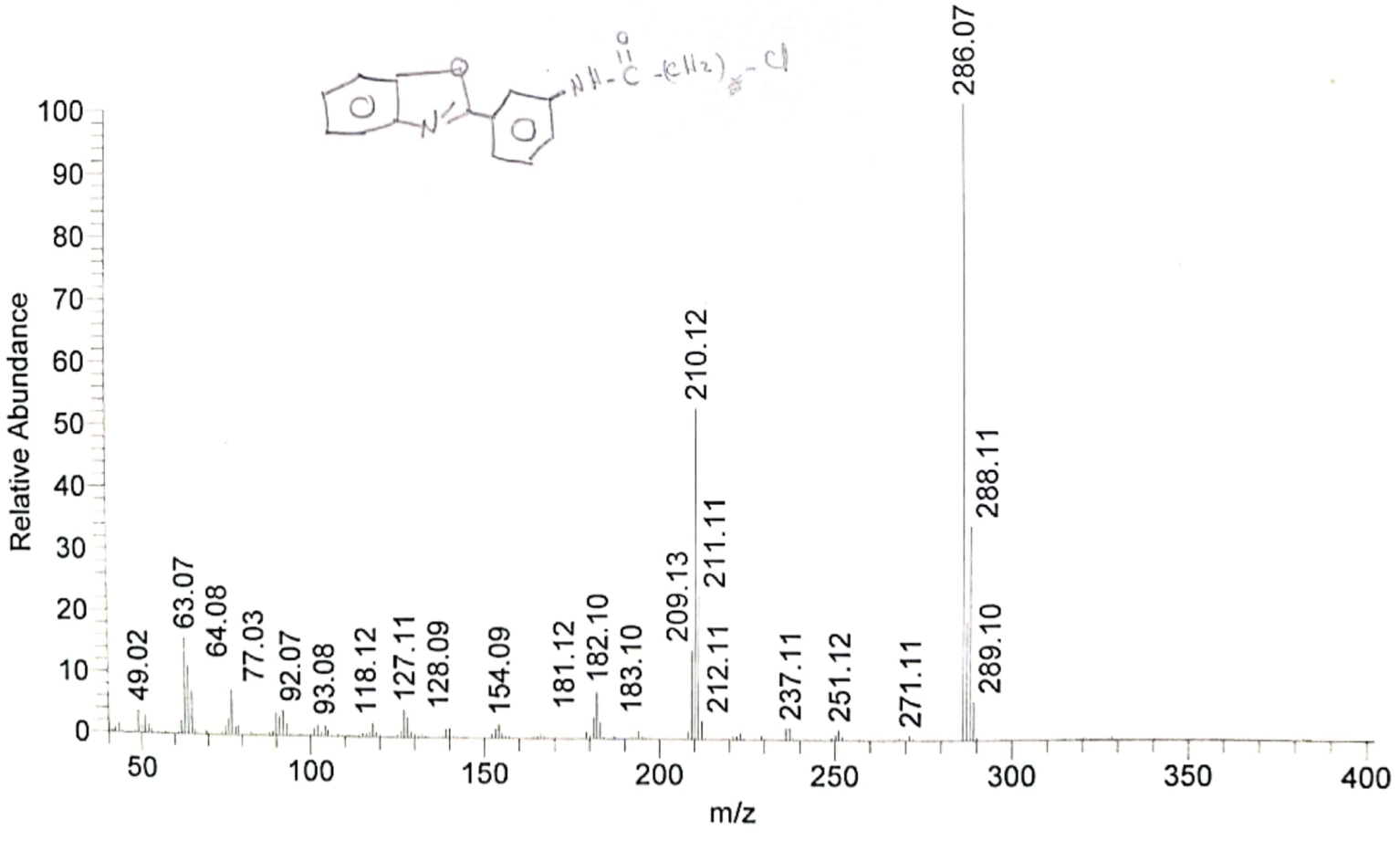
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

RT: 0.21 - 2.87 SM: 15B

NL:
3.79E8
TIC MS
HEBA-
ATEF-13A



HEBA-ATEF-13A #101 RT: 1.71 AV: 1 NL: 8.89E7
T: {0,0} + c EI Full ms [40.00-1000.00]



-ATEF-13A#101 RT: 1.71

(0,0) + c EI Full ms [40.00-1000.00]

z= 40.00-402.04

m/z	Intensity	Relative
40.17	1131343.0	1.27
42.06	691520.3	0.78
43.06	1306507.6	1.47
49.02	3386065.5	3.81
50.06	1169314.5	1.31
51.04	2581737.3	2.90
52.07	1176987.9	1.32
53.08	665746.5	0.75
62.08	1962754.0	2.21
63.07	14034603.0	15.78
64.08	9988192.0	11.23
65.09	6282410.5	7.06
75.06	1414077.1	1.59
76.07	2323802.3	2.61
77.03	6500209.5	7.31
78.09	1165893.0	1.31
79.03	1389607.8	1.56
89.08	700555.0	0.79
90.08	3212211.8	3.61
91.07	2852849.8	3.21
92.07	3660815.3	4.12
93.08	1802245.8	2.03
101.08	1090399.0	1.23
102.08	1612141.9	1.81
104.21	1444106.6	1.62
104.97	907477.4	1.02
117.09	994217.9	1.12
118.12	1916056.1	2.15
119.02	702520.1	0.79
126.11	850203.5	0.96
127.11	3897566.5	4.38
128.09	2901539.8	3.26
129.09	842947.6	0.95
139.08	1182809.6	1.33
140.08	1261618.4	1.42
153.08	1250522.4	1.41
154.09	2105179.0	2.37
155.09	772681.4	0.87
166.09	745088.6	0.84
179.08	950514.6	1.07
181.12	2987026.8	3.36
182.10	6754416.5	7.59
183.10	2394031.0	2.69
194.09	1032675.8	1.16
208.11	1190046.6	1.34
209.13	12688930.0	14.27
210.12	46476856.0	52.26
211.11	20280990.0	22.80
212.11	2645608.8	2.97
223.12	1020521.0	1.15
236.08	1654054.3	1.86
237.11	1693832.1	1.90
250.14	759746.6	0.85
251.12	1468929.3	1.65

-ATEF-13A#101 RT: 1.71

(0,0) + c EI Full ms [40.00-1000.00]

z= 40.00-402.04

m/z	Intensity	Relative
271.11	666862.8	0.75
286.07	88933672.0	100.00
287.11	16730976.0	18.81
288.11	30054792.0	33.79
289.10	5485293.5	6.17

HEBA-14A
 PROTON_BSU CDC13 {C:\data} nmr 6



Current Data Parameters
 NAME Apr19-2015-nmr
 EXPNO 380
 PROCNO 1

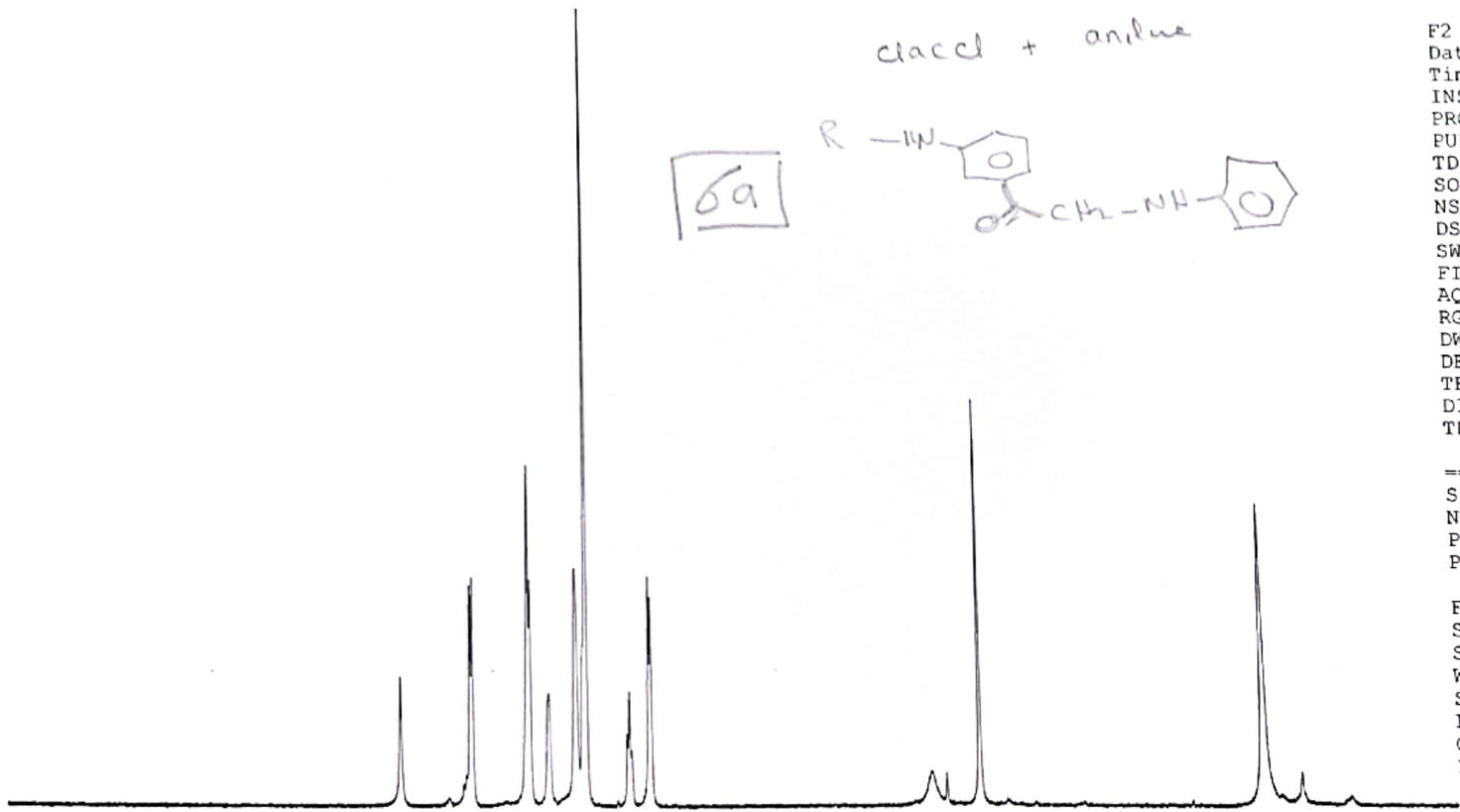
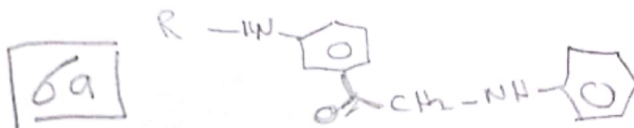
F2 - Acquisition Parameters
 Date_ 20150419
 Time_ 12.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

8.830
8.303
8.299
8.276
8.248
8.228
7.825
7.767
7.746
7.590
7.453
7.439
7.416
7.372
7.285
6.936
6.919
6.901
6.759
6.739
4.391
4.368
4.264
3.984
1.593
1.503
1.456
1.447
1.309
1.277

cdcl + aniline



1.00
2.32
3.46
1.26
2.49
4.65
1.04
2.09
1.03
2.12
3.79

HEBA-14A
 PROTON_BSU CDC13 {C:\data} nmr 6

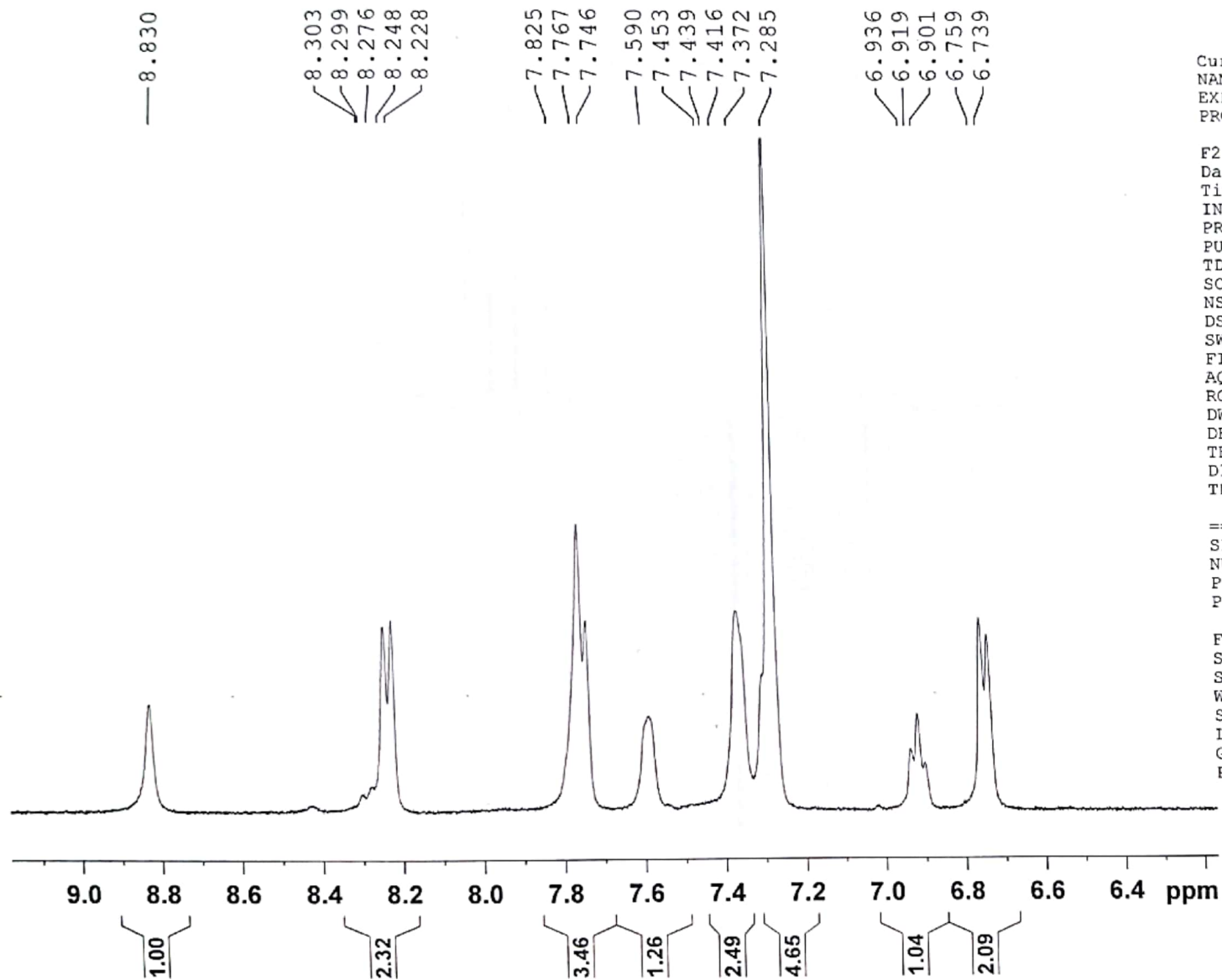


Current Data Parameters
 NAME Apr19-2015-nmr
 EXENO 380
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150419
 Time_ 12.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



HEBA-14A
DEPTQ-BSU CDC13 {C:\data} nmr 24



Current Data Parameters
NAME Apr22-2015-nmr
EXPNO 50
PROCNO 1

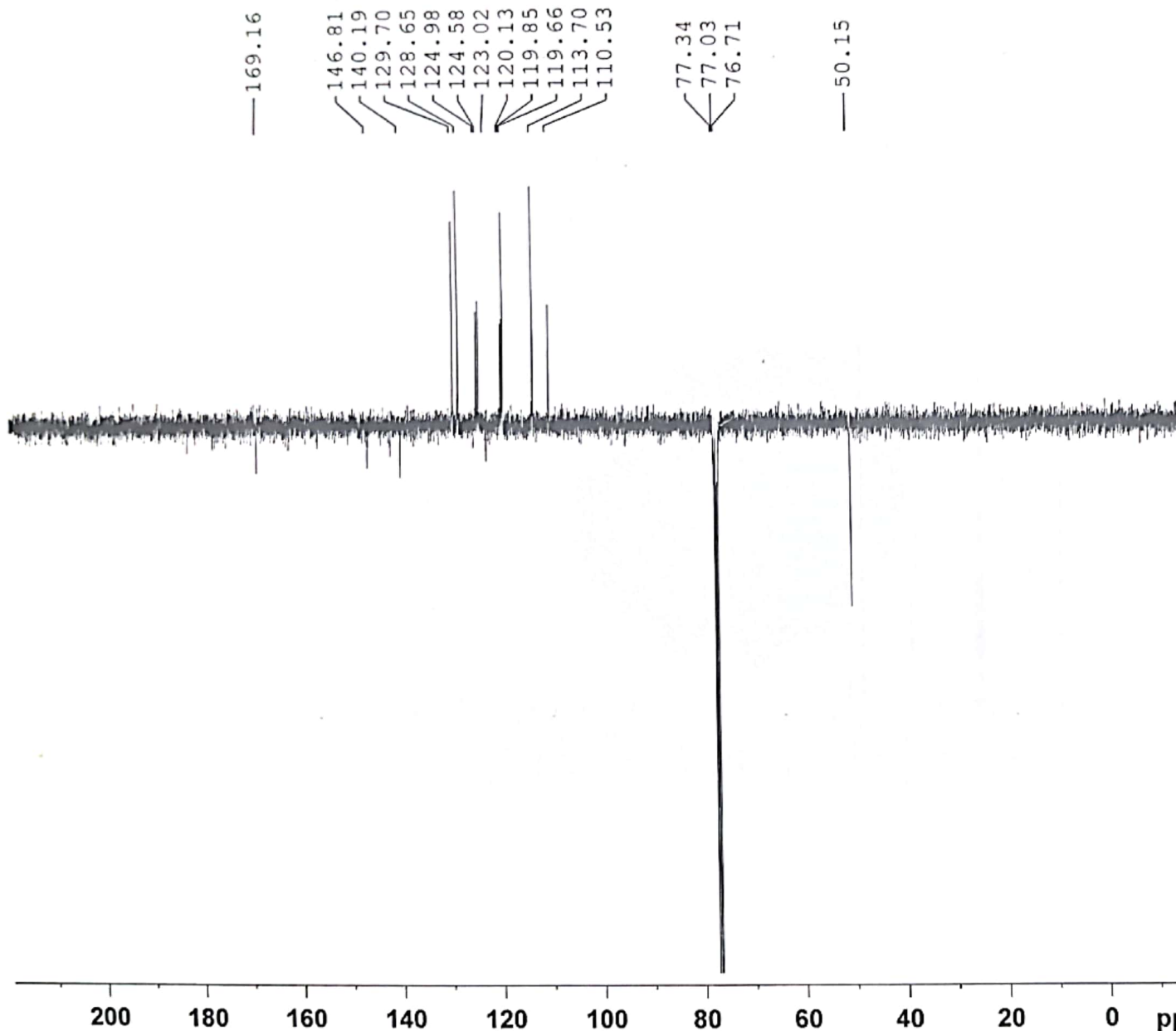
F2 - Acquisition Parameters
Date_ 20150423
Time 8.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

----- CHANNEL f2 -----
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GFNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-14A
DEPTQ-BSU CDC13 {C:\data} nmr 24



Current Data Parameters
NAME Apr22-2015-nmr
EXPNO 50
PROCNO 1

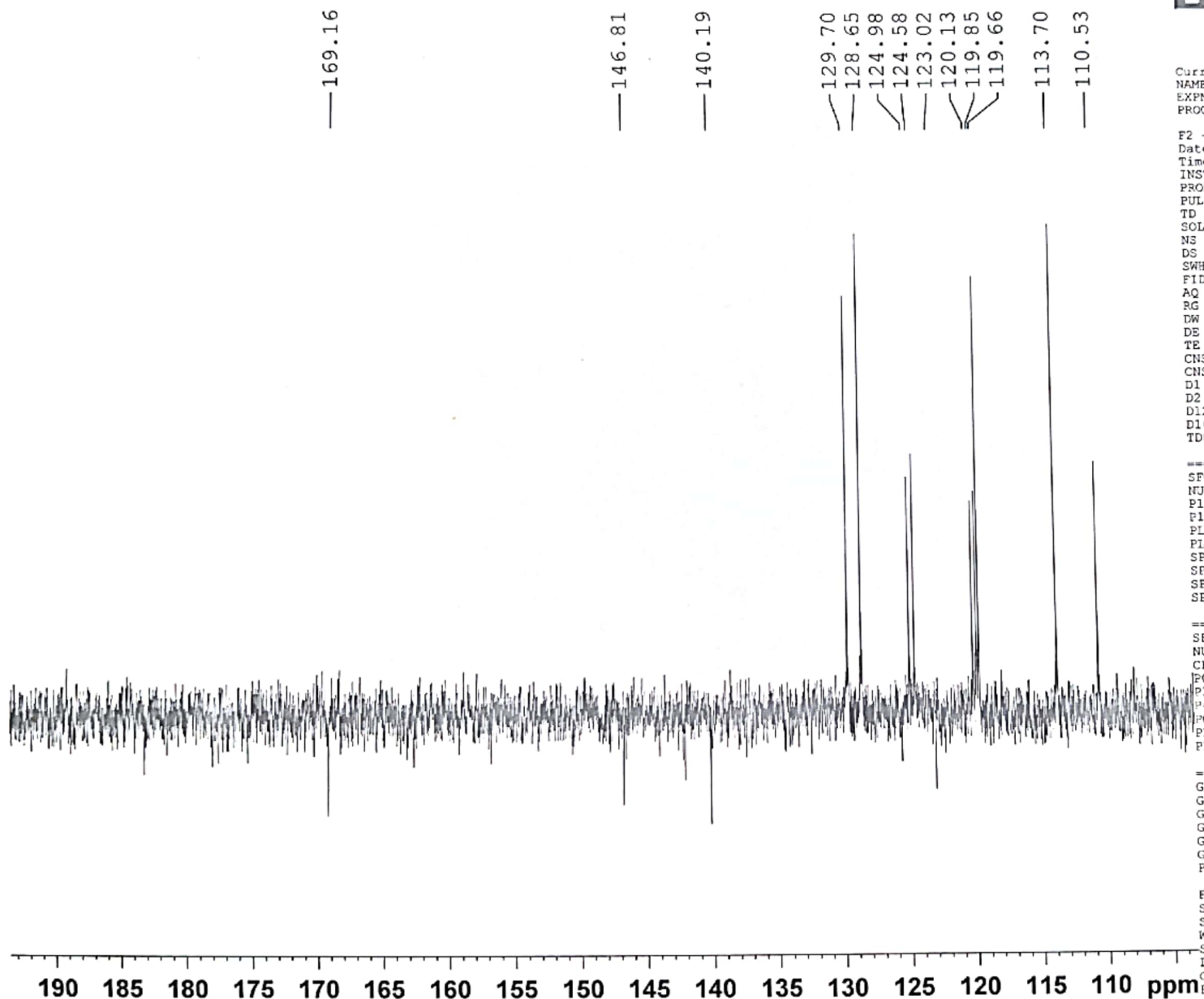
F2 - Acquisition Parameters
Date_ 20150423
Time 8.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.900 usec
DE 6.50 usec
TE 294.7 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-M14
 PROTON_BSU CDCl3 {C:\data} nmr 20



8.946
 8.904
 8.283
 8.275
 8.241
 8.221
 8.183
 7.827
 7.761
 7.741
 7.588
 7.424
 7.365
 7.285
 7.255
 7.157
 7.099
 7.080
 6.707
 6.665
 6.645

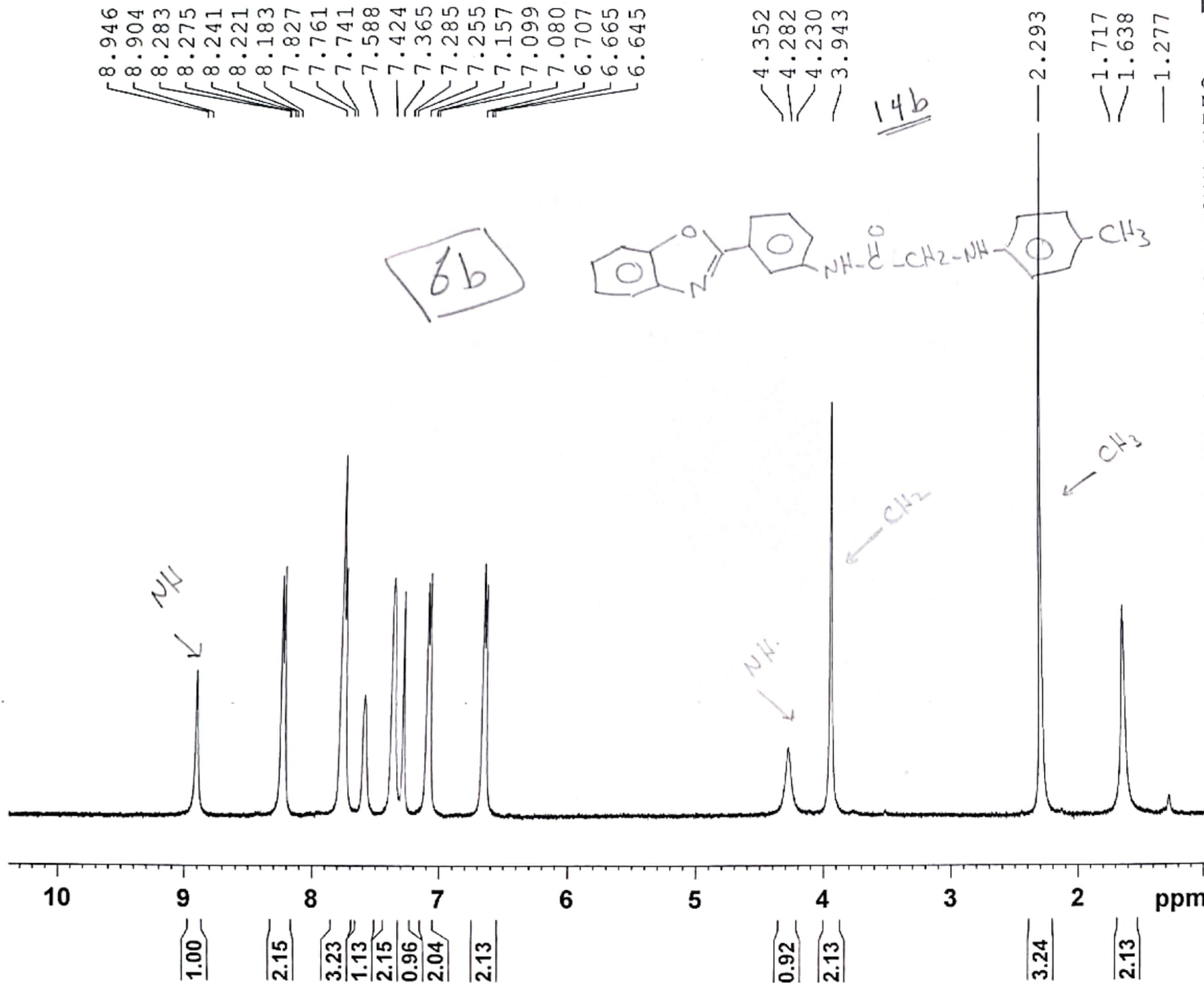
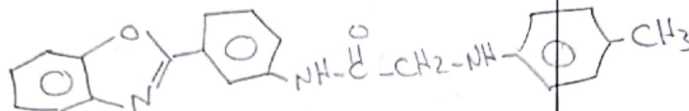
4.352
 4.282
 4.230
 3.943

14b

2.293

1.717
 1.638
 1.277

6b



Current Data Parameters
 NAME Mar19-2015-nmr
 EXPNO 200
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150319
 Time_ 11.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

HEBA-M14
DEPTQ-BSU CDC13 (C:\data) nmr 20

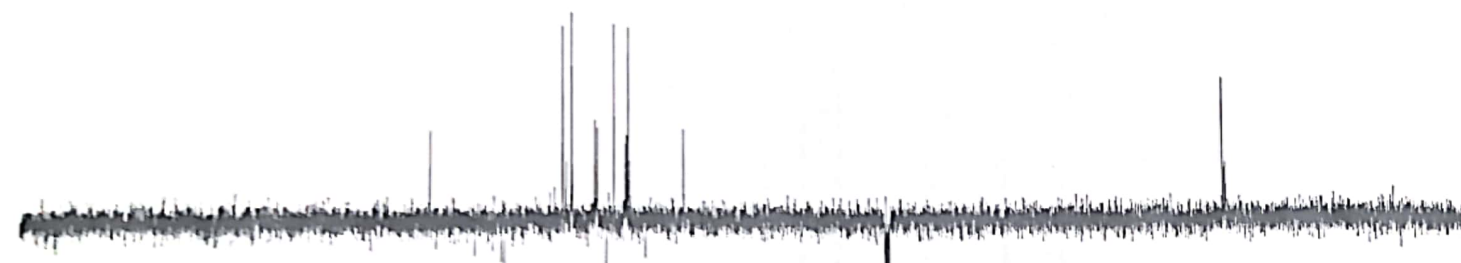
14b



151.79
140.08
139.55
130.30
130.23
129.63
128.80
128.70
125.02
124.61
123.06
121.92
119.99
119.87
119.59
119.34
110.56

77.35
77.03
76.72

21.27
20.91
20.83



Current Data Parameters
NAME Mar31-2015-nmr
EXPNO 360
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150401
Time 8.18
INSTRUM spect
PROBHD 5 mm PARBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00002000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SEW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
FCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GFNAM[1] SMSQ10.100
GFNAM[2] SMSQ10.100
GFNAM[3] SMSQ10.100
GP21 31.00 %
GP22 31.00 %
GP23 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSP 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

HEBA-M14
DEPTQ-BSU CDC13 {C:\data} nmr 20



Current Data Parameters
NAME Mar31-2015-nmr
EXPNO 360
PROCNO 1

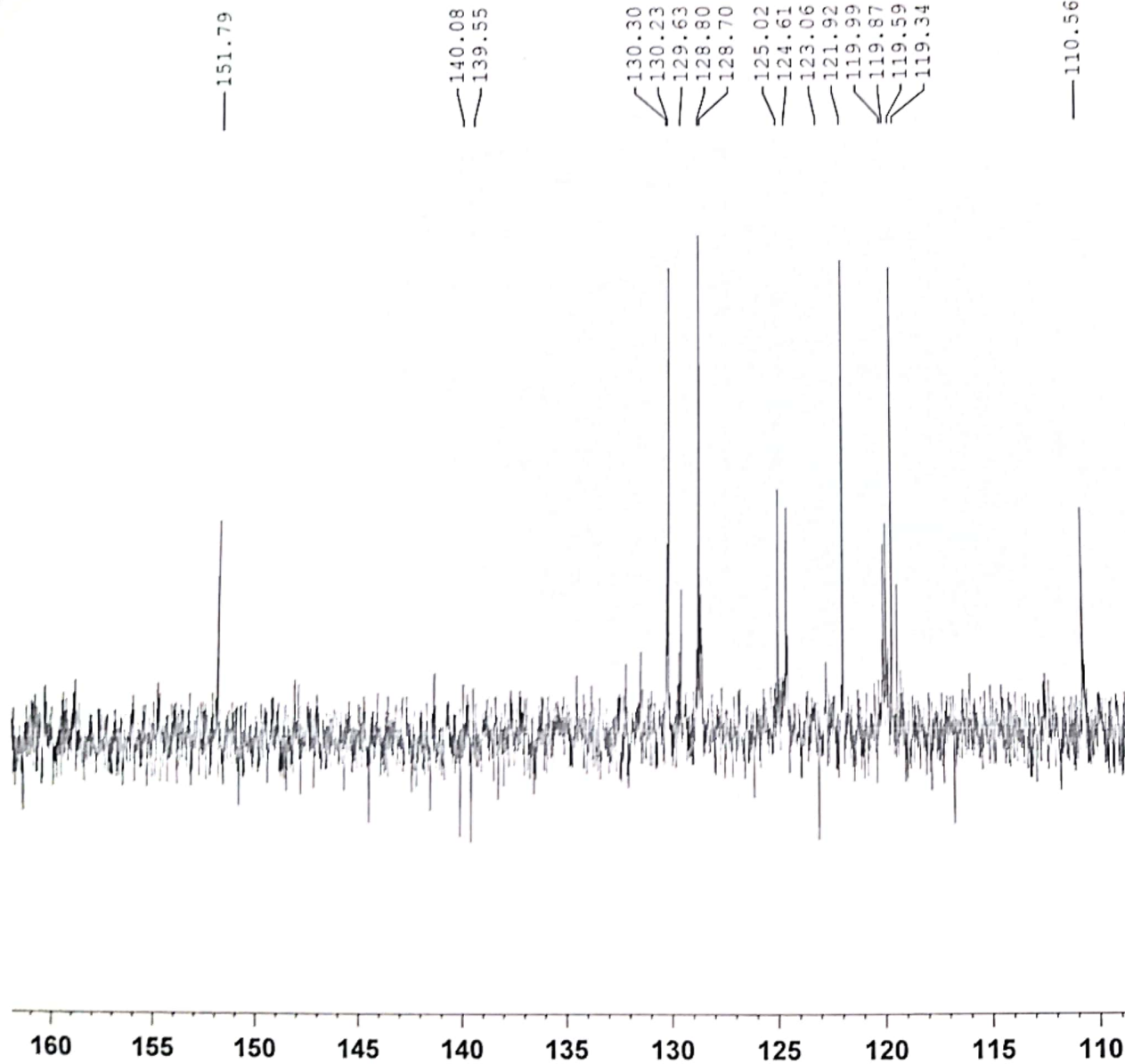
F2 - Acquisition Parameters
Date_ 20150401
Time_ 8.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpap
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

----- CHANNEL f1 -----
SF01 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

----- CHANNEL f2 -----
SF02 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 31.00 %
GP22 31.00 %
GP23 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-14D
PROTON_BSU DMSO (C:\data) nmr 8

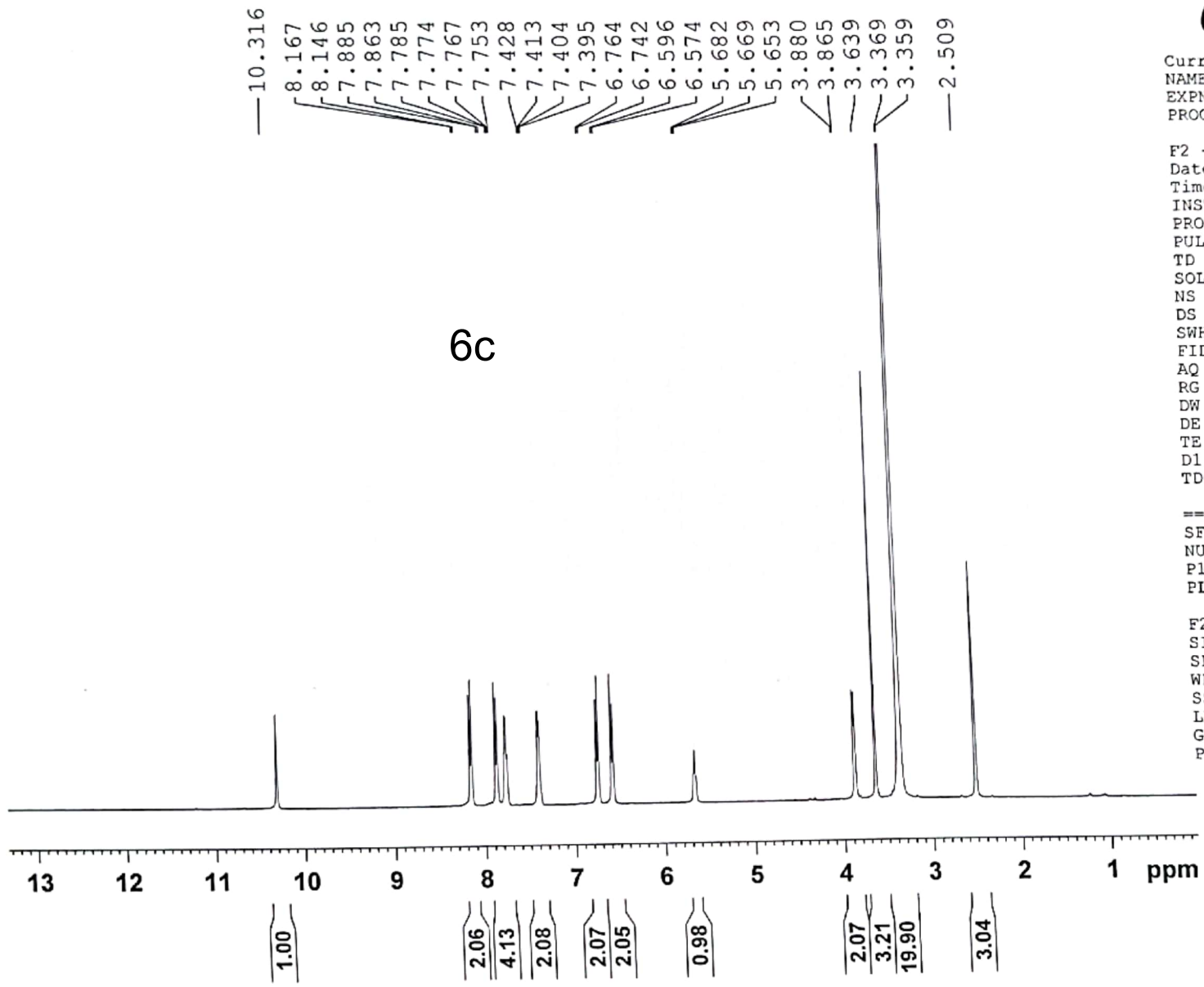


Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 240
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time_ 7.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



HEBA-14D
PROTON_BSU DMSO {C:\data} nmr 8



8.167
8.146
7.885
7.863
7.785
7.774
7.767
7.753
7.428
7.413
7.404
7.395

6.764
6.742
6.596
6.574

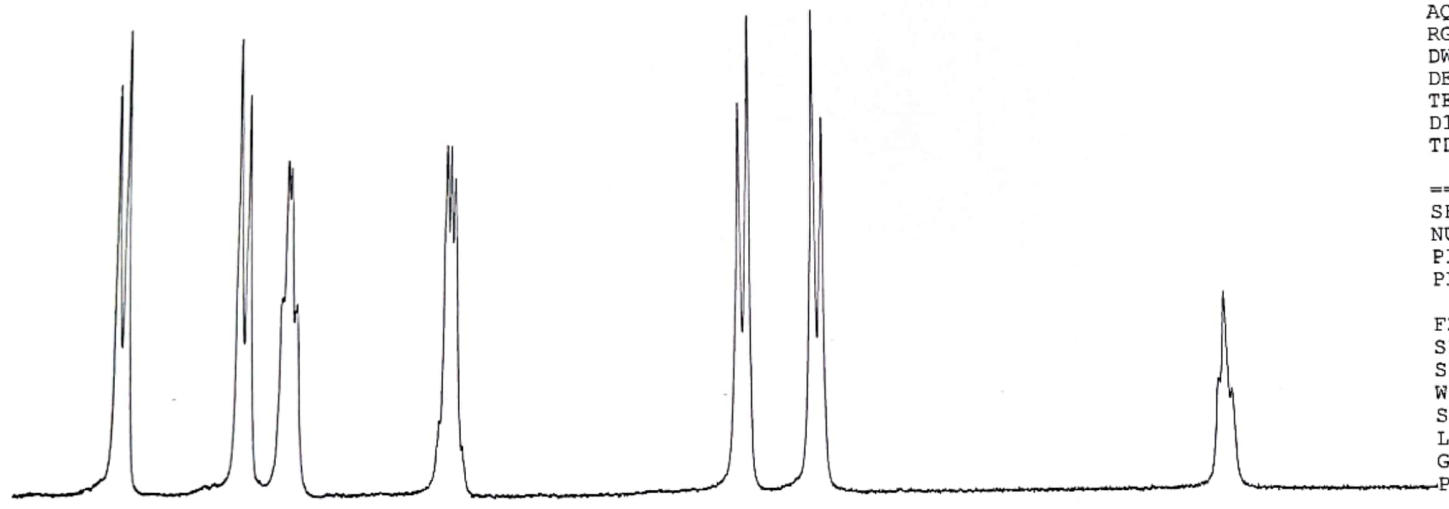
5.682
5.669
5.653

Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 240
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time_ 7.44
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 147.93
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



2.06

4.13

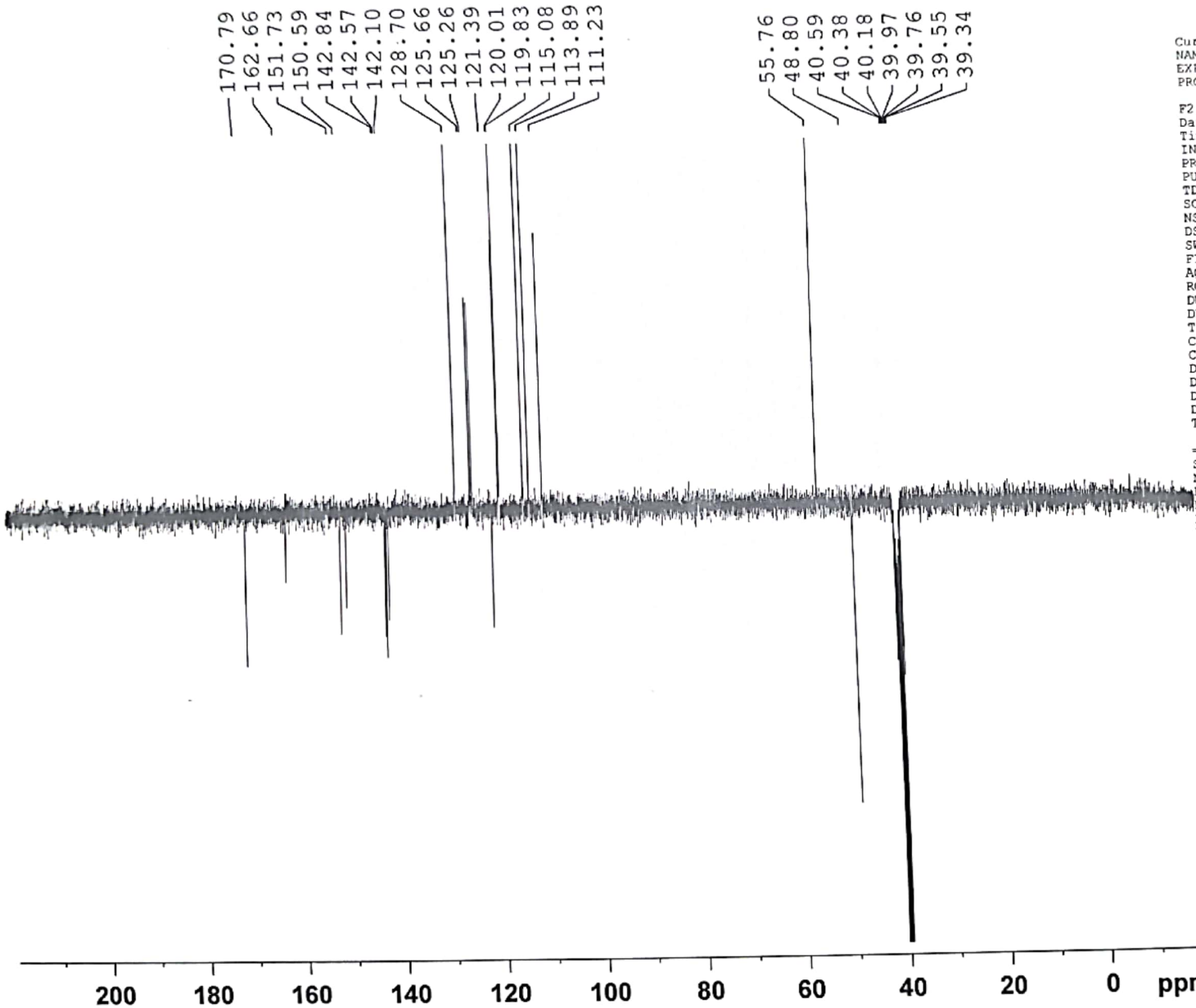
2.08

2.07

2.05

0.98

HEBA-14D
DEPTQ-BSU DMSO {C:\data} nmr 8



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 241
PROCNO 1

F2 - Acquisition Parameters
Date 20150718
Time 11.33
INSTRUM spect
PROBHD 5 mm PABBO EB/
PULPROG deptqqesp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SFNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

==== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

==== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-14D
DEPTQ-BSU DMSO {C:\data} nmr 8



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 241
PROCNO 1

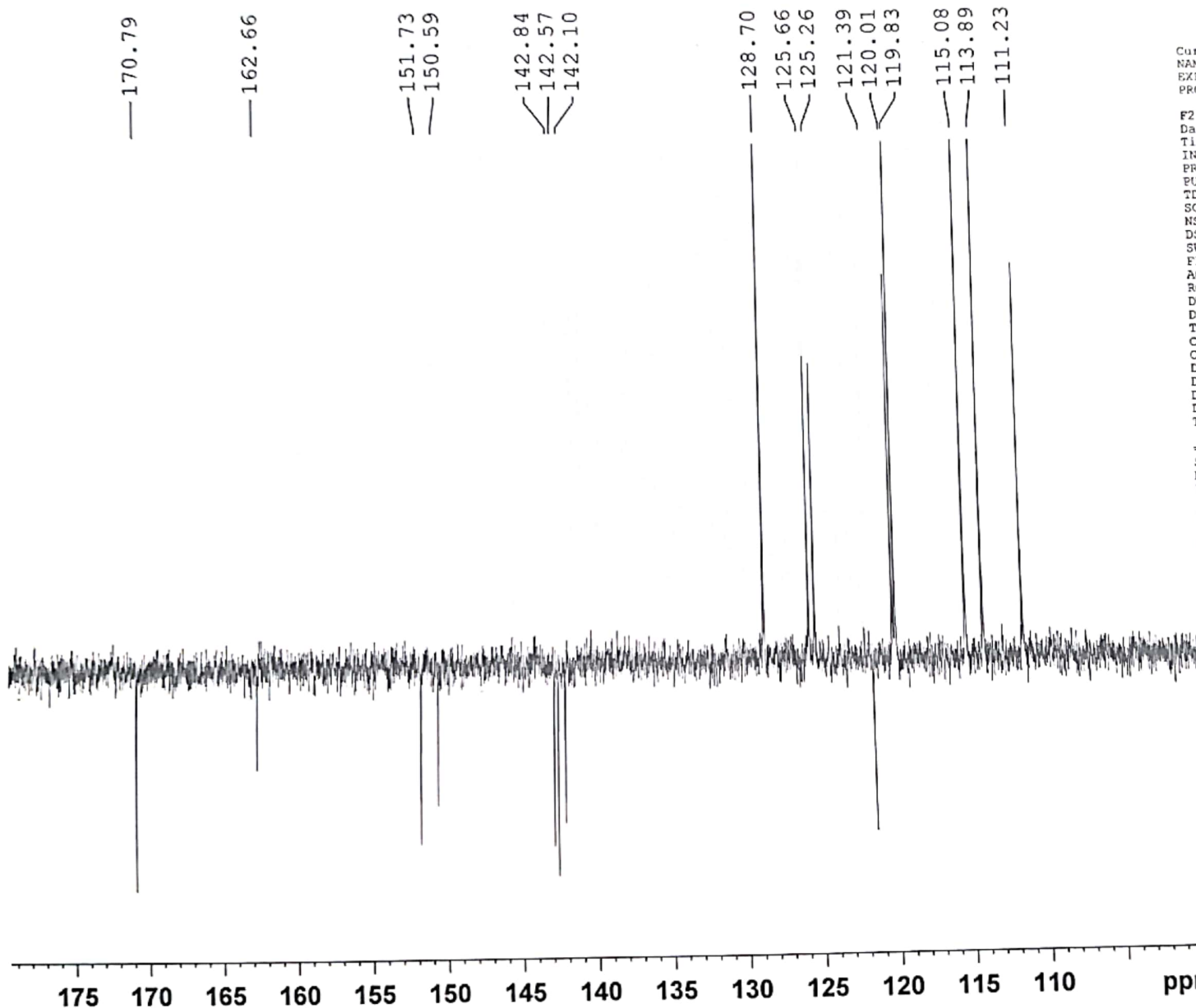
F2 - Acquisition Parameters
Date 20150718
Time 11.33
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.0002000 sec
D16 0.0002000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM(5) Crp60comp.4
SFOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG(2) waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM(1) SMSQ10.100
GPNAM(2) SMSQ10.100
GPNAM(3) SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-14D
DEPTQ-BSU DMSO (C:\data) nmr 8



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 241
PROCNO 1

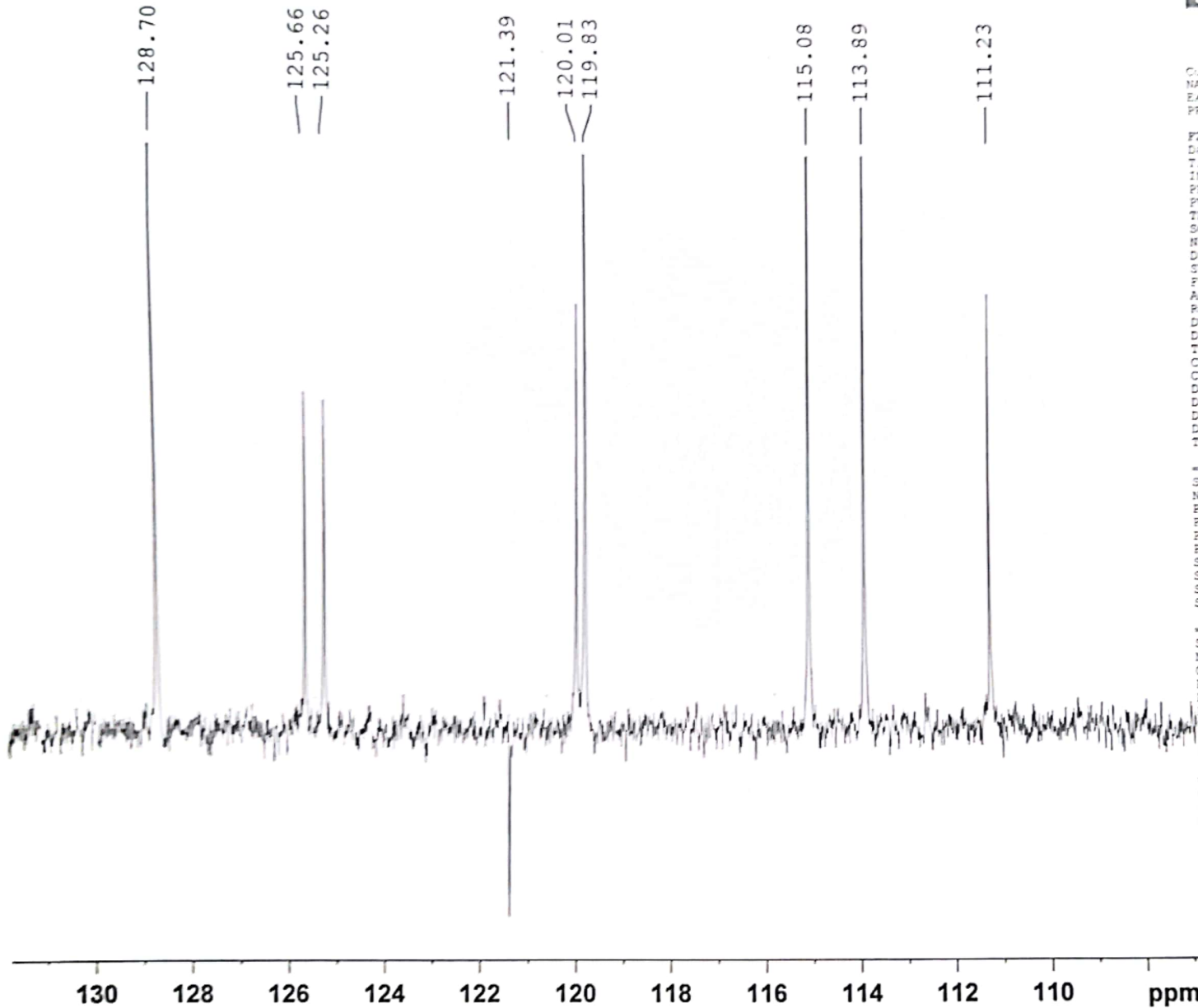
F2 - Acquisition Parameters
Date_ 20150718
Time_ 11.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsqpp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24039.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
EW 20.800 usec
DE 6.50 usec
TE 298.4 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344825 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 100.6228903 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp40comp.4
SFOALS 0.500
SFOFFS5 0 Hz
SPW5 10.08399963 W

----- CHANNEL f2 -----
SFO2 400.1312797 MHz
NUC2 1H
CPOPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 31.00 %
GP22 31.00 %
GP23 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



HEBA-14D
DEPTQ-BSU DMSO {C:\data} nmr 8



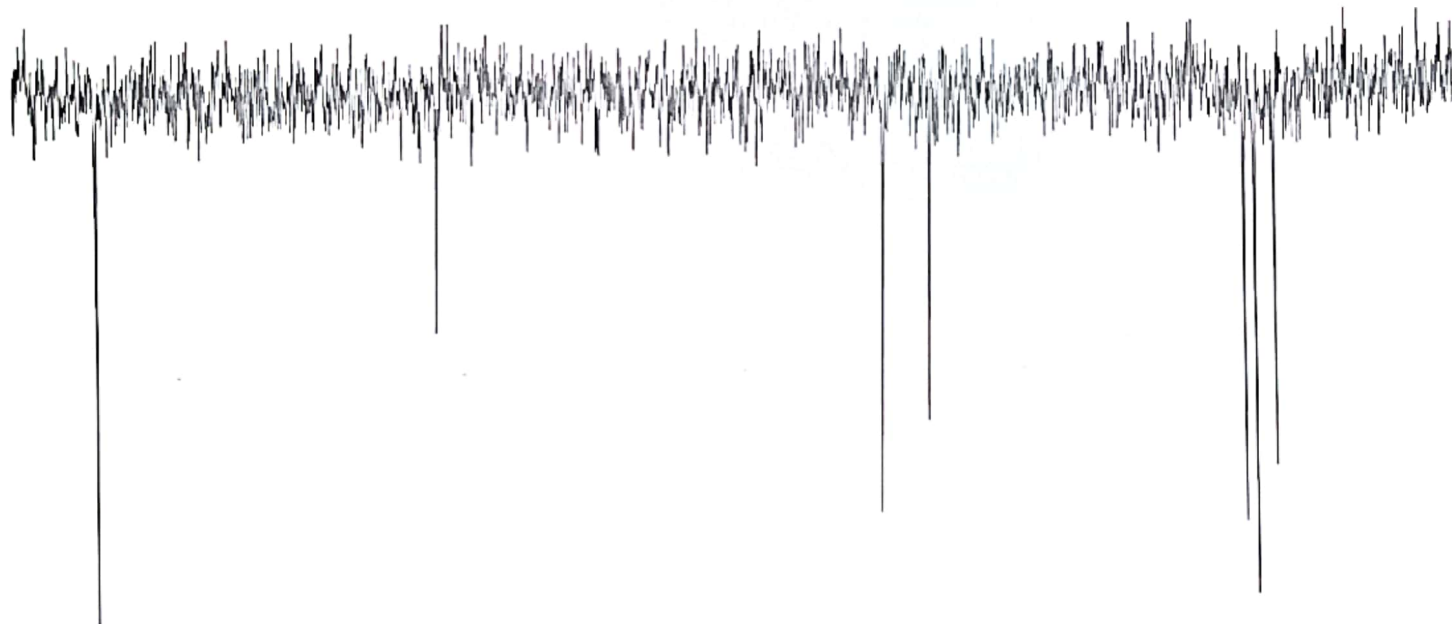
— 170.79

— 162.66

— 151.73

— 150.59

142.84
142.57
142.10



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 241
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time_ 11.33
INSTRUM spect
PROBHD 5 mm BABB0 BB/
PULPROG deptqqppp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SFOAL5 0.500
SPOFFS5 0 Hz
SEW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CEDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GENAM[1] SMSQ10.100
GENAM[2] SMSQ10.100
GENAM[3] SMSQ10.100
GPZ1 31.00 μ
GPZ2 31.00 μ
GPZ3 31.00 μ
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HEBA-14C
 PROTON_BSU DMSO {C:\data} nmr 9



Current Data Parameters
 NAME May03-2015-nmr
 EXPNO 330
 PROCNO 1

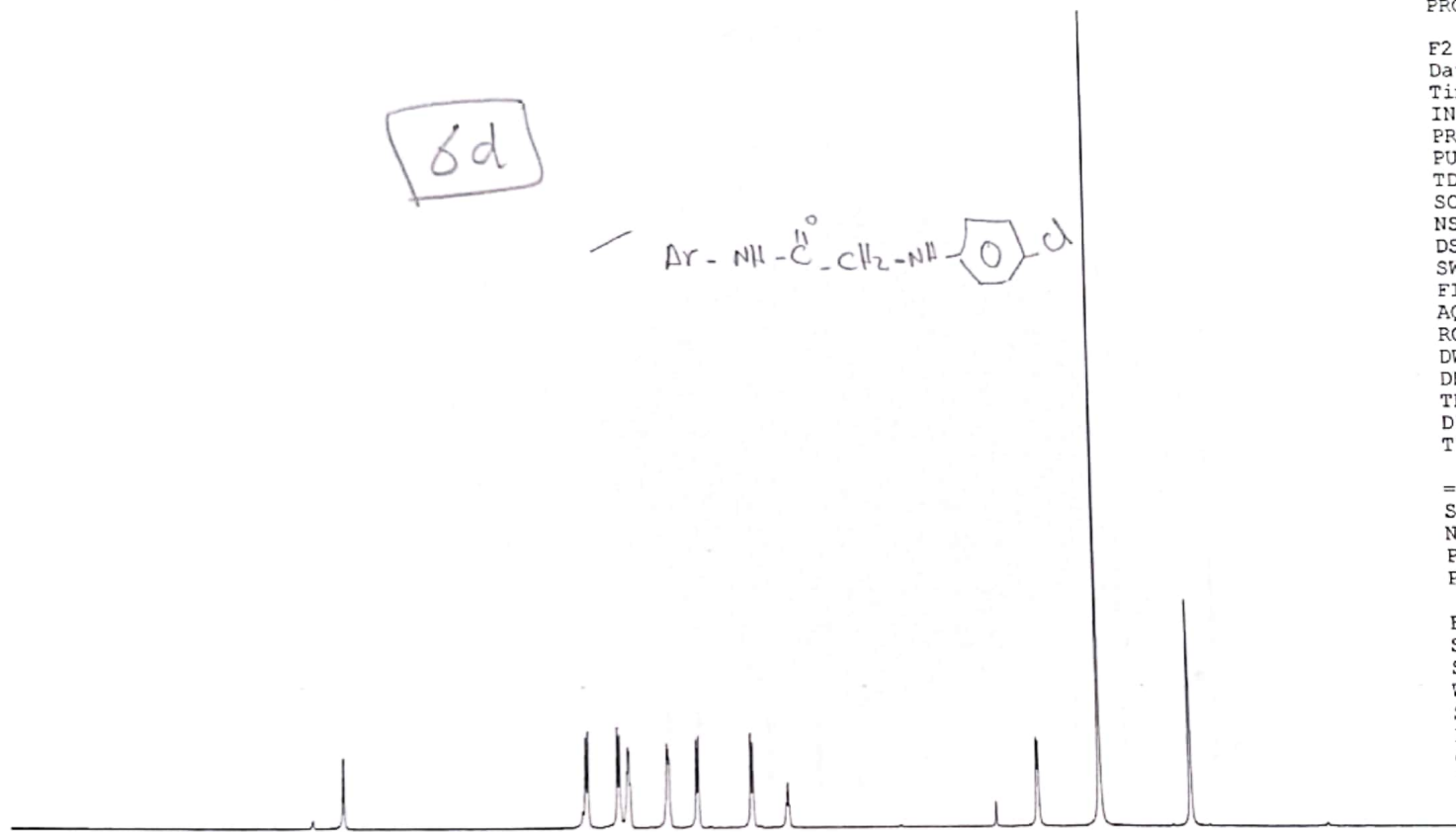
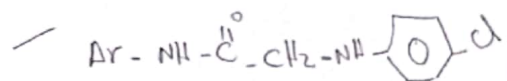
F2 - Acquisition Parameters
 Date_ 20150503
 Time 13.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 DW 62.400 usec
 DE 6.50 usec
 TE 294.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

— 10.431
 8.173
 8.152
 7.877
 7.857
 7.789
 7.779
 7.770
 7.414
 7.405
 7.396
 7.142
 7.121
 6.633
 6.612
 6.290
 4.336
 3.950
 3.936
 3.361
 — 2.508

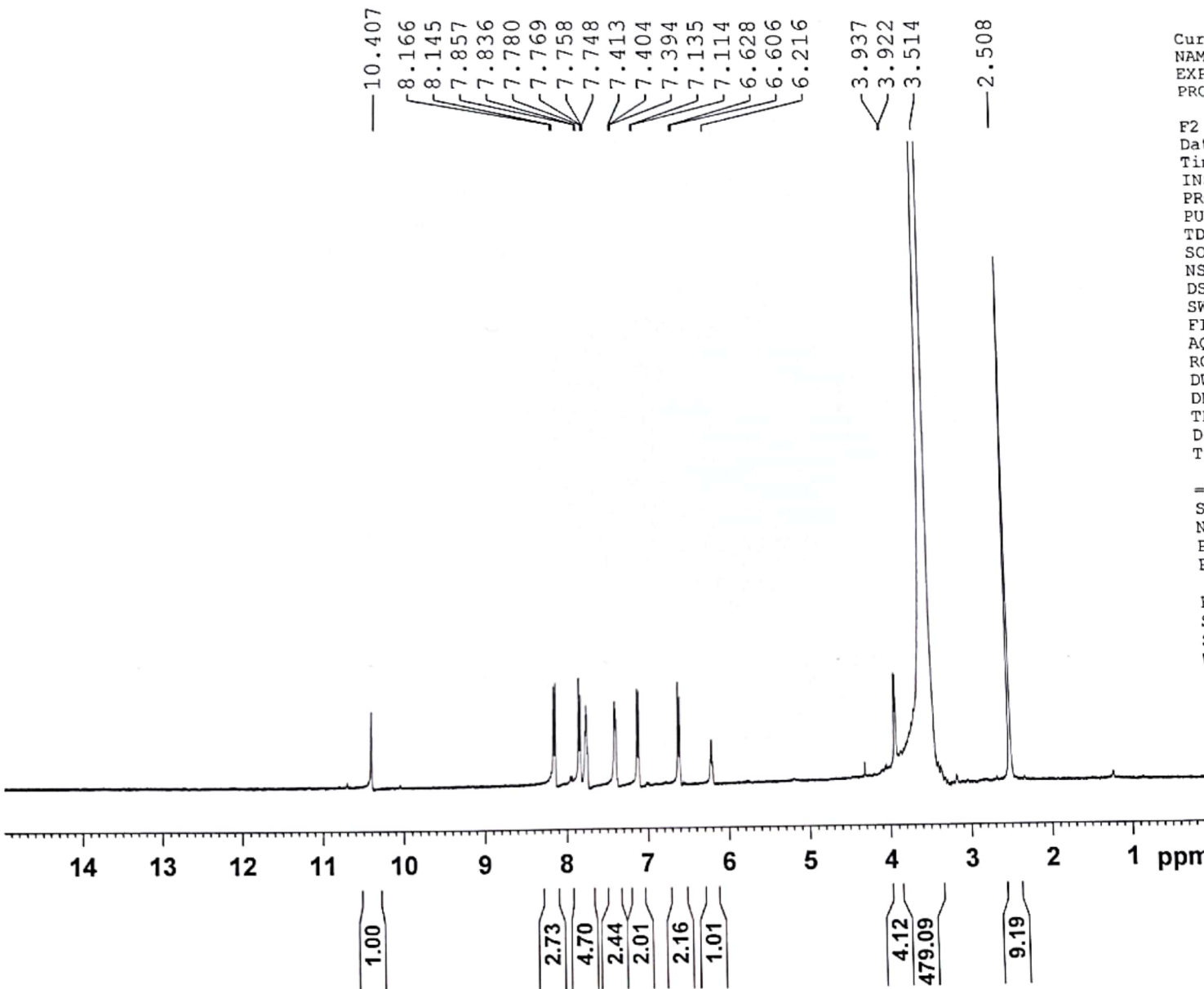
δd



13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

3.26
 7.88
 7.69
 7.34
 7.66
 6.53
 6.58
 3.13
 0.80
 6.50
 27.08
 12.28

HEBA-14C
PROTON_BSU DMSO {C:\data} nmr 7



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 231
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time_ 7.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

HEBA-14C
PROTON_BSU DMSO {C:\data} nmr 7

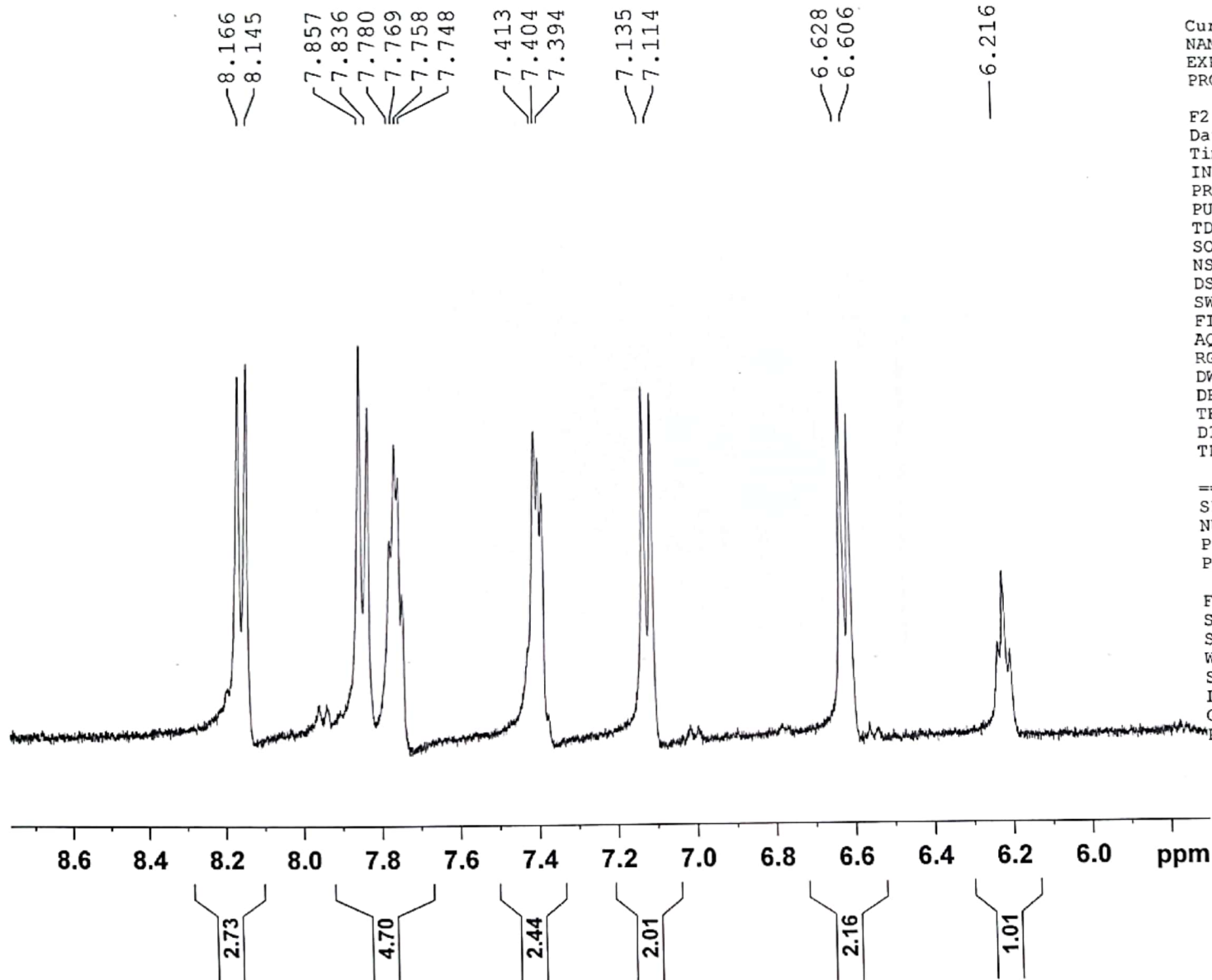


Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 231
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time 7.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.28
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

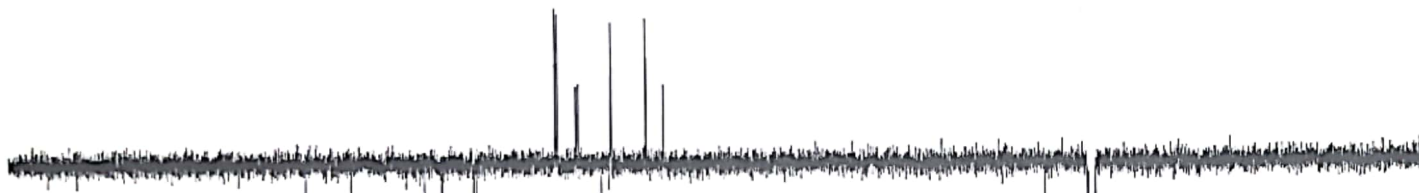


HEBA-14C
DEPTQ-BSU DMSO {C:\data} nmr 7



170.15
162.64
150.56
147.68
142.51
142.01
129.07
128.73
125.73
125.32
121.43
119.99
119.87
114.16
111.25

47.61
40.43
40.22
40.01
39.80
39.59
39.38
39.18



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 230
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time 7.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqgppsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.0000000
CNST12 1.5000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

===== CHANNEL f2 =====
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 31.00 %
GPZ2 31.00 %
GPZ3 31.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

HEBA-14C
DEPTQ-BSU DMSO {C:\data} nmr 7



Current Data Parameters
NAME Jul15-2015-nmr
EXPNO 230
PROCNO 1

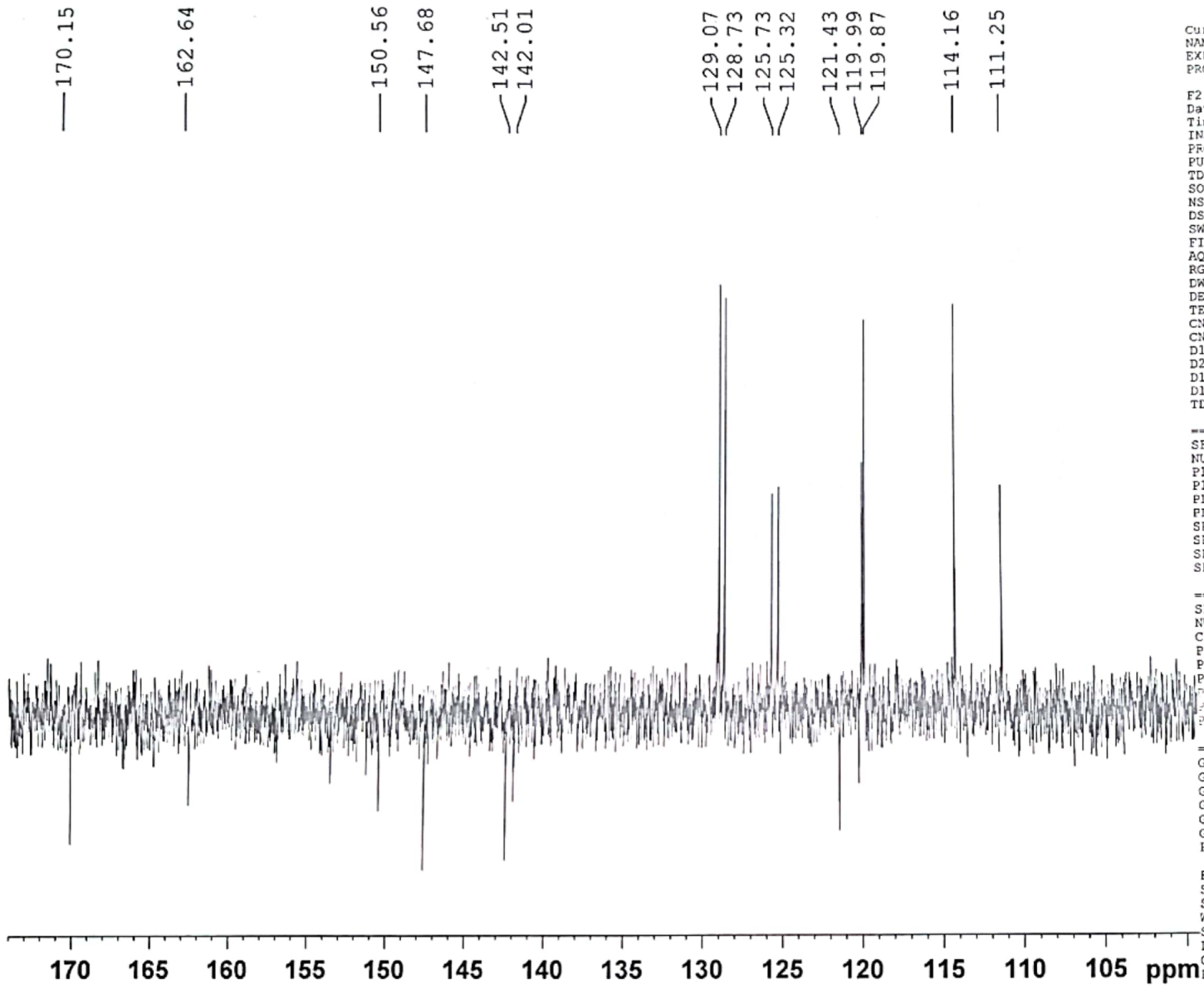
F2 - Acquisition Parameters
Date_ 20150718
Time 7.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptqqpsp
TD 65536
SOLVENT DMSO
NS 4000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 205.44
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
CNST2 145.000000
CNST12 1.500000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 100.6228303 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
PLW0 0 W
PLW1 66.00000000 W
SPNAM[5] Crp60comp.4
SPOALS 0.500
SPOFFS5 0 Hz
SPW5 10.08399963 W

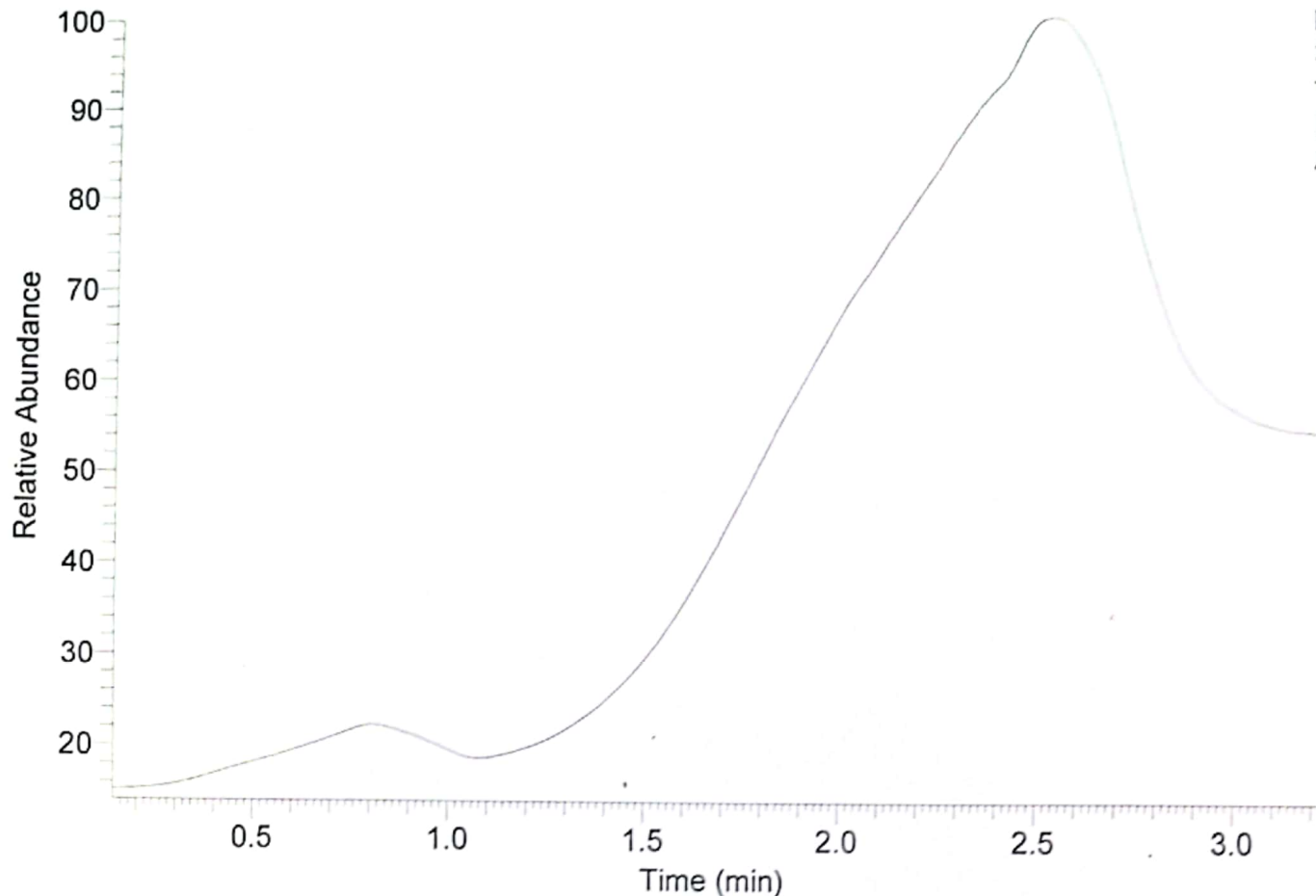
----- CHANNEL f2 -----
SFO2 400.1312797 MHz
NUC2 1H
CPDPRG[2] waltz16
P0 15.75 usec
P3 10.50 usec
P4 21.00 usec
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.21777999 W

----- GRADIENT CHANNEL -----
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GP21 31.00 t
GP22 31.00 t
GP23 31.00 t
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

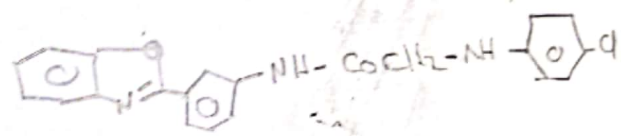
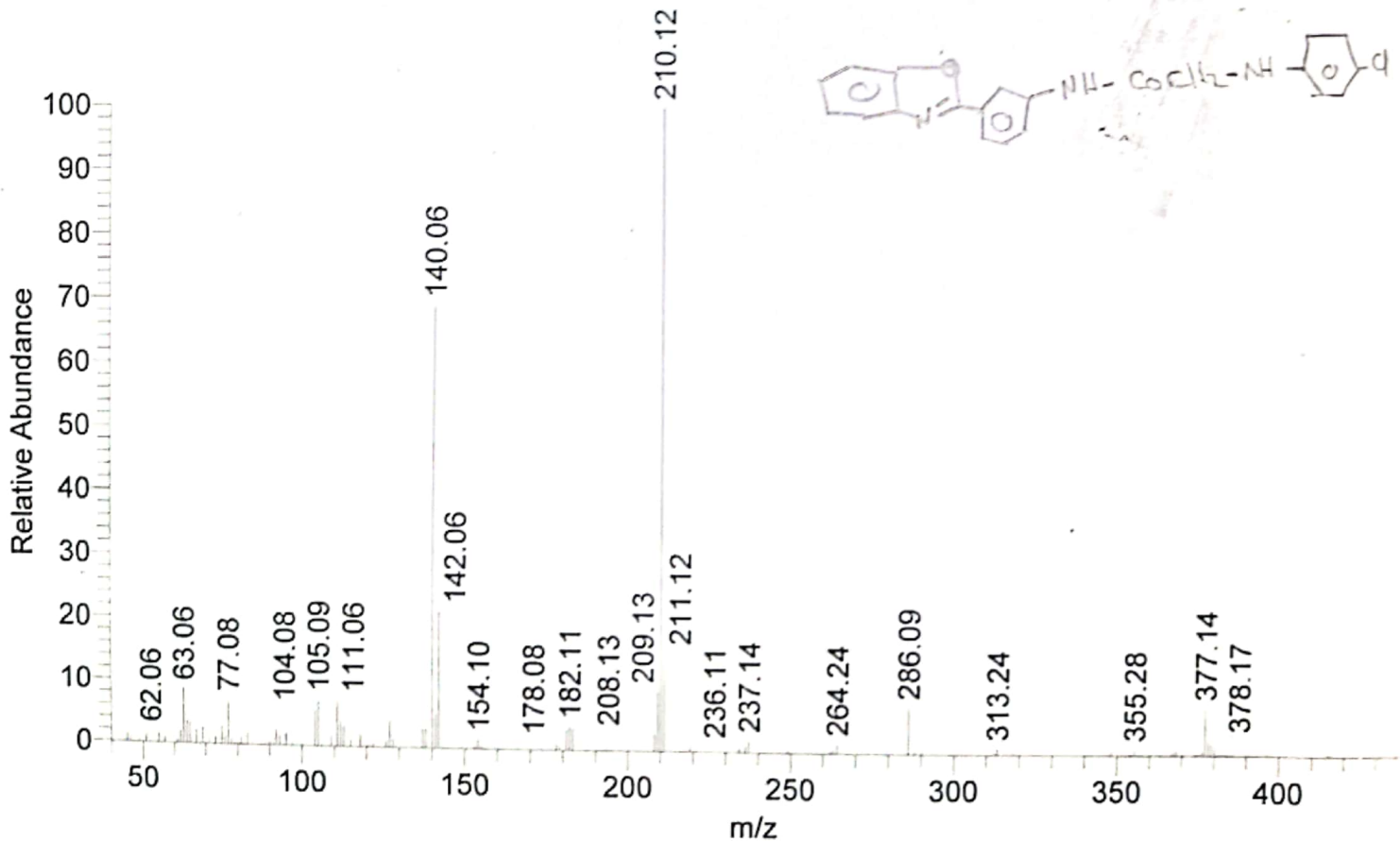


RT: 0.14 - 3.22 SM: 15B



NL:
3.46E8
TIC MS
HEBA-
ATEF-14C

HEBA-ATEF-14C #280 RT: 4.70 AV: 1 SB: 17 4.75-4.90, 4.75-4.85 NL: 5.32E5
T: {0,0} + c EI Full ms [40.00-1000.00]



HEBA-ATEF-14C#280 RT: 4.70
 SB: 17 4.75-4.90 , 4.75-4.85
 T: (0,0) + c EI Full ms [40.00-1000.00]
 m/z = 40.00-437.64

m/z	Intensity	Relative
45.07	6768.7	1.27
51.07	6430.1	1.21
55.08	8617.3	1.62
57.10	5261.2	0.99
62.06	9781.4	1.84
63.06	45728.4	8.60
64.06	17917.9	3.37
65.07	17073.4	3.21
67.09	11662.2	2.19
69.08	14534.2	2.73
71.10	4813.0	0.91
73.06	5816.0	1.09
75.05	14686.1	2.76
76.06	6406.4	1.20
77.08	37069.7	6.97
78.07	4880.4	0.92
81.10	6430.6	1.21
83.10	9006.6	1.69
92.06	11952.3	2.25
93.09	7755.5	1.46
95.11	10386.9	1.95
104.08	29514.4	5.55
105.09	38490.3	7.24
109.12	8033.4	1.51
111.06	37508.6	7.05
112.07	20904.3	3.93
113.06	17109.6	3.22
115.09	5426.9	1.02
118.10	9903.0	1.86
126.09	4835.4	0.91
127.07	21613.1	4.07
128.10	6662.5	1.25
137.08	15344.6	2.89
138.07	15234.3	2.87
140.06	365521.8	68.75
141.08	27620.5	5.19
142.06	113742.6	21.39
154.10	7168.9	1.35
178.08	5430.7	1.02
181.11	16279.0	3.06
182.11	19056.0	3.58
183.11	17278.5	3.25
208.13	14047.1	2.64
209.13	49876.3	9.38
210.12	531679.2	100.00
211.12	82355.6	15.49
236.11	4276.6	0.80
237.14	9716.8	1.83
264.24	7759.8	1.46
286.09	38787.3	7.30
313.24	4495.5	0.85
355.28	4336.9	0.82
368.28	3957.9	0.74

HEBA-A-TEF-14C#280 RT: 4.70
SB: 17 4.75-4.90 , 4.75-4.85
T: {0,0} + c EI Full ms [40.00-1000.00]
m/z= 40.00-437.64

m/z	Intensity	Relative
377.14	38752.7	7.29
378.17	12105.5	2.28
379.15	9416.4	1.77
380.14	5266.6	0.99