

Supporting information

Diversty-oriented synthesis of fused thioglycosyl benzo[e][1,4]oxathiepin-5-ones and benzo[f][1,4]thiazepin-5(2H)- ones by a sequences of palladium-catalyzed glycosyl thiol arylation and deprotection-lactonization reactions

Riyadh Ahmed Atto AL-Shuaeeb, Gilles Galvani, Guillaume Bernadat, Jean-Daniel Brion,
Mouad Alami* and Samir Messaoudi*

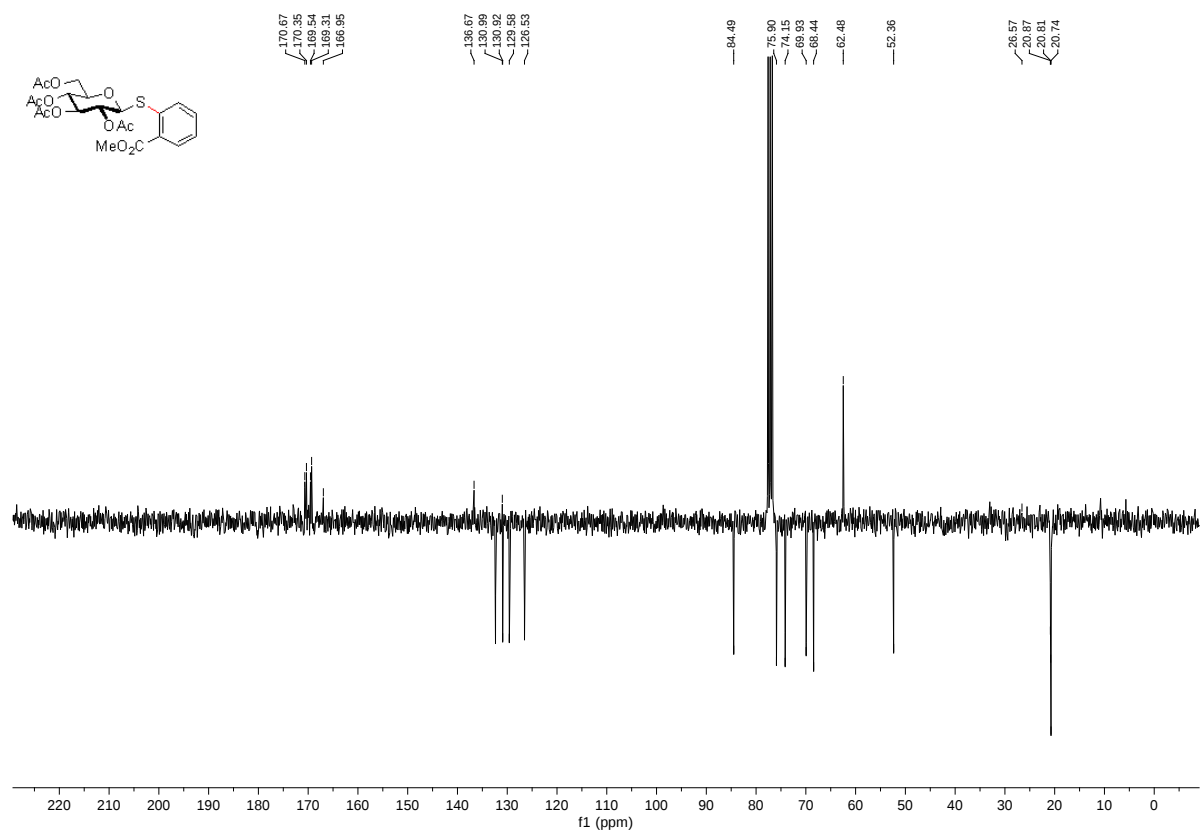
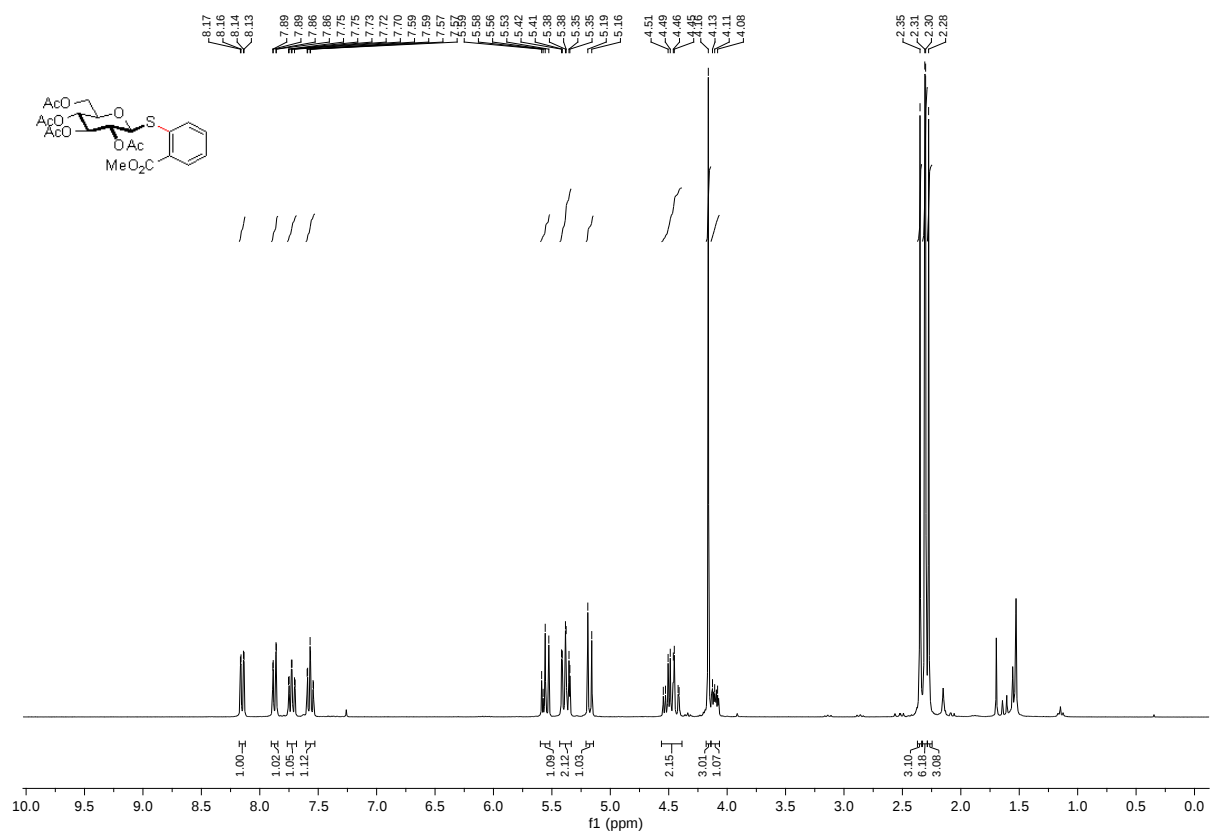
*Univ Paris-Sud, CNRS, BioCIS-UMR 8076, Laboratoire de Chimie Thérapeutique,
Equipe Labellisée Ligue Contre le Cancer, LabEx LERMIT, Faculté de Pharmacie, 5 rue
J.-B. Clément, Châtenay-Malabry, 92296.*

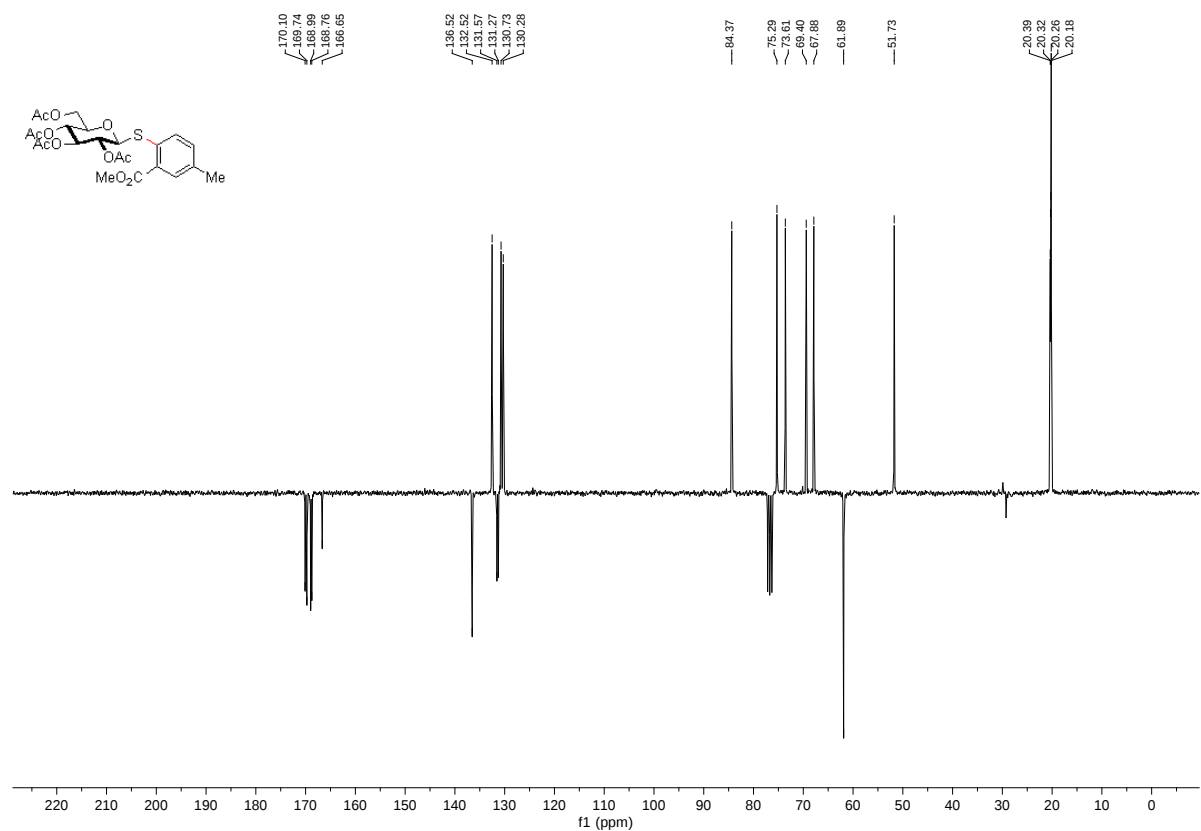
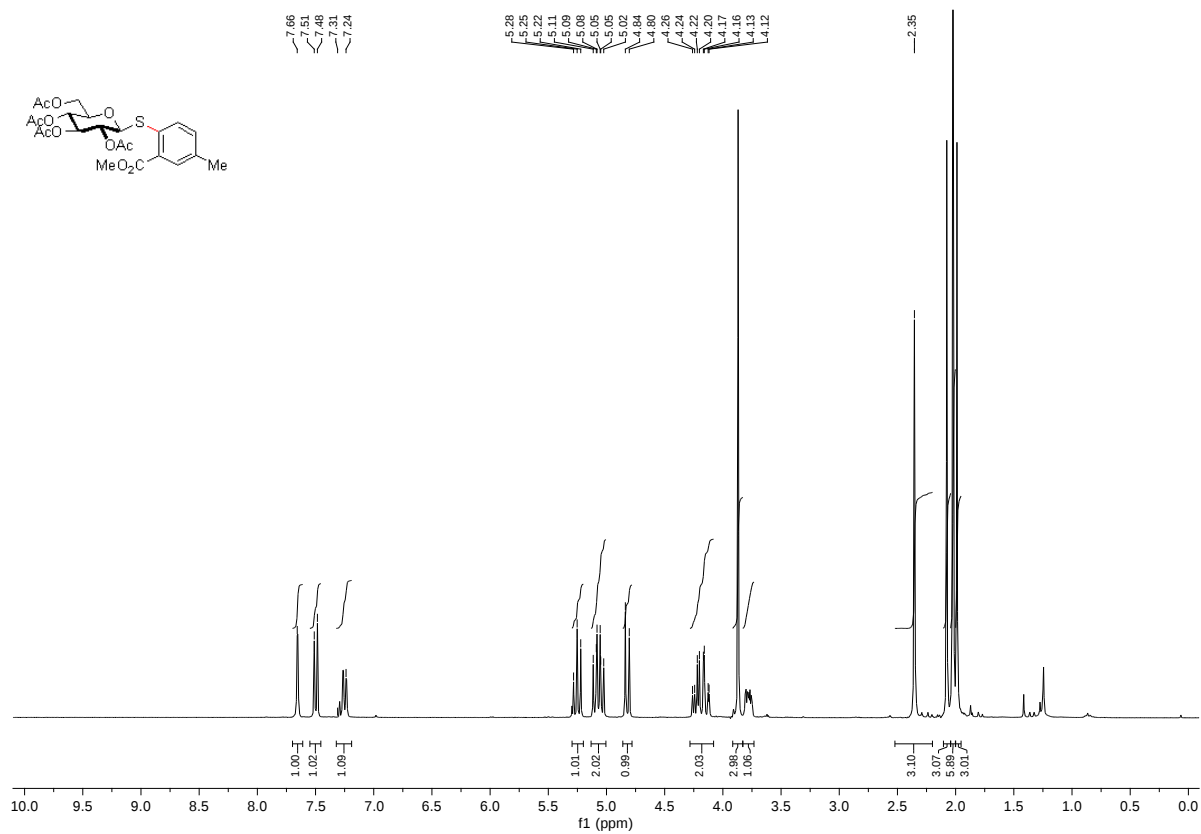
samir.messaoudi@u-psud.fr, mouad.alami@u-psud.fr,

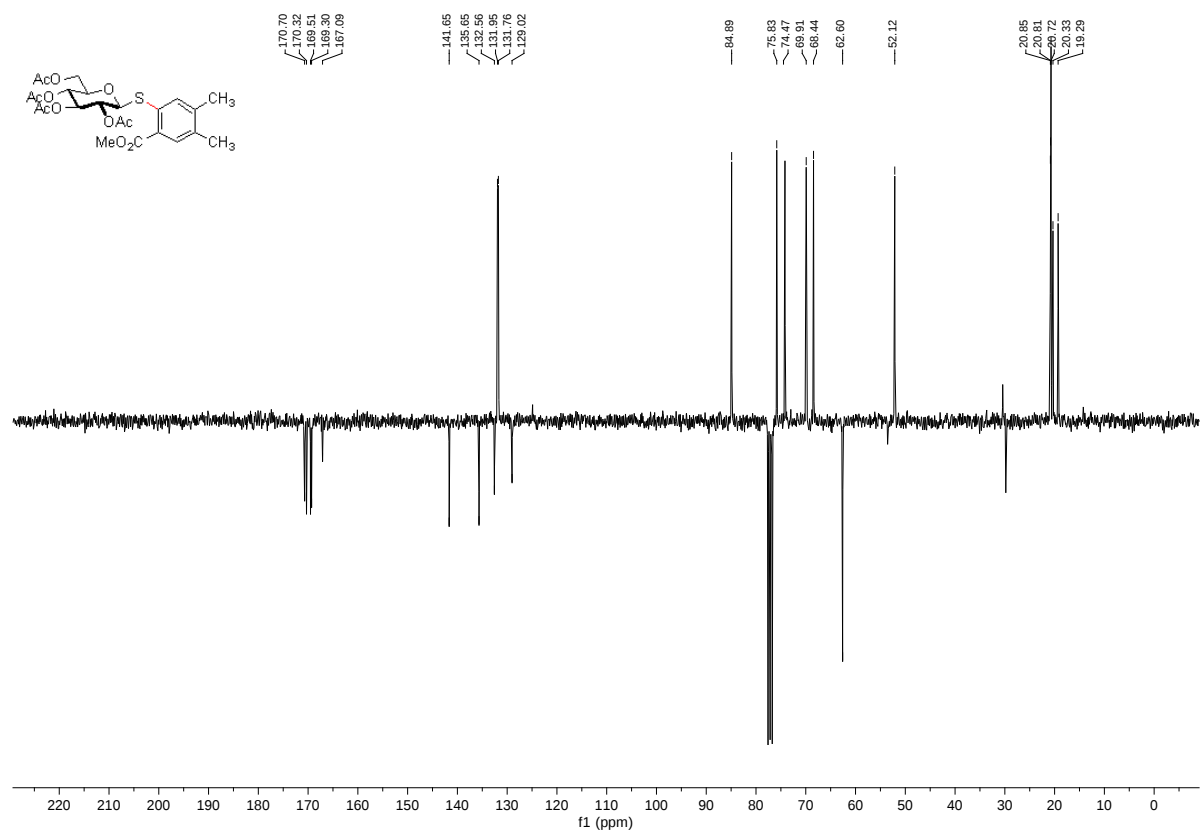
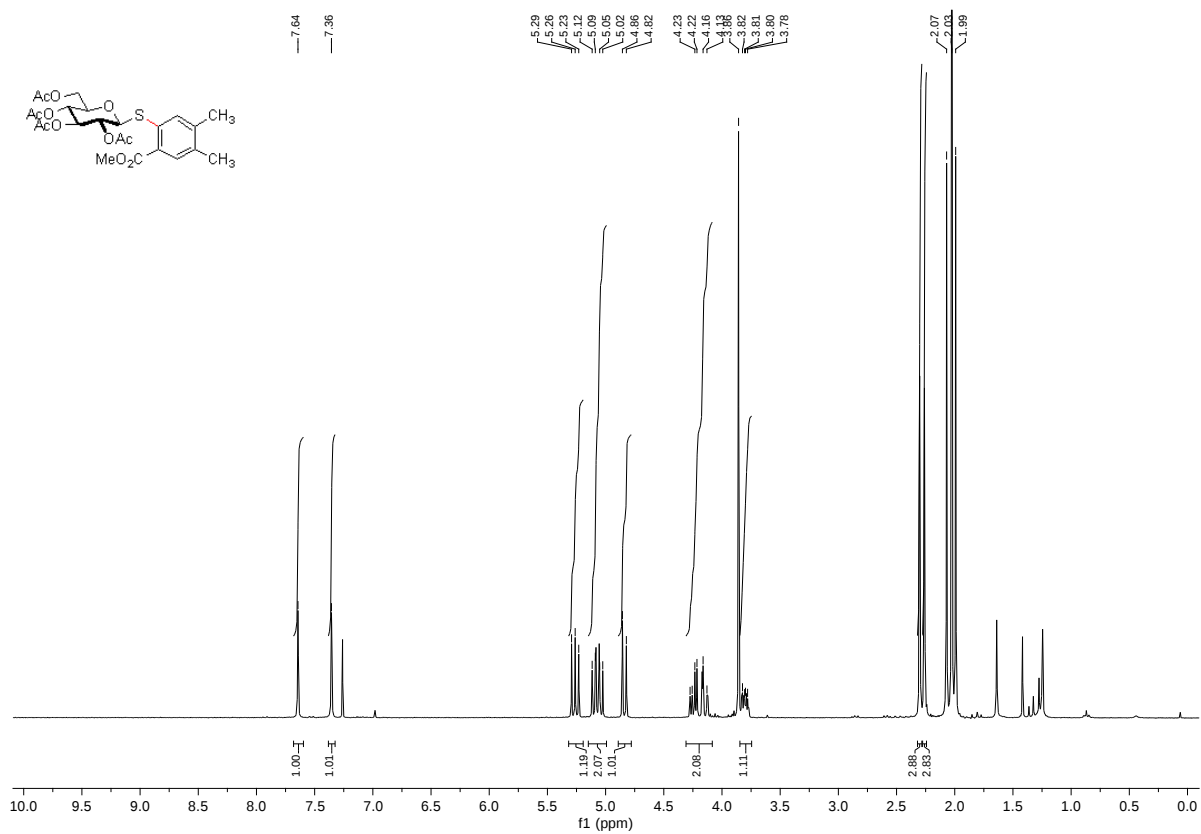
Phone: 33(0)1.46.83.58.28 ; Fax: 33(0)1.46.83.58.28

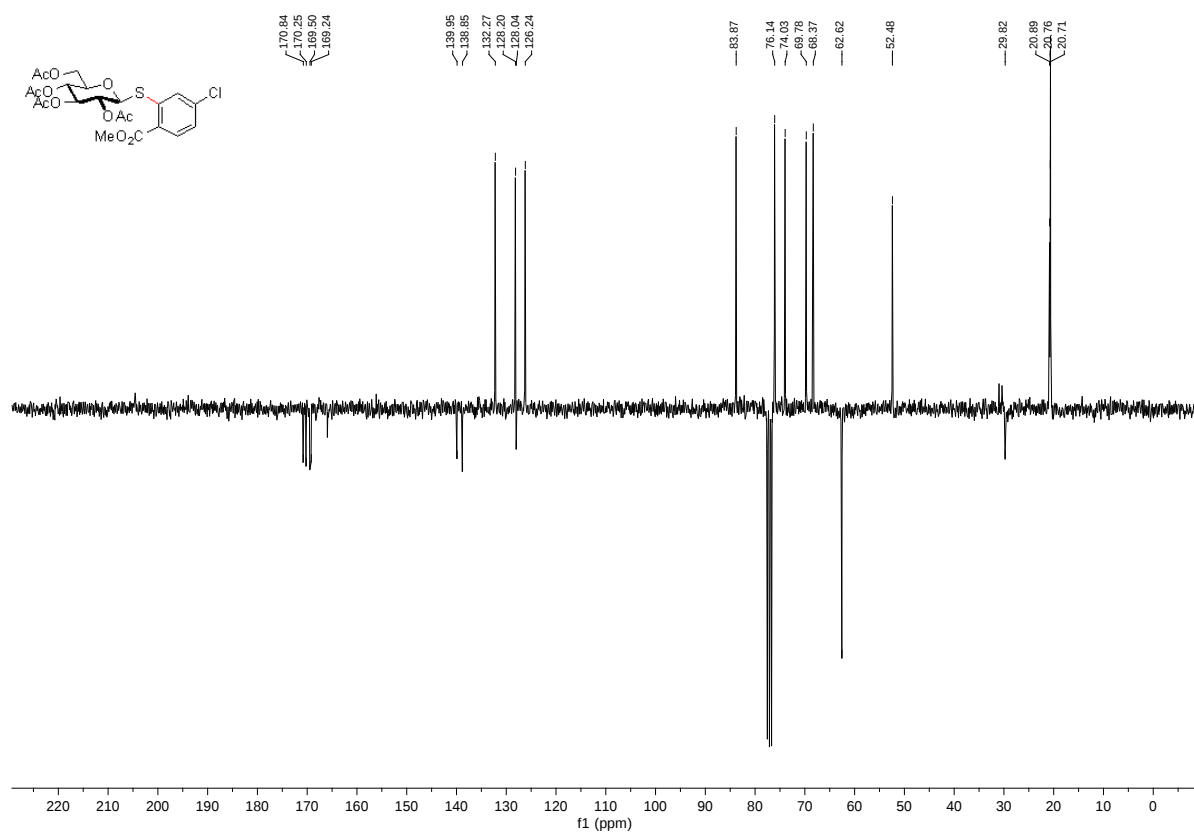
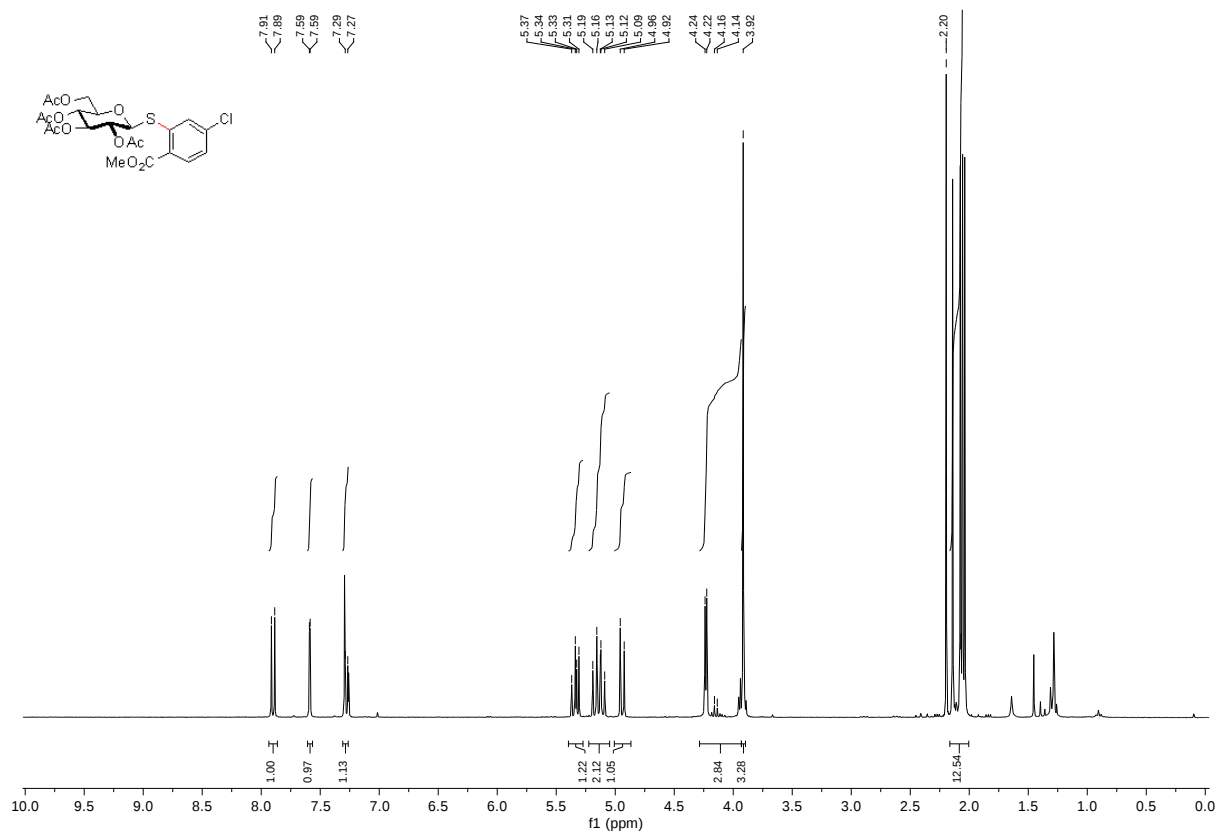
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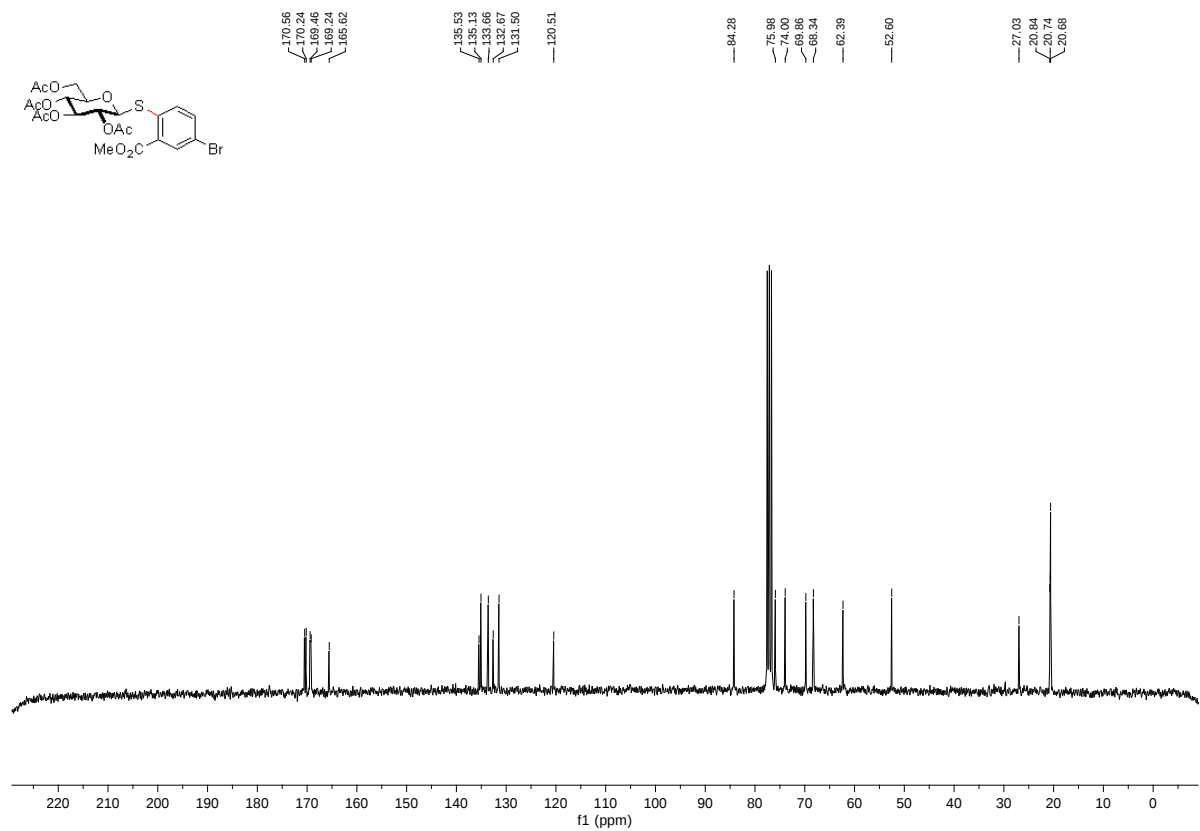
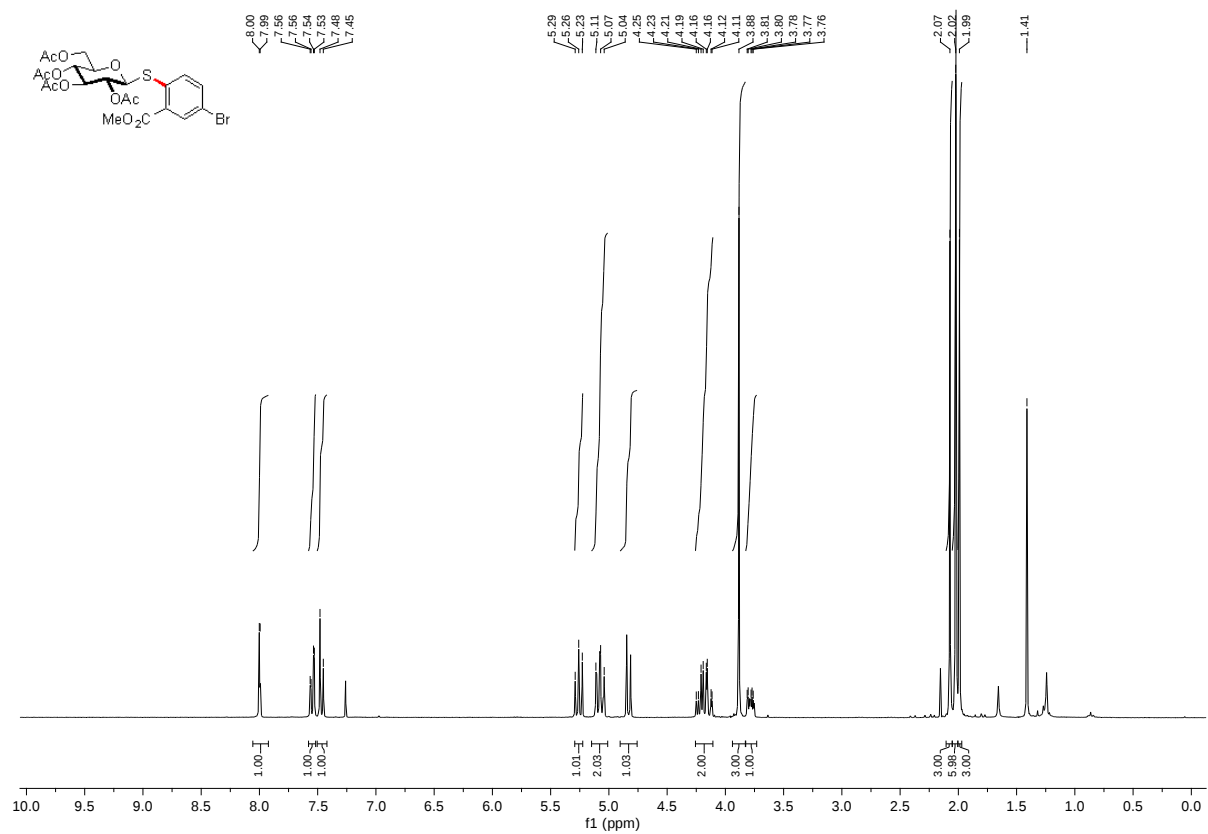
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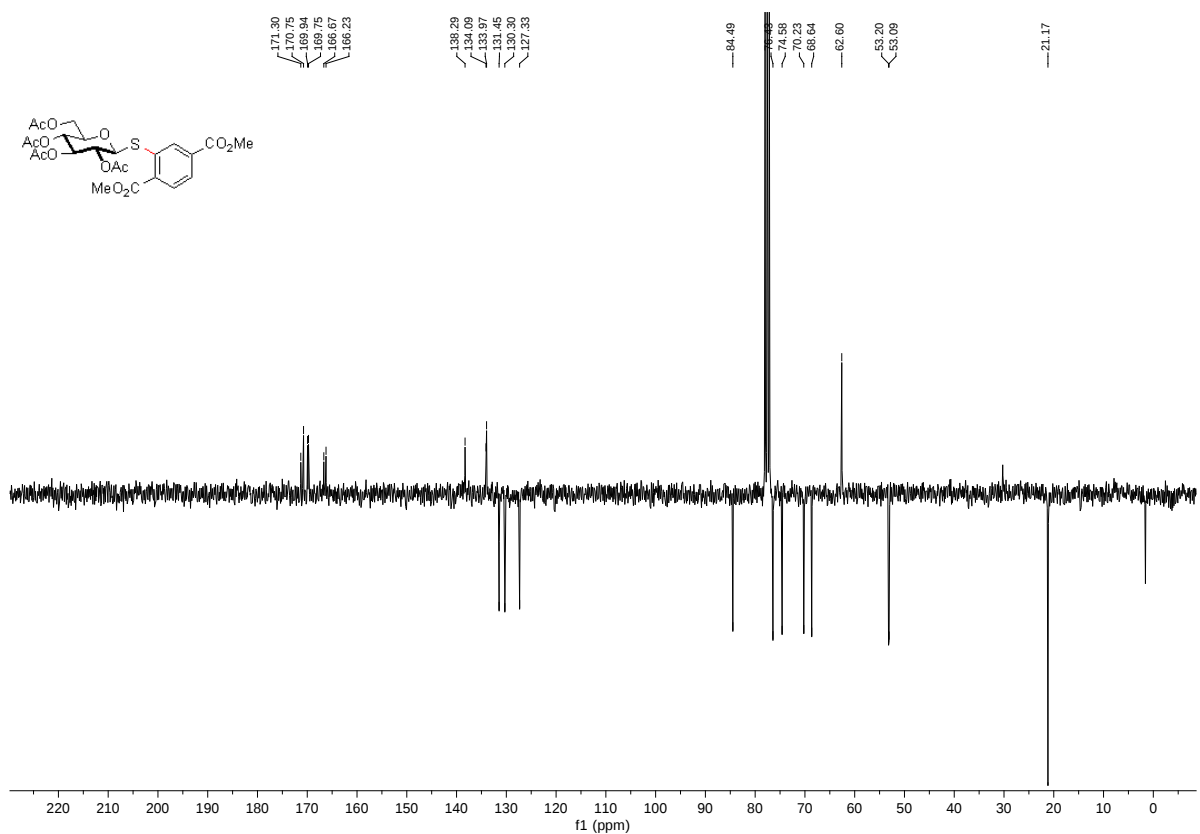
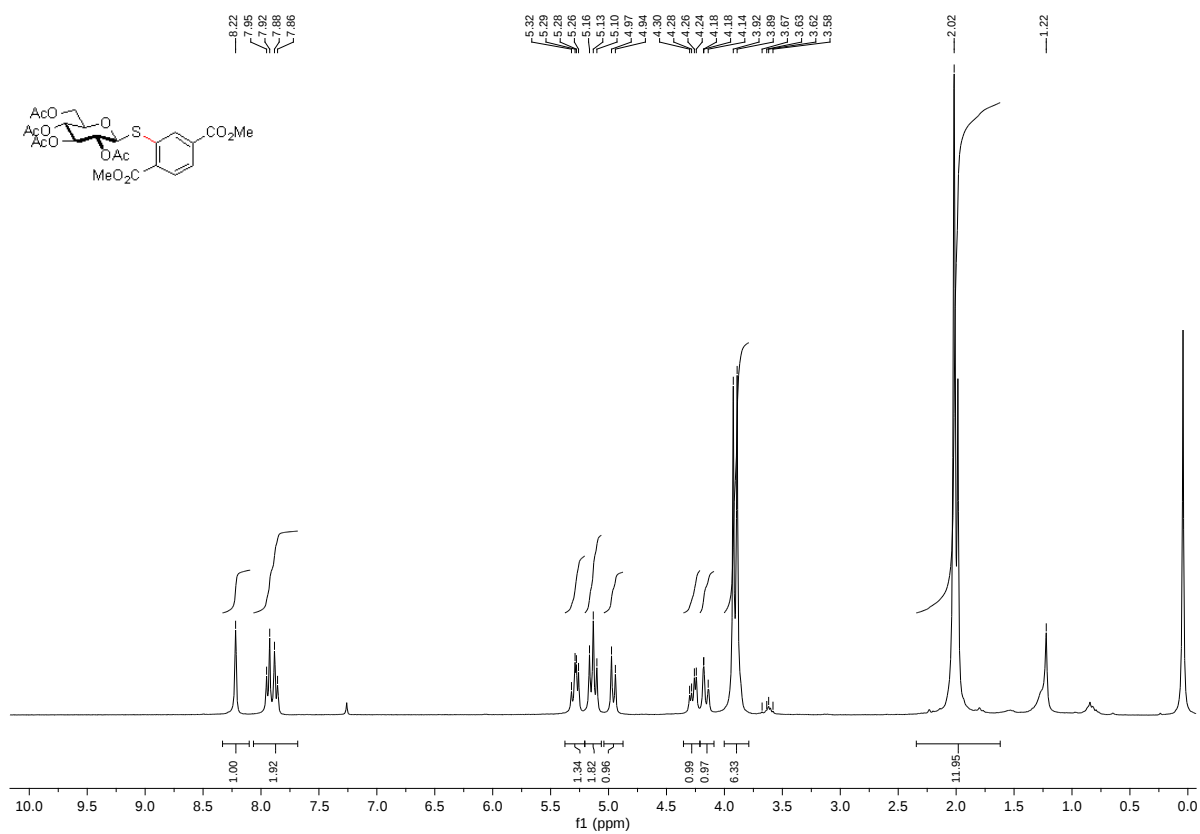


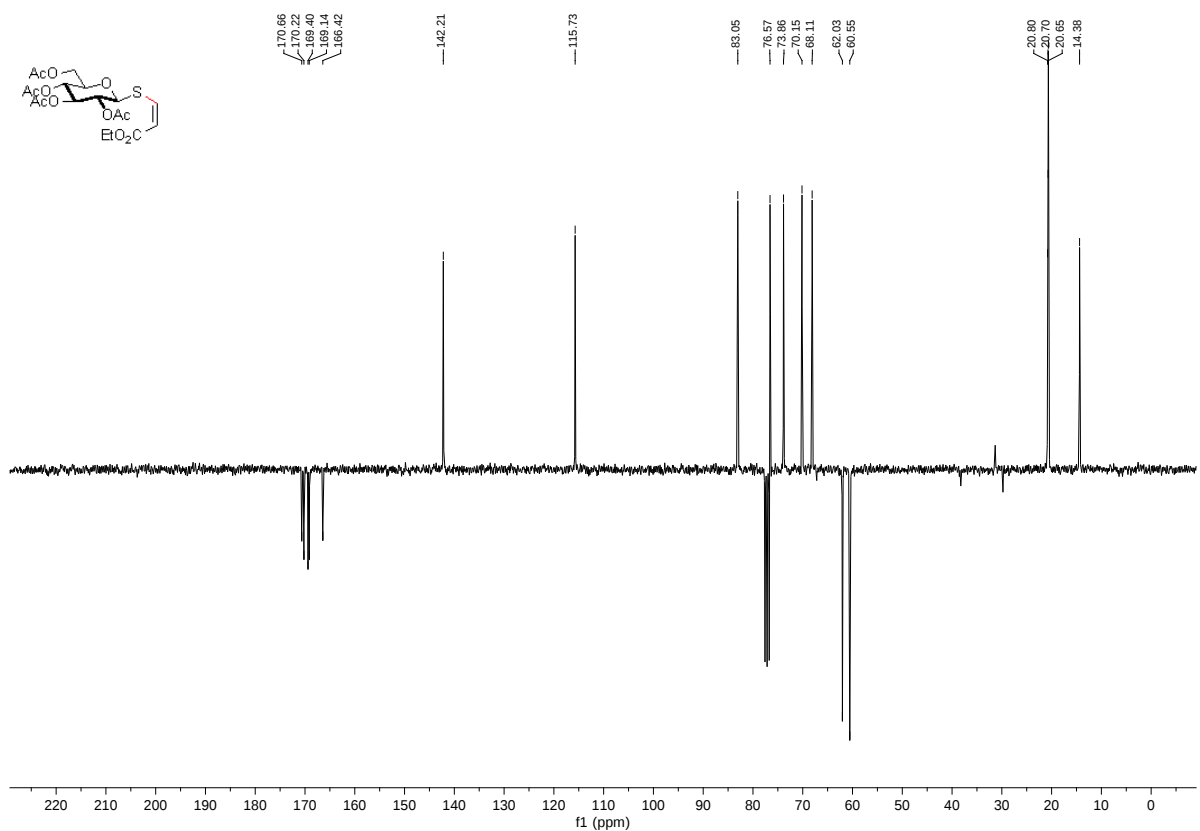
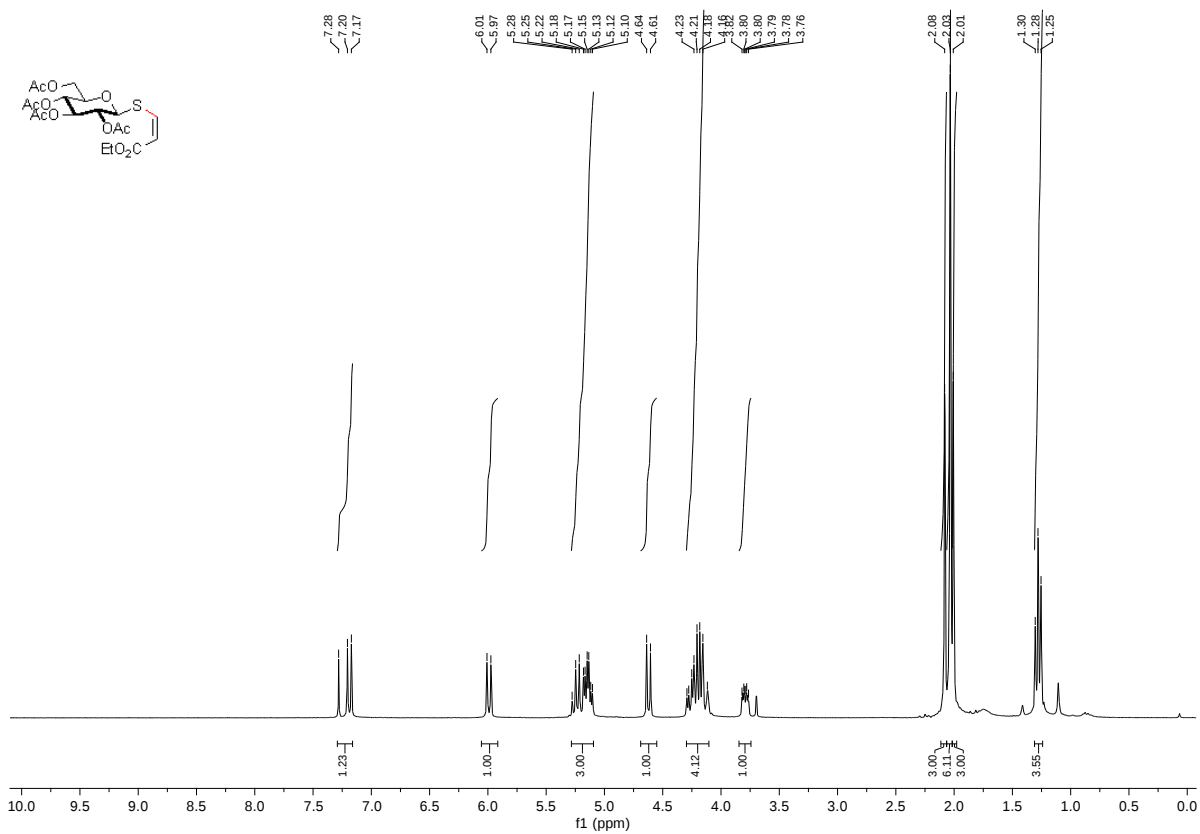


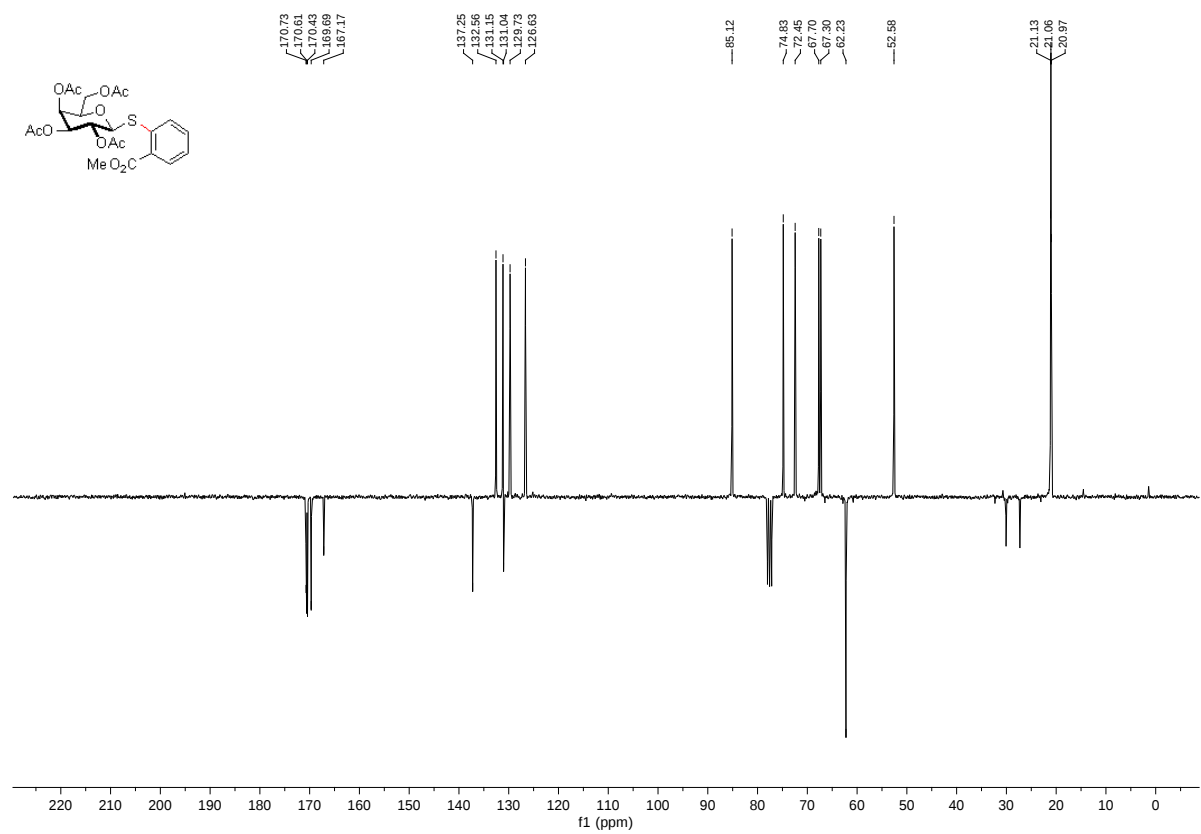
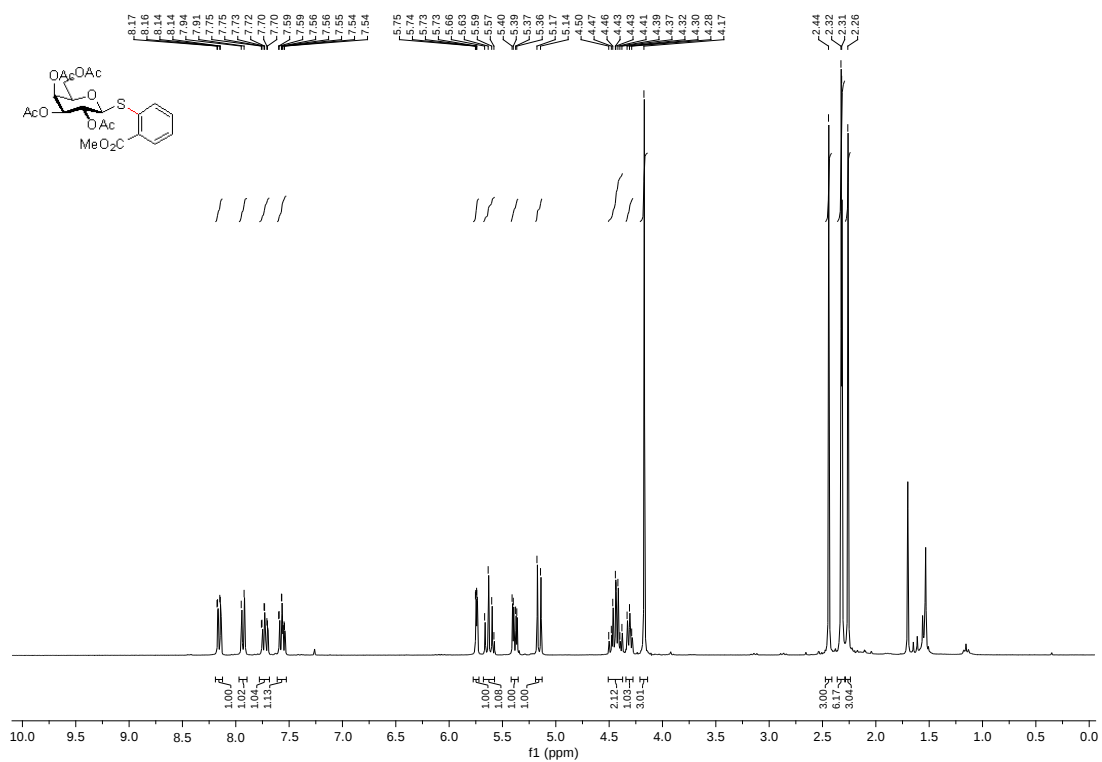


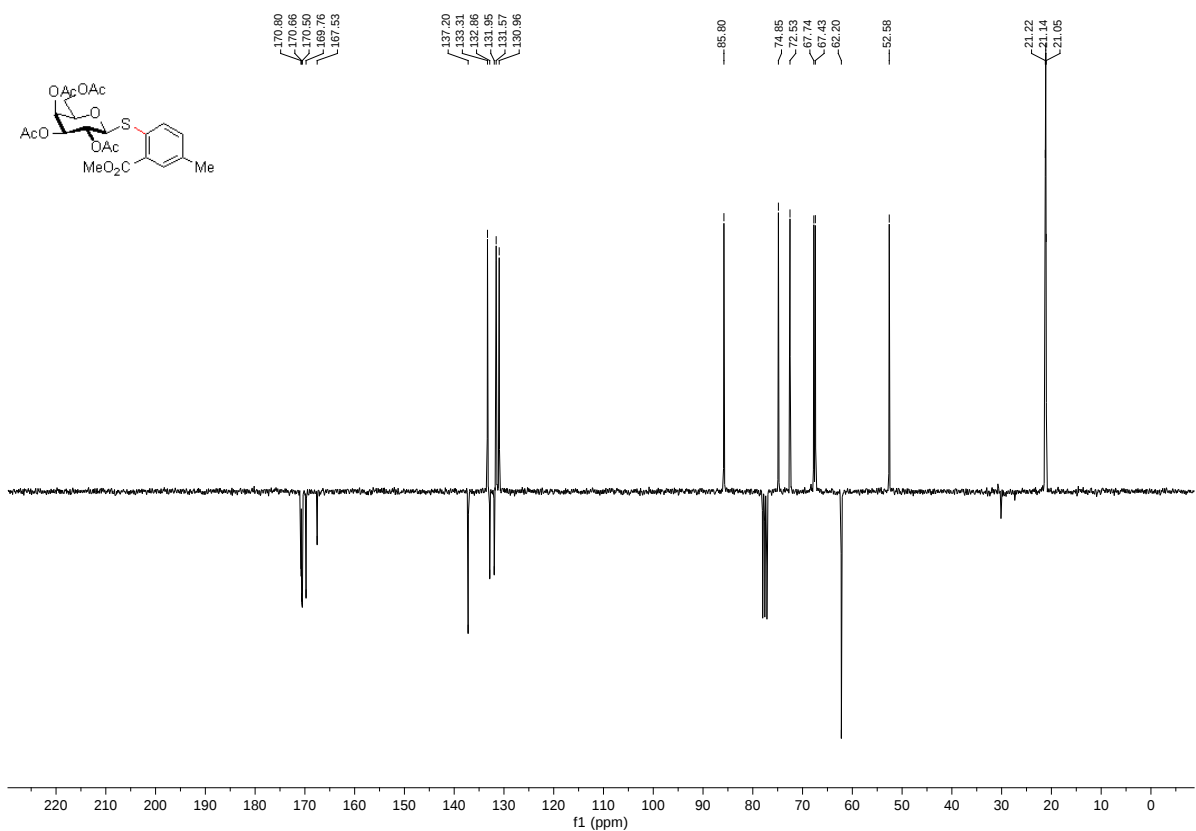
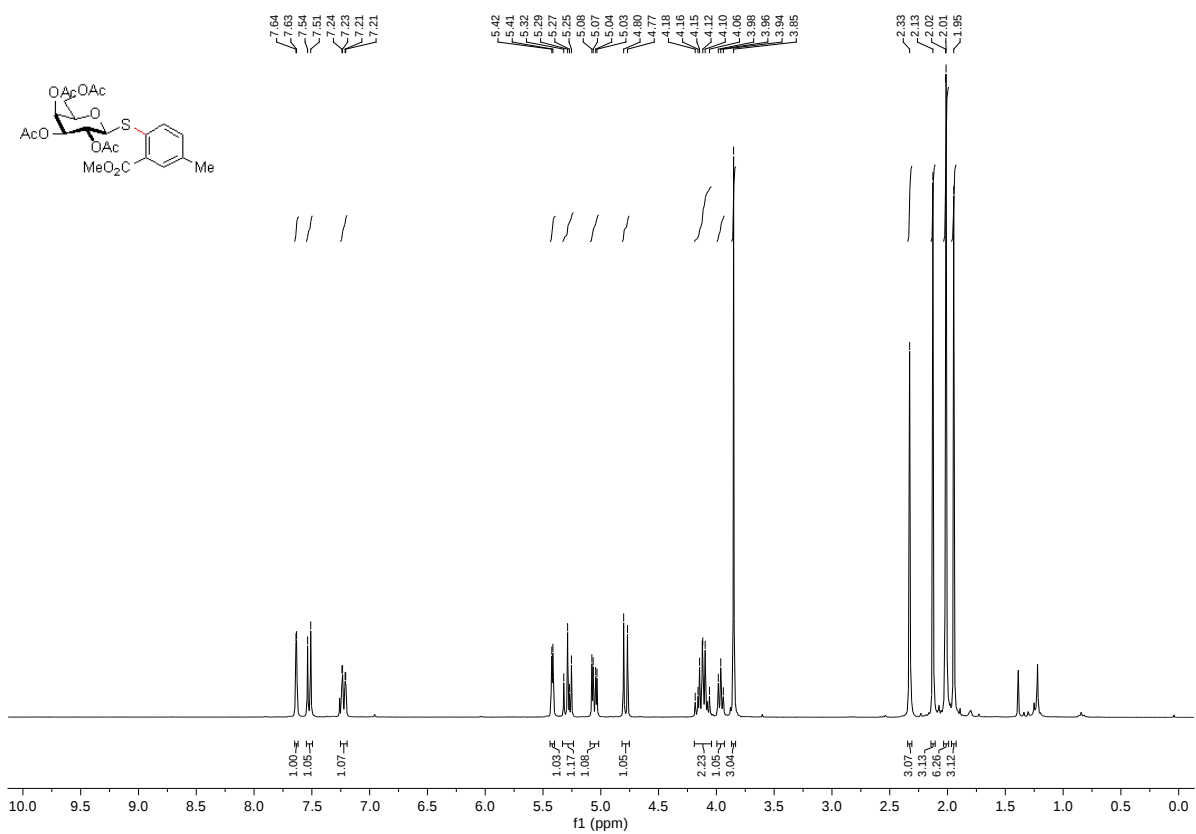


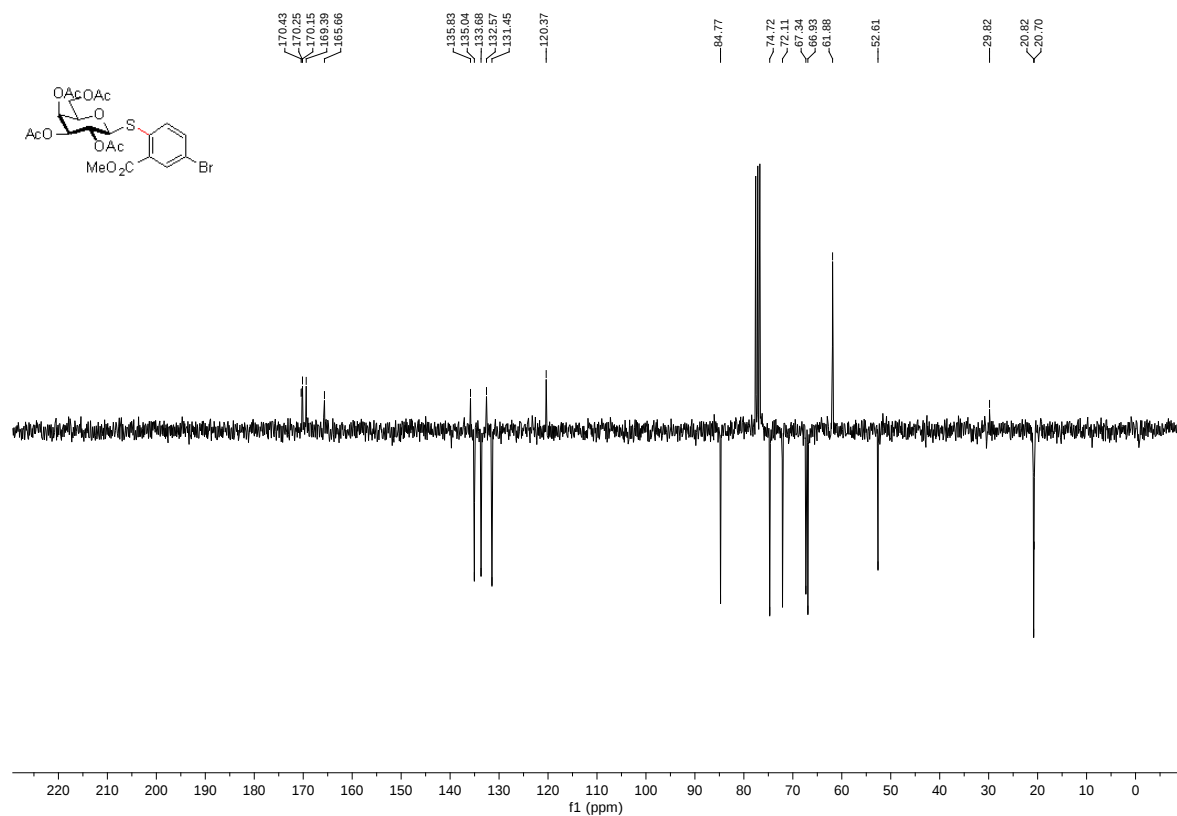
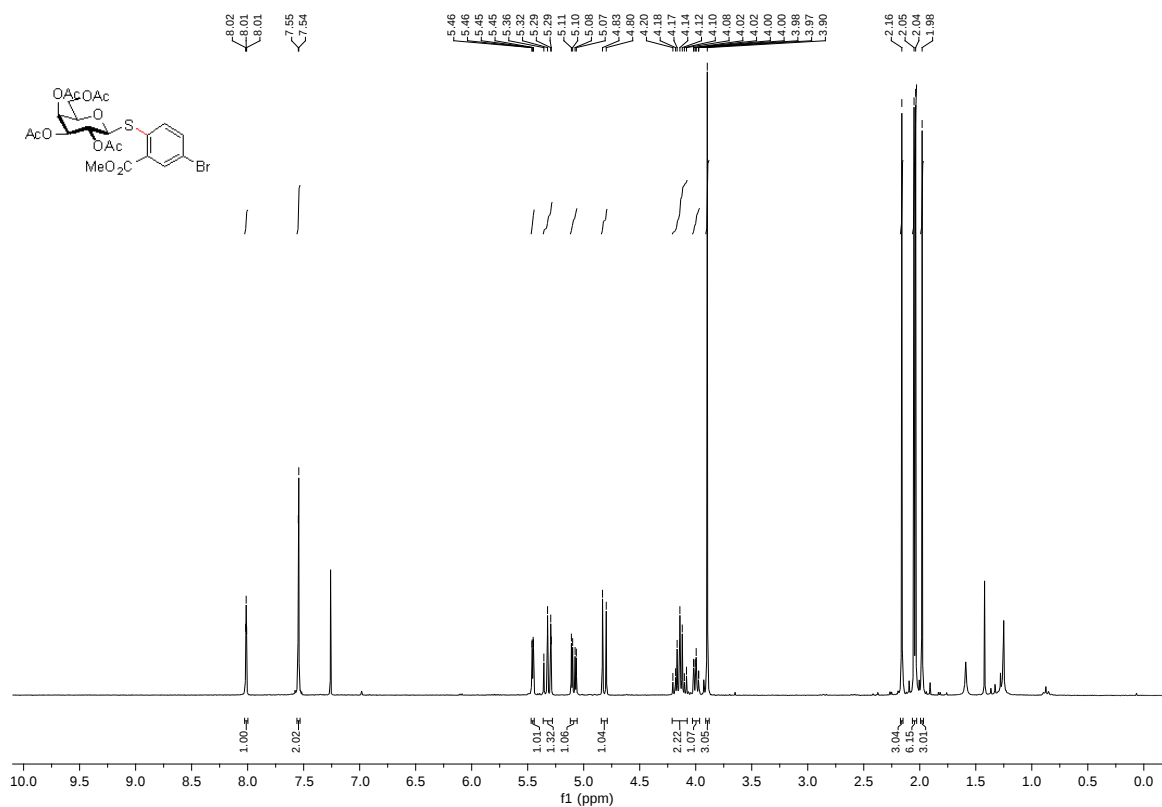


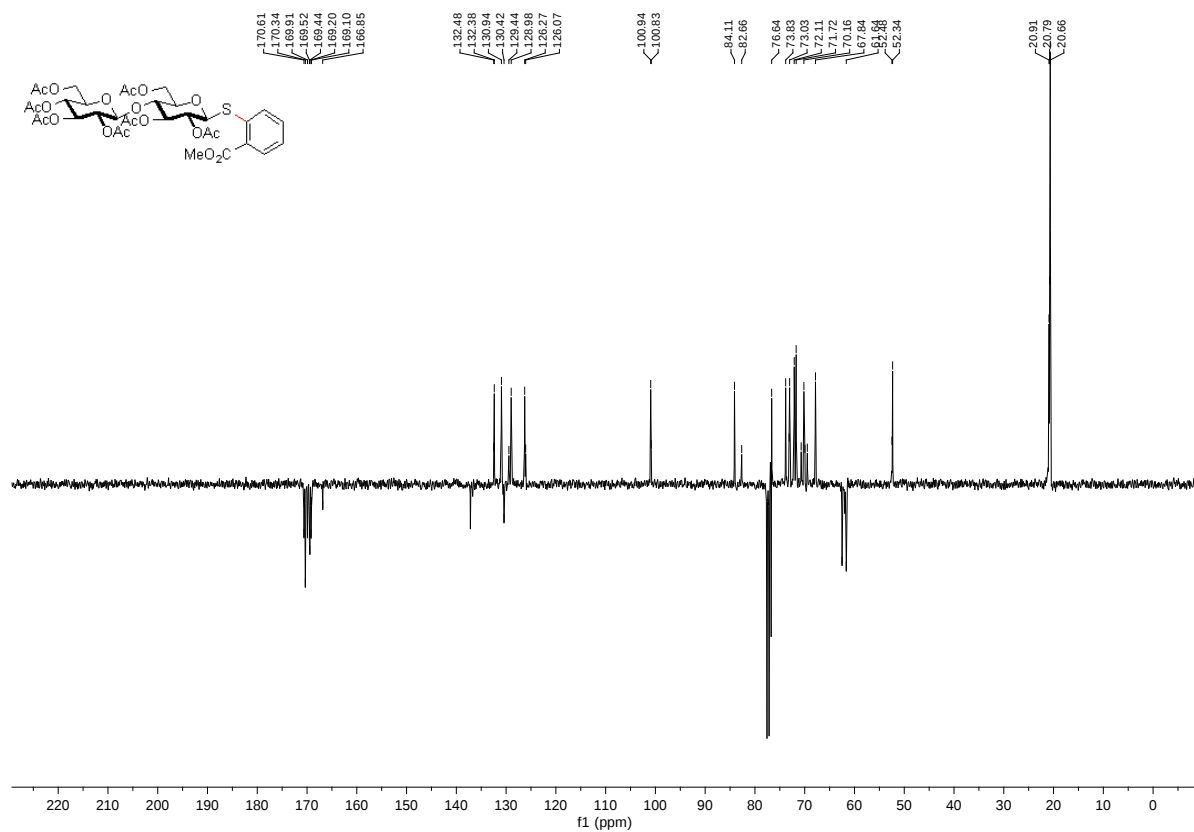
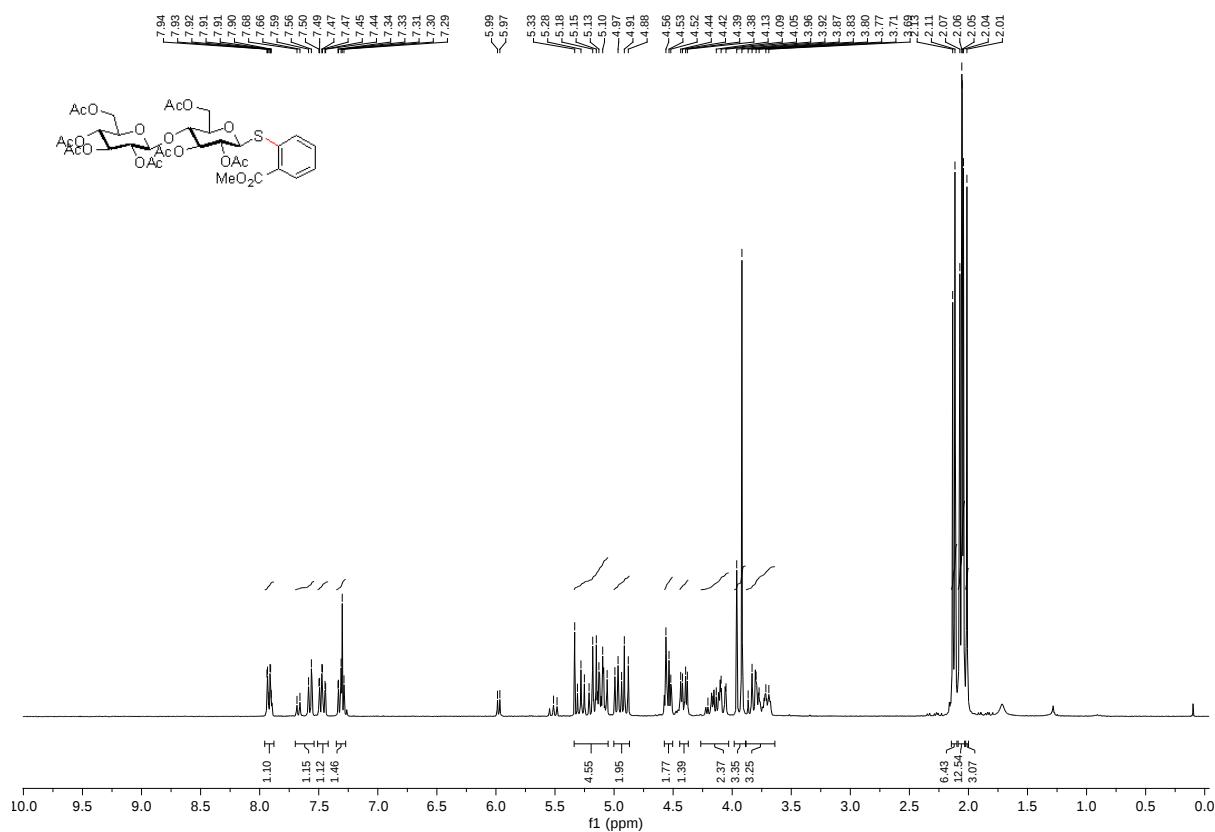


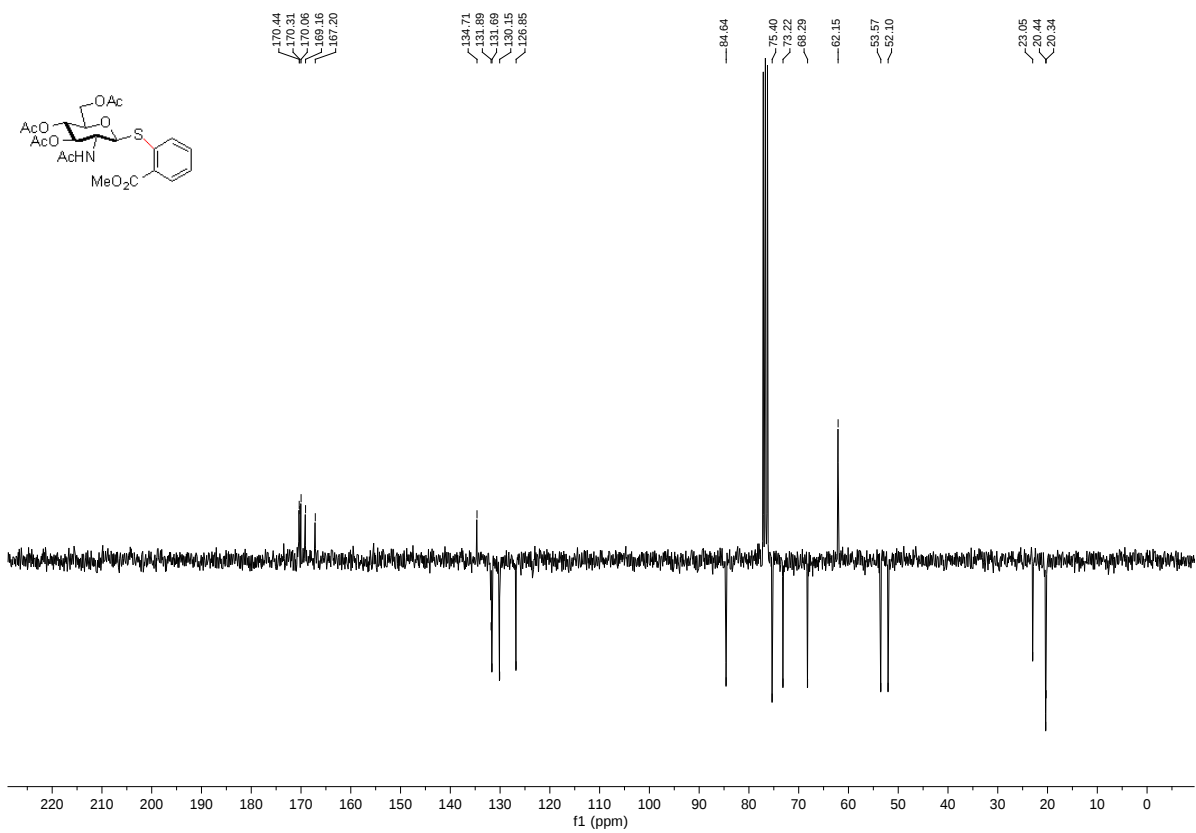
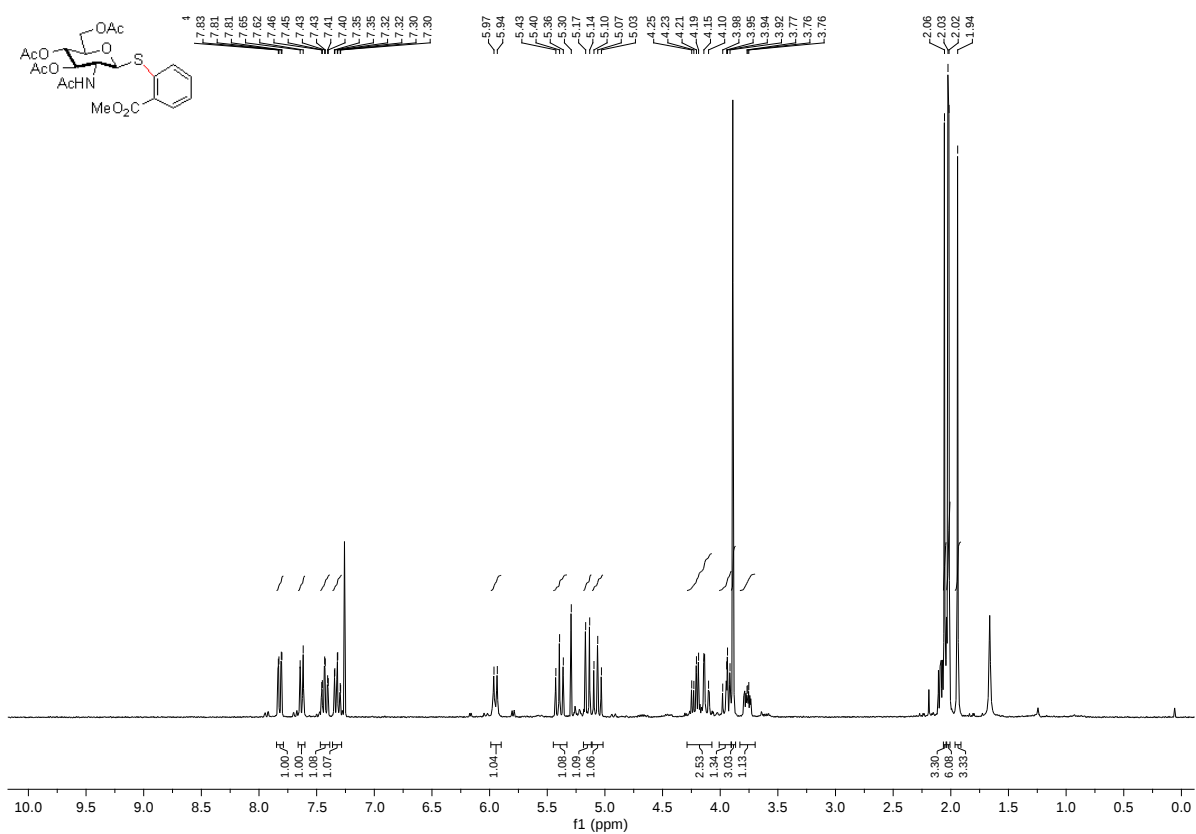


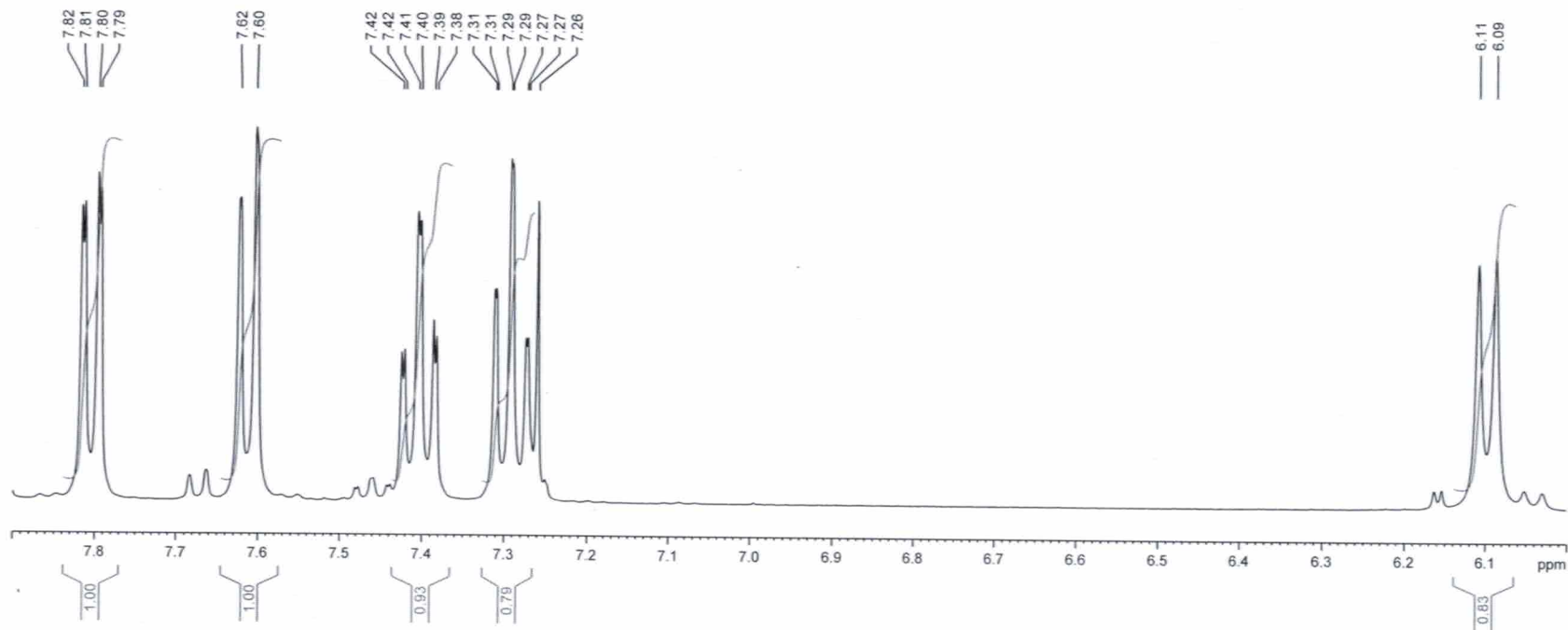






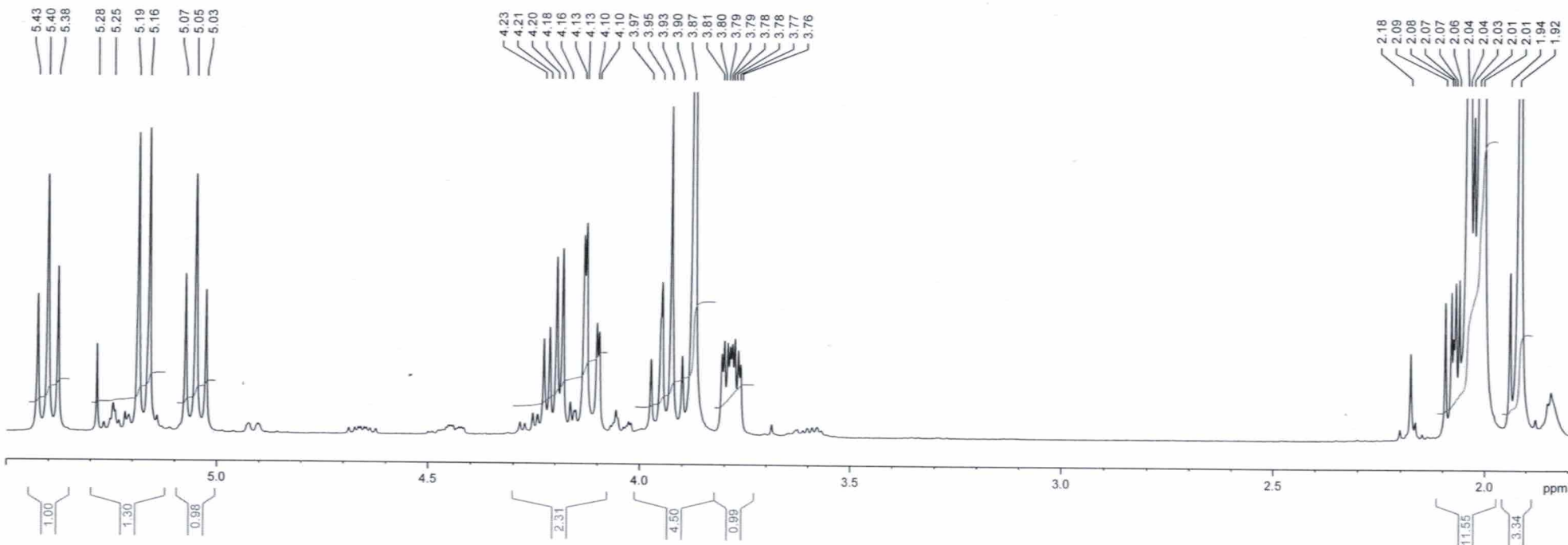


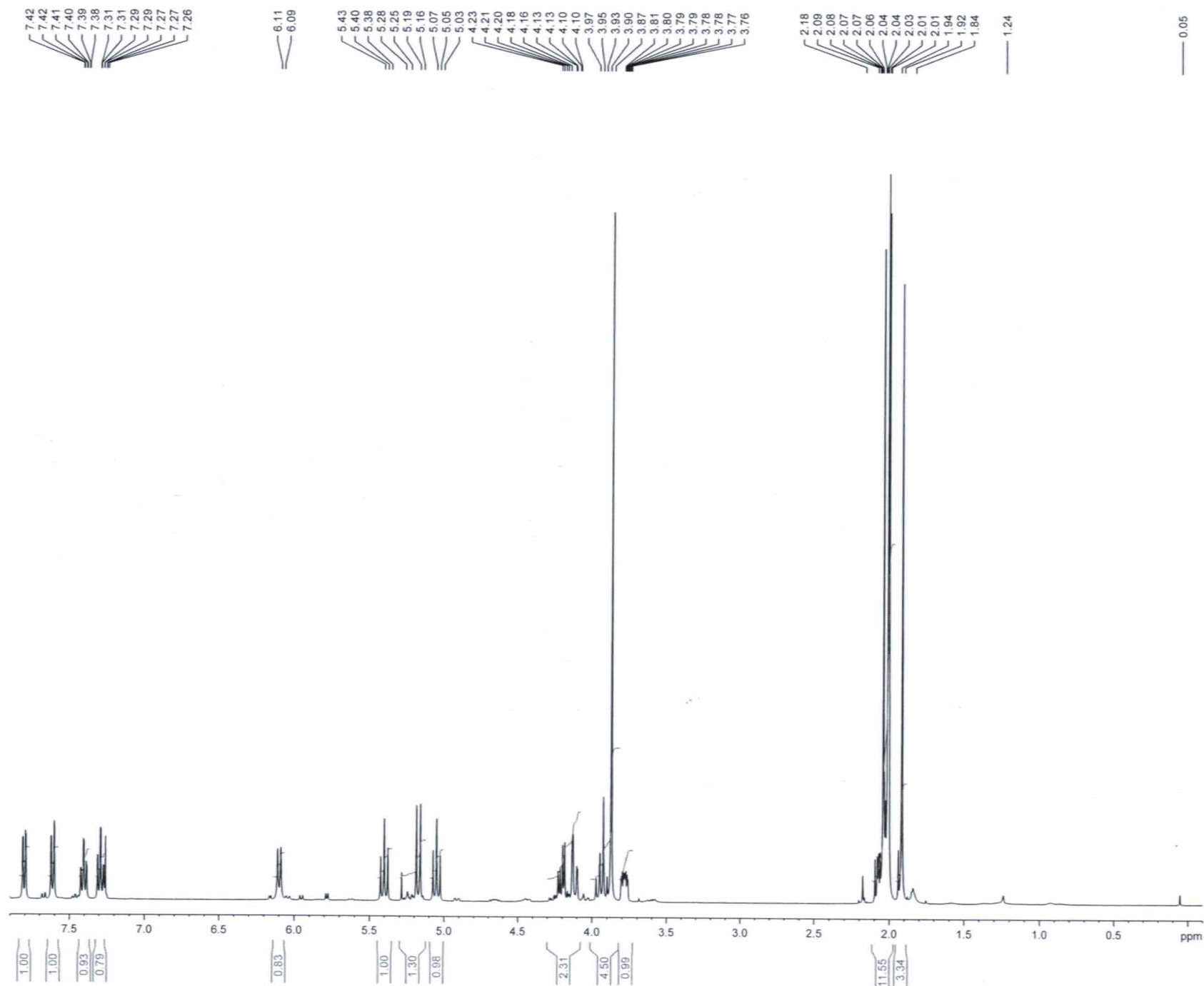




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 EXPNO 10
 PROCNO 1
 Date_ 20141205
 Time_ 16.05
 INSTRUM spect
 PROBHD 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8250.825 Hz
 FIDRES 0.125898 Hz
 AQ 3.9715922 sec
 RG 64
 DW 60.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 5.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.82 usec
 PL1 0.00 dB
 SFO1 400.1336012 MHz
 SI 32768
 SF 400.1300172 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





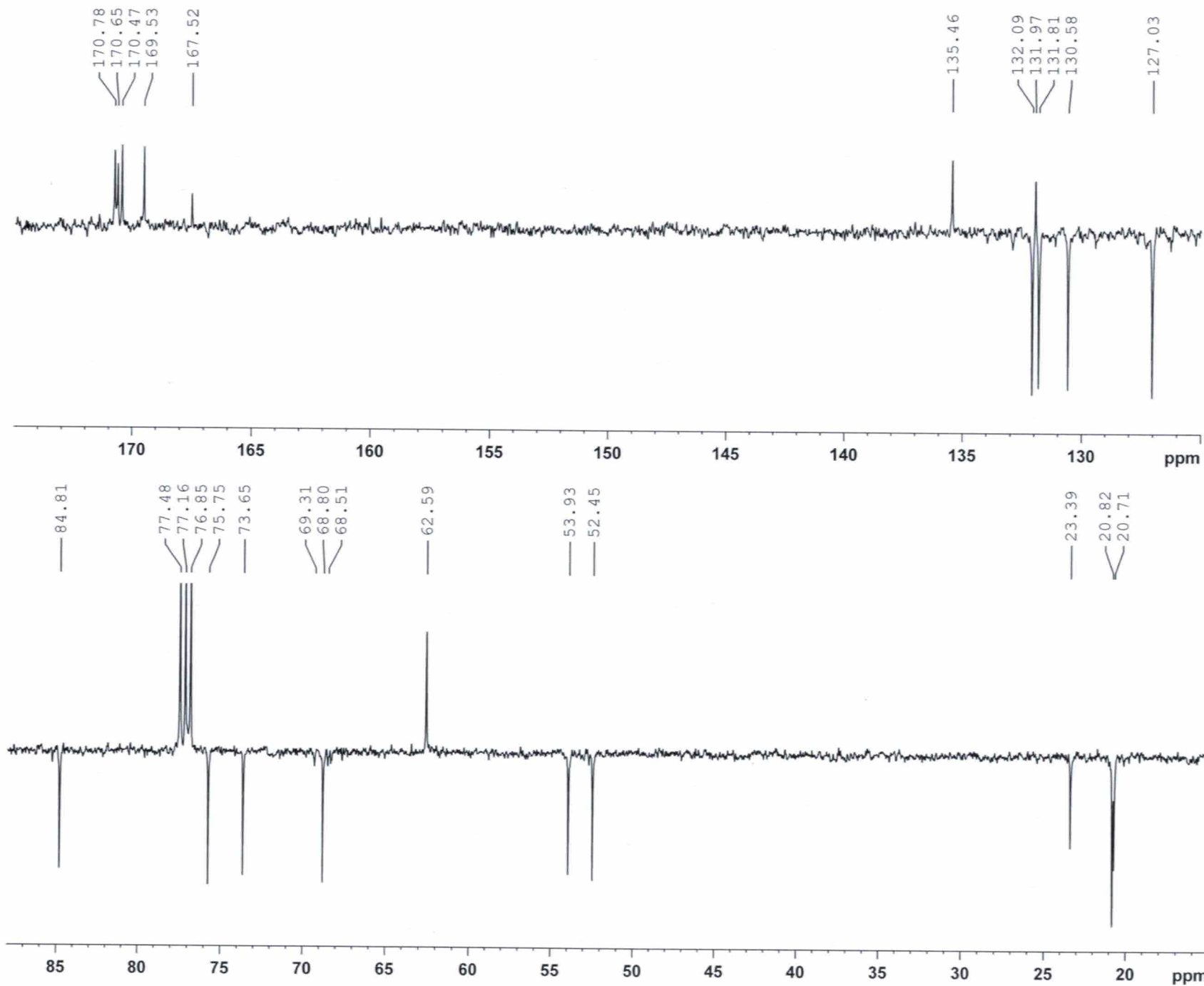
R0151 beta Proton

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NAME          ral151b
EXPNO         10
PROCNO        1
Date_         20141205
Time_         16.05
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8250.825 Hz
FIDRES        0.125898 Hz
AQ            3.9715922 sec
RG            64
DW            60.600 usec
DE            6.50 usec
TE            300.0 K
D1            5.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1           1H
P1             6.82 usec
PL1            0.00 dB
SFO1          400.1336012 MHz
SI            32768
SF            400.1300172 MHz
WDW            EM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
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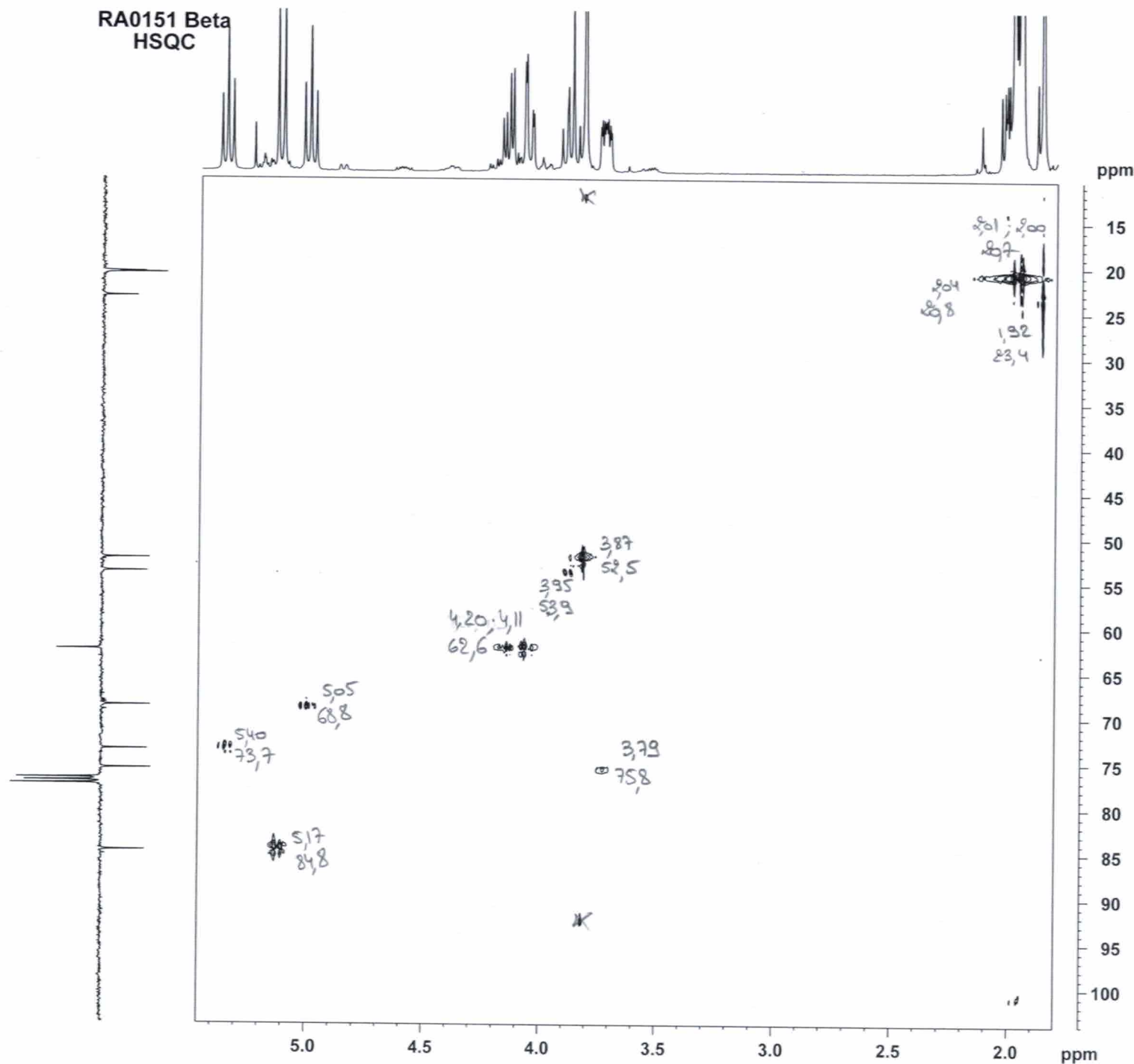
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PROCNO 1
Date_ 20141208
Time 13.03
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG jmod
TD 65536
SOLVENT CDCl3
NS 2000
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156492 sec
RG 14596.5
DW 21.600 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 5.0000000 sec
D20 0.00689655 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 0.00 dB
SFO1 100.6233333 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 23.32 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127593 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

RA0151 Beta
HSQC



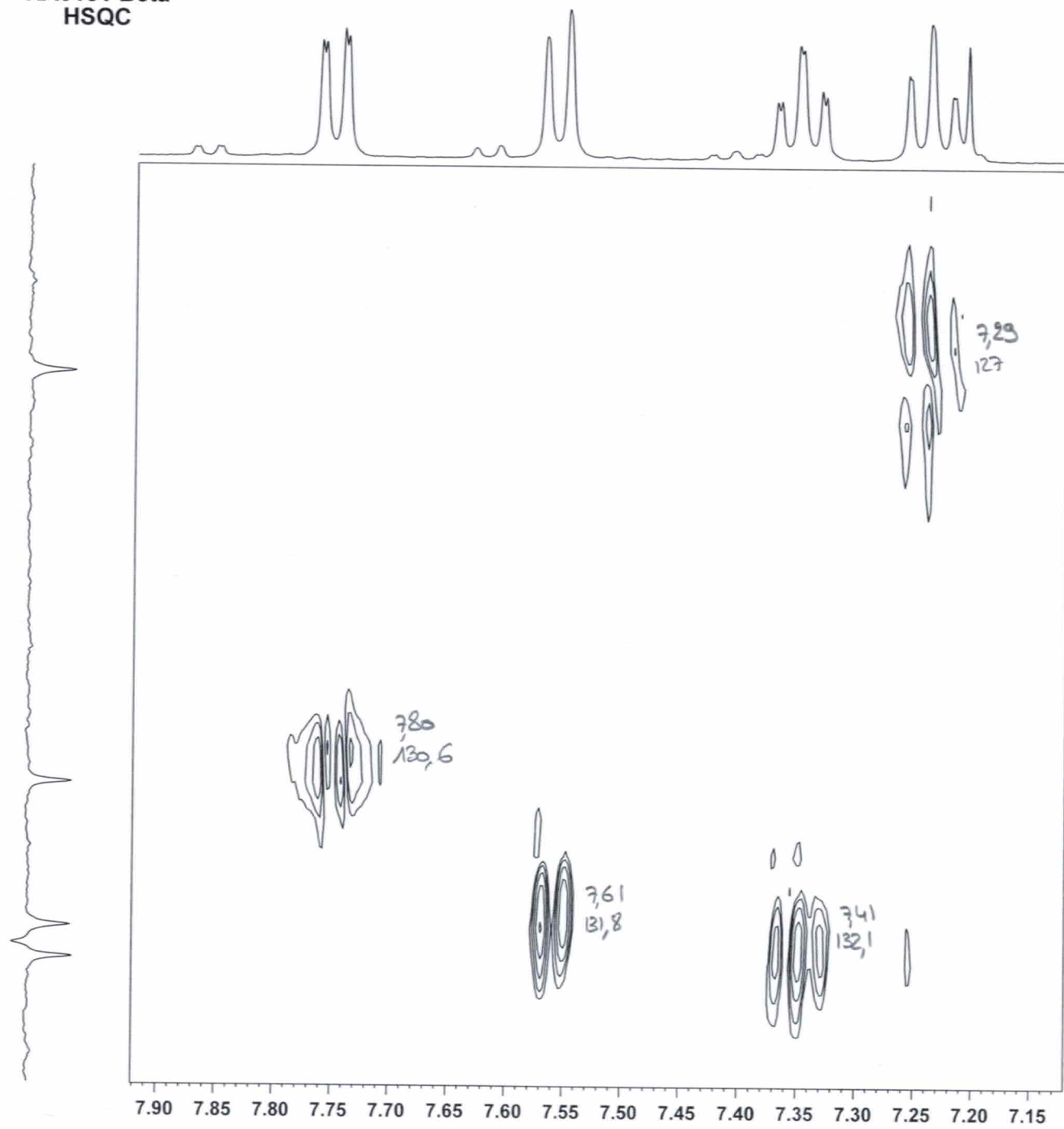
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PROCNO 1
Date_ 20141205
Time_ 16.52
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hsqcetgpsi
TD 4096
SOLVENT CDC13
NS 2
DS 4
SWH 3280.840 Hz
FIDRES 0.800986 Hz
AQ 0.6244328 sec
RG 9195.2
DW 152.400 usec
DE 6.50 usec
TE 300.0 K
CNST2 140.0000000
D0 0.00000300 sec
D1 0.95248401 sec
D4 0.00178571 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00089000 sec
INO 0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
P28 1000.00 usec
PL1 0.00 dB
SFO1 400.1317813 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 11.00 usec
P4 22.00 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
SFO2 100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6203 MHz
FIDRES 62.887669 Hz
SW 160.000 ppm
FnMODE Echo-Antiecho
SI 4096
SF 400.1300385 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6127593 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

RA0151 Beta
HSQC



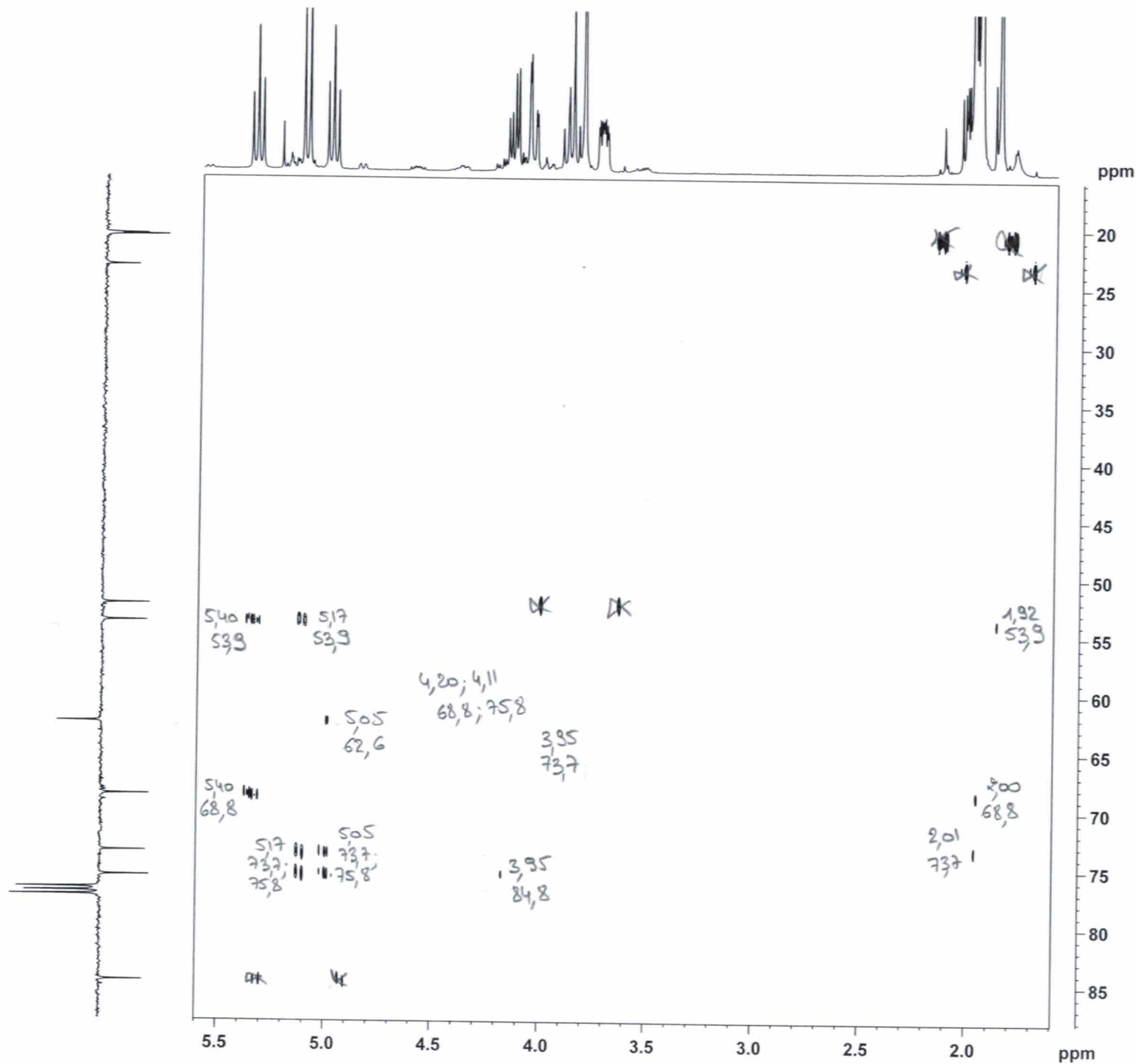
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EXPNO 22
PROCNO 1
Date_ 20141205
Time 16.52
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hsqcetgpsi
TD 4096
SOLVENT CDCl3
NS 2
DS 4
SWH 3280.840 Hz
FIDRES 0.800986 Hz
AQ 0.6244328 sec
RG 9195.2
DW 152.400 usec
DE 6.50 usec
TE 300.0 K
CNST2 140.0000000
D0 0.00000300 sec
D1 0.95248401 sec
D4 0.00178571 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
P28 1000.00 usec
PL1 0.00 dB
SFO1 400.1317813 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 11.00 usec
P4 22.00 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
SFO2 100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6203 MHz
FIDRES 62.887669 Hz
SW 160.000 ppm
FnMODE Echo-Antiecho
SI 4096
SF 400.1300385 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6127593 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

RA0151 Beta HMBC



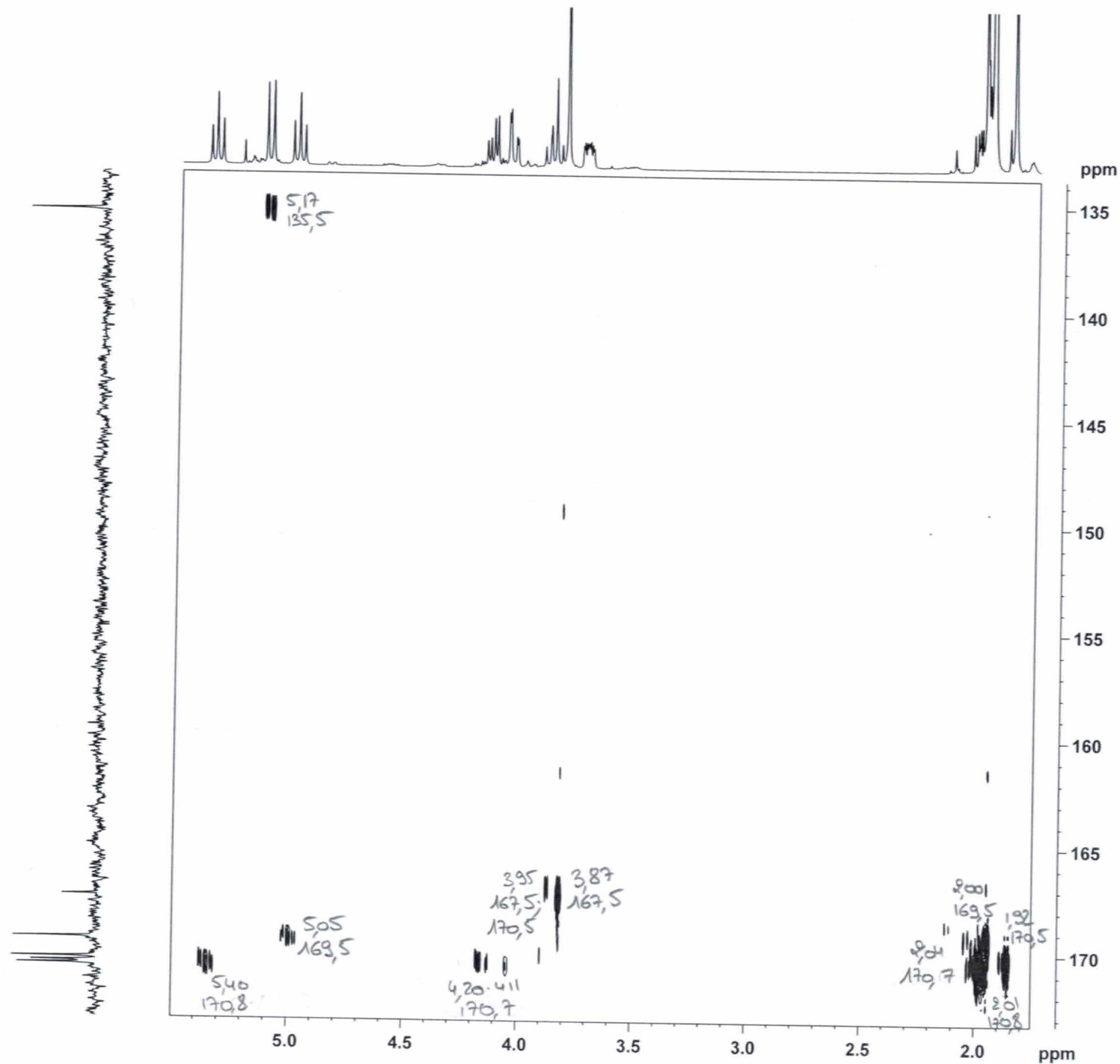
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EXPNO 83
PROCNO 1
Date 20141208
Time 8.49
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 4096
SOLVENT CDC13
NS 2
DS 4
SWH 3094.059 Hz
FIDRES 0.755386 Hz
AQ 0.6621252 sec
RG 11585.2
DW 161.600 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 0.93916899 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00002160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1318282 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6238 MHz
FIDRES 90.403236 Hz
SW 229.997 ppm
FnMODE QF
SI 4096
SF 400.1300385 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6127593 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

RA0151 Beta HMBC



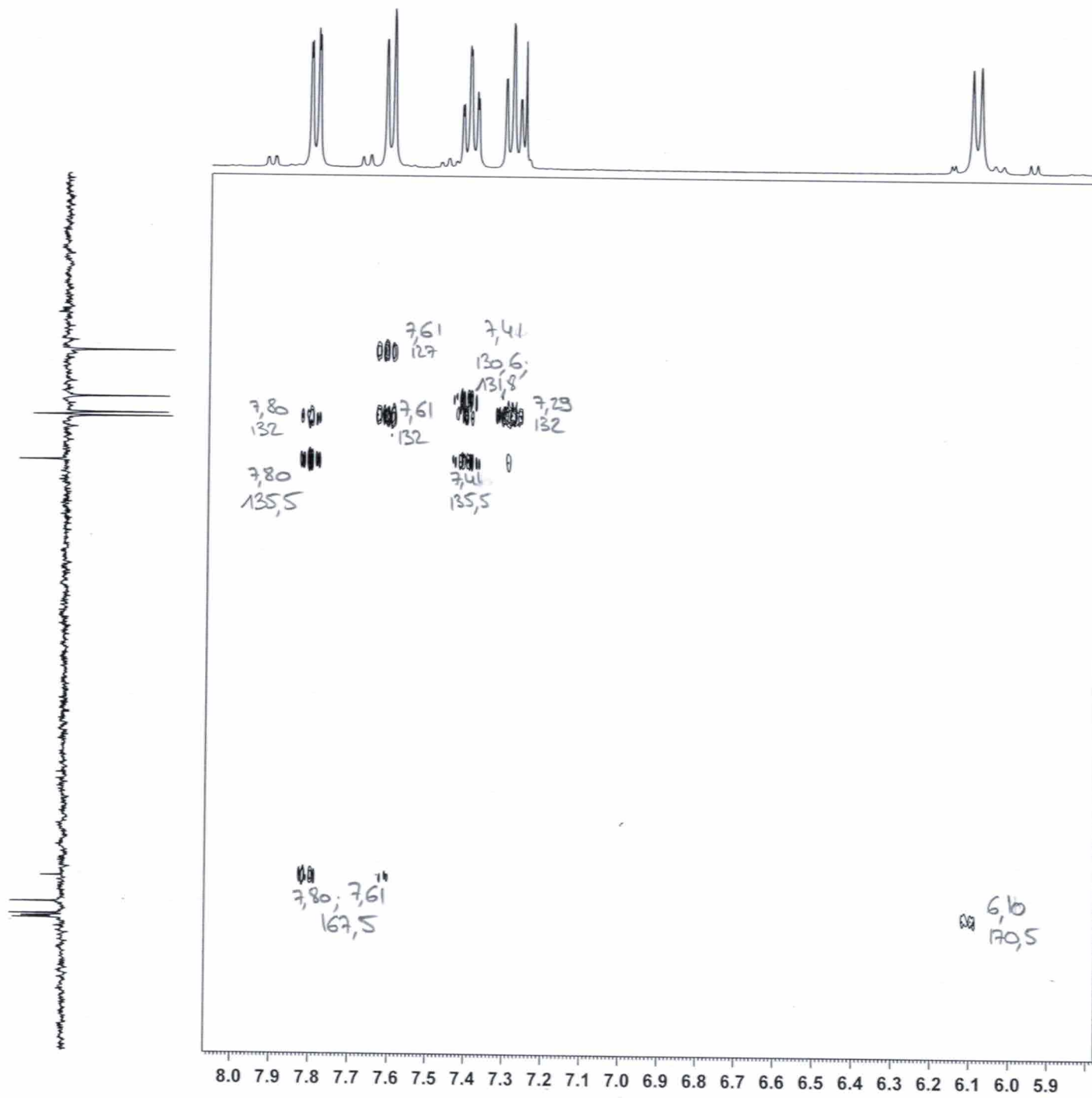
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EXPNO 83
PROCNO 1
Date_ 20141208
Time 8.49
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PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 4096
SOLVENT CDCl3
NS 2
DS 4
SWH 3094.059 Hz
FIDRES 0.755386 Hz
AQ 0.6621252 sec
RG 11585.2
DW 161.600 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 0.93916899 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002160 sec

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1318282 MHz

===== CHANNEL f2 =====
NUC2 ^{13}C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

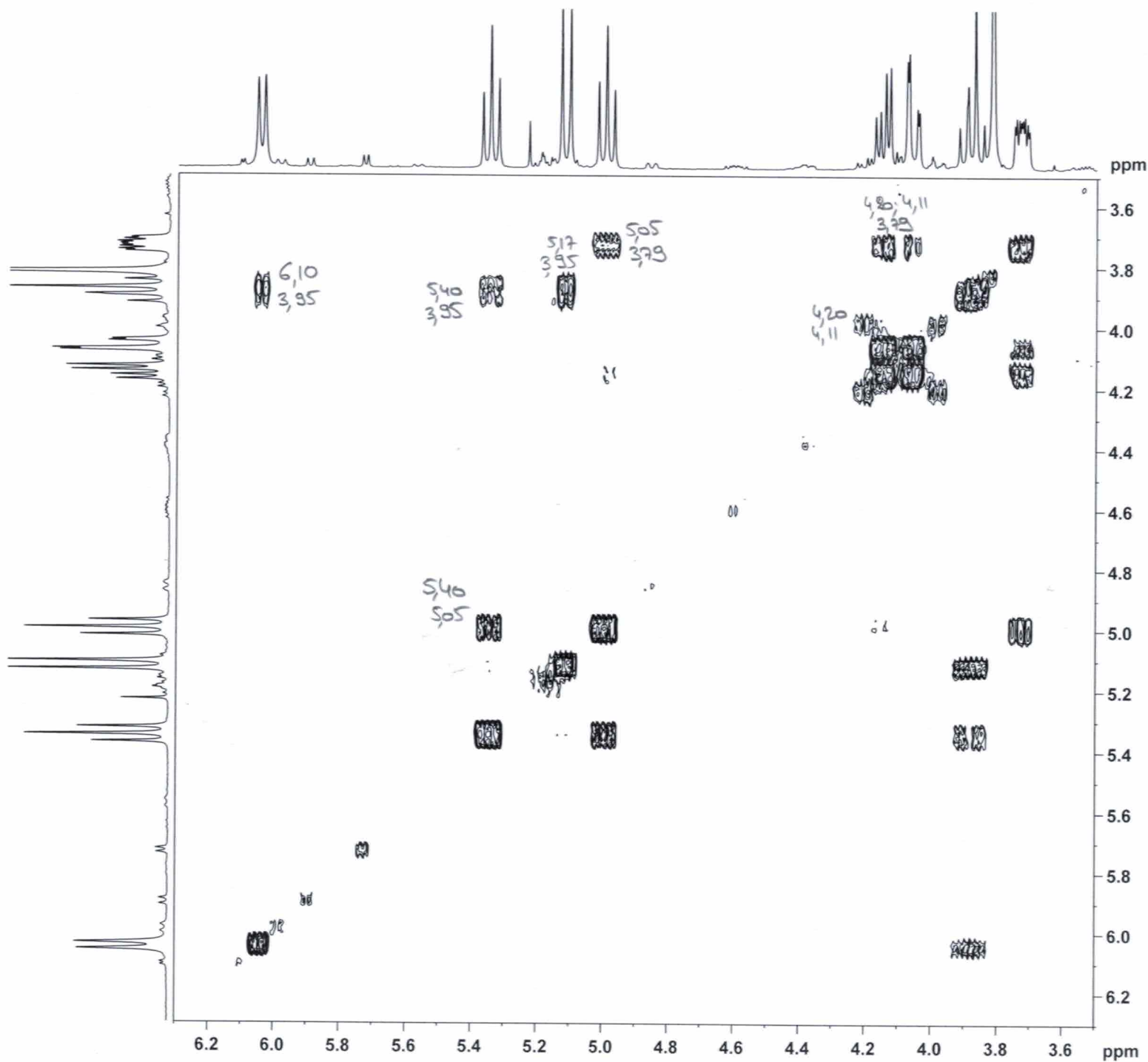
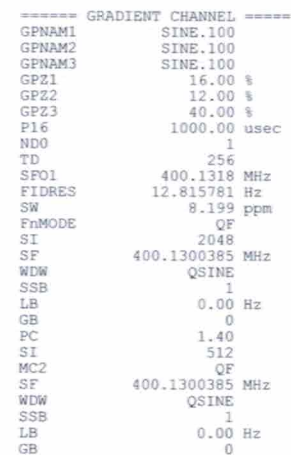
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6238 MHz
FIDRES 90.403236 Hz
SW 229.997 ppm
FnMODE QF
SI 4096
SF 400.1300385 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6127593 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

RA0151 Beta HMBC

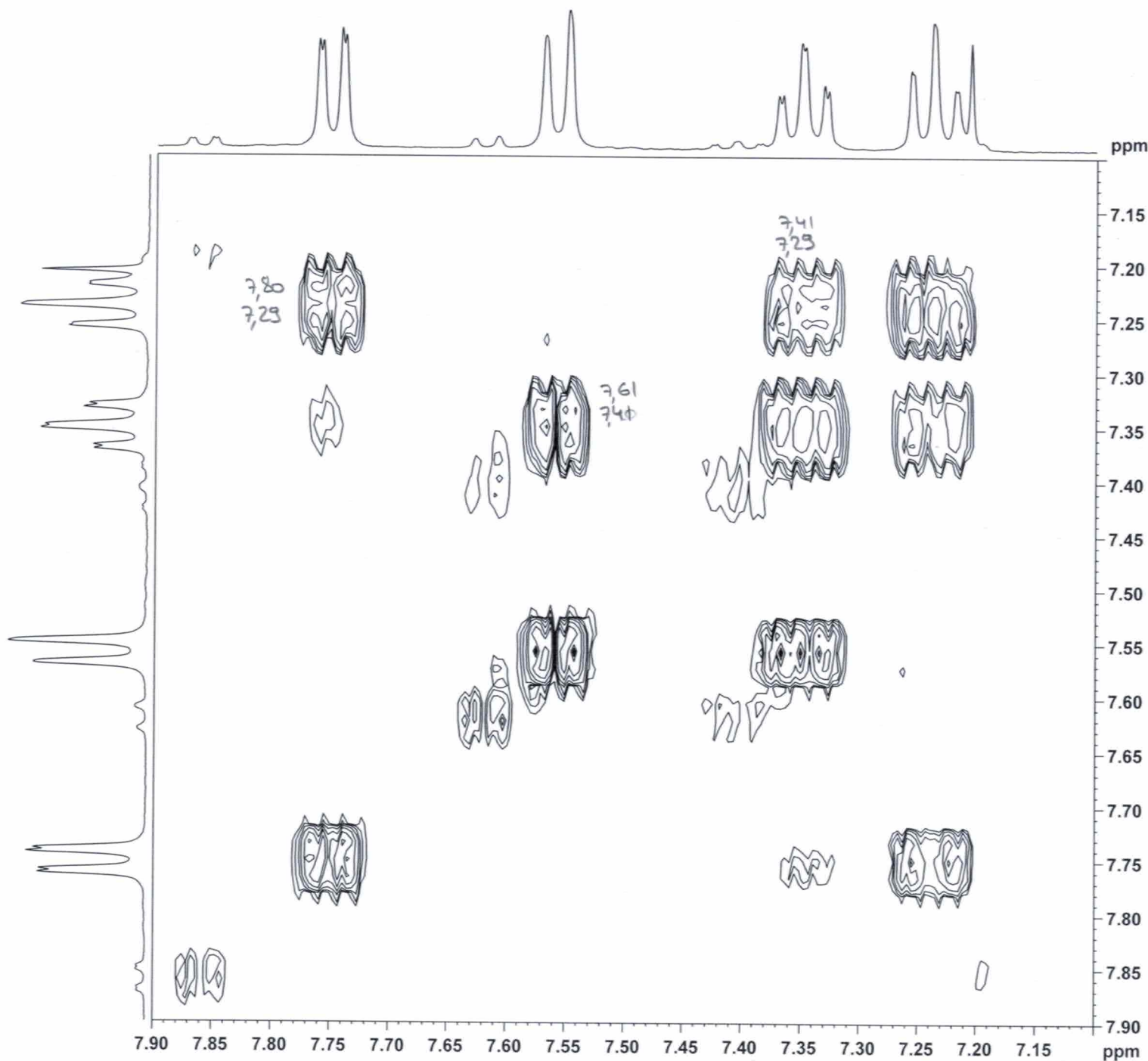


ppm	NAME	ra151b
115	EXPNO	83
	PROCNO	1
	Date_	20141208
	Time	8.49
	INSTRUM	spect
120	PROBHD	5 mm Multinucl
	PULPROG	hmbcpglpndqf
	TD	4096
	SOLVENT	CDCl3
	NS	2
	DS	4
125	SWH	3094.059 Hz
	FIDRES	0.755386 Hz
	AQ	0.6621252 sec
	RG	11585.2
	DW	161.600 usec
130	DE	6.50 usec
	TE	300.0 K
	CNST2	145.0000000
	CNST13	8.0000000
	D0	0.00000300 sec
135	D1	0.93916899 sec
	D2	0.00344828 sec
	D6	0.06250000 sec
	D16	0.00020000 sec
	IN0	0.00002160 sec
140	===== CHANNEL f1 =====	
	NUC1	1H
	P1	6.82 usec
	P2	13.65 usec
	PL1	0.00 dB
145	SFO1	400.1318282 MHz
	===== CHANNEL f2 =====	
	NUC2	13C
	P3	11.00 usec
150	PL2	0.00 dB
	SFO2	100.6238364 MHz
	===== GRADIENT CHANNEL =====	
155	GPNAME1	SINE.100
	GPNAME2	SINE.100
	GPNAME3	SINE.100
	GFZ1	50.00 %
	GFZ2	30.00 %
	GFZ3	40.10 %
160	P16	1000.00 usec
	ND0	2
	TD	256
	SFO1	100.6238 MHz
	FIDRES	90.403236 Hz
165	SW	229.997 ppm
	FnMODE	QF
	SI	4096
	SF	400.1300148 MHz
	WDW	SINE
170	SSB	0
	LB	0.00 Hz
	GB	0
	PC	1.40
	SI	1024
175	MC2	QF
	SF	100.6127593 MHz
	WDW	SINE
	SSB	0
180	LB	0.00 Hz
	GB	0

ppm



R0151 beta COSY



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NAME          ral51b
EXPNO         11
PROCNO        1
Date_         20141205
Time          16.05
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       cosygpmfqr
TD            2134
SOLVENT       CDC13
NS            1
DS            8
SWH           3280.840 Hz
FIDRES        1.537413 Hz
AQ            0.3254240 sec
RG            4096
DW            152.400 usec
DE            6.50 usec
TE            300.0 K
D0            0.00000300 sec
D1            0.97438931 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00030480 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
PL1           0.00 dB
SFO1          400.1317775 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPZ1          16.00 %
GPZ2          12.00 %
GPZ3          40.00 %
P16           1000.00 usec
ND0           1
TD            256
SFO1          400.1318 MHz
FIDRES        12.815781 Hz
SW            8.199 ppm
FnMODE        QF
SI            2048
SF            400.1300385 MHz
WDW           QSINE
SSB           1
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           QF
SF            400.1300385 MHz
WDW           QSINE
SSB           1
LB            0.00 Hz
GB            0
  
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[illegible]

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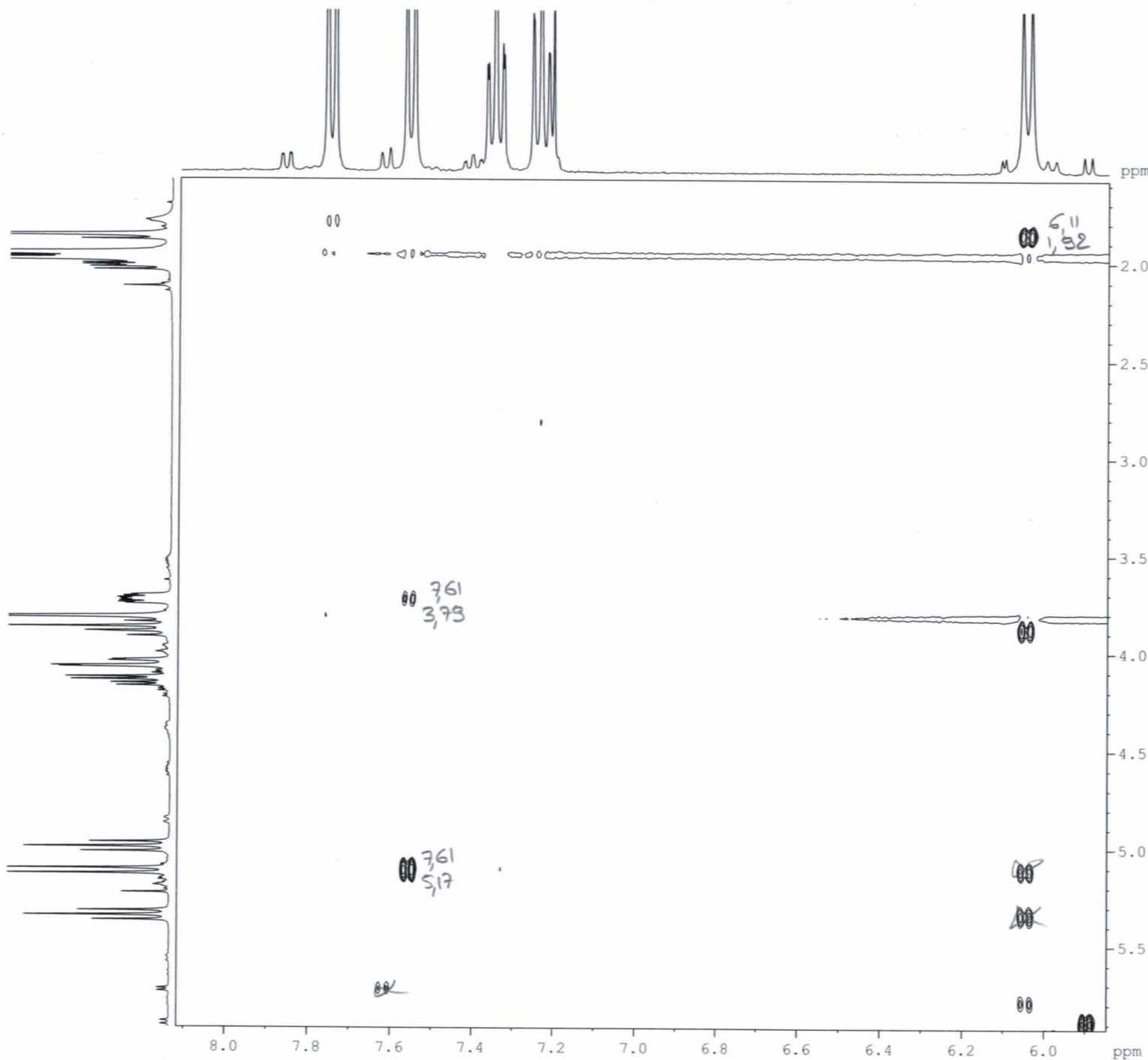
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PROCNO                              1
Date_                               20141208
Time_                               9.04
INSTRUM                            spect
PROBHD      5 mm Multinuc1
PULPROG                            noesypph
TD                                  2134
SOLVENT                            CDC13
NS                                  2
DS                                  16
SWH                                3094.059 Hz
FIDRES                            1.449887 Hz
AQ                                0.3450660 sec
RG                                  35.9
DW                                161.6000 usec
DE                                  6.50 usec
TE                                  300.0 K
D0                                  0.00015291 sec
D1                                  1.45603800 sec
D8                                  0.800000001 sec
D16                                0.000200000 sec
IN0                                0.00032320 sec

===== CHANNEL f1 =====
NUC1                                1H
P1                                  6.82 usec
P2                                  13.65 usec
PL1                                 0.00 dB
SFO1                                400.1318282 MHz

===== GRADIENT CHANNEL =====
GPNAM1                             SINE.100
GPZ1                                40.00 %
P16                                 1000.00 usec
ND0                                  1
TD                                  256
SFO1                                400.1318 MHz
FIDRES                            12.086169 Hz
SW                                  7.733 ppm
FNMODE                             States-TPPI
SI                                  2048
SF                                  400.1300385 MHz
WDW                                 QSINE
SSB                                 2
LB                                  0.00 Hz
GB                                  0
PC                                  1.40
SI                                  512
MC2                                States-TPPI
SF                                  400.1300385 MHz
WDW                                 QSINE
SSB                                 2
LB                                  0.00 Hz
GB                                  0

```

RA0151 Beta NOESY

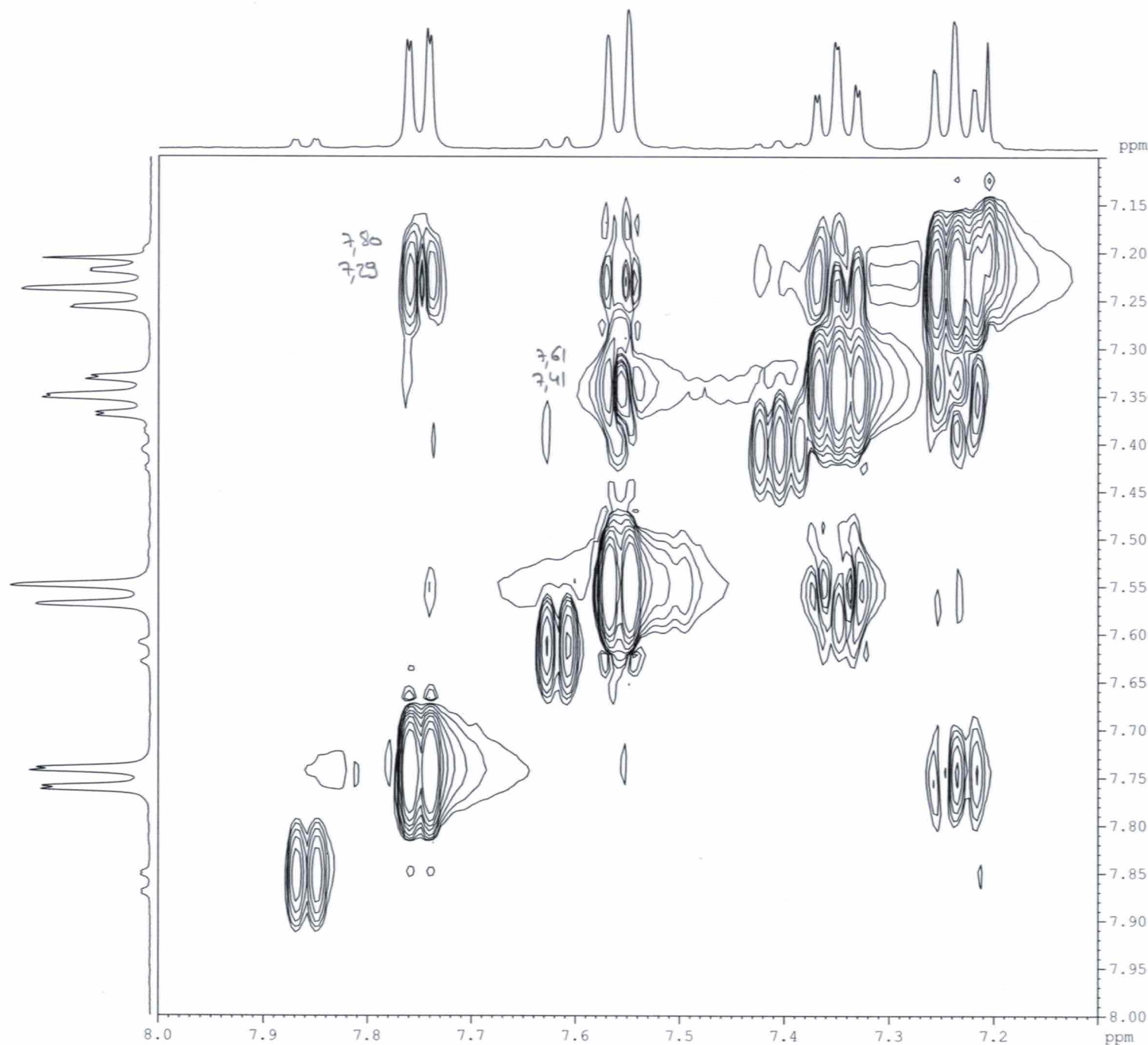


NAME ral51b
EXPNO 84
PROCNO 1
Date 20141208
Time 9.04
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesygpph
TD 2134
SOLVENT CDCl3
NS 2
DS 16
SWH 3094.059 Hz
FIDRES 1.449887 Hz
AQ 0.3450660 sec
RG 35.9
DW 161.600 usec
DE 6.50 usec
TE 300.0 K
DO 0.00015291 sec
D1 1.45603800 sec
D8 0.80000001 sec
D16 0.00020000 sec
INO 0.00032320 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1318282 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GFZ1 40.00 %
P16 1000.00 usec
NDO 1
TD 256
SFO1 400.1318 MHz
FIDRES 12.086169 Hz
SW 7.733 ppm
FnMODE States-TPPI
SI 2048
SF 400.1300385 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 States-TPPI
SF 400.1300385 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

RA0151 Beta NOESY

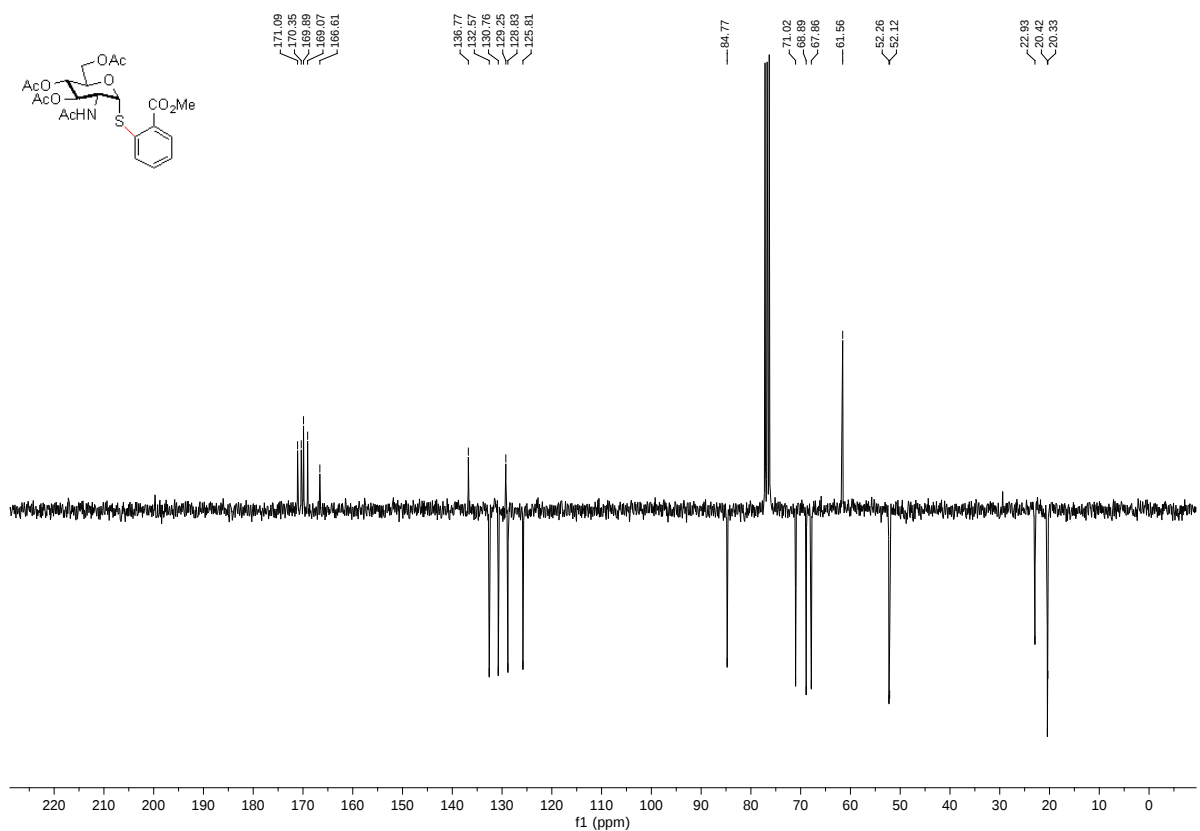
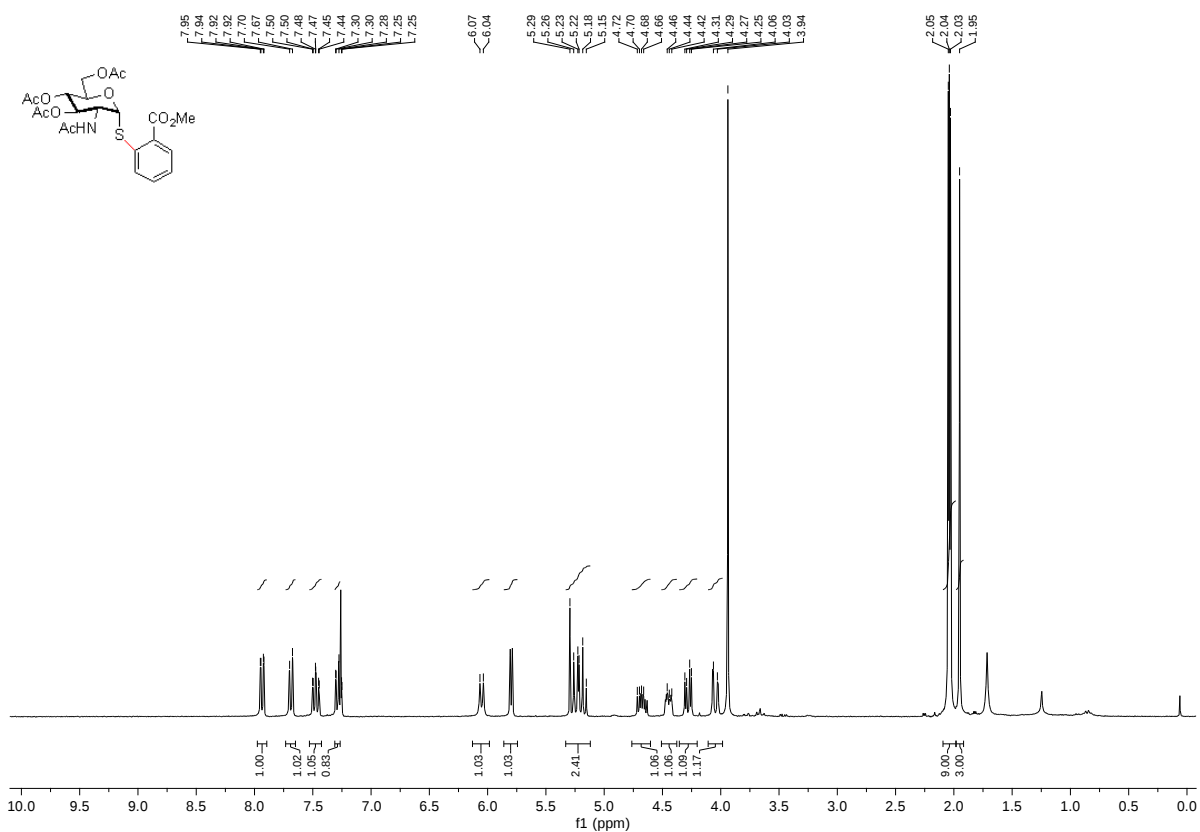


```

NAME          ral51b
EXPNO         84
PROCNO        1
Date_         20141208
Time          9.04
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       noesygpph
TD            2134
SOLVENT       CDC13
NS            2
DS            16
SWH           3094.059 Hz
FIDRES        1.449887 Hz
AQ            0.3450660 sec
RG            35.9
DW            161.600 usec
DE            6.50 usec
TE            300.0 K
DO            0.00015291 sec
D1            1.45603800 sec
D8            0.80000001 sec
D16           0.00020000 sec
INO           0.00032320 sec

===== CHANNEL f1 =====
NUC1           1H
P1             6.82 usec
P2            13.65 usec
PL1            0.00 dB
SFO1          400.1318282 MHz

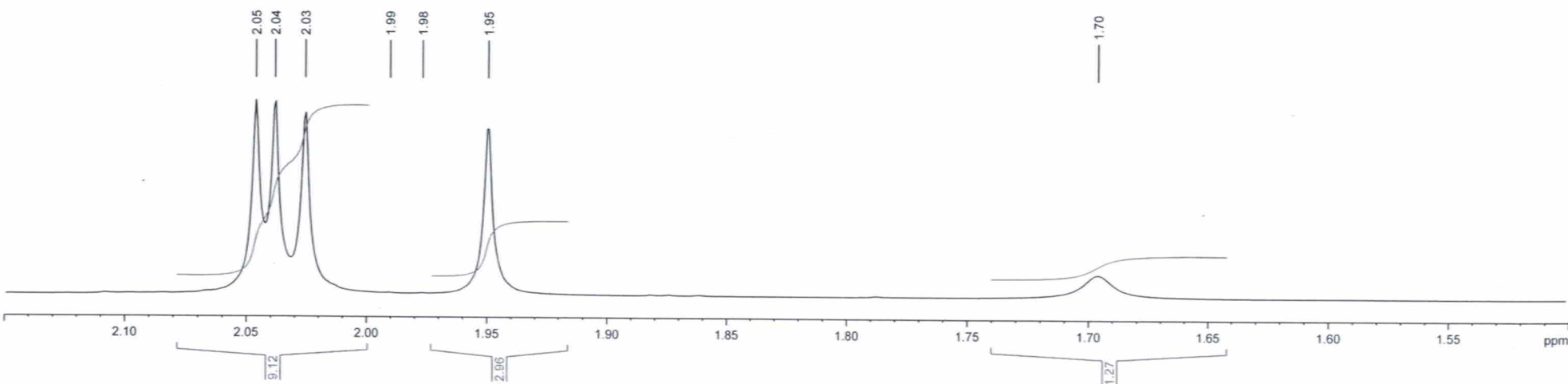
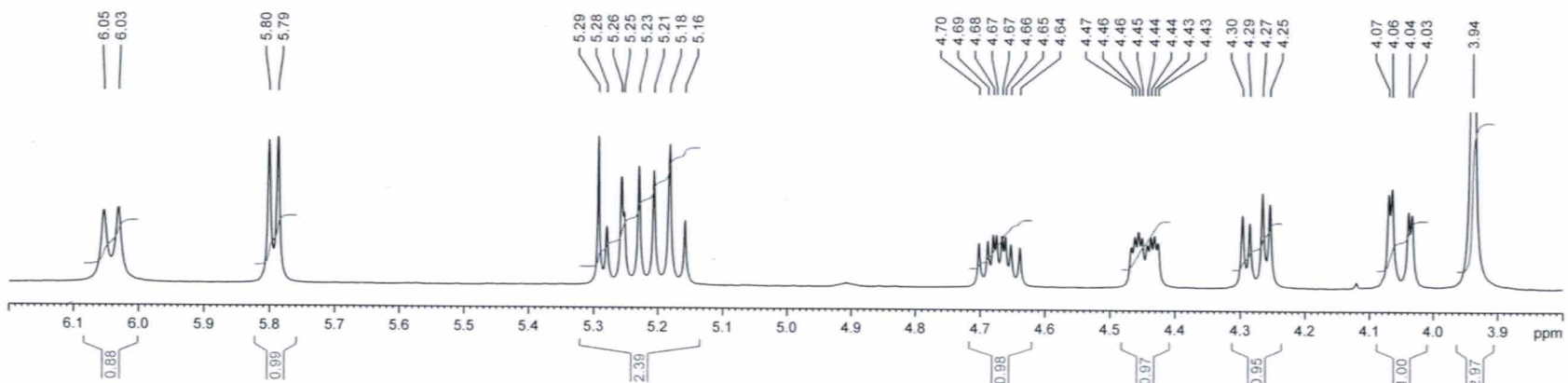
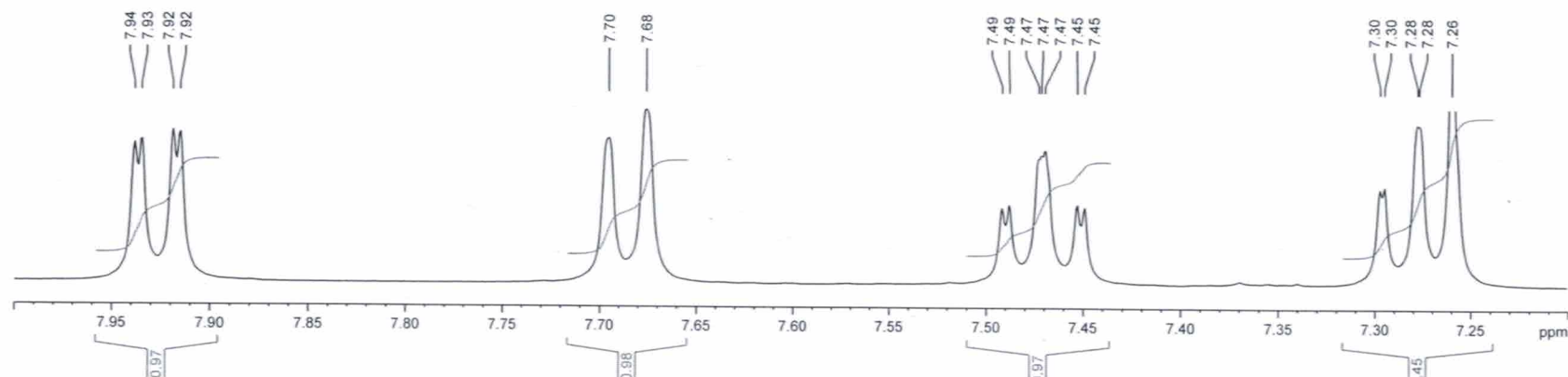
===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPZ1          40.00 %
P16           1000.00 usec
ND0            1
TD            256
SFO1          400.1318 MHz
FIDRES        12.086169 Hz
SW            7.733 ppm
FnMODE        States-TPPI
SI            2048
SF            400.1300385 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           States-TPPI
SF            400.1300385 MHz
WDW           QSINE
SSB            2
LB            0.00 Hz
GB            0
  
```

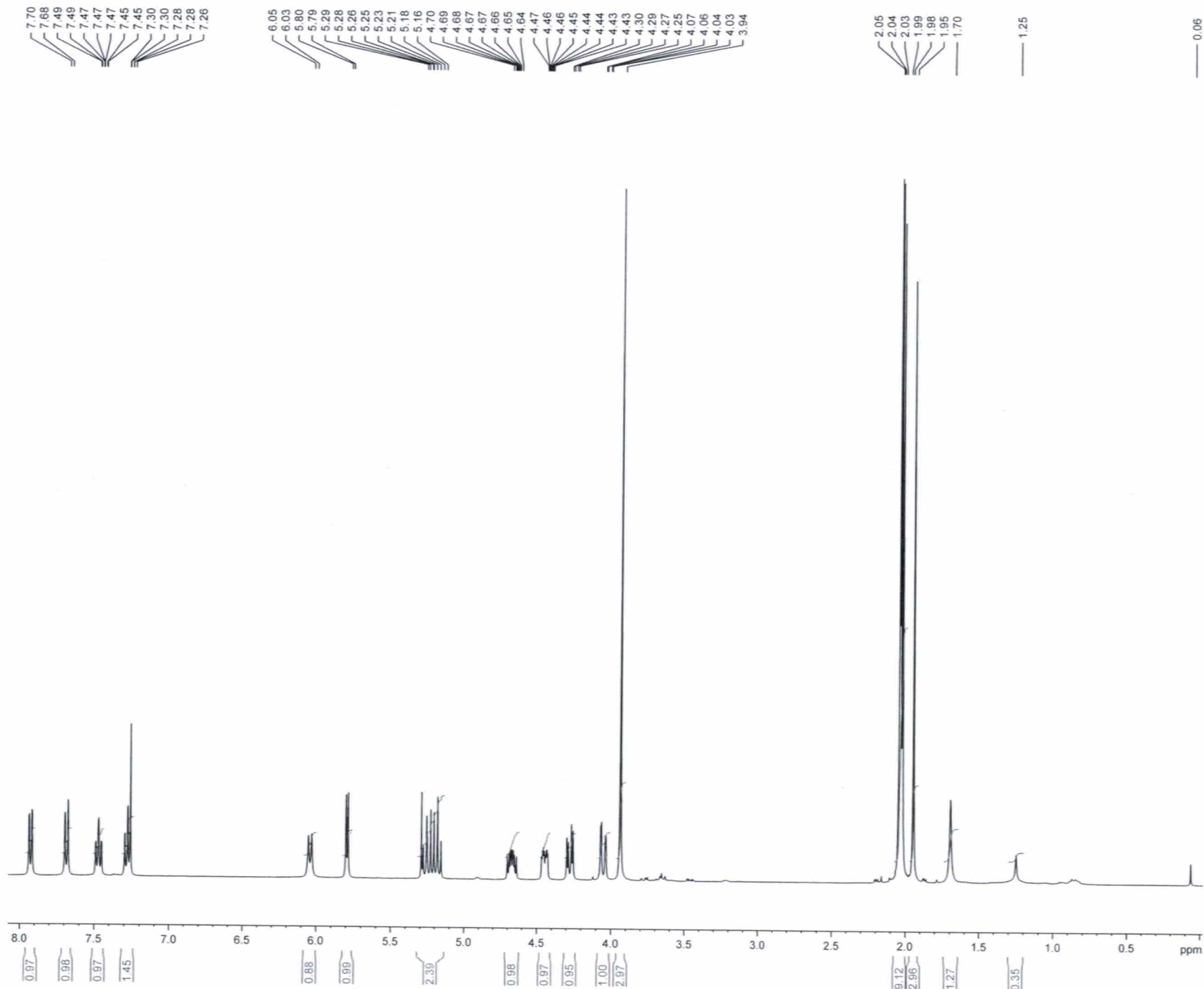


RA0151 ALPHA Proton

NAME ra0151
EXPNO 10
PROCNO 1
Date_ 20141129
Time 13.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 64
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 161.3
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1336012 MHz
SI 32768
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





RA0151 ALPHA Proton

NAME ra0151
EXPNO 10
PROCNO 1
Date_ 20141129
Time 13.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 161.3
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

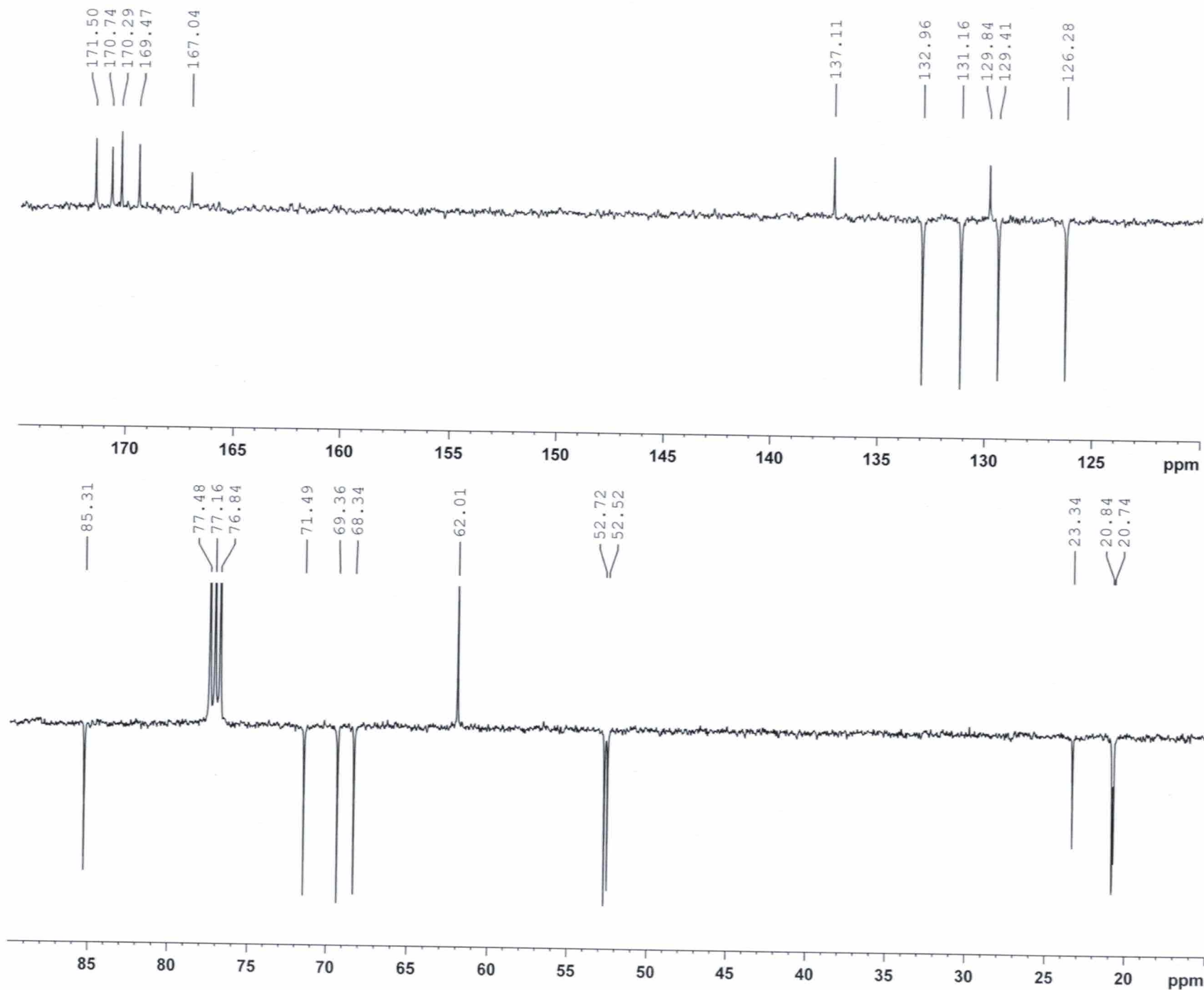
===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1336012 MHz
SI 32768
SF 400.1300173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

RA0151 ALPHA Jmod

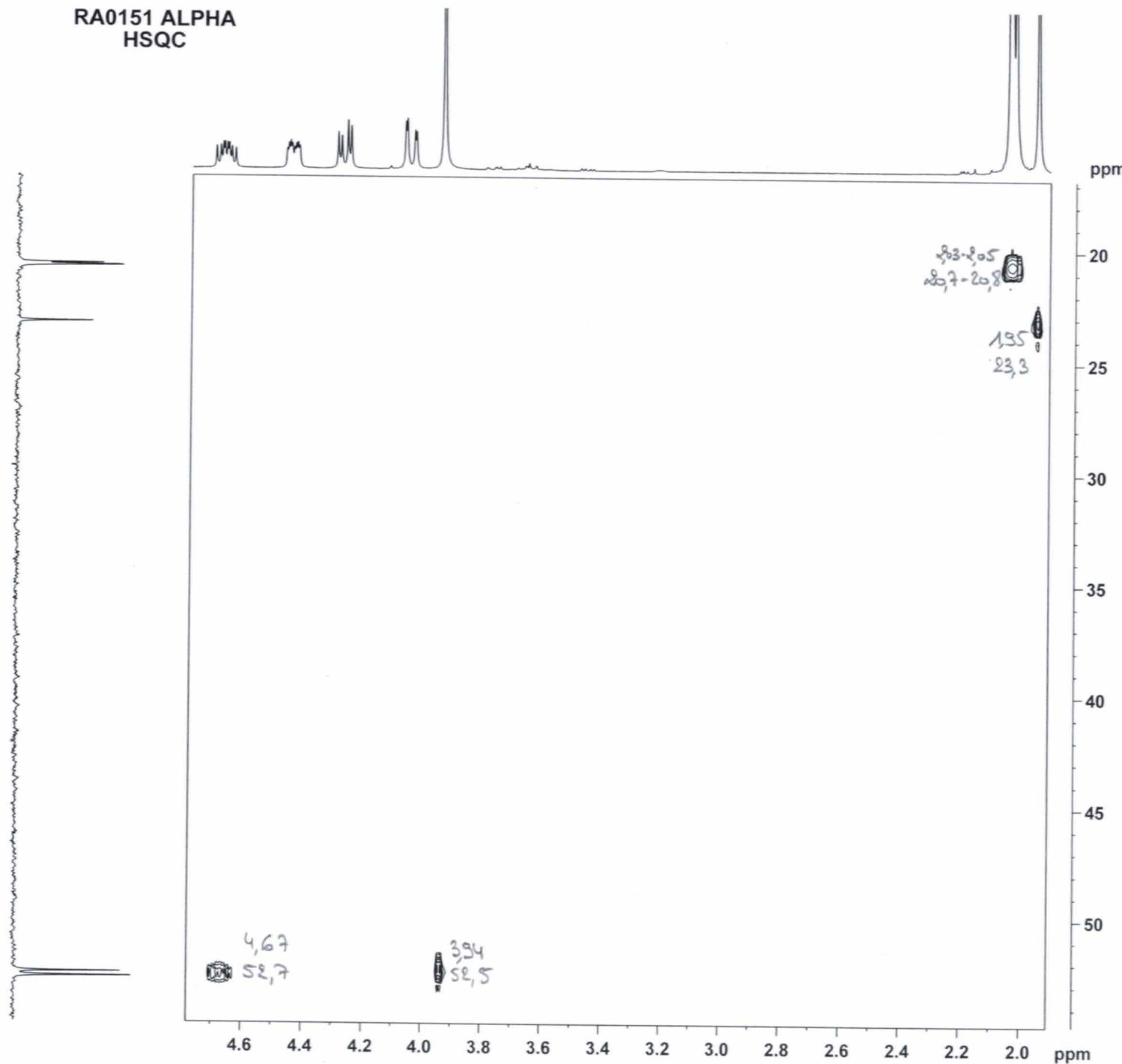
NAME ra0151
EXPNO 15
PROCNO 1
Date_ 20141130
Time 0.26
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG jmod
TD 65536
SOLVENT CDC13
NS 4000
DS 4
SWH 23148.148 Hz
FIDRES 0.353213 Hz
AQ 1.4156492 sec
RG 14596.5
DW 21.600 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST11 1.0000000
D1 5.00000000 sec
D20 0.00689655 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 0.00 dB
SFO1 100.6233333 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 23.32 dB
SFO2 400.1316005 MHz
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



RA0151 ALPHA
HSQC



NAME	ra0151
EXPNO	12
PROCNO	1
Date_	20141129
Time	13.15
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	hsqcetgpsi
TD	4096
SOLVENT	CDCl3
NS	8
DS	4
SWH	3387.534 Hz
FIDRES	0.827035 Hz
AQ	0.6047672 sec
RG	7298.2
DW	147.600 usec
DE	6.50 usec
TE	300.0 K
CNST2	140.0000000
D0	0.00000300 sec
D1	0.97296399 sec
D4	0.00178571 sec
D11	0.03000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
D24	0.00089000 sec
IN0	0.00003105 sec
ZGOPTNS	

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

NUC1	1H
P1	6.82 usec
P2	13.65 usec
P28	1000.00 usec
PL1	0.00 dB
SFO1	400.1317473 MHz

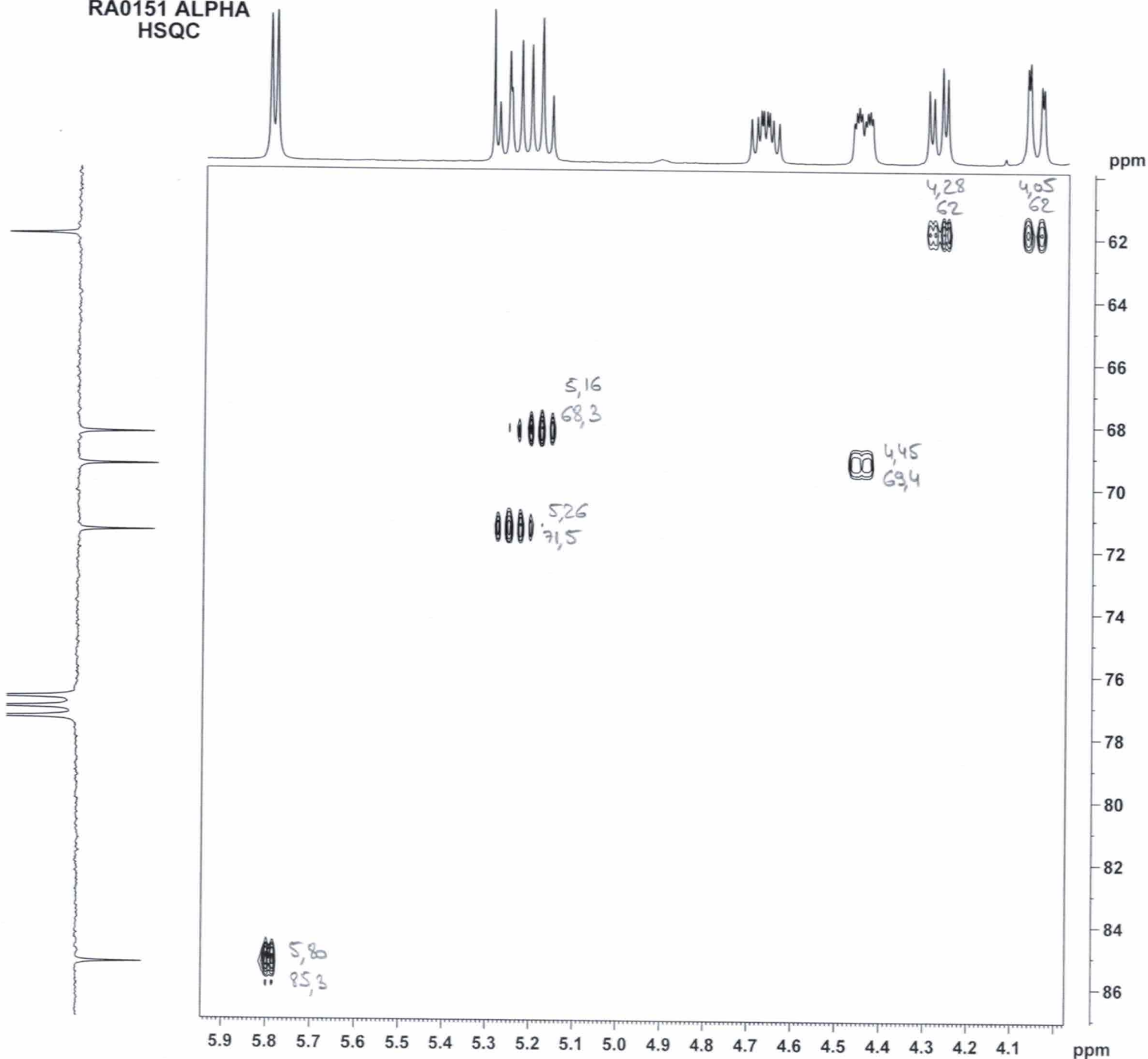
===== CHANNEL f2 =====

CPDPRG2	garp
NUC2	13C
P3	11.00 usec
P4	22.00 usec
PCPD2	80.00 usec
PL2	0.00 dB
PL12	17.23 dB
SFO2	100.6203150 MHz

===== GRADIENT CHANNEL =====

GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	100.6203 MHz
FIDRES	62.887669 Hz
SW	160.000 ppm
FnMODE	Echo-Antiecho
SI	4096
SF	400.1300173 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	512
MC2	echo-antiecho
SF	100.6127568 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

RA0151 ALPHA
HSQC



```

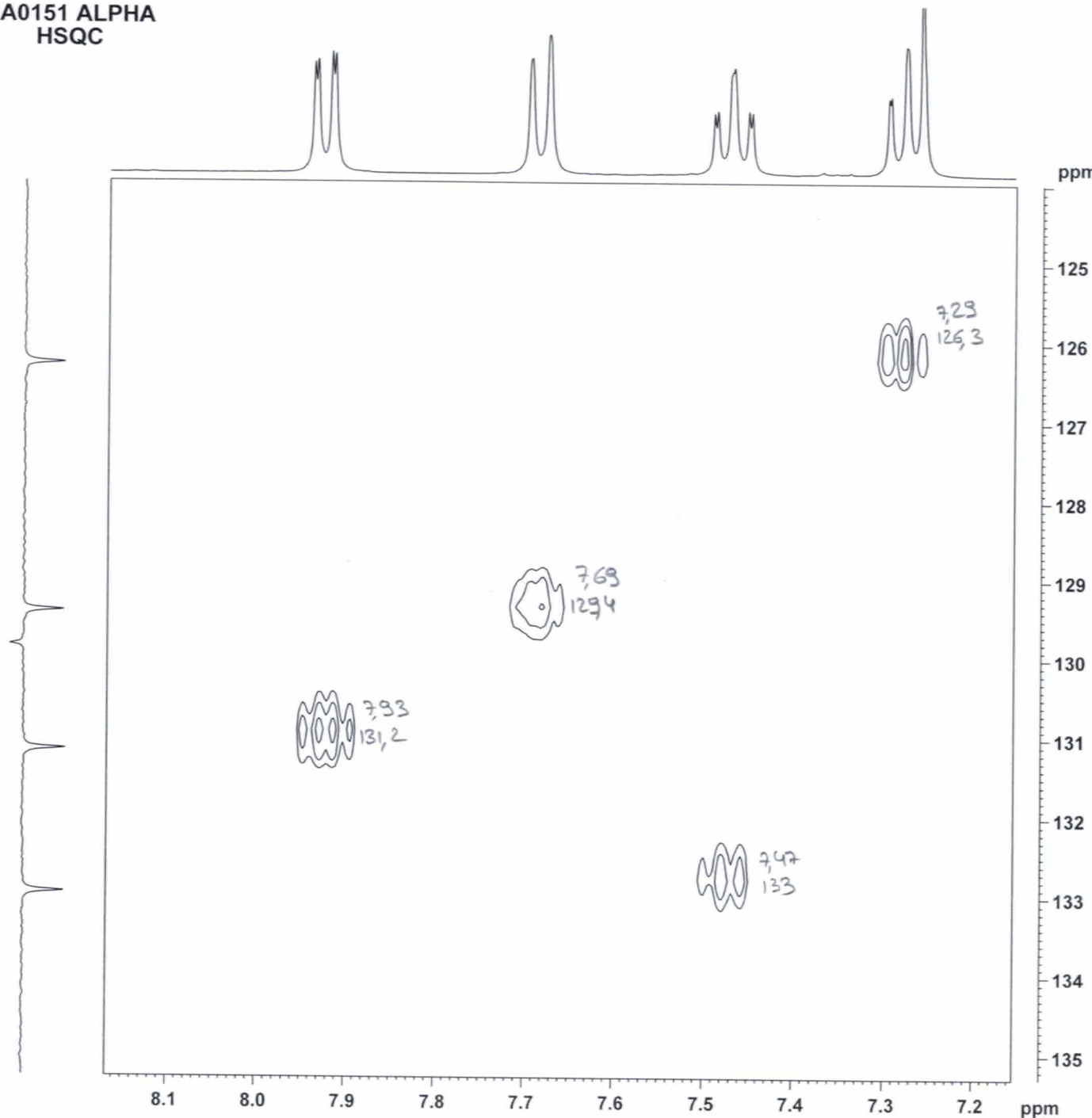
NAME      ra0151
EXPNO     12
PROCNO    1
Date_     20141129
Time      13.15
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   hsqcetgpsi
TD        4096
SOLVENT   CDCl3
NS         8
DS         4
SWH        3387.534 Hz
FIDRES     0.827035 Hz
AQ         0.6047672 sec
RG         7298.2
DW         147.600 usec
DE         6.50 usec
TE         300.0 K
CNST2     140.0000000
D0         0.00000300 sec
D1         0.97296399 sec
D4         0.00178571 sec
D11        0.03000000 sec
D13        0.00000400 sec
D16        0.00020000 sec
D24        0.00089000 sec
IN0        0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1       1H
P1         6.82 usec
P2         13.65 usec
P28        1000.00 usec
PL1        0.00 dB
SFO1       400.1317473 MHz

===== CHANNEL f2 =====
CPDPRG2    garp
NUC2       13C
P3         11.00 usec
P4         22.00 usec
PCPD2      80.00 usec
PL2        0.00 dB
PL12       17.23 dB
SFO2       100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPNAM2     SINE.100
GPZ1       80.00 %
GPZ2       20.10 %
P16        1000.00 usec
ND0        2
TD         256
SFO1       100.6203 MHz
FIDRES     62.887669 Hz
SW         160.000 ppm
FnMODE     Echo-Antiecho
SI         4096
SF         400.1300173 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40
SI         512
MC2        echo-antiecho
SF         100.6127568 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
  
```

RA0151 ALPHA
HSQC



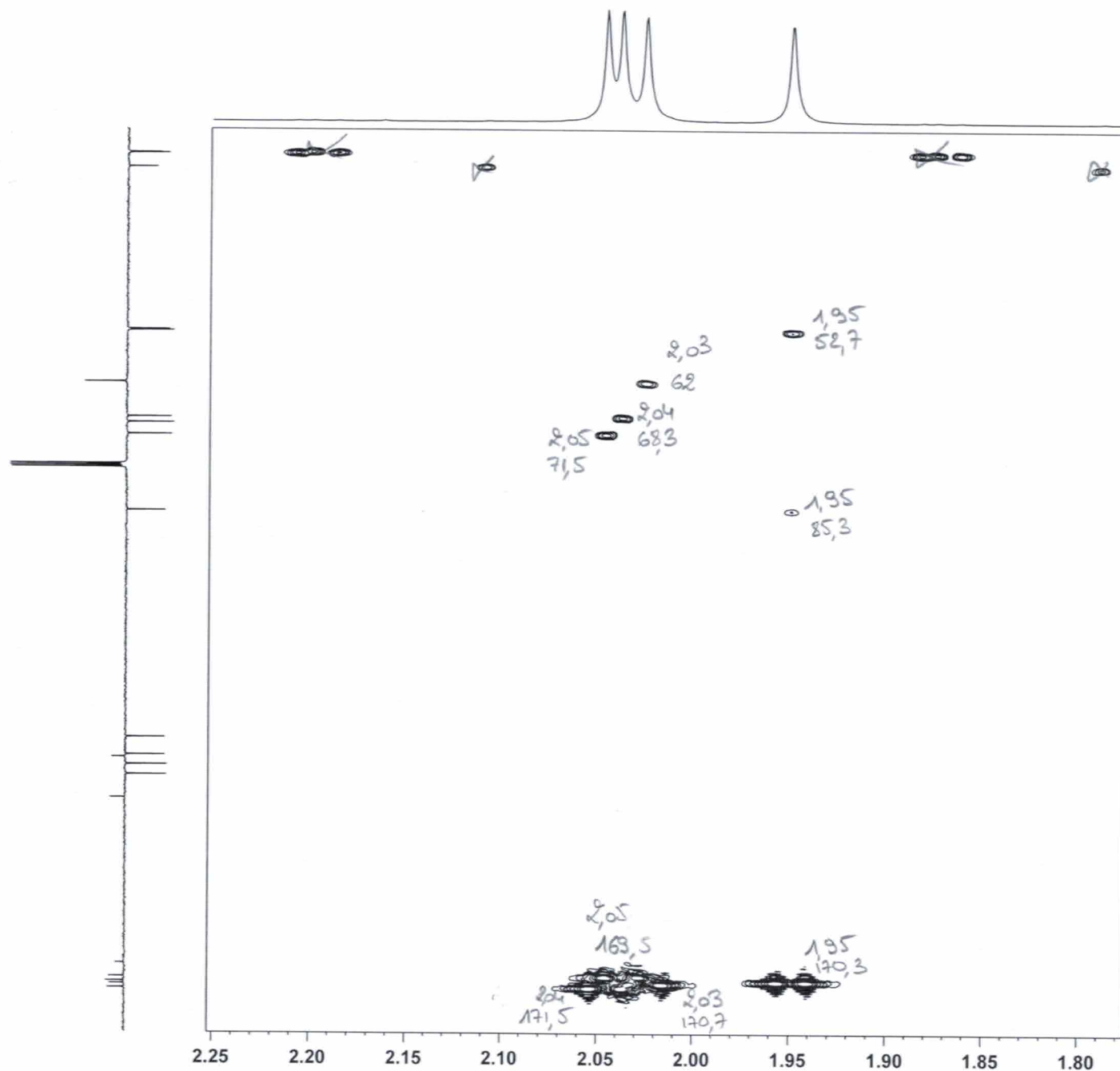
NAME ra0151
EXPNO 12
PROCNO 1
Date_ 20141129
Time 13.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hsqcetgpsi
TD 4096
SOLVENT CDCl3
NS 8
DS 4
SWH 3387.534 Hz
FIDRES 0.827035 Hz
AQ 0.6047672 sec
RG 7298.2
DW 147.600 usec
DE 6.50 usec
TE 300.0 K
CNST2 140.0000000
D0 0.00000300 sec
D1 0.97296399 sec
D4 0.00178571 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
P28 1000.00 usec
PL1 0.00 dB
SFO1 400.1317473 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 ^{13}C
P3 11.00 usec
P4 22.00 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
SFO2 100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
NDO 2
TD 256
SFO1 100.6203 MHz
FIDRES 62.887669 Hz
SW 160.000 ppm
FnMODE Echo-Antiecho
SI 4096
SF 400.1300173 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6127568 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

RA0151 ALPHA HMBC



ppm

```

NAME      ra0151
EXPNO     1
PROCNO    1
Date_     20141129
Time      14.11
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   hmbcgp1pndqf
TD         4096
SOLVENT   CDCl3
NS         16
DS         4
SWH        3387.534 Hz
FIDRES     0.827035 Hz
AQ         0.6047672 sec
RG         18390.4
DW         147.600 usec
DE         6.50 usec
TE         300.0 K
CNST2     145.0000000
CNST13     8.0000000
D0         0.00000300 sec
D1         0.99651301 sec
D2         0.00344828 sec
D6         0.06250000 sec
D16        0.00020000 sec
IN0        0.00002160 sec

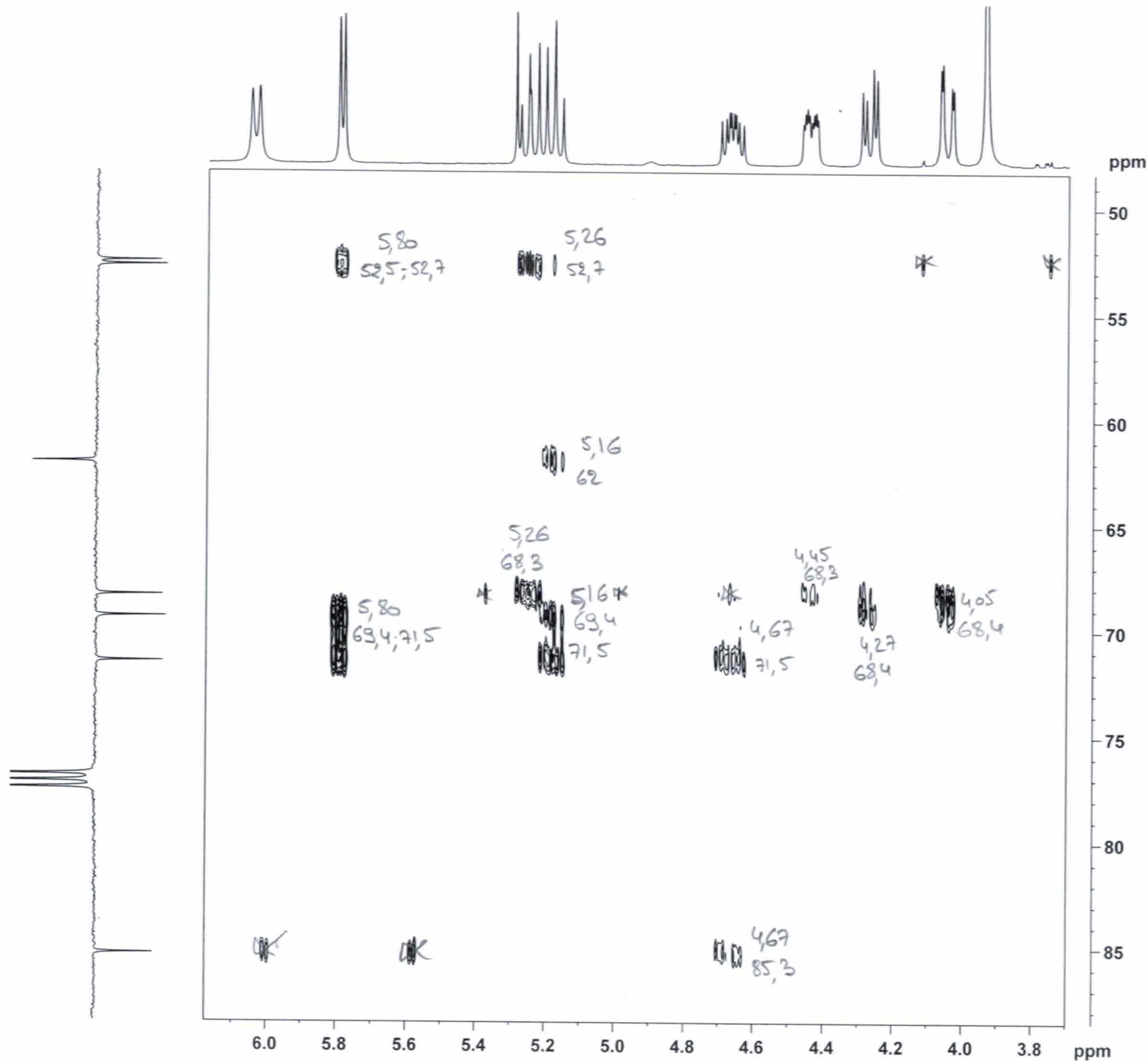
===== CHANNEL f1 =====
NUC1       1H
P1         6.82 usec
P2         13.65 usec
PL1        0.00 dB
SFO1       400.1317473 MHz

===== CHANNEL f2 =====
NUC2       13C
P3         11.00 usec
PL2        0.00 dB
SFO2       100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPNAM2     SINE.100
GPNAM3     SINE.100
GPZ1       50.00 %
GPZ2       30.00 %
GPZ3       40.10 %
P16        1000.00 usec
ND0        2
TD         256
SFO1       100.6238 MHz
FIDRES     90.403236 Hz
SW         229.997 ppm
F0MODE     QF
SI         4096
SF         400.1300173 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40
SI         1024
MC2        QF
SF         100.6127568 MHz
WDW        SINE
SSB        0
LB         0.00 Hz
GB         0
  
```

ppm

RA0151 ALPHA HMBC



```

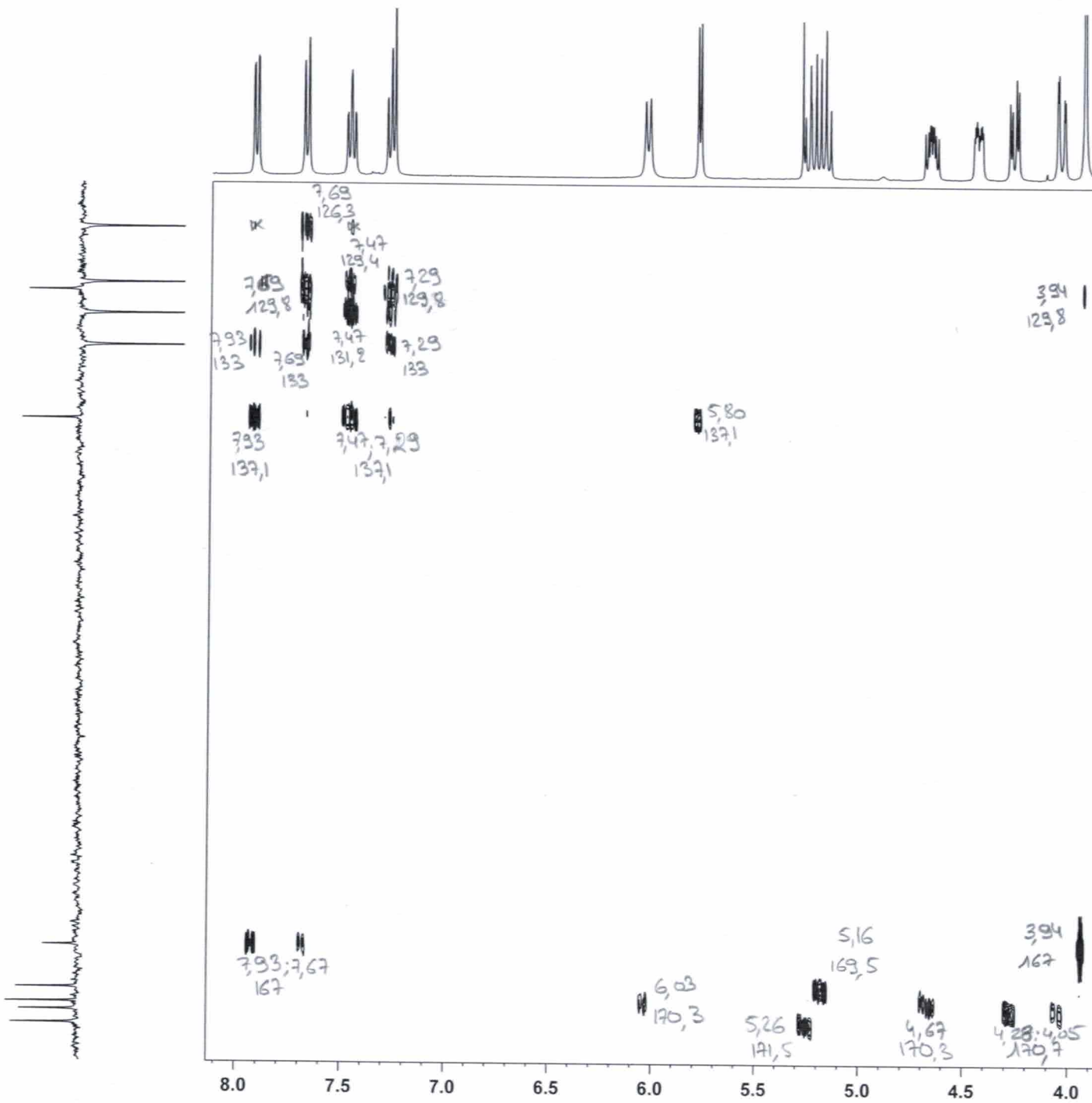
NAME          ra0151
EXPNO         13
PROCNO        1
Date_         20141129
Time_         14.11
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       hmbcpglpndqf
TD            4096
SOLVENT       CDCl3
NS            16
DS            4
SWH           3387.534 Hz
FIDRES        0.827035 Hz
AQ            0.6047672 sec
RG            18390.4
DW            147.600 usec
DE            6.50 usec
TE            300.0 K
CNST2         145.0000000
CNST13        8.0000000
D0            0.00000300 sec
D1            0.99651301 sec
D2            0.00344828 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002160 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
PL1           0.00 dB
SFO1          400.1317473 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            11.00 usec
PL2           0.00 dB
SFO2          100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GP21          50.00 %
GP22          30.00 %
GP23          40.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6238 MHz
FIDRES        90.403236 Hz
SW            229.997 ppm
FnMODE        QF
SI            4096
SF            400.1300173 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6127568 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
  
```

RA0151 ALPHA HMBC



ppm

NAME	ra0151
EXPNO	13
PROCNO	1
Date_	20141129
Time	14.11
INSTRUM	spect
PROBHD	5 mm Multinuc1
PULPROG	hmbcgp1pndqf
TD	4096
SOLVENT	CDC13
NS	16
DS	4
SWH	3387.534 Hz
FIDRES	0.827035 Hz
AQ	0.6047672 sec
RG	18390.4
DW	147.600 usec
DE	6.50 usec
TE	300.0 K
CNST2	145.0000000
CNST13	8.0000000
D0	0.00000300 sec
D1	0.99651301 sec
D2	0.00344828 sec
D6	0.06250000 sec
D16	0.00020000 sec
INO	0.00002160 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	6.82 usec
P2	13.65 usec
PL1	0.00 dB
SFO1	400.1317473 MHz
===== CHANNEL f2 =====	
NUC2	13C
P3	11.00 usec
PL2	0.00 dB
SFO2	100.6238364 MHz
===== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPNAM3	SINE.100
GPZ1	50.00 %
GPZ2	30.00 %
GPZ3	40.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	100.6238 MHz
FIDRES	90.403236 Hz
SW	229.997 ppm
FnMODE	QF
SI	4096
SF	400.1300173 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	100.6127568 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

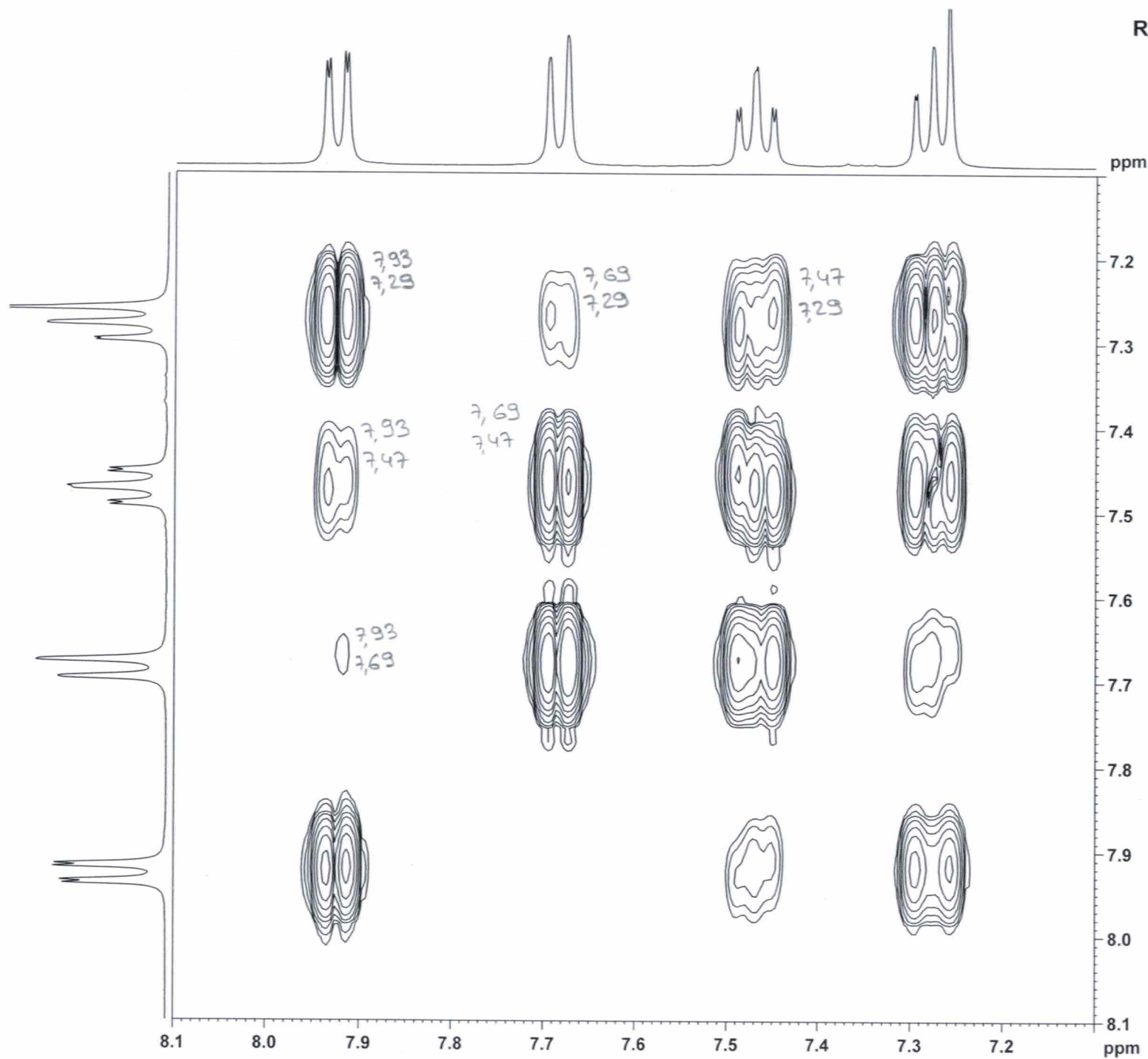
ppm

RA0151 ALPHA COSY

NAME ra0151
EXPNO 11
PROCNO 1
Date_ 20141129
Time 13.02
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG cosygpmfqr
TD 2134
SOLVENT CDC13
NS 2
DS 8
SWH 3387.534 Hz
FIDRES 1.587410 Hz
AQ 0.3151760 sec
RG 7298.2
DW 147.600 usec
DE 6.50 usec
TE 300.0 K
D0 0.00000300 sec
D1 0.98505932 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00029520 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1317473 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1317 MHz
FIDRES 13.232554 Hz
SW 8.466 ppm
FMODE QF
SI 2048
SF 400.1300173 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300173 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0

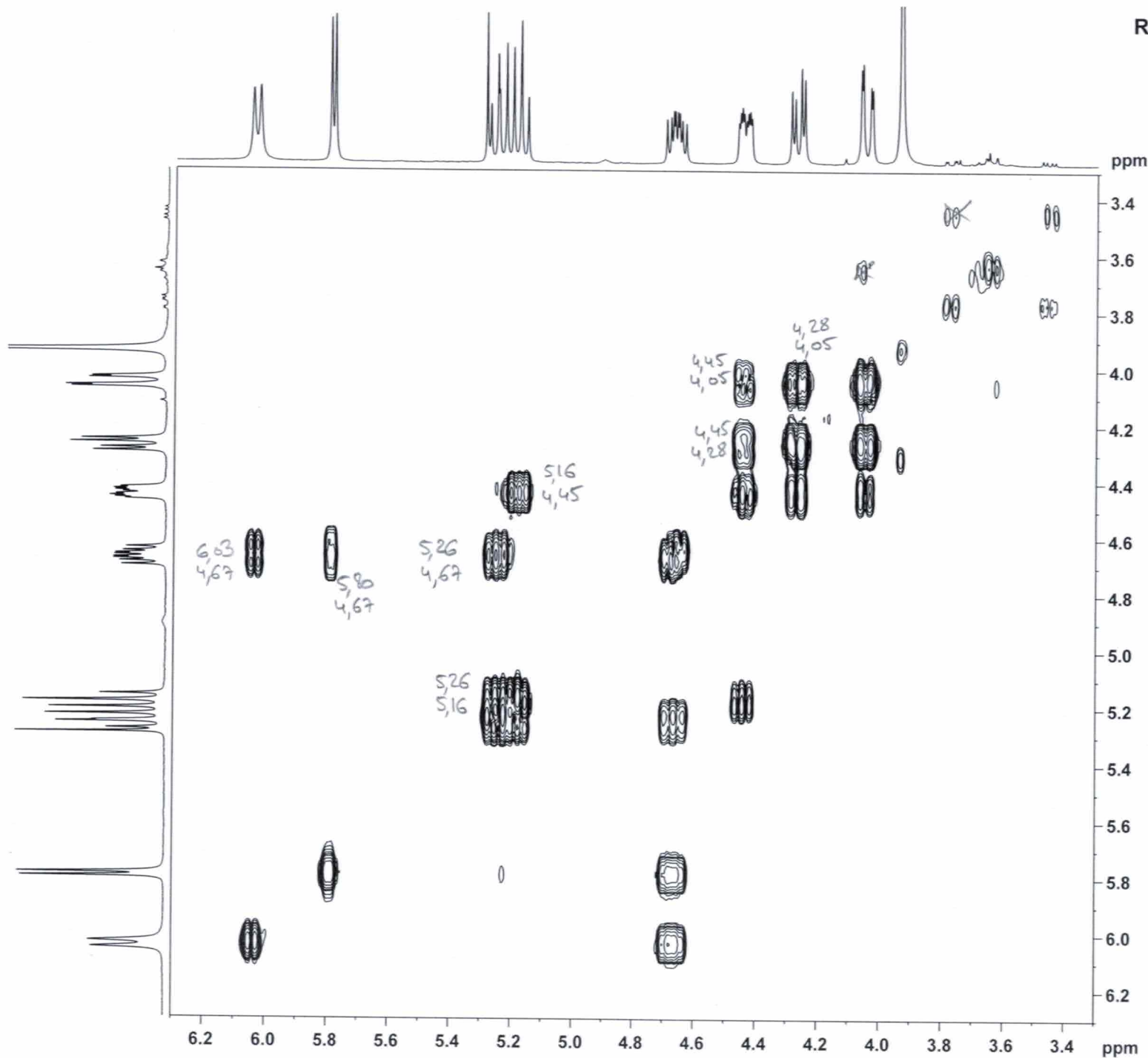


RA0151 ALPHA COSY

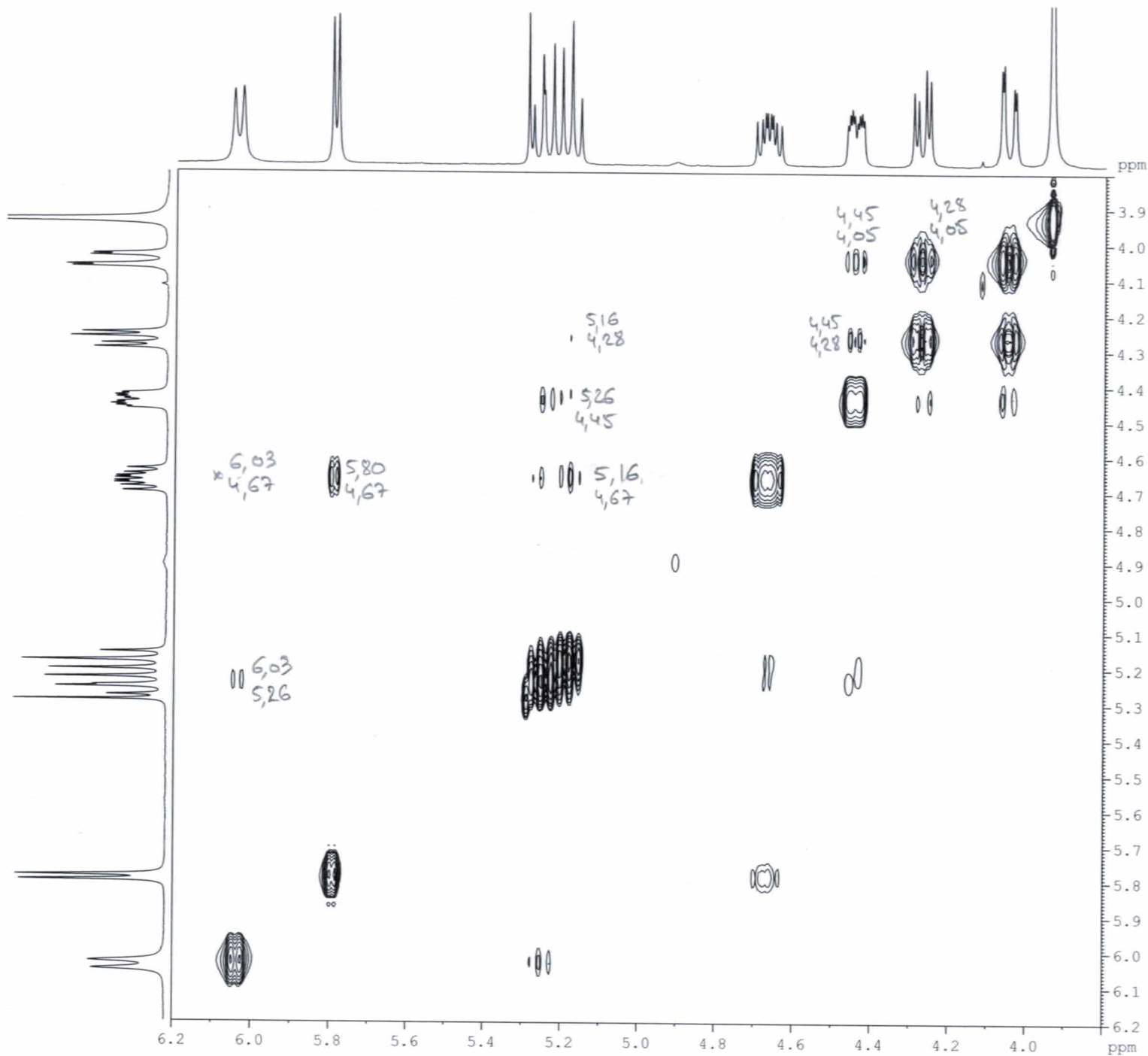
NAME ra0151
EXPNO 11
PROCNO 1
Date 20141129
Time 13.02
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG cosygpmfzf
TD 2134
SOLVENT CDCl3
NS 2
DS 8
SWH 3387.534 Hz
FIDRES 1.587410 Hz
AQ 0.3151760 sec
RG 7298.2
DW 147.600 usec
DE 6.50 usec
TE 300.0 K
D0 0.00000300 sec
D1 0.98505932 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00029520 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1317473 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1317 MHz
FIDRES 13.232554 Hz
SW 8.466 ppm
FnMODE QF
SI 2048
SF 400.1300173 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300173 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0



RA0151 ALPHA NOESY



NAME ra0151
EXPNO 14
PROCNO 1
Date_ 20141129
Time_ 16.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesygpph
TD 2134
SOLVENT CDCl3
NS 6
DS 16
SWH 3387.534 Hz
FIDRES 1.587410 Hz
AQ 0.3151760 sec
RG 71.8
DW 147.600 usec
DE 6.50 usec
TE 300.0 K
DO 0.0001391 sec
D1 1.48591399 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00029520 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1317473 MHz

===== GRADIENT CHANNEL =====
GPNAMI SINE.100
GPZ1 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1317 MHz
FIDRES 13.232554 Hz
SW 8.466 ppm
FnMODE States-TPPI
SI 2048
SF 400.1300173 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 States-TPPI
SF 400.1300173 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

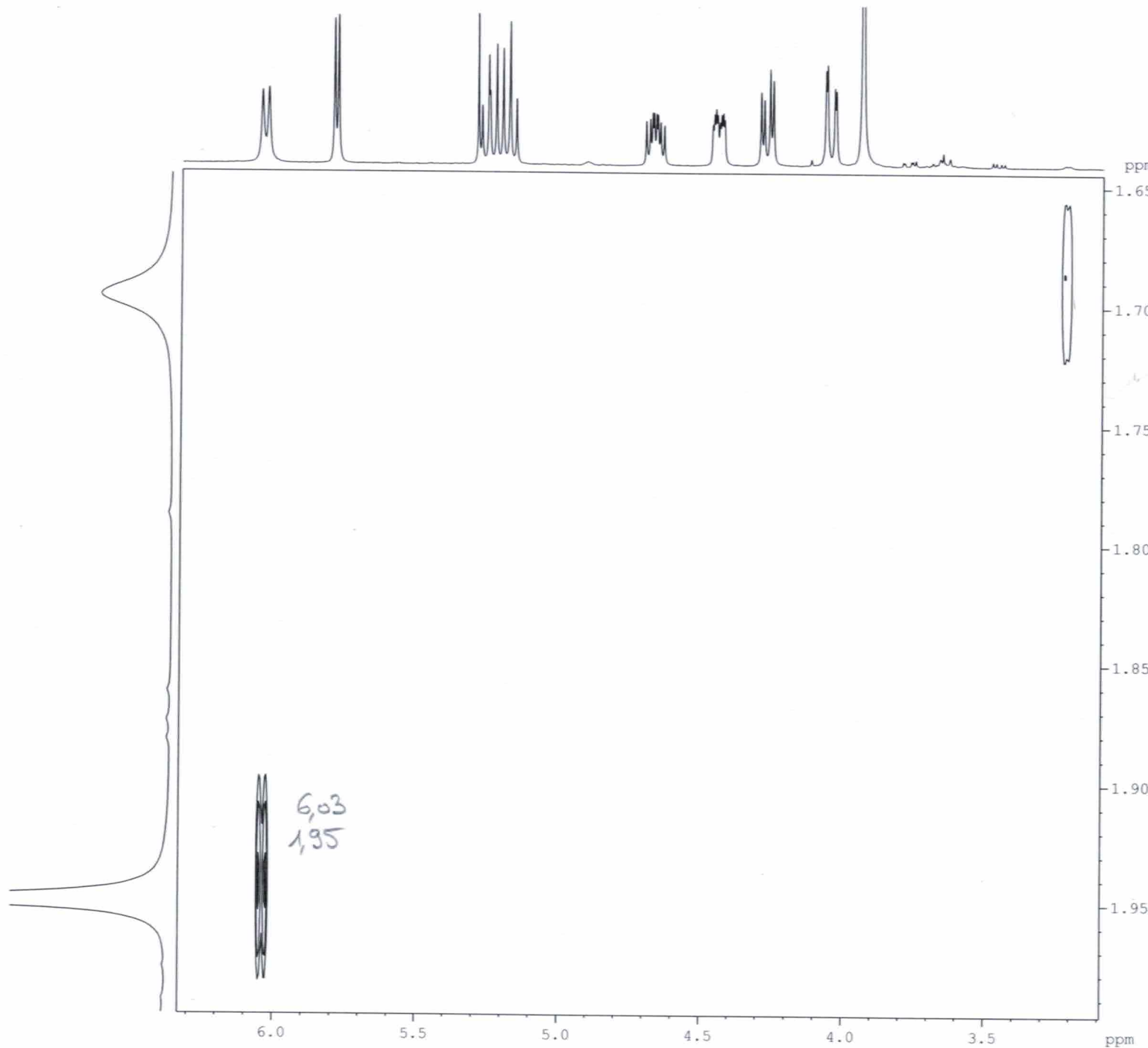
```
===== CHANNEL f1 =====  
NUC1                1H  
P1                   6.82 usec  
P2                   13.65 usec  
PL1                  0.00 dB  
SFO1                 400.1317473 MHz
```

```

===== GRADIENT CHANNEL =====
GNAM1          SINE.100
GPZ1           40.00    %
P16            1000.00  usec
NDO            1
TD             256
SF01           400.1317  MHz
FIDRES         13.232554 Hz
SW             8.466    ppm
FhMODE         States-TPPI
SI             2048
SF             400.1300173 MHz
WDW            QSINE
SSB            2
LB             0.00    Hz
GB             0
PC             1.40
SI             512
MC2            States-TPPI
SF             400.1300173 MHz
WDW            QSINE
SSB            2
LB             0.00    Hz
GB             0

```

RA0151 ALPHA NOESY

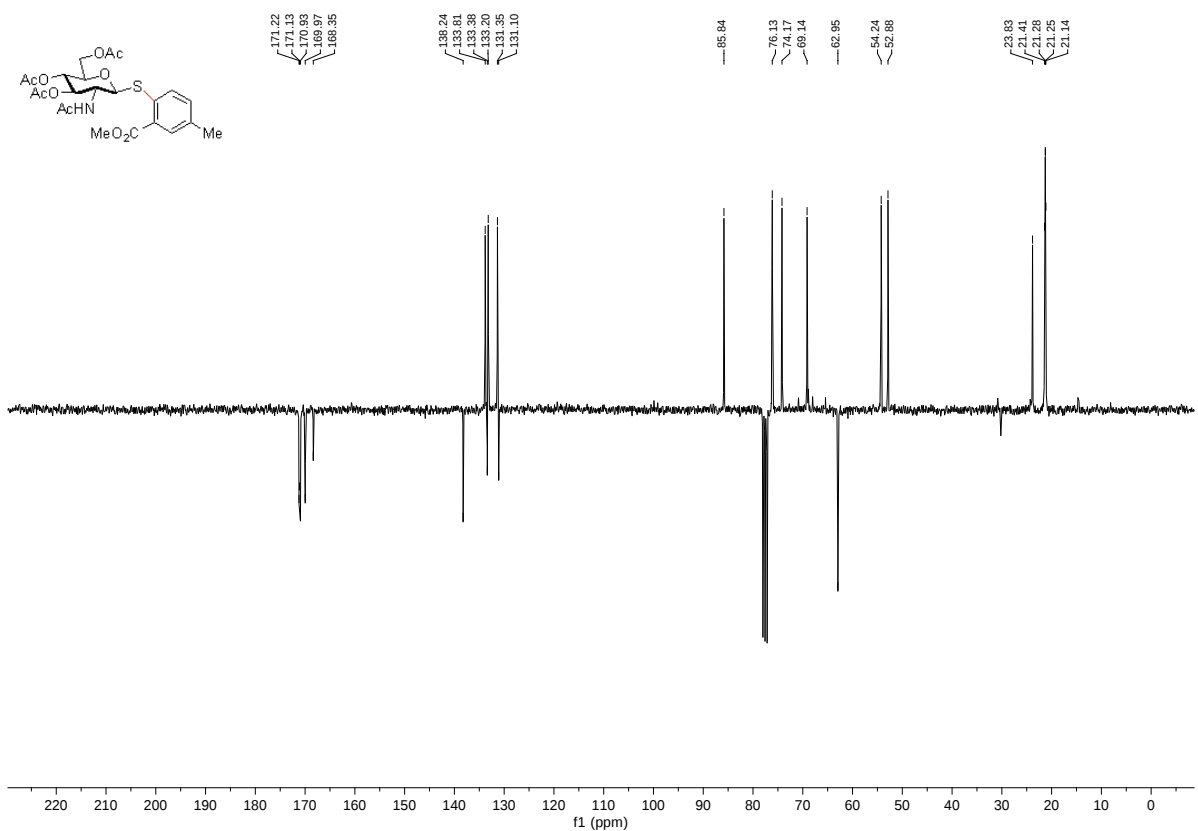
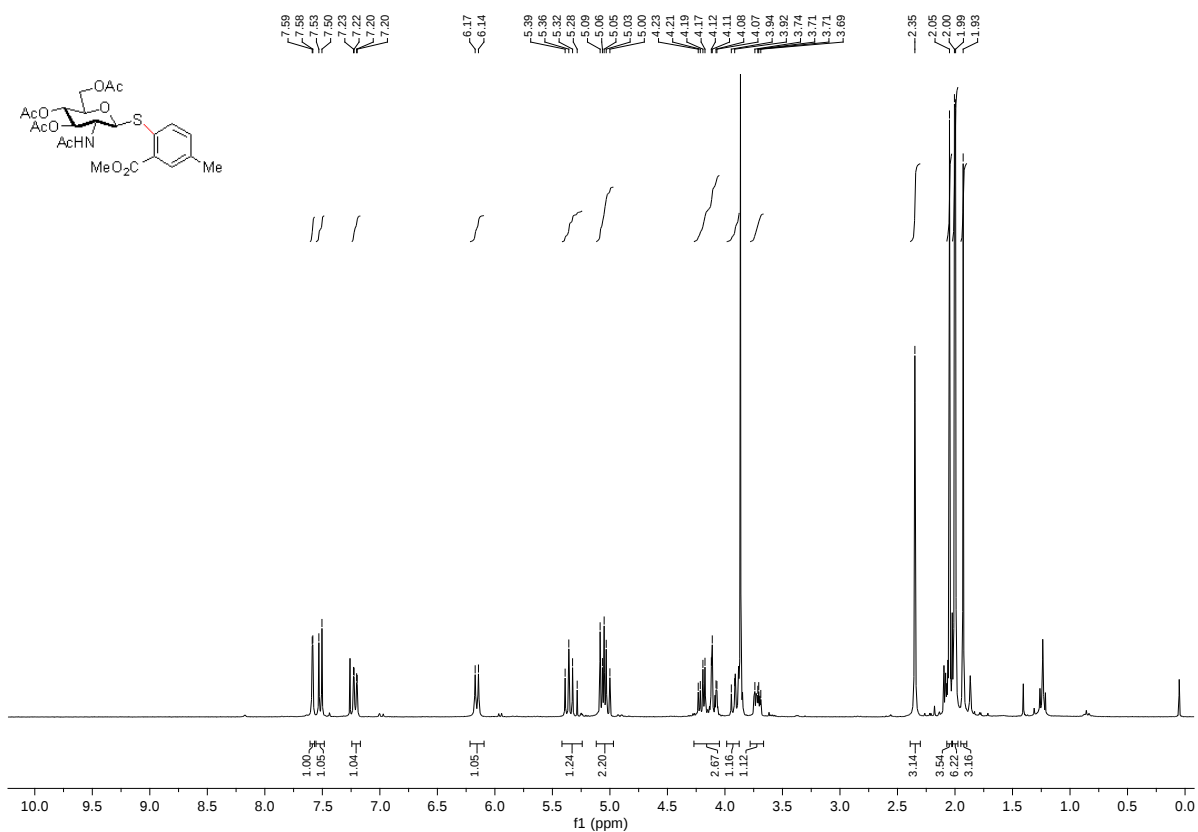


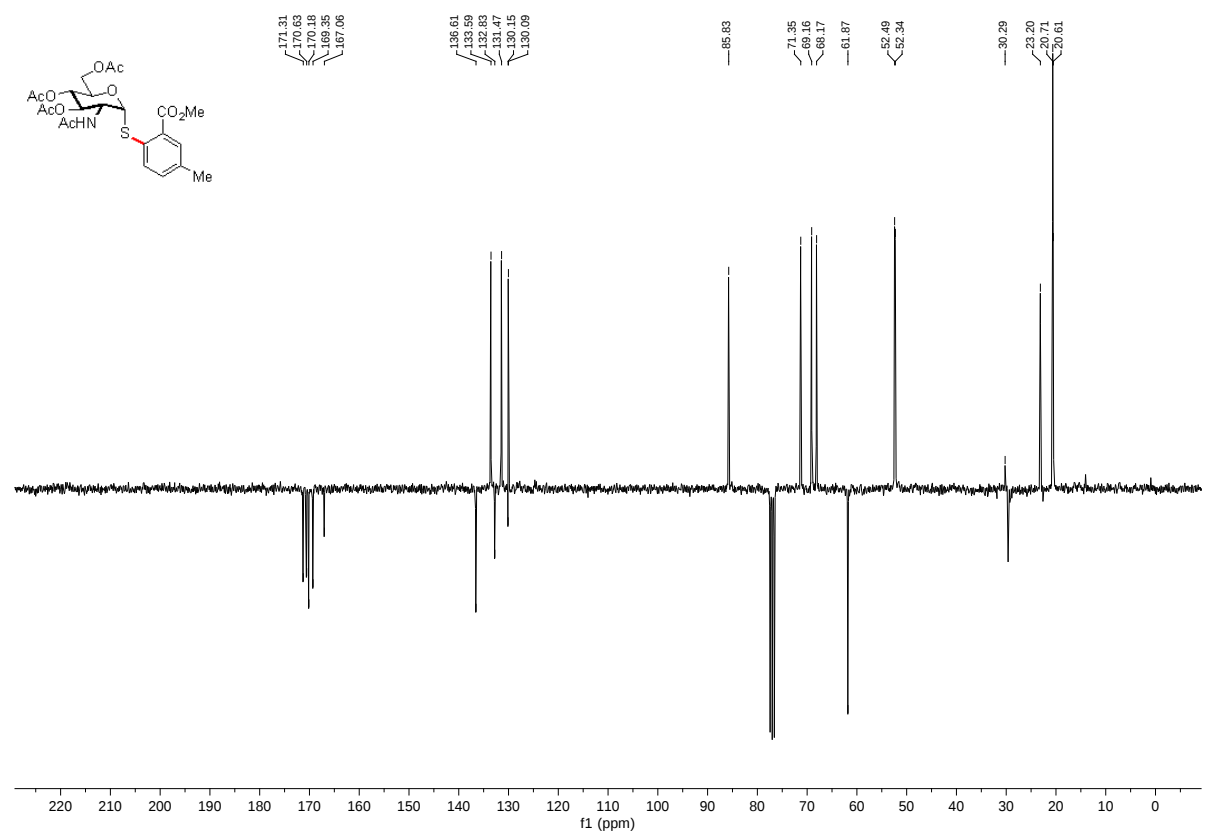
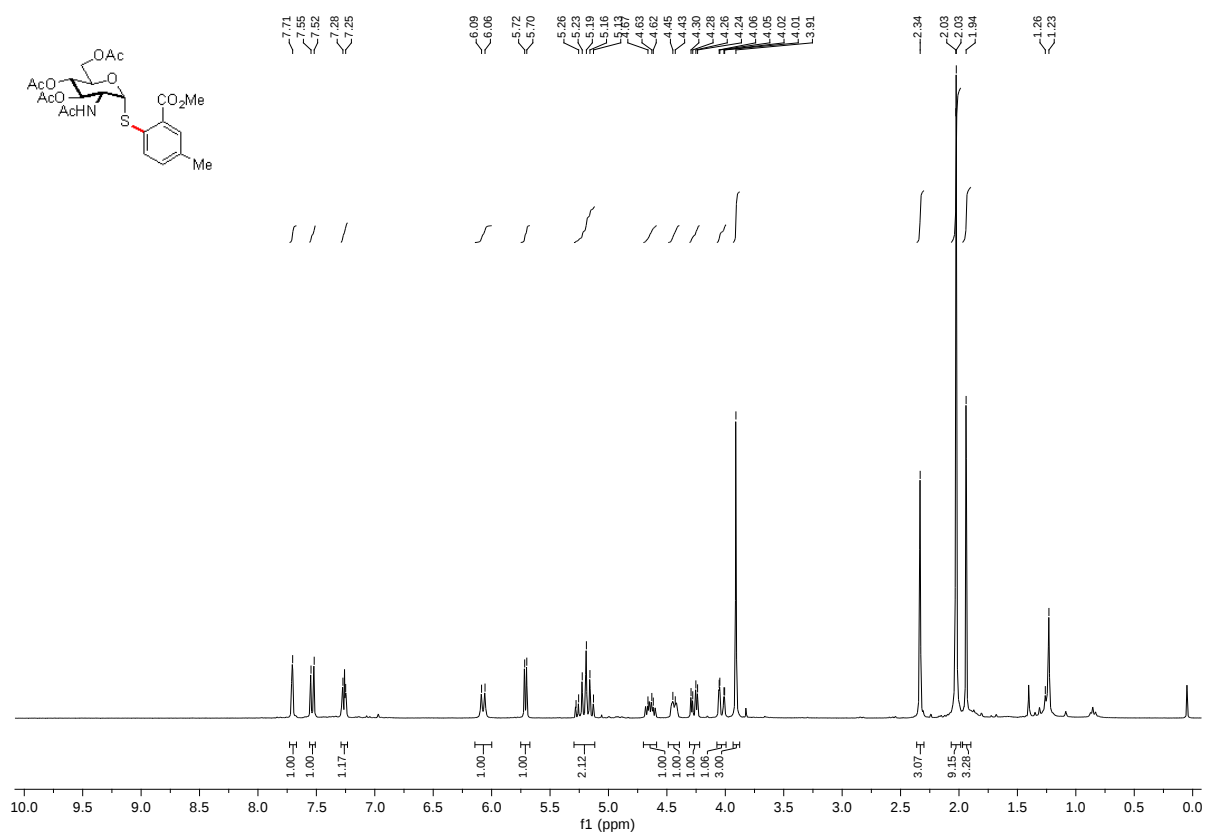
NAME ra0151
EXPNO 14
PROCNO 1
Date_ 20141129
Time_ 16.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesygpph
TD 2134
SOLVENT CDCl3
NS 6
DS 16
SWH 3387.534 Hz
FIDRES 1.587410 Hz
AQ 0.3151760 sec
RG 71.8
DW 147.600 usec
DE 6.50 usec
TE 300.0 K
D0 0.00013891 sec
D1 1.48591399 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00029520 sec

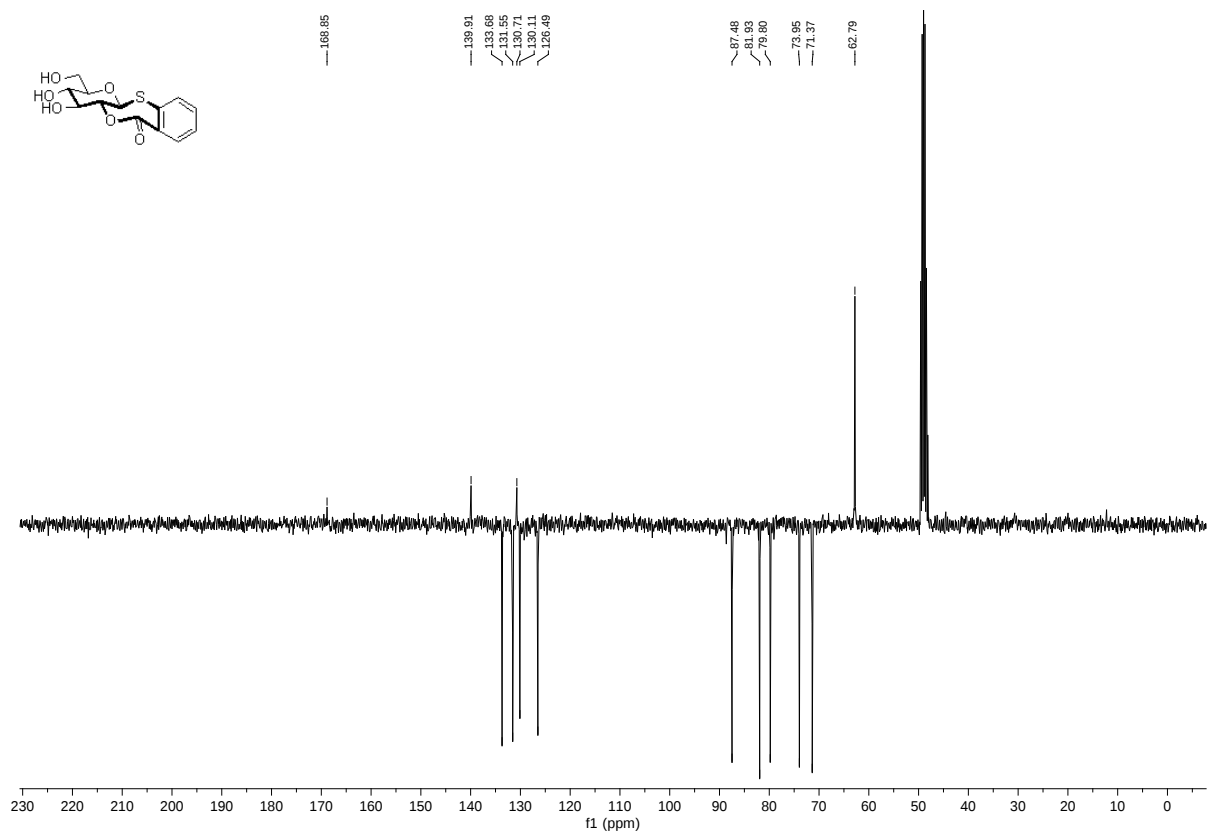
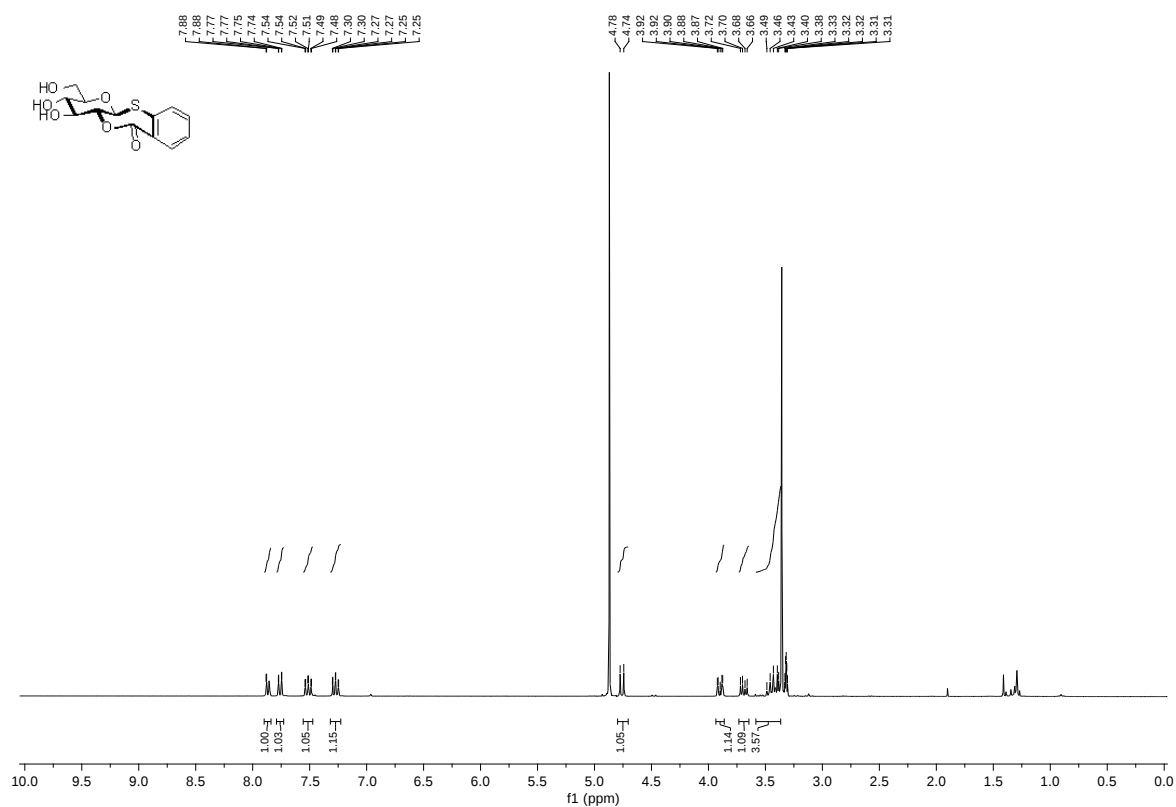
===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1317473 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1317 MHz
FIDRES 13.232554 Hz
SW 8.466 ppm
FMODE States-TPPI
SI 2048
SF 400.1300173 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 States-TPPI
SF 400.1300173 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

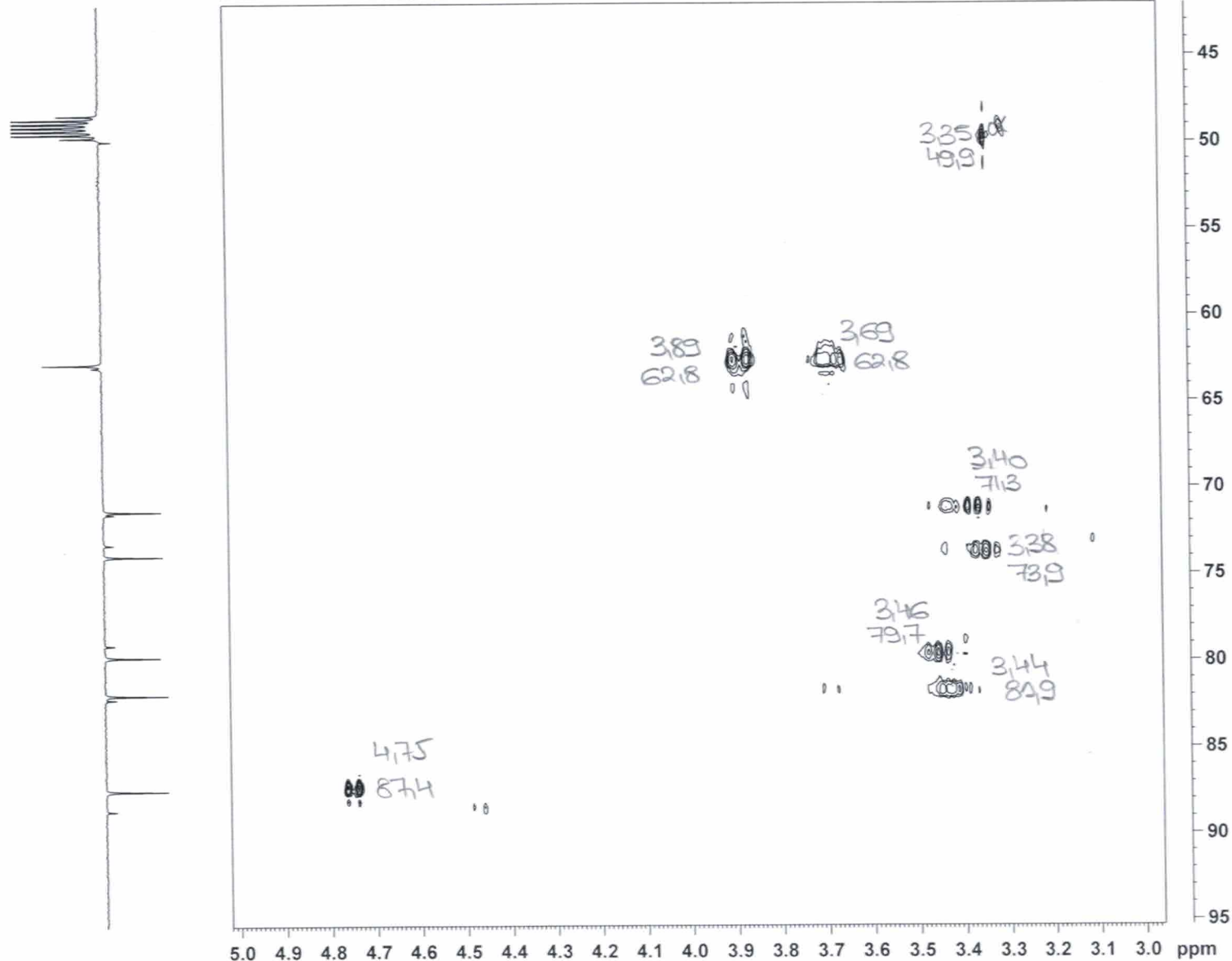
ppm
1.65
1.70
1.75
1.80
1.85
1.90
1.95
ppm







RA087
HSQC



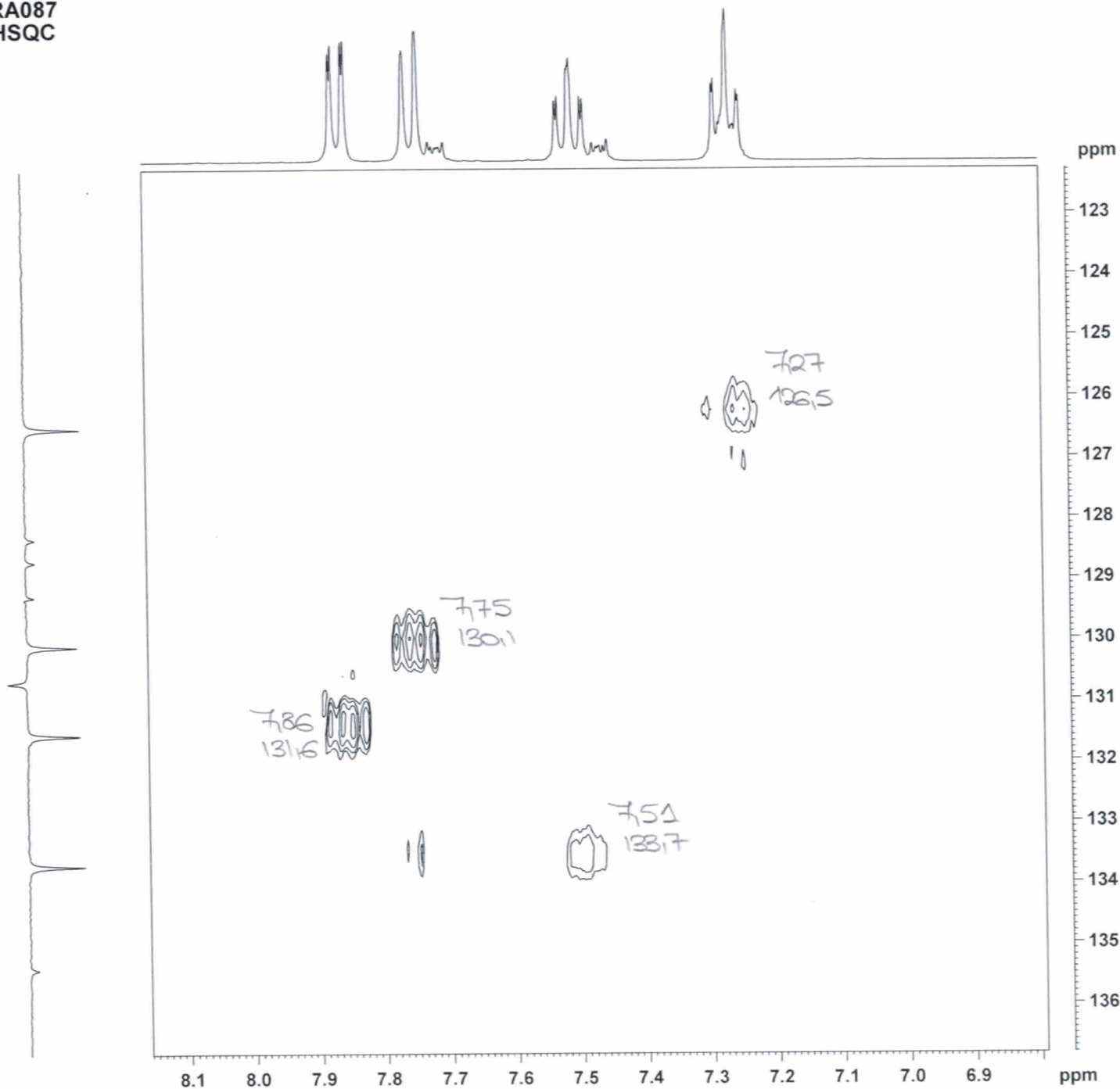
NAME ra087
EXPNO 22
PROCNO 1
Date_ 20140620
Time 7.15
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hsqcetpsi
TD 4096
SOLVENT MeOD
NS 2
DS 4
SWH 3180.662 Hz
FIDRES 0.776529 Hz
AQ 0.6440984 sec
RG 13004
DW 157.200 usec
DE 6.50 usec
TE 300.0 K
CNST2 140.0000000
D0 0.00000300 sec
D1 0.93200397 sec
D4 0.00178571 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
D24 0.00089000 sec
IN0 0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
P28 1000.00 usec
PL1 0.00 dB
SFO1 400.1318233 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 ^{13}C
P3 11.00 usec
P4 22.00 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
SFO2 100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
F16 1000.00 usec
ND0 2
TD 256
SFO1 100.6203 MHz
FIDRES 62.887669 Hz
SW 160.000 ppm
FnMODE Echo-Antiecho
SI 4096
SF 400.1300072 MHz
SSB QSINE
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 echo-antiecho
SF 100.6126309 MHz
SSB QSINE
LB 0.00 Hz
GB 0

RA087
HSQC



```

NAME      ra087
EXPNO     22
PROCNO    1
Date_     20140620
Time      7.15
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   hsqcetgpsi
TD        4096
SOLVENT   MeOD
NS        2
DS        4
SWH       3180.662 Hz
FIDRES    0.776529 Hz
AQ        0.6440984 sec
RG        13004
DW        157.200 usec
DE        6.50 usec
TE        300.0 K
CNST2     140.0000000
D0        0.00000300 sec
D1        0.93200397 sec
D4        0.00178571 sec
D11       0.03000000 sec
D13       0.00000400 sec
D16       0.00020000 sec
D24       0.00089000 sec
IN0       0.00003105 sec
ZGPTNS

```

```

===== CHANNEL f1 =====
NUC1      1H
P1        6.82 usec
P2        13.65 usec
P28       1000.00 usec
PL1       0.00 dB
SFO1      400.1318233 MHz

```

```

===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3        11.00 usec
P4        22.00 usec
PCPD2     80.00 usec
PL2       0.00 dB
PL12      17.23 dB
SFO2      100.6203150 MHz

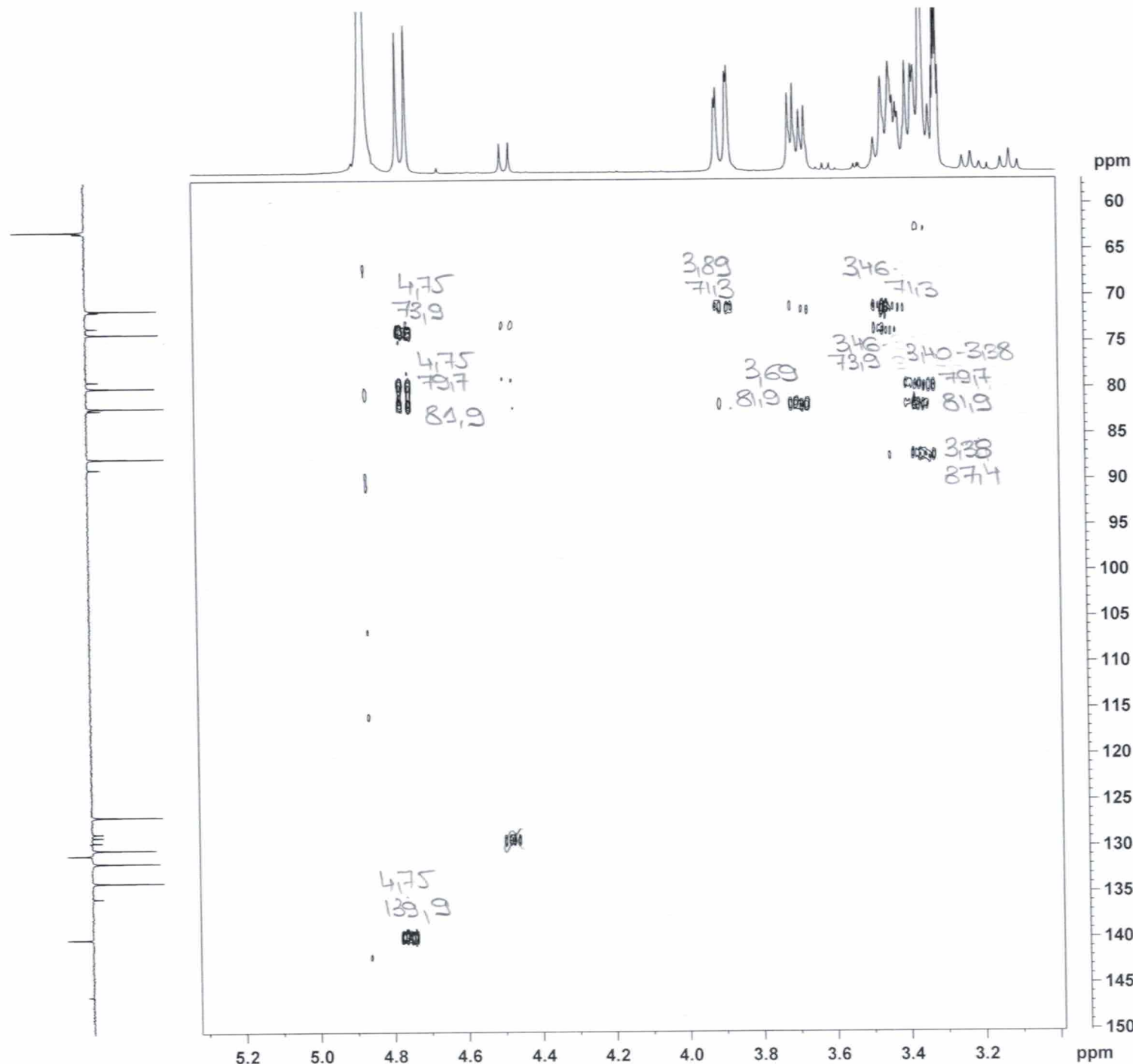
```

```

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPZ1      80.00 %
GPZ2      20.10 %
P16       1000.00 usec
ND0       2
TD        256
SFO1      100.6203 MHz
FIDRES    62.887669 Hz
SW        160.000 ppm
FnMODE    Echo-Antiecho
SI        4096
SF        400.1300072 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.40
SI        512
MC2       echo-antiecho
SF        100.6126309 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0

```

RA087
HMBC



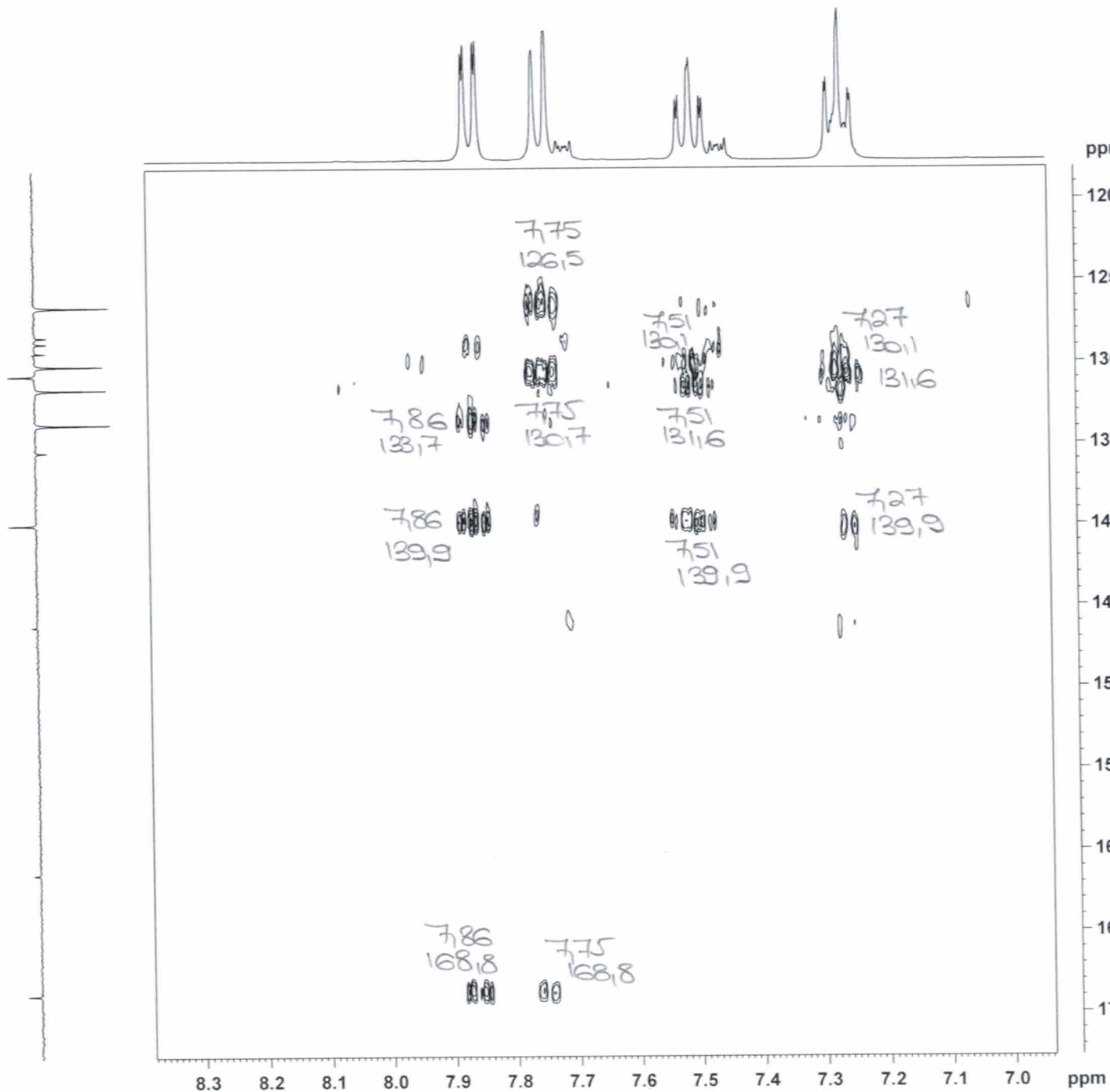
NAME ra087
EXPNO 23
PROCNO 1
Date_ 20140620
Time_ 7.30
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 4096
SOLVENT MeOD
NS 6
DS 4
SWH 3180.662 Hz
FIDRES 0.776529 Hz
AQ 0.6440984 sec
RG 18390.4
DW 157.200 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 0.95555300 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1318233 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6238 MHz
FIDRES 90.403236 Hz
SW 229.997 ppm
FnMODE QF
SI 4096
SF 400.1300072 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6126309 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

RA087 HMBC



```

NAME          ra087
EXPNO         23
PROCNO        1
Date_         20140620
Time          7.30
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       hmbcpg1pndqf
TD            4096
SOLVENT       MeOD
NS            6
DS            4
SWH           3180.662 Hz
FIDRES        0.776529 Hz
AQ            0.6440984 sec
RG            18390.4
DW            157.200 usec
DE            6.50 usec
TE            300.0 K
CNST2         145.0000000
CNST13        8.0000000
D0            0.00000300 sec
D1            0.95555300 sec
D2            0.00344828 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002160 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
PL1           0.00 dB
SFO1          400.1318233 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            11.00 usec
PL2           0.00 dB
SFO2          100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6238 MHz
FIDRES        90.403236 Hz
SW            229.997 ppm
FnMODE        QF
SI            4096
SF            400.1300072 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6126309 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
  
```

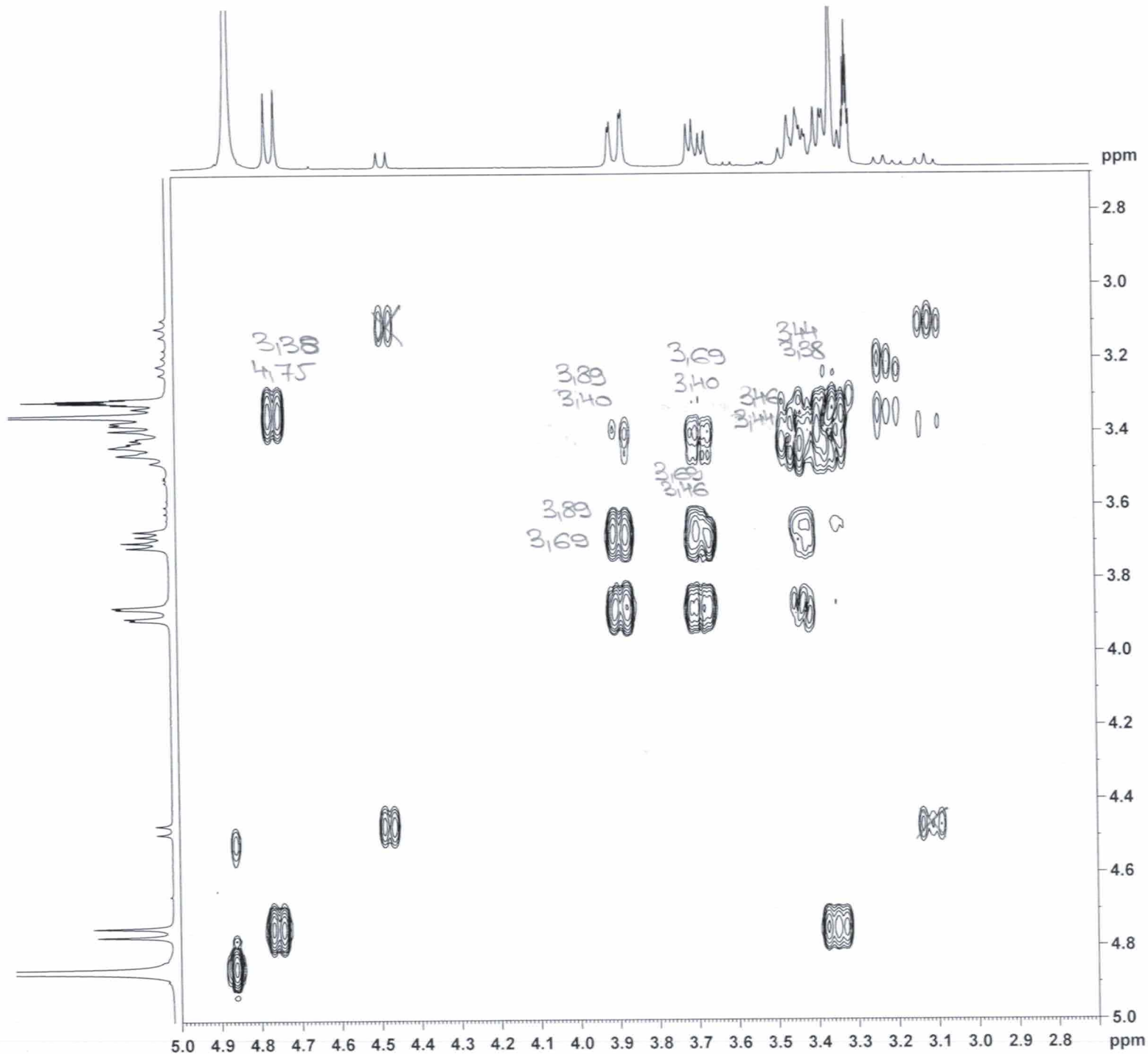
```

NAME                                ra087
EXFNO                               21
PROCNO                               1
Date_                               20140620
Time_                               7.08
INSTRUM                            spect
PROBHD      5 mm Multinuc1
PULPROG                            cosygmrgf
TD                                  2134
SOLVENT                             MeOD
NS                                  1
DS                                  8
SWH                                3180.662 Hz
FIDRES                            1.490469 Hz
AQ                                0.3356720 sec
RG                                  4096
DW                                157.200 usec
DE                                  6.50 usec
TE                                  300.0 K
DO                                0.00000300 sec
D1                                0.96371931 sec
D13                              0.00000400 sec
D16                              0.00020000 sec
INO                              0.00031440 sec

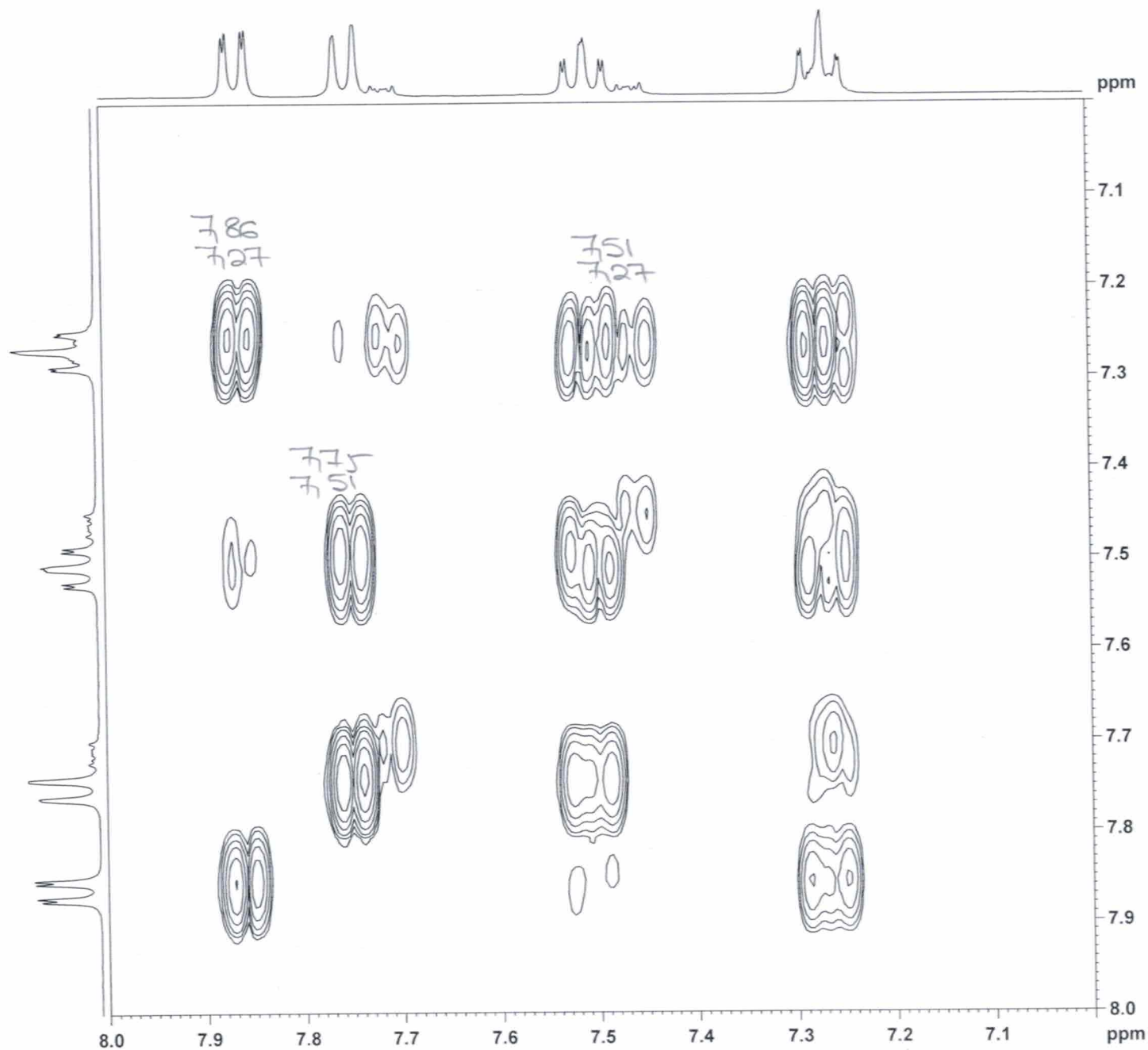
===== CHANNEL f1 =====
NUC1                                1H
P1                                  6.82 usec
PL1                                0.00 dB
SFO1                              400.1318233 MHz

===== GRADIENT CHANNEL =====
GPNAM1                             SINE.100
GPNAM2                             SINE.100
GPNAM3                             SINE.100
GPZ1                                16.00 %
GPZ2                                12.00 %
GPZ3                                40.00 %
P16                                1000.00 usec
NDO                                 1
TD                                  256
SFO1                                400.1318 MHz
FIDRES                            12.424459 Hz
SW                                  7.949 ppm
FnMODE                             QF
SI                                  2048
SF                                400.1300072 MHz
WDW                                QSINE
SSB                                 1
LB                                  0.00 Hz
GB                                  0
PC                                  1.40
SI                                  512
MC2                                QF
SF                                400.1300072 MHz
WDW                                QSINE
SSB                                 1
LB                                  0.00 Hz
GB                                  0

```



RA087 COSY



```

NAME          ra087
EXPNO         21
PROCNO        1
Date_         20140620
Time          7.08
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       cosygpmfqr
TD            2134
SOLVENT       MeOD
NS            1
DS            8
SWH           3180.662 Hz
FIDRES        1.490469 Hz
AQ            0.3356720 sec
RG            4096
DW            157.200 usec
DE            6.50 usec
TE            300.0 K
D0            0.00000300 sec
D1            0.96371931 sec
D13           0.00000400 sec
D16           0.00020000 sec
INO           0.00031440 sec
  
```

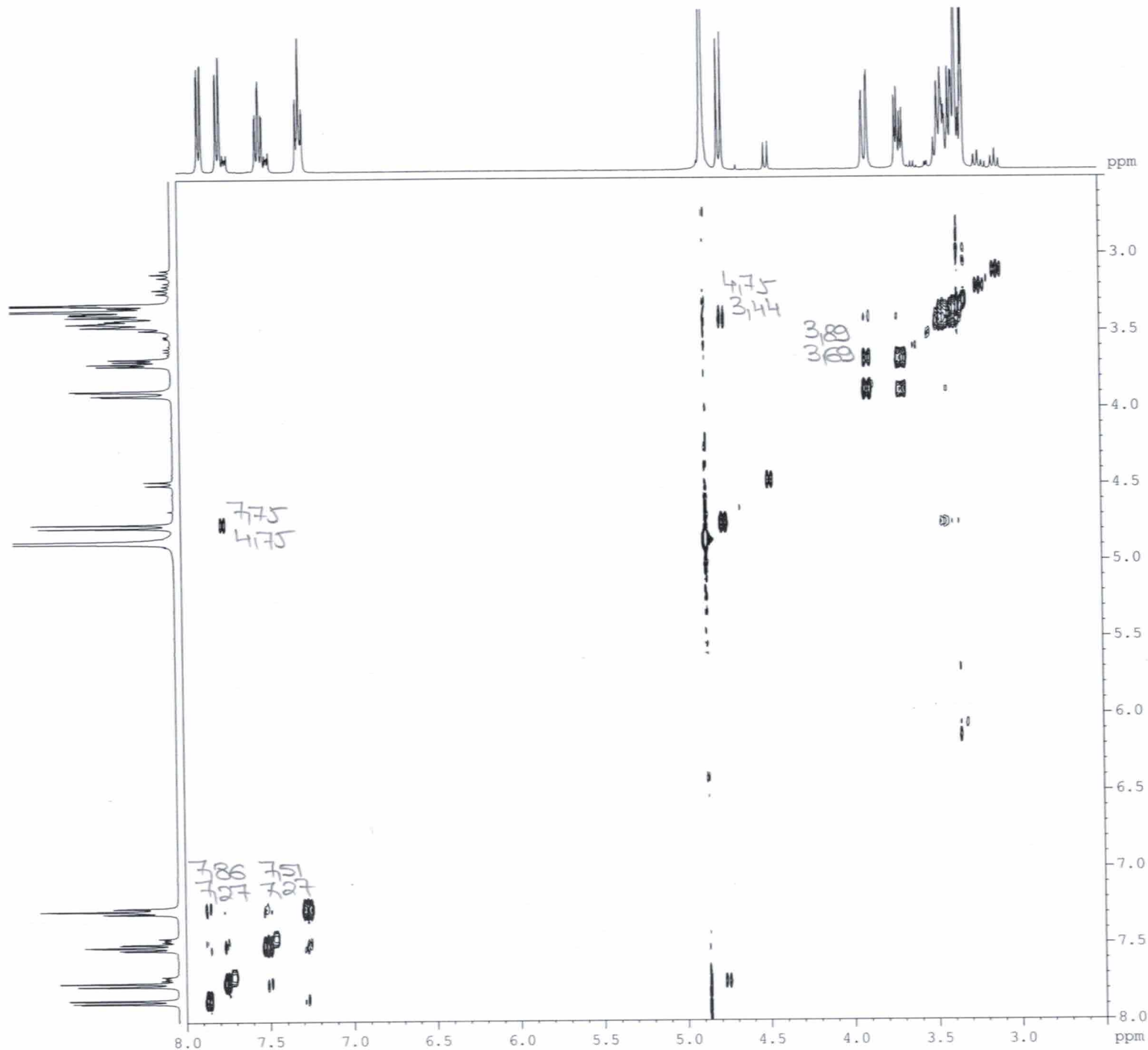
```

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
PL1           0.00 dB
SFO1          400.1318233 MHz
  
```

```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPZ1          16.00 %
GPZ2          12.00 %
GPZ3          40.00 %
P16           1000.00 usec
ND0           1
TD            256
SFO1          400.1318 MHz
FIDRES        12.424459 Hz
SW            7.949 ppm
FIRMODE       QF
SI            2048
SF            400.1300072 MHz
WDW           QSINE
SSB           1
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           QF
SF            400.1300072 MHz
WDW           QSINE
SSB           1
LB            0.00 Hz
GB            0
  
```

RA087 NOESY



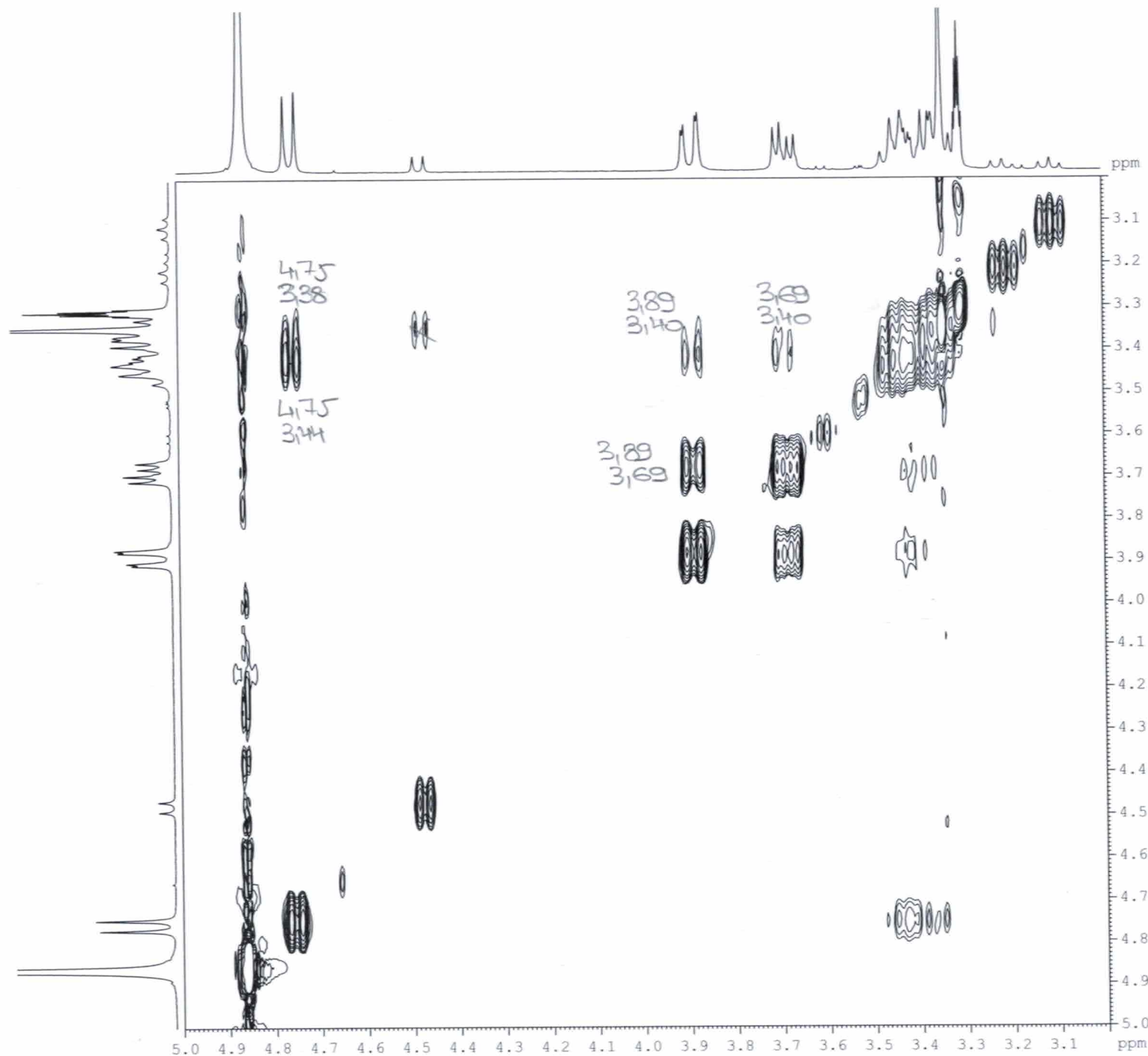
```

NAME          ra087
EXPNO         24
PROCNO        1
Date_         20140620
Time          8.14
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       noesygpph
TD            2134
SOLVENT       MeOD
NS            2
DS            16
SWH           3180.662 Hz
FIDRES        1.490469 Hz
AQ            0.3356720 sec
RG            45.3
DE            157.200 usec
TE            300.0 K
D0            0.00014851 sec
D1            1.46457398 sec
D8            0.80000001 sec
D16           0.00020000 sec
IN0           0.00031440 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
PL1           0.00 dB
SFO1          400.1318233 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPZ1          40.00 %
P16           1000.00 usec
NDO           1
TD            256
SFO1          400.1318 MHz
FIDRES        12.424459 Hz
SW            7.949 ppm
FnMODE        States-TPPI
SI            2048
SF            400.1300072 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           States-TPPI
SF            400.1300072 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

RA087 NOESY

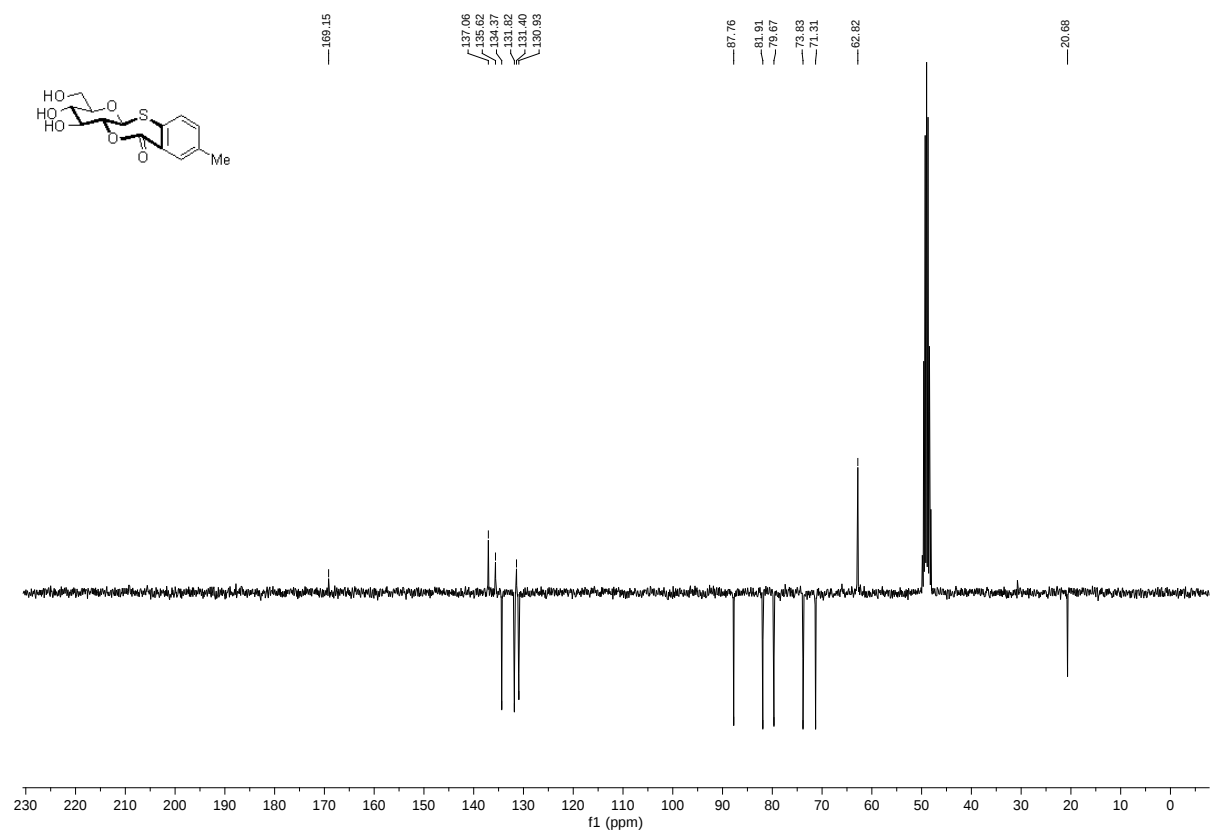
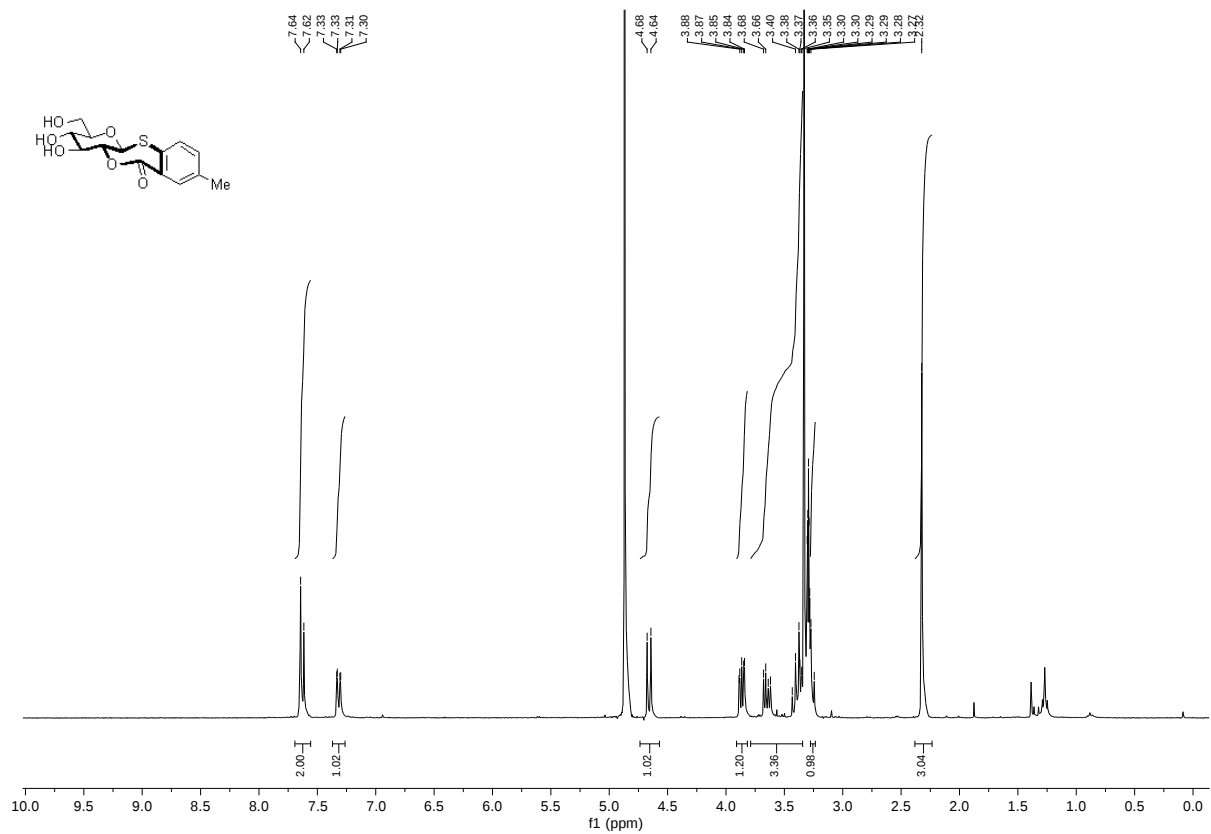


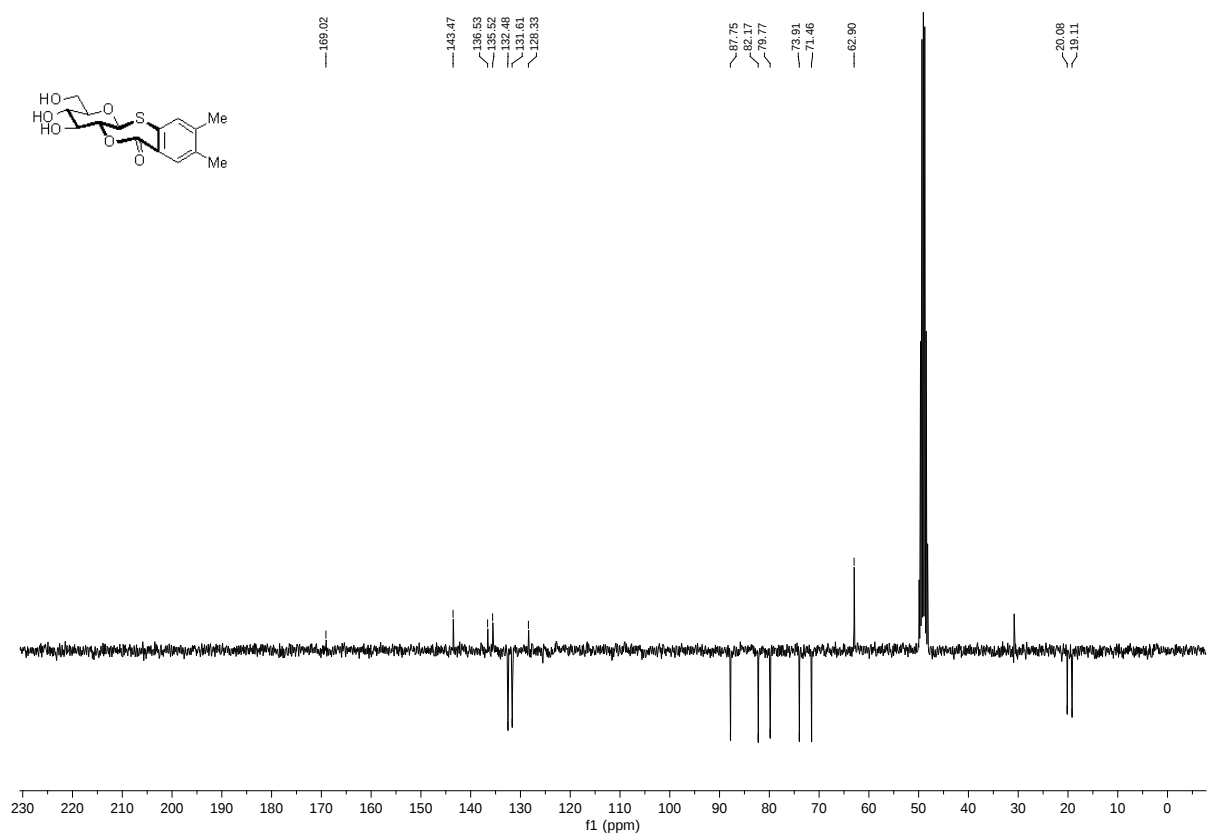
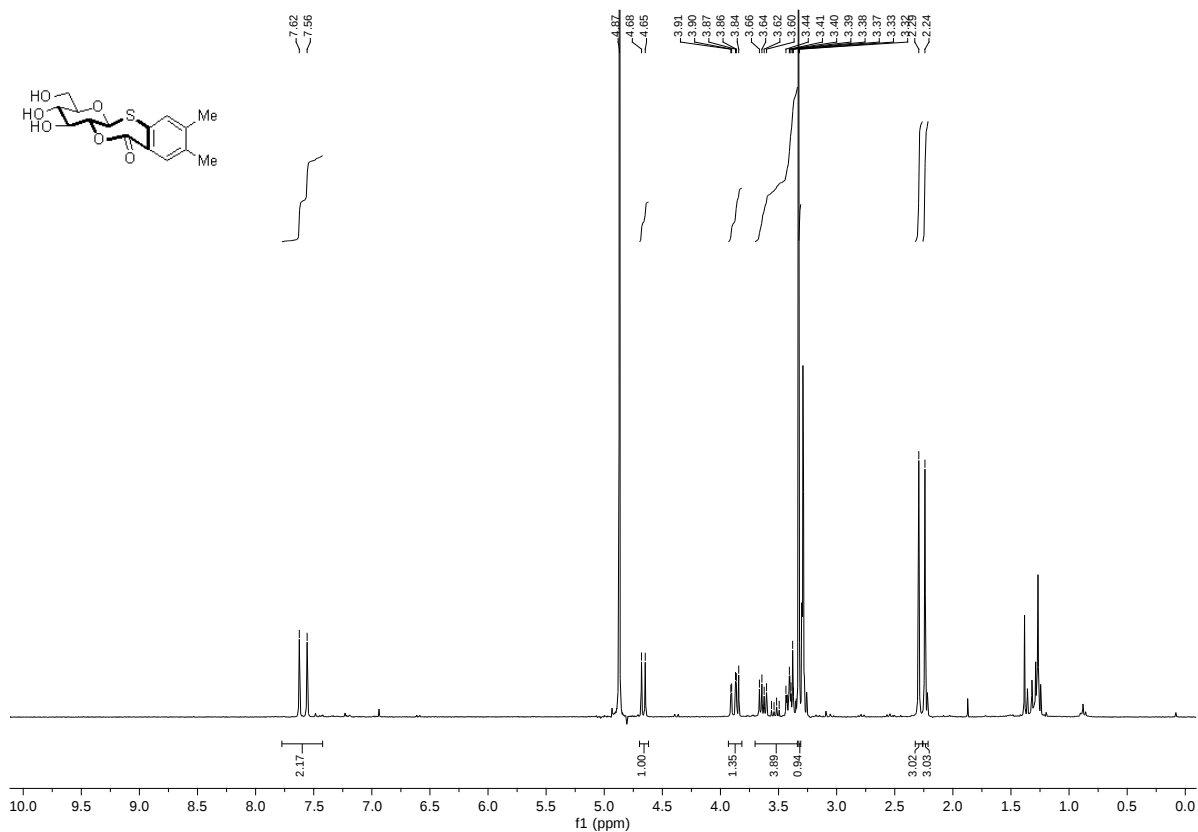
```

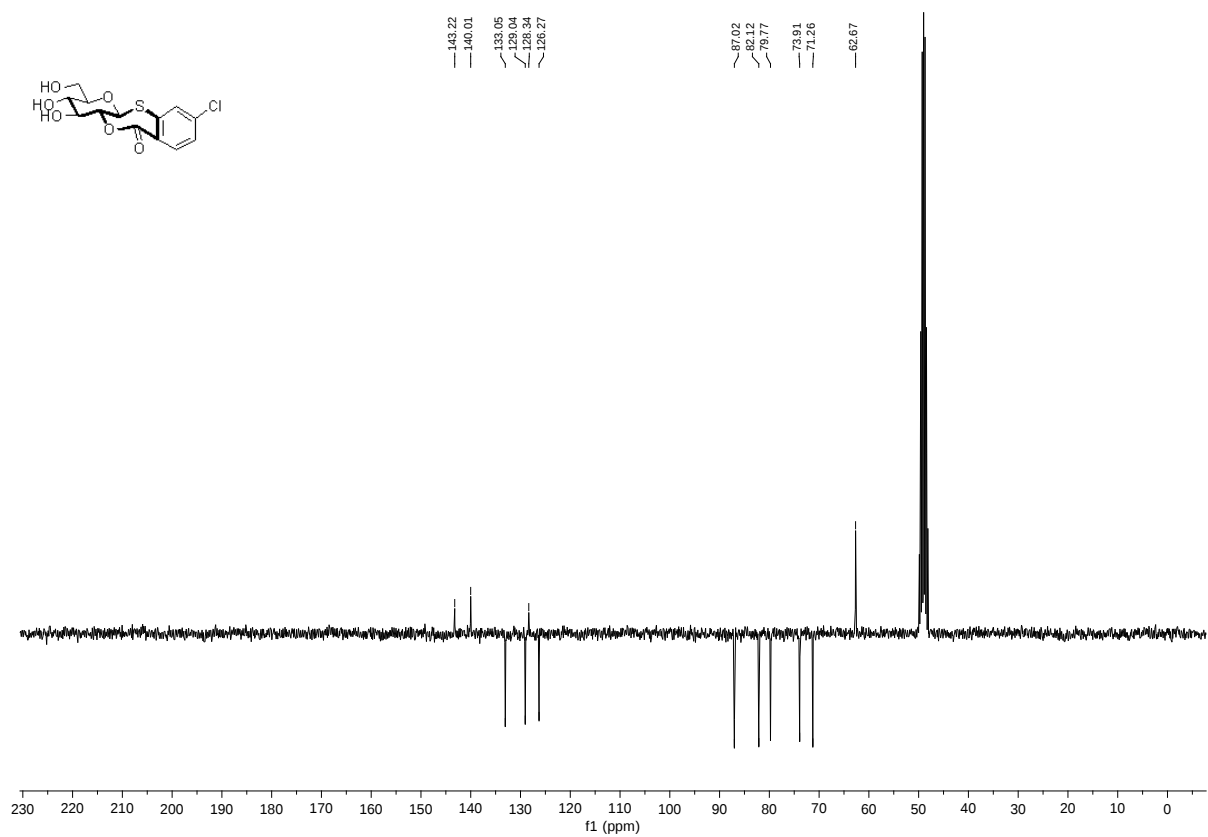
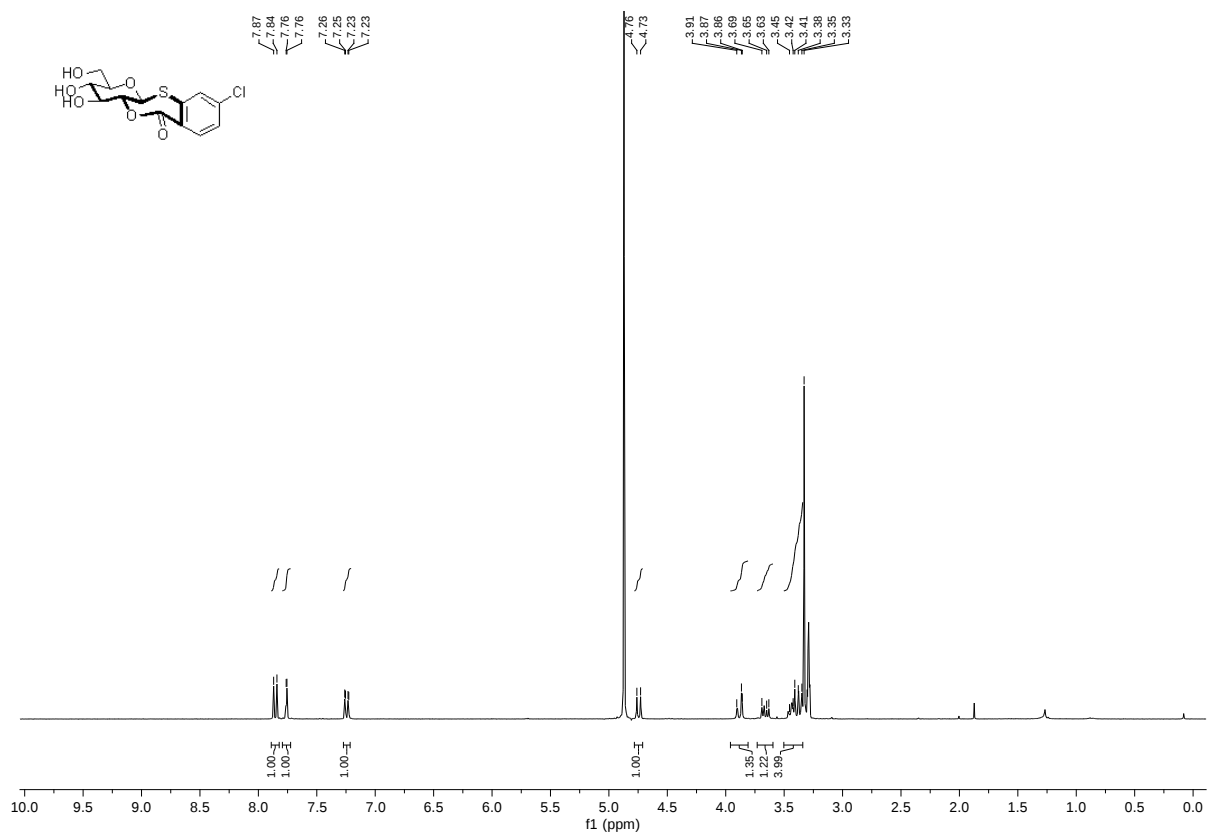
NAME      ra087
EXPNO     24
PROCNO    1
Date_     20140620
Time      8.14
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   noesygpph
TD        2134
SOLVENT   MeOD
NS         2
DS         16
SWH        3180.662 Hz
FIDRES     1.490469 Hz
AQ         0.3356720 sec
RG         45.3
DW         157.200 usec
DE         6.50 usec
TE         300.0 K
D0         0.00014851 sec
D1         1.46457398 sec
D8         0.80000001 sec
D16        0.00020000 sec
IN0        0.00031440 sec

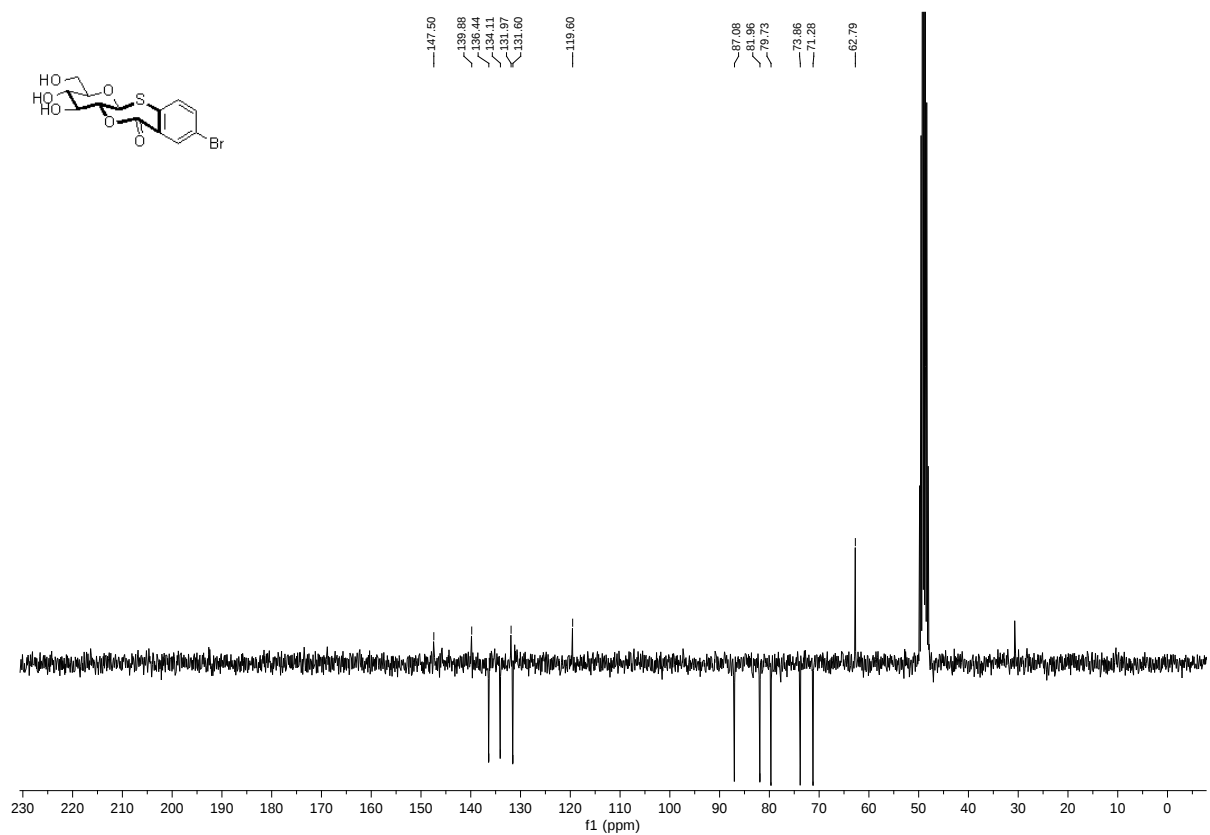
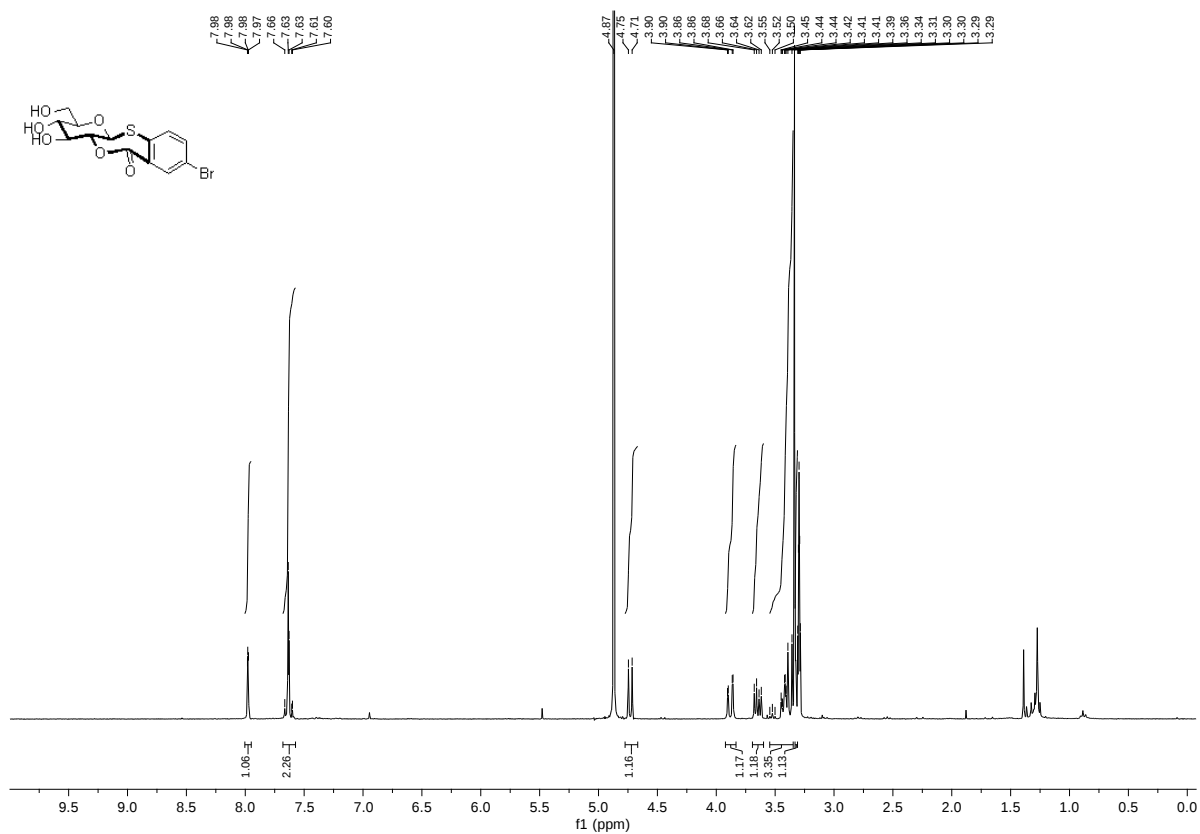
===== CHANNEL f1 =====
NUC1       1H
P1         6.82 usec
P2         13.65 usec
PL1        0.00 dB
SFO1       400.1318233 MHz

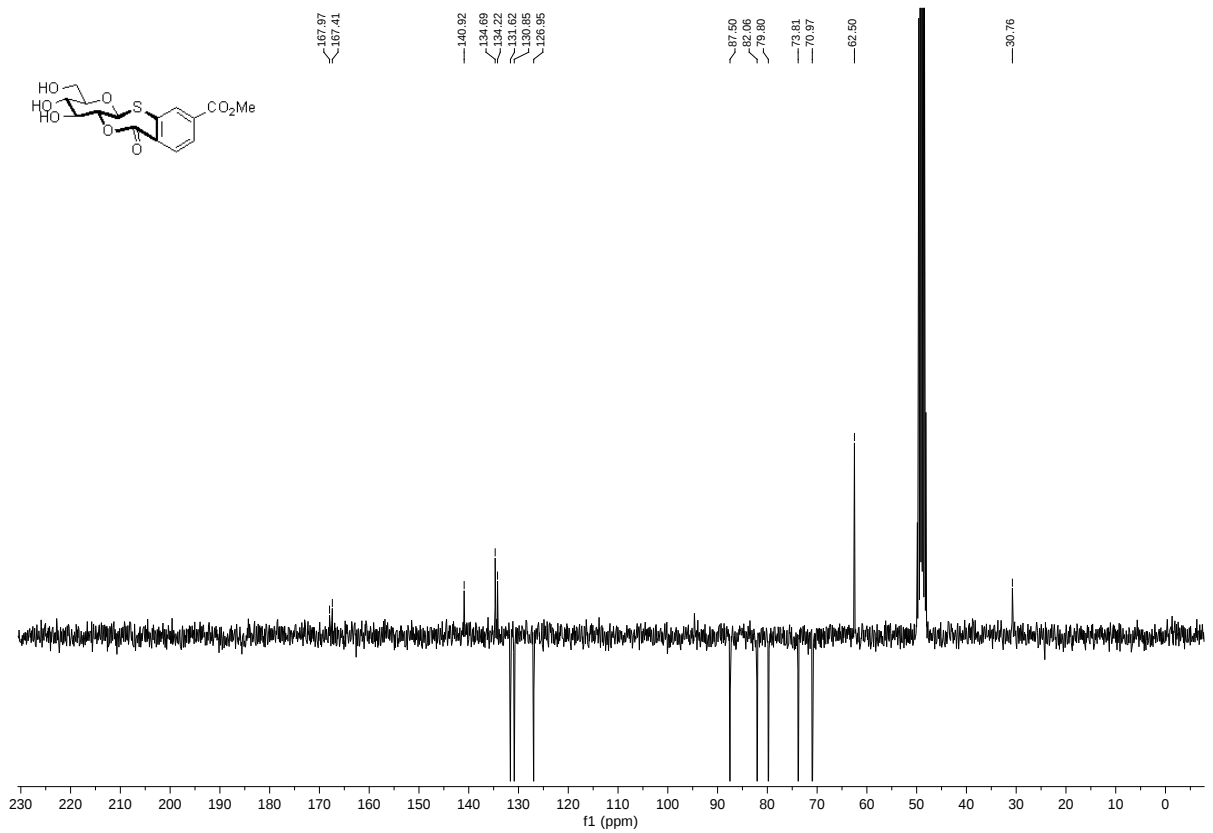
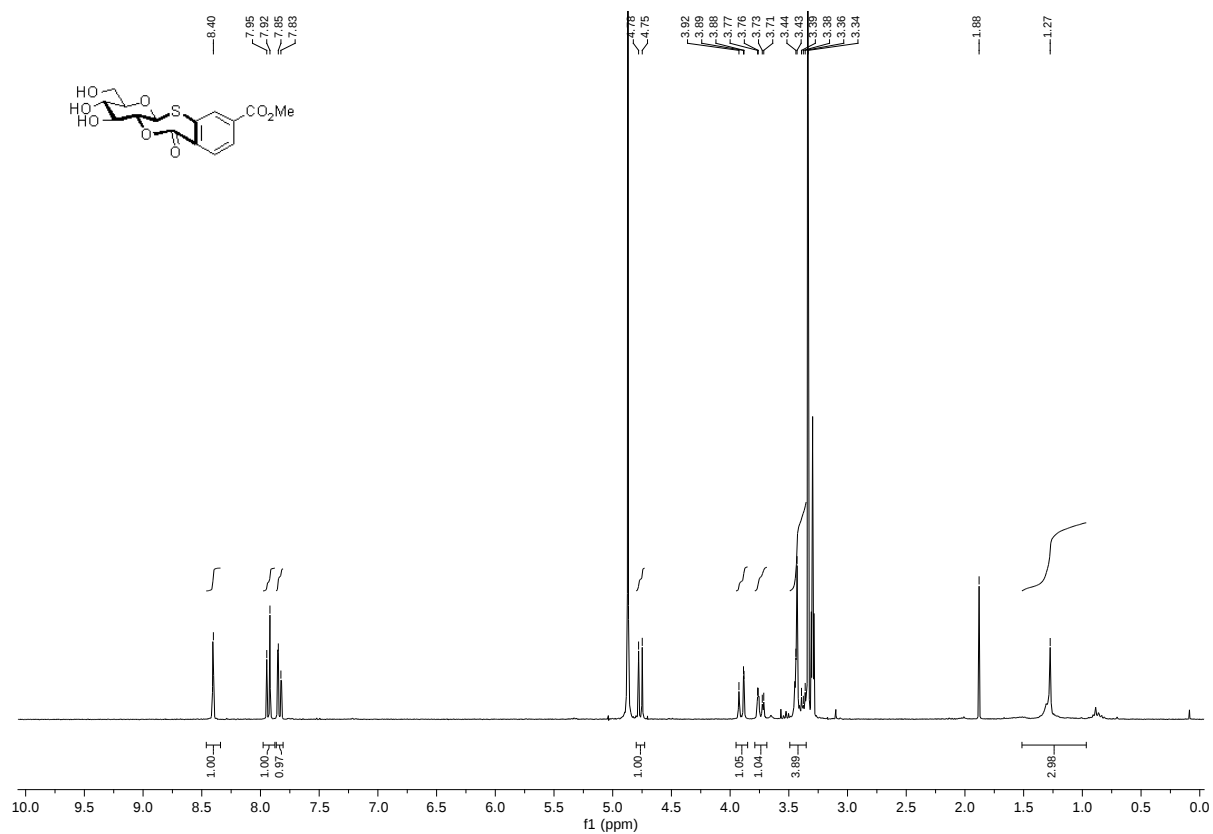
===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPZ1       40.00 %
P16        1000.00 usec
ND0        1
TD         256
SFO1       400.1318 MHz
FIDRES     12.424459 Hz
SW         7.949 ppm
FnMODE     States-TPPI
SI         2048
SF         400.1300072 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.40
SI         -512
MC2        States-TPPI
SF         400.1300072 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
  
```

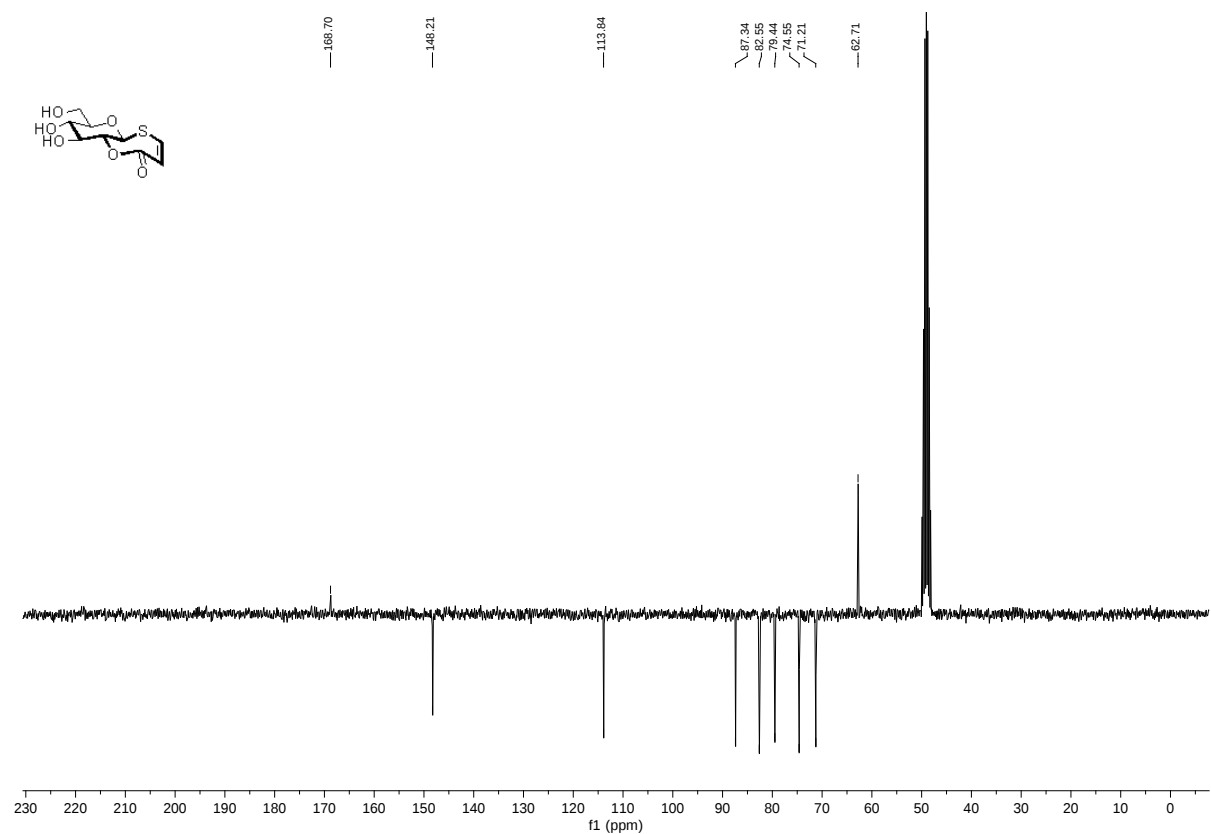
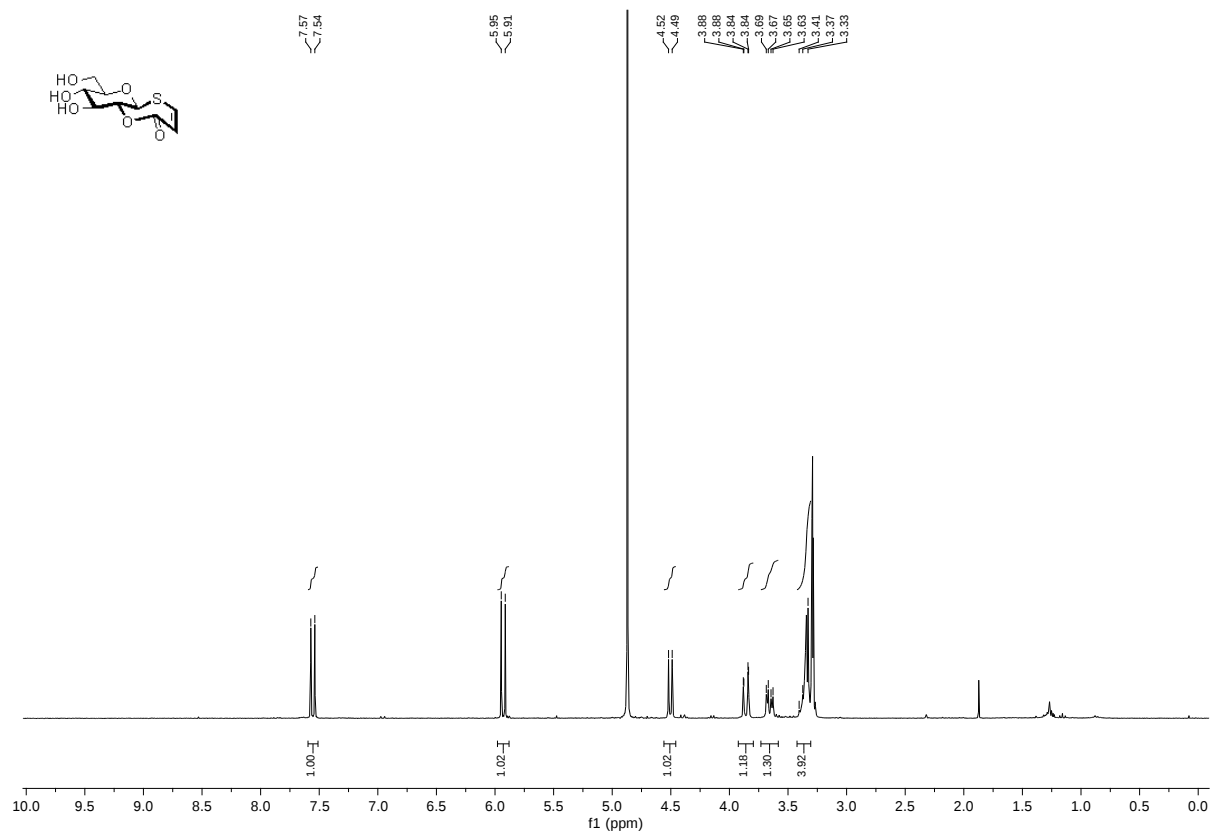


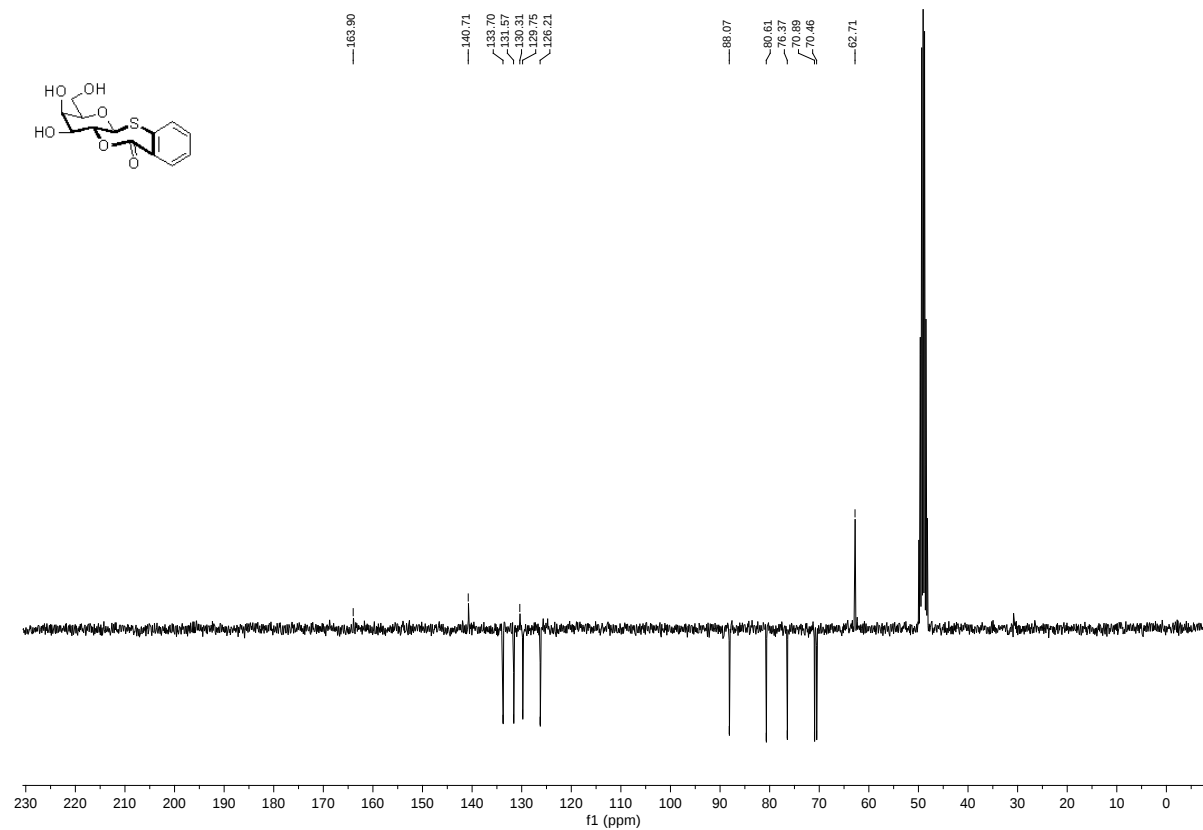
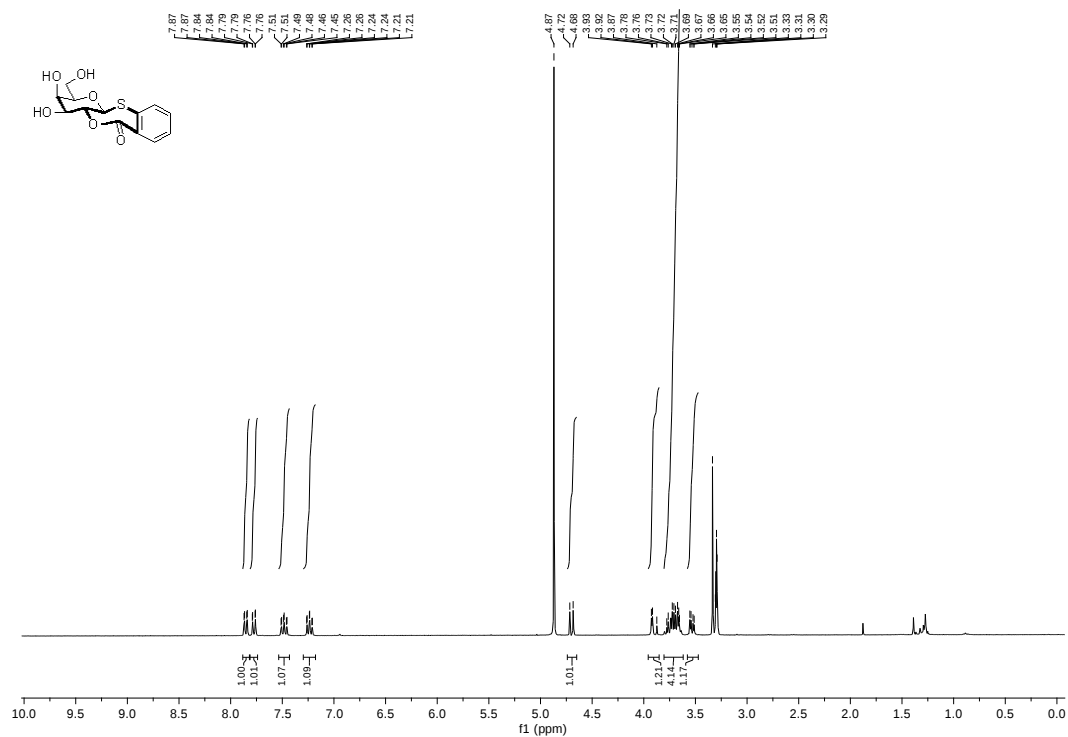


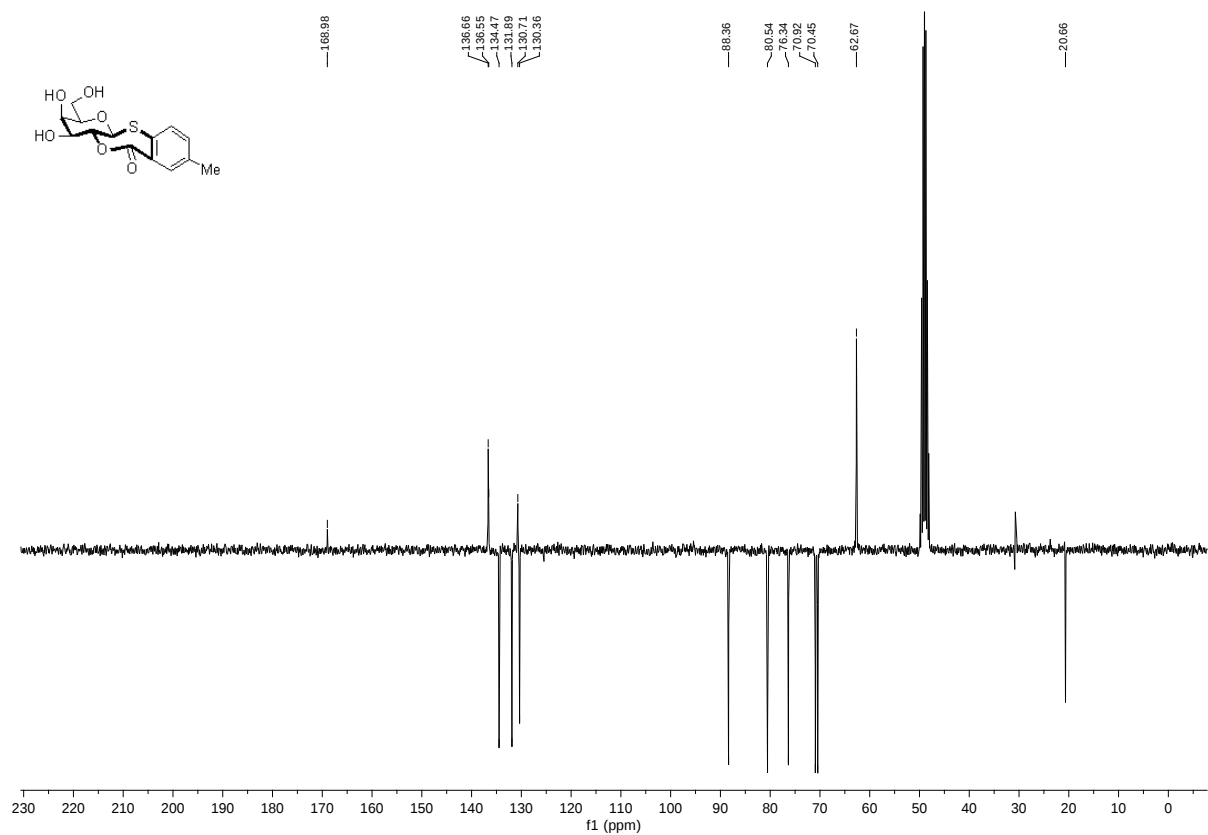
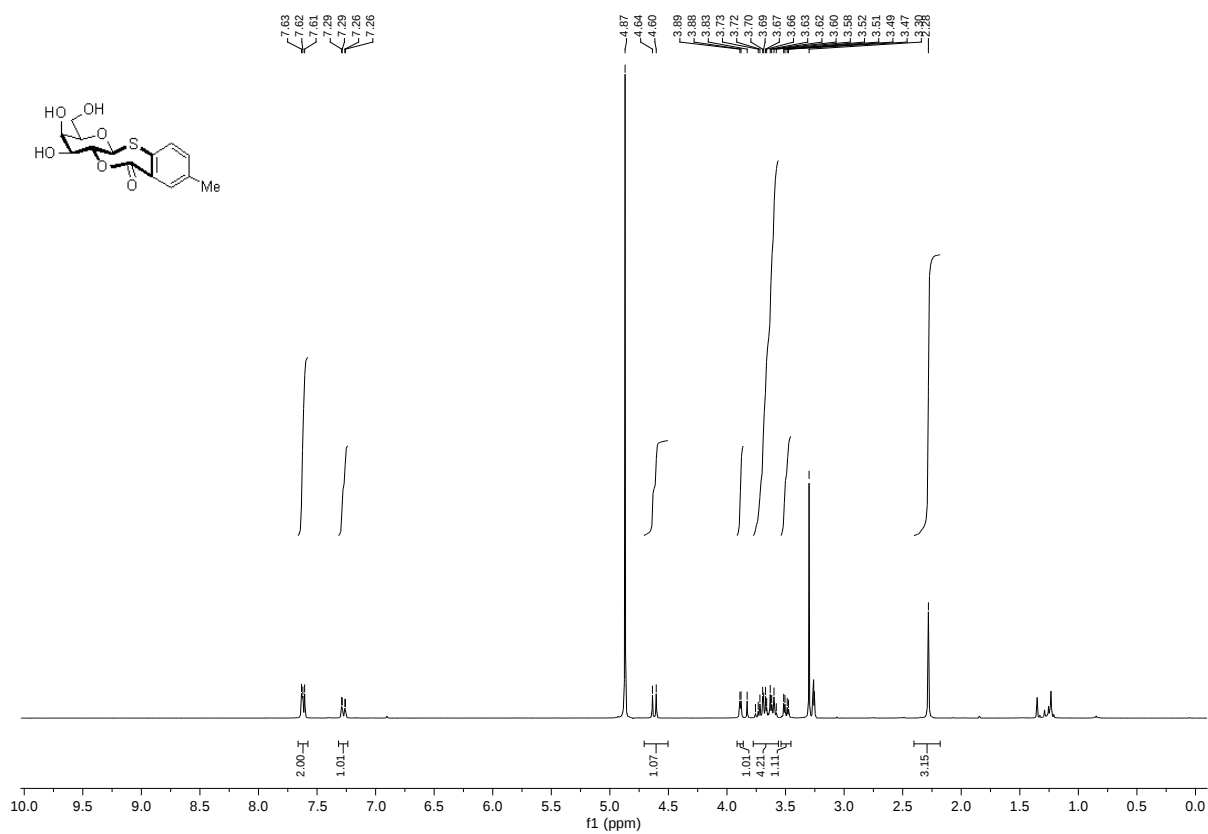


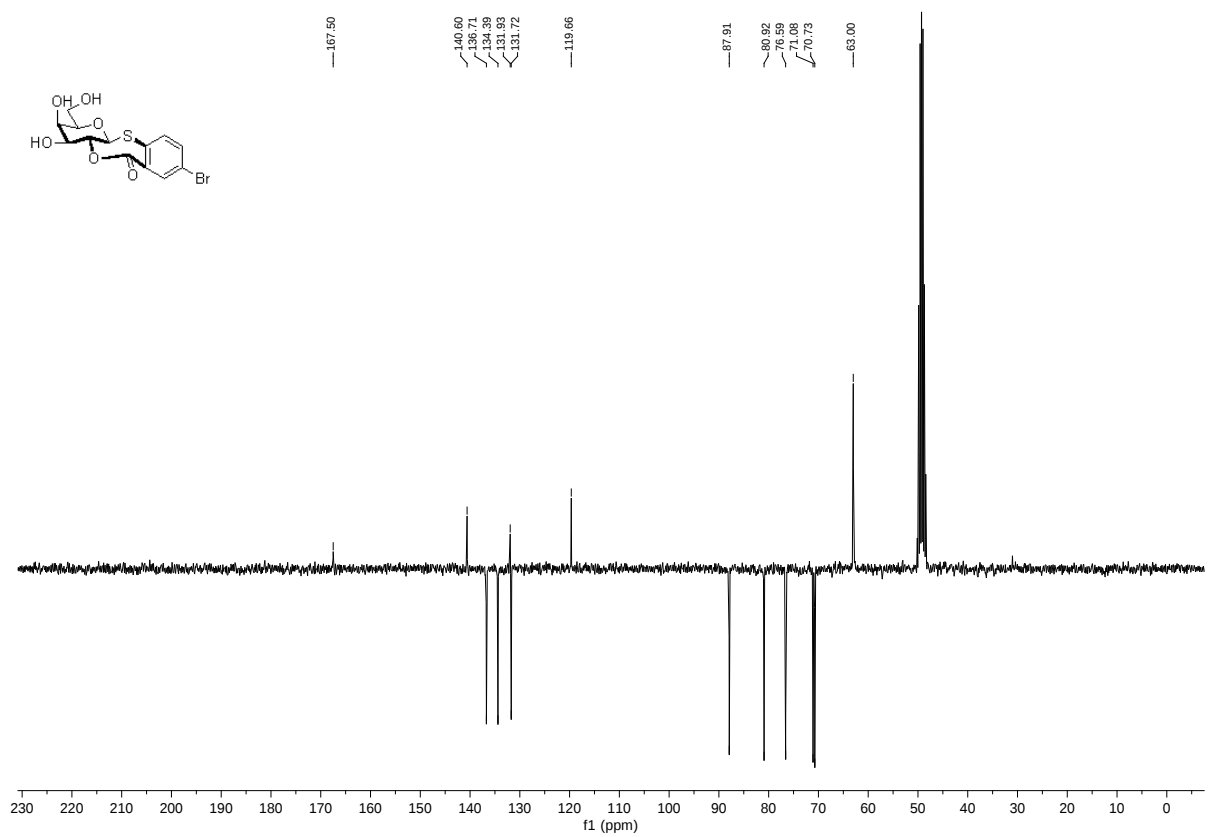
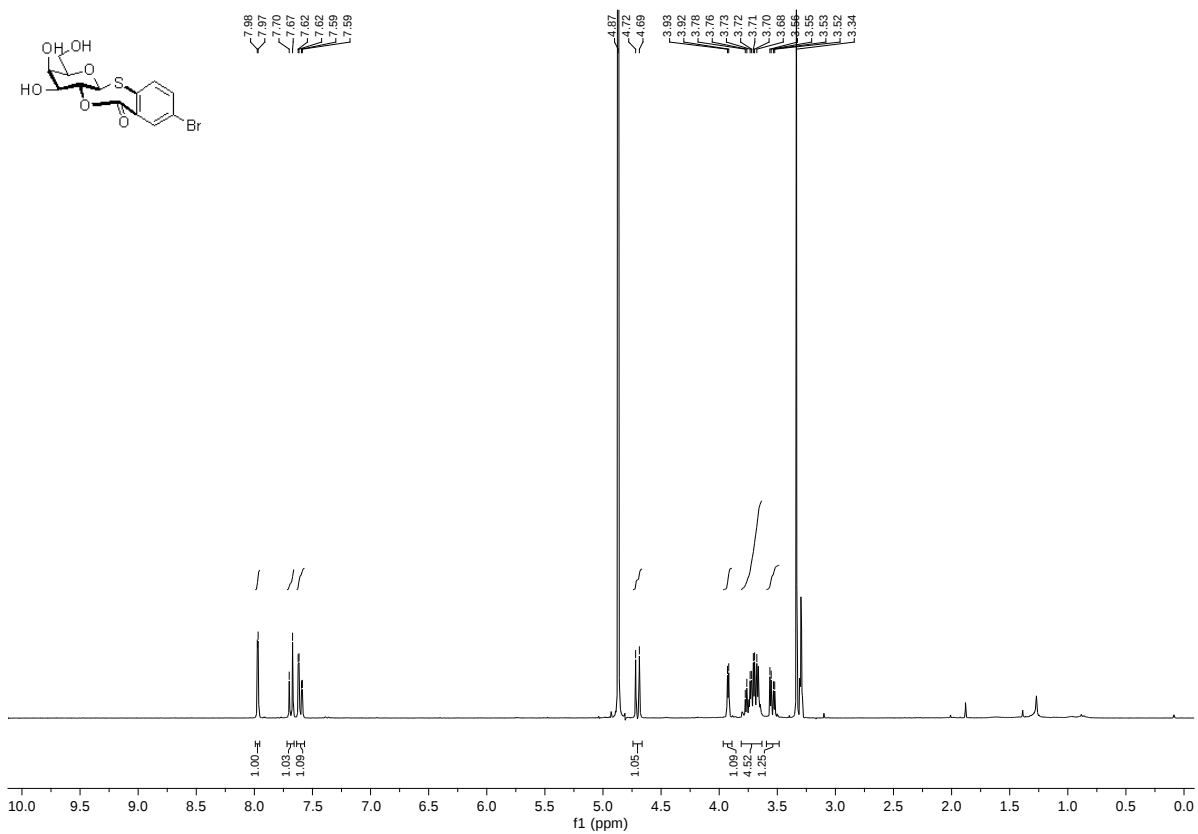


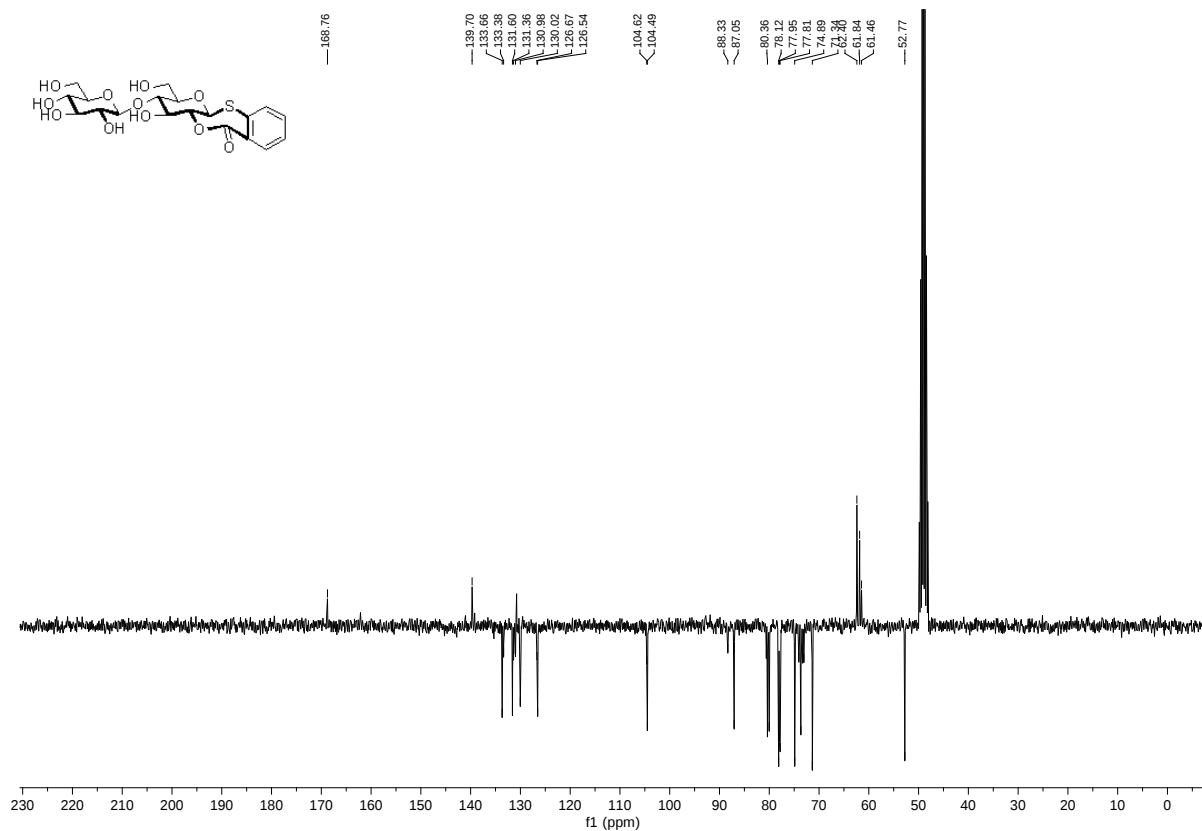
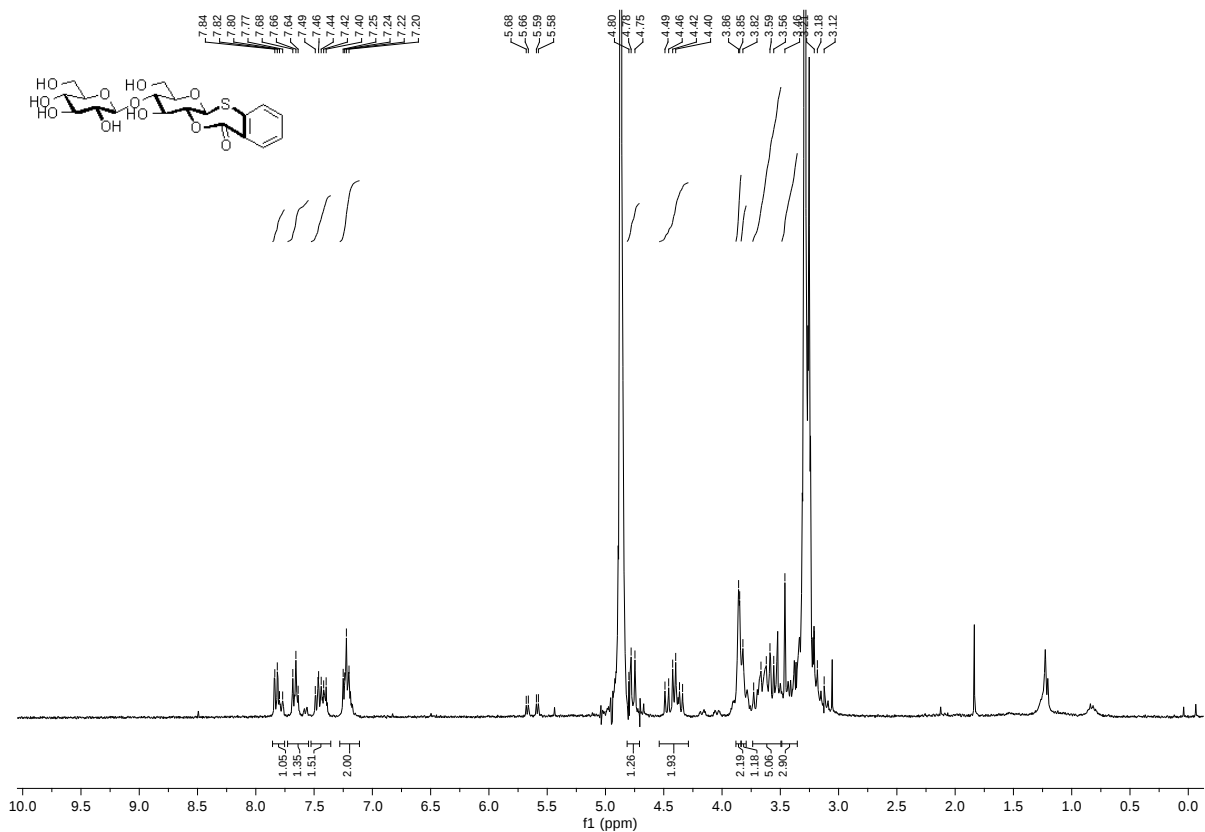


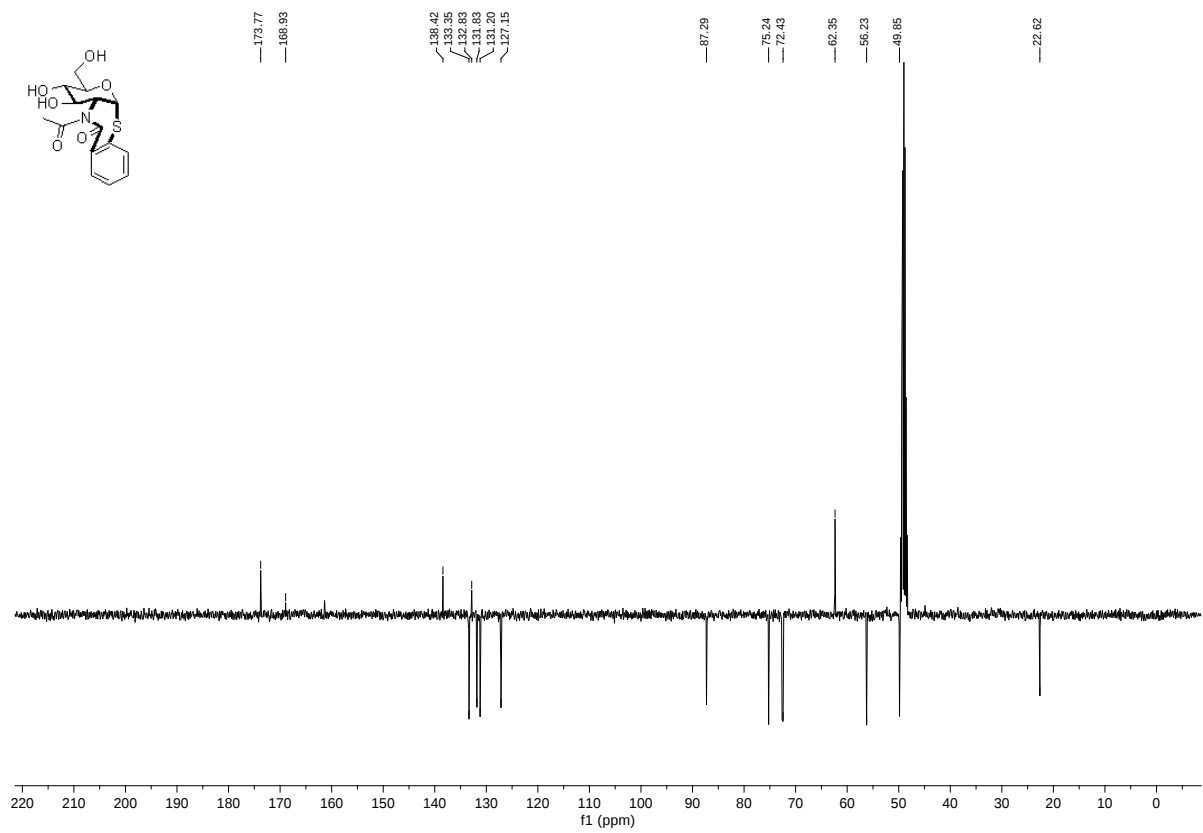
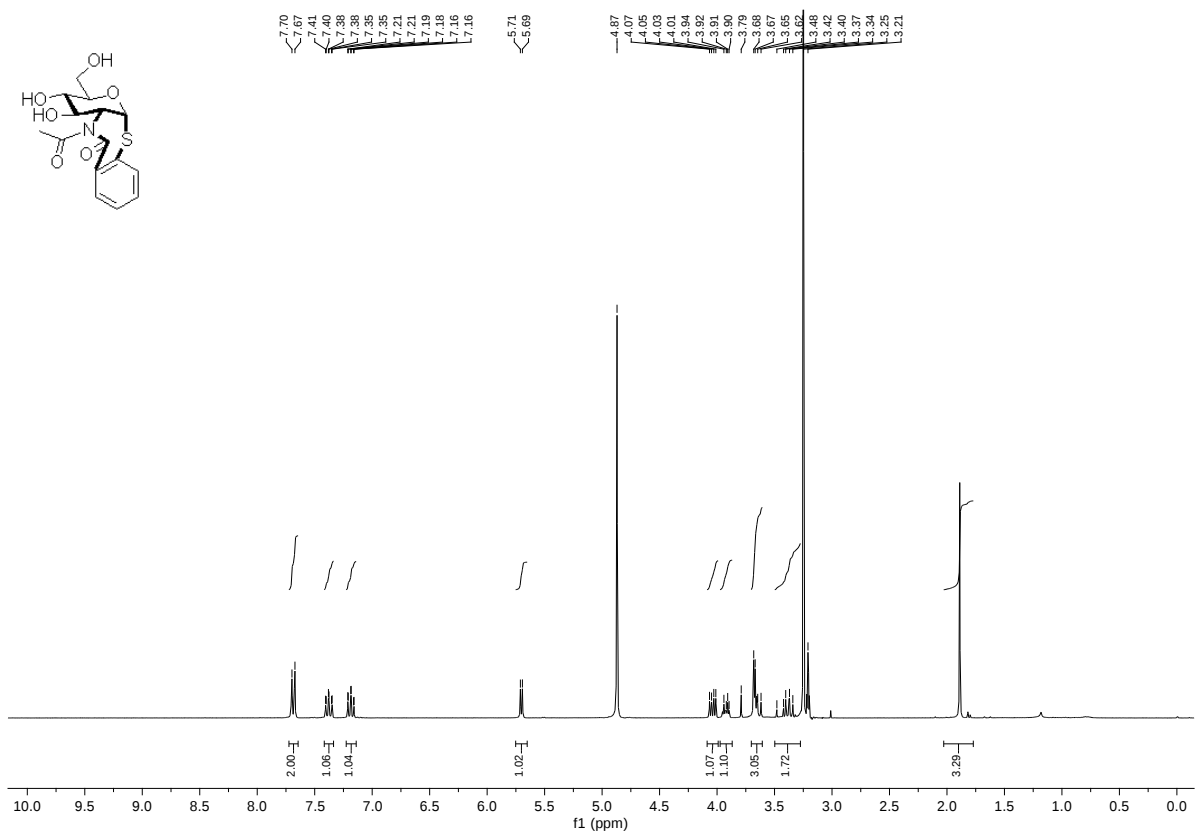


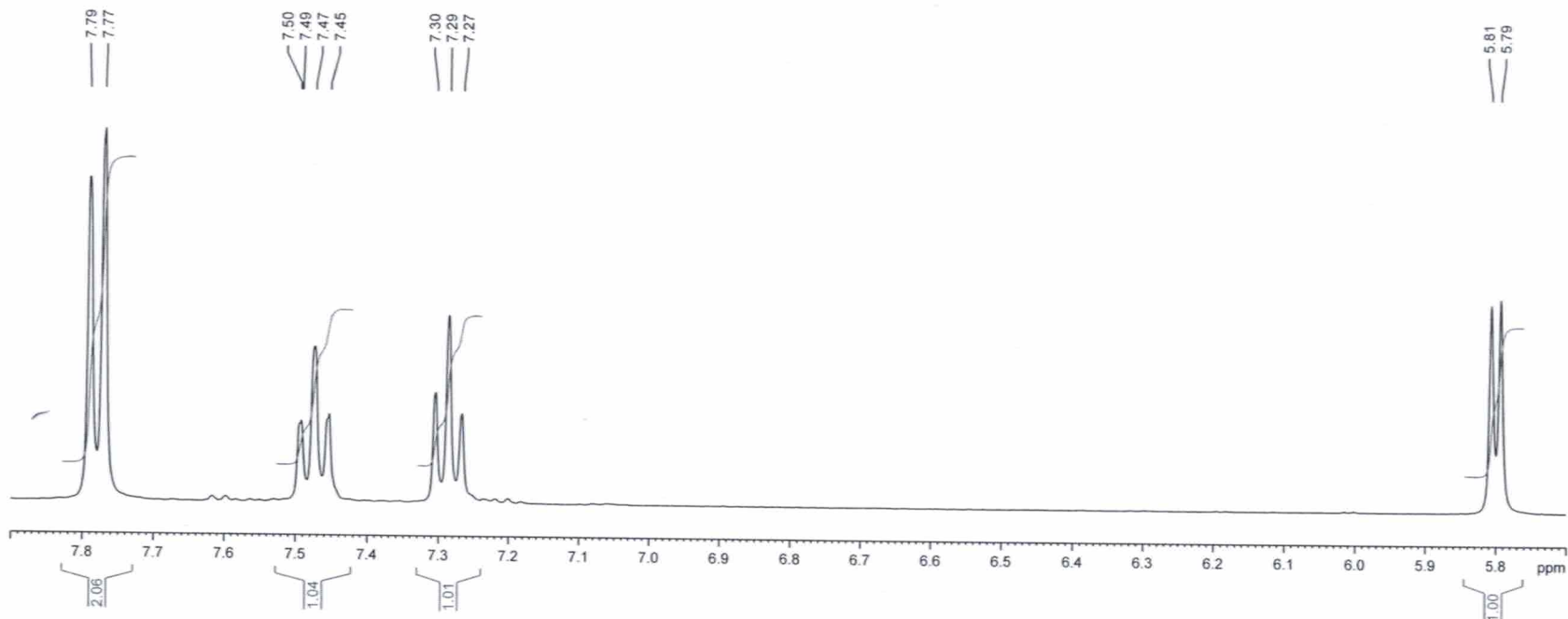








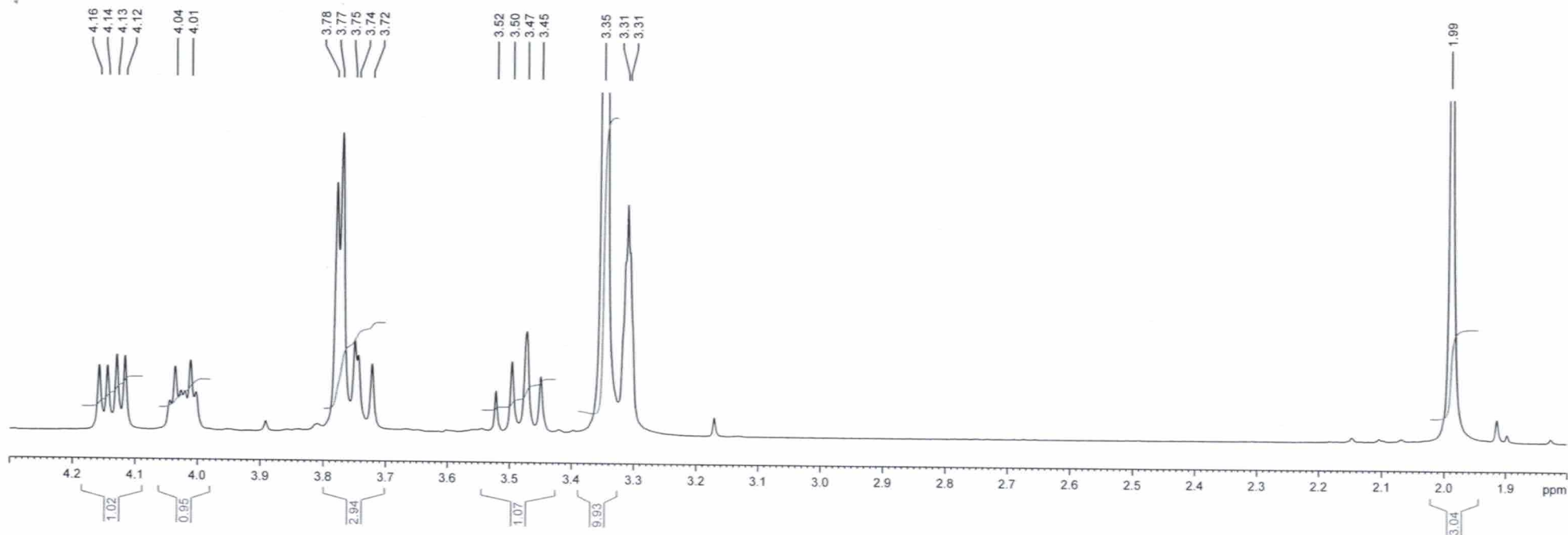


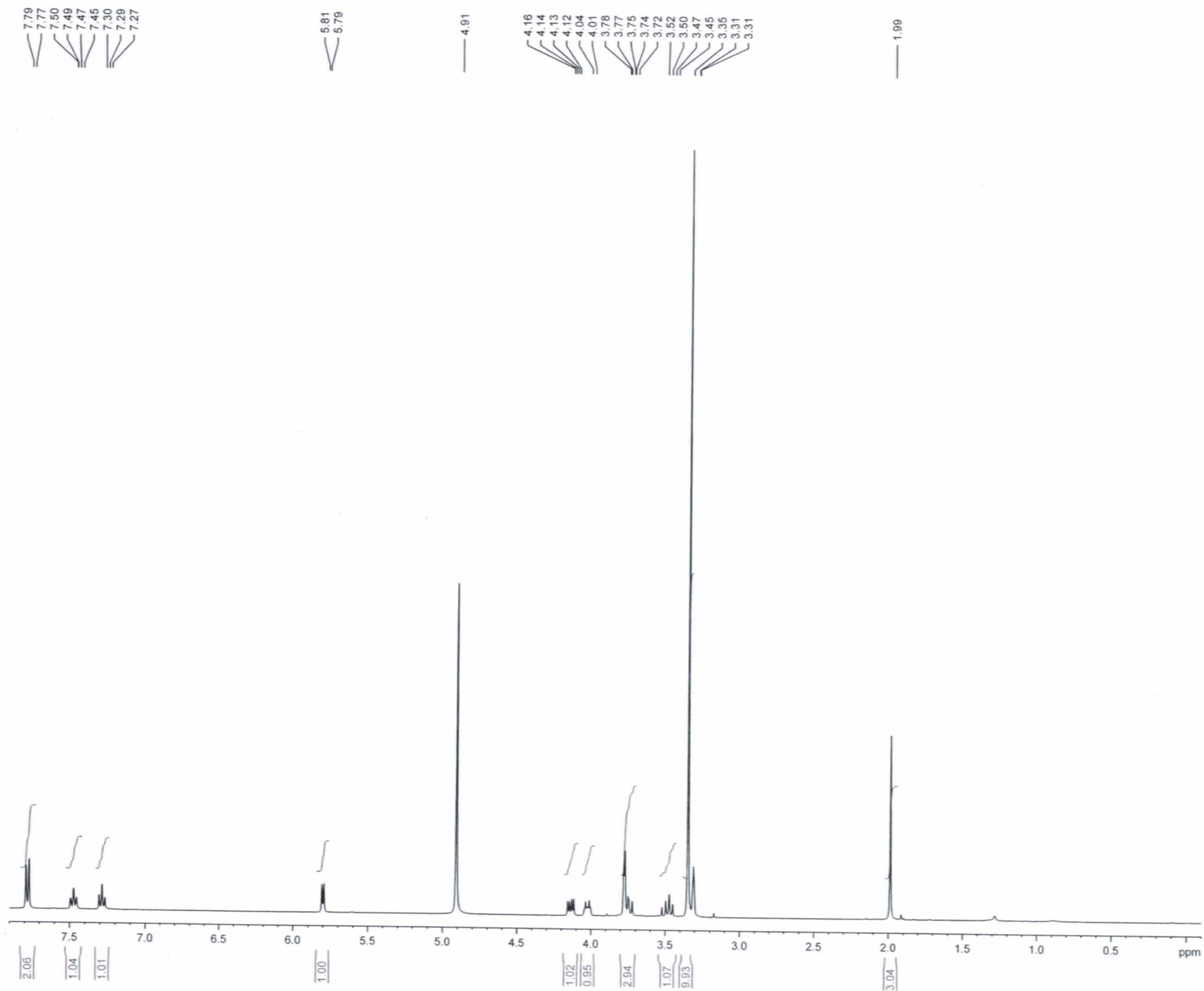


ra155 Cycl. Proton

NAME ra1555
EXPNO 10
PROCNO 1
Date_ 20141209
Time 8.55
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 16
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 71.8
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SF01 400.1336012 MHz
SI 32768
SF 400.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





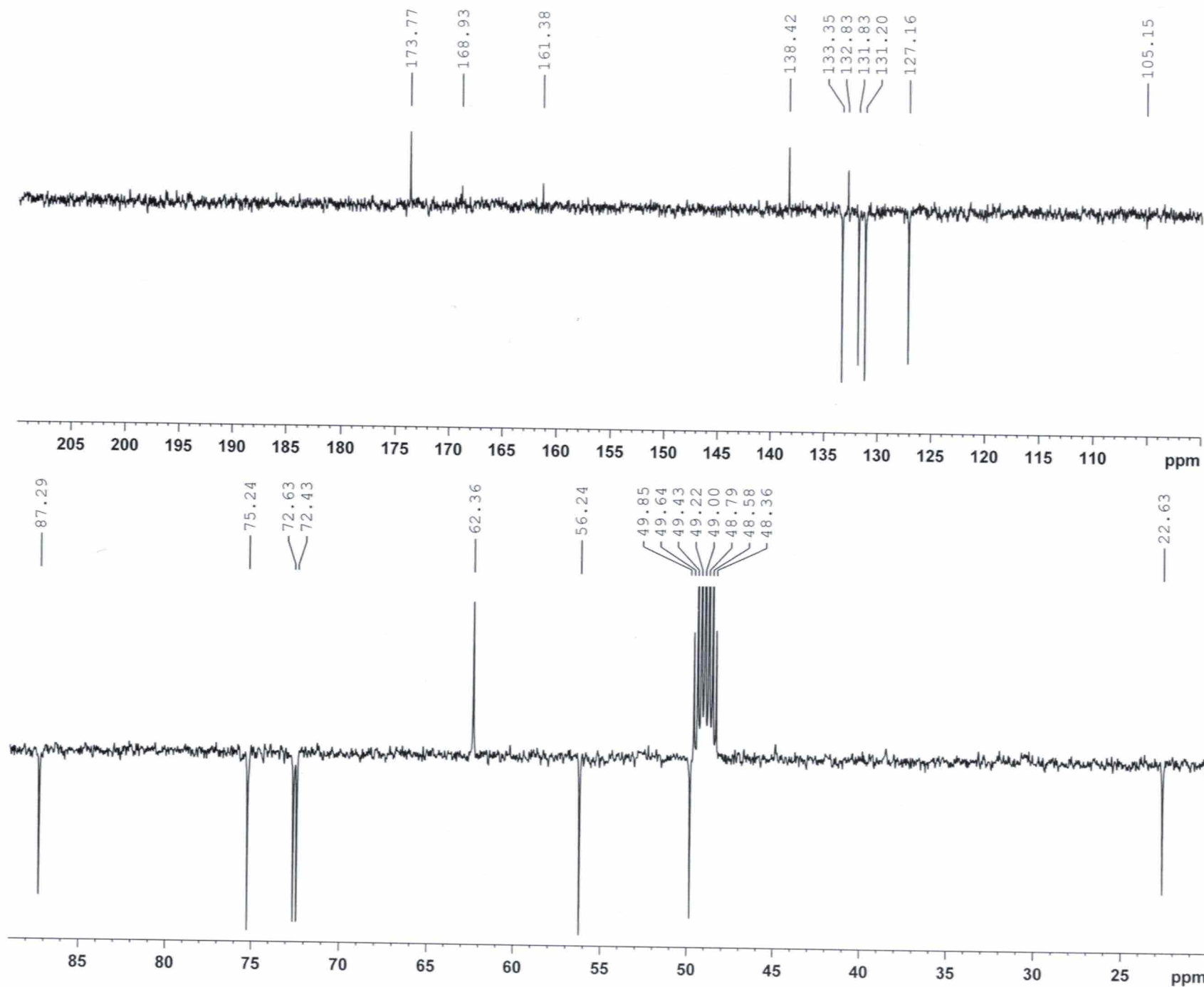
ra155 Cycl. Proton

```

NAME          ra1555
EXPNO         10
PROCNO        1
Date_         20141209
Time          8.55
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       zg30
TD            65536
SOLVENT       MeOD
NS            16
DS            2
SWH           8250.825 Hz
FIDRES        0.125898 Hz
AQ            3.9715922 sec
RG            71.8
DW            60.600 usec
DE            6.50 usec
TE            300.0 K
D1            5.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
PL1           0.00 dB
SFO1          400.1336012 MHz
SI            32768
SF            400.1300074 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



ra155 Cycl. Jmod

```

NAME      ra1555
EXPNO     15
PROCNO    1
Date_     20141209
Time      12.20
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   jmod
TD        65536
SOLVENT   MeOD
NS        1624
DS        4
SWH       23148.148 Hz
FIDRES    0.353213 Hz
AQ        1.4156492 sec
RG        14596.5
DW        21.600 usec
DE        6.50 usec
TE        300.0 K
CNST2     145.0000000
CNST11    1.0000000
D1        5.0000000 sec
D20       0.00689655 sec
TD0       1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1        11.00 usec
P2        22.00 usec
PL1       0.00 dB
SFO1      100.6233333 MHz

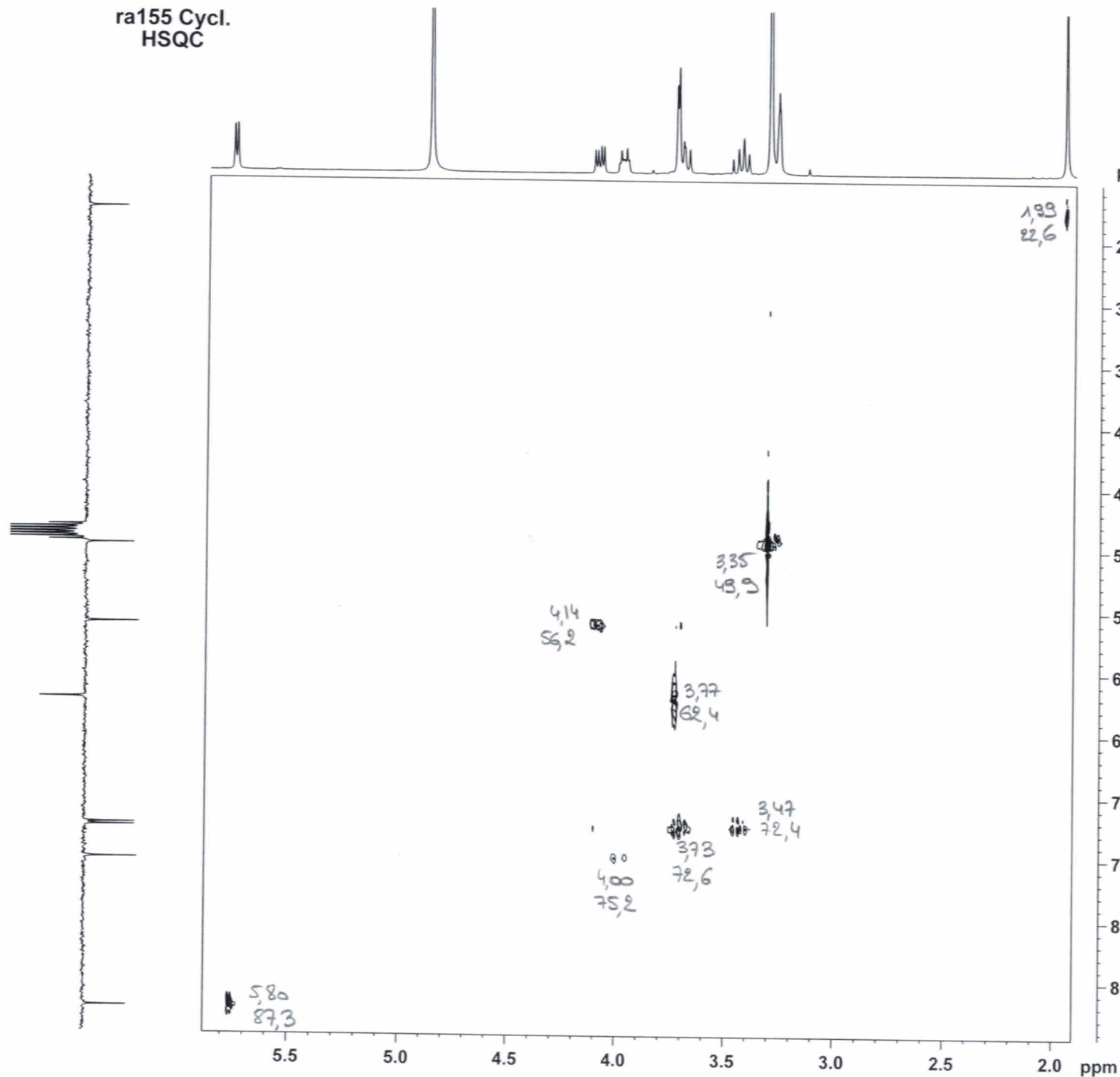
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     100.00 usec
PL2       0.00 dB
PL12      23.32 dB
SFO2      400.1316005 MHz
SI        32768
SF        100.6126294 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40

```

ra155 Cycl.
HSQC



```

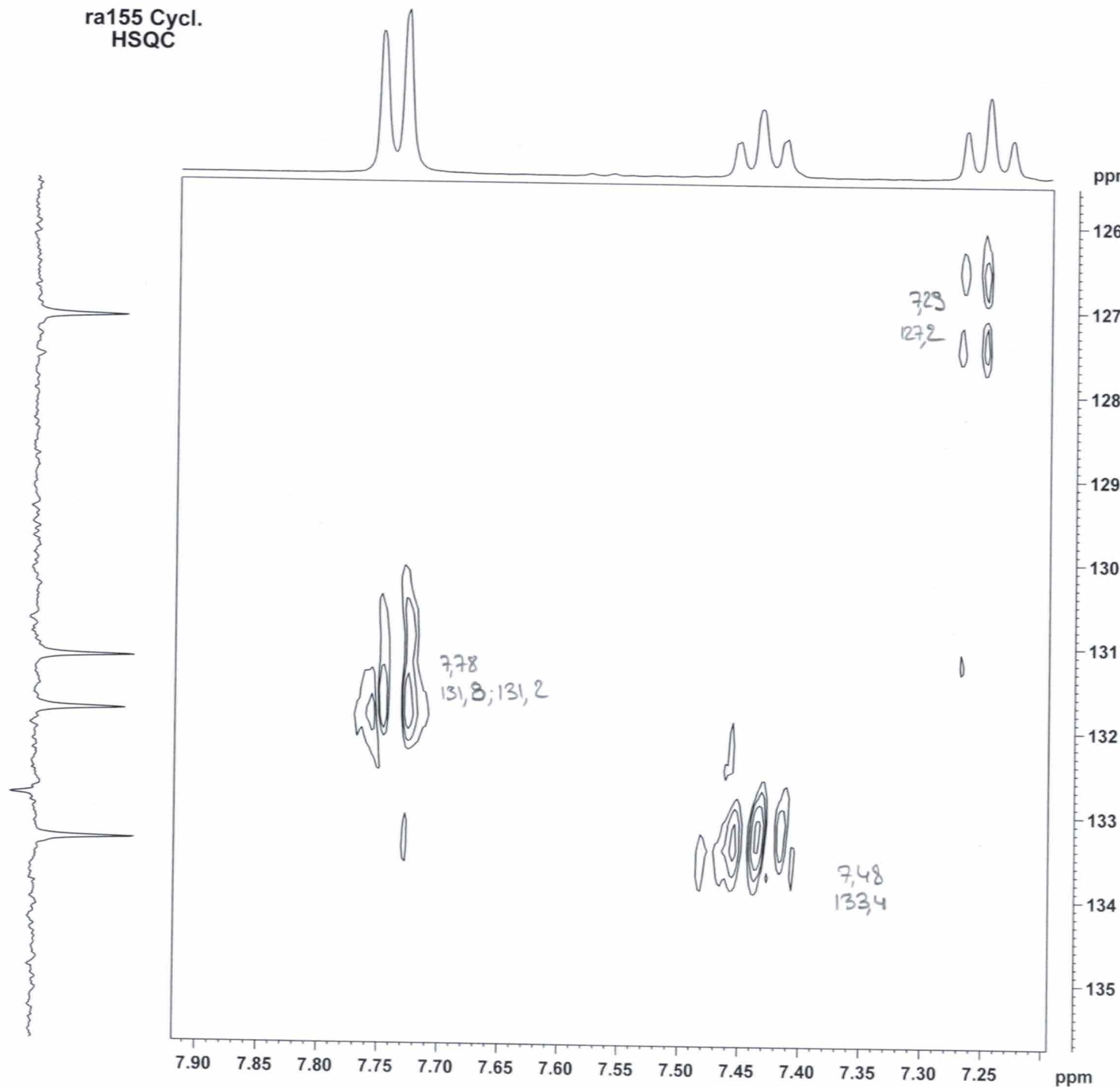
NAME          ra1555
EXPNO         12
PROCNO        1
Date_         20141209
Time          9.03
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       hsqcetgpsi
TD            4096
SOLVENT       MeOD
NS            2
DS            4
SWH           3333.333 Hz
FIDRES        0.813802 Hz
AQ            0.6146000 sec
RG            13004
DW            150.000 usec
DE            6.50 usec
TE            300.0 K
CNST2         140.0000000
DO            0.00000300 sec
D1            0.96067601 sec
D4            0.00178571 sec
D11           0.030000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D24           0.00089000 sec
IN0           0.00003105 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
P28           1000.00 usec
PL1           0.00 dB
SFO1          400.1317858 MHz

===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            11.00 usec
P4            22.00 usec
PCPD2         80.00 usec
PL2           0.00 dB
PL12          17.23 dB
SFO2          100.6203150 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6203 MHz
FIDRES        62.887669 Hz
SW            160.000 ppm
FMODE         Echo-Antiecho
SI            4096
SF            400.1300230 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
FC            1.40
SI            512
MC2           echo-antiecho
SF            100.6126294 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

ra155 Cycl.
HSQC



```

NAME          ra1555
EXPNO         12
PROCNO        1
Date_         20141209
Time          9.03
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       hsqcetgpsi
TD            4096
SOLVENT       MeOD
NS            2
DS            4
SWH           3333.333 Hz
FIDRES        0.813802 Hz
AQ            0.6146000 sec
RG            13004
DW            150.000 usec
DE            6.50 usec
TE            300.0 K
CNST2         140.0000000
D0            0.00000300 sec
D1            0.96067601 sec
D4            0.00178571 sec
D11           0.03000000 sec
D13           0.00000400 sec
D16           0.00020000 sec
D24           0.00089000 sec
IN0           0.00003105 sec
ZGPTNS
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
P28           1000.00 usec
PL1           0.00 dB
SFO1          400.1317858 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       garp
NUC2          13C
P3            11.00 usec
P4            22.00 usec
PCPD2         80.00 usec
PL2           0.00 dB
PL12          17.23 dB
SFO2          100.6203150 MHz
  
```

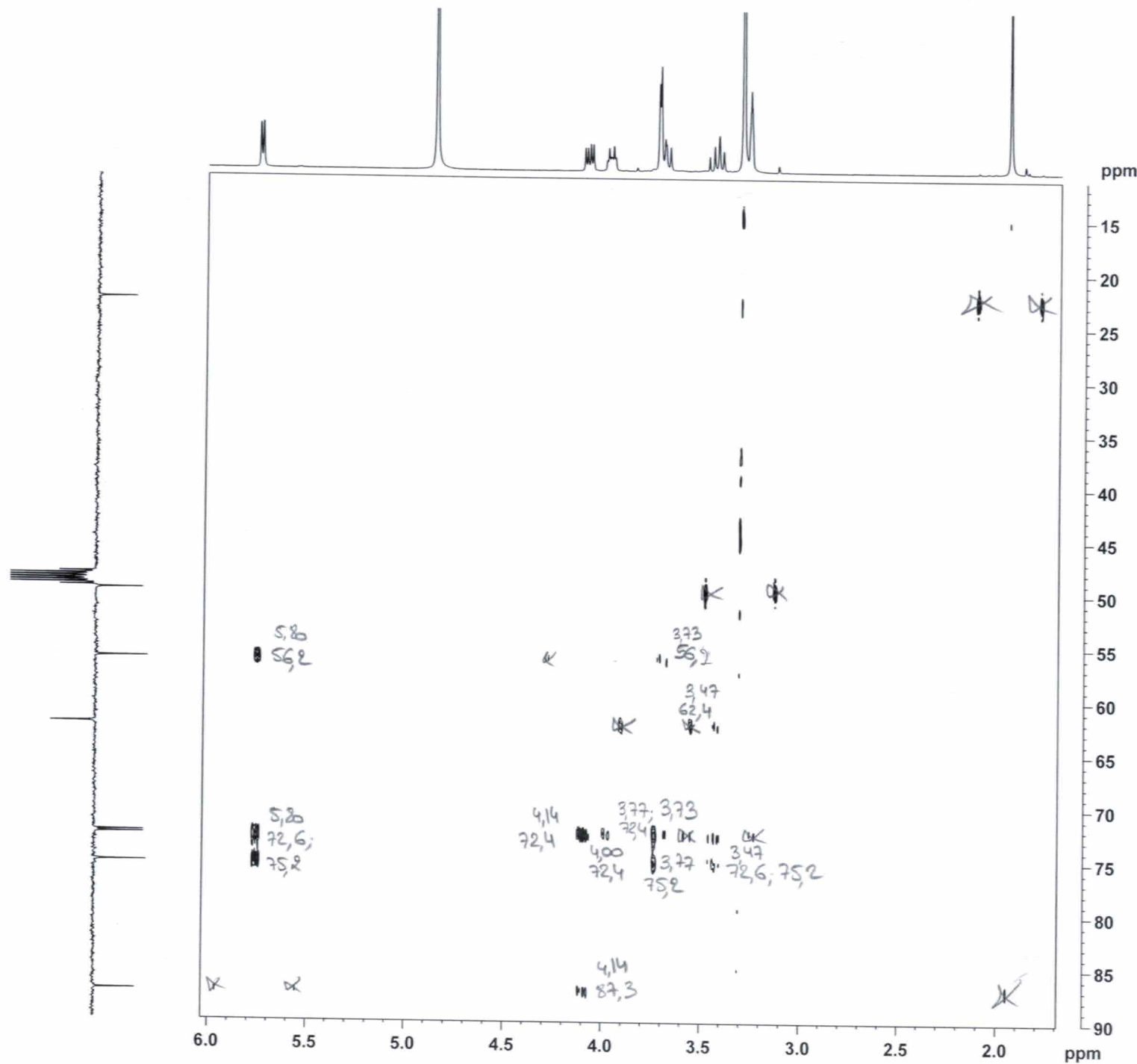
```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6203 MHz
FIDRES        62.887669 Hz
SW            160.000 ppm
FnMODE        Echo-Antiecho
SI            4096
SF            400.1300230 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           echo-antiecho
SF            100.6126294 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

```

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPZ1          80.00 %
GPZ2          20.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6203 MHz
FIDRES        62.887669 Hz
SW            160.000 ppm
FnMODE        Echo-Antiecho
SI            4096
SF            400.1300230 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
PC            1.40
SI            512
MC2           echo-antiecho
SF            100.6126294 MHz
WDW           QSINE
SSB           2
LB            0.00 Hz
GB            0
  
```

ra155 Cycl. HMBC



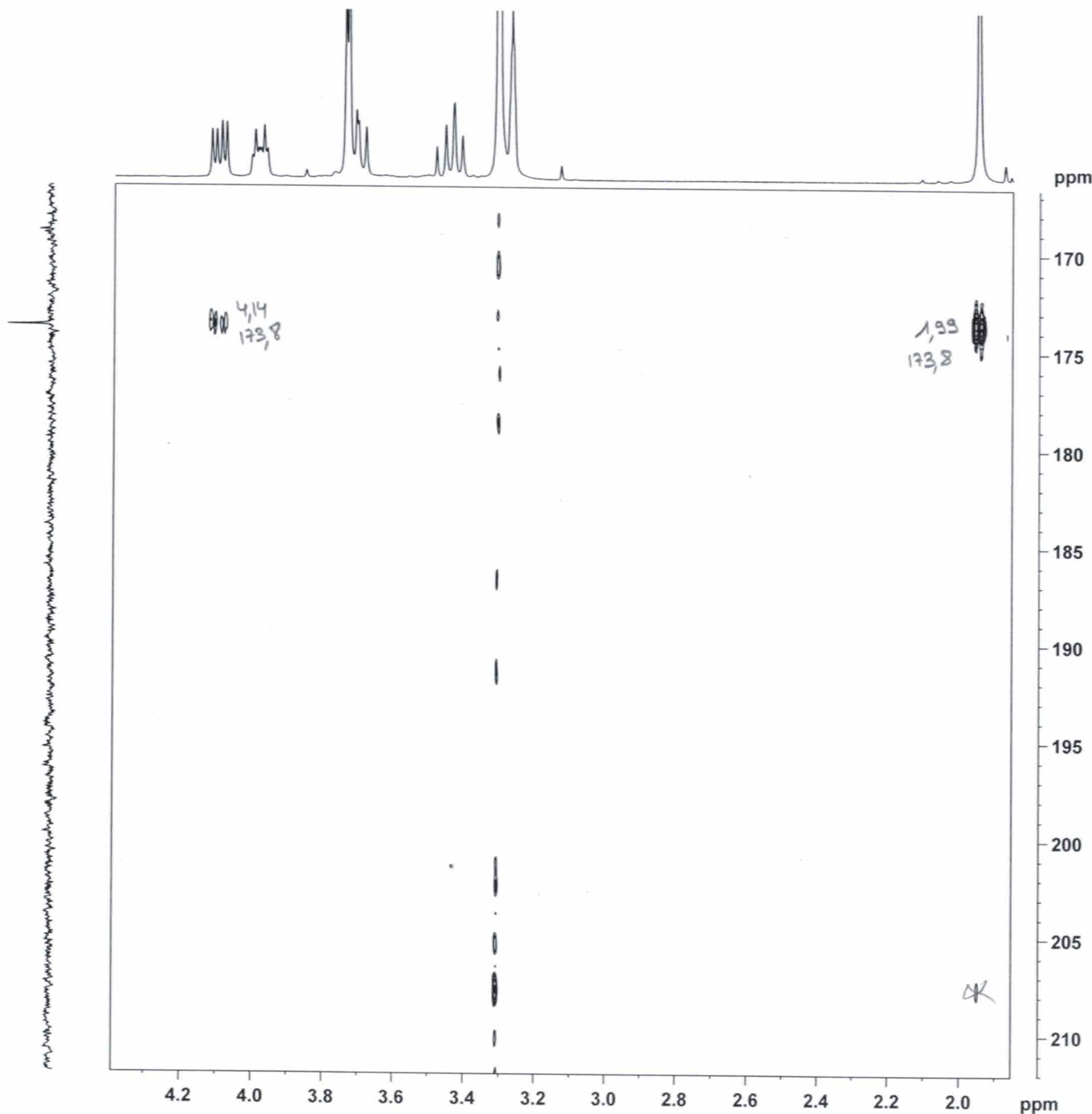
NAME ra1555
EXPNO 13
PROCNO 1
Date_ 20141209
Time 9.17
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 4096
SOLVENT MeOD
NS 2
DS 4
SWH 3333.333 Hz
FIDRES 0.813802 Hz
AQ 0.6146000 sec
RG 18390.4
DW 150.000 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 0.98422498 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
INO 0.00002160 sec

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1317858 MHz

===== CHANNEL f2 =====
NUC2 ^{13}C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
NDO 2
TD 256
SFO1 100.6238 MHz
FIDRES 90.403236 Hz
SW 229.997 ppm
FnMODE QF
SI 4096
SF 400.1300230 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6126294 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

ra155 Cycl.
HMBC



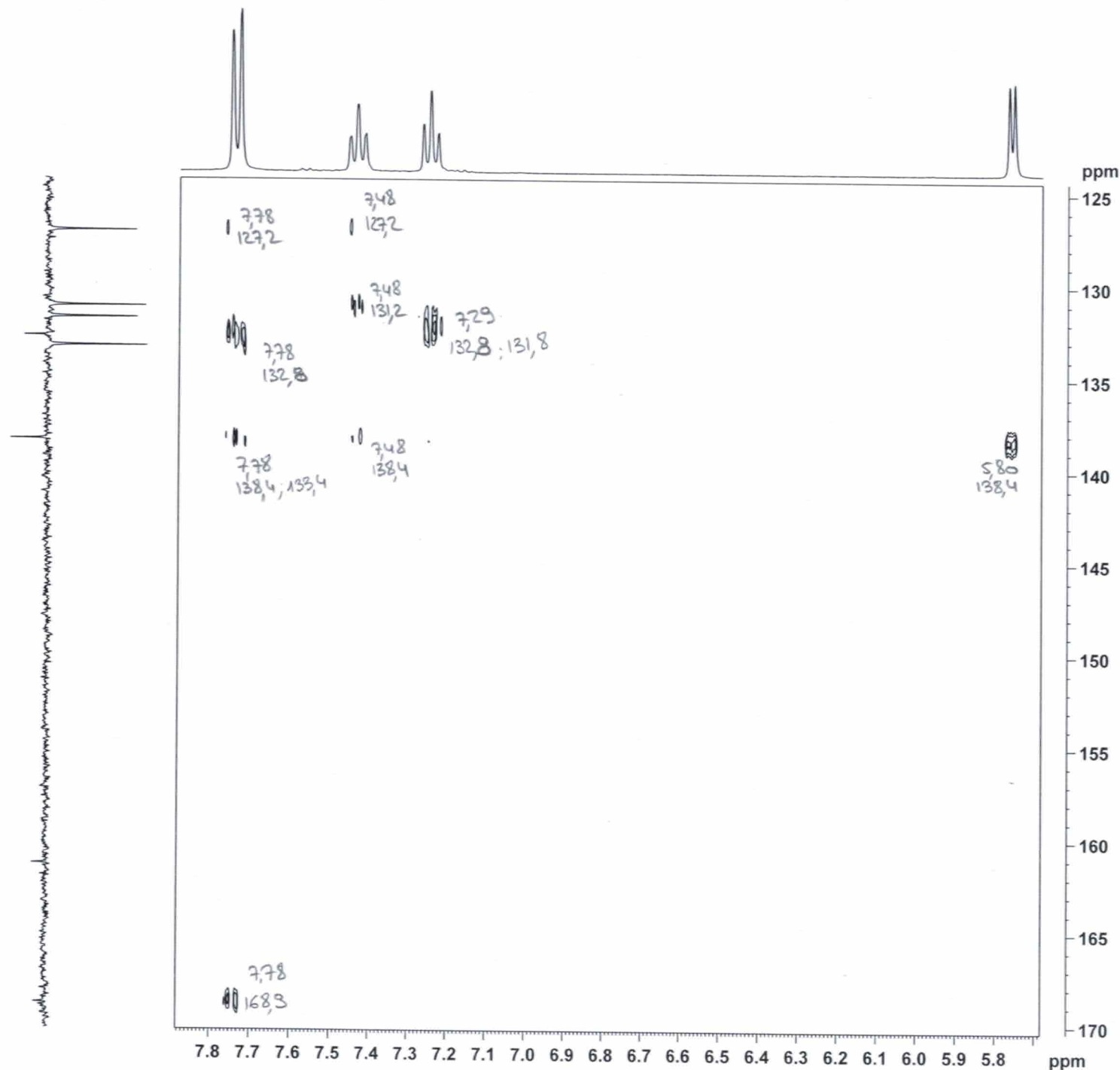
NAME ra1555
EXPNO 13
PROCNO 1
Date_ 20141209
Time_ 9.17
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 4096
SOLVENT MeOD
NS 2
DS 4
SWH 3333.333 Hz
FIDRES 0.813802 Hz
AQ 0.6146000 sec
RG 18390.4
DW 150.000 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 8.0000000
D0 0.00000300 sec
D1 0.98422498 sec
D2 0.00344828 sec
D6 0.06250000 sec
D16 0.00020000 sec
IN0 0.00002160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1317858 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 256
SFO1 100.6238 MHz
FIDRES 90.403236 Hz
SW 229.997 ppm
FhMODE QF
SI 4096
SF 400.1300230 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6126294 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

ra155 Cycl.
HMBC



```

NAME          ra1555
EXPNO         13
PROCNO        1
Date_         20141209
Time_         9.17
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       hmbcgp1pndqf
TD            4096
SOLVENT       MeOD
NS            2
DS            4
SWH           3333.333 Hz
FIDRES        0.813802 Hz
AQ            0.6146000 sec
RG            18390.4
DW            150.000 usec
DE            6.50 usec
TE            300.0 K
CNST2         145.0000000
CNST13        8.0000000
D0            0.00000300 sec
D1            0.98422498 sec
D2            0.00344828 sec
D6            0.06250000 sec
D16           0.00020000 sec
IN0           0.00002160 sec

===== CHANNEL f1 =====
NUC1          1H
P1            6.82 usec
P2            13.65 usec
PL1           0.00 dB
SFO1          400.1317858 MHz

===== CHANNEL f2 =====
NUC2          13C
P3            11.00 usec
PL2           0.00 dB
SFO2          100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GP21          50.00 %
GP22          30.00 %
GP23          40.10 %
P16           1000.00 usec
ND0           2
TD            256
SFO1          100.6238 MHz
FIDRES        90.403236 Hz
SW            229.997 ppm
FMODE         QF
SI            4096
SF            400.1300230 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            100.6126294 MHz
WDW           SINE
SSB           0
LB            0.00 Hz
GB            0
  
```

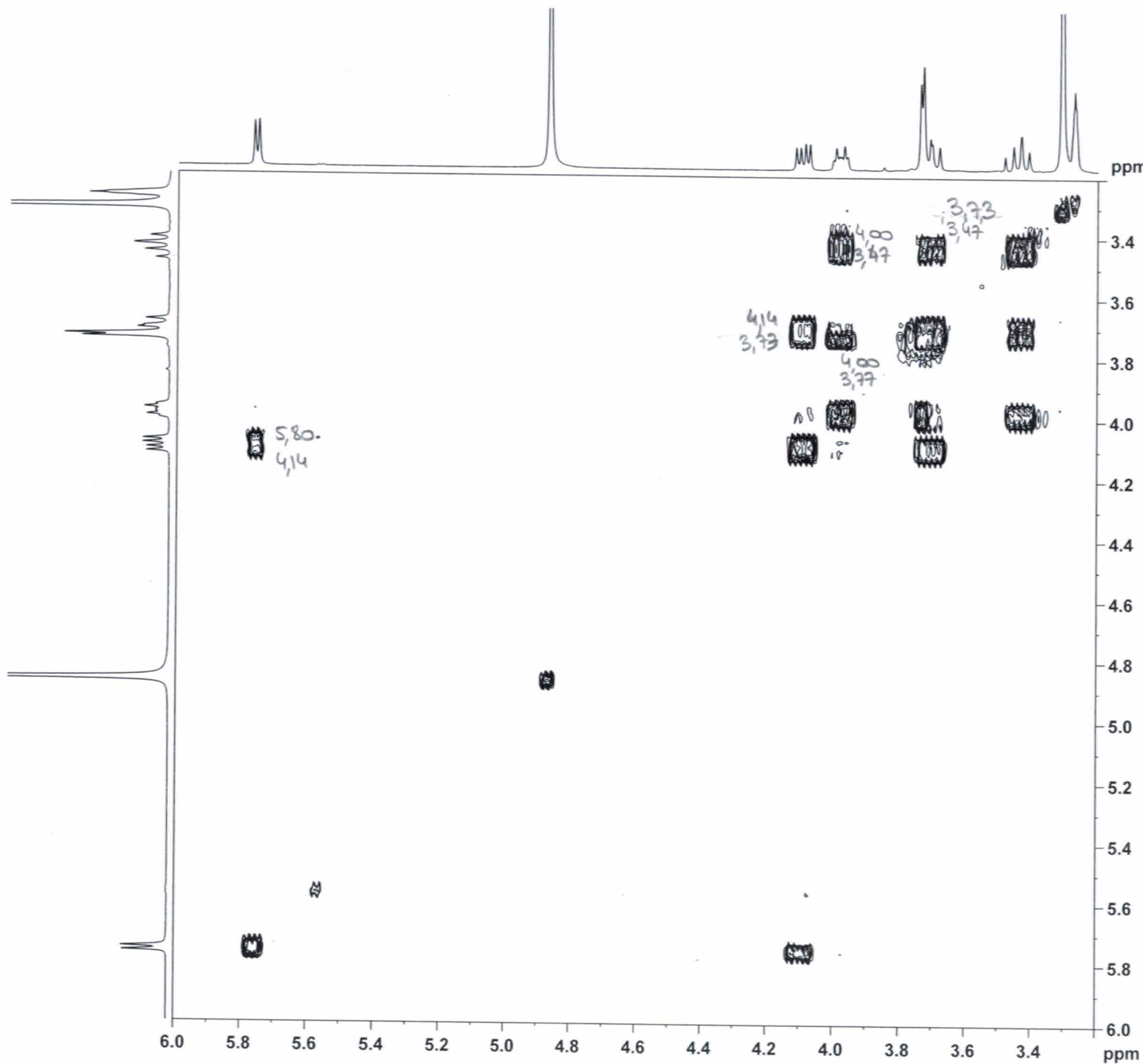
ppm

```
===== CHANNEL f1 =====
NUC1                1H
P1                   6.82 usec
PL1                  0.00 dB
SFO1                400.131785 MHz
```

```

===== GRADIENT CHANNEL =====
GPNAM1                SINE.100
GPNAM2                SINE.100
GPNAM3                SINE.100
GPZ1                   16.00    %
GPZ2                   12.00    %
GPZ3                   40.00    %
PI6                    1000.00 usec
NDO                     1
TD                      256
SFO1                   400.1318 MHz
FIDRES                 13.020833 Hz
SW                      8.331 ppm
FnMODE                 QF
SI                      2048
SF                     400.1300230 MHz
WDW                     QSINE
SSB                     1
LB                      0.00 Hz
GB                      0
PC                      1.40
SI                      512
MC2                     QF
SF                     400.1300230 MHz
WDW                     QSINE
SSB                     1
LB                      0.00 Hz
GB                      0

```

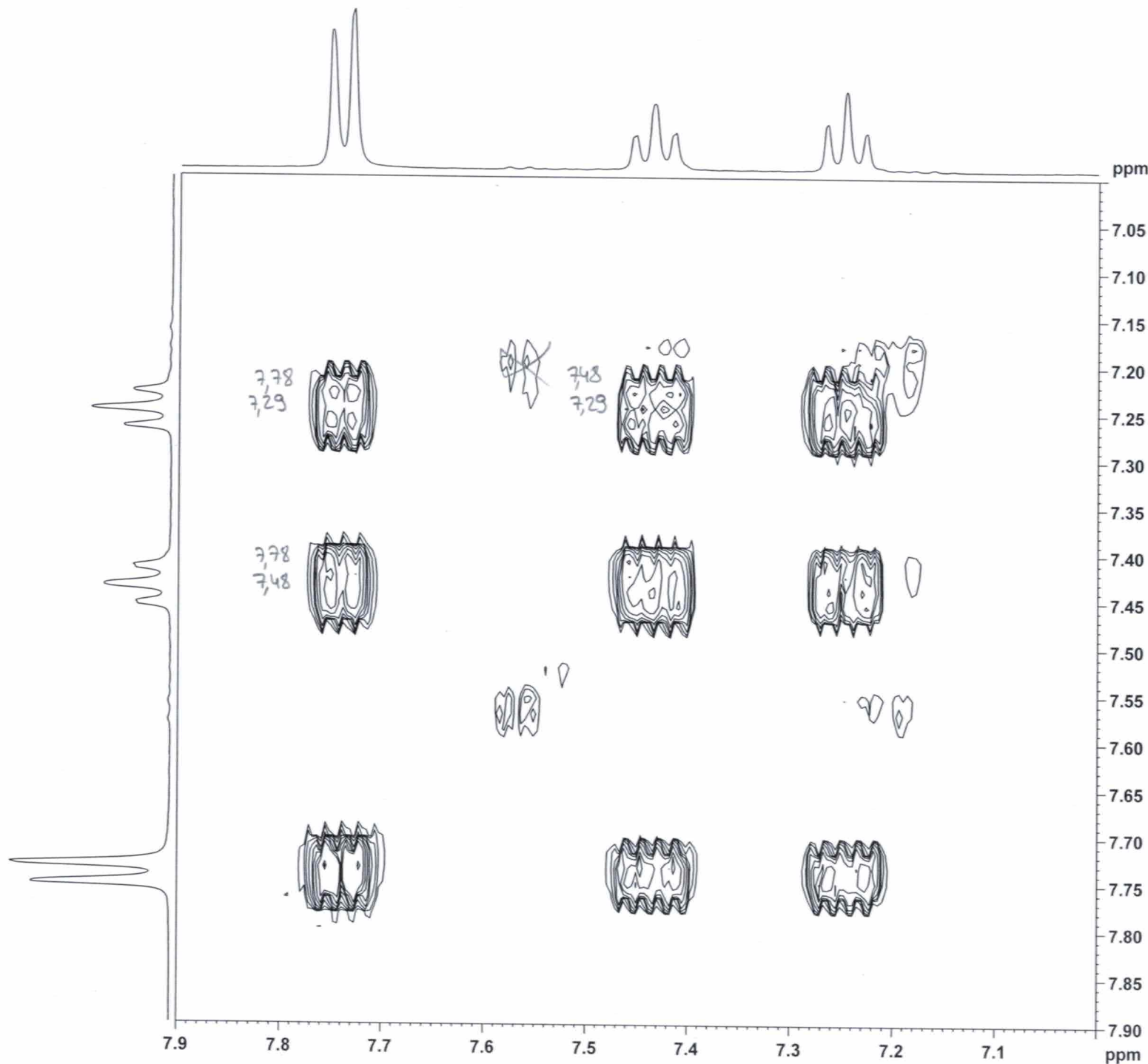


ra155 Cycl.
COSY

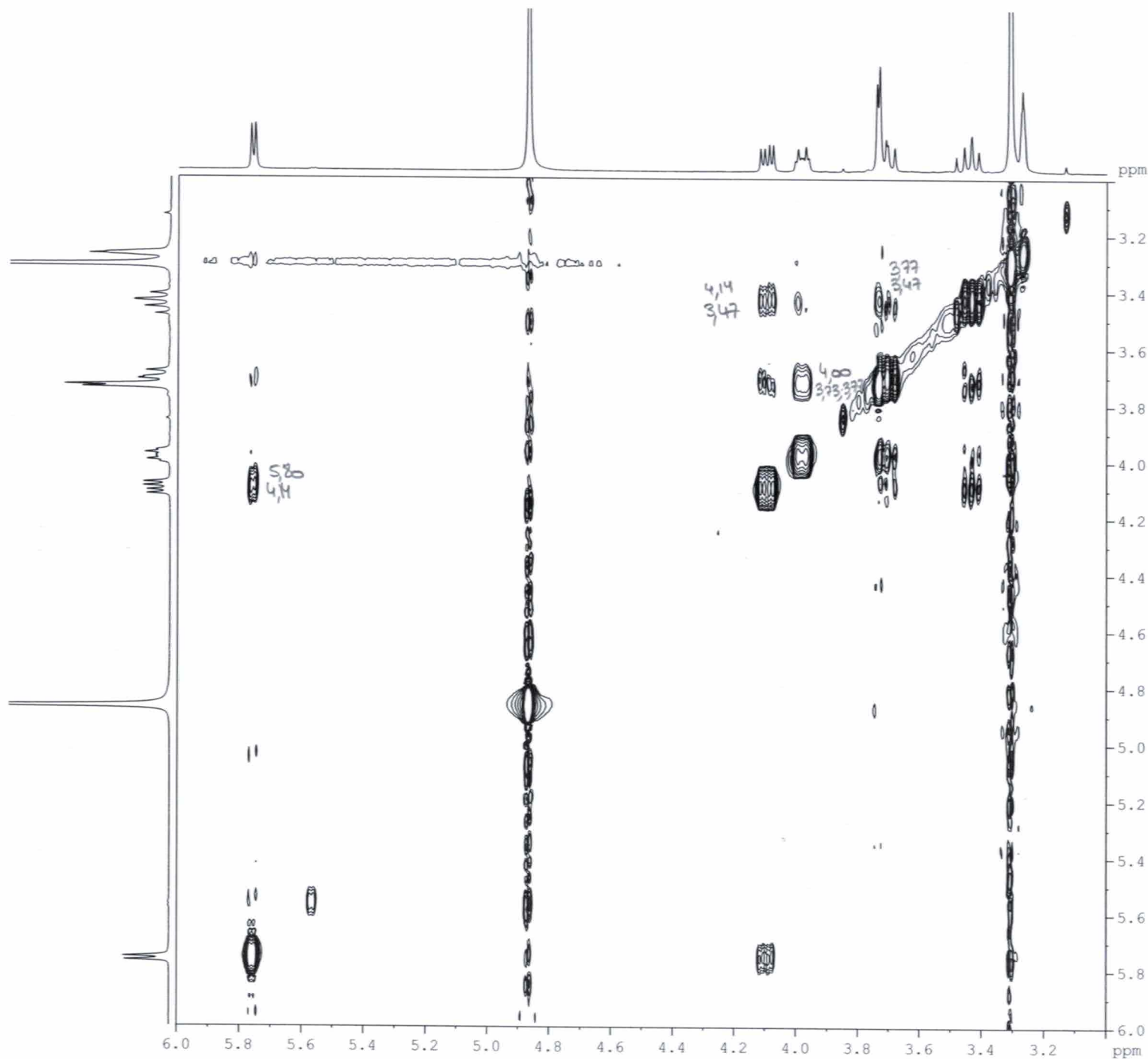
NAME ra1555
EXPNO 11
PROCNO 1
Date_ 20141209
Time 8.56
INSTRUM spect
PROBHD 5 mm Multinucl
FULPROG cosygpmfqq
TD 2134
SOLVENT MeOD
NS 1
DS 8
SWH 3333.333 Hz
FIDRES 1.562012 Hz
AQ 0.3203000 sec
RG 4597.6
DW 150.000 usec
DE 6.50 usec
TE 300.0 K
D0 0.00000300 sec
D1 0.97865731 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00030000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1317858 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1318 MHz
FIDRES 13.020833 Hz
SW 8.331 ppm
FnMODE QF
SI 2048
SF 400.1300230 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 QF
SF 400.1300230 MHz
WDW QSINE
SSB 1
LB 0.00 Hz
GB 0



ra155 Cycl.
NOESY

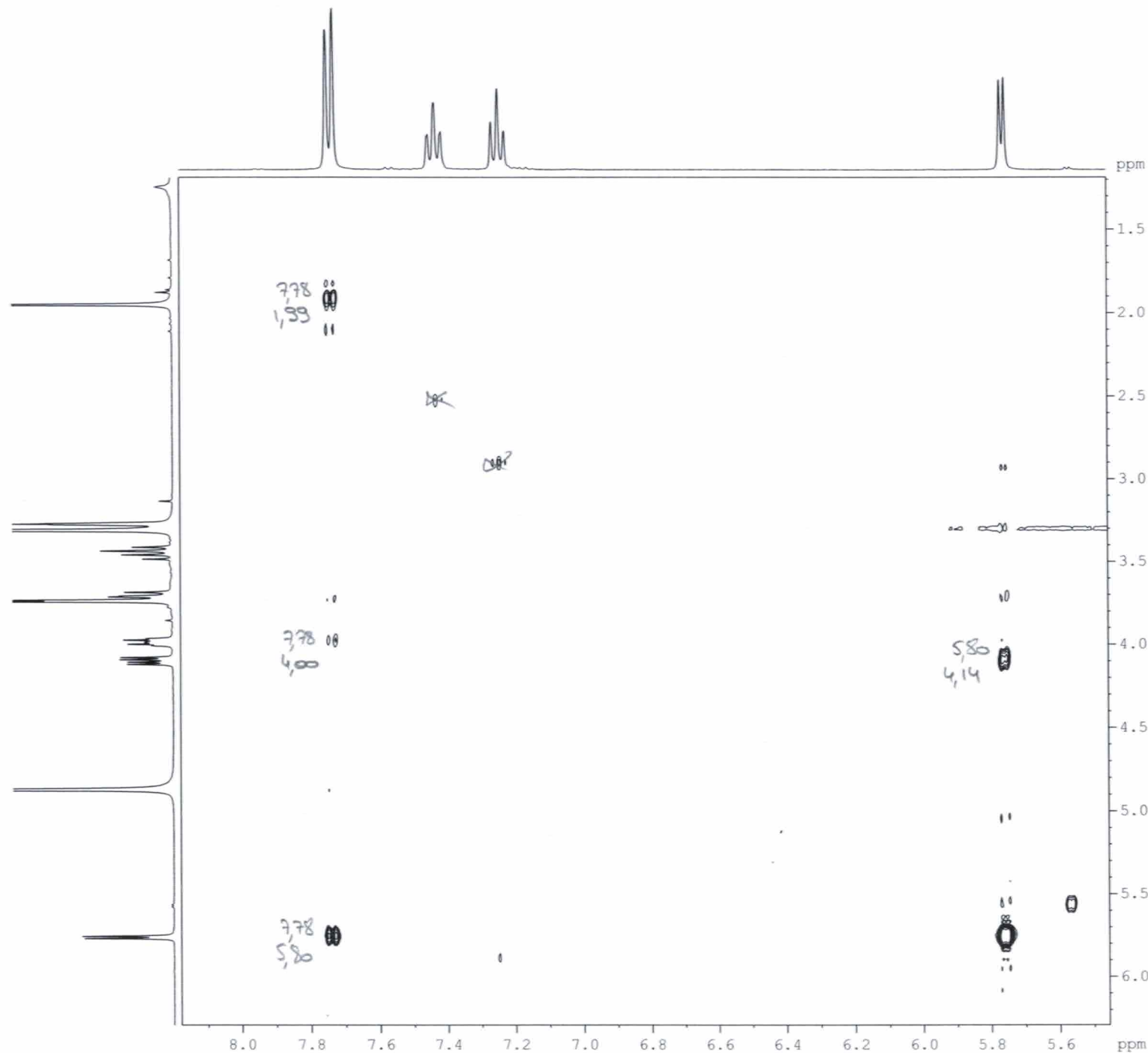


NAME ra1555
EXPNO 14
PROCNO 1
Date_ 20141209
Time_ 9.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesygpph
TD 2134
SOLVENT MeOD
NS 2
DS 16
SWH 3333.333 Hz
FIDRES 1.562012 Hz
AQ 0.3203000 sec
RG 45.3
DW 150.000 usec
DE 6.50 usec
TE 300.0 K
D0 0.00014131 sec
D1 1.47951198 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00030000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1317858 MHz

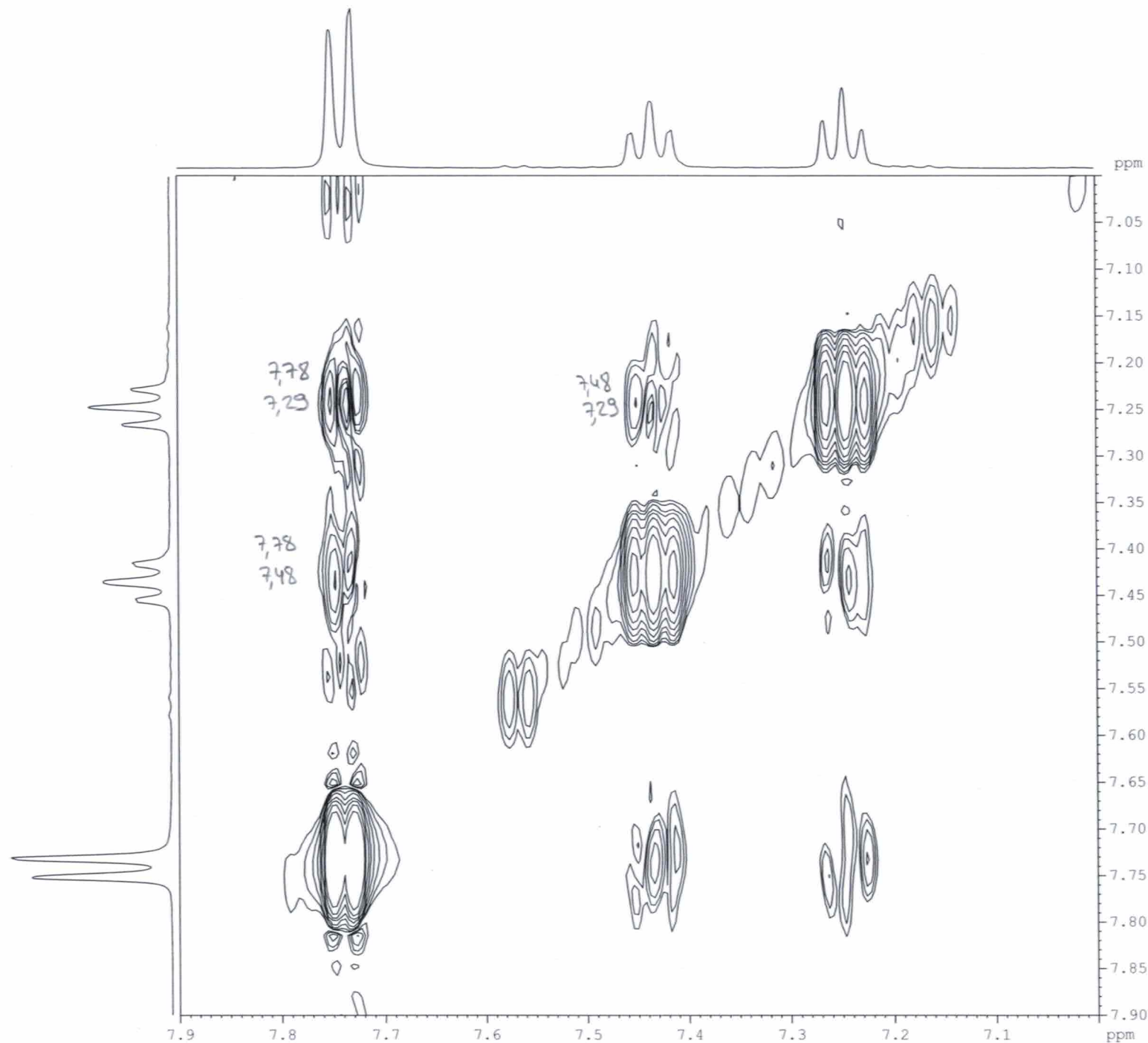
===== GRADIENT CHANNEL =====
GPNAMI SINE.100
GPZ1 40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 400.1318 MHz
FIDRES 13.020833 Hz
SW 8.331 ppm
FnMODE States-TPPI
SI 2048
SF 400.1300230 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
MC2 States-TPPI
SF 400.1300230 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

ra155 Cycl. NOESY



NAME	ra1555
EXPNO	14
PROCNO	1
Date_	20141209
Time	9.33
INSTRUM	spect
PROBHD	5 mm Multinucl
PULPROG	noesygpph
TD	2134
SOLVENT	MeOD
NS	2
DS	16
SWH	3333.333 Hz
FIDRES	1.562012 Hz
AQ	0.3203000 sec
RG	45.3
DW	150.000 usec
DE	6.50 usec
TE	300.0 K
DO	0.00014131 sec
D1	1.47951198 sec
D8	0.80000001 sec
D16	0.00020000 sec
IN0	0.00030000 sec
===== CHANNEL f1 =====	
NUC1	1H
P1	6.82 usec
P2	13.65 usec
PL1	0.00 dB
SFO1	400.1317858 MHz
===== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPZ1	40.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	400.1318 MHz
FIDRES	13.020833 Hz
SW	8.331 ppm
FnMODE	States-TPPI
SI	2048
SF	400.1300230 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	512
MC2	States-TPPI
SF	400.1300230 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

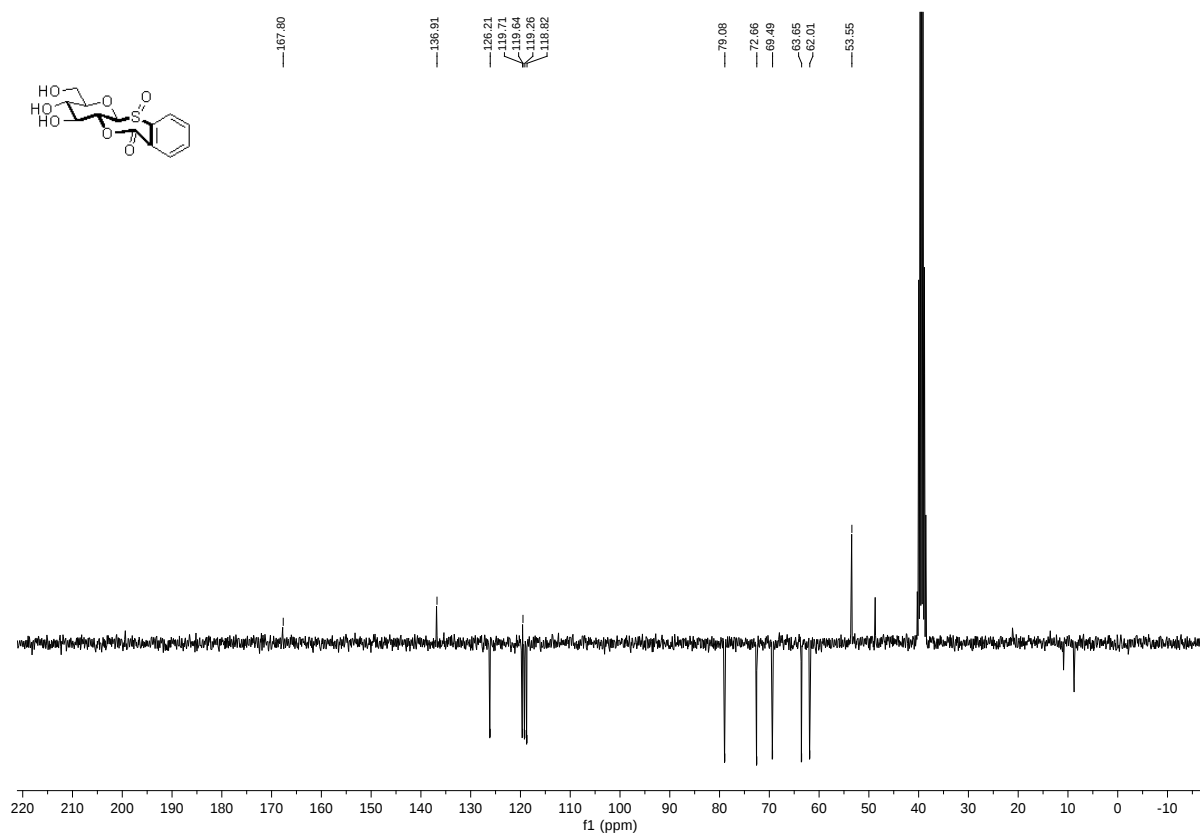
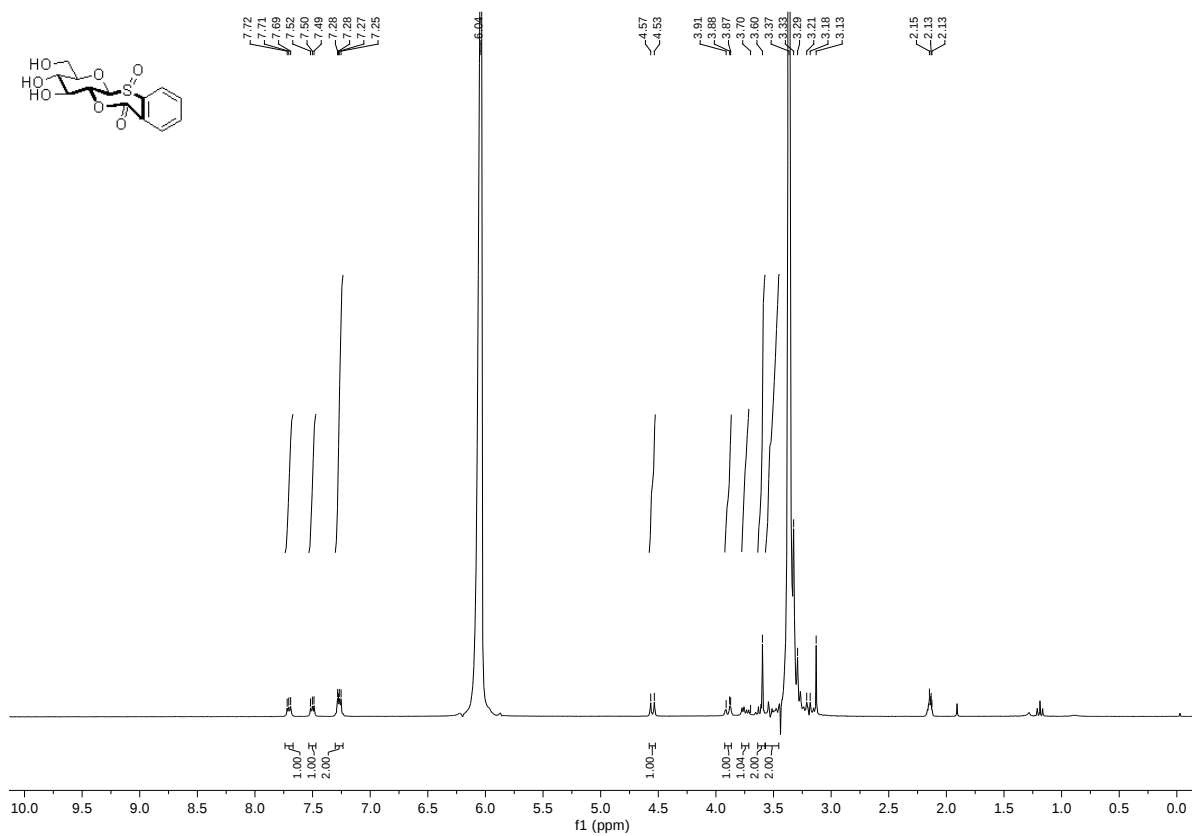
ra155 Cycl.
NOESY

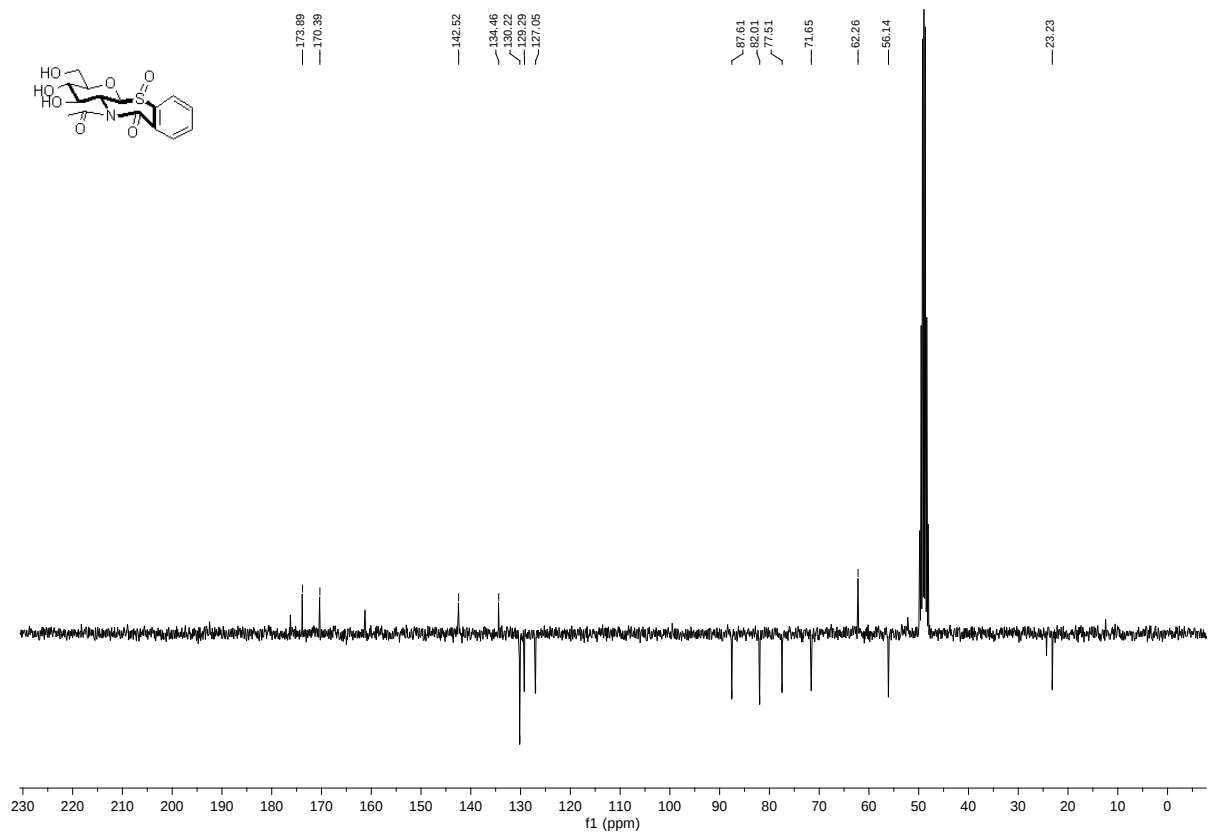
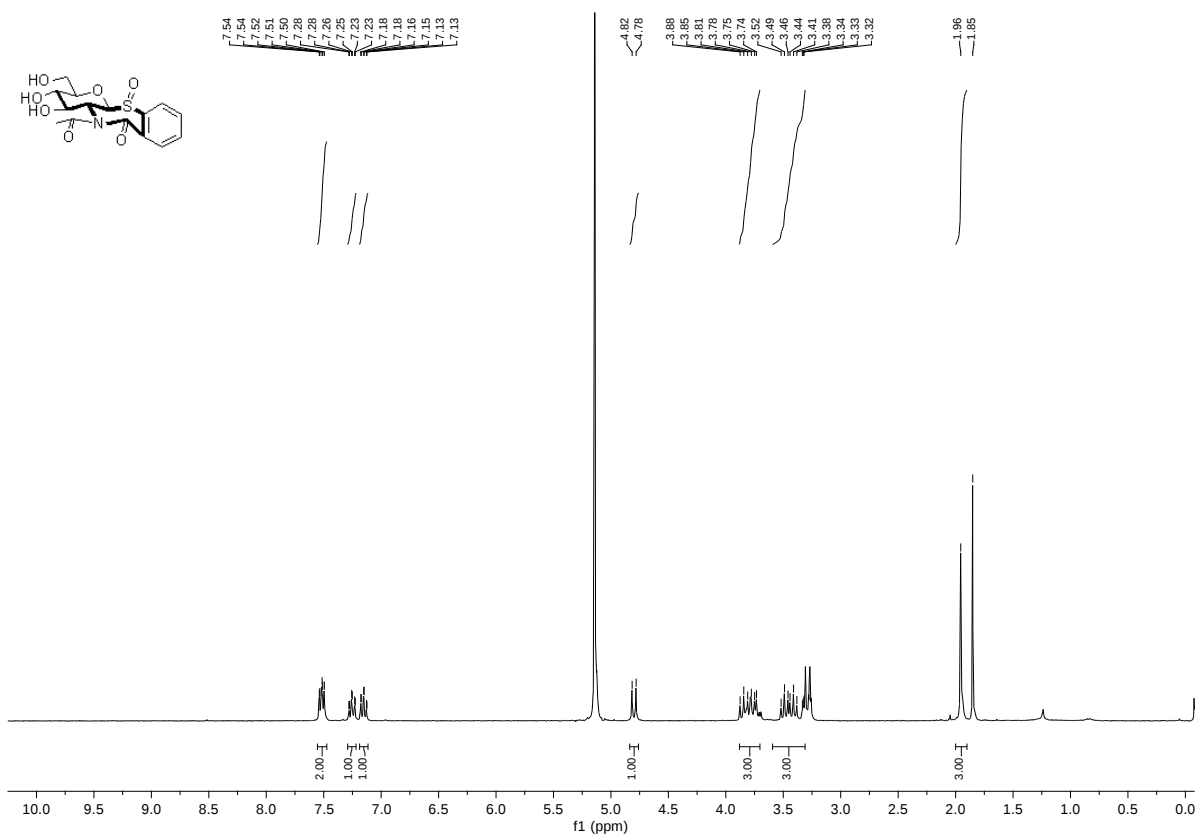


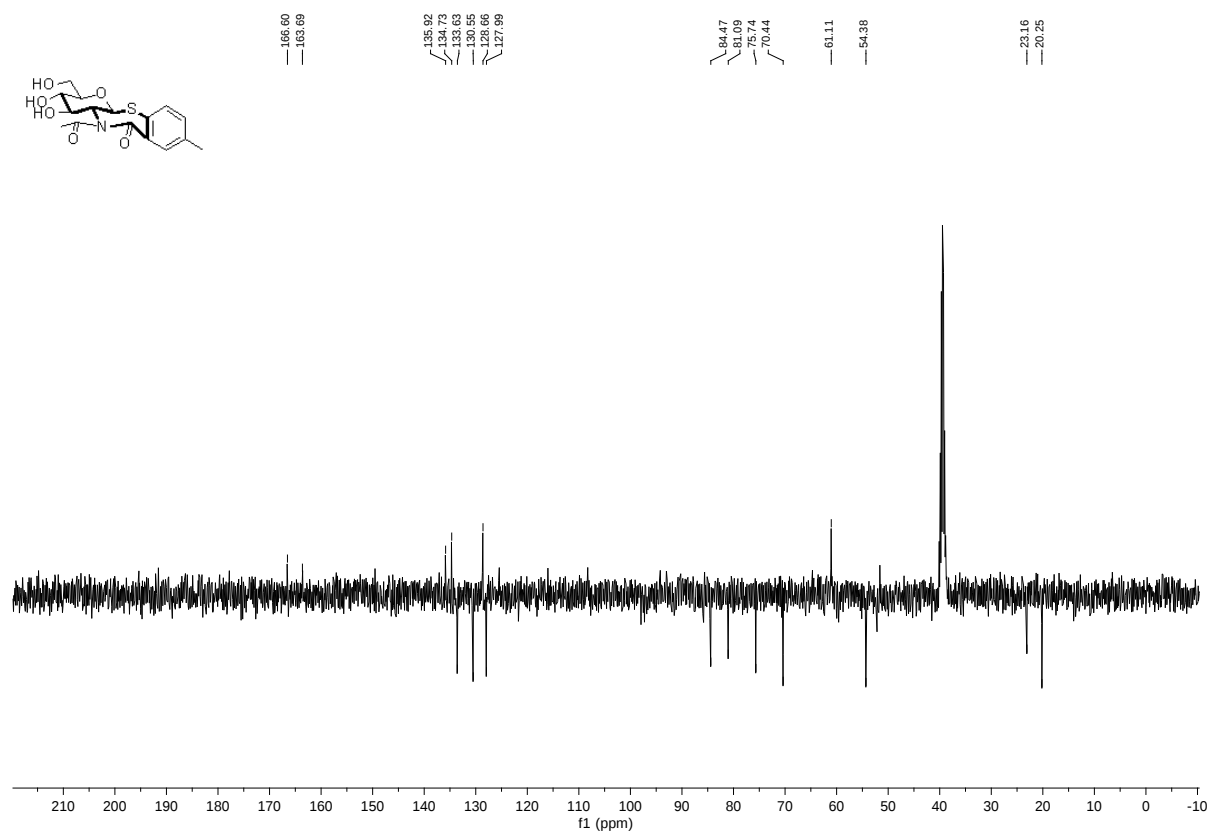
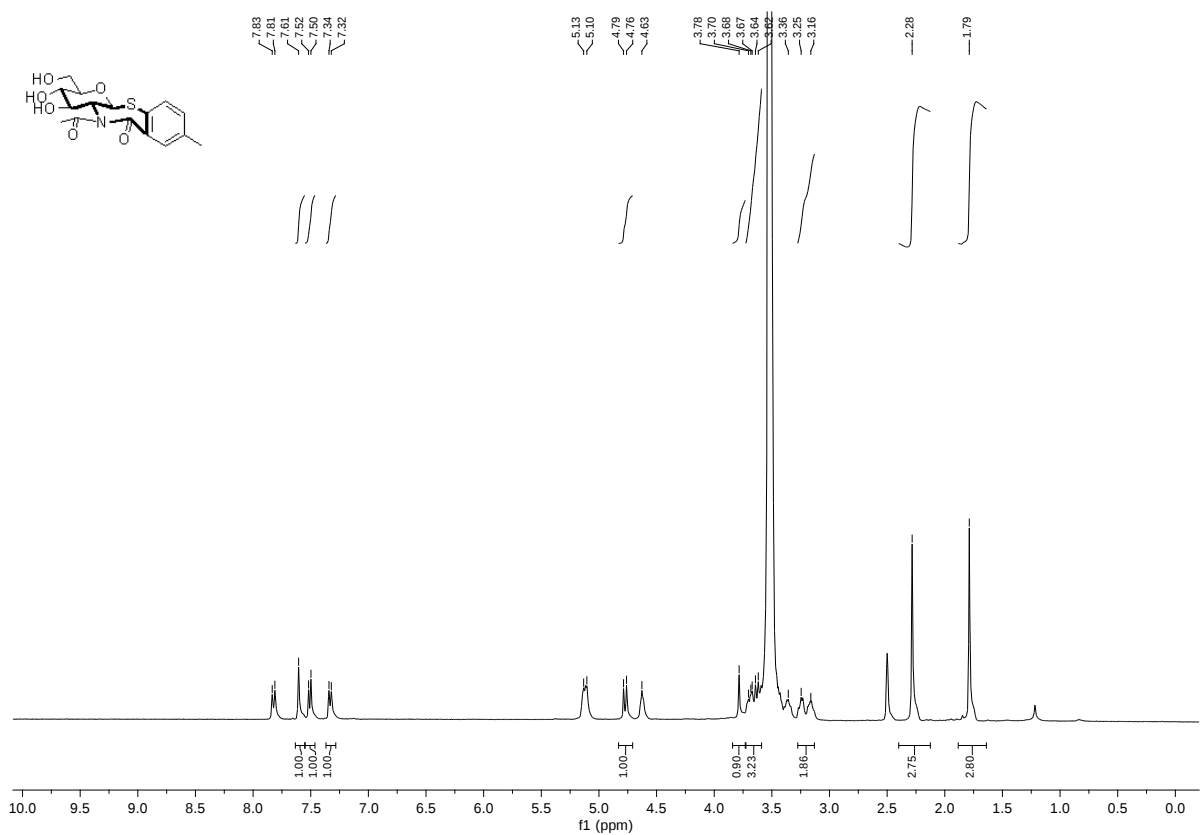
NAME ra1555
EXPNO 14
PROCNO 1
Date_ 20141209
Time 9.33
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesygpph
TD 2134
SOLVENT MeOD
NS 2
DS 16
SWH 3333.333 Hz
FIDRES 1.562012 Hz
AQ 0.3203000 sec
RG 45.3
DW 150.000 usec
DE 6.50 usec
TE 300.0 K
DO 0.00014131 sec
D1 1.47951198 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00030000 sec

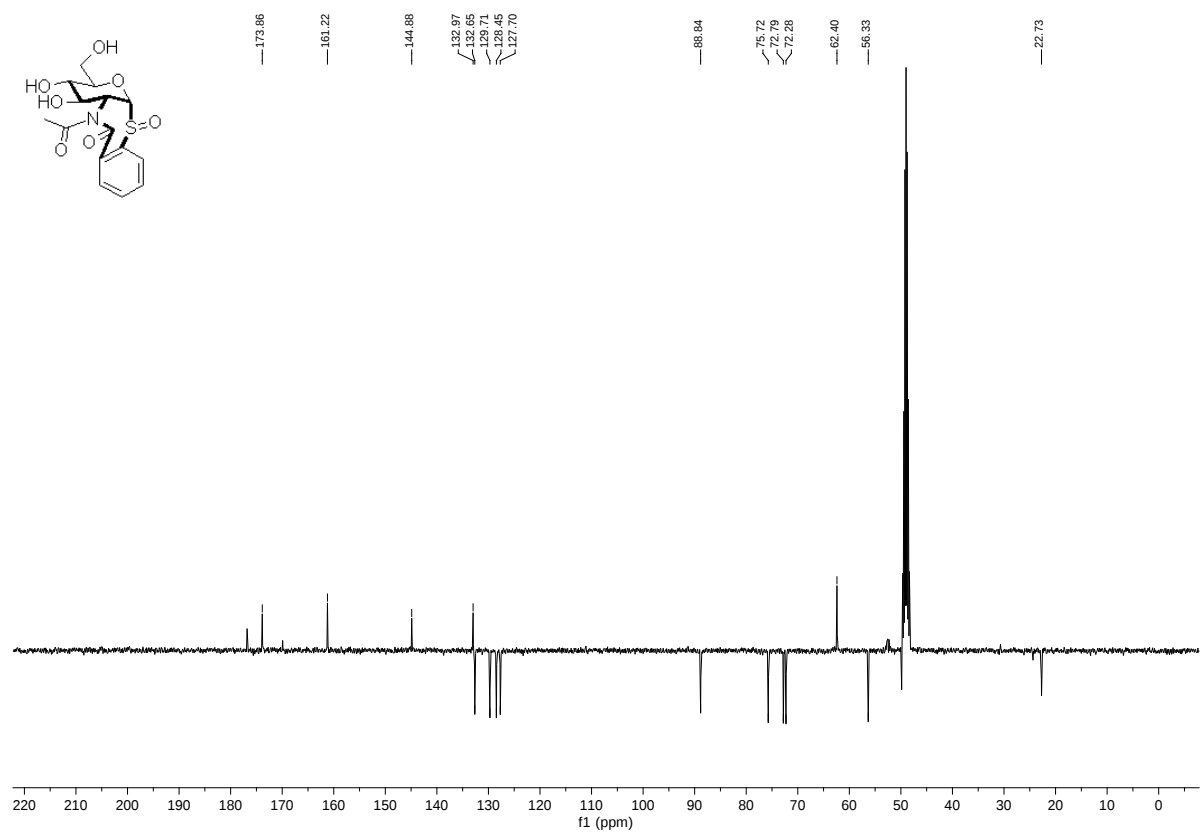
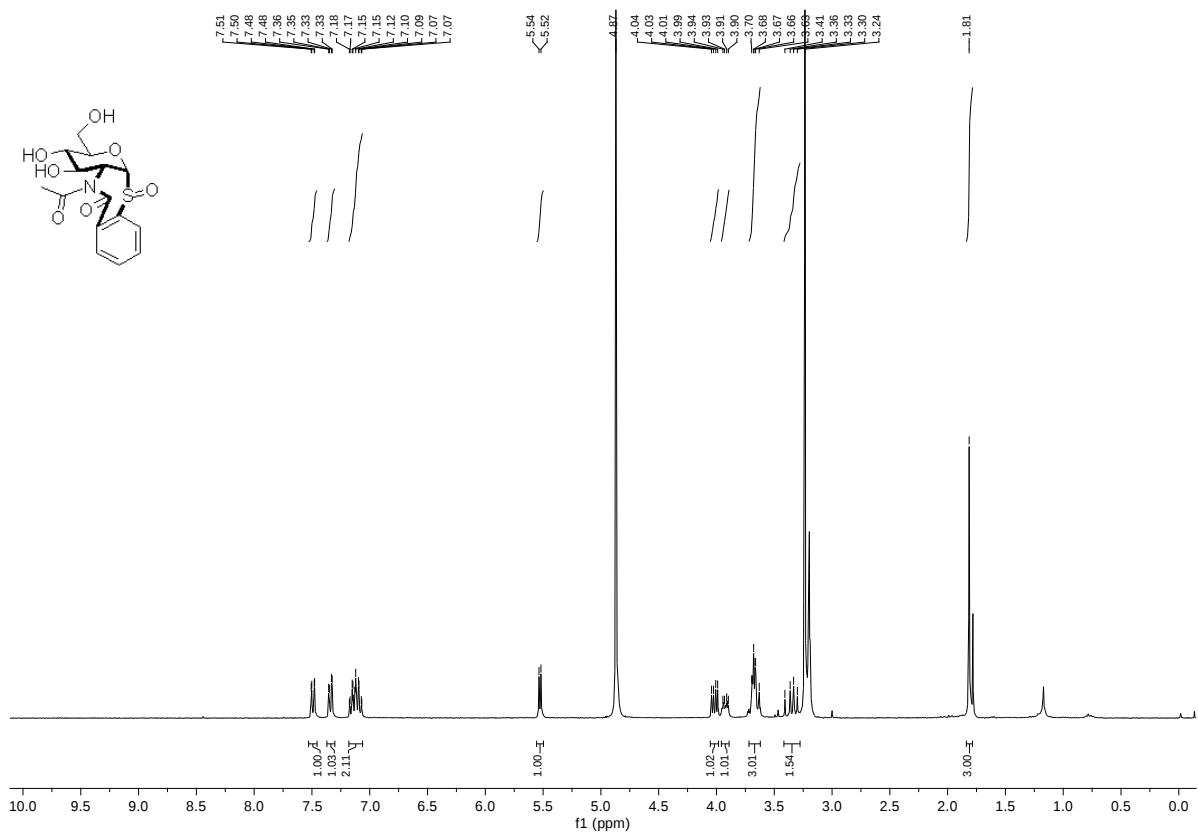
===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
7.30 SFO1 400.1317858 MHz

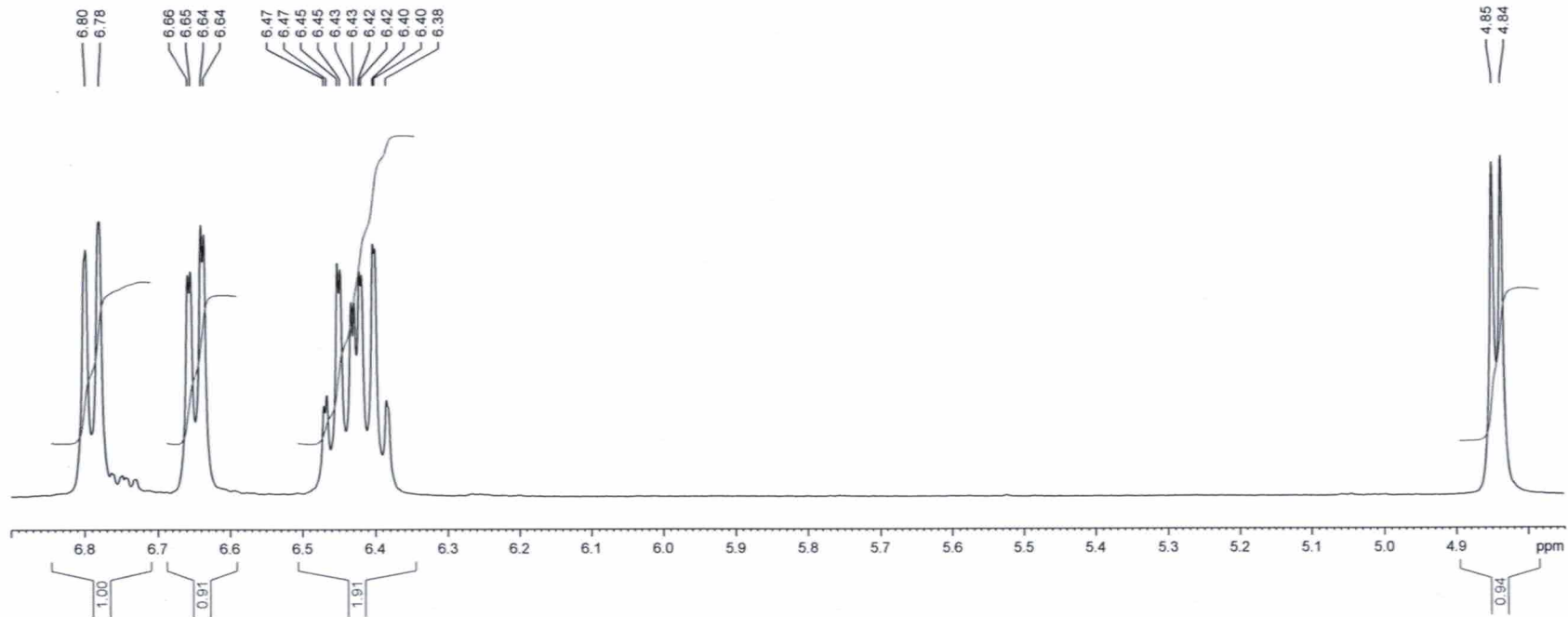
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
7.35 GPZ1 40.00 %
P16 1000.00 usec
ND0 1
TD 256
7.40 SFO1 400.1318 MHz
FIDRES 13.020833 Hz
SW 8.331 ppm
7.45 FMODE States-TPPI
SI 2048
SF 400.1300230 MHz
WDW QSINE
7.50 SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 512
7.55 MC2 States-TPPI
SF 400.1300230 MHz
WDW QSINE
7.60 SSB 2
LB 0.00 Hz
GB 0







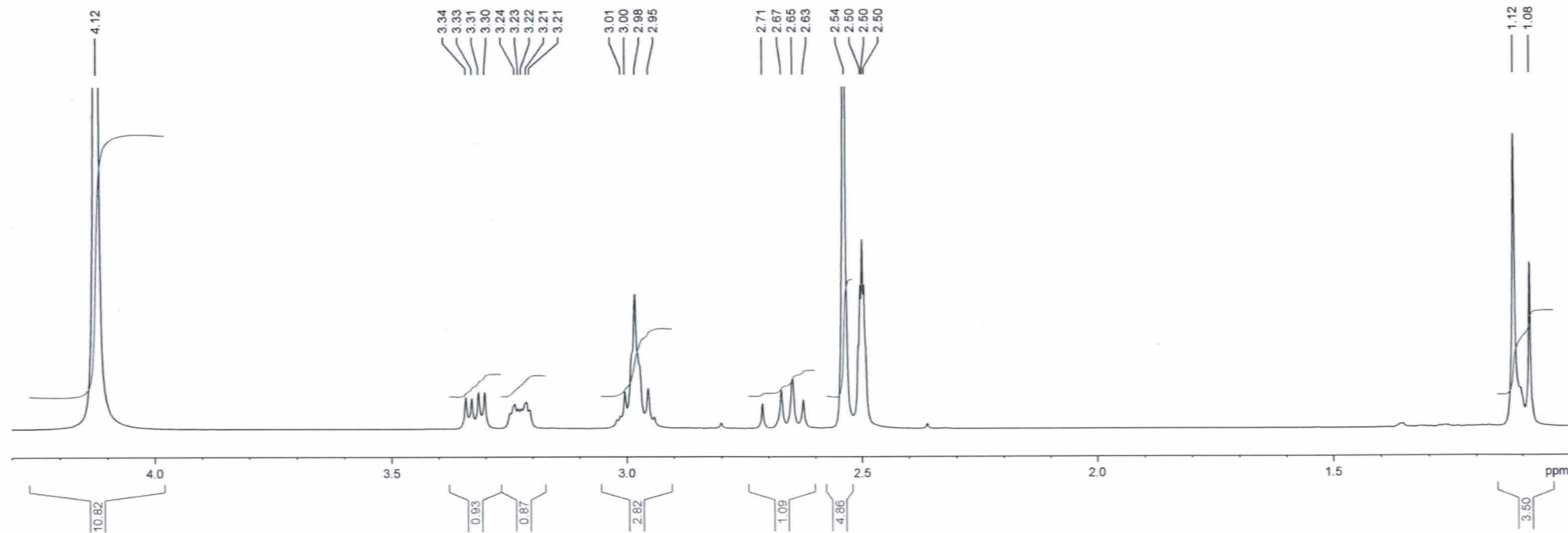




RA0167 **Proton**

NAME ra0167
EXPNO 27
PROCNO 1
Date_ 20150319
Time_ 17.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 161.3
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1336012 MHz
SI 32768
SF 400.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



6.64
6.64
6.47
6.47
6.45
6.45
6.43
6.43
6.42
6.42
6.40
6.40
6.38

4.85
4.84

4.12

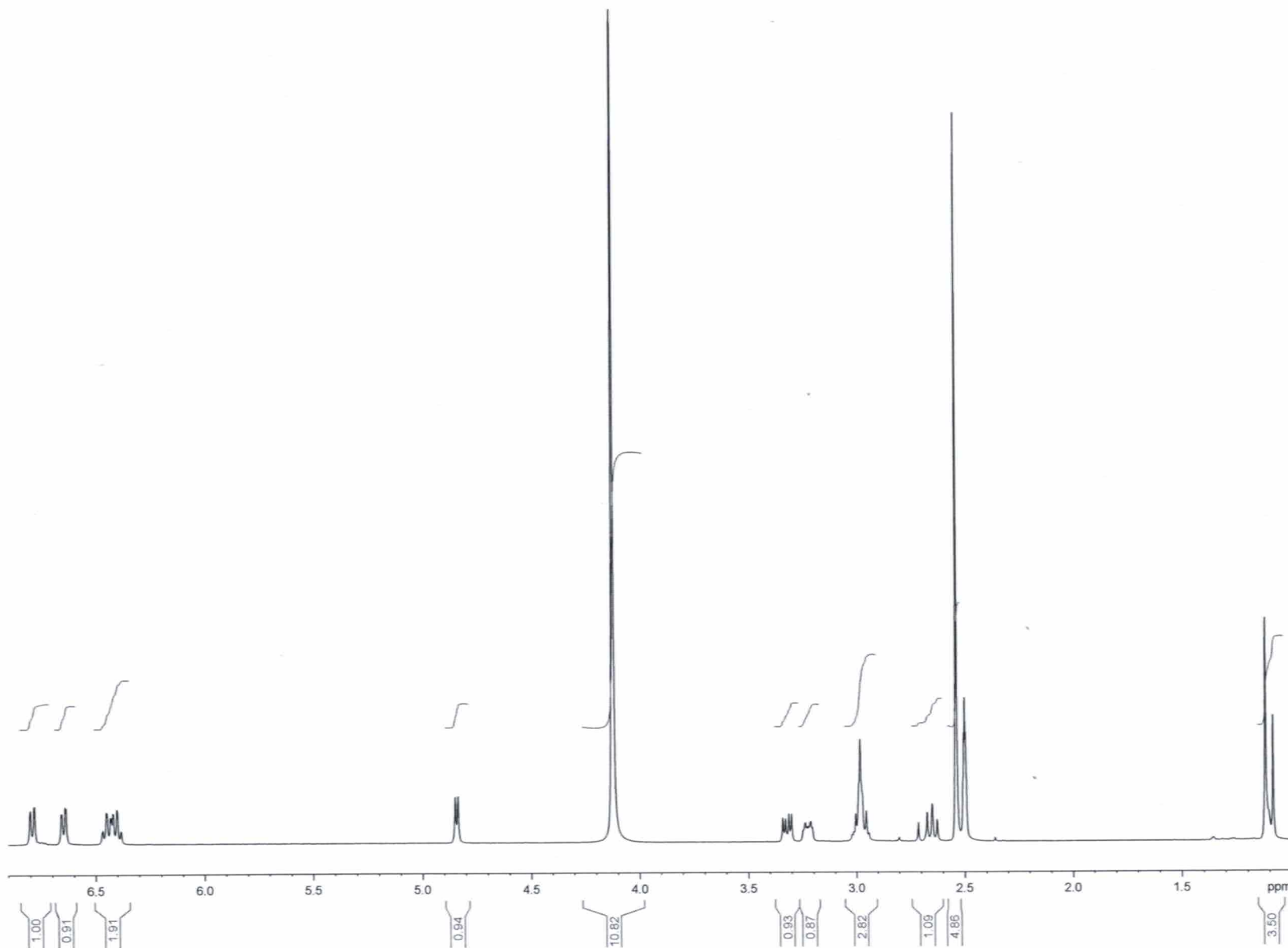
3.34
3.33
3.31
3.30
3.24
3.23
3.22
3.21
3.21
3.01
3.00
2.98
2.95
2.71
2.67
2.65
2.63
2.54
2.50
2.50

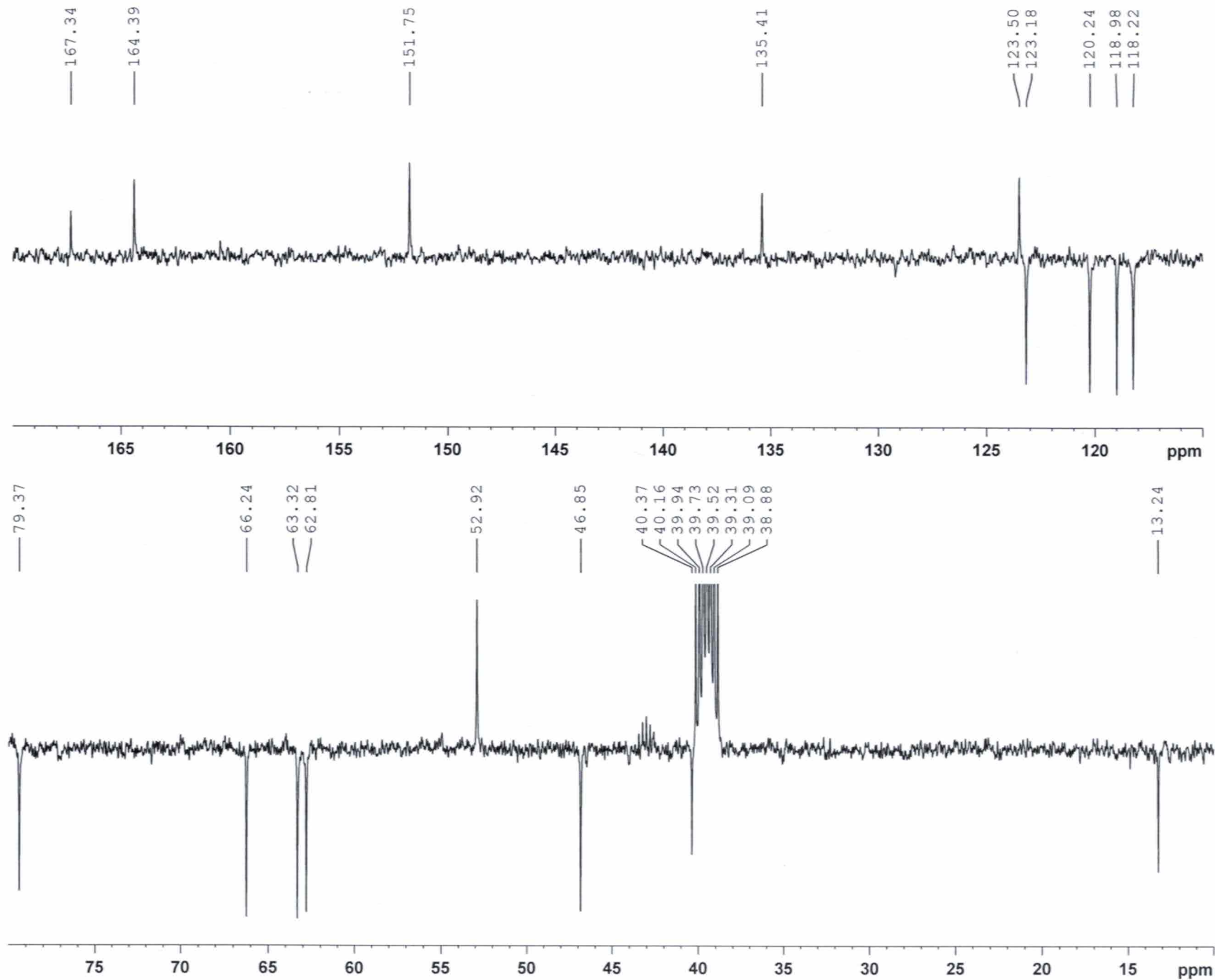
1.12
1.08

RA0167 Proton

NAME ra0167
EXPNO 27
PROCNO 1
Date_ 20150319
Time 17.31
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
DS 2
SWH 8250.825 Hz
FIDRES 0.125898 Hz
AQ 3.9715922 sec
RG 161.3
DW 60.600 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
PL1 0.00 dB
SFO1 400.1336012 MHz
SI 32768
SF 400.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





RA0167 Jmod

```

NAME      ra0167
EXPNO     15
PROCNO    1
Date_     20150312
Time      19.26
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   jmod
TD        65536
SOLVENT   DMSO
NS        1000
DS        4
SWH       23148.148 Hz
FIDRES    0.353213 Hz
AQ        1.4156492 sec
RG        14596.5
DW        21.600 usec
DE        6.50 usec
TE        300.0 K
CNST2     145.0000000
CNST11    1.0000000
D1        5.00000000 sec
D20       0.00689655 sec
TD0       1

```

```

===== CHANNEL f1 =====
NUC1      13C
P1        11.00 usec
P2        22.00 usec
PL1       0.00 dB
SFO1      100.6233333 MHz

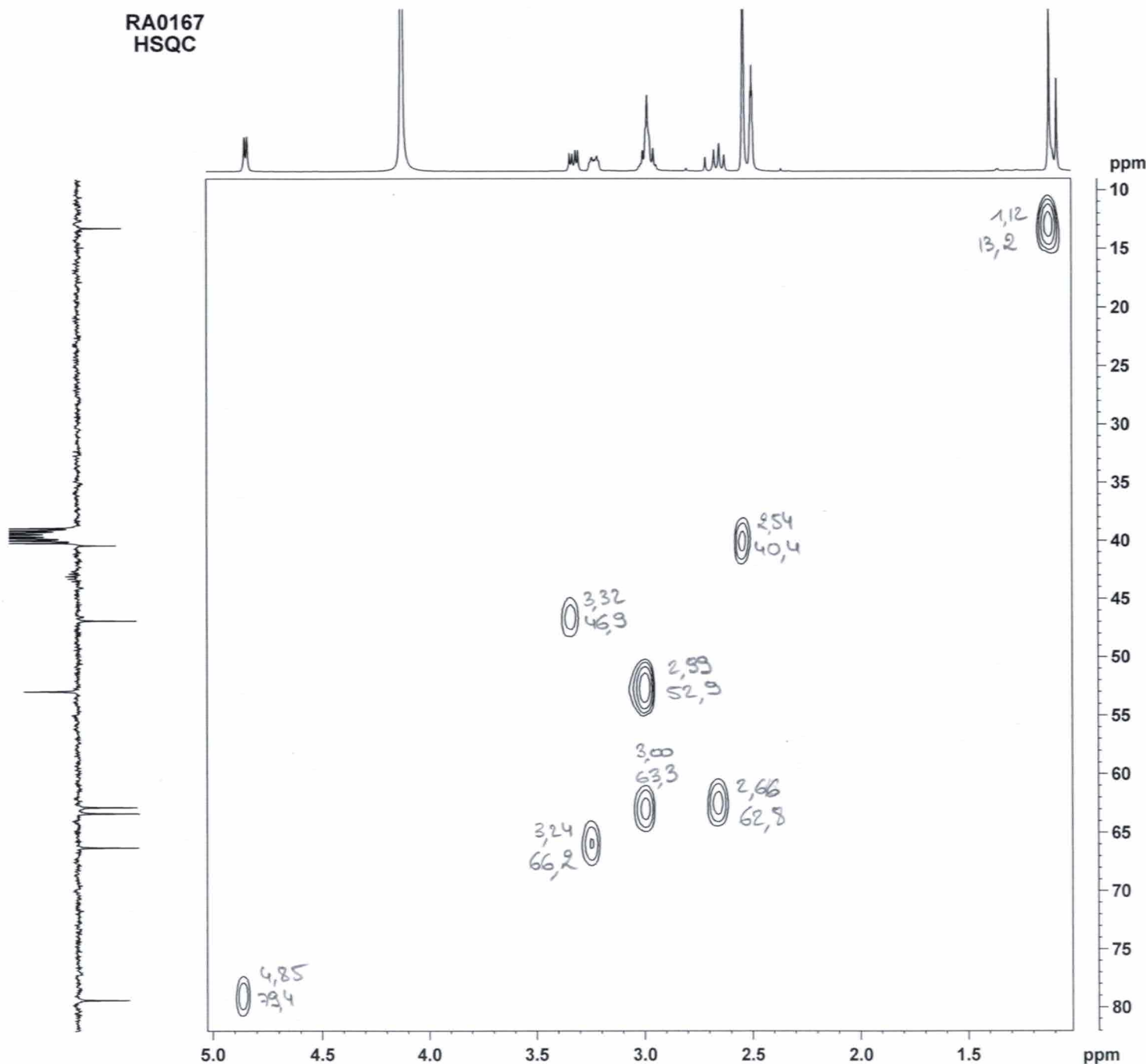
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     100.00 usec
PL2       0.00 dB
PL12     23.32 dB
SFO2      400.1316005 MHz
SI        32768
SF        100.6135019 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40

```

RA0167
HSQC



```

NAME      ra0167
EXPNO     22
PROCNO    1
Date_     20150317
Time      19.03
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   hsqcetgp
TD        1024
SOLVENT   DMSO
NS        16
DS        16
SWH       3968.254 Hz
FIDRES    3.875248 Hz
AQ        0.1292000 sec
RG        46341
DW        126.000 usec
DE        6.50 usec
TE        300.0 K
CNST2     145.0000000
D0        0.00000300 sec
D1        1.01843095 sec
D4        0.00172414 sec
D11       0.03000000 sec
D13       0.00000400 sec
D16       0.00020000 sec
IN0       0.00002615 sec
ZGPTNS

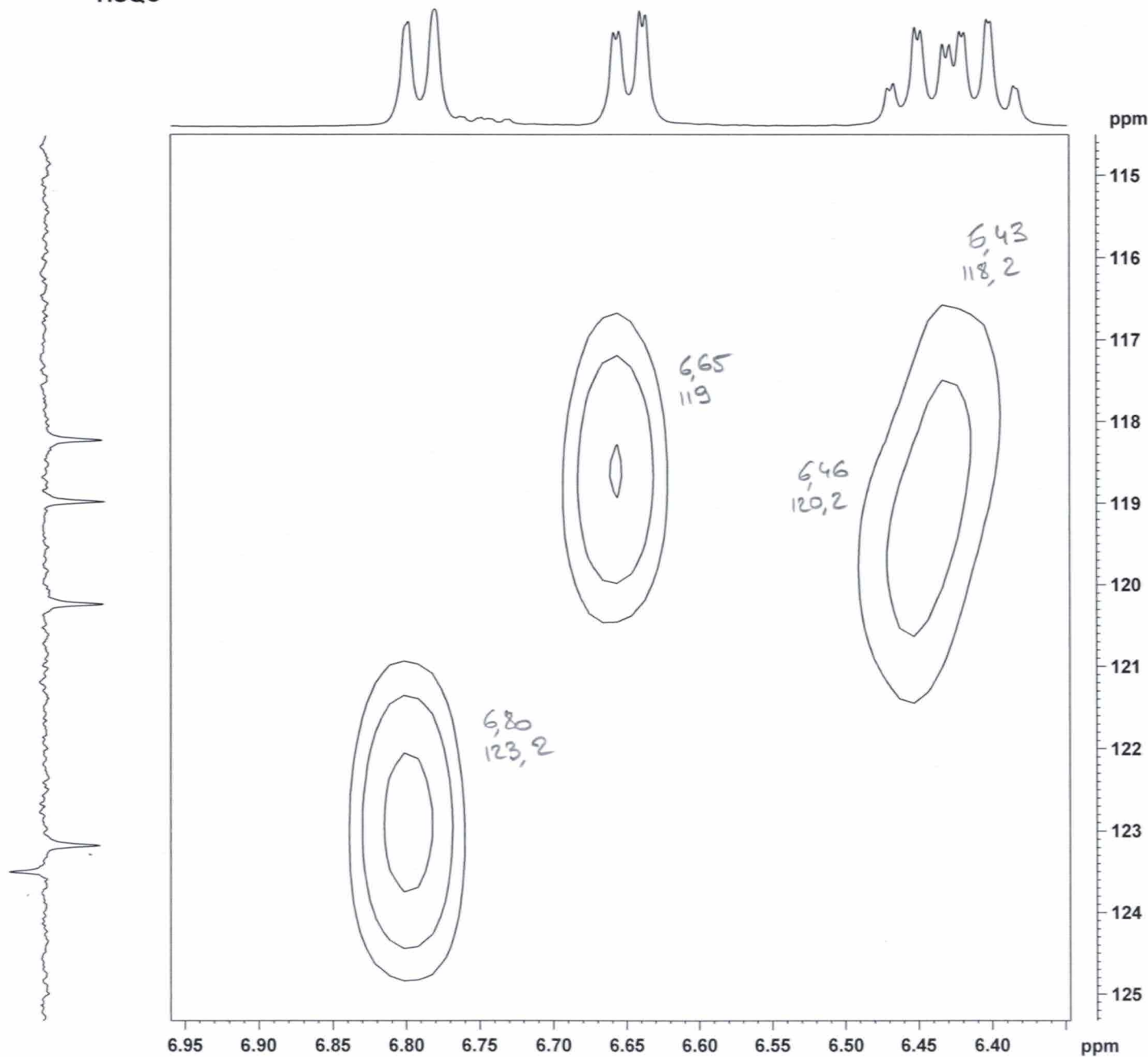
===== CHANNEL f1 =====
NUC1      1H
P1        6.82 usec
P2        13.65 usec
P28       1000.00 usec
PL1       0.00 dB
SFO1      400.1314082 MHz

===== CHANNEL f2 =====
CPDPRG2   garp
NUC2      13C
P3        11.00 usec
P4        22.00 usec
PCPD2     80.00 usec
PL2       0.00 dB
PL12      17.23 dB
SFO2      100.6213211 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPZ1      80.00 %
GPZ2      20.10 %
P16       1000.00 usec
ND0       2
TD        128
SFO1      100.6213 MHz
FIDRES    149.358215 Hz
SW        189.998 ppm
FnMODE    Echo-Antiecho
SI        1024
SF        400.1300062 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0
PC        1.40
SI        1024
MC2       echo-antiecho
SF        100.6135169 MHz
WDW       QSINE
SSB       2
LB        0.00 Hz
GB        0

```

RA0167
HSQC



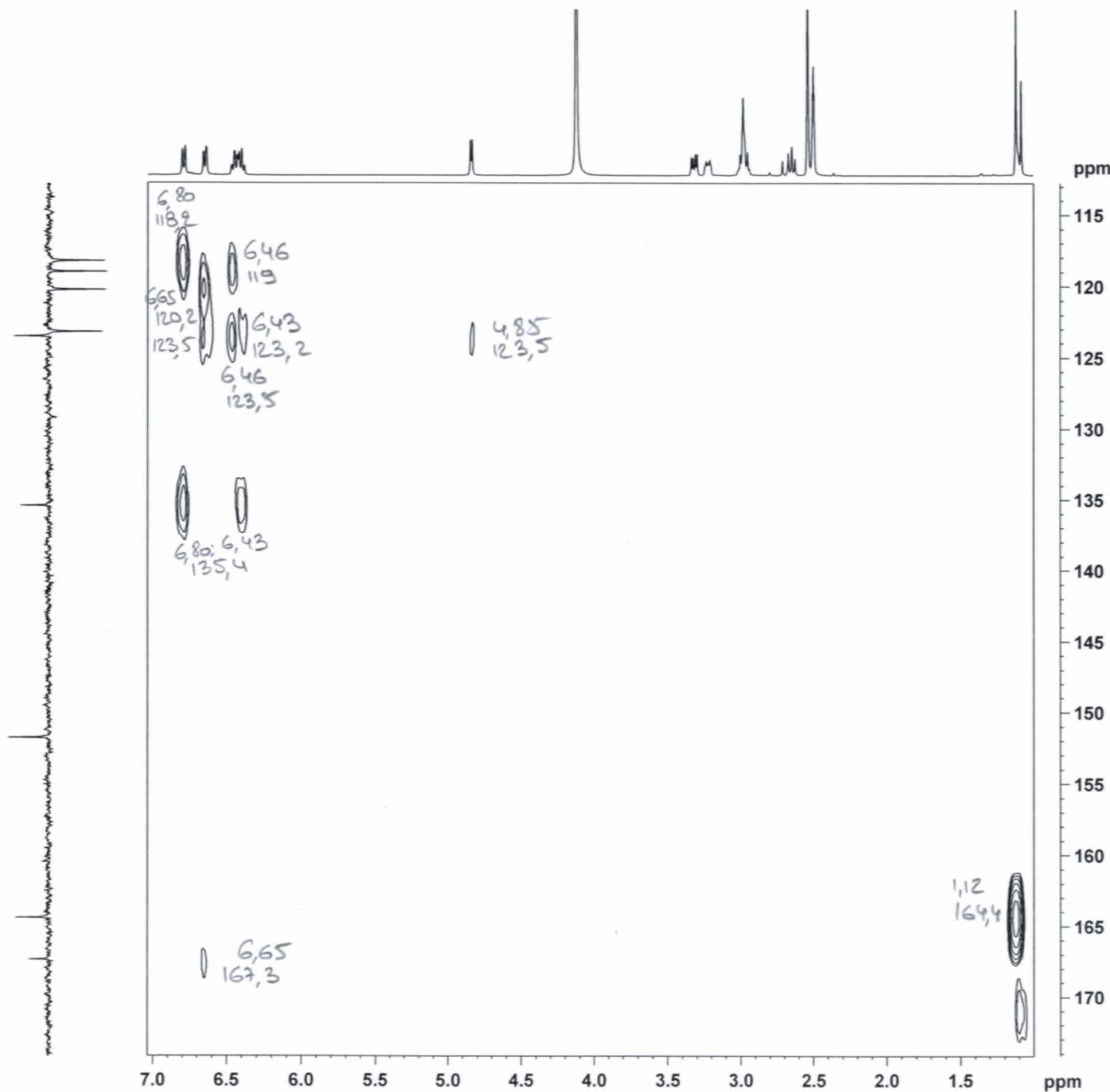
NAME ra0167
EXPNO 22
PROCNO 1
Date_ 20150317
Time_ 19.03
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hsqcetgp
TD 1024
SOLVENT DMSO
NS 16
DS 16
SWH 3968.254 Hz
FIDRES 3.875248 Hz
AQ 0.1292000 sec
RG 46341
DW 126.000 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.01843095 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00002615 sec
ZGPTNS

===== CHANNEL f1 =====
NUC1 ^1H
P1 6.82 usec
P2 13.65 usec
P28 1000.00 usec
PL1 0.00 dB
SFO1 400.1314082 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 ^{13}C
P3 11.00 usec
P4 22.00 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
SFO2 100.6213211 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
P16 1000.00 usec
ND0 2
TD 128
SFO1 100.6213 MHz
FIDRES 149.358215 Hz
SW 189.998 ppm
FnMODE Echo-Antiecho
SI 1024
SF 400.1300062 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 100.6135169 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

RA0167 HMBC



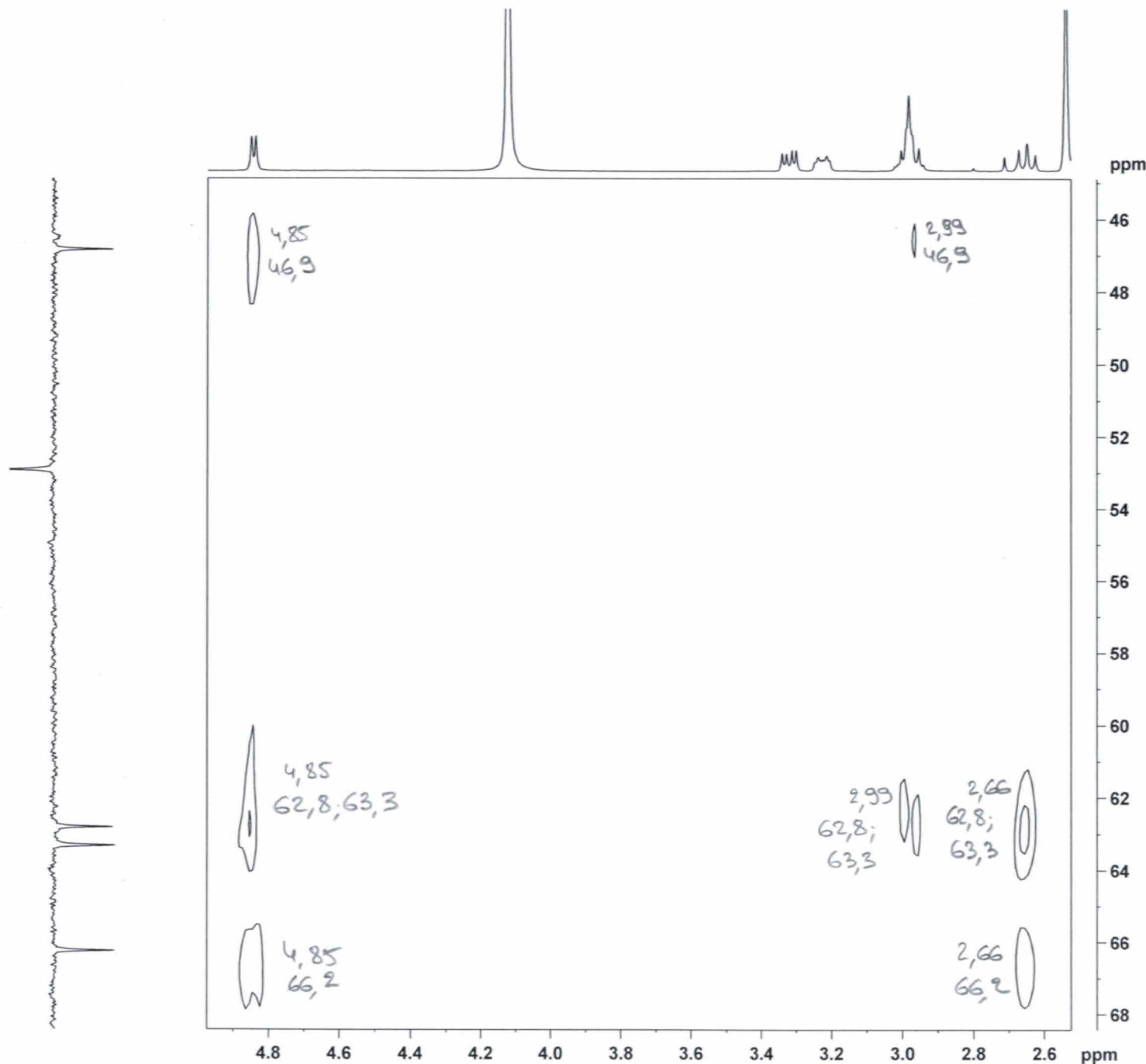
NAME ra0167
EXPNO 23
PROCNO 1
Date_ 20150317
Time 19.43
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgp1pndqf
TD 1024
SOLVENT DMSO
NS 16
DS 16
SWH 3968.254 Hz
FIDRES 3.875248 Hz
AQ 0.1292000 sec
RG 46341
DW 126.000 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 7.6999998
D0 0.00000300 sec
D1 1.01658499 sec
D2 0.00344828 sec
D6 0.06493507 sec
D16 0.00020000 sec
IN0 0.00002160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1314082 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 128
SFO1 100.6238 MHz
FIDRES 180.806473 Hz
SW 229.997 ppm
FnMODE QF
SI 1024
SF 400.1300068 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6134872 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

RA0167
HMBC



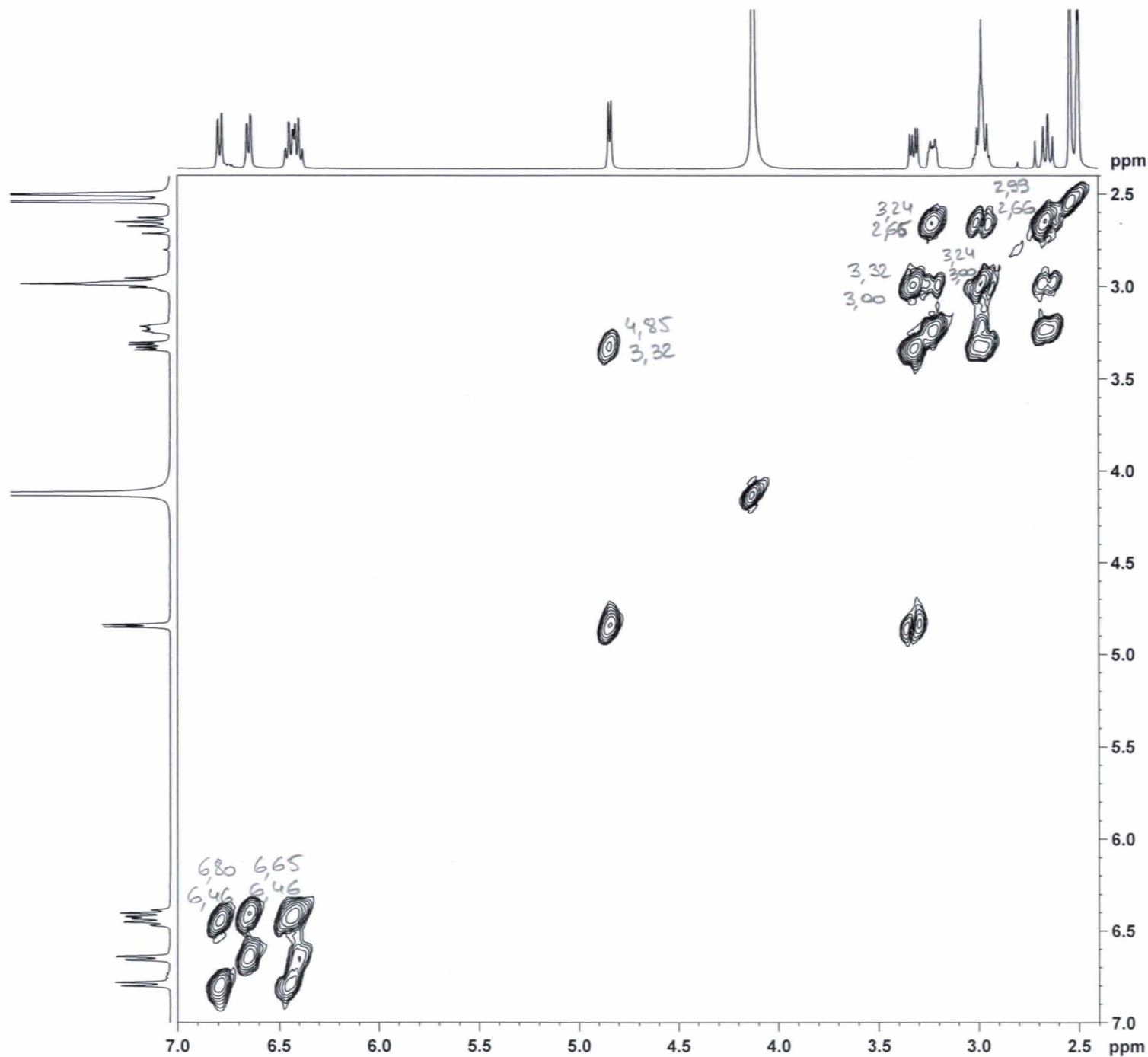
NAME ra0167
EXPNO 23
PROCNO 1
Date_ 20150317
Time 19.43
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG hmbcgpplpndgf
TD 1024
SOLVENT DMSO
NS 16
DS 16
SWH 3968.254 Hz
FIDRES 3.875248 Hz
AQ 0.1292000 sec
RG 46341
DW 126.000 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
CNST13 7.6999998
D0 0.00000300 sec
D1 1.01658499 sec
D2 0.00344828 sec
D6 0.06493507 sec
D16 0.00020000 sec
INO 0.00002160 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1314082 MHz

===== CHANNEL f2 =====
NUC2 13C
P3 11.00 usec
PL2 0.00 dB
SFO2 100.6238364 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 128
SFO1 100.6238 MHz
FIDRES 180.806473 Hz
SW 229.997 ppm
FnMODE QF
SI 1024
SF 400.1300068 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 100.6134872 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

RA0167 COSY



```

NAME          ra0167
EXPNO         21
PROCNO        1
Date_         20150317
Time          18.43
INSTRUM       spect
PROBHD        5 mm Multinucl
PULPROG       cosygpmfzf
TD            1024
SOLVENT       DMSO
NS            4
DS            16
SWH           3968.254 Hz
FIDRES        3.875248 Hz
AQ            0.1292000 sec
RG            8192
DW            126.000 usec
DE            6.50 usec
TE            300.0 K
D0            0.00000300 sec
D1            2.01638293 sec
D13           0.00000400 sec
D16           0.00020000 sec
INO           0.00025200 sec

===== CHANNEL f1 =====
NUC1           1H
P1             6.82 usec
PL1            0.00 dB
SFO1          400.1314082 MHz

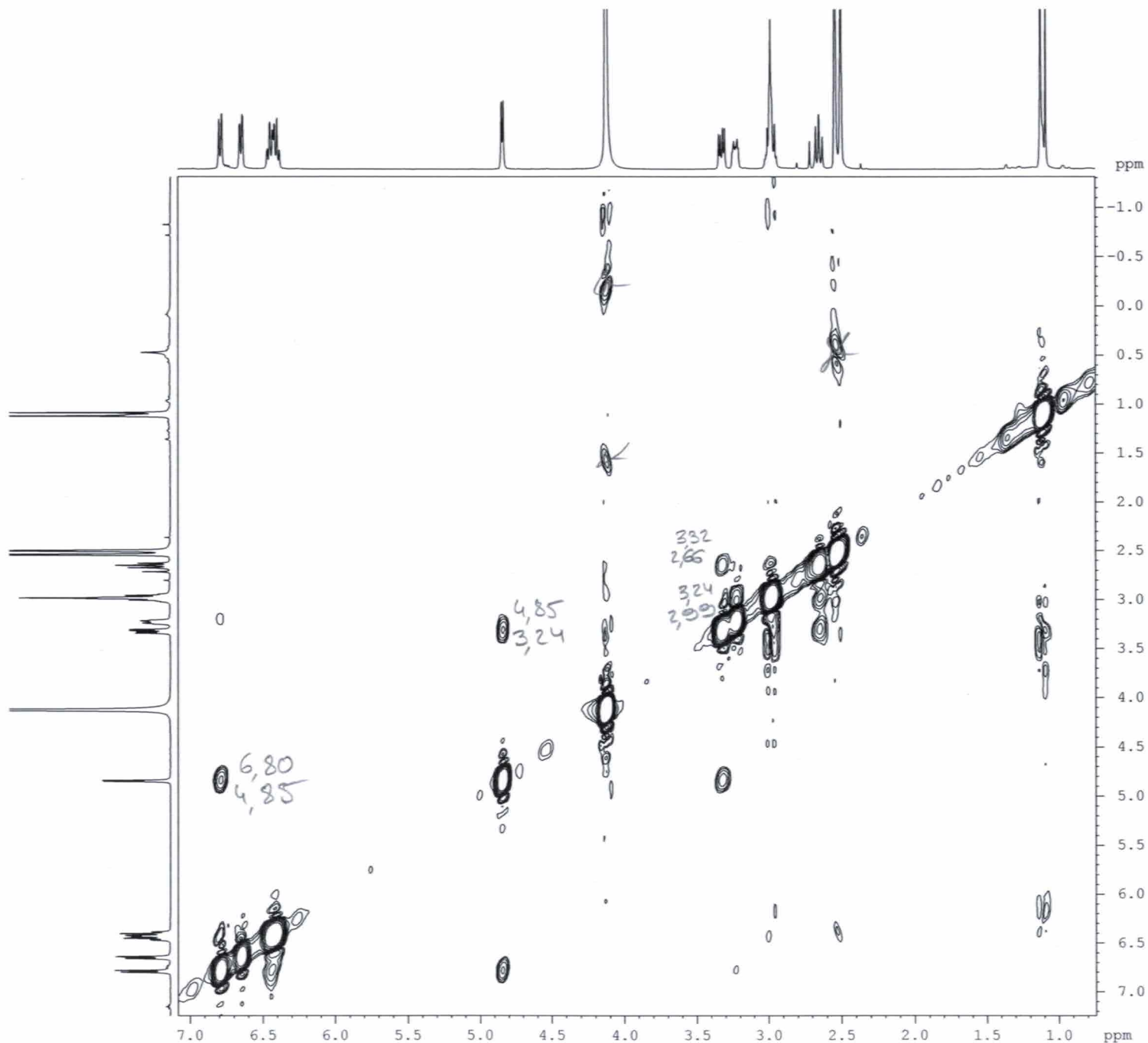
===== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPNAM3        SINE.100
GPZ1          16.00 %
GPZ2          12.00 %
GPZ3          40.00 %
P16           1000.00 usec
ND0            1
TD            128
SFO1          400.1314 MHz
FIDRES        31.001984 Hz
SW            9.917 ppm
FnMODE        QF
SI            1024
SF            400.1300090 MHz
WDW           SINE
SSB            0
LB            0.00 Hz
GB            0
PC            1.40
SI            1024
MC2           QF
SF            400.1300073 MHz
WDW           SINE
SSB            0
LB            0.00 Hz
GB            0
  
```

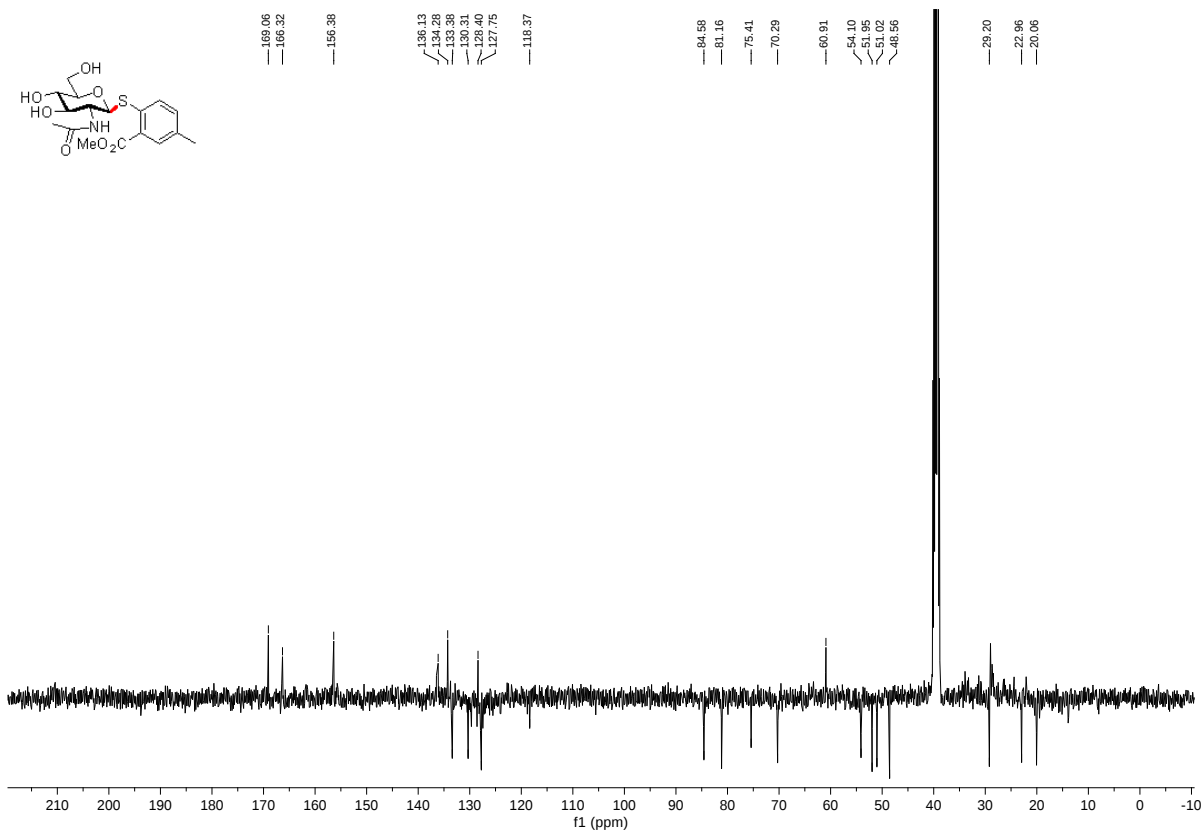
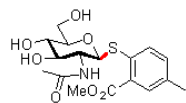
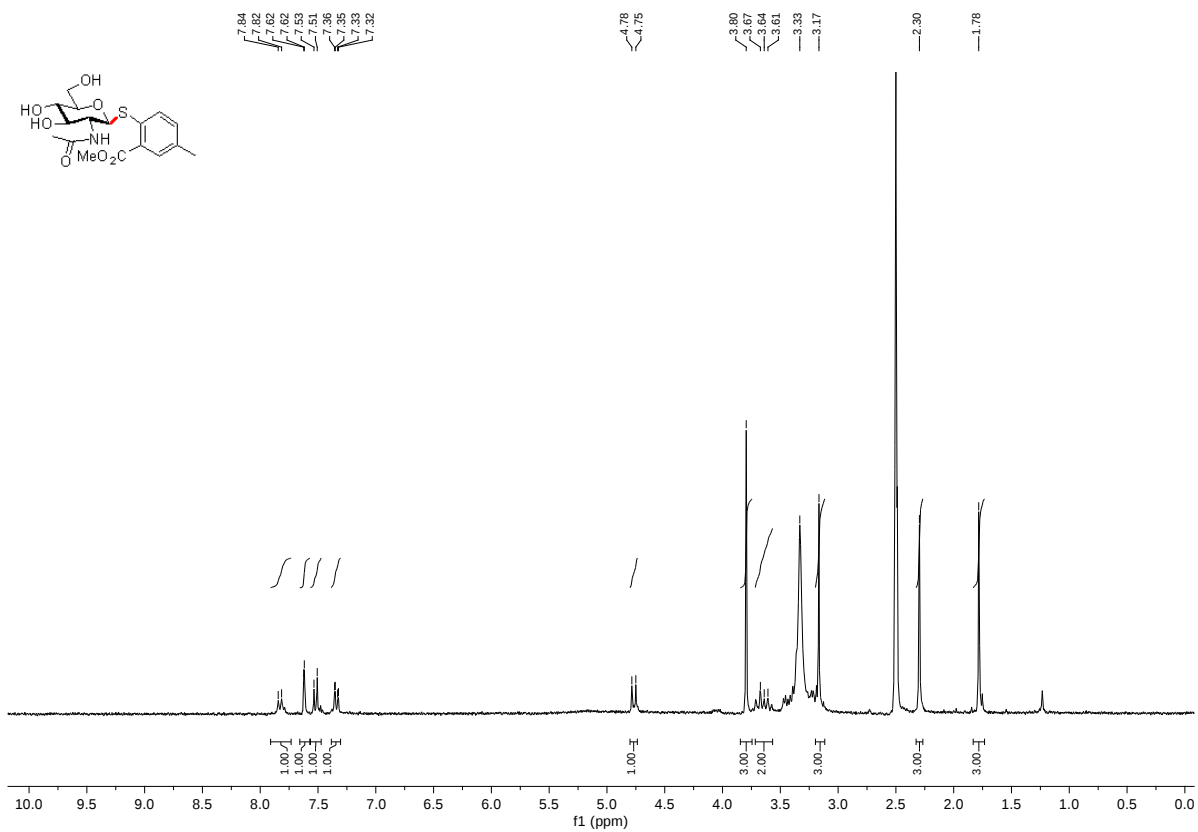
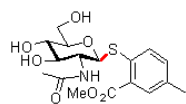
RA0167 NOESY

NAME ra0167
EXPNO 24
PROCNO 1
Date_ 20150317
Time 20.26
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG noesyppph
TD 1024
SOLVENT DMSO
NS 8
DS 16
SWH 3968.254 Hz
FIDRES 3.875248 Hz
AQ 0.1292000 sec
RG 128
DW 126.000 usec
DE 6.50 usec
TE 300.0 K
D0 0.00011731 sec
D1 1.02334595 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00025200 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.82 usec
P2 13.65 usec
PL1 0.00 dB
SFO1 400.1314082 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 40.00 %
P16 1000.00 usec
NDO 1
TD 128
SFO1 400.1314 MHz
FIDRES 31.001984 Hz
SW 9.917 ppm
FnMODE TPPI
SI 1024
SF 400.1300086 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
SI 1024
MC2 TPPI
SF 400.1300101 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

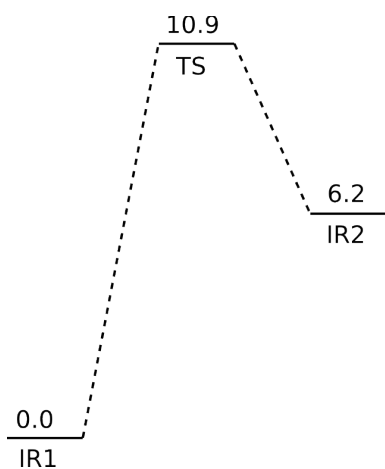




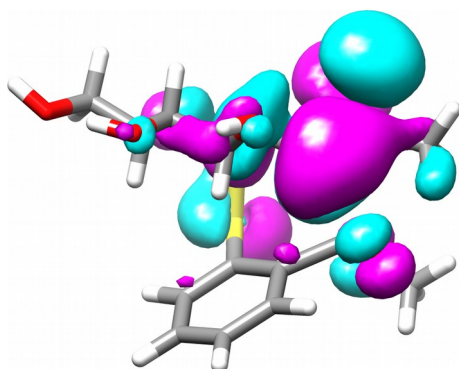
Molecular models

Anomer alpha, attack on the *re* face

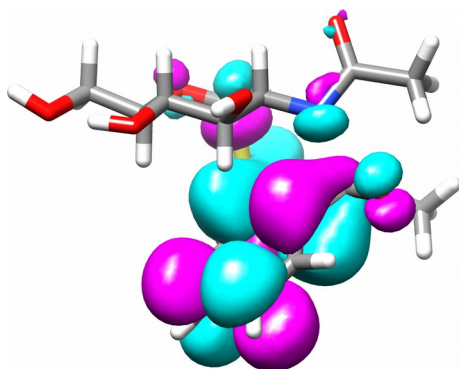
Free energy profile :



HOMO in TS :¹



LUMO in TS :



¹ FMO figures were rendered with Chimera. Chimera is developed by the Resource for Biocomputing, Visualization, and Informatics at the University of California, San Francisco, with support from the National Institutes of Health (National Center for Research Resources grant 2P41RR001081, National Institute of General Medical Sciences grant 9P41GM103311).

IR1 model :

Electronic energy (RB3LYP): -1601.23548954 Ha.

Lowest frequency: 17.7141 cm⁻¹.

Sum of electronic and thermal free energies: -1600.936654 Ha.

List of atomic coordinates:

1	C	0.414703	-1.428584	0.458005
2	C	0.662169	-1.165693	-1.049400
3	O	2.043452	-1.183013	-1.398395
4	C	2.857224	-0.275713	-0.669887
5	C	2.729480	-0.507948	0.842158
6	C	1.272069	-0.487186	1.313779
7	S	-0.194047	0.298023	-1.899365
8	C	-0.562497	1.595473	-0.700968
9	C	-1.755164	1.687660	0.054859
10	C	-2.966009	0.803416	-0.046008
11	N	-0.976470	-1.435227	0.830571
12	O	-3.801948	0.715000	0.834873
13	C	-1.907593	2.743904	0.966122
14	C	-0.939864	3.732823	1.111857
15	C	0.209448	3.681270	0.325336
16	C	0.386656	2.621550	-0.562590
17	C	4.264350	-0.540537	-1.202702
18	O	3.435422	0.487733	1.593499
19	O	1.240506	-0.912280	2.677389
20	H	0.843637	-2.442148	0.569954
21	H	2.575124	0.763060	-0.896379
22	H	3.130009	-1.510989	1.069997
23	H	0.898805	0.542745	1.241270
24	H	-2.816771	2.763395	1.557512
25	H	-1.087846	4.539086	1.826376
26	H	0.974486	4.449792	0.409419
27	H	1.289987	2.567698	-1.161493
28	O	5.196414	0.343180	-0.553712
29	H	4.319097	0.552939	1.190172
30	H	1.879932	-0.333399	3.124613
31	C	-1.546839	-2.617047	0.580366
32	O	-1.053133	-3.613430	-0.019010
33	C	-2.958726	-2.780989	1.163150
34	H	-3.626618	-3.235553	0.418308
35	H	-2.910787	-3.486241	2.004792
36	H	-3.376688	-1.836690	1.521742
37	H	0.224370	-2.007207	-1.587745
38	H	4.273947	-0.384052	-2.290257
39	H	4.519618	-1.591246	-1.003107
40	H	6.089125	0.028467	-0.756796
41	O	-3.137516	0.276946	-1.270604
42	C	-4.305496	-0.531401	-1.434558
43	H	-4.275681	-0.873161	-2.470719
44	H	-4.280577	-1.382192	-0.752306
45	H	-5.212177	0.054841	-1.248935

TS model :

Electronic energy (RB3LYP): -1601.22127763 Ha.

Single imaginary frequency: 158.8895i cm⁻¹.

Sum of electronic and thermal free energies: -1600.919212 Ha.

List of atomic coordinates:

1	C	0.154398	-1.350033	0.230600
2	C	0.610822	-1.115101	-1.230100
3	O	2.023178	-1.242442	-1.386481
4	C	2.799531	-0.410749	-0.532957
5	C	2.489863	-0.729390	0.936233
6	C	0.998684	-0.561440	1.244796
7	S	-0.037746	0.402409	-2.102215
8	C	-0.321917	1.627129	-0.821268
9	C	-1.291605	1.504531	0.195173
10	C	-2.373479	0.418649	0.337040
11	N	-1.283675	-1.251936	0.388804
12	O	-3.114258	0.466441	1.326312
13	C	-1.377495	2.527755	1.149767
14	C	-0.571995	3.663494	1.093982
15	C	0.352978	3.801452	0.059819
16	C	0.478830	2.779788	-0.879905
17	C	4.239552	-0.727718	-0.932490
18	O	3.199038	0.120379	1.841977
19	O	0.739115	-1.075026	2.550908
20	H	0.415276	-2.405645	0.393221
21	H	2.591866	0.651927	-0.727191
22	H	2.751286	-1.786778	1.116856
23	H	0.779137	0.510322	1.222372
24	H	-2.115444	2.393439	1.933412
25	H	-0.671403	4.438417	1.851530
26	H	0.987945	4.682570	-0.006567
27	H	1.220437	2.854973	-1.670646
28	O	5.141842	0.058847	-0.134961
29	H	4.114268	0.167406	1.512918
30	H	1.346667	-0.586655	3.130400
31	C	-1.907608	-2.442843	0.224875
32	O	-1.342049	-3.511032	-0.101228
33	C	-3.411630	-2.494980	0.475521
34	H	-3.937820	-2.548540	-0.485857
35	H	-3.621839	-3.426864	1.011793
36	H	-3.776424	-1.638209	1.042068
37	H	0.196277	-1.929542	-1.826450
38	H	4.372882	-0.508515	-2.000785
39	H	4.415077	-1.802058	-0.776583
40	H	6.035139	-0.288337	-0.272072
41	O	-2.957972	0.204329	-0.947423
42	C	-4.347913	0.468634	-0.991808
43	H	-4.627563	0.395751	-2.048786
44	H	-4.935675	-0.251679	-0.412337
45	H	-4.587677	1.476007	-0.621996

IR2 model :

Electronic energy (RB3LYP): -1601.22901996 Ha.

Lowest frequency: 22.8245 cm⁻¹.

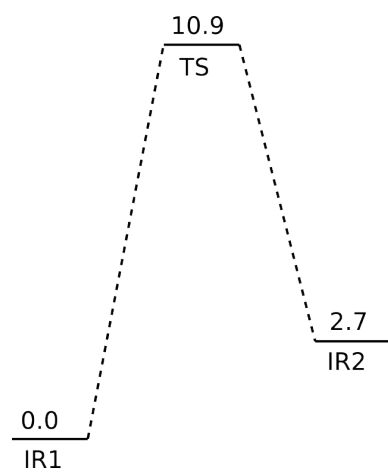
Sum of electronic and thermal free energies: -1600.926812 Ha.

List of atomic coordinates:

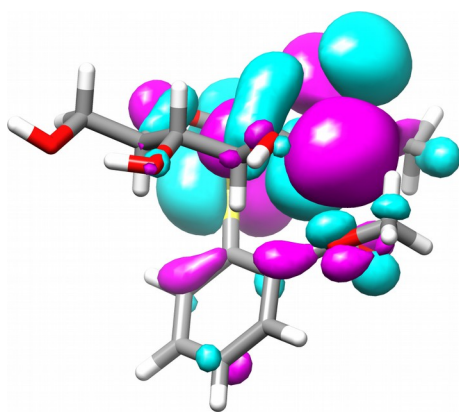
1	C	0.150777	-1.327048	0.072168
2	C	0.669650	-0.992972	-1.348001
3	O	2.089913	-1.100517	-1.431410
4	C	2.806938	-0.312682	-0.487552
5	C	2.456202	-0.775611	0.932609
6	C	0.951661	-0.653321	1.199679
7	S	0.036323	0.560116	-2.138553
8	C	-0.345300	1.665018	-0.779967
9	C	-1.224621	1.337706	0.271280
10	C	-2.123589	0.051908	0.423877
11	N	-1.300384	-1.253412	0.161919
12	O	-2.813312	0.034031	1.489368
13	C	-1.435772	2.306623	1.260594
14	C	-0.840542	3.566186	1.210293
15	C	0.007996	3.888408	0.150772
16	C	0.261936	2.930779	-0.829688
17	C	4.270608	-0.538983	-0.860250
18	O	3.112695	-0.010515	1.944127
19	O	0.637315	-1.321496	2.418584
20	H	0.371288	-2.395391	0.170407
21	H	2.561781	0.753703	-0.599778
22	H	2.727752	-1.842646	1.016821
23	H	0.727884	0.412220	1.291667
24	H	-2.109220	2.011518	2.059760
25	H	-1.039080	4.293788	1.995458
26	H	0.483665	4.865631	0.093141
27	H	0.945508	3.152312	-1.645758
28	O	5.109635	0.209160	0.035865
29	H	4.030918	0.112532	1.643925
30	H	1.142573	-0.851059	3.100901
31	C	-1.935347	-2.466793	0.009444
32	O	-1.313207	-3.502099	-0.276164
33	C	-3.440398	-2.541021	0.193058
34	H	-3.931480	-2.256185	-0.742302
35	H	-3.685740	-3.581238	0.426848
36	H	-3.771550	-1.851952	0.970957
37	H	0.303092	-1.776025	-2.014455
38	H	4.429490	-0.221105	-1.899749
39	H	4.486176	-1.615296	-0.791758
40	H	6.023367	-0.078444	-0.104558
41	O	-2.935298	0.085513	-0.872275
42	C	-4.078339	0.894180	-0.767131
43	H	-4.746121	0.629163	-1.598618
44	H	-4.595399	0.730542	0.187220
45	H	-3.846470	1.973068	-0.848587

Anomer alpha, attack on the *si* face

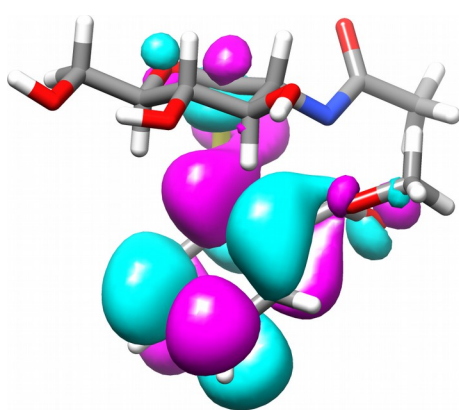
Free energy profile :



HOMO in TS :



LUMO in TS :



IR1 model :

Electronic energy (RB3LYP): -1601.23885533 Ha.

Lowest frequency: 27.061 cm⁻¹.

Sum of electronic and thermal free energies: -1600.940283 Ha.

List of atomic coordinates:

1	C	-0.663752	-1.650646	0.081072
2	C	0.023751	-1.285192	-1.270771
3	O	1.400101	-1.639802	-1.326642
4	C	2.212855	-1.210586	-0.237983
5	C	1.619254	-1.629290	1.114214
6	C	0.175527	-1.151751	1.258900
7	S	-0.350875	0.385351	-2.065016
8	C	0.391635	1.720137	-1.112521
9	C	-0.264607	2.392768	-0.060729
10	C	-1.665575	2.052397	0.380320
11	N	-2.038540	-1.235053	0.148722
12	O	-2.653222	2.186251	-0.305501
13	C	0.380180	3.448684	0.598762
14	C	1.642089	3.884352	0.201111
15	C	2.282980	3.249485	-0.863394
16	C	1.661345	2.179198	-1.504271
17	C	3.562716	-1.866410	-0.527408
18	O	2.362871	-1.080350	2.208320
19	O	-0.352167	-1.655390	2.487584
20	H	-0.589885	-2.755384	0.071312
21	H	2.333638	-0.118836	-0.239712
22	H	1.616270	-2.731861	1.171268
23	H	0.175782	-0.053855	1.285874
24	H	-0.125282	3.932036	1.430188
25	H	2.119735	4.712723	0.719042
26	H	3.266983	3.579307	-1.189251
27	H	2.157009	1.669566	-2.325056
28	O	4.504739	-1.498534	0.496135
29	H	3.300445	-1.256596	2.013398
30	H	0.310033	-1.401553	3.152158
31	C	-2.831633	-1.951523	-0.648863
32	O	-2.506086	-2.891795	-1.428203
33	C	-4.318966	-1.579375	-0.582555
34	H	-4.495359	-0.662309	-0.013251
35	H	-4.705865	-1.450781	-1.600904
36	H	-4.887069	-2.402901	-0.127279
37	H	-0.478870	-1.909071	-2.014029
38	H	3.918059	-1.542524	-1.515537
39	H	3.419108	-2.956059	-0.553935
40	H	5.274559	-2.078977	0.409345
41	O	-1.660683	1.687798	1.677066
42	C	-2.881876	1.095087	2.170307
43	H	-2.752757	1.030672	3.252780
44	H	-3.740124	1.723935	1.917480
45	H	-2.952601	0.102775	1.708087

TS model :

Electronic energy (RB3LYP): -1601.22500269 Ha.

Single imaginary frequency: 151.3061i cm⁻¹.

Sum of electronic and thermal free energies: -1600.922846 Ha.

List of atomic coordinates:

1	C	-0.118197	-1.486223	-0.023253
2	C	0.604866	-1.195013	-1.368136
3	O	2.021566	-1.298798	-1.303861
4	C	2.640484	-0.565290	-0.253353
5	C	2.127186	-1.083314	1.095767
6	C	0.609266	-0.917942	1.202445
7	S	0.013201	0.313657	-2.280010
8	C	-0.137905	1.651663	-1.091757
9	C	-1.024217	1.688086	0.003162
10	C	-2.133597	0.687098	0.398656
11	N	-1.518207	-1.118474	-0.113441
12	O	-3.249526	0.879904	-0.098256
13	C	-1.046545	2.863557	0.779818
14	C	-0.256115	3.970604	0.489566
15	C	0.605065	3.932574	-0.607383
16	C	0.662773	2.775643	-1.376705
17	C	4.132317	-0.807431	-0.477143
18	O	2.695291	-0.390591	2.209650
19	O	0.149086	-1.629848	2.353910
20	H	-0.053792	-2.579844	0.072590
21	H	2.428509	0.510142	-0.341960
22	H	2.360782	-2.161146	1.151661
23	H	0.405962	0.149015	1.326156
24	H	-1.718170	2.887746	1.630652
25	H	-0.313457	4.857063	1.118096
26	H	1.235525	4.784431	-0.853726
27	H	1.343366	2.717180	-2.221572
28	O	4.886668	-0.116771	0.533465
29	H	3.641309	-0.276423	2.009724
30	H	0.548430	-1.167861	3.107948
31	C	-2.246985	-2.006700	-0.831200
32	O	-1.770547	-3.039493	-1.357930
33	C	-3.741909	-1.750800	-0.991512
34	H	-3.926659	-0.760671	-1.411723
35	H	-4.142581	-2.536838	-1.637805
36	H	-4.258501	-1.775164	-0.025518
37	H	0.294004	-1.981469	-2.057388
38	H	4.406998	-0.451262	-1.479493
39	H	4.319152	-1.890533	-0.433651
40	H	5.804852	-0.418001	0.473902
41	O	-1.998283	0.516123	1.801427
42	C	-3.015424	-0.266632	2.393934
43	H	-2.906289	-0.152708	3.478036
44	H	-4.009156	0.074294	2.080773
45	H	-2.884476	-1.320635	2.122872

IR2 model :

Electronic energy (RB3LYP): -1601.24082736 Ha.

Lowest frequency: 37.9441 cm⁻¹.

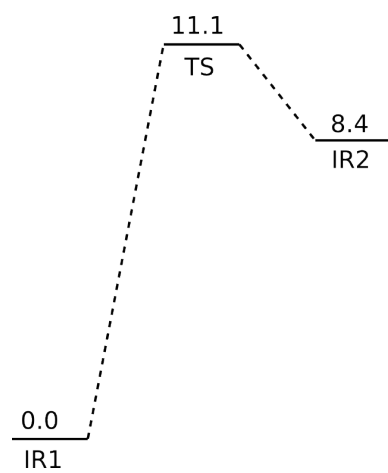
Sum of electronic and thermal free energies: -1600.936036 Ha.

List of atomic coordinates:

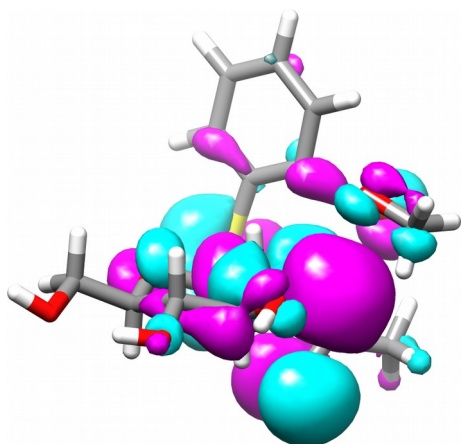
1	C	0.059290	-1.302504	0.007696
2	C	0.787024	-1.096632	-1.336415
3	O	2.192354	-1.223733	-1.215195
4	C	2.797169	-0.437606	-0.193737
5	C	2.229775	-0.795069	1.193271
6	C	0.713473	-0.585792	1.216463
7	S	0.241181	0.398413	-2.298386
8	C	-0.255343	1.654087	-1.111113
9	C	-1.198578	1.476130	-0.078388
10	C	-2.088988	0.223986	0.169653
11	N	-1.386386	-1.098590	-0.179281
12	O	-3.246578	0.377703	-0.302621
13	C	-1.528366	2.604593	0.693298
14	C	-0.969765	3.856540	0.462514
15	C	-0.041574	4.023202	-0.567494
16	C	0.314209	2.921690	-1.337388
17	C	4.284804	-0.755400	-0.348903
18	O	2.802338	0.024290	2.204980
19	O	0.196873	-1.111498	2.419935
20	H	0.181877	-2.369226	0.218027
21	H	2.633151	0.634676	-0.380005
22	H	2.437549	-1.863616	1.386186
23	H	0.560794	0.496896	1.180970
24	H	-2.246963	2.462014	1.490806
25	H	-1.255674	4.699859	1.088071
26	H	0.412453	4.993109	-0.759592
27	H	1.050314	3.024925	-2.130317
28	O	5.049950	0.039150	0.571095
29	H	3.751238	0.090544	1.998178
30	H	-0.710521	-0.719705	2.441897
31	C	-2.022015	-2.173921	-0.765504
32	O	-1.386311	-3.190154	-1.086477
33	C	-3.516229	-2.151909	-1.044773
34	H	-3.770598	-1.340470	-1.727373
35	H	-3.757123	-3.126929	-1.478881
36	H	-4.104523	-1.981232	-0.141625
37	H	0.495811	-1.914415	-1.996502
38	H	4.583667	-0.546037	-1.385224
39	H	4.433650	-1.828394	-0.158546
40	H	5.945981	-0.326246	0.602599
41	O	-2.088840	0.151104	1.786649
42	C	-3.265085	-0.435083	2.284957
43	H	-3.415921	-0.086735	3.316857
44	H	-4.123368	-0.137067	1.669450
45	H	-3.213083	-1.539191	2.302404

Anomer beta, attack on the *re* face

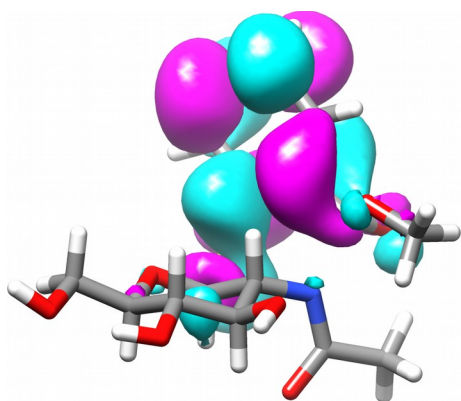
Free energy profile :



HOMO in TS :



LUMO in TS :



IR1 model :

Electronic energy (RB3LYP): -1601.24347077 Ha.

Lowest frequency: 21.5788 cm⁻¹.

Sum of electronic and thermal free energies: -1600.945733 Ha.

List of atomic coordinates:

1	C	0.507837	-0.981891	-0.248374
2	C	0.652523	-0.185130	1.077190
3	O	1.388429	1.045154	0.942673
4	C	2.703151	0.873338	0.429478
5	C	2.634673	0.246792	-0.967582
6	C	1.900220	-1.090075	-0.914982
7	H	1.138041	-0.846263	1.804425
8	C	-1.644278	1.477099	0.782441
9	C	-2.655605	1.163433	-0.145031
10	C	-3.176855	-0.243094	-0.285794
11	N	-0.142165	-2.268246	-0.054112
12	O	-3.864913	-0.808524	0.536151
13	C	-3.186812	2.165112	-0.967420
14	C	-2.741521	3.481119	-0.864218
15	C	-1.740637	3.800399	0.055059
16	C	-1.198392	2.804951	0.866736
17	C	3.285224	2.286112	0.442223
18	O	3.932990	-0.005121	-1.519595
19	O	1.737841	-1.572374	-2.254173
20	H	-0.112329	-0.385023	-0.933136
21	H	3.302713	0.220495	1.084986
22	H	2.067998	0.932845	-1.622005
23	H	2.500774	-1.791853	-0.323666
24	H	-3.950676	1.902409	-1.694493
25	H	-3.169397	4.250948	-1.502377
26	H	-1.381199	4.823736	0.139735
27	H	-0.411539	3.037666	1.575452
28	O	4.630188	2.257798	-0.067161
29	H	4.462144	0.793475	-1.346867
30	H	2.639076	-1.572461	-2.616654
31	C	0.469666	-3.115562	0.768017
32	O	1.536329	-2.959904	1.437977
33	C	-0.232117	-4.474603	0.916354
34	H	-0.467786	-4.650606	1.974141
35	H	-1.151421	-4.542246	0.326734
36	H	0.455012	-5.274324	0.608633
37	S	-0.946889	0.241504	1.890289
38	H	3.268356	2.675361	1.469942
39	H	2.644599	2.927954	-0.179583
40	H	4.904427	3.173033	-0.223549
41	O	-2.804916	-0.747962	-1.473185
42	C	-2.939431	-2.180176	-1.638162
43	H	-2.061897	-2.624534	-1.147680
44	H	-3.878659	-2.526123	-1.199973
45	H	-2.926323	-2.350310	-2.717010

TS model :

Electronic energy (RB3LYP): -1601.22980531 Ha.

Single imaginary frequency: 122.3548i cm⁻¹.

Sum of electronic and thermal free energies: -1600.928118 Ha.

List of atomic coordinates:

1	C	0.412957	-0.602619	-0.029237
2	C	0.870070	0.248084	1.174381
3	O	1.864116	1.212413	0.782882
4	C	3.053702	0.583463	0.323535
5	C	2.764532	-0.322241	-0.885722
6	C	1.654357	-1.331160	-0.580713
7	H	1.277350	-0.415993	1.944531
8	C	-1.497355	1.736907	0.647993
9	C	-2.198169	0.964013	-0.301996
10	C	-2.449174	-0.563159	-0.330815
11	N	-0.727399	-1.420829	0.303563
12	O	-3.385681	-0.996035	0.347031
13	C	-2.928942	1.659502	-1.285509
14	C	-3.004154	3.048302	-1.322631
15	C	-2.324237	3.801863	-0.366449
16	C	-1.568321	3.140566	0.596331
17	C	3.985369	1.747815	-0.006841
18	O	3.917084	-1.073244	-1.281819
19	O	1.312975	-2.023657	-1.782723
20	H	0.095776	0.090694	-0.818841
21	H	3.505407	-0.033555	1.119565
22	H	2.420262	0.316371	-1.718280
23	H	2.012586	-2.038034	0.176582
24	H	-3.453206	1.070852	-2.029720
25	H	-3.591308	3.537296	-2.097635
26	H	-2.364840	4.889120	-0.378280
27	H	-1.003599	3.707848	1.330385
28	O	5.242699	1.234814	-0.481946
29	H	4.653682	-0.437351	-1.318198
30	H	2.156600	-2.384517	-2.101948
31	C	-0.566628	-2.352403	1.262020
32	O	0.501543	-2.592651	1.876799
33	C	-1.783431	-3.218762	1.574038
34	H	-1.727820	-3.527930	2.622895
35	H	-2.719621	-2.697844	1.365529
36	H	-1.744738	-4.129007	0.958654
37	S	-0.520755	1.083466	2.009626
38	H	4.131030	2.361407	0.892862
39	H	3.501464	2.369865	-0.773020
40	H	5.733910	1.973006	-0.870549
41	O	-2.279554	-0.947410	-1.676366
42	C	-2.573911	-2.307307	-1.935734
43	H	-1.792283	-2.943843	-1.505658
44	H	-3.548335	-2.588413	-1.519652
45	H	-2.583897	-2.420636	-3.024936

IR2 model :

Electronic energy (RB3LYP): -1601.23514778 Ha.

Lowest frequency: 33.0288 cm⁻¹.

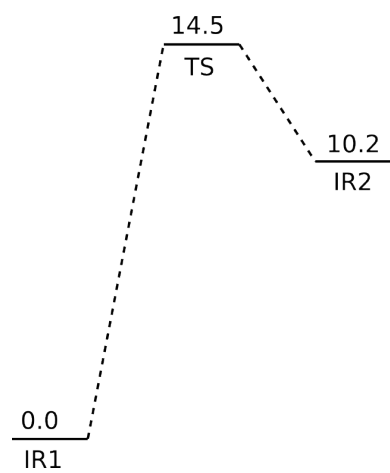
Sum of electronic and thermal free energies: -1600.932281 Ha.

List of atomic coordinates:

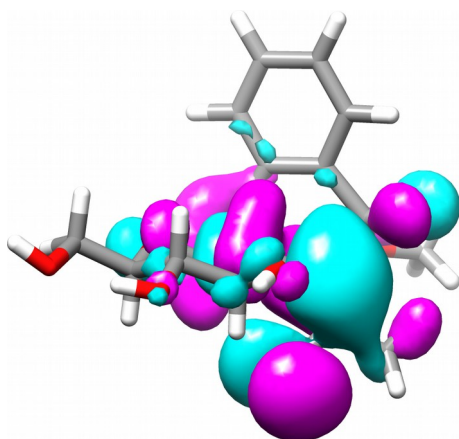
1	C	0.451844	-0.483446	0.054347
2	C	0.857066	0.518474	1.154180
3	O	1.816745	1.455966	0.635002
4	C	3.038709	0.816496	0.288222
5	C	2.808530	-0.278324	-0.767687
6	C	1.720597	-1.266617	-0.332696
7	H	1.296789	-0.019071	2.001506
8	C	-1.696359	1.681145	0.497043
9	C	-2.224333	0.696804	-0.362369
10	C	-2.046716	-0.868333	-0.342179
11	N	-0.720888	-1.258041	0.427045
12	O	-3.090362	-1.464494	0.058703
13	C	-3.171828	1.125708	-1.312596
14	C	-3.595295	2.444579	-1.411245
15	C	-3.067754	3.408938	-0.547252
16	C	-2.118168	3.021753	0.389713
17	C	3.930021	1.951747	-0.210445
18	O	3.991232	-1.046605	-1.005305
19	O	1.453434	-2.163727	-1.405526
20	H	0.158191	0.092998	-0.825895
21	H	3.501524	0.348237	1.174280
22	H	2.470609	0.204383	-1.700955
23	H	2.078214	-1.820186	0.542742
24	H	-3.576931	0.367707	-1.972709
25	H	-4.333611	2.722785	-2.161433
26	H	-3.380602	4.449327	-0.611300
27	H	-1.678779	3.758395	1.057246
28	O	5.207002	1.416253	-0.599488
29	H	4.706927	-0.400772	-1.143811
30	H	2.321692	-2.534164	-1.635615
31	C	-0.623979	-2.110404	1.489082
32	O	0.436511	-2.237911	2.128761
33	C	-1.826207	-2.940198	1.906643
34	H	-1.508708	-3.540520	2.764634
35	H	-2.672979	-2.298865	2.154349
36	H	-2.171461	-3.580599	1.092321
37	S	-0.569263	1.388563	1.873490
38	H	4.047755	2.698401	0.586875
39	H	3.430838	2.433949	-1.062609
40	H	5.674466	2.101086	-1.099169
41	O	-1.654855	-1.123290	-1.765495
42	C	-1.779737	-2.480712	-2.123507
43	H	-0.987557	-3.097641	-1.674432
44	H	-2.758843	-2.877253	-1.824282
45	H	-1.679111	-2.534114	-3.215631

Anomer beta, attack on the si face

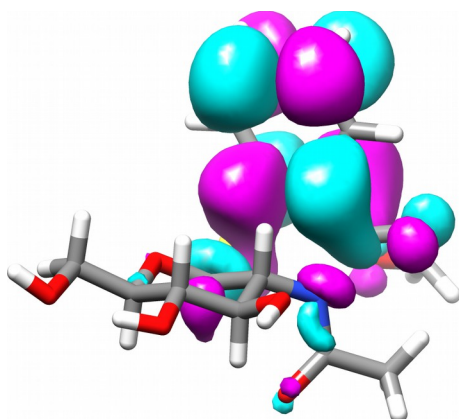
Free energy profile :



HOMO in TS :



LUMO in TS :



IR1 model :

Electronic energy (RB3LYP): -1601.24378238 Ha.

Lowest frequency: 19.8356 cm⁻¹.

Sum of electronic and thermal free energies: -1600.946267 Ha.

List of atomic coordinates:

1	C	-1.089658	-0.763656	0.802696
2	C	-0.753633	-0.333721	-0.653514
3	O	-1.405701	0.885764	-1.080696
4	C	-2.824713	0.791879	-1.032894
5	C	-3.272649	0.545482	0.412123
6	C	-2.631416	-0.725795	0.966863
7	H	-1.073201	-1.168360	-1.292227
8	C	1.740593	0.996323	0.014092
9	C	3.130177	1.030815	0.320754
10	C	4.171273	0.100642	-0.197578
11	N	-0.500446	-2.041648	1.150192
12	O	5.285684	-0.027117	0.283866
13	C	3.626720	2.010537	1.200316
14	C	2.801548	2.966189	1.771762
15	C	1.440157	2.950734	1.454057
16	C	0.924661	1.993066	0.589840
17	C	-3.303924	2.121513	-1.612772
18	O	-4.691909	0.387066	0.527258
19	O	-2.948736	-0.818158	2.360424
20	H	-0.690568	-0.004916	1.492491
21	H	-3.183183	-0.036446	-1.665188
22	H	-2.936502	1.402814	1.023725
23	H	-3.040051	-1.583445	0.418532
24	H	4.688890	1.984790	1.420452
25	H	3.208964	3.712921	2.448328
26	H	0.770349	3.696149	1.877718
27	H	-0.125539	2.009534	0.330543
28	O	-4.741614	2.146702	-1.625671
29	H	-5.091963	1.080784	-0.026215
30	H	-3.919110	-0.787635	2.387261
31	C	-0.857264	-3.070732	0.391908
32	O	-1.624601	-3.109475	-0.623850
33	C	-0.233090	-4.406062	0.825440
34	H	-1.029460	-5.124474	1.063898
35	H	0.338585	-4.835726	-0.008669
36	H	0.420740	-4.285731	1.694038
37	S	1.028923	-0.227823	-1.070768
38	H	-2.903357	2.237852	-2.629380
39	H	-2.905532	2.937352	-0.991656
40	H	-5.018598	3.049727	-1.838425
41	O	3.784317	-0.577980	-1.298038
42	C	4.710757	-1.550232	-1.788721
43	H	4.203877	-2.039425	-2.621268
44	H	5.633900	-1.068617	-2.126427
45	H	4.955354	-2.276751	-1.009161

TS model :

Electronic energy (RB3LYP): -1601.2257604 Ha.

Single imaginary frequency: 136.9948i cm⁻¹.

Sum of electronic and thermal free energies: -1600.92317 Ha.

List of atomic coordinates:

1	C	-0.438425	-0.531163	0.273031
2	C	-0.824003	-0.016269	-1.133255
3	O	-1.977879	0.846245	-1.092186
4	C	-3.138049	0.191419	-0.596988
5	C	-2.896881	-0.294565	0.838393
6	C	-1.672402	-1.207912	0.908901
7	H	-1.023256	-0.874794	-1.784366
8	C	1.295774	1.737008	-0.542427
9	C	2.056682	1.073498	0.444565
10	C	2.526460	-0.397016	0.439879
11	N	0.768169	-1.331471	0.256512
12	O	3.133707	-0.828529	1.425720
13	C	2.541285	1.829585	1.519986
14	C	2.330836	3.204480	1.610874
15	C	1.609621	3.860228	0.614046
16	C	1.084748	3.120038	-0.445306
17	C	-4.233925	1.249905	-0.704194
18	O	-4.002427	-1.043818	1.354245
19	O	-1.393011	-1.498941	2.279096
20	H	-0.239047	0.349246	0.895611
21	H	-3.402887	-0.676923	-1.224345
22	H	-2.705971	0.590103	1.471236
23	H	-1.892437	-2.129374	0.359423
24	H	3.101355	1.289207	2.276221
25	H	2.731668	3.760243	2.456542
26	H	1.436344	4.933318	0.667107
27	H	0.485794	3.606631	-1.209746
28	O	-5.475738	0.703971	-0.225208
29	H	-4.802513	-0.536700	1.129014
30	H	-2.224330	-1.866410	2.621702
31	C	0.705584	-2.543519	-0.322936
32	O	-0.282673	-3.022434	-0.929610
33	C	1.947045	-3.421504	-0.184934
34	H	1.613160	-4.427867	0.092753
35	H	2.450919	-3.501494	-1.155669
36	H	2.645463	-3.040358	0.561651
37	S	0.538564	0.899883	-1.944507
38	H	-4.327938	1.569455	-1.751290
39	H	-3.932003	2.120555	-0.104719
40	H	-6.099441	1.437352	-0.122864
41	O	3.041150	-0.678429	-0.861516
42	C	4.378549	-1.141619	-0.857537
43	H	4.678706	-1.182661	-1.910625
44	H	5.047497	-0.459509	-0.313982
45	H	4.482291	-2.137936	-0.414044

IR2 model :

Electronic energy (RB3LYP): -1601.23286426 Ha.

Lowest frequency: 30.3032 cm⁻¹.

Sum of electronic and thermal free energies: -1600.930027 Ha.

List of atomic coordinates:

1	C	-0.467867	-0.507311	0.163090
2	C	-0.862372	0.154507	-1.174371
3	O	-1.974475	1.050635	-0.999438
4	C	-3.147517	0.397296	-0.531365
5	C	-2.883821	-0.260108	0.830335
6	C	-1.696371	-1.222585	0.756315
7	H	-1.125406	-0.624211	-1.900264
8	C	1.395333	1.713390	-0.491344
9	C	1.977673	0.882885	0.490989
10	C	2.107926	-0.691645	0.471810
11	N	0.734558	-1.313708	0.034772
12	O	2.622795	-1.196068	1.512460
13	C	2.625667	1.505740	1.563523
14	C	2.743486	2.892143	1.656148
15	C	2.186842	3.702695	0.666612
16	C	1.499922	3.108465	-0.392333
17	C	-4.192702	1.509900	-0.474125
18	O	-4.000624	-1.026323	1.288343
19	O	-1.381605	-1.681485	2.067560
20	H	-0.231097	0.295477	0.866987
21	H	-3.477604	-0.381681	-1.240043
22	H	-2.639979	0.535348	1.556114
23	H	-1.974164	-2.063910	0.113904
24	H	3.044955	0.834201	2.307440
25	H	3.267804	3.338447	2.499727
26	H	2.266599	4.786765	0.723502
27	H	1.026622	3.724378	-1.152716
28	O	-5.437104	0.970362	0.004425
29	H	-4.784367	-0.462409	1.161535
30	H	-2.209995	-2.065601	2.398580
31	C	0.650056	-2.549439	-0.539991
32	O	-0.370685	-2.942018	-1.130509
33	C	1.838139	-3.488974	-0.407029
34	H	1.433492	-4.502779	-0.315701
35	H	2.446162	-3.438103	-1.315244
36	H	2.459361	-3.228132	0.450554
37	S	0.520132	1.078669	-1.930610
38	H	-4.316287	1.943874	-1.475824
39	H	-3.821553	2.296205	0.198170
40	H	-6.016626	1.714309	0.223508
41	O	2.896609	-0.909747	-0.818651
42	C	4.284024	-0.865982	-0.611375
43	H	4.762657	-1.347328	-1.475590
44	H	4.670581	0.168710	-0.541380
45	H	4.565016	-1.395040	0.308246