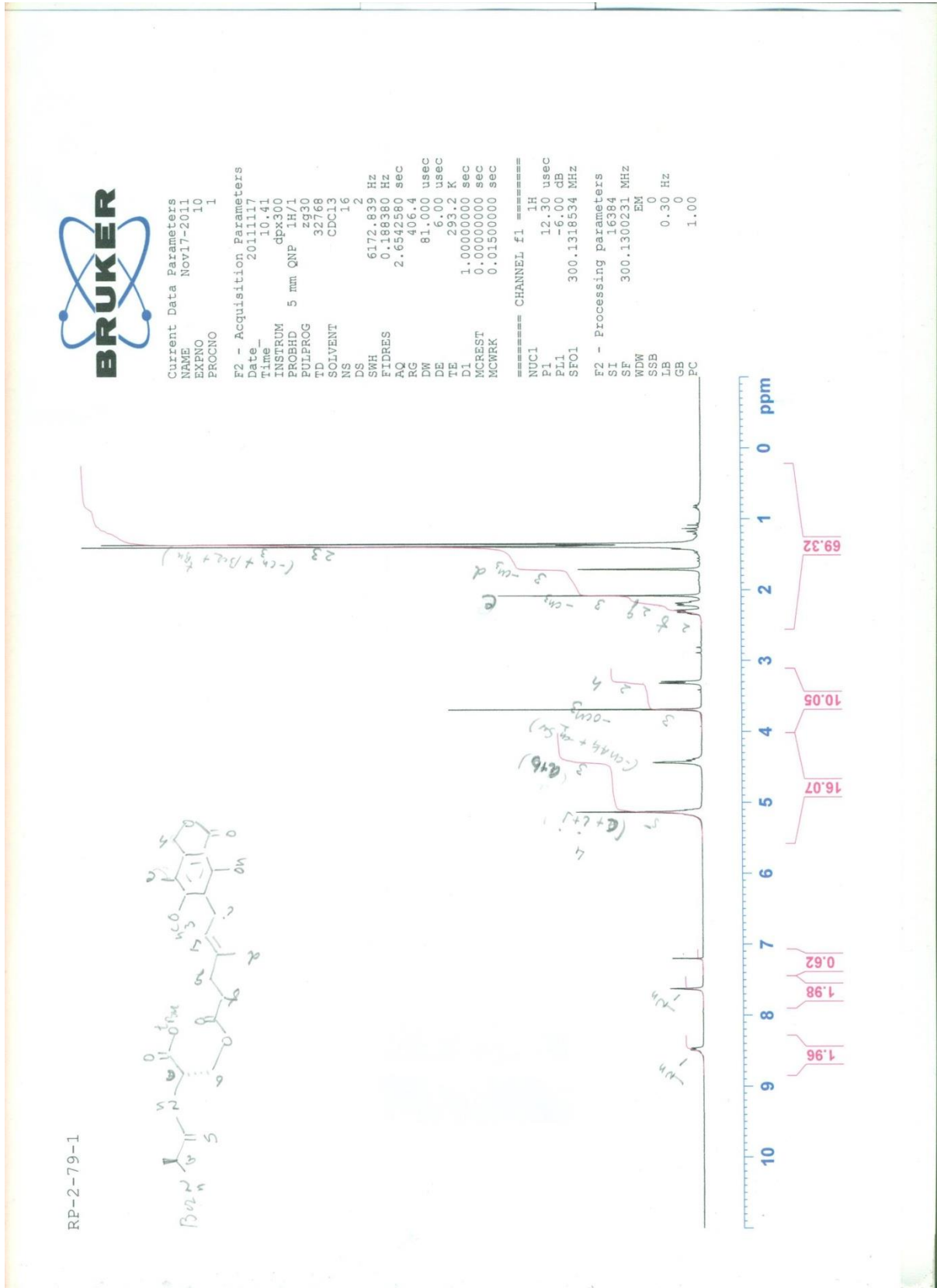


# Reproduced NMR Spectra for Key Compounds

20 <sup>1</sup>H NMR



20 13C NMR



Current Data Parameters  
 NAME Nov17-2011  
 EXPNO 102  
 PROCNO 1

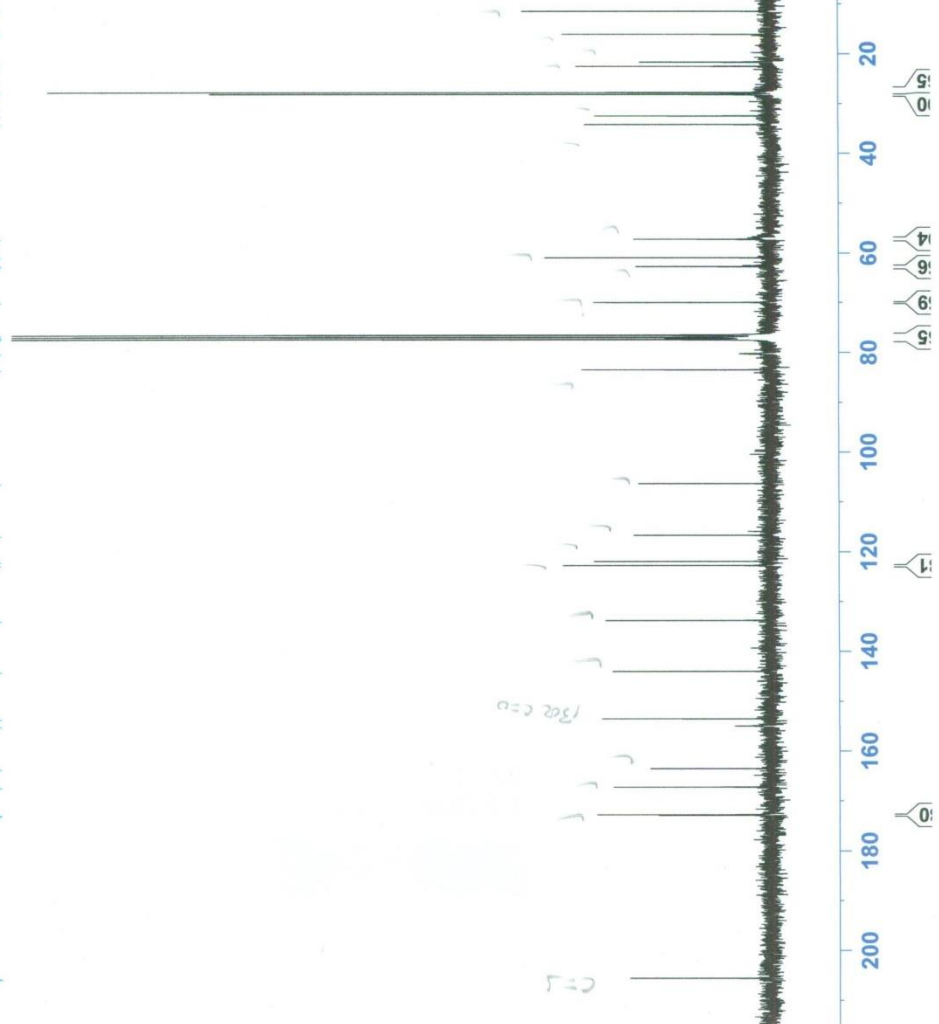
F2 - Acquisition Parameters

Date\_ 20111118  
 Time 0.07  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.9219509 sec  
 RG 10321.3  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 293.2 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 MCREST 0.00000000 sec  
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.40 usec  
 PL1 -6.00 dB  
 SF01 75.4752953 MHz  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 100.00 usec  
 PL2 -6.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 NDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

RP-2-79





19 1H NMR

RP-2-83-1

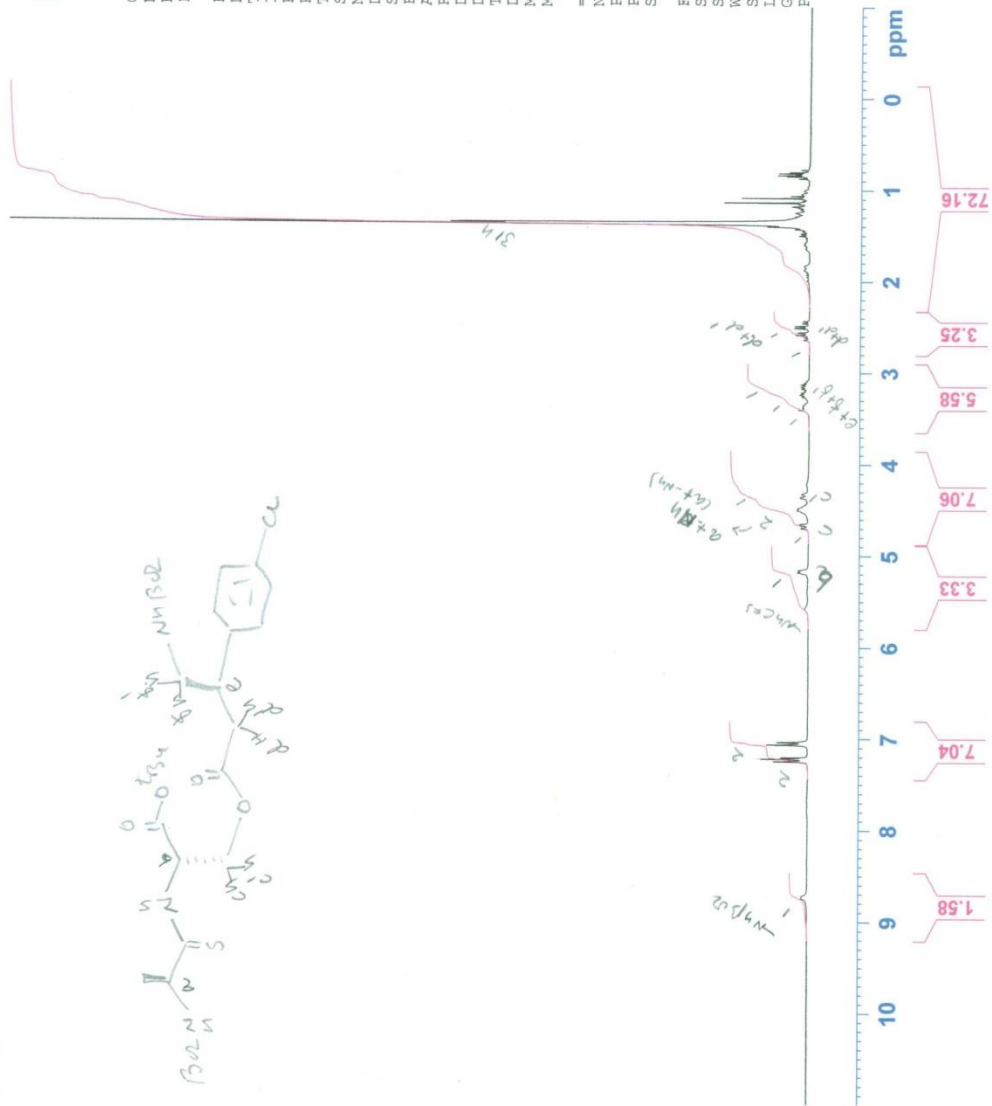
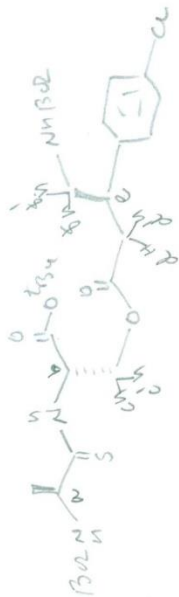


Current Data Parameters  
 NAME Nov24-2011  
 EXPNO 30  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20111124  
 Time\_ 21:33  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 228.1  
 DM 81.000 usec  
 DE 6.00 usec  
 TE 293.2 K  
 DI 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.30 usec  
 PL1 -6.00 dB  
 SF01 300.1318534 MHz

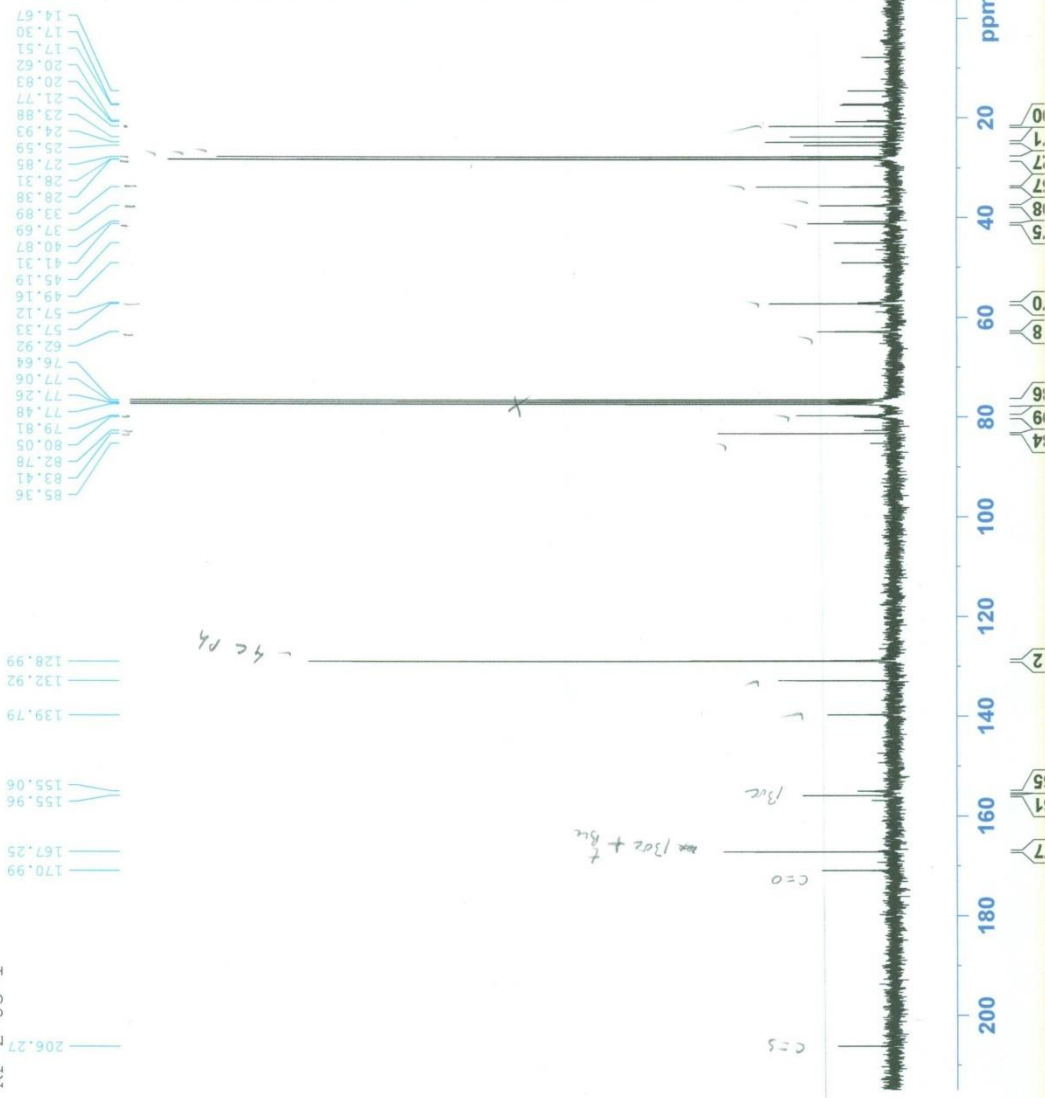
F2 - Processing parameters  
 SI 32768  
 SF 300.1300219 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



19 <sup>13</sup>C NMR



RP-2-83-1



Current Data Parameters  
 NAME Nov24-2011  
 EXPNO 33  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20111124  
 Time\_ 23:39  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274433 Hz  
 AQ 1.8219508 sec  
 RG 9195.2  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 293.2 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999998 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 6.40 usec  
 PL1 -6.00 dB  
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 -6.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





Current Data Parameters  
 NAME Nov30-2011  
 EXPNO 63  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20111130  
 Time\_ 23.27  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 ID zgpg30  
 SOLVENT D2O  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 10321.3  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.40 usec  
 PL1 -6.00 dB  
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 -6.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

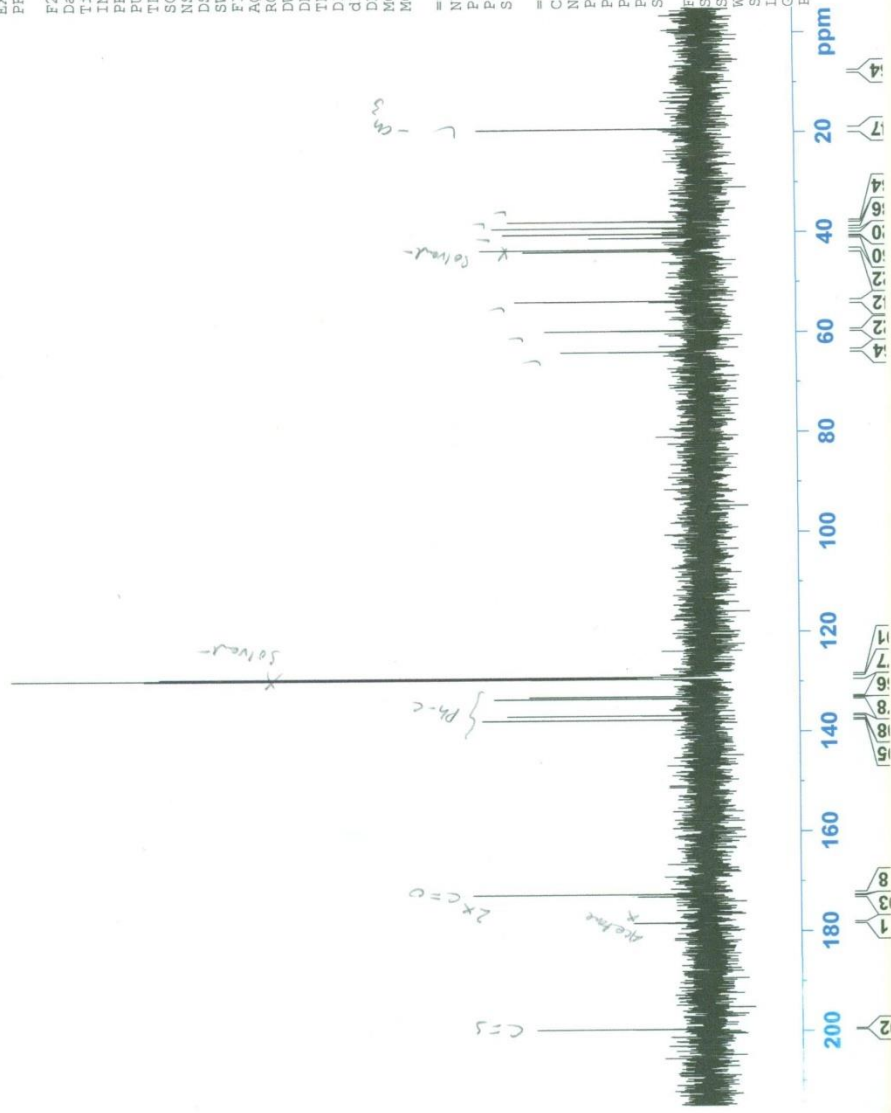
F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

RP-2-85-D2O

137.66  
136.79  
133.35  
132.97  
129.40  
129.26  
129.21  
129.05

63.93  
59.71  
53.77  
43.80  
43.45  
41.13  
40.31  
39.10  
37.82

19.28



Solvent

CHLOR

C5

Methine

2x C=O

Ph-C

17 <sup>1</sup>H NMR

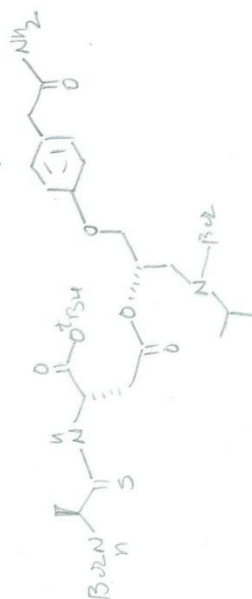


Current Data Parameters  
 NAME Nov30-2011  
 EXPNO 30  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20111130  
 Time\_ 19.08  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.094190 Hz  
 AQ 5.3084660 sec  
 RG 256  
 DM 81.000 usec  
 DE 6.00 usec  
 TE 293.2 K  
 DI 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.30 usec  
 PL1 -6.00 dB  
 SF01 300.1318534 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 300.1300221 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

$[\alpha]_D = 34.97$   
 589 nm  
 25.1°C  
 CHCl<sub>3</sub>

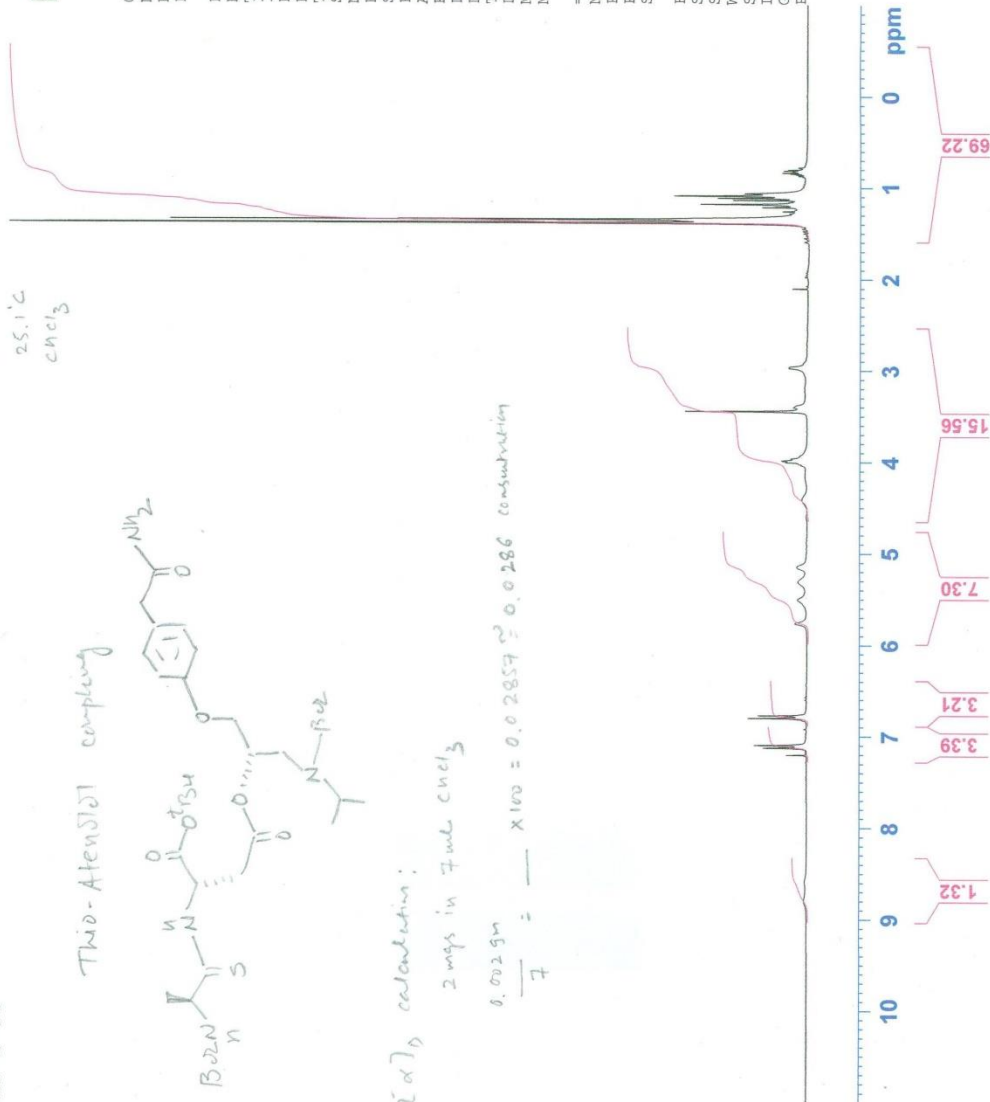
Thio-Atenolol coupling



$[\alpha]_D$  calculation:

2 mgs in 7ml CHCl<sub>3</sub>

$$\frac{0.025 \text{ g}}{7} = \text{---} \times 100 = 0.02857 \times 0.0286 \text{ concentration}$$



RP-2-84





Current Data Parameters  
 NAME Nov30-2011  
 EXPNO 33  
 PROCNO 1

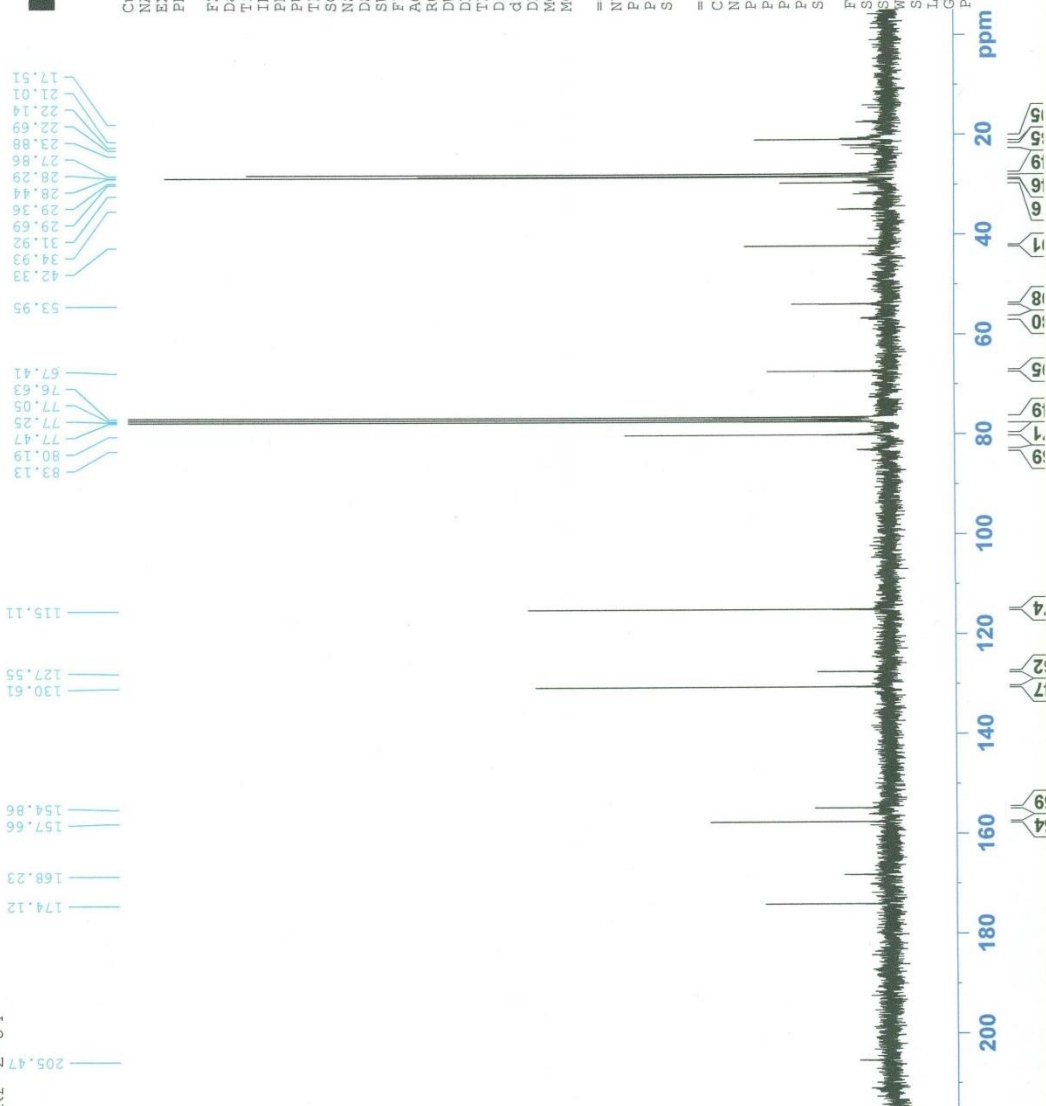
F2 - Acquisition Parameters  
 Date\_ 20111130  
 Time 21.14  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 10321.3  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 293.2 K  
 D1 2.0000000 sec  
 d11 0.0300000 sec  
 DELTA 1.8999998 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.40 usec  
 PL1 -6.00 dB  
 SF01 75.4752953 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 6.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SF02 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 EM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

RP-2-84



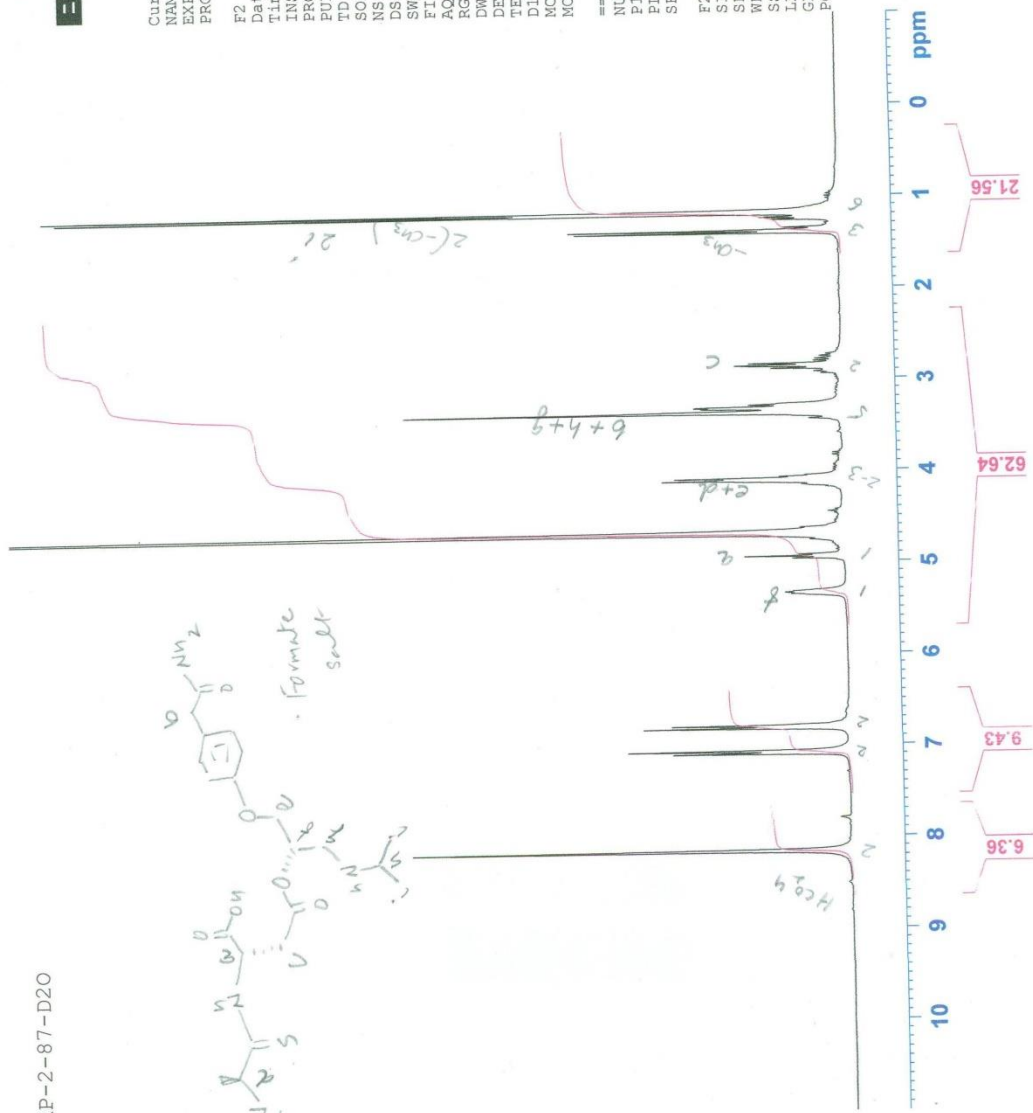
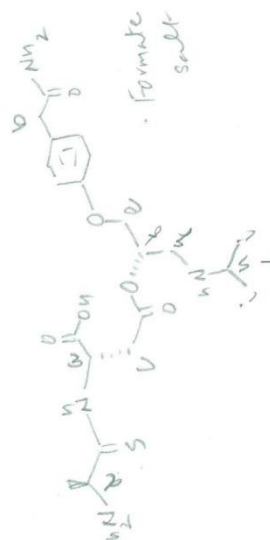
8 1H NMR



Current Data Parameters  
 NAME Dec02-2011  
 EXPNO 10  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20111202  
 Time 13.21  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg30  
 TD 32768  
 SOLVENT D2O  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FWH 0.188380 Hz  
 FIDRES 2.6542580 sec  
 AQ 256  
 RG 81.000 usec  
 DW 6.00 usec  
 DE 292.2 K  
 TE 1.00000000 sec  
 DI 0.00000000 sec  
 MCREST 0.01500000 sec  
 MCWRK

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.30 usec  
 PL1 -6.00 dB  
 SFO1 300.1318534 MHz  
 F2 - Processing parameters  
 SI 16384  
 SF 300.1300000 MHz  
 EM  
 WDW 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

RP-2-87-D2O









Current Data Parameters  
 NAME Mar15-2012  
 EXFNO 32  
 PROCNO 1

F2 - Acquisition Parameters

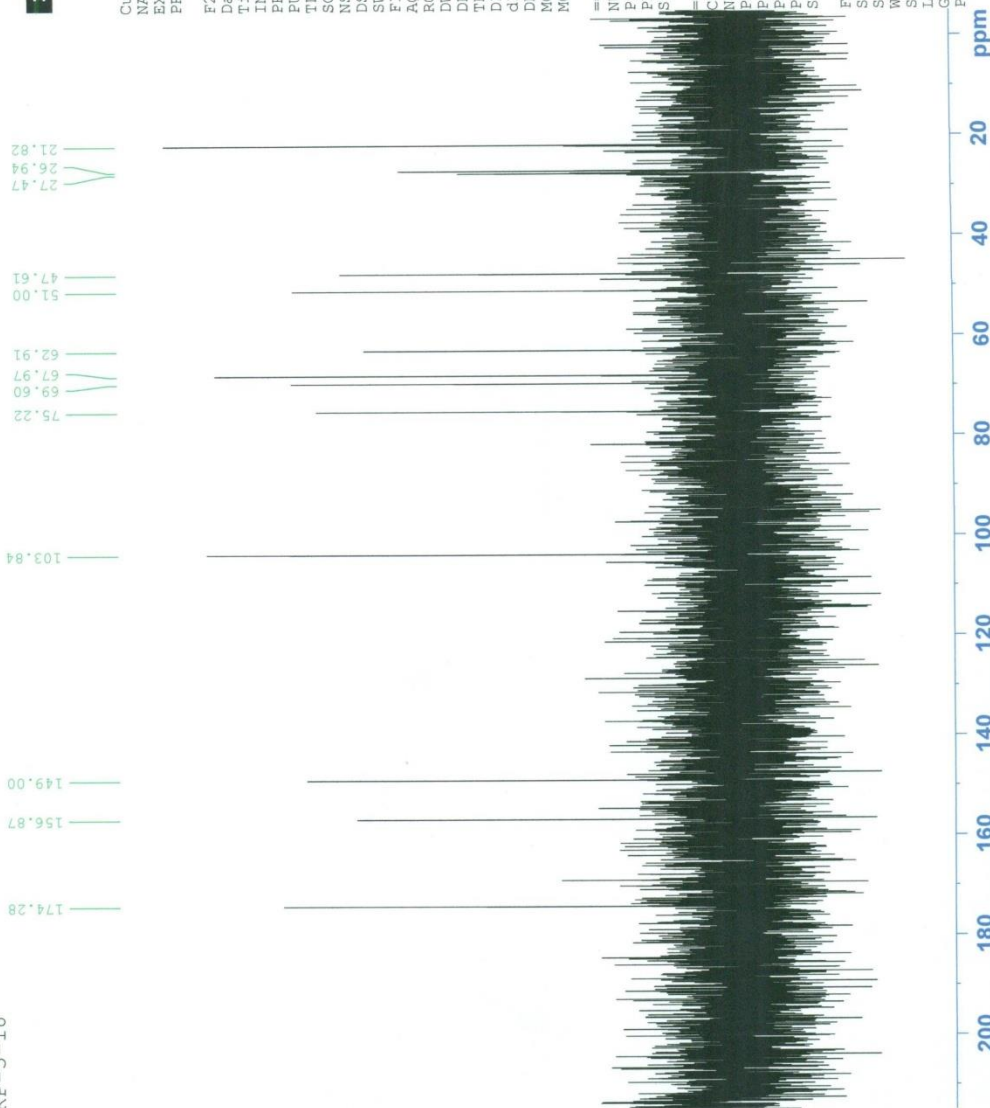
Date\_ 20120317  
 Time 6.23  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT D2O  
 NS 1024  
 DS 4  
 SWH 17985.611 Hz  
 FIDRES 0.274439 Hz  
 AQ 1.8219508 sec  
 RG 13004  
 DW 27.800 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 2.0000000 sec  
 g11 0.0300000 sec  
 DELTA 1.8999998 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 6.40 usec  
 PL1 -6.00 dB  
 SF01 75.4752953 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 -6.00 dB  
 PL12 17.00 dB  
 PL13 20.00 dB  
 SFO2 300.1312005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 75.4677490 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

RP-3-18



18 13C NMR



Thio-Releaza Final

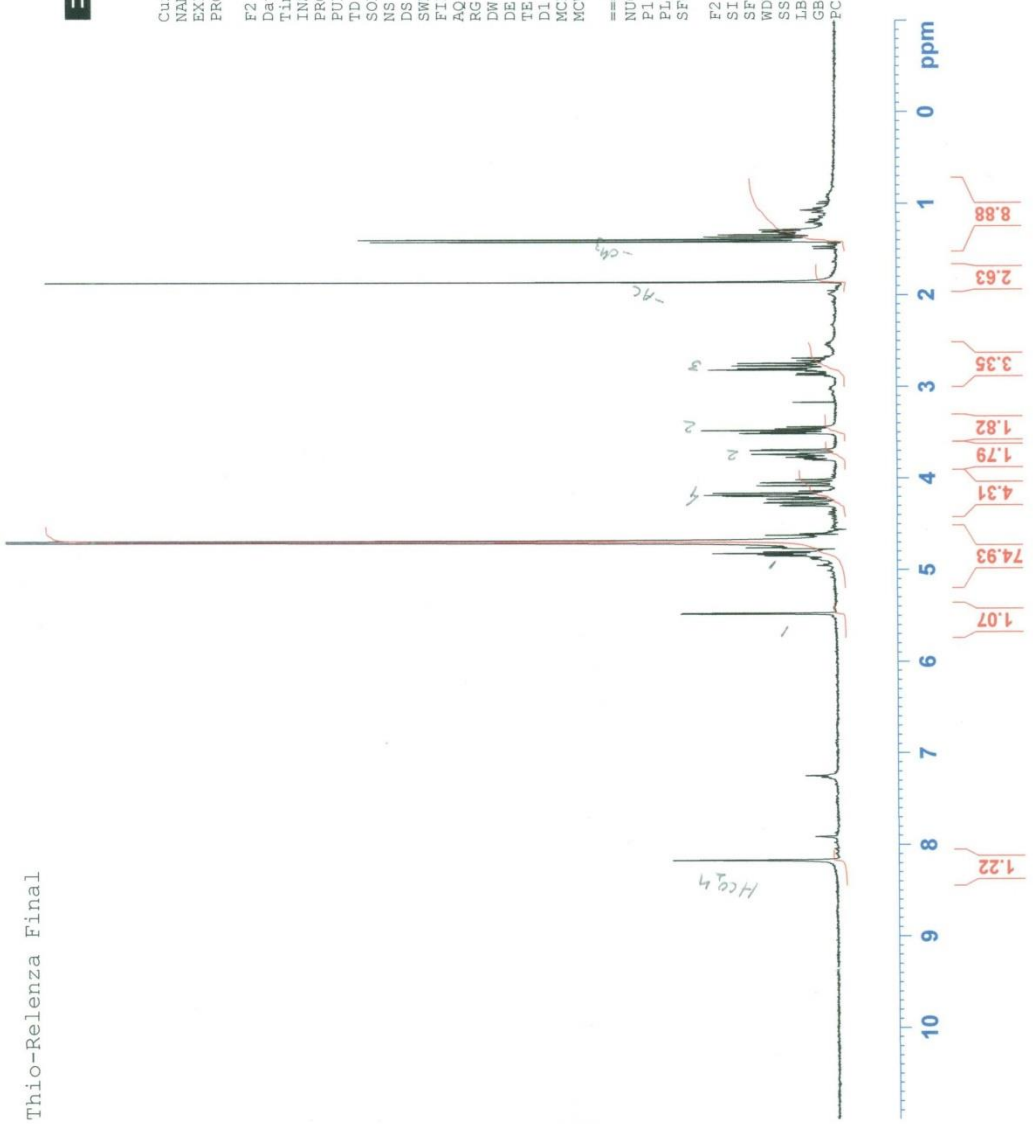
fP → apk → abas → Xwing plot

Current Data Parameters  
 NAME April-2012  
 EXNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120411  
 Time 13.53  
 INSTRUM dpx300  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg30  
 TD 32768  
 SOLVENT D2O  
 NS 16  
 DS 2  
 SWH 6172.839 Hz  
 FIDRES 0.188380 Hz  
 AQ 2.6542580 sec  
 RG 456.1  
 DW 81.000 usec  
 DE 6.00 usec  
 TE 291.2 K  
 D1 1.00000000 sec  
 MCREST 0.00000000 sec  
 MCWREK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 12.30 usec  
 PL1 -6.00 dB  
 SF01 300.1318534 MHz

F2 - Processing parameters  
 SI 16384  
 SF 300.1300000 MHz  
 WDW nc  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 FC 1.00

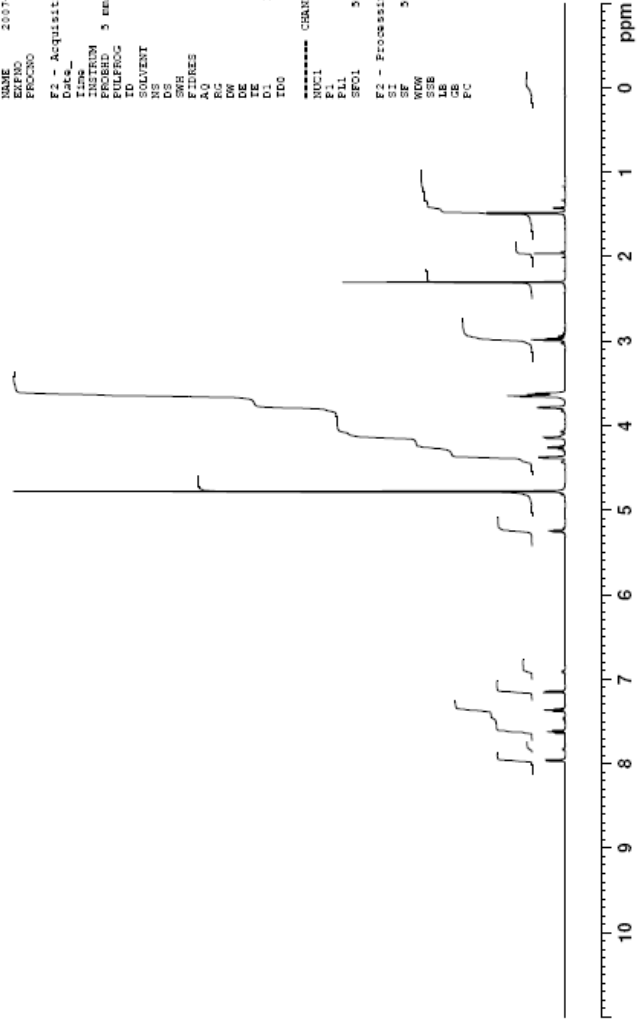




# 4 1H NMR

Current Data Parameters  
NAME 2007-09-30-PS-40  
EXPNO 1.0  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20070930  
Time 16.37  
INSTRUM spect  
PULPROG zgpg30  
FIDRES 5 Hz TXI 2336  
ID 6536  
SOLVENT D2O  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 320  
DE 48.20 usec  
TE 300.2 K  
IE 300.0 K  
D1 1.0000000 sec  
IDC 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
IR 1H  
F1 4.0 usec  
SFO1 500.136083 MHz  
F2 - Processing Parameters  
SI 32768  
SF 500.136083 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





# 5 1H NMR

