

## Supplementary Information

### Synthesis of three <sup>18</sup>F-labelled cyclooxygenase-2 (COX-2) inhibitors based on a pyrimidine scaffold

Ole Tietz,<sup>a</sup> Sai Kiran Sharma,<sup>a,b</sup> Jatinder Kaur,<sup>a</sup> Jenilee Way,<sup>a</sup> Alison Marshall,<sup>a</sup> Melinda Wuest,<sup>a</sup> and Frank Wuest<sup>\*a,b</sup>

<sup>a</sup> *Department of Oncology, University of Alberta, 11560 University Ave, Edmonton AB T6G 1Z2, Canada.*

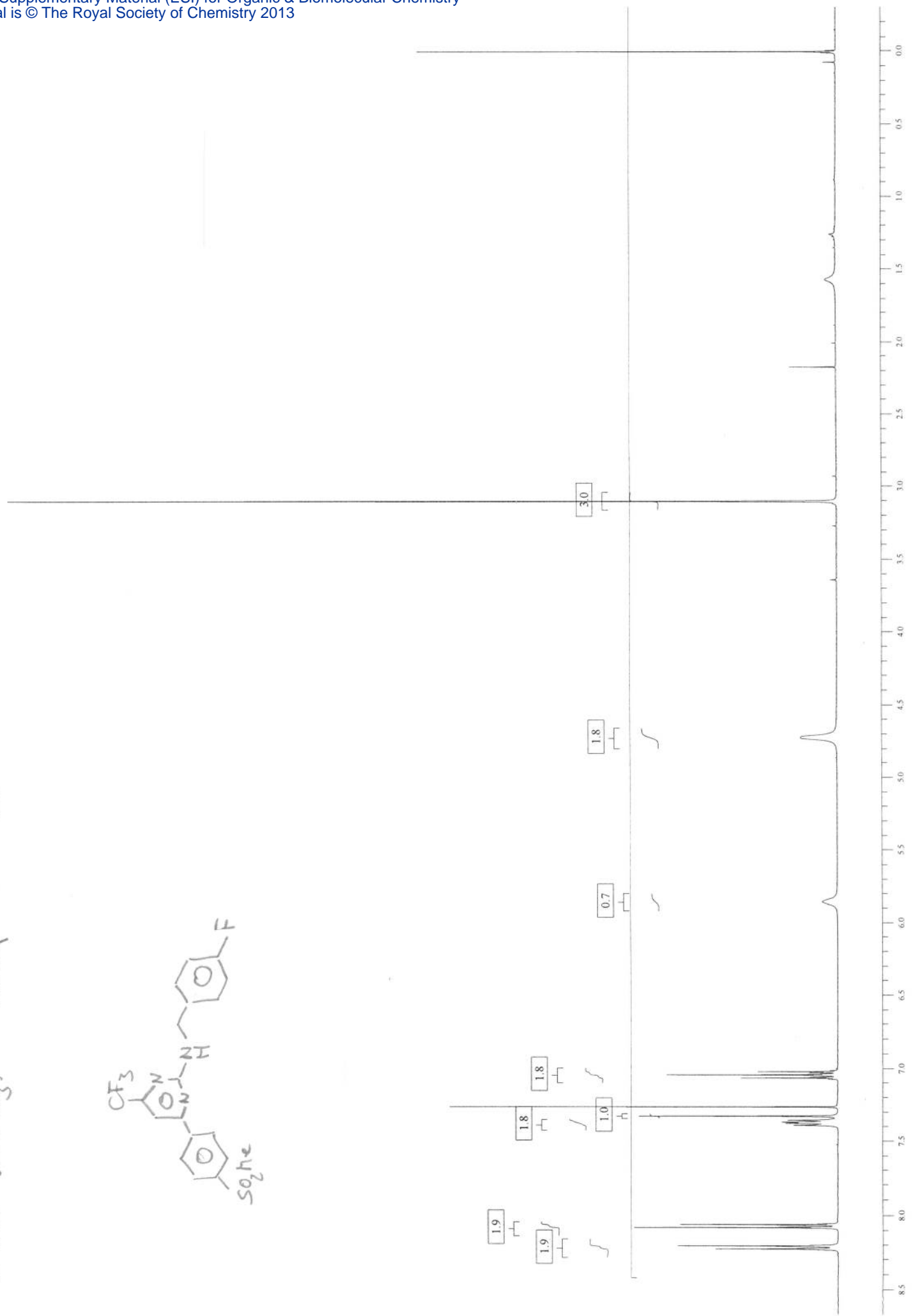
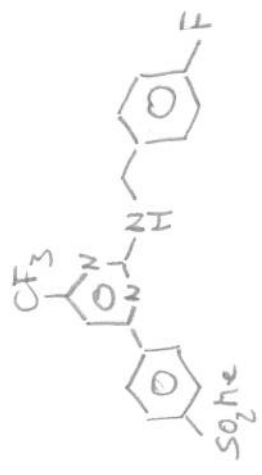
<sup>b</sup> *Faculty of Pharmacy and Pharmaceutical Sciences, University of Alberta, Edmonton, Canada.*

*Fax: +1 780 432 8483; Tel: +1 780 989 8150; E-mail: wuest@ualberta.ca*

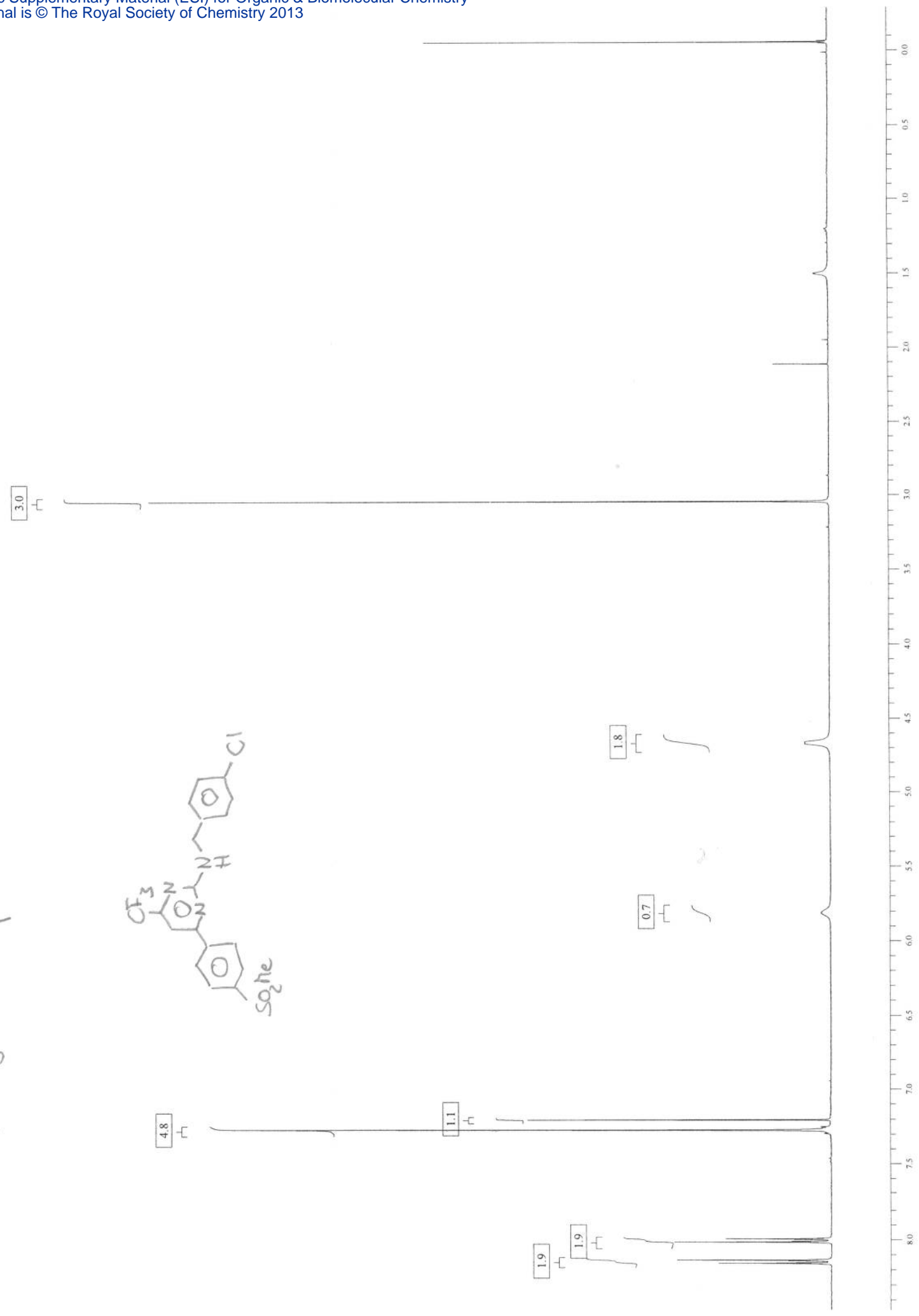
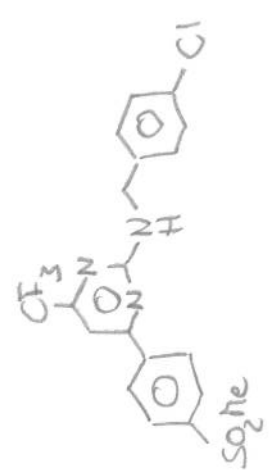
#### Contents

<sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra of all compounds

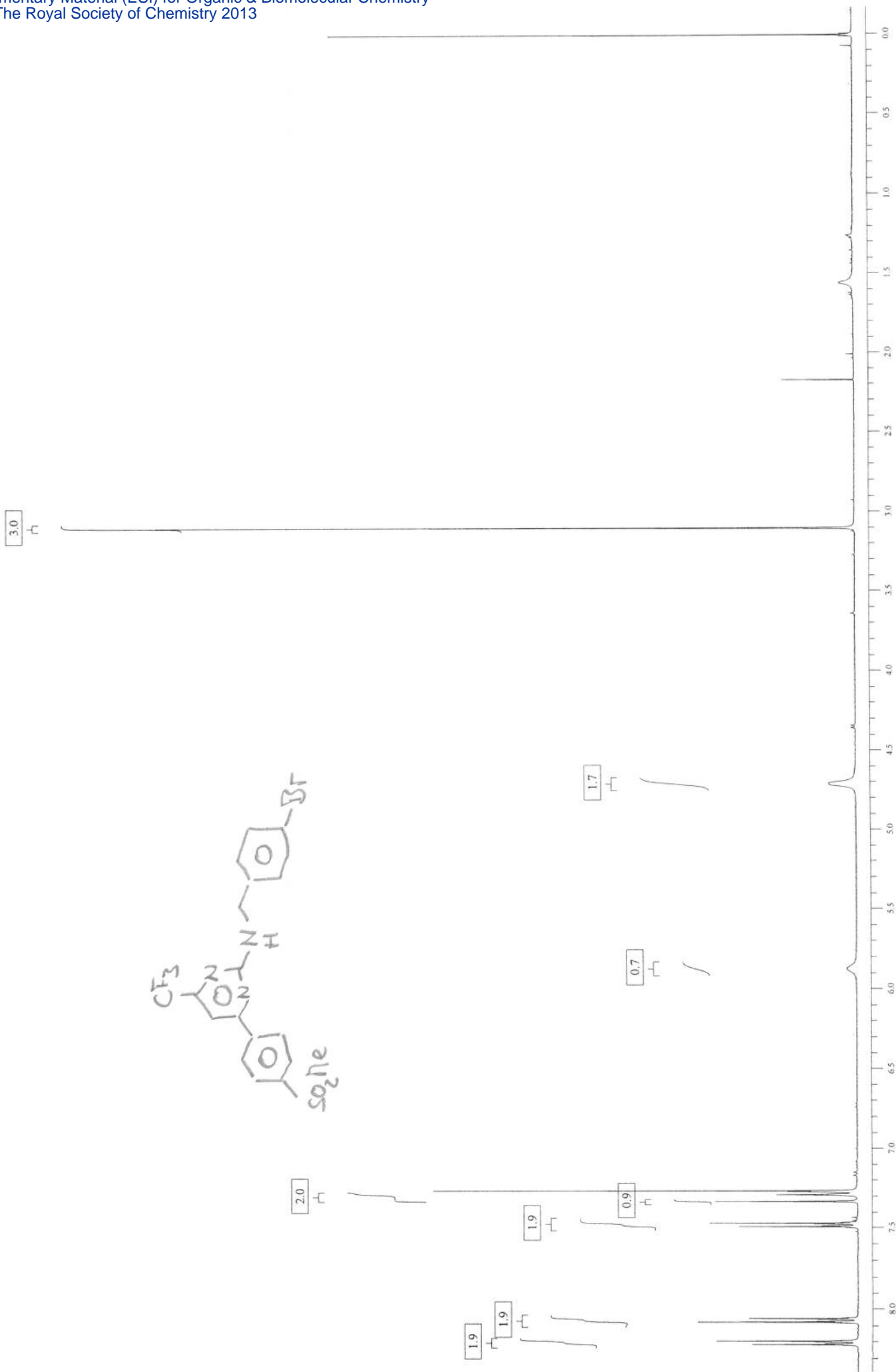
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound: 1a



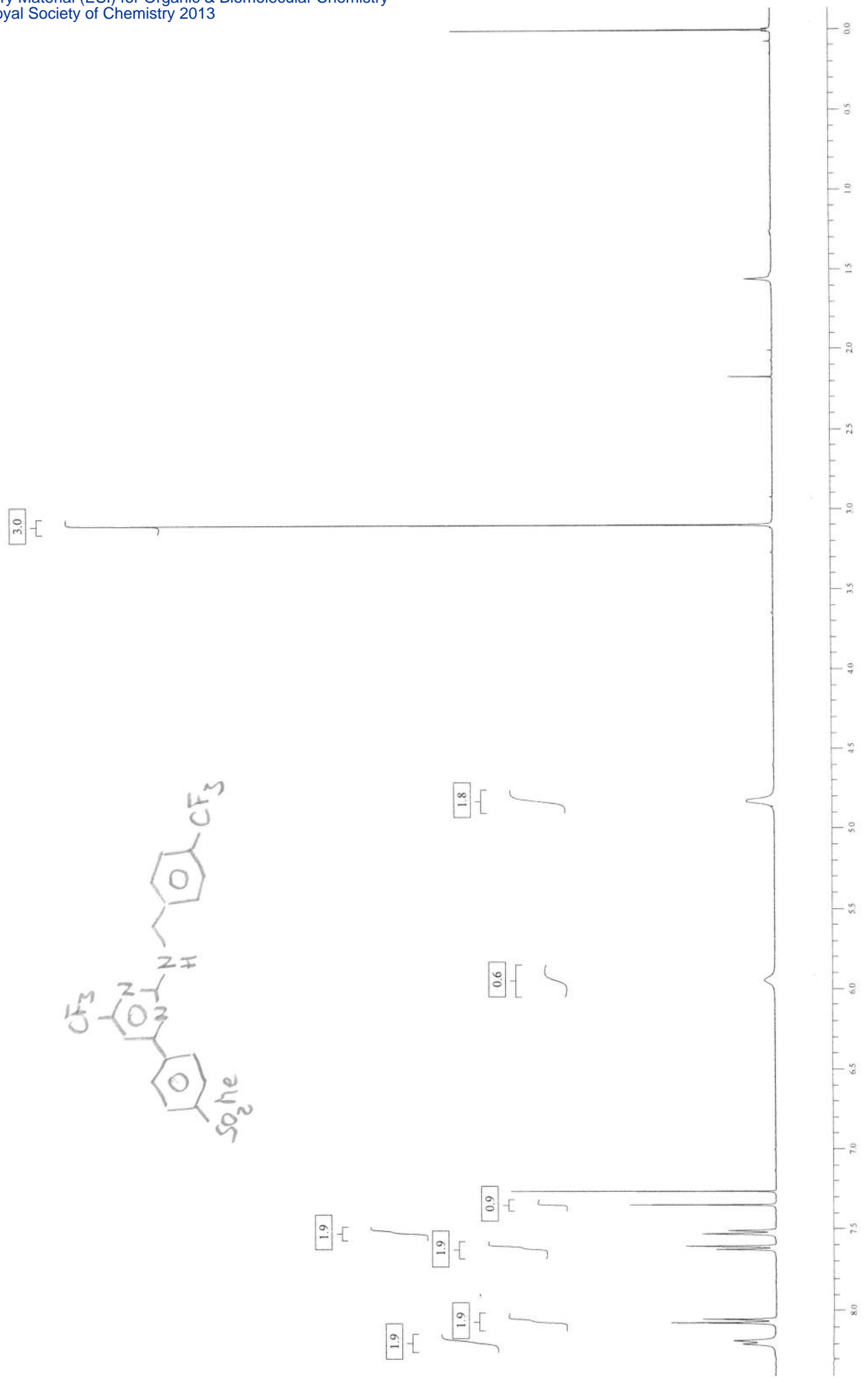
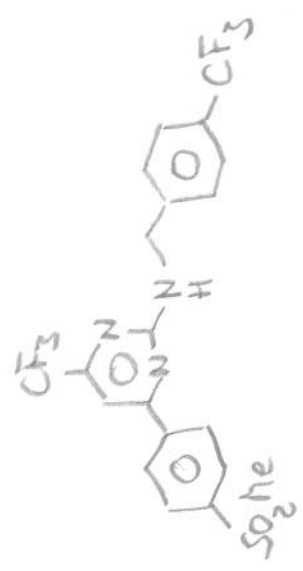
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 1b



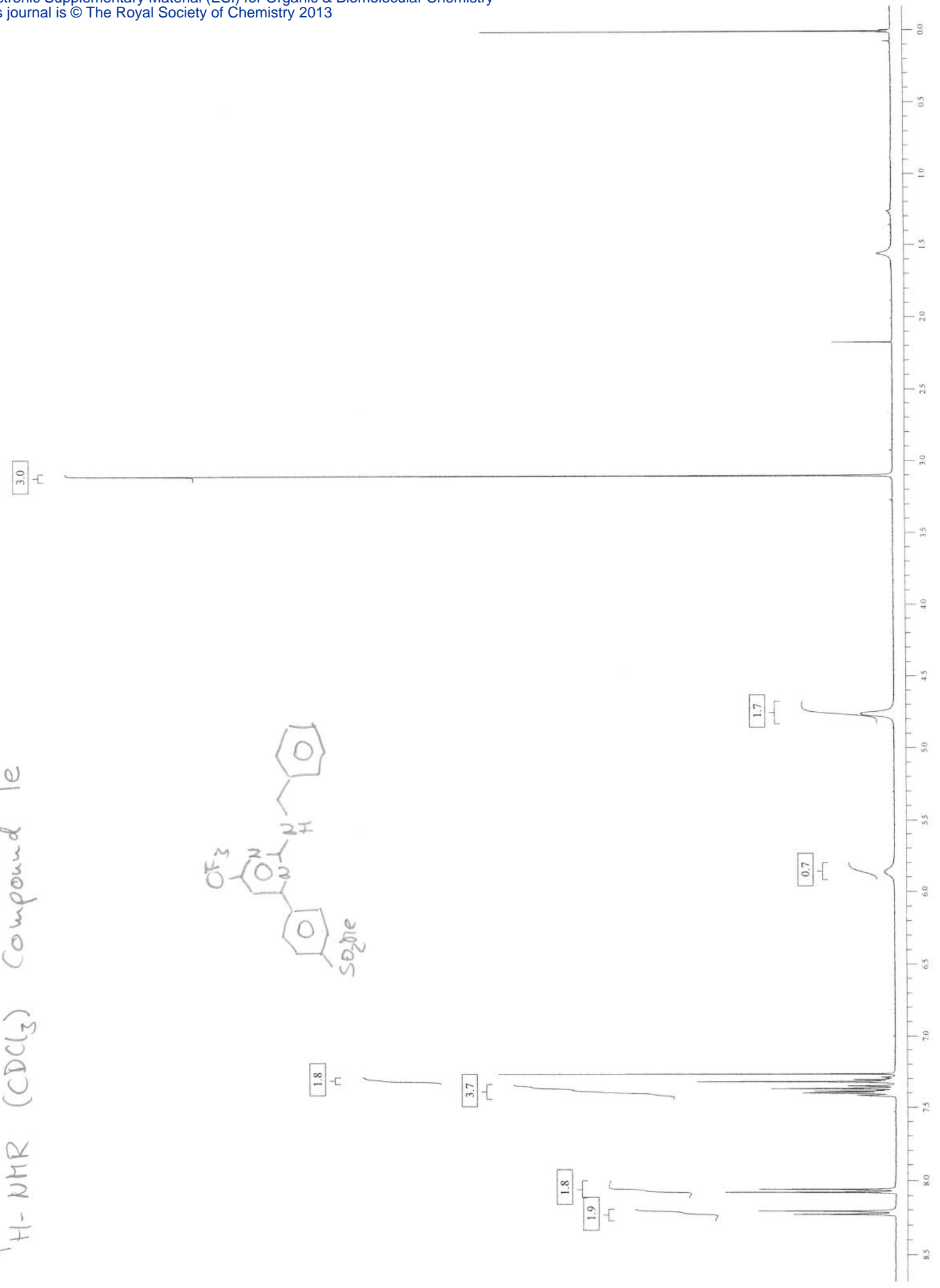
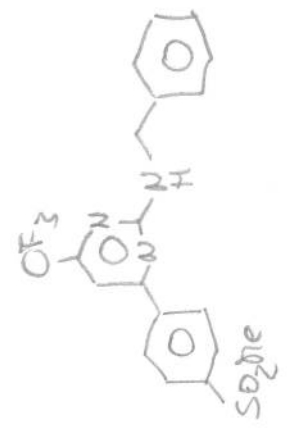
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 1c



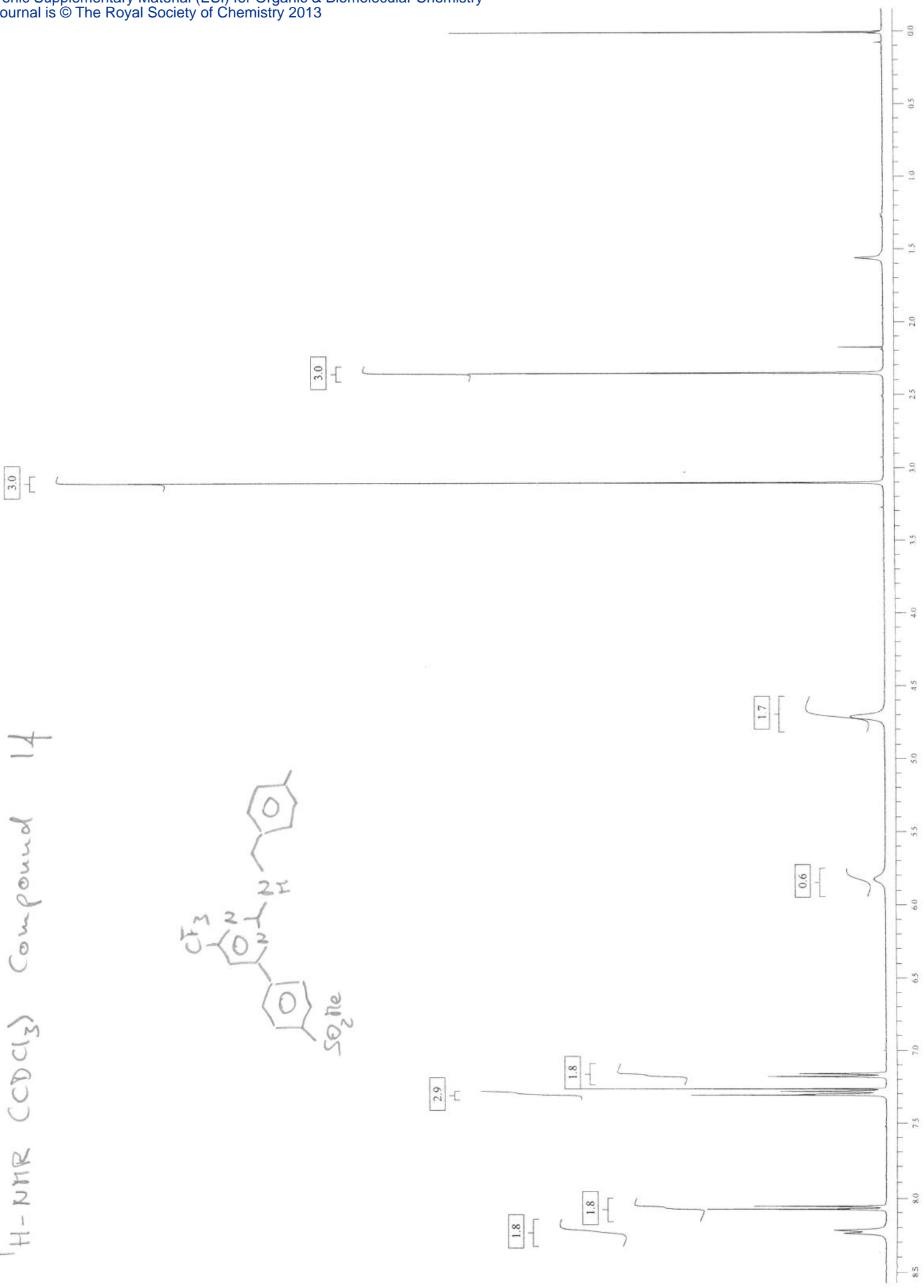
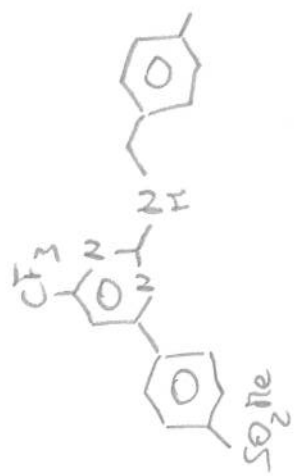
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 1d



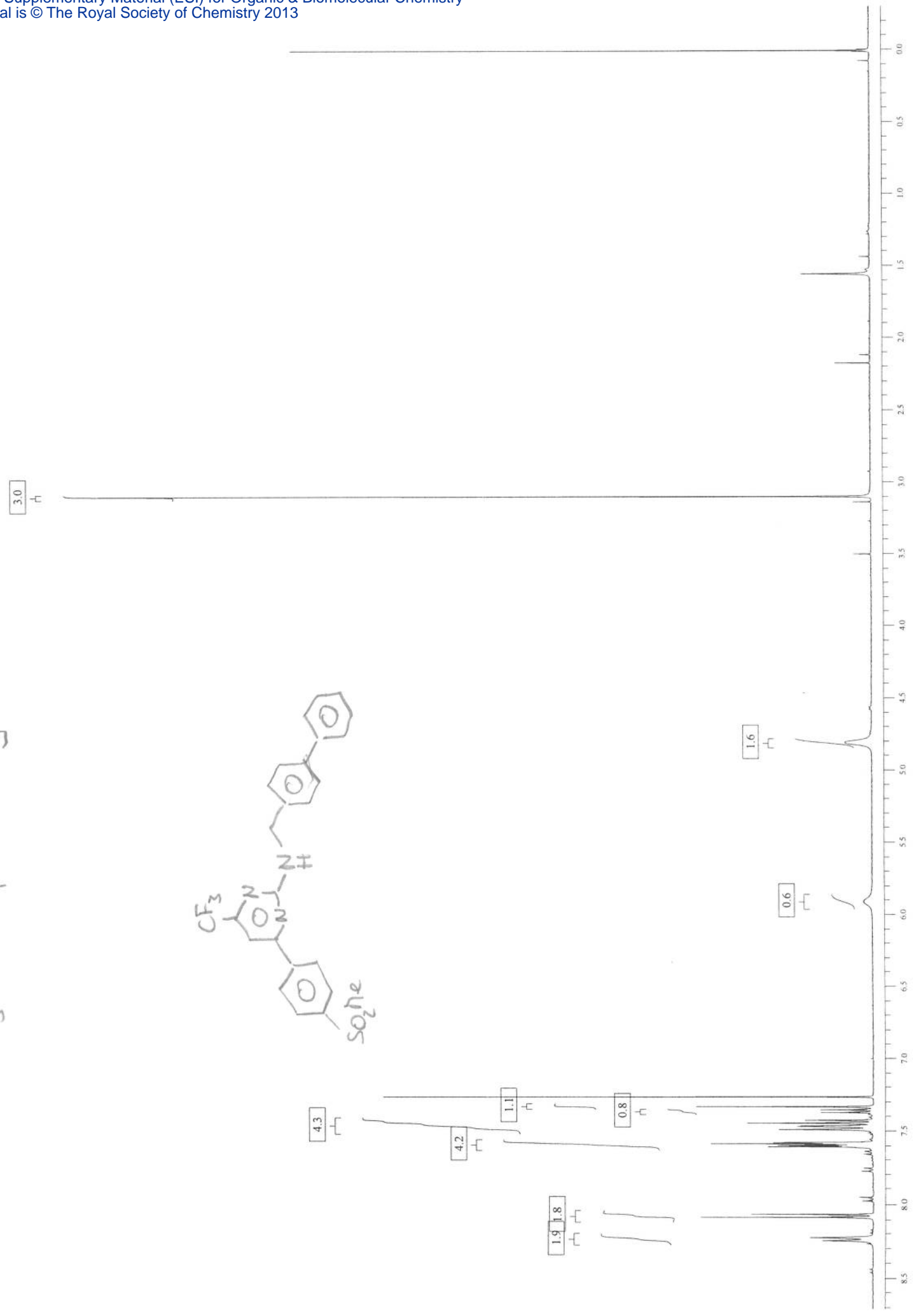
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 1e



<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 14

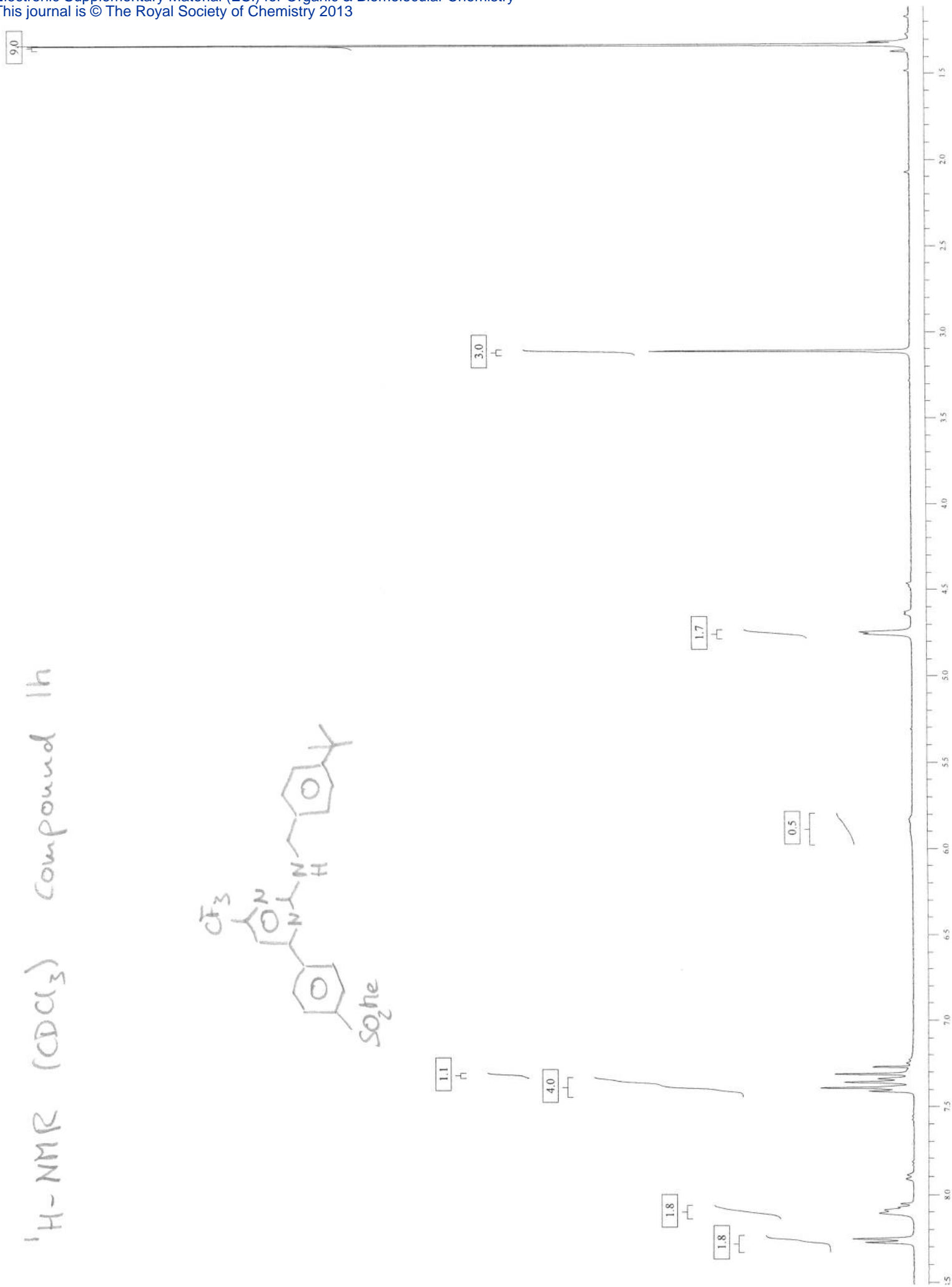
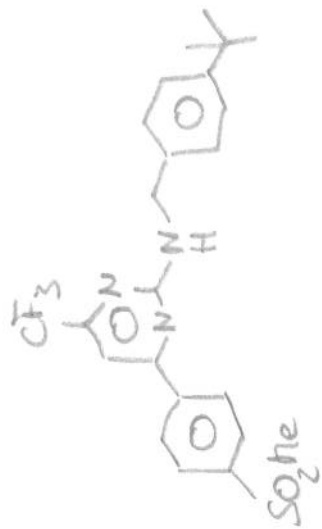


<sup>1</sup>H-NMR (CDCl<sub>3</sub>) Compound 1g

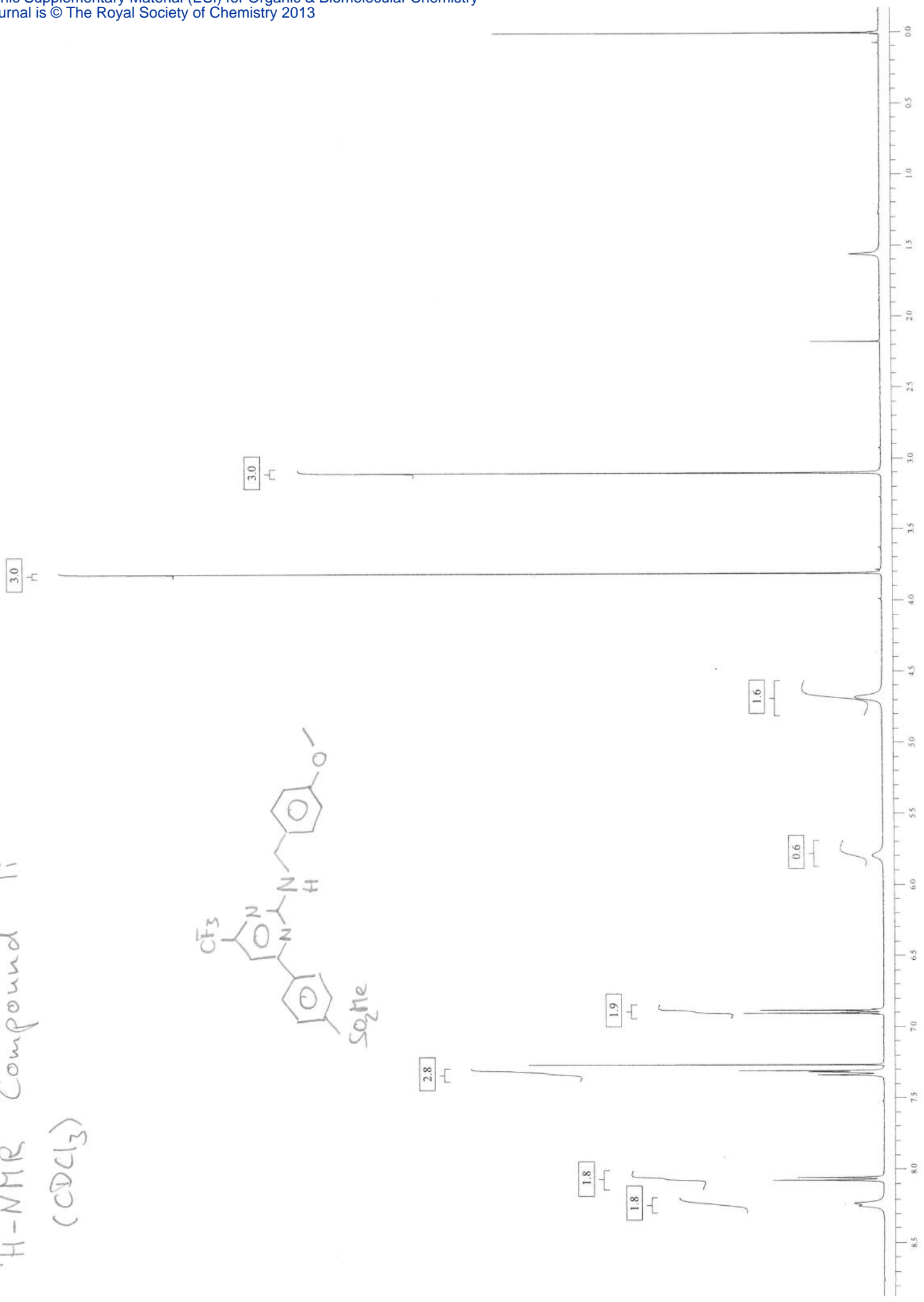
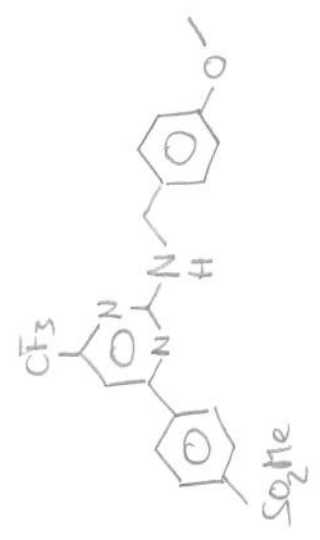




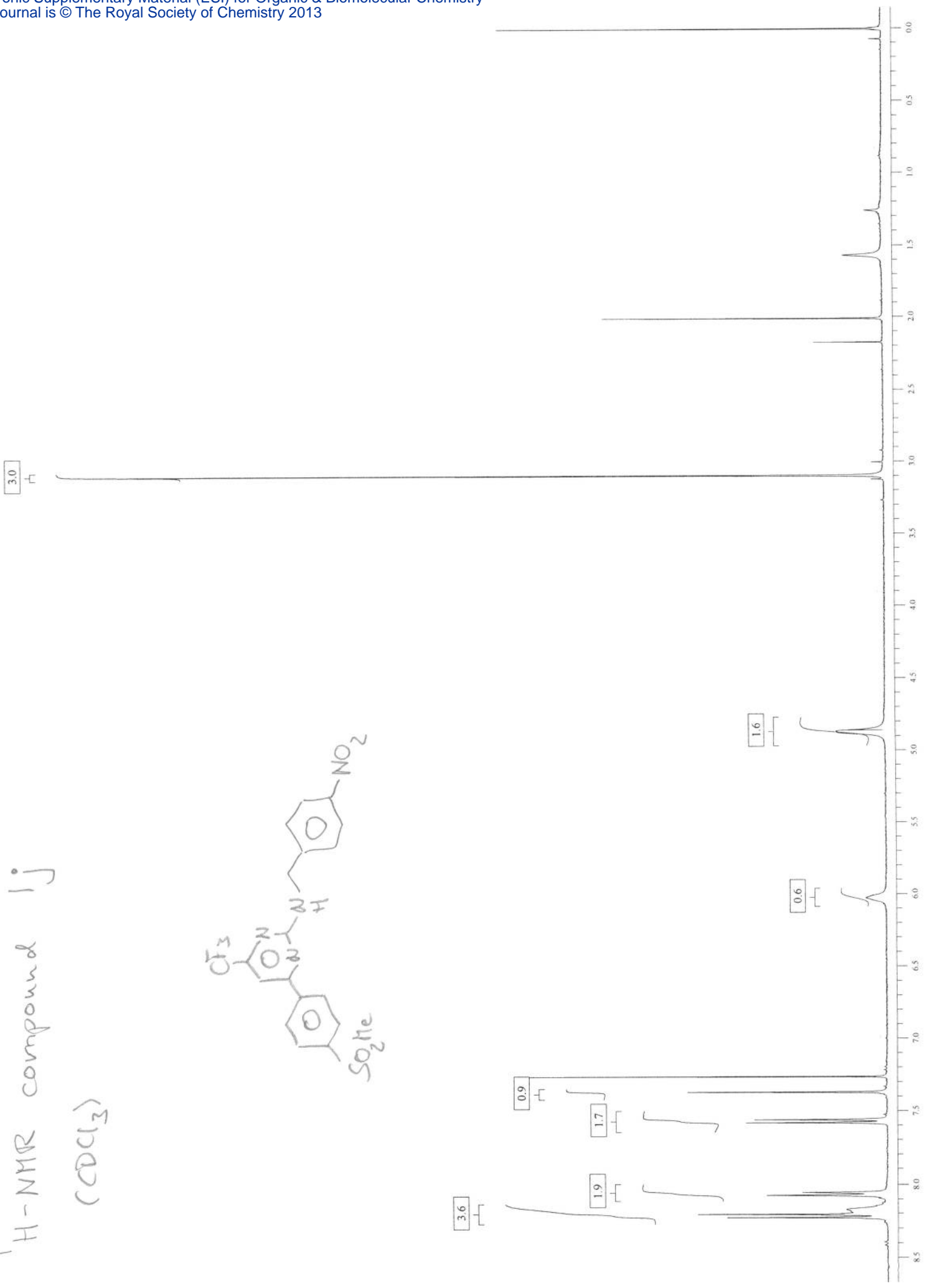
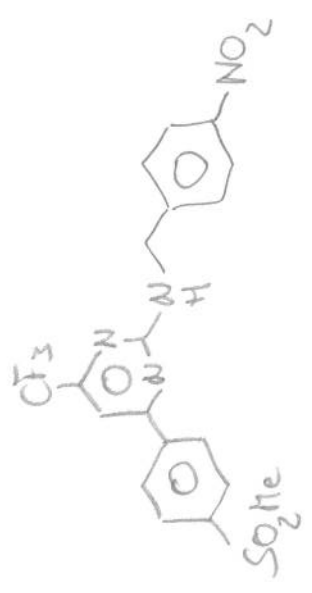
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ ) Compound 1h



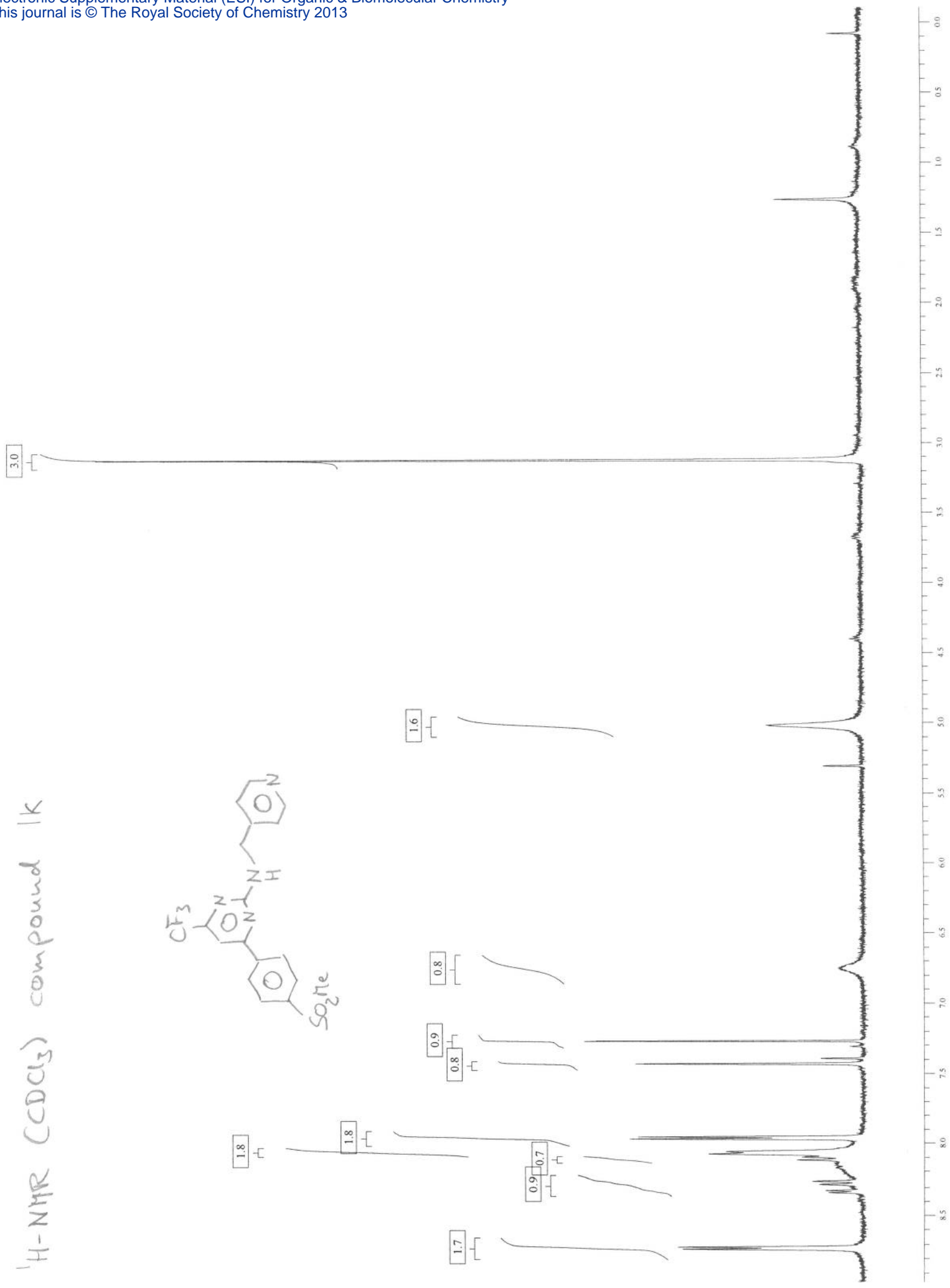
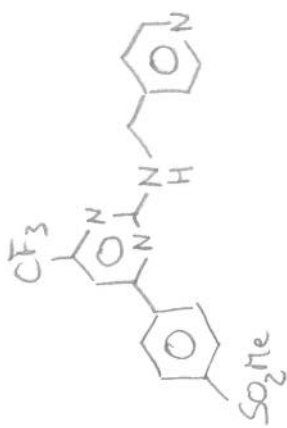
<sup>1</sup>H-NMR Compound 1i  
(CDCl<sub>3</sub>)



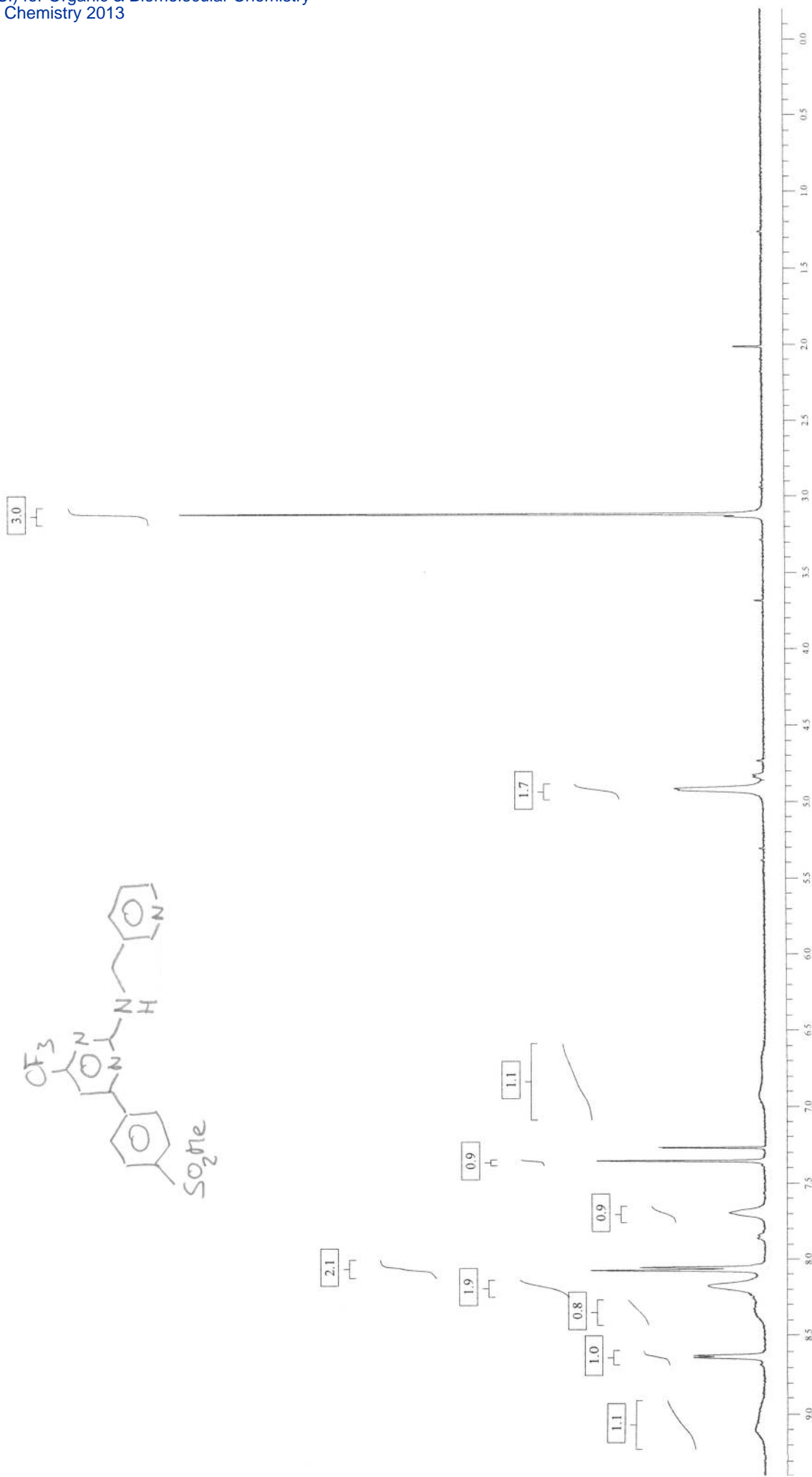
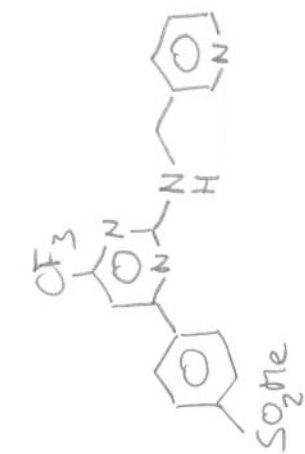
<sup>1</sup>H-NMR compound 1j  
(CDCl<sub>3</sub>)



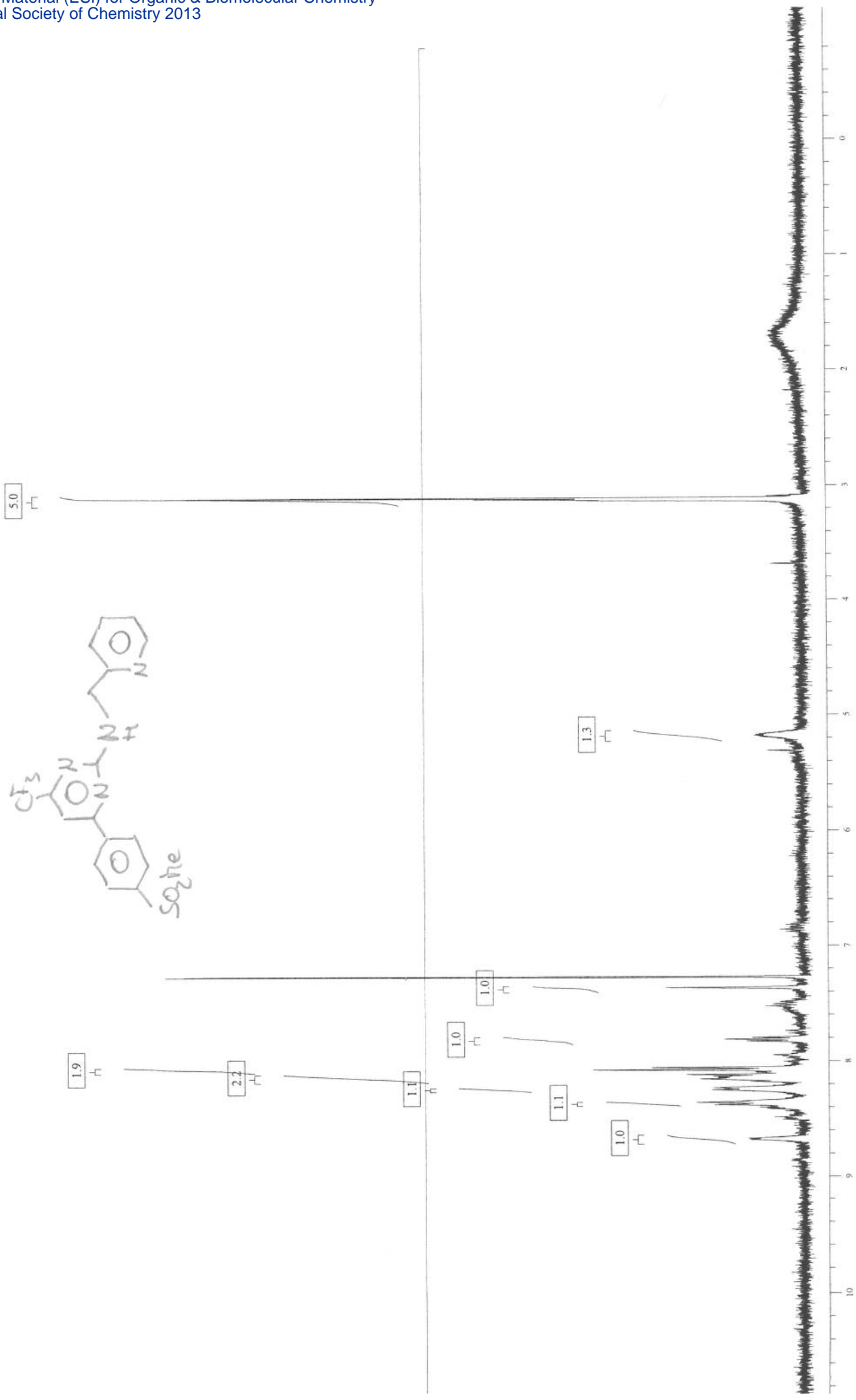
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) compound 1k



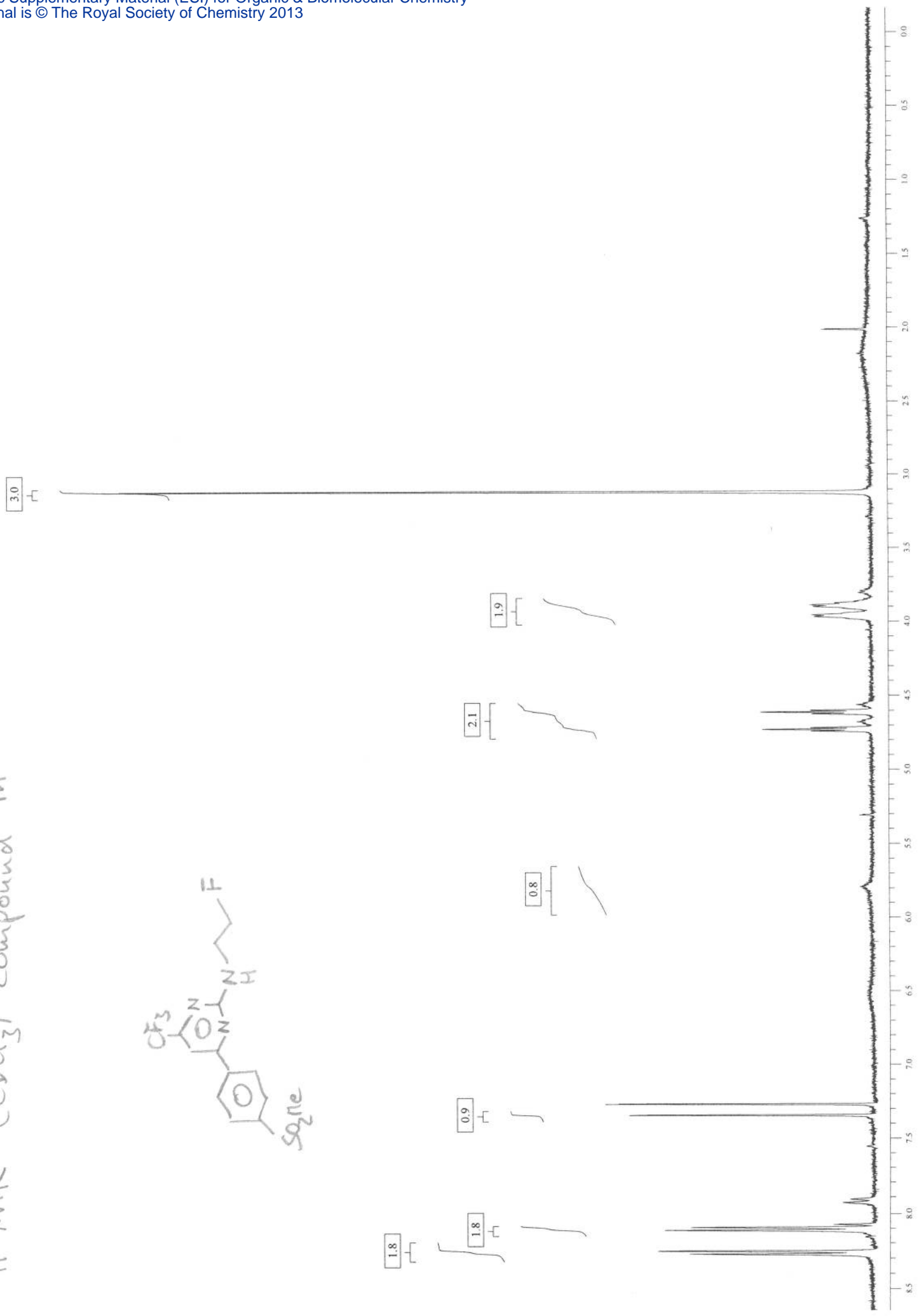
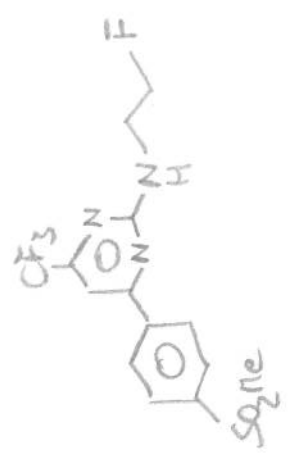
<sup>1</sup>H-NMR (CDCl<sub>3</sub>) compound 11



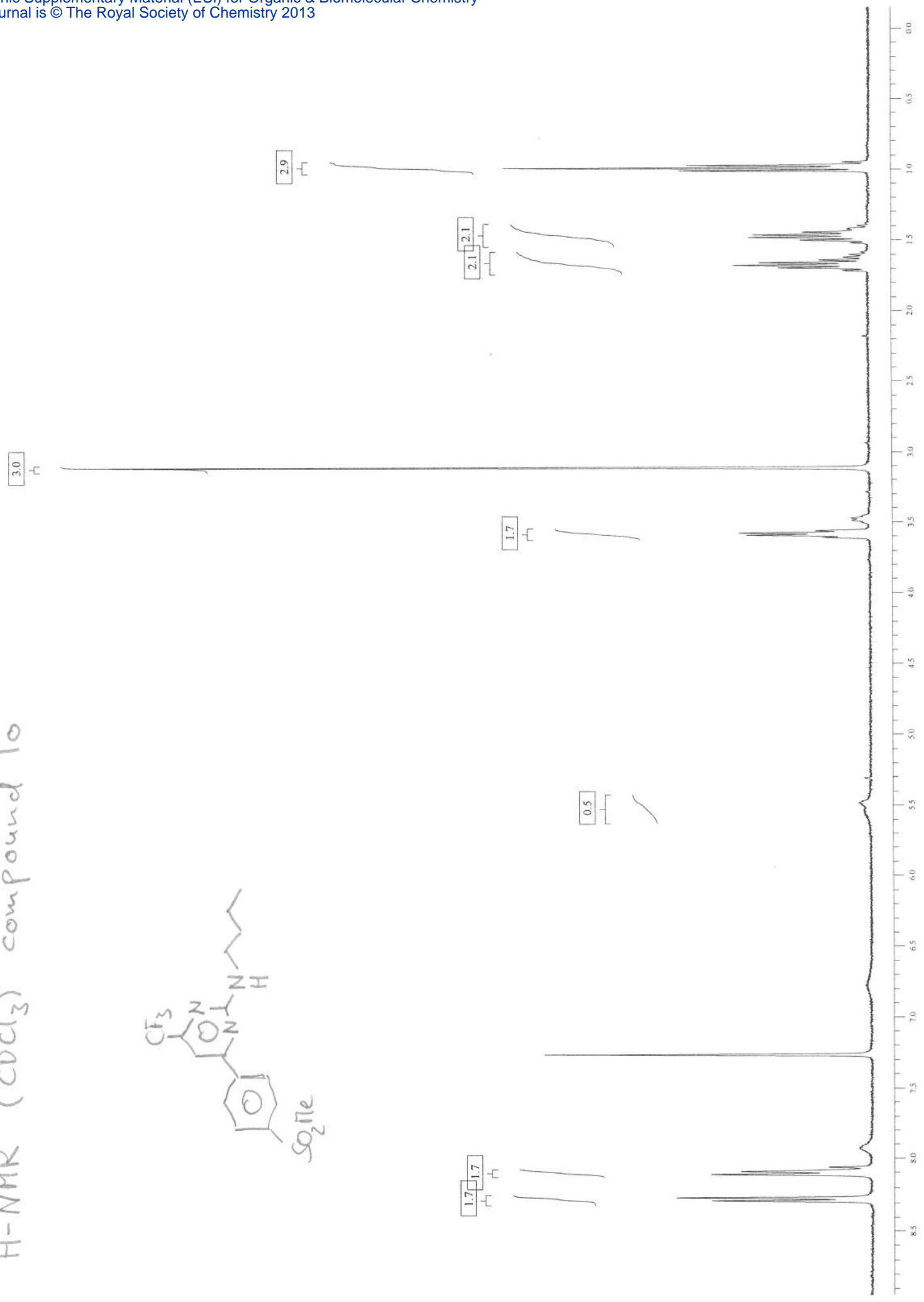
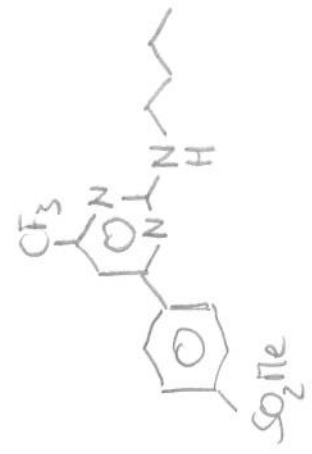
$^1\text{H-NMR}$  ( $\text{CDCl}_3$ ) compound 1m



<sup>1</sup>H-NMR (CDCl<sub>3</sub>) compound 1n



<sup>1</sup>H-NMR (CDCl<sub>3</sub>) compound 10







Current Data Parameters  
NAME May01\_2013  
EXPNO 20  
PROCNO 1

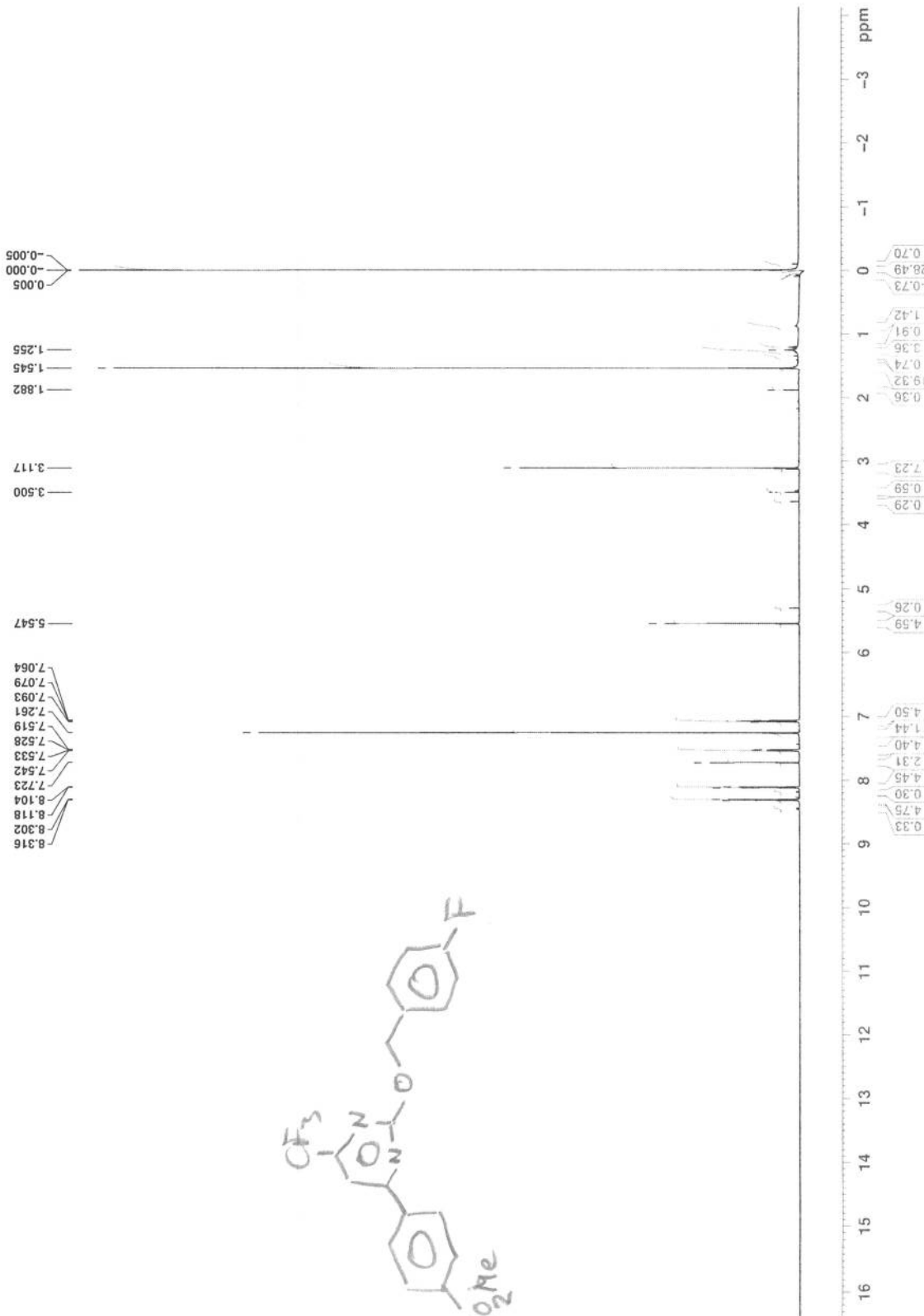
F2 - Acquisition Parameters  
Date\_ 20130501  
Time 9.58  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 64  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 180.12  
DW 40.533 usec  
DE 15.13 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 13.40 usec  
PLW1 21.29999924 W

F2 - Processing parameters  
SI 65536  
SF 600.2700180 MHz  
WDW EM  
SSB 0 0.20 Hz  
LB 0  
GB 0  
PC 1.00

<sup>1</sup>H-NMR (CDCl<sub>3</sub>) compound 3a

Ole: proton on OTIPY-I1329  
CPP\_Proton.A CDCl3 (C:\Bruker\TopSpin3.1) vishwa 14





Current Data Parameters  
NAME May01\_2013  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130501  
Time 9.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 64  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 180.12  
DW 40.533 usec  
DE 15.13 usec  
TE 296.0 K  
D1 1.0000000 sec  
TD0 1

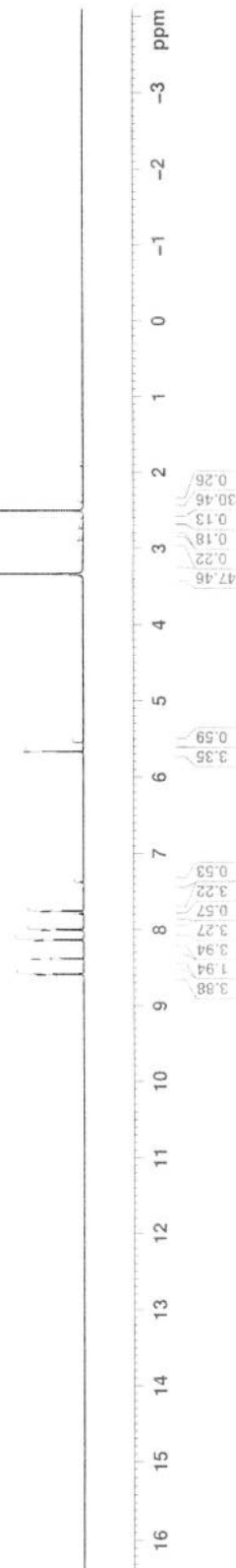
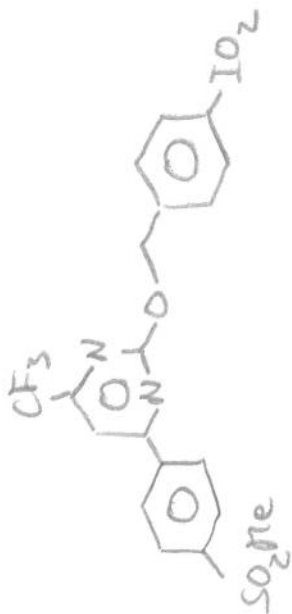
===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 13.40 usec  
PLW1 21.25999924 W

F2 - Processing parameters  
SI 65536  
SF 600.2700000 MHz  
WDW EM  
SSB 0 0.20 Hz  
LB 0  
GB 0  
PC 1.00

<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO) compound II

Ole: proton on OTIPY-I1329  
CPP\_Proton.A DMSO {C:\Bruker\TopSpin3.1} vishwa 13

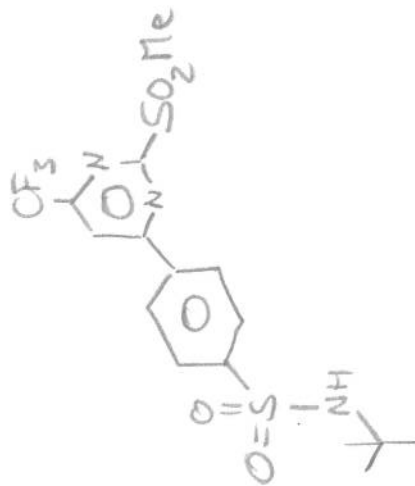
8.598  
8.584  
8.388  
8.145  
8.131  
8.011  
7.997  
7.766  
7.752  
5.669  
3.337  
3.332  
2.517  
2.514  
2.511





Ole Tietz: Proton on OT-SA-I-02X

<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO)  
compound 8

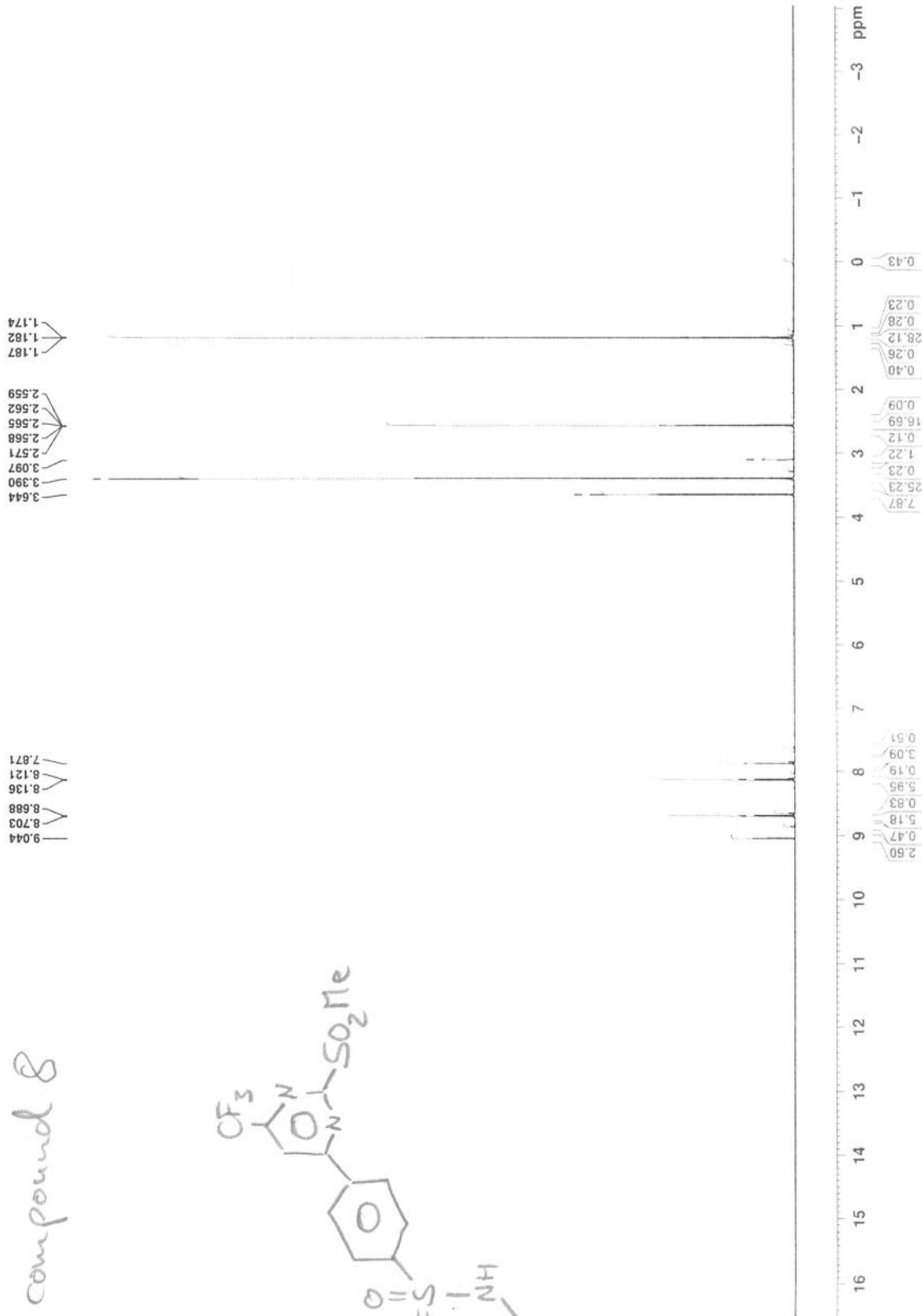


Current Data Parameters  
NAME Aug22-2012  
EXPNO 100  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120822  
Time\_ 17.39  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W

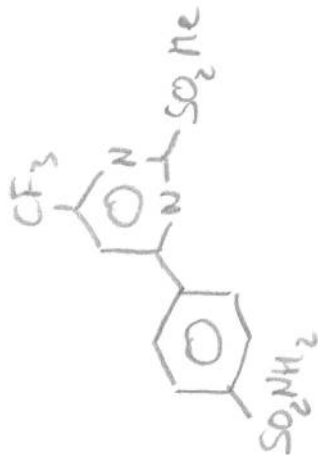
F2 - Processing parameters  
SI 65536  
SF 600.2698692 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00





Ole Tietz: Proton on OT-SA-I-03X

<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO):  
compound 9



3.646  
3.393  
3.101  
2.572  
2.569  
2.566  
2.563  
2.559

9.049  
8.707  
8.704  
8.696  
8.693  
8.124  
8.121  
8.113  
8.110  
7.681

Current Data Parameters  
NAME Aug22-2012  
EXPNO 110  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.44  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W  
F2 - Processing parameters  
SI 65536  
SF 600.2699693 MHz  
WDW EM  
SSB 0 0.20 Hz  
LB 0  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO) compound 2a

Ole Tietz: Proton on OT-SA-P-01

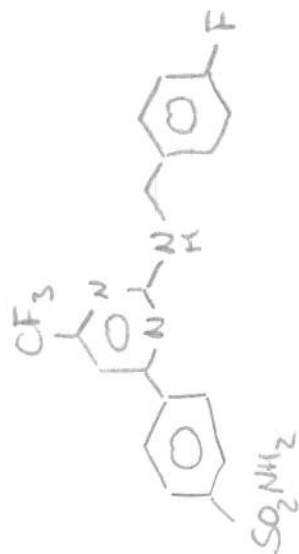


8.421  
7.718  
7.572  
7.226  
7.211  
7.196

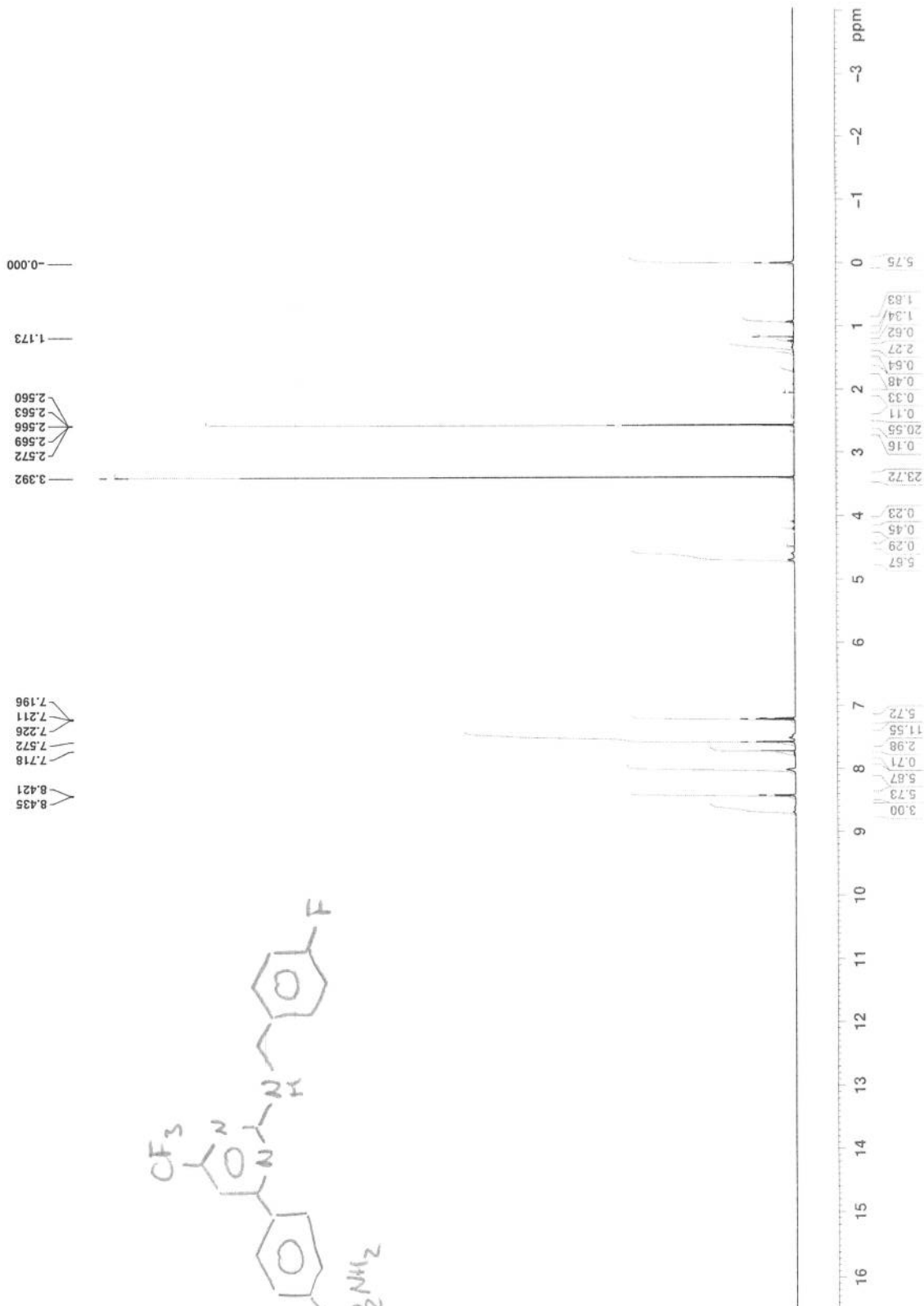
3.92  
2.572  
2.569  
2.566  
2.563  
2.560

0.000

1.173



Current Data Parameters  
NAME Aug22-2012  
EXPNO 50  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.16  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W  
F2 - Processing parameters  
SI 65536  
SF 600.2699688 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00



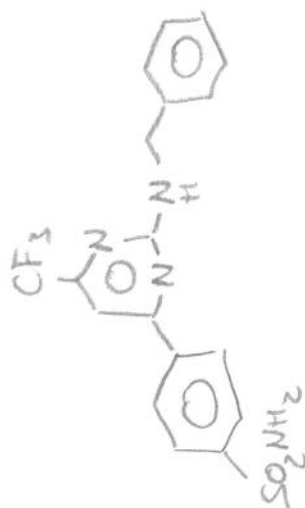
H-NMR ( $d_6$ -DMSO) compound 2b

Ole Tietz: Proton on OT-SA-P-02

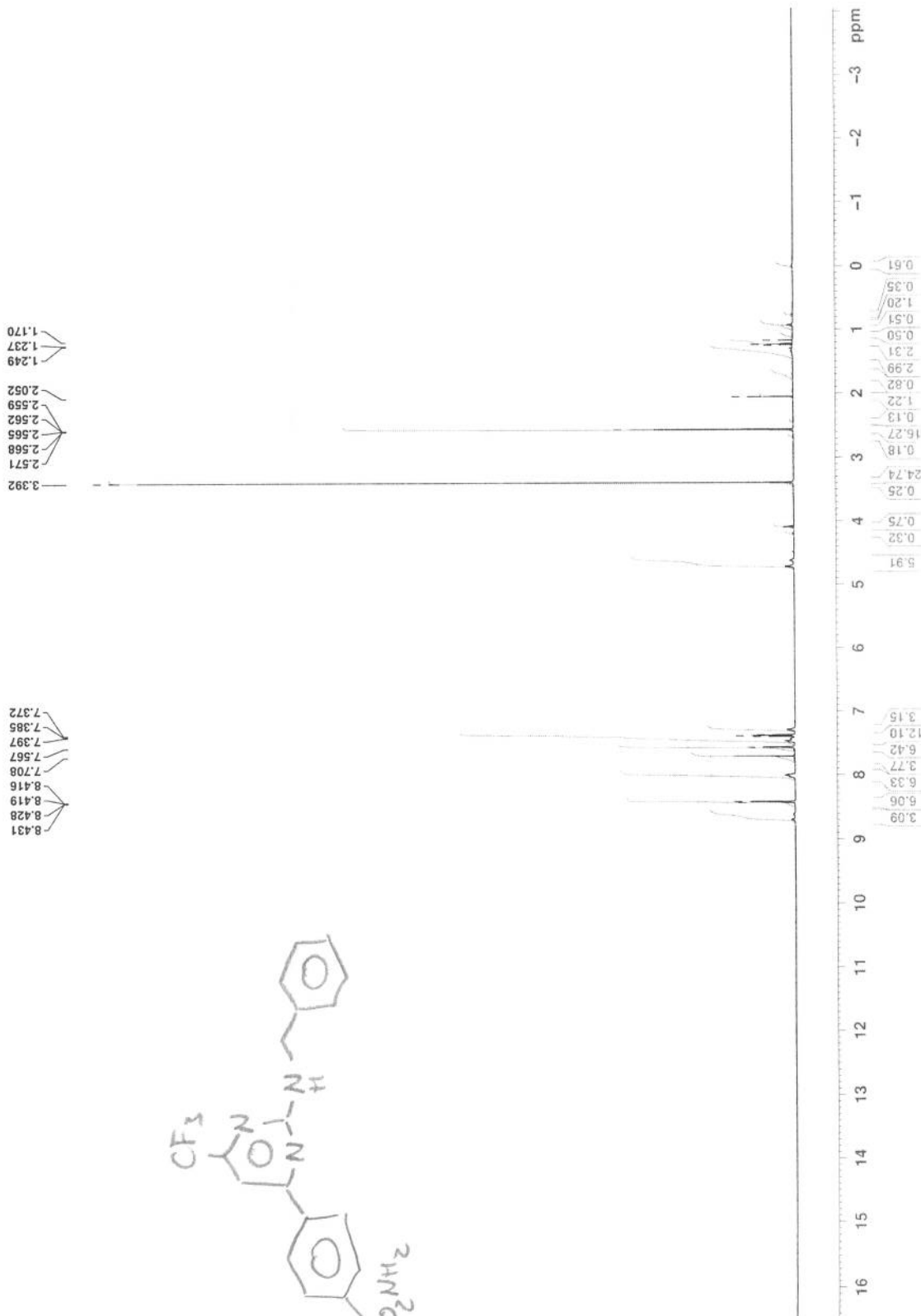


8.431  
8.428  
8.419  
8.416  
7.708  
7.567  
7.397  
7.385  
7.372

3.392  
2.571  
2.568  
2.565  
2.562  
2.559  
2.052  
1.249  
1.237  
1.170



Current Data Parameters  
NAME Aug22-2012  
EXPNO 60  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.20  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.0 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W  
F2 - Processing parameters  
SI 65536  
SF 600.2699693 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00



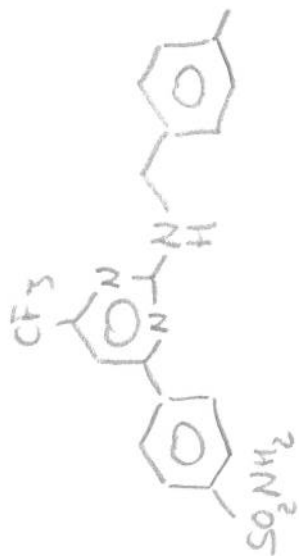
<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO) compound 2c

Ole Tietz: Proton on OT-SA-P-03

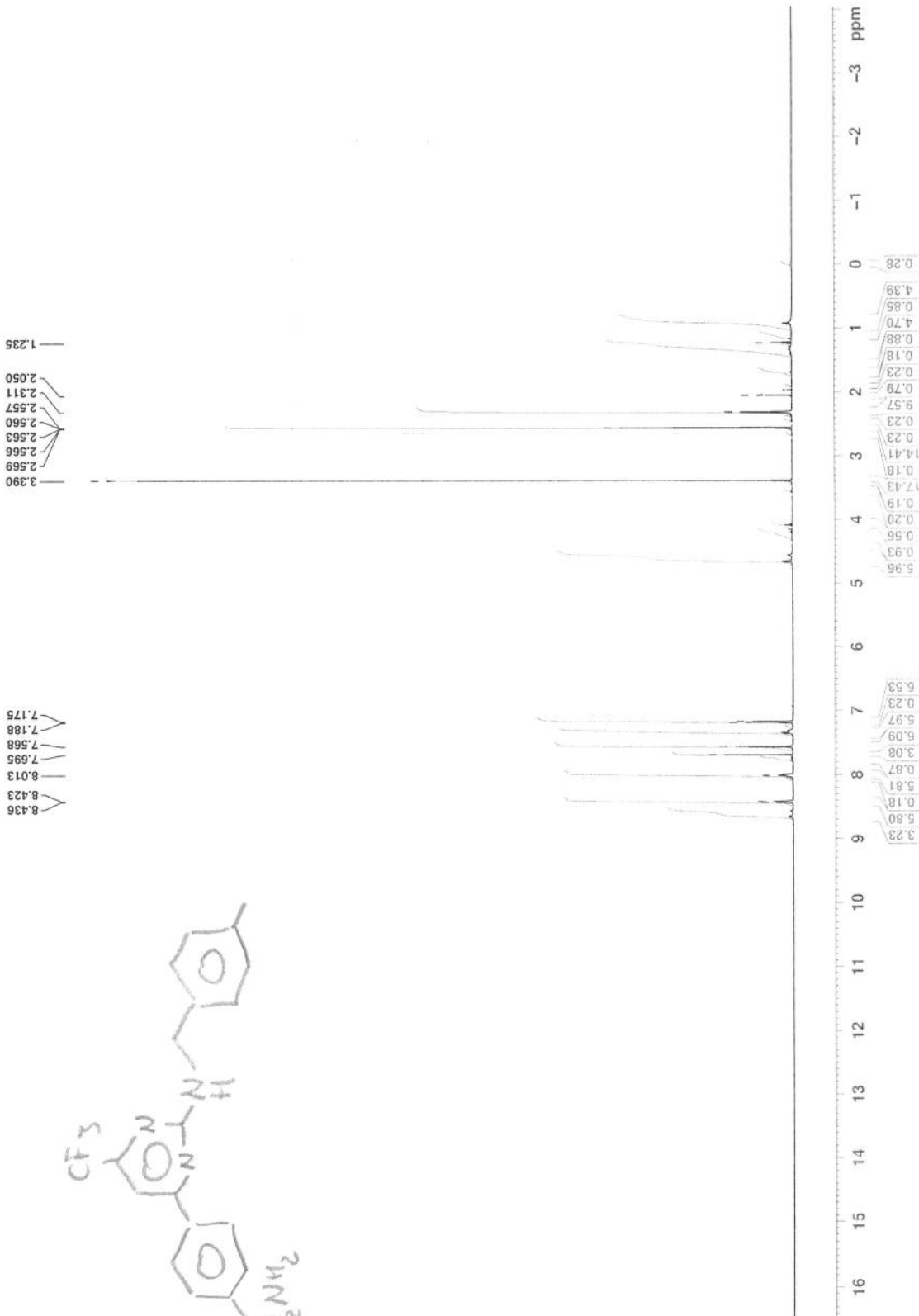


8.436  
8.423  
8.013  
7.995  
7.568  
7.188  
7.175

3.390  
2.569  
2.566  
2.563  
2.560  
2.557  
2.311  
2.050  
1.235

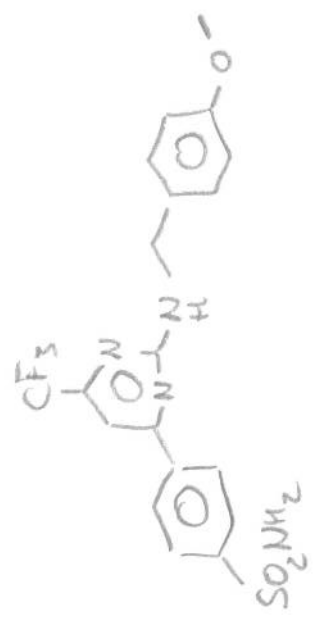


Current Data Parameters  
NAME Aug22-2012  
EXPNO 70  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.25  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.186225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 295.9 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
PLW1 12.00 usec  
PLW1 27.29999924 W  
F2 - Processing parameters  
SI 65536  
SF 600.2699709 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00



<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO) compound 2d

Ole Tietz: Proton on OT-SA-P-04



7.976  
7.644  
7.521  
6.898  
6.894  
6.867  
6.863

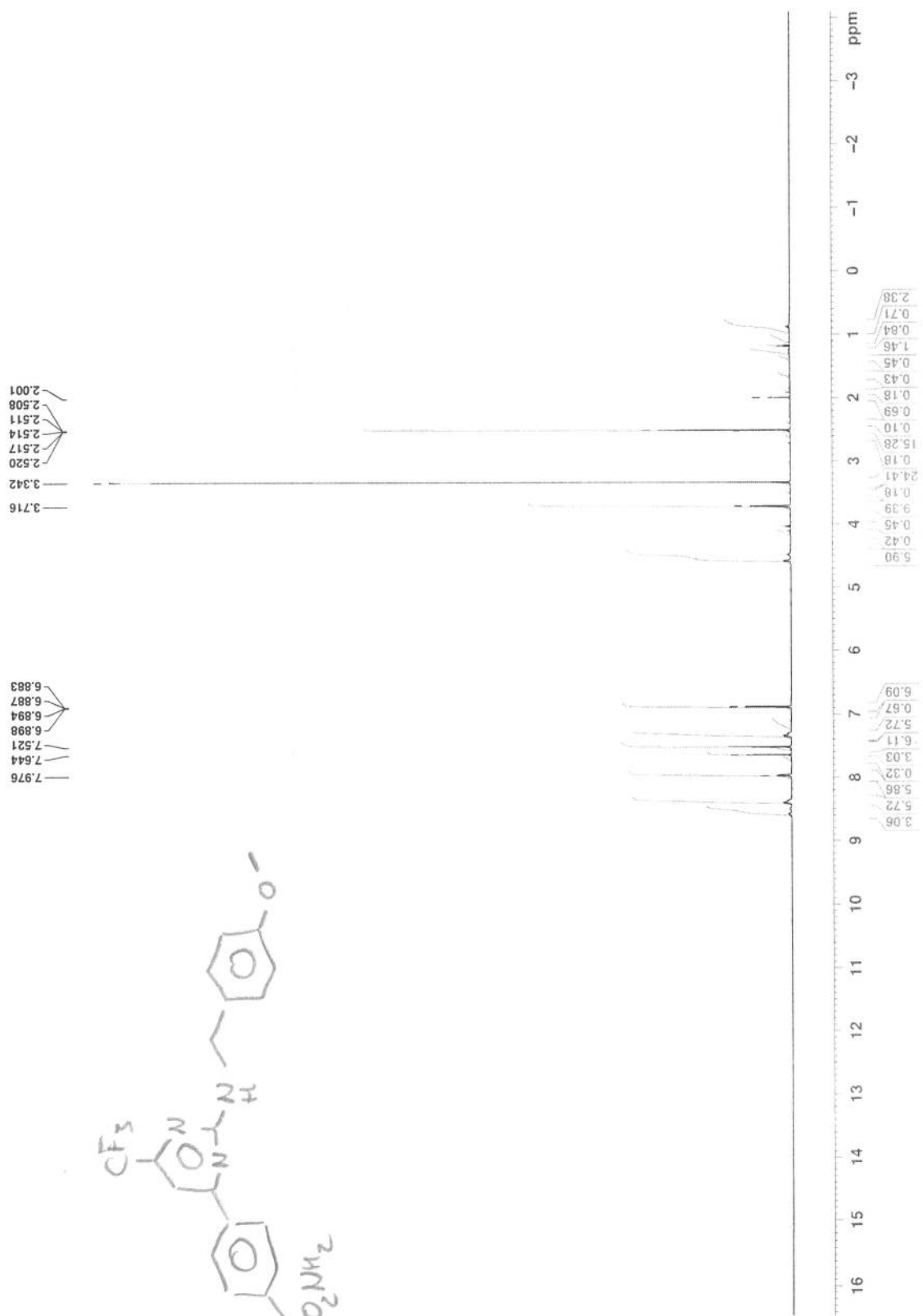
3.716  
3.342  
2.520  
2.517  
2.514  
2.511  
2.508  
2.001

Current Data Parameters  
NAME Aug22-2012  
EXPNO 80  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.30  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.186225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W

F2 - Processing parameters  
SI 65536  
SF 600.2700000 MHz  
WDW EM  
SSB 0 0.20 Hz  
LB 0  
GB 0  
PC 1.00







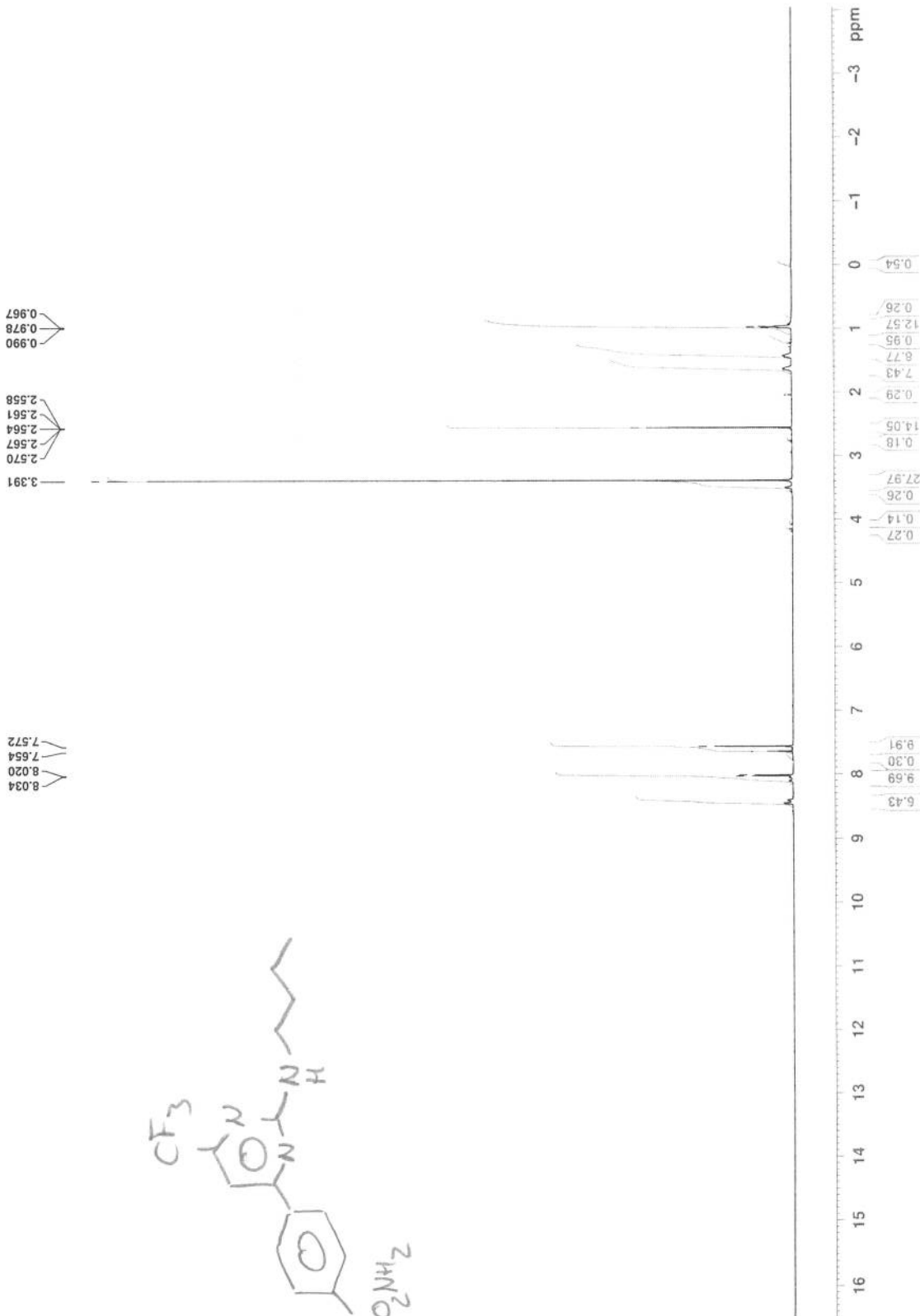
Current Data Parameters  
NAME Aug22-2012  
EXPNO 90  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120822  
Time 17.34  
INSTRUM spect  
PROBHD 5 mm CPPBBO BB  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12335.526 Hz  
FIDRES 0.188225 Hz  
AQ 2.6563926 sec  
RG 118.28  
DW 40.533 usec  
DE 20.49 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

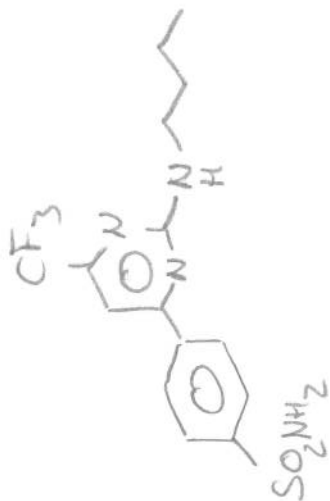
==== CHANNEL f1 =====  
SFO1 600.2737069 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 27.29999924 W

F2 - Processing parameters  
SI 65536  
SF 600.2699699 MHz  
WDW EM  
SSB 0  
LB 0.20 Hz  
GB 0  
PC 1.00

Ole Tietz: Proton on OT-SA-P-06



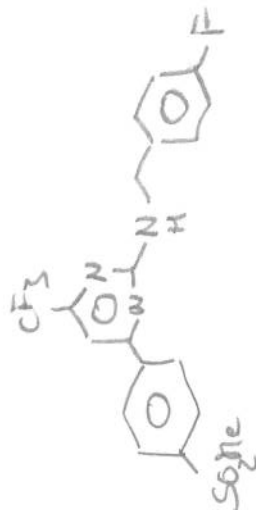
<sup>1</sup>H-NMR (d<sub>6</sub>-DMSO) compound 2e





<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1a

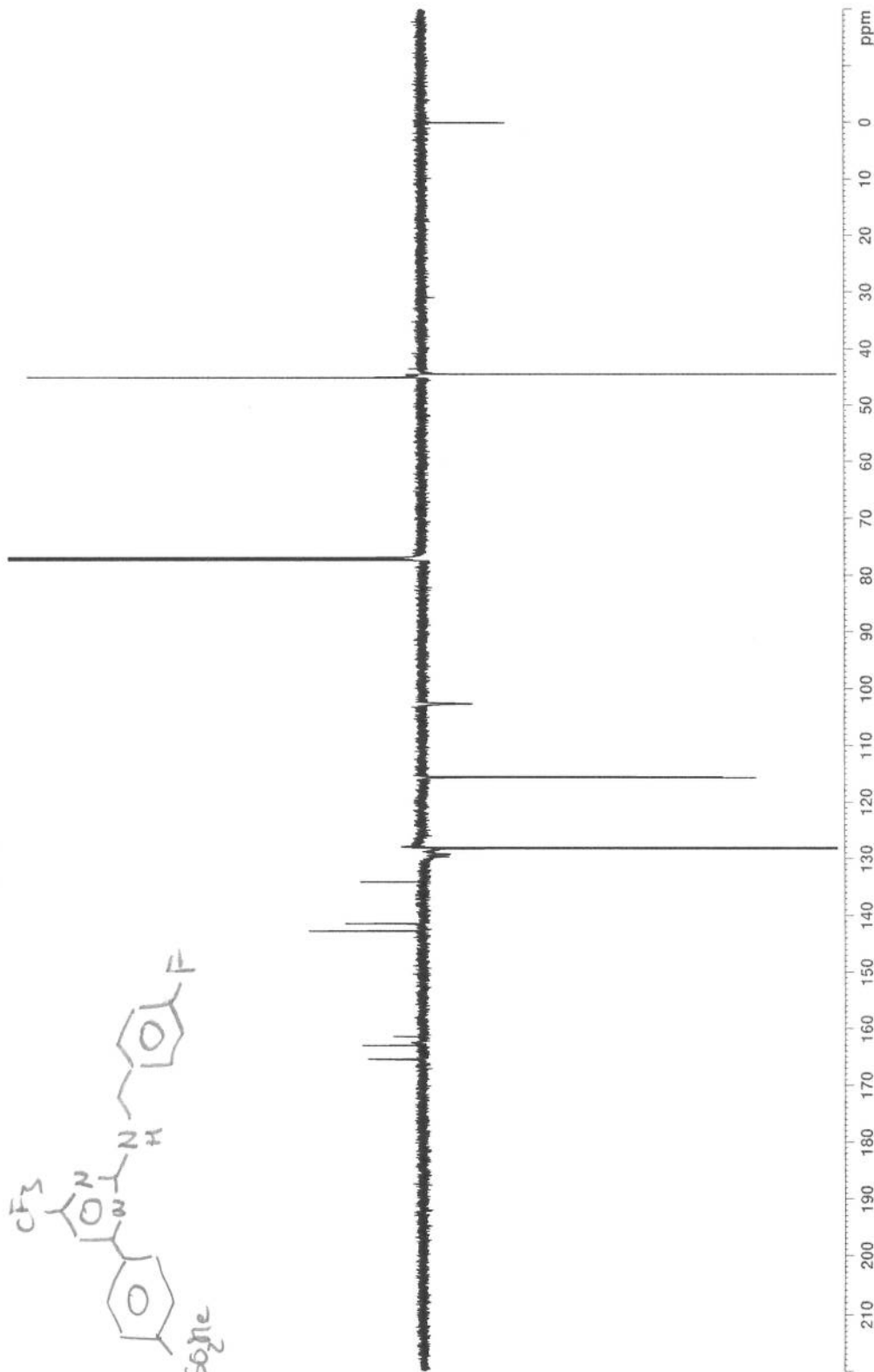
Ole Tietz: Deptq on OTPy P101  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2) vishwa 41



```
Current Data Parameters
NAME      Sep17-2013
EXPNO    200
PROCNO    1

F2 - Acquisition Parameters
Date_    20130917
Time     23:40
INSTRUM  spect
PROBHD   5 mm PABBO BH/
PULPROG  zgpg30
TD        65536
SFO1     101.2530000 MHz
RG        681.2
AQ        0.35000000 sec
RG        681.2
DS         4
SWH       36231.863 Hz
FIDRES    0.2944568 Hz
AQRES     0.5944568 Hz
RG         180.12
RG         180.12
DM         13.860 usec
DE         26.00 usec
TE         300.2 K
CNS12     145.0000000 K
CNS112    1.5000000
D1         2.0000000 sec
D2         0.0500000 sec
D3         0.0002000 sec
D5         0.0002000 sec
D7         0.0002000 sec
D9         0.0002000 sec
D10        0.0002000 sec
D11        0.0002000 sec
D12        0.0002000 sec
D16        0.0002000 sec
D17        0.0002000 sec
D18        0.0002000 sec
D19        0.0002000 sec
D20        0.0002000 sec
D21        0.0002000 sec
D22        0.0002000 sec
D23        0.0002000 sec
D24        0.0002000 sec
D25        0.0002000 sec
D26        0.0002000 sec
D27        0.0002000 sec
D28        0.0002000 sec
D29        0.0002000 sec
D30        0.0002000 sec
D31        0.0002000 sec
D32        0.0002000 sec
D33        0.0002000 sec
D34        0.0002000 sec
D35        0.0002000 sec
D36        0.0002000 sec
D37        0.0002000 sec
D38        0.0002000 sec
D39        0.0002000 sec
D40        0.0002000 sec
D41        0.0002000 sec
D42        0.0002000 sec
D43        0.0002000 sec
D44        0.0002000 sec
D45        0.0002000 sec
D46        0.0002000 sec
D47        0.0002000 sec
D48        0.0002000 sec
D49        0.0002000 sec
D50        0.0002000 sec
D51        0.0002000 sec
D52        0.0002000 sec
D53        0.0002000 sec
D54        0.0002000 sec
D55        0.0002000 sec
D56        0.0002000 sec
D57        0.0002000 sec
D58        0.0002000 sec
D59        0.0002000 sec
D60        0.0002000 sec
D61        0.0002000 sec
D62        0.0002000 sec
D63        0.0002000 sec
D64        0.0002000 sec
D65        0.0002000 sec
D66        0.0002000 sec
D67        0.0002000 sec
D68        0.0002000 sec
D69        0.0002000 sec
D70        0.0002000 sec
D71        0.0002000 sec
D72        0.0002000 sec
D73        0.0002000 sec
D74        0.0002000 sec
D75        0.0002000 sec
D76        0.0002000 sec
D77        0.0002000 sec
D78        0.0002000 sec
D79        0.0002000 sec
D80        0.0002000 sec
D81        0.0002000 sec
D82        0.0002000 sec
D83        0.0002000 sec
D84        0.0002000 sec
D85        0.0002000 sec
D86        0.0002000 sec
D87        0.0002000 sec
D88        0.0002000 sec
D89        0.0002000 sec
D90        0.0002000 sec
D91        0.0002000 sec
D92        0.0002000 sec
D93        0.0002000 sec
D94        0.0002000 sec
D95        0.0002000 sec
D96        0.0002000 sec
D97        0.0002000 sec
D98        0.0002000 sec
D99        0.0002000 sec
D100       0.0002000 sec

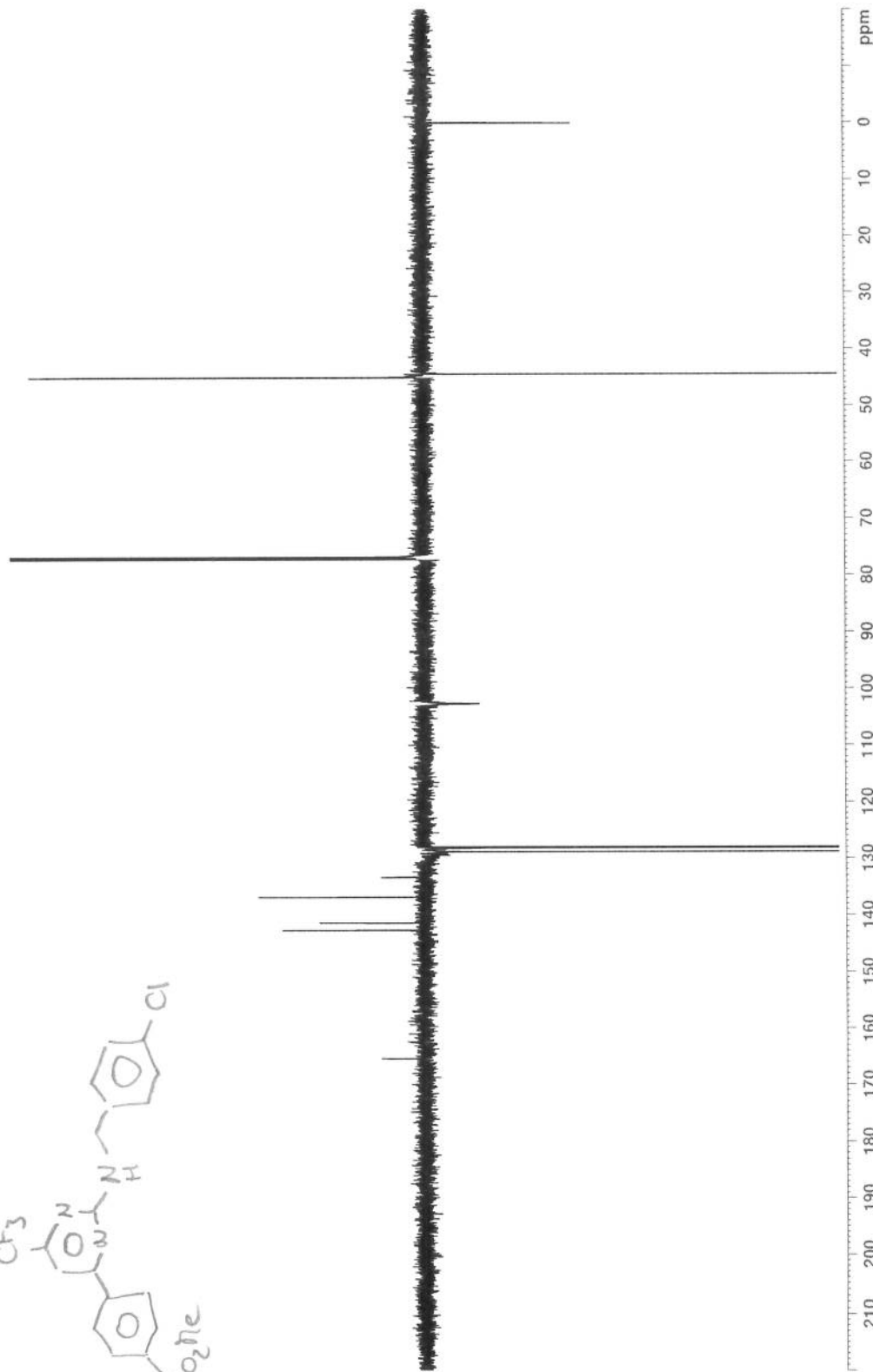
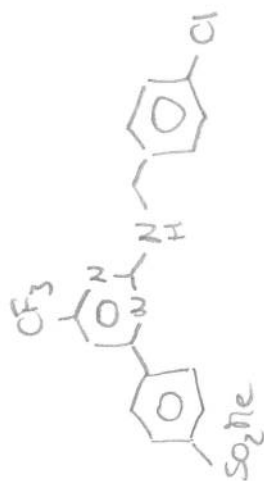
===== CHANNEL f1 =====
SFO1     150.9531058 MHz
NUC1     13C
P1        12.00 usec
PL1       0.00 dB
SFO2     600.2119197 MHz
NUC2     1H
P2        12.00 usec
PL2       0.00 dB
SFO3     120.0000000 MHz
PL3       0.00 dB
SFO4     200.0000000 MHz
PL4       0.00 dB
SFO5     24.24759519 MHz
PL5       0.00 dB
===== CHANNEL f2 =====
SFO2     600.2119197 MHz
NUC2     1H
P2        12.00 usec
PL2       0.00 dB
SFO3     120.0000000 MHz
PL3       0.00 dB
SFO4     200.0000000 MHz
PL4       0.00 dB
SFO5     24.24759519 MHz
PL5       0.00 dB
===== GRABUNT CHANNEL =====
GRABUNT1  SMS10-100
GRABUNT2  SMS10-100
GRABUNT3  SMS10-100
GRABUNT4  SMS10-100
GRABUNT5  SMS10-100
GRABUNT6  SMS10-100
GRABUNT7  SMS10-100
GRABUNT8  SMS10-100
GRABUNT9  SMS10-100
GRABUNT10 SMS10-100
GRABUNT11 SMS10-100
GRABUNT12 SMS10-100
GRABUNT13 SMS10-100
GRABUNT14 SMS10-100
GRABUNT15 SMS10-100
GRABUNT16 SMS10-100
GRABUNT17 SMS10-100
GRABUNT18 SMS10-100
GRABUNT19 SMS10-100
GRABUNT20 SMS10-100
===== Processing parameters =====
SI        32768
SF         150.9531058 MHz
WDW        EM
SSB         0
LB          0
GB          0
PC         1.40
```





# <sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1b

Ole Tietz: Deptq on OTPY P102  
CPP\_Deptq.A CDCl3 (C:\Bruker\TopSpin3.2) vishwa 33



```
Current Data Parameters
Name      Sep09_302
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    2012.02.21
Time     22.51
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS       4400
DS       4
SWH       36231.885 MHz
FIDRES    0.552855 MHz
AQ        0.9643968 sec
RG        180.12 ussec
DB        13.650 ussec
TE        296.0 K
CNS2      145.000000
DMS112    1.500000
DMS112    2.0000000 sec
D2        0.0034428 sec
D12       0.0002000 sec
D16       0.0002000 sec
106

***** CHANNEL f1 *****
SFO1     130.953108 MHz
PC1      11.40 ussec
P13      2000.40 ussec
PLMO     0. W
SFOALS   CF1CF0C0M0.4
SFOALS   0.500
SEFFS5   0 Hz
SEWS     24.21799519 W

***** CHANNEL f2 *****
SFO2     600.2719197 MHz
NUC2     1H
WALT16   wa16
PC2PRG2  20.10 ussec
P3       13.40 ussec
P4       26.60 ussec
P5       26.60 ussec
PLMO     0. W
SFOALS   CF1CF0C0M0.4
SEFFS5   0 Hz
SEWS     24.21799519 W

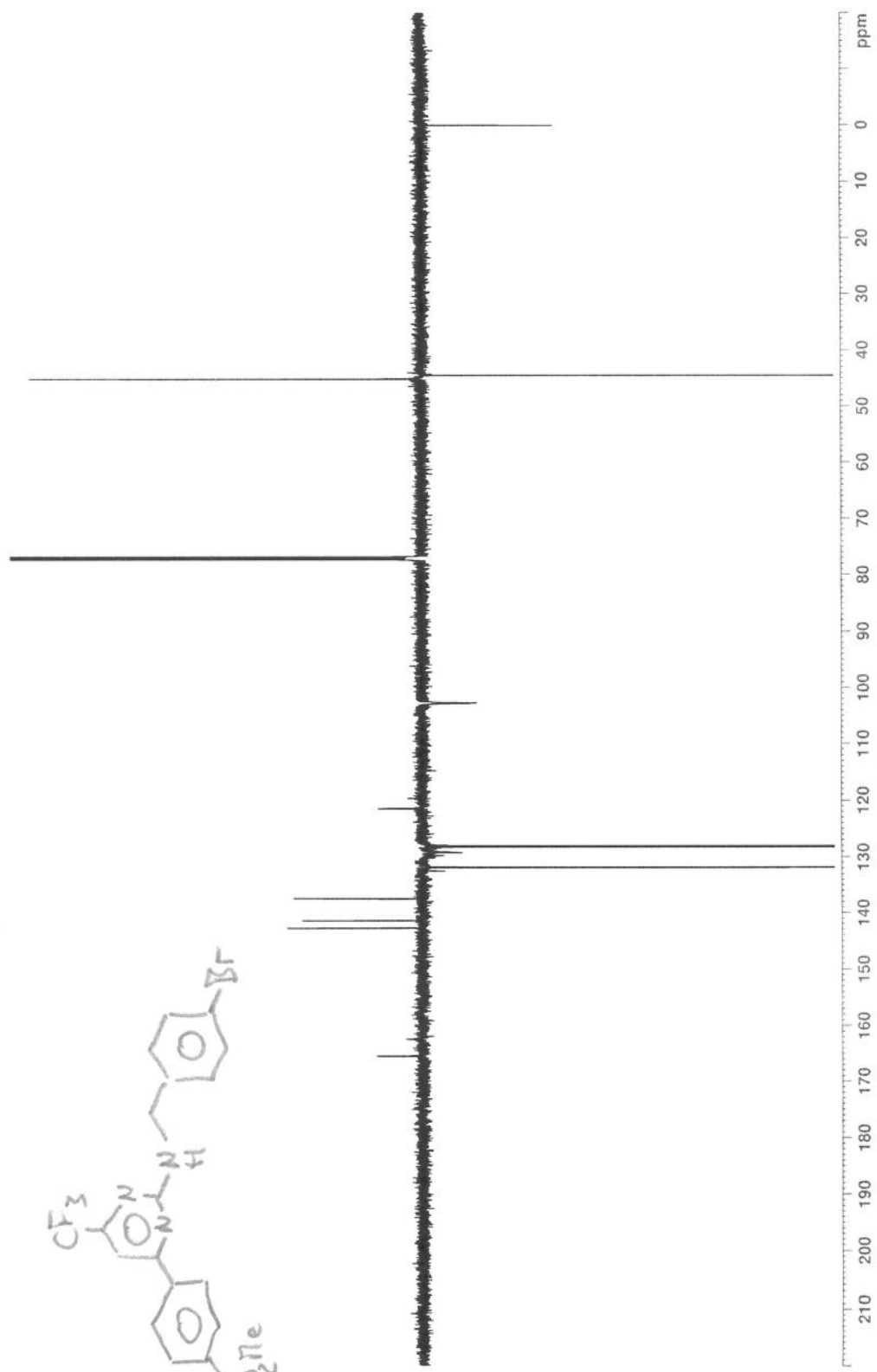
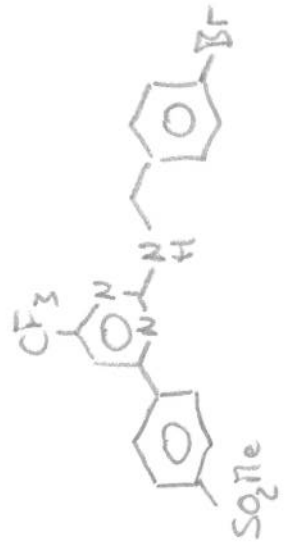
***** GRADIENT CHANNEL *****
GNUM1    1
GNUM2    1
GNUM3    1
GNUM4    1
GNUM5    1
GNUM6    1
GNUM7    1
GNUM8    1
GNUM9    1
GNUM10   1
GNUM11   1
GNUM12   1
GNUM13   1
GNUM14   1
GNUM15   1
GNUM16   1
GNUM17   1
GNUM18   1
GNUM19   1
GNUM20   1
GNUM21   1
GNUM22   1
GNUM23   1
GNUM24   1
GNUM25   1
GNUM26   1
GNUM27   1
GNUM28   1
GNUM29   1
GNUM30   1
GNUM31   1
GNUM32   1
GNUM33   1
GNUM34   1
GNUM35   1
GNUM36   1
GNUM37   1
GNUM38   1
GNUM39   1
GNUM40   1
GNUM41   1
GNUM42   1
GNUM43   1
GNUM44   1
GNUM45   1
GNUM46   1
GNUM47   1
GNUM48   1
GNUM49   1
GNUM50   1
GNUM51   1
GNUM52   1
GNUM53   1
GNUM54   1
GNUM55   1
GNUM56   1
GNUM57   1
GNUM58   1
GNUM59   1
GNUM60   1
GNUM61   1
GNUM62   1
GNUM63   1
GNUM64   1
GNUM65   1
GNUM66   1
GNUM67   1
GNUM68   1
GNUM69   1
GNUM70   1
GNUM71   1
GNUM72   1
GNUM73   1
GNUM74   1
GNUM75   1
GNUM76   1
GNUM77   1
GNUM78   1
GNUM79   1
GNUM80   1
GNUM81   1
GNUM82   1
GNUM83   1
GNUM84   1
GNUM85   1
GNUM86   1
GNUM87   1
GNUM88   1
GNUM89   1
GNUM90   1
GNUM91   1
GNUM92   1
GNUM93   1
GNUM94   1
GNUM95   1
GNUM96   1
GNUM97   1
GNUM98   1
GNUM99   1
GNUM100  1

F2 - Processing parameters
SF       150.9380178 MHz
WDW      EM
SSB      0
GB       0
PC       1.40
PC       1.40
```



<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1c

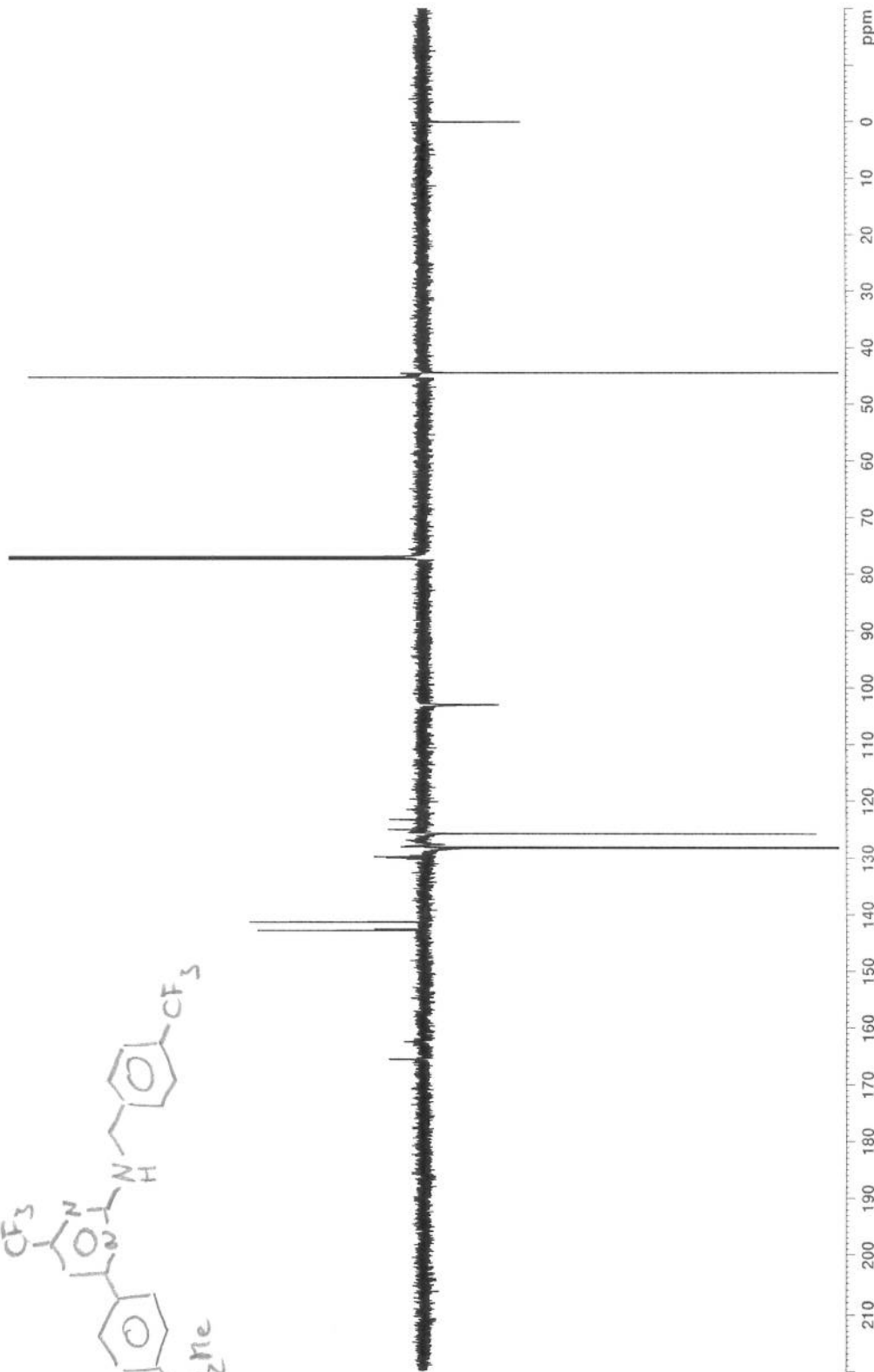
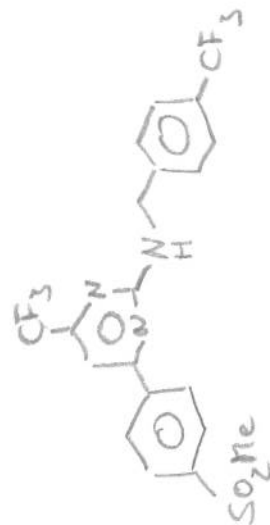
Ole: Deptq on P103  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2) vishwa 49



```
Current Data Parameters
Name      Sep10-2013
Date_    20130910
PROCNO   29
F2 - Acquisition Parameters
Date_    20130910
Time     11:20:10
INSTRUM spect
PROBHD  5 mm PABBO B6/
PULPROG zgpg30
SOLVENT CDCl3
NS      8192
DS      4
SWH     36231.86 Hz
FIDRES  0.1552865 Hz
AQ      0.5043968 sec
RG      180.12
DQ      11.800 usec
TE      296.20 K
CRST2   145.0000000
CNST12  1.5000000 sec
D2      0.0034828 sec
D12     0.0002000 sec
D16     0.0002000 sec
TDG     1
----- CHANNEL f1 -----
SFO1    130.9531058 MHz
NUC1    13C
P13     11.50 usec
PLW0    0 W
PLW1    120.0000000 W
CPRGAM(S) CPEPRGAM(S)
SFOALS   0 Hz
SFOFFS5 0 Hz
SPW5     24.24759519 W
----- CHANNEL f2 -----
SFO2    500.2719197 MHz
NUC2    1H
P12     13.40 usec
PLW2    26.80 usec
PCPD2   21.28920500 usec
PLM12   0.78053999 W
----- GRADIENT CHANNEL -----
GMM1(1) SMSO15
GMM1(2) SMSO15
GMM1(3) SMSO15
GMM1(4) SMSO15
GRZ1    31.00 %
GRZ2    31.00 %
GRZ3    31.00 %
P15     1000.00 usec
F2 - Processing parameters
SI      32768
SF      150.930299 MHz
WDW     EM
SSB     0
GB      0
PC      1.40
```

# <sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1d

Ole Tietz: Deptq on OTPY P104  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2} vishwa 34

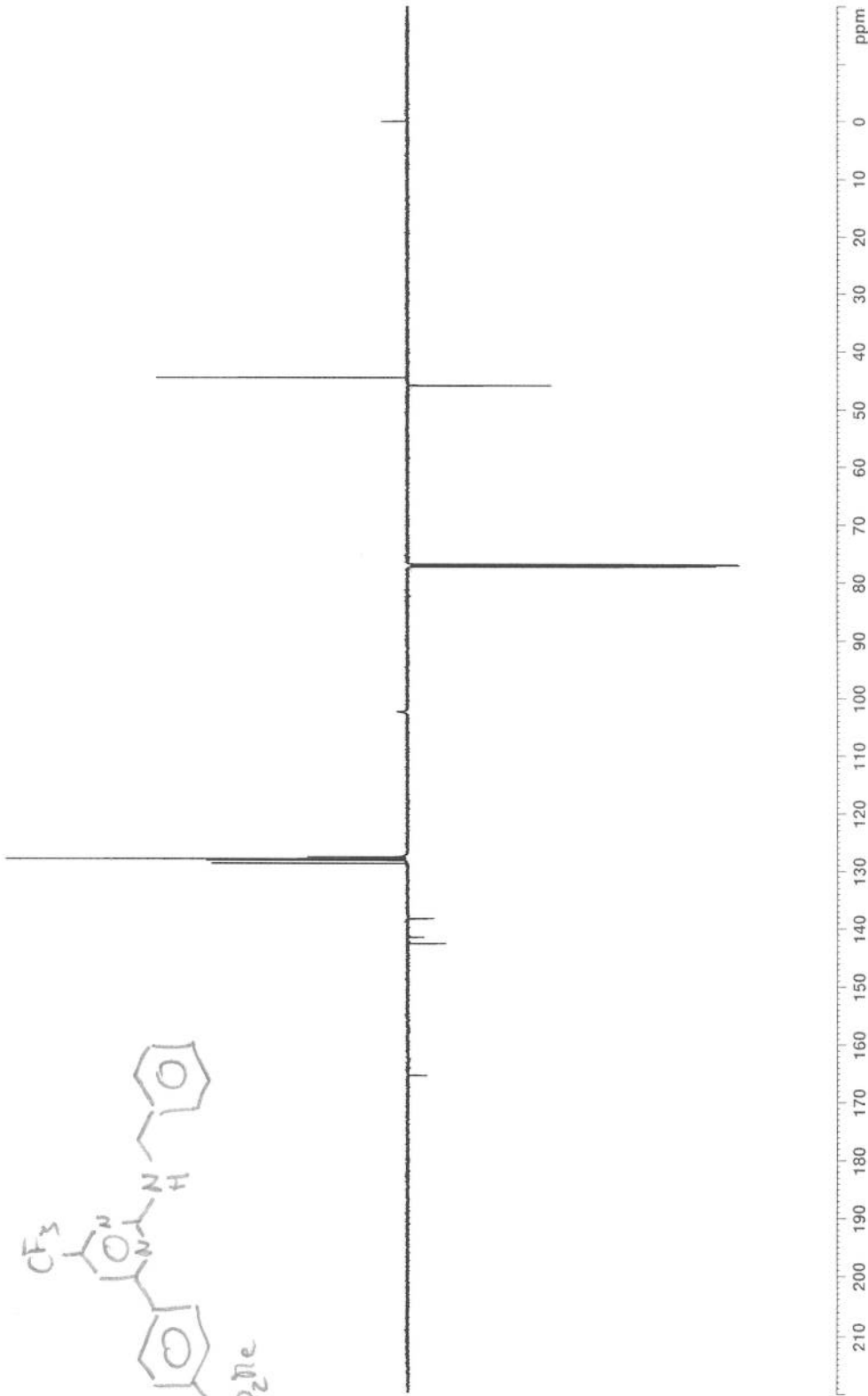
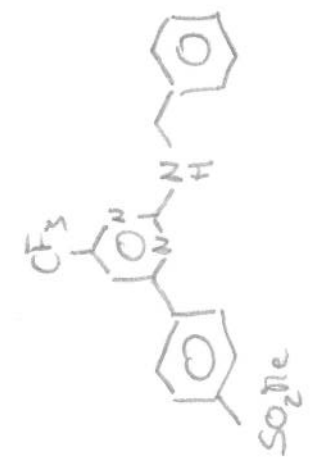


```
Current Data Parameters
NAME      Sep09-2013
PROCNO    1
F2 - Acquisition Parameters
Date_     20130910
Time      11.40
INSTRUM   spect
PROBHD    5 mm PABBO 36/
PULPROG   zgpg30
SOLVENT   CDCl3
NS        4400
DS        4
AQ        0.555285 Hz
FIDRES    0.9043668 arc
RG        180.12
DM        13.800 usec
DE        296.0 K
TE        145.0000000
CNS12     1.500000 sec
CNS112    1.500000 sec
D2        0.0034828 sec
D12       0.0002000 sec
D16       0.0002000 sec
100
===== CHANNEL f1 =====
SFO1      150.931058 MHz
NUC1      13C
P1        11.50 usec
PL1       0 M
PL2       2000.00 usec
PL3       0 M
PL4       100.0000000 W
PL5       100.0000000 W
SFOFF5    0 Hz
SFOFF6    0.500
SFOFF7    0 Hz
SFOFF8    24.24799919 W
===== CHANNEL f2 =====
SFO2      600.2719197 MHz
NUC2      1H
P2        13.40 usec
PL2       13.40 usec
PL3       26.80 usec
PL4       26.80 usec
PL5       31.9000000 W
PL6       0.78052929 W
===== GRADIENT CHANNEL =====
G1        1000.00 usec
G2        1000.00 usec
G3        1000.00 usec
G4        1000.00 usec
G5        1000.00 usec
G6        1000.00 usec
F2 - Processing parameters
SI        32768
SF        150.930177 MHz
WDW       EM
SSB       0
RB        1.00 Hz
GB        0
PC        1.40
```



<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1e

Ole Tietz: Deptq on OTPY P105  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2) vishwa 35

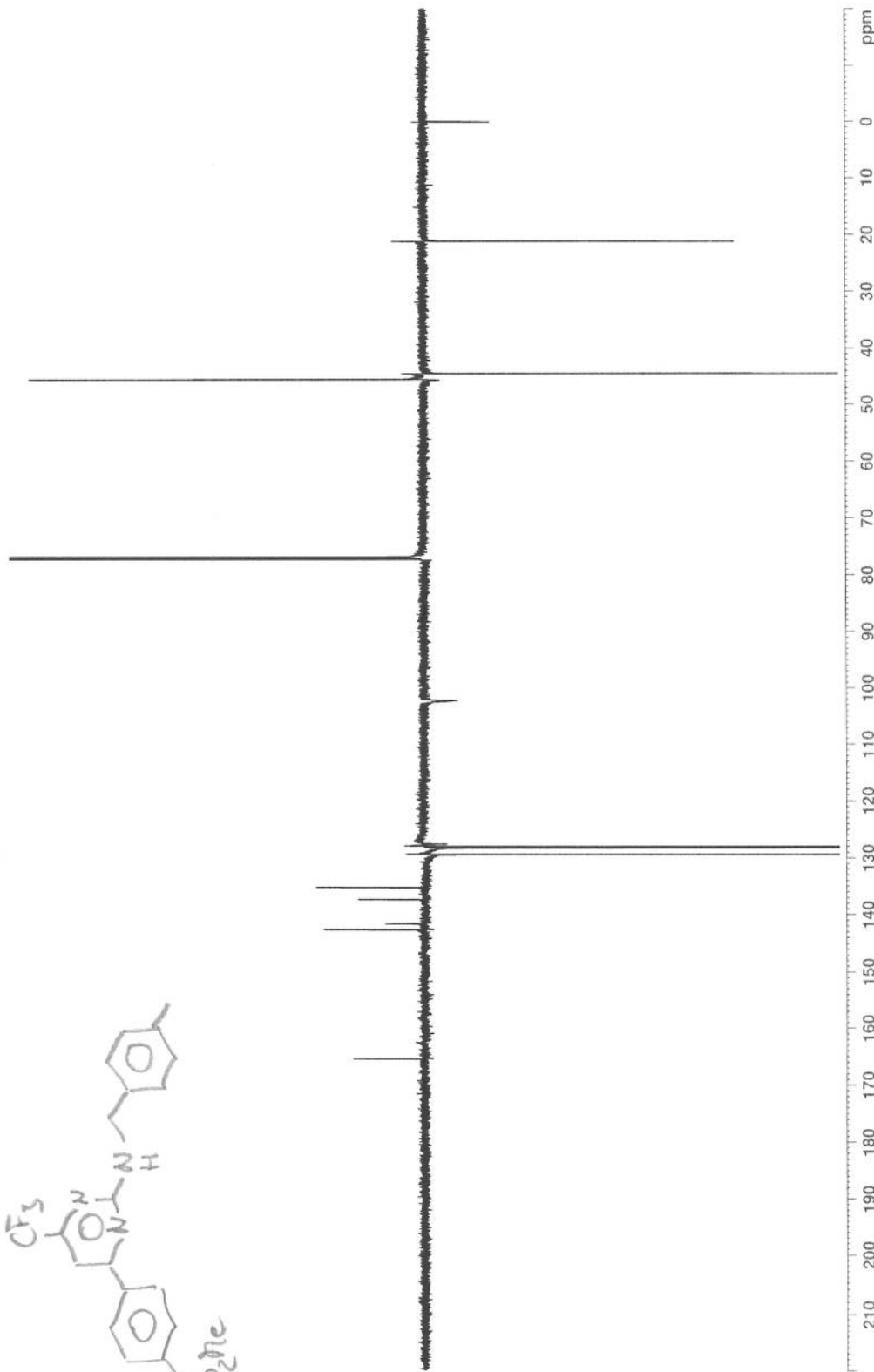
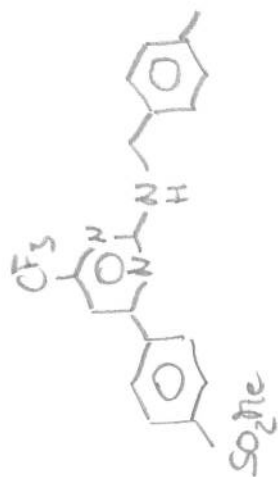


Current Data Parameters  
NAME: Sept9-2013  
PROCNO: 1  
F2 - Acquisition Parameters  
Date\_: 20130910  
Time: 11:10:58  
INSTRUM: spect  
PROBHD: 5 mm PABBO BH/4  
PULPROG: zgpg30  
D1: 1.00000000 sec  
SOLVENT: CDCl3  
NS: 4460  
DS: 4  
SWH: 3621.865 Hz  
FIDRES: 0.33186 Hz  
AQ: 0.9043668 sec  
RG: 180.12  
DM: 13.800 usec  
DE: 1.00000000 usec  
TE: 297.0 K  
CNS12: 145.0000000  
CNS112: 1.5000000  
D1: 1.00000000 sec  
D2: 0.0004898 sec  
D12: 0.0002050 sec  
D16: 0.0002000 sec  
TD0: 1  
=====  
CHANNEL F1 =====  
SFO1 130.9531058 MHz  
NUC1 13C  
P1 1.20 usec  
PL1 0.00 dB  
PL0 0 W  
2000.00 usec  
PWR1 120.00000000 W  
SFO2 600.1376195 MHz  
SFO1S1 CPDPRG2  
SFOFFS 0 Hz  
SFOFF5 0 Hz  
SFM5 24.2479915 M  
=====  
CHANNEL F2 =====  
SFO2 600.2191917 MHz  
NUC2 1H  
P2 12.00 usec  
PL2 0.00 dB  
PL0 0 W  
2000.00 usec  
PWR2 120.00000000 W  
SFO2S1 CPDPRG2  
SFOFFS 0 Hz  
SFOFF5 0 Hz  
SFM5 24.2479915 M  
=====  
GRADIENT CHANNEL =====  
GMR11 0 Hz  
GMR10 100 Hz  
GMR11S1 0 Hz  
GMR10S1 100 Hz  
GMR11S1 31.00 A  
GMR10S1 31.00 A  
GMR2 0 Hz  
GMR1 0 Hz  
GMR3 0 Hz  
GMR4 1000.00 usec  
=====  
F2 - Processing Parameters  
SI 32768  
SF 130.9531058 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1f

Ole: Deptq on P106  
CPP\_Deptq.A CDCl3 (C:\Bruker\TopSpin3.2) vishwa 50



```
Current Data Parameters
NAME      Sept10_2013
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130913
Time     11:20
INSTRUM spect
PROBHD   5 mm PARBO BB/
PULPROG zgpg30
SOLVENT  CDCl3
NS       6000
DS       4
SWH      36281.86 Hz
FIDRES   0.55285 Hz
AQ       0.9643648 sec
RG       180.12
DW       13.600 usec
DE       0.500 usec
TE       296.0 K
CNS2     145.0000000
CNS112   1.5000000 sec
D1       0.00344828 sec
D2       0.00344828 sec
D12      0.00002000 sec
D16      0.00020000 sec
TD       1

===== CHANNEL f1 =====
SFO1     150.9531028 MHz
NUC1     13C
P13      11.20 usec
PLW0     0 W
SFO1(S)  120.68000000 W
SFOALS   0 Hz
SFOFS5   0 Hz
SWS      24.2479919 W

===== CHANNEL f2 =====
SFO2     600.2719197 MHz
NUC2     1H
P13      11.20 usec
PLW0     0 W
SFO2(S)  120.68000000 W
SFOALS   0 Hz
SFOFS5   0 Hz
SWS      24.2479919 W

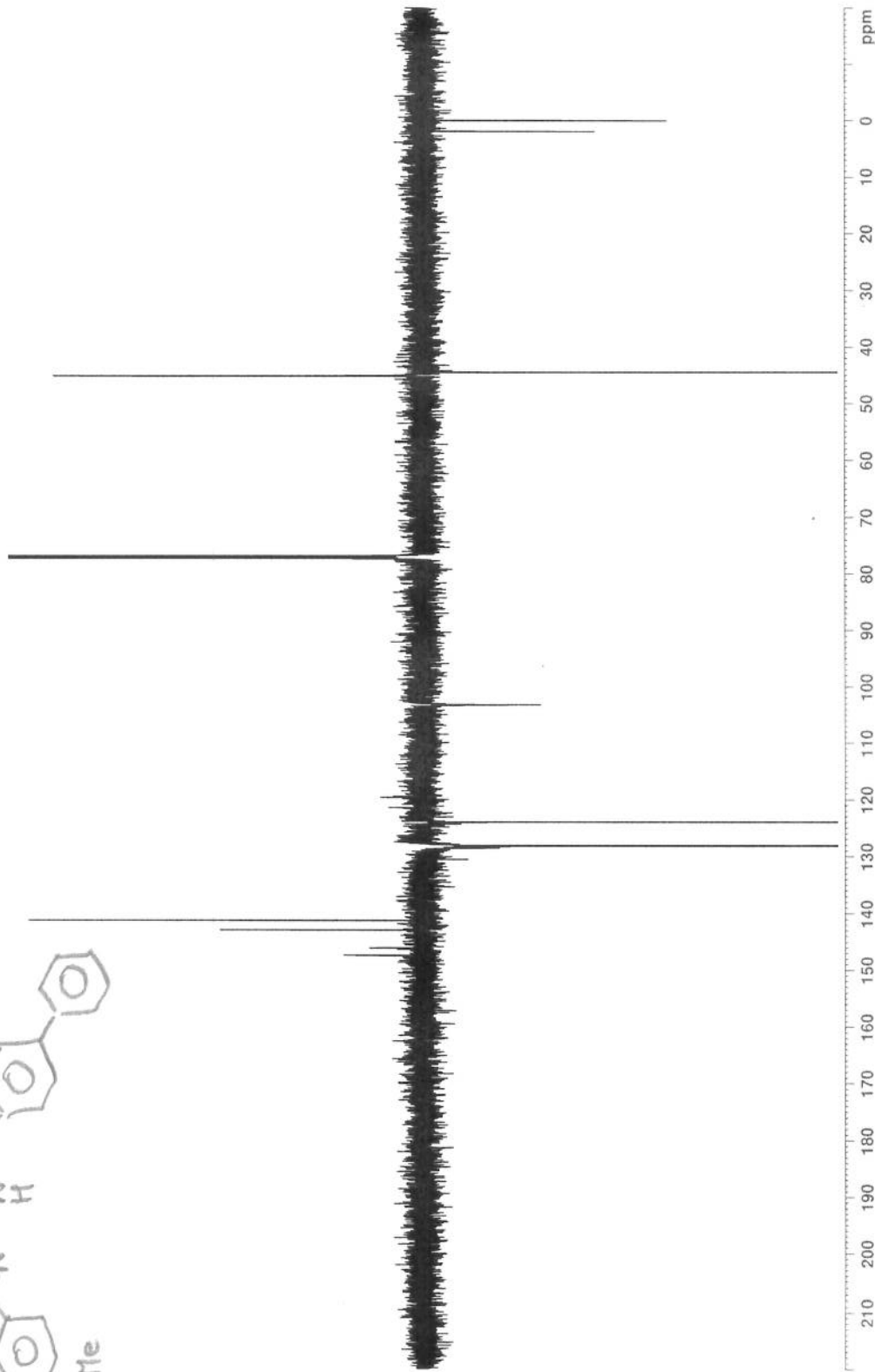
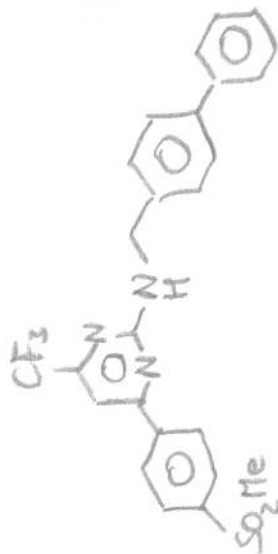
===== GRADIENT CHANNEL =====
GAMMA1   13C
GAMMA2   1H
SFOG1     120.68000000 MHz
SFOG2     500.1359598 MHz
SFOG3     120.68000000 MHz
SFOG4     500.1359598 MHz
SFOG5     120.68000000 MHz
SFOG6     500.1359598 MHz
SFOG7     120.68000000 MHz
SFOG8     500.1359598 MHz
SFOG9     120.68000000 MHz
SFOG10    500.1359598 MHz
SFOG11    120.68000000 MHz
SFOG12    500.1359598 MHz
SFOG13    120.68000000 MHz
SFOG14    500.1359598 MHz
SFOG15    120.68000000 MHz
SFOG16    500.1359598 MHz
SFOG17    120.68000000 MHz
SFOG18    500.1359598 MHz
SFOG19    120.68000000 MHz
SFOG20    500.1359598 MHz
SFOG21    120.68000000 MHz
SFOG22    500.1359598 MHz
SFOG23    120.68000000 MHz
SFOG24    500.1359598 MHz
SFOG25    120.68000000 MHz
SFOG26    500.1359598 MHz
SFOG27    120.68000000 MHz
SFOG28    500.1359598 MHz
SFOG29    120.68000000 MHz
SFOG30    500.1359598 MHz
SFOG31    120.68000000 MHz
SFOG32    500.1359598 MHz
SFOG33    120.68000000 MHz
SFOG34    500.1359598 MHz
SFOG35    120.68000000 MHz
SFOG36    500.1359598 MHz
SFOG37    120.68000000 MHz
SFOG38    500.1359598 MHz
SFOG39    120.68000000 MHz
SFOG40    500.1359598 MHz
SFOG41    120.68000000 MHz
SFOG42    500.1359598 MHz
SFOG43    120.68000000 MHz
SFOG44    500.1359598 MHz
SFOG45    120.68000000 MHz
SFOG46    500.1359598 MHz
SFOG47    120.68000000 MHz
SFOG48    500.1359598 MHz
SFOG49    120.68000000 MHz
SFOG50    500.1359598 MHz

F2 - Processing parameters
SI        32768
SF        150.938127 MHz
WDW       EM
SSB       0
RB        0
GB        0
PC        1.40
```



$^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ ) compound 1g

Ole Tietz: Deptq on P110  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2) vishwa 27



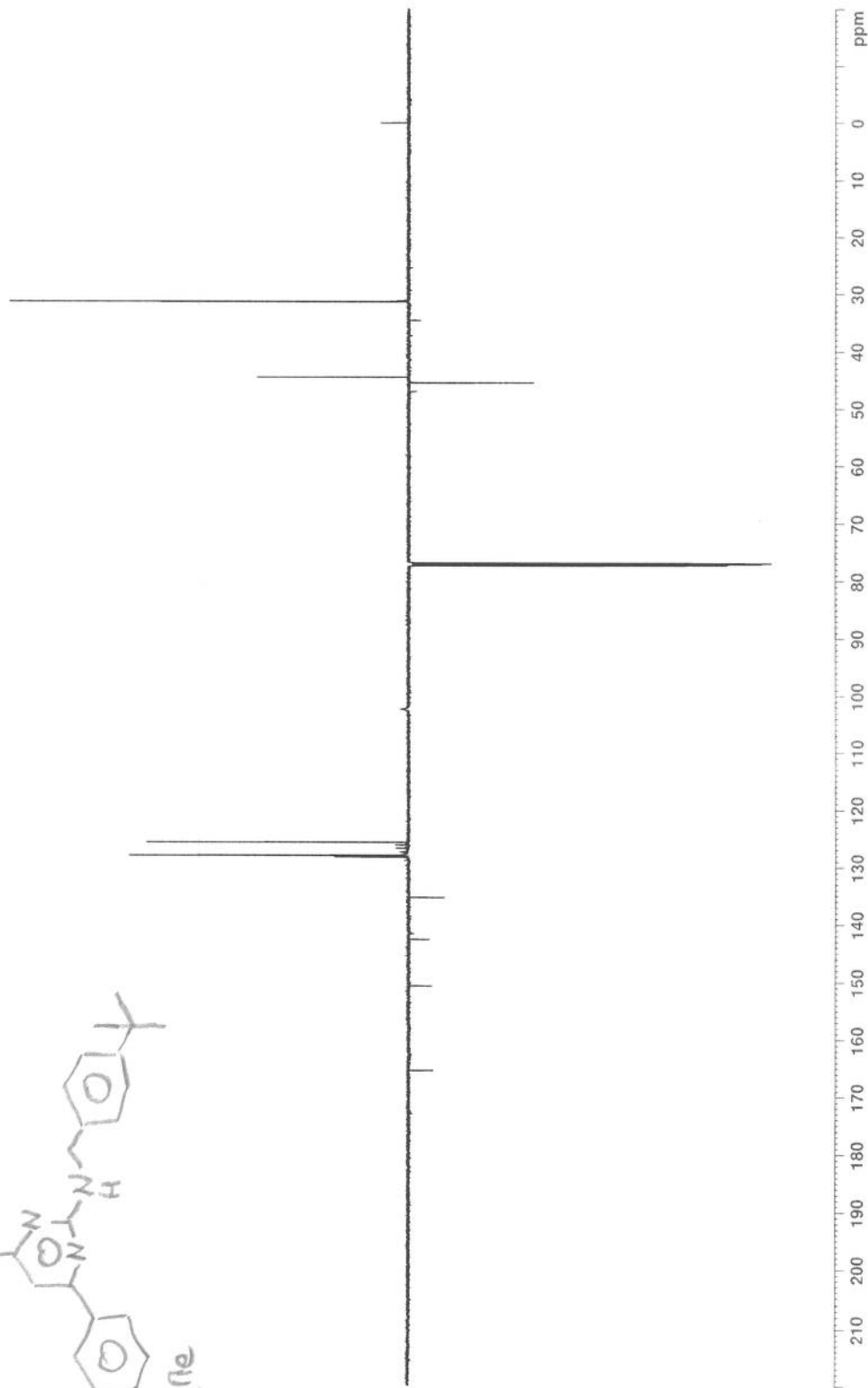
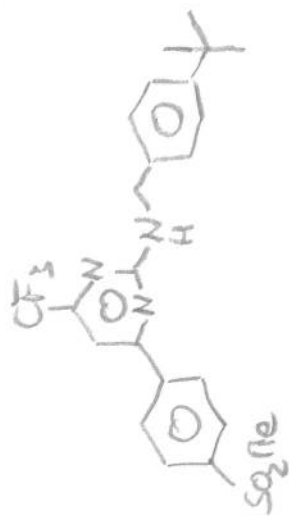
```
Current Data Parameters
Date_   Sep11-2013
Time    9:11
PROCNO  1
F2 - Acquisition Parameters
Date_   20130922
Time    11:50
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zgpg30
SOLVENT CDC13
NS      4860
DS      4
DE      36231.88 Hz
FIDRES  0.4552865 Hz
AQ      0.9043668 sec
RG      180.12
WDW     EM
SS      13.800 usec
LB      1.000 usec
TE      296.2 K
CNS2    145.0000000
CNS112  2.0000000 sec
D2      0.00344628 sec
D12     0.00002000 sec
D16     0.00002000 sec
108
===== CHANNEL f1 =====
SFO1    150.931028 MHz
PC1     11.50 usec
PL1     2000.00 uWAC
SFO1S1  10.00000000 W
CPDPRG1 CPMAS1
SFOALS1 0.500
SEFFS1  0 Hz
SEFFS5  24.2479919 W
===== CHANNEL f2 =====
NUC2    13C
PC2     11.50 usec
PL2     20.00 uWAC
SFO2    600.271917 MHz
PL2S1  12.40 uWAC
PL2S2  26.80 uWAC
PL2S3  21.9894502 usec
PL2S4  0.7865599 W
===== GRADIENT CHANNEL =====
GNDM1[1] 5MSQ10.100
GNDM1[2] 5MSQ10.100
GNDM1[3] 5MSQ10.100
GR21     31.00 %
GR22     31.00 %
GR23     31.00 %
P16      1000.00 usec
F2 - Processing parameters
SF      150.9380128 MHz
NUC     13C
WDW     EM
SSB     0
GB      0
PC      1.00 Hz
PC      1.40
```





Ole Iietz: Deptq on P107  
CPP\_Deptq.A CDCl3 (C:\Bruker\TopSpin3.2) vishwa 25

<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1h

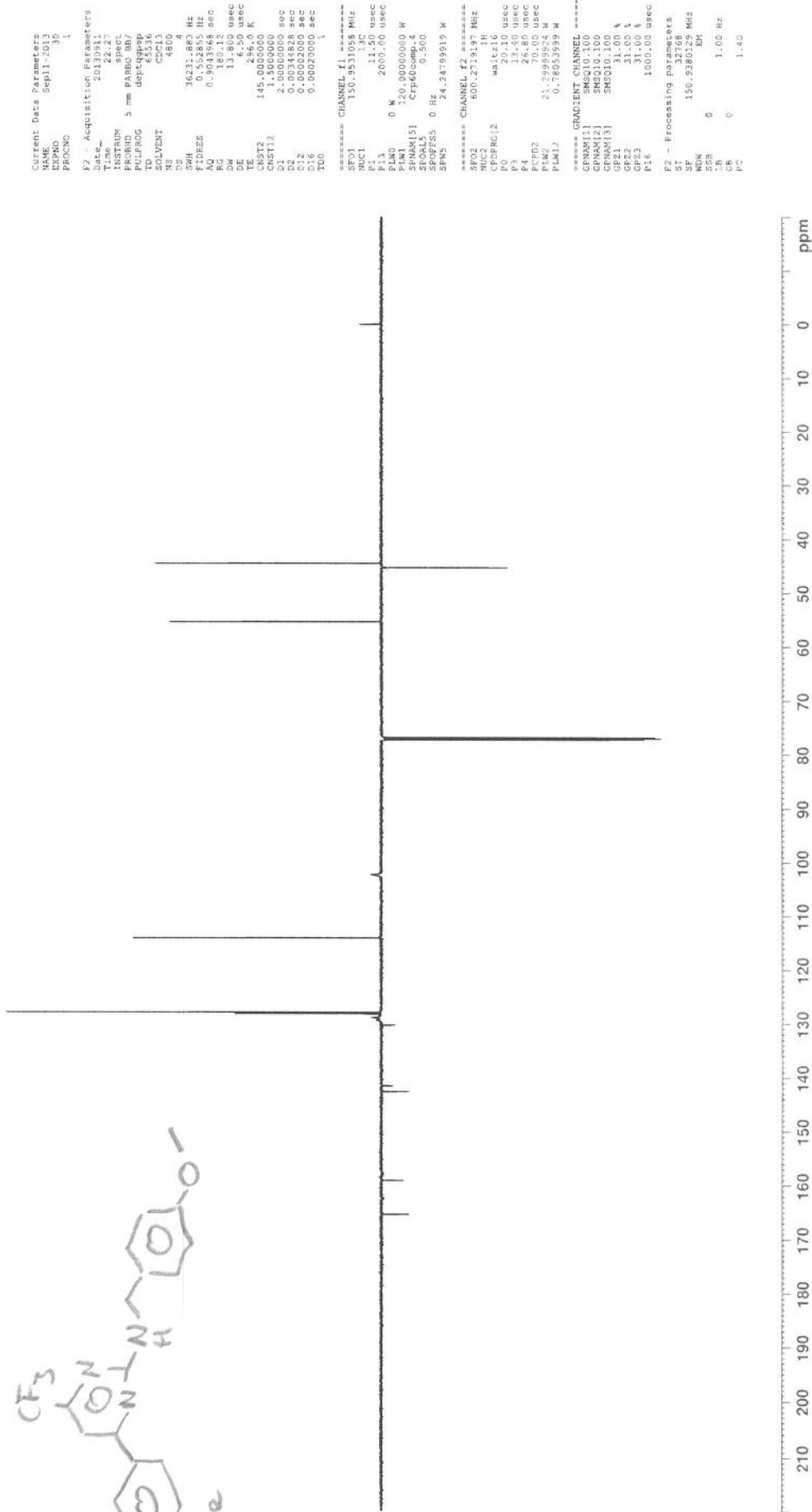
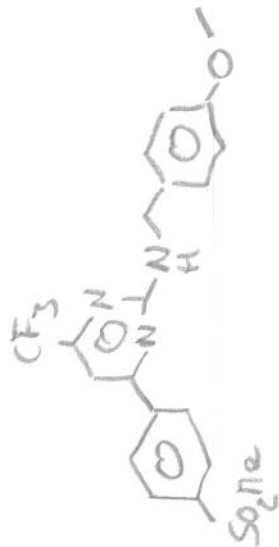


```
Current Data Parameters
NAME      Sept11_2013
PROCNO    1
F2 - Acquisition Parameters
Date_     20110824
Time      18:28
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4800
DS         4
SS         36231.88 Hz
AQ         0.552865 Hz
FIDRES    0.9043648 sec
RG         180.12
AQ         138.00 usec
SFO1       101.625000 MHz
TE         296.2 K
CNS2       145.000000
CNS112    2.000000 sec
D2         0.00344828 sec
D12        0.0002000 sec
D16        0.0002000 sec
TD6        1
===== CHANNEL F1 =====
SFO1       130.9531058 MHz
NUC1        13
P13         11.00 usec
PL10        0 W
PL13        2000.00 usec
SFOA151    20.00000000 W
SFOA15     CFPR000004
SFOFF55    0 Hz
SFOFF5     0.500
SFF55      24.24799919 W
===== CHANNEL F2 =====
SFO2       800.2719197 MHz
NUC2        1H
P23         11.00 usec
PL20        0 W
PL23        20.10 usec
P2         13.50 usec
P3         13.50 usec
P4         26.80 usec
PULPROG    zgpg30
SFOA152    21.29899992 usec
SFOA15     CFPR000004
SFOFF55    0 Hz
SFOFF5     0.78653939 W
===== GRADIENT CHANNEL =====
GFM1M1     0.00000000
GFM1M2     0.00000000
GFM1M3     0.00000000
GFM1M4     0.00000000
GFM1M5     0.00000000
GFM1M6     0.00000000
GFM1M7     0.00000000
GFM1M8     0.00000000
GFM1M9     0.00000000
GFM1M10    0.00000000
GFM1M11    0.00000000
GFM1M12    0.00000000
GFM1M13    0.00000000
GFM1M14    0.00000000
GFM1M15    0.00000000
GFM1M16    0.00000000
GFM1M17    0.00000000
GFM1M18    0.00000000
GFM1M19    0.00000000
GFM1M20    0.00000000
GFM1M21    0.00000000
GFM1M22    0.00000000
GFM1M23    0.00000000
GFM1M24    0.00000000
GFM1M25    0.00000000
GFM1M26    0.00000000
GFM1M27    0.00000000
GFM1M28    0.00000000
GFM1M29    0.00000000
GFM1M30    0.00000000
GFM1M31    0.00000000
GFM1M32    0.00000000
GFM1M33    0.00000000
GFM1M34    0.00000000
GFM1M35    0.00000000
GFM1M36    0.00000000
GFM1M37    0.00000000
GFM1M38    0.00000000
GFM1M39    0.00000000
GFM1M40    0.00000000
GFM1M41    0.00000000
GFM1M42    0.00000000
GFM1M43    0.00000000
GFM1M44    0.00000000
GFM1M45    0.00000000
GFM1M46    0.00000000
GFM1M47    0.00000000
GFM1M48    0.00000000
GFM1M49    0.00000000
GFM1M50    0.00000000
GFM1M51    0.00000000
GFM1M52    0.00000000
GFM1M53    0.00000000
GFM1M54    0.00000000
GFM1M55    0.00000000
GFM1M56    0.00000000
GFM1M57    0.00000000
GFM1M58    0.00000000
GFM1M59    0.00000000
GFM1M60    0.00000000
GFM1M61    0.00000000
GFM1M62    0.00000000
GFM1M63    0.00000000
GFM1M64    0.00000000
GFM1M65    0.00000000
GFM1M66    0.00000000
GFM1M67    0.00000000
GFM1M68    0.00000000
GFM1M69    0.00000000
GFM1M70    0.00000000
GFM1M71    0.00000000
GFM1M72    0.00000000
GFM1M73    0.00000000
GFM1M74    0.00000000
GFM1M75    0.00000000
GFM1M76    0.00000000
GFM1M77    0.00000000
GFM1M78    0.00000000
GFM1M79    0.00000000
GFM1M80    0.00000000
GFM1M81    0.00000000
GFM1M82    0.00000000
GFM1M83    0.00000000
GFM1M84    0.00000000
GFM1M85    0.00000000
GFM1M86    0.00000000
GFM1M87    0.00000000
GFM1M88    0.00000000
GFM1M89    0.00000000
GFM1M90    0.00000000
GFM1M91    0.00000000
GFM1M92    0.00000000
GFM1M93    0.00000000
GFM1M94    0.00000000
GFM1M95    0.00000000
GFM1M96    0.00000000
GFM1M97    0.00000000
GFM1M98    0.00000000
GFM1M99    0.00000000
GFM1M100   0.00000000
===== Processing parameters =====
SF          150.9380129 MHz
NUC1        13C
P1          11.00 usec
PL1         0.00 W
PL13        2000.00 usec
PL16        1000.00 usec
===== Processing parameters =====
SF          150.9380129 MHz
NUC1        13C
P1          11.00 usec
PL1         0.00 W
PL13        2000.00 usec
PL16        1000.00 usec
```



Ole Tietz: Deptq on P108  
CPP\_Deptq.A CDC13 (C:\Bruker\TopSpin3.2) vishwa 26

$^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ ) compound 1i



```
Current Data Parameters
NAME      Sept11_2013
NO      31
PROCNO    11

F2 - Acquisition Parameters
File      20130727
Time      20:19:27
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
SOLVENT   CDCl3
NS        4800
DS        4
AQ        36231.86 s
FIDRES    0.4552865 Hz
AQ        0.9013968 sec
RG        180.12
WDW        13.850 usec
SSB        0
GB        0
TE        296.0 K
CST2      145.0000000
CNST12    2.1500000 sec
D1        0.0002000 sec
D2        0.0034828 sec
D12       0.0002000 sec
D16       0.0002000 sec
TD        100

***** CHANNEL f1 *****
SFO1      150.9531058 MHz
NUC1      13C
P1        11.50 usec
PL1       0 W
PL12      2000.00 usec
SFO2      20.0000000 MHz
SFO1S1    CPDPRG2
SFOALS    0.560
SFOFSS    0 Hz
SFOFSS2   24.24799919 W

***** CHANNEL f2 *****
SFO2      800.2719197 MHz
NUC2      1H
P2        12.00 usec
PL2       0 W
PL22      20.00 usec
SFO2S1    WALTZ16
SFO2S2    WALTZ16
SFO2S3    WALTZ16
SFO2S4    WALTZ16
SFO2S5    WALTZ16
SFO2S6    WALTZ16
SFO2S7    WALTZ16
SFO2S8    WALTZ16
SFO2S9    WALTZ16
SFO2S10   WALTZ16
SFO2S11   WALTZ16
SFO2S12   WALTZ16
SFO2S13   WALTZ16
SFO2S14   WALTZ16
SFO2S15   WALTZ16
SFO2S16   WALTZ16
SFO2S17   WALTZ16
SFO2S18   WALTZ16
SFO2S19   WALTZ16
SFO2S20   WALTZ16
SFO2S21   WALTZ16
SFO2S22   WALTZ16
SFO2S23   WALTZ16
SFO2S24   WALTZ16
SFO2S25   WALTZ16
SFO2S26   WALTZ16
SFO2S27   WALTZ16
SFO2S28   WALTZ16
SFO2S29   WALTZ16
SFO2S30   WALTZ16
SFO2S31   WALTZ16
SFO2S32   WALTZ16
SFO2S33   WALTZ16
SFO2S34   WALTZ16
SFO2S35   WALTZ16
SFO2S36   WALTZ16
SFO2S37   WALTZ16
SFO2S38   WALTZ16
SFO2S39   WALTZ16
SFO2S40   WALTZ16
SFO2S41   WALTZ16
SFO2S42   WALTZ16
SFO2S43   WALTZ16
SFO2S44   WALTZ16
SFO2S45   WALTZ16
SFO2S46   WALTZ16
SFO2S47   WALTZ16
SFO2S48   WALTZ16
SFO2S49   WALTZ16
SFO2S50   WALTZ16

***** GRADIENT CHANNEL *****
G1        1000.00 usec
G1A1      20.0000000 MHz
G1A2      20.0000000 MHz
G1A3      20.0000000 MHz
G1A4      20.0000000 MHz
G1A5      20.0000000 MHz
G1A6      20.0000000 MHz
G1A7      20.0000000 MHz
G1A8      20.0000000 MHz
G1A9      20.0000000 MHz
G1A10     20.0000000 MHz
G1A11     20.0000000 MHz
G1A12     20.0000000 MHz
G1A13     20.0000000 MHz
G1A14     20.0000000 MHz
G1A15     20.0000000 MHz
G1A16     20.0000000 MHz
G1A17     20.0000000 MHz
G1A18     20.0000000 MHz
G1A19     20.0000000 MHz
G1A20     20.0000000 MHz
G1A21     20.0000000 MHz
G1A22     20.0000000 MHz
G1A23     20.0000000 MHz
G1A24     20.0000000 MHz
G1A25     20.0000000 MHz
G1A26     20.0000000 MHz
G1A27     20.0000000 MHz
G1A28     20.0000000 MHz
G1A29     20.0000000 MHz
G1A30     20.0000000 MHz
G1A31     20.0000000 MHz
G1A32     20.0000000 MHz
G1A33     20.0000000 MHz
G1A34     20.0000000 MHz
G1A35     20.0000000 MHz
G1A36     20.0000000 MHz
G1A37     20.0000000 MHz
G1A38     20.0000000 MHz
G1A39     20.0000000 MHz
G1A40     20.0000000 MHz
G1A41     20.0000000 MHz
G1A42     20.0000000 MHz
G1A43     20.0000000 MHz
G1A44     20.0000000 MHz
G1A45     20.0000000 MHz
G1A46     20.0000000 MHz
G1A47     20.0000000 MHz
G1A48     20.0000000 MHz
G1A49     20.0000000 MHz
G1A50     20.0000000 MHz

***** Processing parameters *****
SF        150.9380159 MHz
WDW       EM
SSB       0
GB        0
PC        0
PC2       0
PC3       0
PC4       0
PC5       0
PC6       0
PC7       0
PC8       0
PC9       0
PC10      0
PC11      0
PC12      0
PC13      0
PC14      0
PC15      0
PC16      0
PC17      0
PC18      0
PC19      0
PC20      0
PC21      0
PC22      0
PC23      0
PC24      0
PC25      0
PC26      0
PC27      0
PC28      0
PC29      0
PC30      0
PC31      0
PC32      0
PC33      0
PC34      0
PC35      0
PC36      0
PC37      0
PC38      0
PC39      0
PC40      0
PC41      0
PC42      0
PC43      0
PC44      0
PC45      0
PC46      0
PC47      0
PC48      0
PC49      0
PC50      0
PC51      0
PC52      0
PC53      0
PC54      0
PC55      0
PC56      0
PC57      0
PC58      0
PC59      0
PC60      0
PC61      0
PC62      0
PC63      0
PC64      0
PC65      0
PC66      0
PC67      0
PC68      0
PC69      0
PC70      0
PC71      0
PC72      0
PC73      0
PC74      0
PC75      0
PC76      0
PC77      0
PC78      0
PC79      0
PC80      0
PC81      0
PC82      0
PC83      0
PC84      0
PC85      0
PC86      0
PC87      0
PC88      0
PC89      0
PC90      0
PC91      0
PC92      0
PC93      0
PC94      0
PC95      0
PC96      0
PC97      0
PC98      0
PC99      0
PC100     0
```



Current Data Parameters  
Name: Ole\_Tietzq  
Date\_: 2013-09-23  
PROBHD: 5 mm PABBO BB/  
PULPROG: zgpg30  
SOLVENT: DMSO  
NS: 10000  
DS: 36231.88 Hz  
SWH: 120.0000000 MHz  
FIDRES: 0.552865 Hz  
AQ: 0.9043568 sec  
RG: 180.12  
DW: 13.800 usec  
DE: 1.000 usec  
TE: 296.0 K  
CNS12: 145.0000000  
CNS112: 1.5000000 sec  
D1: 0.0034828 sec  
D2: 0.0034828 sec  
D12: 0.0002000 sec  
D16: 0.0002000 sec  
TD0: 1

===== CHANNEL F1 =====  
SFO1: 130.9531058 MHz  
NUC1: <sup>13</sup>C  
P13: 11.50 usec  
PL13: 0 W  
PL10: 2000.00 usec  
PREAMP1: 120.0000000 W  
SFOALS1: CPDPRG00  
SFOFFS1: 0 Hz  
SFOFF5: 0 Hz  
SPR5: 24.2799519 W

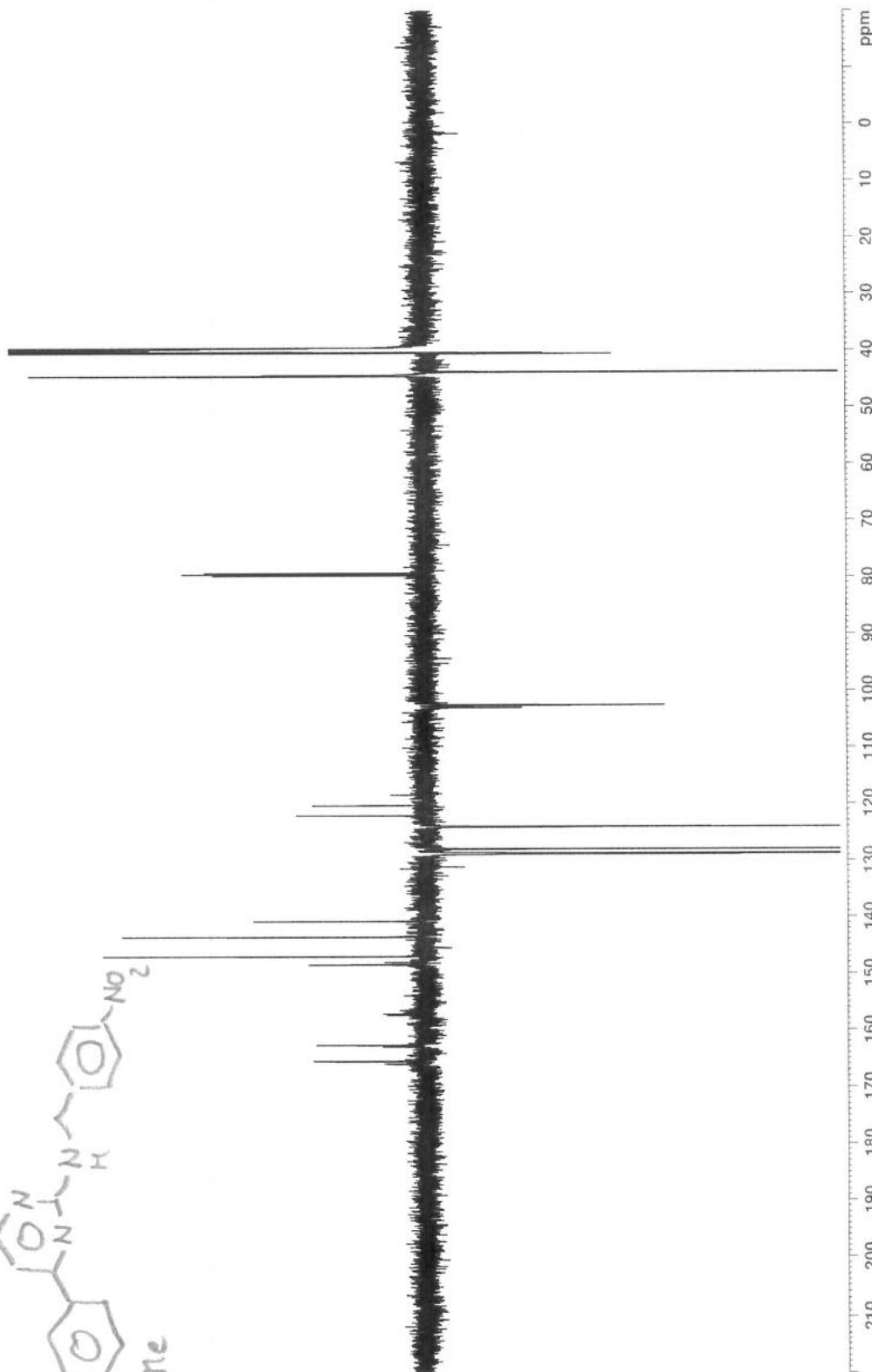
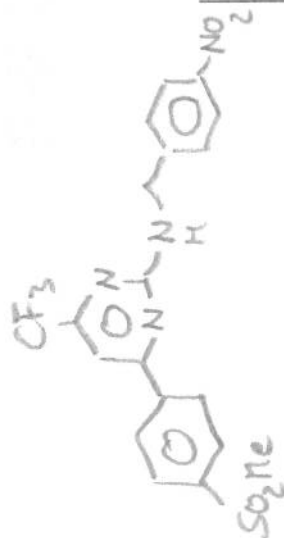
===== CHANNEL F2 =====  
SFO2: 600.2719197 MHz  
NUC2: <sup>1</sup>H  
P12: 13.40 usec  
PL12: 0 W  
PL14: 26.80 usec  
P14: 26.80 usec  
P16: 1000.00 usec  
P16: 1000.00 usec

===== GRADIENT CHANNEL =====  
GNDM1: 100.0000000 MHz  
GNDM2: 100.0000000 MHz  
GNDM3: 100.0000000 MHz  
GNDM4: 100.0000000 MHz  
GNDM5: 100.0000000 MHz  
GNDM6: 100.0000000 MHz  
GNDM7: 100.0000000 MHz  
GNDM8: 100.0000000 MHz  
GNDM9: 100.0000000 MHz  
GNDM10: 100.0000000 MHz  
GNDM11: 100.0000000 MHz  
GNDM12: 100.0000000 MHz  
GNDM13: 100.0000000 MHz  
GNDM14: 100.0000000 MHz  
GNDM15: 100.0000000 MHz  
GNDM16: 100.0000000 MHz  
GNDM17: 100.0000000 MHz  
GNDM18: 100.0000000 MHz  
GNDM19: 100.0000000 MHz  
GNDM20: 100.0000000 MHz  
GNDM21: 100.0000000 MHz  
GNDM22: 100.0000000 MHz  
GNDM23: 100.0000000 MHz  
GNDM24: 100.0000000 MHz  
GNDM25: 100.0000000 MHz  
GNDM26: 100.0000000 MHz  
GNDM27: 100.0000000 MHz  
GNDM28: 100.0000000 MHz  
GNDM29: 100.0000000 MHz  
GNDM30: 100.0000000 MHz  
GNDM31: 100.0000000 MHz  
GNDM32: 100.0000000 MHz  
GNDM33: 100.0000000 MHz  
GNDM34: 100.0000000 MHz  
GNDM35: 100.0000000 MHz  
GNDM36: 100.0000000 MHz  
GNDM37: 100.0000000 MHz  
GNDM38: 100.0000000 MHz  
GNDM39: 100.0000000 MHz  
GNDM40: 100.0000000 MHz  
GNDM41: 100.0000000 MHz  
GNDM42: 100.0000000 MHz  
GNDM43: 100.0000000 MHz  
GNDM44: 100.0000000 MHz  
GNDM45: 100.0000000 MHz  
GNDM46: 100.0000000 MHz  
GNDM47: 100.0000000 MHz  
GNDM48: 100.0000000 MHz  
GNDM49: 100.0000000 MHz  
GNDM50: 100.0000000 MHz  
GNDM51: 100.0000000 MHz  
GNDM52: 100.0000000 MHz  
GNDM53: 100.0000000 MHz  
GNDM54: 100.0000000 MHz  
GNDM55: 100.0000000 MHz  
GNDM56: 100.0000000 MHz  
GNDM57: 100.0000000 MHz  
GNDM58: 100.0000000 MHz  
GNDM59: 100.0000000 MHz  
GNDM60: 100.0000000 MHz  
GNDM61: 100.0000000 MHz  
GNDM62: 100.0000000 MHz  
GNDM63: 100.0000000 MHz  
GNDM64: 100.0000000 MHz  
GNDM65: 100.0000000 MHz  
GNDM66: 100.0000000 MHz  
GNDM67: 100.0000000 MHz  
GNDM68: 100.0000000 MHz  
GNDM69: 100.0000000 MHz  
GNDM70: 100.0000000 MHz  
GNDM71: 100.0000000 MHz  
GNDM72: 100.0000000 MHz  
GNDM73: 100.0000000 MHz  
GNDM74: 100.0000000 MHz  
GNDM75: 100.0000000 MHz  
GNDM76: 100.0000000 MHz  
GNDM77: 100.0000000 MHz  
GNDM78: 100.0000000 MHz  
GNDM79: 100.0000000 MHz  
GNDM80: 100.0000000 MHz  
GNDM81: 100.0000000 MHz  
GNDM82: 100.0000000 MHz  
GNDM83: 100.0000000 MHz  
GNDM84: 100.0000000 MHz  
GNDM85: 100.0000000 MHz  
GNDM86: 100.0000000 MHz  
GNDM87: 100.0000000 MHz  
GNDM88: 100.0000000 MHz  
GNDM89: 100.0000000 MHz  
GNDM90: 100.0000000 MHz  
GNDM91: 100.0000000 MHz  
GNDM92: 100.0000000 MHz  
GNDM93: 100.0000000 MHz  
GNDM94: 100.0000000 MHz  
GNDM95: 100.0000000 MHz  
GNDM96: 100.0000000 MHz  
GNDM97: 100.0000000 MHz  
GNDM98: 100.0000000 MHz  
GNDM99: 100.0000000 MHz  
GNDM100: 100.0000000 MHz

F2 - Processing Parameters  
SI: 32768  
SF: 150.9801200 MHz  
WDW: EM  
SSB: 0  
GB: 0  
CB: 6  
PC: 1.40

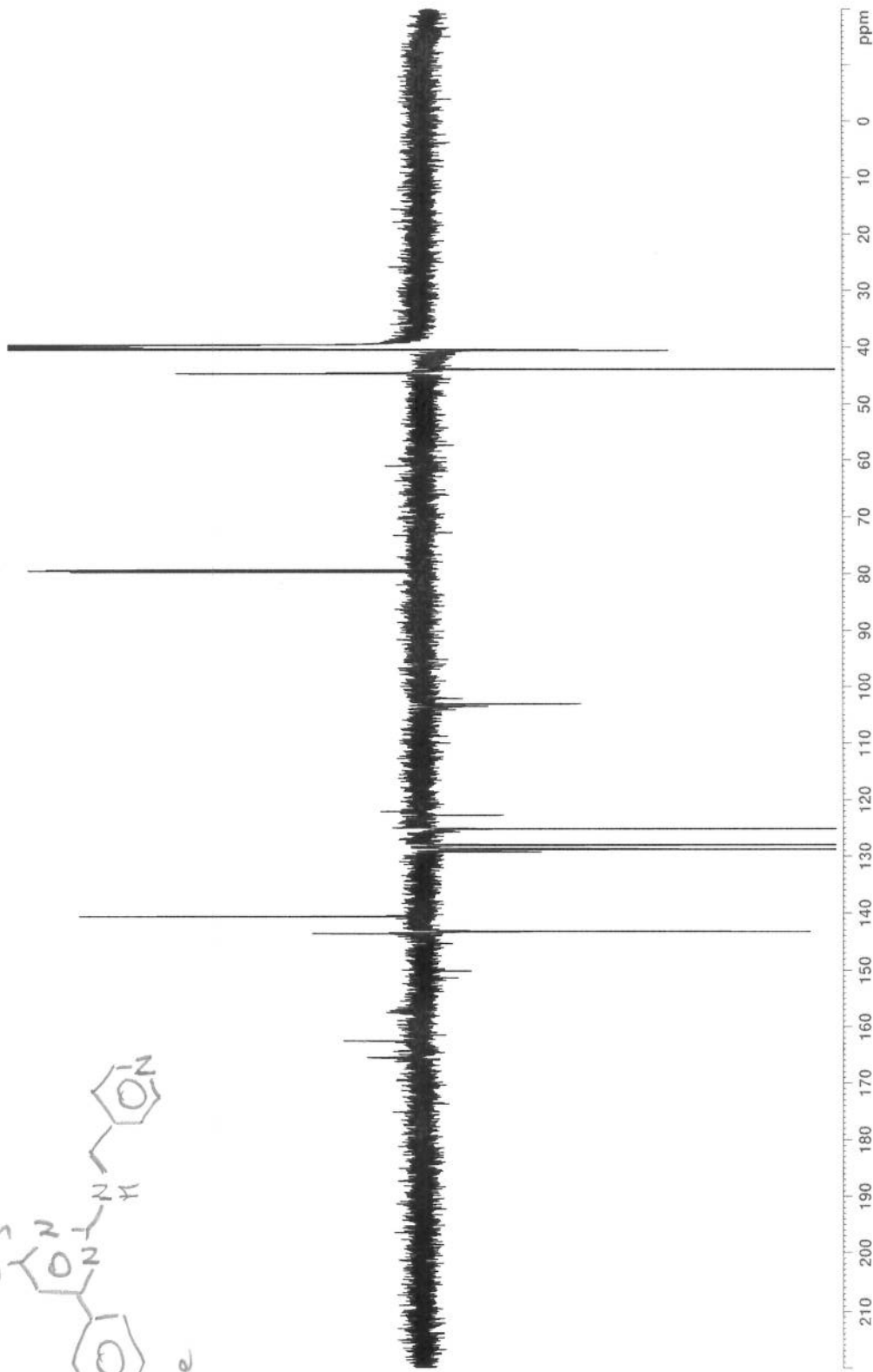
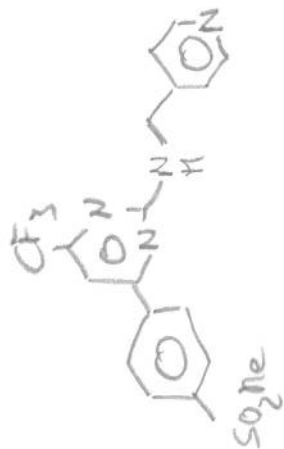
Ole Tietz: Deptq on OtPY-P111  
CPP\_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 31

<sup>13</sup>C-NMR (CDCl<sub>3</sub>) compound 1j





Ole Tietz: Deptq on OtPY-Pl15  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 32



```
Current Data Parameters
AcqDate Sep19_2013
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130828
Time 8:28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 10000
DS 4
SWH 36231.885 MHz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 180.12
DB 136.50 ussec
DE 6.50 ussec
TE 296.0 K
LNUST2 145.0000000
NUST12 145.0000000
D1 2.0000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

***** CHANNEL f1 *****
SFO1 150.9531095 MHz
P1C1 11.50 ussec
P13 2000.00 ussec
PLM0 0 W
SFOALS1 0.00000000 W
SFOALS5 CFC60000.4
SFOALS 0.500
SFOFFS 0 Hz
SWS 24.24799915 W

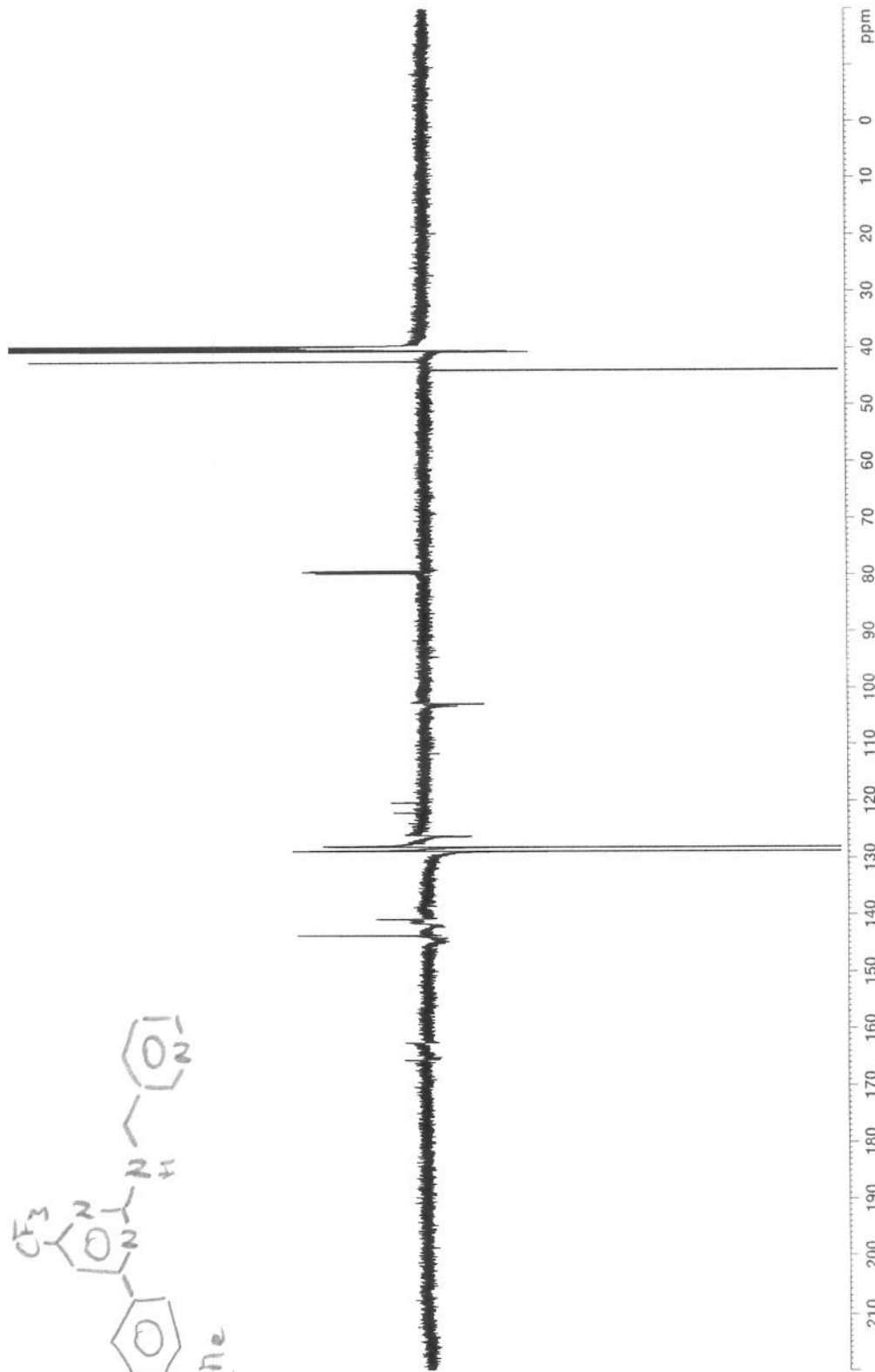
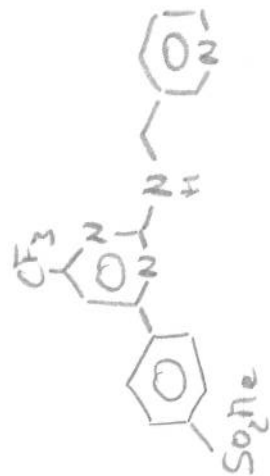
***** CHANNEL f2 *****
SFO2 600.2719197 MHz
NUC2 13
PCPRG12 waltz16
P3 25.10 ussec
P4 12.40 ussec
P5 26.60 ussec
PLM2 21.29899924 W
PLM12 0.78652999 W

***** GRADIENT CHANNEL *****
GNUM1 21
GNUM21 1
GNUM131 SMO10.100
GPN1 31.00 %
GPN2 31.00 %
GPN3 31.00 %
GPN4 31.00 %
GPN5 1000.00 ussec

F2 - Processing parameters
SF 150.9380120 MHz
WDW EM
SSB 0
GB 0
PC 1.40
```

$^{13}\text{C}$ -NMR ( $d_6$ -DMSO) compound 1b

Ole Tietz: Deptq on OtPY-P116  
CPP\_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 33

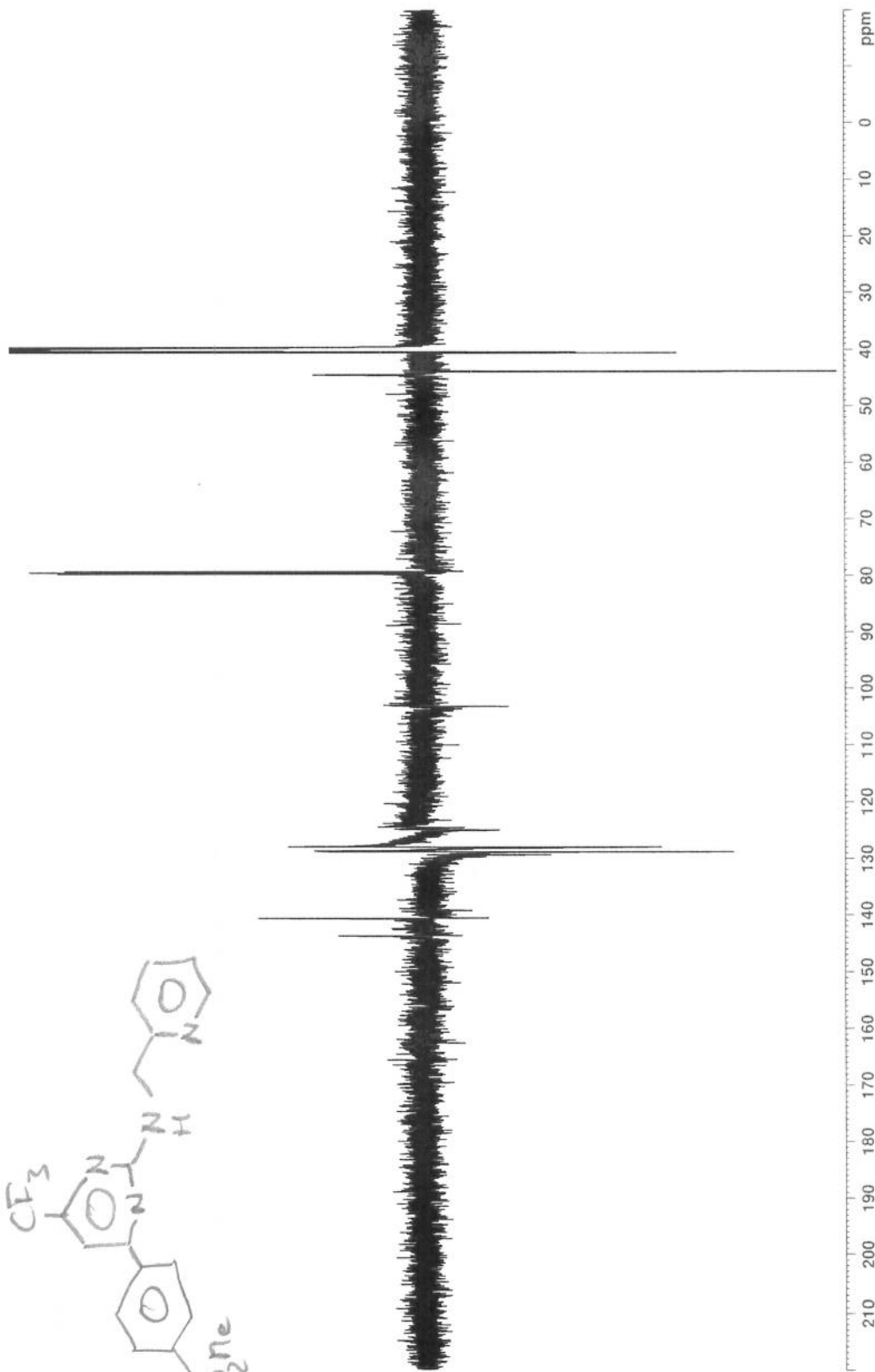
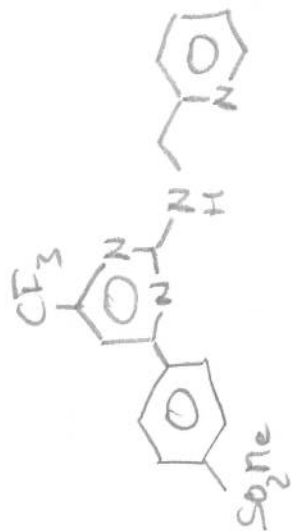


```
Current Date Parameters
Date_   Sep19-2013
EXPNO   4.0
PROCNO  1
F2 - Acquisition Parameters
Date_   20130920
Time    17.03
INSTRUM spect
PROBHD  5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT DMSO
NS       10000
DS       4
SWH      36231.883 Hz
FIDRES   0.552855 Hz
AQ       0.9643968 sec
RG       180.00
SR       13.40 usec
SB       6.50 usec
TE       296.0 K
CNS2     145.000000
D1        1.00
D2        2.00000000 sec
D3        0.0034428 sec
D4        0.0002000 sec
D5        0.0002000 sec
D6        0.0002000 sec
D7        0.0002000 sec
D8        0.0002000 sec
D9        0.0002000 sec
D10       0.0002000 sec
===== CHANNEL f1 =====
NUC1      13C
P1        150.999108 MHz
PCPD1    11.50 usec
PL1       0 W
PL2       2000.00 usec
PL3       0 W
PL4       20.00000000 M
SFOALS1  CFF60comp.4
SFOALS2  0.500
SFOALS3  0 Hz
SFOALS4  24.24199919 W
===== CHANNEL f2 =====
NUC2      13C
P2        600.2719197 MHz
PCPD2    11.50 usec
PL2       0 W
PL3       20.10 usec
PL4       13.40 usec
PL5       26.80 usec
PL6       21.39999954 usec
PL7       0.78053999 M
===== GRABBER CHANNEL =====
GRAB1     13C
GRAB2     13C
GRAB3     13C
GRAB4     13C
GRAB5     13C
GRAB6     13C
GRAB7     13C
GRAB8     13C
GRAB9     13C
GRAB10    13C
GRAB11    13C
GRAB12    13C
===== Processing Parameters =====
SI        32768
SF        150.9980120 MHz
WDW       EM
SSB       0
GB        0
CB        0
PC        1.40
```



Ole Iietz: Deptg on OtPY-P117  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 34

<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 1m

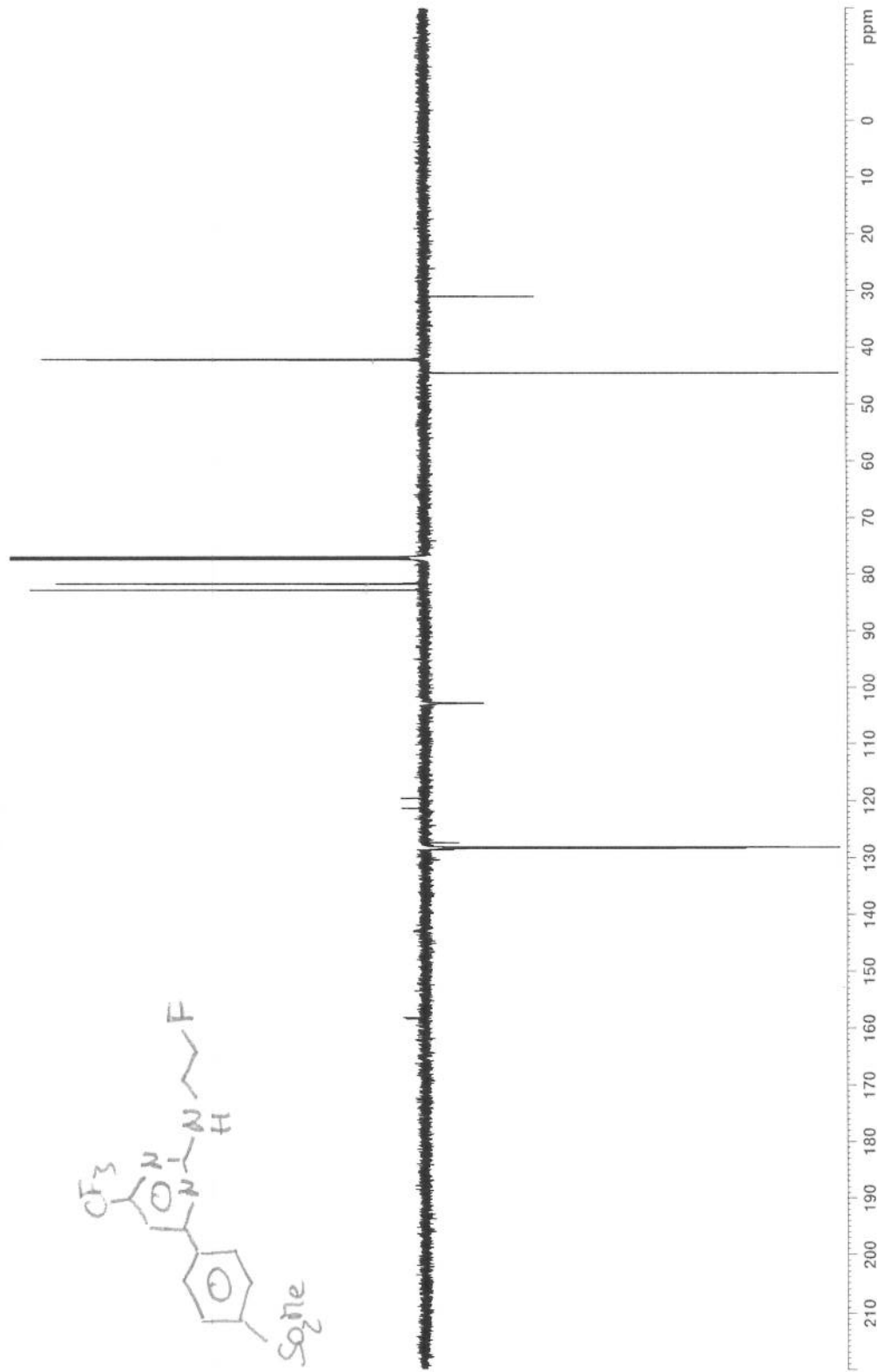
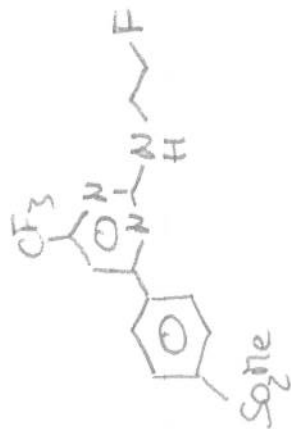


```
Current Data Parameters
Date_   Sep19-2013
EXPNO   1
PROCNO   1
F2 - Acquisition Parameters
Date_   20130919
Time    11:15
INSTRUM spect
PROBHD  5 mm PARBO BB7
PULPROG zgpg30
DELTA   8.8536
SOLVENT DMSO
NS       10000
DS       4
SWH      36231.863 MHz
FIDRES   0.552855 Hz
AQ       0.9843968 sec
RG       180.12
DE       6.50 ussec
TE       296.0 K
CNS22    145.000000
INST12   150.951098 MHz
D1       2.0000000 sec
D2       0.00344828 sec
D12      0.0000200 sec
T1       1.16
T16      0.0002000 sec
T166     1
===== CHANNEL f1 =====
SFO1     150.951098 MHz
NUC1     13C
P1C1     11.50 ussec
PL1      0 W
PL12     2000.00 ussec
SFOALS   0 Hz
SFOALS1  C15160000.4 M
SFOALS2  0.500
SFOFFS   0 Hz
SWS      24.24799819 M
===== CHANNEL f2 =====
SFO2     600.271517 MHz
NUC2     1H
P1C2     18.00 ussec
PL12     20.10 ussec
PL2      0 W
PL22     13.50 ussec
PL23     26.40 ussec
PL24     21.9999972 M
PL25     0.76053999 M
===== GRABF1 CHANNEL =====
GPNAM1   1
SFO1     150.951098 MHz
SFO2     600.271517 MHz
GPNAM2   2
SFO2     600.271517 MHz
GPNAM3   3
SFO3     150.951098 MHz
GPNAM4   4
SFO4     150.951098 MHz
GPNAM5   5
SFO5     150.951098 MHz
GPNAM6   6
SFO6     150.951098 MHz
GPNAM7   7
SFO7     150.951098 MHz
GPNAM8   8
SFO8     150.951098 MHz
GPNAM9   9
SFO9     150.951098 MHz
GPNAM10  10
SFO10    150.951098 MHz
GPNAM11  11
SFO11    150.951098 MHz
GPNAM12  12
SFO12    150.951098 MHz
GPNAM13  13
SFO13    150.951098 MHz
GPNAM14  14
SFO14    150.951098 MHz
GPNAM15  15
SFO15    150.951098 MHz
GPNAM16  16
SFO16    150.951098 MHz
F2 - Processing parameters
SI       32768
SF       150.9380120 MHz
WDW      EM
SSB      0
GB       0
PC       1.40
```



<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound in

Ole Tietz: Deptg on OTPY-P118  
 CPP\_Deptg.A CDCI3 {C:\Bruker\TopSpin3.2} vishwa 23



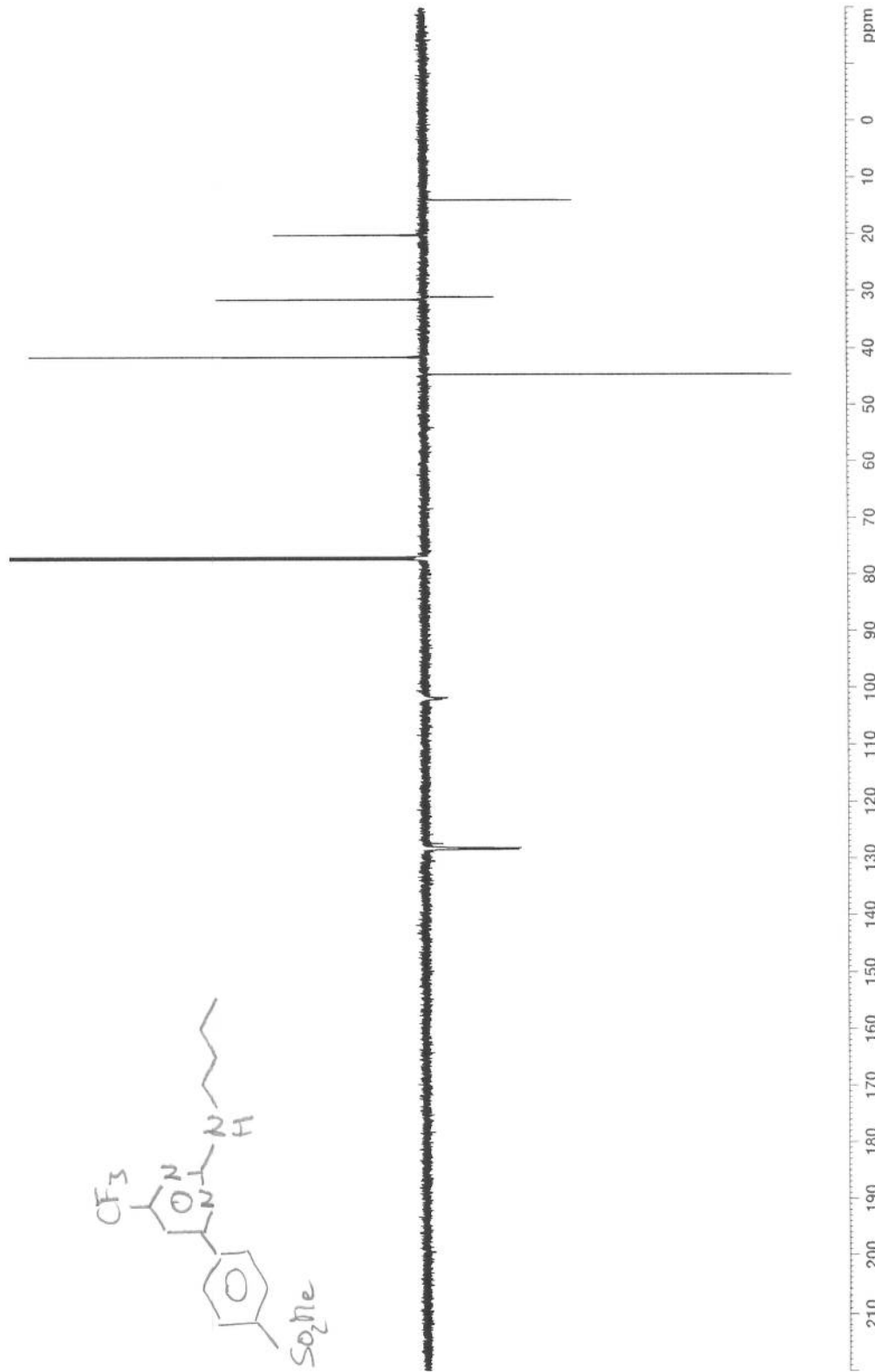
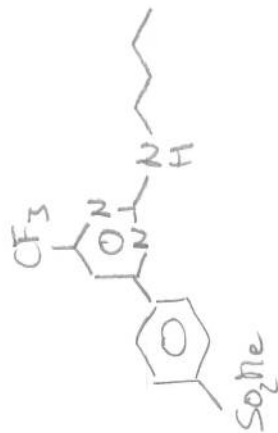
```

Current Data Parameters
NAME      Sep12-2013
EXPNO    61
PROCNO   1
=====
F2 - Acquisition Parameters
Date_    20130713
Time     11.43
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
DELTA    0.00100000 sec
SOLVENT DMSO
NS       5000
DS       4
SWH      36231.864 Hz
FIDRES   0.3515865 Hz
AQ        0.9645965 sec
RG        186.12
AQ        13.800 usec
SFO1      125.760 MHz
TE        296.20 K
=====
CHN12     145.0000000
CHN112    1.5000000 sec
D1        0.00010000 sec
D2        0.0014828 sec
D12       0.00002000 sec
D16       0.00020000 sec
TD0       1
=====
===== CHANNEL f1 =====
SFO1      125.76000000 MHz
NUC1      13C
P1        12.00 usec
PL1       0.00 dB
PL12      0.00 dB
PL13      0.00 dB
PL14      0.00 dB
PL15      0.00 dB
PL16      0.00 dB
PL17      0.00 dB
PL18      0.00 dB
PL19      0.00 dB
PL20      0.00 dB
PL21      0.00 dB
PL22      0.00 dB
PL23      0.00 dB
PL24      0.00 dB
PL25      0.00 dB
PL26      0.00 dB
PL27      0.00 dB
PL28      0.00 dB
PL29      0.00 dB
PL30      0.00 dB
===== CHANNEL f2 =====
SFO2      600.2719197 MHz
NUC2      1H
P2        12.00 usec
PL2       0.00 dB
PL22      0.00 dB
PL23      0.00 dB
PL24      0.00 dB
PL25      0.00 dB
PL26      0.00 dB
PL27      0.00 dB
PL28      0.00 dB
PL29      0.00 dB
PL30      0.00 dB
===== GRADIENT CHANNEL =====
GRAD1[1]  SM010.100
GRAD1[2]  SM010.100
GRAD1[3]  SM010.100
GRAD1[4]  SM010.100
GRAD1[5]  SM010.100
GRAD1[6]  SM010.100
GRAD1[7]  SM010.100
GRAD1[8]  SM010.100
GRAD1[9]  SM010.100
GRAD1[10] SM010.100
=====
F2 - Processing parameters
SI        32768
SF        125.76000000 MHz
WDW       EM
SSB       0
LB        0
GB        0
PC        1.00 Hz
=====
PC        0
PC2       1.40
    
```



<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 10

Ole Tietz: Deptq on OTPY-P119  
CPP\_Deptq.A CDC13 {C:\Bruker\TopSpin3.2} vishwa 24



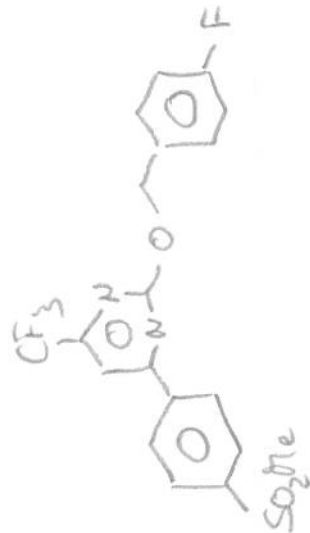
```
Current: Date Parameters
Name      Sept17-2013
PROBHD    5 mm PABBO BB/
PROCNO    1
=====
F2 - Acquisition Parameters
File      20130917
Time      12:47
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
SOLVENT   DMSO-d6
NS         5000
DS         4
SFO1       125.761 MHz
FIDRES     0.452865 Hz
AQ         0.9043668 sec
RG         180.12
CW         13.500 usec
TE         296.0 K
=====
Channel 1
=====
SFO1       125.761058 MHz
NUC1       13C
P1         12.00 usec
PL1        0 W
PL12       11.40 usec
PL13       2000.00 usec
PL14       0 W
PL15       120.0000000 W
SFO2       400.2719197 MHz
SFO2S      0 Hz
SFO2S5     0 Hz
SFO2S6     0.500
SFO2S7     24.24759919 W
=====
Channel 2
=====
SFO2       400.2719197 MHz
NUC2       1H
P2         12.00 usec
PL2        0 W
PL22       23.10 usec
PL23       13.40 usec
PL24       26.80 usec
PL25       1000.00 usec
PL26       31.0000000 W
PL27       0.76053999 W
=====
GRABENT CHANNEL
=====
SFO1       125.761058 MHz
SFO2       400.2719197 MHz
SFO2S      0 Hz
SFO2S5     0.500
SFO2S6     0.500
SFO2S7     24.24759919 W
=====
Processing parameters
SI         32768
SF         150.92601200 MHz
RG         0
WDW         EM
SSB         0
CB         0
GB         0
PC         1.40
```



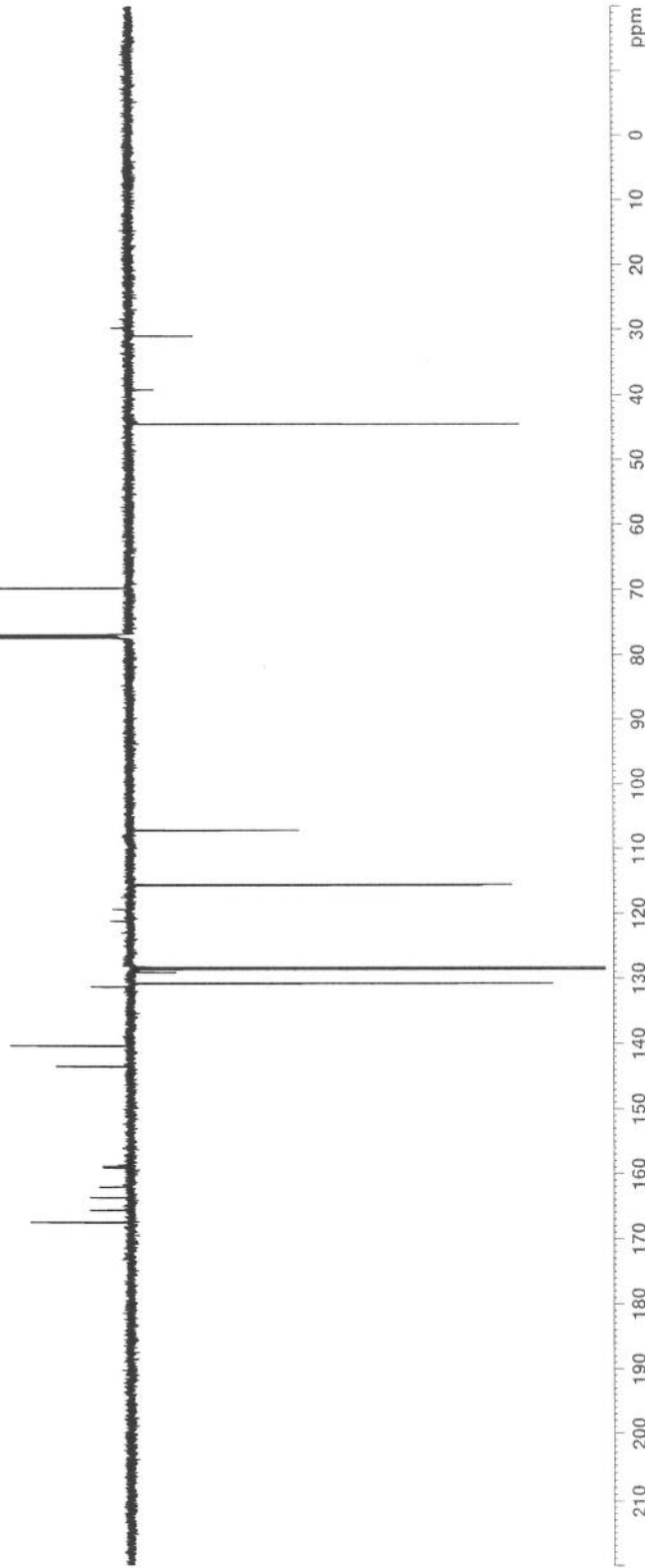


Ole Tietz: Deptq on OTPY-P130  
CPP\_Deptq.A CDCl3 (C:\Bruker\TopSpin3.2) vishwa 25

<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 3a



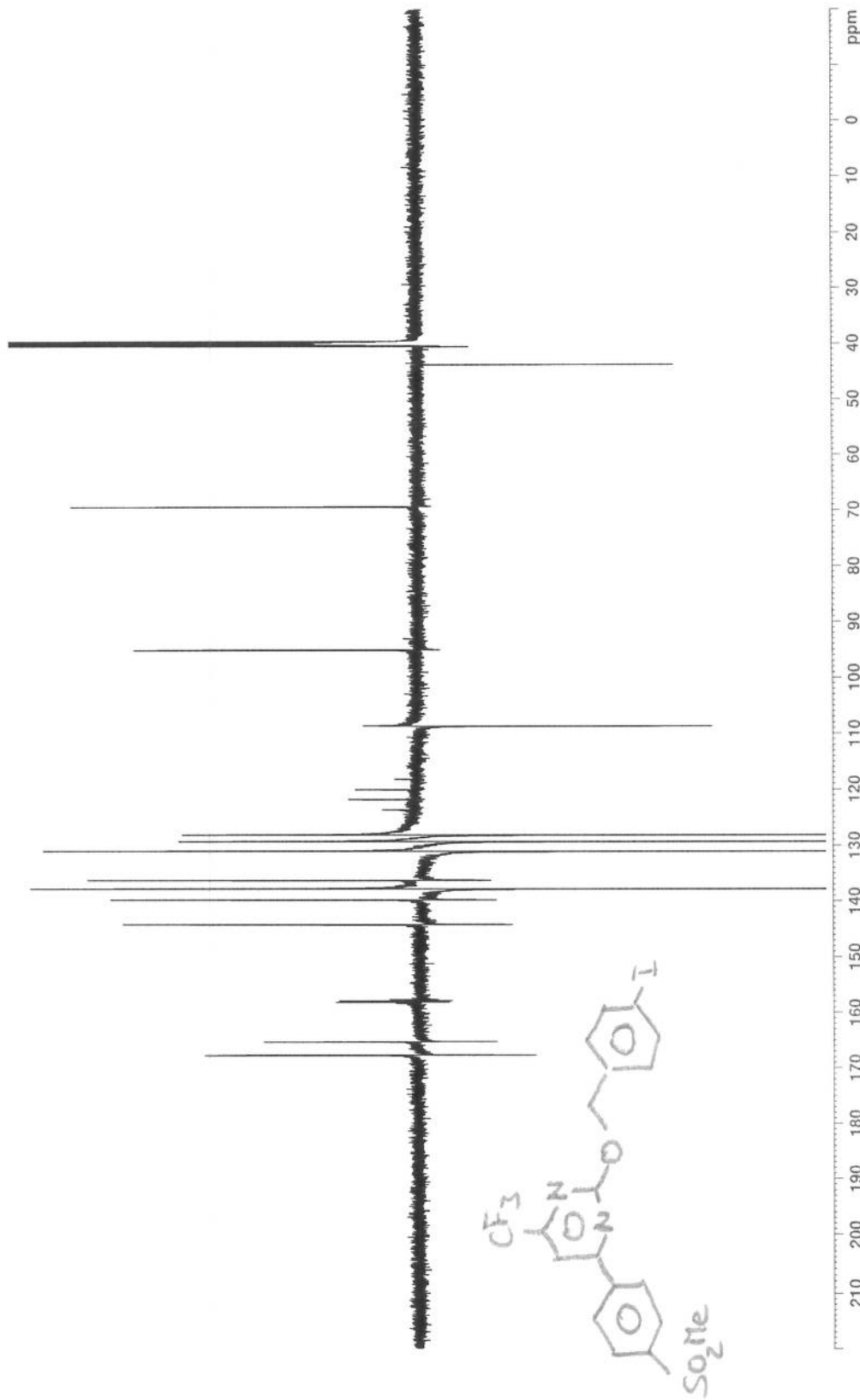
```
Current Data Parameters
Date_      Sep17-2013
Time_     01
PROCNO    1
F2 - Acquisition Parameters
Date_     20130917
Time_    12:37
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
SOLVENT   CDCl3
NS        5000
DS        4
SS        36731.88 Hz
AQ        0.552895 Hz
RG        0.9043668 sec
RG2       180.12
WDW        8.50 usec
SSB        13.00 usec
GB         0.50 usec
TE        296.0 K
CNS12     145.0000000
CNS112    2.0000000 sec
D2        0.00344828 sec
D12       0.00002000 sec
D16       0.00020000 sec
TD5       1
===== CHANNEL f1 =====
SFO1      150.9531058 MHz
NUC1      13
P13       11.40 usec
PL13     0 W
SFOA1(S) 120.0000000 W
SFOA1(S)  CTRF40.0 0.500
SFOFFS5   0 Hz
SFOFFS5   24.24799919 W
===== CHANNEL f2 =====
SFO2      800.2719197 MHz
NUC2      1H
P12       12.40 usec
PL12     0 W
SFOA2(S)  12.40 usec
SFOA2(S)  26.80 usec
SFOFFS2   0 Hz
SFOFFS2   21.29899999 usec
SFOFFS2   0.78553599 W
===== GRADIENT CHANNEL =====
GPM1(S)   150.9531058 MHz
GPM2(S)   800.2719197 MHz
GPM3(S)   150.9531058 MHz
GPM4(S)   800.2719197 MHz
GPM5(S)   150.9531058 MHz
GPM6(S)   800.2719197 MHz
GPM7(S)   150.9531058 MHz
GPM8(S)   800.2719197 MHz
GPM9(S)   150.9531058 MHz
GPM10(S)  800.2719197 MHz
GPM11(S)  150.9531058 MHz
GPM12(S)  800.2719197 MHz
===== Processing parameters =====
SF        150.9380120 MHz
RG        0
WDW        0
SSB        0
GB         0
PC        1.40
```





<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 10

Ole Tietz: Deptq on OTPY-P132  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 26

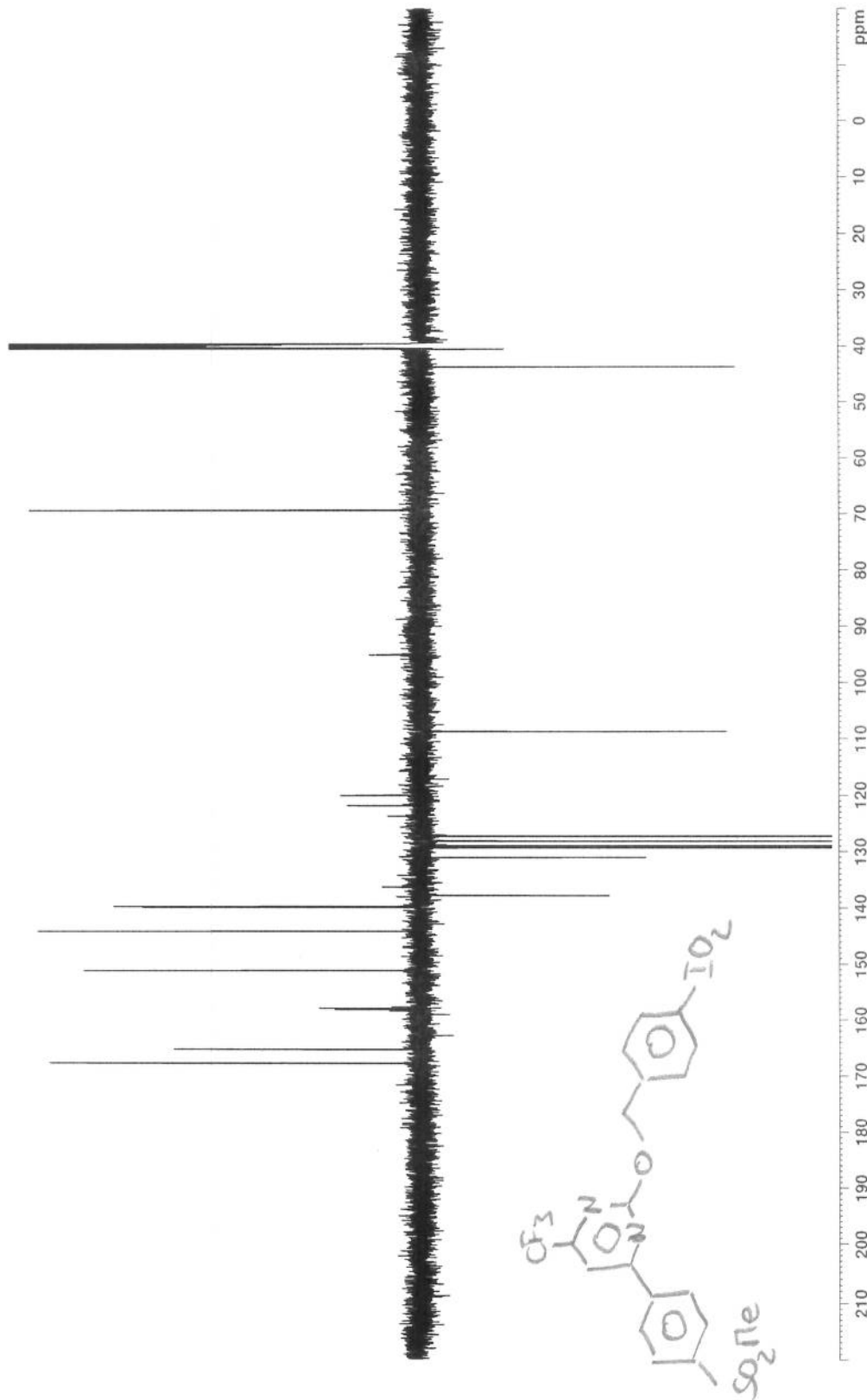


```
Current Data Parameters
Acq No.      1
Date_       Sept17_2013
Time        21:06
PROCNO     1
F2 - Acquisition Parameters
Date_      20130917
Time      21:06
INSTRUM   spect
PROBHD    5 mm PABBO-RE/
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS         5000
DS         4
AQ         36231.887 s
FIDRES    0.552855 Hz
AQ         0.9043968 sec
RG         180.12
WDW        EM
SSB        0
LB         13.600 usec
GB         0
TE         296.0 K
CONST     145.0000000
CNS11.2   1.0000000 sec
D2         2.0000000 sec
D12        0.00344828 sec
D16        0.00002000 sec
D18        0.00020000 sec
D19        0
===== CHANNEL F1 =====
SFO1      150.951058 MHz
NUC1      13
P1        11.50 usec
PL1       0 W
PL12      0.00000000 W
SFOA1(S)  CF360000.4
SFOA15    0.500
SFOF55    0 Hz
SFW5      24.24799519 W
===== CHANNEL F2 =====
SFO2      600.2719197 MHz
NUC2      1H
P2        19.00 usec
PL2       0 W
PL22      25.10 usec
P3        12.40 usec
P4        26.60 usec
P1202     21.298999524 usec
P1204     0.500
P1212     0.76553929 W
===== GRADIENT CHANNEL =====
GFM1A1    1.0000000 W
GFM1A2    1.0000000 W
GFM1A3    1.0000000 W
GFM1A4    1.0000000 W
GFM1A5    1.0000000 W
GFM1A6    1.0000000 W
GFM1A7    1.0000000 W
GFM1A8    1.0000000 W
GFM1A9    1.0000000 W
GFM1A10   1.0000000 W
===== Processing parameters =====
SI        150.9380120 MHz
WDW       EM
SSB       0
LB         1.00 Hz
GB         0
PC         1.40
```



<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 11

Ole Tietz: Deptq on OTPY-PI329  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 27

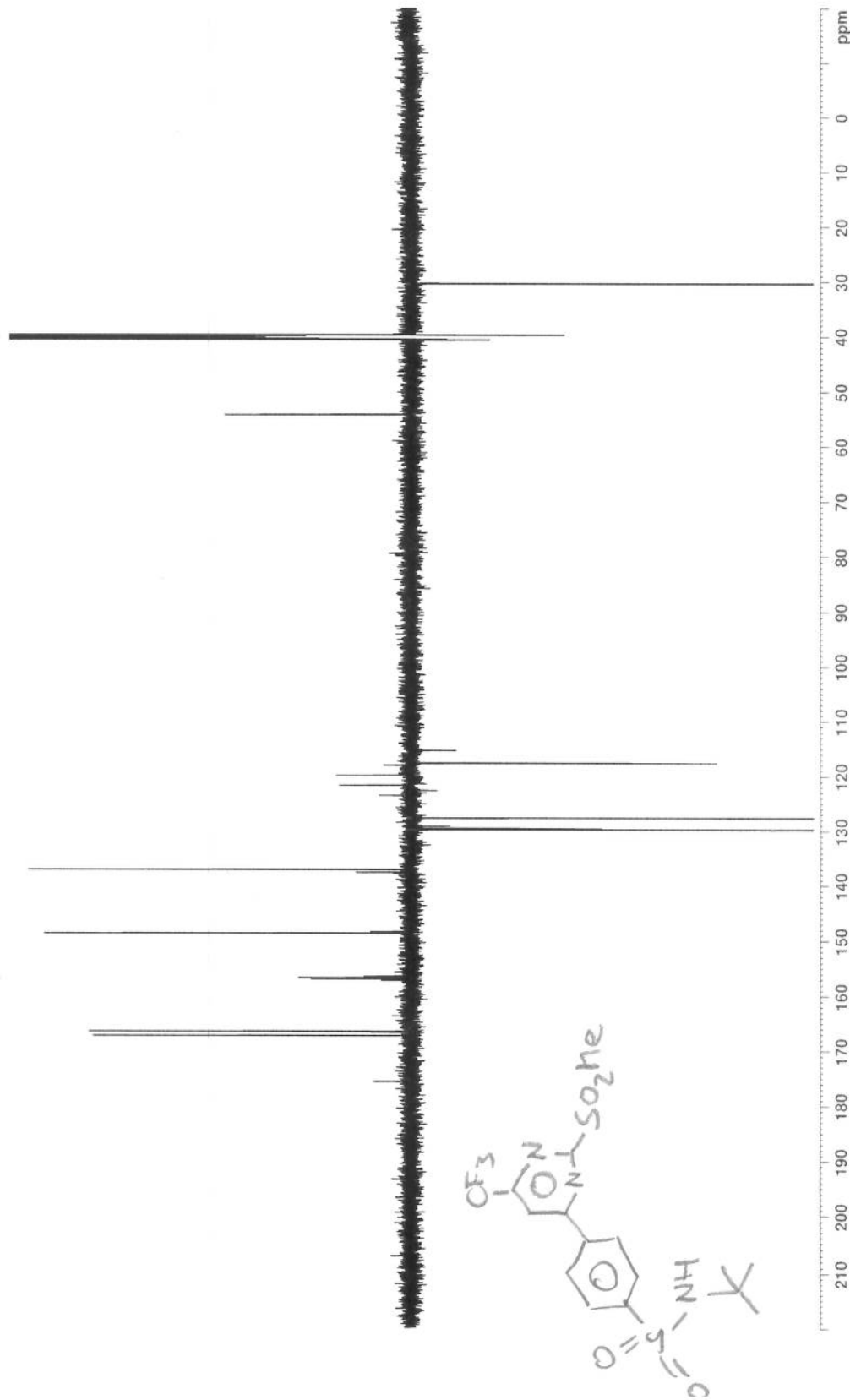


```
Current Data Parameters
Name      Sep17_2013
PROBHD    5 mm
PROBNG    5 mm
=====
F2 - Acquisition Parameters
=====
Date_     20130715
Time      11.40
INSTRUM   spect
PROBHD    5 mm
PULPROG   zgpg30
SOLVENT   DMSO
NS         5000
DS         4
AQ         36231.86 Hz
FIDRES    0.552865 Hz
AQ         0.9043648 sec
RG         180.12
AQ         132.60 usec
SFO2       100.620000 MHz
TE         296.0 K
CST2      145.0000000
CST12     1.5000000 sec
D1         0.0011828 sec
D2         0.0011828 sec
D12       0.0002000 sec
D16       0.0002000 sec
TD         100
===== CHANNEL f1 =====
SFO1      150.931028 MHz
NUC1      13C
P13       11.50 usec
PL1       0 W
SFO2      100.6200000 MHz
SFOALS    0.500
SFOFES    0 Hz
SFOFES5   24.2479919 W
===== CHANNEL f2 =====
SFO2      500.2719197 MHz
NUC2      1H
P2PRG2    waltz16
PL2       13.40 usec
PL3       13.40 usec
PL4       26.80 usec
PCPD2     21.8000000 usec
PLM12     0.7605299 W
===== GRADIENT CHANNEL =====
GUNIT1    GMR10.100
GUNIT2    GMR10.100
GUNIT3    GMR10.100
GMR10     31.00 A
GMR20     31.00 A
GMR30     31.00 A
P16       1000.00 usec
=====
F2 - Processing parameters
=====
SI         32768
SF         150.931028 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
```



<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compounds 8

Ole Tietz: Deptq on OTISA-II02x  
CPP\_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 28

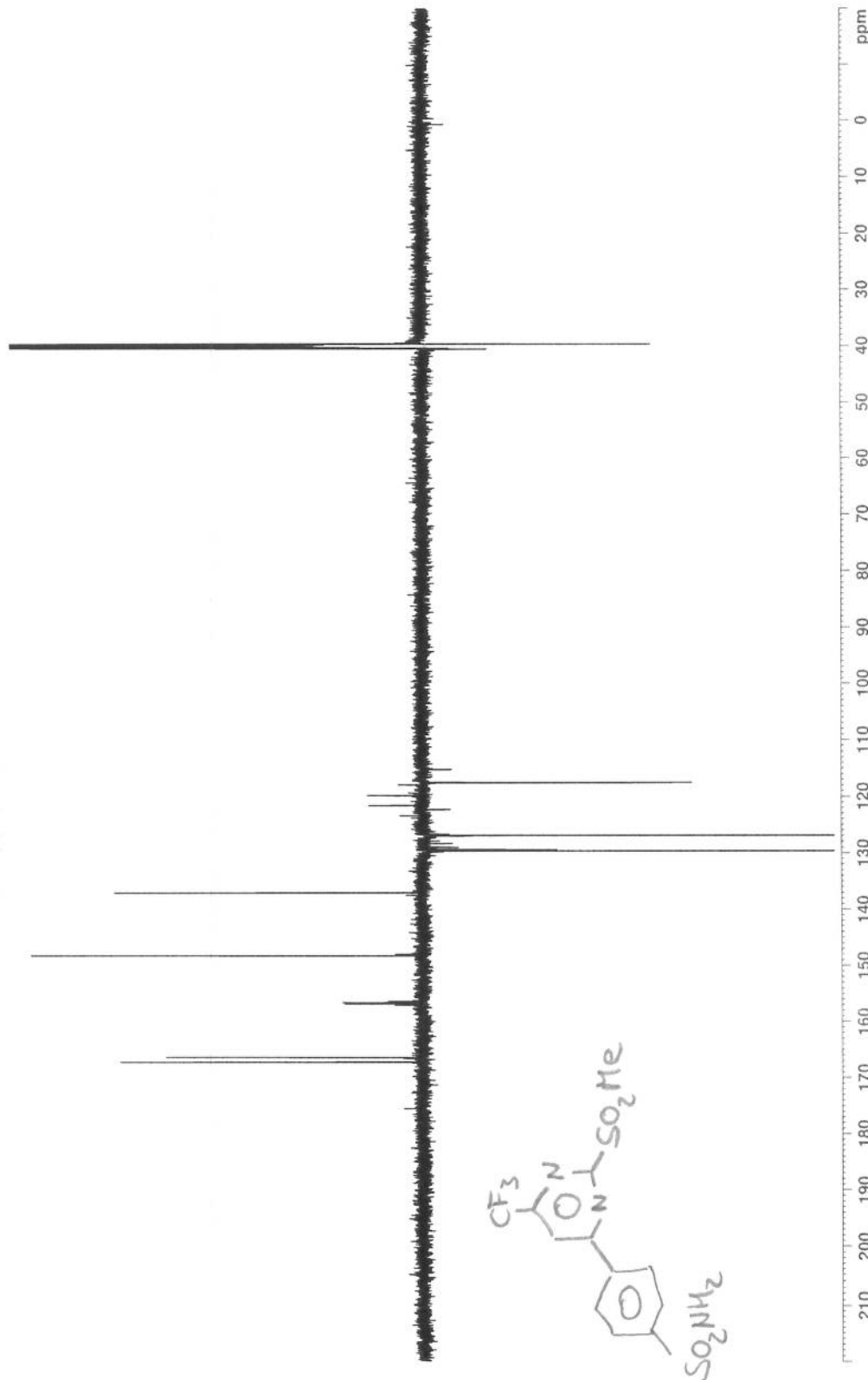


```
Current Data Parameters
NAME      Sep12_2013
PROCNO    111
=====
F2 - Acquisition Parameters
Acq_      20130714
Date_     20130714
Time      11:50
INSTRUM   spect
PROBHD    5 mm PABBO BBI
PULPROG   zgpg30
SOLVENT   DMSO
NS        5000
DS        4
SFO1      363.130 MHz
FIDRES    0.55285 MHz
AQ         0.9013965 sec
RG         180.12
WDW        13.800 usec
SSB        0
TE         296.2 K
CST2      145.000000
CNS112    1.500000 sec
D1         0.0034828 sec
D2         0.0034828 sec
D12        0.0002000 sec
D16        0.0002000 sec
TD0        1
===== CHANNEL f1 =====
SFO1      150.9531028 MHz
NUC1       13C
P13        11.50 usec
PL10       0 W
SFO2      120.0000000 MHz
SFOALS1    CFP0000000
SFOFFS1    0 Hz
SFOFFS2    0 Hz
SFOFFS3    24.2479919 MHz
===== CHANNEL f2 =====
SFO2      600.2719137 MHz
NUC2       1H
P2         12.50 usec
PL20       0 W
SFOFFS2    0 Hz
SFOFFS3    0 Hz
===== GRADIENT CHANNEL =====
GMR11     1000.00 usec
GMR12     1000.00 usec
GMR13     1000.00 usec
GMR14     1000.00 usec
GMR15     1000.00 usec
GMR16     1000.00 usec
GMR17     1000.00 usec
GMR18     1000.00 usec
GMR19     1000.00 usec
GMR20     1000.00 usec
=====
SF         150.9801320 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
=====
F2 - Processing Parameters
SFO1      150.9531028 MHz
SFO2      600.2719137 MHz
SF         150.9801320 MHz
WDW        EM
SSB        0
GB         0
PC         1.40
```



<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 9

Ole Tietz: Deptq on OTISA-IL03X  
CPP\_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 29

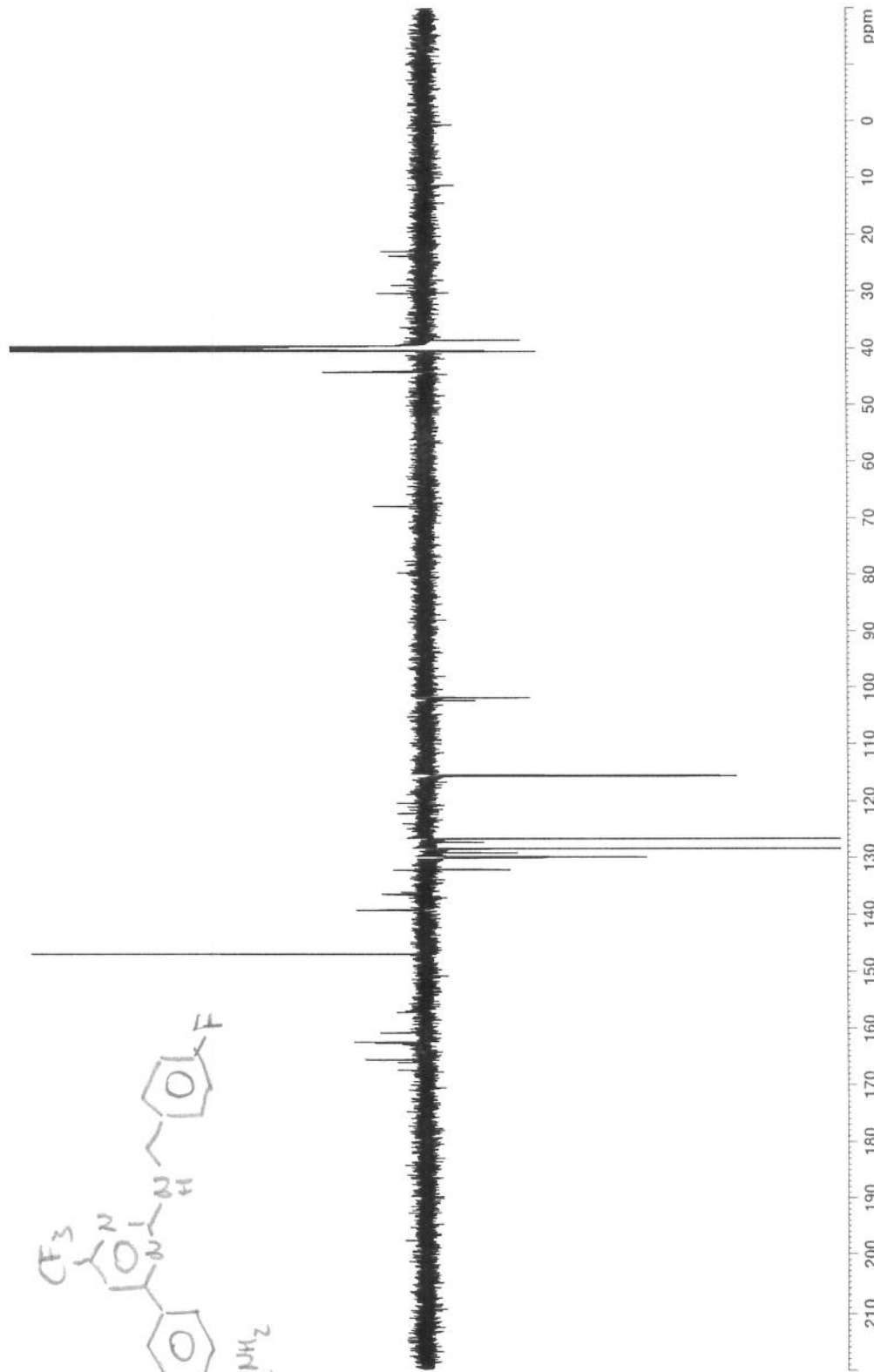
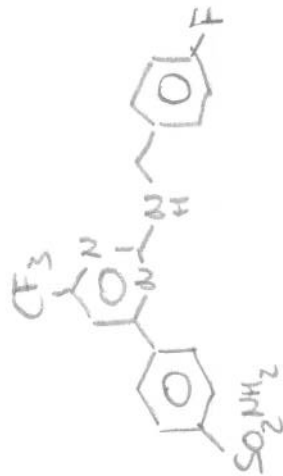


```
Current Data Parameters
Name      Sept2_2013
Date_    20130915
PROBHD   5 mm PABBO BH/
PULPROG  zgpg30
SOLVENT  DMSO
NS       5000
DS       4
SWH      36531.864 Hz
FIDRES   0.352861 Hz
AQ       0.9043968 sec
RG       180.12
DM       13.800 usec
DE       0.500 usec
TE       240.0 K
CNS1     145.0000000
CNS2     145.0000000
CNS12    1.5000000 sec
D1       0.0030000 sec
D2       0.0034828 sec
D12      0.0000200 sec
D16      0.0002000 sec
TD9      1
----- CHANNEL f1 -----
SFO1     150.951025 MHz
NUC1     13C
P13      11.50 usec
PL13     0 W
PL10     2000.00 usec
PL101    120.00000000 W
SFO1M1   CPDPRG000
SFO1M1S  0.500
SFOFFS5  0 Hz
SFW5     24.2479919 M
----- CHANNEL f2 -----
SFO2     600.2719197 MHz
NUC2     1H
PCPD12   40.00 usec
PCPD1    13.40 usec
P3       13.40 usec
P4       26.80 usec
PCPD2    31.00 usec
PCPD3    31.00 usec
PCPD4    31.00 usec
PCPD5    31.00 usec
PCPD6    31.00 usec
PCPD7    31.00 usec
PCPD8    31.00 usec
PCPD9    31.00 usec
PCPD10   31.00 usec
PCPD11   31.00 usec
PCPD12   31.00 usec
PCPD13   31.00 usec
PCPD14   31.00 usec
PCPD15   31.00 usec
PCPD16   31.00 usec
PCPD17   31.00 usec
PCPD18   31.00 usec
PCPD19   31.00 usec
PCPD20   31.00 usec
PCPD21   31.00 usec
PCPD22   31.00 usec
PCPD23   31.00 usec
PCPD24   31.00 usec
PCPD25   31.00 usec
PCPD26   31.00 usec
PCPD27   31.00 usec
PCPD28   31.00 usec
PCPD29   31.00 usec
PCPD30   31.00 usec
PCPD31   31.00 usec
PCPD32   31.00 usec
PCPD33   31.00 usec
PCPD34   31.00 usec
PCPD35   31.00 usec
PCPD36   31.00 usec
PCPD37   31.00 usec
PCPD38   31.00 usec
PCPD39   31.00 usec
PCPD40   31.00 usec
PCPD41   31.00 usec
PCPD42   31.00 usec
PCPD43   31.00 usec
PCPD44   31.00 usec
PCPD45   31.00 usec
PCPD46   31.00 usec
PCPD47   31.00 usec
PCPD48   31.00 usec
PCPD49   31.00 usec
PCPD50   31.00 usec
PCPD51   31.00 usec
PCPD52   31.00 usec
PCPD53   31.00 usec
PCPD54   31.00 usec
PCPD55   31.00 usec
PCPD56   31.00 usec
PCPD57   31.00 usec
PCPD58   31.00 usec
PCPD59   31.00 usec
PCPD60   31.00 usec
PCPD61   31.00 usec
PCPD62   31.00 usec
PCPD63   31.00 usec
PCPD64   31.00 usec
PCPD65   31.00 usec
PCPD66   31.00 usec
PCPD67   31.00 usec
PCPD68   31.00 usec
PCPD69   31.00 usec
PCPD70   31.00 usec
PCPD71   31.00 usec
PCPD72   31.00 usec
PCPD73   31.00 usec
PCPD74   31.00 usec
PCPD75   31.00 usec
PCPD76   31.00 usec
PCPD77   31.00 usec
PCPD78   31.00 usec
PCPD79   31.00 usec
PCPD80   31.00 usec
PCPD81   31.00 usec
PCPD82   31.00 usec
PCPD83   31.00 usec
PCPD84   31.00 usec
PCPD85   31.00 usec
PCPD86   31.00 usec
PCPD87   31.00 usec
PCPD88   31.00 usec
PCPD89   31.00 usec
PCPD90   31.00 usec
PCPD91   31.00 usec
PCPD92   31.00 usec
PCPD93   31.00 usec
PCPD94   31.00 usec
PCPD95   31.00 usec
PCPD96   31.00 usec
PCPD97   31.00 usec
PCPD98   31.00 usec
PCPD99   31.00 usec
PCPD100  31.00 usec
----- GRADIENT CHANNEL -----
GMR1     150.951025 MHz
GMR2     150.951025 MHz
GMR3     150.951025 MHz
GMR4     150.951025 MHz
GMR5     150.951025 MHz
GMR6     150.951025 MHz
GMR7     150.951025 MHz
GMR8     150.951025 MHz
GMR9     150.951025 MHz
GMR10    150.951025 MHz
GMR11    150.951025 MHz
GMR12    150.951025 MHz
GMR13    150.951025 MHz
GMR14    150.951025 MHz
GMR15    150.951025 MHz
GMR16    150.951025 MHz
GMR17    150.951025 MHz
GMR18    150.951025 MHz
GMR19    150.951025 MHz
GMR20    150.951025 MHz
GMR21    150.951025 MHz
GMR22    150.951025 MHz
GMR23    150.951025 MHz
GMR24    150.951025 MHz
GMR25    150.951025 MHz
GMR26    150.951025 MHz
GMR27    150.951025 MHz
GMR28    150.951025 MHz
GMR29    150.951025 MHz
GMR30    150.951025 MHz
GMR31    150.951025 MHz
GMR32    150.951025 MHz
GMR33    150.951025 MHz
GMR34    150.951025 MHz
GMR35    150.951025 MHz
GMR36    150.951025 MHz
GMR37    150.951025 MHz
GMR38    150.951025 MHz
GMR39    150.951025 MHz
GMR40    150.951025 MHz
GMR41    150.951025 MHz
GMR42    150.951025 MHz
GMR43    150.951025 MHz
GMR44    150.951025 MHz
GMR45    150.951025 MHz
GMR46    150.951025 MHz
GMR47    150.951025 MHz
GMR48    150.951025 MHz
GMR49    150.951025 MHz
GMR50    150.951025 MHz
GMR51    150.951025 MHz
GMR52    150.951025 MHz
GMR53    150.951025 MHz
GMR54    150.951025 MHz
GMR55    150.951025 MHz
GMR56    150.951025 MHz
GMR57    150.951025 MHz
GMR58    150.951025 MHz
GMR59    150.951025 MHz
GMR60    150.951025 MHz
GMR61    150.951025 MHz
GMR62    150.951025 MHz
GMR63    150.951025 MHz
GMR64    150.951025 MHz
GMR65    150.951025 MHz
GMR66    150.951025 MHz
GMR67    150.951025 MHz
GMR68    150.951025 MHz
GMR69    150.951025 MHz
GMR70    150.951025 MHz
GMR71    150.951025 MHz
GMR72    150.951025 MHz
GMR73    150.951025 MHz
GMR74    150.951025 MHz
GMR75    150.951025 MHz
GMR76    150.951025 MHz
GMR77    150.951025 MHz
GMR78    150.951025 MHz
GMR79    150.951025 MHz
GMR80    150.951025 MHz
GMR81    150.951025 MHz
GMR82    150.951025 MHz
GMR83    150.951025 MHz
GMR84    150.951025 MHz
GMR85    150.951025 MHz
GMR86    150.951025 MHz
GMR87    150.951025 MHz
GMR88    150.951025 MHz
GMR89    150.951025 MHz
GMR90    150.951025 MHz
GMR91    150.951025 MHz
GMR92    150.951025 MHz
GMR93    150.951025 MHz
GMR94    150.951025 MHz
GMR95    150.951025 MHz
GMR96    150.951025 MHz
GMR97    150.951025 MHz
GMR98    150.951025 MHz
GMR99    150.951025 MHz
GMR100   150.951025 MHz
----- Processing parameters -----
SI        32768
SF        150.951025 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
```



$^{13}\text{C}$ -NMR ( $d_6$ -DMSO) compound 2a

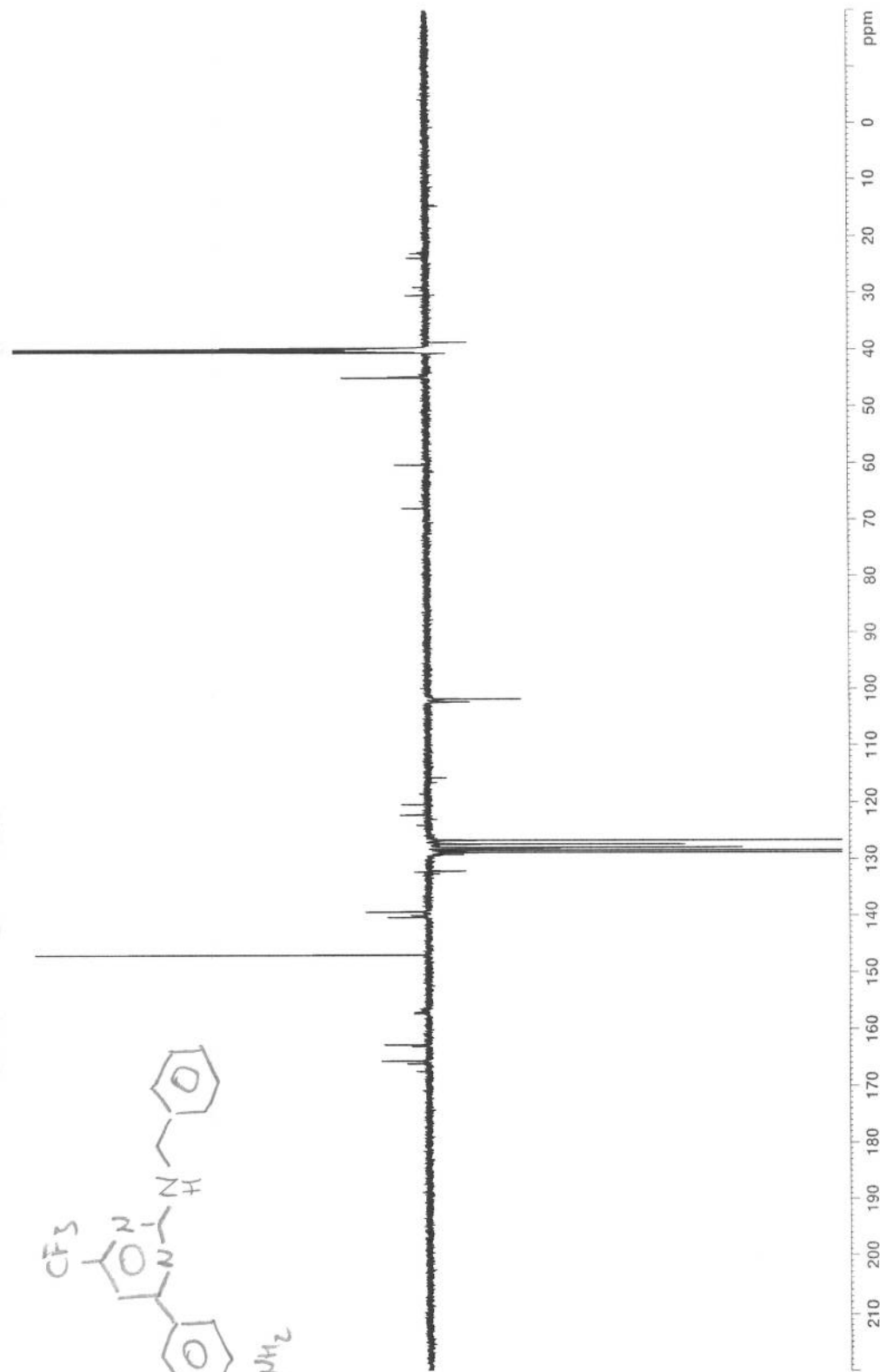
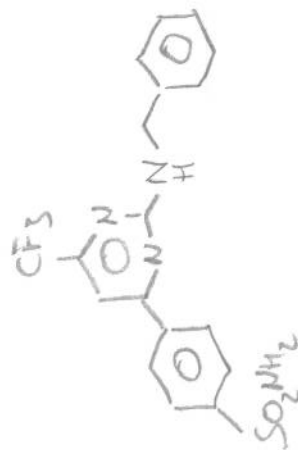
Ole Tietz: Deptq on OTISA-P101  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 30



```
Current Data Parameters
Name      Sep17_2013
Date_    13.09.13
PROCNO   1
=====
F2 - Acquisition Parameters
Date_    20130914
Time     11.30
INSTRUM spect
PROBHD  5 mm PABBO B6/
PULPROG zgpg30
RG      650
SOLVENT DMSO
NS      5000
DS      4
SWH     36331.86 Hz
FIDRES  0.555285 Hz
AQ      0.9443968 sec
RG      180.12
DW      13.800 usec
DE      1.0000000 usec
TE      294.2 K
=====
CONST2  145.0000000
CONST12 1.5000000 usec
D1       0.0000000 sec
D2       0.0034828 sec
D12      0.0002000 sec
D16      0.0002000 sec
TD       100
=====
CHANNEL f1
SFO1     150.831058 MHz
NUC1     13C
P1       11.30 usec
PL1      0.00
PLWD     2000.00 usec
P2       0.00
P3       0.00
SFO2     120.0000000 MHz
NUC2     13C
P2       11.30 usec
PL2      0.00
PLWD     2000.00 usec
SFO3     125.7613500 MHz
SFO4     125.7613500 MHz
SFO5     24.28799919 MHz
=====
CHANNEL f2
SFO2     800.2719197 MHz
NUC2     1H
P2       19.16 usec
PL2      0.00
PLWD     13.40 usec
P3       13.40 usec
P4       26.80 usec
PCPD2   0.00 usec
PDM2    0.00 usec
PDM3    0.00 usec
PDM4    0.76053999 M
=====
***** GRADIENT CHANNEL *****
GDM1(1) SMC10.100
GDM1(2) SMC10.100
GDM1(3) SMC10.100
GDM1(4) SMC10.100
GDM2(1) SMC10.100
GDM2(2) SMC10.100
GDM2(3) SMC10.100
GDM2(4) SMC10.100
=====
F2 - Processing parameters
SI       32768
SF       150.831058 MHz
WDW      EM
SSB      0
GB       0
CB       0
PC       1.40
```

<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound Zb

Ole Tietz: Deptq on OTISA-P102  
CPP\_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 31



```
Current Data Parameters
NAME      Sep17-2013
EXPNO    150
PROCNO   1

F2 - Acquisition Parameters
Date_    20130914
Time     14.52
INSTRUM  spect
PROBHD   5 mm PARBO BB/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       5000
DS       4
SWH      36211.863 Hz
AQ       0.9438968 sec
RG       180.12
DW       13.800 usec
DE       6.500 usec
TE       296.0 K
CNST2    145.0000000
CNST12   1.5000000
D1       2.0000000 sec
D2       0.0000000 sec
D3       0.0000000 sec
D5       0.0000000 sec
D6       0.0000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     130.9531058 MHz
NUC1     13
PC       1.20 usec
PL1      0 dB
PL2      0 dB
PL3      0 dB
PL40     2000.00 usec
PL10     120.0000000 W
SFO10    125.7611700 MHz
SFO11    125.7611700 MHz
SFO12    125.7611700 MHz
SFO13    125.7611700 MHz
SFO14    125.7611700 MHz
SFO15    125.7611700 MHz
SFO16    125.7611700 MHz
SFO17    125.7611700 MHz
SFO18    125.7611700 MHz
SFO19    125.7611700 MHz
SFO20    125.7611700 MHz
SFO21    125.7611700 MHz
SFO22    125.7611700 MHz
SFO23    125.7611700 MHz
SFO24    125.7611700 MHz
SFO25    125.7611700 MHz
SFO26    125.7611700 MHz
SFO27    125.7611700 MHz
SFO28    125.7611700 MHz
SFO29    125.7611700 MHz
SFO30    125.7611700 MHz
SFO31    125.7611700 MHz
SFO32    125.7611700 MHz
SFO33    125.7611700 MHz
SFO34    125.7611700 MHz
SFO35    125.7611700 MHz
SFO36    125.7611700 MHz
SFO37    125.7611700 MHz
SFO38    125.7611700 MHz
SFO39    125.7611700 MHz
SFO40    125.7611700 MHz
SFO41    125.7611700 MHz
SFO42    125.7611700 MHz
SFO43    125.7611700 MHz
SFO44    125.7611700 MHz
SFO45    125.7611700 MHz
SFO46    125.7611700 MHz
SFO47    125.7611700 MHz
SFO48    125.7611700 MHz
SFO49    125.7611700 MHz
SFO50    125.7611700 MHz
SFO51    125.7611700 MHz
SFO52    125.7611700 MHz
SFO53    125.7611700 MHz
SFO54    125.7611700 MHz
SFO55    125.7611700 MHz
SFO56    125.7611700 MHz
SFO57    125.7611700 MHz
SFO58    125.7611700 MHz
SFO59    125.7611700 MHz
SFO60    125.7611700 MHz
SFO61    125.7611700 MHz
SFO62    125.7611700 MHz
SFO63    125.7611700 MHz
SFO64    125.7611700 MHz
SFO65    125.7611700 MHz
SFO66    125.7611700 MHz
SFO67    125.7611700 MHz
SFO68    125.7611700 MHz
SFO69    125.7611700 MHz
SFO70    125.7611700 MHz
SFO71    125.7611700 MHz
SFO72    125.7611700 MHz
SFO73    125.7611700 MHz
SFO74    125.7611700 MHz
SFO75    125.7611700 MHz
SFO76    125.7611700 MHz
SFO77    125.7611700 MHz
SFO78    125.7611700 MHz
SFO79    125.7611700 MHz
SFO80    125.7611700 MHz
SFO81    125.7611700 MHz
SFO82    125.7611700 MHz
SFO83    125.7611700 MHz
SFO84    125.7611700 MHz
SFO85    125.7611700 MHz
SFO86    125.7611700 MHz
SFO87    125.7611700 MHz
SFO88    125.7611700 MHz
SFO89    125.7611700 MHz
SFO90    125.7611700 MHz
SFO91    125.7611700 MHz
SFO92    125.7611700 MHz
SFO93    125.7611700 MHz
SFO94    125.7611700 MHz
SFO95    125.7611700 MHz
SFO96    125.7611700 MHz
SFO97    125.7611700 MHz
SFO98    125.7611700 MHz
SFO99    125.7611700 MHz
SFO100   125.7611700 MHz

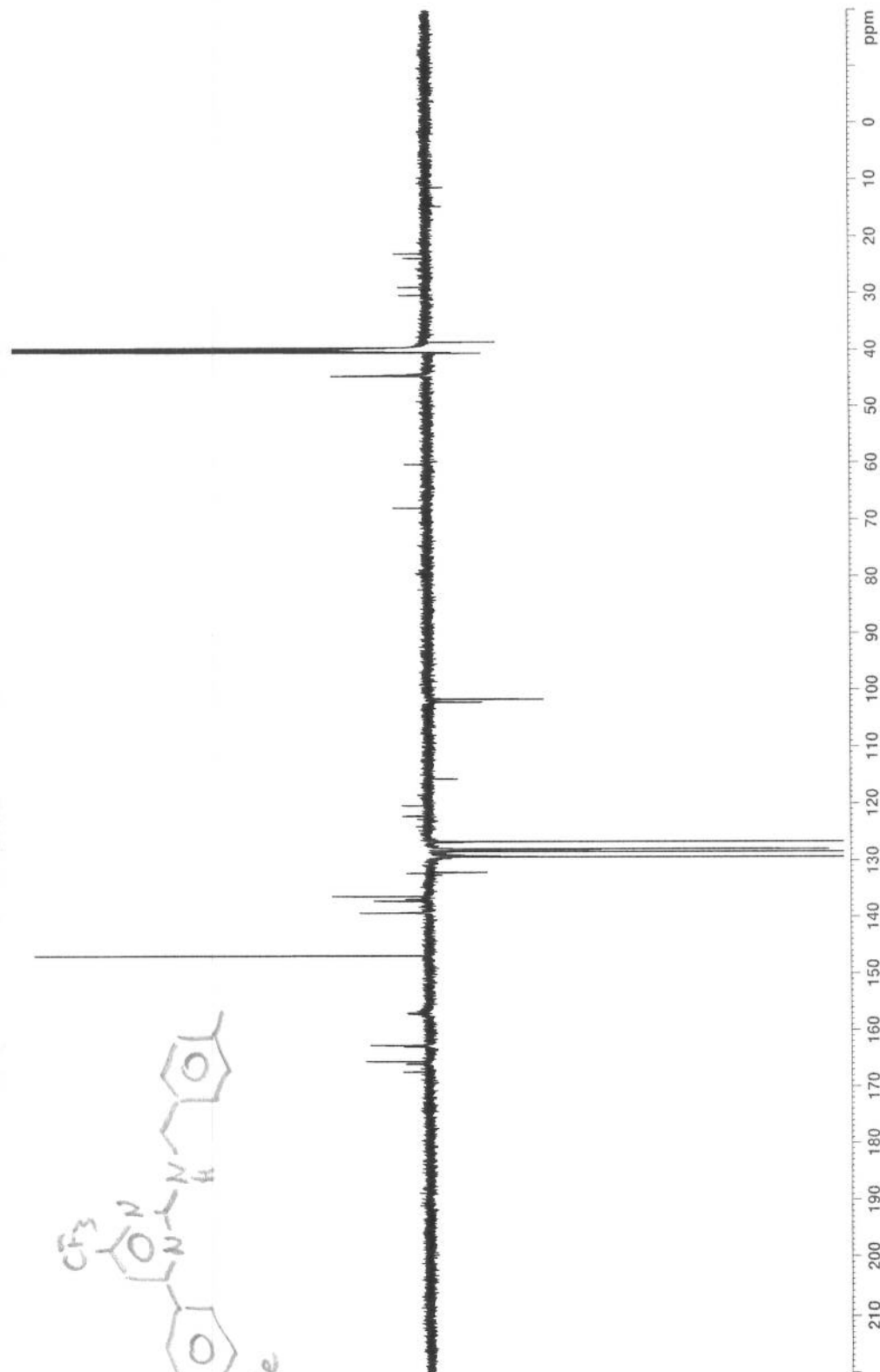
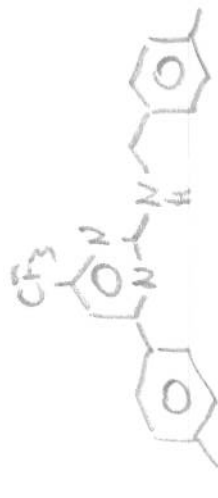
===== CHANNEL f2 =====
NUC2     600.219197 MHz
PC       1.18 usec
PL1      0 dB
PL2      0 dB
PL3      0 dB
PL40     2000.00 usec
PL10     120.0000000 W
SFO10    600.2191970 MHz
SFO11    600.2191970 MHz
SFO12    600.2191970 MHz
SFO13    600.2191970 MHz
SFO14    600.2191970 MHz
SFO15    600.2191970 MHz
SFO16    600.2191970 MHz
SFO17    600.2191970 MHz
SFO18    600.2191970 MHz
SFO19    600.2191970 MHz
SFO20    600.2191970 MHz
SFO21    600.2191970 MHz
SFO22    600.2191970 MHz
SFO23    600.2191970 MHz
SFO24    600.2191970 MHz
SFO25    600.2191970 MHz
SFO26    600.2191970 MHz
SFO27    600.2191970 MHz
SFO28    600.2191970 MHz
SFO29    600.2191970 MHz
SFO30    600.2191970 MHz
SFO31    600.2191970 MHz
SFO32    600.2191970 MHz
SFO33    600.2191970 MHz
SFO34    600.2191970 MHz
SFO35    600.2191970 MHz
SFO36    600.2191970 MHz
SFO37    600.2191970 MHz
SFO38    600.2191970 MHz
SFO39    600.2191970 MHz
SFO40    600.2191970 MHz
SFO41    600.2191970 MHz
SFO42    600.2191970 MHz
SFO43    600.2191970 MHz
SFO44    600.2191970 MHz
SFO45    600.2191970 MHz
SFO46    600.2191970 MHz
SFO47    600.2191970 MHz
SFO48    600.2191970 MHz
SFO49    600.2191970 MHz
SFO50    600.2191970 MHz
SFO51    600.2191970 MHz
SFO52    600.2191970 MHz
SFO53    600.2191970 MHz
SFO54    600.2191970 MHz
SFO55    600.2191970 MHz
SFO56    600.2191970 MHz
SFO57    600.2191970 MHz
SFO58    600.2191970 MHz
SFO59    600.2191970 MHz
SFO60    600.2191970 MHz
SFO61    600.2191970 MHz
SFO62    600.2191970 MHz
SFO63    600.2191970 MHz
SFO64    600.2191970 MHz
SFO65    600.2191970 MHz
SFO66    600.2191970 MHz
SFO67    600.2191970 MHz
SFO68    600.2191970 MHz
SFO69    600.2191970 MHz
SFO70    600.2191970 MHz
SFO71    600.2191970 MHz
SFO72    600.2191970 MHz
SFO73    600.2191970 MHz
SFO74    600.2191970 MHz
SFO75    600.2191970 MHz
SFO76    600.2191970 MHz
SFO77    600.2191970 MHz
SFO78    600.2191970 MHz
SFO79    600.2191970 MHz
SFO80    600.2191970 MHz
SFO81    600.2191970 MHz
SFO82    600.2191970 MHz
SFO83    600.2191970 MHz
SFO84    600.2191970 MHz
SFO85    600.2191970 MHz
SFO86    600.2191970 MHz
SFO87    600.2191970 MHz
SFO88    600.2191970 MHz
SFO89    600.2191970 MHz
SFO90    600.2191970 MHz
SFO91    600.2191970 MHz
SFO92    600.2191970 MHz
SFO93    600.2191970 MHz
SFO94    600.2191970 MHz
SFO95    600.2191970 MHz
SFO96    600.2191970 MHz
SFO97    600.2191970 MHz
SFO98    600.2191970 MHz
SFO99    600.2191970 MHz
SFO100   600.2191970 MHz

===== GRADIENT CHANNEL =====
GMS10    1000.0000000 MHz
GMS11    1000.0000000 MHz
GMS12    1000.0000000 MHz
GMS13    1000.0000000 MHz
GMS14    1000.0000000 MHz
GMS15    1000.0000000 MHz
GMS16    1000.0000000 MHz
GMS17    1000.0000000 MHz
GMS18    1000.0000000 MHz
GMS19    1000.0000000 MHz
GMS20    1000.0000000 MHz
GMS21    1000.0000000 MHz
GMS22    1000.0000000 MHz
GMS23    1000.0000000 MHz
GMS24    1000.0000000 MHz
GMS25    1000.0000000 MHz
GMS26    1000.0000000 MHz
GMS27    1000.0000000 MHz
GMS28    1000.0000000 MHz
GMS29    1000.0000000 MHz
GMS30    1000.0000000 MHz
GMS31    1000.0000000 MHz
GMS32    1000.0000000 MHz
GMS33    1000.0000000 MHz
GMS34    1000.0000000 MHz
GMS35    1000.0000000 MHz
GMS36    1000.0000000 MHz
GMS37    1000.0000000 MHz
GMS38    1000.0000000 MHz
GMS39    1000.0000000 MHz
GMS40    1000.0000000 MHz
GMS41    1000.0000000 MHz
GMS42    1000.0000000 MHz
GMS43    1000.0000000 MHz
GMS44    1000.0000000 MHz
GMS45    1000.0000000 MHz
GMS46    1000.0000000 MHz
GMS47    1000.0000000 MHz
GMS48    1000.0000000 MHz
GMS49    1000.0000000 MHz
GMS50    1000.0000000 MHz
GMS51    1000.0000000 MHz
GMS52    1000.0000000 MHz
GMS53    1000.0000000 MHz
GMS54    1000.0000000 MHz
GMS55    1000.0000000 MHz
GMS56    1000.0000000 MHz
GMS57    1000.0000000 MHz
GMS58    1000.0000000 MHz
GMS59    1000.0000000 MHz
GMS60    1000.0000000 MHz
GMS61    1000.0000000 MHz
GMS62    1000.0000000 MHz
GMS63    1000.0000000 MHz
GMS64    1000.0000000 MHz
GMS65    1000.0000000 MHz
GMS66    1000.0000000 MHz
GMS67    1000.0000000 MHz
GMS68    1000.0000000 MHz
GMS69    1000.0000000 MHz
GMS70    1000.0000000 MHz
GMS71    1000.0000000 MHz
GMS72    1000.0000000 MHz
GMS73    1000.0000000 MHz
GMS74    1000.0000000 MHz
GMS75    1000.0000000 MHz
GMS76    1000.0000000 MHz
GMS77    1000.0000000 MHz
GMS78    1000.0000000 MHz
GMS79    1000.0000000 MHz
GMS80    1000.0000000 MHz
GMS81    1000.0000000 MHz
GMS82    1000.0000000 MHz
GMS83    1000.0000000 MHz
GMS84    1000.0000000 MHz
GMS85    1000.0000000 MHz
GMS86    1000.0000000 MHz
GMS87    1000.0000000 MHz
GMS88    1000.0000000 MHz
GMS89    1000.0000000 MHz
GMS90    1000.0000000 MHz
GMS91    1000.0000000 MHz
GMS92    1000.0000000 MHz
GMS93    1000.0000000 MHz
GMS94    1000.0000000 MHz
GMS95    1000.0000000 MHz
GMS96    1000.0000000 MHz
GMS97    1000.0000000 MHz
GMS98    1000.0000000 MHz
GMS99    1000.0000000 MHz
GMS100   1000.0000000 MHz

F2 - Processing parameters
SI       32768
SF       150.9260320 MHz
WDW      EM
SSB      0
RB       0
GB       0
PC       1.40
```



Ole Tietz: Deptq on OTISA-P103  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 32



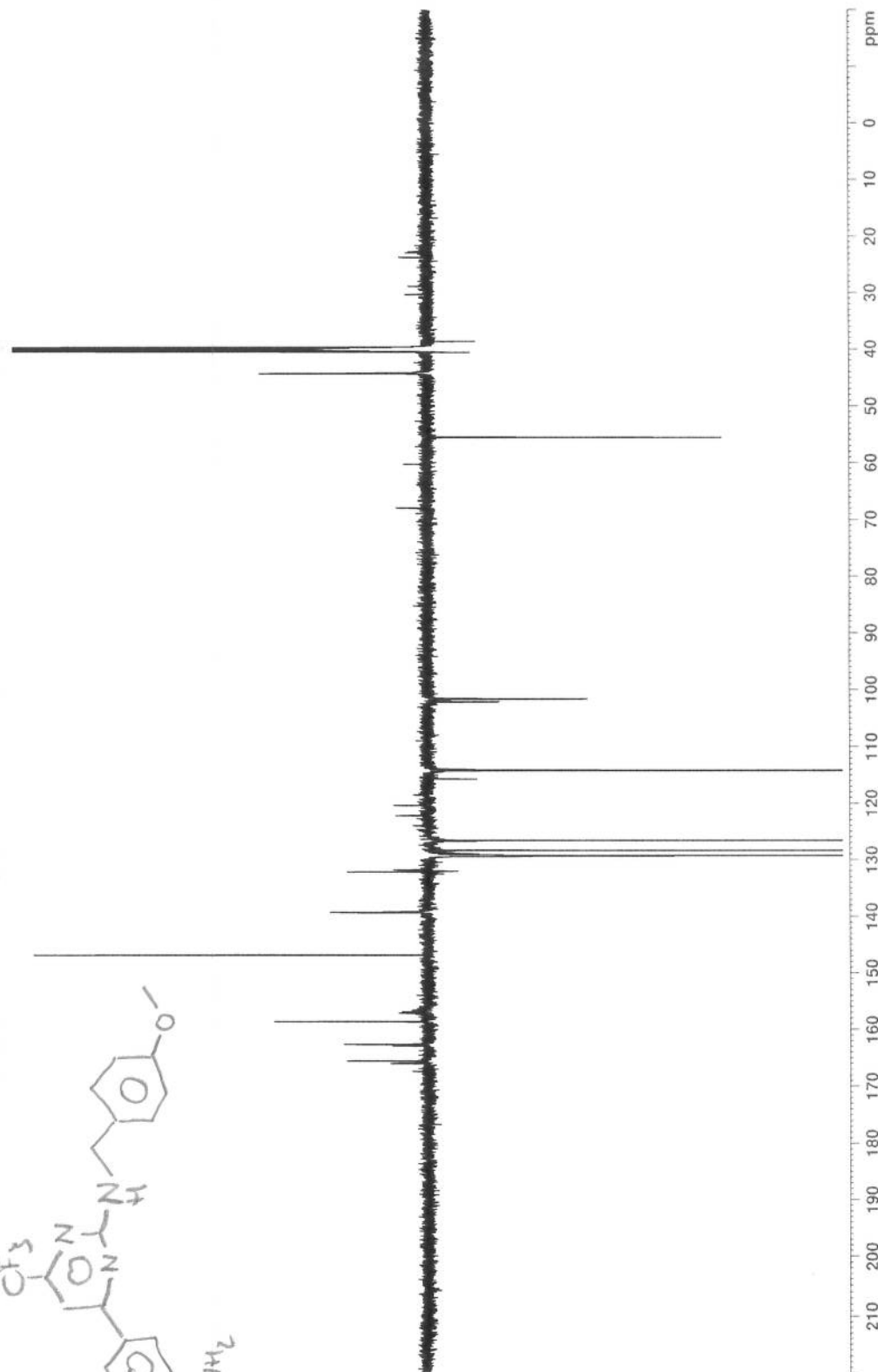
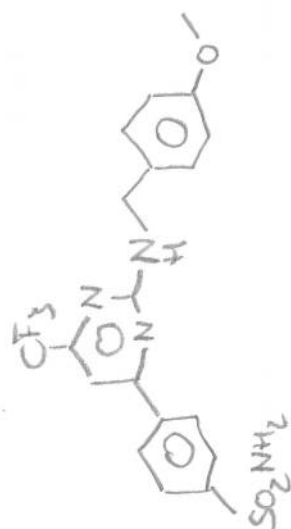
Current Data Parameters  
NAME: Sept12-2013  
EXPRNO: 150  
PROCNO: 1  
F2 - Acquisition Parameters  
Date\_ 20130914  
Time 11:00:00  
INSTRUM spect  
PROBHD 5 mm PABBO AB/ deptsqsp  
PULPROG zgpg30  
D1 0.0002000 sec  
SOLVENT DMSO  
NS 5000  
DS 4  
SWH 3221.863 Hz  
AQ 0.948968 sec  
RG 180.12  
CW 13.800 usec  
TE 296.0 K  
CNS2 145.0000000  
CNS12 1.5000000  
D1 0.0002000 sec  
D2 0.0002000 sec  
D12 0.0002000 sec  
D16 0.0002000 sec  
TD0 1  
==== CHANNEL f1 =====  
SFO1 150.9531058 MHz  
NUC1 13C  
P1 12.00 usec  
PL1 0.00 dB  
PLM0 0 W  
PLM1 120.0000000 W  
SFO2 125.7611550 MHz  
SFO3 125.7611550 MHz  
SFO4 125.7611550 MHz  
SFO5 0 Hz  
SFOFF5 0 Hz  
SP5 24.2479919 W  
==== CHANNEL f2 =====  
SFO2 400.2719197 MHz  
NUC2 1H  
CDEPRG12 waiz16 usec  
F3 13.40 usec  
F4 26.80 usec  
PCPD2 70.00 usec  
PLM2 21.8833333 W  
PLM3 0.7853333 W  
==== GRADIENT CHANNEL =====  
GENM111 SMC10.100  
SFO1 150.9531058 MHz  
SFO2 150.9531058 MHz  
SFO3 150.9531058 MHz  
SFO4 150.9531058 MHz  
SFO5 0 Hz  
SFOFF5 0 Hz  
SP5 24.2479919 W  
==== Processing parameters  
SI 32768  
SF 150.9531058 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
PC 0  
PP 1.40





$^{13}\text{C}$ -NMR ( $d_6$ -DMSO) compounds 2d

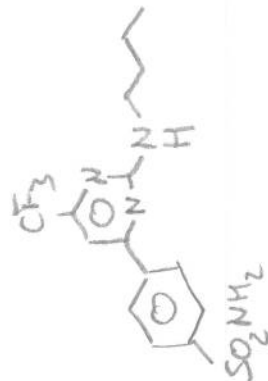
Ole Tietz: Deptq on OTISA-P104  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 33



```
Current Data Parameters
NAME      Exp12-2013
EXPNO    160
PROCNO   1
F2 - Acquisition Parameters
Date_    20130915
Time     2.10
INSTRUM  spect
PROBHD   5 mm PABBO BB7
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       5000
DS       4
SWH      36231.863 Hz
FIDRES   0.349625 Hz
AQ       180.12 sec
RG        655
DM       13.800 usec
DE       8.00 usec
TE       300.2 K
UNST2    145.000000
CNST12   1.500000
D1       2.0000000 sec
D2       0.0500000 sec
D12      0.0002000 sec
D16      0.0002000 sec
TD0      1
===== CHANNEL f1 =====
SFO1    130.92531055 MHz
NUC1    13C
P1      11.20 usec
PL1     0.00 dB
PL10    2000.00 usec
PL100   0 W
SFO1M1  120.000000000 MHz
SFO1M2  120.000000000 MHz
SFO1M3  120.000000000 MHz
SFO1M4  120.000000000 MHz
SFO1M5  120.000000000 MHz
SFO1M6  120.000000000 MHz
SFO1M7  120.000000000 MHz
SFO1M8  120.000000000 MHz
SFO1M9  120.000000000 MHz
SFO1M10 120.000000000 MHz
SFO1M11 120.000000000 MHz
SFO1M12 120.000000000 MHz
SFO1M13 120.000000000 MHz
SFO1M14 120.000000000 MHz
SFO1M15 120.000000000 MHz
SFO1M16 120.000000000 MHz
SFO1M17 120.000000000 MHz
SFO1M18 120.000000000 MHz
SFO1M19 120.000000000 MHz
SFO1M20 120.000000000 MHz
SFO1M21 120.000000000 MHz
SFO1M22 120.000000000 MHz
SFO1M23 120.000000000 MHz
SFO1M24 120.000000000 MHz
SFO1M25 120.000000000 MHz
SFO1M26 120.000000000 MHz
SFO1M27 120.000000000 MHz
SFO1M28 120.000000000 MHz
SFO1M29 120.000000000 MHz
SFO1M30 120.000000000 MHz
SFO1M31 120.000000000 MHz
SFO1M32 120.000000000 MHz
SFO1M33 120.000000000 MHz
SFO1M34 120.000000000 MHz
SFO1M35 120.000000000 MHz
SFO1M36 120.000000000 MHz
SFO1M37 120.000000000 MHz
SFO1M38 120.000000000 MHz
SFO1M39 120.000000000 MHz
SFO1M40 120.000000000 MHz
SFO1M41 120.000000000 MHz
SFO1M42 120.000000000 MHz
SFO1M43 120.000000000 MHz
SFO1M44 120.000000000 MHz
SFO1M45 120.000000000 MHz
SFO1M46 120.000000000 MHz
SFO1M47 120.000000000 MHz
SFO1M48 120.000000000 MHz
SFO1M49 120.000000000 MHz
SFO1M50 120.000000000 MHz
SFO1M51 120.000000000 MHz
SFO1M52 120.000000000 MHz
SFO1M53 120.000000000 MHz
SFO1M54 120.000000000 MHz
SFO1M55 120.000000000 MHz
SFO1M56 120.000000000 MHz
SFO1M57 120.000000000 MHz
SFO1M58 120.000000000 MHz
SFO1M59 120.000000000 MHz
SFO1M60 120.000000000 MHz
SFO1M61 120.000000000 MHz
SFO1M62 120.000000000 MHz
SFO1M63 120.000000000 MHz
SFO1M64 120.000000000 MHz
SFO1M65 120.000000000 MHz
SFO1M66 120.000000000 MHz
SFO1M67 120.000000000 MHz
SFO1M68 120.000000000 MHz
SFO1M69 120.000000000 MHz
SFO1M70 120.000000000 MHz
SFO1M71 120.000000000 MHz
SFO1M72 120.000000000 MHz
SFO1M73 120.000000000 MHz
SFO1M74 120.000000000 MHz
SFO1M75 120.000000000 MHz
SFO1M76 120.000000000 MHz
SFO1M77 120.000000000 MHz
SFO1M78 120.000000000 MHz
SFO1M79 120.000000000 MHz
SFO1M80 120.000000000 MHz
SFO1M81 120.000000000 MHz
SFO1M82 120.000000000 MHz
SFO1M83 120.000000000 MHz
SFO1M84 120.000000000 MHz
SFO1M85 120.000000000 MHz
SFO1M86 120.000000000 MHz
SFO1M87 120.000000000 MHz
SFO1M88 120.000000000 MHz
SFO1M89 120.000000000 MHz
SFO1M90 120.000000000 MHz
SFO1M91 120.000000000 MHz
SFO1M92 120.000000000 MHz
SFO1M93 120.000000000 MHz
SFO1M94 120.000000000 MHz
SFO1M95 120.000000000 MHz
SFO1M96 120.000000000 MHz
SFO1M97 120.000000000 MHz
SFO1M98 120.000000000 MHz
SFO1M99 120.000000000 MHz
SFO1M100 120.000000000 MHz
===== CHANNEL f2 =====
SFO2    600.211917 MHz
NUC2    1H
P2      12.00 usec
PL2     0.00 dB
PL20    20.00 usec
PL200   0 W
SFO2M1  600.211917 MHz
SFO2M2  600.211917 MHz
SFO2M3  600.211917 MHz
SFO2M4  600.211917 MHz
SFO2M5  600.211917 MHz
SFO2M6  600.211917 MHz
SFO2M7  600.211917 MHz
SFO2M8  600.211917 MHz
SFO2M9  600.211917 MHz
SFO2M10 600.211917 MHz
SFO2M11 600.211917 MHz
SFO2M12 600.211917 MHz
SFO2M13 600.211917 MHz
SFO2M14 600.211917 MHz
SFO2M15 600.211917 MHz
SFO2M16 600.211917 MHz
SFO2M17 600.211917 MHz
SFO2M18 600.211917 MHz
SFO2M19 600.211917 MHz
SFO2M20 600.211917 MHz
SFO2M21 600.211917 MHz
SFO2M22 600.211917 MHz
SFO2M23 600.211917 MHz
SFO2M24 600.211917 MHz
SFO2M25 600.211917 MHz
SFO2M26 600.211917 MHz
SFO2M27 600.211917 MHz
SFO2M28 600.211917 MHz
SFO2M29 600.211917 MHz
SFO2M30 600.211917 MHz
SFO2M31 600.211917 MHz
SFO2M32 600.211917 MHz
SFO2M33 600.211917 MHz
SFO2M34 600.211917 MHz
SFO2M35 600.211917 MHz
SFO2M36 600.211917 MHz
SFO2M37 600.211917 MHz
SFO2M38 600.211917 MHz
SFO2M39 600.211917 MHz
SFO2M40 600.211917 MHz
SFO2M41 600.211917 MHz
SFO2M42 600.211917 MHz
SFO2M43 600.211917 MHz
SFO2M44 600.211917 MHz
SFO2M45 600.211917 MHz
SFO2M46 600.211917 MHz
SFO2M47 600.211917 MHz
SFO2M48 600.211917 MHz
SFO2M49 600.211917 MHz
SFO2M50 600.211917 MHz
SFO2M51 600.211917 MHz
SFO2M52 600.211917 MHz
SFO2M53 600.211917 MHz
SFO2M54 600.211917 MHz
SFO2M55 600.211917 MHz
SFO2M56 600.211917 MHz
SFO2M57 600.211917 MHz
SFO2M58 600.211917 MHz
SFO2M59 600.211917 MHz
SFO2M60 600.211917 MHz
SFO2M61 600.211917 MHz
SFO2M62 600.211917 MHz
SFO2M63 600.211917 MHz
SFO2M64 600.211917 MHz
SFO2M65 600.211917 MHz
SFO2M66 600.211917 MHz
SFO2M67 600.211917 MHz
SFO2M68 600.211917 MHz
SFO2M69 600.211917 MHz
SFO2M70 600.211917 MHz
SFO2M71 600.211917 MHz
SFO2M72 600.211917 MHz
SFO2M73 600.211917 MHz
SFO2M74 600.211917 MHz
SFO2M75 600.211917 MHz
SFO2M76 600.211917 MHz
SFO2M77 600.211917 MHz
SFO2M78 600.211917 MHz
SFO2M79 600.211917 MHz
SFO2M80 600.211917 MHz
SFO2M81 600.211917 MHz
SFO2M82 600.211917 MHz
SFO2M83 600.211917 MHz
SFO2M84 600.211917 MHz
SFO2M85 600.211917 MHz
SFO2M86 600.211917 MHz
SFO2M87 600.211917 MHz
SFO2M88 600.211917 MHz
SFO2M89 600.211917 MHz
SFO2M90 600.211917 MHz
SFO2M91 600.211917 MHz
SFO2M92 600.211917 MHz
SFO2M93 600.211917 MHz
SFO2M94 600.211917 MHz
SFO2M95 600.211917 MHz
SFO2M96 600.211917 MHz
SFO2M97 600.211917 MHz
SFO2M98 600.211917 MHz
SFO2M99 600.211917 MHz
SFO2M100 600.211917 MHz
===== GRADIENT CHANNEL =====
GPMAX[1] 800.000000 MHz
GPMAX[2] 800.000000 MHz
GPMAX[3] 800.000000 MHz
GFM1     31.00 kHz
GFM2     31.00 kHz
GFM3     31.00 kHz
GFM4     31.00 kHz
GFM5     31.00 kHz
GFM6     31.00 kHz
GFM7     31.00 kHz
GFM8     31.00 kHz
GFM9     31.00 kHz
GFM10    31.00 kHz
GFM11    31.00 kHz
GFM12    31.00 kHz
GFM13    31.00 kHz
GFM14    31.00 kHz
GFM15    31.00 kHz
GFM16    31.00 kHz
GFM17    31.00 kHz
GFM18    31.00 kHz
GFM19    31.00 kHz
GFM20    31.00 kHz
GFM21    31.00 kHz
GFM22    31.00 kHz
GFM23    31.00 kHz
GFM24    31.00 kHz
GFM25    31.00 kHz
GFM26    31.00 kHz
GFM27    31.00 kHz
GFM28    31.00 kHz
GFM29    31.00 kHz
GFM30    31.00 kHz
GFM31    31.00 kHz
GFM32    31.00 kHz
GFM33    31.00 kHz
GFM34    31.00 kHz
GFM35    31.00 kHz
GFM36    31.00 kHz
GFM37    31.00 kHz
GFM38    31.00 kHz
GFM39    31.00 kHz
GFM40    31.00 kHz
GFM41    31.00 kHz
GFM42    31.00 kHz
GFM43    31.00 kHz
GFM44    31.00 kHz
GFM45    31.00 kHz
GFM46    31.00 kHz
GFM47    31.00 kHz
GFM48    31.00 kHz
GFM49    31.00 kHz
GFM50    31.00 kHz
GFM51    31.00 kHz
GFM52    31.00 kHz
GFM53    31.00 kHz
GFM54    31.00 kHz
GFM55    31.00 kHz
GFM56    31.00 kHz
GFM57    31.00 kHz
GFM58    31.00 kHz
GFM59    31.00 kHz
GFM60    31.00 kHz
GFM61    31.00 kHz
GFM62    31.00 kHz
GFM63    31.00 kHz
GFM64    31.00 kHz
GFM65    31.00 kHz
GFM66    31.00 kHz
GFM67    31.00 kHz
GFM68    31.00 kHz
GFM69    31.00 kHz
GFM70    31.00 kHz
GFM71    31.00 kHz
GFM72    31.00 kHz
GFM73    31.00 kHz
GFM74    31.00 kHz
GFM75    31.00 kHz
GFM76    31.00 kHz
GFM77    31.00 kHz
GFM78    31.00 kHz
GFM79    31.00 kHz
GFM80    31.00 kHz
GFM81    31.00 kHz
GFM82    31.00 kHz
GFM83    31.00 kHz
GFM84    31.00 kHz
GFM85    31.00 kHz
GFM86    31.00 kHz
GFM87    31.00 kHz
GFM88    31.00 kHz
GFM89    31.00 kHz
GFM90    31.00 kHz
GFM91    31.00 kHz
GFM92    31.00 kHz
GFM93    31.00 kHz
GFM94    31.00 kHz
GFM95    31.00 kHz
GFM96    31.00 kHz
GFM97    31.00 kHz
GFM98    31.00 kHz
GFM99    31.00 kHz
GFM100   31.00 kHz
===== Processing parameters =====
SI      32768
SF      130.92531055 MHz
RG      655
WDW     EM
SSB     0
LB      0
GB      0
PC      1.40
```

<sup>13</sup>C-NMR (d<sub>6</sub>-DMSO) compound 2e

Ole Tietz: Deptq on OTISA-P106  
CPP\_Deptq.A DMSO (C:\Bruker\TopSpin3.2) vishwa 34



Current Data Parameters  
NAME: Sept12-2013  
EXPNO: 170  
PROCNO: 1  
F2 - Acquisition Parameters  
Date\_ 20130915  
Time 6.19  
Time00 8.12  
PULPROG 5 mm PABBO/B7  
PROBHD 5 mm PABBO/B7  
PULPROG deptqppp  
TD 6536  
SFO1 125.760 MHz  
NUS 500  
SOLVENT DMSO  
DS 4  
SWH 36231.863 Hz  
FIDRES 0.394269 Hz  
AQ 0.0485389 sec  
RG 180.12 sec  
DM 13.800 usec  
DE 6.50 usec  
TE 300.2 K  
CHST2 145.000000 K  
CHST12 1.5000000  
D1 2.00000000 sec  
D2 0.05000000 sec  
D3 0.00000000 sec  
D16 0.00020000 sec  
TD0 1  
----- CHANNEL f1 -----  
SFO1 150.9531058 MHz  
NUC1 13C  
P1 1.20 usec  
PL1 0.00000000 W  
PL10 0 W  
PL10 2000.00 usec  
SENSE1 CTE40comp.4  
SFO2 125.760 MHz  
SFOFFS 0 Hz  
SFOFFS 24.2479919 W  
----- CHANNEL f2 -----  
SFO2 600.215197 MHz  
NUC2 1H  
P2 12.00 usec  
PL2 0.00000000 W  
P4 26.80 usec  
P4 26.80 usec  
PCPD2 75.00 usec  
PLM2 21.2999958 W  
PLW12 0.18652999 W  
----- GRADIENT CHANNEL -----  
GNUM1 1  
GNUM2 1  
GNUM3 1  
GF21 31.00 %  
GF22 31.00 %  
GF23 31.00 %  
F16 1800.00 usec  
F2 - Processing parameters  
SI 32768  
SF 150.9380100 MHz  
RG 68  
SBB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

