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Supplementary Information

Synthesis of three 18F-labelled cyclooxygenase-2 (COX-2) inhibitors based on a pyrimidine scaffold

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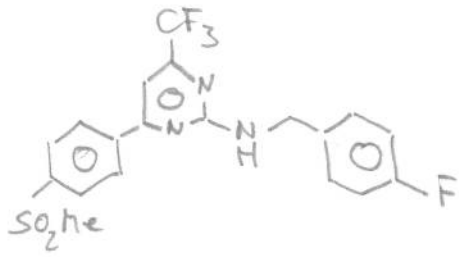
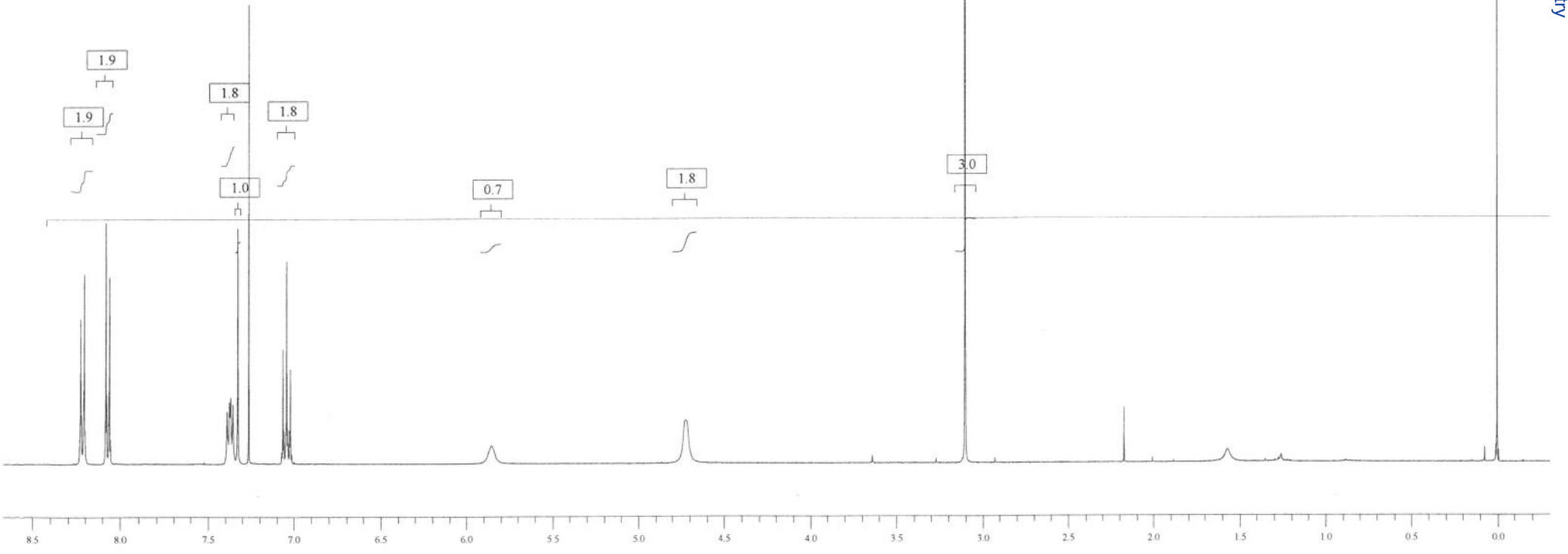
Contents

^{1}H-NMR and ^{13}C-NMR spectra of all compounds

^{1}H-NMR ($CDCl_3$) Compound: 1a





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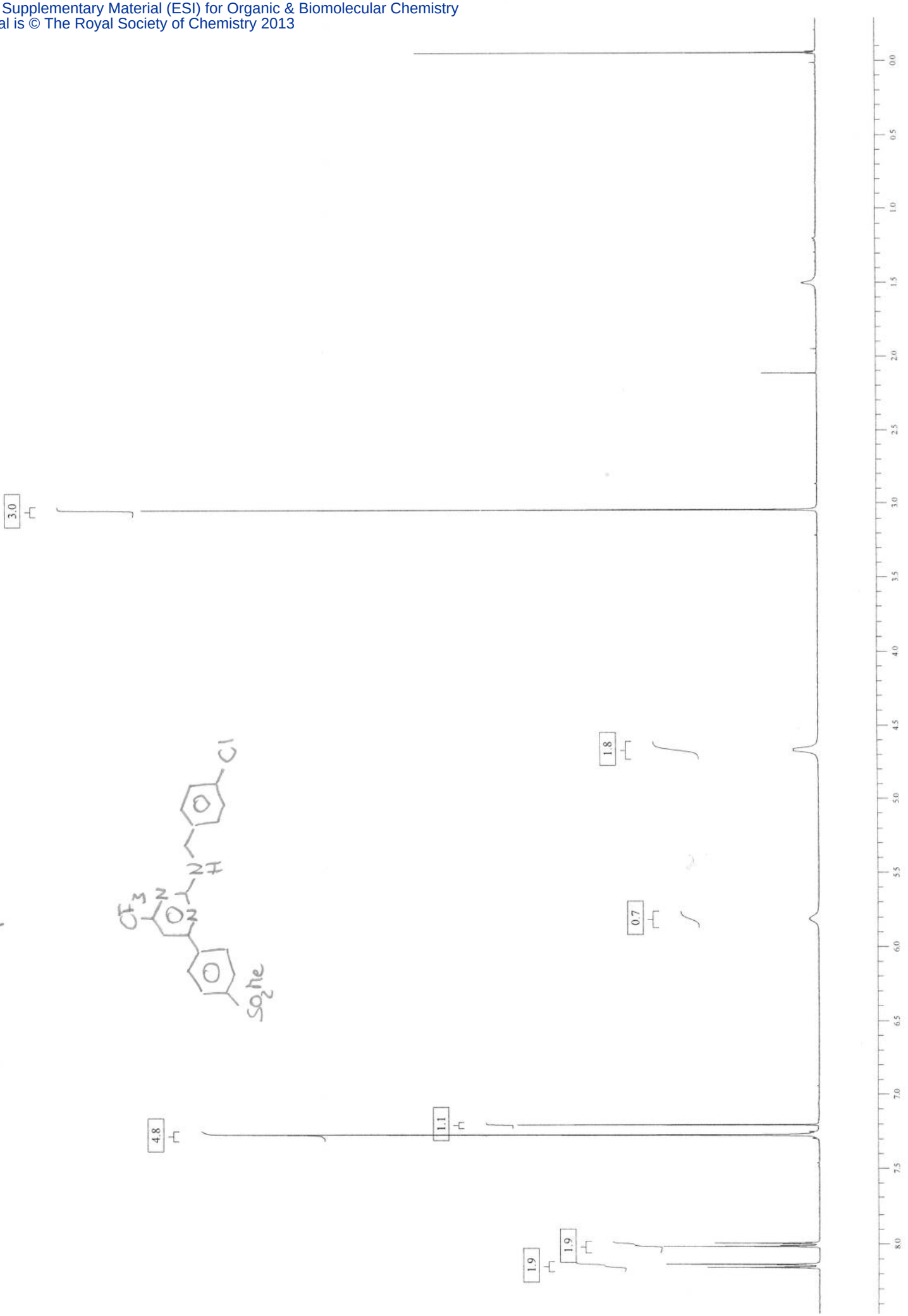
^{1}H-NMR ($CDCl_3$) Compound 1b



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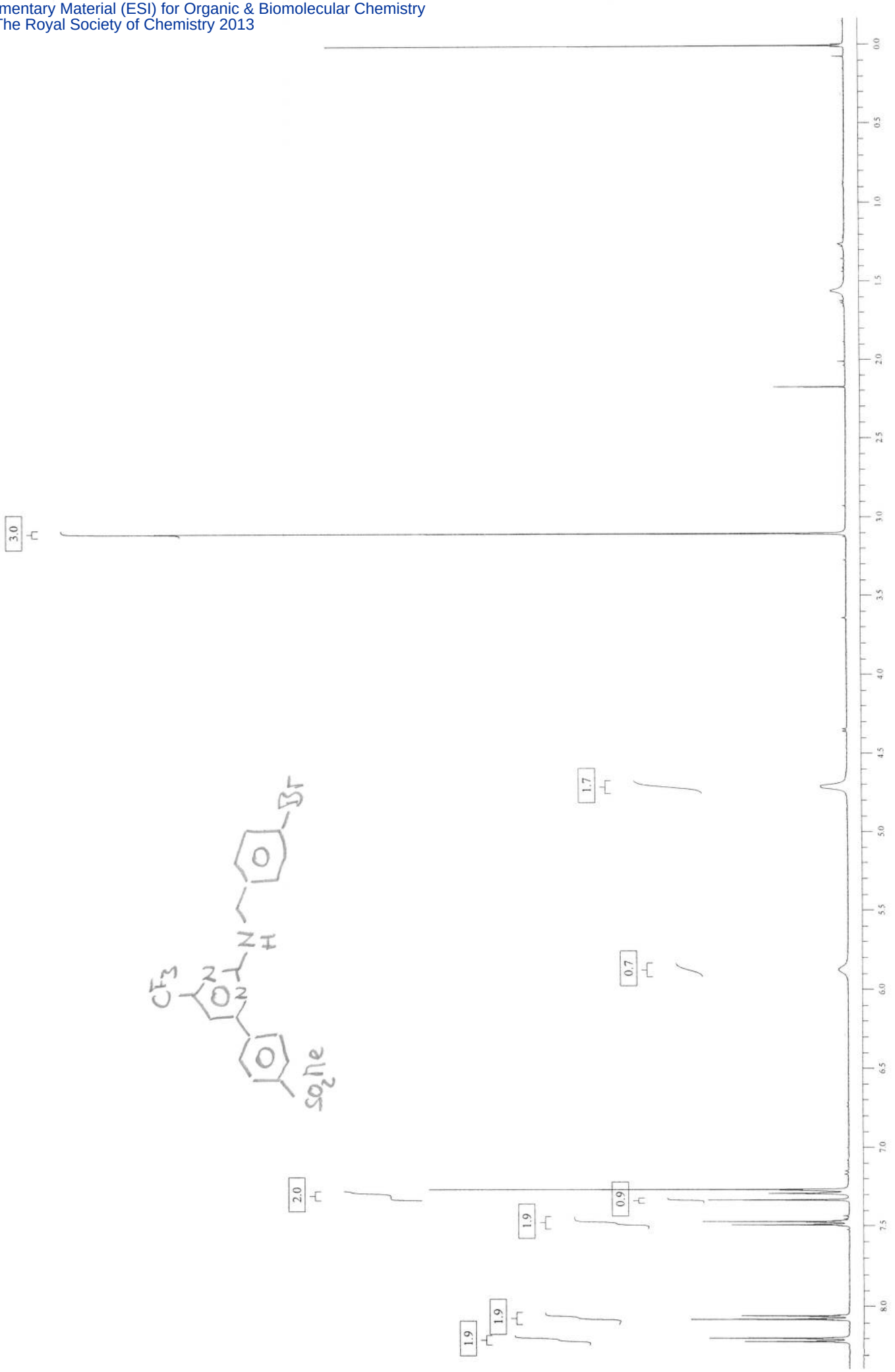

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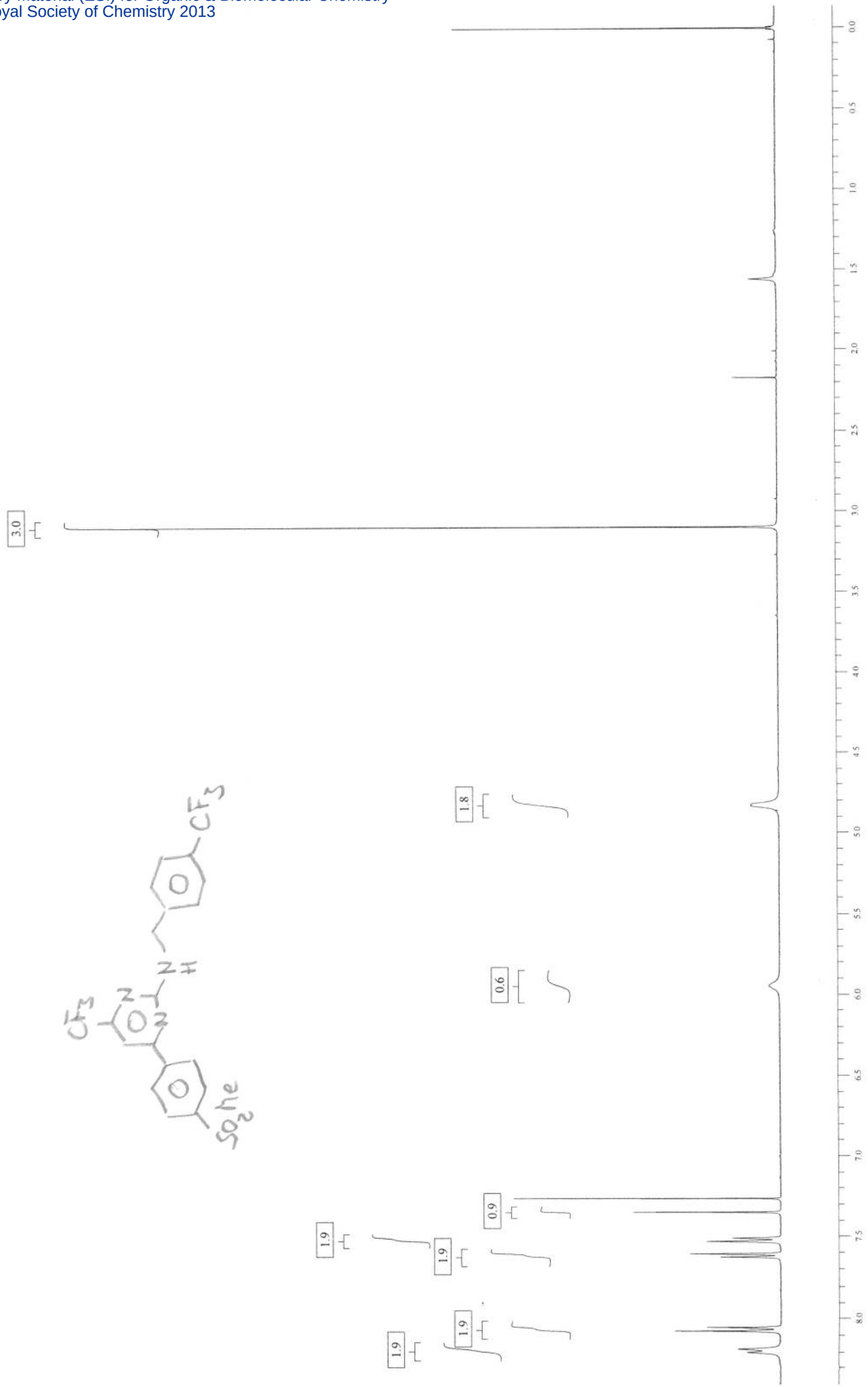

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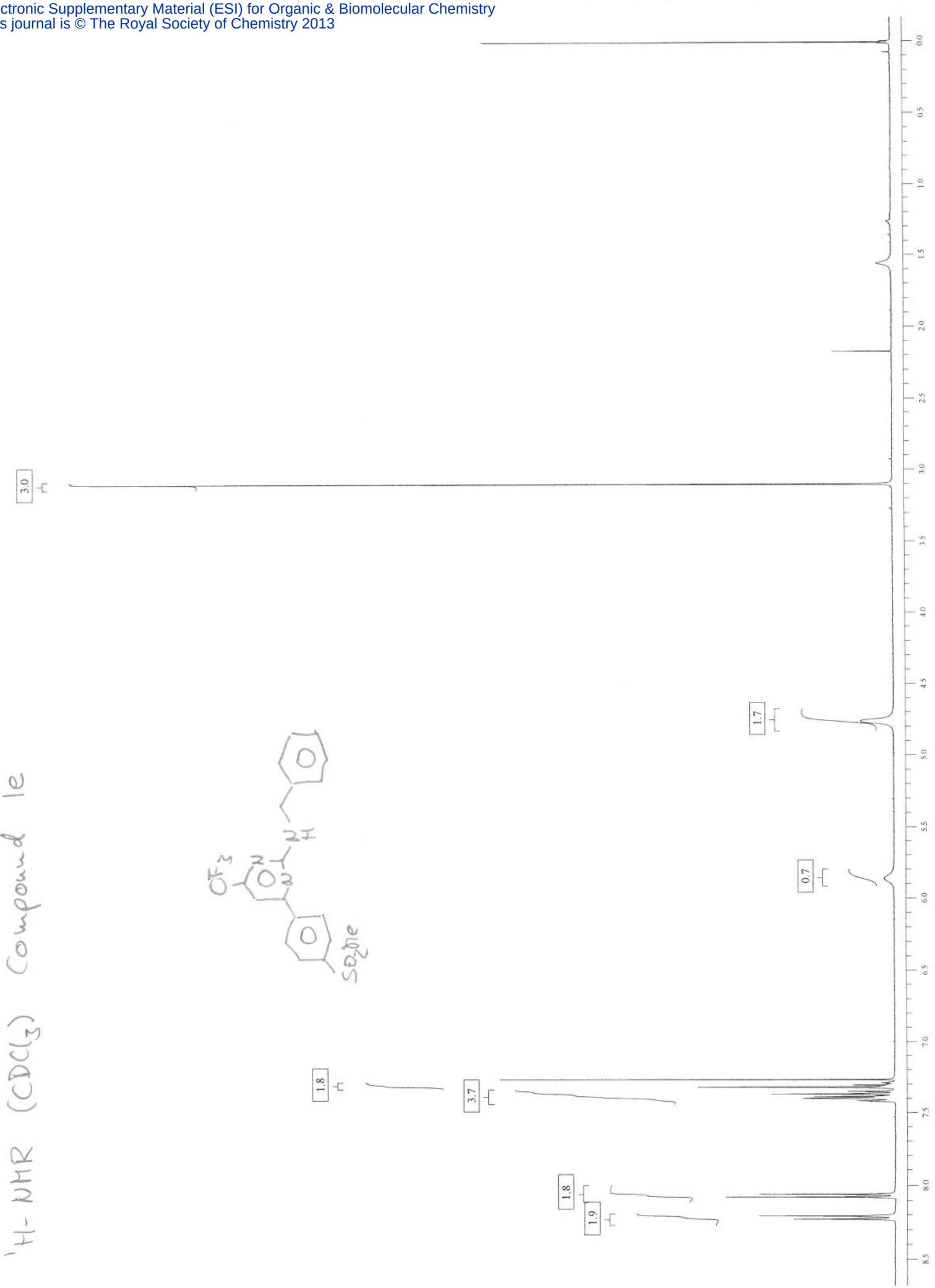
^{1}H- NMR ($CDCl_3$) Compound 1e



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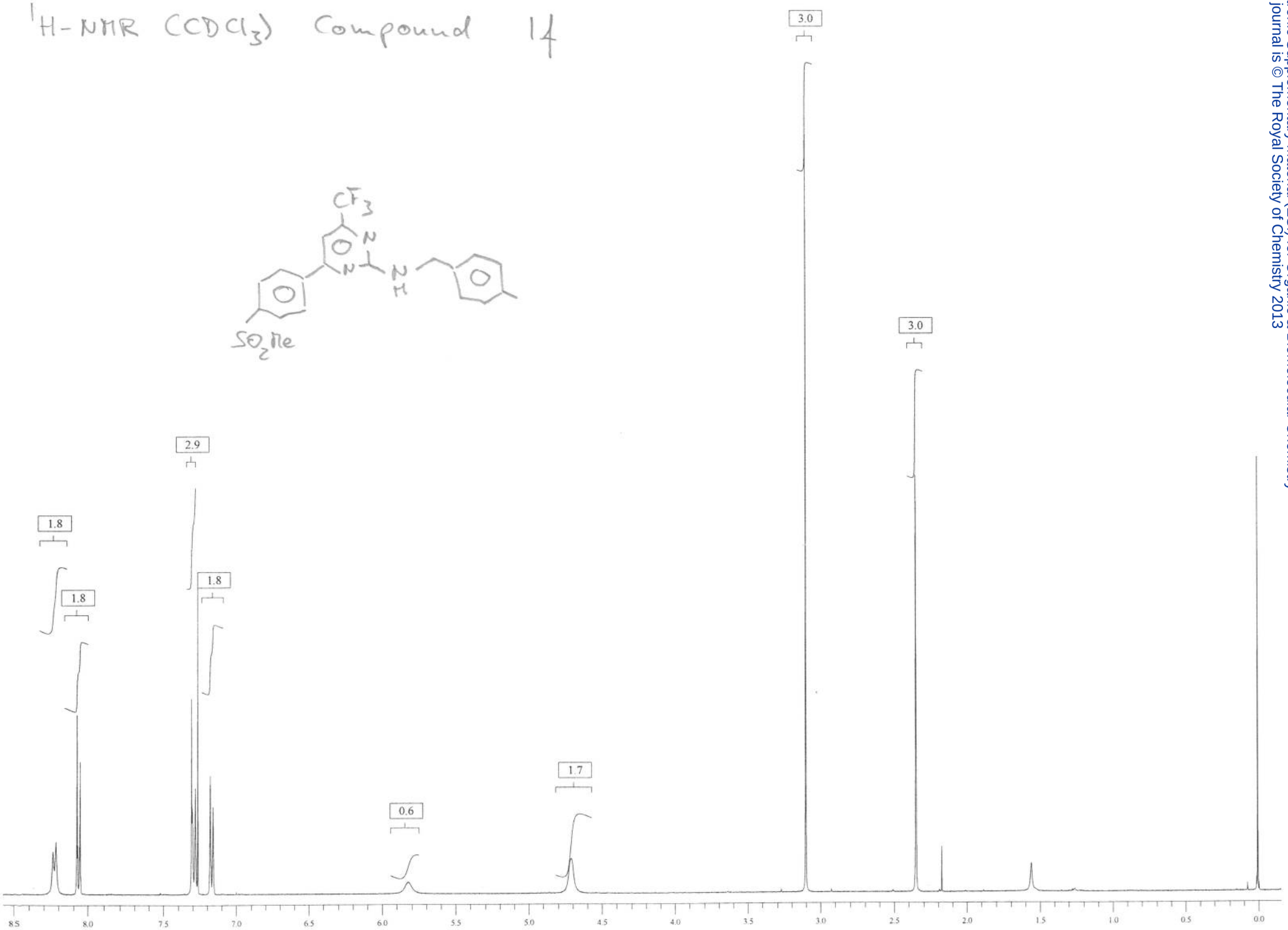

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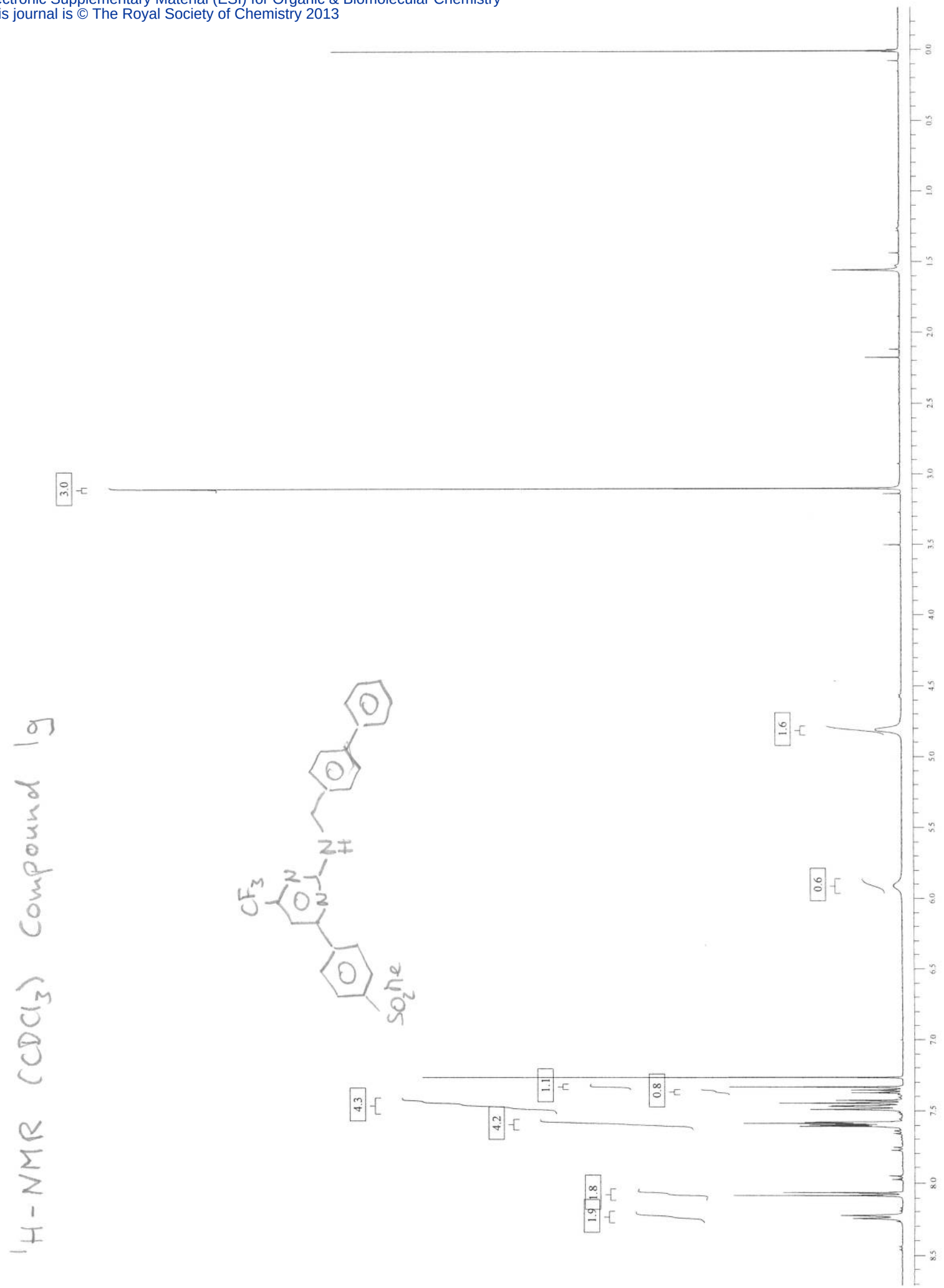

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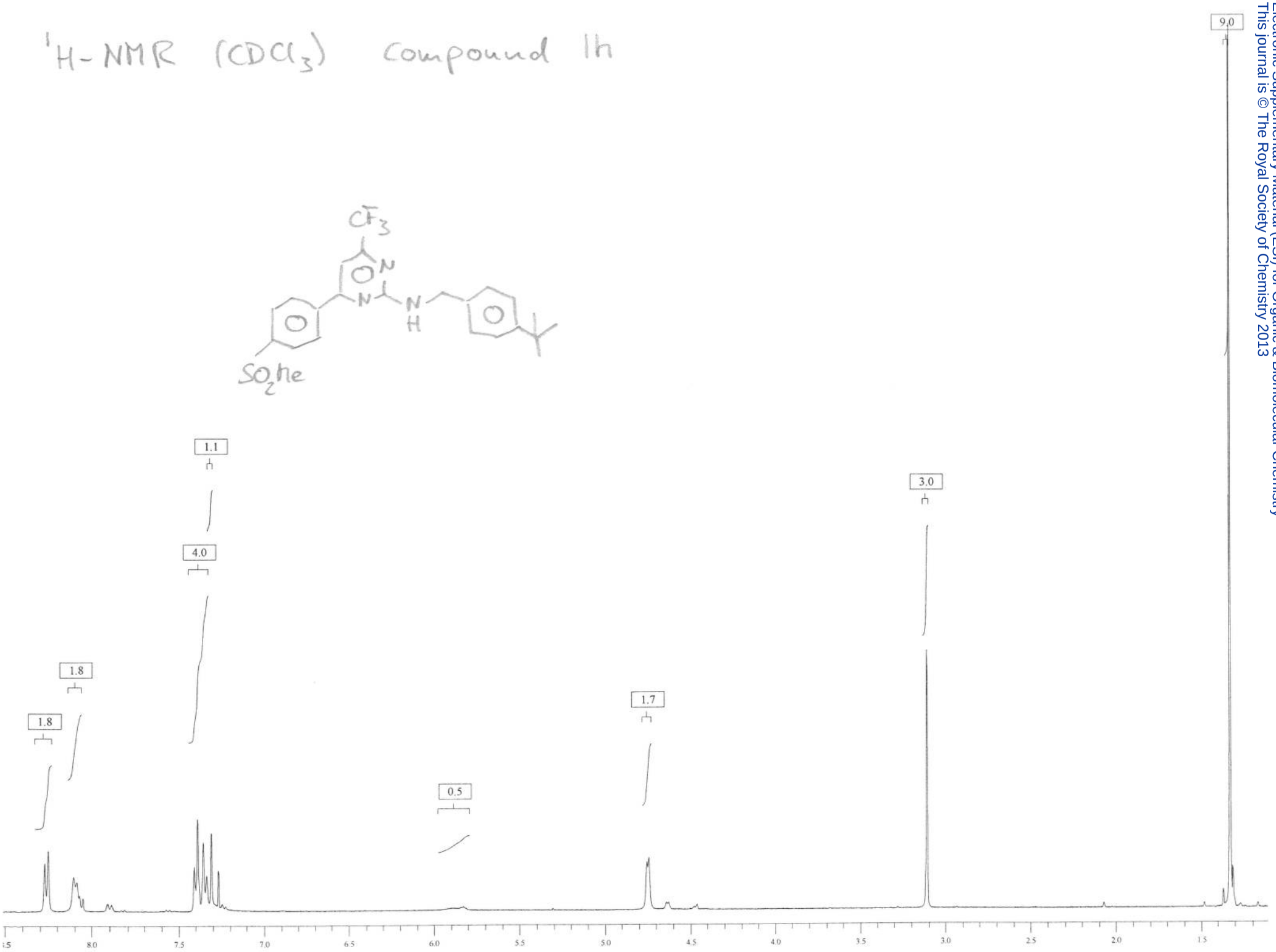

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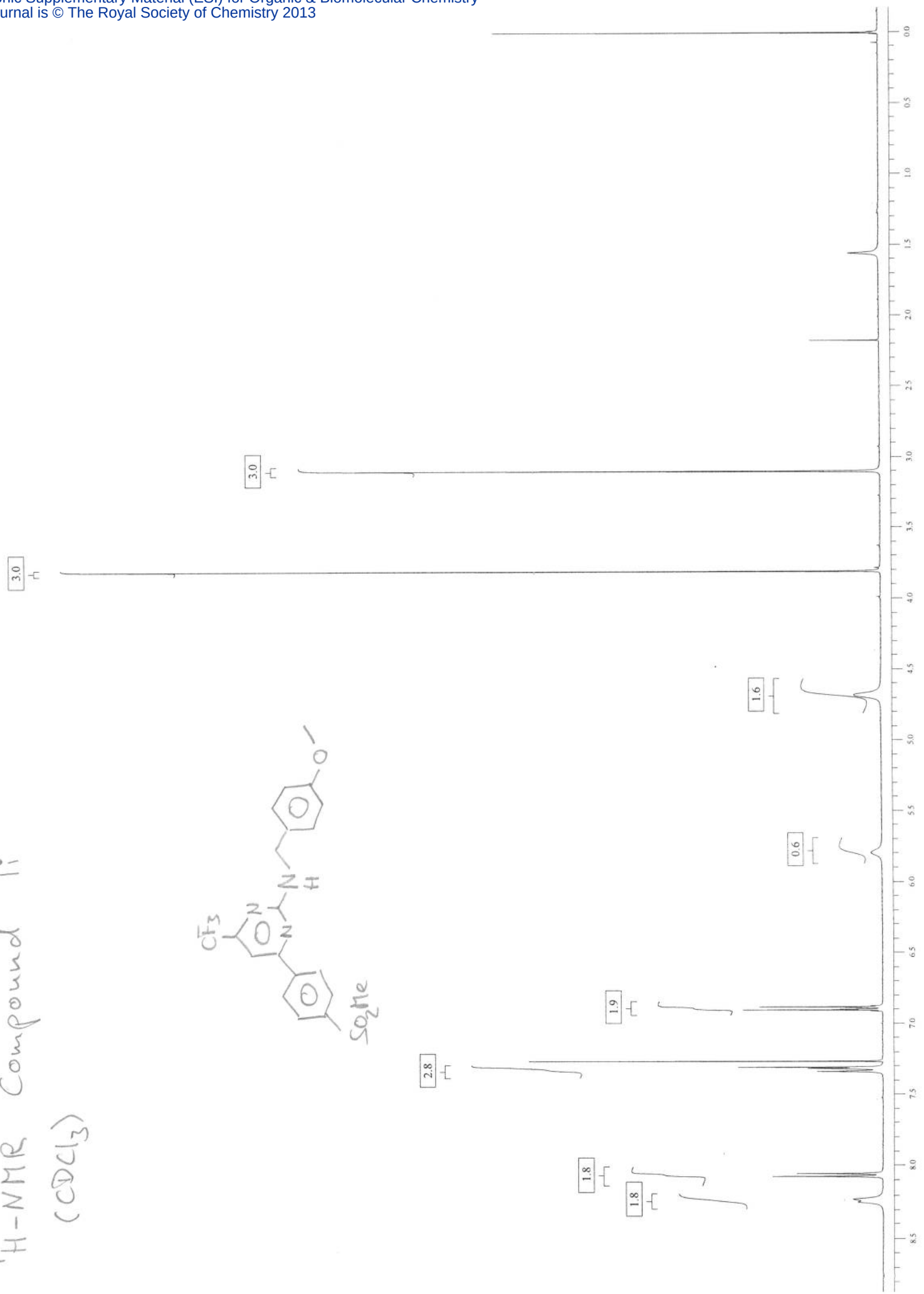
^{1}H-NMR Compound 11
($CDCl_3$)



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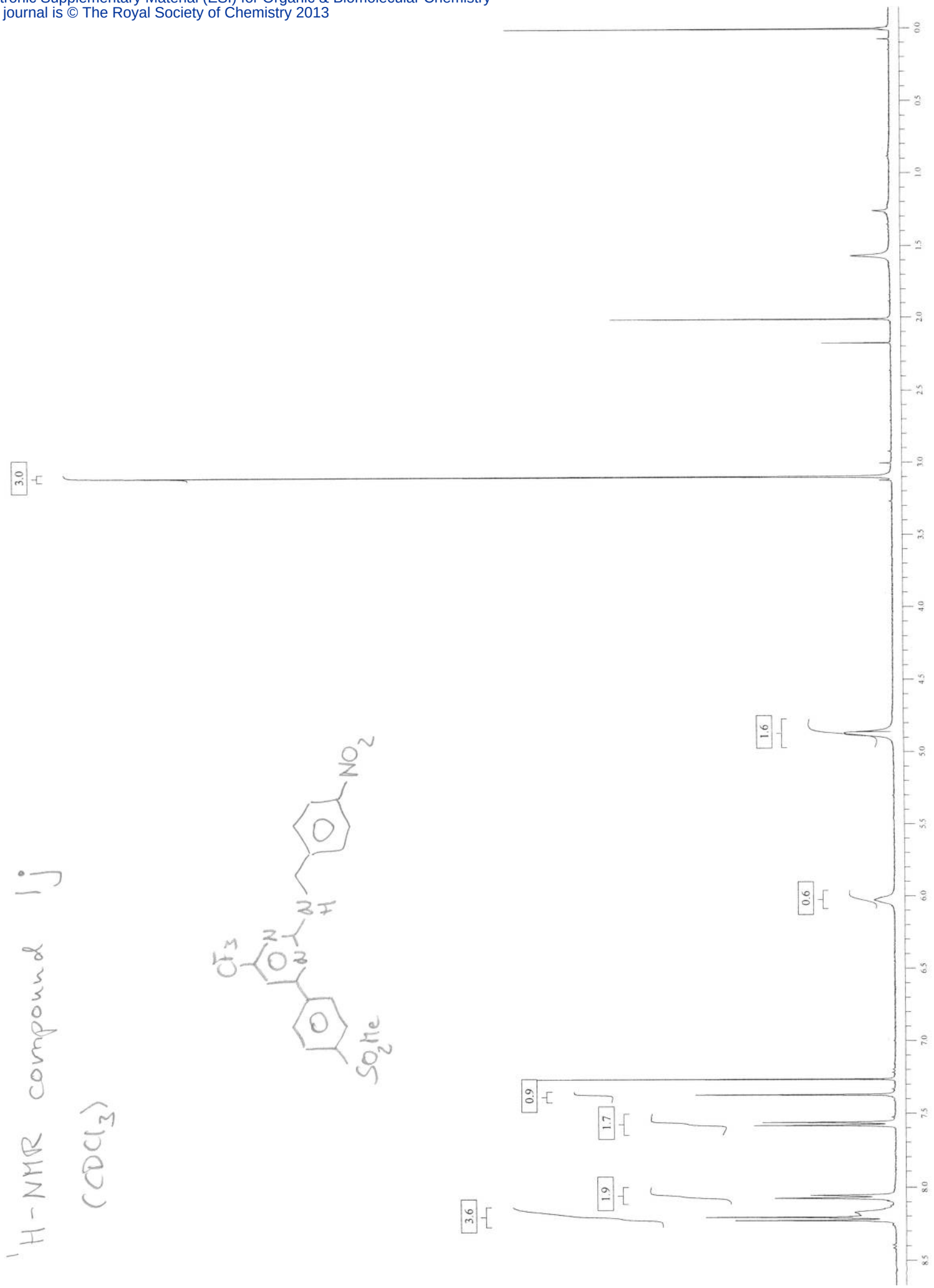
^{1}H-NMR compound 1j

($CDCl_3$)



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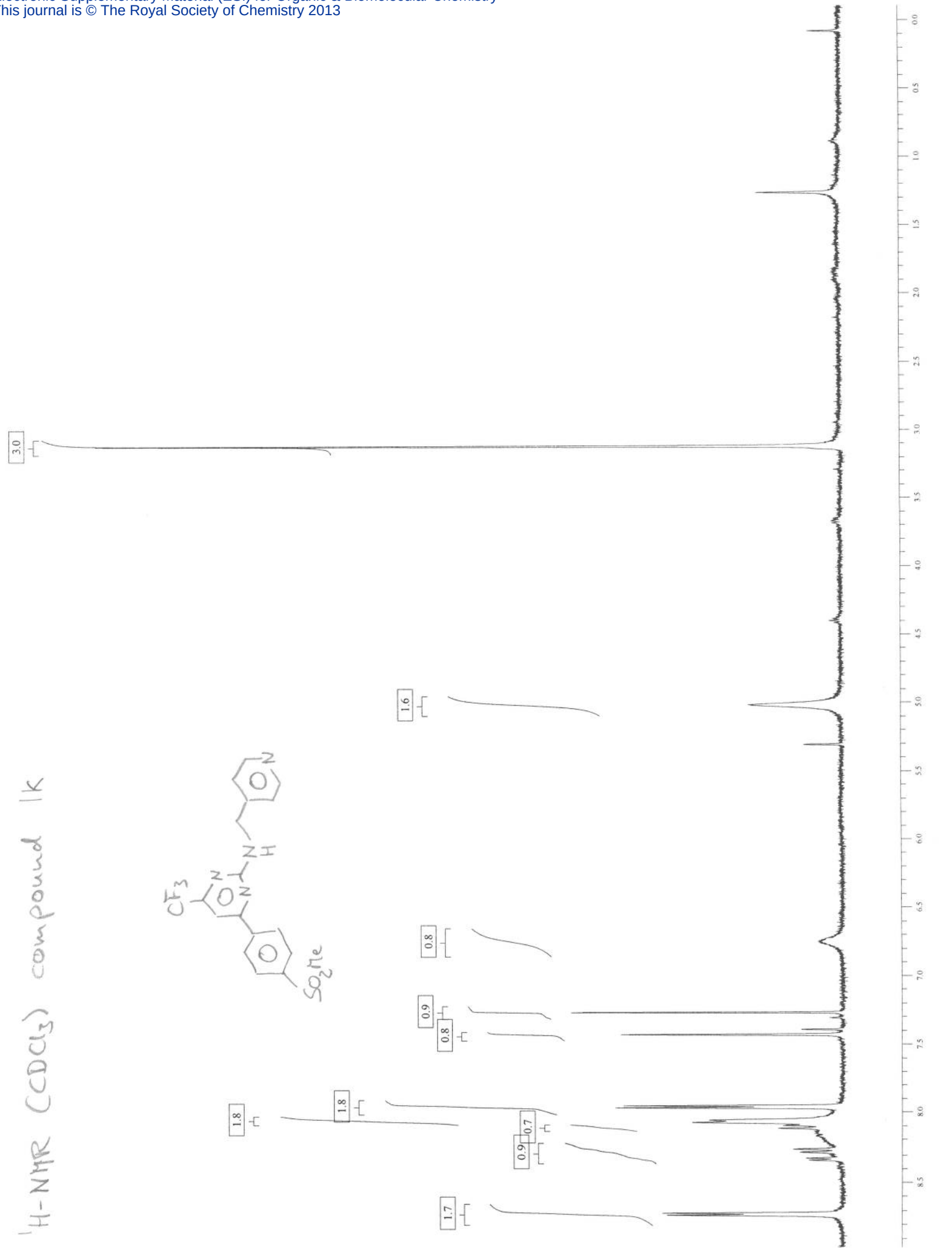

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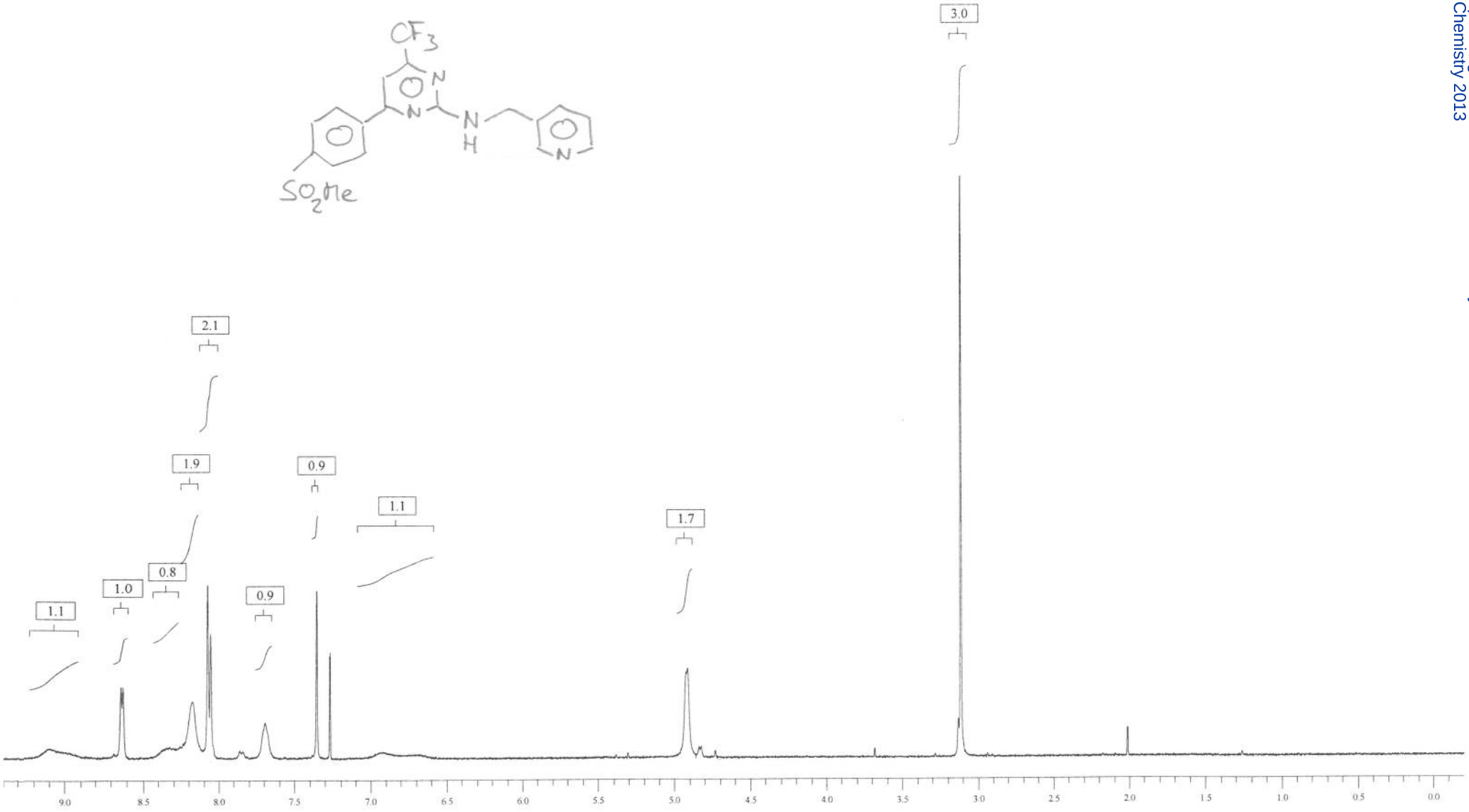

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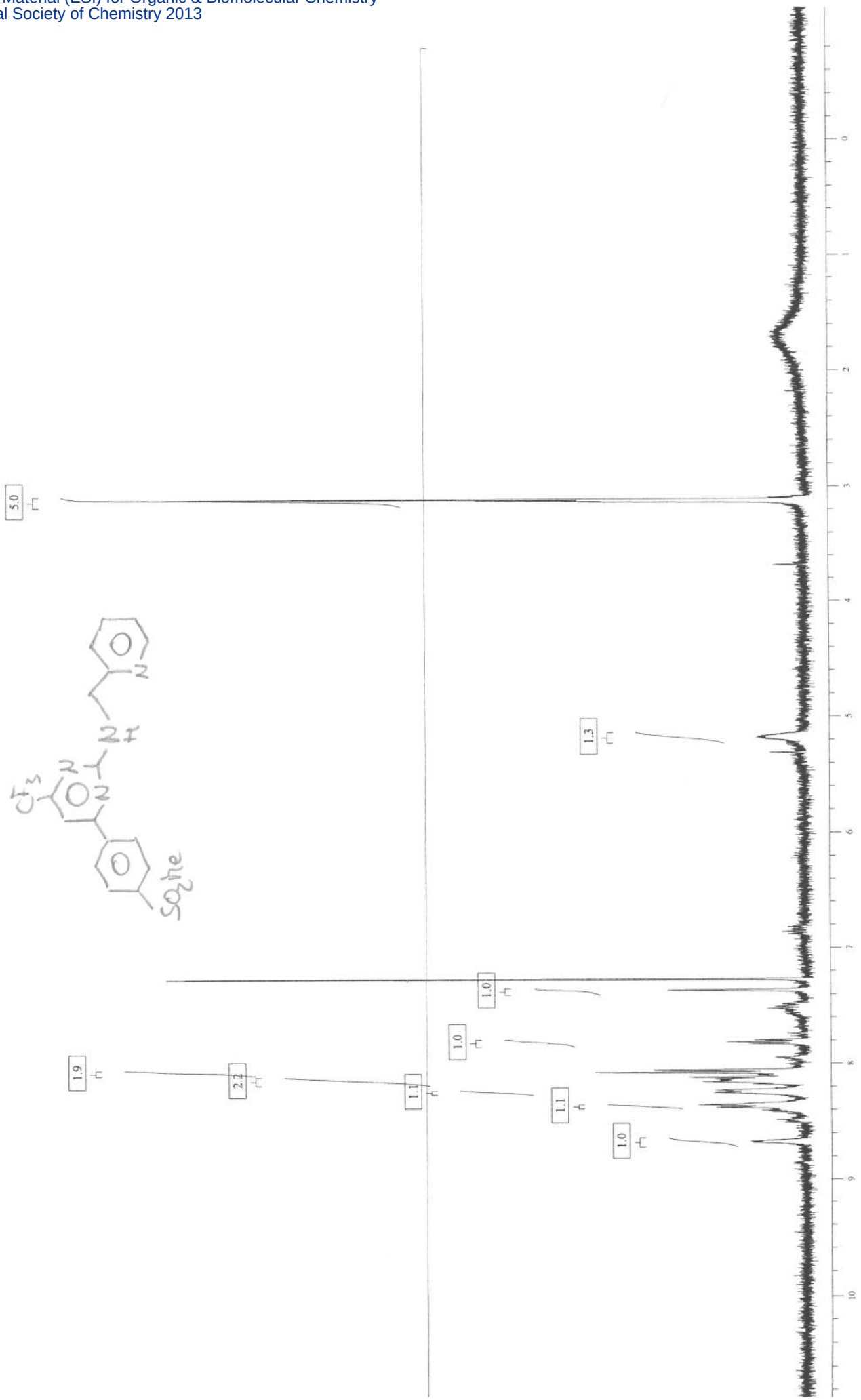
^{1}H - NMR ($CDCl_3$) compound 1m



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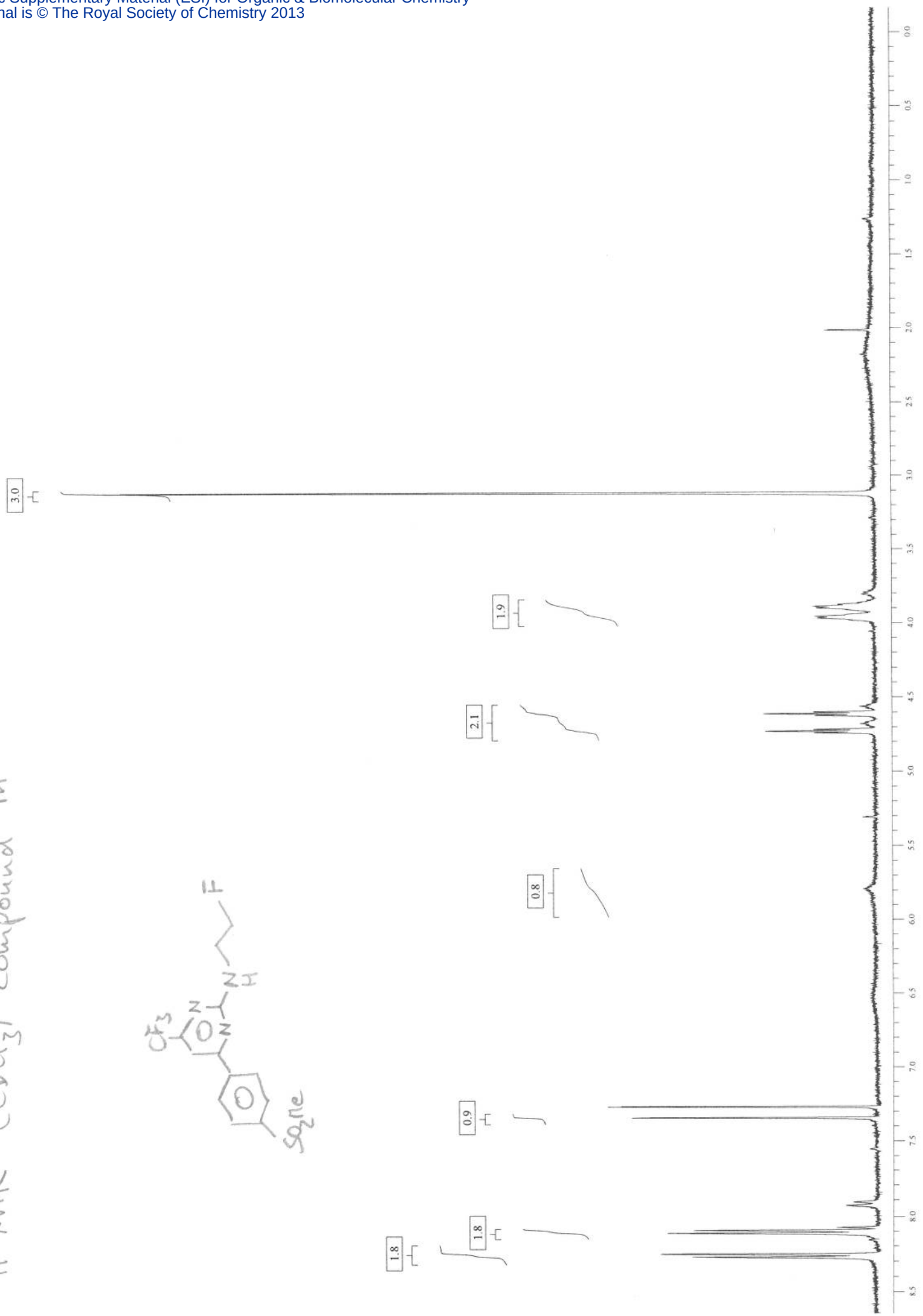

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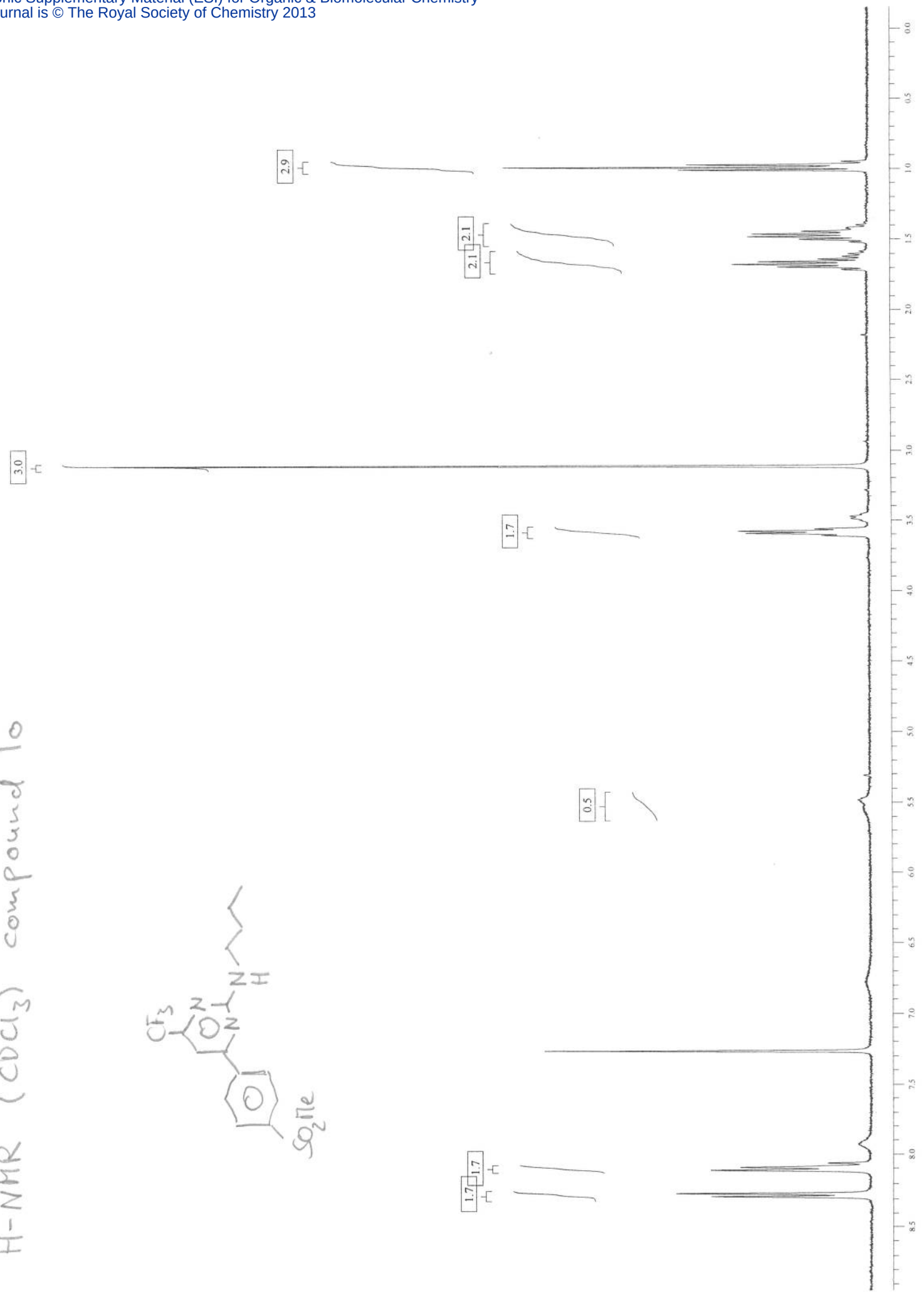
^{1}H-NMR ($CDCl_3$) compound 10



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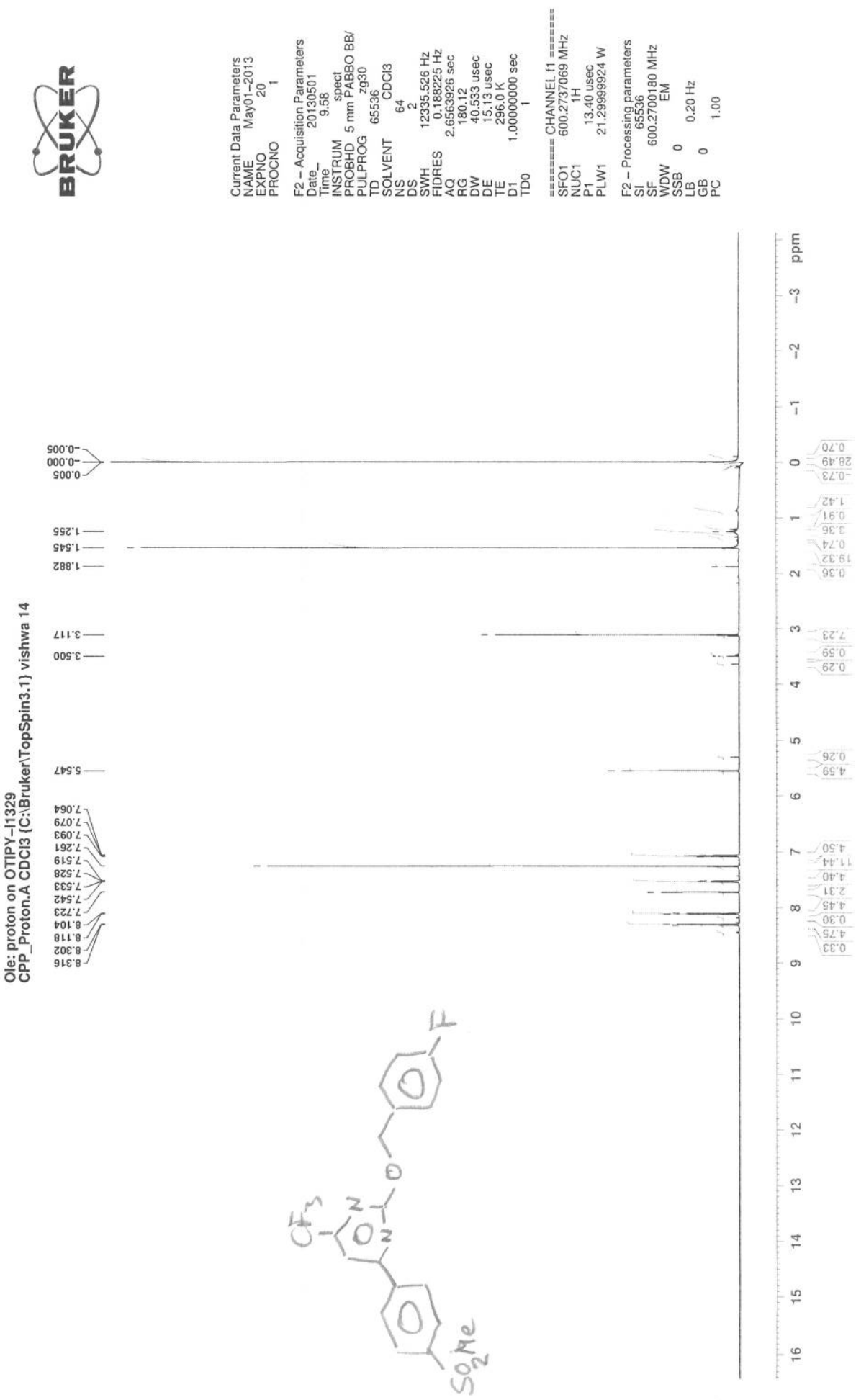
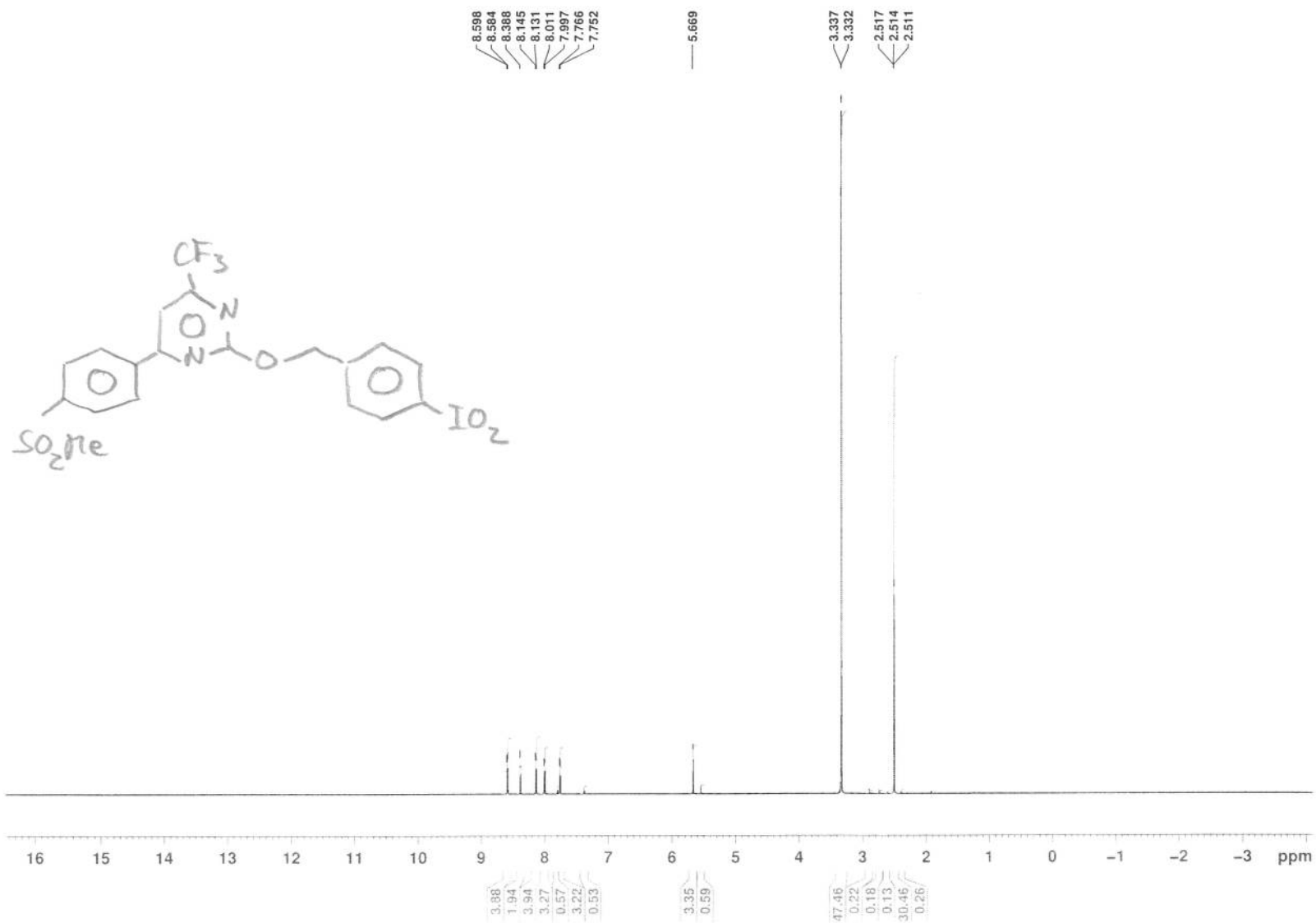
^{1}H-NMR ($CDCl_3$) compound 3a



^{1}H-NMR (d_6-DMSO) compound 11

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



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DE 15.13 usec
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PLW1 21.29999924 W

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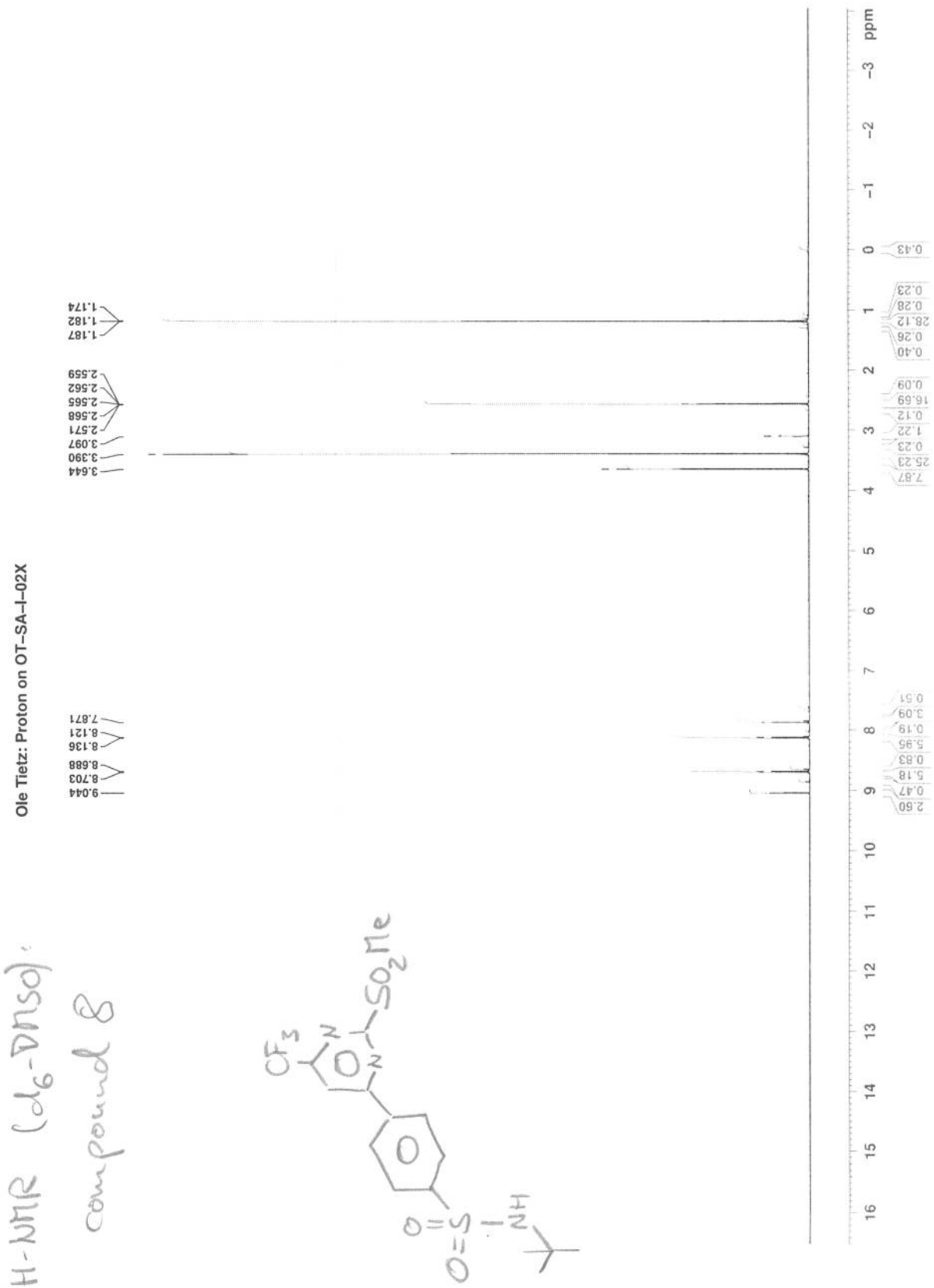
^{1}H-NMR (d_6-DMSO):
compound 8



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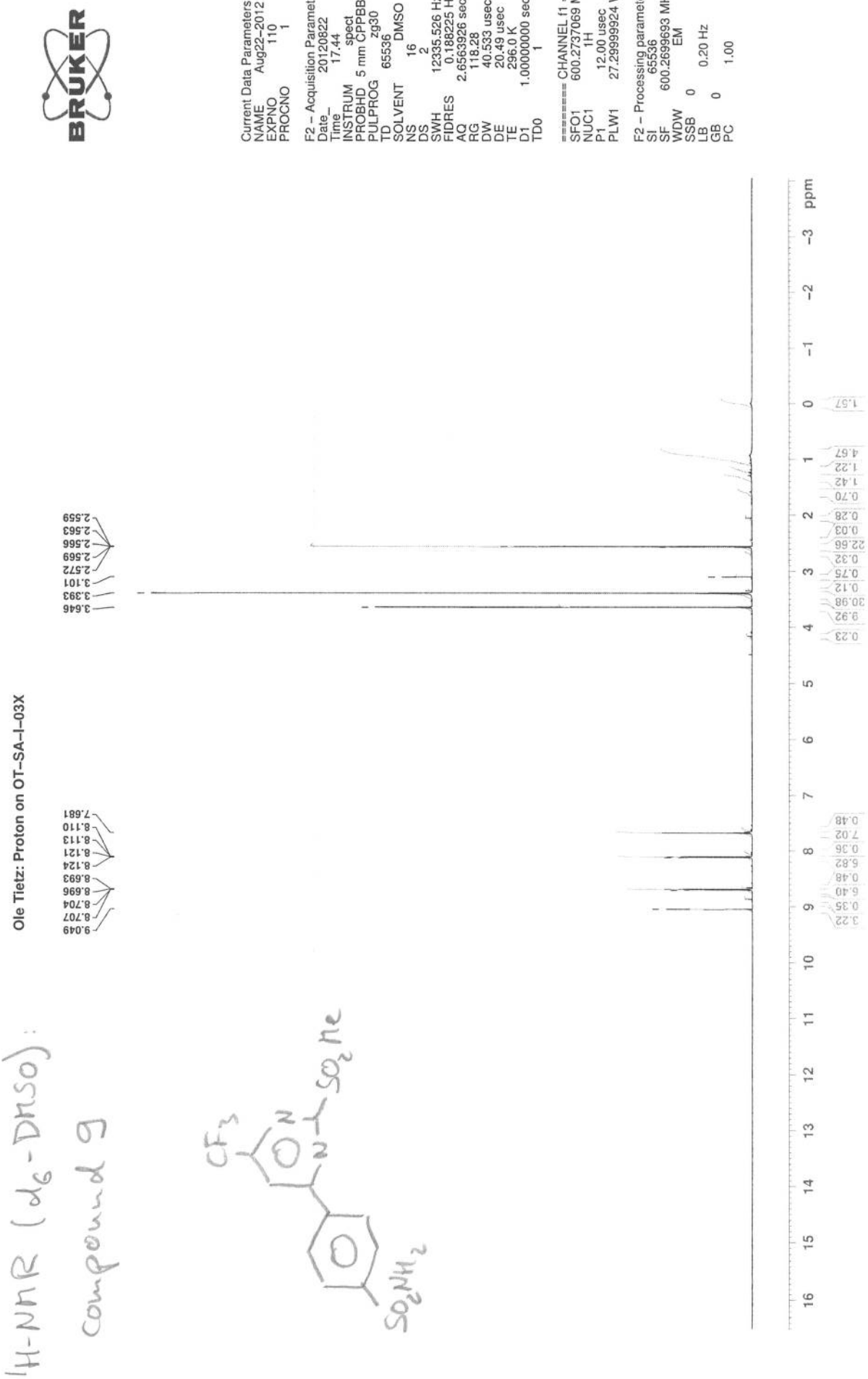

^{1}H-NMR (d_6-DMSO):

Compound 9

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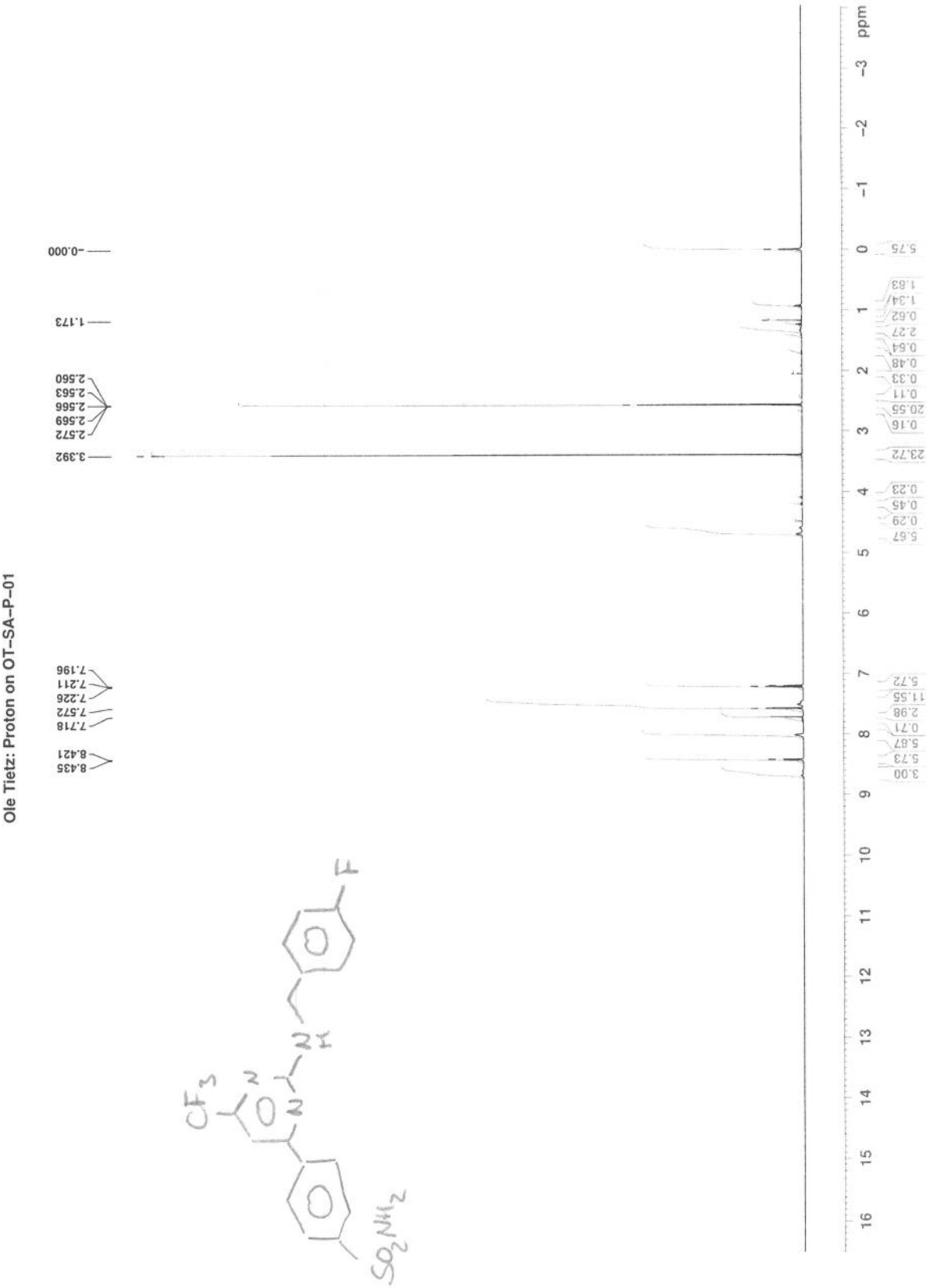
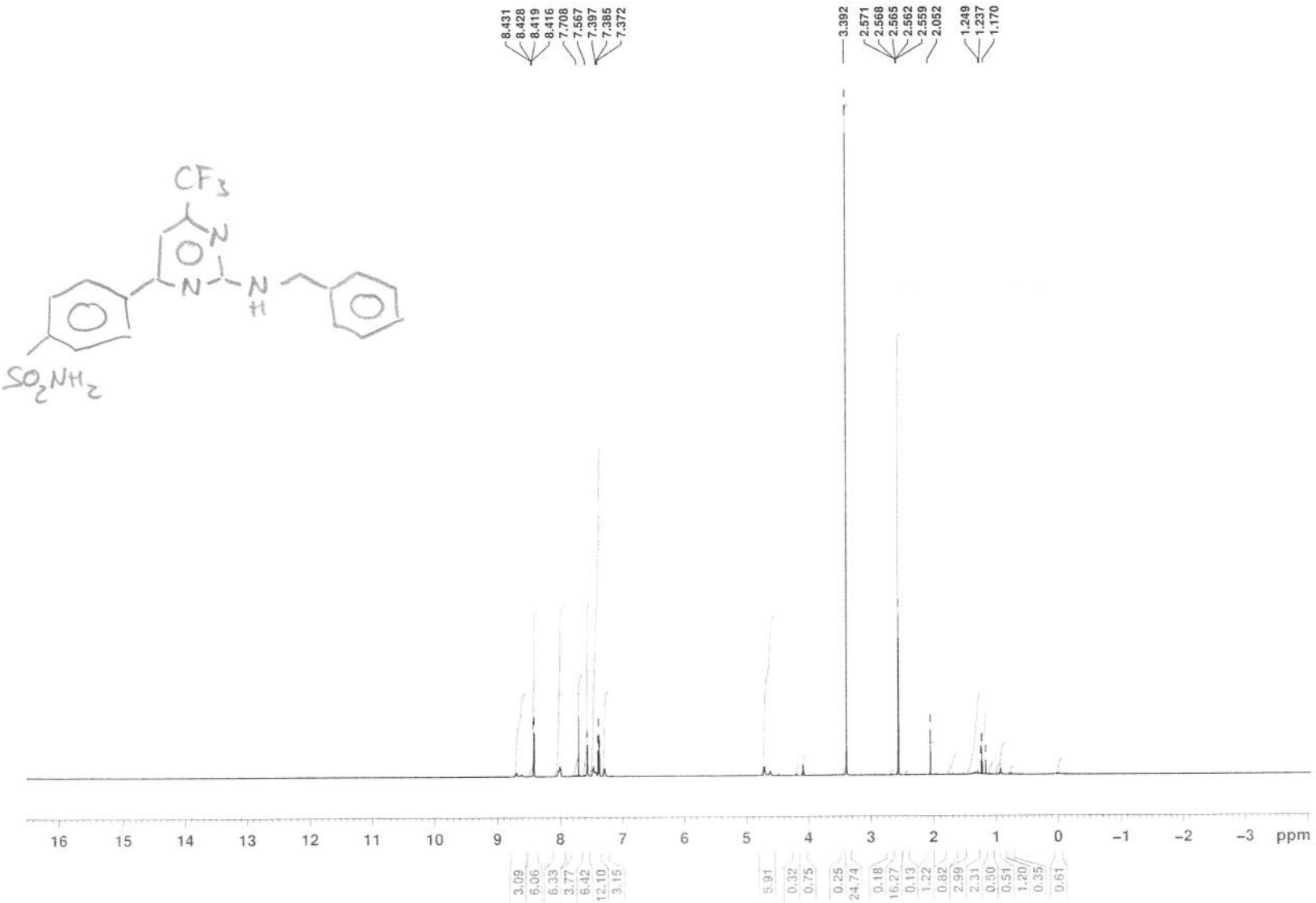
^{1}H-NMR (d_6-DMSO) compound 2a



H-NMR (d_6-DMSO) compound 2b

Ole Tietz: Proton on OT–SA–P–02



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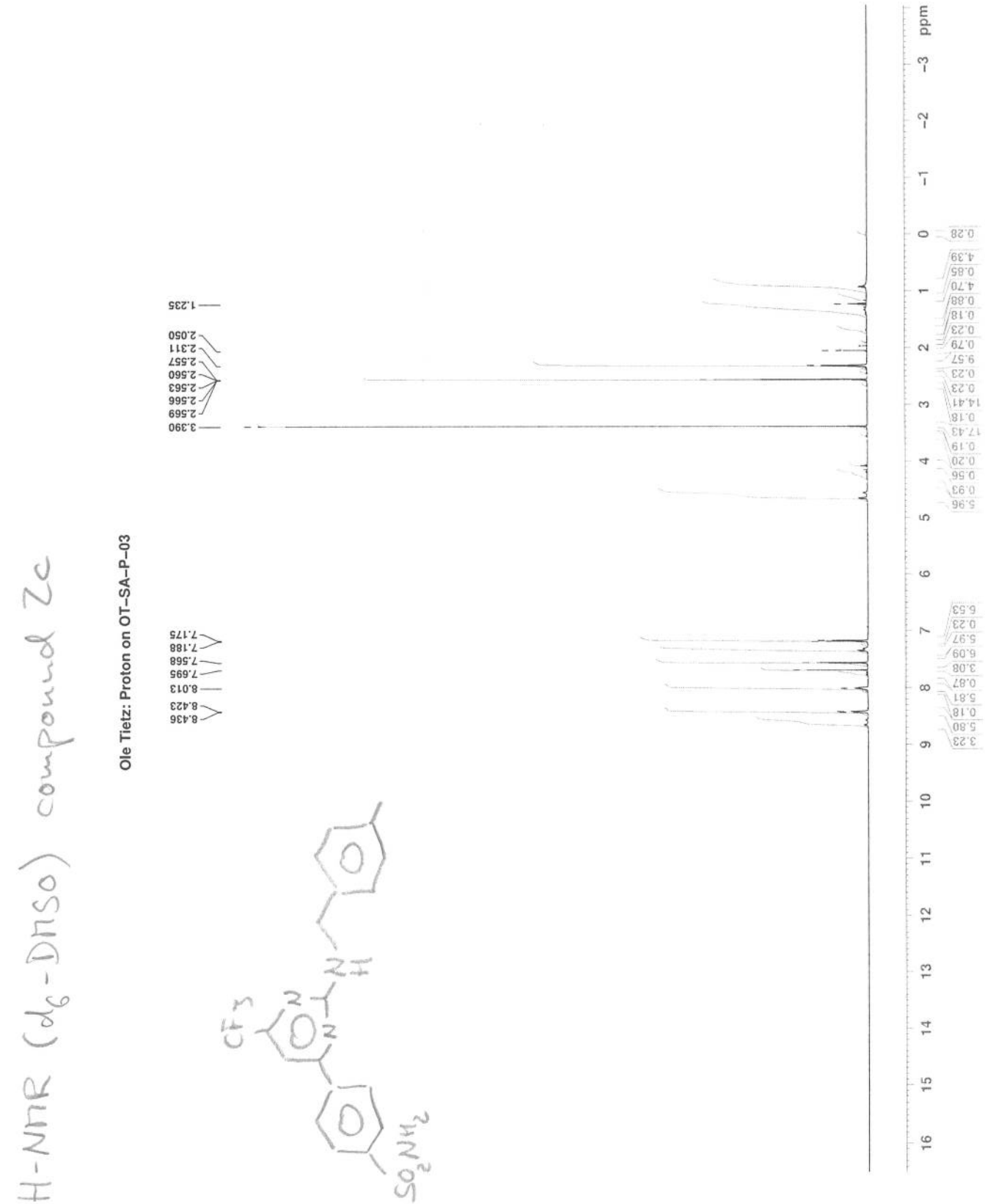
^{1}H-NMR (d_6-DMSO) compound 2c



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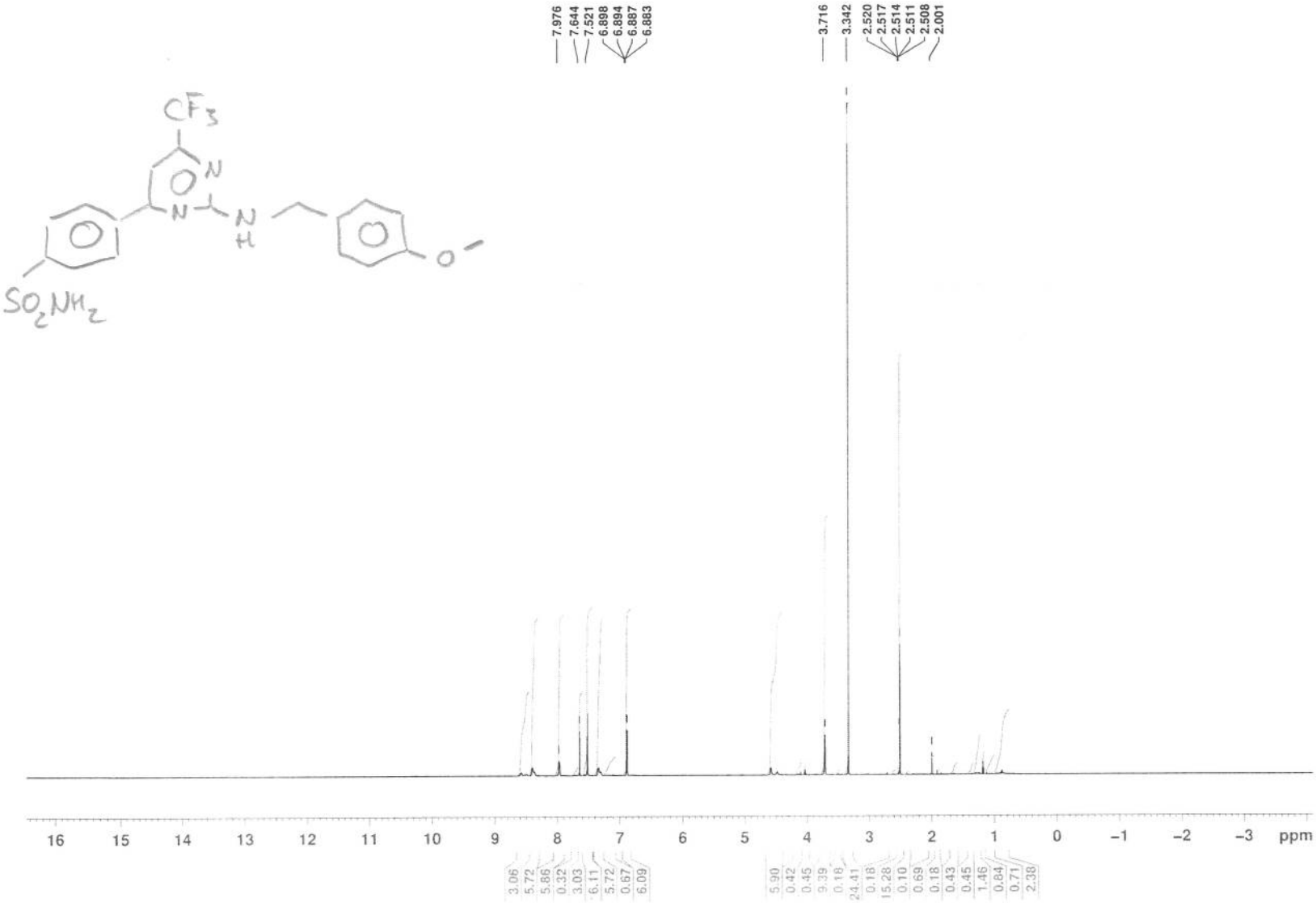

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DE 20.49 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
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PLW1 27.29999924 W

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LB 0.20 Hz
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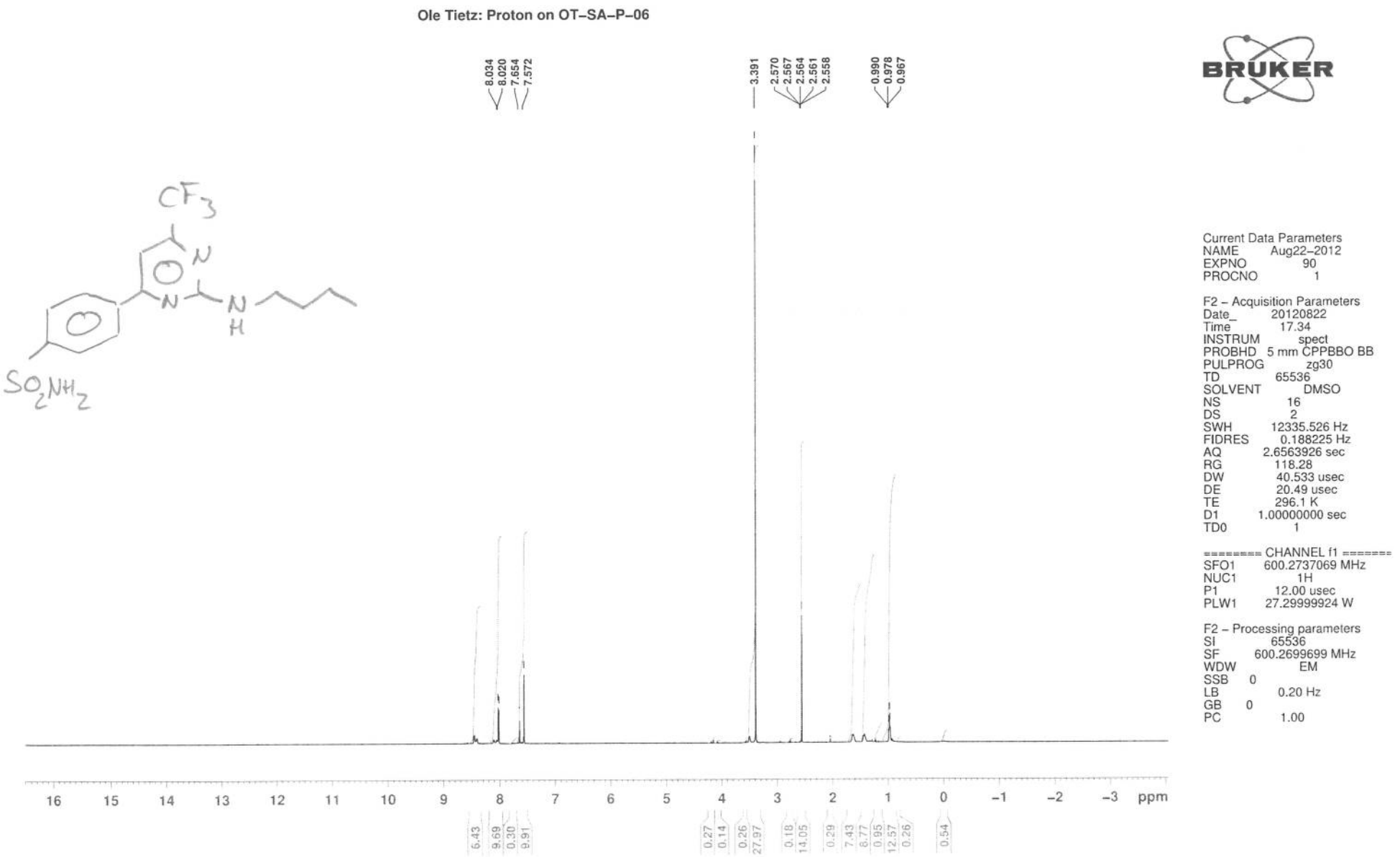
^{1}H-NMR (d_6-DMSO) compound 2e



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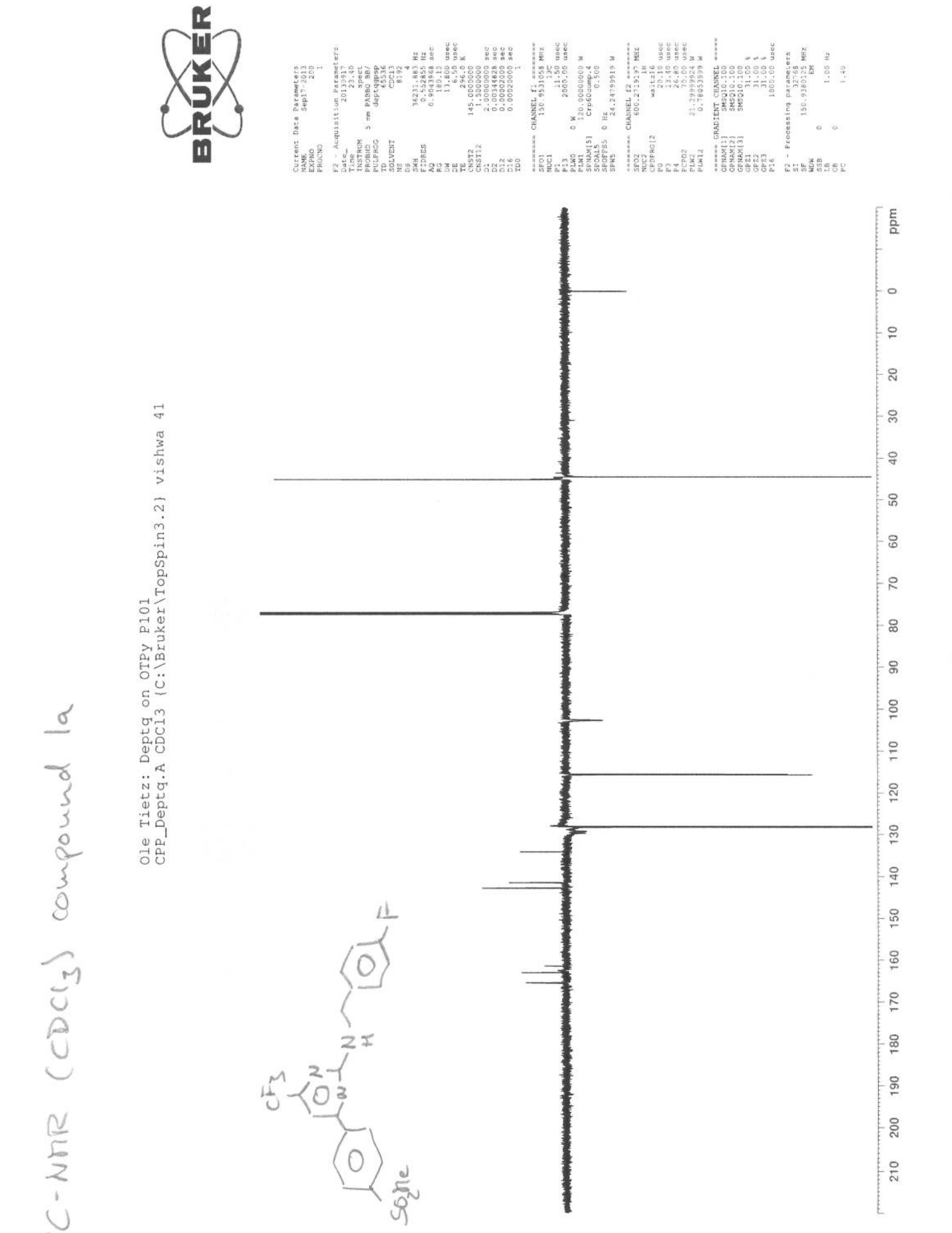
^{13}C-NMR ($CDCl_3$) compound 1a



^{13}C-NMR ($CDCl_3$) compound 1b

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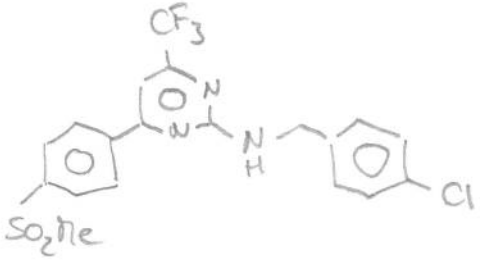

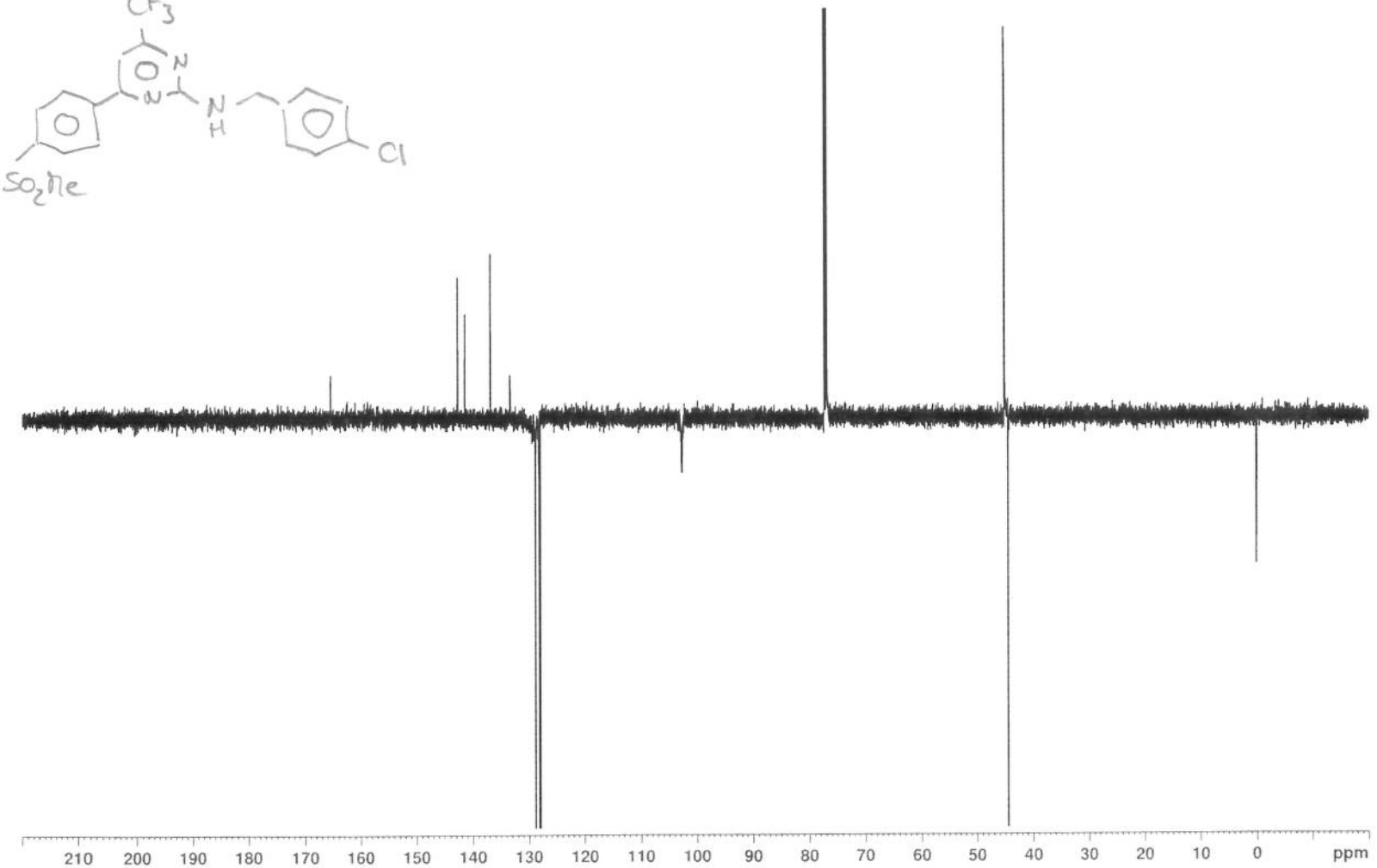

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FIDRES        0.552855 Hz
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P3                13.40 usec
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PC                1.40
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^{13}C-NMR ($CDCl_3$) compound 1c

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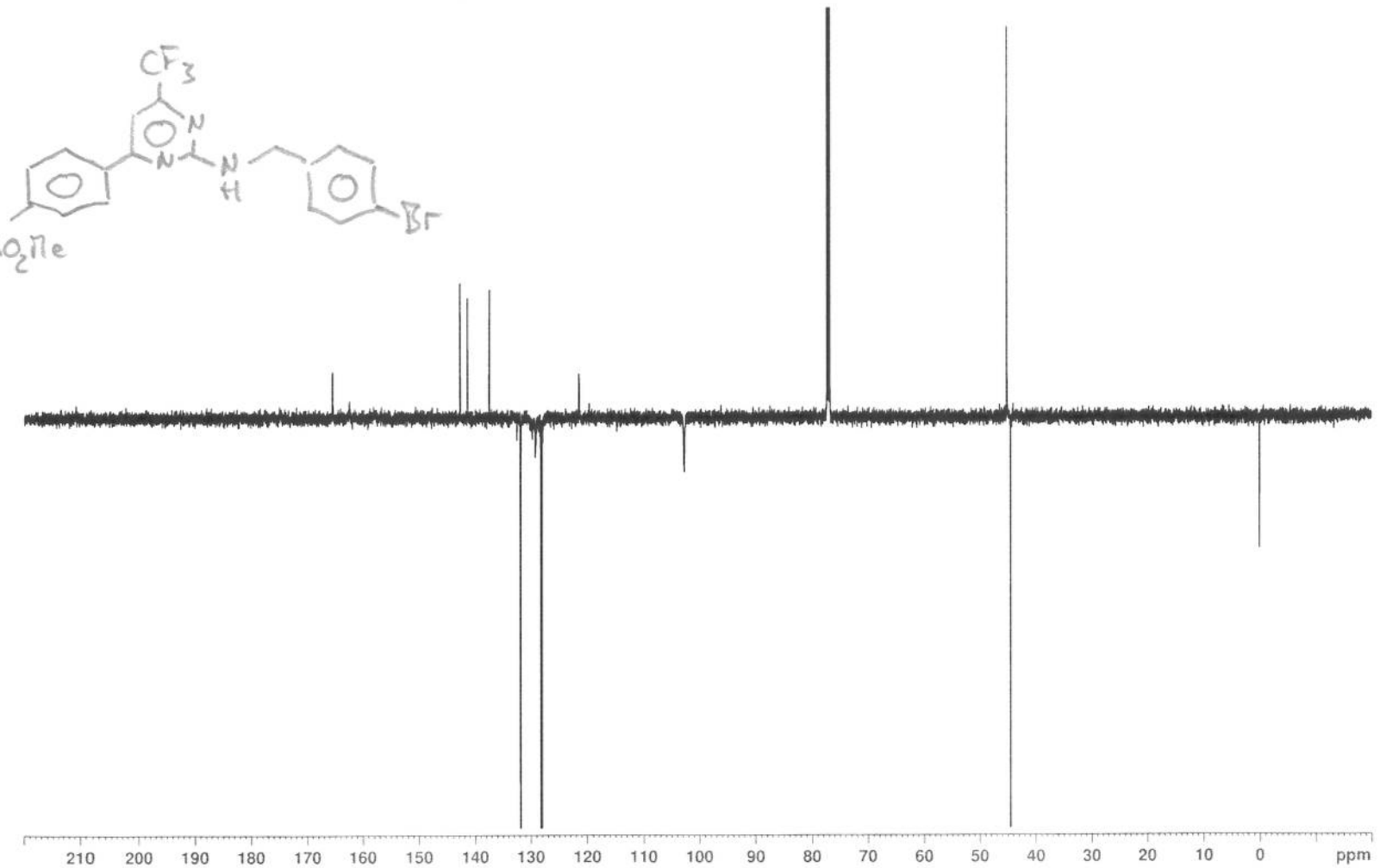
CPP_Deptq.A CDCl3 {C:\Bruker\TopSpin3.2} vishwa 49

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GPZ3                       31.00 %
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^{13}C-NMR ($CDCl_3$) compound 1d

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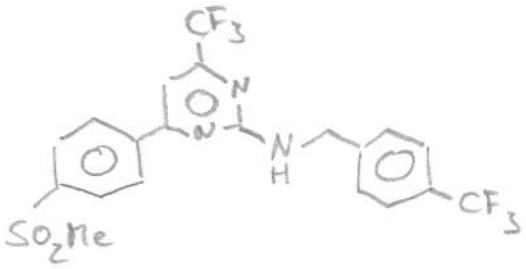

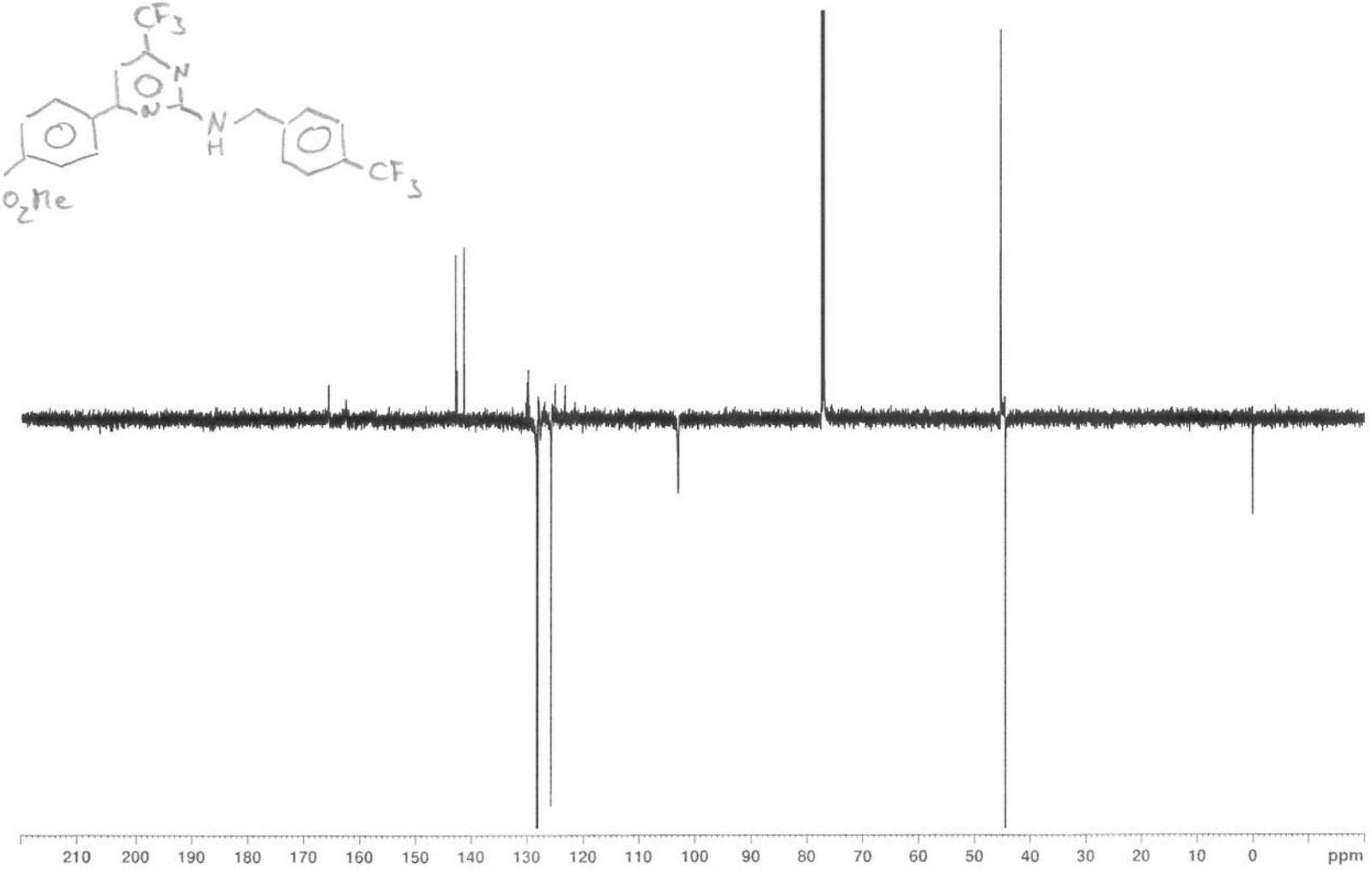


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SWH           36231.883 Hz
FIDRES        0.552855 Hz
AQ            0.9043968 sec
RG                180.12
DW               13.800 usec
DE                6.50 usec
TE               296.0 K
CNST2        145.0000000
CNST12         1.5000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
D16            0.00020000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         150.9531058 MHz
NUC1               13C
P1                11.50 usec
P13             2000.00 usec
PLW0     0 W
PLW1       120.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5          0.500
SPOFFS5  0 Hz
SPW5        24.24799919 W

======== CHANNEL f2 ========
SFO2         600.2719197 MHz
NUC2               1H
CPDPRG[2          waltz16
P0                20.10 usec
P3                13.40 usec
P4                26.80 usec
PCPD2             70.00 usec
PLW2        21.29999924 W
PLW12        0.78053999 W

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

F2 - Processing parameters
SI                32768
SF           150.9380117 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

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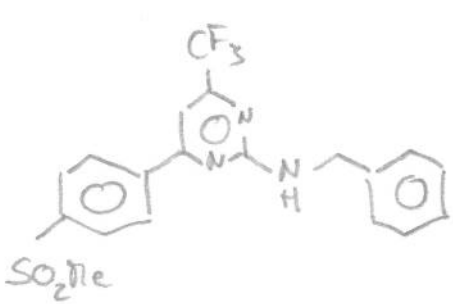
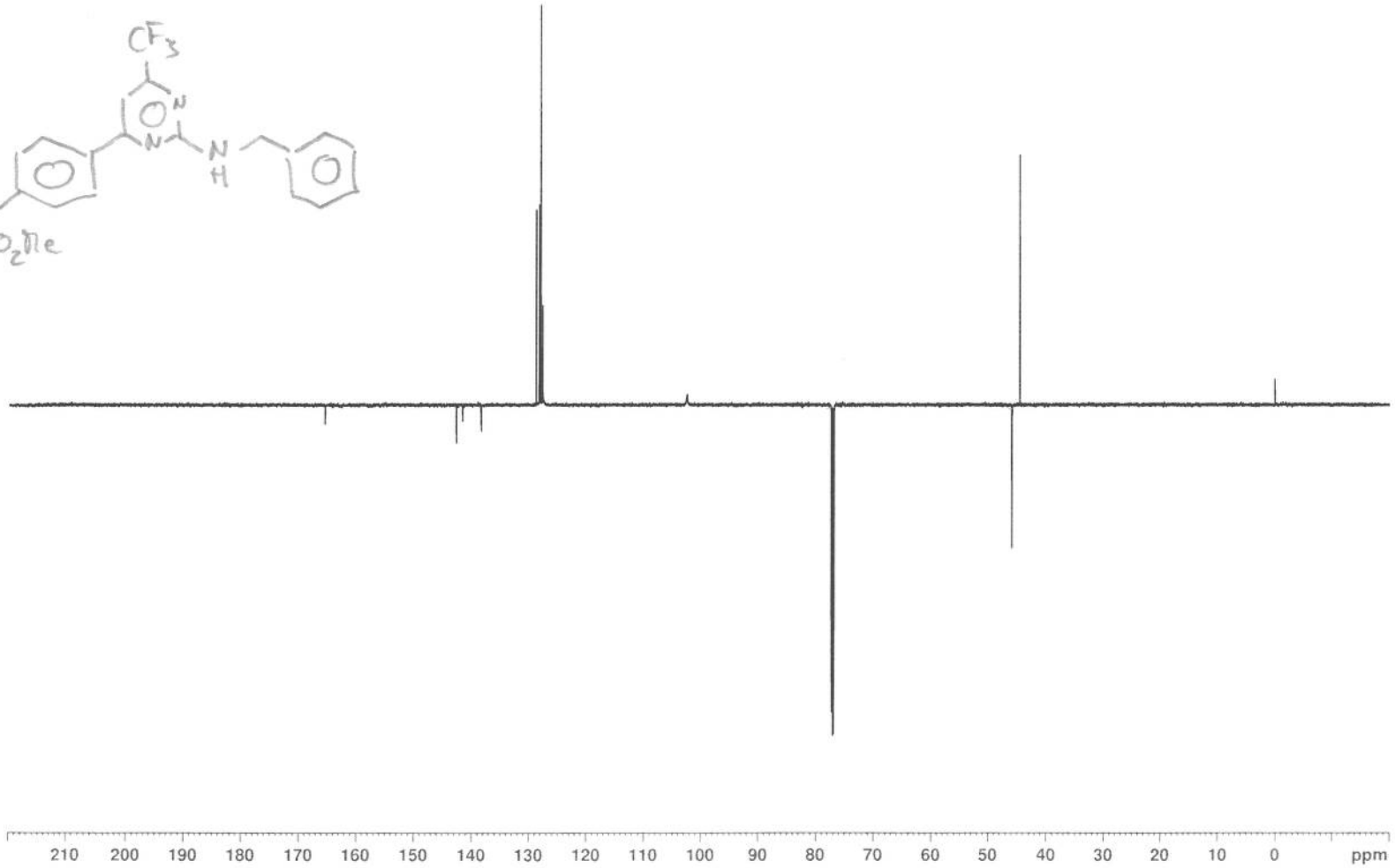
^{13}C-NMR ($CDCl_3$) compound 1e

Ole Tietz: Deptq on OTPY P105
CPP_Deptq.A CDCl3 {C:\Bruker\TopSpin3.2} vishwa 35



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Current Data Parameters
NAME          Sep09-2013
EXPNO                 70
PROCNO                 1

F2 - Acquisition Parameters
Date_          20130910
Time              6.11
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG       deptqgpsp
TD                65536
SOLVENT           CDCl3
NS                 4400
DS                    4
SWH           36231.883 Hz
FIDRES        0.552855 Hz
AQ            0.9043968 sec
RG                180.12
DW               13.800 usec
DE                6.50 usec
TE               296.0 K
CNST2        145.0000000
CNST12         1.5000000
D1             2.0000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
D16            0.00020000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         150.9531058 MHz
NUC1                13C
P1                11.50 usec
P13             2000.00 usec
PLW0     0 W
PLW1      120.00000000 W
SPNAM[5]    Crp60comp.4
SPOAL5            0.500
SPOFFS5  0 Hz
SPW5        24.24799919 W

======== CHANNEL f2 ========
SFO2         600.2719197 MHz
NUC2                 1H
CPDPRG[2          waltz16
PO                20.10 usec
P3                13.40 usec
P4                26.80 usec
PCPD2             70.00 usec
PLW2        21.29999924 W
PLW12        0.78053999 W

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

F2 - Processing parameters
SI                32768
SF          150.9380129 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

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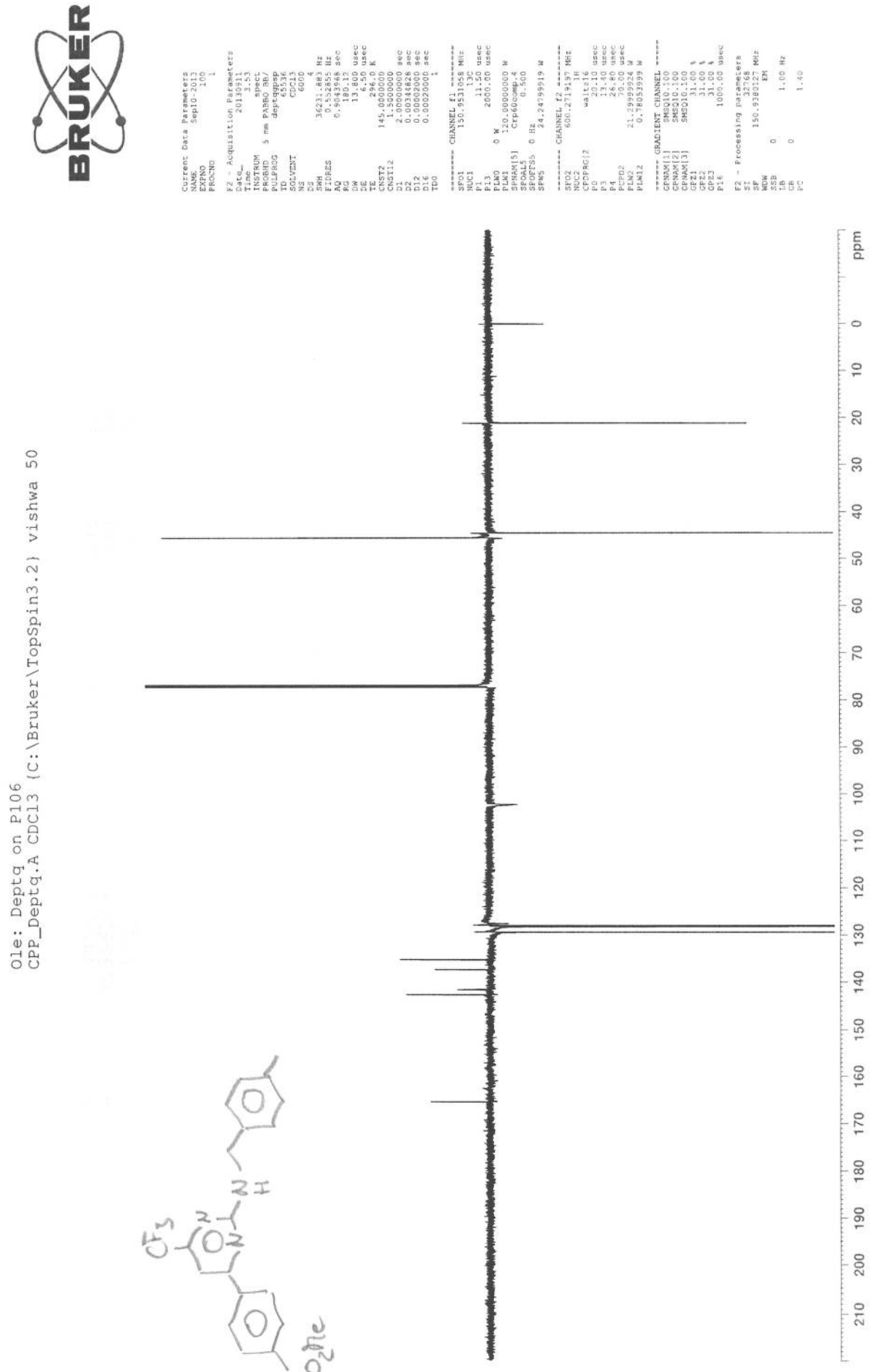
^{13}C-NMR ($CDCl_3$) compound 14



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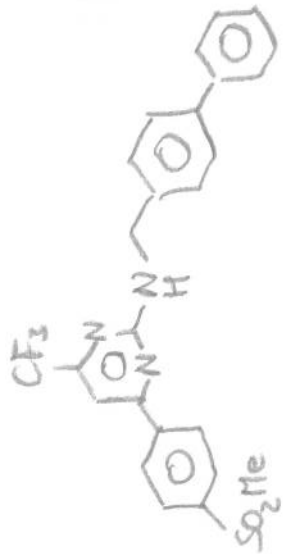
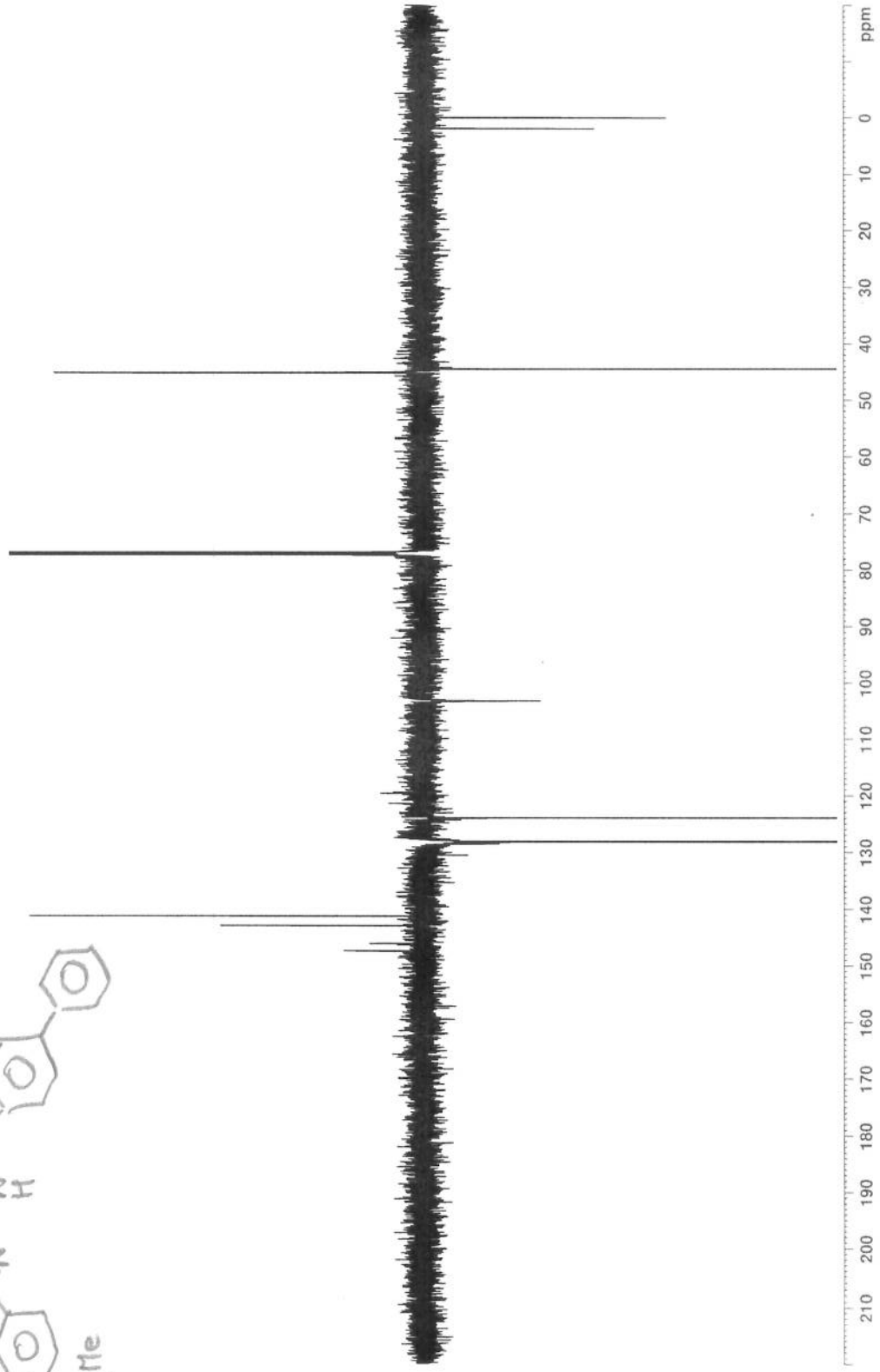
^{13}C-NMR ($CDCl_3$) compound 1g



Ole Tietz: Deptq on P110
CPP_Deptq.A CDCl3 (C:\Bruker\TopSpin3.2) vishwa 27



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Current Data Parameters
NAME       Sep11-2013
EXPNO              40
PROCNO              1

F2 - Acquisition Parameters
Date_        20130912
Time              2.27
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG   deptqgpsp
TD               65536
SOLVENT          CDCl3
NS                4800
DS                   4
SWH         36231.883 Hz
FIDRES          0.552855 Hz
AQ              0.9043568 sec
RG                180.12
DW               13.800 usec
DE                6.50 usec
TE                296.0 K
CNST2       145.0000000
CNST12        1.3000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
D16           0.00020000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        150.9531058 MHz
NUC1               13C
P1               11.50 usec
P13            2000.00 usec
PLW0    0 W  120.00000000 W
PLW1         Crp60comp.4
SPNAM[5]     Crp60comp.4
SPOAL5          0.500
SPOFFS5  0 Hz
SPW5        24.24799919 W

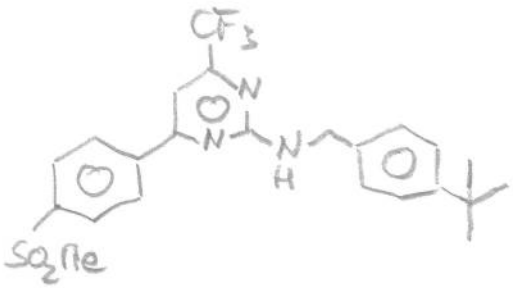
======== CHANNEL f2 ========
SFO2        600.2719197 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            70.00 usec
P3               13.40 usec
P4               26.80 usec
PCPD2            70.00 usec
PLW2        21.29999524 W
PLW12        0.78053999 W

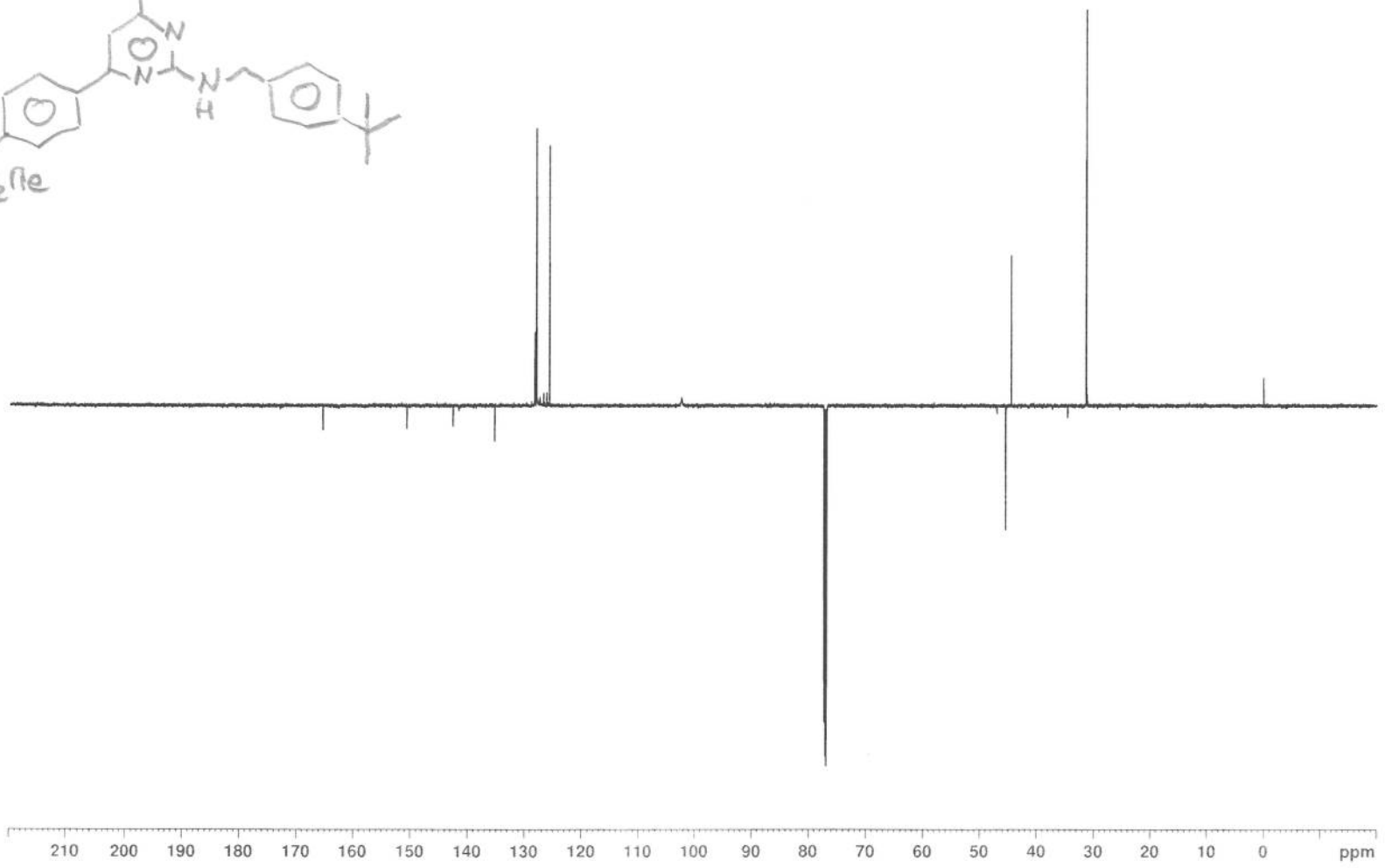
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPZ1             31.00 %
GPZ2             31.00 %
GPZ3             31.00 %
P16            1000.00 usec

F2 - Processing parameters
SI                32768
SF          150.9380128 MHz
WDW                 EM
SSB                 0
LB                  1.00 Hz
GB                  0
PC                  1.40
```

^{13}C-NMR ($CDCl_3$) compound 1h

Ole Tietz: Deptq on P107
CPP_Deptq.A CDCl3 {C:\Bruker\TopSpin3.2} vishwa 25



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Current Data Parameters
NAME            Sep11-2013
EXPNO                   20
PROCNO                   1

F2 - Acquisition Parameters
Date_             20130911
Time                 18.28
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG         deptqgpsp
TD                   65536
SOLVENT              CDCl3
NS                    4800
DS                       4
SWH              36231.883 Hz
FIDRES           0.552855 Hz
AQ               0.9043968 sec
RG                   180.12
DW                  13.800 usec
DE                   6.50 usec
TE                  296.0 K
CNST2           145.0000000
CNST12            1.5000000
D1                2.00000000 sec
D2                0.00344828 sec
D12               0.00002000 sec
D16               0.00020000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            150.9531058 MHz
NUC1                    13C
P1                   11.50 usec
P13                2000.00 usec
PLW0       0 W
PLW1        120.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5             0.500
SPOFFS5    0 Hz
SPW5         24.24799919 W

======== CHANNEL f2 ========
SFO2            600.2719197 MHz
NUC2                    1H
CPDPRG[2           waltz16
P0                   20.10 usec
P3                   13.40 usec
P4                   26.80 usec
PCPD2                70.00 usec
PLW2          21.29999924 W
PLW12          0.78053999 W

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

F2 - Processing parameters
SI                   32768
SF              150.9380129 MHz
WDW                     EM
SSB        0
LB                    1.00 Hz
GB         0
PC                    1.40
```

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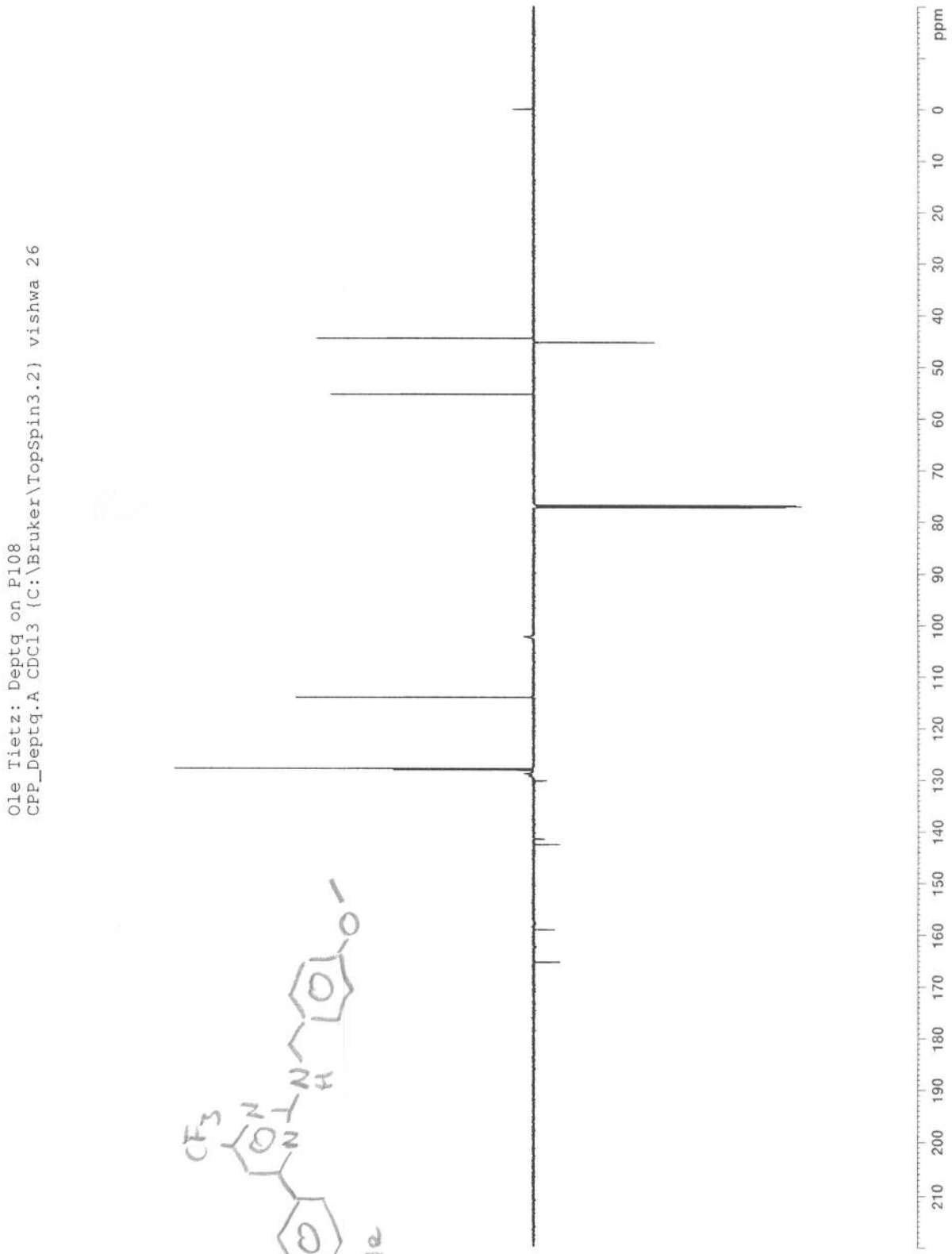
^{13}C-NMR ($CDCl_3$) compound 1i



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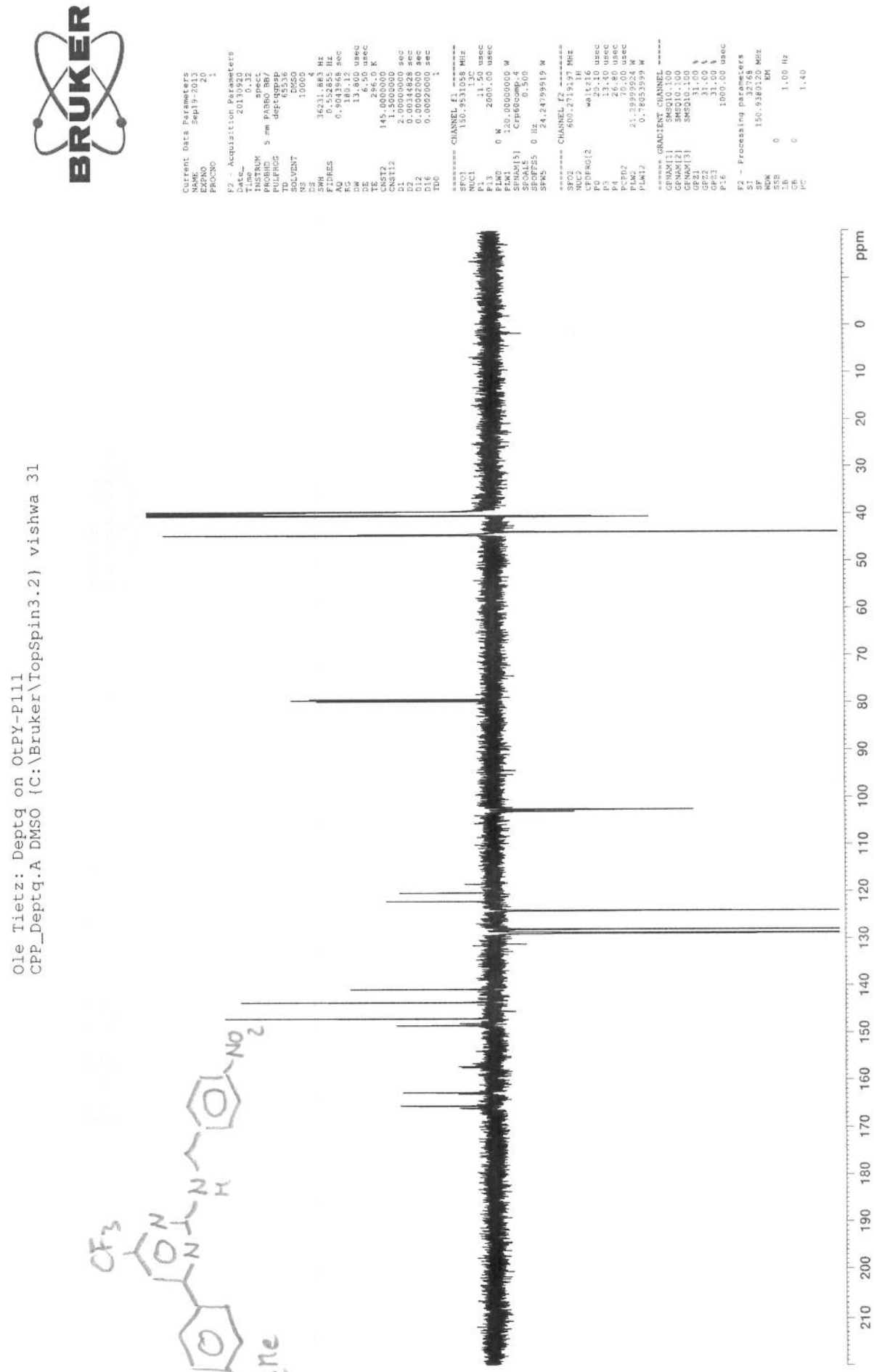
^{13}C-NMR ($CDCl_3$) compound 1j



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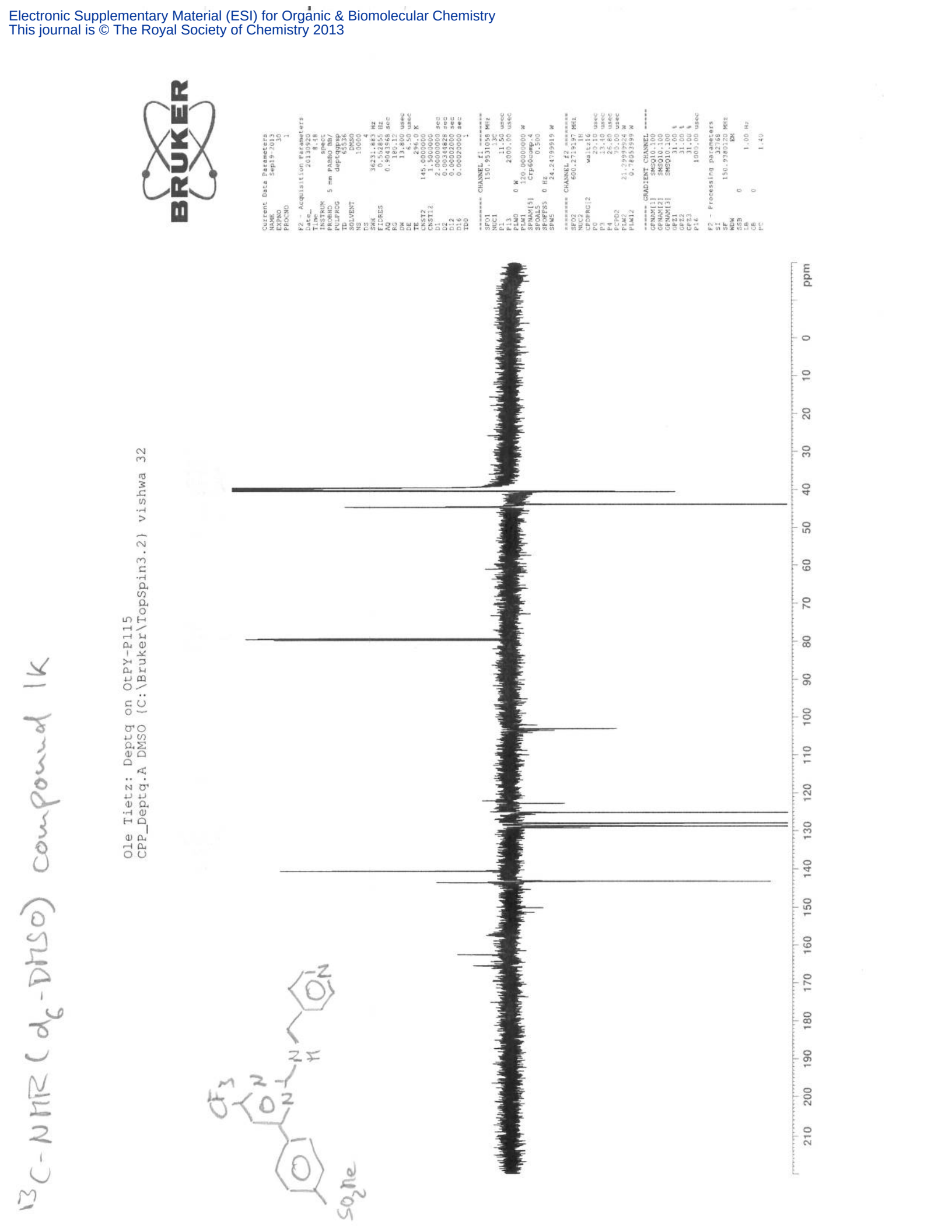
^{13}C-NMR (d_6-DMSO) compound 1K



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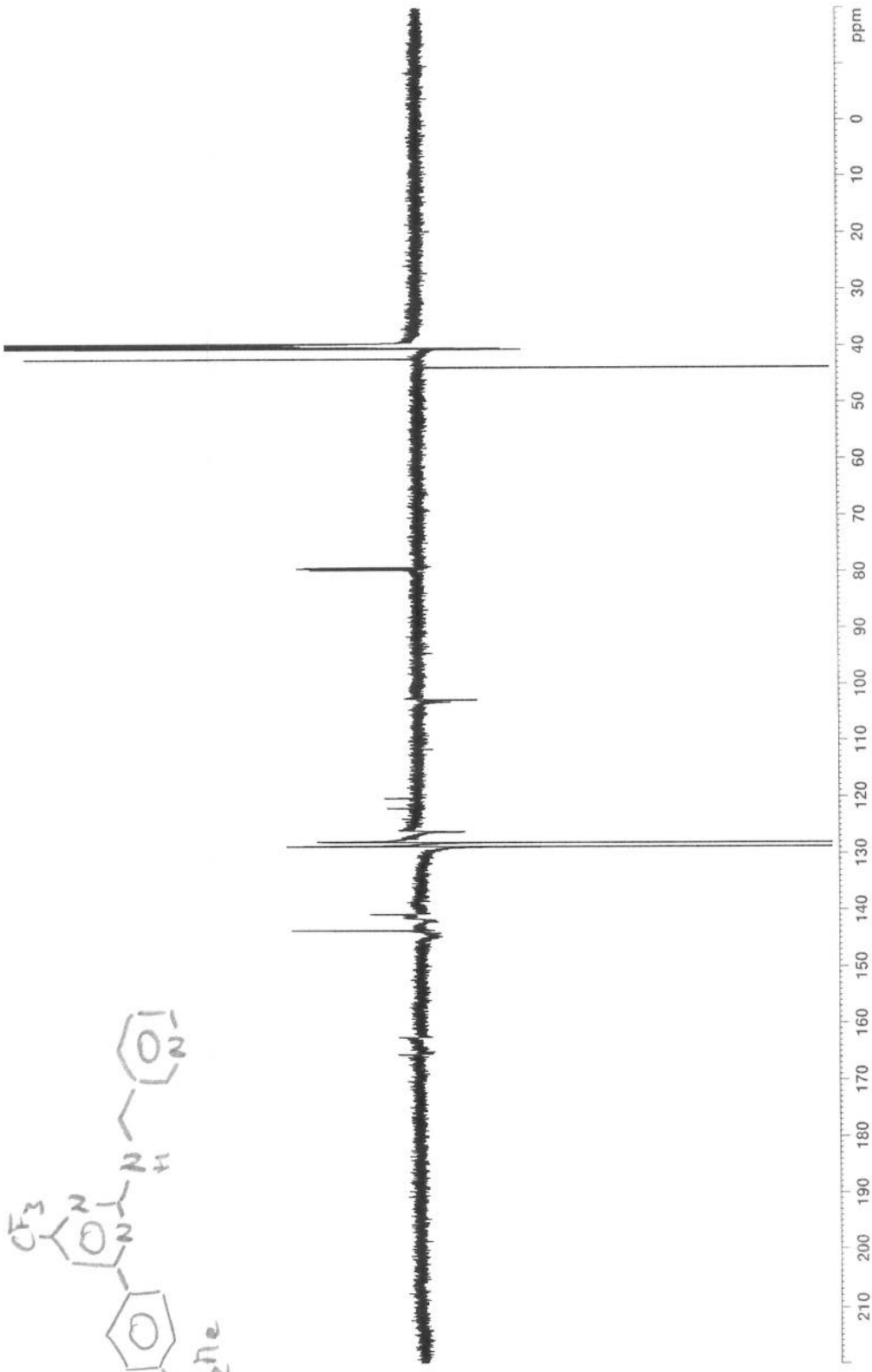
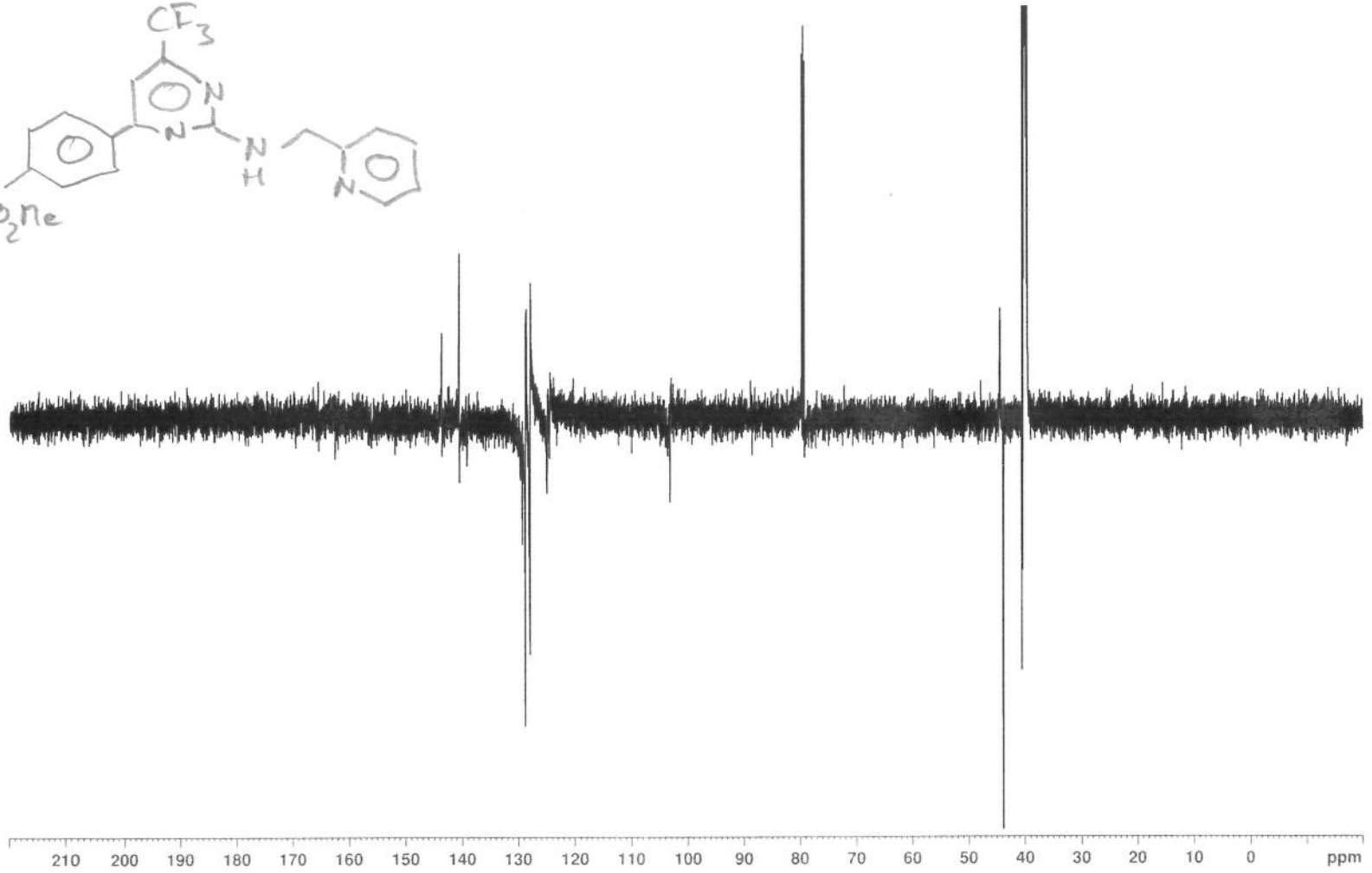
^{13}C - NMR (CD_3-DMSO) compound 16



^{13}C-NMR (d_6-DMSO) compound 1m

Ole Tietz: Deptq on OtPY-P117
CPP_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 34

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Current Data Parameters
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EXPNO                         50
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130921
Time                        1.19
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                deptqgpsp
TD                         65536
SOLVENT                     DMSO
NS                         10000
DS                             4
SWH                    36231.883 Hz
FIDRES                 0.552855 Hz
AQ                     0.9043968 sec
RG                        180.12
DW                        13.800 usec
DE                         6.50 usec
TE                        296.0 K
CNST2                145.0000000
CNST12                 1.5000000
D1                     2.00000000 sec
D2                     0.00344828 sec
D12                    0.00002000 sec
D16                    0.00020000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                 150.9531058 MHz
NUC1                         13C
P1                         11.50 usec
P13                      2000.00 usec
PLW0       0 W
PLW1          120.00000000 W
SPNAM[5]       Crp60comp.4
SPOAL5                   0.500
SPOFFS5    0 Hz
SPW5            24.24799919 W

======== CHANNEL f2 ========
SFO2                 600.2719197 MHz
NUC2                         1H
CPDPRG[2                waltz16
P0                         20.10 usec
P3                         13.40 usec
P4                         26.80 usec
PCPD2                      70.00 usec
PLW2                21.29999924 W
PLW12                0.78053999 W

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

F2 - Processing parameters
SI                         32768
SF                   150.9380120 MHz
WDW                           EM
SSB        0
LB                          1.00 Hz
GB         0
PC                          1.40
```

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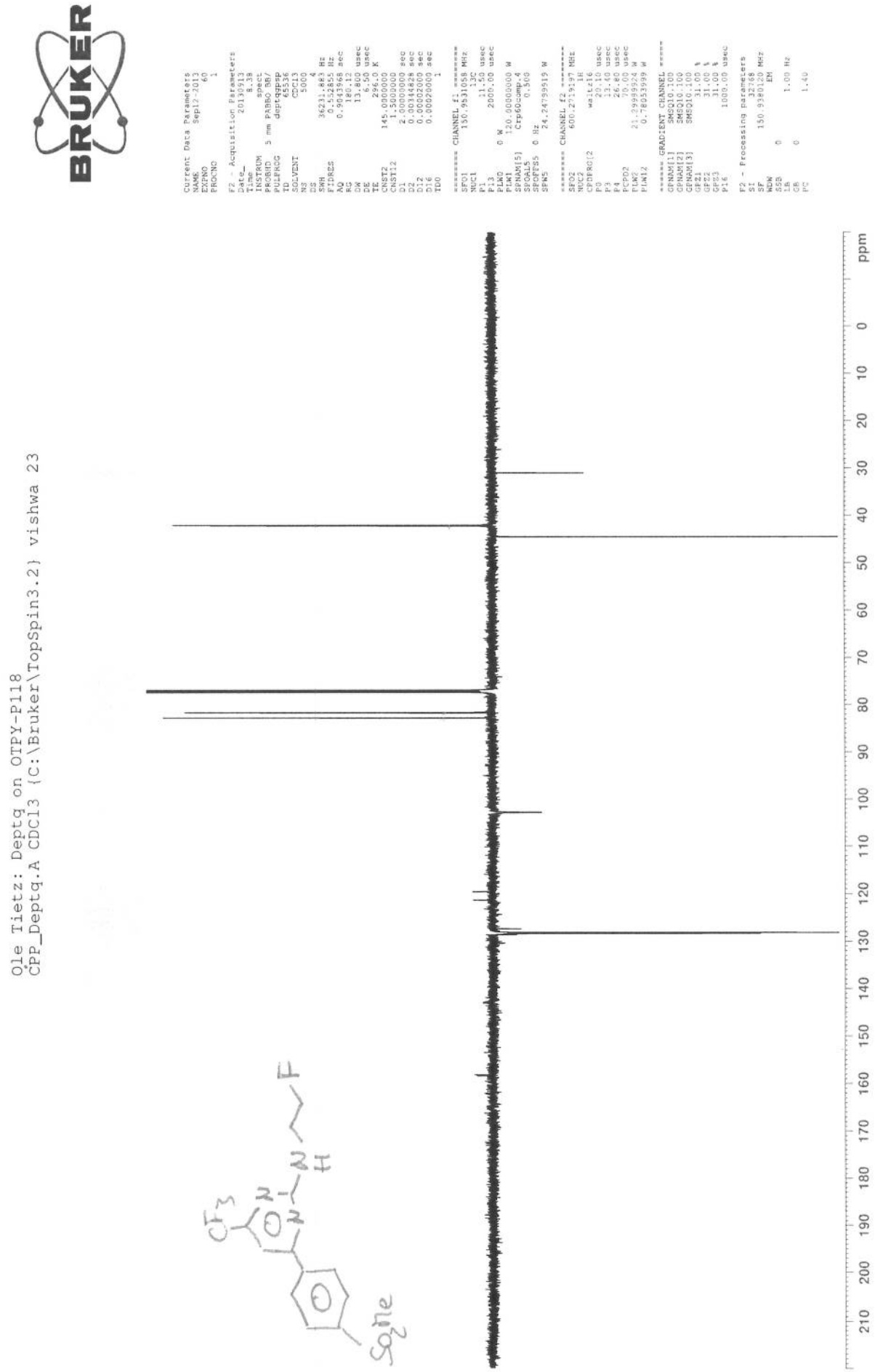
^{13}C-NMR (d_6-DMSO) compound 1h



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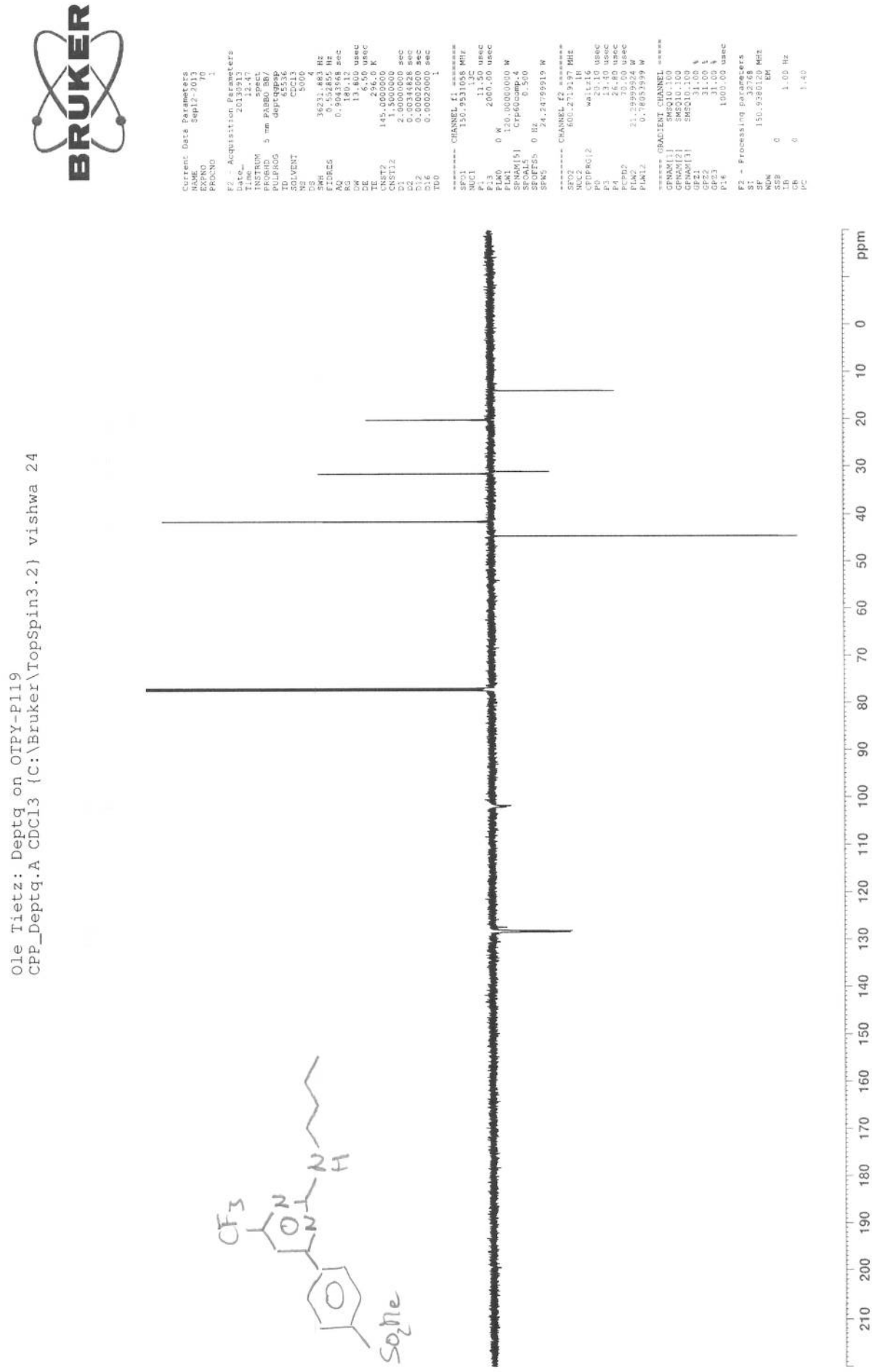
^{13}C-NMR (d_6-DMSO) compound 10



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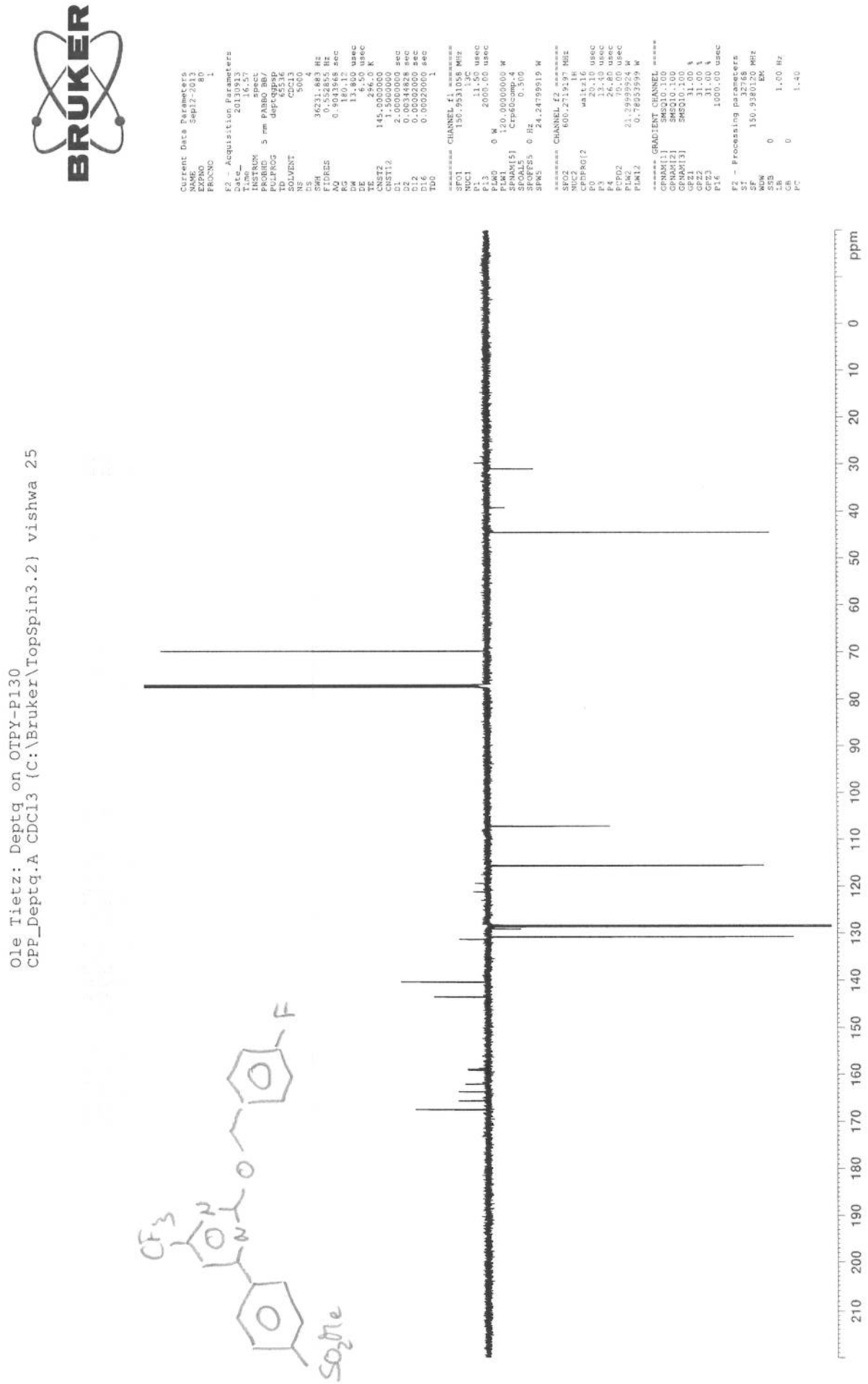
^{13}C-NMR (d_6-DMSO) compound 3a



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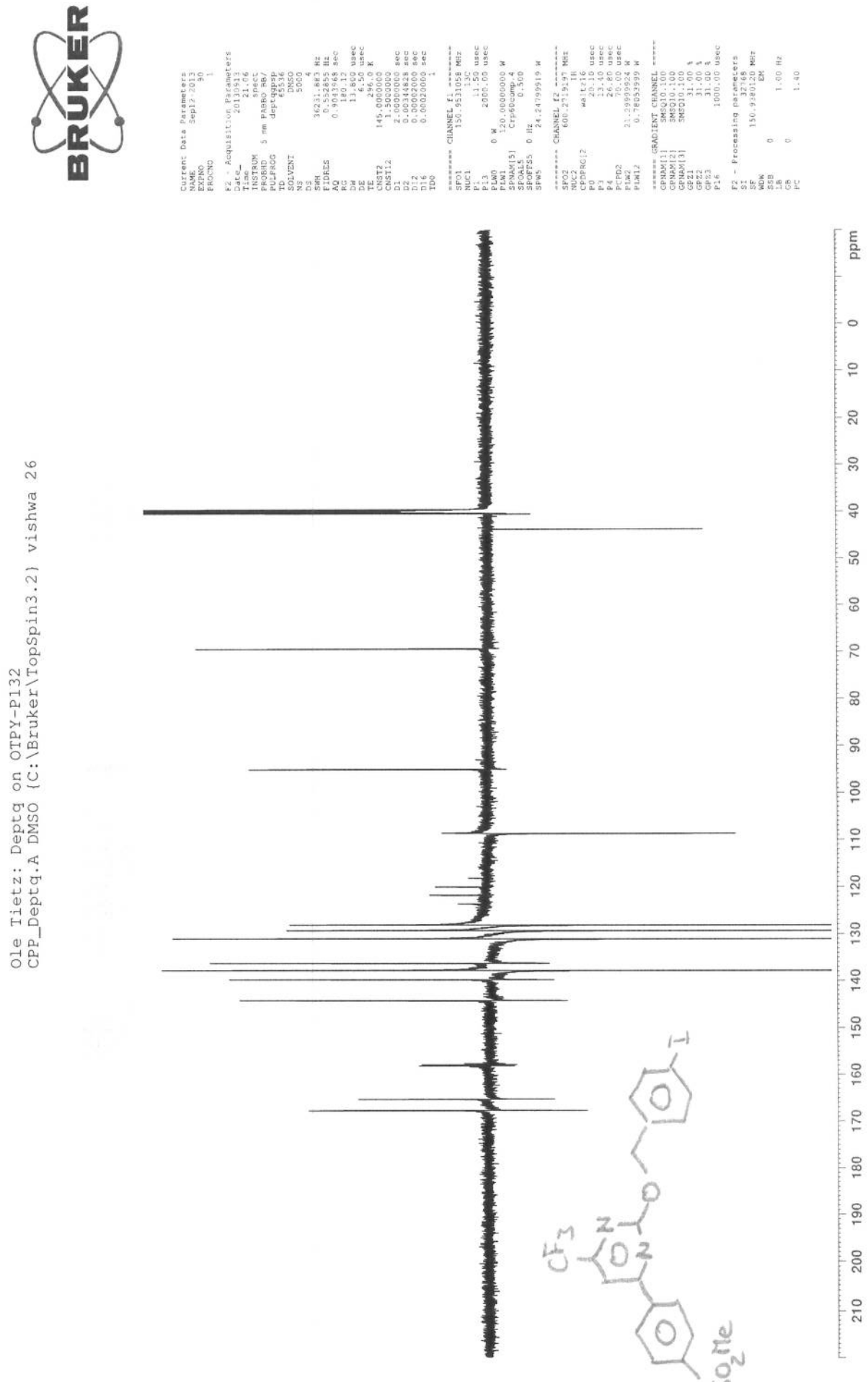
^{13}C-NMR (d_6-DMSO) compound 10



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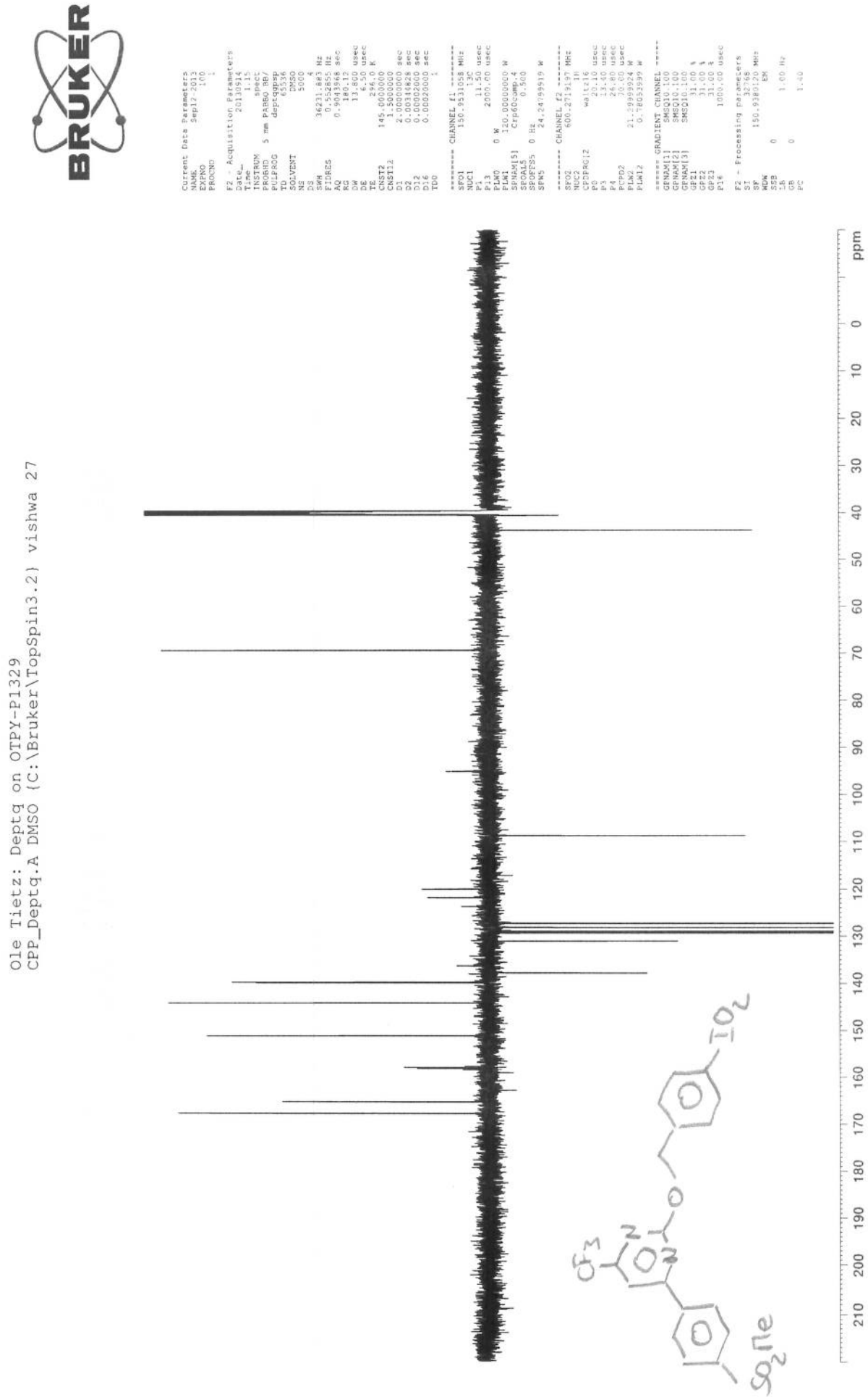
^{13}C-NMR (d_6-DMSO) compound 11



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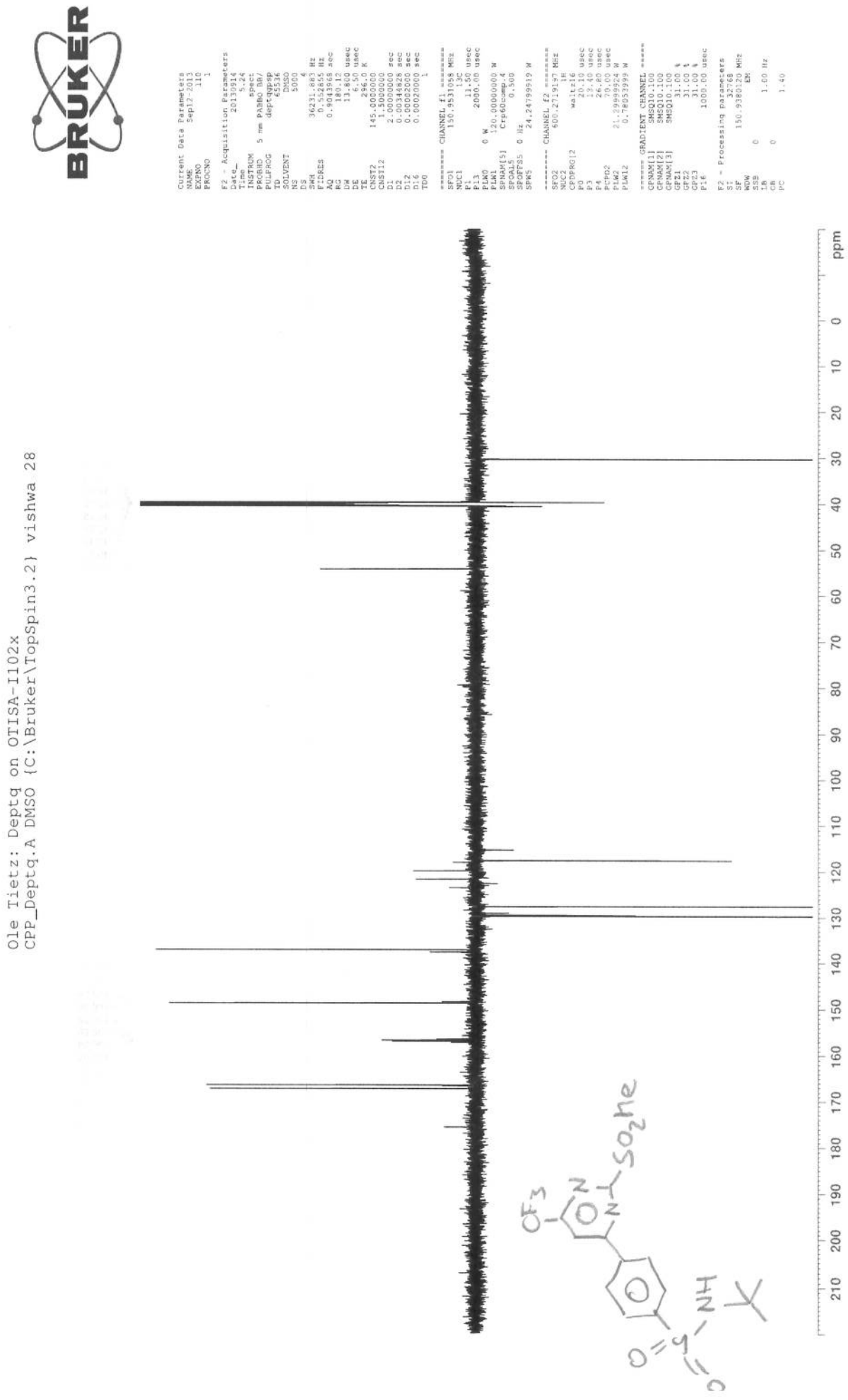
^{13}C-NMR (d_6-DMSO) compounds 8



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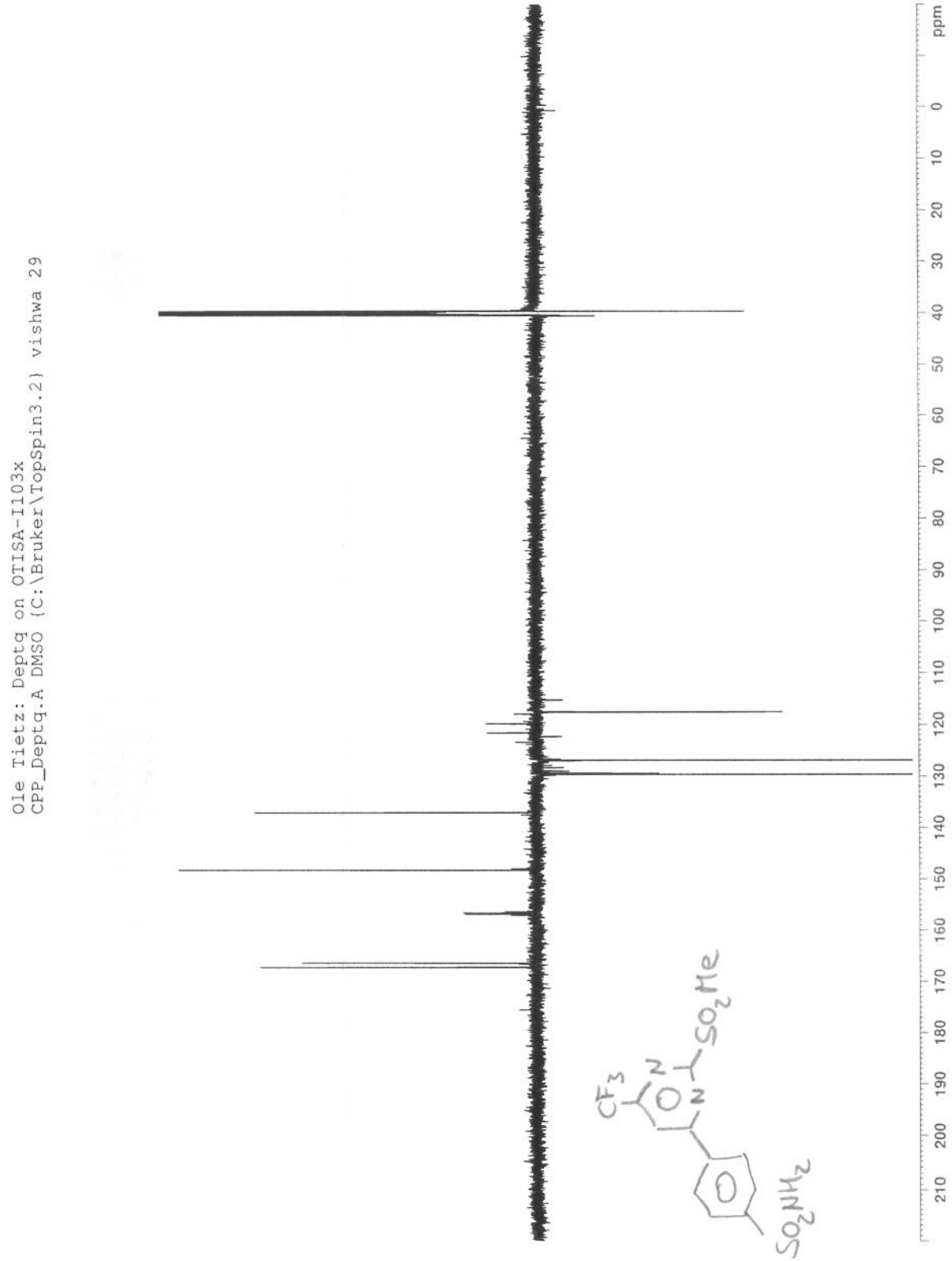
^{13}C-NMR (d_6-DMSO) compound 9



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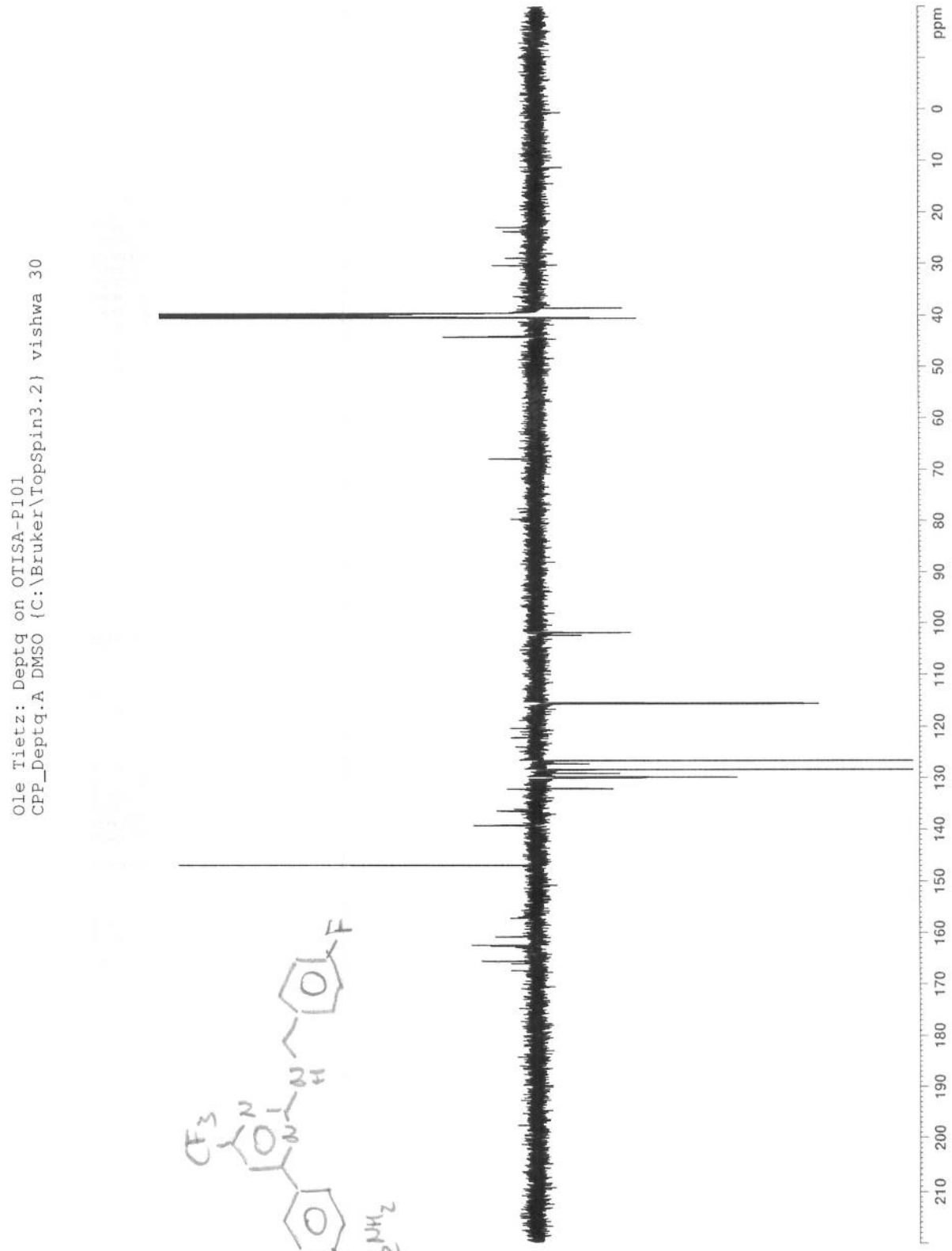
^{13}C-NMR (d_6-DMSO) compound 2a



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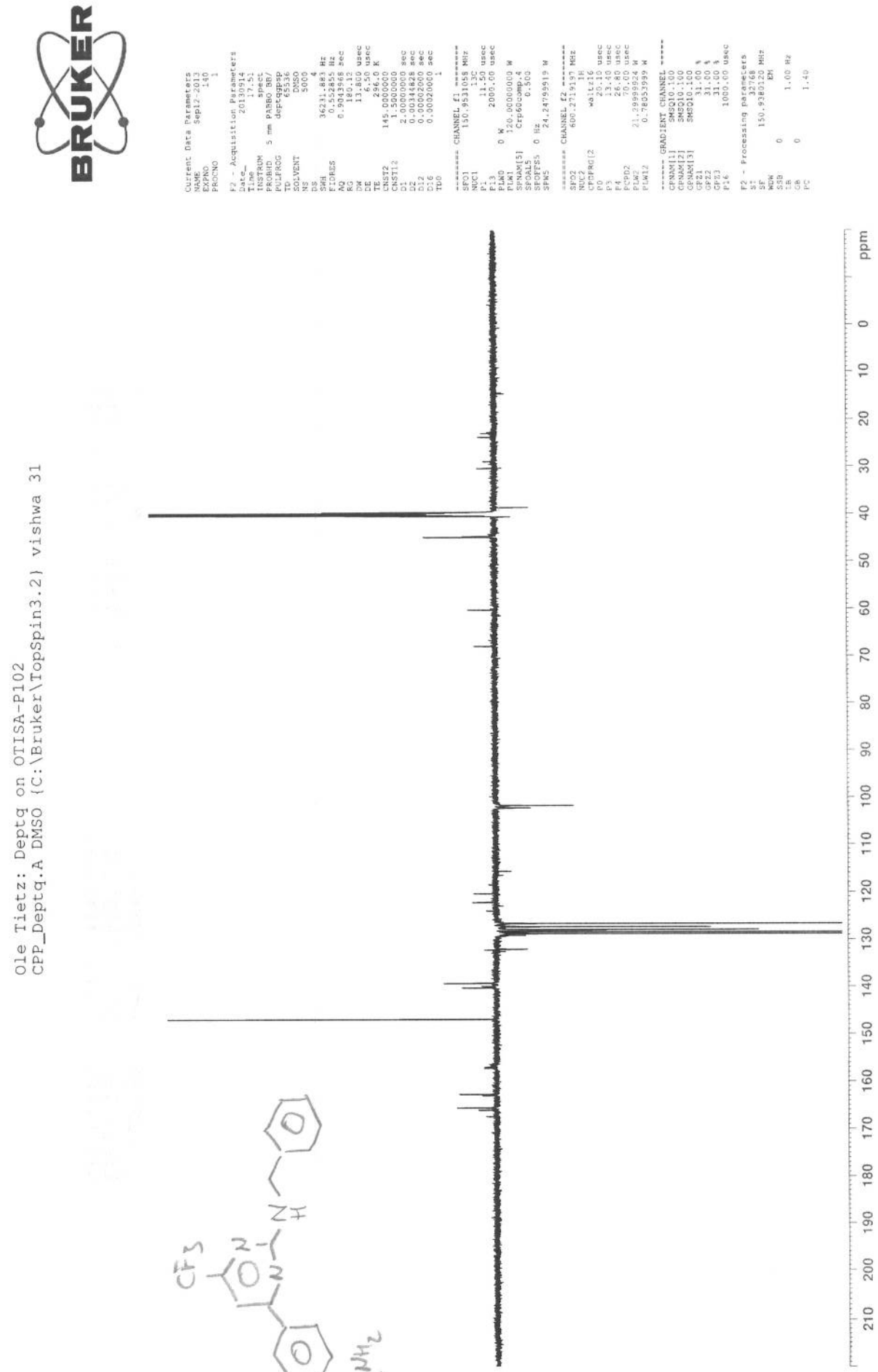
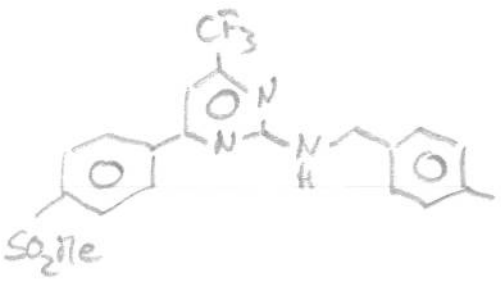
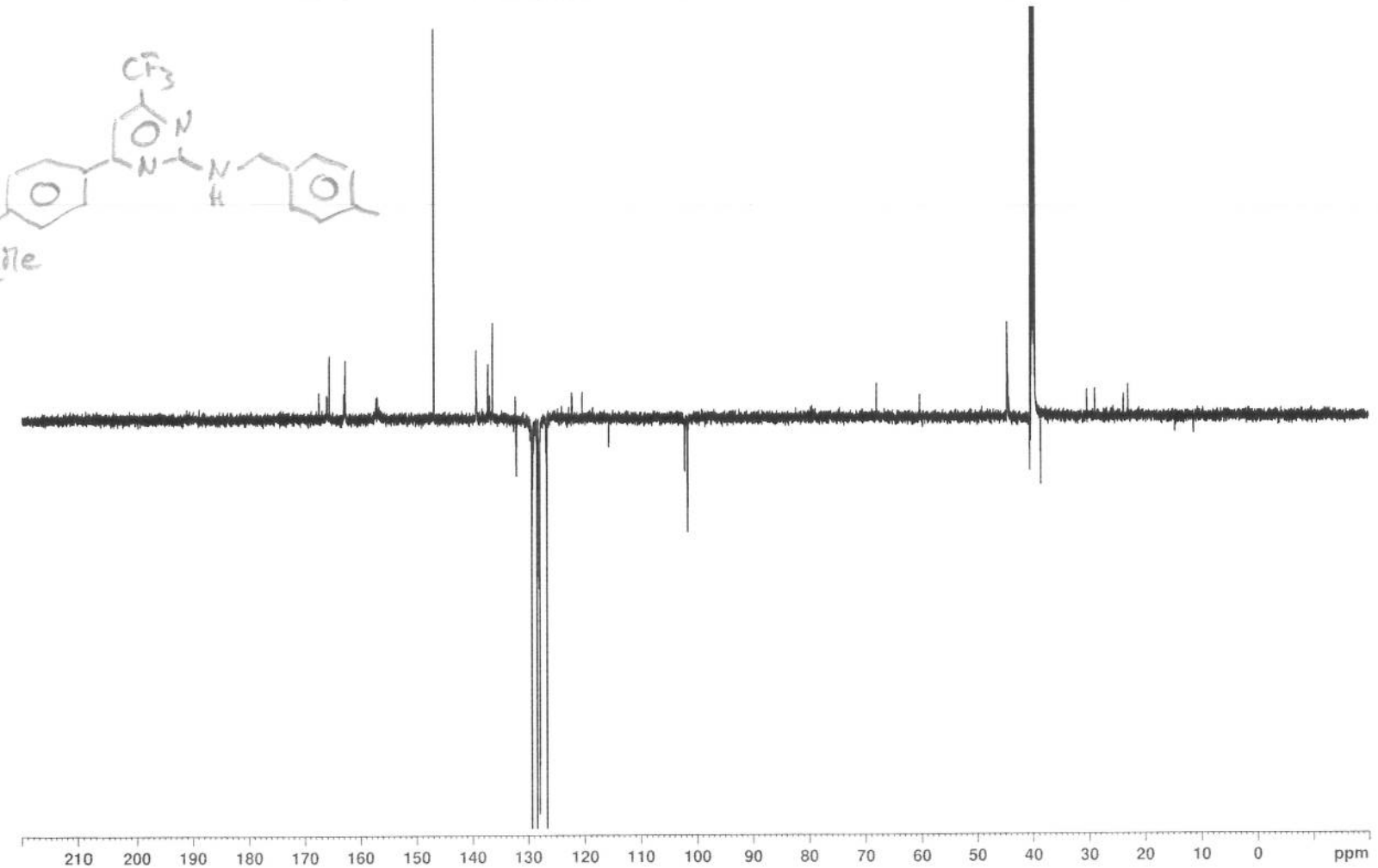
^{13}C-NMR (d_6-DMSO) compound 2b



^{13}C-NMR (d_6-DMSO) compound 2c

Ole Tietz: Deptq on OTISA-P103
CPP_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 32



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Current Data Parameters
NAME            Sep12-2013
EXPNO                  150
PROCNO                   1

F2 - Acquisition Parameters
Date_          20130914
Time               22.00
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG       deptqgpsp
TD                 65536
SOLVENT             DMSO
NS                   5000
DS                      4
SWH            36231.883 Hz
FIDRES         0.552855 Hz
AQ             0.9043968 sec
RG                 180.12
DW                13.800 usec
DE                 6.50 usec
TE                296.0 K
CNST2         145.0000000
CNST12          1.5000000
D1              2.0000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
D16             0.00020000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         150.9531058 MHz
NUC1                13C
P1                 11.50 usec
P13              2000.00 usec
PLW0      0 W
PLW1       120.00000000 W
SPNAM[5]     Crp60comp.4
SPOAL5             0.500
SPOFFS5   0 Hz
SPW5        24.24799919 W

======== CHANNEL f2 ========
SFO2         600.2719197 MHz
NUC2                 1H
CPDPRG[2          waltz16
P0                 20.10 usec
P3                 13.40 usec
P4                 26.80 usec
PCPD2              70.00 usec
PLW2         21.29999924 W
PLW12         0.78053999 W

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

F2 - Processing parameters
SI                 32768
SF          150.9380120 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

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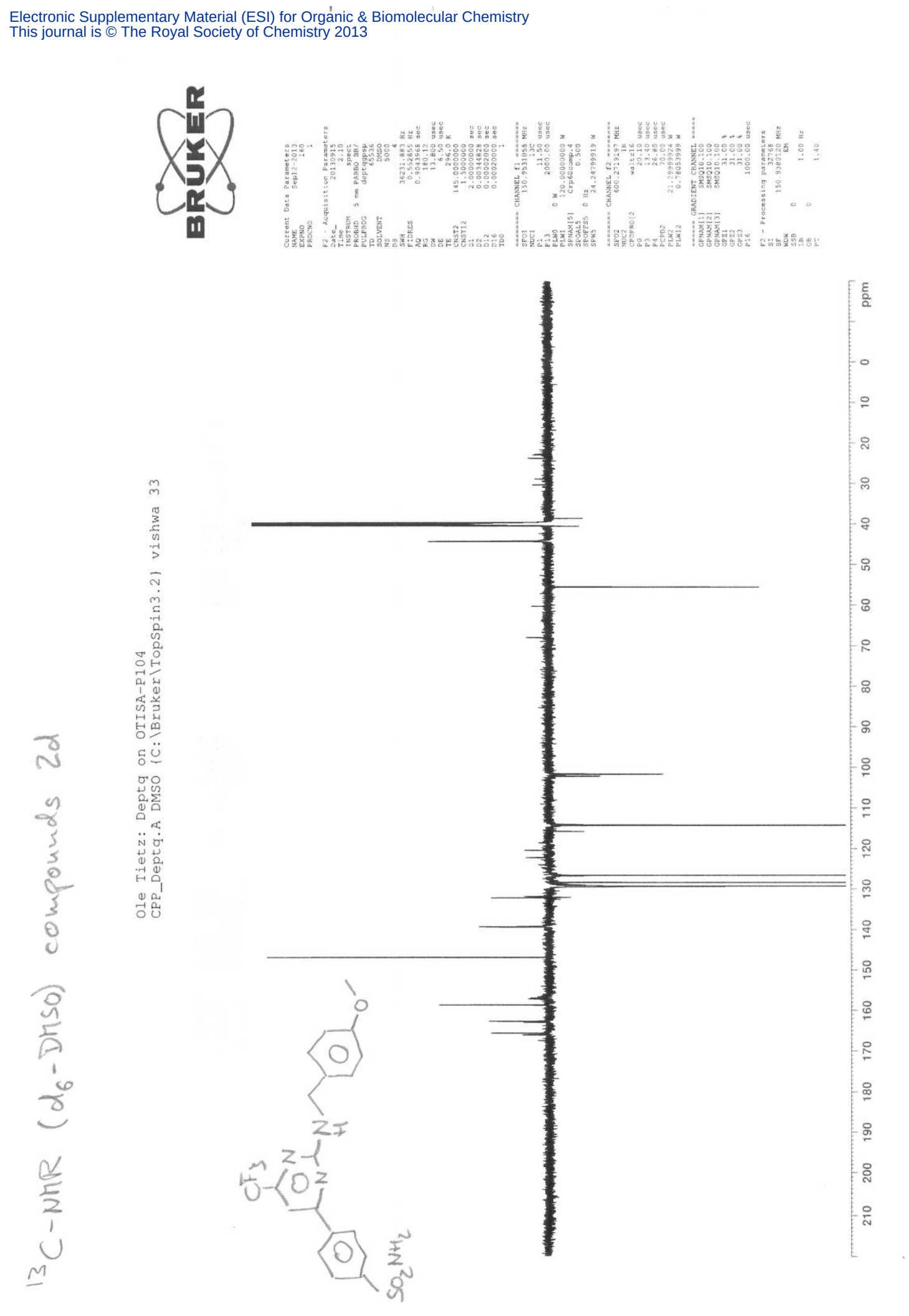
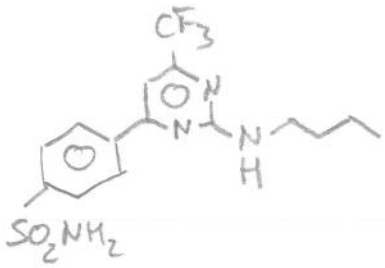
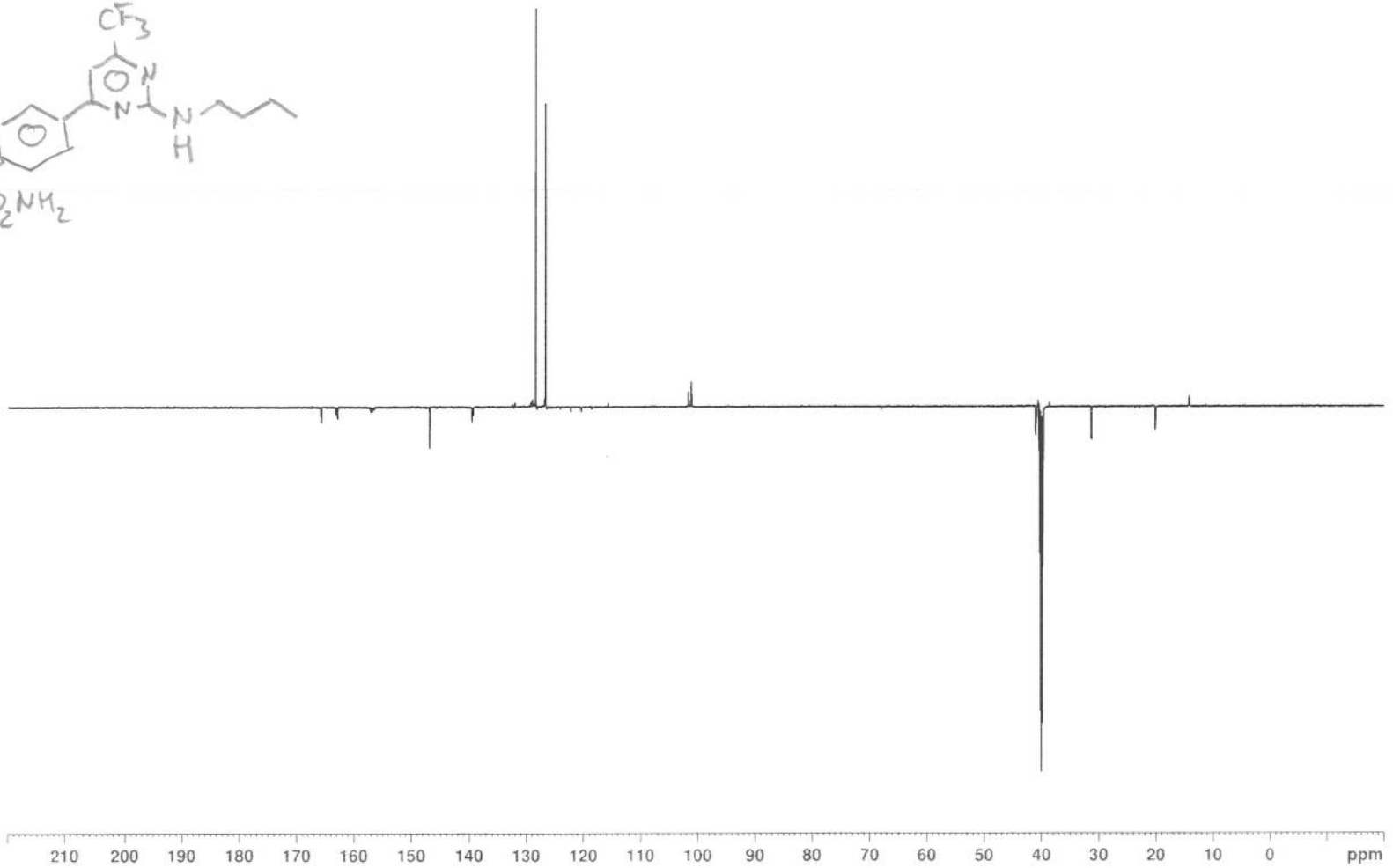
^{13}C-NMR (d_6-DMSO) compounds 2d



^{13}C-NMR (d_6-DMSO) compound 2e

Ole Tietz: Deptq on OTISA-P106
CPP_Deptq.A DMSO {C:\Bruker\TopSpin3.2} vishwa 34






```
Current Data Parameters
NAME                  Sep12-2013
EXPNO                        170
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130915
Time                        6.19
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                deptqqpsp
TD                         65536
SOLVENT                     DMSO
NS                          5000
DS                             4
SWH                    36231.883 Hz
FIDRES                 0.552855 Hz
AQ                     0.9043968 sec
RG                        180.12
DW                        13.800 usec
DE                         6.50 usec
TE                       296.0 K
CNST2                145.0000000
CNST12                 1.5000000
D1                     2.00000000 sec
D2                     0.00344828 sec
D12                    0.00002000 sec
D16                    0.00020000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                 150.9531058 MHz
NUC1                         13C
P1                         11.50 usec
P13                      2000.00 usec
PLW0          0 W
PLW1               120.00000000 W
SPNAM[5]            Crp60comp.4
SPOAL5                     0.500
SPOFFS5       0 Hz
SPW5                24.24799919 W

======== CHANNEL f2 ========
SFO2                 600.2719197 MHz
NUC2                         1H
CPDPRG[2                 waltz16
P0                         20.10 usec
P3                         13.40 usec
P4                         26.80 usec
PCPD2                      70.00 usec
PLW2                21.29999924 W
PLW12                0.78053999 W

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

F2 - Processing parameters
SI                         32768
SF                   150.9380120 MHz
WDW                           EM
SSB           0
LB                          1.00 Hz
GB            0
PC                          1.40
```

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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