Direct Conversion of Thiols to Sulfonyl Chlorides and Sulfonamides

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Content

General procedure for oxidative chlorination of thiols

A mixture of thiol compound (2 mmol), 30% H_2O_2 (6 mmol, 0.6 mL) and $SOCl_2$ (2 mmol, 0.14 mL) was stirred in CH_3CN at 25 °C for the time indicated in Table 2. After completion of the reaction as indicated by TLC, the reaction mixture was quenched by adding water (10 mL), extracted with ethyl acetate (4 × 5 mL) and the extract dried with anhydrous $MgSO_4$. The filtrate was evaporated under vacuum to afford the analytically pure product. All of products are known compounds and characterized easily by comparison with authentic samples (^{1}H NMR, ^{13}C NMR, mp).

General procedure for the synthesis of sulfonamides

A mixture of thiol compound (2 mmol), 30% H_2O_2 (6 mmol, 0.6 mL) and $SOCl_2$ (2 mmol, 0.14 mL) was stirred in CH_3CN at 25 °C for an appropriate time. After completion of the reaction as indicated by TLC, a solution of amine (2 mmol) in pyridine (1 mL) was added to the reaction mixture. The resulting mixture was stirred at room temperature until TLC showed complete disappearance of starting material (Table 3) then acidified with 2 N HCl solution, and extracted with EtOAc. The organic layer was washed with H_2O and brine, and dried over $MgSO_4$. The filtrate was evaporated and the corresponding pure sulfonamide was obtained as a crystalline solid. Recrystallization from a mixture of ethanol and water affords analytically pure product. Spectral and physical data for selected compounds follow.

N-2-Chlorophenyl-4-methylbenzenesulfonamide. M.p= 105 °C. ^{1}H NMR (200 MHz, $CDCl_3$): δ 2.36 (s, 3H), 6.98-7.07 (m, 2H), 7.18-7.26 (m, 4H), 7.63-7.67 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 22, 122.8, 125.5, 126.3, 127.7, 128.3, 129.8, 130.1, 133.9, 136.3, 144.7. Anal. Calcd for $C_{13}H_{12}NSO_2Cl$: C, 55.42; H, 4.26; N, 4.97; S, 11.36. Found: C, 55.06; H, 4.38; N, 4.86; S, 10.85.

N-Cyclohexyl-4-bromobenzenesulfonamide. Mp= 100 °C. ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.15 (m, 5H), 1.53-1.74 (m, 5H), 3.10 (m, 1H), 4.96 (d, 1H, *J*=7.5 Hz, NH), 7.63 (d, 2H, J=8 Hz), 7.75 (d, 2H, J=8 Hz). ^{13}C NMR (50 MHz, $CDCl_3$): δ 24.6, 25, 33.8, 52.7, 127.3, 128.5, 132.3, 140.6. Anal. Calcd for $C_{12}H_{16}NSO_2Br$: C, 45.28; H, 5.03; N, 4.40; S, 10.06. Found: C, 45.25; H, 5.01; N, 4.23; S, 9.77.

N-3-Nitrophenyl-4-bromobenzenesulfonamide. Mp= 118-120 °C. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.17-7.74 (m, 7H), 7.86-8.00 (m, 2H). ^{13}C NMR (50 MHz, $CDCl_3$): δ 115.4, 120.2, 126.4, 128.8, 129.1, 130.6, 132.9, 137.4, 137.6, 148.8. Anal. Calcd for $C_{12}H_9N_2SO_2Br$: C, 44.31; H, 2.76; N, 8.61; S, 9.85. Found: C, 43.65; H, 2.68; N, 8.53; S, 9.50.

N-4-Chlorophenyl-2-naphthalenesulfonamide. Mp= 115 °C. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.12 (d, 2H, *J*= 8.9 Hz), 7.25 (d, 2H, *J*= 8.9 Hz), 7.57-8.13 (m, 6H), 8.43 (d, 1H, *J*= 1.3 Hz), 10.56 (s, 1H, NH). ^{13}C NMR (50 MHz, $CDCl_3$): δ 122, 122.3, 128.2, 128.3, 128.5, 128.6, 129.5, 129.6, 129.7, 130, 132, 134.7, 136.6, 137.1. Anal. Calcd for $C_{16}H_{12}NSO_2Cl$: C, 60.48; H, 3.78; N, 4.41; S, 10.07. Found: C, 60.31; H, 3.87; N, 4.14; S, 9.88.

N-4-Bromophenyl-2-benzimidazolesulfonamide. Mp= 156-158 °C. ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.57-7.65 (m, 5H), 8.07 (d, 2H, *J*=9 Hz), 8.17 (d, 2H, *J*=9 Hz). ^{13}C NMR (50 MHz, $CDCl_3$): δ 123.6, 123.9, 126.5, 127.2, 132, 132, 142.6, 147.1. Anal. Calcd for $C_{13}H_{10}N_3SO_2Br$: C, 44.32; H, 2.84; N, 11.93; S, 9.09. Found: C, 44.03; H, 2.51; N, 11.62; S, 8.72.

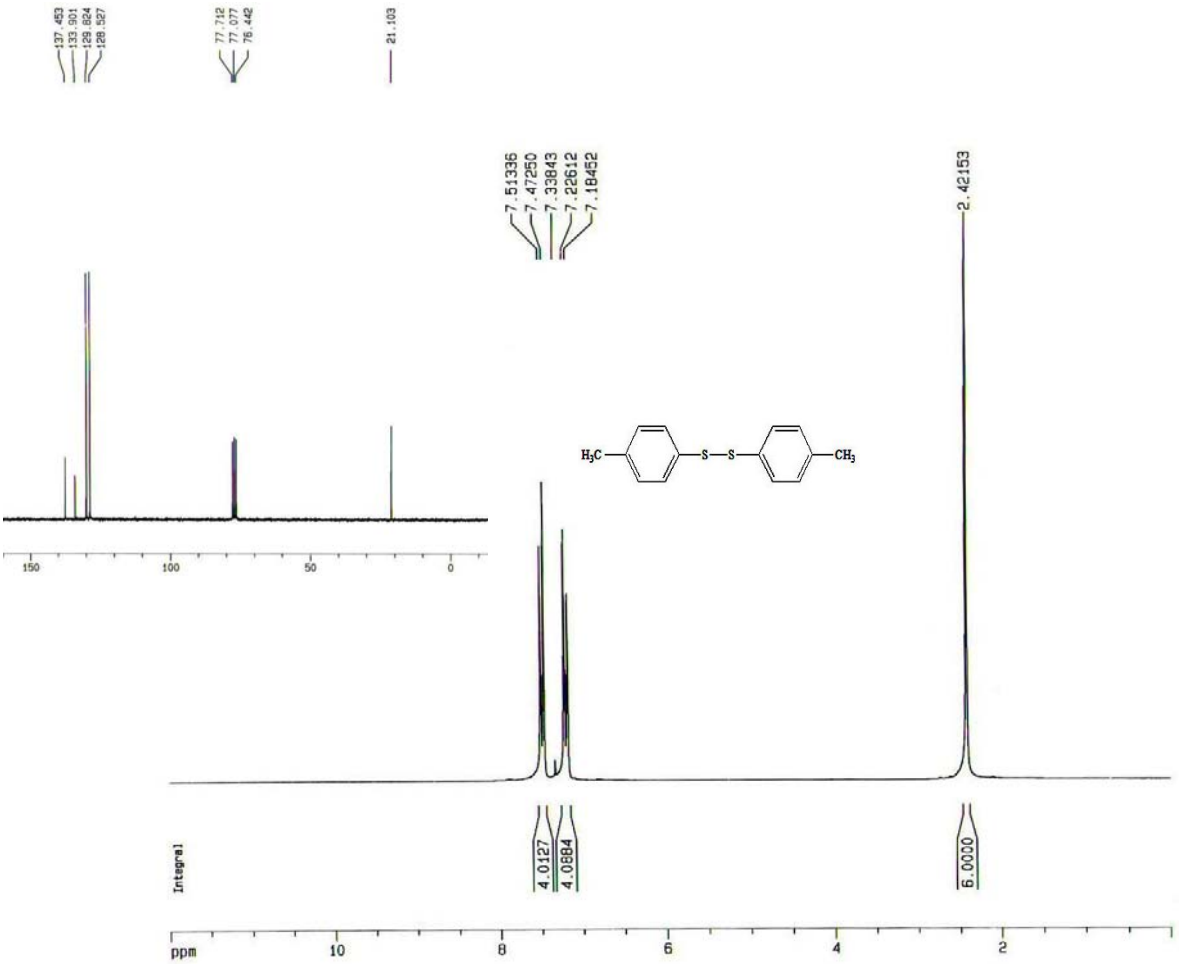
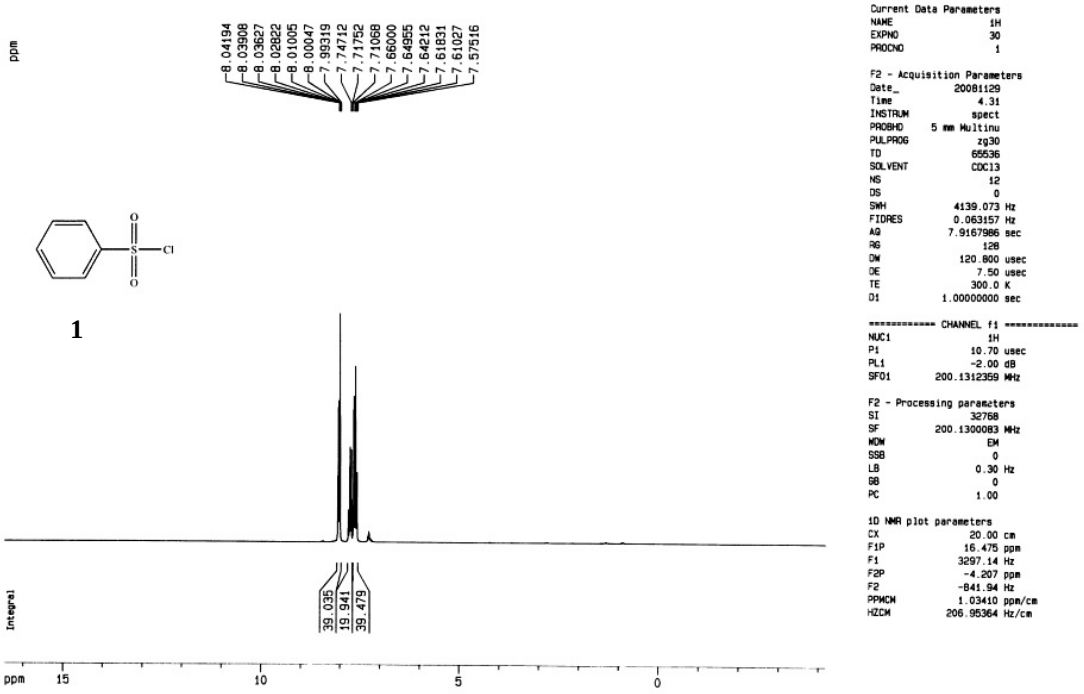
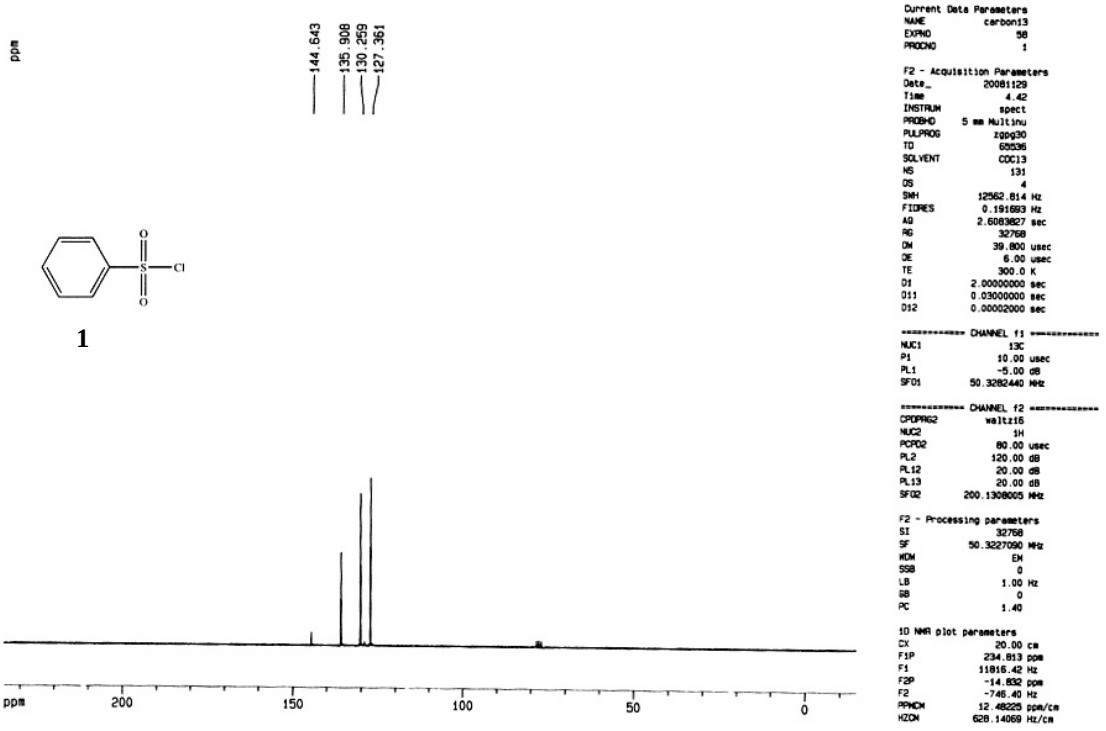
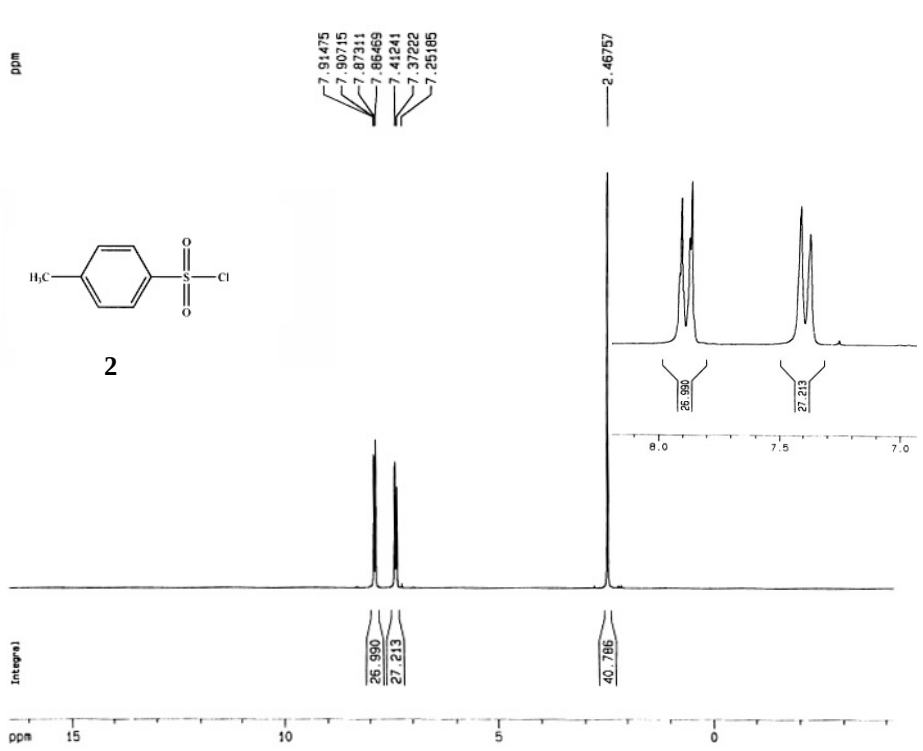


Figure 1. ^{1}H and ^{13}C NMR spectra of 4-methylphenyl disulfide in $CDCl_3$

^{1}H and ^{13}C NMR spectra of sulfonyl chlorides (S5-S17)







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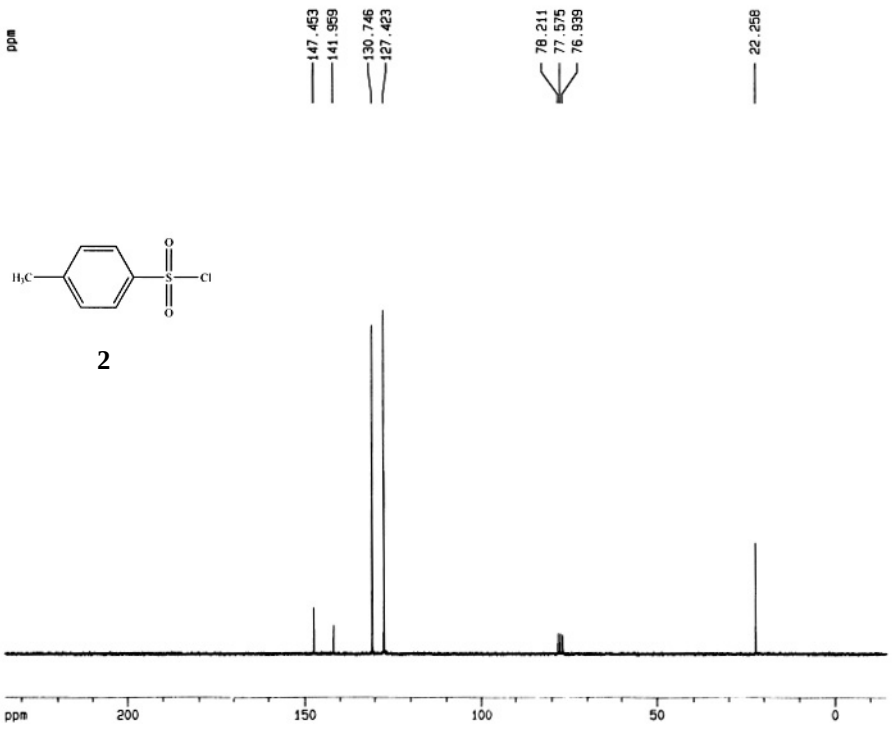

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GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P              -14.832 ppm
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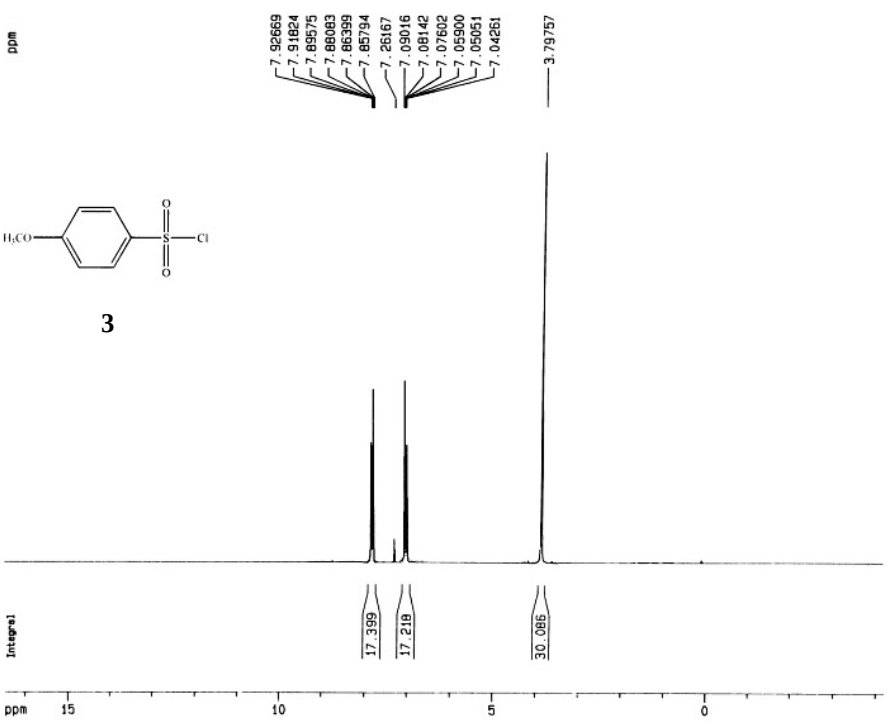

3

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PROCNO                 1

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1D NMR plot parameters
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HZCM          206.95364 Hz/cm
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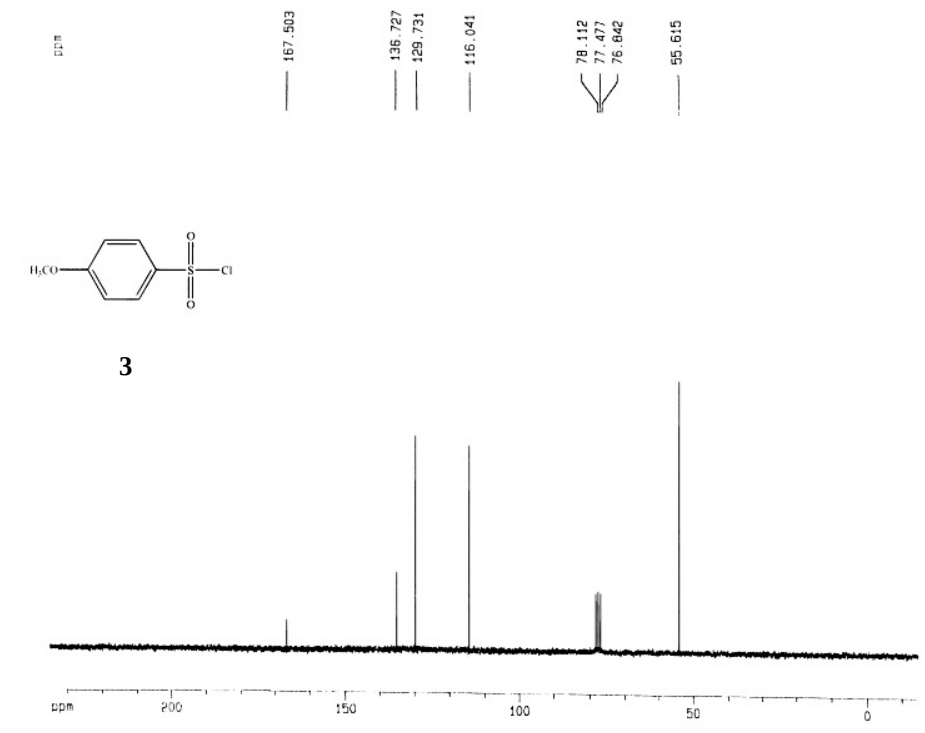

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============ CHANNEL f2 =============
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1D NMR plot parameters
CX                 20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P               -14.832 ppm
F2             -746.40 Hz
PPMCM           12.48225 ppm/cm
HZCM          628.14069 Hz/cm
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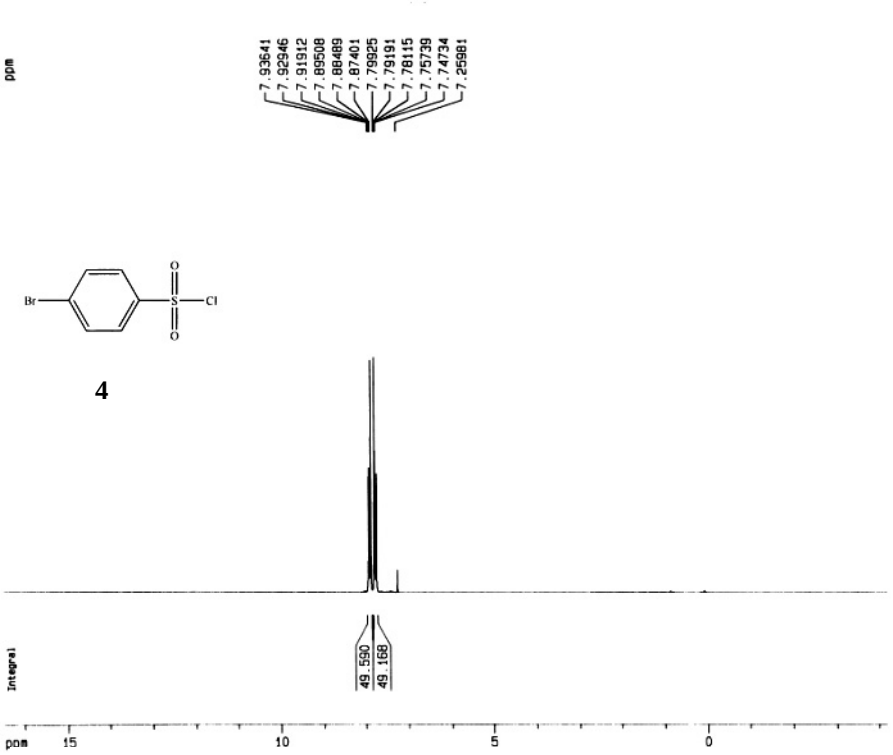

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============ CHANNEL f1 ============
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PL1               -2.00 dB
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F2 - Processing parameters
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LB                0.30 Hz
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1D NMR plot parameters
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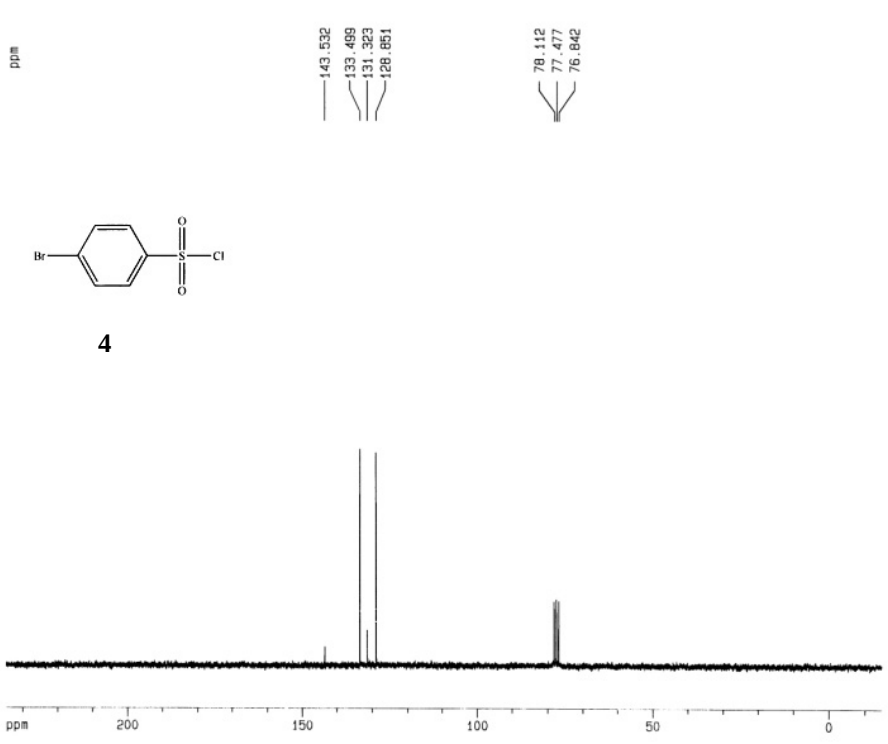

4

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PROCNO                1

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SOLVENT           CDCl3
NS                  148
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SWH           12562.814 Hz
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TE               300.0 K
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SFO1        50.3282440 MHz

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NUC2                  1H
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F2 - Processing parameters
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WDW                  EM
SSB                   0
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PC                 1.40

1D NMR plot parameters
CX                20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P              -14.832 ppm
F2             -746.40 Hz
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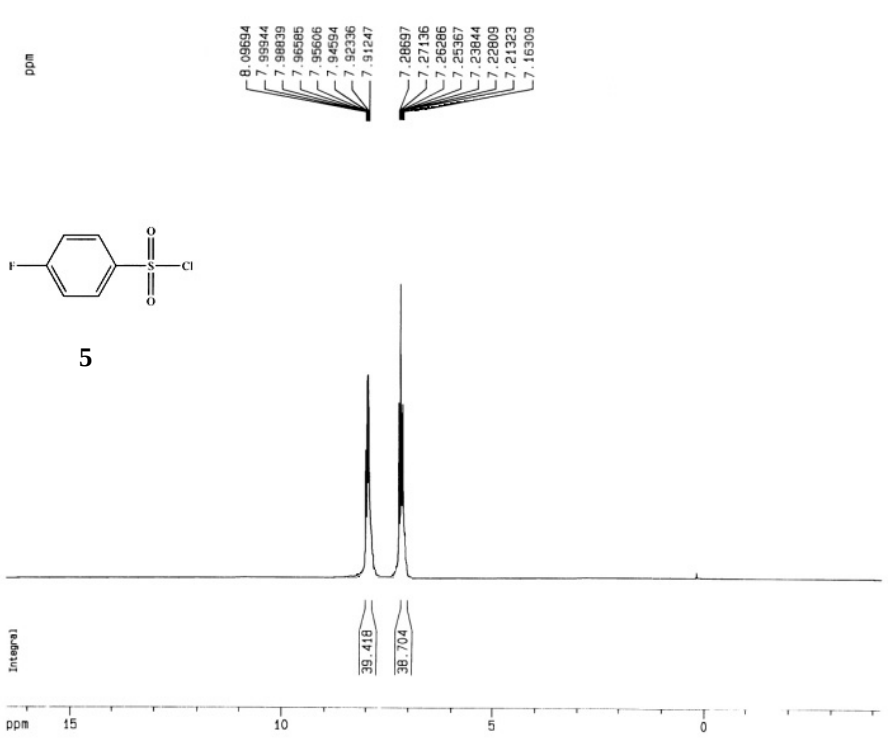

5

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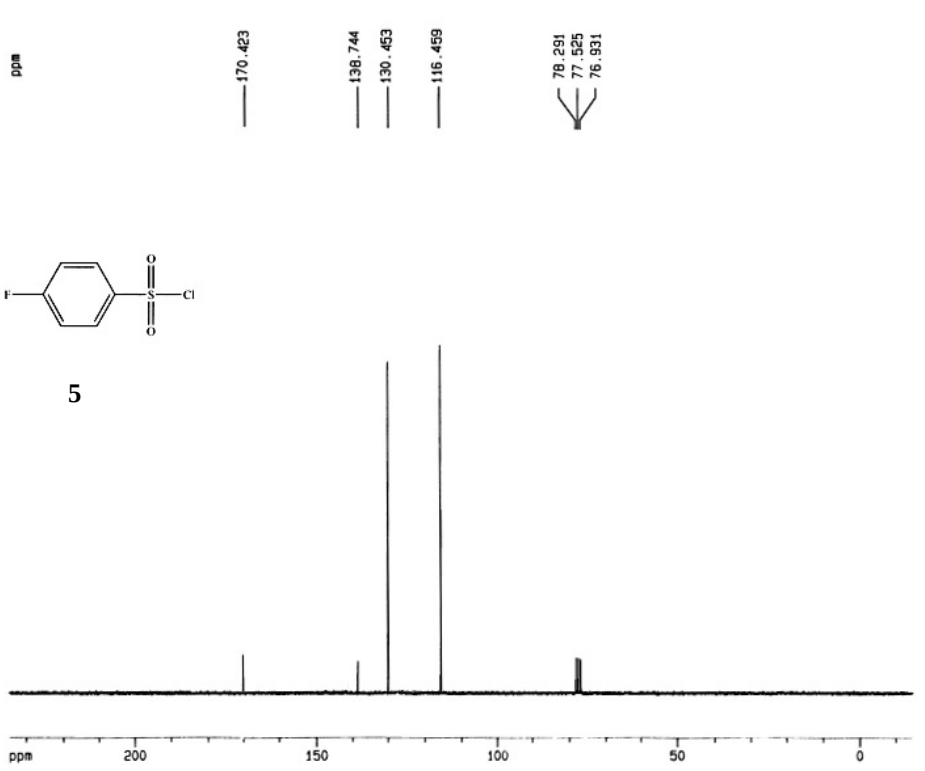

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============ CHANNEL f2 =============
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NUC2                       1H
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PL12                     20.00 dB
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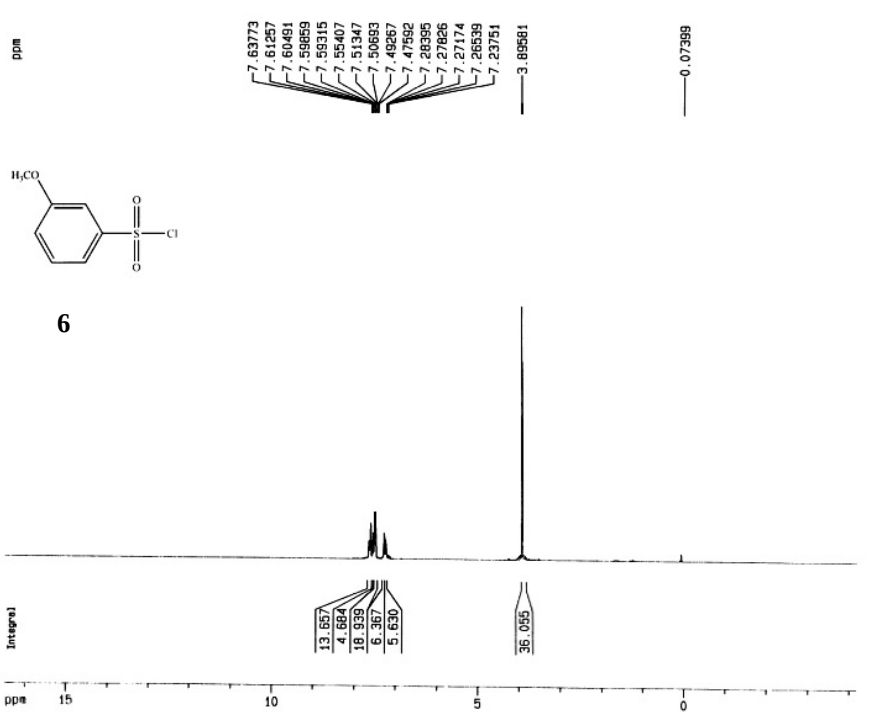

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1D NMR plot parameters
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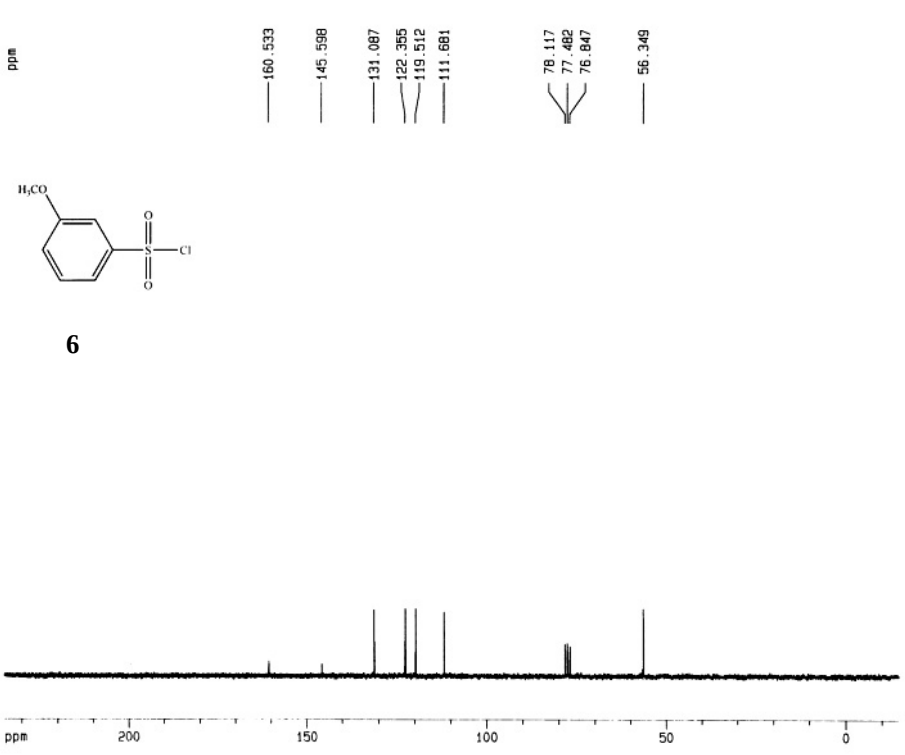

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============ CHANNEL f1 =============
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============ CHANNEL f2 =============
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PL12               20.00 dB
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1D NMR plot parameters
CX                 20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P              -14.832 ppm
F2              -746.40 Hz
PPMCM          12.48225 ppm/cm
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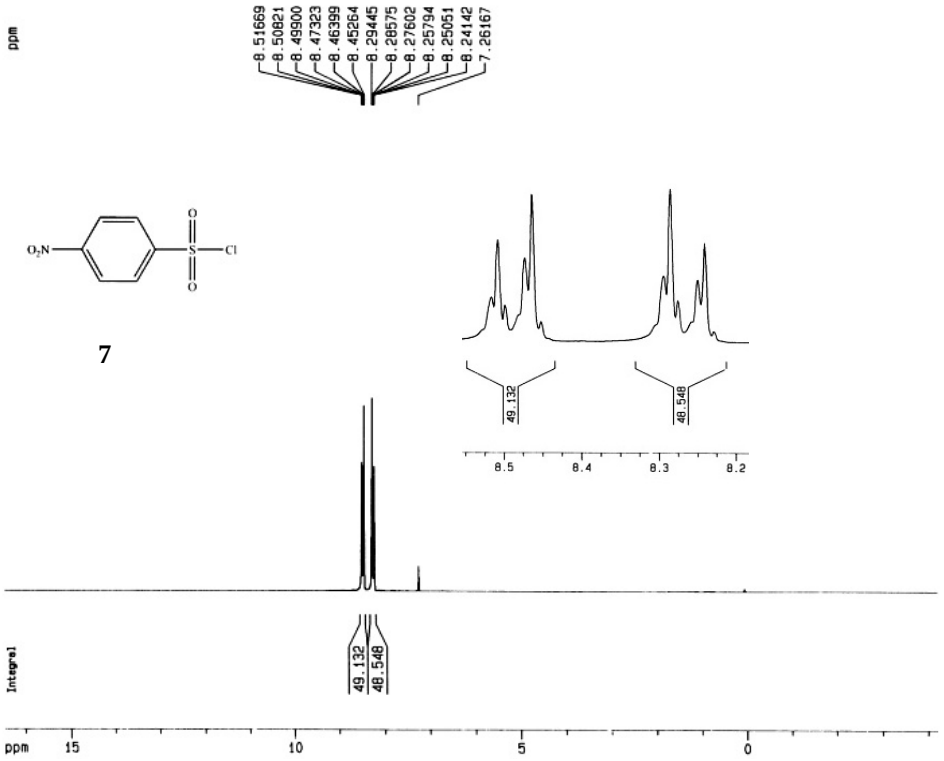

7

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FIDRES         0.063157 Hz
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RG                812.7
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DE                  7.50 usec
TE                300.0 K
D1             1.00000000 sec

============ CHANNEL f1 =============
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P1                 10.70 usec
PL1                -2.00 dB
SFO1          200.1312359 MHz

F2 - Processing parameters
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SF            200.1300083 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
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1D NMR plot parameters
CX                 20.00 cm
F1P                16.475 ppm
F1               3297.14 Hz
F2P                -4.207 ppm
F2               -841.94 Hz
PPMCM              1.03410 ppm/cm
HZCM             206.95364 Hz/cm
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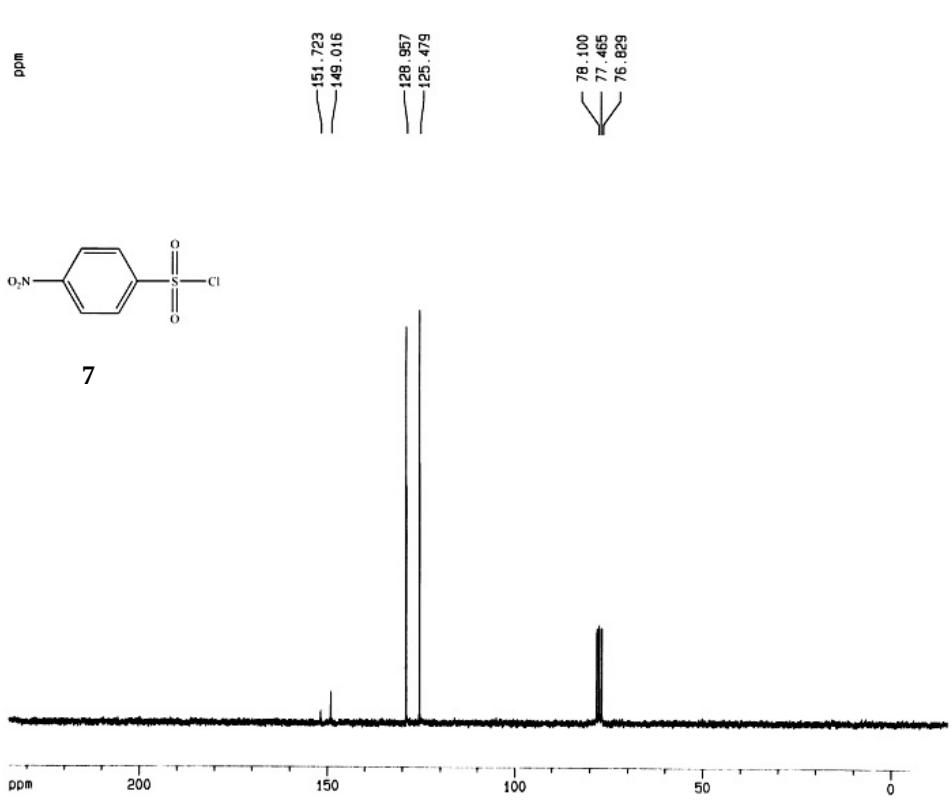


7

```
Current Data Parameters
NAME              carbon13
EXPNO                 59
PROCNO                1

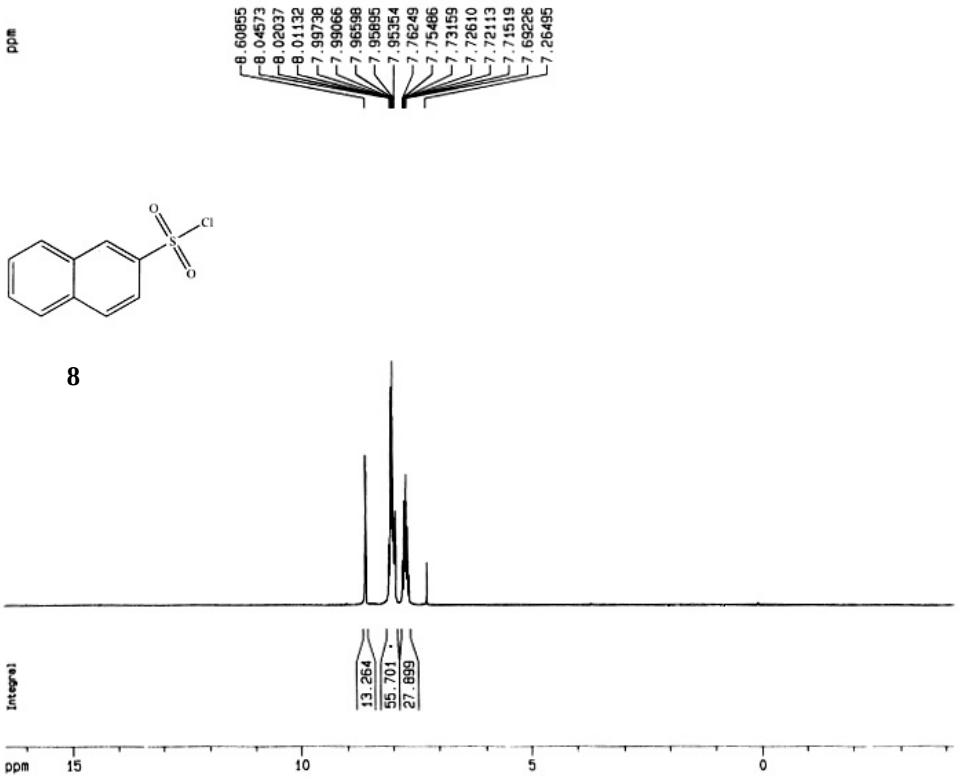
F2 - Acquisition Parameters
Date_           20081129
Time                5.47
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  719
DS                    4
SWH           12562.814 Hz
FIDRES         0.191693 Hz
AQ             2.6083827 sec
RG                32768
DW                39.800 usec
DE                  6.00 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec

============ CHANNEL f1 =============
NUC1                 13C
P1                 10.00 usec
PL1                -5.00 dB
SFO1          50.3282440 MHz

============ CHANNEL f2 =============
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               20.00 dB
PL13               20.00 dB
SFO2          200.1308005 MHz

F2 - Processing parameters
SI                 32768
SF            50.3227090 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               234.813 ppm
F1              11816.42 Hz
F2P                -14.832 ppm
F2               -746.40 Hz
PPMCM             12.48225 ppm/cm
HZCM             628.14069 Hz/cm
```



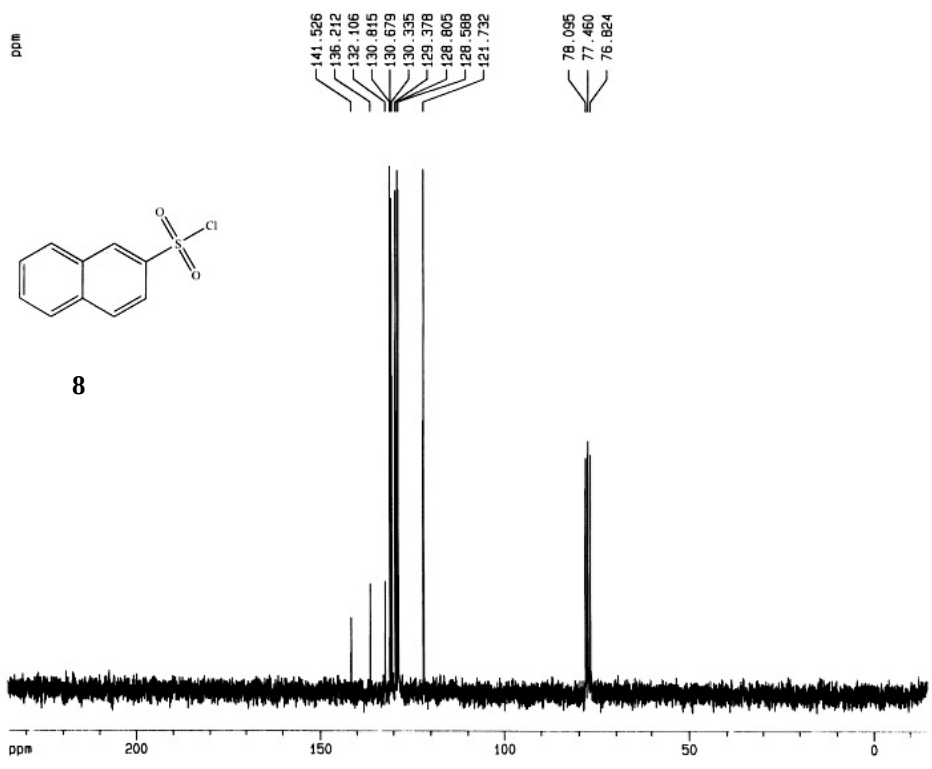

```
Current Data Parameters
NAME                  1H
EXPNO                 19
PROCNO                1

F2 - Acquisition Parameters
Date_           20081125
Time                6.12
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   20
DS                    0
SWH           4139.073 Hz
FIDRES        0.063157 Hz
AQ            7.9167986 sec
RG                574.7
DW              120.800 usec
DE                7.50 usec
TE                300.0 K
D1            1.00000000 sec

============ CHANNEL f1 ============
NUC1                  1H
P1                10.70 usec
PL1               -2.00 dB
SFO1         200.1312359 MHz

F2 - Processing parameters
SI                32768
SF          200.1300075 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
F1P               16.479 ppm
F1              3297.89 Hz
F2P               -4.203 ppm
F2              -841.18 Hz
PPMCM             1.03410 ppm/cm
HZCM            206.95364 Hz/cm
```




```
Current Data Parameters
NAME             carbon13
EXPNO                  55
PROCNO                  1

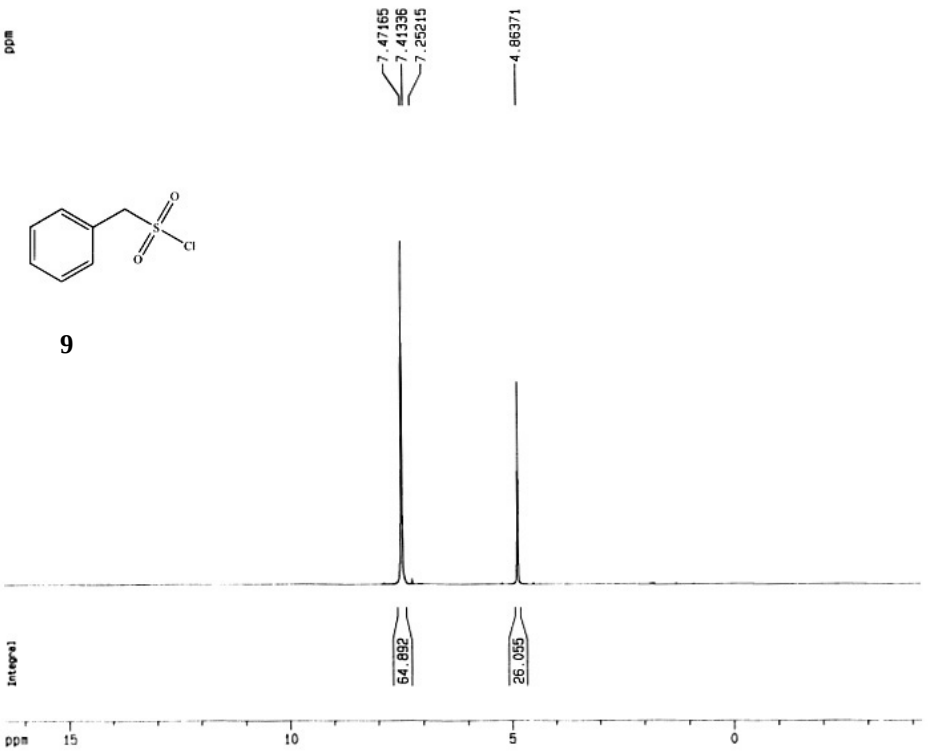
F2 - Acquisition Parameters
Date_           20081125
Time                8.45
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  552
DS                    4
SWH          12562.814 Hz
FIDRES        0.191693 Hz
AQ            2.6083827 sec
RG                32768
DW              39.800 usec
DE                6.00 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                10.00 usec
PL1               -5.00 dB
SFO1         50.3282440 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2              120.00 dB
PL12              20.00 dB
PL13              20.00 dB
SFO2         200.1308005 MHz

F2 - Processing parameters
SI                32768
SF          50.3227090 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P              -14.832 ppm
F2             -746.40 Hz
PPMCM            12.48225 ppm/cm
HZCM           628.14069 Hz/cm
```



9

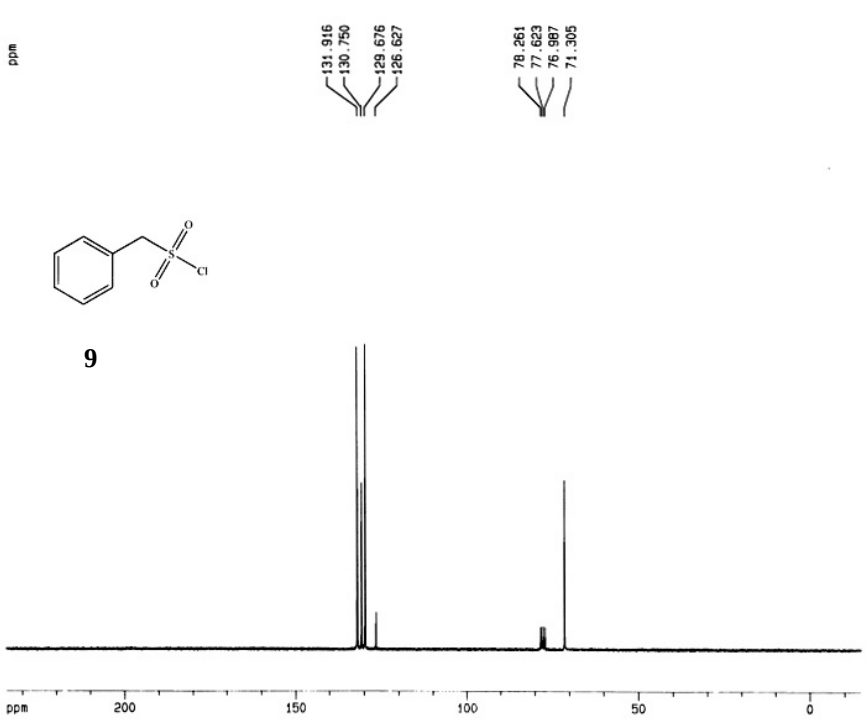
```
Current Data Parameters
NAME                  H1
EXPNO                 69
PROCNO                1

F2 - Acquisition Parameters
Date_           20081108
Time                4.24
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   12
DS                    0
SWH           4139.073 Hz
FIDRES        0.063157 Hz
AQ            7.9167986 sec
RG                  362
DW              120.800 usec
DE                7.50 usec
TE                300.0 K
D1           1.00000000 sec

============ CHANNEL f1 ============
NUC1                  1H
P1                10.70 usec
PL1               -2.00 dB
SFO1        200.1312359 MHz

F2 - Processing parameters
SI                32768
SF          200.1300101 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
F1P               16.466 ppm
F1              3295.37 Hz
F2P               -4.216 ppm
F2              -843.71 Hz
PPMCM             1.03410 ppm/cm
HZCM            206.95363 Hz/cm
```



9

```
Current Data Parameters
NAME             carbon13
EXPNO                32
PROCNO                1

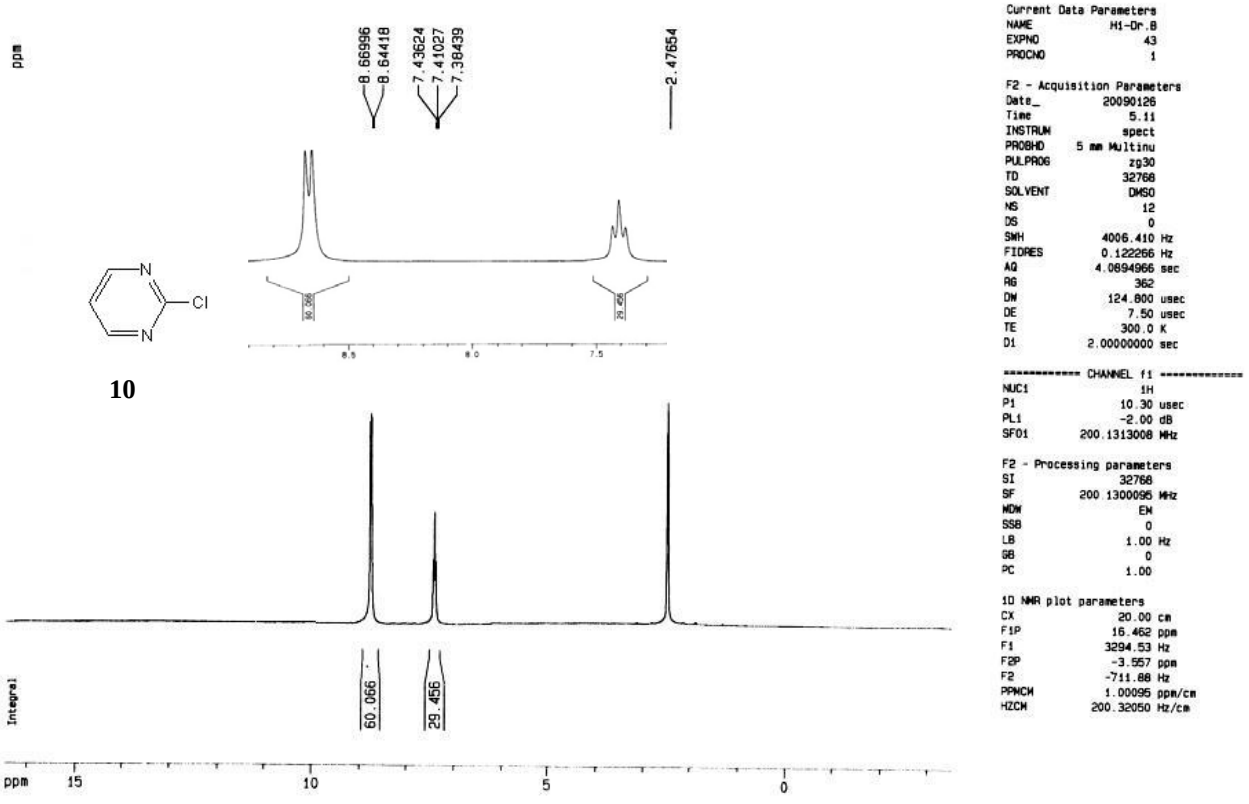
F2 - Acquisition Parameters
Date_           20081116
Time                3.56
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  378
DS                    4
SWH          12562.814 Hz
FIDRES        0.191693 Hz
AQ            2.6083827 sec
RG                32768
DW              39.800 usec
DE                6.00 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                10.00 usec
PL1               -5.00 dB
SFO1        50.3282440 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2              120.00 dB
PL12              20.00 dB
PL13              20.00 dB
SFO2        200.1308005 MHz

F2 - Processing parameters
SI                32768
SF          50.3227090 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
F1P              234.813 ppm
F1             11816.42 Hz
F2P              -14.832 ppm
F2              -746.40 Hz
PPMCM            12.48225 ppm/cm
HZCM           628.14069 Hz/cm
```



10

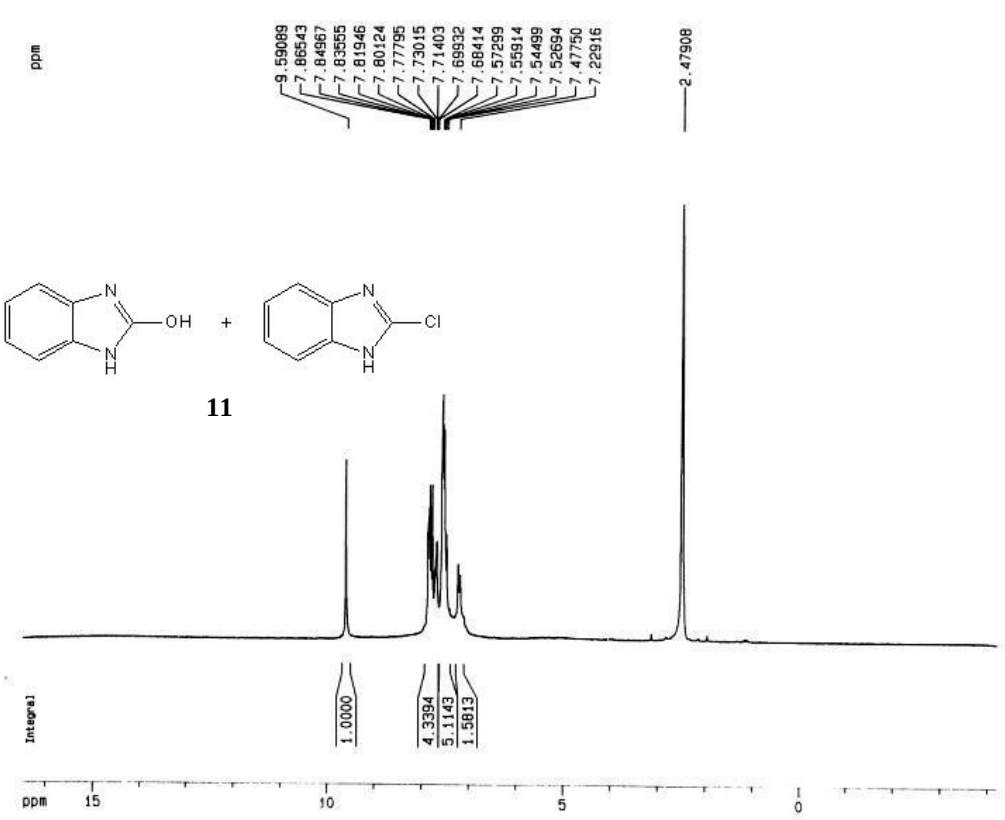
```
Current Data Parameters
NAME                  H1-Dr.B
EXPNO                      43
PROCNO                      1

F2 - Acquisition Parameters
Date_                20090126
Time                     5.11
INSTRUM                 spect
PROBHD     5 mm Multinu
PULPROG                 zg30
TD                     32768
SOLVENT                 DMSO
NS                         12
DS                          0
SWH                 4006.410 Hz
FIDRES              0.122266 Hz
AQ                  4.0894966 sec
RG                        362
DW                  124.800 usec
DE                    7.50 usec
TE                    300.0 K
D1                 2.00000000 sec

========== CHANNEL f1 ==========
NUC1                       1H
P1                    10.30 usec
PL1                   -2.00 dB
SFO1             200.1313008 MHz

F2 - Processing parameters
SI                         32768
SF               200.1300095 MHz
WDW                        EM
SSB                         0
LB                     1.00 Hz
GB                          0
PC                     1.00

1D NMR plot parameters
CX                    20.00 cm
F1P                  16.462 ppm
F1                 3294.53 Hz
F2P                  -3.557 ppm
F2                 -711.88 Hz
PPMCM              1.00095 ppm/cm
HZCM             200.32050 Hz/cm
```



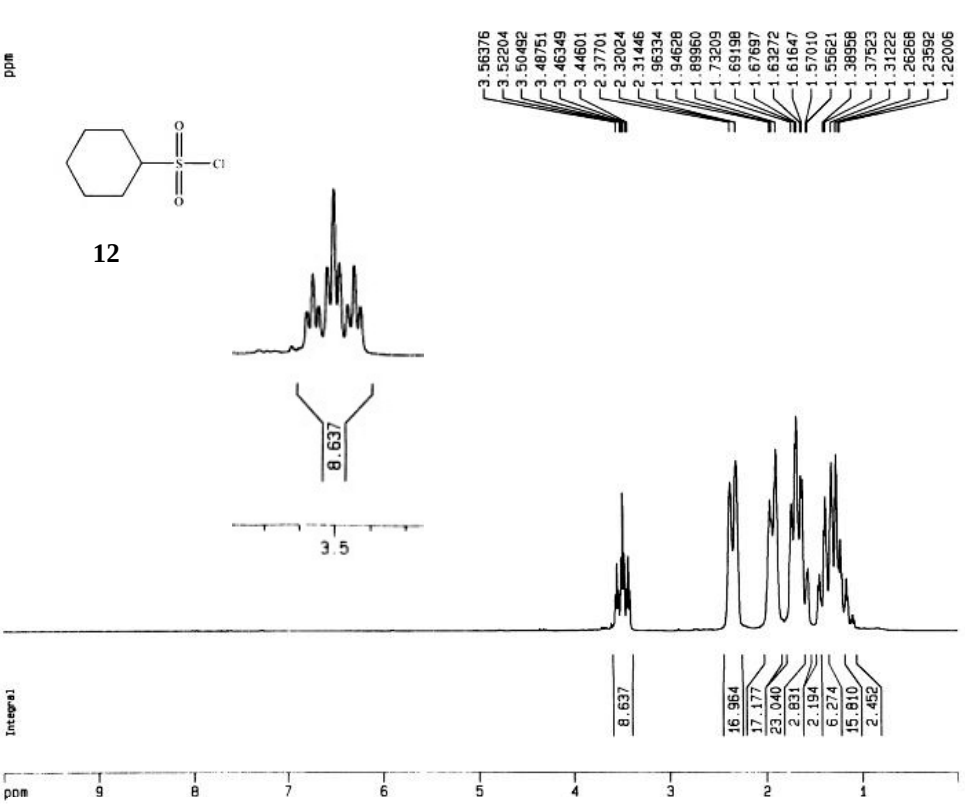

```
Current Data Parameters
NAME                  1H-Dr.8
EXPNO                      22
PROCNO                      1

F2 - Acquisition Parameters
Date_              20090307
Time                   9.22
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        12
DS                         0
SWH               4139.073 Hz
FIDRES            0.063157 Hz
AQ                7.9167986 sec
RG                     406.4
DW                   120.800 usec
DE                     7.50 usec
TE                    300.0 K
D1                1.00000000 sec

============ CHANNEL f1 =============
NUC1                      1H
P1                     10.30 usec
PL1                    -2.00 dB
SFO1           200.1312359 MHz

F2 - Processing parameters
SI                     32768
SF             200.1300087 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
F1P                   16.473 ppm
F1                  3296.76 Hz
F2P                   -4.209 ppm
F2                  -842.32 Hz
PPMCM                1.03410 ppm/cm
HZCM               206.95363 Hz/cm
```



12

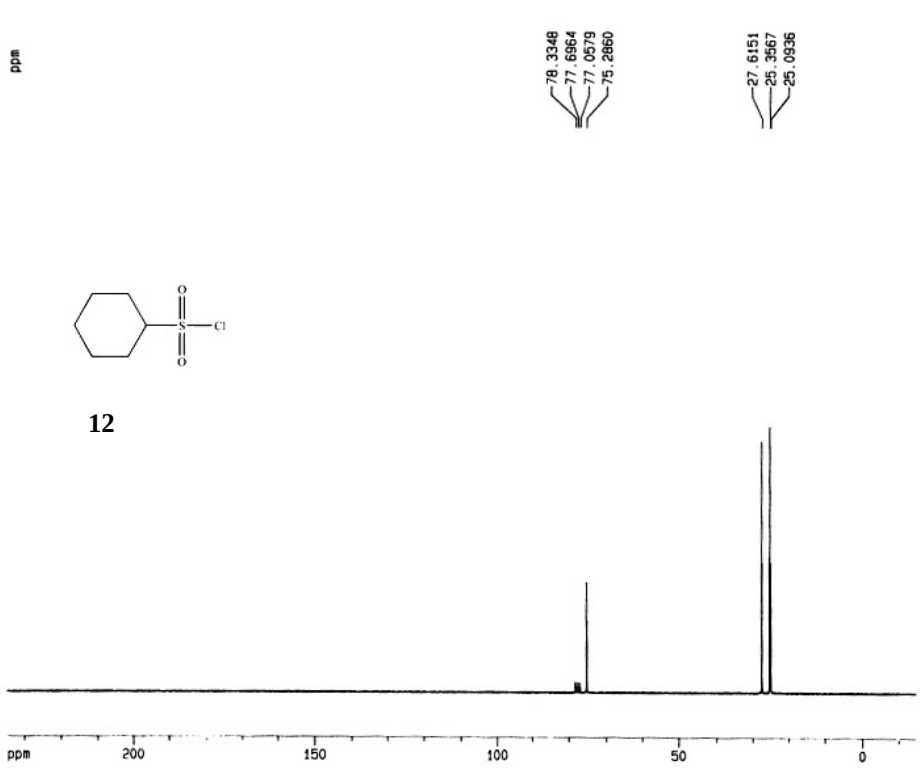
```
Current Data Parameters
NAME                  1H
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20081123
Time                4.23
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     0
SWH           4139.073 Hz
FIDRES        0.063157 Hz
AQ            7.9167986 sec
RG                  35.9
DW                120.800 usec
DE                  7.50 usec
TE                 300.0 K
D1            1.00000000 sec

============ CHANNEL f1 ============
NUC1                  1H
P1                 10.70 usec
PL1                -2.00 dB
SFO1         200.1312359 MHz

F2 - Processing parameters
SI                 32768
SF           200.1300066 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
F1P                10.000 ppm
F1               2001.30 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM              0.50000 ppm/cm
HZCM             100.06500 Hz/cm
```



12

```
Current Data Parameters
NAME             carbon13
EXPNO                  50
PROCNO                  1

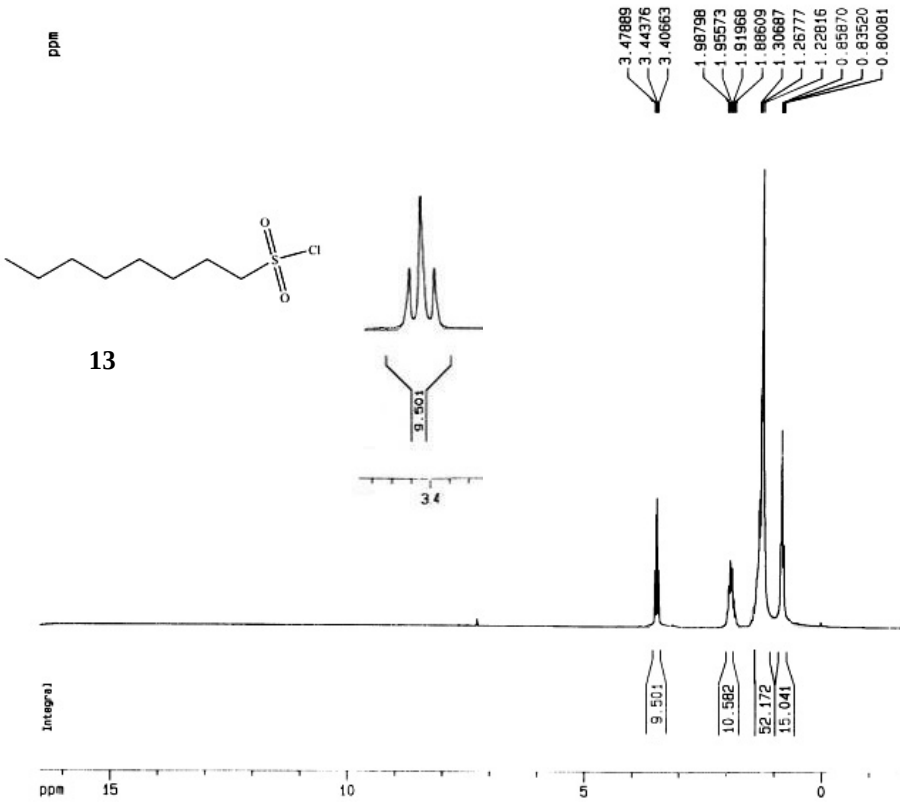
F2 - Acquisition Parameters
Date_           20081123
Time                4.31
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    90
DS                     4
SWH           12562.814 Hz
FIDRES        0.191693 Hz
AQ            2.6083827 sec
RG                 32768
DW                 39.800 usec
DE                  6.00 usec
TE                 300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec

============ CHANNEL f1 ============
NUC1                 13C
P1                 10.00 usec
PL1                -5.00 dB
SFO1         50.3282440 MHz

============ CHANNEL f2 ============
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               20.00 dB
PL13               20.00 dB
SFO2         200.1300005 MHz

F2 - Processing parameters
SI                 32768
SF           50.3227090 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               234.813 ppm
F1              11816.42 Hz
F2P               -14.832 ppm
F2               -746.40 Hz
PPMCM             12.48225 ppm/cm
HZCM            628.14069 Hz/cm
```



13

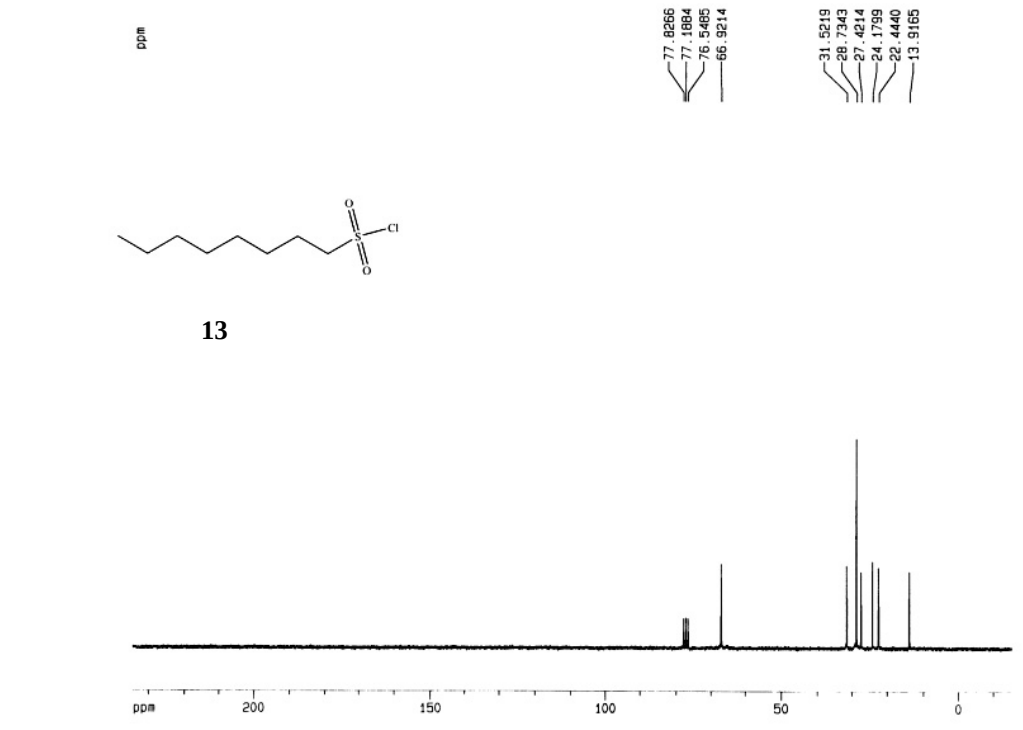
```
Current Data Parameters
NAME                 1H-Dr.B
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_               20081223
Time                    5.48
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        12
DS                         0
SWH                4139.073 Hz
FIDRES             0.063157 Hz
AQ                 7.9167986 sec
RG                        32
DW                   120.800 usec
DE                     7.50 usec
TE                    300.0 K
D1                 1.00000000 sec

============ CHANNEL f1 =============
NUC1                      1H
P1                     10.70 usec
PL1                    -2.00 dB
SFO1              200.1312359 MHz

F2 - Processing parameters
SI                        32768
SF                200.1300073 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
F1P                   16.480 ppm
F1                  3298.08 Hz
F2P                   -4.202 ppm
F2                  -840.99 Hz
PPMCM                1.03410 ppm/cm
HZCM               206.95364 Hz/cm
```



13

```
Current Data Parameters
NAME      13-Carbon-Dr.B
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20081215
Time                9.27
INSTRUM            spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   79
DS                    4
SWH           12562.814 Hz
FIDRES         0.191693 Hz
AQ             2.6083827 sec
RG                 32768
DW                39.800 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec

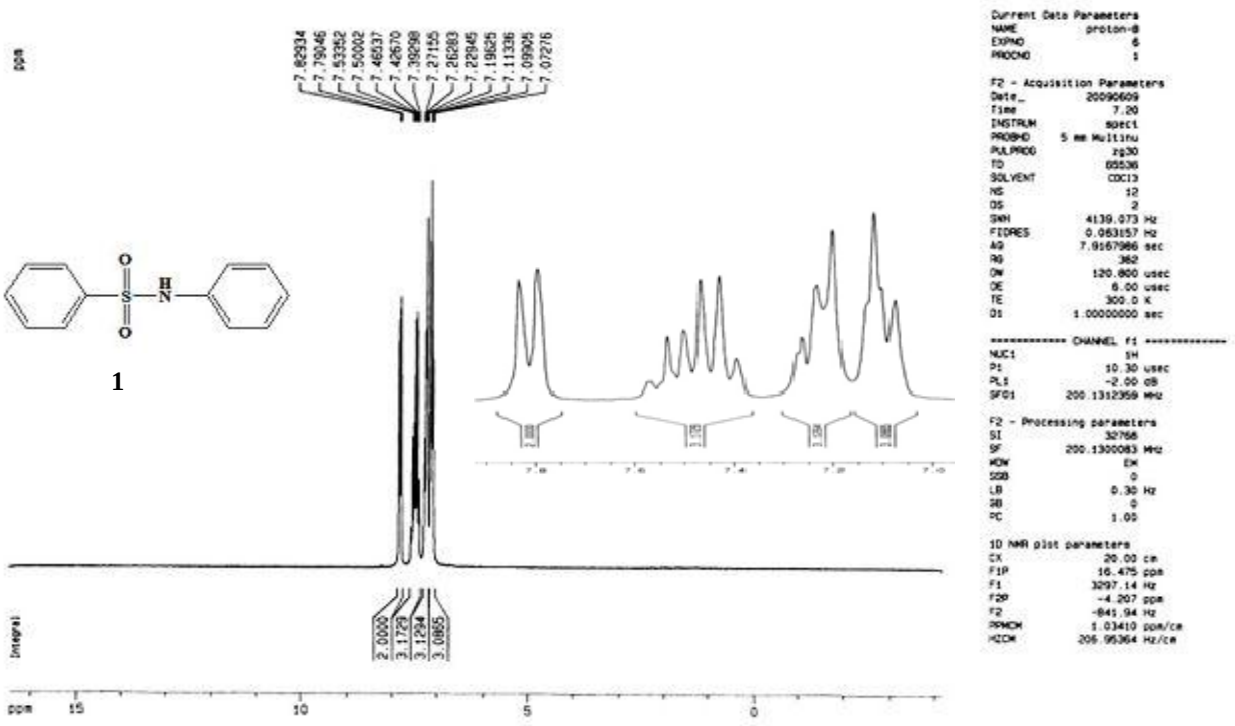
============ CHANNEL f1 =============
NUC1                  13C
P1                 10.00 usec
PL1                -5.00 dB
SFO1          50.3282440 MHz

============ CHANNEL f2 =============
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               20.00 dB
PL13               20.00 dB
SFO2          200.1308005 MHz

F2 - Processing parameters
SI                 32768
SF           50.3227309 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               234.377 ppm
F1              11794.47 Hz
F2P               -15.268 ppm
F2              -768.34 Hz
PPMCM            12.48225 ppm/cm
HZCM            628.14069 Hz/cm
```

^{1}H and ^{13}C NMR spectra of sulfonamides (S18-S28)



1

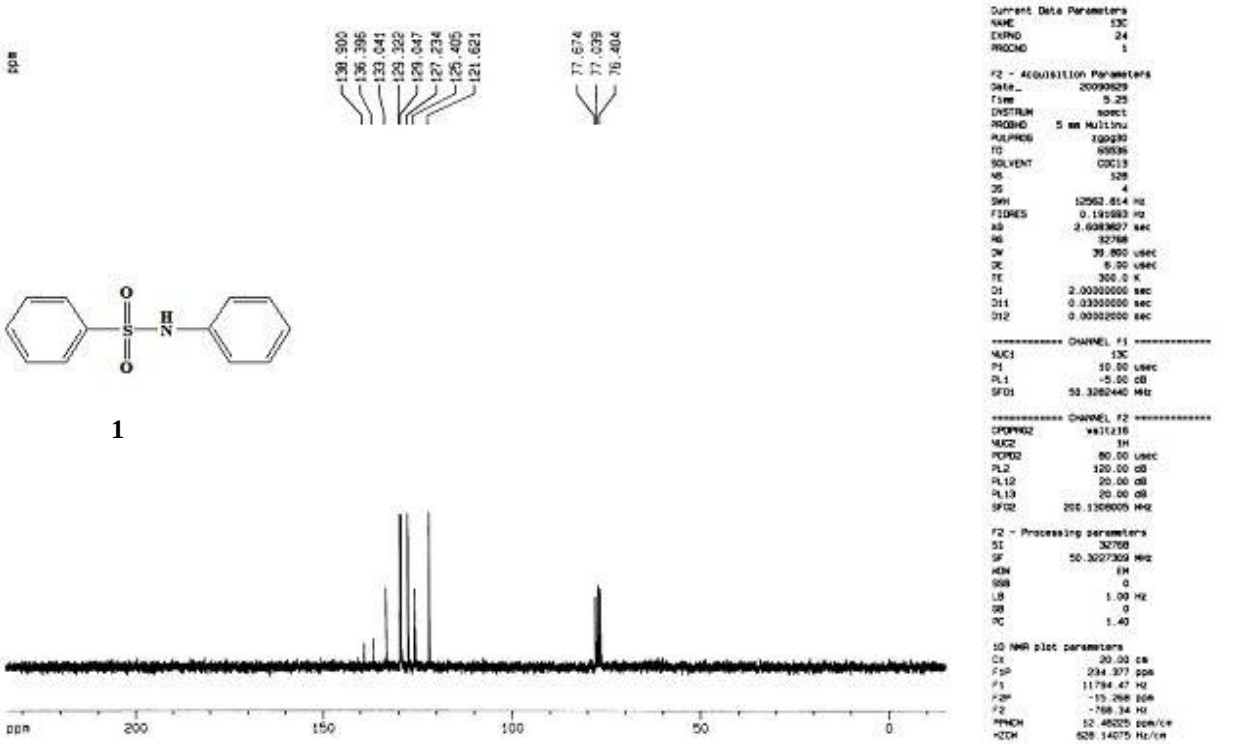
Current Data Parameters
NAME proton-8
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090609
Time 7.20
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 4139.073 Hz
FIDRES 0.063157 Hz
AQ 7.9167986 sec
RG 362
DW 120.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

CHANNEL f1
NUC1 1H
P1 10.30 usec
PL1 -2.00 dB
SFO1 200.1312959 MHz

F2 - Processing parameters
SI 32768
SF 200.1300083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 16.475 ppm
F1 3297.14 Hz
F2P -4.207 ppm
F2 -841.94 Hz
PPMCM 1.03410 ppm/cm
HZCM 206.95364 Hz/cm



1

Current Data Parameters
NAME 13C
EXPNO 24
PROCNO 1

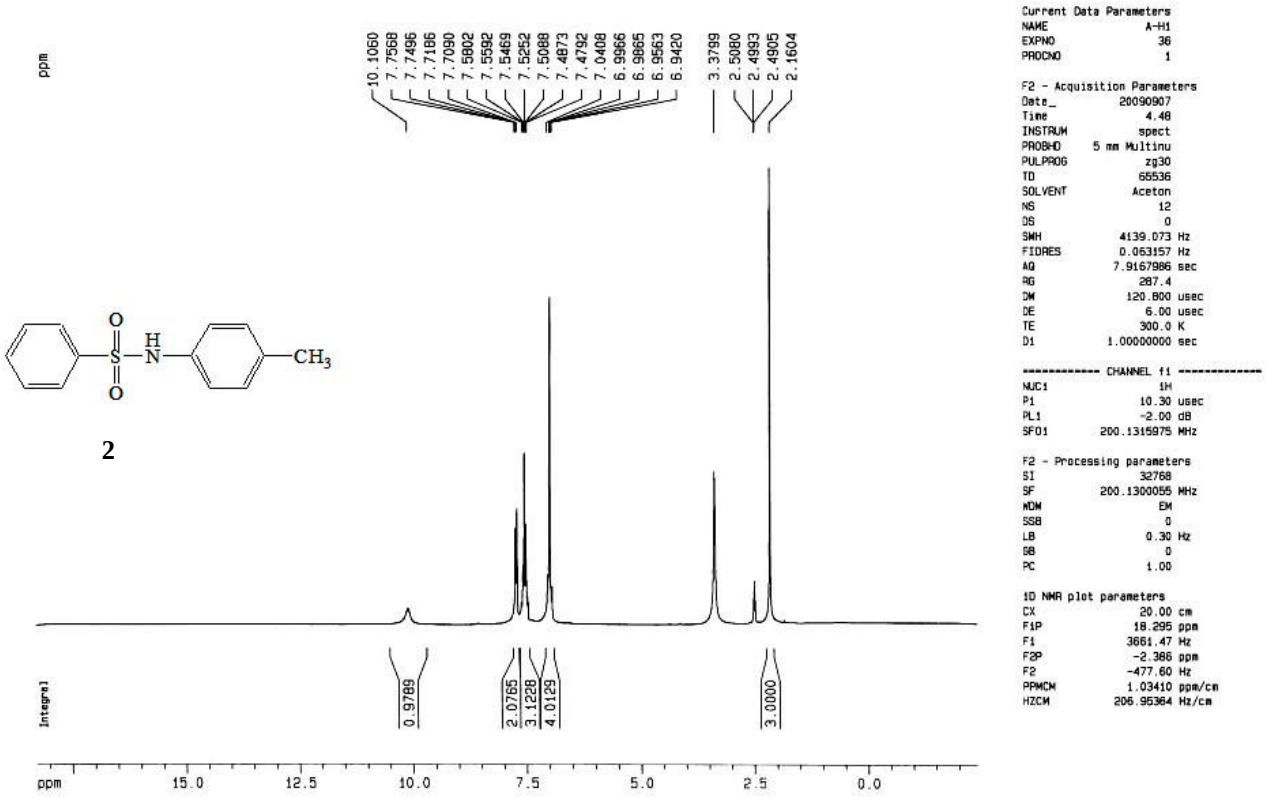
F2 - Acquisition Parameters
Date_ 20090629
Time 5.25
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083607 sec
RG 32768
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -5.00 dB
SFO1 50.3282440 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 200.1300005 MHz

F2 - Processing parameters
SI 32768
SF 50.3027309 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 234.377 ppm
F1 11794.47 Hz
F2P -15.268 ppm
F2 -768.34 Hz
PPMCM 12.46225 ppm/cm
HZCM 626.14075 Hz/cm



2

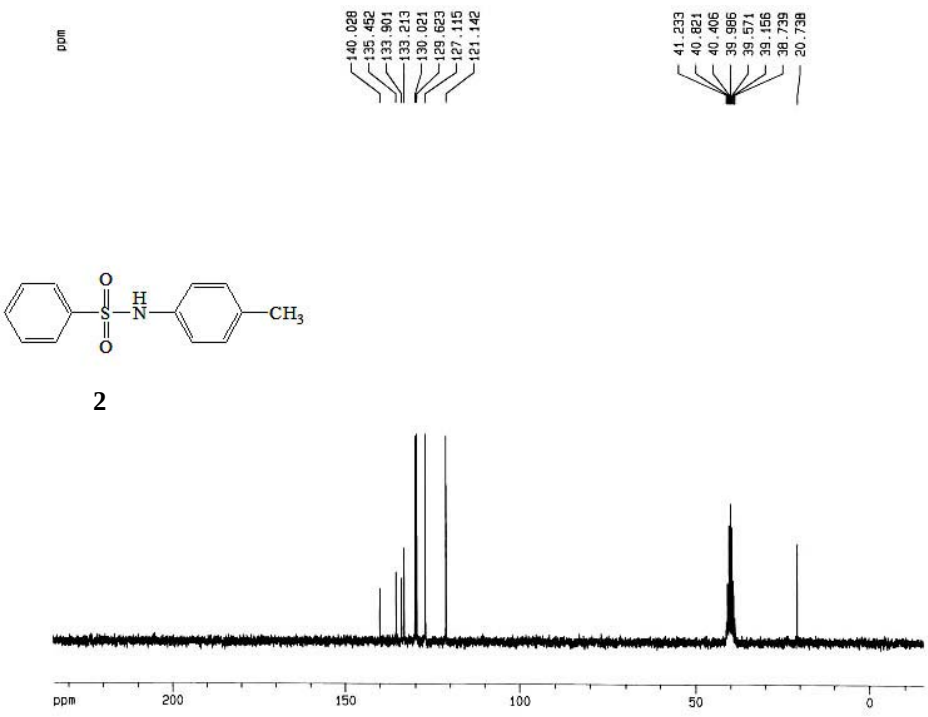
Current Data Parameters
NAME A-H1
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090907
Time 4.48
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT Aceton
NS 12
DS 0
SWH 4139.073 Hz
FIDRES 0.063157 Hz
AQ 7.9167986 sec
RG 287.4
DW 120.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

---------- CHANNEL f1 ----------
NUC1 1H
P1 10.30 usec
PL1 -2.00 dB
SFO1 200.1315975 MHz

F2 - Processing parameters
SI 32768
SF 200.1300055 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 18.295 ppm
F1 3661.47 Hz
F2P -2.386 ppm
F2 -477.60 Hz
PPMCM 1.03410 ppm/cm
HZCM 206.95364 Hz/cm



2

Current Data Parameters
NAME 13C
EXPNO 8
PROCNO 1

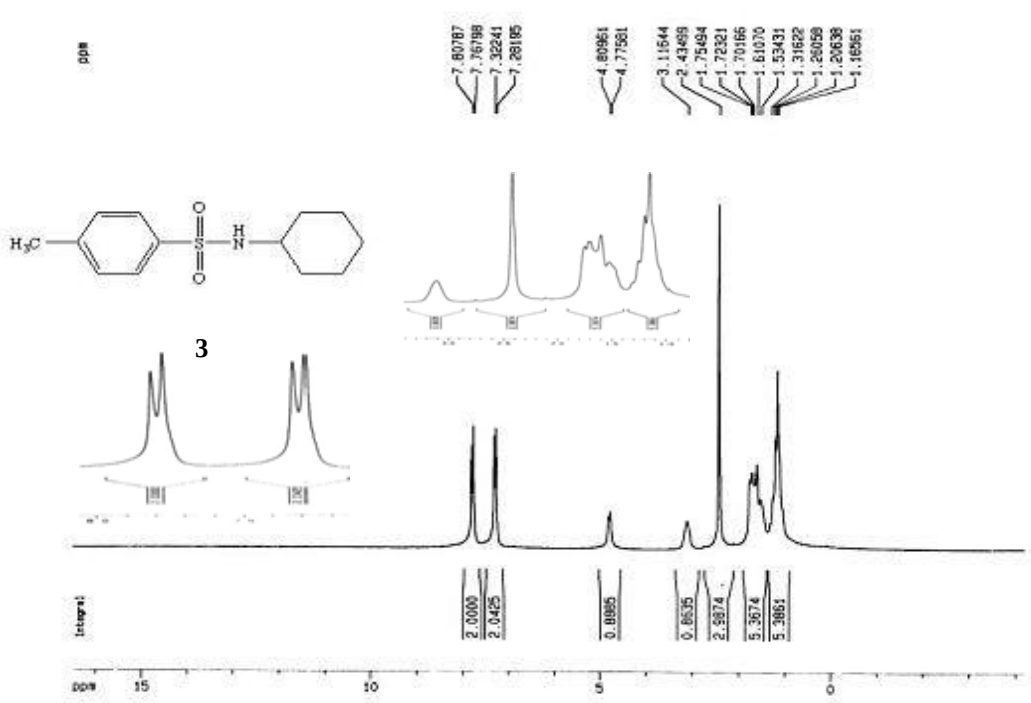
F2 - Acquisition Parameters
Date_ 20090907
Time 4.59
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 127
DS 4
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 32768
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

---------- CHANNEL f1 ----------
NUC1 13C
P1 10.00 usec
PL1 -5.00 dB
SFO1 50.3282440 MHz

---------- CHANNEL f2 ----------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 200.1308005 MHz

F2 - Processing parameters
SI 32768
SF 50.3227294 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 234.408 ppm
F1 11796.04 Hz
F2P -15.237 ppm
F2 -766.77 Hz
PPMCM 12.48225 ppm/cm
HZCM 628.14075 Hz/cm



3

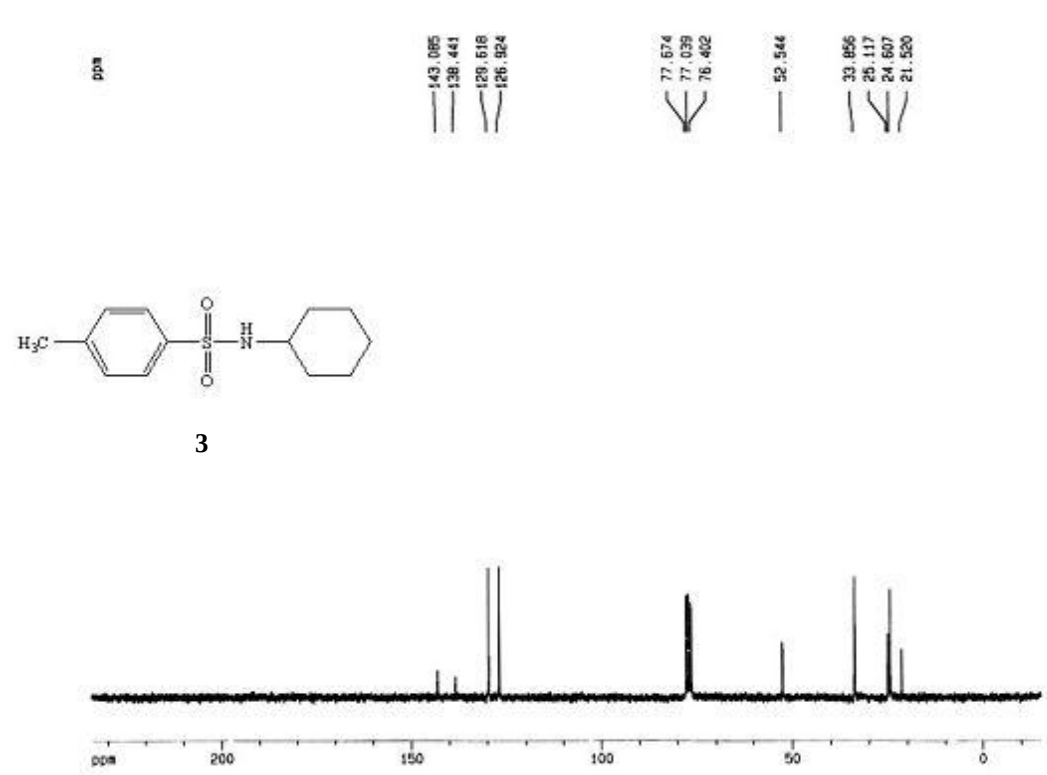
```
Current Data Parameters
NAME                  1H-Dr.B
EXPNO                      15
PROCNO                      1

F2 - Acquisition Parameters
Date_              20090225
Time                    6.56
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        0
SWH                4139.073 Hz
FIDRES             0.063157 Hz
AQ                 7.9167986 sec
RG                      256
DW                 120.800 usec
DE                   7.50 usec
TE                   300.0 K
D1                 1.00000000 sec

========== CHANNEL f1 ==========
NUC1                      1H
P1                     10.30 usec
PL1                    -2.00 dB
SFO1          200.1312359 MHz

F2 - Processing parameters
SI                       32768
SF                200.1300045 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
F1P                   10.494 ppm
F1                  3300.97 Hz
F2P                   -4.188 ppm
F2                  -838.10 Hz
PPMCM                 1.03410 ppm/cm
HZCM                206.95364 Hz/cm
```



3

```
Current Data Parameters
NAME                  C13-Dr.B
EXPNO                       10
PROCNO                      1

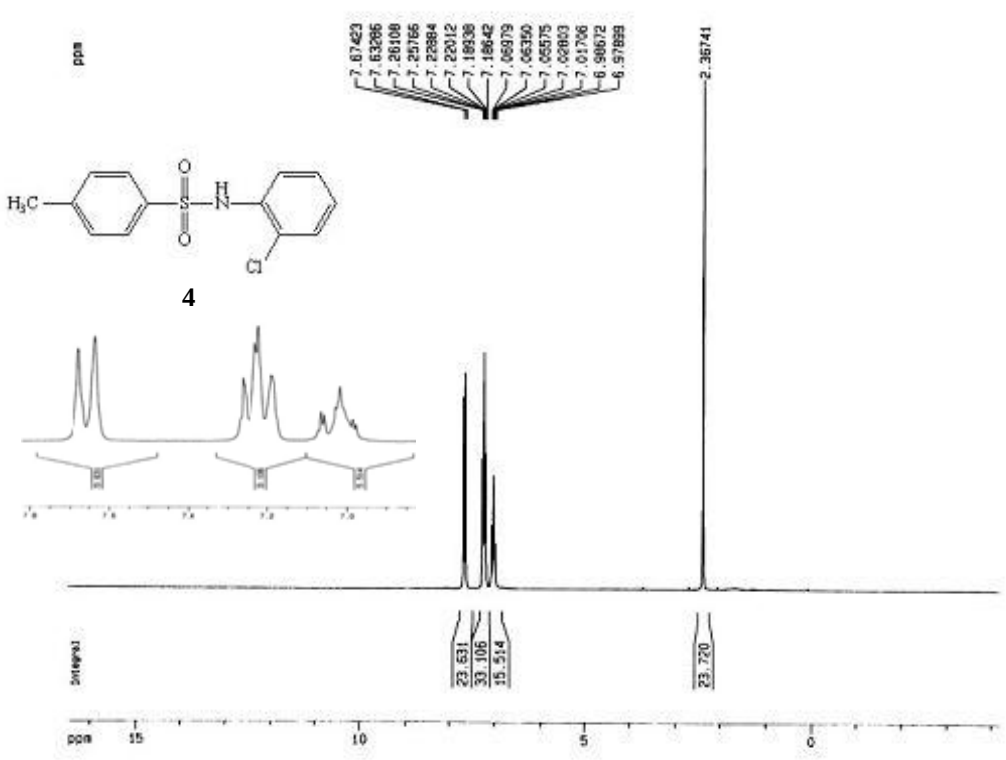
F2 - Acquisition Parameters
Date_              20090225
Time                    6.24
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       349
DS                         4
SWH                12562.814 Hz
FIDRES             0.191693 Hz
AQ                 2.6083827 sec
RG                      32768
DW                 39.800 usec
DE                    6.00 usec
TE                   300.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec

========== CHANNEL f1 ==========
NUC1                      13C
P1                     10.00 usec
PL1                    -5.00 dB
SFO1          50.3282440 MHz

========== CHANNEL f2 ==========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                   120.00 dB
PL12                   20.00 dB
PL13                   20.00 dB
SFO2          200.1308005 MHz

F2 - Processing parameters
SI                       32768
SF                50.3227309 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40

1D NMR plot parameters
CX                     20.00 cm
F1P                  234.377 ppm
F1                 11794.47 Hz
F2P                  -15.268 ppm
F2                  -768.34 Hz
PPMCM                12.48026 ppm/cm
HZCM                628.14075 Hz/cm
```



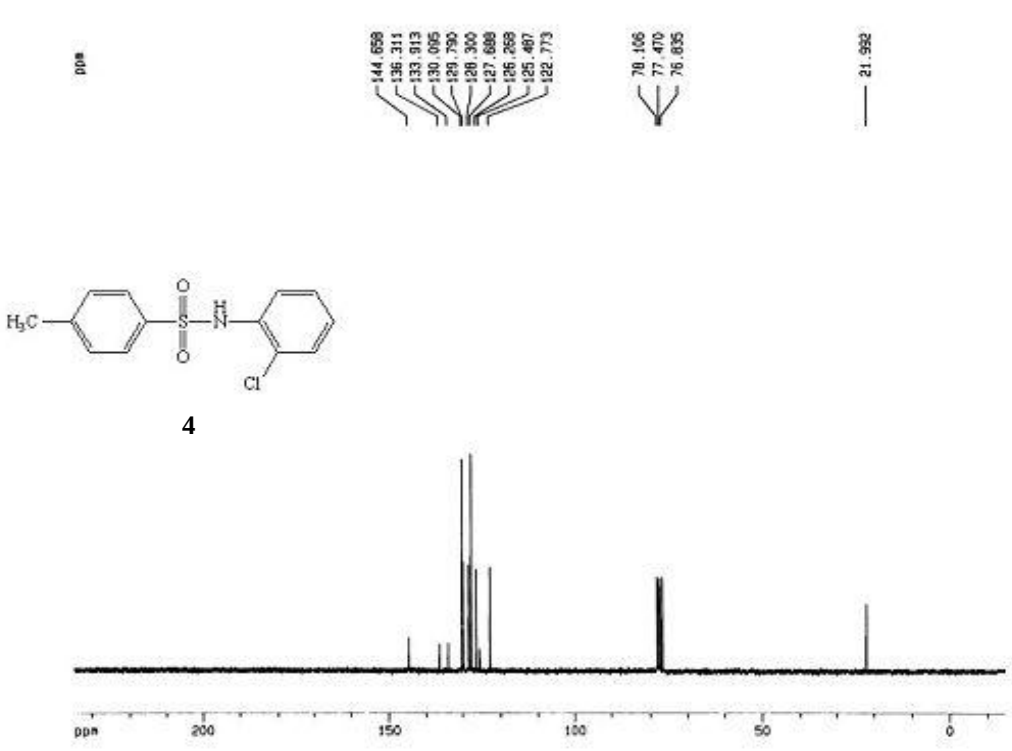

```
Current Data Parameters
NAME                  1H
EXPNO                 28
PROCNO                1

F2 - Acquisition Parameters
Date_           20081125
Time                13.23
INSTRUM             spect
PROBHD     5 mm Multinu
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                     28
DS                      0
SWH              4139.073 Hz
FIDRES           0.063157 Hz
AQ               7.9167986 sec
RG                  574.7
DW                120.800 usec
DE                  7.50 usec
TE                 300.0 K
D1              1.00000000 sec

========== CHANNEL f1 ==========
NUC1                  1H
P1                 10.70 usec
PL1                -2.00 dB
SFO1          200.1312359 MHz

F2 - Processing parameters
SI                 32768
SF            200.1300063 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
FSP               16.475 ppm
F1              3297.14 Hz
F2P                -4.207 ppm
F2              -841.94 Hz
PPMCM           1.03410 ppm/cm
HZCM          206.95384 Hz/cm
```




```
Current Data Parameters
NAME              carbon13
EXPNO                   57
PROCNO                   1

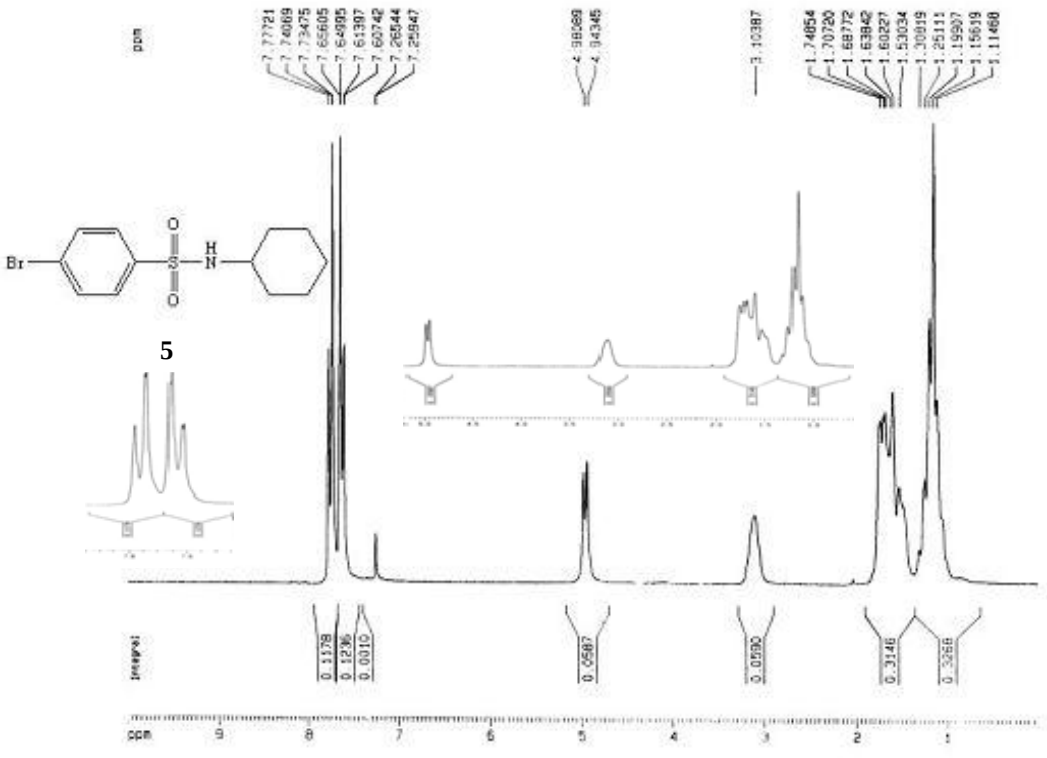
F2 - Acquisition Parameters
Date_           20081125
Time                13.17
INSTRUM             spect
PROBHD     5 mm Multinu
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                    452
DS                      4
SWH              12562.814 Hz
FIDRES           0.191693 Hz
AQ               2.6083827 sec
RG                  32768
DW                 39.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec

========== CHANNEL f1 ==========
NUC1                  13C
P1                 10.00 usec
PL1                -5.00 dB
SFO1          50.3282440 MHz

========== CHANNEL f2 ==========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2               120.00 dB
PL12               20.00 dB
PL13               20.00 dB
SFO2          200.1308005 MHz

F2 - Processing parameters
SI                 32768
SF            50.3227290 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
F1P               254.853 ppm
F1              11816.42 Hz
F2P               -14.832 ppm
F2              -746.40 Hz
PPMCM           12.46225 ppm/cm
HZCM          626.14698 Hz/cm
```



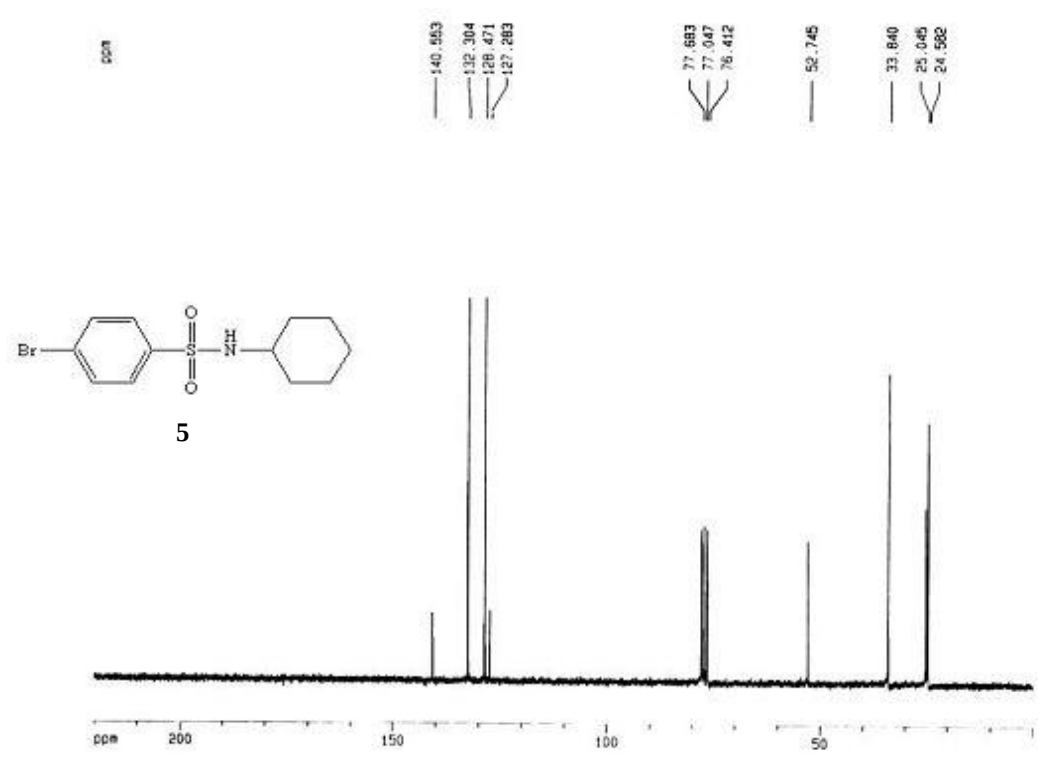
Current Data Parameters
NAME 5H-Dr.B
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090309
Time 8.06
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 0
SWH 4139.073 Hz
FIDRES 0.063157 Hz
AQ 7.9167988 sec
RG 256
DW 120.800 usec
DE 7.50 usec
TE 300.0 K
D1 1.00000000 sec

CHANNEL f1
NUC1 1H
P1 10.30 usec
PL1 -2.00 dB
SFO1 200.1312959 MHz

F2 - Processing parameters
SI 32768
SF 200.1300087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 2001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.50000 ppm/cm
HZCM 100.06500 Hz/cm



Current Data Parameters
NAME C13-Dr.B
EXPNO 24
PROCNO 1

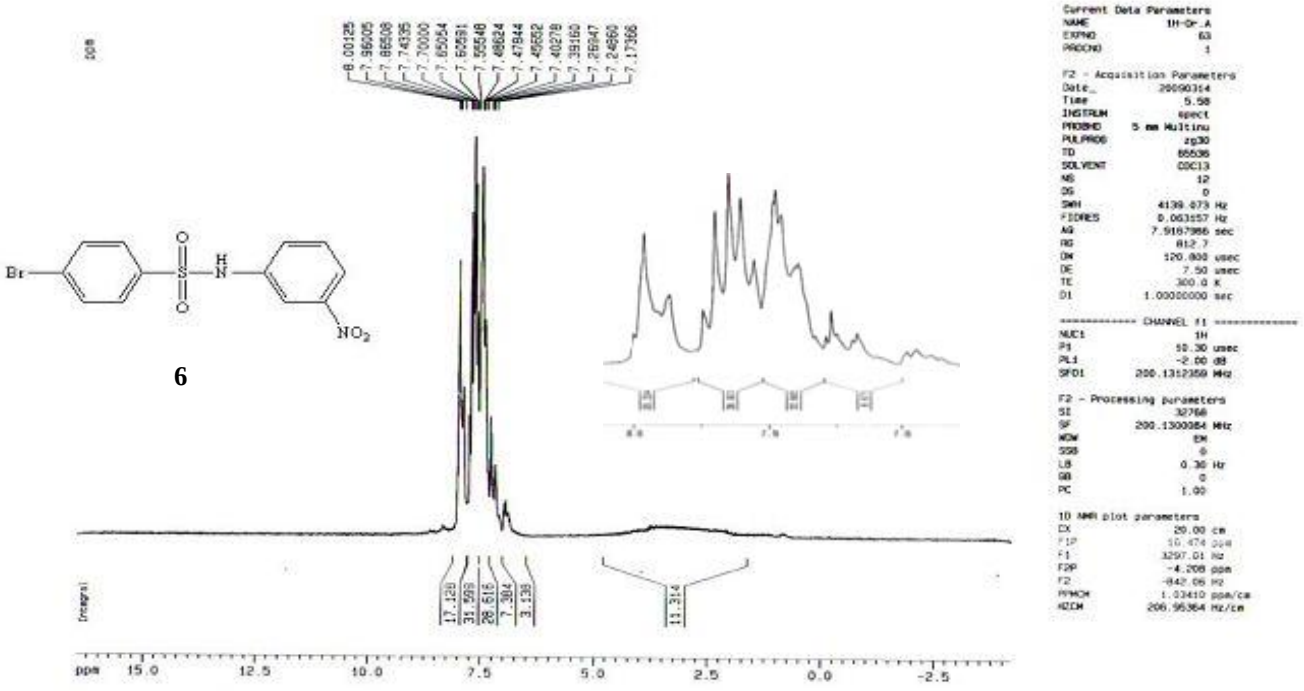
F2 - Acquisition Parameters
Date_ 20090309
Time 9.12
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 761
DS 4
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 32768
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -5.00 dB
SFO1 50.3282440 MHz

CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 200.1308005 MHz

F2 - Processing parameters
SI 32768
SF 50.3227309 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 220.000 ppm
F1 10971.00 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 11.00000 ppm/cm
HZCM 553.55005 Hz/cm



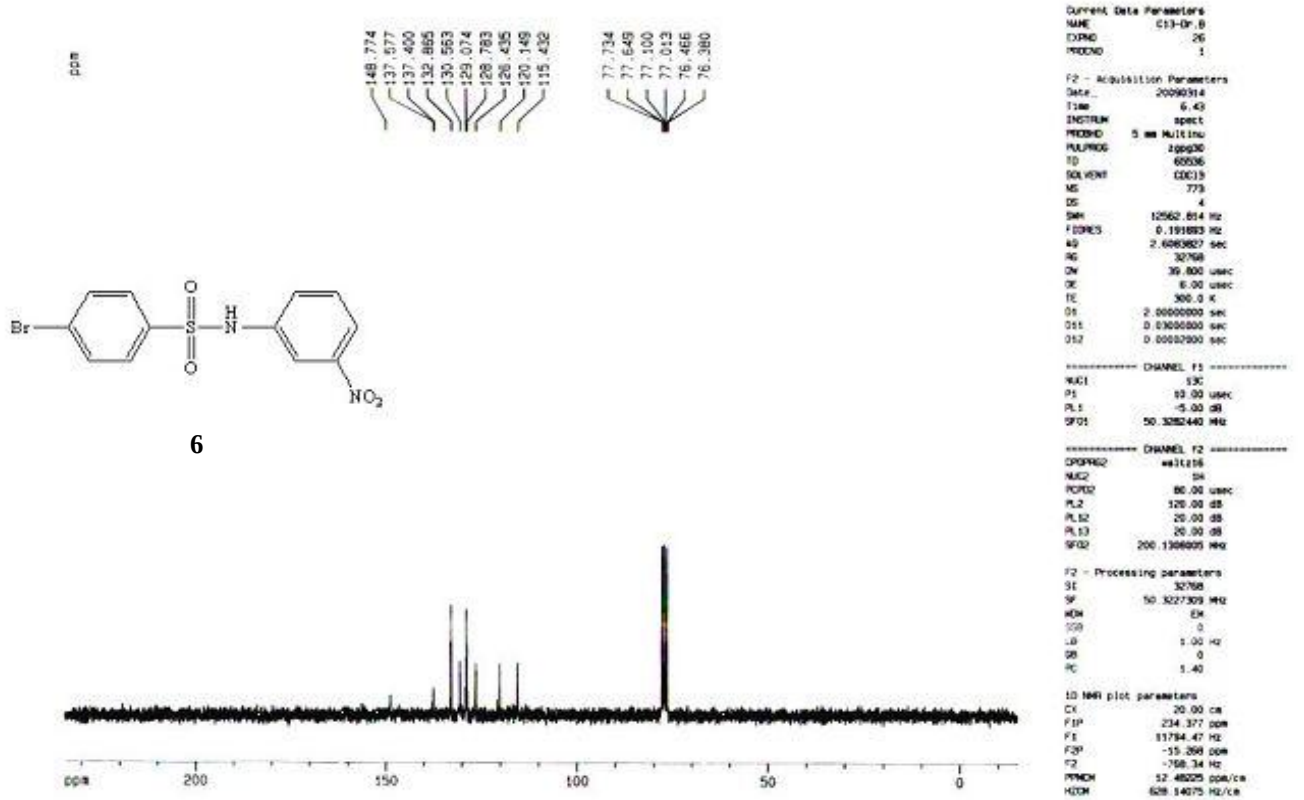

```
Current Data Parameters
NAME                  1H-Dr.A
EXPNO                      63
PROCNO                      1

F2 - Acquisition Parameters
Date_              20090314
Time                   5.58
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        0
SWH              4139.073 Hz
FIDRES           0.063157 Hz
AQ               7.9167986 sec
RG                    812.7
DW                120.800 usec
DE                  7.50 usec
TE                 300.0 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.30 usec
PL1                 -2.00 dB
SFO1        200.1312359 MHz

F2 - Processing parameters
SI                    32768
SF          200.1300084 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    20.00 cm
F1P                 10.474 ppm
F1                 3297.01 Hz
F2P                -4.208 ppm
F2                 -842.06 Hz
PPMCM               1.03410 ppm/cm
HZCM              206.95364 Hz/cm
```




```
Current Data Parameters
NAME                  C13-Dr.B
EXPNO                       26
PROCNO                       1

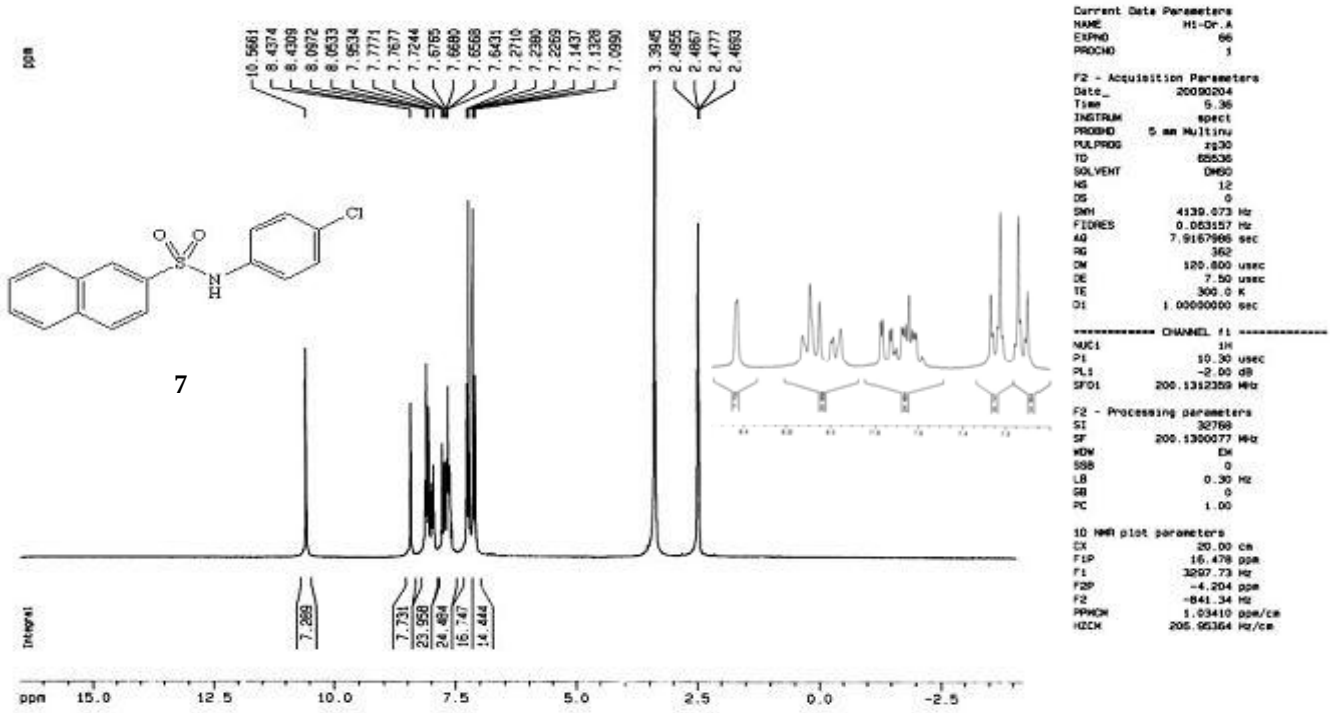
F2 - Acquisition Parameters
Date_              20090314
Time                   6.43
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      773
DS                        4
SWH              12562.814 Hz
FIDRES           0.191693 Hz
AQ               2.6083827 sec
RG                    32768
DW                39.800 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec

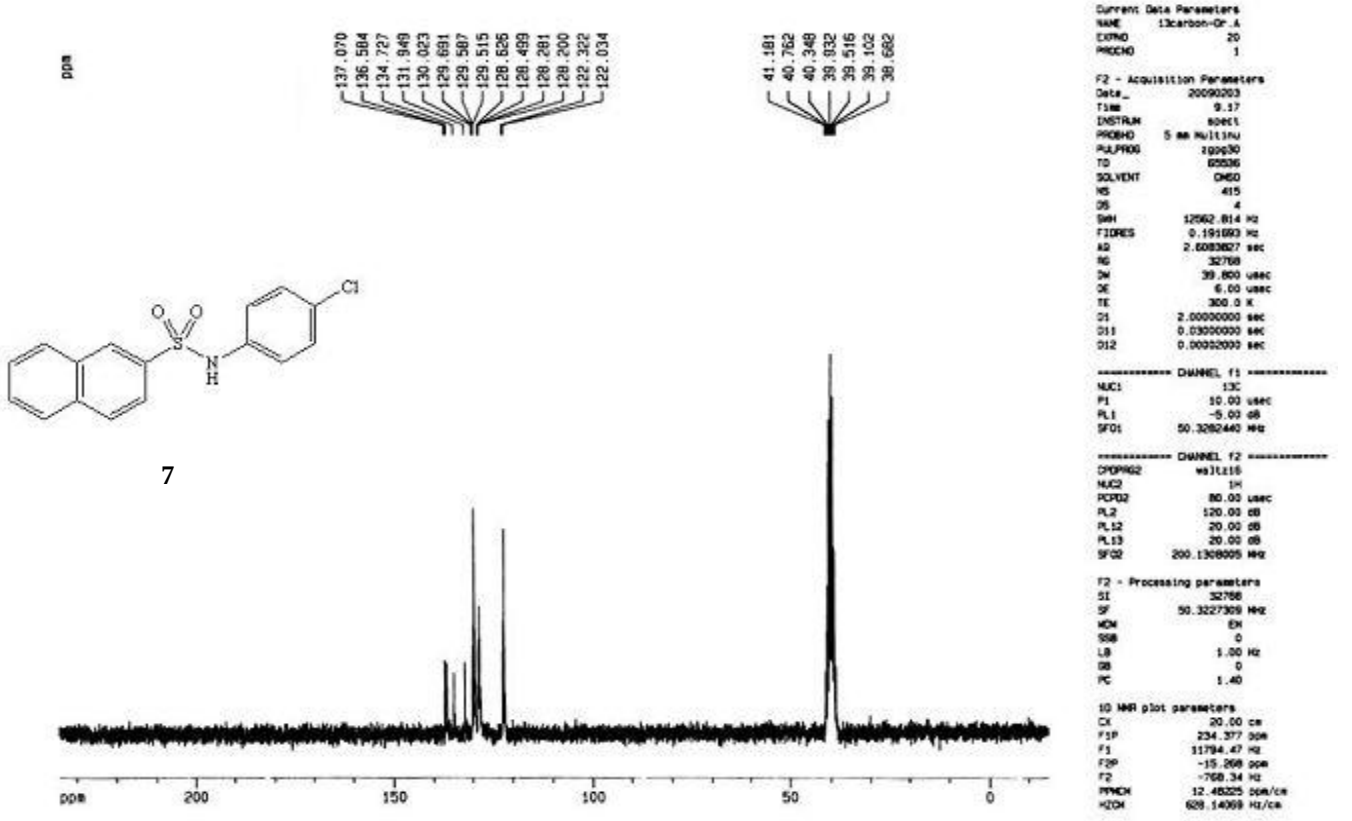
======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PL1                 -5.00 dB
SFO1        50.3252440 MHz

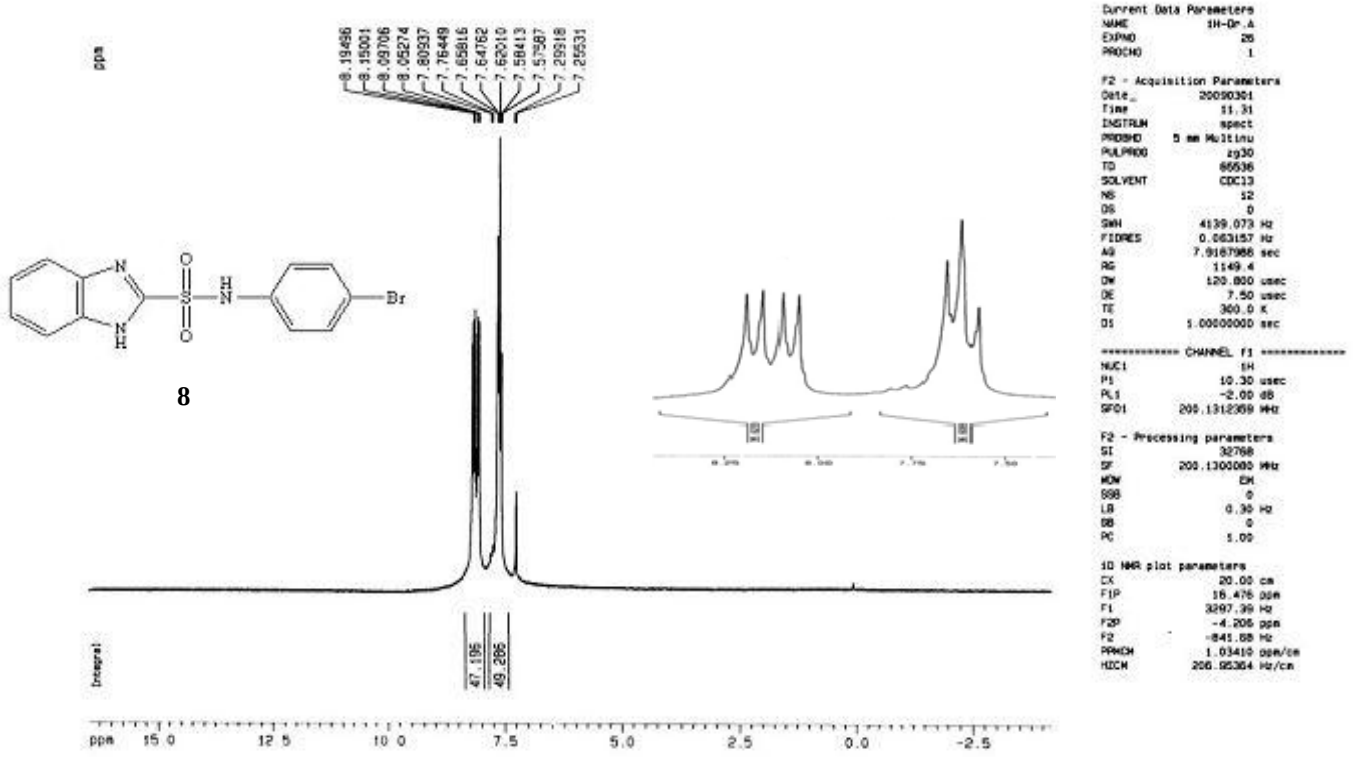
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                120.00 dB
PL12                20.00 dB
PL13                20.00 dB
SFO2        200.1300005 MHz

F2 - Processing parameters
SI                    32768
SF          50.3227309 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                    20.00 cm
F1P                 234.377 ppm
F1                 11794.47 Hz
F2P                -15.256 ppm
F2                 -768.34 Hz
PPMCM              52.48225 ppm/cm
HZCM              628.14075 Hz/cm
```


ppm
10.5661
8.4374
8.4308
8.0972
8.0533
7.9534
7.7771
7.7677
7.7244
7.6765
7.6680
7.6568
7.6431
7.2710
7.2380
7.2269
7.1437
7.1328
7.0990
3.3945
2.4955
2.4867
2.4777
2.4663
Cl
O
S
O
N
H
7
Integral
7.288
7.731
23.958
24.464
16.747
14.444
ppm 15.0 12.5 10.0 7.5 5.0 2.5 0.0 -2.5
Current Data Parameters
NAME H1-Dr.A
EXPNO 66
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090204
Time 5.36
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 12
DS 0
SWH 4139.073 Hz
FIDRES 0.063157 Hz
AQ 7.9167986 sec
RG 362
DW 120.800 usec
DE 7.50 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 10.30 usec
PL1 -2.00 dB
SFO1 200.1312359 MHz
F2 - Processing parameters
SI 32768
SF 200.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 10.478 ppm
F1 3297.73 Hz
F2P -4.204 ppm
F2 -841.34 Hz
PPMCM 1.03410 ppm/cm
HZCM 205.95364 Hz/cm


ppm
137.070
136.584
134.727
131.949
130.023
129.691
129.587
129.515
128.626
128.499
128.281
128.200
122.322
122.034
41.181
40.762
40.348
39.932
39.516
39.102
38.682
Cl
O
S
O
N
H
7
ppm 200 150 100 50 0
Current Data Parameters
NAME 13carbon-Dr.A
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090203
Time 9.17
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 415
DS 4
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 32768
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -5.00 dB
SFO1 50.3282440 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 200.1308005 MHz
F2 - Processing parameters
SI 32768
SF 50.3227309 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 234.377 ppm
F1 11794.47 Hz
F2P -15.268 ppm
F2 -768.34 Hz
PPMCM 12.48225 ppm/cm
HZCM 628.14069 Hz/cm



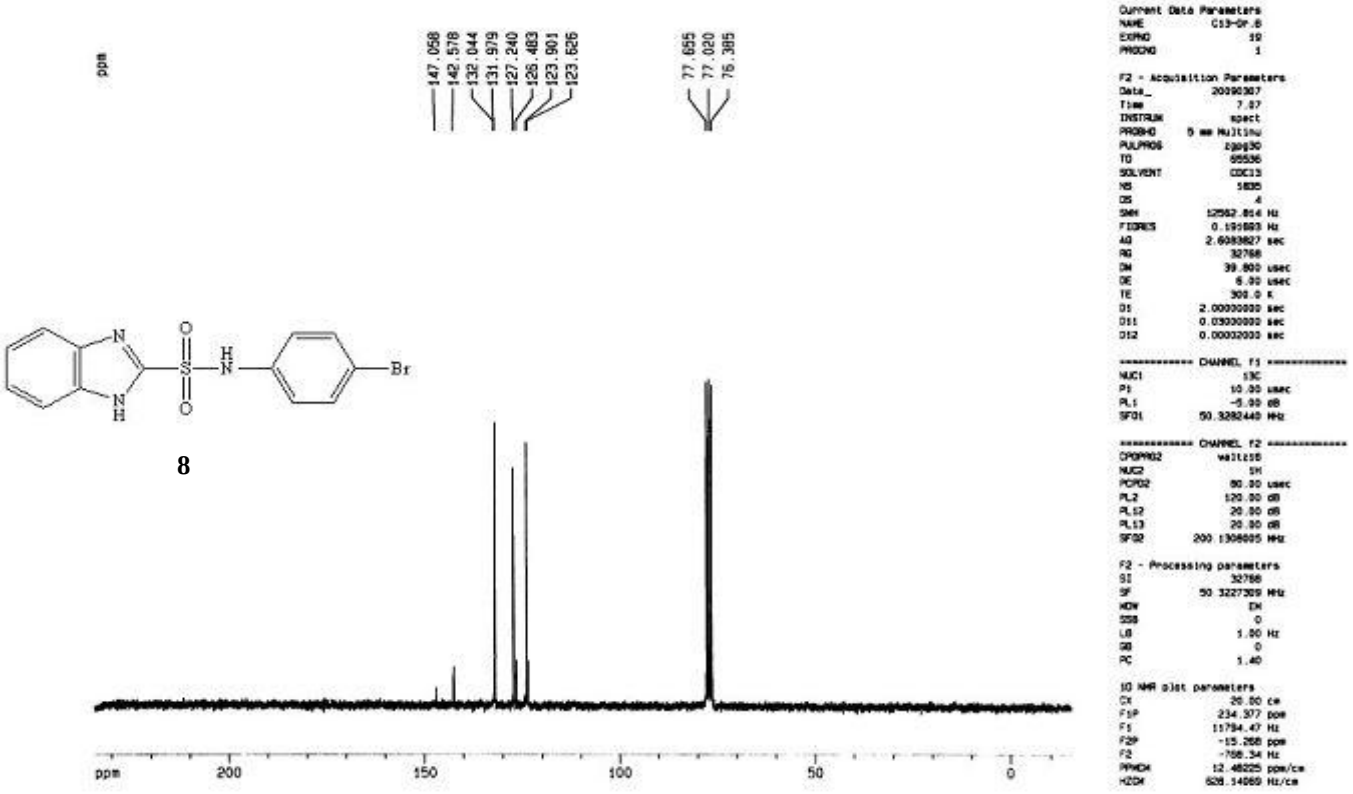

```
Current Data Parameters
NAME                  1H-Gr.A
EXPNO                      26
PROCNO                      1

F2 - Acquisition Parameters
Date_              20090301
Time                  11.31
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      12
DS                       0
SWH              4139.073 Hz
FIDRES           0.063157 Hz
AQ               7.9167986 sec
RG                  1149.4
DW                 120.800 usec
DE                    7.50 usec
TE                  300.0 K
D1               1.00000000 sec

============ CHANNEL f1 =============
NUC1                   1H
P1                  10.30 usec
PL1                 -2.00 dB
SFO1          200.1312369 MHz

F2 - Processing parameters
SI                   32768
SF            200.1300000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                    1.00

1D NMR plot parameters
CX                   20.00 cm
F1P                16.476 ppm
F1                 3297.39 Hz
F2P                -4.206 ppm
F2                 -841.68 Hz
PPMCM             1.03410 ppm/cm
HZCM              206.95364 Hz/cm
```




```
Current Data Parameters
NAME                  C13-Gr.A
EXPNO                       19
PROCNO                       1

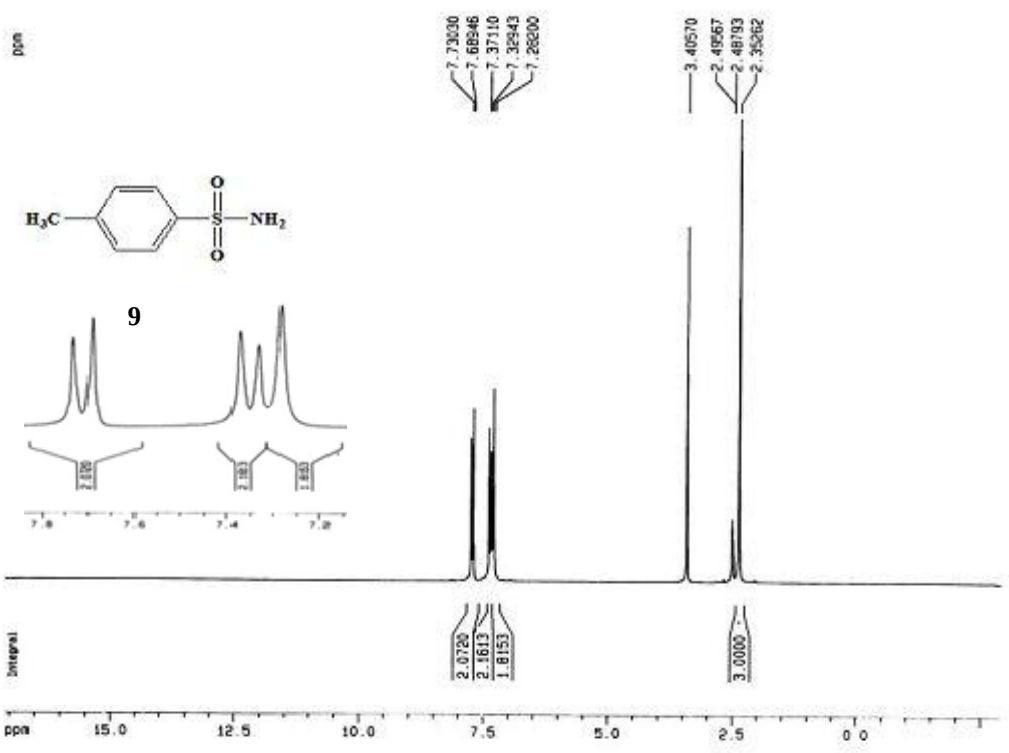
F2 - Acquisition Parameters
Date_              20090307
Time                   7.07
INSTRUM                spect
PROBHD     5 mm Multinu
PULPROG             zpg30
TD                   65536
SOLVENT              CDCl3
NS                    5835
DS                       4
SWH              12562.814 Hz
FIDRES           0.191693 Hz
AQ               2.6083827 sec
RG                   32768
DW                  39.800 usec
DE                    6.00 usec
TE                  300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
D12              0.00002000 sec

============ CHANNEL f1 =============
NUC1                   13C
P1                  10.00 usec
PL1                  -5.00 dB
SFO1          50.3282440 MHz

============ CHANNEL f2 =============
CPDPRG2             waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                120.00 dB
PL12                20.00 dB
PL13                20.00 dB
SFO2          200.1308005 MHz

F2 - Processing parameters
SI                   32768
SF            50.3227309 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                    1.40

1D NMR plot parameters
CX                   20.00 cm
F1P                234.377 ppm
F1                 11794.47 Hz
F2P                -15.268 ppm
F2                 -768.34 Hz
PPMCM             12.48225 ppm/cm
HZCM              628.14069 Hz/cm
```



9

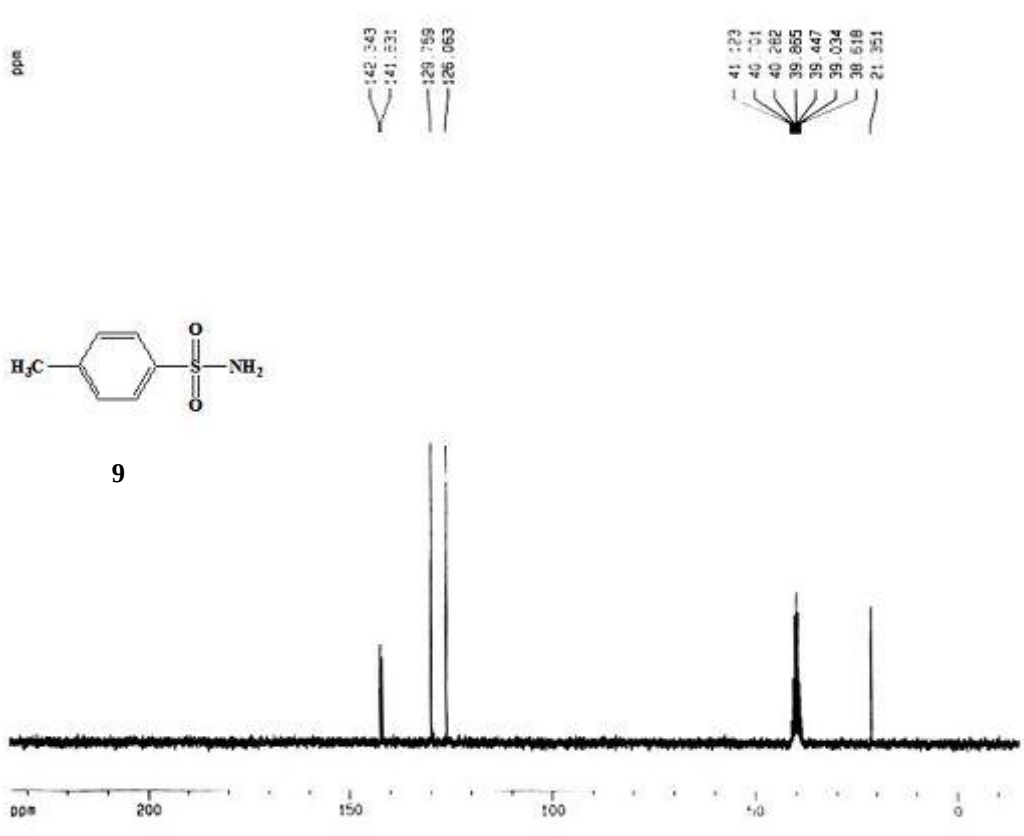
```
Current Data Parameters
NAME                  Proton-B
EXPNO                       24
PROCNO                       1

F2 - Acquisition Parameters
Date_               20090506
Time                      9.10
INSTRUM                   spect
PROBHD     5 mm Multinu
PULPROG                   zg30
TD                       65536
SOLVENT                   DMSO
NS                          12
DS                           0
SWH                 4006.410 Hz
FIDRES              0.061133 Hz
AQ                  8.1789427 sec
RG                         256
DW                  124.800 usec
DE                    7.50 usec
TE                    300.0 K
D1                  1.00000000 sec

========== CHANNEL f1 ==========
NUC1                       1H
P1                      10.30 usec
PL1                     -2.00 dB
SFO1             200.1314252 MHz

F2 - Processing parameters
SI                       32768
SF                200.1300074 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
F1P                    17.094 ppm
F1                   3421.06 Hz
F2P                   -2.925 ppm
F2                   -585.35 Hz
PPMCM                1.00095 ppm/cm
HZCM               200.32050 Hz/cm
```



9

```
Current Data Parameters
NAME                  13C-Dr.B
EXPNO                       21
PROCNO                       1

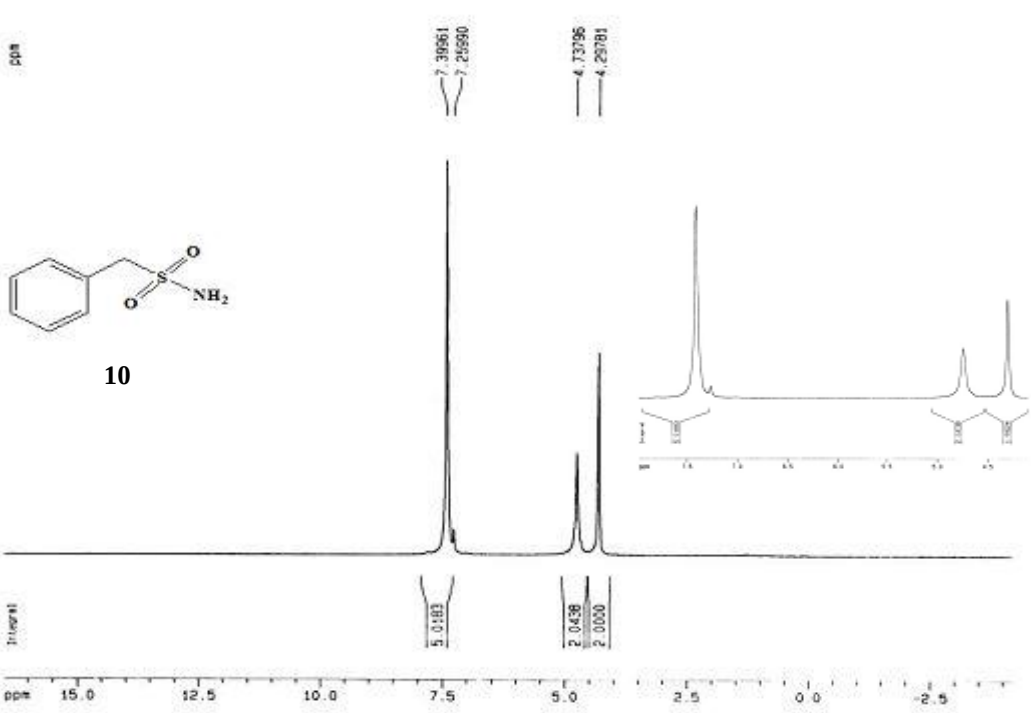
F2 - Acquisition Parameters
Date_               20090509
Time                      5.23
INSTRUM                   spect
PROBHD     5 mm Multinu
PULPROG                 zgpg30
TD                       65536
SOLVENT                   DMSO
NS                          53
DS                           4
SWH                 12562.814 Hz
FIDRES              0.191693 Hz
AQ                  2.6083827 sec
RG                       32768
DW                    39.800 usec
DE                     6.00 usec
TE                    300.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec

========== CHANNEL f1 ==========
NUC1                       13C
P1                      10.00 usec
PL1                      -5.00 dB
SFO1             50.3262440 MHz

========== CHANNEL f2 ==========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                     120.00 dB
PL12                     20.00 dB
PL13                     20.00 dB
SFO2             200.1308005 MHz

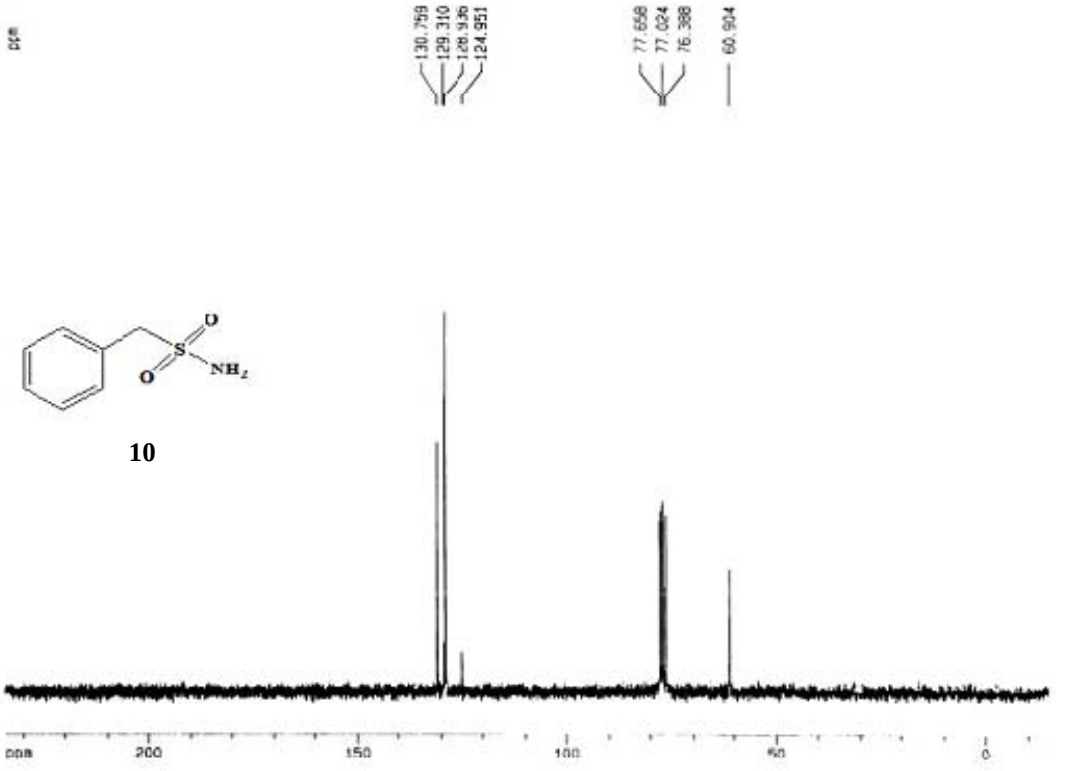
F2 - Processing parameters
SI                       32768
SF                50.3227309 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
F1P                   234.377 ppm
F1                  11794.47 Hz
F2P                  -15.268 ppm
F2                   -768.34 Hz
PPMCM                12.46225 ppm/cm
HZCM               626.14075 Hz/cm
```


ppm
7.39961
7.26990
4.73796
4.29781
Integral
5.0183
2.0438
2.0000
ppm 15.0 12.5 10.0 7.5 5.0 2.5 0.0 -2.5

10


Current Data Parameters
NAME H1-A
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090525
Time 9.48
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 4139.073 Hz
FIDRES 0.063157 Hz
AQ 7.9167986 sec
RG 812.7
DW 120.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
CHANNEL f1
NUC1 1H
P1 10.30 usec
PL1 -2.00 dB
SFO1 200.1312359 MHz
F2 - Processing parameters
SI 32768
SF 200.1300084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
F1P 16.174 ppm
F1 3297.01 Hz
F2P -4.208 ppm
F2 -842.06 Hz
PPMCM 1.03410 ppm/cm
HZCM 206.95364 Hz/cm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128.936
124.951
77.656
77.024
76.388
60.904
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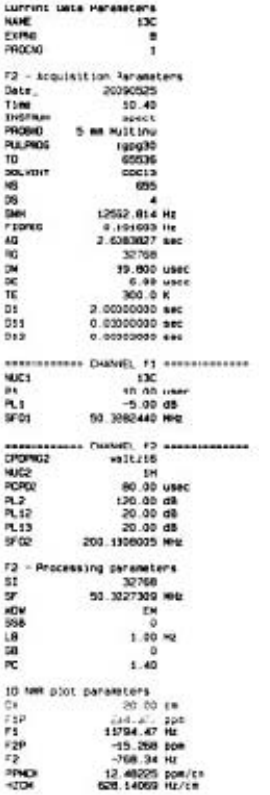
10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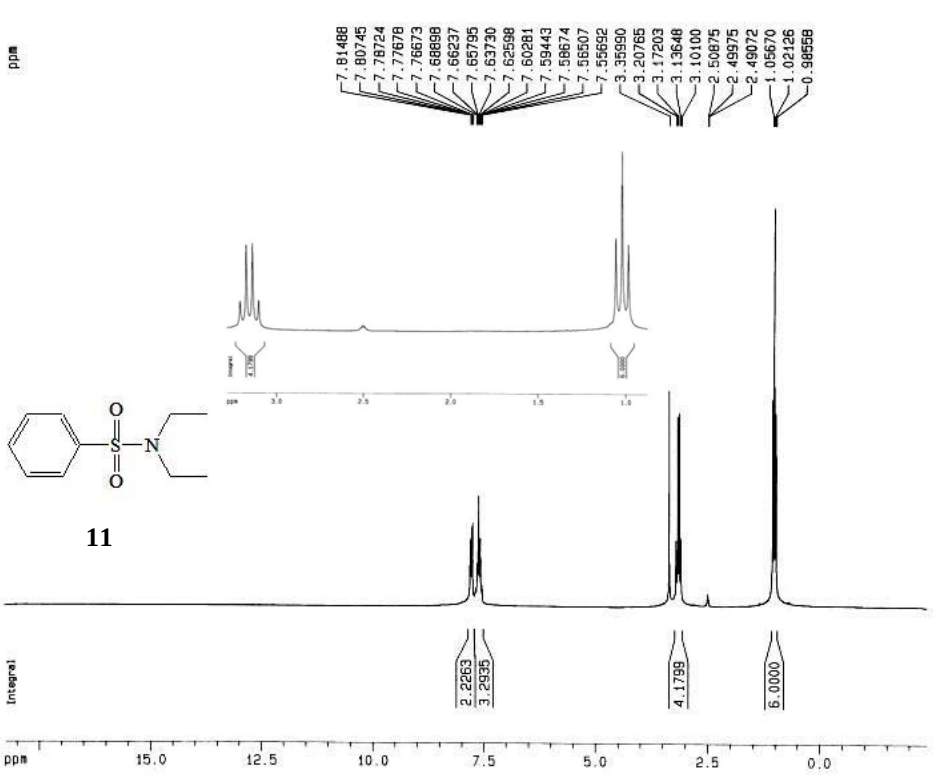
NAME 13C
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090525
Time 10.40
INSTRUM spect
PROBHD 5 mm Multinu
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 655
DS 4
SWH 12562.814 Hz
FIDRES 0.191693 Hz
AQ 2.6083827 sec
RG 32768
DW 39.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00020000 sec
CHANNEL f1
NUC1 13C
P1 10.00 usec
PL1 -5.00 dB
SFO1 50.3082440 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 120.00 dB
PL12 20.00 dB
PL13 20.00 dB
SFO2 200.1308005 MHz
F2 - Processing parameters
SI 32768
SF 50.3227309 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
F1P 240.0... ppm
F1 12084.47 Hz
F2P -15.268 ppm
F2 -768.94 Hz
PPMCM 12.48225 ppm/cm
HZCM 628.14069 Hz/cm



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```
Current Data Parameters
NAME                  A-H1
EXPNO                   35
PROCNO                   1

F2 - Acquisition Parameters
Date_              20090907
Time                   3.42
INSTRUM               spect
PROBHD     5 mm Multinu
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      12
DS                       0
SWH               4139.073 Hz
FIDRES            0.063157 Hz
AQ                7.9167986 sec
RG                     181
DW                 120.800 usec
DE                   6.00 usec
TE                  300.0 K
D1                1.00000000 sec

========== CHANNEL f1 ==========
NUC1                    1H
P1                   10.30 usec
PL1                  -2.00 dB
SFO1            200.1315975 MHz

F2 - Processing parameters
SI                      32768
SF                200.1300053 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
F1P                    10.297 ppm
F1                    3861.72 Hz
F2P                   -2.385 ppm
F2                    -477.35 Hz
PPMCM                 1.03410 ppm/cm
HZCM                206.95364 Hz/cm
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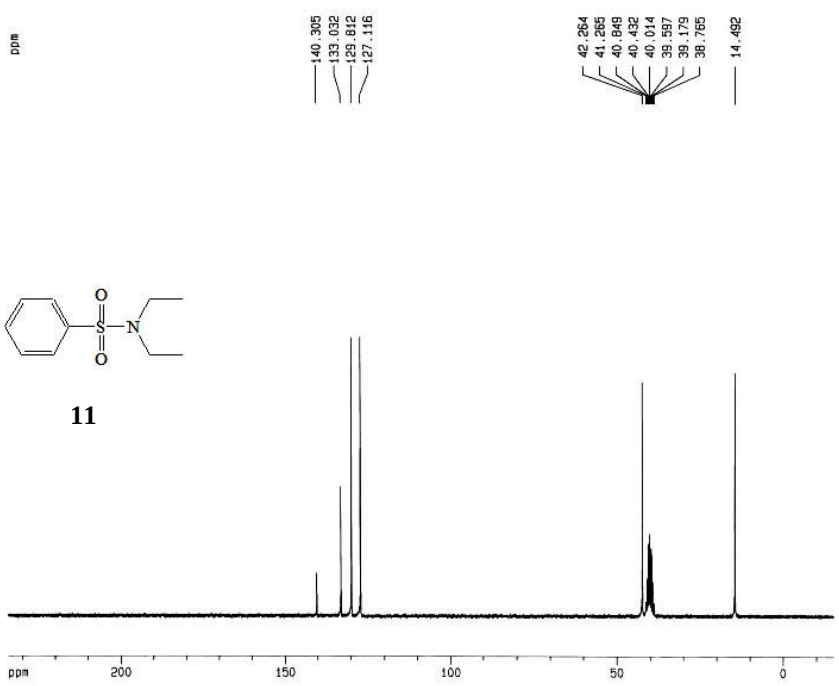

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```
Current Data Parameters
NAME                   13C
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_              20090907
Time                   4.35
INSTRUM               spect
PROBHD     5 mm Multinu
PULPROG            zgpg30
TD                   65536
SOLVENT               DMSO
NS                      673
DS                        4
SWH               12562.814 Hz
FIDRES            0.191693 Hz
AQ                2.6083827 sec
RG                     32768
DW                 39.800 usec
DE                   6.00 usec
TE                  300.0 K
D1                2.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec

========== CHANNEL f1 ==========
NUC1                   13C
P1                   10.00 usec
PL1                  -5.00 dB
SFO1            50.3282440 MHz

========== CHANNEL f2 ==========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                 120.00 dB
PL12                 20.00 dB
PL13                 20.00 dB
SFO2            200.1308005 MHz

F2 - Processing parameters
SI                      32768
SF                50.3227294 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
F1P                   234.408 ppm
F1                   11795.04 Hz
F2P                  -15.237 ppm
F2                    -766.77 Hz
PPMCM                12.48225 ppm/cm
HZCM                628.14075 Hz/cm
```