Design and Synthesis of sugar-triazole low molecular weight gels as merucury ion sensor

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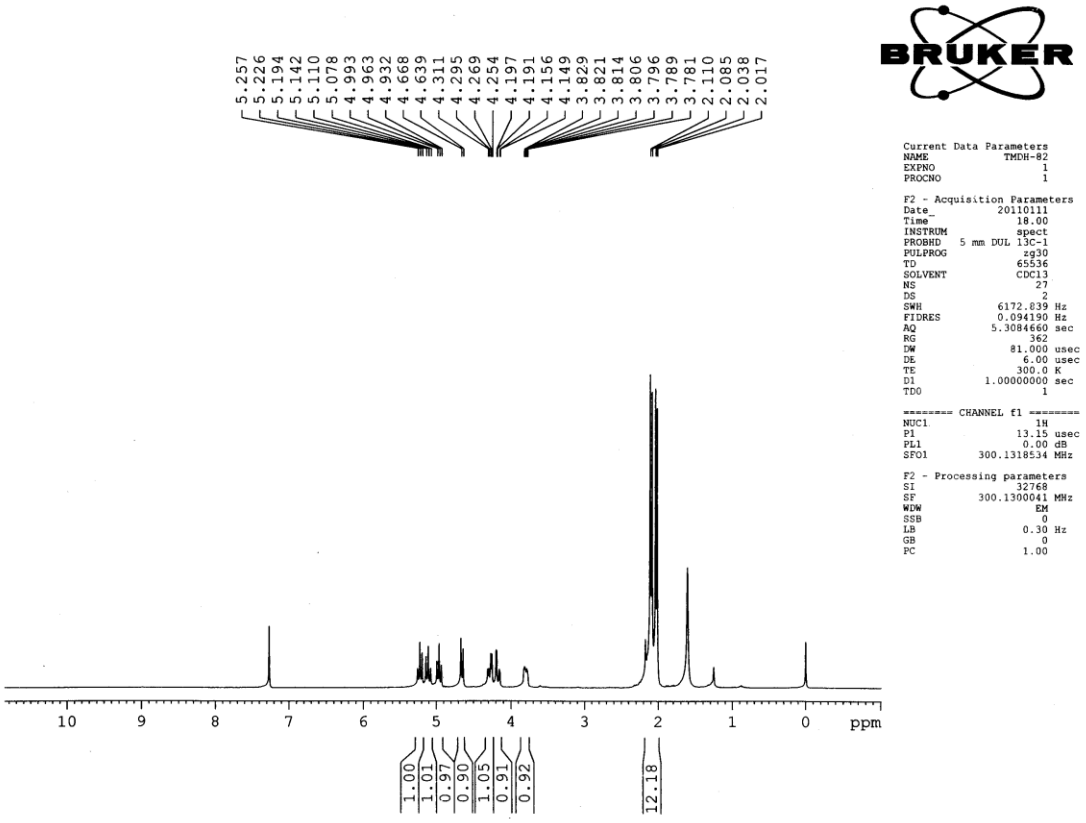
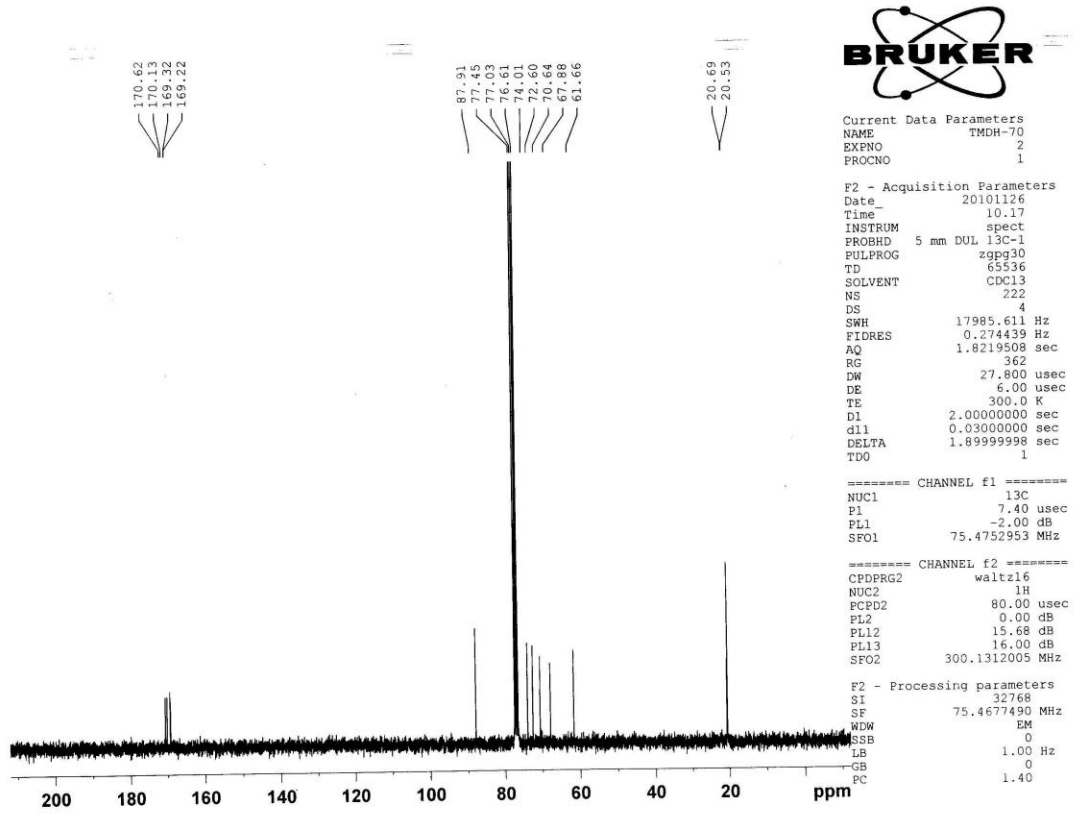
NMR Spectras:

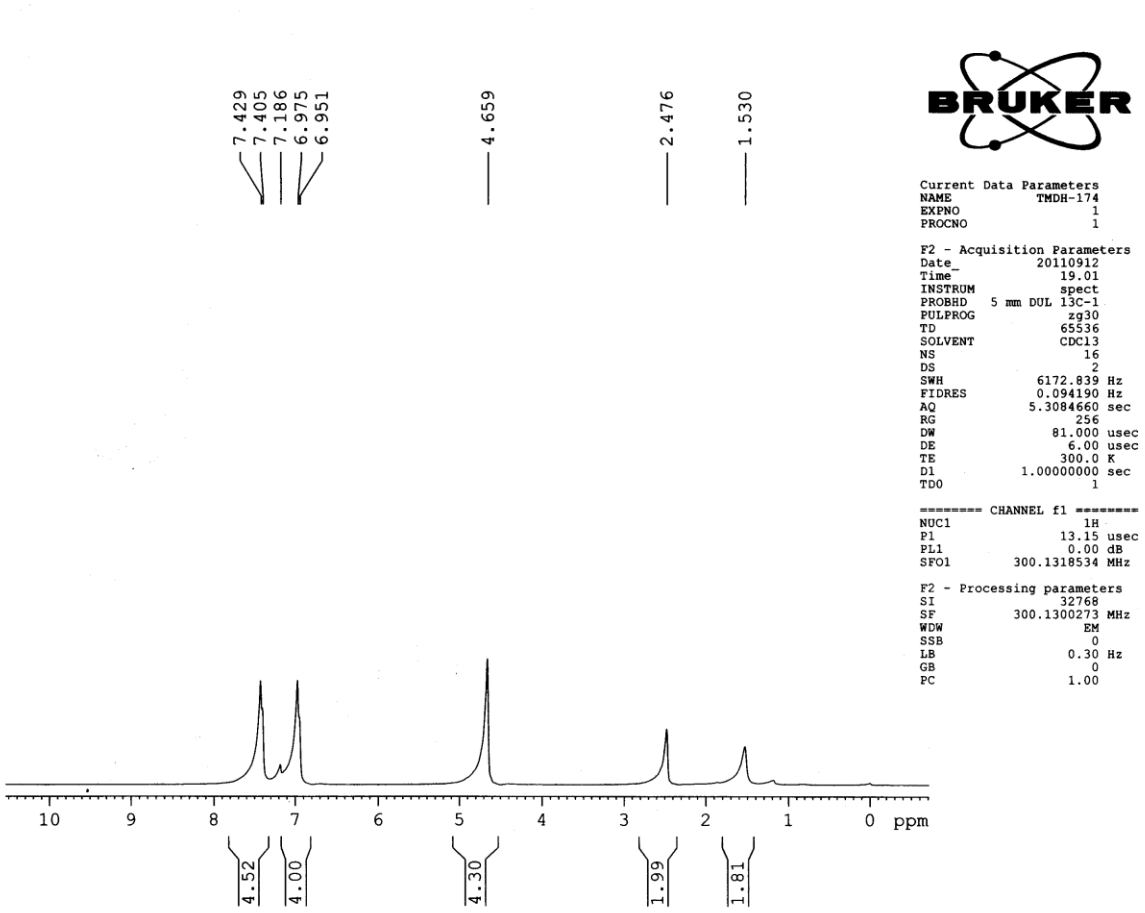
^{1}H NMR spectra of compound 1



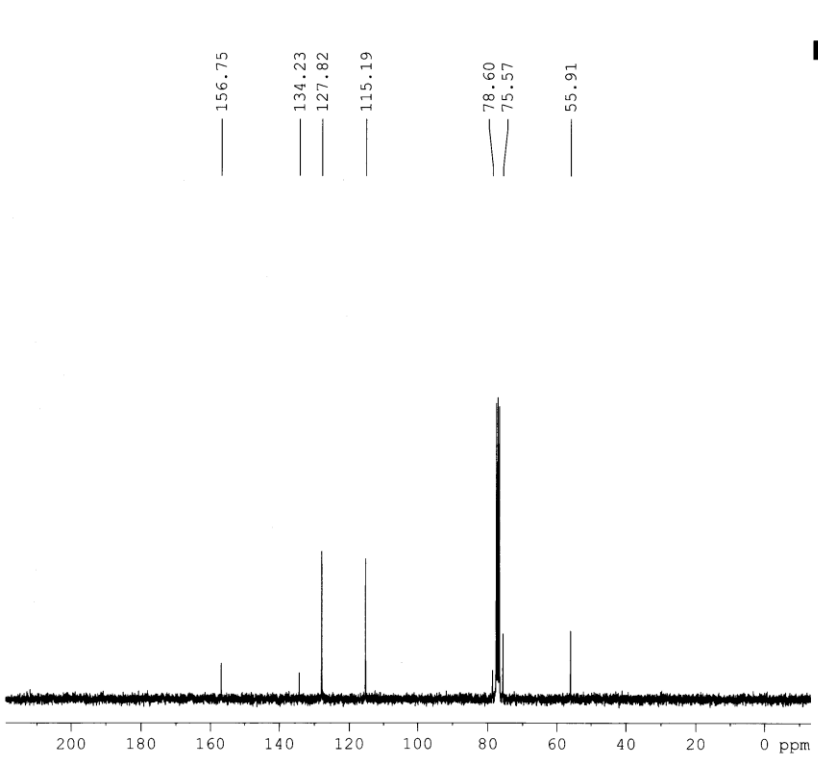
^{13}C NMR spectra of compound 1



^{1}H NMR spectra of compound 2a



^{13}C NMR spectra of compound 2a



BRUKER

Current Data Parameters
NAME TMDH-174
EXPNO 2
PROCNO 1

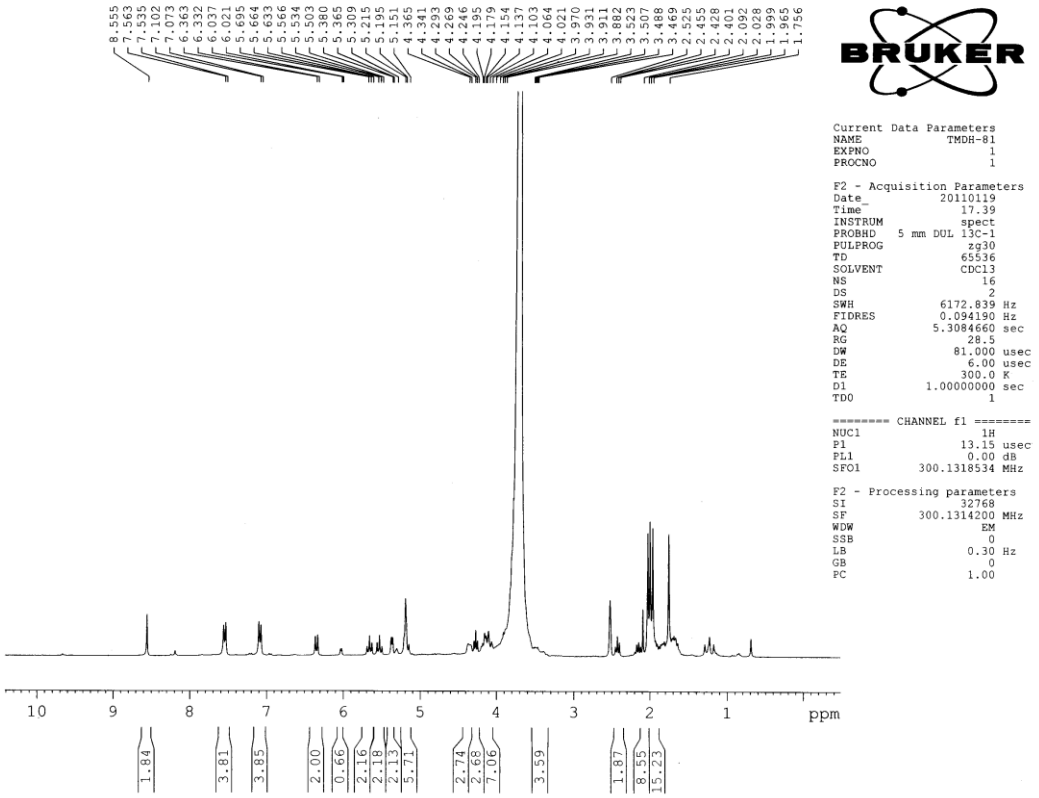
F2 - Acquisition Parameters
Date_ 20110912
Time 19.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 457
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 8192
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

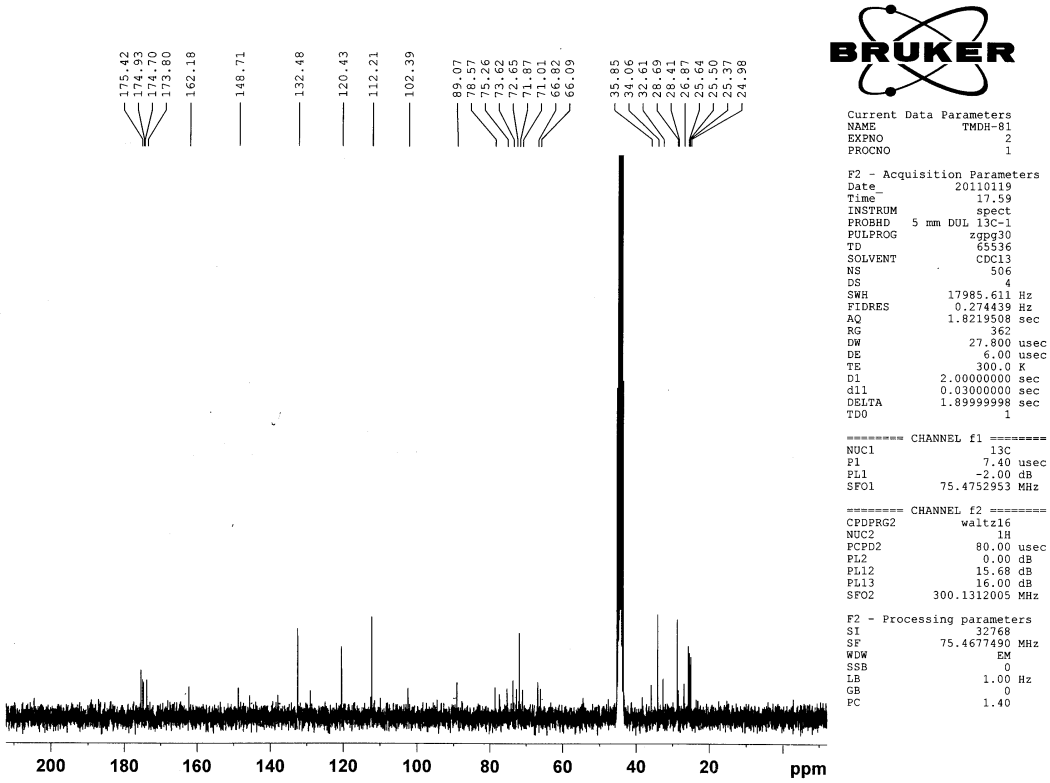
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

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

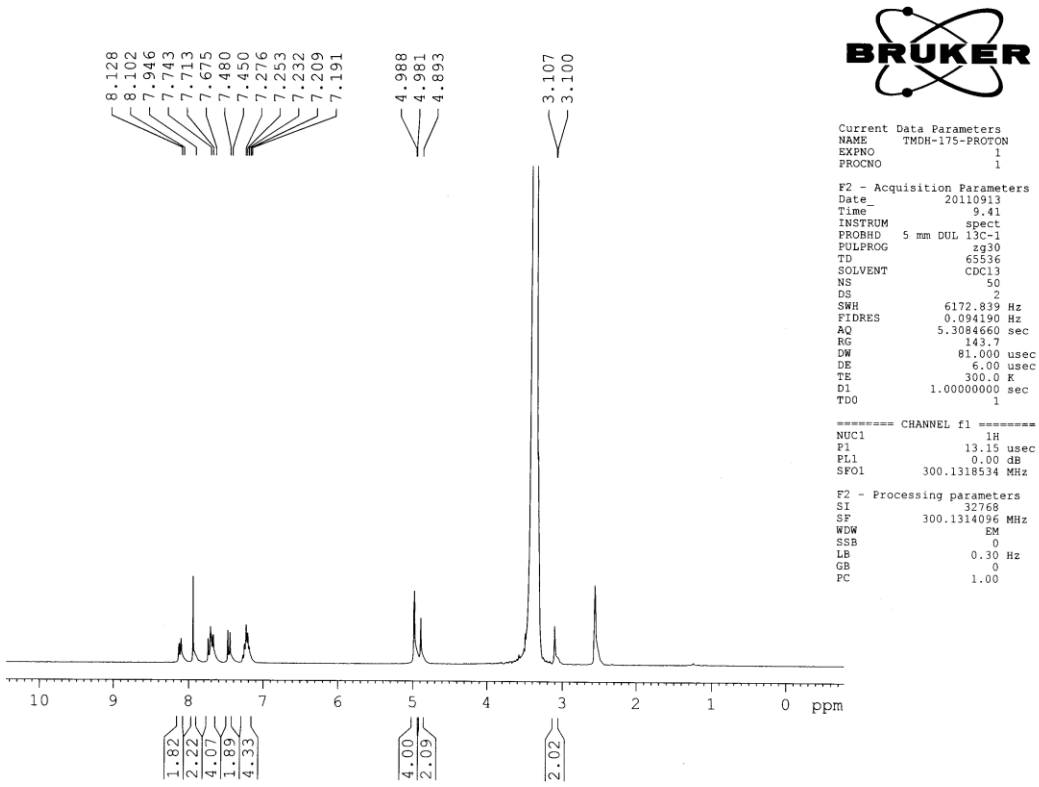
^{1}H NMR spectra of compound 3a



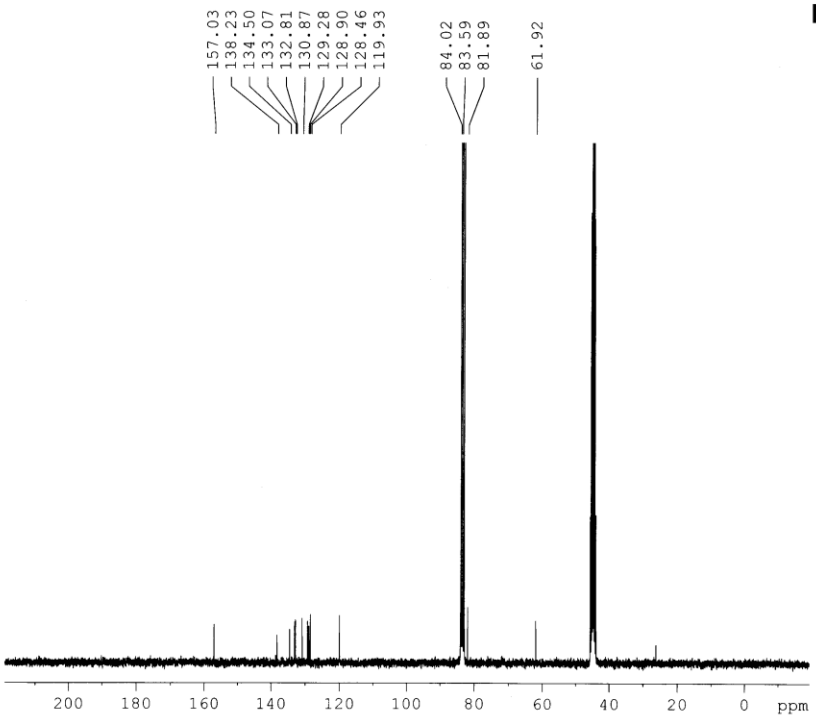
^{13}C NMR spectra of compound 3a



^{1}H NMR spectra of compound 2b



^{13}C NMR spectra of compound 2b



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EXPNO                        1
PROCNO                       1

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Time                      0.05
INSTRUM                  spect
PROBHD   5 mm DUL 13C-1
PULPROG                 zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                        3597
DS                           4
SWH                17985.611 Hz
FIDRES                 0.274439 Hz
AQ                     1.8219508 sec
RG                       20642.5
DW                        27.800 usec
DE                         6.00 usec
TE                        300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.30 usec
PL1                       0.00 dB
SFO1               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                       0.00 dB
PL12                     15.68 dB
PL13                     16.00 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF                 75.4677490 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
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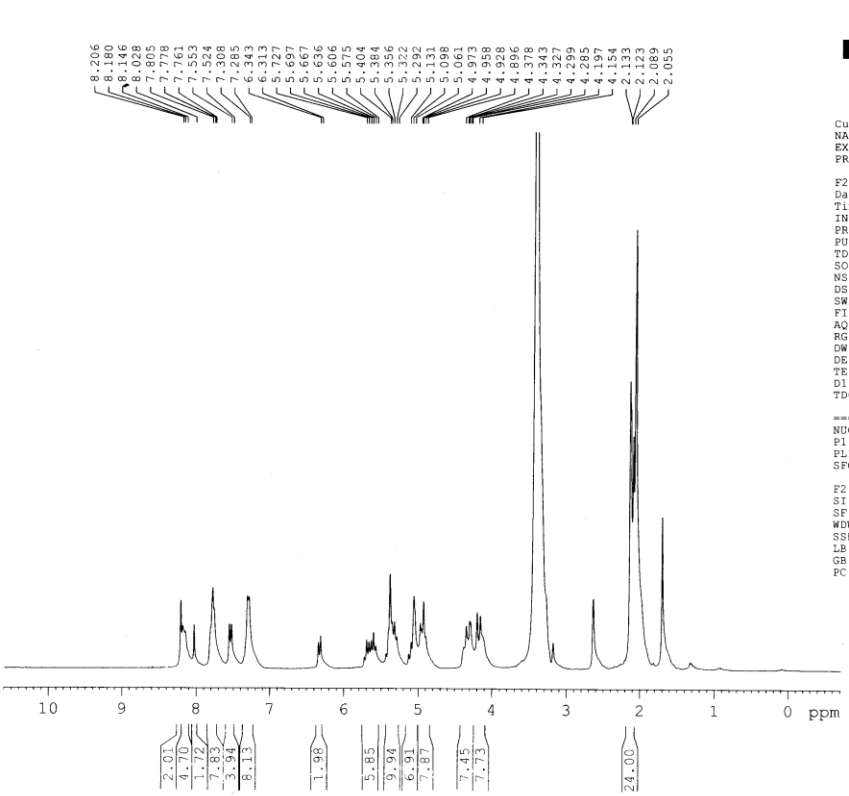
^{1}H NMR spectra of compound 3b



BRUKER

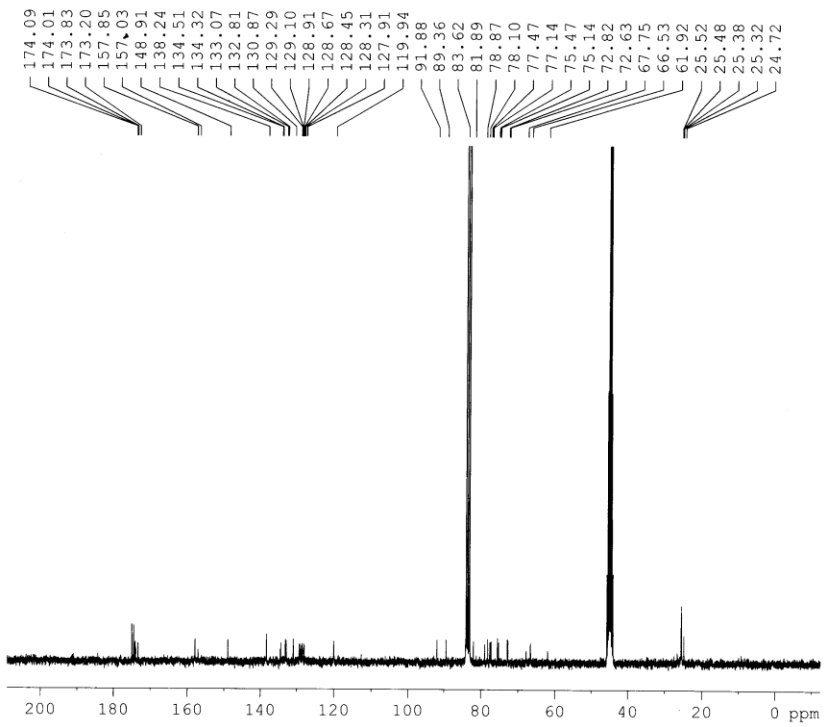
Current Data Parameters
NAME TMDH-161-HIGH SCAN
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110822
Time 19.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 50
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 161.3
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1313880 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{13}C NMR spectra of compound 3b



BRUKER

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Current Data Parameters
NAME      TMDH-161-HIGH SCAN
EXPNO                  2
PROCNO                 1

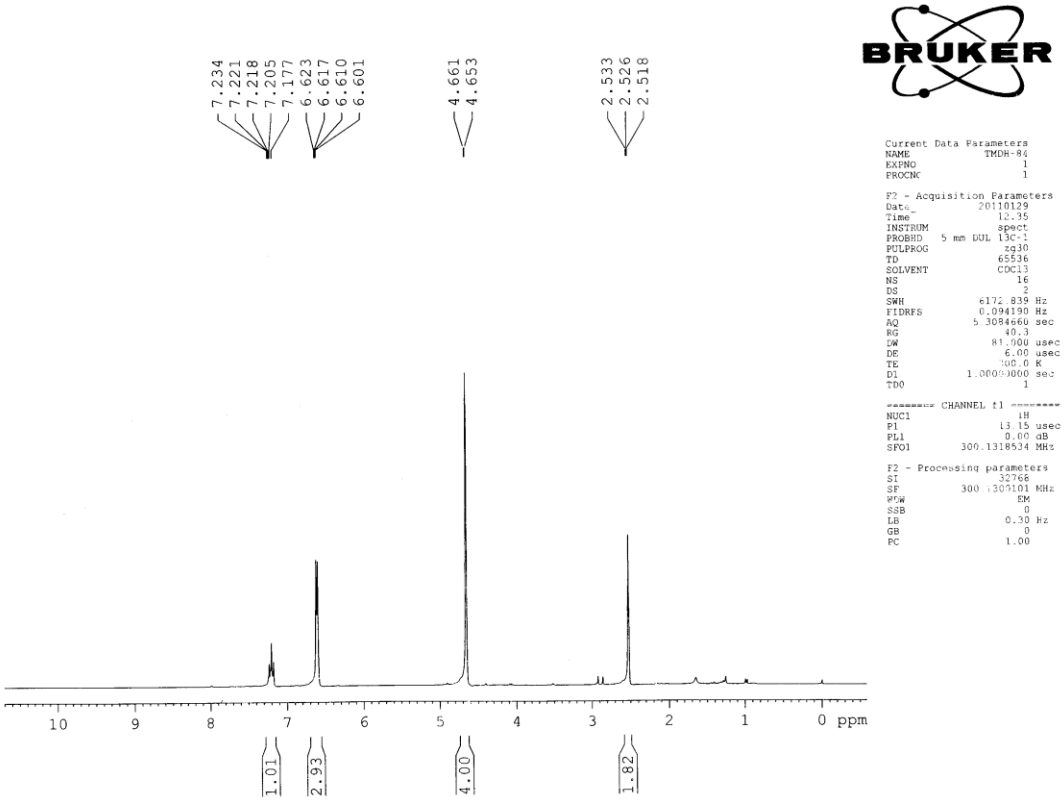
F2 - Acquisition Parameters
Date_           20110822
Time              21.44
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1689
DS                    4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                912.3
DW               27.800 usec
DE                6.00 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.30 usec
PL1                 0.00 dB
SFO1          75.4752953 MHz

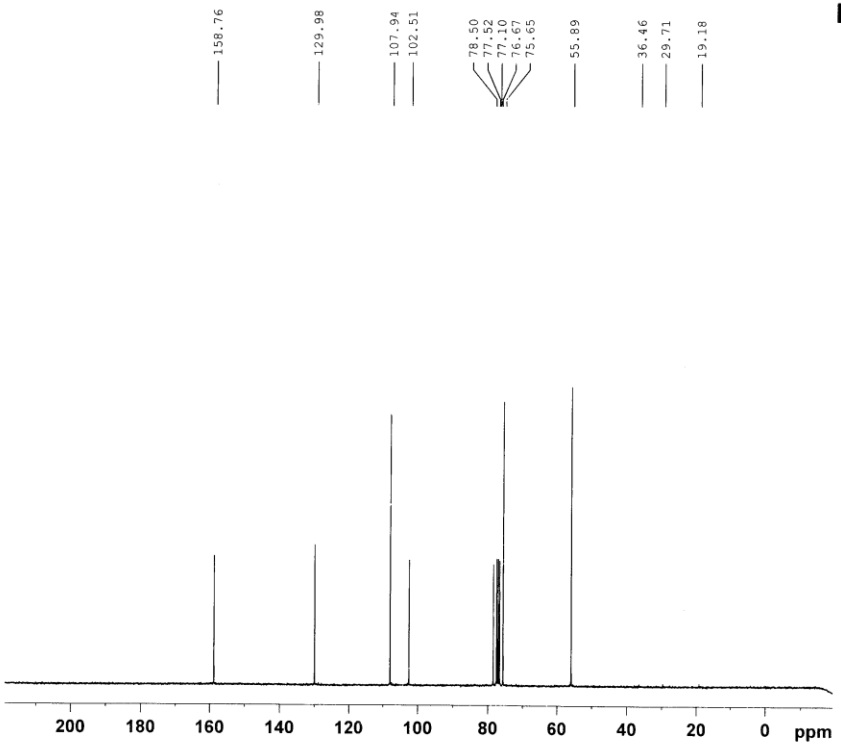
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.68 dB
PL13               16.00 dB
SFO2         300.1312005 MHz

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

^{1}H NMR spectra of compound 2c



^{13}C NMR spectra of compound 2c



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Current Data Parameters
NAME                  TMDH-84
EXPNO                       2
PROCNO                      1

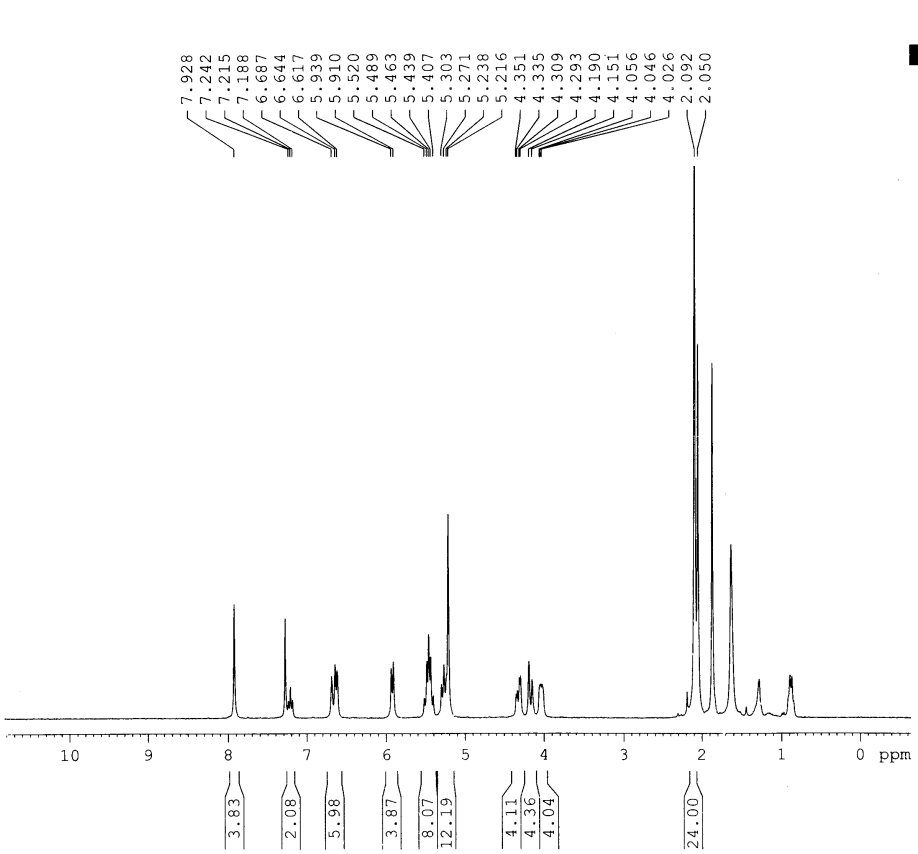
F2 - Acquisition Parameters
Date_              20110129
Time                  13.09
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     562
DS                       4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                     362
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    7.40 usec
PL1                  -2.00 dB
SFO1            75.4752953 MHz

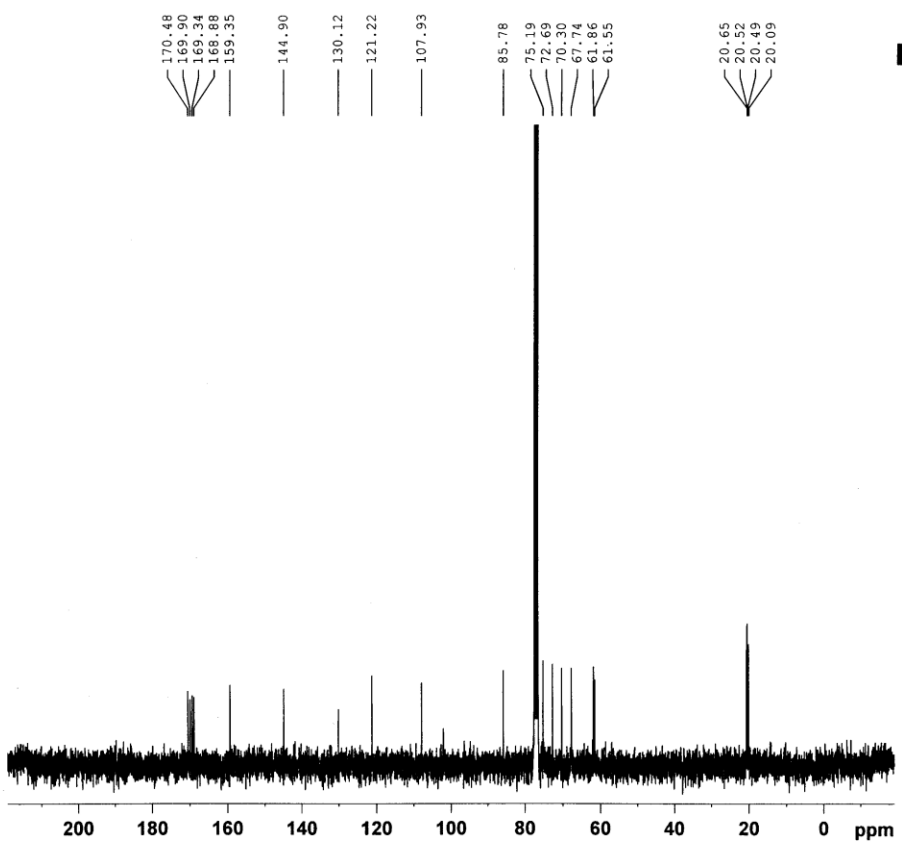
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
PL13                 16.00 dB
SFO2           300.1312005 MHz

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

^{1}H NMR spectra of compound 3c



^{13}C NMR spectra of compound 3c

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Current Data Parameters
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EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
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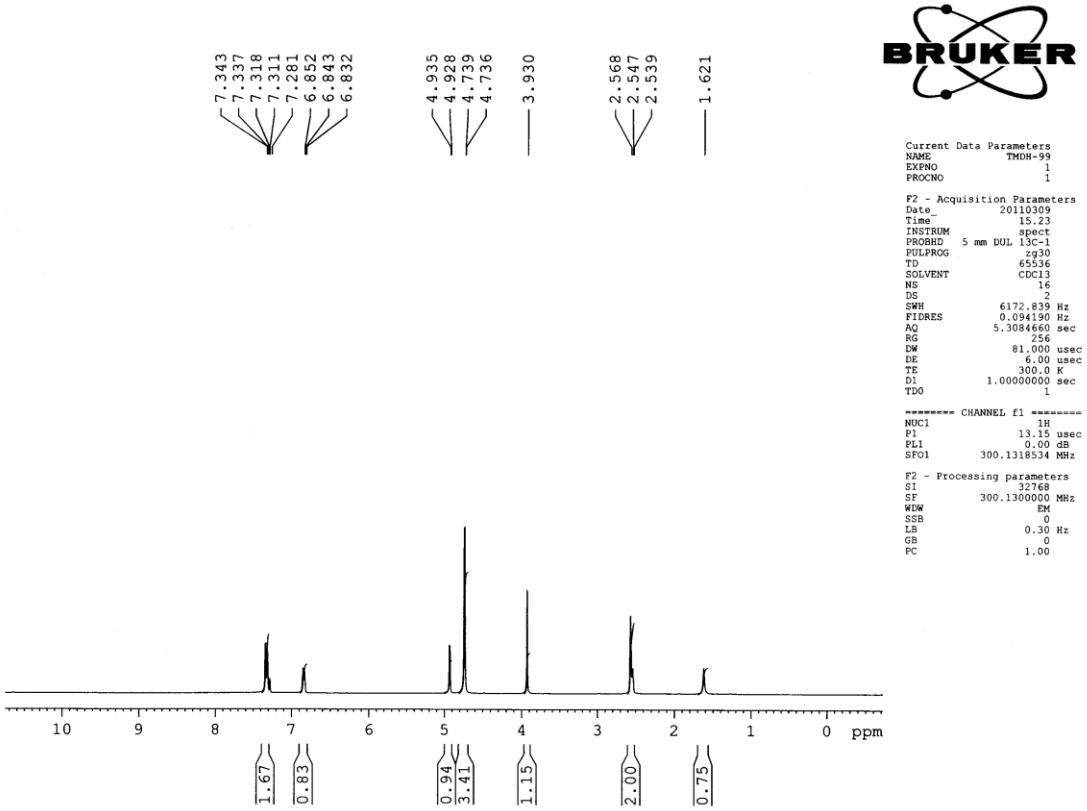
Time                   13.08
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1001
DS                       4
SWH              17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                     362
DW                27.800 usec
DE                 6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                   13C
P1                  7.40 usec
PL1                -2.00 dB
SFO1           75.4752953 MHz

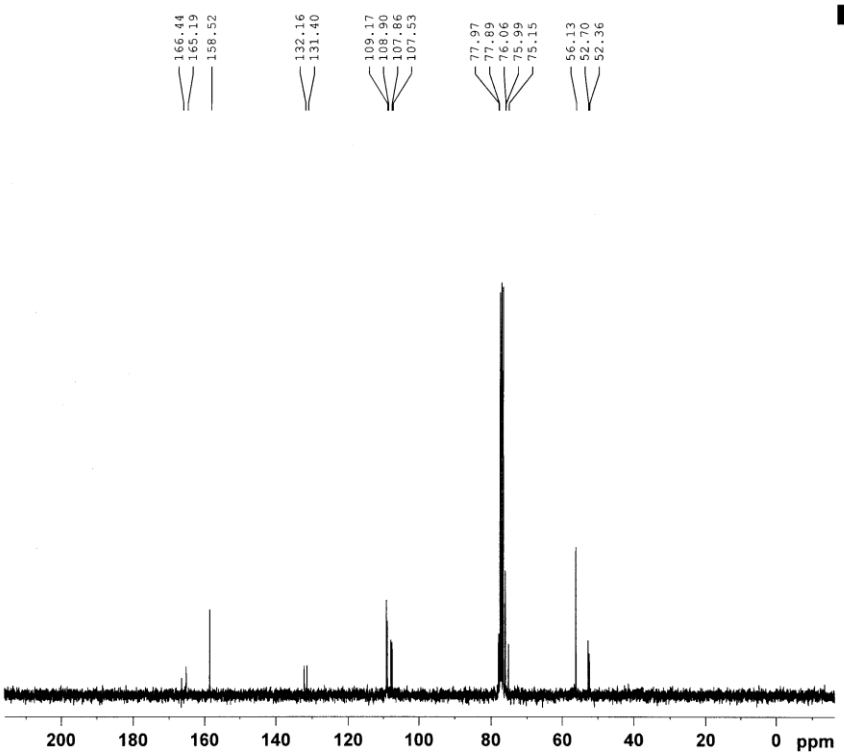
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               15.68 dB
PL13               16.00 dB
SFO2          300.1312005 MHz

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

^{1}H NMR spectra of compound 2d



^{13}C NMR spectra of compound 2d



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Current Data Parameters
NAME          TMDH-99-C13
EXPNO                   1
PROCNO                  1

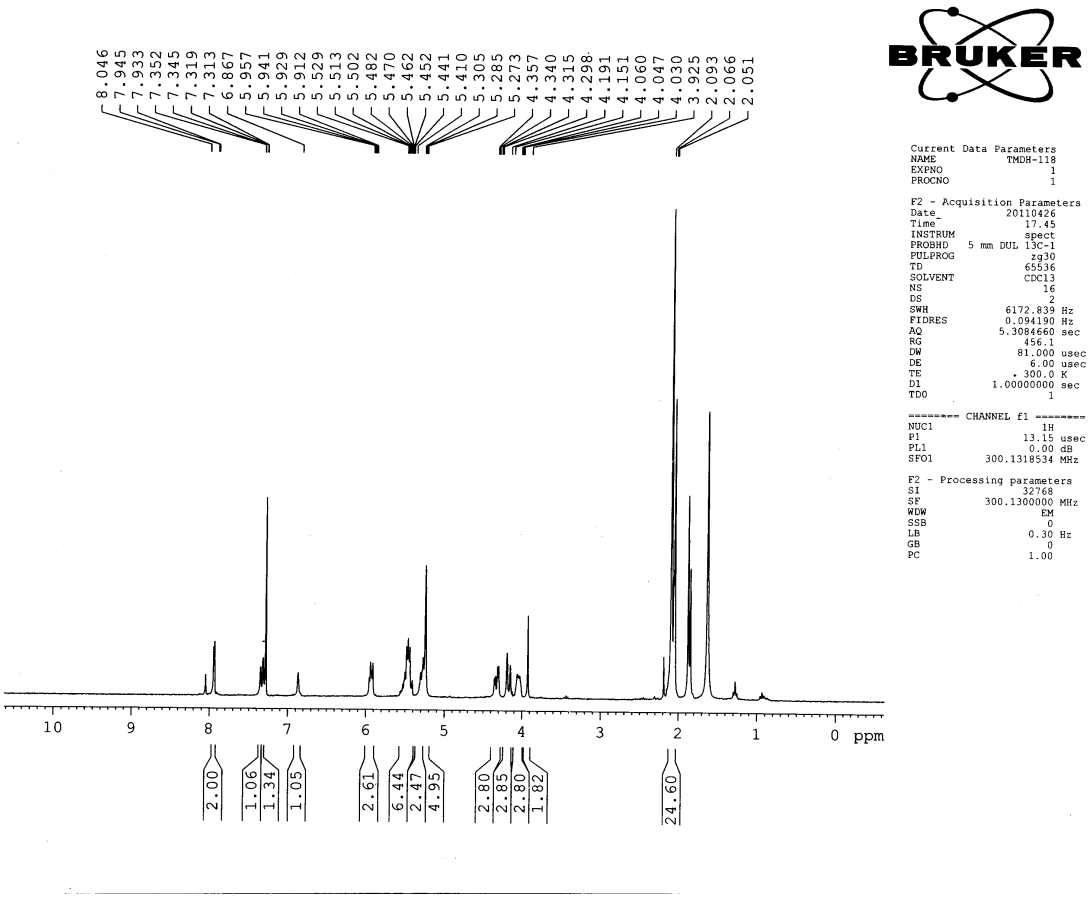
F2 - Acquisition Parameters
Date_          20110310
Time               8.54
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 210
DS                   4
SWH          17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                 362
DW              27.800 usec
DE               6.00 usec
TE               300.0 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               7.40 usec
PL1              -2.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2                1H
PCPD2           80.00 usec
PL2              0.00 dB
PL12            15.68 dB
PL13            16.00 dB
SFO2       300.1312005 MHz

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

^{1}H NMR spectra of compound 3d

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EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20110426
Time                     17.45
INSTRUM                  spect
PROBHD     5 mm DUL 13C-1
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                          16
DS                           2
SWH                 6172.839 Hz
FIDRES              0.094190 Hz
AQ                  5.3084660 sec
RG                       456.1
DW                    81.000 usec
DE                     6.00 usec
TE                     300.0 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.15 usec
PL1                      0.00 dB
SFO1             300.1318534 MHz

F2 - Processing parameters
SI                       32768
SF                300.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
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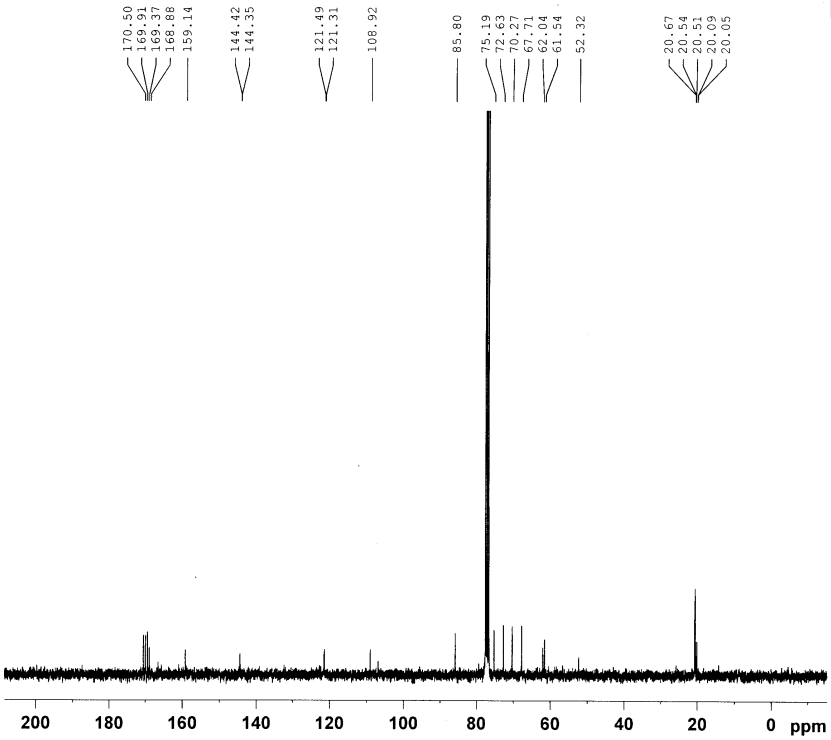
^{13}C NMR spectra of compound 3d



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Current Data Parameters
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EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20110427
Time                 18.30
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT                CDCl3
NS                       923
DS                         4
SWH                17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                     645.1
DW                    27.800 usec
DE                     6.00 usec
TE                    300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.30 usec
PL1                      0.00 dB
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                      0.00 dB
PL12                    15.68 dB
PL13                    16.00 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                       32768
SF                75.4677490 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
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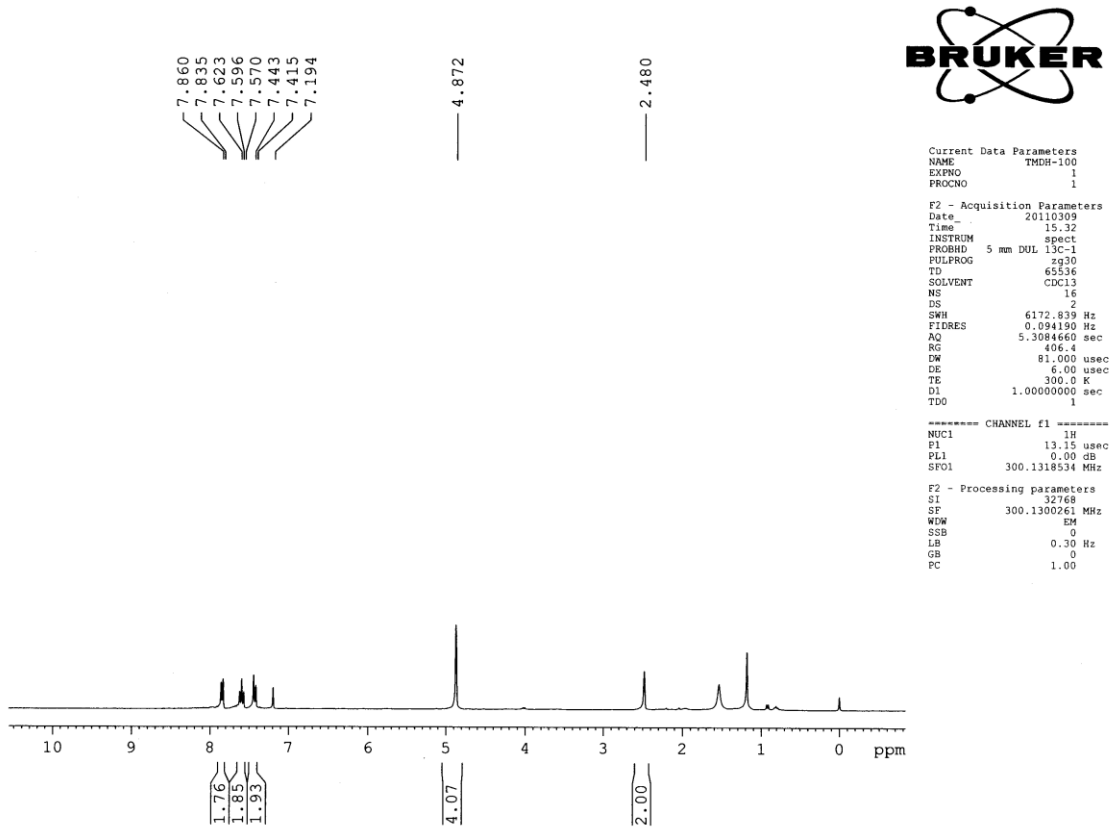
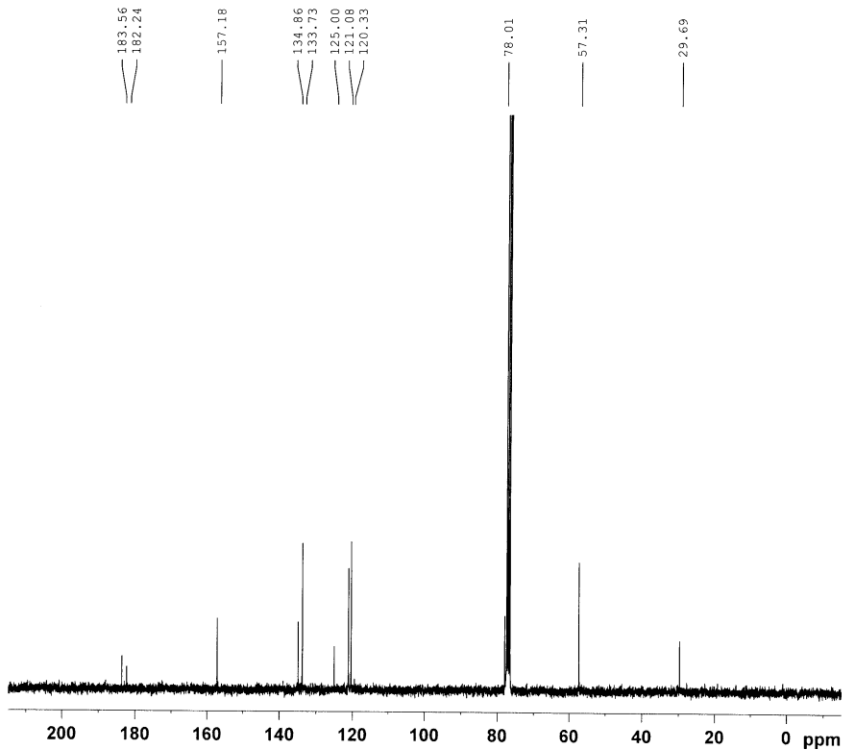
^{1}H NMR spectra of compound 2e



^{13}C NMR spectra of compound 2e



BRUKER

Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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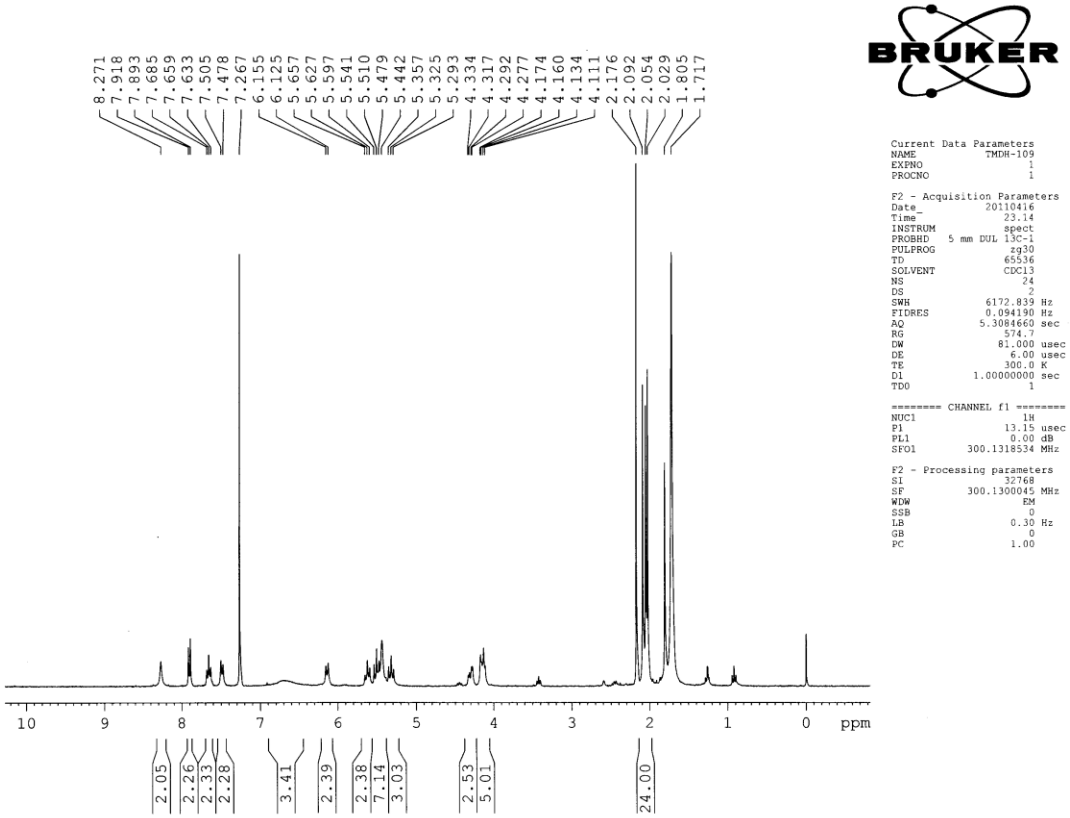
Time 9.15
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 863
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 574.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

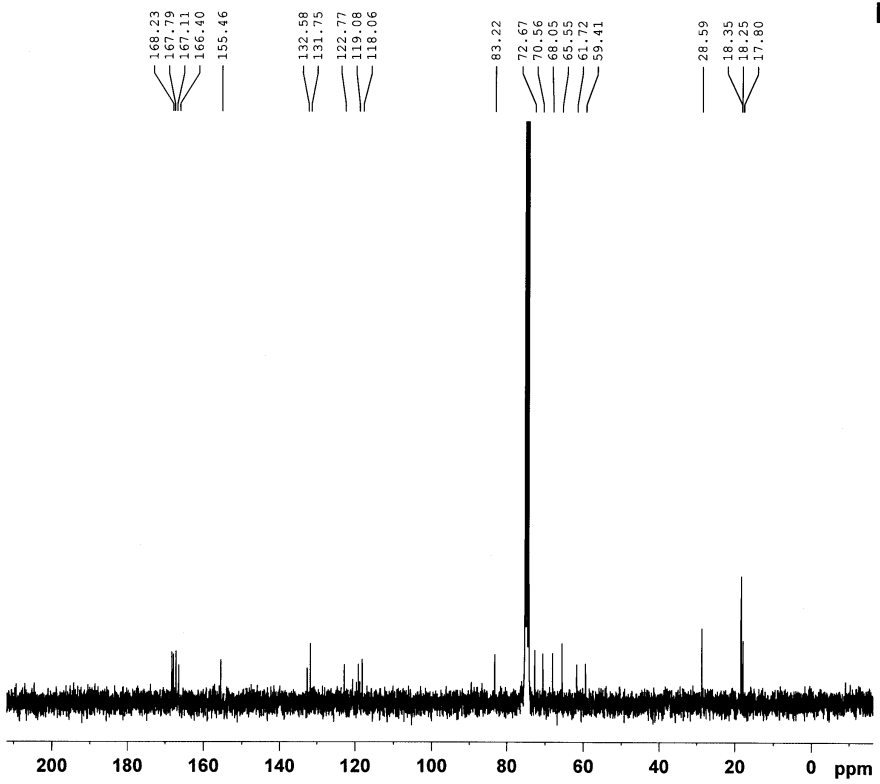
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

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

^{1}H NMR spectra of compound 3e



^{13}C NMR spectra of compound 3e



BRUKER

Current Data Parameters
NAME TMDH-109
EXPNO 2
PROCNO 1

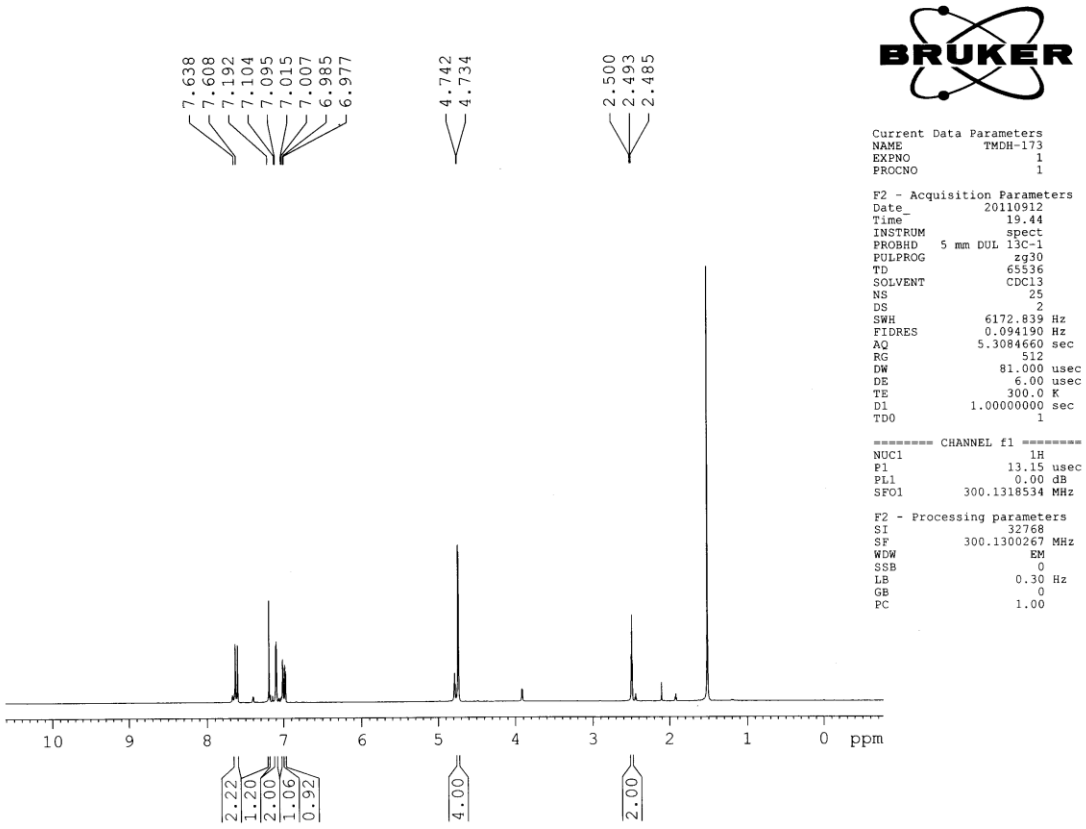
F2 - Acquisition Parameters
Date_ 20110417
Time 4.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5000
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 574.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4679239 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H NMR spectra of compound 2f



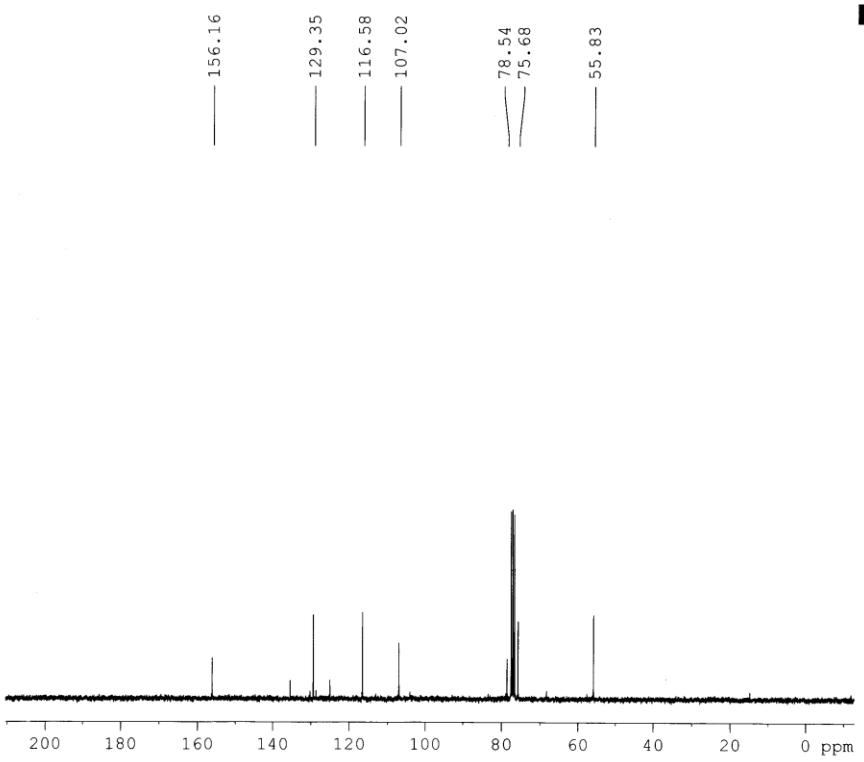

```
Current Data Parameters
NAME                 TMDH-173
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20110912
Time                   19.44
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       25
DS                        2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                      512
DW                   81.000 usec
DE                    6.00 usec
TE                   300.0 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      13.15 usec
PL1                      0.00 dB
SFO1            300.1318534 MHz

F2 - Processing parameters
SI                      32768
SF              300.1300267 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

^{13}C NMR spectra of compound 2f



BRUKER

Current Data Parameters
NAME TMDH-173
EXPNO 2
PROCNO 1

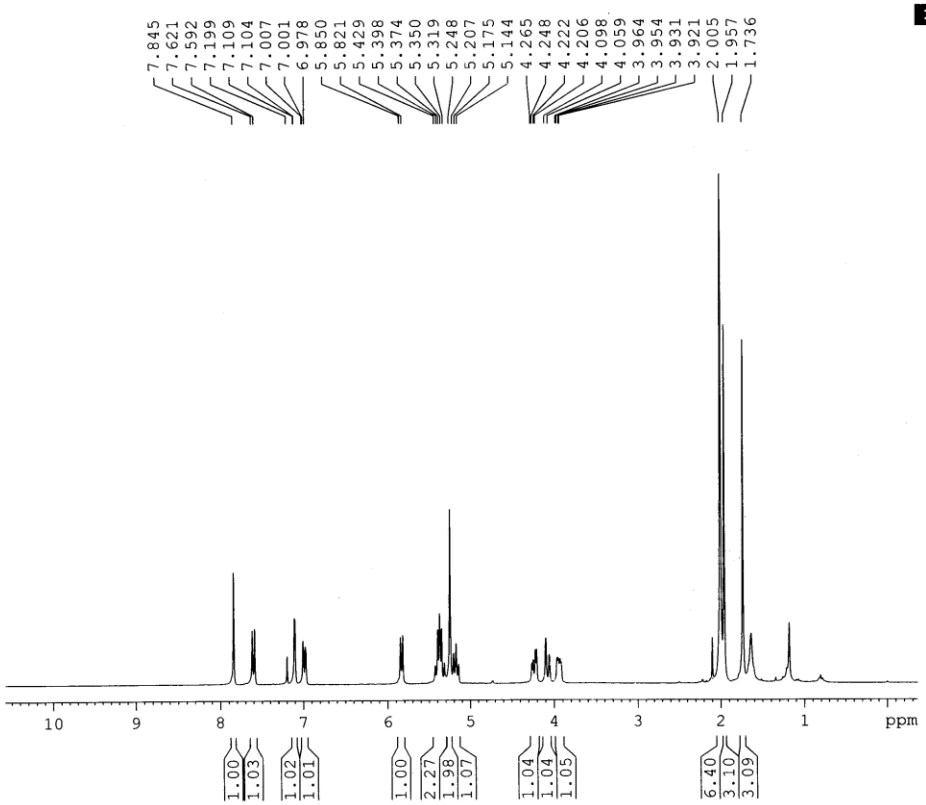
F2 - Acquisition Parameters
Date_ 20110912
Time 20.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 154
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 10321.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

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

^{1}H NMR spectra of compound 3f



BRUKER

```
Current Data Parameters
NAME        TMDH-TMDH-103
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110315
Time                 9.47
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             6172.839 Hz
FIDRES          0.094190 Hz
AQ              5.3084660 sec
RG                  161.3
DW                 81.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.15 usec
PL1                 0.00 dB
SFO1         300.1318534 MHz

F2 - Processing parameters
SI                  32768
SF          300.1300247 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00
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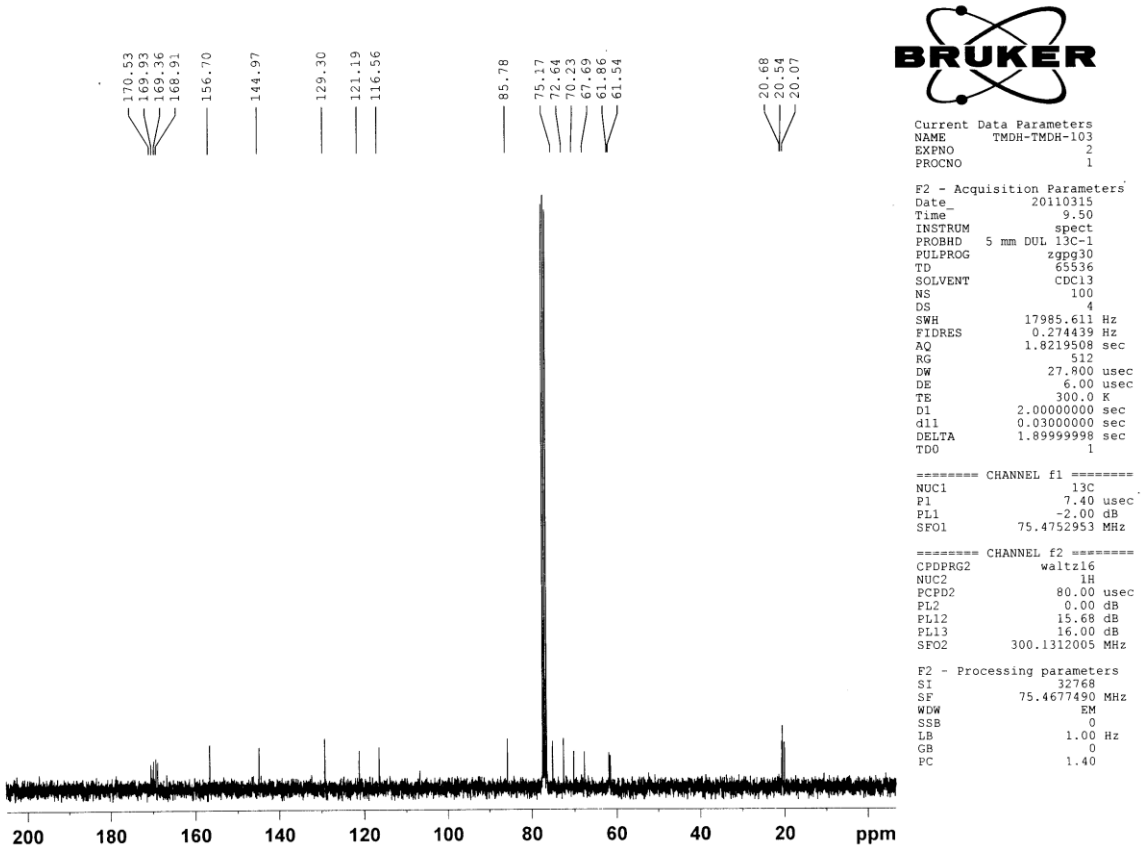
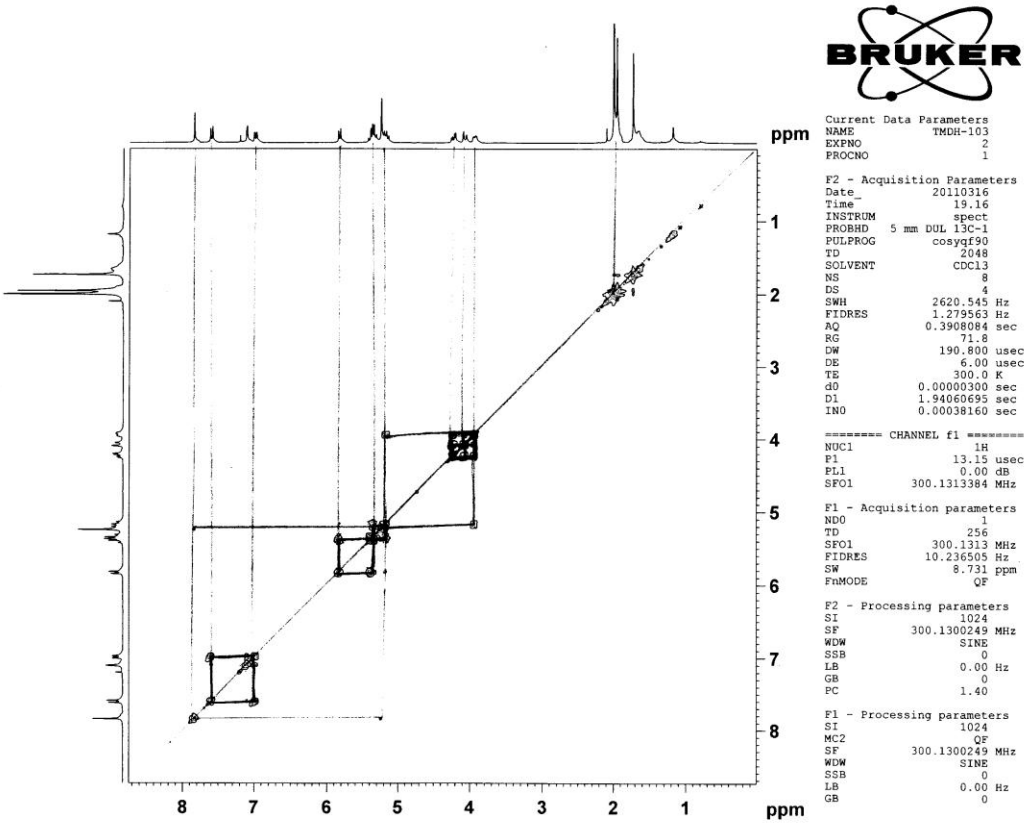
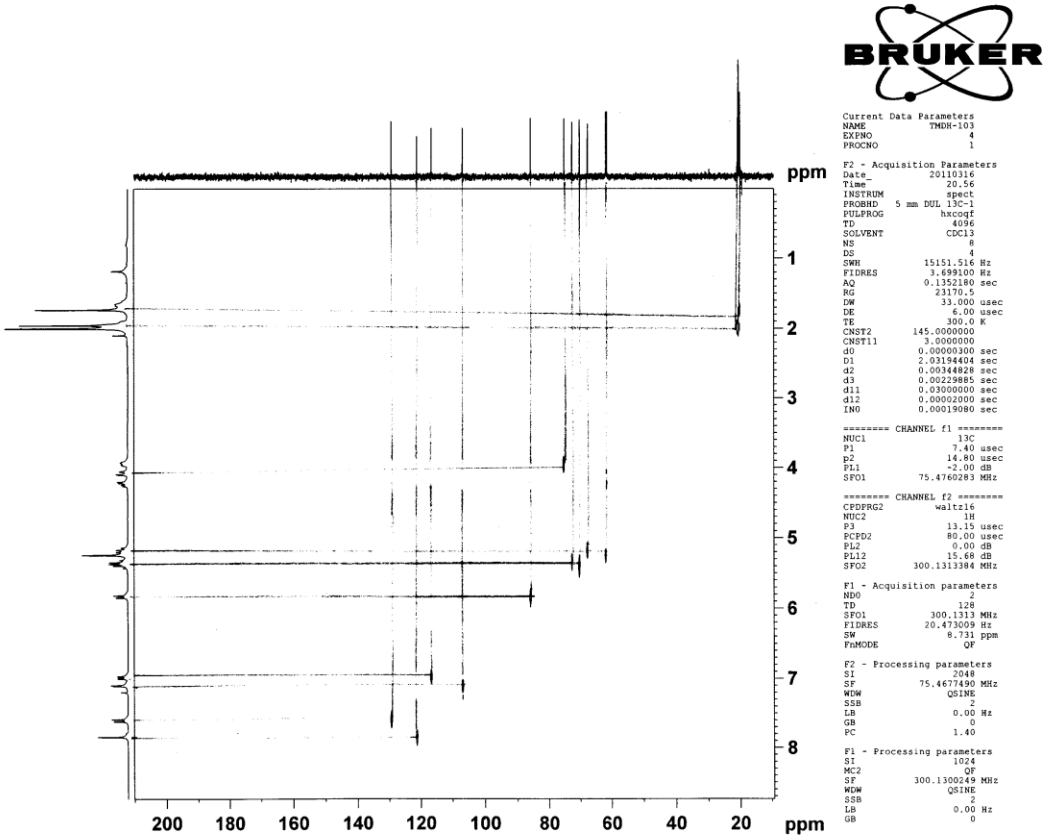
^{13}C NMR spectra of compound 3f



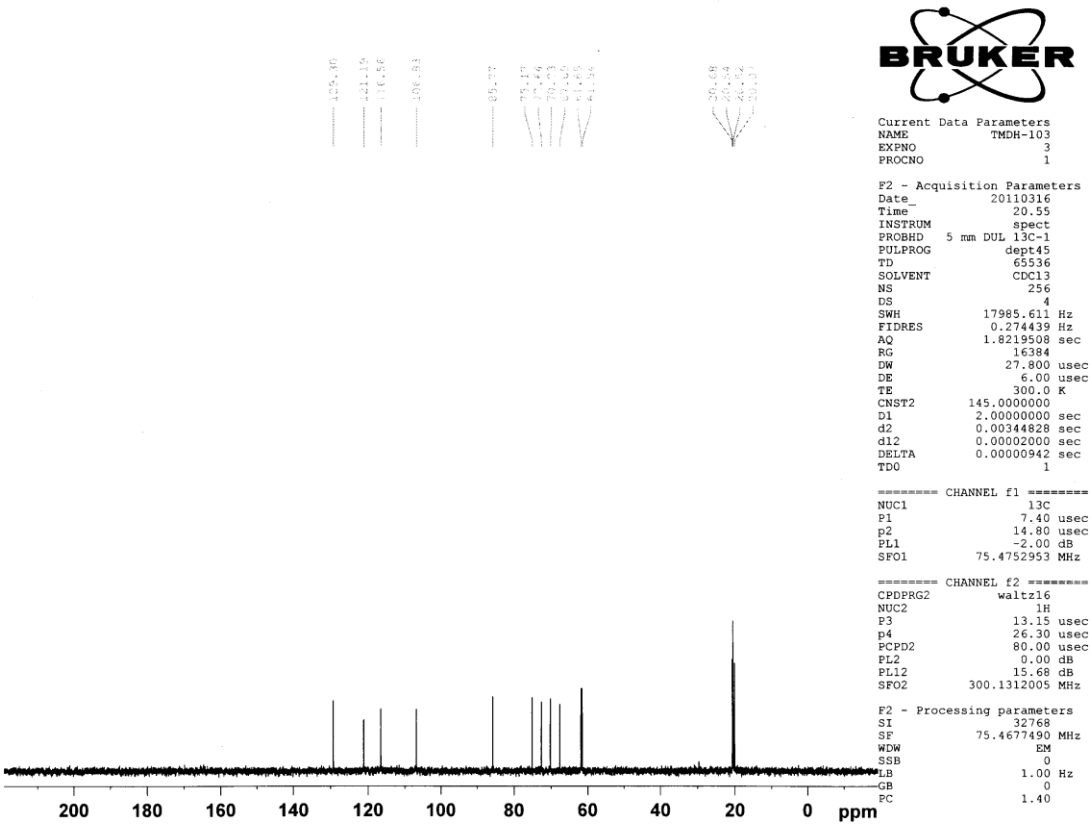
^{1}H-^{1}H COSY spectra of compound 3f



^{1}H-^{13}C COSY spectra of compound 3f



DEPT-45 spectra of compound 3f



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Current Data Parameters
NAME TMDH-103
EXPNO 3
PROCNO 1

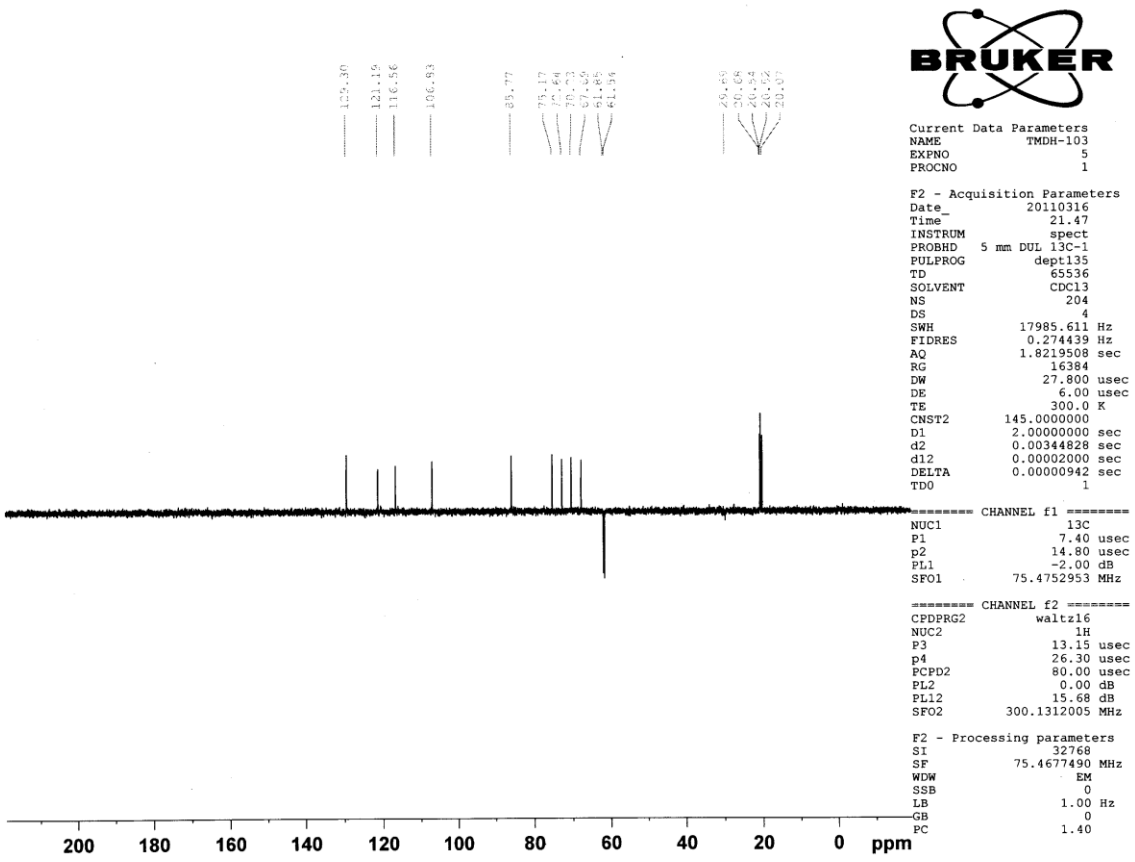
F2 - Acquisition Parameters
Date_ 20110316
Time 20.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG dept45
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 16384
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000942 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
p2 14.80 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

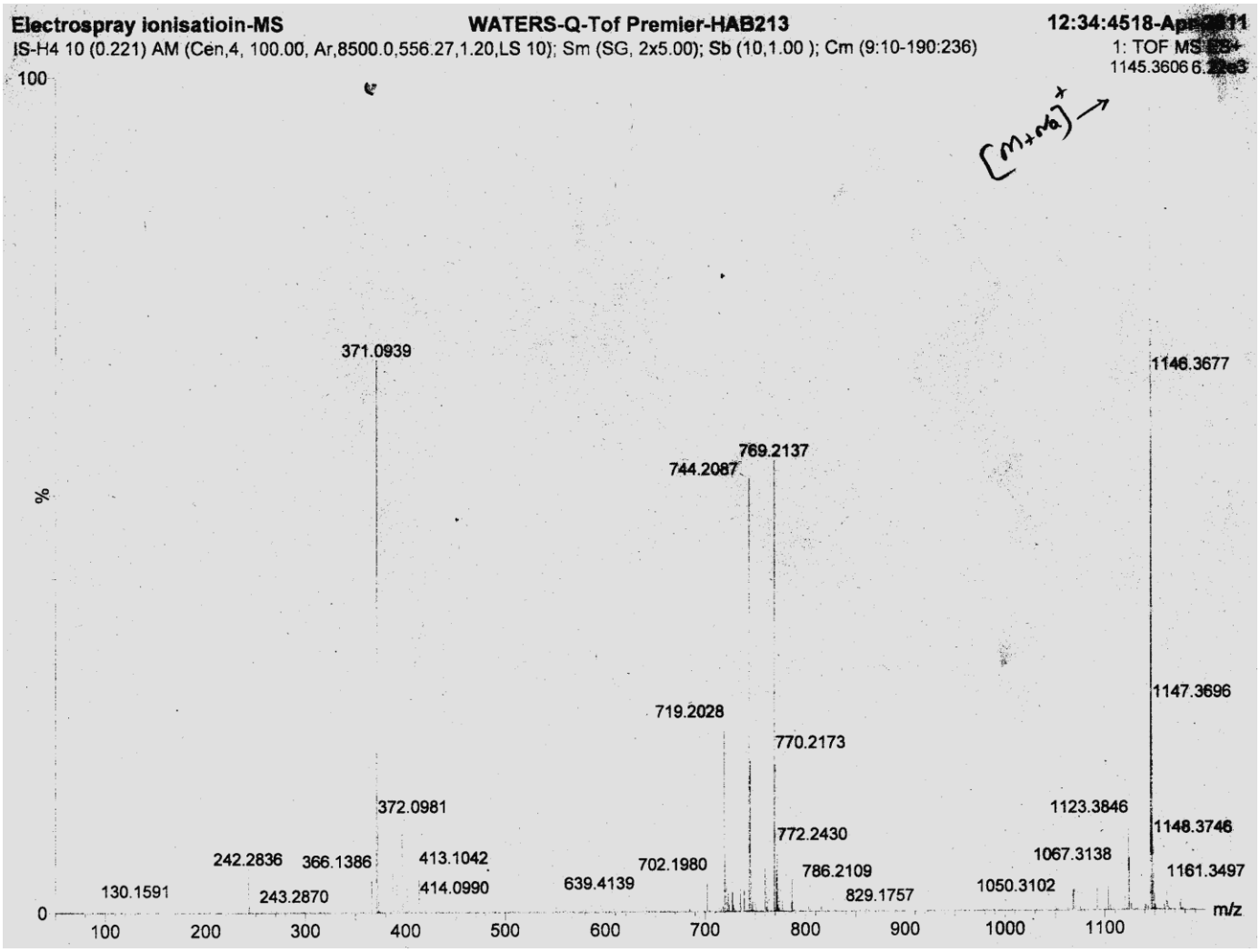
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.15 usec
p4 26.30 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
SFO2 300.1312005 MHz

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

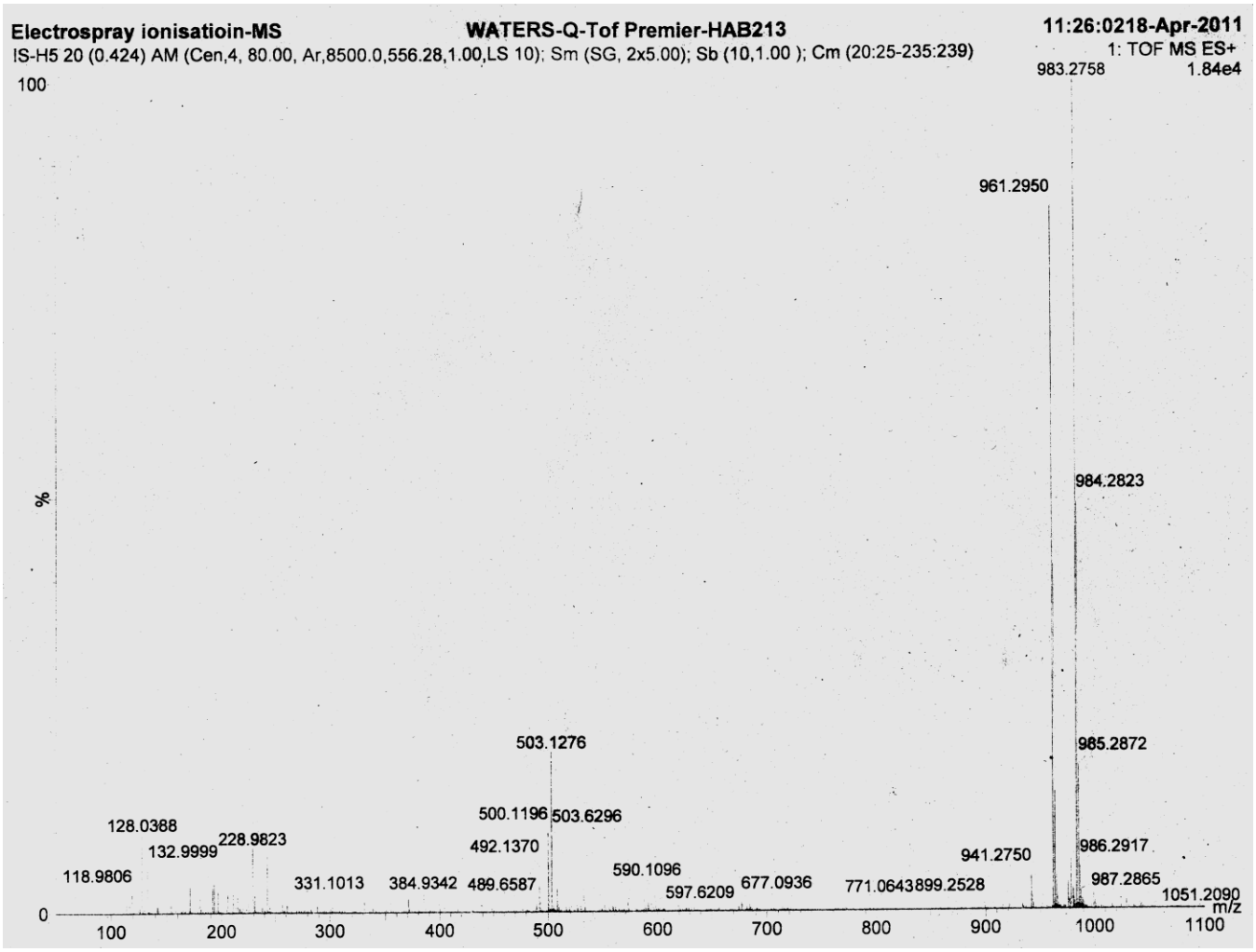
DEPT-135 spectra of compound 3f



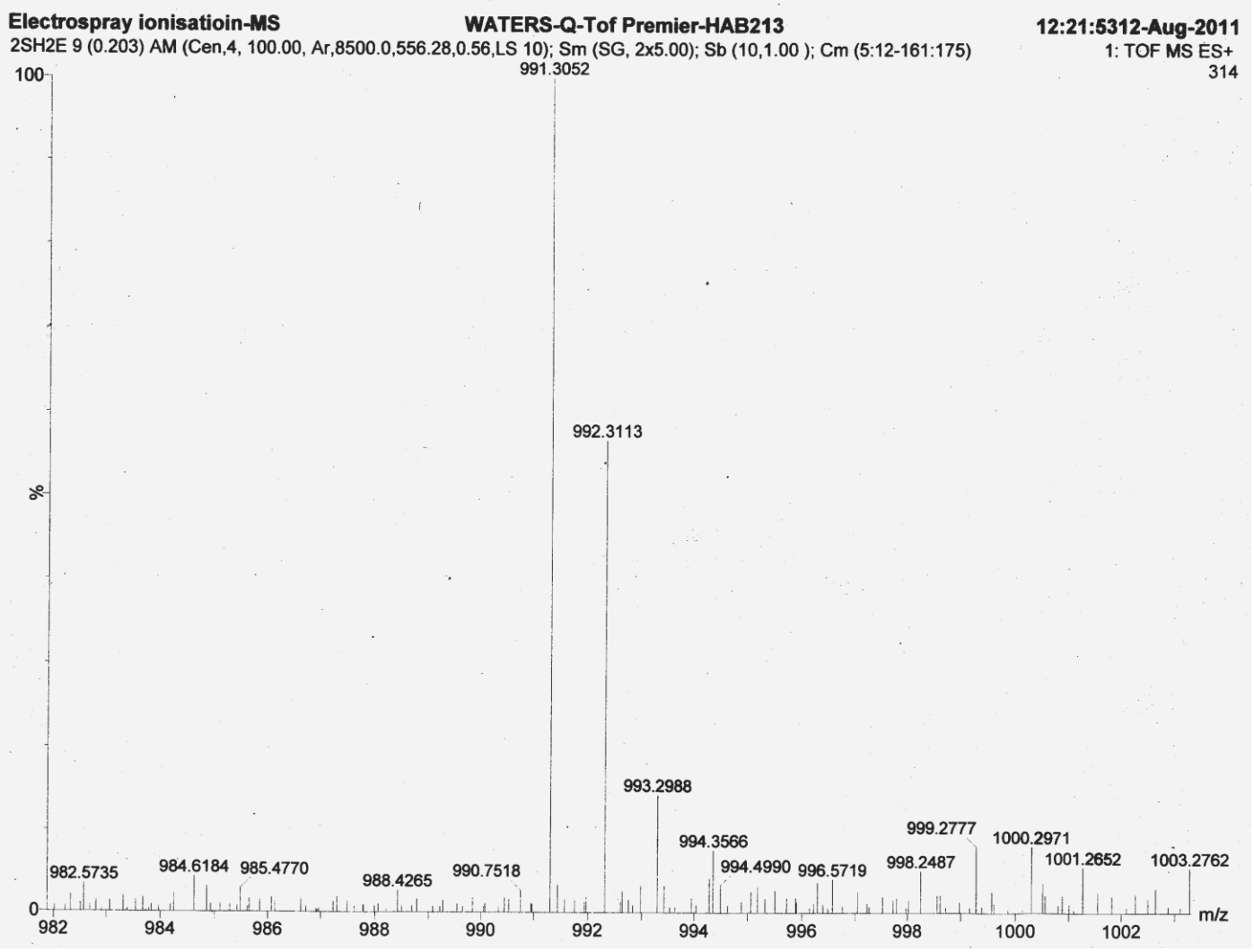
ESI-Mass spectra of compound of compound 3b



ESI-Mass spectra of compound 3c



ESI-Mass spectra of compound 3d



ESI-Mass spectra of compound 3f

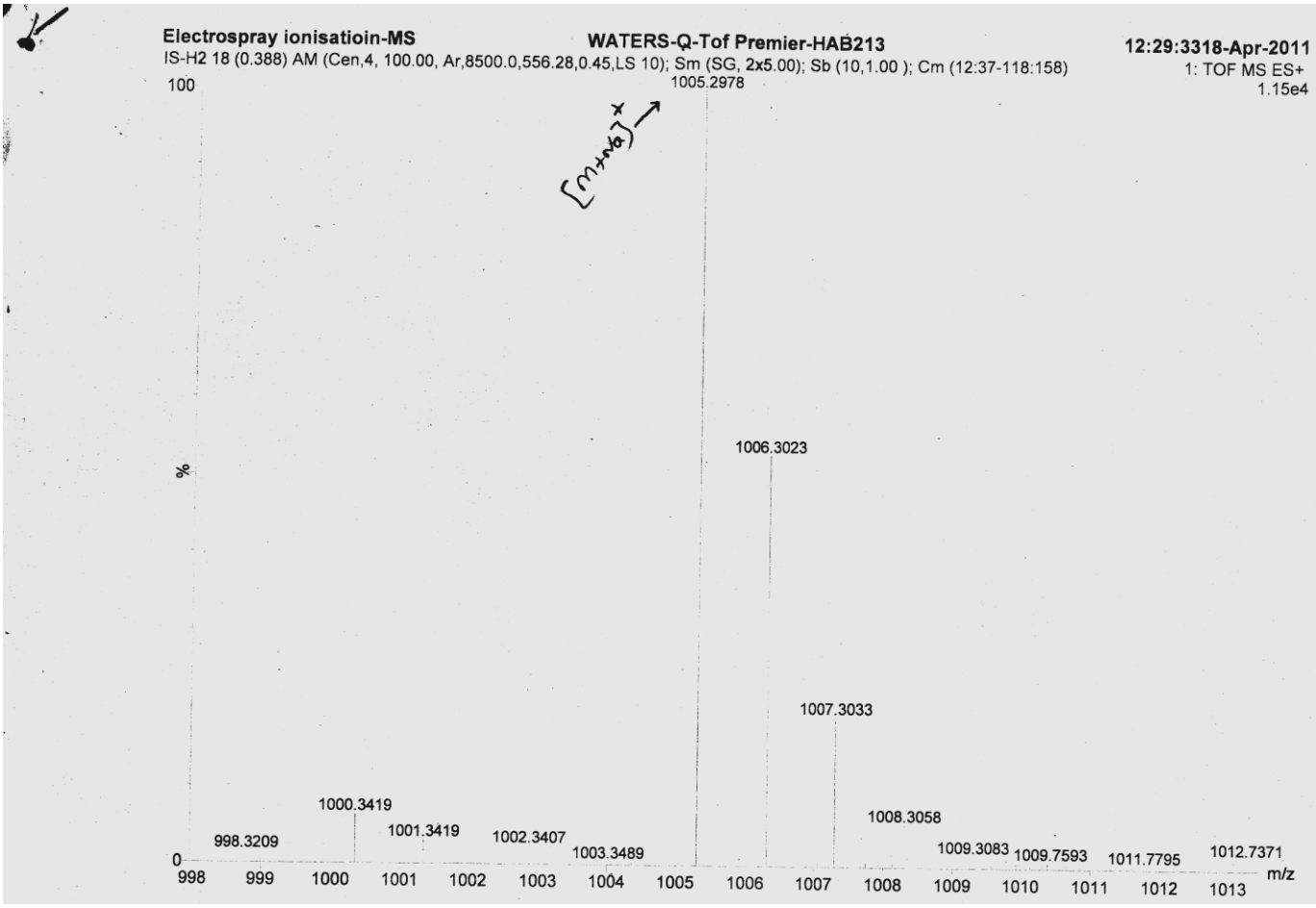
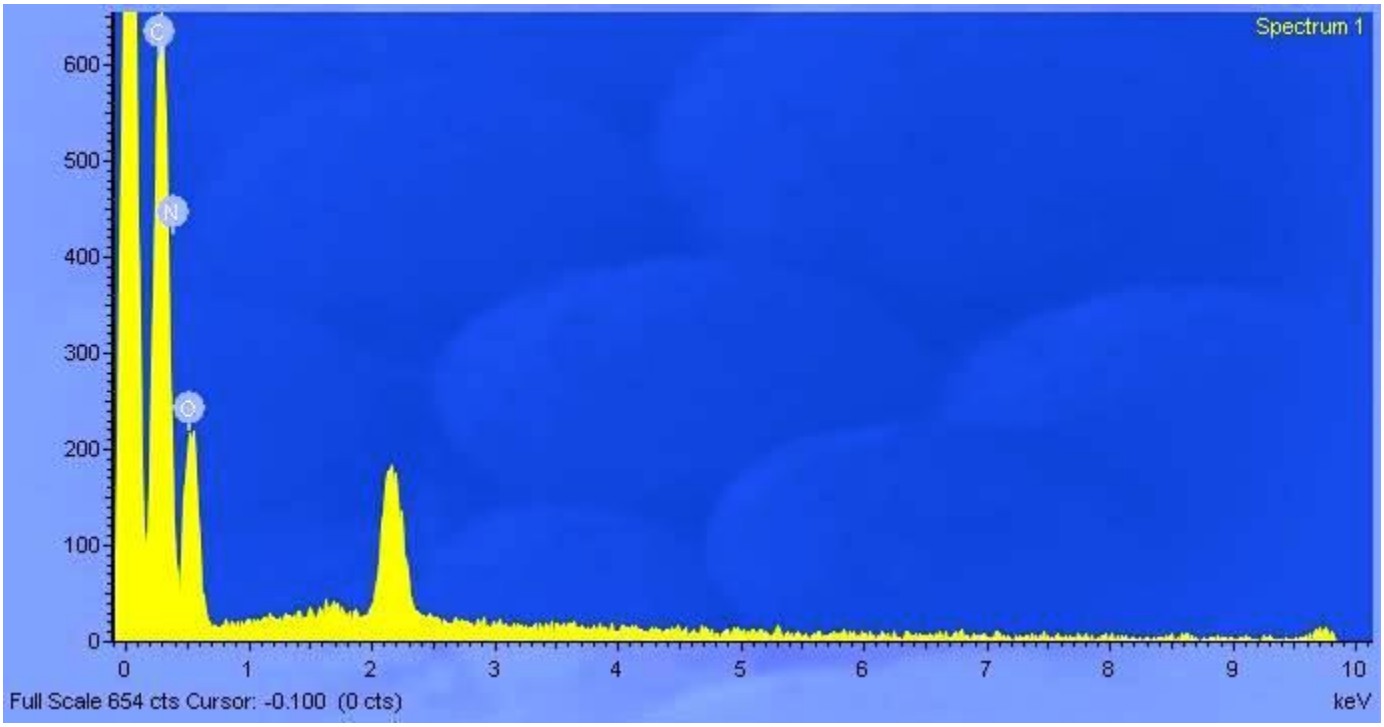


Table 2: **Gelation ability of compound 3(a-f)**

Cmpd No	Hexane	Hexane+ ethylacetate	Ethyl acetate	Chloro form	Chloroform + methanol	Methanol	DMSO	DMSO +water	Benzene	Toluene
3a	NG	NG	NG	NG	NG	NG	NG	NG	NG	NG
3b	NG	NG	NG	NG	NG	NG	NG	NG	NG	NG
3c	NG	G	PG	NG	NG	NG	NG	NG	NG	NG
3d	NG	G	PG	NG	NG	NG	NG	NG	NG	NG
3e	NG	NG	NG	NG	NG	NG	NG	NG	NG	NG
3f	NG	G	PG	NG	NG	NG	NG	NG	NG	NG

G = Gelator; PG = partial gelator; NG = non-gelator

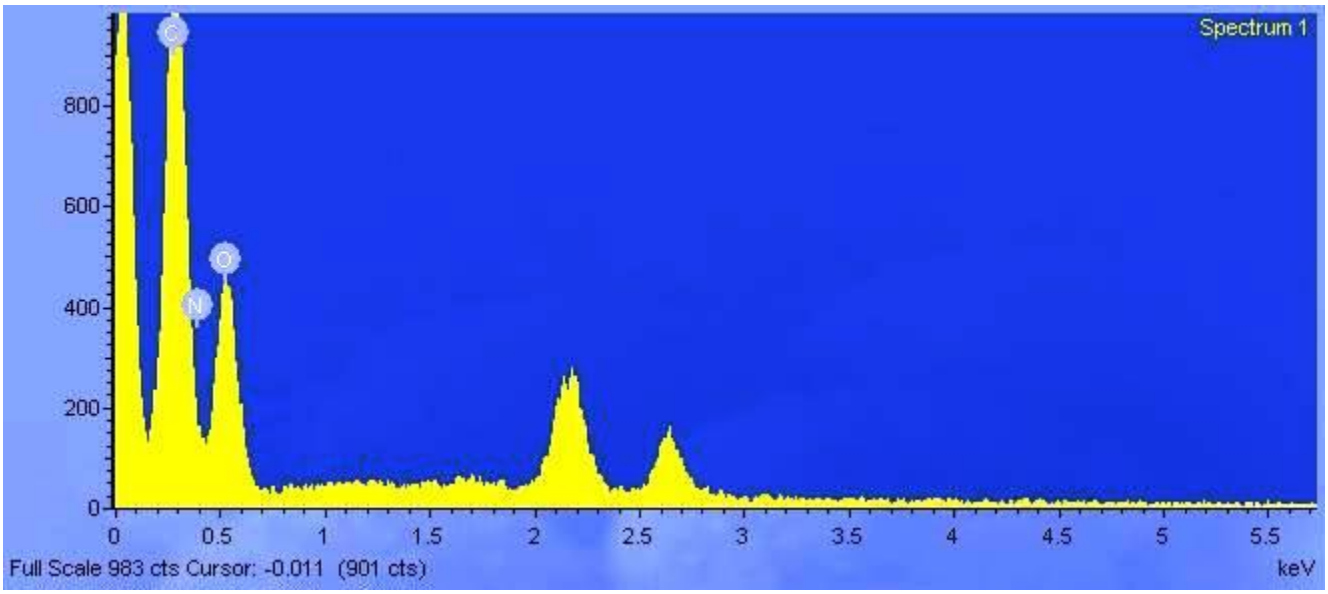
EDAX of compound 3f (before complexation with Hg^{2+} ion)



Standard :
C CaCO3
N Not defined
O SiO2

Element	Weight%	Atomic%
C K	36.02	41.18
N K	31.95	31.32
O K	32.03	27.49
Totals	100.00	

EDAX of compound 3d



Standard :

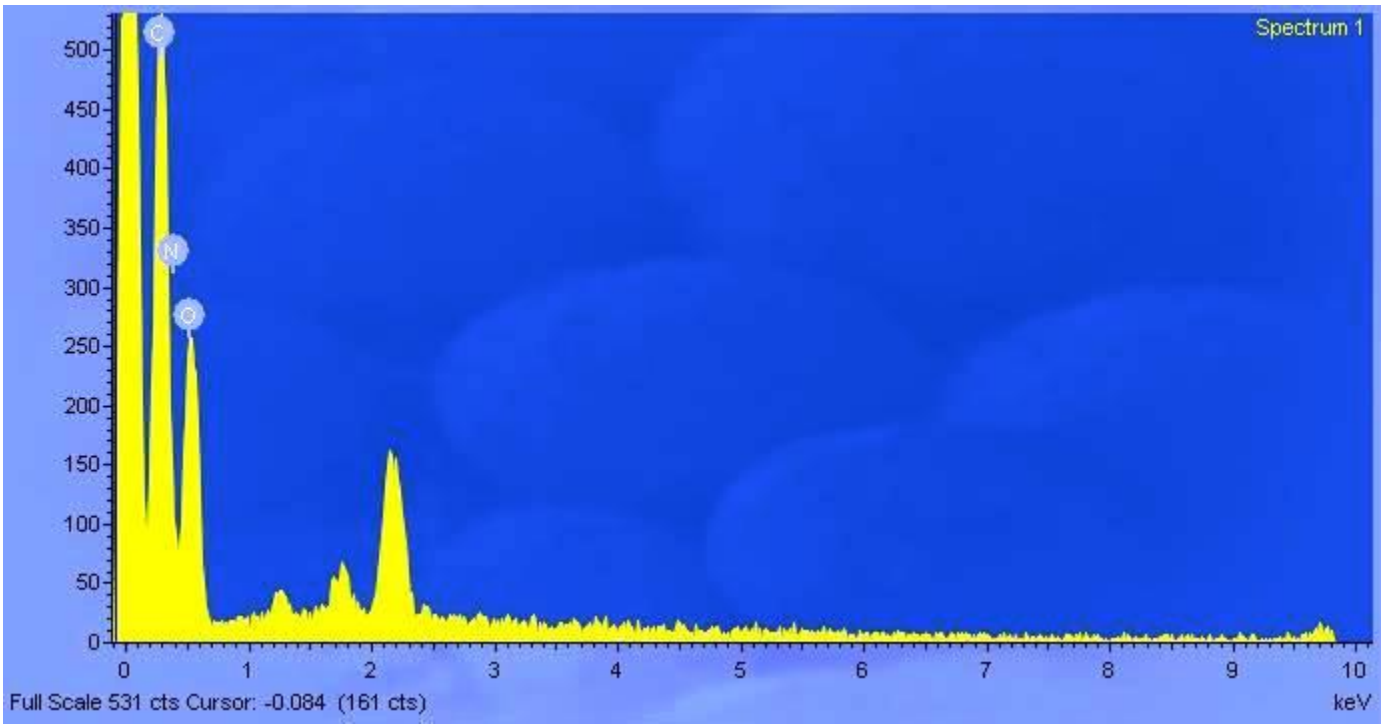
C CaCO3

N Not defined

O SiO2

Element	**Weight%**	**Atomic%**
C K	35.54	40.82
N K	29.35	28.91
O K	35.11	30.27
Totals	100.00	

EDAX of compound 3c



Standard :

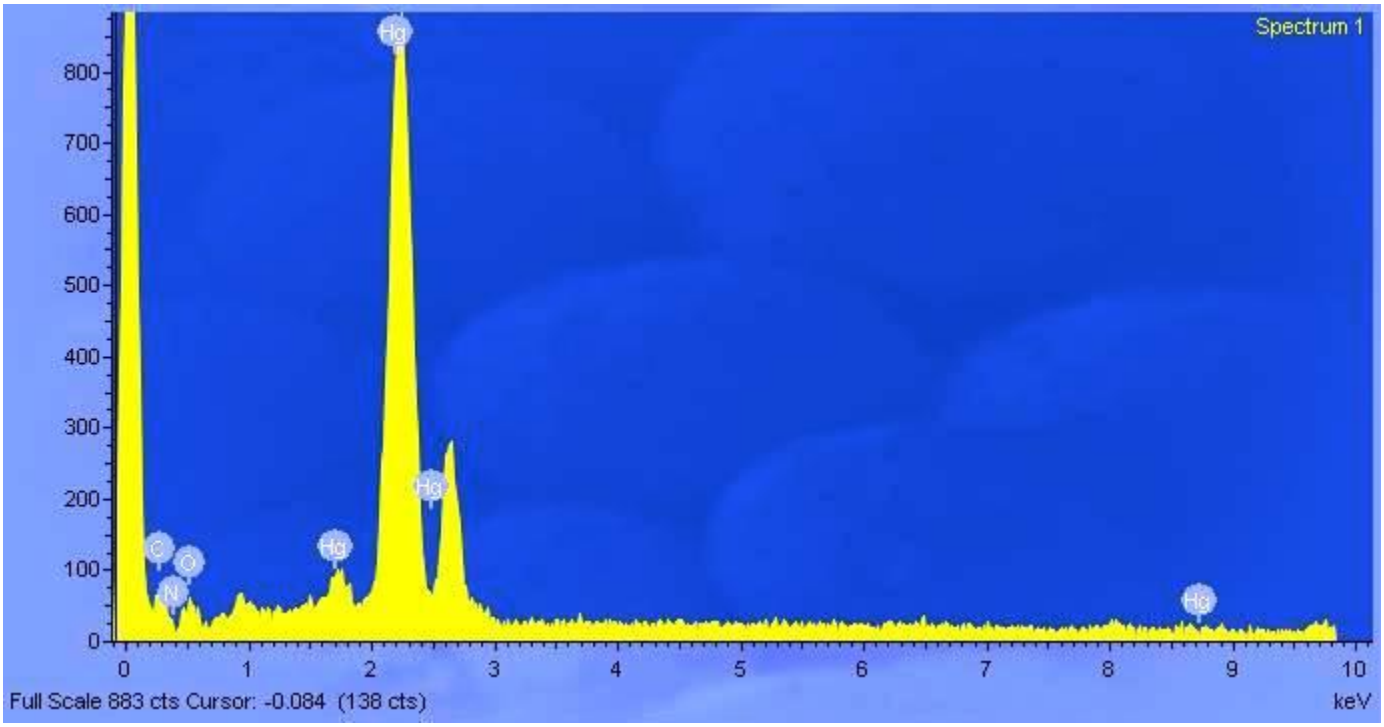
C CaCO3

N Not defined

O SiO2

Element	**Weight%**	**Atomic%**
C K	33.24	38.43
N K	29.35	29.10
O K	37.41	32.47
Totals	100.00	

EDAX of compound 3c (after complexation with Hg^{2+} ion)



Standard :

C CaCO3

N Not defined

O SiO2

Hg HgTe

Element	Weight%	Atomic%
C K	13.36	51.94
N K	2.57	8.58
O K	7.41	21.62
Hg M	76.67	17.85