Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Synthesis of oxazolidinofullerenes/thiazolidinofullerenes: Novel reaction [60]fullerene with isocyanates/isothiocyanates promoted by ferric perchlorate

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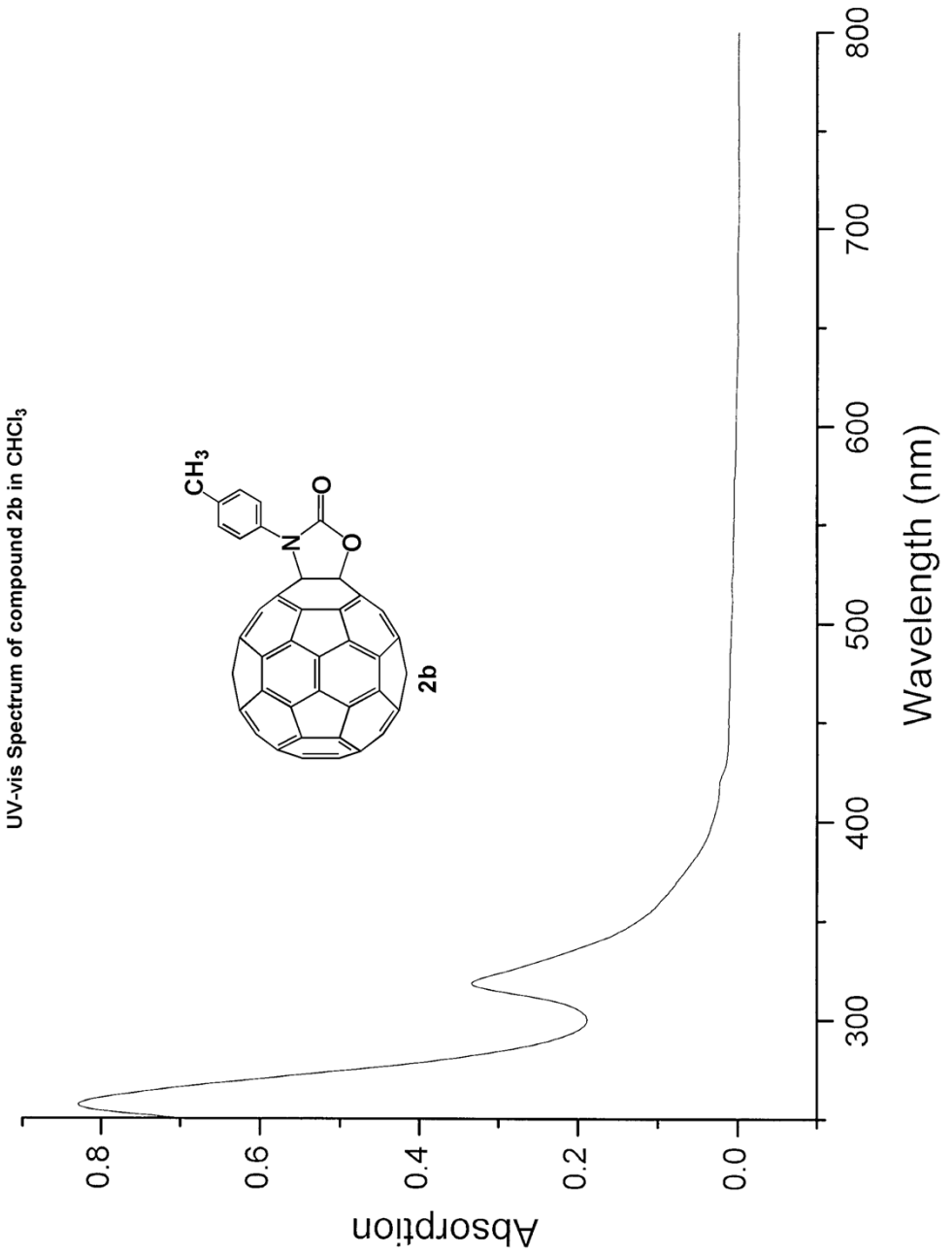
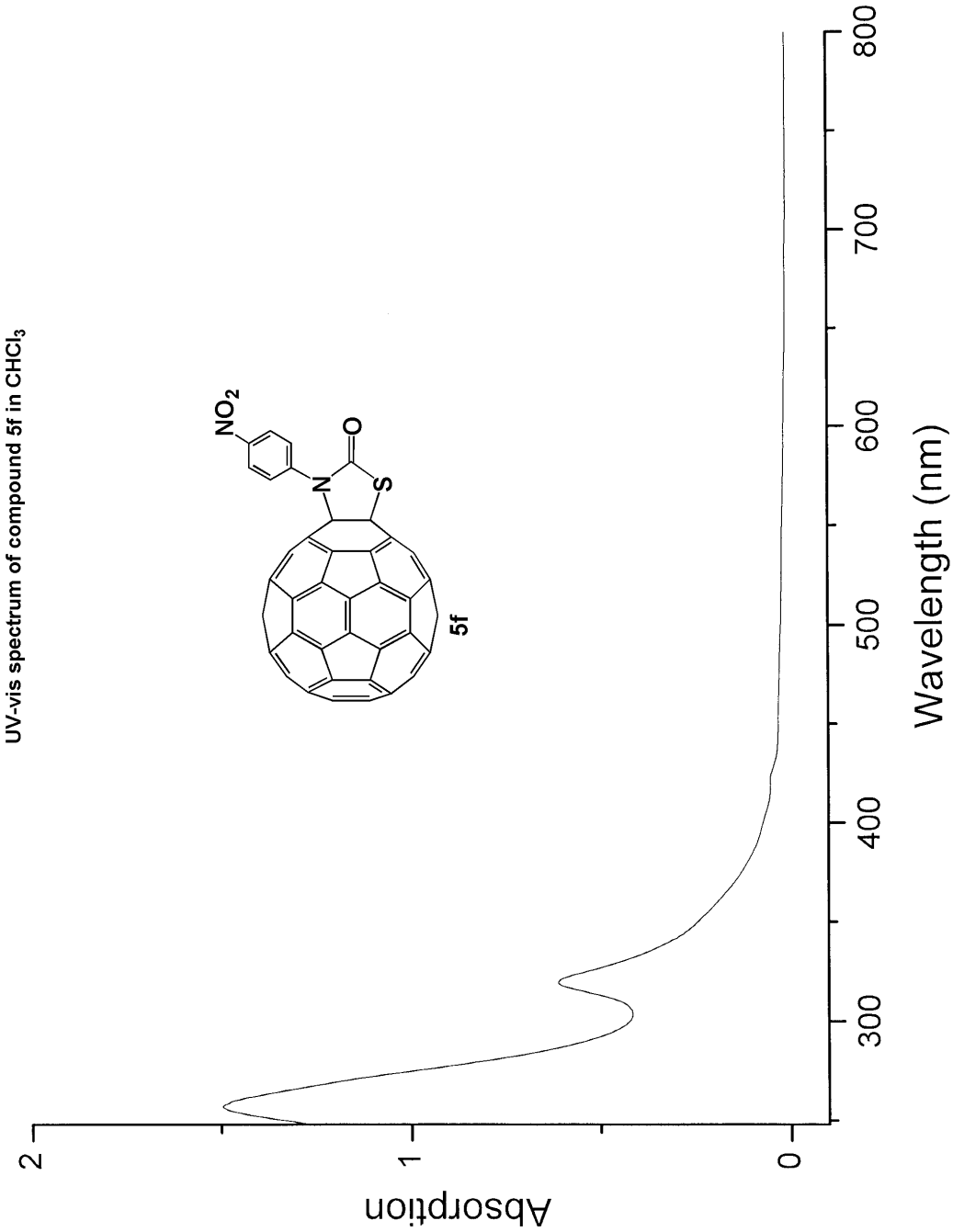
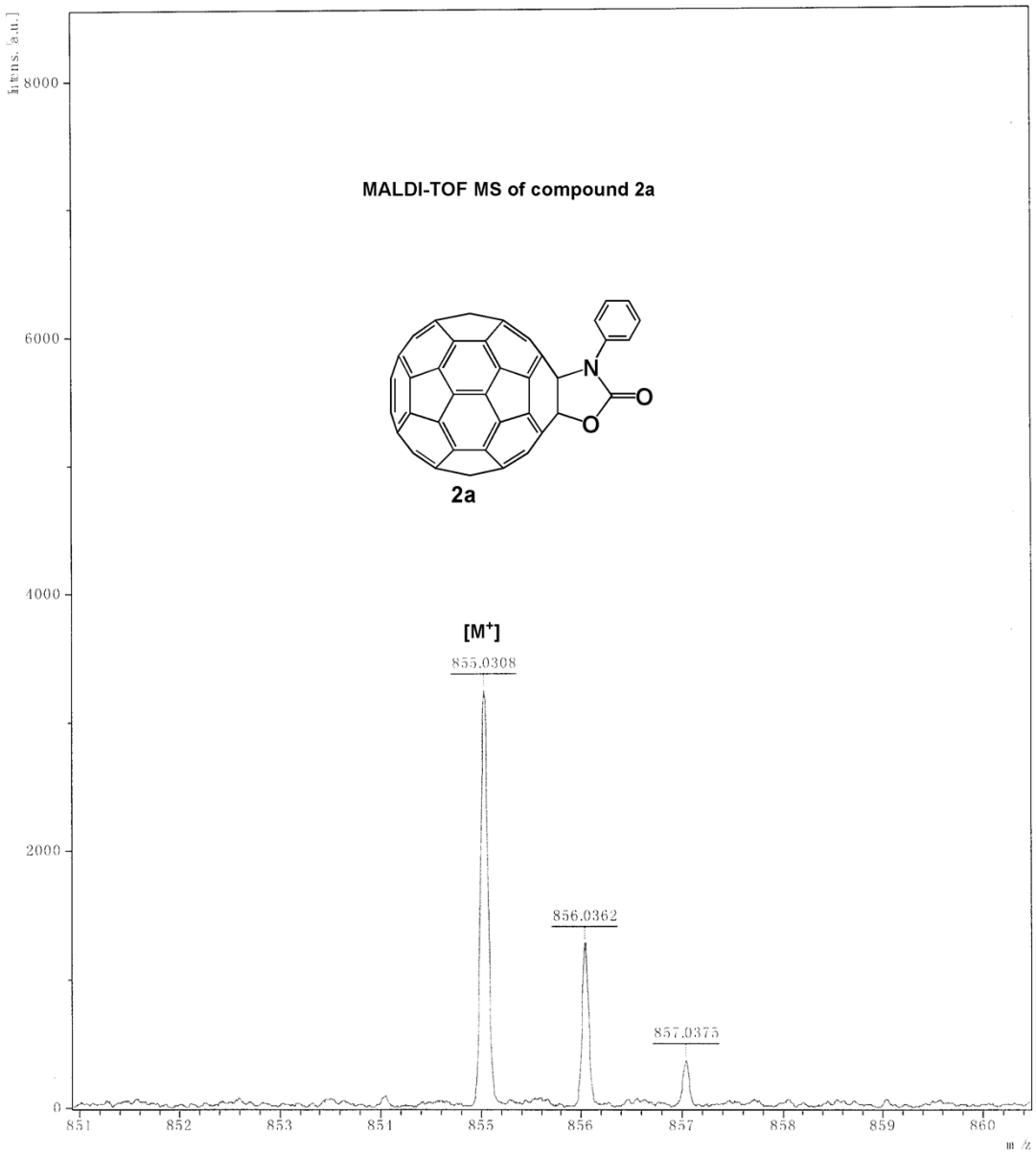
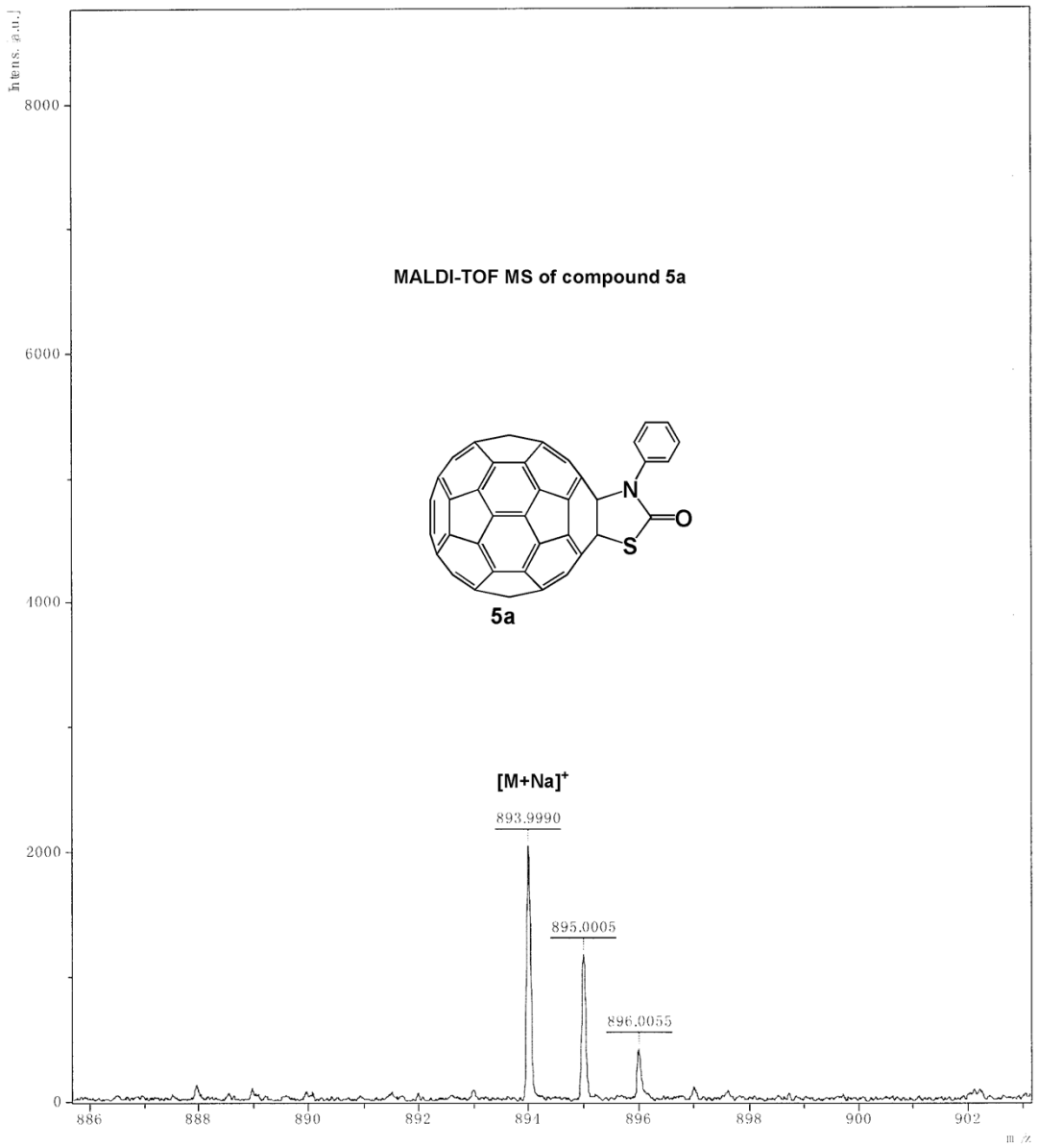
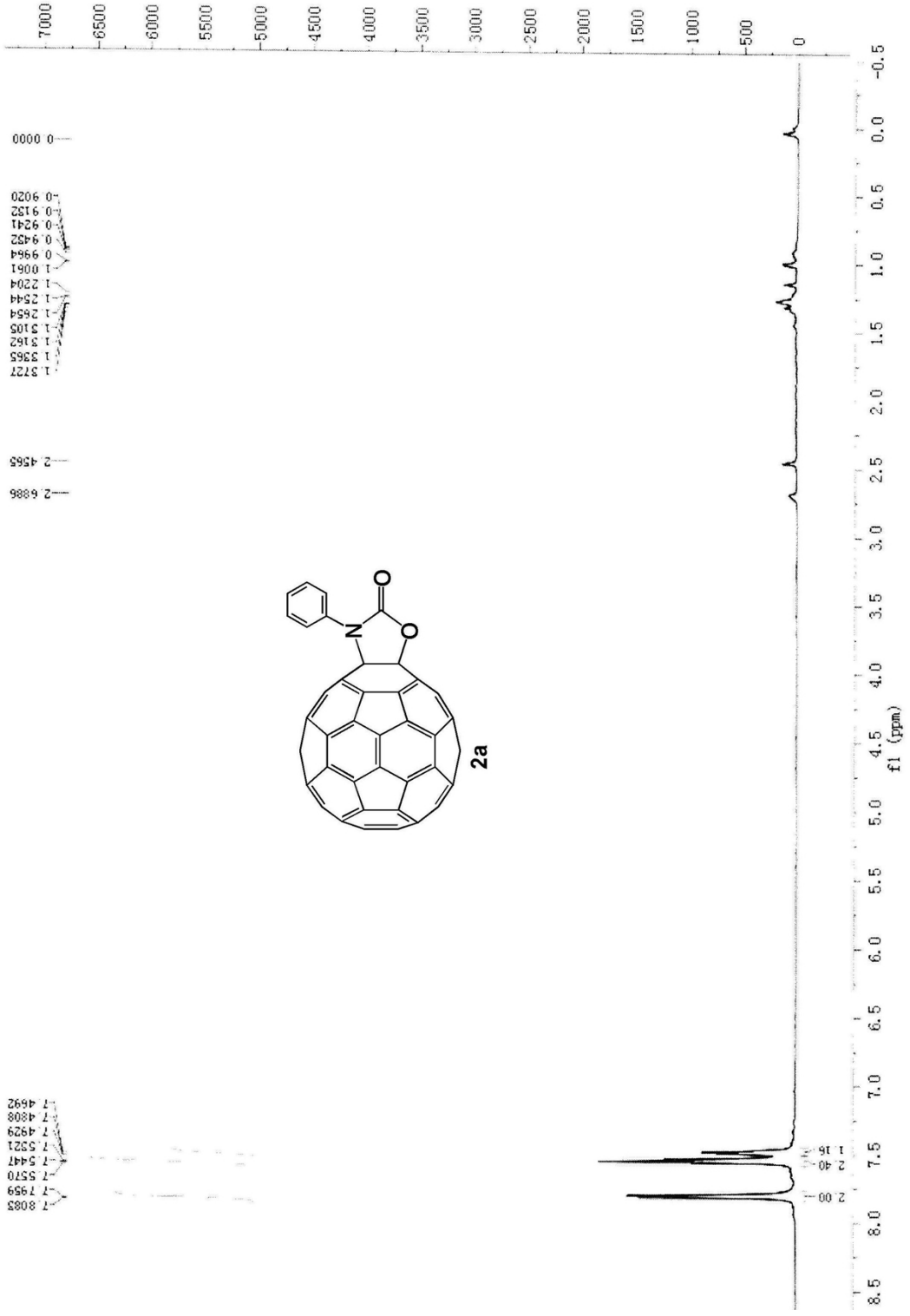

UV-vis Spectrum of compound 2b in CHCl3
CH3
N
O
O
2b
Absorption
0.0
0.2
0.4
0.6
0.8
300
400
500
600
700
800
Wavelength (nm)


UV-vis spectrum of compound 5f in CHCl3
NO2
O
N
S
5f
Absorption
0
1
2
300
400
500
600
700
800
Wavelength (nm)

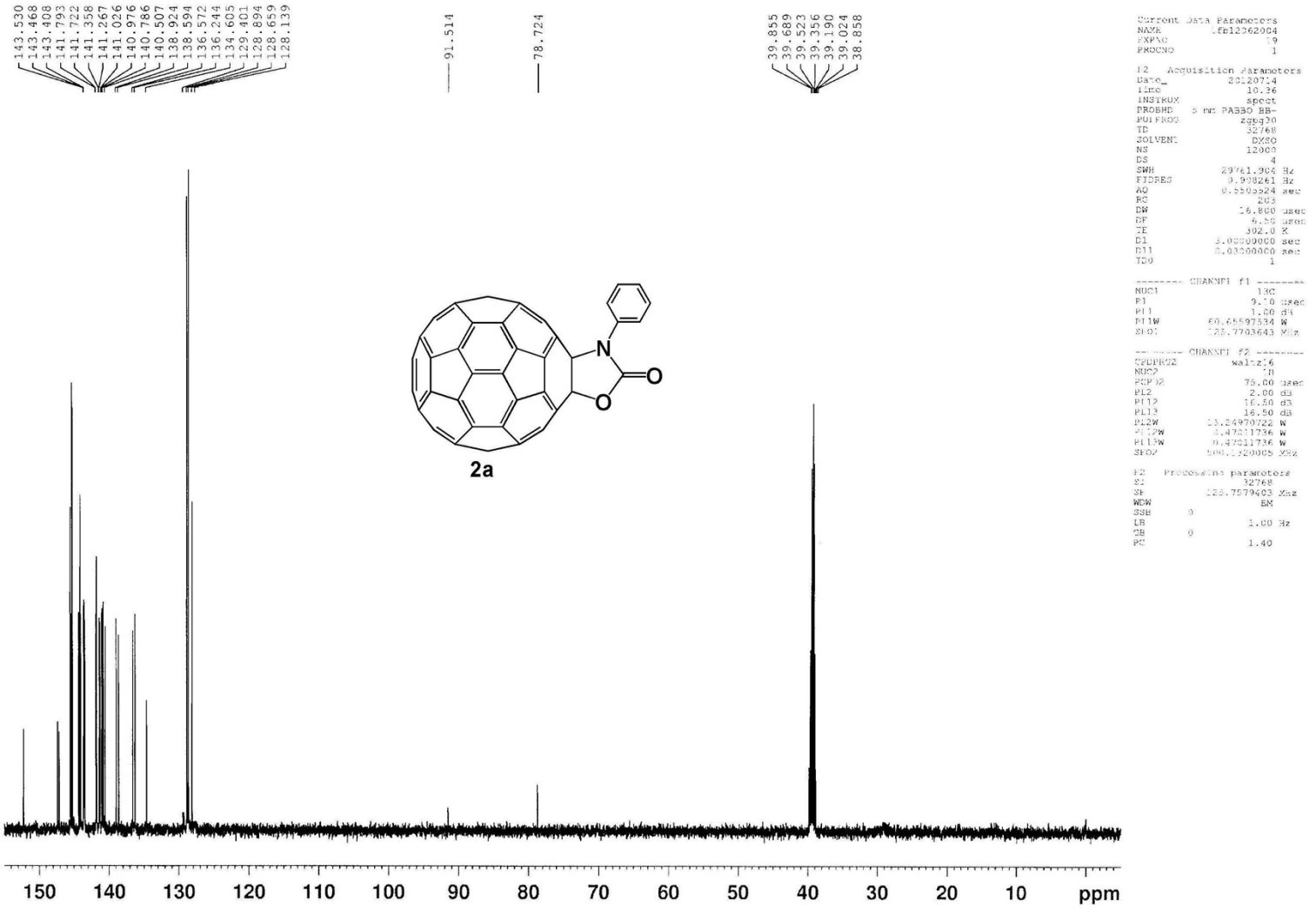

Intens. [a.u.]
8000
6000
4000
2000
0
MALDI-TOF MS of compound 2a
N
O
O
2a
[M+]
855.0308
856.0362
857.0375
851
852
853
854
855
856
857
858
859
860
m/z


Intens. [a.u.]
8000
6000
4000
2000
0
MALDI-TOF MS of compound 5a
N
O
S
5a
[M+Na]+
893.9990
895.0005
896.0055
886
888
890
892
894
896
898
900
902
m/z

^{1}H NMR (600 MHz, CS_2/DMSO-d_6) of compound 2a



^{13}C NMR (125 MHz, CS_2/DMSO-d_6) of compound 2a

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PROCNO                   1

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PULPROG             zgpg30
TD                   32768
SOLVENT                DMSO
NS                     12000
DS                         4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ                0.550324 sec
RG                      203
DW                   16.800 usec
DE                    6.50 usec
TE                   302.0 K
D1                3.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.70 usec
PL1                     1.00 dB
PL1W              60.65997534 W
SFO1              125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  75.00 usec
PL2                     2.00 dB
PL12                   16.50 dB
PL13                   16.50 dB
PL2W              13.24970722 W
PL12W              0.47211736 W
PL13W              0.47211736 W
SFO2              500.1320005 MHz

F2 - Processing parameters
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WDW                         EM
SSB                      0
LB                      1.00 Hz
GB                       0
PC                      1.40
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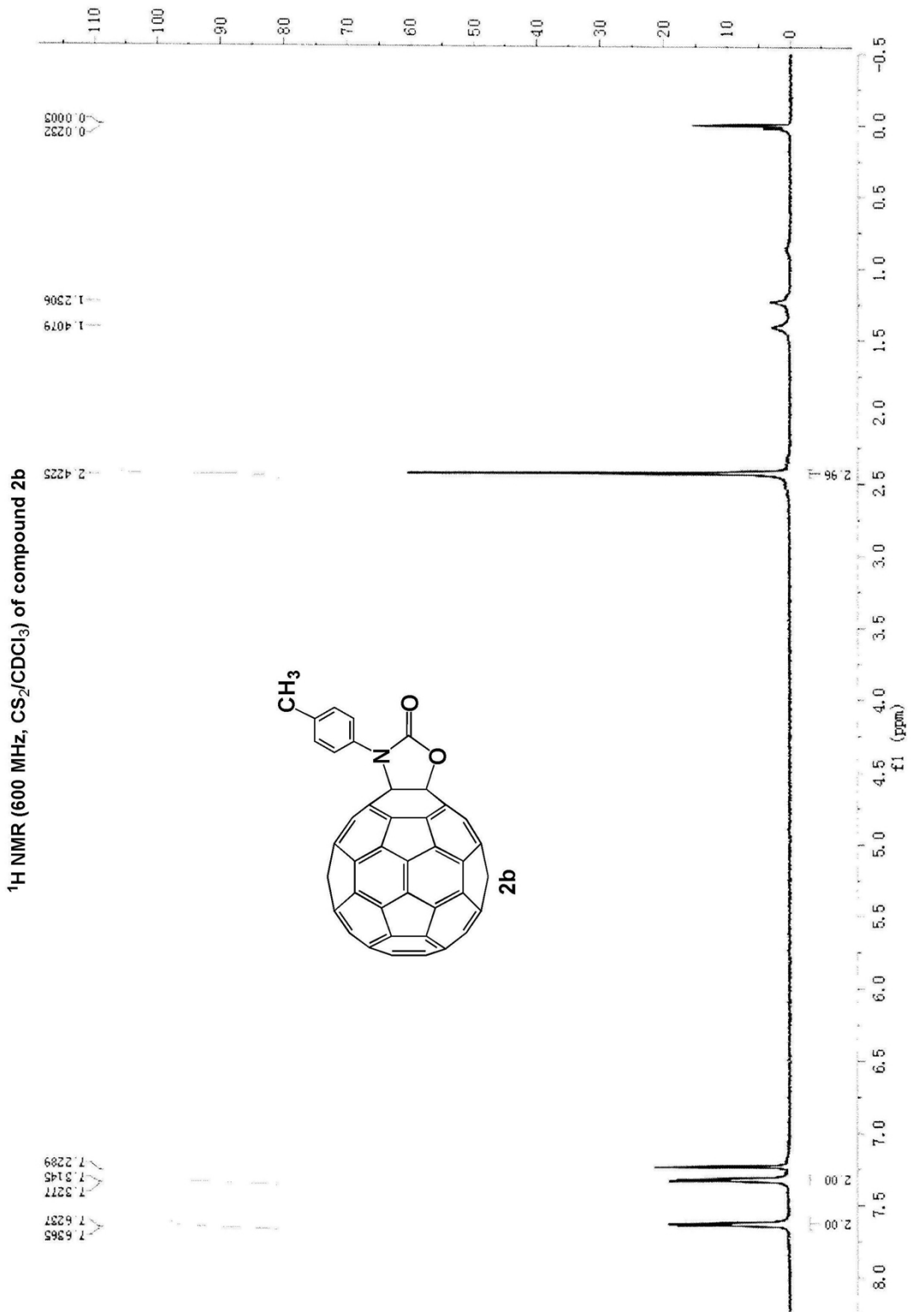
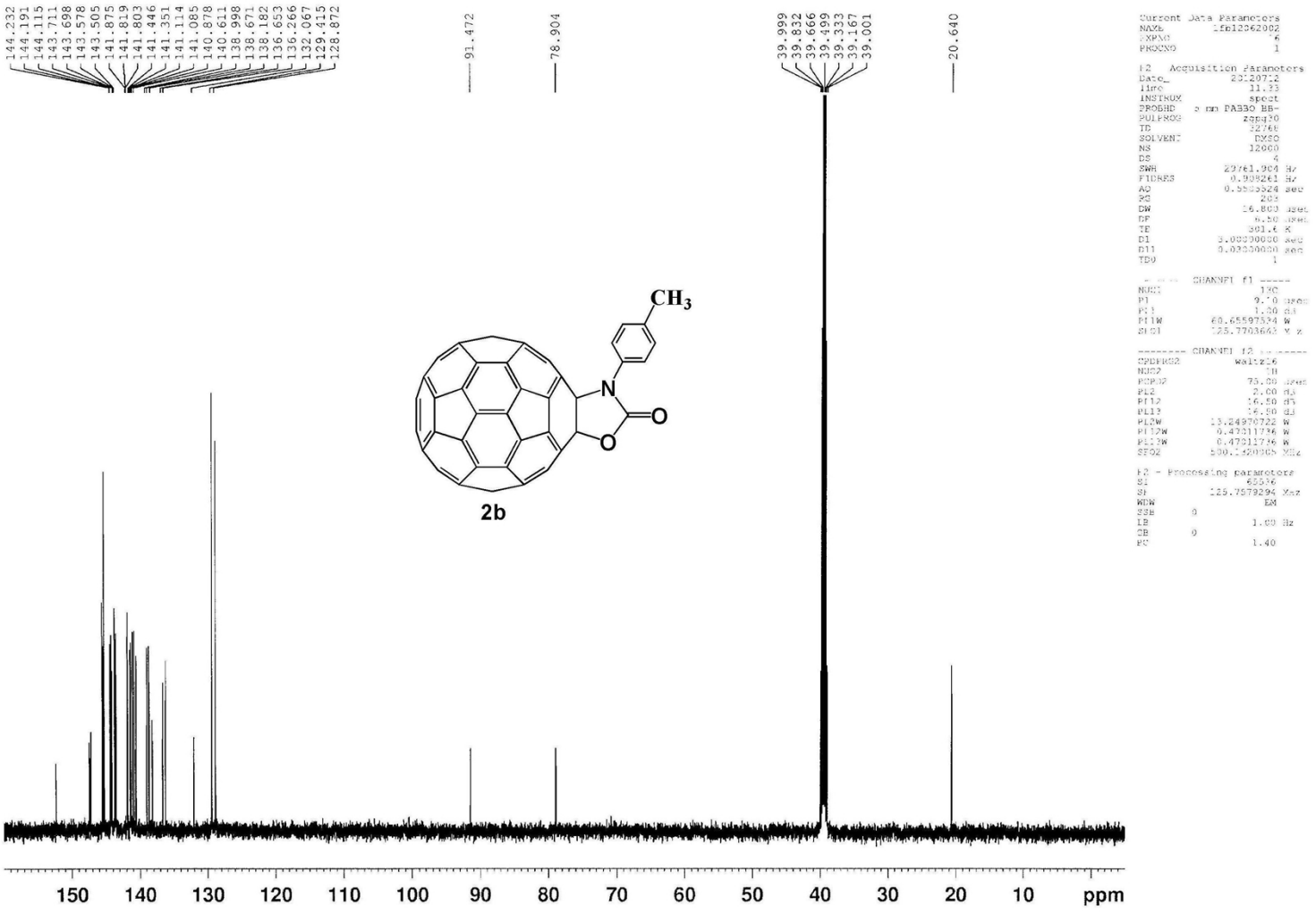

^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 2b
CH_3
N
O
O
2b
f1 (ppm)

^{13}C NMR (125 MHz, CS_2/DMSO-d_6) of compound 2b



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EXPNO 6
PROCNO 1

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INSTRUM spect
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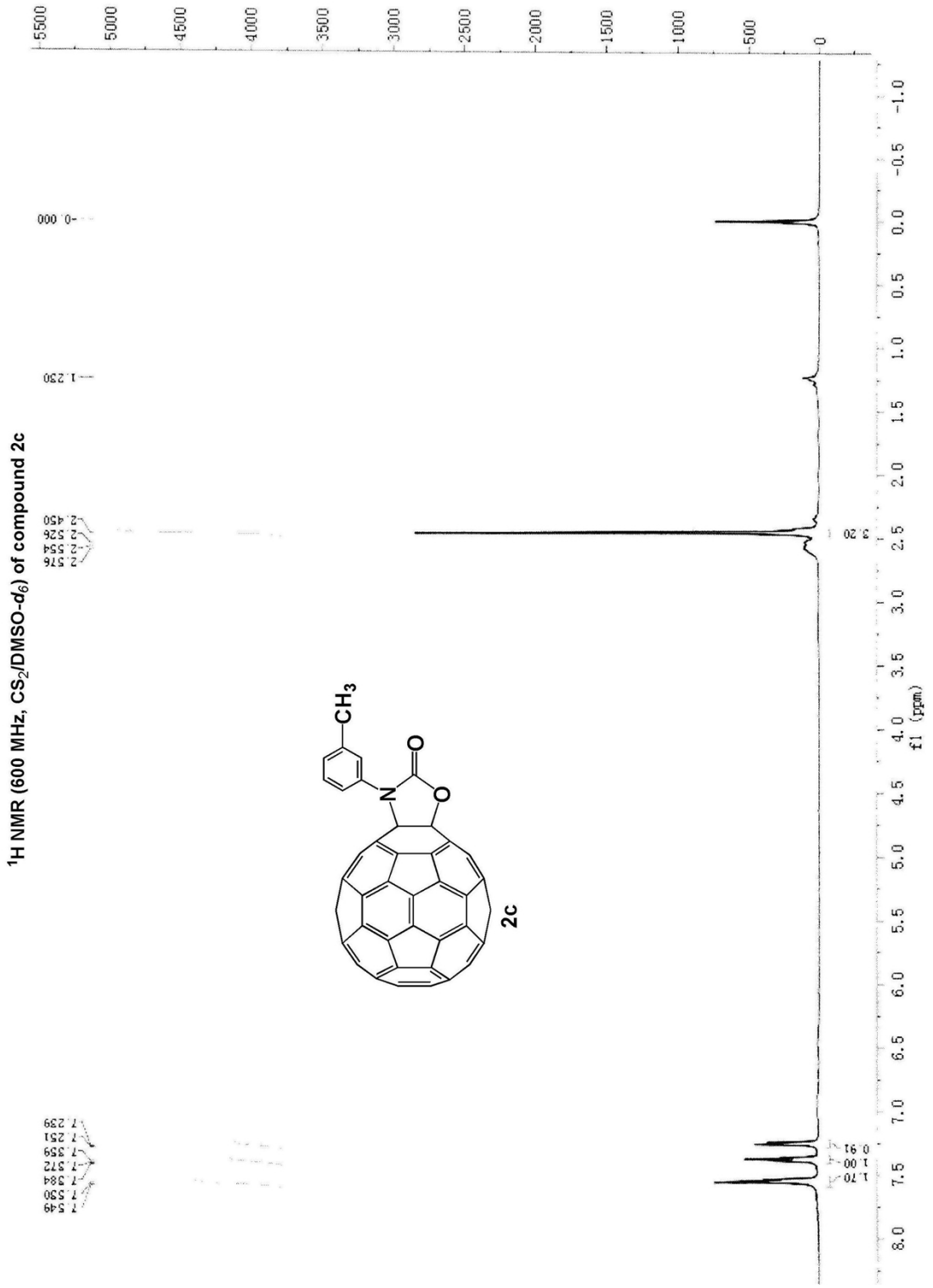
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 12000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505624 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 301.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

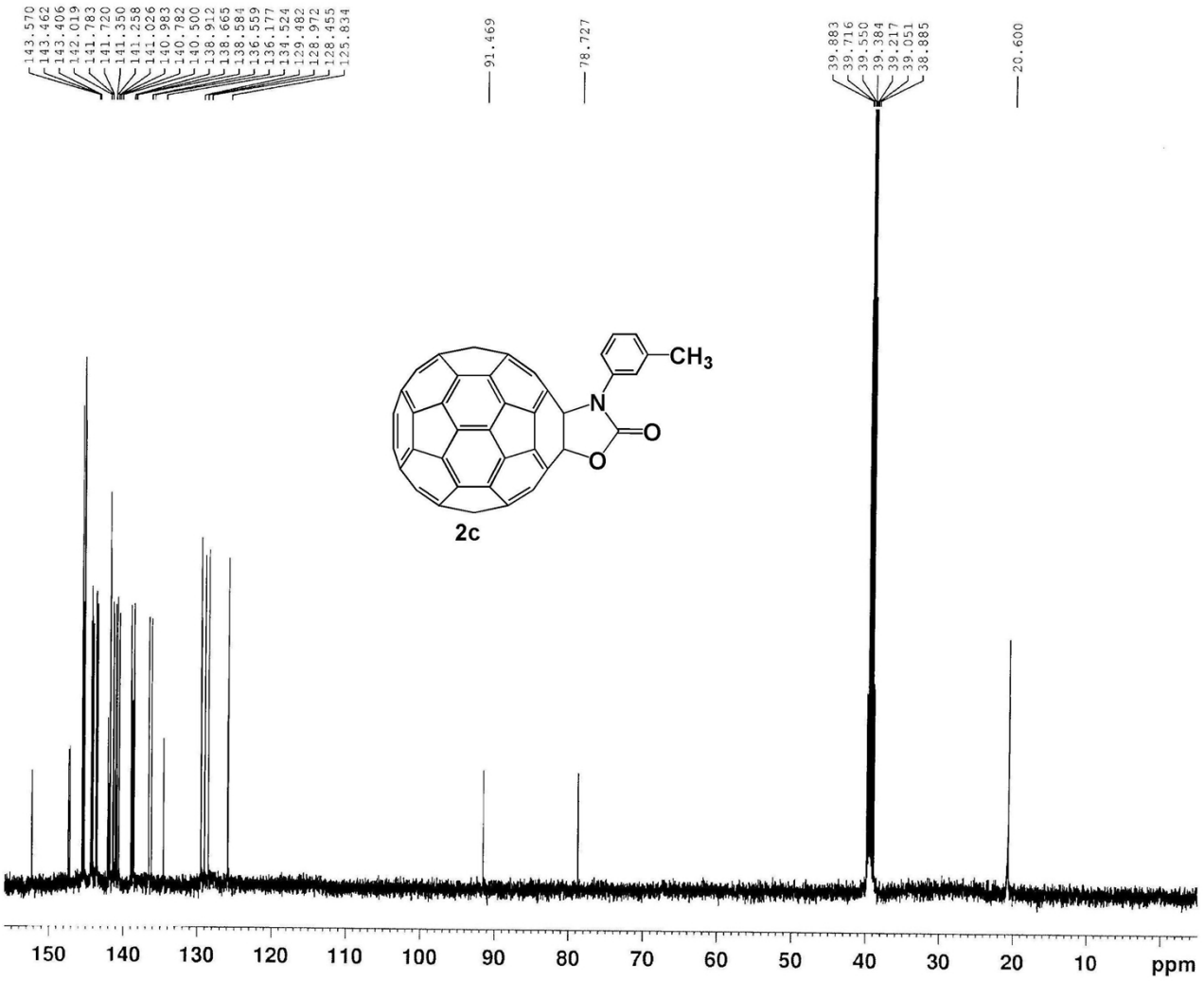
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 1.00 dB
PL1W 60.65597534 W
SFO1 125.7703663 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz65
NUC2 1H
PCPD2 75.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
PL2W 13.24970722 W
PL12W 0.47311736 W
PL13W 0.47311736 W
SFO2 500.1320005 MHz

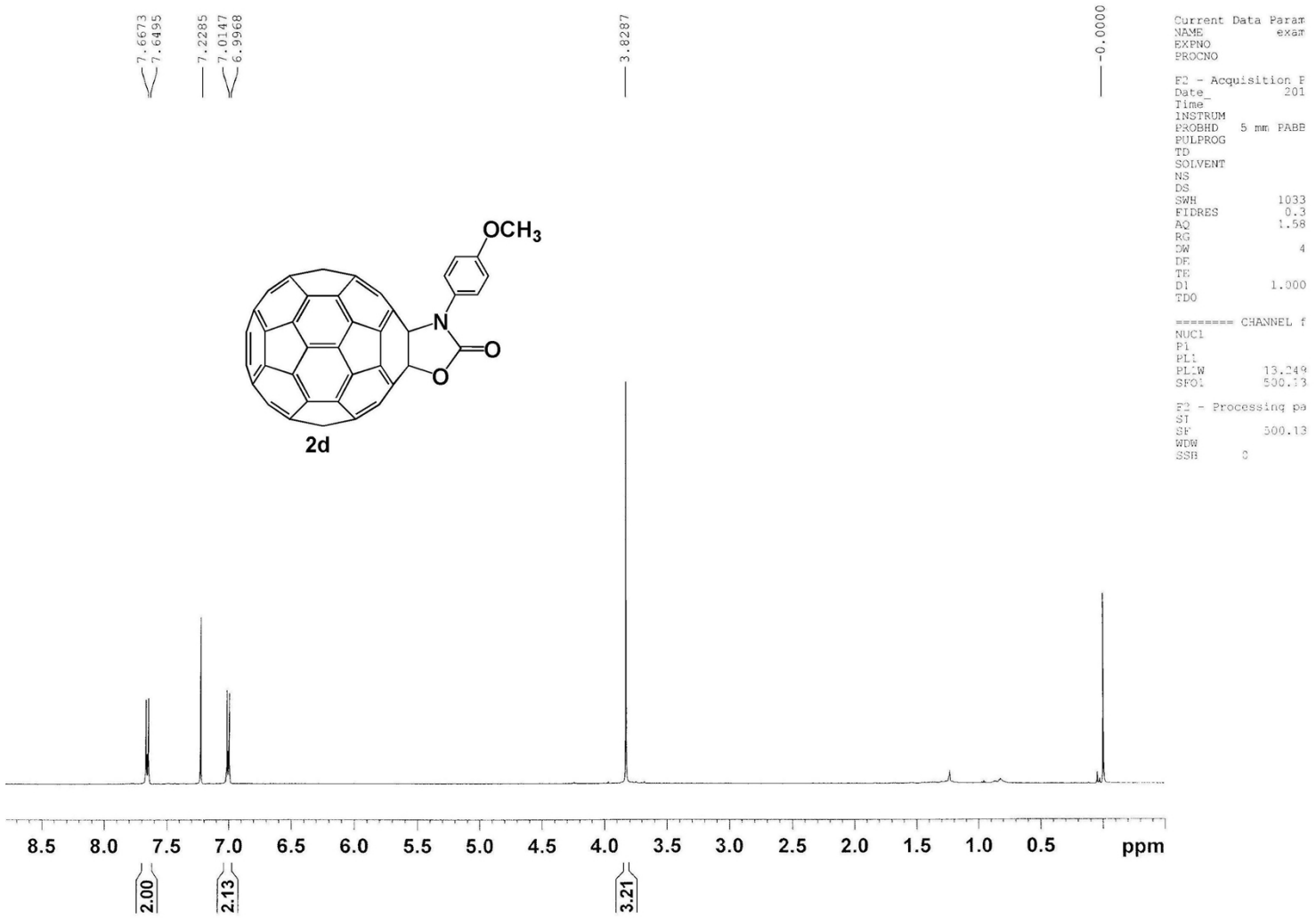
F2 - Processing parameters
SI 65536
SF 125.7579294 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

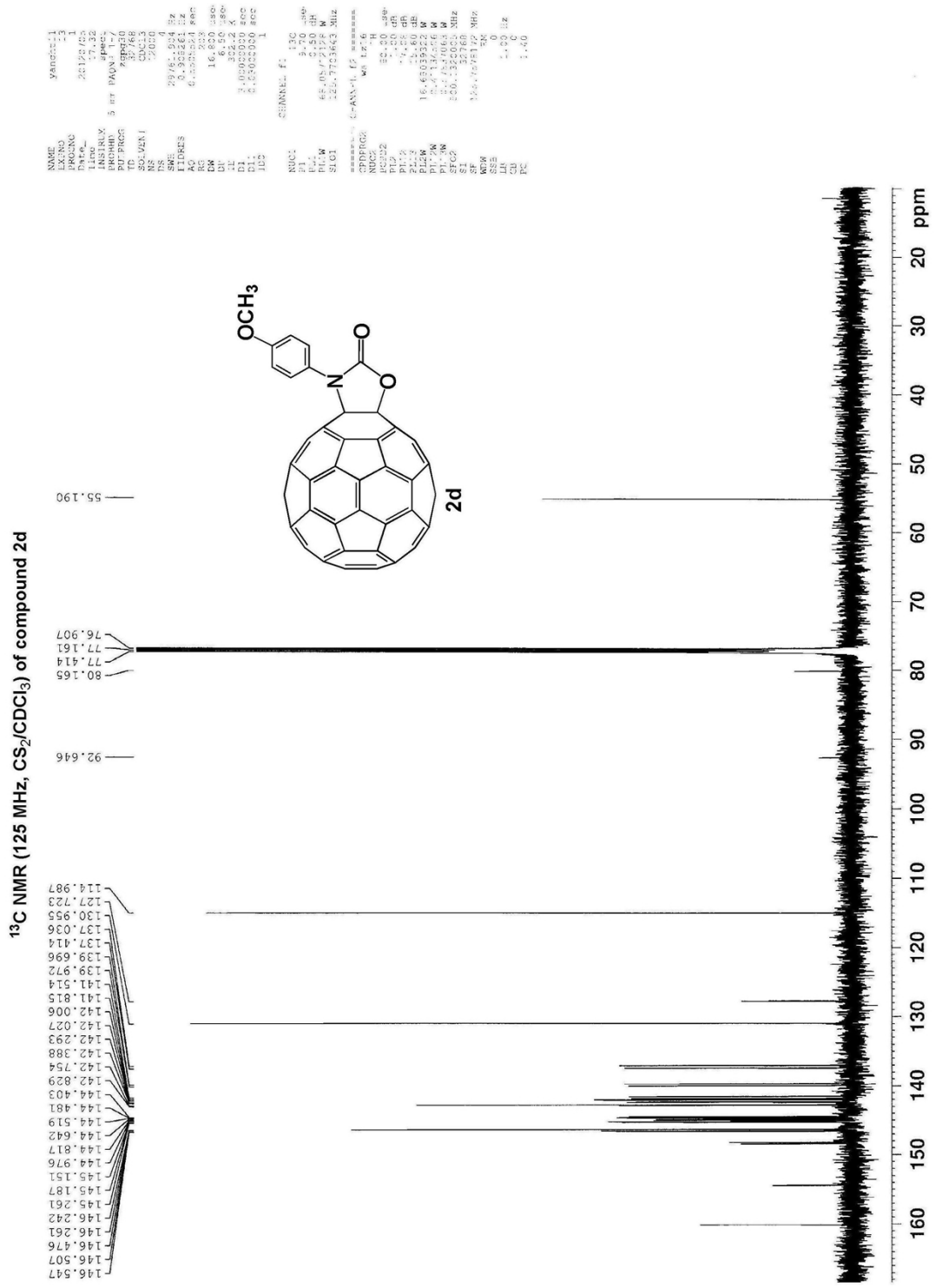

^{1}H NMR (600 MHz, CS_2/DMSO-d_6) of compound 2c
CH_3
N
O
O
2c
f1 (ppm)

^{13}C NMR (125 MHz, CS_2/DMSO-d_6) of compound 2c

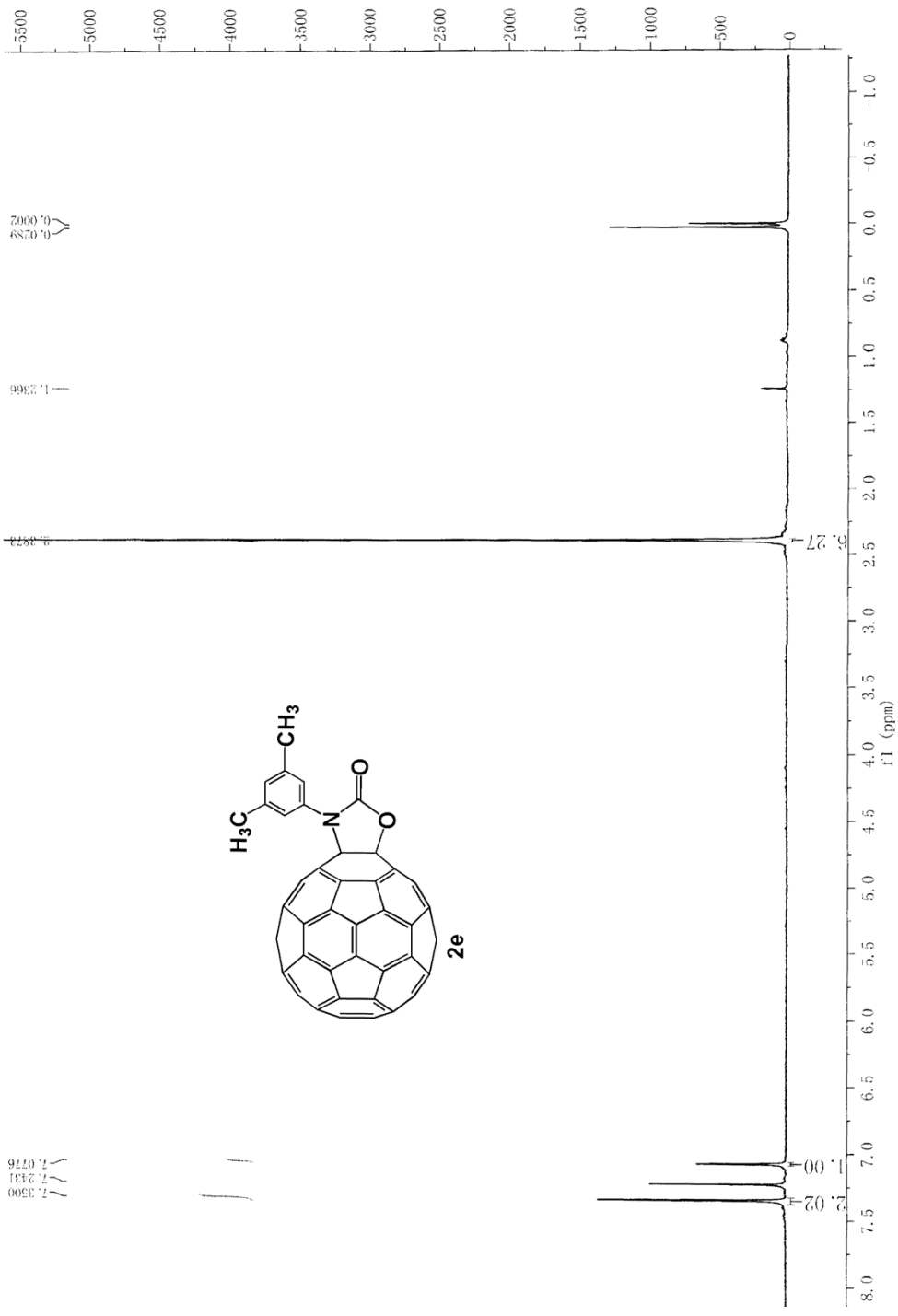


^{1}H NMR (500 MHz, CS_2/$CDCl_3$) of compound 2d

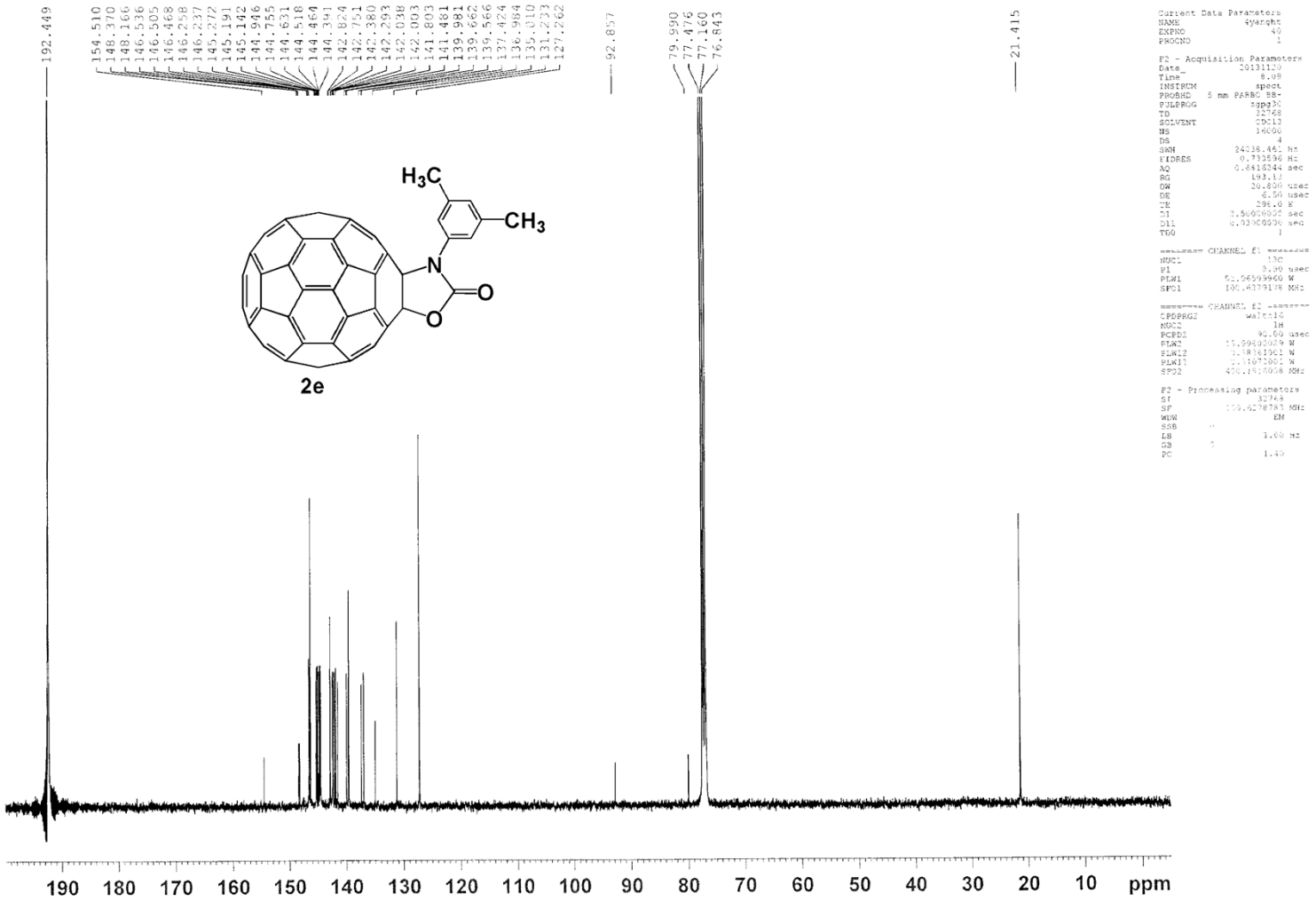



13C NMR (125 MHz, CS2/CDCl3) of compound 2d
OCH3
N
O
O
2d
55.190
76.907
77.161
77.414
80.165
92.646
114.987
127.723
130.955
137.036
137.414
139.696
139.972
141.514
141.815
142.006
142.027
142.293
142.388
142.754
142.829
144.403
144.481
144.519
144.642
144.817
144.976
145.151
145.187
145.261
146.242
146.261
146.476
146.507
146.547
ppm

^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 2e



^{13}C NMR (100 MHz, CS_2/$CDCl_3$) of compound 2e



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PROCNO 1

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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 14000
DS 4
SWH 24038.461 Hz
FIDRES 0.733536 Hz
AQ 0.6816384 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.90 usec
PLW1 51.06599960 W
SFO1 100.4779178 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 91.60 usec
PLW2 15.99600029 W
PLW12 1.19381901 W
PLW13 1.11675001 W
SFO2 400.1316008 MHz

F2 - Processing parameters
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SSB 0
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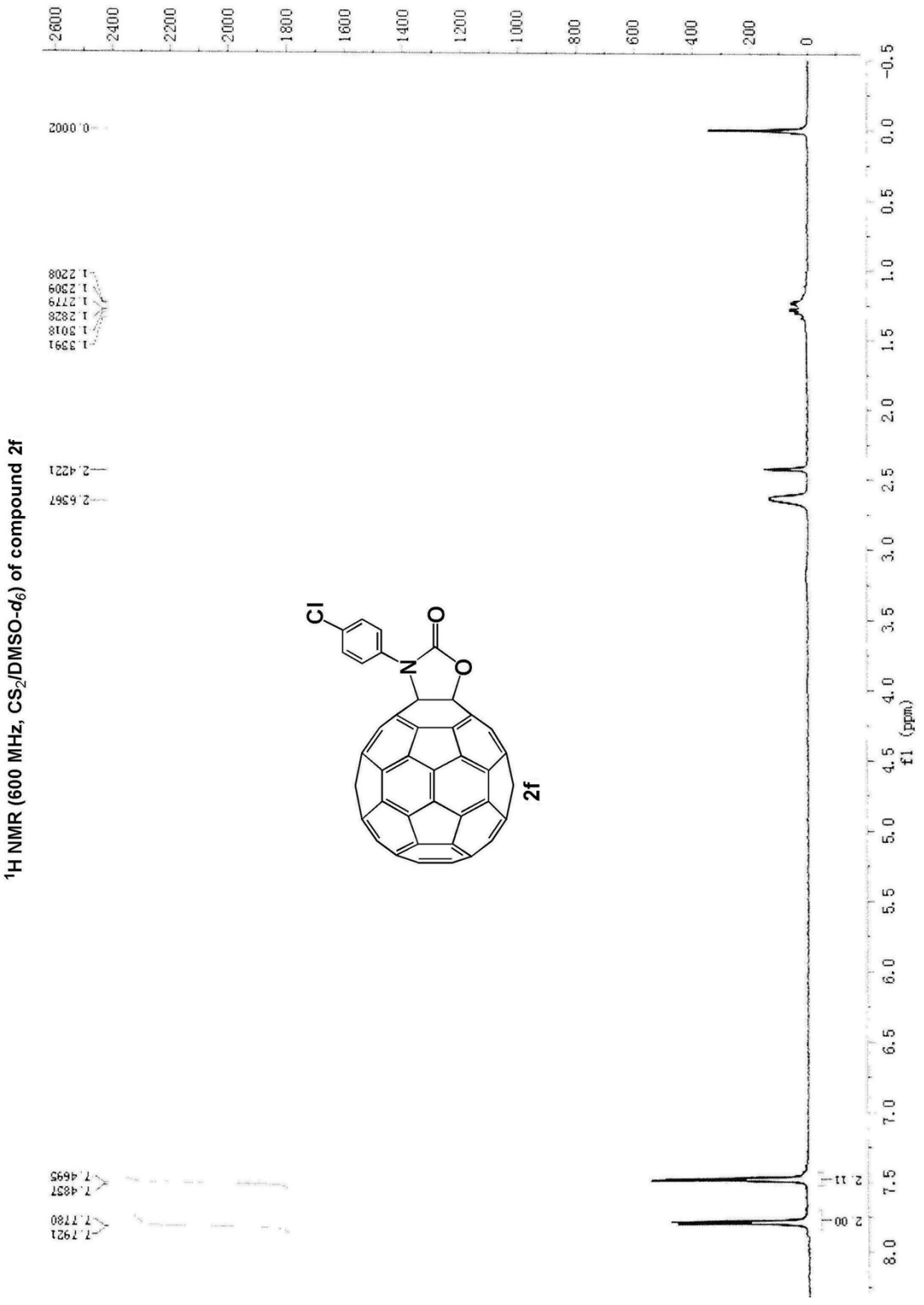
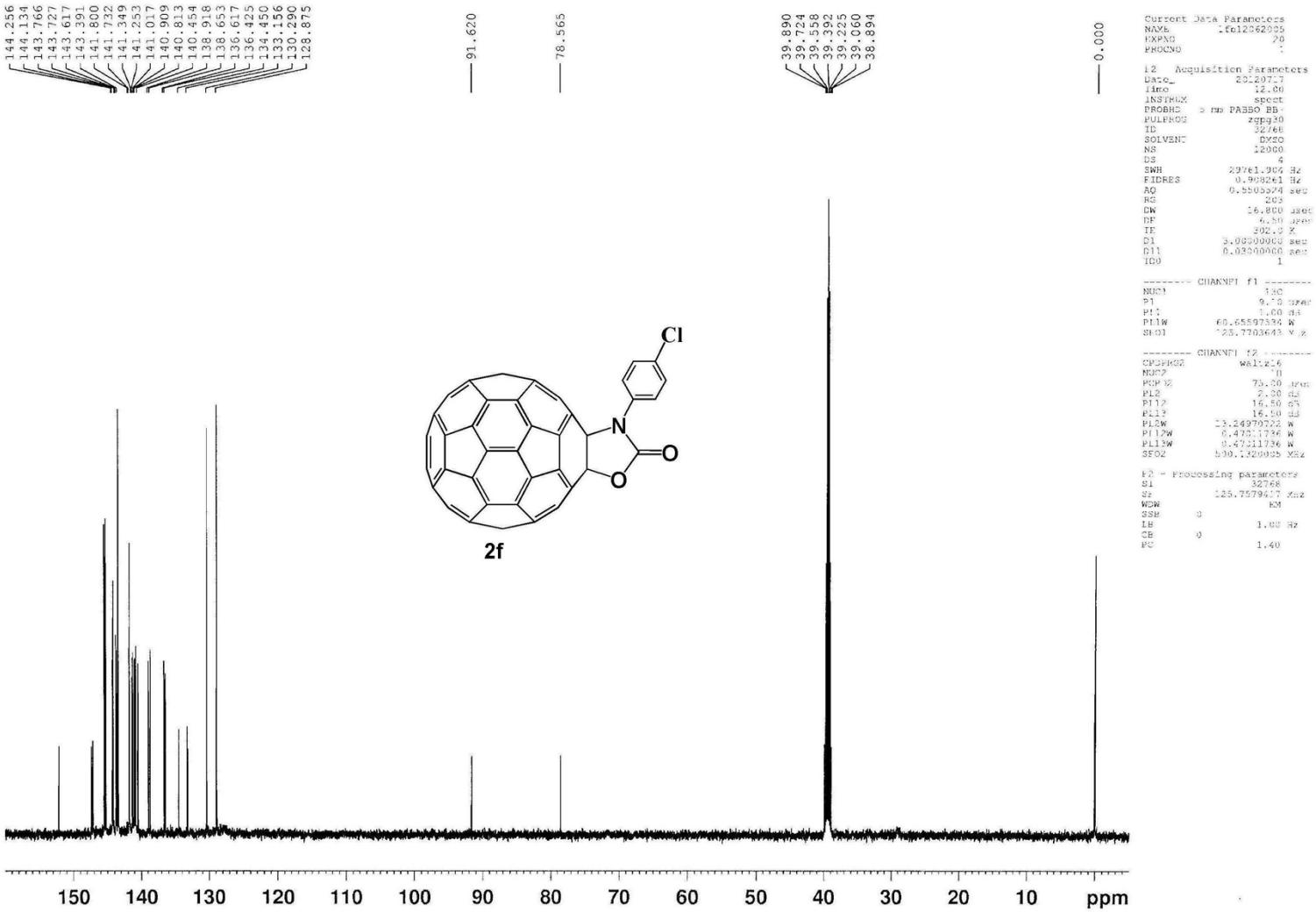
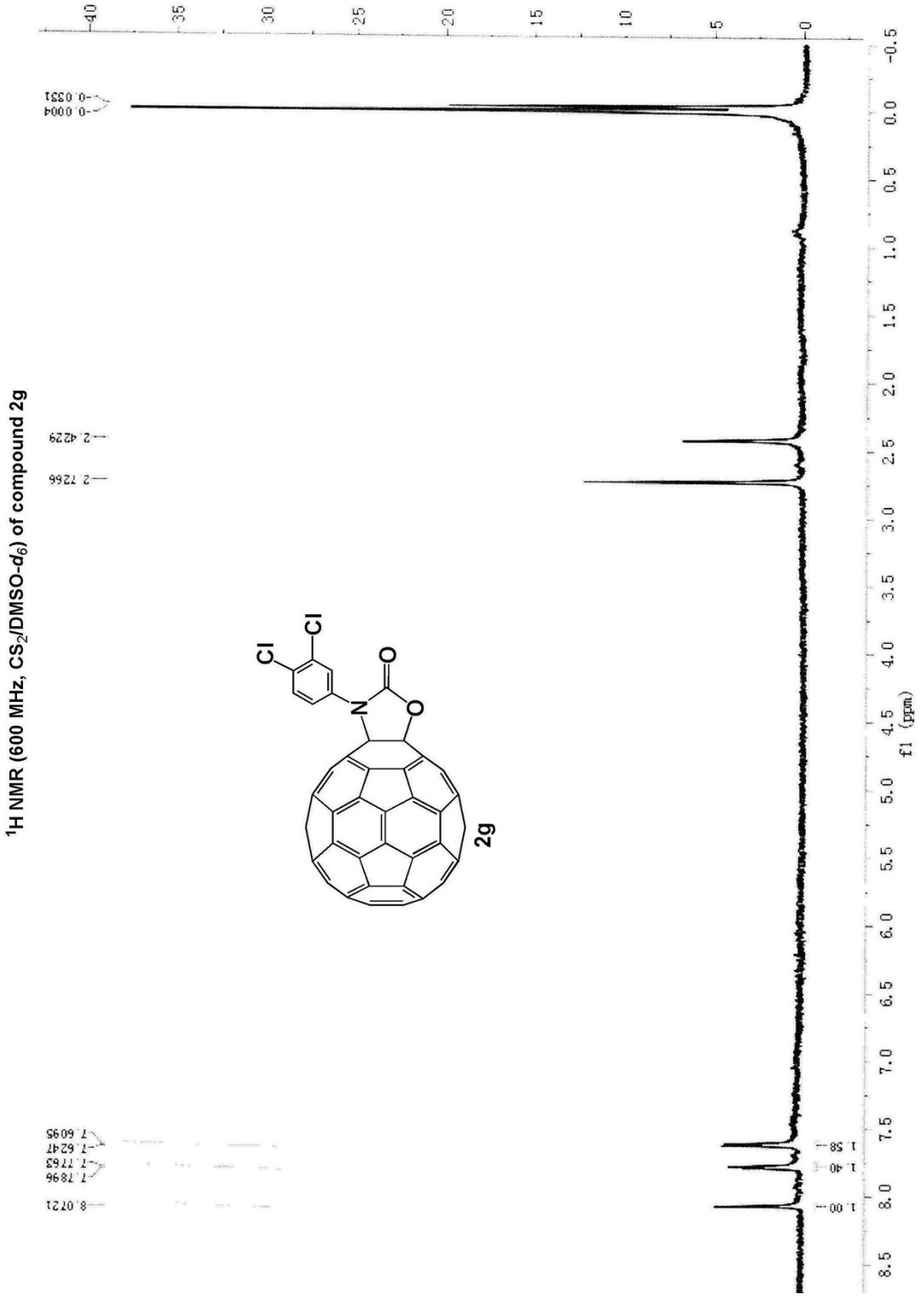
GB 0
PC 1.40

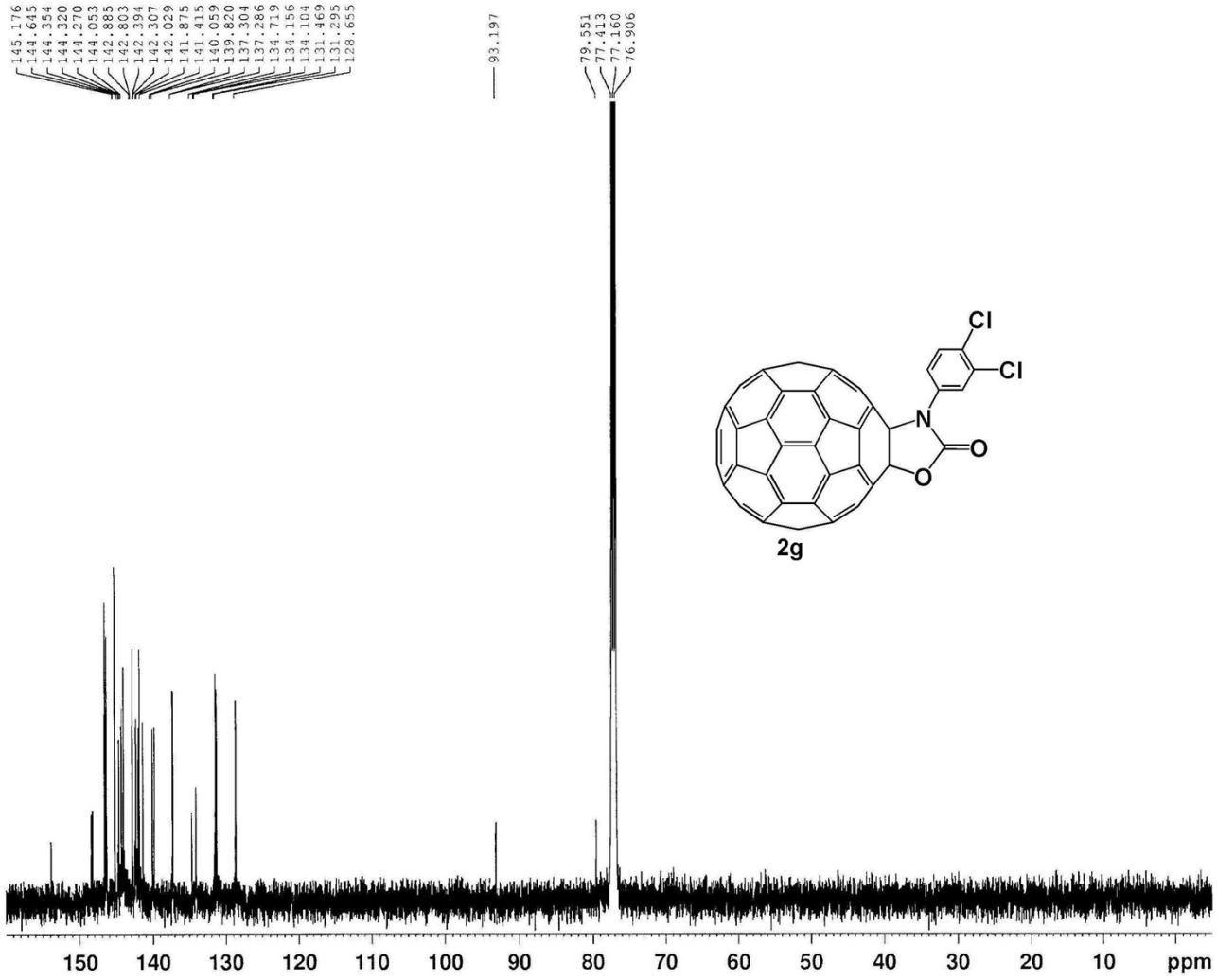

^{1}H NMR (600 MHz, CS_2/DMSO-d_6) of compound 2f
Cl
O
N
O
2f
f1 (ppm)

^{13}C NMR (125 MHz, CS_2/DMSO-d_6) of compound 2f




^{1}H NMR (600 MHz, CS_2/DMSO-d_6) of compound 2g
Cl
Cl
N
O
O
2g
f1 (ppm)

^{13}C NMR (125 MHz, CS_2/$CDCl_3$) of compound 2g

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PROCNO                         1

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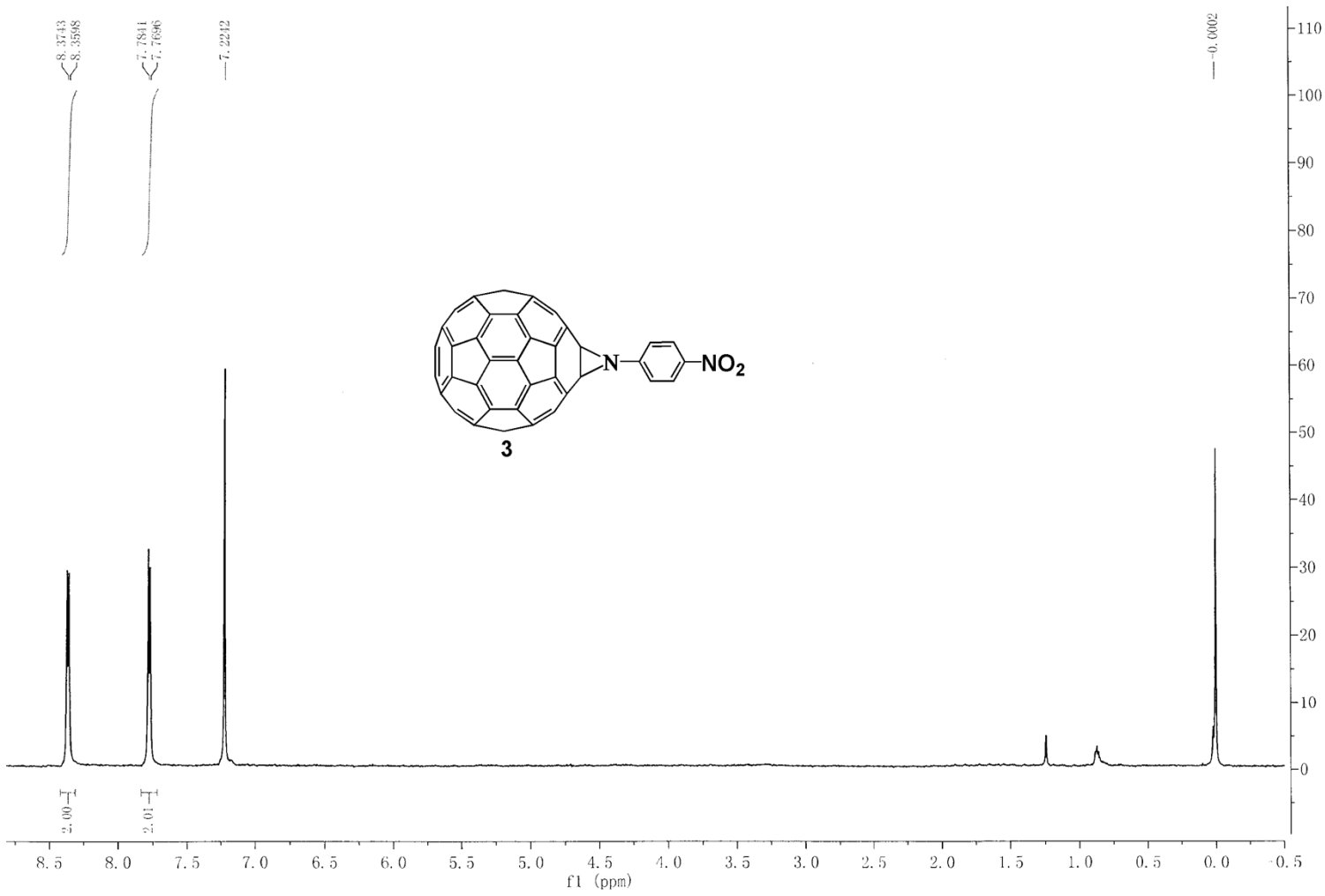
Time                      10.25
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                zgpg30
TD                        32768
SOLVENT                   CDCl3
NS                        10000
DS                            4
SWH                 29761.904 Hz
FIDRES                0.908261 Hz
AQ                    0.550000 sec
RG                          203
DW                       16.800 usec
DE                        6.50 usec
TE                       303.1 K
D1                    3.00000000 sec
D11                   0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                         9.70 usec
PL1                        0.50 dB
PL1W                68.05722198 W
SFO1               125.7703643 MHz

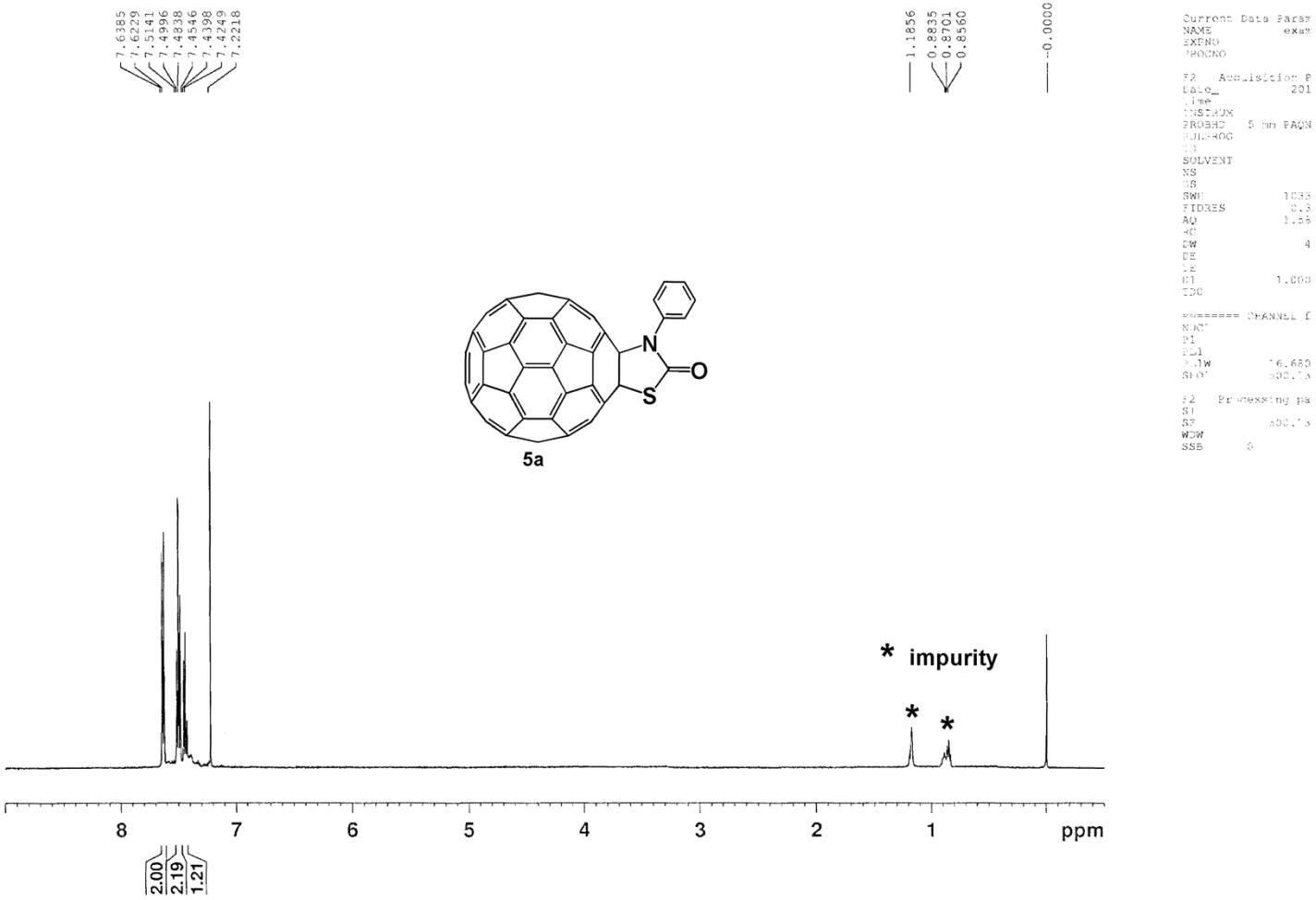
======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     80.00 usec
PL2                        1.00 dB
PL12                      17.08 dB
PL13                      15.60 dB
PL2W                16.68339422 W
PL12W                0.47134506 W
PL13W                0.57857063 W
SFO2               500.1320005 MHz

F2 - Processing parameters
SI                        65536
SF                 125.7570391 MHz
WDW                          EM
SSB                       0
LB                         1.00 Hz
GB                        0
PC                         1.40
```

^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 3



^{1}H NMR (500 MHz, CS_2/$CDCl_3$) of compound 5a



Current Data Param
NAME exam
EXPNO
PROCNO

F2 - Acquisition P
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Time
INSTRUM
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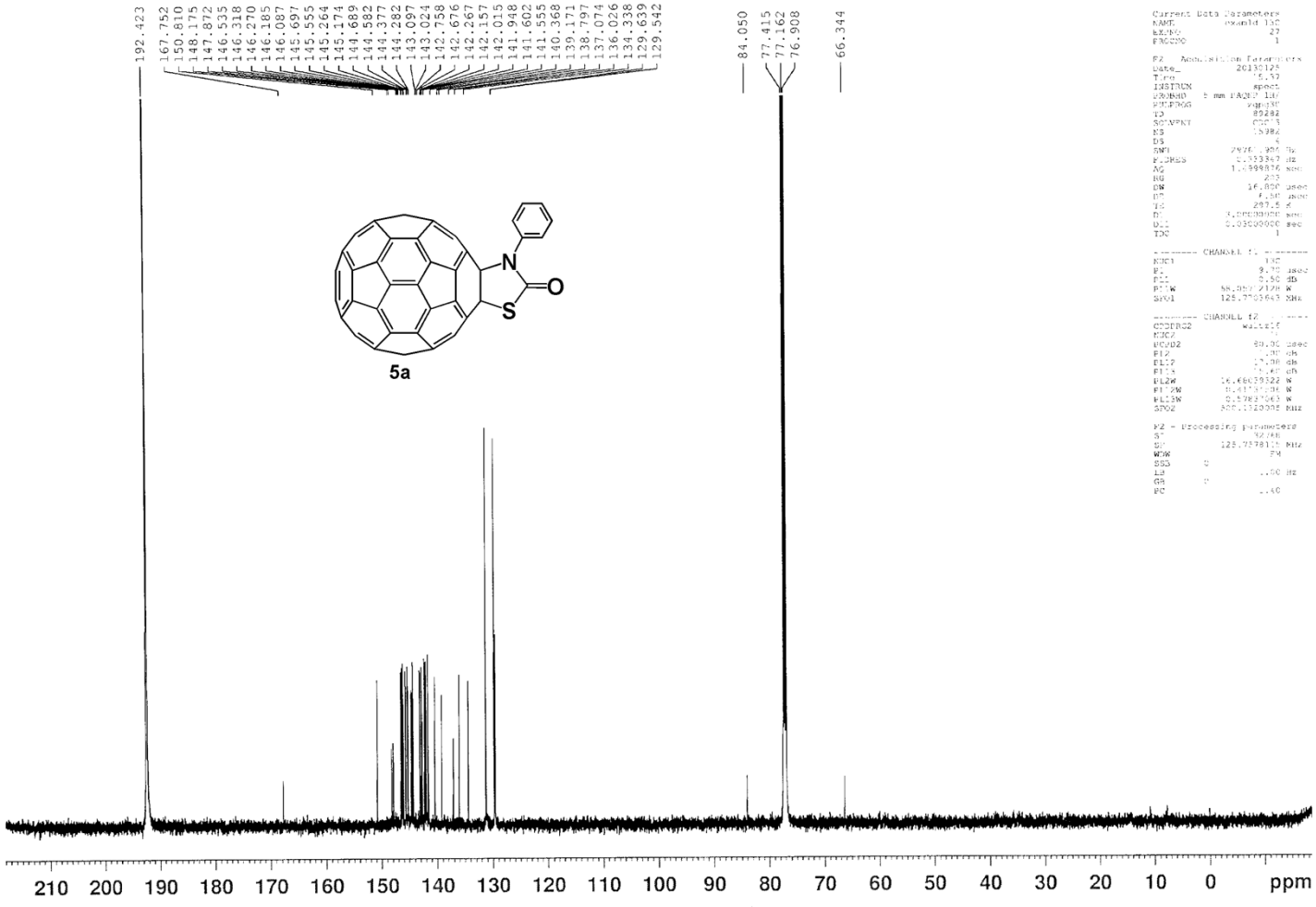
PULPROG
TD
SOLVENT
NS
DS
SWH 1035
FIDRES 0.3
AQ 1.56
RG
DW 4
DE
TE
D1 1.000
TD0

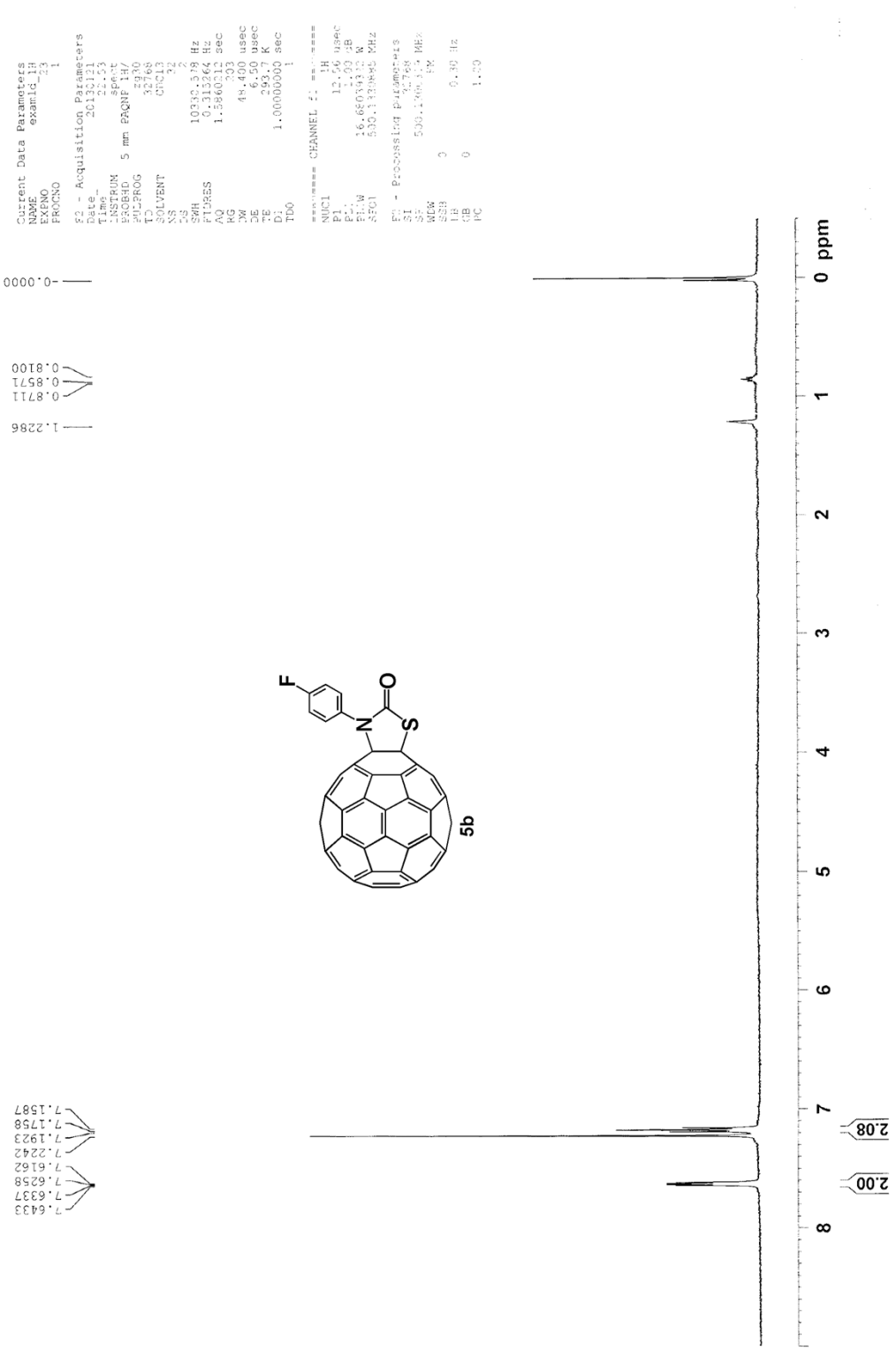
======== CHANNEL f
NUC1
P1
PL1
PL1W 16.680
SFO1 500.13

F2 - Processing pa
SI
SF 500.13
WDW
SSB 0

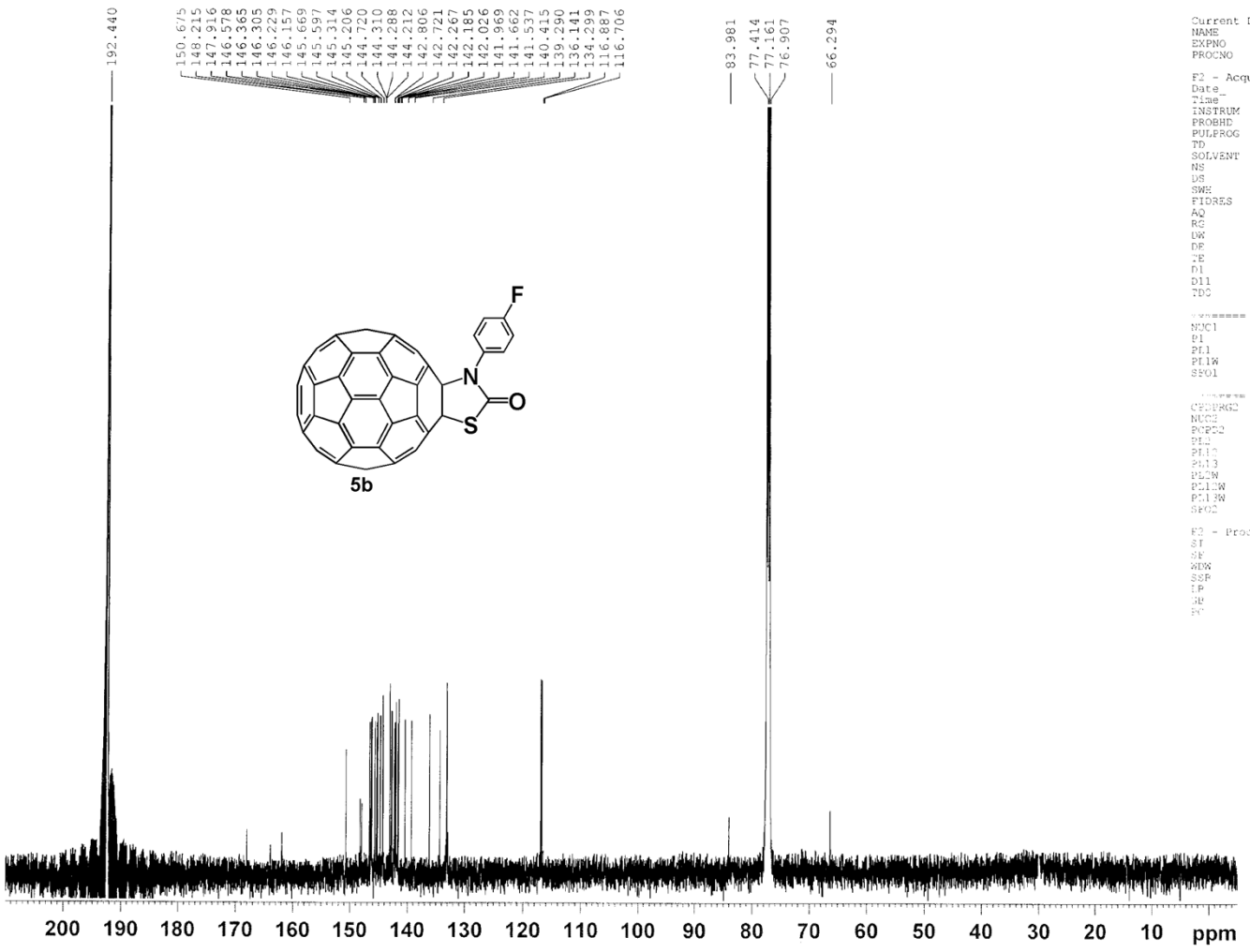
^{13}C NMR (125 MHz, CS_2/$CDCl_3$) of compound 5a



^{1}H NMR (500 MHz, CS_2/$CDCl_3$) of compound 5b



^{13}C NMR (125 MHz, CS_2/$CDCl_3$) of compound 5b

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EXPNO                       24
PROCNO                       1

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Time                   19.26
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PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                     20000
DS                         4
SWH                29761.904 Hz
FIDRES             0.908261 Hz
AQ                 0.5505524 sec
RG                       203
DW                    16.800 usec
DE                     6.50 usec
TE                    298.0 K
D1                 3.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 =========
NUC1                      13C
P1                       9.70 usec
PL1                      0.50 dB
PL1W               68.05712128 W
SFO1               125.7703643 MHz

======== CHANNEL f2 =========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                   80.00 usec
PL2                      1.00 dB
PL12                    17.08 dB
PL13                    19.60 dB
PL2W               16.68079185 W
PL12W               2.81134526 W
PL13W               1.78837063 W
SFO2               500.1330005 MHz

F2 - Processing parameters
SI                       32768
SF                 125.7577089 MHz
WDW                         EM
SSB                  0
LB                       1.00 Hz
GB                   0
PC                       1.40
```
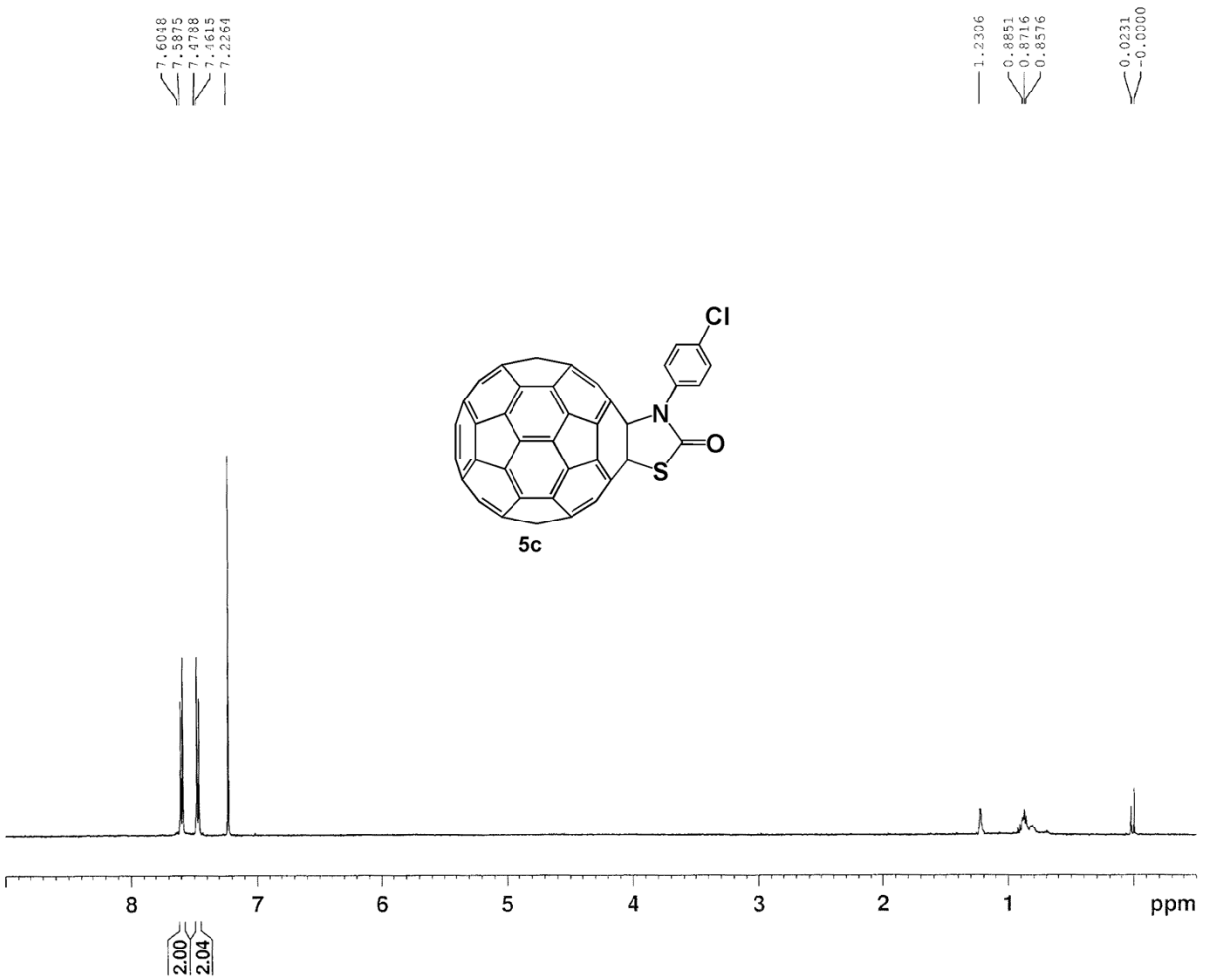

^{1}H NMR (500 MHz, CS_2/$CDCl_3$) of compound 5c



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EXPNO 42
PROCNO 1

F2 - Acquisition Parameters
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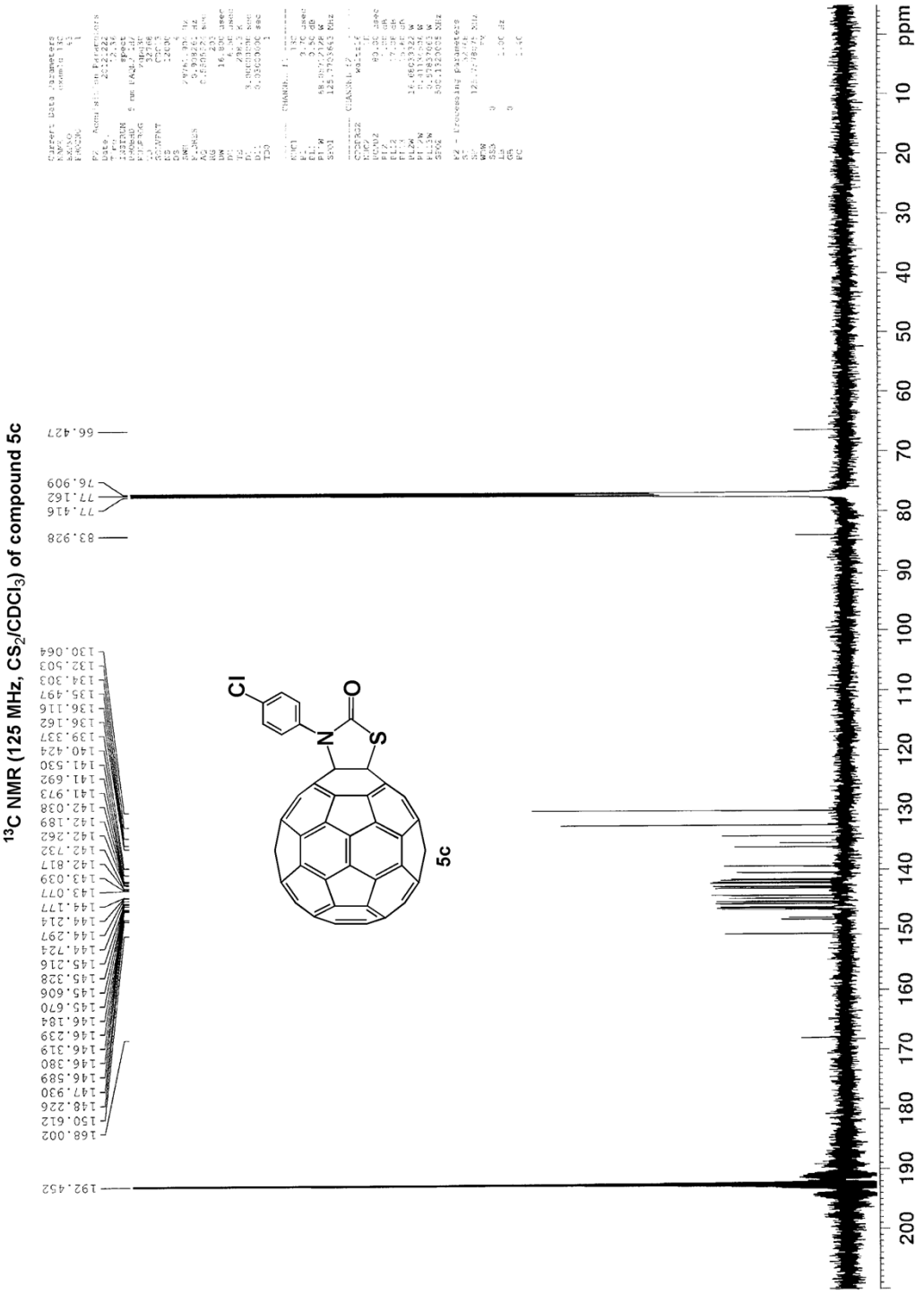
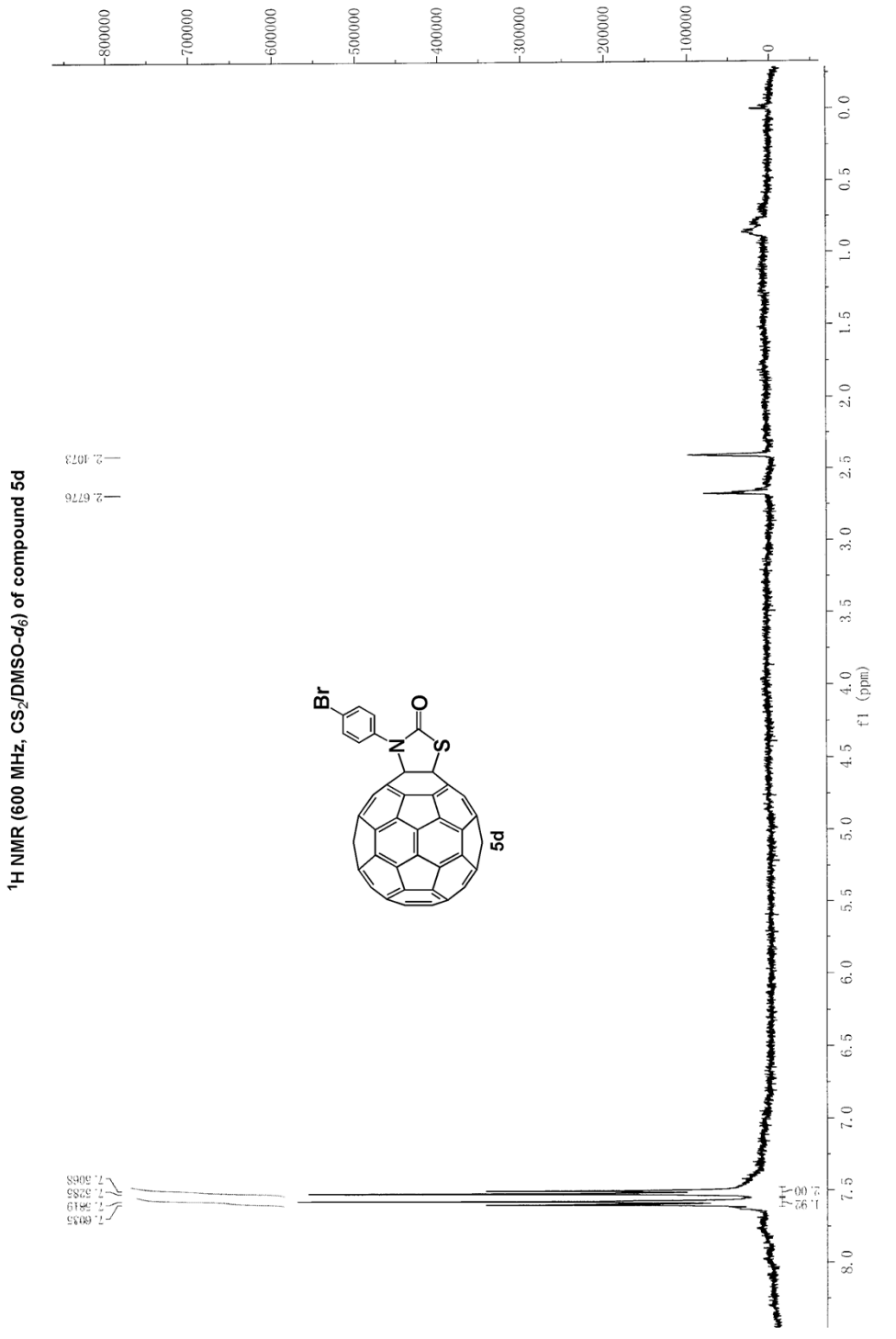
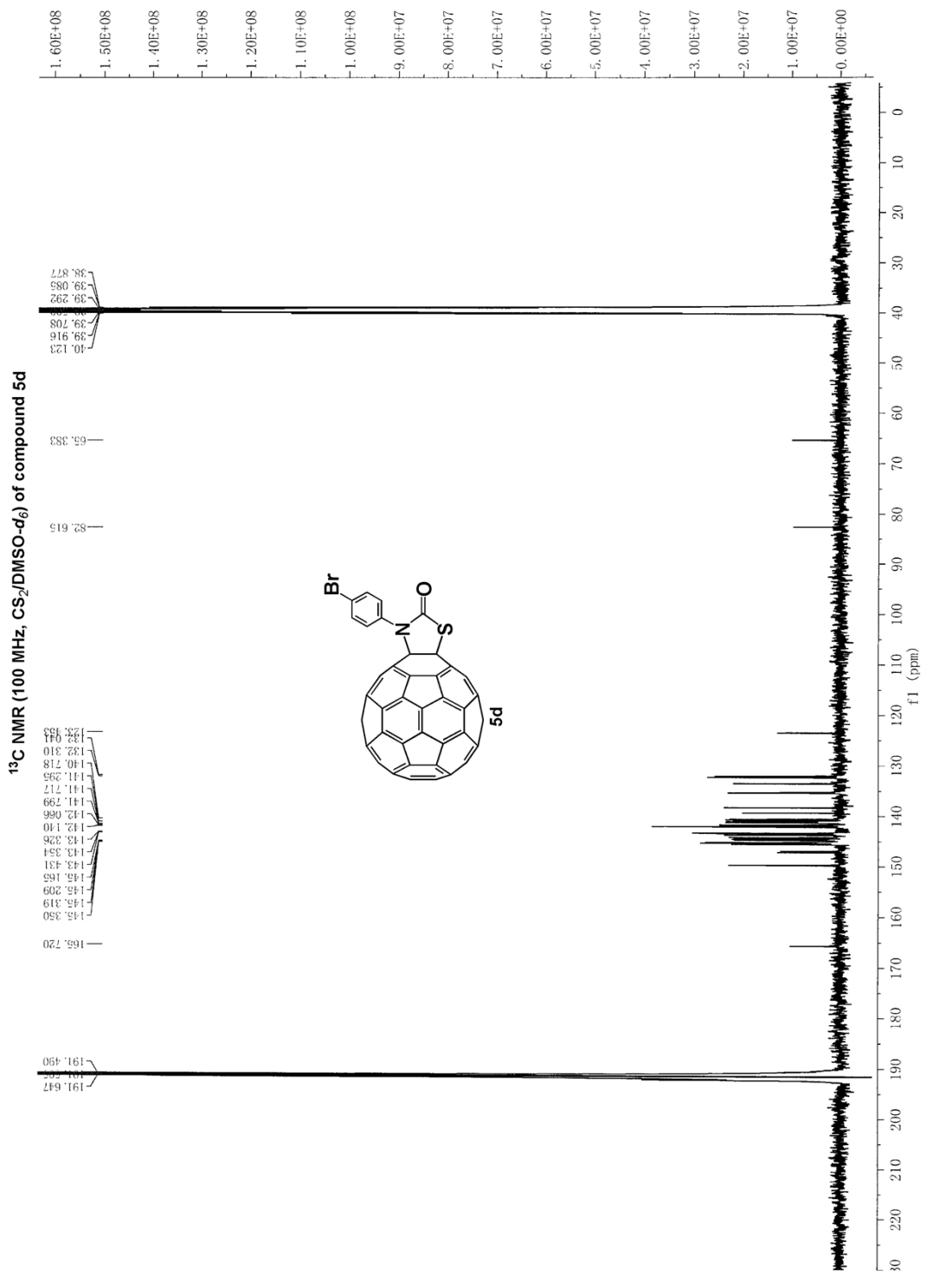
Time 23.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 10330.578 H
FIDRES 0.315264 H
AQ 1.5859212 s
RG 203
DW 48.400 u
DE 6.50 u
TE 293.3 K
D1 1.00000000 s
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.56 u
PL1 1.00 d
PL1W 16.45039322 W
SFO1 500.1330088 M

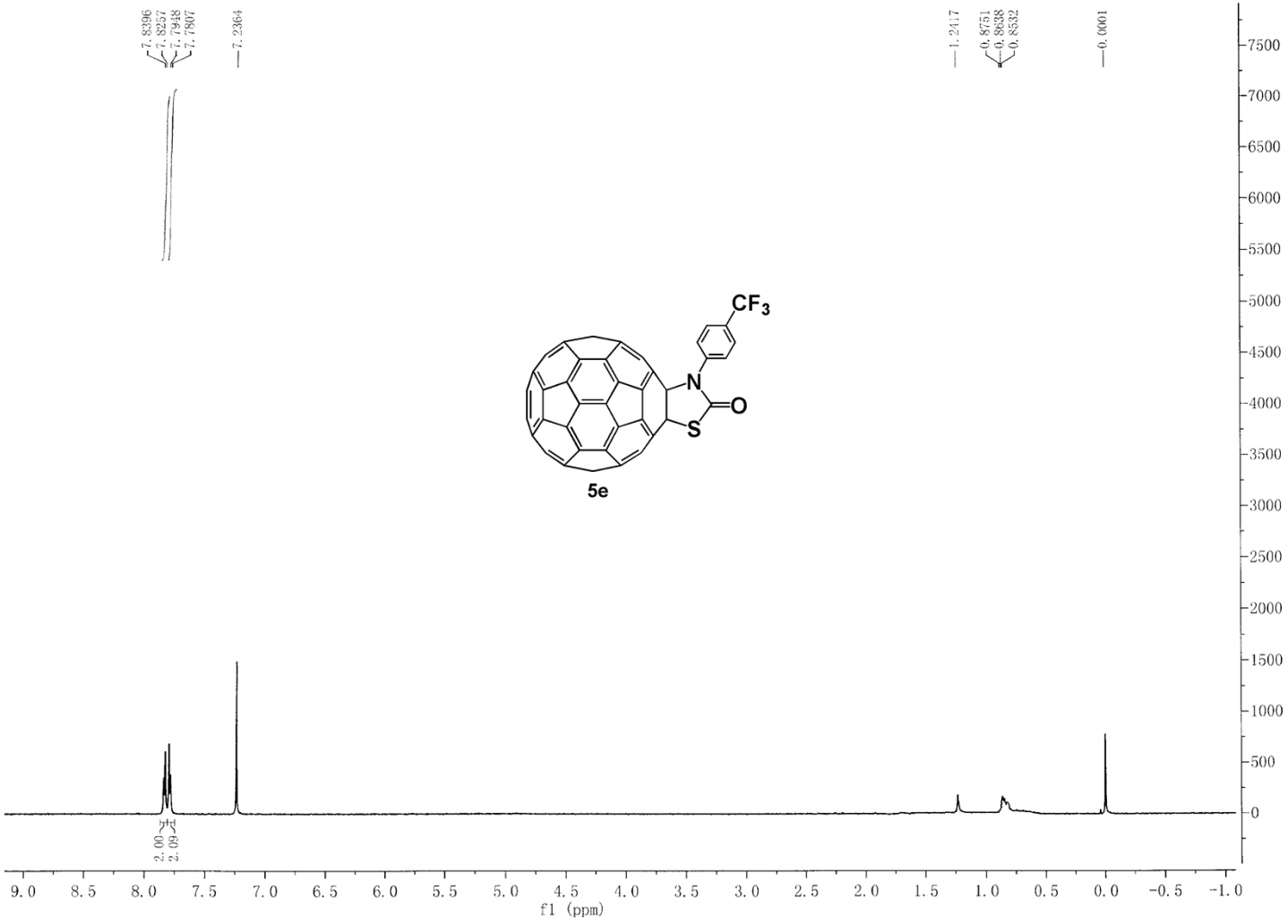
F2 - Processing parameters
SI 32768
SF 500.1300303 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00


13C NMR (125 MHz, CS2/CDCl3) of compound 5c
Cl
N
O
S
5c
ppm

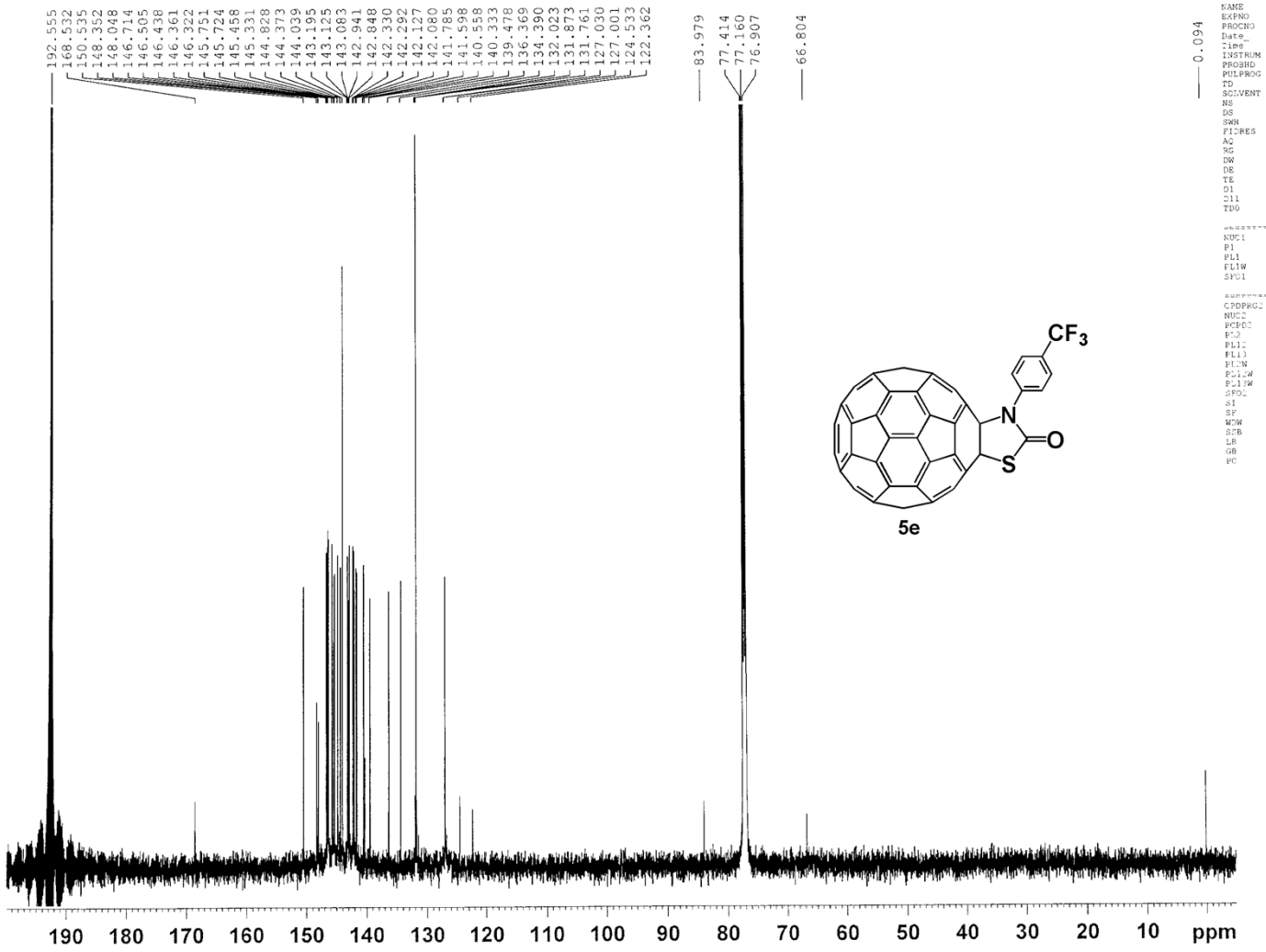

^{1}H NMR (600 MHz, CS_2/DMSO-d_6) of compound 5d
Br
N
O
S
5d
f1 (ppm)


13C NMR (100 MHz, CS2/DMSO-d6) of compound 5d
Br
O
N
S
5d
f1 (ppm)

^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 5e



^{13}C NMR (125 MHz, CS_2/$CDCl_3$) of compound 5e



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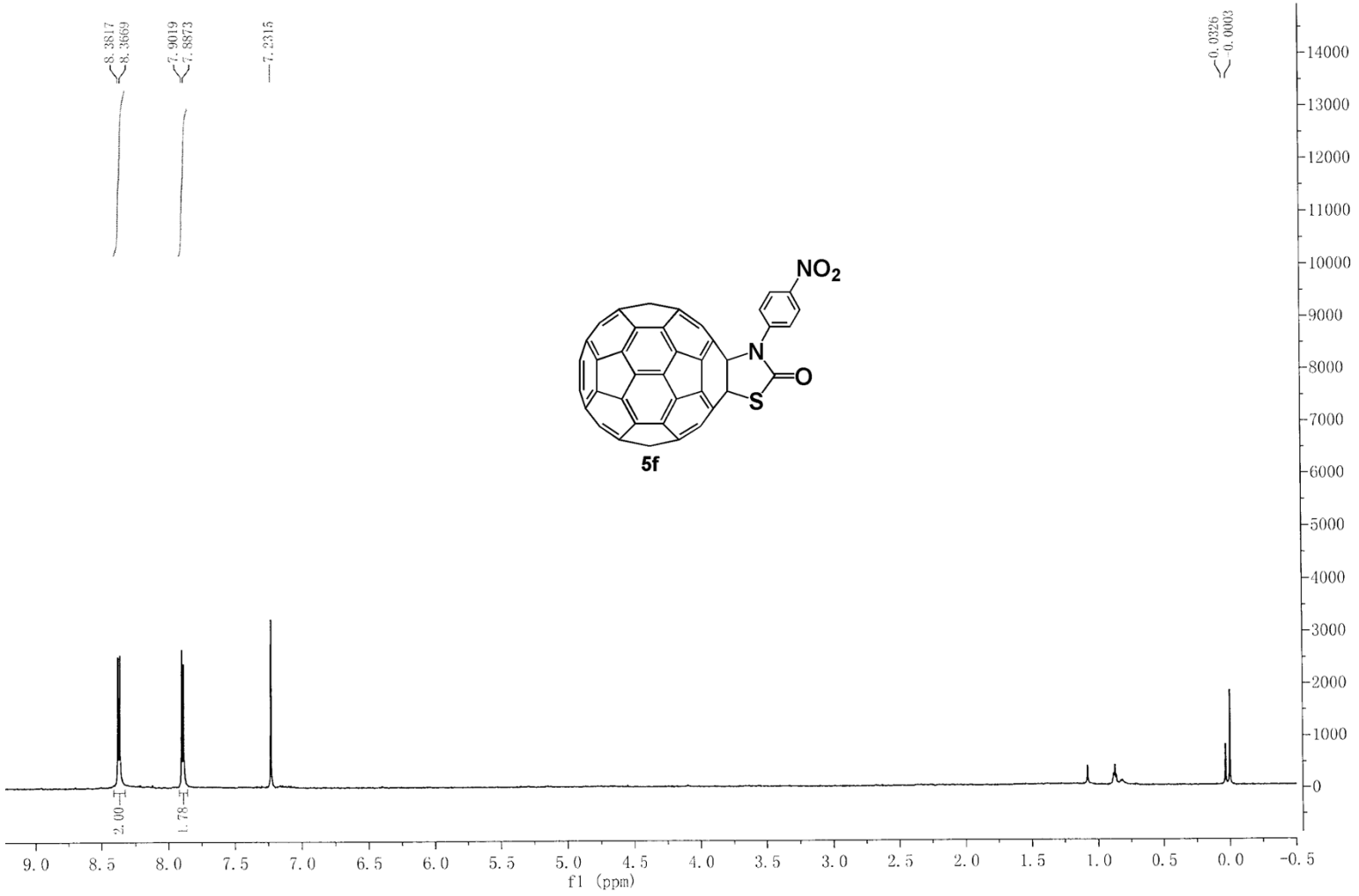
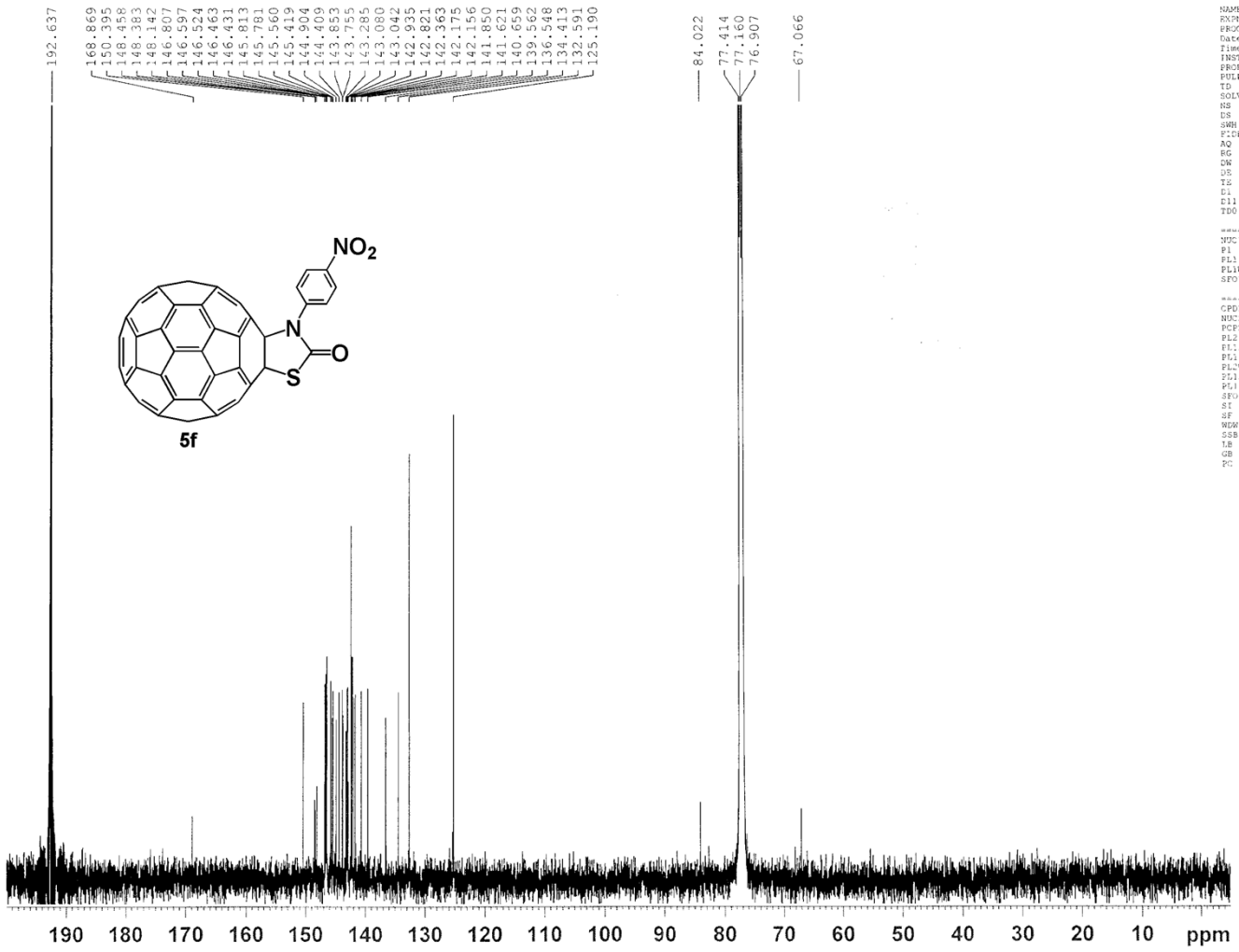
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	36000
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	0.5505524 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	299.6 K
D1	2.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	0.50 dB
PL1W	68.05712128 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	17.08 dB
PL13	15.60 dB
PL2W	16.68039322 W
PL12W	0.41134506 W
PL13W	0.57837063 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578055 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 5f



^{13}C NMR (125 MHz, CS_2/$CDCl_3$) of compound 5f

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EXPNO                     19
PROCNO                     1
Date_               20131101
Time                    6.02
INSTRUM                spect
PROBHD   5 mm PAQNP 1H/
PULPROG                zgpg30
TD                      32768
SOLVENT                 CDCl3
NS                      16000
DS                          4
SWH                 29761.904 Hz
FIDRES              0.908261 Hz
AQ                  0.5505524 sec
RG                        203
DW                   16.800 usec
DE                    6.50 usec
TE                   300.9 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.70 usec
PL1                      0.50 dB
PL1W                68.05712128 W
SFO1               125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      1.00 dB
PL12                    17.68 dB
PL13                    19.60 dB
PL2W                19.48919322 W
PL12W               0.42134366 W
PL13W               0.27972063 W
SFO2               500.1326005 MHz
SI                       32768
SF                 125.7577964 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40
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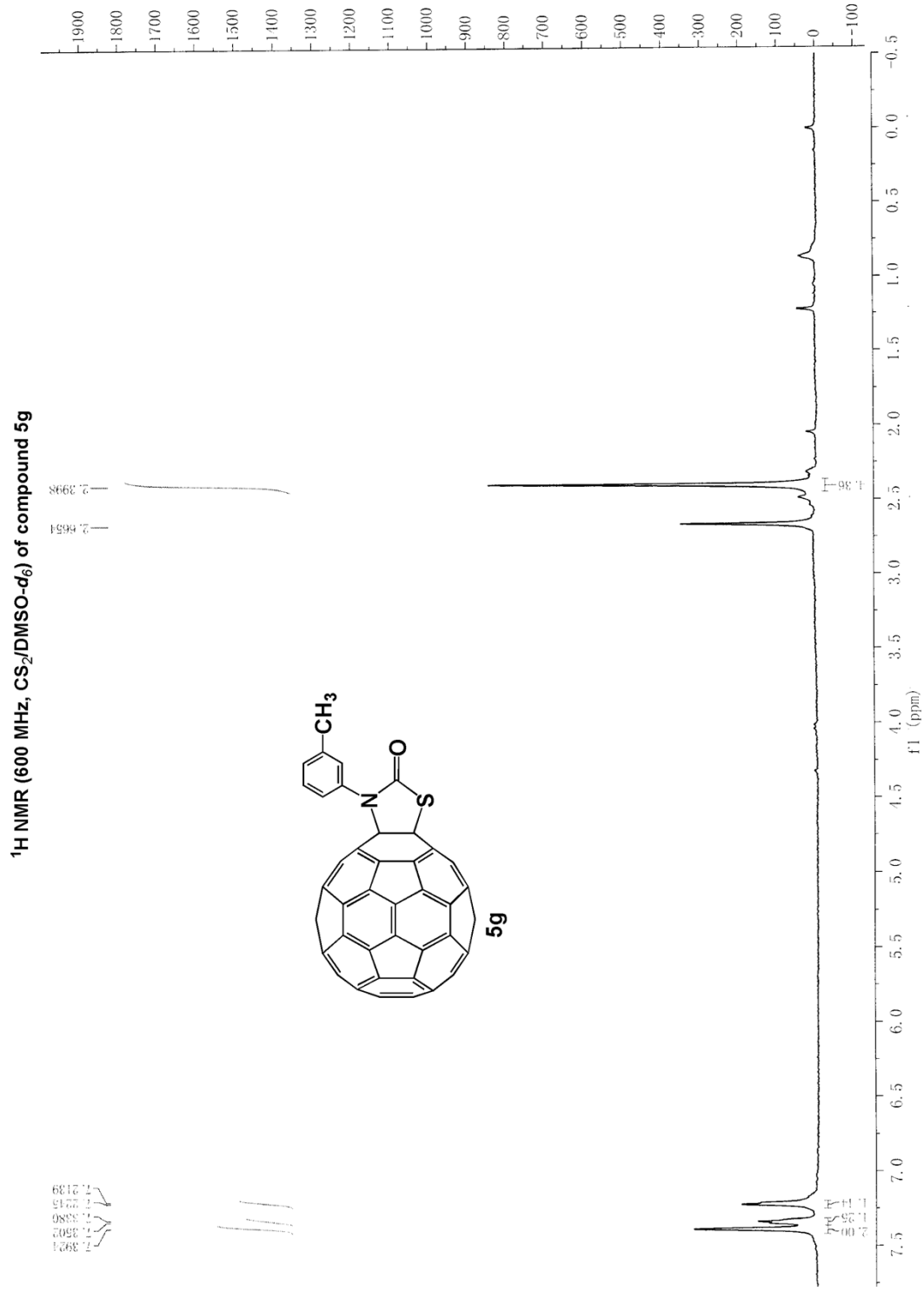
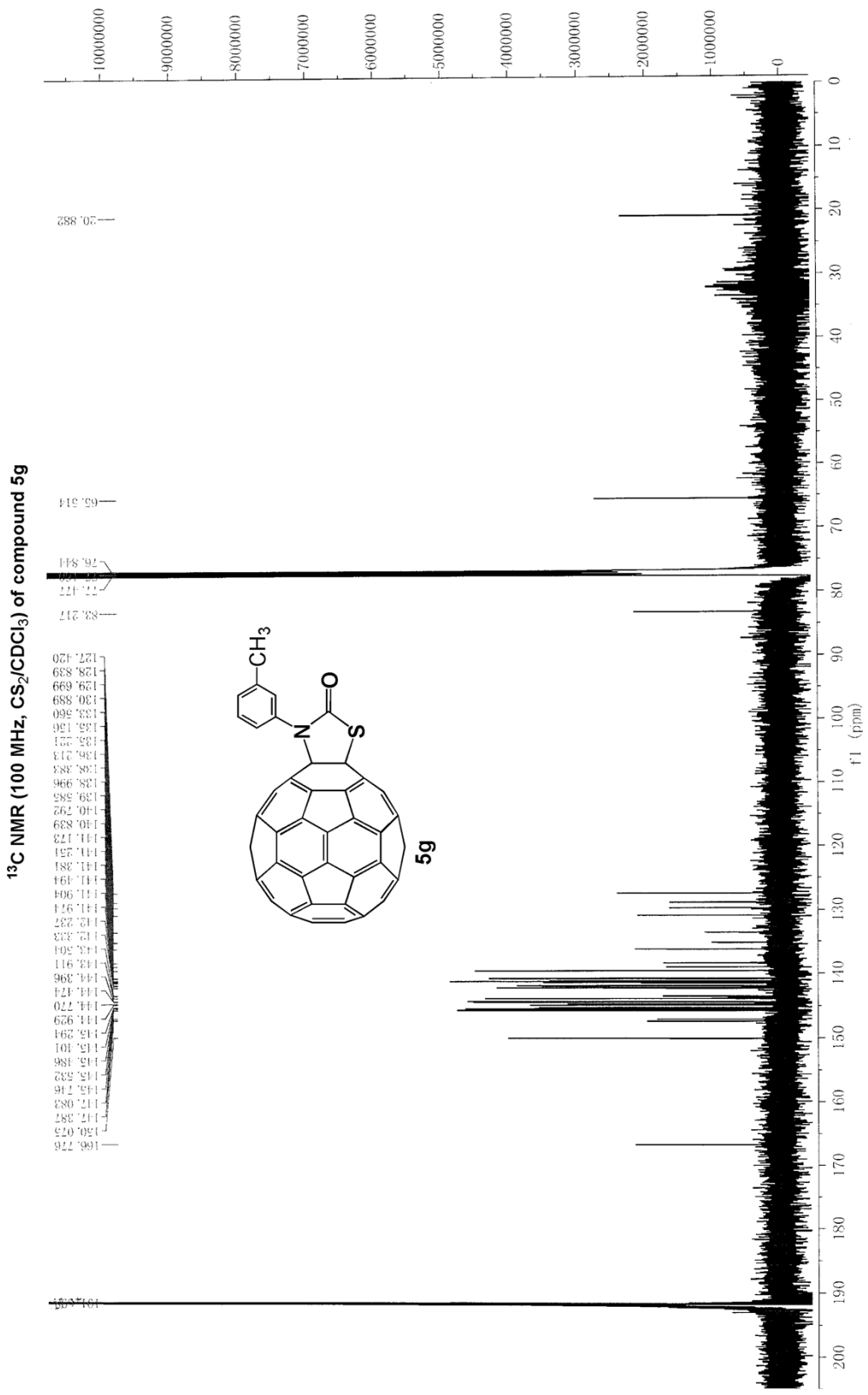
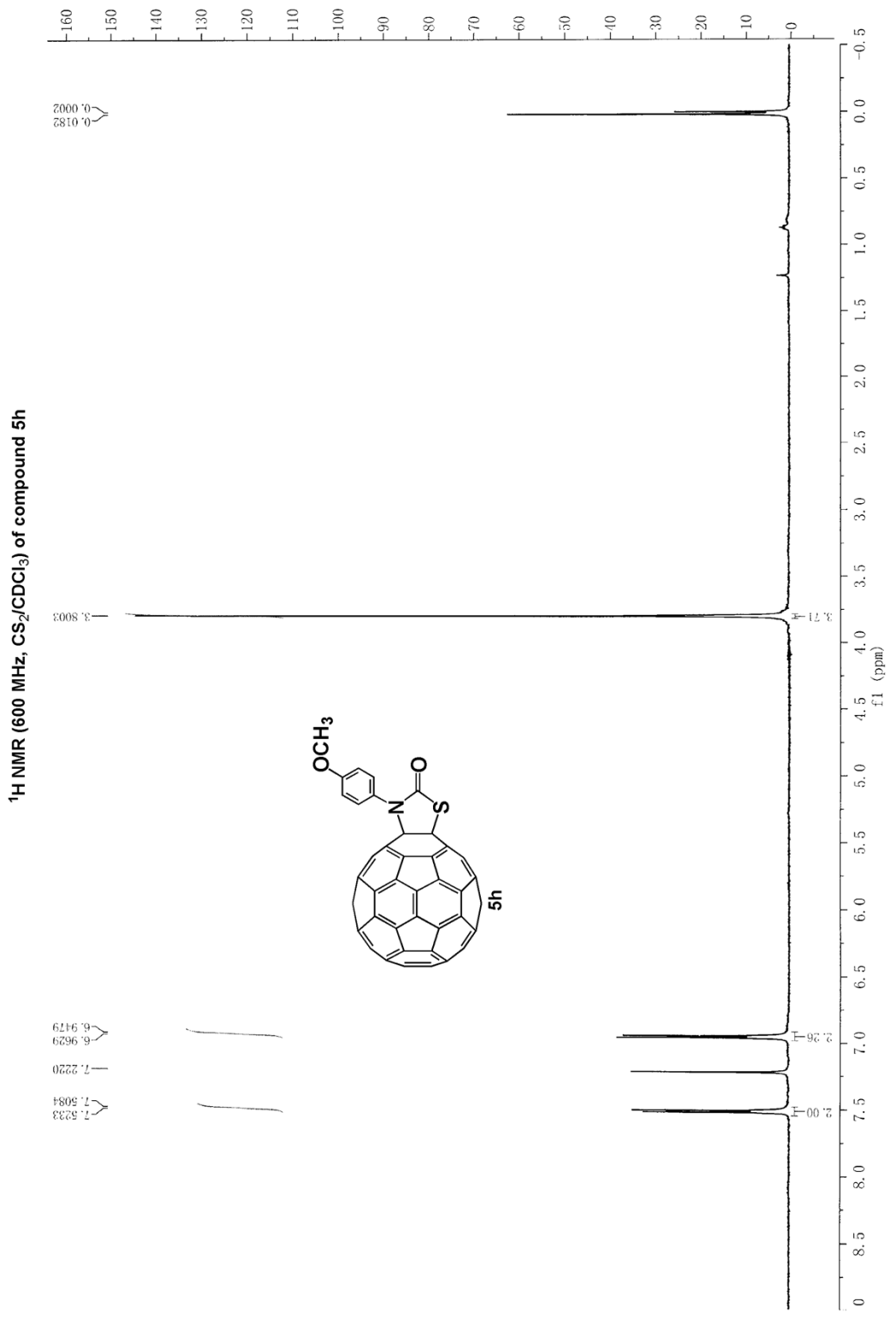
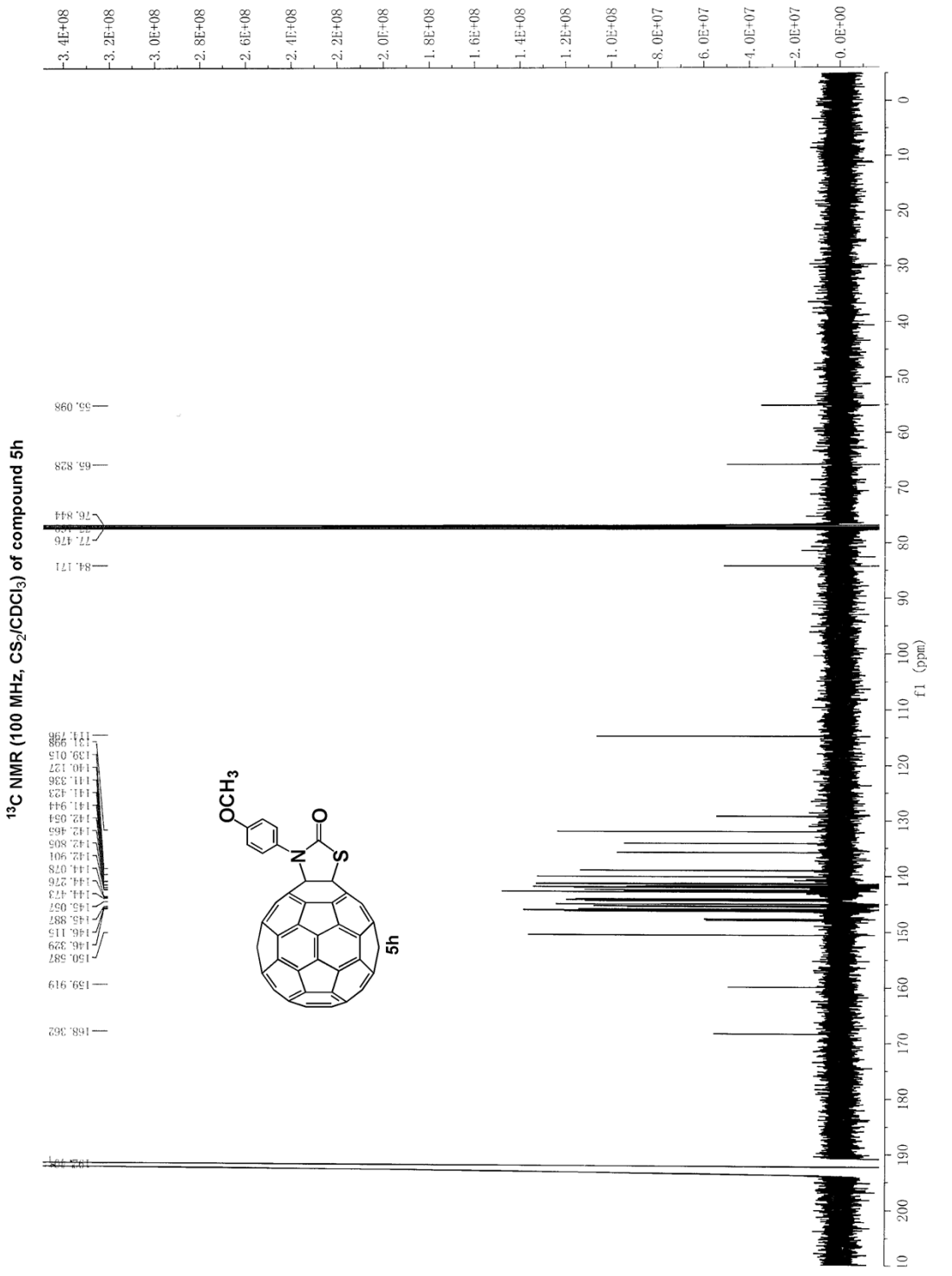

1H NMR (600 MHz, CS2/DMSO-d6) of compound 5g
CH3
N
O
S
5g
f1 (ppm)


^{13}C NMR (100 MHz, CS_2/$CDCl_3$) of compound 5g
CH_3
N
O
S
5g
f1 (ppm)


^{1}H NMR (600 MHz, CS_2/$CDCl_3$) of compound 5h
OCH3
N
O
S
5h
f1 (ppm)


^{13}C NMR (100 MHz, CS_2/$CDCl_3$) of compound 5h
OCH_3
N
O
S
5h
f1 (ppm)