

## Synthesis, Conformation and Antiproliferative Activity of Isothiazoloisoxazole 1,1-dioxides

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ELECTRONIC SUPPLEMENTARY INFORMATION FILE 2:

<sup>1</sup>H and <sup>13</sup>C spectra for compounds **21**, **22b**, **22c**, **22f – 22t**, **23a/b** and **24**





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Current Data Parameters  
NAME sn15605ap  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080924  
Time 17.30  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.171923 sec  
RG 812  
DW 48.400 usec  
DE 6.00 usec  
TE 296.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.70 usec  
PL1 0.10 dB  
SFO1 500.1330885 MHz

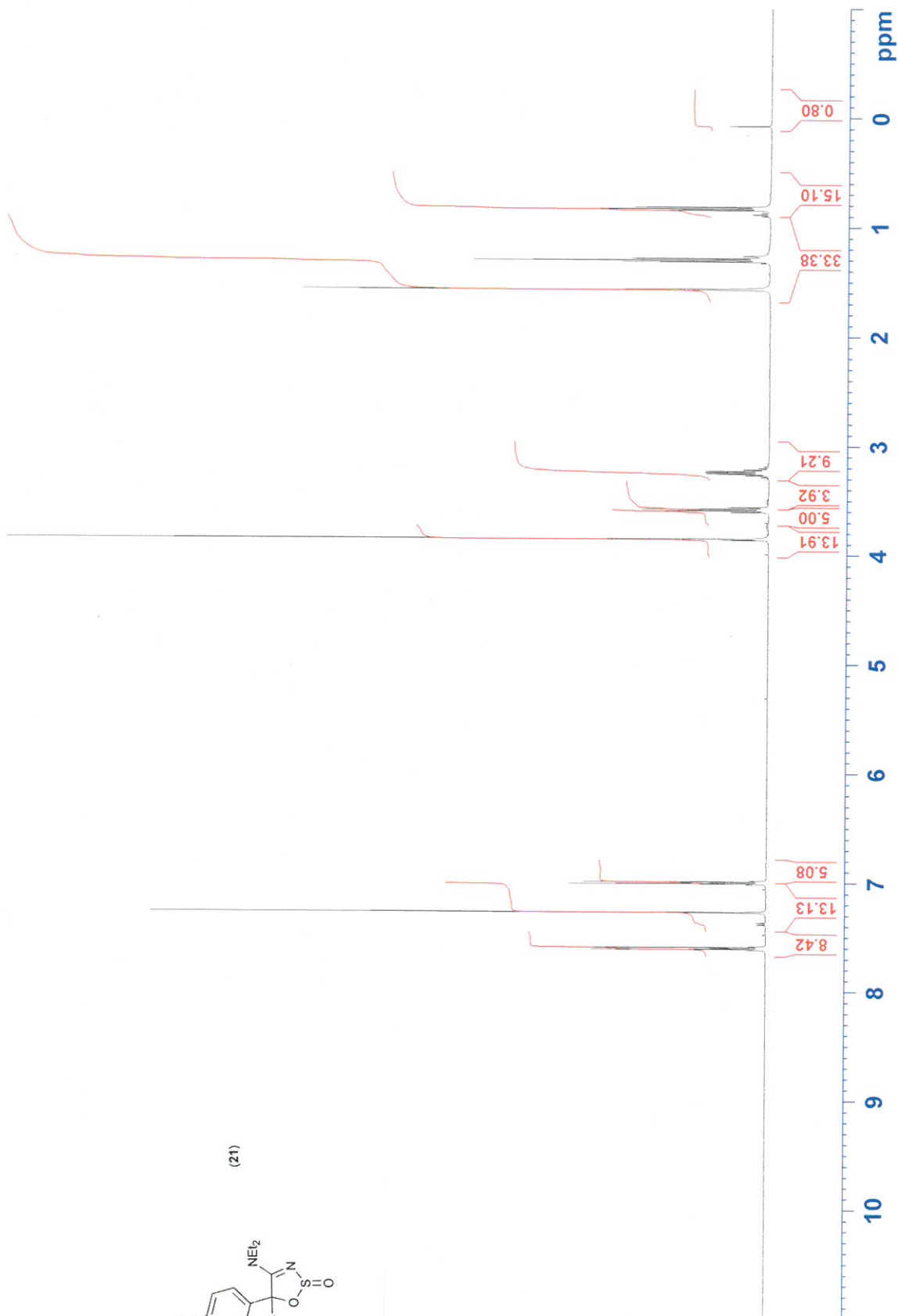
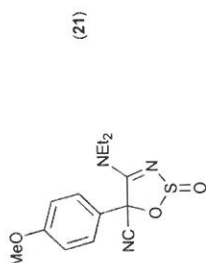
F2 - Processing parameters  
SI 32768  
SF 500.1300085 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.5663  
1.3124  
1.2982  
1.2839  
0.8435  
0.8294  
0.8153  
0.0776

3.8615  
3.8510  
3.6060  
3.5918  
3.5775  
3.5633  
3.2996  
3.2856  
3.2706  
3.2561  
3.2462  
3.2420  
3.2321  
3.2284  
3.2178  
3.2029  
3.1891  
3.1749

5.3097

7.6086  
7.5909  
7.3861  
7.3684  
7.2703  
7.0074  
6.9896





# <sup>13</sup>C H-decoupled

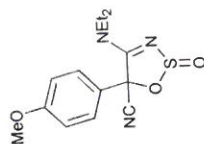
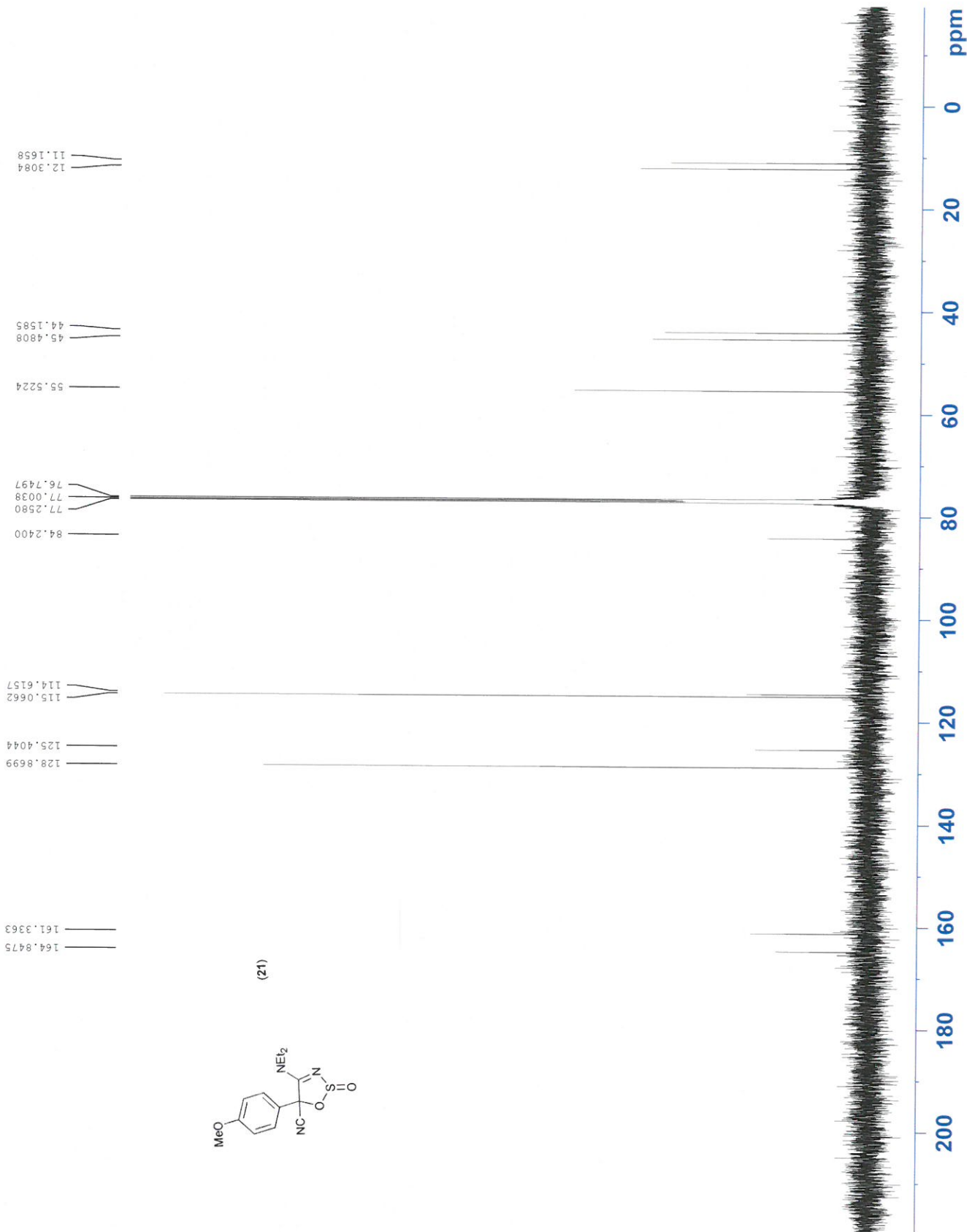
Current Data Parameters  
 NAME sn15605ap  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080924  
 Time\_ 17.35  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 4096  
 DS 4  
 SWH 30030.023 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912244 sec  
 RG 16400  
 DW 16.650 usec  
 DE 6.00 usec  
 TE 297.8 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 128

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 9.00 usec  
 PL1 0.00 dB  
 SFO1 125.7703637 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577876 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







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Current Data Parameters  
NAME AP 223 f.6-19  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20071207  
Time 9.22  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 287.4  
DM 60.400 usec  
DE 6.00 usec  
TE 689.0 K  
D1 1.00000000 sec  
TD0 1

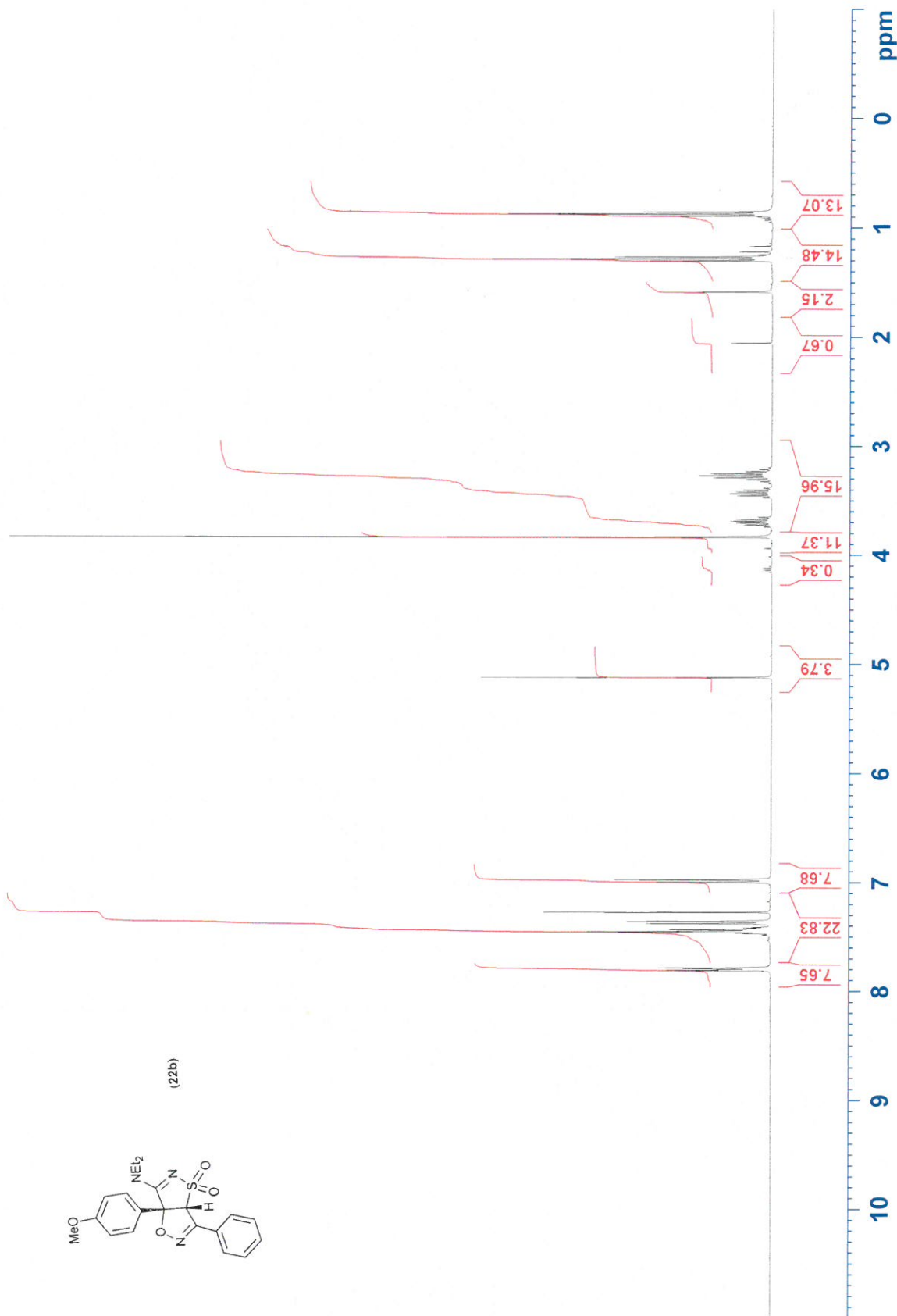
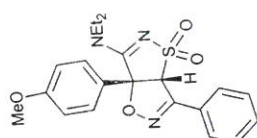
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300050 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1.5877  
1.3035  
1.2858  
1.2679  
0.8930  
0.8754  
0.8577

5.1191  
4.1552  
4.1373  
4.1195  
4.1016  
3.8357  
3.7408  
3.7231  
3.7054  
3.6891  
3.6715  
3.6534  
3.4723  
3.4546  
3.4369  
3.4206  
3.4031  
3.3854  
3.3526  
3.3075  
3.2892  
3.2697  
3.2514  
3.2331  
3.2149  
2.0559

7.8069  
7.8030  
7.7881  
7.7830  
7.74491  
7.7445  
7.74307  
7.73764  
7.73717  
7.73592  
7.73543  
7.72705  
6.9937  
6.9711





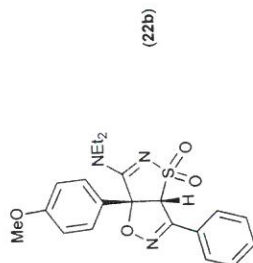
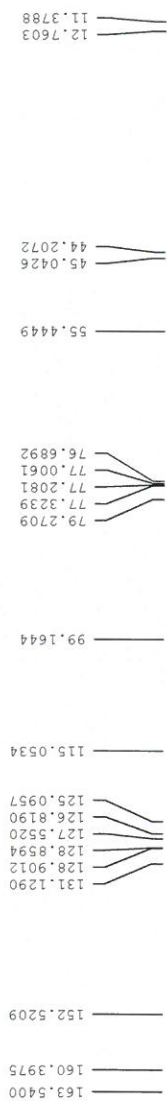
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 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20071207  
 Time\_ 9.25  
 INSTRUM dpz400  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 5160.6  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 689.0 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 8

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.70 usec  
 PL1 -3.00 dB  
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 84.00 usec  
 PL2 -3.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127733 MHz  
 EM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm





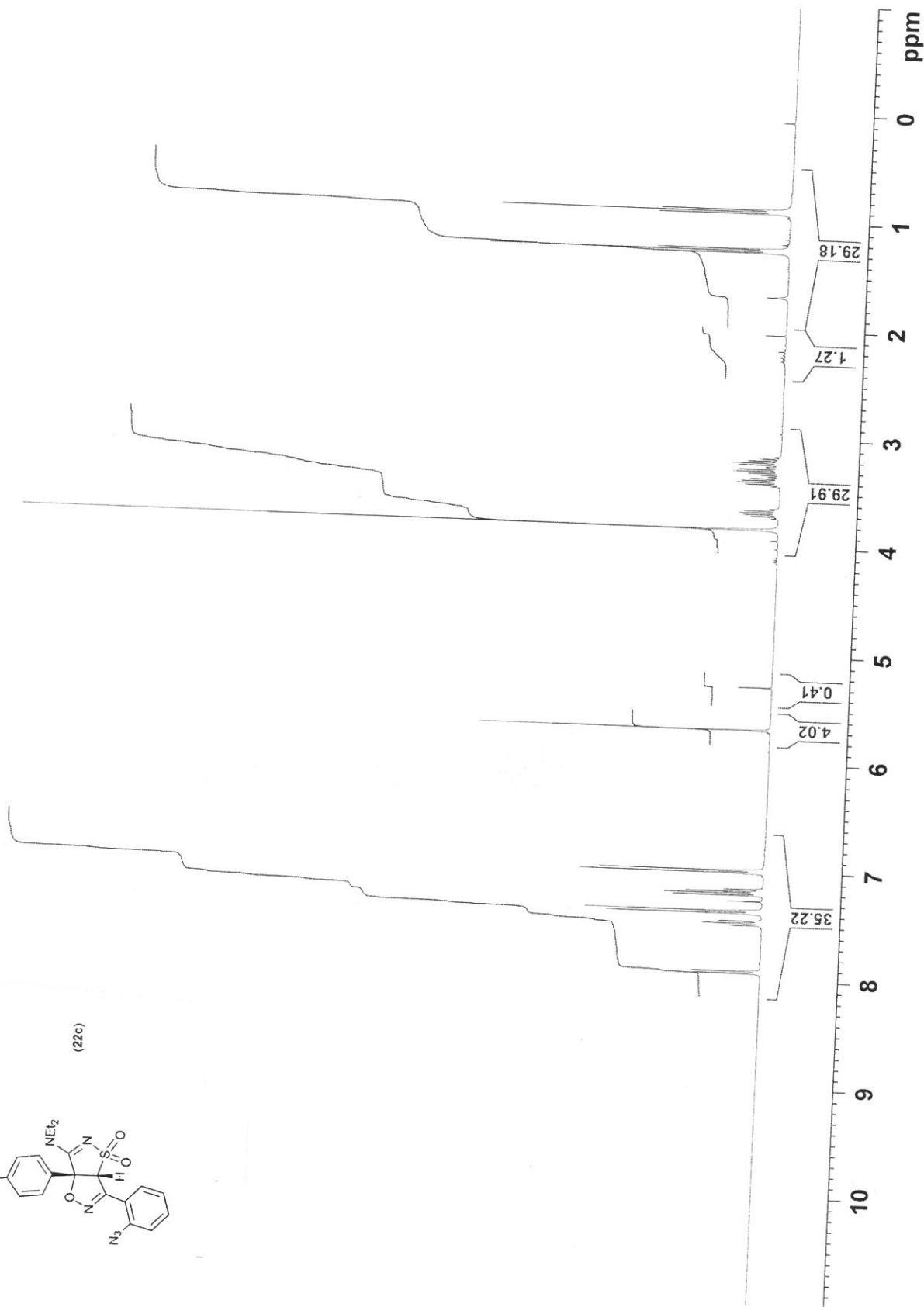
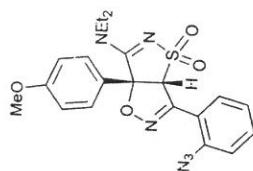
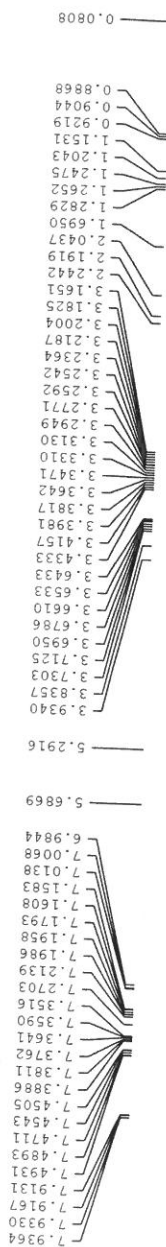
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Current Data Parameters  
NAME AP 182 f.35-48  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071009  
Time 12.06  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 64  
DW 60.400 usec  
DE 6.00 usec  
TE 293.8 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300048 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







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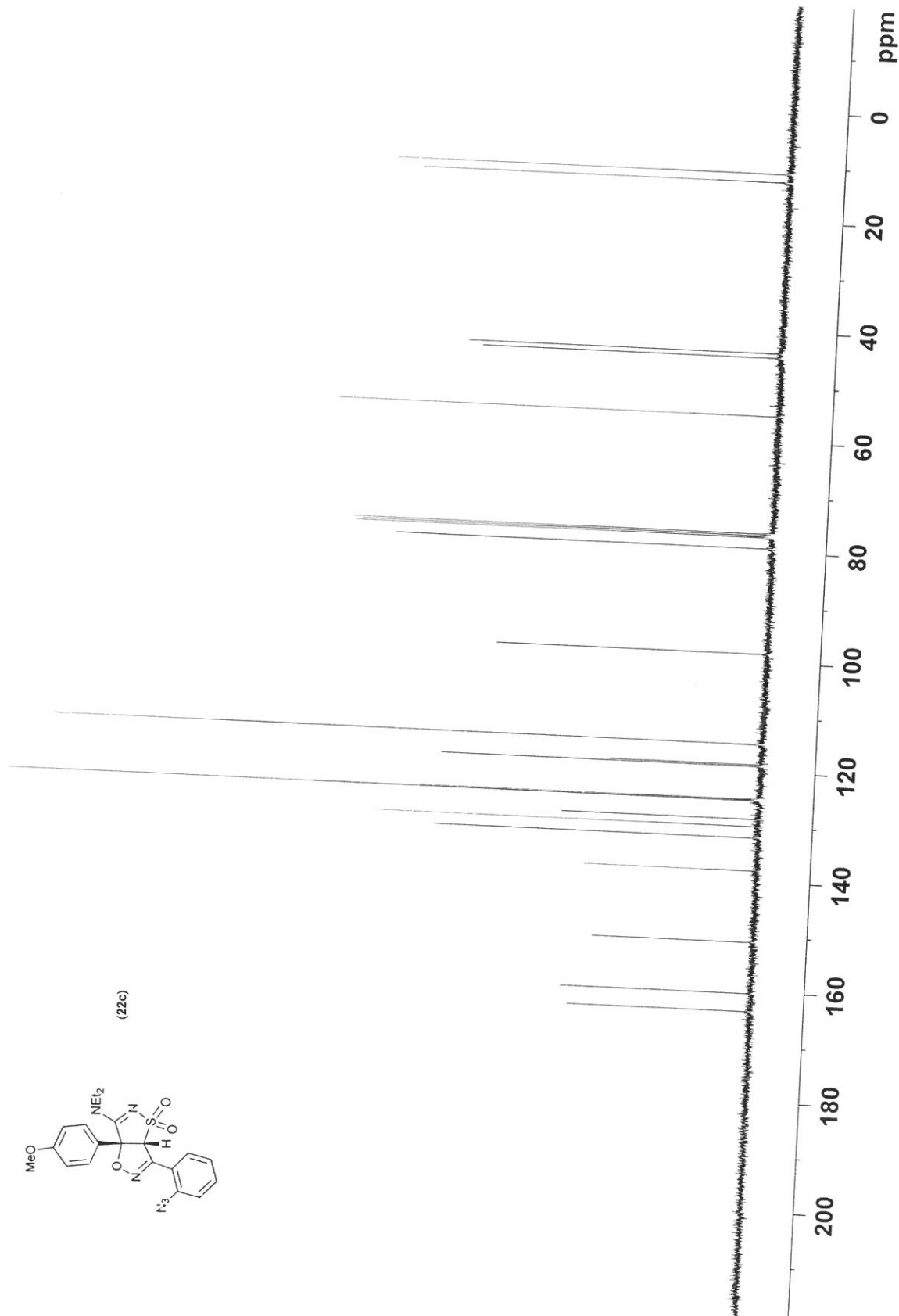
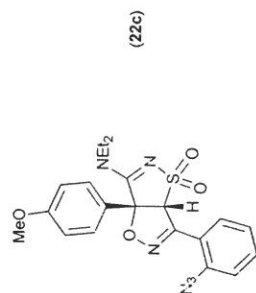
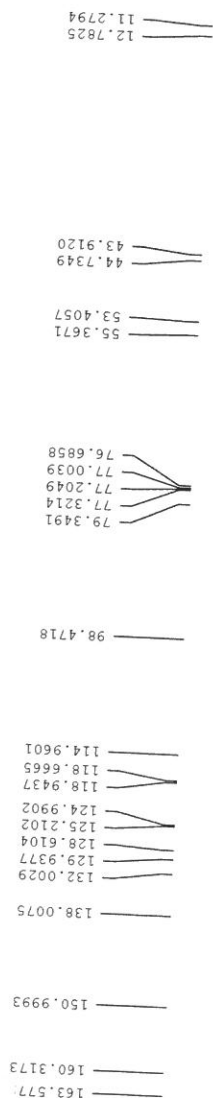
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EXENO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071009  
Time\_ 12.09  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 10321.3  
DW 20.850 usec  
DE 6.00 usec  
TE 294.1 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 8

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -3.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 84.00 usec  
PL2 -3.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127810 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







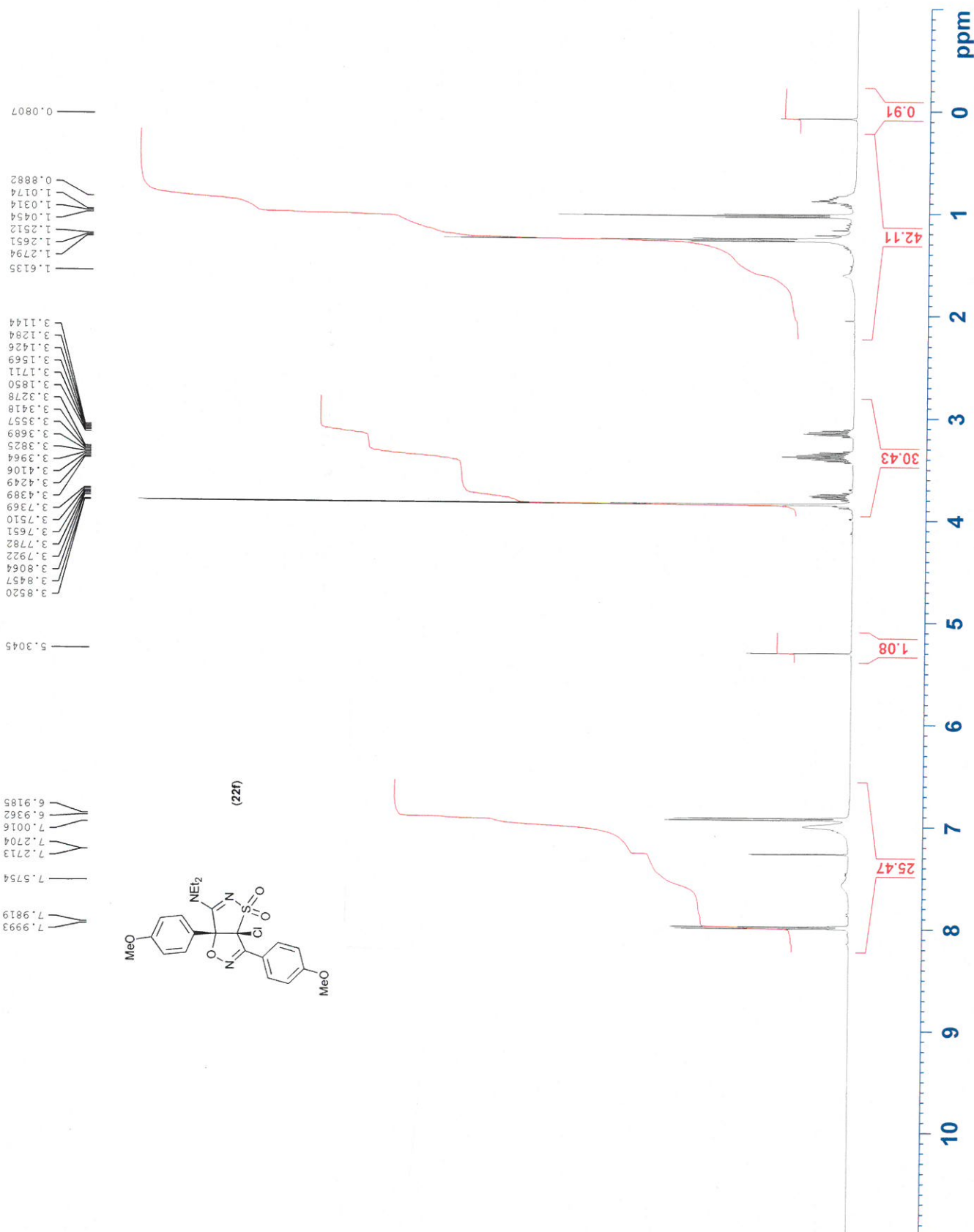
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Current Data Parameters  
NAME sn15479ap  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080313  
Time 12.34  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 144  
DW 48.400 usec  
DE 6.00 usec  
TE 295.4 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.70 usec  
PL1 0.10 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300079 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00







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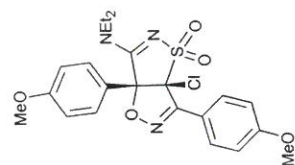
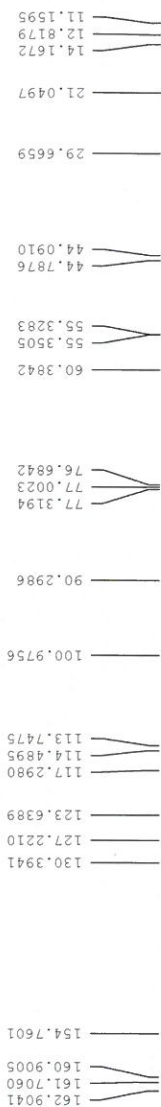
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NAME AP 265 f.14-30  
EXPNO 11  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080306  
Time\_ 15.24  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
DS 256  
NS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 6502  
DW 20.850 usec  
DE 6.00 usec  
TE 687.5 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 8

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -3.00 dB  
SFO1 100.6228298 MHz

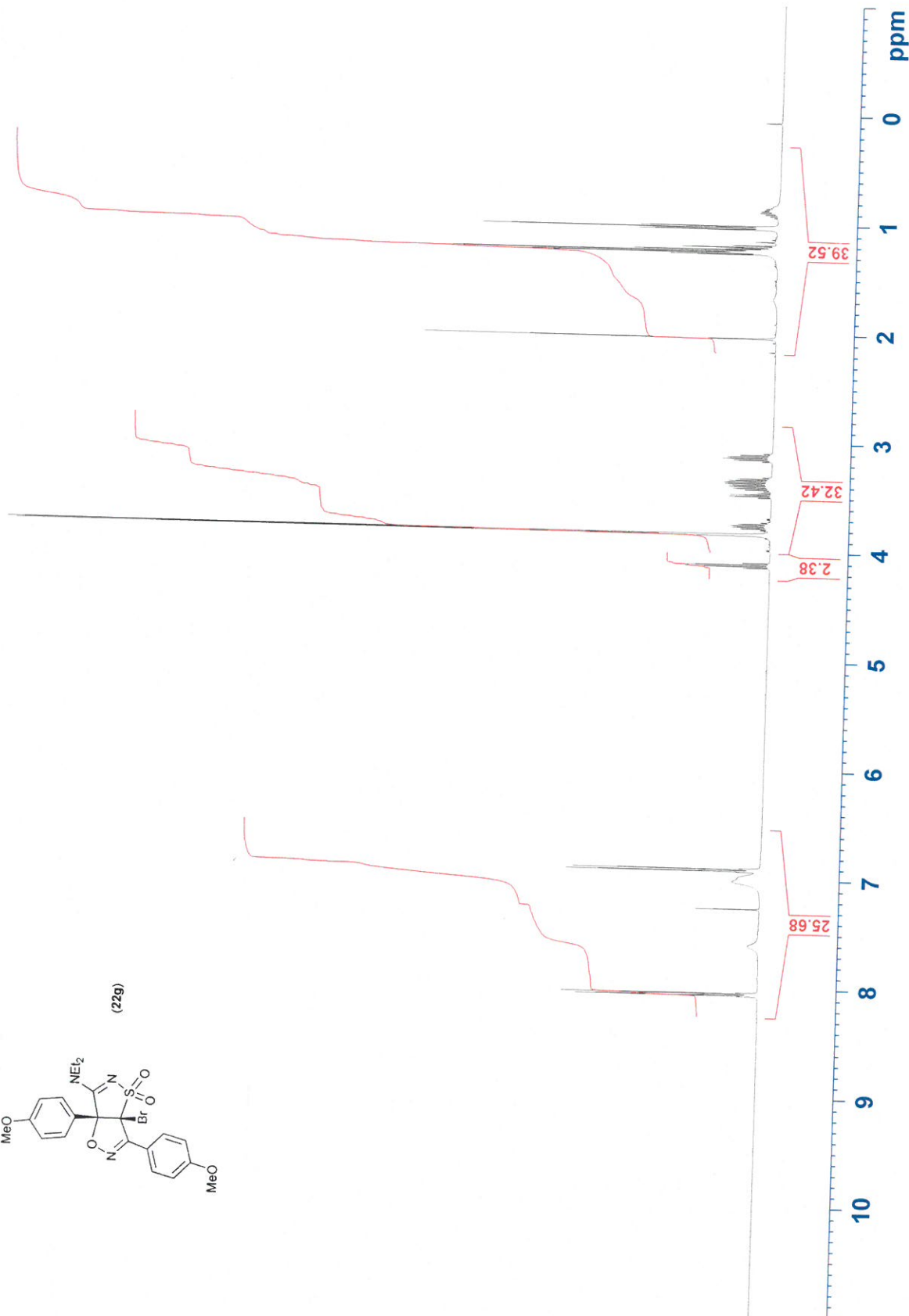
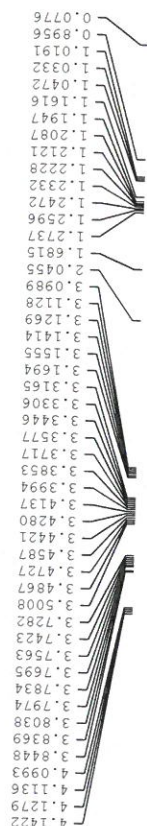
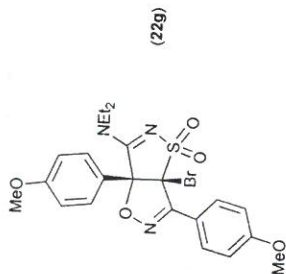
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 84.00 usec  
PL2 -3.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127755 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm





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Current Data Parameters
NAME          sn15449ap
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20080226
Time          9.38
INSTRUM       av500
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           10330.578 Hz
FIDRES        0.157632 Hz
AQ            3.1719923 sec
RG            80.6
DW            48.400 usec
DE            6.00 usec
TE            295.1 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            9.70 usec
PL1           0.10 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
SI            32768
SF            500.1300082 MHz
WDW           EM
SSB           0
GB            0
CB            0.30 Hz
GB            1.00

```





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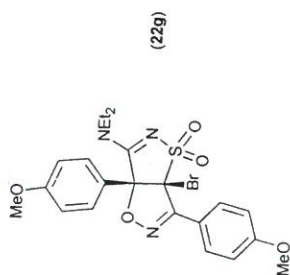
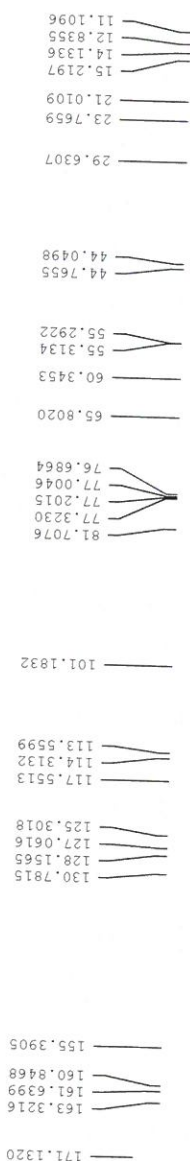
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NAME AP 254 f.8-19  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080222  
Time\_ 11.35  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 16384  
DW 20.850 usec  
DE 6.00 usec  
TE 688.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TD0 8

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -3.00 dB  
SF01 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 84.00 usec  
PL2 -3.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SF02 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127784 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







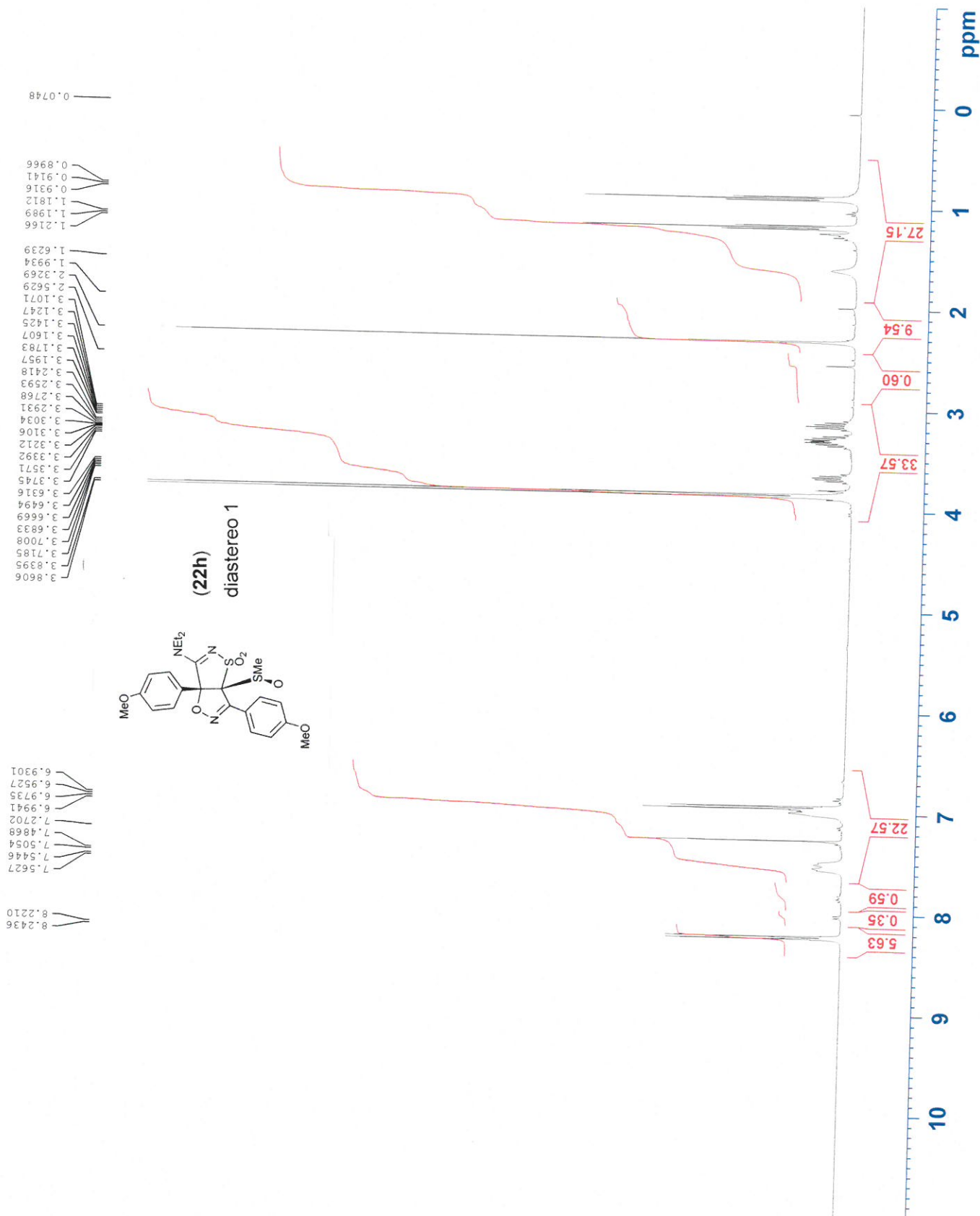
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Current Data Parameters  
NAME AP 272 f.39-53 2  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080812  
Time\_ 11.23  
INSTRUM qpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126214 Hz  
AQ 3.9584243 sec  
RG 287.4  
DW 60.400 usec  
DE 6.00 usec  
TE 293.5 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.130053 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



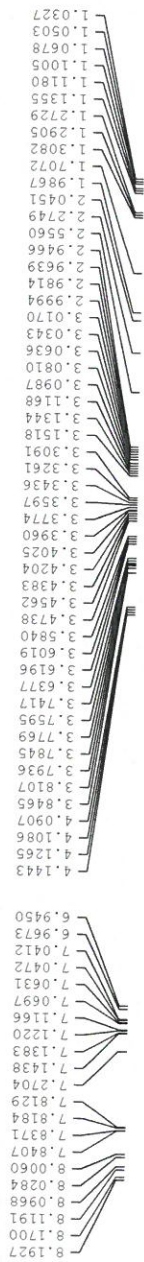
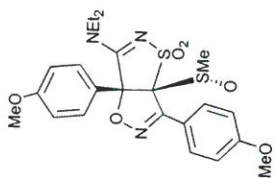




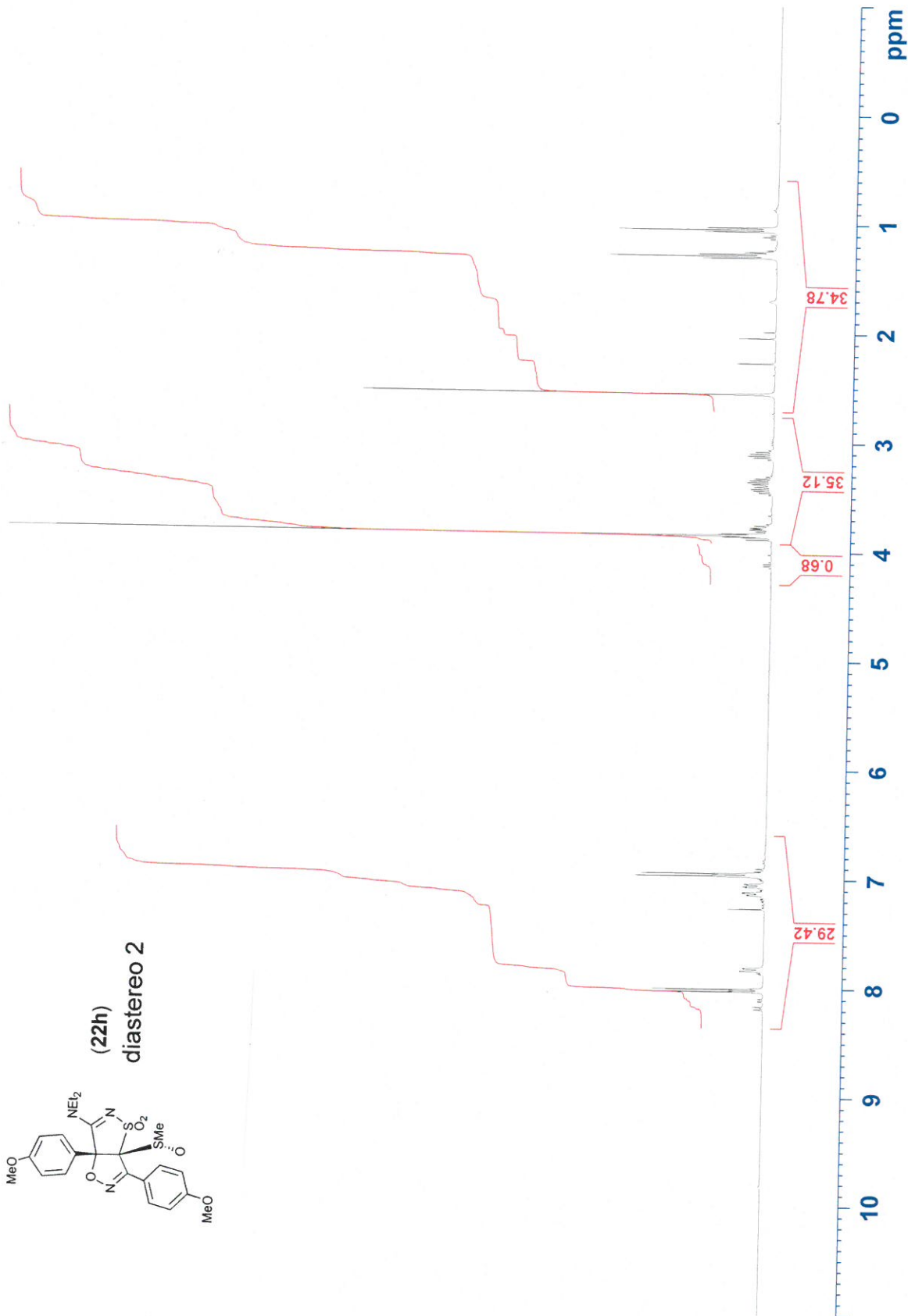




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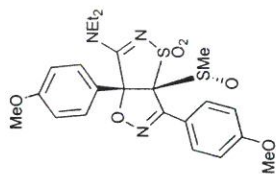


Current Data Parameters  
NAME AP 272 f.19-36  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20080417  
Time 10.08  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 101.6  
DW 60.400 usec  
DE 6.00 usec  
TE 688.7 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz  
F2 - Processing parameters  
SI 32768  
SF 400.1300048 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





# <sup>13</sup>C H-decoupled



(22h)  
diastereo 2



Current Data Parameters  
NAME snl5507ap  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080418  
Time 10.29  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 30030.029 Hz  
FIDRES 0.458222 Hz  
AQ 1.0912244 sec  
RG 16400  
DW 16.650 usec  
DE 6.00 usec  
TE 295.8 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 8

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.00 usec  
PL1 0.00 dB  
SFO1 125.7703637 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 0.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SFO2 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577995 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



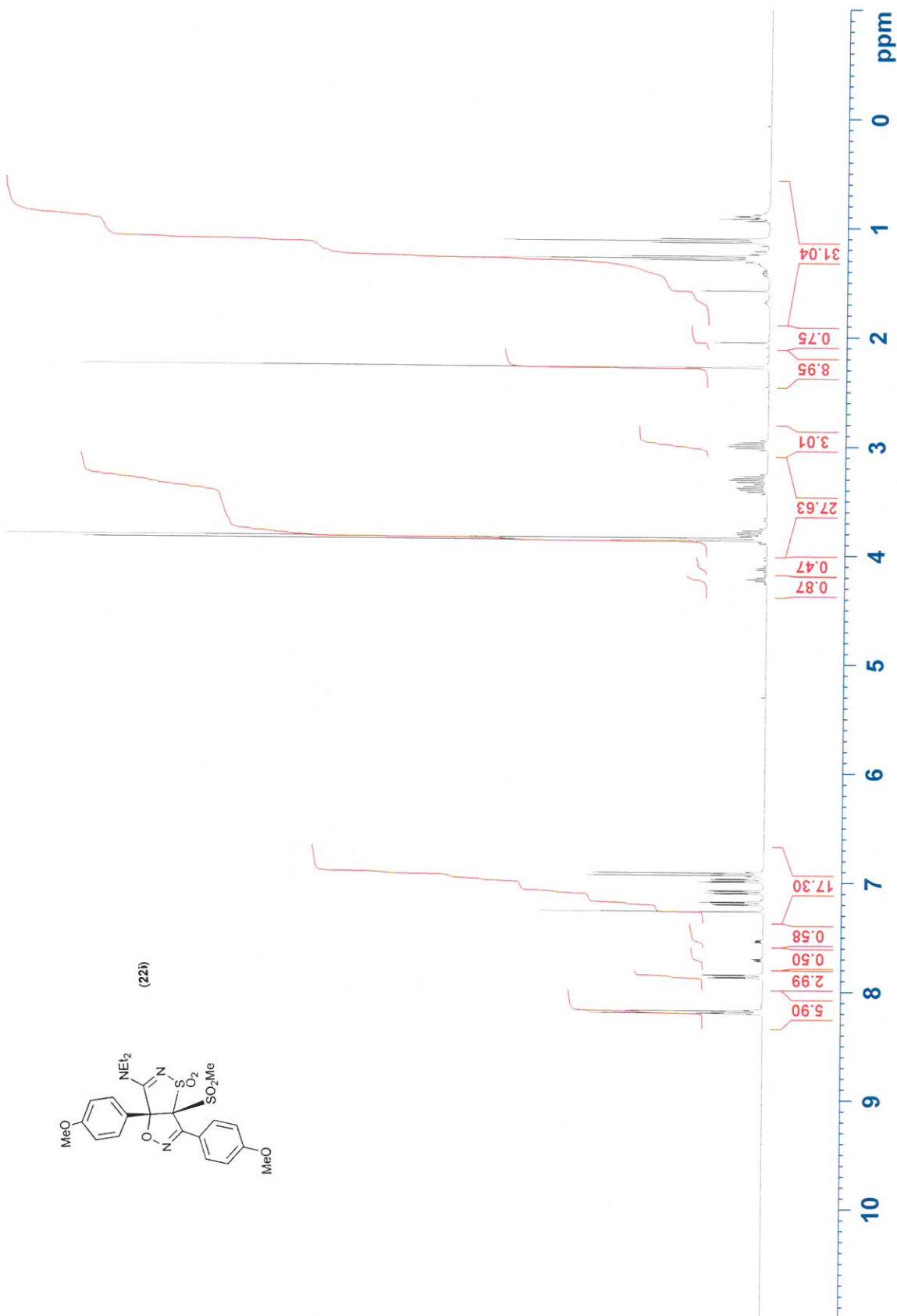
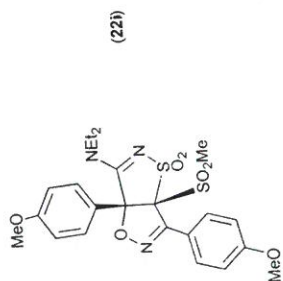




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Current Data Parameters  
NAME AP 270 f.10-32  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20080410  
Time\_ 15.30  
INSTRUM dp400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 287.4  
DW 60.400 usec  
DE 6.00 usec  
TE 687.9 K  
D1 1.00000000 sec  
TD0 1  
===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz  
F2 - Processing parameters  
SI 32768  
SF 400.1300055 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.2036  
8.1809  
8.1897  
8.1835  
8.1857  
8.1814  
8.1724  
8.1791  
8.1713  
8.1708  
8.1536  
8.1453  
8.1310  
8.1203  
8.1096  
8.1033  
8.1877  
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8.0922  
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8.0370  
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8.0353  
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8.0387  
8.0214  
8.0038  
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8.5849  
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8.1084  
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8.9261  
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8.9016



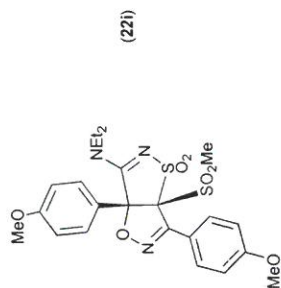
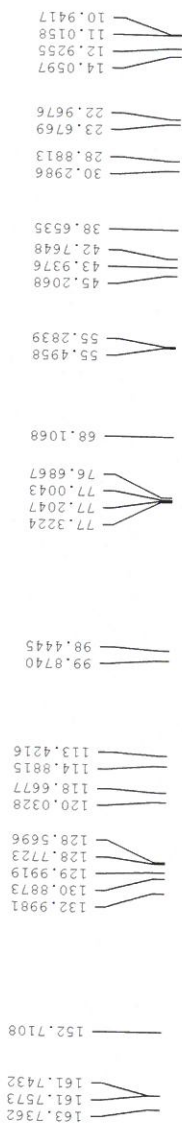


Current Data Parameters  
 NAME AP 270 f.10-32  
 EXPNO 2  
 PROCNO 1  
  
 F2 - Acquisition Parameters  
 Date\_ 20080410  
 Time\_ 15.33  
 INSTRUM dpx400  
 PROHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 256  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 18390.4  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 687.9 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 8

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.70 usec  
 PL1 -3.00 dB  
 SFO1 100.6228298 MHz

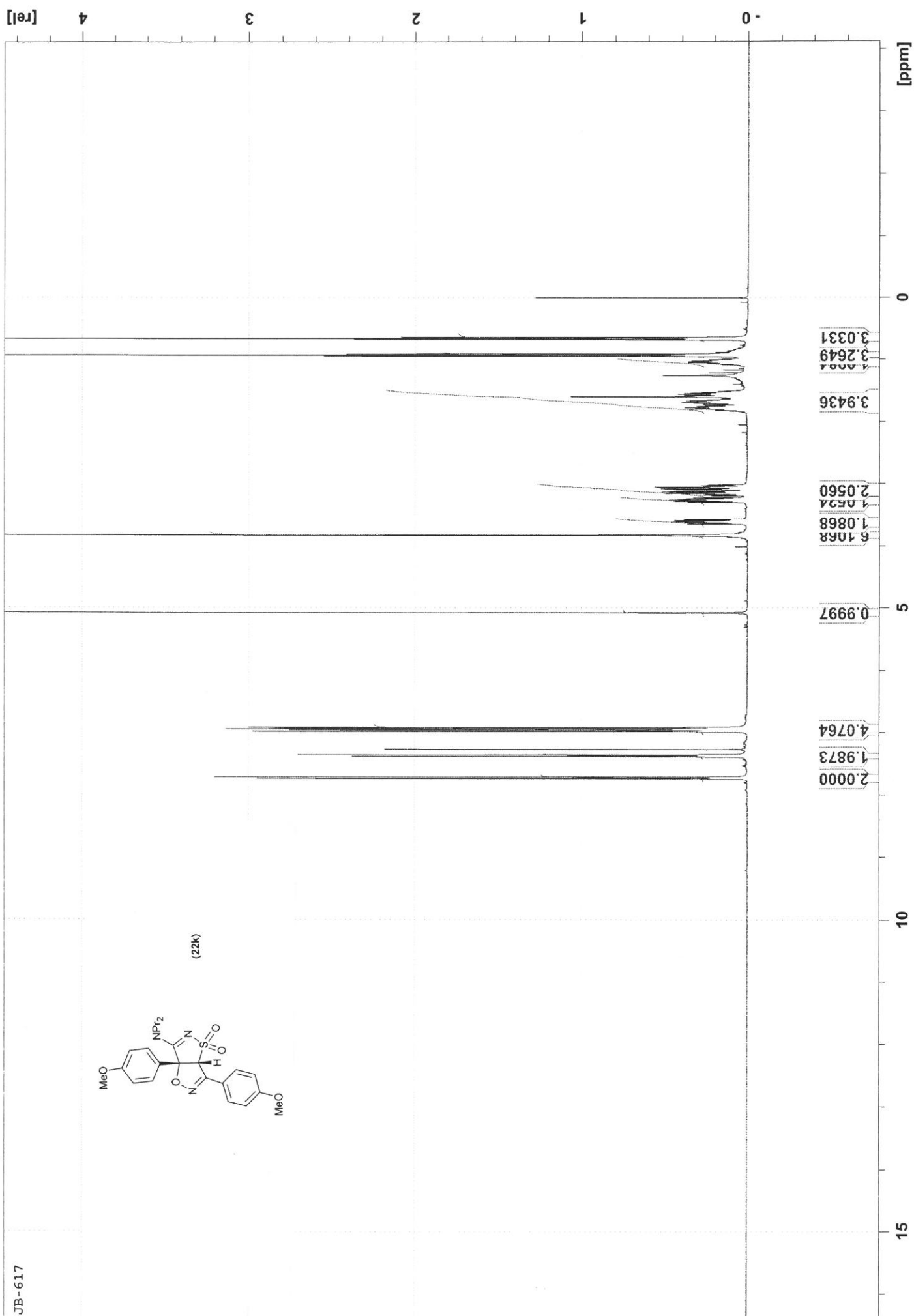
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 84.00 usec  
 PL2 -3.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127740 MHz  
 EM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



200 180 160 140 120 100 80 60 40 20 0 ppm

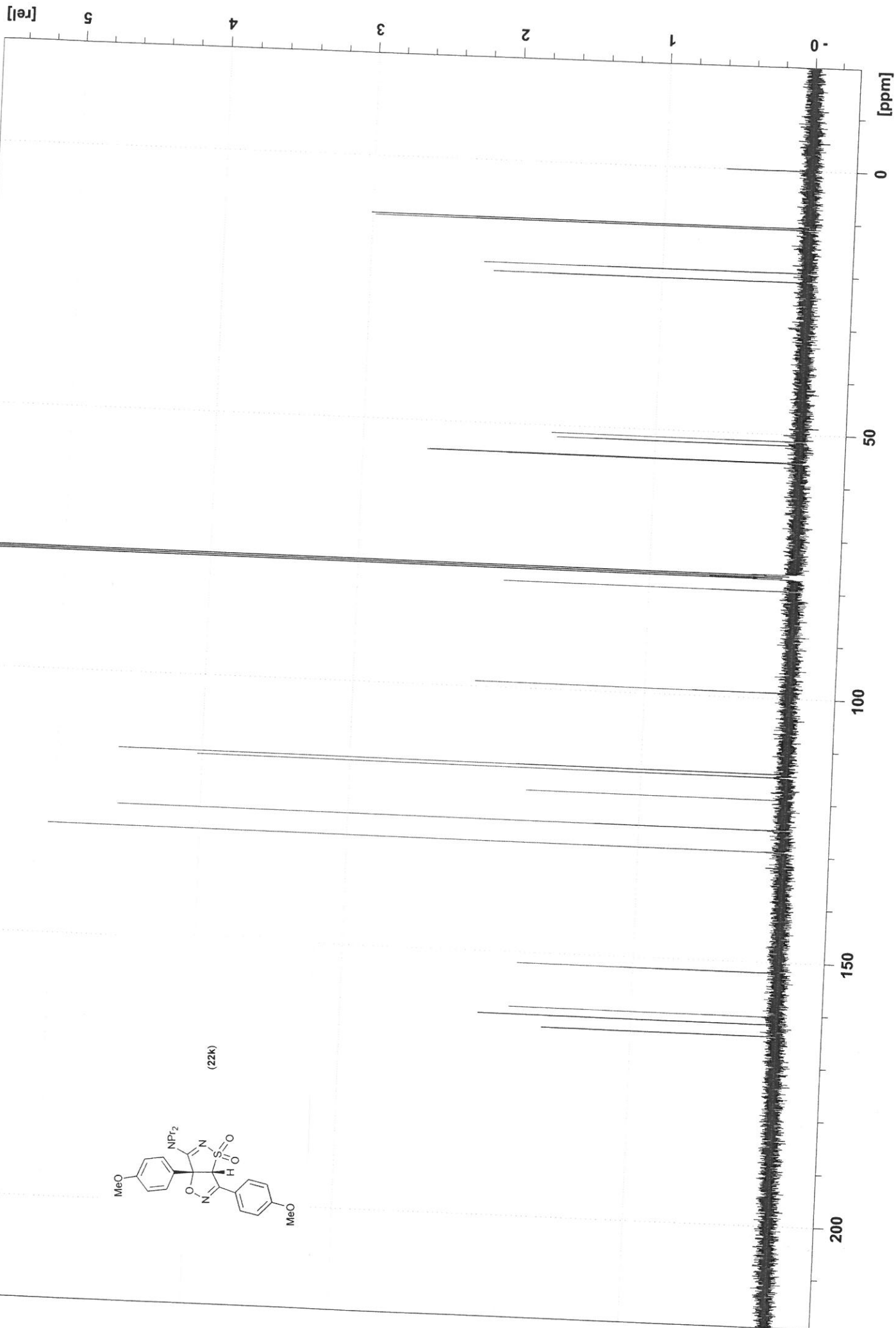




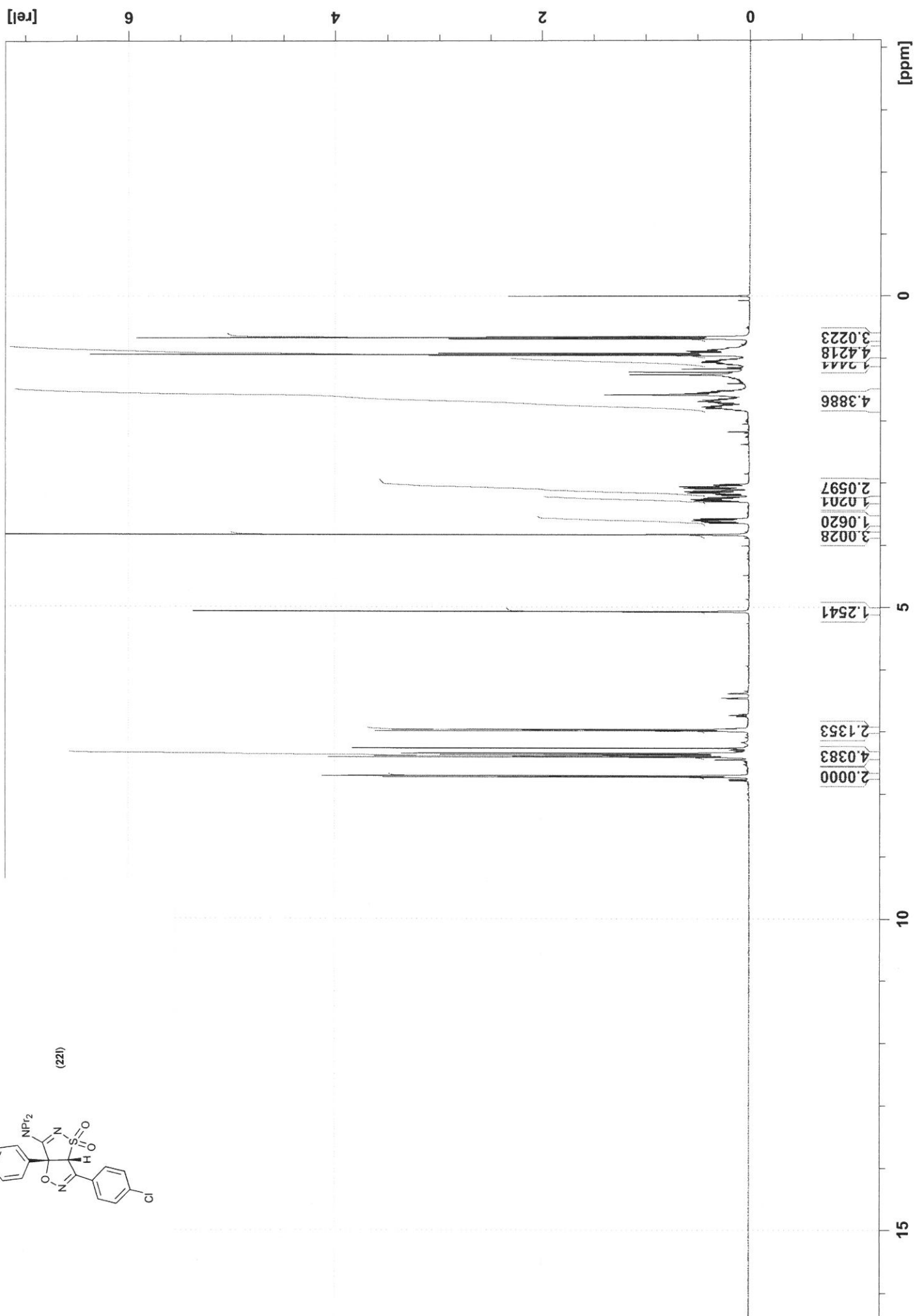


JB-617 41 1 "C:\NMR data student"

JB-617 CLM2 T10-18 chsd3









[rel]

5

4

3

2

1

-0

[ppm]

0

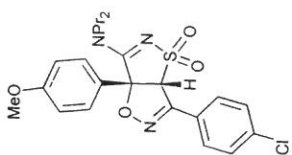
50

100

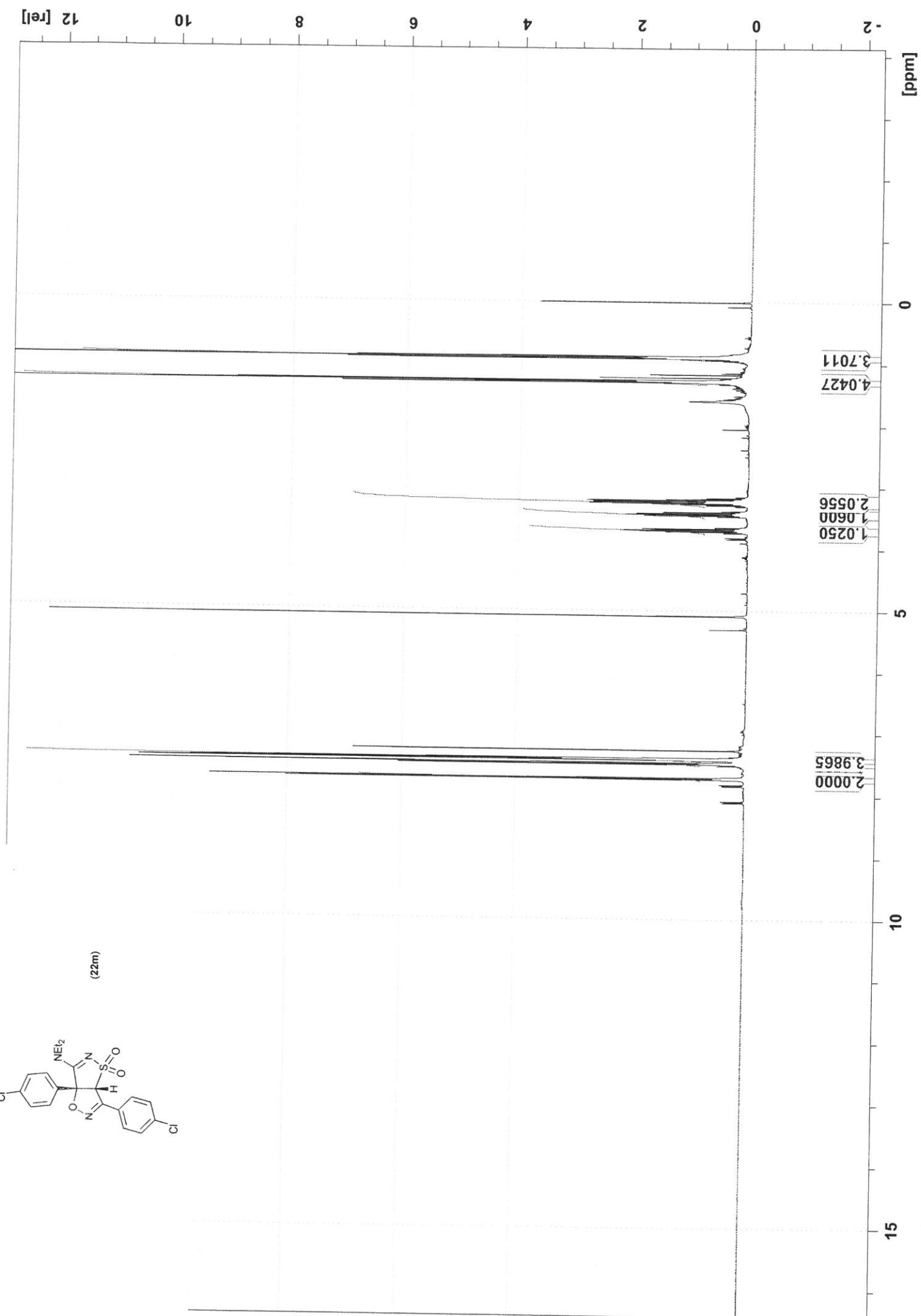
150

200

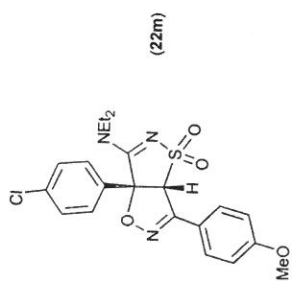
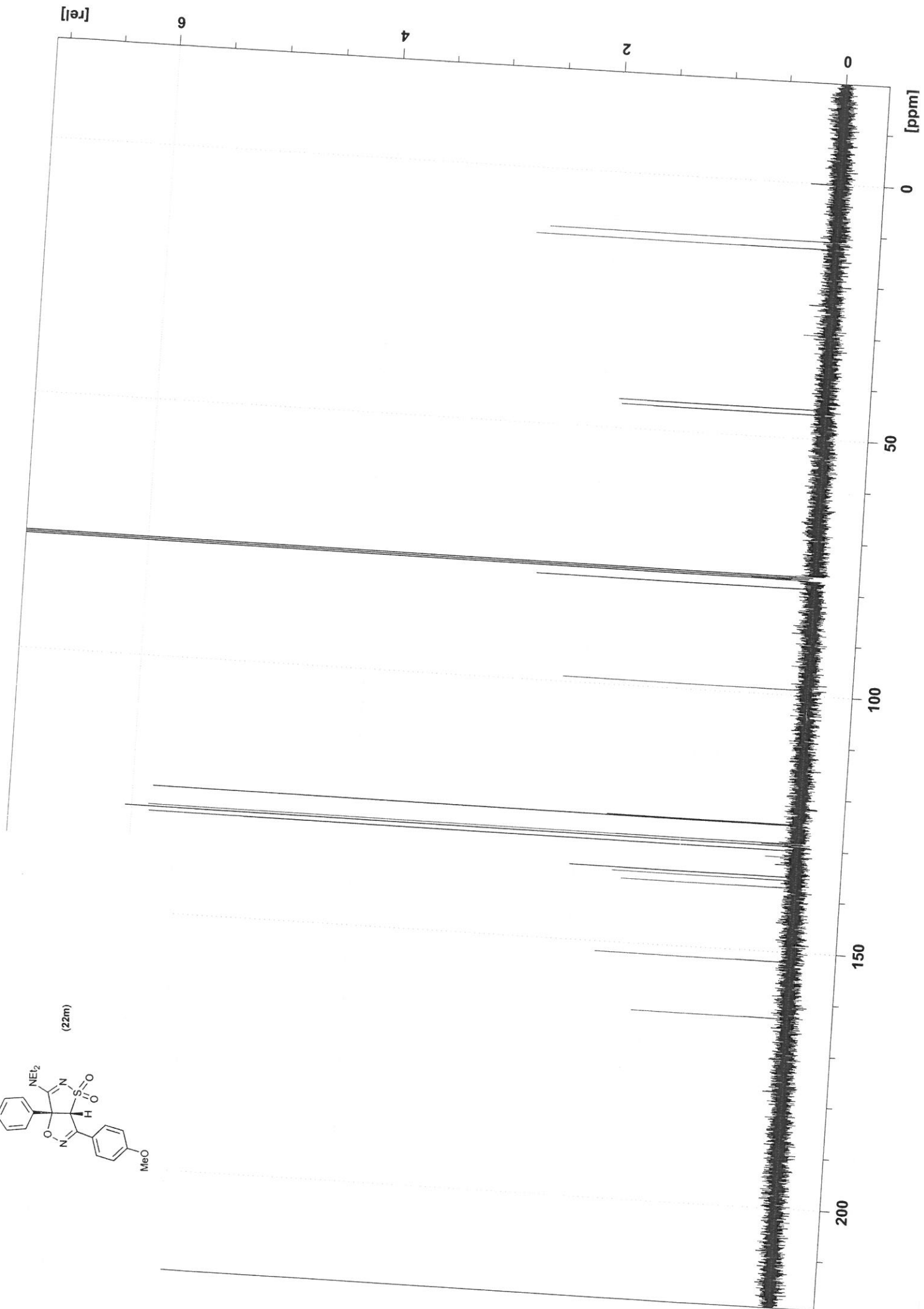
(221)



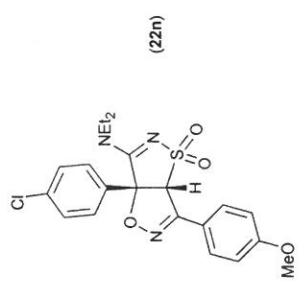
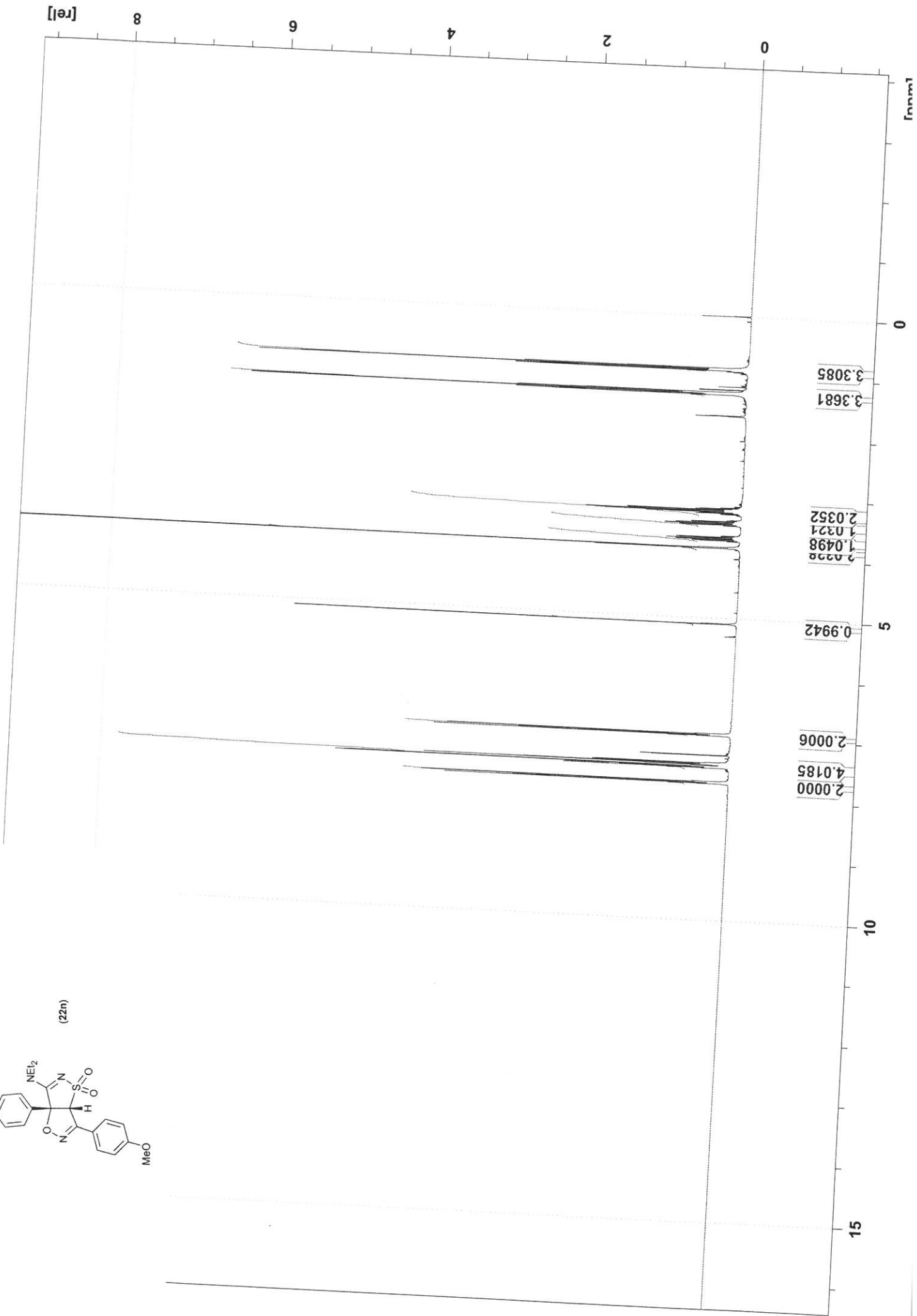




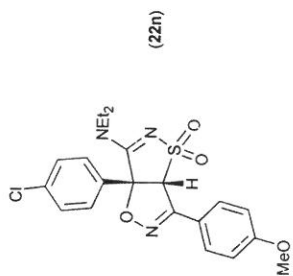
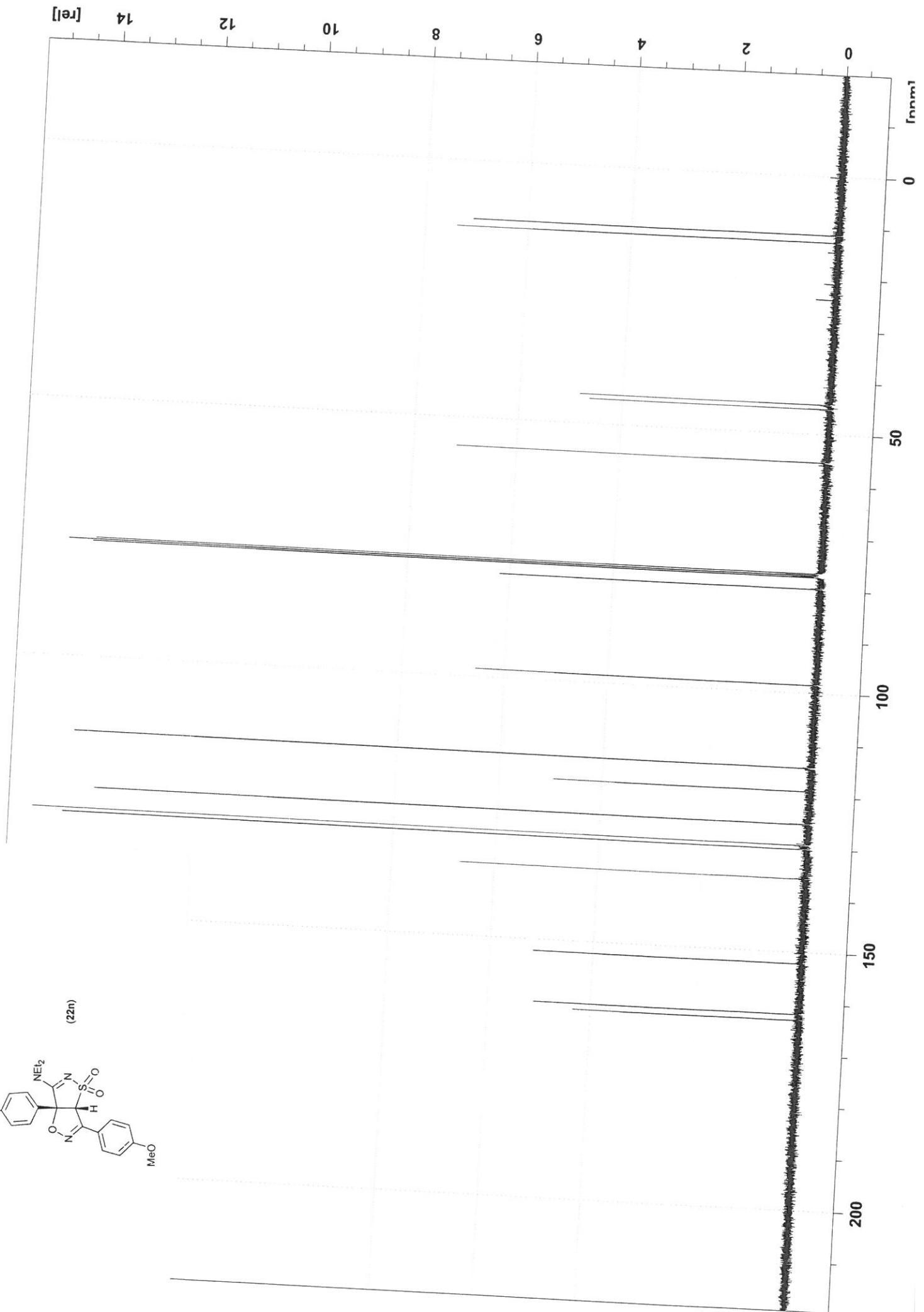




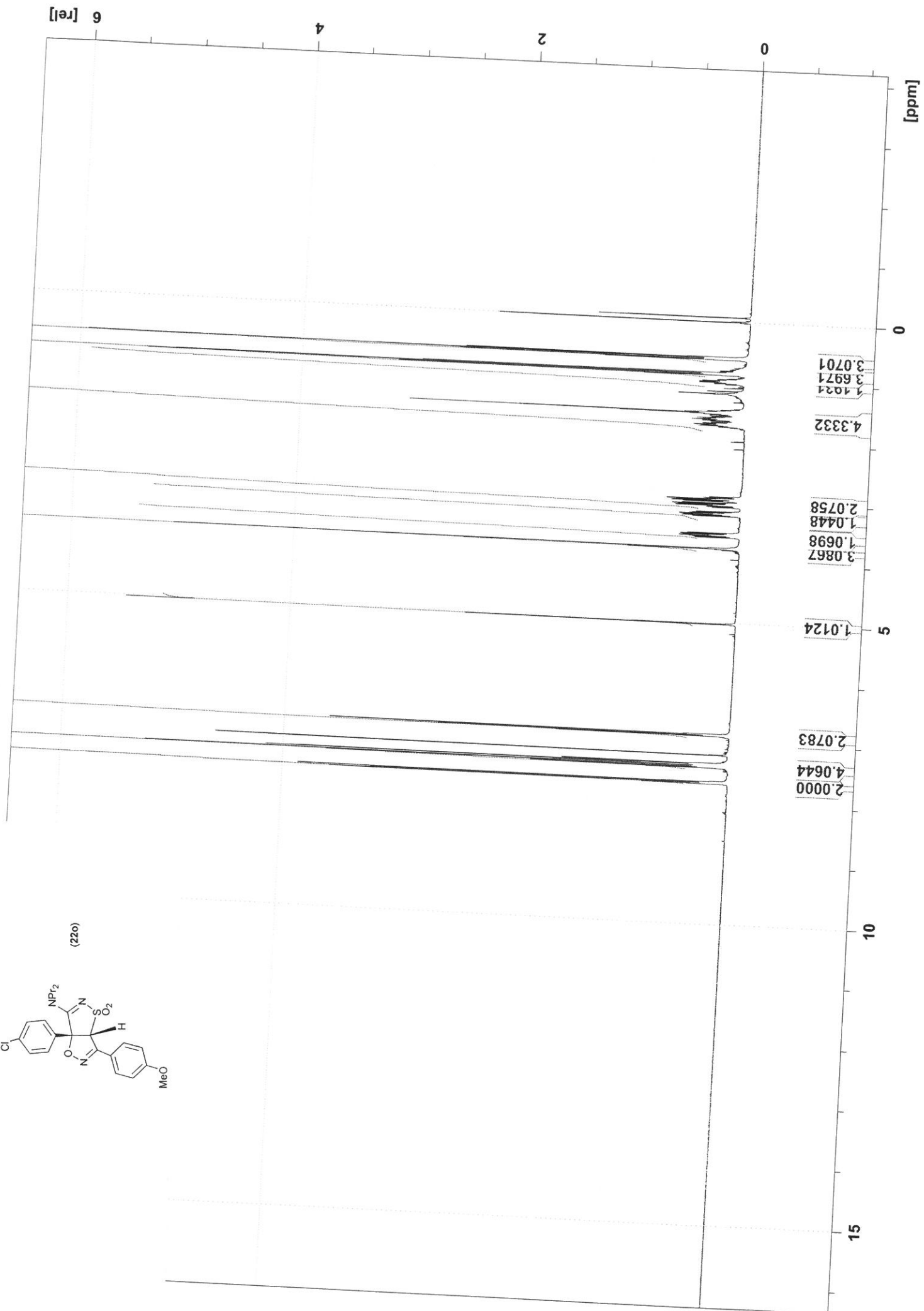




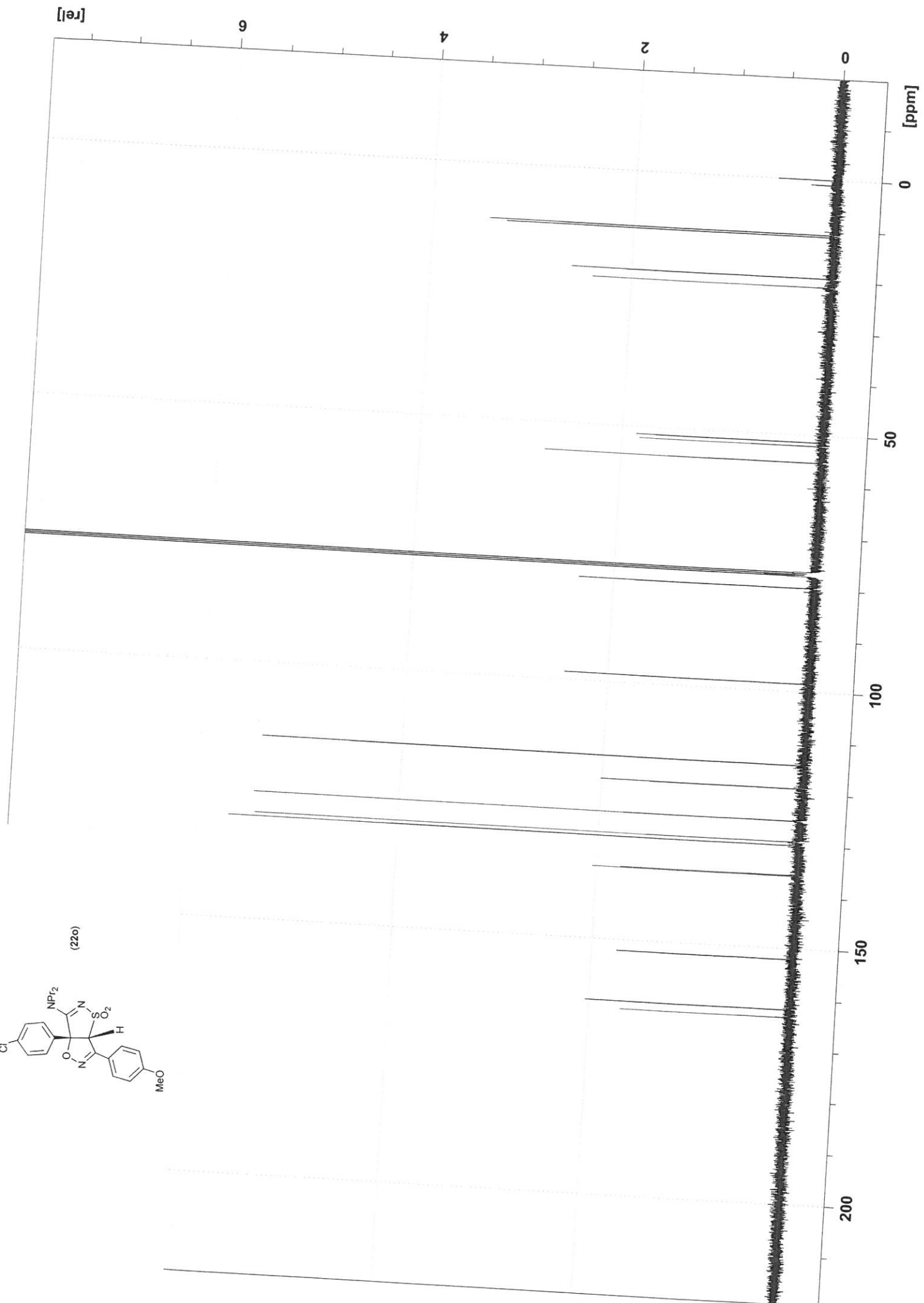




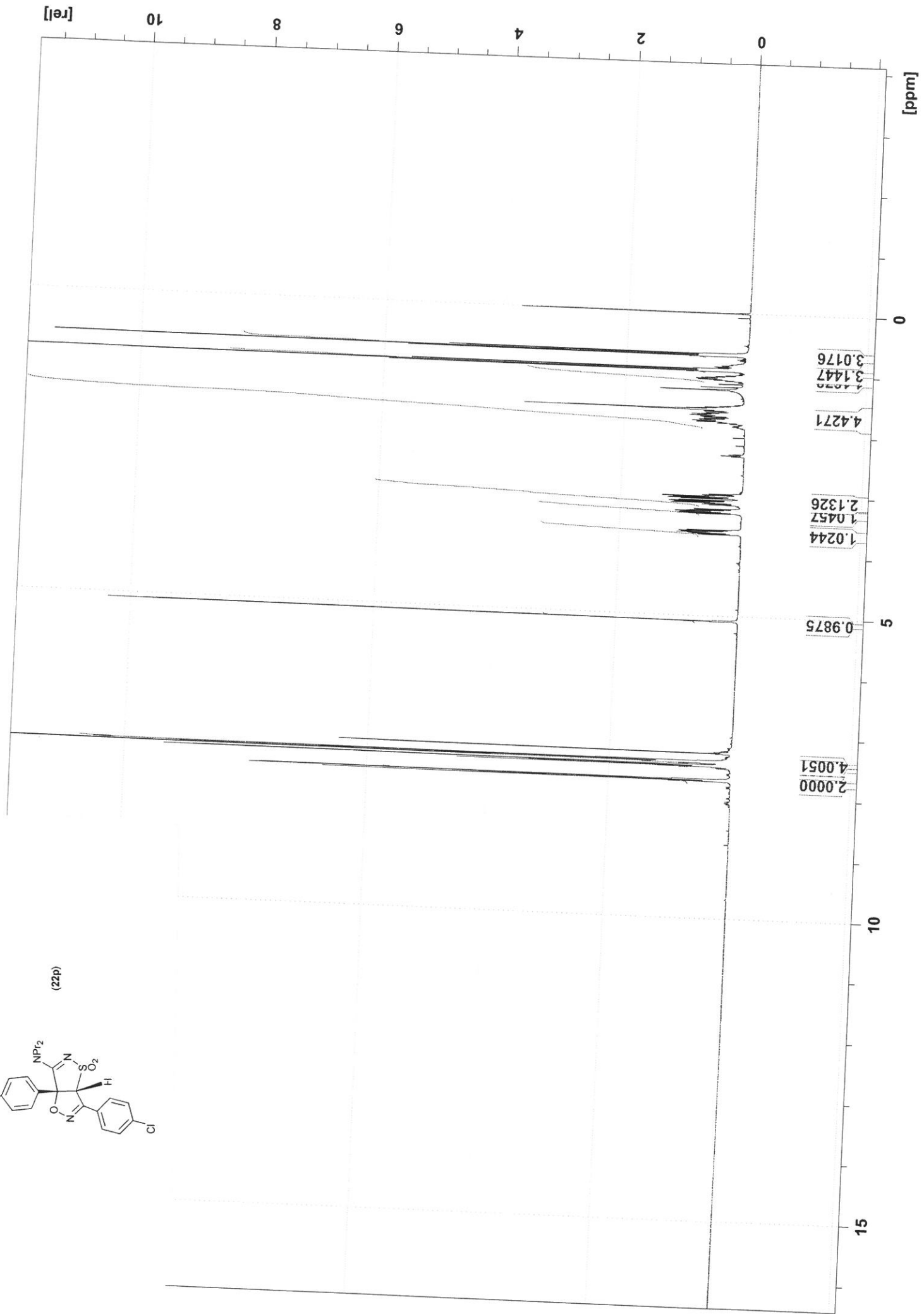




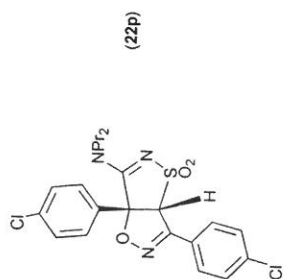
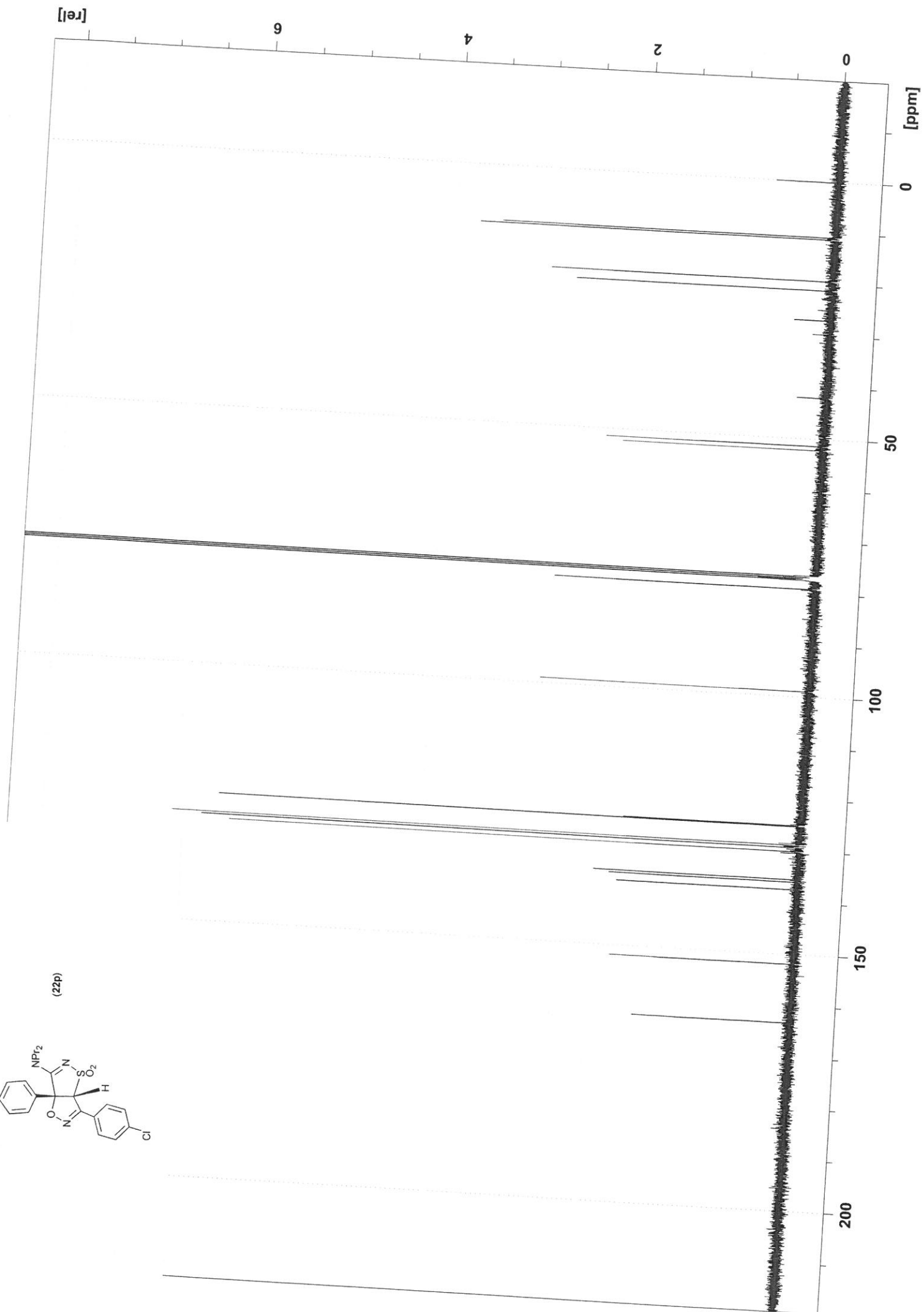




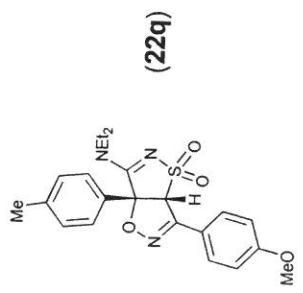
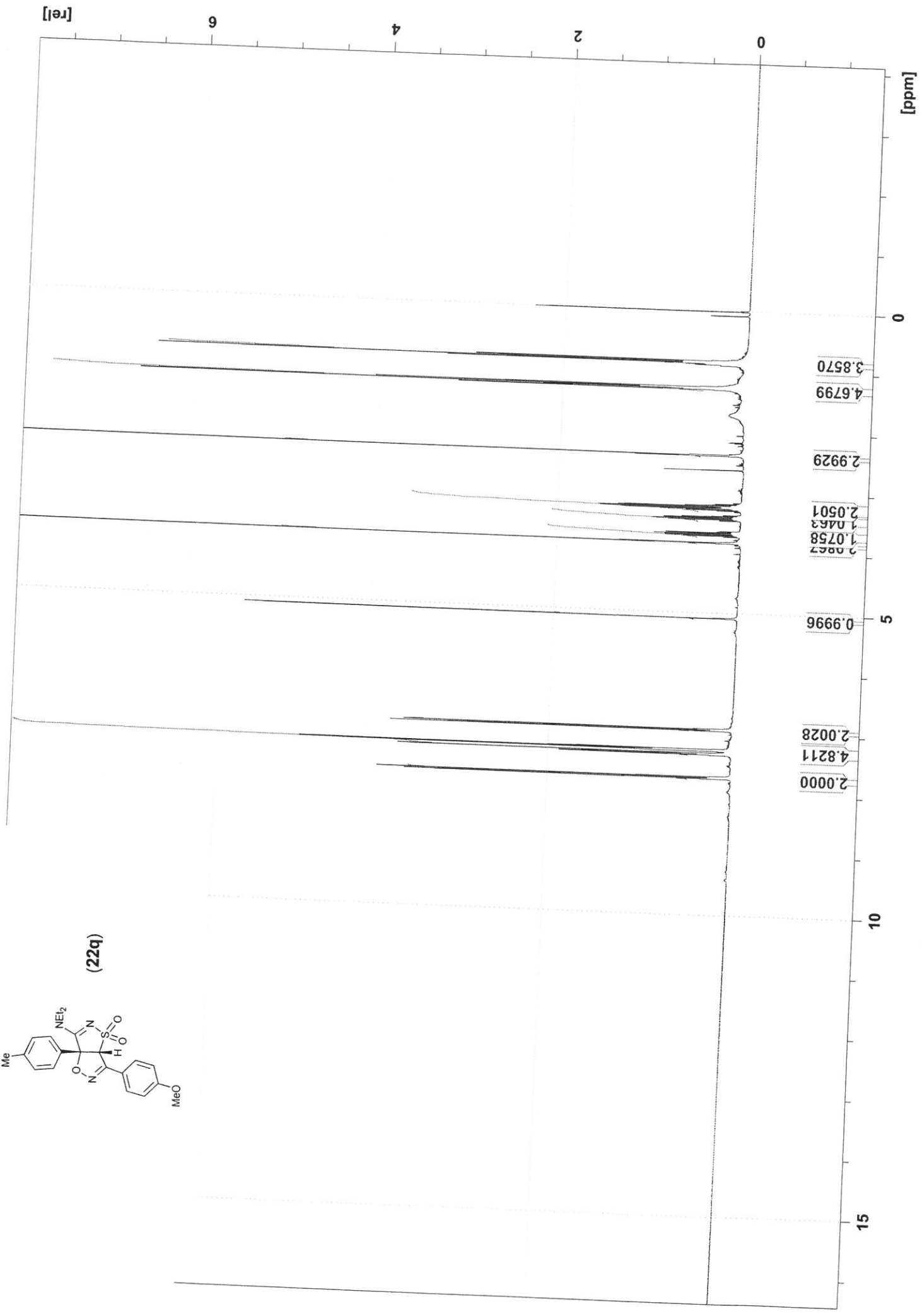




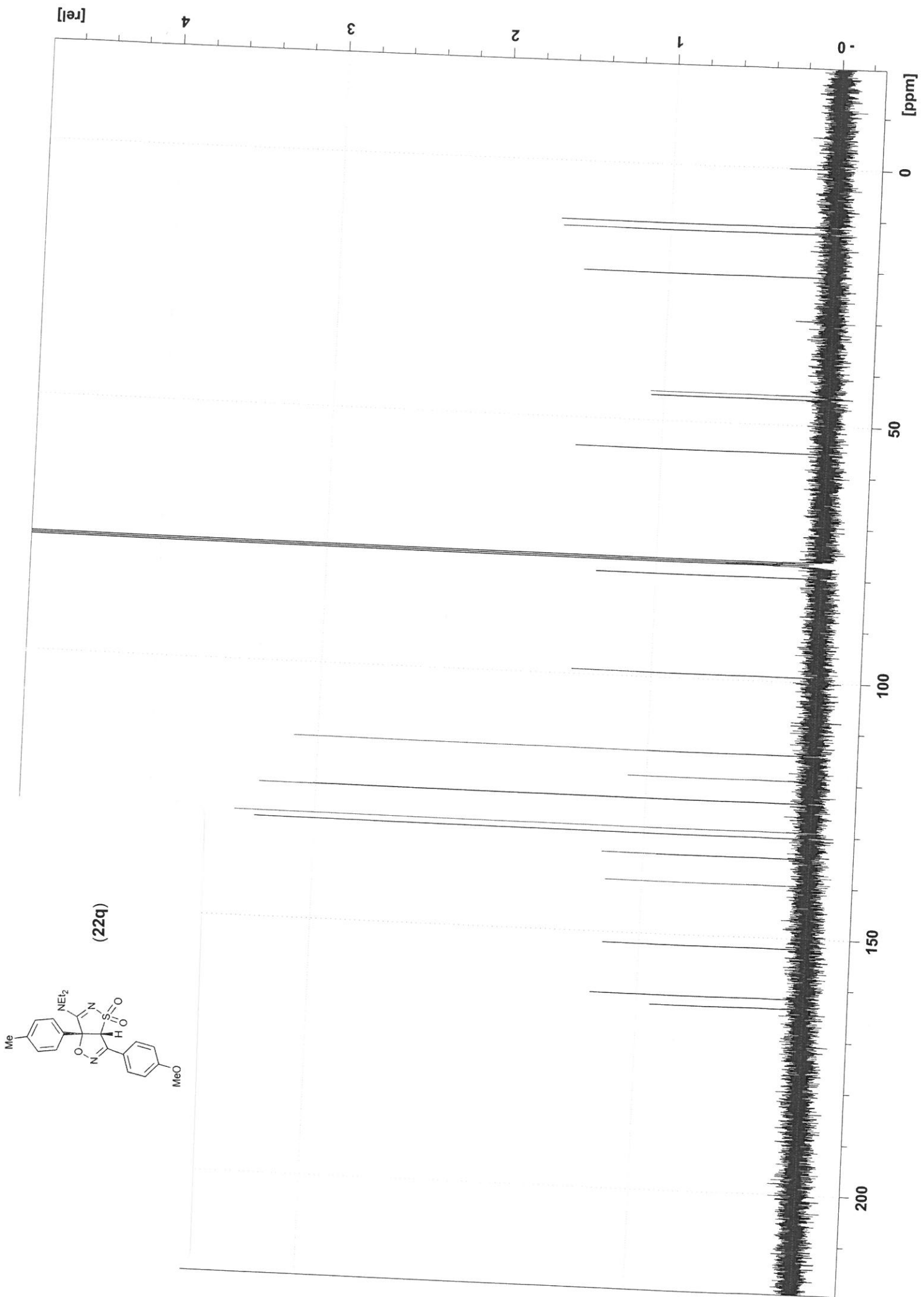




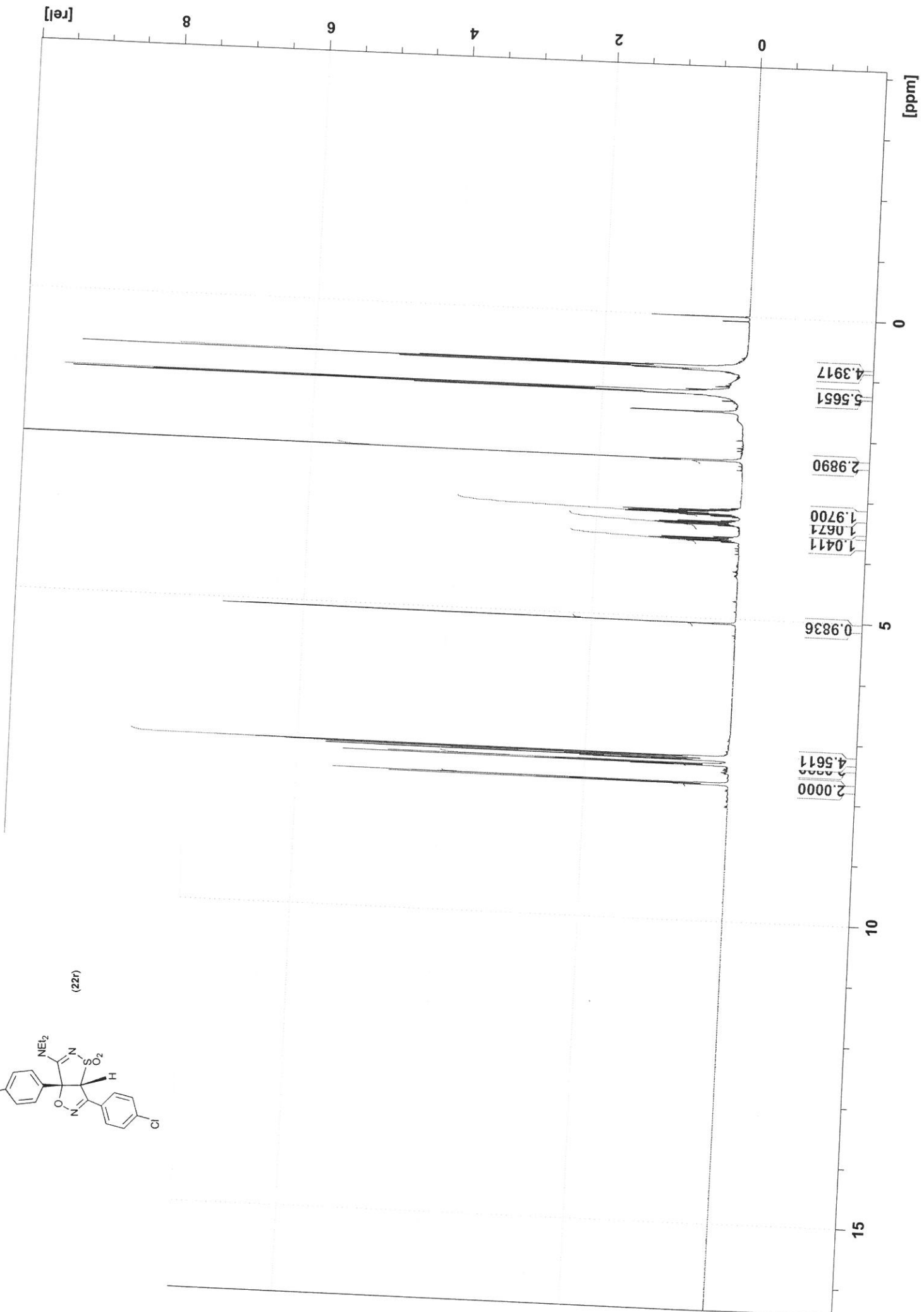




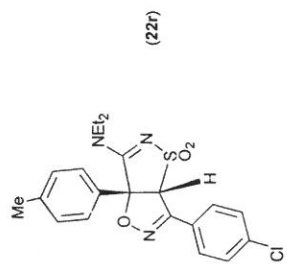
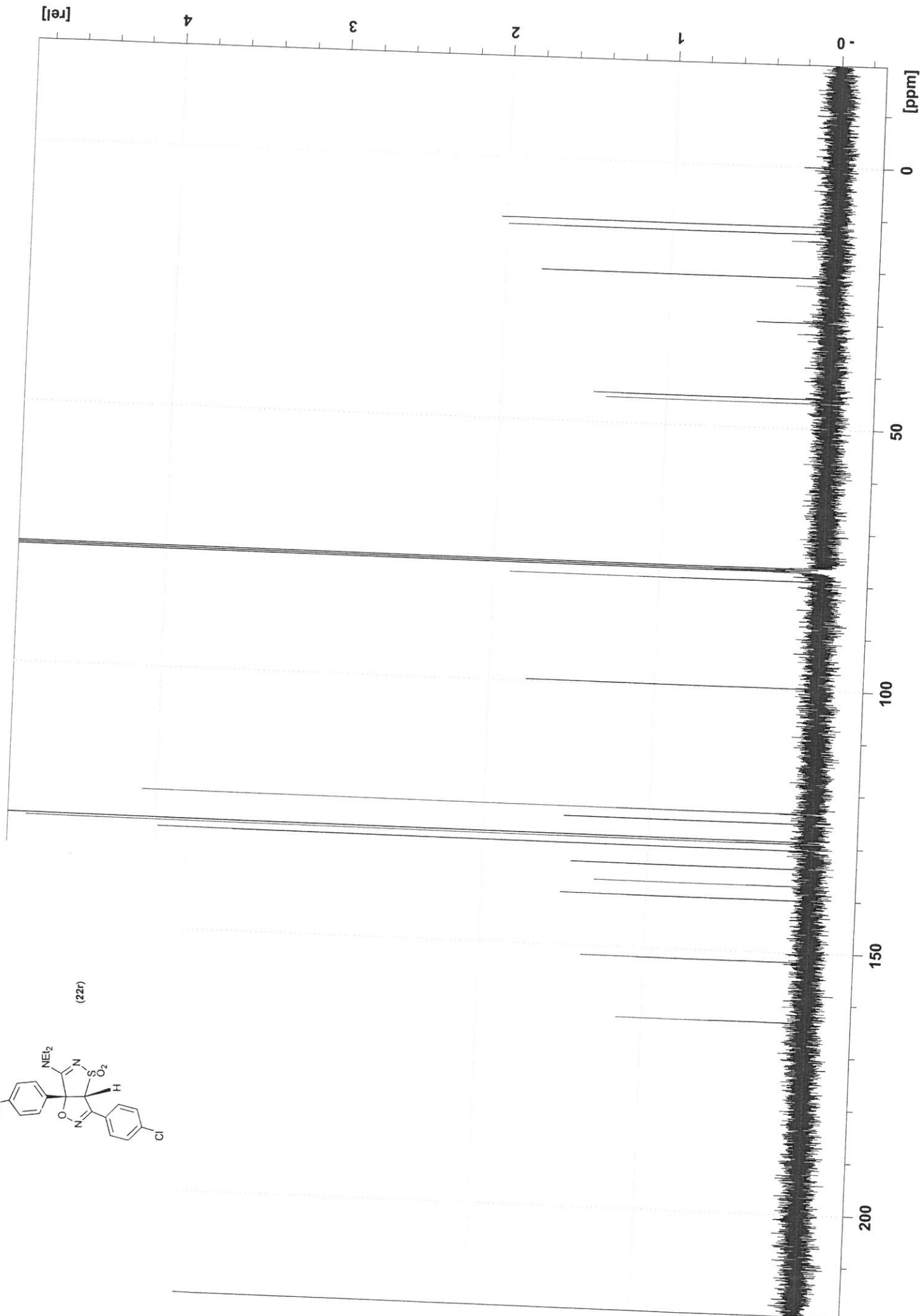




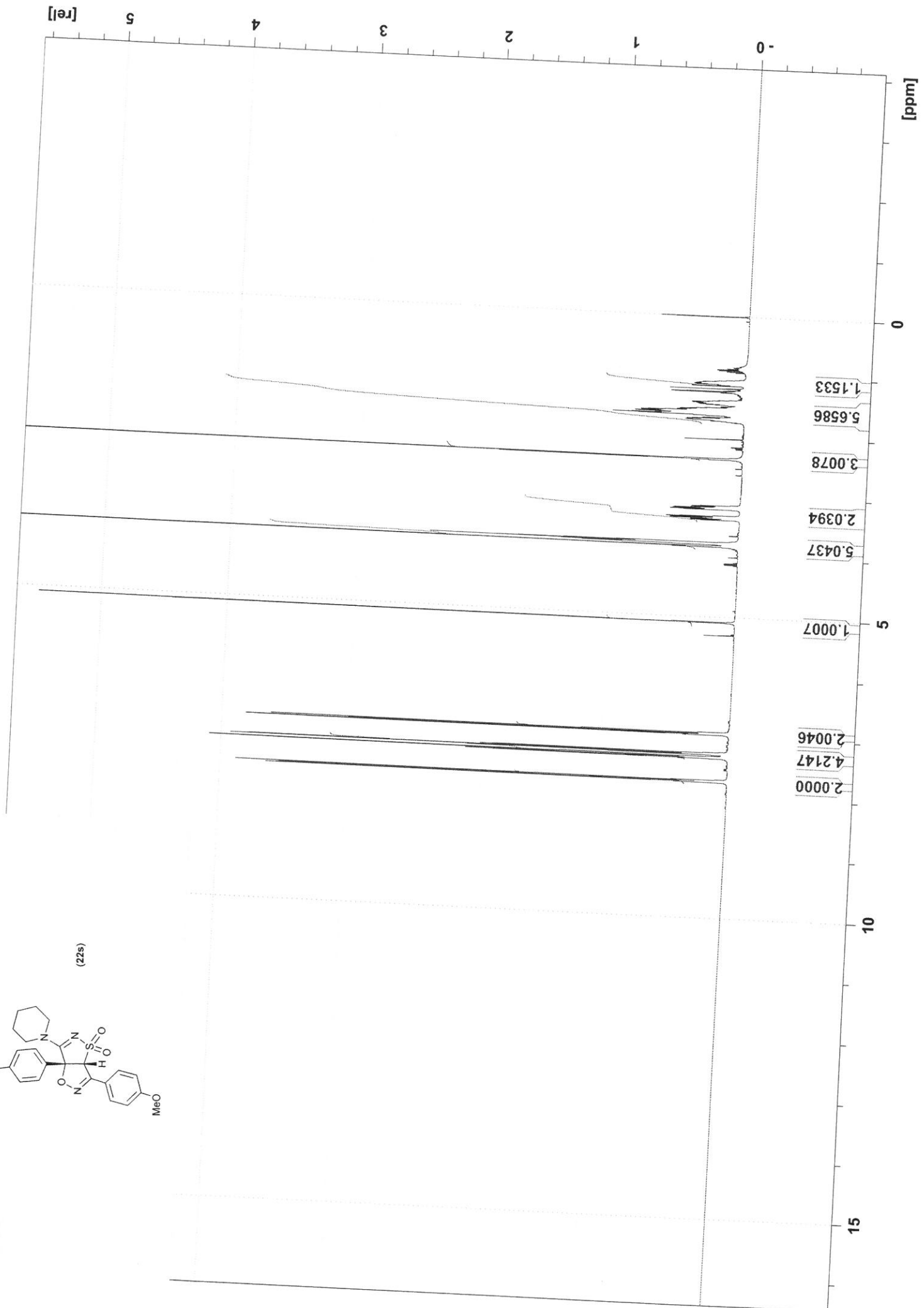




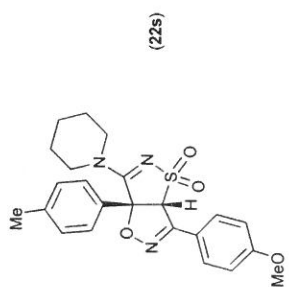
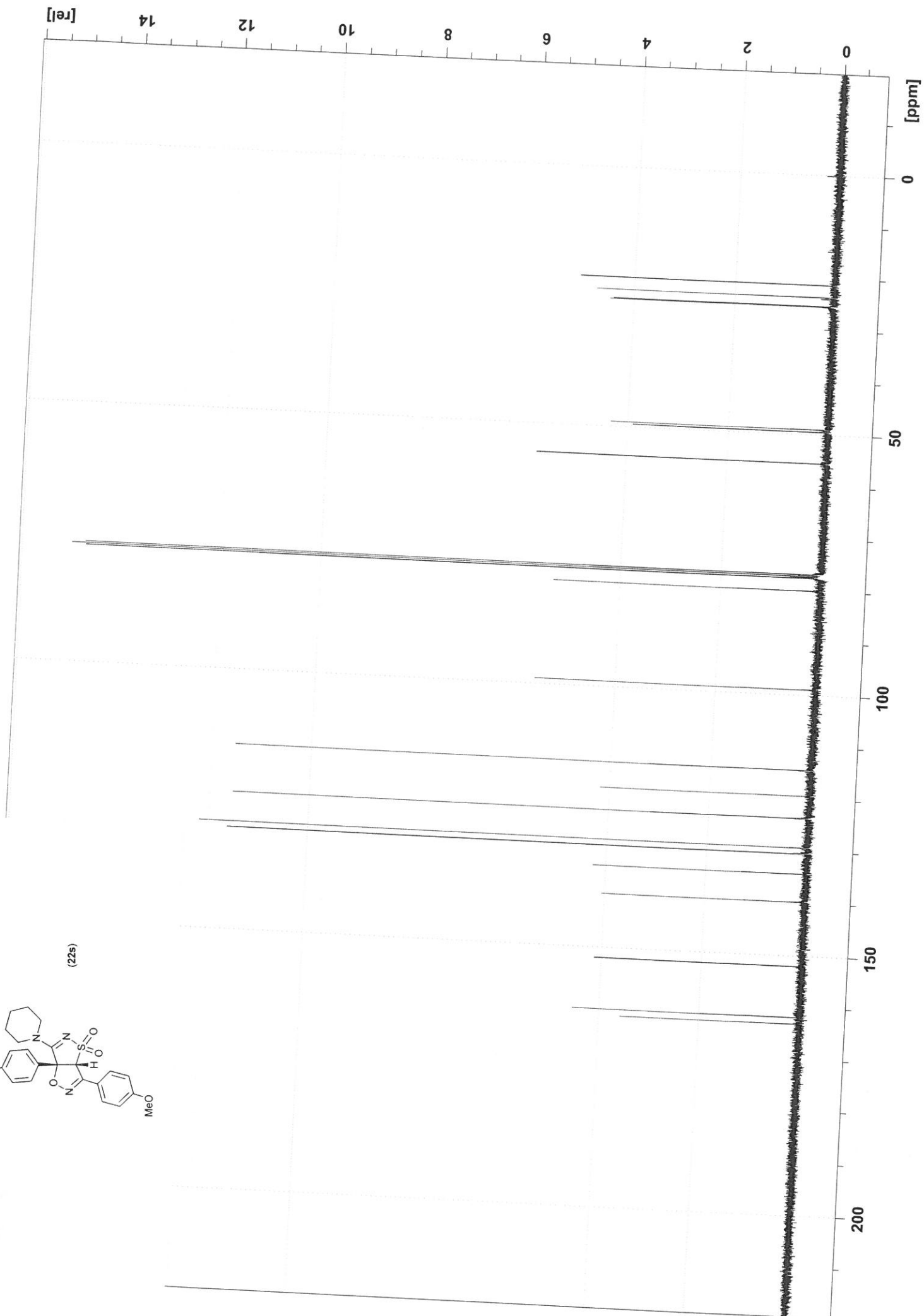




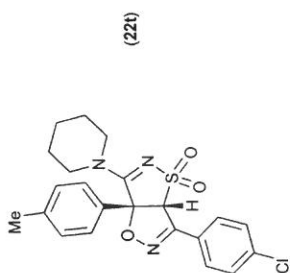
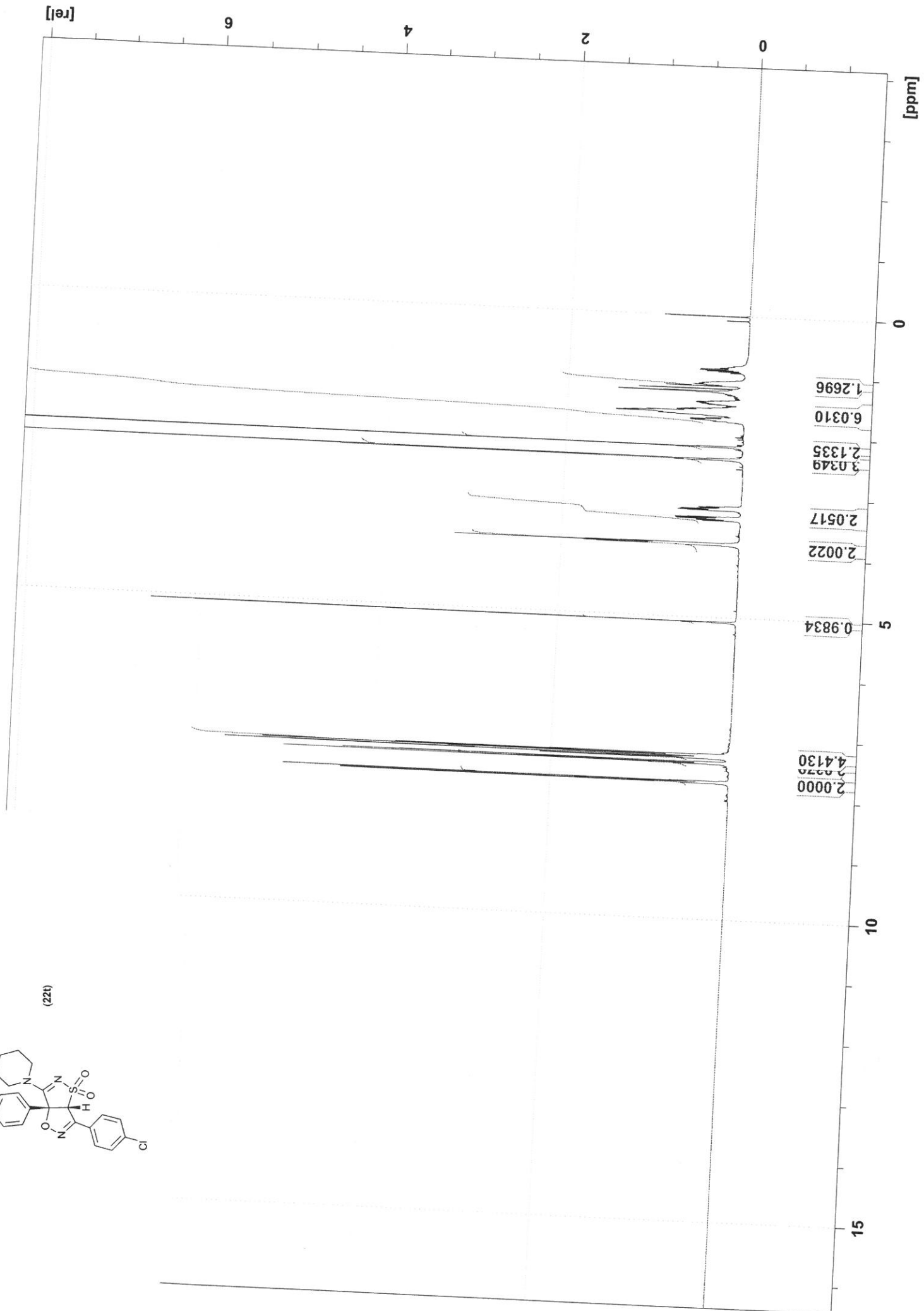




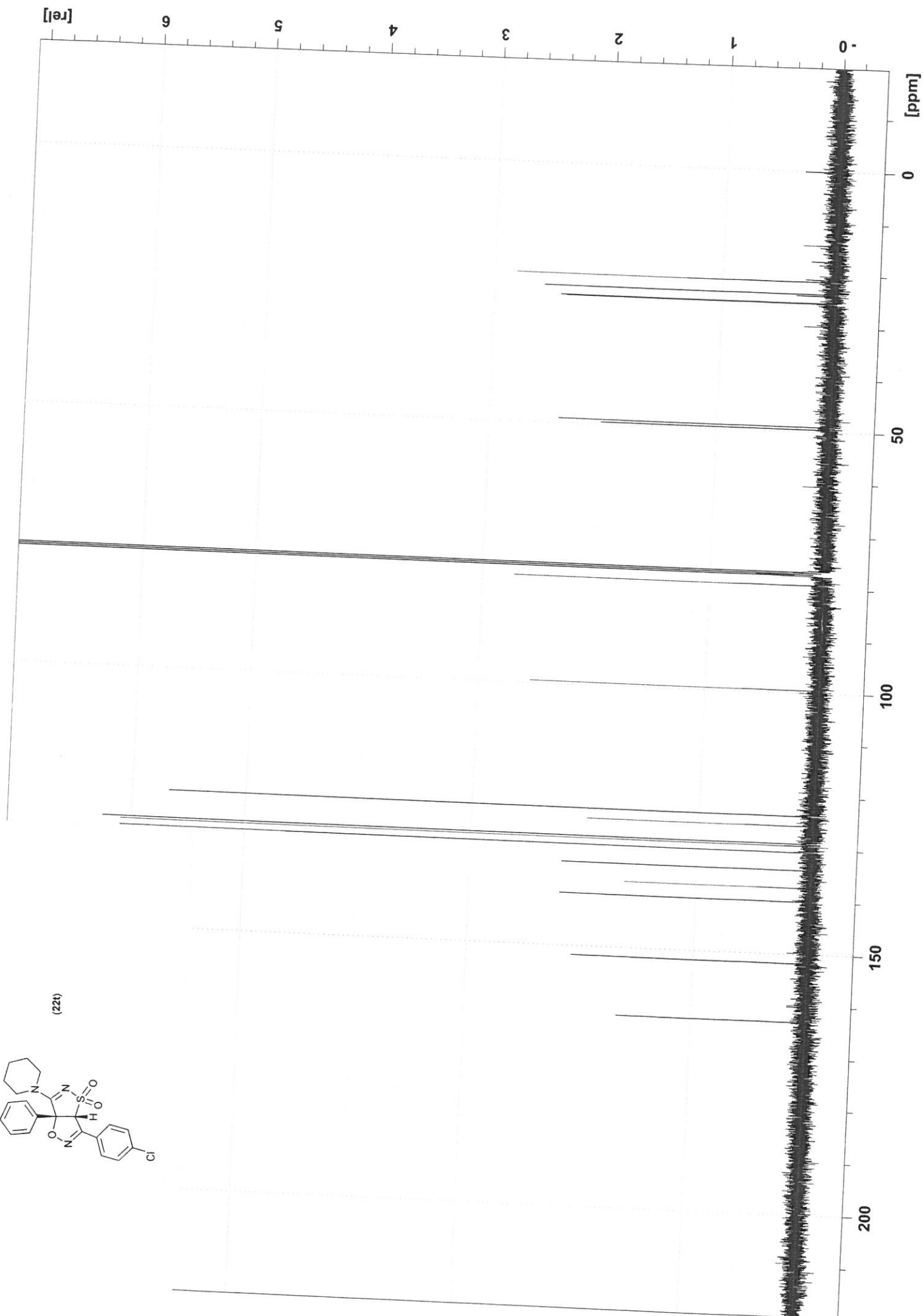
















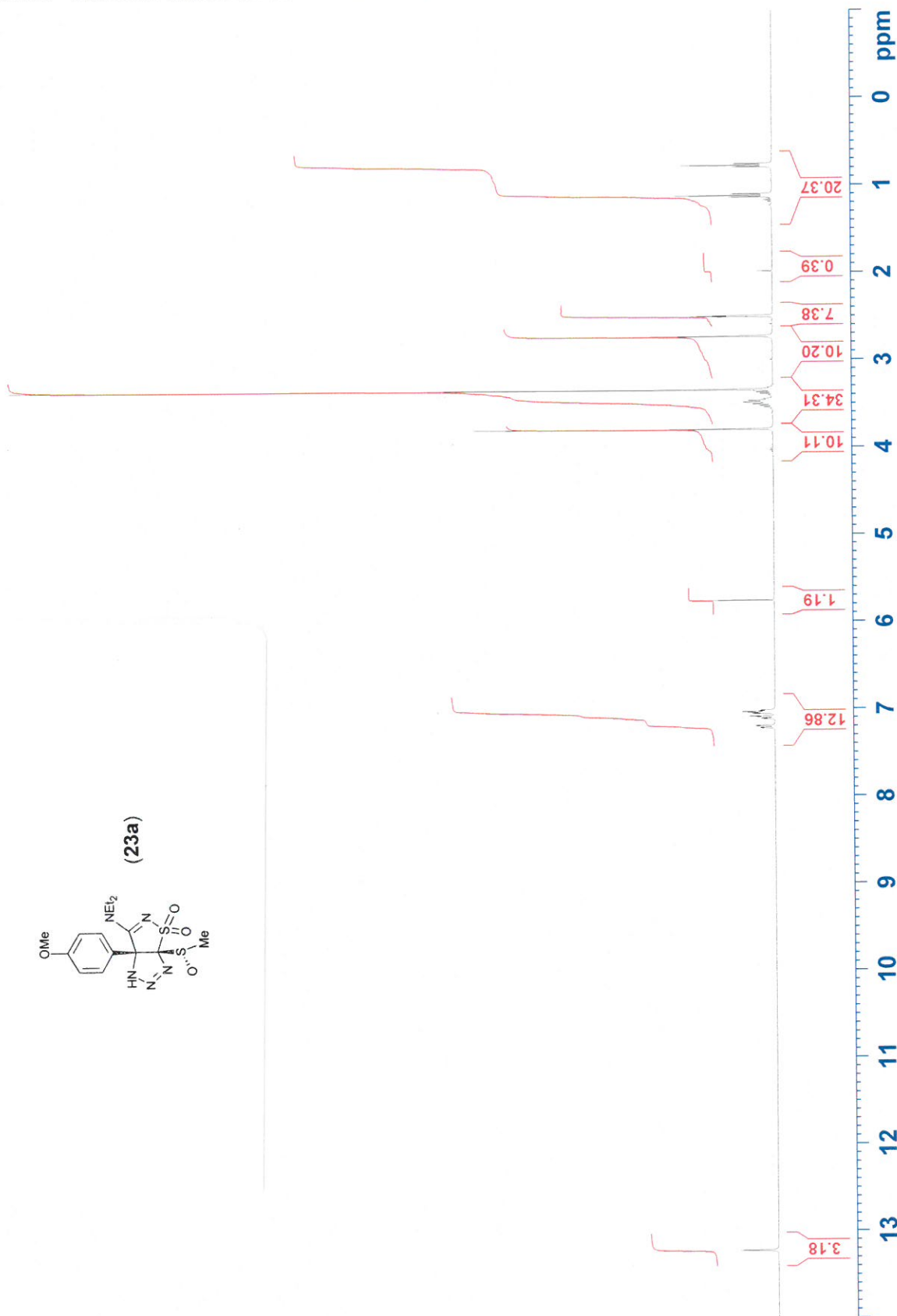
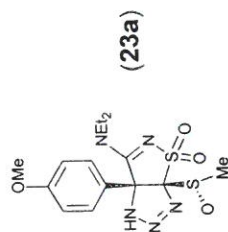
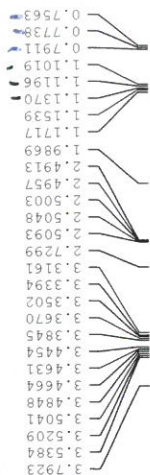
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Current Data Parameters  
NAME AP 294 f.17-24  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080701  
Time 10.38  
INSTRUM dp400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9588243 sec  
RG 287.4  
DW 60.400 usec  
DE 6.00 usec  
TE 691.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300019 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





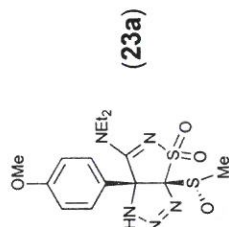
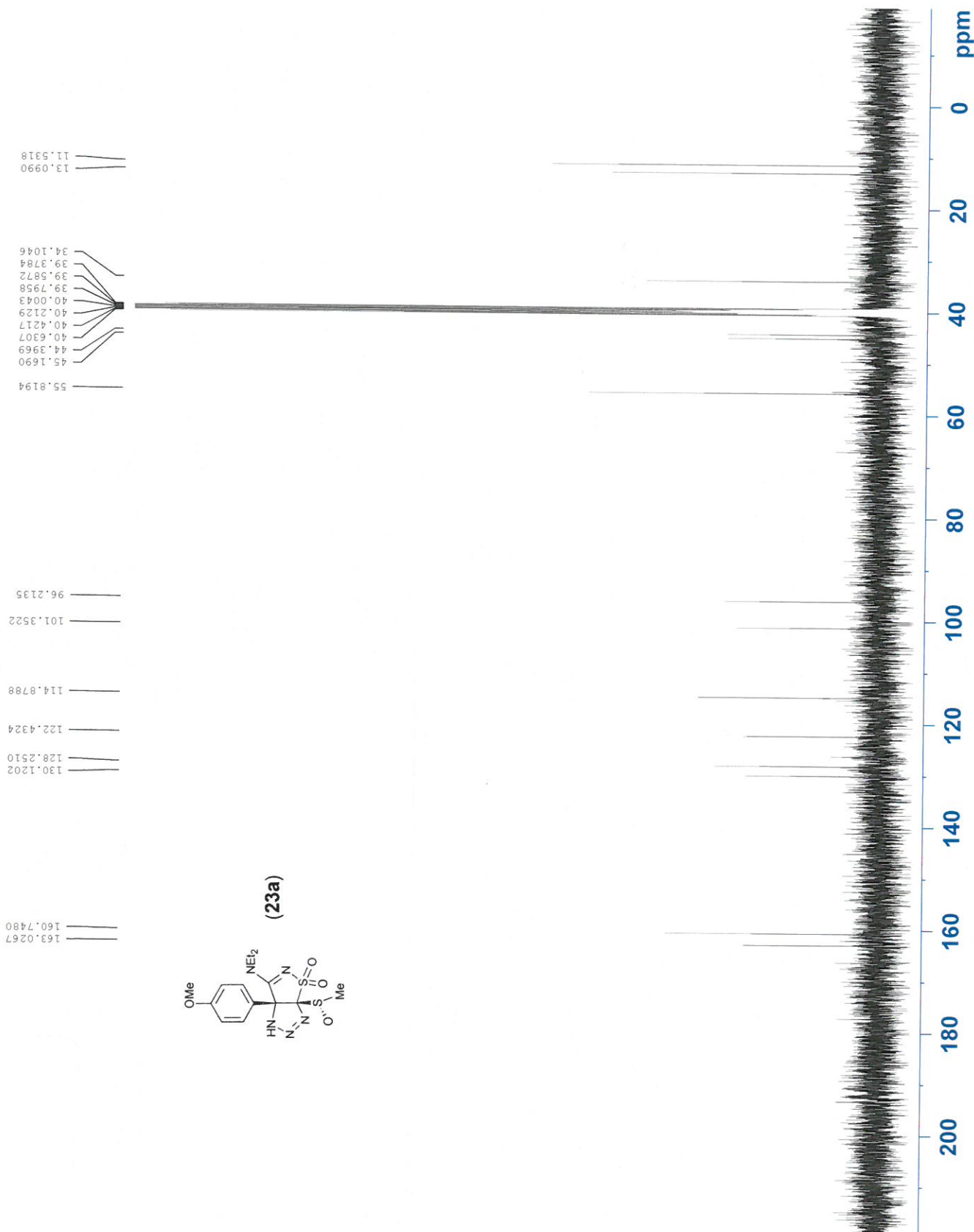
Current Data Parameters  
 NAME AP 294 f.17-24  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20080701  
 Time 14.36  
 INSTRUM dpx400  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 256  
 DS 4  
 SWH 23980.814 Hz  
 FIDRES 0.365918 Hz  
 AQ 1.3664756 sec  
 RG 10321.3  
 DW 20.850 usec  
 DE 6.00 usec  
 TE 689.8 K  
 D1 2.00000000 sec  
 d11 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 8

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.70 usec  
 PL1 3.00 dB  
 SFO1 100.628298 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 84.00 usec  
 PL2 -3.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127638 MHz  
 EM 0  
 WDW 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40







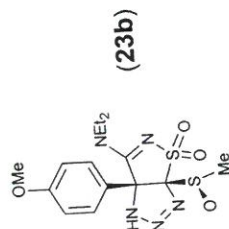
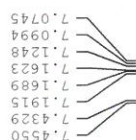
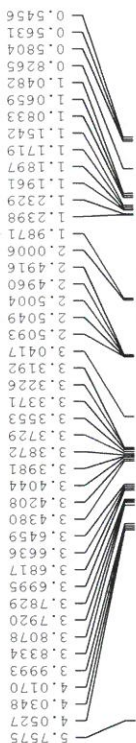
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Current Data Parameters  
NAME AP 294 f.26-40  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080701  
Time 10.43  
INSTRUM dp400  
PROBHD 5 mm QNP 1H/1  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8278.146 Hz  
FIDRES 0.126314 Hz  
AQ 3.9584243 sec  
RG 287.4  
DW 60.400 usec  
DE 6.00 usec  
TE 691.0 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 8.40 usec  
PL1 -3.00 dB  
SFO1 400.1324710 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1300017 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



13.7781





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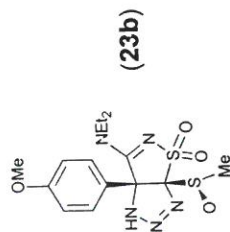
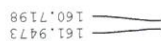
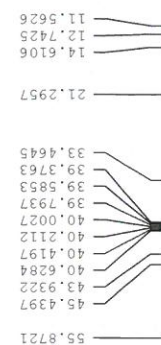
Current Data Parameters  
NAME AP 294 f.26-40  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080701  
Time 15.12  
INSTRUM dpx400  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 256  
DS 4  
SWH 23980.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 13004  
DW 20.850 usec  
DE 6.00 usec  
TE 689.7 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDO 8

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.70 usec  
PL1 -3.00 dB  
SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 84.00 usec  
PL2 -3.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6127636 MHz  
WDW EN  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40







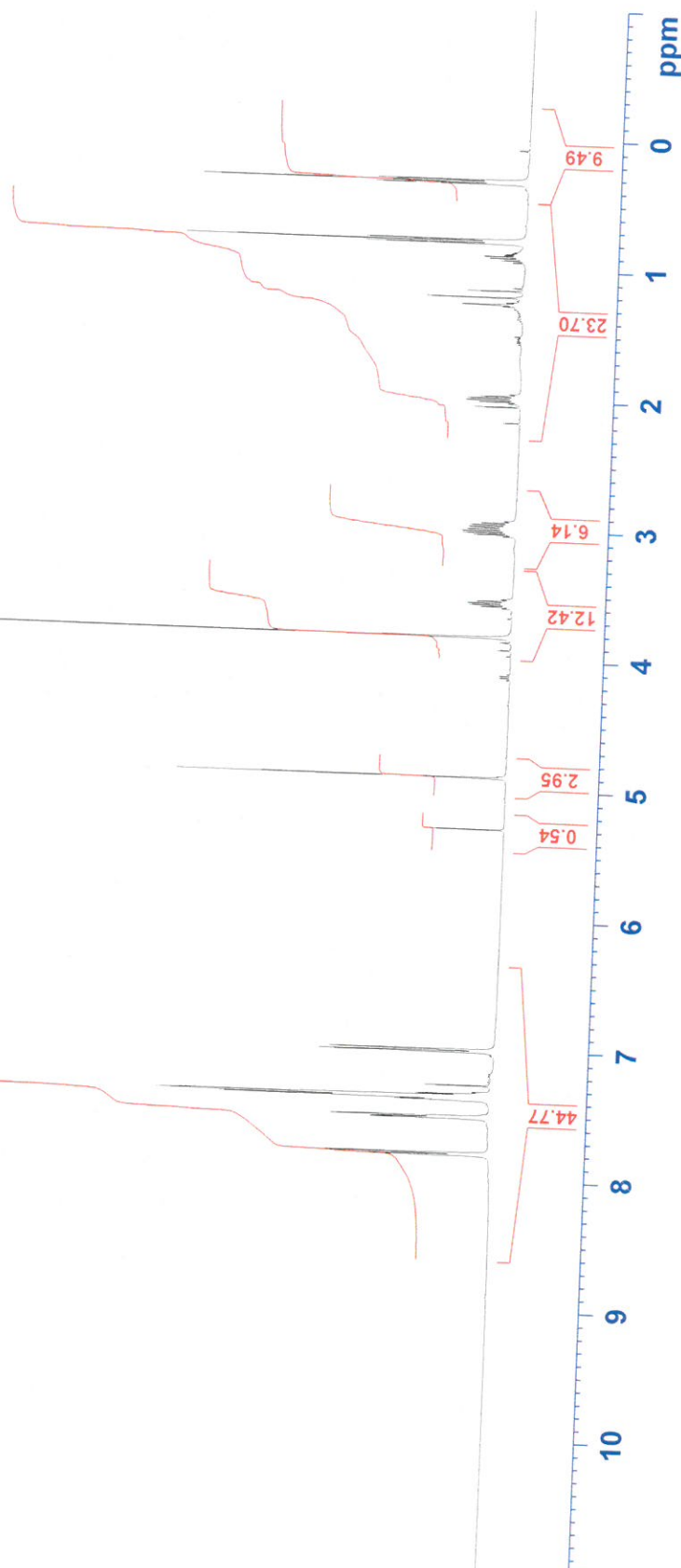
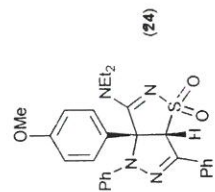
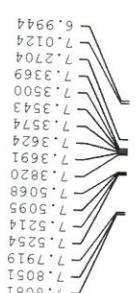
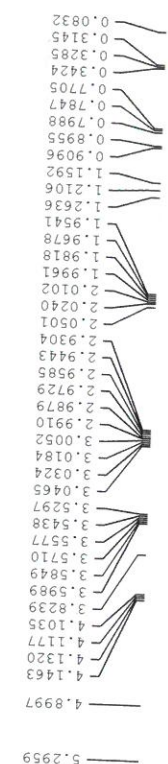
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Current Data Parameters  
NAME sn15347ap  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071217  
Time\_ 8.18  
INSTRUM av500  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.157632 Hz  
AQ 3.1719923 sec  
RG 80.6  
DW 48.400 usec  
DE 6.00 usec  
TE 294.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.70 usec  
PL1 0.10 dB  
SFO1 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300079 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00





# <sup>13</sup>C H-decoupled

Current Data Parameters  
 NAME sn15347ap  
 EXPNO 2  
 PROCNO 1  
  
 F2 - Acquisition Parameters  
 Date\_ 20071217  
 Time\_ 8.23  
 INSTRUM av500  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 128  
 DS 4  
 SWH 30030.029 Hz  
 FIDRES 0.458222 Hz  
 AQ 1.0912244 sec  
 RG 18400  
 DW 16.650 usec  
 DE 6.00 usec  
 TE 295.5 K  
 d11 2.00000000 sec  
 d12 0.03000000 sec  
 DELTA 1.89999998 sec  
 TD0 4  
  
 ===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 9.00 usec  
 PL1 0.00 dB  
 SFO1 125.7703637 MHz  
  
 ===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 <sup>1</sup>H  
 P2 80.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 500.1320005 MHz  
  
 F2 - Processing parameters  
 SI 32768  
 SF 125.7578014 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

