

Current Data Parameters  
NAME nada-ahmed-3F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210916  
Time 10.32  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 44  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>1</sup>H NMR for compound 4a



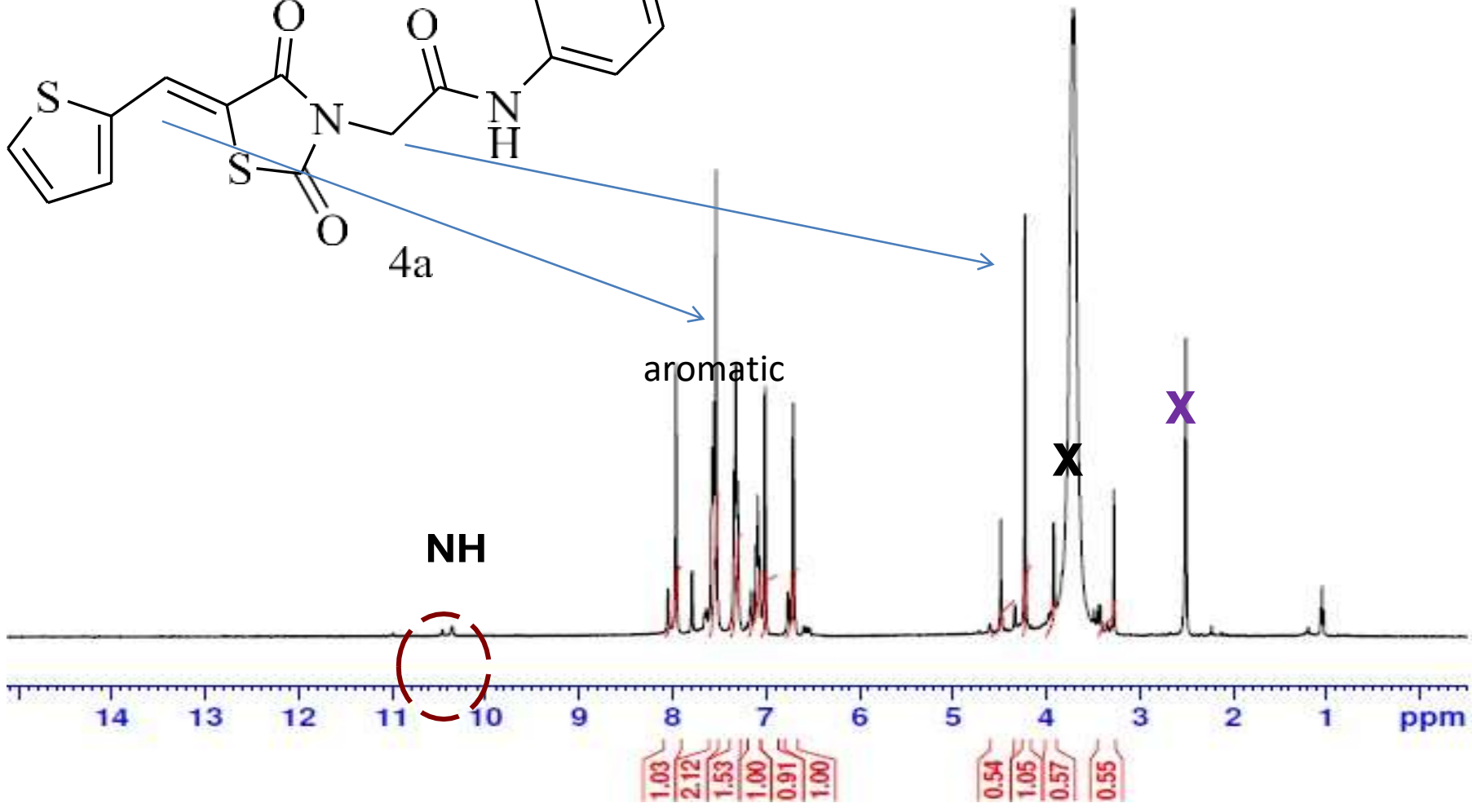
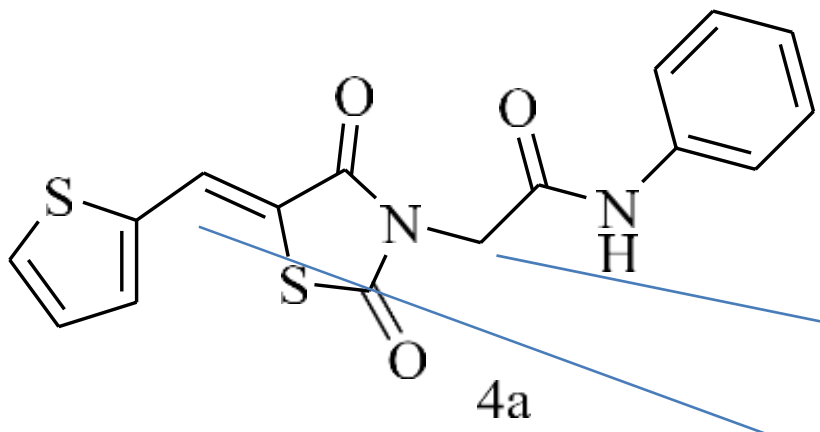
Current Data Parameters  
NAME nada-ahmed-3F-d2o  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210916  
Time 11.47  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zq30  
ID 65536  
SOLVENT DMSO  
NS 39  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.051  
7.963  
7.790  
7.657  
7.634  
7.580  
7.559  
7.534  
7.342  
7.324  
7.304  
7.165  
7.110  
7.092  
7.076  
7.018  
7.008  
6.766  
4.492  
4.341  
4.231  
3.919  
3.717  
3.488  
3.465  
3.440  
3.423  
3.411  
3.363  
3.343  
3.278  
2.507  
1.063



**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 4a**

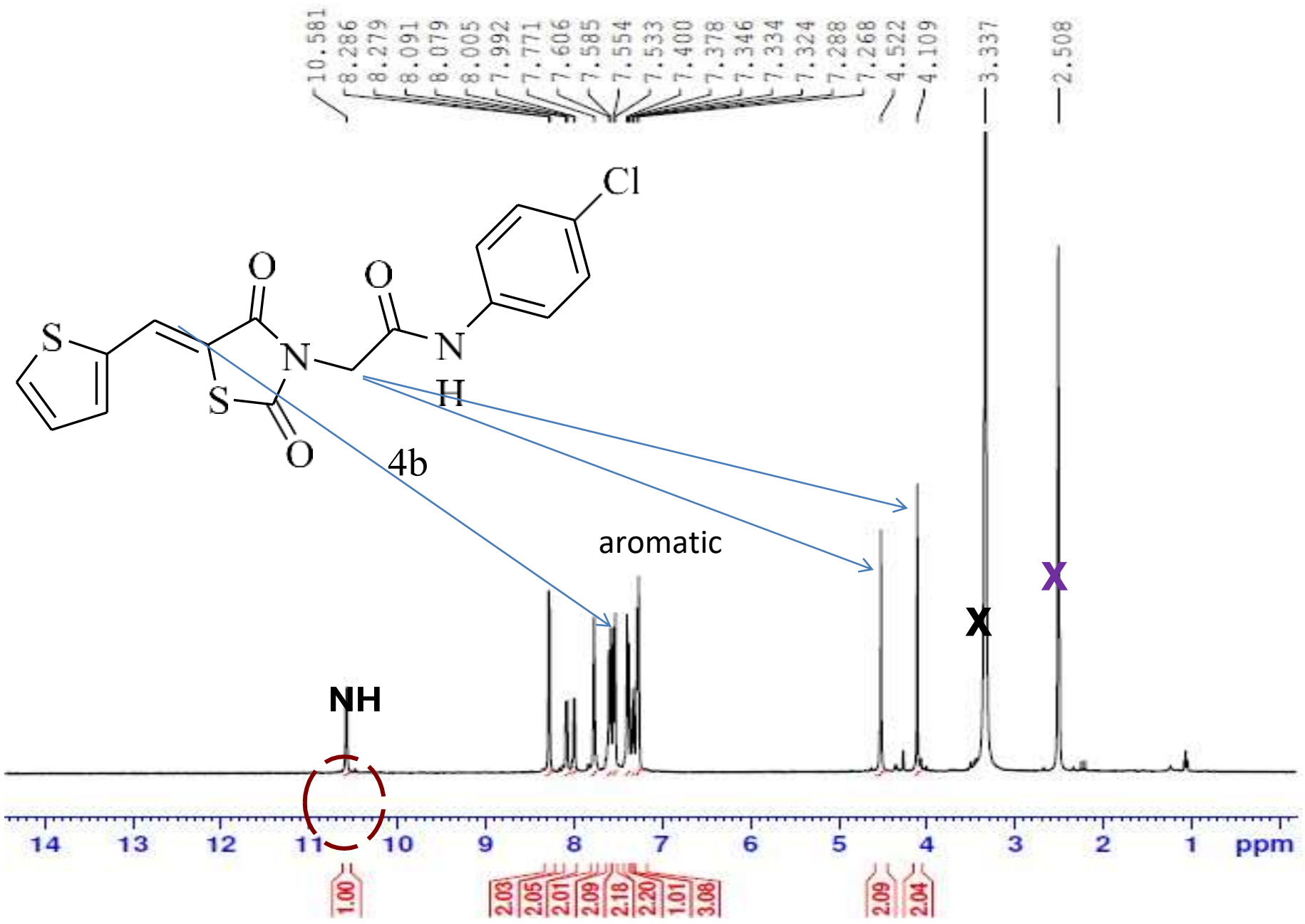


Current Data Parameters  
NAME nada-ahmed-3T  
EXPNO 1  
PROCNO 1

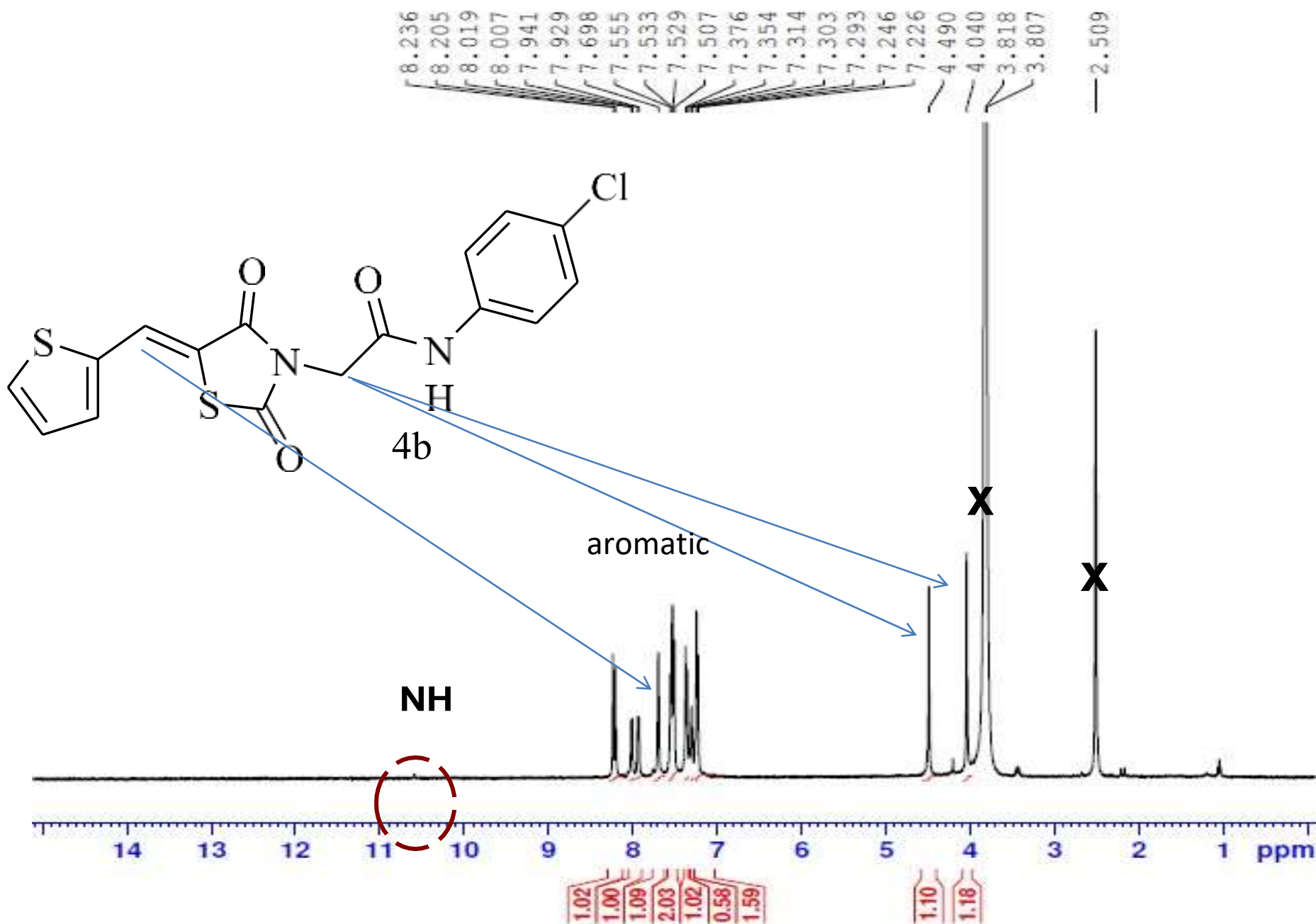
F2 - Acquisition Parameters  
Date\_ 20210916  
Time 10.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 4b**



**BRUKER**

Current Data Parameters  
 NAME nada-ahmed-3T-d2o  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210916  
 Time 11.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 ID 65536  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 IE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

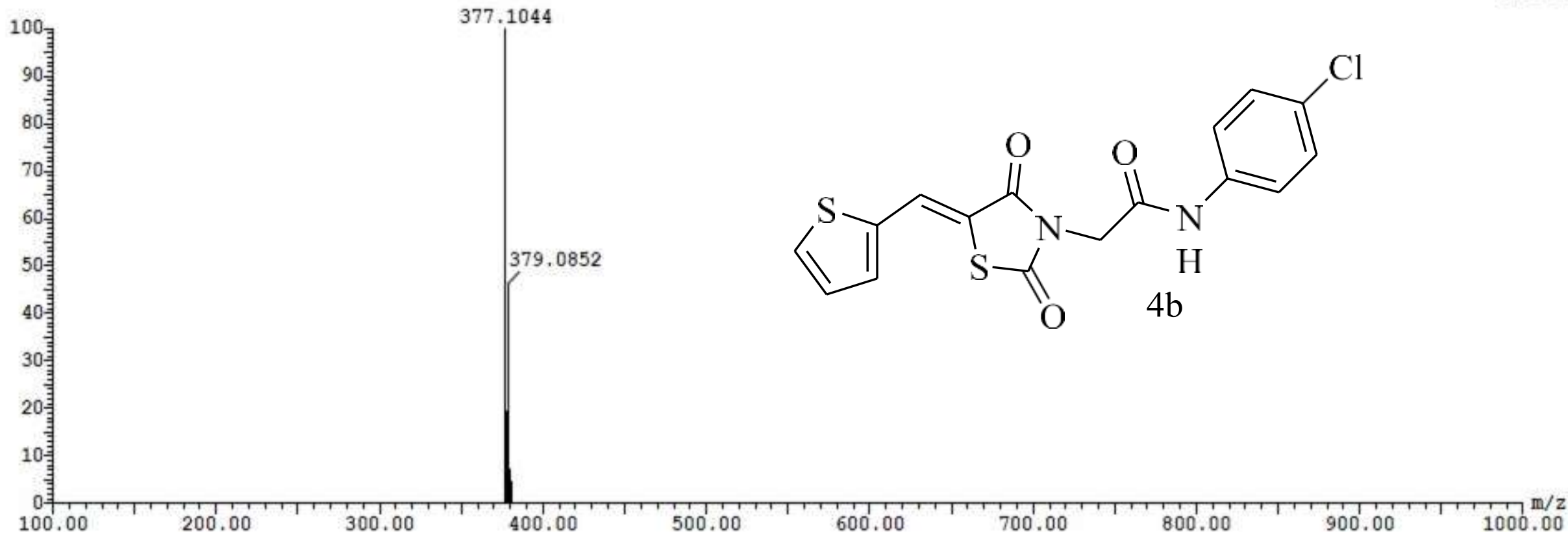
**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 4b**

Peak ID Time Error PPM

7 13.86

(Time: 13.89)

2:MS ES-  
4.0e+006



**LC-MS ESI** spectrometry in the negative ion mode: The mass spectrum of compound **4b** showed M+2 molecular ion peak at 379.0852 and base peak at 377.1044

**Liquid Chromatography-Electrospray Ionization-Mass spectra for compound 4b**

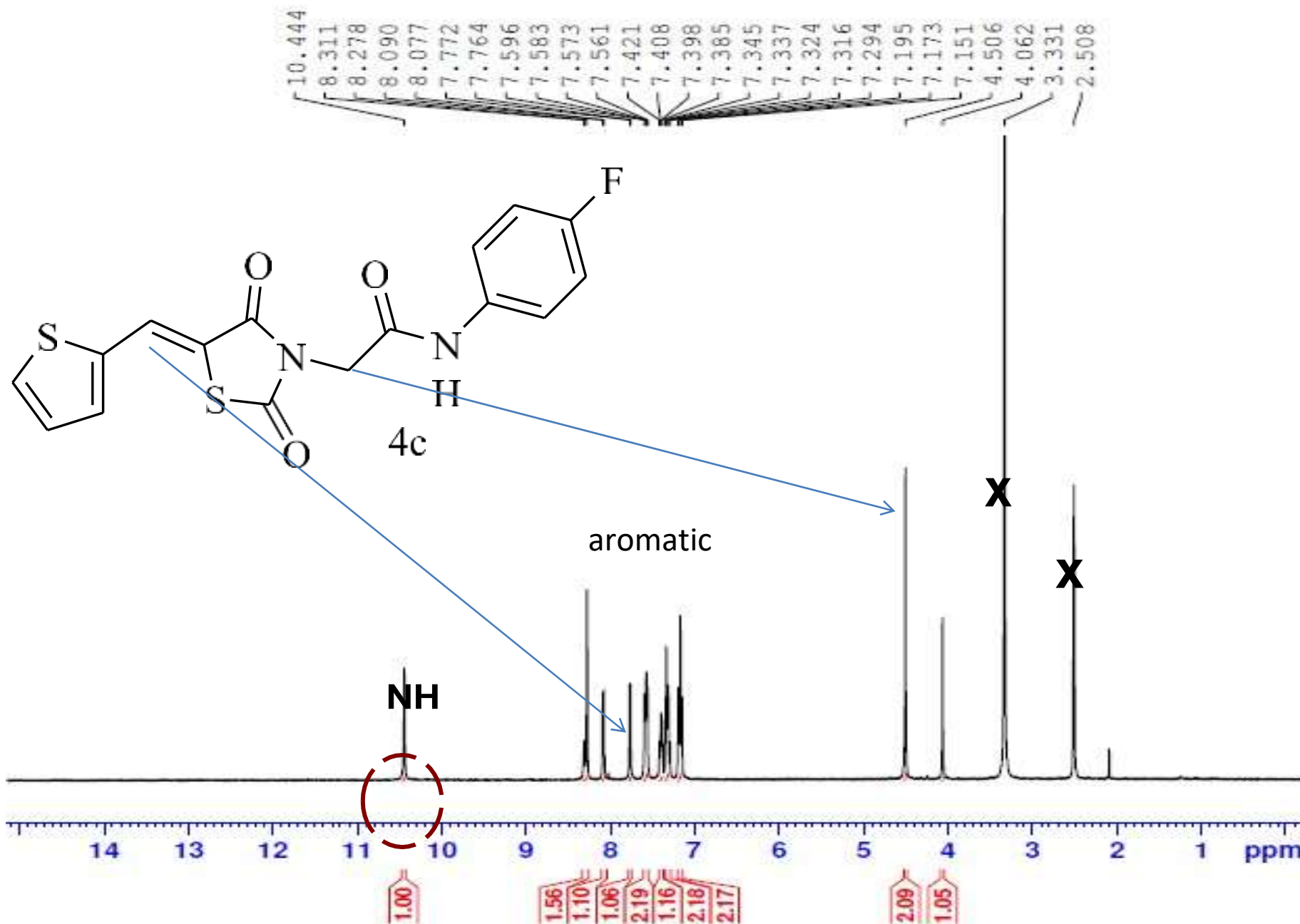


Current Data Parameters  
NAME nada-ahmed-4T  
EXPNO 1  
PROCNO 1

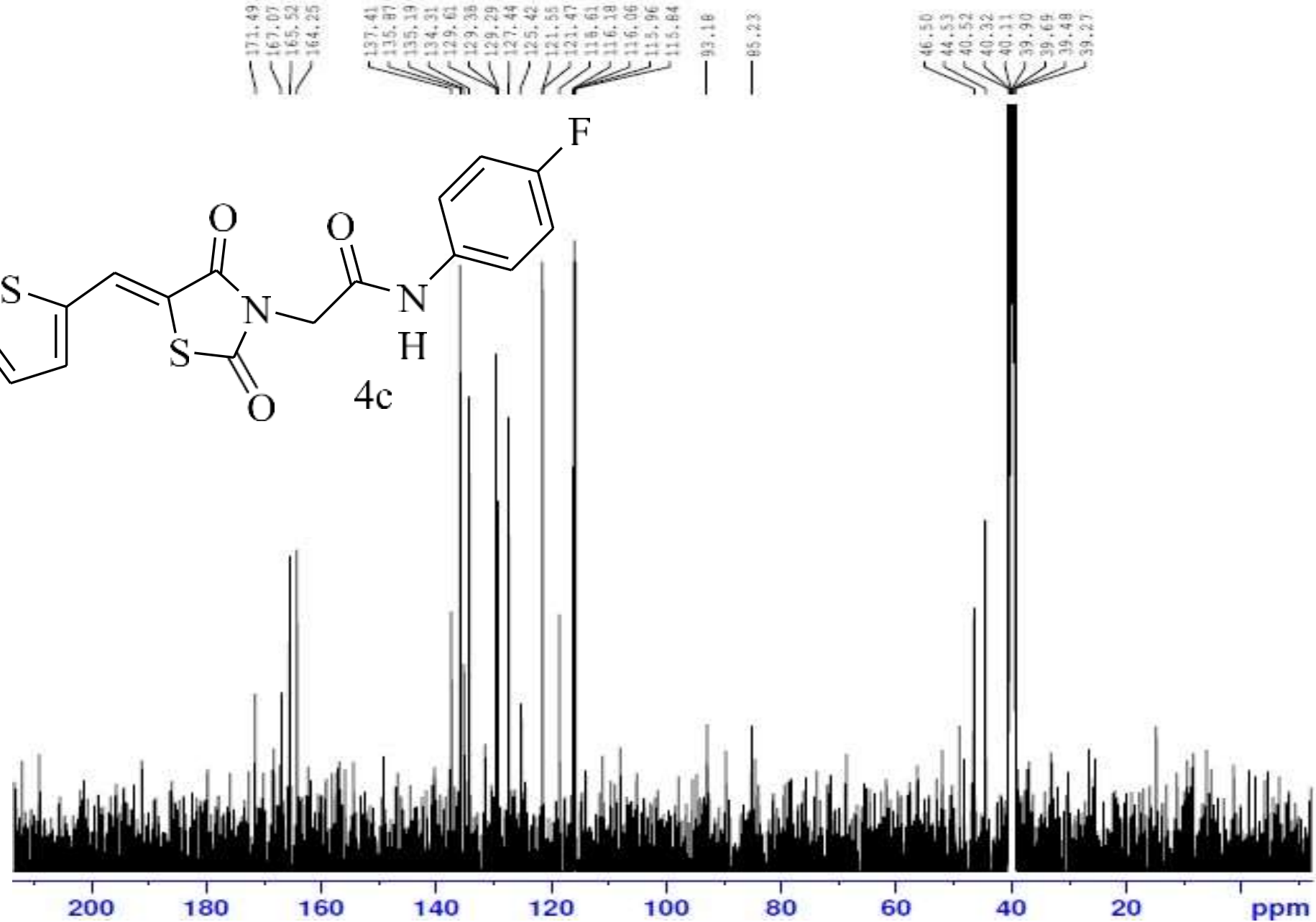
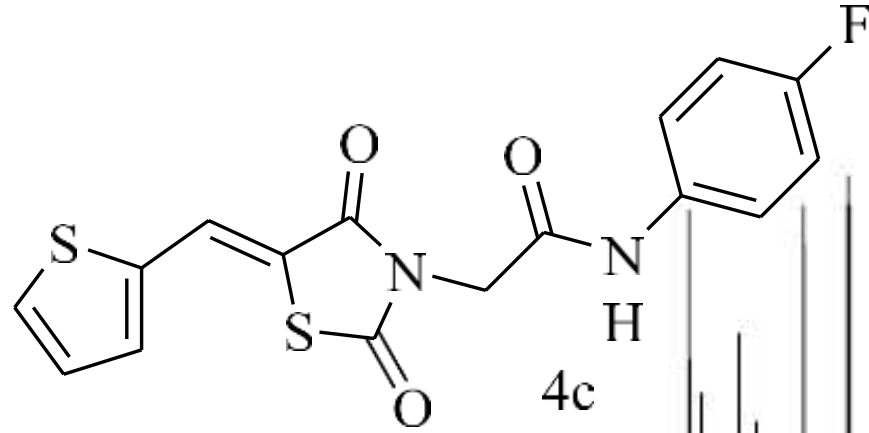
F2 - Acquisition Parameters  
Date\_ 20210906  
Time 15.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 17  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
IE 300.0 K  
D1 1.00000000 sec  
ID0 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 4c**



Current Data Parameters  
NAME nada-ahmed-4f  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210920  
Time 16.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
ID 65536  
SOLVENT DMSO  
NS 1501  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 205.37  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 47.00000000 W

----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 18.00000000 W  
PLW12 0.34722000 W  
PLW13 0.28125000 W

F2 - Processing parameters  
SI 32768  
SF 100.6177975 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

**<sup>13</sup>C NMR for compound 4c**

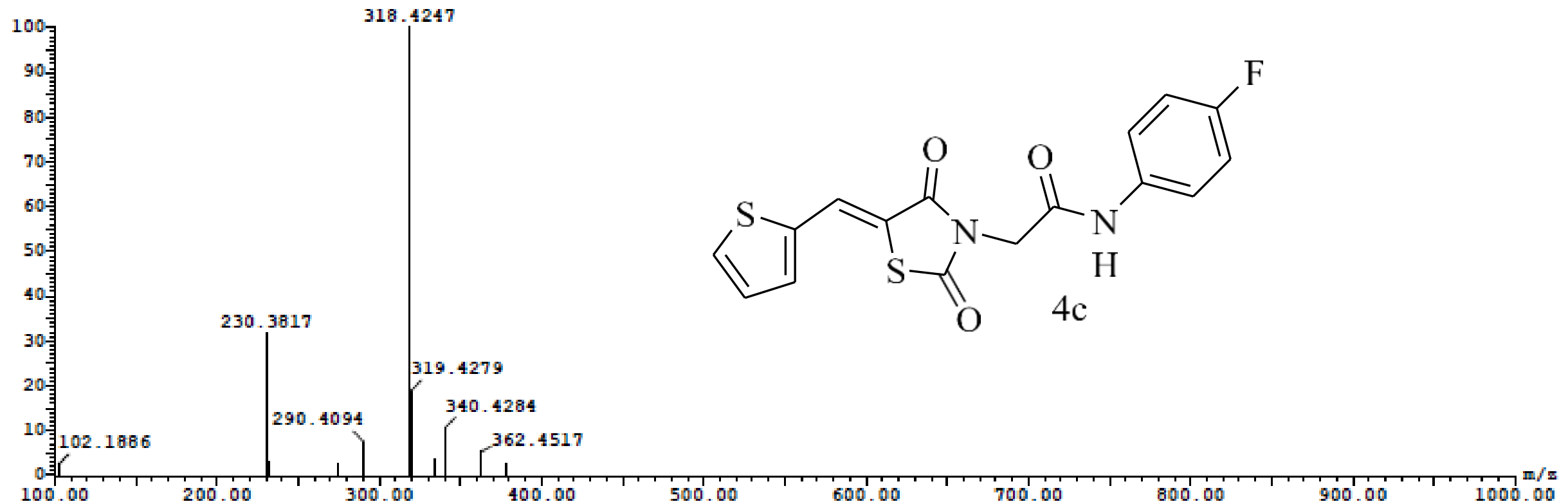
Peak ID Time Error PPM

9 11.67

(Time: 11.67)

1:MS ES+

1.2e+07



**LC-MS ESI** spectrometry in the positive ion mode: The mass spectrum of compound **4c** showed M molecular ion peak at 362.4517. It showed base peak at 318.4247.

**Liquid Chromatography-Electrospray Ionization-Mass spectra for compound 4c**

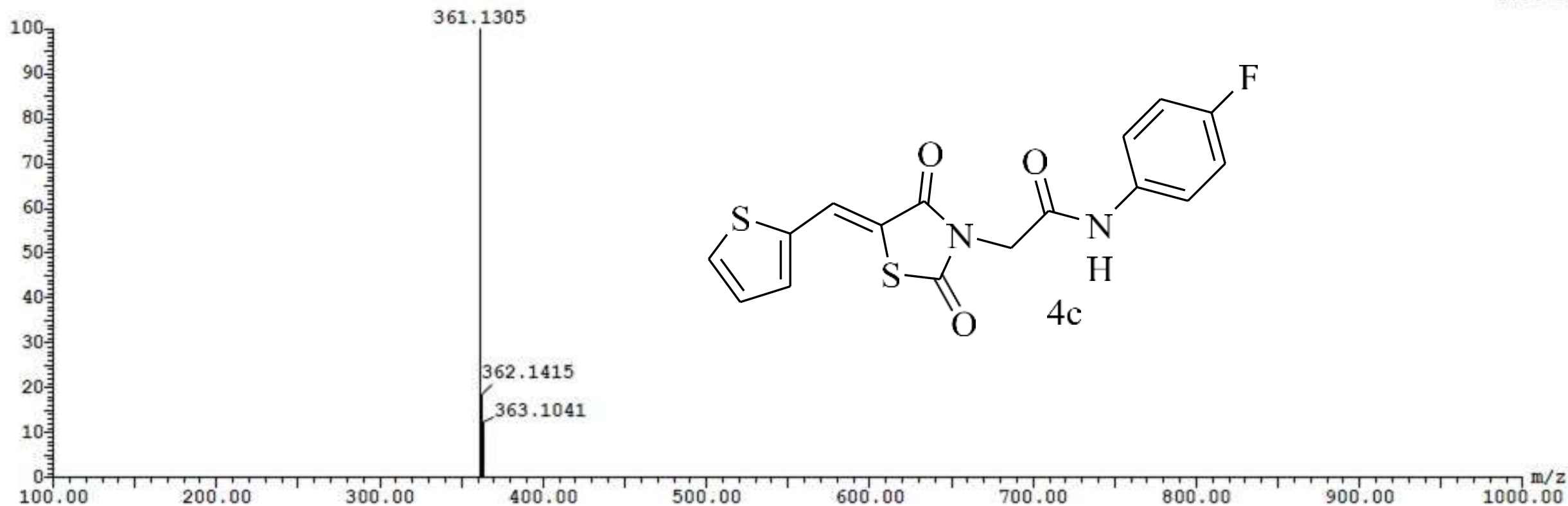


Peak ID Time Error PPM

11 12.66

(Time: 12.67)

2:MS ES-  
1.0e+007



**LC-MS ESI** spectrometry in the negative ion mode: The mass spectrum of compound **4c** showed M-1 molecular ion peak at 361.1305 which also was the base peak. It showed M molecular ion peak at 362.1415 and M+1 molecular ion peak at 363.1041

**Liquid Chromatography-Electrospray Ionization-Mass spectra for compound 4c**

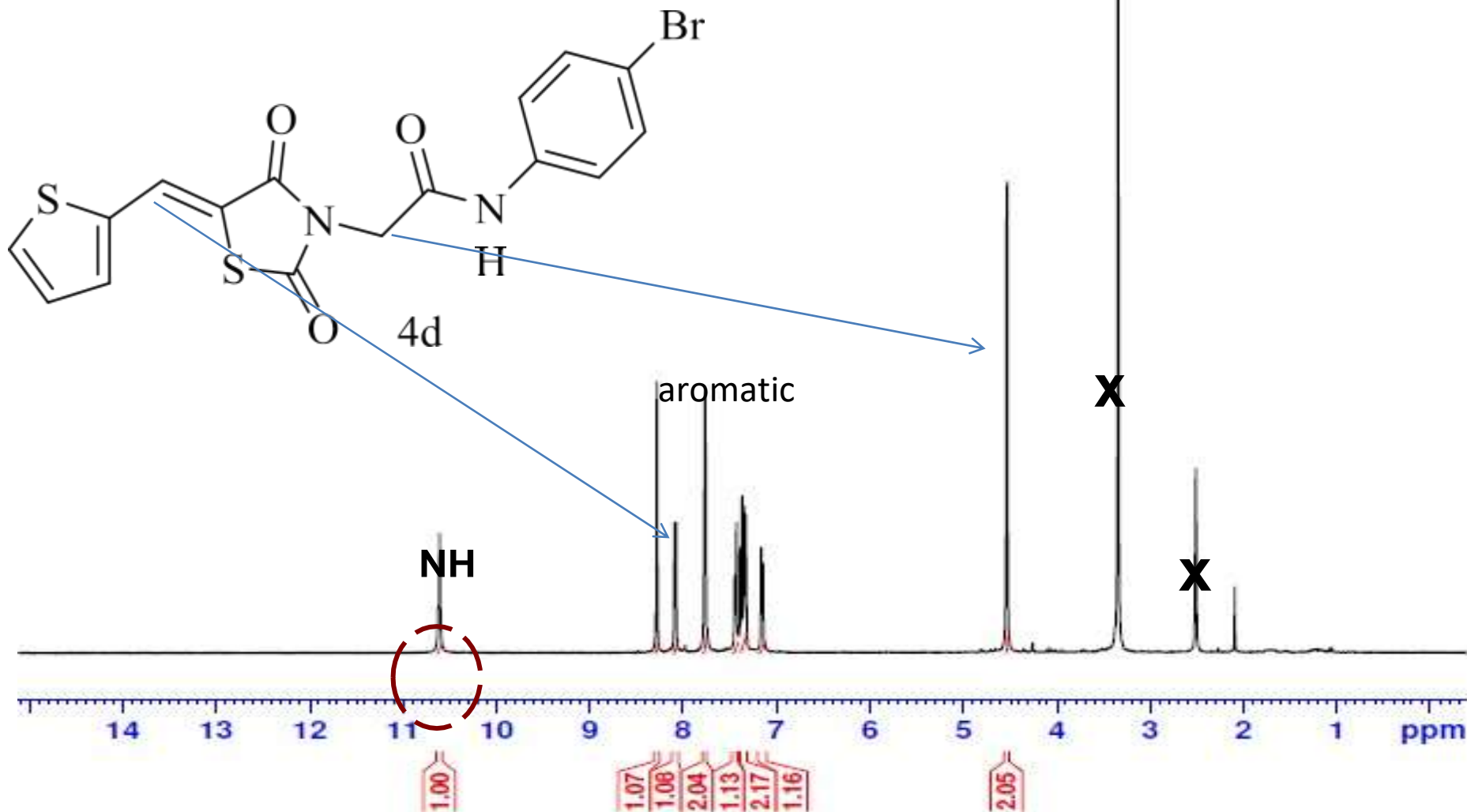


Current Data Parameters  
NAME nada-ahmed-6T  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210906  
Time 16.04  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SF01 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 4d**



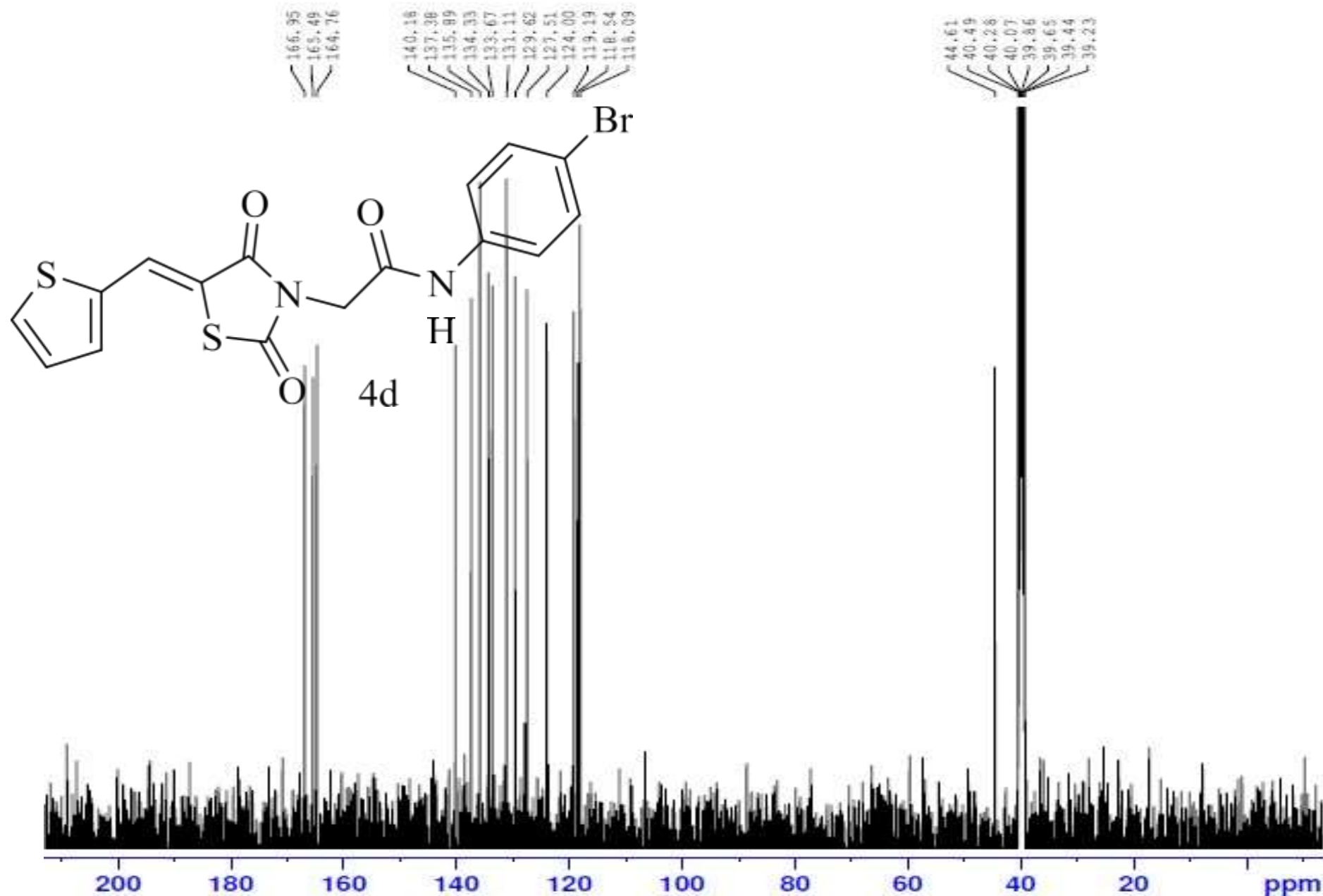
Current Data Parameters  
NAME nada-ahmed-6T  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210920  
Time 14.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
ID 65536  
SOLVENT DMSO  
NS 951  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 205.37  
DW 20.800 usec  
DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 100.6278588 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 47.00000000 W

----- CHANNEL f2 -----  
SFO2 400.1516006 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 18.00000000 W  
PLW12 0.34722000 W  
PLW13 0.28125000 W

F2 - Processing parameters  
SI 32768  
SF 100.6177975 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



$^{13}\text{C}$  NMR for compound 4d

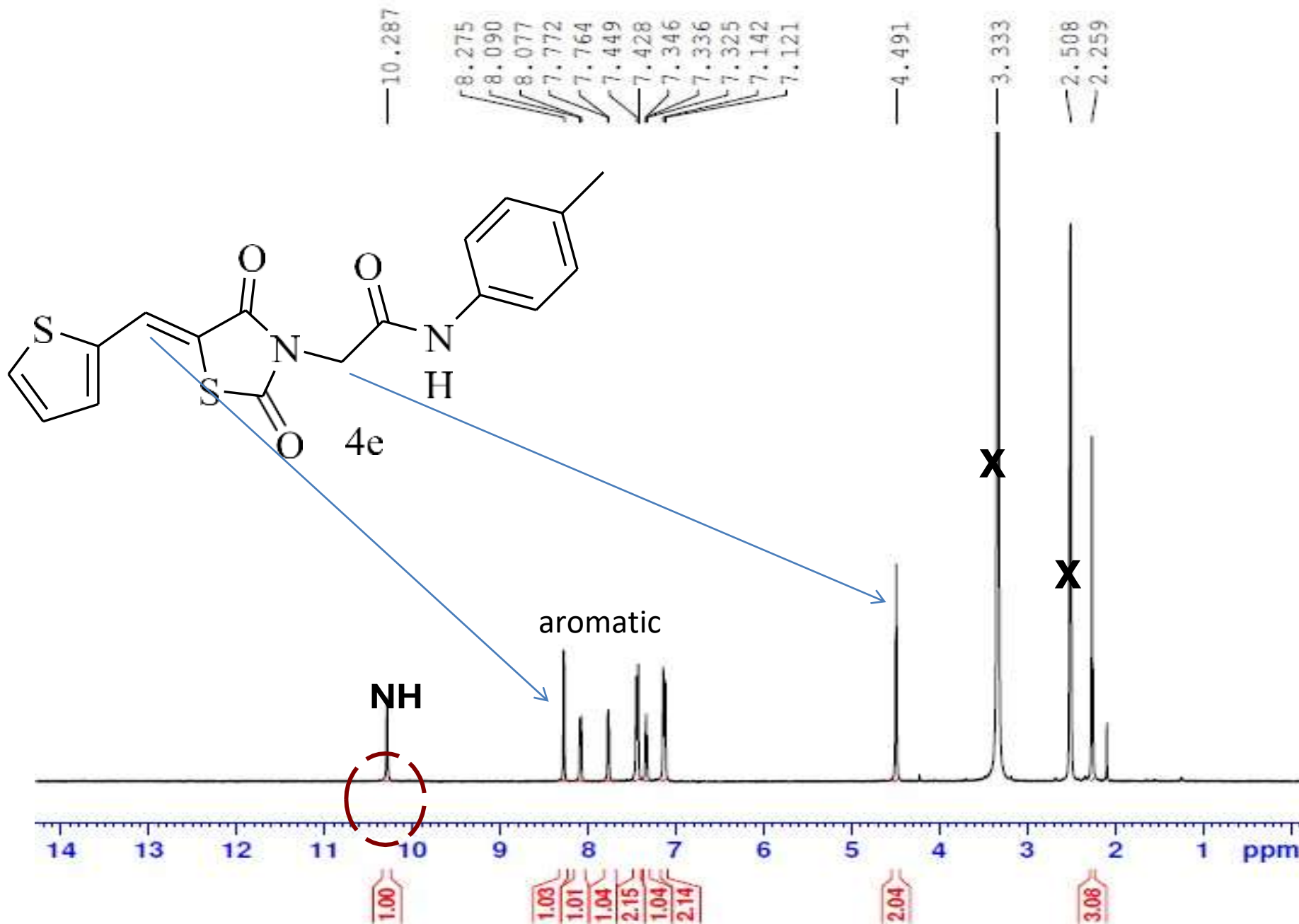


Current Data Parameters  
NAME nada-ahmed-7I  
EXPNO 1  
PROCNO 1

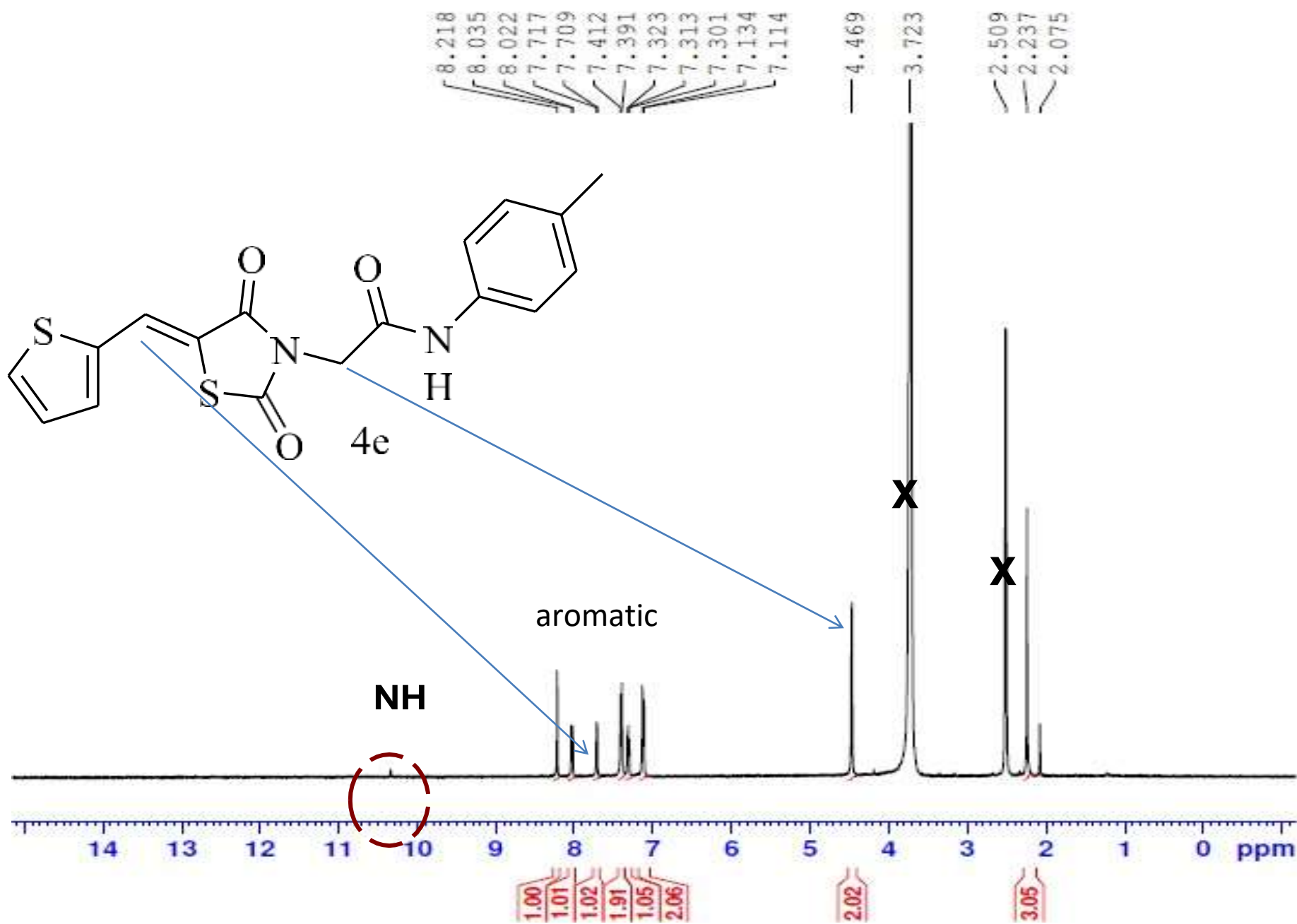
F2 - Acquisition Parameters  
Date\_ 20210916  
Time 11.12  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 79  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 4e**



Current Data Parameters  
 NAME nada-ahmed-7I-d2o  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20210916  
 Time 11.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 ID 65536  
 SOLVENT DMSO  
 NS 27  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 IE 300.0 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 4e**



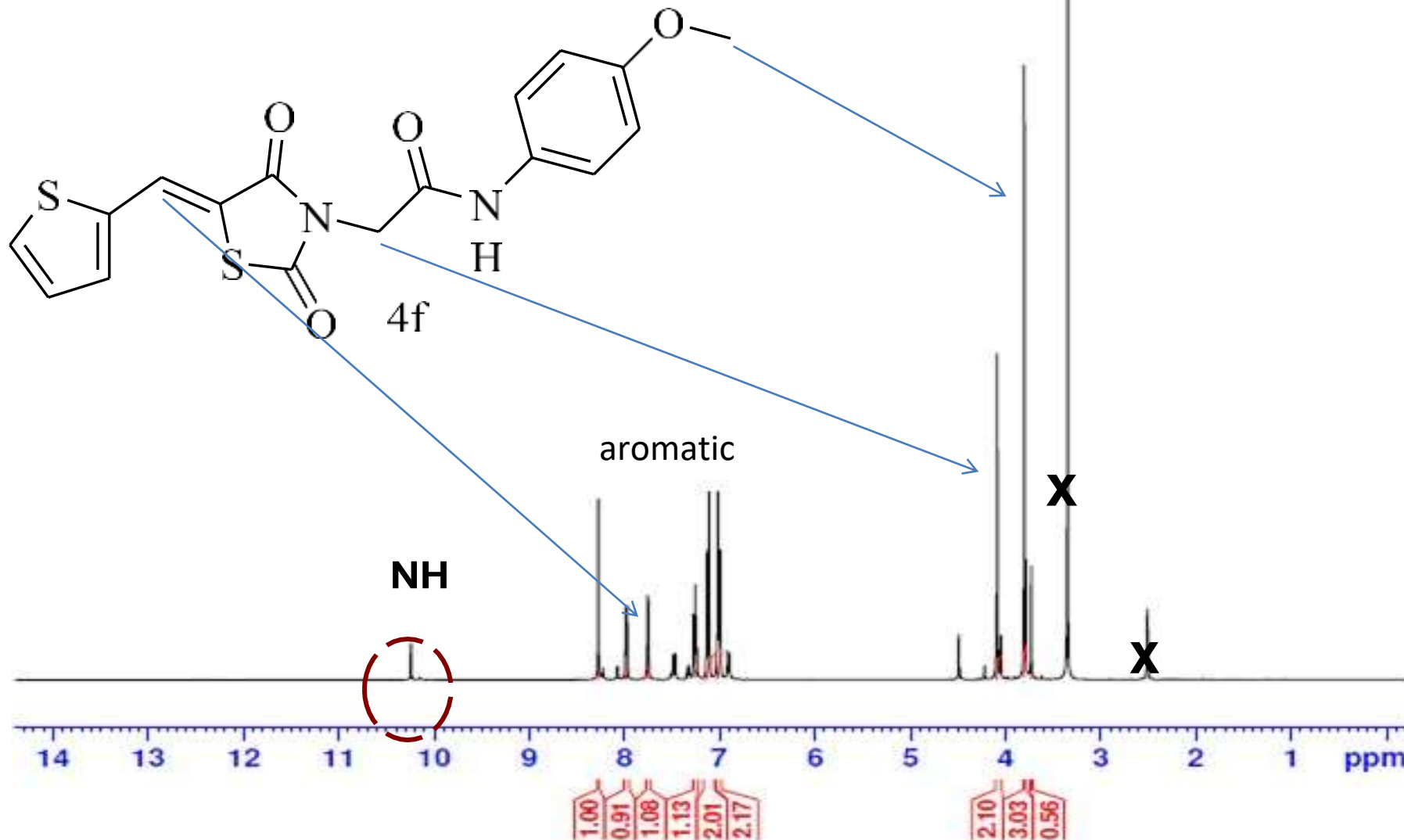
Current Data Parameters  
NAME nada-ahmed-5T  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210916  
Time 10.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 94  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.150000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

8.275  
7.986  
7.974  
7.757  
7.749  
7.272  
7.262  
7.259  
7.250  
7.237  
7.133  
7.128  
7.111  
7.028  
7.026  
7.017  
7.012  
7.006  
7.000  
6.995  
4.087  
4.046  
3.801  
3.787  
3.727  
3.348  
2.512  
2.508  
2.503



<sup>1</sup>H NMR for compound 4f



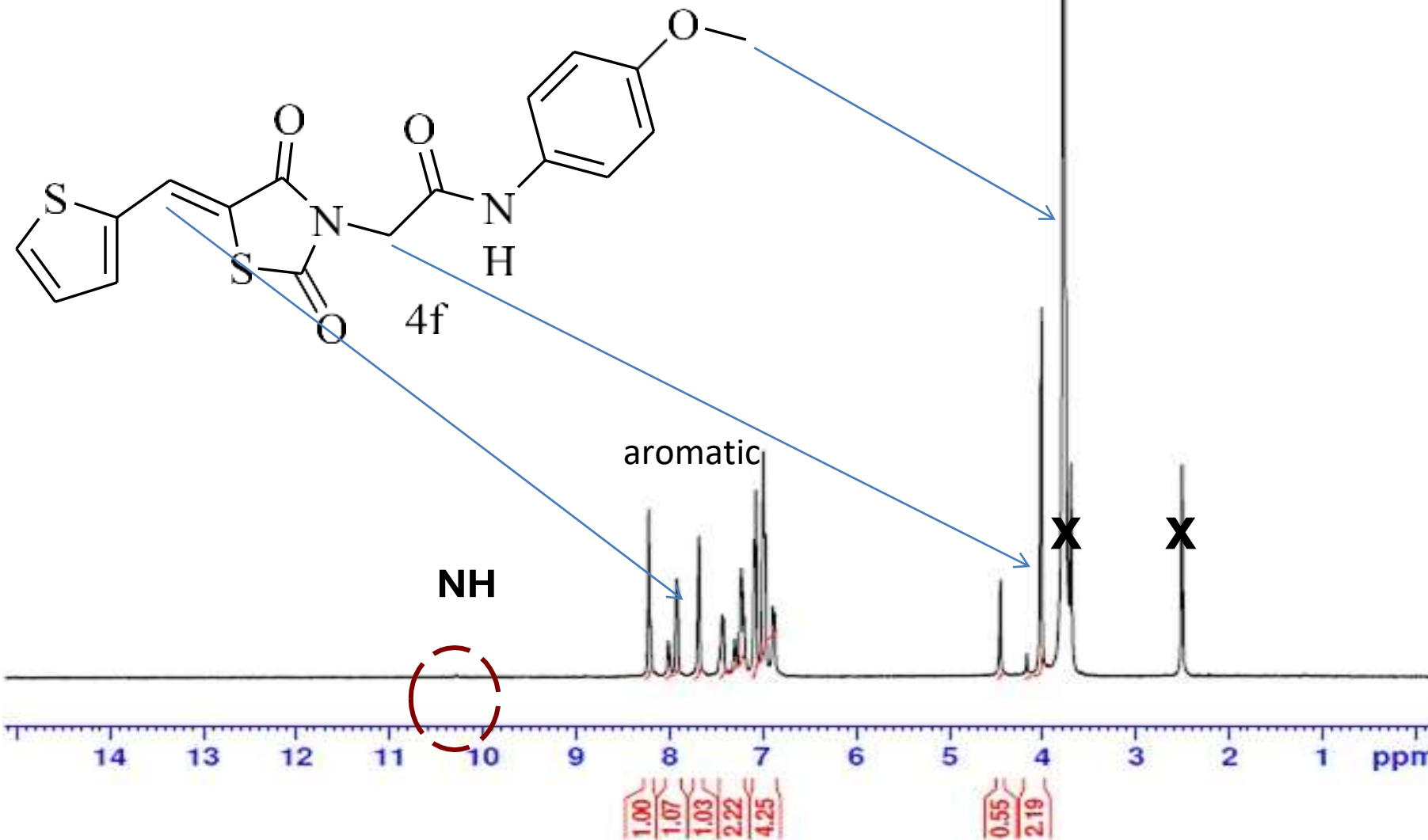
Current Data Parameters  
NAME nada-ahmed-5I-d2o  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210916  
Time 11.41  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 40  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
SF01 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.0000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

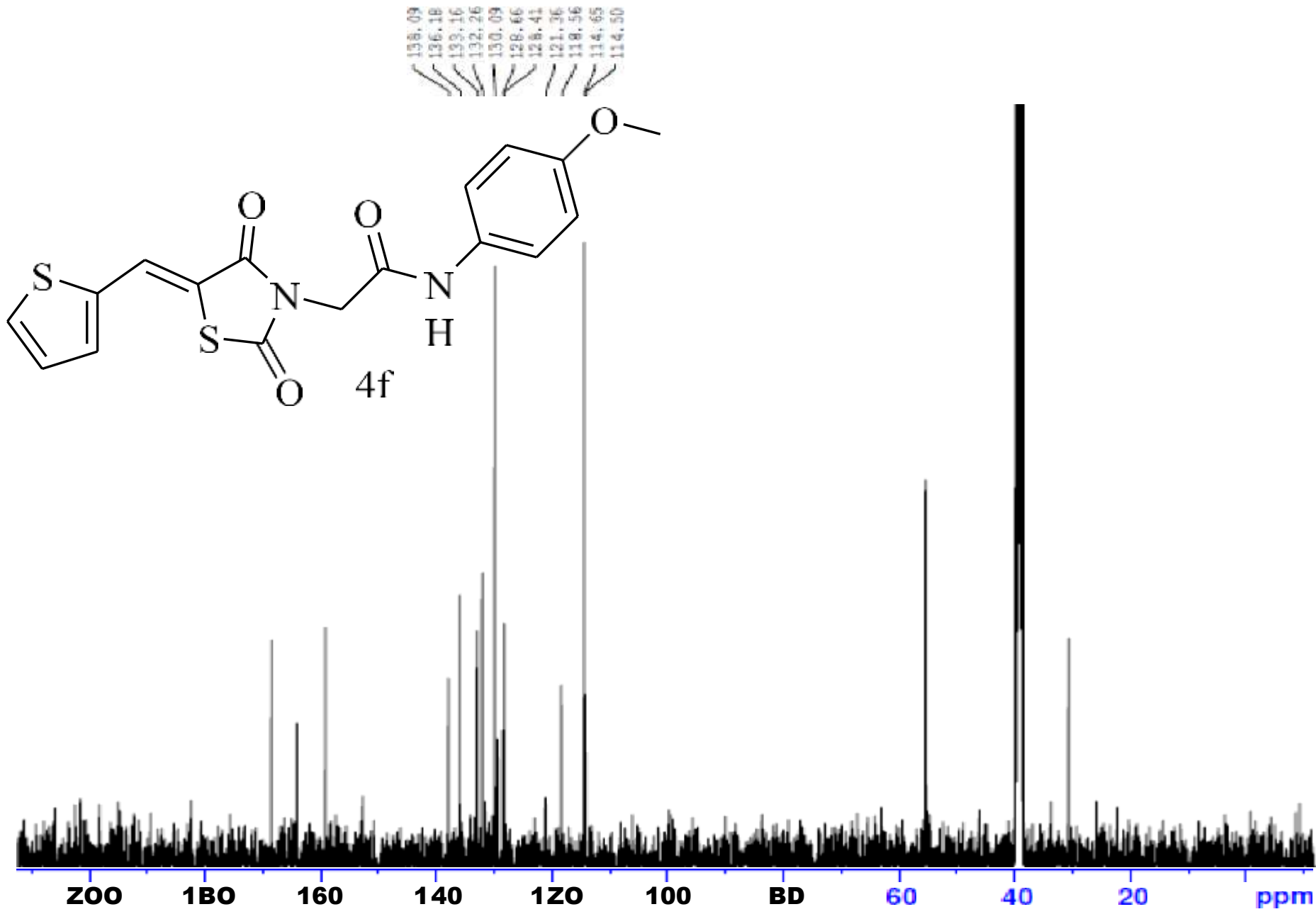
8.223  
8.208  
8.015  
7.921  
7.687  
7.444  
7.423  
7.299  
7.238  
7.206  
7.091  
7.078  
6.999  
6.978  
6.896  
6.878  
4.466  
4.170  
4.035  
3.775  
3.714  
2.517



**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 4f**



current ontanta Parameters



oate\_ 20211028

PRDBHO b oxs PABBO BB/  
PULP|ROG zgpqZo

ns L9J 4

EH TED3B.Oil Hz  
FIDRES D.366W9B Hz  
AQ 1.36BLO88 Dec  
RG PD5.3W  
DW JD.BOO uaec

TE SDO.0K  
OL Z.DDDDD000 C  
OLL 0.DZDDDD00 C  
TDD 1

sFol 100.6278588 MHz  
NUC1 13C  
PL LD.00 U C  
PI]01 47.DDDDD000 W

sPoJ 400.1516006 MHz  
WUCJ 1H  
EPOPRG[] waltz16  
PCPO2 9D.00 uW=u  
PImJ 2B.DDDDD000 N

PL]01Z 0.28125000 W

FJ - Processing parameters

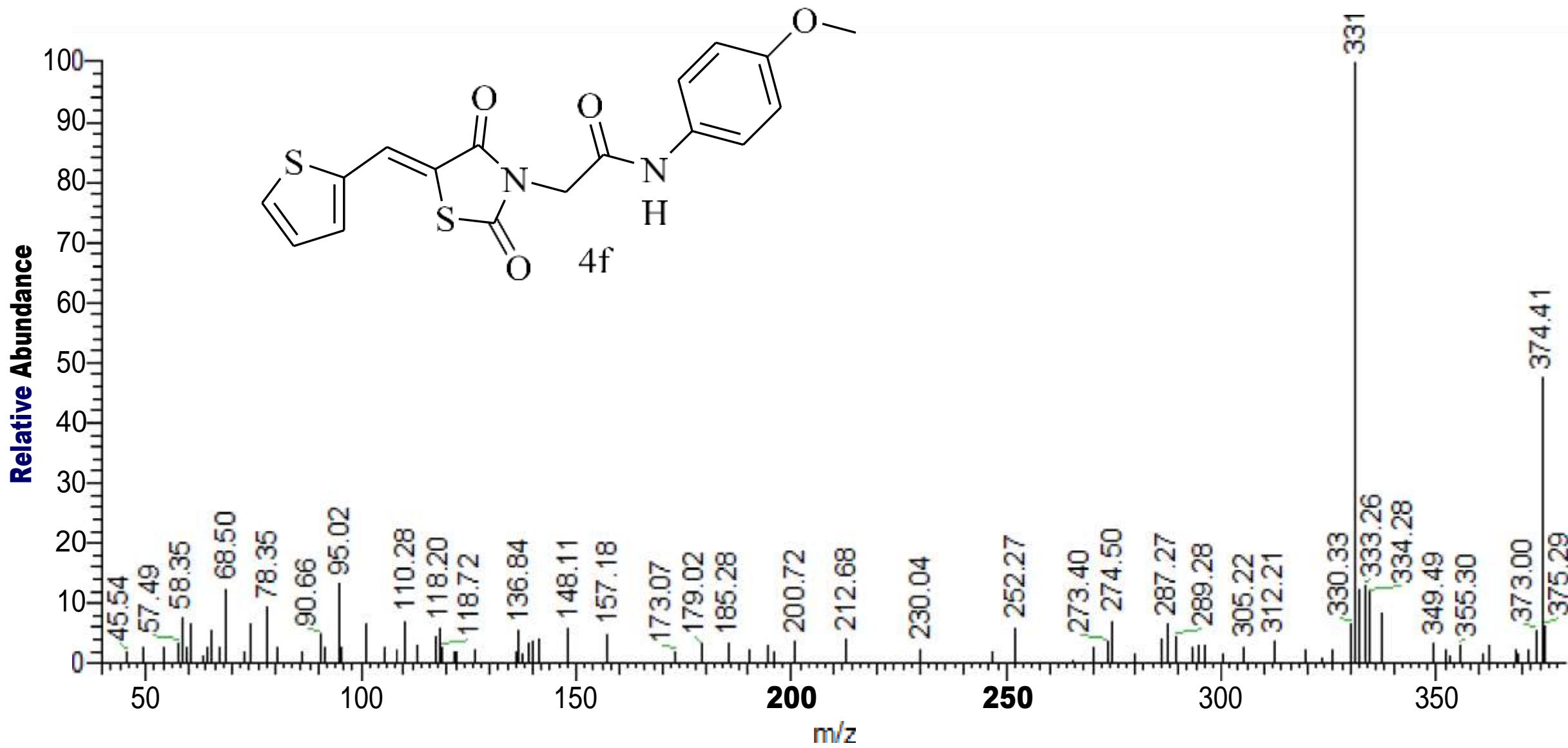
SF 100.6177975 MHz

LB 1.00 Hz

PO L40

<sup>13</sup>C NMR for compound 4f





Mass spectra for compound 4f

10.651  
10.504  
8.366  
8.305  
8.286  
8.262  
8.108  
8.071  
8.054  
7.986  
7.975  
7.746  
7.722  
7.703  
7.646  
7.621  
7.613  
7.595  
7.549  
7.529  
7.422  
7.393  
7.374  
7.336  
7.312  
7.290  
7.271  
7.174  
7.163  
7.146  
4.656  
4.545  
4.263  
4.128  
4.054  
3.538  
3.428  
2.924  
2.764  
2.555  
2.494  
2.138  
2.088

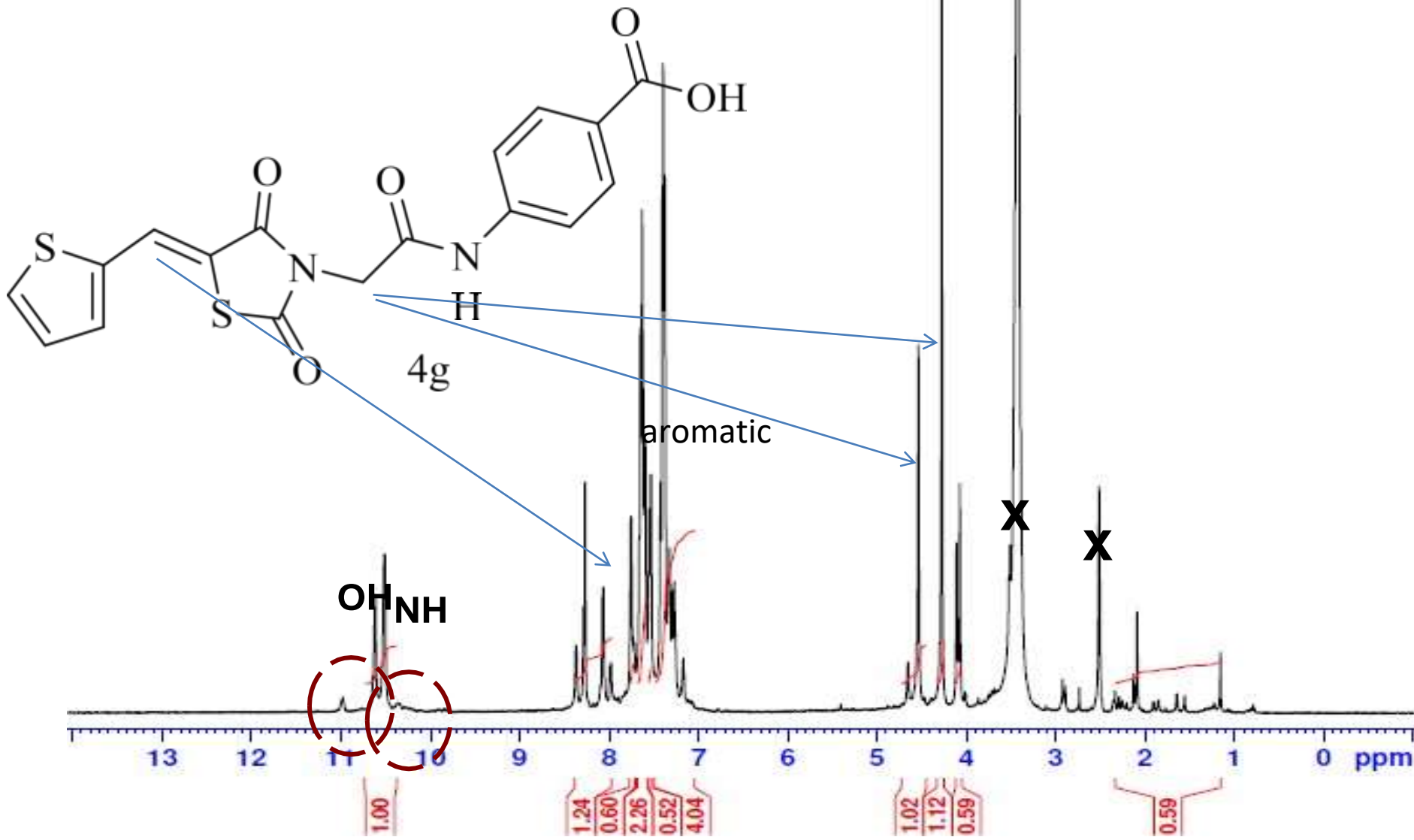


Current Data Parameters  
 NAME nada-aziz-9T  
 EXPNO 1  
 PROCNO 1

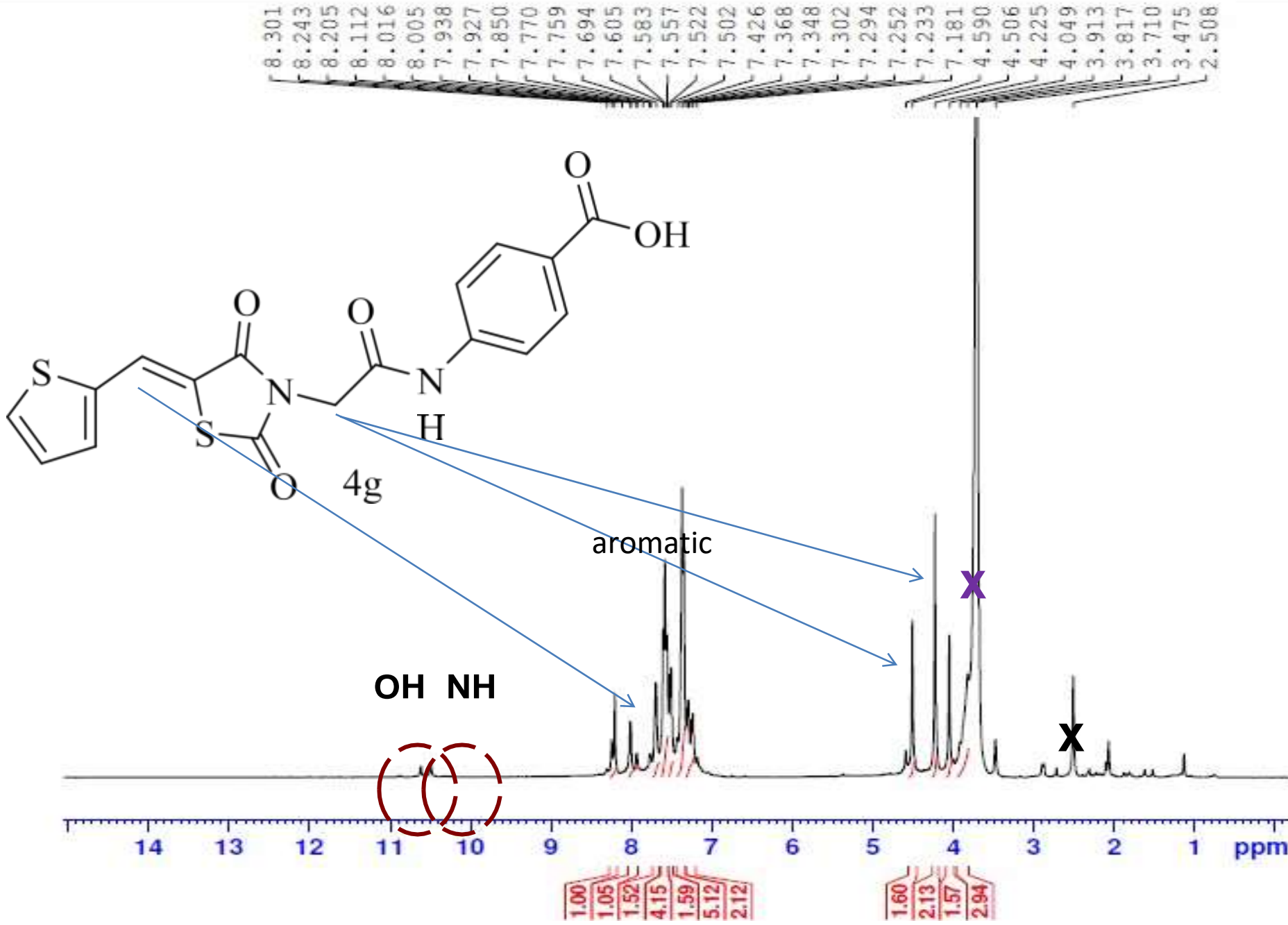
F2 - Acquisition Parameters  
 Date\_ 20211004  
 Time 14.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 ID 65536  
 SOLVENT DMSO  
 NS 22  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 ID0 1

----- CHANNEL f1 -----  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



<sup>1</sup>H NMR for compound 4g



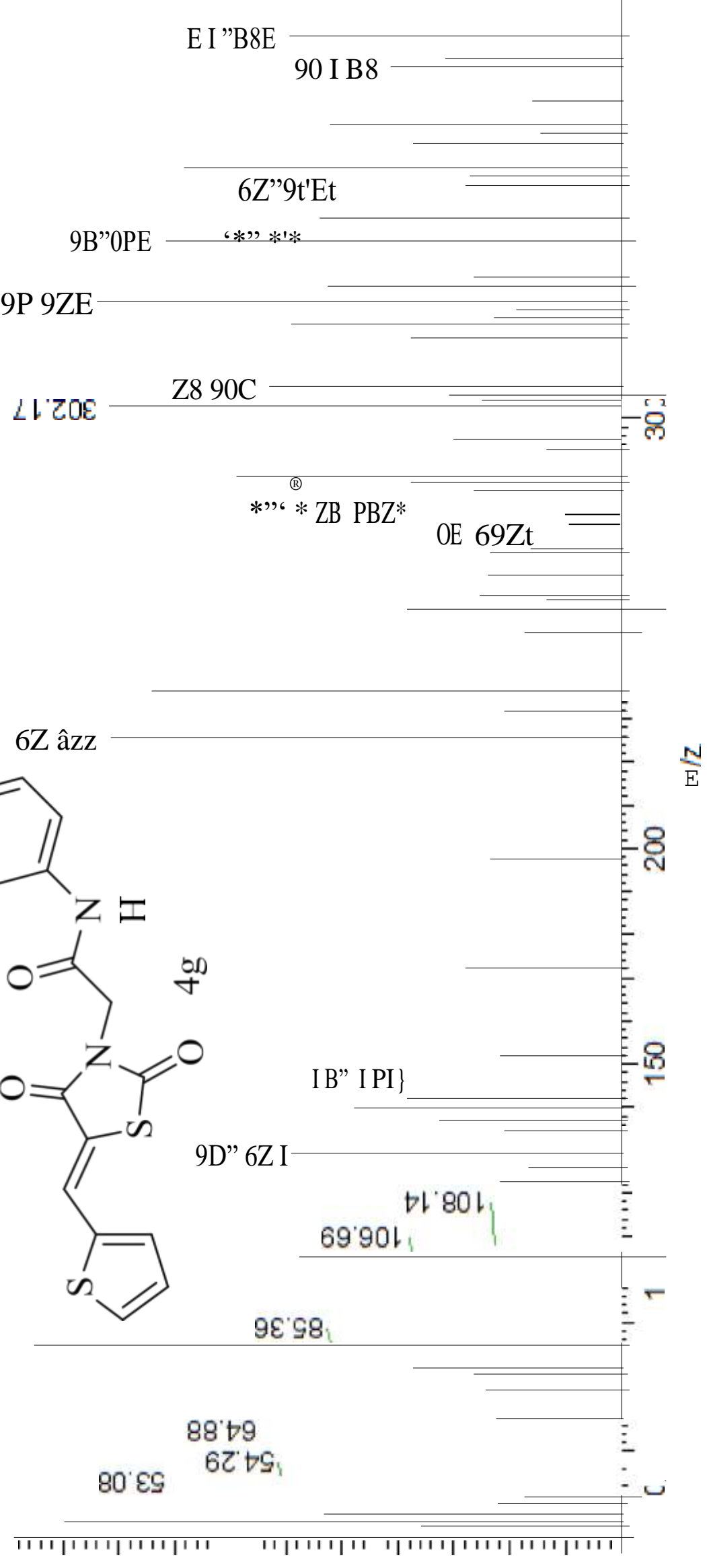
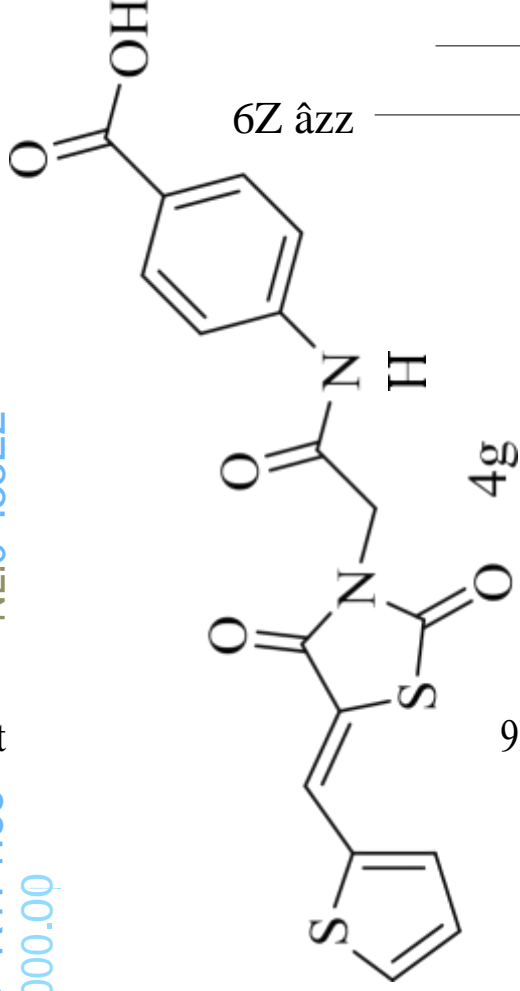
Current Data Parameters  
 NAME nada-aziz-9I-d2o  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211005  
 Time 10.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 ID 65536  
 SOLVENT DMSO  
 NS 63  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 ID0 1

CHANNEL f1  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 4g**



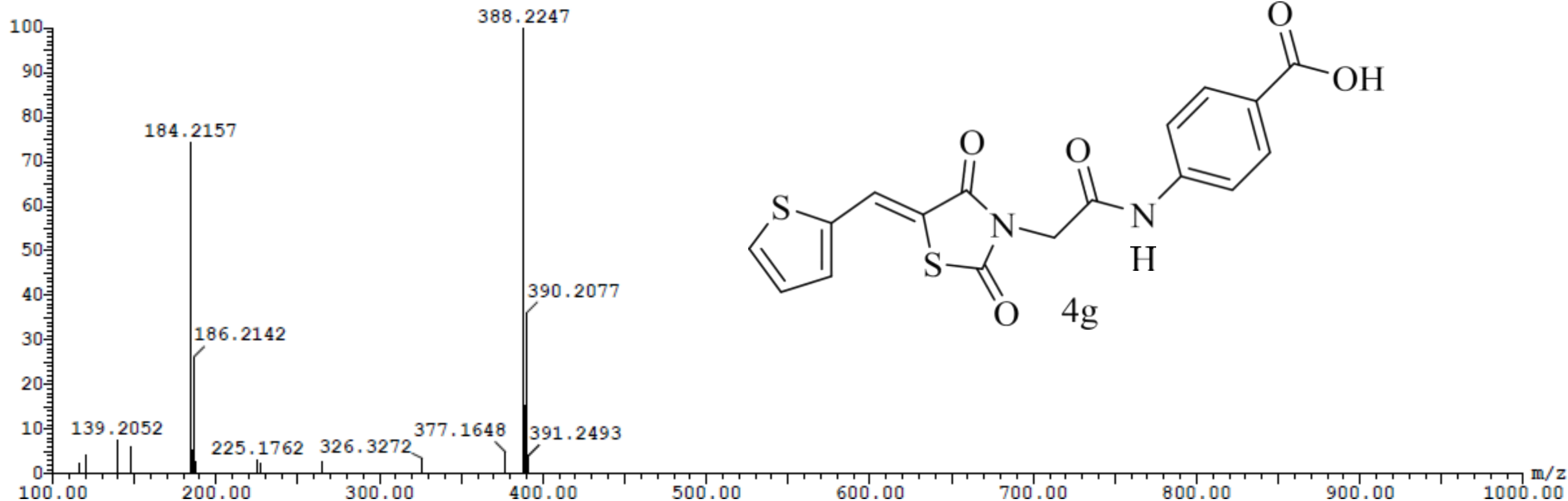
Mass spectra for compound 4g

Peak ID Time Error PPM

15 8.39

(Time: 8.39)

1:MS ES+  
1.4e+007



**LC-MS ESI** spectrometry in the positive ion mode: The mass spectrum of compound **4g** showed M molecular ion peak at 388.2247 which also was the base peak. It showed M+2 and M+3 molecular ion peaks at 390.2077 and 391.2493 respectively.

**Liquid Chromatography-Electrospray Ionization-Mass spectra for compound 4g**

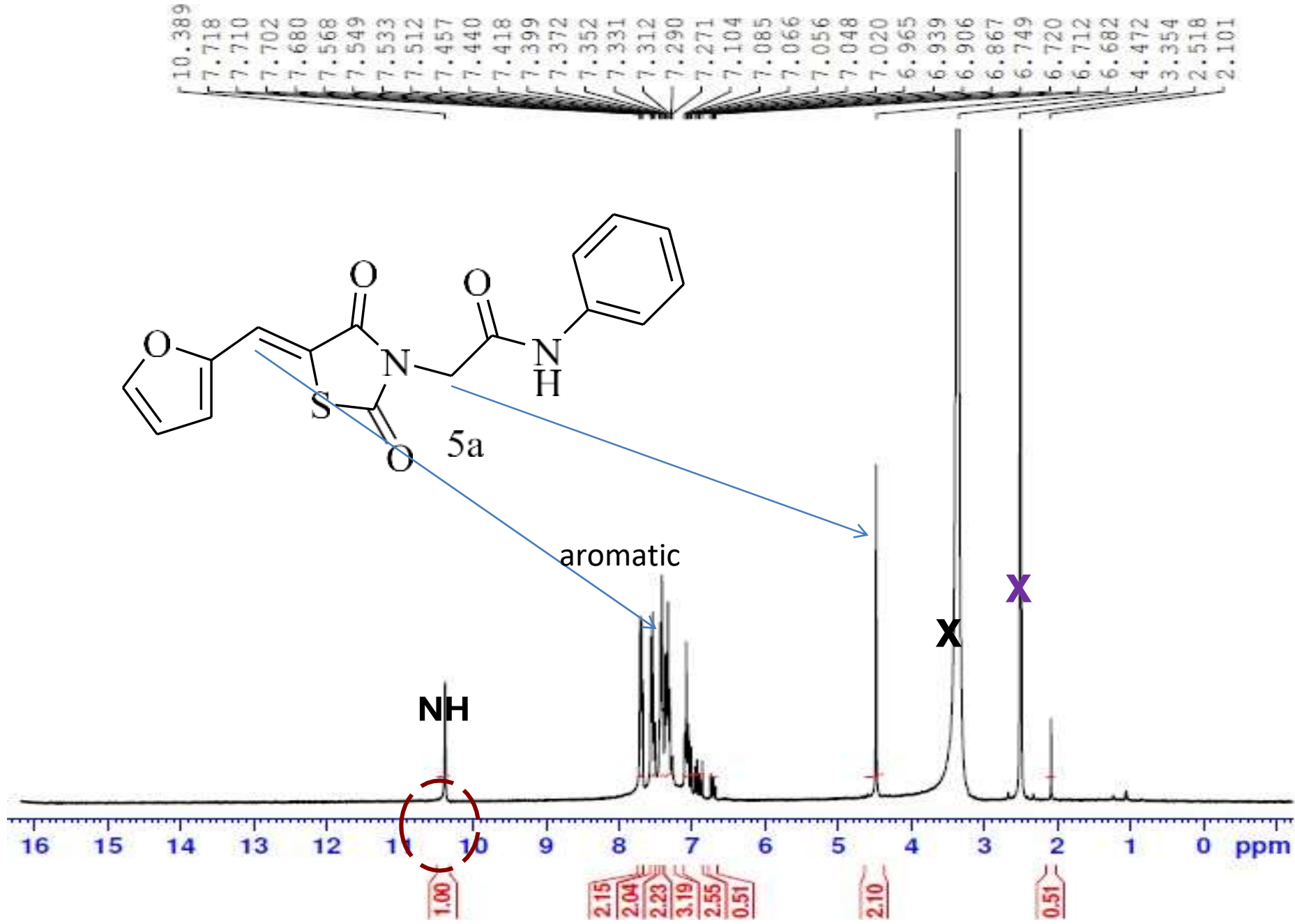


Current Data Parameters  
NAME nada-aziz-3F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211004  
Time 14.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 128  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SF01 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 5a**



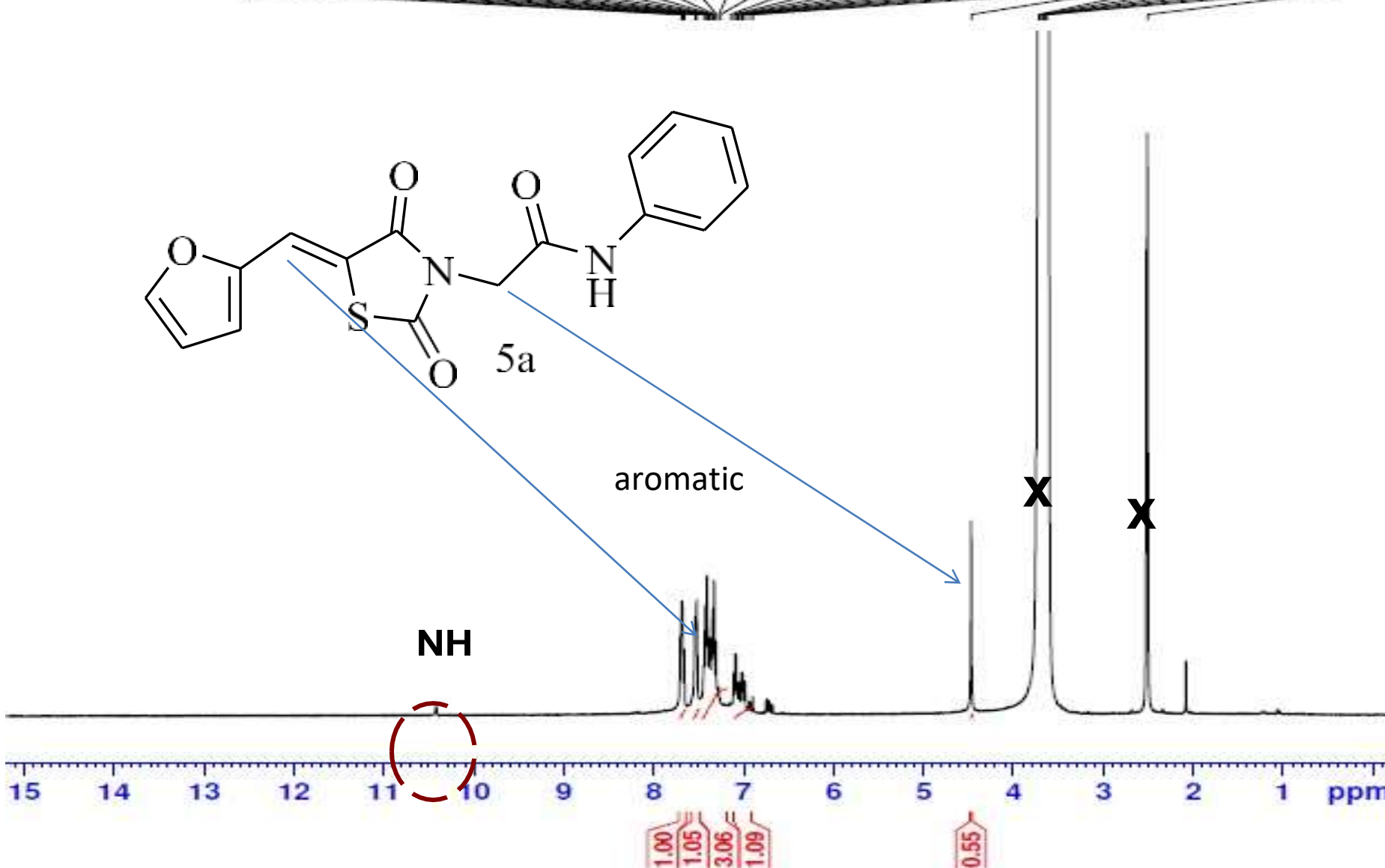
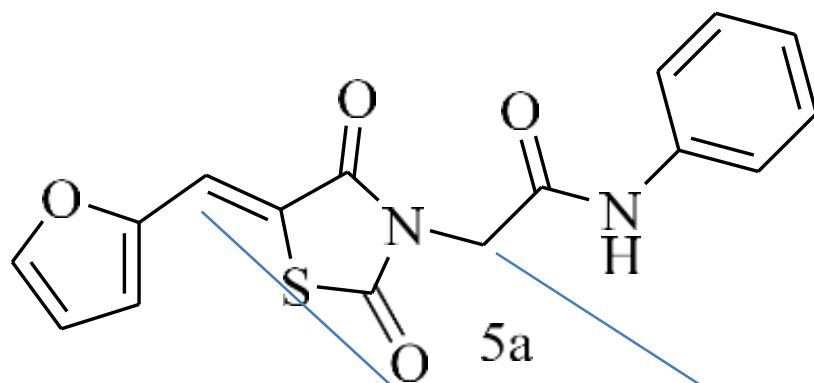
Current Data Parameters  
NAME nada-azir-3f-d2o  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211005  
Time 10.22  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 122  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.694  
7.683  
7.656  
7.538  
7.519  
7.437  
7.423  
7.404  
7.385  
7.373  
7.354  
7.343  
7.335  
7.324  
7.304  
7.274  
7.257  
7.148  
7.104  
7.085  
7.067  
7.046  
7.016  
7.011  
6.979  
6.931  
6.894  
4.466  
3.714  
3.694  
3.671  
3.653  
3.636  
3.625  
2.508



<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 5a

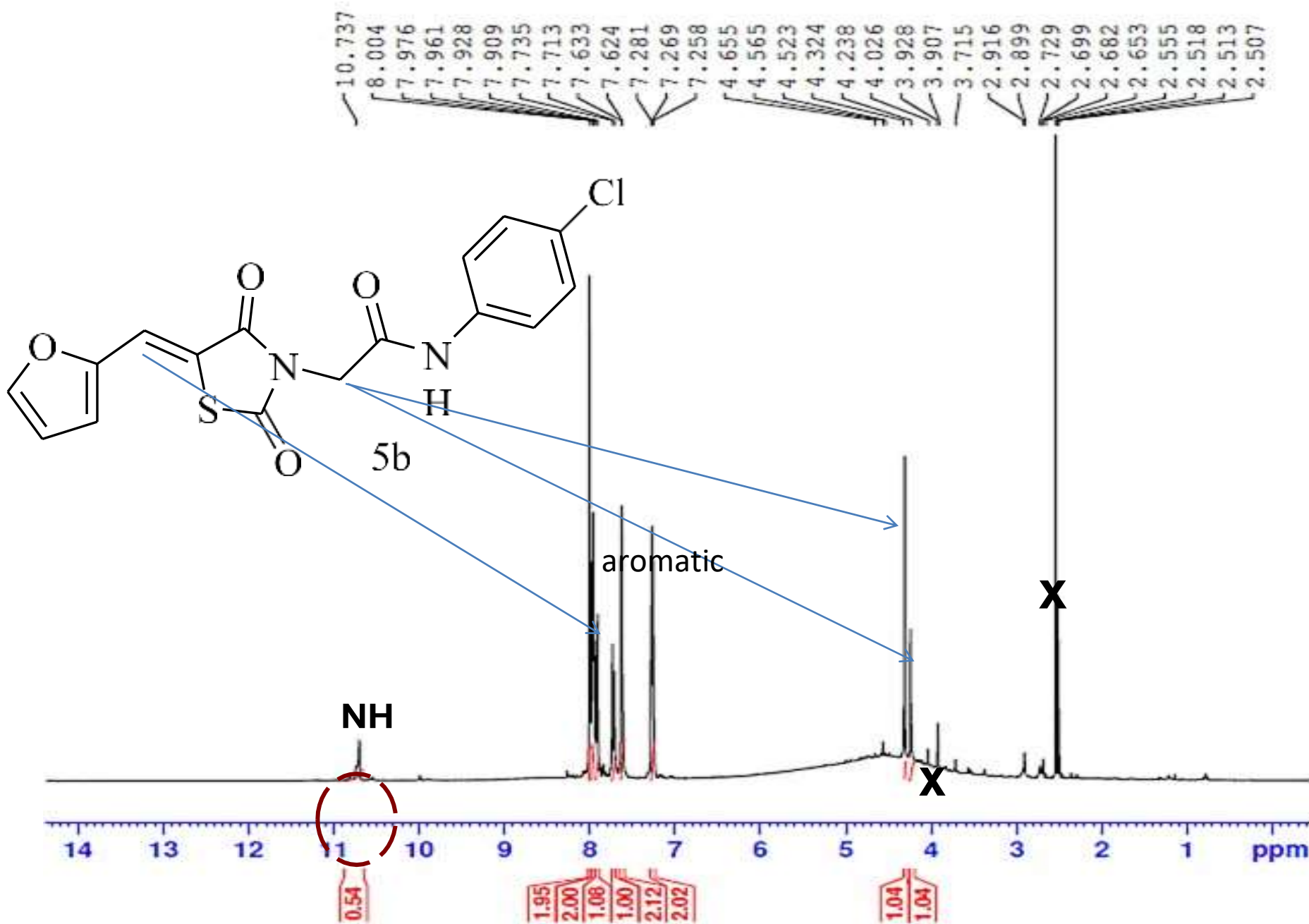


Current Data Parameters  
NAME nada-aziz-T  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211004  
Time 13.42  
INSTRUM spect  
PROBHD 5 mm PARRO BS/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 45  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MRz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MRz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 5b**



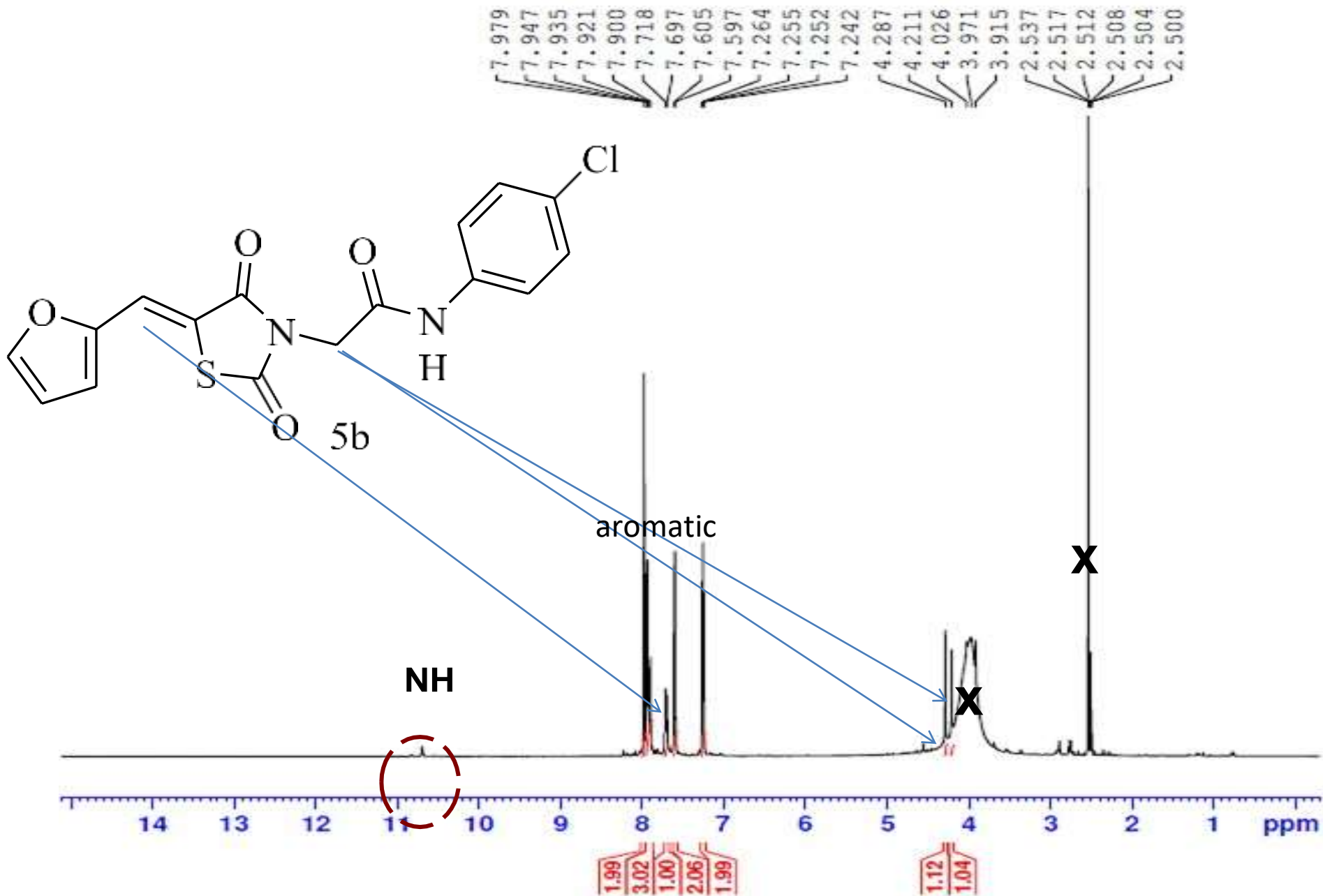


Current Data Parameters  
NAME nada-azix-T-D2O  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211004  
Time 15.01  
INSTRUM spect  
PROBHD 5 mm PARBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 50  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MRz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MRz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**$^1\text{H}$  NMR ( $\text{D}_2\text{O}$ ) for compound 5b**



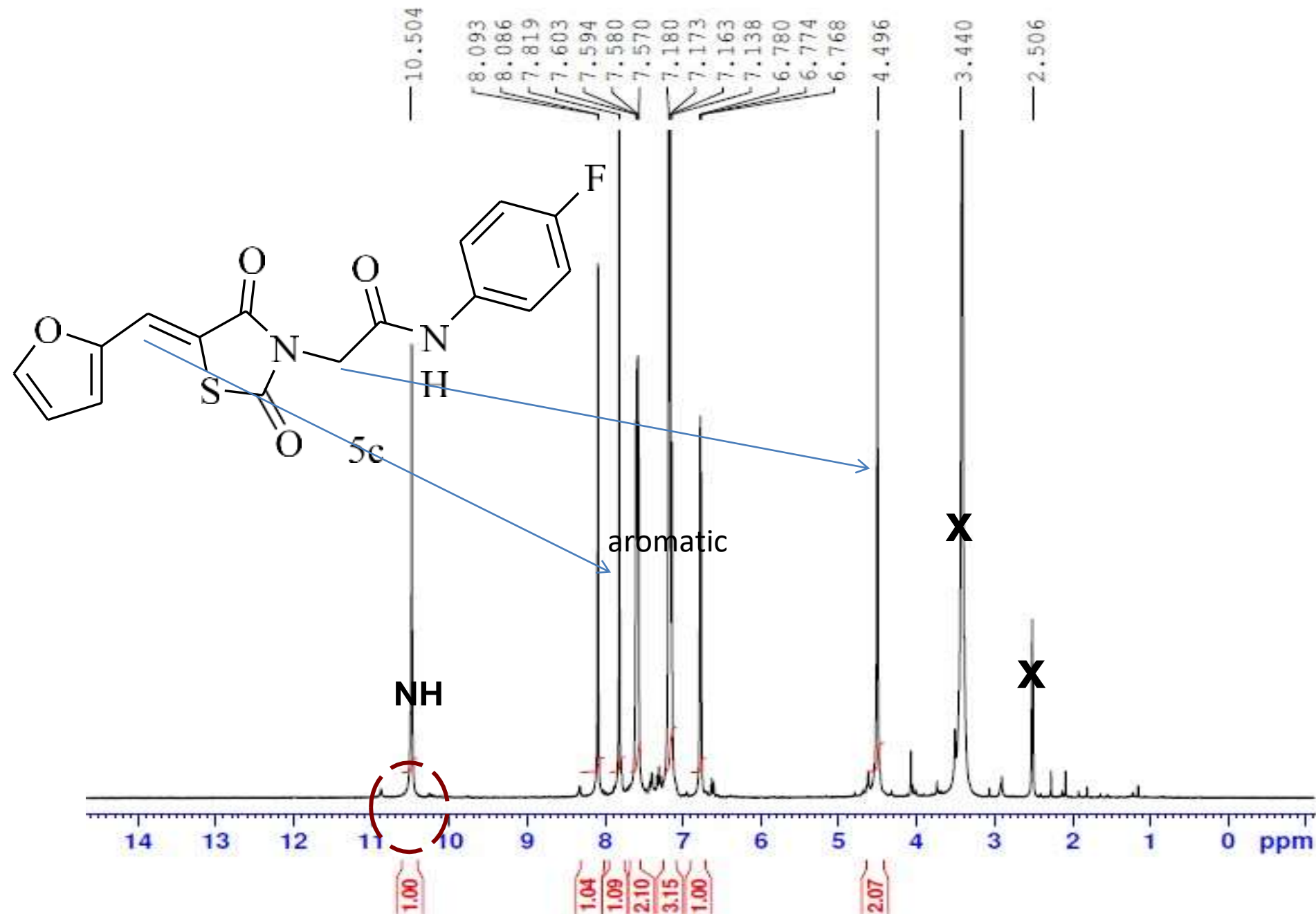
Current Data Parameters  
NAME nada-aziz-6F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20211004  
Time 14.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 5c**

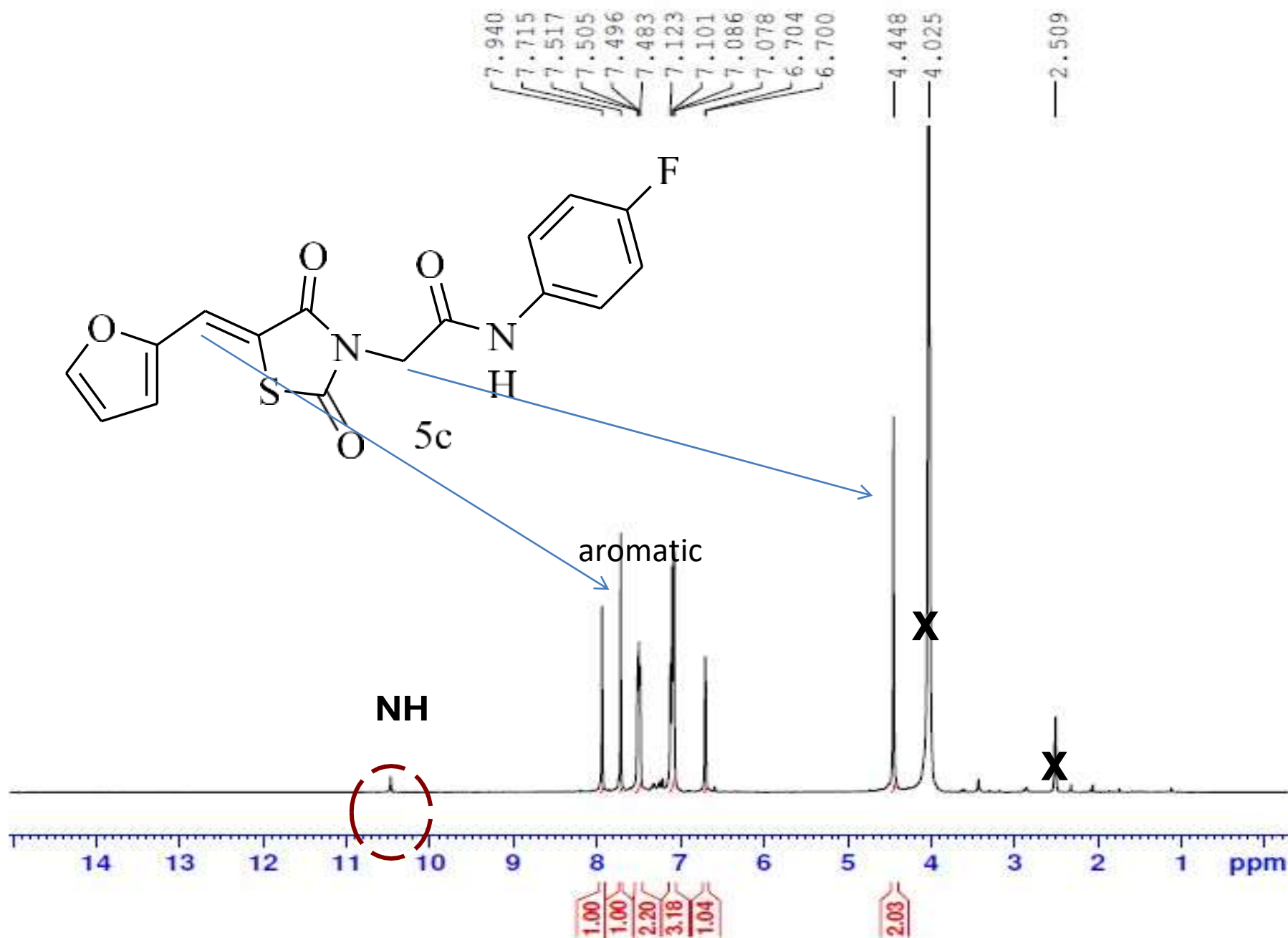


Current Data Parameters  
NAME nada-aziz-6f-d2o  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211005  
Time 10.36  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 33  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

----- CHANNEL f1 -----  
SF01 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



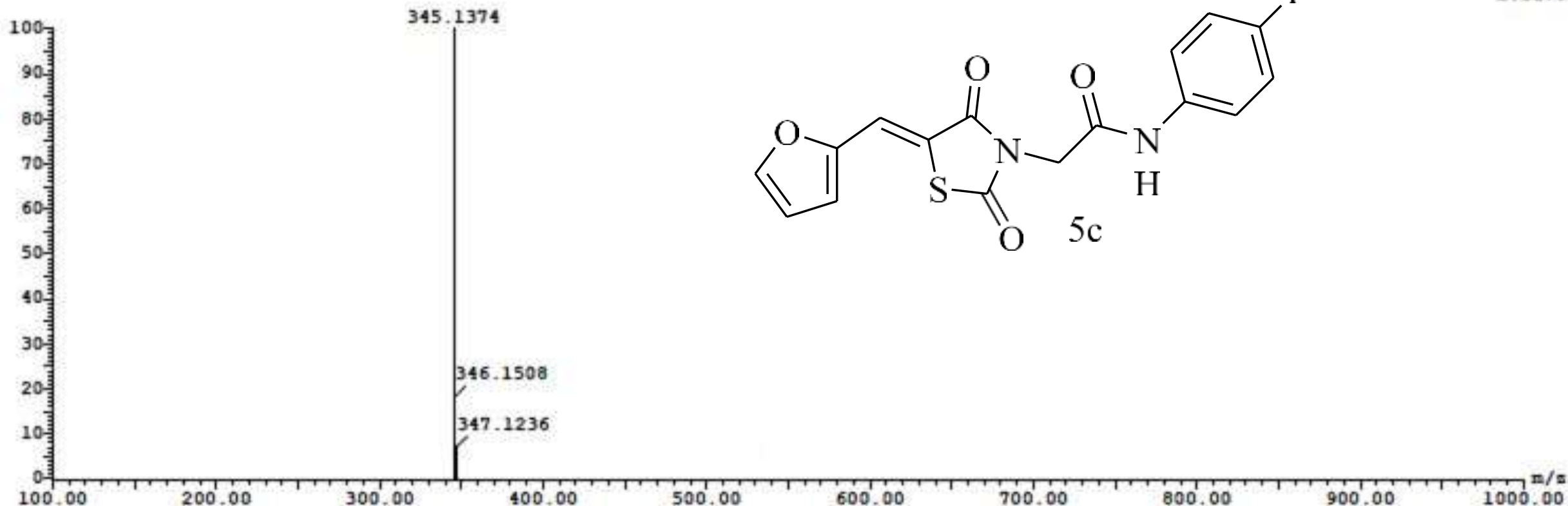
**<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 5c**

Peak ID Time Error PPM

0 11.67

(Time: 11.72)

2:MS ES-  
2.3e+007



**LC-MS ESI** spectrometry in the negative ion mode: The mass spectrum of compound **5c** showed M-1 molecular ion peak at 345.1374 which also was the base peak

**Liquid Chromatography-Electrospray Ionization-Mass spectra for compound 5c**

10.319  
10.233  
7.709  
7.700  
7.691  
7.670  
7.664  
7.647  
7.589  
7.567  
7.556  
7.532  
7.496  
7.492  
7.469  
7.440  
7.431  
7.411  
7.390  
7.384  
7.372  
7.368  
7.349  
7.289  
7.253  
7.143  
7.122  
7.071  
7.044  
7.030  
7.008  
6.950  
6.921  
6.911  
6.881  
4.460  
4.238  
3.428  
2.518  
2.310  
2.248  
2.125

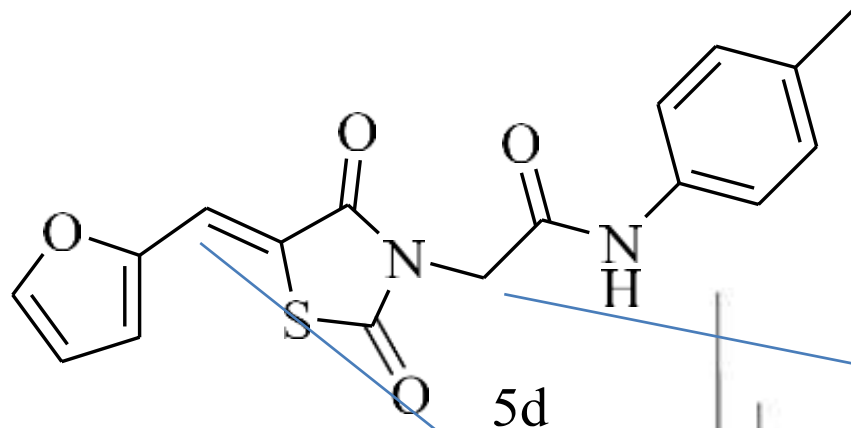


Current Data Parameters  
NAME nada-aziv-5f  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211004  
Time 14.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 40  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

CHANNEL f1  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



aromatic

NH

X

X

14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00

0.95  
2.17  
2.14  
2.00  
0.54

2.09

3.05

<sup>1</sup>H NMR for compound 5d

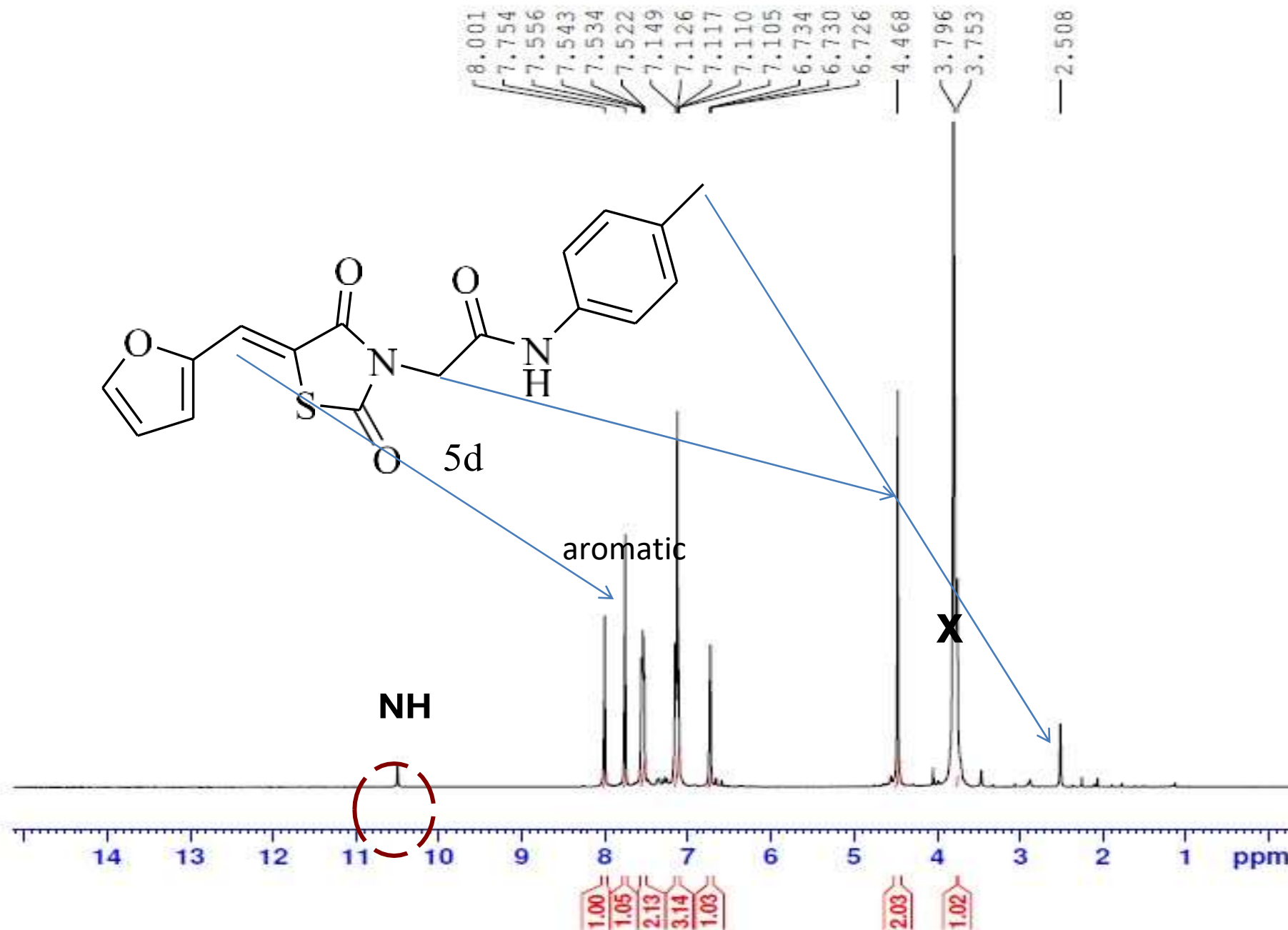


Current Data Parameters  
NAME nada-ariz-5F-D2O  
EXPNO 3  
PROCNO 1

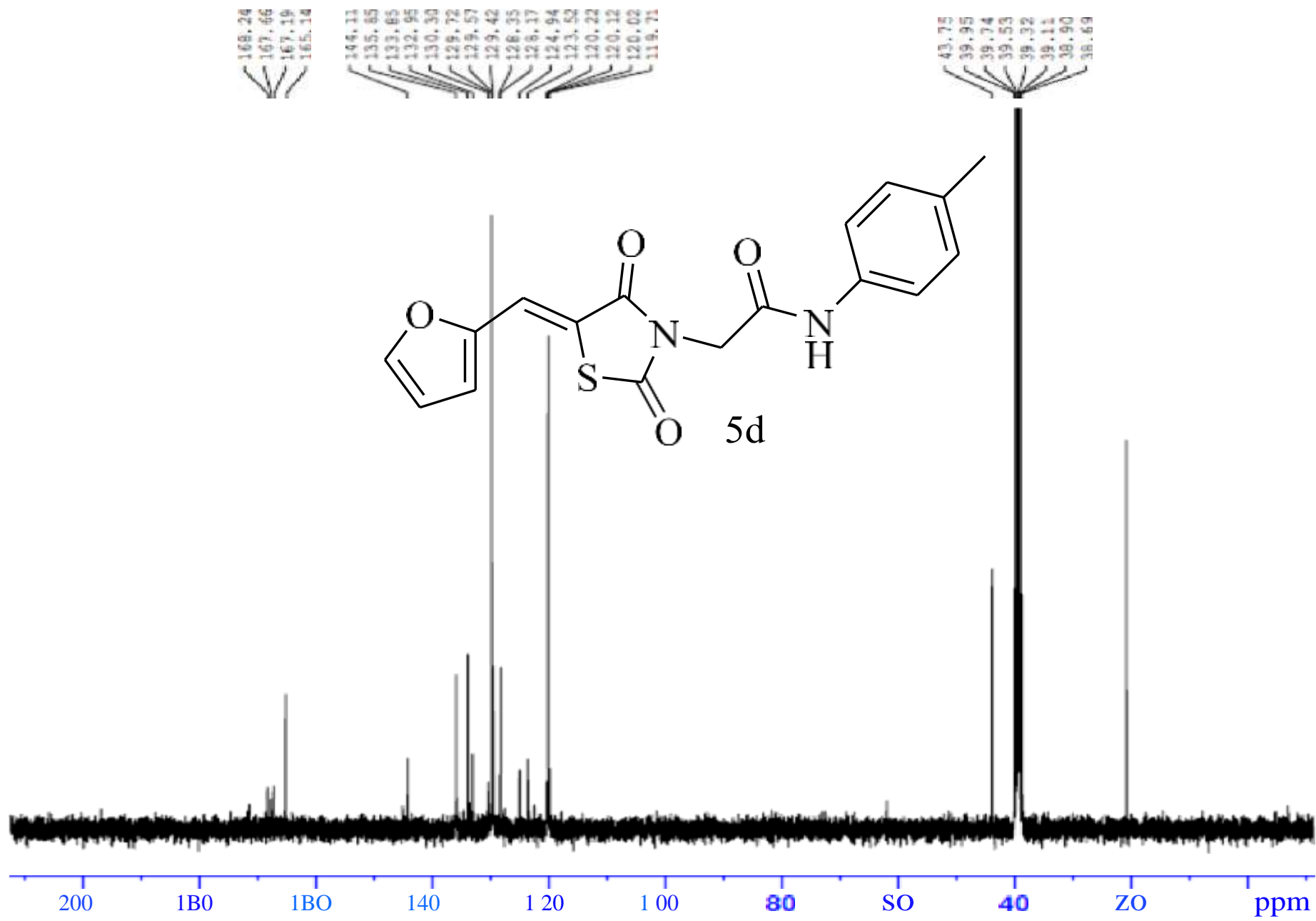
F2 - Acquisition Parameters  
Date\_ 20211004  
Time 16.32  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**$^1\text{H}$  NMR ( $\text{D}_2\text{O}$ ) for compound 5d**



oate\_ JDJL1031  
IWSTROI spert  
PROBHO B cmx GABBO BB/

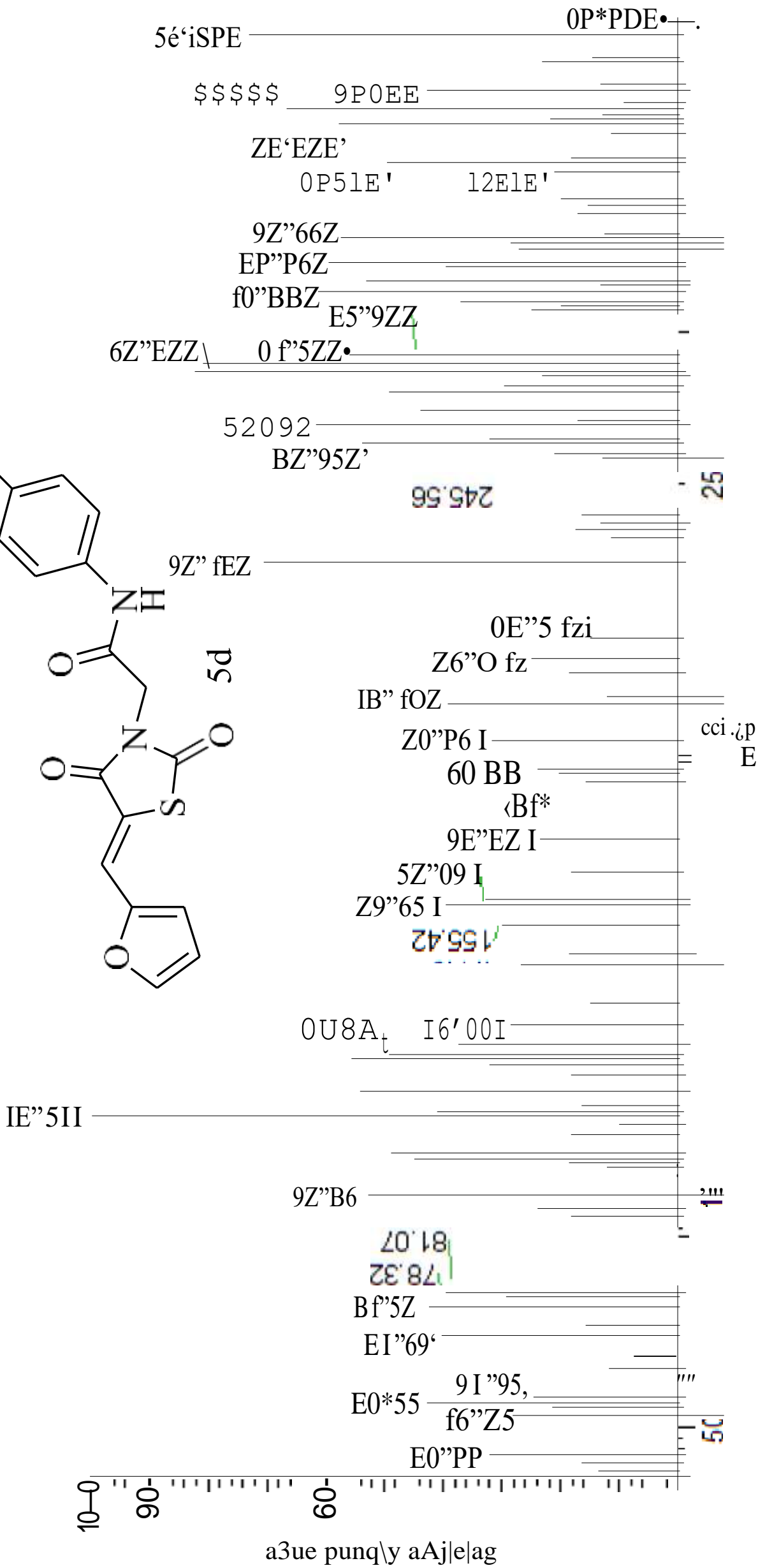
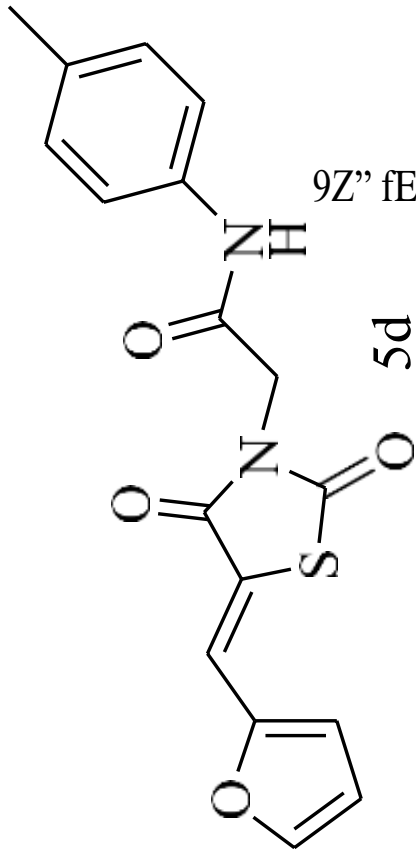
SWH ZS DC B.4J&1 Z  
FIDRES D.E 66QGB Z  
RG 205.37  
CW 20.800 usec  
TE S DO 0  
OL Z . D D D D D O O K  
OLL 0 . DC D D D O O sec  
TD D 1

SFO1 100.6278588 AHZ  
PI LD 00 usec  
PI]sL 63. D D D D D O O W

sFoJ 400.1516006 AHZ  
NUC2 1H  
PCSPOT 9D 00 usec  
PLNJ B D D D D D O O W  
PI]sL3 0 . BLV 5 000 W

SF 100.6177975 xHa  
SSB 0  
LB I.00 HI  
PC L 4 0

<sup>13</sup>C NMR for compound 5d



Mass spectra for compound 5d



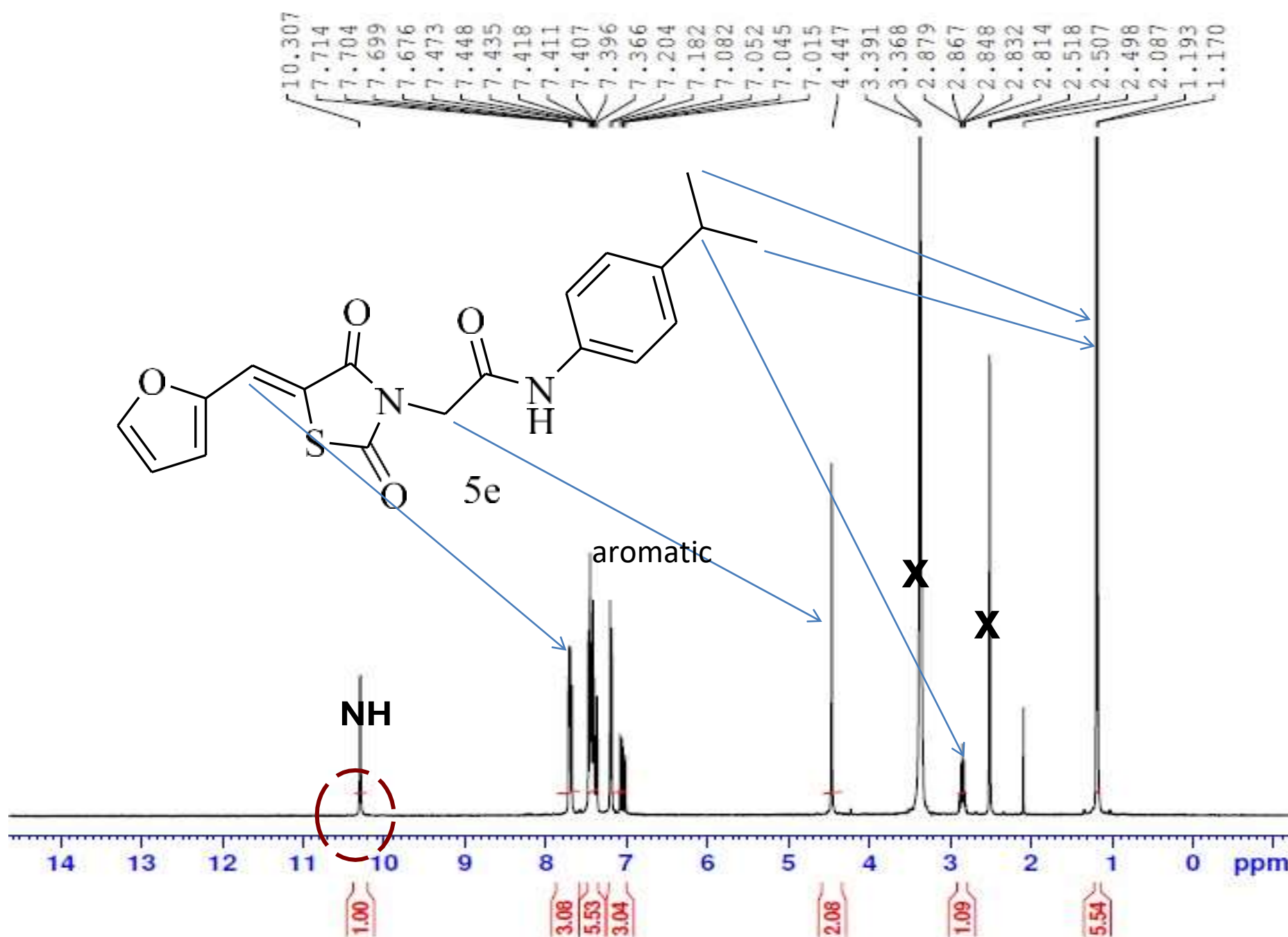


Current Data Parameters  
NAME nada-aziz-2F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211004  
Time 14.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 44  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



**<sup>1</sup>H NMR for compound 5e**



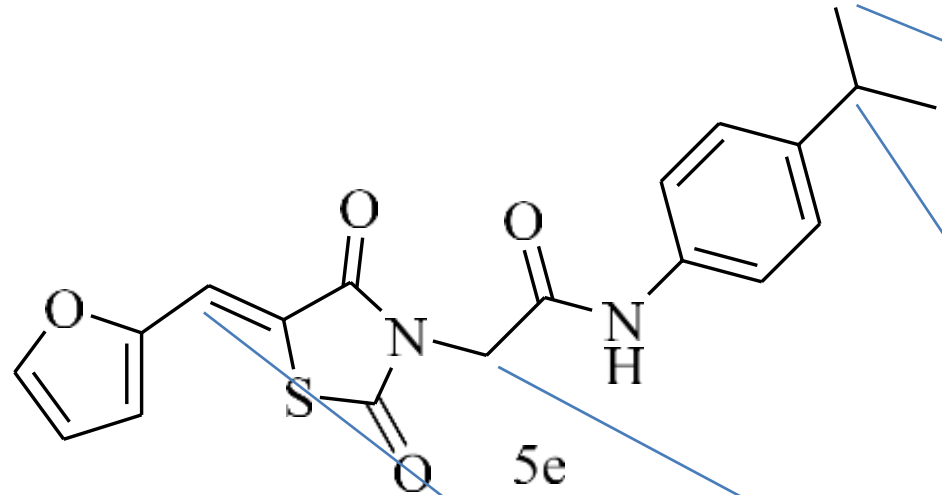
Current Data Parameters  
NAME nada-az1z-2f-d2o  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20211005  
Time 10.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 61  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

7.686  
7.674  
7.647  
7.437  
7.417  
7.399  
7.380  
7.360  
7.322  
7.189  
7.168  
7.033  
7.005  
6.995  
6.967  
4.441  
3.762  
3.753  
3.744  
3.734  
3.715  
3.705  
2.855  
2.838  
2.821  
2.803  
2.786  
2.508  
2.074

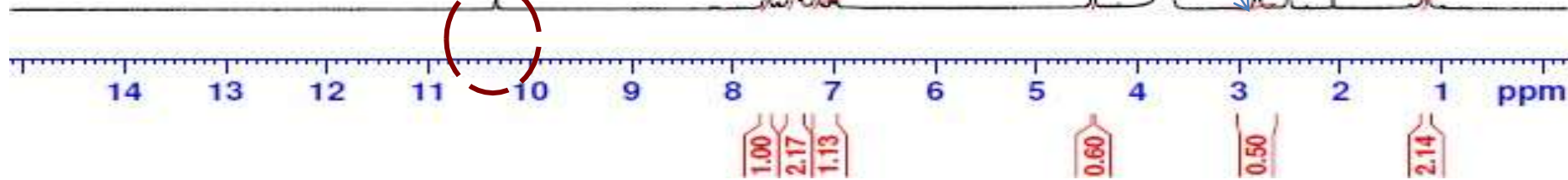


NH

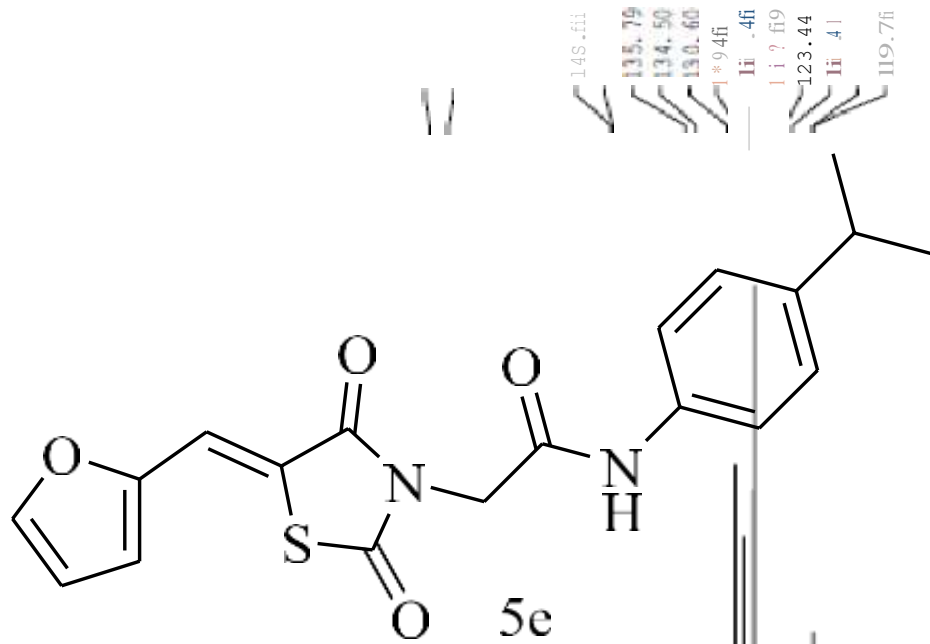
aromatic

X

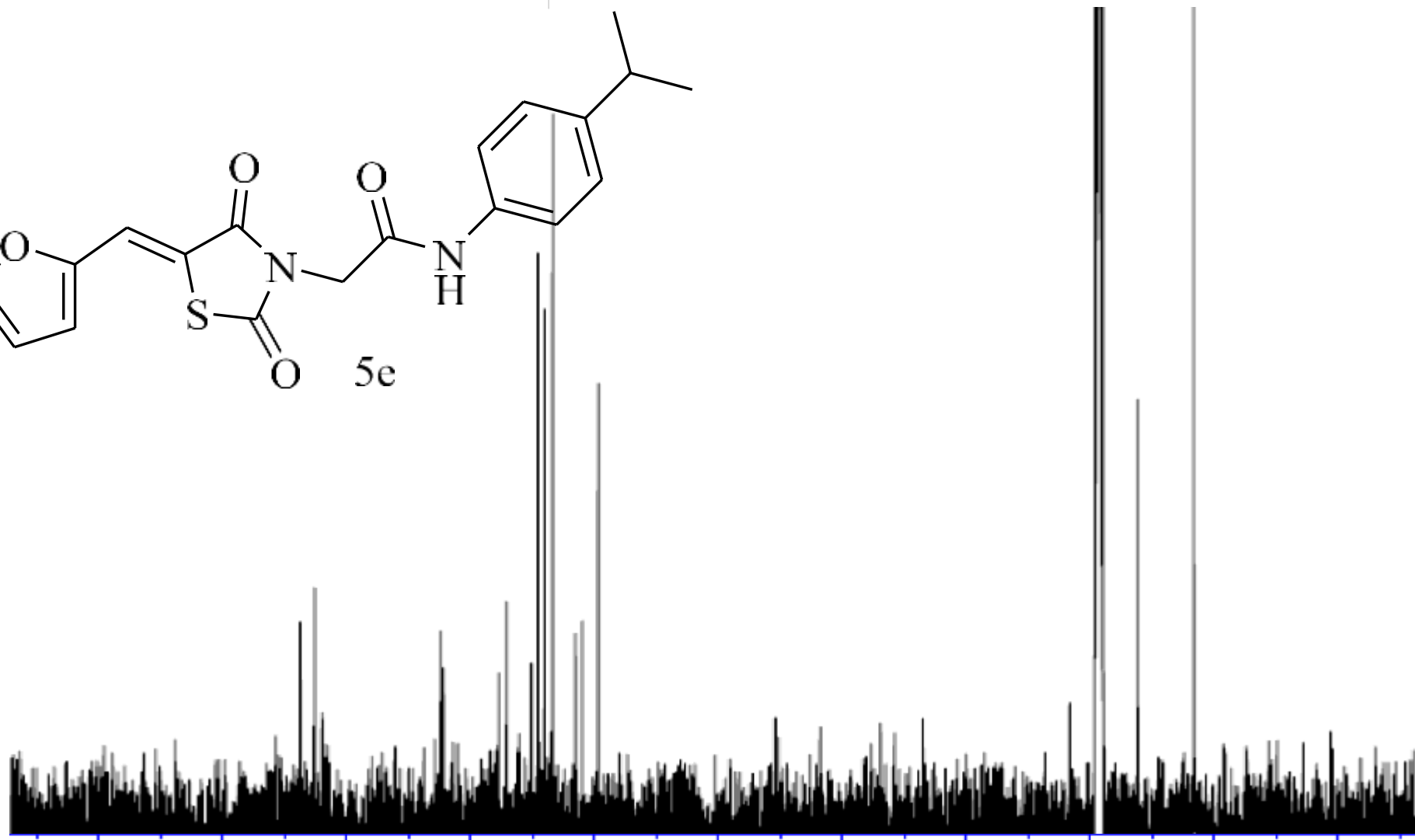
X



<sup>1</sup>H NMR (D<sub>2</sub>O) for compound 5e



148.61i  
135.79  
134.50  
130.60  
119.41  
119.71i  
123.44  
117.99  
117.41



```
oaA_                2 DC L L I O 2

PROBHD 5 mm PABBO BB/
PULPROG zgpg30

NS                4017
EH          Z & DC B 4 6 I Hz
FIDRES        D Z 6 6 T PB Hz

RG                205.137
DW                20.800 usec

TE          Z DO 0 K
0 L          Z D D D D D O O rec
DLL          0 . DC D D D O O sec
TDD          1

-----
NUC1          13C
P1            LD DD uaec
PIm1         4 T . D D D D D O O W

-----
NUC2          ]H
PCPO 2          9 D O O usec
PIW2          B D D D D D O O W
PIW12         0 . 34722000 W

SF            100.6177975 MHz

LB            L . 00 z
PC            L d 0
```

<sup>13</sup>C NMR for compound 5e



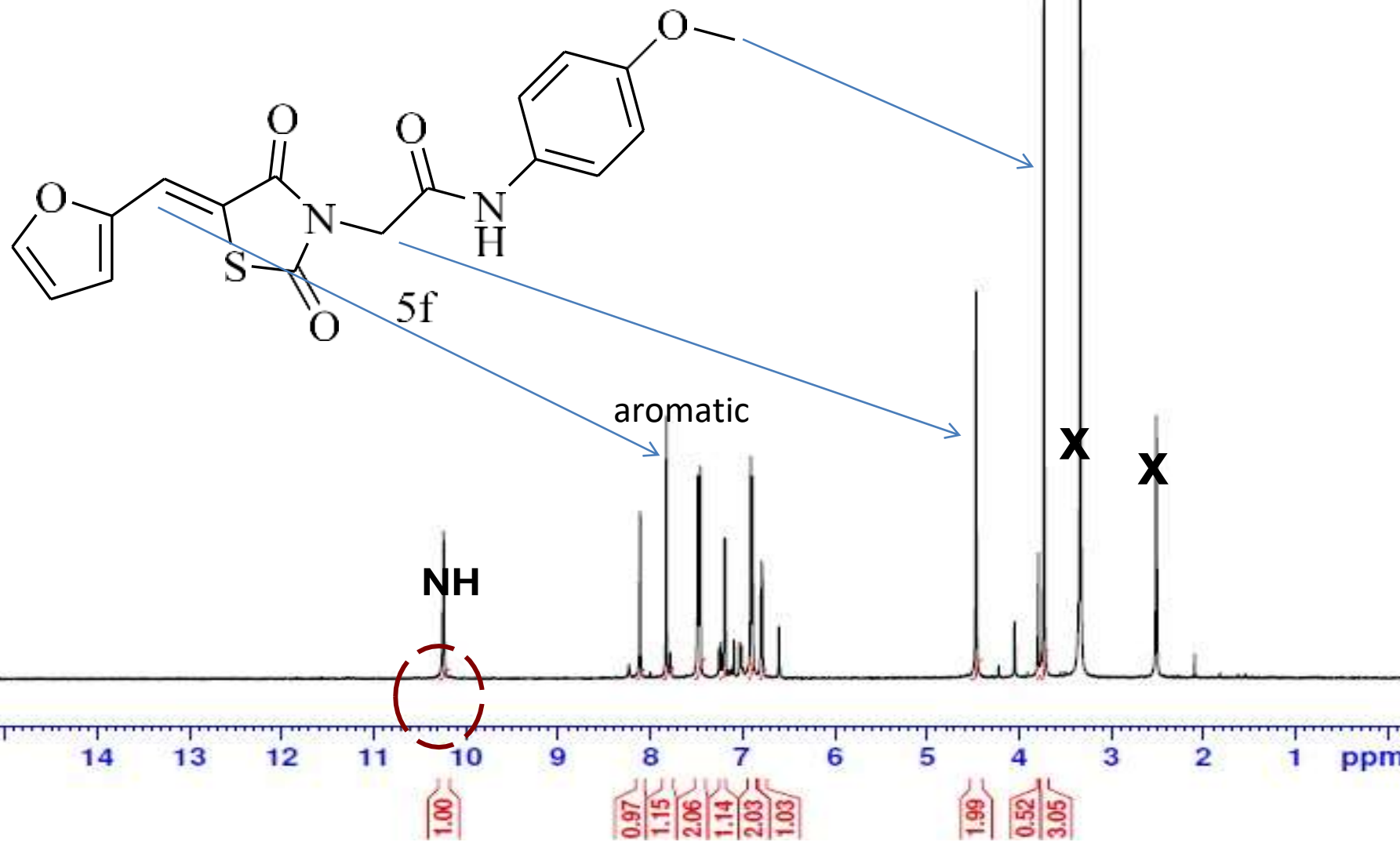
Current Data Parameters  
NAME nada-ahmed-4F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20210906  
Time 16.00  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
ID 65536  
SOLVENT DMSO  
NS 11  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 205.37  
DW 62.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 1.00000000 sec  
ID0 1

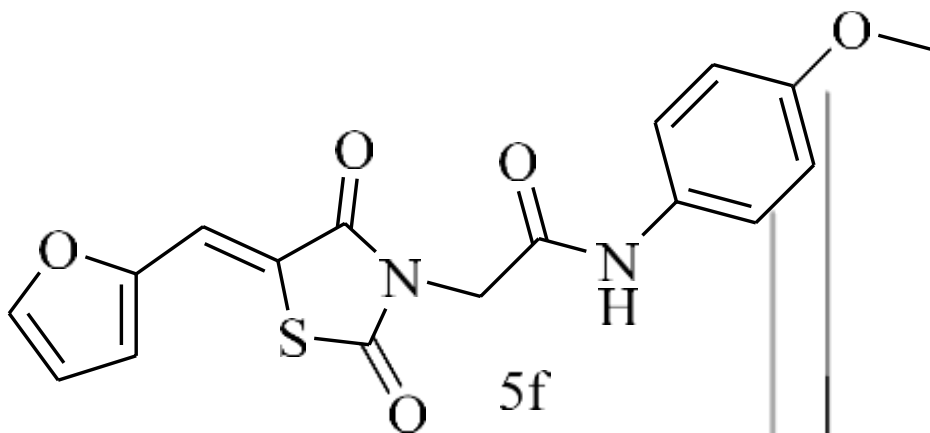
----- CHANNEL f1 -----  
SFO1 400.1524711 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 18.00000000 W

F2 - Processing parameters:  
SI 65536  
SF 400.1500000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

10.244  
8.112  
8.108  
7.823  
7.480  
7.458  
7.254  
7.232  
7.194  
7.186  
7.027  
7.010  
7.004  
6.989  
6.910  
6.888  
6.795  
6.791  
6.787  
6.782  
4.463  
3.798  
3.788  
3.726  
3.333  
2.511  
2.507

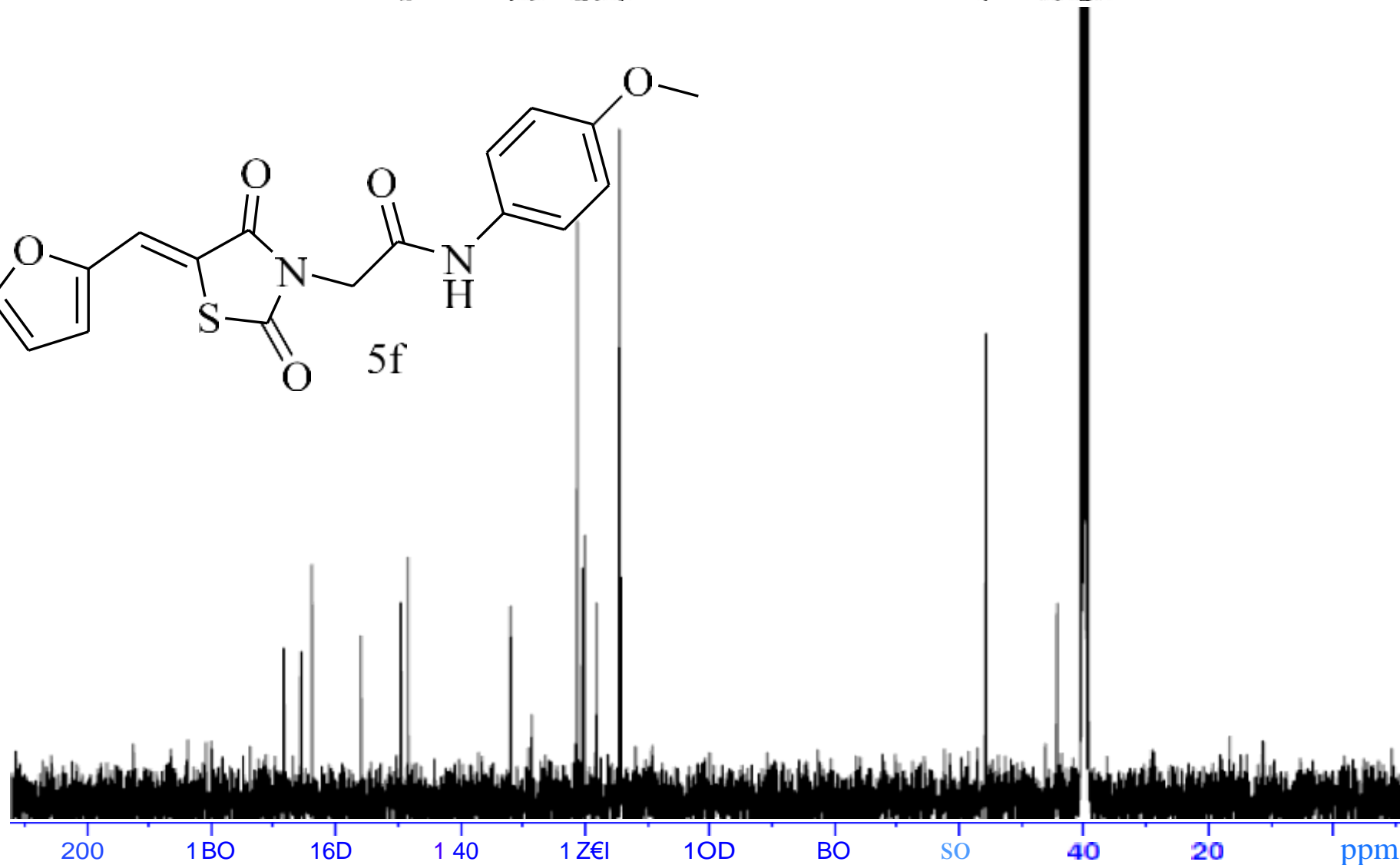


**<sup>1</sup>H NMR for compound 5f**



149.60  
148.43  
131.92  
126.60  
121.24  
120.42  
120.07  
118.05  
114.45  
114.19

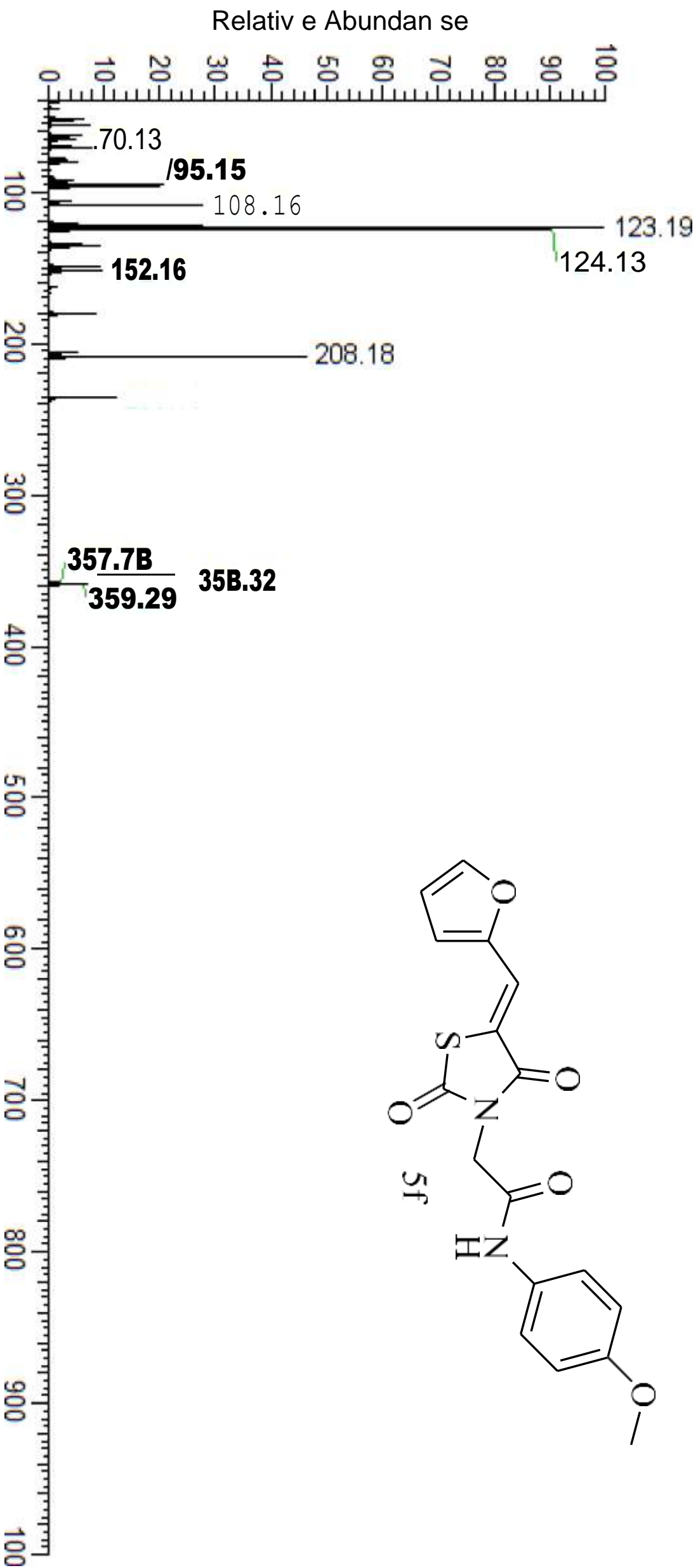
55.69  
44.21  
40.47  
40.26  
40.05  
39.84  
39.63  
39.42  
39.21

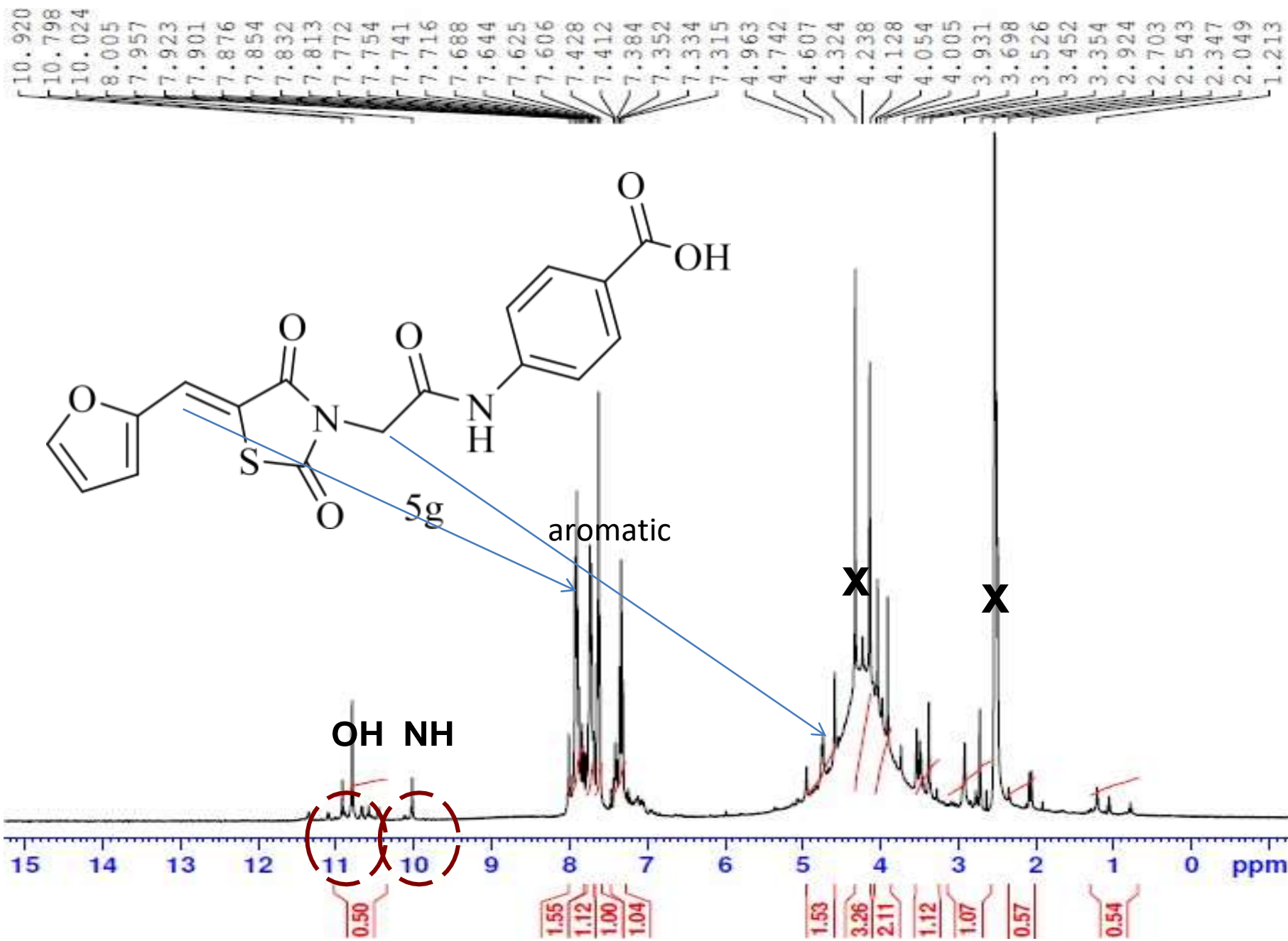


```
te
d-
oate_      2D21D920
PROBHD     5 mm PABBO BB/
PULPROG    zgpg30
To         65s36
NS         L141
SRH        24038.461 1:[z
FIOR1ef1   0.366798 W
AQ         1.3631488 sec
RG         205.37
CW         20.800 usec
Os         6.50 usec
TE         300.0 K
OL         2.0000000 sec
DLL        0.03000000 sec
T0 D       1
CH HbFRL I L -----
SF01       i00.627B5BB BHx
NUC1       zze
PL         LD OD usec
PUE1       41 . DDDDD000 W
IE)hWNRL I'2 ----
SF03       OD0.L5L6006 BHx
NUC2       1H
CPOPRG[S   waltz16
PCPOT      9 D OD usec
PL]02     B D D D D 0000 W
PIW13     0.28125000 W
SF         100.6177975 MHz
LB         I .00 E[z
PC         L -A0
```

<sup>13</sup>C NMR for compound 5f

# Mass spectra for compound 5f





Current Data Parameters  
 NAME nada-aziz-7R  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20211004  
 Time\_ 14.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 42  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 205.37  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 SFO1 400.1524711 MHz  
 NUC1 1H  
 P1 12.00 usec  
 PLW1 18.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.1500000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR for compound 5g