Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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[1,2,4]Triazolo[4,3-a]quinoxaline and [1,2,4]triazolo[4,3-a]quinoxaline-1-thiol derived DNA intercalators: Design, synthesis, molecular docking, *In silico* ADMET profile and anti-proliferative evaluations

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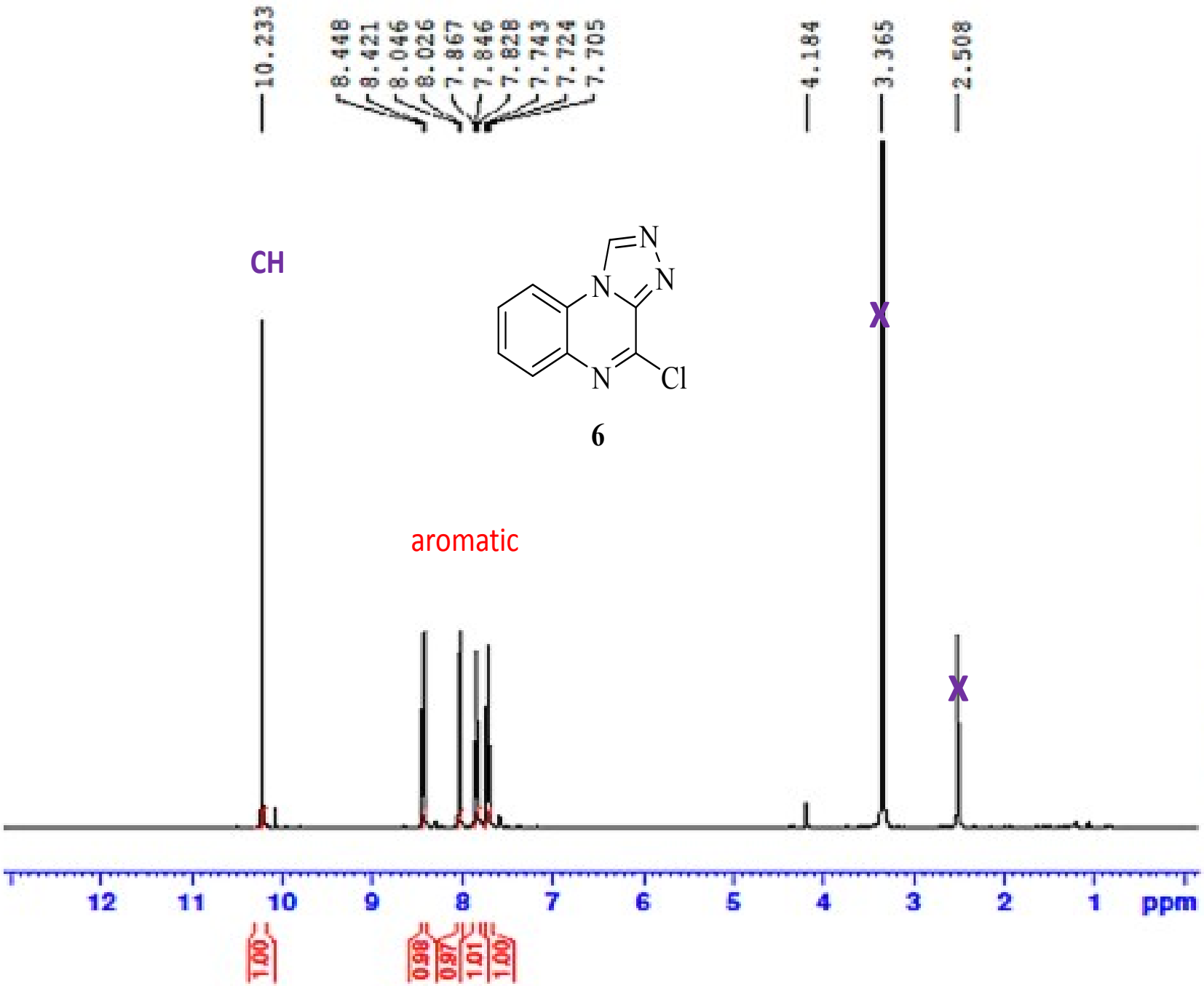
New Journal of Chemistry



BRUKER

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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180606
Time                 9.08
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    37
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               298.0 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
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PC                 1.00
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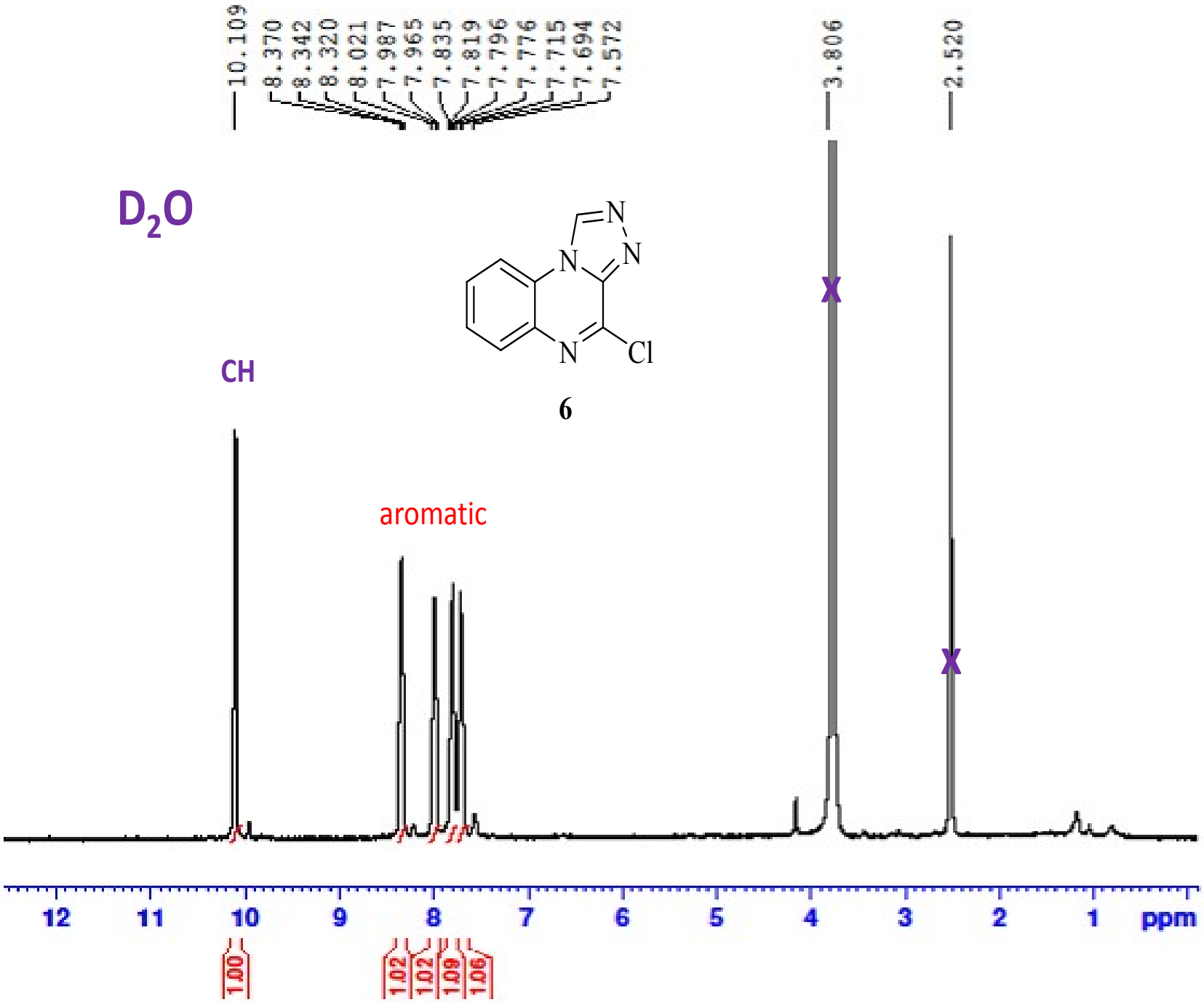

BRUKER

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EXPNO                       1
PROCNO                      1

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Date_              20180606
Time                   9.20
INSTRUM               spect
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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                   298.0 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
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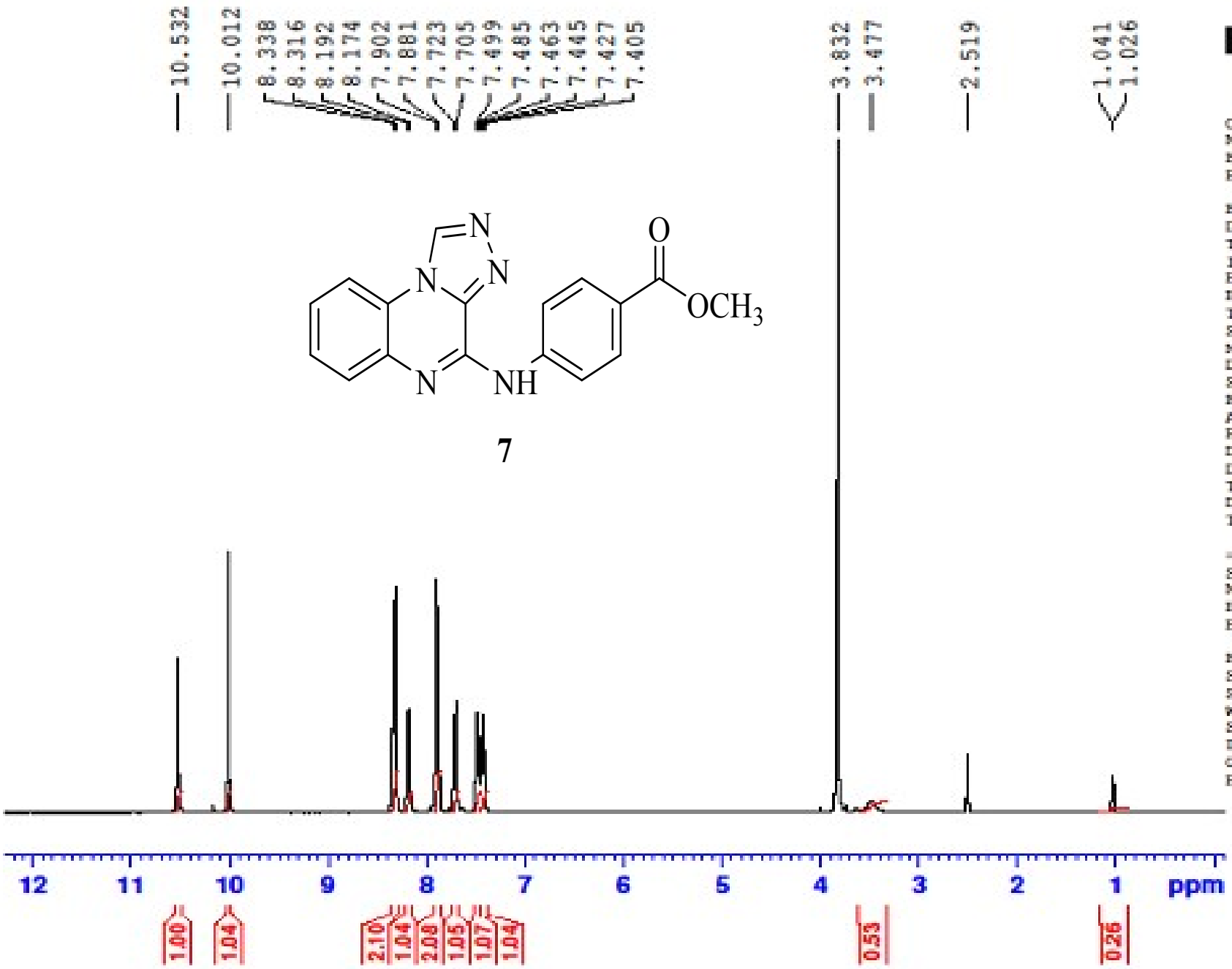

7

BRUKER

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EXPNO                    1
PROCNO                   1

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Time                11.44
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                  299.0 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
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LB                   0.30 Hz
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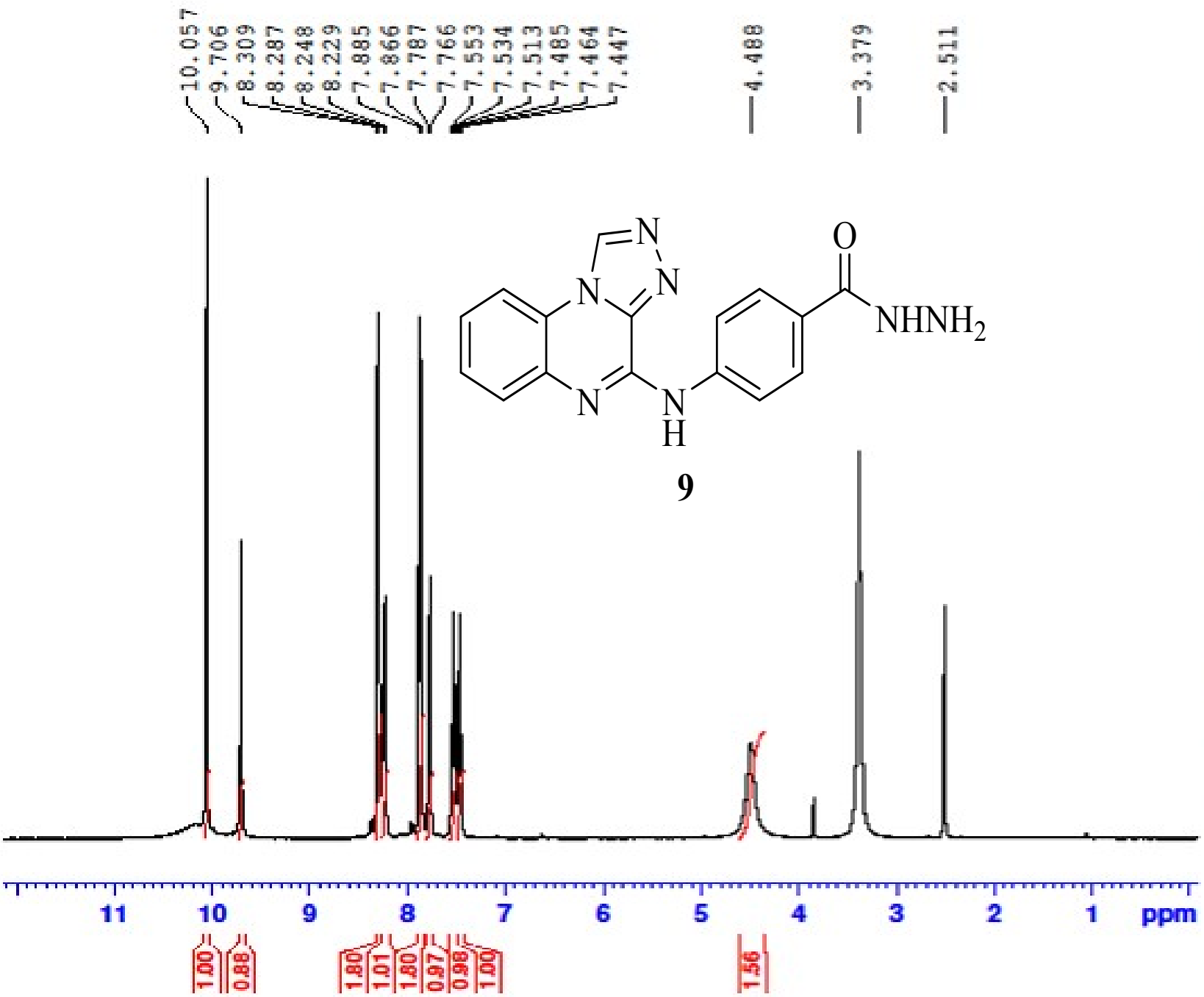

Current Data Parameters
NAME alaa-HZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170924
Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 48
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 298.0 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
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WDW EM
SSB 0
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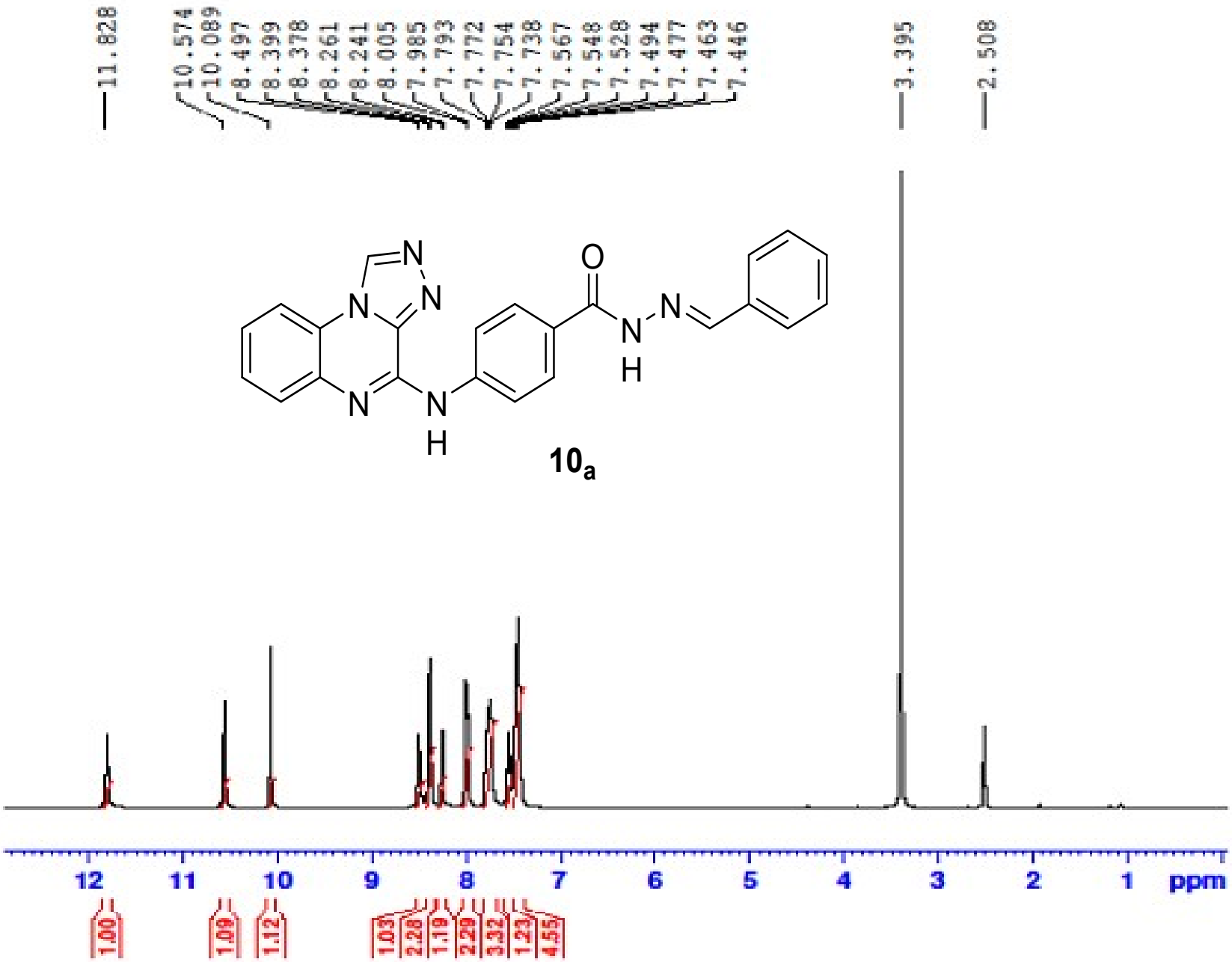

BRUKER

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Current Data Parameters
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EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20171017
Time                    9.14
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PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        47
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                    299.0 K
D1                1.00000000 sec
TD0                        1

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

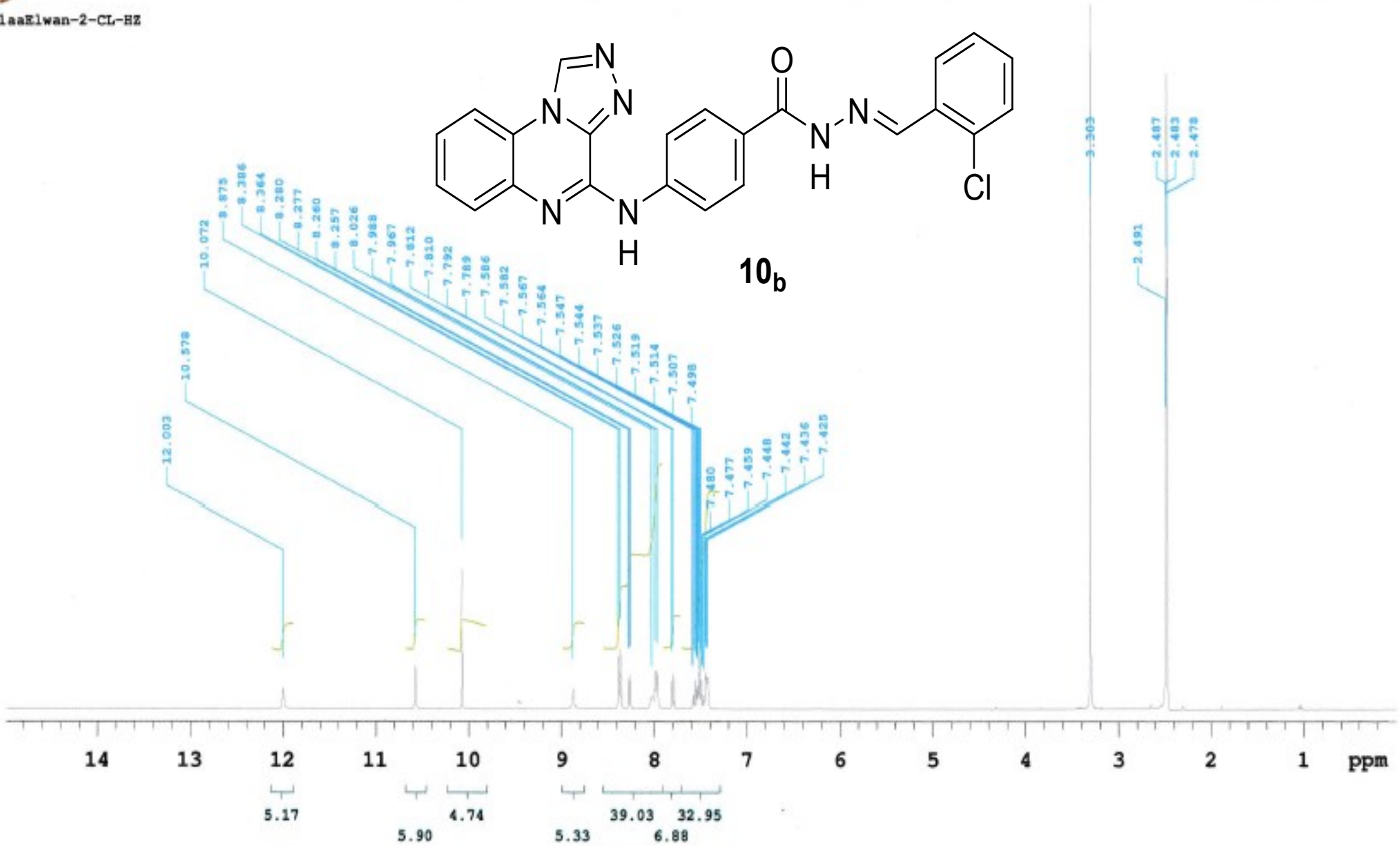
F2 - Processing parameters
SI                     65536
SF              400.1500000 MHz
WDW                       EM
SSB         0
LB                     0.30 Hz
GB          0
PC                     1.00
```

Dr_AlaaElwan-2-CL-HZ

Sample Name	Dr_AlaaElwan-2-CL-HZ	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr1
Date collected	2017-12-12	Solvent	dmso	Spectrometer	nmr400-mercury400	Operator	vnmr1

Dr_AlaaElwan-2-CL-HZ

10b

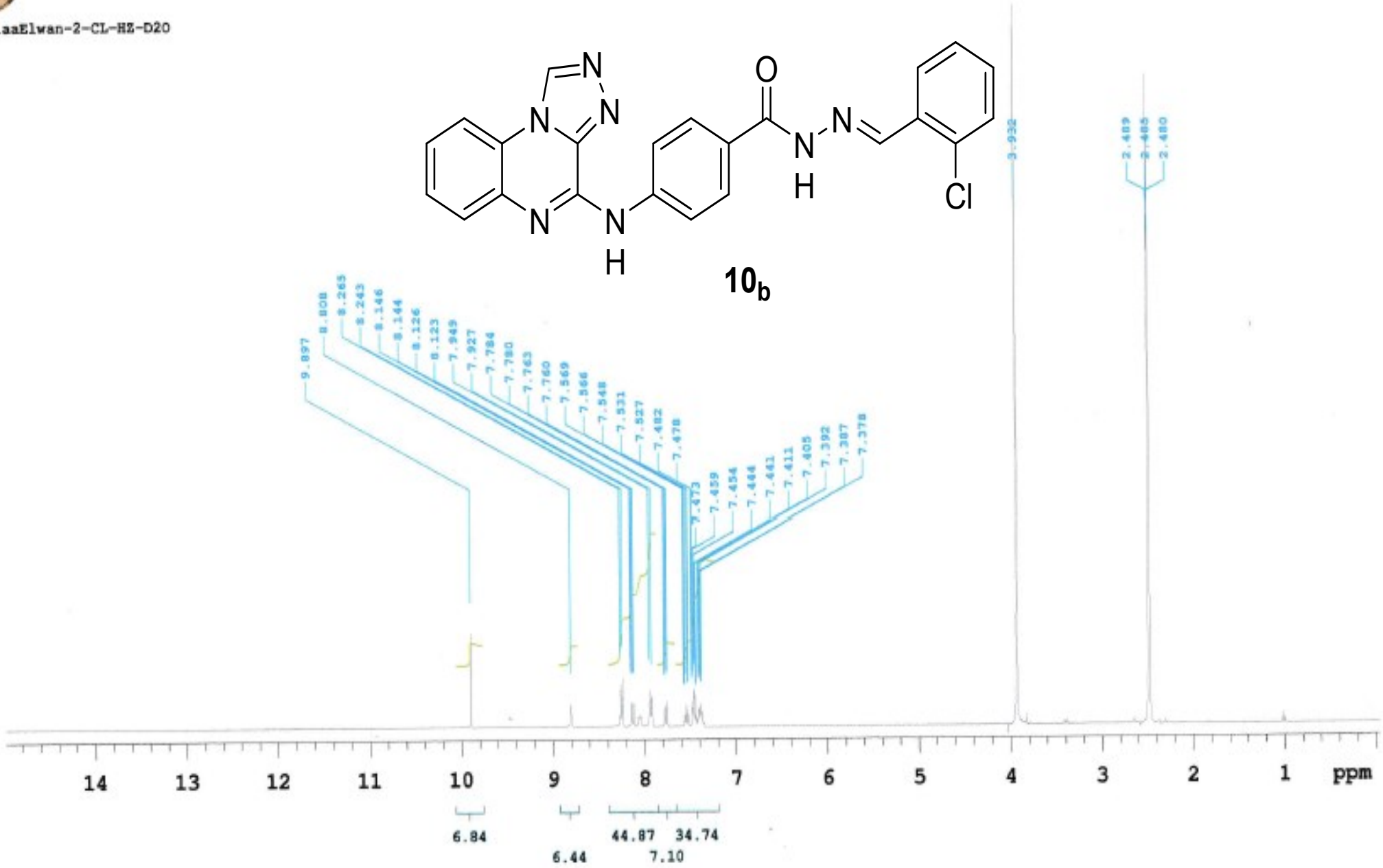


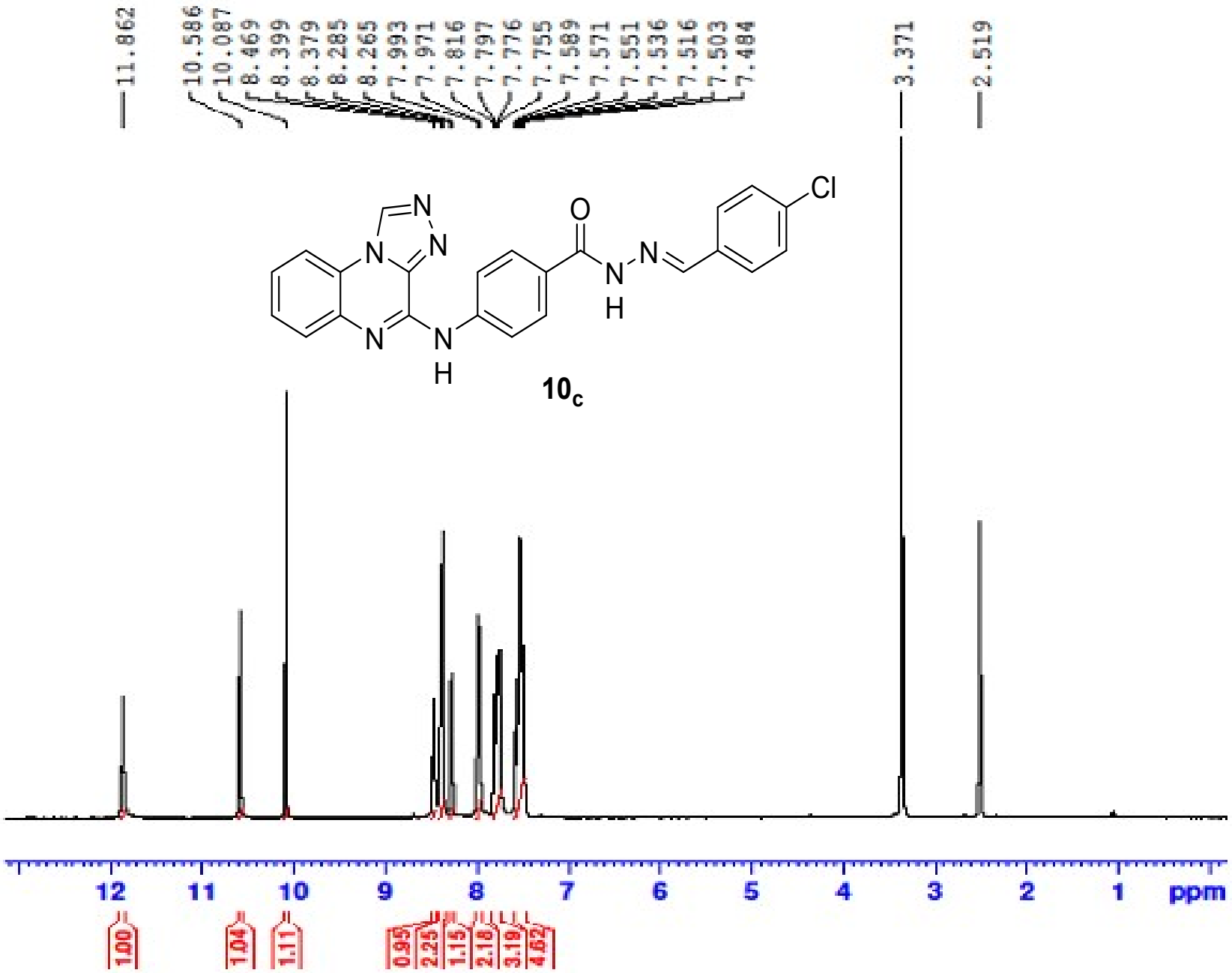
Dr_AlaaElwan-2-CL-HZ-D2O

Sample Name Dr_AlaaElwan-2-CL-HZ-D2O | Pulse sequence PROTON | Temperature 25 | Study owner vnmr1
Date collected 2017-12-16 | Solvent dmso | Spectrometer nmr400-mercury400 | Operator vnmr1

Dr_AlaaElwan-2-CL-HZ-D2O

10b





Current Data Parameters
NAME alaa-4-Cl-benz
EXPNO 1
PROCNO 1

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Time 11.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
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 298.0 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
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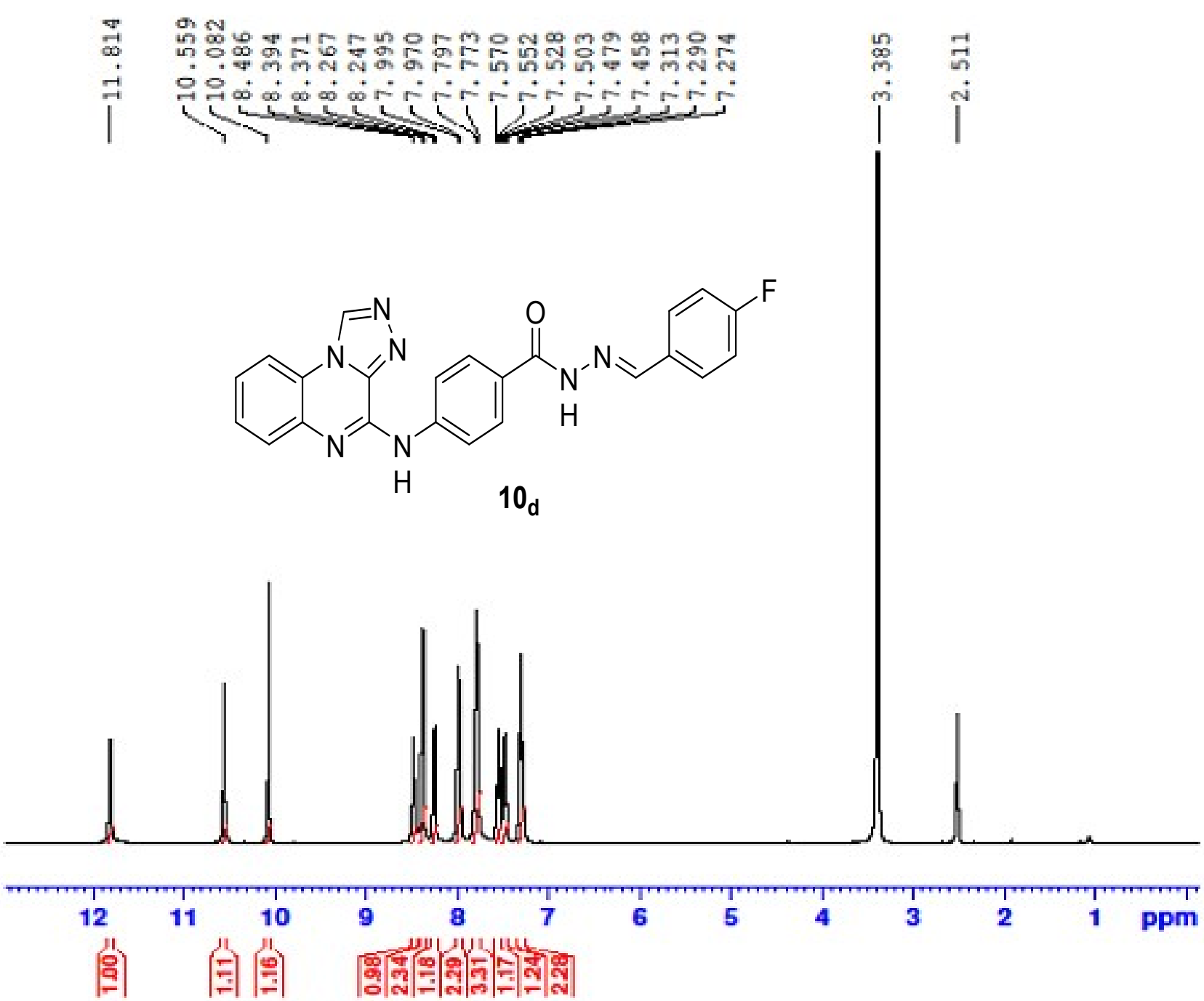
SF 400.1500000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME alaa-4FHZ
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171017
Time 9.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 64
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 299.0 K
D1 1.00000000 sec
TD0 1

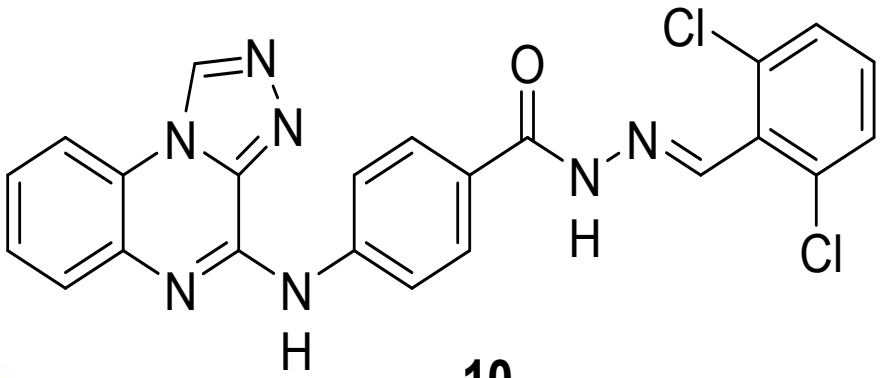
======== CHANNEL f1 ========
SFO1 400.1524711 MHz
NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

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

Dr_AlaaElwan2_6-CL-Hz

Sample Name Dr_AlaaElwan2_6-CL-Hz
Date collected 2017-12-12
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

Dr_AlaaElwan2_6-CL-Hz



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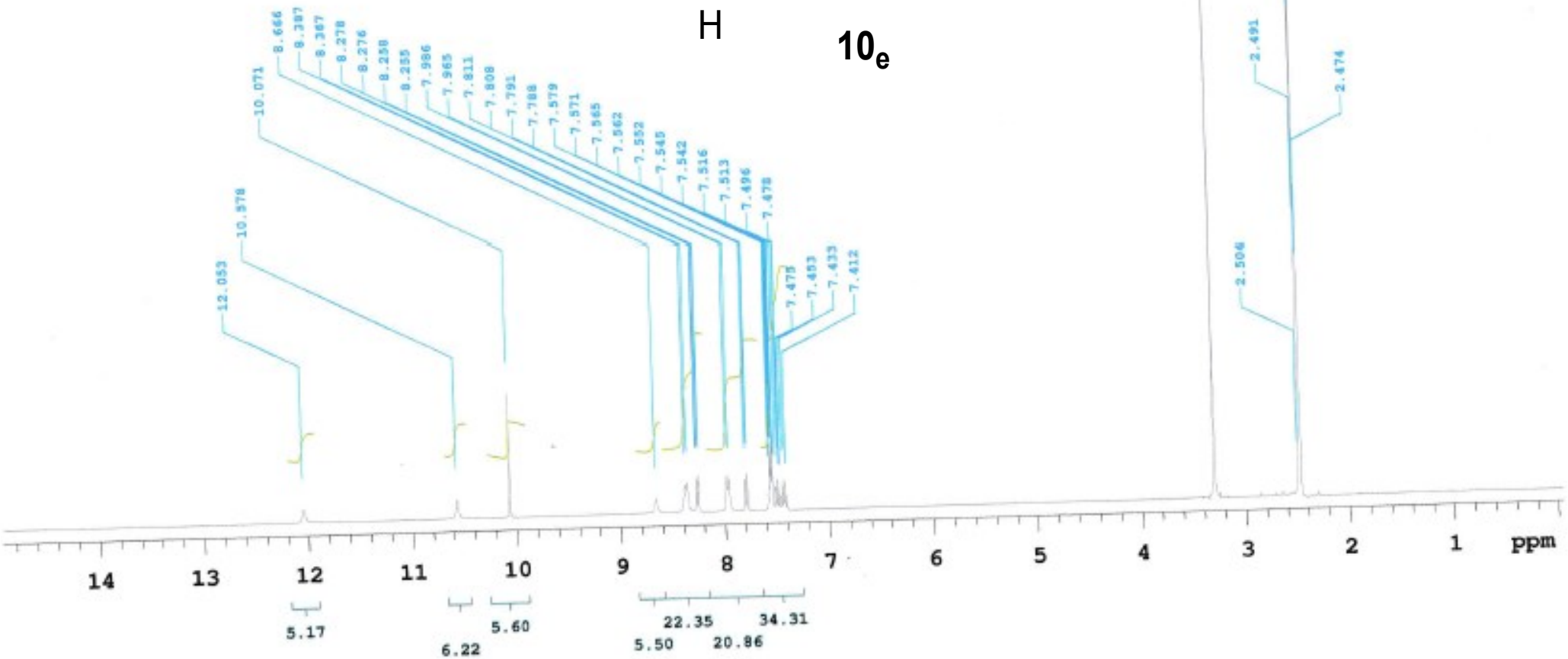
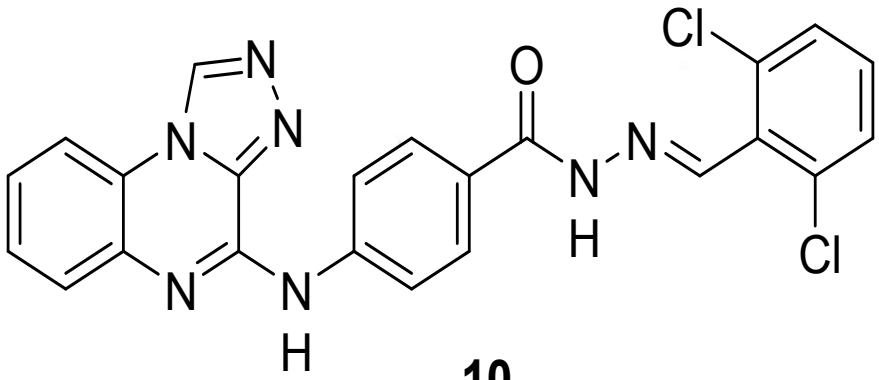


Dr_AlaaElwan2_6-CL-Hz-D2O

Sample Name Dr_AlaaElwan2_6-CL-Hz-D2O
Date collected 2017-12-16
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

Dr_AlaaElwan2_6-CL-Hz-D2O



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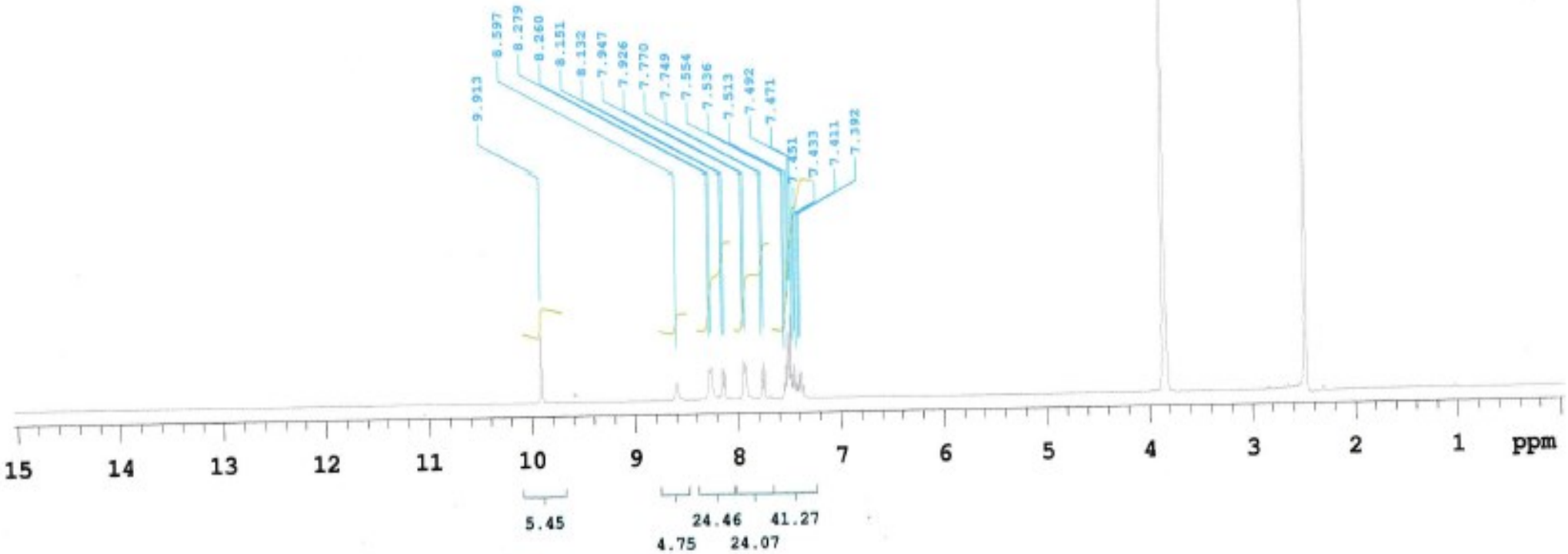
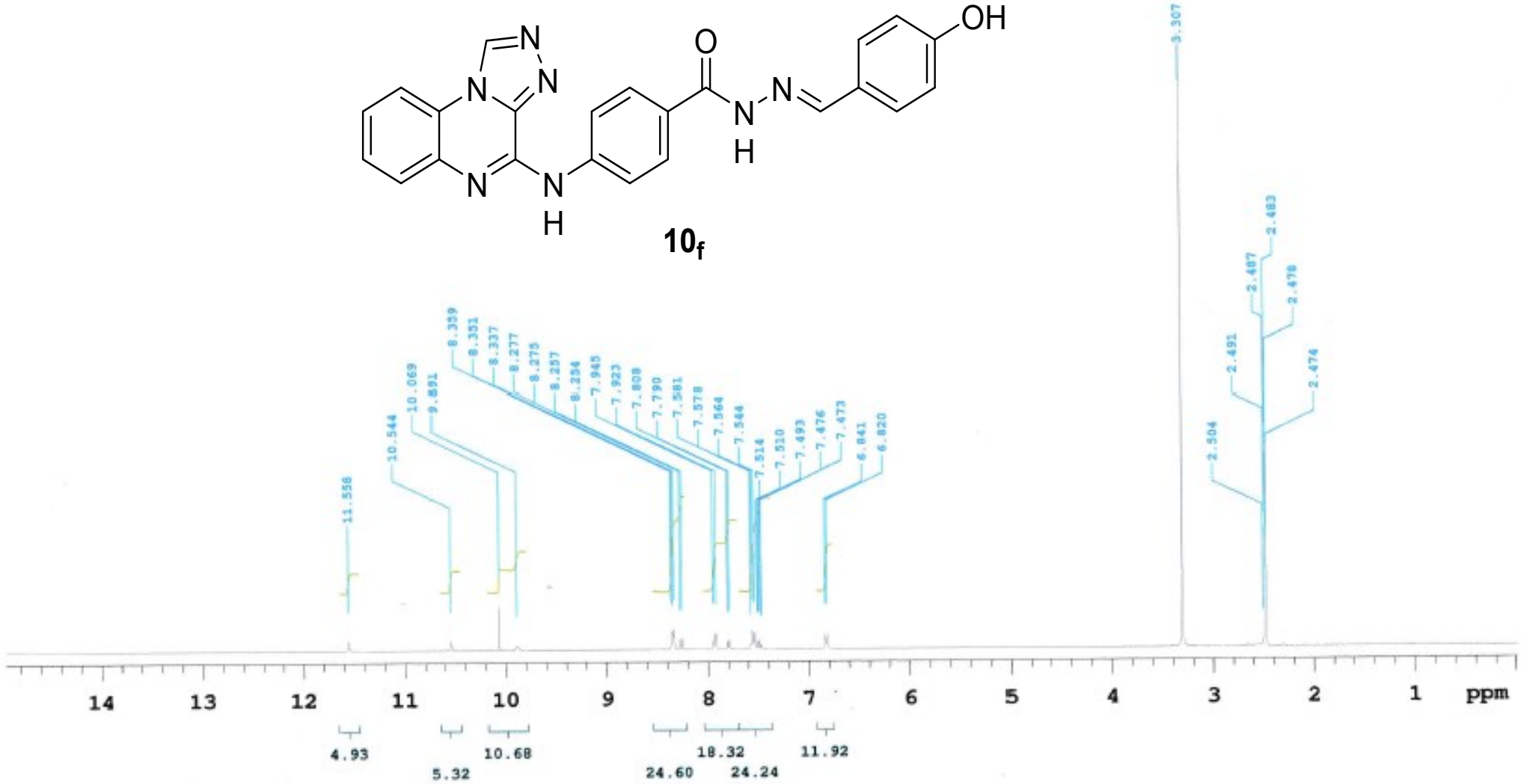


Dr_AlaaElwan-40Hz

Sample Name Dr_AlaaElwan-40Hz
Date collected 2017-12-12
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

Dr_AlaaElwan-40Hz

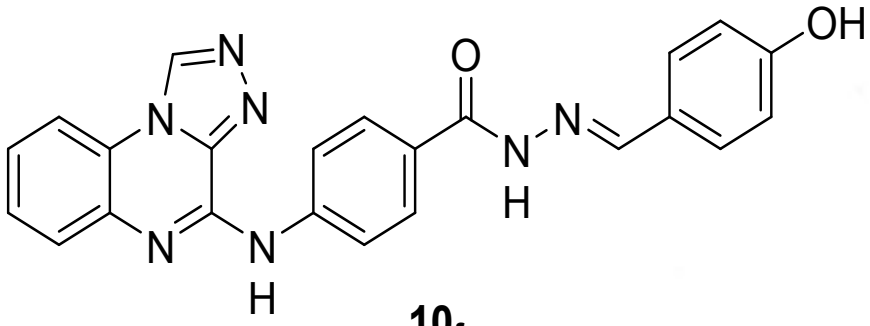
10f



Dr_AlaaElwan-40Hz-D2O

Sample Name Dr_AlaaElwan-40Hz-D2O
Date collected 2017-12-16
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

Dr_AlaaElwan-40Hz-D2O



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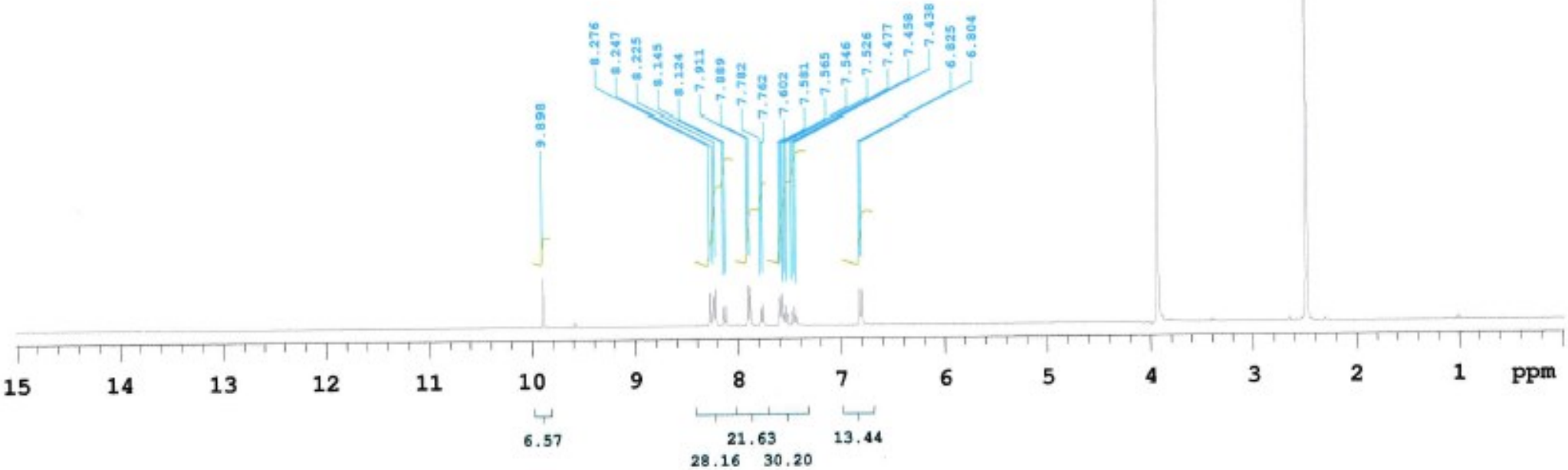
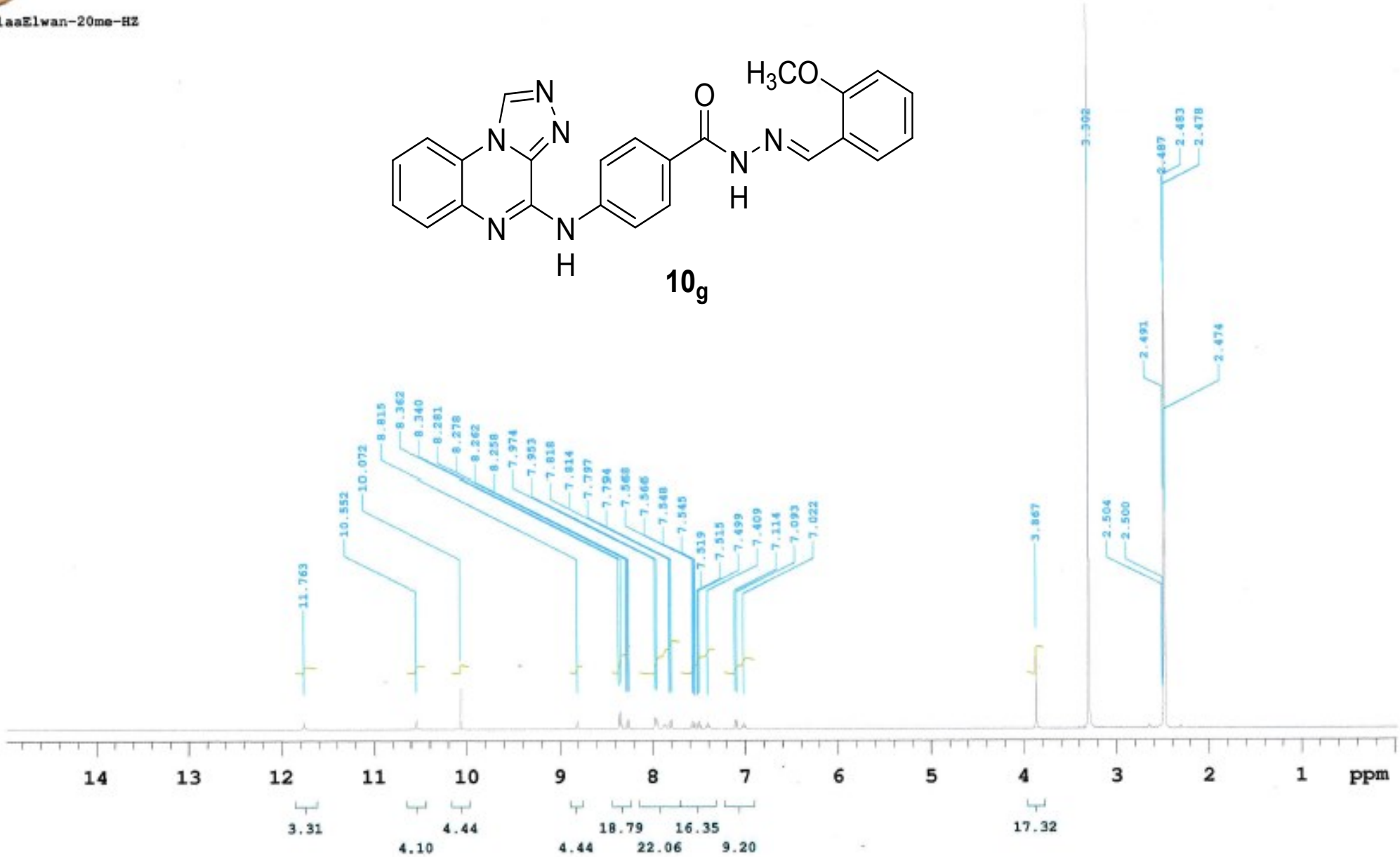


Dr_AlaaElwan-20me-HZ

Sample Name	Dr_AlaaElwan-20me-HZ	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr1
Date collected	2017-12-12	Solvent	dmso	Spectrometer	nmr400-mercury400	Operator	vnmr1

Dr_AlaaElwan-20me-HZ

10g

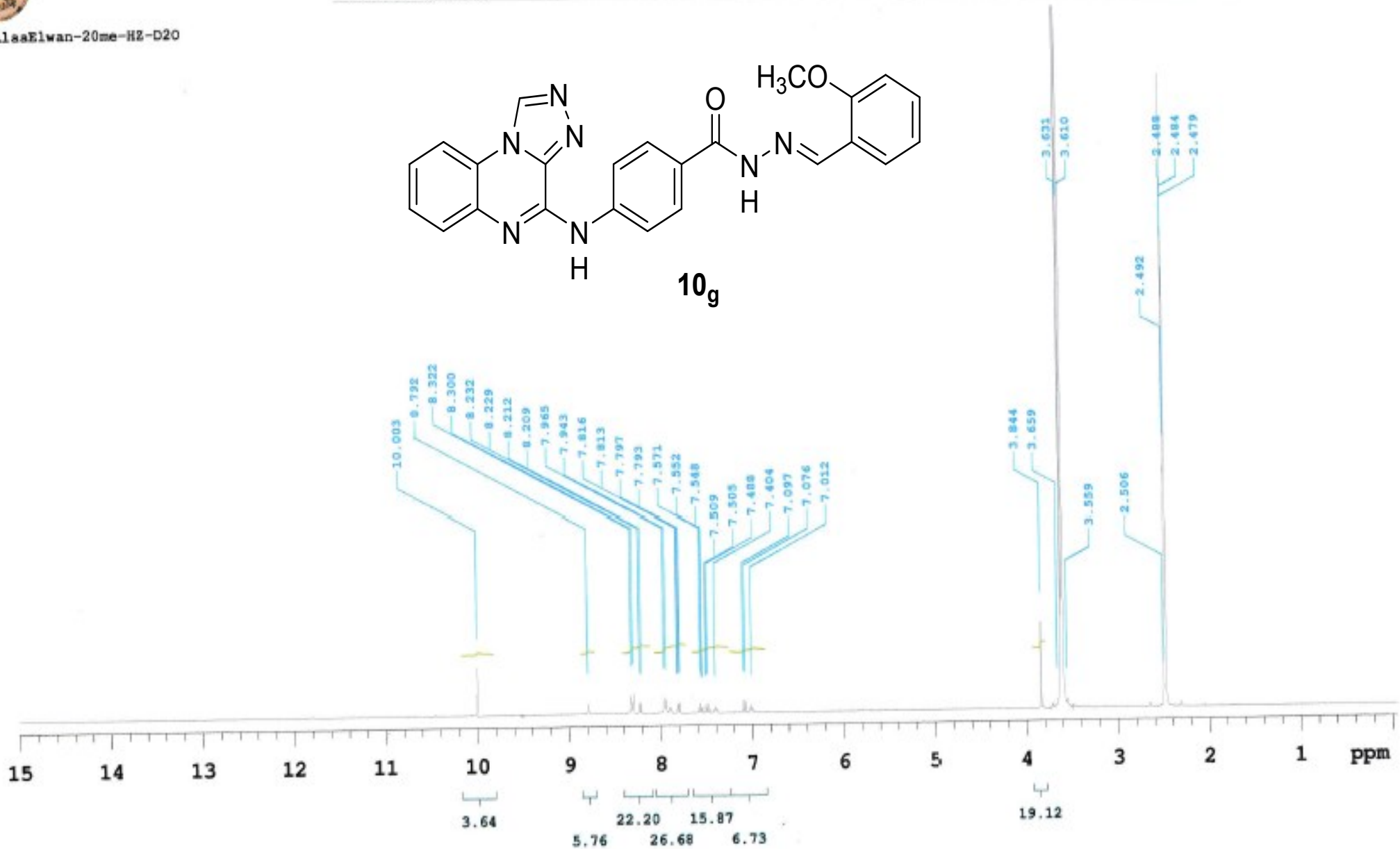


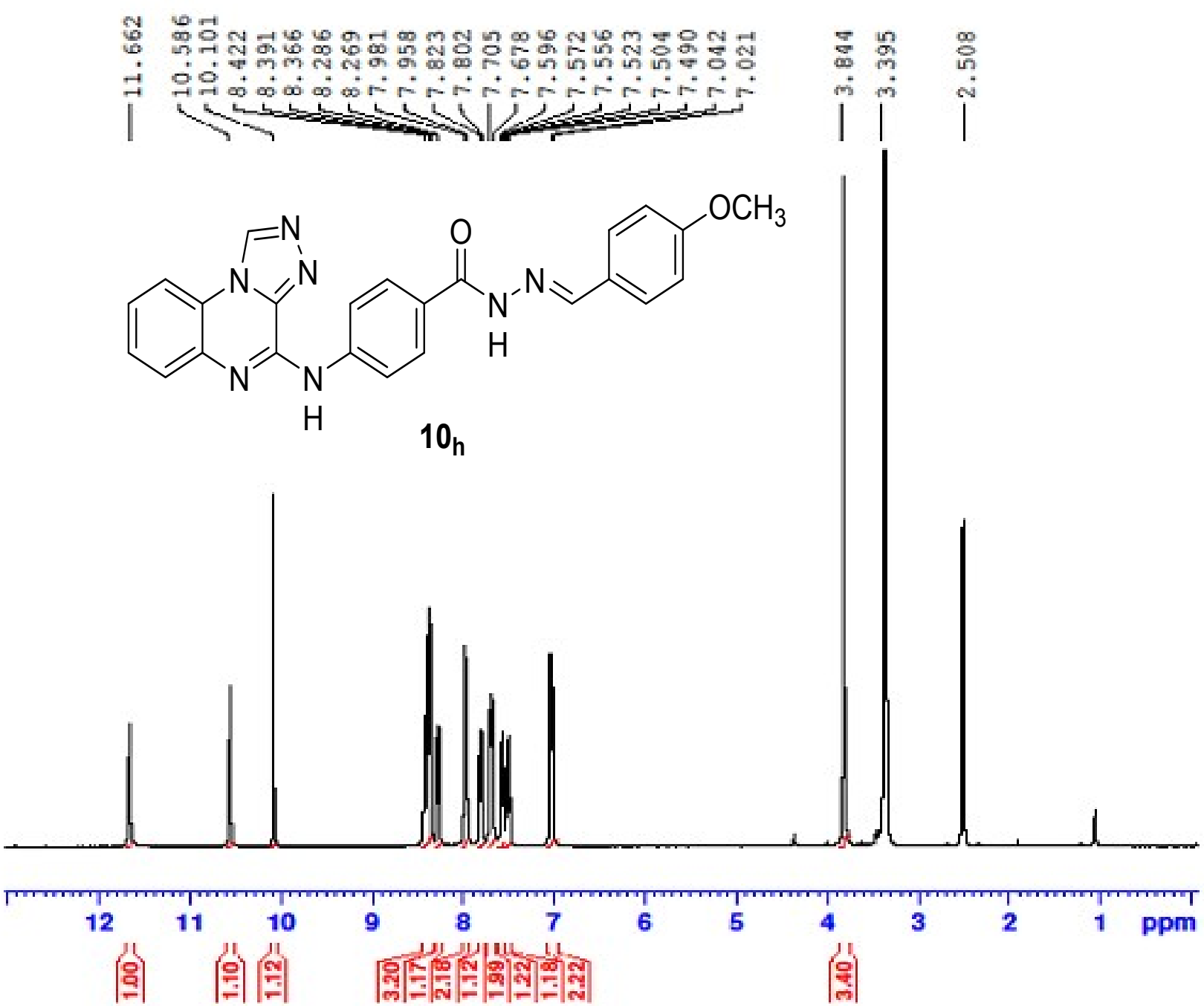
Dr_AlaaElwan-20me-HZ-D2O

Dr_AlaaElwar-20me-HZ-D2O

Sample Name Dr_AlaaElwan-20me-HZ-D2O
Date collected 2017-12-16
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

10g





BRUKER

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PROCNO                 1

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Time                8.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    64
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                 299.0 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
```

Alaa ElWan_C_4-OMe-HZ

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

BRUKER

10h

```
Current Data Parameters
NAME      Alaa ElWan_C_4-OMe-HZ
EXPNO                        10
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20180726
Time                     23.05
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                    DMSO
NS                         1200
DS                            4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                  1.3631488 sec
RG                     202.37
DW                     20.800 usec
DE                       6.50 usec
TE                      298.0 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1              100.6379178 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                45.00000000 W

======== CHANNEL f2 ========
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NUC2                         1H
CPDPRG[2                waltz16
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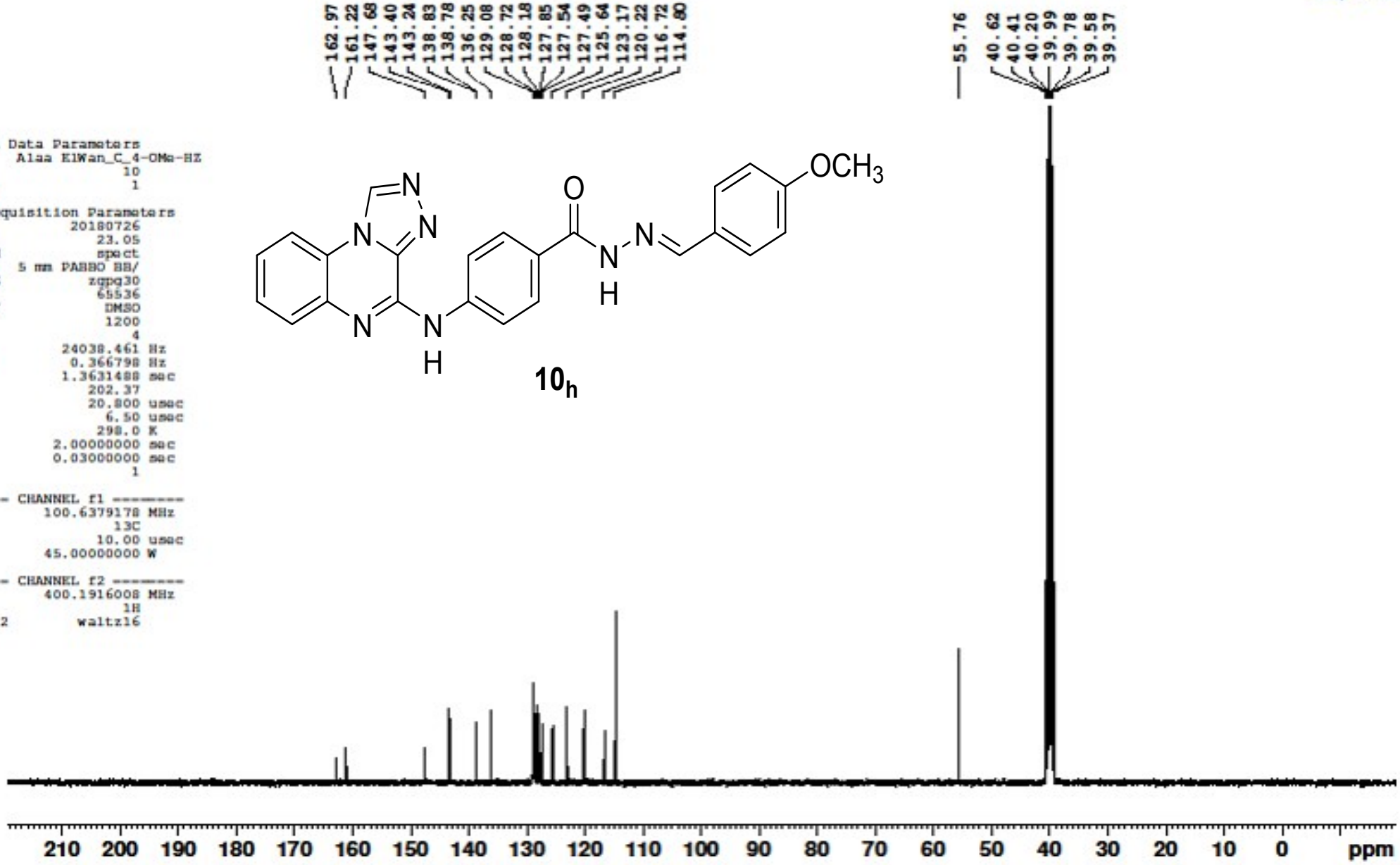
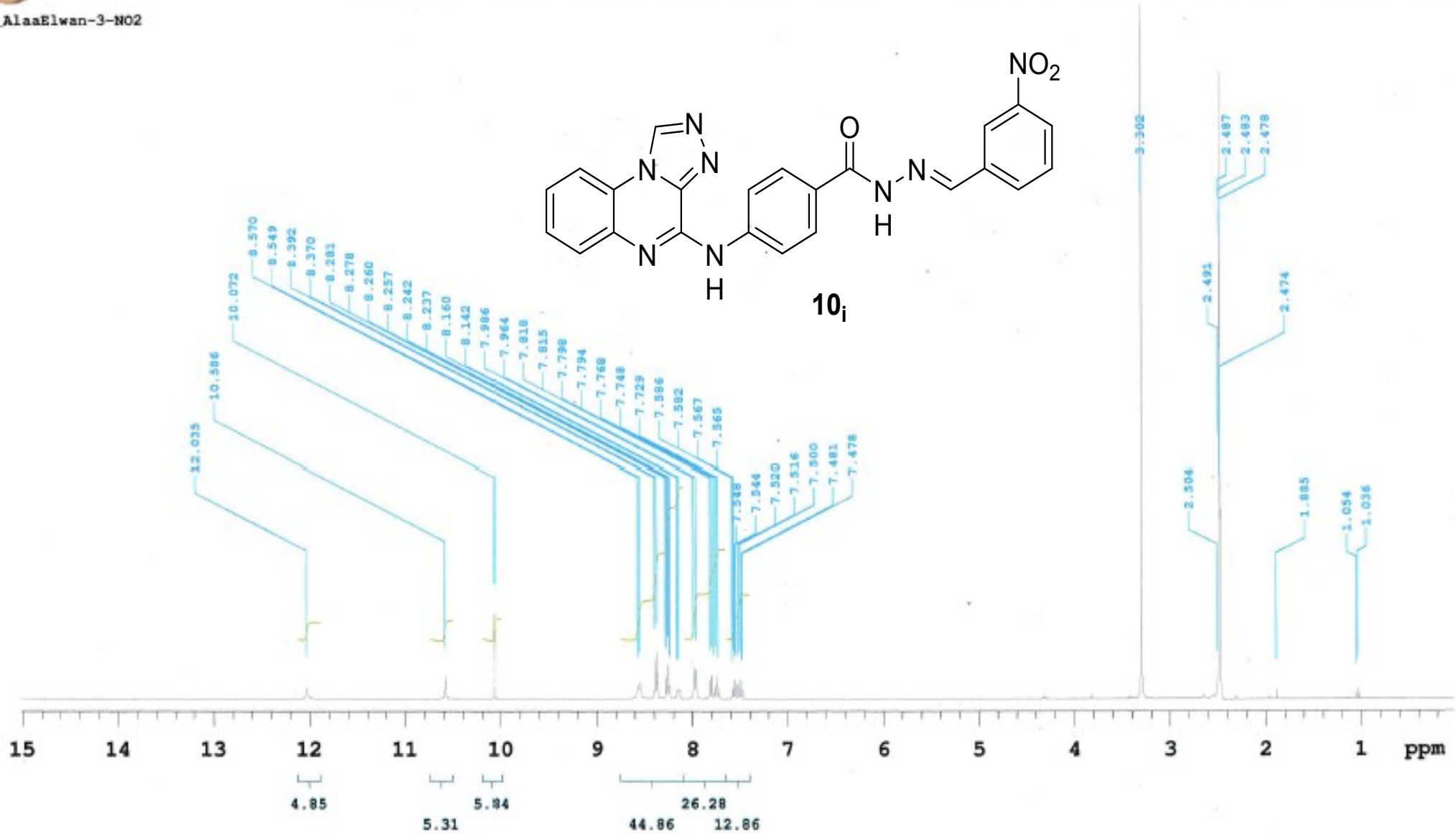


Dr_AlaaElwan-3-NO2

Sample Name	Dr_AlaaElwan-3-NO2	Pulse sequence	PROTON	Temperature	25	Study owner	vnmr1
Date collected	2017-12-12	Solvent	dmso	Spectrometer	nmr400-mercury400	Operator	vnmr1

Dr_AlaaElwan-3-NO2

10$_i$

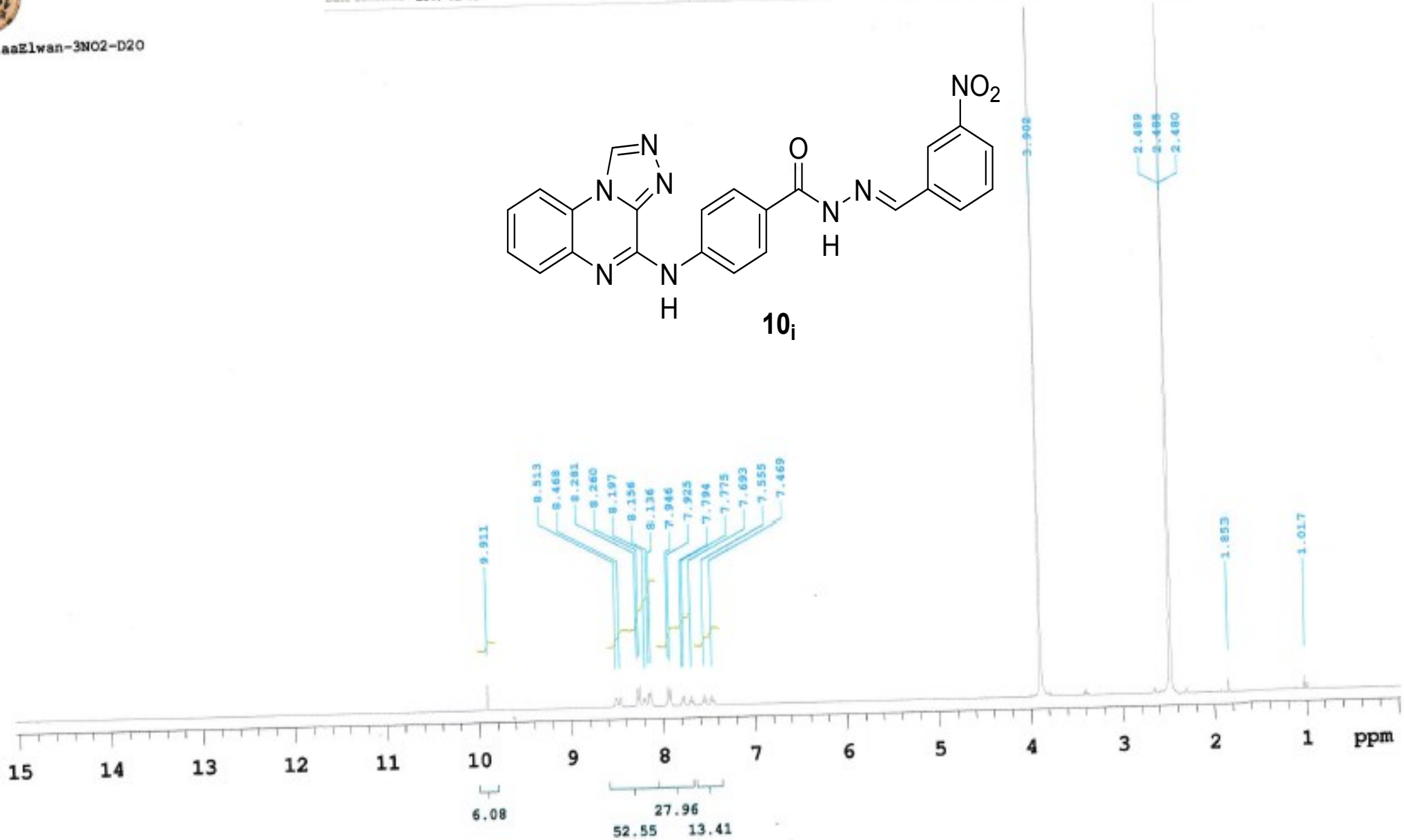


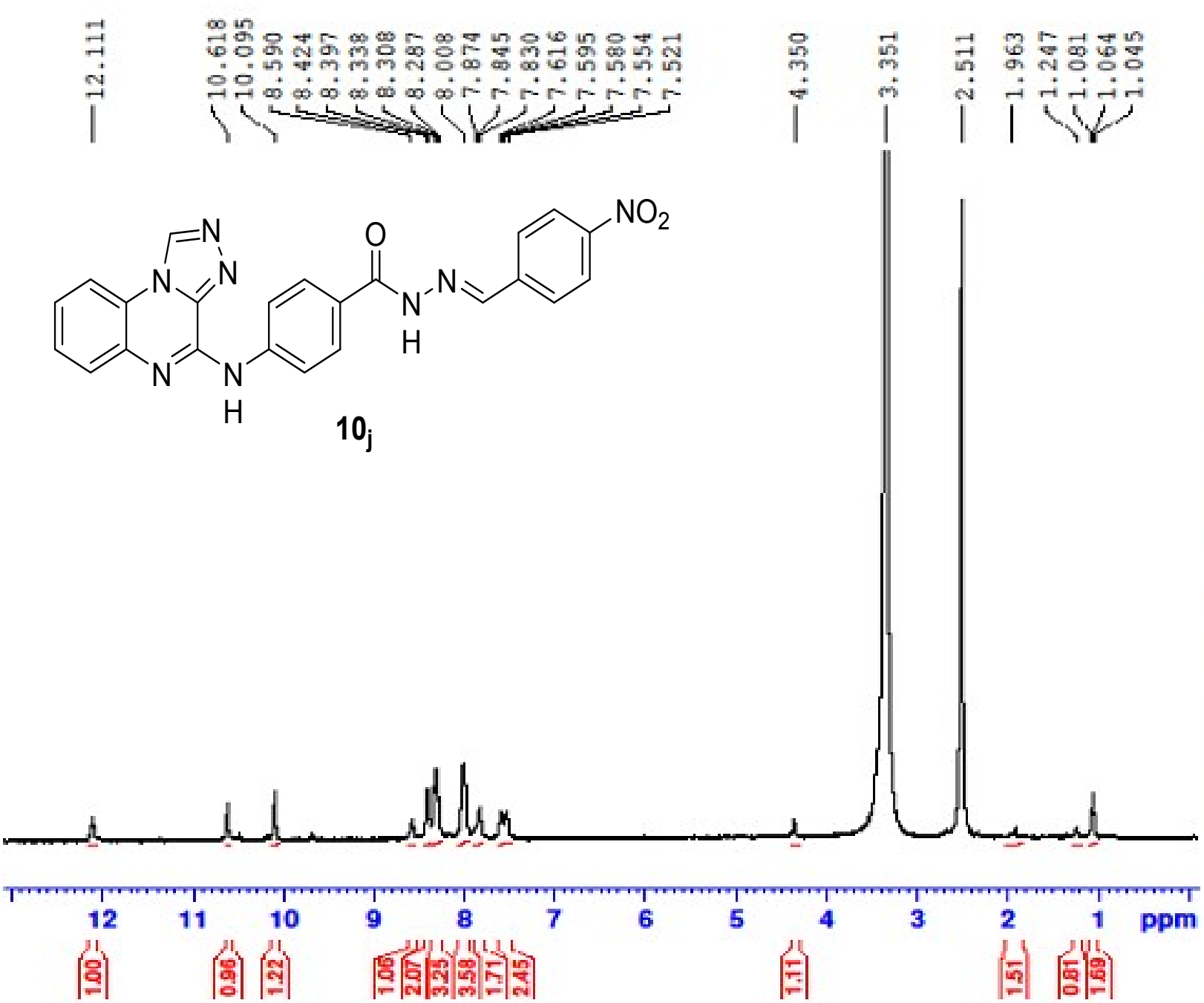
Dr_AlaaElwan-3NO2-D2O

Sample Name Dr_AlaaElwan-3NO2-D2O
Date collected 2017-12-16
Pulse sequence PROTON
Solvent dmso
Temperature 25
Spectrometer nmr400-mercury400
Study owner vnmr1
Operator vnmr1

Dr_AlaaElwan-3NO2-D2O

10$_i$





BRUKER

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
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Time                 8.52
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                  65536
SOLVENT             DMSO
NS                     64
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                 299.0 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
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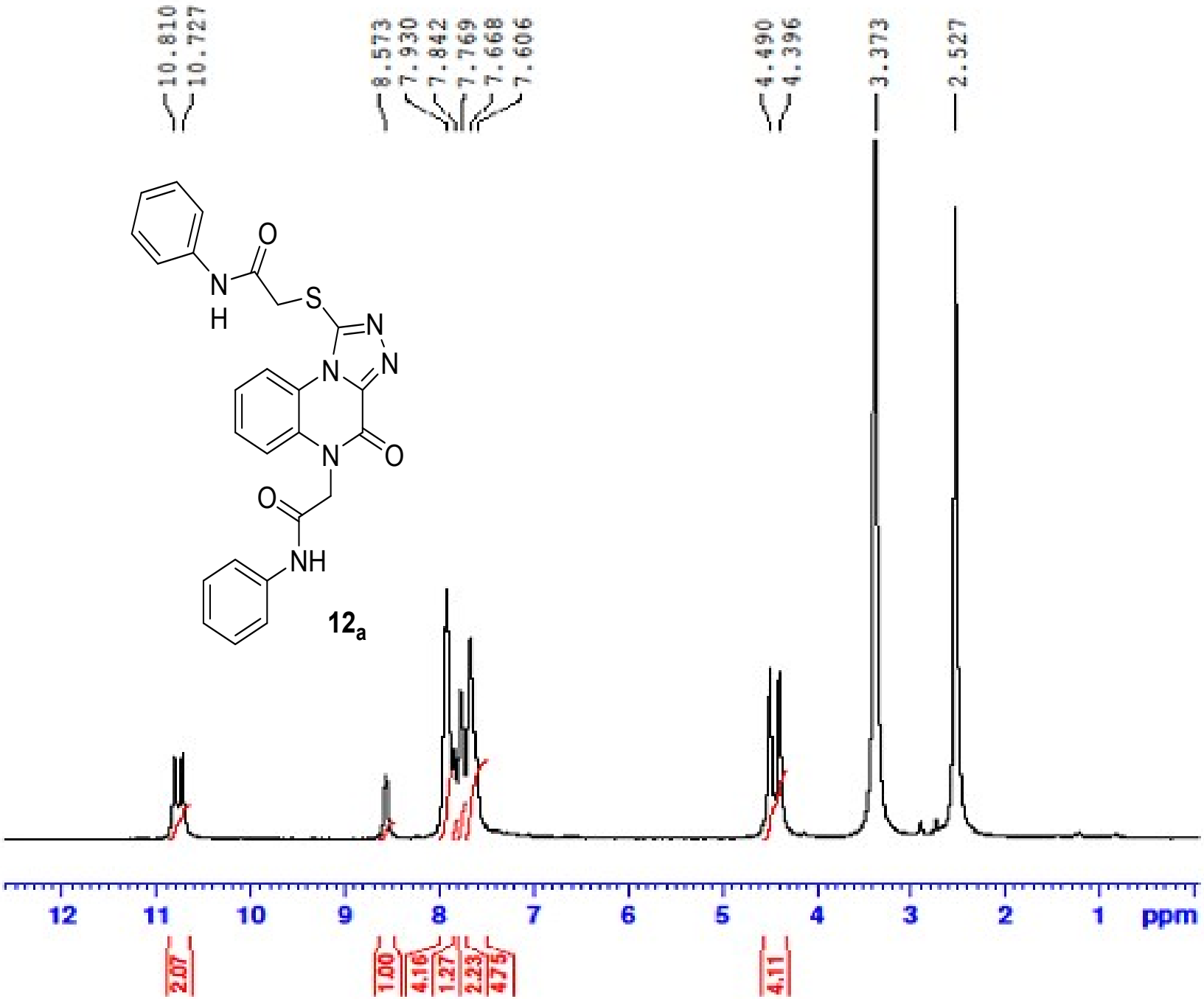

12a

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Current Data Parameters
NAME        alaa-PAA-8-AC
EXPNO                   1
PROCNO                  1

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Date_            20180528
Time                 9.38
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                  65536
SOLVENT             DMSO
NS                     29
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                  298.4 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
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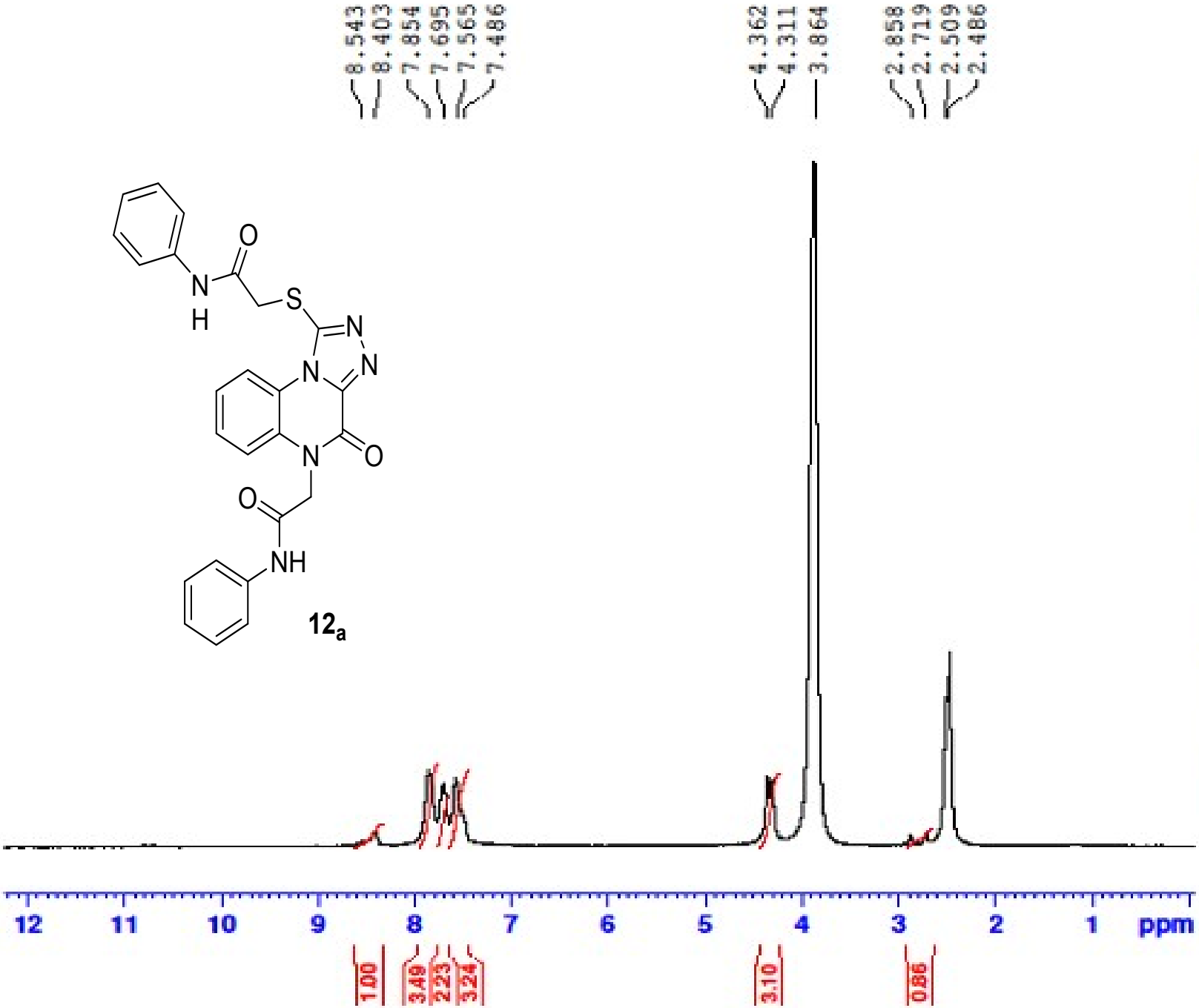
12a



Current Data Parameters
NAME alaa-PAA-S-AC-d2o
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180528
Time 9.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 30
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 298.0 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

Alaa ElWan_C_P-Me-S-AC

Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg

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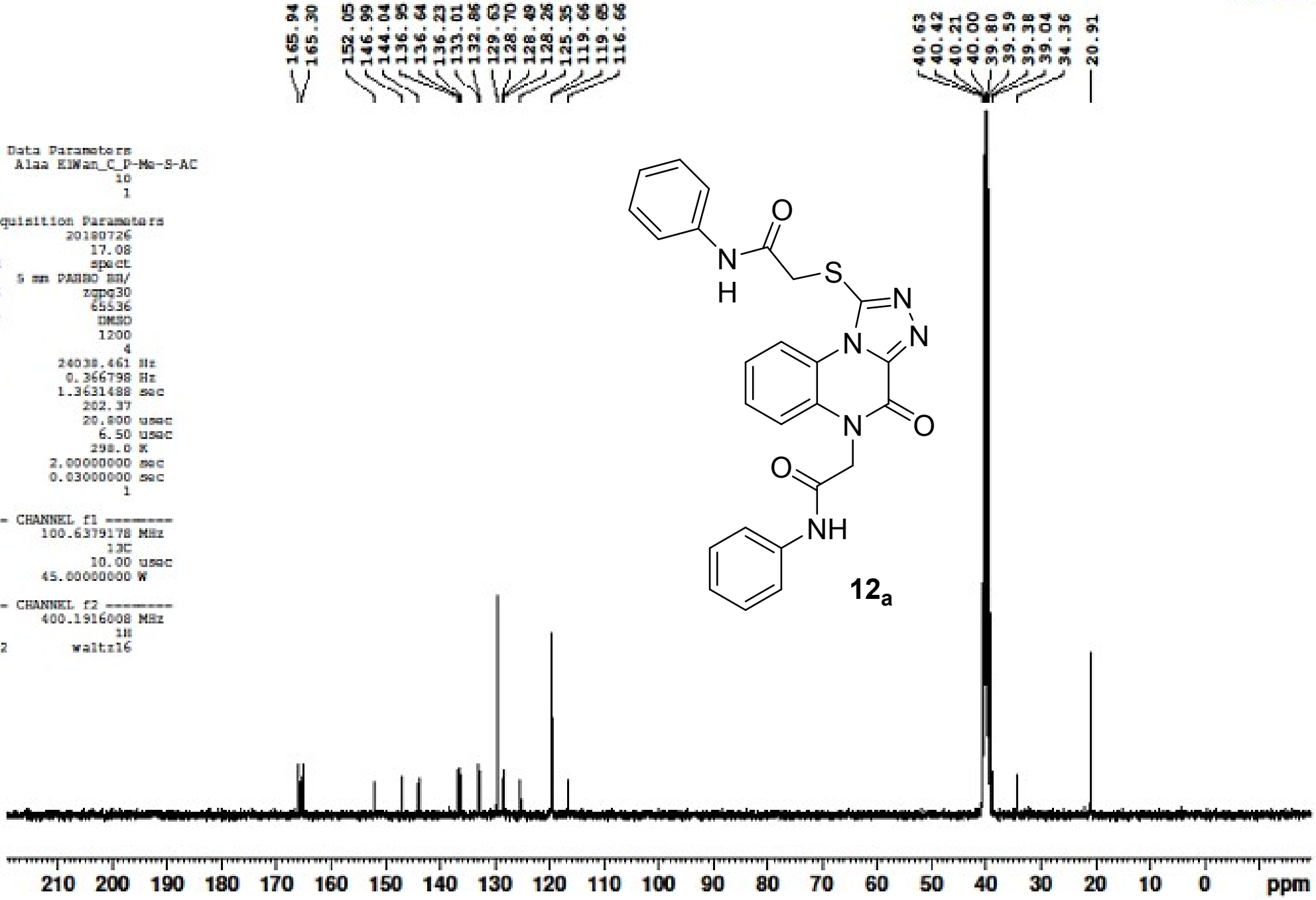
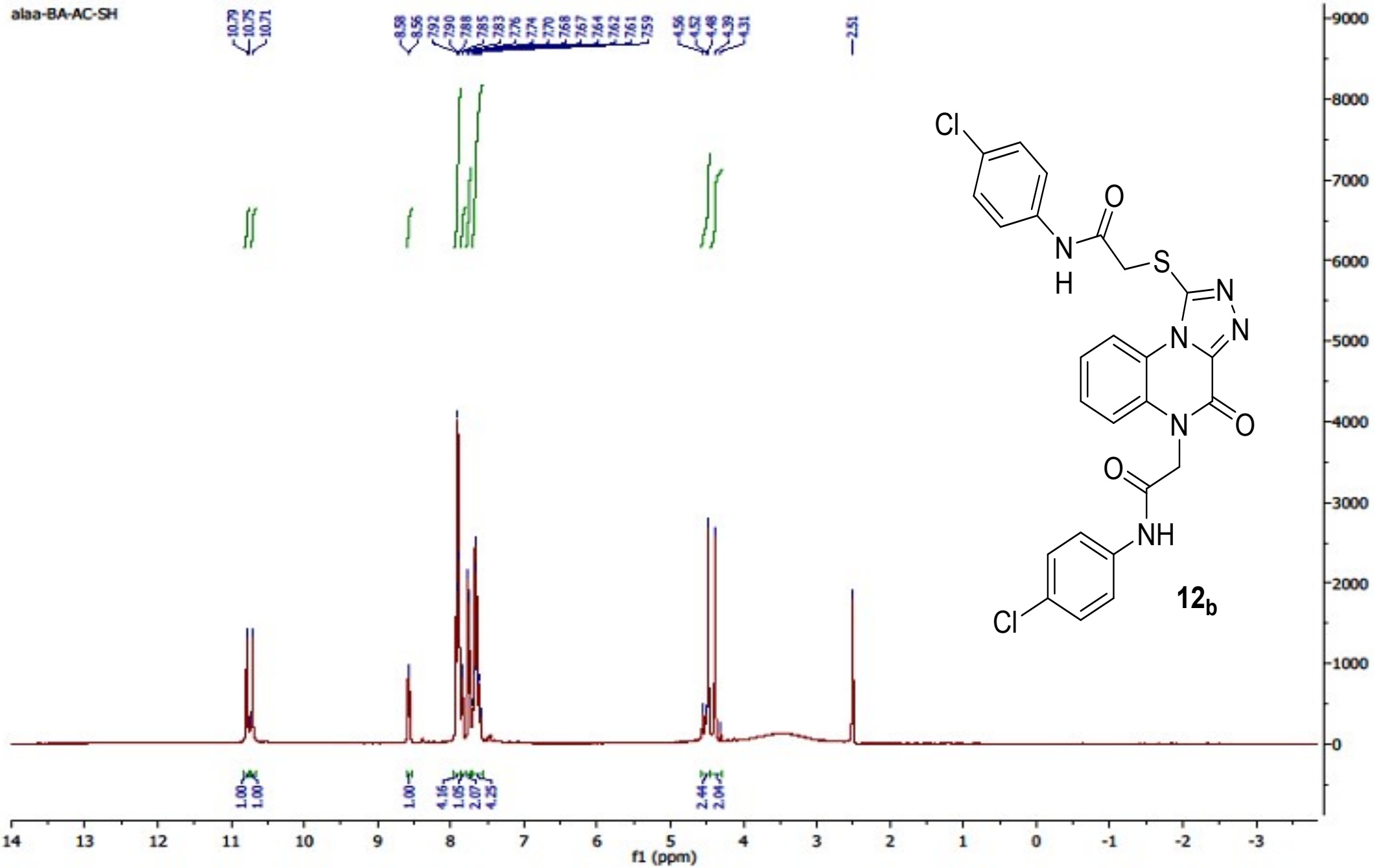


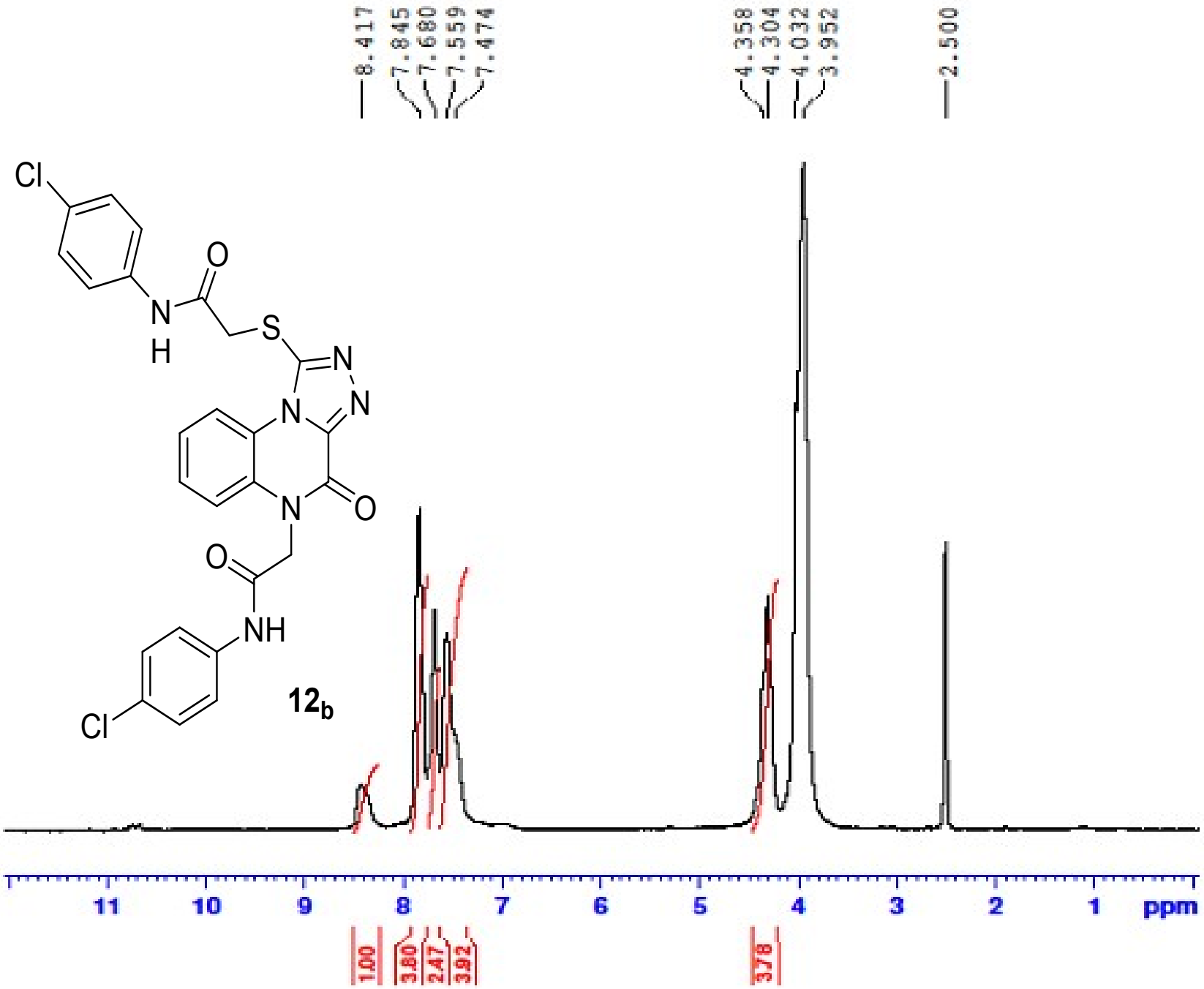

```
Current Data Parameters
NAME      Alaa ElWan_C_P-Me-S-AC
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180726
Time                  17.08
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1200
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                  202.37
DW                  20.800 usec
DE                   6.50 usec
TE                  298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6379178 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           45.00000000 W

======== CHANNEL f2 ========
SFO2           400.1916008 MHz
NUC2                     1H
CPDPRG[2            waltz16
```


alaa-BA-AC-SH
10.79
10.75
10.71
8.58
8.56
7.92
7.90
7.88
7.85
7.83
7.76
7.74
7.70
7.68
7.67
7.64
7.62
7.61
7.59
4.56
4.52
4.48
4.39
4.31
2.51
1.00
1.00
1.00
4.16
1.05
2.07
4.25
2.44
2.04
f1 (ppm)
Cl
O
N
H
S
N
N
N
N
O
O
NH
Cl
12b



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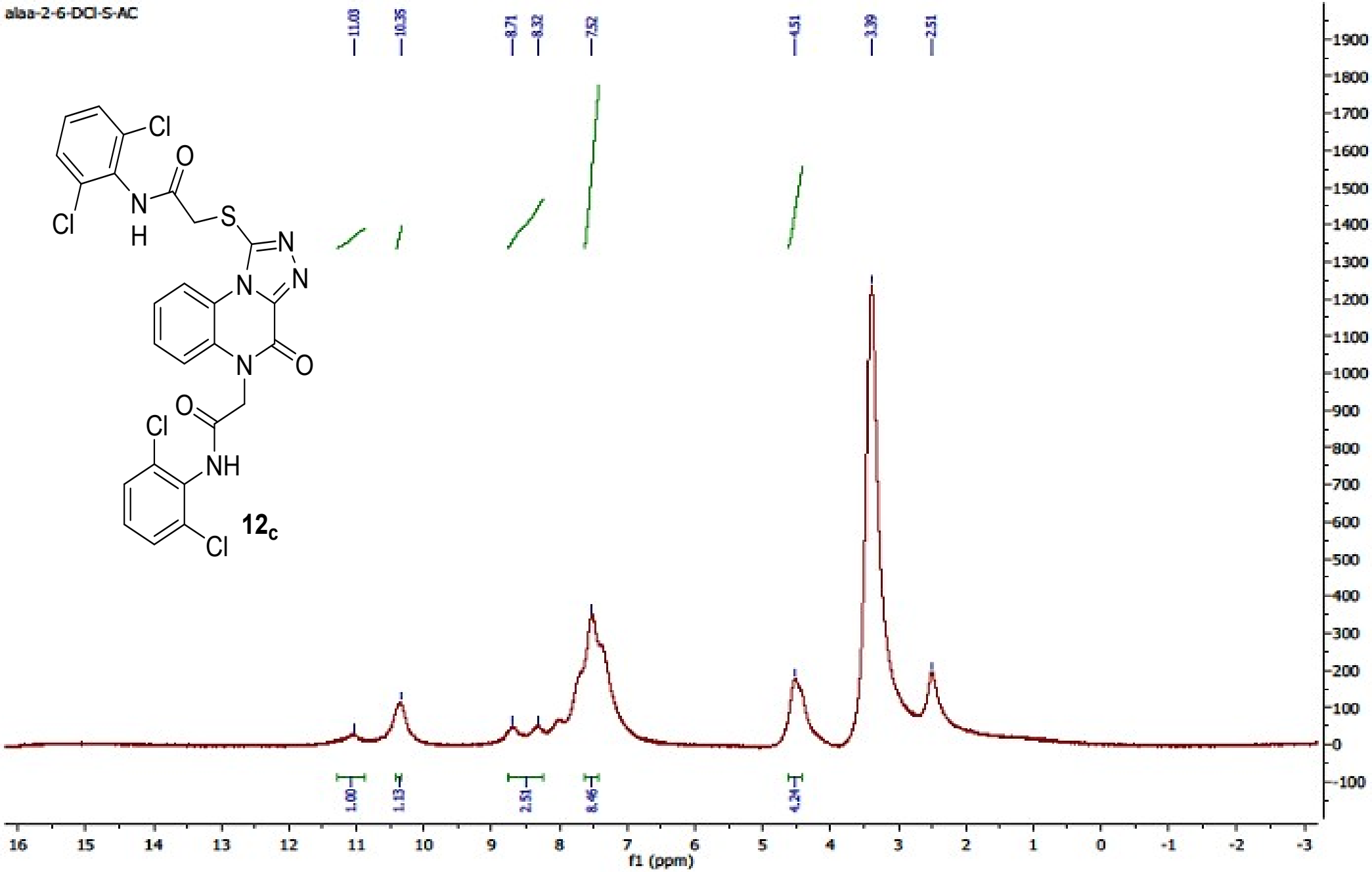
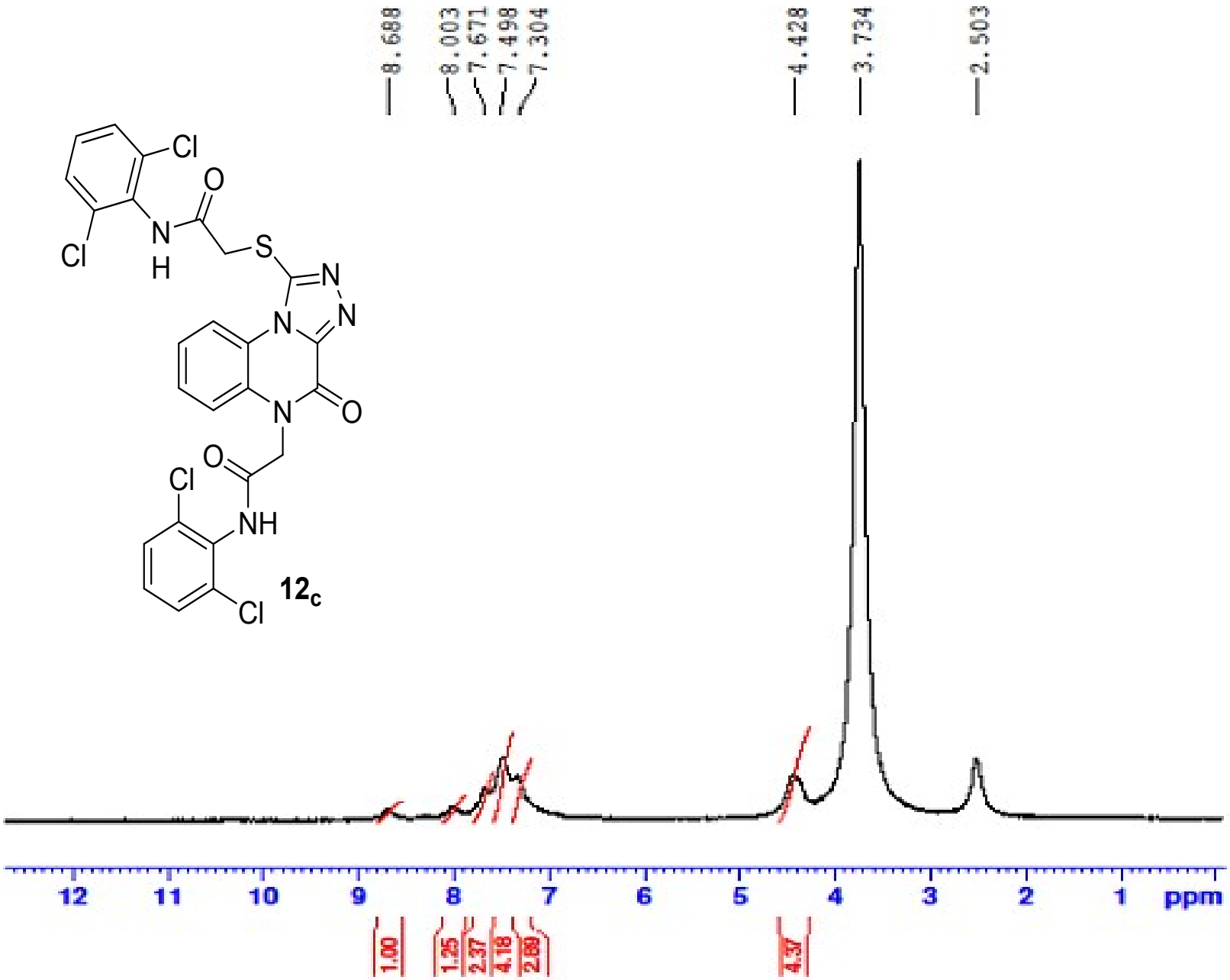
```
Current Data Parameters
NAME      alas-BA-AC-SH-d2o
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20180502
Time                11.58
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    43
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                298.0 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
```


alaa-2-6-DCl-S-AC
11.03
10.35
8.71
8.32
7.52
4.51
3.39
2.51
1.00
1.13
2.51
8.46
4.24
f1 (ppm)
12c



12c

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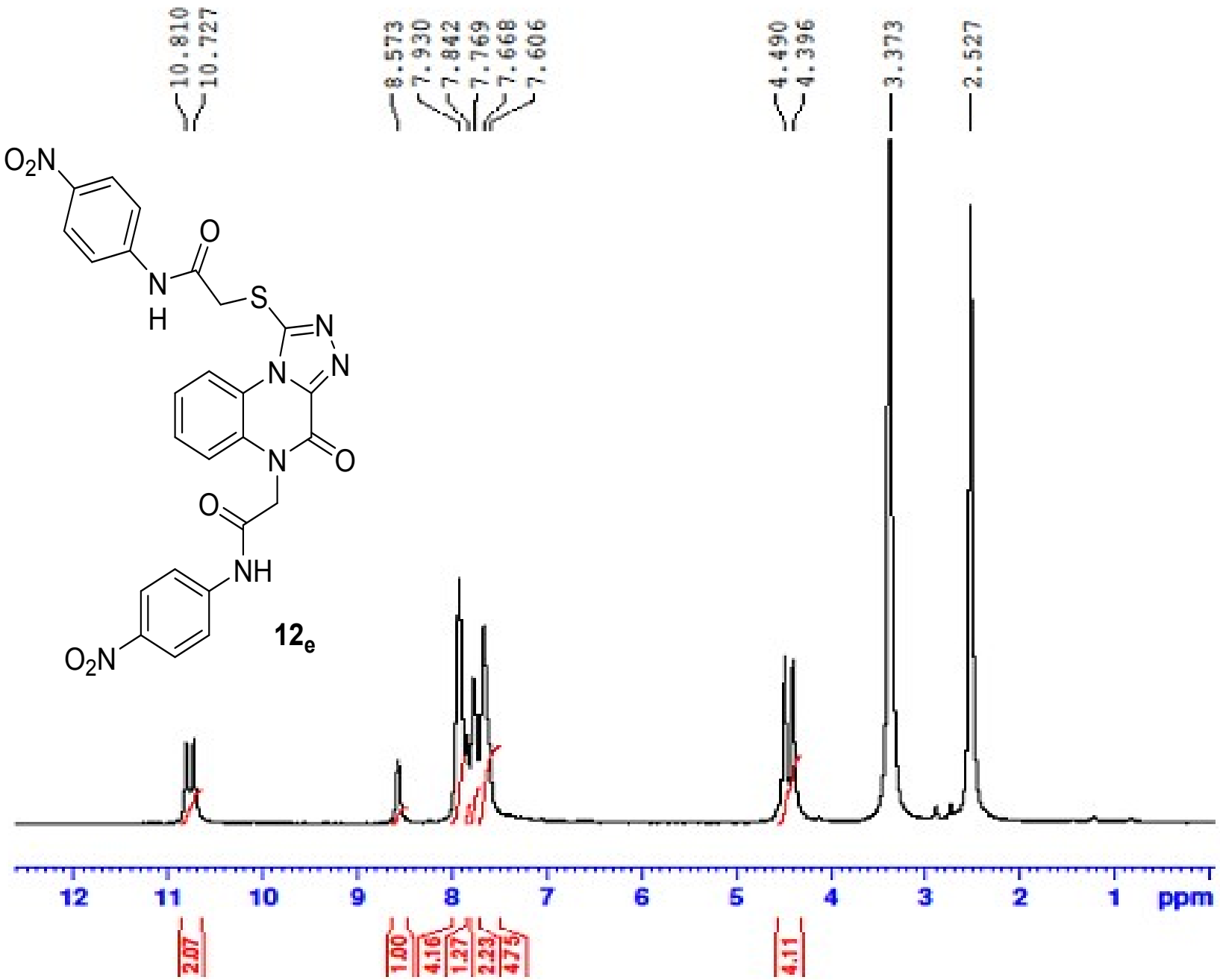
```
Current Data Parameters
NAME      alaa-2-6-DCl-S-AC-d2o
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20180528
Time                   10.16
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG                 zg30
TD                     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
TE                     298.0 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
```



12_e

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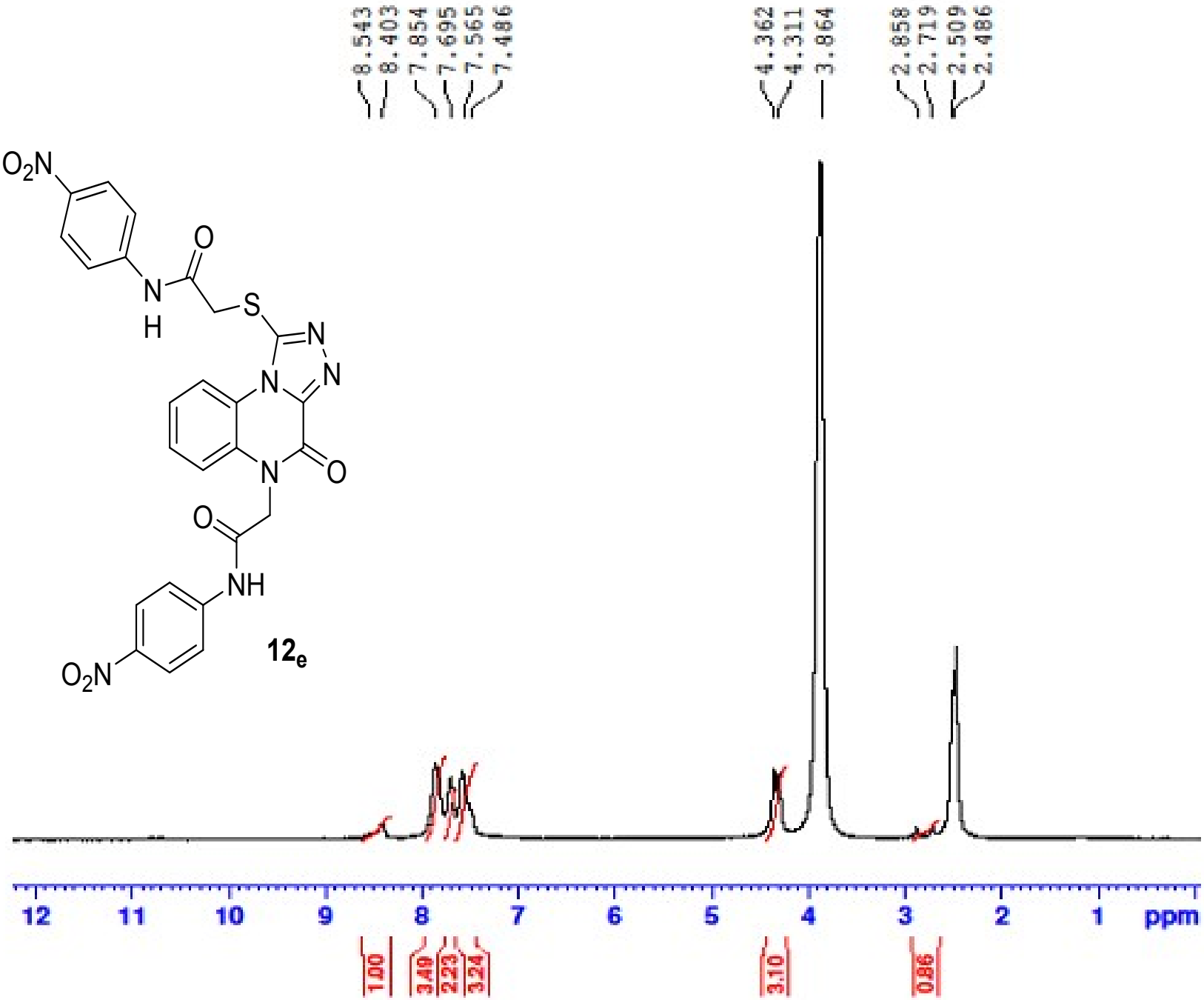
```
Current Data Parameters
NAME        alas-PAA-S-AC
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180528
Time                 9.38
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    29
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                298.4 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
```

12$_e$



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```
Current Data Parameters
NAME      alaa-PAA-S-AC-d2o
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20180528
Time                 9.49
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    30
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                 298.0 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
```