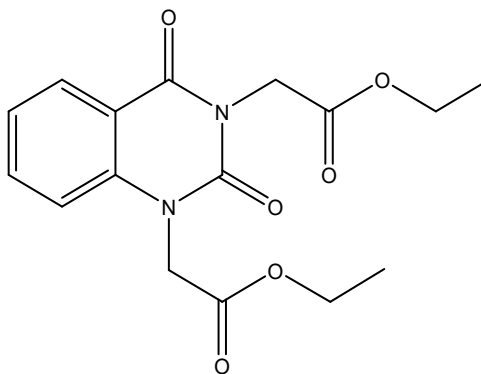


-

[Supplementary data file](#)

Design, Synthetic Approach, In silico Molecular Docking and Antibacterial Activity of Quinazolin-2,4-dione Hybrids Bearing Bioactive Scaffolds

-Compound (1):



1

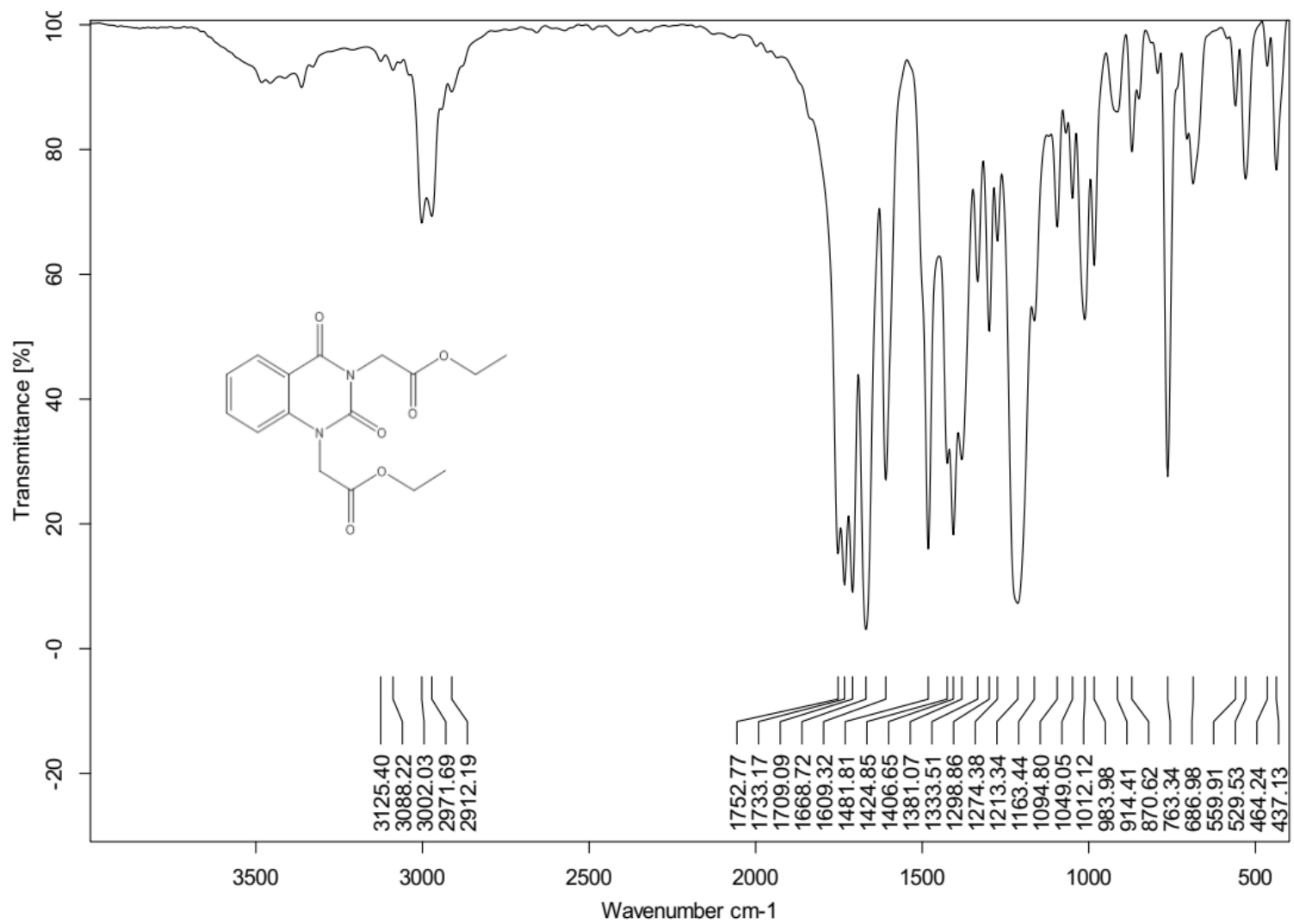


Figure . ¹H-NMR of compound 1 .

-

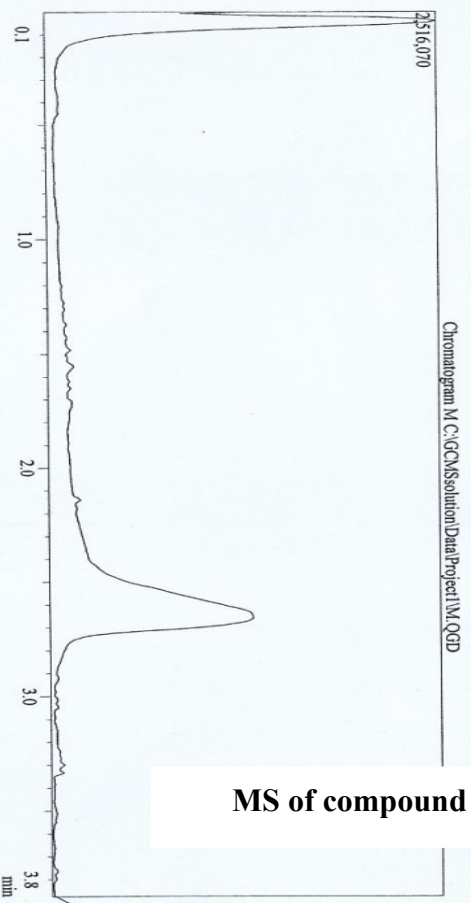
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Micro Analytical Center**

**DI Analysis
Shimadzu Qp-2010 Plus**

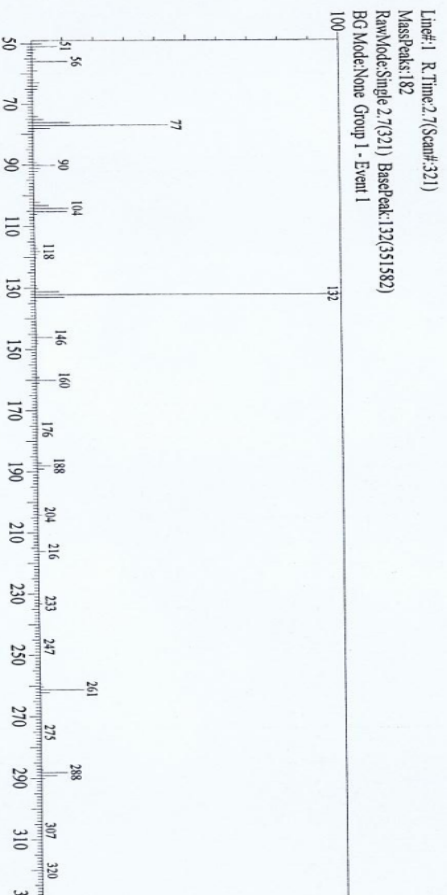
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 01:53:50
 Sample Name : M
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project\IM.QGD
 Org Data File : C:\GCMSsolution\Data\Project\IM.QGD
 Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\SystemTime\default.qgr
 Serials\Modified by : Dr. Mai Younis
 Modified : 15/01/2007 01:57:45

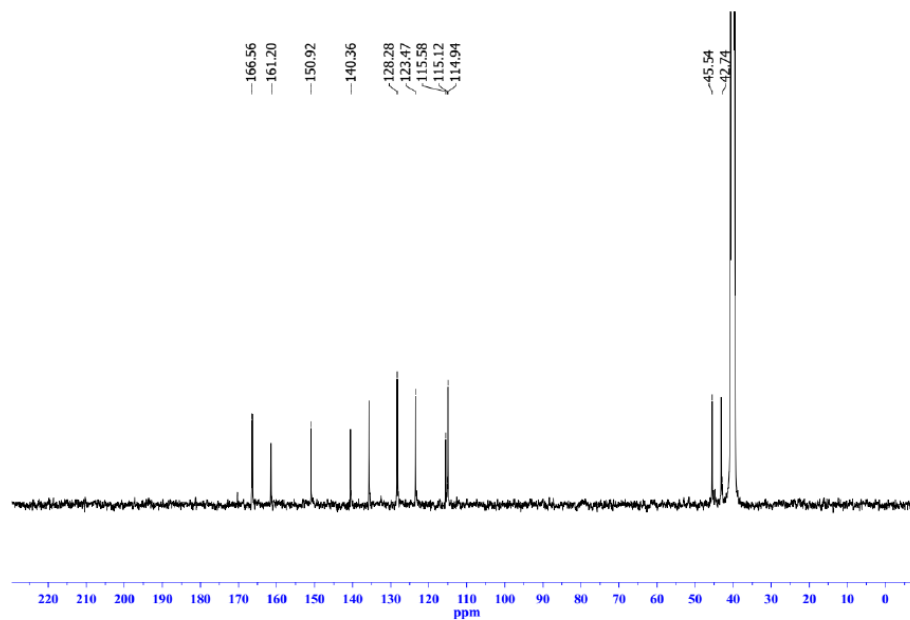
Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 -Group 1 - Event 1-
 Start Time : 0:00min
 End Time : 1:00min
 ACQ Mode : Scan
 Event Time : 0:50sec
 Scan Speed : 1:250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project\IM.QGD



MS of compound (1)





```

Current Data Parameters
Name: Dec06-2022
EXPNO: 150
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20221207
Time: 7.46
INSTRUM: spect
PROBHD: 5 mm DASKO BB/
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 2200
DS: 4
SWH: 24038.461 Hz
FIDRES: 0.366798 Hz
AQ: 1.3611488 s
RG: 199.04
DQ: 26.800 Hz
DE: 6.50 Hz
TE: 300.2 K
D1: 2.0000000 s
d11: 0.0300000 s
TSD: 1

----- CHANNEL f1 -----
SFO1: 100.6210364 MHz
NUC1: 13C
P1: 0.60 s
PLW1: 56.0000000 W

----- CHANNEL f2 -----
SFO2: 400.1140051 MHz
NUC2: 1H
CPCORR[2]: waltz16
PCORR: 90.00 Hz
PINC2: 22.0000000 Hz
PINC12: 0.41091001 Hz
PINC13: 0.33284000 Hz

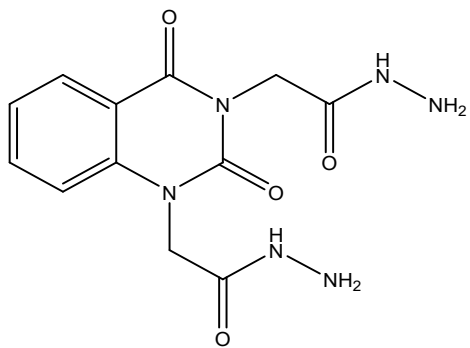
F2 - Processing parameters
SI: 32768
SF: 100.6127690 MHz
MIX: FM
SGB: 0 6.00 Hz
GB: 0
PC: 1.40

```

¹³C-NMR (100 MHz, DMSO) of compound (1)

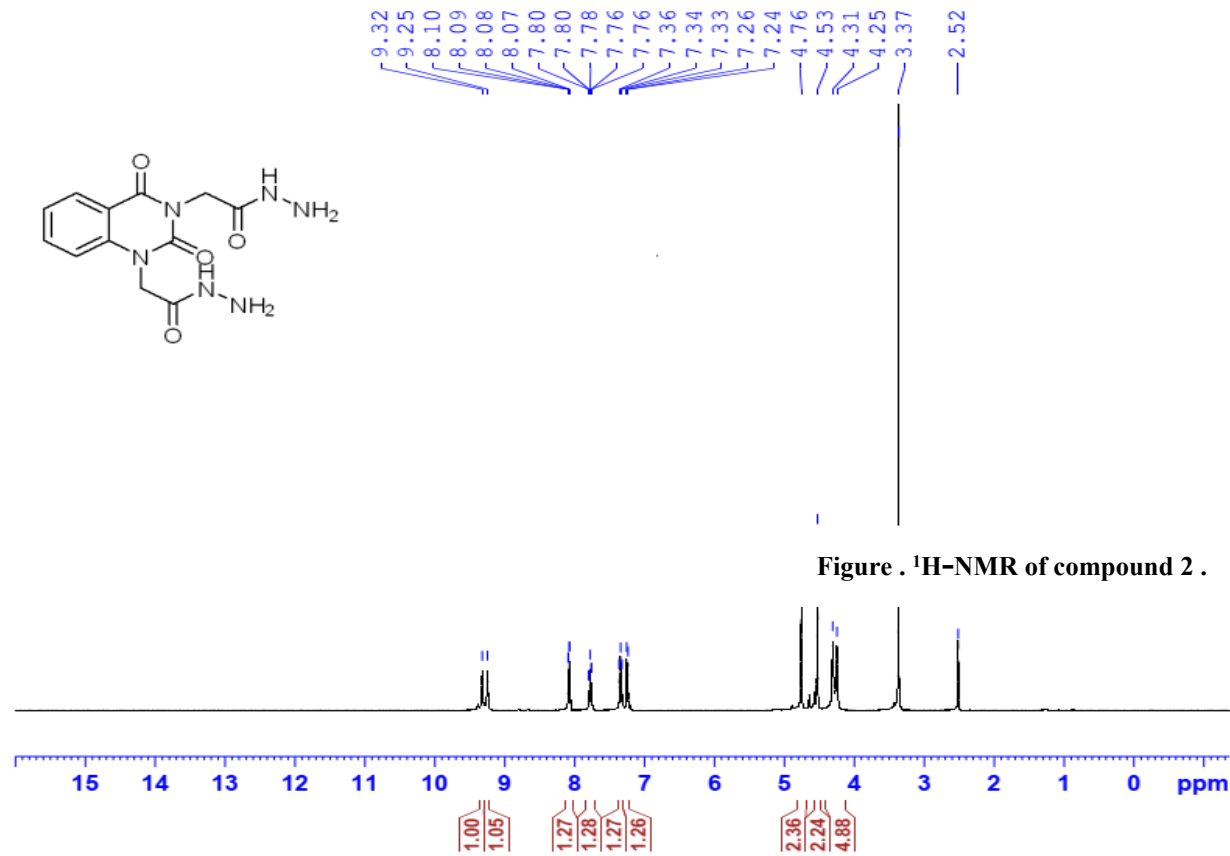
-

-Compound (2):



2

2



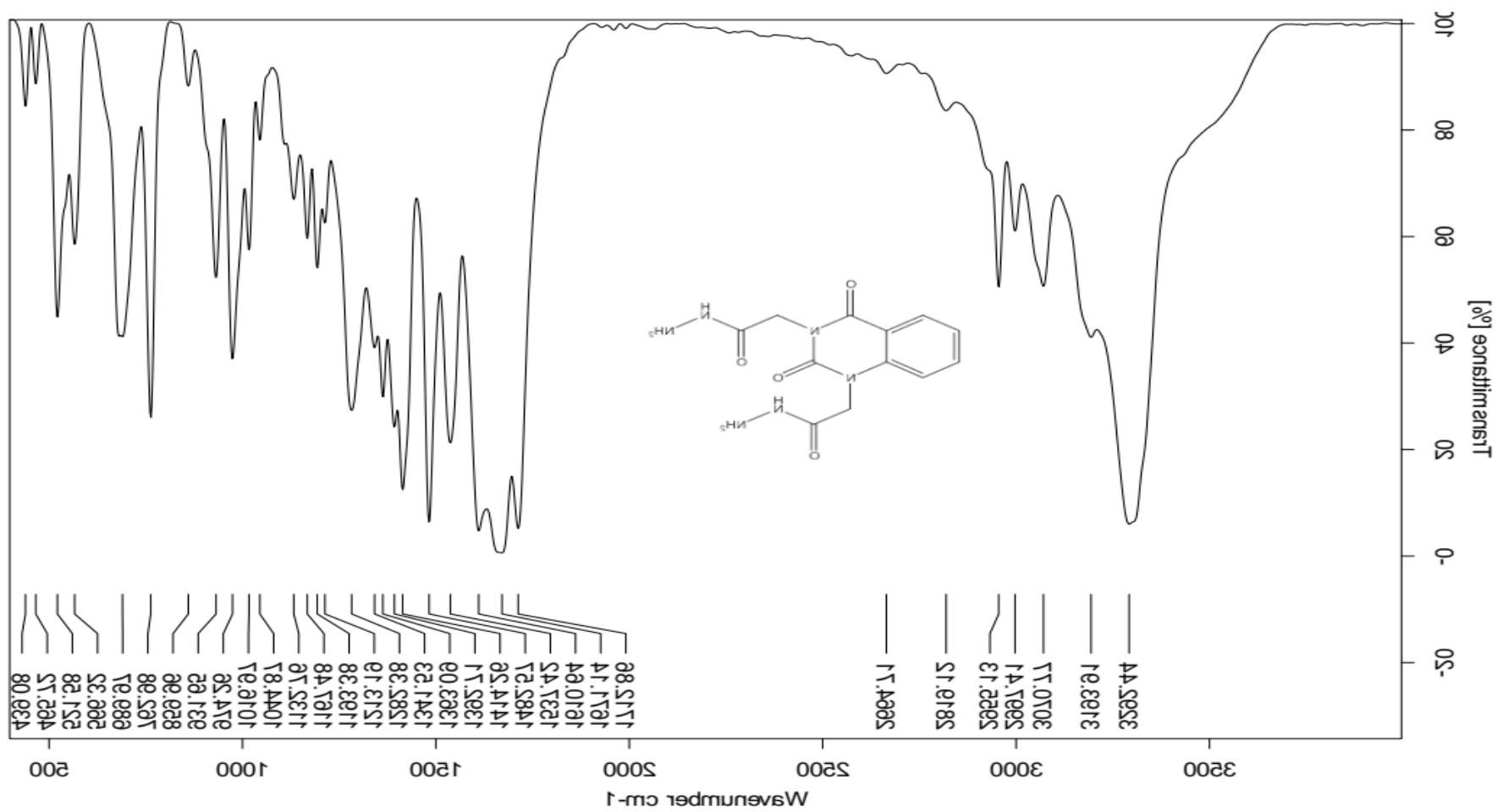
```

Current Data Parameters
NAME      mohamed omer-M1-Hnmr-ov
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20211018
Time     19.08 h
INSTRUM  spect
PROBHD   Z108618_0948 (
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.820 Hz
FIDRES   0.244692 Hz
AQ        4.089466 sec
RG        176.72
DN        62.400 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TDO       1
SF01     400.2024712 MHz
NUC1     15N
P1        12.50 usec
PLW1     12.00000000 W

F2 - Processing parameters
SI        65536
SF        400.2000000 MHz
WDW       EM
SSB       0
GB        0
GAMMA     0.30 Hz
INUM      0
F2        1.00
  
```

Figure . ¹H-NMR of compound 2 .



FT-IR of compound (2)

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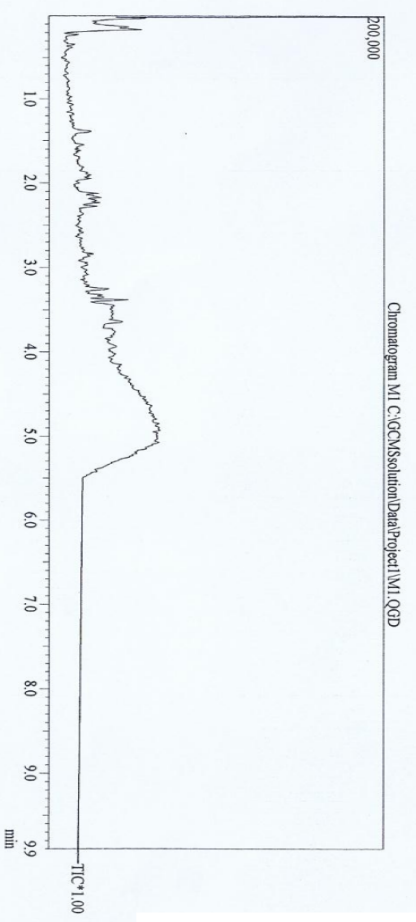
DI Analysis
Shimadzu Qp-2010 Plus

[Handwritten signature]
2/1/07

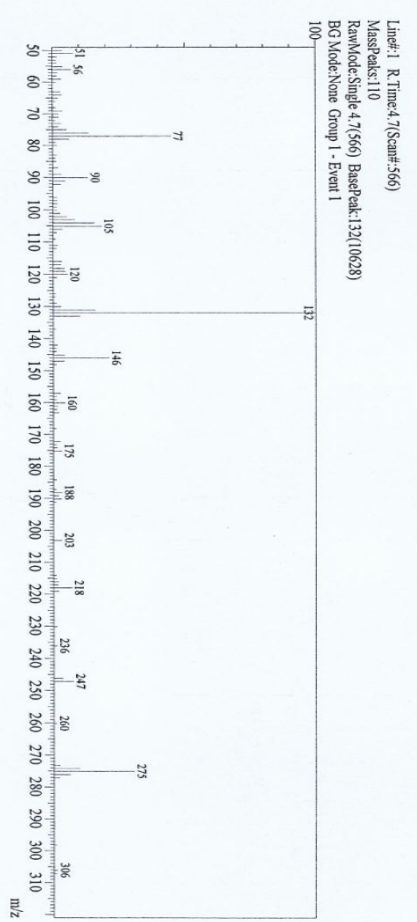
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 01:59:25
 Sample Name : M1
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quesa
 Data File : C:\GCMSsolution\Data\Project1\M1.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\M1.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System1\default.qgt
 Start/Stop/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:04:57

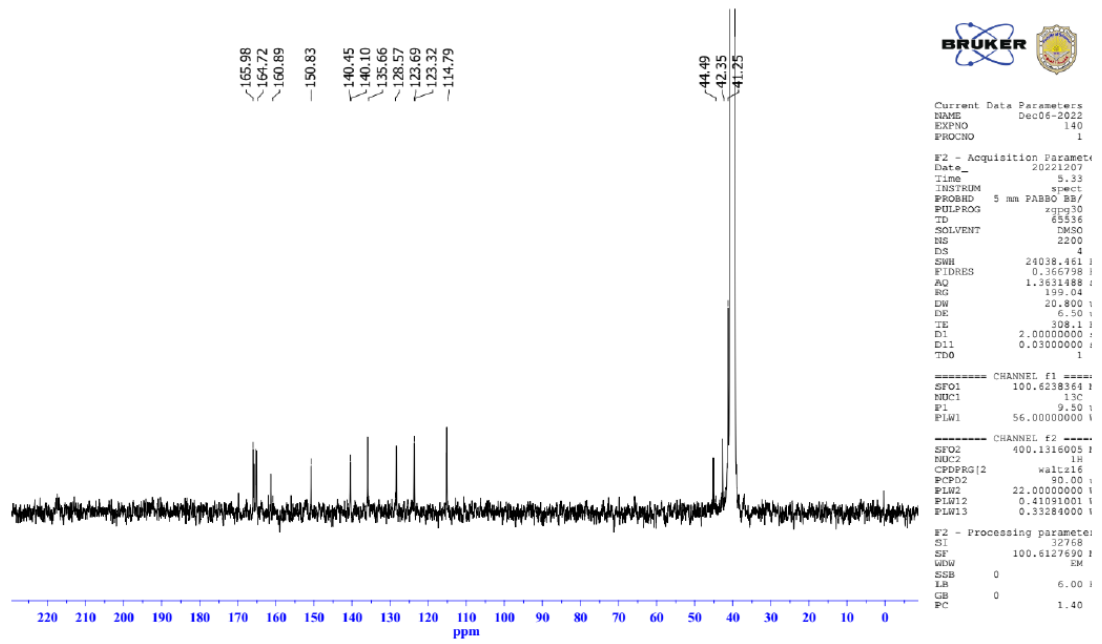
Method
 Analytical Line 1 :
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACO Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project1\M1.QGD



MS of compound (2)

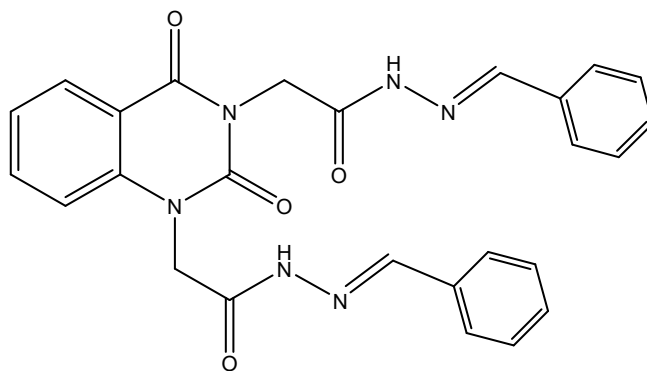




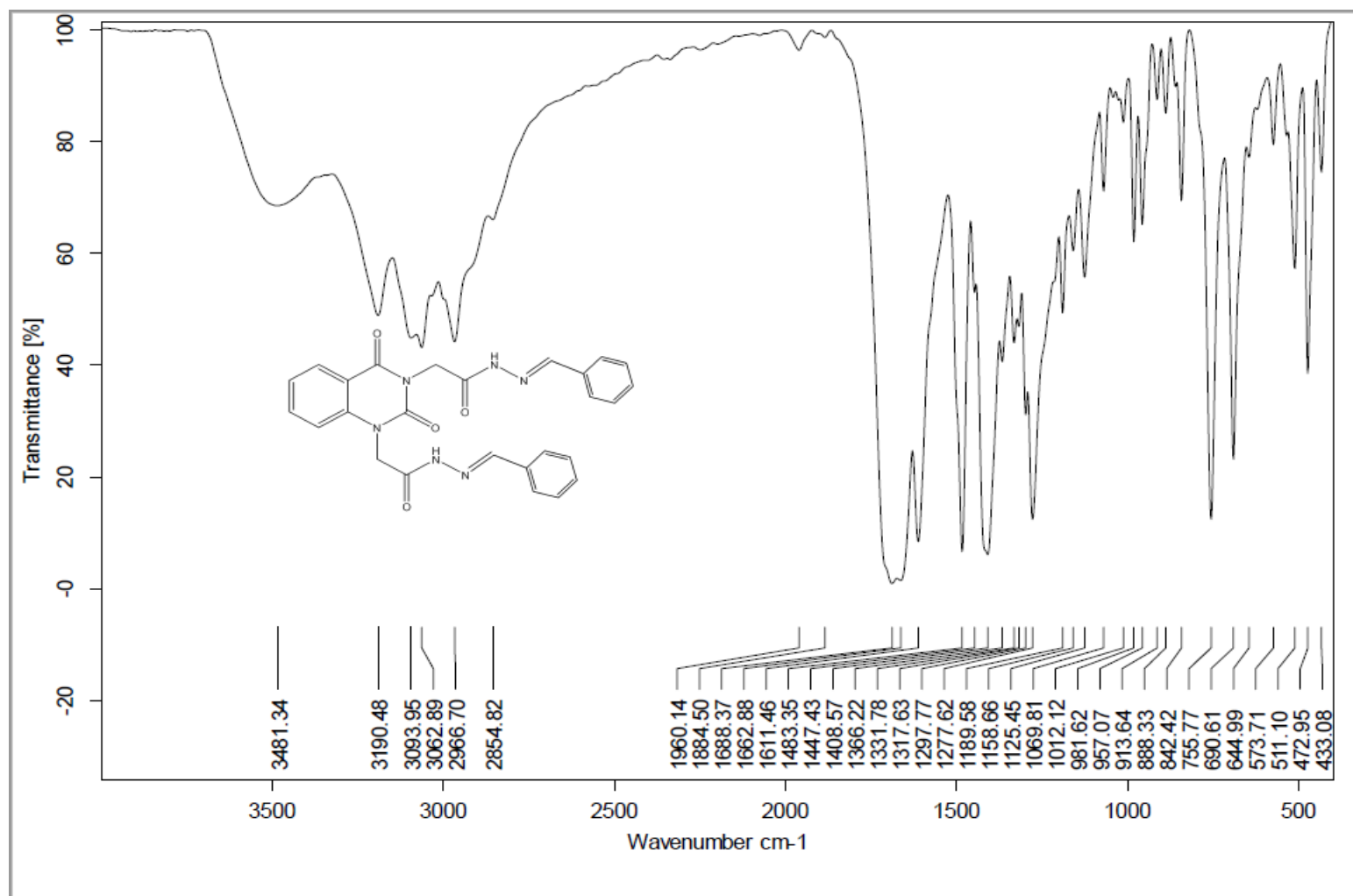
¹³C-NMR (100 MHz, DMSO) of compound (2)

-

-Compound (3a)



3a



FT-IR of compound (3a)

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Micro Analytical Center

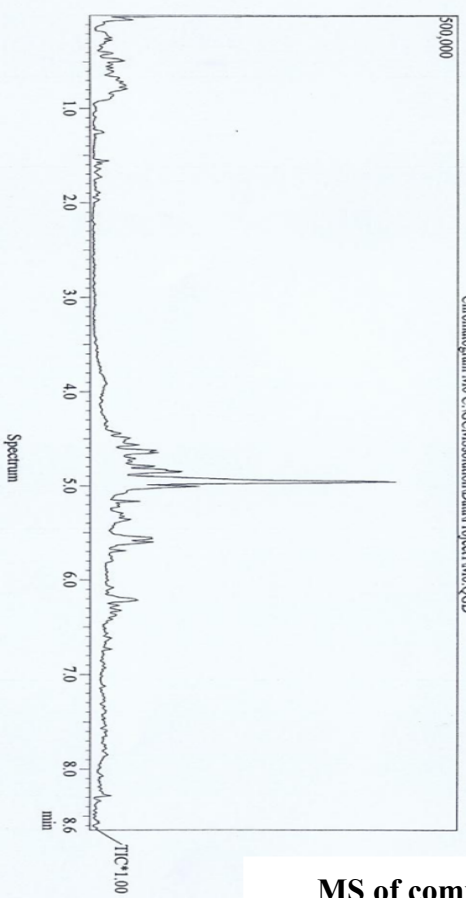
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 02:25:40
 Sample Name : M6
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Quna
 Data File : C:\GCMSolution\Data\Project\1\M6.QGD
 Orig. Data File : C:\GCMSolution\Data\Project\1\M6.QGD
 Method File : C:\GCMSolution\Data\Project\1\High Temperature Op
 Orig. Method File : C:\GCMSolution\Data\Project\1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
 Standard/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:34:22

Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 -Group 1 - Event 1-
 Start Time : 0:00min
 End Time : 1:00min
 AQC Mode : Scan
 Event Time : 0:50sec
 Scan Speed : 1:250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project\1\M6.QGD

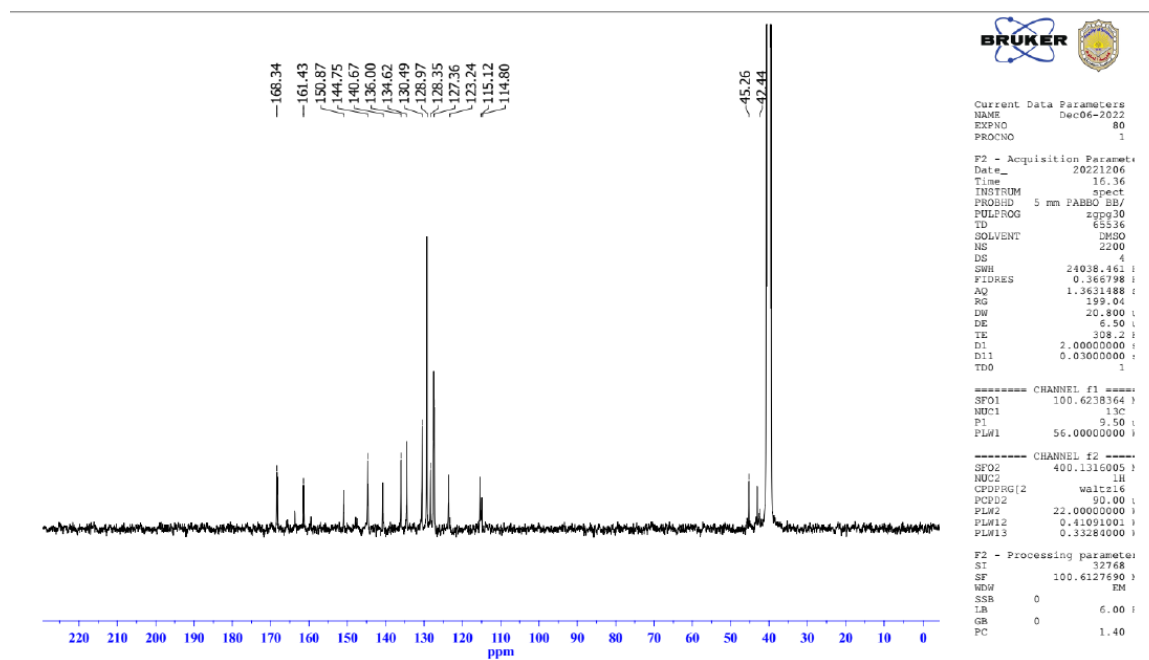
Chromatogram M6 C:\GCMSolution\Data\Project\1\M6.QGD



Line# 1, R. Time: 5.2 (Scan# 625)
 MassPeaks: 170
 RawMode: Single 5.2 (625) BasePeak: 132 (1940)
 BG Mode: None Group 1 - Event 1



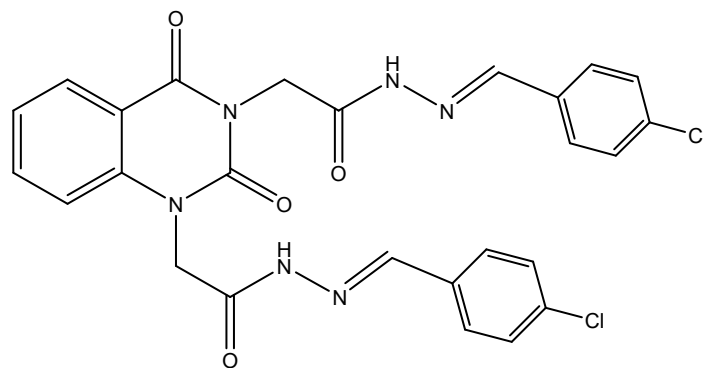
MS of compound (3a)



¹³C-NMR (100 MHz, DMSO) of compound (3a)

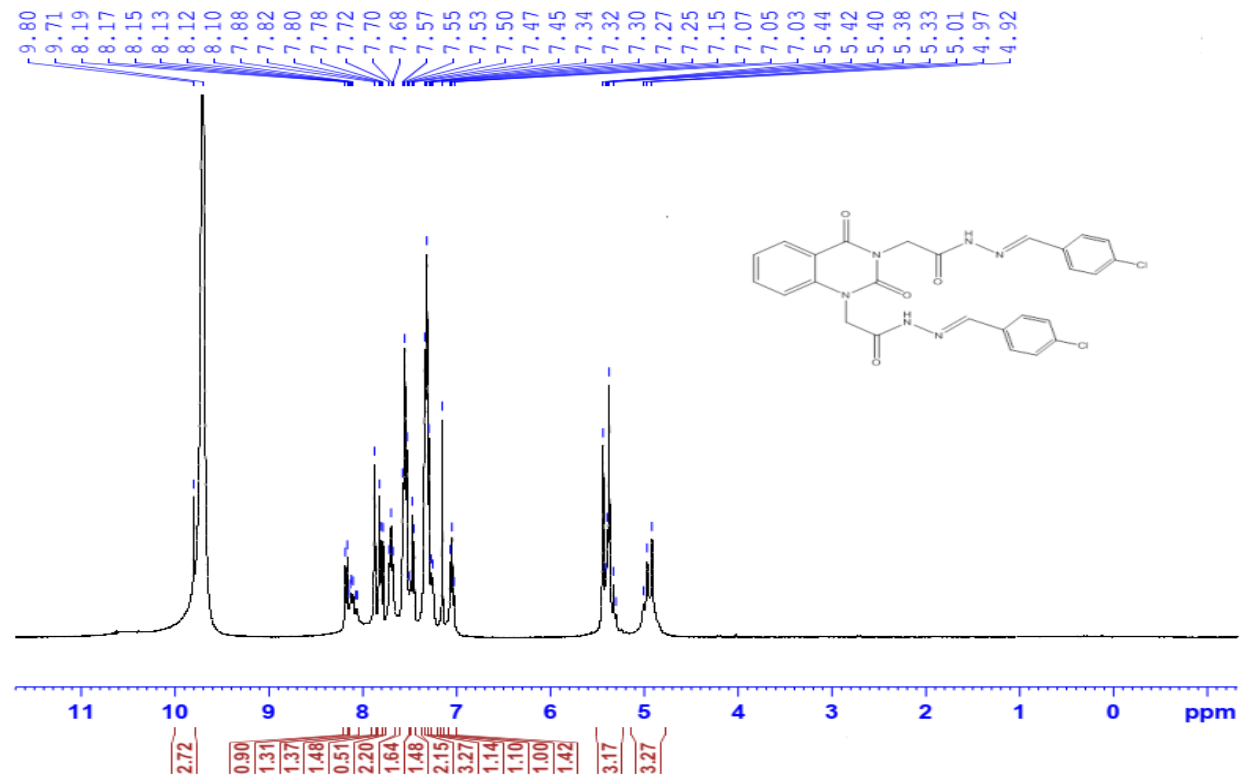
-

Compound (3b): -



3b

Mohamed Omar - M6a -TFA+CDCL3- Hnmr - T



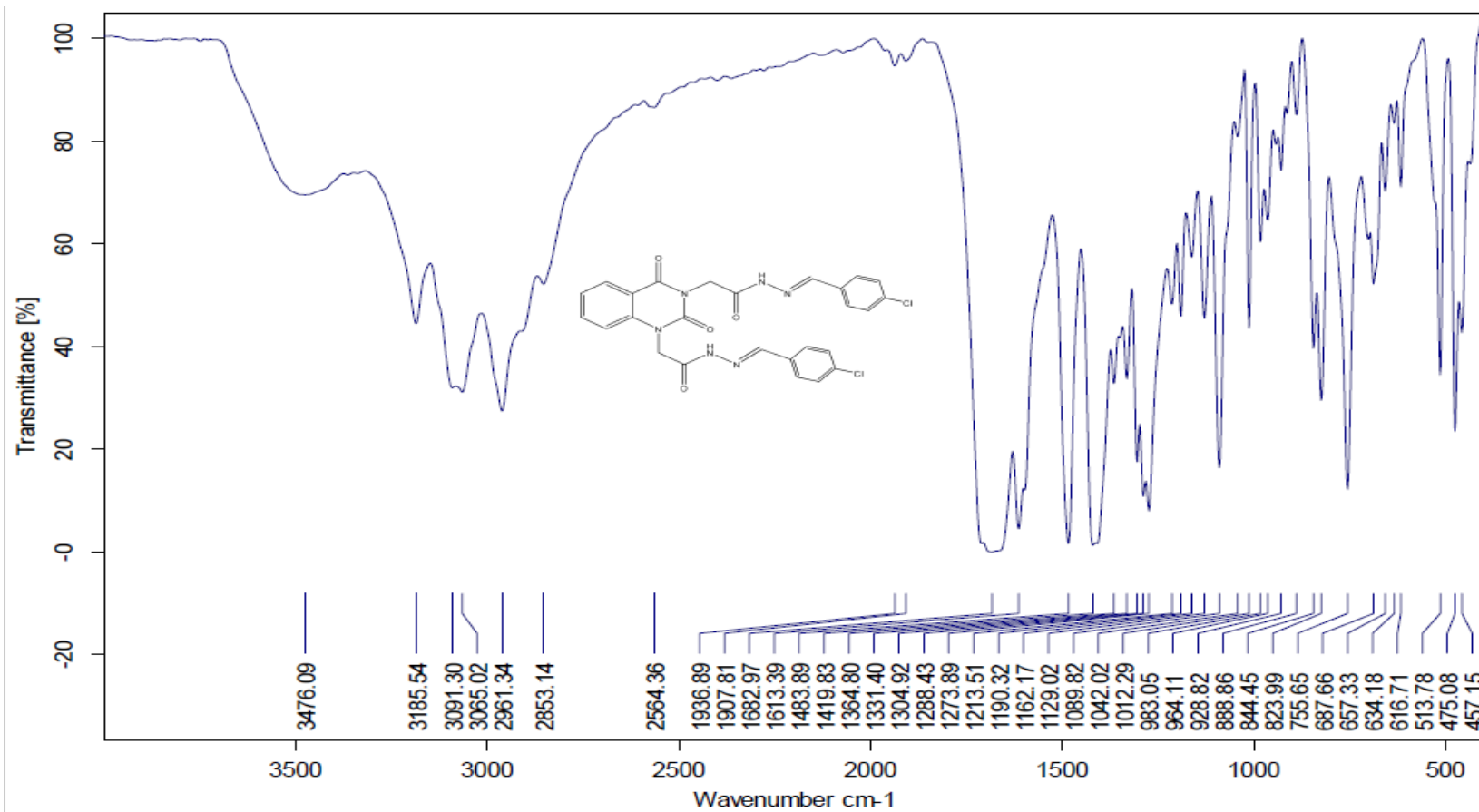
```

Current Data Parameters
NAME Mohamed Omar - M6a -TFA+CDCL3- Hnmr - T
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220115
Time 13.13 D
INSTRUM spect
PROBHD 5100419_0145_1
PULPROG zgpg30
TD 65536
SOLVENT CDCL3
NS 14
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0884445 sec
RG 112.54
SQ 42.400 usec
SE 6.50 usec
TE 294.2 K
VE 1.00000000 sec
VFO 400.2024712 MHz
MFC1 1K
F2 13.50 usec
FID1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.200524 MHz
SOLV TFA
SSB 0
GB 0
PC 1.00
    
```

¹H-NMR (400 MHz, TFA) of compound (3b)



FT-IR of compound (3b)

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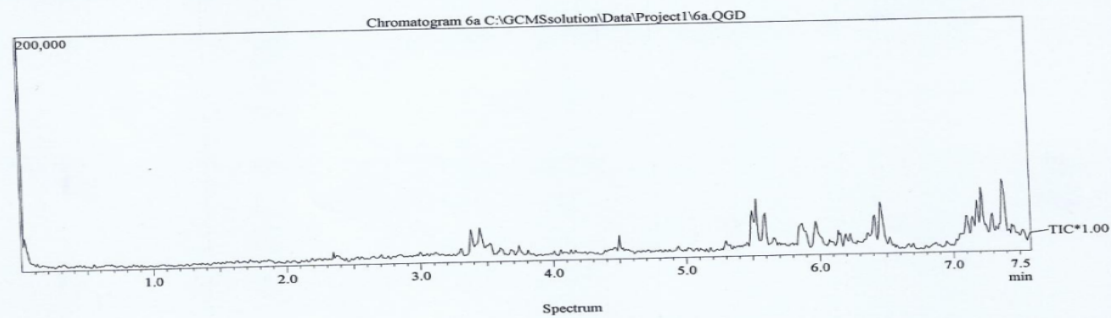
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 04:07:21 من
 Sample Name : 6a
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\6a.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\6a.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 SEndIfSModified by : Dr. Mai Younis
 Modified : 15/01/2007 04:14:59 من

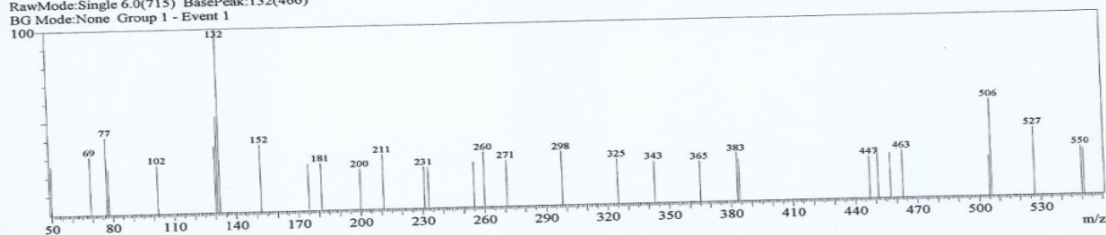
Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\6a.QGD



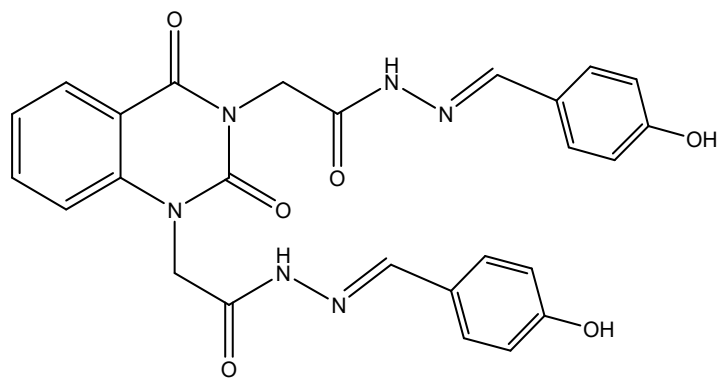
Line#1 R-Time:6.0(Scan#:715)
 MassPeaks:33
 RawMode:Single 6.0(715) BasePeak:132(466)
 BG Mode:None Group 1 - Event 1



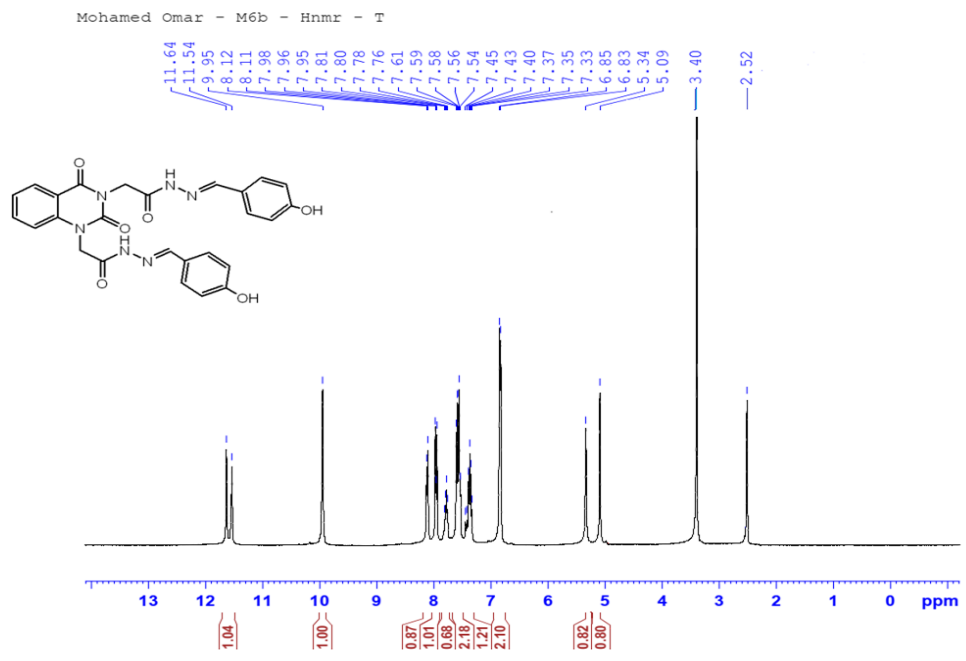
MS of compound (3b)

-

-Compound (3c):



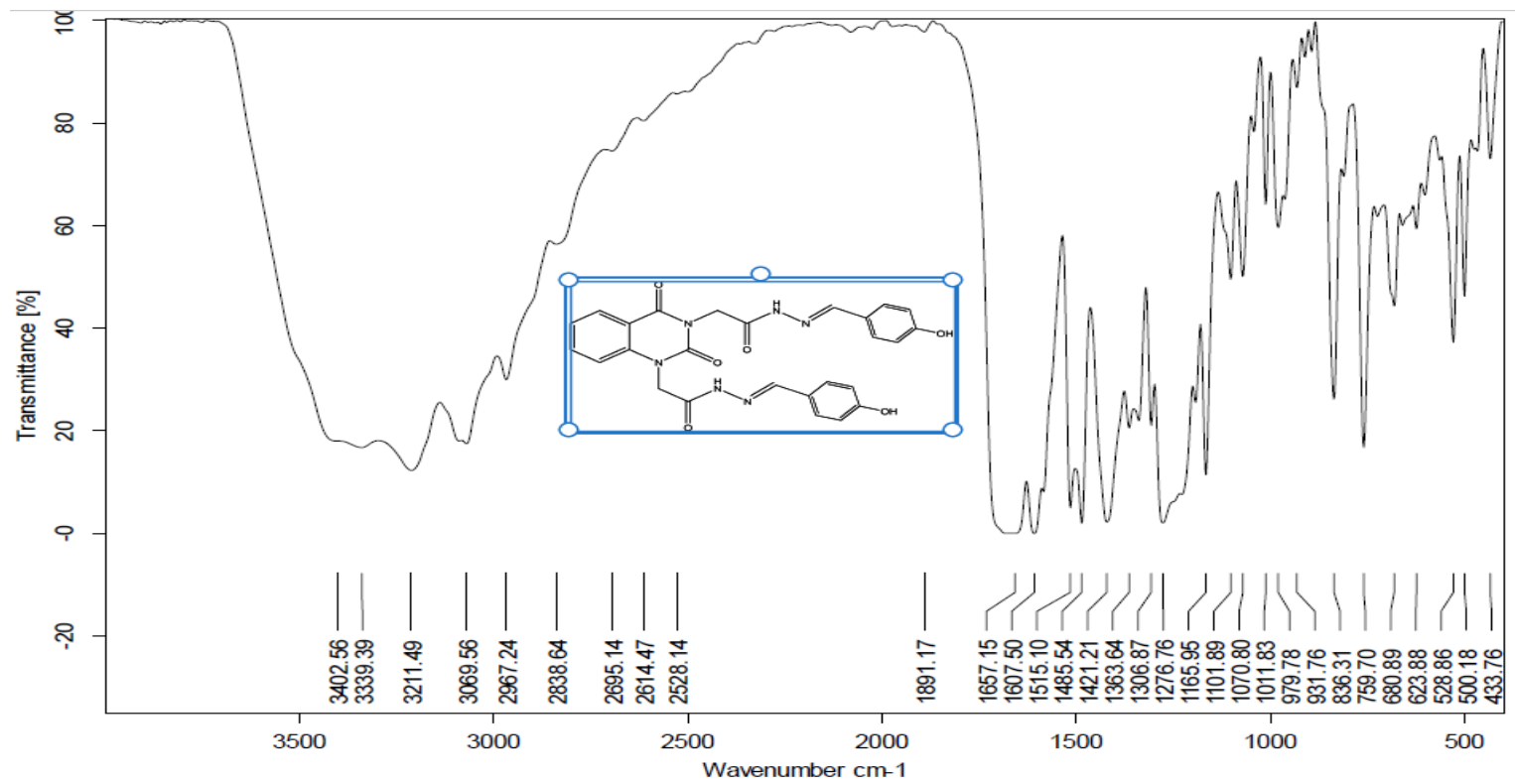
3c



```

Current Data Parameters
NAME Mohamed Omar - M6b - Hnmr - F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20231115
Time 13.00 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 65536
SOLVENT DMSO
DS 16
DE 1.00
SFO1 400.1464000 MHz
AQ 0.2448000 sec
RG 409.6000000
PC 1.0000000 sec
DE 6.80 usec
DI 1.0000000 sec
TE 300.2 K
SFO2 400.1464112 MHz
NUC1 13C
PUL1 13.0000000 sec
F2 - Processing parameters
SI 65536
SF 400.1464000 MHz
WDW EM
SSB 0
GB 0
PC 1.00
  
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (3c)



FT-IR of compound (3c)

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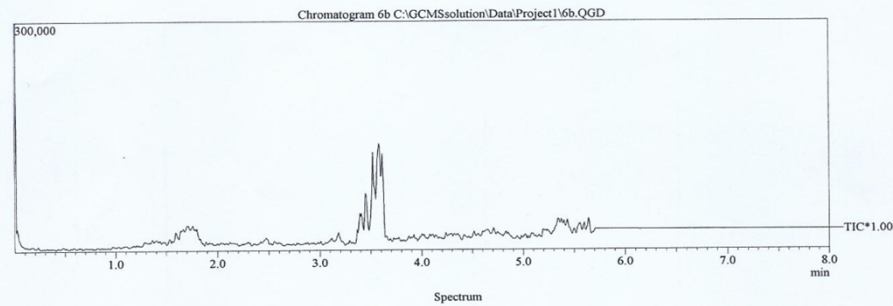
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 04:16:35
 Sample Name : 6b
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\6b.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\6b.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System1\Tune1_default.qgt
 \$END\$ Modified by : Dr. Mai Younis
 Modified : 15/01/2007 04:22:21

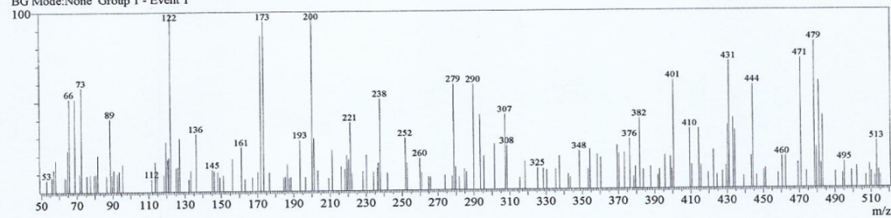
Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\6b.QGD

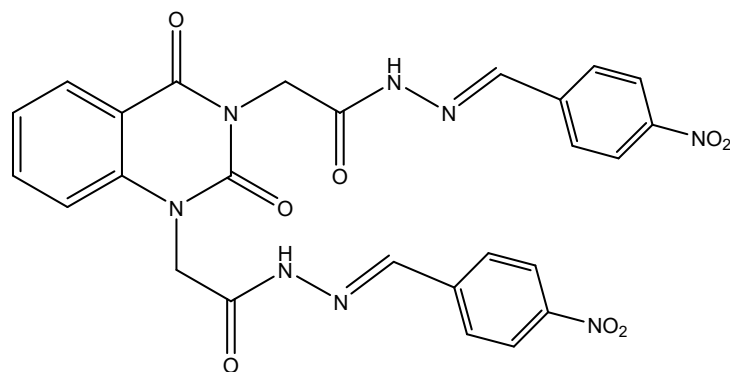


Line#:1 R.Time:3.6(Scan#:429)
 MassPeaks:165
 RawMode:Single 3.6(429) BasePeak:200(1575)
 BG Mode:None Group 1 - Event 1

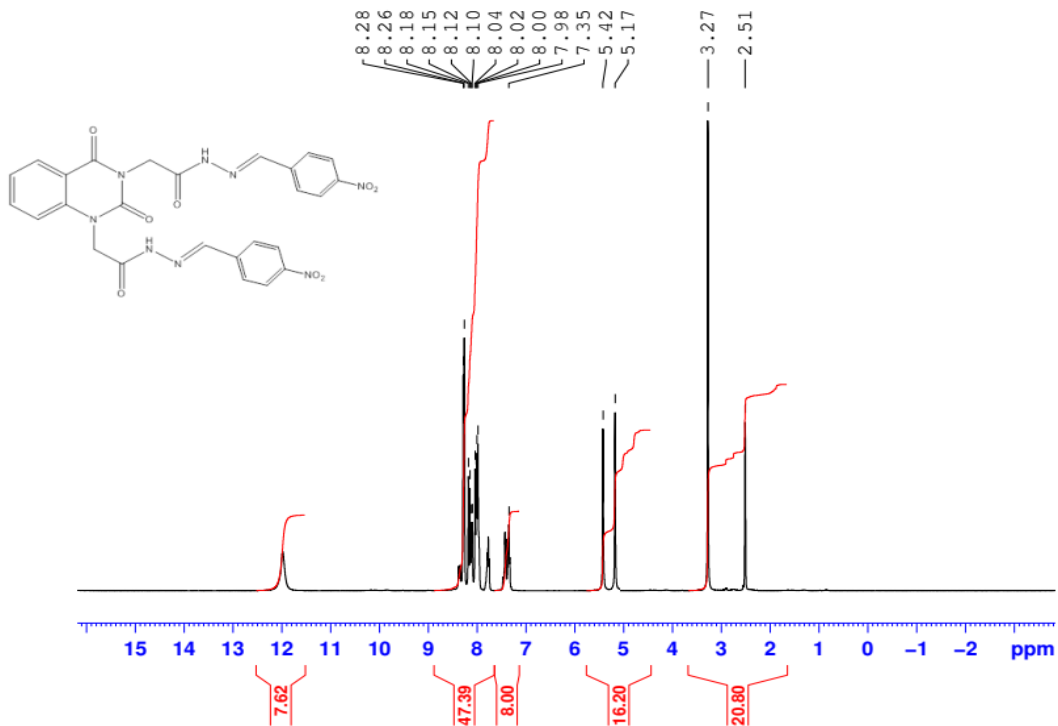


-

-Compound (3d):



3d



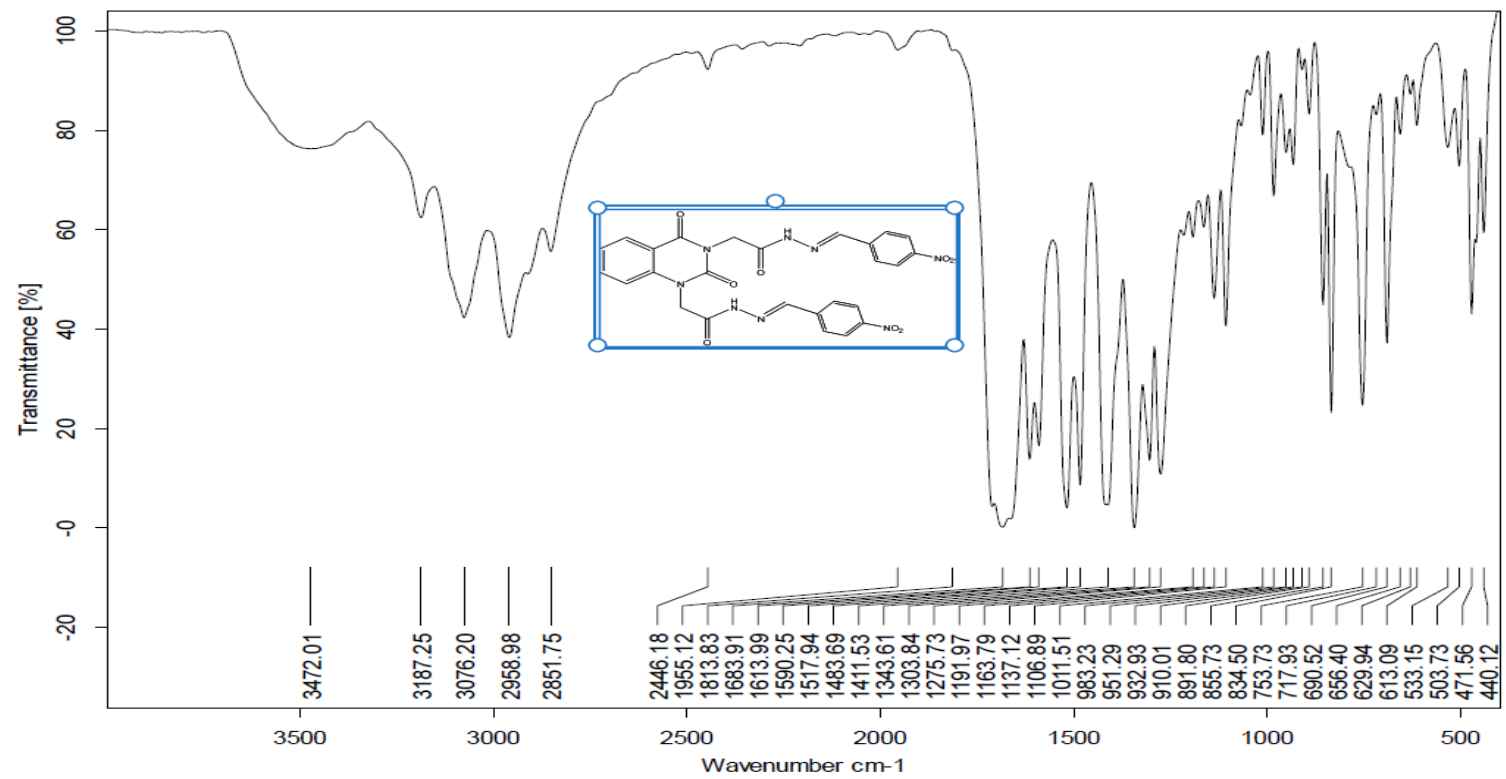
Current Data Parameters
NAME Feb17-2022
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220217
Time 10.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 158.76
DW 62.400 usec
DE 6.50 usec
TE 313.1 K
D1 1.0000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (3d)



FT-IR of compound (3d)

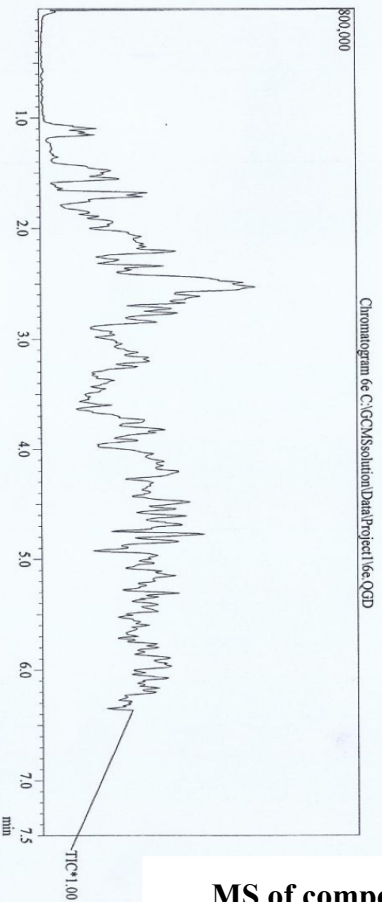
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DI Analysis
Shimadzu Qp-2010 Plus

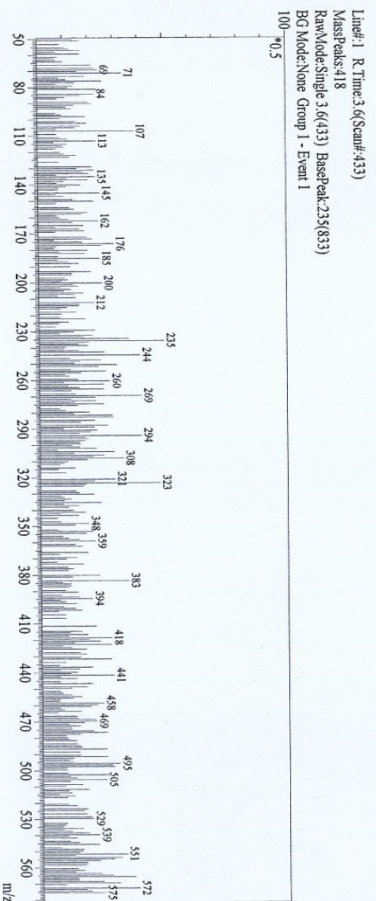
Sample Information
Analyzed by : Dr. Mai Younis
Analyze Date : 15/01/2007 04:32:35
Sample Name : 6e
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quana
Data File : C:\GCMSolution\Data\Project\Iee.QGD
Org Data File : C:\GCMSolution\Data\Project\Iee.QGD
Method File : C:\GCMSolution\Data\Project\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project\High Temperature Op
Report File : C:\GCMSolution\System\Time1_default.qpt
Tuning File : C:\GCMSolution\System\Time1_default.qpt
SendToS Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:39:00

Method
Analytical Line 1 :
IonSourceTemp : 250.00 °C
[MS Table]
-Group 1 - Event 1-
Start Time : 0:00min
End Time : 1:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2:00
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project\Iee.QGD

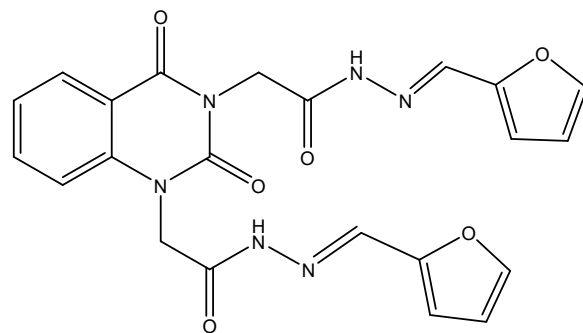


MS of compound (3d)

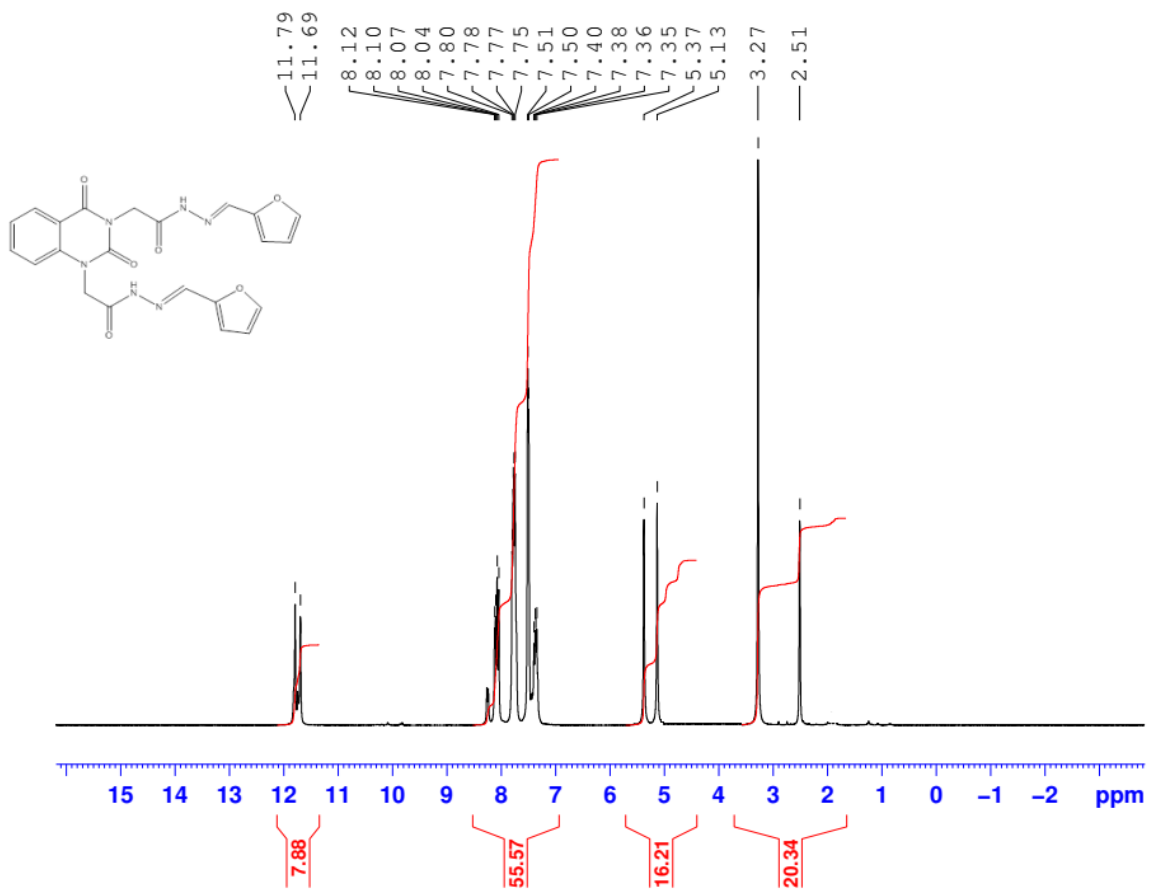


-

-Compound (3e):



3e



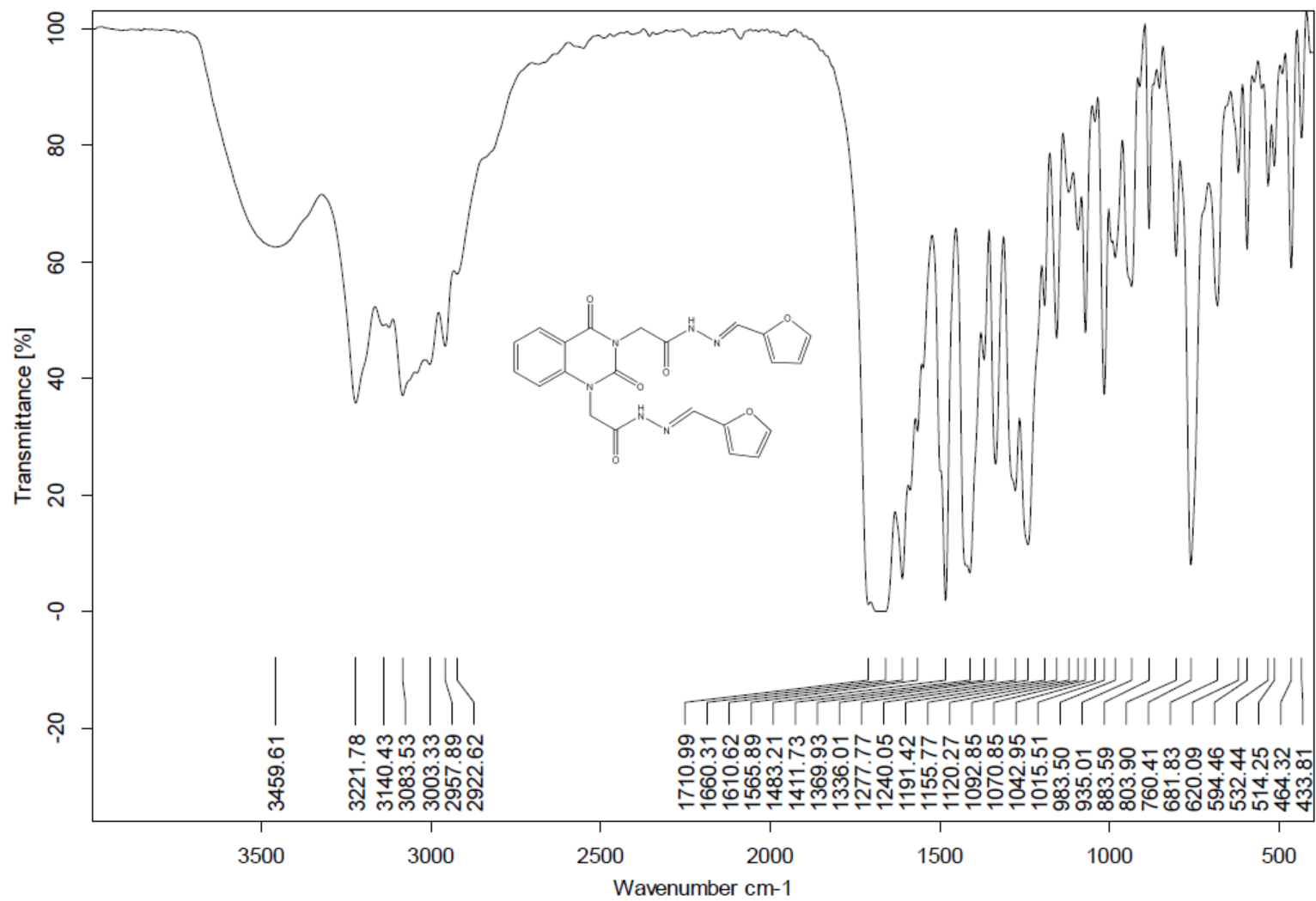
Current Data Parameters
NAME Feb17-2022
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220217
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 159.76
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (3e)



FT-IR of compound (3e)

**Cairo University
Micro Analytical Center**

DI Analysis
Shimadzu QP-2010 Plus

Sample Information

Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 04:40:35
Sample Name : 6f
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Qena
Data File : C:\GCMSolution\Data\Project1\6f\QGD
Org Data File : C:\GCMSolution\Data\Project1\6f\QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File : C:\GCMSolution\System\Tune1_default.qgd
Tuning File : C:\GCMSolution\System\Tune1_default.qgd
Serials/Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:44:39

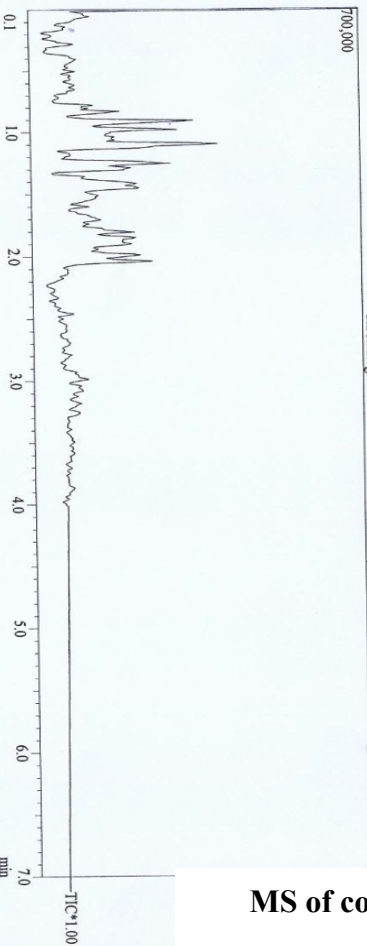
Method

Analytical Line 1 :
IonSourceTemp : 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time : 0:00min
End Time : 1:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project1\6f\QGD

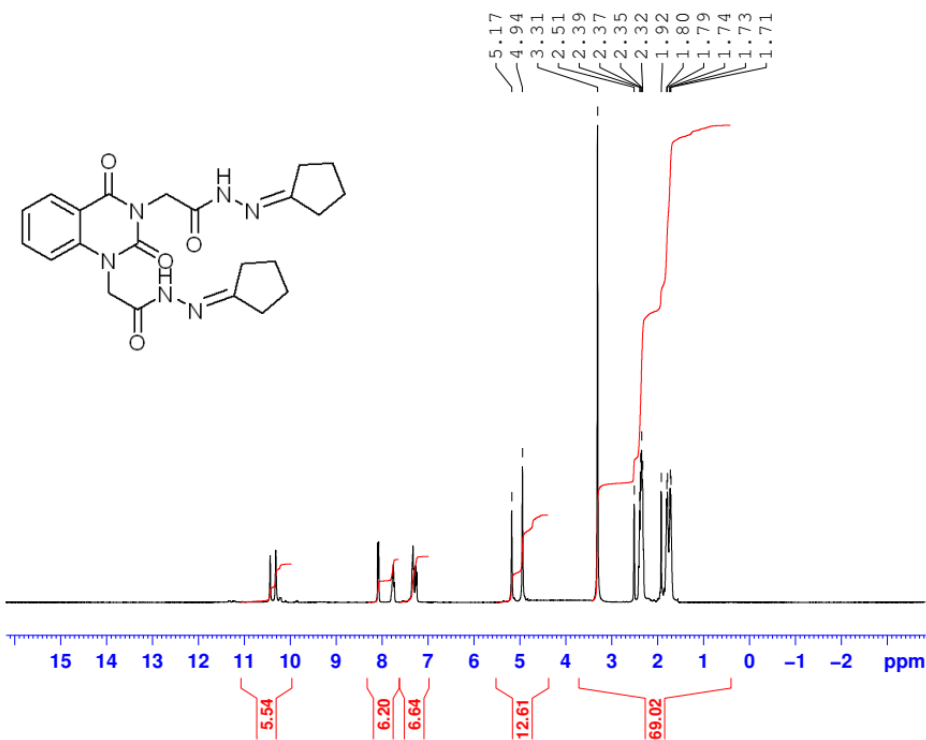
C:\GCMSolution\Data\Project1\6f\QGD

Chromatogram 6f C:\GCMSolution\Data\Project1\6f\QGD



MS of compound (3e)





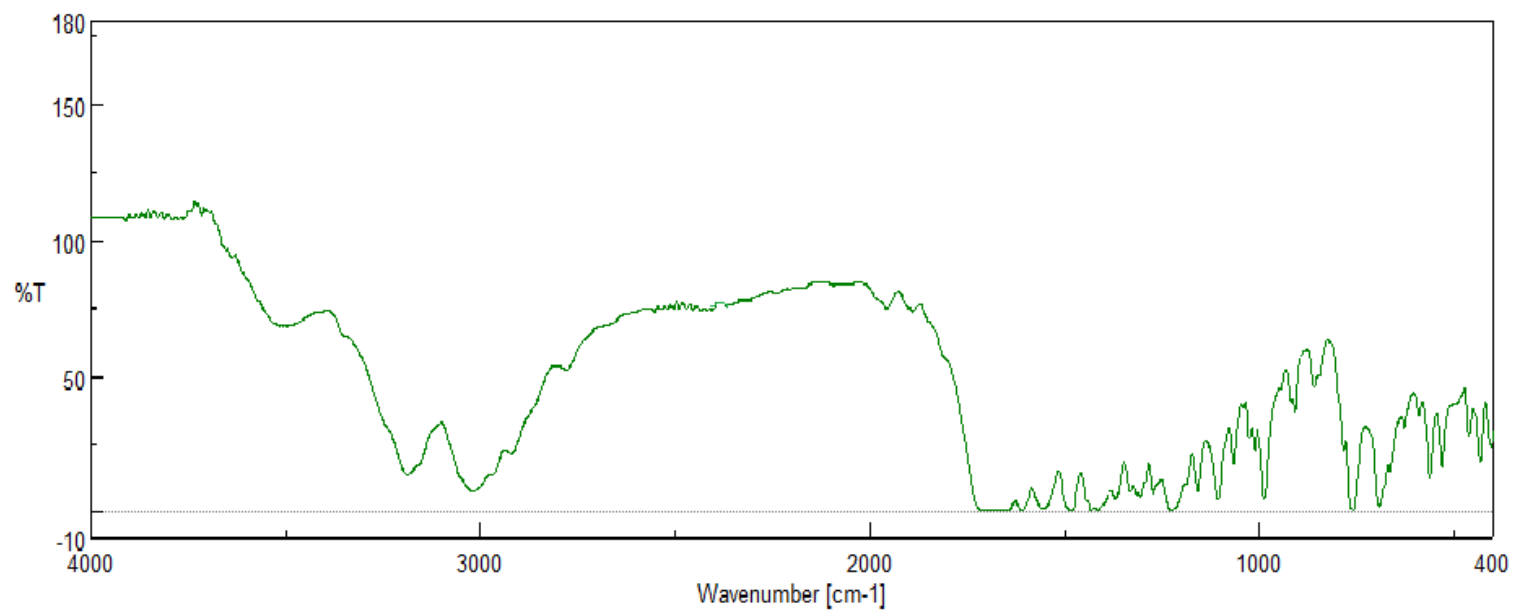
Current Data Parameters
NAME Jul03-2022
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220703
Time 12.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 35
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 120.97
DW 62.400 usec
DE 6.50 usec
TE 308.2 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====
SF01 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

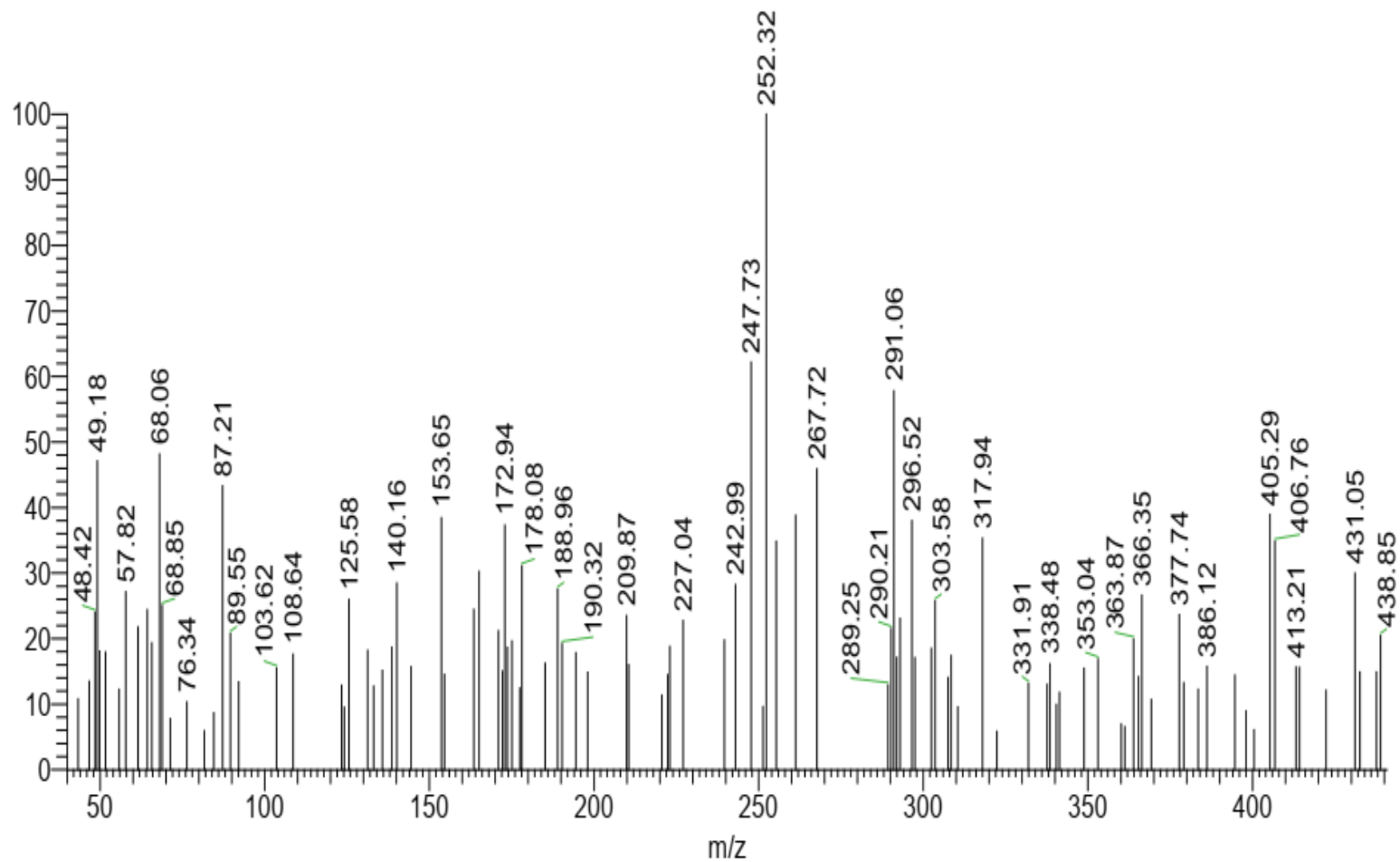
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (4a)



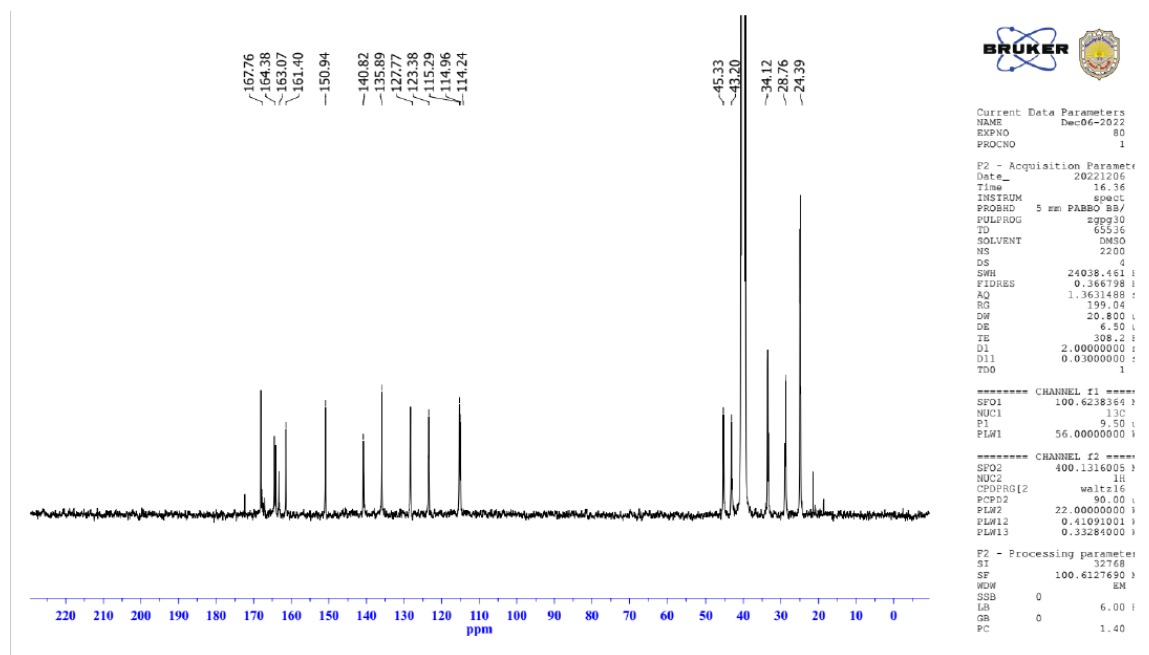
FT-IR of compound (4a)

mohamed-omar-16a #95 RT: 1.61 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 5.58E2
T: + c EI Full ms [40.00-1000.00]



m/z Intensity Relative

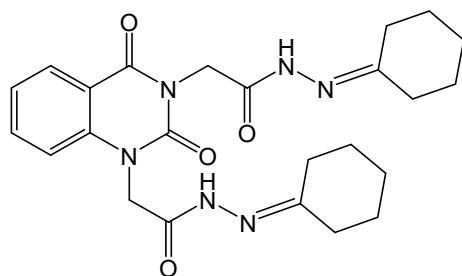
MS of compound (4a)



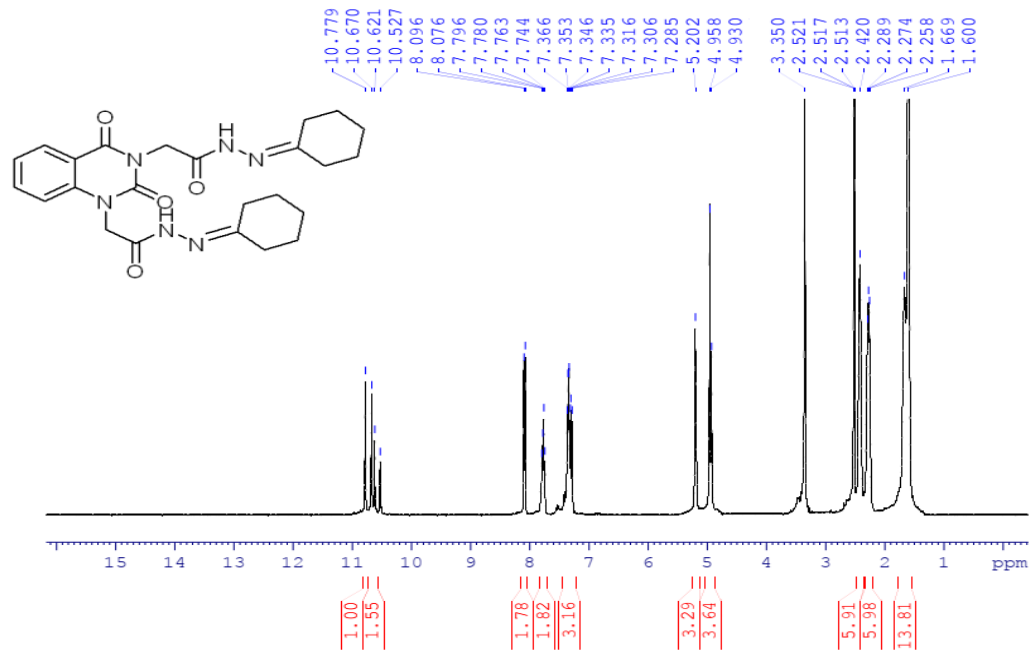
¹³C-NMR (100 MHz, DMSO) of compound (4a)

-

-Compound (4b): -



4b



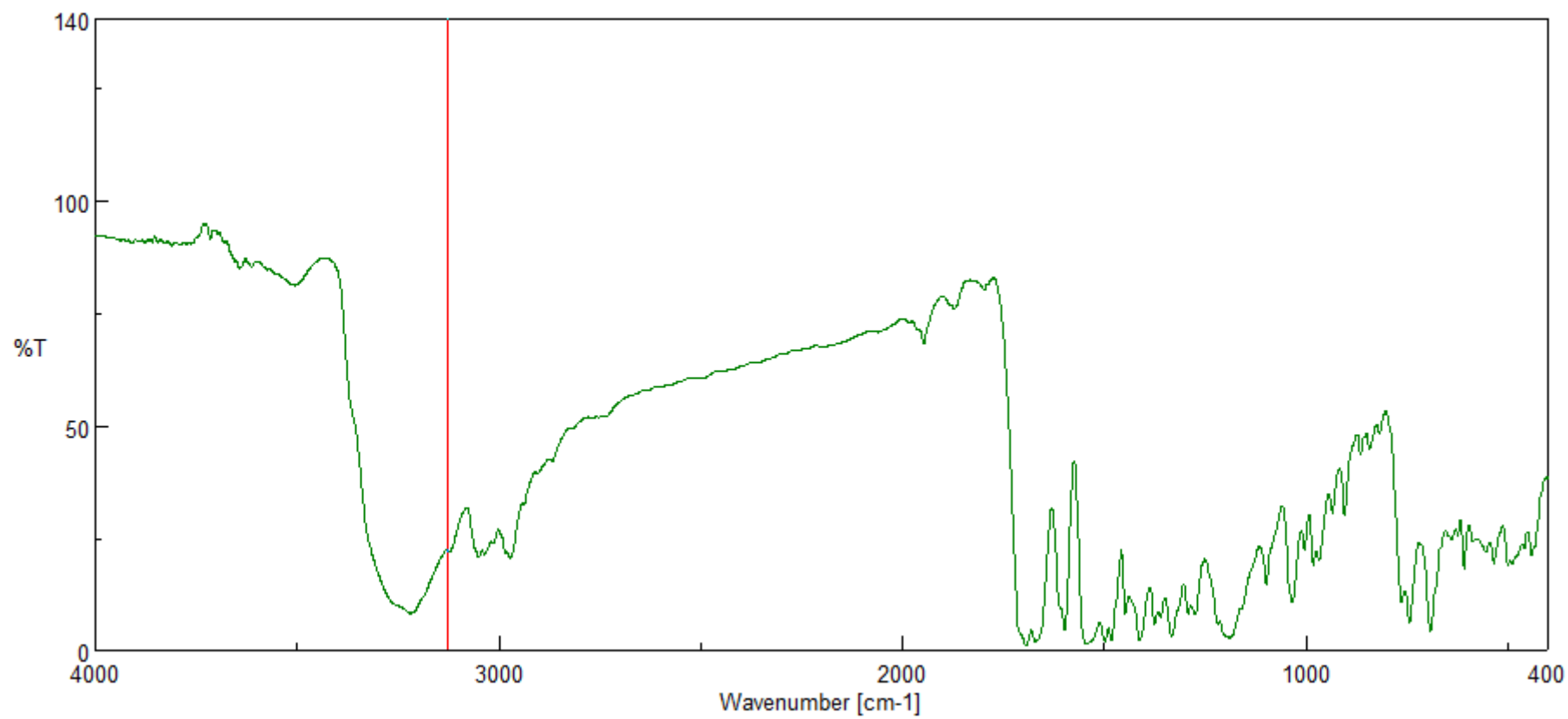
```

Current Data Parameters
NAME      Mohamed Omar - 10H Rnmr - T
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20220611
Time     13.02 h
INSTRUM  spect
PROBHD   E10621_0948 (
PULPROG  zgpg
TD       65536
SOLVENT  DMSO
NS       4
DS       2
SWH      8012.800 Hz
FIDRES   0.248830 Hz
AQ       4.0894468 sec
RG       276.00
DE       6.400 usec
TE       298.15 K
D1       1.00000000 sec
TDO      400.2024711 MHz
NUC1     13C
NUC2     1H
PC       13.00000000 usec
P1       13.00000000 usec
P2       13.00000000 usec

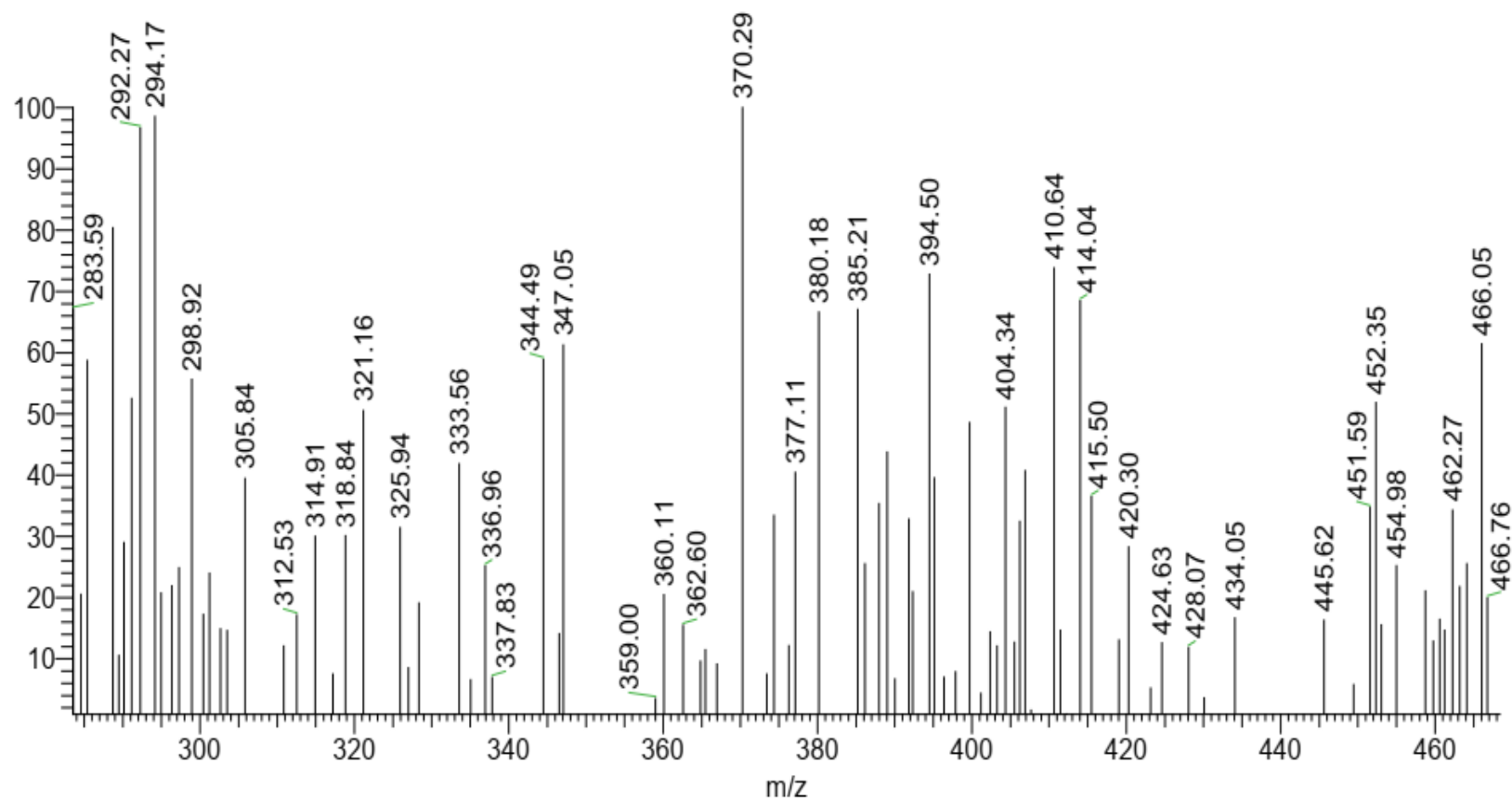
F1 - Processing parameters
SI       65536
SF       400.2000000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (4b)



FT-IR of compound (4b)

mohamed-omar-16b #187-189 RT: 3.15-3.18 AV: 3 SB: 26 1.21-1.34, 0.87-1.14 NL: 1.41E2
T: + c EI Full ms [40.00-1000.00]

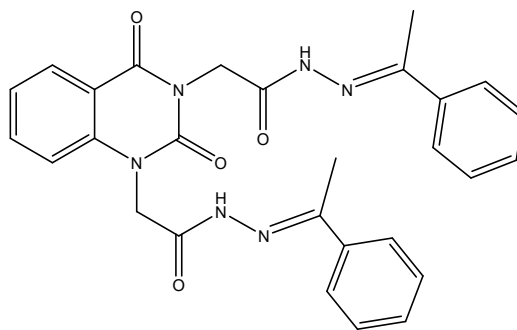


m/z Intensity Relative

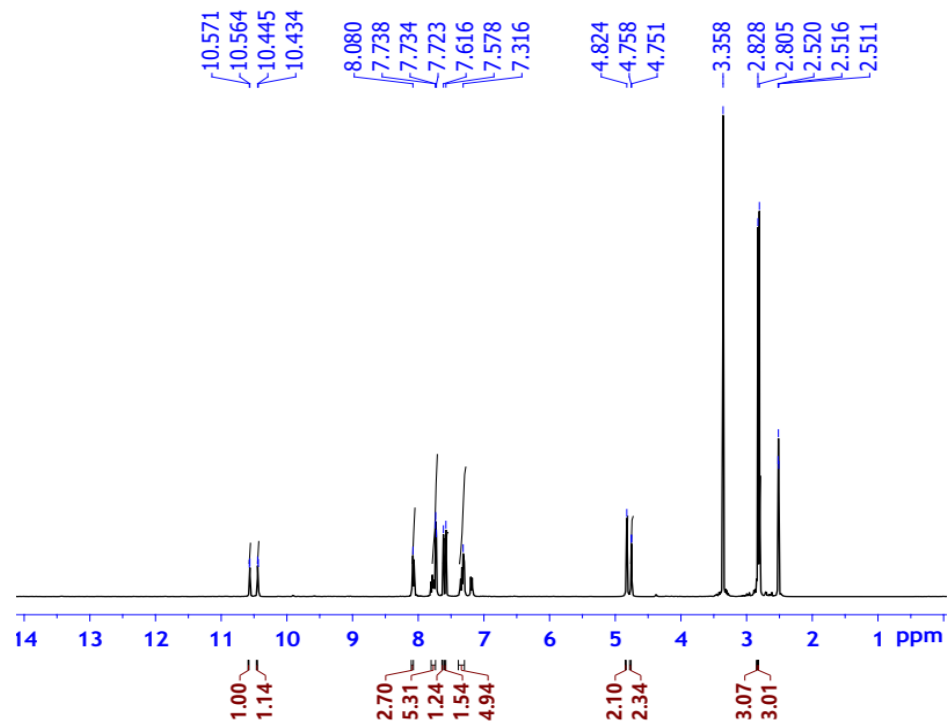
MS of compound (4b)

-

- **Compound (4c):**



4c

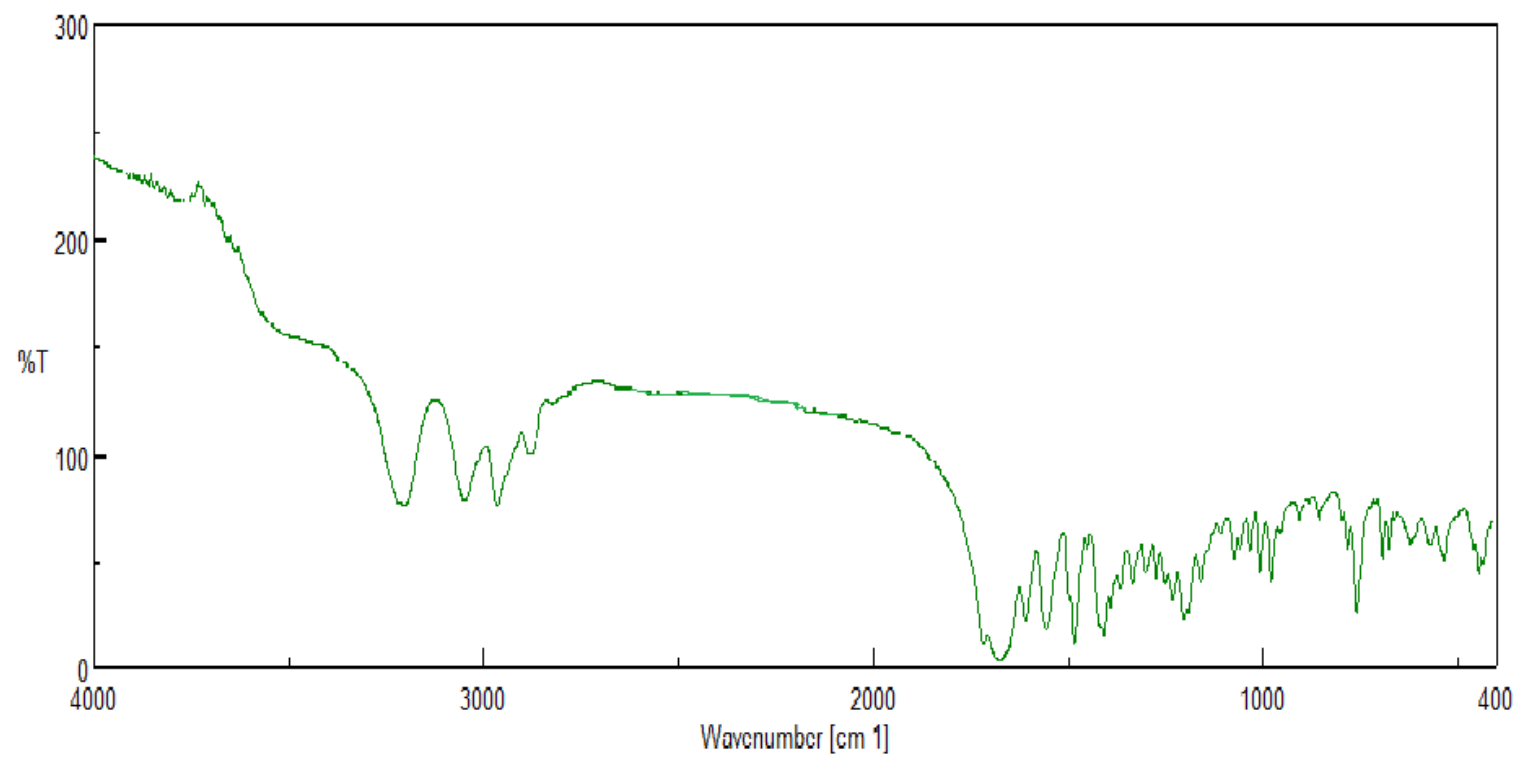


```

Current Data Parameters
NAME      Mohammed Omar-10B-proton-NH
EXPNO    10
PROCNO   1

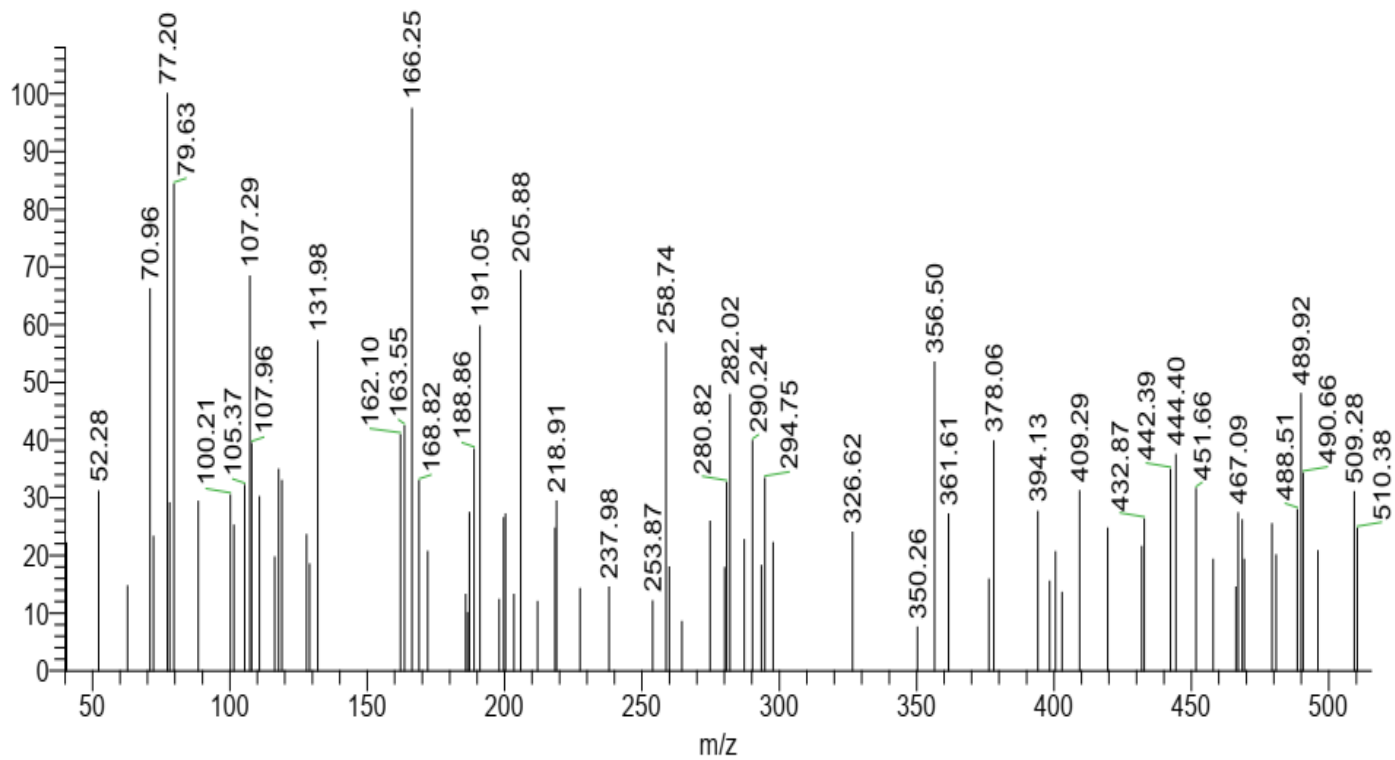
F1 - Acquisition Parameters
Date_    20220808
Time     14.11 h
INSTRUM  spect
PROBHD   E10618_0945 (
PULPROG  zgpg
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.800 Hz
FIDRES   0.24880 Hz
AQ        4.0894465 sec
RG        111.58
DN        62.400 usec
DE        6.50 usec
TE        292.2 K
D1        1.00000000 sec
TDO       0
SFO1     400.2024711 MHz
NUC1      1H
P1        12.50 usec
PL1       0.00000000 M
F1 - Processing parameters
SI        65536
SF        400.2000000 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB        0
PC        1.00
  
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (4c)



FT-IR of compound (4c)

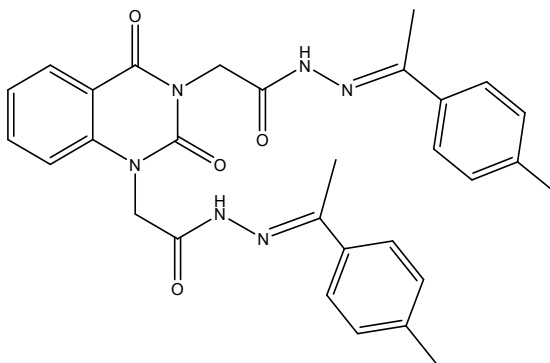
mohamed-omar-16c #169 RT: 2.85 AV: 1 SB: 26 1.21-1.34, 0.87-1.14 NL: 3.86E2
T: + c EI Full ms [40.00-1000.00]



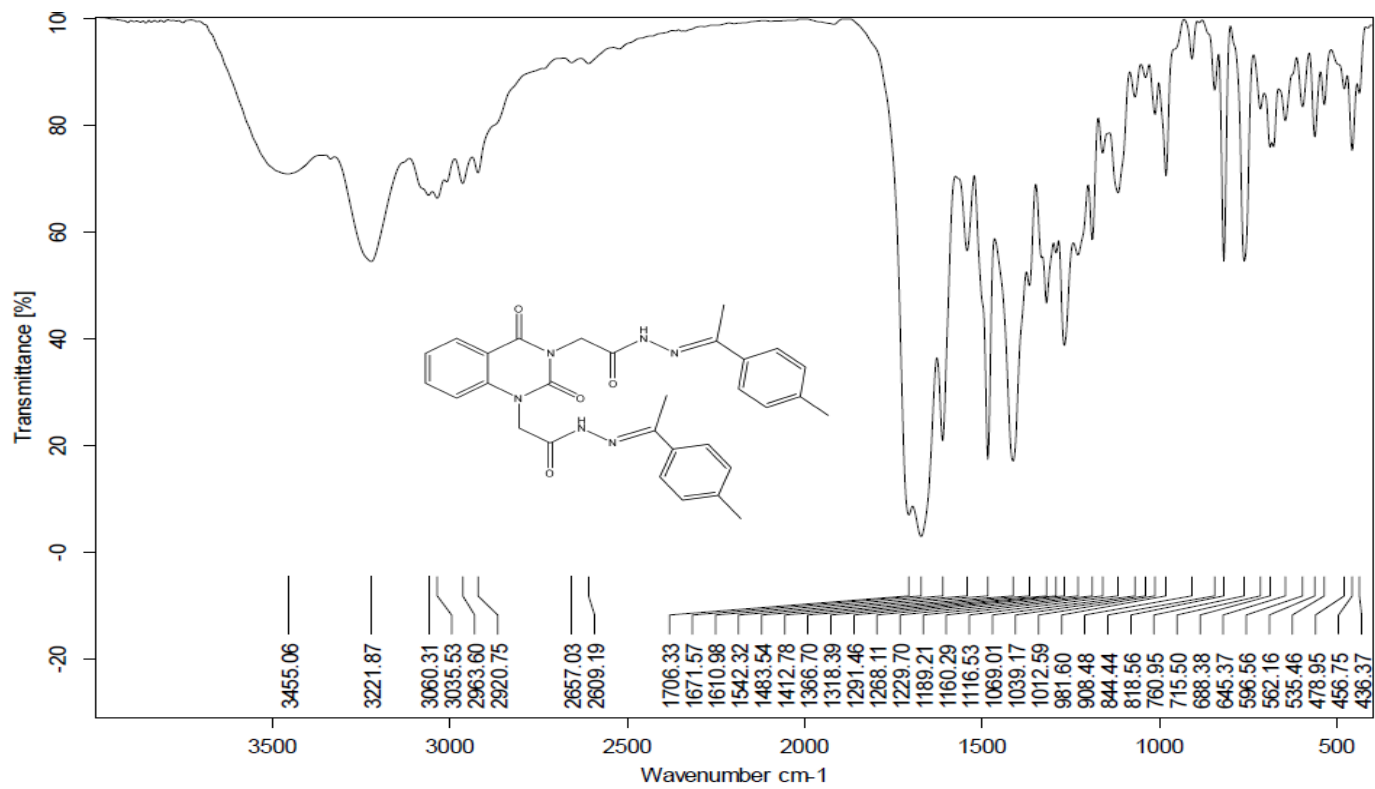
m/z Intensity Relative **MS of compound (4c)**

-

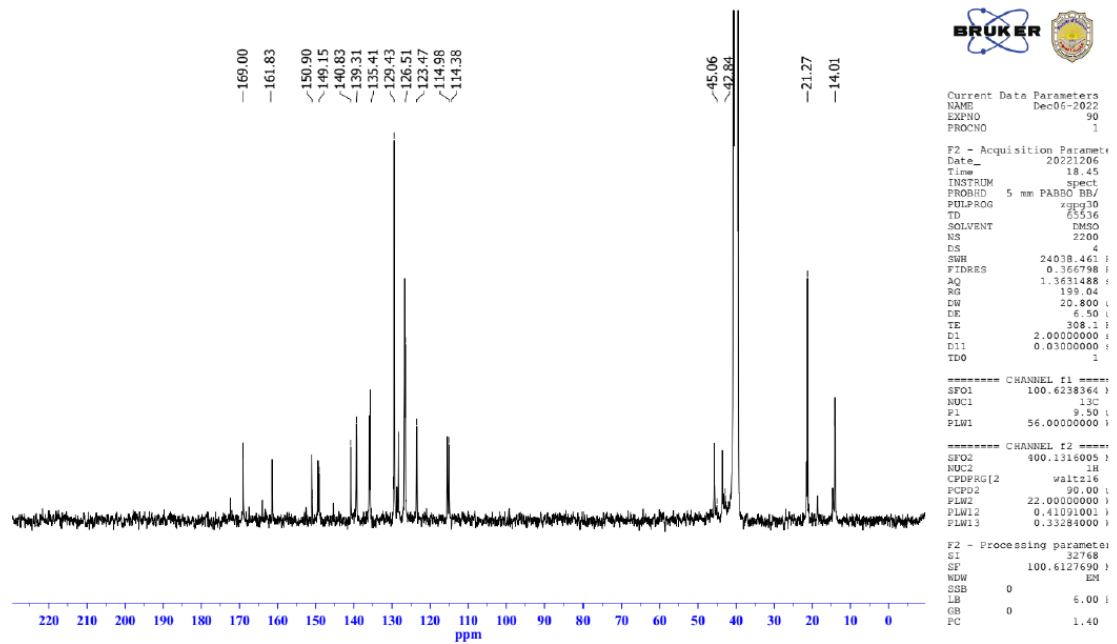
-Compound (4d): -



4d



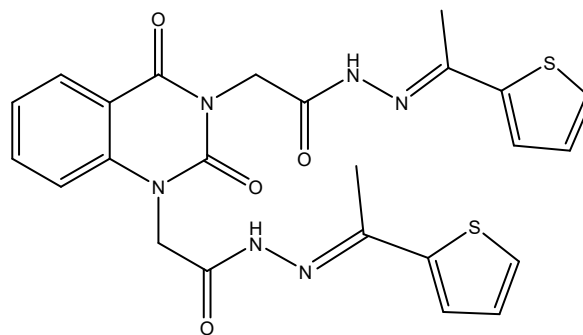
FT-IR of compound (4d)



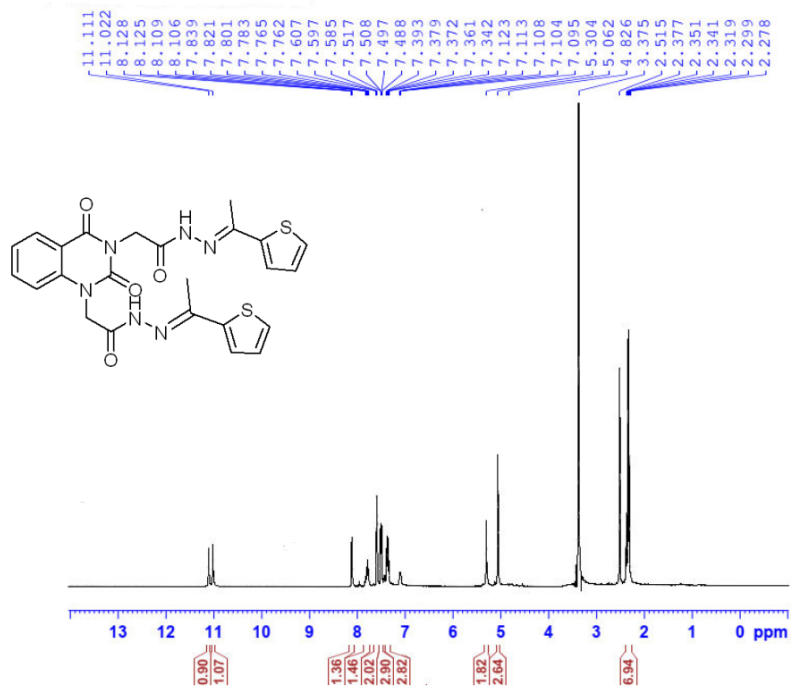
¹³C-NMR (100 MHz, DMSO) of compound (4d)

-

-Compound (4e):-



4e



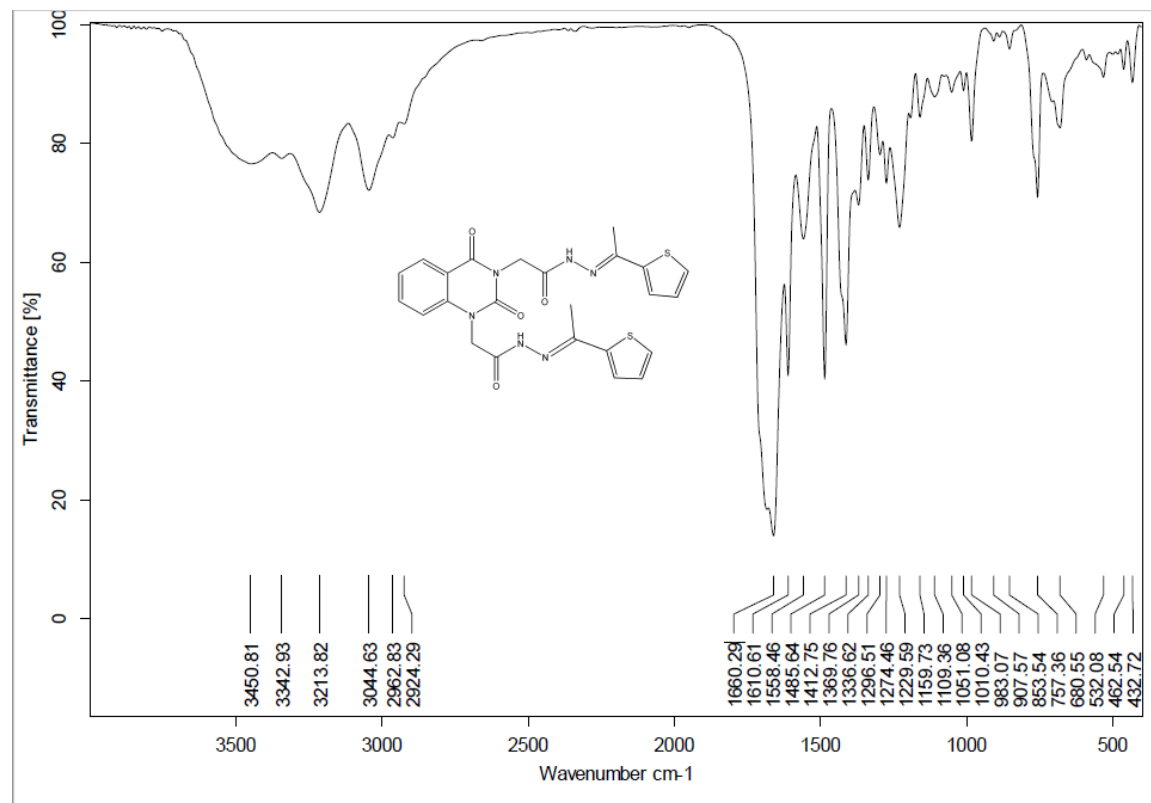
```

Current Data Parameters
NAME: Mohamed Omer-100-proton-MH
EXPNO: 10
PROCNO: 1

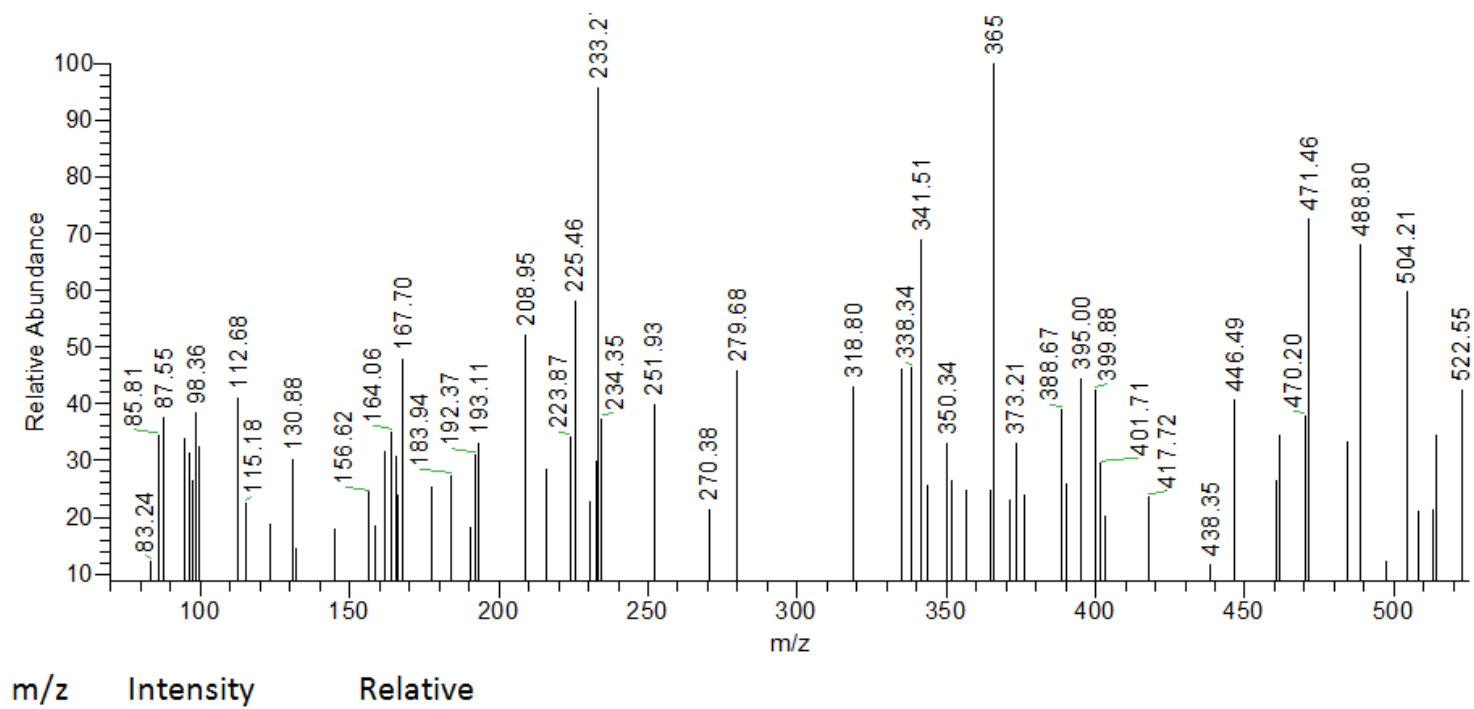
PC - Acquisition Parameters
Date_: 20220908
Time: 14.25 h
INSTRUM: spect
PROBHD: zgpg30
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 400
DS: 4
SWH: 8012.800 Hz
FIDRES: 0.246800 Hz
AQ: 4.028468 sec
RG: 128 Hz
AQ: 60.400 usec
DE: 6.90 usec
TE: 300.2 K
SI: 1.00000000 sec
SFO: 400.146400 MHz
NUC1: 13C
P1: 19.90 usec
P1PL1: 19.00000000 N

PC - Processing parameters
SI: 65536
SF: 400.146400 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
  
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (4e)



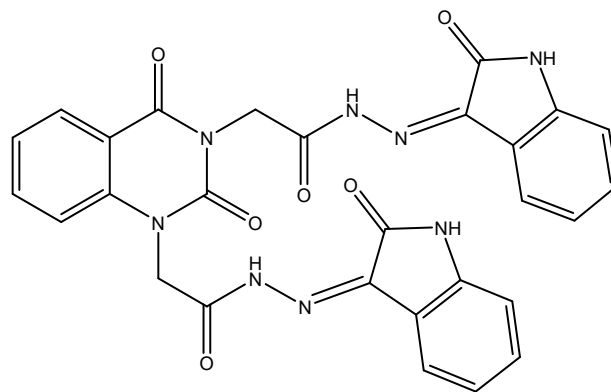
FT-IR of compound (4e)



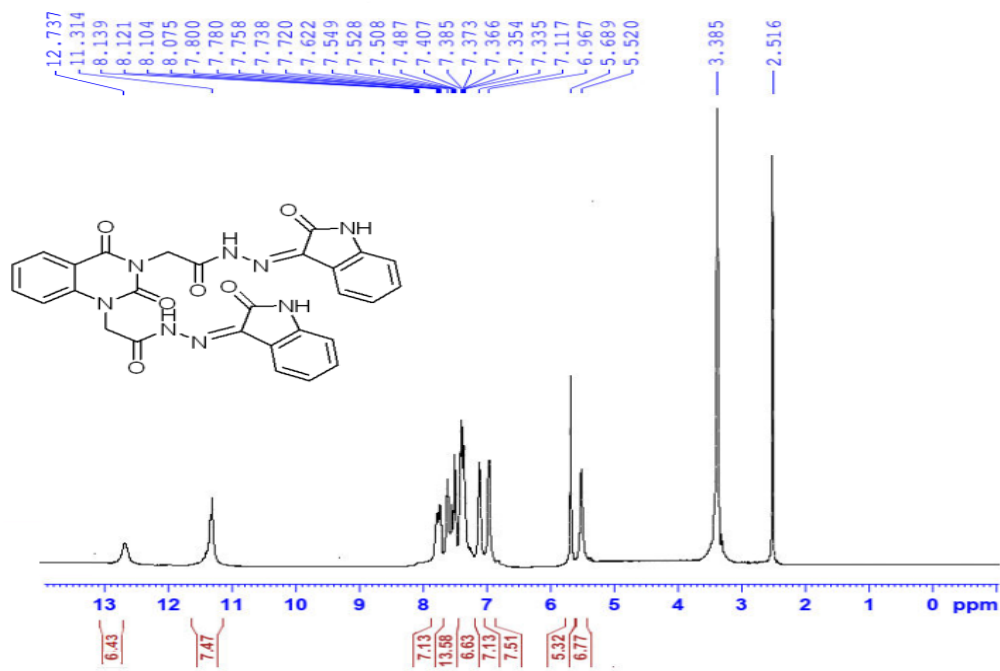
MS of compound (4e)

-

-Compound (4f)



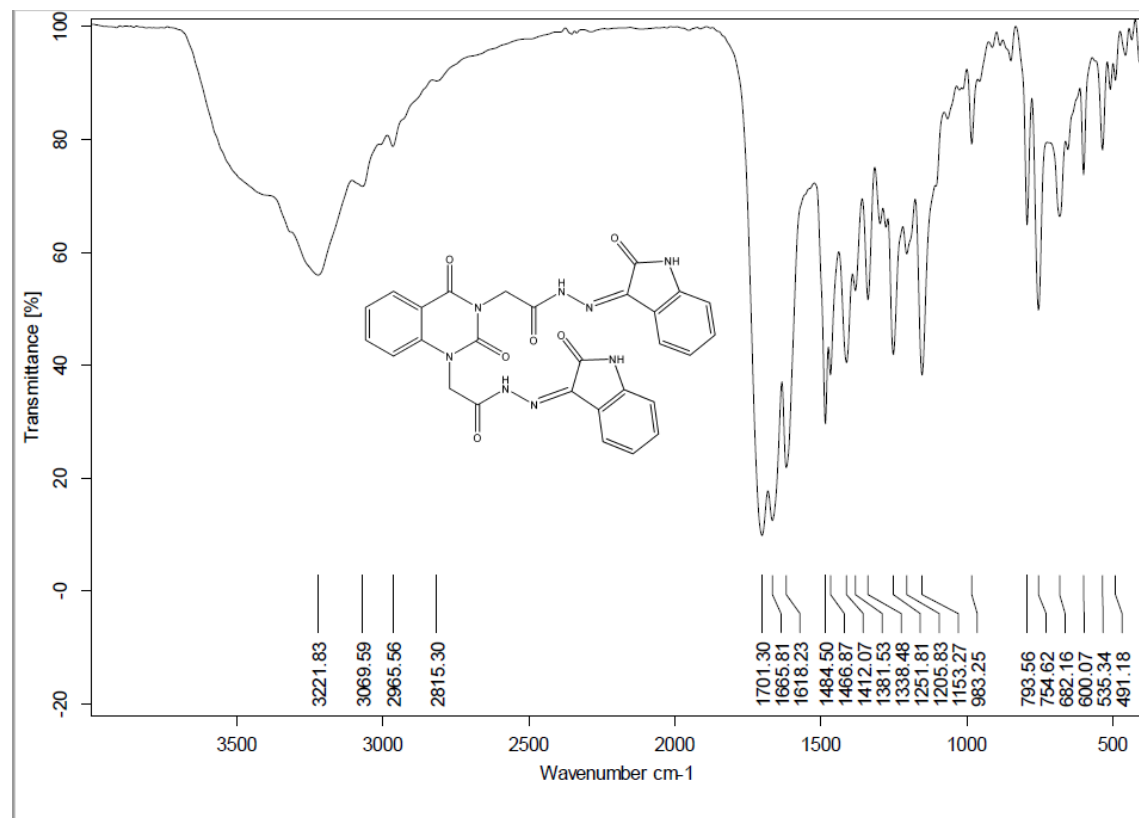
4f



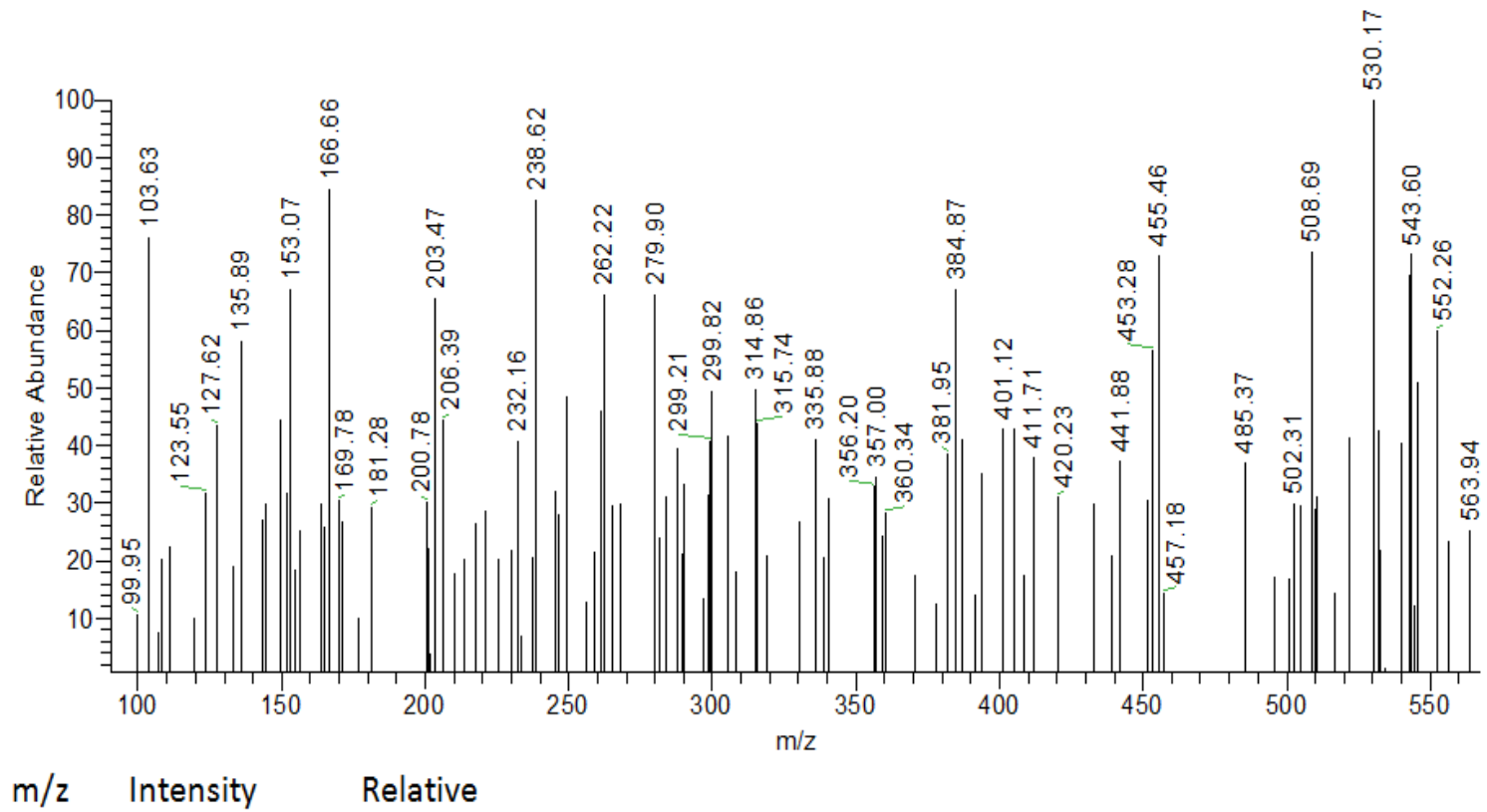
```

Current Data Parameters
NAME      Mohammed Omar-10A-proton-NH
EXPNO    10
PROCNO   1
F1 - Acquisition Parameters
Date_    201308
Time     11:08 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
SOLVENT  DMSO
NS       640
DS       4
SWH      13.0000000 MHz
FIDRES   0.2448800 Hz
AQ       4.0190488 sec
RG        64
AQRES    0.2043750 Hz
SFO      400.2024711 MHz
WDW      EM
SSB      0
GB       0
PC       19.0000000 usec
RG2      19.0000000 usec
Processing parameters
SI        32768
SF        400.2000000 MHz
WDW      EM
SSB      0
GB       0
PC       0.20 usec
RG2      1.00
  
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (4f)



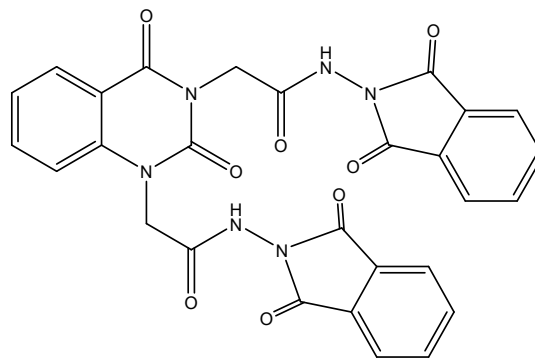
FT-IR of compound (4f)



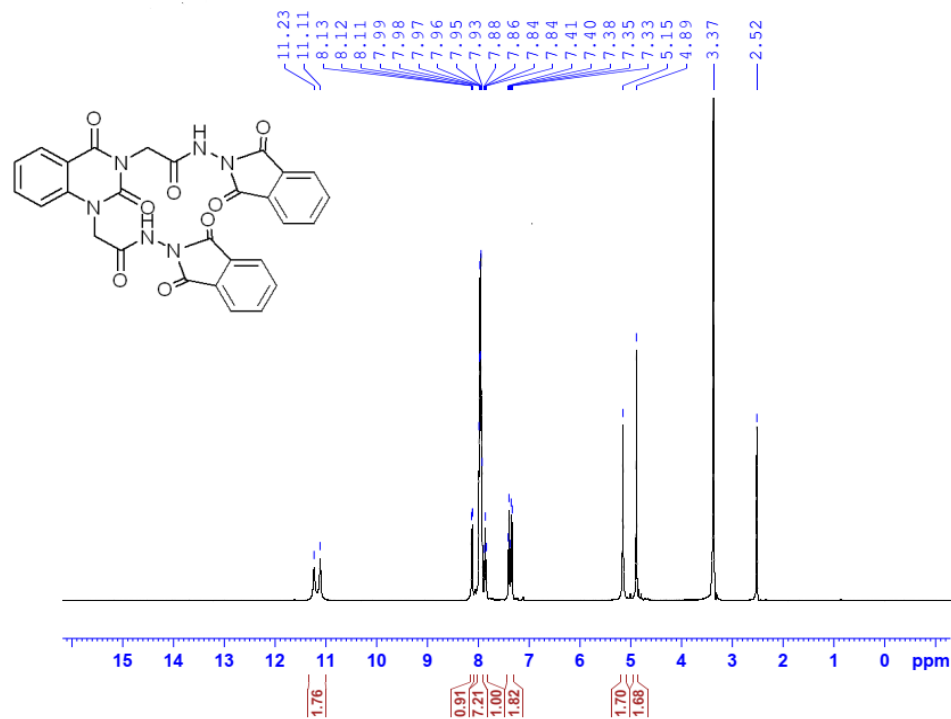
MS of compound (4f)

-

-Compound (5a):



5a

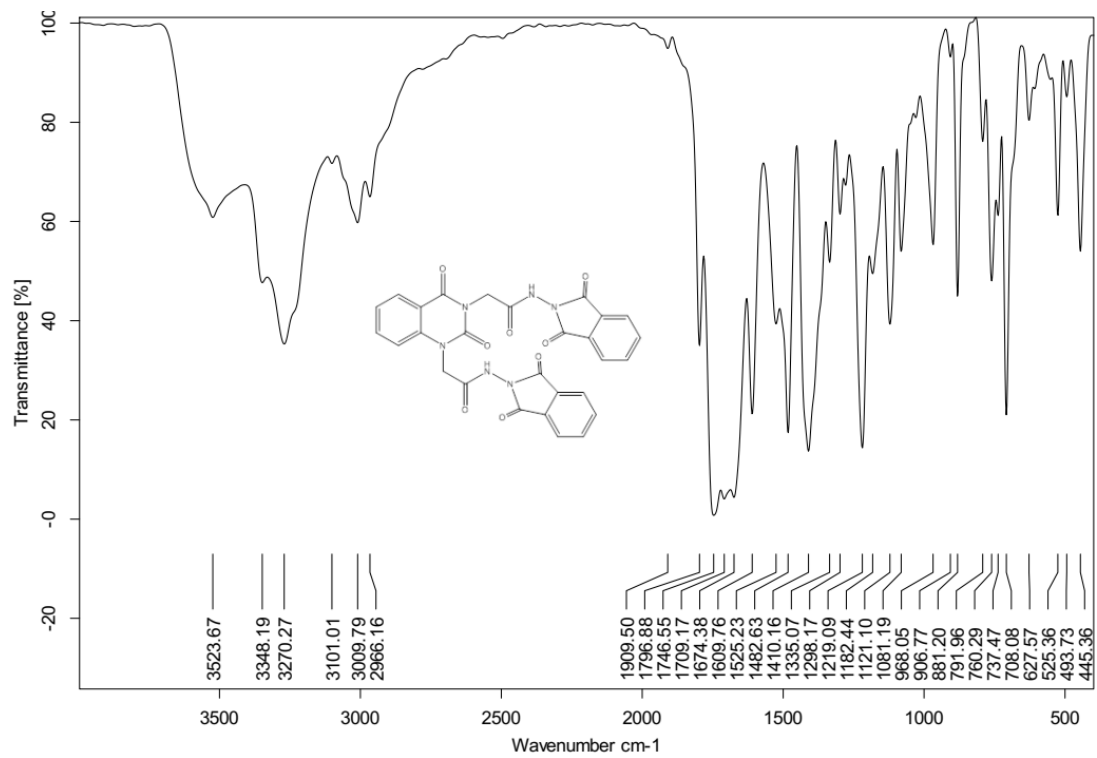


```

Current Data Parameters
NAME      mohamed omer-MC-Hmr-ov
EXPNO    20
PROCNO    1

F2 - Acquisition Parameters
Date_     20211018
Time      12:12 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         48
DS         4
SWH        801.800 Hz
FIDRES     0.244882 Hz
AQ         4.0394465 sec
RG         176.72
DR         62.400 usec
DE         6.50 usec
TE         292.2 K
D1         1.00000000 sec
TD0        1
SFO1      400.1024711 MHz
NUC1       1H
PC         18.50 usec
PL1        13.00000000 W

F2 - Processing parameters
SI         65536
SF         400.1000000 MHz
WDW        EM
SSB        0
GB         0
PC         0.30 Hz
WC         1.00
  
```



FT-IR of compound (5a)

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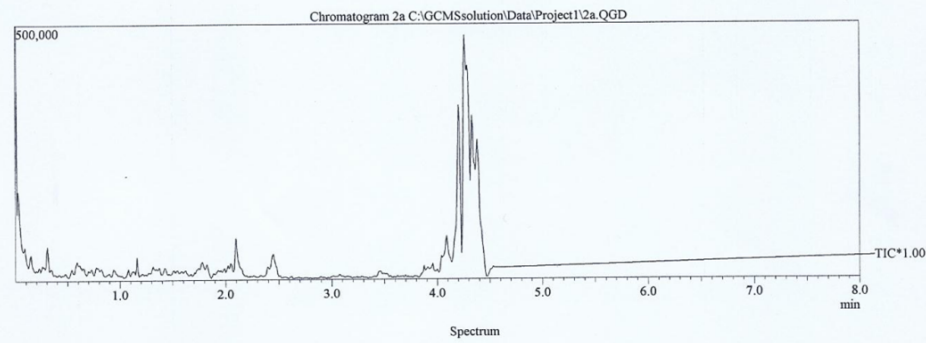
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 03:55:58
 Sample Name : 2a
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\2a.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\2a.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 \$EndIf\$Modified by : Dr. Mai Younis
 Modified : 15/01/2007 04:00:33

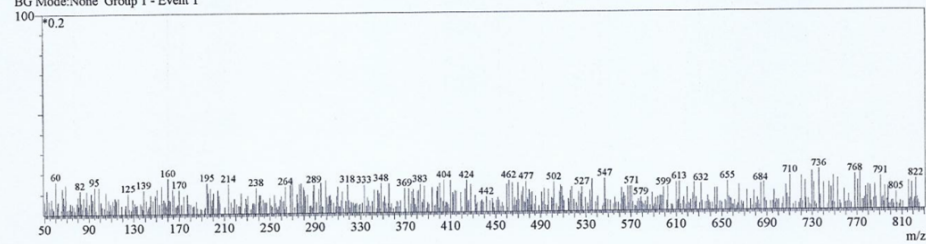
Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage :70 eV
 Ionization Mode :EI



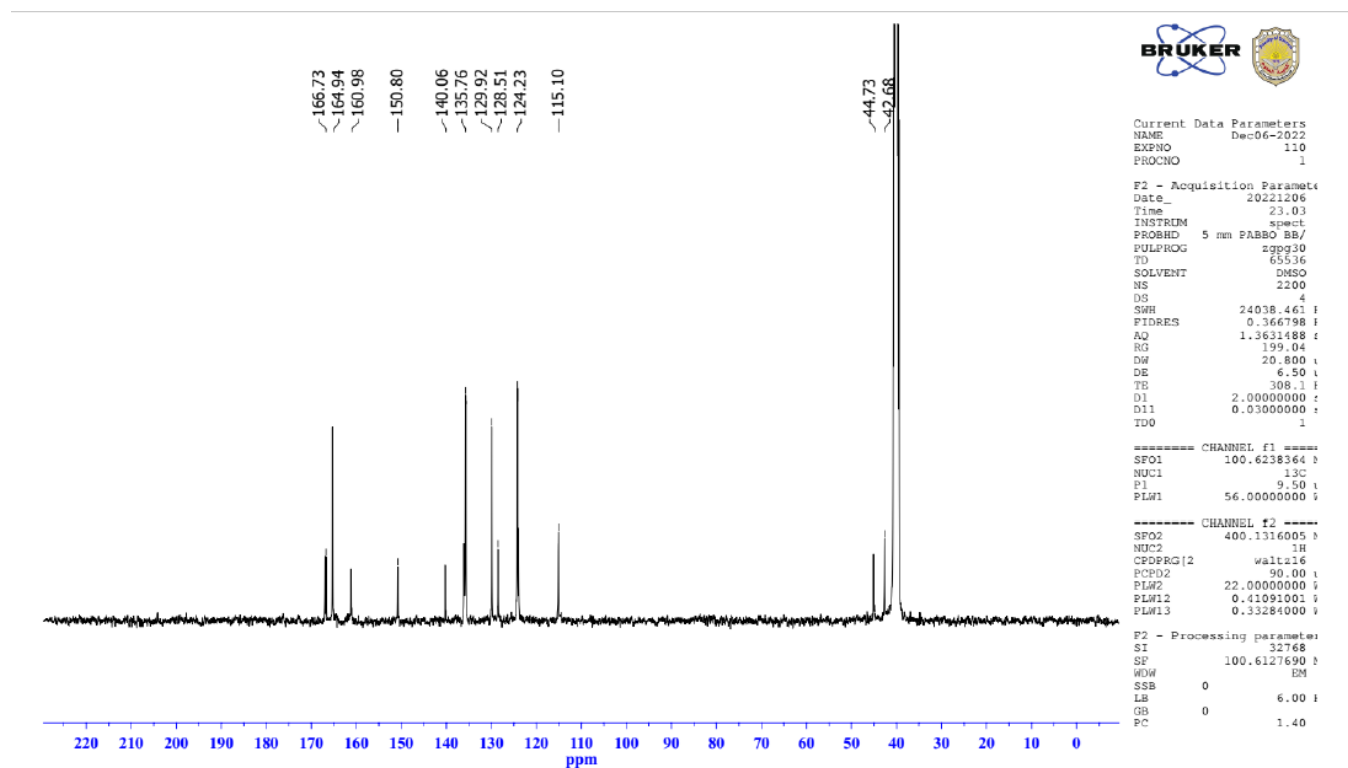
C:\GCMSsolution\Data\Project1\2a.QGD



Line#:1 R.Time:4.4(Scan#:526)
 MassPeaks:554
 RawMode:Single 4.4(526) BasePeak:736(1159)
 BG Mode:None Group 1 - Event 1



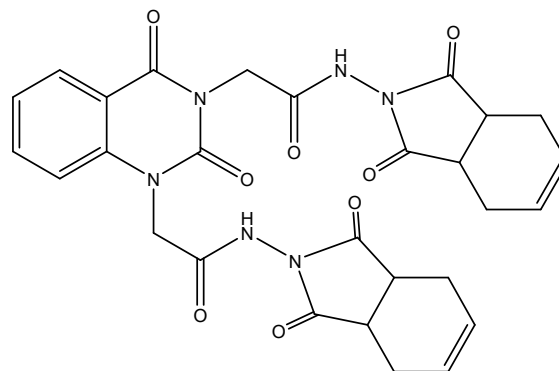
MS of compound (5a)



¹³C-NMR (100 MHz, DMSO) of compound (5a)

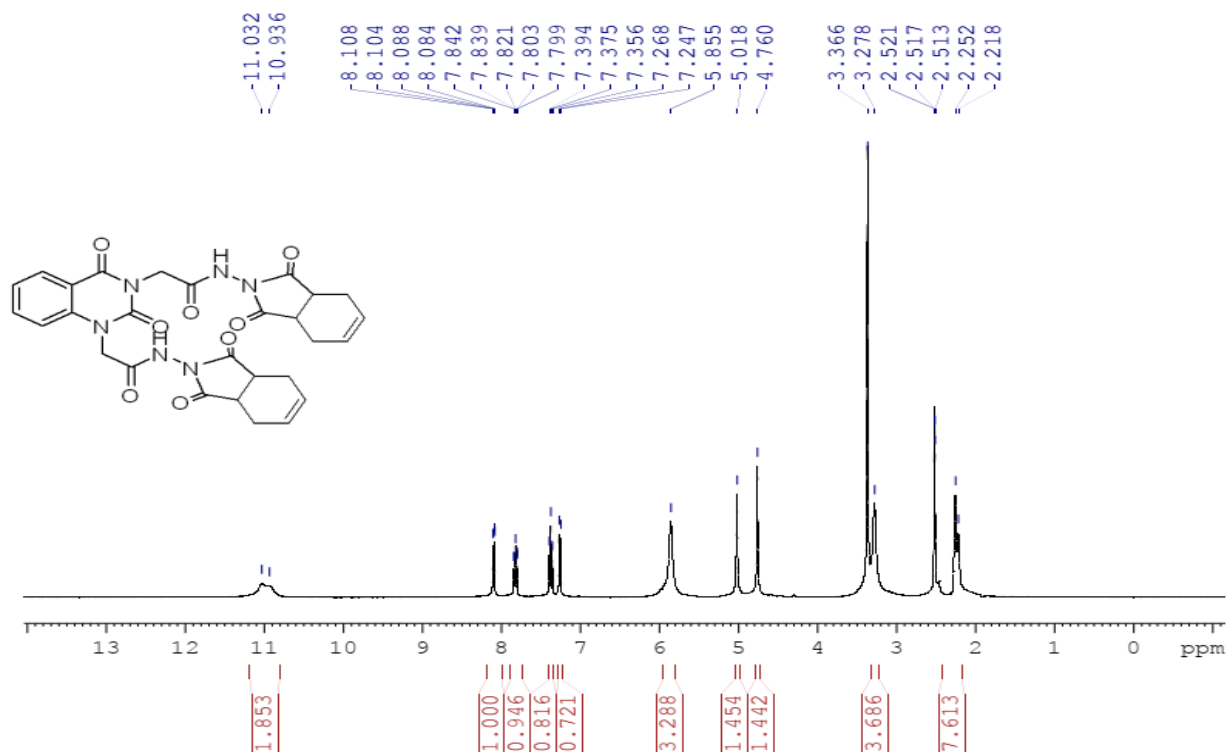
-

-Compound (5b):-



5b

muhammad omar-M2d-RR-hnmr



```
Current Data Parameters
NAME      muhammad omar-M2d-RR-hnmr
EXPNO     10
PROCNO    1

F1 - Acquisition Parameters
Date_     20211228
Time      13.14 h
INSTRUM   spect
PROBHD    E10618_0945 (
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         16
DS         4
SWH        8012.85000 Hz
WDW        EM
SSB        0.000000 Hz
LB         4.000000 Hz
GB         0.000000 Hz
PC         4.000000 sec
DC         0.000000 sec
RR         0.000000 sec
AQ         128.40 sec
RG         655.000000 Hz
DPR        1.000000000 sec
FIDRES     0.000000000 Hz
AQRES      400.0024711 MHz
NUC1       13C
P1         13.50 usec
PL1        0.000000000 W
SFO1       101.625125 MHz
F2 - Processing parameters
SI         65536
SF         400.0000000 MHz
WDW        EM
SSB        0.000000 Hz
LB         0.000000 Hz
GB         0.000000 Hz
PC         1.000000000 sec
```

¹H-NMR (400 MHz, DMSO-d₆) of compound (5b)

Cairo University Micro Analytical Center

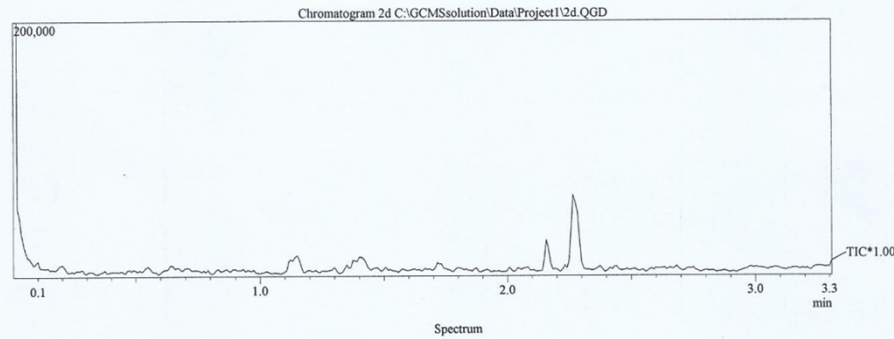
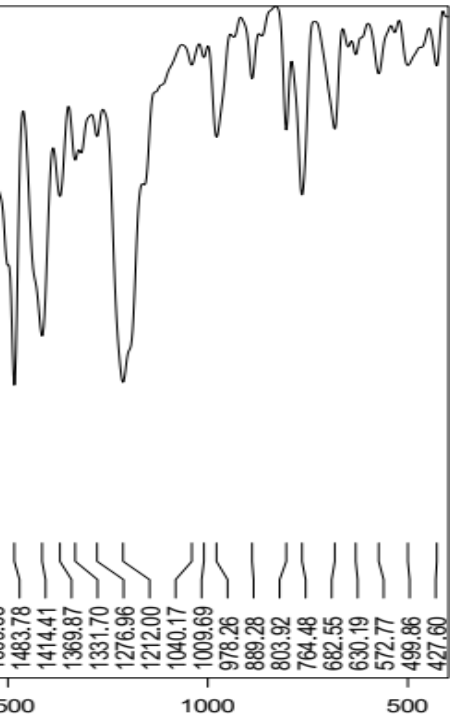
DI Analysis Shimadzu Qp-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 04:02:11 ص
Sample Name : 2d
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSsolution\Data\Project1\2d.QGD
Org Data File : C:\GCMSsolution\Data\Project1\2d.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.gct
SEndIfSModified by : Dr. Mai Younis
Modified : 15/01/2007 04:05:33 ص

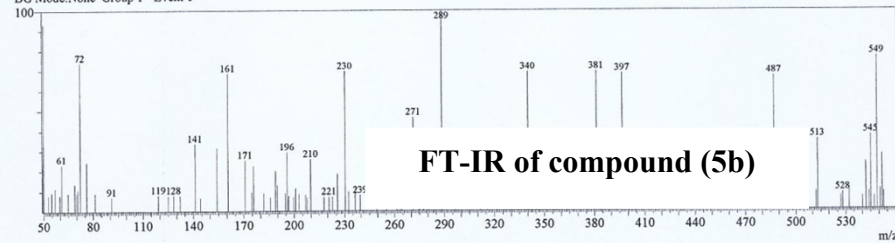
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time : -0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : -0.50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Data\Project1\2d.QGD



Line#:1 R.Time:2.3(Scan#:275)
MassPeaks:109
RawMode:Single 2.3(275) BasePeak:289(1585)
BG Mode:None Group 1 - Event 1

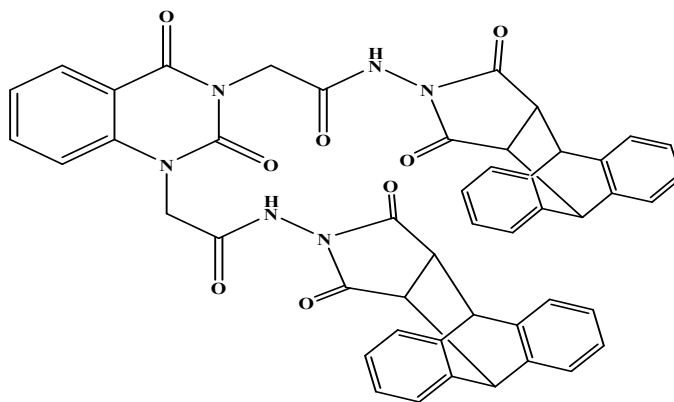


-

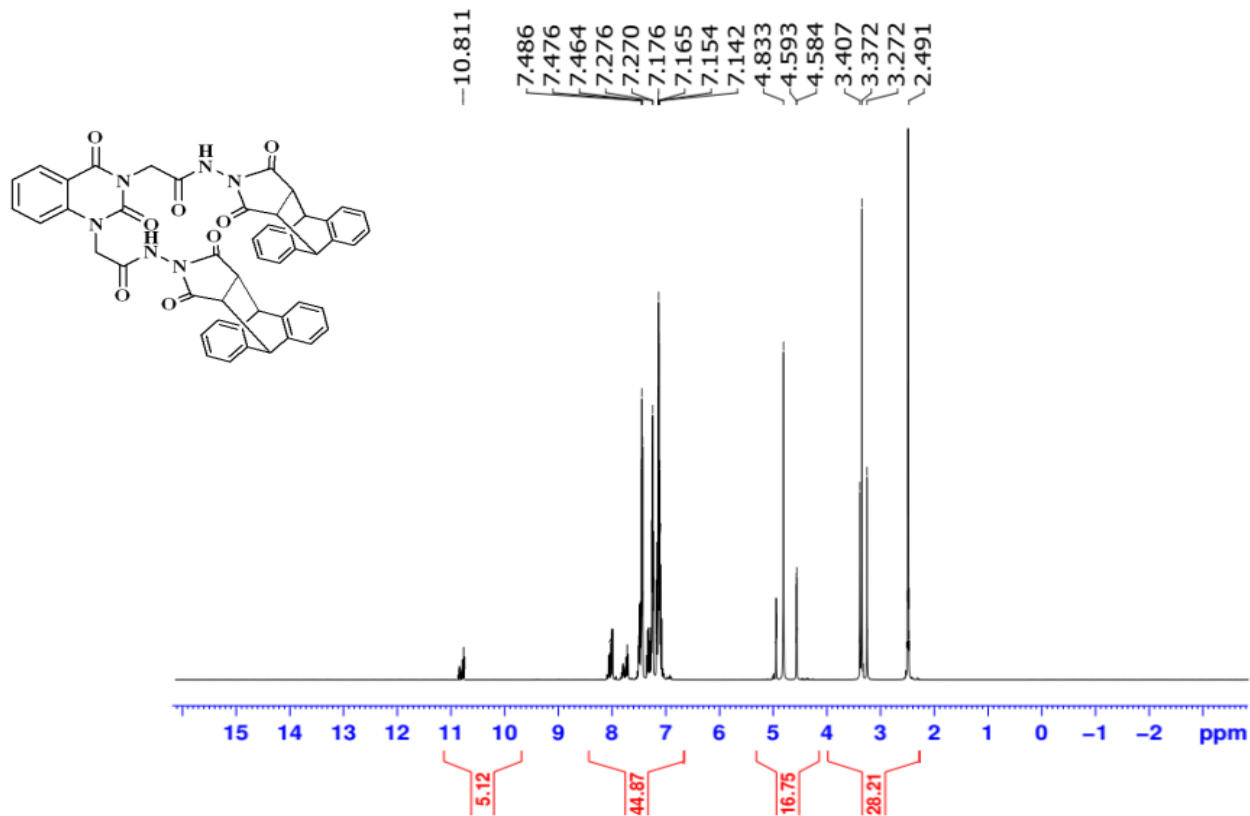
-Compound (5c)

MS of compound (5b)

-



5c



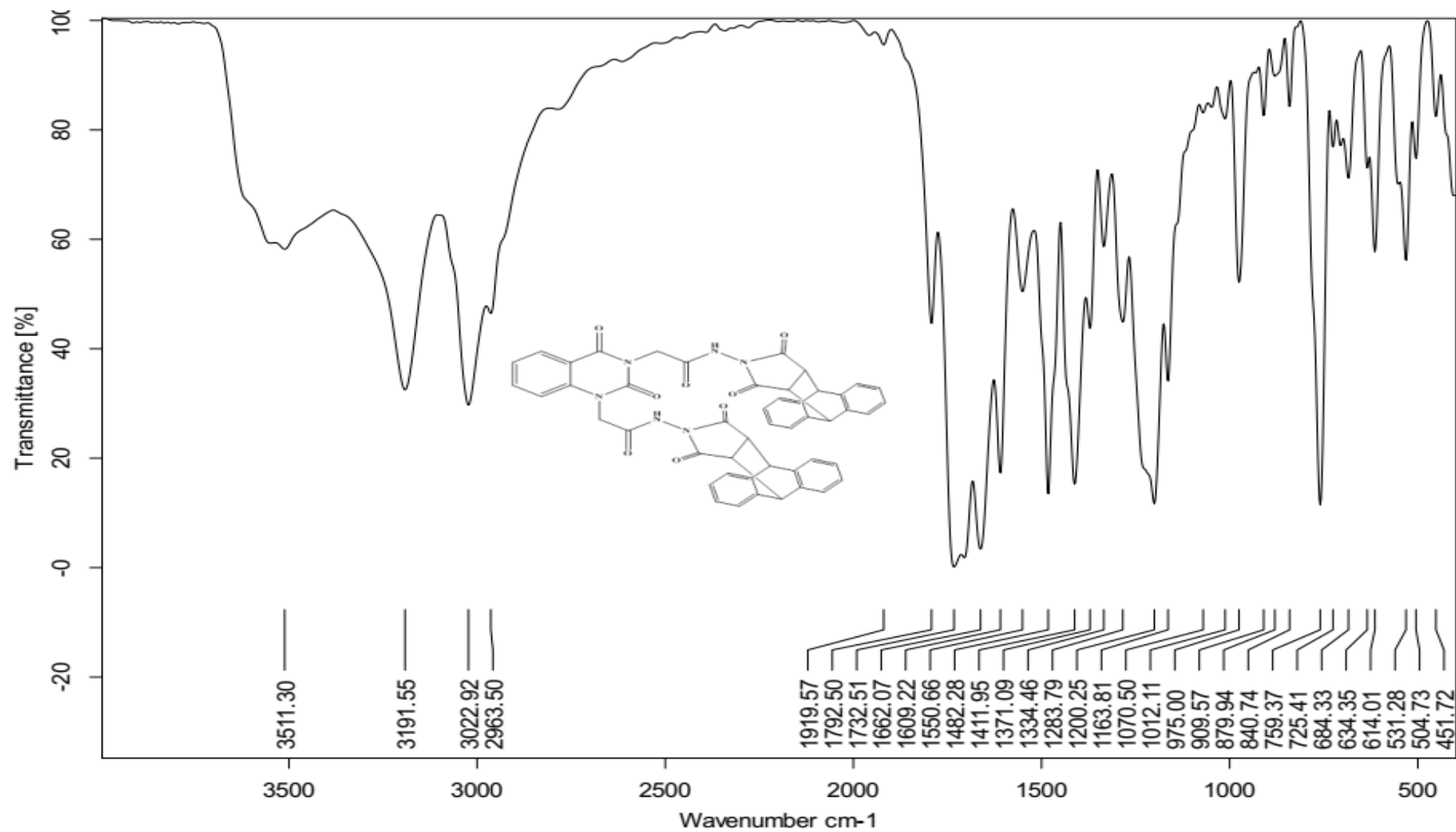
Current Data Parameters
NAME Feb17-2022
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220217
Time 10:14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 135
DW 62.400 usec
DE 6.50 usec
TE 313.3 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SF01 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (5c)



FT-IR of compound (5c)

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

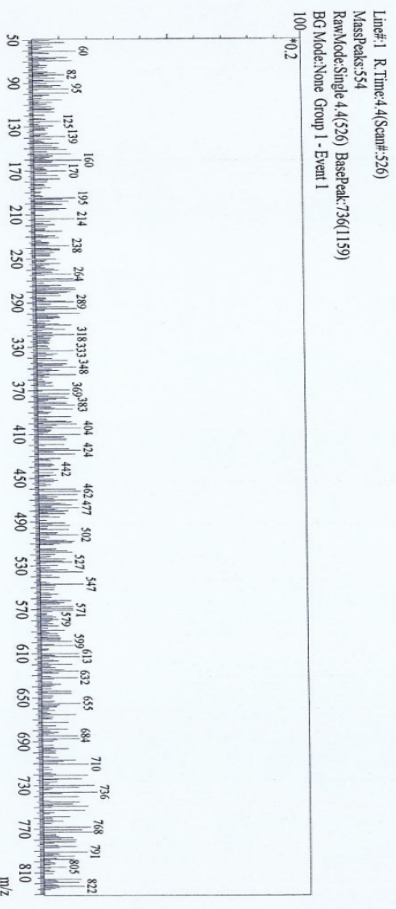
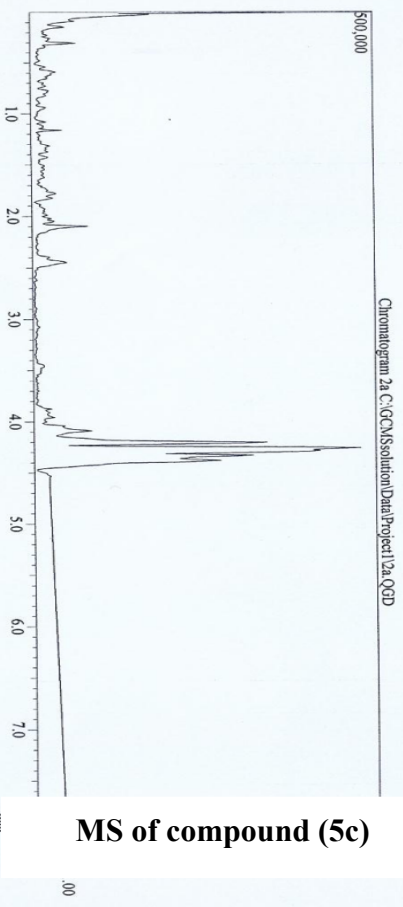
Analyzed by : Dr. Mai Younis
Analysis Date : 15/01/2007 03:55:58
Sample Name : 2a
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSolution\Data\Project1\2a.QGD
Org Data File : C:\GCMSolution\Data\Project1\2a.QGD
Method File : C:\GCMSolution\Data\Project1\Hight Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\Hight Temperature Op
Report File :
Turning File : C:\GCMSolution\System\Time1_default.qgr
Standard/Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:00:33

Method

Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
-Group 1 - Event 1-
Start Time : 0:00min
End Time : 1:0:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00

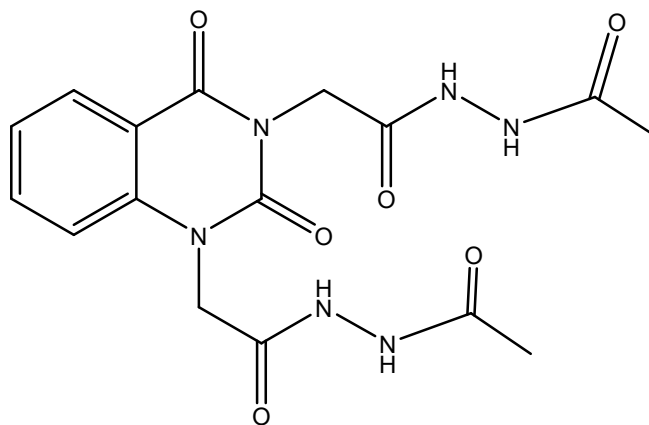
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project1\2a.QGD



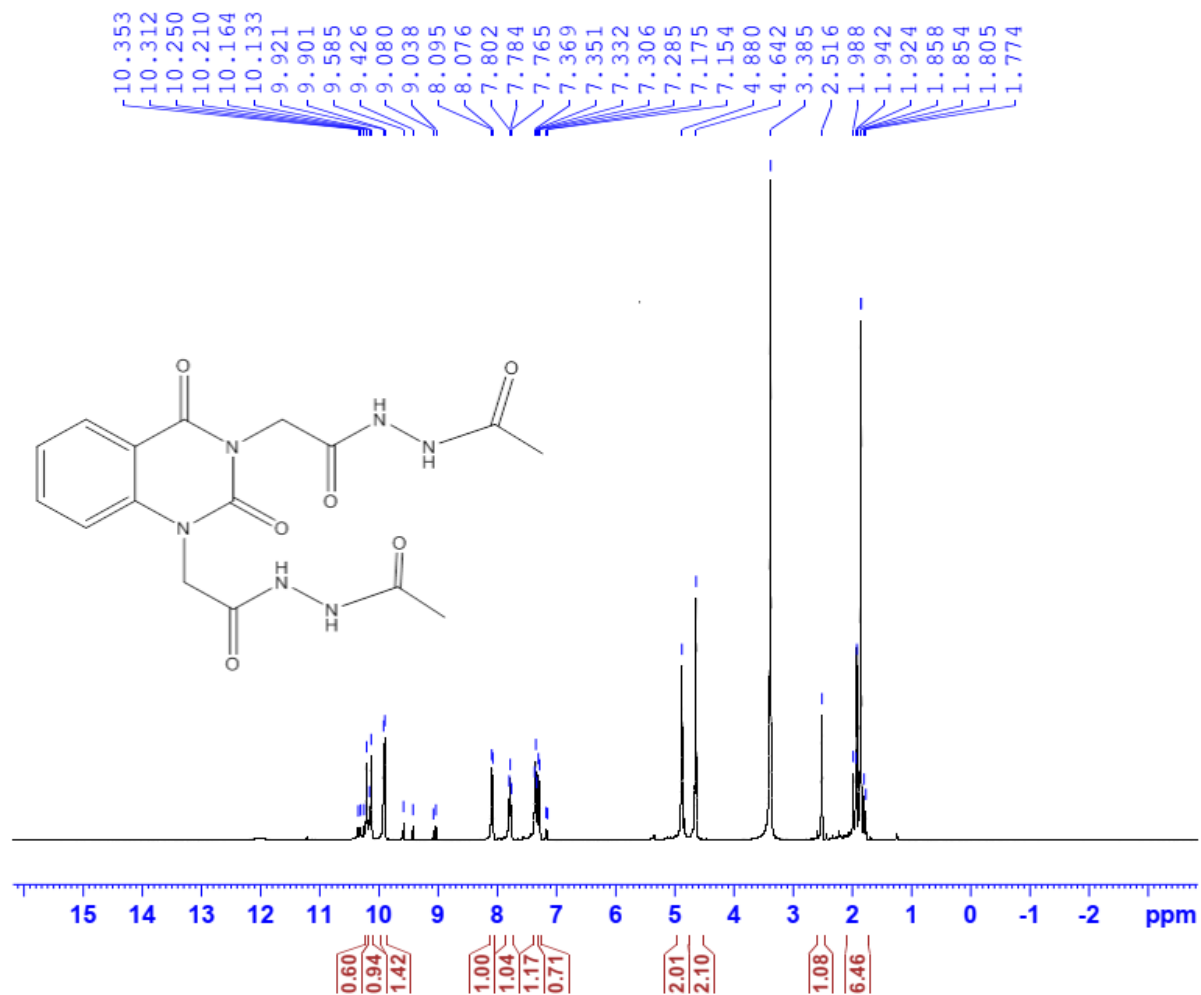
-

-Compound (6a)



6a

Mohamed Omar-10-Hnmr-RR

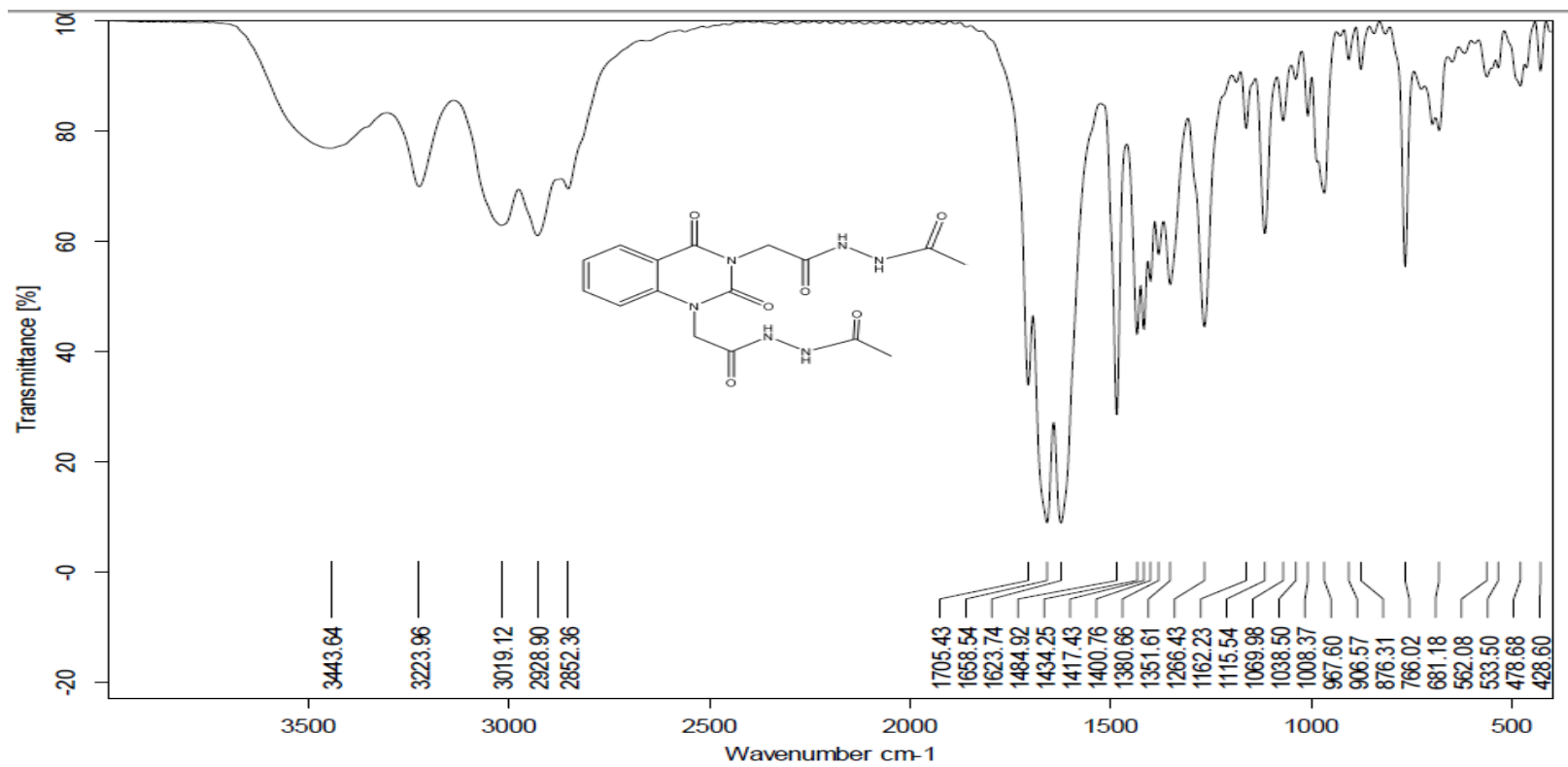


Current Data Parameters
NAME Mohamed Omar-10-Hnmr-RR
EXPNO 10
PROCNO 1

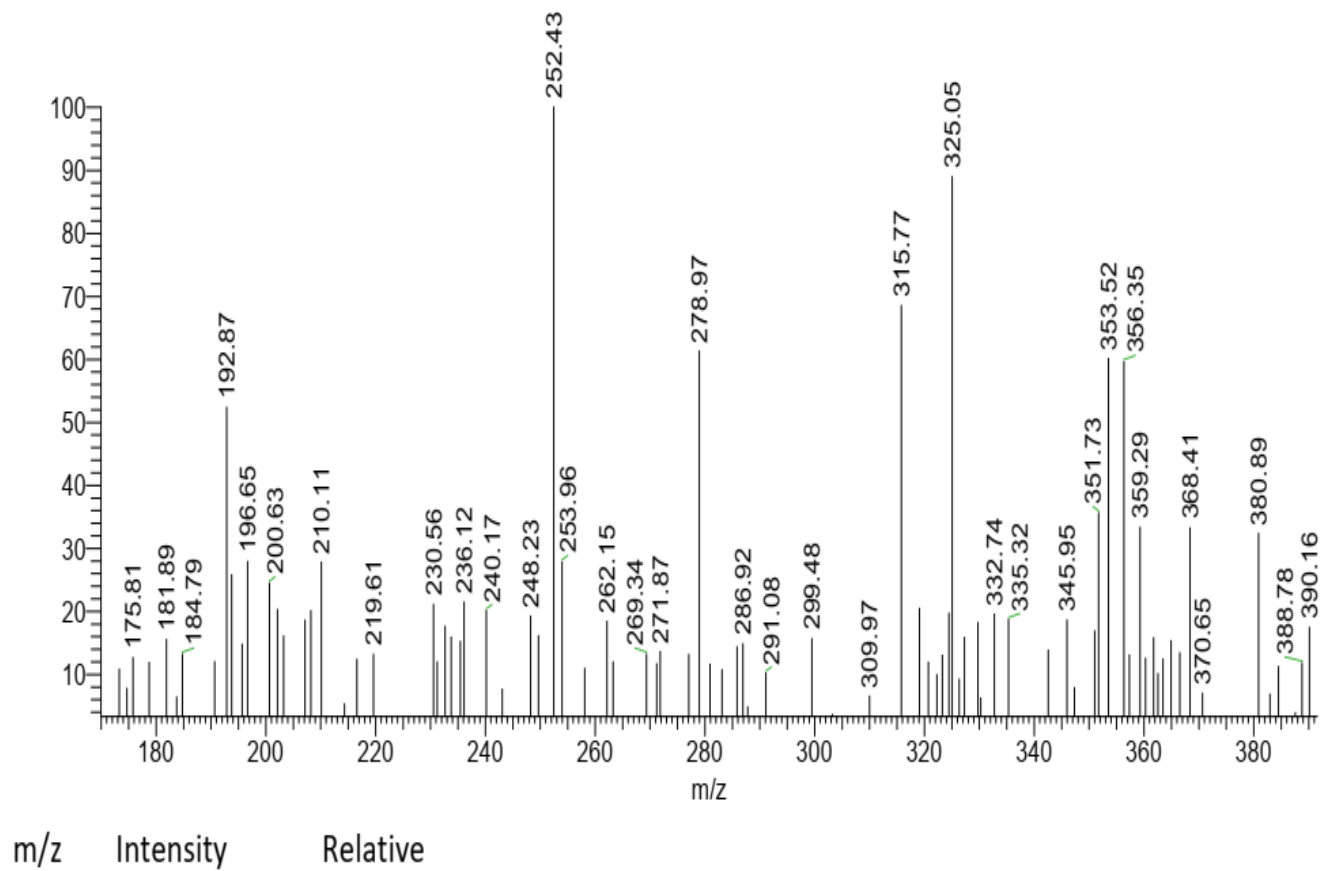
F2 - Acquisition Parameters
Date_ 20220830
Time 11.34 h
INSTRUM spect
PROBHD E108618_0945 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.800 Hz
FIDRES 0.244522 Hz
AQ 4.0894465 sec
RG 112.56
DM 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TDC 400.202471 MHz
SFO1 400.202471 MHz
NUC1 1H
P1 13.50 usec
PLW1 18.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (6a)



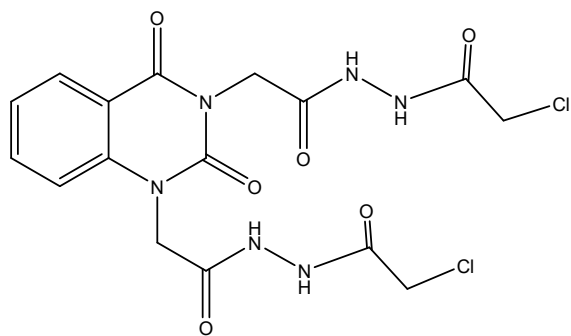
mohamed-omar-15 #173-176 RT: 2.91-2.96 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.75E2
T: + c EI Full ms [40.00-1000.00]



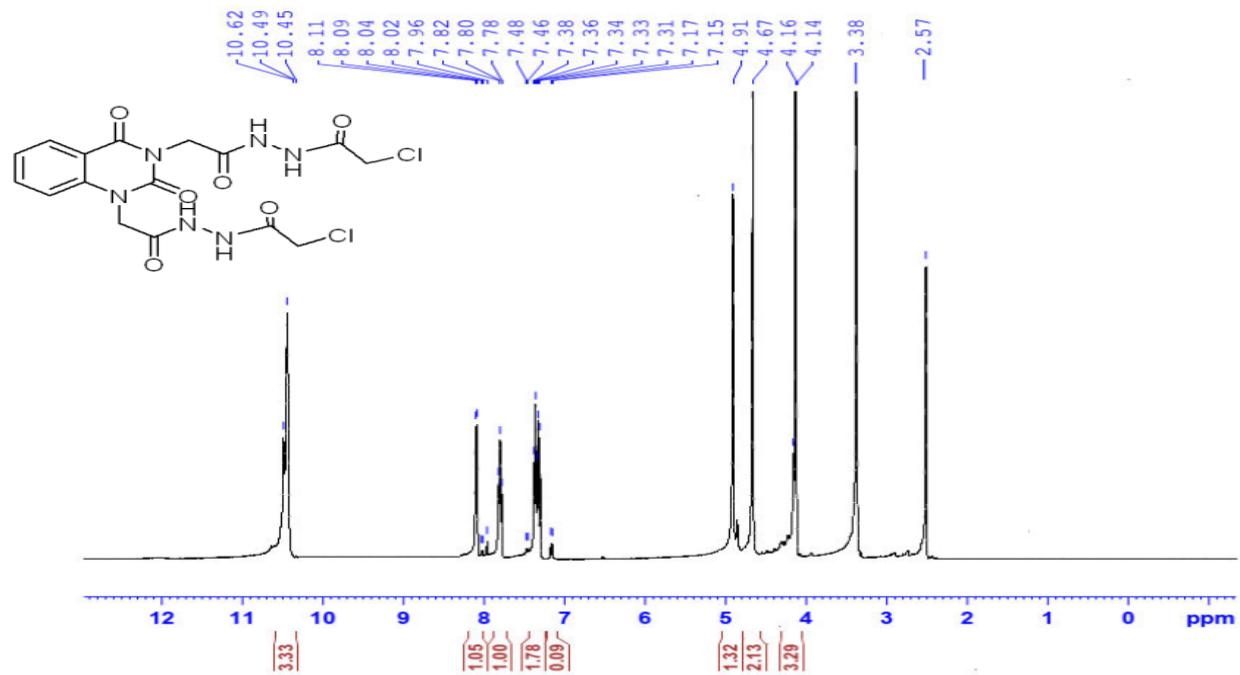
MS of compound (6a)

-

-Compound (6b)



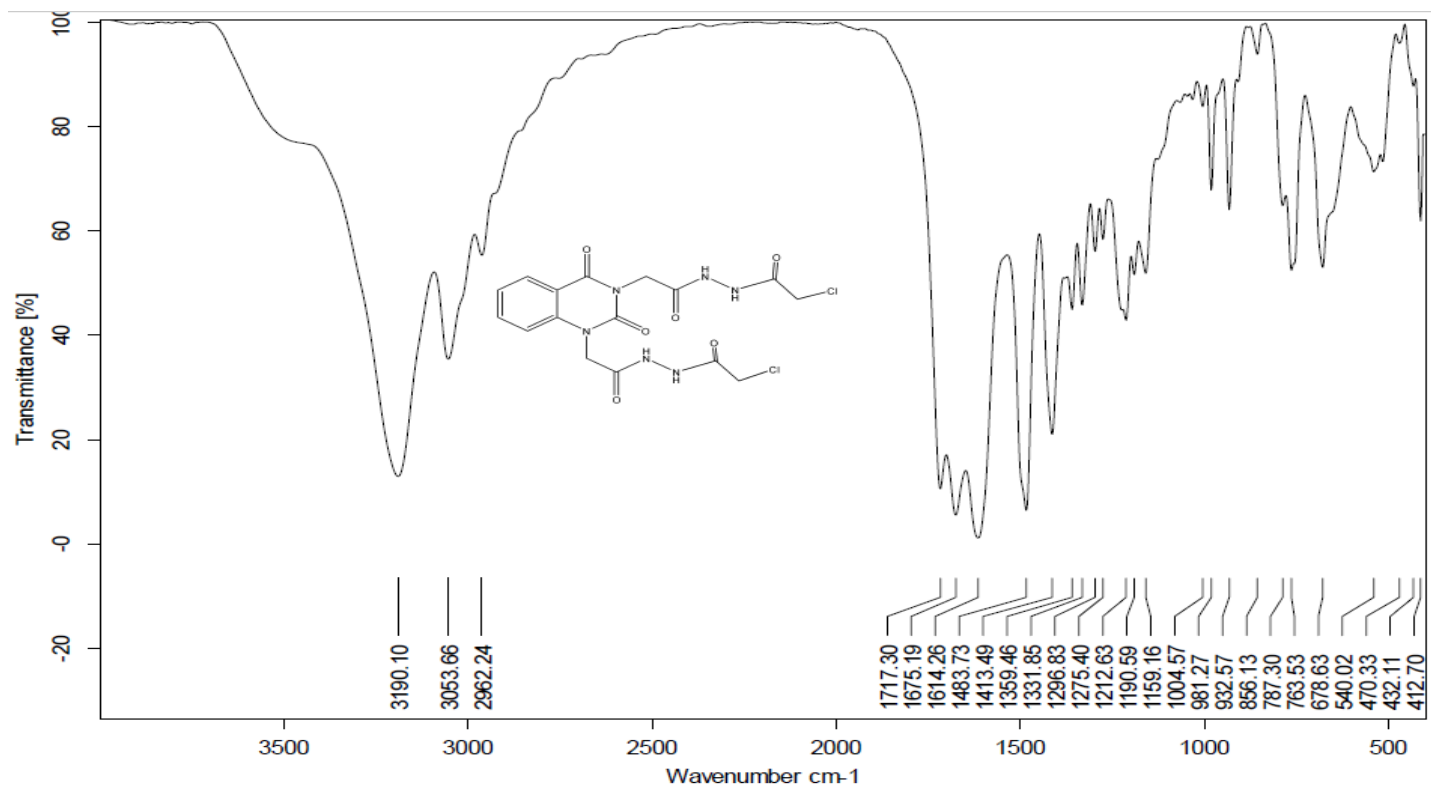
6b



Current Data Parameters
 NAME Mohamed Omar - M7 - Hnm
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220115
 Time 19.06 h
 INSTRUM spect
 PROBHD z108618_0945 f
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.081465 sec
 RG 120.93
 DK 62.400 usec
 DE 6.50 usec
 TE 294.5 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 13
 P1 13.50 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.2000000 MHz
 WDW EM
 SSB 0
 GB 0 0.30 Hz
 PC 1.00

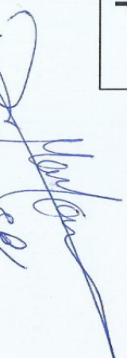


FT-IR of compound (6b)

15-Jan-07 02:56:27

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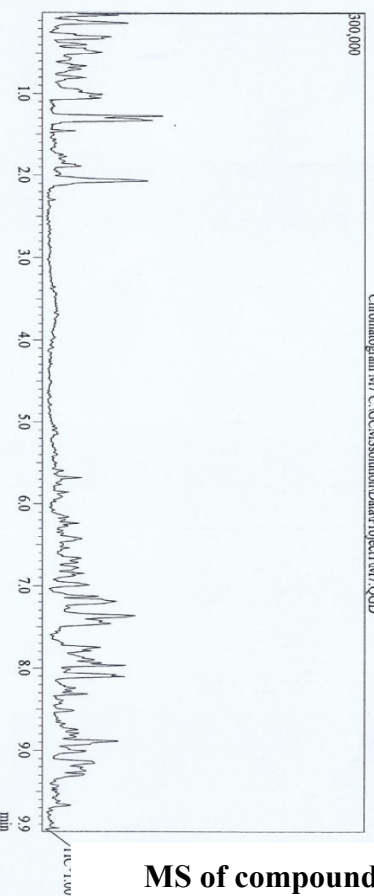


Sample Information
Analyzed by : Dr. Maq Youns
Sample Name : 1501/2007 02:56:02
Sample ID : M7
Customer Name : Dr. Mohamed Omar - Science - Qena
Data File : C:\GCMSolution\Data\Project1\M7.QGD
Org Data File : C:\GCMSolution\Data\Project1\M7.QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org. Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File :
Timing File : C:\GCMSolution\System\Tune1\default.qgt
Standard/Modified by : Dr. Maq Youns
Modified : 1501/2007 02:46:02

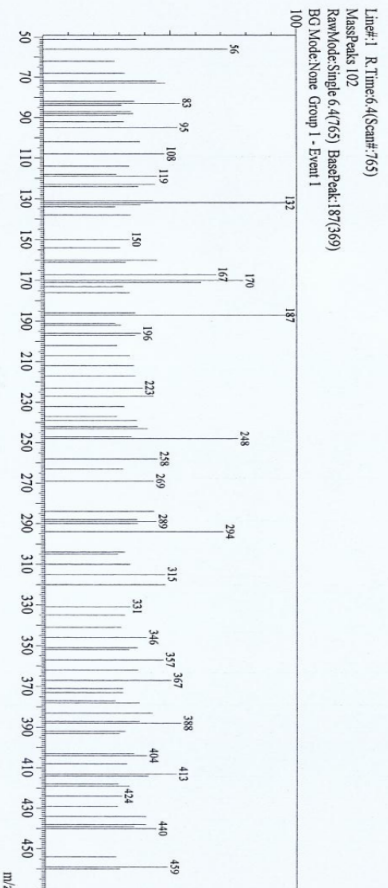
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
MS Table)
--Group 1 - Event 1--
Start Time : 0.00min
End Time : 10.00min
Scan : Scan
ACQ Mode : 0.50sec
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI

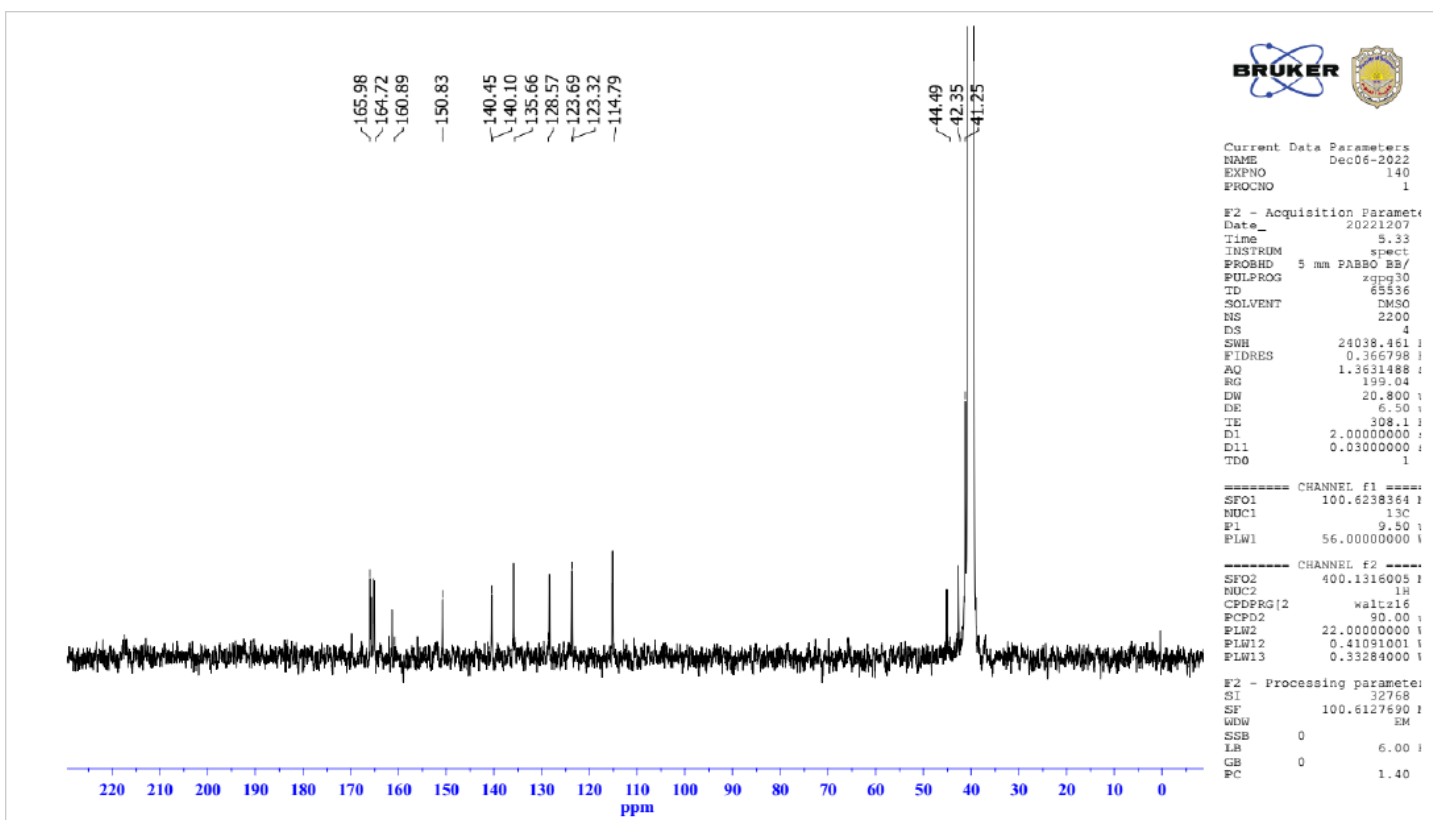
C:\GCMSolution\Data\Project1\M7.QGD

Chromatogram M7 C:\GCMSolution\Data\Project1\M7.QGD



MS of compound (6b)

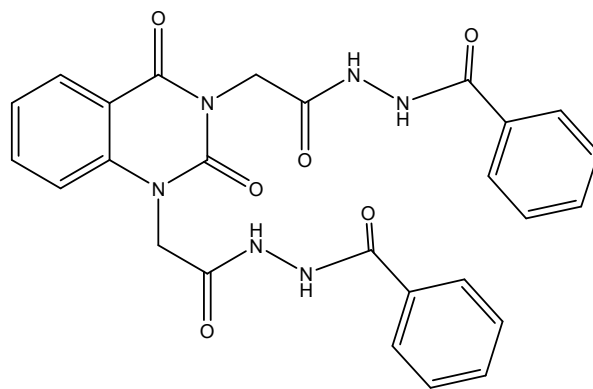




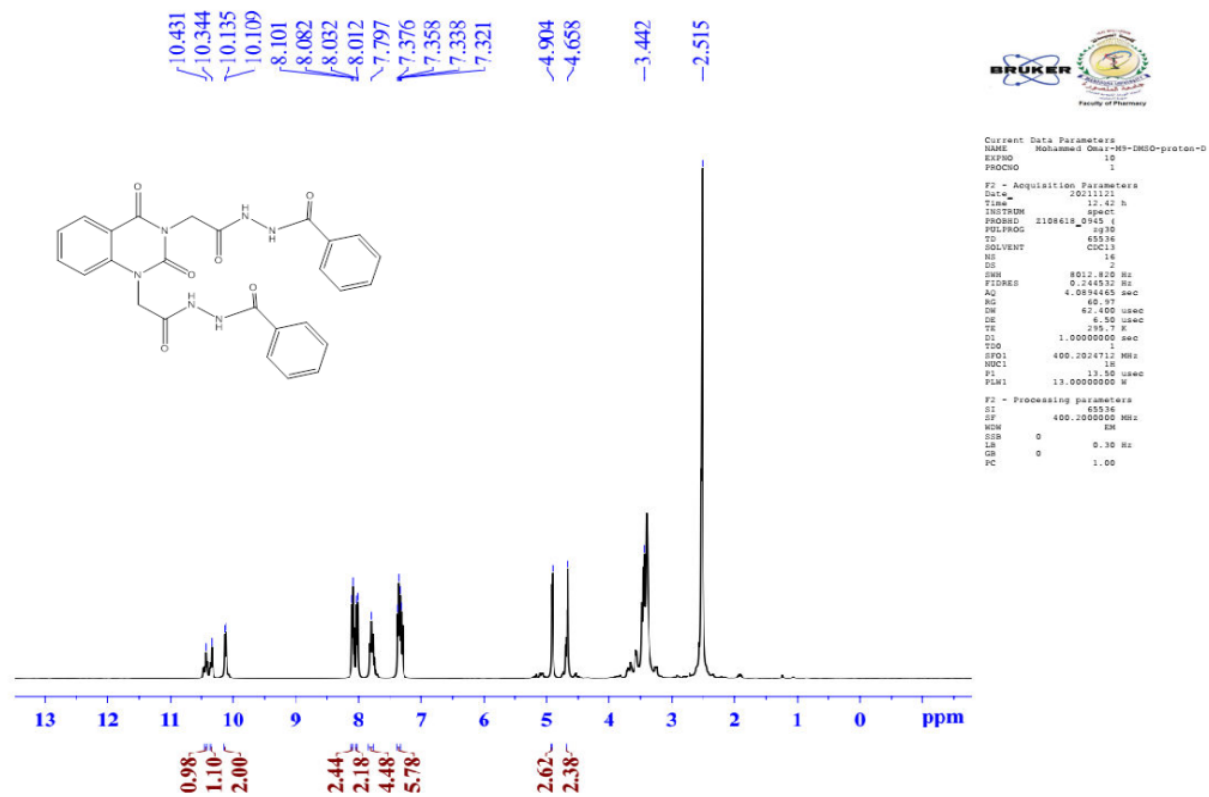
¹³C-NMR (100 MHz, DMSO) of compound (6b)

-

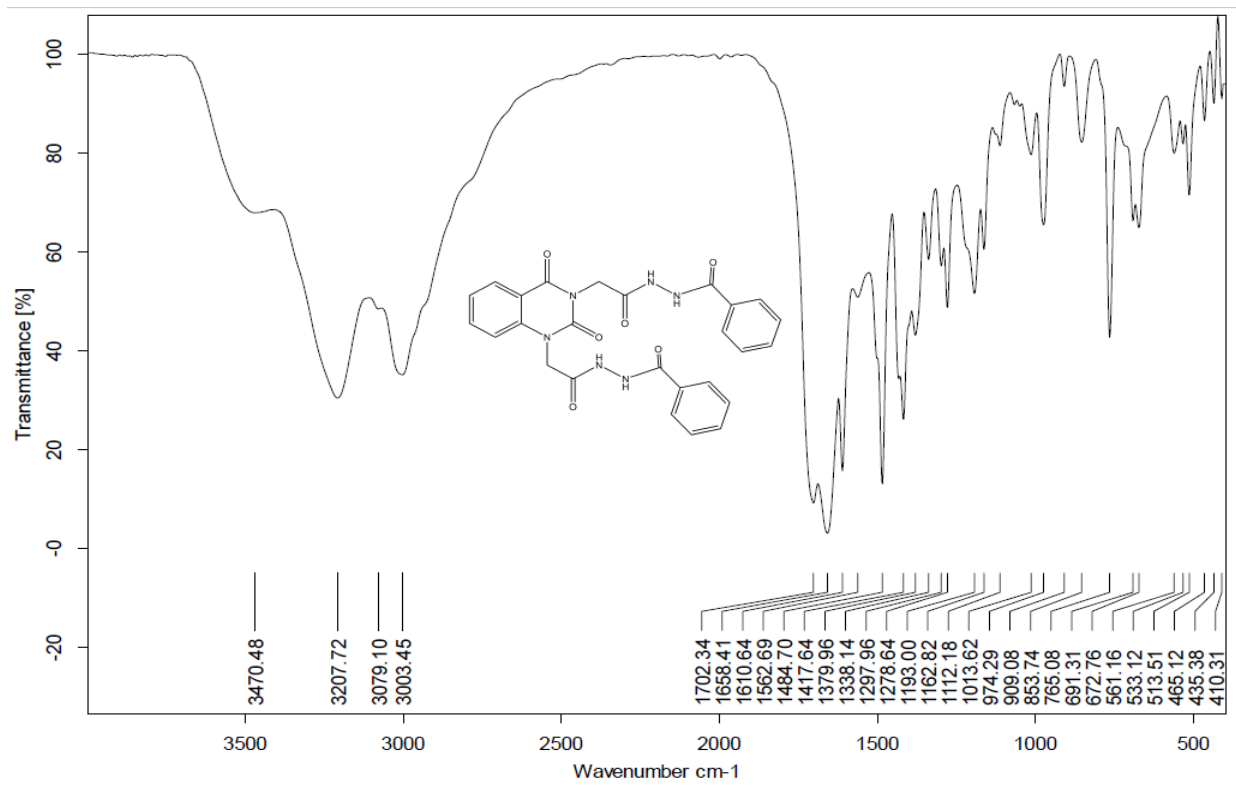
-Compound (6c)



6c

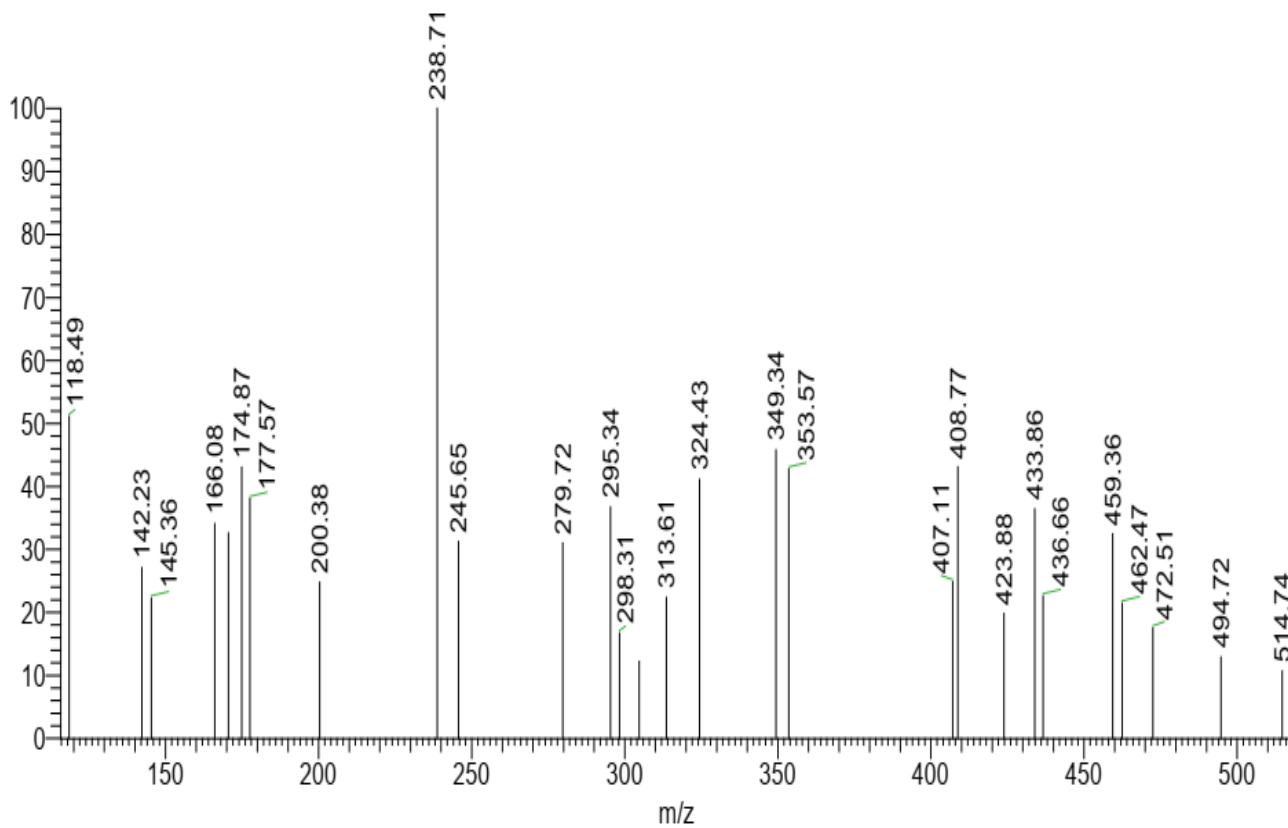


¹H-NMR (400 MHz, DMSO-d₆) of compound (6c)



FT-IR of compound (6c)

mohamed-omar-12 #35-38 RT: 0.60-0.65 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 7.88E1
T: + c EI Full ms [40.00-1000.00]

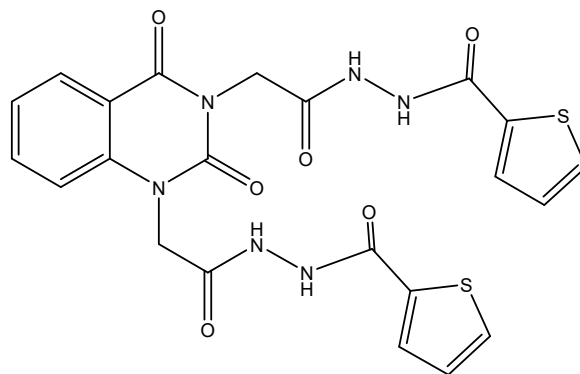


m/z Intensity Relative

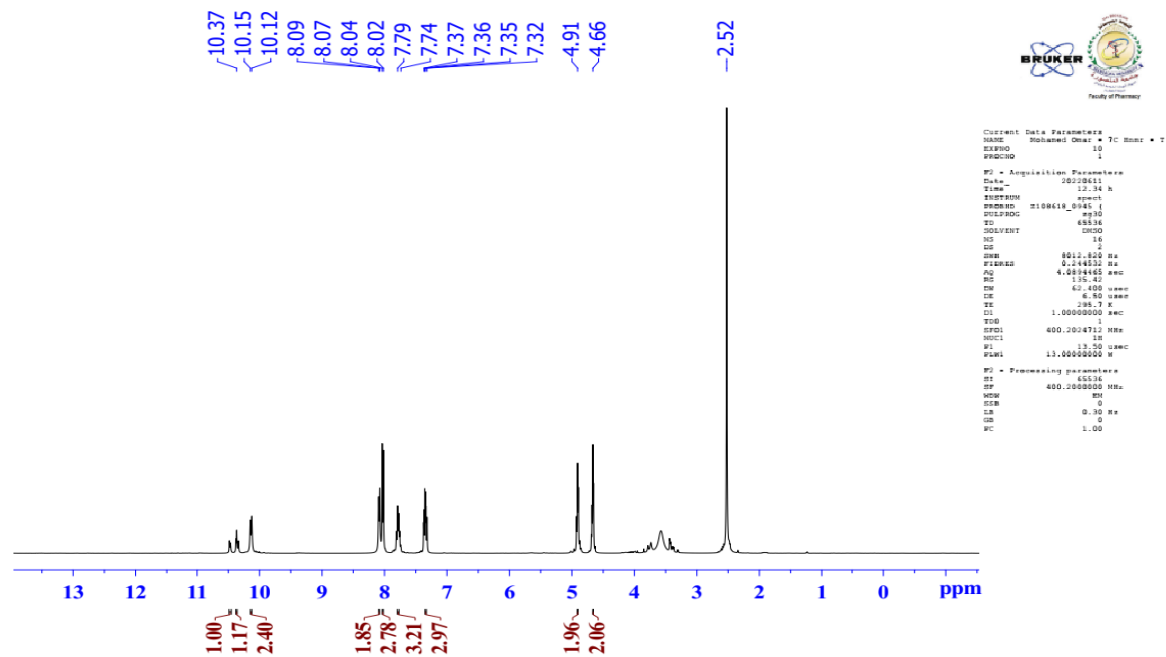
MS of compound (6c)

-

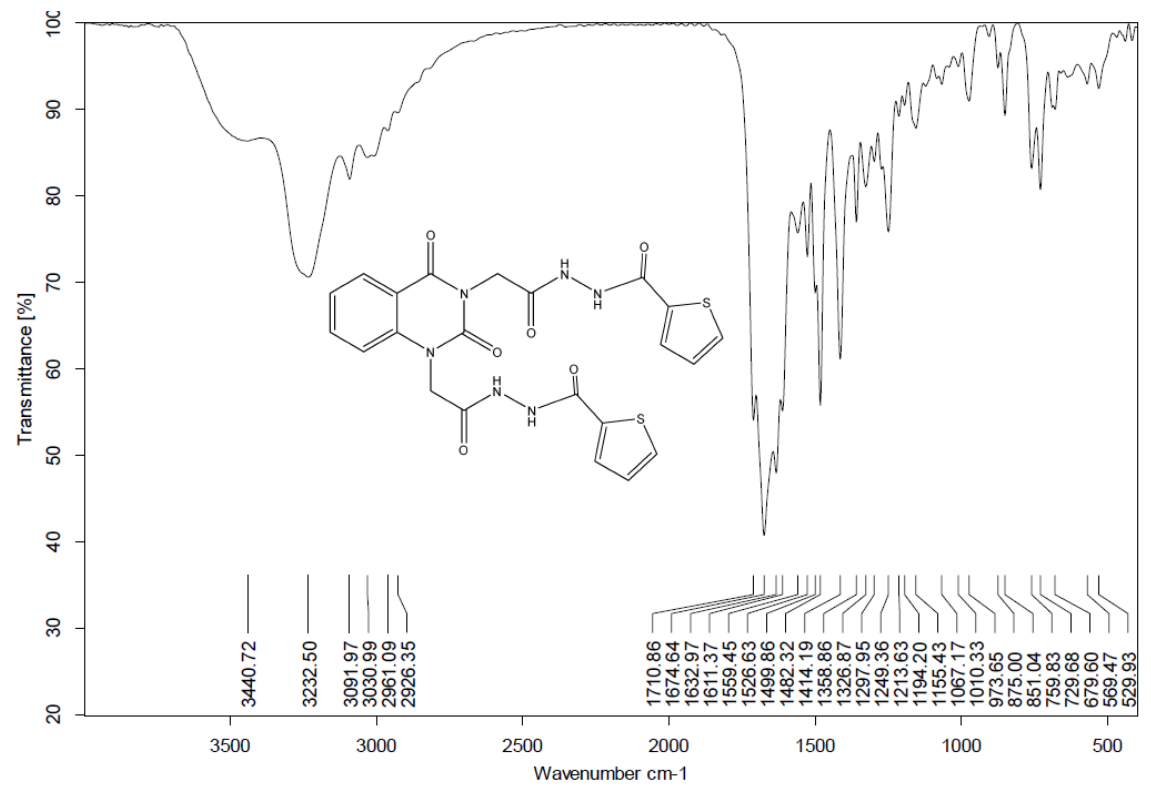
-Compound (6d)



6d



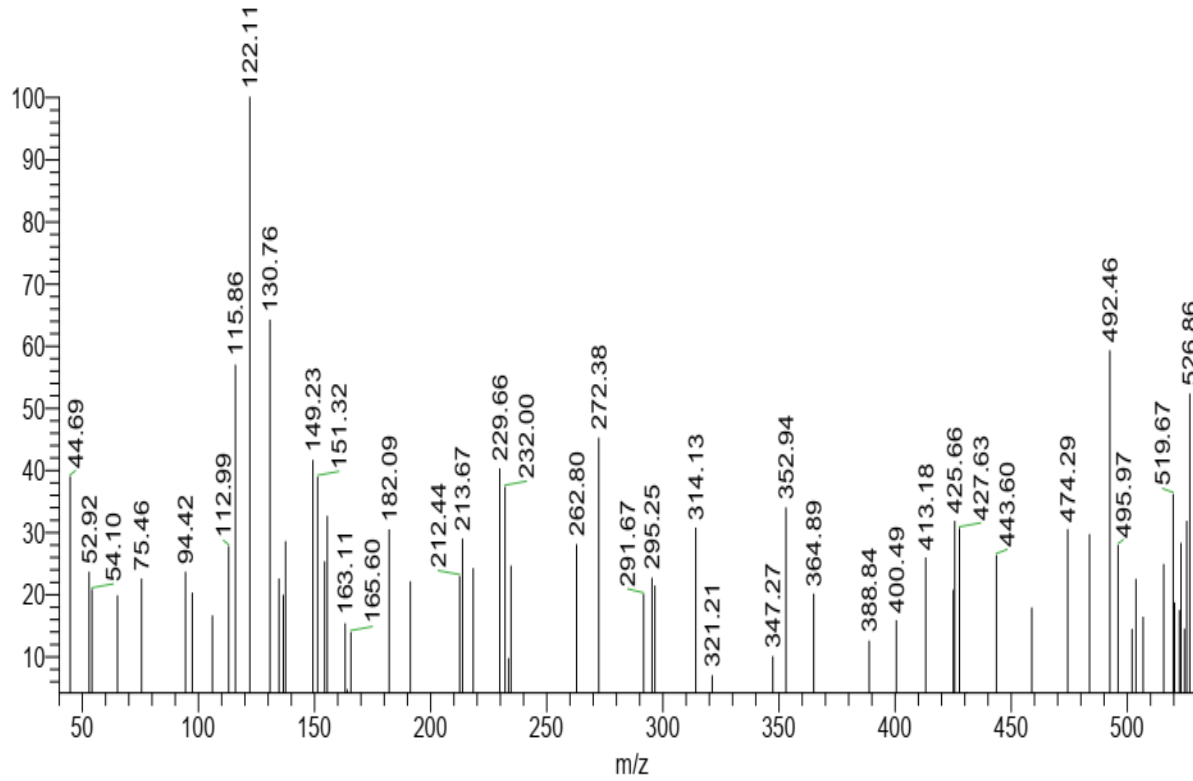
¹H-NMR (400 MHz, DMSO-d₆) of compound (6d)



FT-IR of compound (6d)

Time (min)

mohamed-omar-13 #161 RT: 2.71 AV: 1 SB: 26 1.21-1.34, 0.87-1.14 NL: 3.33E2
T: + c EI Full ms [40.00-1000.00]

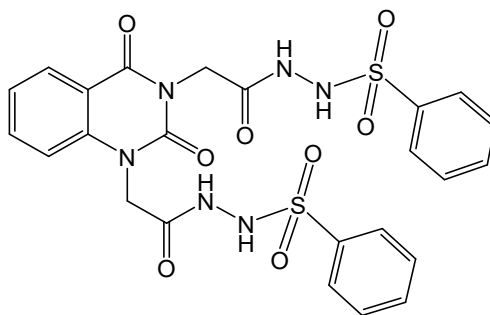


m/z Intensity Relative

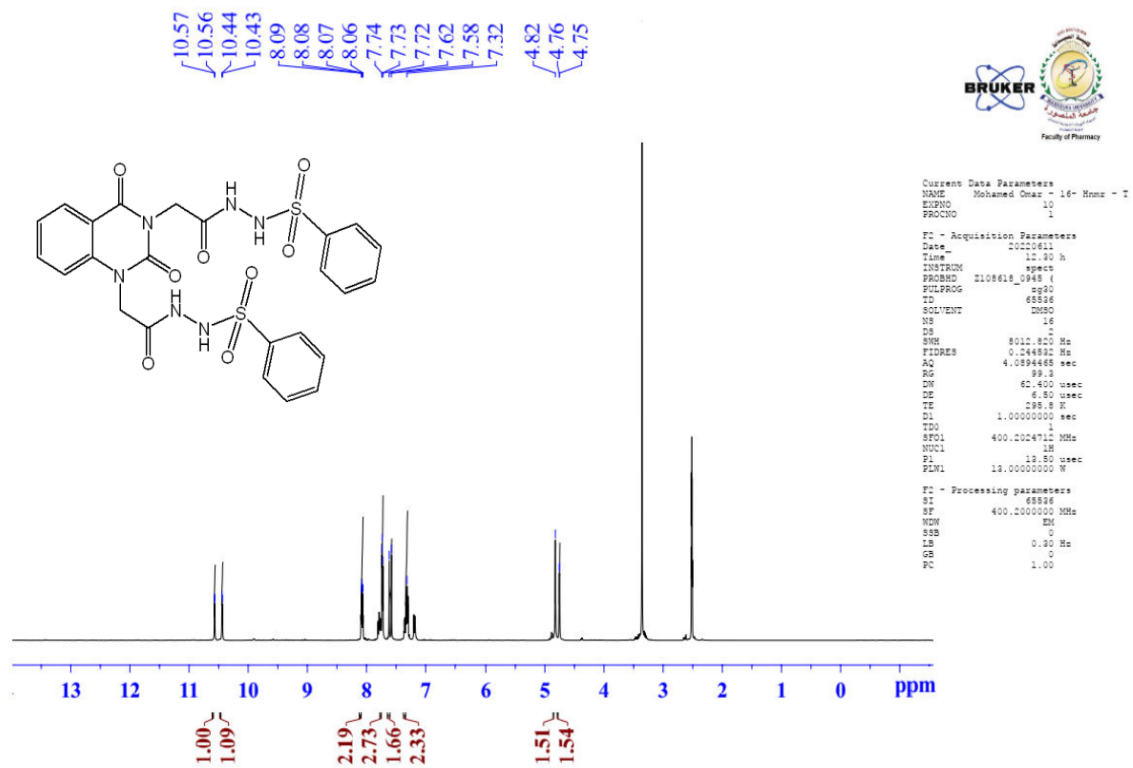
MS of compound (6d)

-

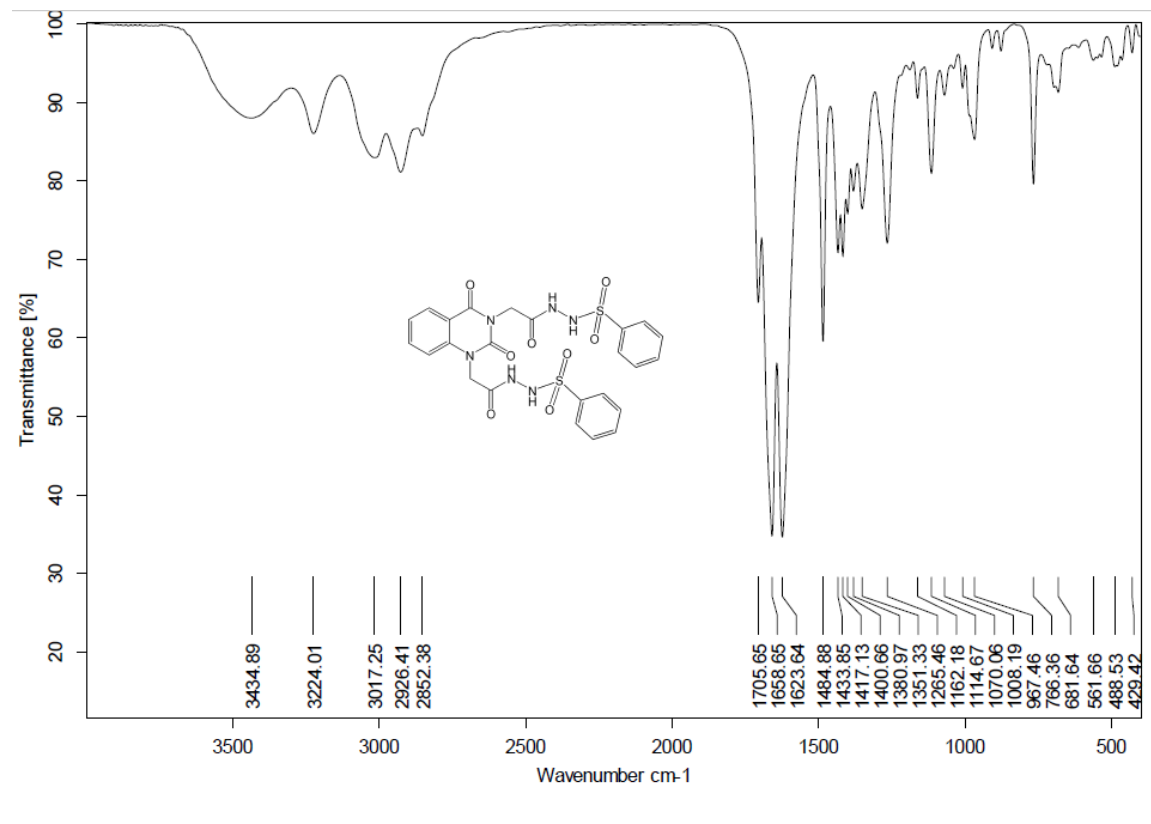
-Compound (6e)



6e

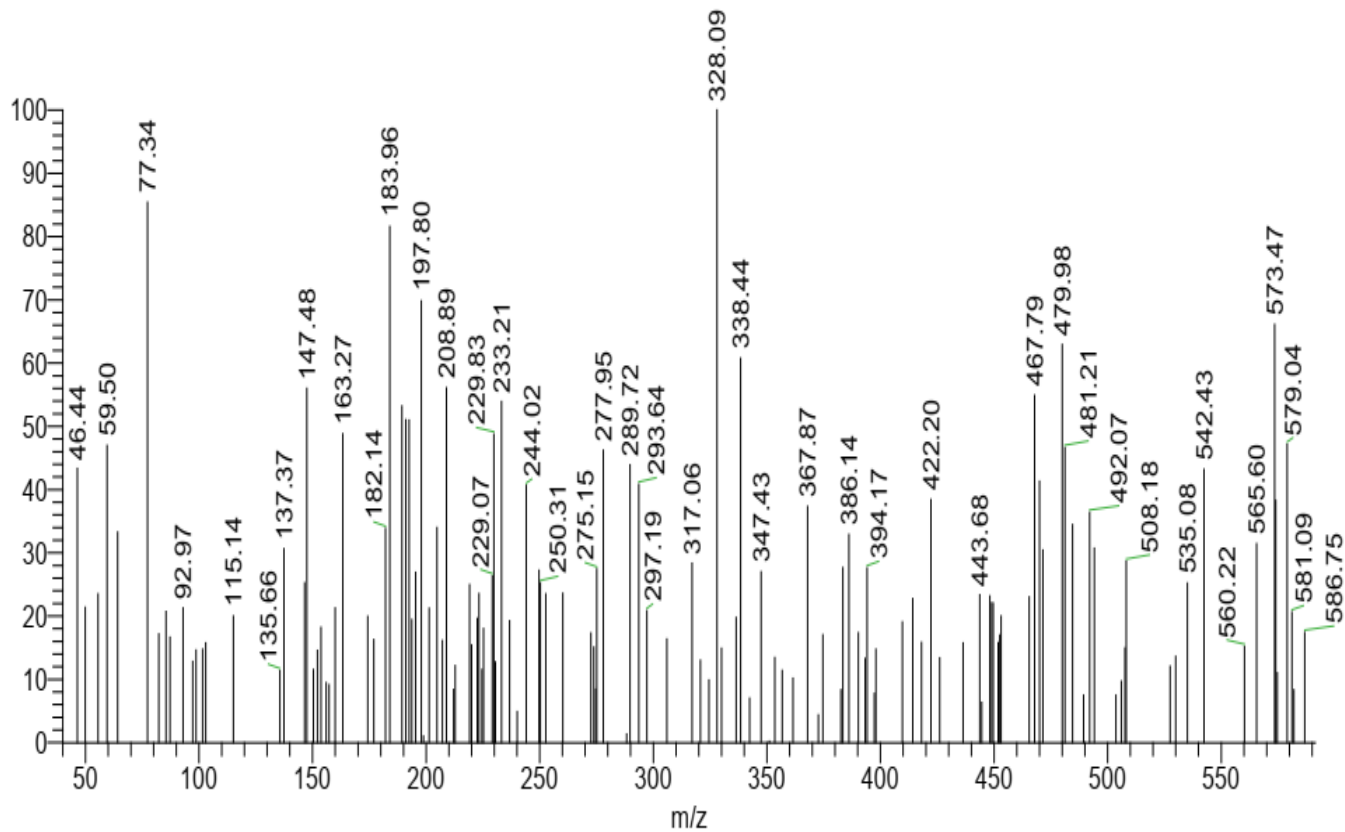


¹H-NMR (400 MHz, DMSO-d₆) of compound (6e)



FT-IR of compound (6e)

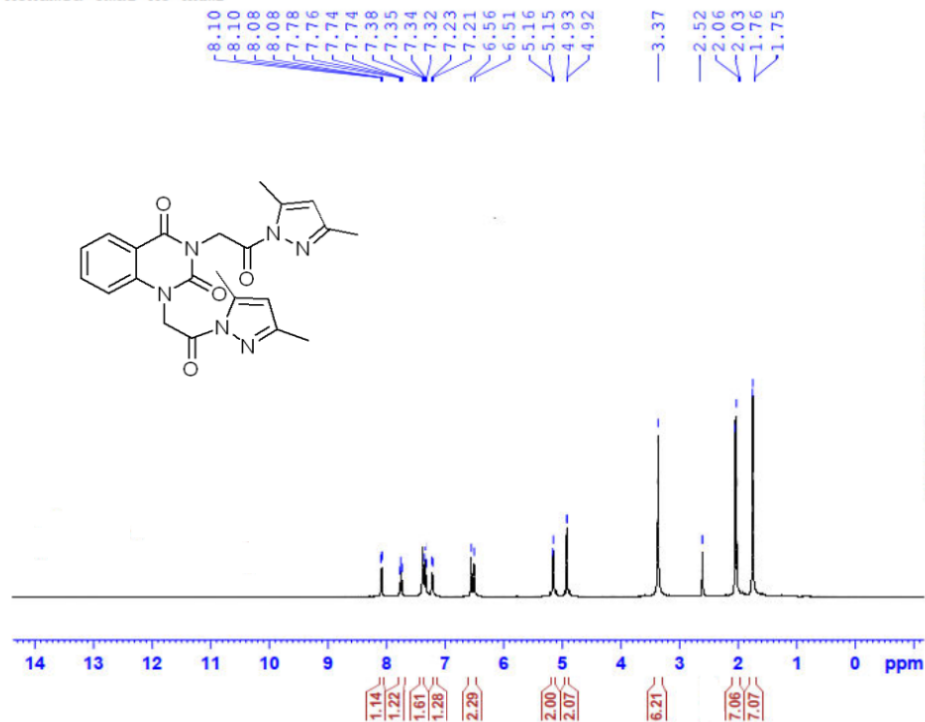
mohamed-omar-14 #54 RT: 0.92 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 3.46E2
T: + c EI Full ms [40.00-1000.00]



m/z Intensity Relative

MS of compound (6e)

Mohamed Omar-M3-Hnmr

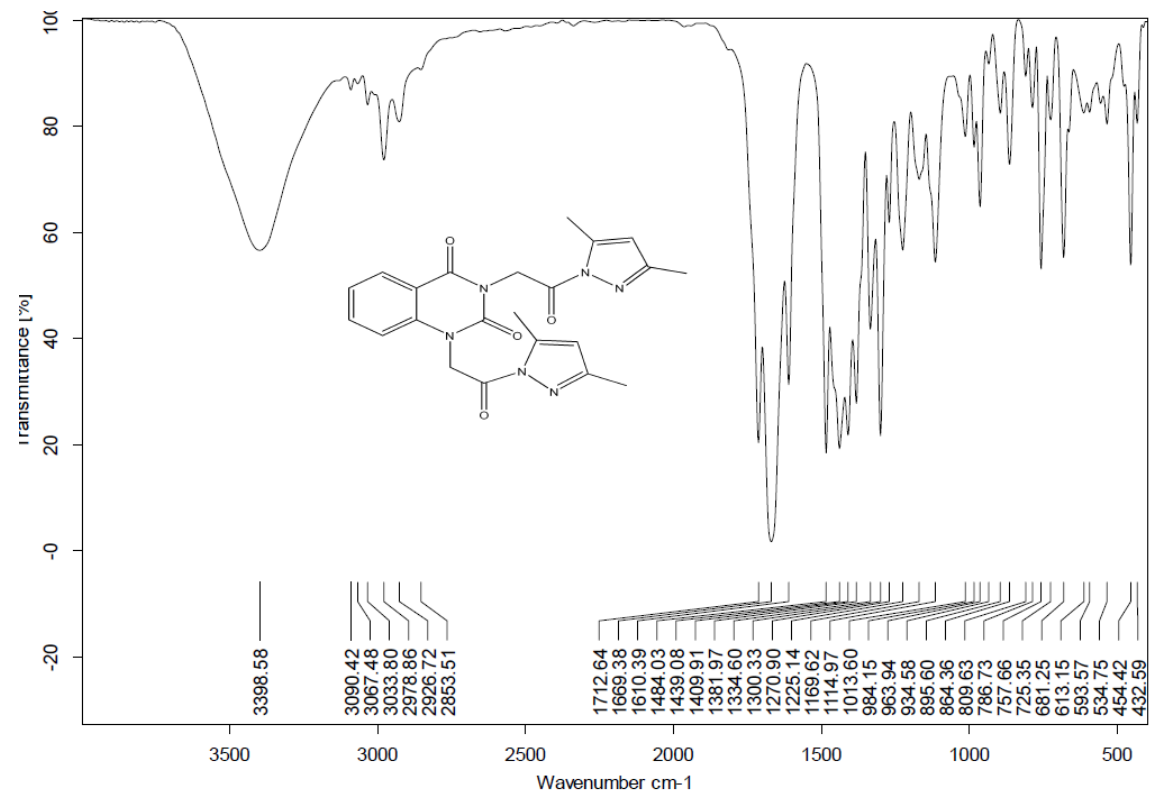


Current Data Parameters
NAME Mohamed Omar-M3-Hnmr-ov
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 2011206
Time 9.50 h
INSTRUM spect
PROBHD z108618_0945 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.56
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
MDC1 1H
F1 13.50 usec
PLAN1 13.00000000 H

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
SOLV DM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

$^1\text{H-NMR}$ (400 MHz, DMSO-d_6) of compound (7a)



FT-IR of compound (7a)

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Micro Analytical Center**

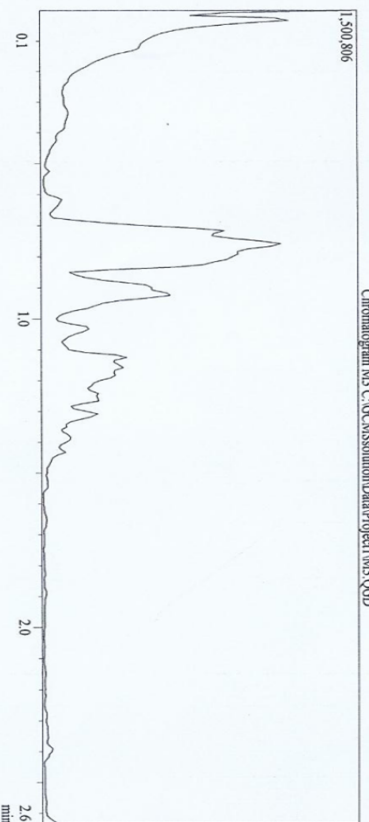
*DI Analysis
Shimadzu QP-2010 Plus*

Dr. Mai Younis
8/10/07

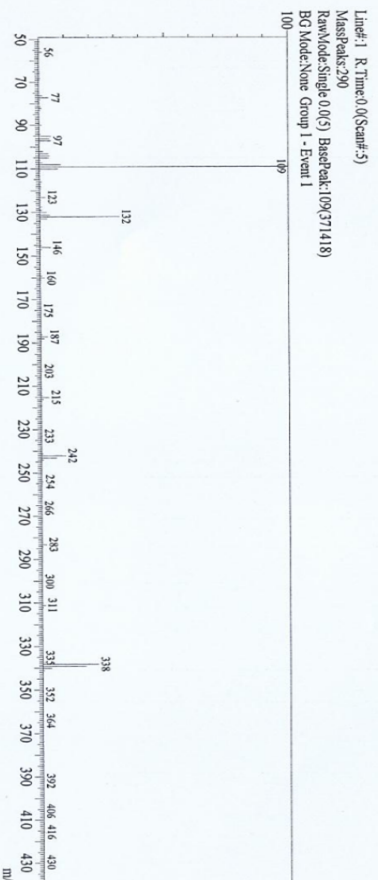
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 02:12:13
 Sample Name : M3
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Qena
 Data File : C:\GCMSolution\Data\Project\M3.QGD
 Org Data File : C:\GCMSolution\Data\Project\M3.QGD
 Method File : C:\GCMSolution\Data\Project\High Temperature Op
 Org Method File : C:\GCMSolution\Data\Project\High Temperature Op
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
 Standard/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:14:54

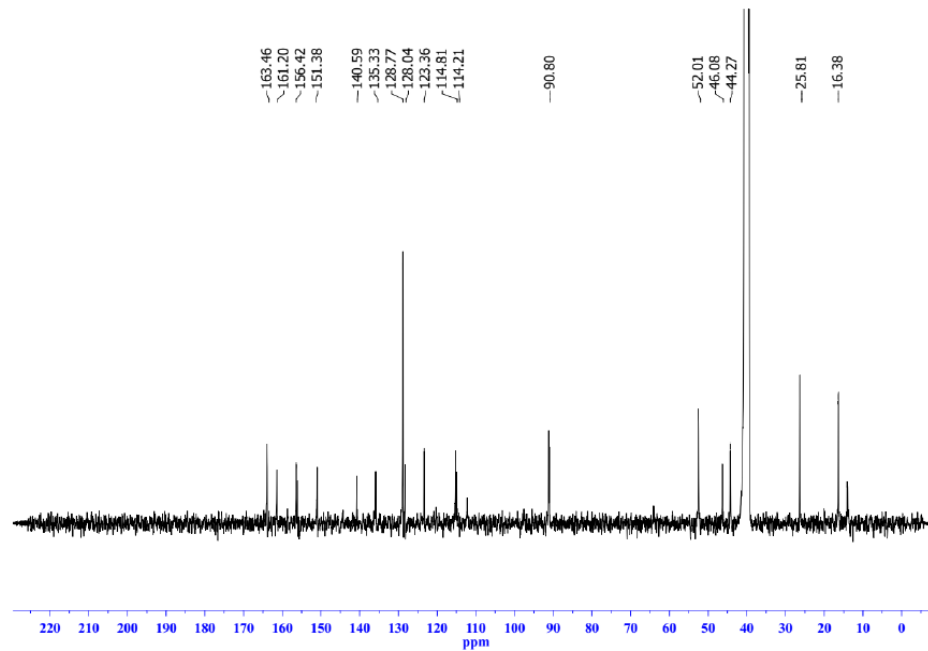
Method
 Analytical Line 1
 IonSource Temp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 Scan : Scan
 ACO Mode : -0.50sec
 Event Time : 12.50
 Scan Speed : 1250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project\M3.QGD



MS of compound (7a)





```

Current Data Parameters
NAME      Dec06-2022
EXPNO    100
PROCNO   1

F2 - Acquisition Parameters
Date_    20221206
Time     20.54
INSTRUM  spect
PROBHD   5 mm PABBO BBI/
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       2200
DS       4
SWH      24038.461 |
FIDRES   0.366798 |
AQ       1.3631488 |
RG       199.04
DW       20.800 |
DE       6.50 |
TE       308.1
D1       2.00000000 |
D11      0.03000000 |
TD0      1

----- CHANNEL f1 -----
SFO1     100.628364 |
NUC1     13C
P1       9.50 |
PLM1     56.0000000 |

----- CHANNEL f2 -----
SFO2     400.1374005 |
NUC2     1H
CPDPRG2  waltz16
PCPD2    90.00 |
PLM2     22.00000000 |
PLM12    0.41091001 |
PLM13    0.32840000 |

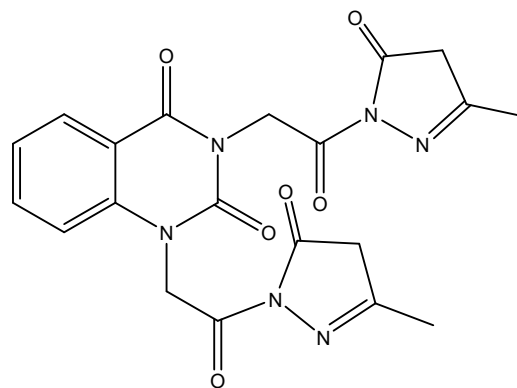
F2 - Processing parameters
SI       32768
SF       100.6127690 |
WDW      0
SSB      0
LB       6.00 |
GB       0
PC       1.40

```

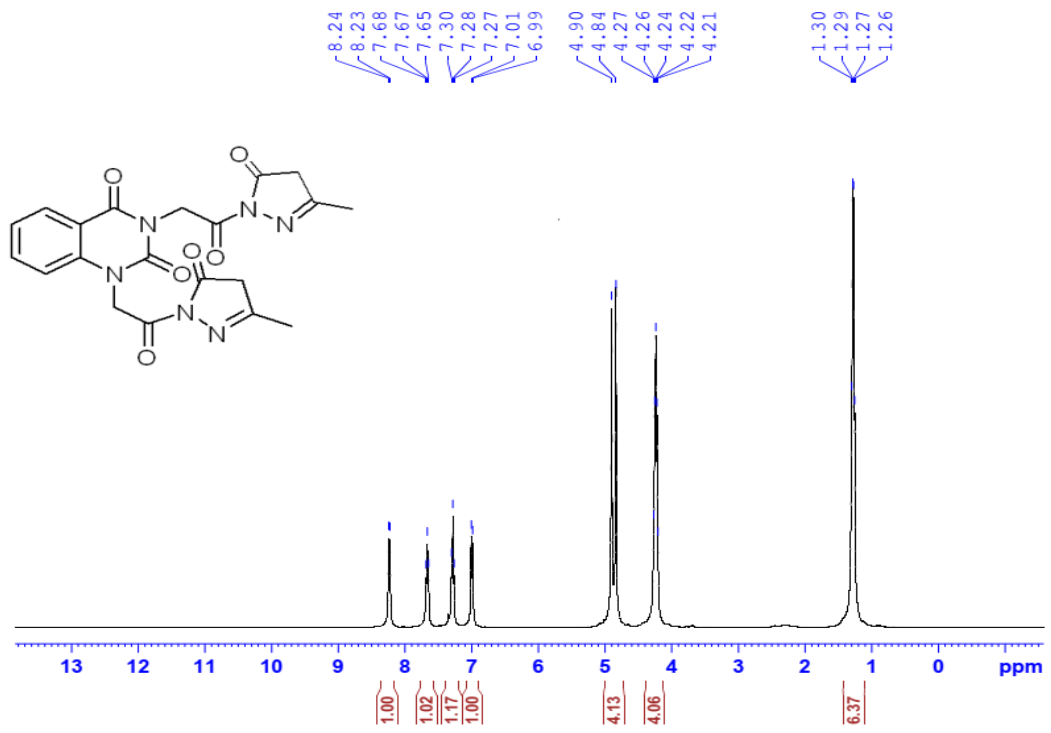
^{13}C -NMR (100 MHz, DMSO) of compound (7a)

-

Compound (7b)



7b

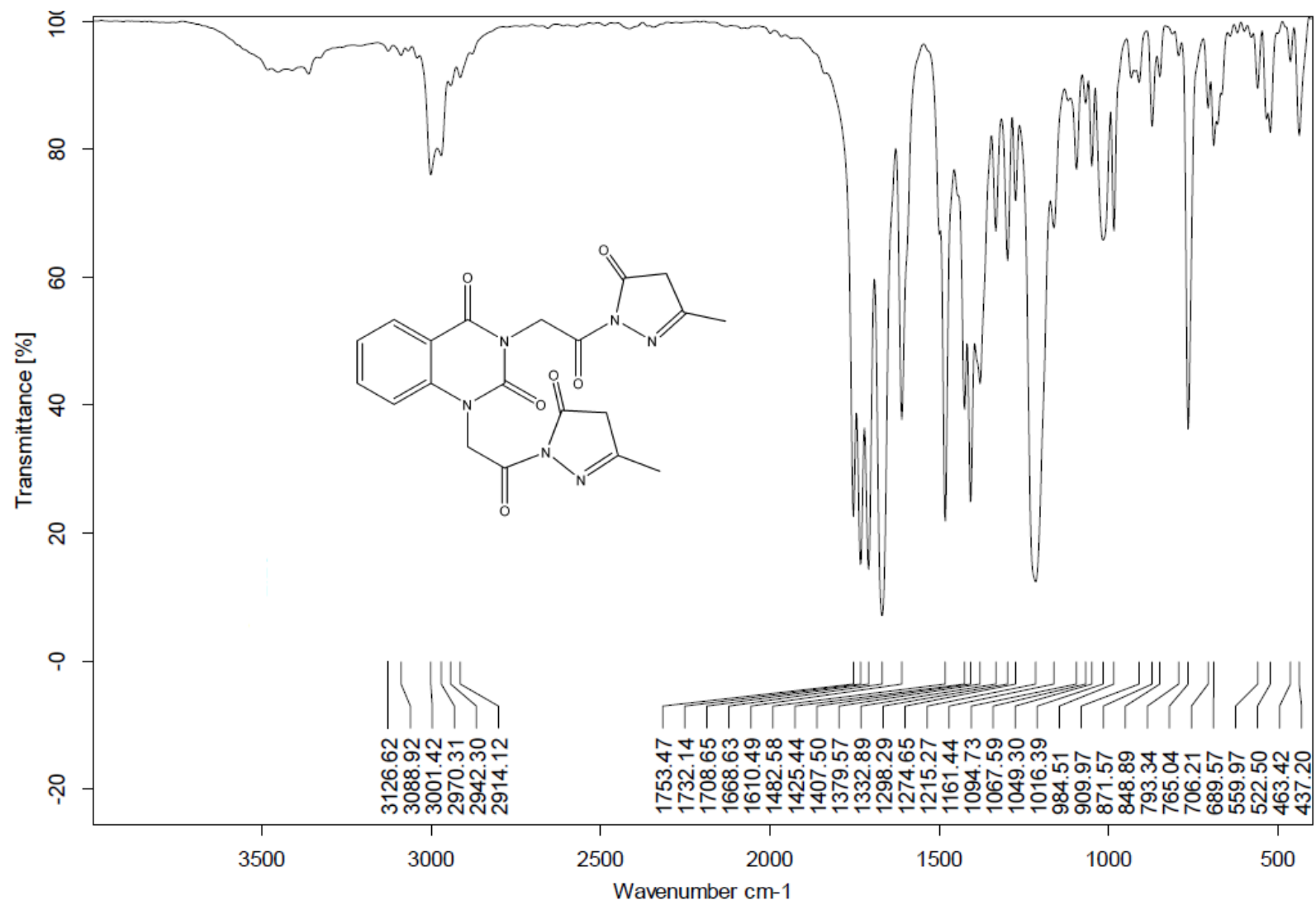


```

Current Data Parameters
NAME      Mohammed Omar-M9-DMSO-proton-D
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20111121
Time      11:42 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
SFO       400.1460000 MHz
AQ        4.0894665 sec
RG         60.97
SOLVENT   DMSO
NS         16
DS         4
SWH        8012.800 Hz
FIDRES     0.244822 Hz
AQRES      4.0894665 sec
RGRES      60.97
SFORES     400.1460000 MHz
NUC1       15N
NUC2       1H
P1         12.00 usec
PL1        0.00 dB
PL12       19.00 usec
PL12       13.00000000 MHz

F2 - Processing parameters
SI         65536
SF         400.1460000 MHz
WDW        EM
SSB        0
GB         0.30 Hz
WC         1.00
  
```



FT-IR of compound (7b)

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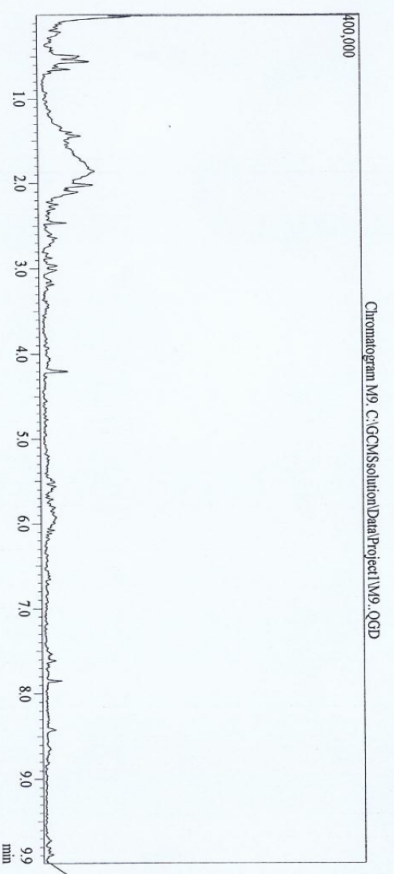
DI Analysis
Shimadzu QP-2010 Plus



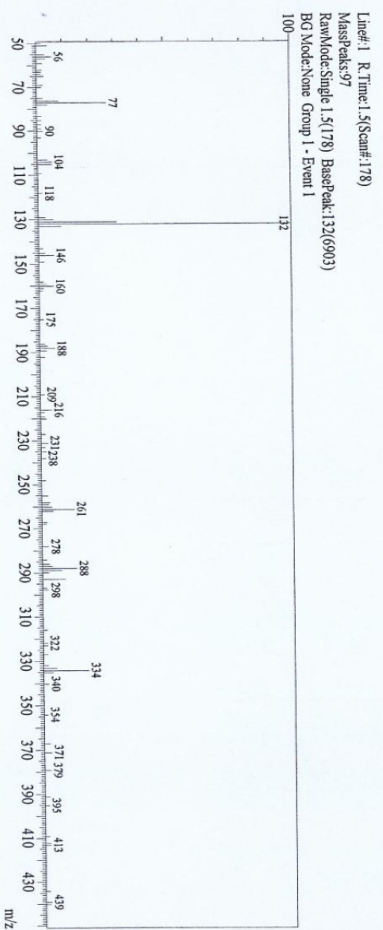
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 03:26:47 م
Sample Name : M9
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSolution\Data\Project1\M9_QGD
Org Data File : C:\GCMSolution\Data\Project1\M9_QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSolution\System1\tune1_default.qft
SENDITSM: Modified by : Dr. Mai Younis
Modified : 15/01/2007 03:36:46 م

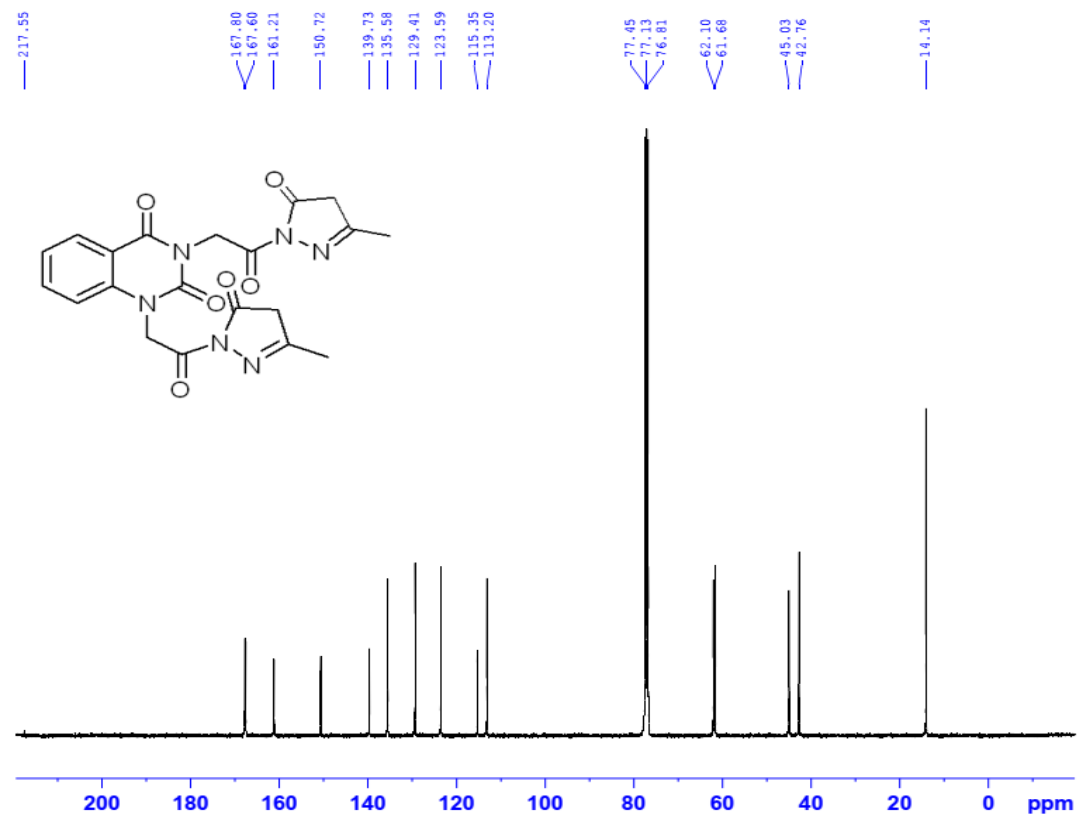
Method
Analytical Line 1
IonSource Temp : 250.00 °C
MS Table
--Group 1 - Event 1--
Start Time : 0:00min
End Time : 1:00:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 300.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project1\M9_QGD



MS of compound (7b)





Current Data Parameters
 NAME Mohamed Omar-M9-AS-carbon
 EXPNO 10
 PROCNO 1

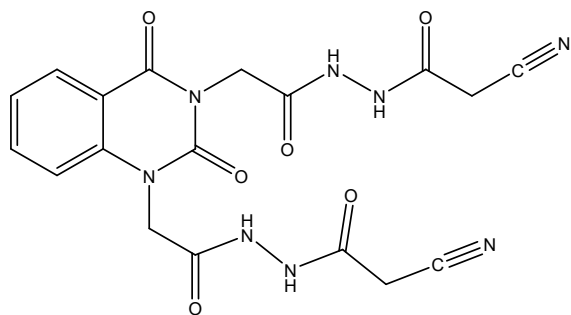
F2 - Acquisition Parameters
 Date 20211206
 Time 22.08 h
 INSTRUM spect
 PROBHD Z108618_0945 ()
 PULPROG zgpg30
 ID 65536
 SOLVENT CDCl3
 NS 2100
 DS 4
 SMH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 197.77
 DW 20.800 usec
 DE 6.50 usec
 TE 298.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1
 SFO1 100.6404331 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 47.00000000 W
 SFO2 400.2016008 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.29249999 W
 PLW13 0.14713000 W

F2 - Processing parameters
 SI 32768
 SF 100.6303700 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

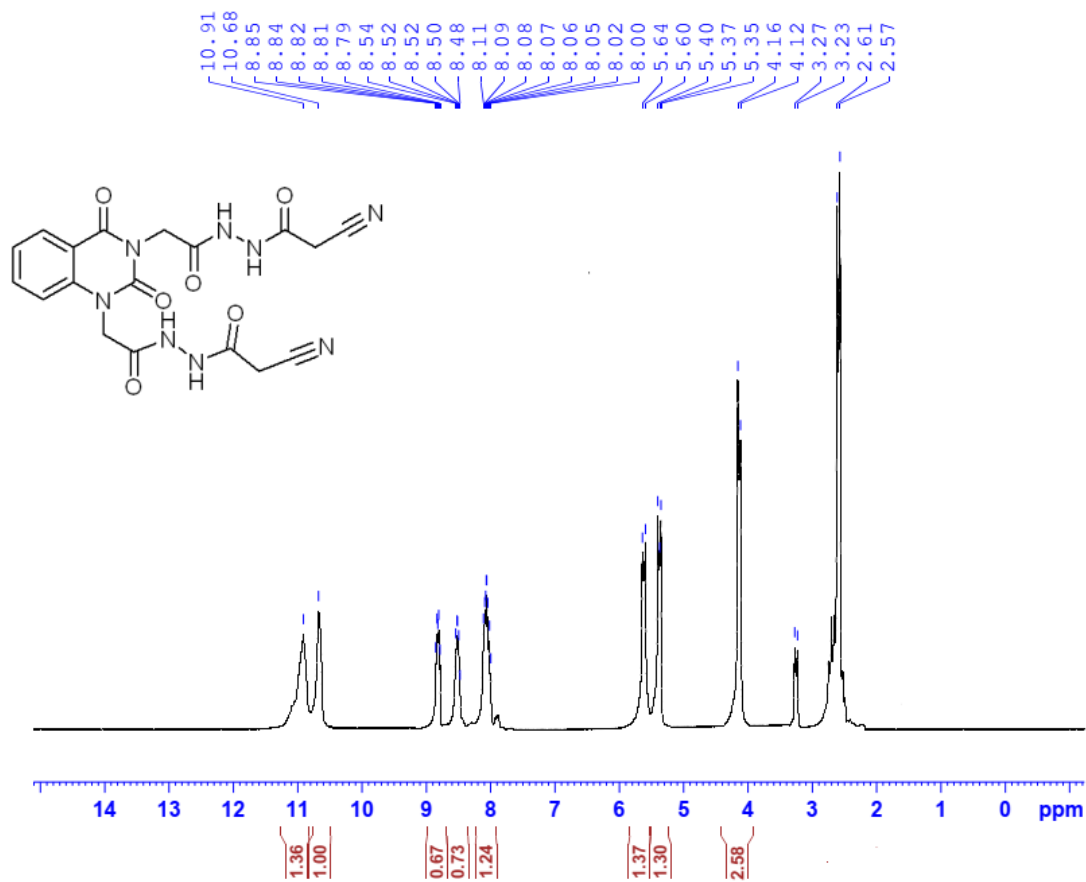
¹³C-NMR (100 MHz, CDCl₃) of compound (7b)

-

-Compound (8)



8

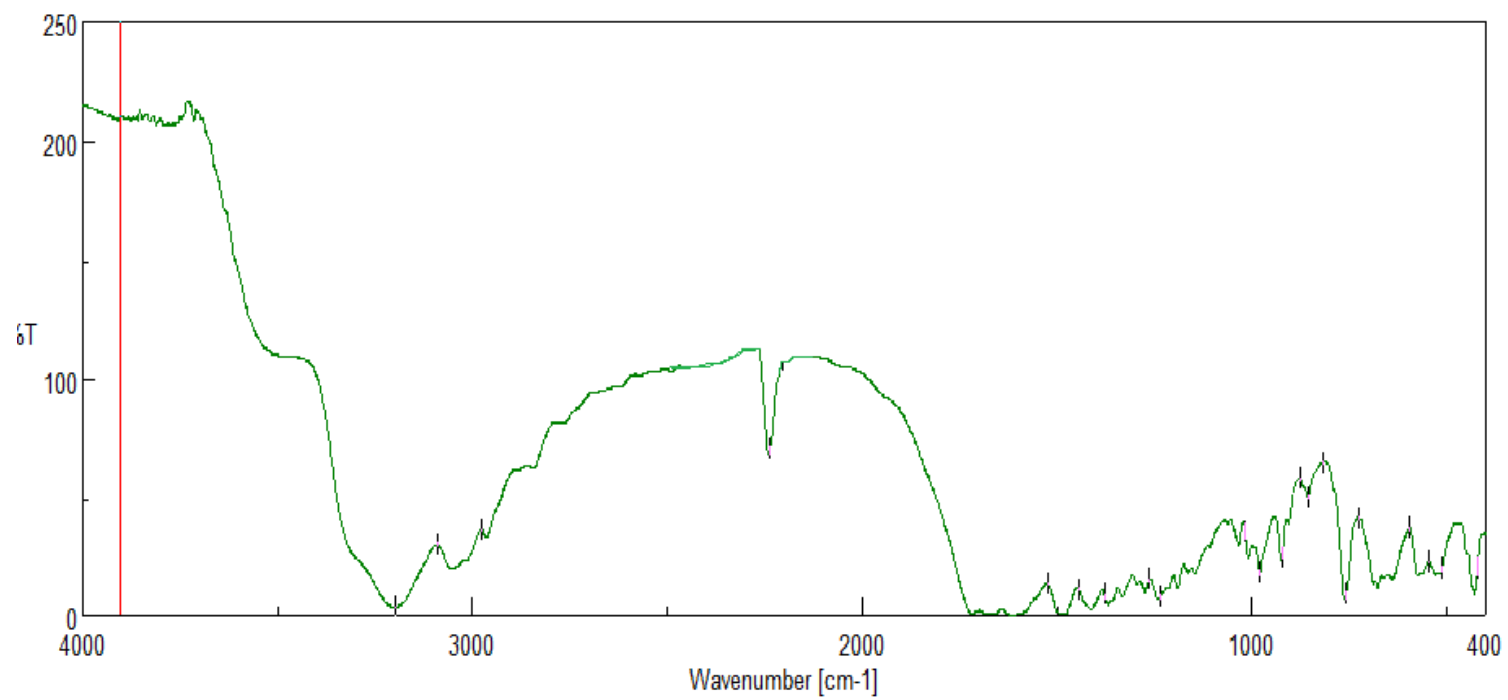


Current Data Parameters
 NAME Mohamed Omar-M 4-Hmr-ov
 EXPNO 10
 PROCNO 1

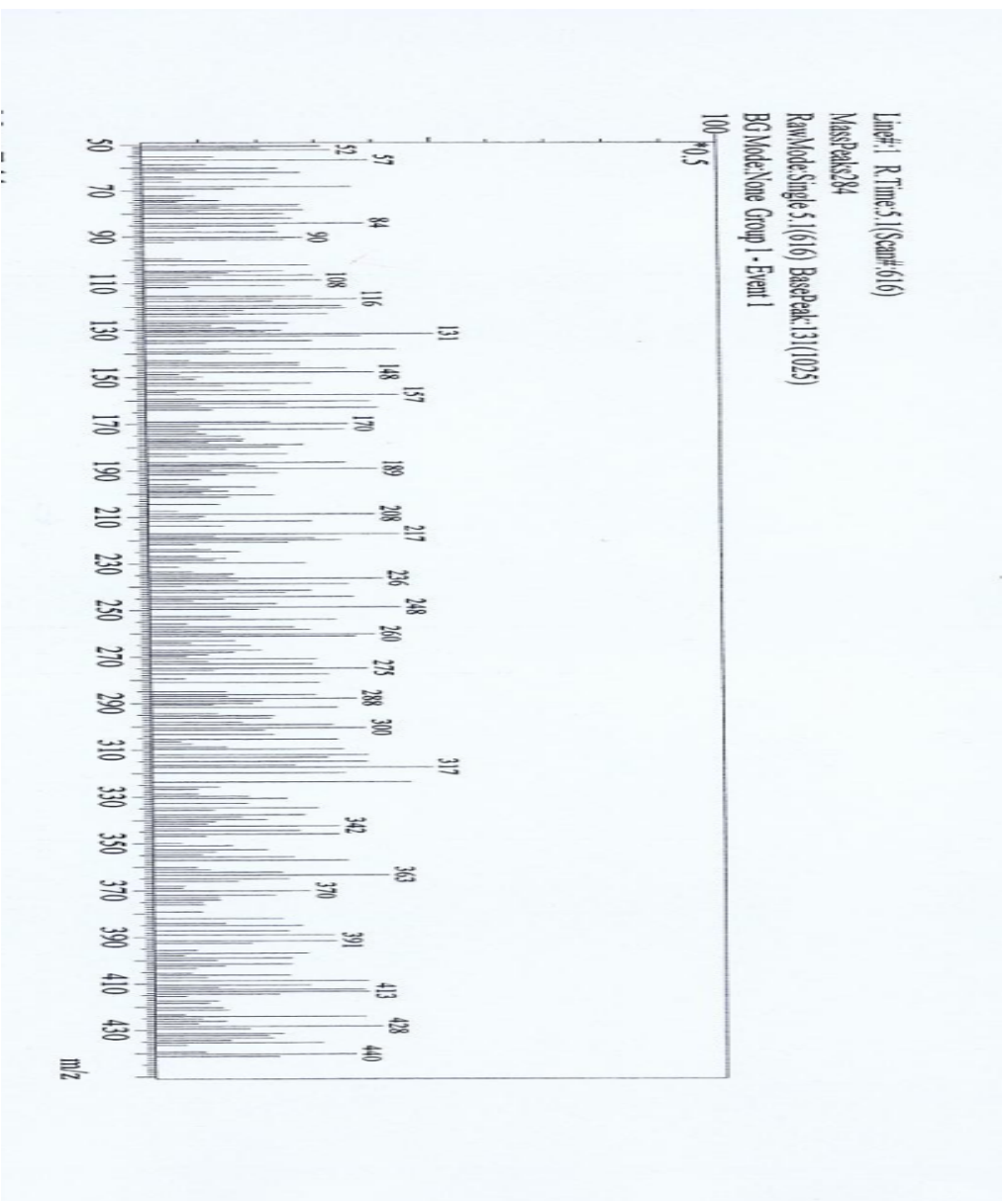
F2 - Acquisition Parameters
 Date_ 20211101
 Time 19.28 h
 INSTRUM spect
 PROBRD 2108618_0948 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO-d6
 NS 16
 DS -
 SFR 8012.800 Hz
 FIDRES 0.244502 Hz
 AQ 4.0894465 sec
 RG 80.00
 SH 62.400 usec
 DE 6.50 usec
 TE 292.9 K
 DL 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 12.50 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1996977 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (8)



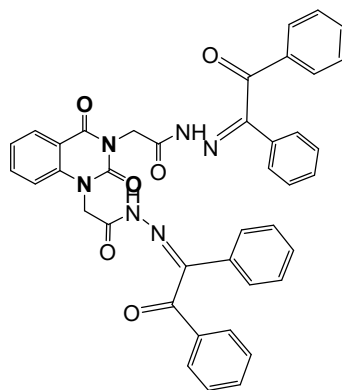
FT-IR of compound (8)



MS of compound (8)

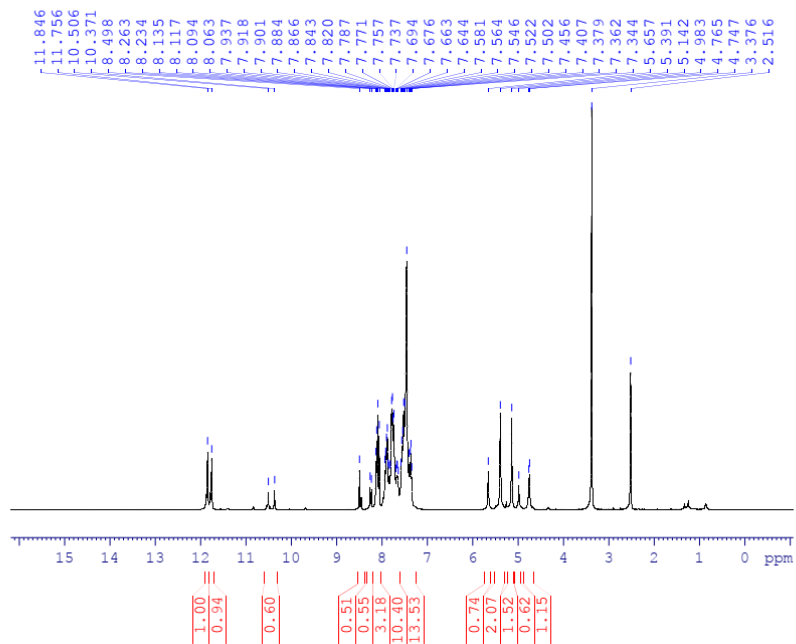
-

-Compound (9a):-



9a

Mohamed Omar - 13 Hnmr - T

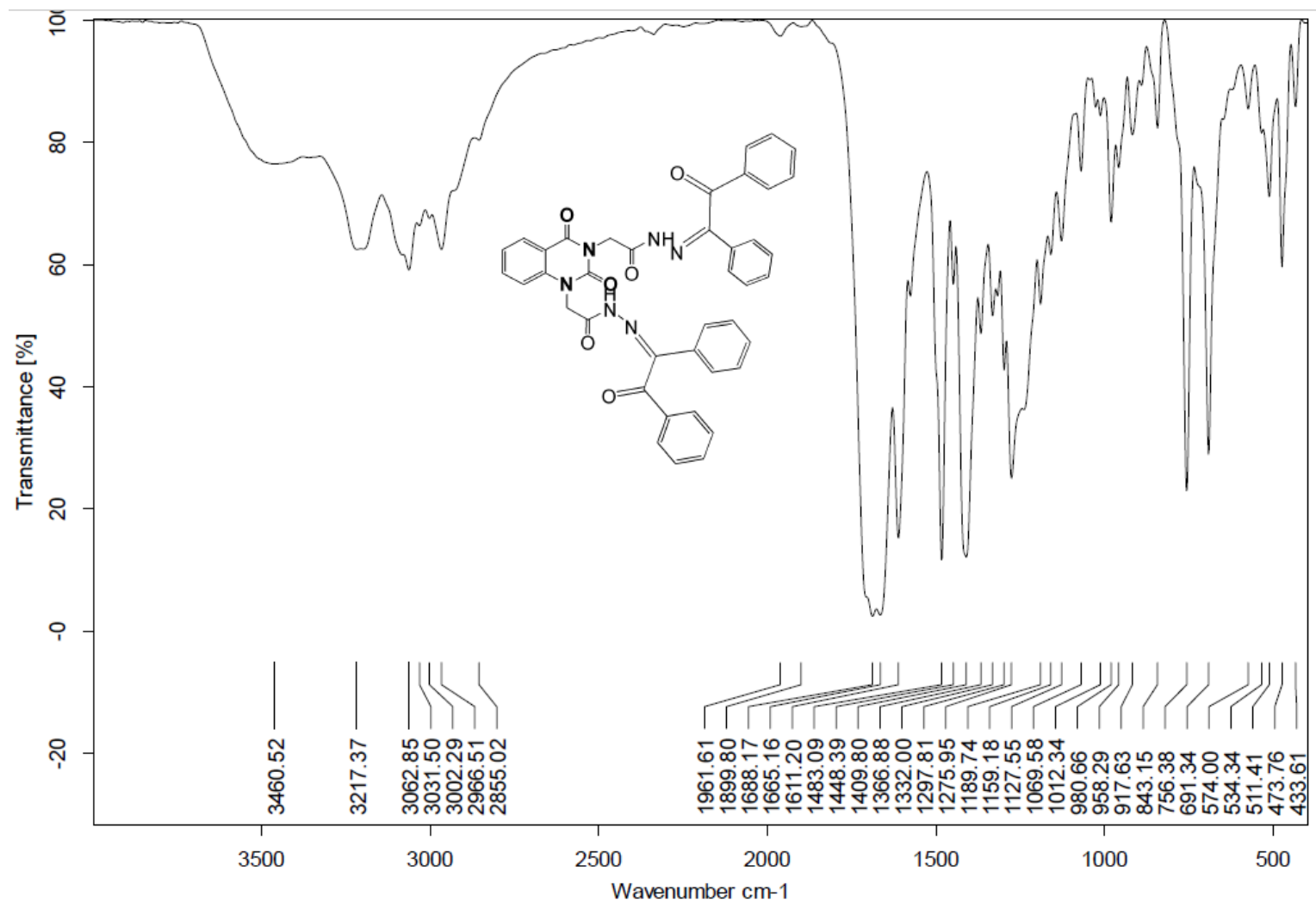


Current Data Parameters
NAME Mohamed Omar - 13 Hnmr - T
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220611
Time 18:07 h
INSTRUM spect
PROBHD zgpg30
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 8012.800 Hz
FIDRES 0.244892 Hz
AQ 4.0894669 sec
RG 512.56
DM 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P1 18.80 usec
PLW1 13.00000000 W

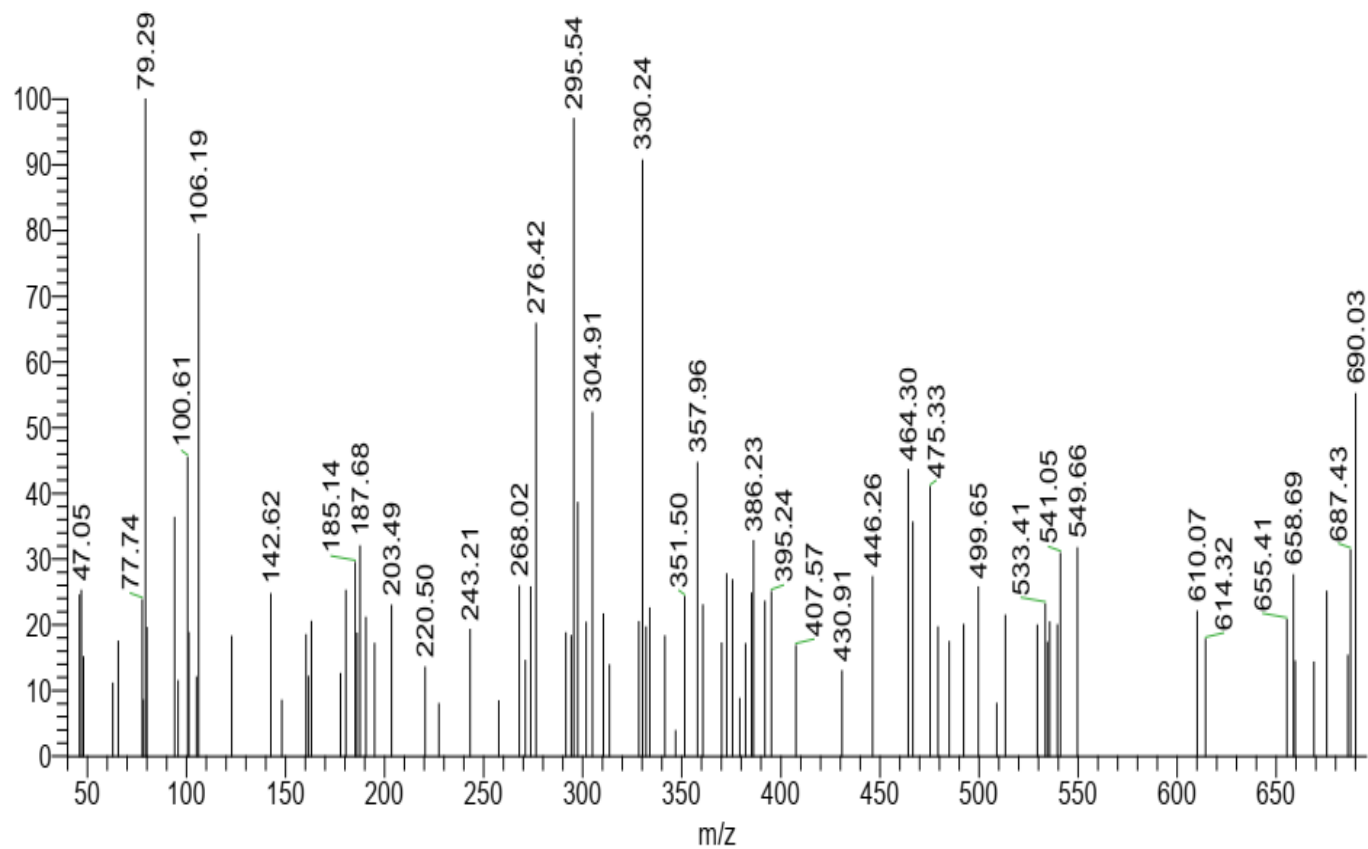
F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.80 Hz
GB 0
PC 1.00

¹H-NMR (400 MHz, DMSO-d₆) of compound (9a)



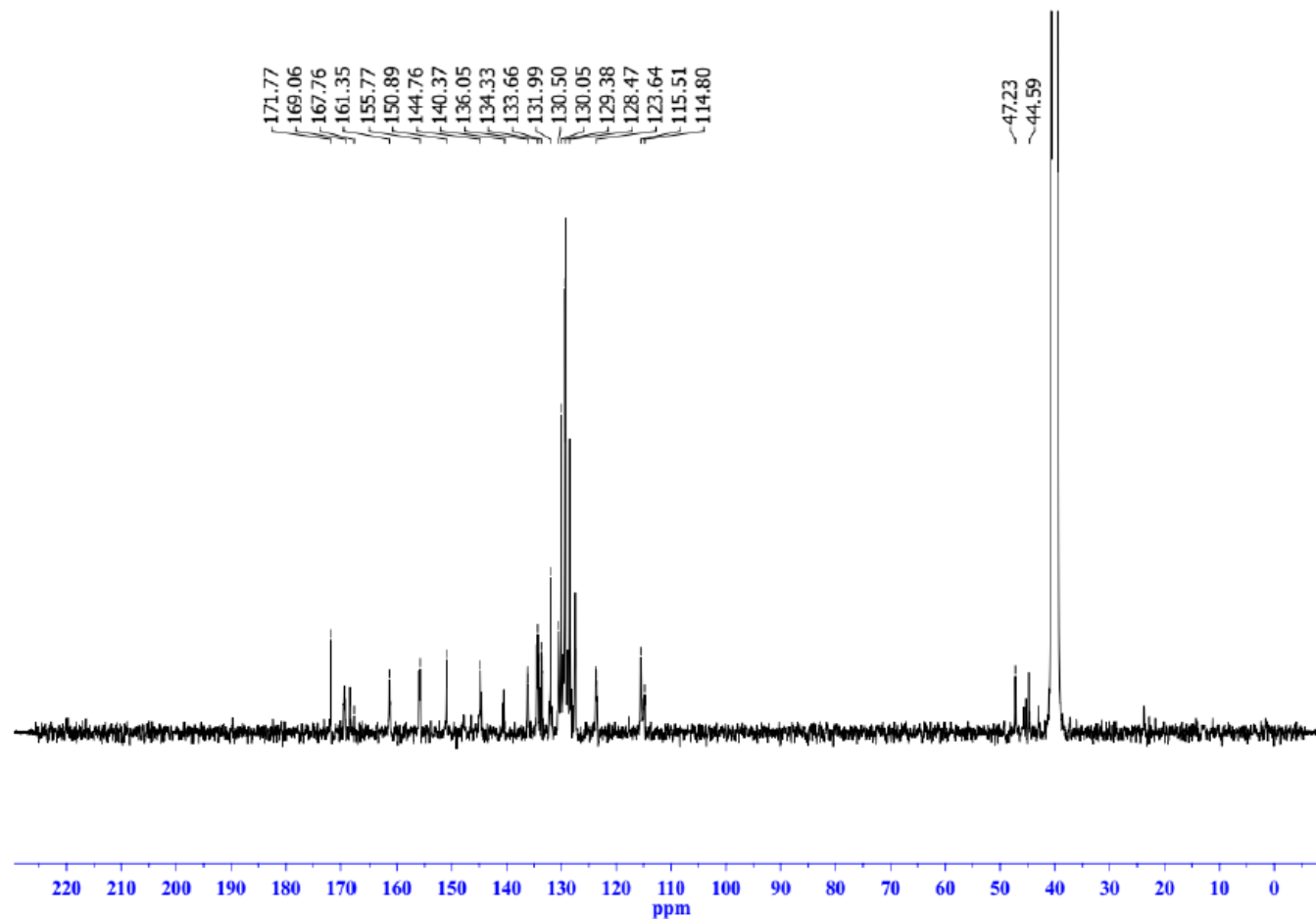
FT-IR of compound (9a)

mohamed-omar-21 #126 RT: 2.13 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 4.29E2
T: + c EI Full ms [40.00-1000.00]



m/z Intensity Relative

MS of compound (9a)



Current Data Parameters
 NAME Dec06-2022
 EXPNO 80
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20221206
 Time 16.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2200
 DS 4
 SWH 24038.461 MHz
 FIDRES 0.366798 MHz
 AQ 1.3631488 sec
 RG 199.04
 DW 20.800 usec
 DE 6.50 usec
 TE 308.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 100.6238364 MHz
 NUC1 13C
 P1 9.50 usec
 PLW1 56.00000000 usec

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 22.00000000 usec
 PLW12 0.41091001 usec
 PLW13 0.33284000 usec

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 6.00 MHz
 GB 0
 PC 1.40

¹³C-NMR (100 MHz, DMSO) of compound (9a)

Compounds Code, InChI, and SMILES

Compound code	InChI	SMILES
1	InChI=1S/C16H18N2O6/c1-3-23-13(19)9-17-12-8-6-5-7-11(12)15(21)18(16(17)22)10-14(20)24-4-2/h5-8H,3-4,9-10H2,1-2H3	<chem>O=C(C1=CC=CC=C1N2CC(OCC)=O)N(CC(OCC)=O)C2=O</chem>
2	InChI=1S/C12H14N6O4/c13-15-9(19)5-17-8-4-2-1-3-7(8)11(21)18(12(17)22)6-10(20)16-14/h1-4H,5-6,13-14H2,(H,15,19)(H,16,20)	<chem>O=C(N2CC(NN)=O)N(CC(NN)=O)C1=CC=CC=C1C2=O</chem>
3a	InChI=1S/C26H22N6O4/c33-23(29-27-15-19-9-3-1-4-10-19)17-31-22-14-8-7-13-21(22)25(35)32(26(31)36)18-24(34)30-28-16-20-11-5-2-6-12-20/h1-16H,17-18H2,(H,29,33)(H,30,34)/b27-15+,28-16+	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=CC=C4)=O)N(CC(N/N=C/C3=CC=CC=C3)=O)C2=O</chem>
3b	InChI=1S/C26H20Cl2N6O4/c27-19-9-5-17(6-10-19)13-29-31-23(35)15-33-22-4-2-1-3-21(22)25(37)34(26(33)38)16-24(36)32-30-14-18-7-11-20(28)12-8-18/h1-14H,15-16H2,(H,31,35)(H,32,36)/b29-13+,30-14+	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=C(Cl)C=C4)=O)N(CC(N/N=C/C3=CC=C(Cl)C=C3)=O)C2=O</chem>
3c	InChI=1S/C26H22N6O6/c33-19-9-5-17(6-10-19)13-27-29-23(35)15-31-22-4-2-1-3-21(22)25(37)32(26(31)38)16-24(36)30-28-14-18-7-11-20(34)12-8-18/h1-14,33-34H,15-16H2,(H,29,35)(H,30,36)/b27-13+,28-14+	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=C(O)C=C4)=O)N(CC(N/N=C/C3=C=C(O)C=C3)=O)C2=O</chem>
3d	InChI=1S/C26H20N8O8/c35-23(29-27-13-17-5-9-19(10-6-17)33(39)40)15-31-22-4-2-1-3-21(22)25(37)32(26(31)38)16-24(36)30-28-14-18-7-11-20(12-8-18)34(41)42/h1-14H,15-16H2,(H,29,35)(H,30,36)/b27-13+,28-14+	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=C([N+])([O-])=O)C=C4)=O)N(CC(N/N=C/C3=CC=C([N+])([O-])=O)C=C3)=O)C2=O</chem>
3e	InChI=1S/C22H18N6O6/c29-19(25-23-11-15-5-3-9-33-15)13-27-18-8-2-1-7-17(18)21(31)28(22(27)32)14-20(30)26-24-12-16-6-4-10-34-16/h1-12H,13-14H2,(H,25,29)(H,26,30)/b23-11+,24-12+	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=CO4)=O)N(CC(N/N=C/C3=CC=CO3)=O)C2=O</chem>
4a	InChI=1S/C22H26N6O4/c29-19(25-23-15-7-1-2-8-15)13-27-18-12-6-5-11-17(18)21(31)28(22(27)32)14-20(30)26-24-16-9-3-4-10-16/h5-6,11-12H,1-4,7-10,13-14H2,(H,25,29)(H,26,30)	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C4/CCCC4)=O)N(CC(N/N=C3/CCCC3)=O)C2=O</chem>
4b	InChI=1S/C24H30N6O4/c31-21(27-25-17-9-3-1-4-10-17)15-29-20-14-8-7-13-19(20)23(33)30(24(29)34)16-22(32)28-26-18-11-5-2-6-12-18/h7-8,13-14H,1-6,9-12,15-16H2,(H,27,31)(H,28,32)	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C4/CCCCC4)=O)N(CC(N/N=C3/CCCCC3)=O)C2=O</chem>
4c	InChI=1S/C28H26N6O4/c1-19(21-11-5-3-6-12-21)29-31-25(35)17-33-24-	<chem>O=C(C1=CC=CC=C1N2CC(N/N=C(C)/C4=CC=CC=C4)=O)N(CC(N/N=C(C)/C3</chem>

	16-10-9-15-23(24)27(37)34(28(33)38)18-26(36)32-30-20(2)22-13-7-4-8-14-22/h3-16H,17-18H2,1-2H3,(H,31,35)(H,32,36)/b29-19+,30-20+	=CC=CC=C3)=O)C2=O
4d	InChI=1S/C30H30N6O4/c1-19-9-13-23(14-10-19)21(3)31-33-27(37)17-35-26-8-6-5-7-25(26)29(39)36(30(35)40)18-28(38)34-32-22(4)24-15-11-20(2)12-16-24/h5-16H,17-18H2,1-4H3,(H,33,37)(H,34,38)/b31-21+,32-22+	O=C(C1=CC=CC=C1N2CC(N/N=C(C)/C4=CC=C(C)C=C4)=O)N(CC(N/N=C(C)/C3=CC=C(C)C=C3)=O)C2=O
4e	InChI=1S/C24H22N6O4S2/c1-15(19-9-5-11-35-19)25-27-21(31)13-29-18-8-4-3-7-17(18)23(33)30(24(29)34)14-22(32)28-26-16(2)20-10-6-12-36-20/h3-12H,13-14H2,1-2H3,(H,27,31)(H,28,32)/b25-15+,26-16+	O=C(C1=CC=CC=C1N2CC(N/N=C(C)/C4=CC=CS4)=O)N(CC(N/N=C(C)/C3=C(C=CS3)=O)C2=O
4f	InChI=1S/C28H20N8O6/c37-21(31-33-23-15-7-1-4-10-18(15)29-25(23)39)13-35-20-12-6-3-9-17(20)27(41)36(28(35)42)14-22(38)32-34-24-16-8-2-5-11-19(16)30-26(24)40/h1-12H,13-14H2,(H,31,37)(H,32,38)(H,29,33,39)(H,30,34,40)	O=C(C1=CC=CC=C1N2CC(N/N=C4/C(C=CC=C5)=C5NC4=O)=O)N(CC(N/N=C3/C(C=CC=C6)=C6NC3=O)=O)C2=O
5a	InChI=1S/C28H18N6O8/c35-21(29-33-24(38)15-7-1-2-8-16(15)25(33)39)13-31-20-12-6-5-11-19(20)23(37)32(28(31)42)14-22(36)30-34-26(40)17-9-3-4-10-18(17)27(34)41/h1-12H,13-14H2,(H,29,35)(H,30,36)	O=C(C1=CC=CC=C1N2CC(NN4C(C3=CC=CC=C3C4=O)=O)=O)N(CC(NN6C(C5=CC=CC=C5C6=O)=O)=O)C2=O
5b	InChI=1S/C48H34N6O8/c55-33(49-53-44(58)39-35-23-11-1-2-12-24(23)36(40(39)45(53)59)26-14-4-3-13-25(26)35)21-51-32-20-10-9-19-31(32)43(57)52(48(51)62)22-34(56)50-54-46(60)41-37-27-15-5-6-16-28(27)38(42(41)47(54)61)30-18-8-7-17-29(30)37/h1-20,35-42H,21-22H2,(H,49,55)(H,50,56)	O=C(C1=CC=CC=C1N2CC(NN3C(C(C7C5=CC=CC=C5C6C8=C7C=CC=C8)C6C3=O)=O)=O)N(CC(NN4C(C(C%11C9=CC=CC=C9C%10C%12=C%11C=CC=C%12)C%10C4=O)=O)=O)C2=O
5c	InChI=1S/C28H26N6O8/c35-21(29-33-24(38)15-7-1-2-8-16(15)25(33)39)13-31-20-12-6-5-11-19(20)23(37)32(28(31)42)14-22(36)30-34-26(40)17-9-3-4-10-18(17)27(34)41/h1-6,11-12,15-18H,7-10,13-14H2,(H,29,35)(H,30,36)	O=C(C1=CC=CC=C1N2CC(NN3C(C(CC=CC6)C6C3=O)=O)=O)N(CC(NN4C(C(CC=CC5)C5C4=O)=O)=O)C2=O
6a	InChI=1S/C16H18N6O6/c1-9(23)17-19-13(25)7-21-12-6-4-3-5-11(12)15(27)22(16(21)28)8-14(26)20-18-10(2)24/h3-6H,7-8H2,1-2H3,(H,17,23)(H,18,24)(H,19,25)(H,20,26)	O=C(C1=CC=CC=C1N2CC(NNC(C)=O)=O)N(CC(NNC(C)=O)=O)C2=O
6b	InChI=1S/C16H16Cl2N6O6/c17-5-11(25)19-21-13(27)7-23-10-4-2-1-3-9(10)15(29)24(16(23)30)8-14(28)22-20-12(26)6-18/h1-4H,5-8H2,(H,19,25)(H,20,26)(H,21,27)(H,22,28)	O=C(C1=CC=CC=C1N2CC(NNC(CCl)=O)=O)N(CC(NNC(CCl)=O)=O)C2=O
6c	InChI=1S/C26H22N6O6/c33-21(27-29-23(35)17-9-3-1-4-10-17)15-31-20-14-8-7-13-19(20)25(37)32(26(31)38)16-22(34)28-30-24(36)18-11-5-2-6-12-18/h1-14H,15-16H2,(H,27,33)(H,28,34)(H,29,35)(H,30,36)	O=C(C1=CC=CC=C1N2CC(NNC(C3=CC=CC=C3)=O)=O)N(CC(NNC(C4=CC=CC=C4)=O)=O)C2=O
6d	InChI=1S/C22H18N6O6S2/c29-17(23-25-19(31)15-7-3-9-35-15)11-27-14-	O=C(C1=CC=CC=C1N2CC(NNC(C3=CC=CS3)=O)=O)N(CC(NNC(C4=CC=CS

	6-2-1-5-13(14)21(33)28(22(27)34)12-18(30)24-26-20(32)16-8-4-10-36-16/h1-10H,11-12H2,(H,23,29)(H,24,30)(H,25,31)(H,26,32)	4)=O)=O)C2=O
7a	InChI=1S/C22H22N6O4/c1-13-9-15(3)27(23-13)19(29)11-25-18-8-6-5-7-17(18)21(31)26(22(25)32)12-20(30)28-16(4)10-14(2)24-28/h5-10H,11-12H2,1-4H3	O=C(C1=CC=CC=C1N2CC(N4N=C(C)C=C4C)=O)N(CC(N3N=C(C)C=C3C)=O)C2=O
7b	InChI=1S/C20H18N6O6/c1-11-7-15(27)25(21-11)17(29)9-23-14-6-4-3-5-13(14)19(31)24(20(23)32)10-18(30)26-16(28)8-12(2)22-26/h3-6H,7-10H2,1-2H3	O=C(C1=CC=CC=C1N2CC(N4N=C(C)CC4=O)=O)N(CC(N3N=C(C)CC3=O)=O)C2=O
8	InChI=1S/C18H16N8O6/c19-7-5-13(27)21-23-15(29)9-25-12-4-2-1-3-11(12)17(31)26(18(25)32)10-16(30)24-22-14(28)6-8-20/h1-4H,5-6,9-10H2,(H,21,27)(H,22,28)(H,23,29)(H,24,30)	O=C(C1=CC=CC=C1N2CC(NNC(CC#N)=O)=O)N(CC(NNC(CC#N)=O)=O)C2=O
9a	InChI=1S/C40H30N6O6.CH4/c47-33(41-43-35(27-15-5-1-6-16-27)37(49)29-19-9-3-10-20-29)25-45-32-24-14-13-23-31(32)39(51)46(40(45)52)26-34(48)42-44-36(28-17-7-2-8-18-28)38(50)30-21-11-4-12-22-30;/h1-24H,25-26H2,(H,41,47)(H,42,48);1H4/b43-35-,44-36-;	O=C(N2CC(N/N=C(C(C5=CC=CC=C5)=O)/C3=CC=CC=C3)=O)N(CC(NN=C(C(C6=CC=CC=C6)=O)C4=CC=CC=C4)=O)C1=CC=CC=C1C2=O

The solubility of compounds in water, acidic and/or basic medium

Solubility Sample	Cold water	Hot water	Acidic medium	Basic medium
1	+ve	+ve	+ve	+ve
2	+ve	+ve	+ve	+ve
3a	-ve	-ve	-ve	-ve
3b	-ve	-ve	-ve	-ve
3c	-ve	-ve	-ve	-ve
3d	-ve	-ve	-ve	-ve
3e	-ve	-ve	-ve	-ve
4a	-ve	-ve	-ve	-ve
4b	-ve	-ve	-ve	-ve
4c	-ve	-ve	-ve	-ve
4d	-ve	-ve	-ve	-ve
4e	-ve	-ve	-ve	-ve
4f	-ve	-ve	-ve	-ve
5a	-ve	-ve	-ve	+ve
5b	-ve	-ve	-ve	-ve
5c	-ve	-ve	-ve	-ve
6a	-ve	-ve	-ve	-ve

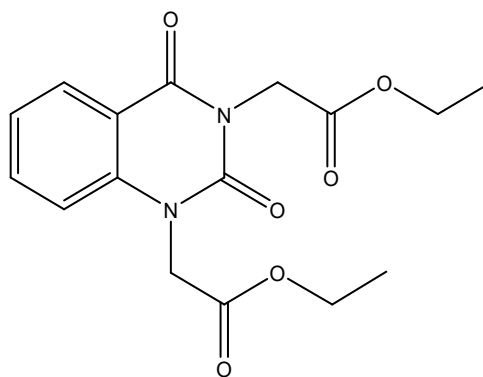
-

6b	-ve	-ve	-ve	-ve
6c	-ve	-ve	-ve	-ve
6d	-ve	-ve	-ve	-ve
7a	-ve	-ve	-ve	-ve
7b	-ve	-ve	-ve	-ve
8	-ve	-ve	-ve	-ve
9a	-ve	-ve	-ve	-ve

-

Supplementary data file

-Compound (1):



1

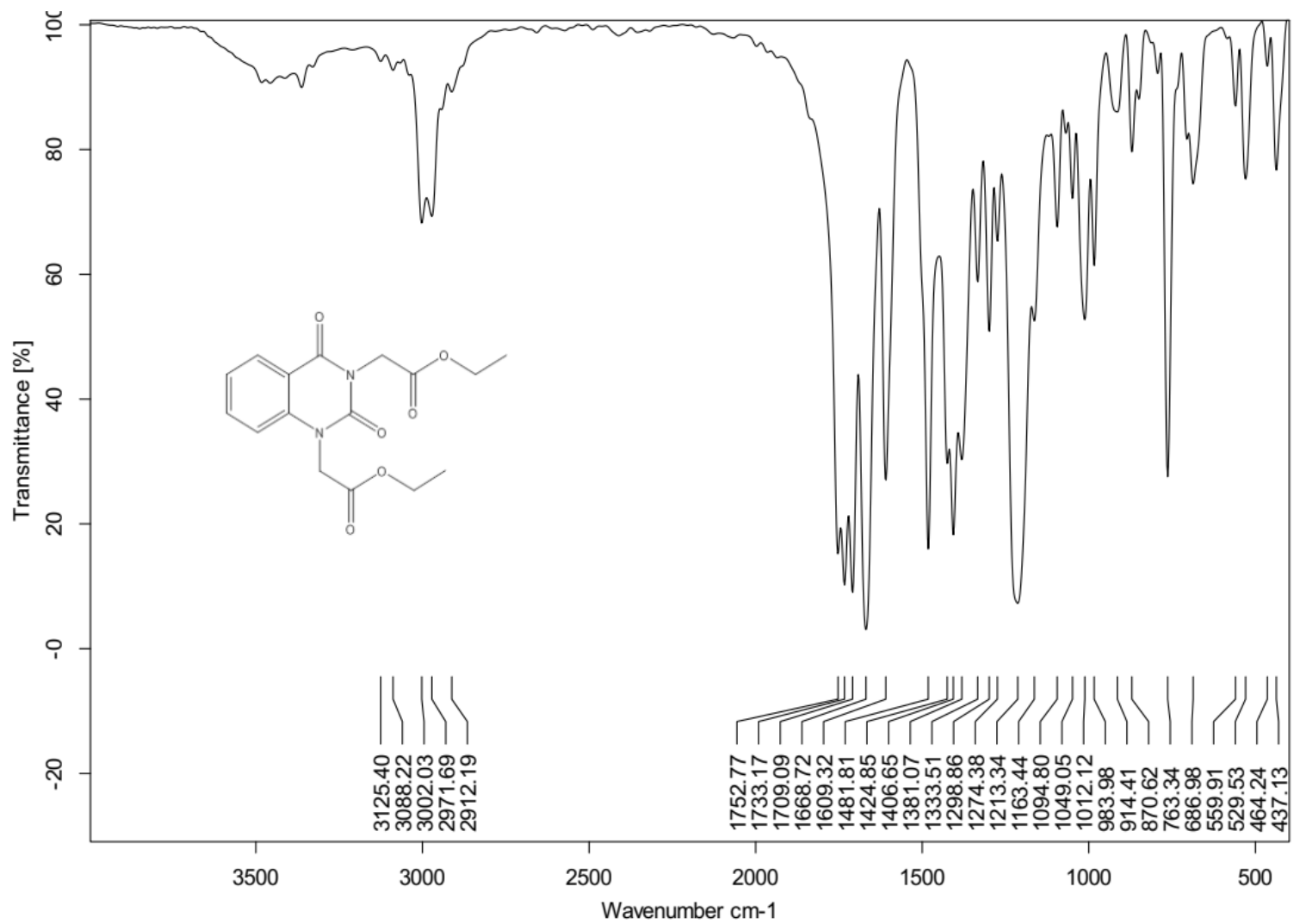


Figure . ¹H-NMR of compound 1 .

-

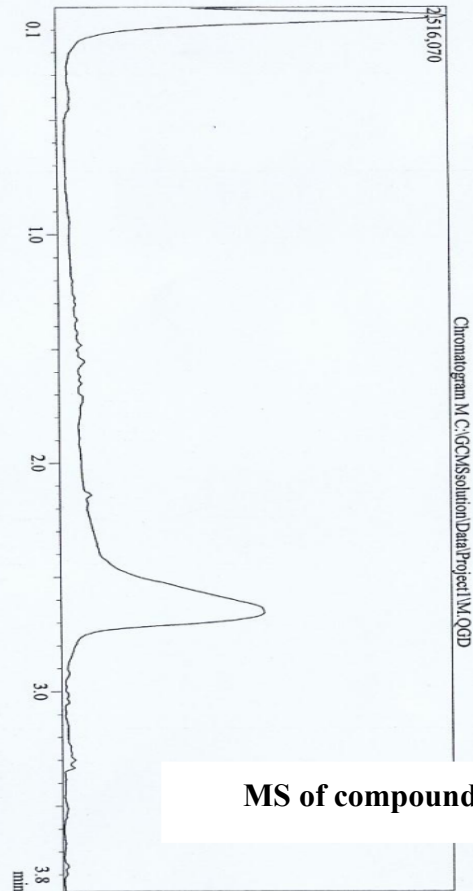
**Cairo University
Micro Analytical Center**

**DI Analysis
Shimadzu Qp-2010 Plus**

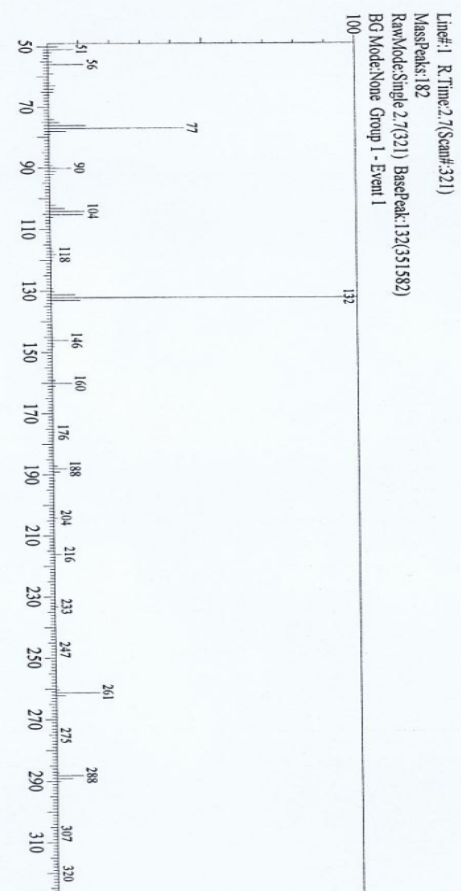
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 01:53:50
 Sample Name : M
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project\1M.QGD
 Org Data File : C:\GCMSsolution\Data\Project\1M.QGD
 Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\SystemTime\default.qgr
 Serial/IS Modified by : Dr. Mai Younis
 Modified : 15/01/2007 01:57:45

Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 -Group 1 - Event 1-
 Start Time : 0:00min
 End Time : 1:00min
 ACQ Mode : Scan
 Event Time : 0:50sec
 Scan Speed : 1:250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project\1M.QGD

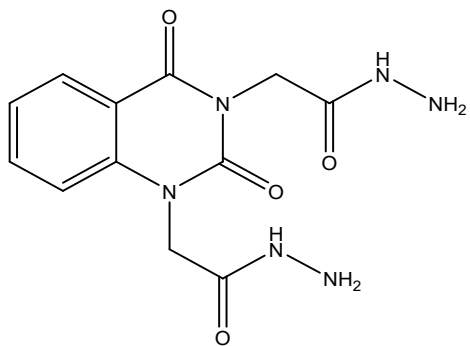


MS of compound (1)



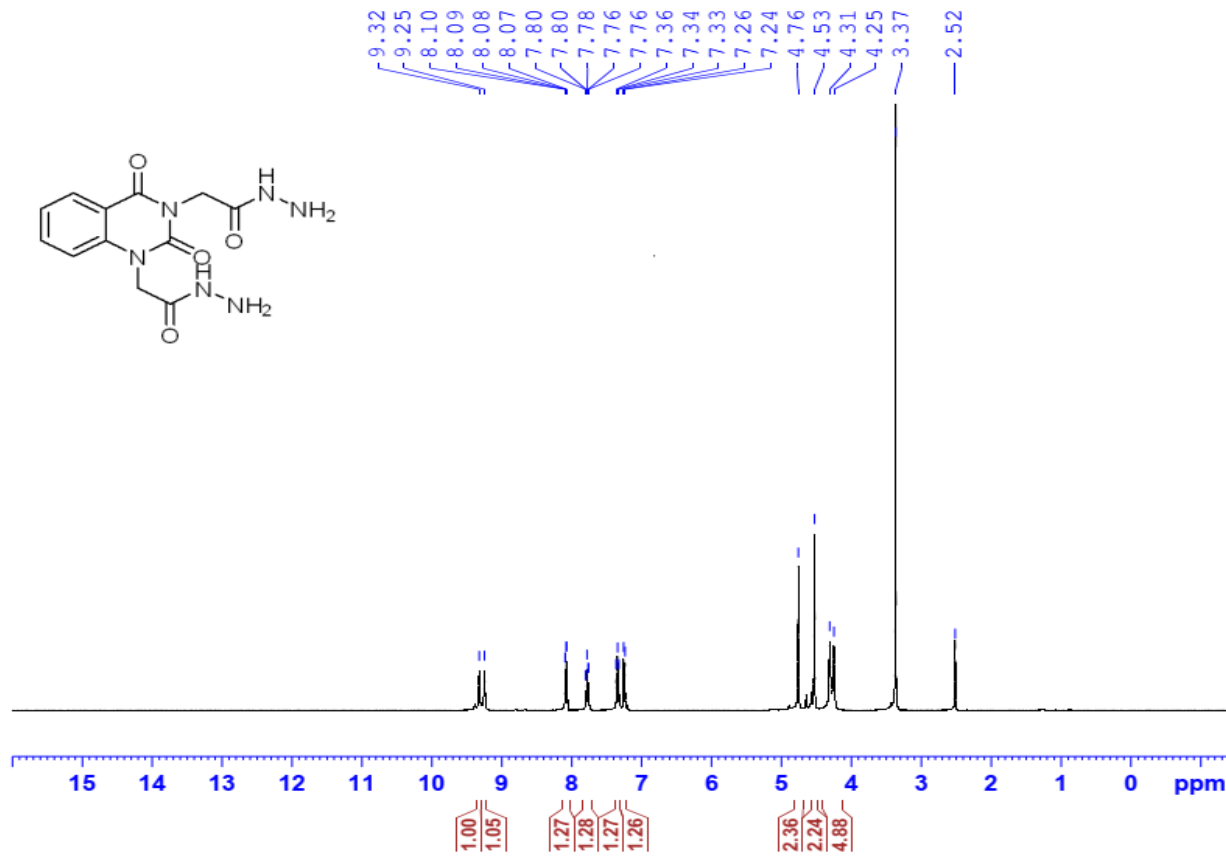
-

-Compound (2):



2

2



```

Current Data Parameters
NAME      mohamed omer-M1-Hnmr-om
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    2011018
Time     18.08 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244533 Hz
AQ        4.089465 sec
RG        176.72
DN        62.400 usec
DE        6.50 usec
TE        302.8 K
D1        1.0000000 sec
TDO       1
SFO1      400.2024711 MHz
NUC1      1H
P1        13.50 usec
PLN1      13.00000000 W

F2 - Processing parameters
SI        65536
SF        400.2000000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

¹H-NMR of compound (2)

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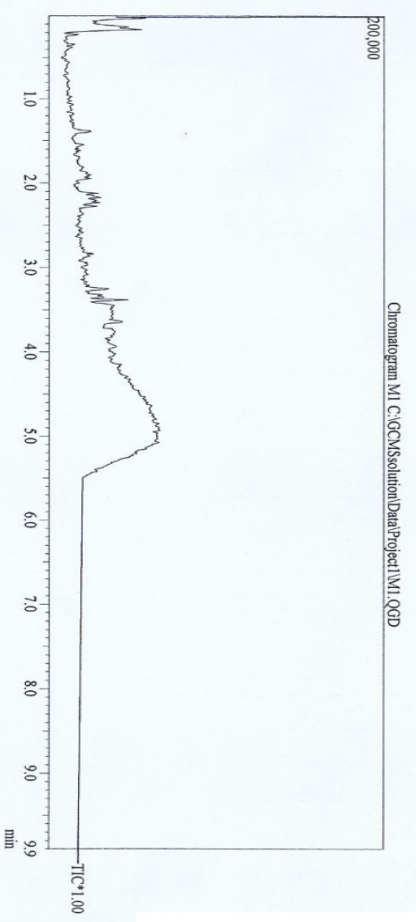
DI Analysis
Shimadzu Qp-2010 Plus

Handwritten signature and date: 1/15/07

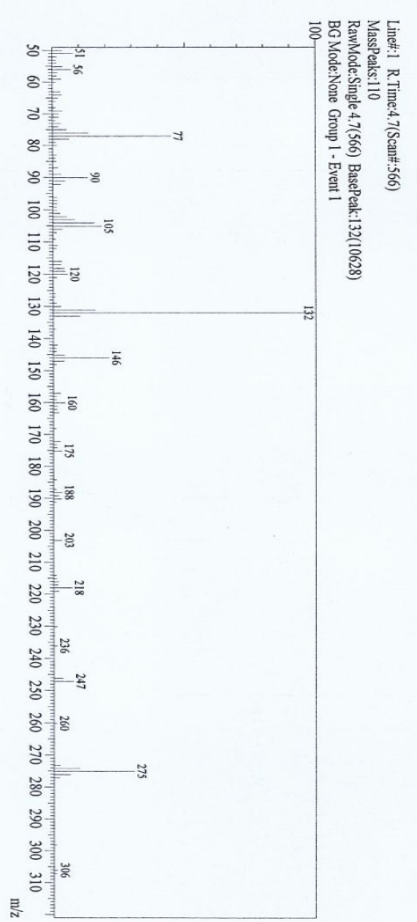
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 01:59:25
 Sample Name : M1
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quesa
 Data File : C:\GCMSsolution\Data\Project1\M1.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\M1.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System1\default.qgt
 Start/Stop/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:04:57

Method
 Analytical Line 1 :
 IonSourceTemp : 250.00 °C
 Ions Table :
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACO Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project1\M1.QGD

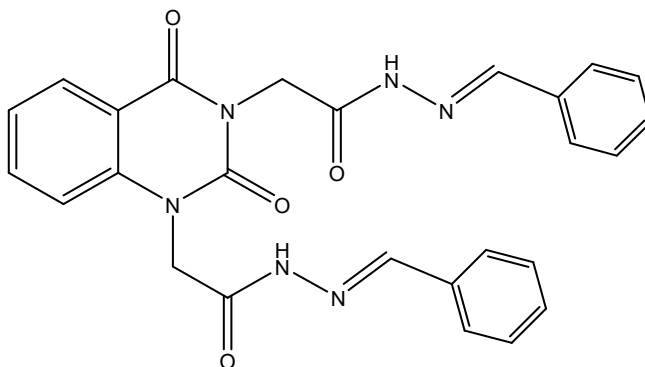


MS of compound (2)

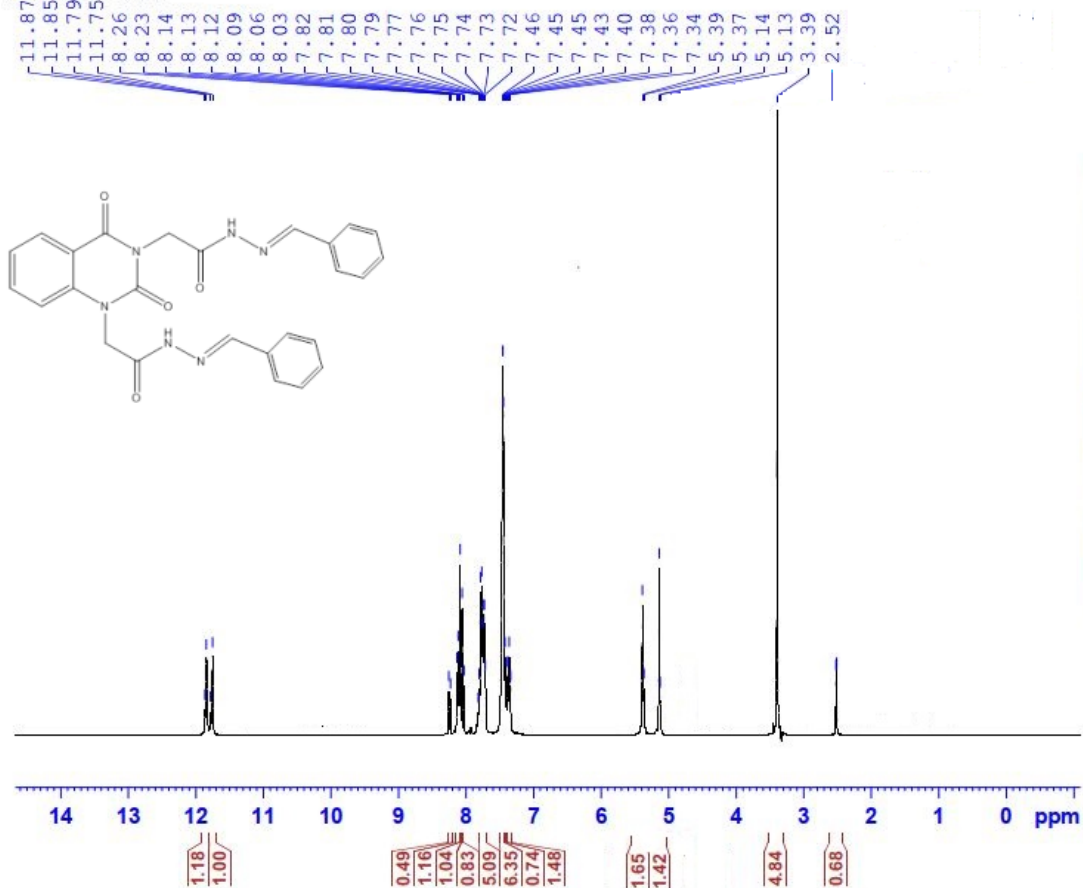


-

-Compound (3a)



Mohamed Omar

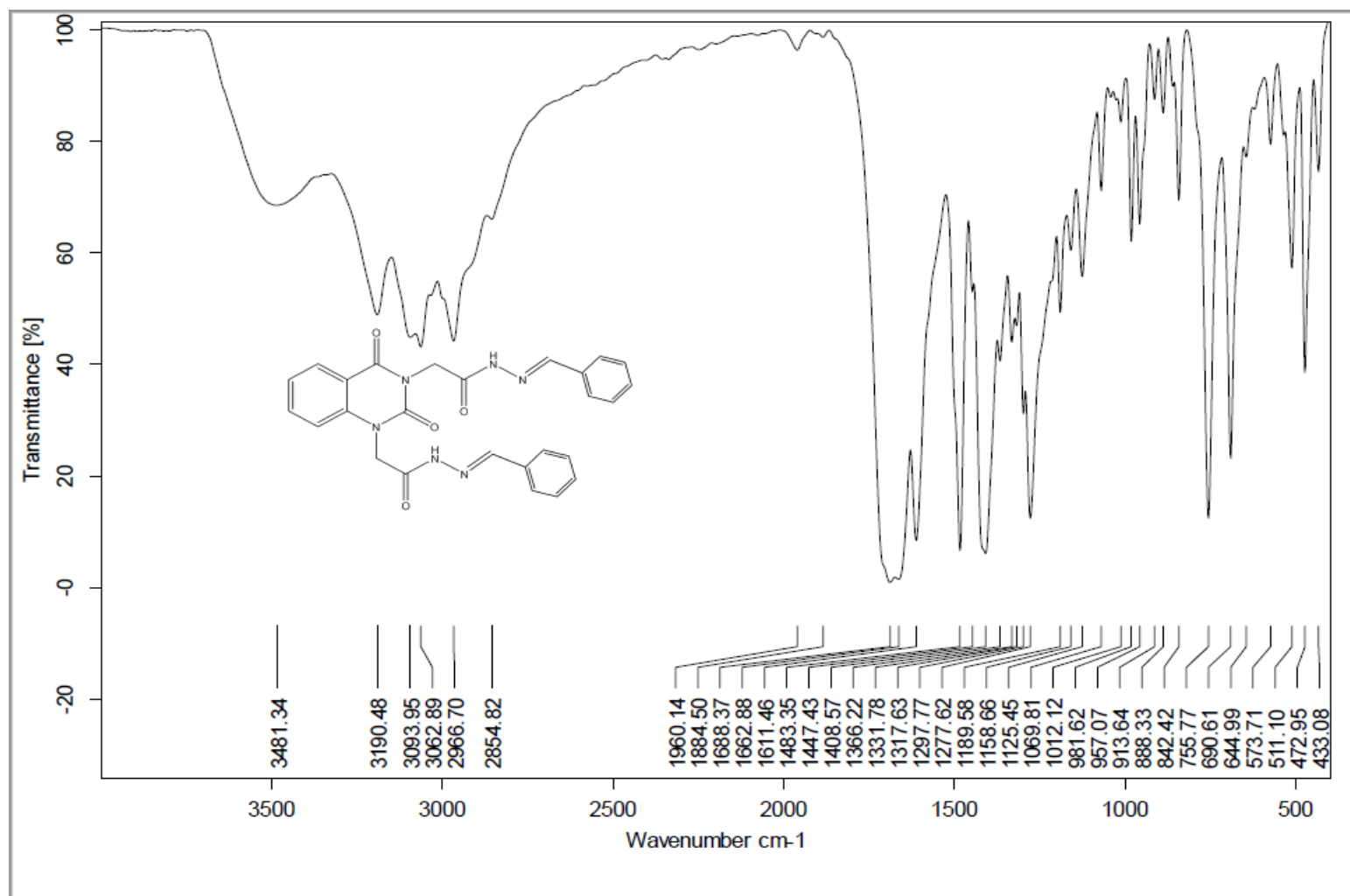


Current Data Parameters
NAME Mohamed Omar-M6-Hnmr-ow
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211206
Time 9.54 h
INSTRUM spect
PROBHD E108618_0903 (1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.244620 Hz
AQ 4.0894465 sec
RG 65.9
UR 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TDC 1
SFO1 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
GB 0 0.30 Hz
PC 1.00

¹H-NMR of compound (3a)



FT-IR of compound (3a)

Cairo University
Micro Analytical Center

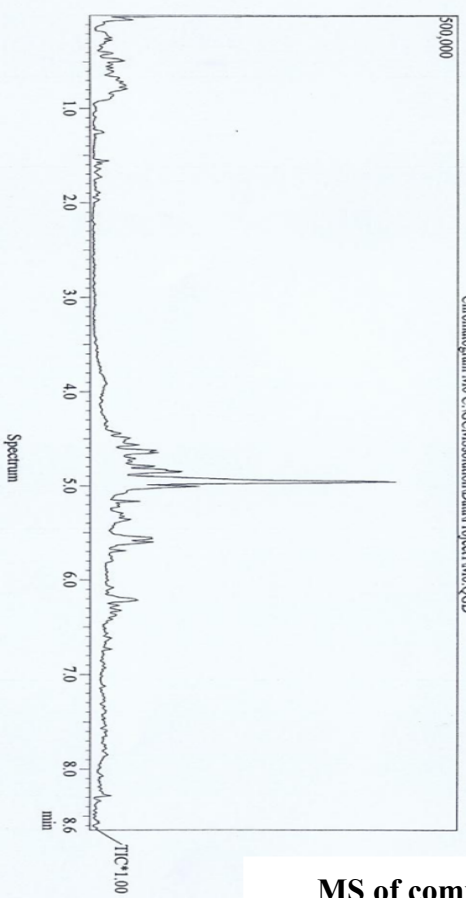
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 02:25:40
 Sample Name : M6
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Quna
 Data File : C:\GCMSolution\Data\Project\1\M6.QGD
 Orig. Data File : C:\GCMSolution\Data\Project\1\M6.QGD
 Method File : C:\GCMSolution\Data\Project\1\High Temperature Op
 Orig. Method File : C:\GCMSolution\Data\Project\1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
 Standard/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:34:22

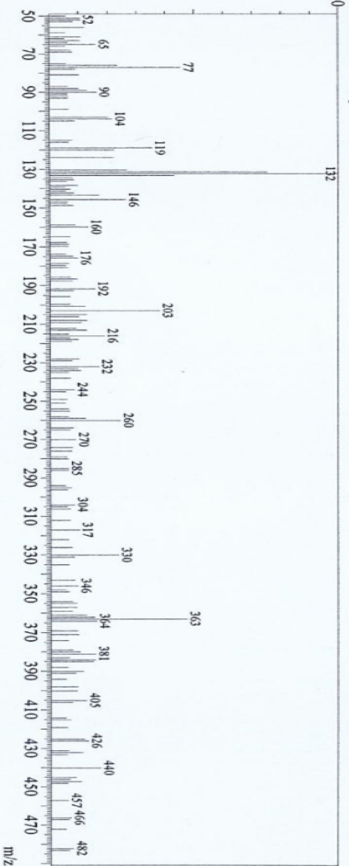
Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 -Group 1 - Event 1-
 Start Time : 0:00min
 End Time : 1:00min
 AQC Mode : Scan
 Event Time : 0:50sec
 Scan Speed : 1:250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project\1\M6.QGD

Chromatogram M6 C:\GCMSolution\Data\Project\1\M6.QGD



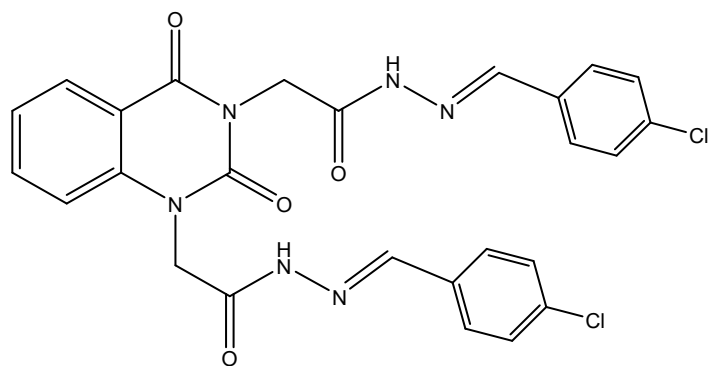
Line# 1, R. Time: 5.2 (Scan# 625)
 MassPeaks: 170
 RawMode: Single 5.2 (625) BasePeak: 132 (1940)
 BG Mode: None Group 1 - Event 1



MS of compound (3a)

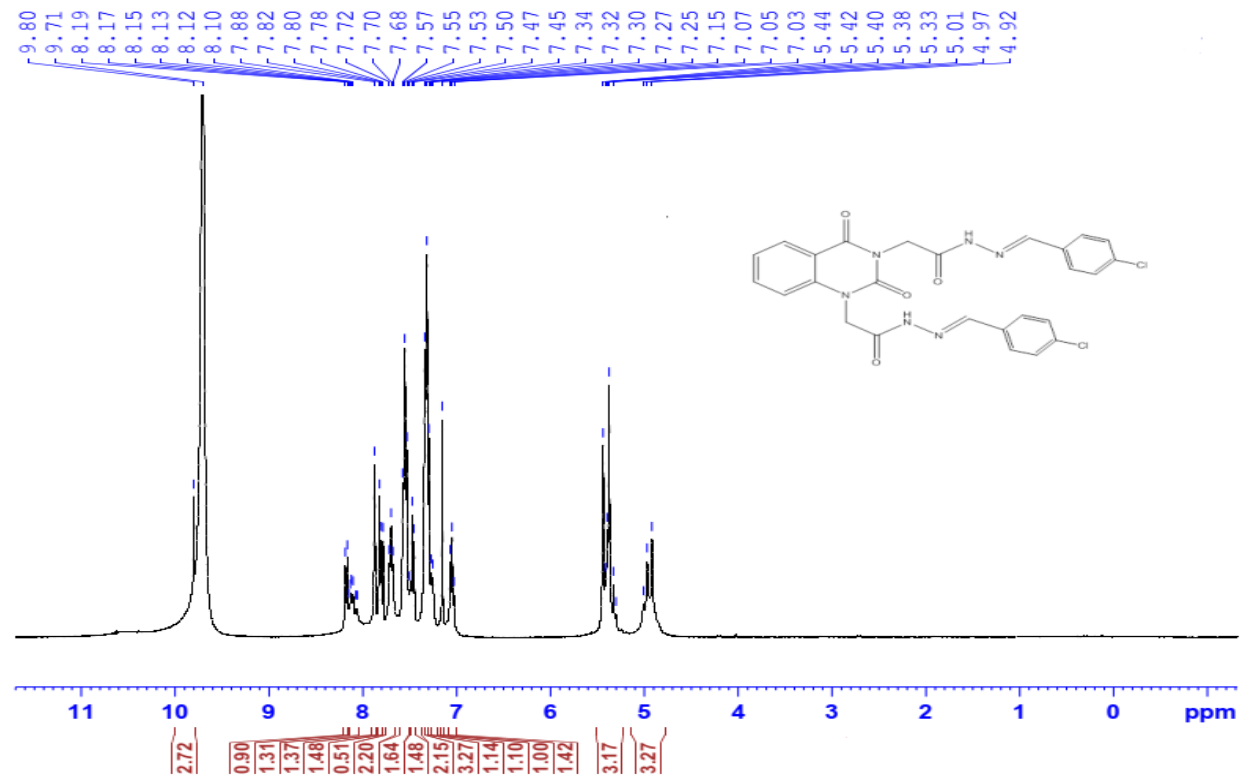
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-Compound (3b): -



3b

Mohamed Omar - M6a -TFA+CDCL3- Hnmr - T



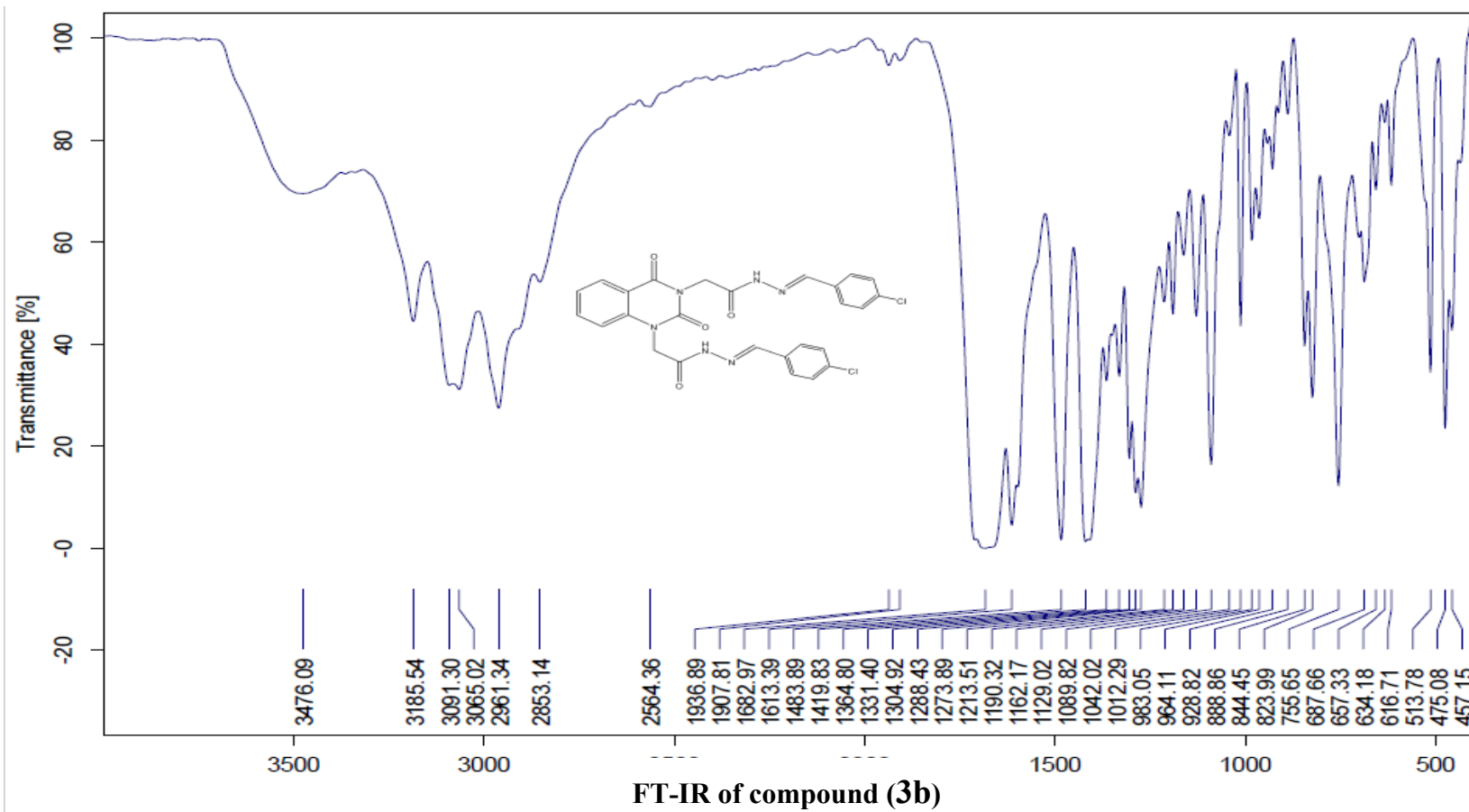
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Current Data Parameters
NAME Mohamed Omar - M6a -TFA+CDCL3- Hnmr - T
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220115
Time 13.13 D
INSTRUM spect
PROBHD 5100419_0145_1
PULPROG zgpg30
TD 65536
SOLVENT CDCL3
NS 14
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0884445 sec
RG 112.54
SQ 42.400 usec
SE 6.50 usec
TE 294.2 K
VE 1.00000000 sec
VD0 1
SFO1 400.2024712 MHz
MVC1 1K
F2 13.50 usec
FID1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.200524 MHz
WDW EM
SSB 0
GB 0
PC 1.00
    
```

¹H-NMR of compound (3b)



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**DI Analysis
Shimadzu Qp-2010 Plus**

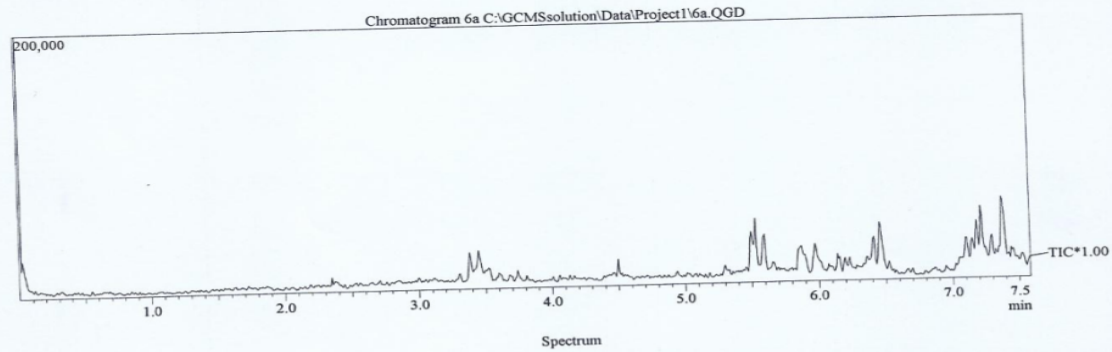
Dr. Mai Younis



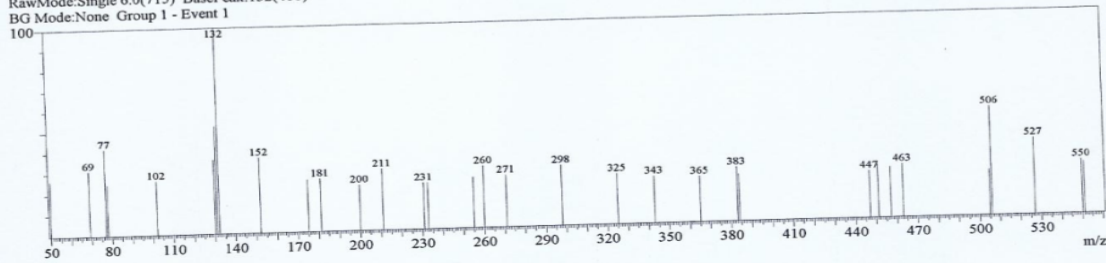
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 04:07:21 من
 Sample Name : 6a
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\6a.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\6a.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 SEndIfSModified by : Dr. Mai Younis
 Modified : 15/01/2007 04:14:59 من

Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSsolution\Data\Project1\6a.QGD

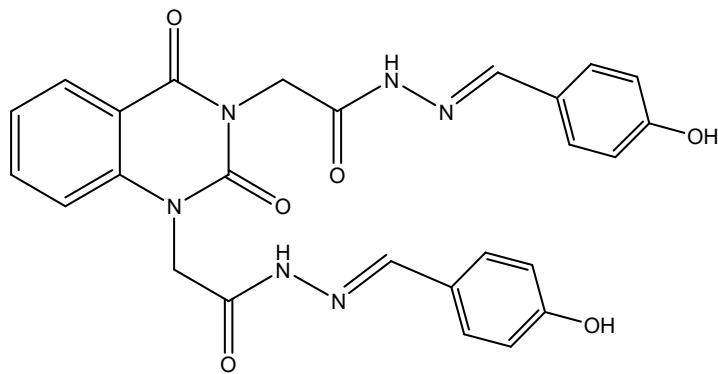


Line#:1 R.Time:6.0(Scan#:715)
 MassPeaks:33
 RawMode:Single 6.0(715) BasePeak:132(466)
 BG Mode:None Group 1 - Event 1

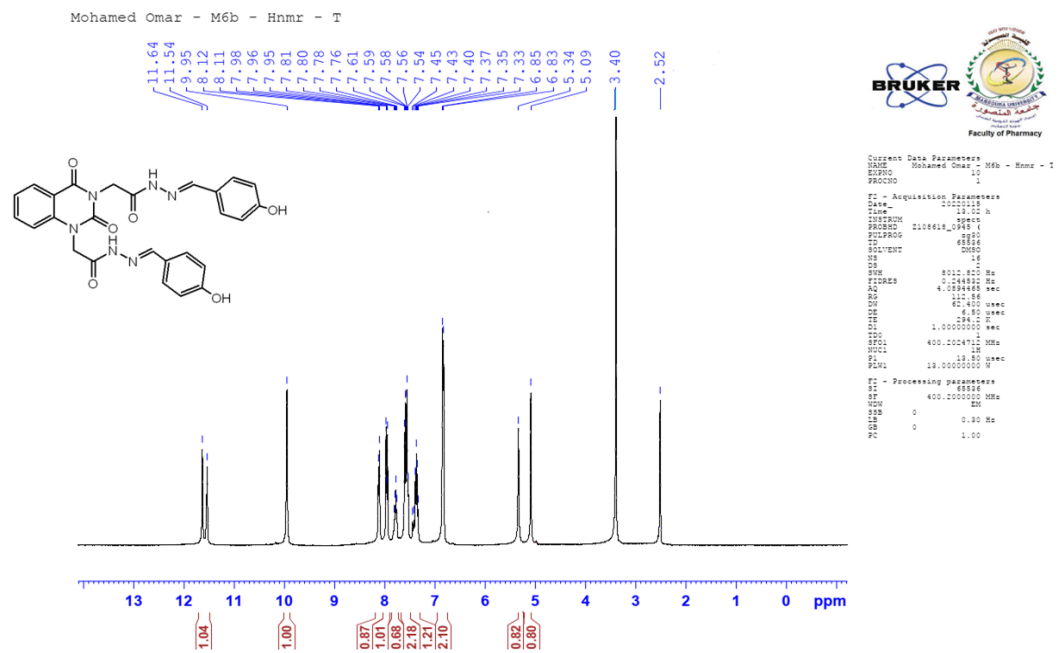


-

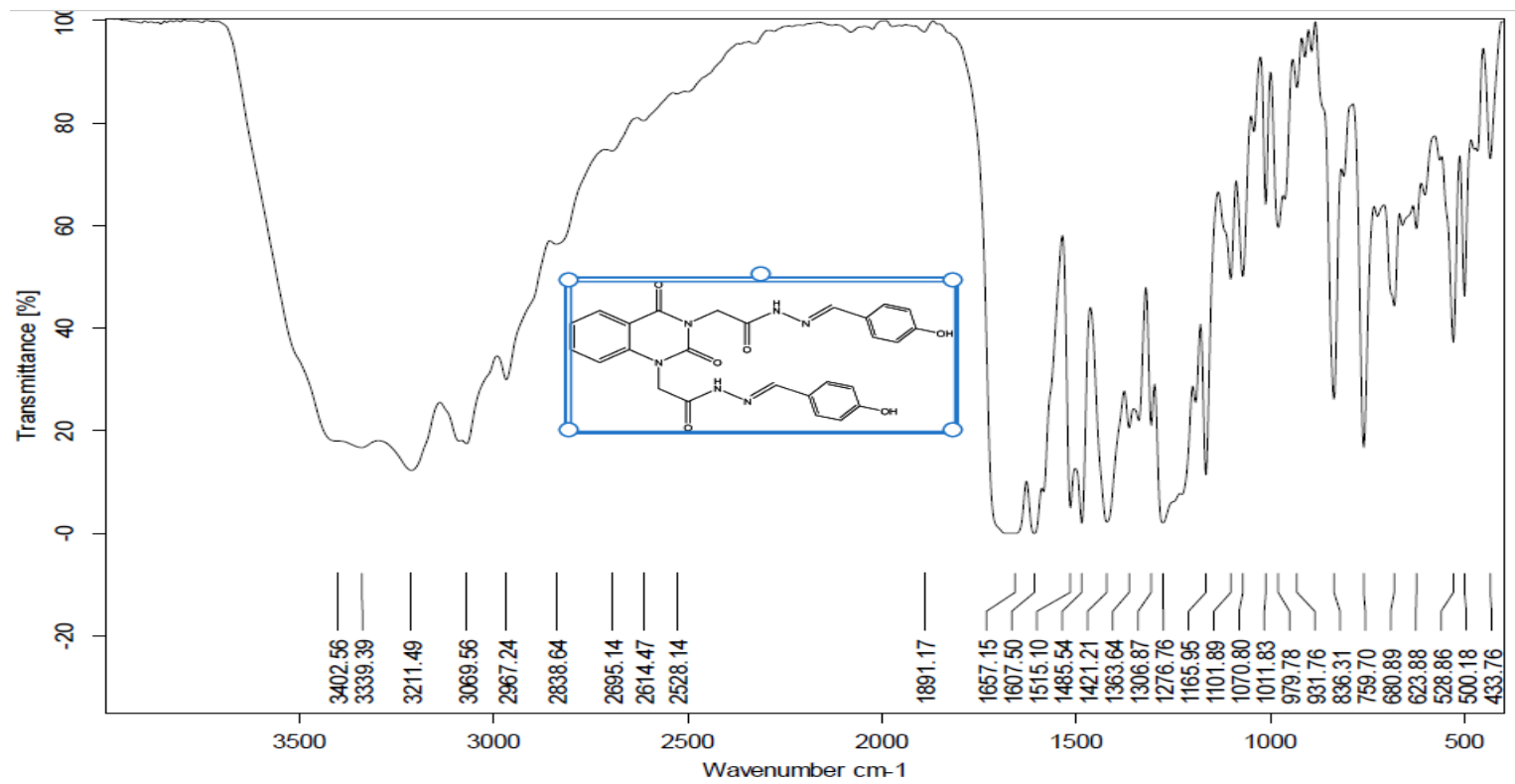
-Compound (3c):



3c



¹H-NMR of compound (3c)



FT-IR of compound (3c)

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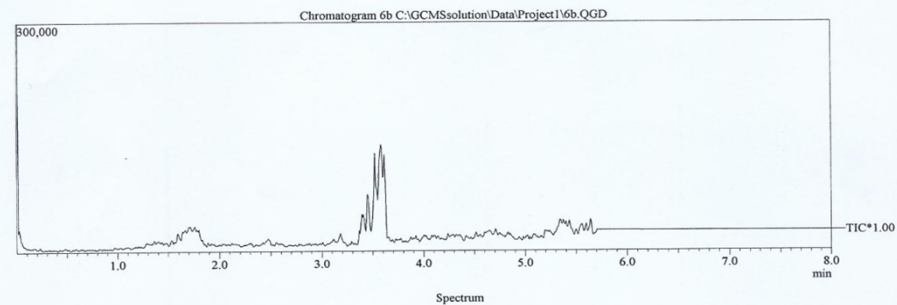
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 04:16:35
 Sample Name : 6b
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\6b.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\6b.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System1\Tune1_default.qgt
 \$END\$ Modified by : Dr. Mai Younis
 Modified : 15/01/2007 04:22:21

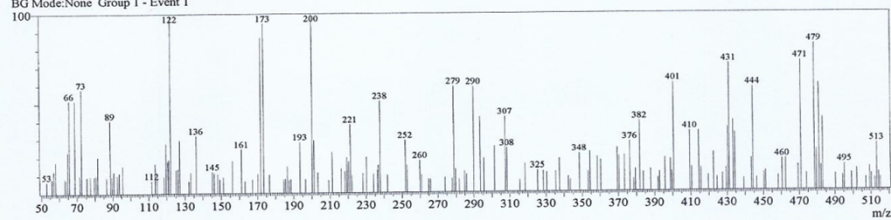
Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage :70 eV
 Ionization Mode :EI



C:\GCMSsolution\Data\Project1\6b.QGD

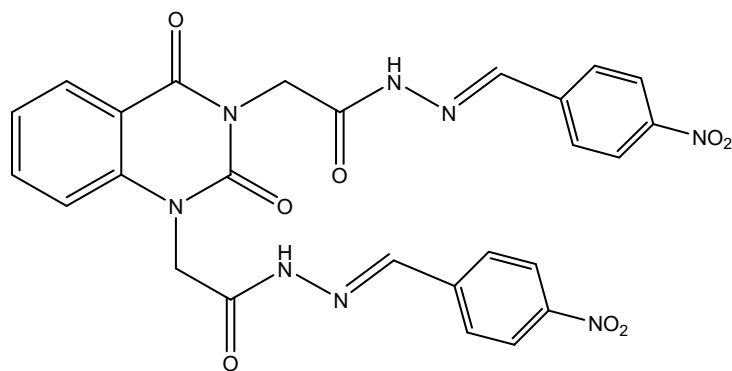


Line#:1 R.Time:3.6(Scan#:429)
 MassPeaks:165
 RawMode:Single 3.6(429) BasePeak:200(1575)
 BG Mode:None Group 1 - Event 1

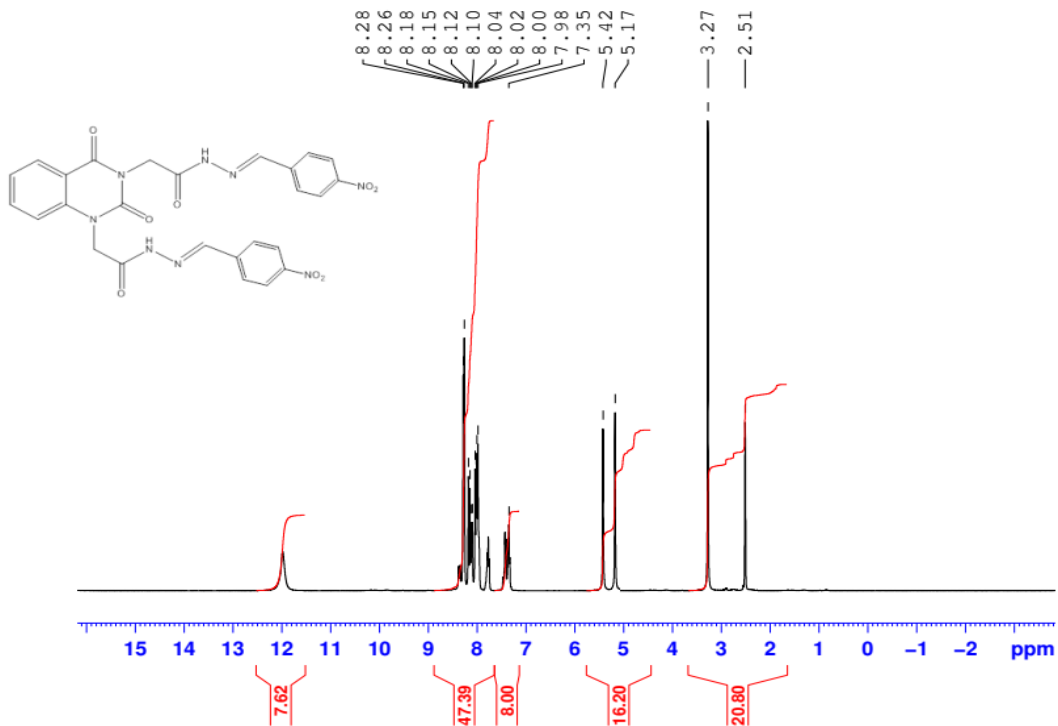


-

-Compound (3d):



3d



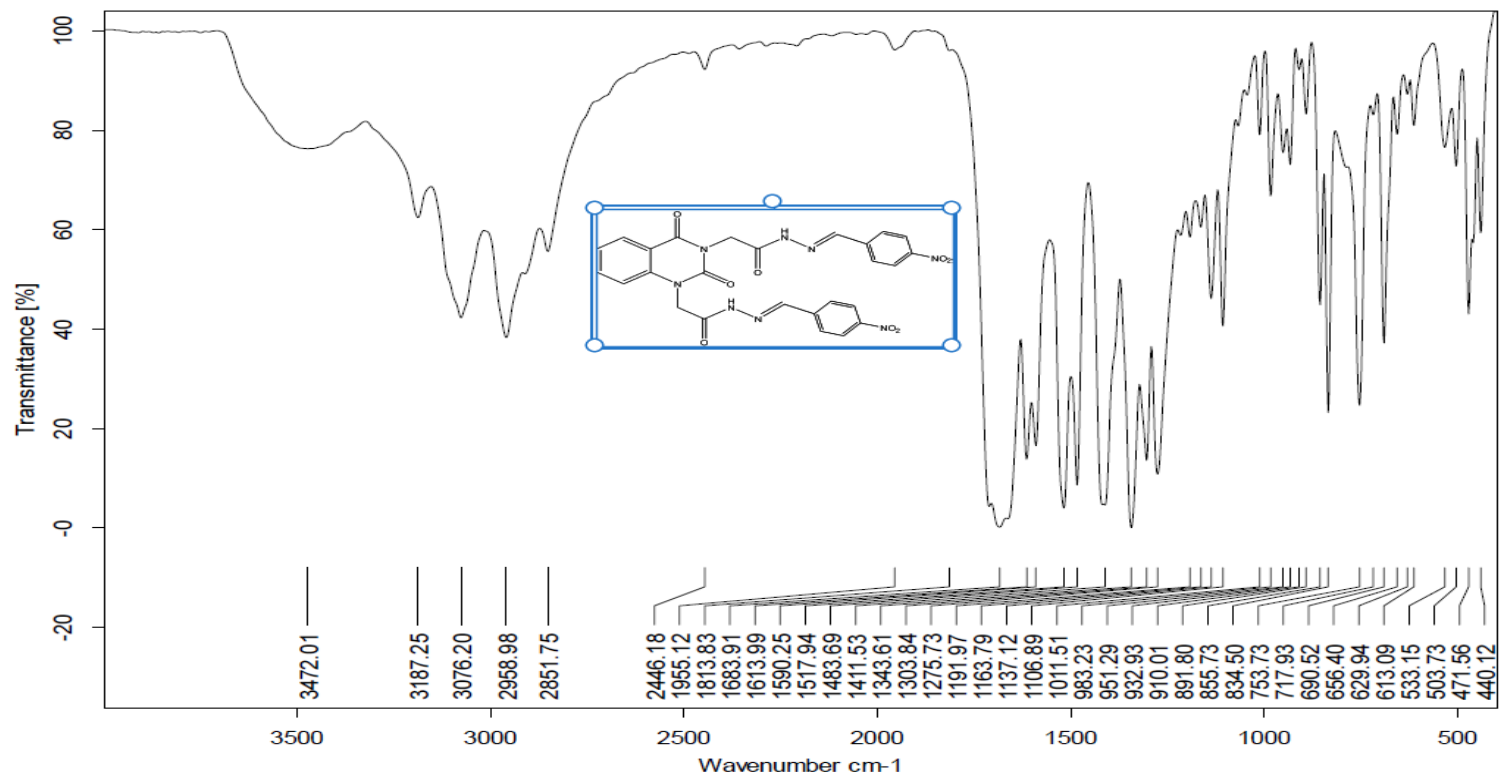
Current Data Parameters
 NAME Feb17-2022
 EXPNO 40
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220217
 Time 10.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 50
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 158.76
 DW 62.400 usec
 DE 6.50 usec
 TE 313.1 K
 DI 1.0000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 22.0000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹H-NMR of compound (3d)



FT-IR of compound (3d)

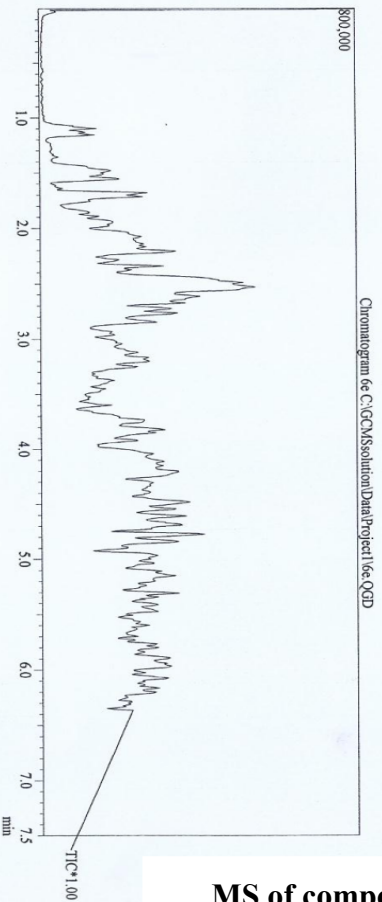
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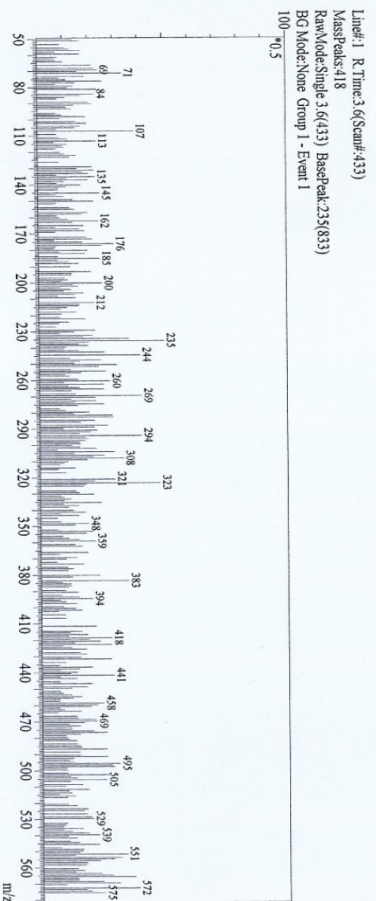
Sample Information
Analyzed by : Dr. Mai Younis
Analyze Date : 15/01/2007 04:32:35
Sample Name : 6e
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quana
Data File : C:\GCMSolution\Data\Project\Iee.QGD
Org Data File : C:\GCMSolution\Data\Project\Iee.QGD
Method File : C:\GCMSolution\Data\Project\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project\High Temperature Op
Report File : C:\GCMSolution\System\Tune1\default.qqt
Tuning File : C:\GCMSolution\System\Tune1\default.qqt
SendToS Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:39:00

Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
-Group 1 - Event 1-
Start Time : 0:00min
End Time : 1:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2:000
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project\Iee.QGD

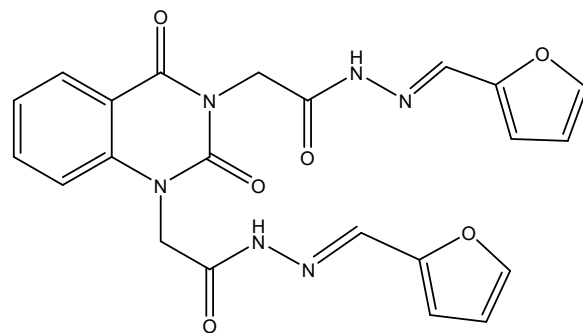


MS of compound (3d)

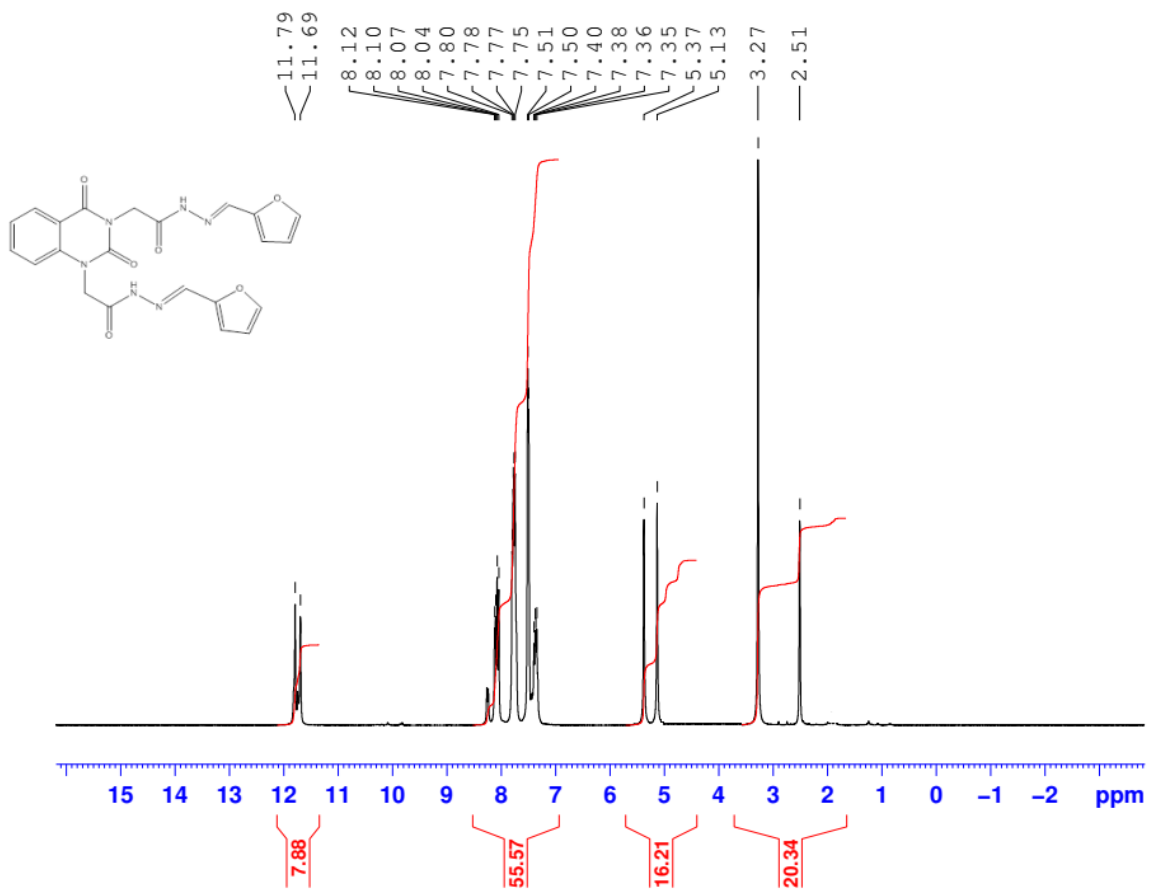


-

Compound (3e):



3e



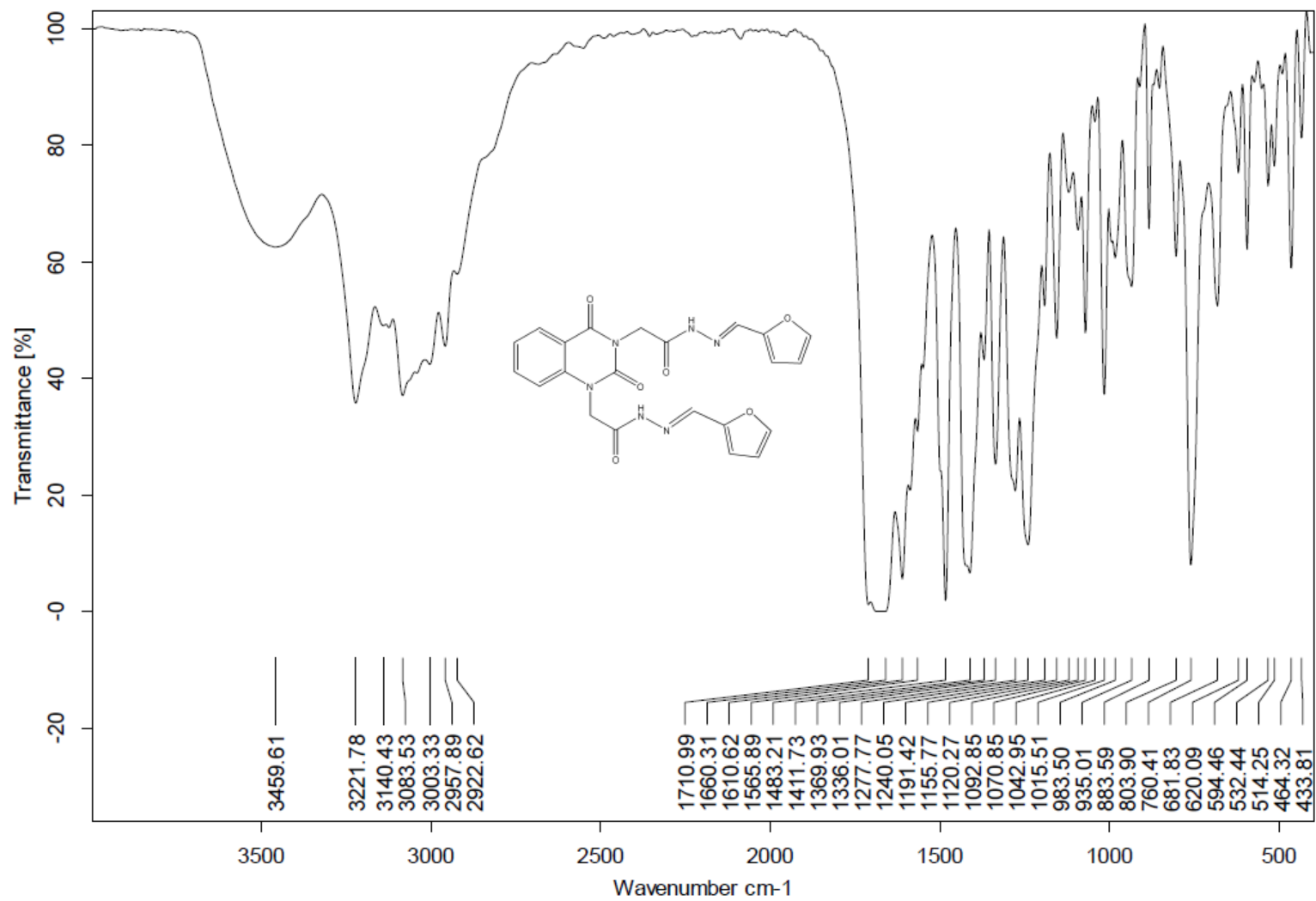
Current Data Parameters
NAME Feb17-2022
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220217
Time 10.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 159.76
DW 62.400 usec
DE 6.50 usec
TE 313.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.0000000 W

F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR of compound (3e)



FT-IR of compound (3e)

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DI Analysis
Shimadzu QP-2010 Plus

Sample Information

Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 04:40:35
Sample Name : 6f
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Qena
Data File : C:\GCMSolution\Data\Project1\6f\QGD
Org Data File : C:\GCMSolution\Data\Project1\6f\QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File : C:\GCMSolution\System\Tune1_default.qgd
Tuning File : C:\GCMSolution\System\Tune1_default.qgd
Serials/Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:44:39

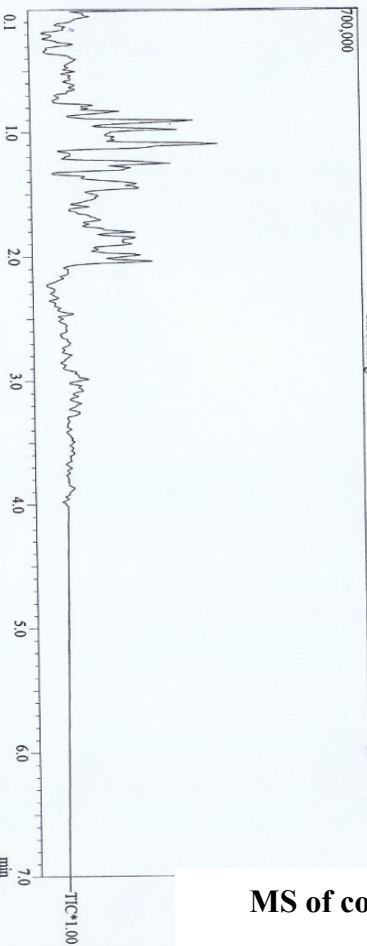
Method

Analytical Line 1 :
IonSourceTemp : 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time : 0:00min
End Time : 1:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI

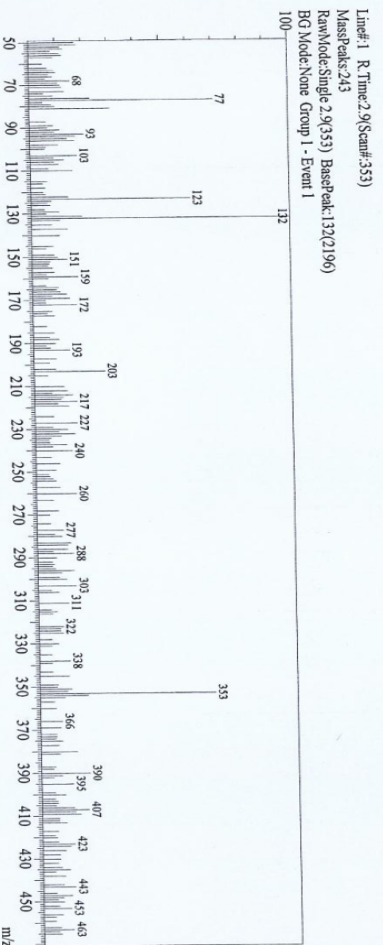
C:\GCMSolution\Data\Project1\6f\QGD

Electron Voltage : 70 eV
Ionization Mode : EI

Chromatogram 6f C:\GCMSolution\Data\Project1\6f\QGD

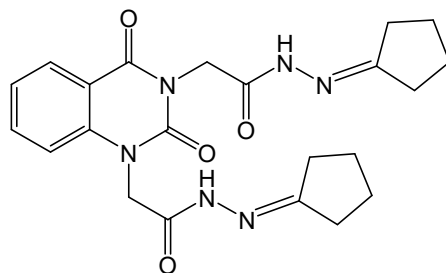


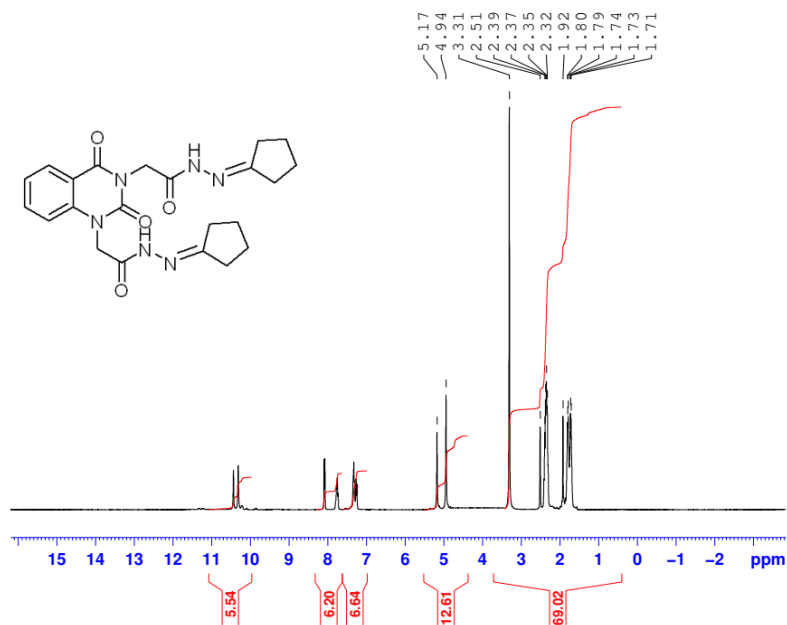
MS of compound (3e)



-

Compound (4a): -





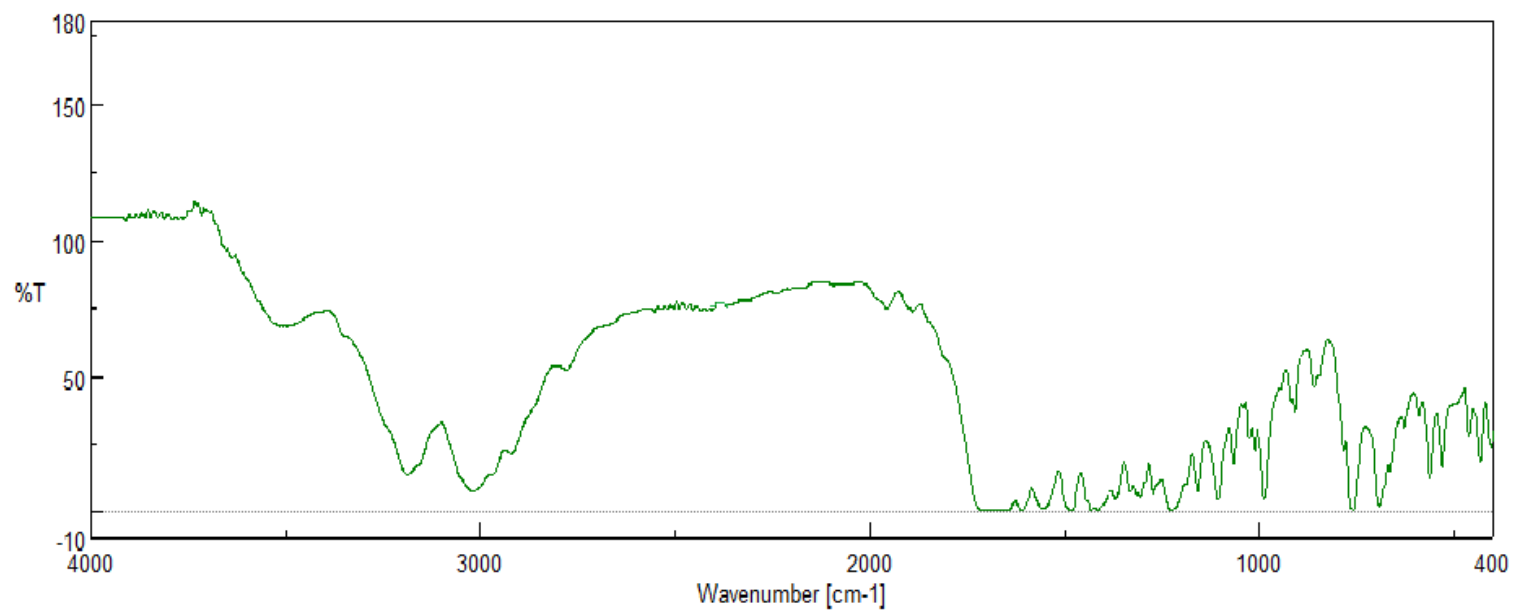
Current Data Parameters
 NAME Jul103-2022
 EXPNO 50
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20220703
 Time 12.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 35
 DS 2
 SMH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 120.97
 DM 62.400 usec
 DE 6.50 usec
 TE 308.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 S1 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

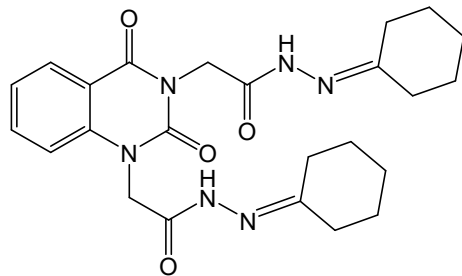
¹H-NMR of compound (4a)



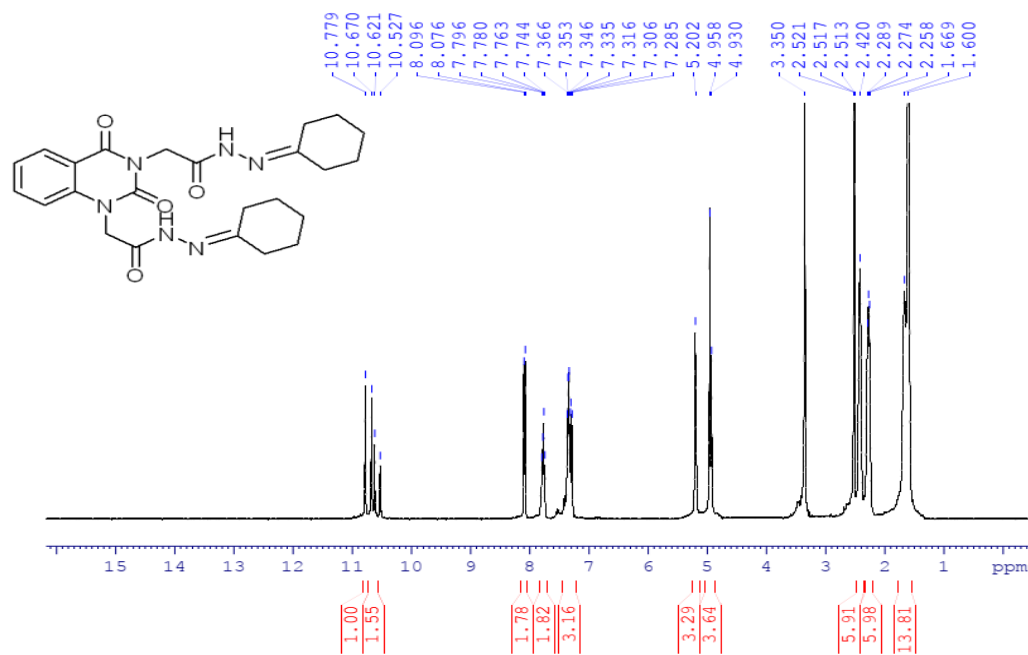
FT-IR of compound (4a)

-

Compound (4b): -



4b



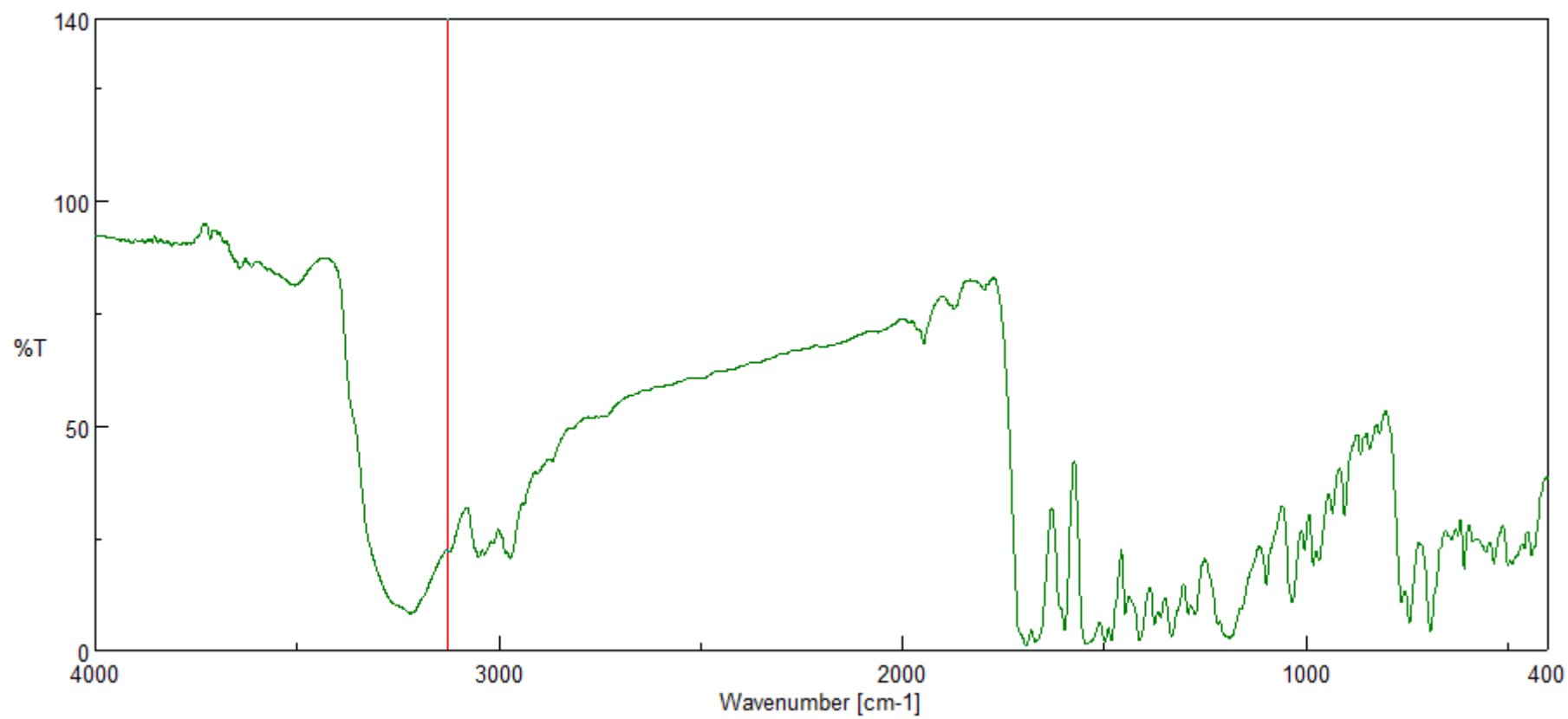
```

Current Data Parameters
NAME      Mohamed Omar - 10M Hnmr - T
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20220611
Time     10.02 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        16
DS        4
SWH       8012.820 Hz
FIDRES    0.244882 Hz
AQ         4.089468 sec
RG         176.72
DM         62.400 usec
DE         6.50 usec
TE        296.1 K
D1         1.00000000 sec
TDO        1
SFO1      400.2024712 MHz
NUC1       1H
P1         13.50 usec
PLM1       13.00000000 W

F2 - Processing parameters
SI         65536
SF         400.2000000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

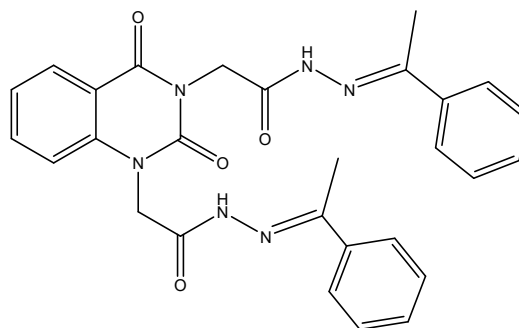
¹H-NMR of compound (4b)



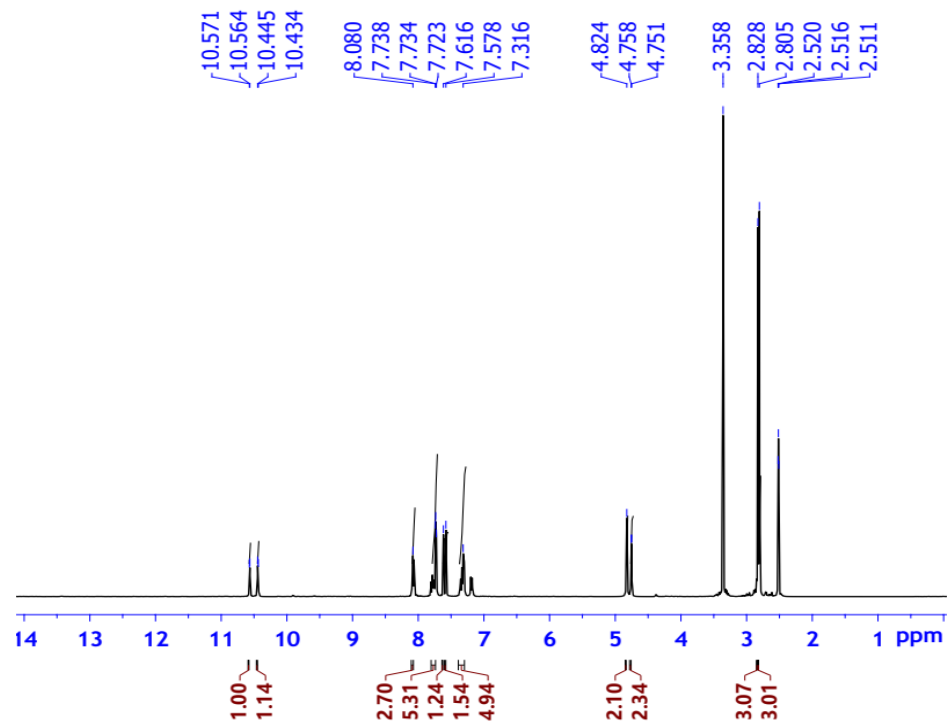
FT-IR of compound (4b)

-

- compound (4c):



4c

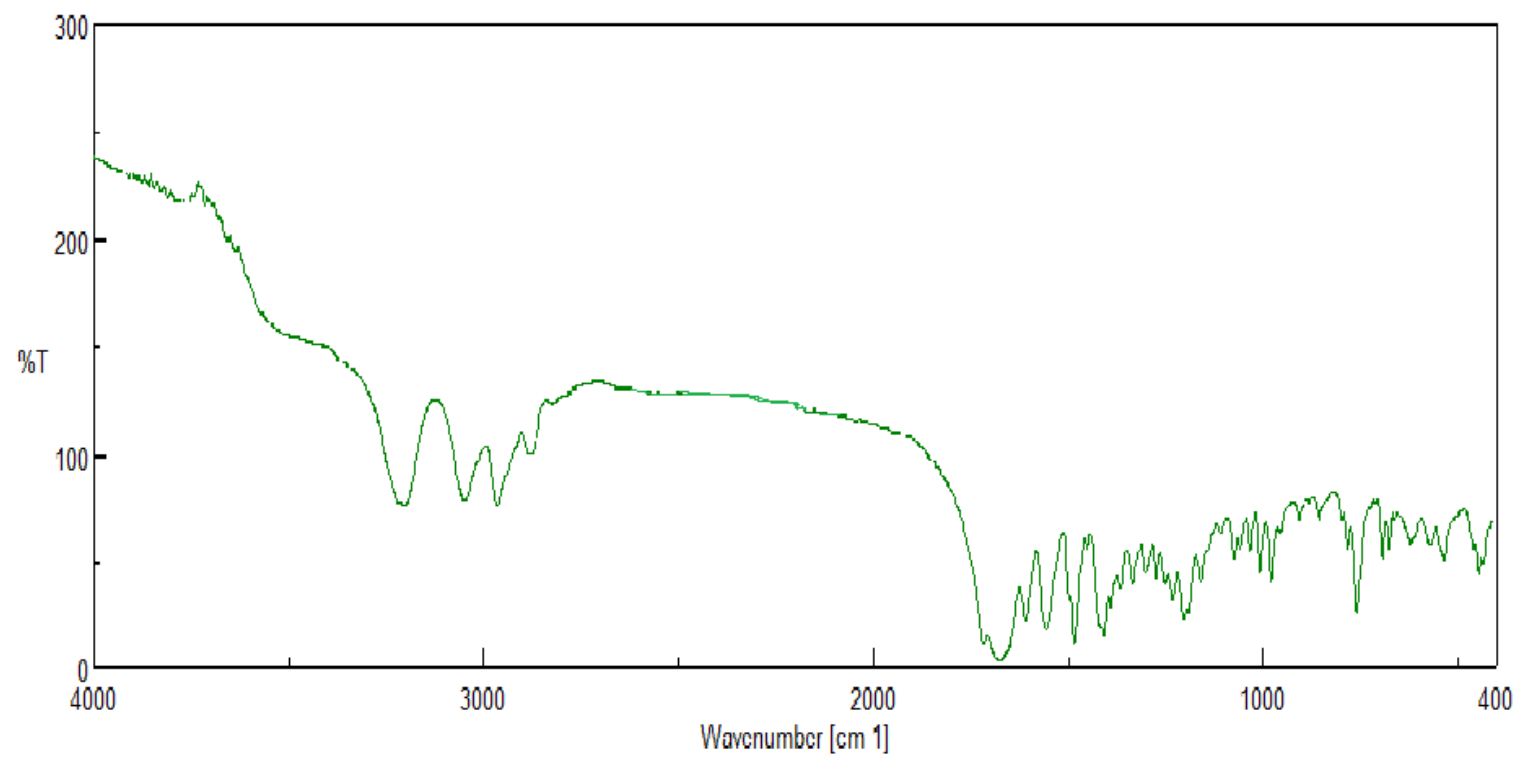


```

Current Data Parameters
NAME      Mohammed Omar-10B-proton-NH
EXPNO    10
PROCNO   1

F1 - Acquisition Parameters
Date_    20220208
Time     14.11 h
INSTRUM  spect
PROBHD   E10618_0945 (
PULPROG  zgpg
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.800 Hz
FIDRES    0.244880 Hz
AQ        4.0894465 sec
RG         11.58
DN         62.400 usec
DE         6.80 usec
TE        292.2 K
D1        1.00000000 sec
TDO
SFO1     400.2024711 MHz
NUC1      1H
P1        13.80 usec
PL1       13.00000000 dB
F1 - Processing parameters
SI        65536
SF        400.20000000 MHz
WDW       EM
SSB       0
LB        0.20 Hz
GB
PC        1.00
  
```

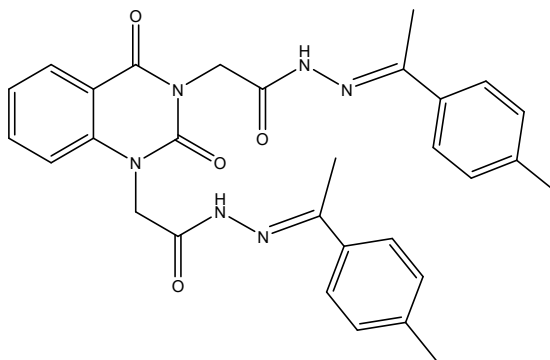
¹H-NMR of compound (4c)



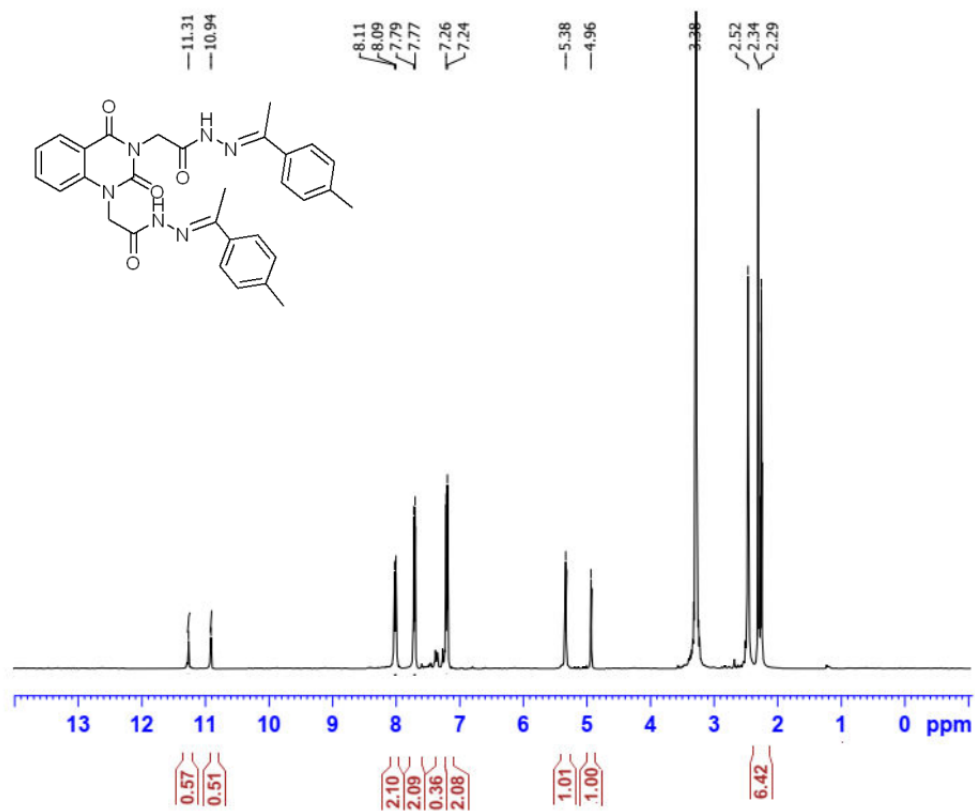
FT-IR of compound (4c)

-

Compound (4d): -



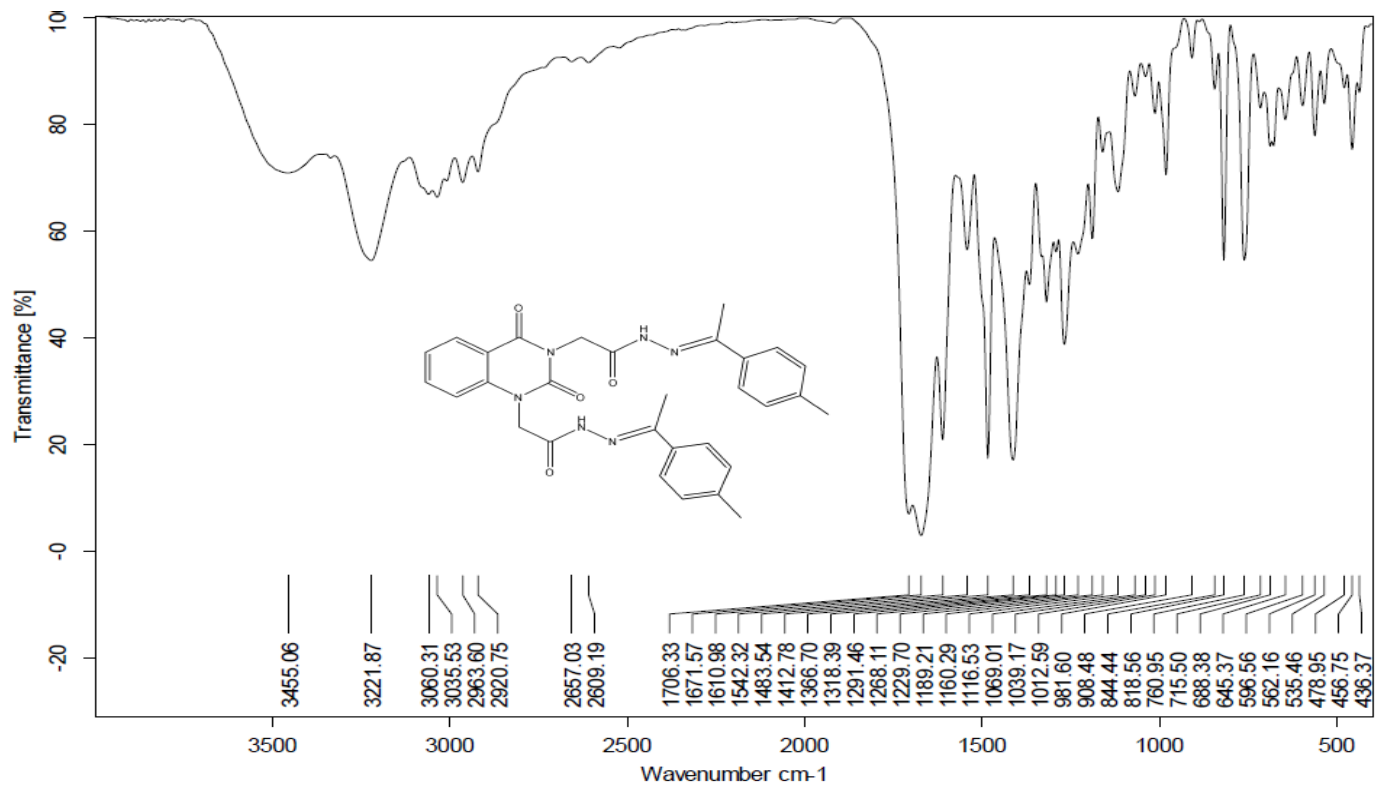
4d



```

Current Data Parameters
NAME: Mubassat_Ola-100-yaoum-101
PROCNO: 1
PC: Acquisition Parameters
Date_: 202308
Time: 14:11 h
INSTRUM: spect
PROBHD: 5 mm BBO
PULPROG: zgpg30
NUC1: 13C
NUC2: 13C
SOLVENT:
SS: 16
DS: 2
SFO1: 101.625 MHz
SFO2: 101.625 MHz
PTPRG1:
AQ: 1.029465 sec
RG: 211.30
RG2: 60.000 usec
RG3: 6.00 usec
RG4: 292.70
RG5: 1.0000000 sec
RG6: 1
SFO1: 401.0024712 MHz
SFO2: 101.625 MHz
RG7: 13.000 usec
RG8: 13.0000000 N
PC: Processing parameters
SI: 65536
SF: 401.0024712 MHz
RG: 60
RG2: 6.00 usec
RG3: 0
RG4: 0.00 MHz
RG5: 0
RG6: 1.00
  
```

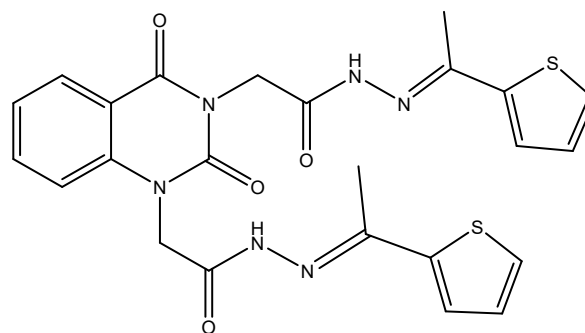
¹H-NMR of compound (4d)



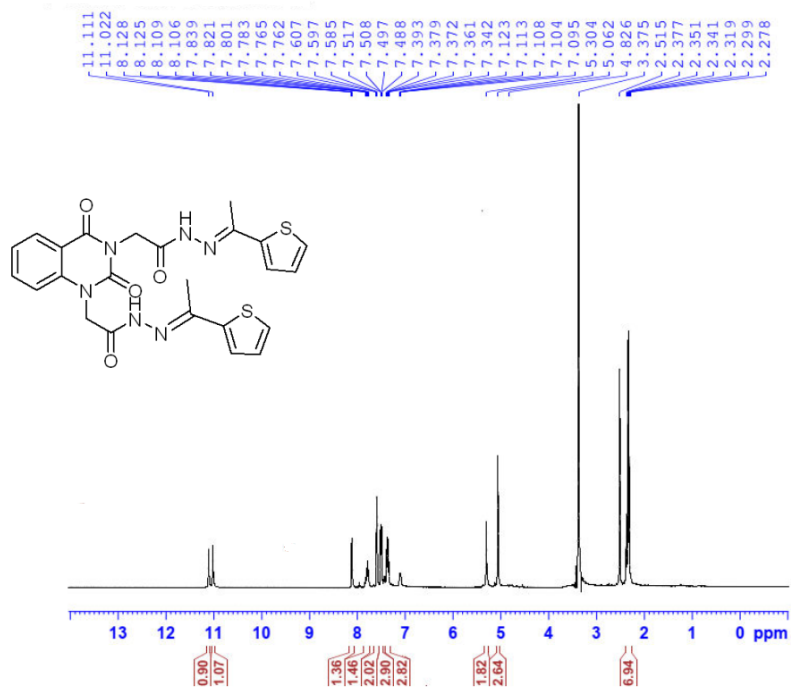
FT-IR of compound (4d)

-

Compound (4e):-



4e



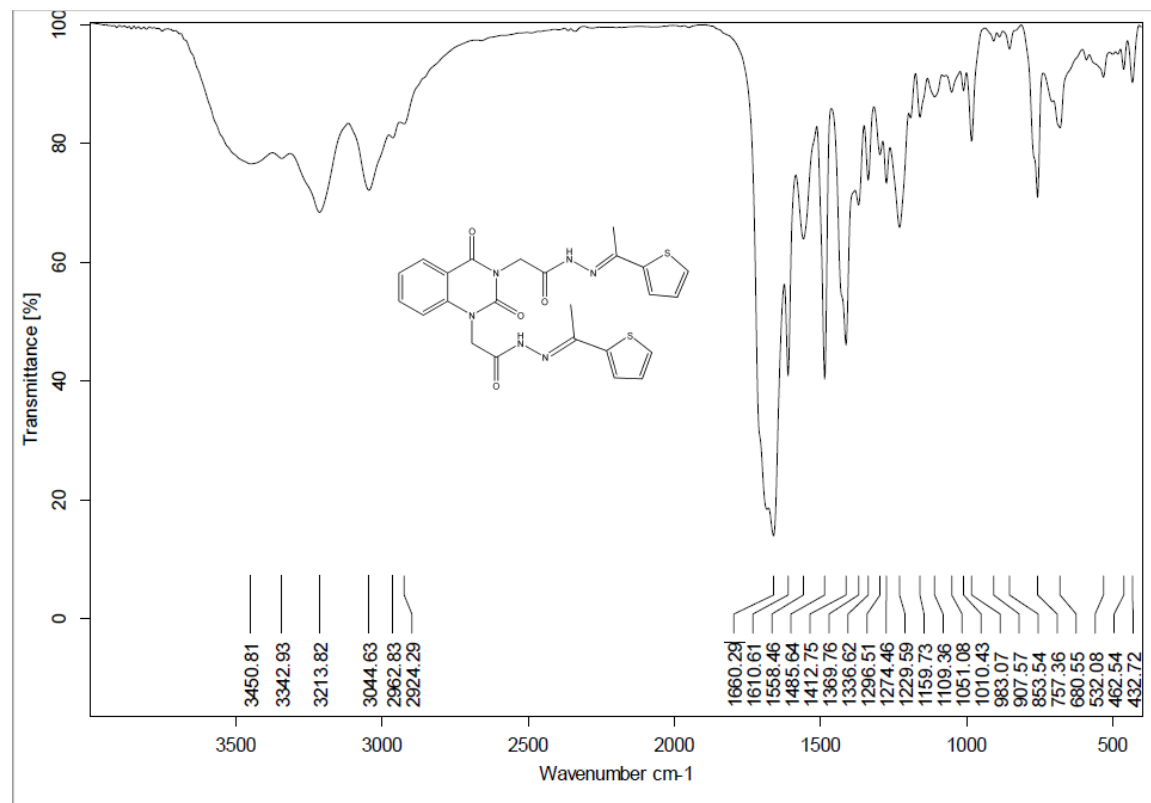
```

Current Data Parameters
NAME: Mohamed Omer-100-proton-NH
EXPNO: 10
PROCNO: 1

PC - Acquisition Parameters
Date_: 20220908
Time: 14.25 h
INSTRUM: spect
PROBHD: zgpg30_5mm (
PULPROG: zgpg30
TD: 65536
SOLVENT: DMSO
NS: 46
DS: 4
SWH: 8012.820 Hz
FIDRES: 0.246892 Hz
AQ: 4.028468 sec
RG: 128.41
AQ: 60.400 usec
DE: 6.90 usec
TE: 300.2 K
SI: 1.00000000 sec
SFO: 400.146400 MHz
NUC1: 13
NUC2: 13
P1: 19.90 usec
P1FL1: 19.00000000 N

PC - Processing parameters
SI: 65536
SF: 400.146400 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
  
```

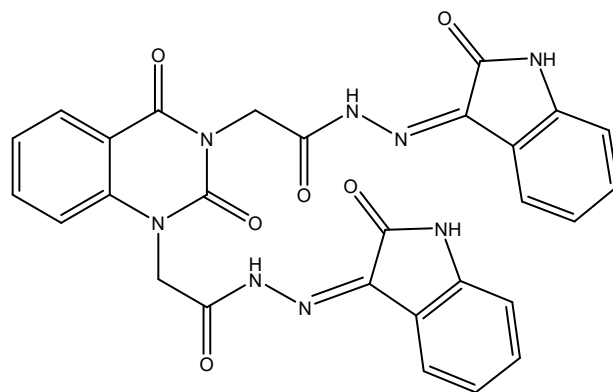
¹H-NMR of compound (4e)



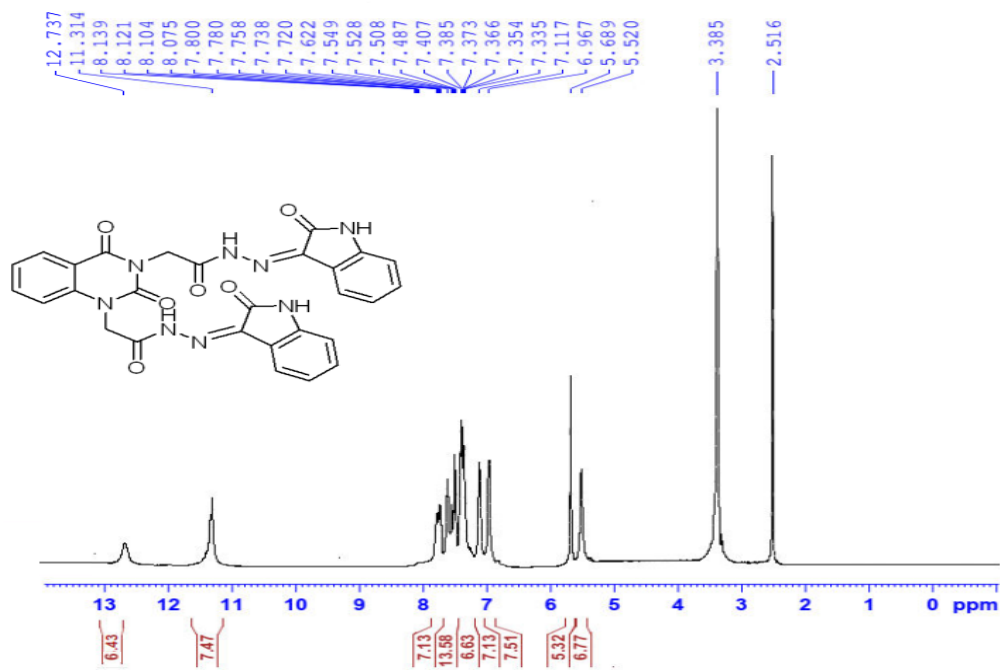
FT-IR of compound (4e)

-

Compound (4f)



4f



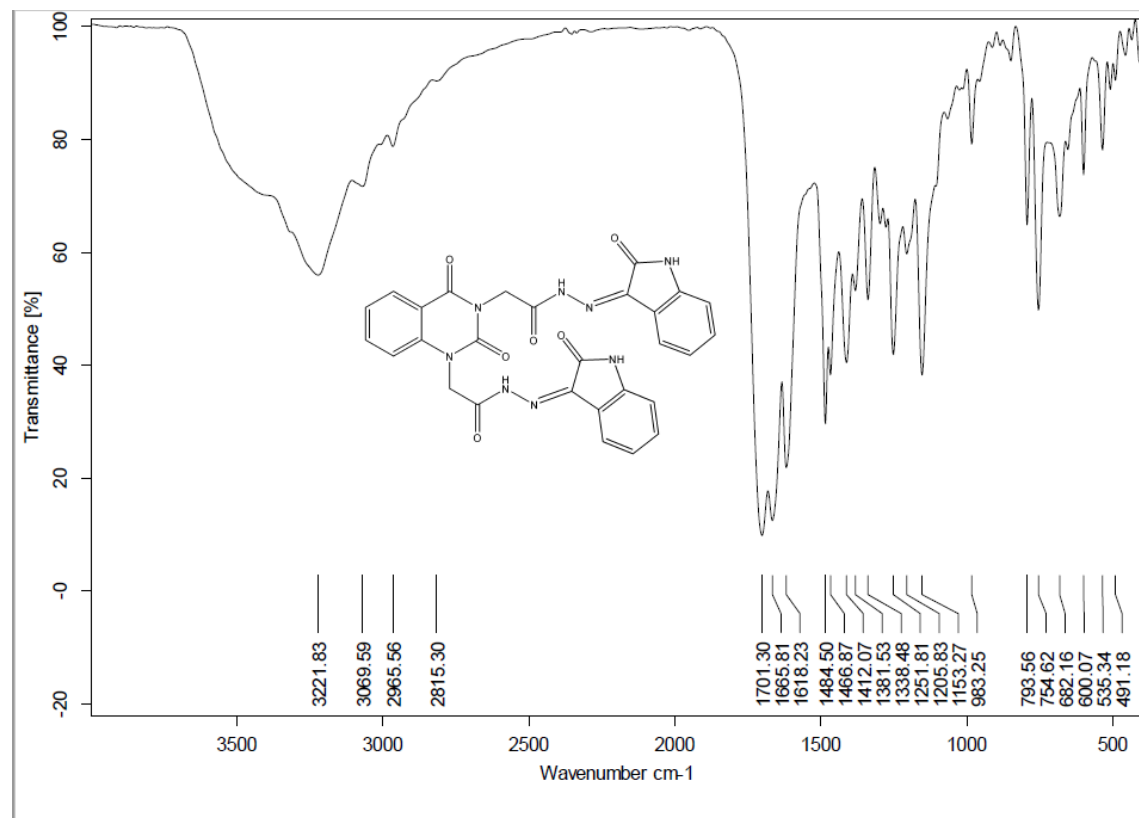
```

Current Data Parameters
NAME      Mohammed Omar-10A-proton-NH
EXPNO    1
PROCNO   1

F1 - Acquisition Parameters
Date_    201308
Time     11:08 h
INSTRUM  spect
PROBHD   zgpg30
PULPROG  zgpg30
SOLVENT  DMSO
NS       640
DS       4
SWH      13000.000 Hz
FIDRES   0.244880 Hz
AQ       4.0194480 sec
RG        64
AQRES    0.244880 Hz
SFO      400.202471 MHz
WDW       EM
SSB       0
GB        0
PC        1.00000000 sec
DC        0
BL        0
SFO2     400.202471 MHz
NUC1      1H
NUC2      13C
NUC3      15N
P1        19.00000000 sec
PC2       0
PC3       0
PC4       0
PC5       0
PC6       0
PC7       0
PC8       0
PC9       0
PC10      0
PC11      0
PC12      0
PC13      0
PC14      0
PC15      0
PC16      0
PC17      0
PC18      0
PC19      0
PC20      0
PC21      0
PC22      0
PC23      0
PC24      0
PC25      0
PC26      0
PC27      0
PC28      0
PC29      0
PC30      0
PC31      0
PC32      0
PC33      0
PC34      0
PC35      0
PC36      0
PC37      0
PC38      0
PC39      0
PC40      0
PC41      0
PC42      0
PC43      0
PC44      0
PC45      0
PC46      0
PC47      0
PC48      0
PC49      0
PC50      0
PC51      0
PC52      0
PC53      0
PC54      0
PC55      0
PC56      0
PC57      0
PC58      0
PC59      0
PC60      0
PC61      0
PC62      0
PC63      0
PC64      0
PC65      0
PC66      0
PC67      0
PC68      0
PC69      0
PC70      0
PC71      0
PC72      0
PC73      0
PC74      0
PC75      0
PC76      0
PC77      0
PC78      0
PC79      0
PC80      0
PC81      0
PC82      0
PC83      0
PC84      0
PC85      0
PC86      0
PC87      0
PC88      0
PC89      0
PC90      0
PC91      0
PC92      0
PC93      0
PC94      0
PC95      0
PC96      0
PC97      0
PC98      0
PC99      0
PC100     0

Processing parameters
SI        32768
SF        400.200000 MHz
WDW       EM
SSB       0
GB        0
PC        1.00
  
```

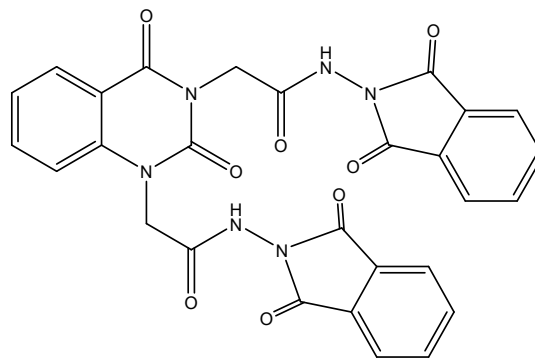
¹H-NMR of compound (4f)

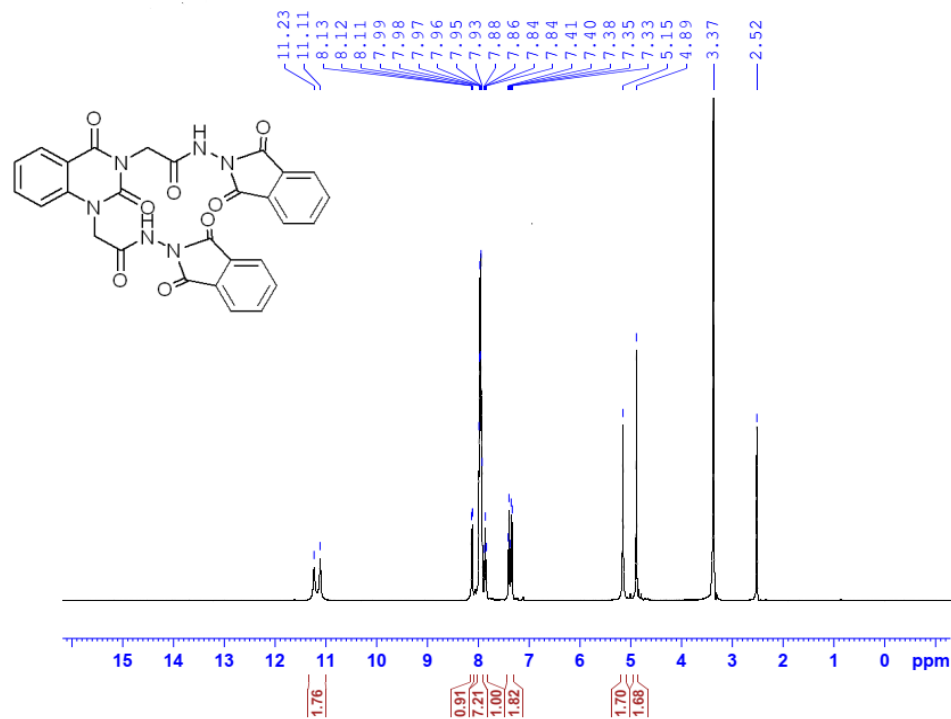


FT-IR of compound (4f)

-

compound (5a)



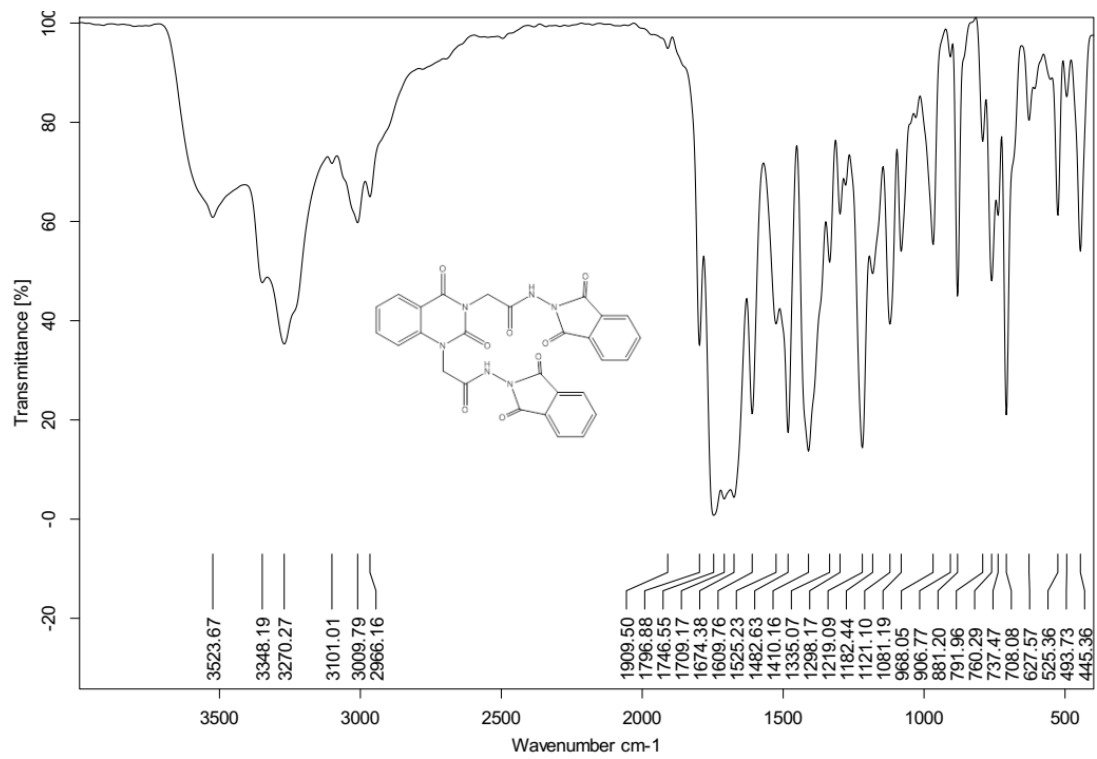


```

Current Data Parameters
NAME      mohamed omer-MC-Hmr-ov
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20211018
Time      12.12 h
INSTRUM   spect
PROBHD    zgpg30
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         48
DS         4
SWH        801.800 Hz
FIDRES     0.224882 Hz
AQ         4.0394465 sec
RG         176.72
DR         62.400 usec
DE         6.50 usec
TE         292.2 K
D1         1.00000000 sec
rDC        1
SFO1       400.202471 MHz
NUC1       1H
PC         18.50 usec
PL1        13.0000000 W

F2 - Processing parameters
SI         65536
SF         400.200000 MHz
WDW        EM
SSB        0
GB         0
PC         0.30 Hz
WC         1.00
  
```



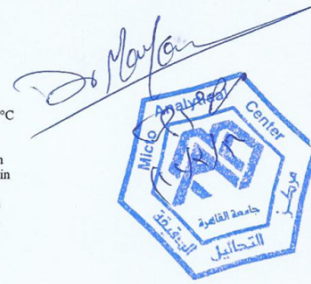
FT-IR of compound (5a)

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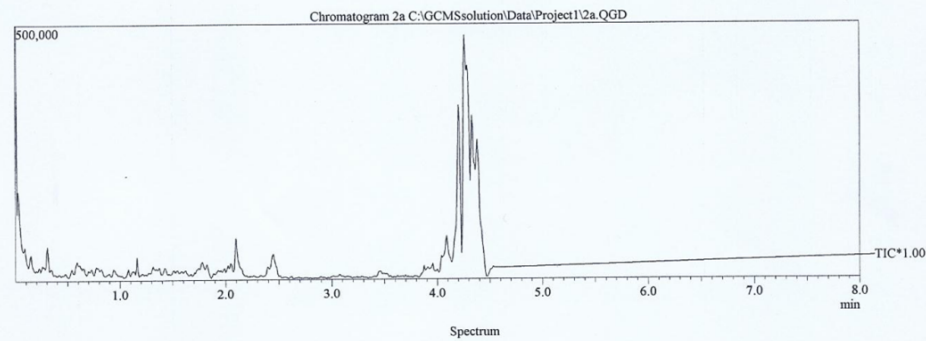
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 03:55:58
 Sample Name : 2a
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Quena
 Data File : C:\GCMSsolution\Data\Project1\2a.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\2a.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 \$EndIf\$Modified by : Dr. Mai Younis
 Modified : 15/01/2007 04:00:33

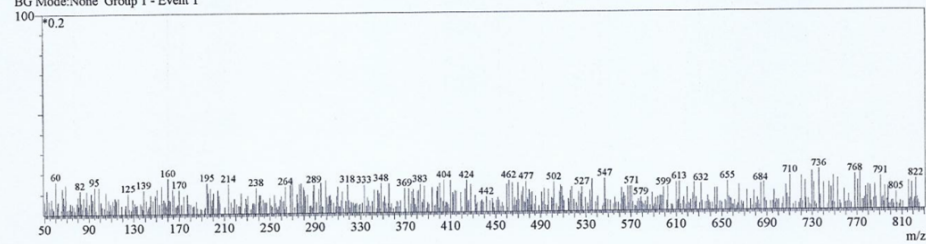
Method
 Analytical Line 1
 IonSourceTemp :250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time :0.00min
 End Time :10.00min
 ACQ Mode :Scan
 Event Time :0.50sec
 Scan Speed :2000
 Start m/z :50.00
 End m/z :900.00
 Electron Voltage :70 eV
 Ionization Mode :EI



C:\GCMSsolution\Data\Project1\2a.QGD



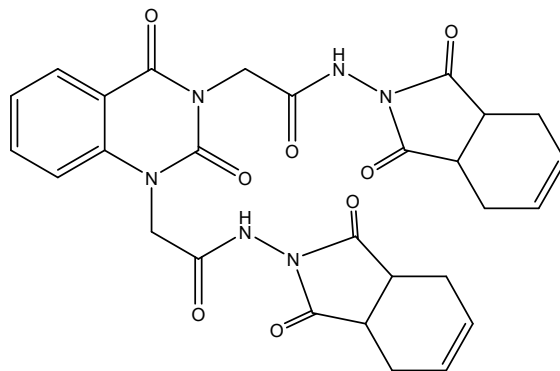
Line#:1 R.Time:4.4(Scan#:526)
 MassPeaks:554
 RawMode:Single 4.4(526) BasePeak:736(1159)
 BG Mode:None Group 1 - Event 1



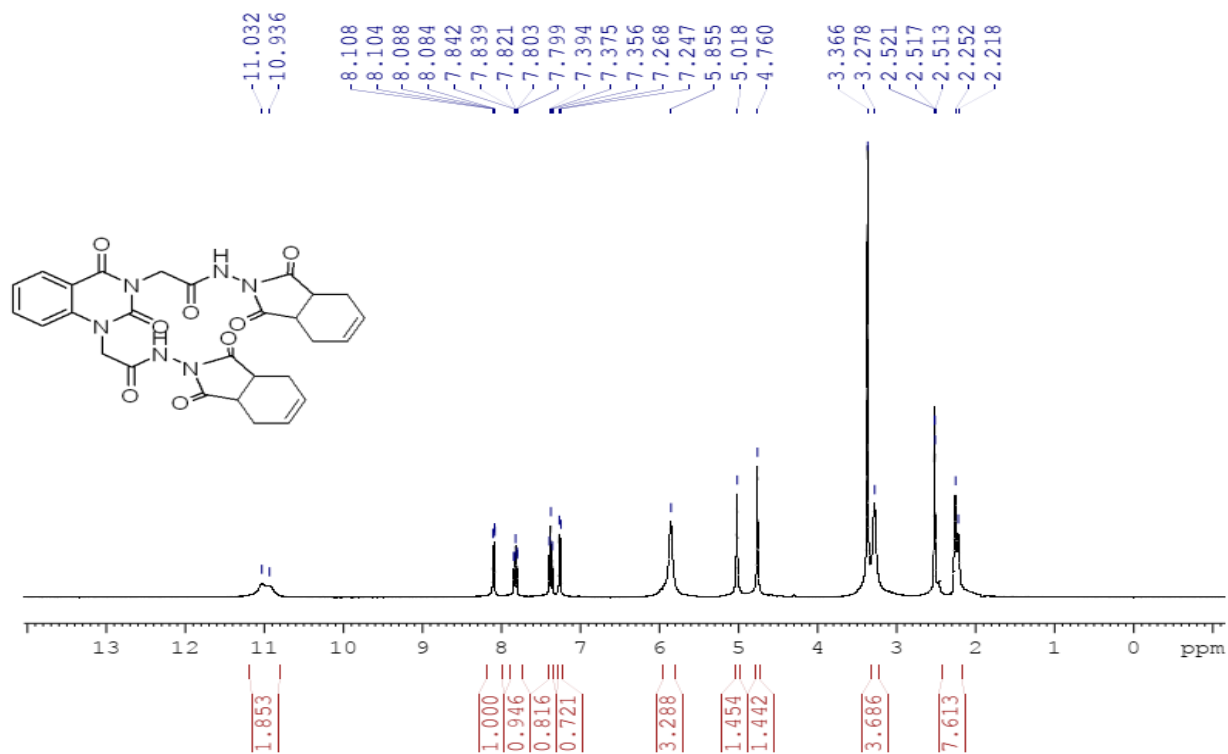
MS of compound (5a)

Compound (5b):-

-



muhammad omar-M2d-RR-hnmr



```
Current Data Parameters
NAME      muhammad omar-M2d-RR-hnmr
EXPNO     10
PROCNO    1

F1 - Acquisition Parameters
Date_     20211228
Time      13.14 h
INSTRUM   spect
PROBHD    E10618_0945 (
PULPROG   zgpg
TD         65536
SOLVENT    DMSO
NS         16
DS         4
SWH        8012.850000 Hz
WDW         EM
SSB         0.00445300 Hz
LB          4.08944680 sec
GB          128.40
PC          80.4000 usec
RG          6.50 usec
AQ          0.22 sec
SFO1       1.000000000 sec
H1          400.1024711 MHz
NUC1        13
P1          13.50 usec
PL1         19.00000000 W

F2 - Processing parameters
SI         65536
SF         400.1000000 MHz
WDW         EM
SSB         0.00 Hz
LB          0.00 Hz
GB          0.00 Hz
PC          1.00
```

¹H-NMR of compound (5b)

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DI Analysis Shimadzu Qp-2010 Plus

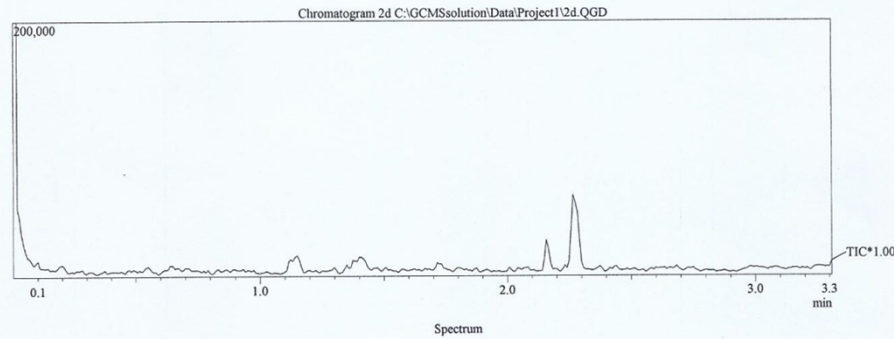
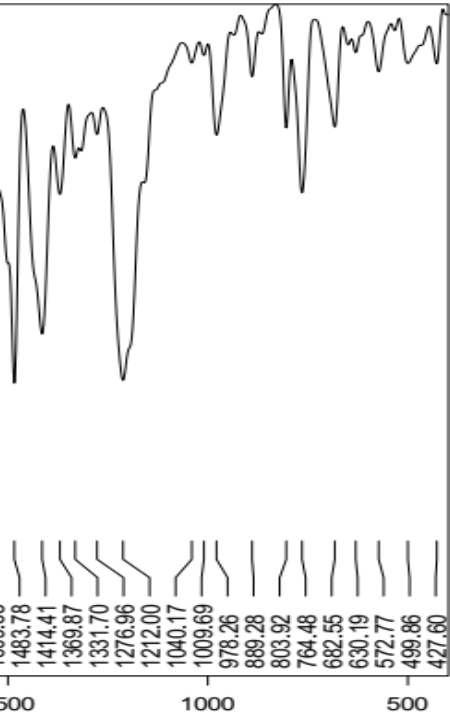
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 04:02:11 ص
Sample Name : 2d
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSsolution\Data\Project1\2d.QGD
Org Data File : C:\GCMSsolution\Data\Project1\2d.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.gct
SEndIfsModified by : Dr. Mai Younis
Modified : 15/01/2007 04:05:33 ص

Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time : -0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : -0.50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00

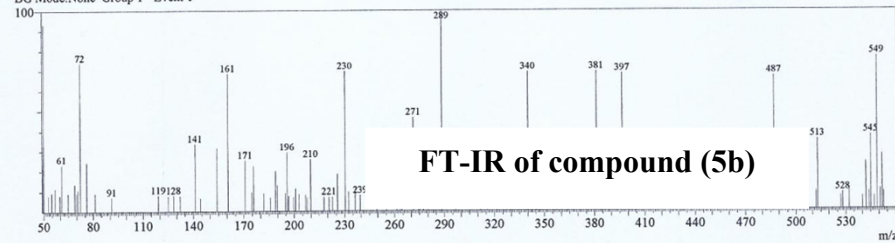
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Data\Project1\2d.QGD



Line#:1 R.Time:2.3(Scan#:275)
MassPeaks:109
RawMode:Single 2.3(275) BasePeak:289(1585)
BG Mode:None Group 1 - Event 1

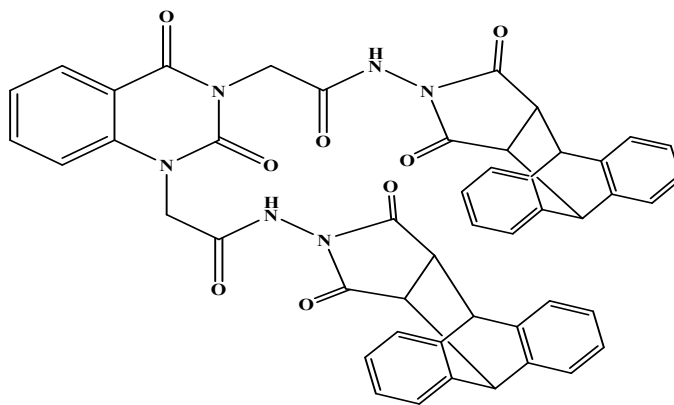


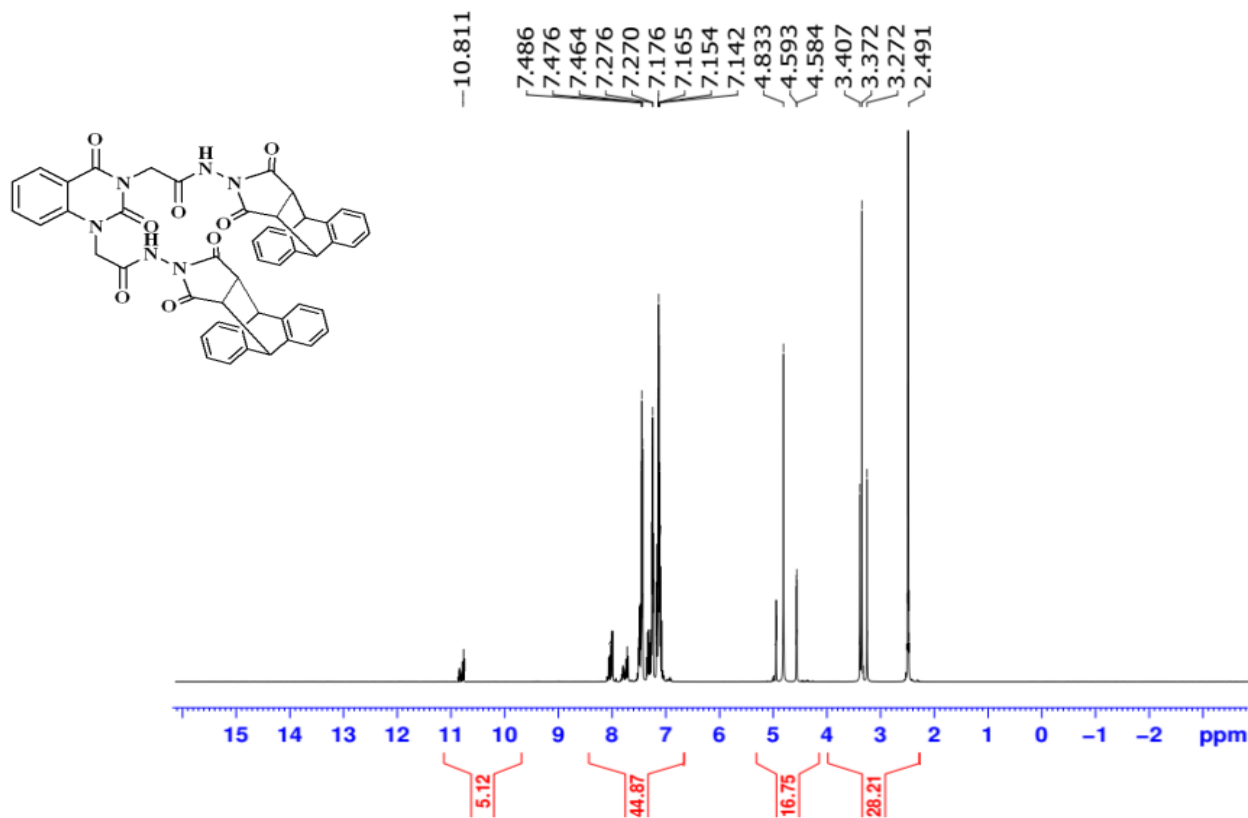
-

Compound (5c)

MS of compound (5b)

-





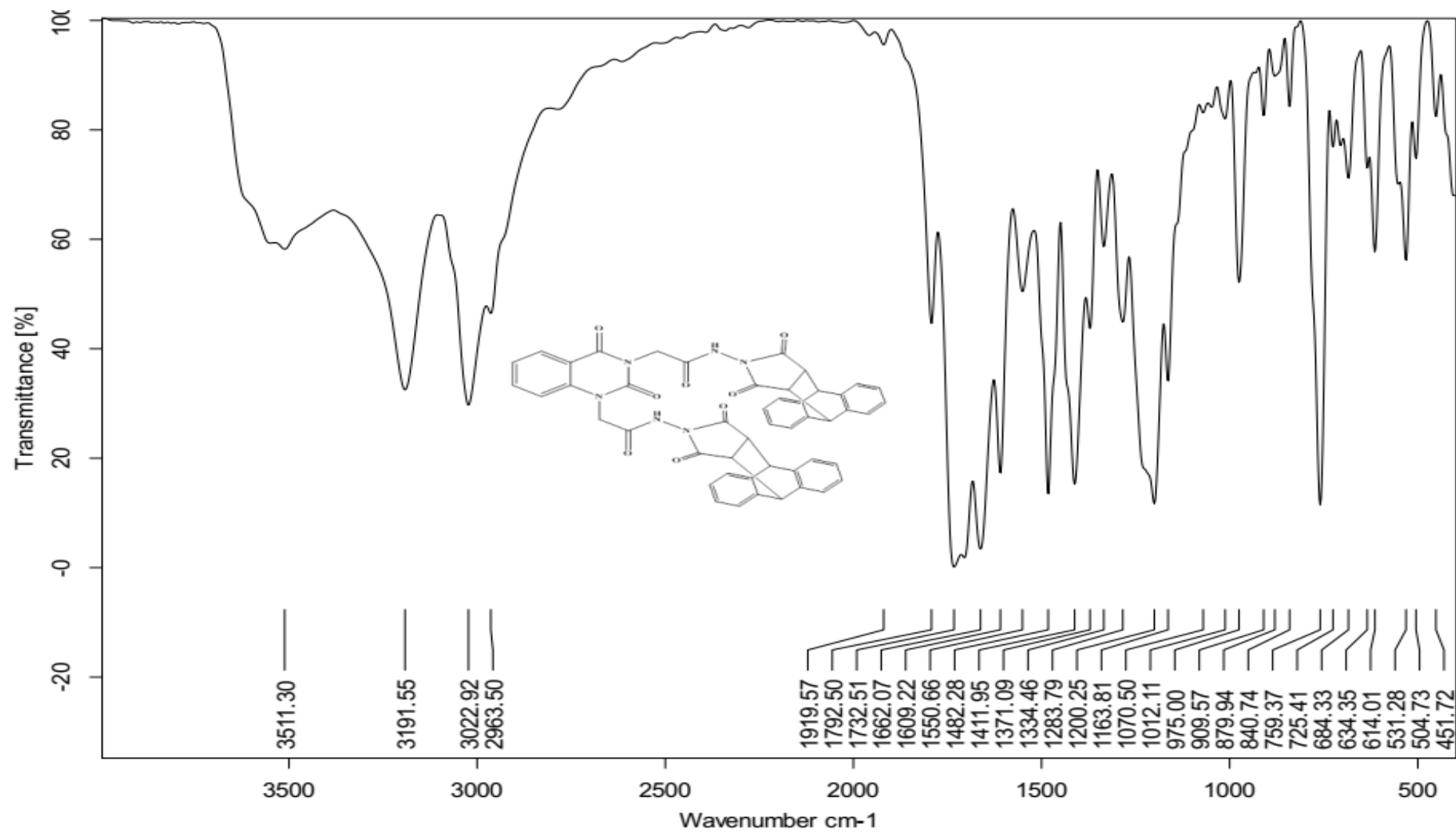
Current Data Parameters
NAME Feb17-2022
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220217
Time 10:14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 50
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 135
DW 62.400 usec
DE 6.50 usec
TE 313.3 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SF01 400.1324710 MHz
NUC1 1H
P1 12.00 usec
PLW1 22.00000000 W

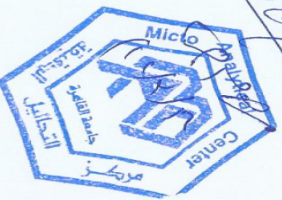
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR of compound (5c)



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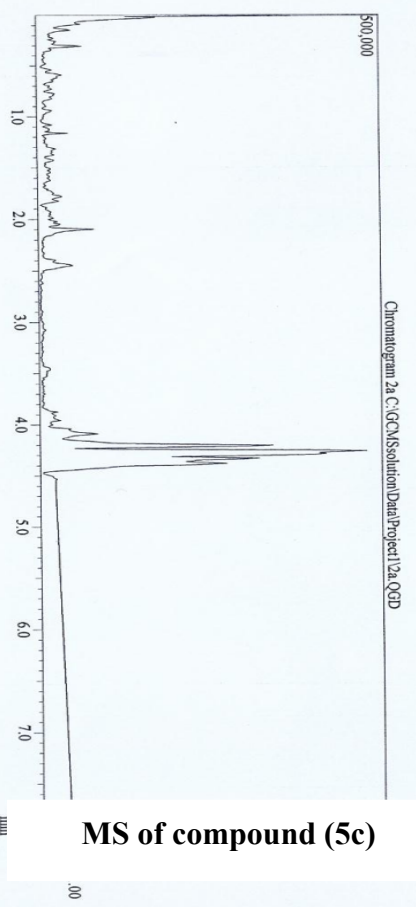
DI Analysis
Shimadzu Qp-2010 Plus



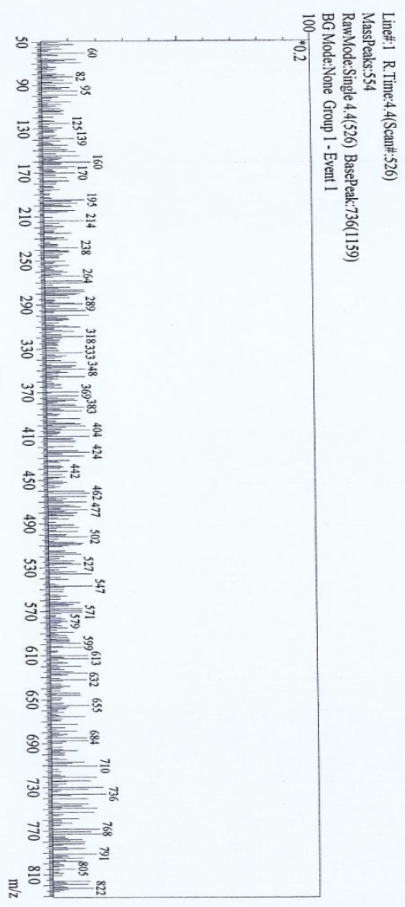
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 03:55:58
Sample Name : 2a
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSolution\Data\Project1\2a.QGD
Org Data File : C:\GCMSolution\Data\Project1\2a.QGD
Method File : C:\GCMSolution\Data\Project1\Hght Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\Hght Temperature Op
Report File :
Turning File : C:\GCMSolution\System\Time1_default.qgr
Standard/Modified by : Dr. Mai Younis
Modified : 15/01/2007 04:00:33

Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
-Group 1 - Event 1-
Start Time : 0:00min
End Time : 1:0:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 900.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project1\2a.QGD



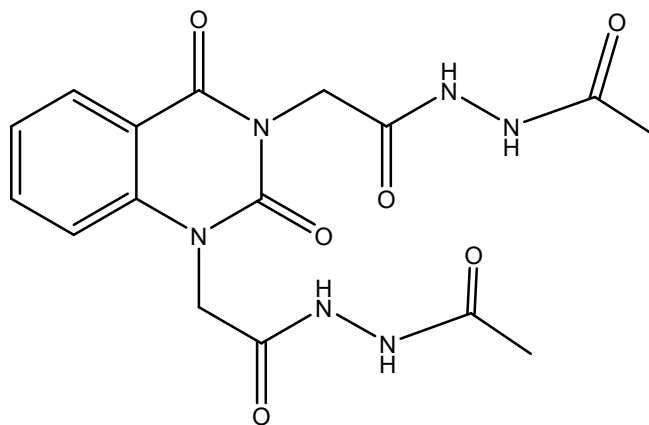
MS of compound (5c)



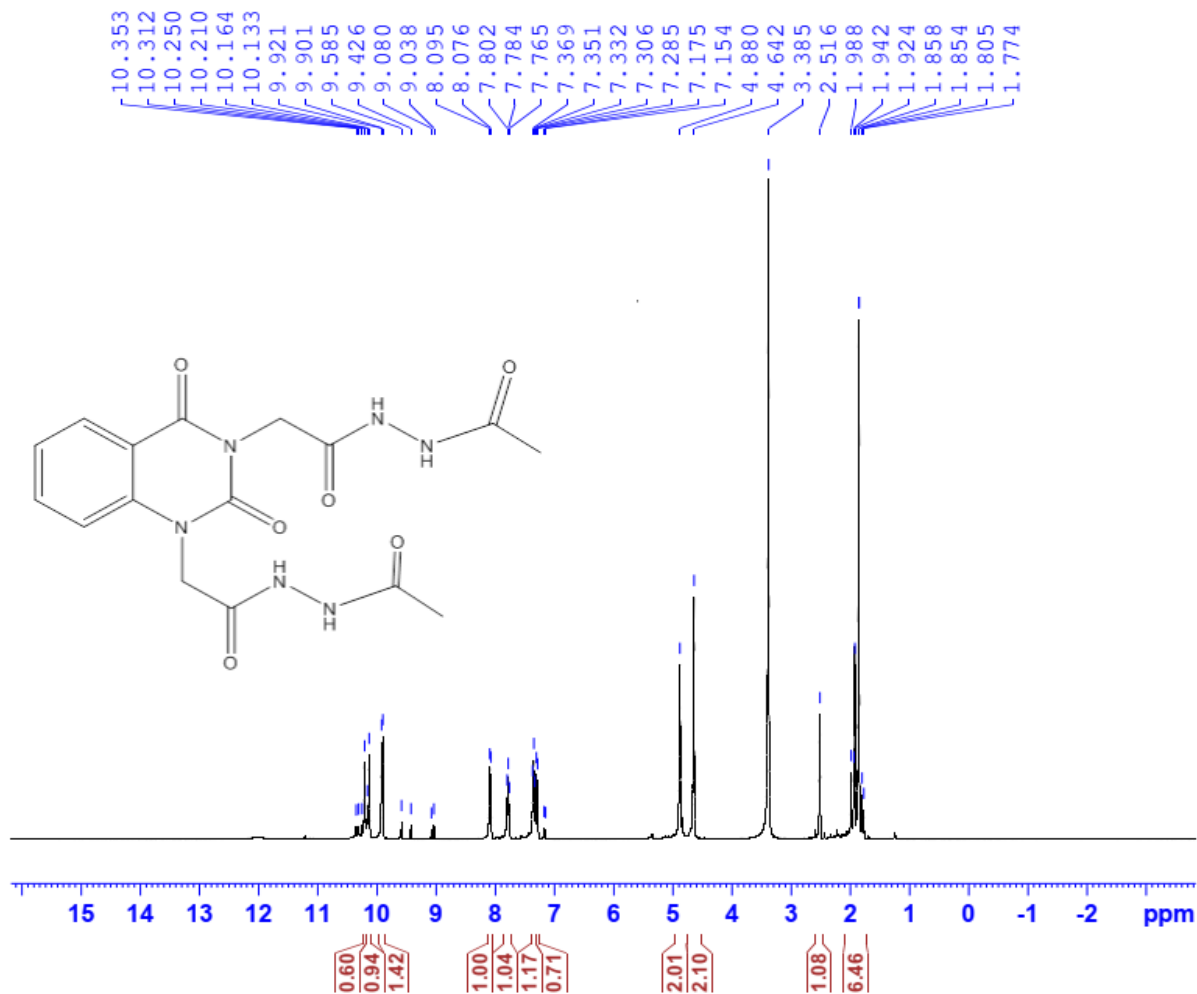
Line# 1 R Time: 4.4(Scan# 526)
MassPeak: 54
RawMode: Single 4.4(526) BasePeak: 736(1159)
BG Mode: None Group 1 - Event 1

-

Compound (6a)



Mohamed Omar-10-Hnmr-RR

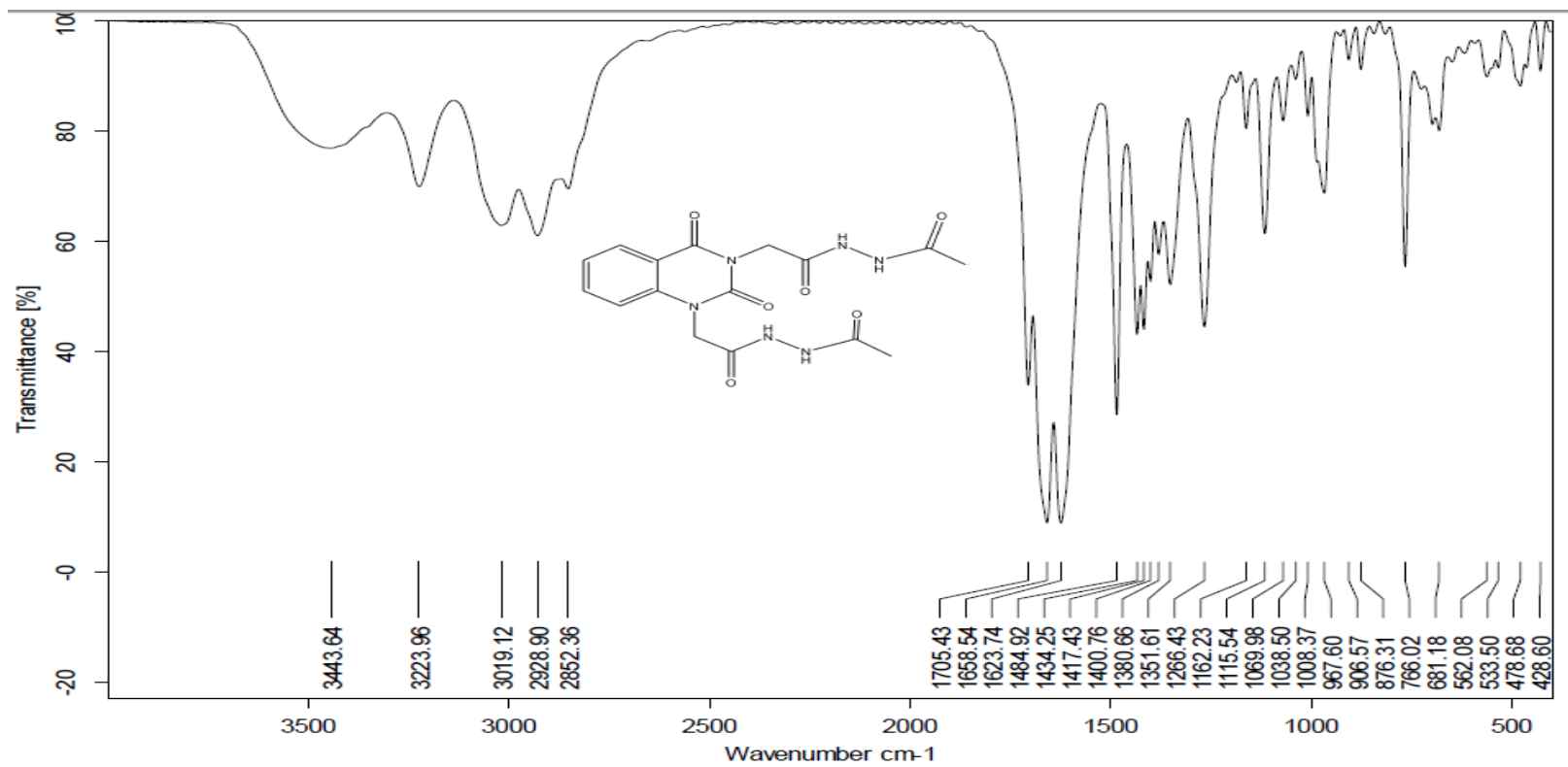


Current Data Parameters
NAME Mohamed Omar-10-Hnmr-RR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220830
Time 11.34 h
INSTRUM spect
PROBHD E108618_0945 (4
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.800 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 112.56
DM 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TDC 400.202471 MHz
SFO1 400.202471 MHz
NUC1 1H
P1 13.50 usec
PLW1 18.00000000 W

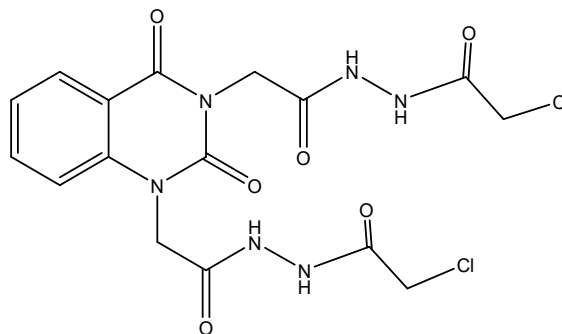
F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

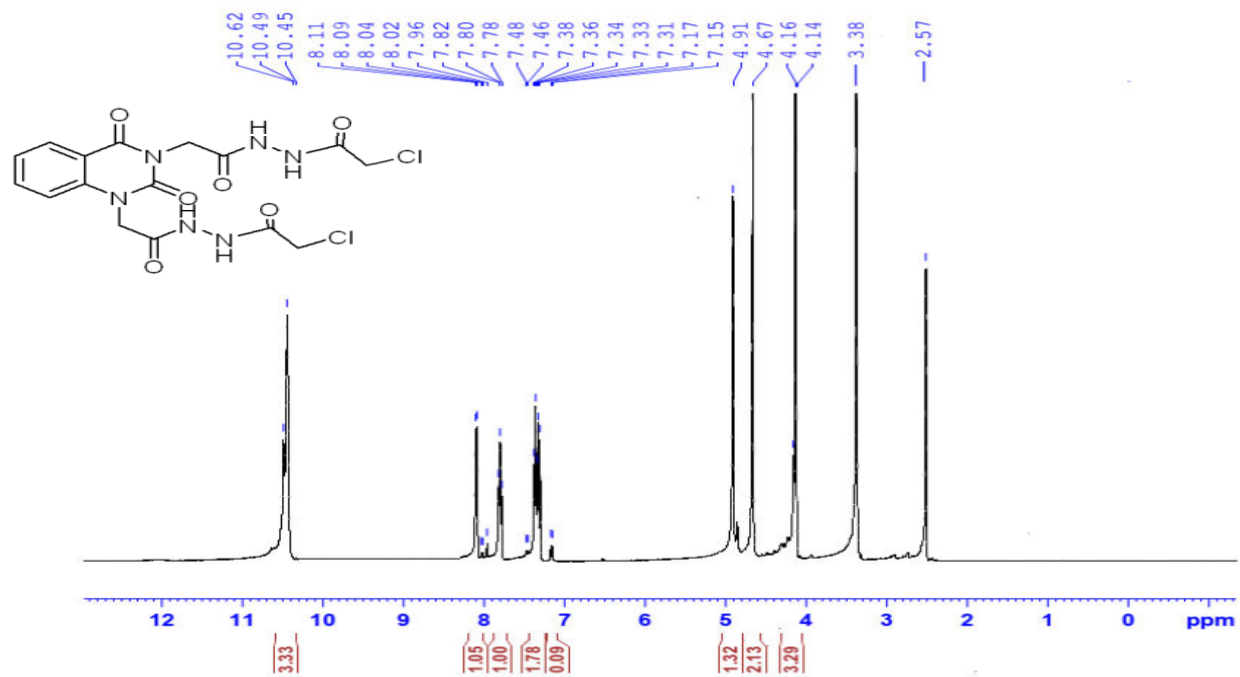
¹H-NMR of compound (6a)



-

FT-IR of compound (6a)



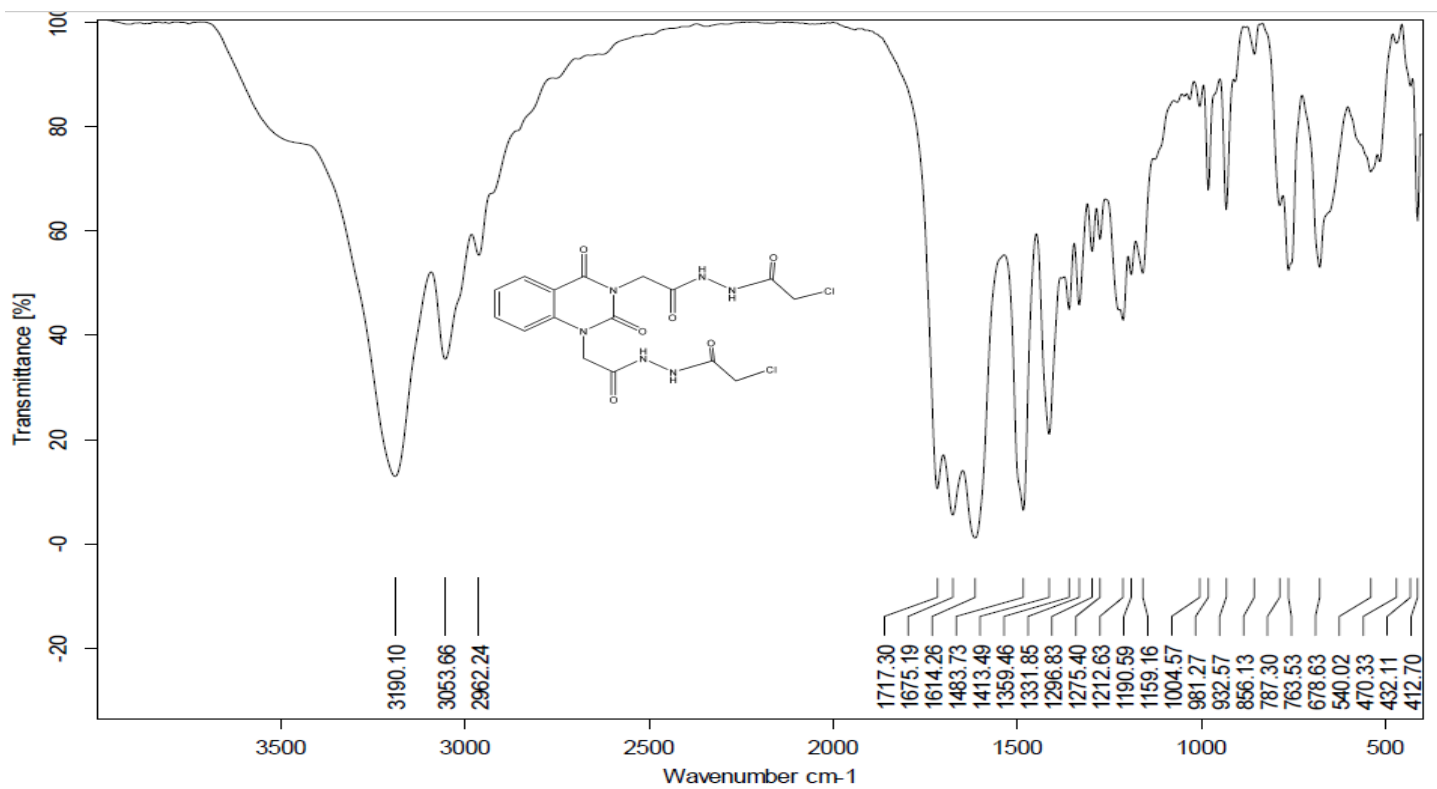


Current Data Parameters
NAME Mohamed Omar - M7 - Hnm
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220115
Time 19:06 h
INSTRUM spect
PROBHD z108618_0945 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.081465 sec
RG 120.93
DK 62.400 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.202412 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR of compound (6b)

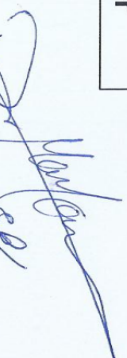


FT-IR of compound (6b)

15-Jan-07 02:56:27

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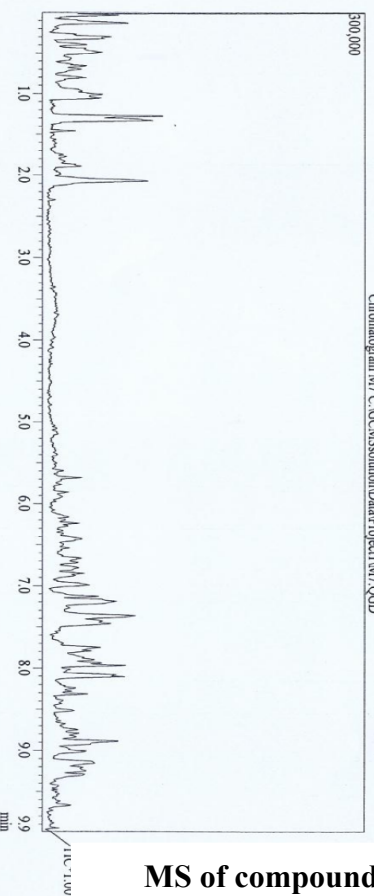


Sample Information
Analyzed by : Dr. Maq Youns
Sample Name : 15/01/2007 02:56:02
Sample ID : M7
Customer Name : Dr. Mohamed Omar - Science - Qena
Data File : C:\GCMSolution\Data\Project1\M7.QGD
Org Data File : C:\GCMSolution\Data\Project1\M7.QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File :
Timing File : C:\GCMSolution\System\Tune1_default.qgt
Standard/Modified by : Dr. Maq Youns
Modified : 15/01/2007 02:46:02

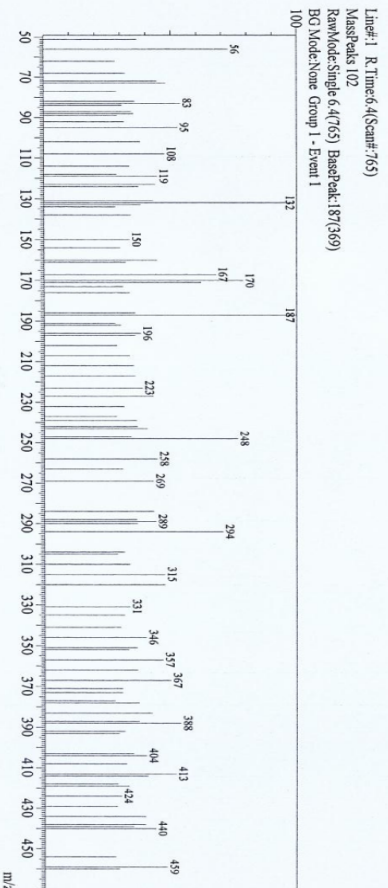
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
MS Table)
--Group 1 - Event 1--
Start Time : 0.00min
End Time : 10.00min
Scan :
ACQ Mode :
Event Time : 0.50sec
Scan Speed :
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSolution\Data\Project1\M7.QGD

Chromatogram M7 C:\GCMSolution\Data\Project1\M7.QGD

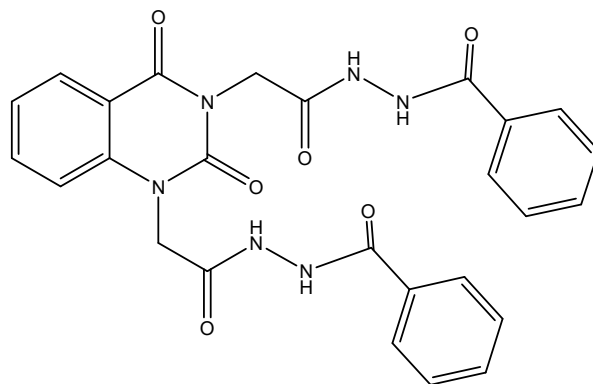


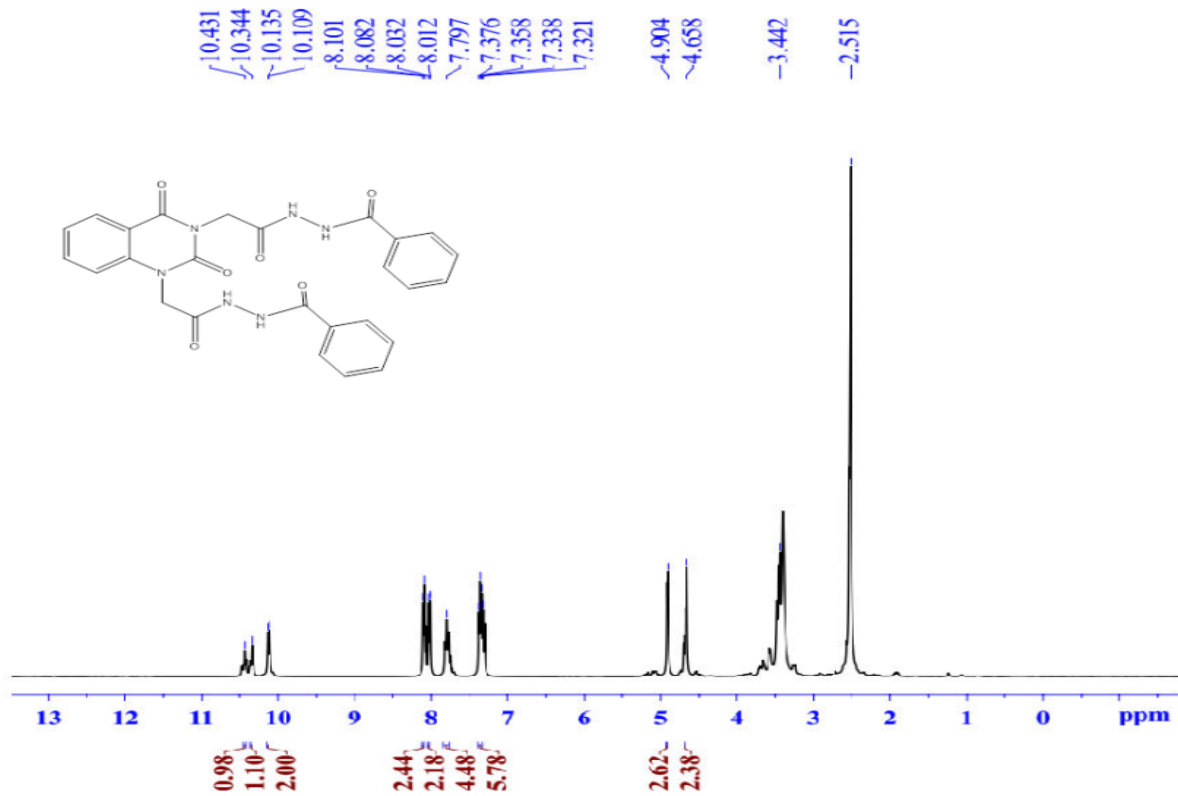
MS of compound (6b)



-

Compound (6c)



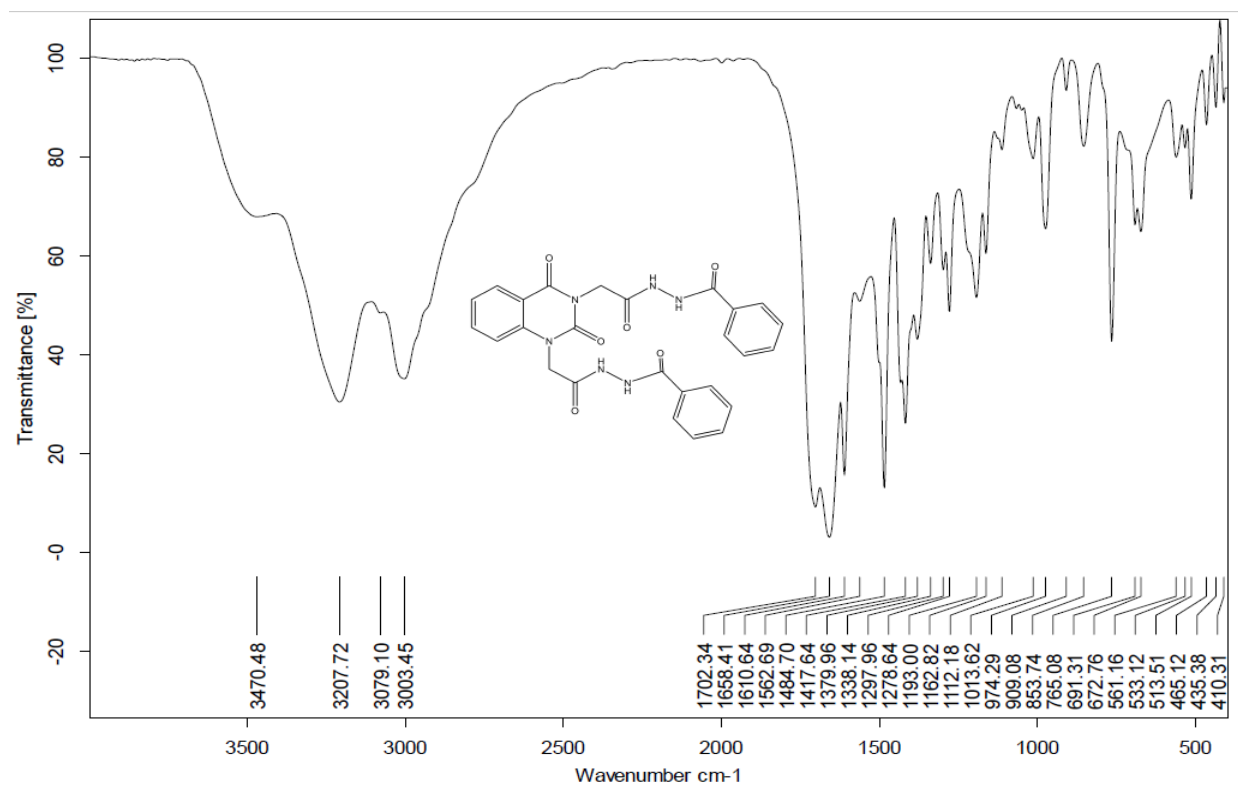


Current Data Parameters
NAME Mohamed Omar-M9-DMSO-proton-D
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211121
Time 12:42 h
INSTRUM spect
PROBHD 1Hocx1_0945 f
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 40.97
DM 62.400 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TSD 1
SFO1 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

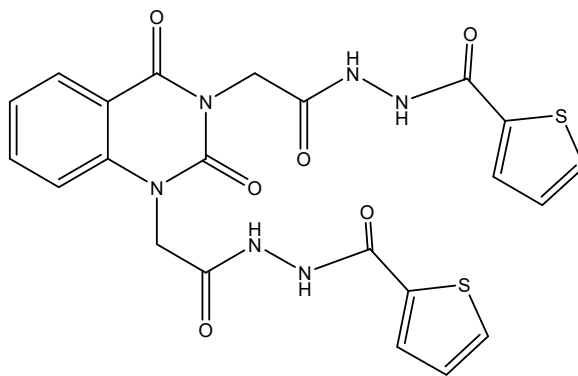
¹H-NMR of compound (6c)

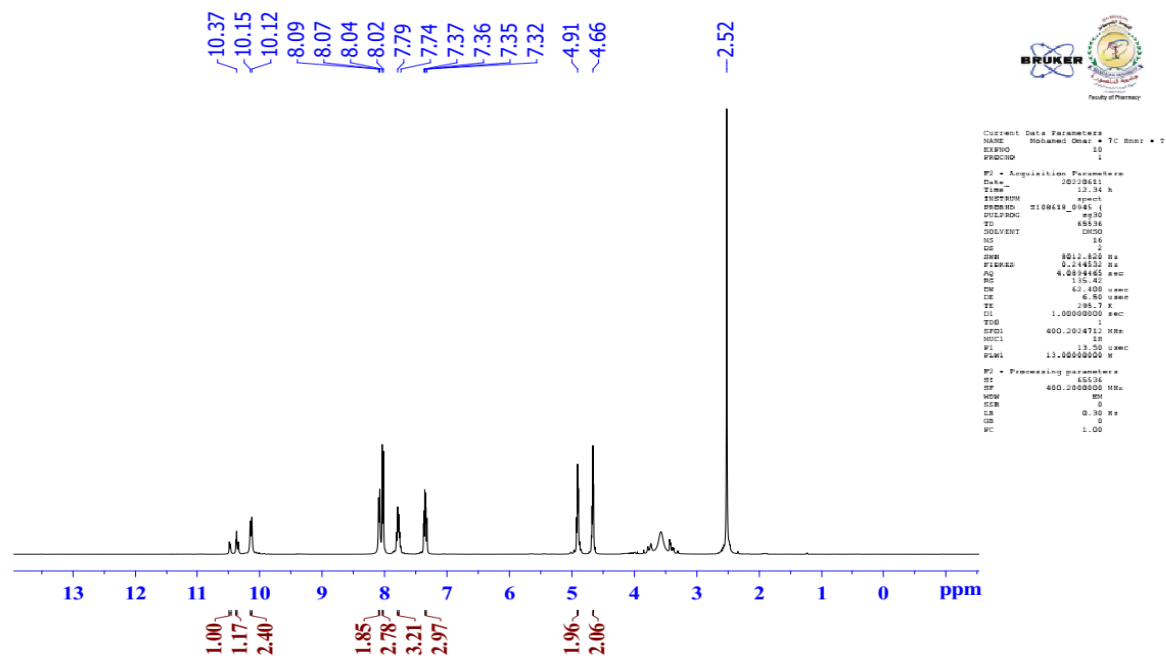


FT-IR of compound (6c)

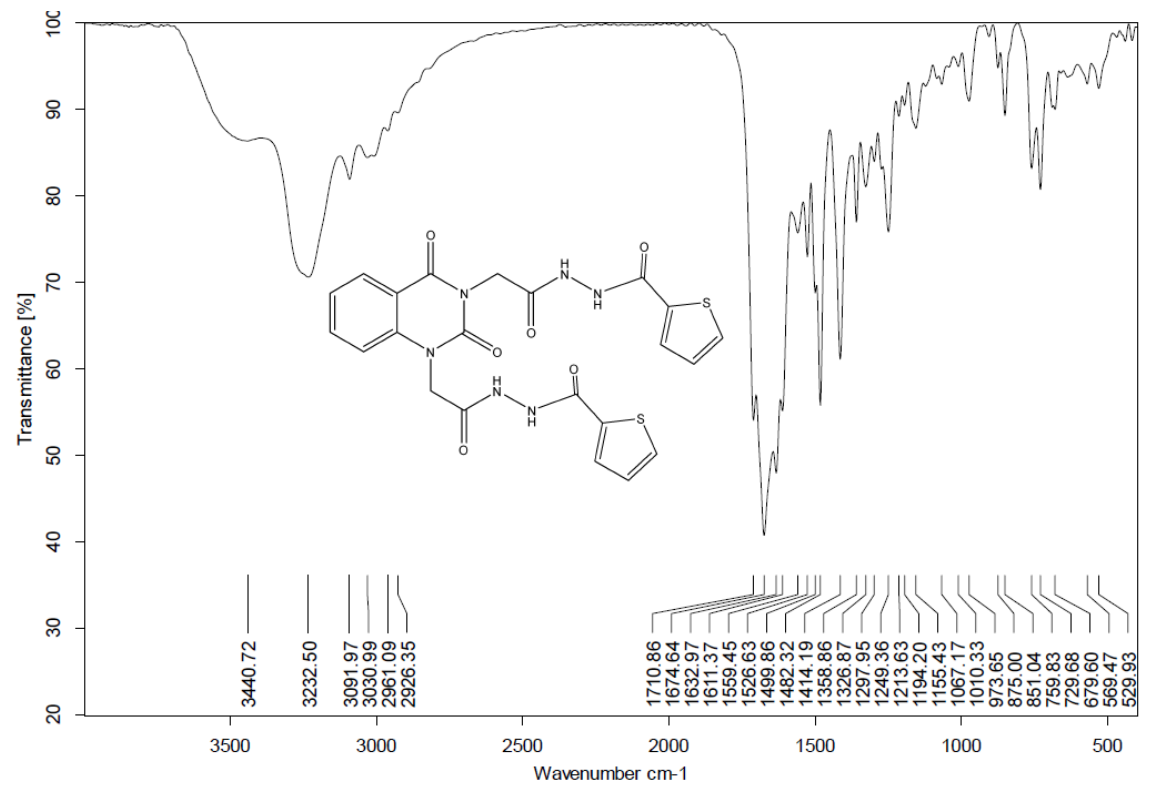
-

Compound (6d)





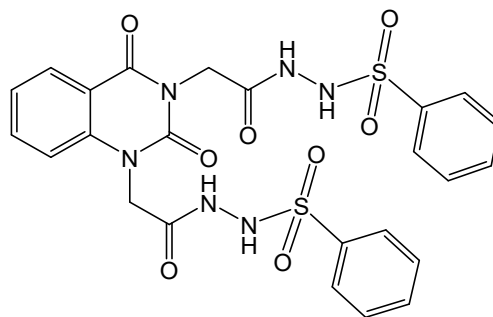
¹H-NMR of compound (6d)

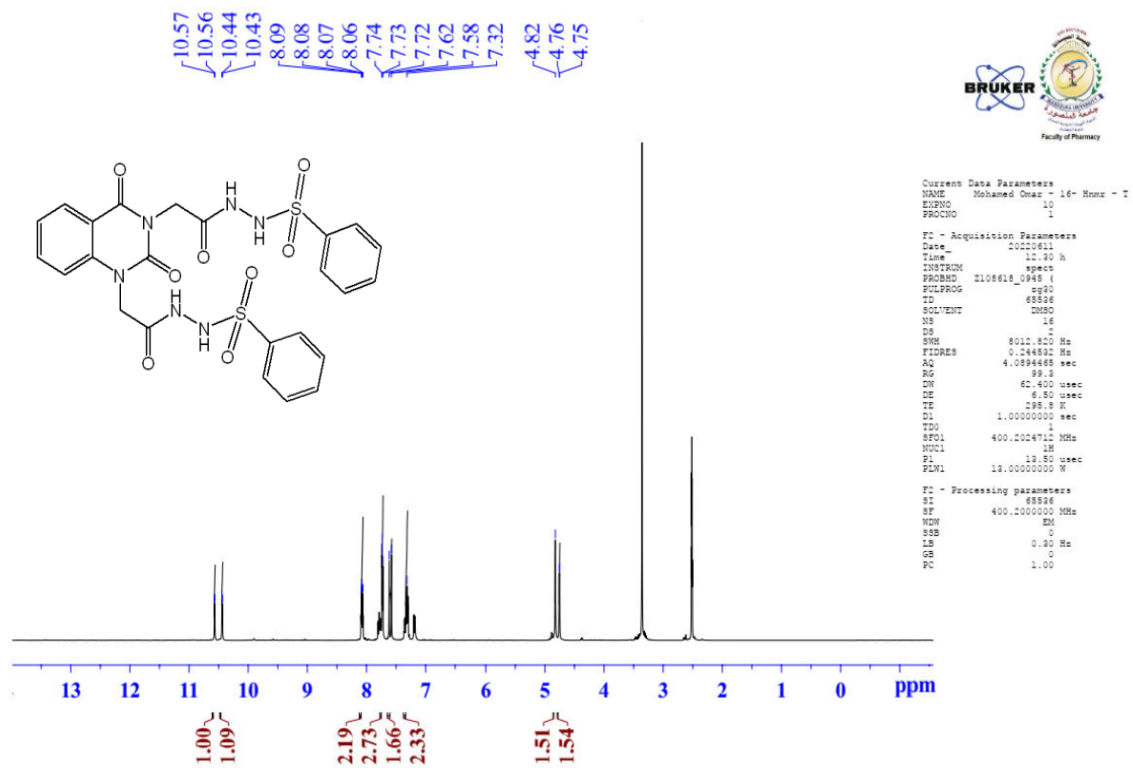


FT-IR of compound (6d)

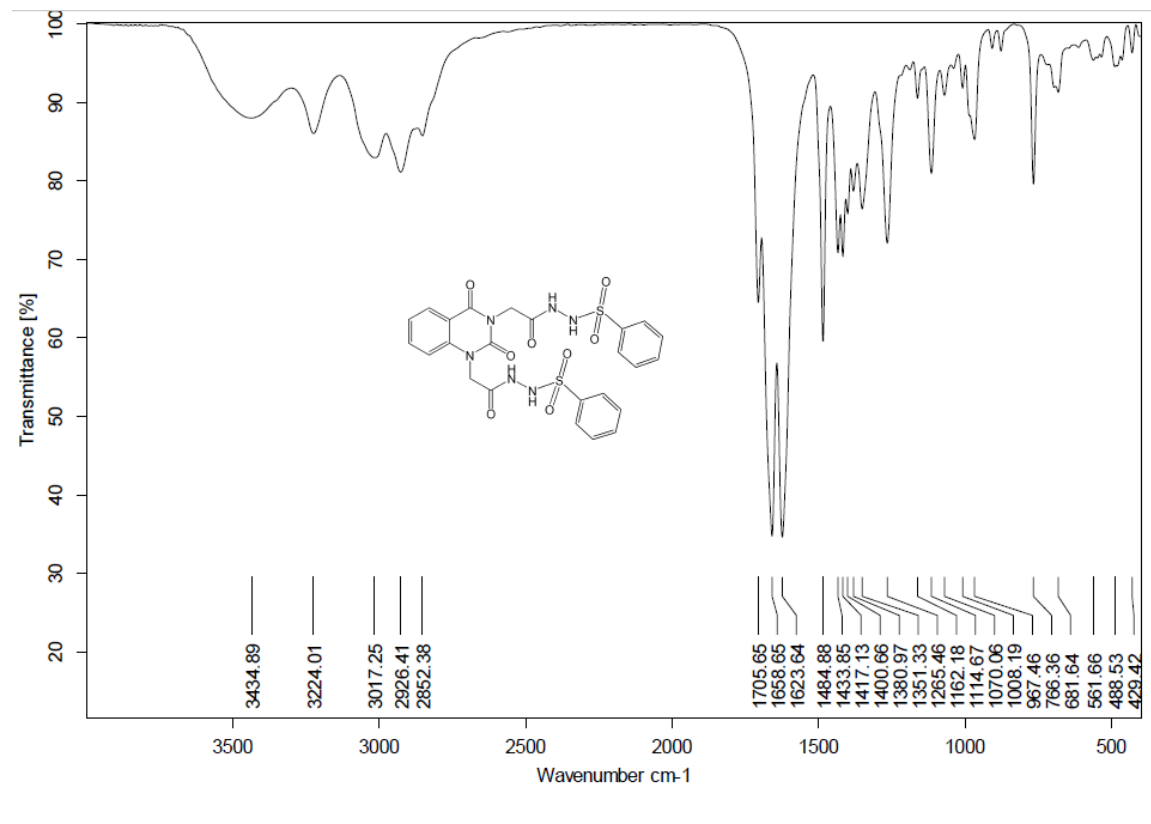
-

Compound (6e)





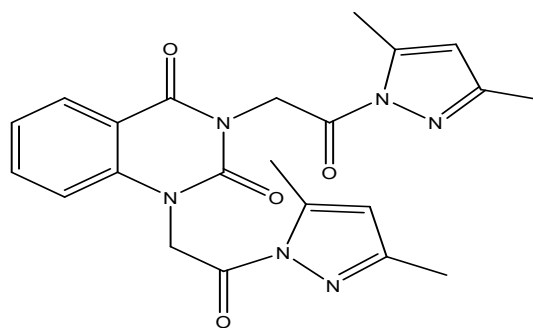
¹H-NMR of compound (6e)

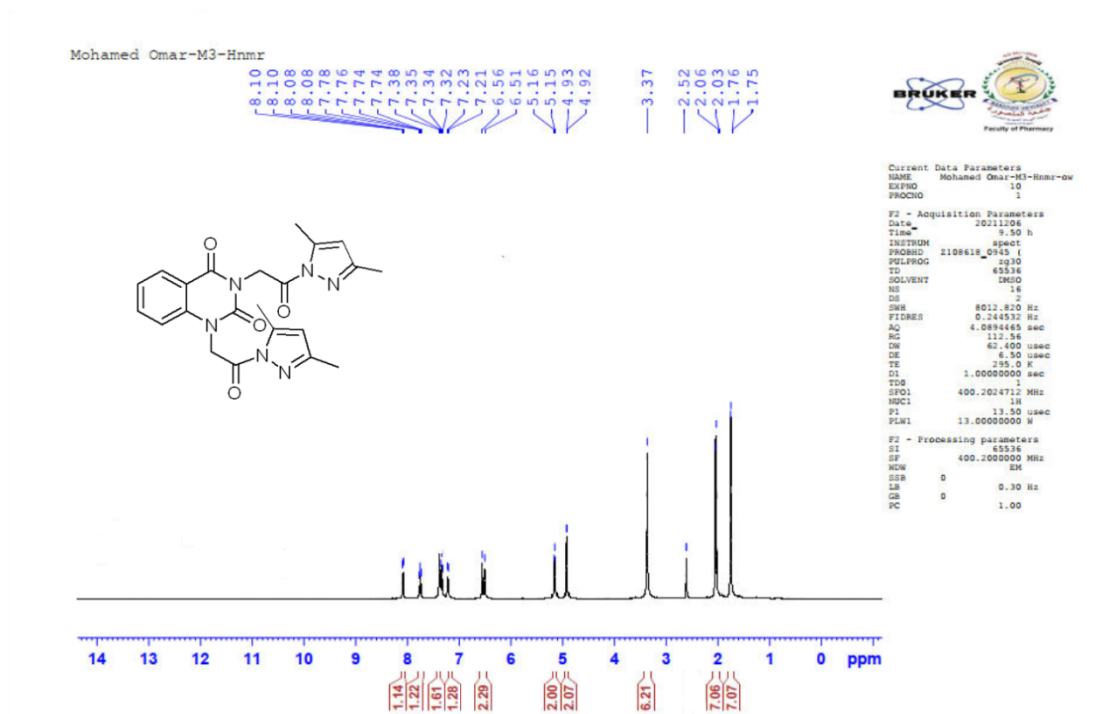


FT-IR of compound (6e)

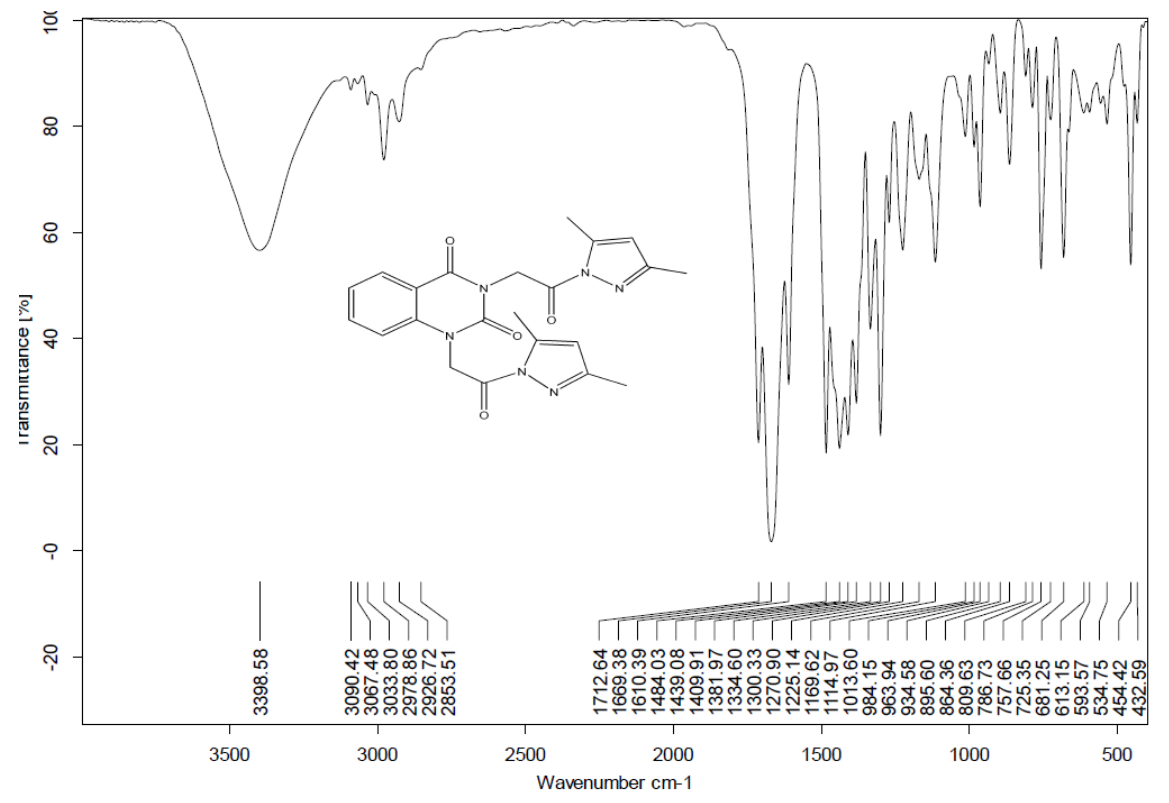
-

Compound (7a)





¹H-NMR of compound (7a)



FT-IR of compound (7a)

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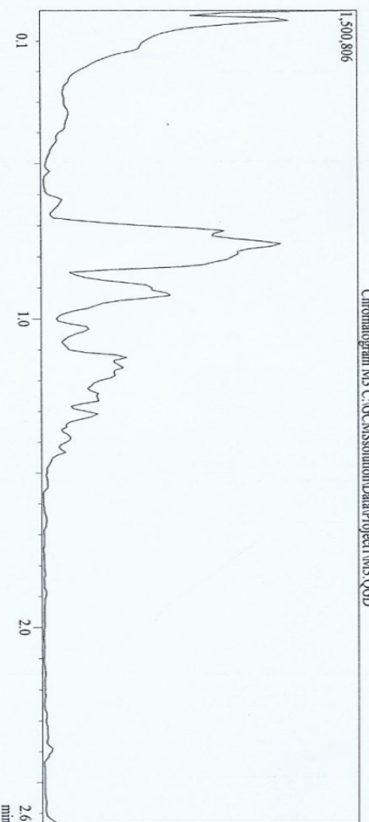
DI Analysis
Shimadzu QP-2010 Plus

Dr. Mai Younis
8/10/07

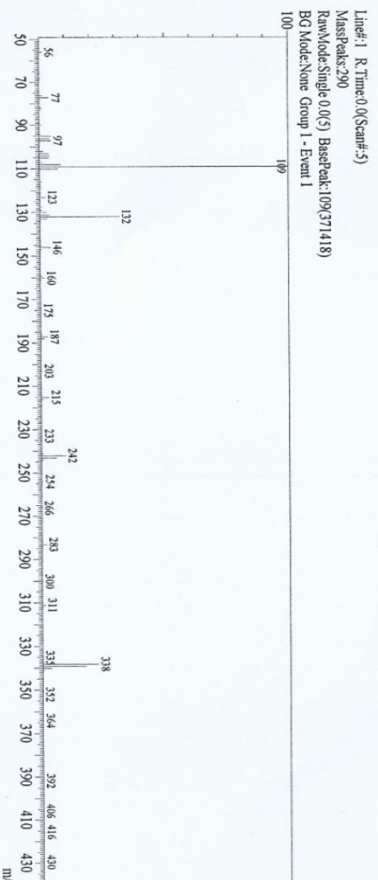
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 15/01/2007 02:12:13
 Sample Name : M3
 Sample ID :
 Customer Name : Dr. Mohamed Omar - Science - Qena
 Data File : C:\GCMSolution\Data\Project\M3.QGD
 Org Data File : C:\GCMSolution\Data\Project\M3.QGD
 Method File : C:\GCMSolution\Data\Project\High Temperature Op
 Org Method File : C:\GCMSolution\Data\Project\High Temperature Op
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
 Standard/Modified by : Dr. Mai Younis
 Modified : 15/01/2007 02:14:54

Method
 Analytical Line 1
 IonSource Temp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 Scan : Scan
 ACO Mode : -0.50sec
 Event Time :
 Scan Speed : 1250
 Start m/z : 50.00
 End m/z : 600.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project\M3.QGD

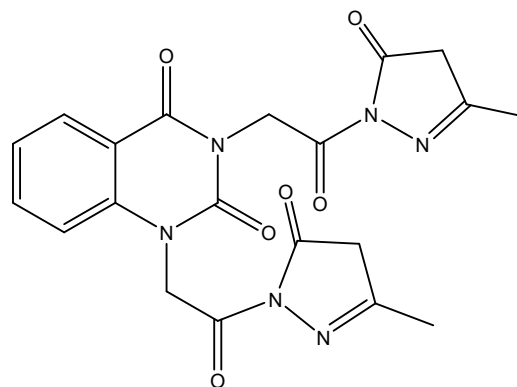


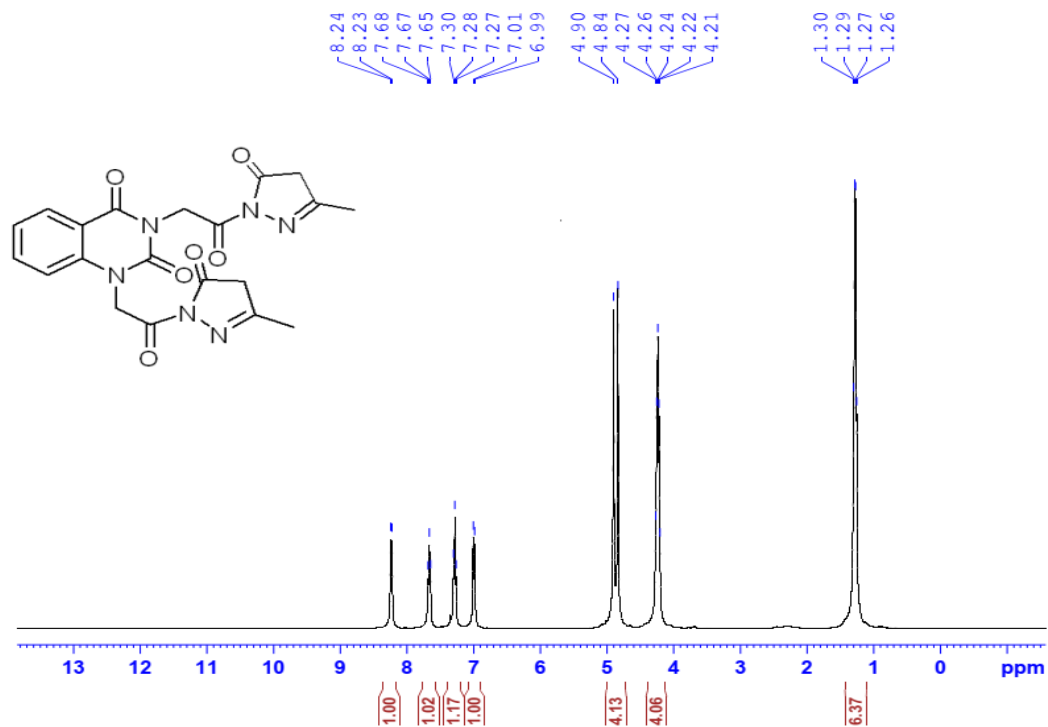
MS of compound (7a)



-

Compound (7b)





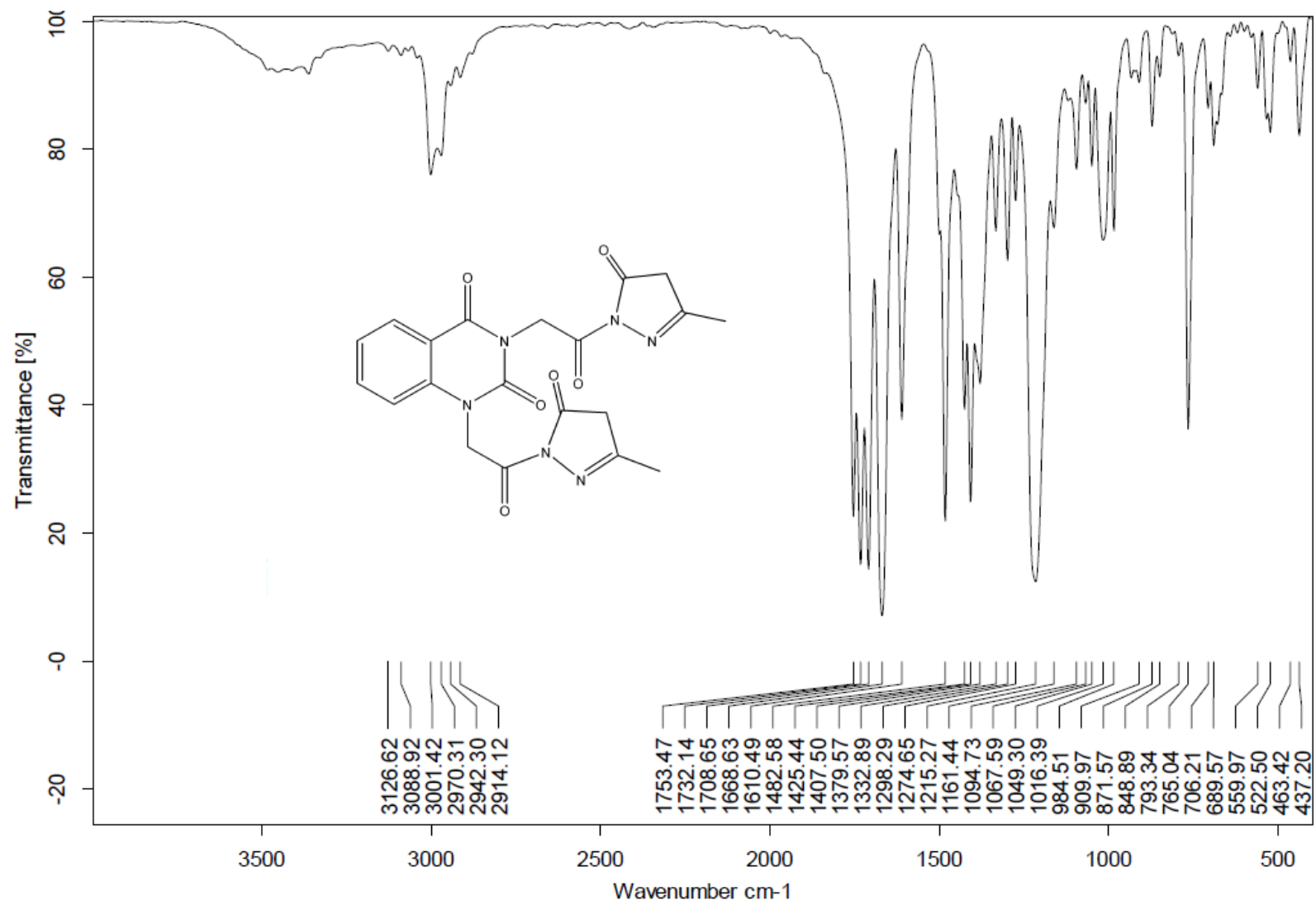
```

Current Data Parameters
NAME      Mohammed Omar-M9-DMSO-proton-D
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20111121
Time     11:42 h
INSTRUM  spect
PROBHD   Z108618_0948 H
PULPROG  zg30
RG        65326
AQ        0.0013
SOLVENT  DMSO
NS        16
DS        4
SFO      801.130000 MHz
SFRES    0.00448220 MHz
AQRES    4.08944650 sec
RGRES    60.37
DQRES    62.400000 usec
RGRES    6.50 usec
SFORES    285.7 Hz
SFORES    1.00000000 sec
SFORES    400.2024711 MHz
NUC1     13
NUC2     15
P1RES    13.50 usec
P1M1     13.00000000 M

F2 - Processing parameters
SFO      801.130000 MHz
SFRES    400.2024711 MHz
AQRES    4.08944650 sec
RGRES    60.37
DQRES    62.400000 usec
RGRES    6.50 usec
SFORES    285.7 Hz
SFORES    1.00000000 sec
SFORES    400.2024711 MHz
NUC1     13
NUC2     15
P1RES    13.50 usec
P1M1     13.00000000 M
  
```

¹H-NMR of compound (7b)



FT-IR of compound (7b)

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DI Analysis
Shimadzu QP-2010 Plus



Sample Information

Analyzed by : Dr. Mai Younis
Analyzed : 15/01/2007 03:26:47 م
Sample Name : M9
Sample ID :
Customer Name : Dr. Mohamed Omar - Science - Quena
Data File : C:\GCMSolution\Data\Project1\M9_QGD
Org Data File : C:\GCMSolution\Data\Project1\M9_QGD
Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
Report File : C:\GCMSolution\System1\default.qgf
Tuning File : C:\GCMSolution\System1\default.qgf
SENDITSM: Modified by : Dr. Mai Younis
Modified : 15/01/2007 03:26:46 م

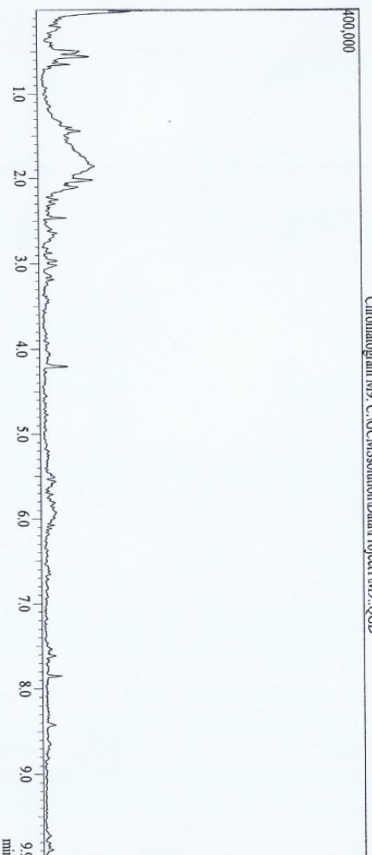
Method

Analytical Line 1
IonSource Temp : 250.00 °C
MS Table
--Group 1 - Event 1--
Start Time : 0:00min
End Time : 1:00:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 2000
Start m/z : 50.00
End m/z : 300.00

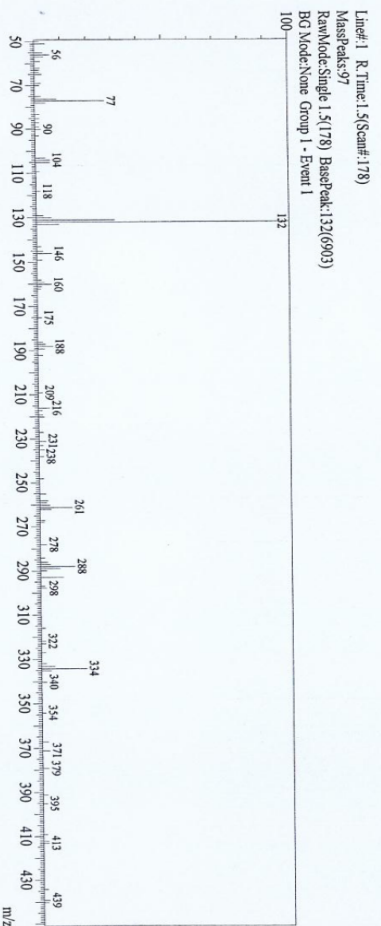
Electron Voltage : 70 eV
Ionization Mode : EI

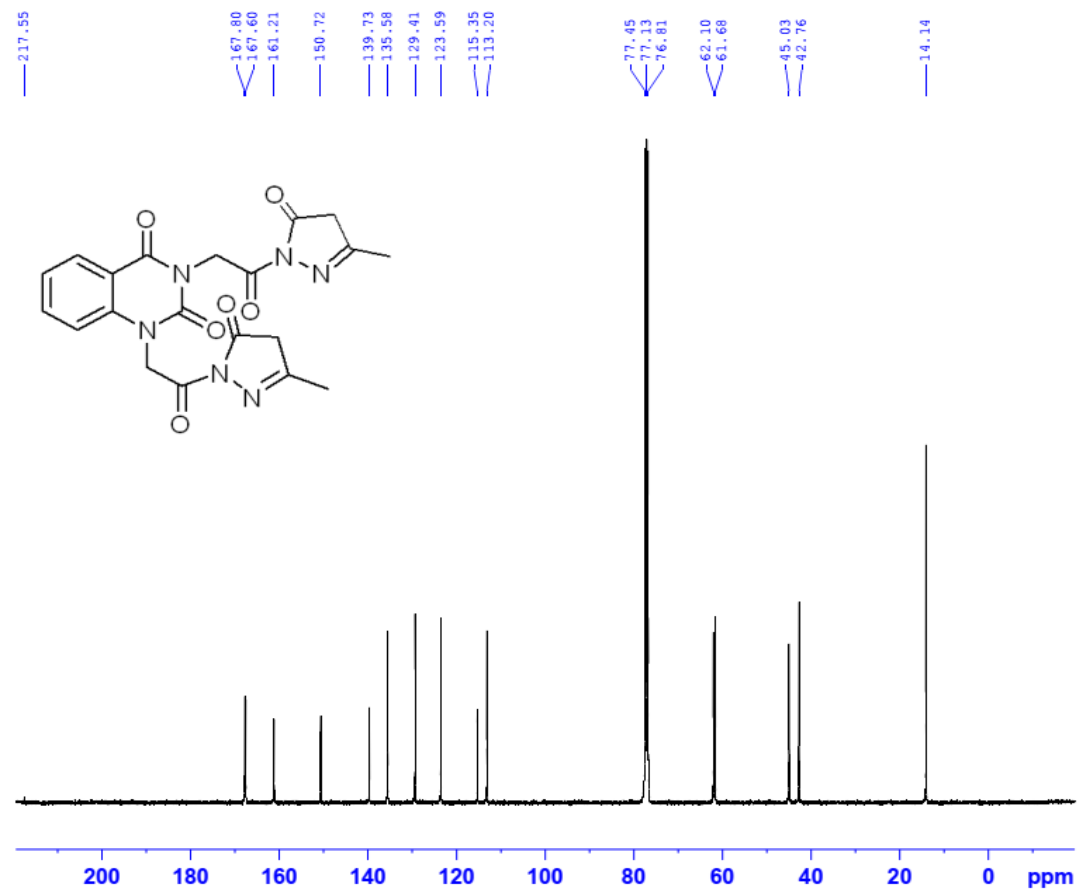
C:\GCMSolution\Data\Project1\M9_QGD

Chromatogram M9 C:\GCMSolution\Data\Project1\M9_QGD



MS of compound (7b)





Current Data Parameters
 NAME Mohamed Omar-M9-AS-carbon
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211206
 Time 22.08 h
 INSTRUM spect
 PROBHD Z106618_0945 (4
 FILPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2100
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 1.3631488 sec
 RG 197.77
 DM 20.800 usec
 DE 6.50 usec
 TE 295.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SF01 100.6404331 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 47.00000000 W
 SF02 400.2016008 MHz
 NUC2 1H
 CPDPRG12 waltz16
 PCPDC 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.29249999 W
 PLW13 0.14713000 W

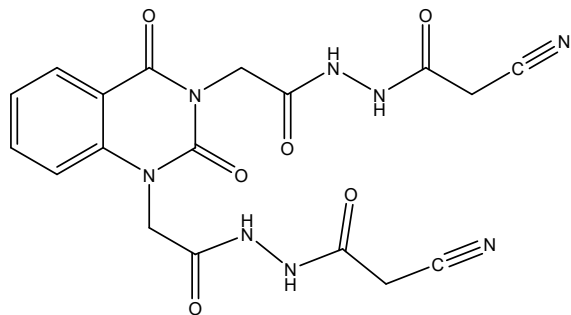
F2 - Processing parameters
 SI 32768
 SF 100.6303700 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

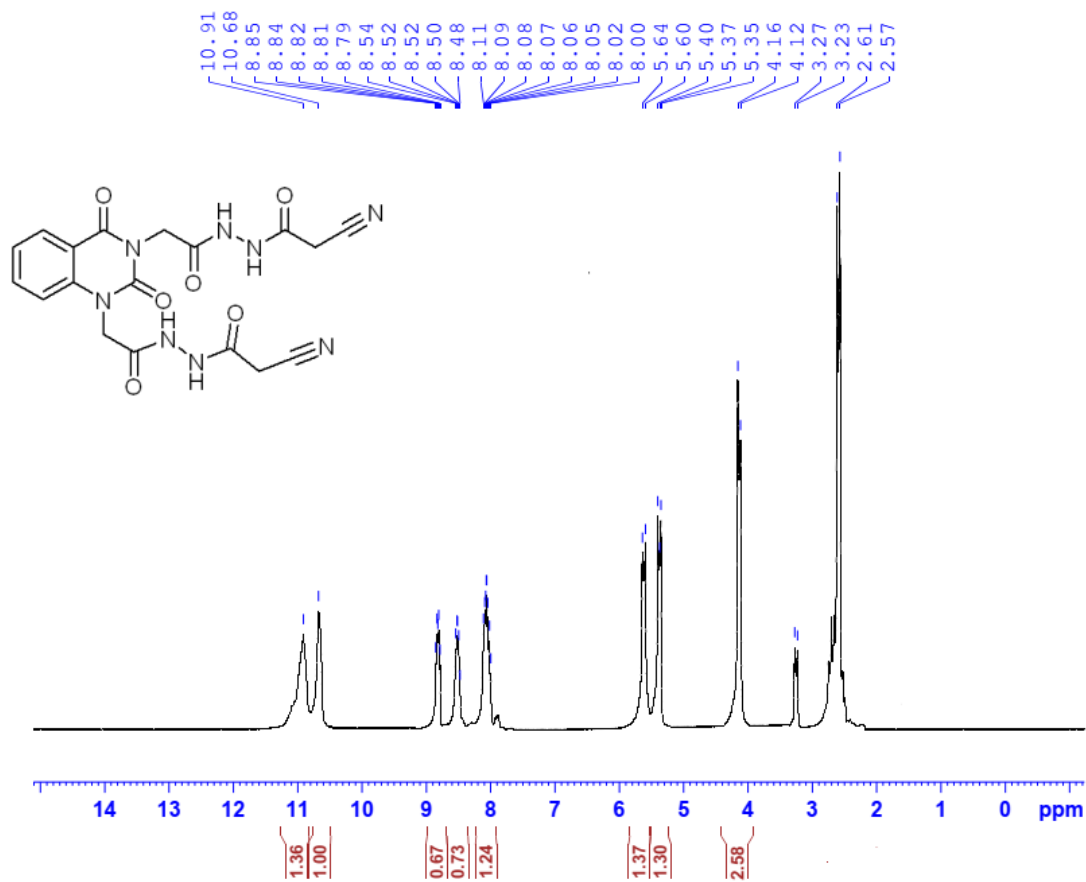
C13-NMR of compound (7b)

-

-

Compound (8)



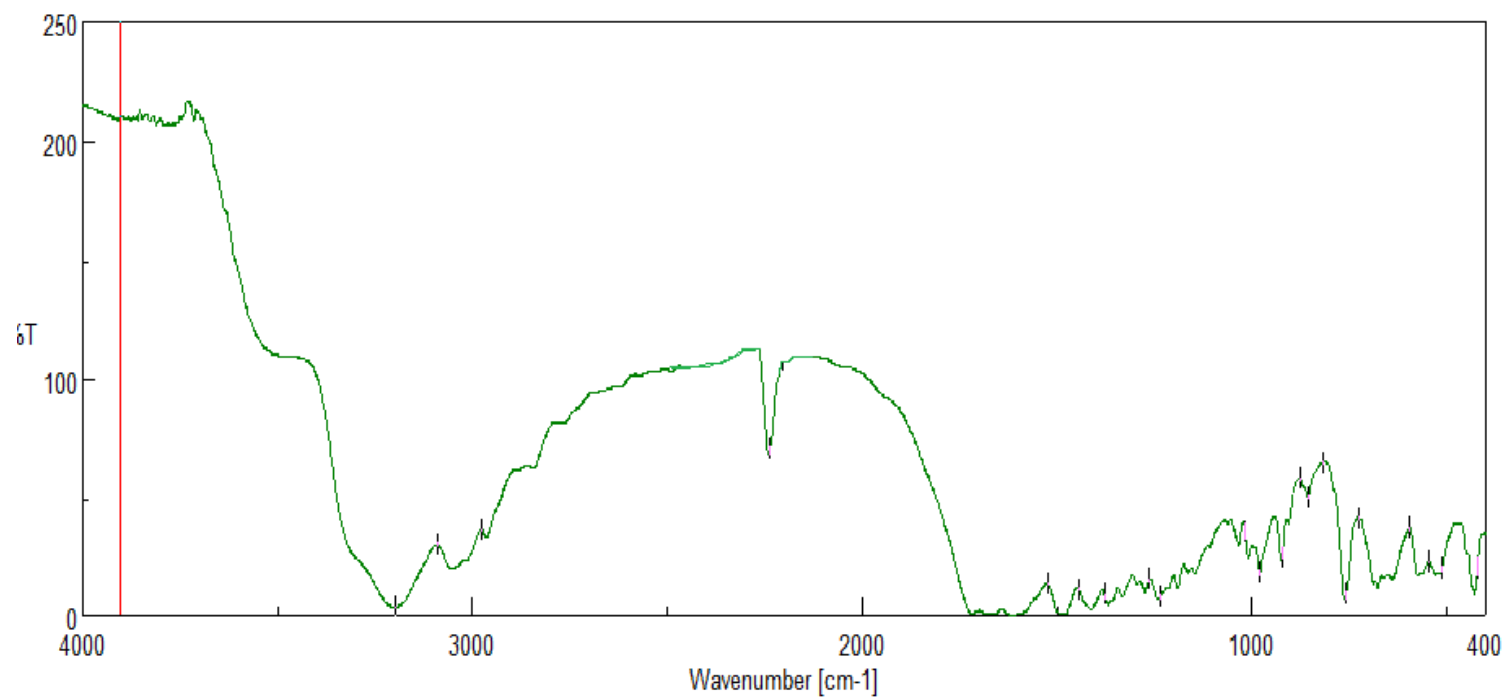


Current Data Parameters
 NAME Mohamed Omar-M 4-Hnmr-ov
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211101
 Time 19.28 h
 INSTRUM spect
 PROBRD 2108618_0948 ()
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO-d6
 NS 16
 DS -
 SFR 8012.800 Hz
 FIDRES 0.244502 Hz
 AQ 4.0894465 sec
 RG 80.00
 SH 62.400 usec
 DE 6.50 usec
 TE 292.9 K
 DL 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 12.50 usec
 PLW1 18.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1996977 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

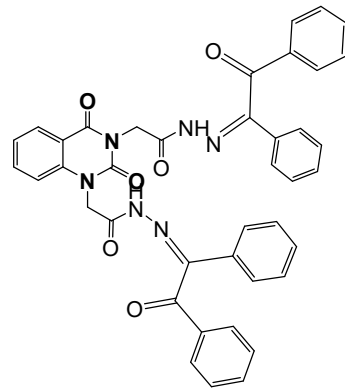
¹H-NMR of compound (8)



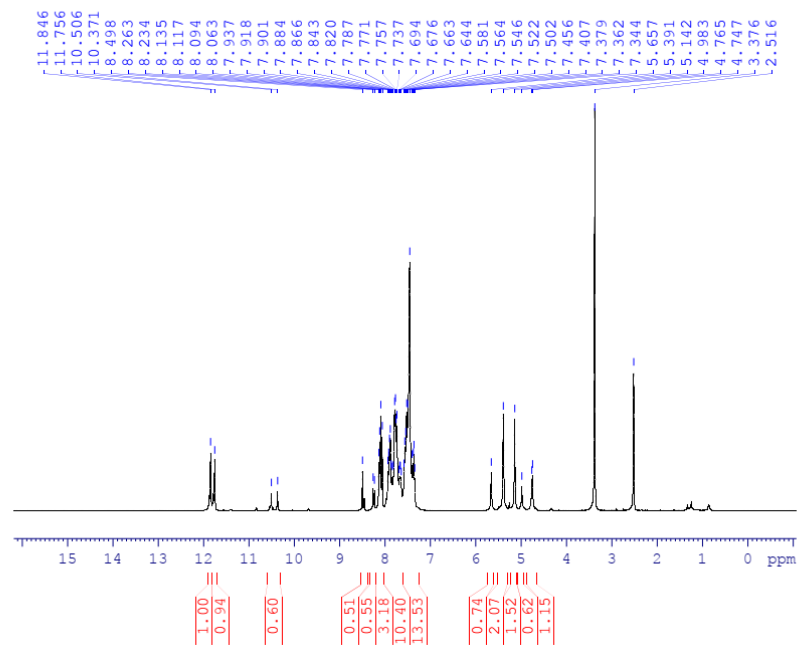
FT-IR of compound (8)

-

Compound (9a)



Mohamed Omar - 13 Hnmr - T

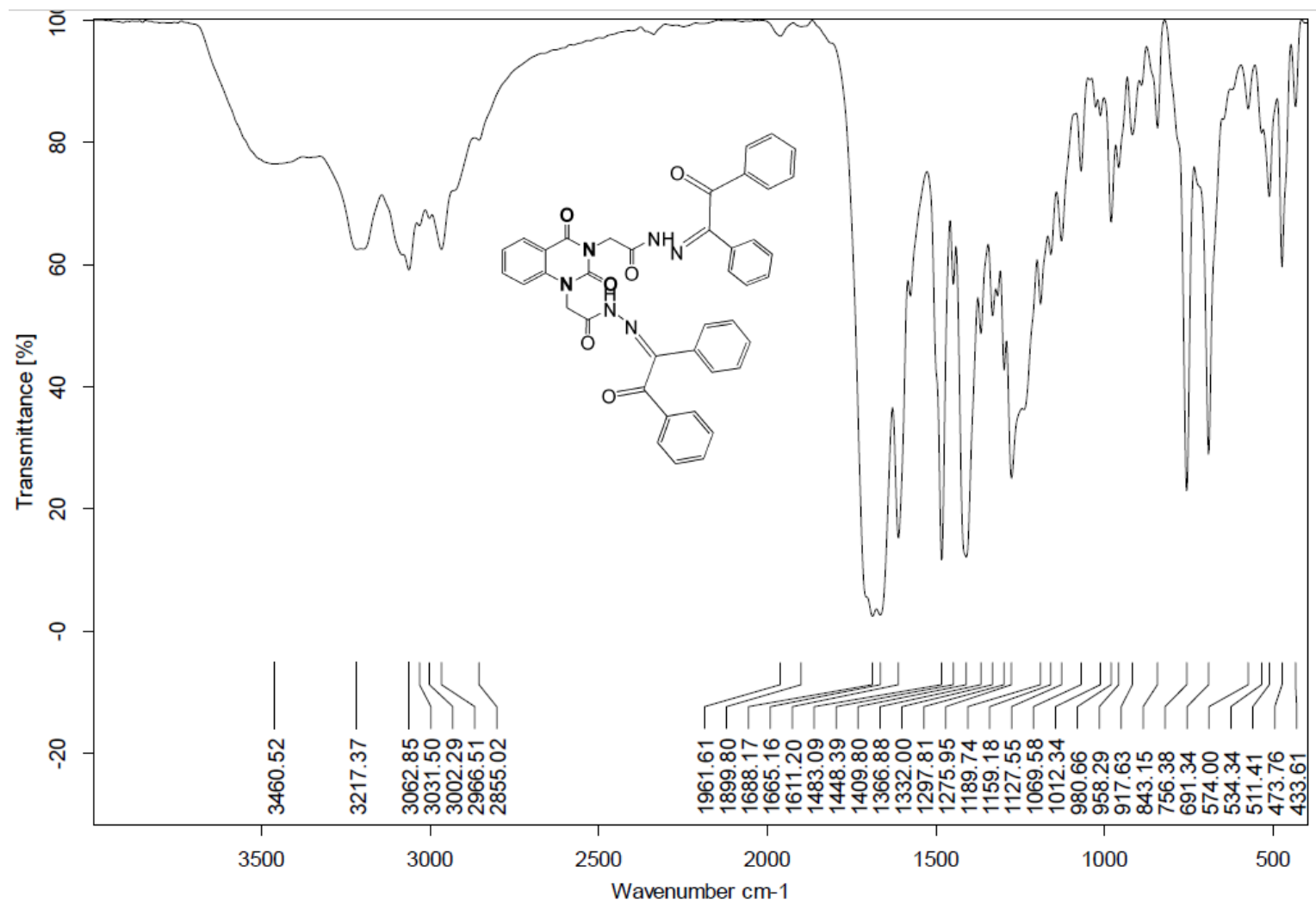


Current Data Parameters
NAME Mohamed Omar - 13 Hnmr - T
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230611
Time 18:07 h
INSTRUM spect
PROBHD 2108618_0948 (1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8011.800 Hz
FIDRES 0.244850 Hz
AQ 4.0894465 sec
RG 212.56
EM 45.800 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0
SFO1 400.2024712 MHz
NUC1 1H
P1 13.80 usec
PLM1 13.00000000 W

F2 - Processing parameters
SI 48828
SF 400.2000000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H-NMR of compound (9a)



FT-IR of compound (9a)