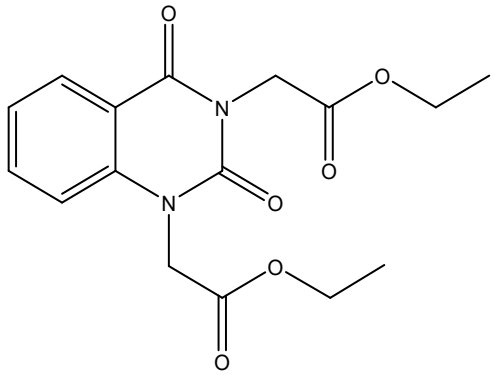
-

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

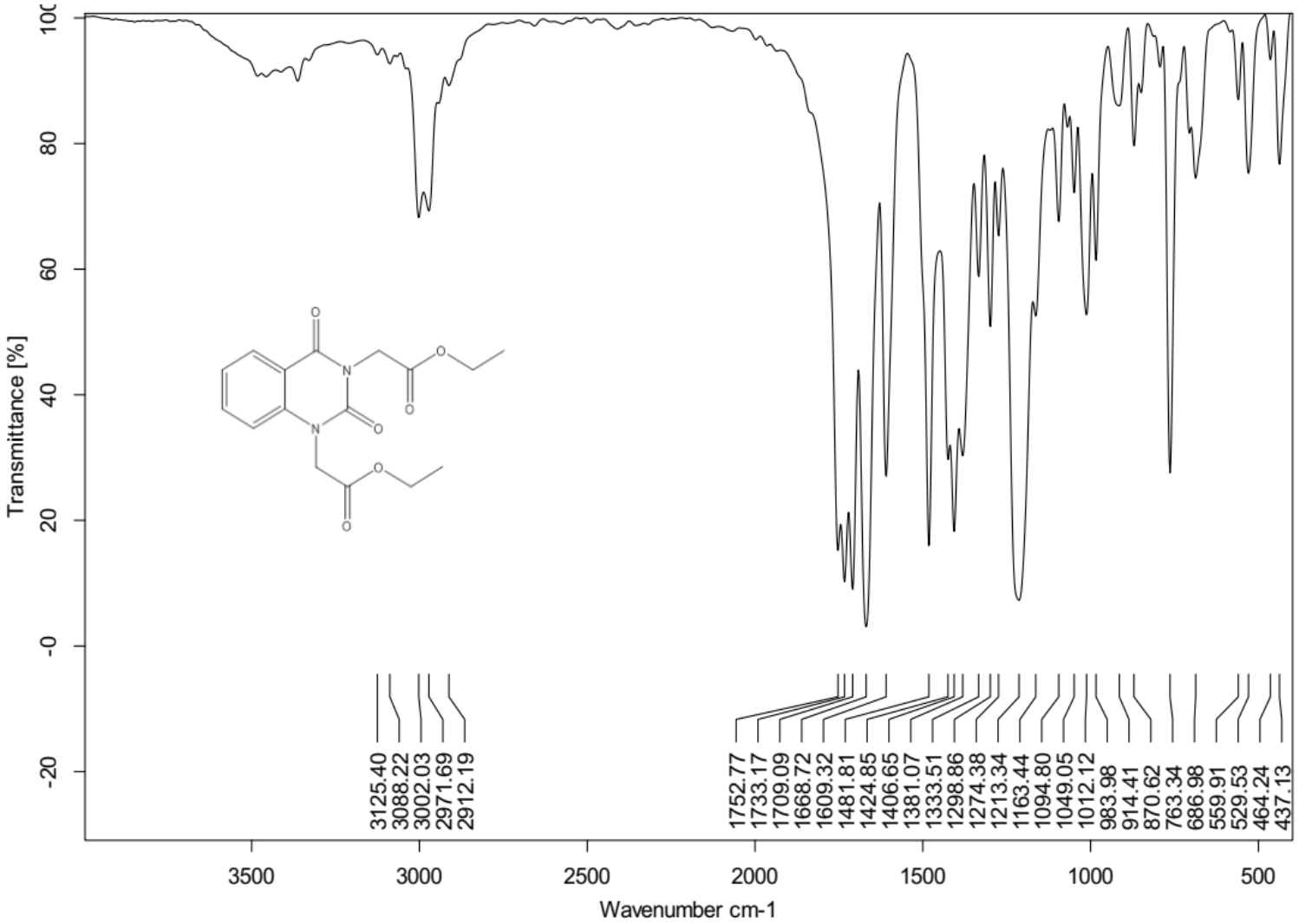


Figure . ^{1}H-NMR of compound 1 .

-

15-

Cairo University
Micro Analytical Center

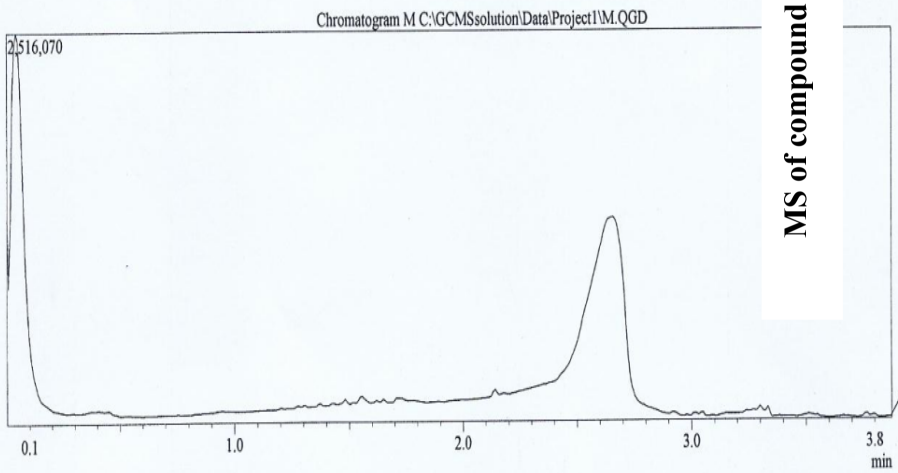
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information	
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 01:53:50 ص
Sample Name	: M
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M.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 01:57:45 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

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

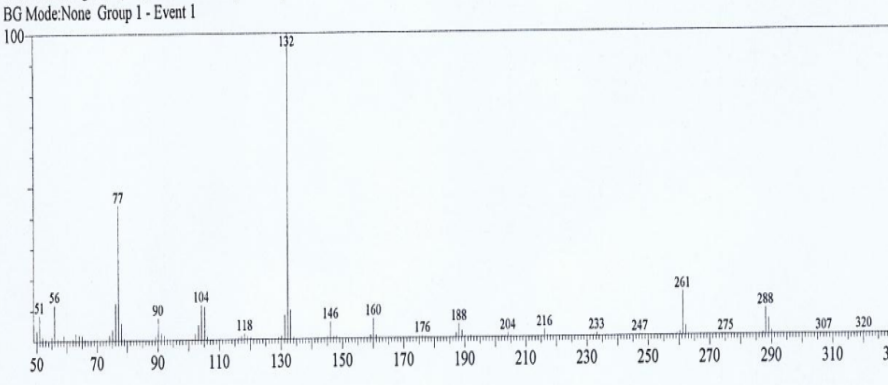
Chromatogram M C:\GCMSsolution\Data\Project1\M.QGD

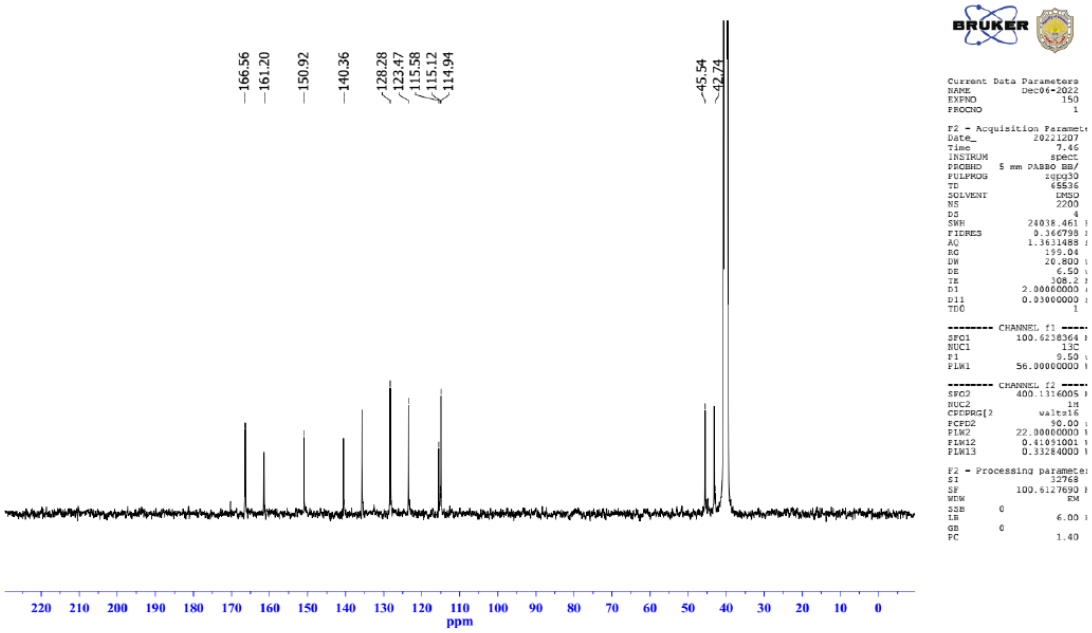


MS of compound (1)

Spectrum

Line#:1 R.Time:2.7(Scan#:321)
MassPeaks:182
RawMode:Single 2.7(321) BasePeak:132(351582)
BG Mode:None Group 1 - Event 1

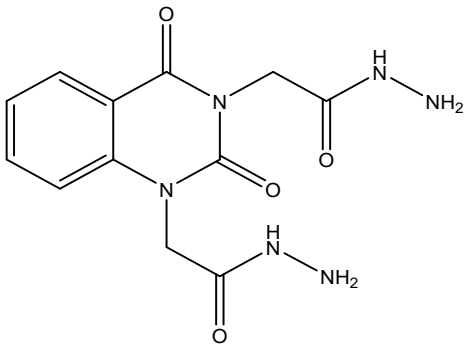




^{13}C-NMR (100 MHz, DMSO) of compound (1)

-

-Compound (2):



2

2

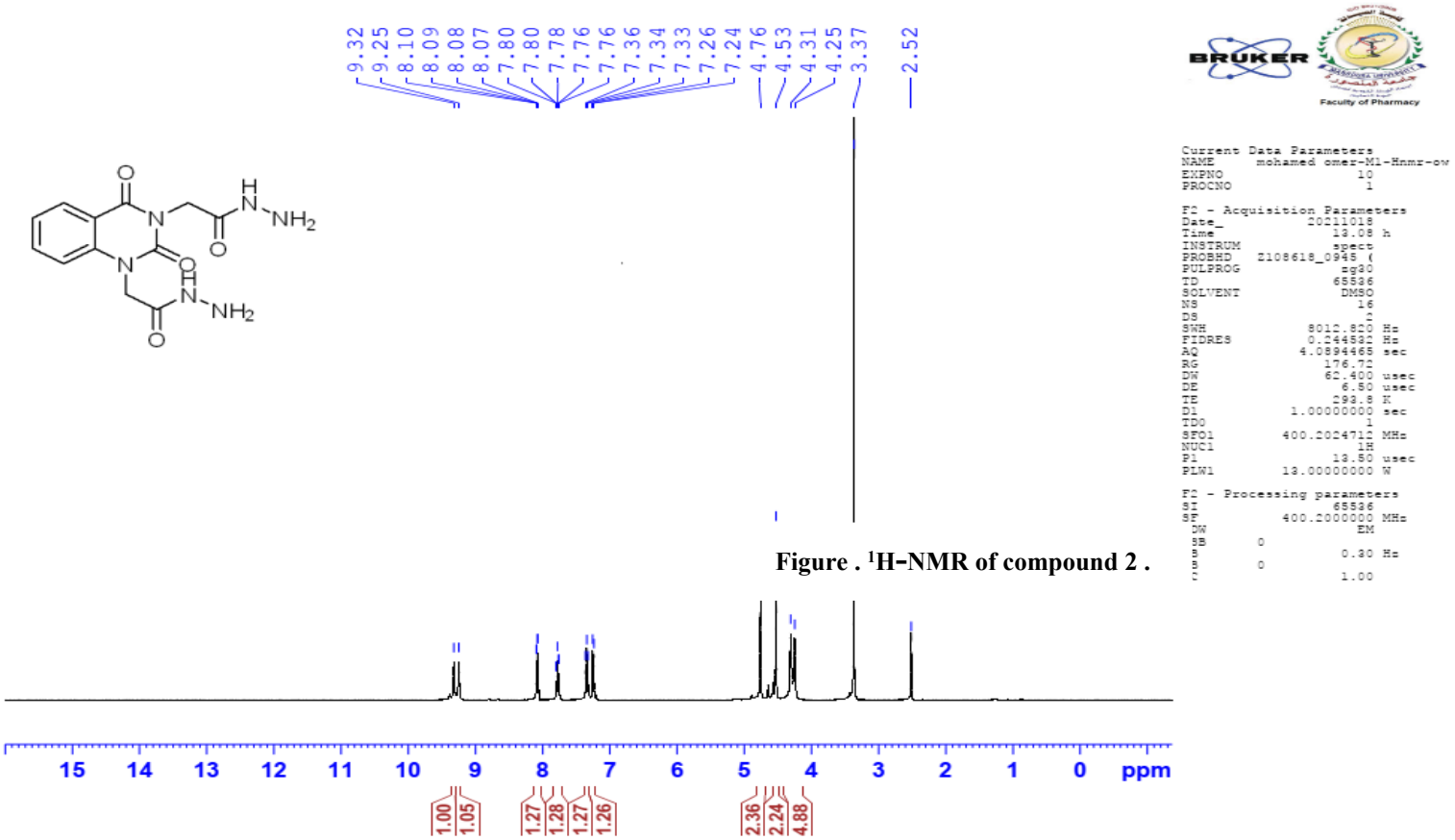


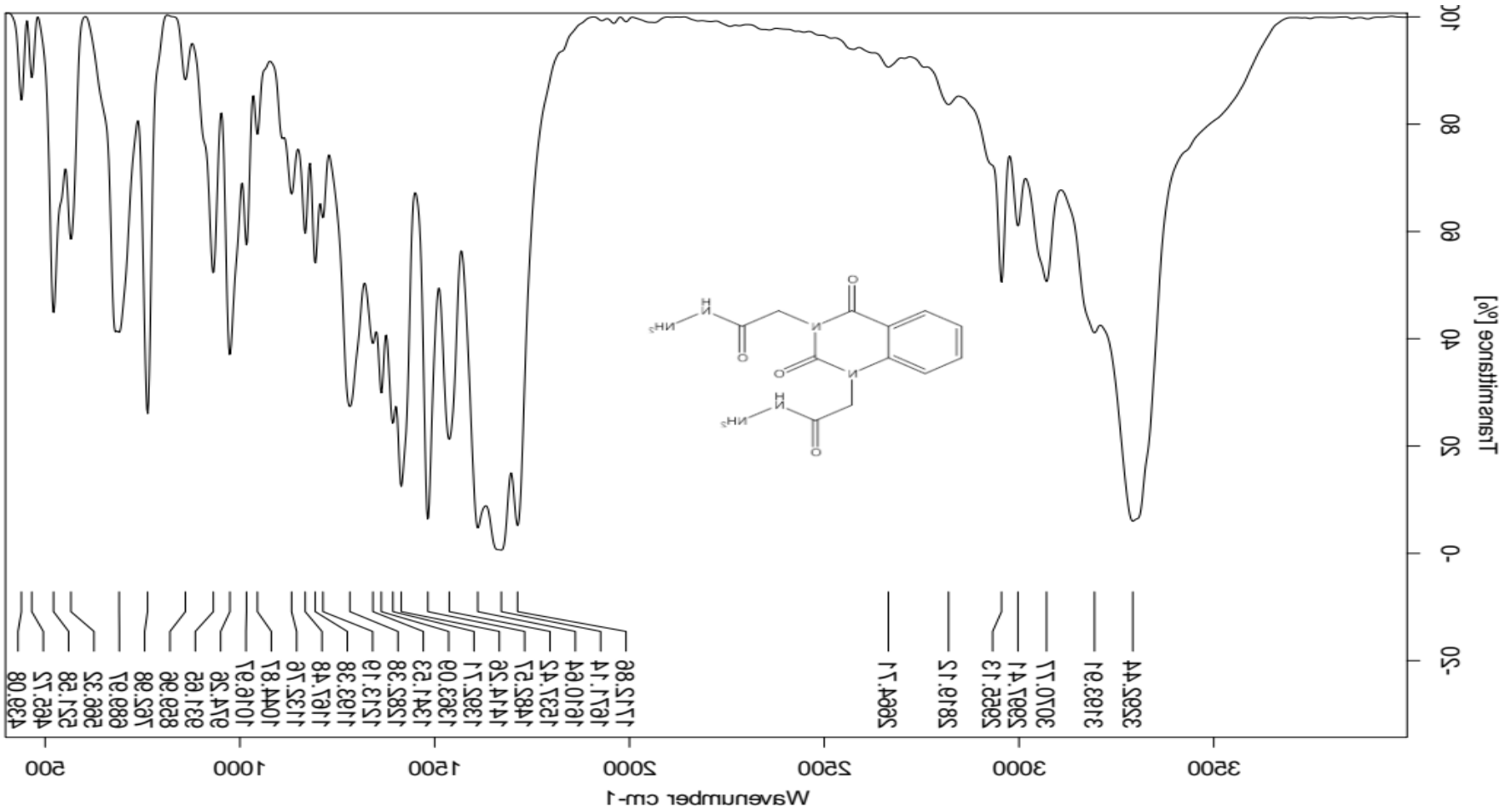
Figure . ^{1}H-NMR of compound 2 .

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

F2 - Acquisition Parameters
Date_           20211018
Time                13.08 h
INSTRUM             spect
PROBHD    Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.244583 Hz
AQ               4.0894465 sec
RG                  176.72
DW                  62.400 usec
DE                   6.50 usec
TE                  293.8 K
D1              1.00000000 sec
TD0                     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
```

-



FT-IR of compound (2)

15-Jan-07 02:07:54

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

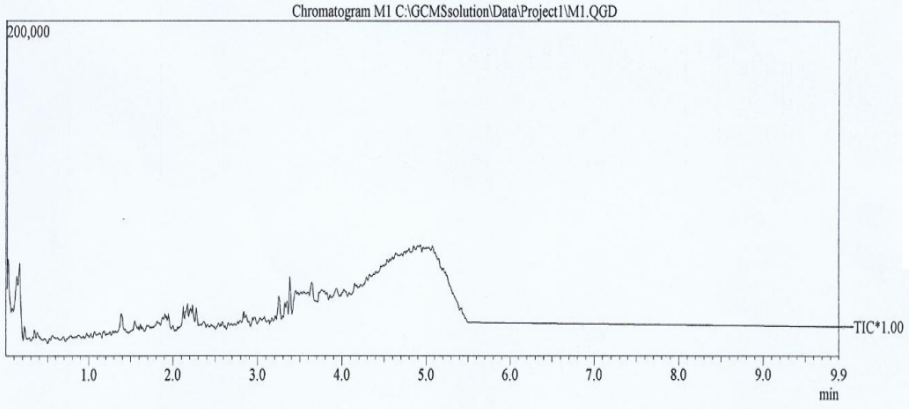
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 01:59:25 ص
Sample Name	: M1
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M1.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M1.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1_default.qgt
$EndIf$Modified by	: Dr. Mai Younis
Modified	: 15/01/2007 02:04:57 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

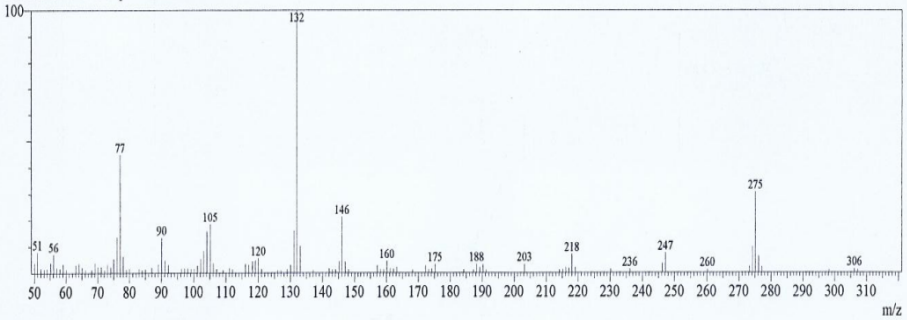
C:\GCMSsolution\Data\Project1\M1.QGD

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



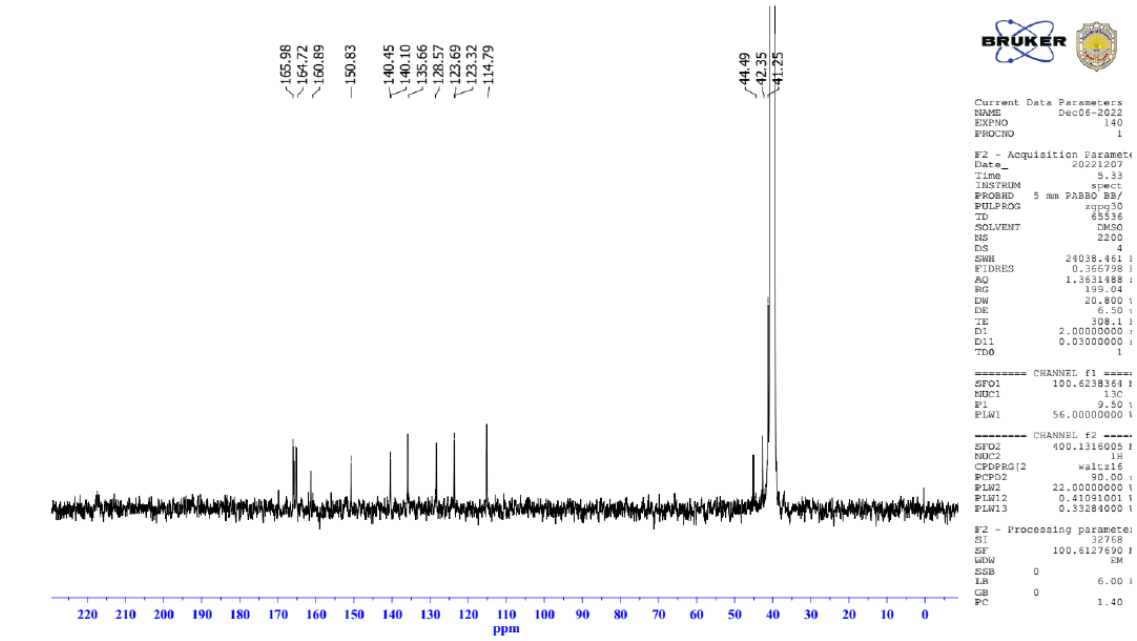
Spectrum

Line#:1 R.Time:4.7(Scan#:566)
MassPeaks:110
RawMode:Single 4.7(566) BasePeak:132(10628)
BG Mode:None Group 1 - Event 1



MS of compound (2)

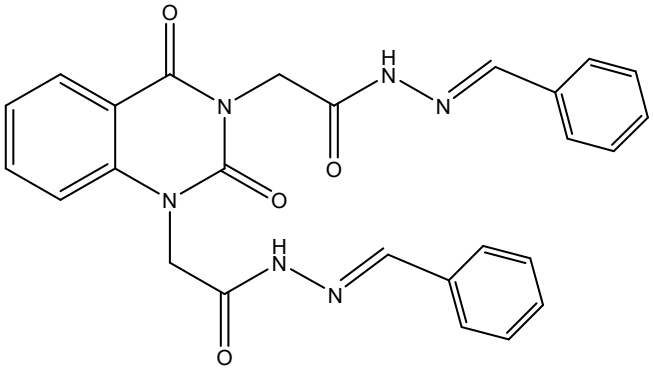
-



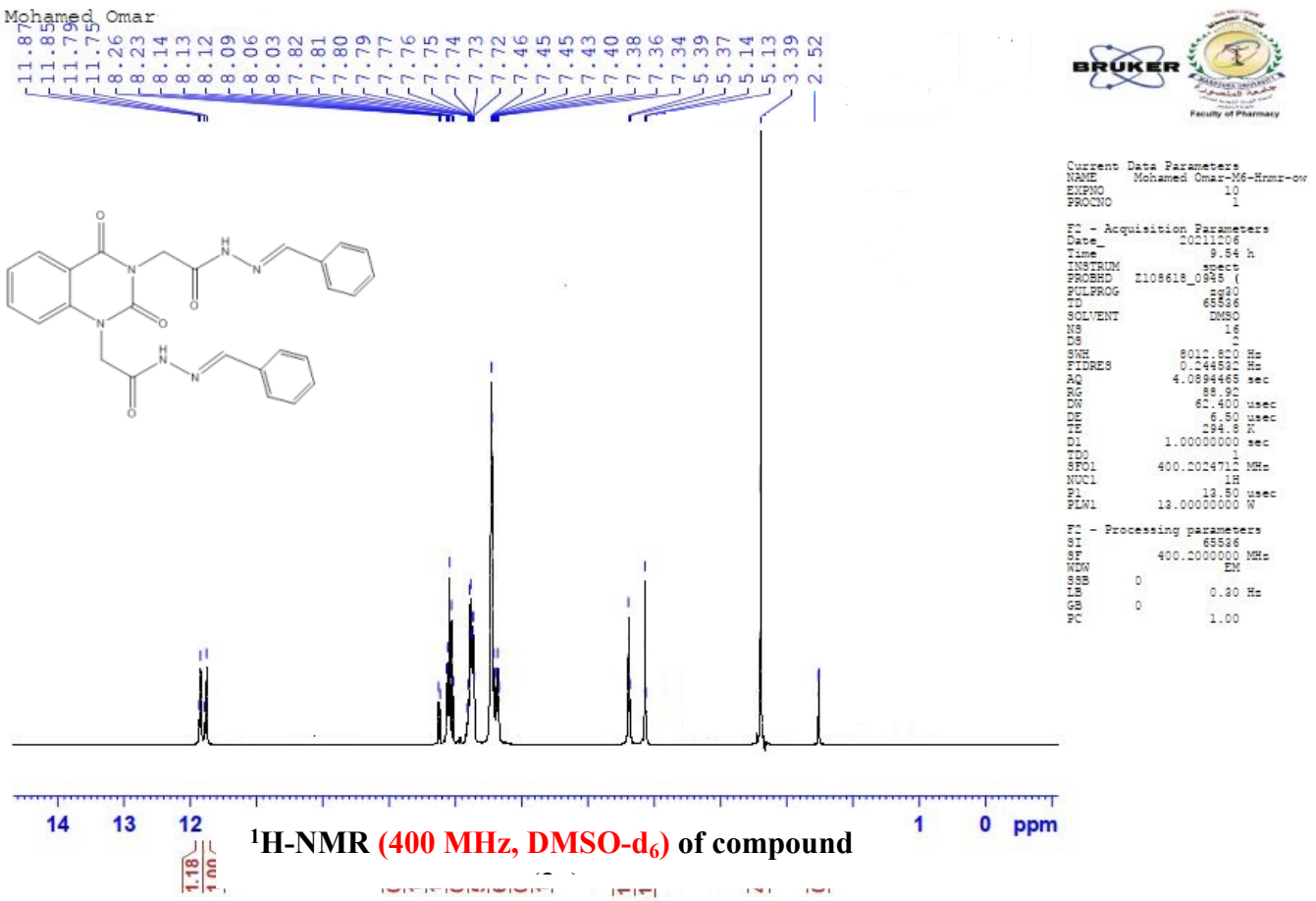
^{13}C-NMR (100 MHz, DMSO) of compound (2)

-

-Compound (3a)



3a



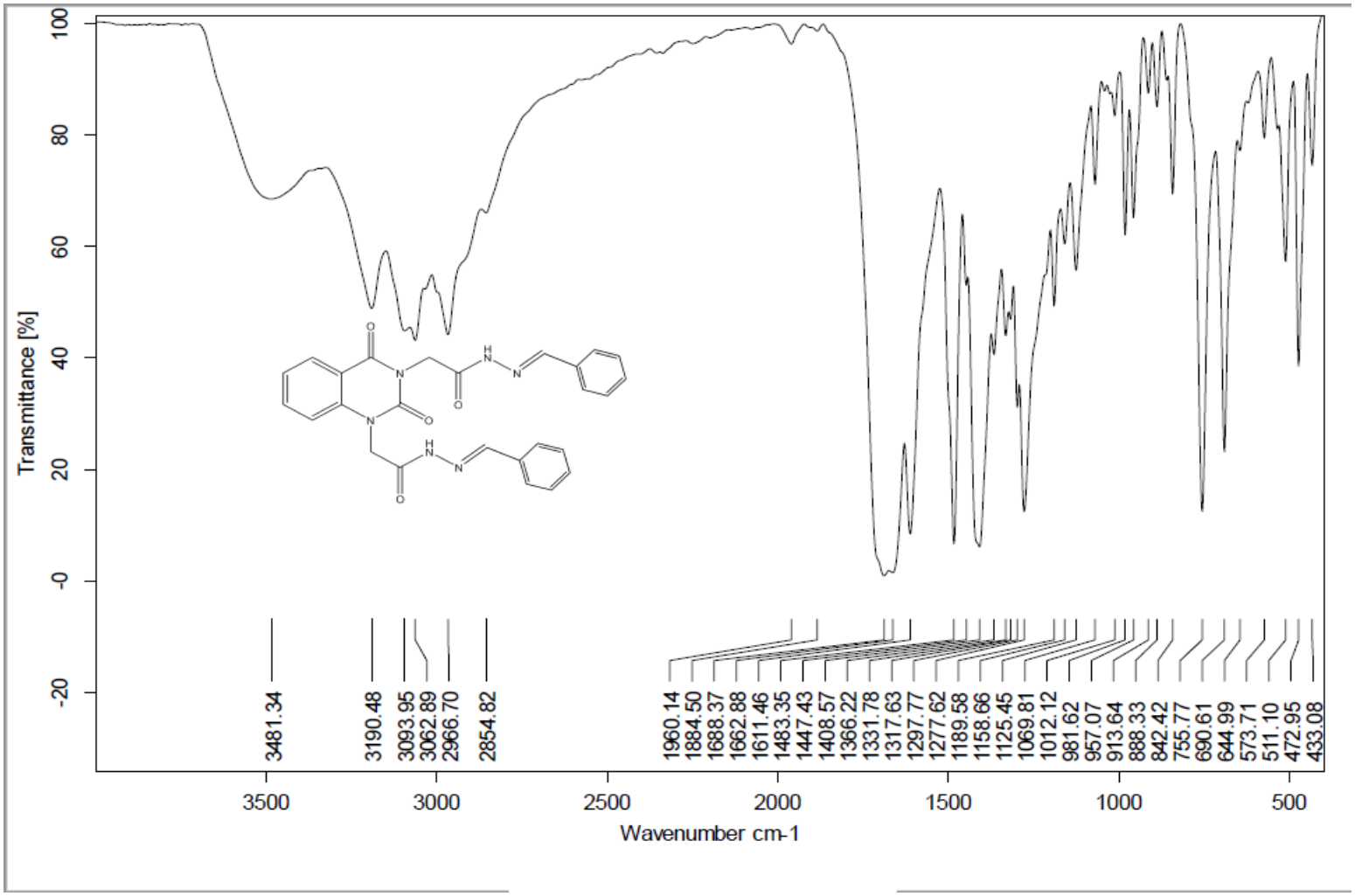
Current Data Parameters
NAME Mohamed Omar-M6-Hnmr-ov
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211206
Time 9.54 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244592 Hz
AQ 4.0894465 sec
RG 88.92
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 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

^{1}H-NMR (400 MHz, DMSO-d_6) of compound

-



FT-IR of compound (3a)

15-Jan-07 02:

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 ص
Sample Name	: M6
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M6.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M6.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 02:34:22 ص

Method

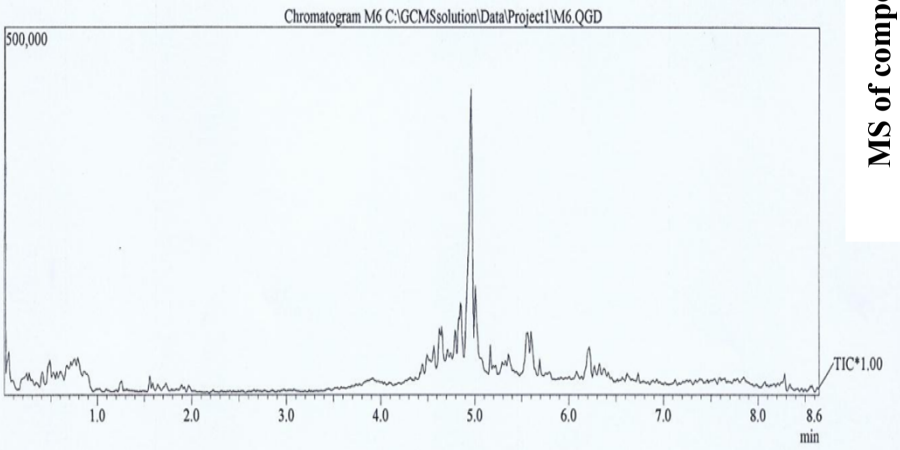
===== Analytical Line 1 =====

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	:1250
Start m/z	:50.00
End m/z	:600.00

Electron Voltage : 70 eV
Ionization Mode : EI

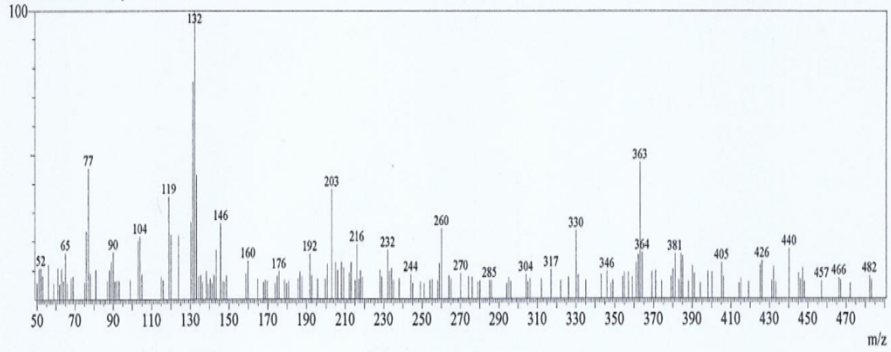
C:\GCMSsolution\Data\Project1\M6.QGD

Chromatogram M6 C:\GCMSsolution\Data\Project1\M6.QGD



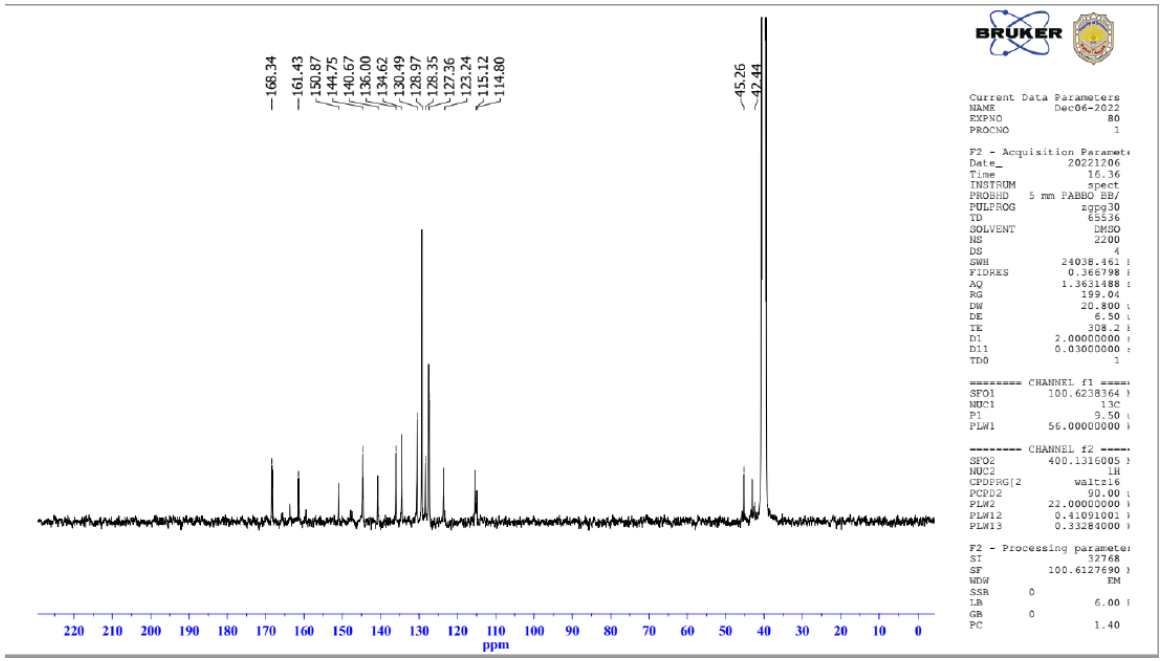
Spectrum

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)

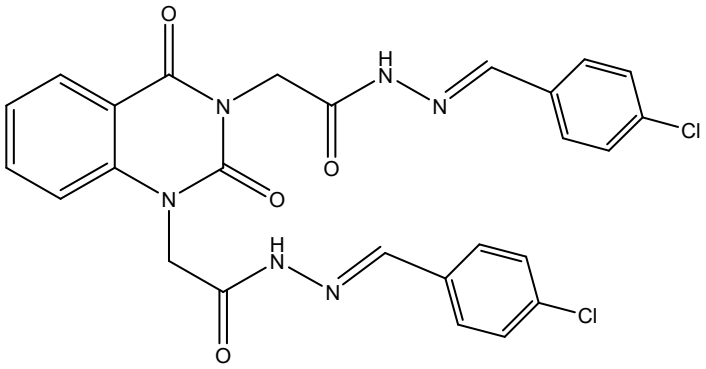
-



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

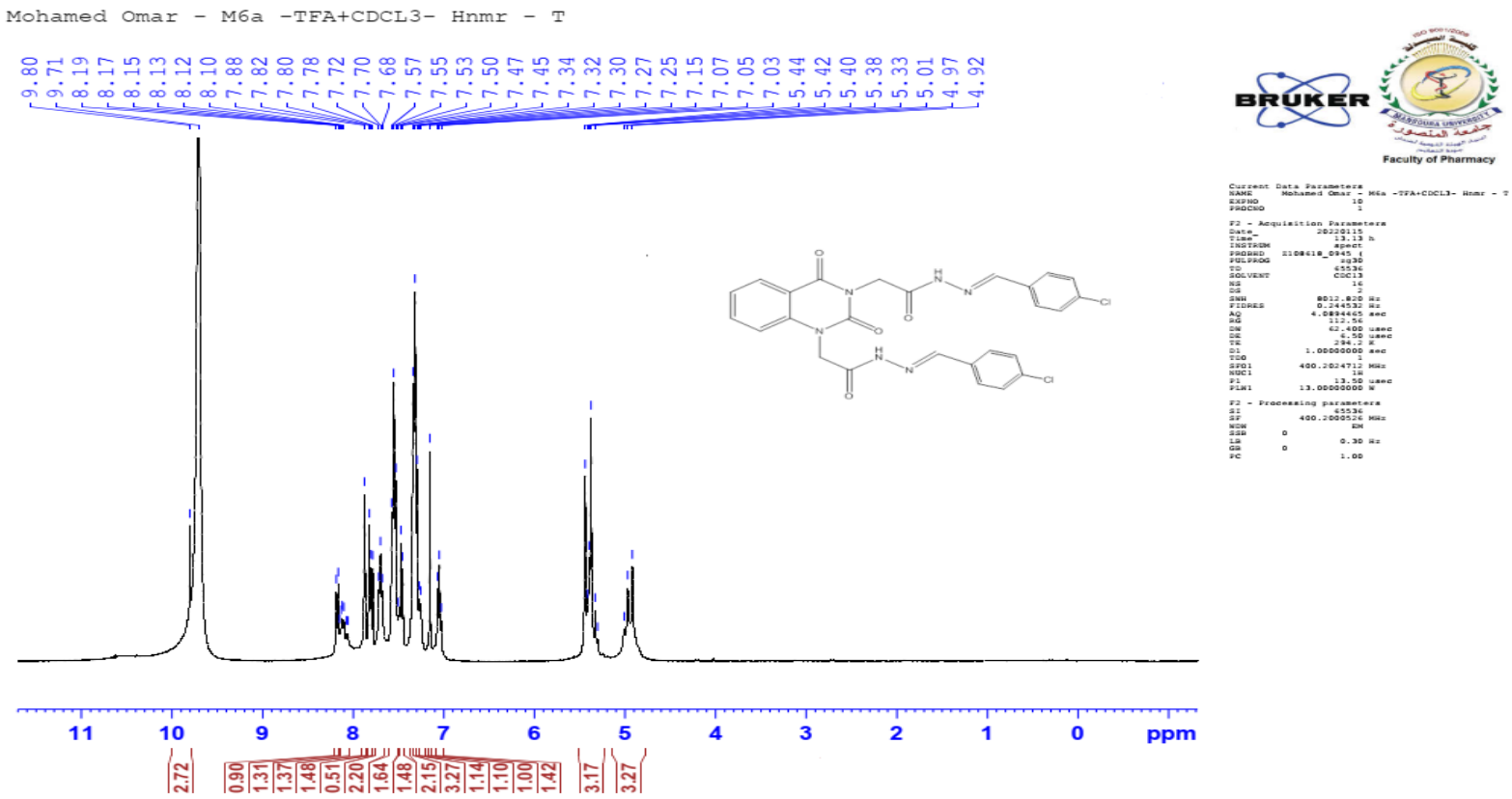
-

Compound (3b): -



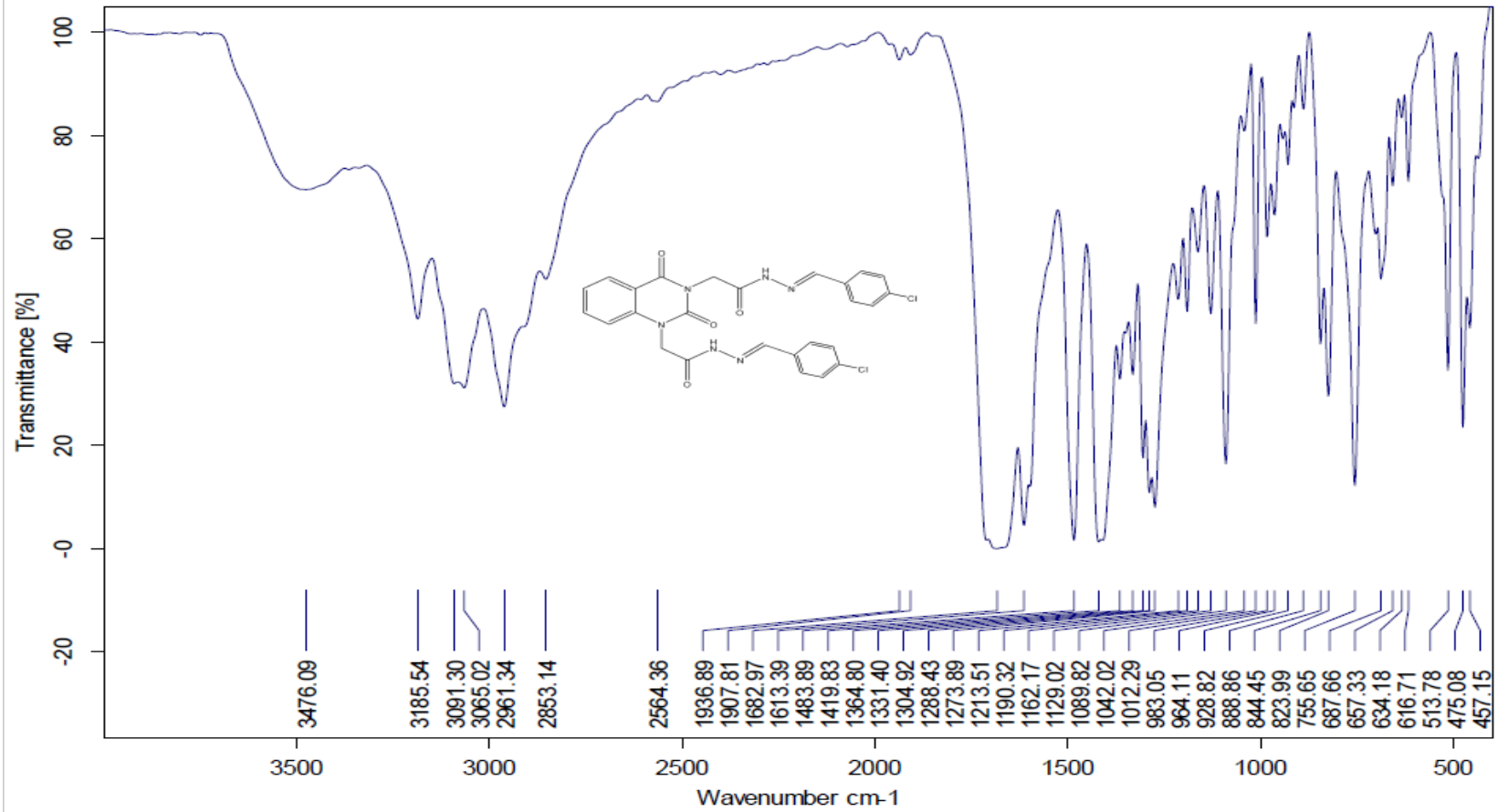
3b

-

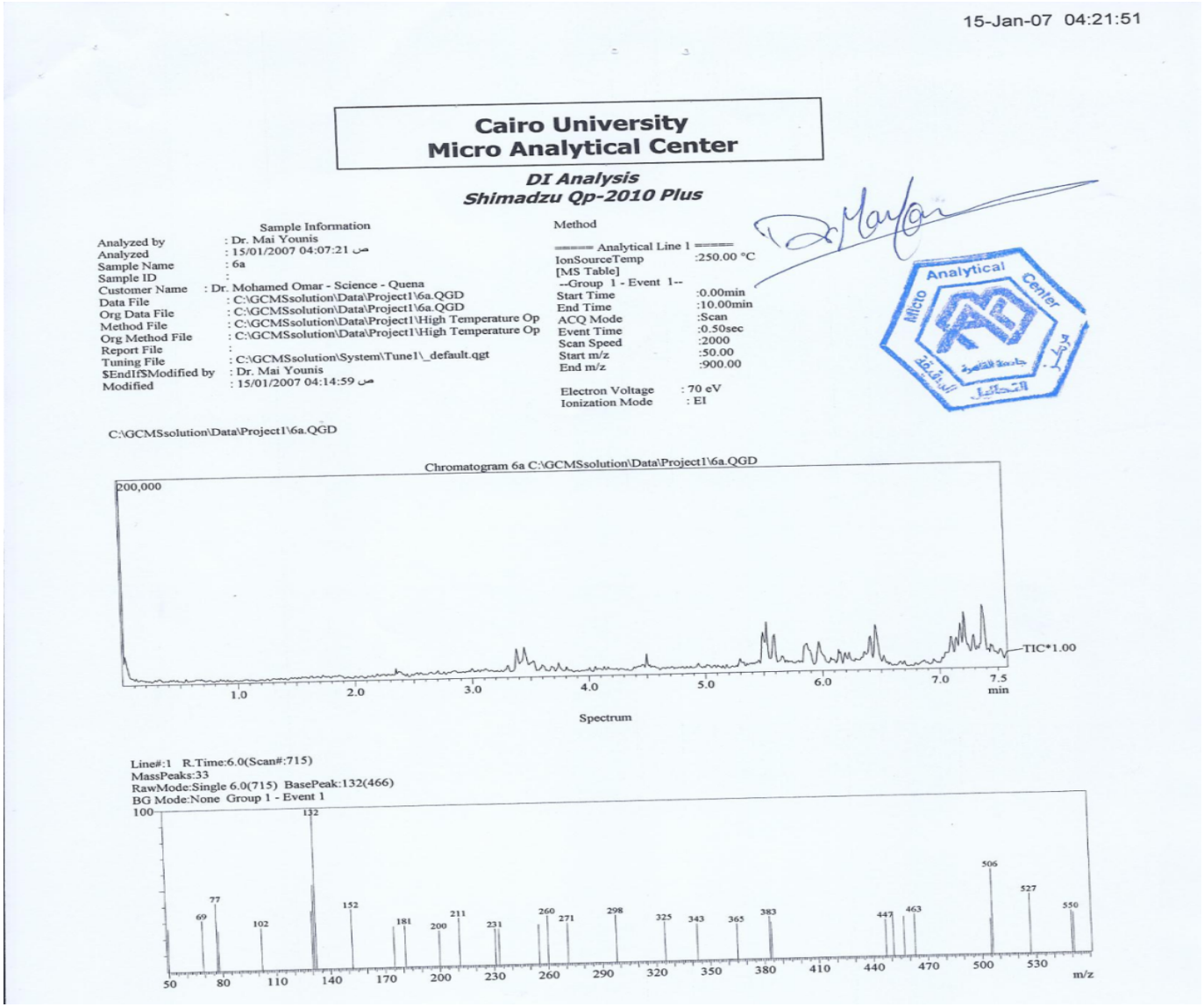


^{1}H-NMR (400 MHz, TFA) of compound (3b)

-



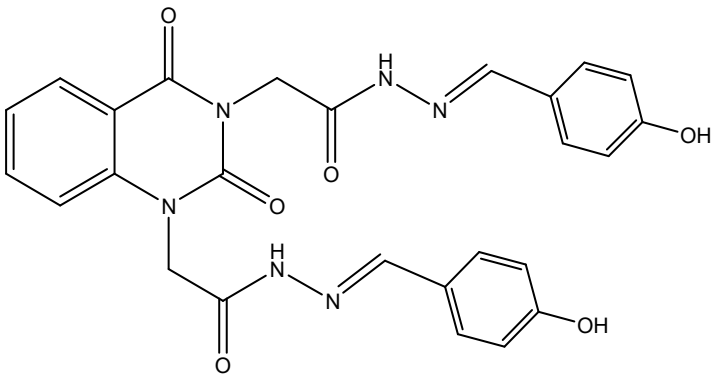
FT-IR of compound (3b)



MS of compound (3b)

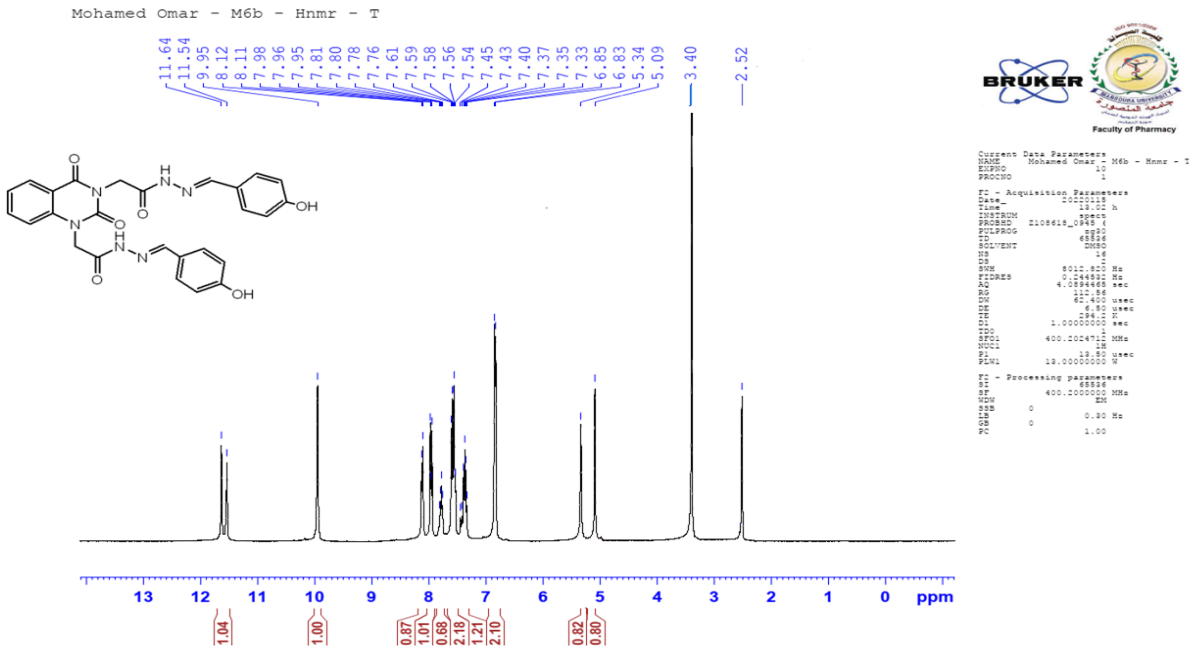
-

-Compound (3c):



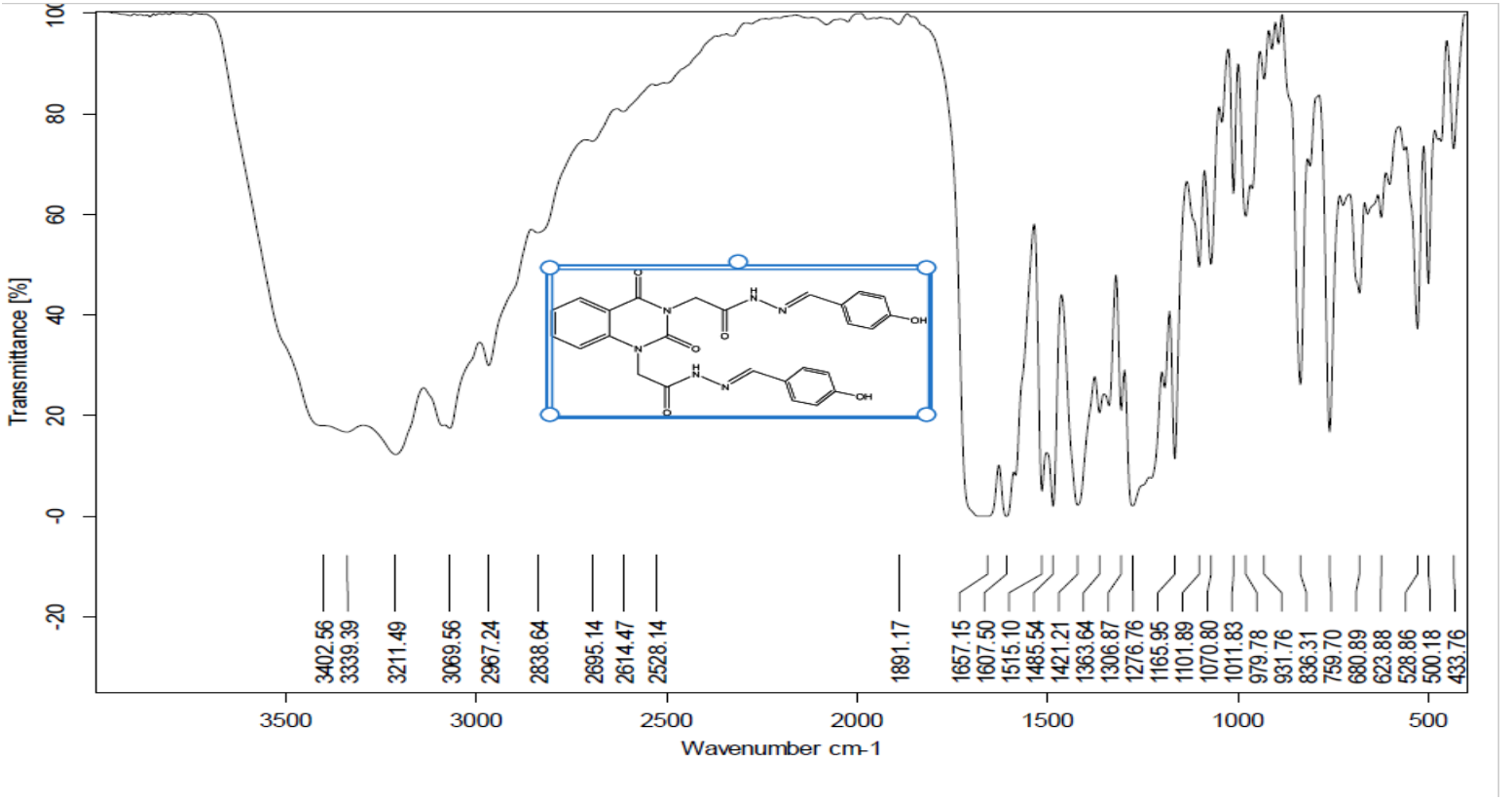
3c

-



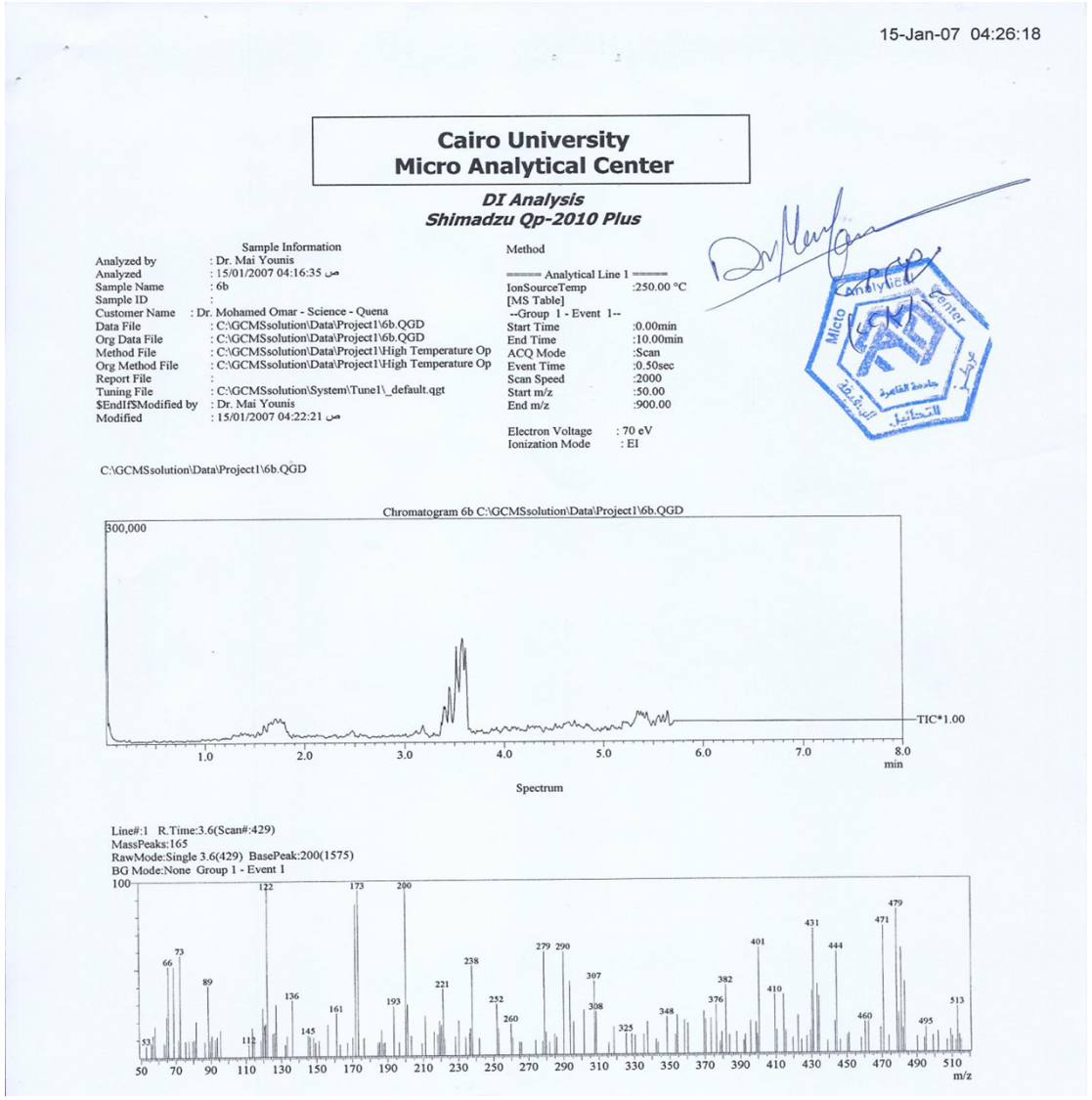
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (3c)

-



FT-IR of compound (3c)

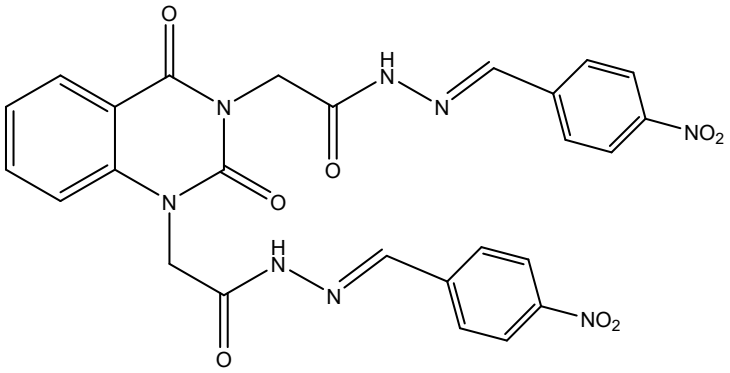
-



MS of compound (3c)

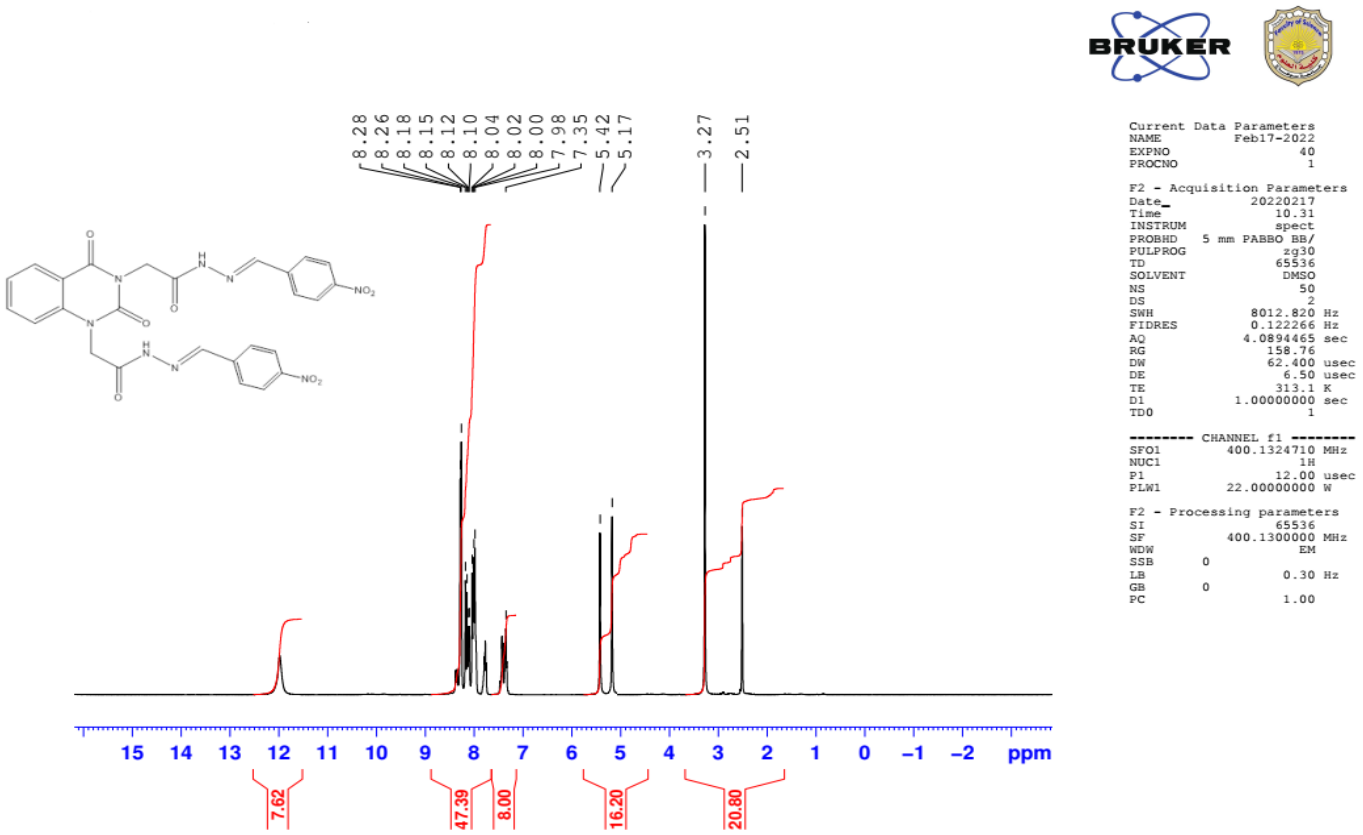
-

-Compound (3d):



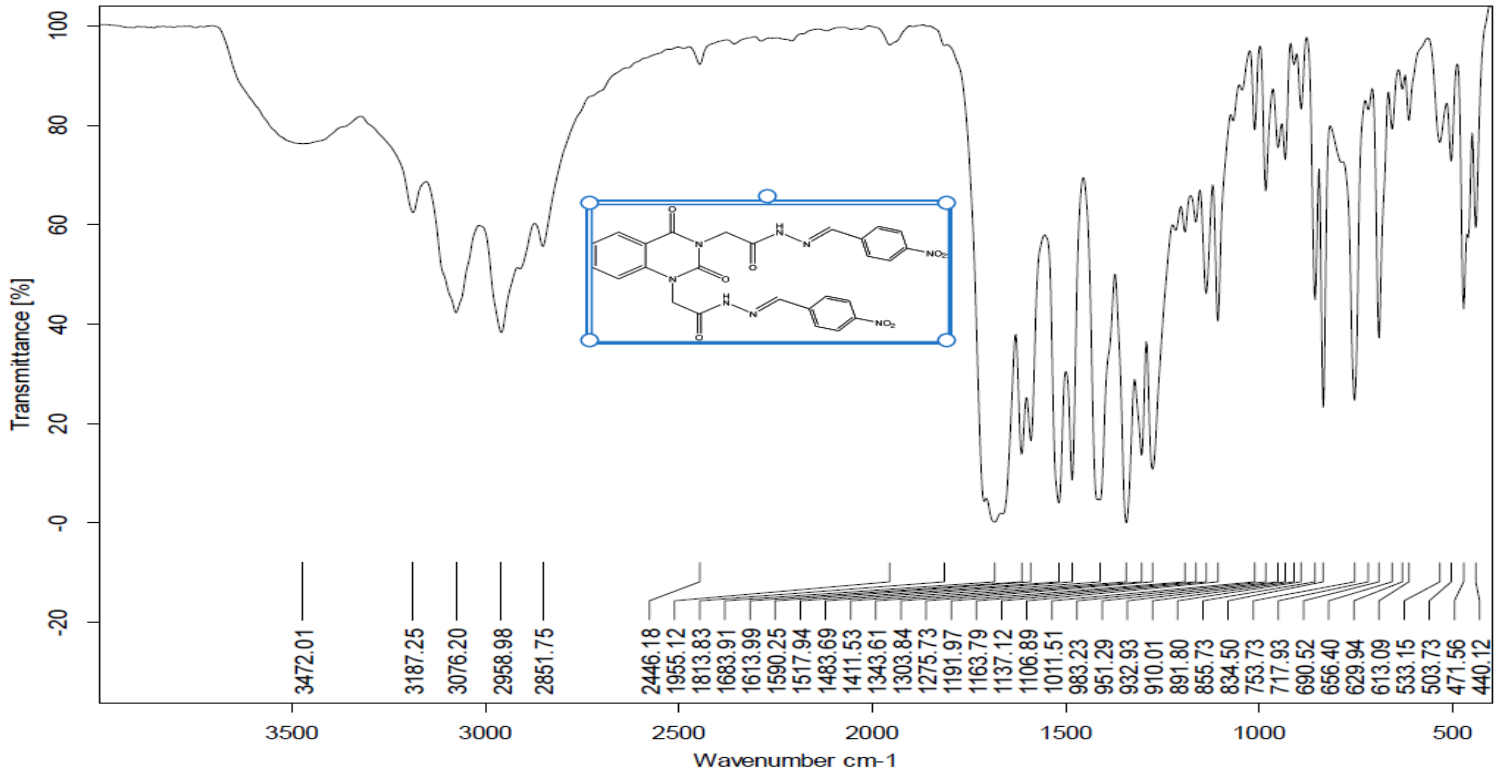
3d

-



^{1}H-NMR (400 MHz, DMSO-d_6) of compound (3d)

-



FT-IR of compound (3d)

15-Jan-07 04:44:26

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

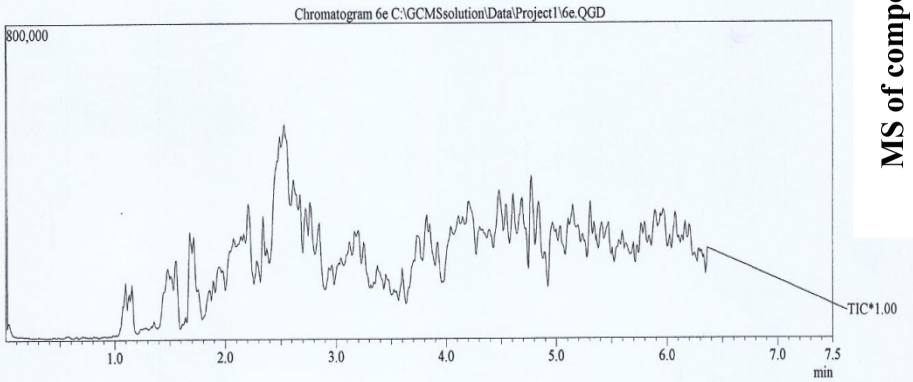
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:32:35 ص
Sample Name	: 6e
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\6e.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\6e.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 04:39:00 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

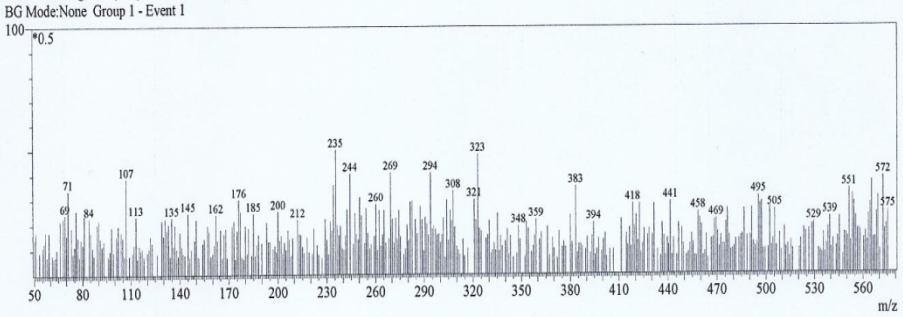
C:\GCMSsolution\Data\Project1\6e.QGD

Chromatogram 6e C:\GCMSsolution\Data\Project1\6e.QGD



Spectrum

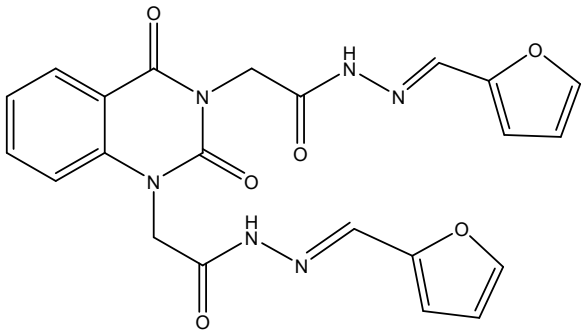
Line#:1 R.Time:3.6(Scan#:433)
MassPeaks:418
RawMode:Single 3.6(433) BasePeak:235(833)
BG Mode:None Group 1 - Event 1



MS of compound (3d)

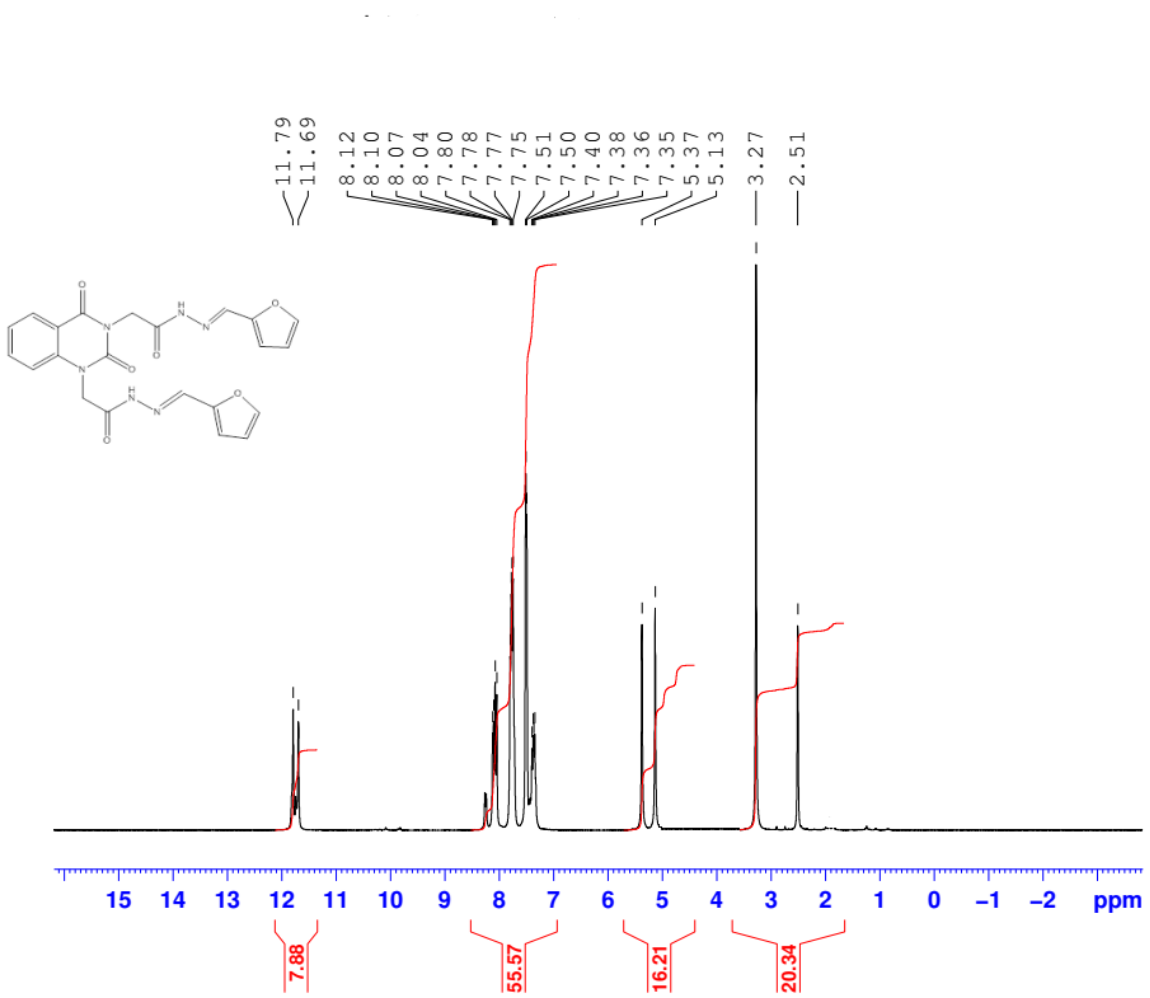
-

-Compound (3e):



3e

-

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Current Data Parameters
NAME          Feb17-2022
EXPNO                 50
PROCNO                 1

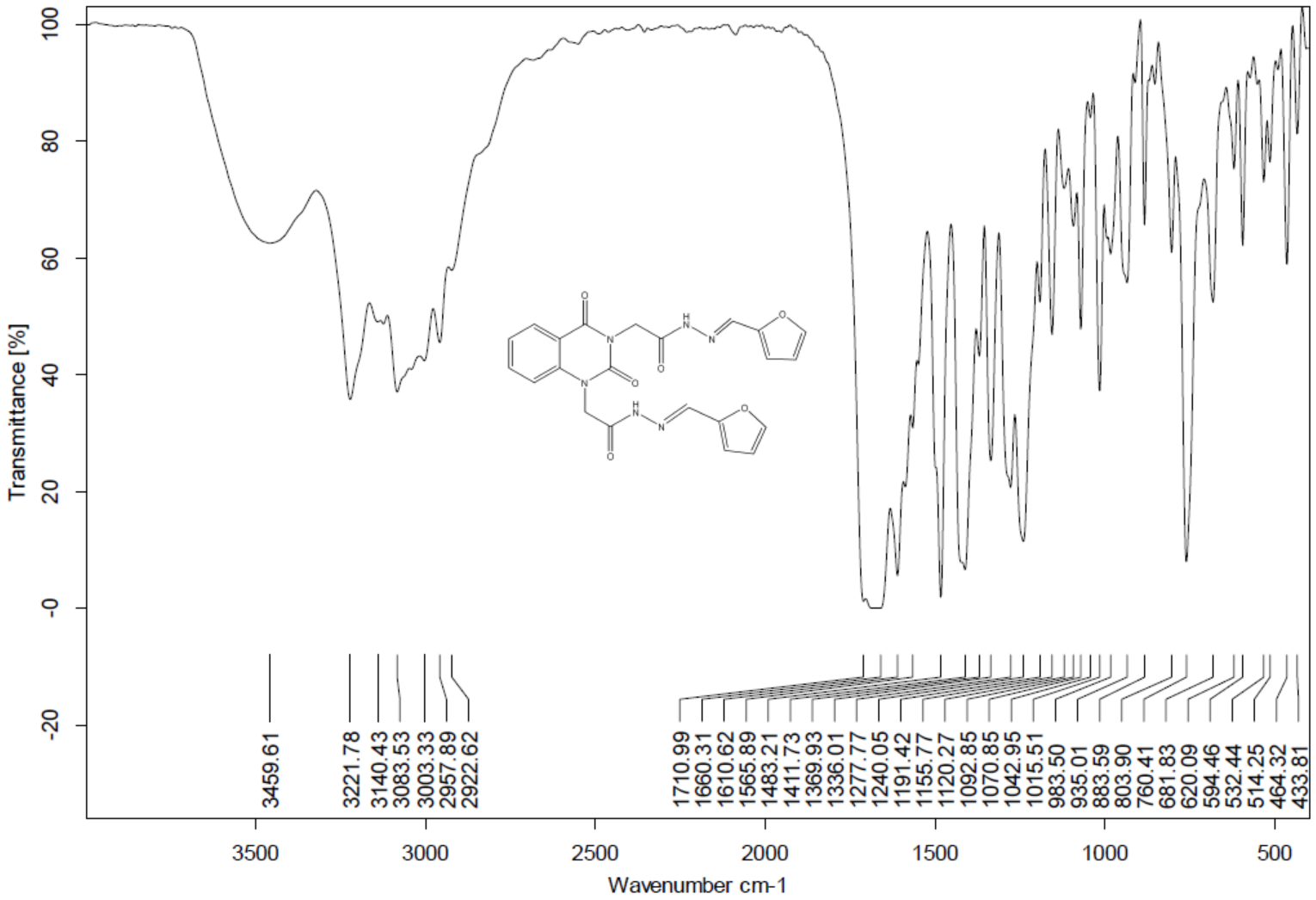
F2 - Acquisition Parameters
Date_           20220217
Time               10.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    50
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                158.76
DW                62.400 usec
DE                 6.50 usec
TE                313.2 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
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR (400 MHz, DMSO-d_6) of compound (3e)

-



FT-IR of compound (3e)

15-Jan-07 04:46:31

Cairo University
Micro Analytical Center

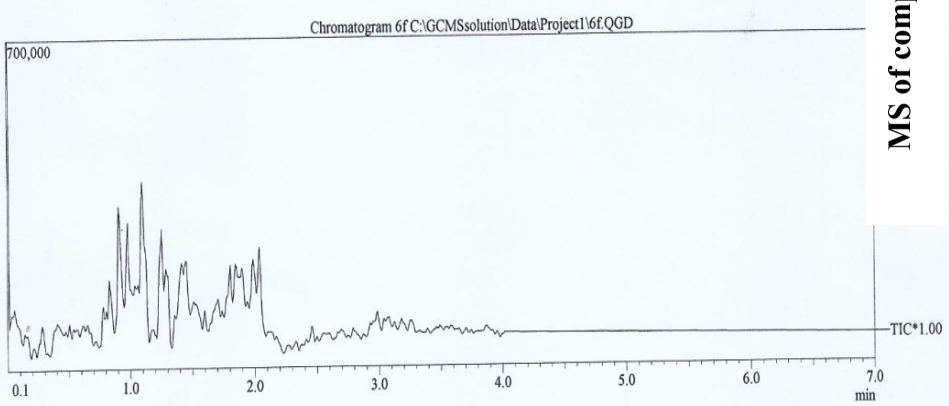
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information	
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:40:35 ص
Sample Name	: 6f
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\6f.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\6f.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 04:44:39 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

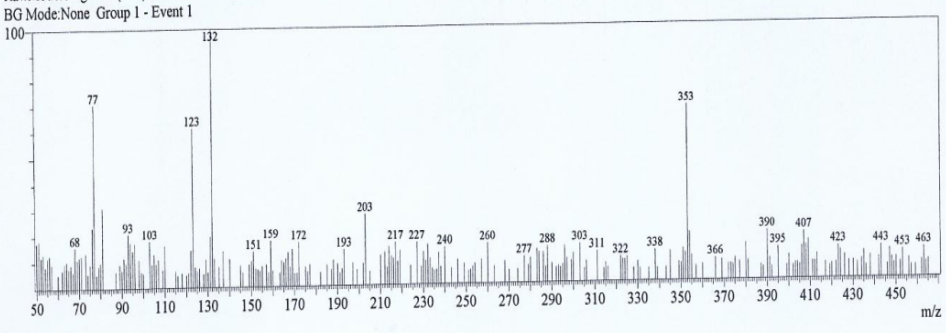
C:\GCMSsolution\Data\Project1\6f.QGD

Chromatogram 6f C:\GCMSsolution\Data\Project1\6f.QGD



Spectrum

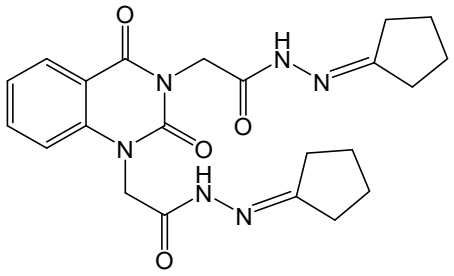
Line#:1 R.Time:2.9(Scan#:353)
MassPeaks:243
RawMode:Single 2.9(353) BasePeak:132(2196)
BG Mode:None Group 1 - Event 1



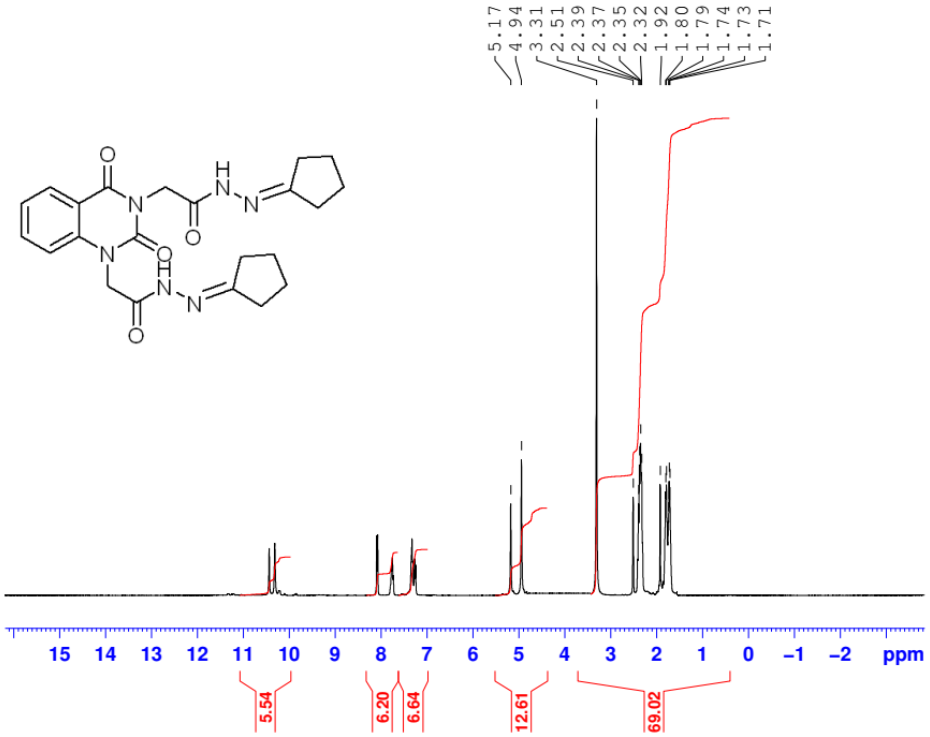
MS of compound (3e)

-

-Compound (4a): -



4a



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Current Data Parameters
NAME                  Jul03-2022
EXPNO                         50
PROCNO                         1

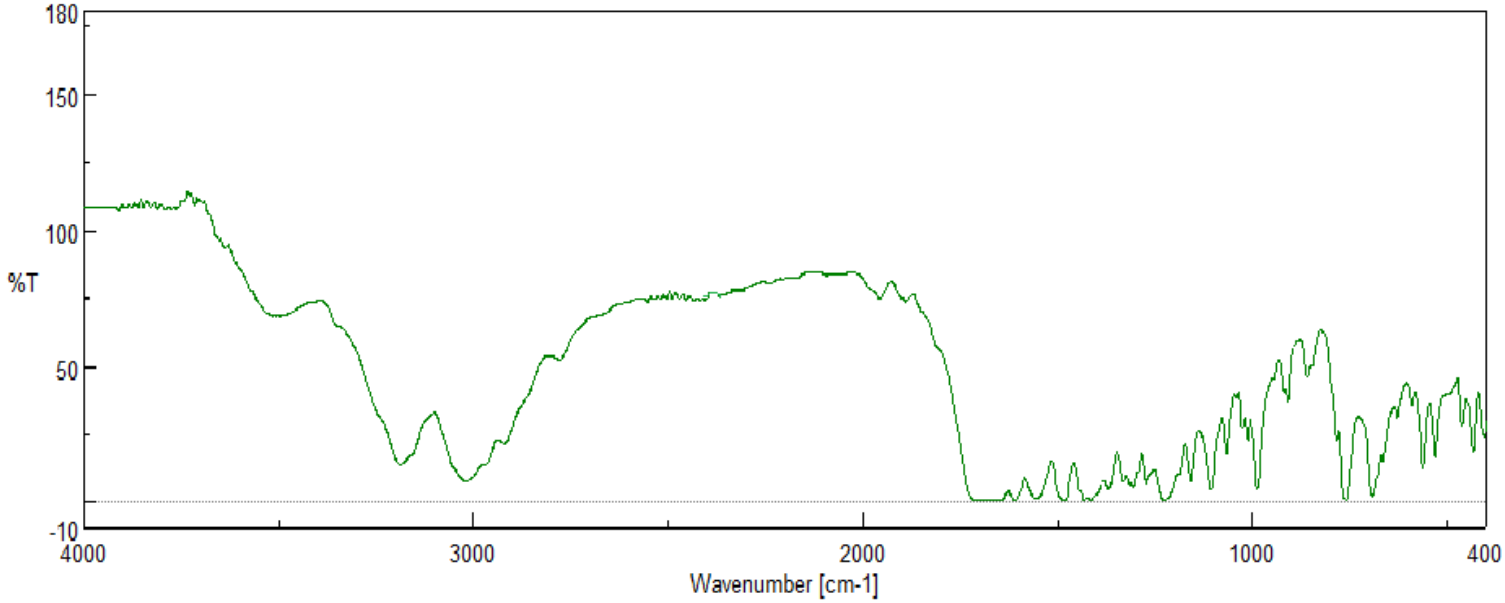
F2 - Acquisition Parameters
Date_                   20220703
Time                       12.19
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                            35
DS                             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
TD0                            1

======== CHANNEL f1 ========
SFO1                 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
```

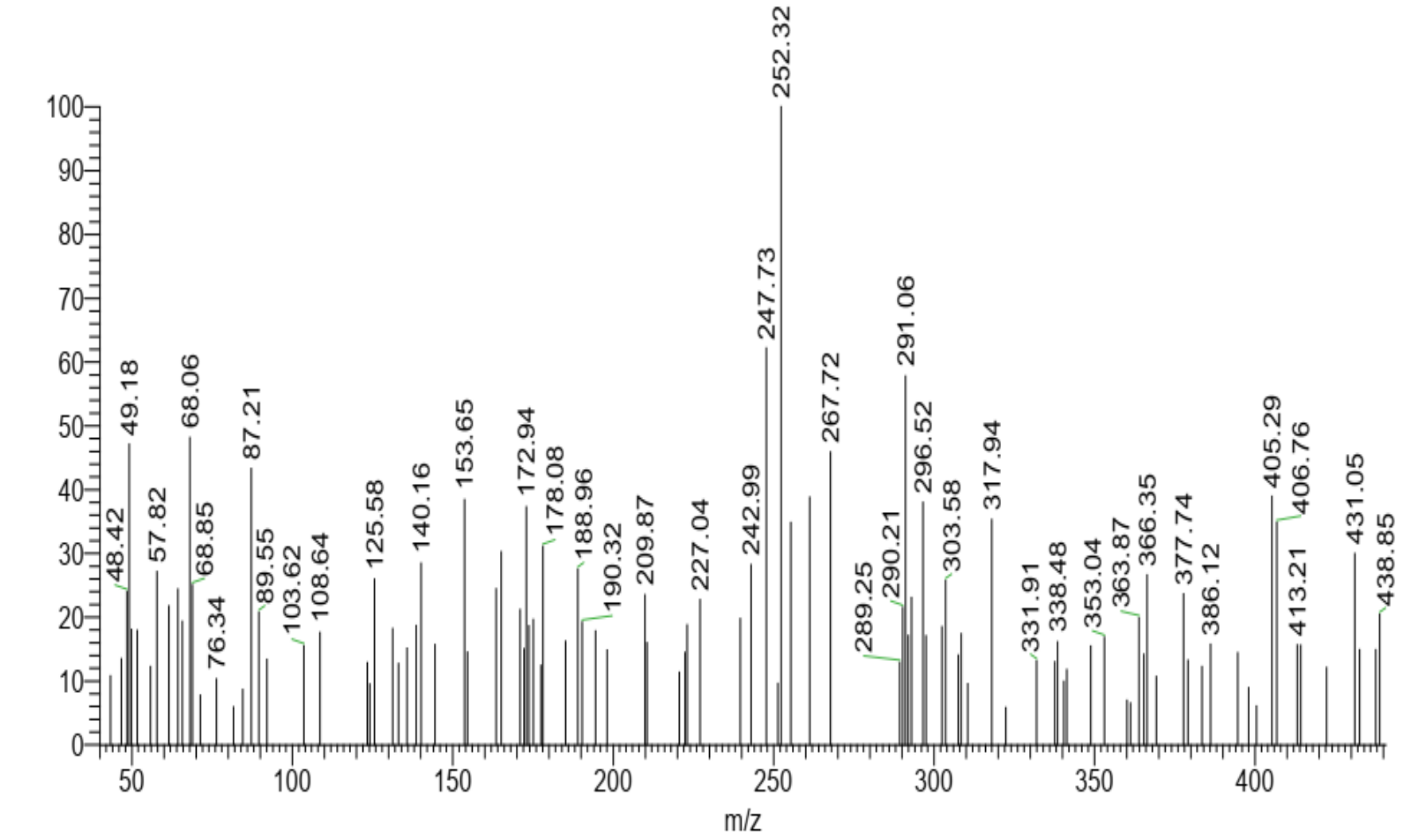
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4a)

-



FT-IR of compound (4a)

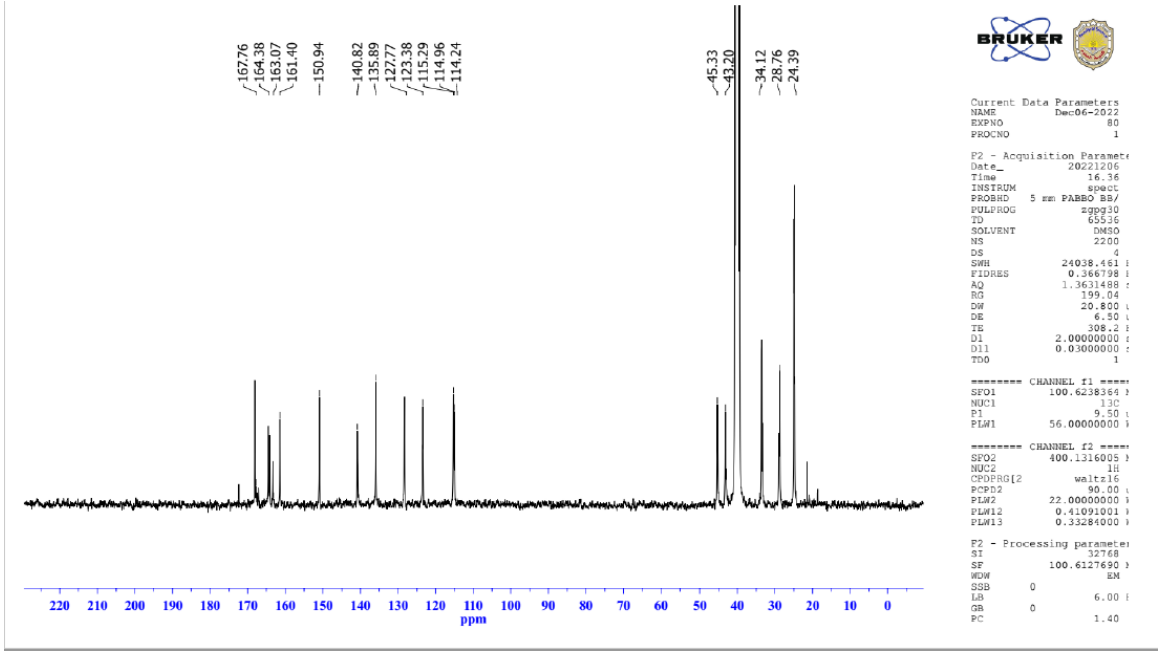
-



m/z	Intensity	Relative

MS of compound (4a)

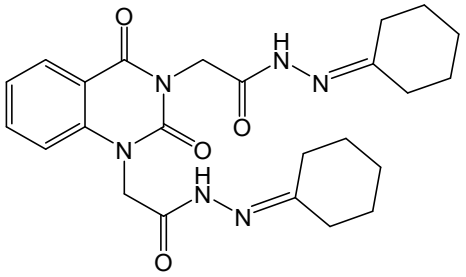
-



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

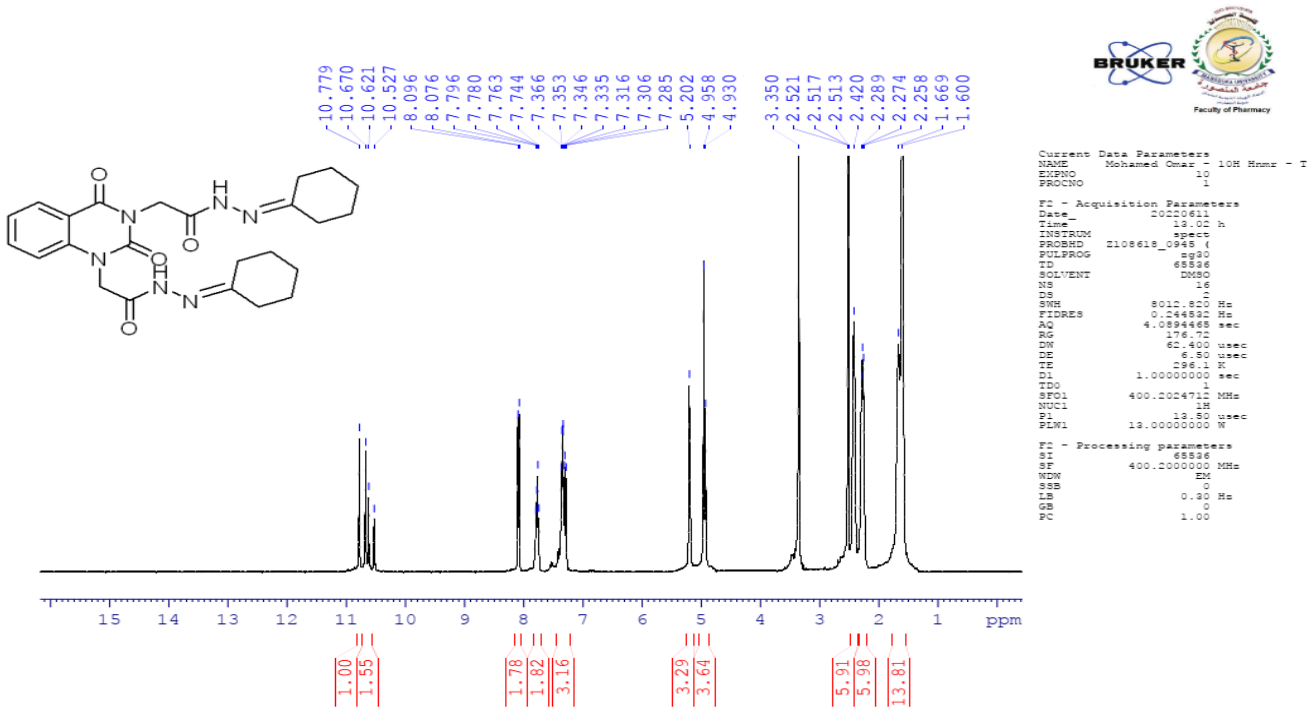
-

-Compound (4b): -



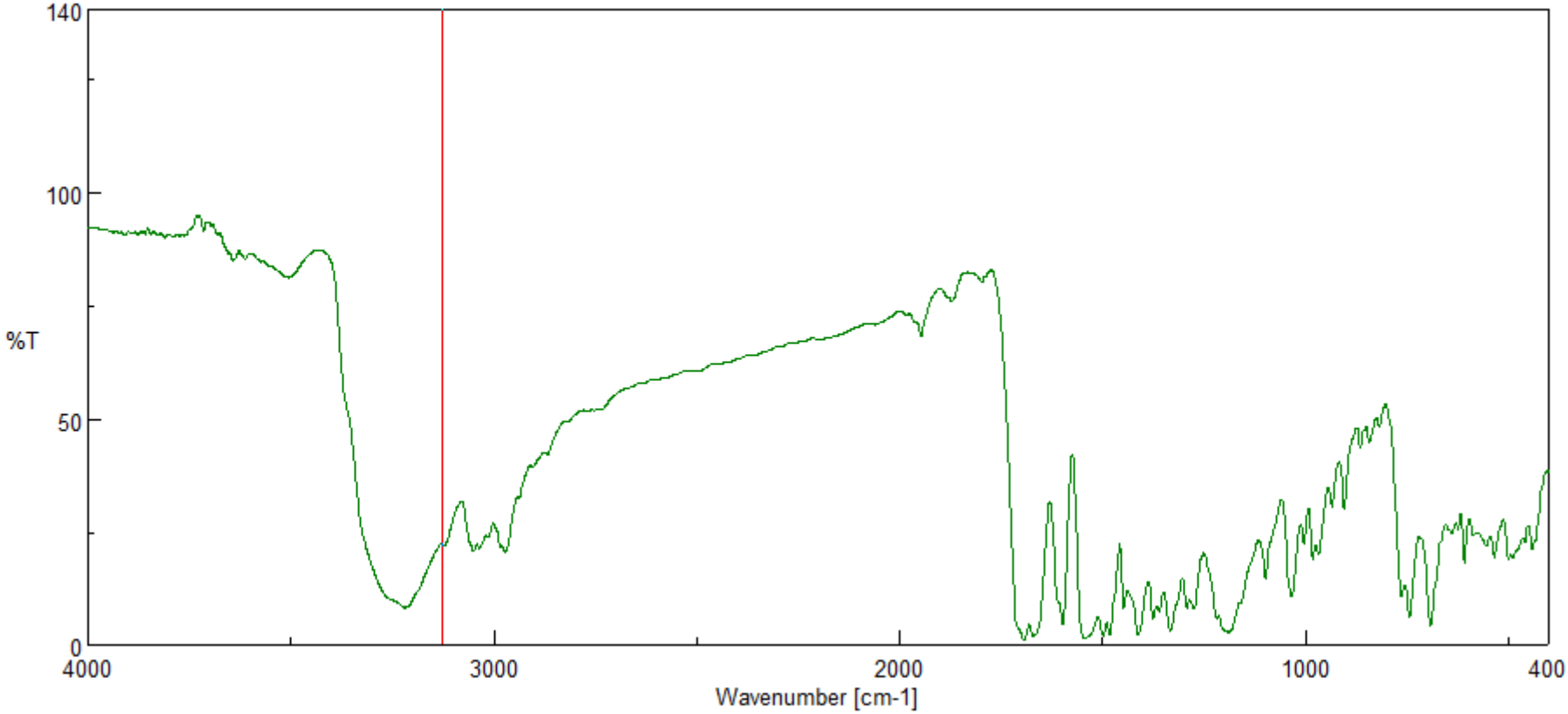
4b

-



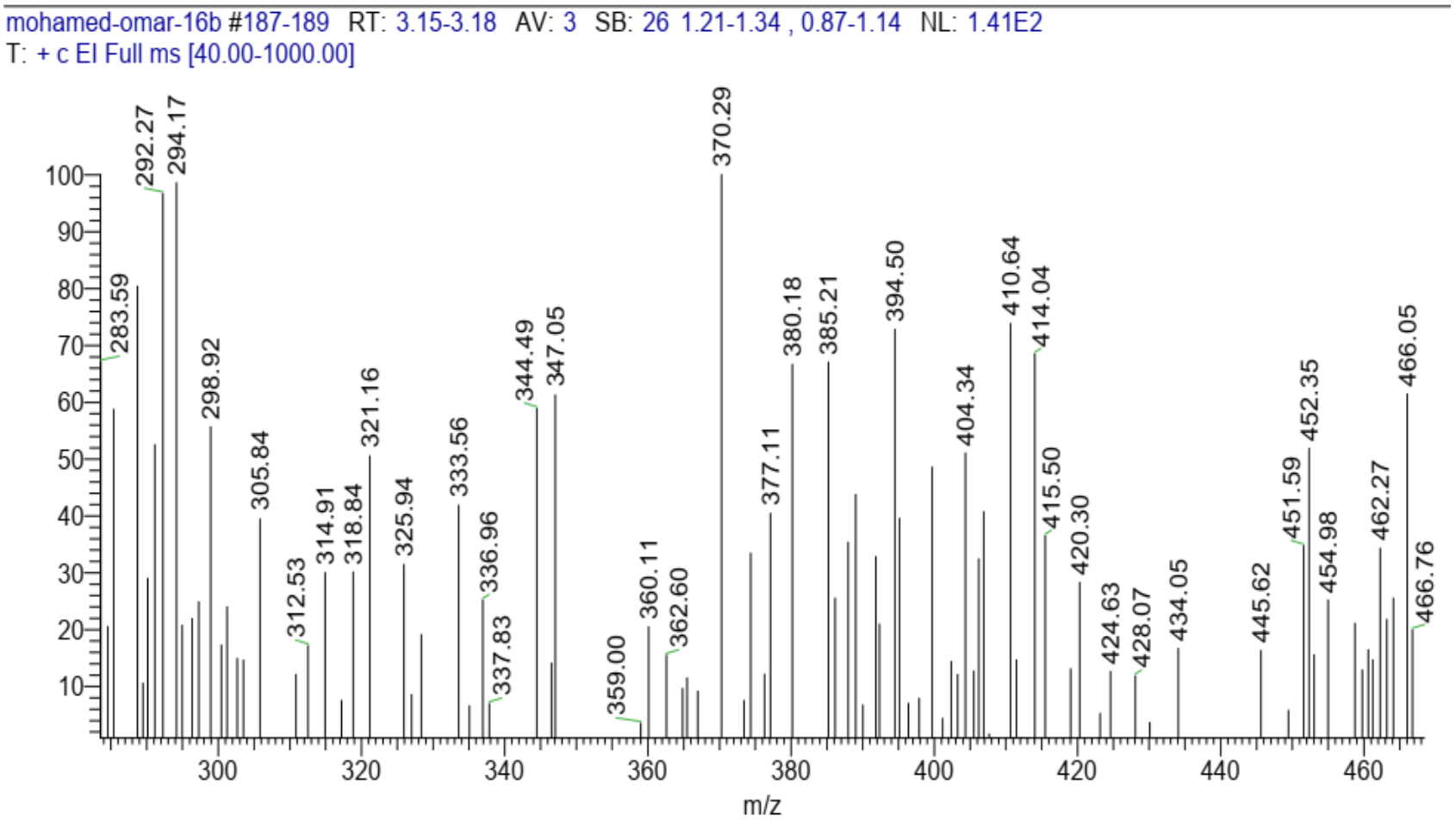
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4b)

-



FT-IR of compound (4b)

-

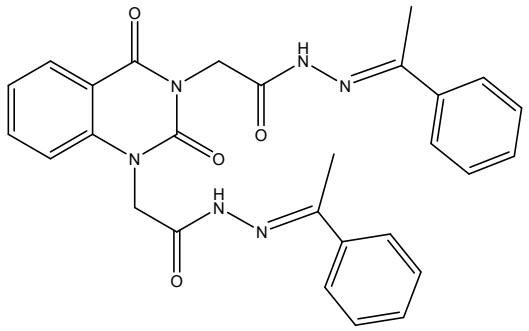


m/z Intensity Relative

MS of compound (4b)

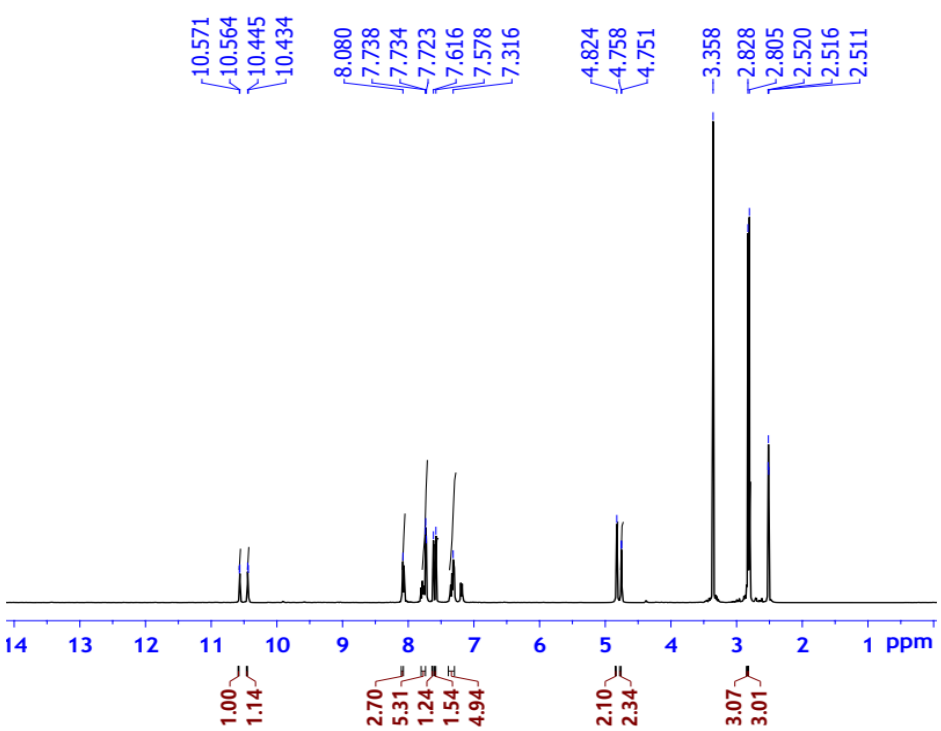
-

- Compound (4c):



4c

-

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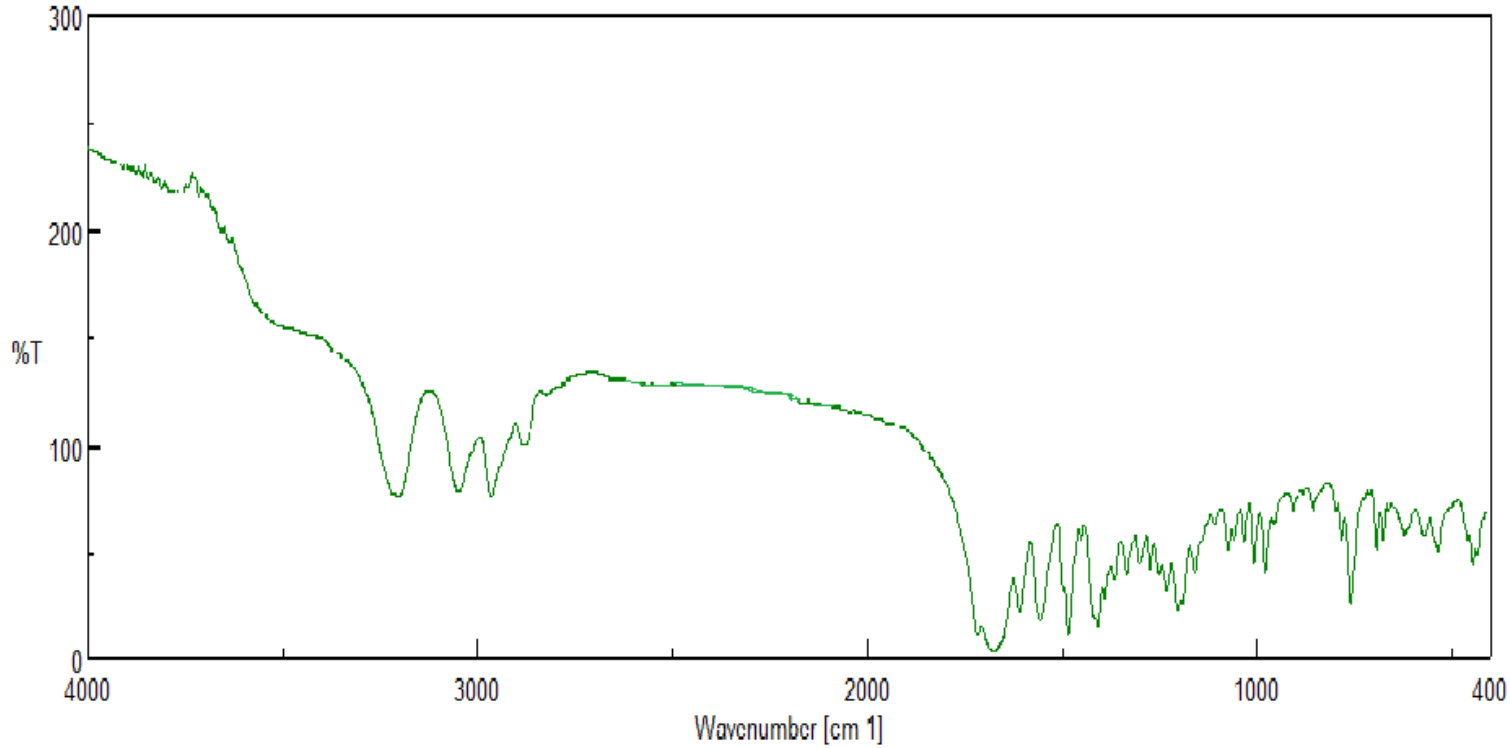
NAME      Mohammed Omar-10B-proton-WH
EXPNO              10
PROCNO              1

F2 - Acquisition Parameters
Date_          20220308
Time              14.11 h
INSTRUM           spect
PROBHD    Z108618_0948 (
PULPROG           zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.244832 Hz
AQ             4.0894465 sec
RG                 112.56
DW                62.400 usec
DE                 6.50 usec
TE                 293.7 K
D1            1.00000000 sec
TD0                   1
SFO1         400.2024712 MHz
NUC1                 1H
P1                13.50 usec
PLW1         19.00000000 W

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

^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4c)

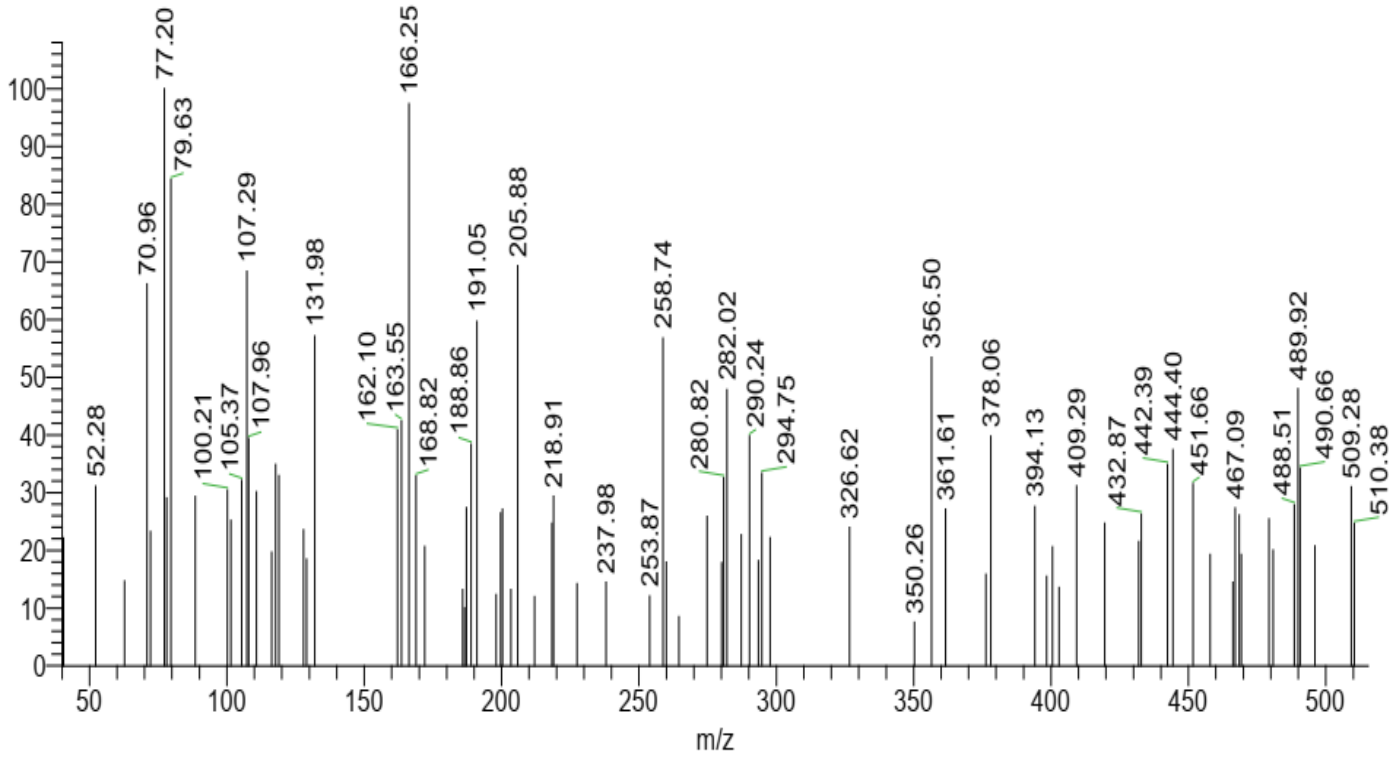
-



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]

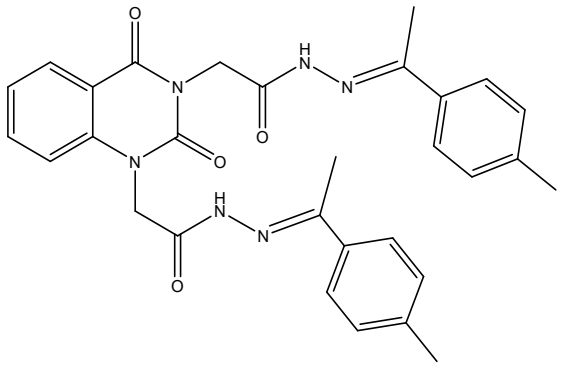


m/z Intensity Relative

MS of compound (4c)

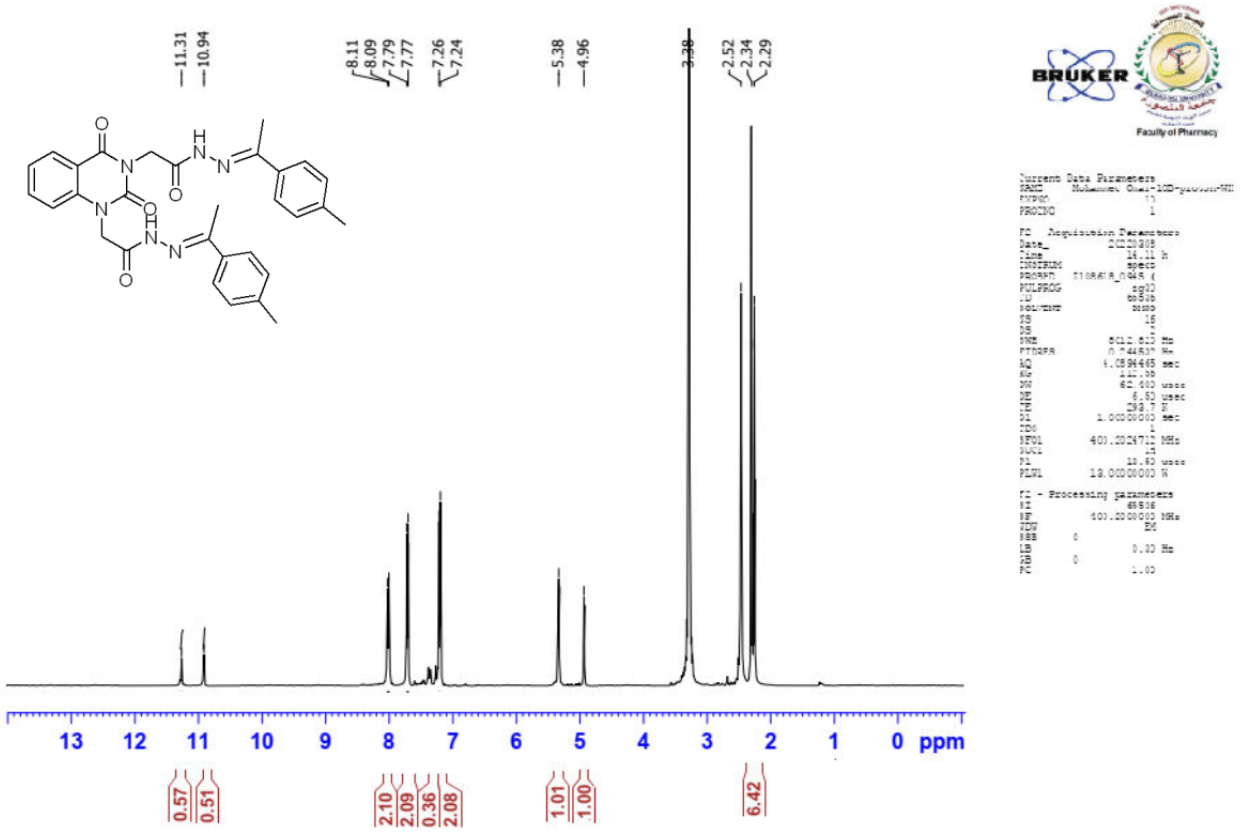
-

-Compound (4d): -



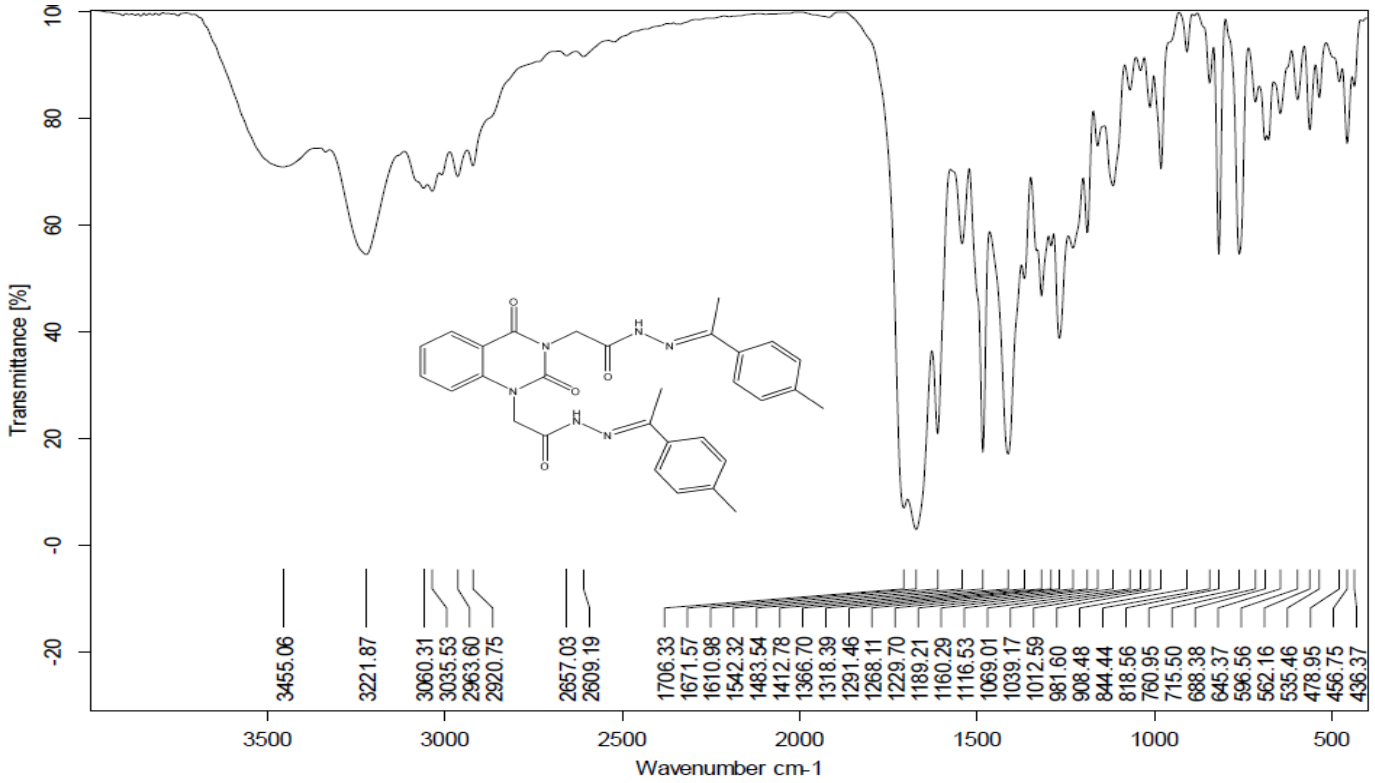
4d

-



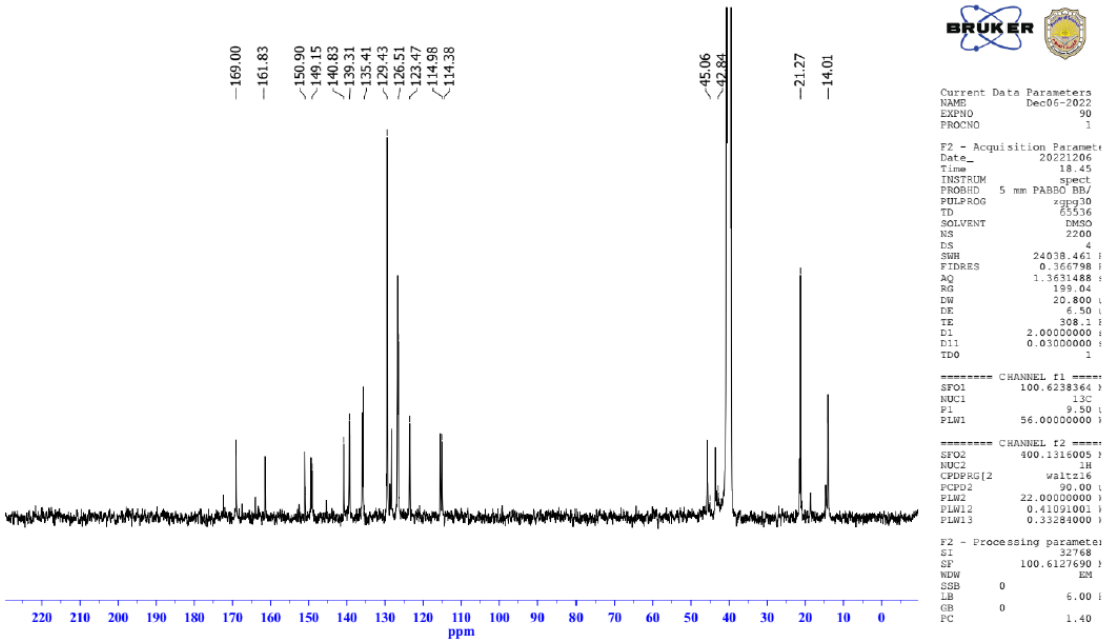
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4d)

-



FT-IR of compound (4d)

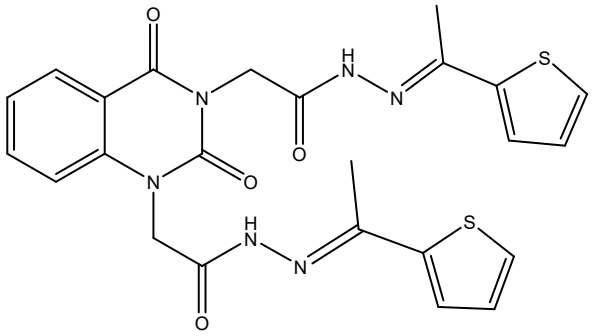
-



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

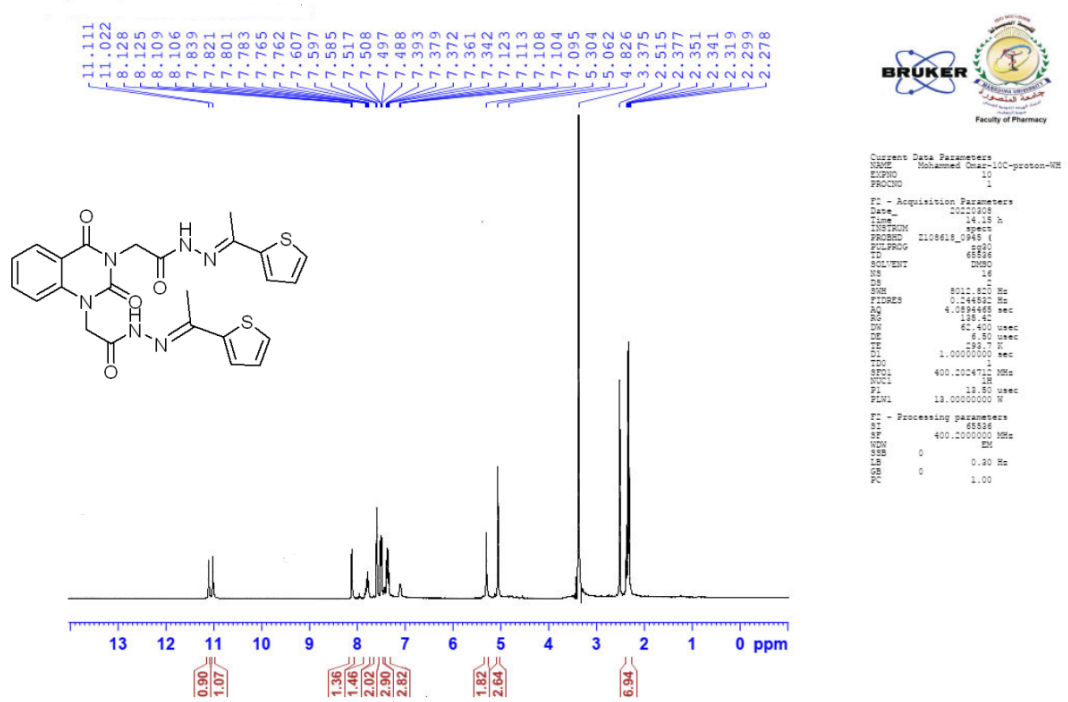
-

-Compound (4e):-



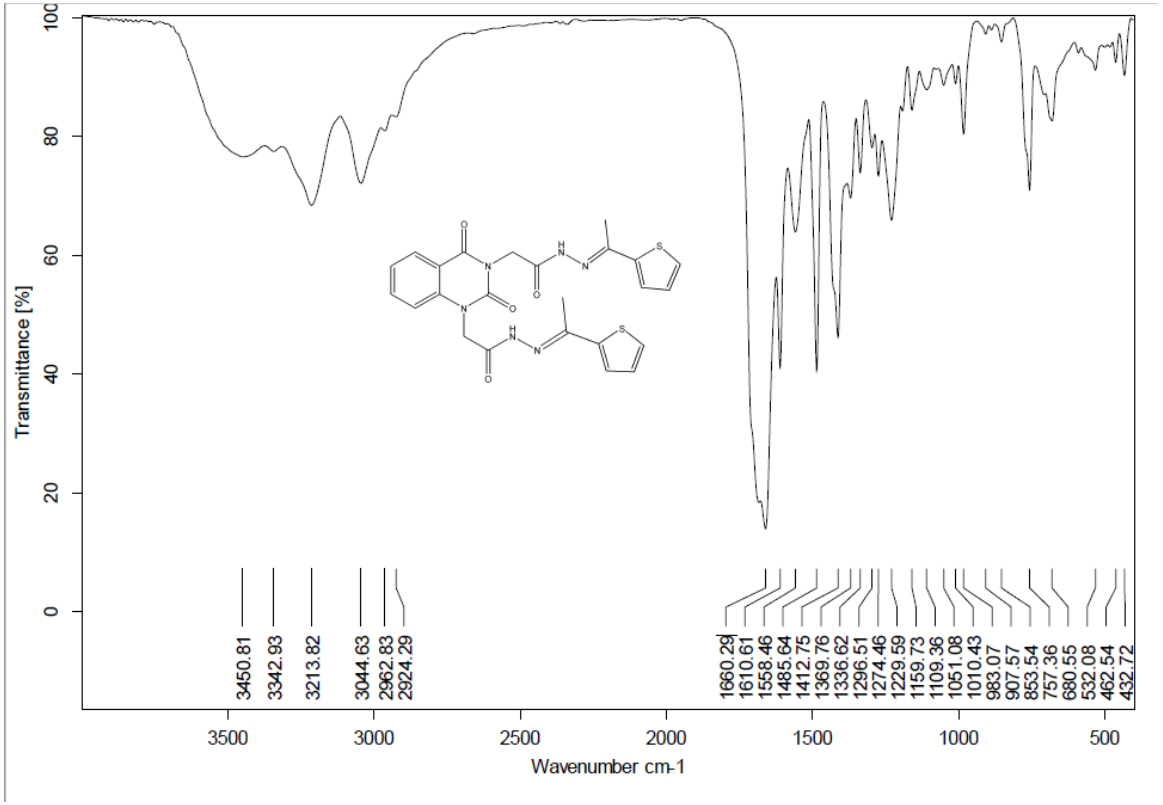
4e

-



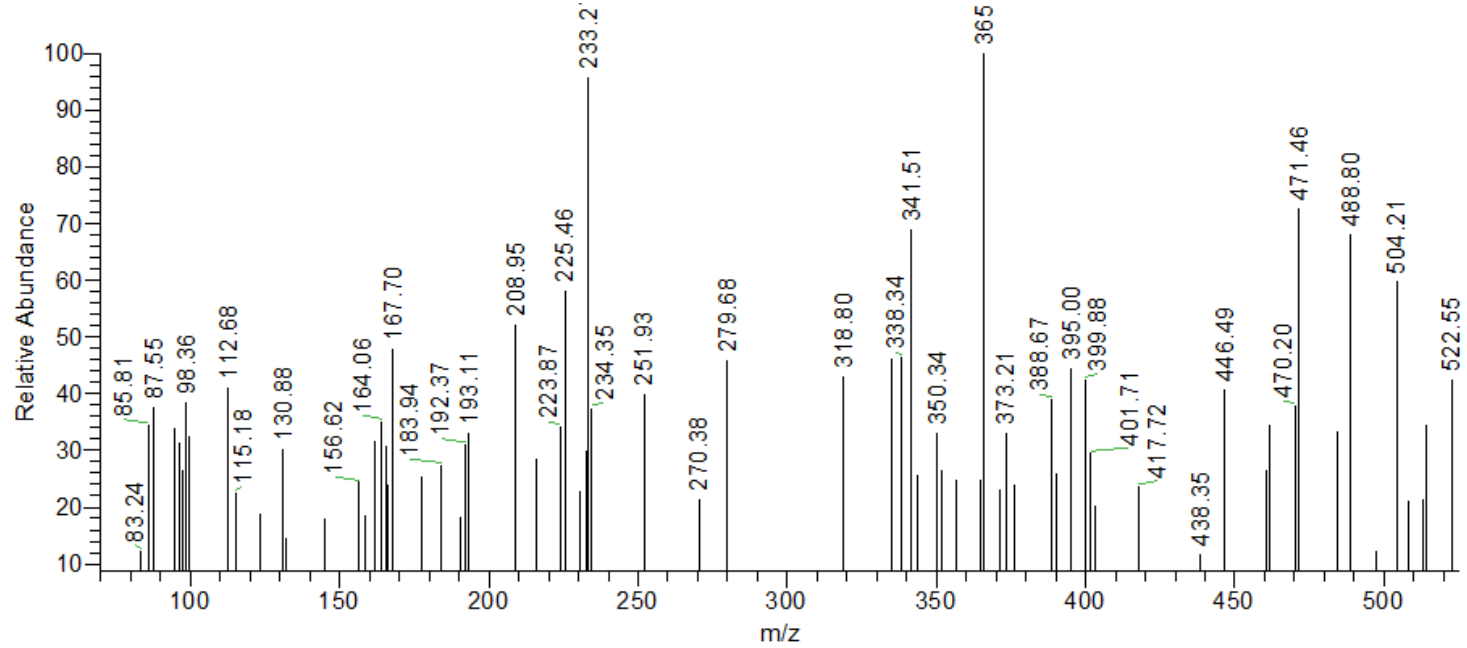
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4e)

-



FT-IR of compound (4e)

-

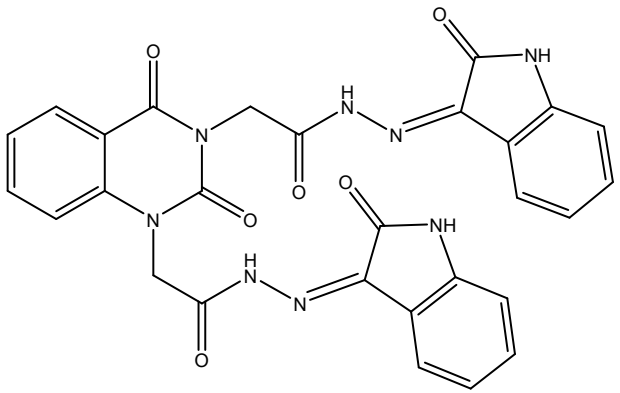


m/z Intensity Relative

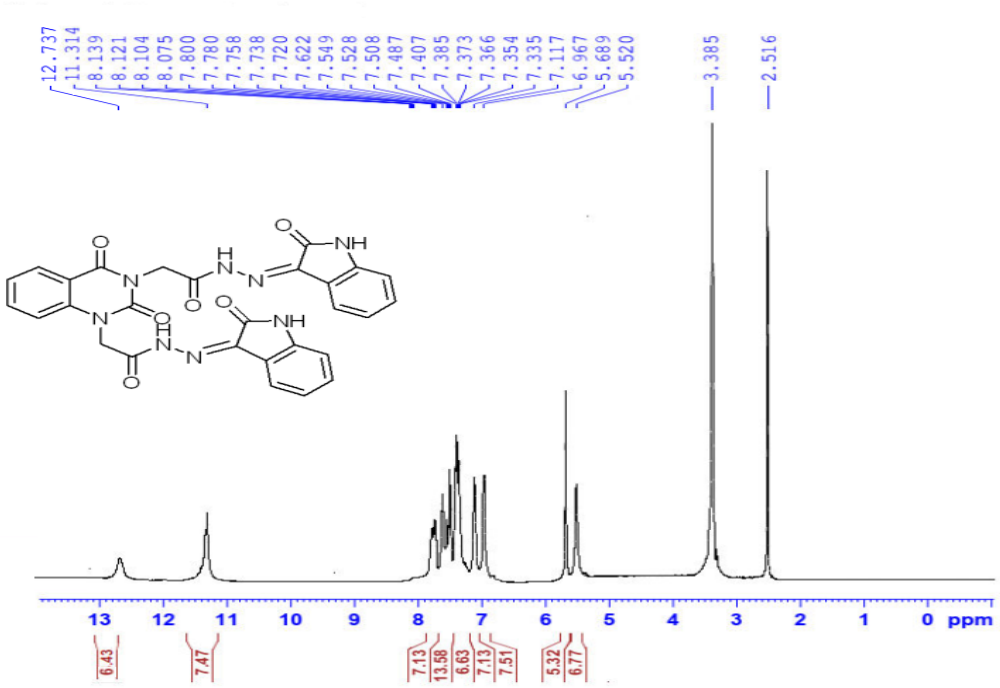
MS of compound (4e)

-

-Compound (4f)

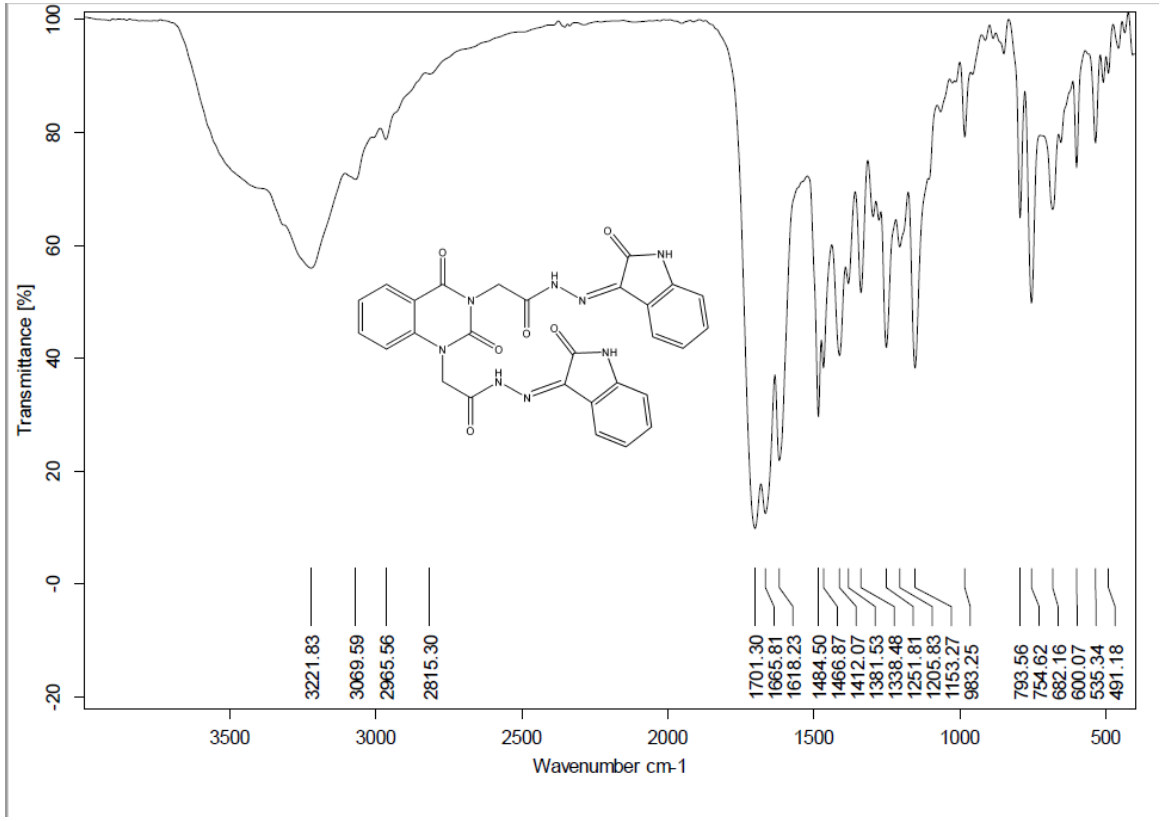


4f

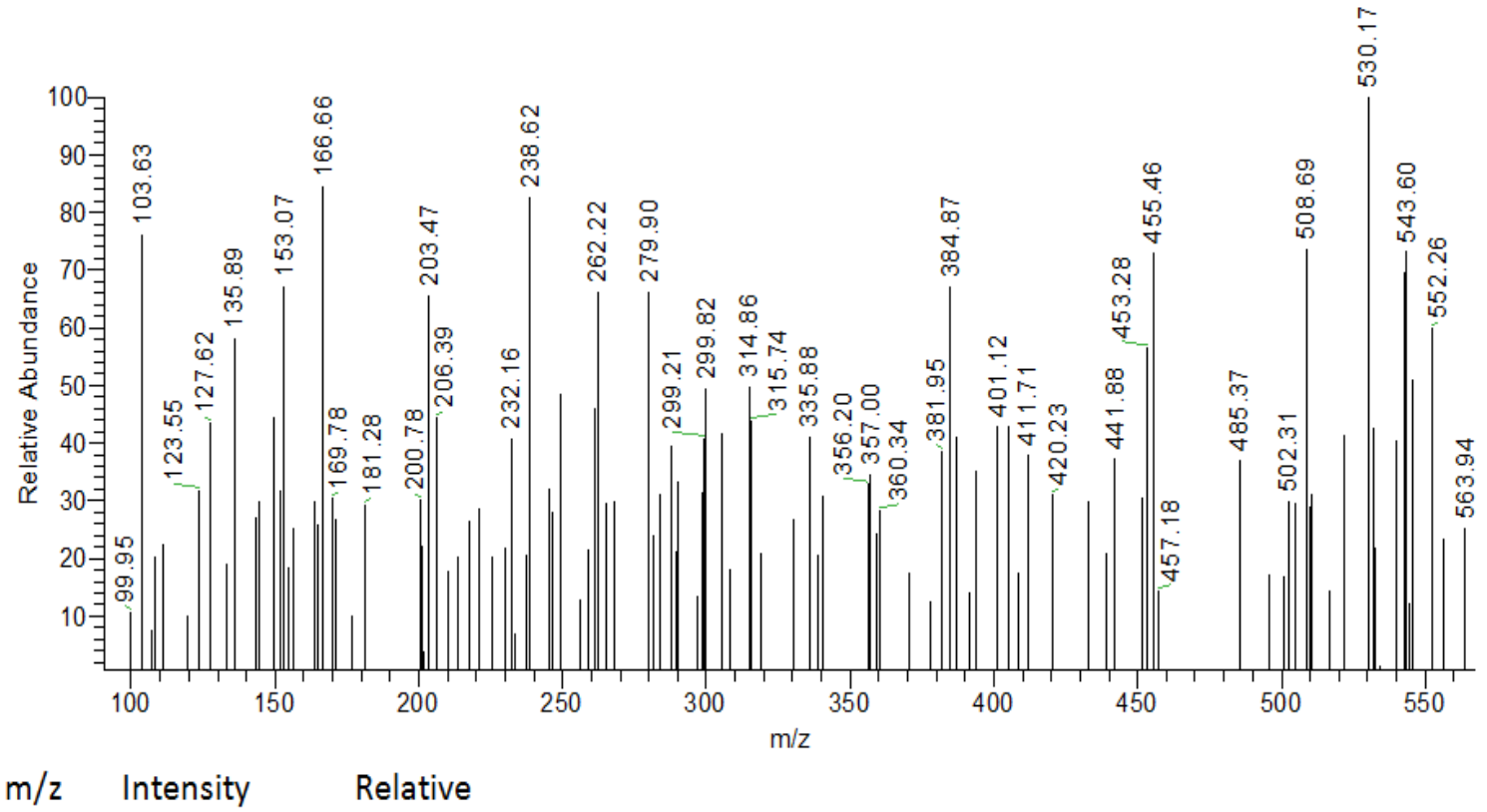


^{1}H-NMR (400 MHz, DMSO-d_6) of compound (4f)

-



FT-IR of compound (4f)

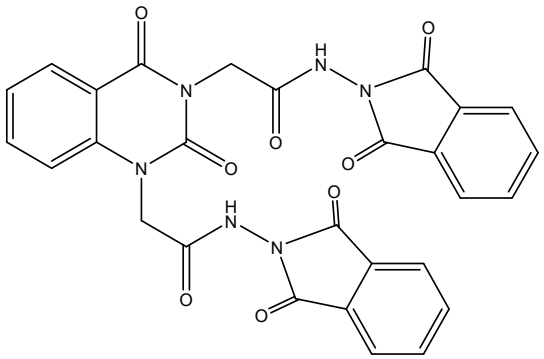


m/z Intensity Relative

MS of compound (4f)

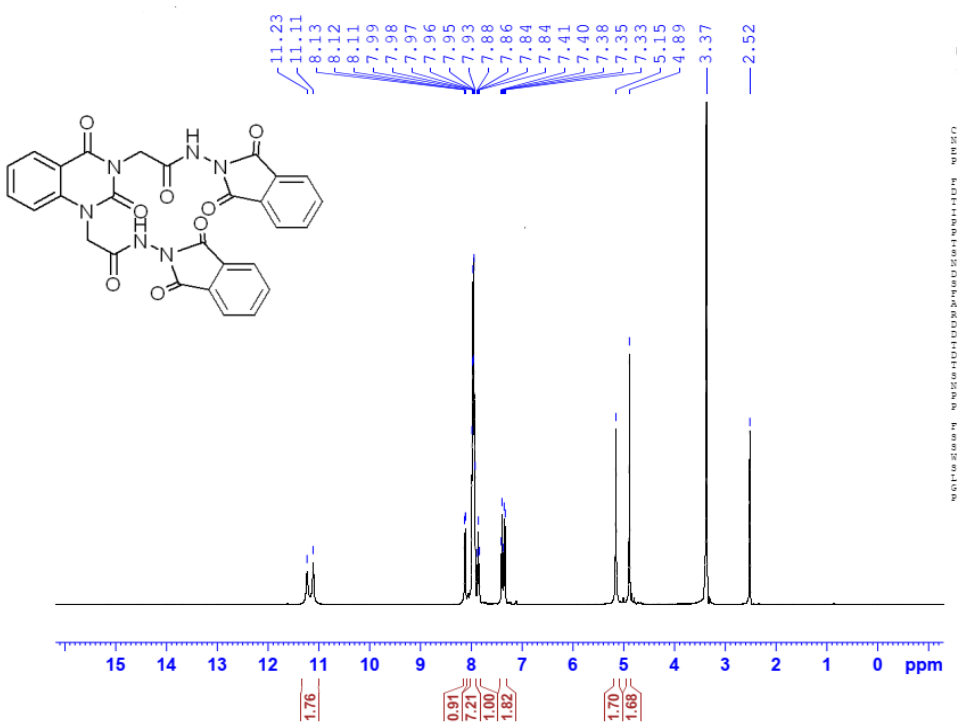
-

-Compound (5a):



5a

-

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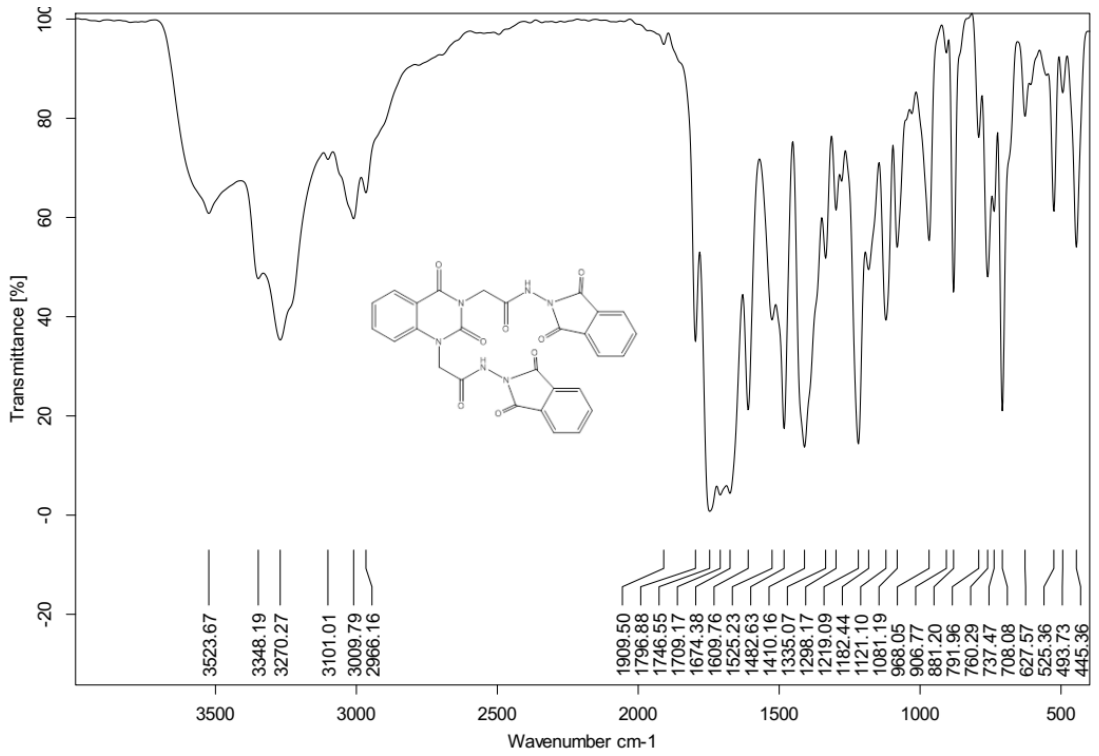
Current Data Parameters
NAME      mohamed omer-M2-Hnmr-ov
EXPNO                 10
PROCNO                 1

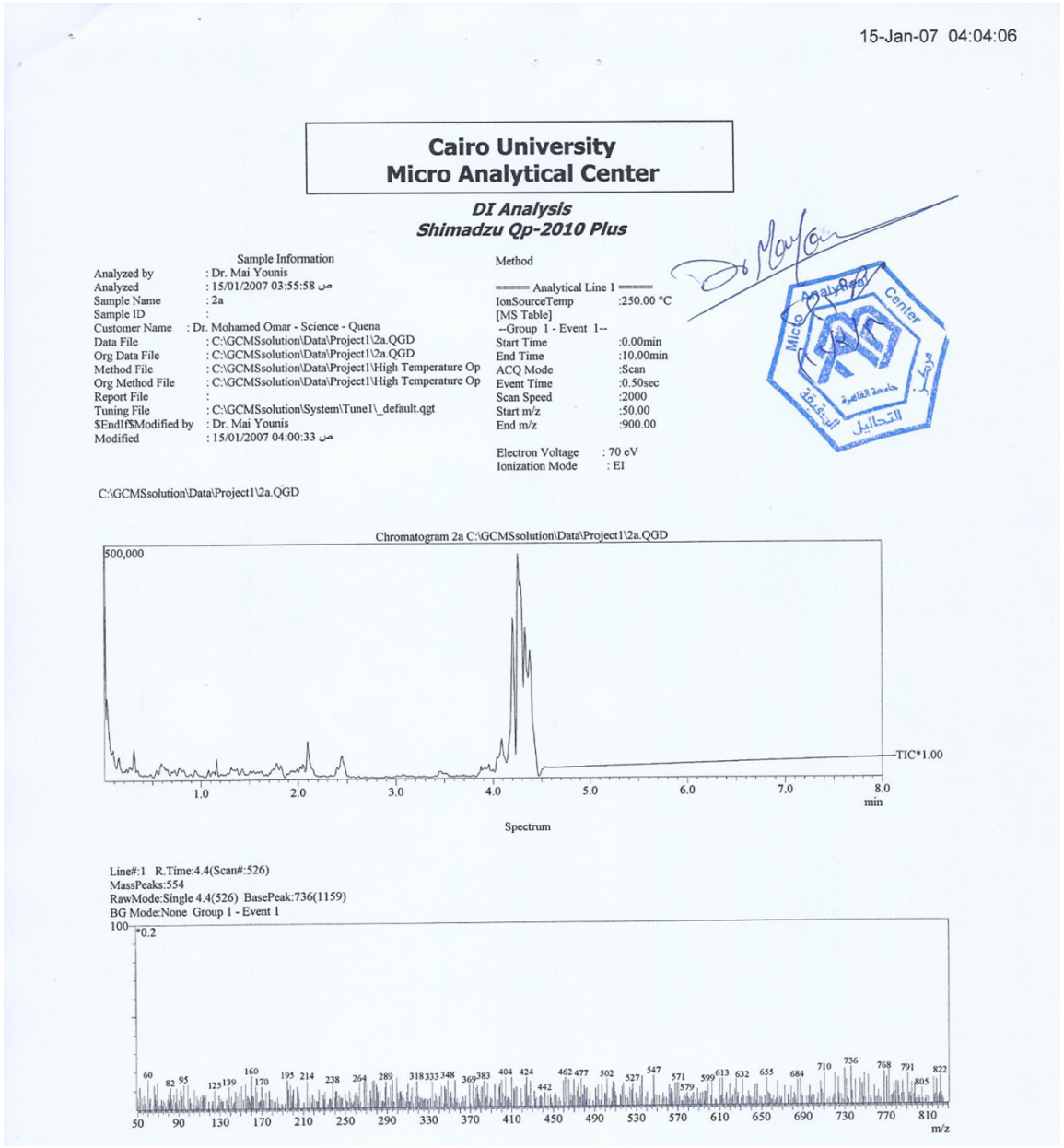
F2 - Acquisition Parameters
Date_           20211018
Time              18.19 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244891 Hz
AQ               4.0894465 sec
RG                  176.71
DW                 62.400 usec
DE                  6.50 usec
TE                293.8 K
D1               1.00000000 sec
TD0                    1
SFO1           400.2024710 MHz
NUC1                  1H
P1                 12.80 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
```

-

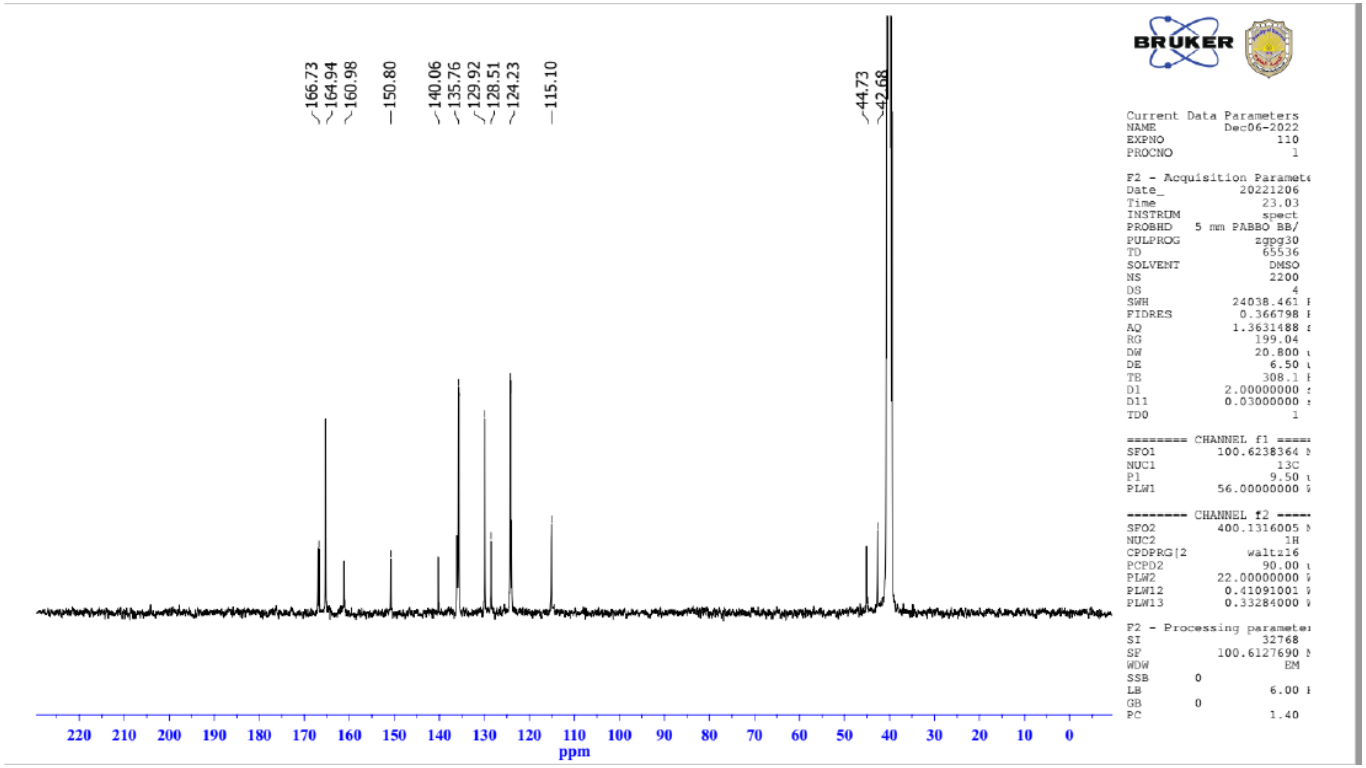


FT-IR of compound (5a)



MS of compound (5a)

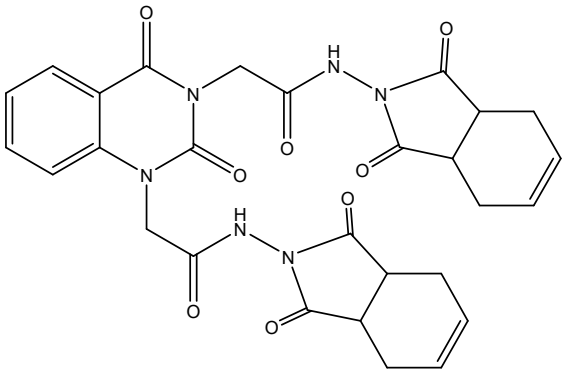
-



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

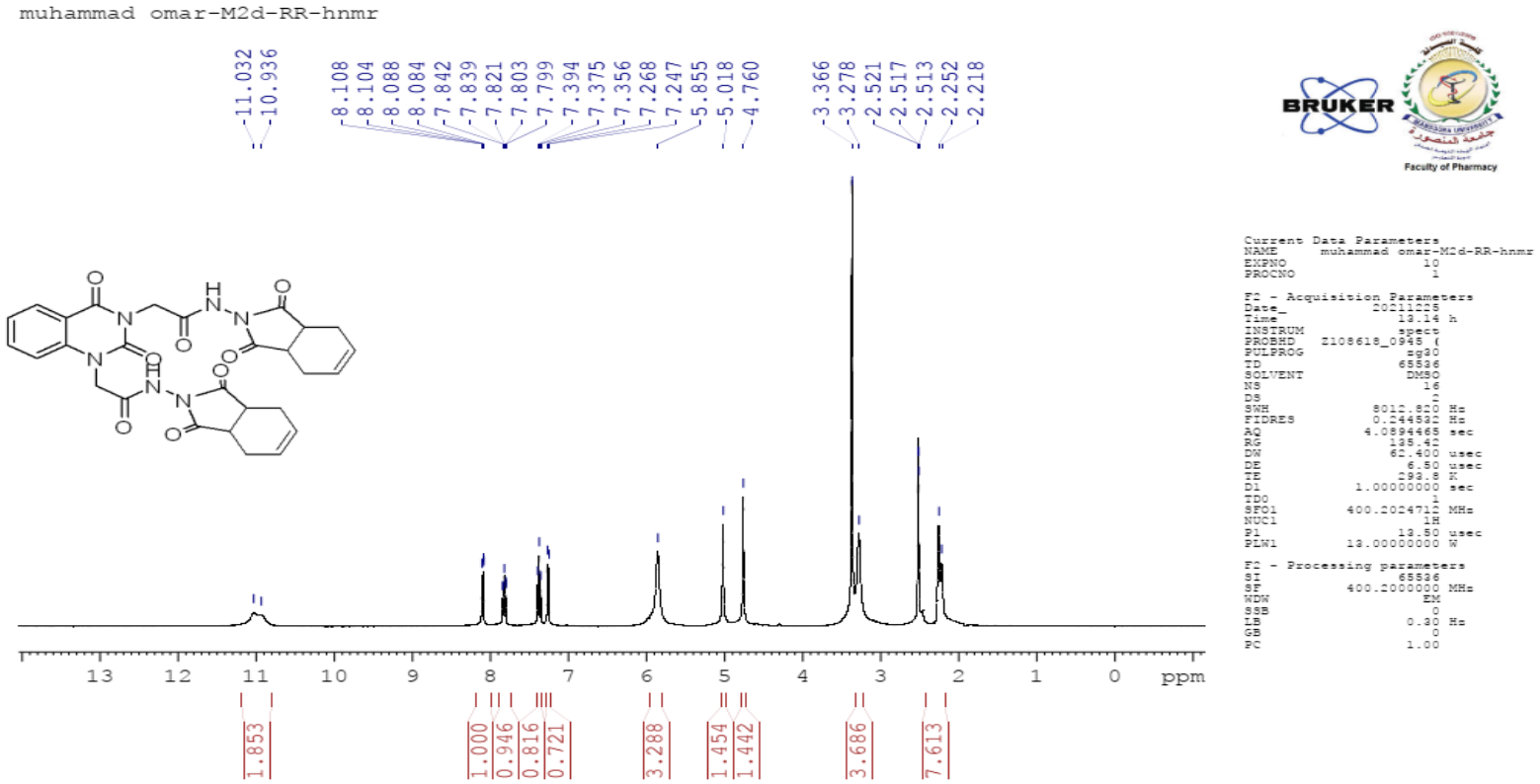
-

-Compound (5b):-

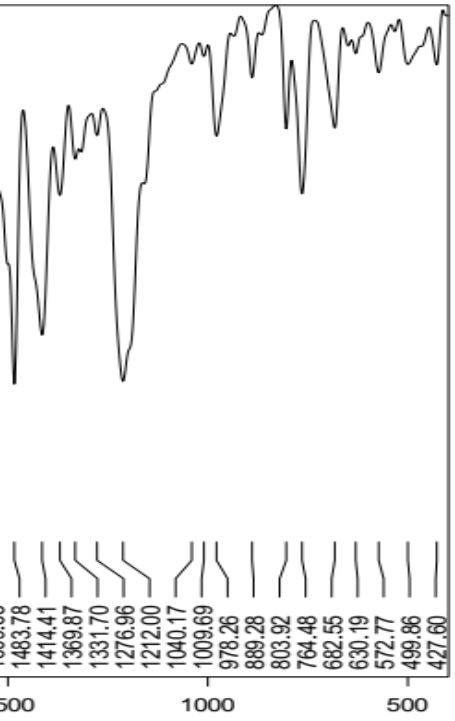


5b

-



^{1}H-NMR (400 MHz, DMSO-d_6) of compound (5b)



15-Jan-07 04:10:17

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

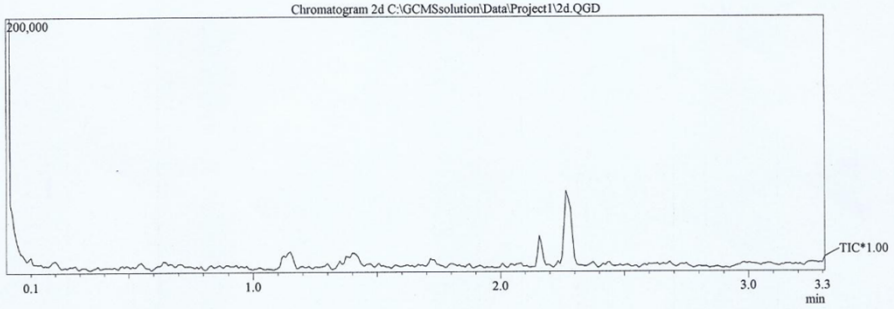
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:02:11 ص
Sample Name	: 2d
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\2d.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\2d.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature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

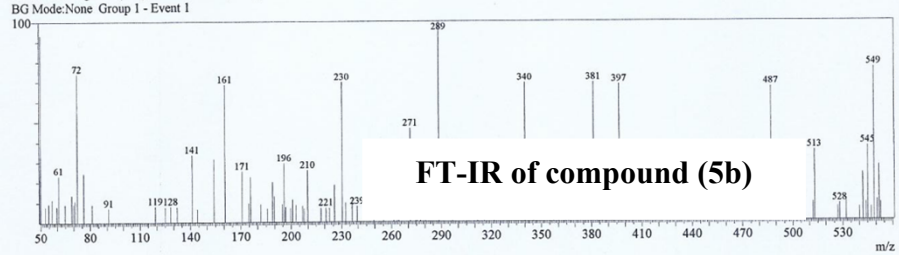
C:\GCMSsolution\Data\Project1\2d.QGD

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



Spectrum

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



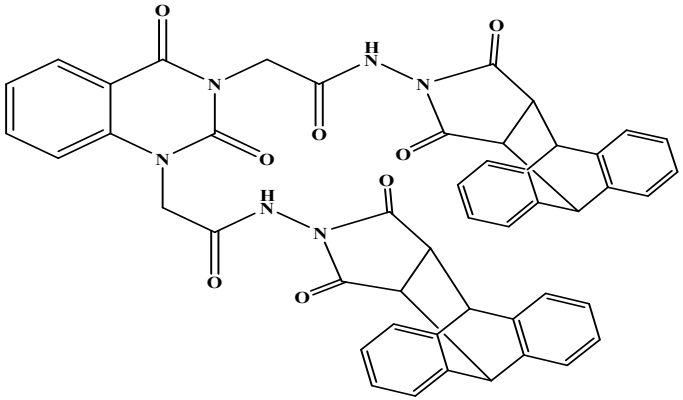
FT-IR of compound (5b)

-

-Compound (5c)

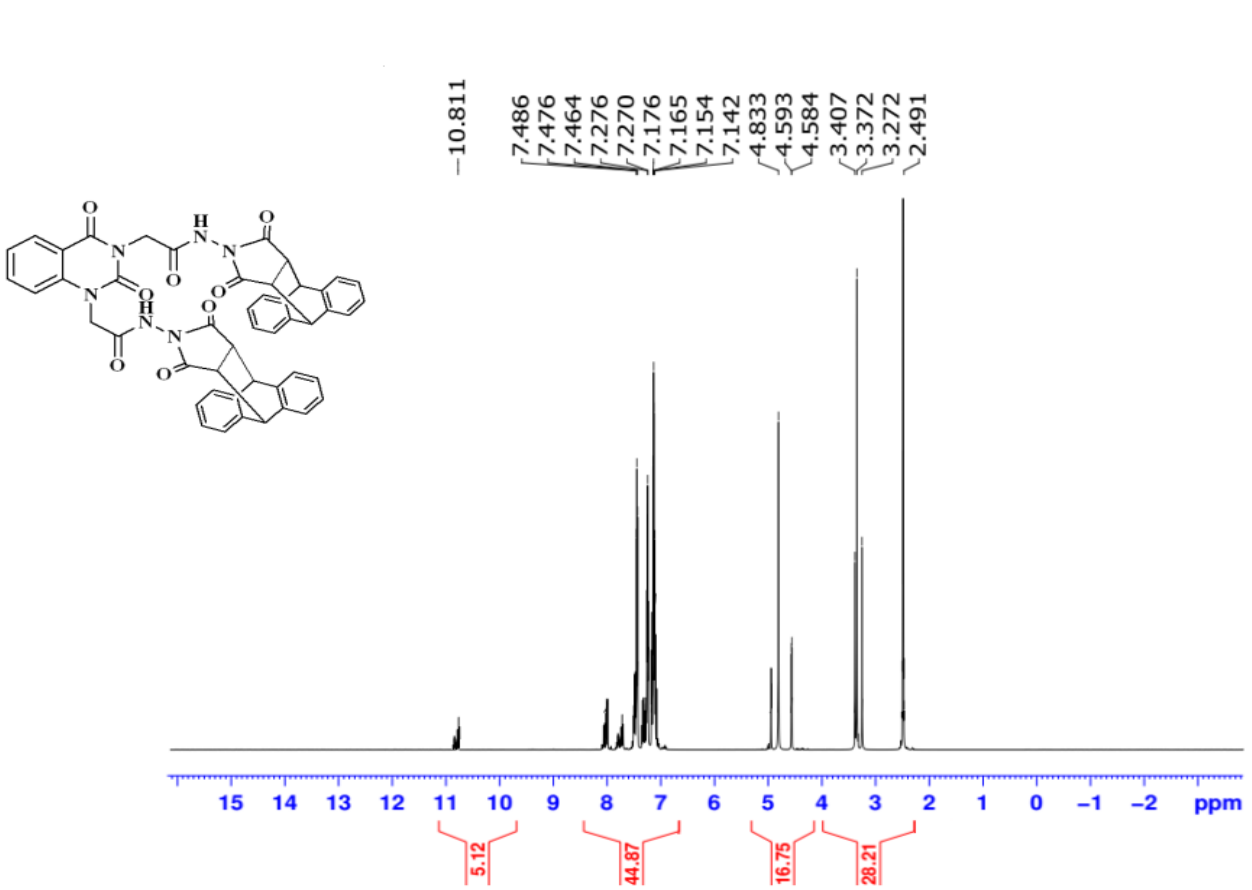
MS of compound (5b)

-



5c

-

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Current Data Parameters
NAME                  Feb17-2022
EXPNO                         20
PROCNO                         1

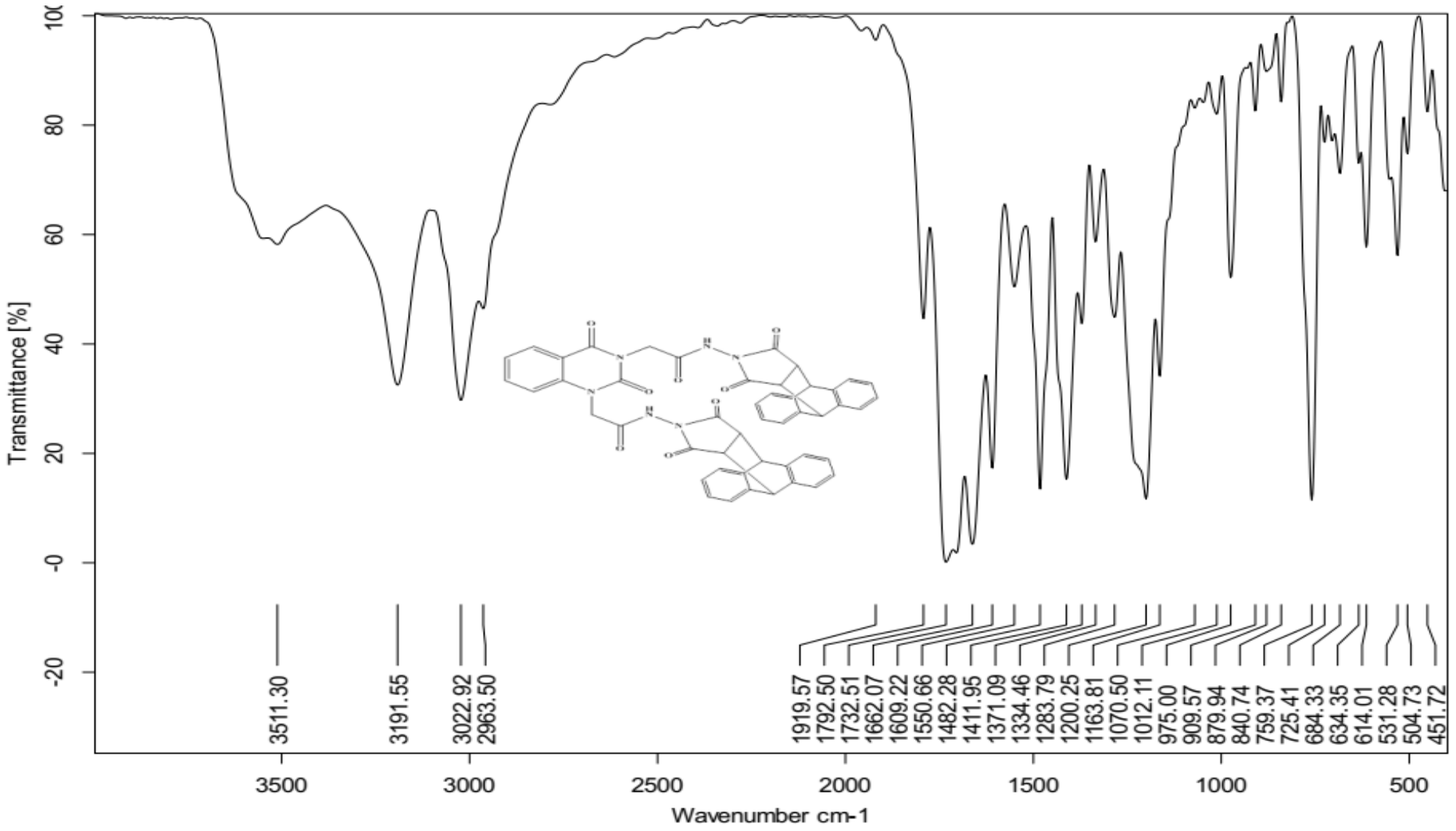
F2 - Acquisition Parameters
Date_                   20220217
Time                       10.14
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                           50
DS                            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 ========
SFO1                 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
```

^{1}H-NMR (400 MHz, DMSO-d_6) of compound (5c)

-



FT-IR of compound (5c)

15-Jan-07 04:04:06

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

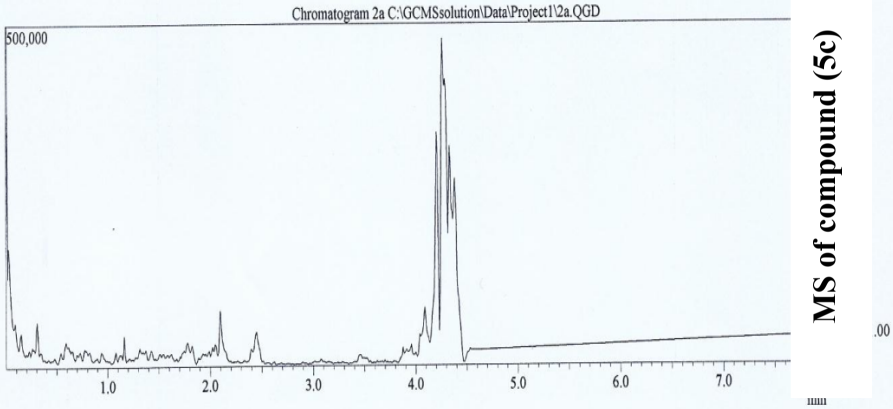
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 03:55:58 ص
Sample Name	: 2a
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\2a.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\2a.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 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

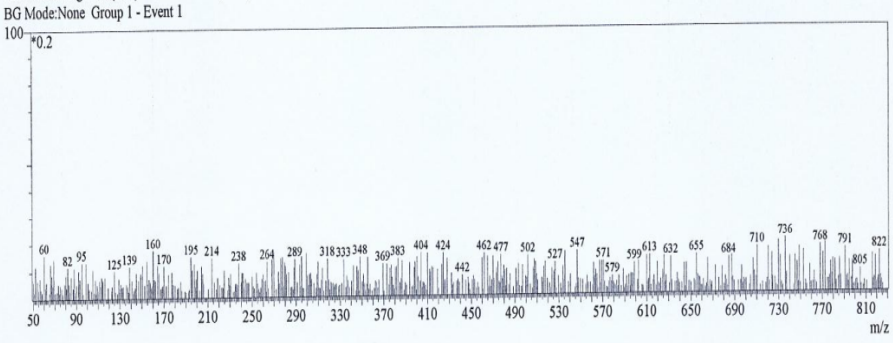
C:\GCMSsolution\Data\Project1\2a.QGD

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



Spectrum

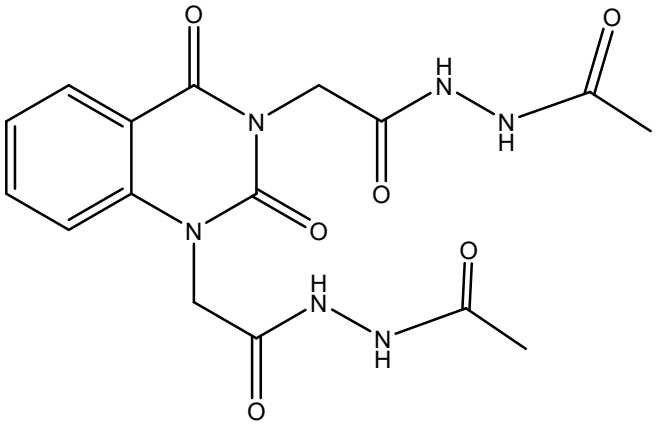
Line#:1 R.Time:4.4(Scan#:526)
MassPeaks:554
RawMode:Single 4.4(526) BasePeak:736(1159)
BG Mode:None Group 1 - Event 1



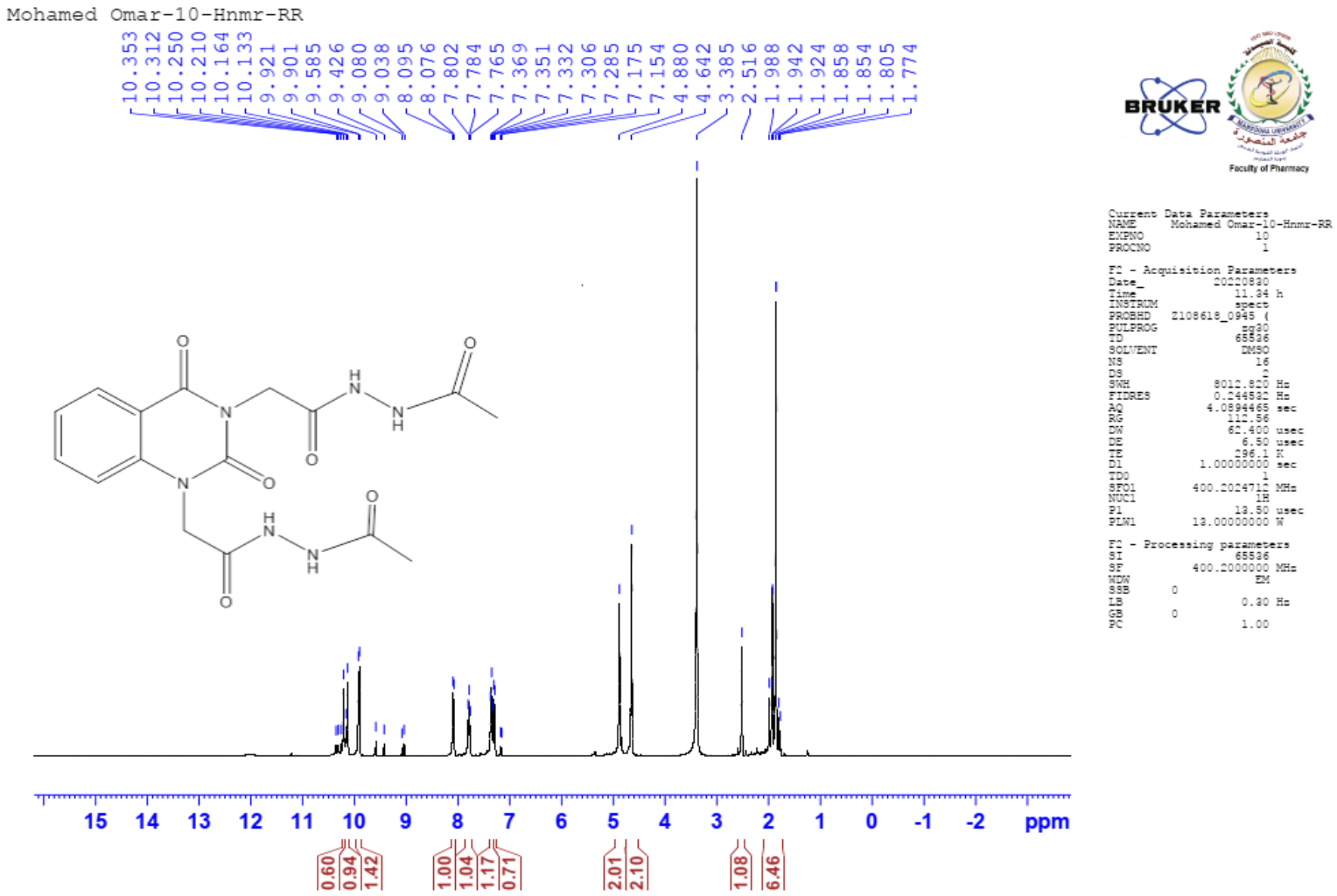
MS of compound (5c)

-

-Compound (6a)



6a



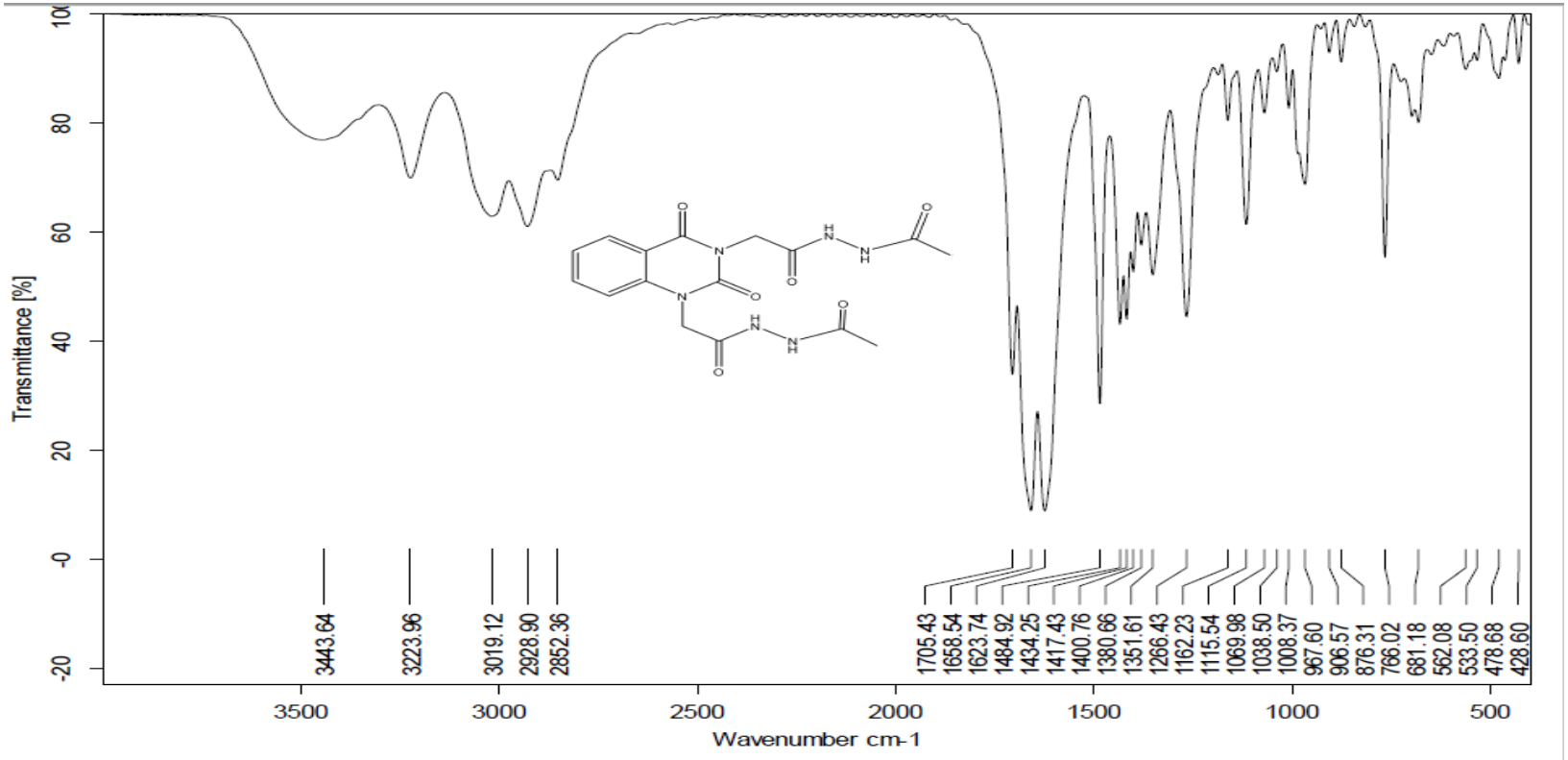

```
Current Data Parameters
NAME      Mohamed Omar-10-Hnmr-RR
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220830
Time              11.34 h
INSTRUM             spect
PROBHD   Z108618_0945 (
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                 296.1 K
D1              1.00000000 sec
TD0                    1
SFO1           400.2024712 MHz
NUC1                   1H
P1                  13.50 usec
PLW1           13.00000000 W

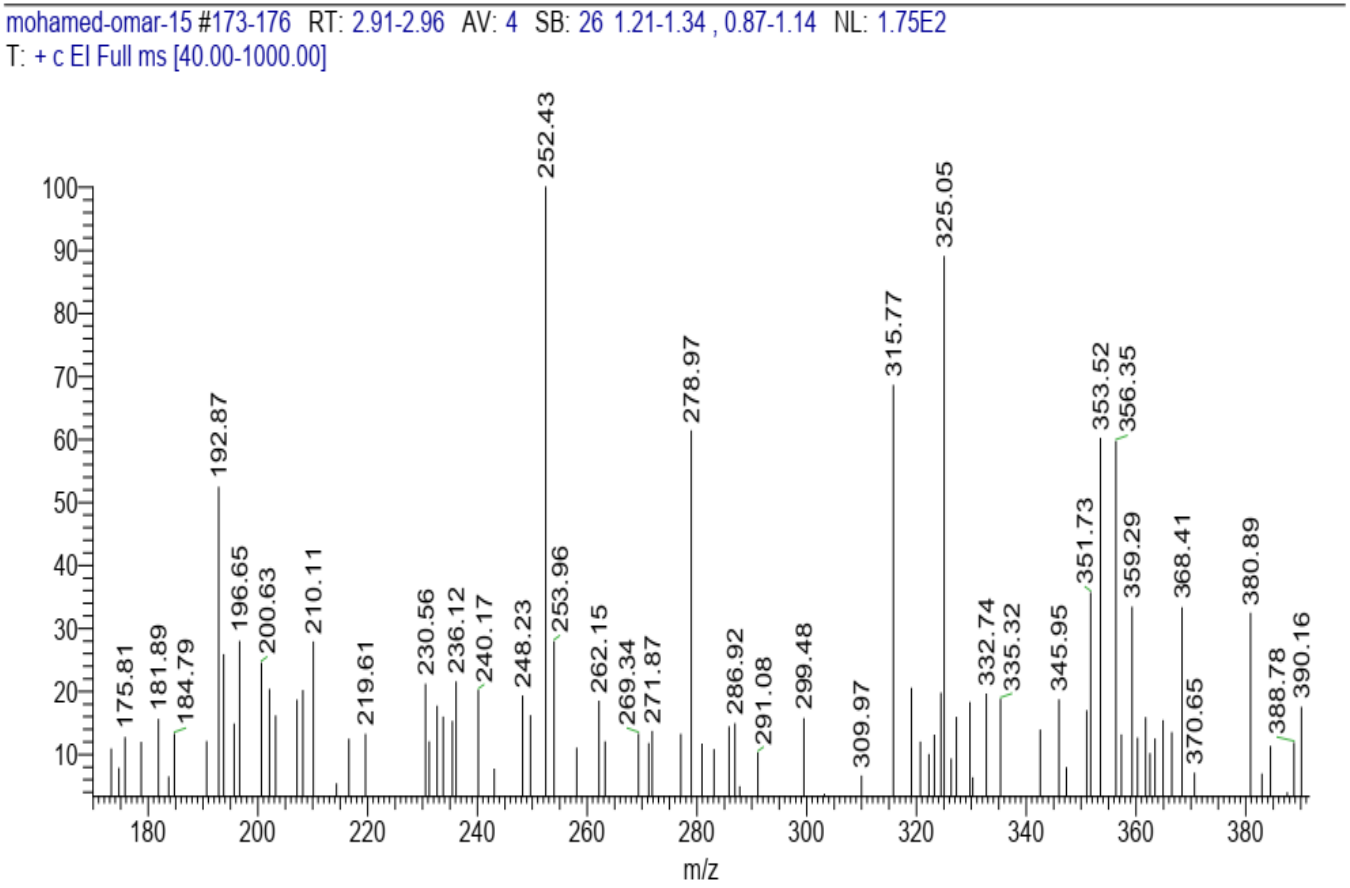
F2 - Processing parameters
SI                 65536
SF           400.2000000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H-NMR (400 MHz, DMSO-d_6) of compound (6a)

-


Transmittance [%]
100
80
60
40
20
-0
-20
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3443.64
3223.96
3019.12
2928.90
2852.36
1705.43
1658.54
1623.74
1484.92
1434.25
1417.43
1400.76
1380.66
1351.61
1266.43
1162.23
1115.54
1069.98
1038.50
1008.37
967.60
906.57
876.31
766.02
681.18
562.08
533.50
478.68
428.60

-

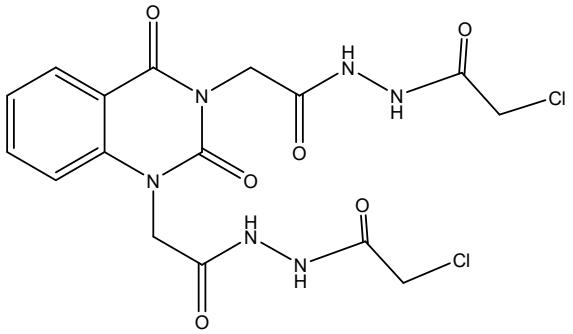


m/z Intensity Relative

MS of compound (6a)

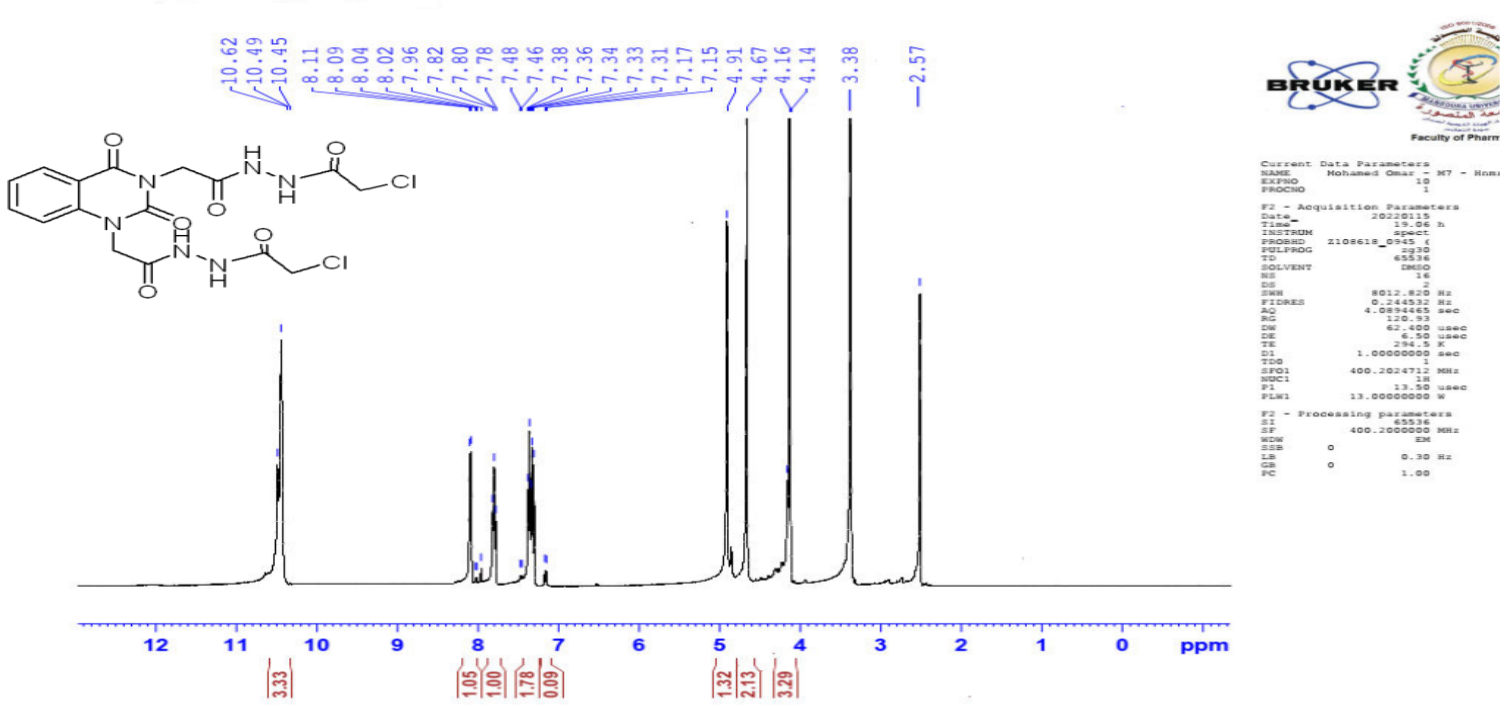
-

-Compound (6b)



6b

-

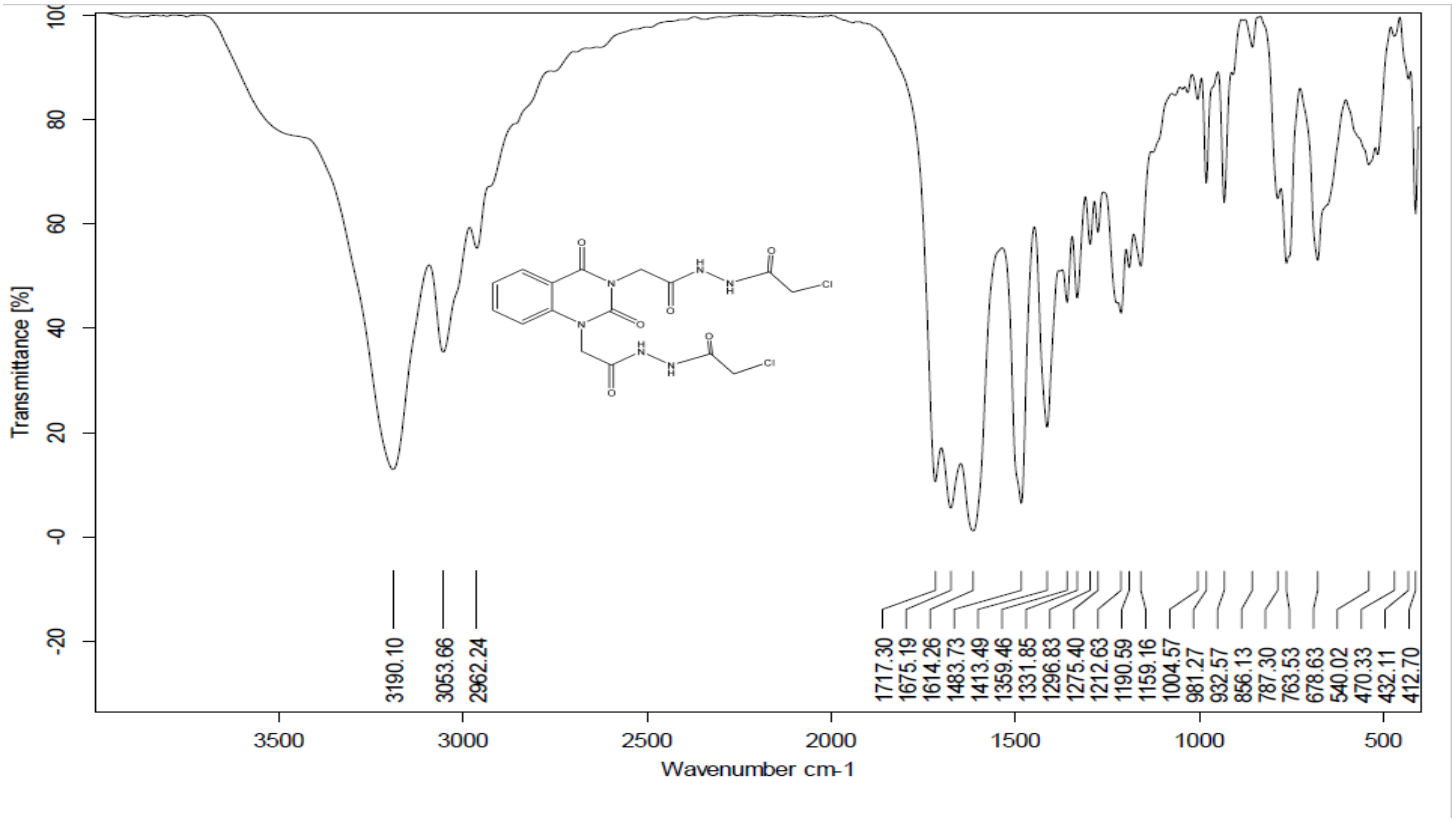


Current Data Parameters
NAME Mohamed Omar - M7 - Hnmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220115
Time 19.06 h
INSTRUM spect
PROBHD 2108618_0945 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 120.93
DW 62.400 usec
DE 6.50 usec
TE 294.5 K
D1 1.00000000 sec
TD0 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

-



FT-IR of compound (6b)

15-Jan-07 02:56:27

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

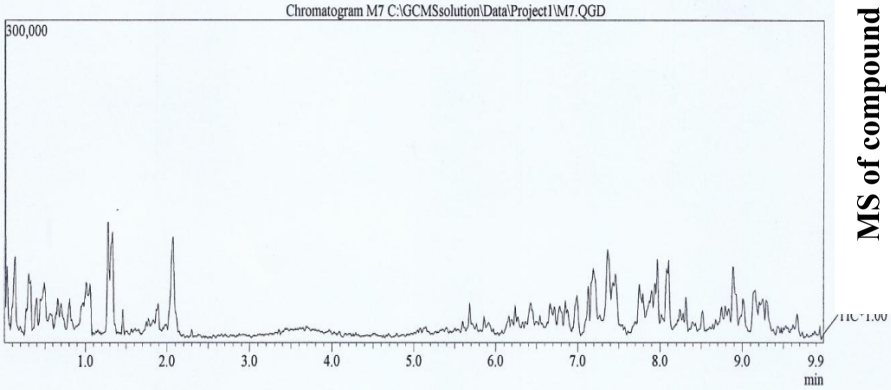
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 02:36:02 ص
Sample Name	: M7
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M7.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M7.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 02:46:02 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

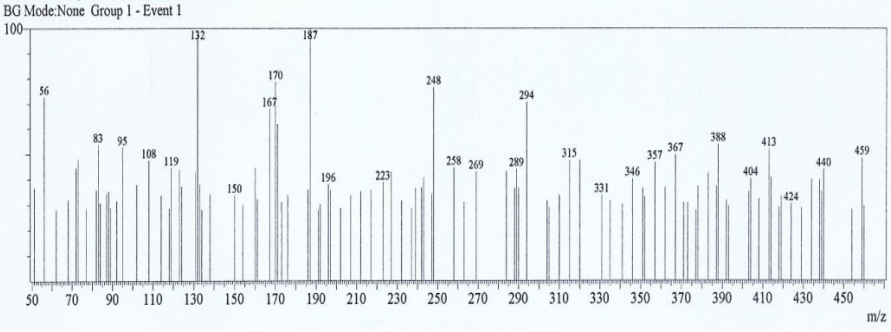
C:\GCMSsolution\Data\Project1\M7.QGD

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



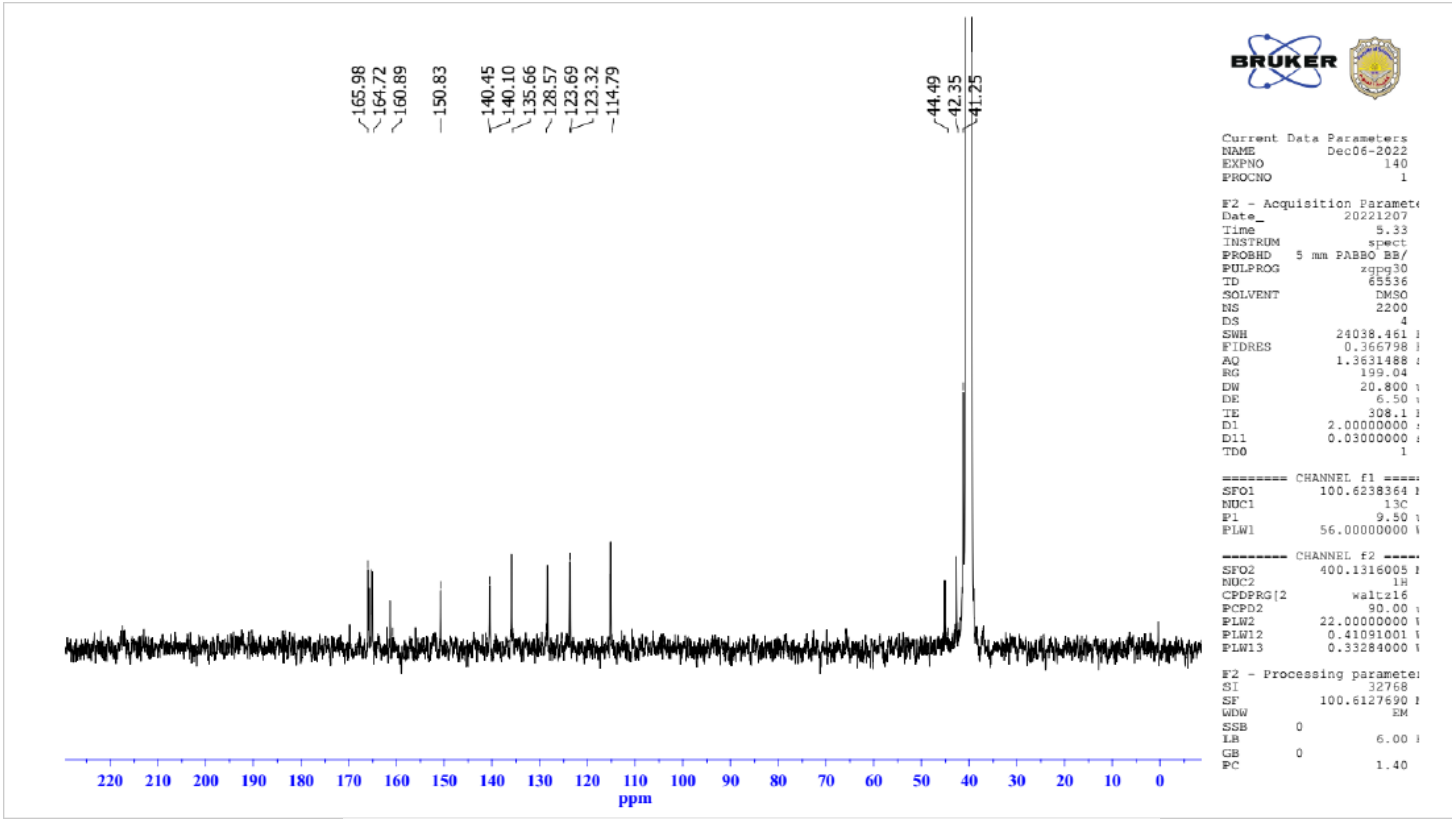
Spectrum

Line#:1 R.Time:6.4(Scan#:765)
MassPeaks 102
RawMode:Single 6.4(765) BasePeak:187(369)
BG Mode:None Group 1 - Event 1



MS of compound (6b)

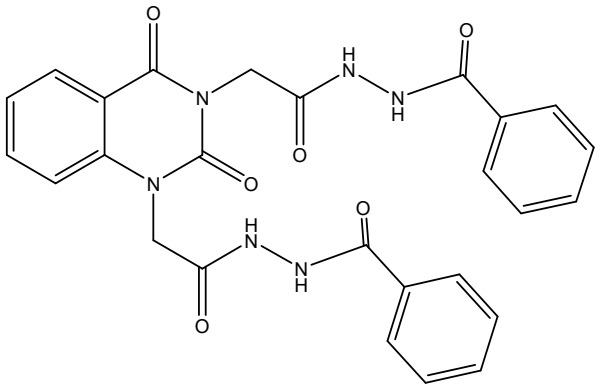
-



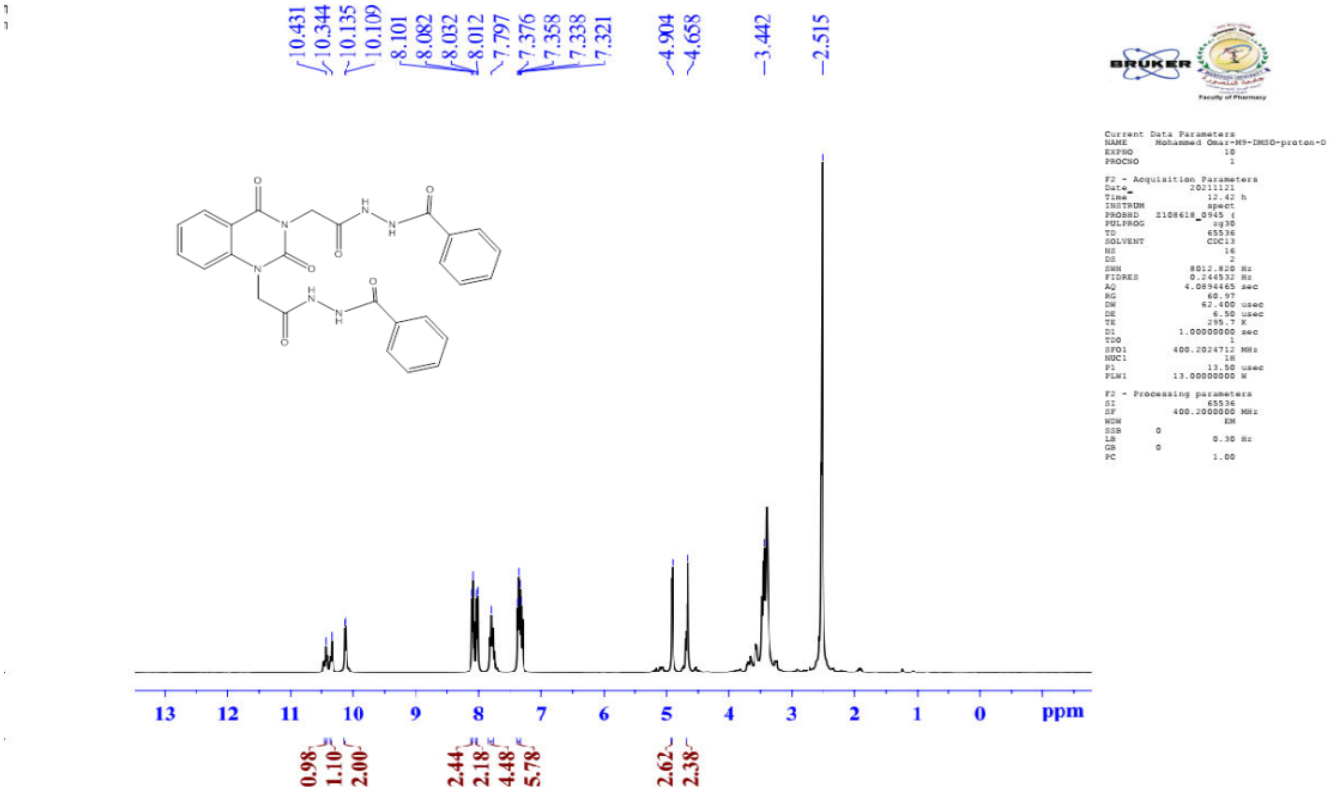
^{13}C-NMR (100 MHz, DMSO) of compound (6b)

-

-Compound (6c)



6c



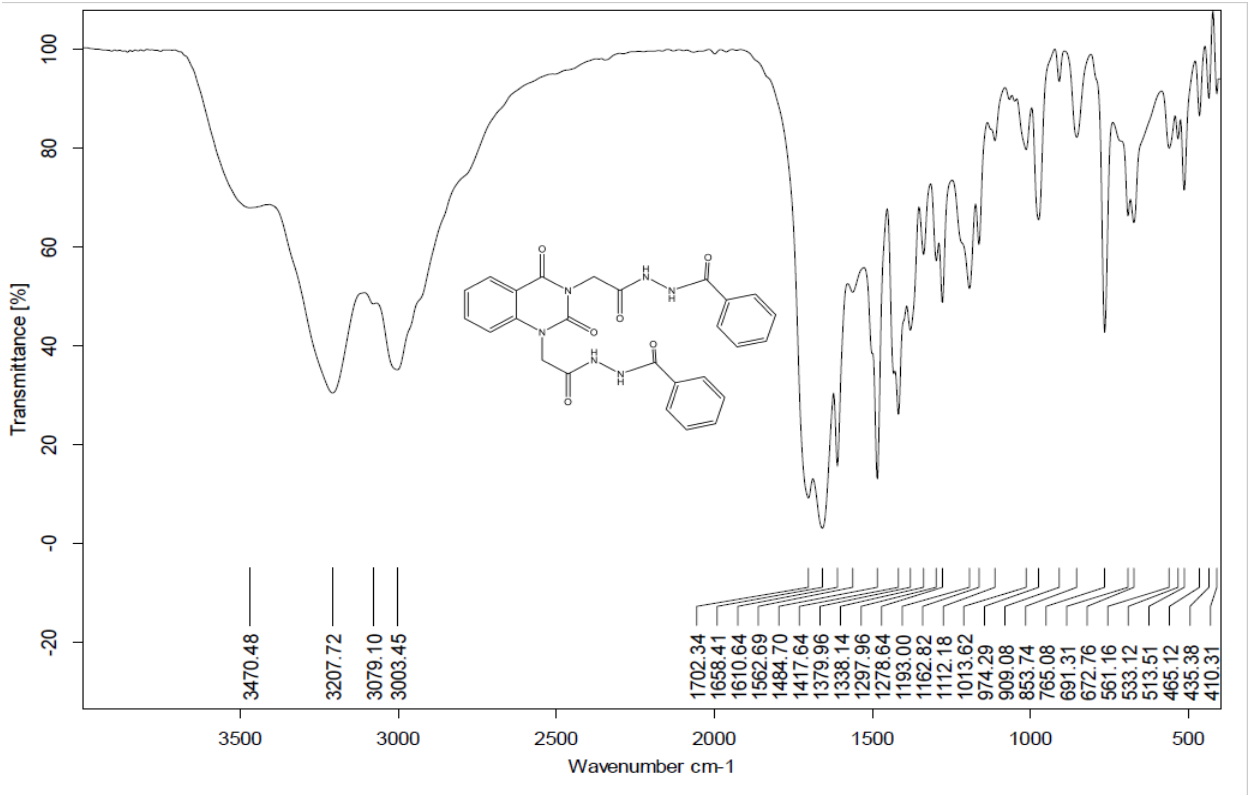
Current Data Parameters
NAME Mohammed Omar-M9-DMSO-proton-D
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211121
Time 12.42 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 60.97
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 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

^{1}H-NMR (400 MHz, DMSO-d_6) of compound (6c)

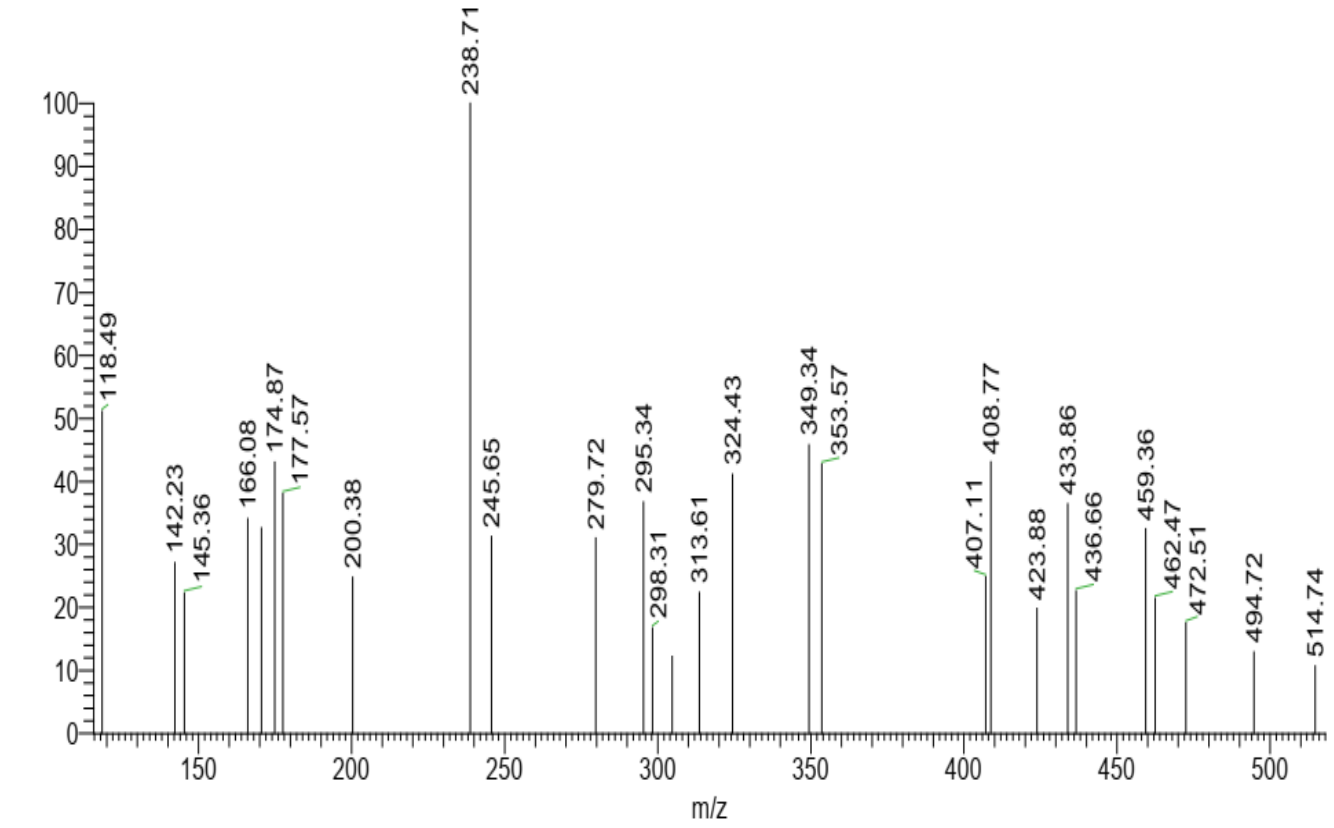
-



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]

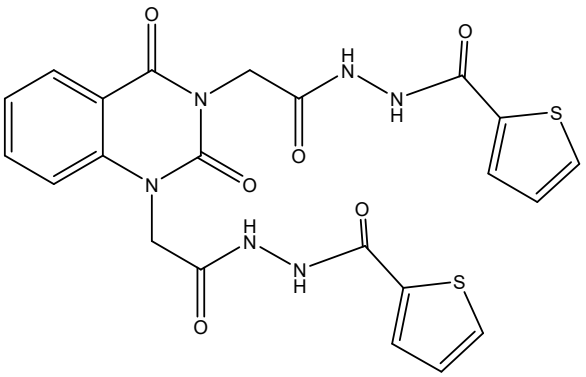


m/z Intensity Relative

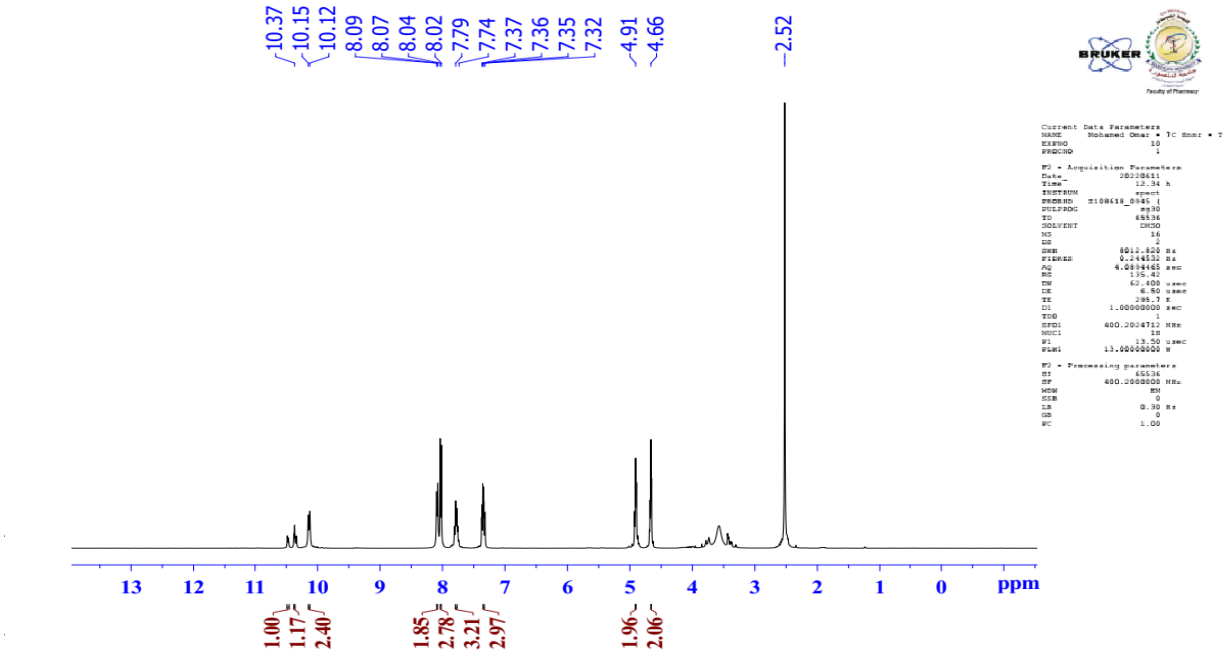
MS of compound (6c)

-

-Compound (6d)

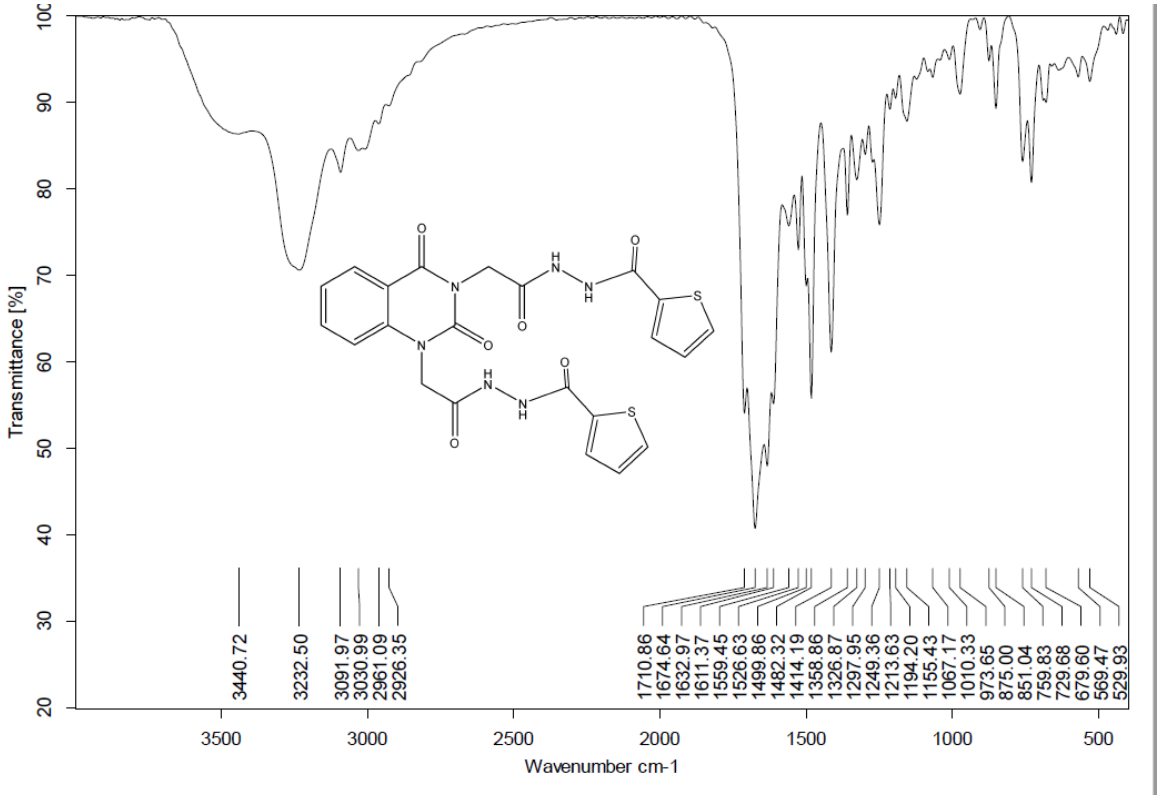


6d



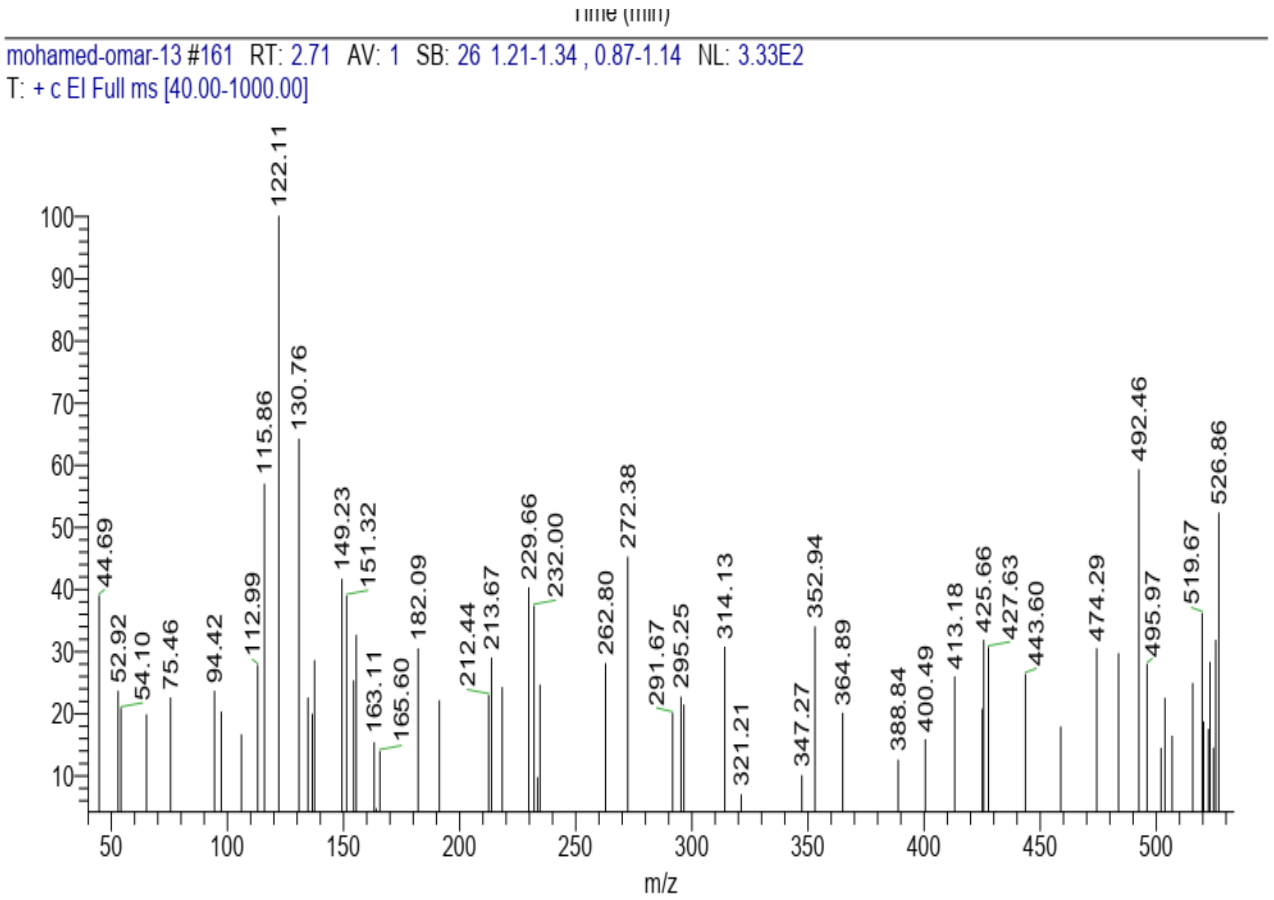
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (6d)

-



FT-IR of compound (6d)

-

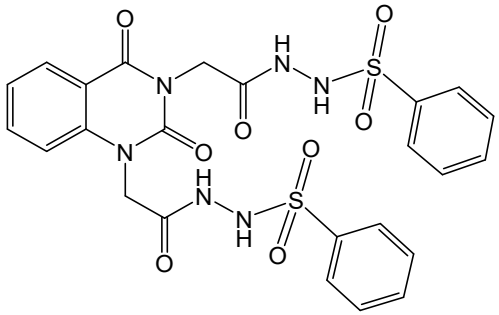


m/z Intensity Relative

MS of compound (6d)

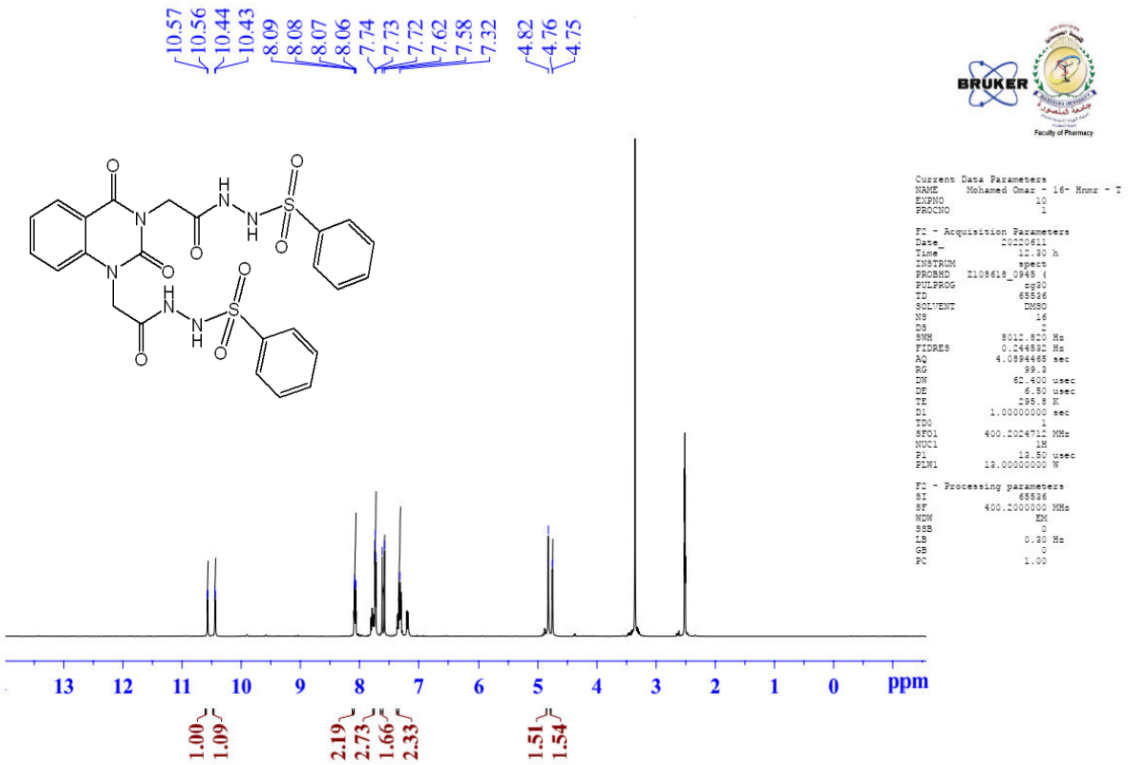
-

-Compound (6e)



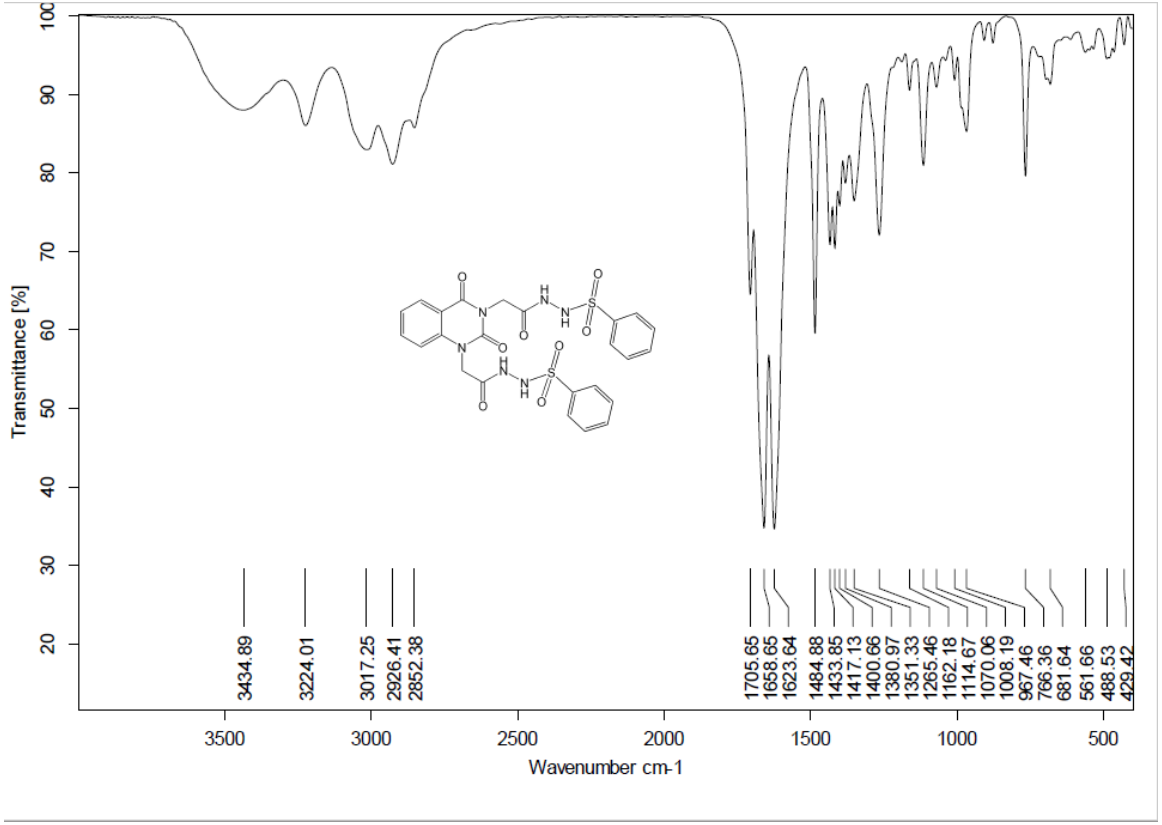
6e

-



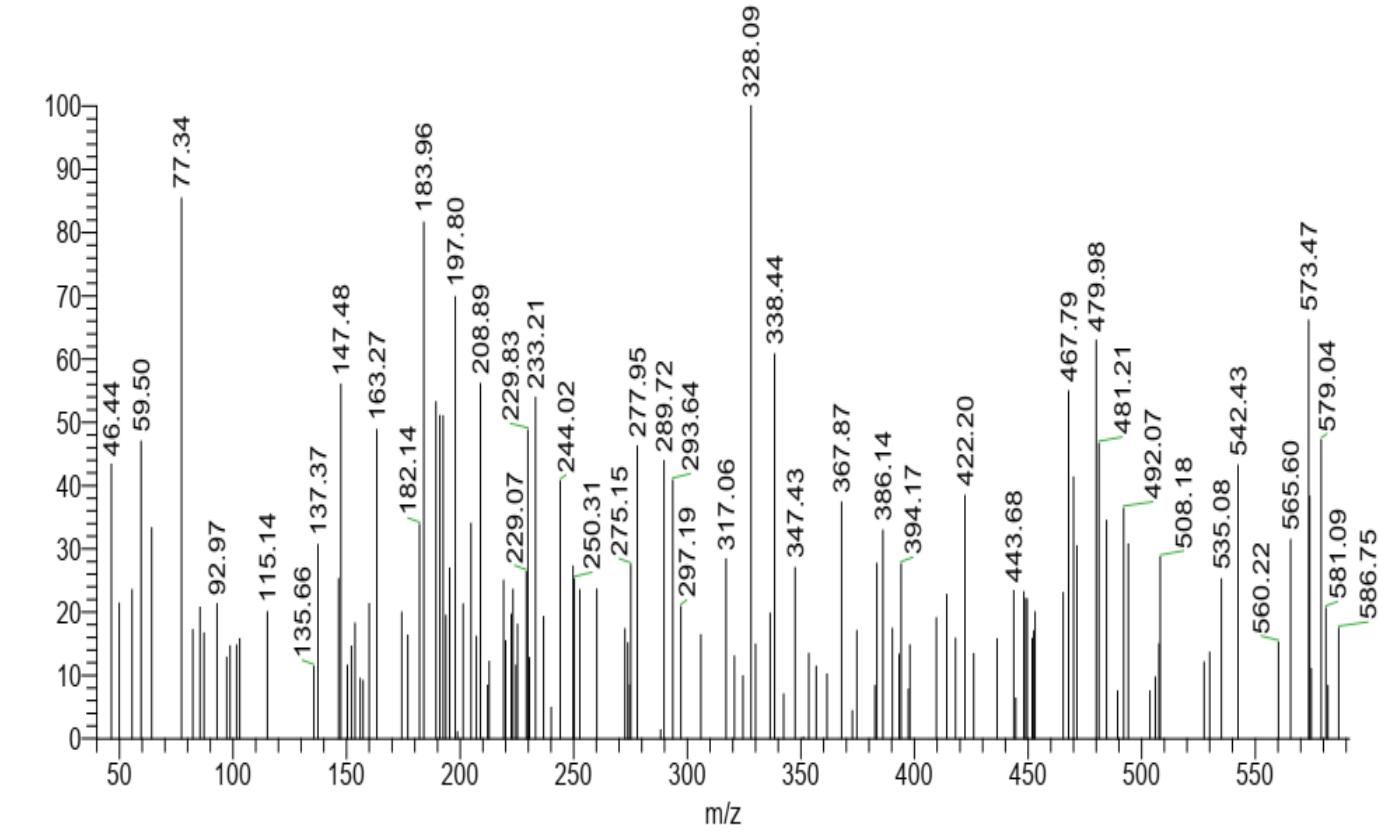
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (6e)

-



FT-IR of compound (6e)

-

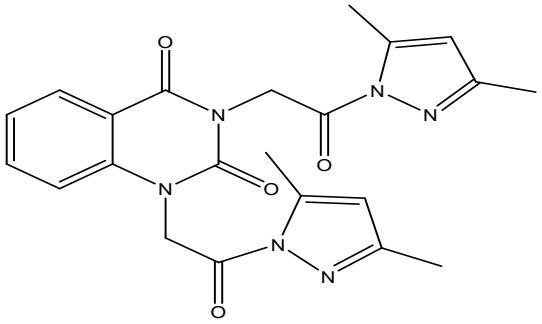


m/z Intensity Relative

MS of compound (6e)

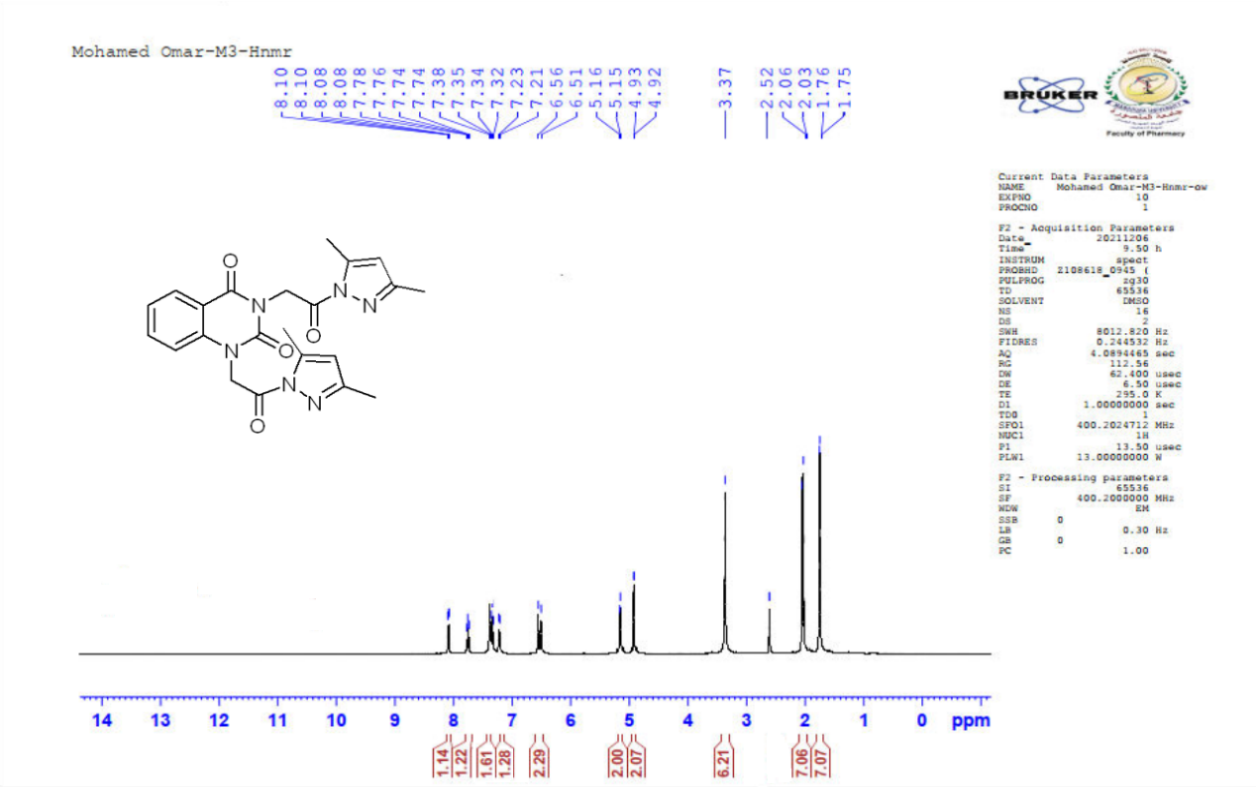
-

-Compound (7a)



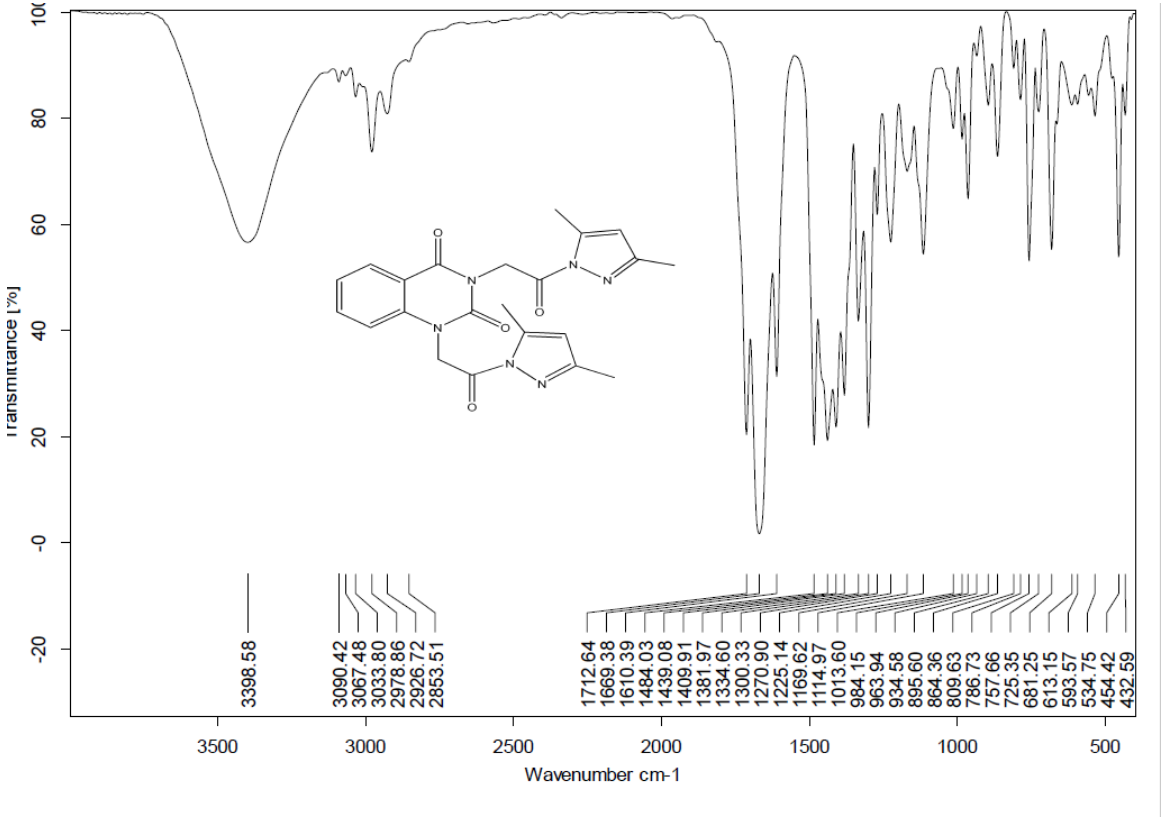
7a

-



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

-



FT-IR of compound (7a)

15-Jan-07 02:21:16

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

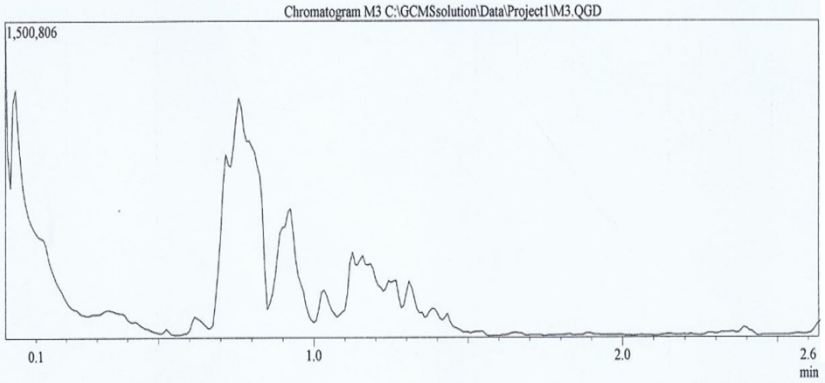
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 02:12:13 ص
Sample Name	: M3
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M3.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M3.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 02:14:54 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

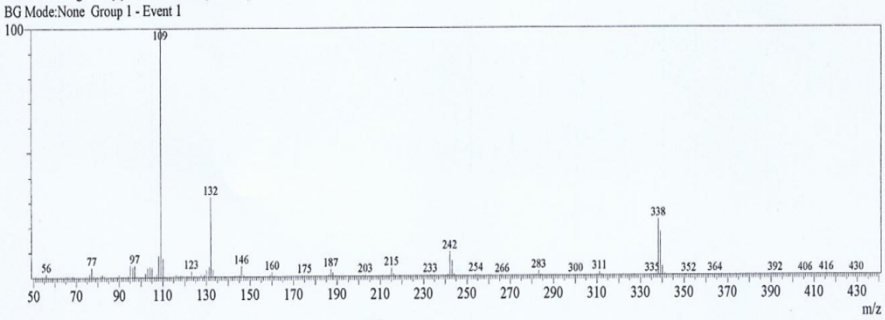
C:\GCMSsolution\Data\Project1\M3.QGD

Chromatogram M3 C:\GCMSsolution\Data\Project1\M3.QGD



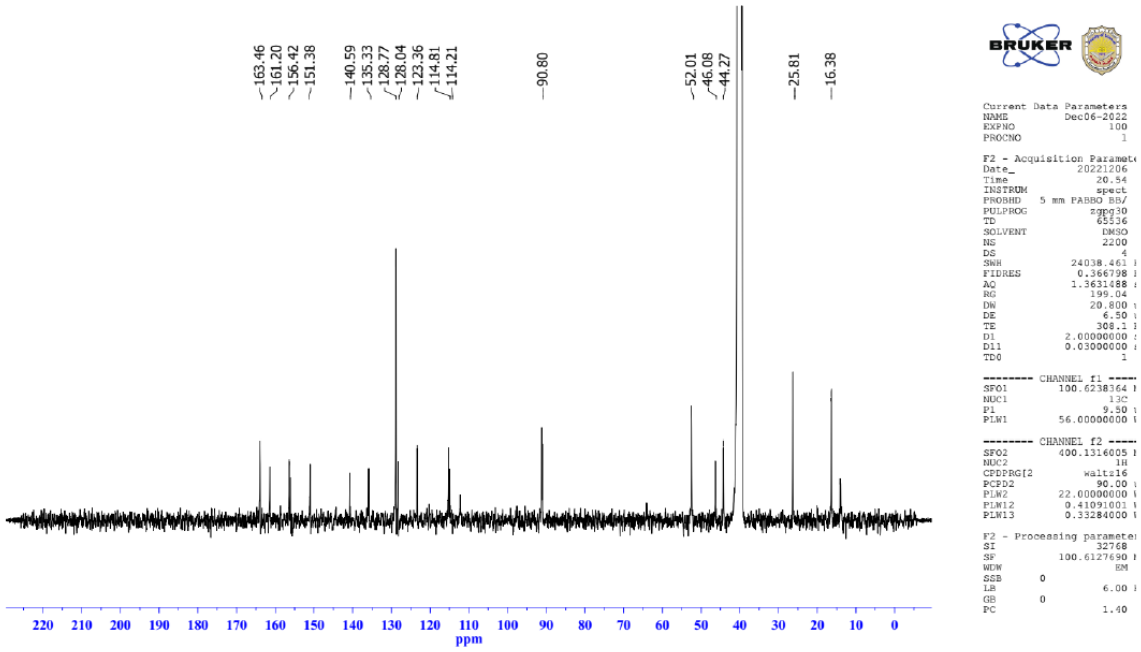
Spectrum

Line#:1 R.Time:0.0(Scan#:5)
MassPeaks:290
RawMode:Single 0.0(5) BasePeak:109(371418)
BG Mode:None Group 1 - Event 1



MS of compound (7a)

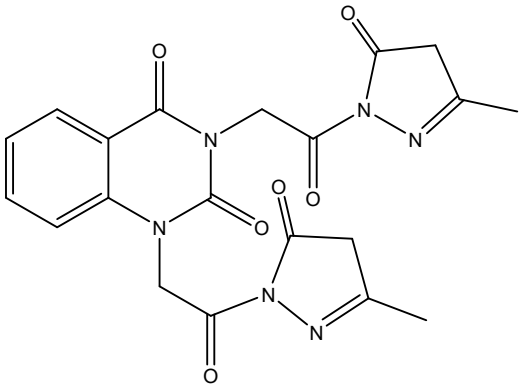
-



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

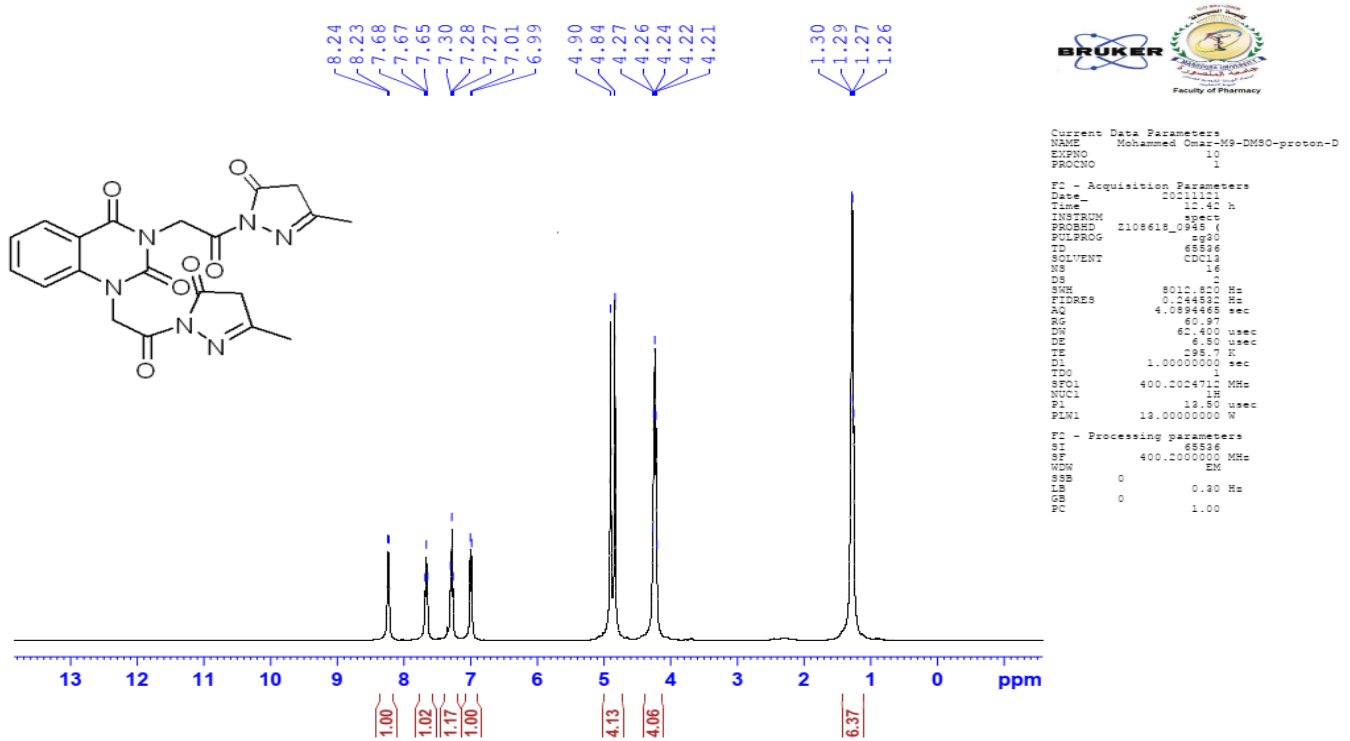
-

Compound (7b)



7b

-

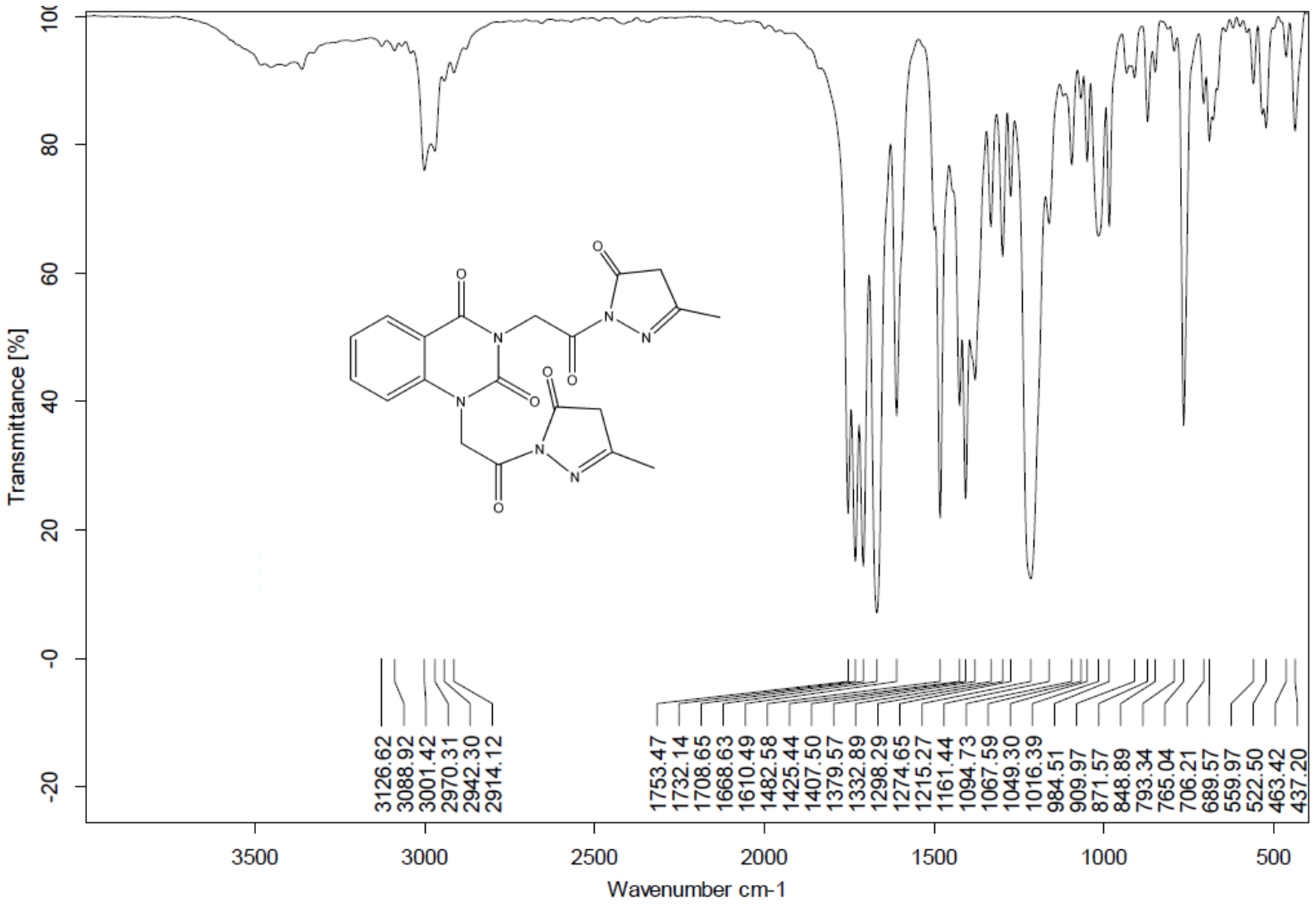



```
Current Data Parameters
NAME      Mohammed Omar-M9-DMSO-proton-D
EXPNO              10
PROCNO              1

F2 - Acquisition Parameters
Date_          20211121
Time              12.41 h
INSTRUM           spect
PROBHD   Z108618_0945 (
PULPROG           zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122283 Hz
AQ             4.0894465 sec
RG                60.97
DW               62.400 usec
DE                6.50 usec
TE               295.7 K
D1             1.00000000 sec
TD0                   1
SFO1         400.2024712 MHz
NUC1                 1H
P1                12.50 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                32768
SF           400.2000000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

-



FT-IR of compound (7b)

15-Jan-07 03:57:28

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 03:26:47 ص
Sample Name	: M9.
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M9..QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M9..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 03:36:46 ص

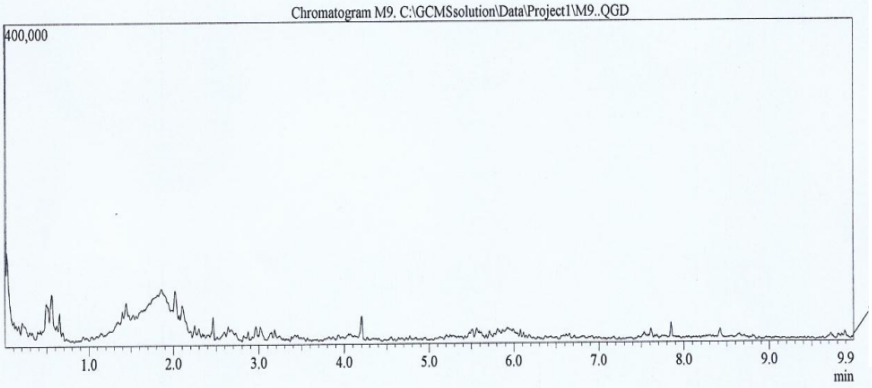
Method

====== 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

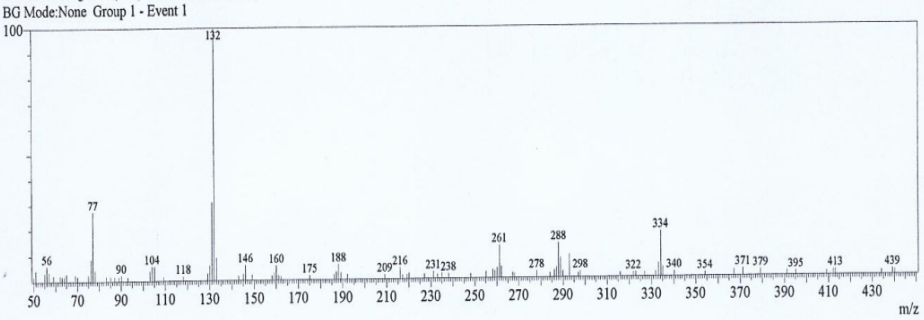
C:\GCMSsolution\Data\Project1\M9..QGD

Chromatogram M9. C:\GCMSsolution\Data\Project1\M9..QGD



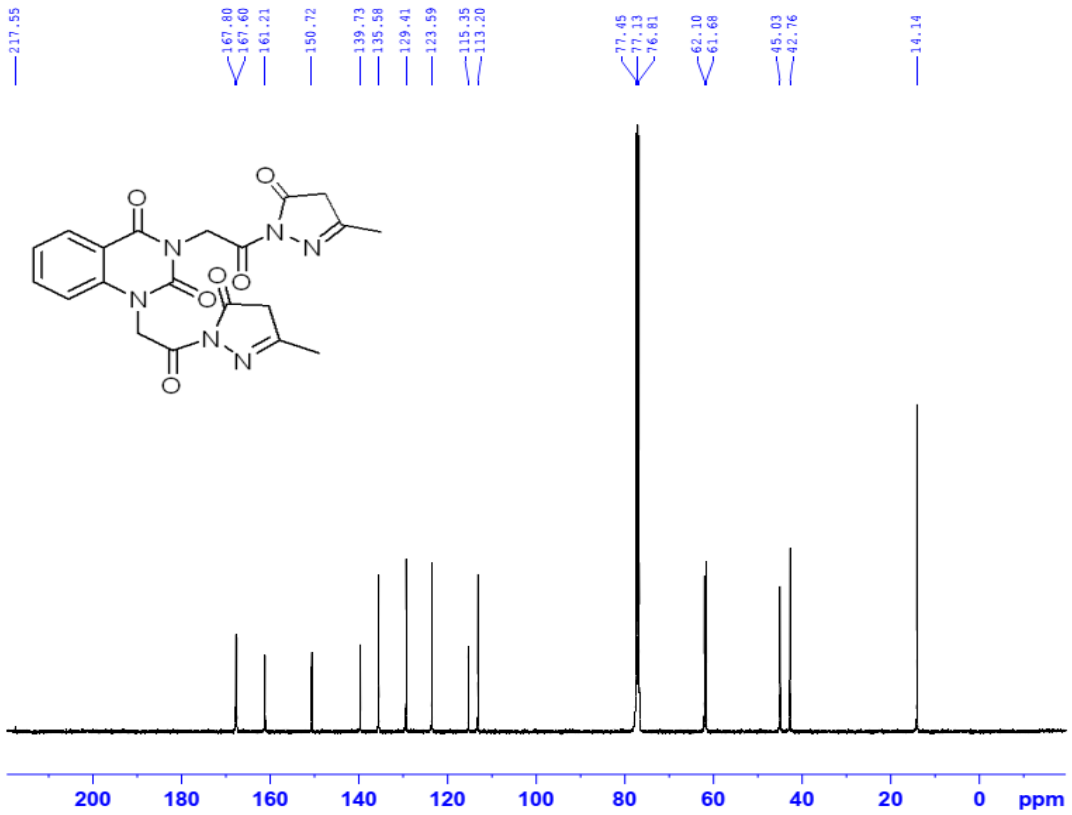
Spectrum

Line#:1 R.Time:1.5(Scan#:178)
MassPeaks:97
RawMode:Single 1.5(178) BasePeak:132(6903)
BG Mode:None Group 1 - Event 1



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
TD                65536
SOLVENT             CDCl3
NS                   2100
DS                      4
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               1.3631488 sec
RG                  197.77
DW                  20.800 usec
DE                   6.50 usec
TE                  295.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          100.6404331 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          47.00000000 W
SFO2          400.2016008 MHz
NUC2                  1H
CPDPRG[2          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
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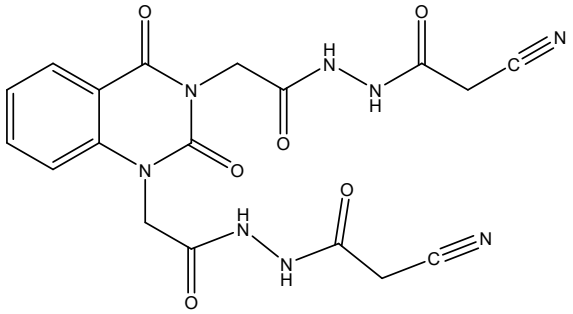
^{13}C-NMR (100 MHz, $CDCl_3$) of compound (7b)

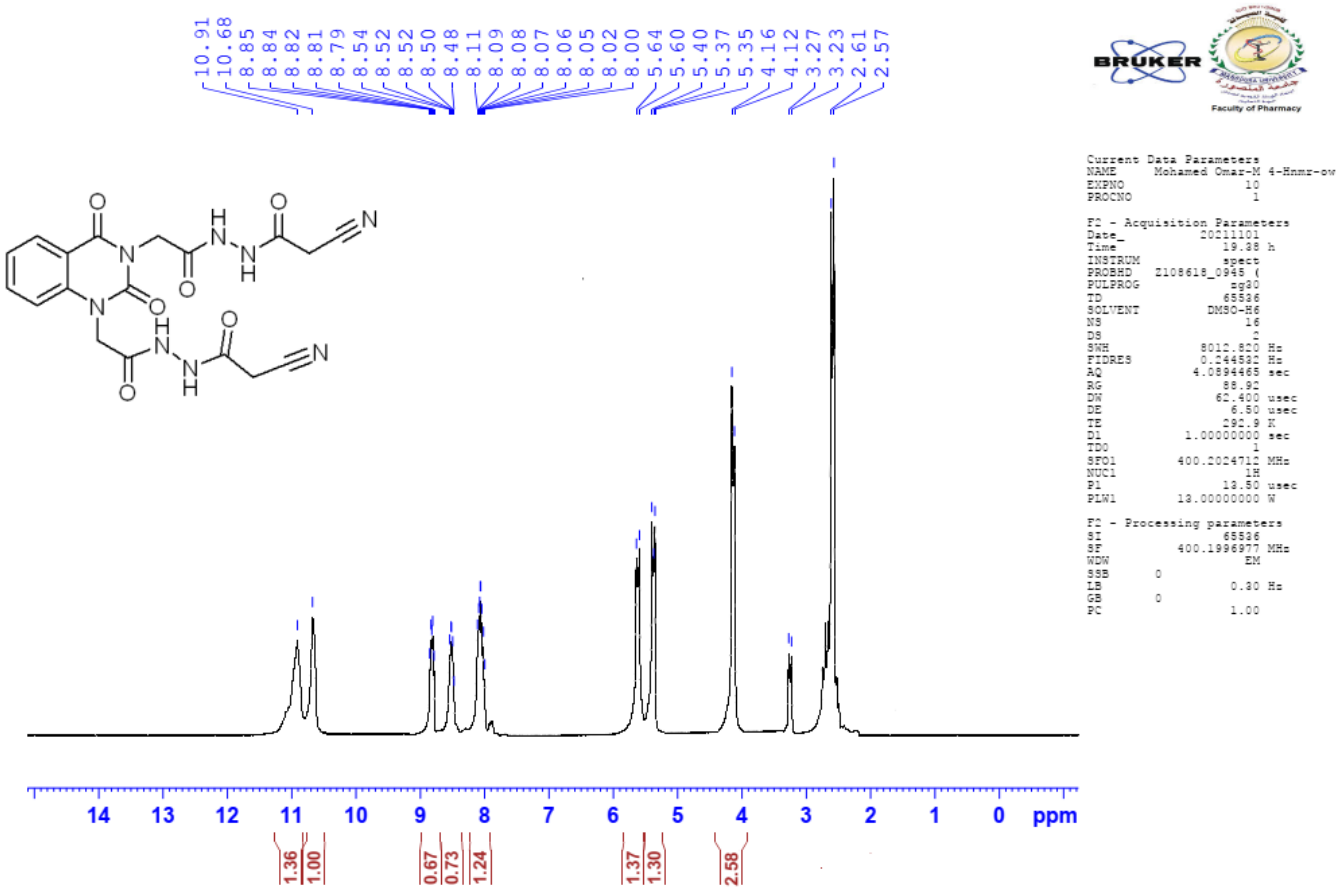
-

-Compound (8)



8

-

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

F2 - Acquisition Parameters
Date_           20211101
Time              19.38 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT          DMSO-H6
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 88.92
DW                62.400 usec
DE                 6.50 usec
TE                292.9 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2024712 MHz
NUC1                  1H
P1                 13.50 usec
PLW1         13.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1996977 MHz
WDW                   EM
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LB                 0.30 Hz
GB        0
PC                 1.00
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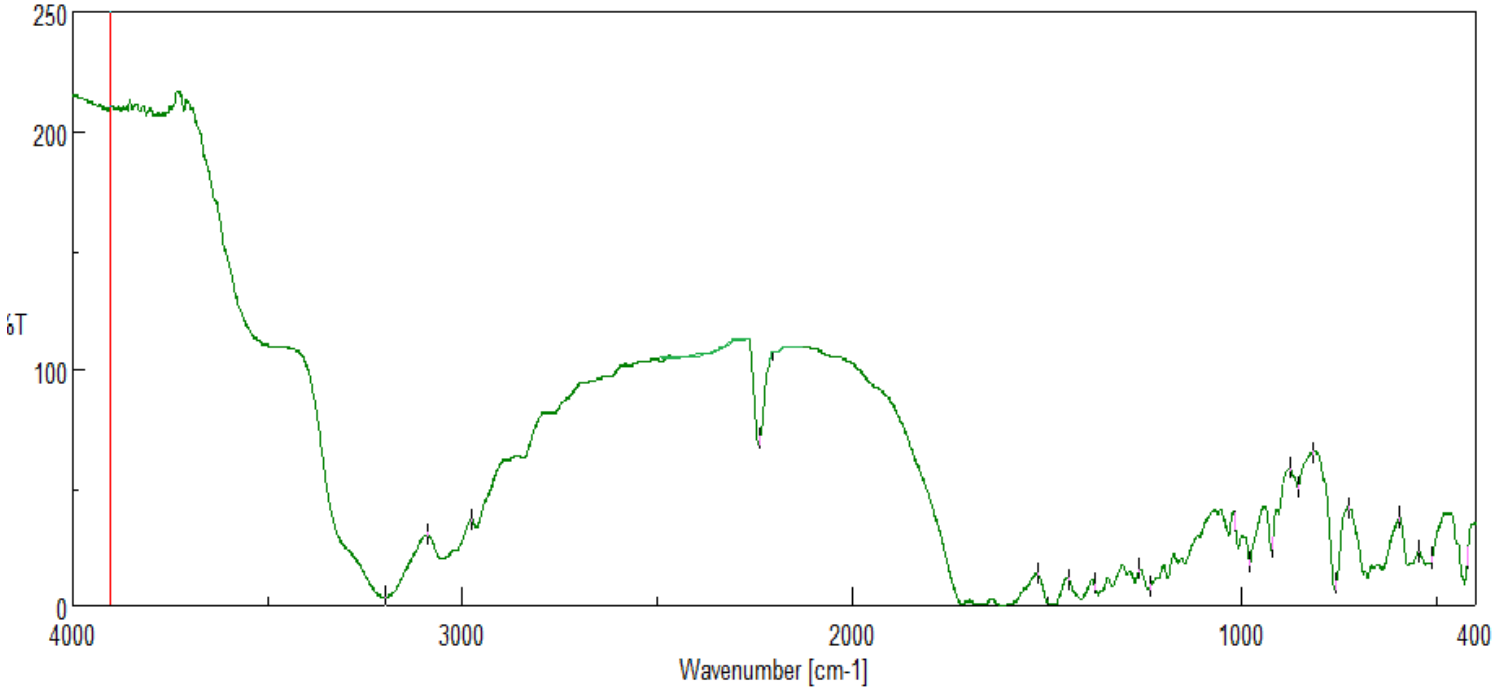
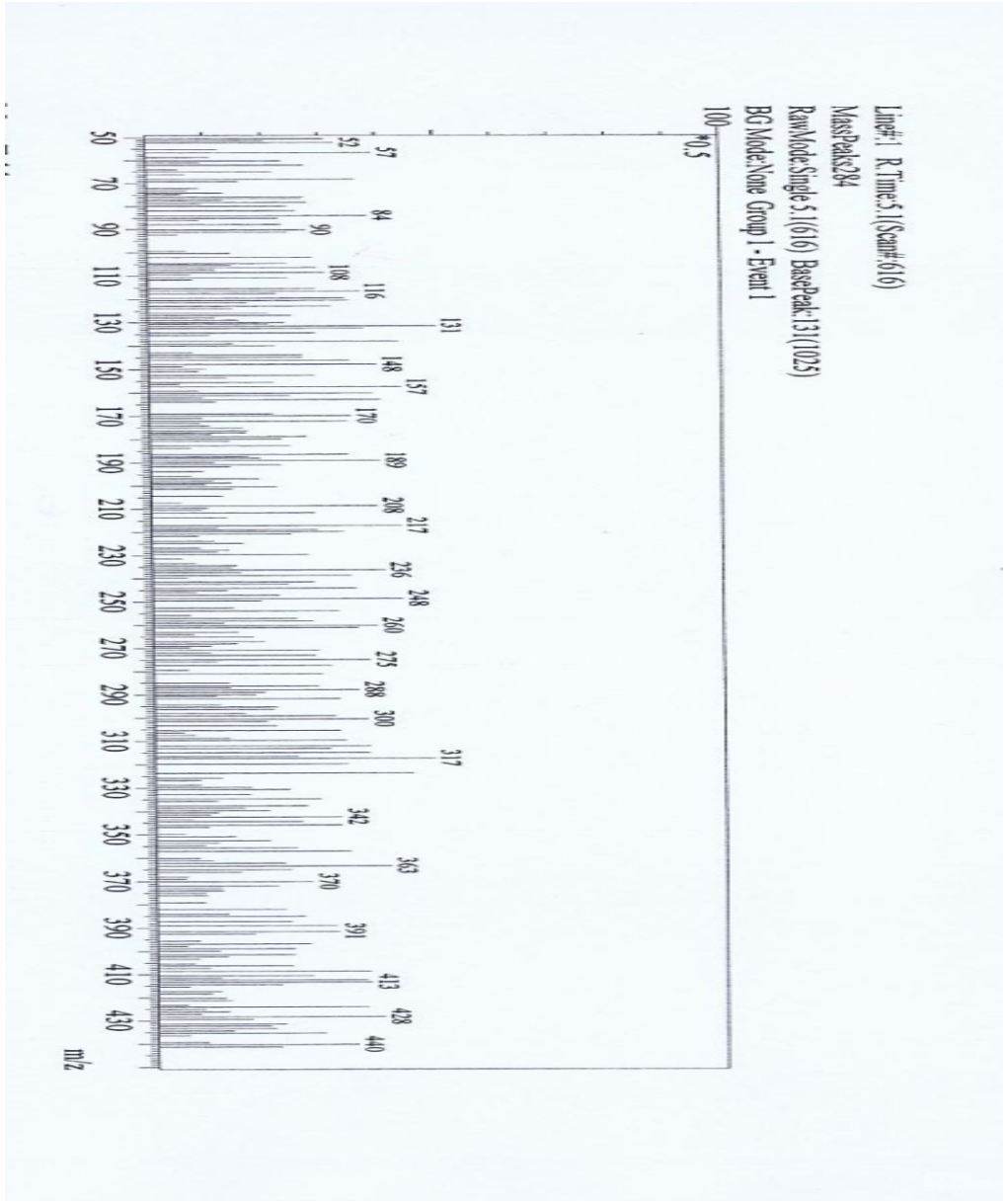
^{1}H-NMR (400 MHz, DMSO-d_6) of compound (8)

-



FT-IR of compound (8)

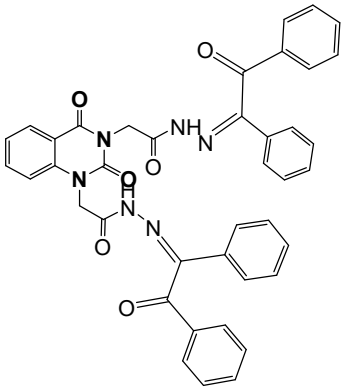
-



MS of compound (8)

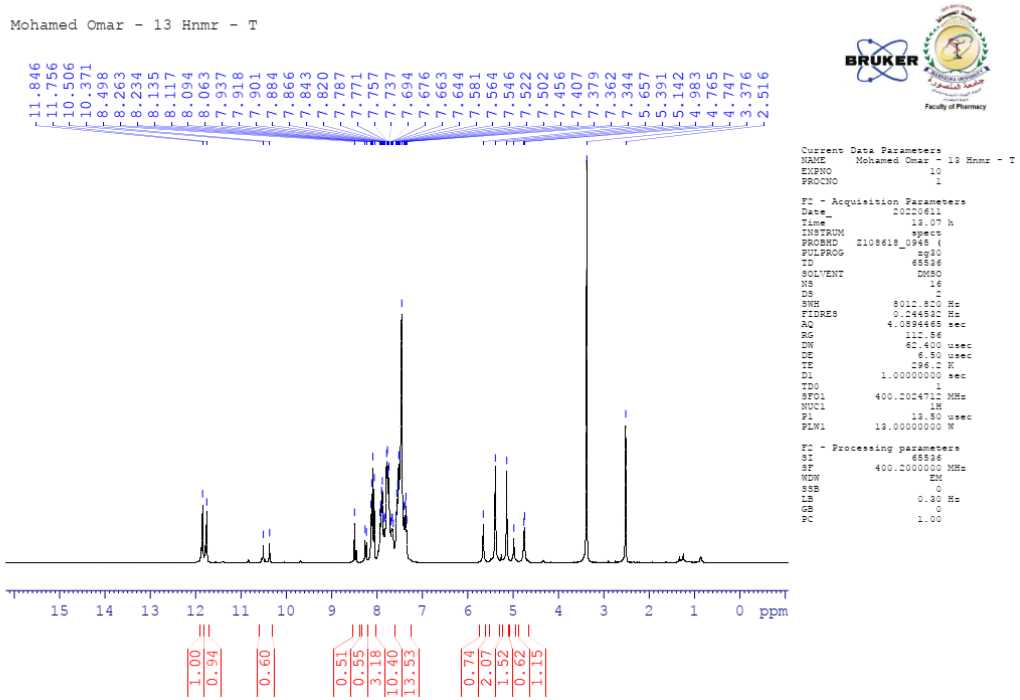
-

-Compound (9a):-



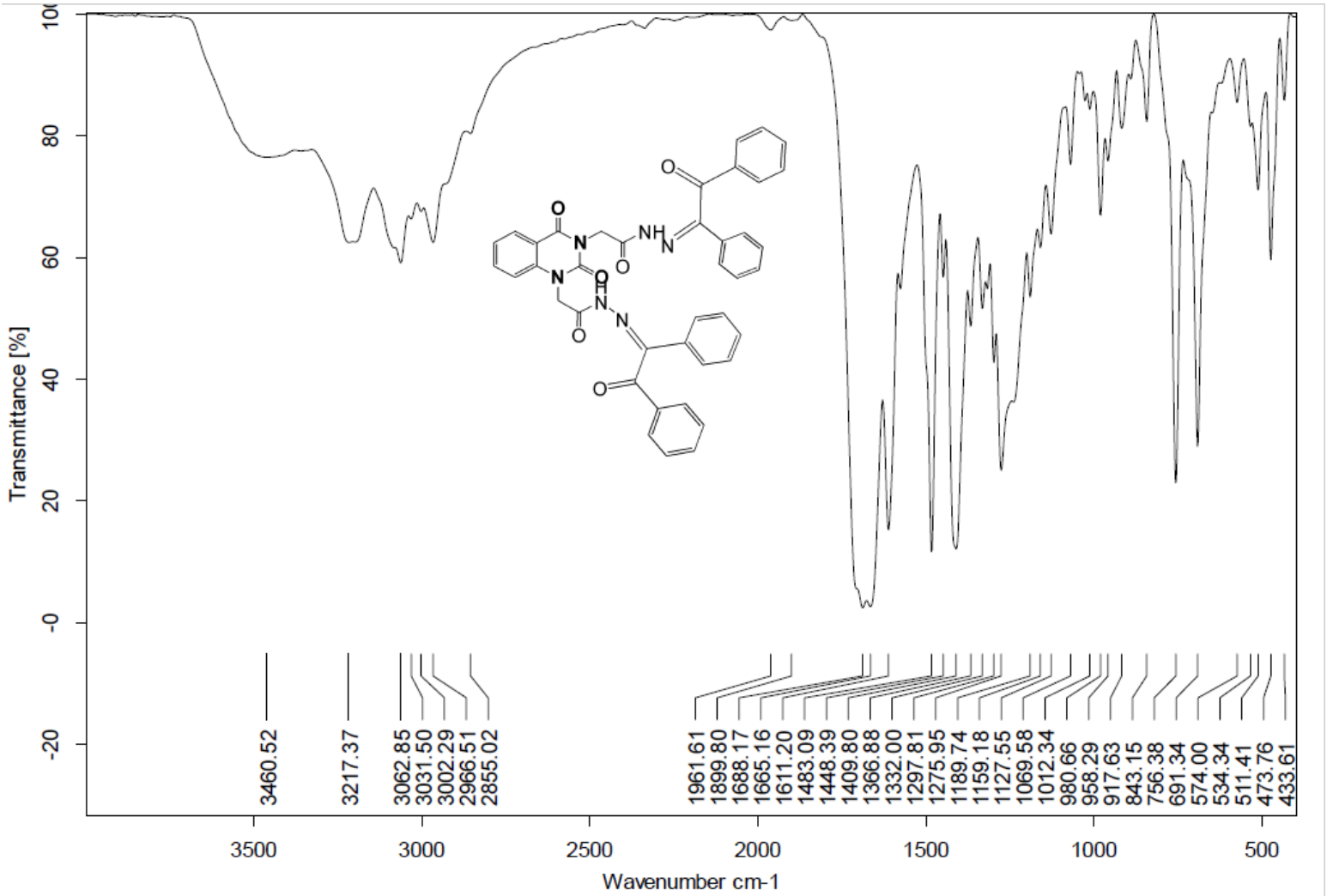
9a

-



^{1}H-NMR (400 MHz, DMSO-d_6) of compound (9a)

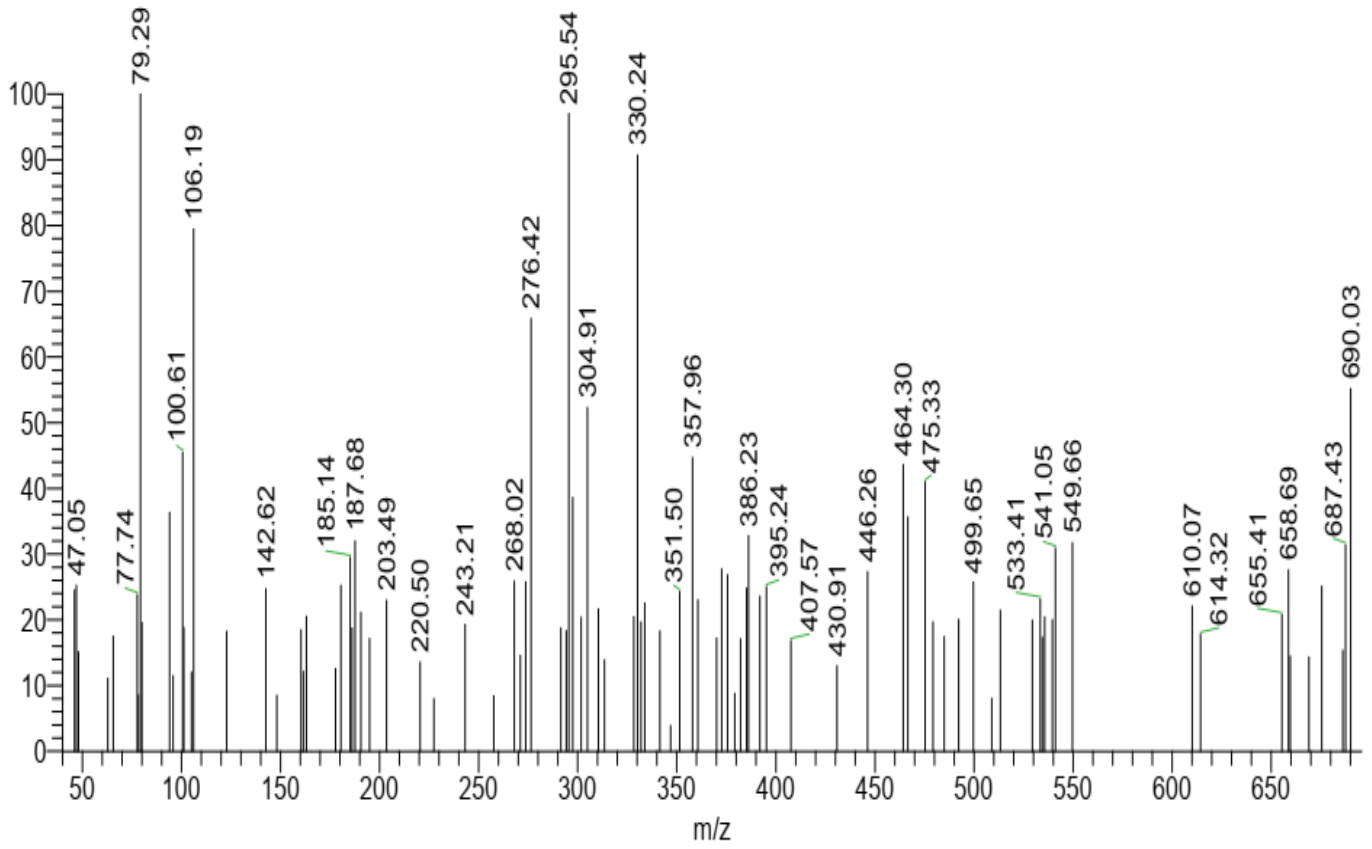
-



FT-IR of compound (9a)

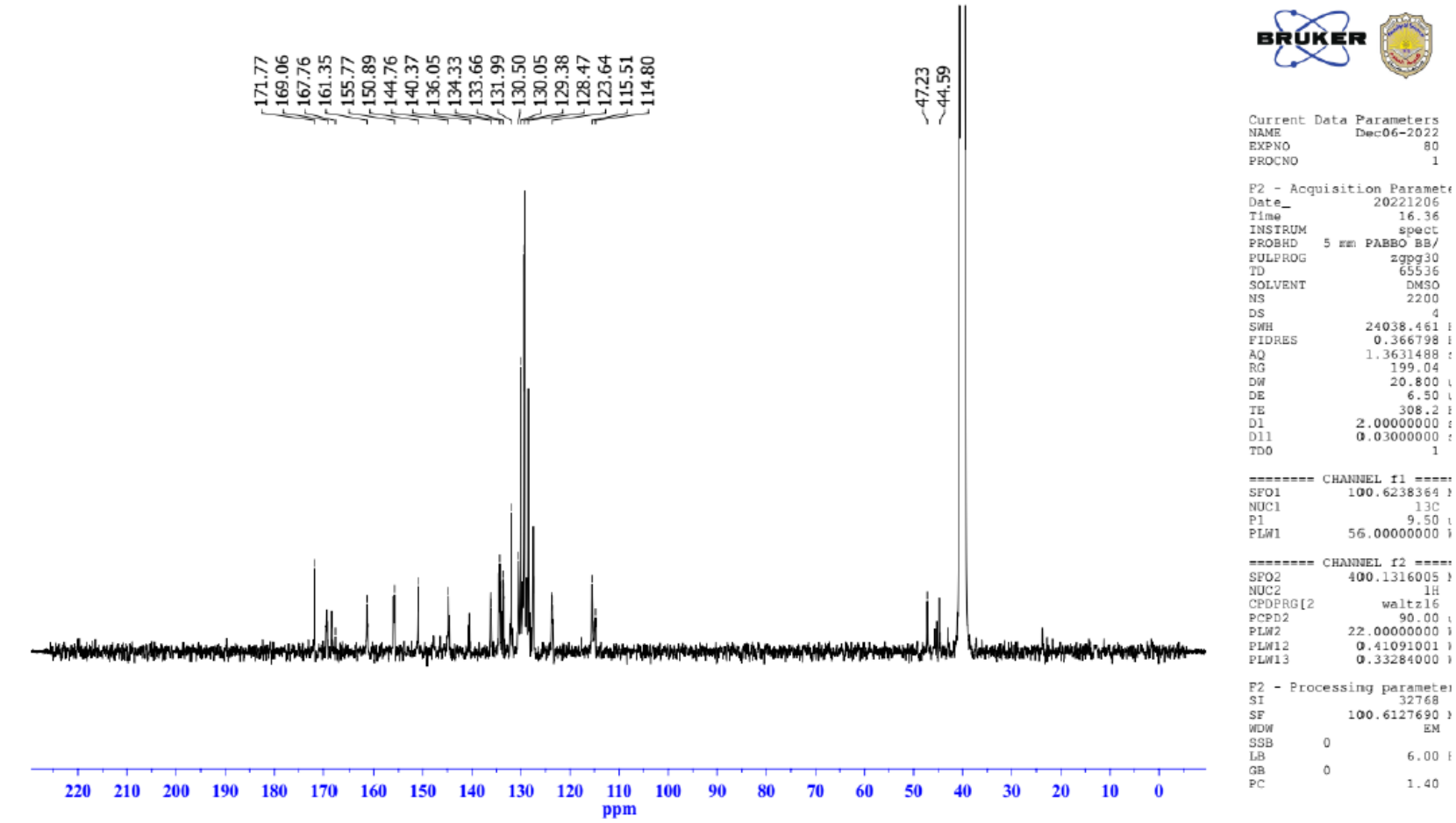
-

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)



^{13}C-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	O=C(C1=CC=CC=C1N2CC(OCC)=O)N(CC(OCC)=O)C2=O
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)	O=C(N2CC(NN)=O)N(CC(NN)=O)C1=CC=CC=C1C2=O
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+	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
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+	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
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+	O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=C(O)C=C4)=O)N(CC(N/N=C/C3=CC=C(O)C=C3)=O)C2=O
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+	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
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+	O=C(C1=CC=CC=C1N2CC(N/N=C/C4=CC=CO4)=O)N(CC(N/N=C/C3=CC=CO3)=O)C2=O
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)	O=C(C1=CC=CC=C1N2CC(N/N=C4/CCCC4)=O)N(CC(N/N=C3/CCCC3)=O)C2=O
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)	O=C(C1=CC=CC=C1N2CC(N/N=C4/CCCCC4)=O)N(CC(N/N=C3/CCCCC3)=O)C2=O
4c	InChI=1S/C28H26N6O4/c1-19(21-11-5-3-6-12-21)29-31-25(35)17-33-24-	O=C(C1=CC=CC=C1N2CC(N/N=C(C)/C4=CC=CC=C4)=O)N(CC(N/N=C(C)/C3

	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=CC=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

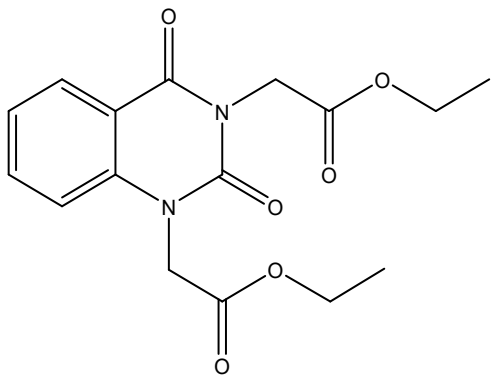
-

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

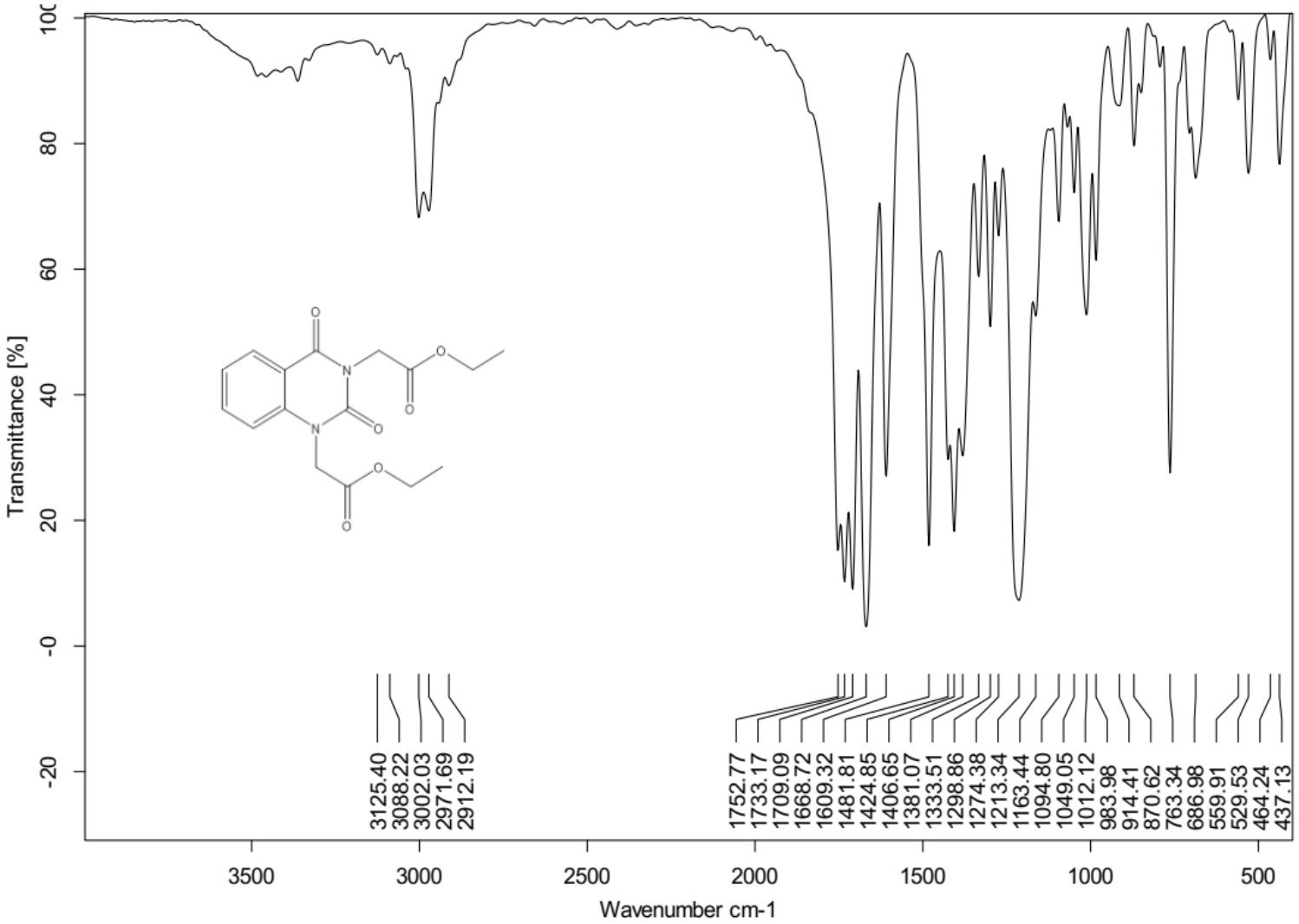


Figure . ^{1}H-NMR of compound 1 .

-

15-

Cairo University
Micro Analytical Center

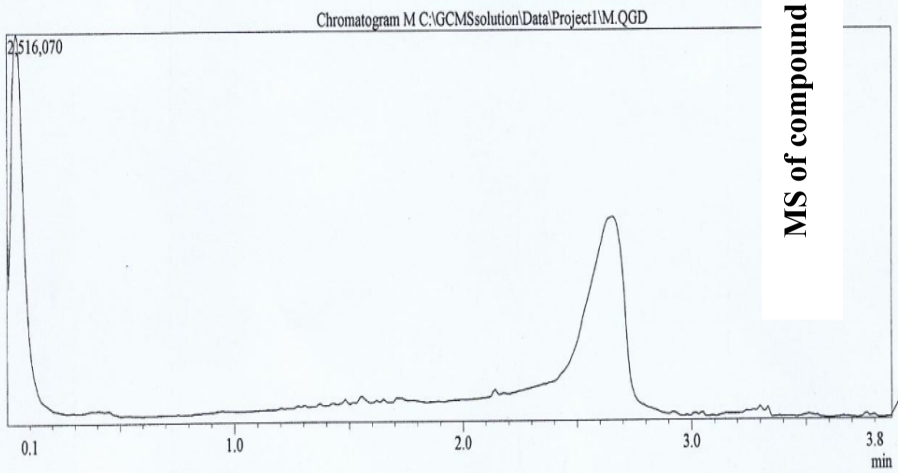
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information	
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 01:53:50 ص
Sample Name	: M
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M.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 01:57:45 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

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

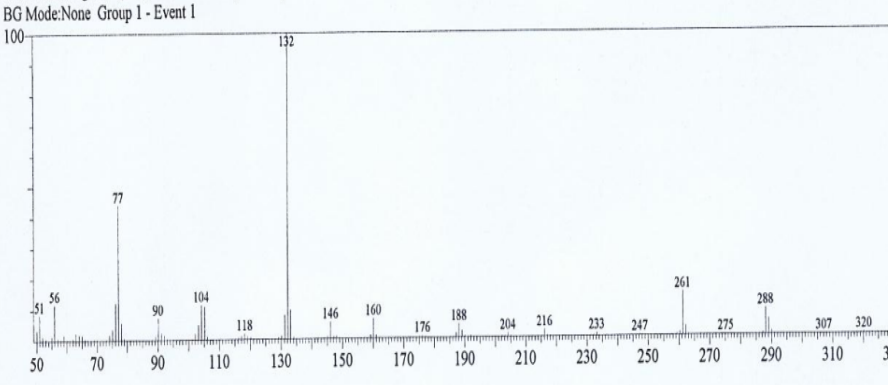
Chromatogram M C:\GCMSsolution\Data\Project1\M.QGD



MS of compound (1)

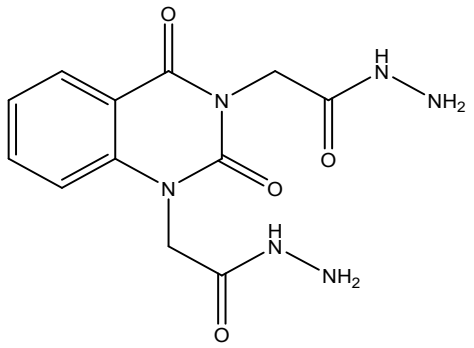
Spectrum

Line#:1 R.Time:2.7(Scan#:321)
MassPeaks:182
RawMode:Single 2.7(321) BasePeak:132(351582)
BG Mode:None Group 1 - Event 1



-

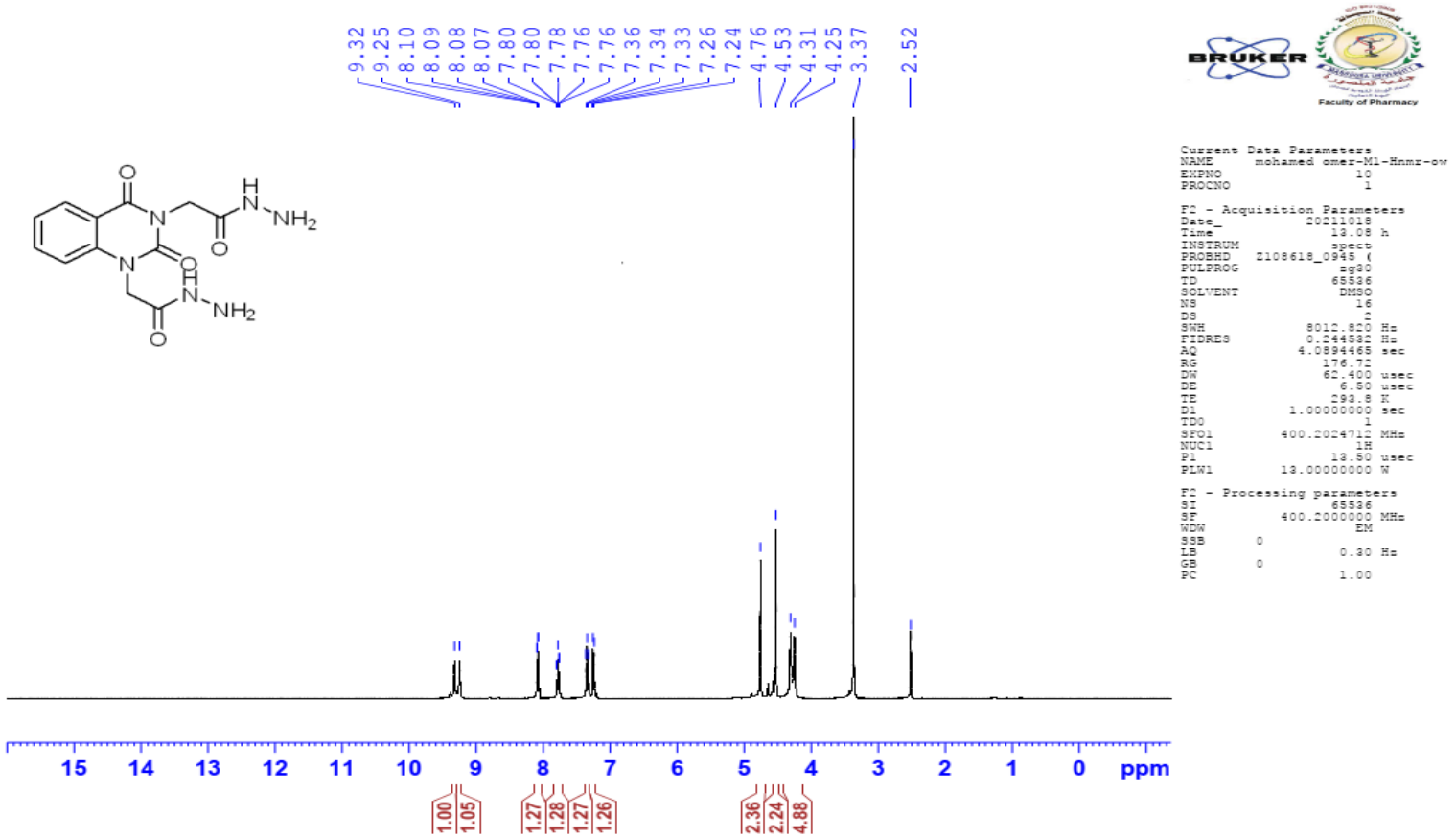
-Compound (2):



2

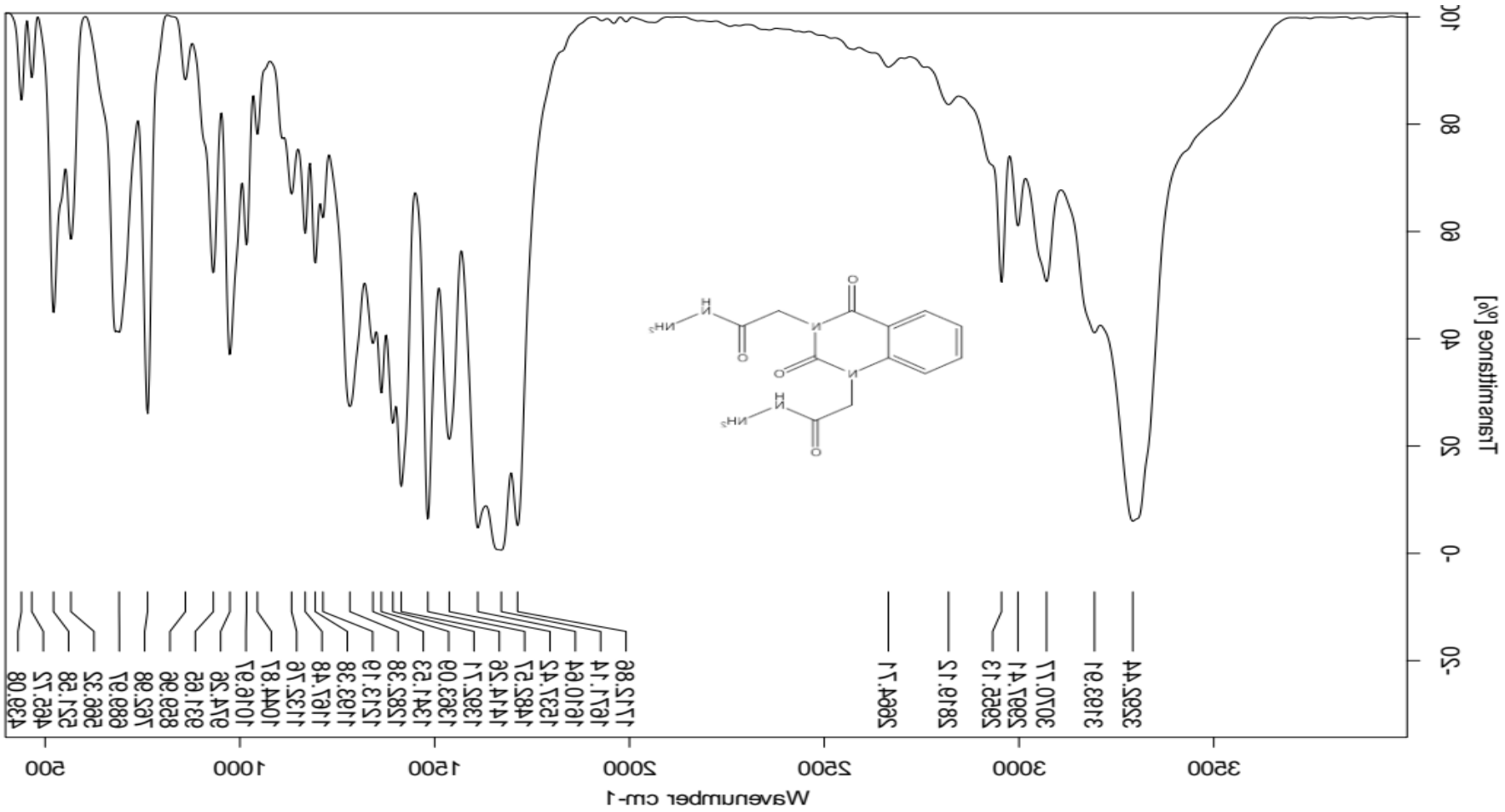
2

-



^{1}H-NMR of compound (2)

-



FT-IR of compound (2)

15-Jan-07 02:07:54

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

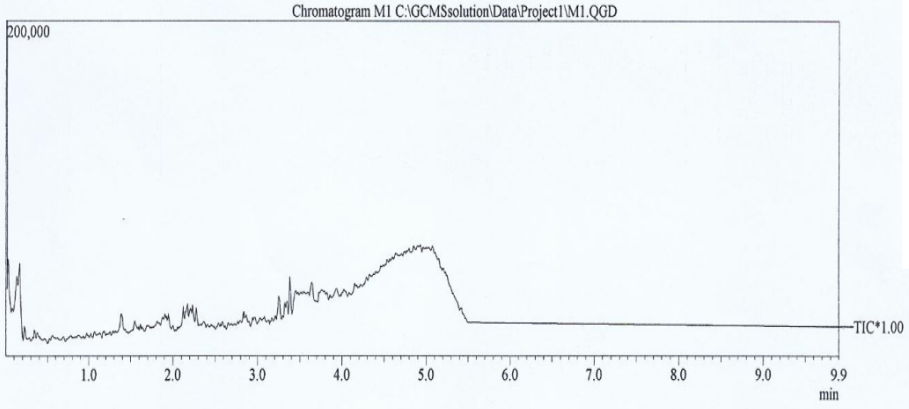
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 01:59:25 ص
Sample Name	: M1
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M1.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M1.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1_default.qgt
$EndIf$Modified by	: Dr. Mai Younis
Modified	: 15/01/2007 02:04:57 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

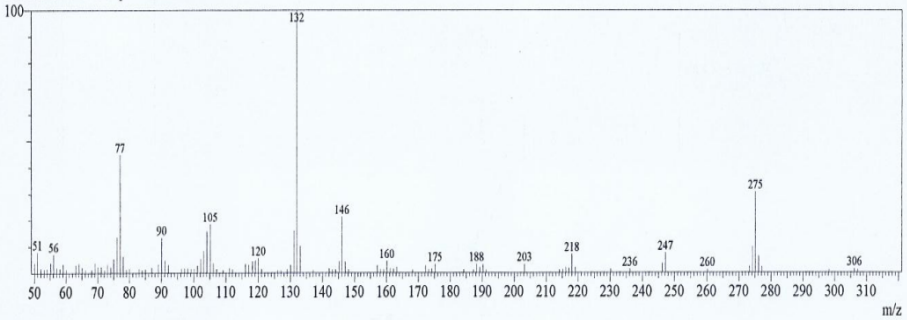
C:\GCMSsolution\Data\Project1\M1.QGD

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



Spectrum

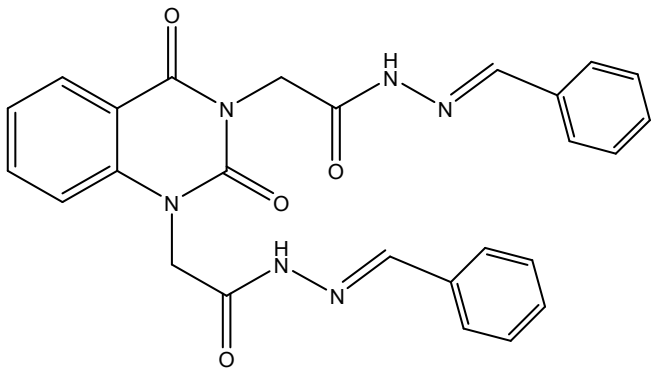
Line#:1 R.Time:4.7(Scan#:566)
MassPeaks:110
RawMode:Single 4.7(566) BasePeak:132(10628)
BG Mode:None Group 1 - Event 1



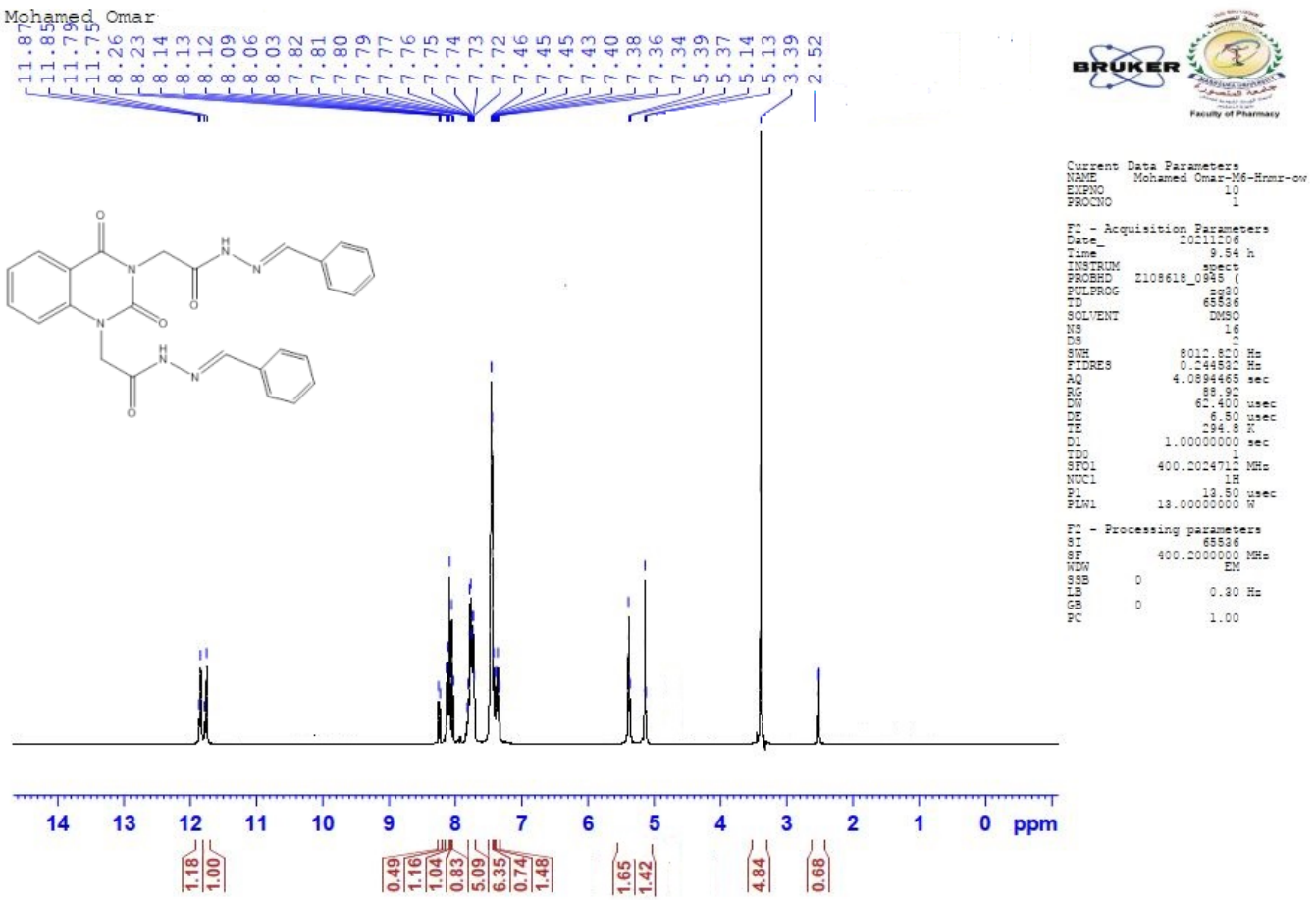
MS of compound (2)

-

-Compound (3a)

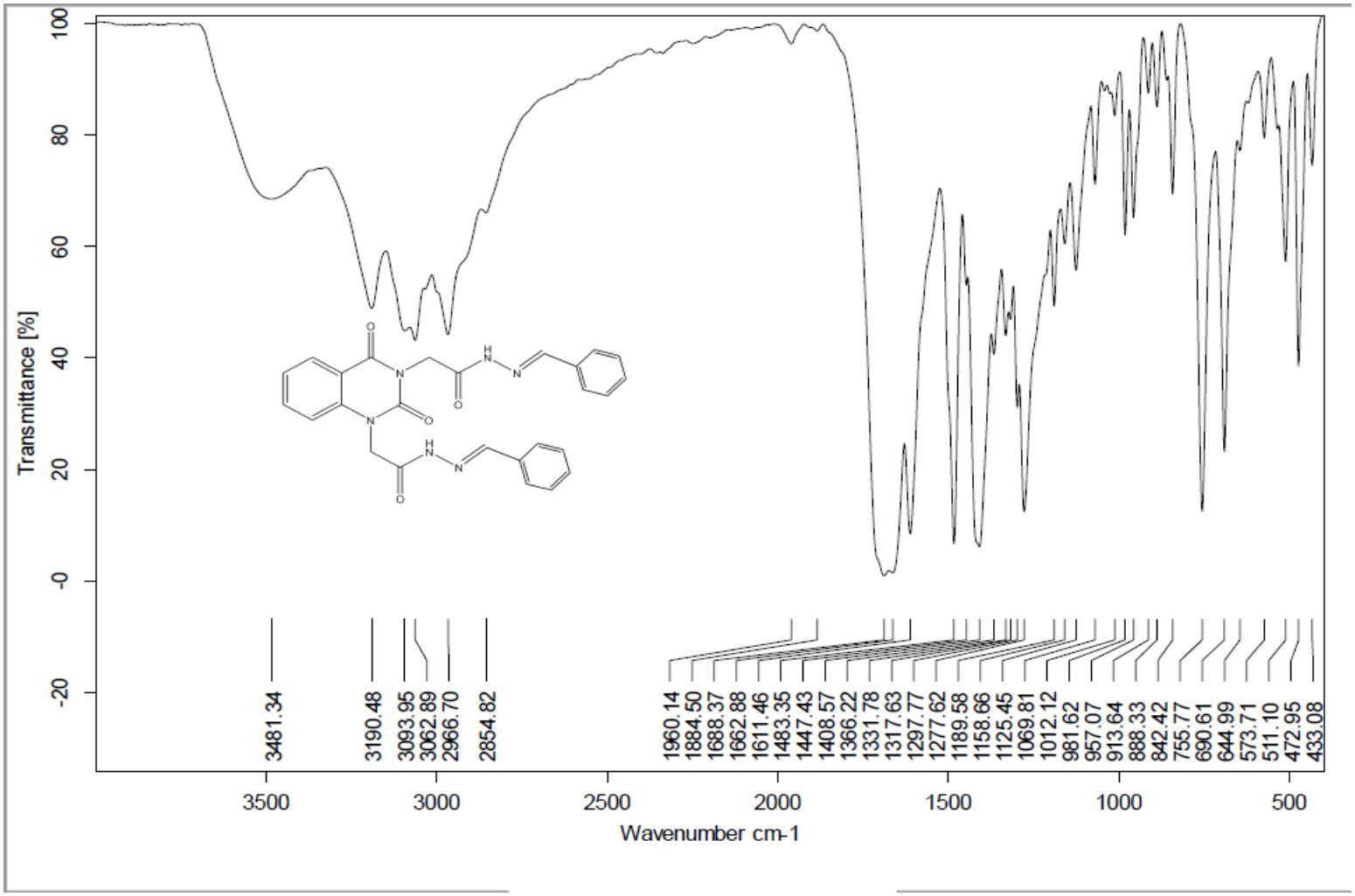


-



[1]H-NMR of compound (3a)

-



FT-IR of compound (3a)

15-Jan-07 02:

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 ص
Sample Name	: M6
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M6.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M6.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 02:34:22 ص

Method

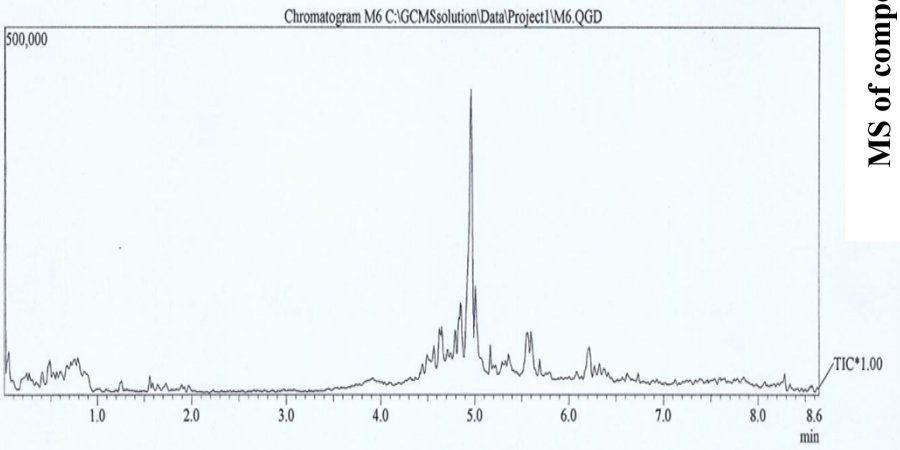
===== Analytical Line 1 =====

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	:1250
Start m/z	:50.00
End m/z	:600.00

Electron Voltage : 70 eV
Ionization Mode : EI

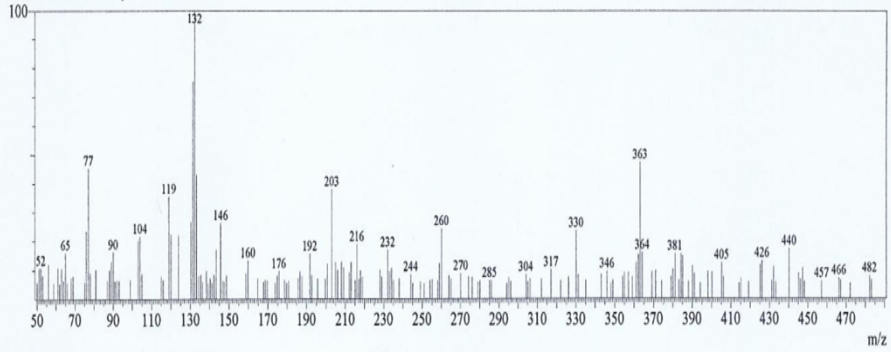
C:\GCMSsolution\Data\Project1\M6.QGD

Chromatogram M6 C:\GCMSsolution\Data\Project1\M6.QGD



Spectrum

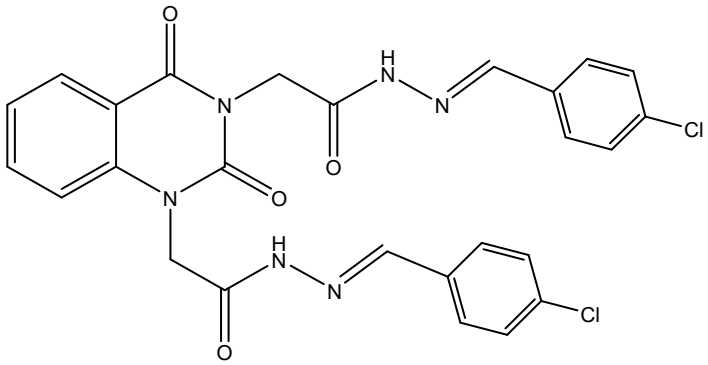
Line#:1 R.Time:5.2(Scan#:625)
MassPeaks:170
RawMode:Single 5.2(625) BasePeak:132(1940)
BG Mode:None Group 1 - Event 1



MS of compound (3a)

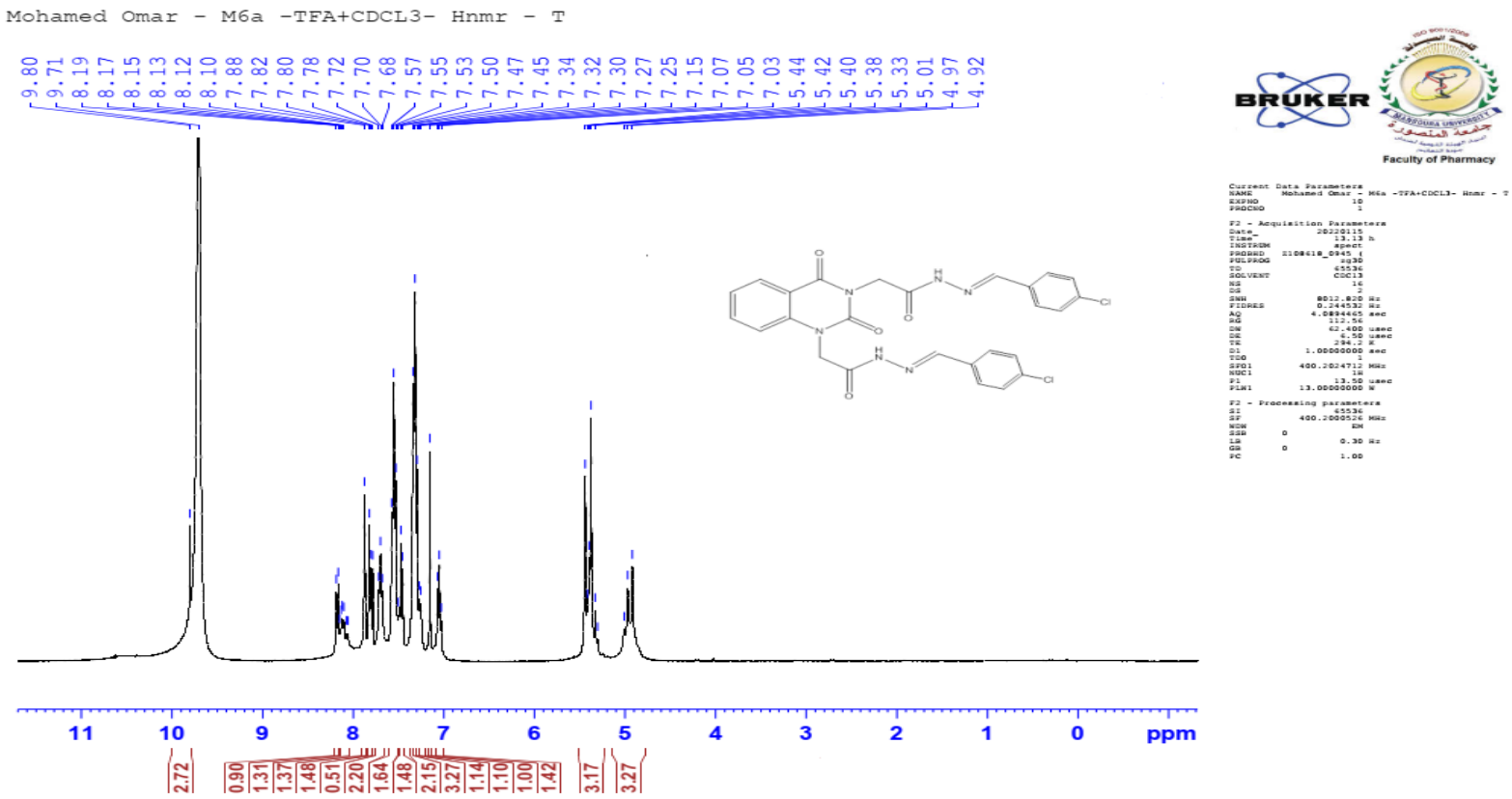
-

-Compound (3b): -



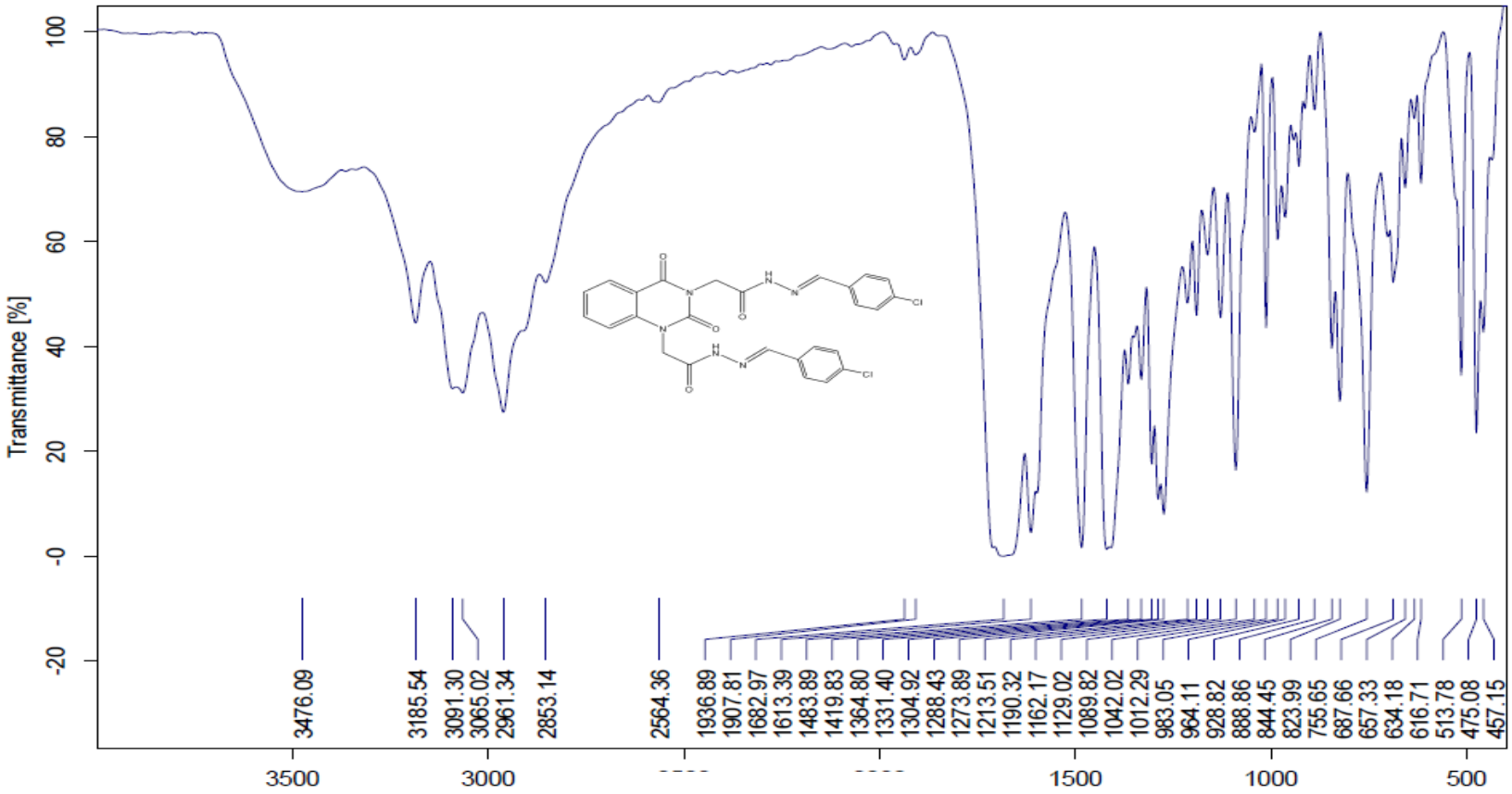
3b

-

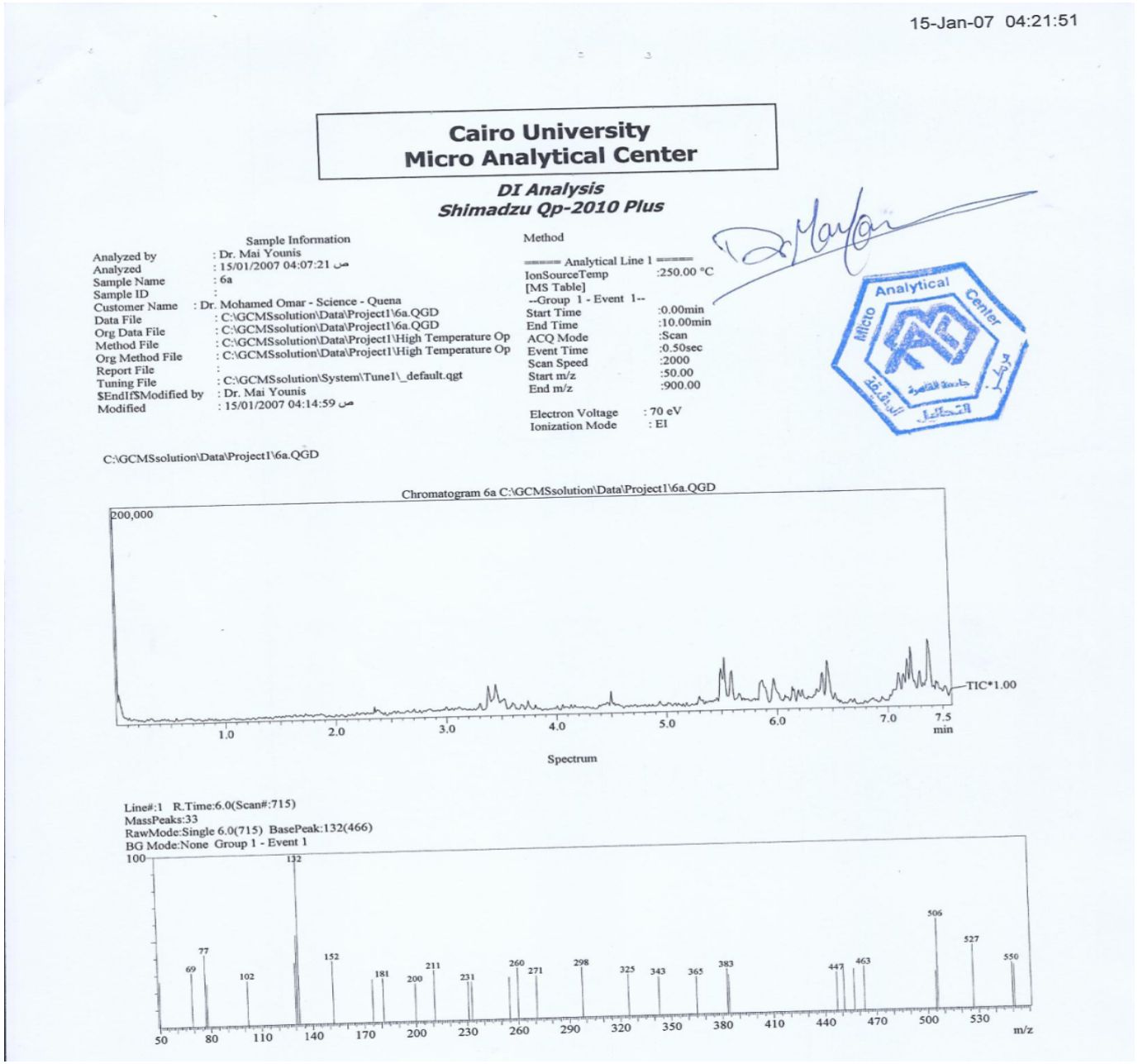


^{1}H-NMR of compound (3b)

-



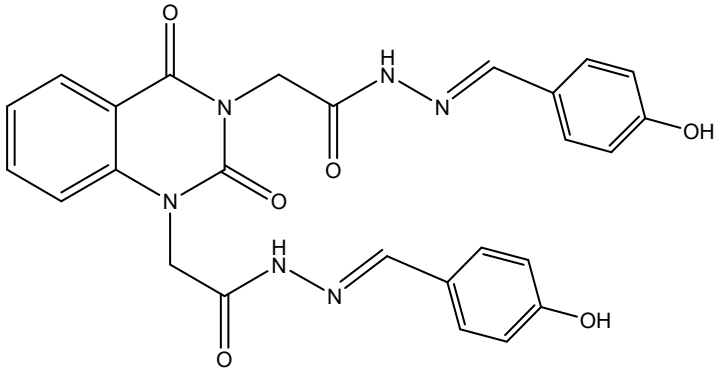
FT-IR of compound (3b)



MS of compound (3b)

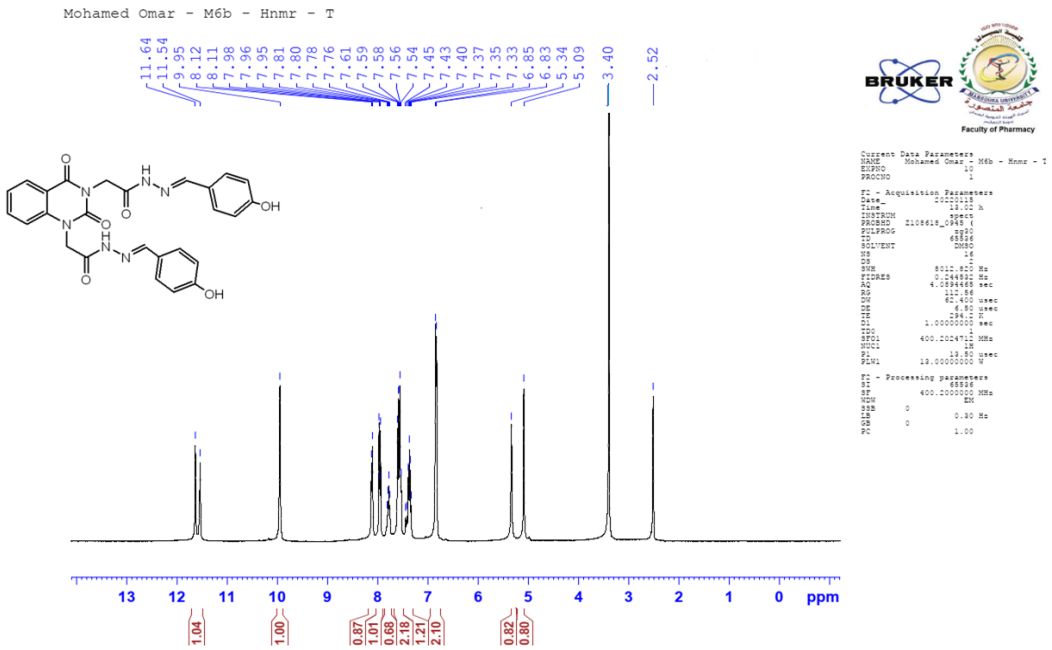
-

-Compound (3c):



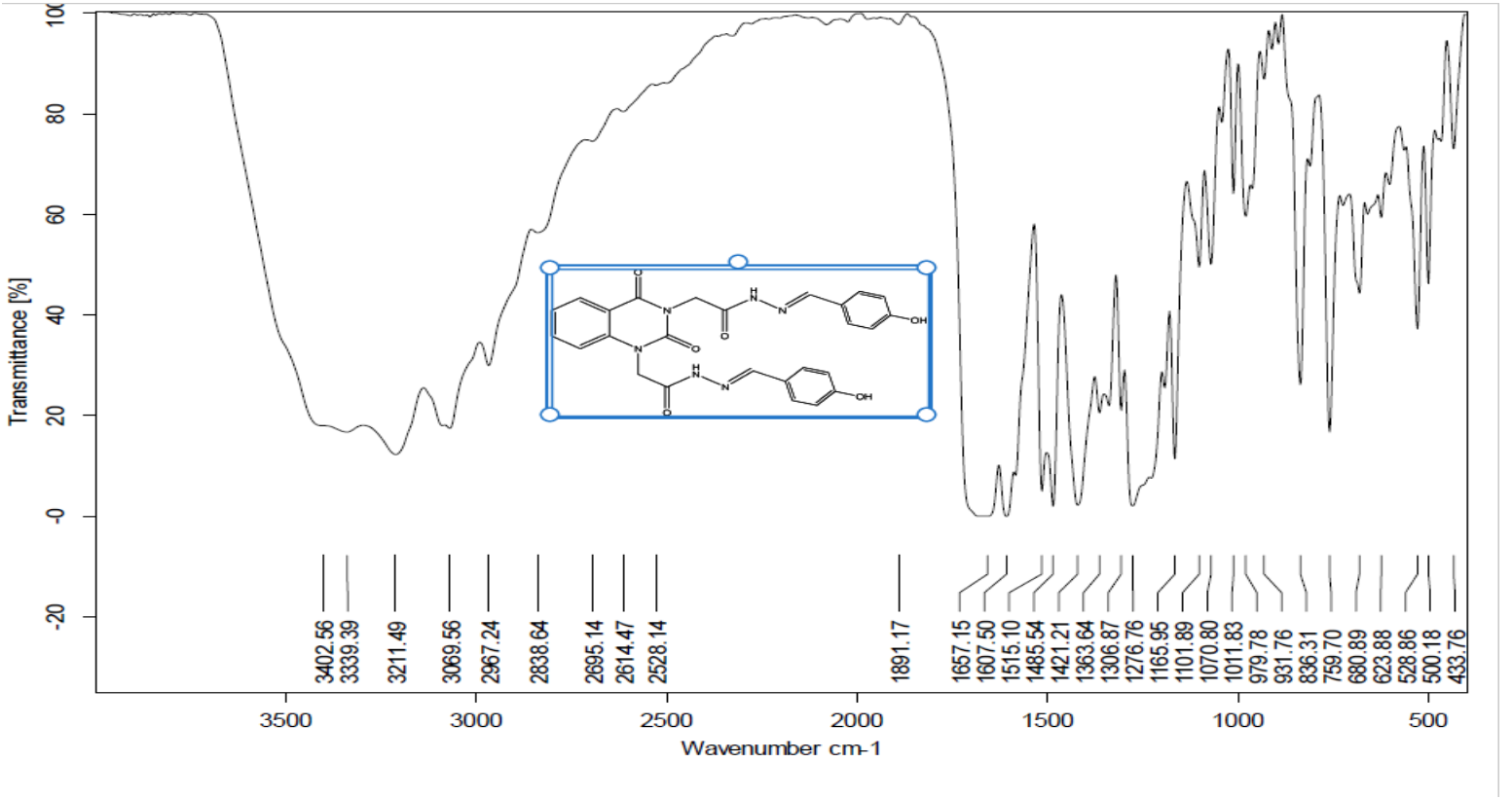
3c

-



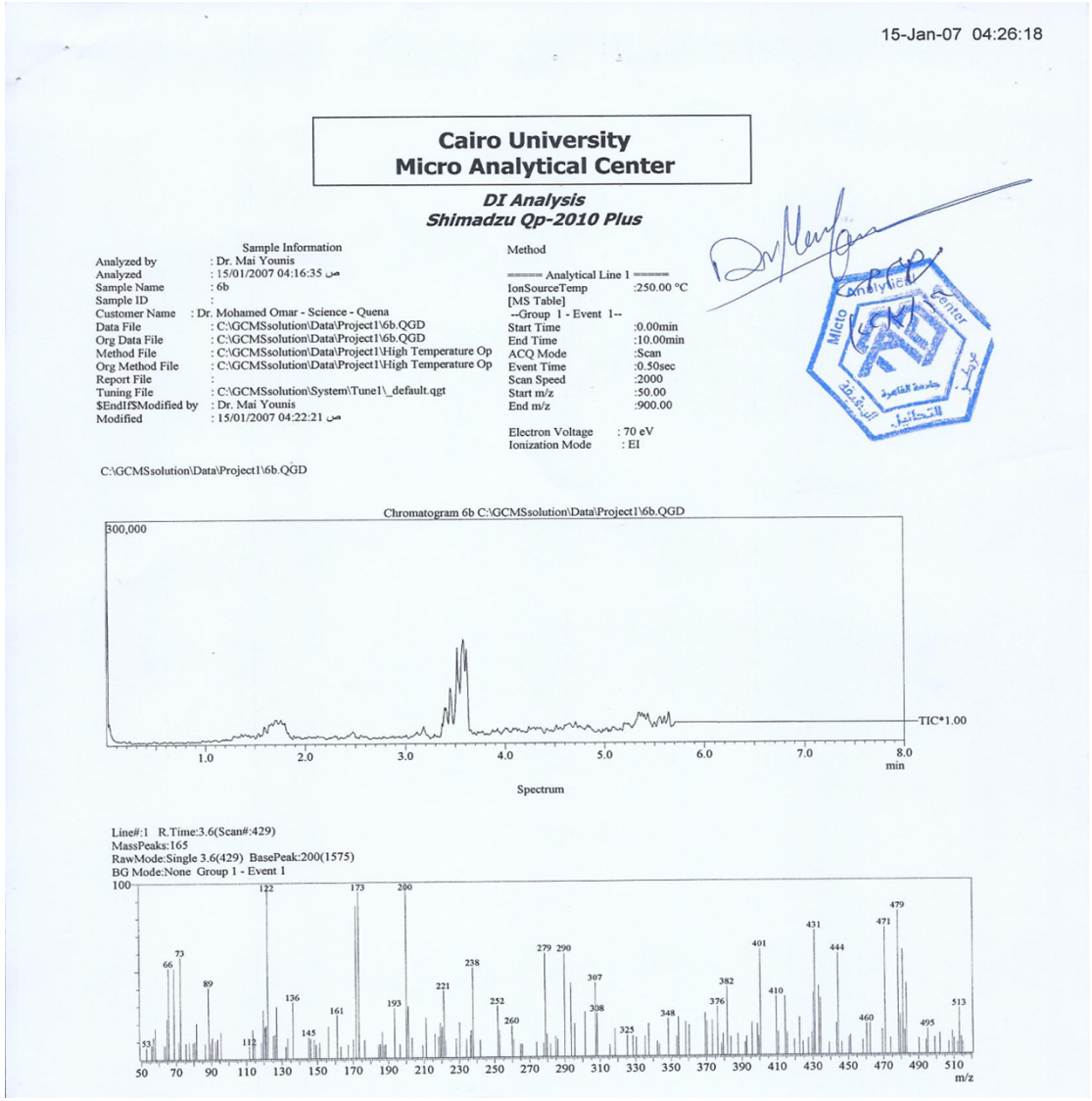
^{1}H-NMR of compound (3c)

-



FT-IR of compound (3c)

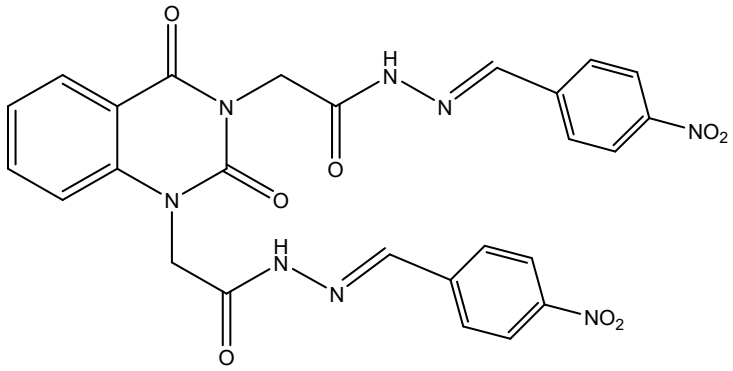
-



MS of compound (3c)

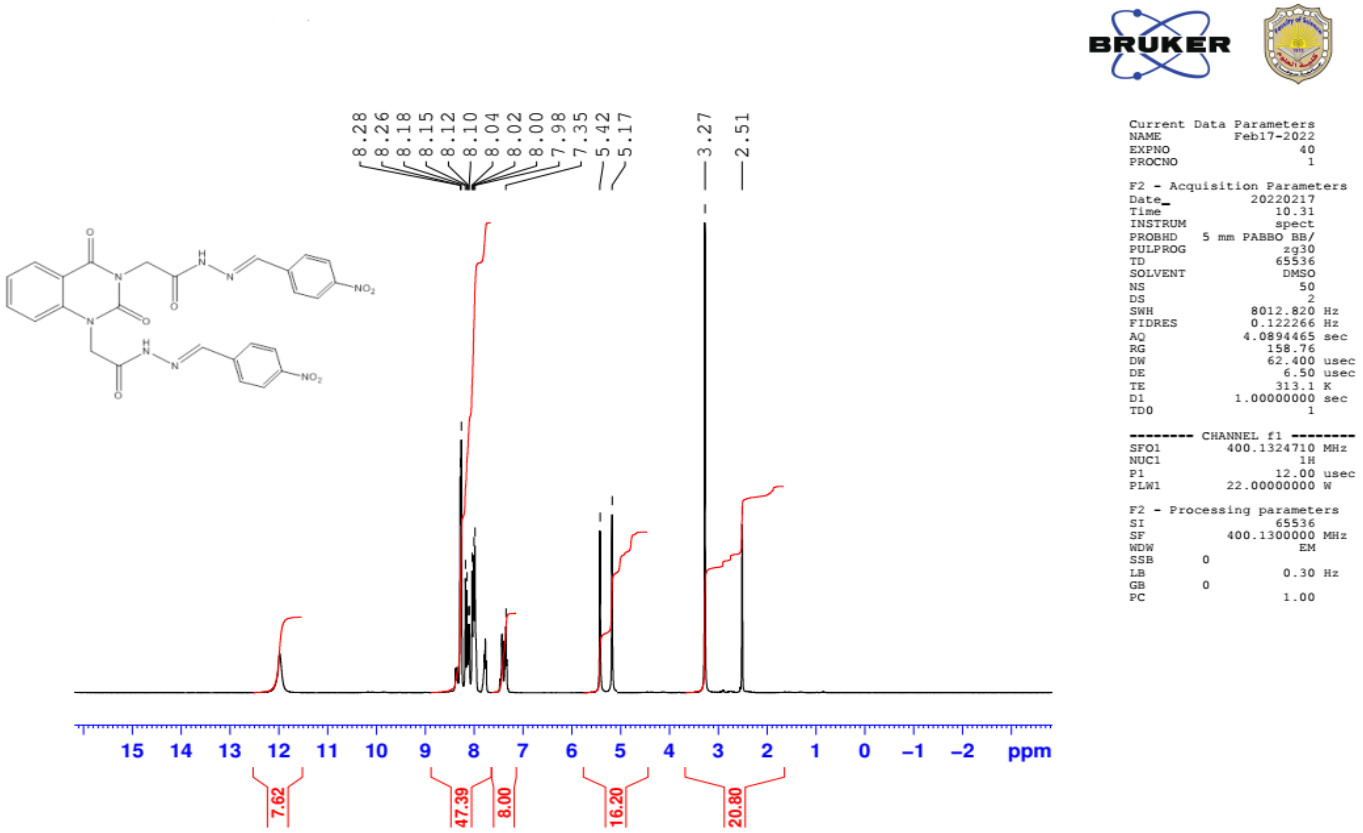
-

-Compound (3d):



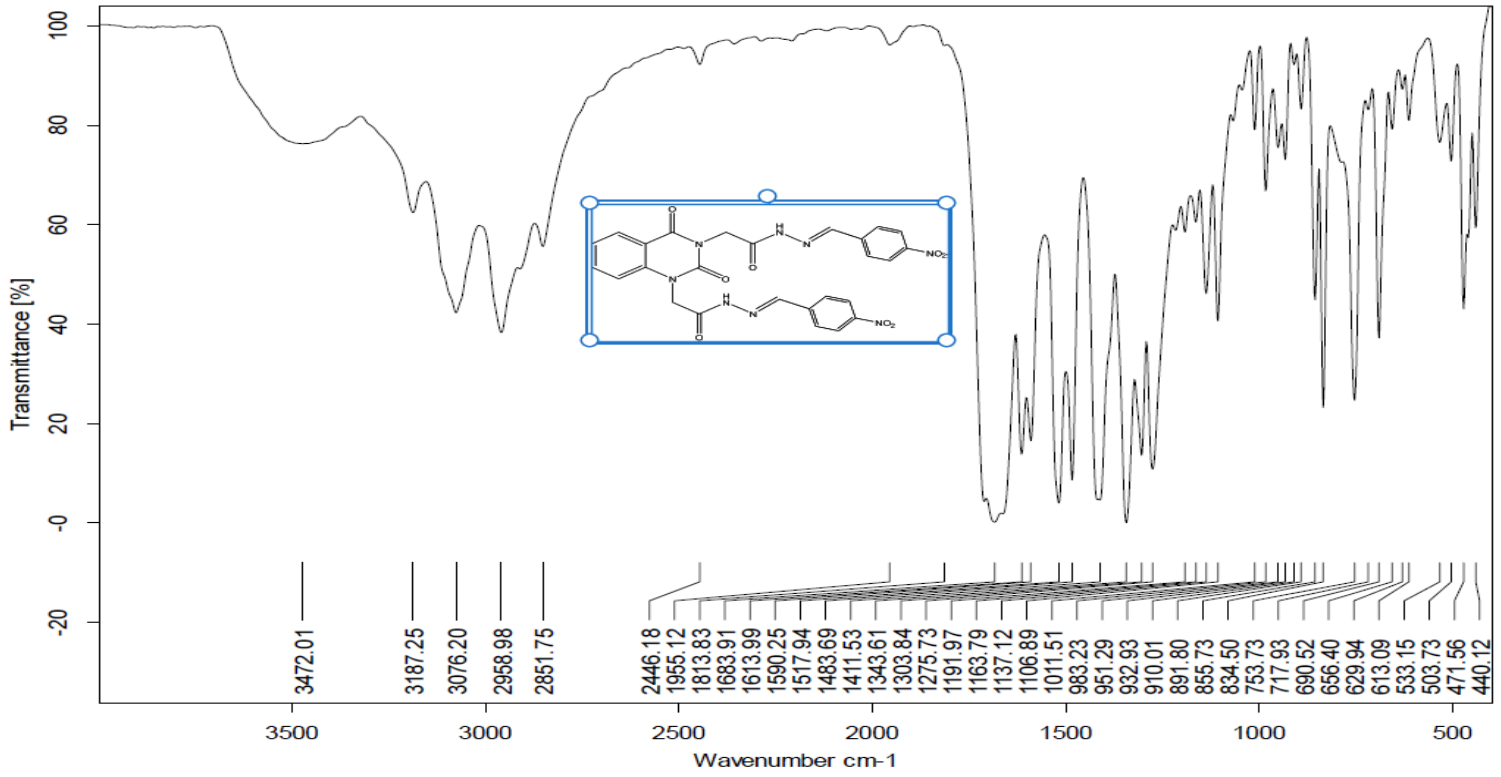
3d

-



^{1}H-NMR of compound (3d)

-



FT-IR of compound (3d)

15-Jan-07 04:44:26

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

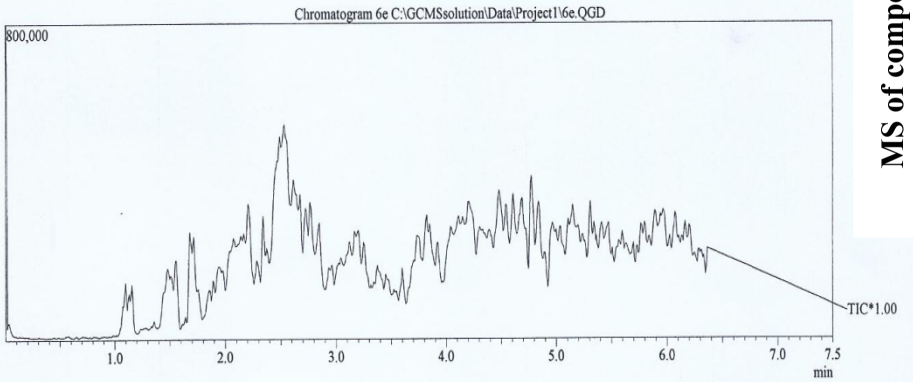
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:32:35 ص
Sample Name	: 6e
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\6e.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\6e.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 04:39:00 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

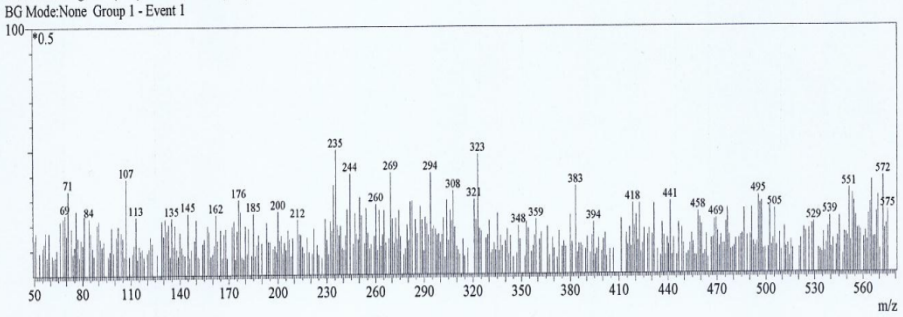
C:\GCMSsolution\Data\Project1\6e.QGD

Chromatogram 6e C:\GCMSsolution\Data\Project1\6e.QGD



Spectrum

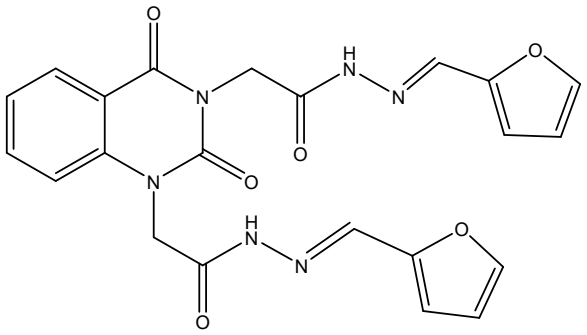
Line#:1 R.Time:3.6(Scan#:433)
MassPeaks:418
RawMode:Single 3.6(433) BasePeak:235(833)
BG Mode:None Group 1 - Event 1



MS of compound (3d)

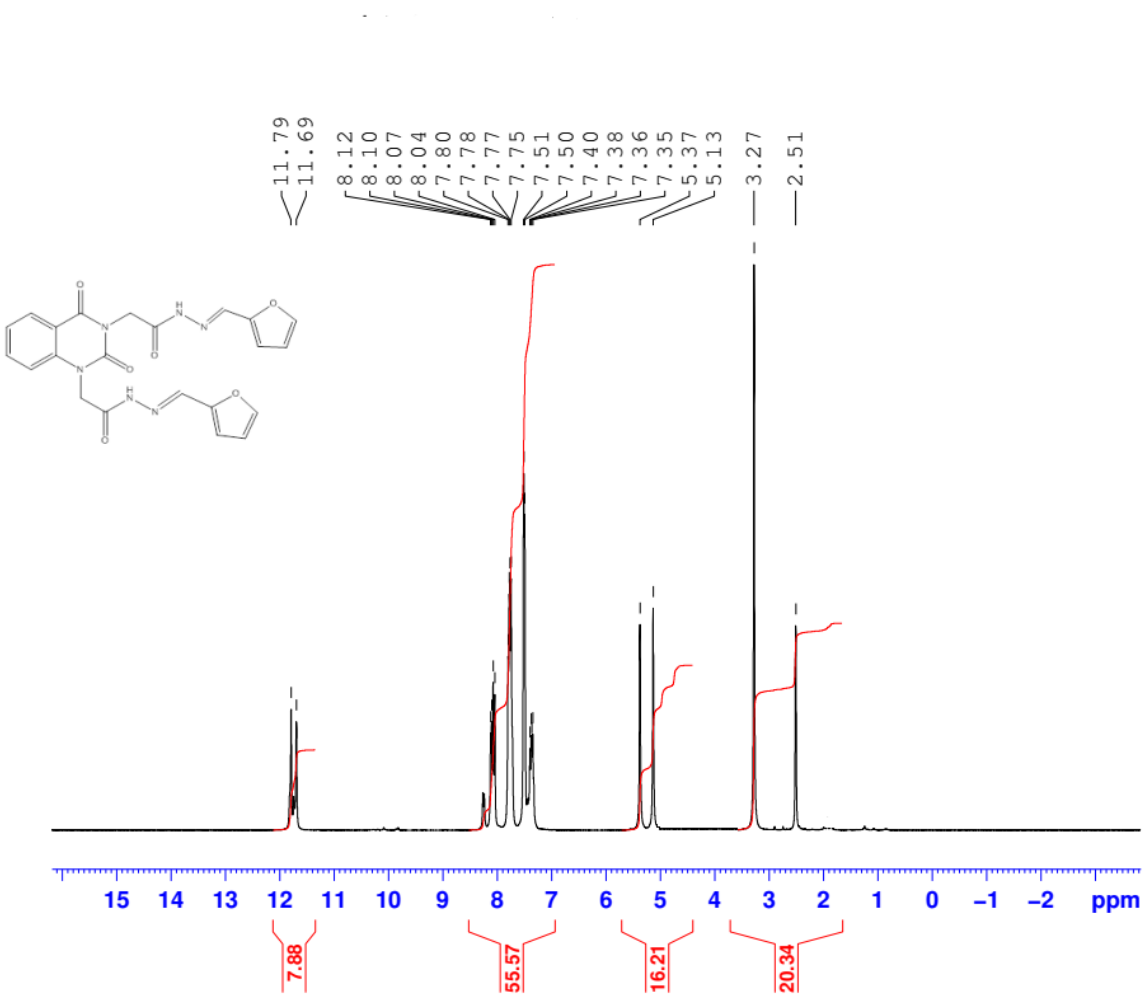
-

Compound (3e):



3e

-




```
Current Data Parameters
NAME          Feb17-2022
EXPNO                 50
PROCNO                 1

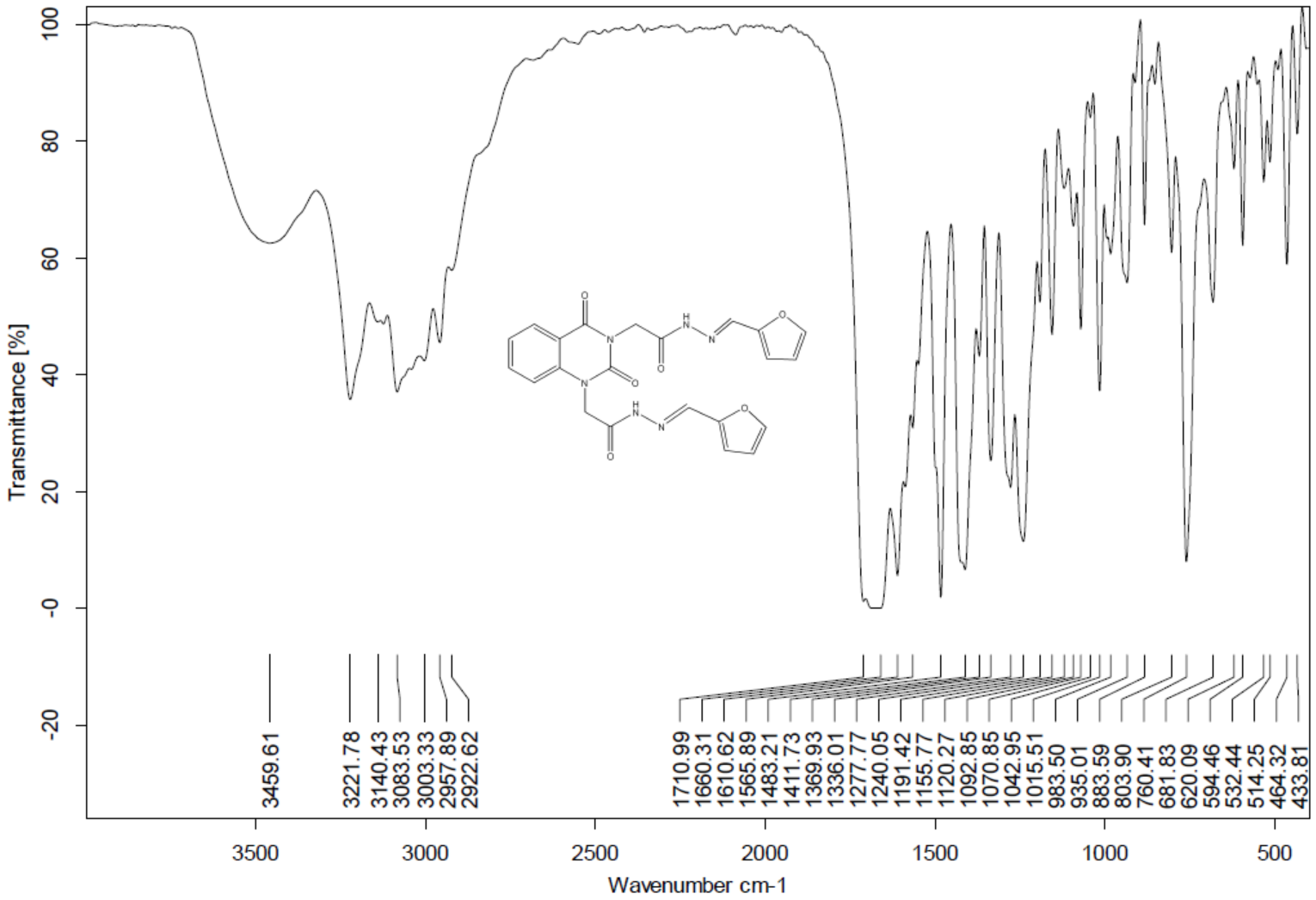
F2 - Acquisition Parameters
Date_           20220217
Time               10.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    50
DS                     2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  158.76
DW                  62.400 usec
DE                   6.50 usec
TE                  313.2 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
SI                 65536
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

[1]H-NMR of compound (3e)

-



FT-IR of compound (3e)

15-Jan-07 04:46:31

Cairo University
Micro Analytical Center

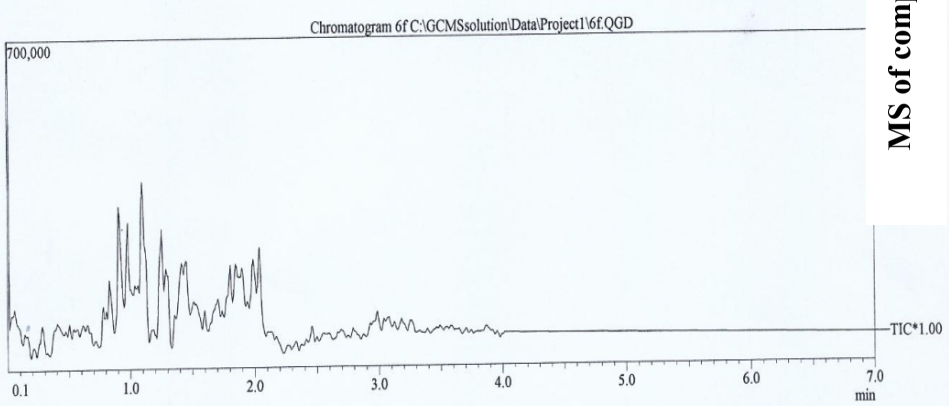
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information	
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:40:35 ص
Sample Name	: 6f
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\6f.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\6f.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 04:44:39 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

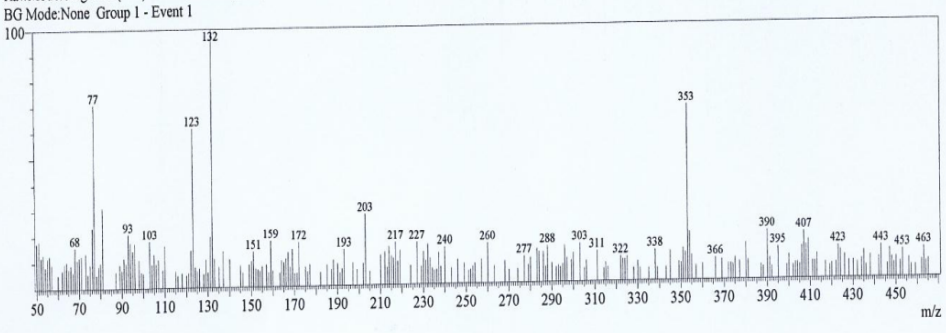
C:\GCMSsolution\Data\Project1\6f.QGD

Chromatogram 6f C:\GCMSsolution\Data\Project1\6f.QGD



Spectrum

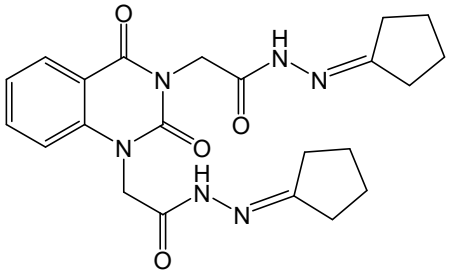
Line#:1 R.Time:2.9(Scan#:353)
MassPeaks:243
RawMode:Single 2.9(353) BasePeak:132(2196)
BG Mode:None Group 1 - Event 1



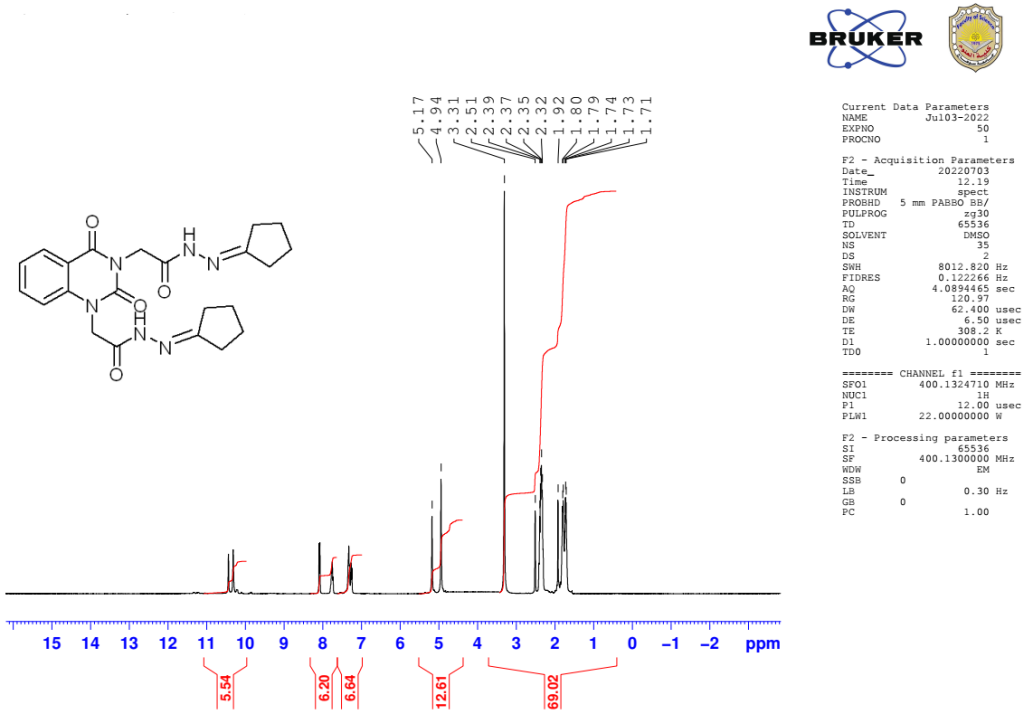
MS of compound (3e)

-

Compound (4a): -



-




```
Current Data Parameters
NAME          Jul03-2022
EXPNO                 50
PROCNO                 1

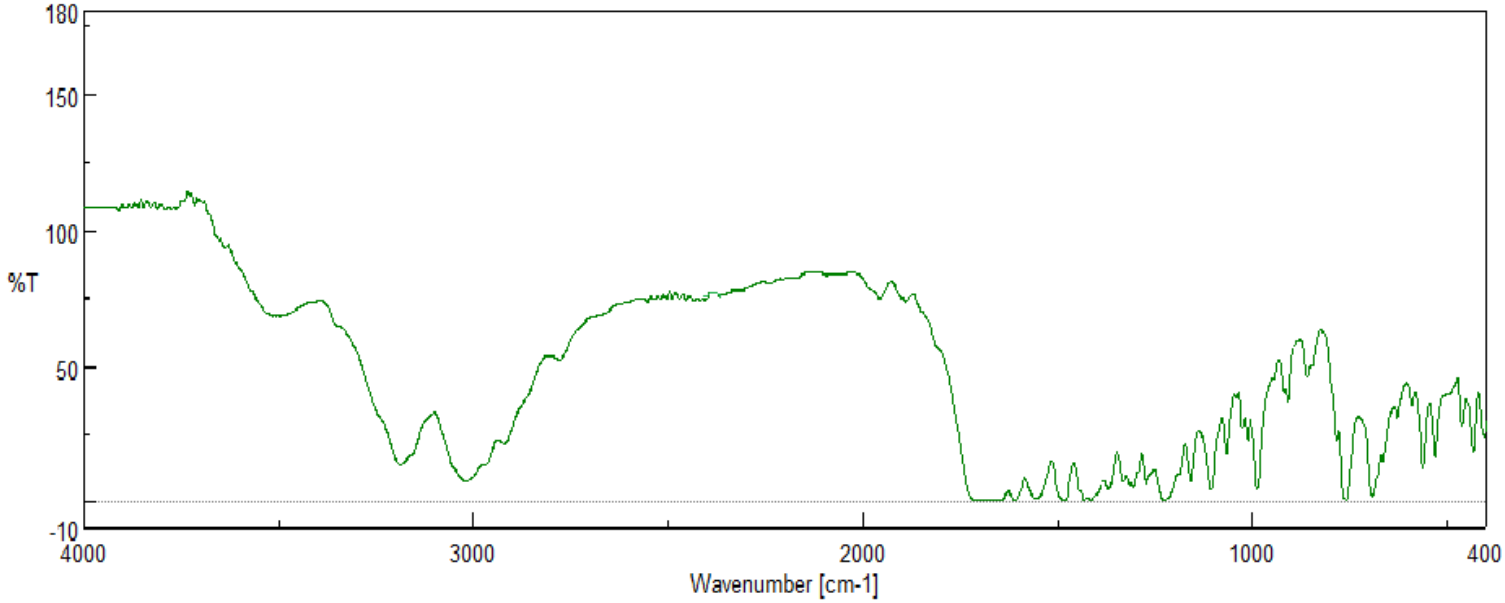
F2 - Acquisition Parameters
Date_           20220703
Time               12.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                   35
DS                    2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ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

======== CHANNEL f1 ========
SFO1         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
```

^{1}H-NMR of compound (4a)

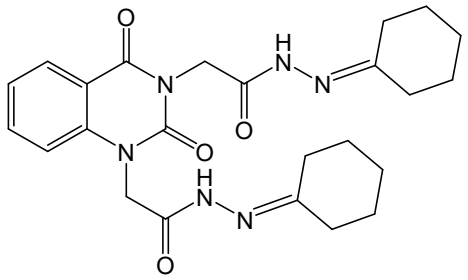
-



FT-IR of compound (4a)

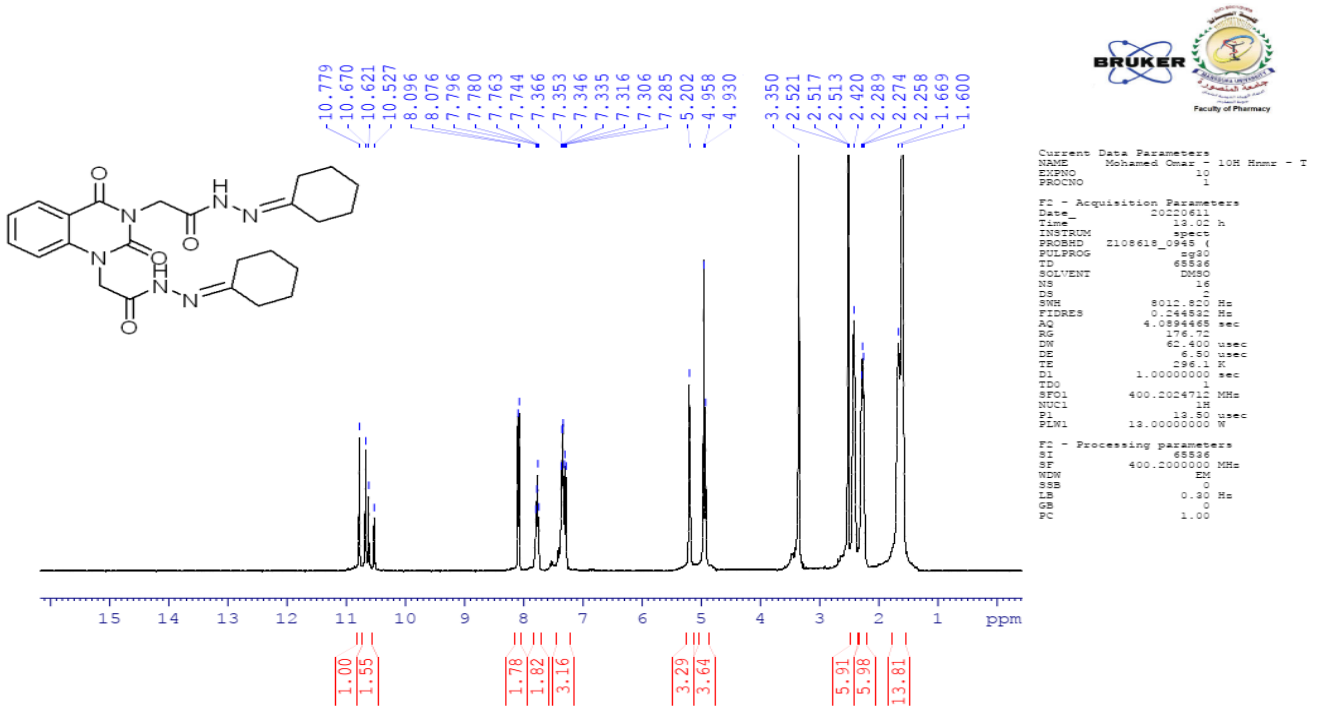
-

Compound (4b): -



4b

-



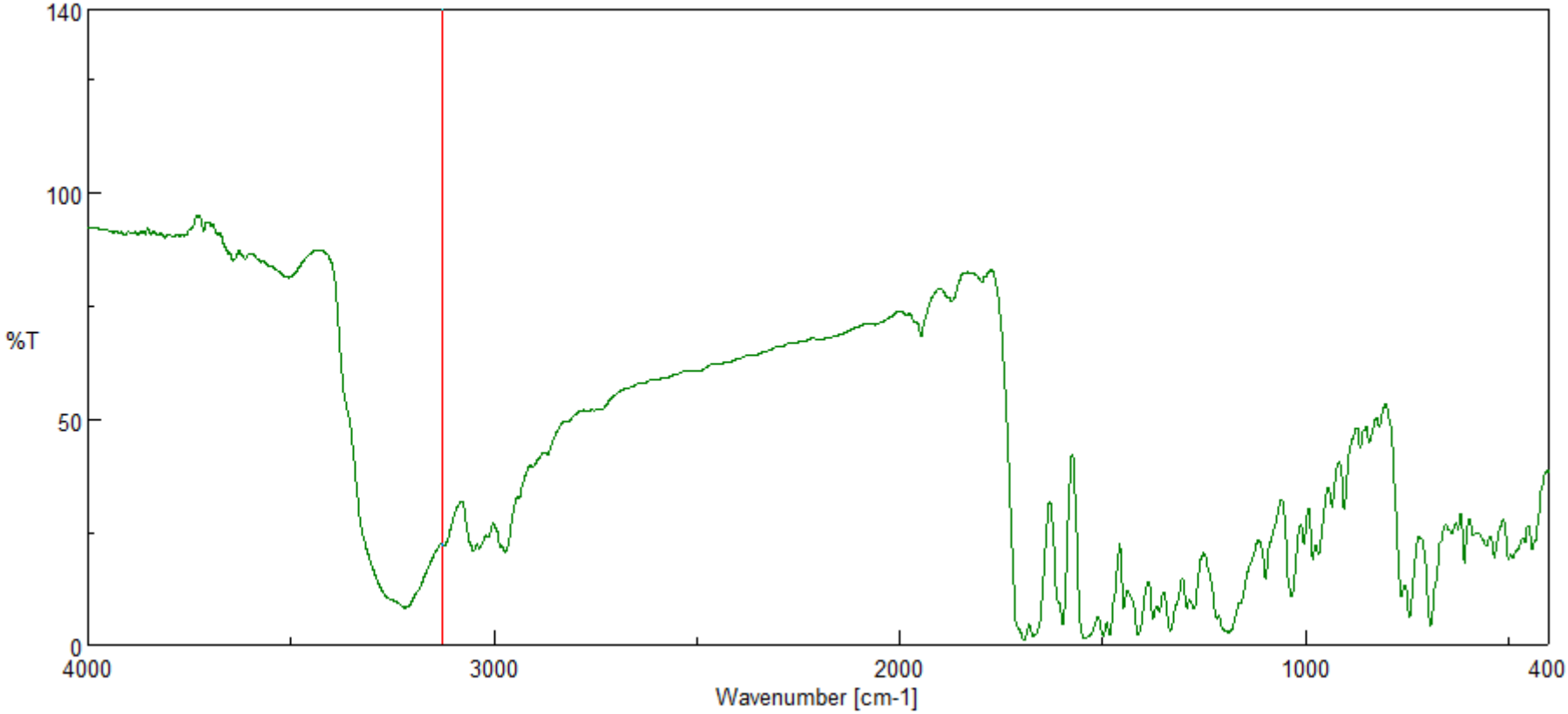

```
Current Data Parameters
NAME      Mohamed Omar - 10H Hnmr - T
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_              20220611
Time_                 13.02 h
INSTRUM                spect
PROBHD   Z108618_0945 (
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       2
SWH                8012.820 Hz
FIDRES             0.244592 Hz
AQ                 4.0894465 sec
RG                    176.71
DW                   62.400 usec
DE                    6.50 usec
TE                   296.1 K
D1                1.00000000 sec
TD0                      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
```

^{1}H-NMR of compound (4b)

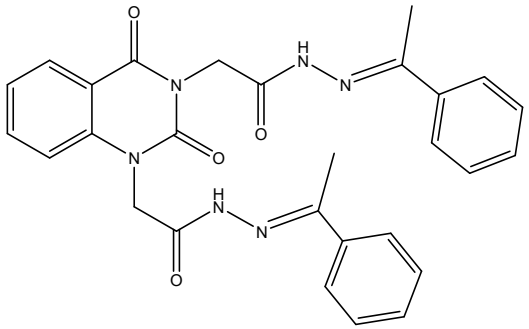
-



FT-IR of compound (4b)

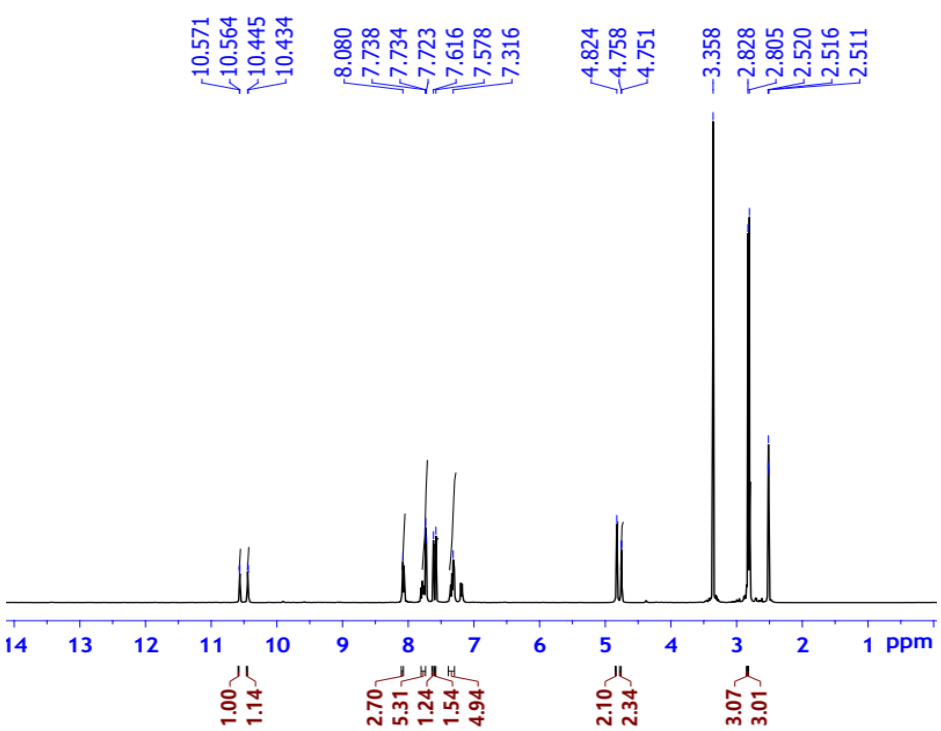
-

- compound (4c):



4c

-



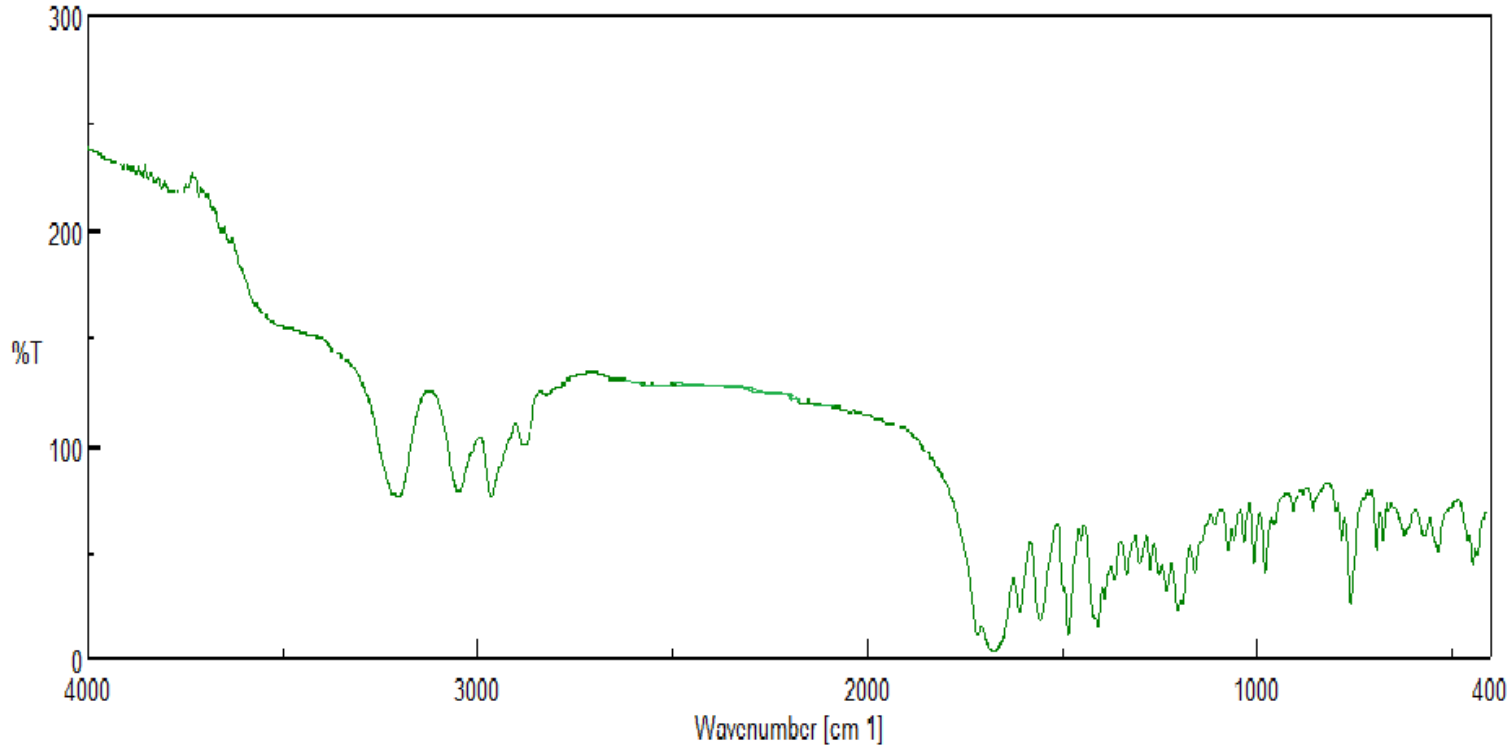

```
Current Data Parameters
NAME      Mohammed Omar-10B-proton-WH
EXPNO              10
PROCNO              1

F2 - Acquisition Parameters
Date_          20220308
Time              14.11 h
INSTRUM           spect
PROBHD    Z108618_0948 (
PULPROG           zg30
TD                65536
SOLVENT            DMSO
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.244832 Hz
AQ             4.0894465 sec
RG                 112.56
DW                62.400 usec
DE                 6.50 usec
TE                 293.7 K
D1           1.00000000 sec
TD0                   1
SFO1         400.2024712 MHz
NUC1                  1H
P1                13.50 usec
PLW1         19.00000000 W

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

^{1}H-NMR of compound (4c)

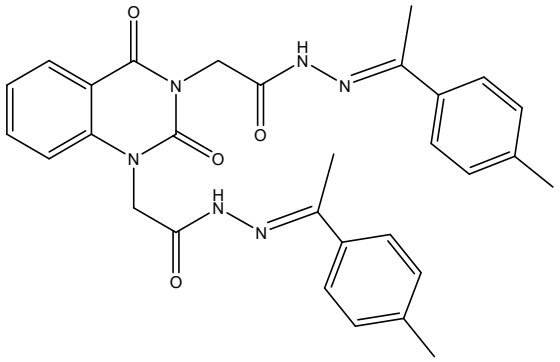
-



FT-IR of compound (4c)

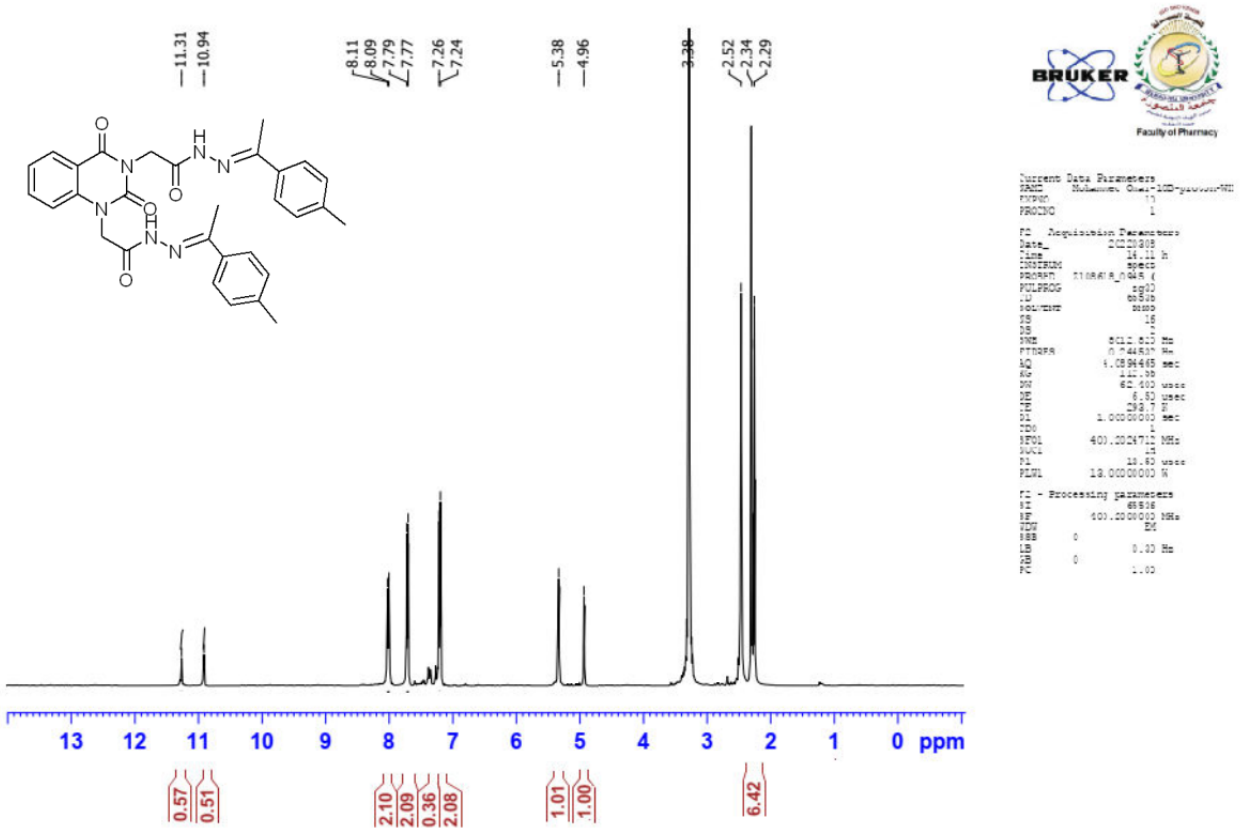
-

Compound (4d): -



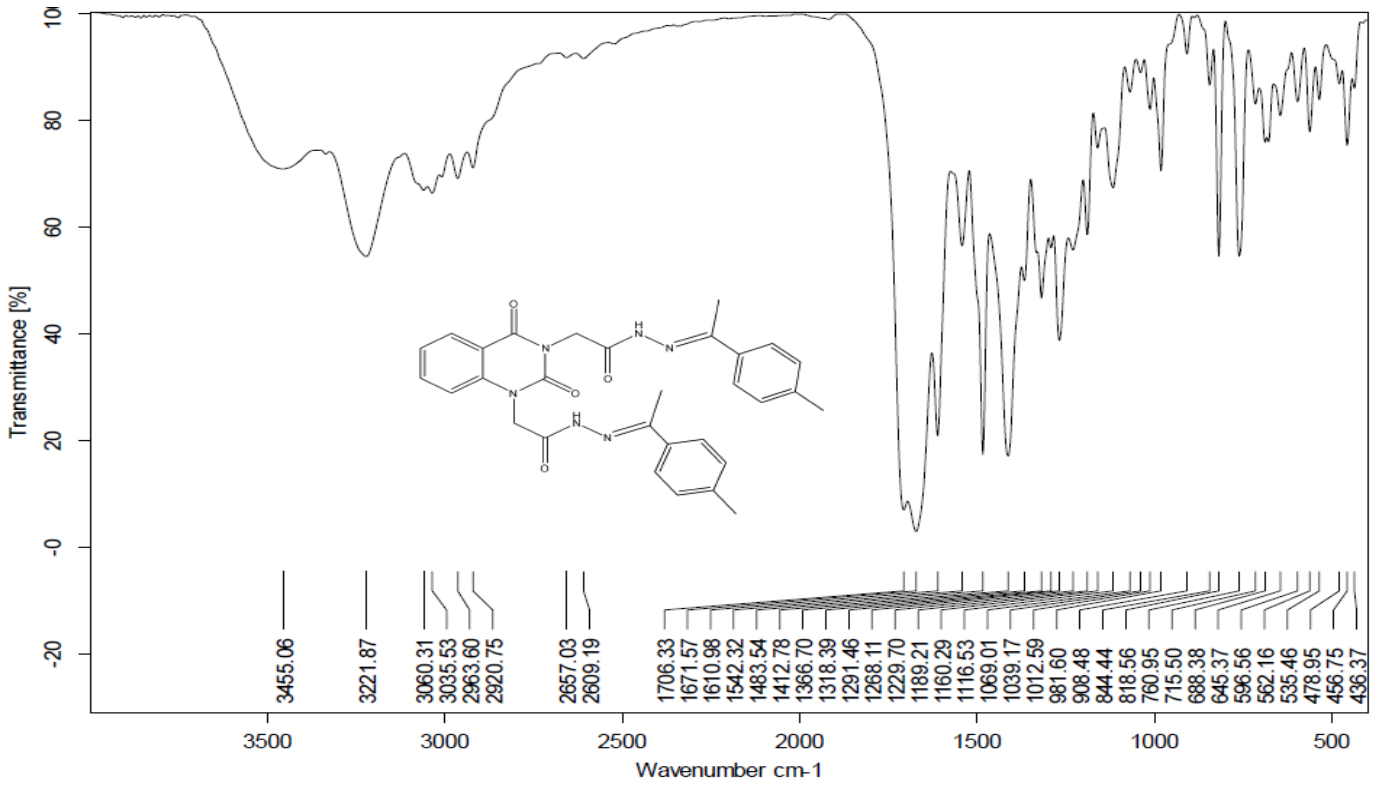
4d

-



^{1}H-NMR of compound (4d)

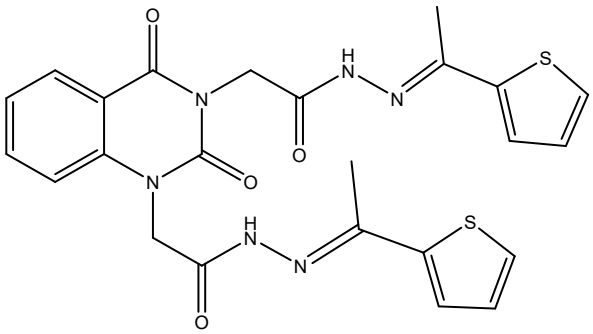
-



FT-IR of compound (4d)

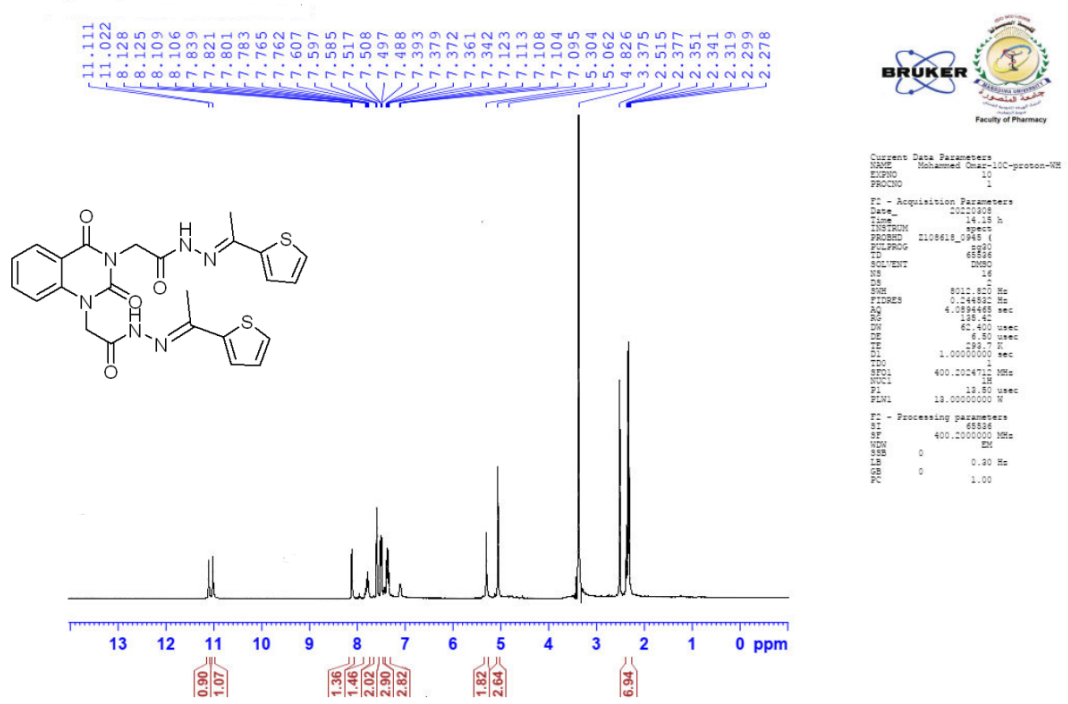
-

Compound (4e):-



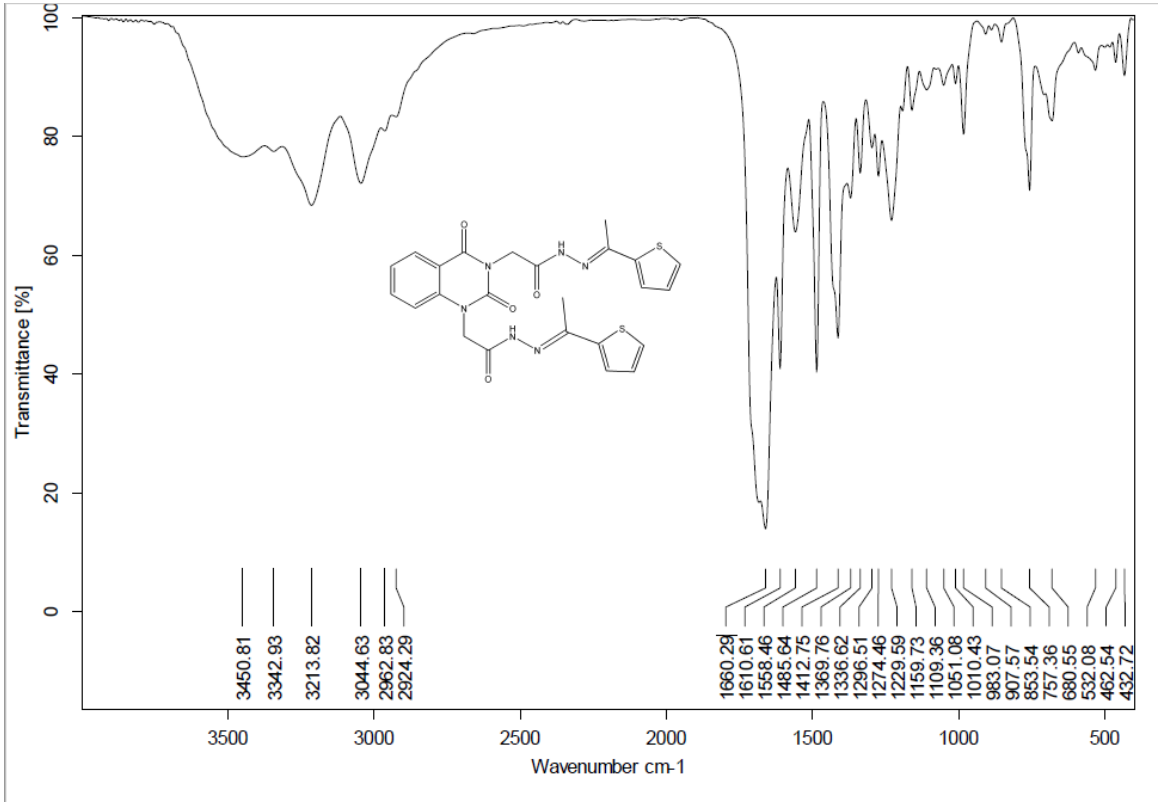
4e

-



^{1}H-NMR of compound (4e)

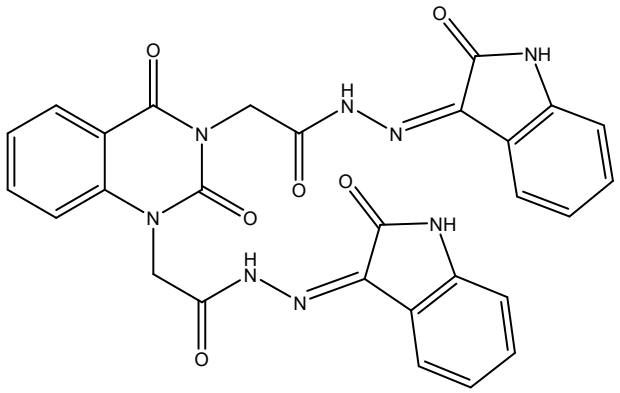
-



FT-IR of compound (4e)

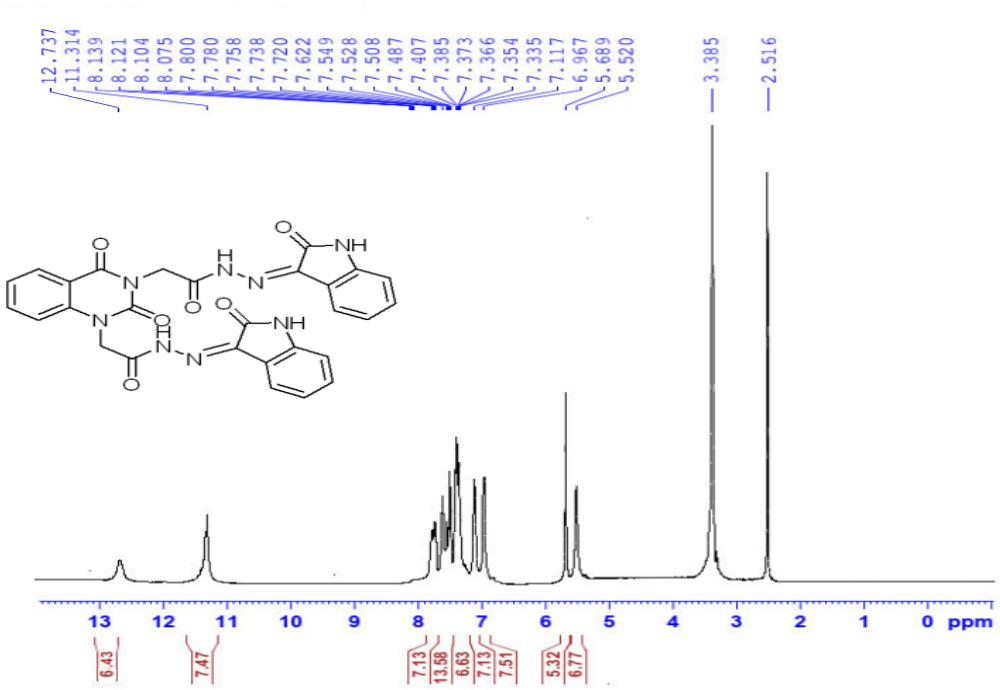
-

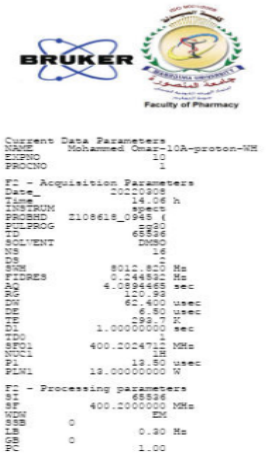
Compound (4f)



4f

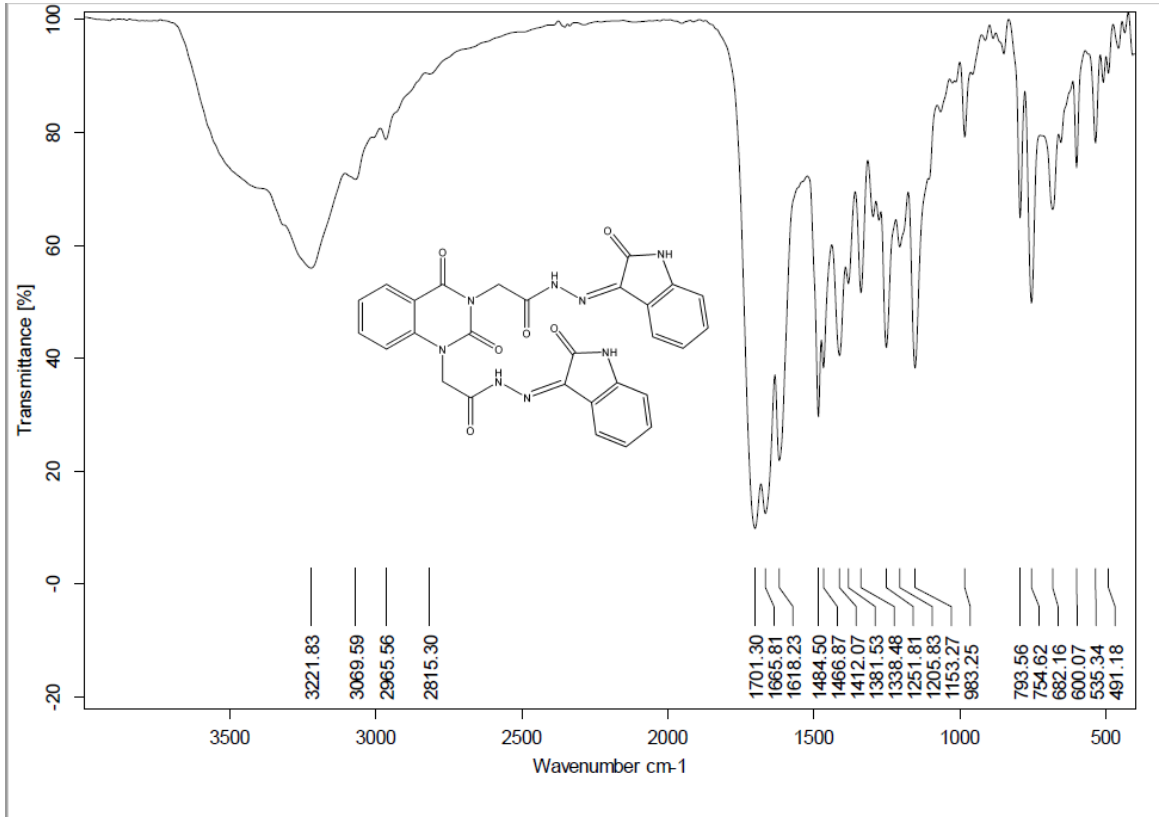
-





^{1}H-NMR of compound (4f)

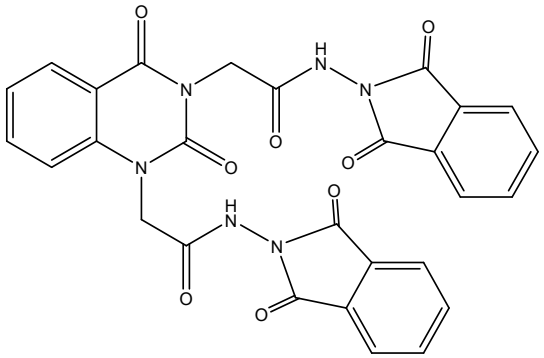
-



FT-IR of compound (4f)

-

compound (5a)



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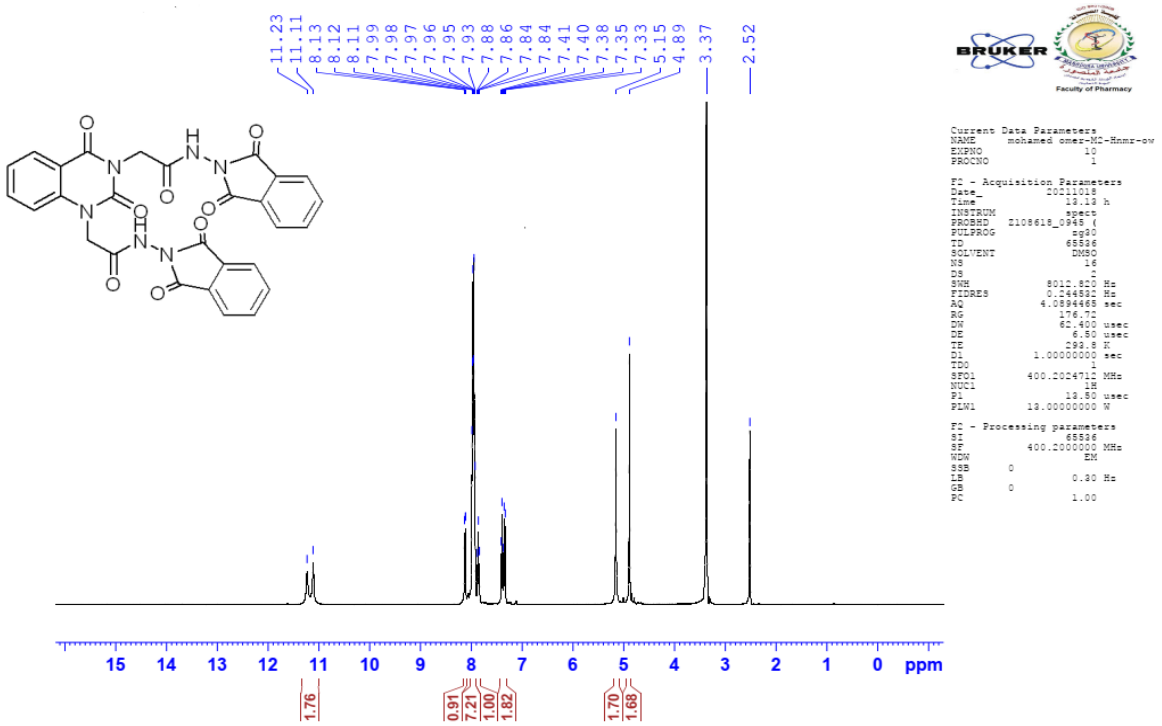


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Current Data Parameters
NAME      mohamed omer-M2-Hnmr-ov
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211018
Time              18.19 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH              8012.820 Hz
FIDRES           0.244891 Hz
AQ               4.0894465 sec
RG                  176.71
DW                 62.400 usec
DE                  6.50 usec
TE                293.8 K
D1               1.00000000 sec
TD0                    1
SFO1           400.2024710 MHz
NUC1                  1H
P1                 12.80 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
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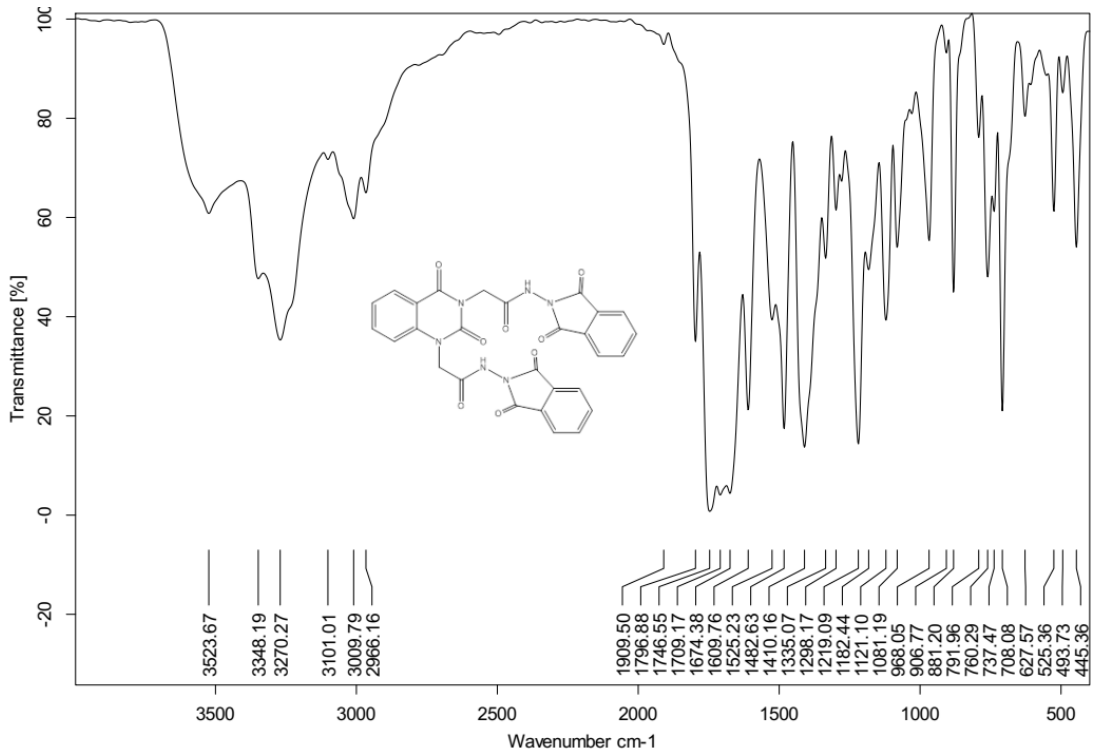
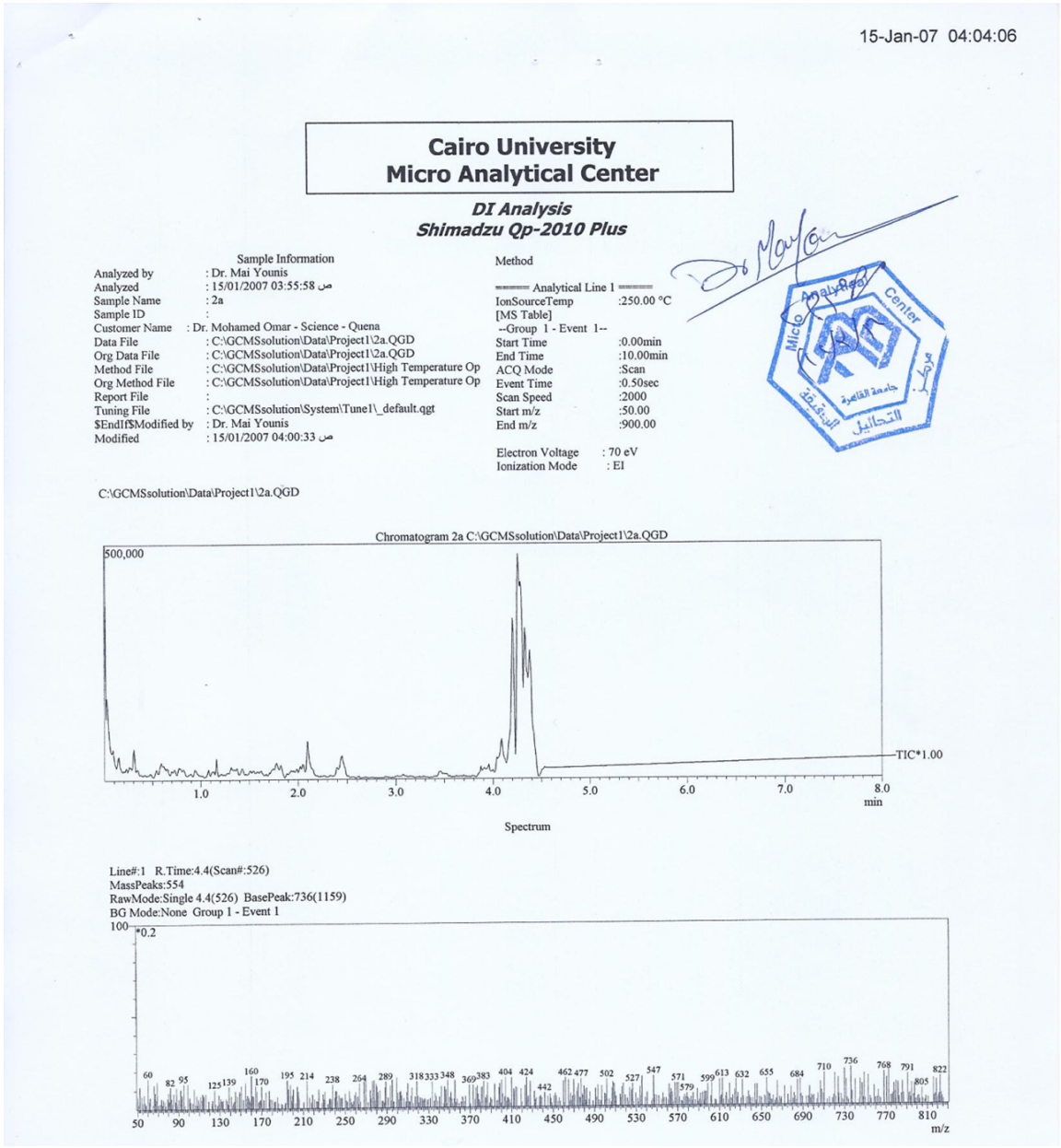
-



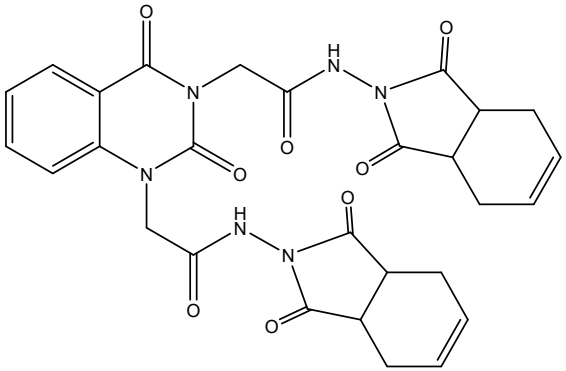
FT-IR of compound (5a)



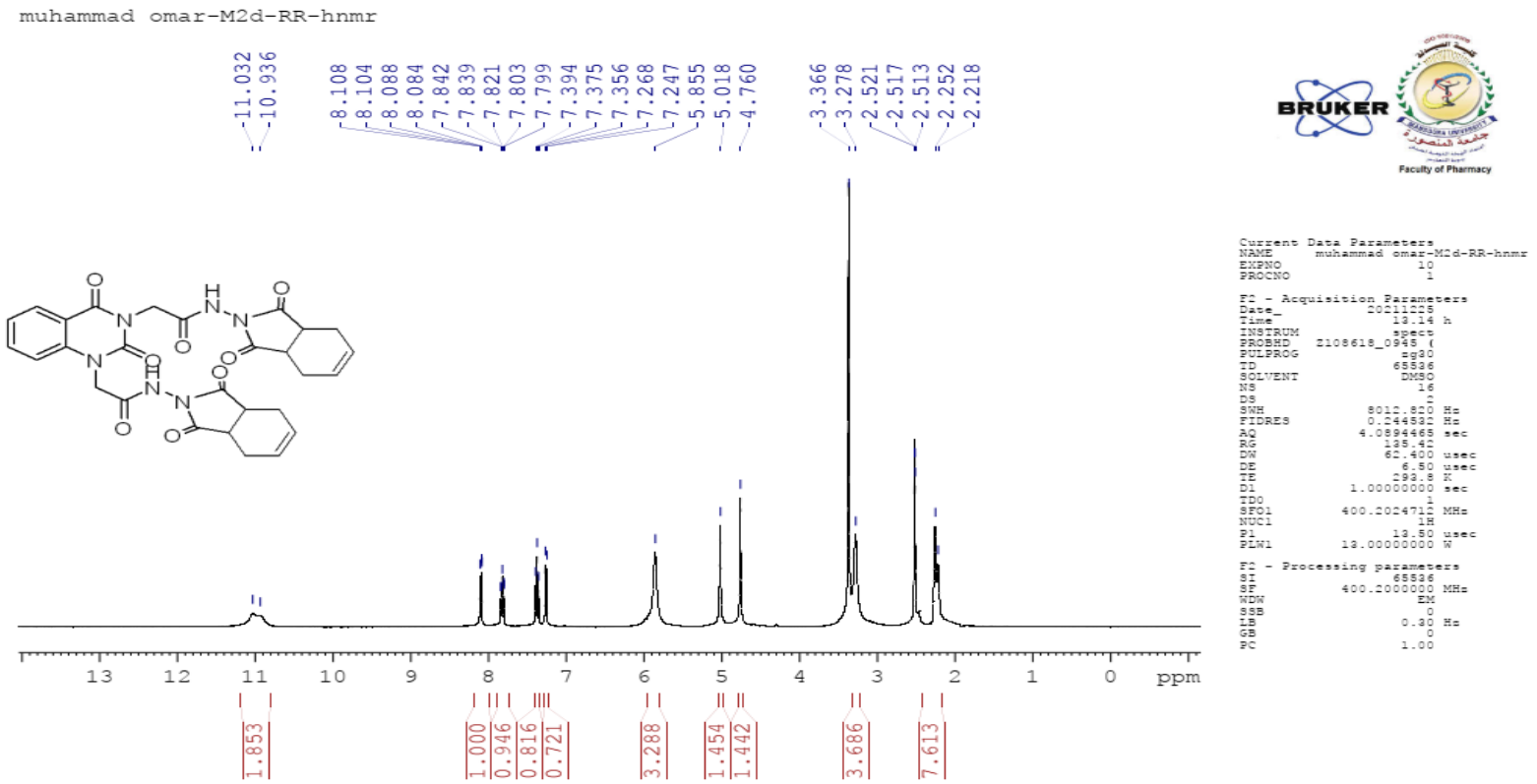
MS of compound (5a)

Compound (5b):-

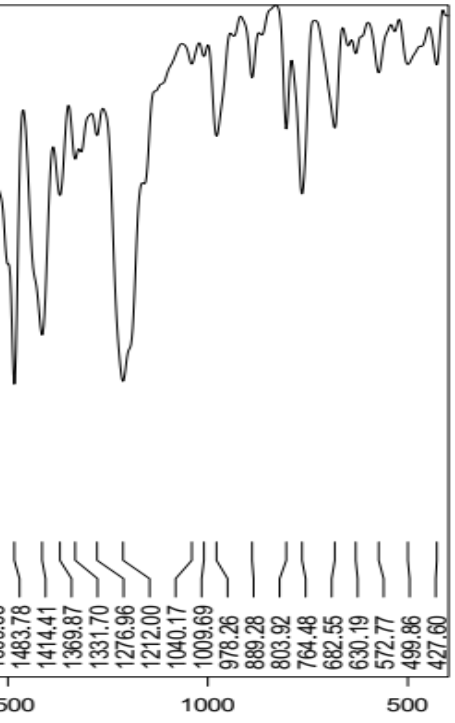
-


O
N
H
N
O
O
O
N
O
O
H
N
N
O
O
O

-



^{1}H-NMR of compound (5b)



15-Jan-07 04:10:17

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

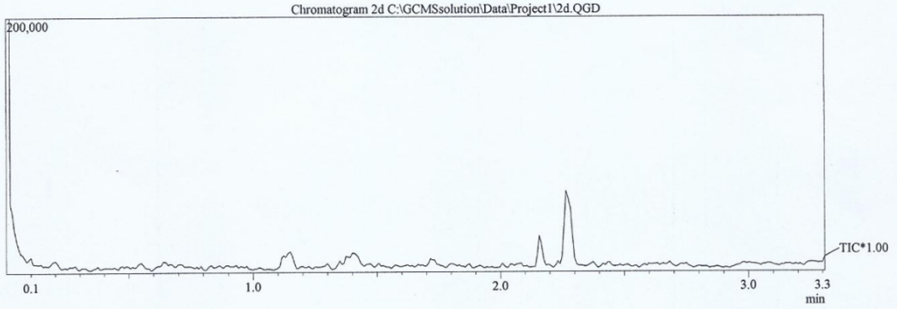
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 04:02:11 ص
Sample Name	: 2d
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\2d.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\2d.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature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

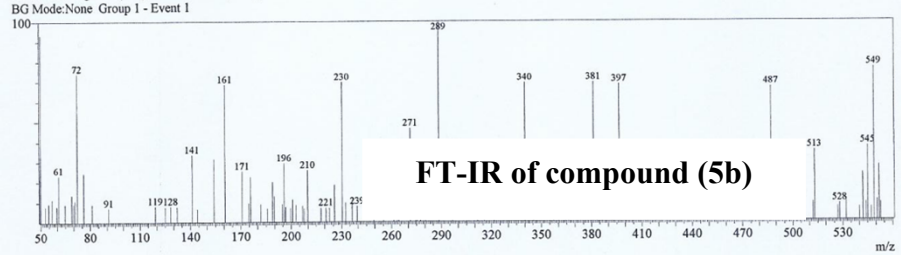
C:\GCMSsolution\Data\Project1\2d.QGD

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



Spectrum

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



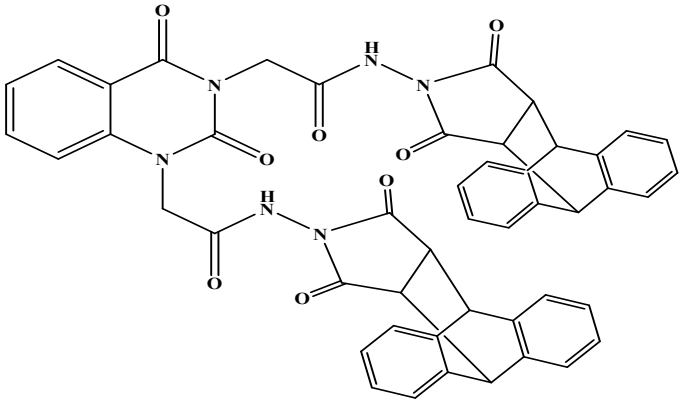
FT-IR of compound (5b)

-

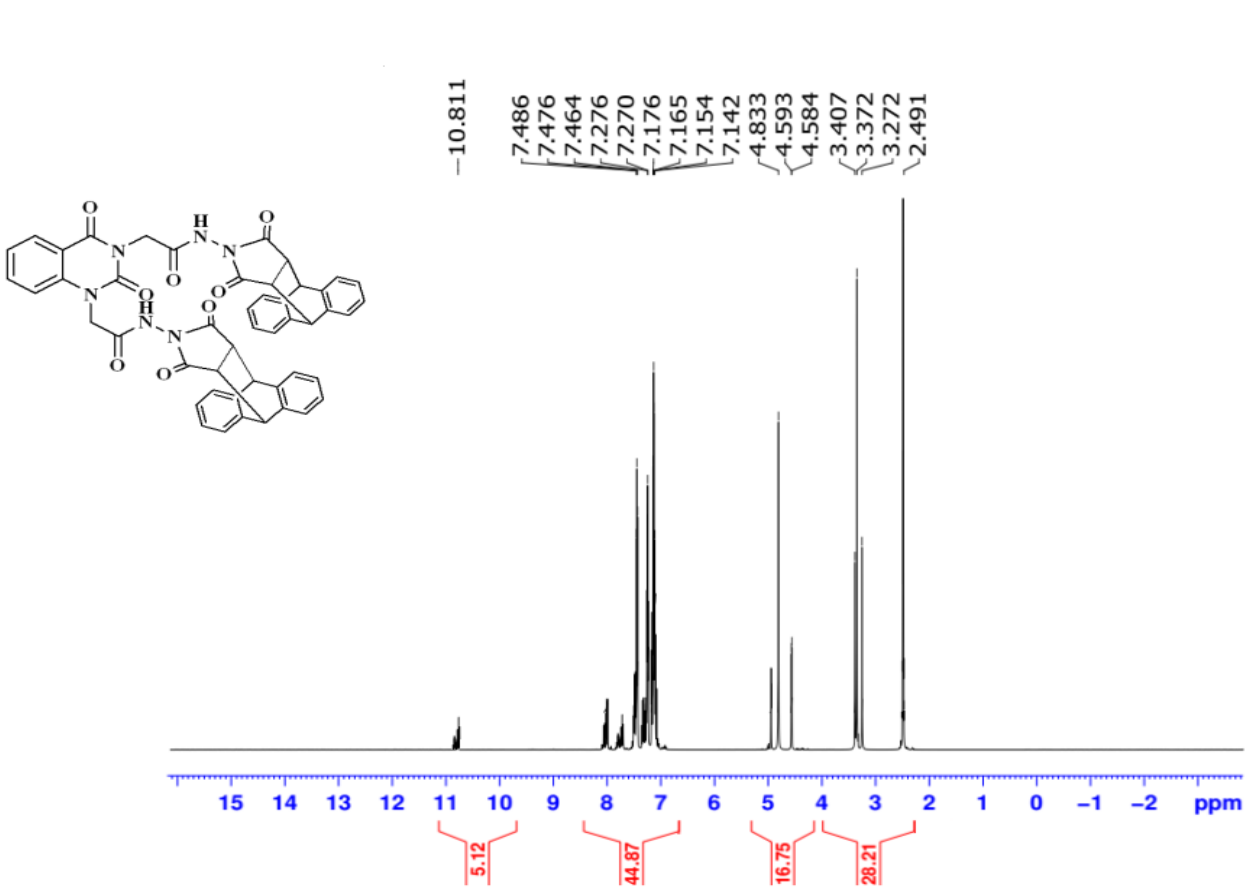
Compound (5c)

MS of compound (5b)

-



-



BRUKER

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Current Data Parameters
NAME                  Feb17-2022
EXPNO                         20
PROCNO                         1

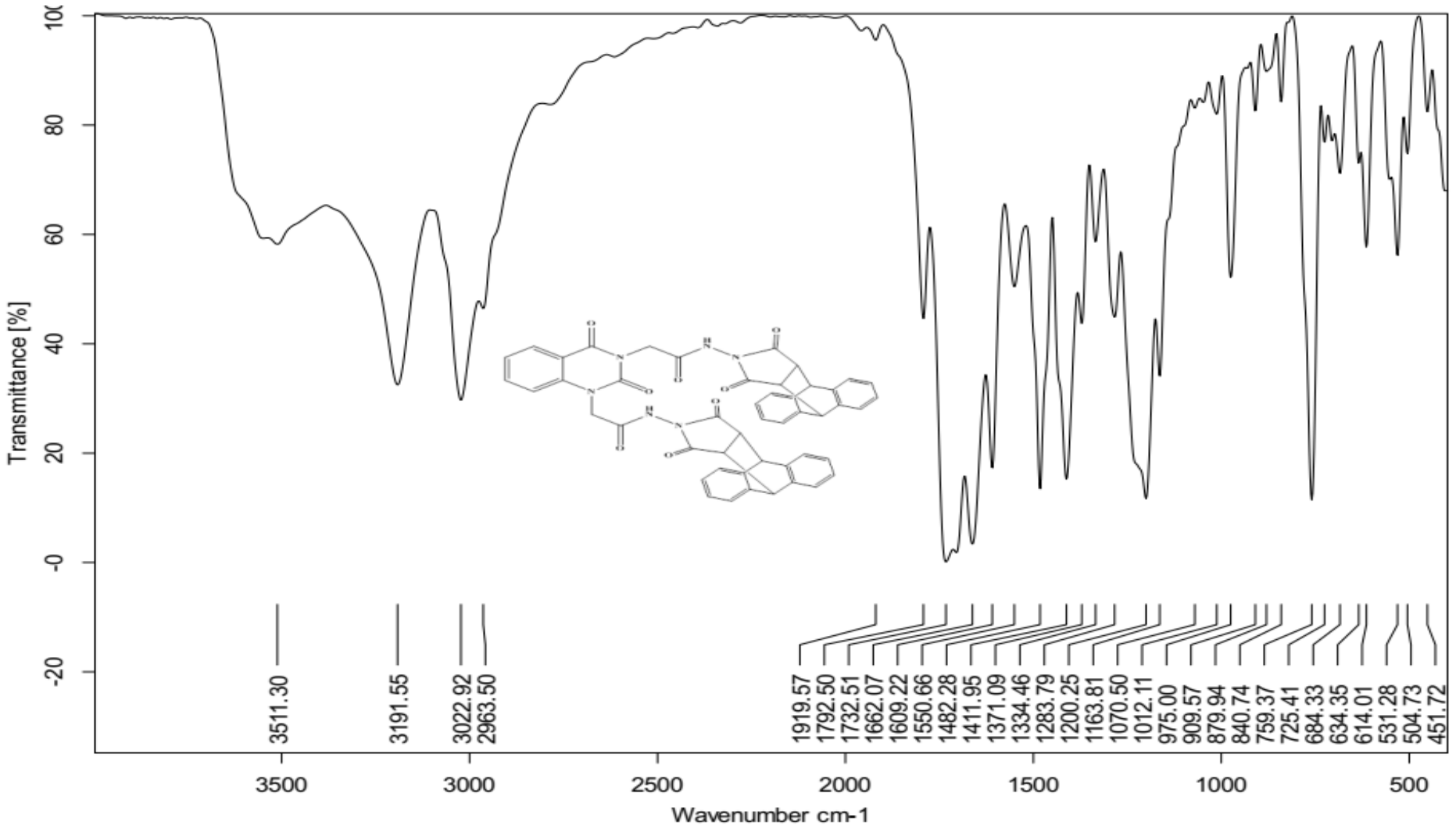
F2 - Acquisition Parameters
Date_                   20220217
Time                       10.14
INSTRUM                    spect
PROBHD     5 mm PABBO BB/
PULPROG                    zg30
TD                        65536
SOLVENT                    DMSO
NS                            50
DS                             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 ========
SFO1                  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
```

[1]H-NMR of compound (5c)

-



FT-IR of compound (5c)

15-Jan-07 04:04:06

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

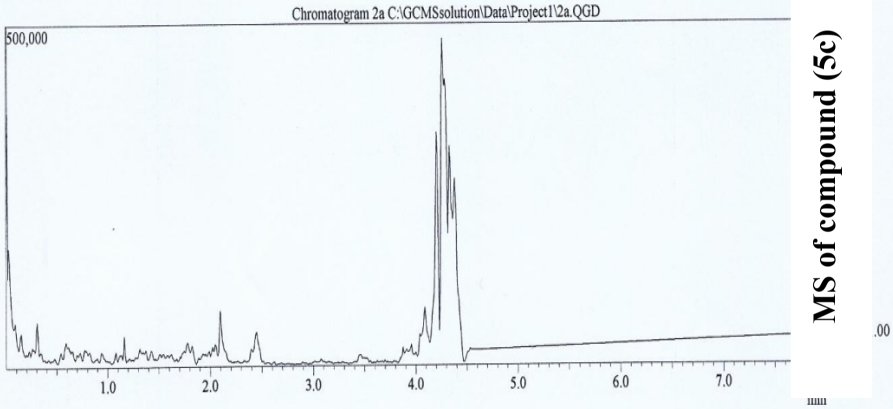
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 03:55:58 ص
Sample Name	: 2a
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\2a.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\2a.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 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

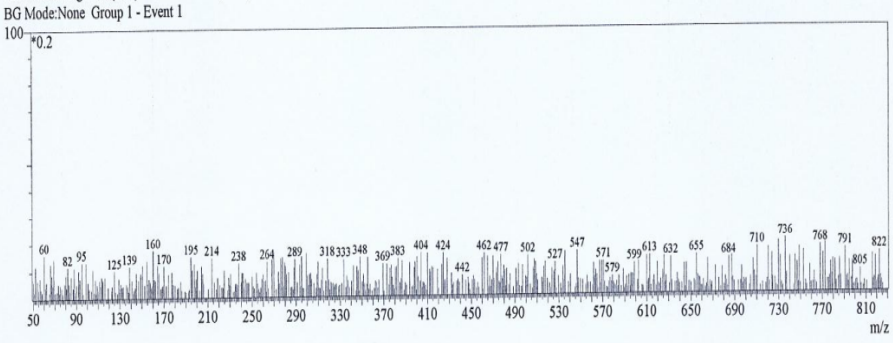
C:\GCMSsolution\Data\Project1\2a.QGD

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



Spectrum

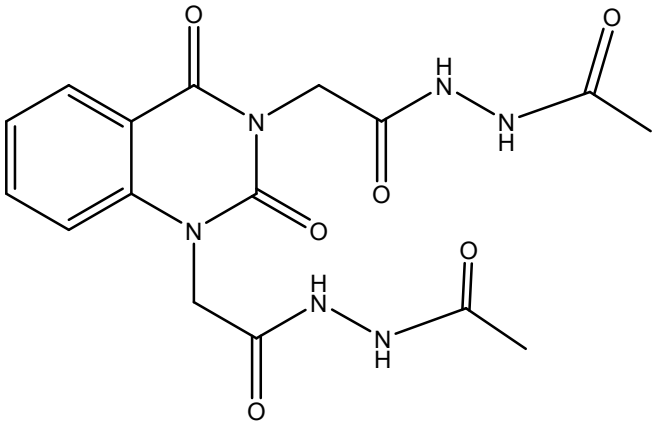
Line#:1 R.Time:4.4(Scan#:526)
MassPeaks:554
RawMode:Single 4.4(526) BasePeak:736(1159)
BG Mode:None Group 1 - Event 1

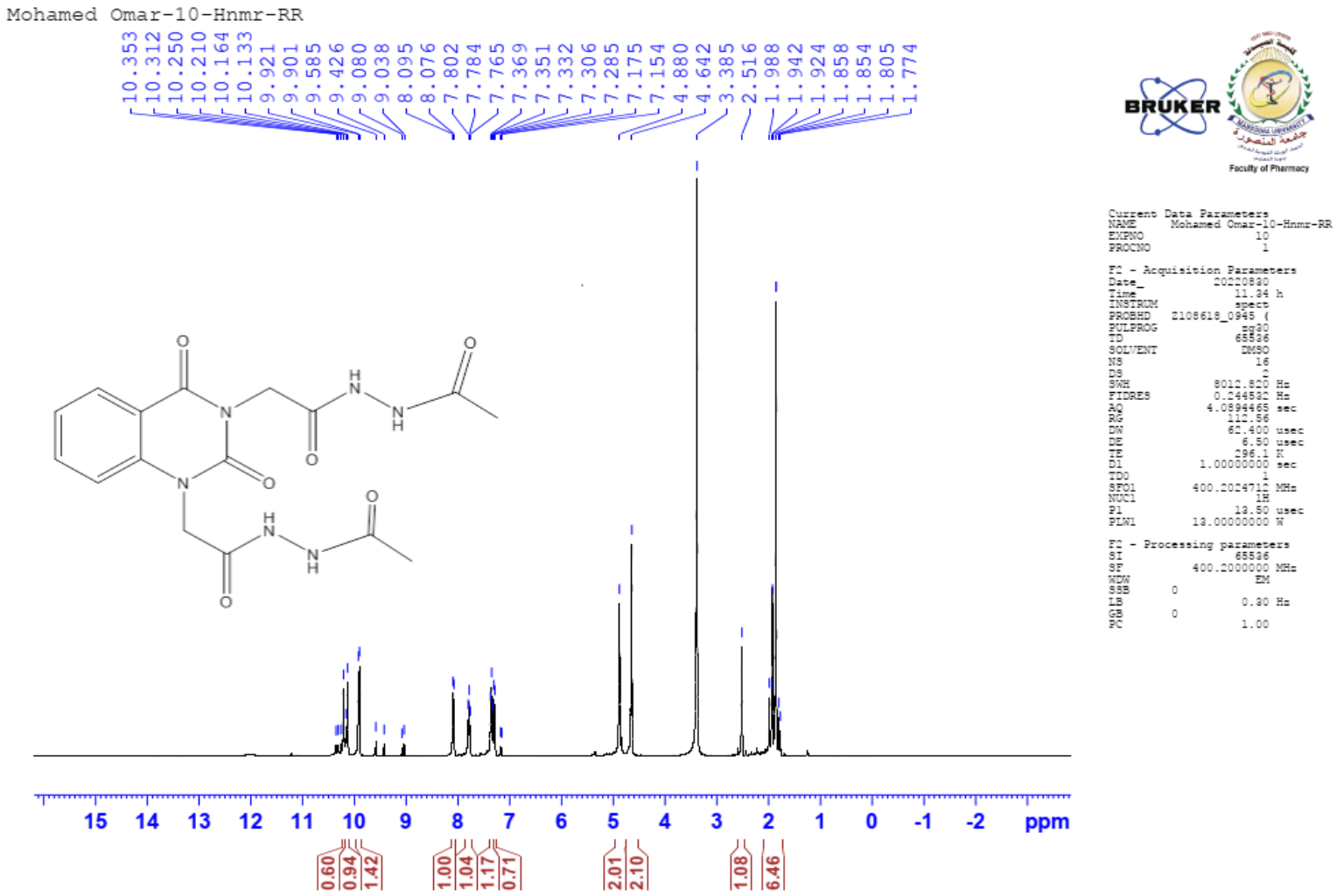


MS of compound (5c)

-

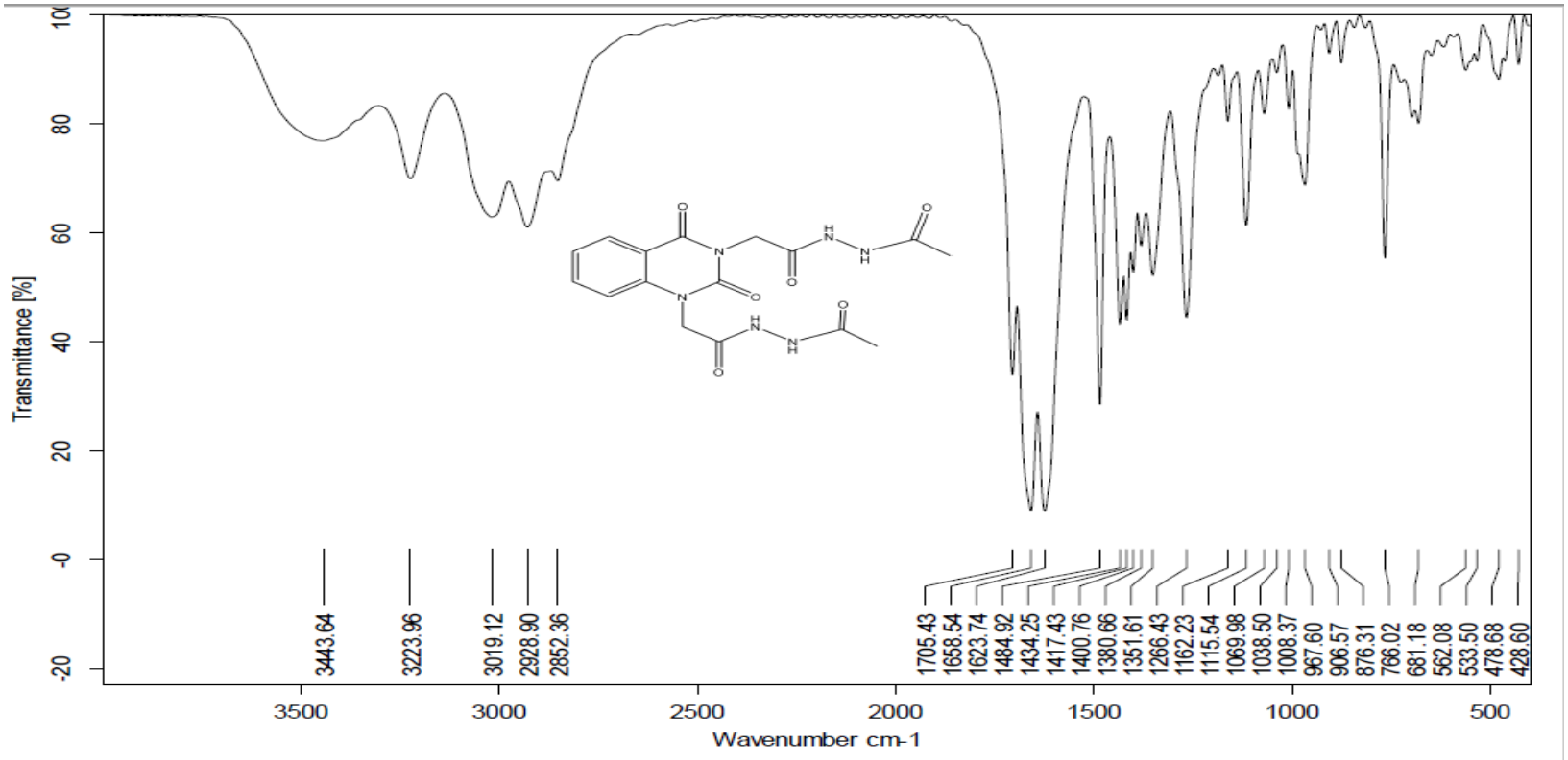
Compound (6a)





^{1}H-NMR of compound (6a)

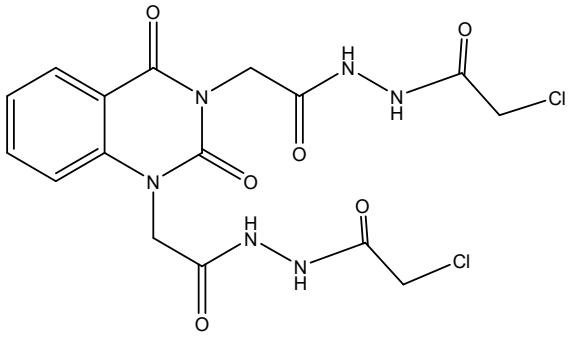
-


Transmittance [%]
100
80
60
40
20
-0
-20
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1
3443.64
3223.96
3019.12
2928.90
2852.36
1705.43
1658.54
1623.74
1484.92
1434.25
1417.43
1400.76
1380.66
1351.61
1266.43
1162.23
1115.54
1069.98
1038.50
1008.37
967.60
906.57
876.31
766.02
681.18
562.08
533.50
478.68
428.60

-

Compound (6b)

FT-IR of compound (6a)



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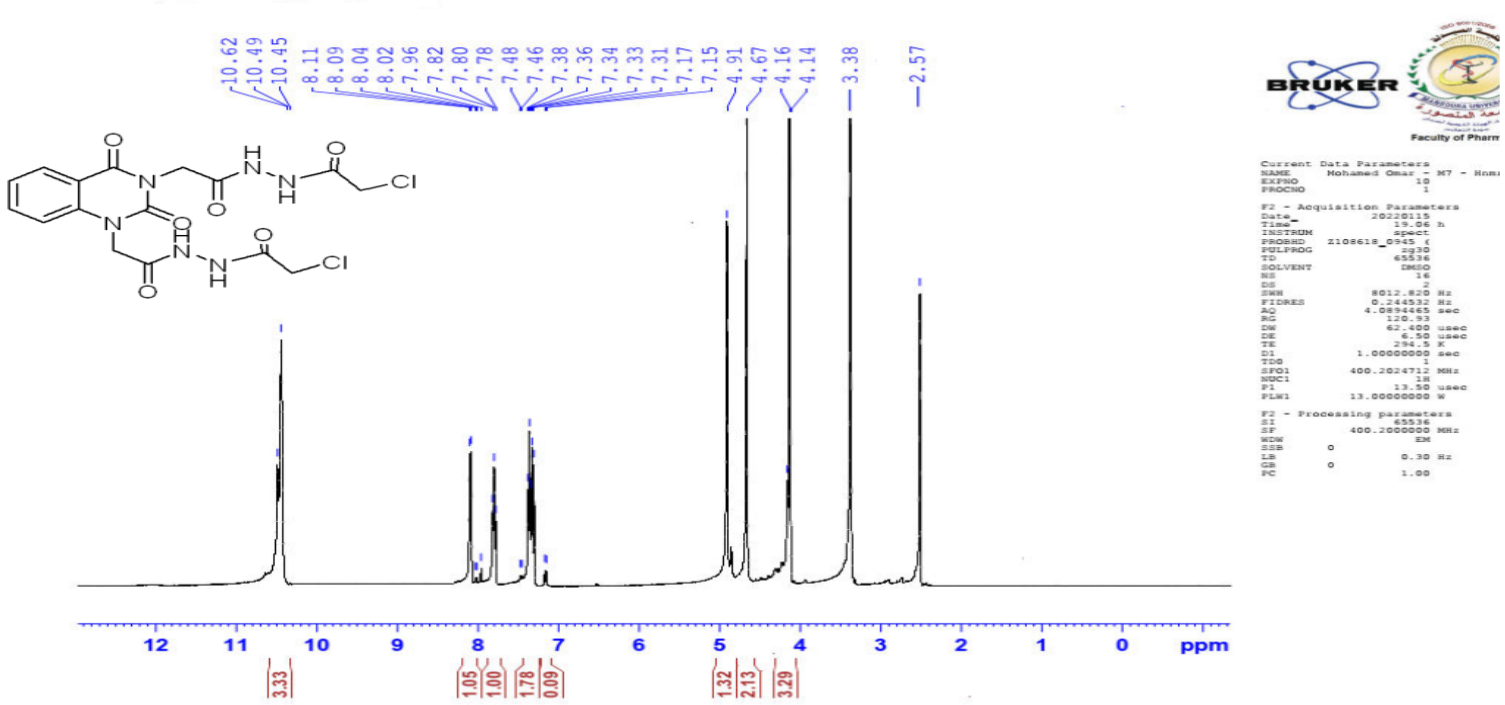
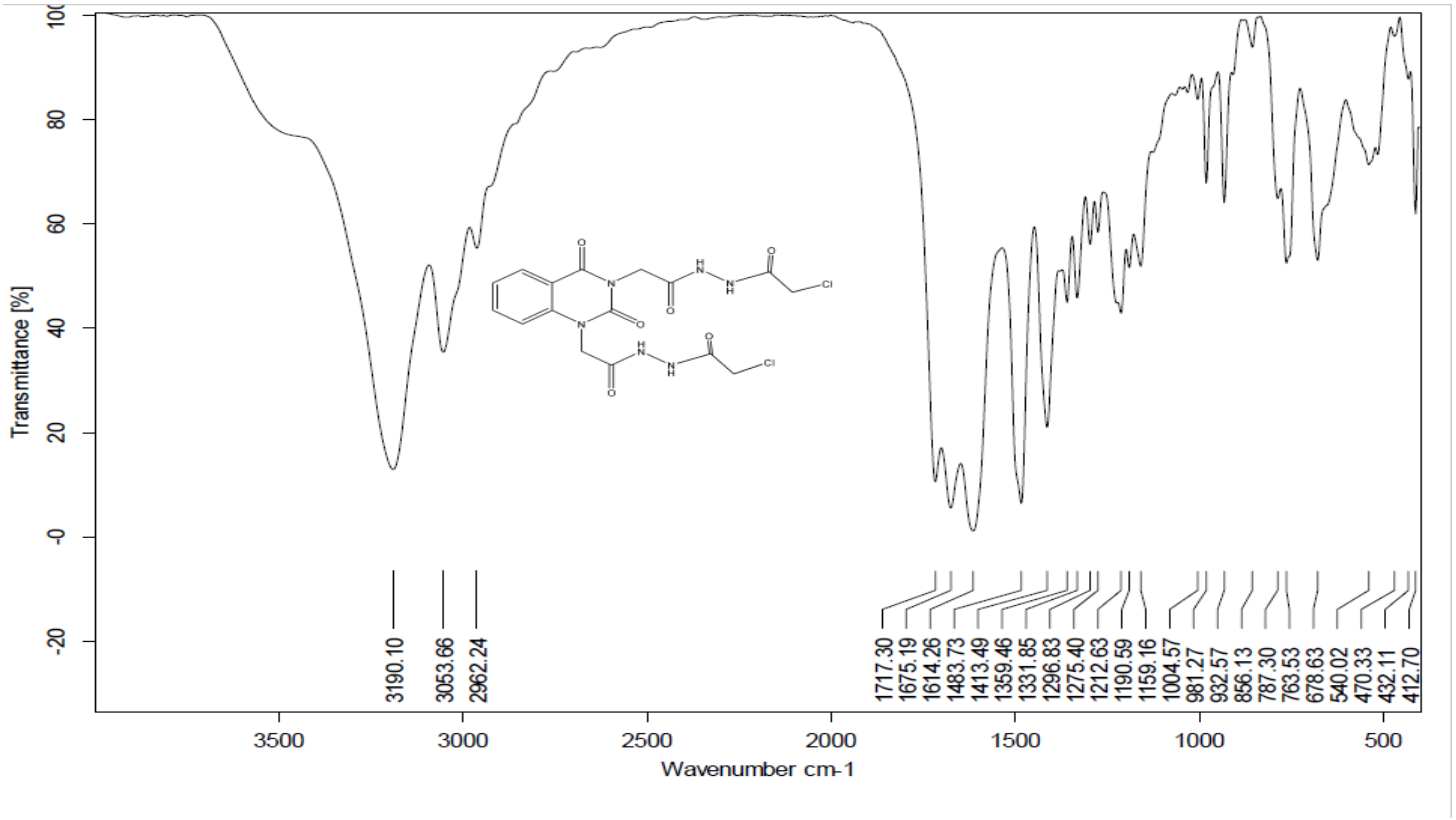


[1]H-NMR of compound (6b)

-



FT-IR of compound (6b)

15-Jan-07 02:56:27

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

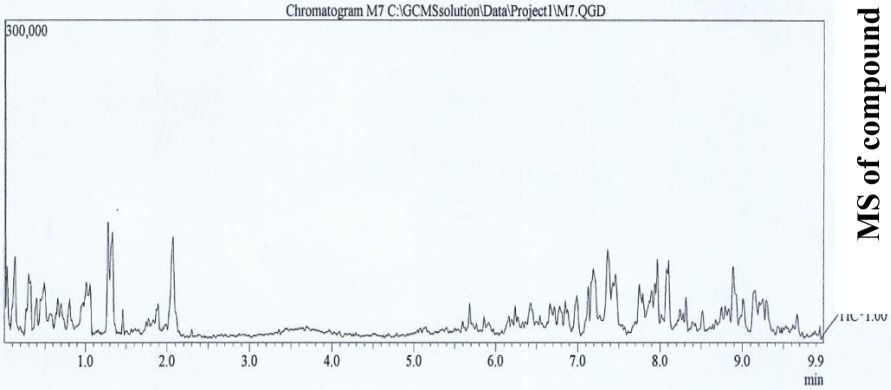
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 02:36:02 ص
Sample Name	: M7
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M7.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M7.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 02:46:02 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

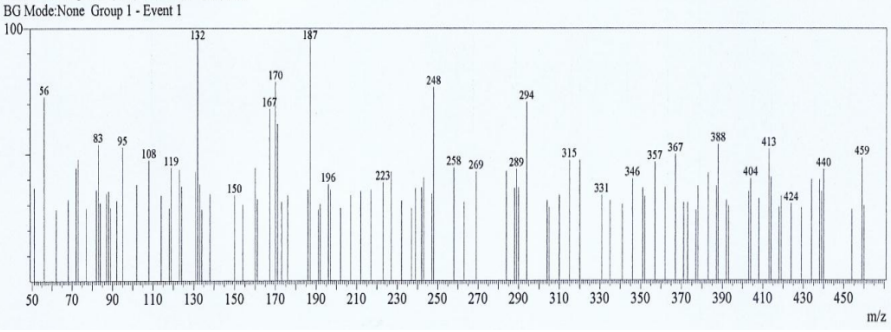
C:\GCMSsolution\Data\Project1\M7.QGD

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



Spectrum

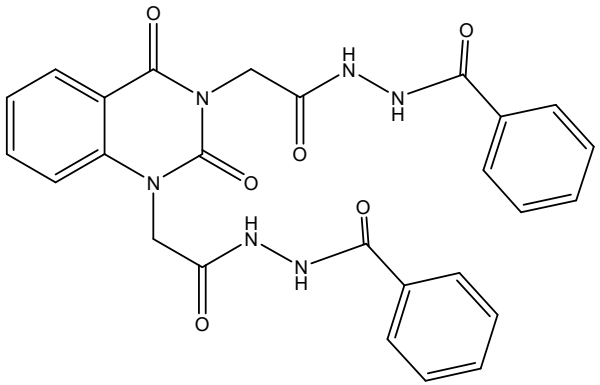
Line#:1 R.Time:6.4(Scan#:765)
MassPeaks 102
RawMode:Single 6.4(765) BasePeak:187(369)
BG Mode:None Group 1 - Event 1



MS of compound (6b)

-

Compound (6c)



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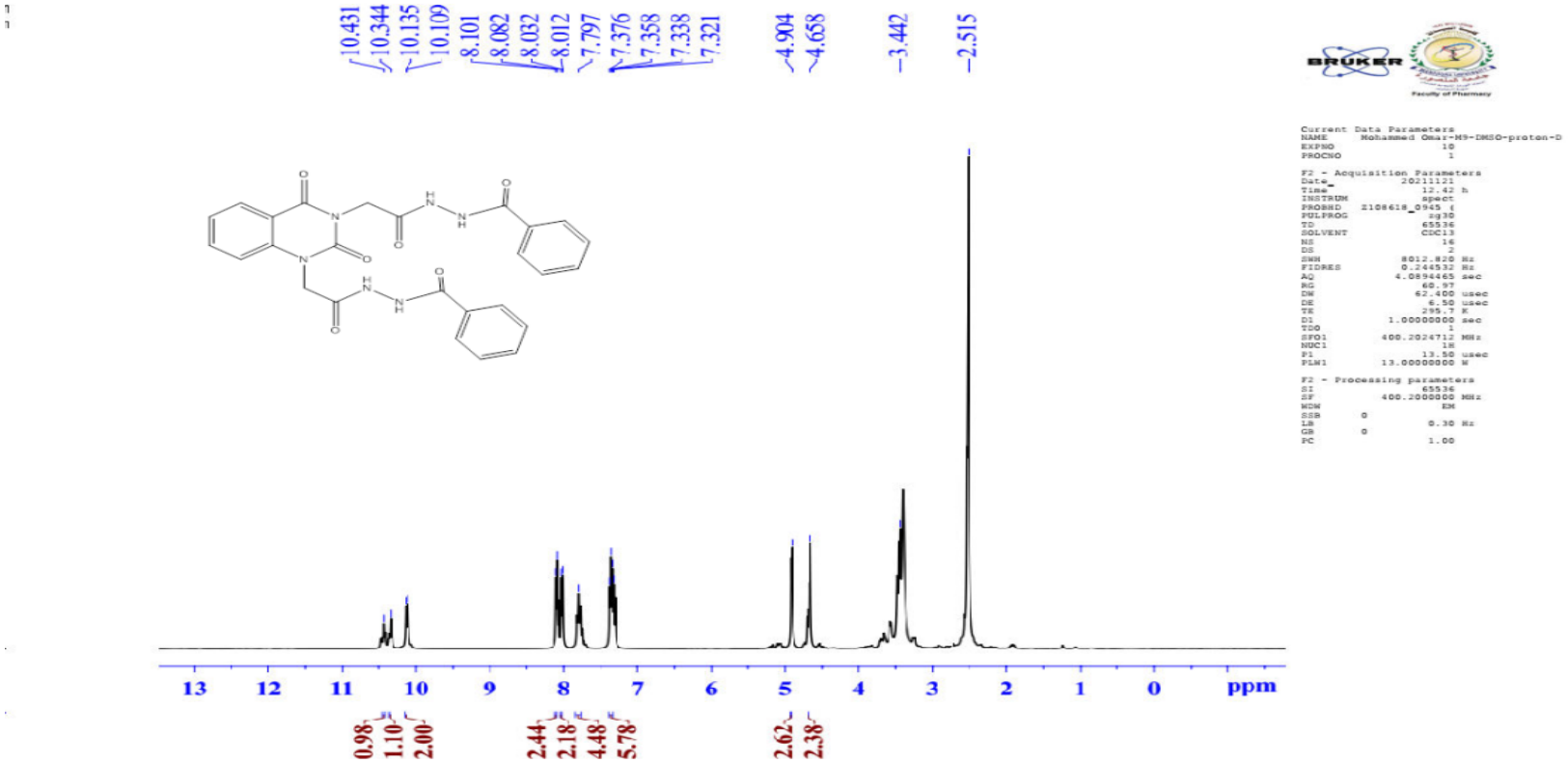
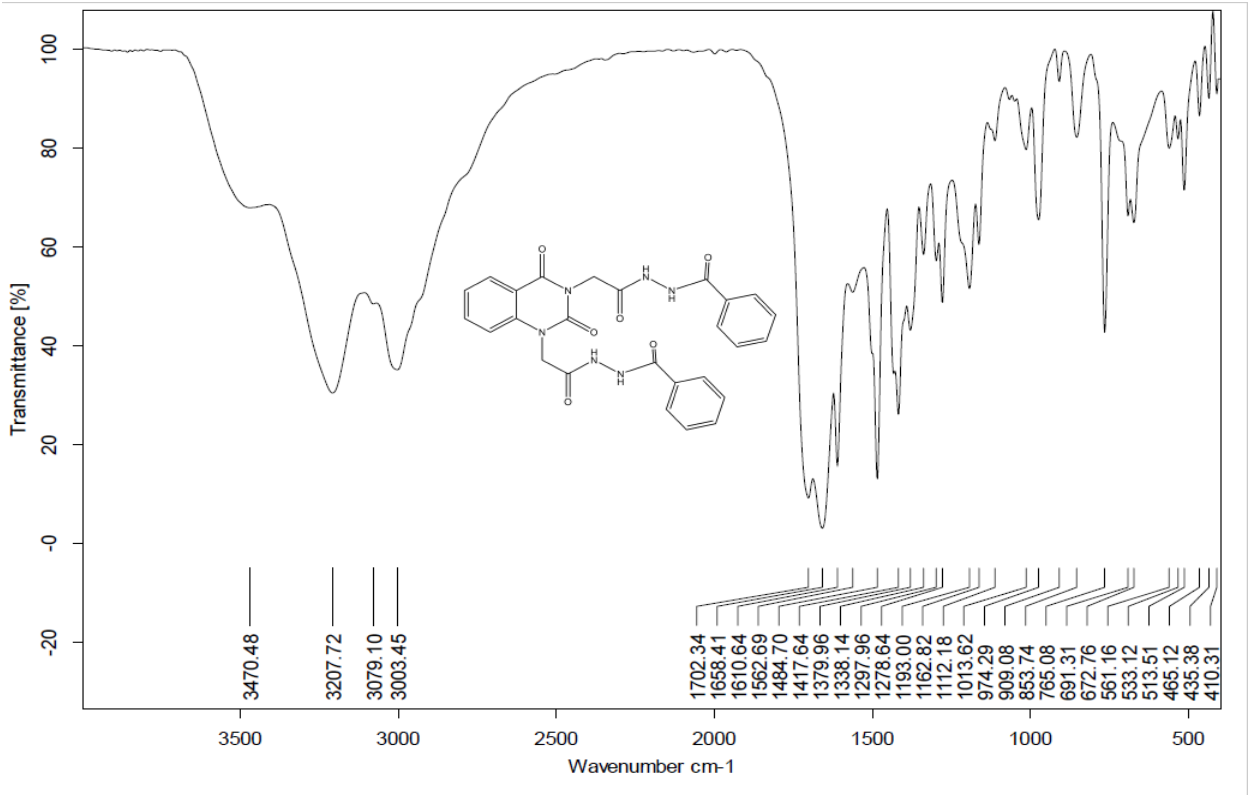


^{1}H-NMR of compound (6c)

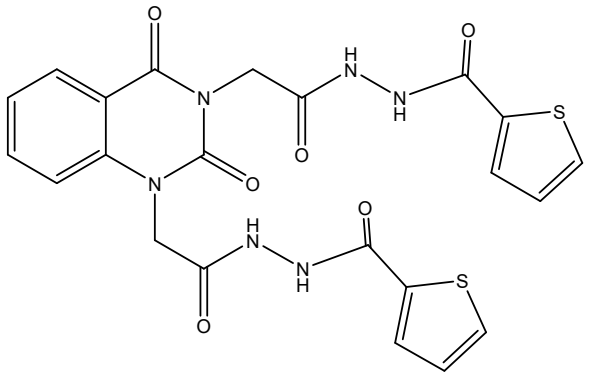
-

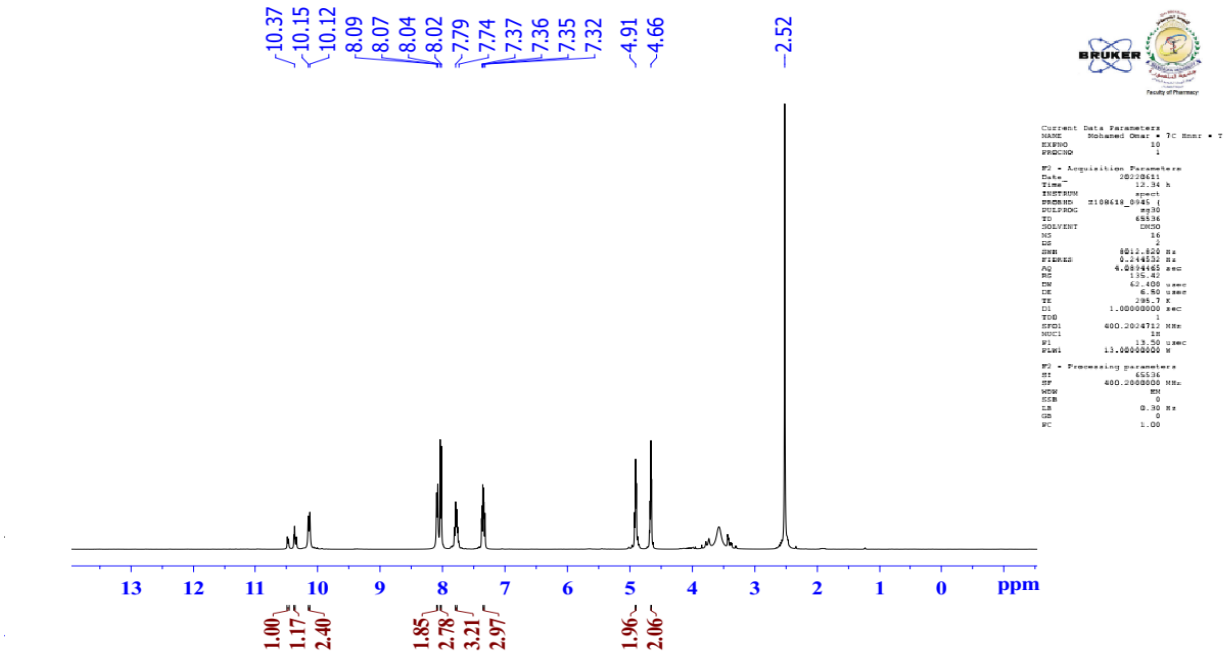


FT-IR of compound (6c)

-

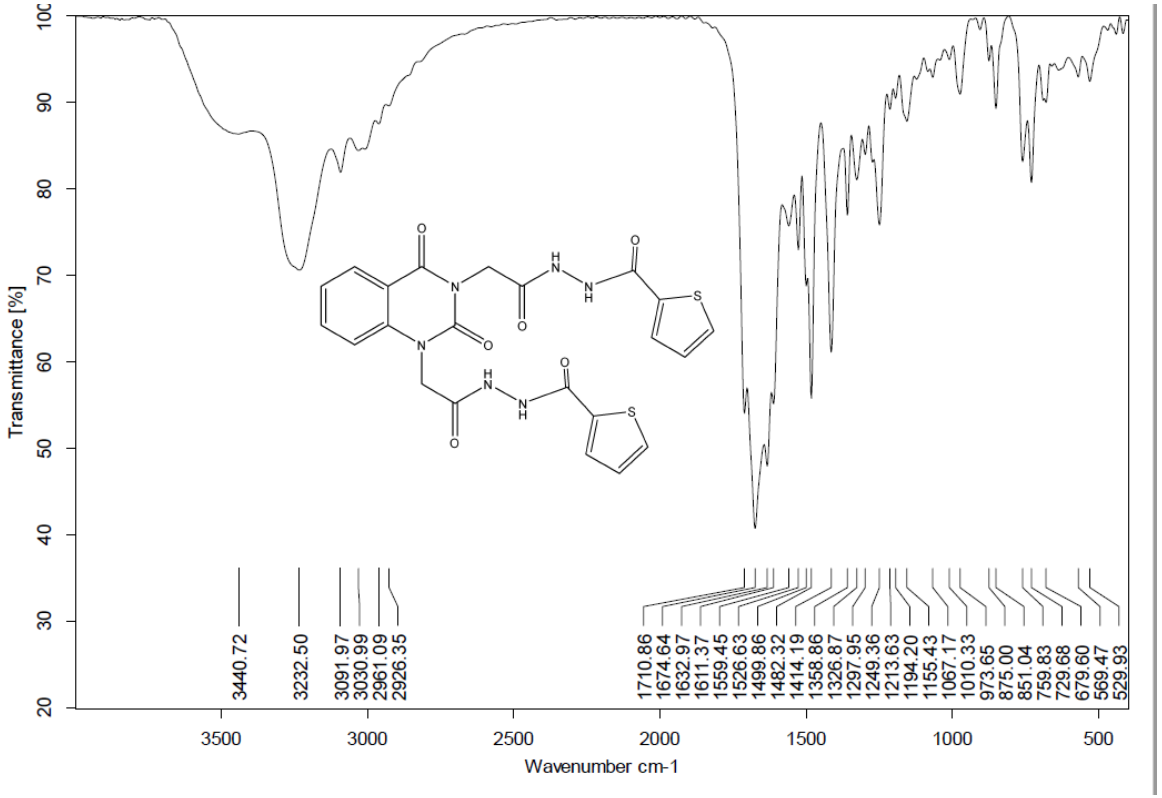
Compound (6d)





[1]H-NMR of compound (6d)

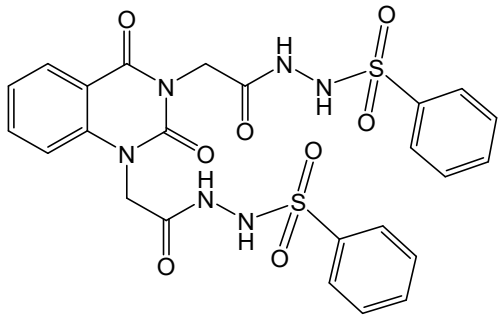
-



FT-IR of compound (6d)

-

Compound (6e)



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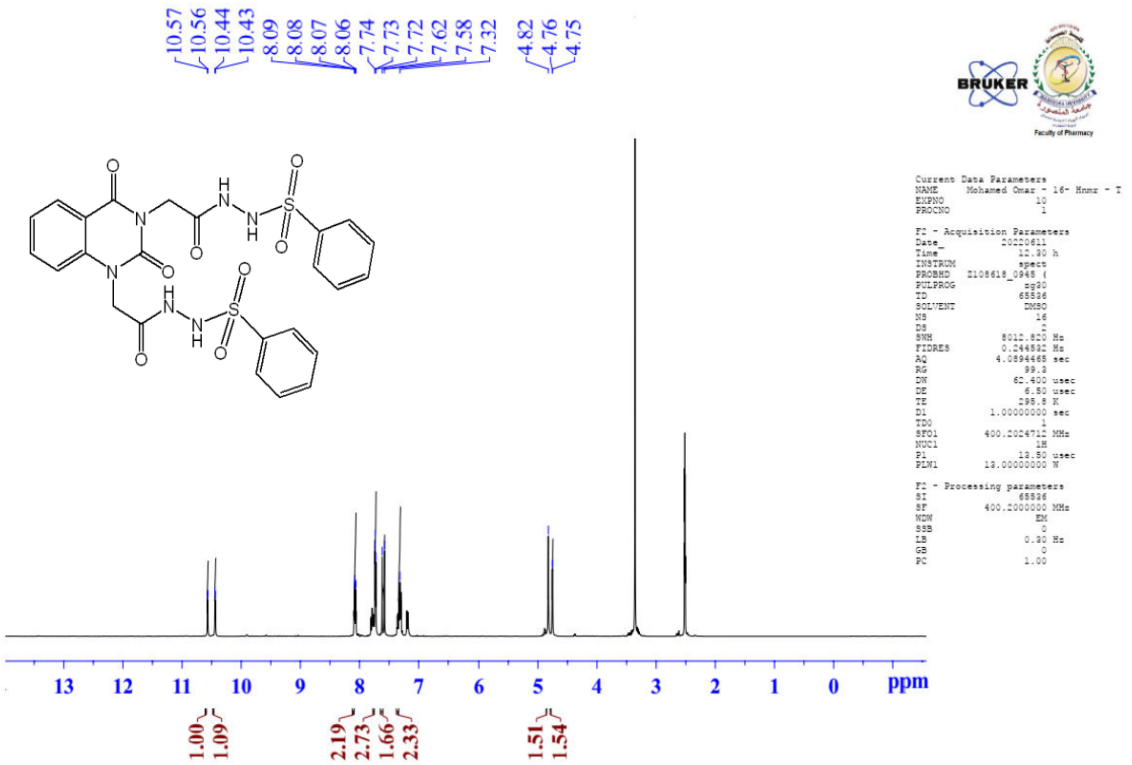
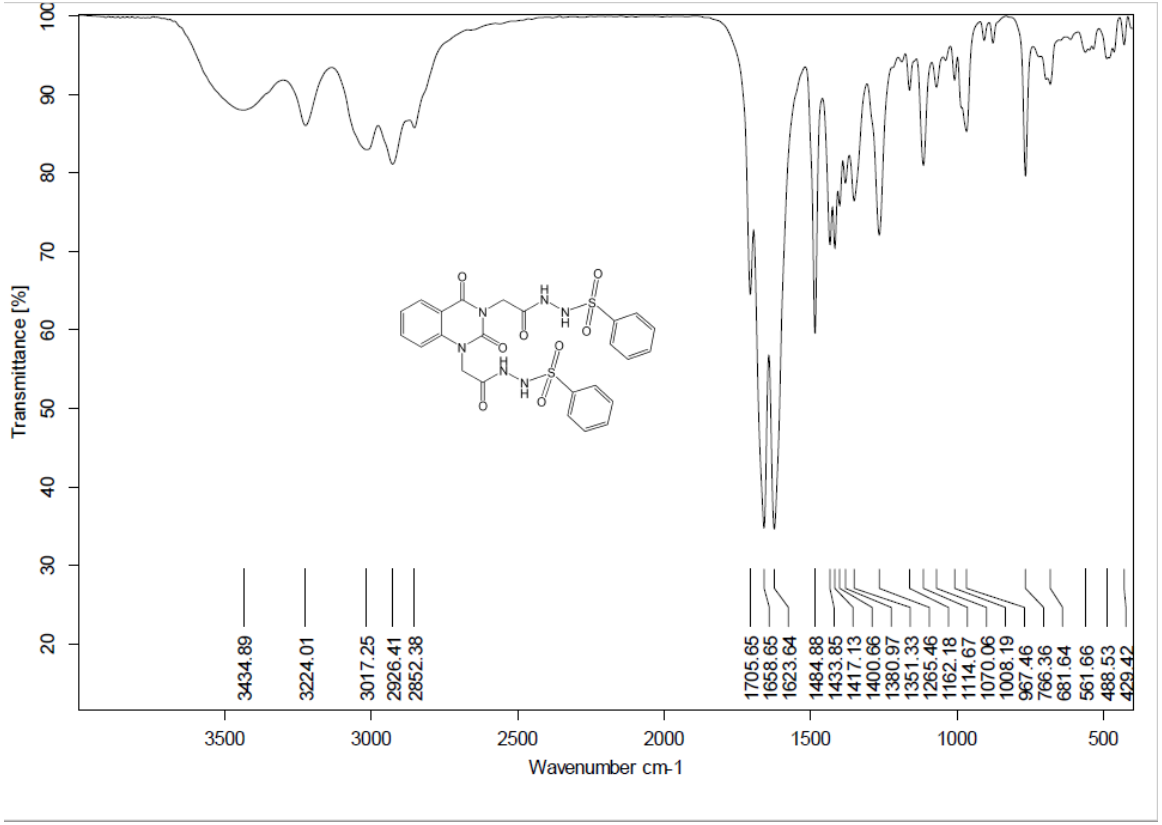


[1]H-NMR of compound (6e)

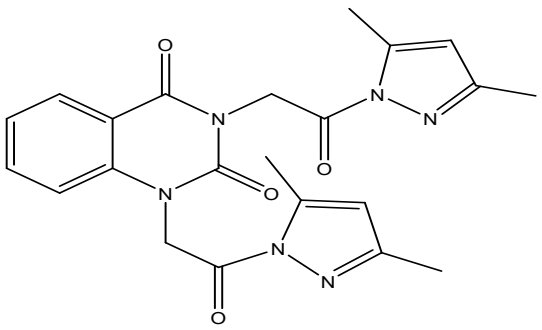
-



FT-IR of compound (6e)

-

Compound (7a)



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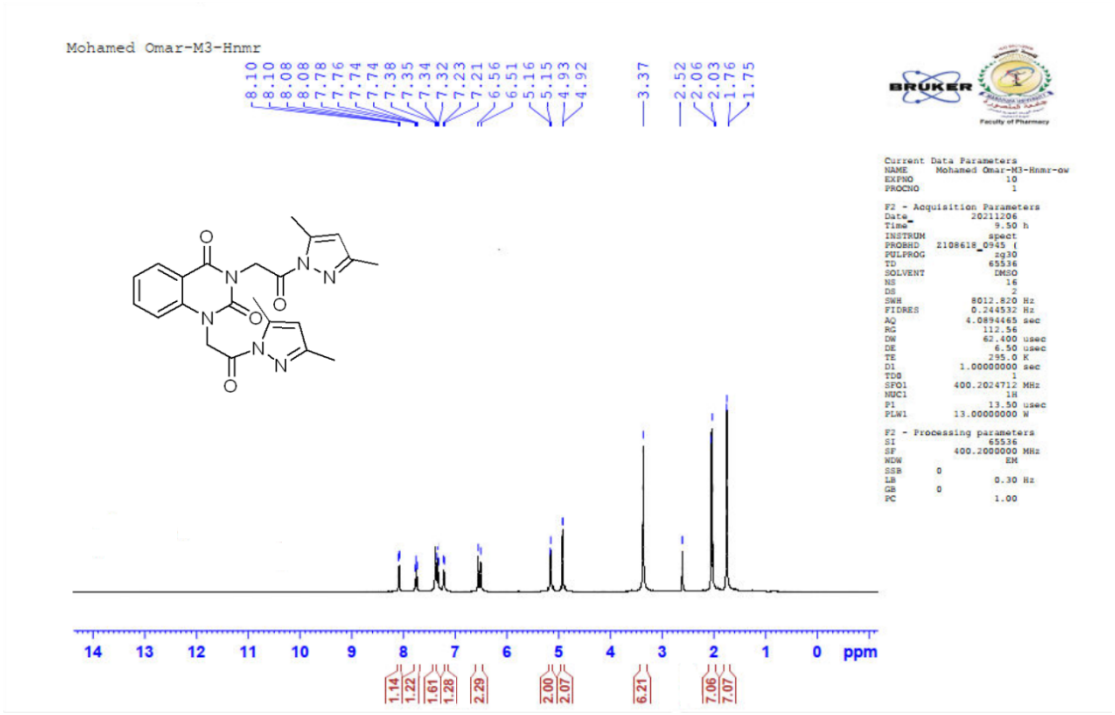
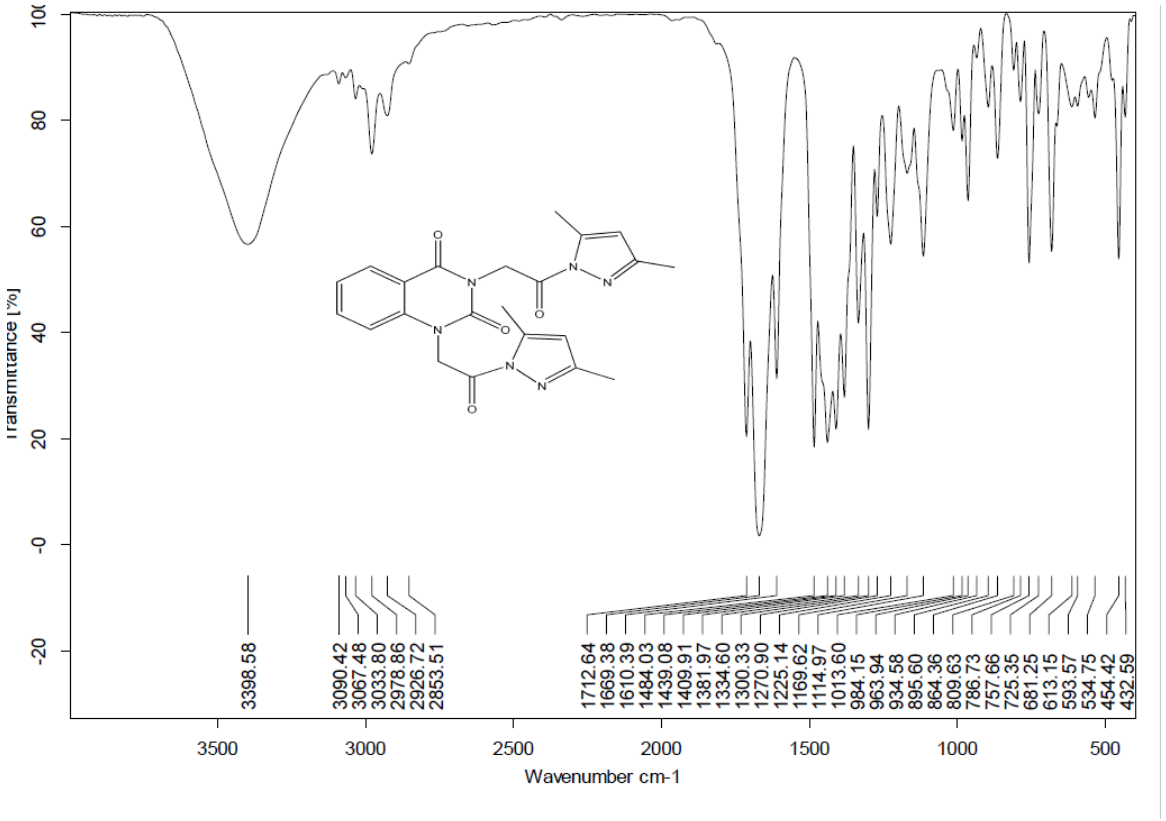


^{1}H-NMR of compound (7a)

-



FT-IR of compound (7a)

15-Jan-07 02:21:16

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

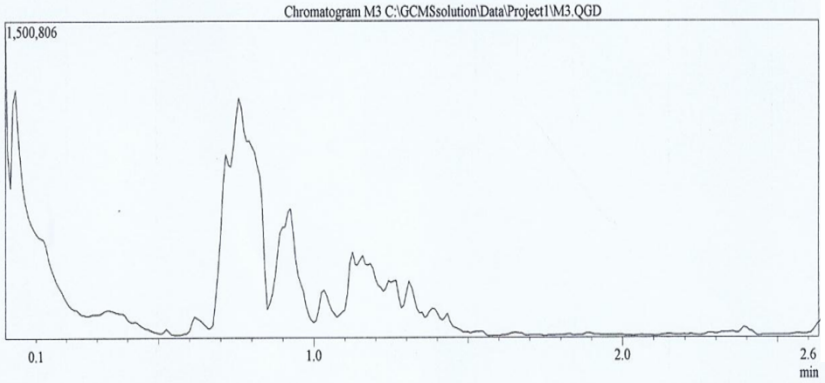
Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 02:12:13 ص
Sample Name	: M3
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M3.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M3.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature 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 02:14:54 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	:1250
Start m/z	:50.00
End m/z	:600.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

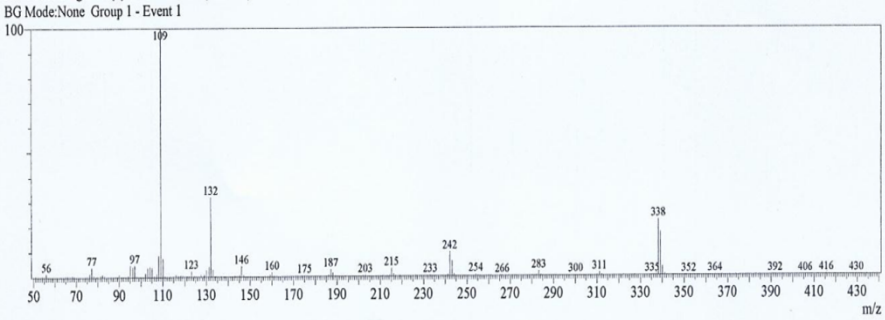
C:\GCMSsolution\Data\Project1\M3.QGD

Chromatogram M3 C:\GCMSsolution\Data\Project1\M3.QGD



Spectrum

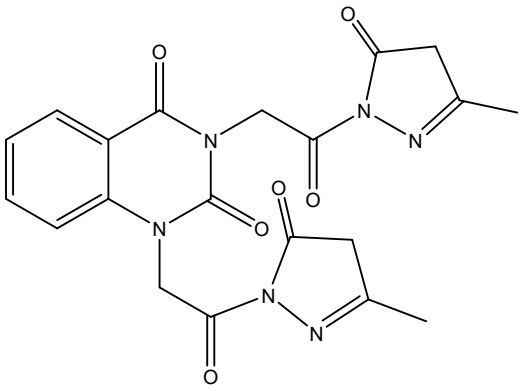
Line#:1 R.Time:0.0(Scan#:5)
MassPeaks:290
RawMode:Single 0.0(5) BasePeak:109(371418)
BG Mode:None Group 1 - Event 1



MS of compound (7a)

-

Compound (7b)



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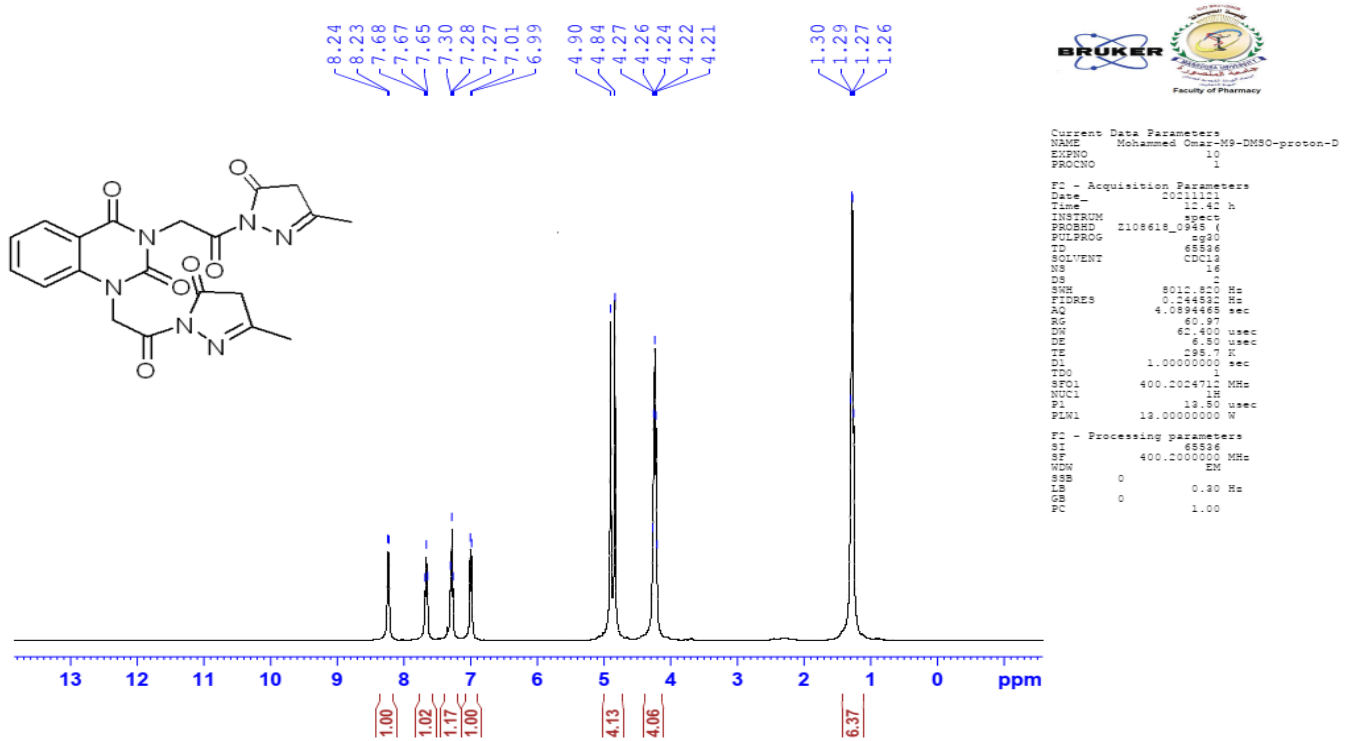

Current Data Parameters
NAME Mohammed Omar-M9-DMSO-proton-D
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211121
Time 12.41 h
INSTRUM spect
PROBHD Z108618_0945 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244831 Hz
AQ 4.0894465 sec
RG 60.97
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2024712 MHz
NUC1 1H
P1 12.50 usec
PLW1 19.00000000 W

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

^{1}H-NMR of compound (7b)

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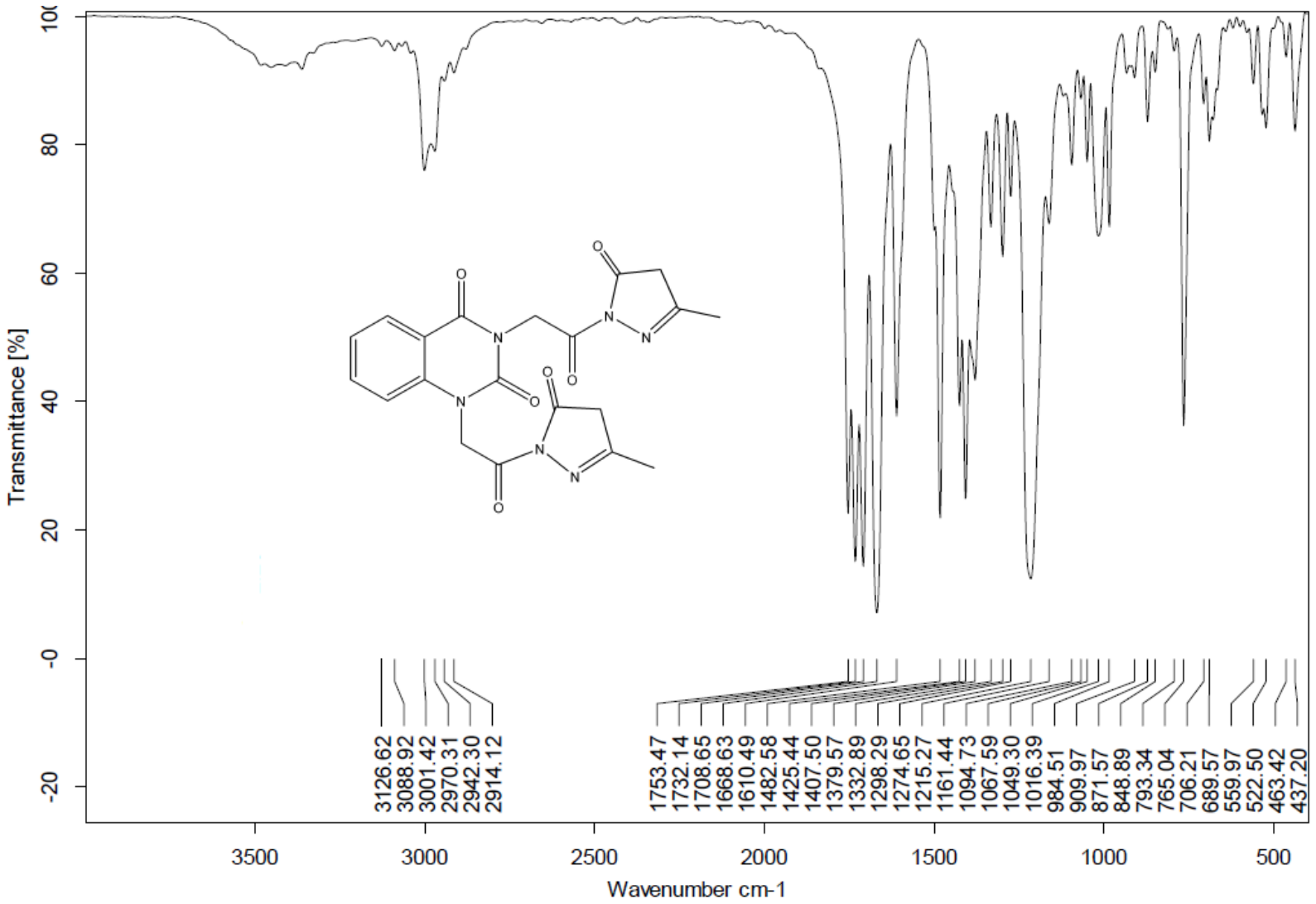


FT-IR of compound (7b)

15-Jan-07 03:57:28

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	: Dr. Mai Younis
Analyzed	: 15/01/2007 03:26:47 ص
Sample Name	: M9.
Sample ID	:
Customer Name	: Dr. Mohamed Omar - Science - Quena
Data File	: C:\GCMSsolution\Data\Project1\M9..QGD
Org Data File	: C:\GCMSsolution\Data\Project1\M9..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 03:36:46 ص

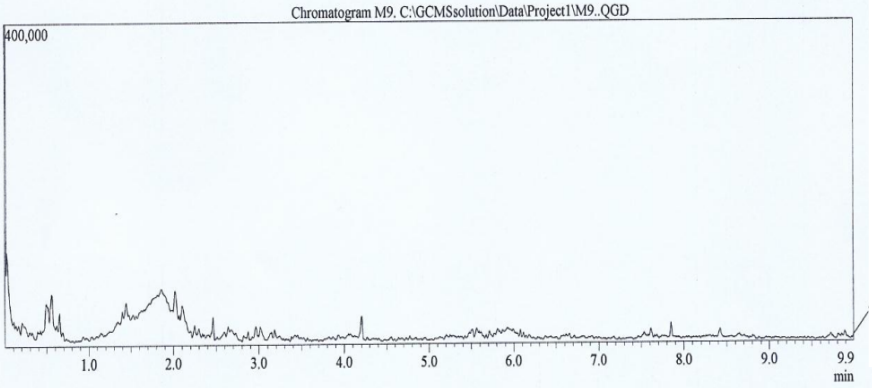
Method

====== 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

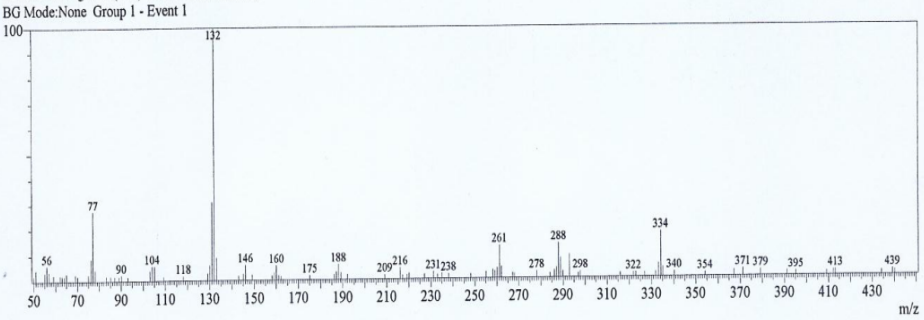
C:\GCMSsolution\Data\Project1\M9..QGD

Chromatogram M9. C:\GCMSsolution\Data\Project1\M9..QGD



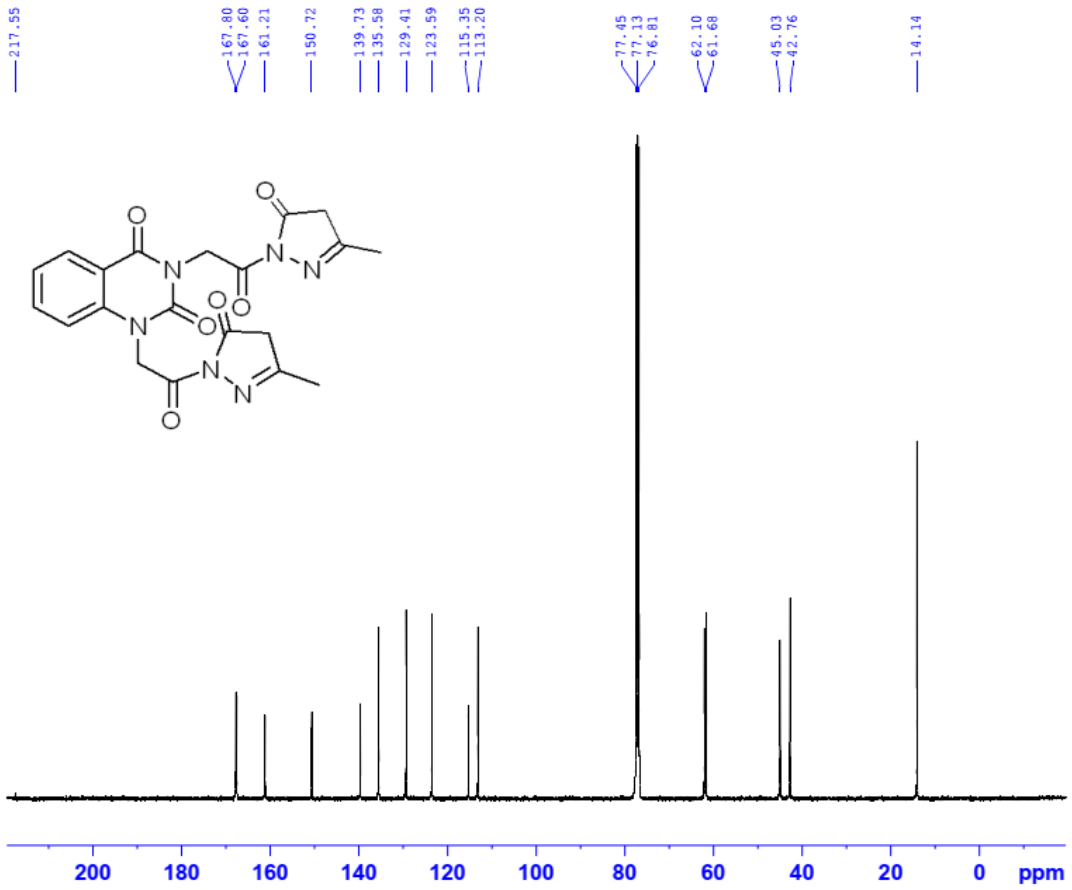
Spectrum

Line#:1 R.Time:1.5(Scan#:178)
MassPeaks:97
RawMode:Single 1.5(178) BasePeak:132(6903)
BG Mode:None Group 1 - Event 1



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
TD                65536
SOLVENT           CDCl3
NS                 2100
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                197.77
DW                20.800 usec
DE                 6.50 usec
TE                295.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6404331 MHz
NUC1               13C
P1               10.00 usec
PLW1        47.00000000 W
SFO2        400.2016008 MHz
NUC2               1H
CPDPRG[2         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
```

C13-NMR of compound (7b)

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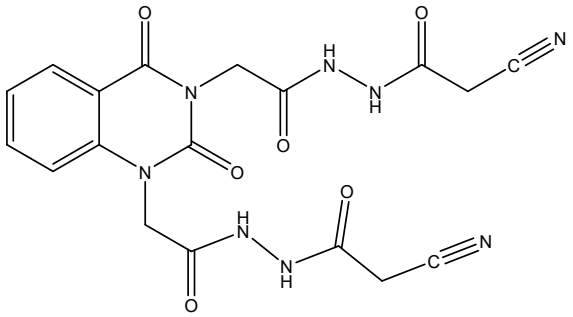
Compound (8)



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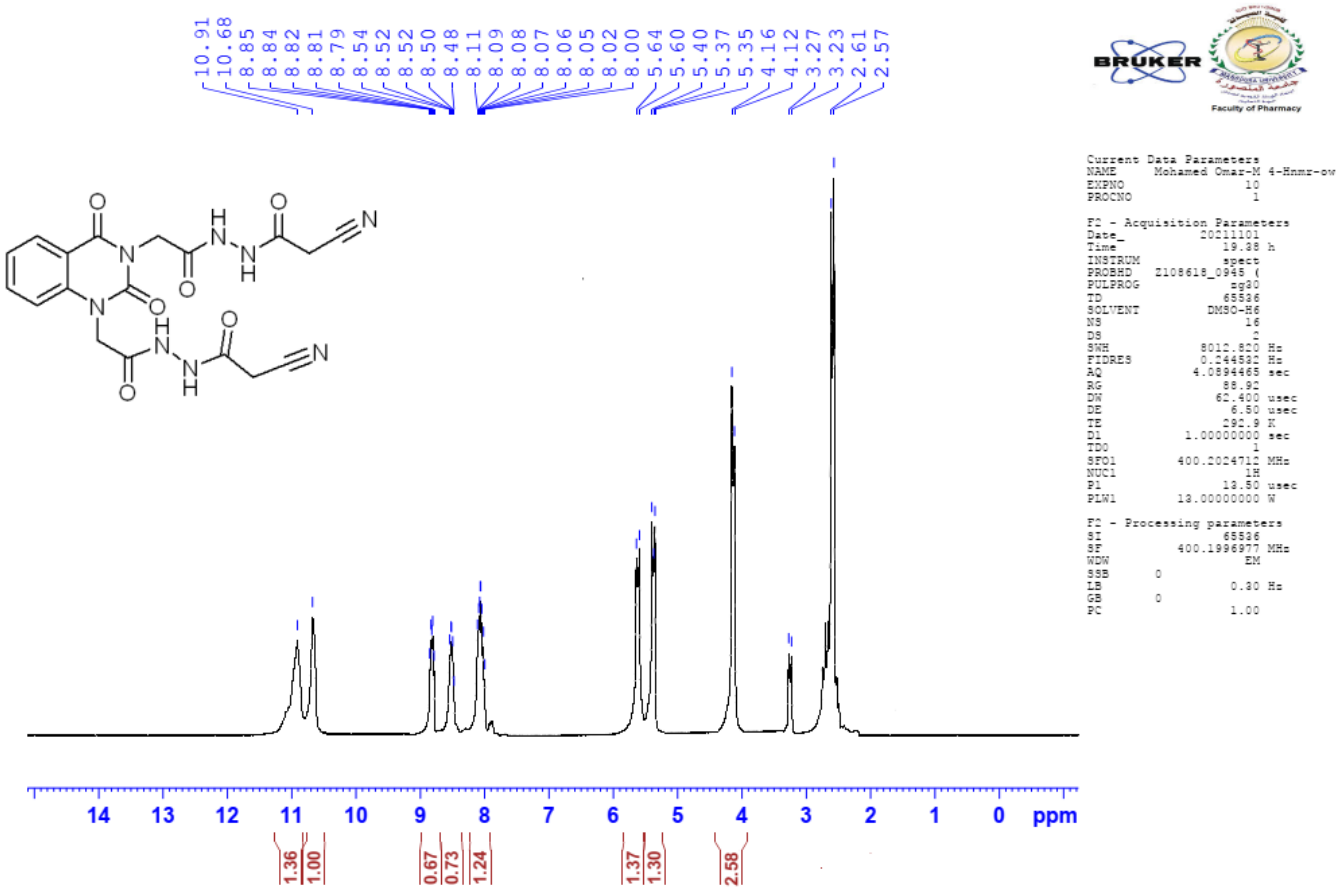


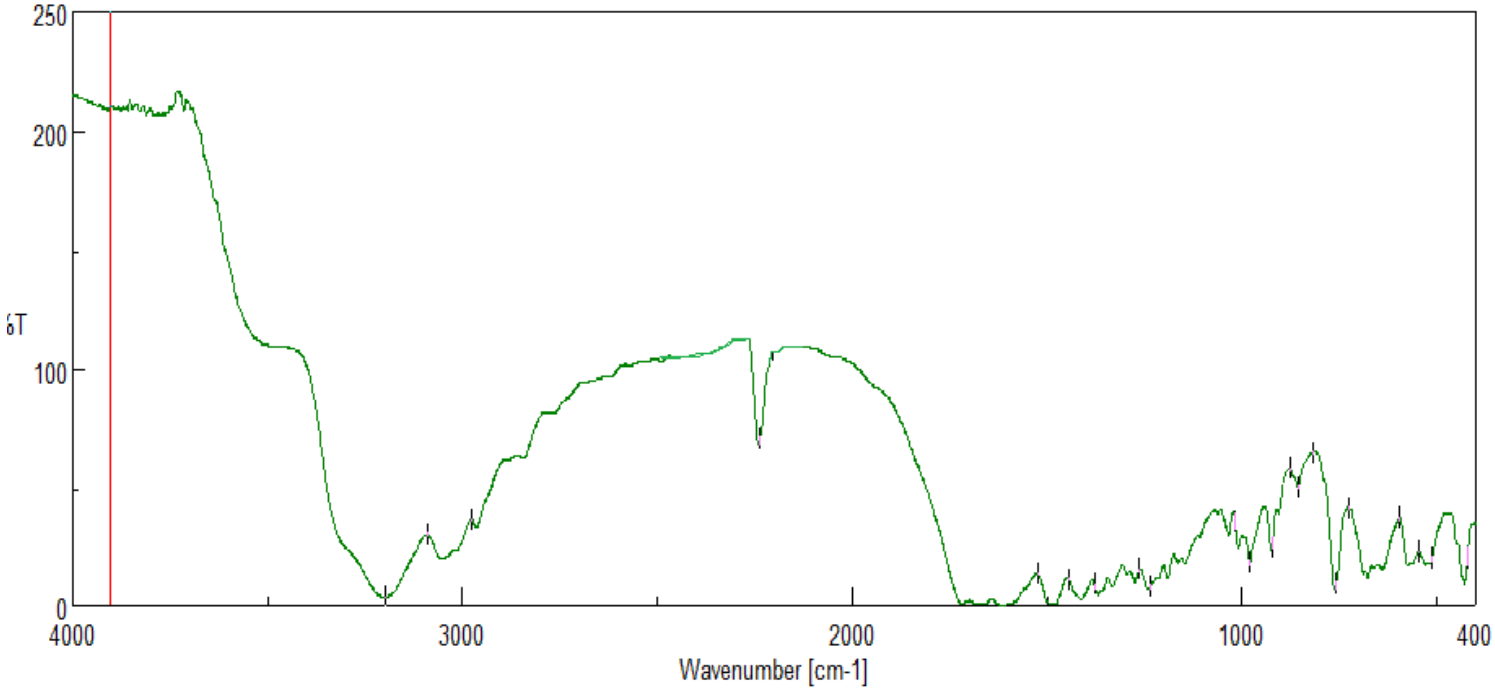

```
Current Data Parameters
NAME      Mohamed Omar-M 4-Hnmr-ow
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211101
Time              19.38 h
INSTRUM             spect
PROBHD   Z108618_0945 (
PULPROG             zg30
TD                 65536
SOLVENT          DMSO-H6
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                 88.92
DW                62.400 usec
DE                 6.50 usec
TE                292.9 K
D1             1.00000000 sec
TD0                    1
SFO1         400.2024712 MHz
NUC1                  1H
P1                 13.50 usec
PLW1         13.00000000 W

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

^{1}H-NMR of compound (8)

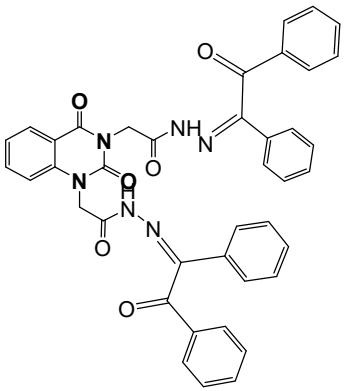
-



FT-IR of compound (8)

-

Compound (9a)



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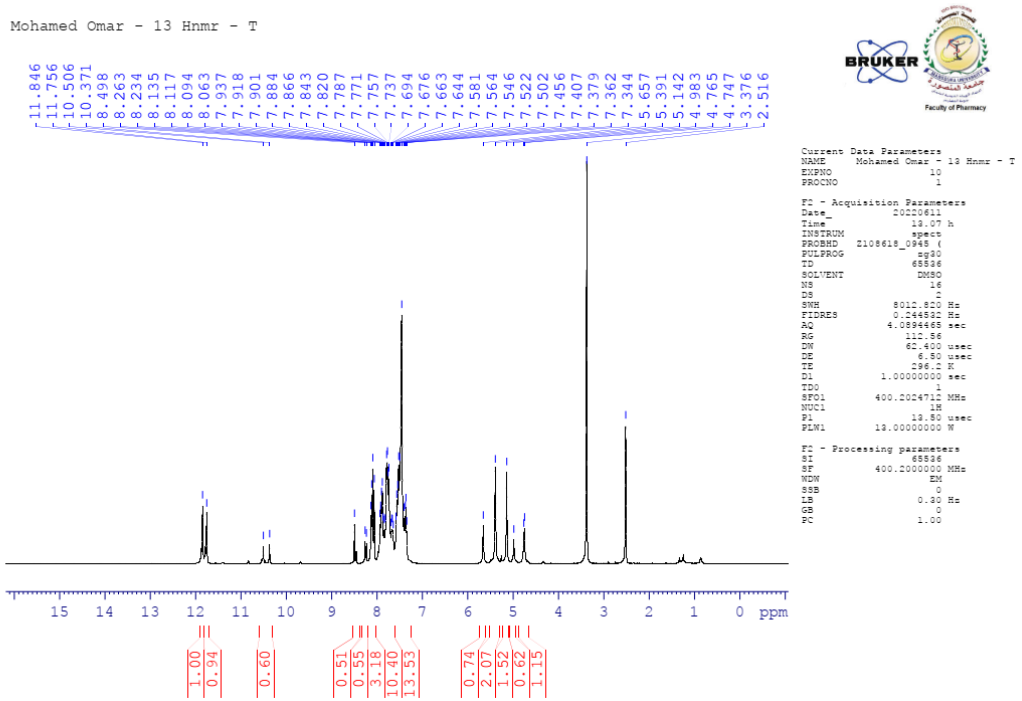
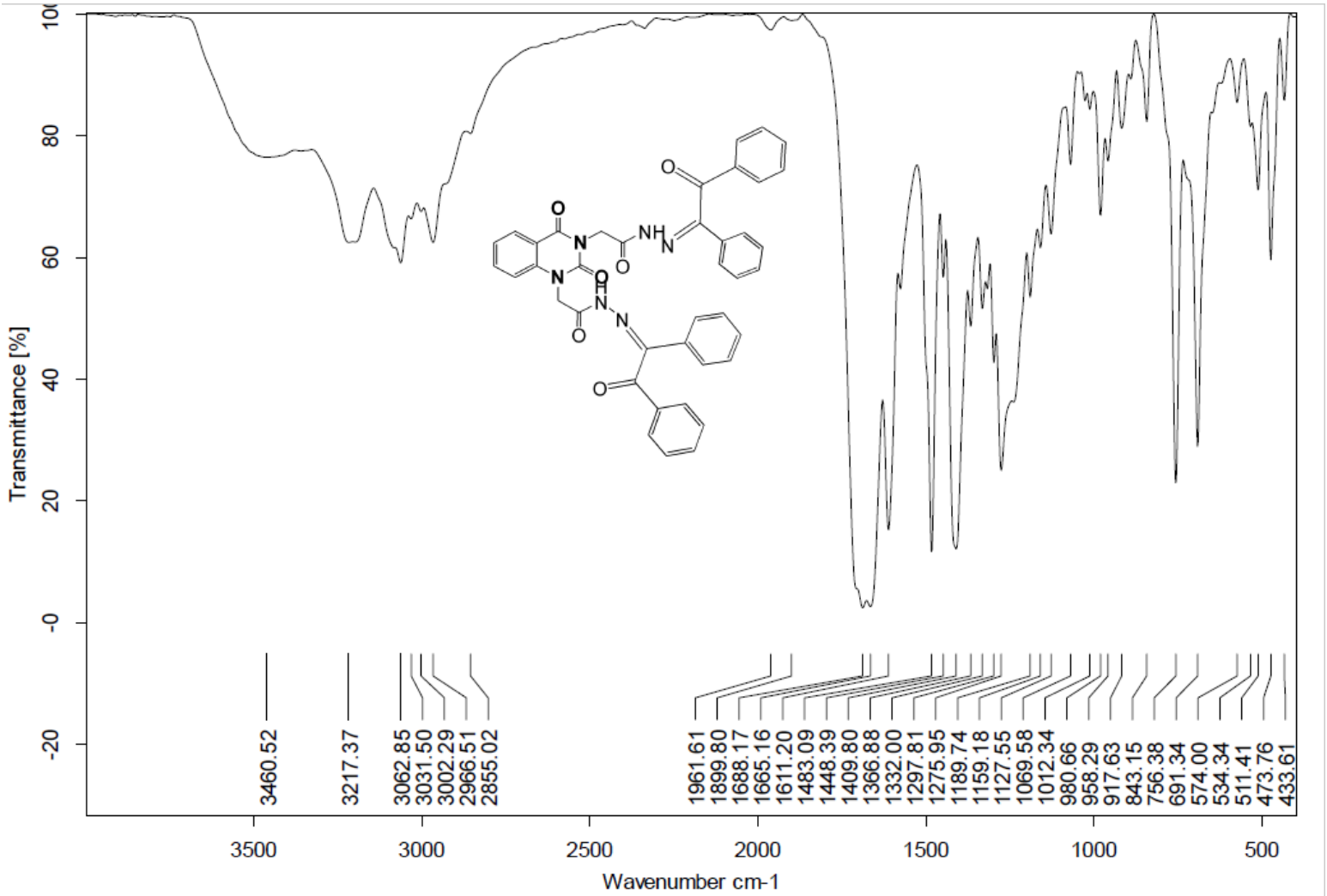


^{1}H-NMR of compound (9a)

-



FT-IR of compound (9a)