

Rigid 3D-Sprio Chromanone as a Crux for Efficient Antimicrobial Agents: Synthesis, Biological and Computational Evaluation

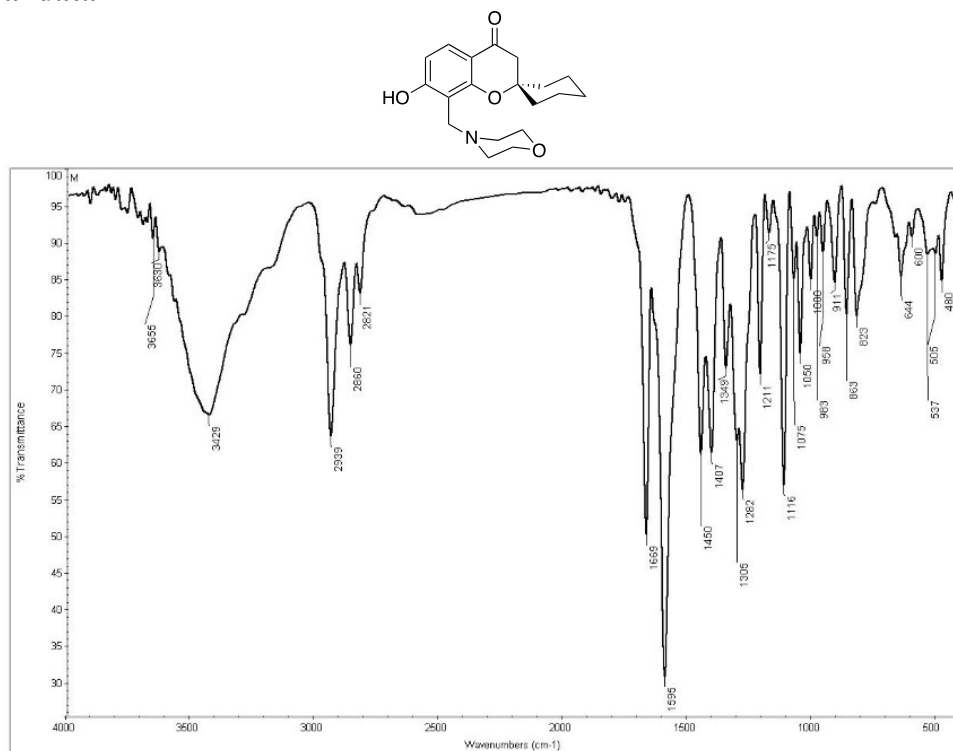
F. H. Elghareeb,^a E. M. Kandil,^a M. Abou-Elzahab,^a M. Abdelmoteleb,^b M. A. Abozeid^{a,*}

^aDepartment of Chemistry, Faculty of Science, Mansoura University, Mansoura-35516, Egypt

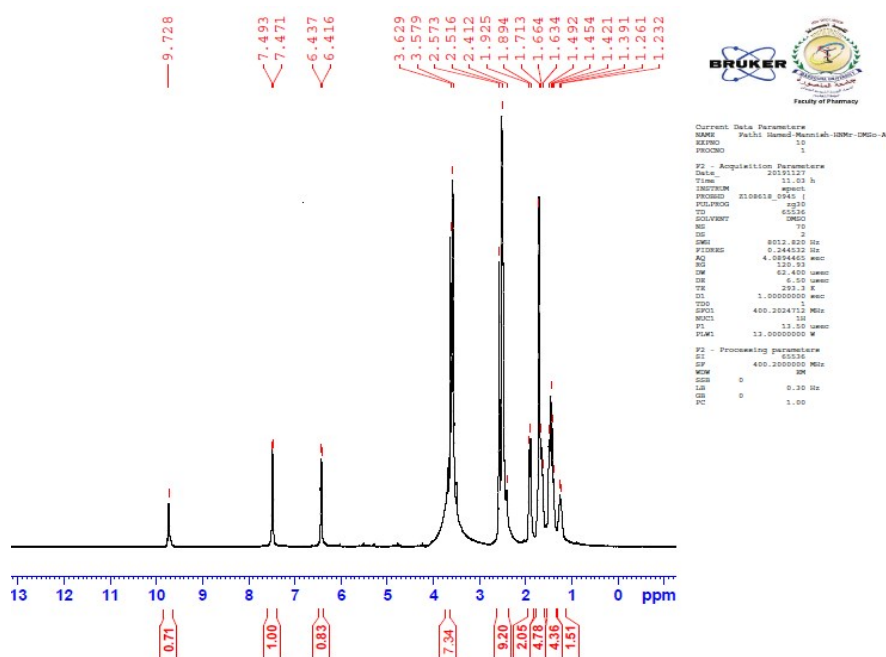
^bDepartment of Botany, Faculty of Science, Mansoura University, Mansoura-35516, Egypt

*Corresponding Author: E-mail: dr.abozeid.chem@gmail.com; mabozeid@mans.edu.eg

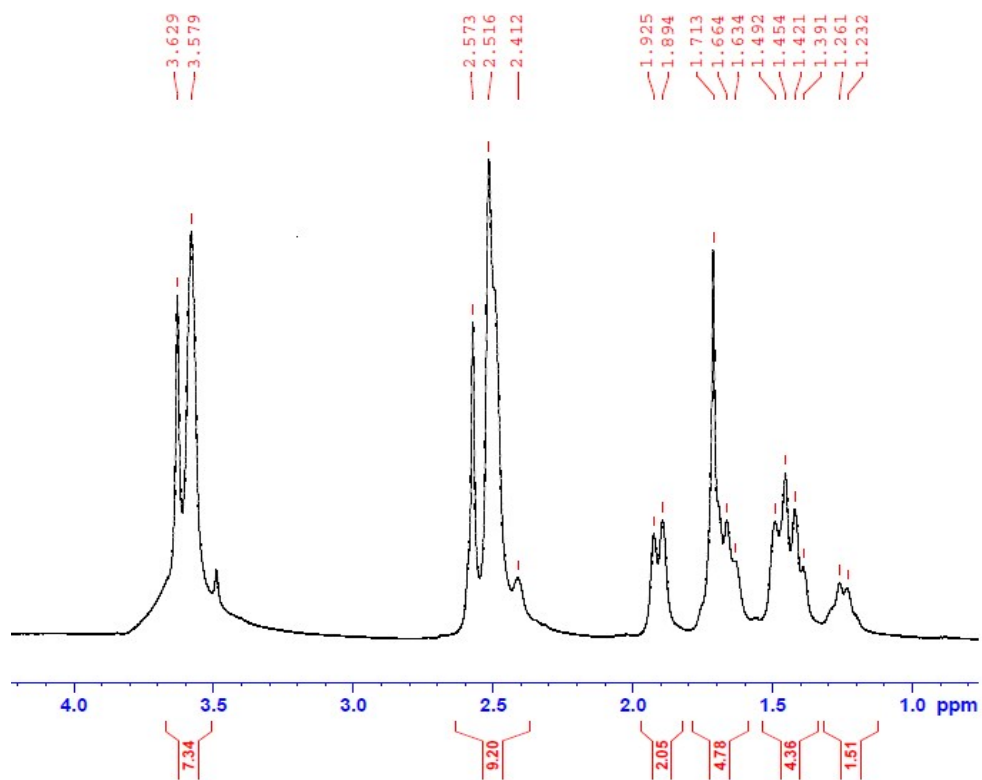
1. Spectral data



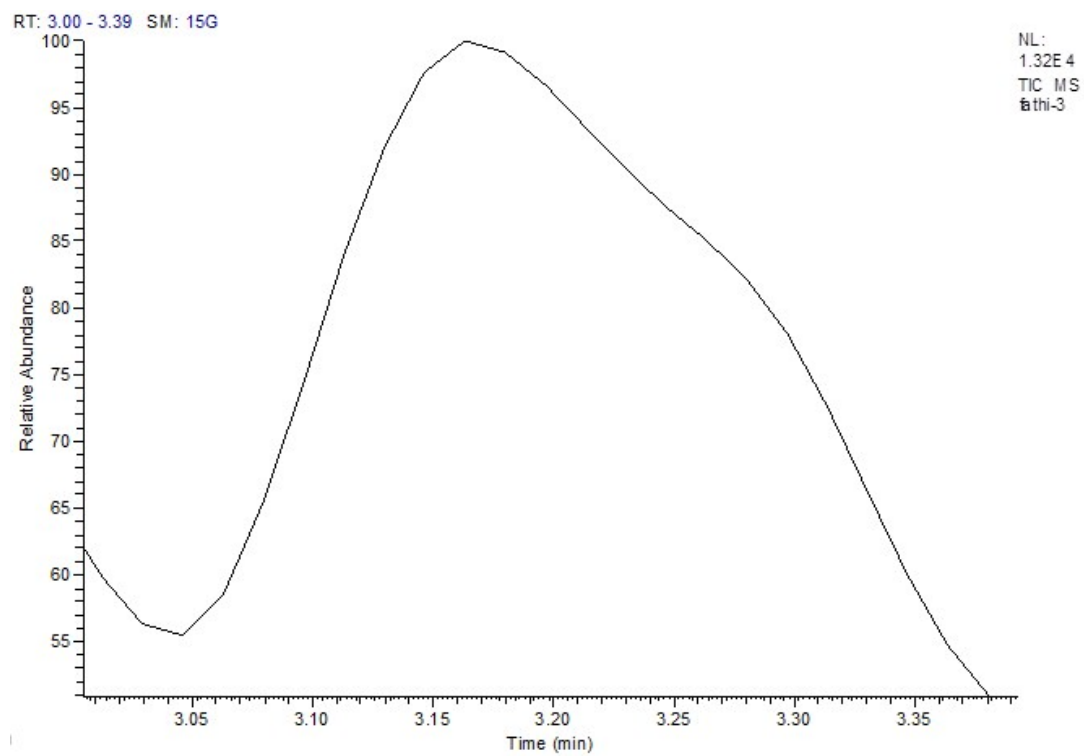
IR spectrum of 2



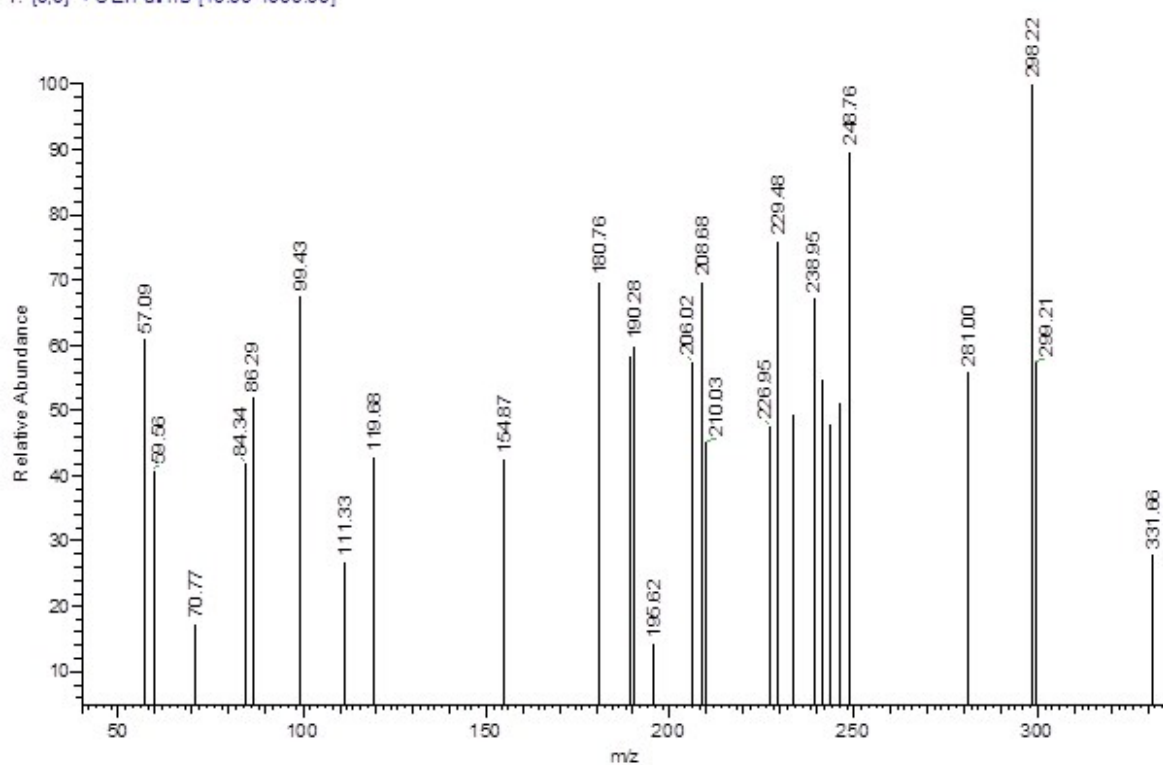
¹H NMR spectrum of 2



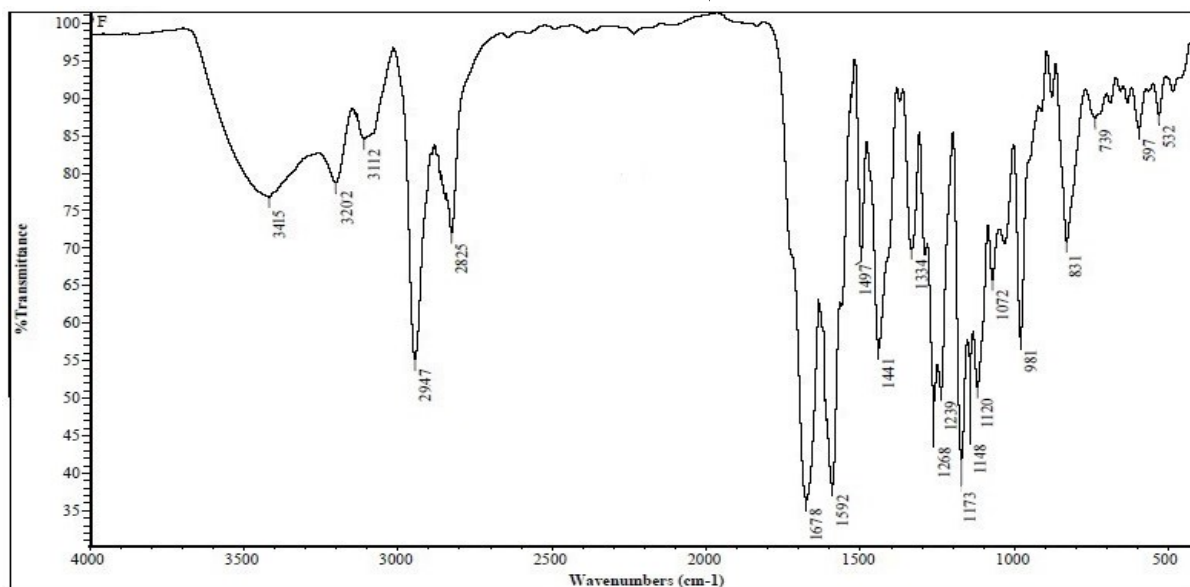
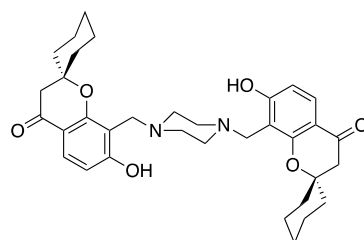
¹H NMR spectrum of 2



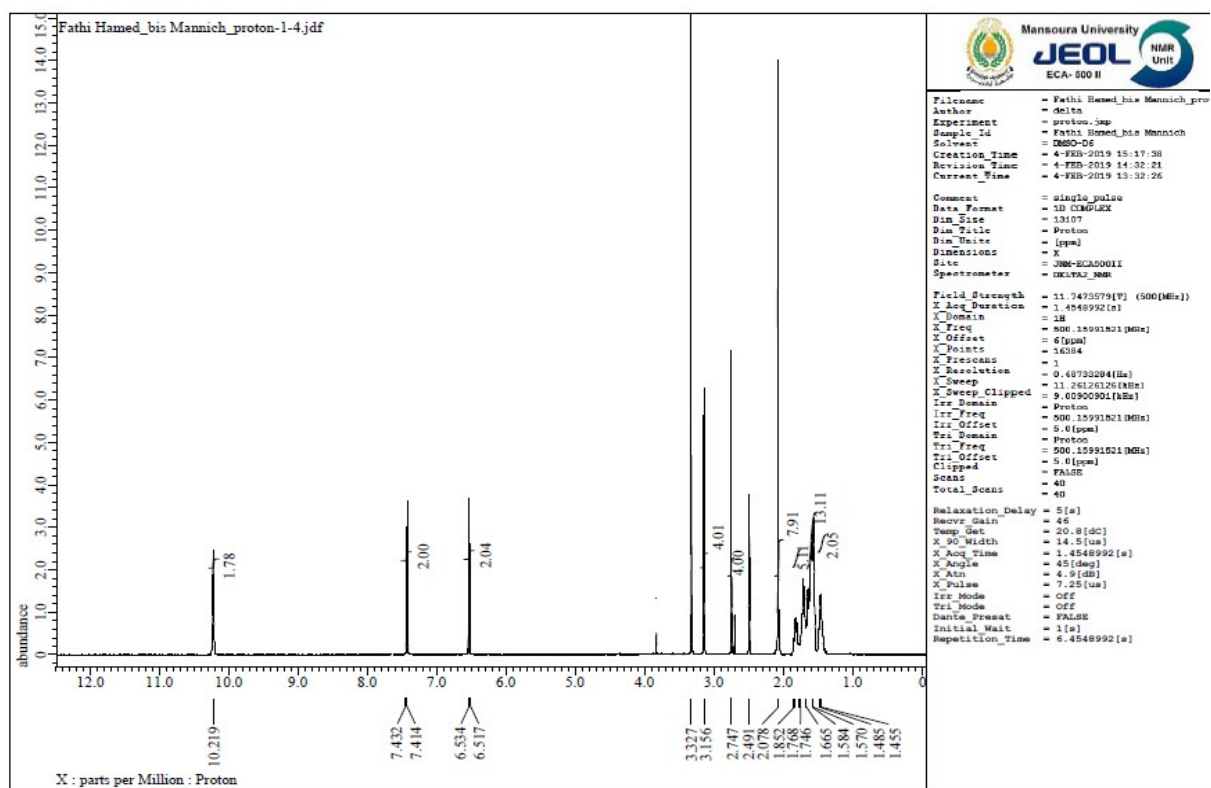
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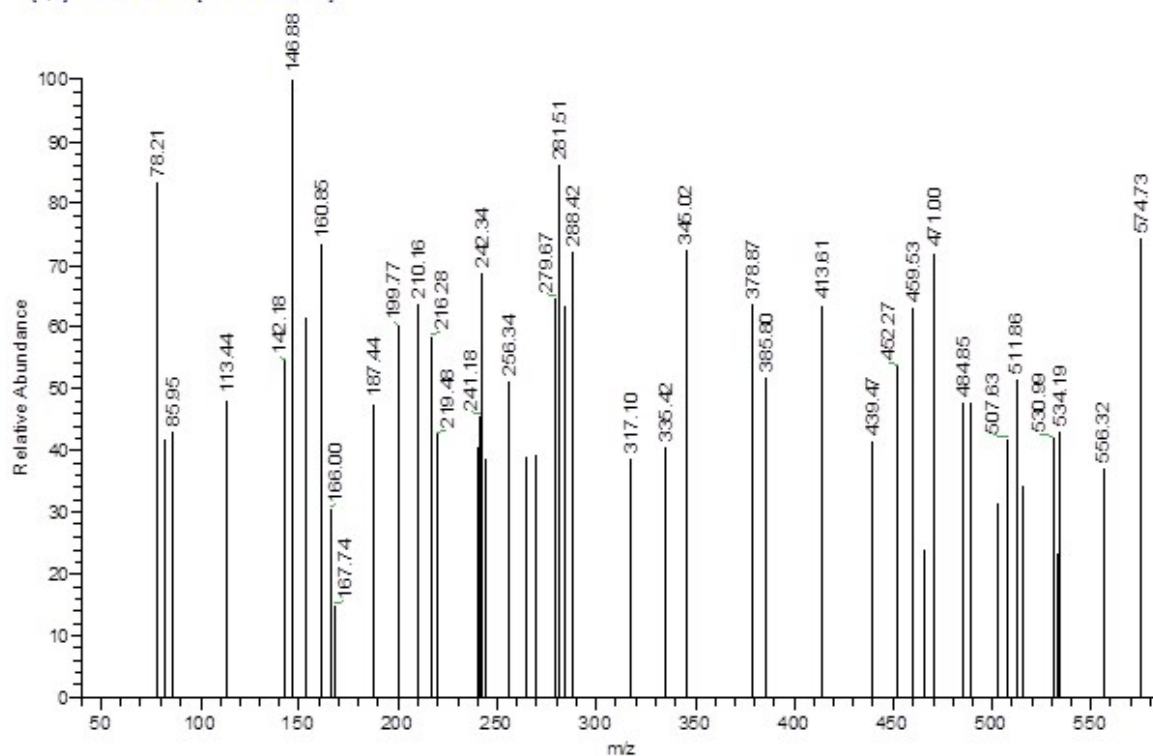
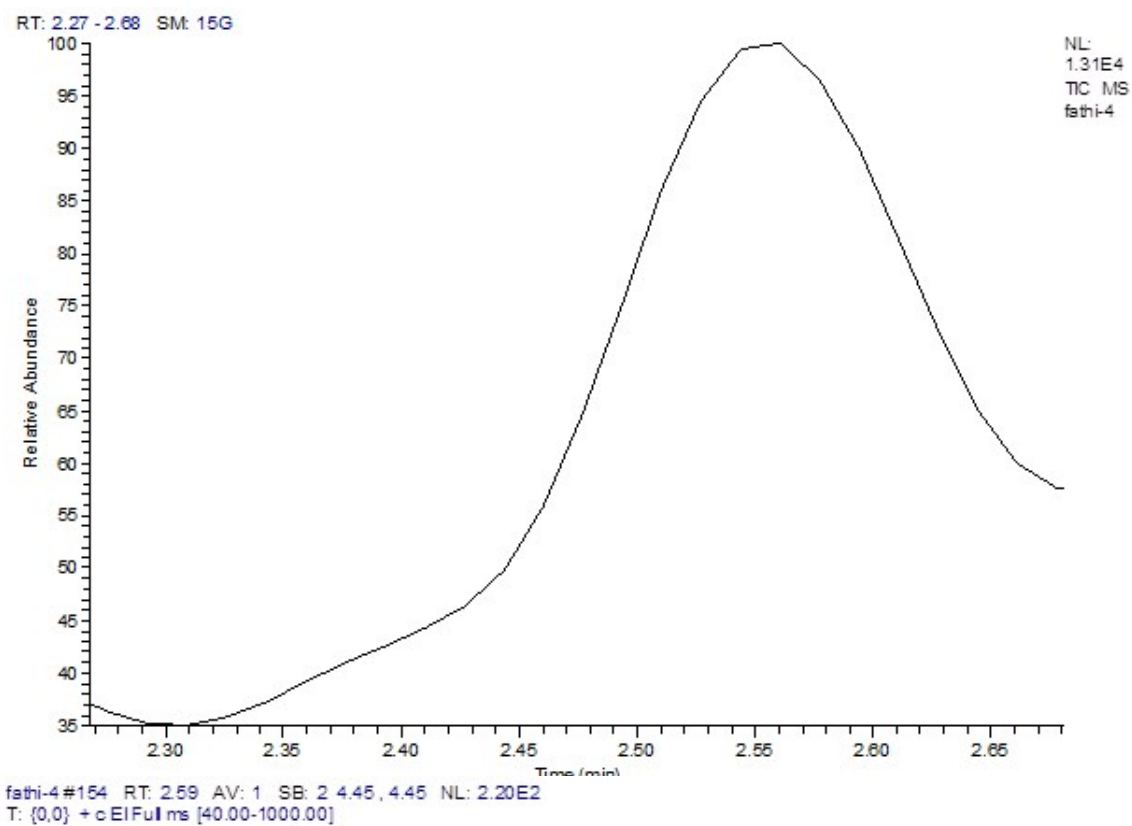
EI-MS spectrum of **2**



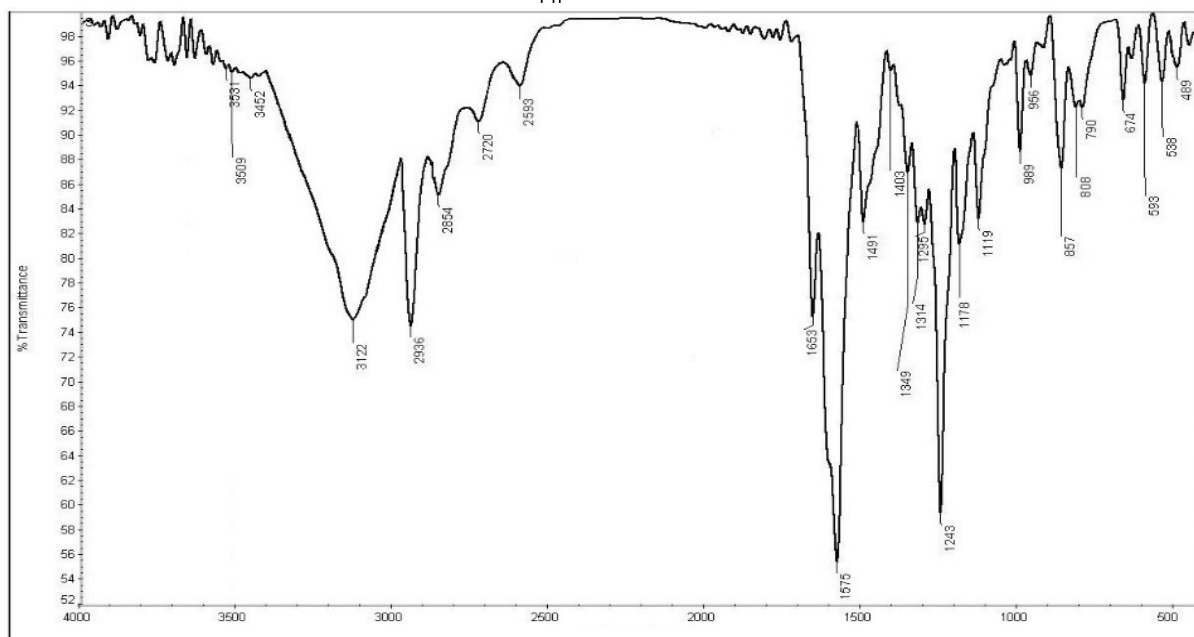
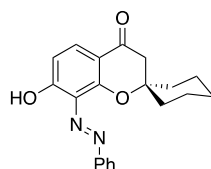
IR spectrum of 3



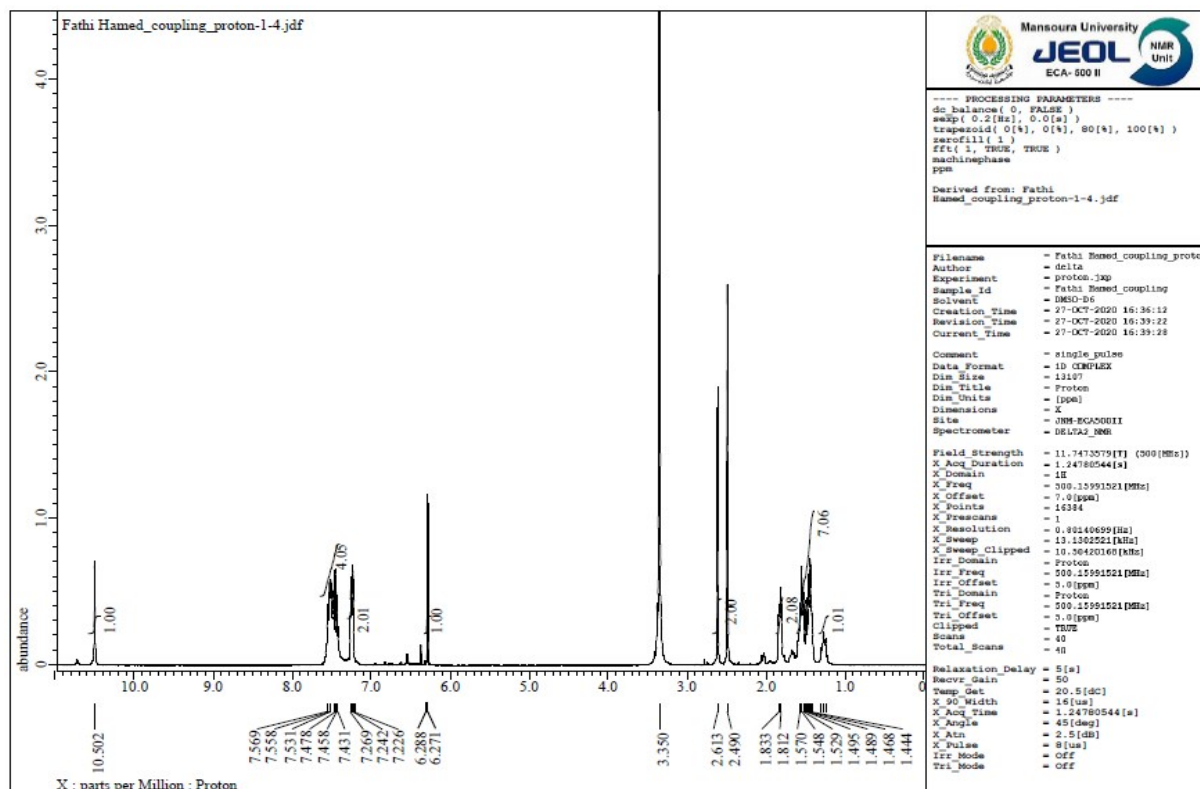
¹H NMR spectrum of 3



EI-MS spectrum of **3**

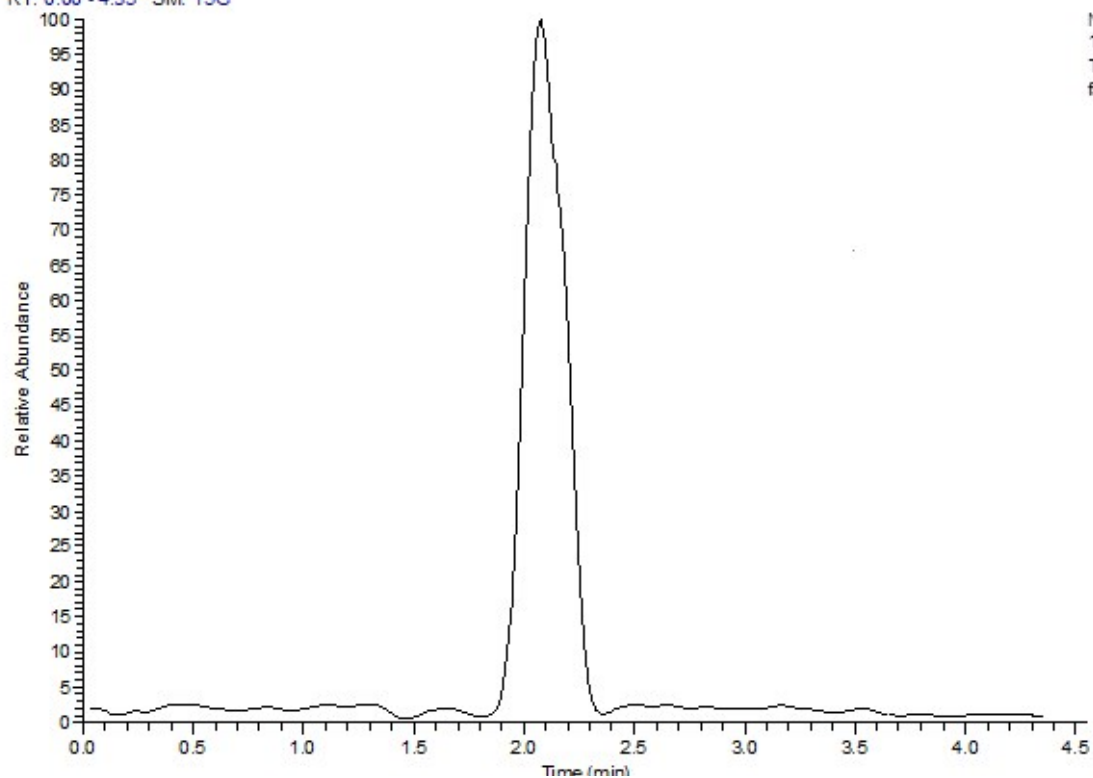


IR spectrum of 4



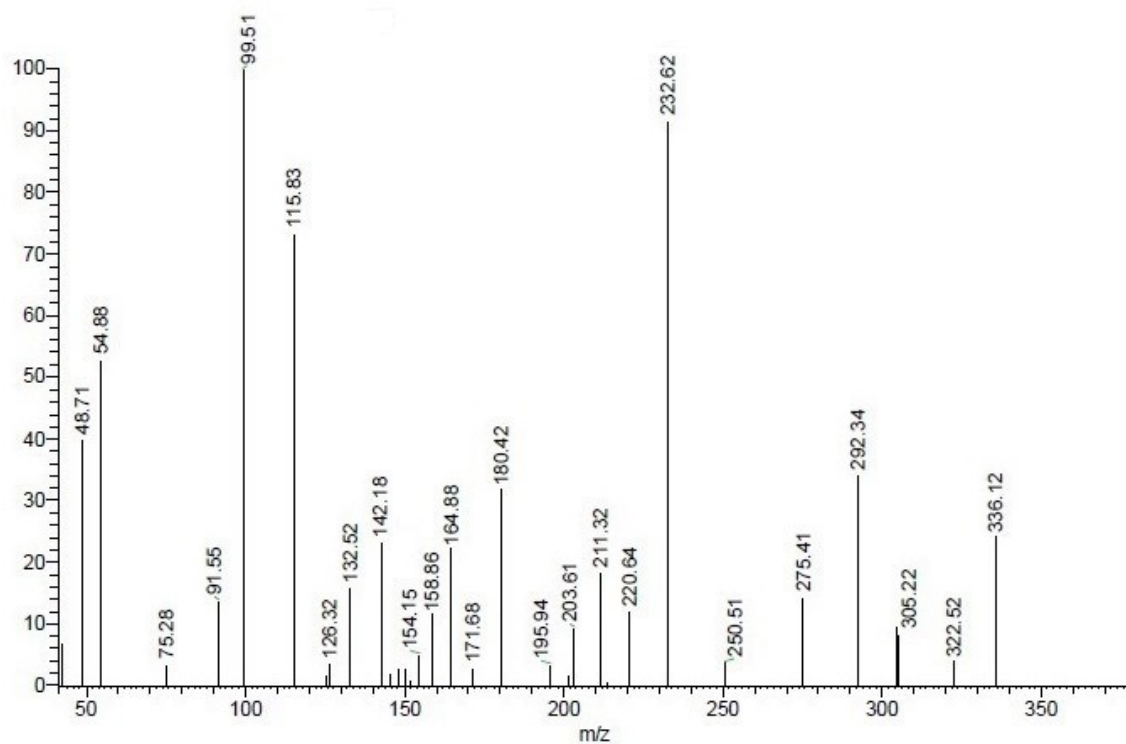
¹H NMR spectrum of 4

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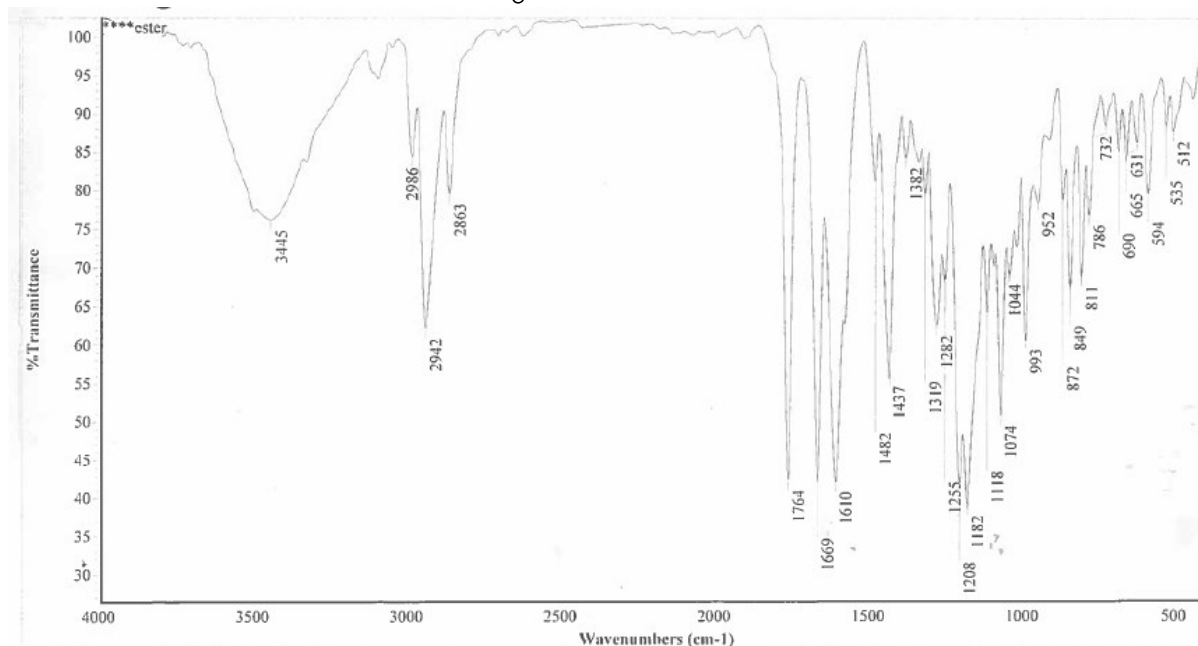
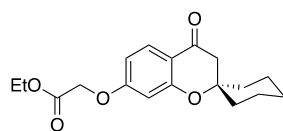


NL:
1.14E8
TIC MS
fathi-05

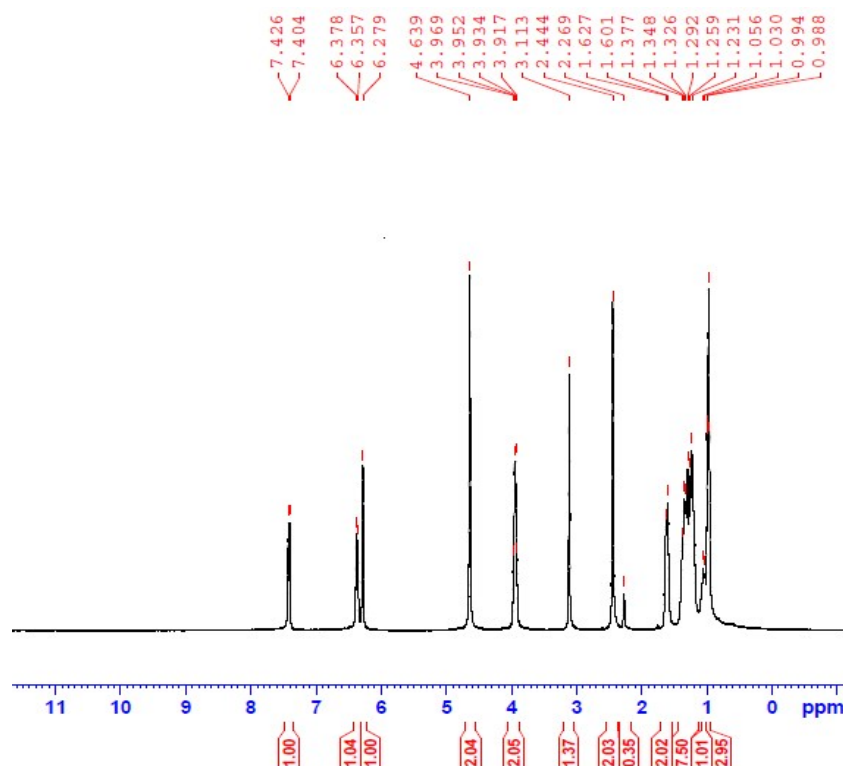
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EI-MS spectrum of 4



IR spectrum of 5



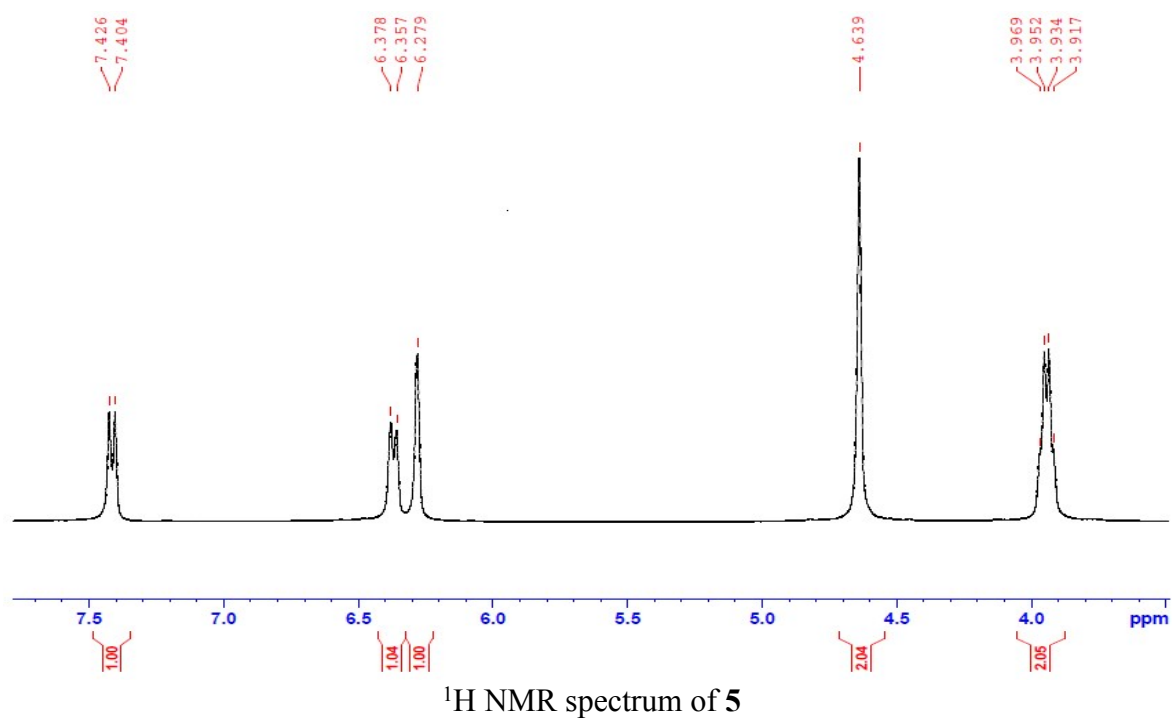
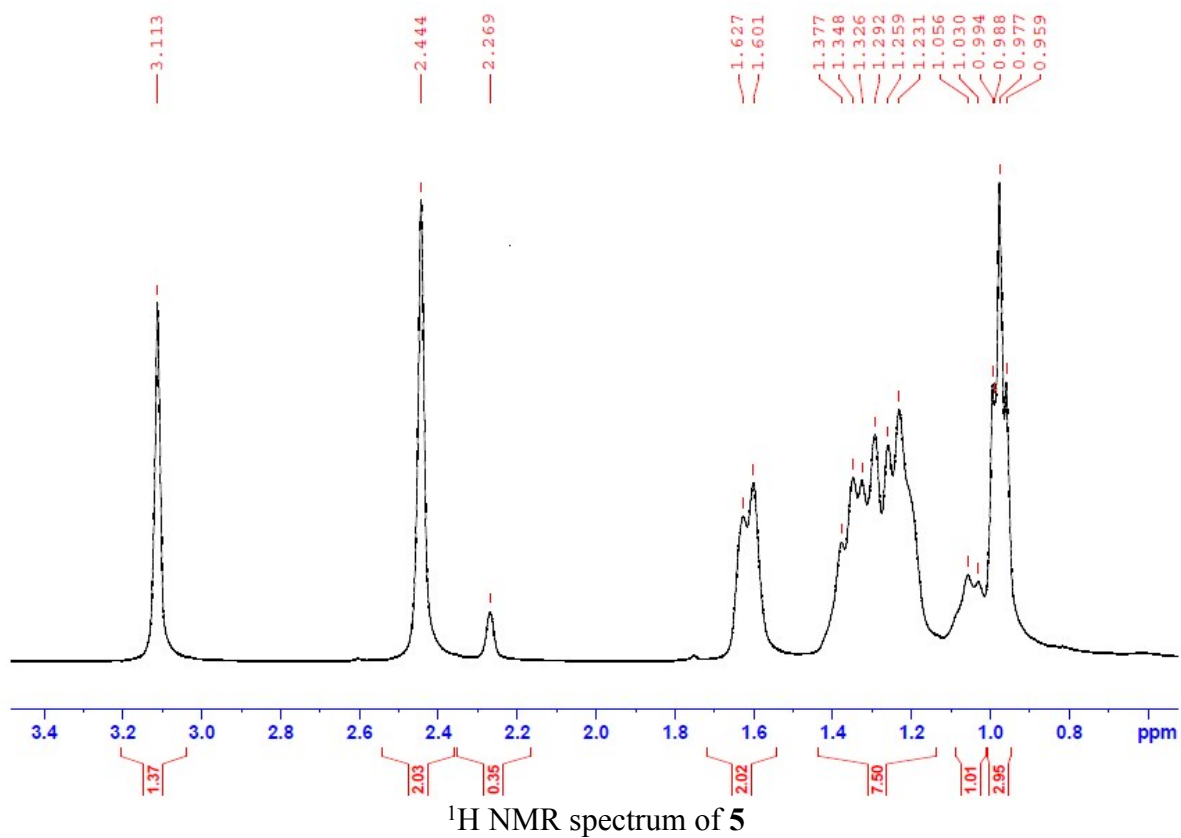
¹H NMR spectrum of 5

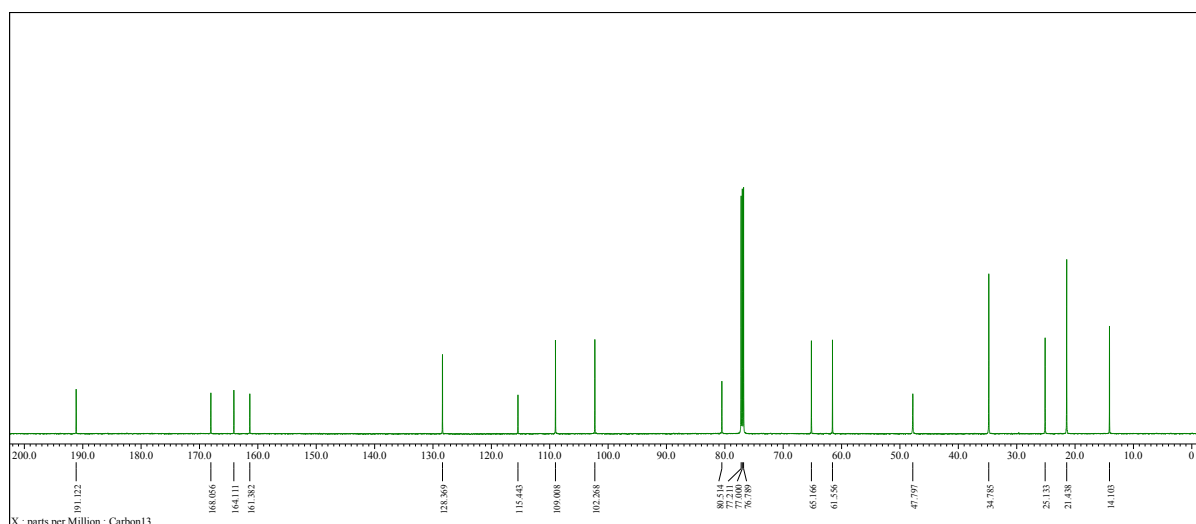


Current Data Parameters
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EXPNO 10
PROCNO 1

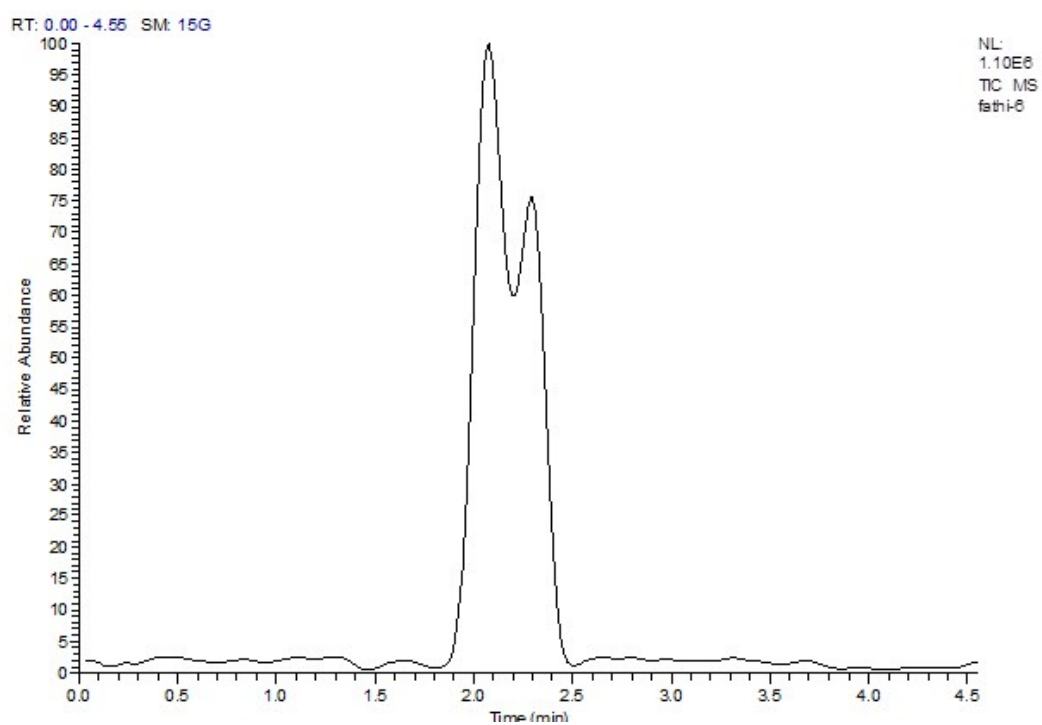
F2 - Acquisition Parameters
Date_ 20200109
Time 10:08 h
INSTRUM spect
PROBHD Z106618_0945 (1
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TD 65536
SOLVINT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 30.59
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TDS 1
SFO1 400.2024712 MHz
NUC1 1H
P1 13.50 usec
PLM1 13.00000000 W

F2 - Processing parameters
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WDW EM
SS 0
LB 0.30 Hz
GB 0
PC 1.00

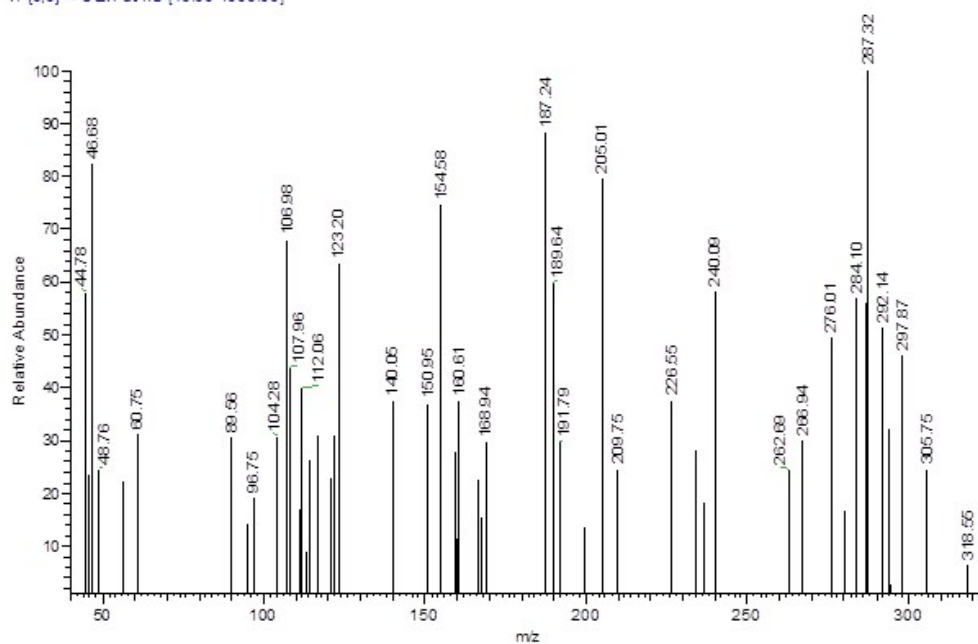




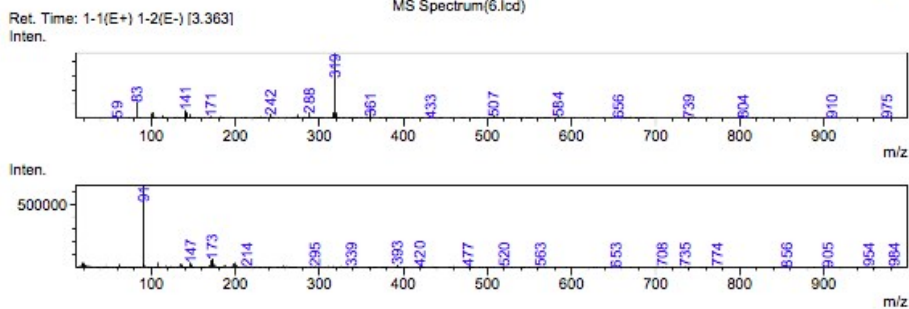
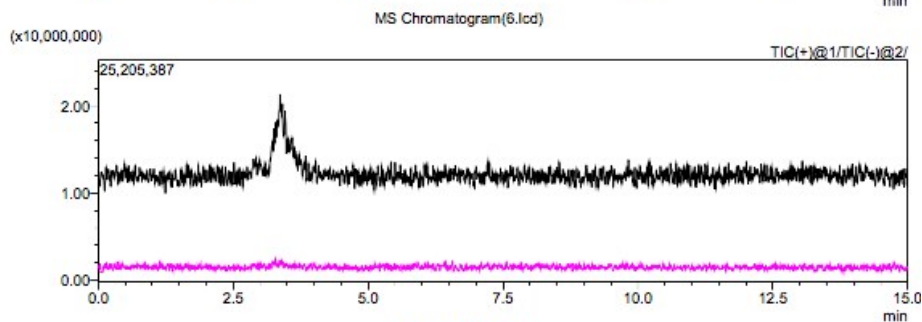
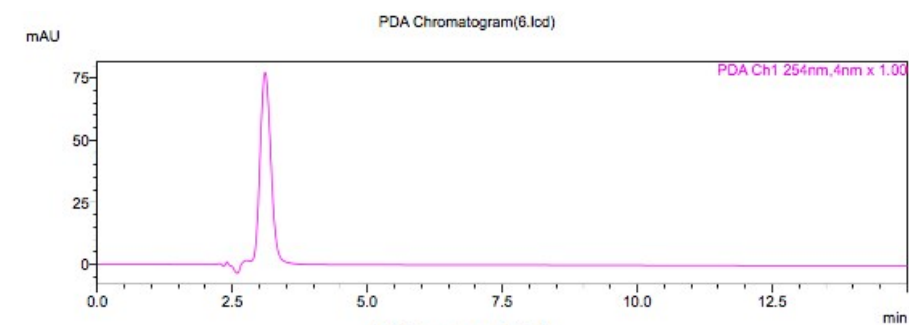
¹³C NMR spectrum of **5**



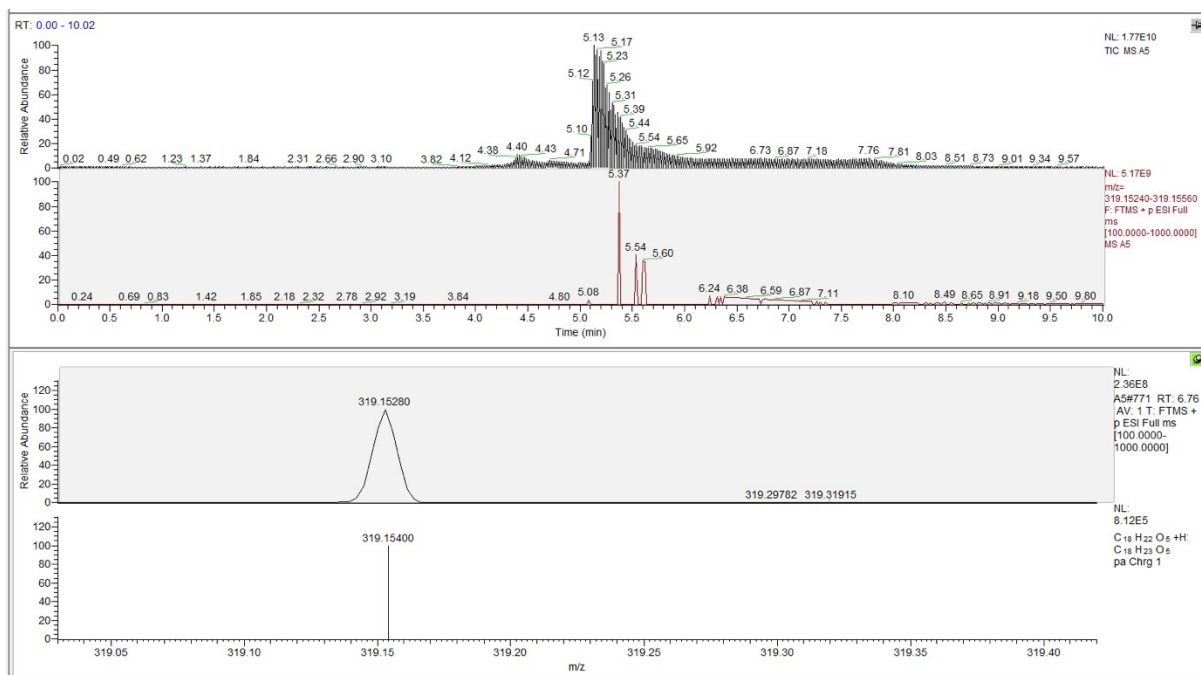
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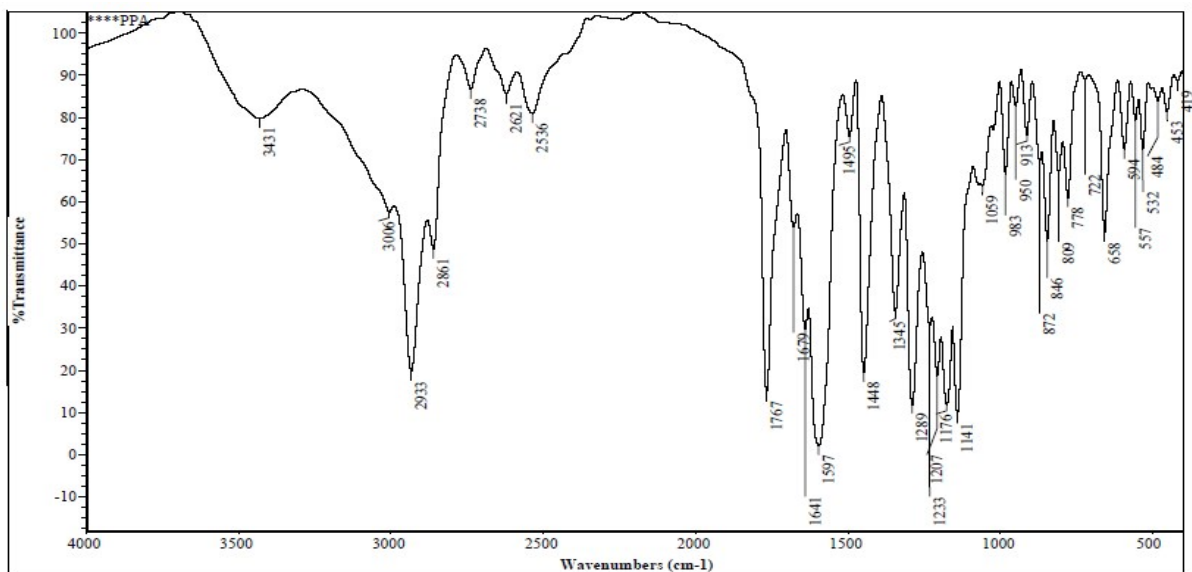
EI-MS spectrum of **5**



LC-MS spectrum of **5**



HR-MS spectrum of **5**



Fathi Hamed_PPA_proton-1-4.jdf

abundance

13.142

7.635
7.619

6.587
6.581
6.569
6.470
6.464

4.765

3.337

2.673
2.490

1.828
1.579
1.573
1.554
1.512
1.491
1.465

1.06

0.99

1.91

2.00

2.00

7.00

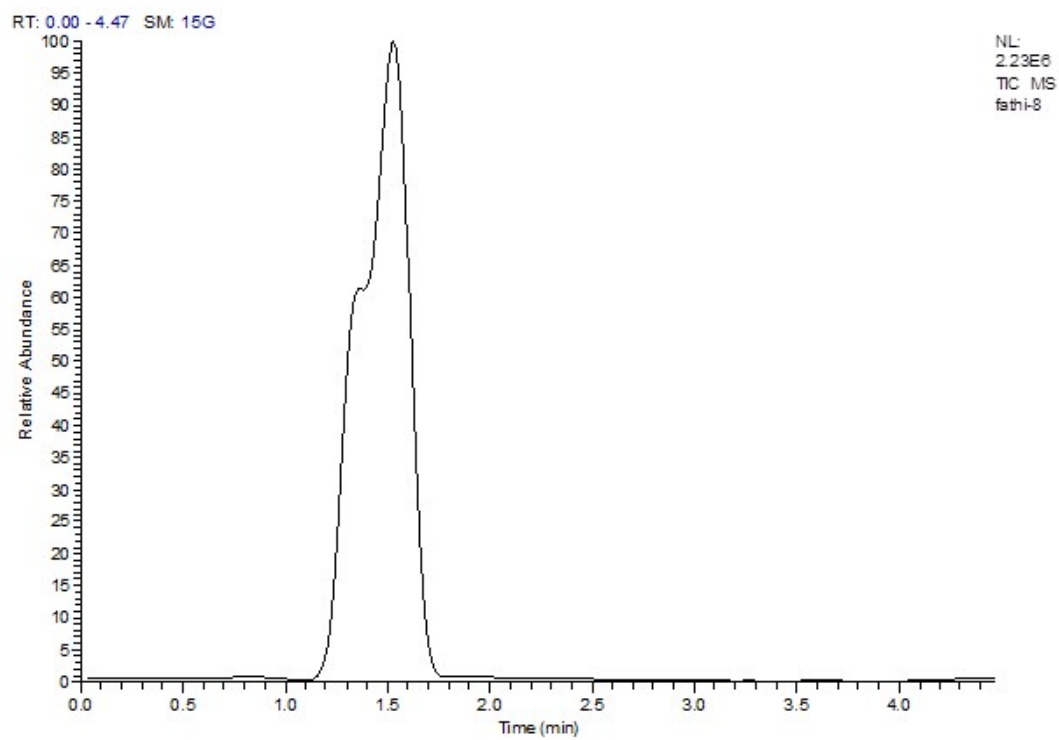
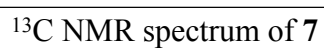
1.55

0.28

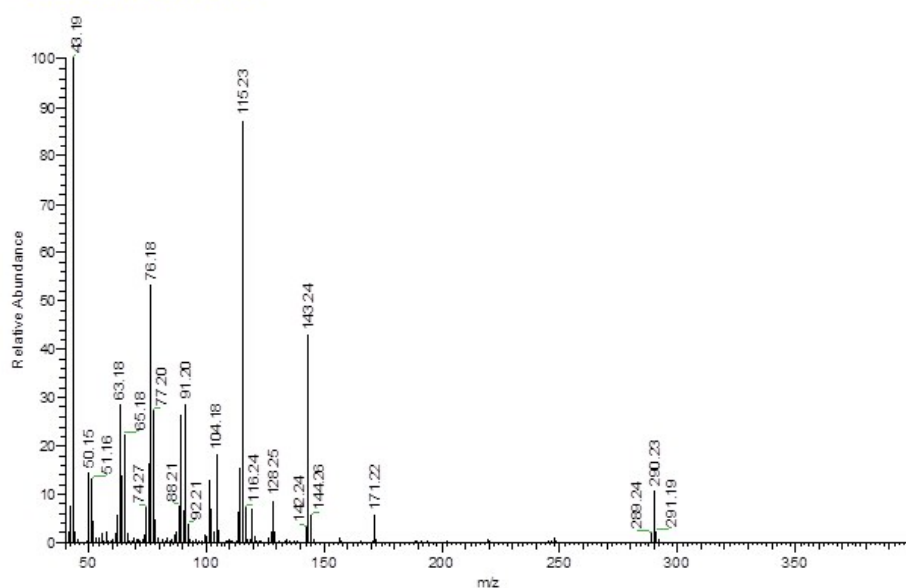
X: parts per Million: Proton

Parameter	Value
Filename	Fathi Hamed_PPA_proton-1-4.jdf
Author	delta
Experiment	proton-1-4.jdf
Sample Id	Fathi Hamed_PPA
Solvent	DMSO-D6
Creation Time	30-JAN-2019 13:30:10
Revision Time	30-JAN-2019 13:12:25
Current Time	30-JAN-2019 13:12:42
Comment	single_pulse
Data Format	1D COMPLEX
Dim Size	13107
Dim Title	Proton
Dim Units	[ppm]
Dimensions	X
Site	JNM-ECA500II
Spectrometer	DELTA2_NMR
Field Strength	11.7473579[T] (500[MH])
X_Acq Duration	1.4548992[s]
X Domain	18
X_Freq	500.15991521[MHz]
X_Offset	6[ppm]
X Points	15384
X_Prescans	1
X Resolution	0.68733284[Hz]
X_Sweep	11.26126126[kHz]
X_Sweep_Clippped	9.00900901[kHz]
Irr Domain	Proton
Irr Freq	500.15991521[MHz]
Irr_Offset	5.0[ppm]
Tri Domain	Proton
Tri Freq	500.15991521[MHz]
Tri_Offset	5.0[ppm]
Clipped	FALSE
Scans	40
Total Scans	40
Relaxation Delay	5[s]
Recvr Gain	46
Temp Get	18.6[degC]
X_90 Width	14.5[us]
X_Acq Time	1.4548992[s]
X_Angle	45[deg]
X_Ain	4.9[deg]
X_Pulse	7.25[us]
Irr Mode	Off
Tri Mode	Off
Daqie Presat	FALSE
Initial Wait	1[s]
Repetition Time	6.4548992[s]

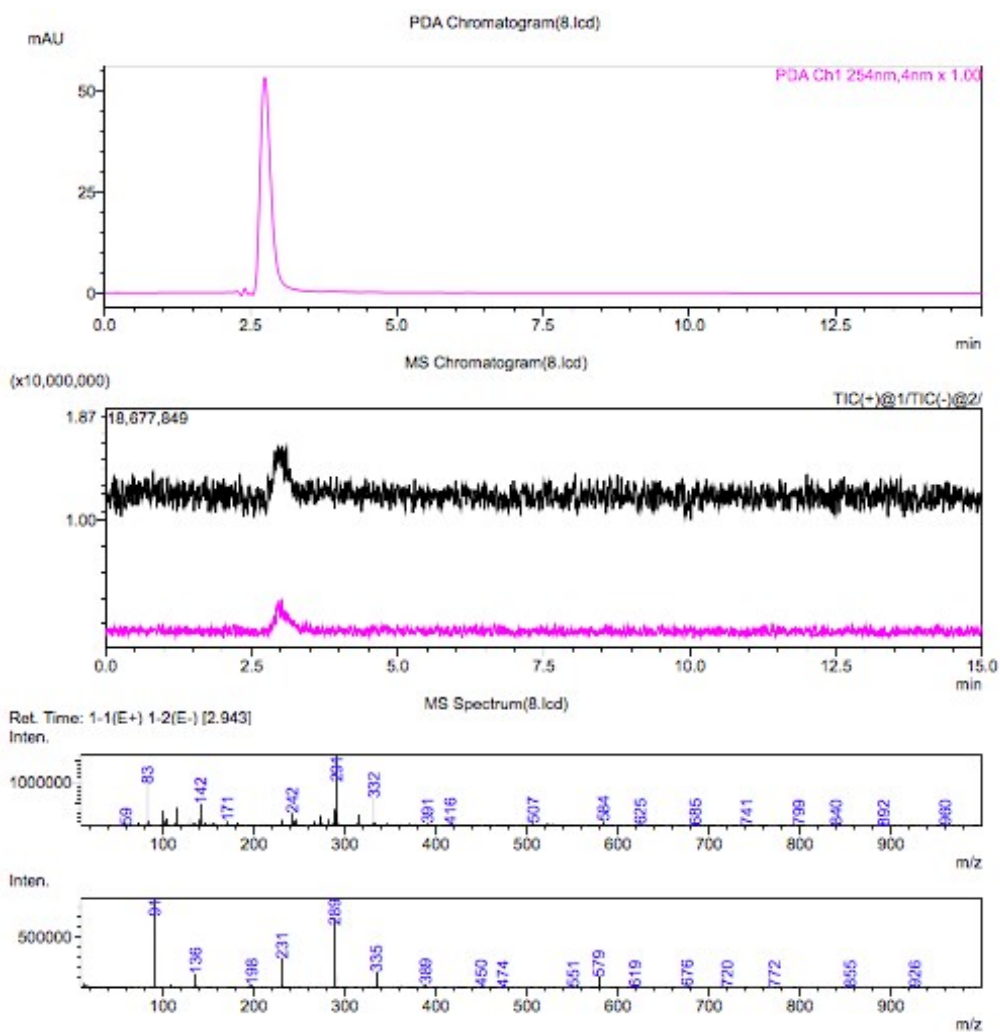
¹H NMR spectrum of **7**



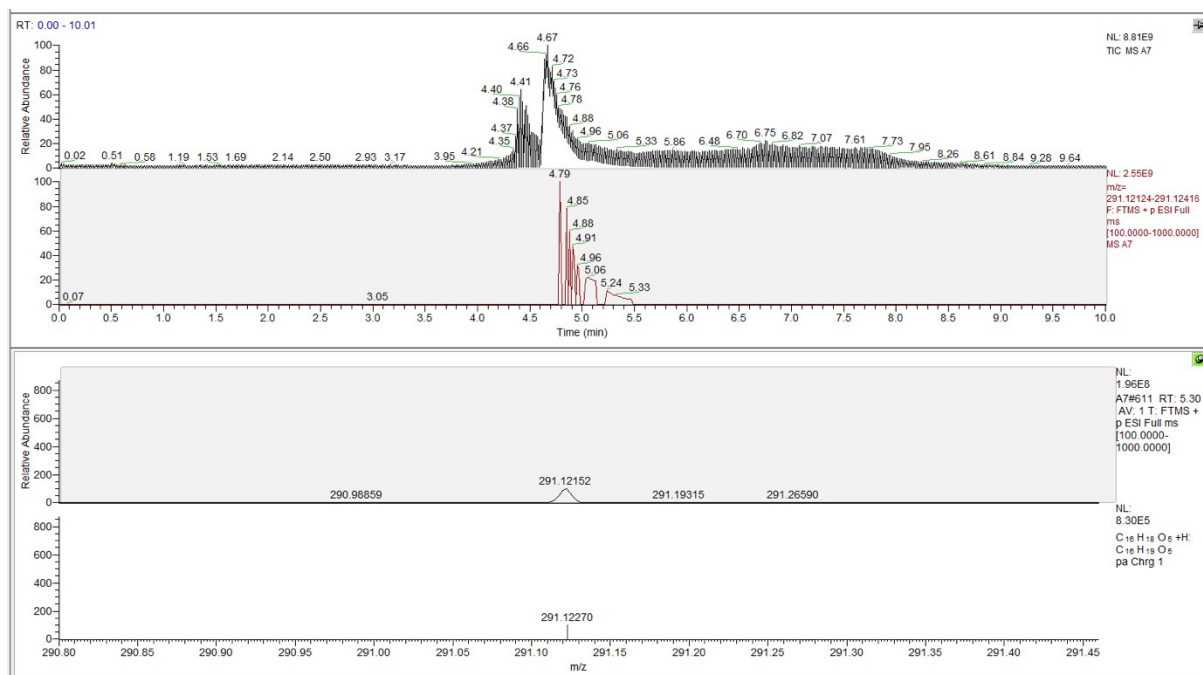
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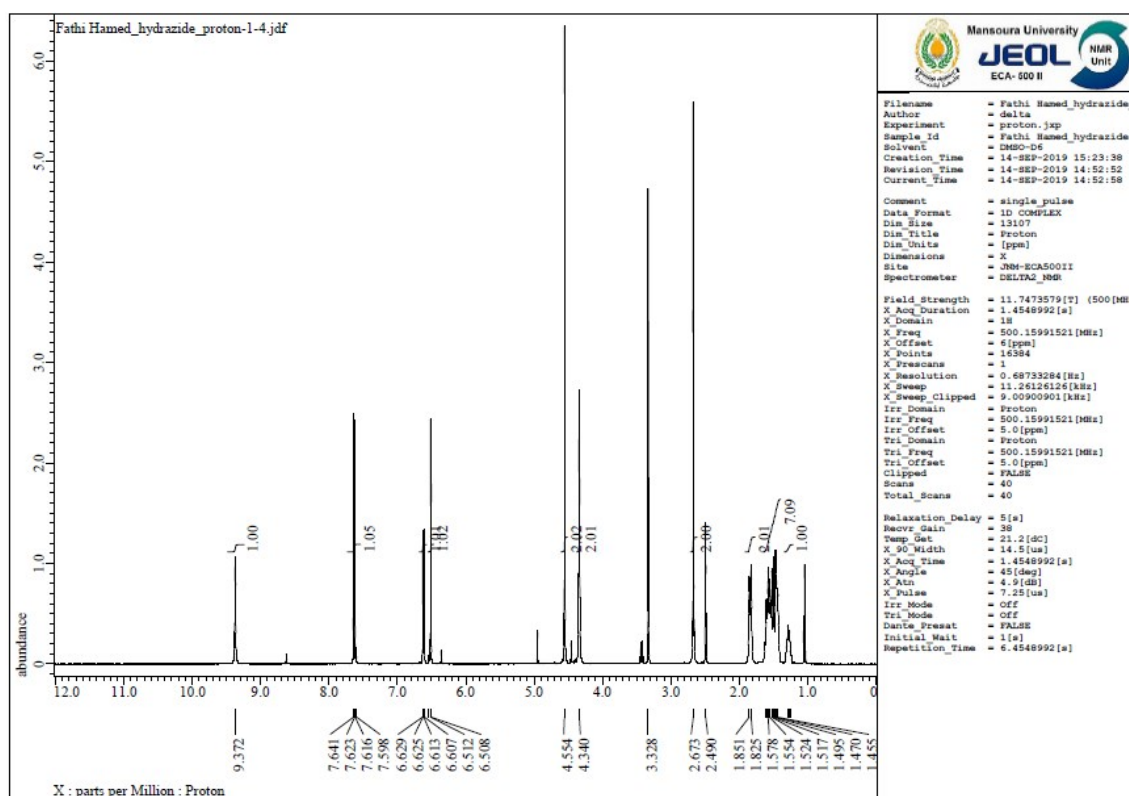
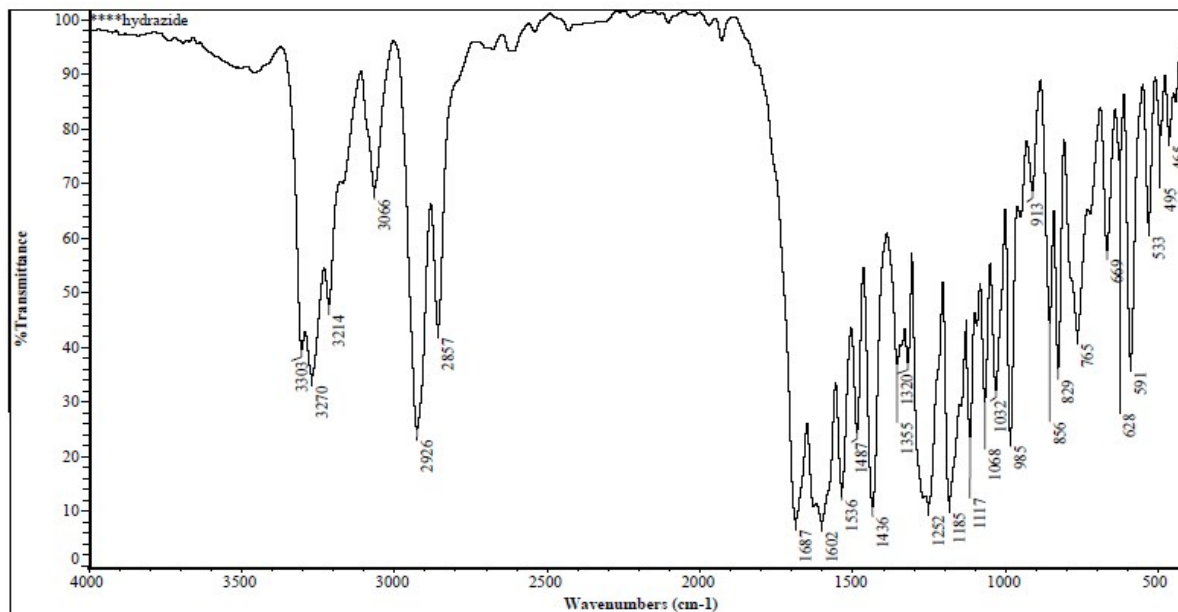
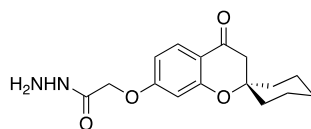
EI-MS spectrum of 7

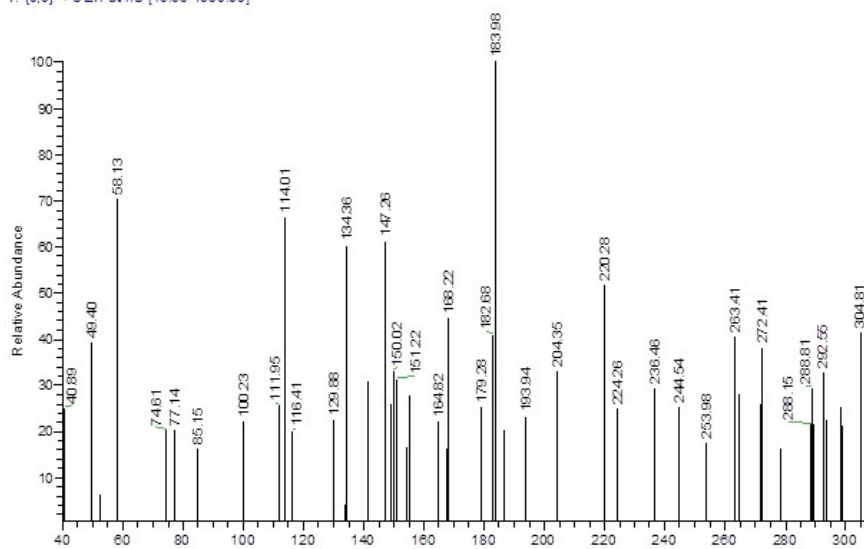
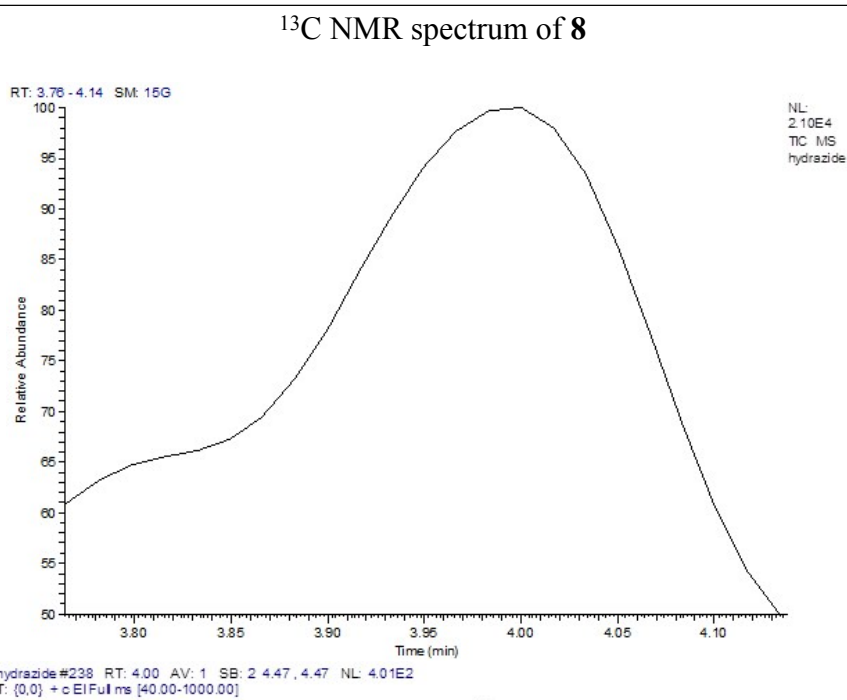
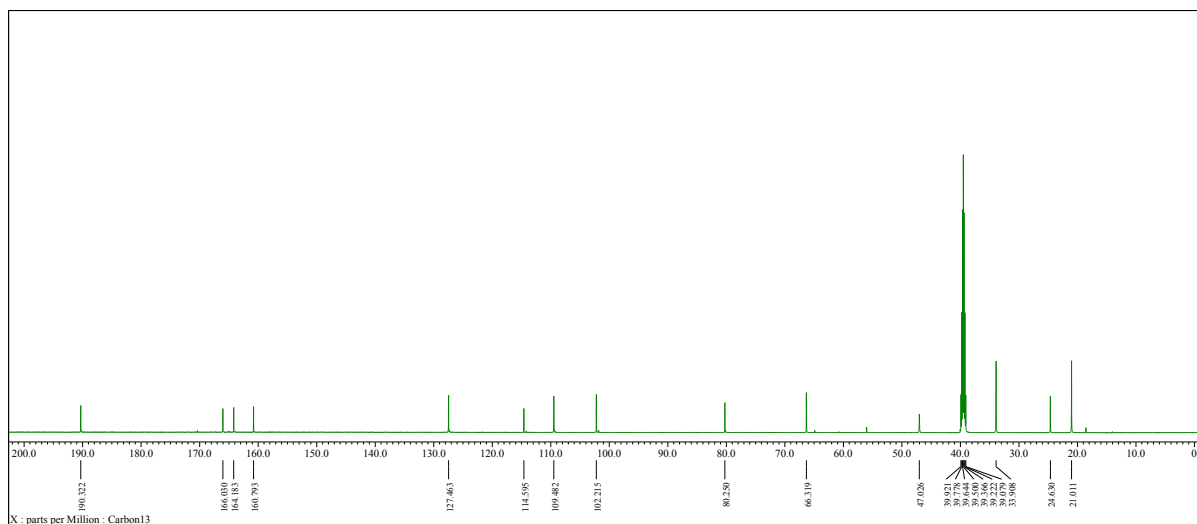


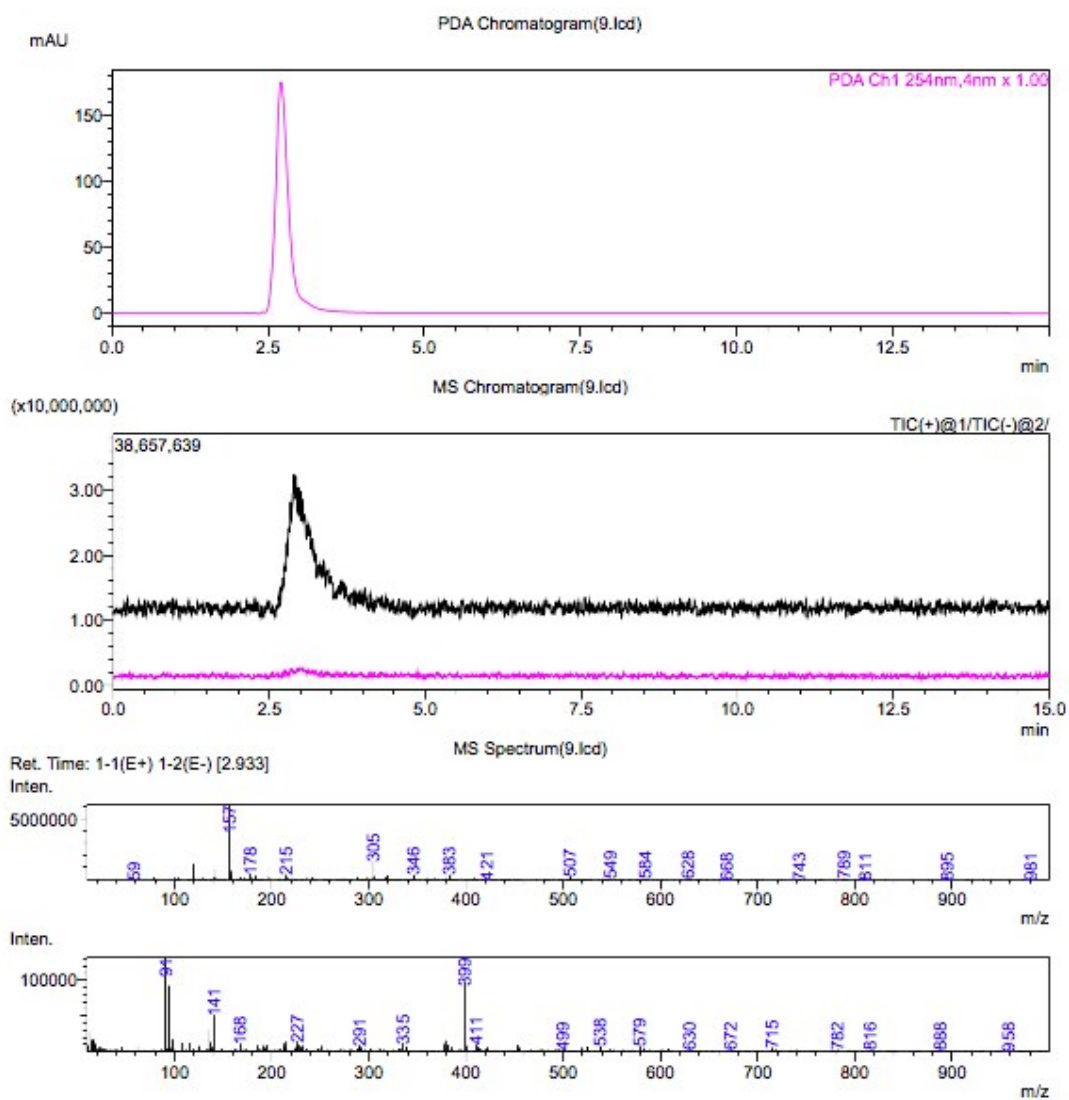
LC-MS spectrum of 7



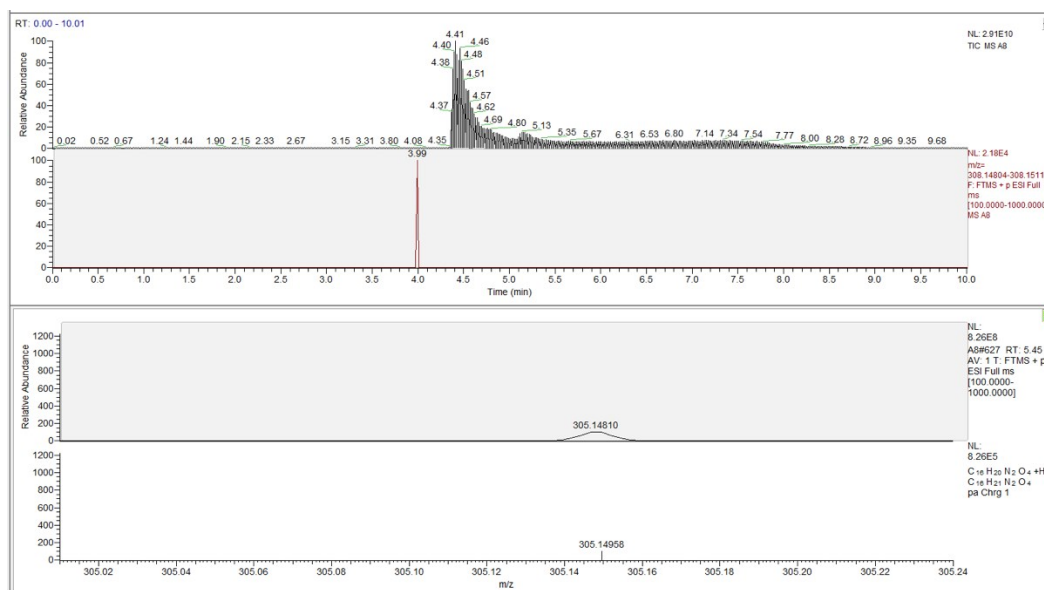
HR-MS spectrum of 7



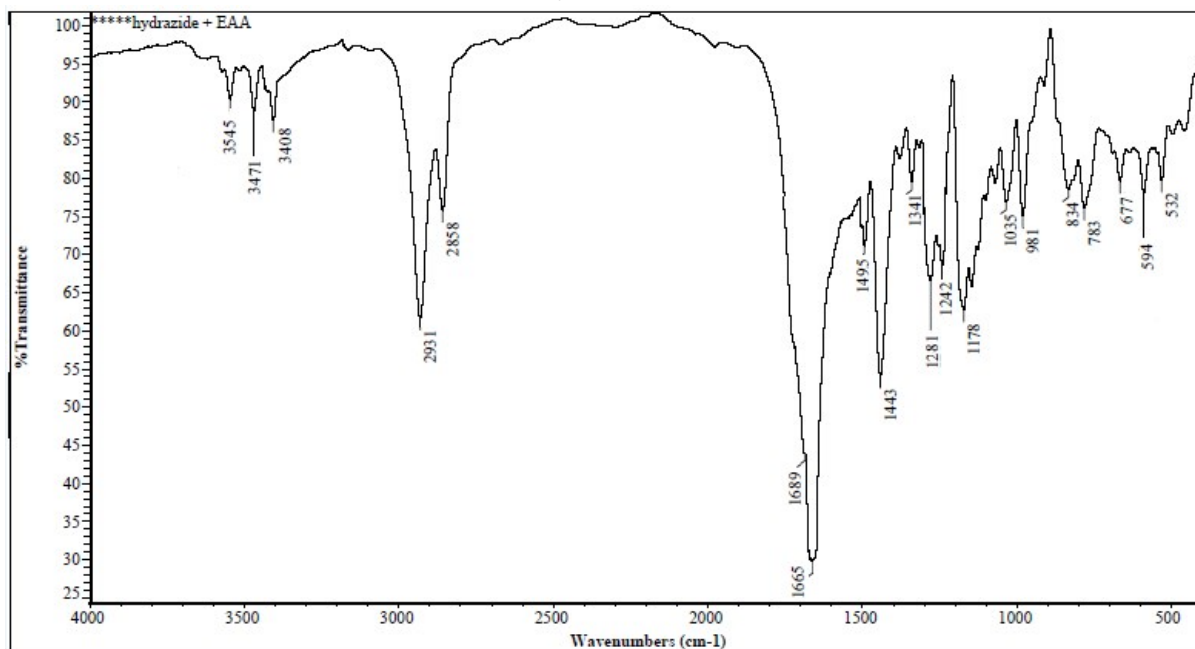
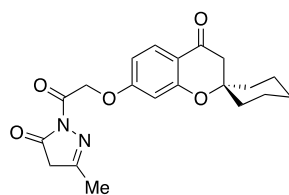




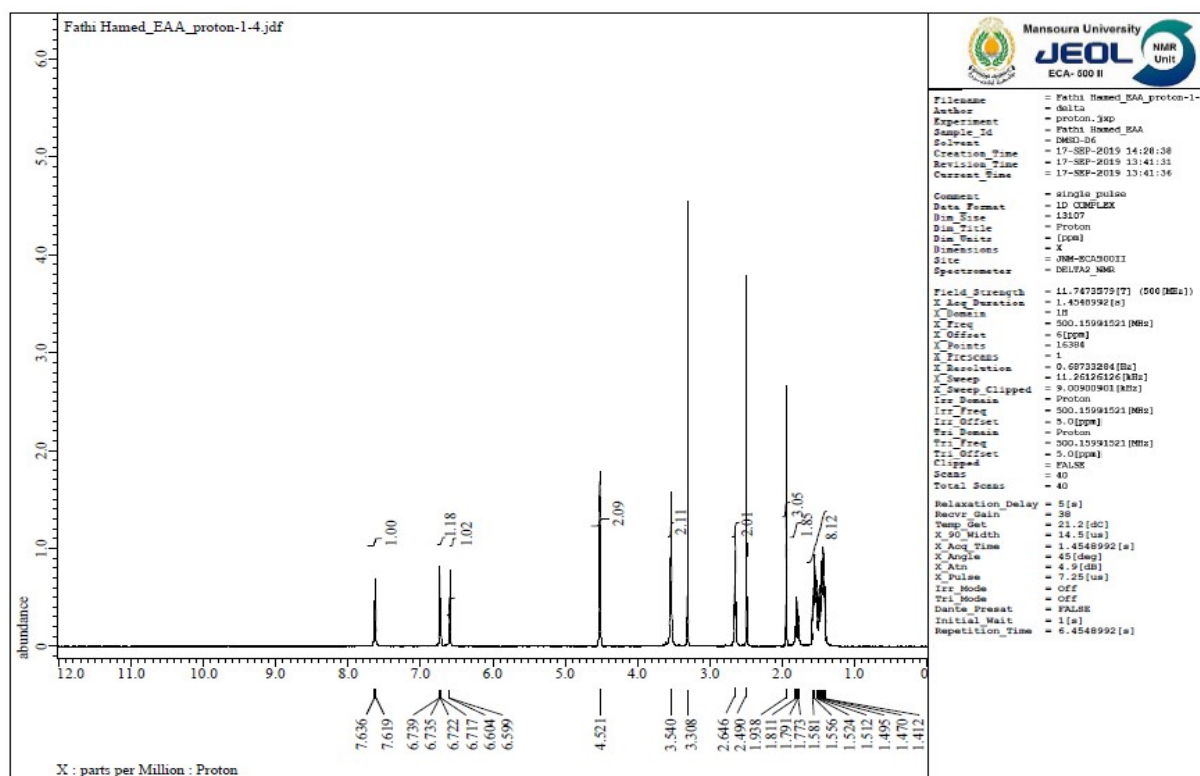
LC-MS spectrum of **8**



HR-MS spectrum of **8**

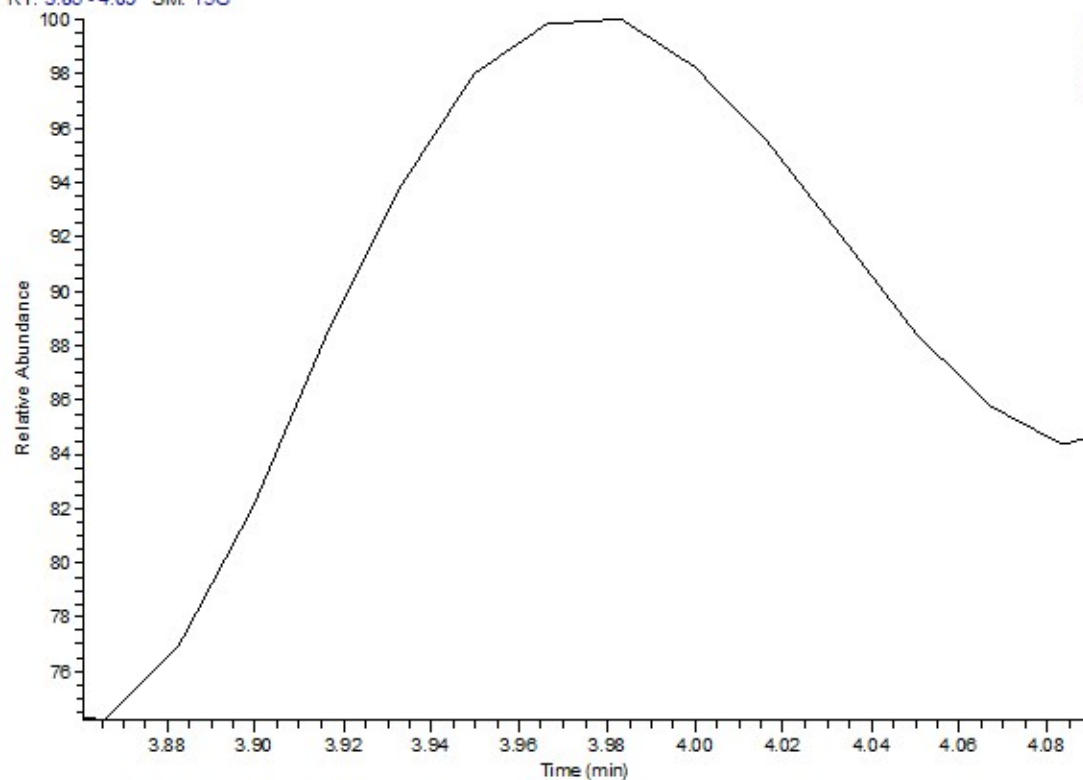


IR spectrum of 9



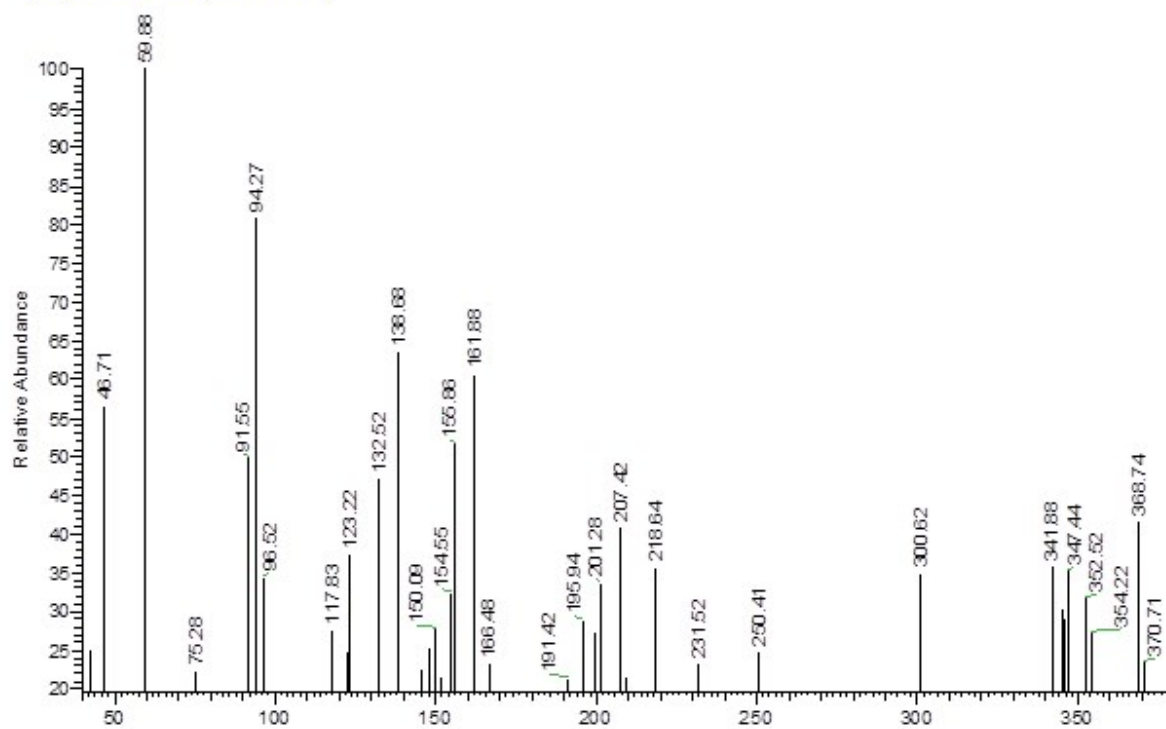
¹H NMR spectrum of 9

RT: 3.86 - 4.09 SM: 15G

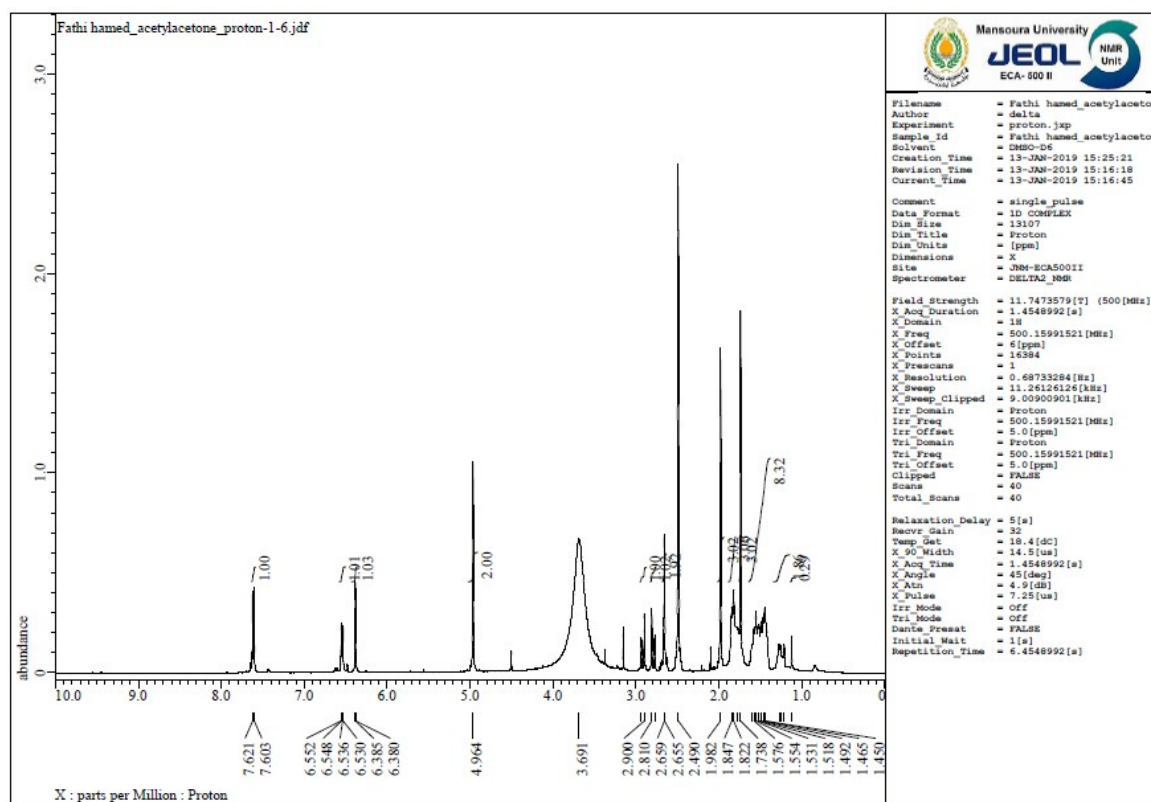
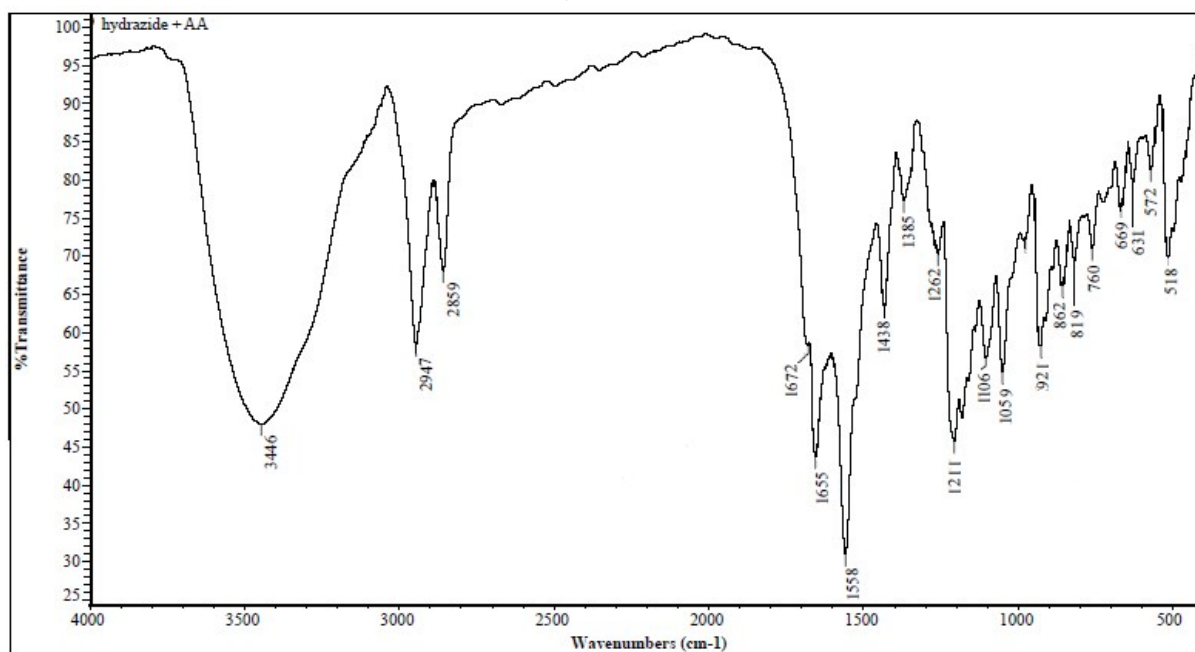
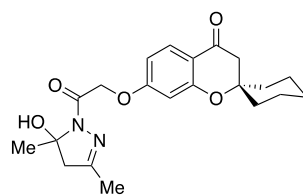


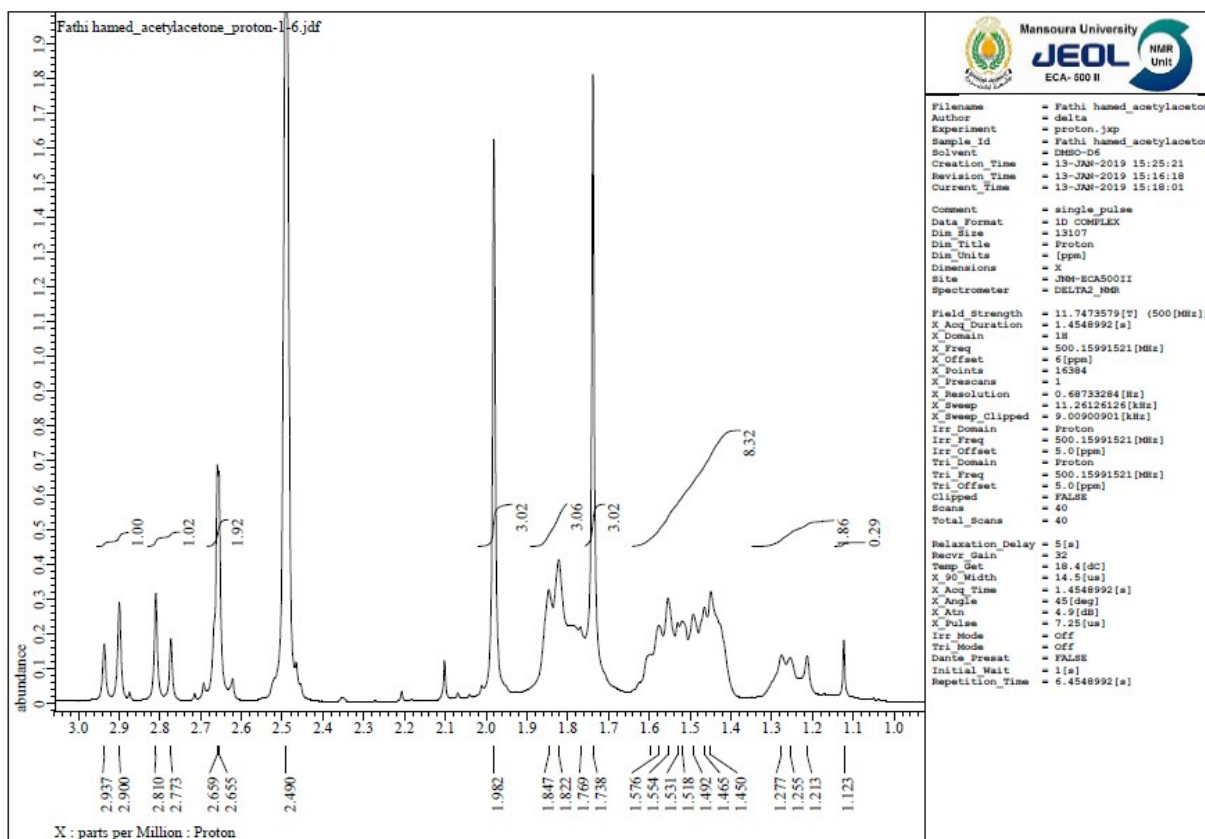
NL:
9.89E3
TIC MS
fathi-13

fathi-13#129 RT: 2.18 AV: 1 SB: 2 4.55, 4.55 NL: 3.43E2
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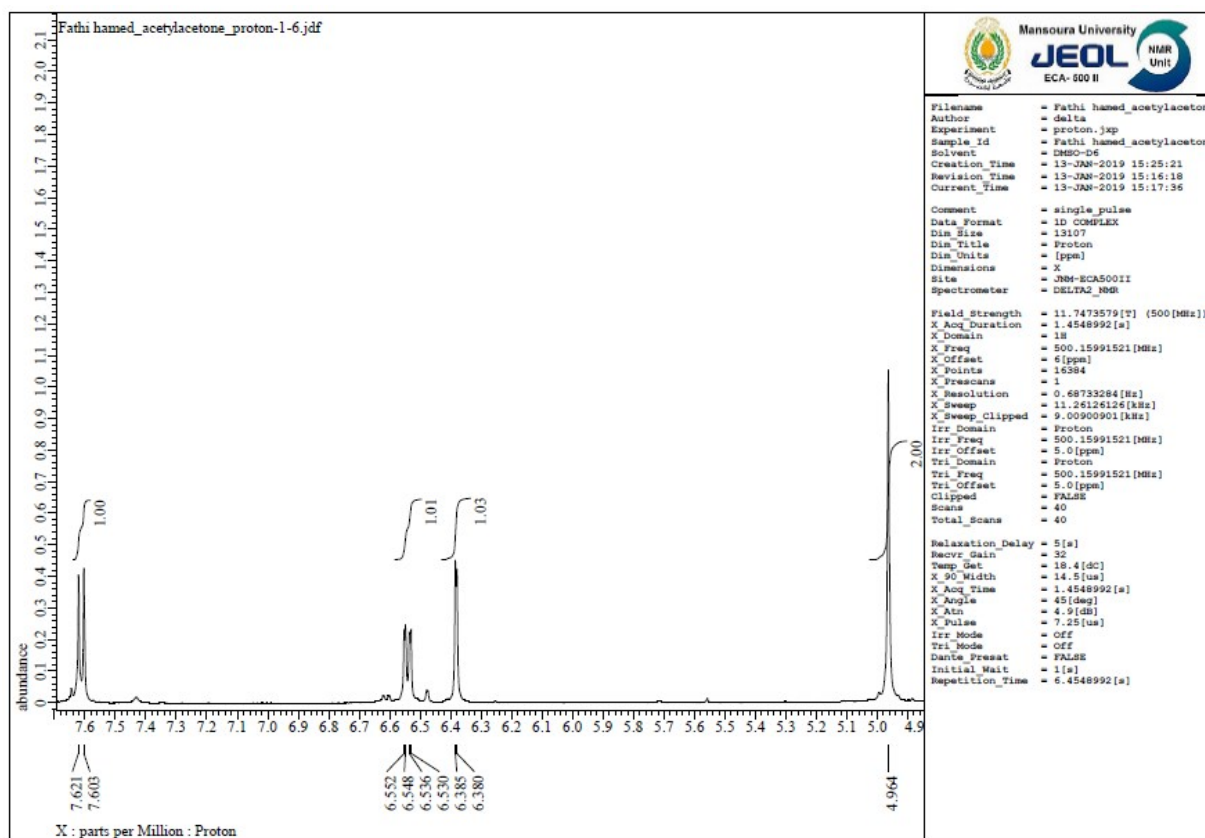


EI-MS spectrum of 9

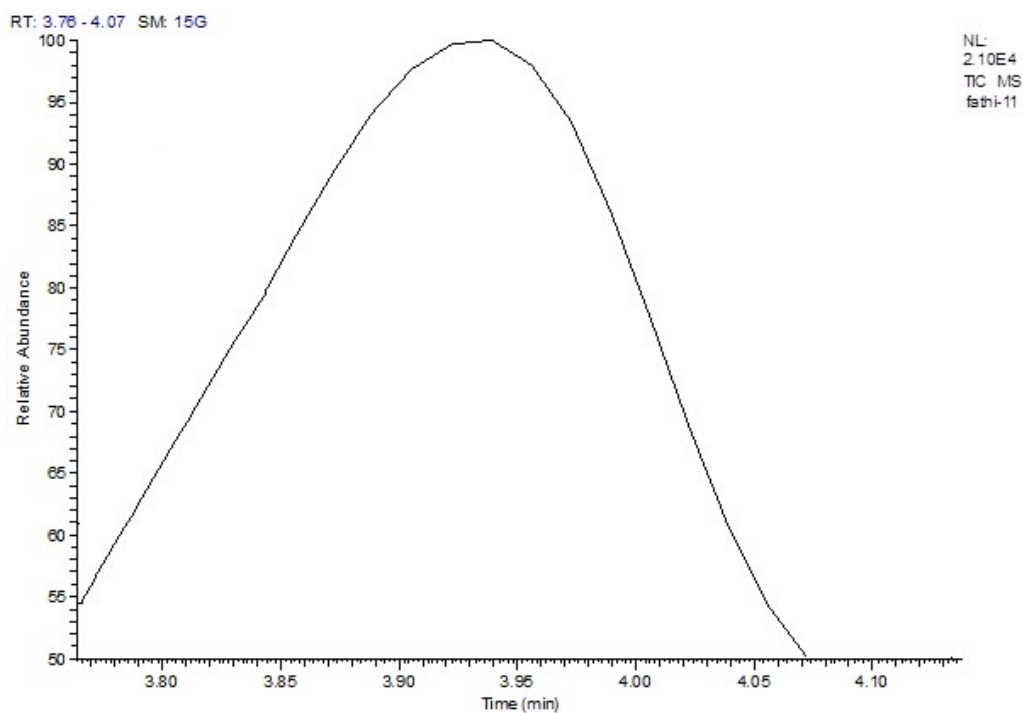




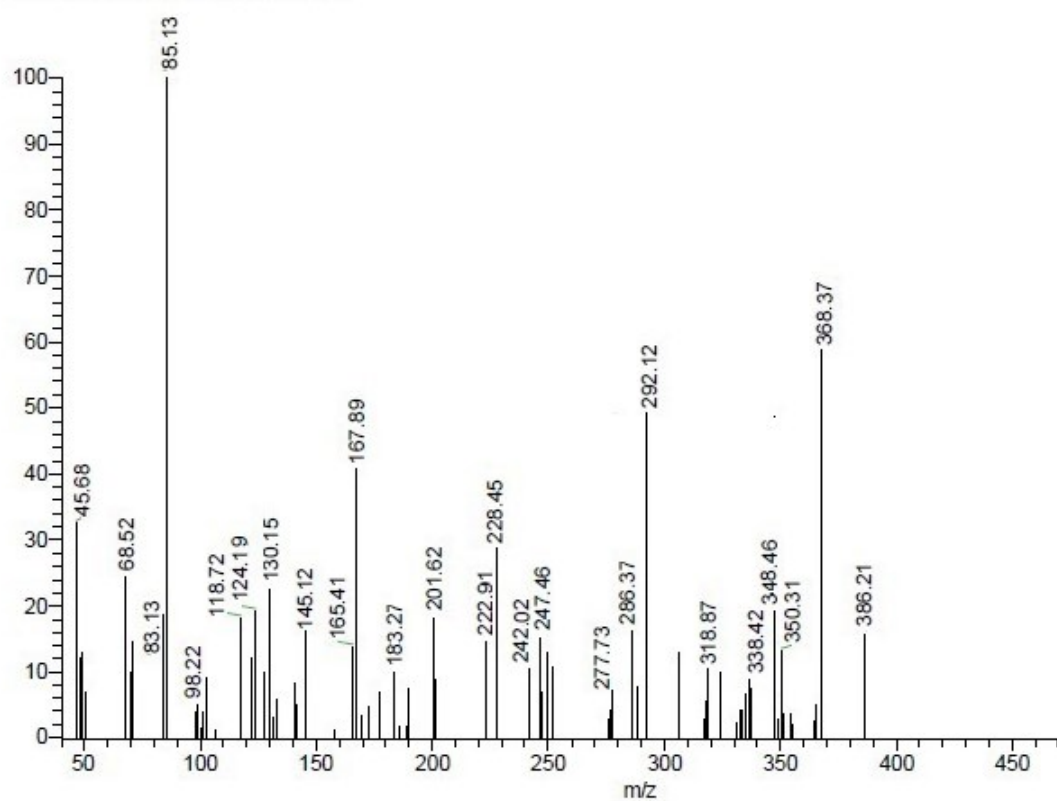
¹H NMR spectrum of **10**



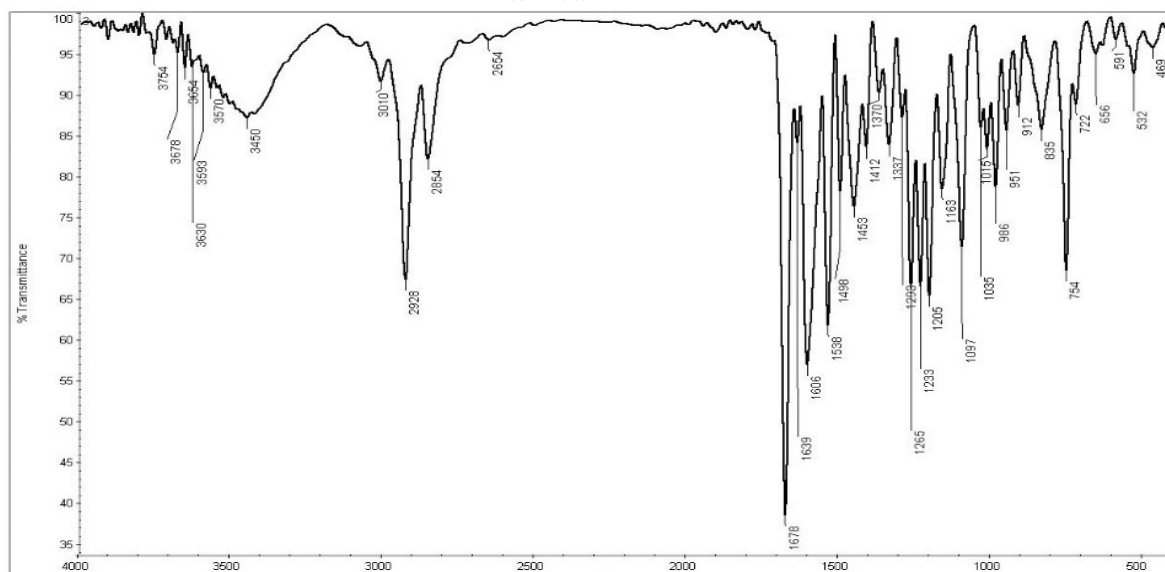
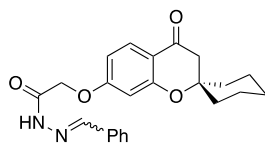
¹H NMR spectrum of **10**



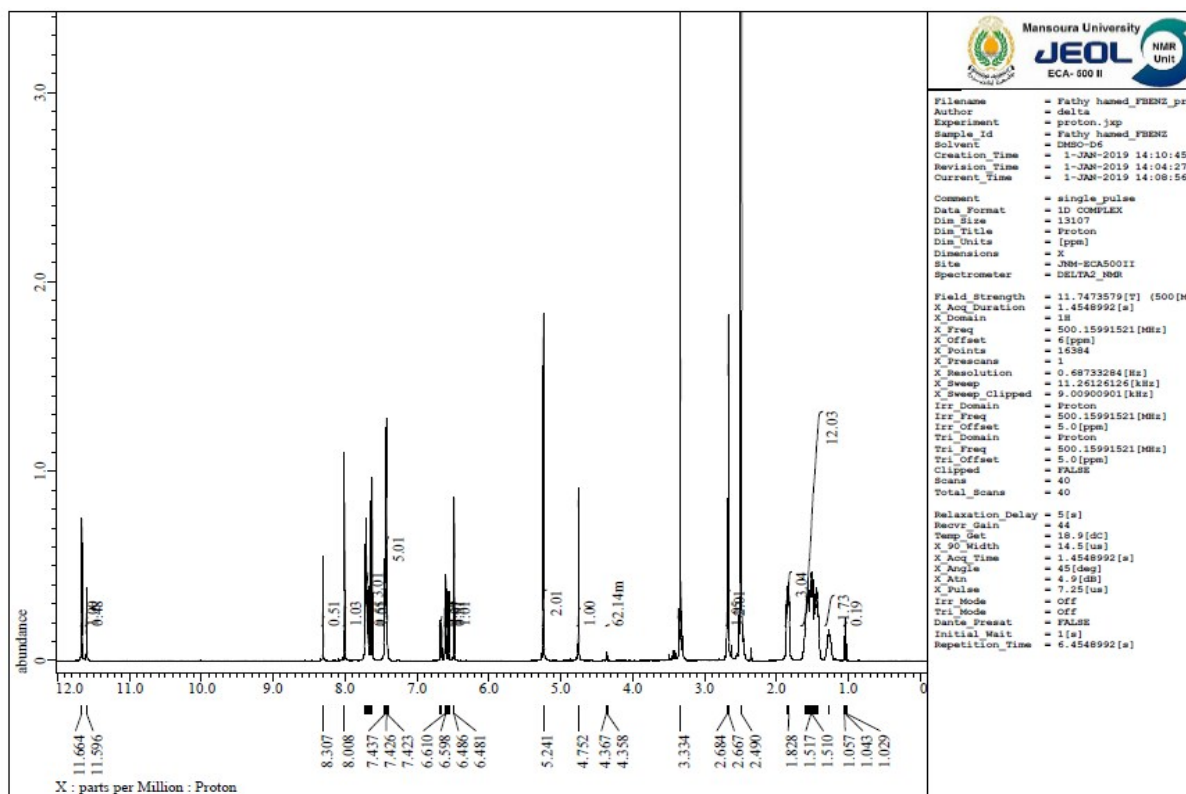
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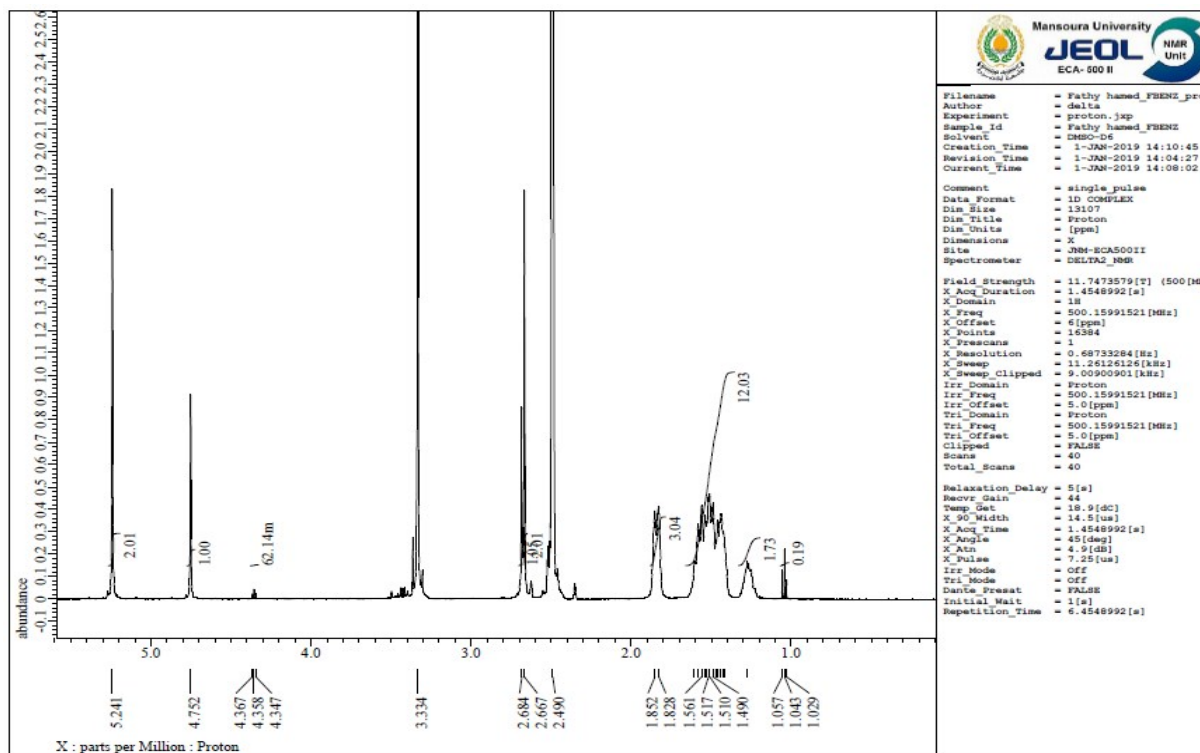
EI-MS spectrum of **10**



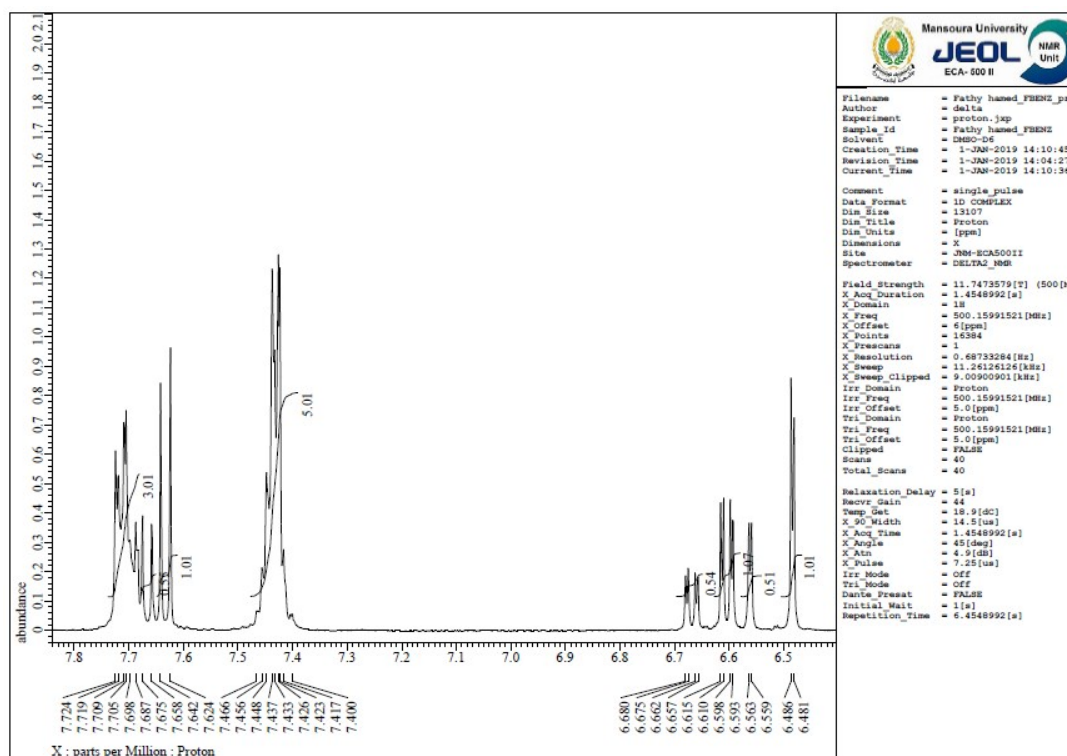
IR spectrum of **11**



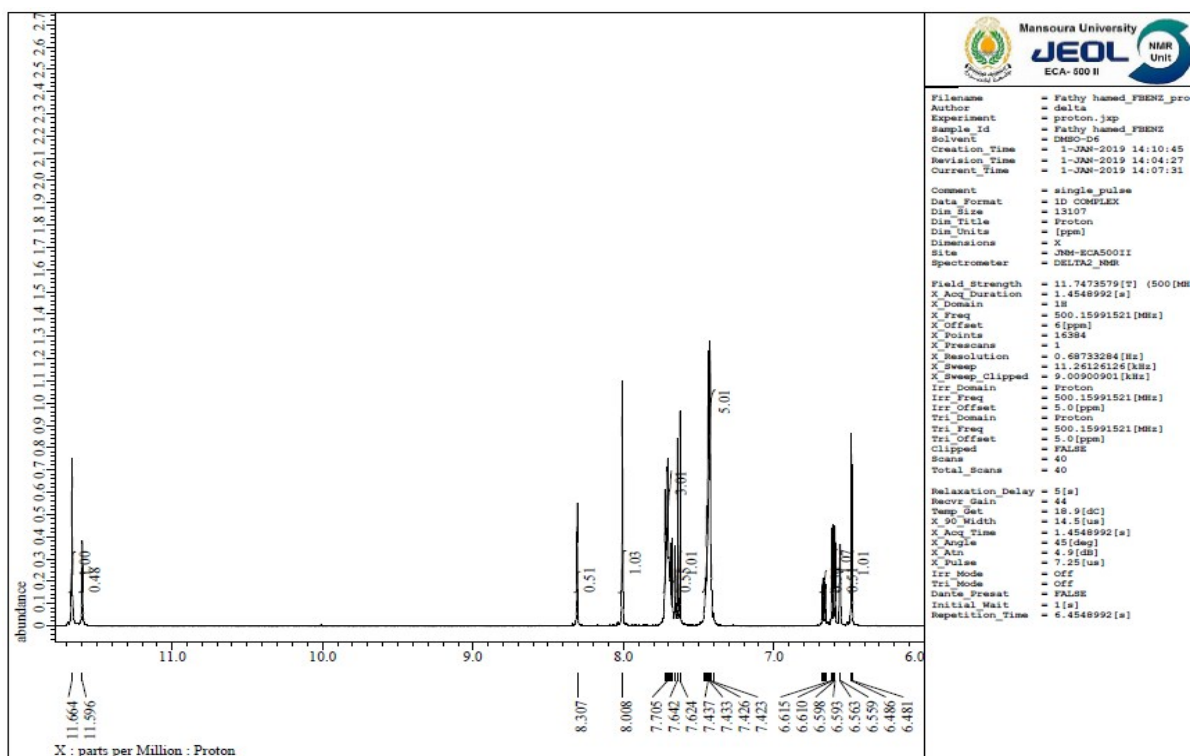
¹H NMR spectrum of **11**



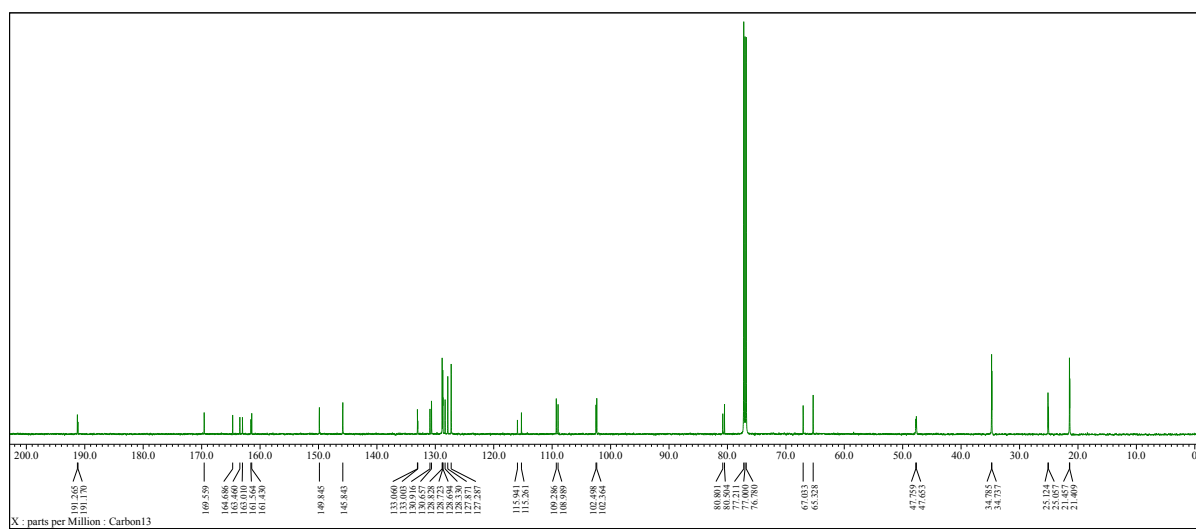
¹H NMR spectrum of **11**



¹H NMR spectrum of **11**

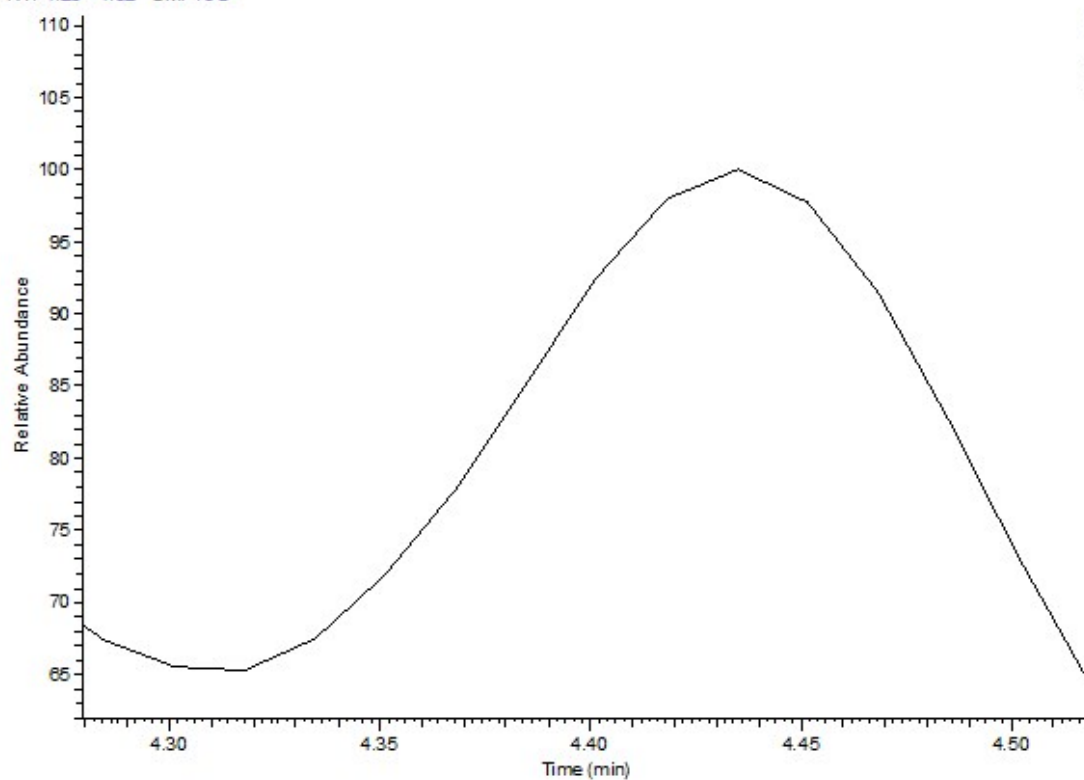


¹H NMR spectrum of **11**



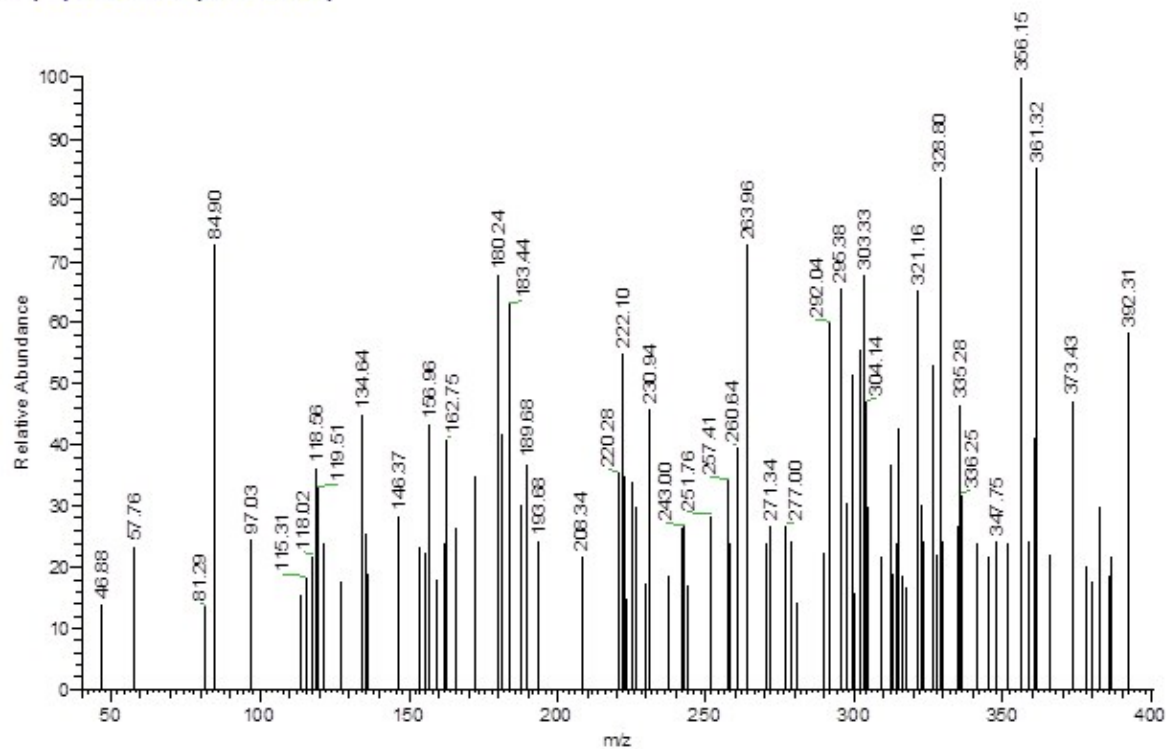
¹³C NMR spectrum of **11**

RT: 4.28 - 4.52 SM: 15G

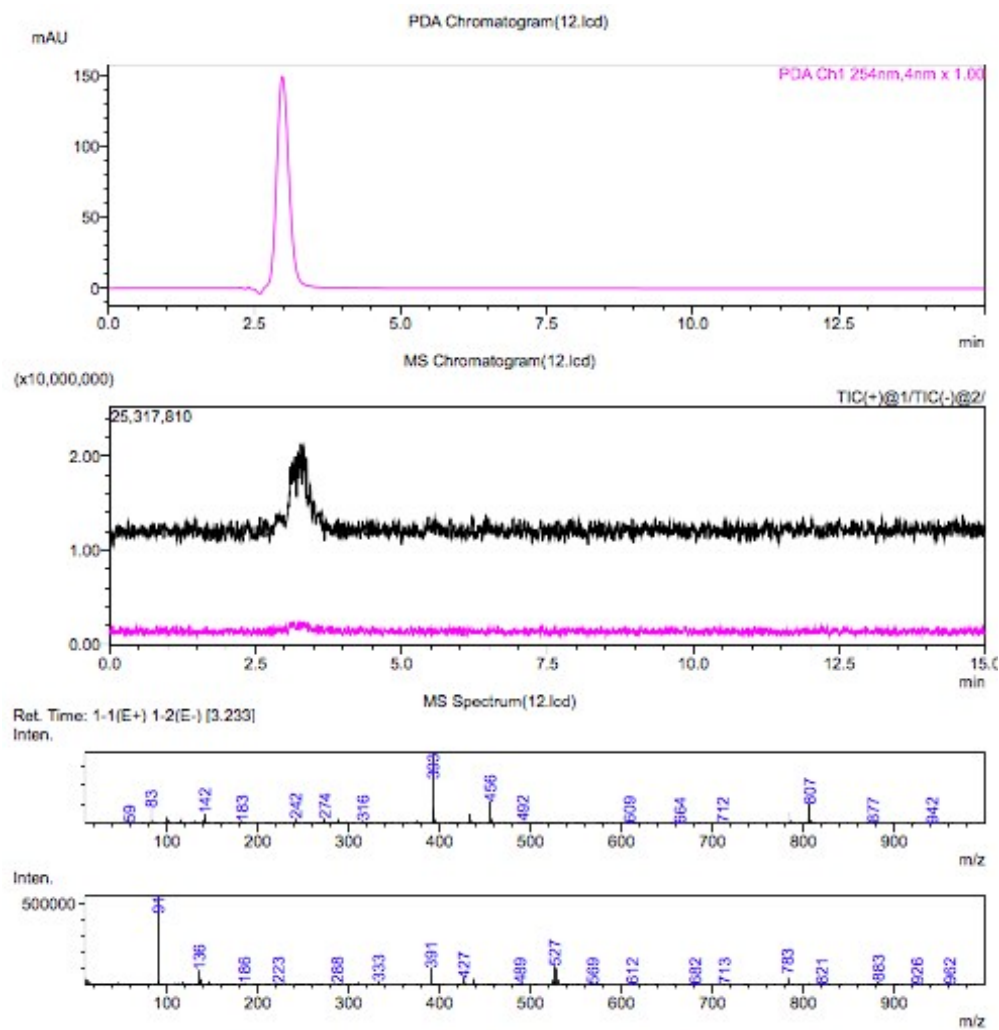


NL:
1.98E4
TIC MS
benzal-10

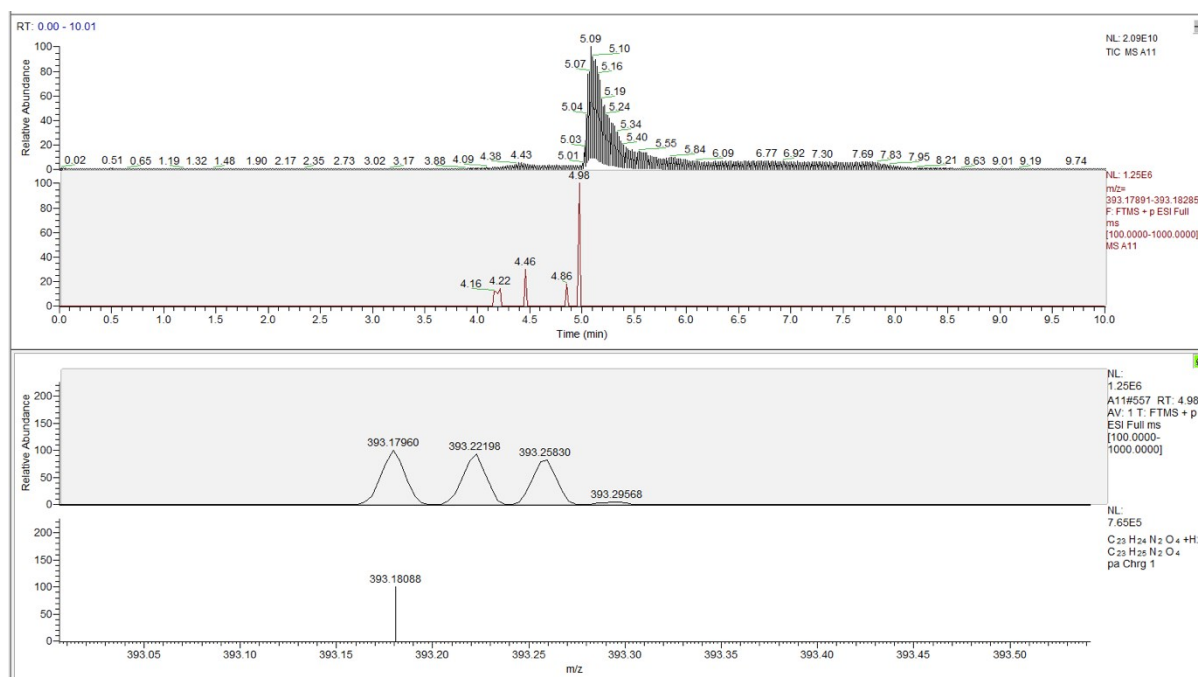
benzal-10 #225 RT: 3.78 AV: 1 SB: 2 4.54, 4.54 NL: 4.05E2
T: {0,0} + cEiFull.ms [40.00-1000.00]



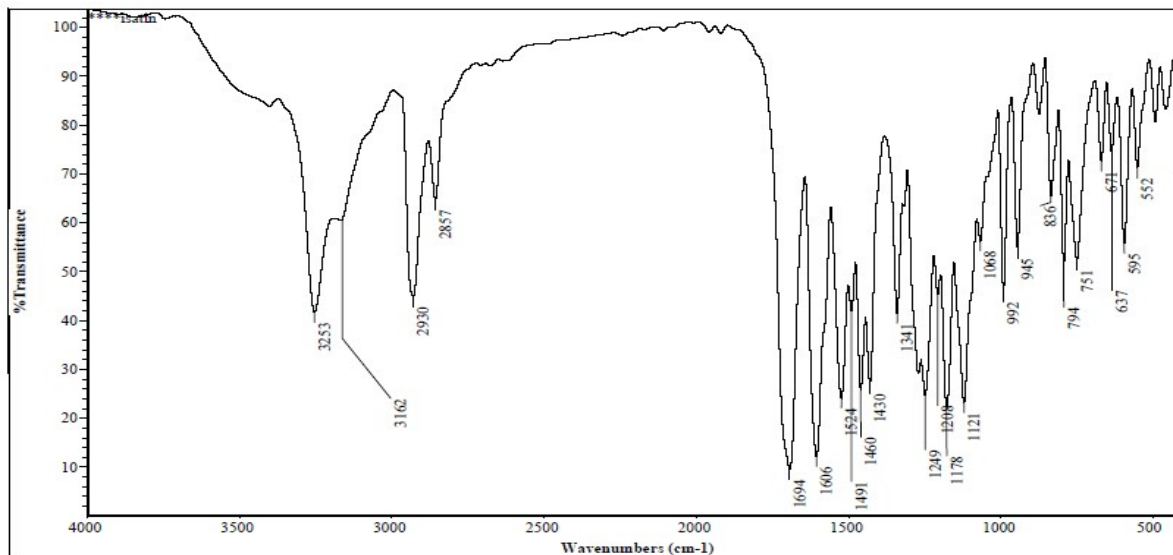
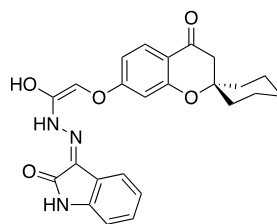
EI-MS spectrum of 11



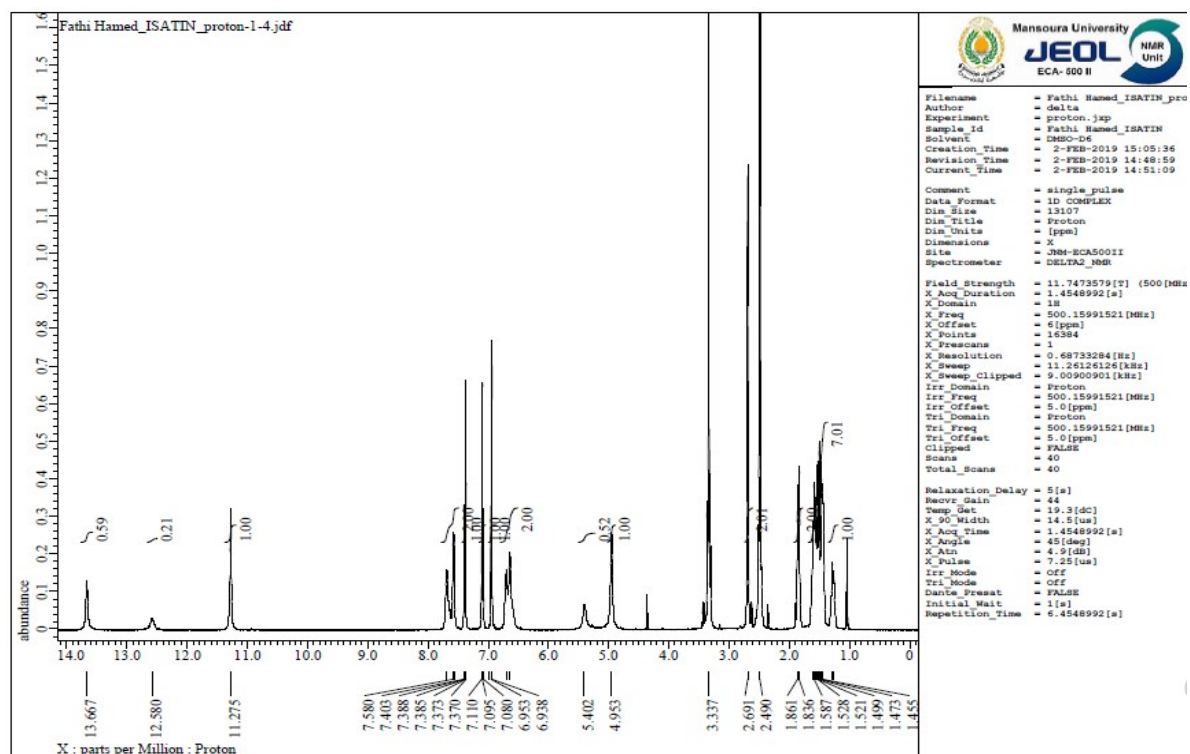
LC-MS spectrum of **11**



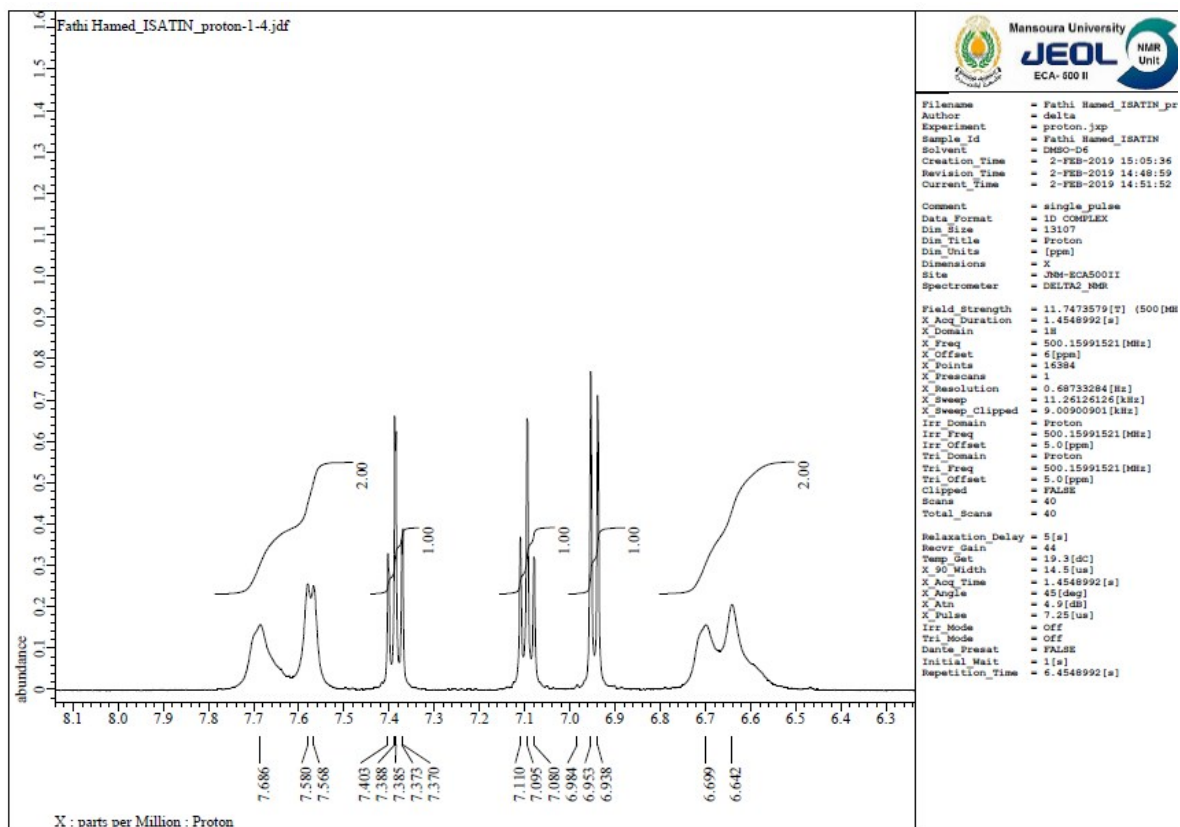
HR-MS spectrum of **11**



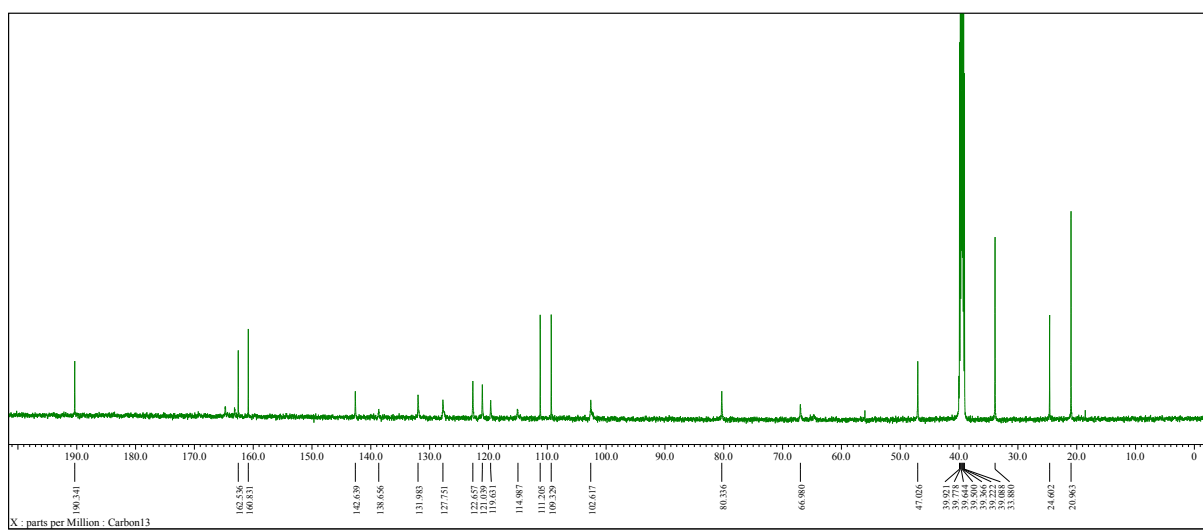
IR spectrum of 13



¹H NMR spectrum of 13

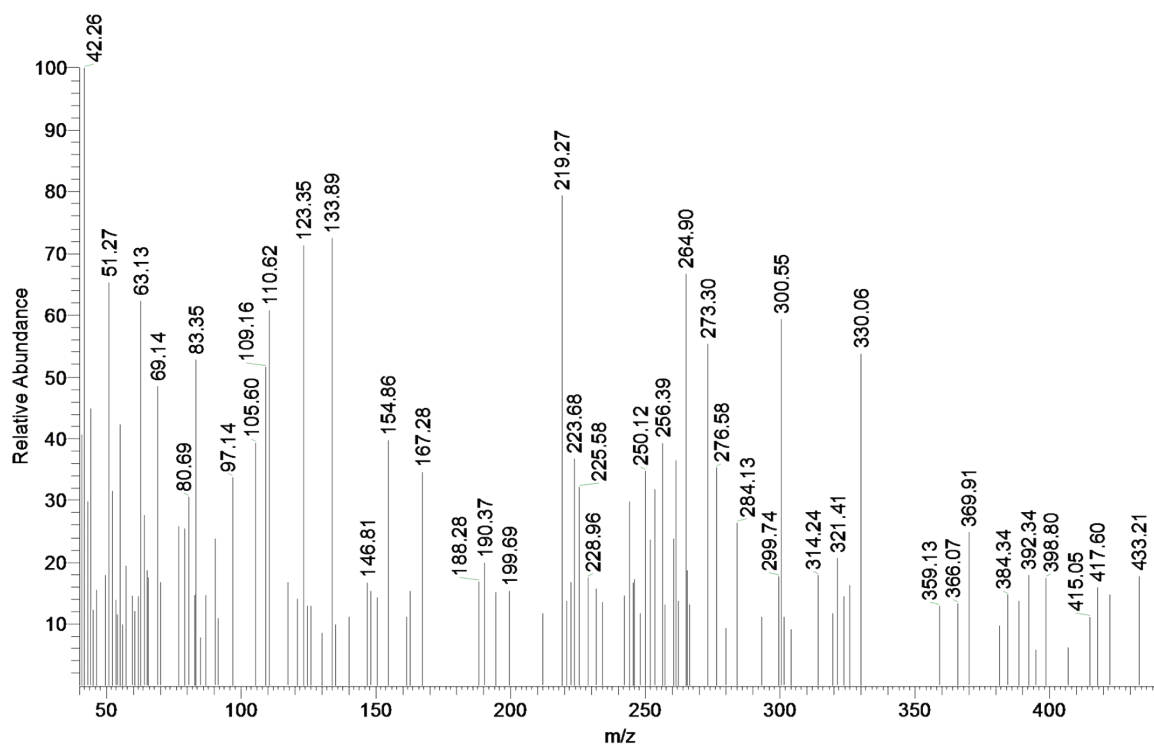


¹H NMR spectrum of **13**

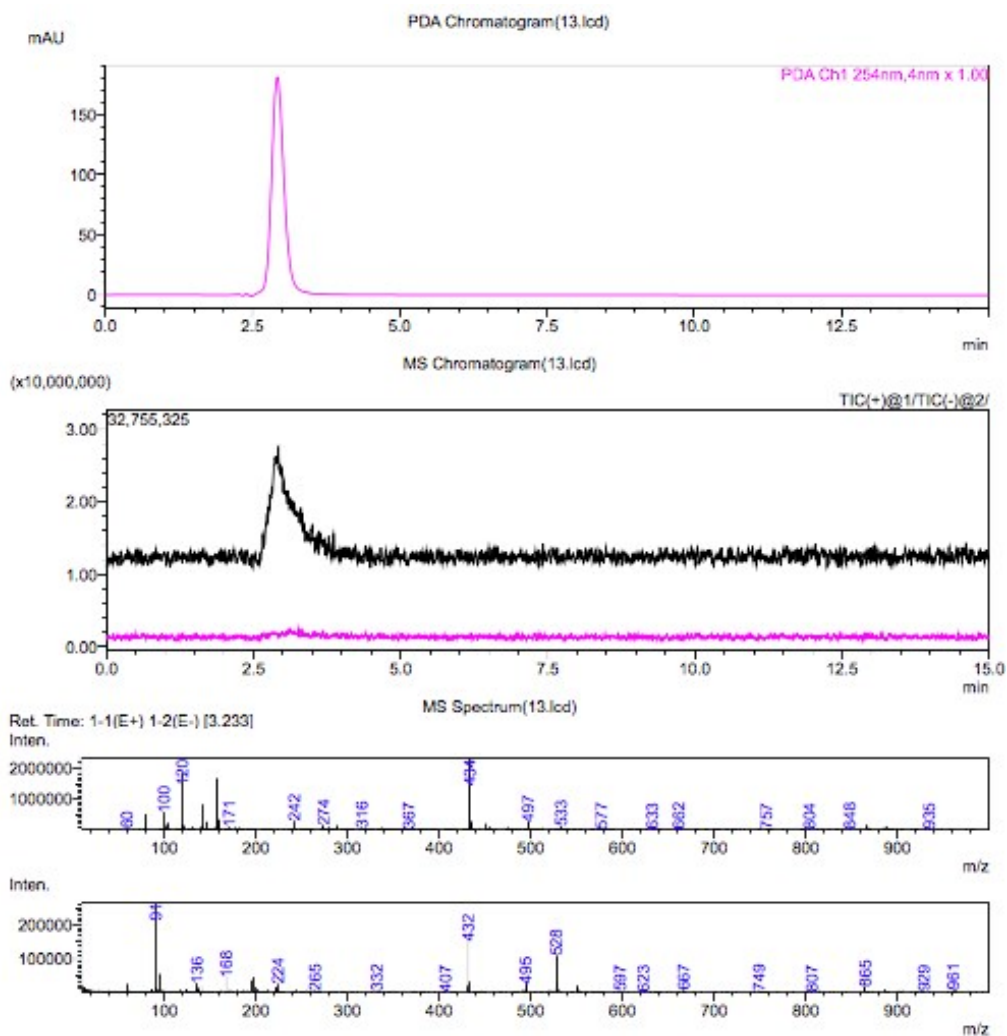


¹³C NMR spectrum of **13**

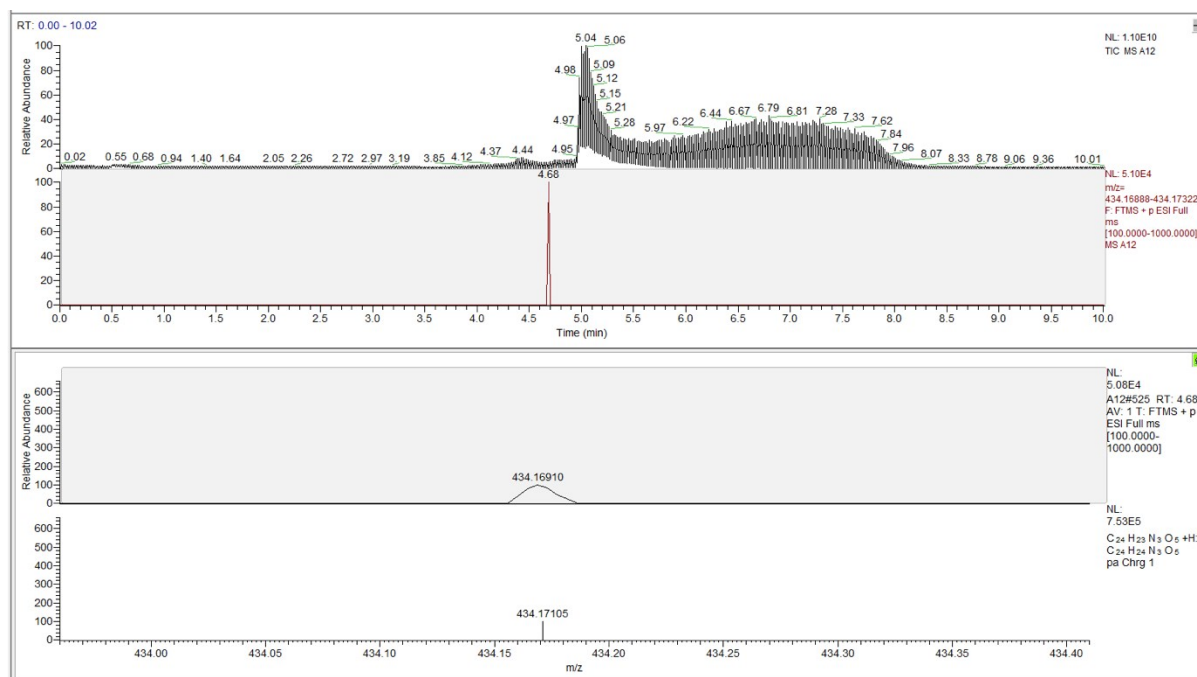
fathi-hamed-13 #117-118 RT: 1.97-1.99 AV: 2 SB: 2 4.45, 4.45 NL: 3.63E2
T: {0,0} + c EI Full ms [40.00-1000.00]



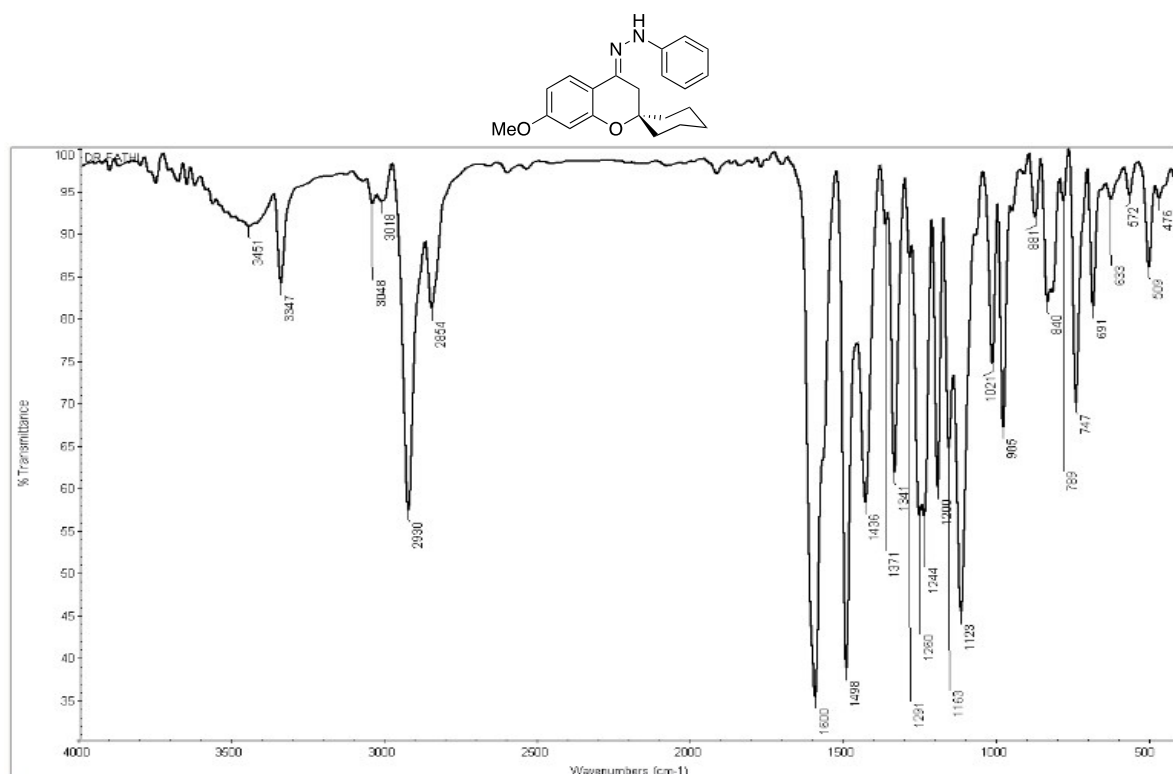
EI-MS spectrum of 13



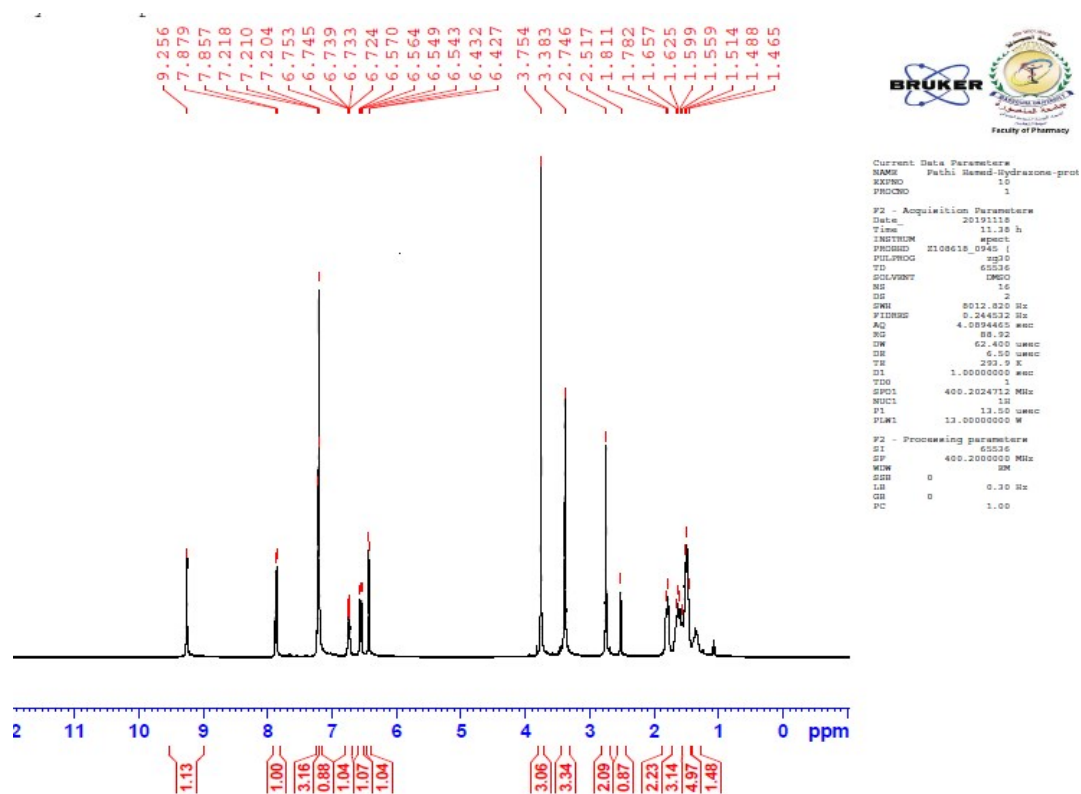
EI-MS spectrum of **13**



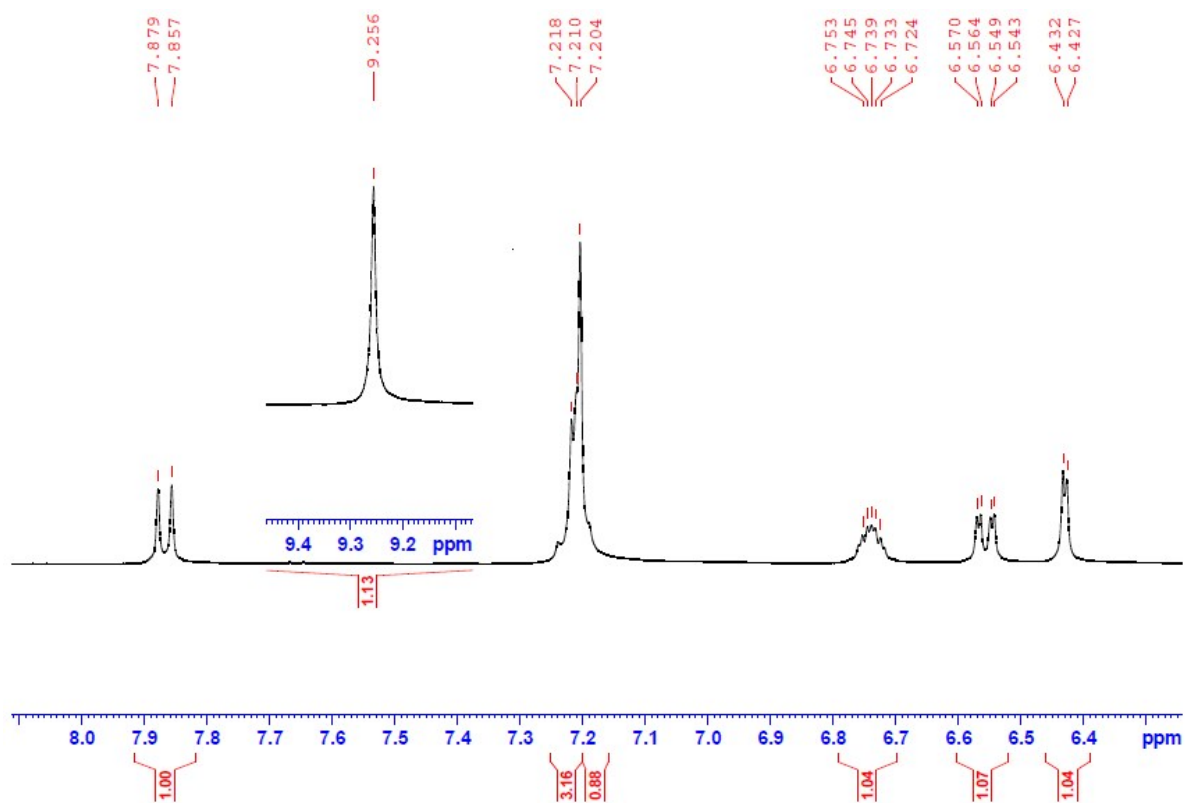
HR-MS spectrum of **13**



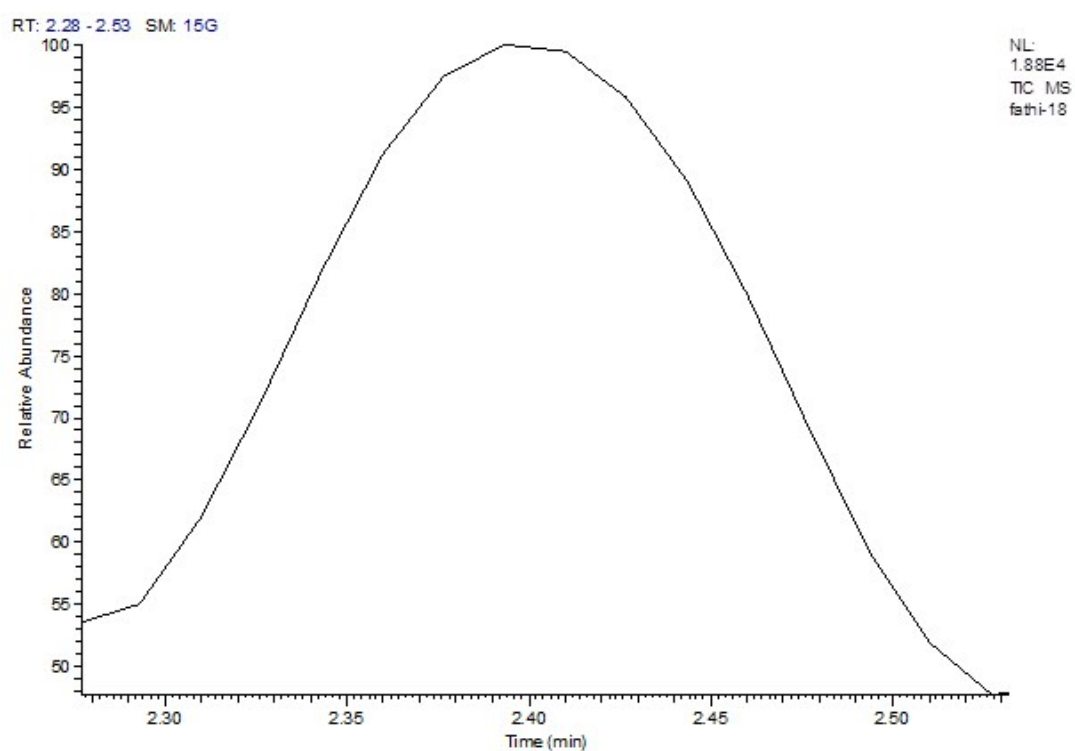
IR spectrum of compound 15



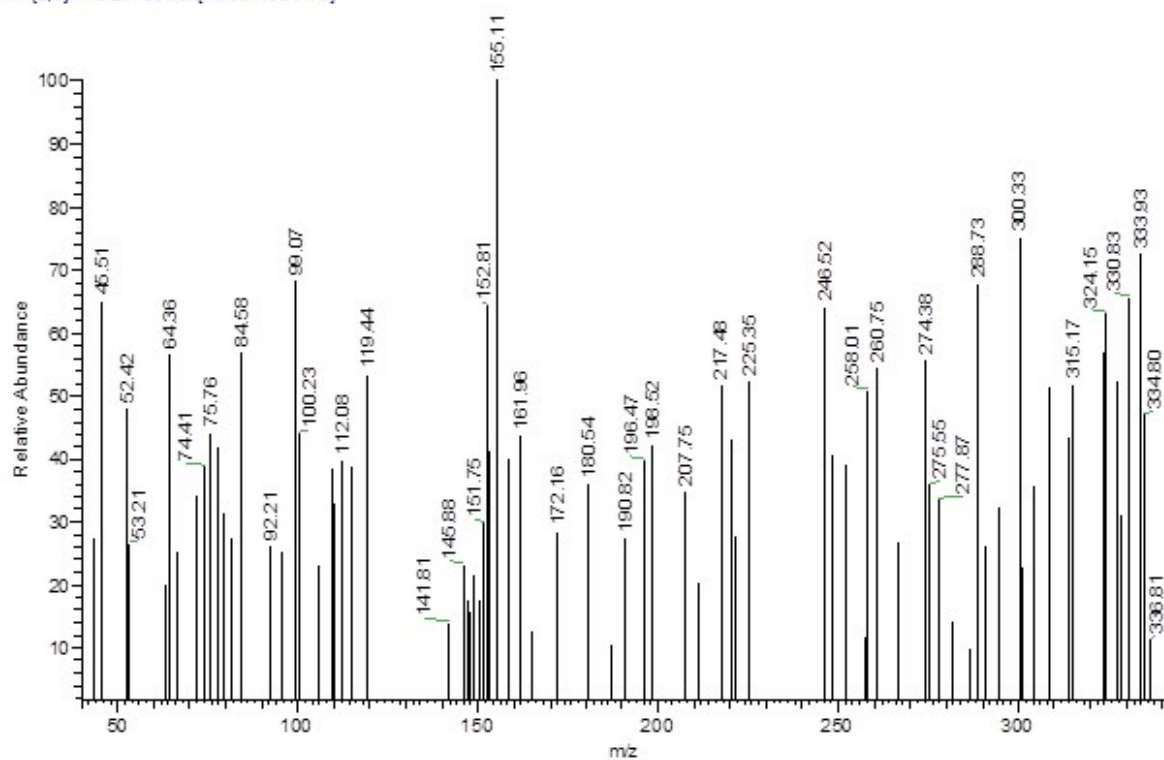
¹H NMR spectrum of compound 15



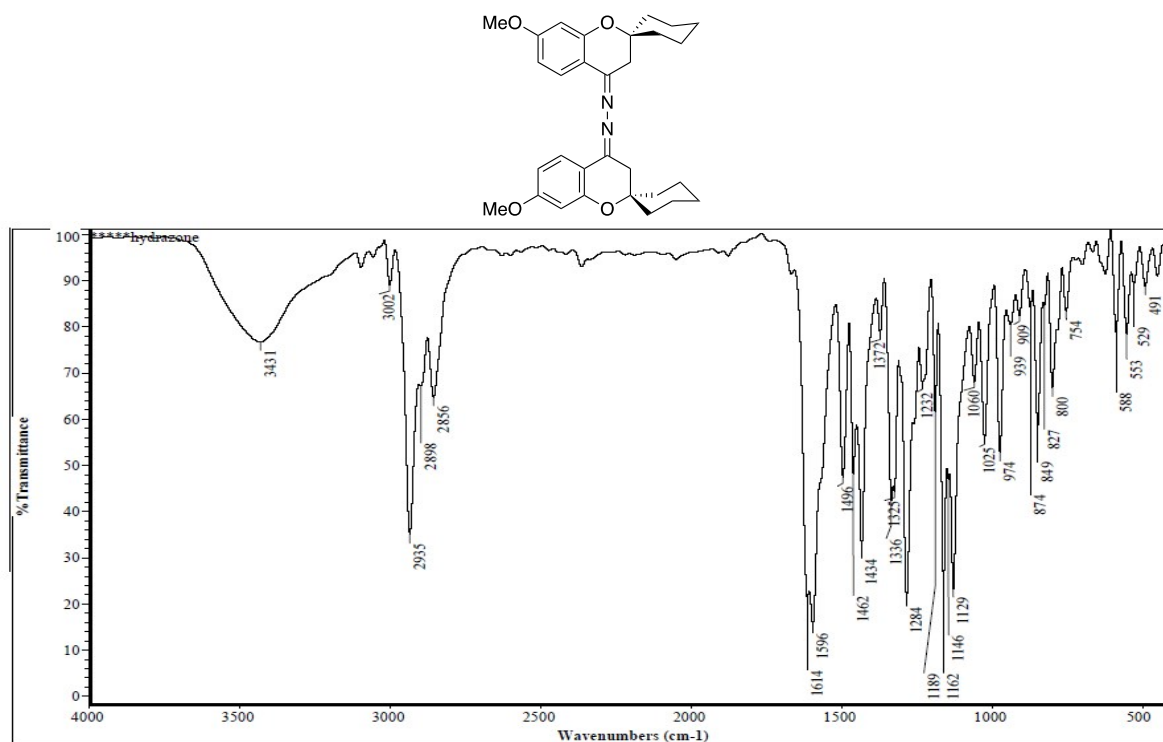
¹H NMR spectrum of **15**



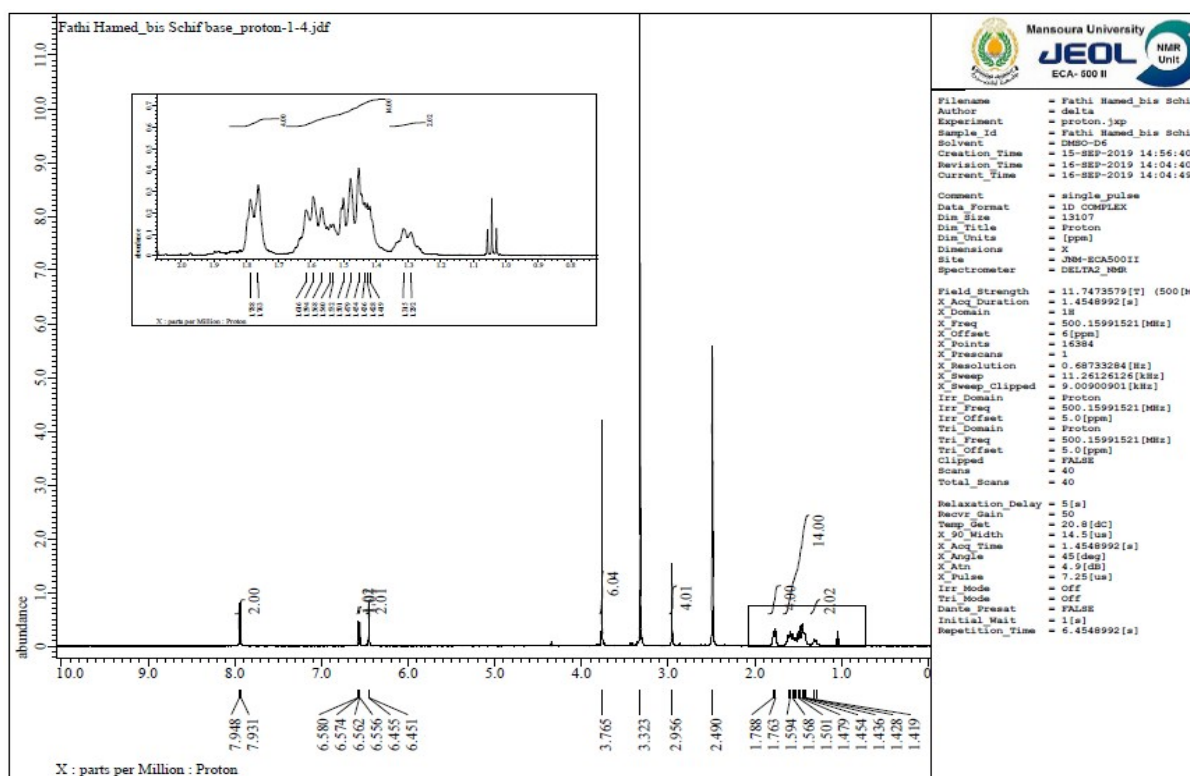
fathi-18 #186 RT: 3.13 AV: 1 SB: 2 4.55, 4.57 NL: 2.73E2
T: {0,0} + c EIFull ms [40.00-1000.00]



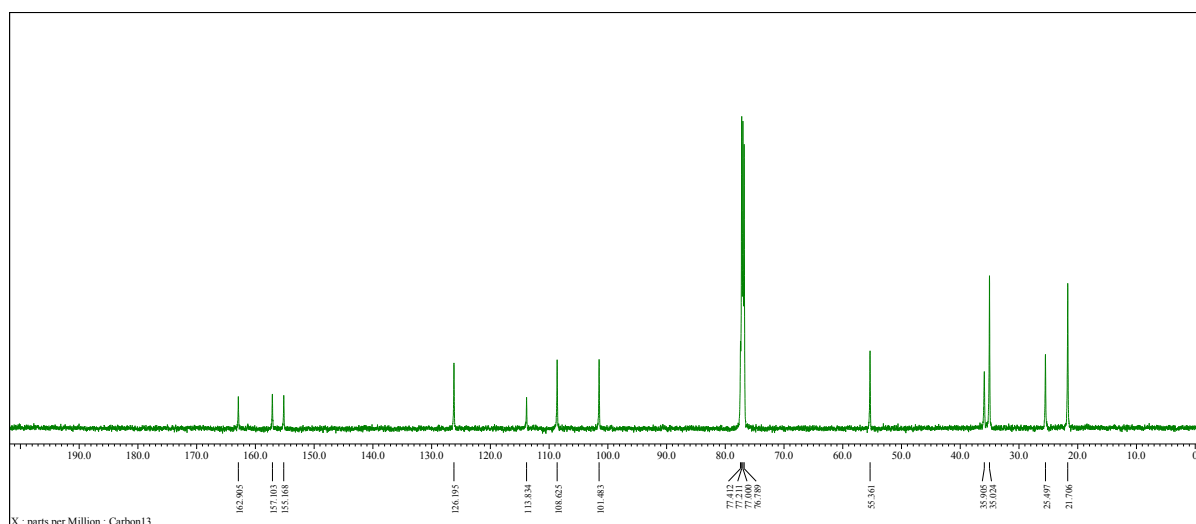
EI-MS spectrum of **15**



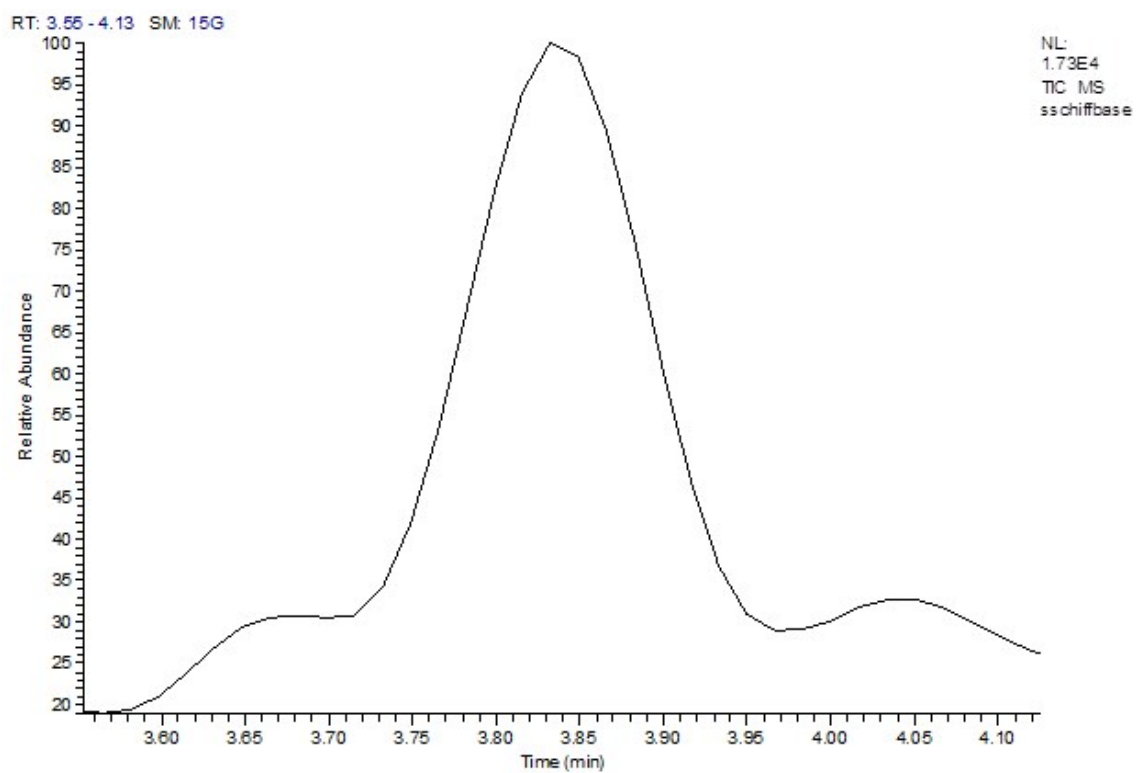
IR spectrum of 16



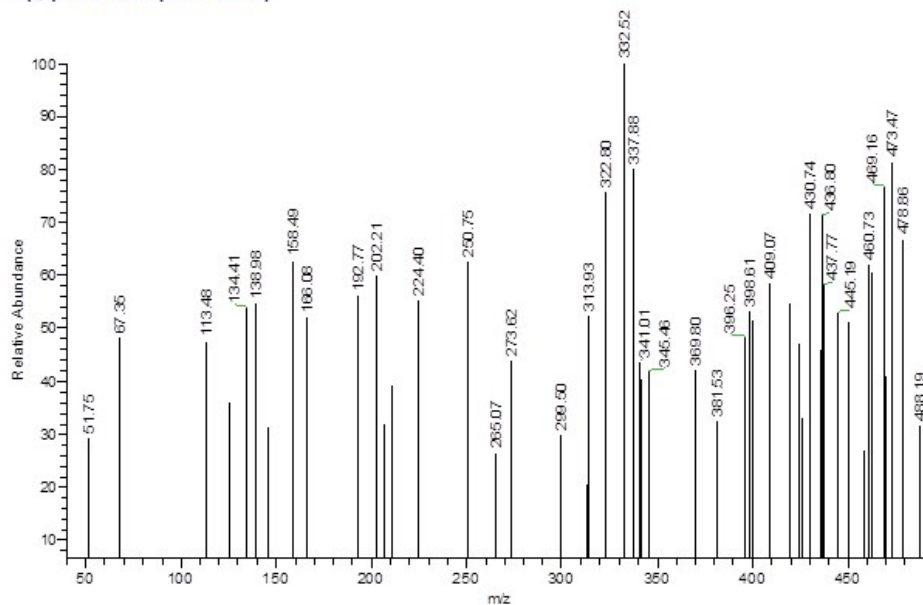
¹H NMR spectrum of 16



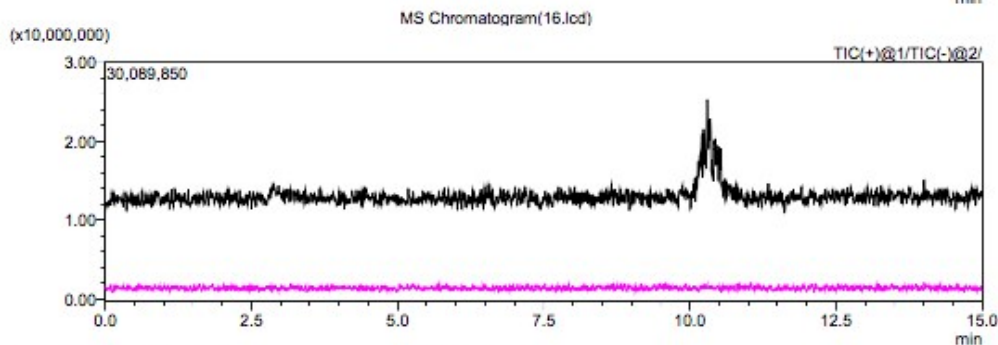
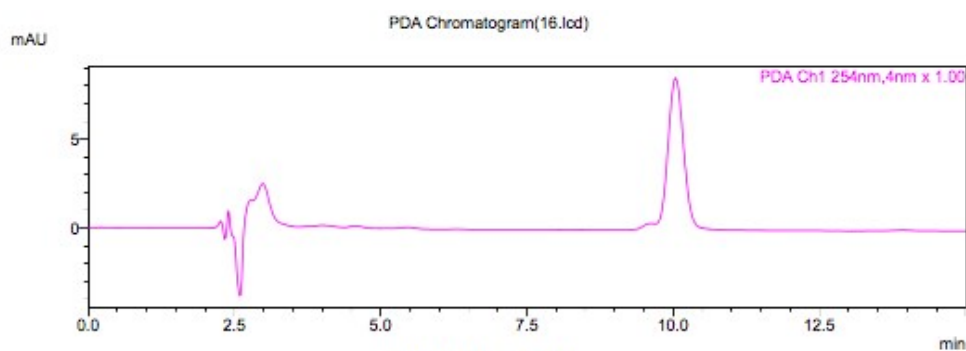
¹³C NMR spectrum of **16**



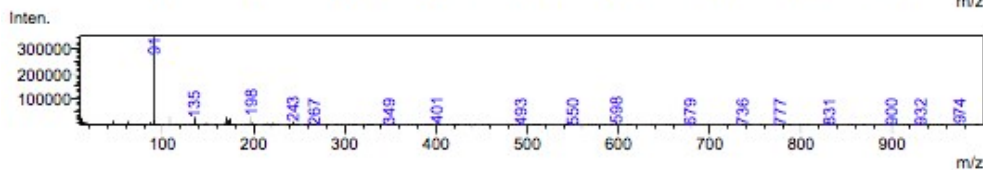
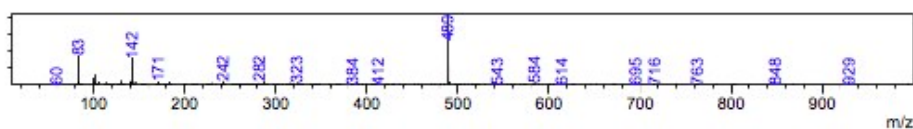
sschiffbase#61 RT: 1.04 AV: 1 SB: 2 4.45, 4.46 NL: 2.35E2
T: [0,0] + cEIFull.ms [40.00-1000.00]



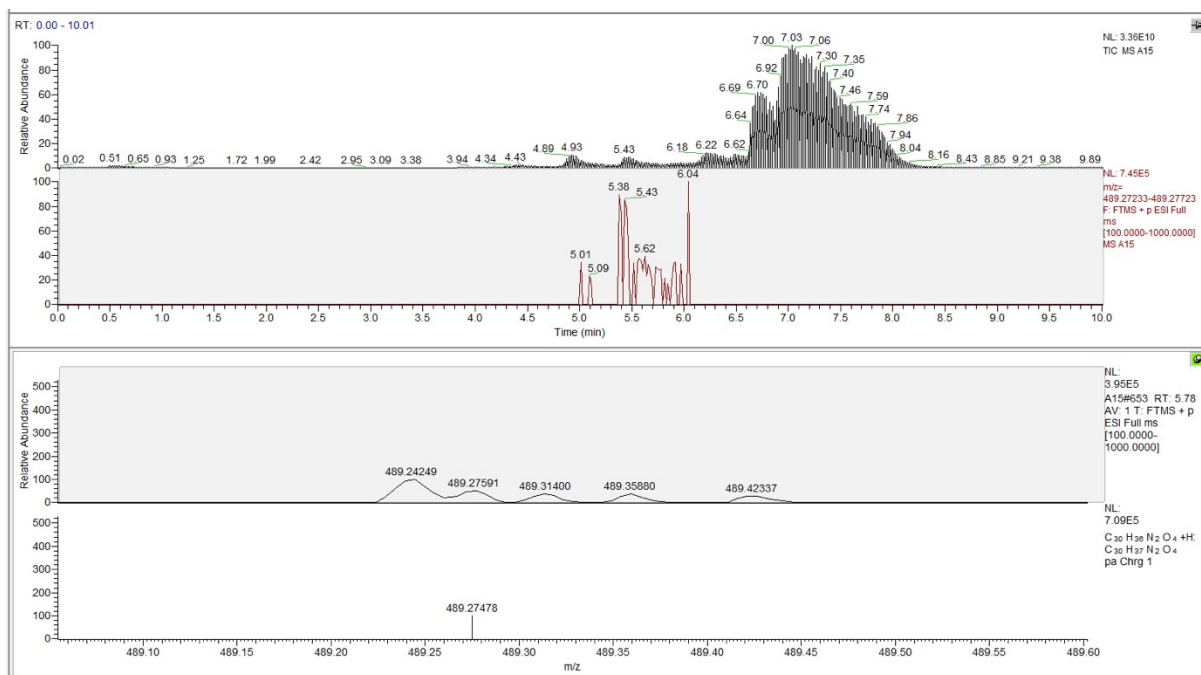
EI-MS spectrum of 16



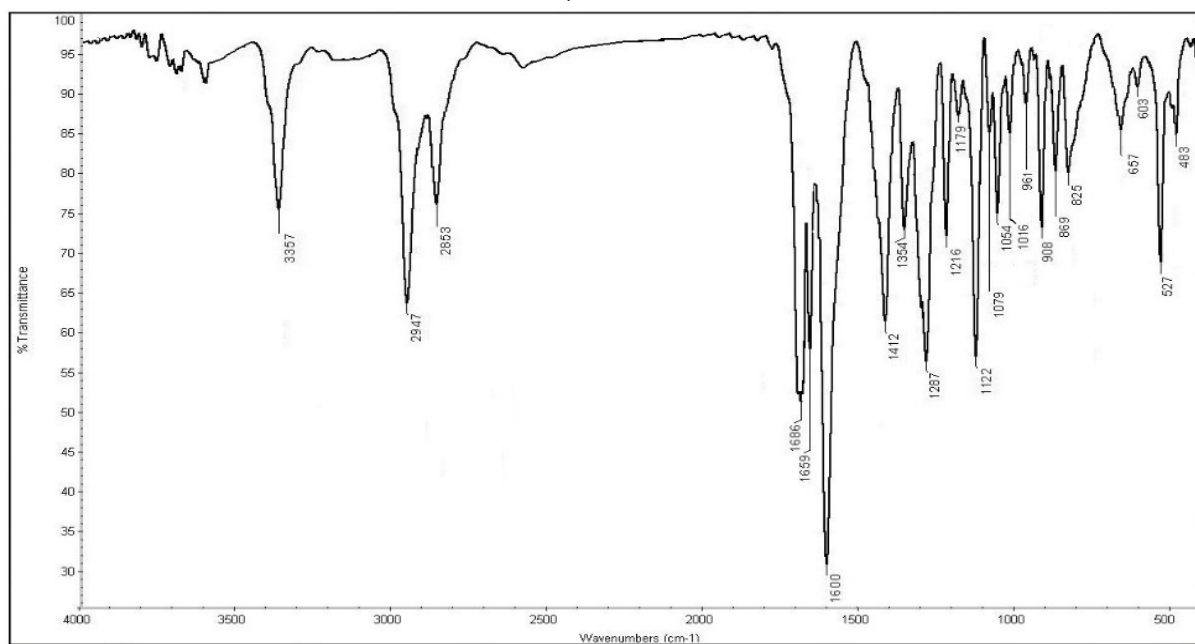
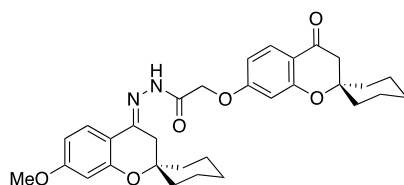
Ret. Time: 1-1(E+) 1-2(E-) [10.287]
Inten.



LC-MS spectrum of 16

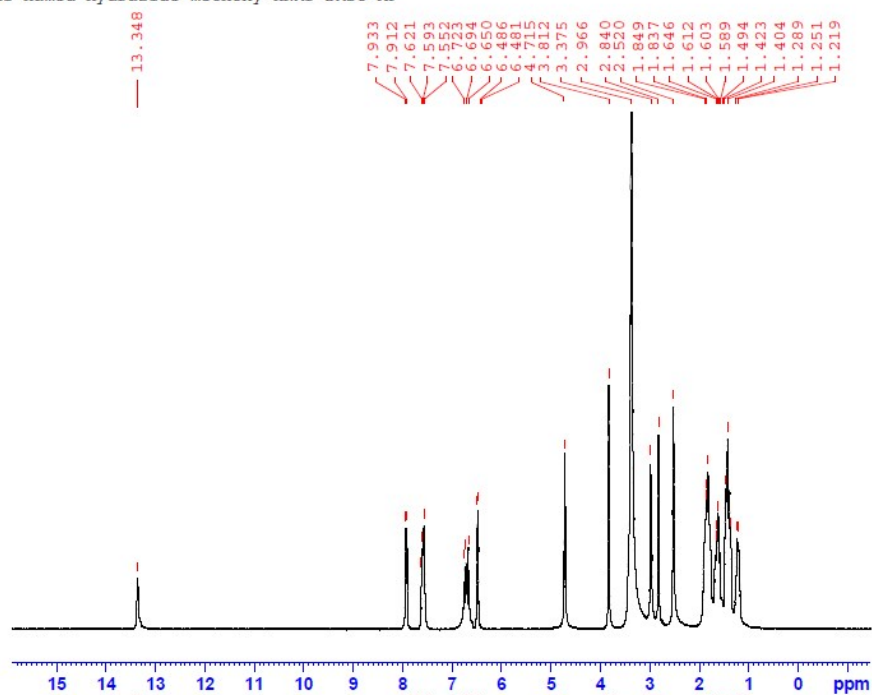


HR-MS spectrum of 16



IR spectrum of 17

Fathi Hamed-hydrazide methoxy-HNMR-DMSO-AF



¹H NMR spectrum of 17

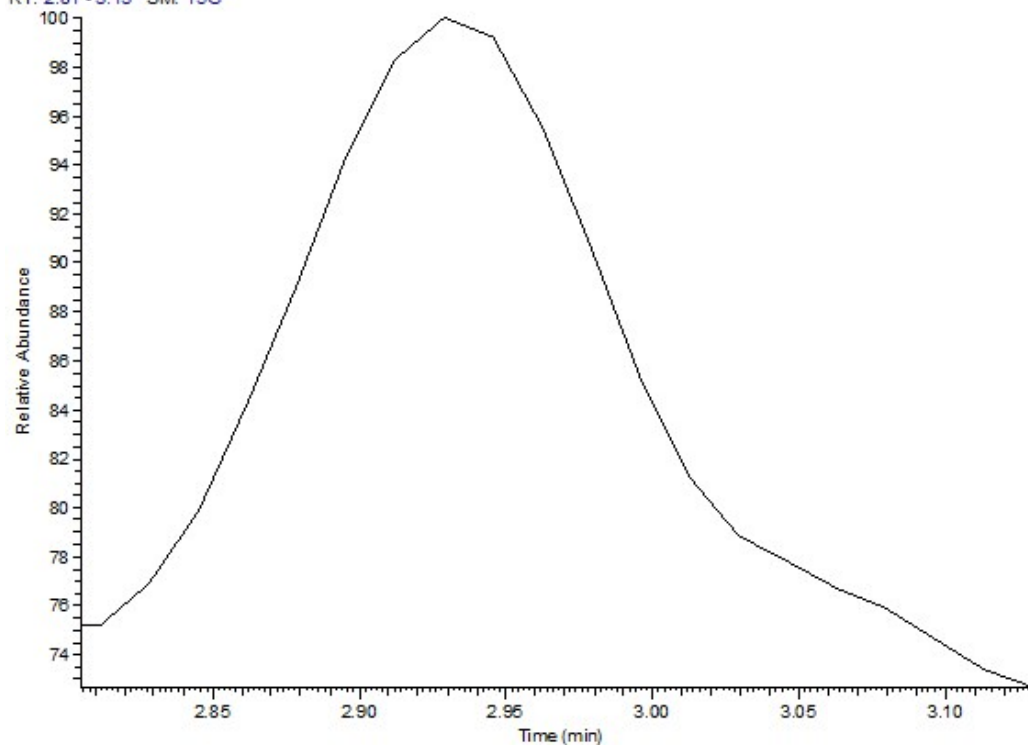


Current Data Parameters
NAME Fathi Hamed-hydrazide methoxy-HNMR-DMSO-AF
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191127
Time 11:46
INSTRUM spect
PROBHD Z106C18_0945_1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 70
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 176.72
SQ 62.400 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TDO 1
SFO1 400.2024712 MHz
NUC1 13
P1 13.50 usec
PLM1 13.00000000 W

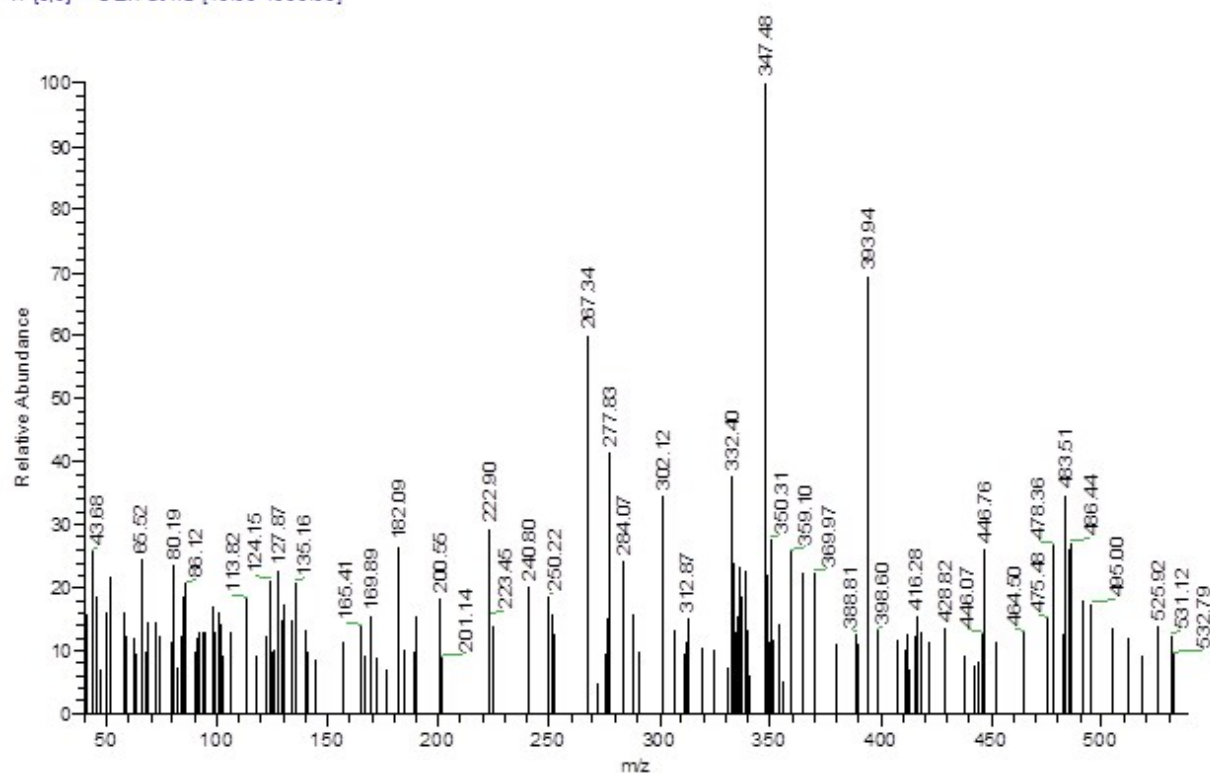
F2 - Processing parameters
SI 65536
SF 400.2000000 MHz
WDW EM
SSB 0
GB 0
PC 1.00

RT: 2.81 - 3.13 SM: 15G

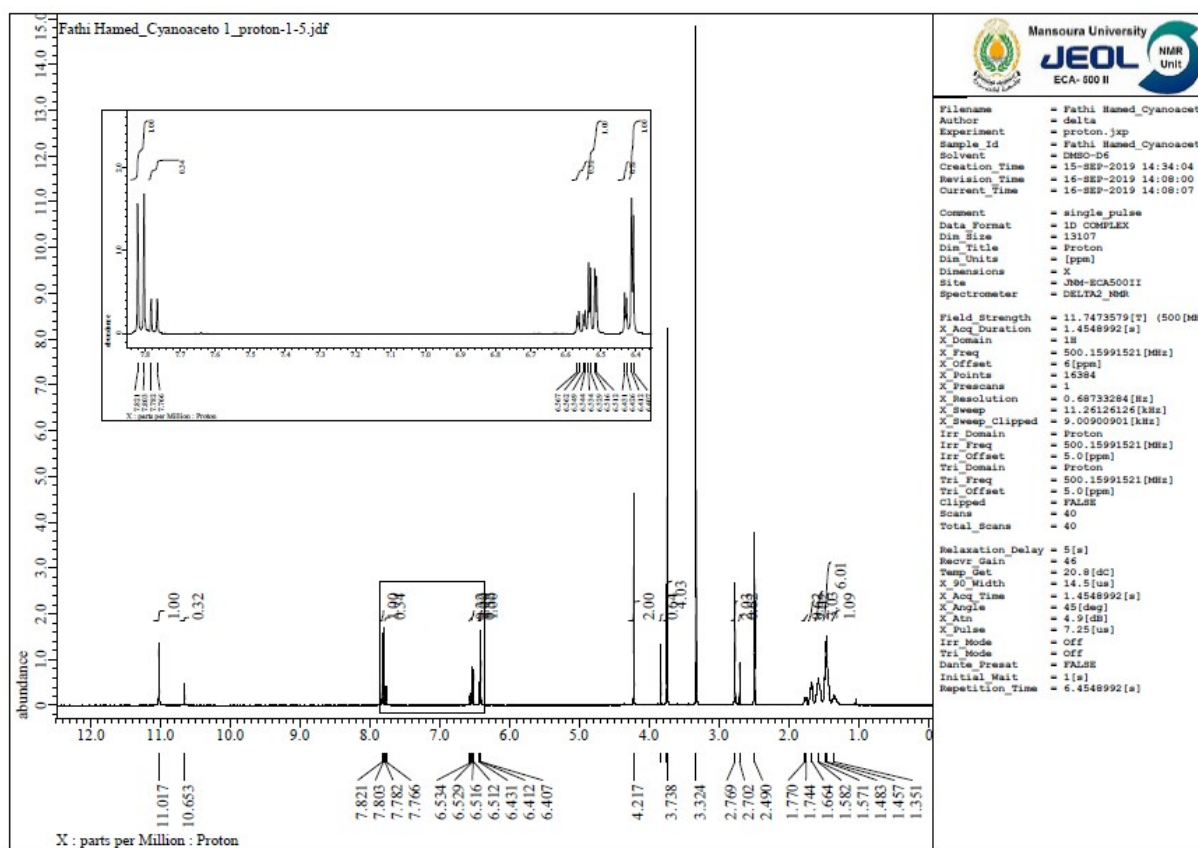
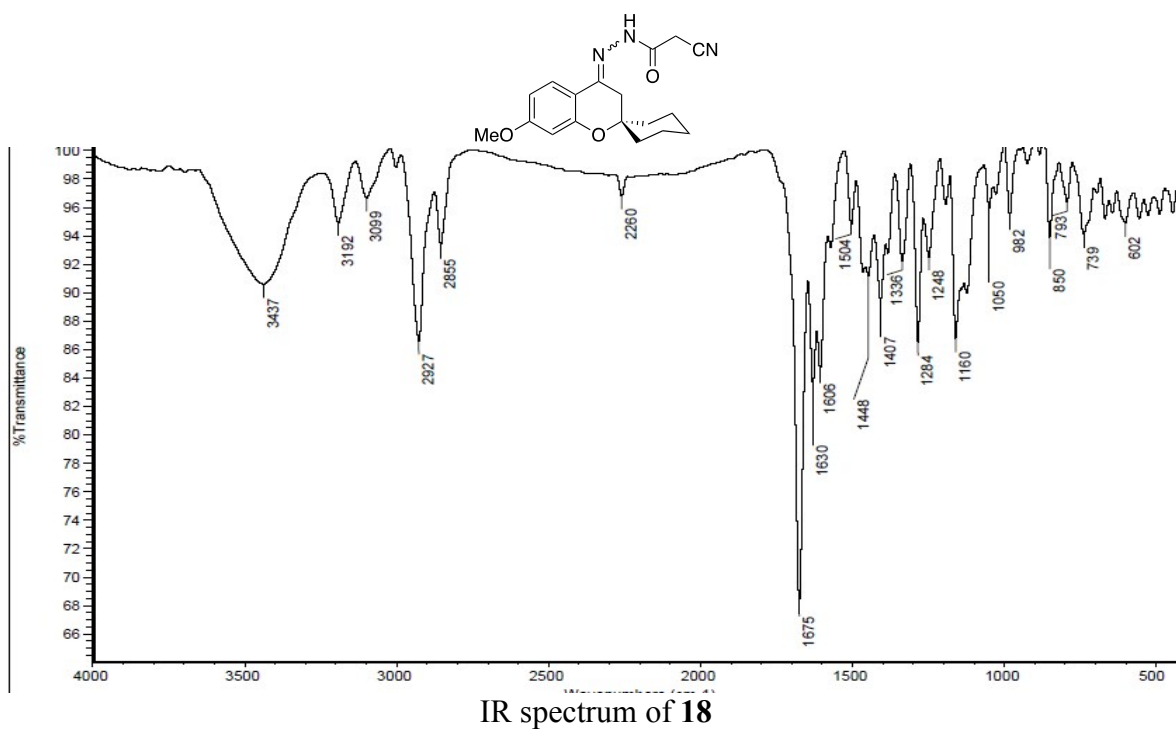


NL:
2.20E4
TIC MS
fathi-17

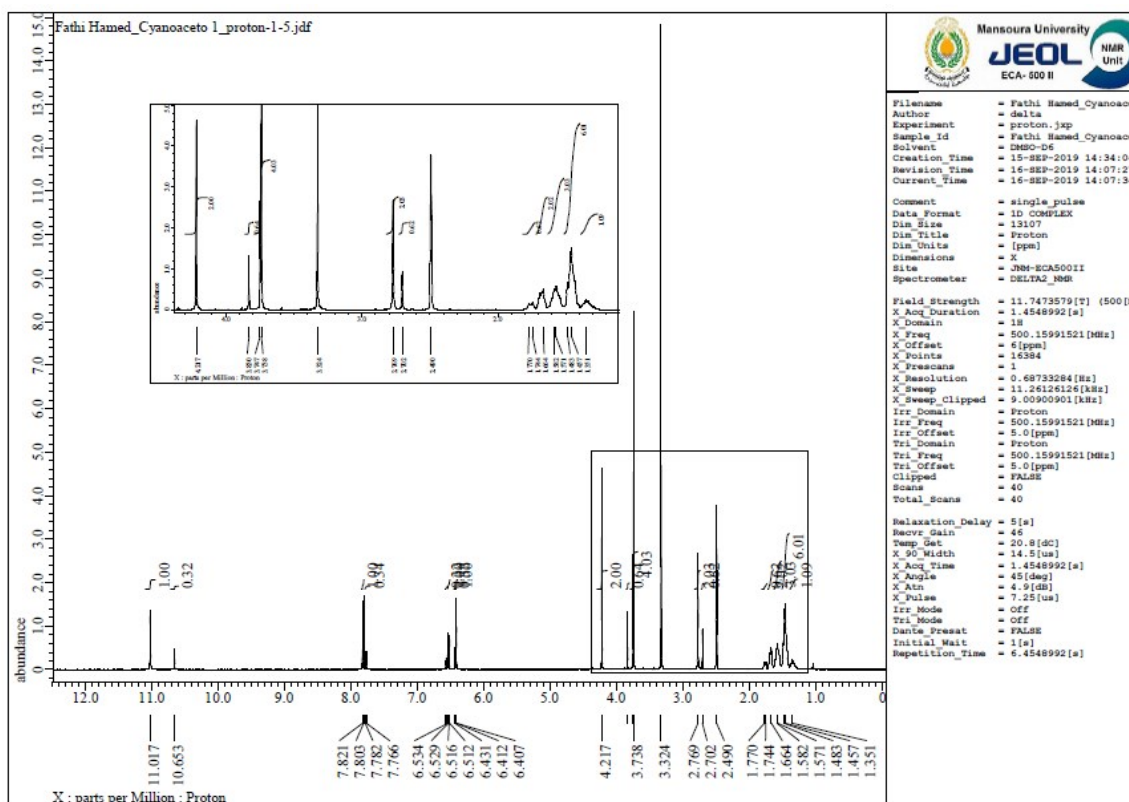
fathi-17 #212 RT: 3.58 AV: 1 SB: 2 4.45, 4.45 NL: 8.29E2
T: {0,0} + c EI Full ms [40.00-1000.00]



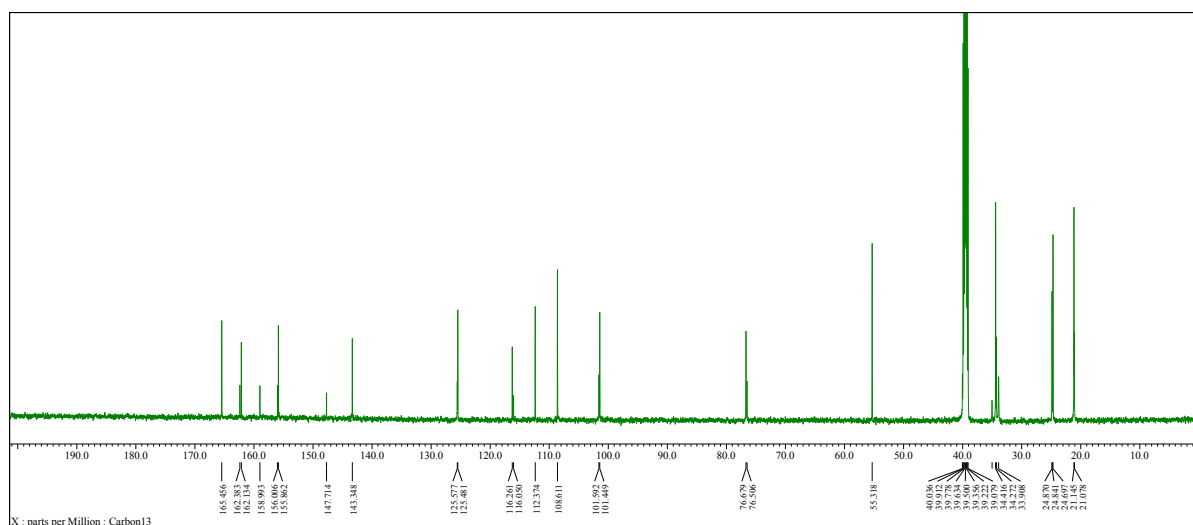
EI-MS spectrum of 17



¹H NMR spectrum of 18

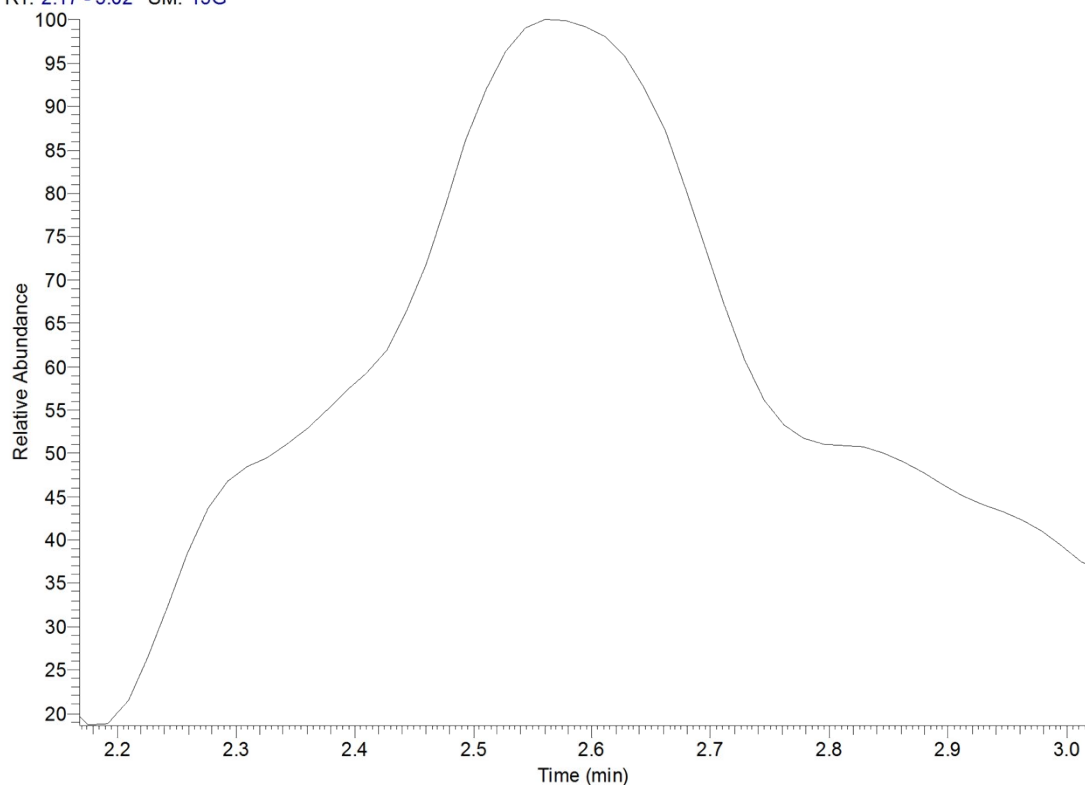


¹H NMR spectrum of **18**



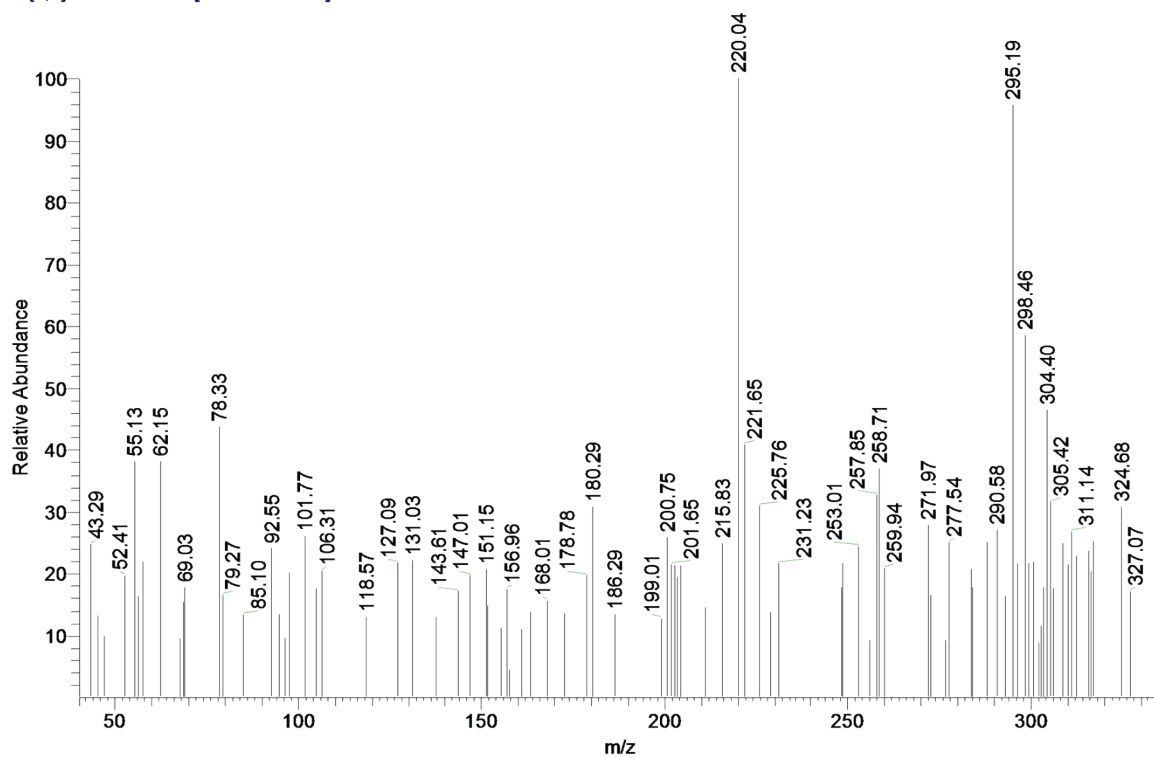
¹³C NMR spectrum of **18**

RT: 2.17 - 3.02 SM: 15G

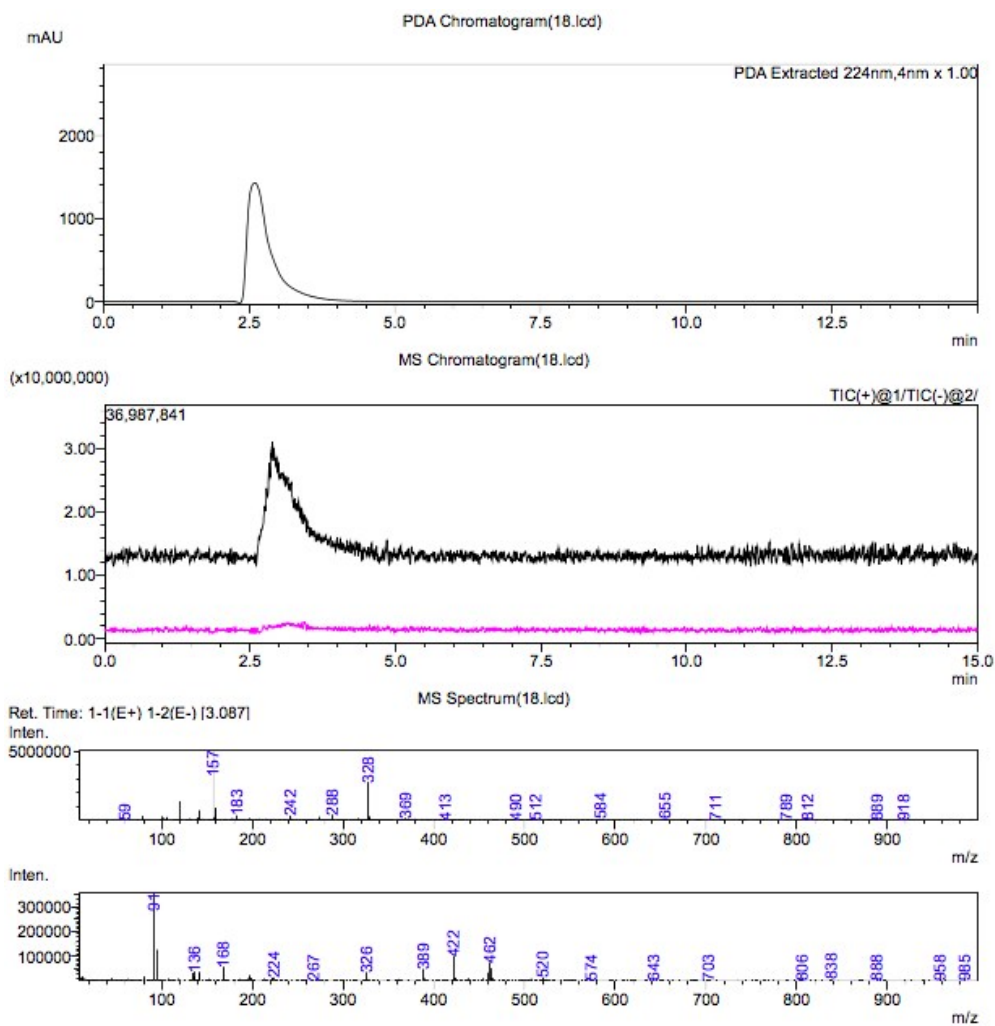


NL:
2.55E4
TIC MS
fathi-
hamed-18

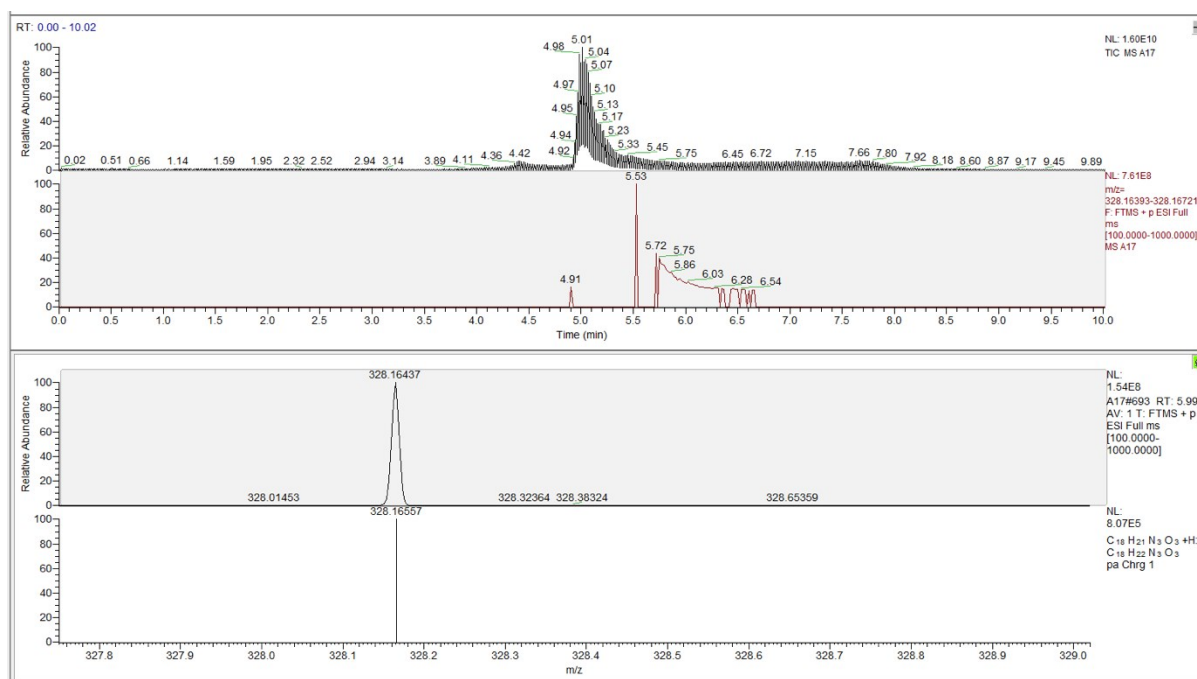
fathi-hamed-18 #238 RT: 4.00 AV: 1 SB: 2 4.45 , 4.45 NL: 5.27E2
T: {0,0} + c EI Full ms [40.00-1000.00]



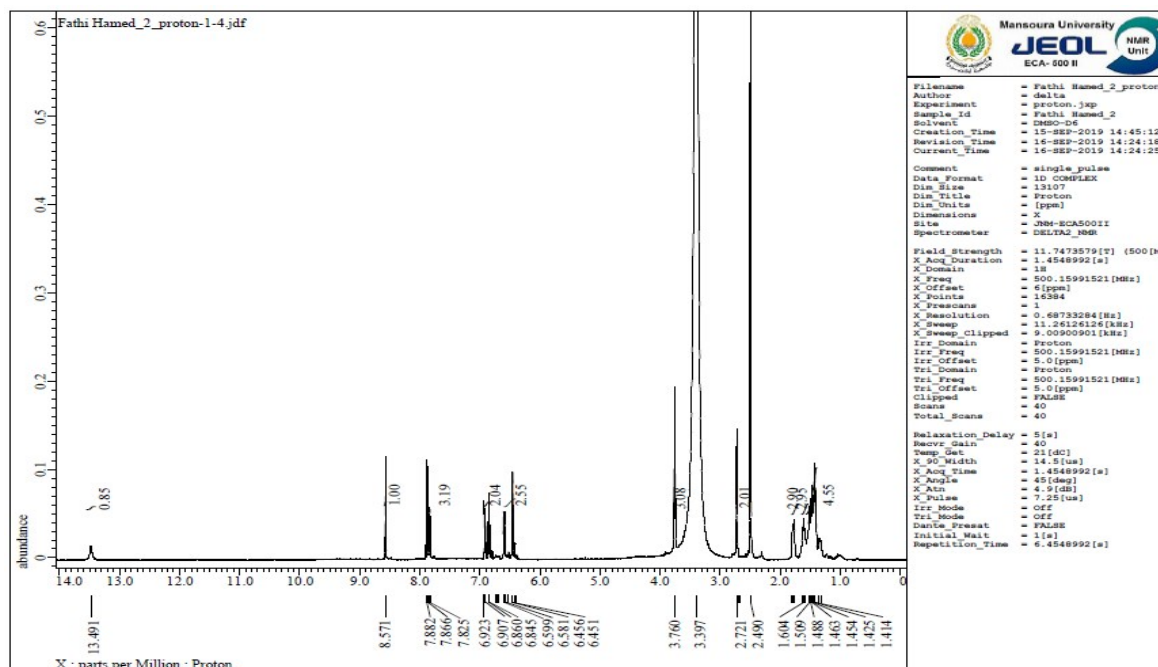
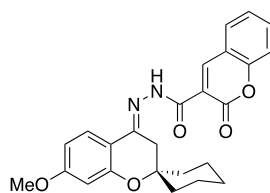
EI-MS spectrum of 18



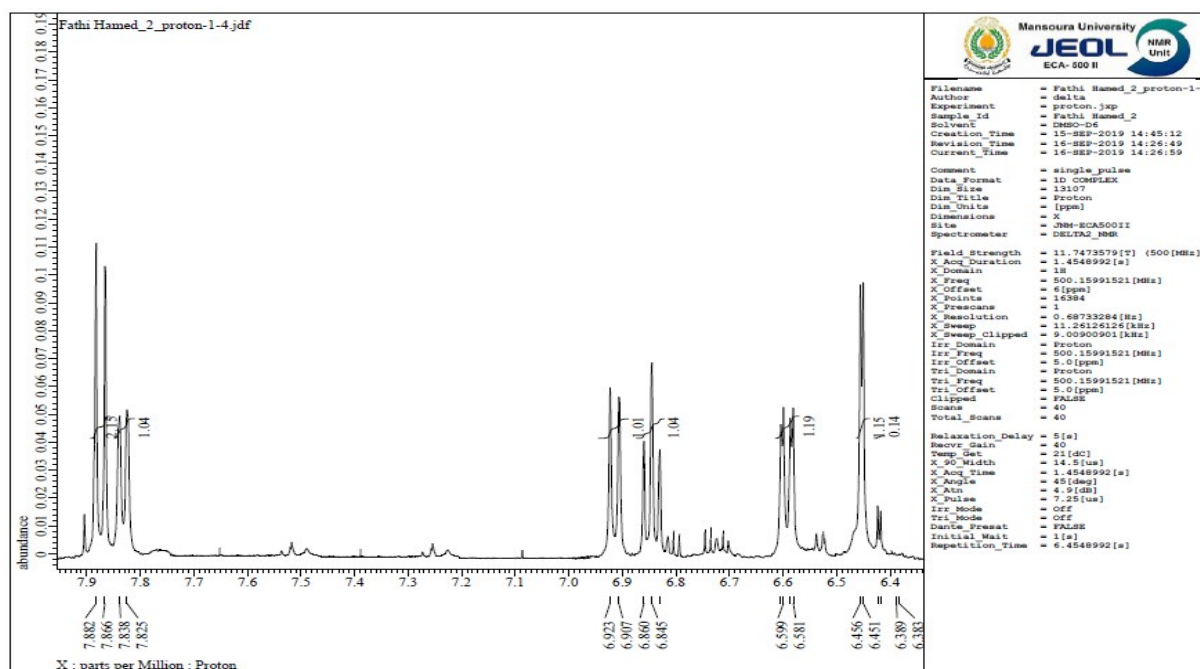
LC-MS spectrum of **18**



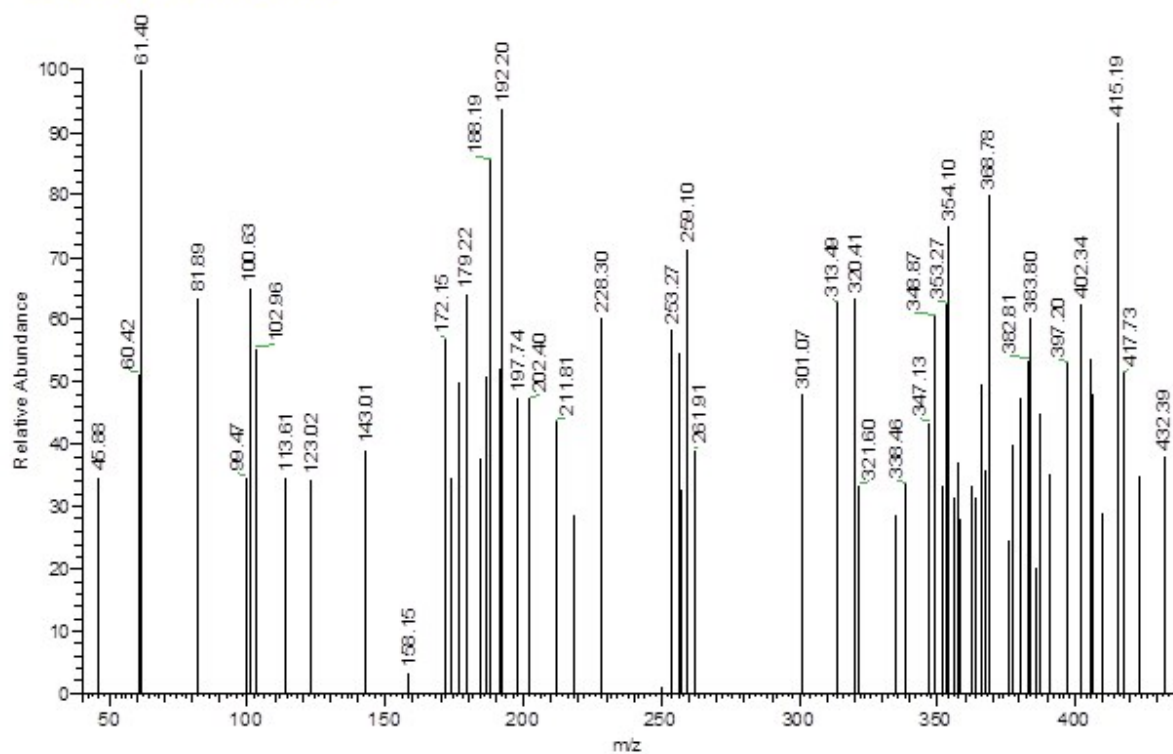
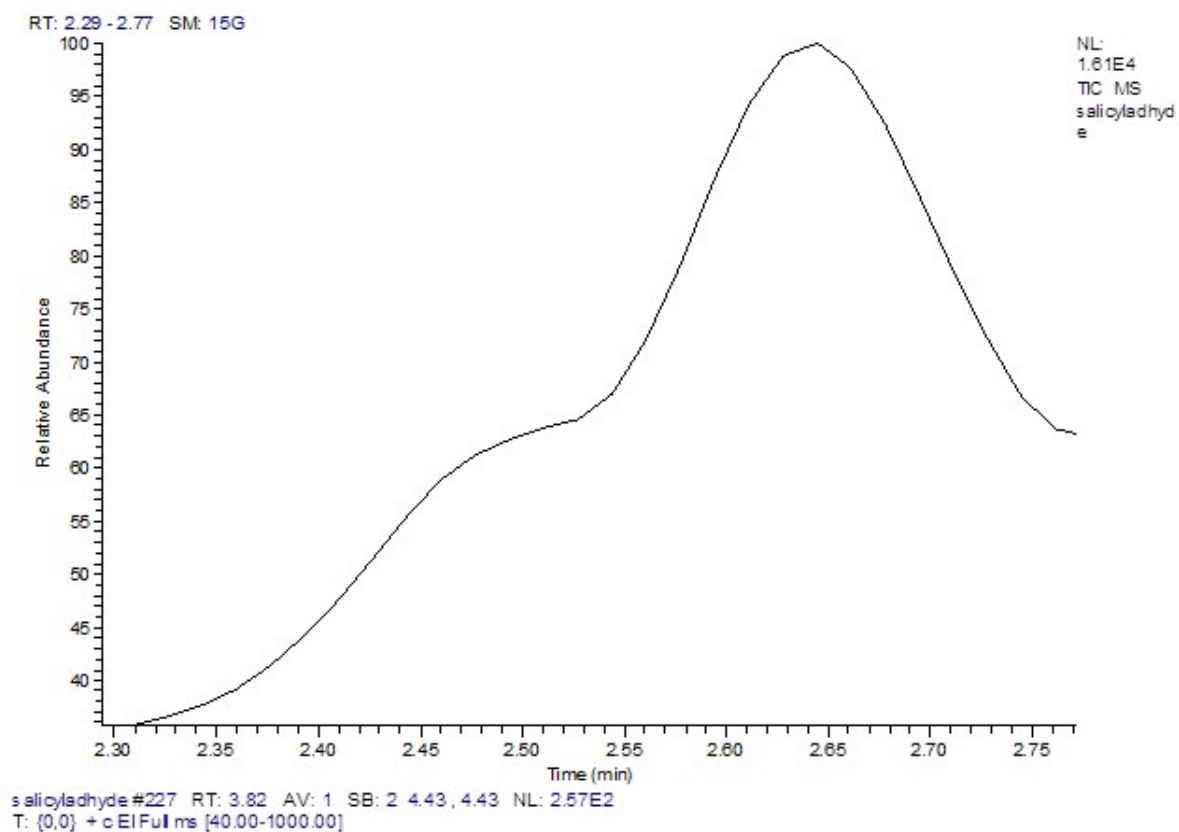
HR-MS spectrum of **18**



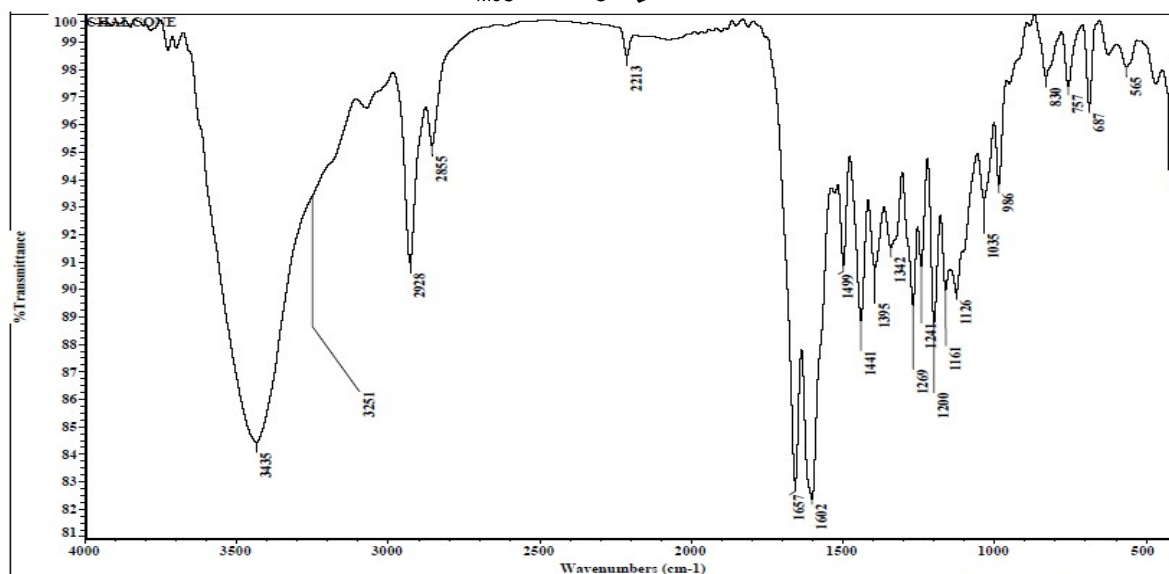
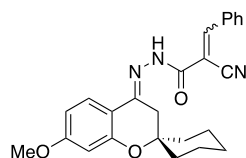
¹H NMR spectrum of 19



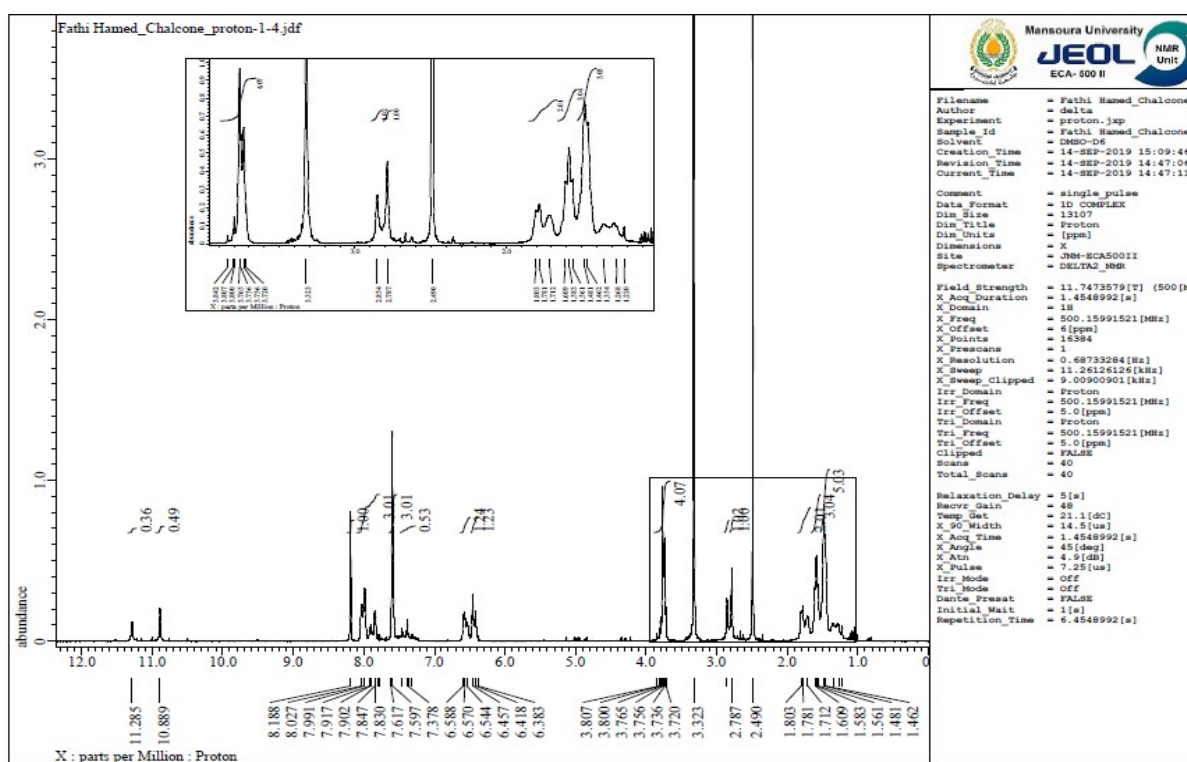
¹H NMR spectrum of 19



EI-MS spectrum of 19

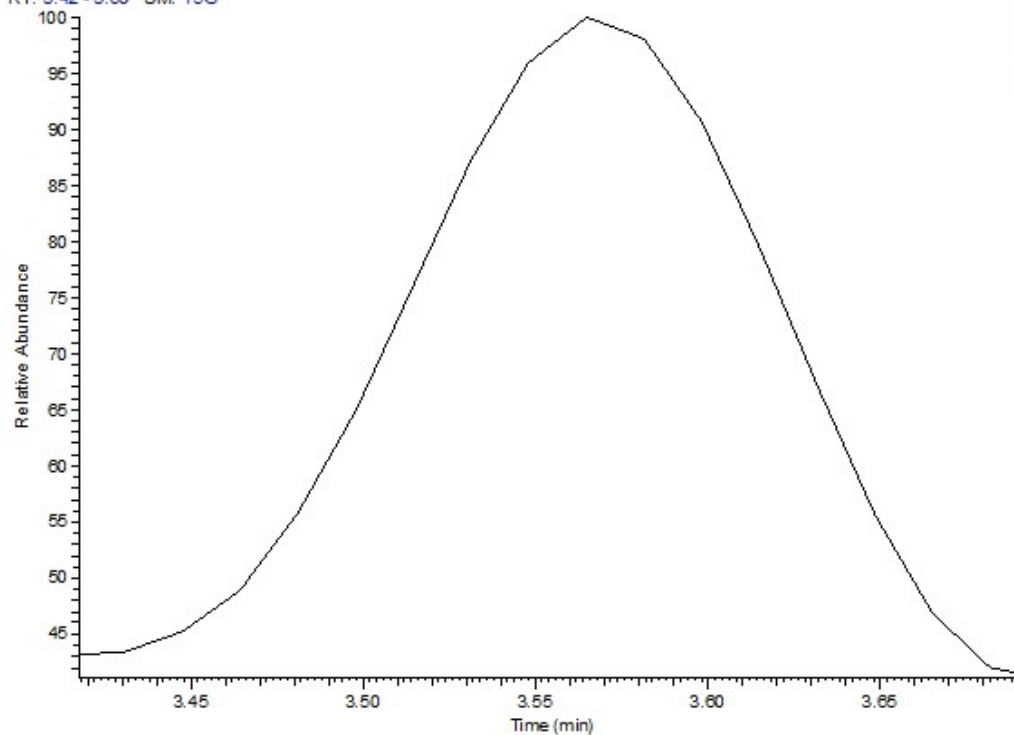


IR spectrum of 20



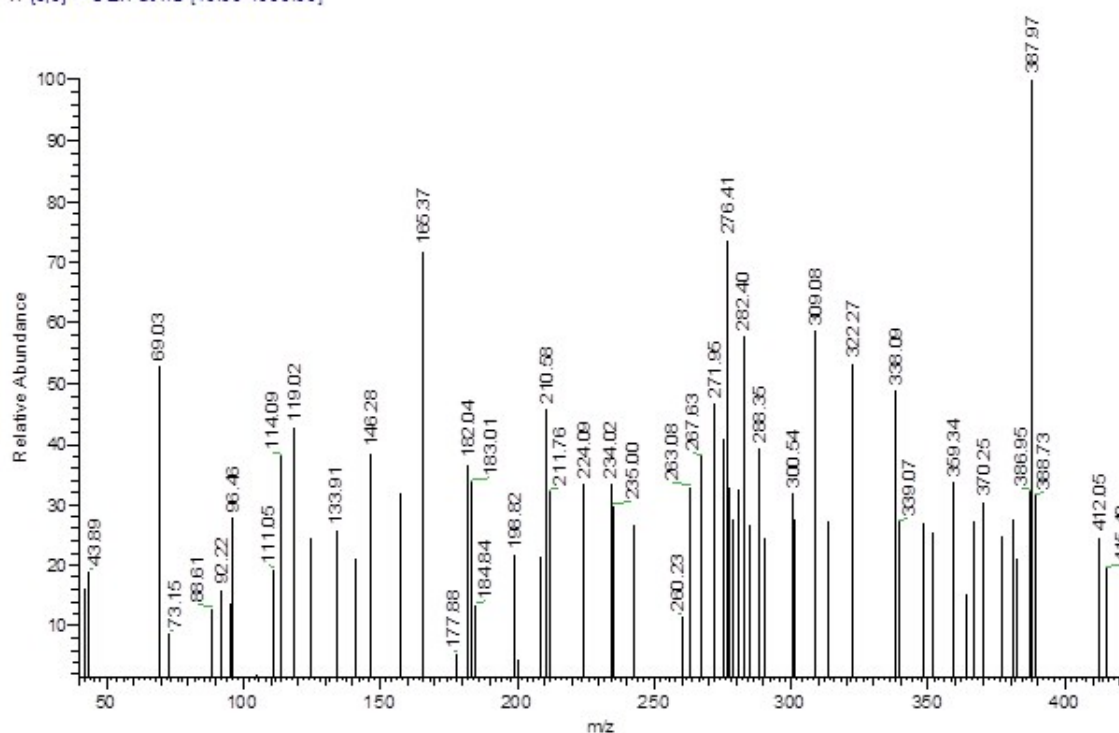
¹H NMR spectrum of 20

RT: 3.42 - 3.69 SM: 15G

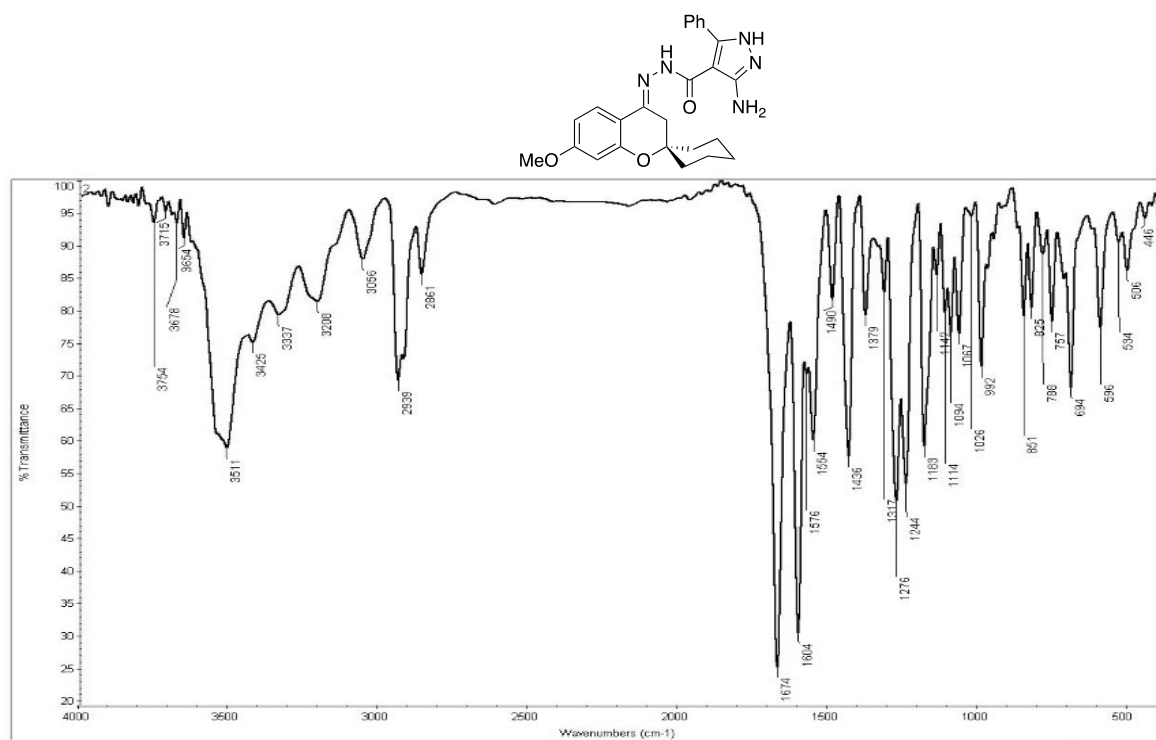


NL:
2.13E4
TIC MS
chalcone

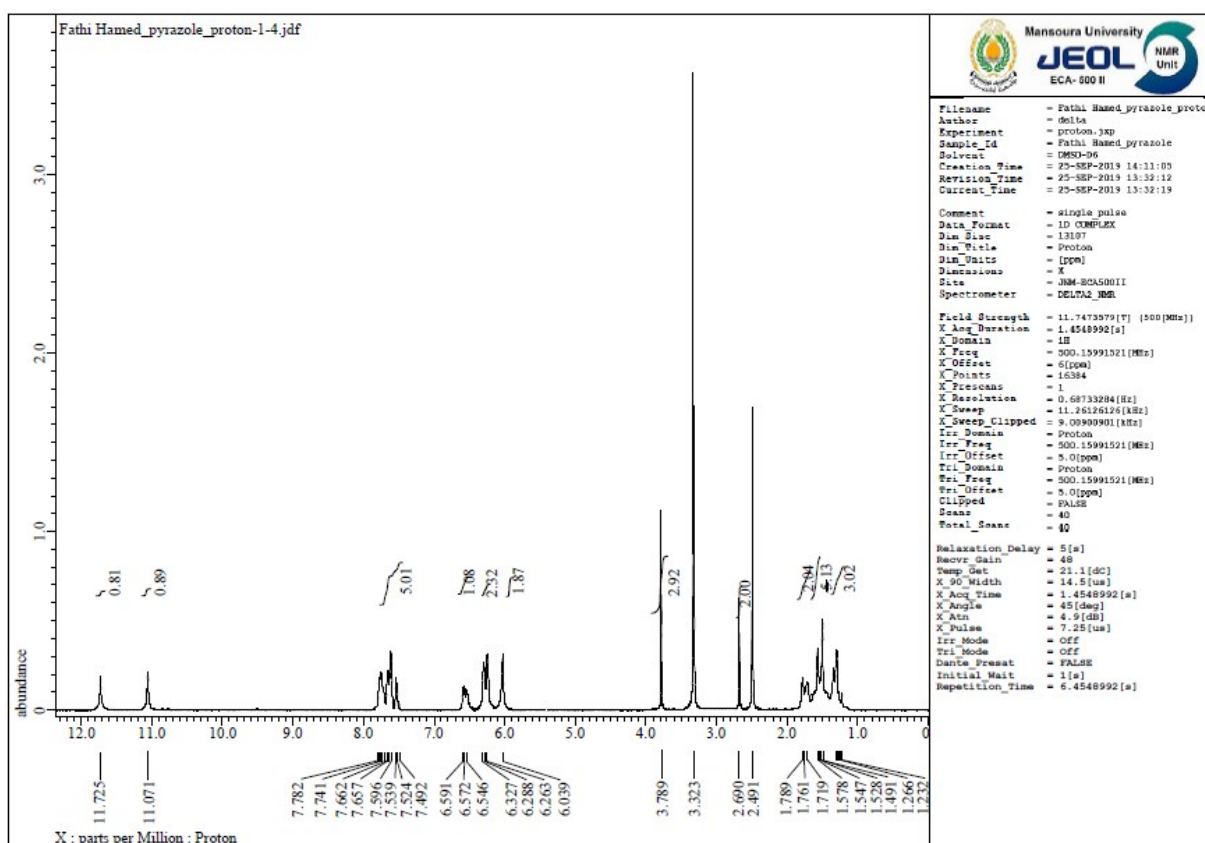
chalcone #243 RT: 4.08 AV: 1 SB: 2 4.47, 4.47 NL: 3.86E2
T: {0.0} + c EI Full ms [40.00-1000.00]



EI-MS spectrum of 20

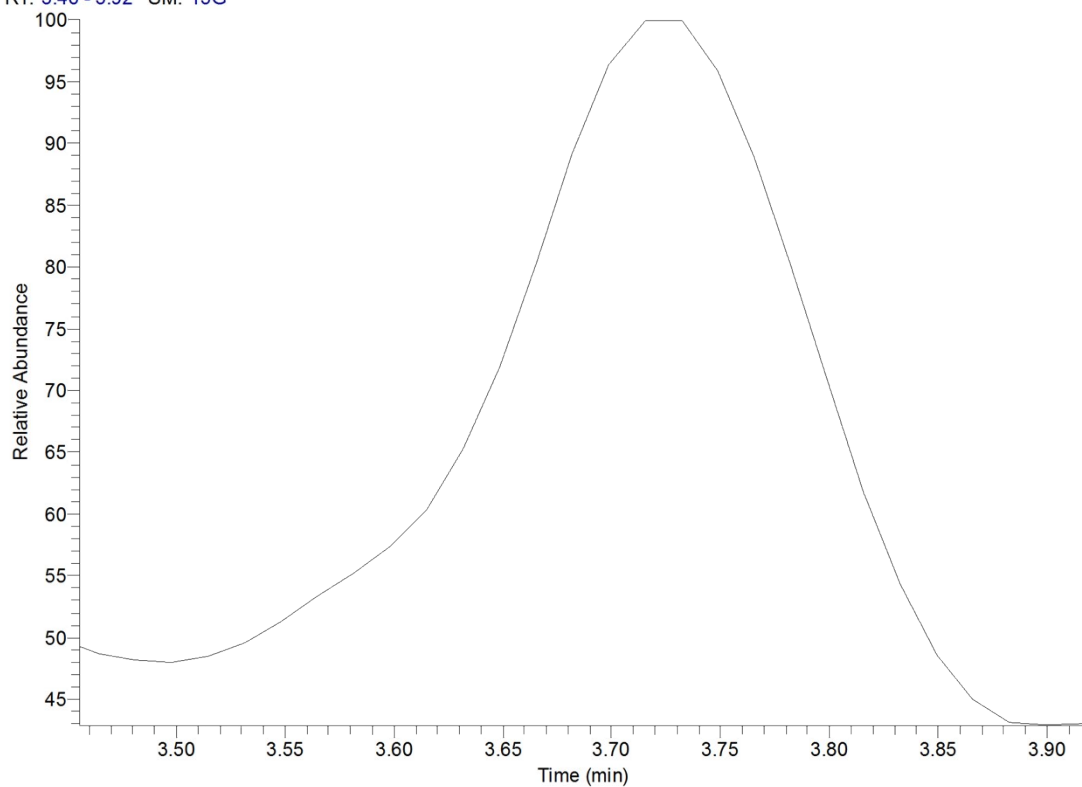


IR spectrum of **21**



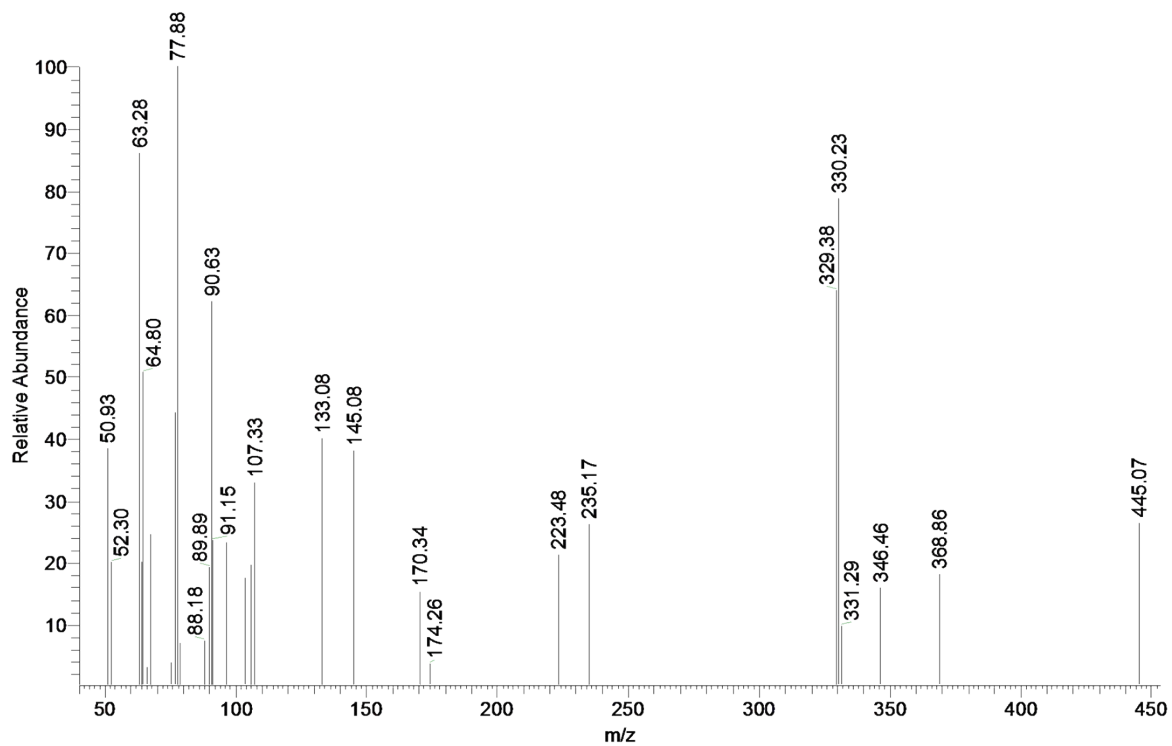
¹H NMR spectrum of **21**

RT: 3.46 - 3.92 SM: 15G



NL:
3.10E4
TIC MS
fathi-
hamed-21

fathi-hamed-21 #217 RT: 3.65 AV: 1 SB: 2 4.45, 4.45 NL: 6.57E2
T: {0,0} + c EI Full ms [40.00-1000.00]



EI-MS spectrum of 21

2. Antimicrobial screening against methicillin-resistant *Staphylococcus aureus* (MRSA)

The antimicrobial activity of the synthesized compounds against methicillin-resistant *Staphylococcus aureus* (MRSA) was, unfortunately, weak compared with Ciprofloxacin as seen in the following photos:

