

Supporting information

Synthesis of Novel Naphthalene-Heterocycle Hybrids with Potent Antitumor, Anti-inflammatory and Antituberculosis Activities

Mohamed Ahmed Abozeid,^a Aya Atef El-Sawi,^a Mohamed Abdelmoteleb,^{b,c} Hanem Awad,^d Marwa Mostafa Abdel-Aziz,^e Abdel-Rahman Hassan Abdel-Rahman^a and El-Sayed Ibrahim El-Desoky^{*a}

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

^bFood Allergy Research & Resource Program (FARRP), Department of Food Science & Technology, University of Nebraska, Lincoln, NE, USA

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

^dDepartment of Tanning Materials and Leather Technology, Chemical Industries Research Division, National Research Centre, 33 EL-Bohouth St., Dokki 12622, Giza. Egypt.

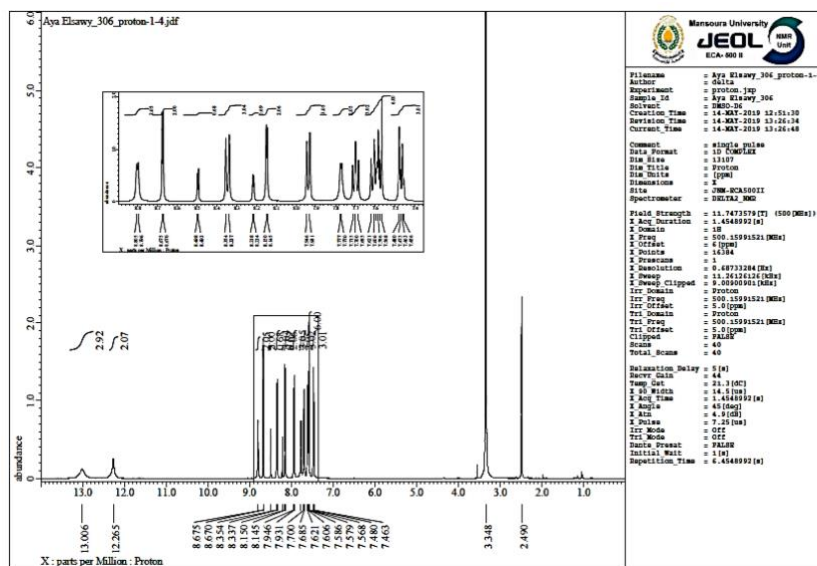
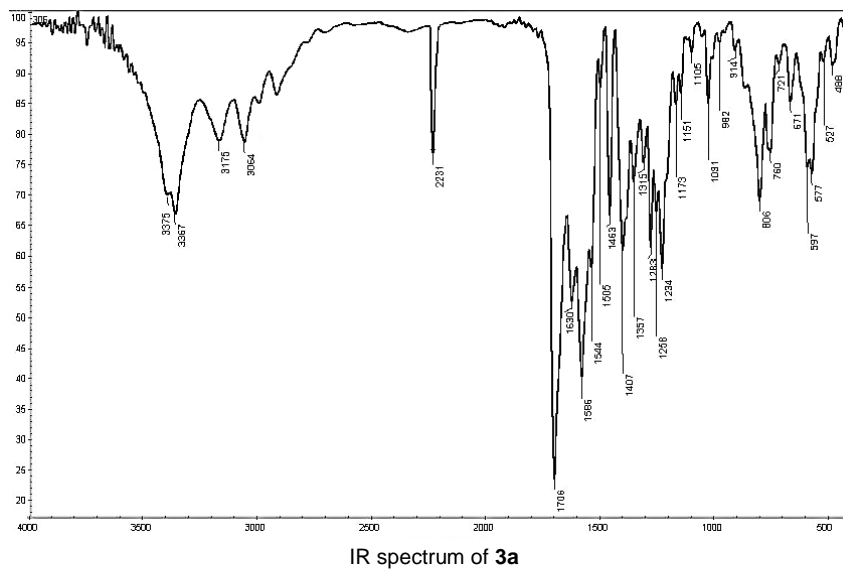
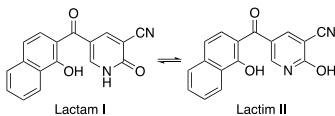
^eThe Regional Center for Mycology and Biotechnology, Al-Azhar University, Cairo 11759, Egypt.

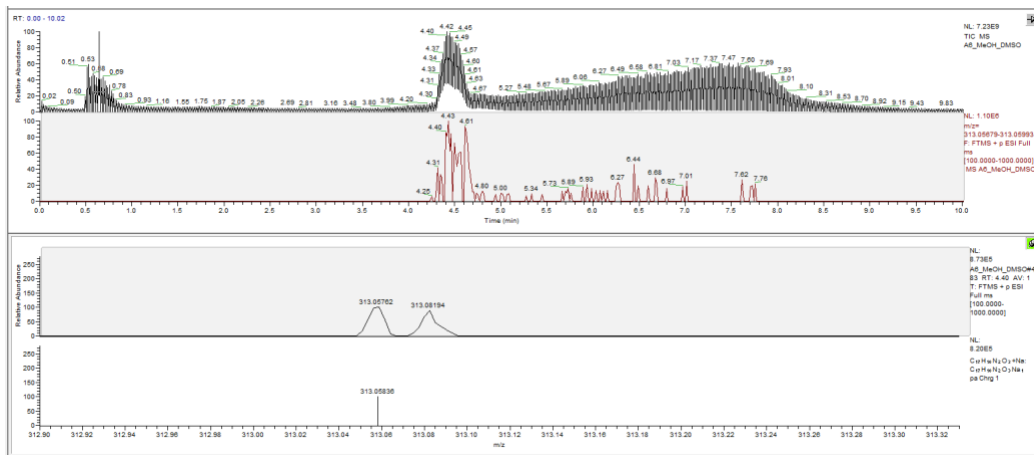
*Corresponding Author: E-mail: prof.deosky.orgchem@gmail.com; desoky199@mans.edu.eg; Tel: 00201060614054.

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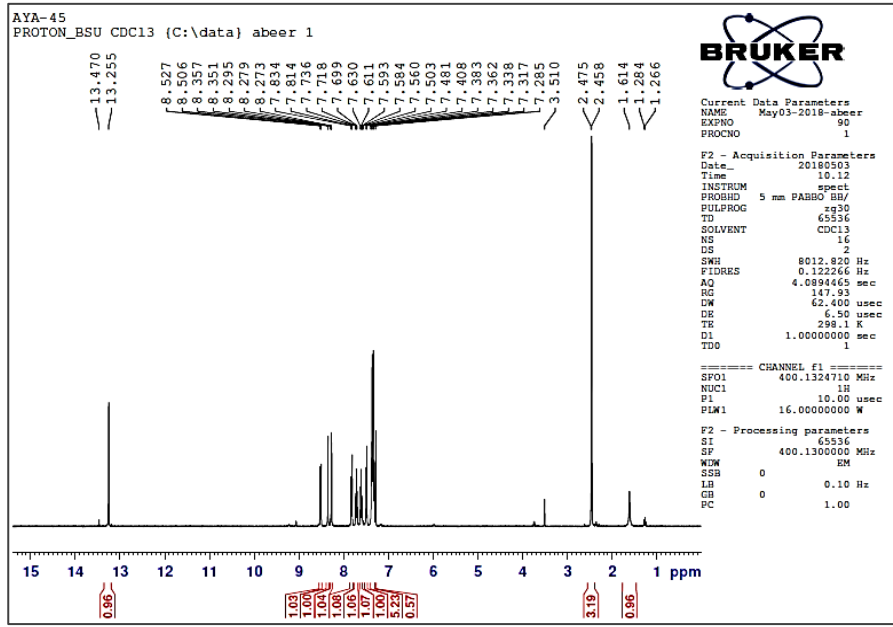
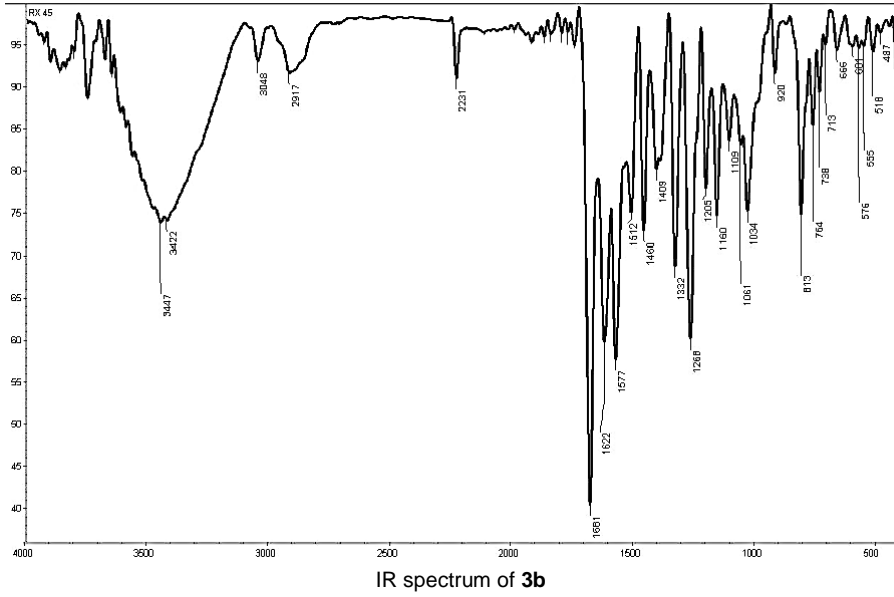
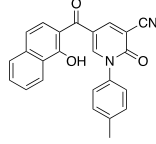
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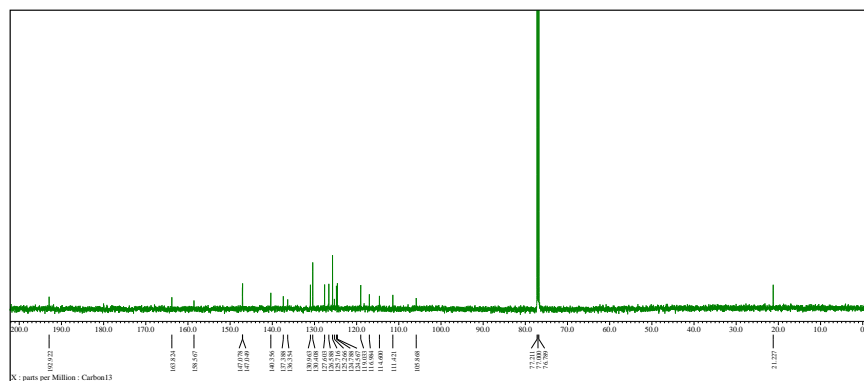
1. Spectral data





HR-MS spectrum of 3a

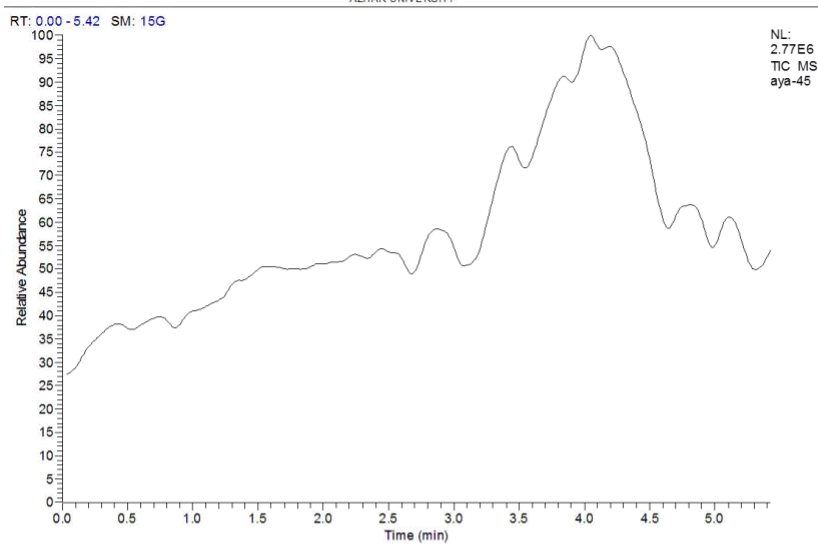




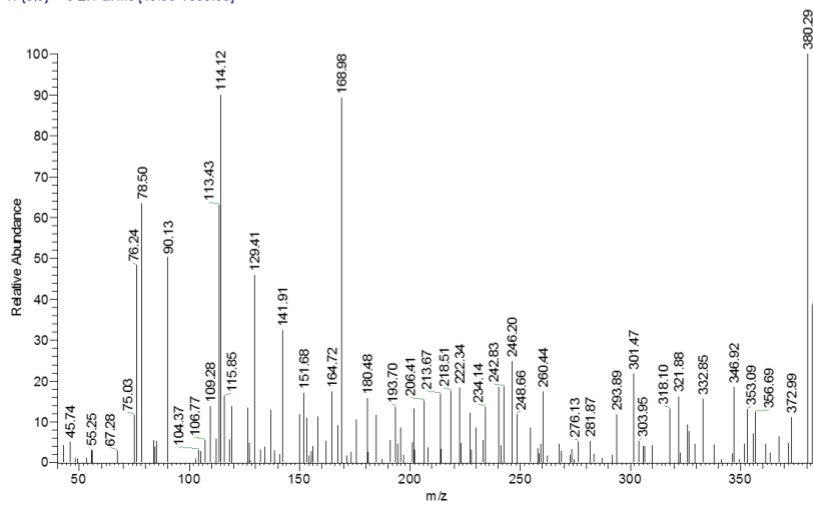
¹³C NMR spectrum of 3b

C:\xcalib\data\1\aya-45

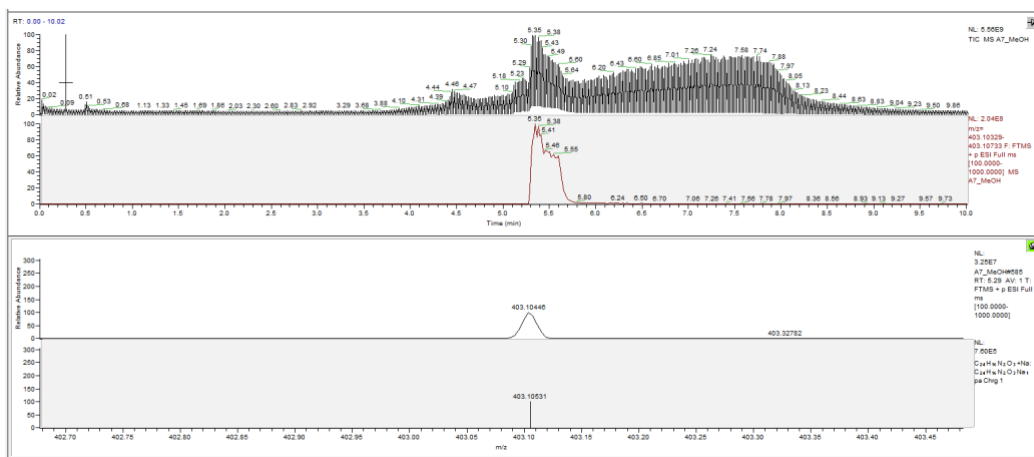
27-Nov-16 12:32:34 PM
THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY
AZHAR UNIVERSITY



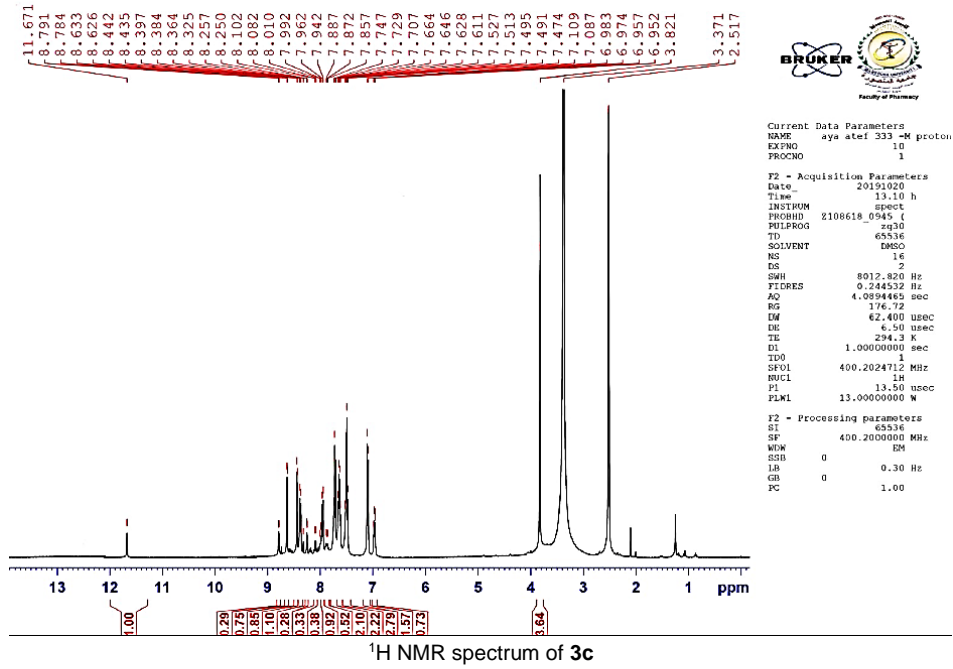
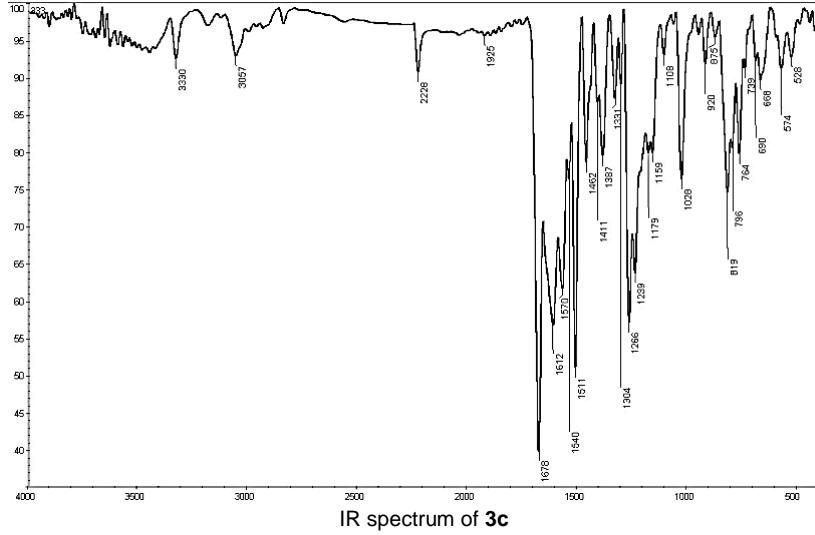
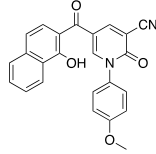
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T: (0.0) + c EI Full ms [40.00-1000.00]



Mass spectrum of 3b



HR-MS spectrum of **3b**

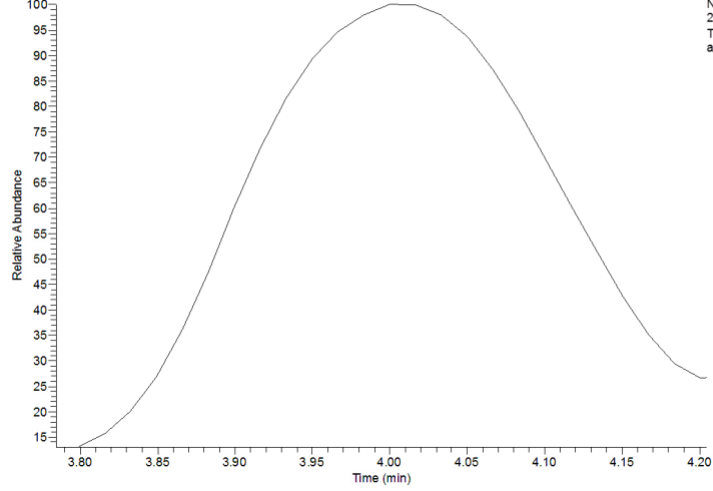


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 PROCNO 1

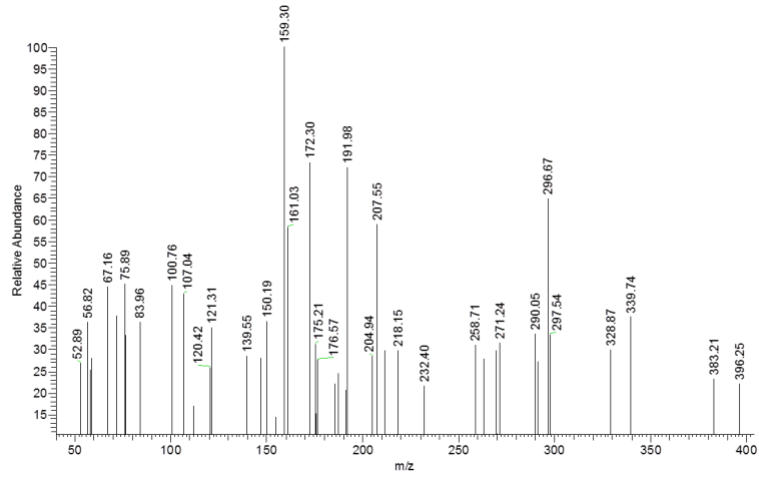
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 Time 13:10 h
 INSTRUM spect
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 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 176.92
 DM 62.400 usec
 DE 6.50 usec
 TE 294.3 K
 D1 1.00000000 sec
 T10 1
 SF01 400.2024712 MHz
 RUC1 1H
 F1 13.50 usec
 FLW1 13.00000000 N

F2 - Processing parameters
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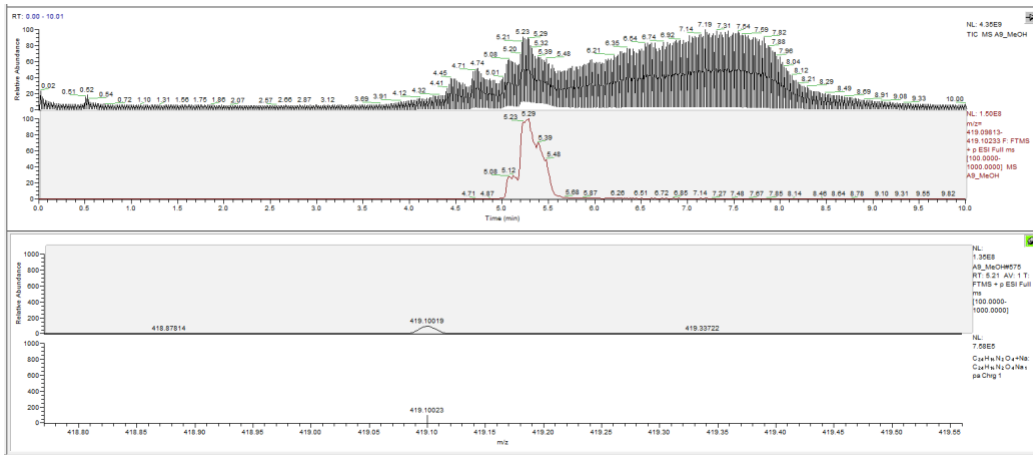
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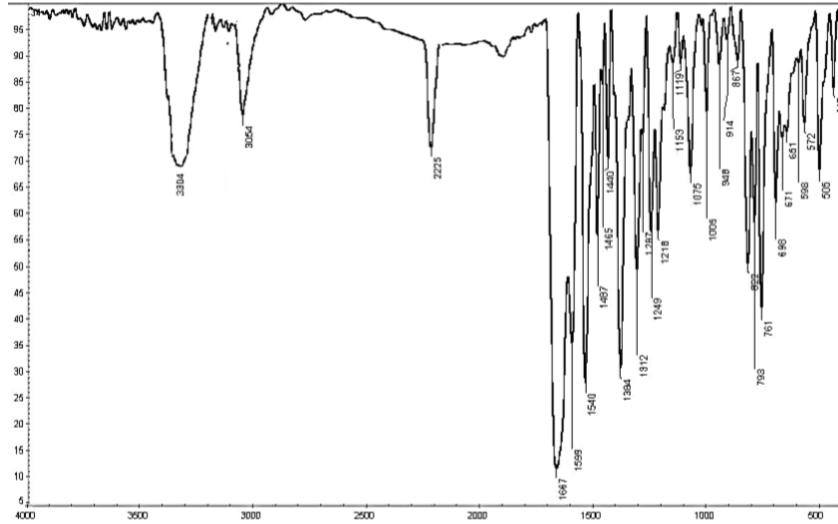
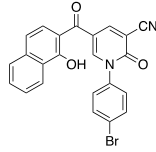
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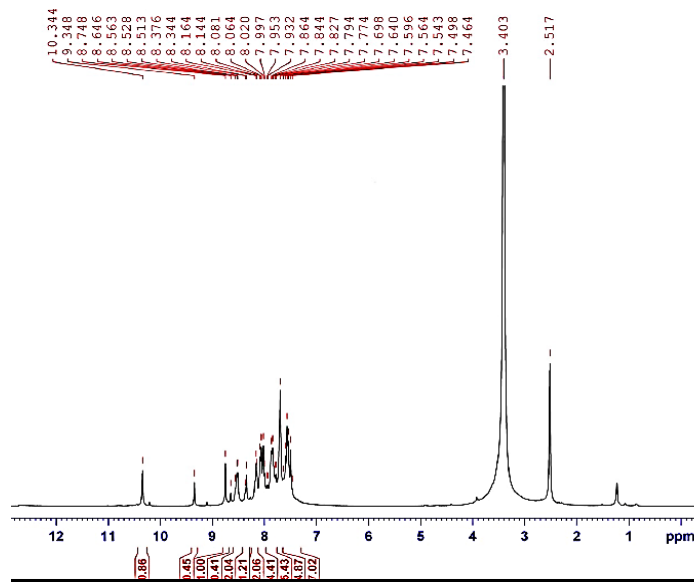
Mass spectrum of 3c



HR-MS spectrum of 3c



IR spectrum of 3d



¹H NMR spectrum of 3d

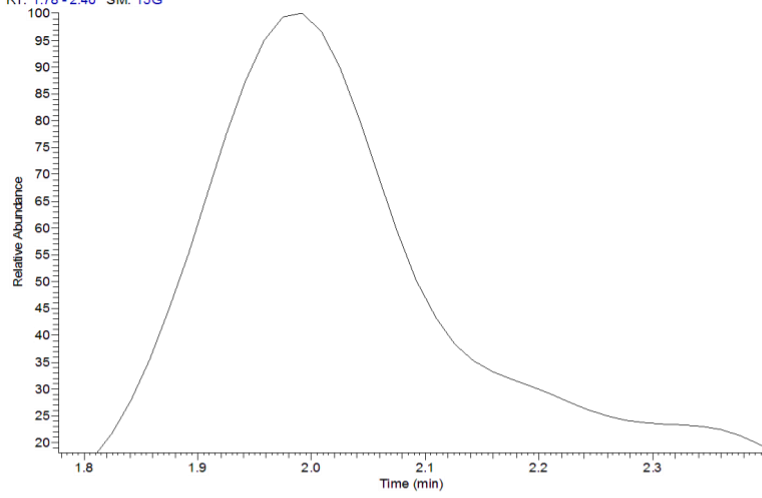


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 EXPNO: 10
 PROCNO: 1

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 PULPROG: zgpg30
 TD: 65536
 SOLVENT: DMSO
 NS: 16
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0854465 sec
 M: 120.83
 GM: 65.400 usec
 DE: 6.50 usec
 TE: 293.2 K
 D1: 1.00000000 sec
 T10: 1
 SECT1: 400.2024712 MHz
 NUC1: 1H
 P1: 13.50 usec
 PL1: 13.0000000 W

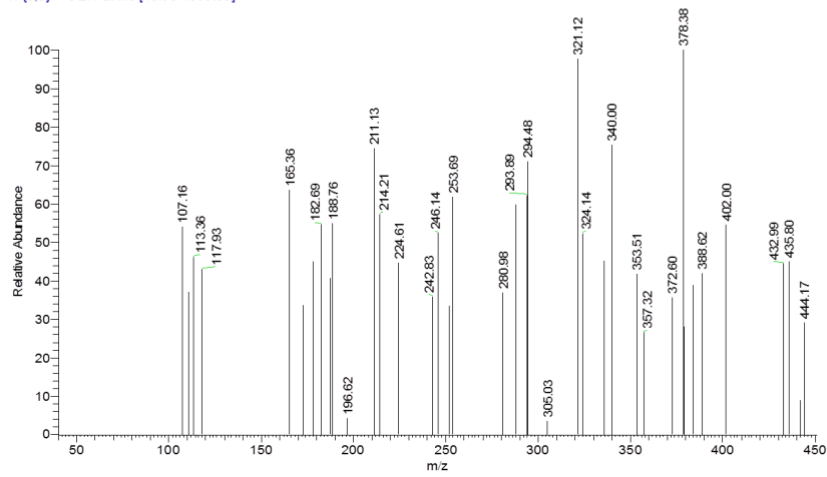
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RT: 1.78 - 2.40 SM: 15G

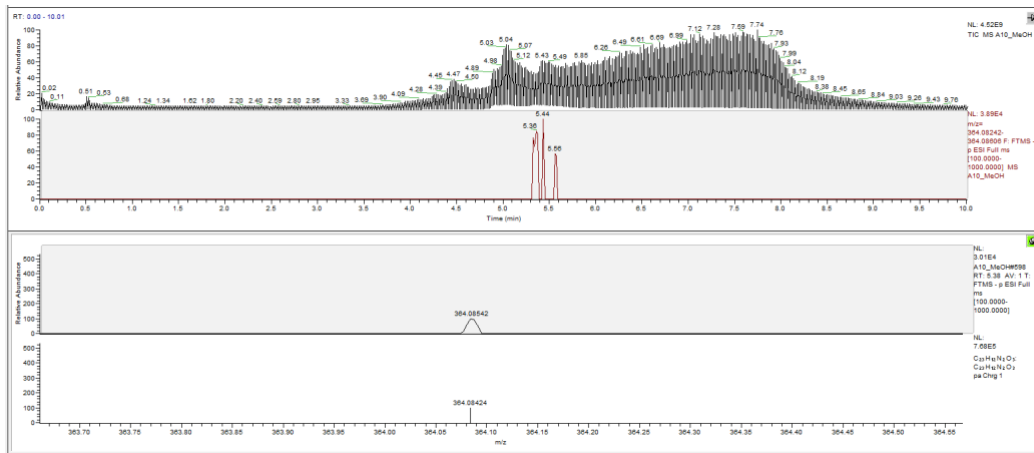


NL: 3.11E6
TIC MS
aya-34

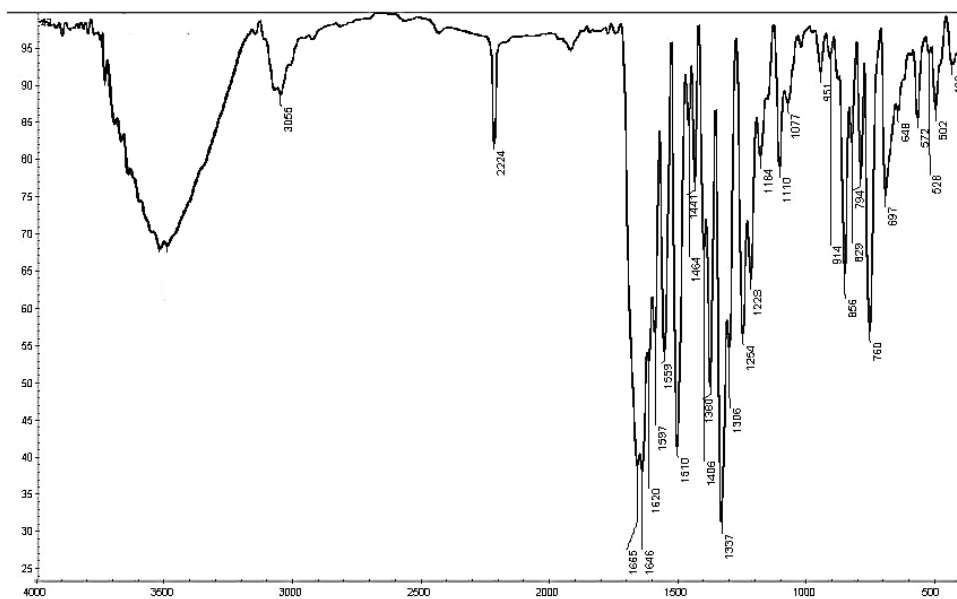
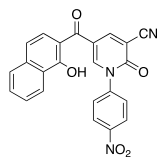
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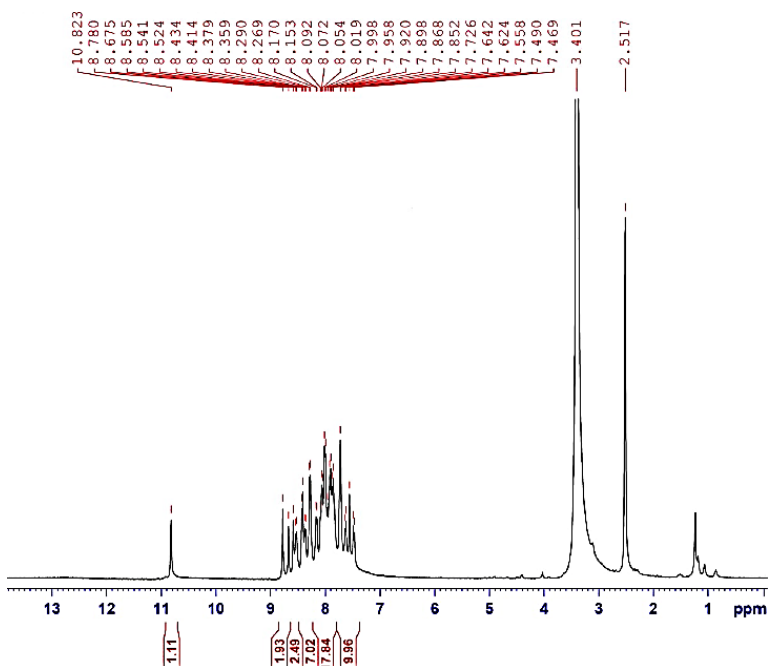
Mass spectrum of 3d



HR-MS spectrum of 3d



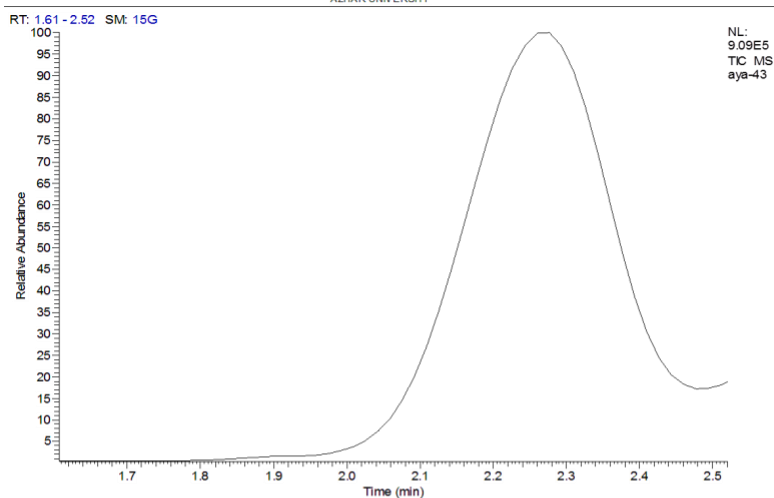
IR spectrum of **3e**



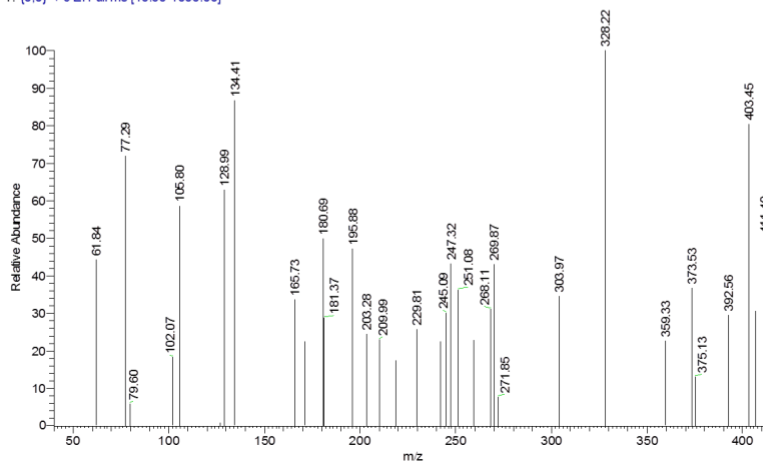
¹H NMR spectrum of **3e**



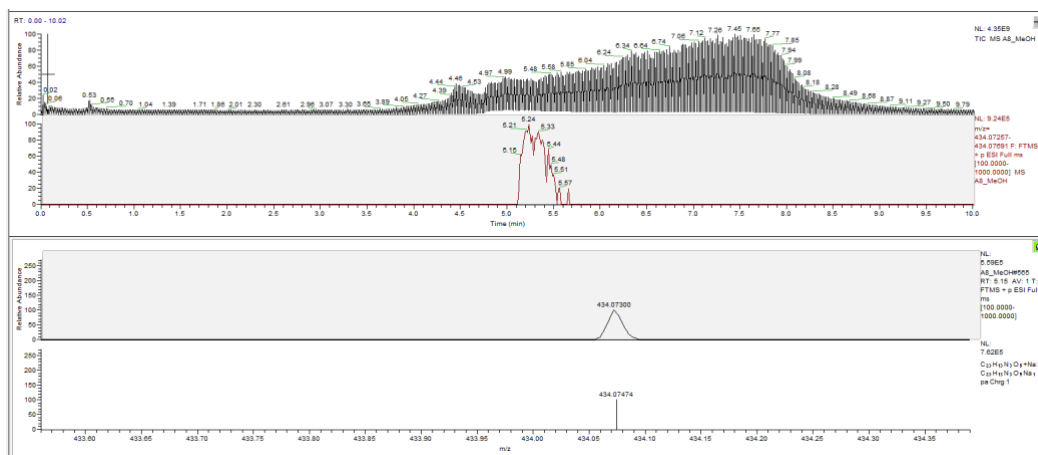
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 PULPROG zg30
 TD 65536
 SOLVENT DMF0
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0854465 sec
 RG 120.93
 DW 62.400 usec
 DE 6.50 usec
 TE 293.3 K
 D1 1.09000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 13.09000000 W
 F2 - Processing parameters
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 SF 400.2009000 MHz
 NRG EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



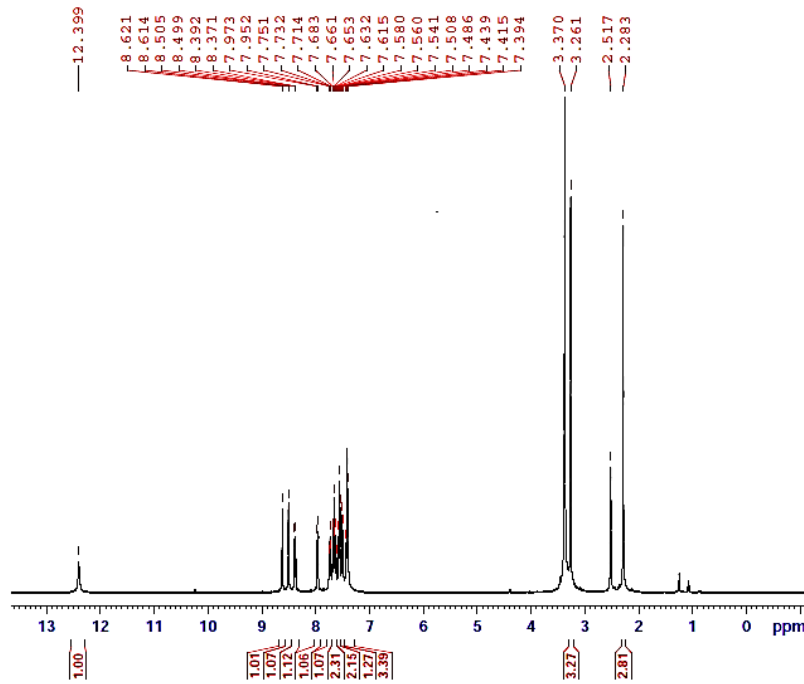
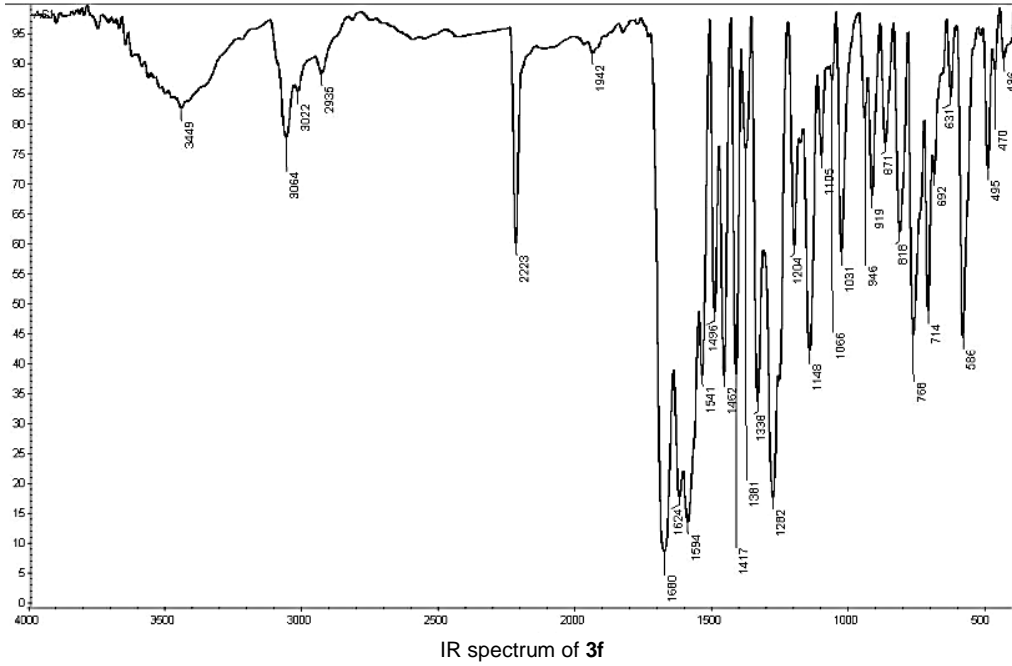
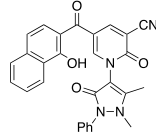
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Mass spectrum of 3e



HR-MS spectrum of 3e

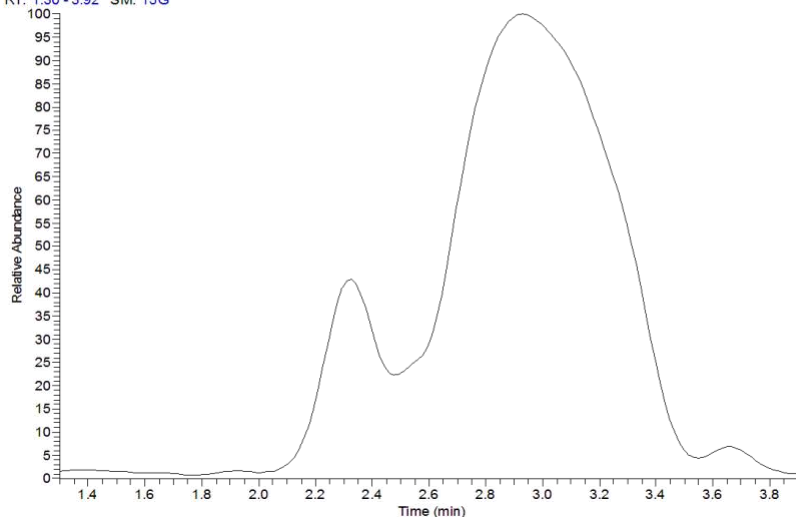


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 PROCNO: 1

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 PULPROG: zg30
 TD: 65536
 SOLVENT: DMSO
 NS: 16
 DS: 2
 SWH: 8012.820 MHz
 FIDRES: 0.244532 MHz
 AQ: 4.0894465 sec
 RG: 176.72
 DM: 62.400 usec
 DE: 8.50 usec
 TE: 284.2 K
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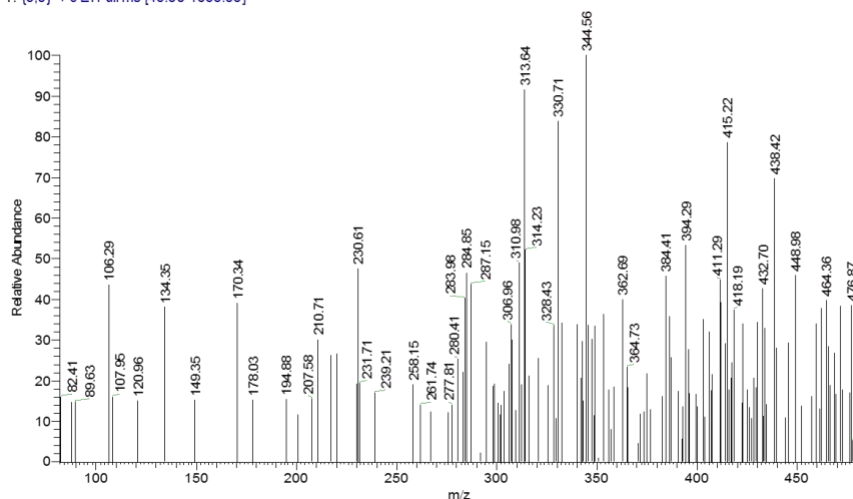
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RT: 1.30 - 3.92 SM: 15G

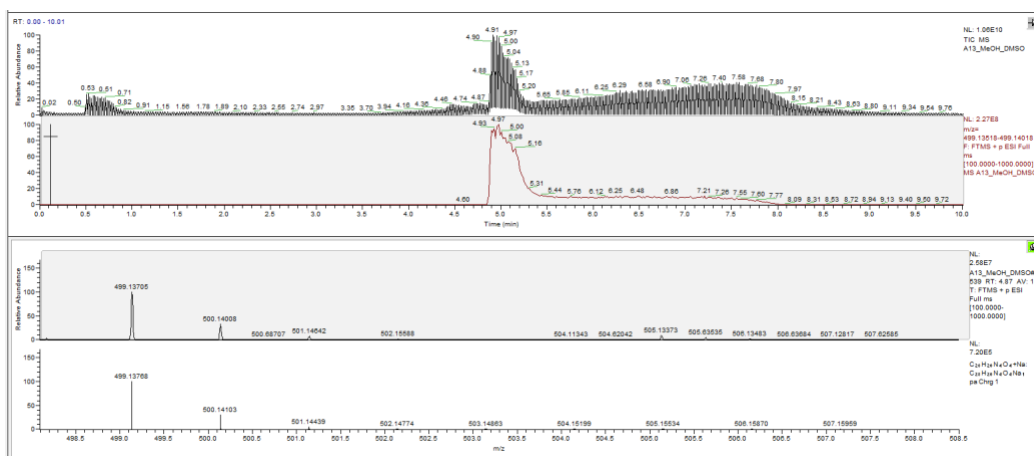


NL:
1.57E6
TIC MS
aya-as1

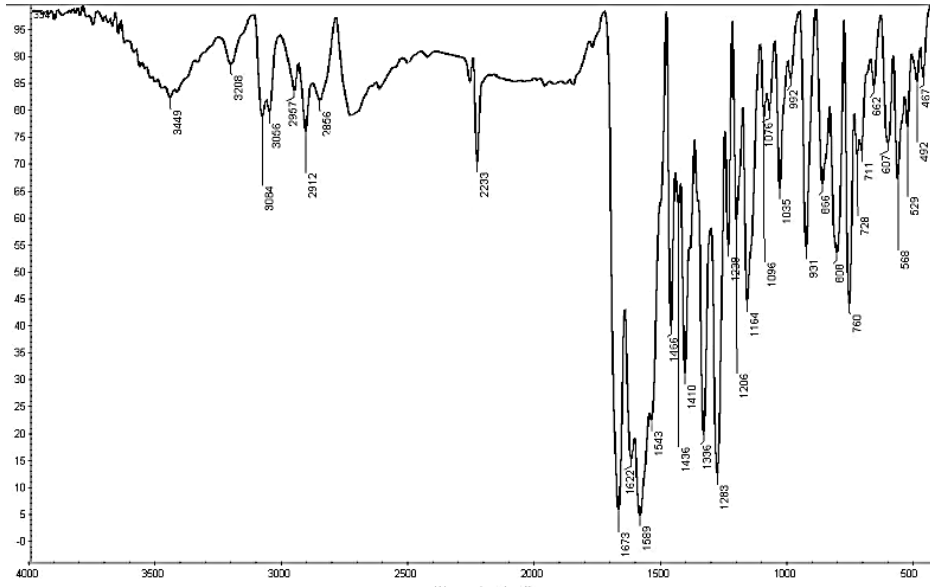
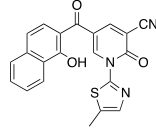
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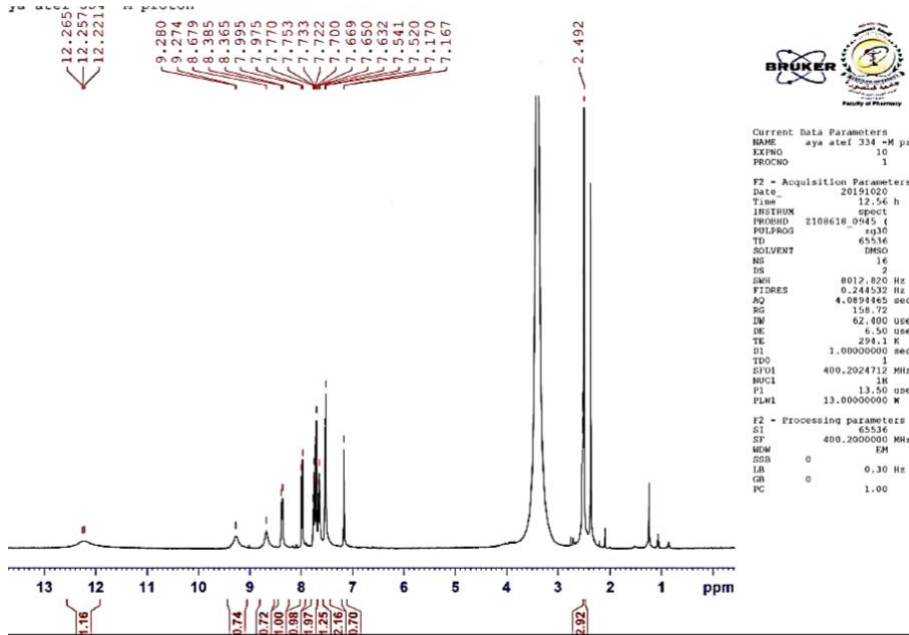
Mass spectrum of 3f



HR-MS spectrum of 3f



IR spectrum of 3g

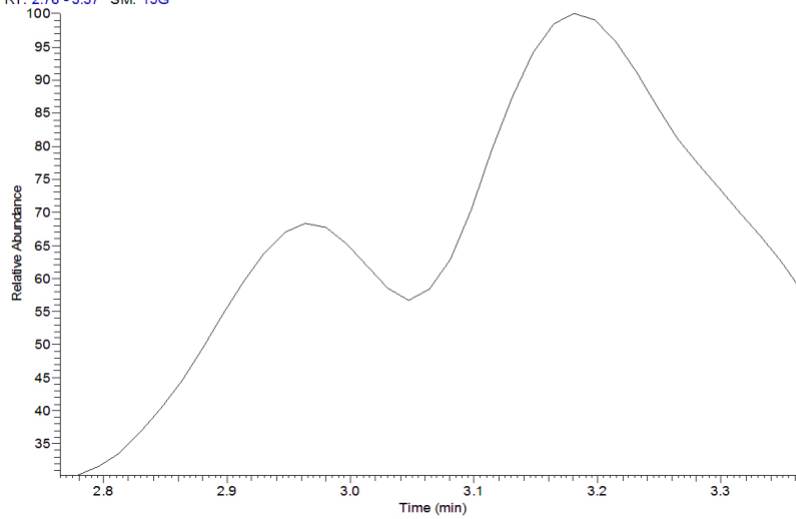


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 XXPR0 10
 PROCNO 1
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 Time 12.56 h
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 PROBRD E108618 0545 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWS 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894445 sec
 RG 158.72
 IM 82.400 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.0000000 sec
 TPO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 13.50 usec
 PL1 13.0000000 Hz
 F2 - Processing parameters
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 GB 0
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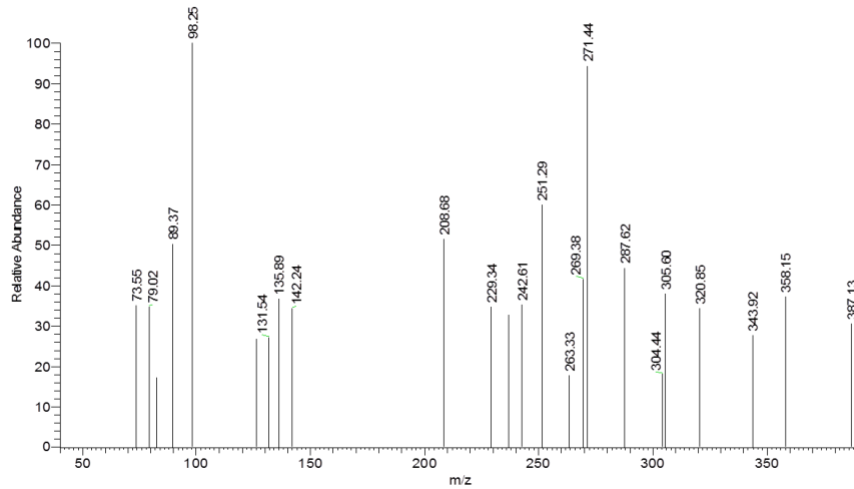
¹H NMR spectrum of 3g

RT: 2.76 - 3.37 SM: 15G

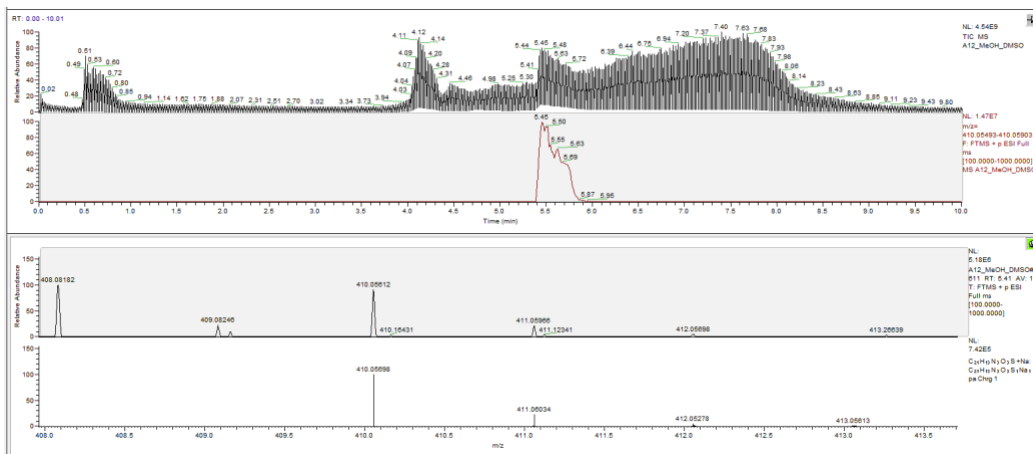
NL:
2.17E4
TIC MS
aya-334



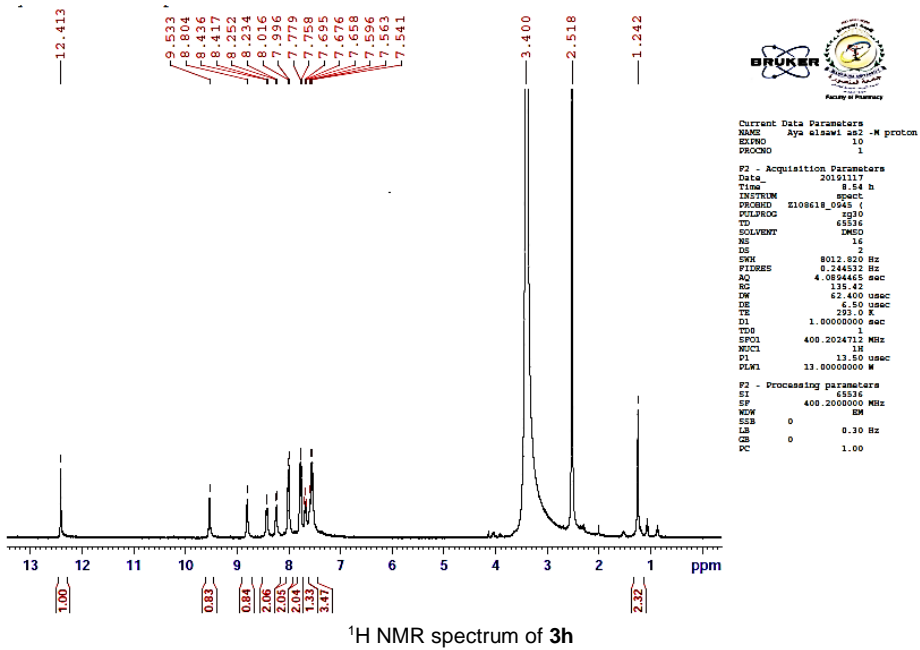
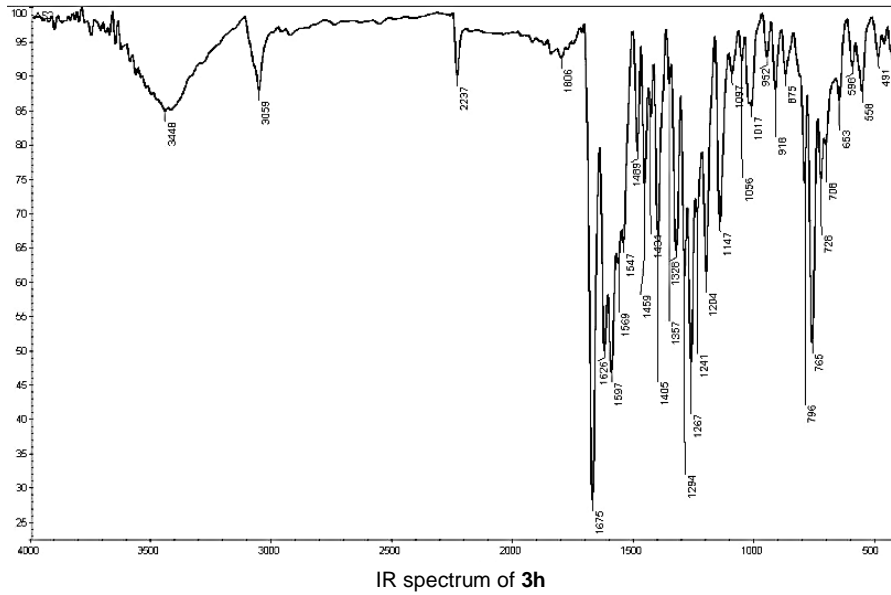
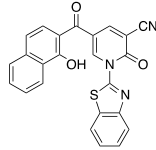
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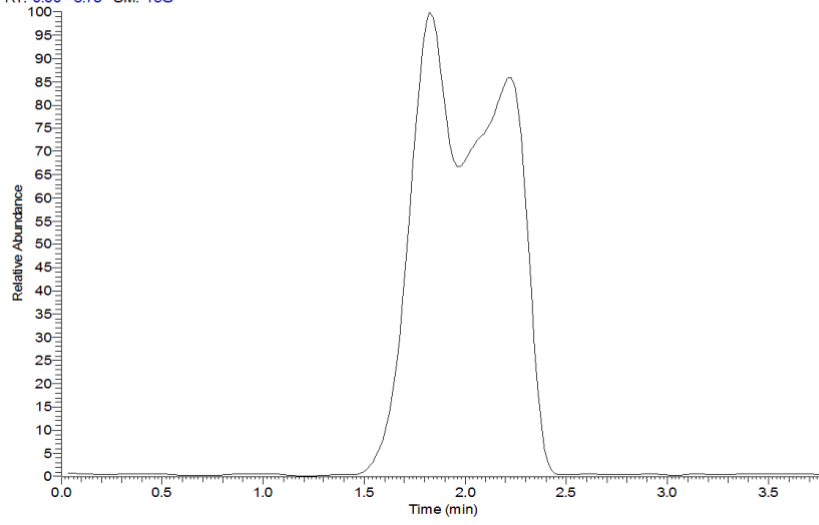
Mass spectrum of 3g



HR-MS spectrum of 3g

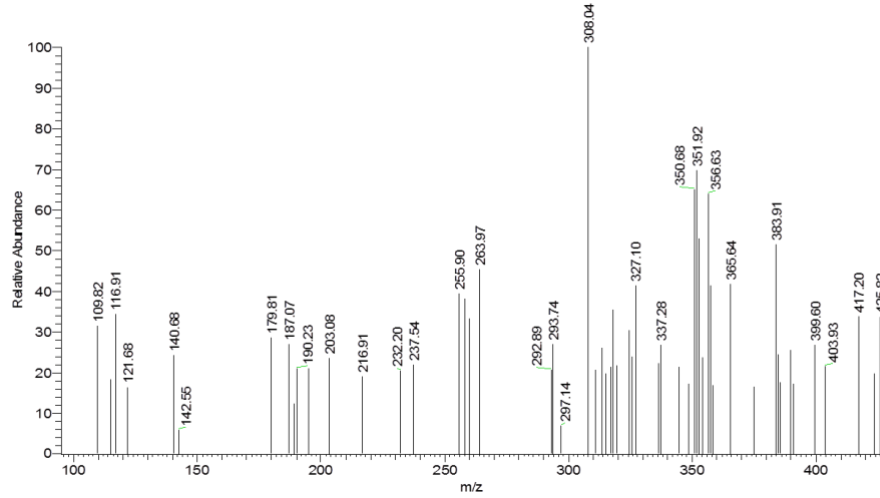


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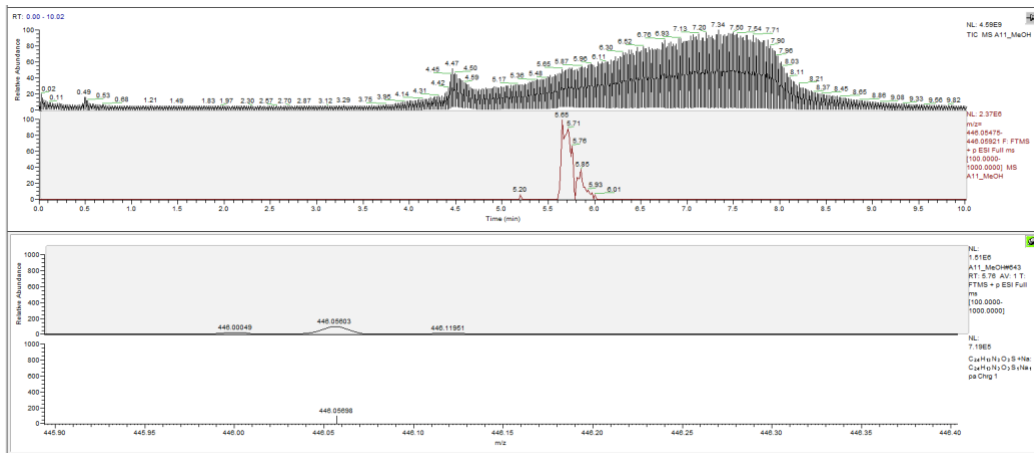


NL:
3.74E6
TIC MS
aya-as2

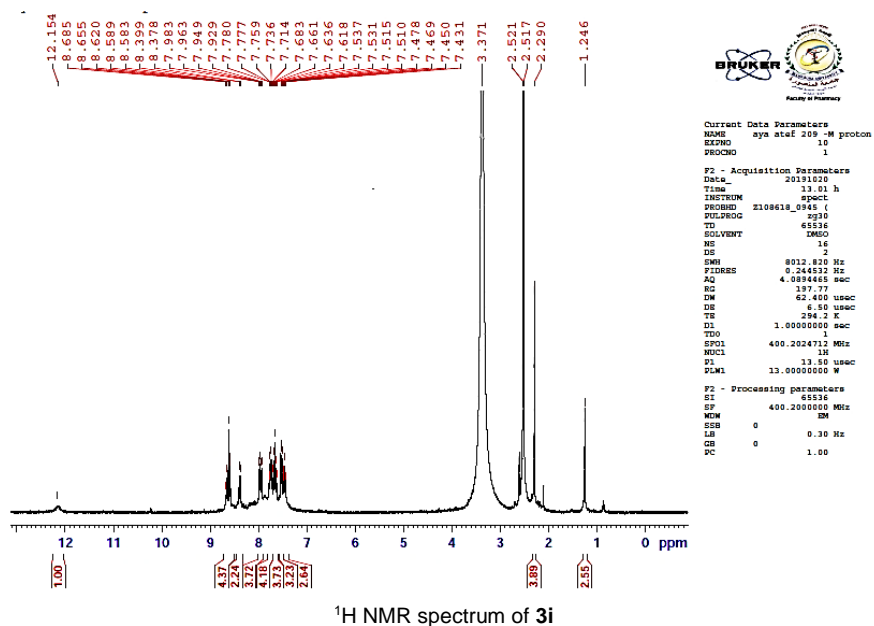
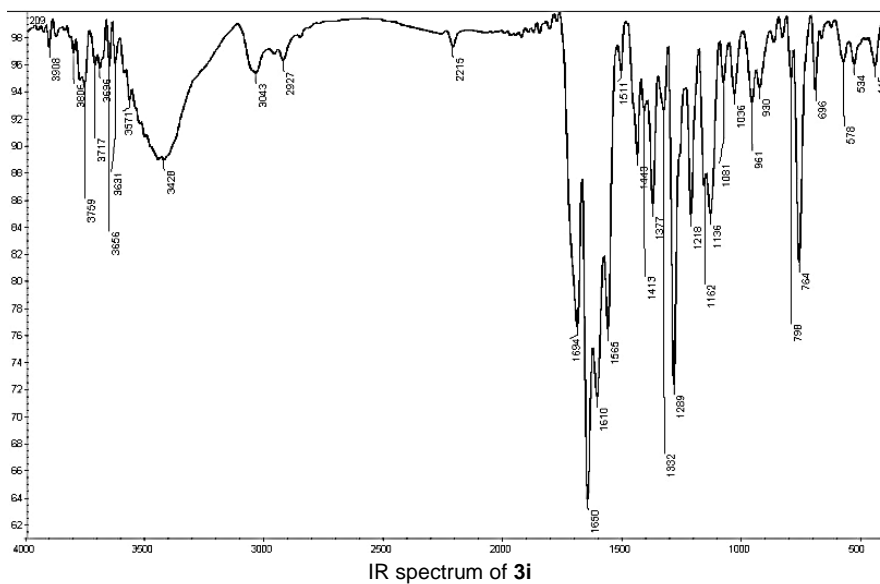
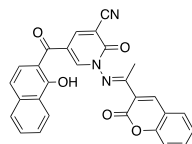
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Mass spectrum of 3h



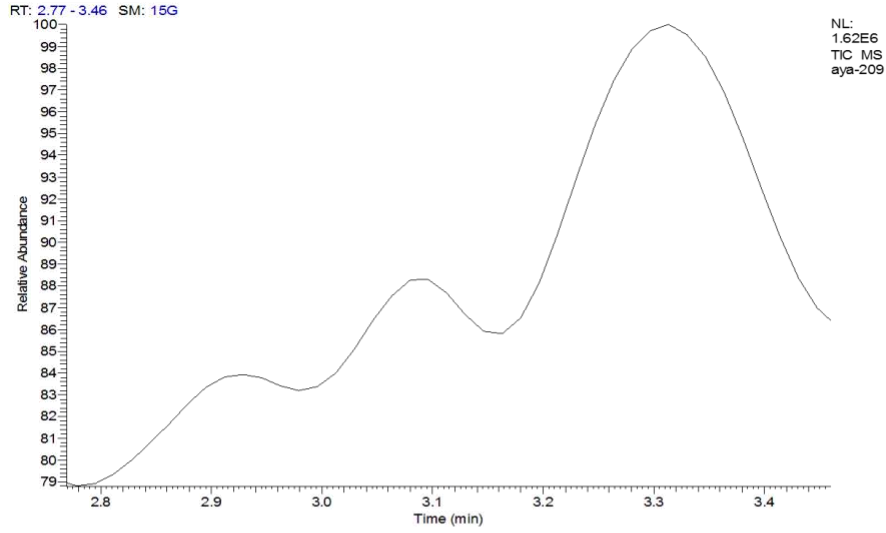
HR-MS spectrum of 3h



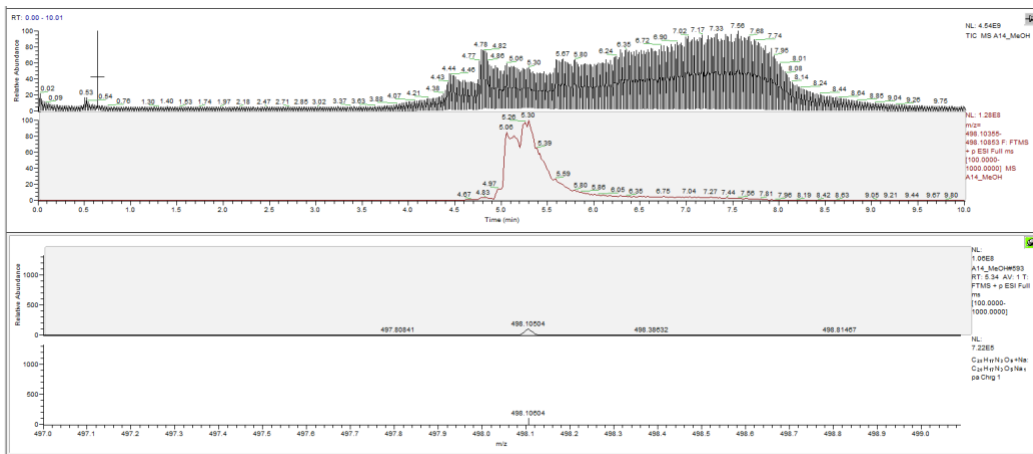
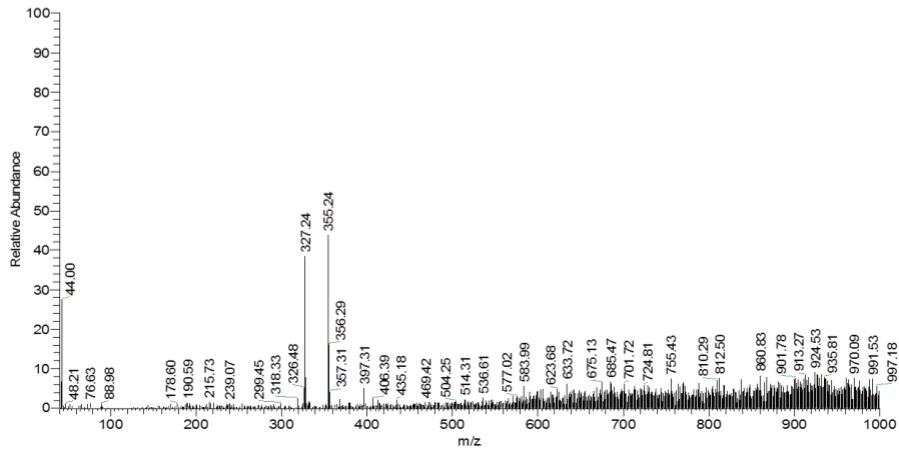
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 PROCESS: 1

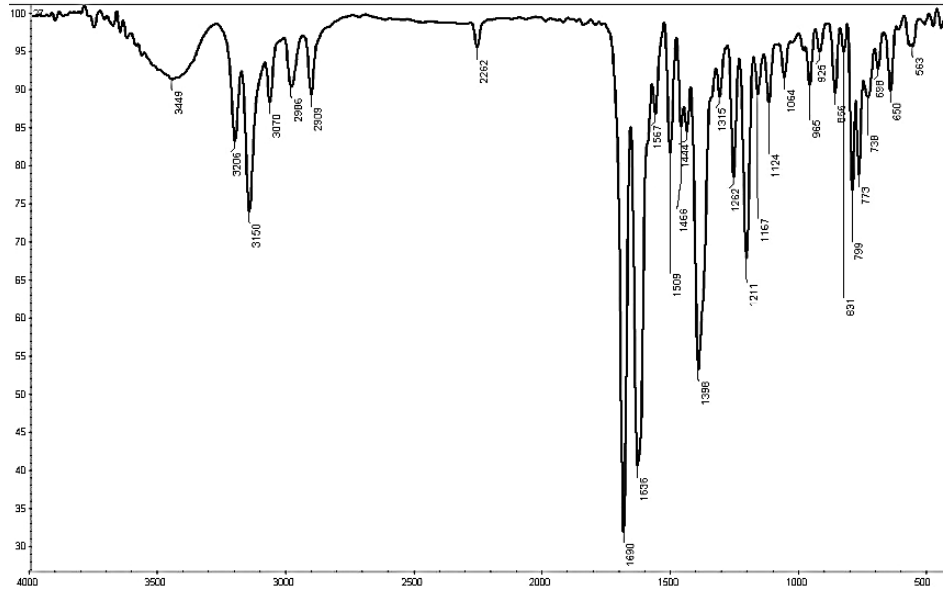
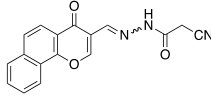
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 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.244532 Hz
 AQ: 4.0894465 sec
 RG: 197.77
 DW: 62.400 usec
 DE: 6.50 usec
 TE: 298.2 K
 D1: 1.00000000 sec
 TSD: 1
 SFO1: 400.2024712 MHz
 NUC1: 1H
 P1: 13.50 usec
 PL1: 13.00000000 W

F2 - Processing parameters
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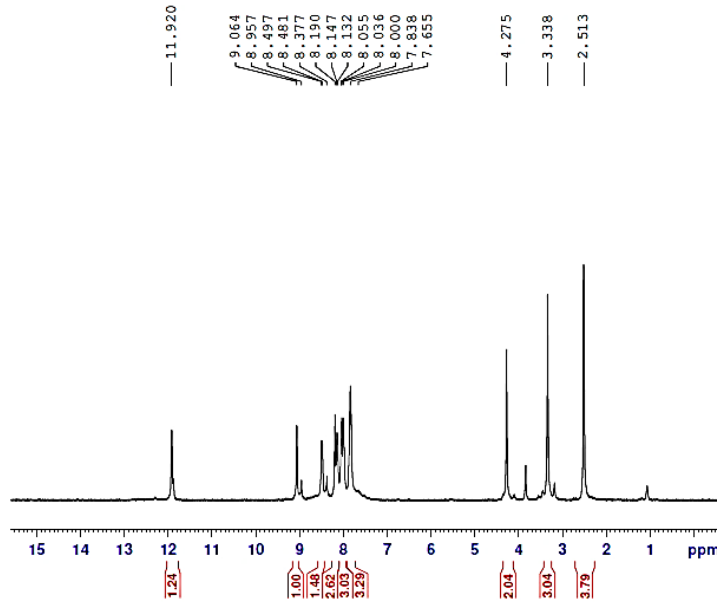
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IR spectrum of 5

EX-AYA-33
 PROTON DMSO (C:\data) nmr 17



¹H NMR spectrum of 5



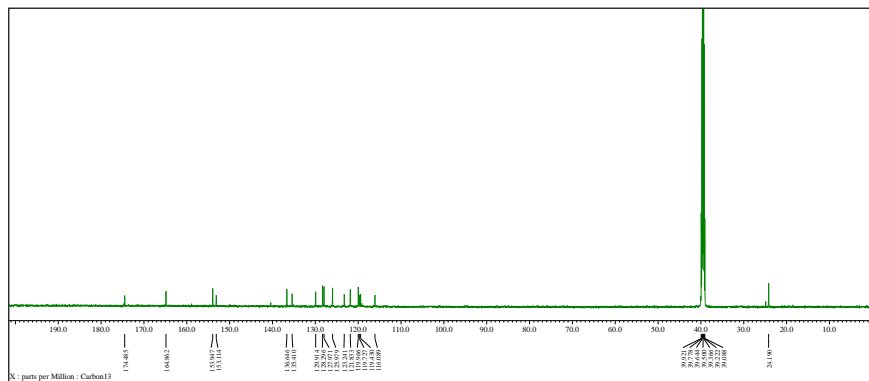
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PROCNO   1

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PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        205.44
CW        62.400 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TD0       1

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NUC1     1H
P1       10.00 usec
PLW1     16.00000000 W

F2 - Processing parameters
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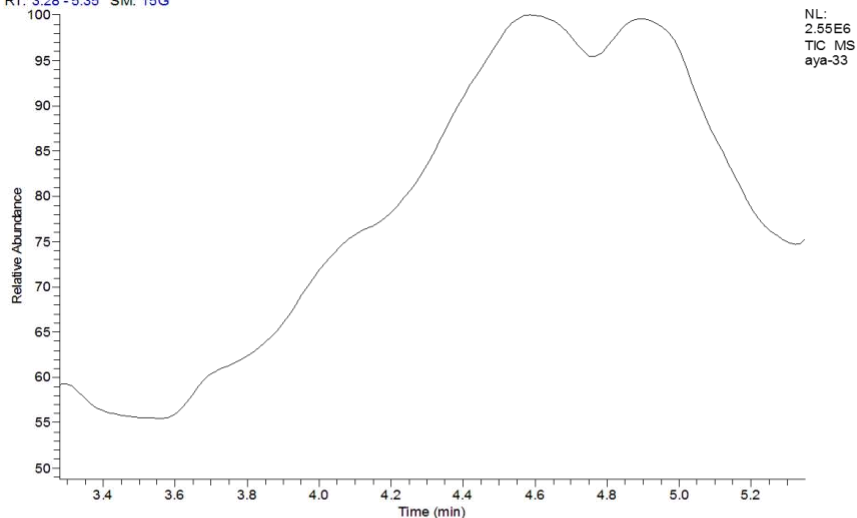


13C NMR spectrum of 5

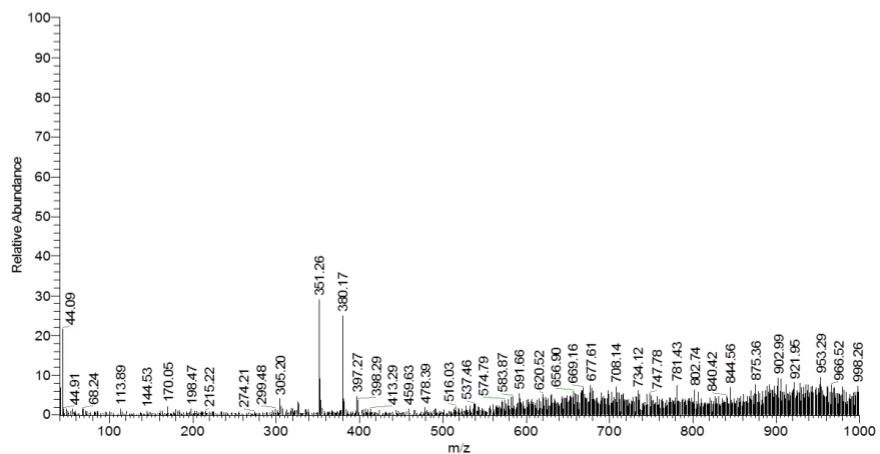
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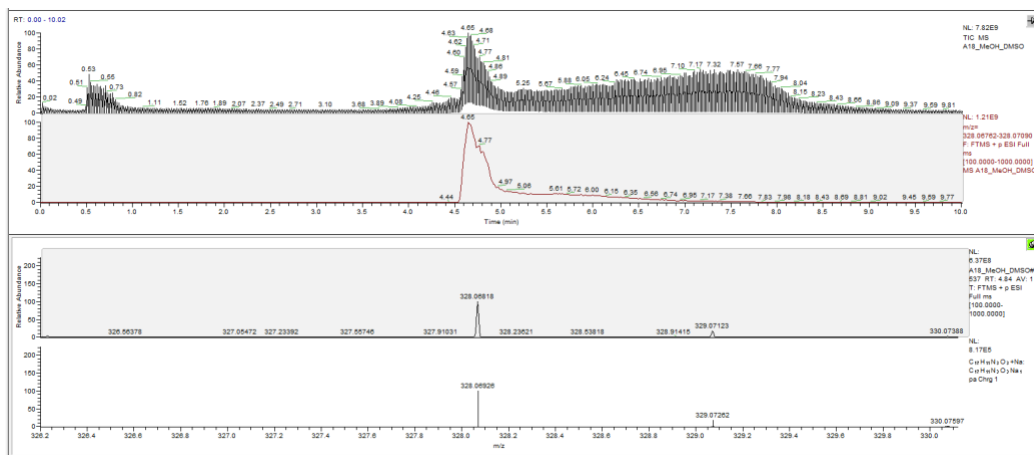
27-Nov-18 1:07:41 PM
THE REGIONAL CENTER FOR MYCOLOGY AND BIOTECHNOLOGY
AZHAR UNIVERSITY

RT: 3.28 - 5.35 SM: 15G

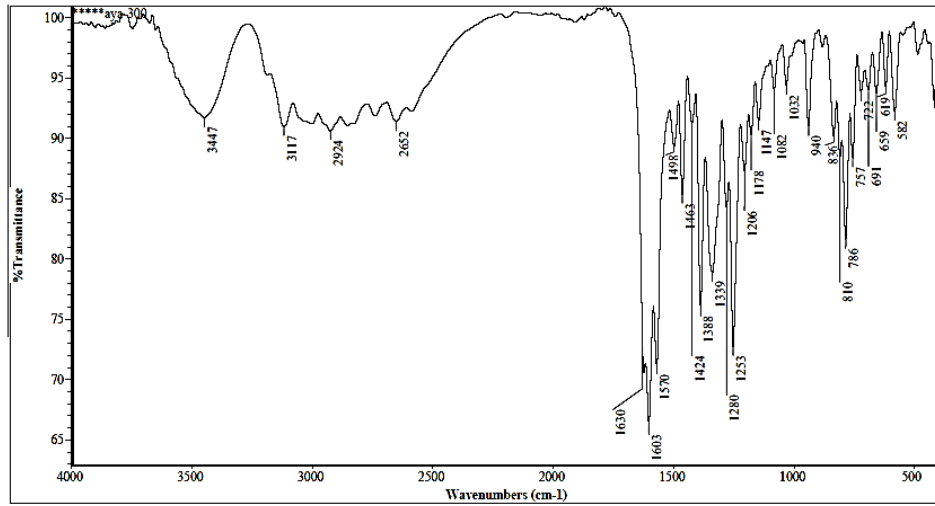
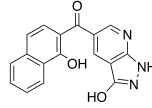


aya-33 #210 RT: 3.53 AV: 1 NL: 5.48E4
T: {0,0} + c EI Full ms [40.00-1000.00]





HR-MS spectrum of 5



****aya-300

Number of sample scans: 32
 Number of background scans: 32
 Resolution: 4.000
 Sample gain: 2.0
 Optical velocity: 0.4747
 Aperture: 80.00



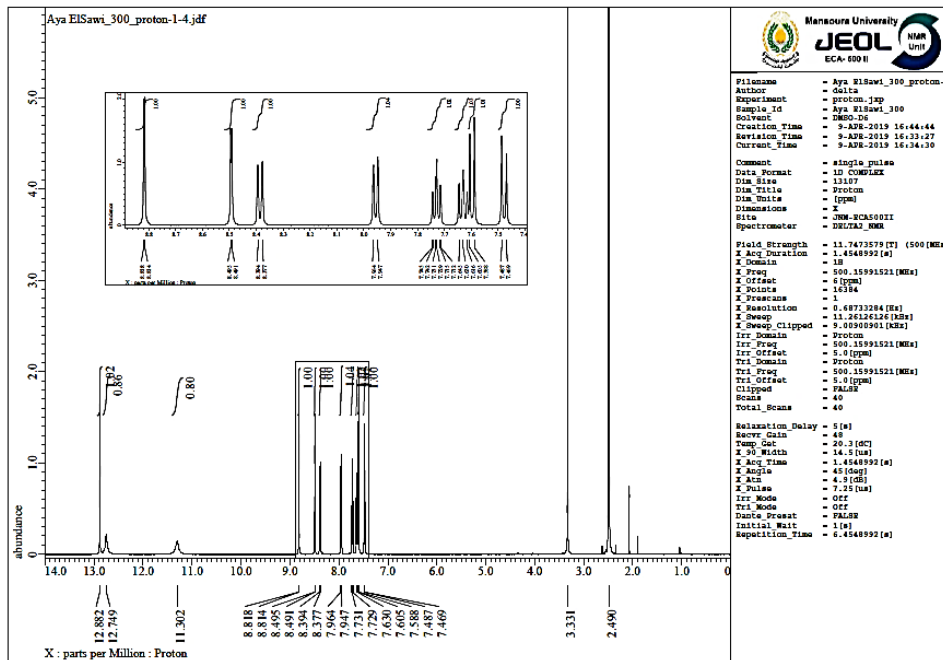
Sun Apr 07 10:55:03 2019 (GMT+02:00)

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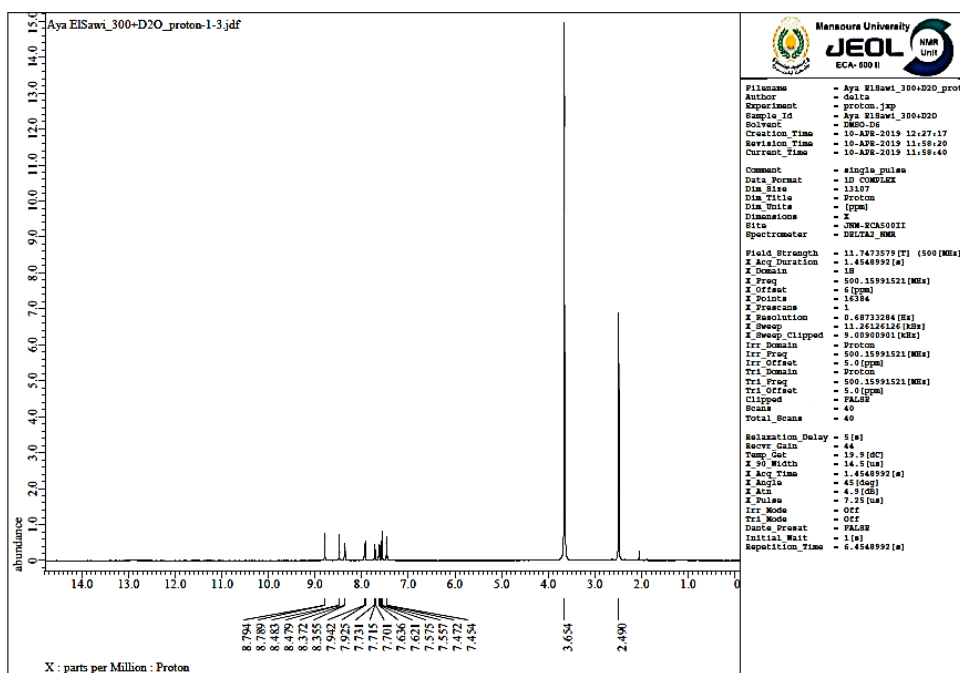


Mansoura University
 Faculty of Science
 Spectral Analyses unit
 Chemistry Department
 ThermoFisher Nicolette IS10, USA
 Spectral range: 4000 - 400 cm-1

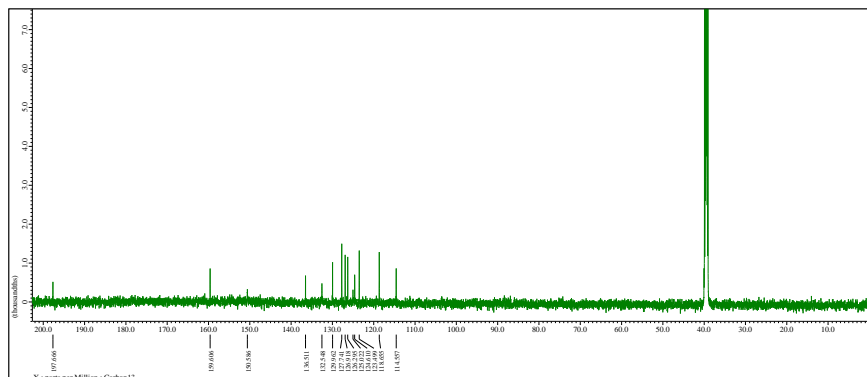
IR spectrum of 6



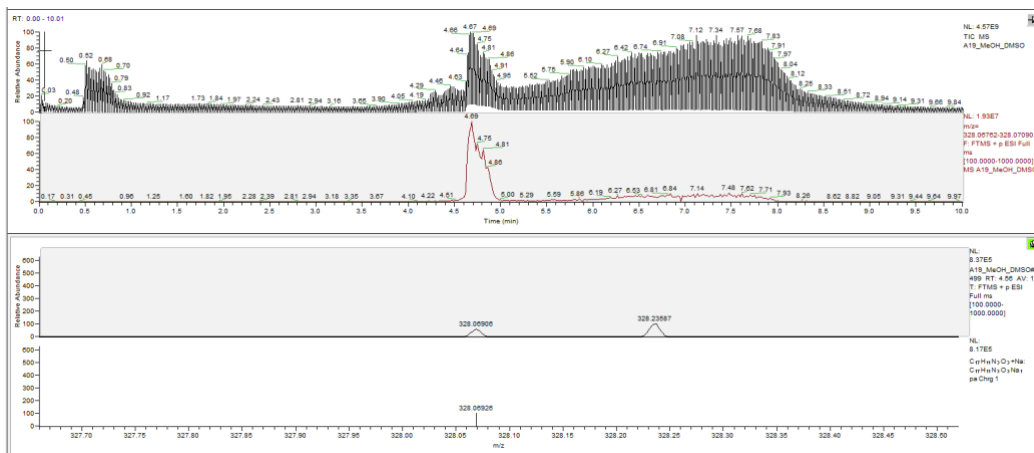
¹H NMR spectrum of 6



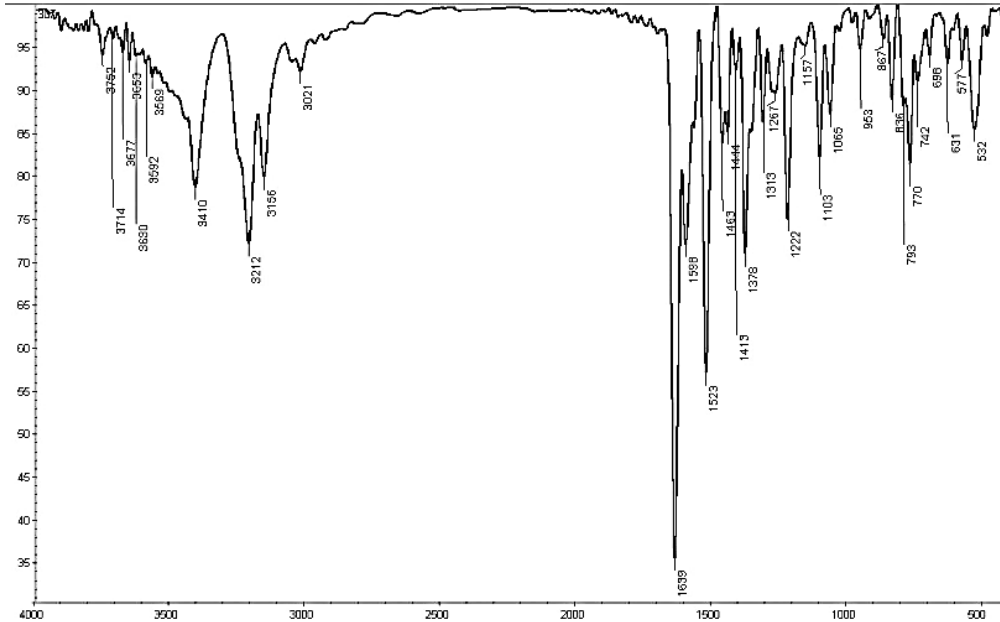
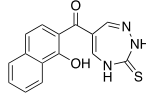
¹H NMR spectrum of **6** in the presence of D₂O



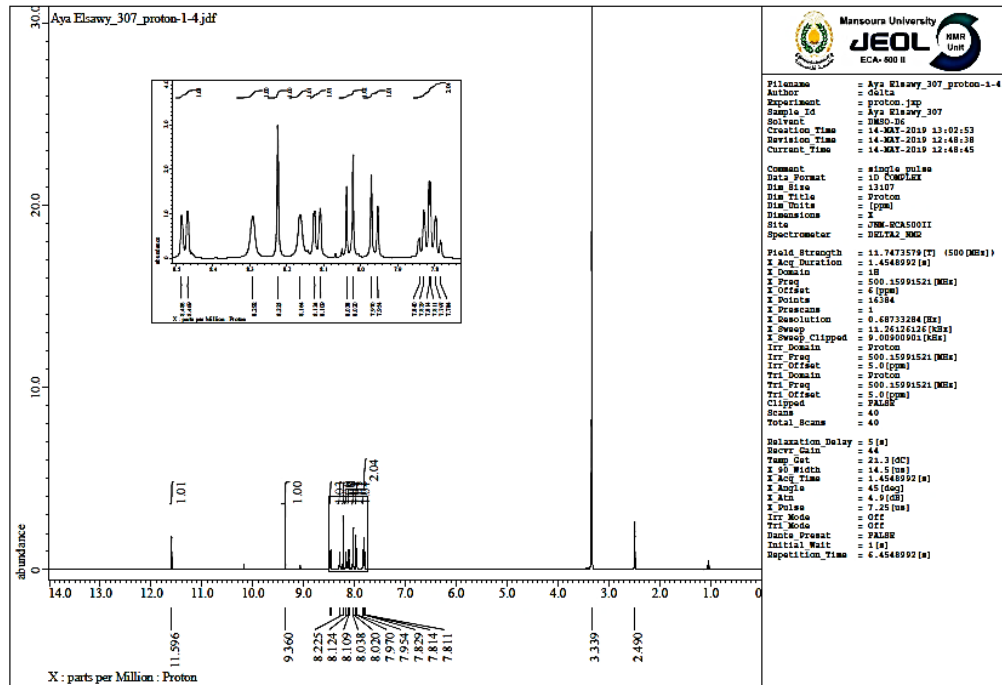
¹³C NMR spectrum of **6**



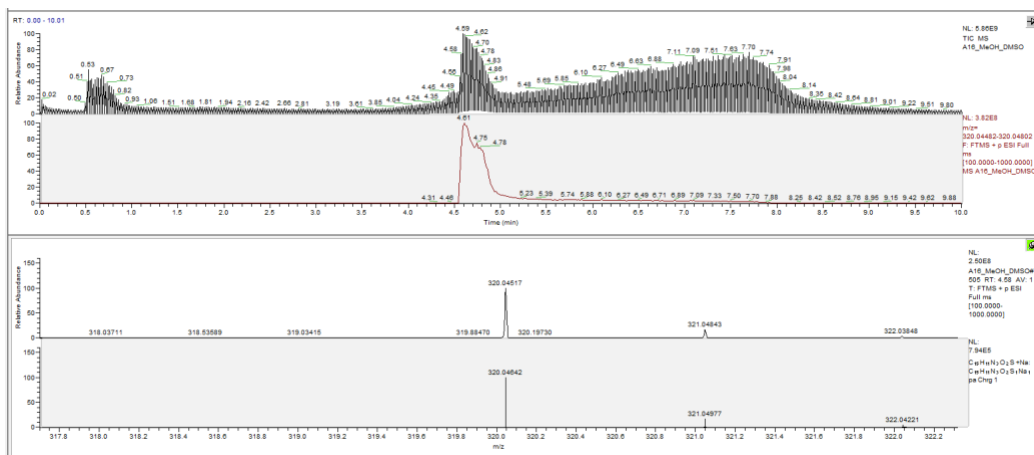
HR-MS spectrum of **6**



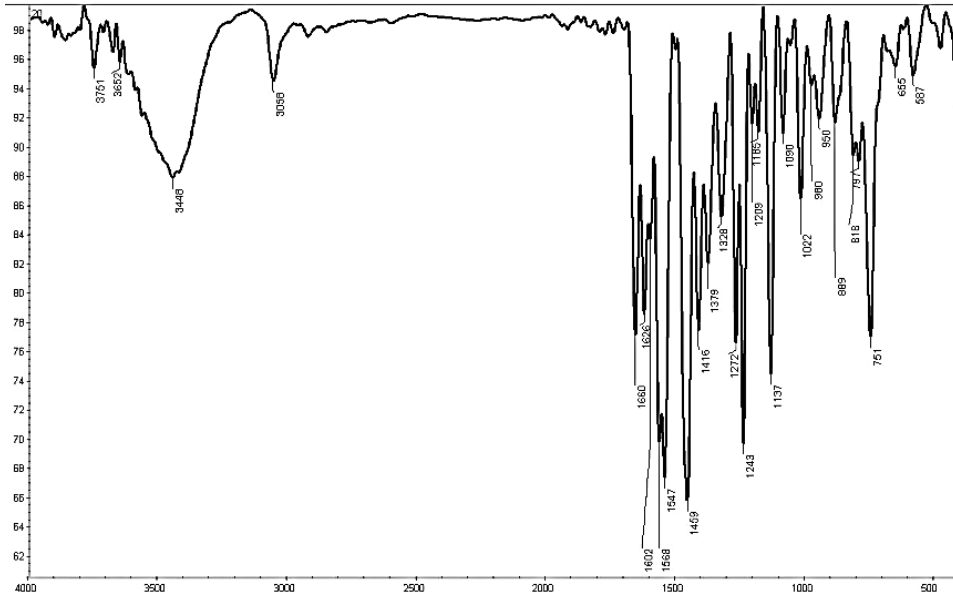
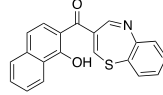
IR spectrum of 7



¹H NMR spectrum of 7

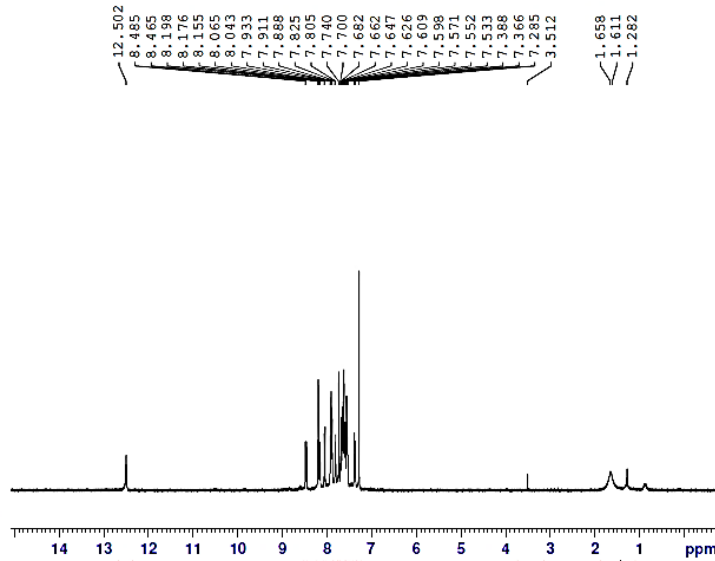


HR-MS spectrum of 7



IR spectrum of 8

AYA-20
 PROTON_BSU CDC13 (C:\data) abeer 2



¹H NMR spectrum of 8

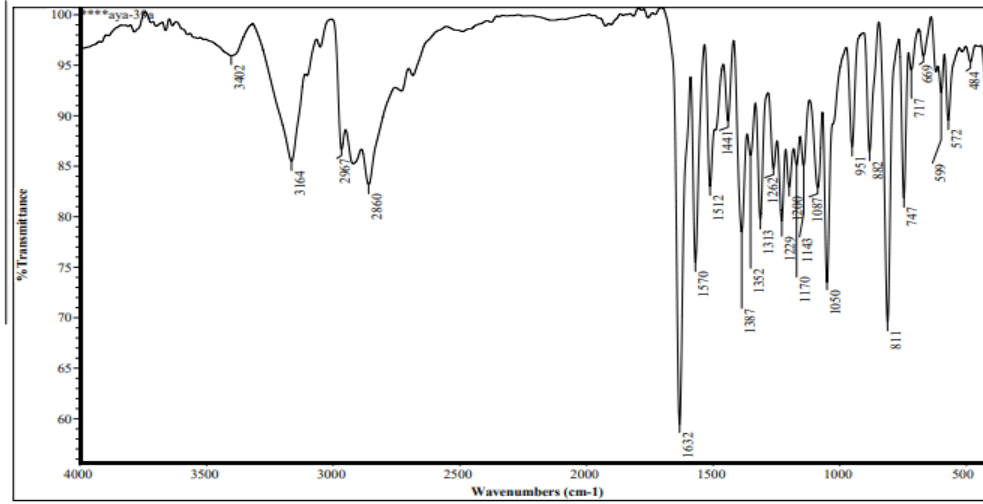
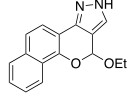


Current Data Parameters
 NAME May03-2018-abeer
 EXPNO 100
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180303
 Time 10.16
 INSTRUM spect
 PROBHD 5 mm PABBO BBI/
 PULPROG zg30
 TD 65536
 SOLVENT cdcl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 147.93
 EW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TDD 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 16.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00



****aya-39a
 Number of sample scans: 32
 Number of background scans: 32
 Resolution: 4.000
 Sample gain: 2.0
 Optical velocity: 0.4747
 Aperture: 80.00

Tue Apr 17 12:07:45 2018 (GMT-07:00)

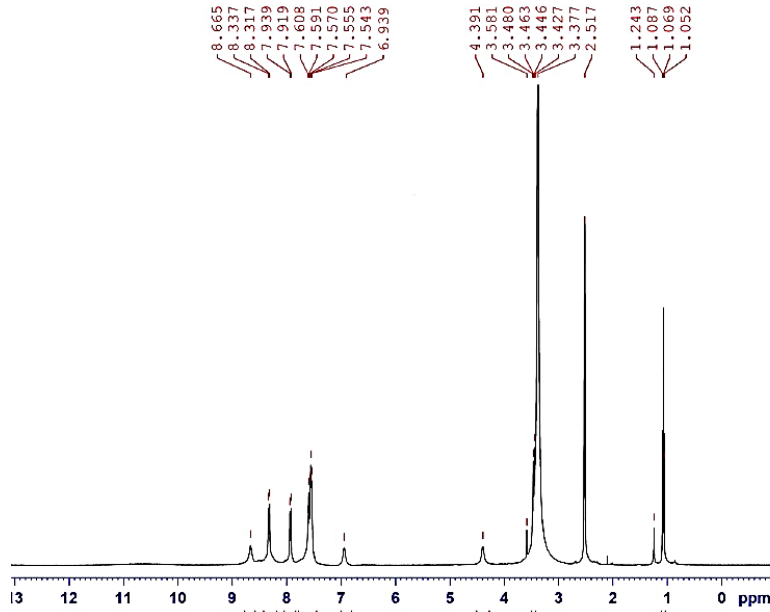


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 Spectral Analyses unit
 Chemistry Department
 ThermoFisher Nicolette IS10, USA
 Spectral range: 4000 - 400 cm-1

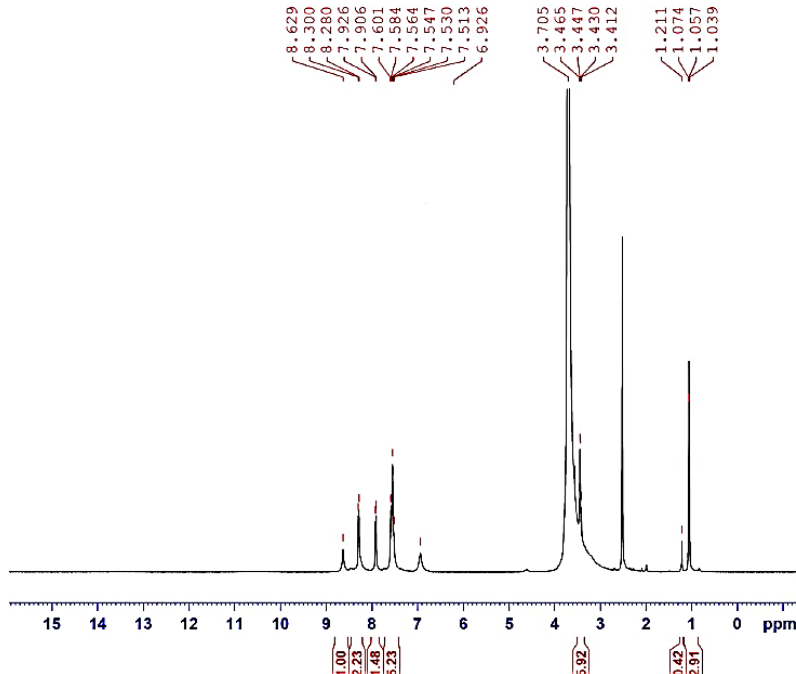
IR spectrum of 10



¹H NMR spectrum of 10



Current Data Parameters
 NAME aya atel 39a -M proton
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 2019020
 Time 12.51 h
 INSTRUM spect
 FREQHHD 2108618 0945 (1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0394465 sec
 RG 197.77
 DW 62.400 usec
 DE 4.50 usec
 TE 294.0 K
 TD 1.0000000 sec
 TSD 1
 SF01 400.2024712 MHz
 NUCL 1H
 PI 13.50 usec
 PLML 13.0000000 W
 F2 - Processing parameters
 SI 65536
 SF 400.2000000 MHz
 MW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

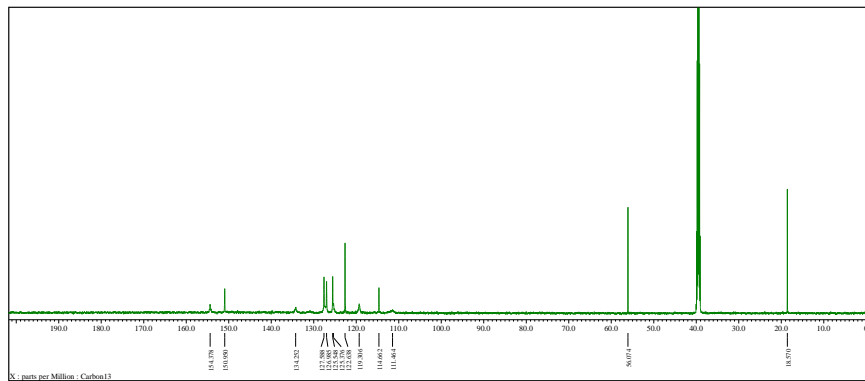


Current Data Parameters
 NAME Aya aya-39a -H₂O -dss-
 EXFNO 10
 PROCNO 1

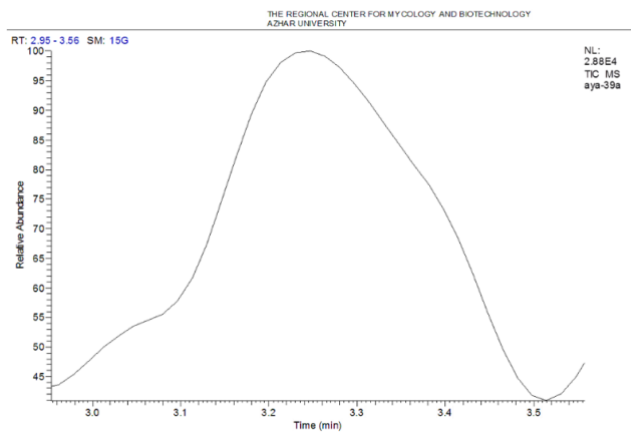
F2 - Acquisition Parameters
 Date 20191103
 Time 11.19 h
 INSTRUM spect
 PROGRAM 2109619_0919 ()
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SFO 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894465 sec
 RG 80.52
 DF 62.400 usec
 DE 6.50 usec
 TE 298.4 K
 DL 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 PI 13.50 usec
 PL1 13.0000000 w

F2 - Processing parameters
 SI 65536
 SF 400.2000800 MHz
 SFR 80
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

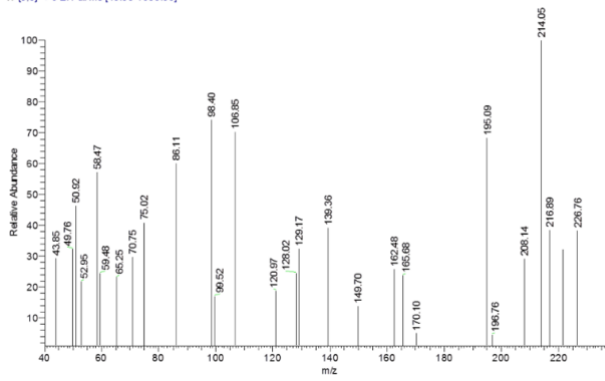
¹H NMR spectrum of compound 10 in the presence of D₂O



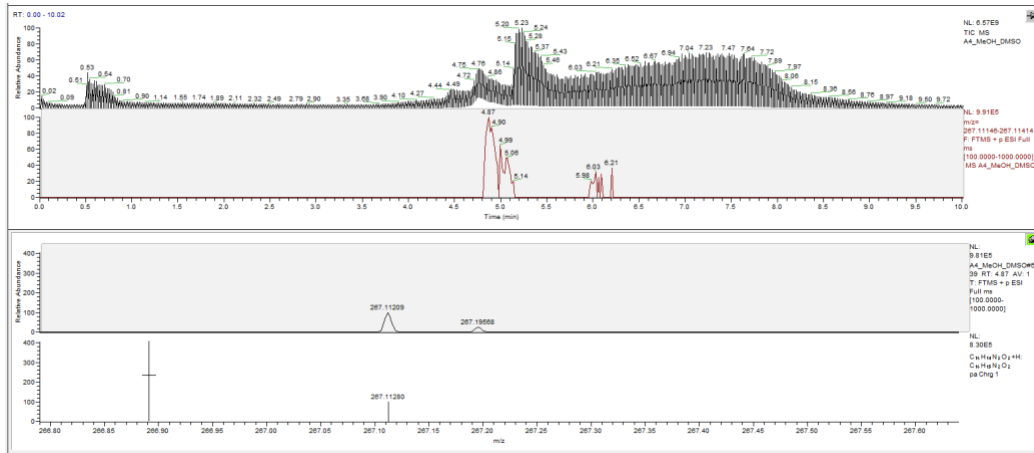
¹³C NMR spectrum of 10



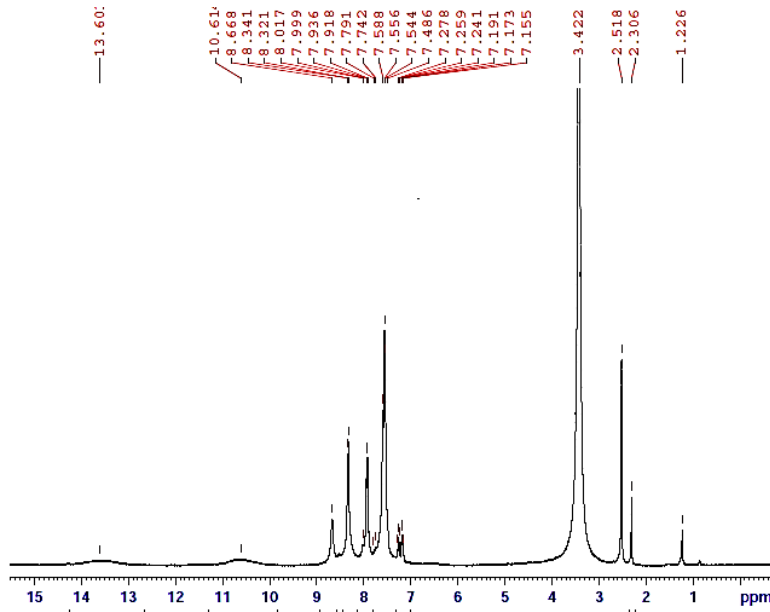
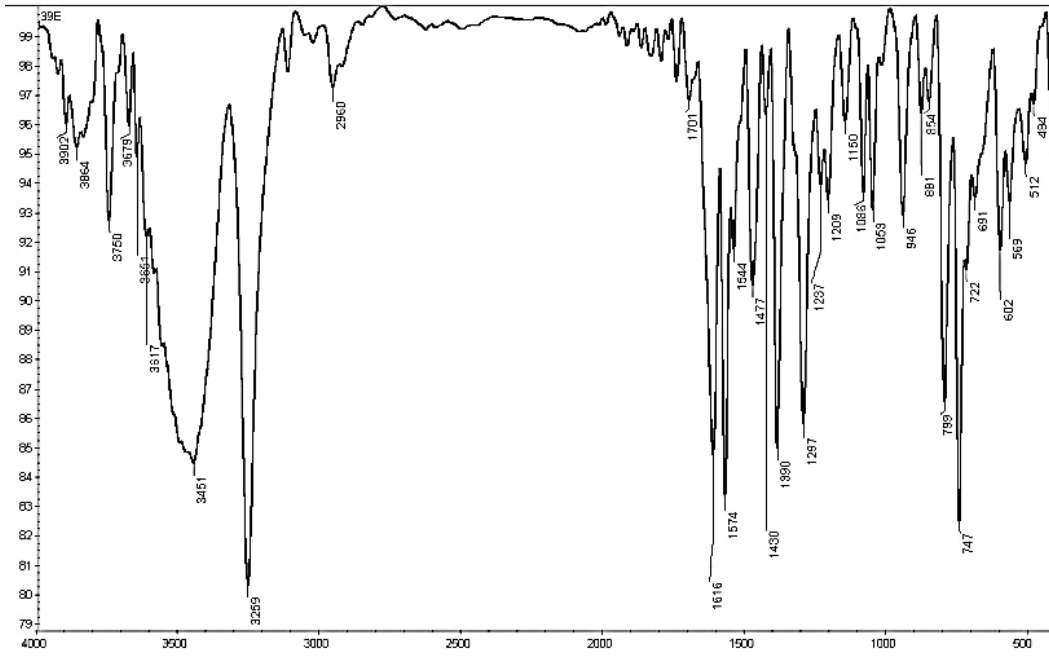
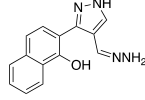
eye-39e #213 RT: 3.58 AV: 1 SB: 2 4.43, 4.43 NL: 3.63E2
 T: (0,0) + c EI Full ms [40.00-1000.00]



Mass spectrum of 10



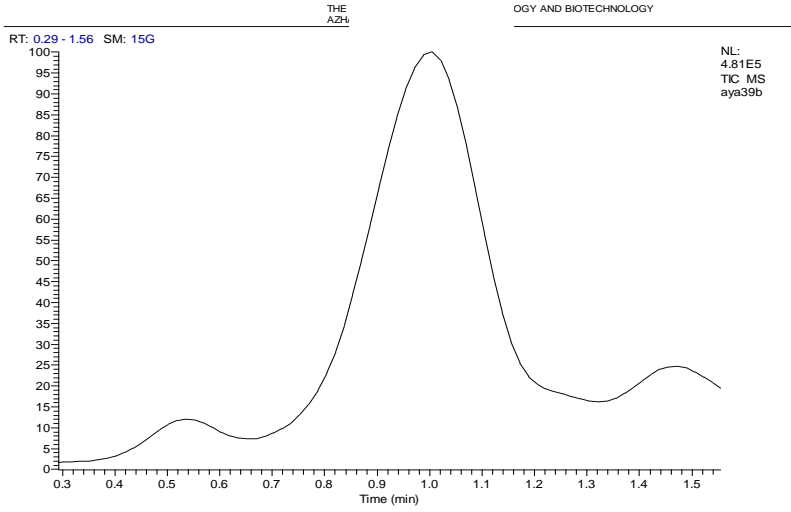
HR-MS spectrum of 10



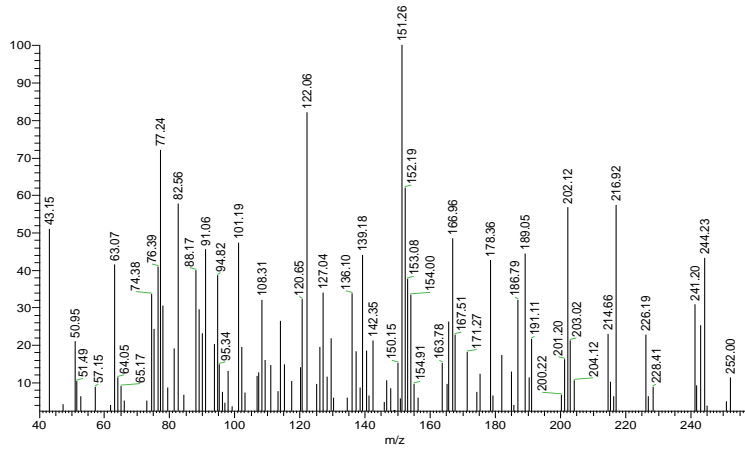
Current Data Parameters
 NAME Aya alsawi 396 - M proton
 EXNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191117
 Time 3.08 h
 INSTRUM spect
 FREQID 2108618 0445
 CULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0854465 sec
 RG 112.56
 IN 62.400 usec
 DE 6.50 usec
 IE 253.3 K
 D1 1.00000000 sec
 TDS
 SFO1 400.2024712 MHz
 NUC1 1H
 P1 13.50 usec
 PLW1 13.00000000 W

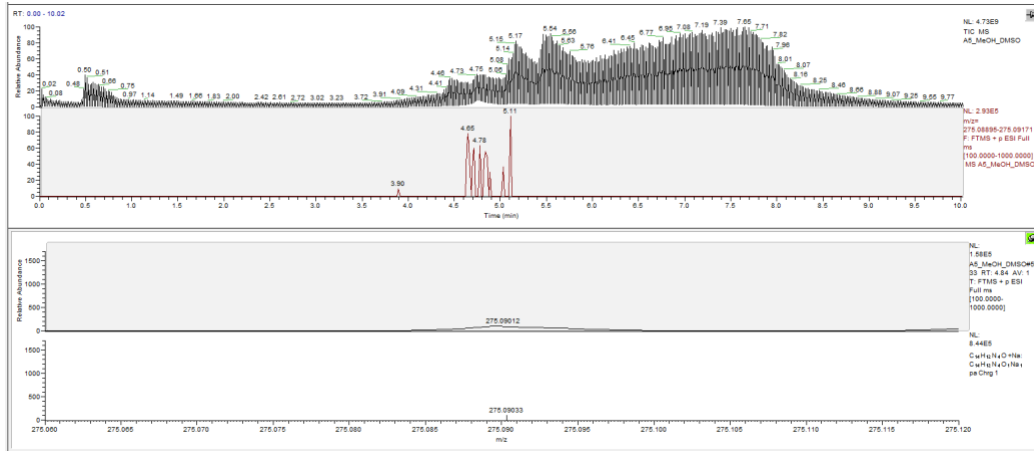
F2 - Processing parameters
 SI 65536
 SF 400.2000000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



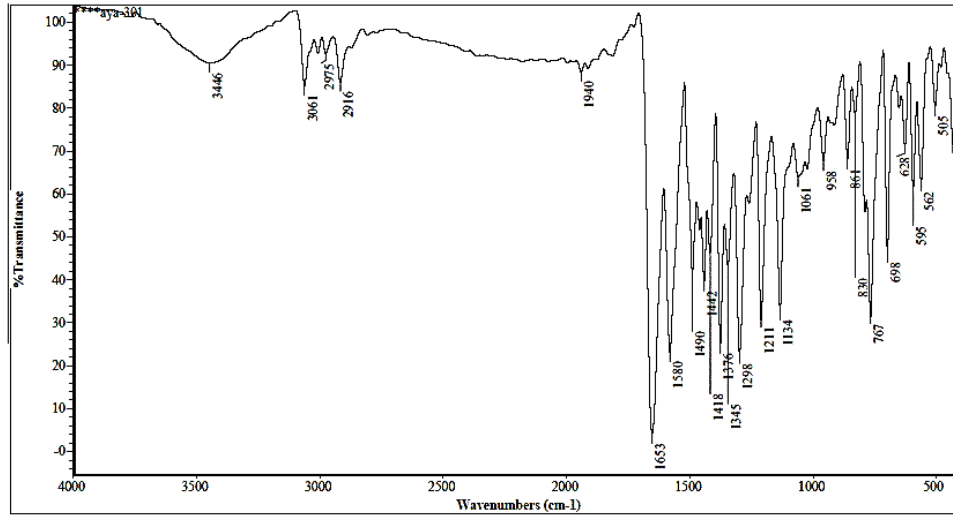
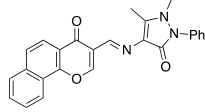
aya39b #32 RT: 0.55 AV: 1 SB: 2 3.82, 3.82 NL: 2.32E3
T: (0,0) + c EI Full ms [40.00-1000.00]



Mass spectrum of 11



HR-MS spectrum of 11



***aya-301

Number of sample scans: 32
 Number of background scans: 32
 Resolution: 4.000
 Sample gain: 4.0
 Optical velocity: 0.4747
 Aperture: 80.00



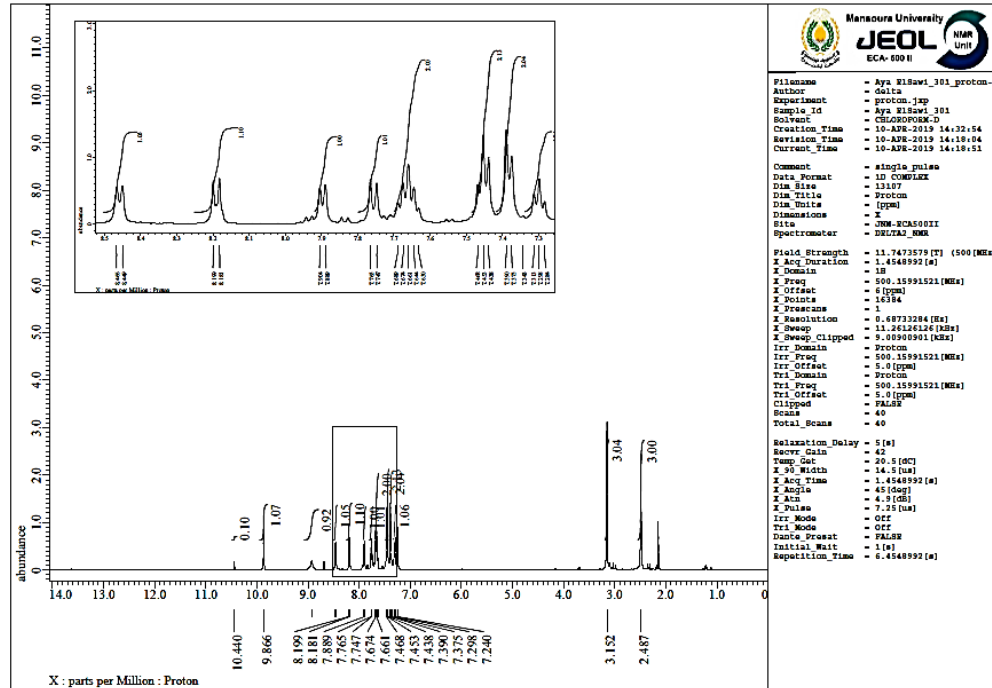
Tue Apr 09 13:24:05 2019 (GMT+02:00)

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Mansoura University
 Faculty of Science
 Spectral Analyses unit
 Chemistry Department
 ThermoFisher Nicolette IS10, USA
 Spectral range: 4000 - 400 cm-1

IR spectrum of 12a



Mansoura University
JEOL NMR Unit
 ECA-600H

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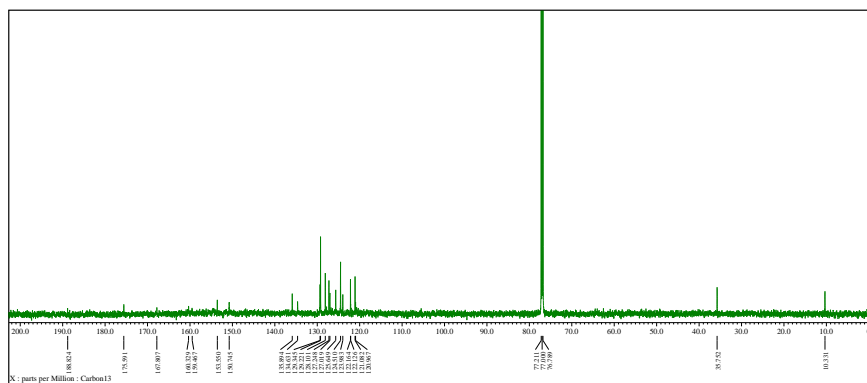
Filename = Aya_Kilawi_101_proton-1.
Author = Gaita
Experiment = proton_1xp
Sample ID = Aya_Kilawi_101
Solvent = CHLOROFORM-D
Creation Time = 10-ADR-2019 14:32:54
Revision Time = 10-ADR-2019 14:18:04
Current Time = 10-ADR-2019 14:18:51

Comment = single_pulse
Data Format = ID COMPLEX
Dir Size = 1317
Dir Title = Proton
Dir Units = [ppm]
Dimensions = 1
Site = JNM-ECX600EI
Spectrometer = JEOL7AJ_NMR

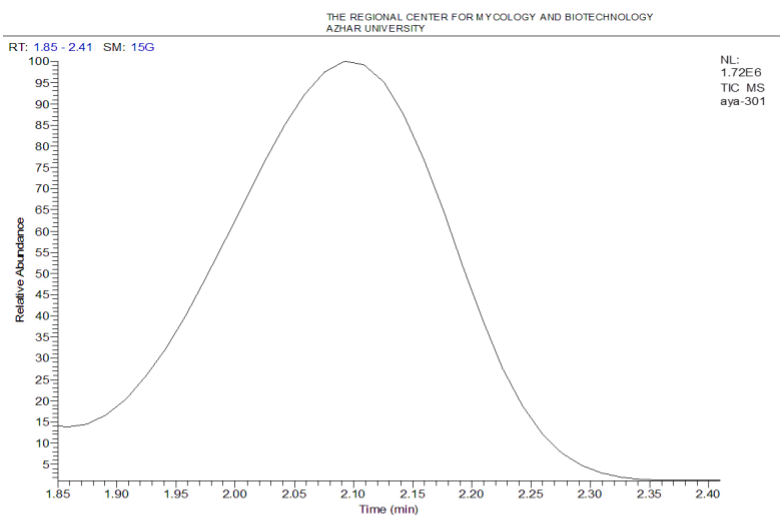
Field Strength = 11.747379 [T] (500 [MHz])
X_Acq Duration = 1.4548992 [s]
X_Domain = 18
X_Freq = 500.15991521 [MHz]
X_Offset = 6 [ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.69732884 [Hz]
X_Sweep = 11.26126126 [kHz]
X_Sweep_Clippped = 9.88989891 [kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521 [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 = 42
Temp Cal = 20.5 [degC]
X_90_Width = 14.5 [us]
X_Acq Time = 1.4548992 [s]
X_Angle = 45 [deg]
X_Pulse = 4.9 [dB]
X_Pulse_Prog = 7.00 [us]
Irr_Mode = Off
Tri_Mode = Off
Dance_Program = FALSE
Initial Wait = 1 [s]
Repetition Time = 6.4548992 [s]
  
```

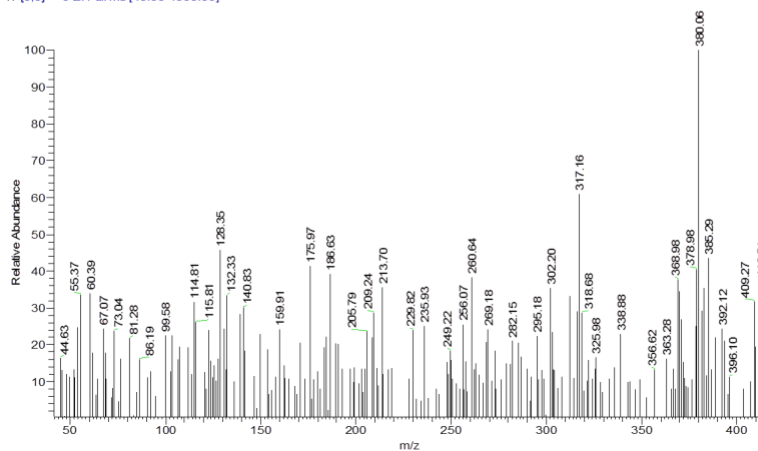
1H NMR spectrum of 12a



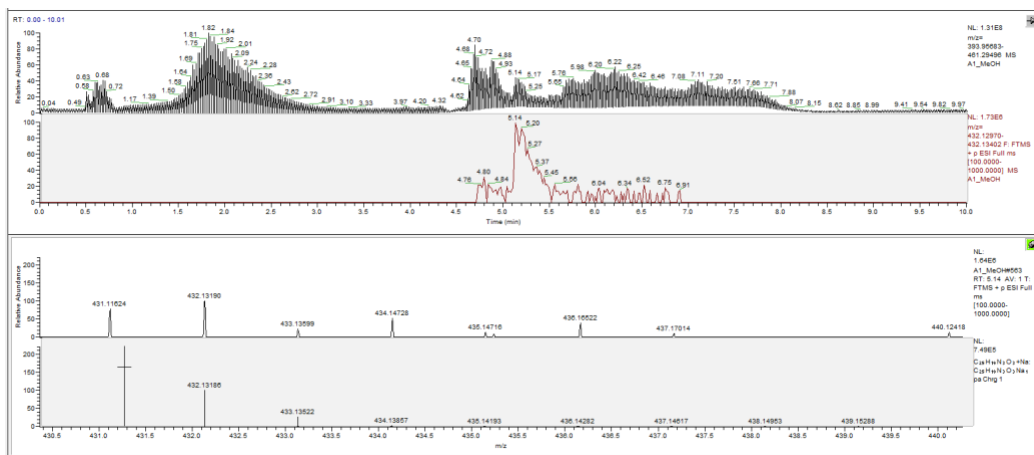
^{13}C NMR spectrum of **12a**



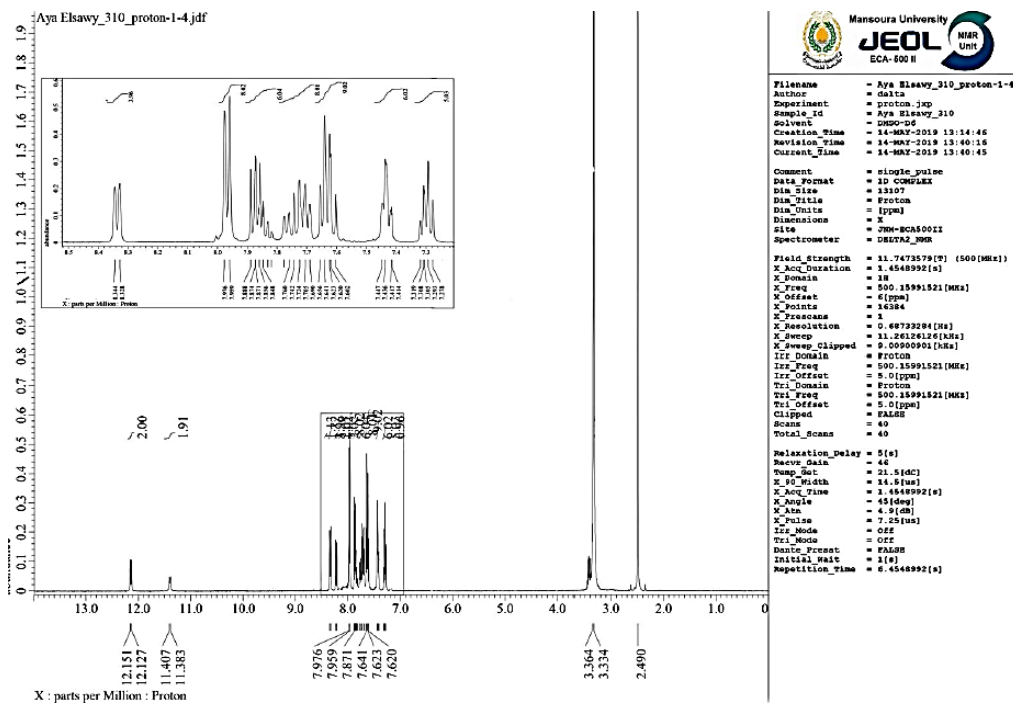
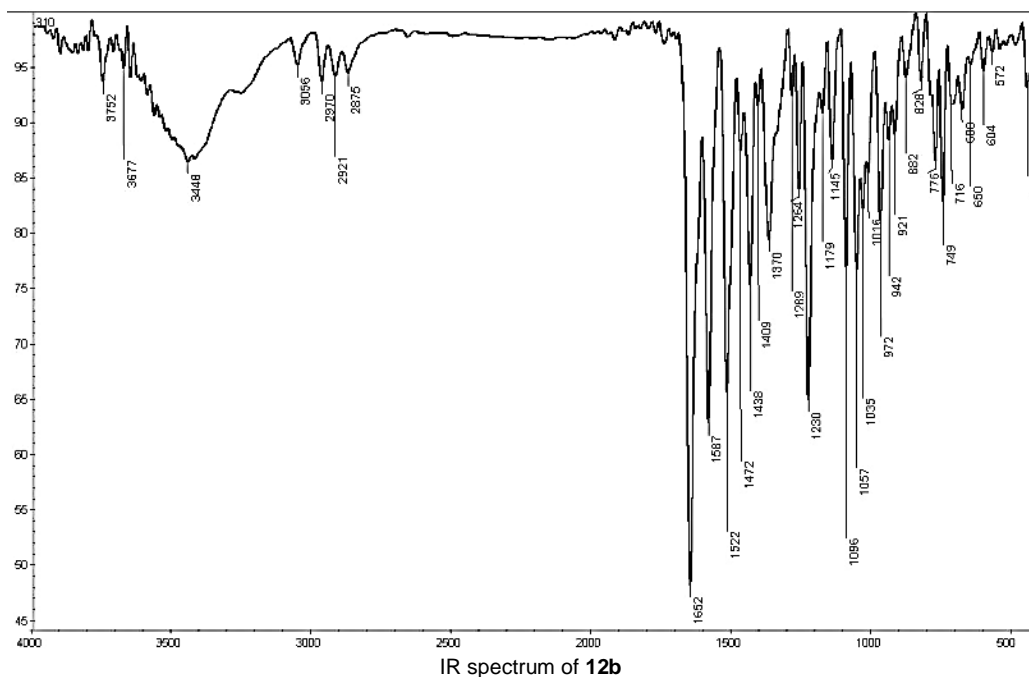
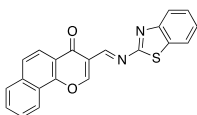
aya-301 #191-192 RT: 3.21-3.23 AV: 2 SB: 2 4.47, 4.47 NL: 4.39E2
T: (0,0) +c EI Full ms [40.00-1000.00]



Mass spectrum of **12a**



HR-MS spectrum of 12a



Mansoura University
JEOL NMR UNIT
ECA-600 II

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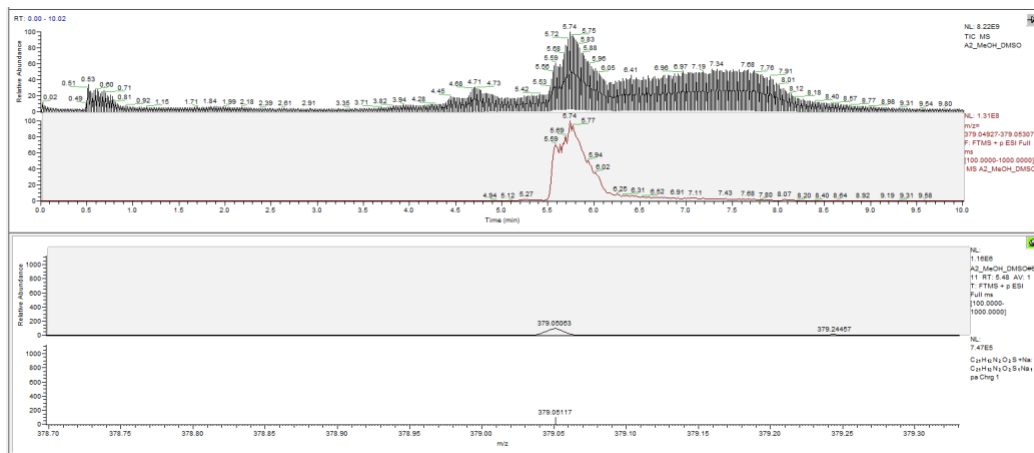
Filename = Aya_Elsawy_310_proton-1-4.
Author = delta
Experiment = proton_jkp
Sample_Id = Aya_Elsawy_310
Solvent = DMSO-d6
Creation_Time = 14-MAY-2019 13:54:46
Revision_Time = 14-MAY-2019 13:40:16
Current_Time = 14-MAY-2019 13:40:45

Comment = single pulse
Data_Format = 3D COMPLEX
Dir_Type = 13107
Dir_Title = Proton
Dir_Unit = [ppm]
Discipline = X
Site = JNM-ECX600II
Spectrometer = spect2_300

Field_Strength = 11.7473579[P] (500[MHz])
X_Acq_Duration = 3.4548992[s]
X_Pulsin = 18
X_Freq = 500.13591521[MHz]
X_Offset = 6[ppm]
X_Points = 16384
X_Programs = 3
X_Resolution = 0.68732284[Hz]
X_Sweep = 11.28228282[s][Hz]
X_Sweep_Clipped = 9.0090901[Hz]
Irr_Domain = PROTON
Irr_Freq = 500.13591521[MHz]
Irr_Offset = 5.0[ppm]
Tr1_Domain = PROTON
Tr1_Freq = 500.13591521[MHz]
Tr1_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 40
Total_Scans = 40

Relaxation_Delay = 5[s]
Recov_Gain = 46
Temp_Set = 21.5[degC]
X_P1_Width = 11.6[us]
X_Acq_Time = 3.4548992[s]
X_Angle = 45[deg]
X_Alt = 4.0[deg]
X_Pulse = 7.25[us]
Irr_Mode = Off
Tr1_Mode = Off
Date_Recd = 14-MAY-2019
Initial_Stat = 1[s]
Repetition_Time = 6.4548992[s]

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HR-MS spectrum of 12b

2. Pharmacokinetic parameters of the synthesized derivatives

Comp	Mol. Weight	#Rotatable bonds	#H-bond acceptors	#H-bond donors	TPSA	Silicos-IT Log P	Bioavailability Score	Solubility
3a	290.27	2	4	2	93.95	3.54	0.55	Soluble
3b	380.4	3	4	1	83.09	4.6	0.55	Moderately soluble
3c	396.39	4	5	1	92.32	4.13	0.55	Moderately soluble
3d	445.26	3	4	1	83.09	4.75	0.55	Poorly soluble
3e	411.37	4	6	1	128.91	1.91	0.55	Moderately soluble
3f	476.48	4	5	1	110.02	3.68	0.55	Poorly soluble
3g	387.41	3	5	1	124.22	4.66	0.55	Moderately soluble
3h	423.44	3	5	1	124.22	5.15	0.55	Poorly soluble
3i	475.45	4	7	1	125.66	5.18	0.55	Poorly soluble
5	305.29	4	5	1	95.46	3.31	0.55	Soluble
6	305.29	2	5	3	99.1	2.89	0.55	Moderately soluble
7	297.33	2	3	3	113.86	4.25	0.55	Soluble
8	331.39	2	3	1	74.96	4.78	0.55	Moderately soluble
10	266.29	2	3	1	47.14	3.52	0.55	Soluble
11	280.28	3	4	3	104.36	2.55	0.55	Soluble
12a	409.44	3	4	0	69.5	4.95	0.55	Moderately soluble
12b	356.4	2	4	0	83.7	6.45	0.55	Moderately soluble

3. Role of hydrophobic interactions in docking of compound 3c

