

Synthesis, In vitro Evaluation and Molecular Docking Studies of Novel Thiophenyl Thiazolyl-Pyridine Hybrids as Potential Anticancer Agents

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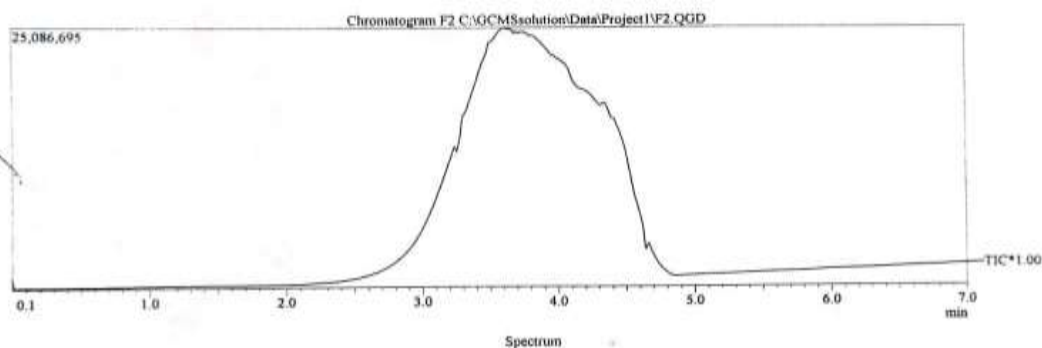
DI Analysis Shimadzu Qp-2010 Plus



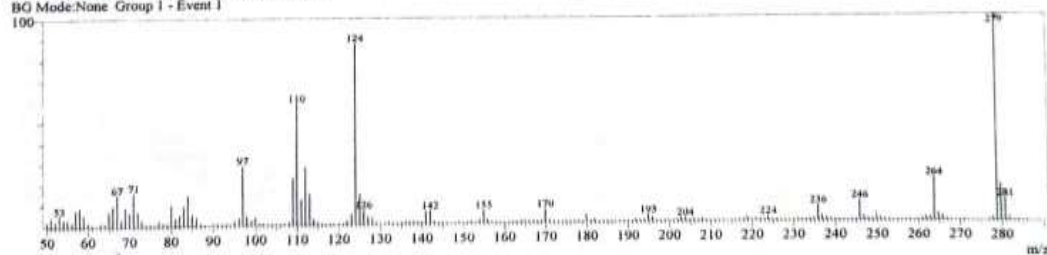
Analyzed by Dr. Mai Younis
Analyzed 27/08/2019 02:29:38
Sample Name F2
Sample ID
Customer Name Dr. Fayza Othman - Science - Cairo
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Org Data File C:\GCMSolution\Data\Project1\F2.QGD
Method File C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File C:\GCMSolution\Data\Project1\High Temperature Op
Report File
Tuning File C:\GCMSolution\System\Tune1_default.qgt
SEndIfSModified by Dr. Mai Younis
Modified 27/08/2019 02:34:32

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 : 1111
 Start m/z : 50.00
 End m/z : 550.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

C:\GCMSolution\Data\Project1\F2.QGD

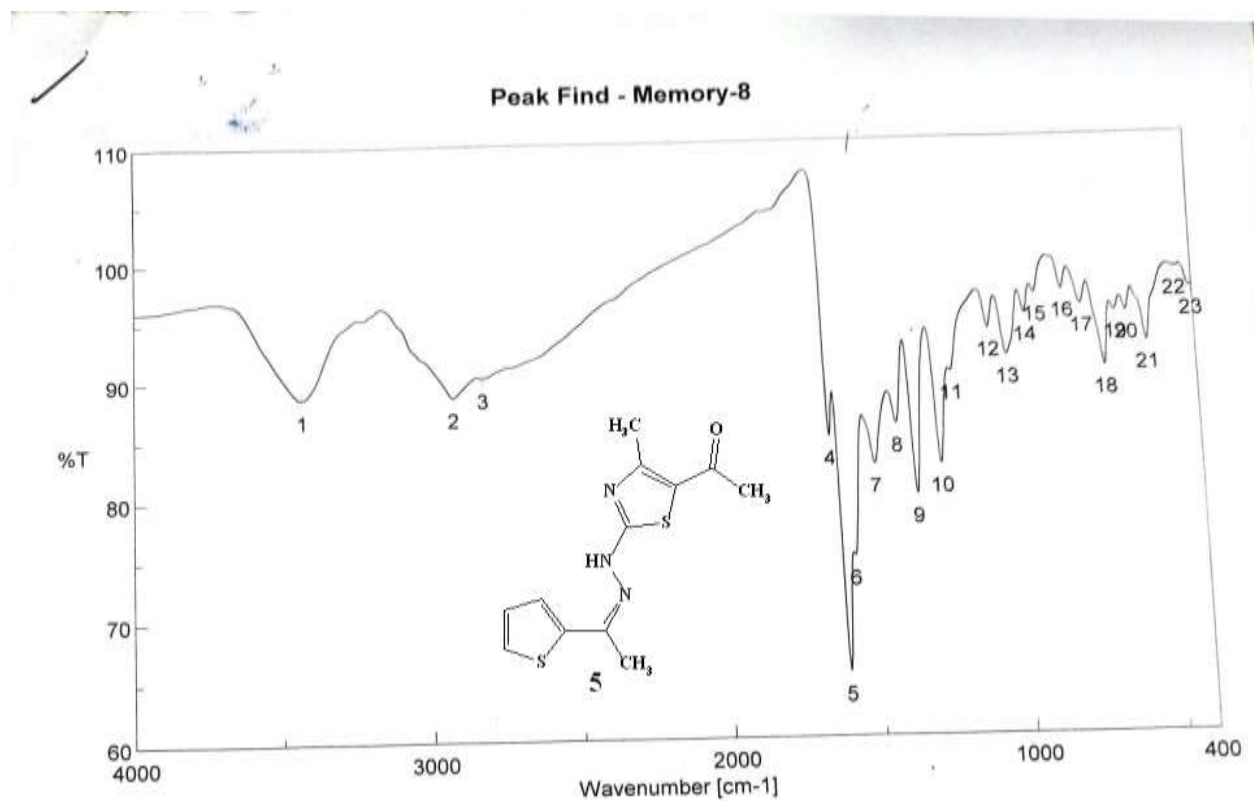


Line#:1 R.Time:3.6(Scan#:436)
 MassPeaks:231
 RawMode:Single 3.6(436) BasePeak:279(3264752)
 BG Mode:None Group 1 - Event 1



Mass Table
 Line#:1 R.Time:3.6(Scan#:436)
 MassPeaks:231
 RawMode:Single 3.6(436) BasePeak:279(3264752)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	60822	1.86	4	53.00	165374	5.07
2	51.00	140705	4.31	5	54.00	109041	3.34
3	52.00	82143	2.52	6	55.00	101590	3.11
				7	56.05	60482	1.85
				8	56.95	244535	7.49
				9	57.95	285652	8.75



[Comments]
 Sample name F2
 Comment 12/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3430.74	88.5809	2	2918.73	88.5304	3	2818.45	90.0999
4	1650.77	84.7602	5	1609.31	65.2476	6	1579.41	74.7496
7	1501.31	82.3557	8	1424.17	85.6966	9	1361.5	79.7901
10	1278.57	82.2721	11	1235.18	89.9593	12	1103.08	93.5253
13	1043.3	91.2129	14	976.769	94.7092	15	940.128	96.3989
16	845.633	96.6811	17	782.958	95.3875	18	711.604	90.1341
19	668.214	94.8291	20	630.609	94.7651	21	564.077	92.1955
22	458.975	98.4484	23	405.942	96.7336			



IR spectra of compound 5

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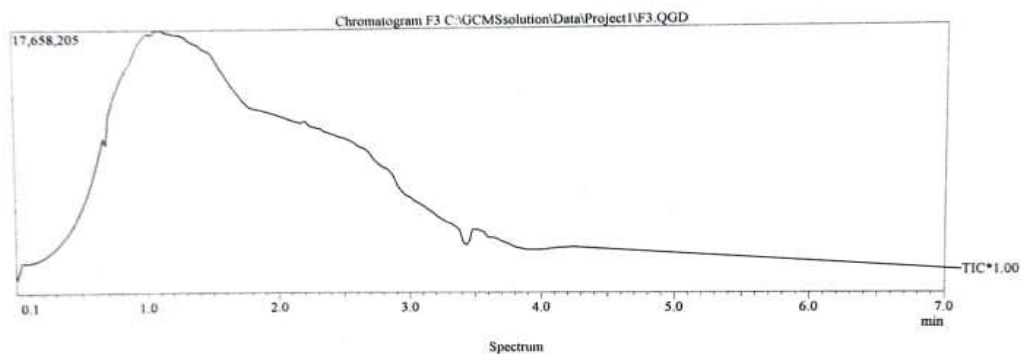
DI Analysis Shimadzu Qp-2010 Plus

Sample Information
 Analyzed by: Dr. Mai Younis
 Analyzed: 27/08/2019 02:37:16
 Sample Name: F3
 Sample ID:
 Customer Name: Dr. Fayza Othman - Science - Cairo
 Data File: C:\GCMSolution\Data\Project1\F3.QGD
 Org Data File: C:\GCMSolution\Data\Project1\F3.QGD
 Method File: C:\GCMSolution\Data\Project1\High Temperature Op
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 Report File:
 Tuning File: C:\GCMSolution\System\Tune1_default.qgt
 \$EndIFS Modified by: Dr. Mai Younis
 Modified: 27/08/2019 02:41:35

Method
 Analytical Line 1
 IonSource Temp: 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: 1111
 Start m/z: 50.00
 End m/z: 550.00
 Electron Voltage: 70 eV
 Ionization Mode: EI



C:\GCMSolution\Data\Project1\F3.QGD

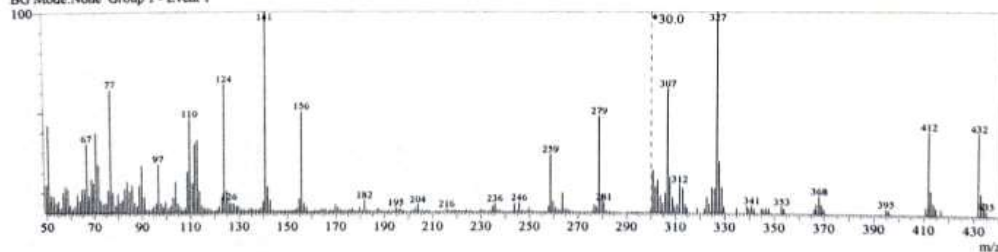


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MassPeaks:302

RawMode:Single 2.5(298) BasePeak:141(764329)

BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:2.5(Scan#:298)

MassPeaks:302

RawMode:Single 2.5(298) BasePeak:141(764329)

BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	106316	13.91	4	53.00	63658	8.33	7	56.05	19283	2.52
2	51.00	334652	43.78	5	54.00	35881	4.69	8	57.00	77417	10.13
3	52.00	65186	8.53	6	55.00	42828	5.60	9	57.95	101714	13.31

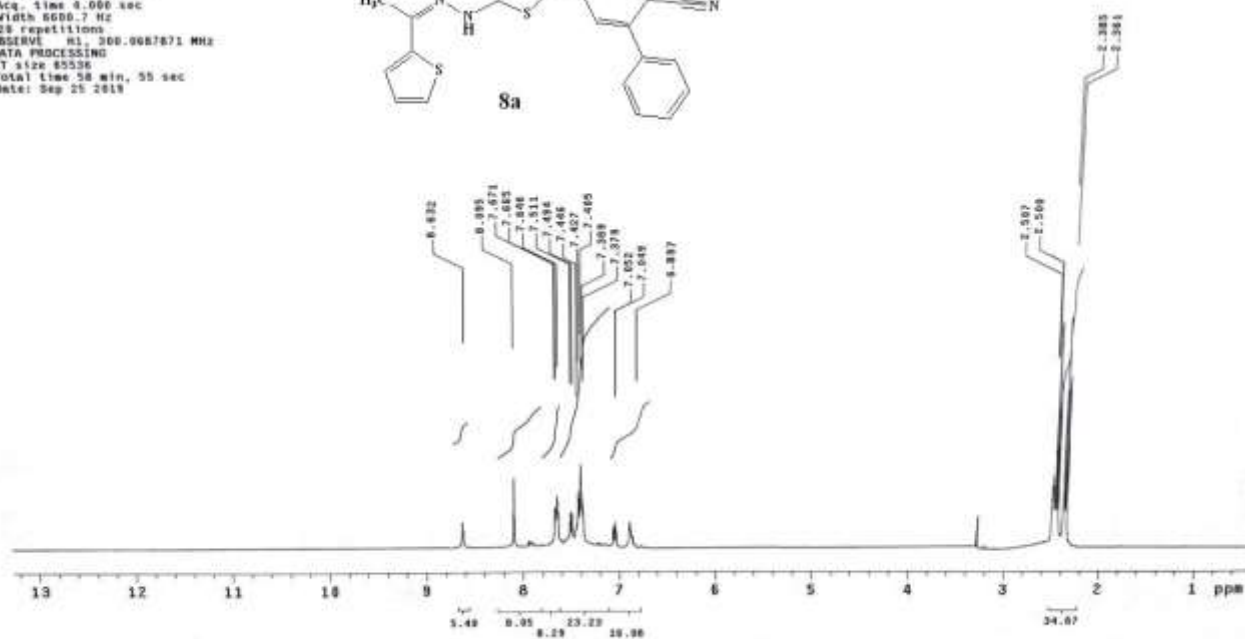
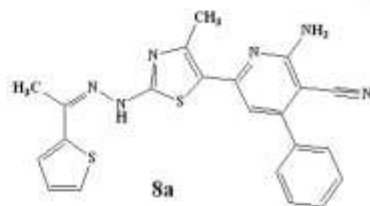
FayzW0thman-F2-DMSO-H1

Archive directory: /export/home/vmr1/vmrsys/data
Sample directory: D05ae_test_12Mar2014-21:34:49
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp. 30.0 C / 303.1 K
Mercury-50000 "NMR300"

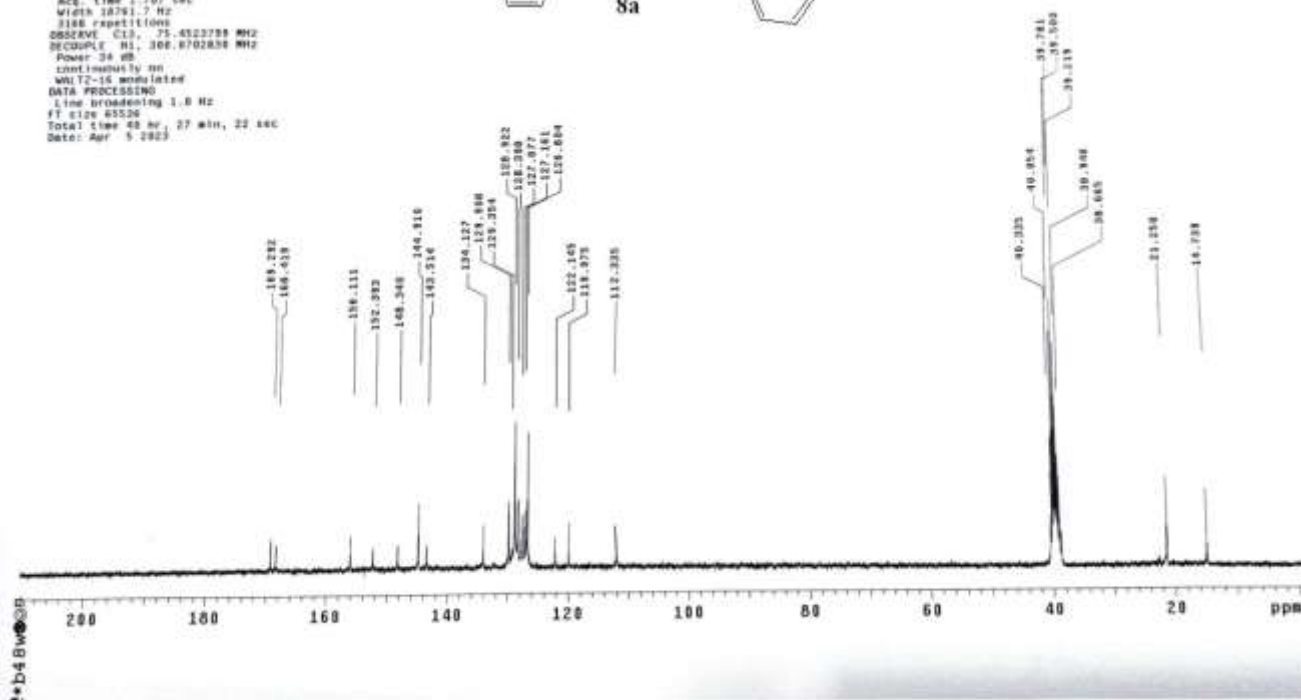
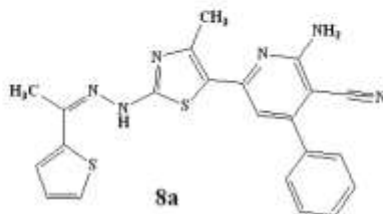
Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6000.7 Hz
28 repetitions
OBSERVE H1, 300.9087871 MHz
DATA PROCESSING
FT size 85336
Total time 58 min. 55 sec
Date: Sep 25 2019



¹H-NMR spectra of compound **8a**

FayzOdhan-T3-DMSO-Cl3
 Archive directory: /export/home/vmr1/vmr/sys/data
 Sample directory: D05aw_test_12Mar2014-21:34:40
 Pulse Sequence: szpu1
 Solvent: DMSO
 Ambient temperature
 File: FayzOdhan-T3-DMSO-Cl3
 Marcury-30000 "NMR300"

Pulse 45.0 degrees
 Acq. time 1.767 sec
 Width 18781.7 Hz
 3188 repetitions
 OBSERVE C13, 75.4522798 MHz
 DECOUPLE H1, 300.6702838 MHz
 Power 34 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65526
 Total time 48 hr, 27 min, 22 sec
 Date: Apr 5 2003



¹³C-NMR spectra of compound **8a**

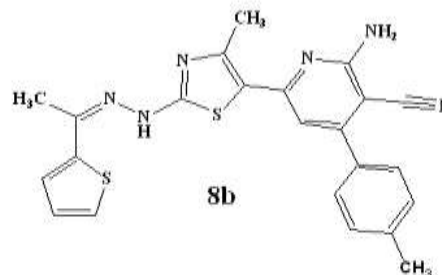


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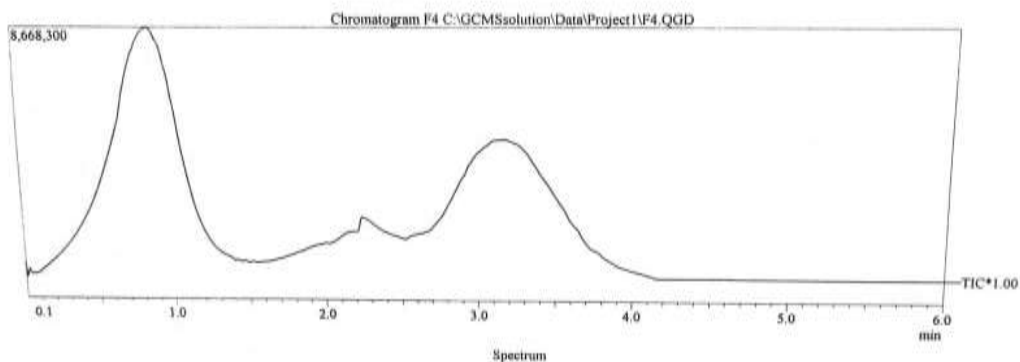
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 27/08/2019 02:54:27
 Sample Name : F4
 Sample ID :
 Customer Name : Dr. Fayza Othman - Science - Cairo
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 Org Data File : C:\GCMSolution\Data\Project1\F4.QGD
 Method File : C:\GCMSolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSolution\System\Tune1_default.qgt
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 Modified : 27/08/2019 02:58:40

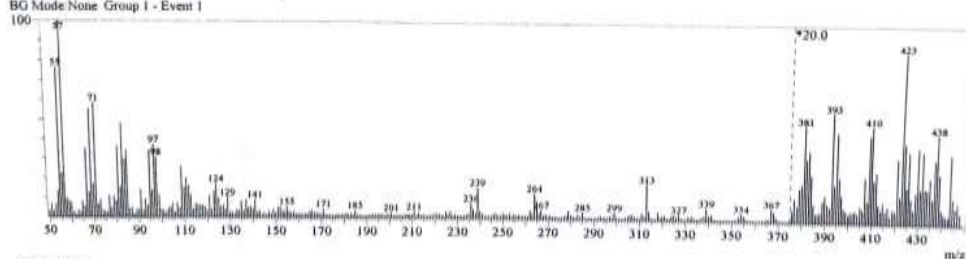
Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1111
 Start m/z : 50.00
 End m/z : 550.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSolution\Data\Project1\F4.QGD



Line#1 R.Time:3.1(Scan#:375)
 MassPeaks:399
 RawMode:Single 3.1(375) BasePeak:57(301854)
 BG Mode:None Group 1 - Event 1



Mass Table
 Line#1 R.Time:3.1(Scan#:375)
 MassPeaks:399
 RawMode:Single 3.1(375) BasePeak:57(301854)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	8705	2.88	4	53.00	19652	6.51	7	56.05	67099	22.23
2	51.00	20052	6.64	5	54.05	40410	13.39	8	57.00	301854	100.00
3	52.00	8433	2.79	6	55.00	229879	76.16	9	58.00	28166	9.33

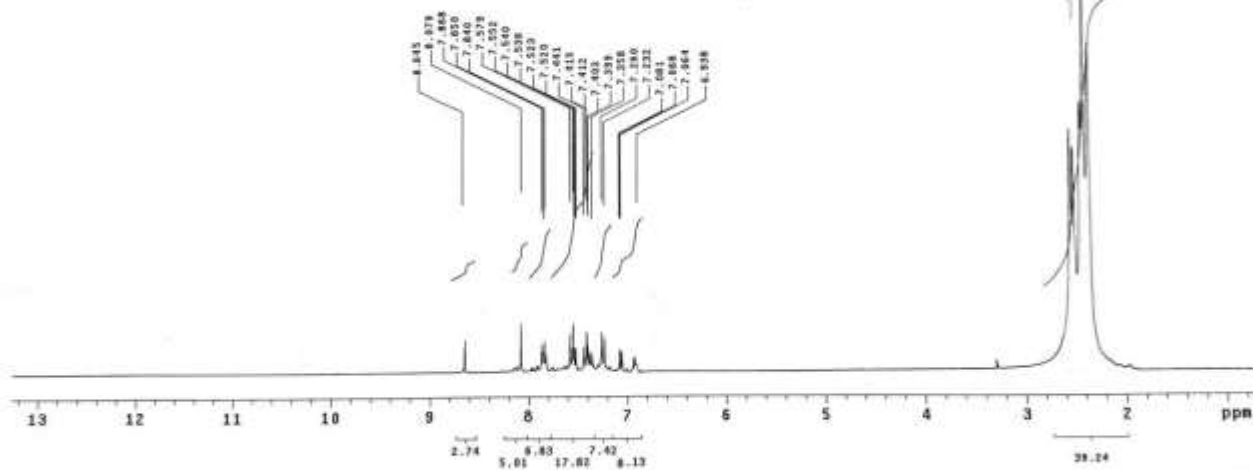
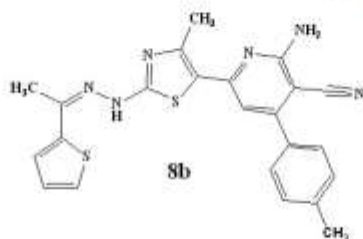
Mass spectra of compound **8b**

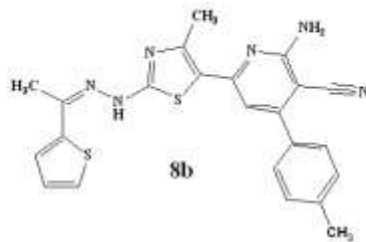
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File: PROTON
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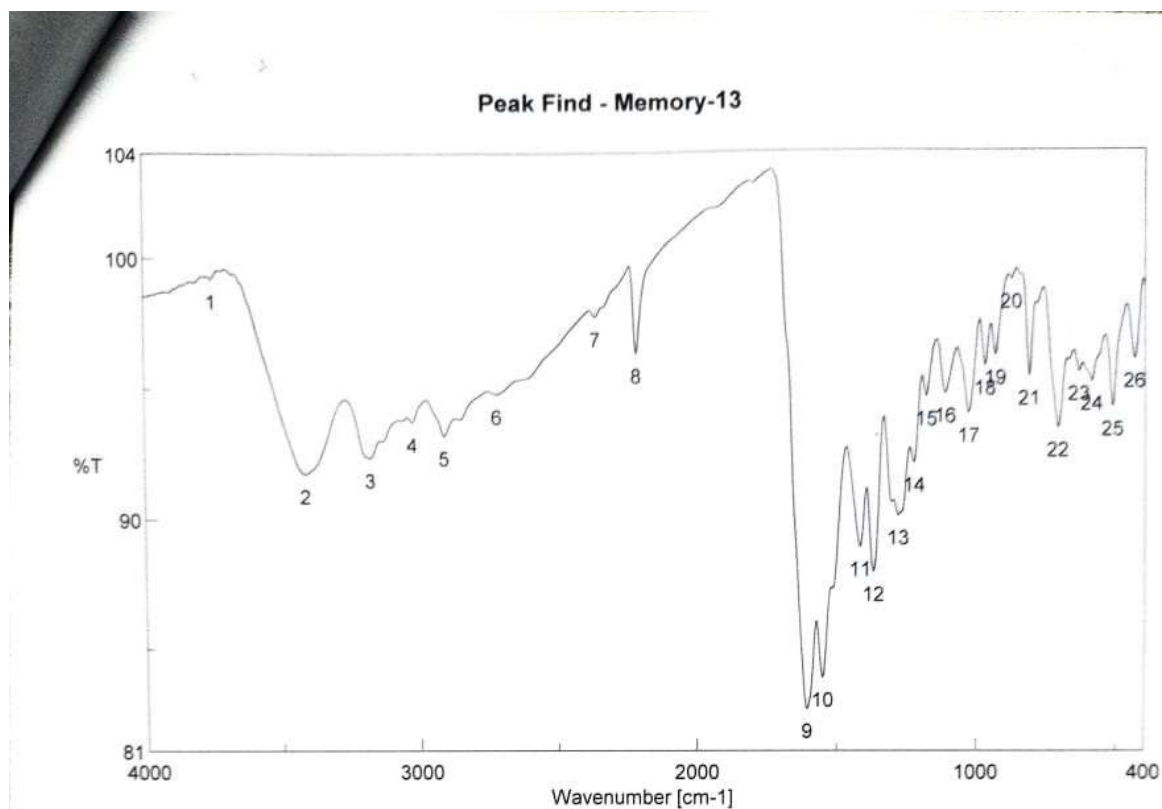
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Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 4.908 sec
Width 6680.7 Hz
23 repetitions
OBSERVE H1 389.0687871 MHz
DATA PROCESSING
FT size 65536
Total time 58 min, 35 sec
Date: Sep 28 2019

```

¹H-NMR spectra of compound **8b**

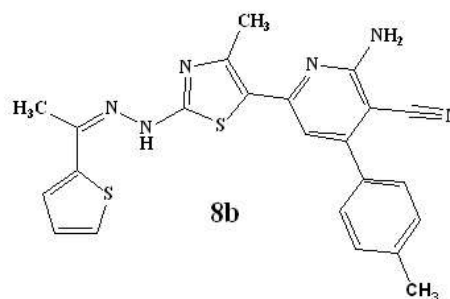
^{13}C -NMR spectra of compound **8b**



[Comments]
 Sample name F4
 Comment 12/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3754.73	99.2222	2	3419.17	91.7877	3	3186.79	92.4049
4	3034.44	93.7705	5	2918.73	93.2482	6	2727.82	94.8251
7	2370.09	97.7512	8	2221.59	96.3559	9	1605.45	82.6371
10	1550.49	83.849	11	1416.46	88.8668	12	1369.21	87.9095
13	1281.47	90.0695	14	1225.54	92.0897	15	1183.11	94.6143
16	1115.62	94.7216	17	1031.73	93.9622	18	973.876	95.7597
19	937.235	96.1588	20	879.381	99.0589	21	814.777	95.3733
22	710.64	93.4037	23	636.394	95.5344	24	591.075	95.1588
25	515.865	94.2022	26	437.762	96.0332			



IR spectra of compound **8b**



27-Aug-19 16:13:36

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DI Analysis Shimadzu Qp-2010 Plus

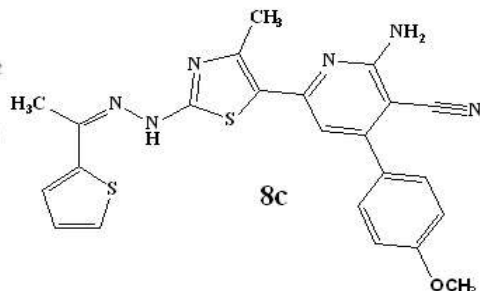
Sample Information

Analyzed by : Dr. Mai Younis
 Analyzed : 27/08/2019 04:07:46
 Sample Name : F8
 Sample ID :
 Customer Name : Dr. Fayza Othman - Science - Cairo
 Data File : C:\GCMSsolution\Data\Project1\F8.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\F8.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System1\Tune1\default.qgt
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 Modified : 27/08/2019 04:12:20

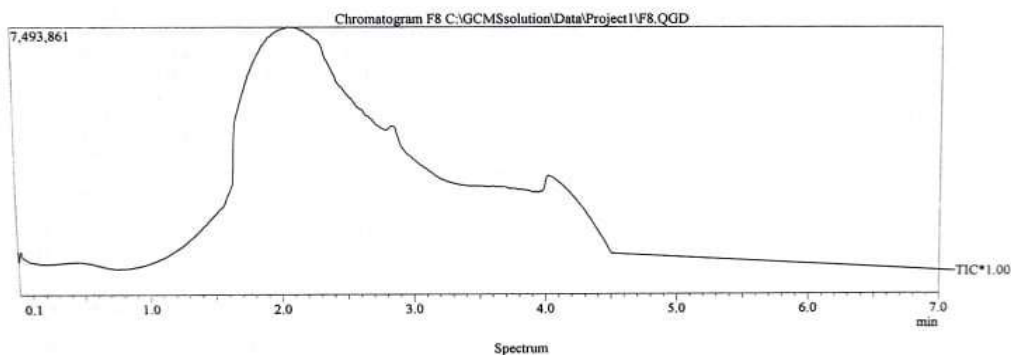
Method

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 : 1111
 Start m/z : 50.00
 End m/z : 550.00

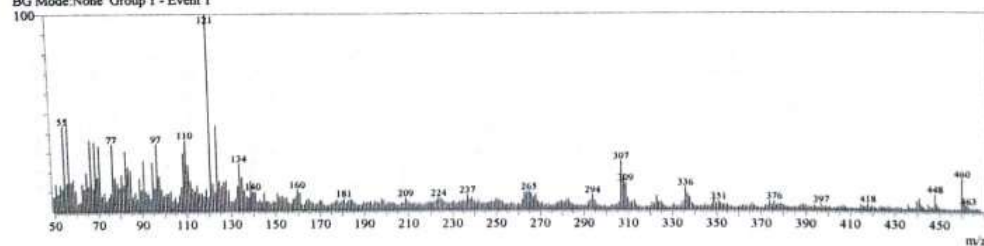
Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\F8.QGD



Line# 1 R.Time:3.6(Scan#:435)
 MassPeaks:419
 RawMode:Single 3.6(435) BasePeak:121(119064)
 BG Mode:None Group 1 - Event 1



Mass Table

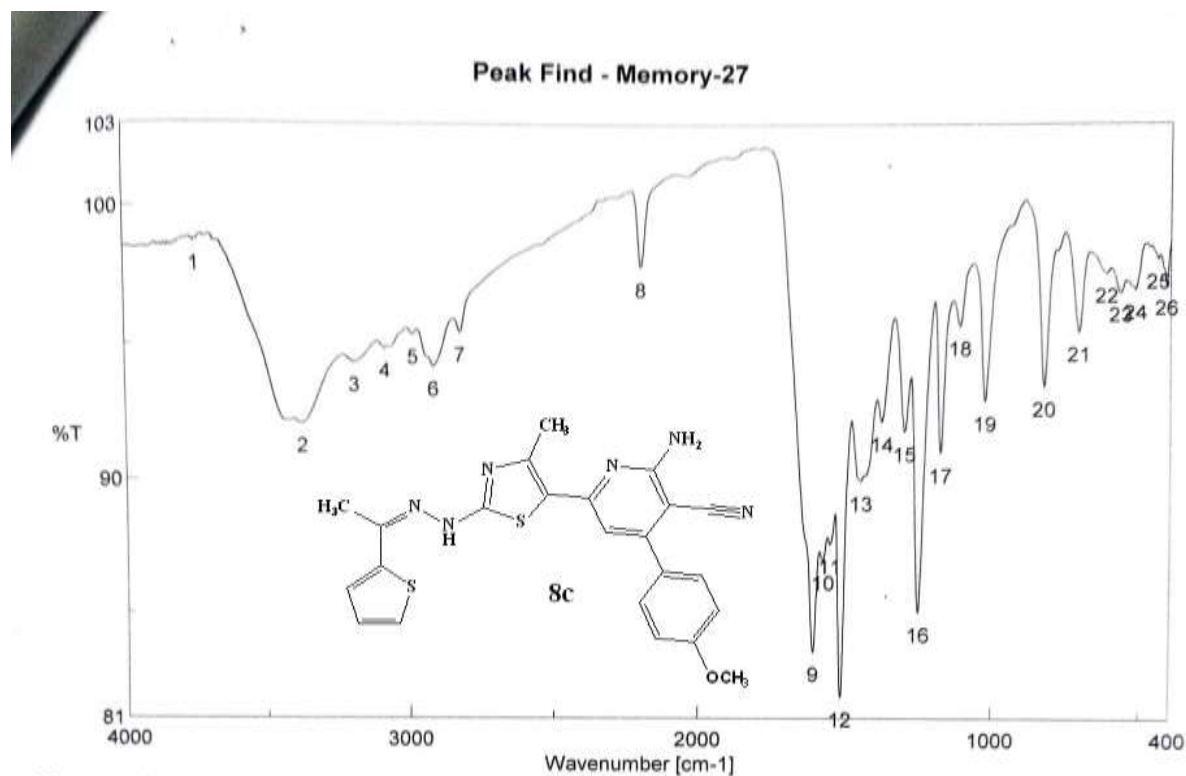
Line# 1 R.Time:3.6(Scan#:435)

MassPeaks:419

RawMode:Single 3.6(435) BasePeak:121(119064)

BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	8631	7.25	4	53.00	15959	13.40	7	56.05	16792	14.10
2	51.00	16697	14.02	5	54.05	13674	11.48	8	57.00	56788	47.70
3	52.00	10374	8.71	6	55.00	51638	43.37	9	58.00	17378	14.60



[Comments]
 Sample name F8
 Comment 12/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3752.8	98.7361	2	3383.5	92.0907	3	3204.15	94.3546
4	3097.12	94.8811	5	3000.69	95.3727	6	2928.38	94.1936
7	2837.74	95.4513	8	2208.09	97.7665	9	1605.45	83.4802
10	1572.66	86.8829	11	1549.52	87.4896	12	1511.92	81.7909
13	1446.35	89.8177	14	1376.93	91.9994	15	1299.79	91.6309
16	1249.65	84.9454	17	1177.33	90.8359	18	1115.62	95.5094
19	1028.84	92.7327	20	828.277	93.2543	21	710.64	95.2878
22	617.109	97.4659	23	569.862	96.7562	24	519.722	96.8541
25	442.583	97.9948	26	413.656	97.0177			



IR spectra of compound **8c**



27-Aug-19 15:56:29

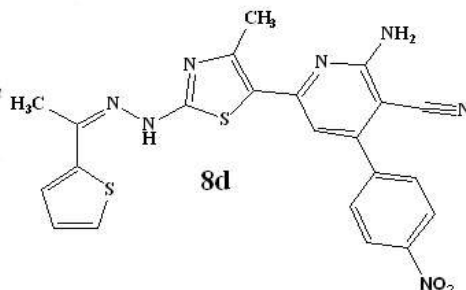
ع. د. محمد

Cairo University Micro Analytical Center

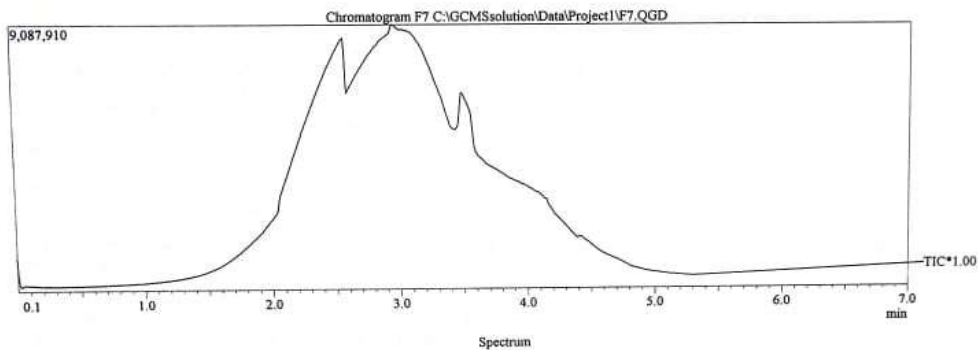
DI Analysis Shimadzu Qp-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 27/08/2019 03:49:36
Sample Name : F7
Sample ID :
Customer Name : Dr. Fayza Othman - Science - Cairo
Data File : C:\GCMSsolution\Data\Project1\F7.QGD
Org Data File : C:\GCMSsolution\Data\Project1\F7.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
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Report File :
Tuning File : C:\GCMSsolution\System1\Tune1_default.qgt
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Modified : 27/08/2019 03:54:59

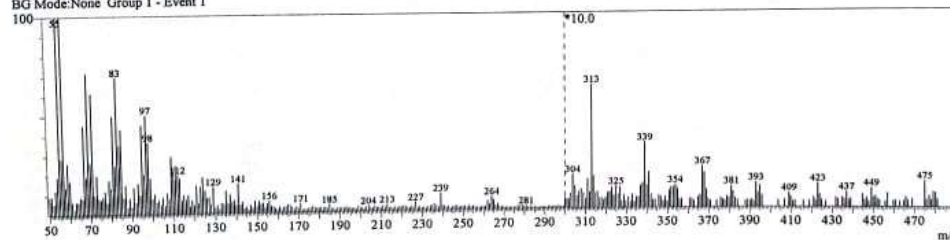
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1111
Start m/z : 50.00
End m/z : 550.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Data\Project1\F7.QGD



Line#1 R.Time:4.5(Scan#:540)
MassPeaks:382
RawMode:Single 4.5(540) BasePeak:57(79712)
BG Mode:None Group 1 - Event 1



Mass Table

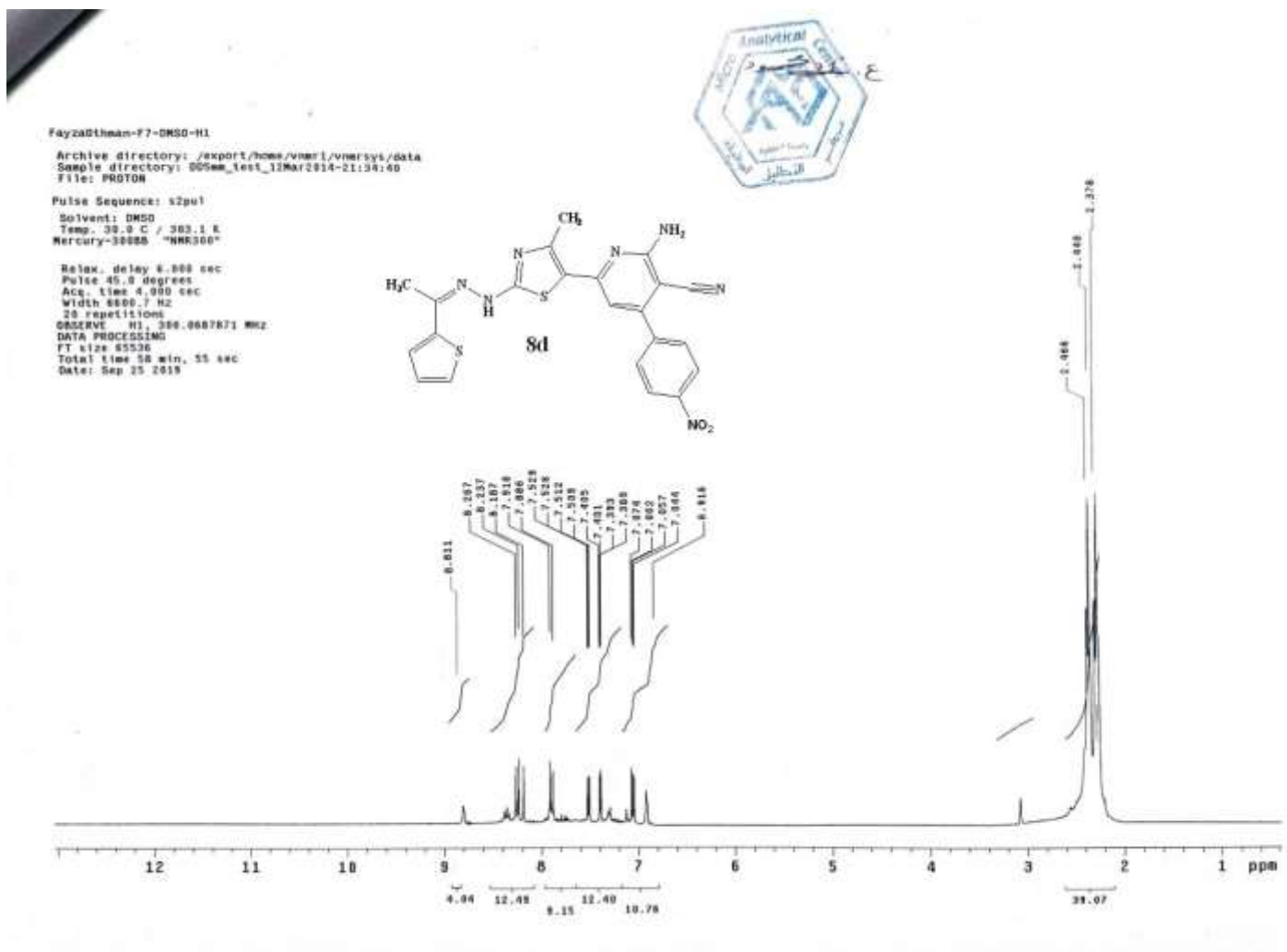
Line#1 R.Time:4.5(Scan#:540)

MassPeaks:382

RawMode:Single 4.5(540) BasePeak:57(79712)

BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	7033	8.82	4	53.00	9834	12.34	7	56.05	22635	28.40
2	51.00	7410	9.30	5	54.05	15173	19.03	8	57.05	79712	100.00
3	52.00	4198	5.27	6	55.00	79270	99.45	9	58.00	10714	13.44



¹H-NMR spectra of compound **8d**

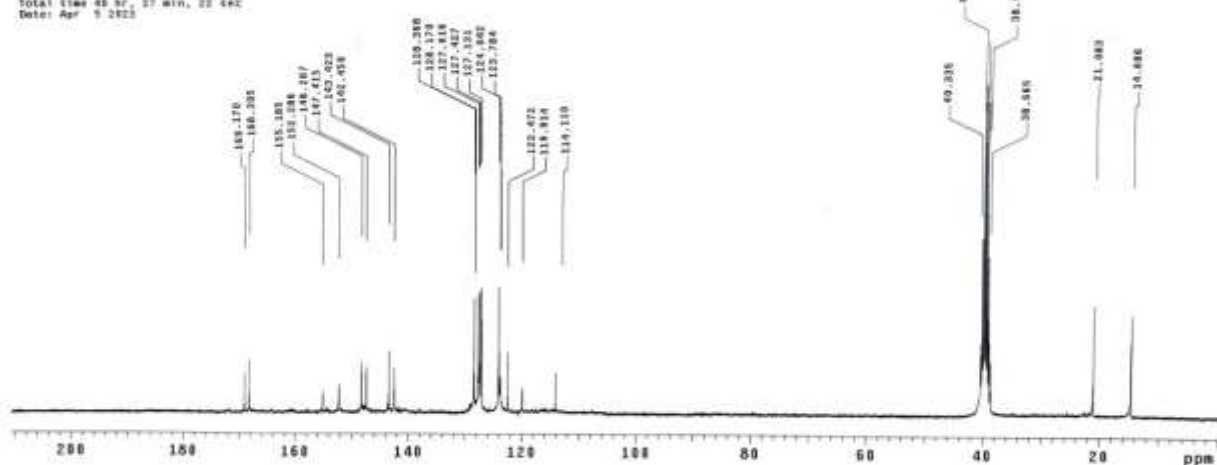
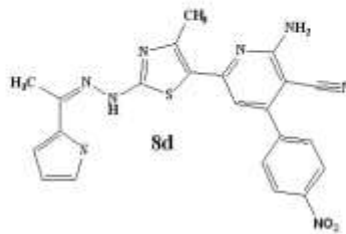
Fayez@thman-F7-DMSO-C13

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Sample directory: D55m_tms_12Mar2014-21:33:46
File: PROTON

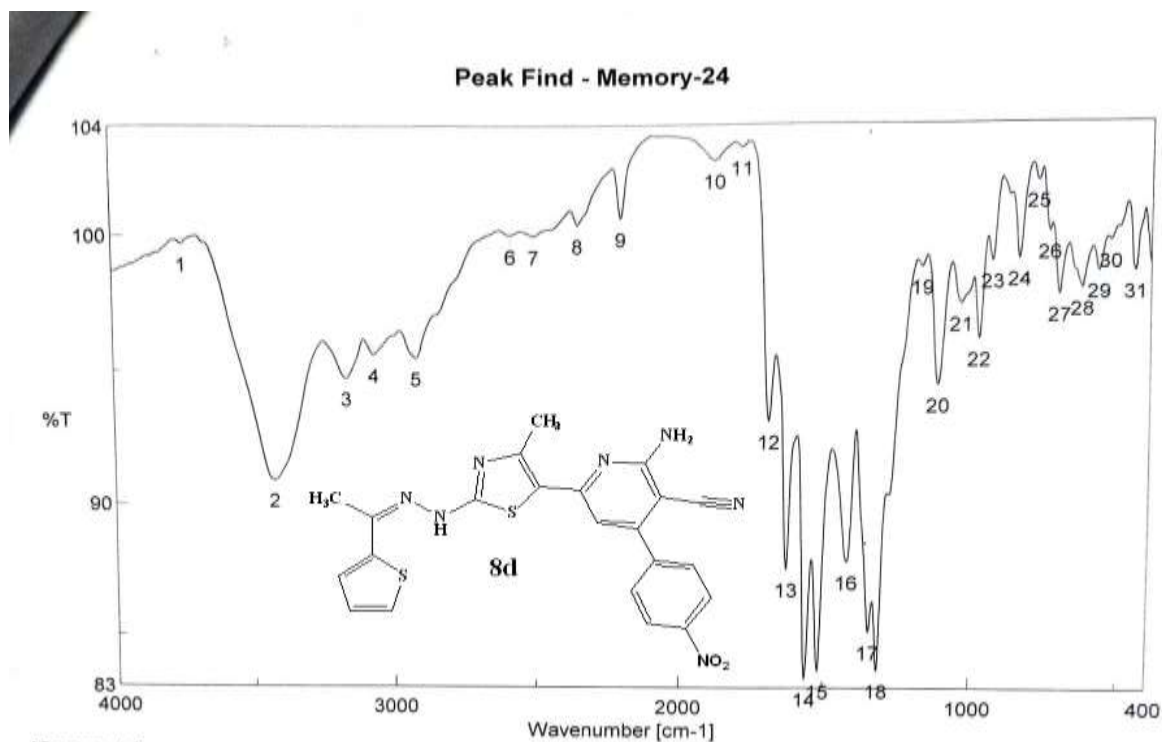
Pulse Sequence: zgpg30

Solvent: DMSO
Ambient temperature
Mercury-300WB "NMR300"

Pulse 45.0 degrees
Acq. time 1.737 sec
Width 18791.7 Hz
28972 repetitions
OBSERVE C13, 75.4523851 MHz
DECOUPLE H1, 300.9740836 MHz
Power 34 dB
Continuously on
MAGZ-18 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 48 hr, 27 min, 22 sec
Date: Apr 5 2023



¹³C-NMR spectra of compound **8d**



[Comments]
 Sample name F7
 Comment 12/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3751.83	99.7013	2	3430.74	90.9116	3	3177.15	94.7356
4	3079.76	95.6042	5	2931.27	95.4752	6	2597.64	99.9606
7	2517.61	99.9206	8	2363.34	100.315	9	2211.95	100.557
10	1887	102.662	11	1793.47	103.134	12	1692.23	93.0308
13	1628.59	87.4969	14	1563.02	83.3527	15	1518.67	83.6492
16	1422.24	87.7705	17	1346.07	85.1311	18	1316.18	83.6762
19	1176.36	98.682	20	1117.55	94.3597	21	1042.34	97.3302
22	980.625	96.0419	23	937.235	98.894	24	846.597	98.9821
25	782.958	101.879	26	743.424	99.9869	27	709.676	97.6644
28	632.537	97.8978	29	576.612	98.5293	30	538.042	99.6529
31	453.19	98.5312						



IR spectra of compound **8d**



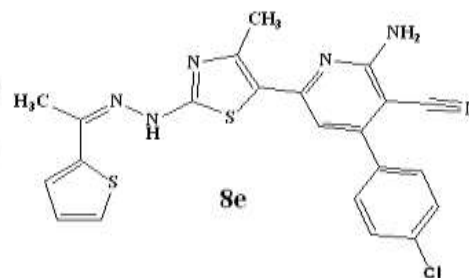
27-Aug-19 15:29:57

Cairo University Micro Analytical Center

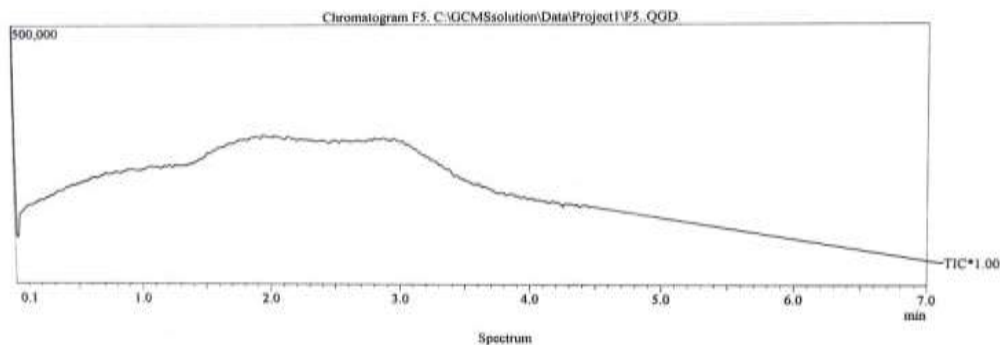
DI Analysis Shimadzu Qp-2010 Plus

Sample Information
Analyzed by: Dr. Mai Younis
Analyzed: 27/08/2019 03:23:43
Sample Name: F5
Sample ID:
Customer Name: Dr. Fayza Othman - Science - Cairo
Data File: C:\GCMSsolution\Data\Project1\F5_QGD
Org Data File: C:\GCMSsolution\Data\Project1\F5_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
\$End1\$Modified by: Dr. Mai Younis
Modified: 27/08/2019 03:28:15

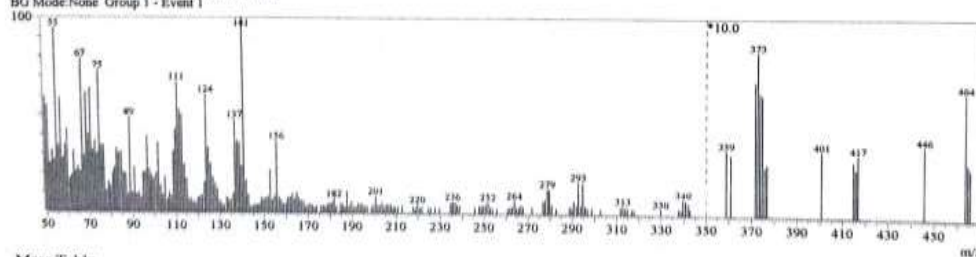
Method
Analytical Line 1
IonSourceTemp: 250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time: 0.00min
End Time: 10.00min
ACQ Mode: Scan
Event Time: 0.50sec
Scan Speed: 1111
Start m/z: 50.00
End m/z: 550.00
Electron Voltage: 70 eV
Ionization Mode: EI



C:\GCMSsolution\Data\Project1\F5_QGD



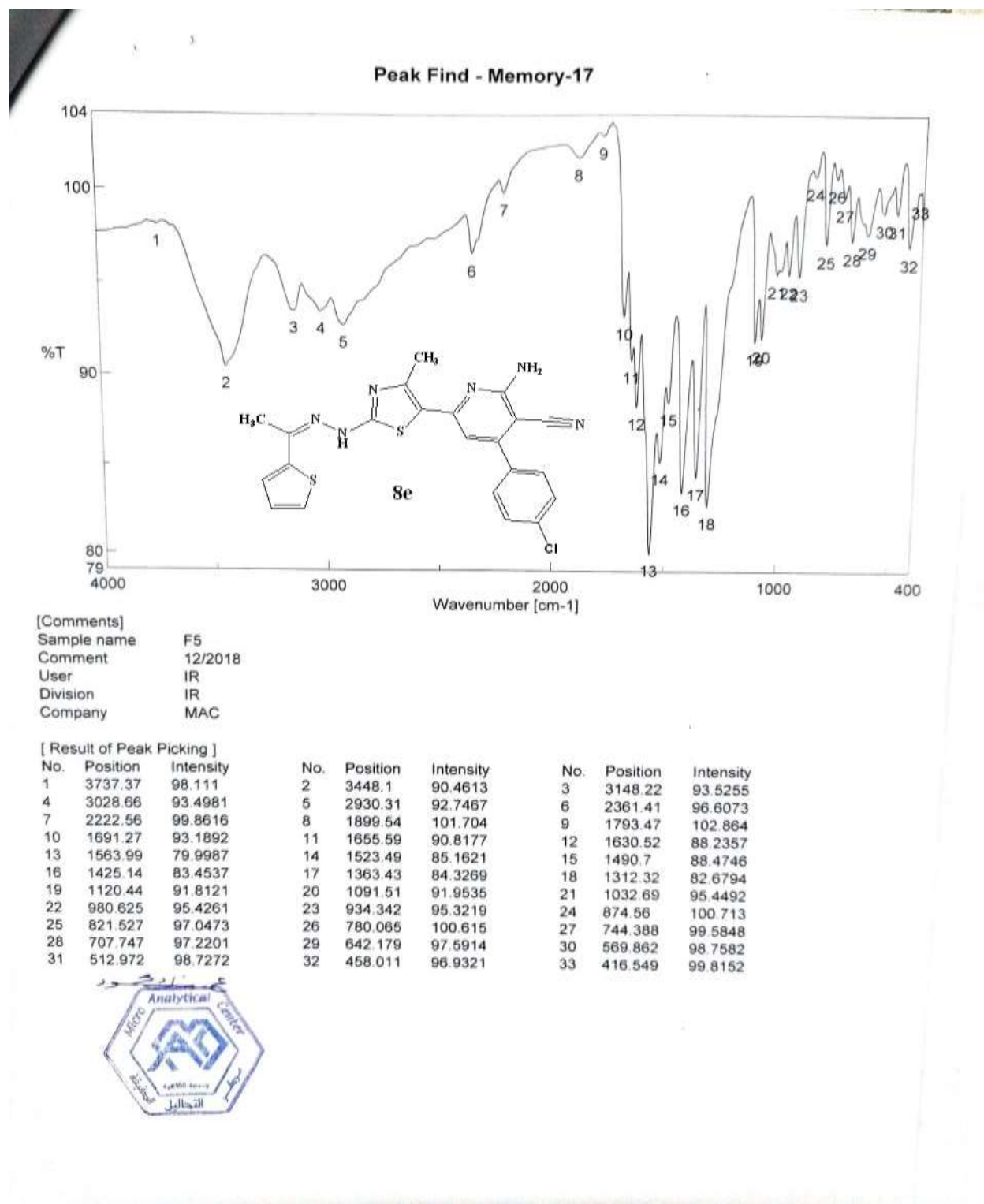
Line# 1 R.Time:3.0(Scan#:360)
MassPeaks:238
RawMode:Single 3.0(360) BasePeak:141(8586)
BG Mode:None Group 1 - Event 1



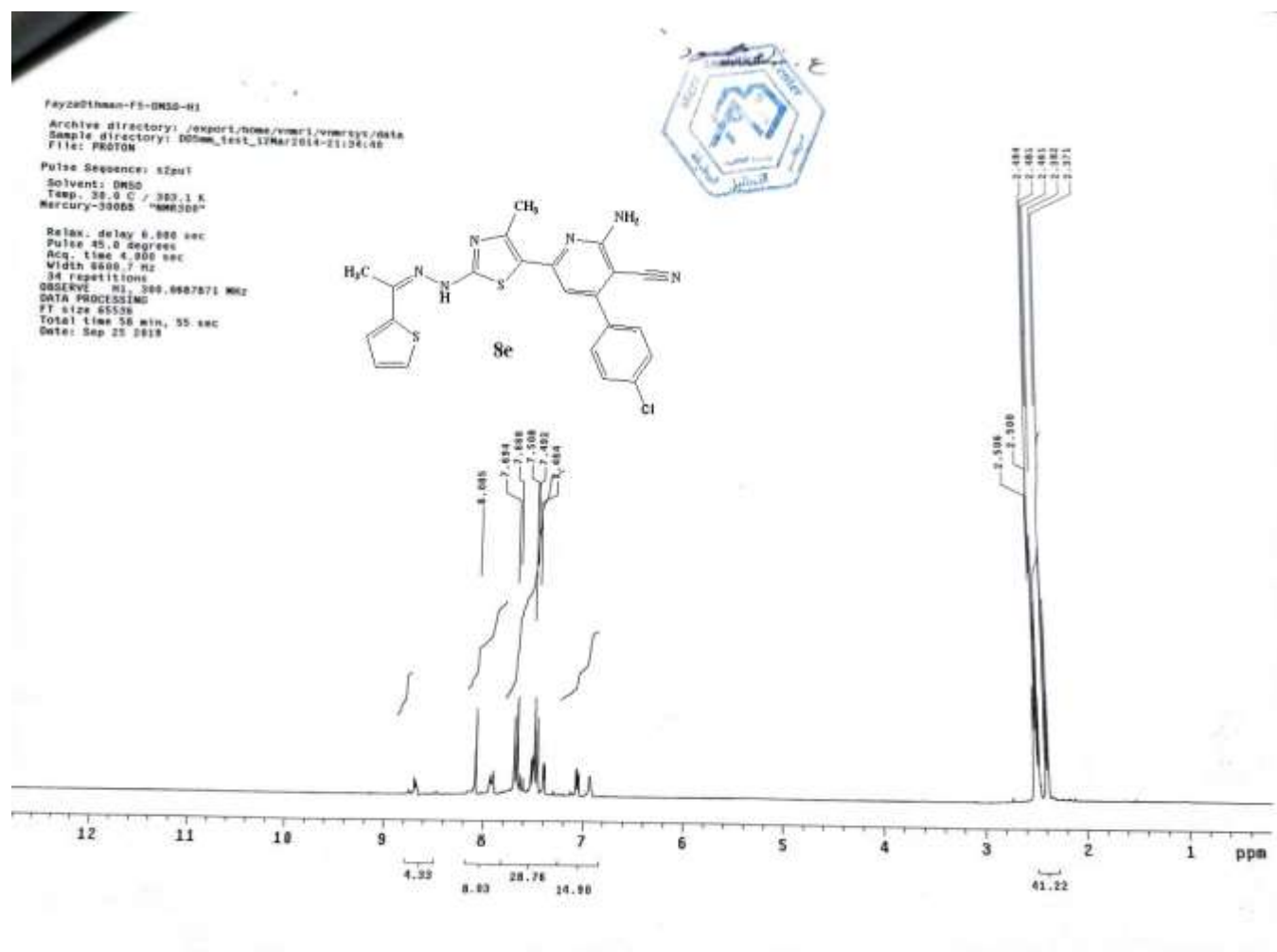
Mass Table
Line# 1 R.Time:3.0(Scan#:360)
MassPeaks:238
RawMode:Single 3.0(360) BasePeak:141(8586)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	5084	59.21	4	53.00	2718	31.66	7	56.00	2951	34.37
2	51.00	4746	55.28	5	54.00	2297	26.75	8	57.00	5052	58.84
3	52.00	2145	24.98	6	55.00	8103	94.37	9	58.00	2366	27.56

Mass spectra of compound **8e**



IR spectra of compound **8e**



¹H-NMR spectra of compound **8e**



27-Aug-19 15:48:14

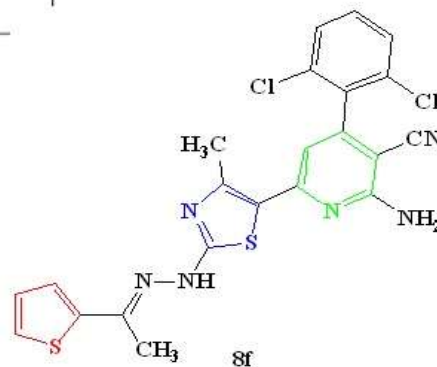
ع. ز. محمد

Cairo University Micro Analytical Center

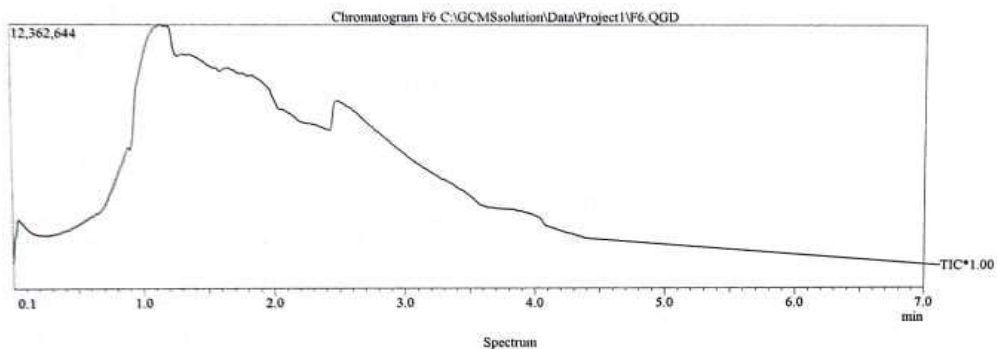
DI Analysis Shimadzu Qp-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 27/08/2019 03:41:03
Sample Name : F6
Sample ID :
Customer Name : Dr. Fayza Othman - Science - Cairo
Data File : C:\GCMSsolution\Data\Project1\F6.QGD
Org Data File : C:\GCMSsolution\Data\Project1\F6.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Report File : C:\GCMSsolution\System\Tune1_default.qgt
Tuning File :
\$End1\$Modified by : Dr. Mai Younis
Modified : 27/08/2019 03:45:30

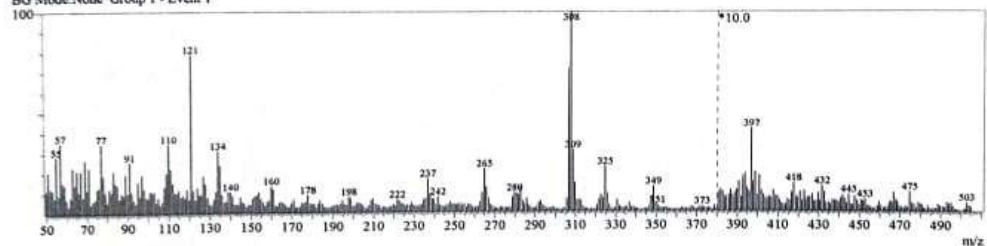
Method
Analytical Line 1
IonSourceTemp :250.00 °C
[MS Table]
--Group 1 - Event 1--
Start Time :0.00min
End Time :10.00min
ACQ Mode :Scan
Event Time :0.50sec
Scan Speed :1111
Start m/z :50.00
End m/z :550.00
Electron Voltage :70 eV
Ionization Mode :EI



C:\GCMSsolution\Data\Project1\F6.QGD

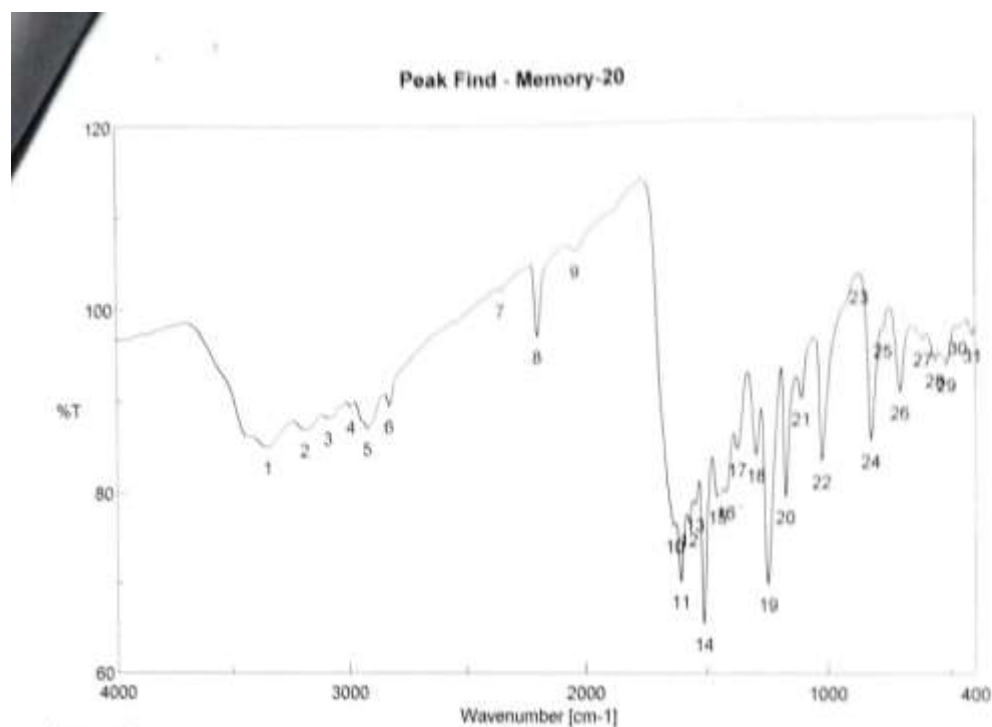


Line#1 R.Time:2.8(Scan#:334)
MassPeaks:455
RawMode:Single 2.8(334) BasePeak:308(311107)
BG Mode:None Group 1 - Event 1



Mass Table
Line#1 R.Time:2.8(Scan#:334)
MassPeaks:455
RawMode:Single 2.8(334) BasePeak:308(311107)
BG Mode:None Group 1 - Event 1

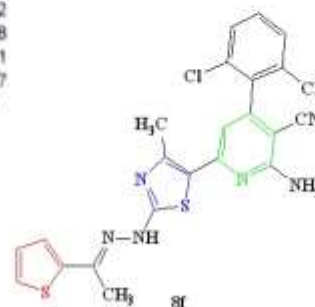
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	34670	11.14	4	53.00	35970	11.56	7	56.05	27516	8.84
2	51.00	63222	20.32	5	54.05	23464	7.54	8	57.00	108273	34.80
3	52.00	37692	12.12	6	55.00	87274	28.05	9	57.95	46554	14.96



[Comments]
 Sample name F6
 Comment 12/2018
 User IR
 Division IR
 Company MAC

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	3353.6	85.0103	2	3194.51	86.8864	3	3096.15	88.1441
4	2999.73	89.4215	5	2928.38	87.007	6	2835.81	89.461
7	2364.3	101.907	8	2207.13	96.8547	9	2049.96	106.068
10	1632.45	76.0639	11	1605.45	70.0397	12	1573.63	76.7853
13	1548.56	78.3886	14	1510.95	65.4291	15	1455.99	79.2056
16	1421.28	79.6748	17	1375	84.2947	18	1297.86	83.6832
19	1247.72	69.6847	20	1176.36	79.1675	21	1113.69	89.7068
22	1027.87	82.9717	23	877.452	102.78	24	827.312	85.0971
25	780.065	96.9508	26	709.676	90.2889	27	615.181	96.0077
28	566.005	93.7328	29	517.793	93.2679	30	471.51	97.272
31	411.728	96.4427						



IR spectra of compound **8f**