

Design and Synthesis of Novel Quinazolinone-Chalcone Hybrids as Potential Apoptotic Candidates Targeting Caspase-3 and PARP-1: *In Vitro*, Molecular Docking, and SAR Studies

Eman A. Madbouly¹, El-Sayed M. Lashine¹, Ahmed A. Al-Karmalawy^{2,*}, Mahmoud M Sebaiy¹, Harris Pratsinis³, Dimitris Kletsas³, and Kamel Metwally⁴

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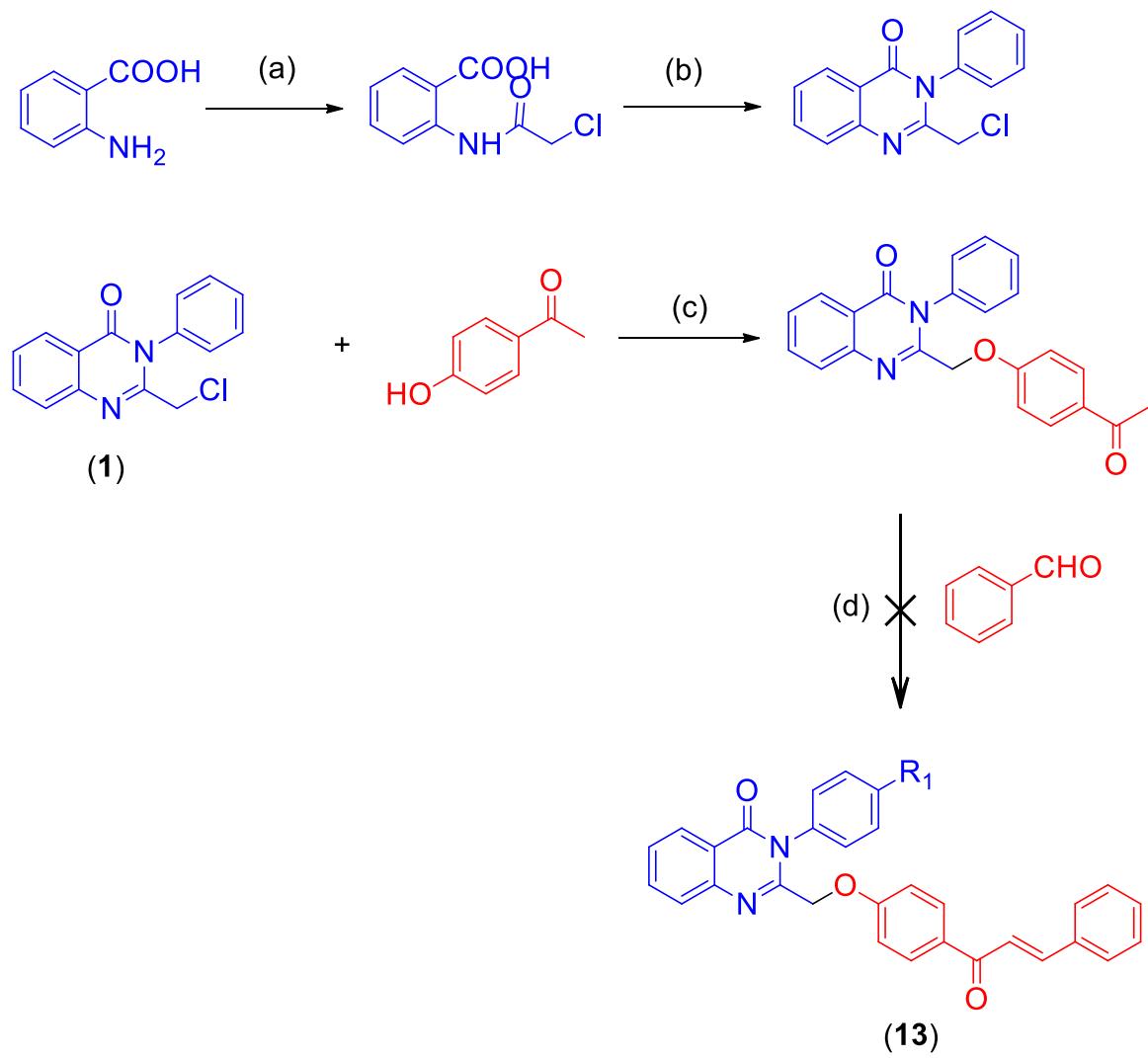
² Pharmaceutical Chemistry Department, Faculty of Pharmacy, Ahram Canadian University, 6th of October City, Giza 12566, Egypt.

³ Laboratory of Cell Proliferation and Ageing, Institute of Biosciences and Applications, National Centre of Scientific Research "Demokritos", Athens, Greece.

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Corresponding author:

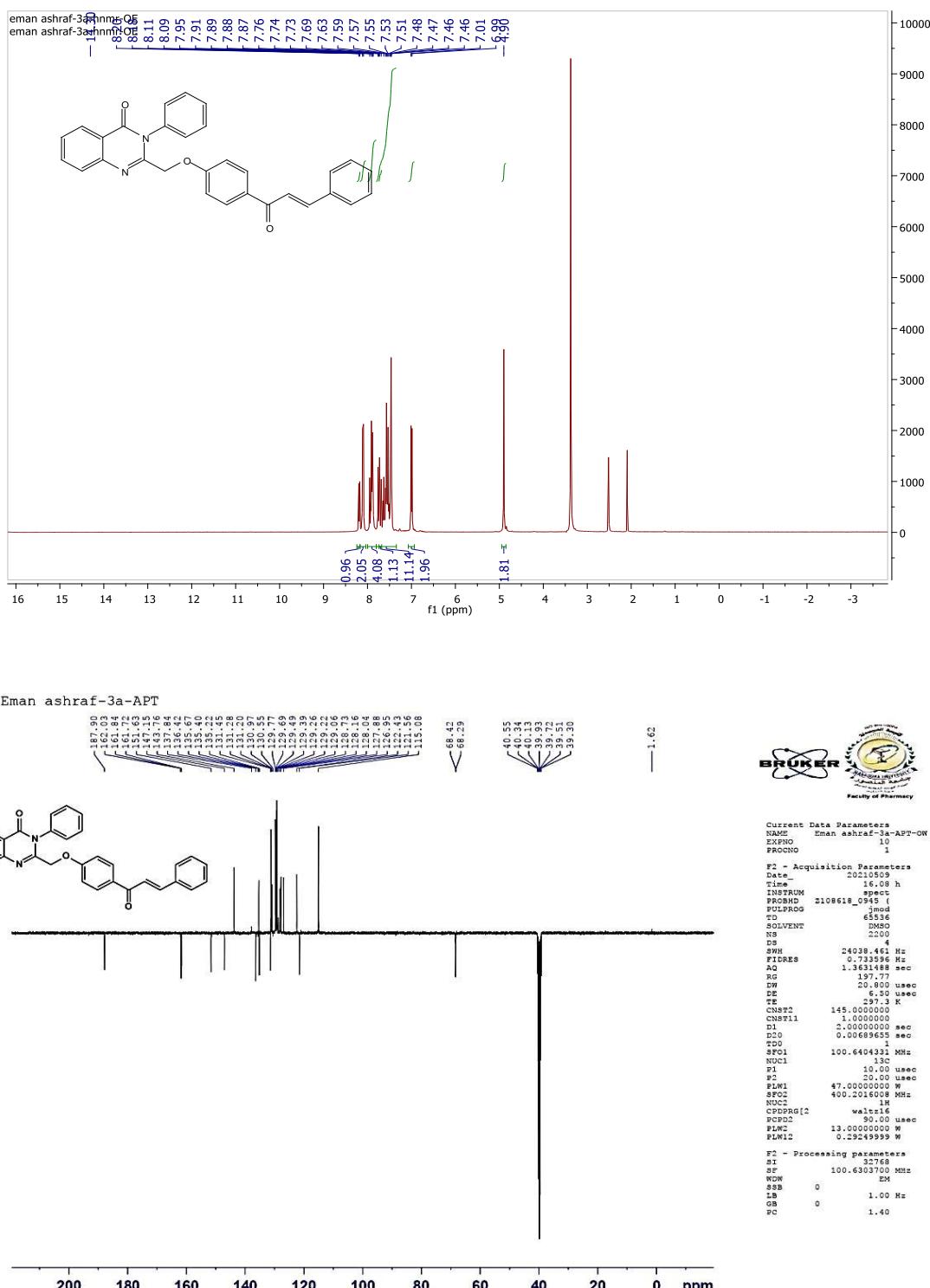
Ahmed A. Al-Karmalawy: akarmalawy@acu.edu.eg



Scheme SI 1. Reagents and conditions: (a) Chloroacetylchloride, dry benzene, reflux. (b) Anilines, POCl_3 , dry toluene, reflux. (c) K_2CO_3 , KI, acetonitrile, reflux. (d) NaOH , EtOH , room temperature.

SI. Spectral data of the novel quinazolinone-chalcone hybrid molecules **13-43** (^1H NMR, ^{13}C NMR, and Mass spectroscopy).

2-((4-Cinnamoylphenoxy)methyl)-3-phenylquinazolin-4(3H)-one (13).



21-Jan-07 12:44:55

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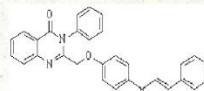
DI Analysis
Shimadzu QP-2010 Plus

Sample Information

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Analyzed : 21/01/2007 12:39:38
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Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
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Modified : 21/01/2007 12:44:09

Method

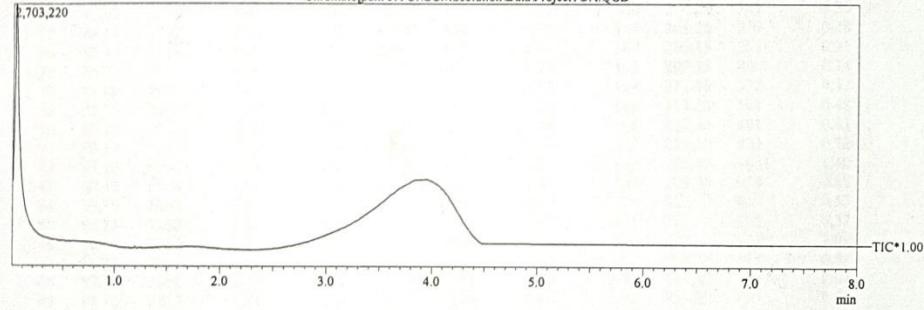
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ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Datap\Project\3A.QGD

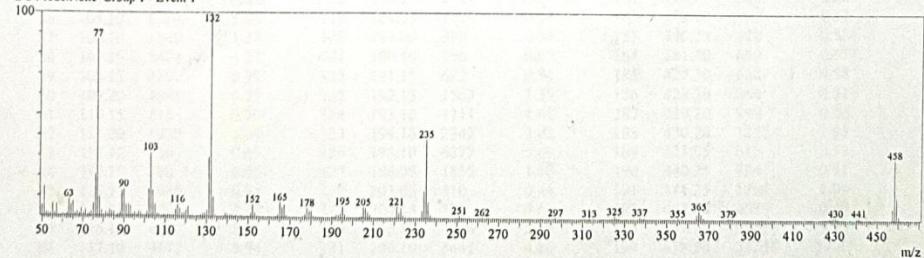


Chromatogram 3A C:\GCMSsolution\Datap\Project\3A.QGD



Spectrum

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RawMode:Single 4.0(477) BasePeak:132(116167)
BG Mode:None Group 1 - Event 1

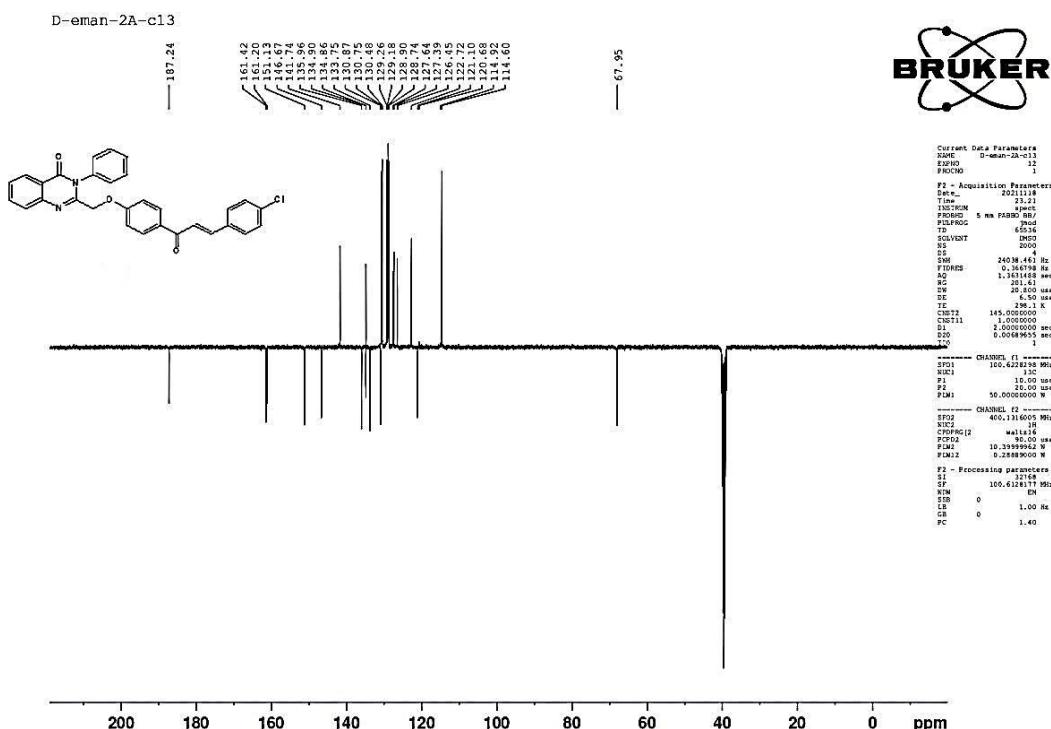
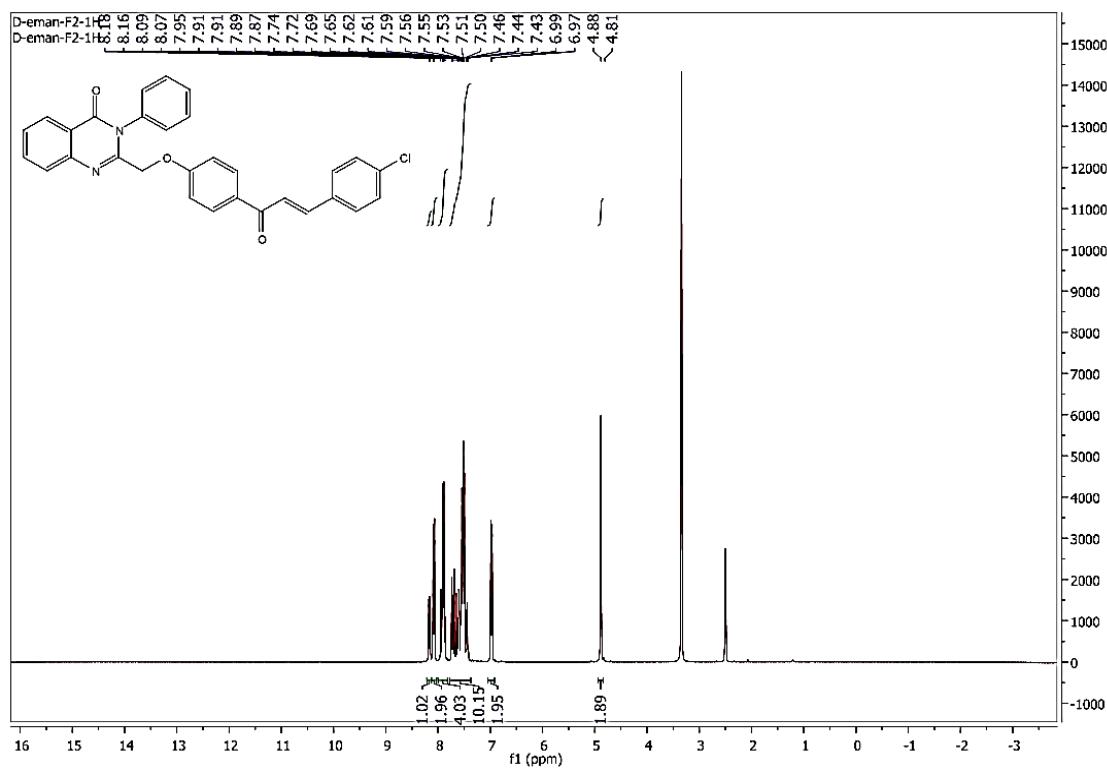


Mass Table

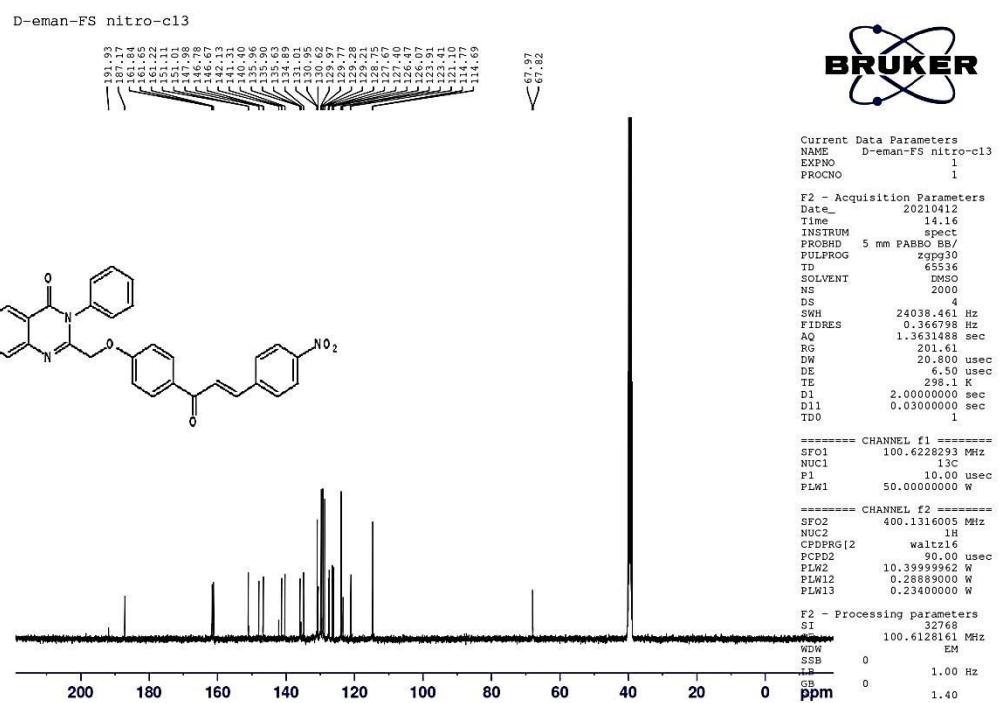
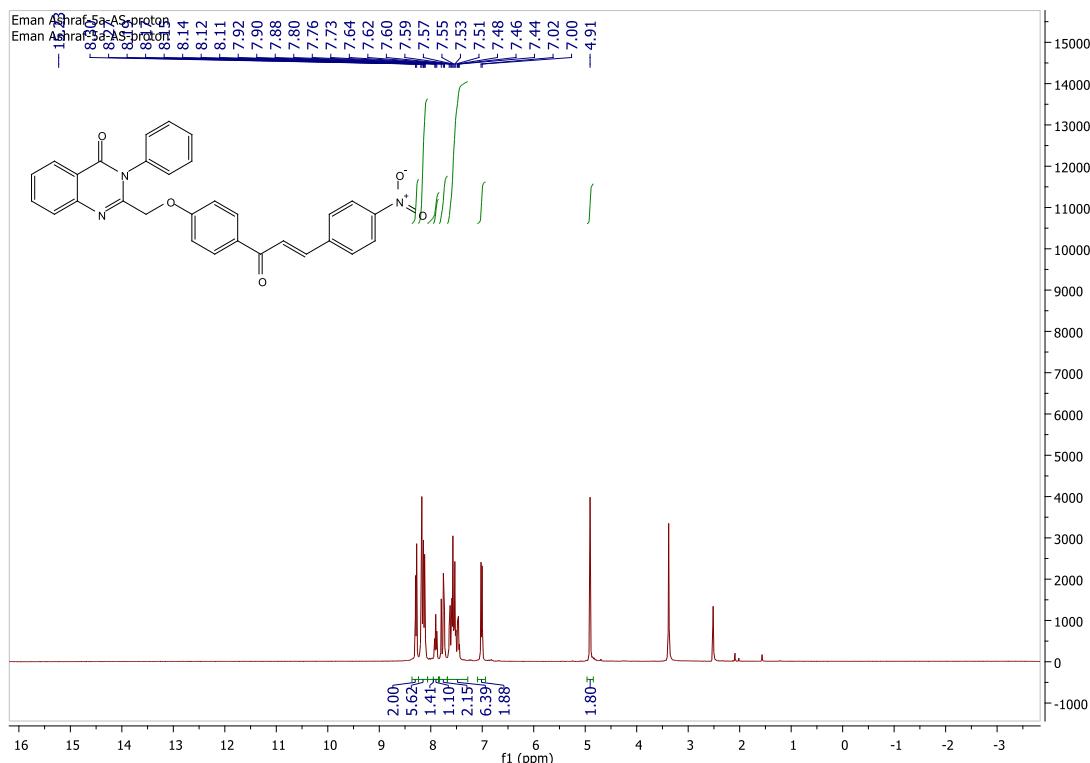
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RawMode:Single 4.0(477) BasePeak:132(116167)
BG Mode:None Group 1 - Event 1

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1	50.05	6425	5.53	4	53.00	1905	1.64	7	56.15	1883	1.62
2	51.00	16610	14.30	5	54.05	1411	1.21	8	57.10	6607	5.69
3	52.05	2472	2.13	6	55.05	6715	5.78	9	58.05	725	0.62

(E)-2-((4-(3-(4-chlorophenyl)acryloyl)phenoxy)methyl)-3-phenylquinazolin-4(3H)-one (14).



(E)-2-((4-(3-(4-Nitrophenyl)acryloyl)phenoxy)methyl)-3-phenylquinazolin-4-(3H)-one (15).



21-Jan-07 12:58:23

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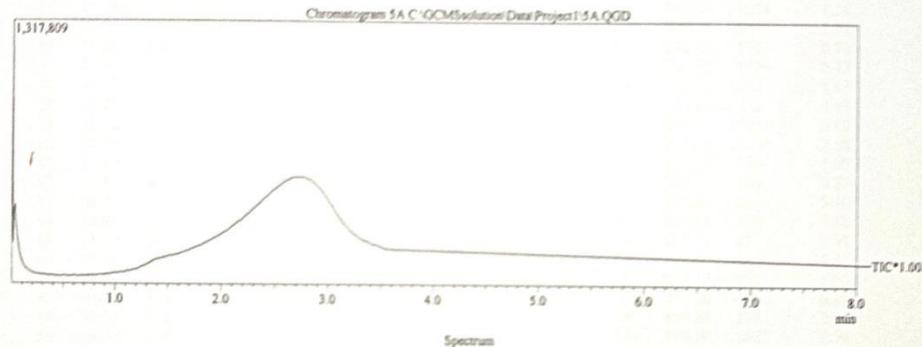
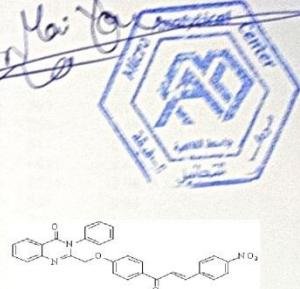
DI Analysis
Shimadzu QP-2010 Plus

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Sample ID :
Customer Name : Dr. Emran Adaruf - Pharmacy - Zagazik
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Report File :
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\$EndOfFile Modified by : Dr. Mai Younis
Modified : 21/01/2007 12:57:35

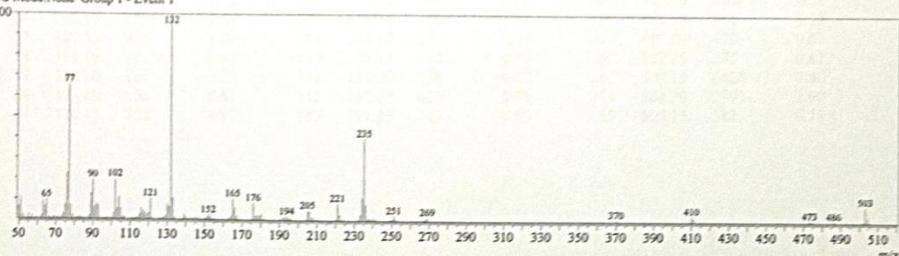
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End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 12500
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMsolution\Project1\5A.QGD



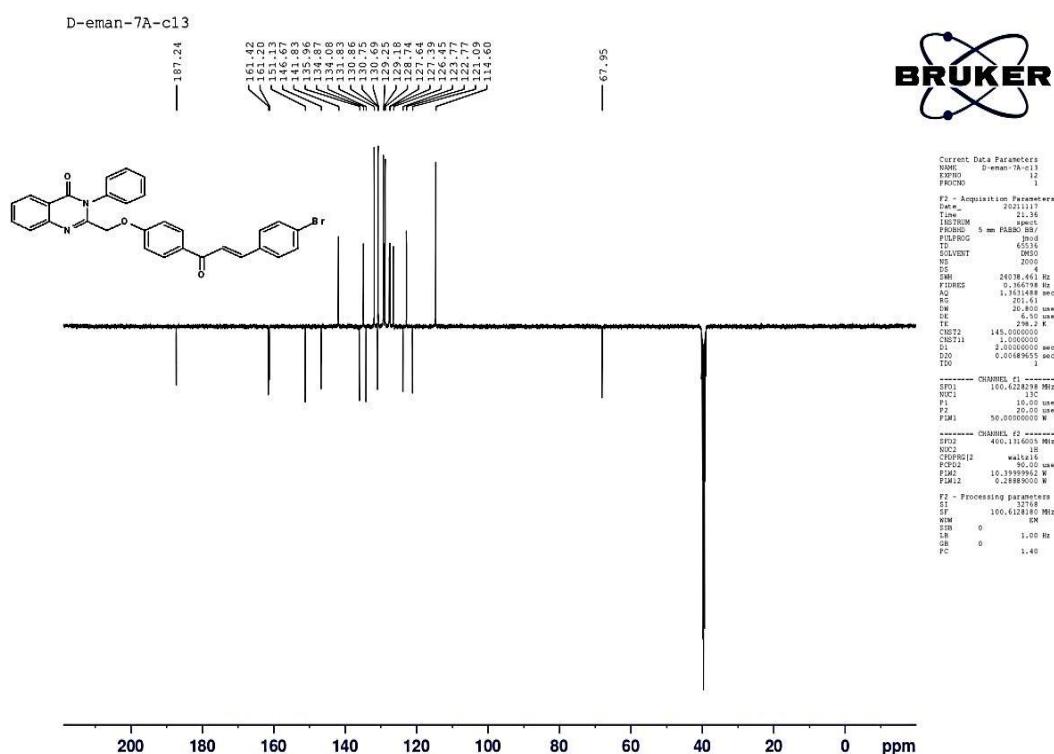
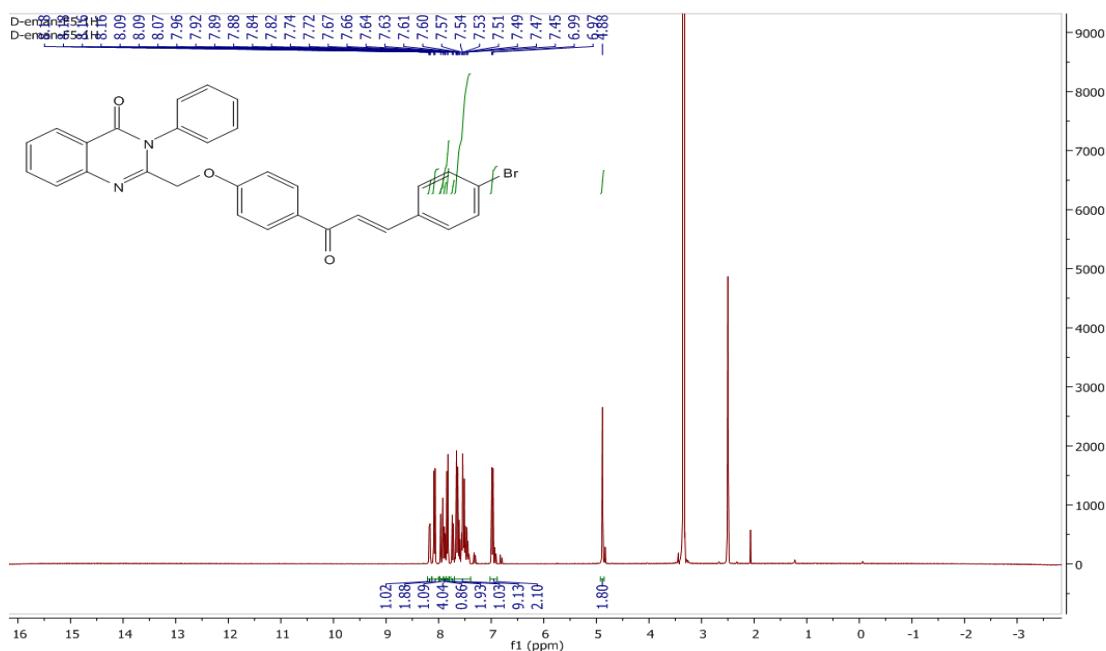
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MassPeaks:165
RawMode:Single 2.7(322) BasePeak:132(82366)
BG Mode:None Group 1 - Event 1



Mass Table
Line# 1 R.Time:2.7(Scan#:322)
MassPeaks:165
RawMode:Single 2.7(322) BasePeak:132(82366)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.
1	50.05	5458	6.63	4	53.00	1209	1.47	7	56.05	663	0.80
2	51.00	8967	10.89	5	54.15	562	0.68	8	57.05	1739	2.11
3	52.05	2105	2.56	6	55.05	2085	2.53	9	58.10	354	0.43

(E)-2-((4-(3-(4-Bromophenyl)acryloyl)phenoxy)methyl)-3-phenylquinazolin-4(3H)-one (16).



21-Jan-07 13:05:28

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DT Analysis
Shimadzu QP-2010 Plus

Sample Information

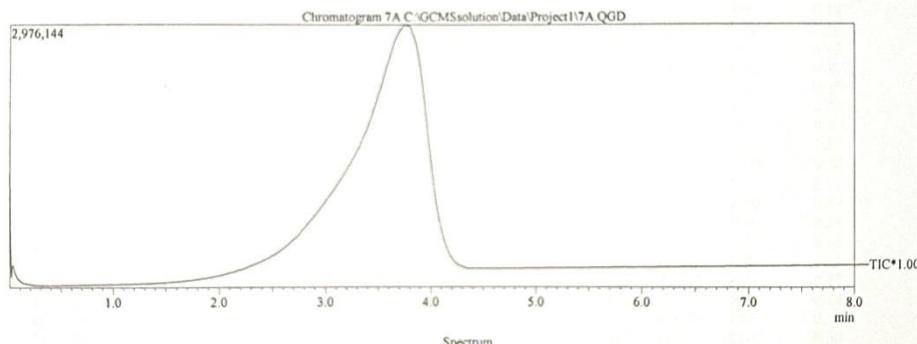
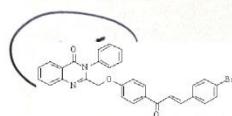
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Sample ID :
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Modified : 21/01/2007 01:04:31

Method

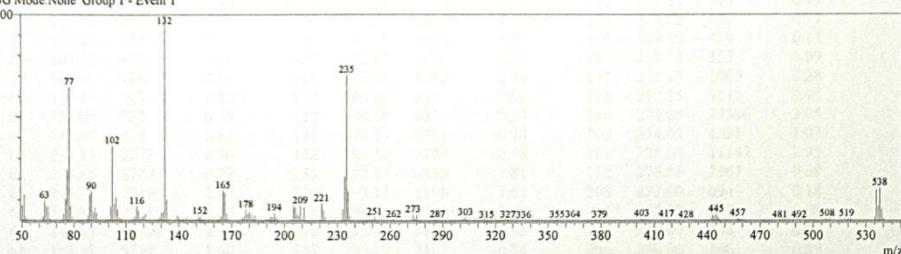
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End Time : 10:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Dataproject1\7A.QGD



Line#:1 R.Time:3.8(Scan#:452)
MassPeaks:312
RawMode:Single 3.8(452) BasePeak:132(377270)
BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.8(Scan#:452)

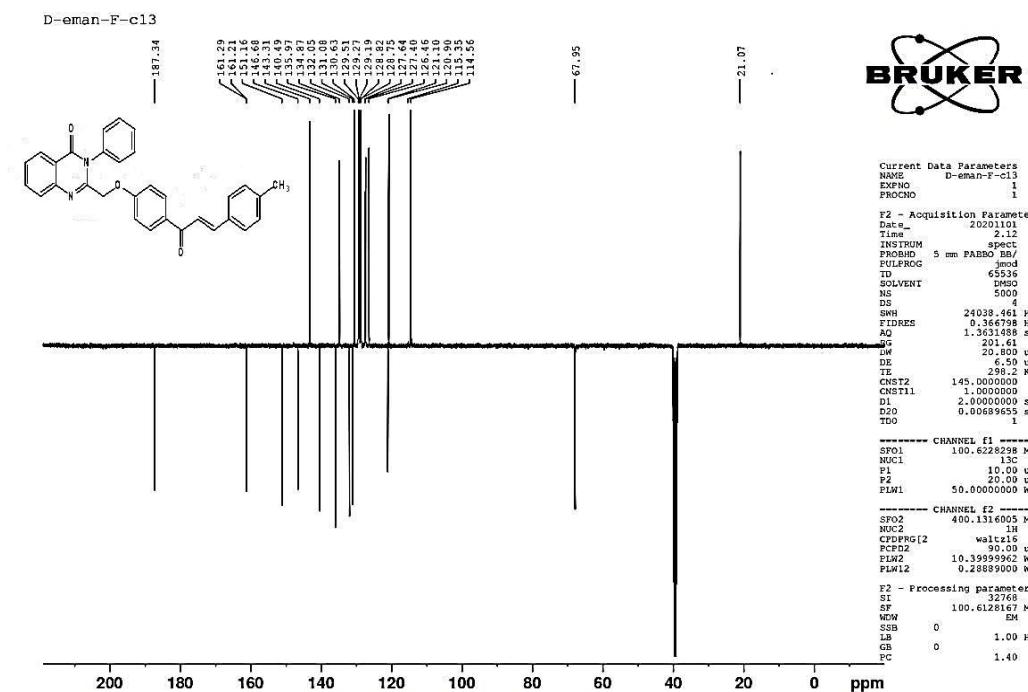
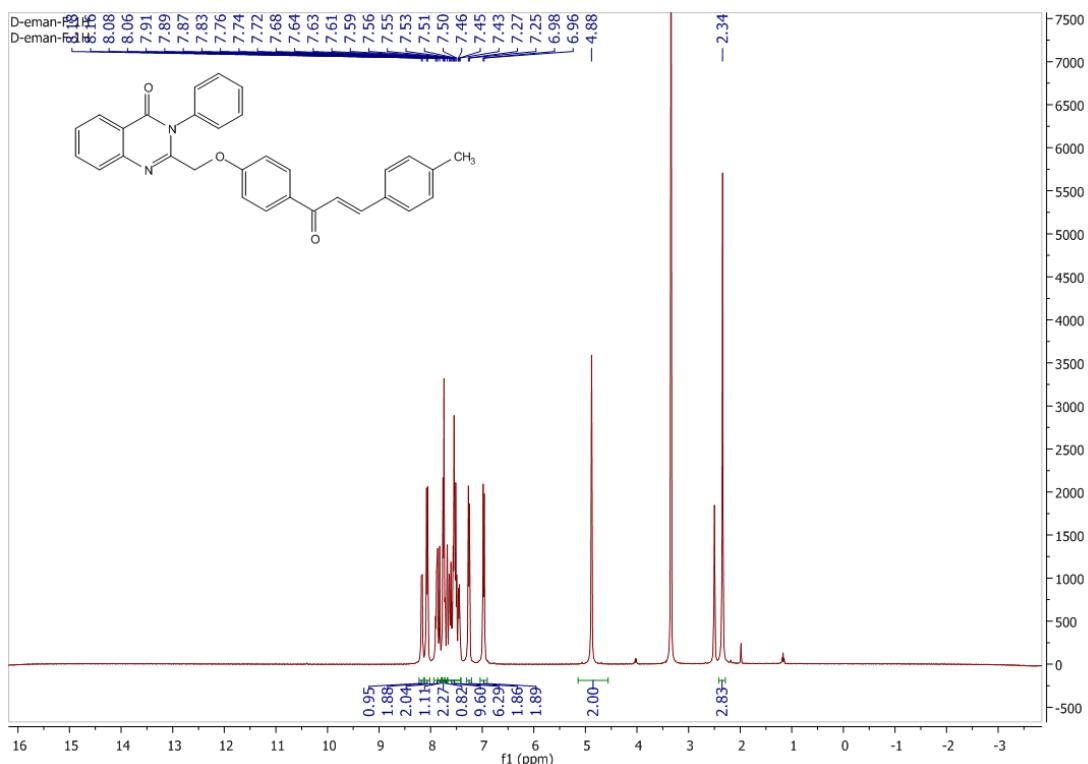
MassPeaks:312

RawMode:Single 3.8(452) BasePeak:132(377270)

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	50.05	27620	7.32	4	53.05	3678	0.97	7	56.15	717	0.19
2	51.05	47358	12.55	5	54.05	965	0.26	8	57.10	1671	0.44
3	52.05	8408	2.23	6	55.05	2650	0.70	9	58.10	434	0.12

(E)-3-Phenyl-2-((4-(3-(*p*-tolyl)acryloyl)phenoxy)methyl)quinazolin-4(3*H*)-one (17).



27-Jan-21 20:49:29

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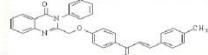
DI Analysis
Shimadzu QP-2010 Plus

Sample Information

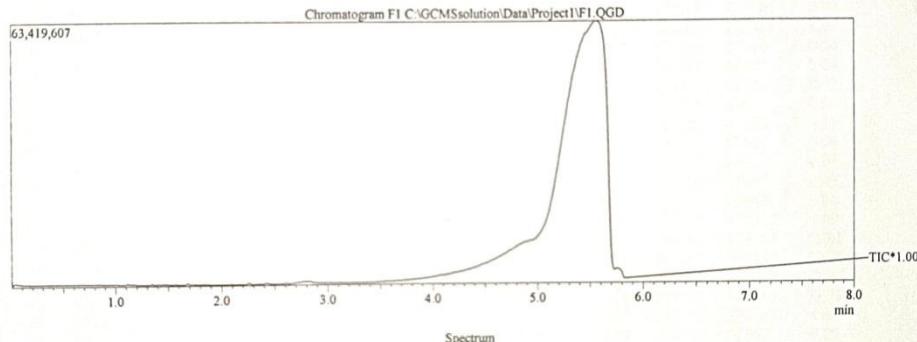
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Report File :
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Modified : 27/01/2021 08:48:01

Method

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[MS Table]
—Group 1 - Event 1—
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End Time : 10:00min
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Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI

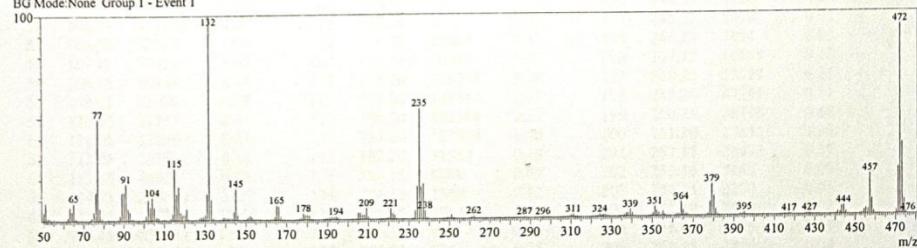


C:\GCMSsolution\Project\F1.QGD



Spectrum

Line#:1 R.Time:5.5(Scan#:667)
MassPeaks 418
RawMode:Single 5.5(667) BasePeak:132(6712038)
BG Mode:None Group 1 - Event 1



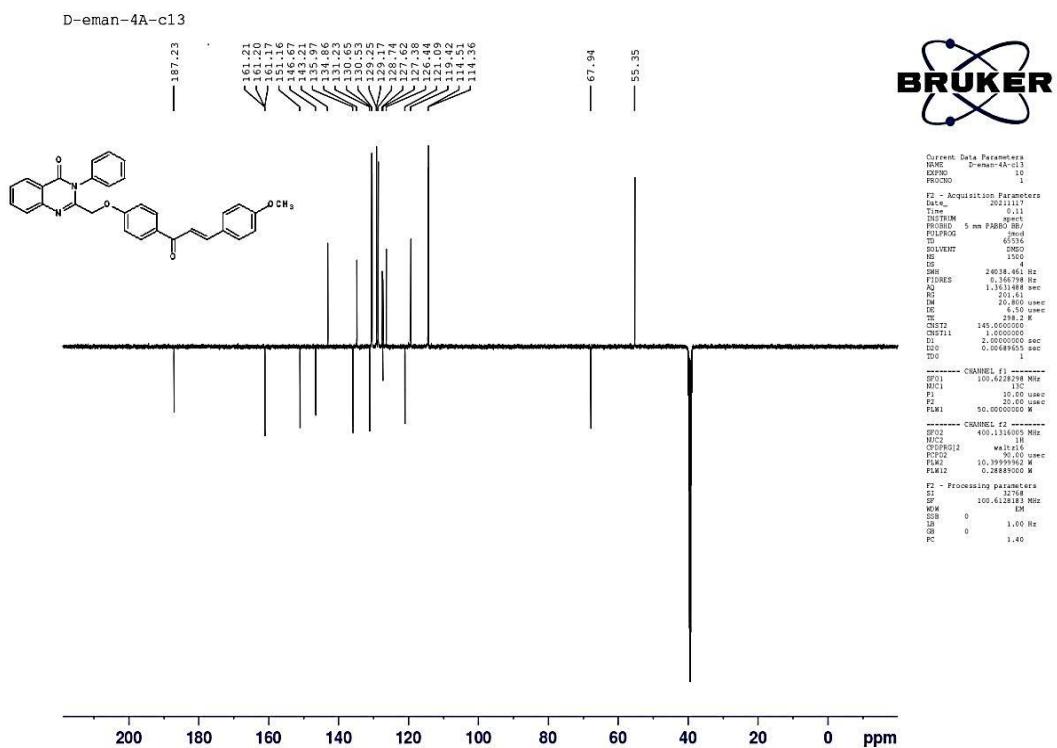
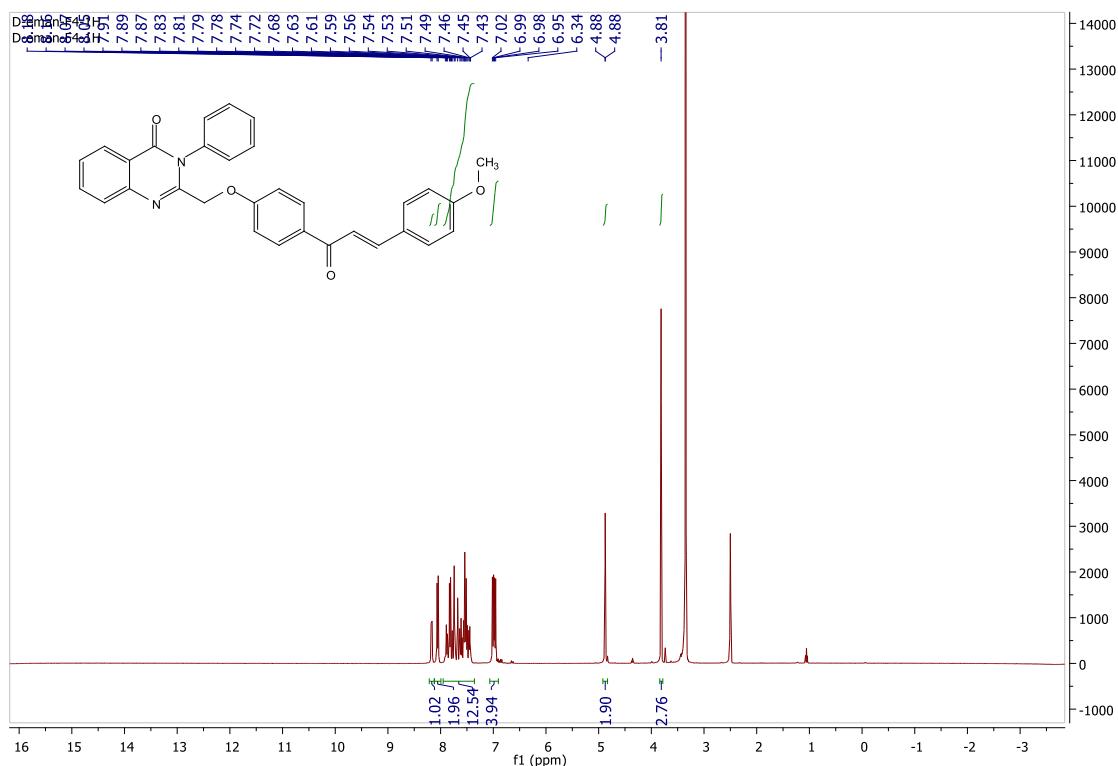
Mass Table
Line#:1 R.Time:5.5(Scan#:667)
MassPeaks:418

RawMode:Single 5.5(667) BasePeak:132(6712038)

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	50.10	257380	3.83	4	53.05	66694	0.99	7	56.05	6438	0.10
2	51.05	573714	8.55	5	54.05	9568	0.14	8	57.10	12190	0.18
3	52.05	86208	1.28	6	55.05	44224	0.66	9	58.10	4007	0.06

(E)-2-((4-(3-(4-Methoxyphenyl)acryloyl)phenoxy)methyl)-3-phenylquinazolin-4-(3H)-one (18).



21-Jan-07 12:52:54

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DI Analysis
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Sample Information

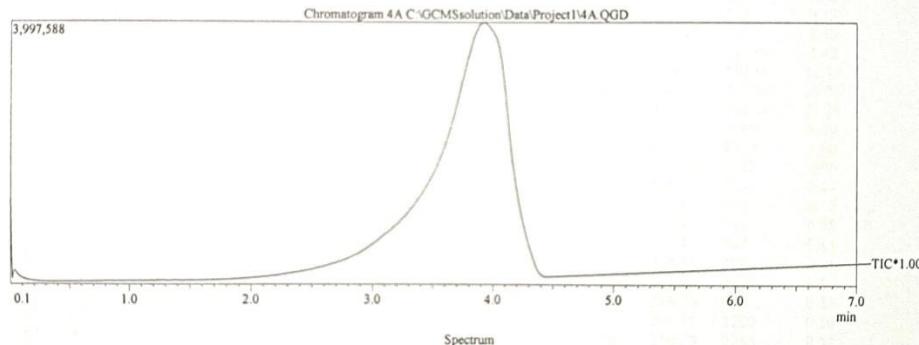
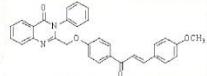
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Modified : 21/01/2007 12:51:38

Method

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Event Time : 0.50sec
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Start m/z : 50.00
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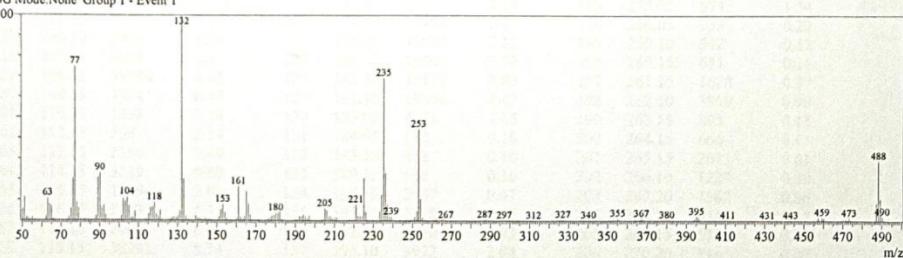
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Spectrum

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BG Mode:None Group 1 - Event 1



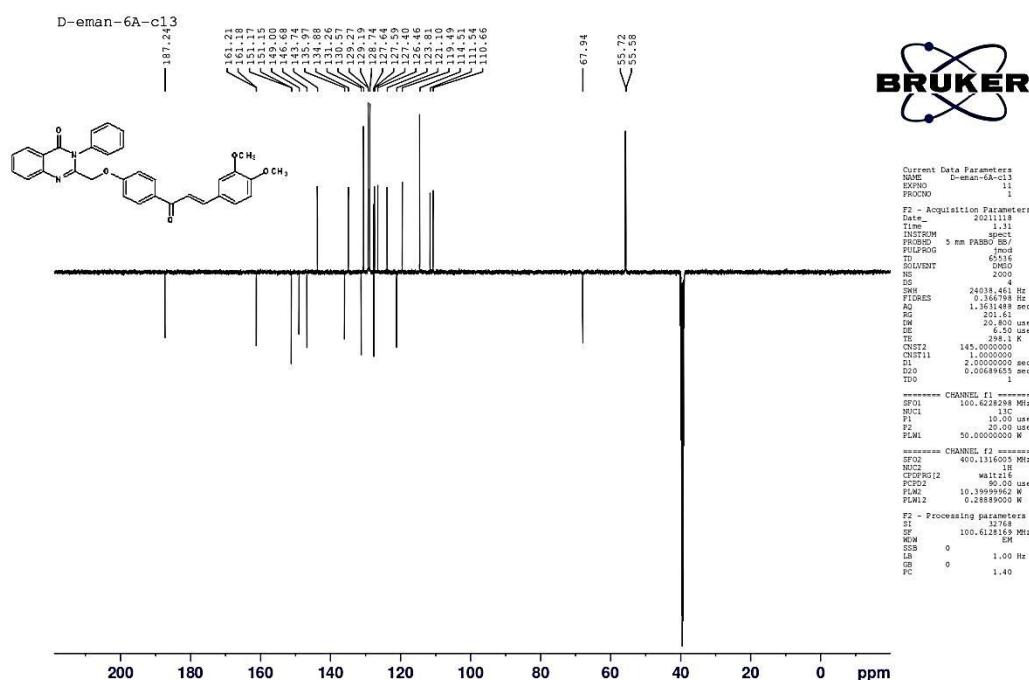
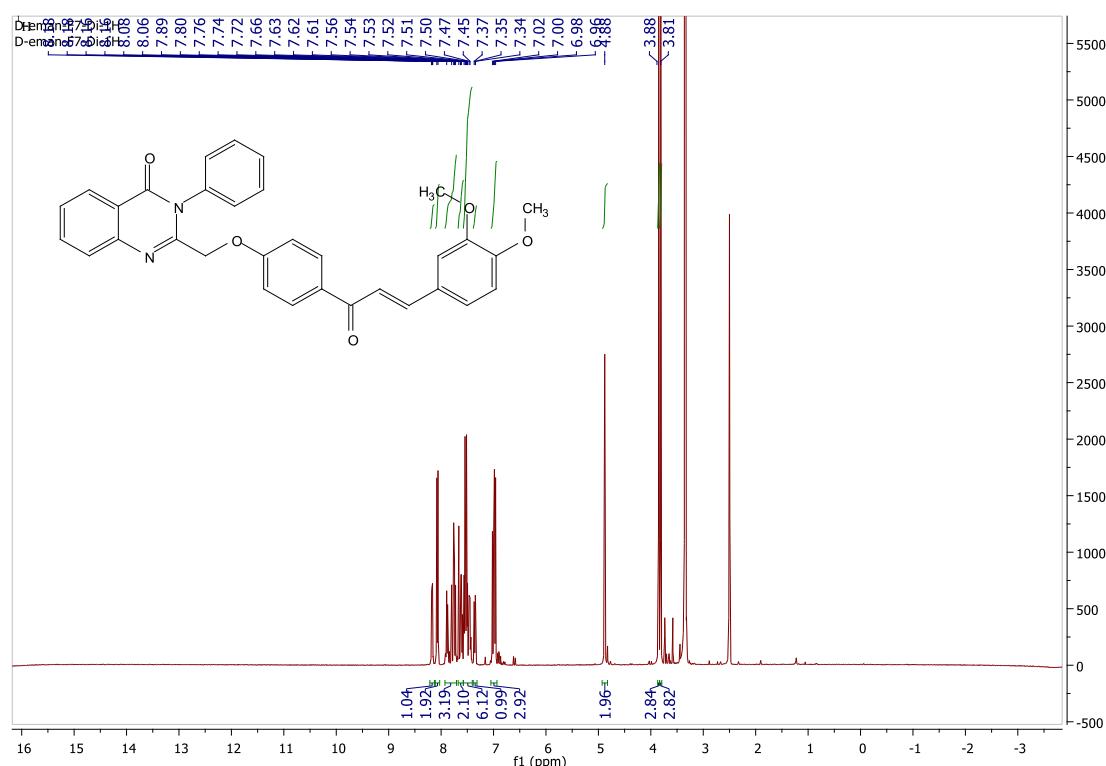
Mass Table

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MassPeaks:308
RawMode:Single 3.9(472) BasePeak:132(438128)

BG Mode:None Group 1 - Event 1

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1	50.05	24148	5.51	4	53.05	6330	1.44	7	56.15	1173	0.27
2	51.05	50083	11.43	5	54.05	1519	0.35	8	57.10	2364	0.54
3	52.05	7691	1.76	6	55.05	6951	1.59	9	58.15	482	0.11

*(E)-2-((4-(3,4-Dimethoxyphenyl)acryloyl)phenoxy)methyl-3-phenylquinazolin-4(3*H*)-one (19).*



11-Jan-07 04:04:40

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DI Analysis
Shimadzu QP-2010 Plus

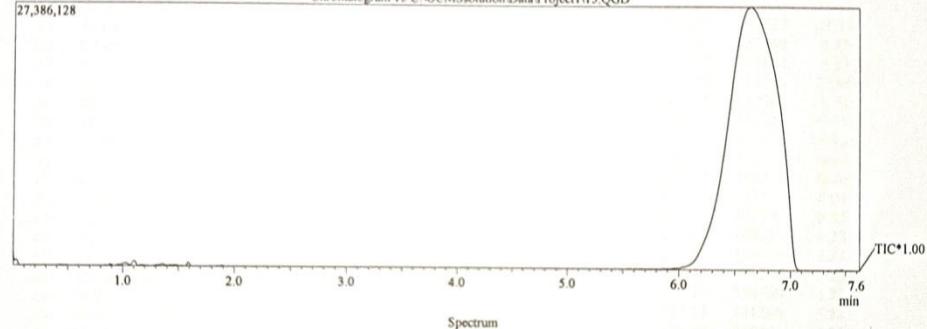
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Report File :
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Modified : 11/01/2007 04:02:40

Method
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End Time : 10:00min
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Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI

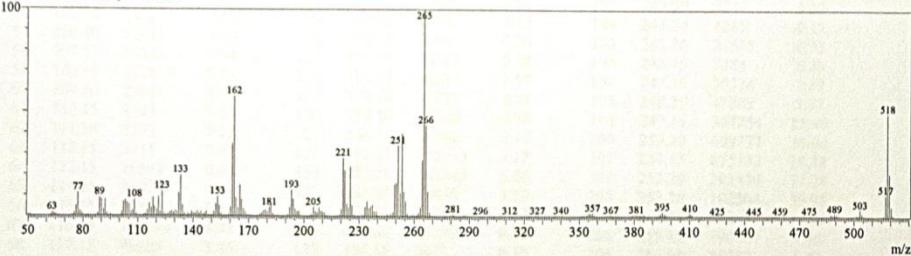
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Chromatogram 15 C:\GCMSsolution\Project1\15.QGD



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BG Mode:None Group 1 - Event 1

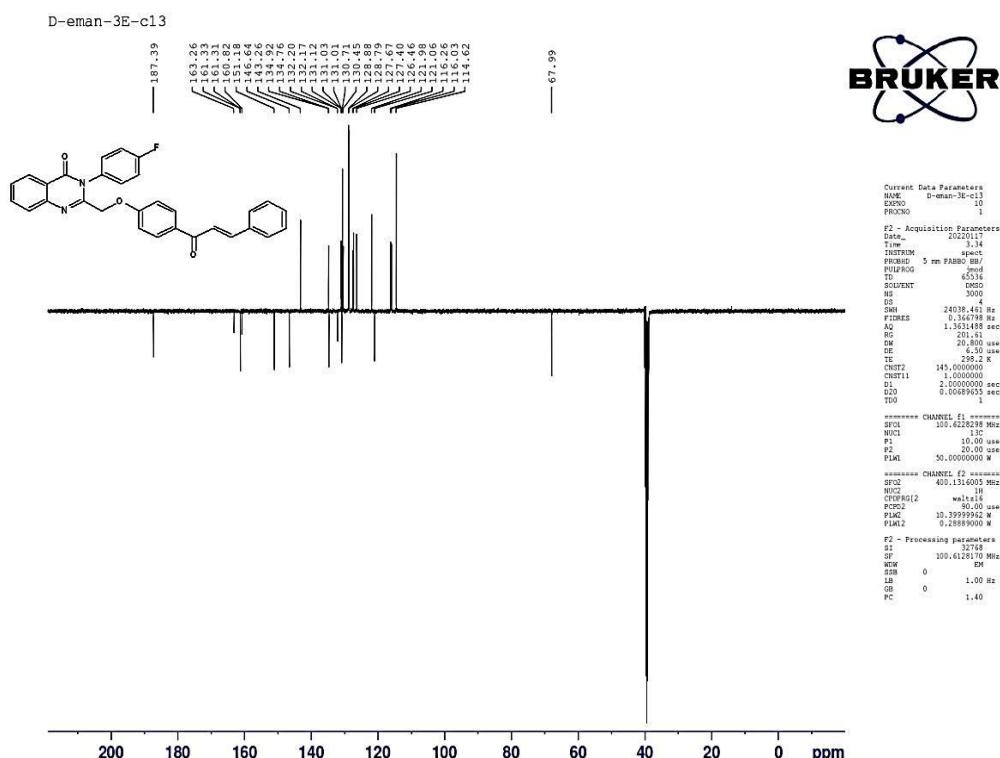
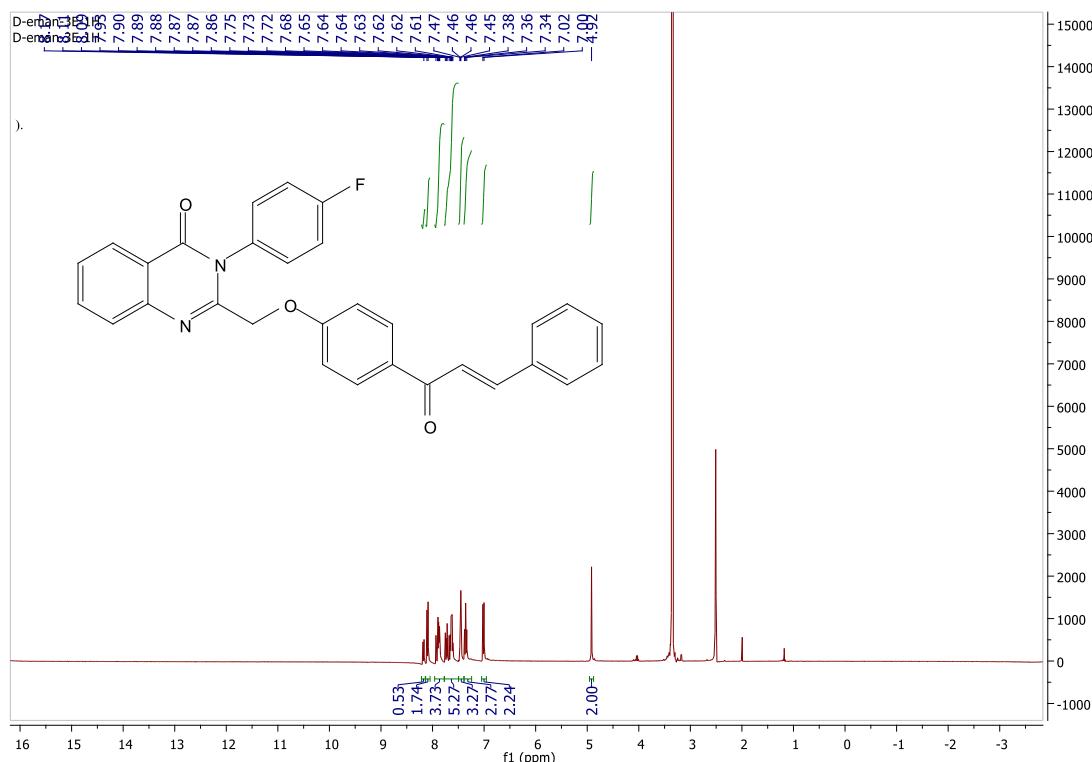


Mass Table
Line#:1 R.Time:6.6(Scan#:797)
MassPeaks:463
RawMode:Single 6.6(797) BasePeak:265(2560666)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	17425	0.68	4	53.00	6142	0.24	7	56.00	586	0.02
2	51.00	19146	0.75	5	54.05	1690	0.07	8	57.00	545	0.02
3	52.00	7697	0.30	6	55.05	3764	0.15	9	58.00	318	0.01

1 / 4

(E)-2-((4-Cinnamoylphenoxy)methyl)-3-(4-fluorophenyl)quinazolin-4(3H)-one (20).



21-Jan-07 17:20:03

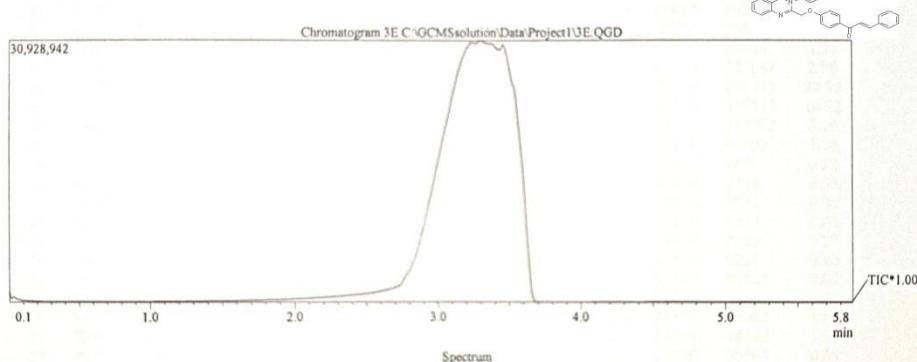
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DI Analysis
Shimadzu QP-2010 Plus

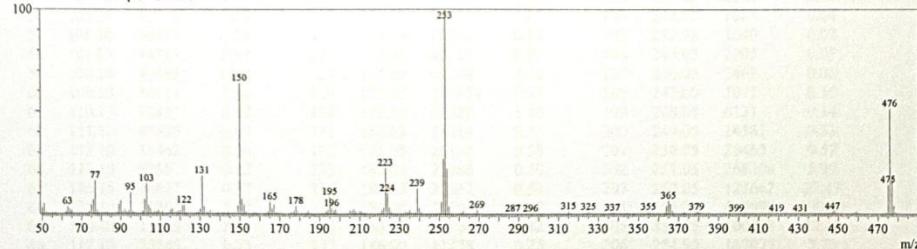
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Analyzed : 21/01/2007 05:13:10
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\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:19:06

Method
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[MS Table]
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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\Project1\3E.QGD



Line#:1 R.Time:3.3(Scan#:396)
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BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.3(Scan#:396)

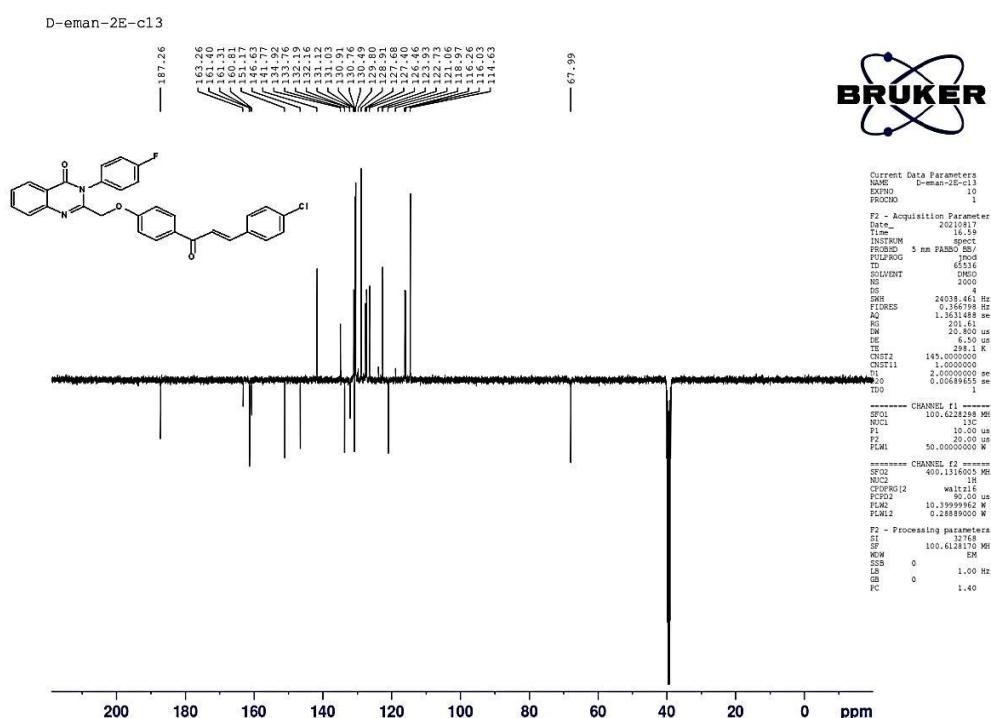
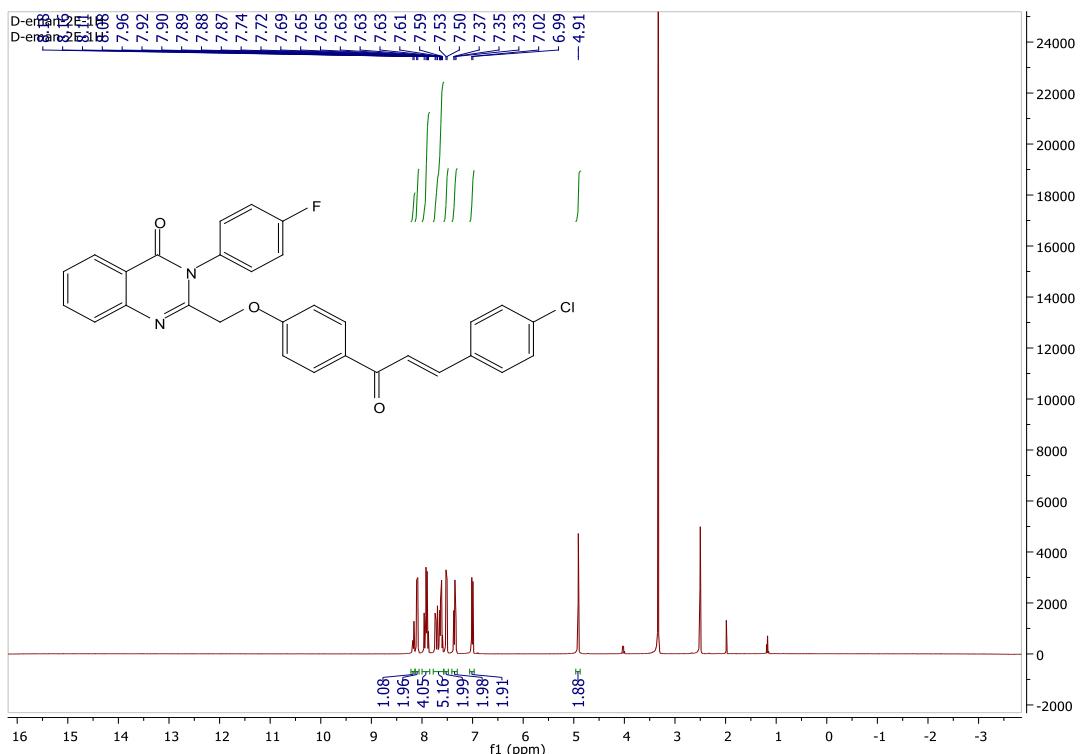
MassPeaks:424

RawMode:Single 3.3(396) BasePeak:253(4476991)

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	50.05	140174	3.13	4	53.00	25855	0.58	7	56.05	8203	0.18
2	51.00	226548	5.06	5	54.05	6734	0.15	8	57.00	27977	0.62
3	52.00	41111	0.92	6	55.00	27657	0.62	9	58.00	4298	0.10

(E)-2-((4-(4-Chlorophenyl)acryloyl)phenoxy)methyl-3-(4-fluorophenyl)quinazolin-4(3H)-one
(21).



21-Jan-07 17:12:52

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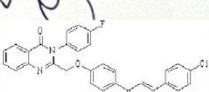
DI Analysis
Shimadzu QP-2010 Plus

Sample Information

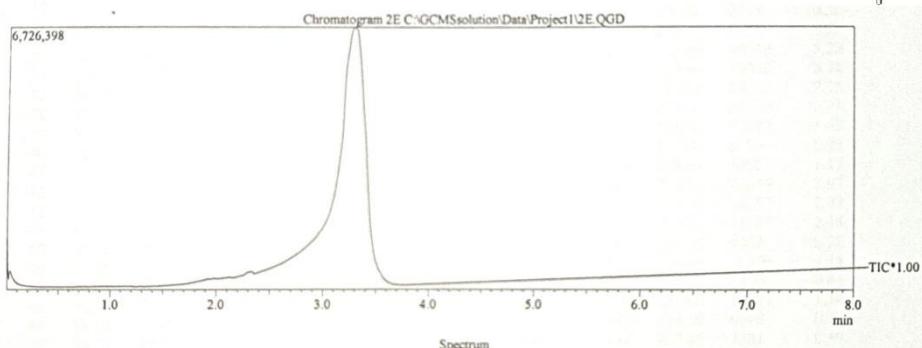
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 05:06:59
Sample Name : 2E
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project1\2E.QGD
Org Data File : C:\GCMSsolution\Project1\2E.QGD
Method File : C:\GCMSsolution\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
\$/End(\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:10:47

Method

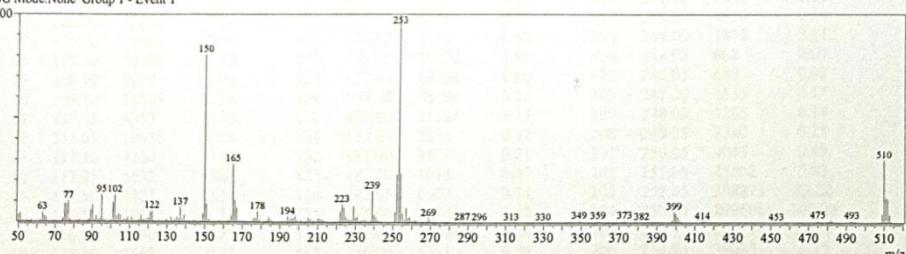
— Analytical Line 1 —
IonSourceTemp : 250.00 °C
[MS Table]
—Group 1 - Event 1—
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Project1\2E.QGD



Line#:1 R.Time:3.3(Scan#:397)
MassPeaks:395
RawMode:Single 3.3(397) BasePeak:253(899505)
BG Mode:None Group 1 - Event 1

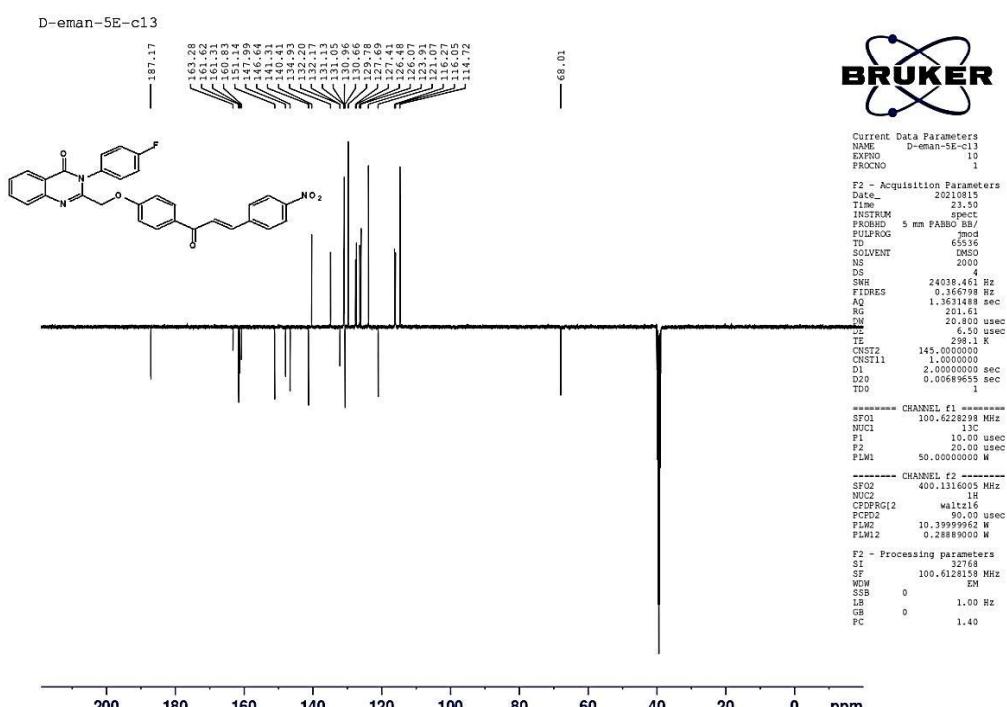
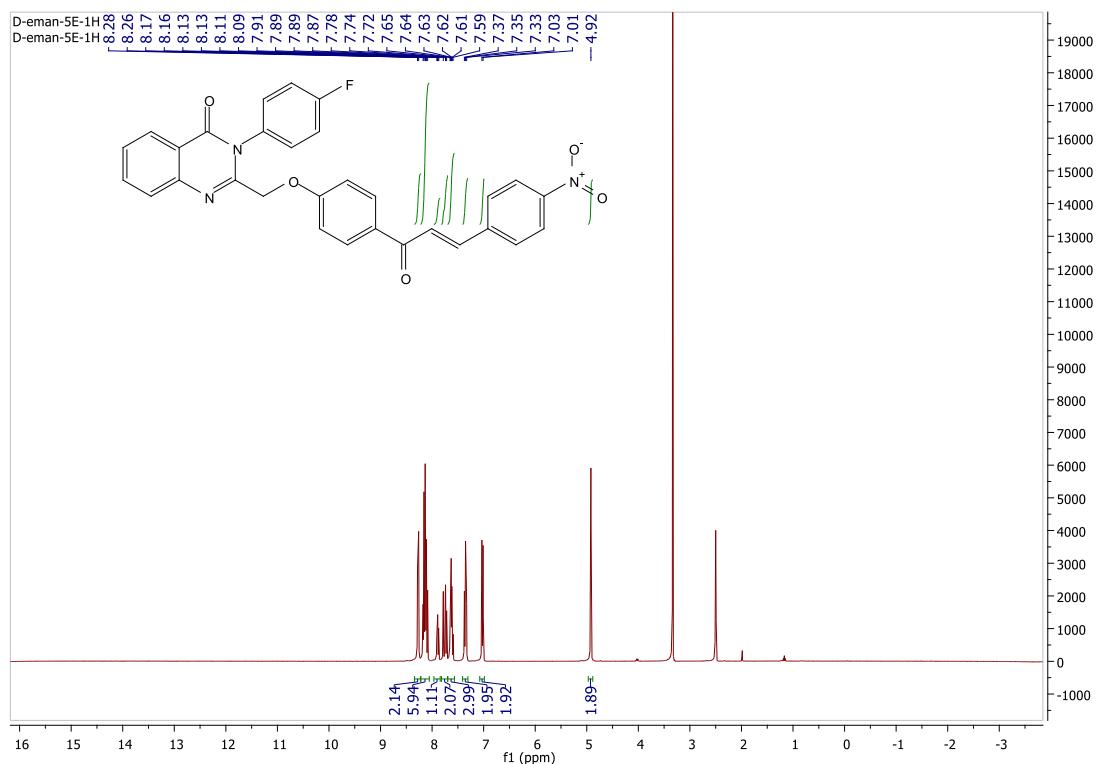


Mass Table

Line#:1 R.Time:3.3(Scan#:397)
MassPeaks:395
RawMode:Single 3.3(397) BasePeak:253(899505)
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	50.05	33093	3.68	4	53.00	4713	0.52	7	56.05	2587	0.29
2	51.00	38110	4.24	5	54.05	1860	0.21	8	57.00	8711	0.97
3	52.00	7382	0.82	6	55.00	6625	0.74	9	58.05	1112	0.12

(E)-3-(4-Fluorophenyl)-2-((4-(3-(4-nitrophenyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one (22).



21-Jan-07 17:32:09

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DT Analysis
Shimadzu QP-2010 Plus

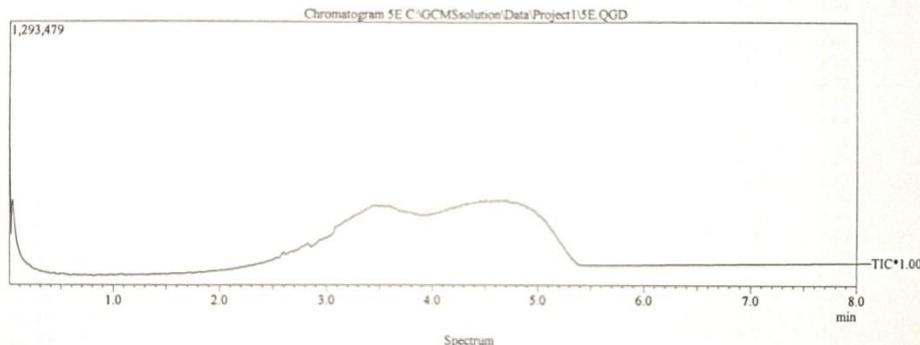
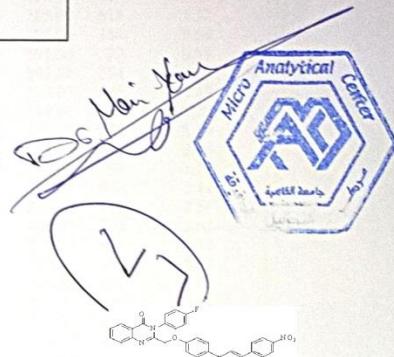
Sample Information

Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 05:25:48
Sample Name : 5E
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Project1\5E.QGD
Org Data File : C:\GCMSSolution\Project1\5E.QGD
Method File : C:\GCMSSolution\Project1\High Temperature Op
Org Method File : C:\GCMSSolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1\default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:31:16

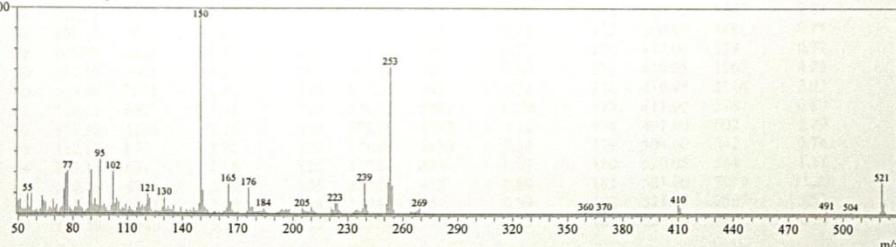
Method

==== 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\Project1\5E.QGD



Line#1 R.Time:3.5(Scan#:419)
MassPeaks:183
RawMode:Single 3.5(419) BasePeak:150(46495)
BG Mode:None Group 1 - Event 1



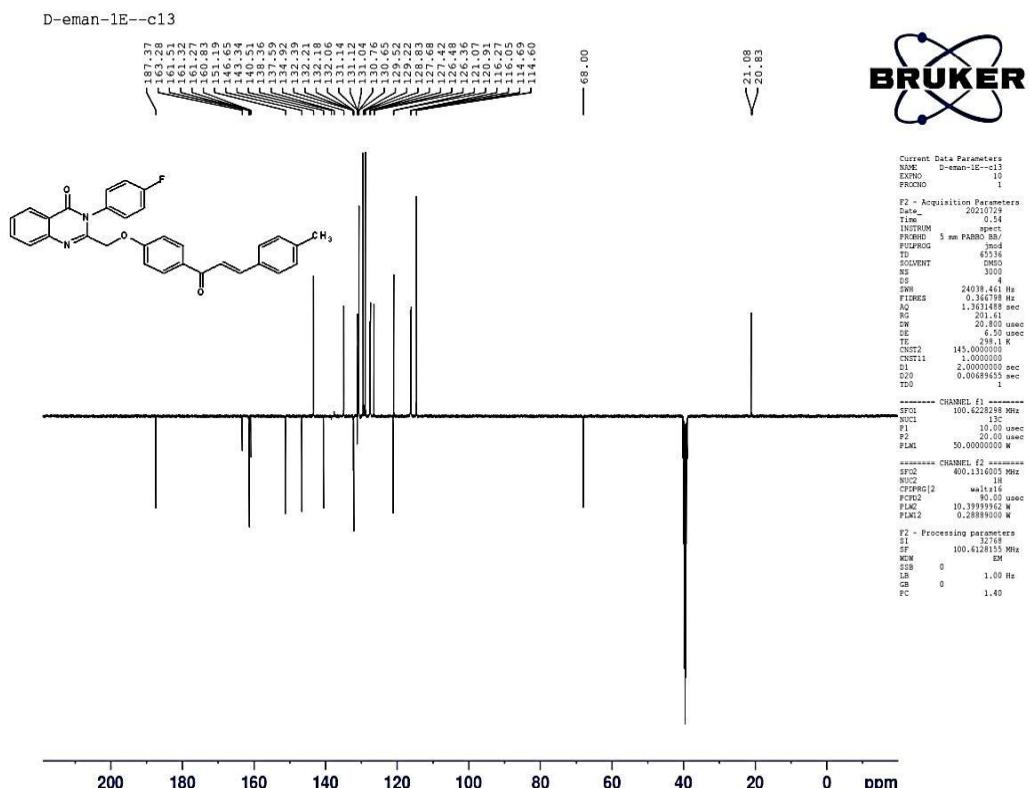
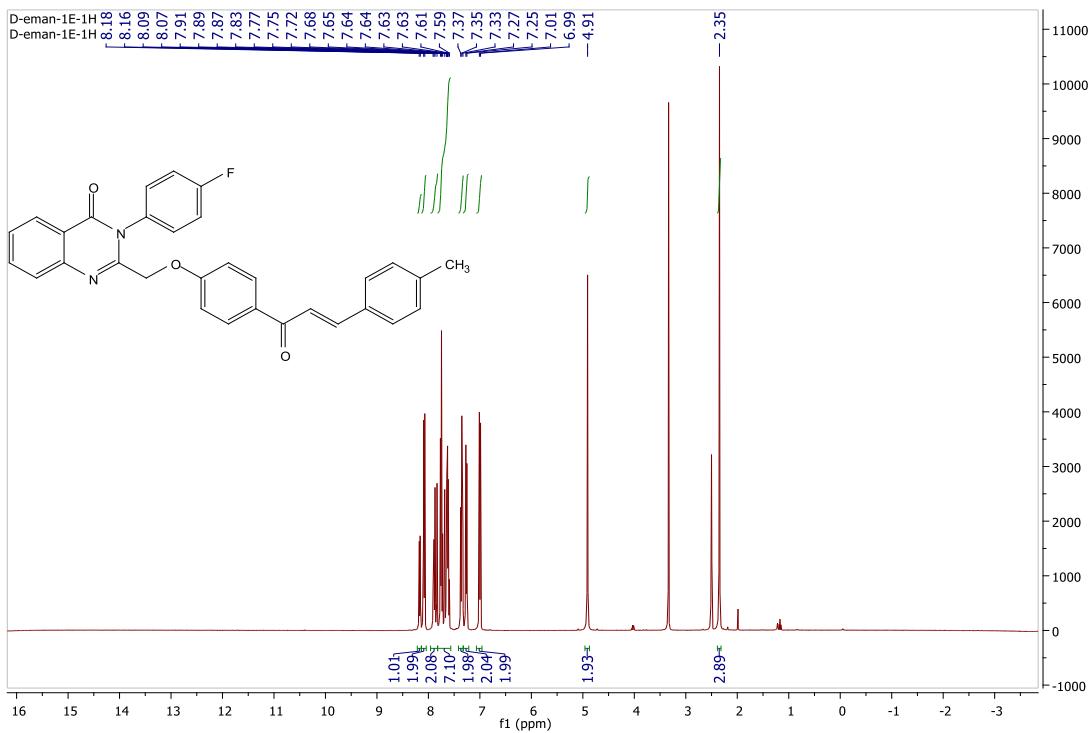
Mass Table
Line#1 R.Time:3.5(Scan#:419)
MassPeaks:183

RawMode:Single 3.5(419) BasePeak:150(46495)

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	2932	6.31	4	53.00	969	2.08	7	56.05	1467	3.16
2	51.00	3246	6.98	5	54.05	1094	2.35	8	57.05	4575	9.84
3	52.00	1249	2.69	6	55.05	4464	9.60	9	58.00	612	1.32

*(E)-3-(4-Fluorophenyl)-2-((4-(3-(*p*-tolyl)acryloyl)phenoxy)methyl)quinazolin-4(3*H*)-one (23).*



21-Jan-07 17:05:14

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DI Analysis
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Sample Information

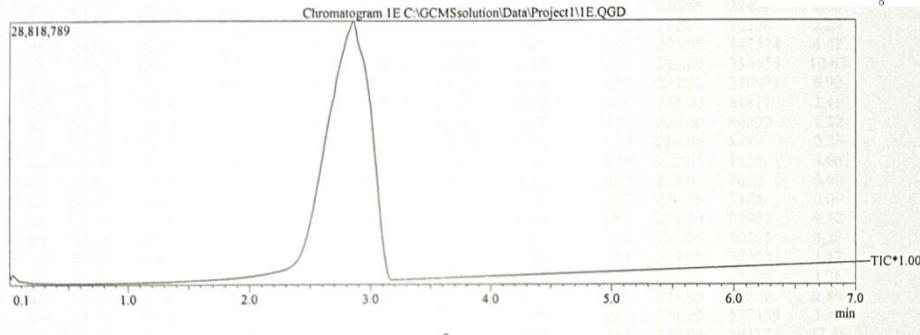
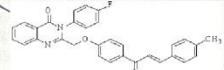
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 05:01:16
Sample Name : 1E
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Datap\Project1\1E.QGD
Org Data File : C:\GCMSsolution\Datap\Project1\1E.QGD
Method File : C:\GCMSsolution\Datap\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Datap\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:04:29

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

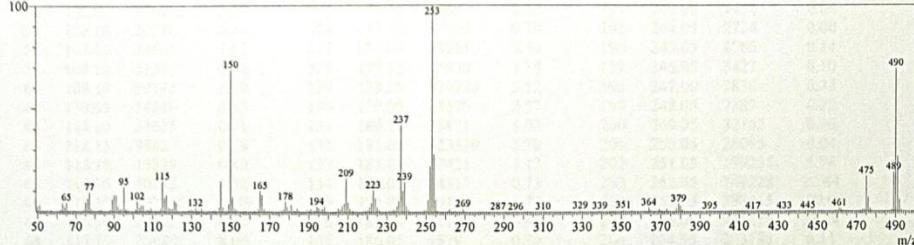
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Datap\Project1\1E.QGD



Spectrum

Line#1 R.Time:2.9(Scan#:345)
MassPeaks:436
RawMode:Single 2.9(345) BasePeak:253(3334153)
BG Mode:None Group 1 - Event 1



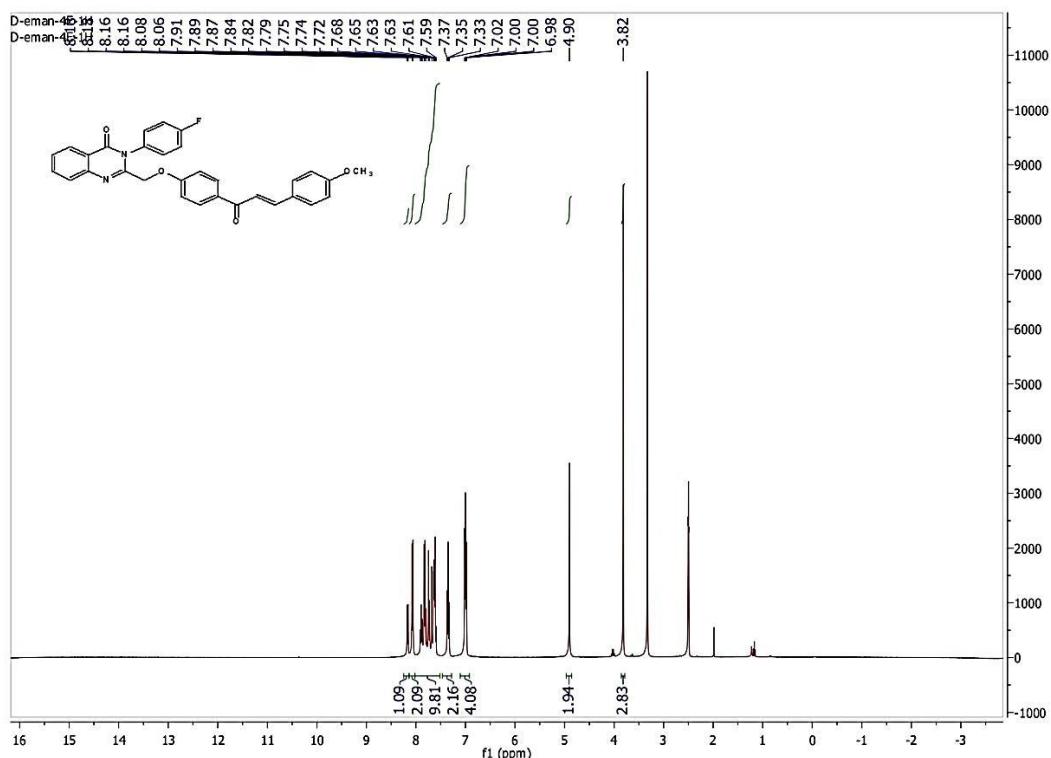
Mass Table
Line#1 R.Time:2.9(Scan#:345)
MassPeaks:436

RawMode:Single 2.9(345) BasePeak:253(3334153)

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	86385	2.59	4	53.00	23420	0.70	7	56.05	8847	0.27
2	51.00	107098	3.21	5	54.05	6944	0.21	8	57.00	30692	0.92
3	52.05	22026	0.66	6	55.00	29849	0.90	9	58.00	4121	0.12

(E)-3-(4-Fluorophenyl)-2-((4-(3-(4-methoxyphenyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one (24).



21-Jan-07 17:24:49

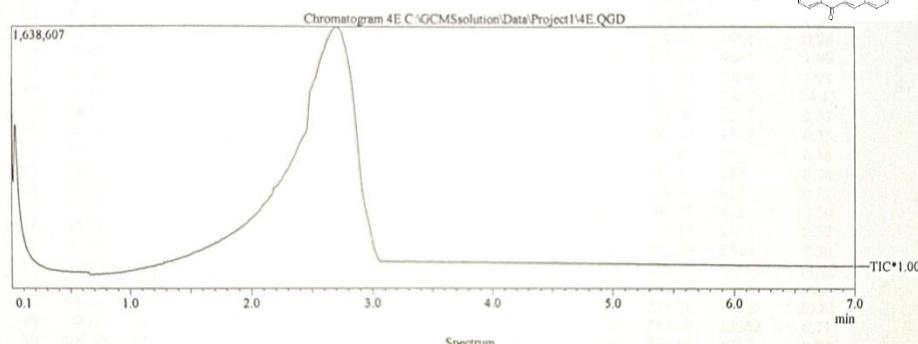
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DI Analysis
Shimadzu QP-2010 Plus

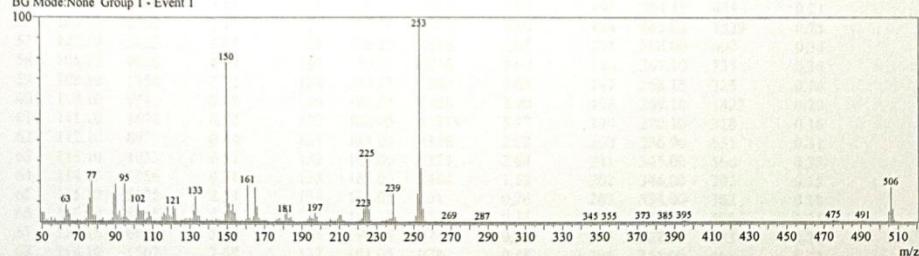
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 05:21:01
Sample Name : 4E
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Project1\4E.QGD
Org Data File : C:\GCMSSolution\Project1\4E.QGD
Method File : C:\GCMSSolution\Project1\High Temperature Op
Org Method File : C:\GCMSSolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1\default.qgt
\$End\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:24:08

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\Project1\4E.QGD



Line#1 R.Time:2.7(Scan#:324)
MassPeaks:232
RawMode:Single 2.7(324) BasePeak:253(204044)
BG Mode:None Group 1 - Event 1



Mass Table
Line#1 R.Time:2.7(Scan#:324)

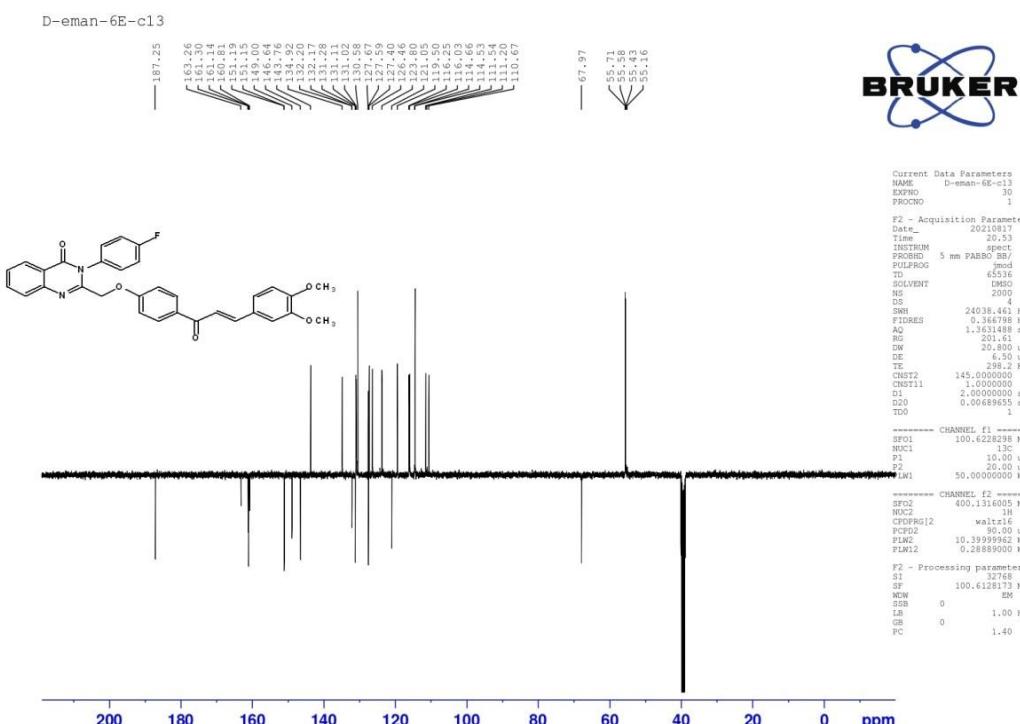
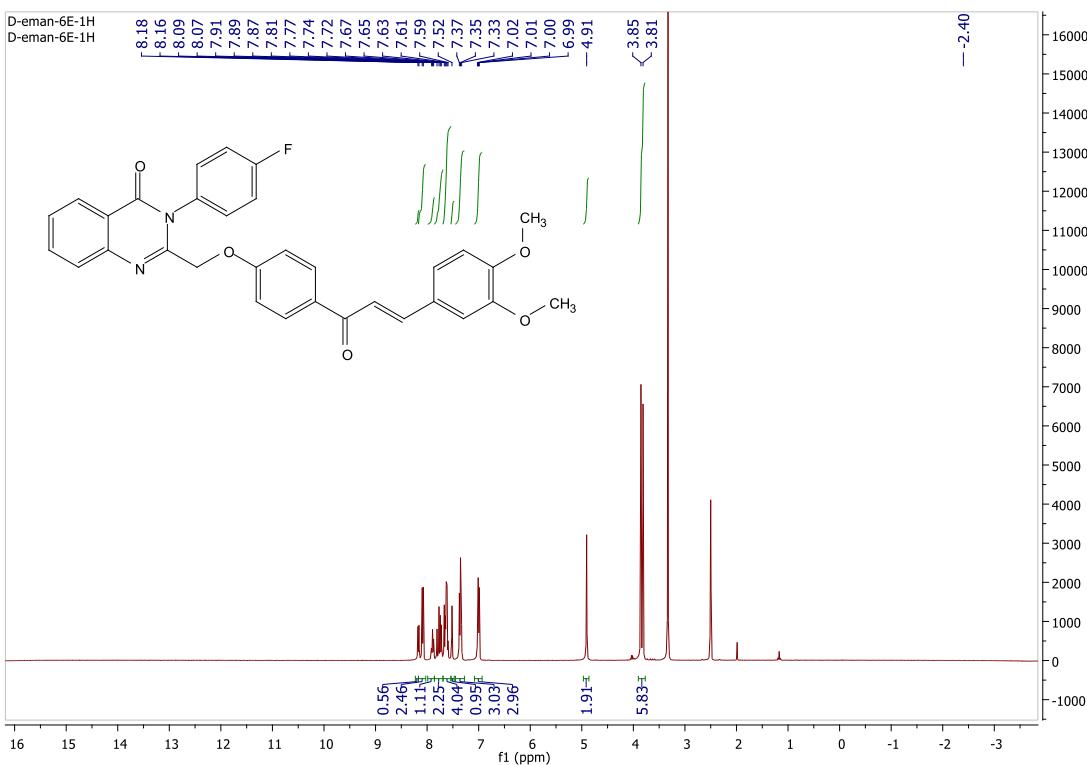
MassPeaks:232

RawMode:Single 2.7(324) BasePeak:253(204044)

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	9585	4.70	4	53.00	2638	1.29	7	56.05	1361	0.67
2	51.00	9975	4.89	5	54.05	1233	0.60	8	57.00	3884	1.90
3	52.05	2537	1.24	6	55.00	4466	2.19	9	57.95	613	0.30

(E)-2-((4-(3,4-Dimethoxyphenyl)acryloyl)phenoxy)methyl-3-(4-fluorophenyl)quinazolin-4(3H)-one (25).



21-Jan-07 17:37:40

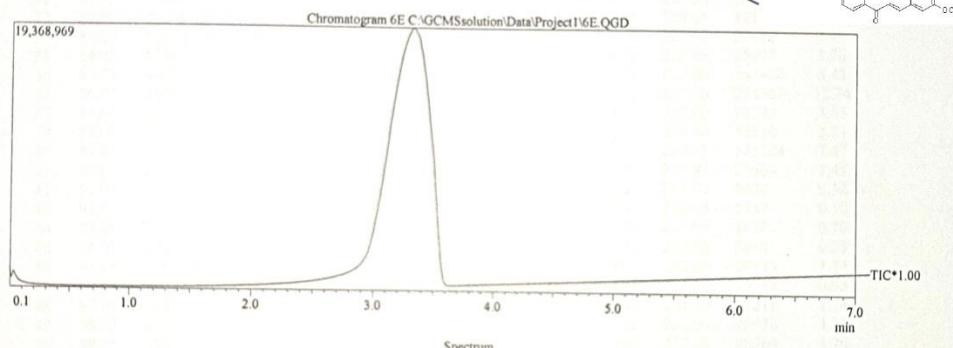
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DI Analysis
Shimadzu QP-2010 Plus

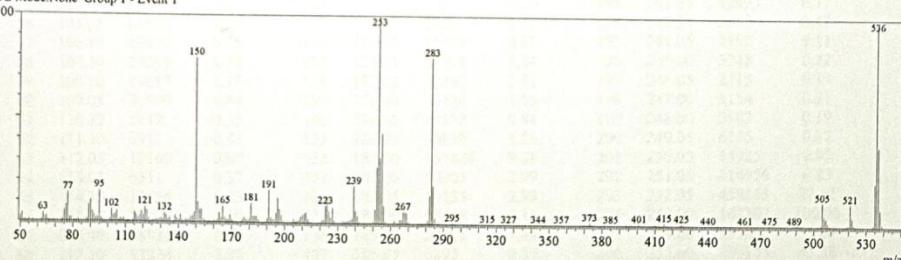
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 05:33:10
Sample Name : 6E
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Dat\Project1\6E.QGD
Org Data File : C:\GCMSsolution\Dat\Project1\6E.QGD
Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qrt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 05:36:51

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\Dat\Project1\6E.QGD



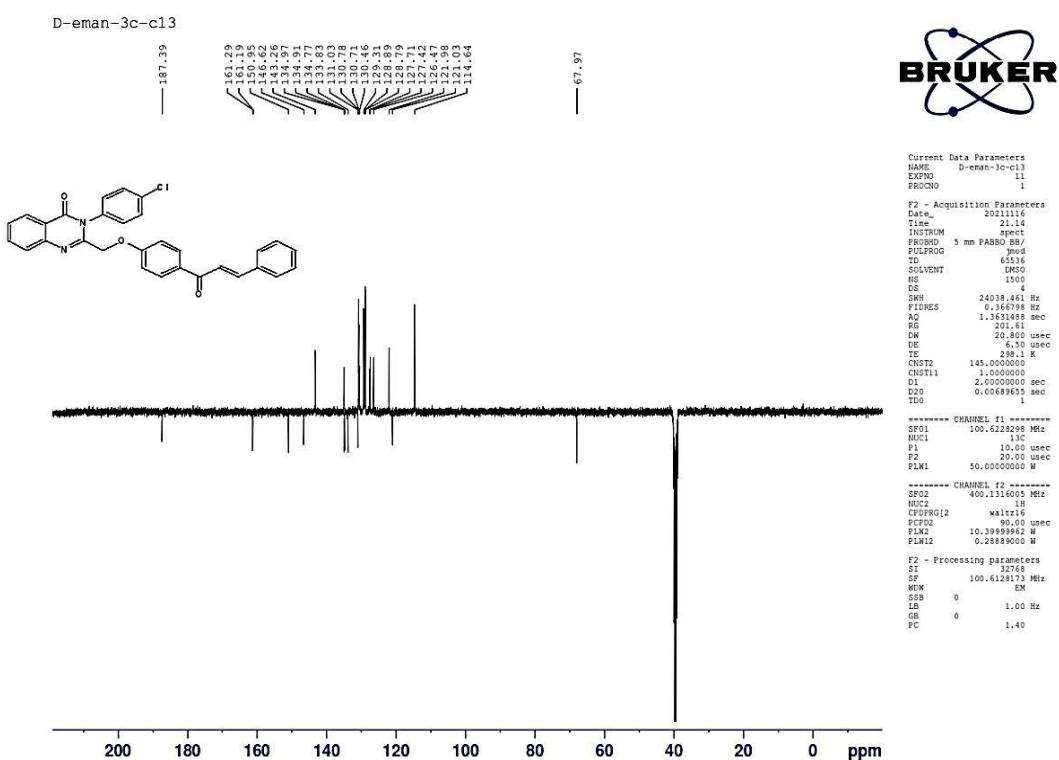
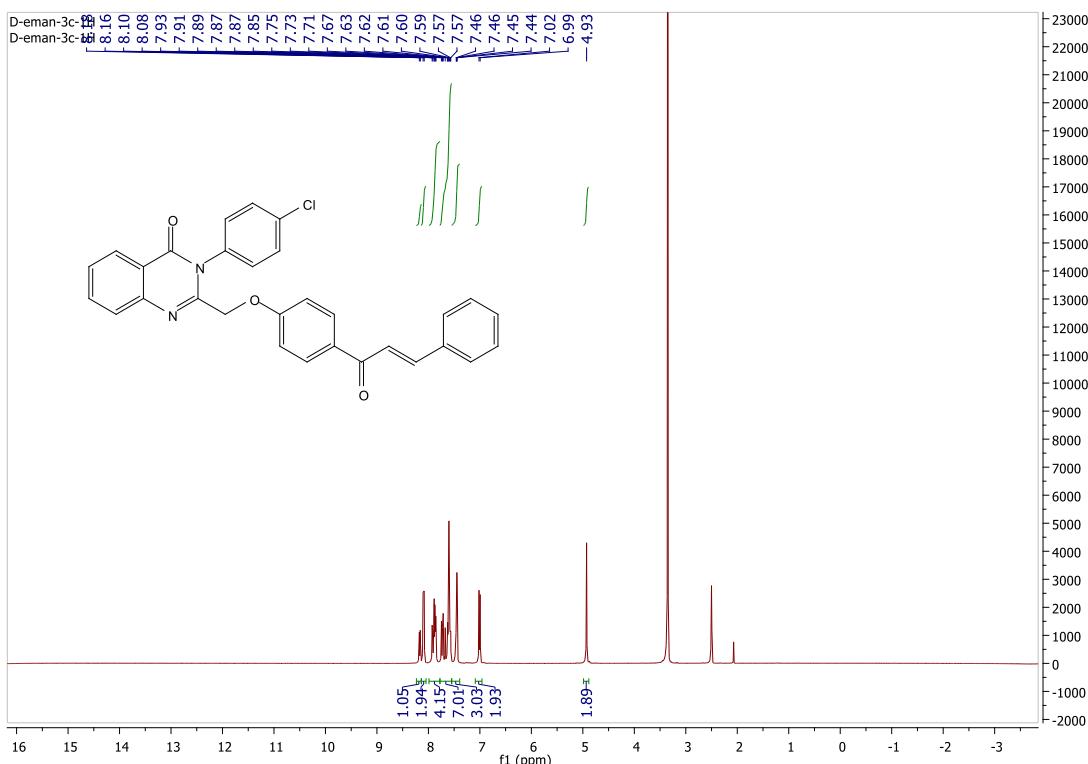
Line#1 R.Time:3.3(Scan#:402)
MassPeaks:465
RawMode:Single 3.3(402) BasePeak:253(1683025)
BG Mode:None Group 1 - Event 1



Mass Table
Line#:1 R.Time:3.3(Scan#:402)
MassPeaks:465
RawMode:Single 3.3(402) BasePeak:253(1683025)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.
1	50.00	45487	2.70	4	53.00	14495	0.86	7	56.05	4669	0.28
2	51.00	69831	4.15	5	54.05	4429	0.26	8	57.00	15622	0.93
3	52.00	12178	0.72	6	55.00	22097	1.31	9	57.95	2172	0.13

(E)-3-(4-Chlorophenyl)-2-((4-cinnamoylphenoxy)methyl)quinazolin-4(3H)-one (26).



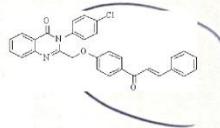
21-Jan-07 15:13:24

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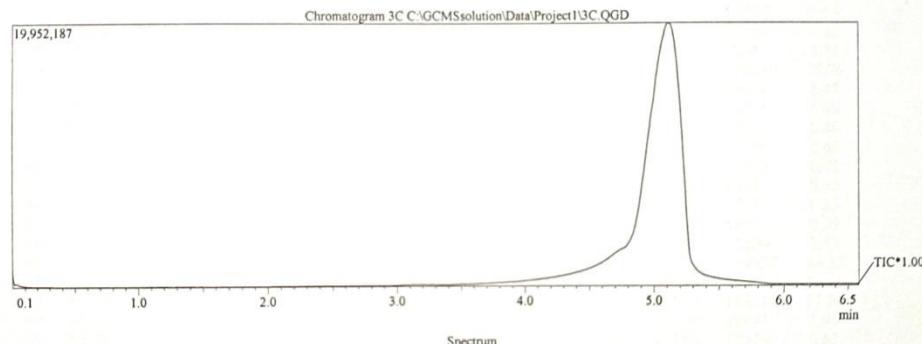
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 03:06:07
Sample Name : 3C
Sample ID :
Customer Name : Dr.Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Dat\Project1\3C.QGD
Org Data File : C:\GCMSsolution\Dat\Project1\GC.QGD
Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
\$End/\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 03:12:45

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

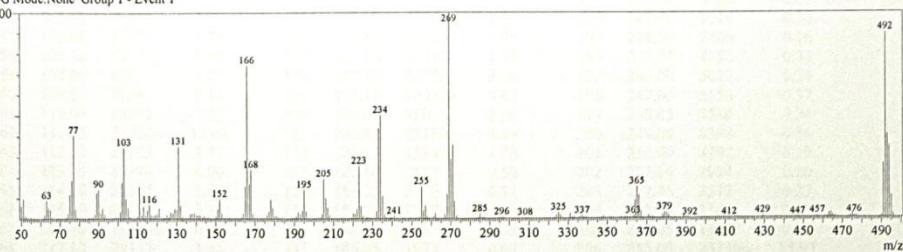


C:\GCMSsolution\Dat\Project1\3C.QGD



Spectrum

Line#:1 R.Time:5.1(Scan#:615)
MassPeaks:432
RawMode:Single 5.1(615) BasePeak:269(1489914)
BG Mode:None Group 1 - Event 1

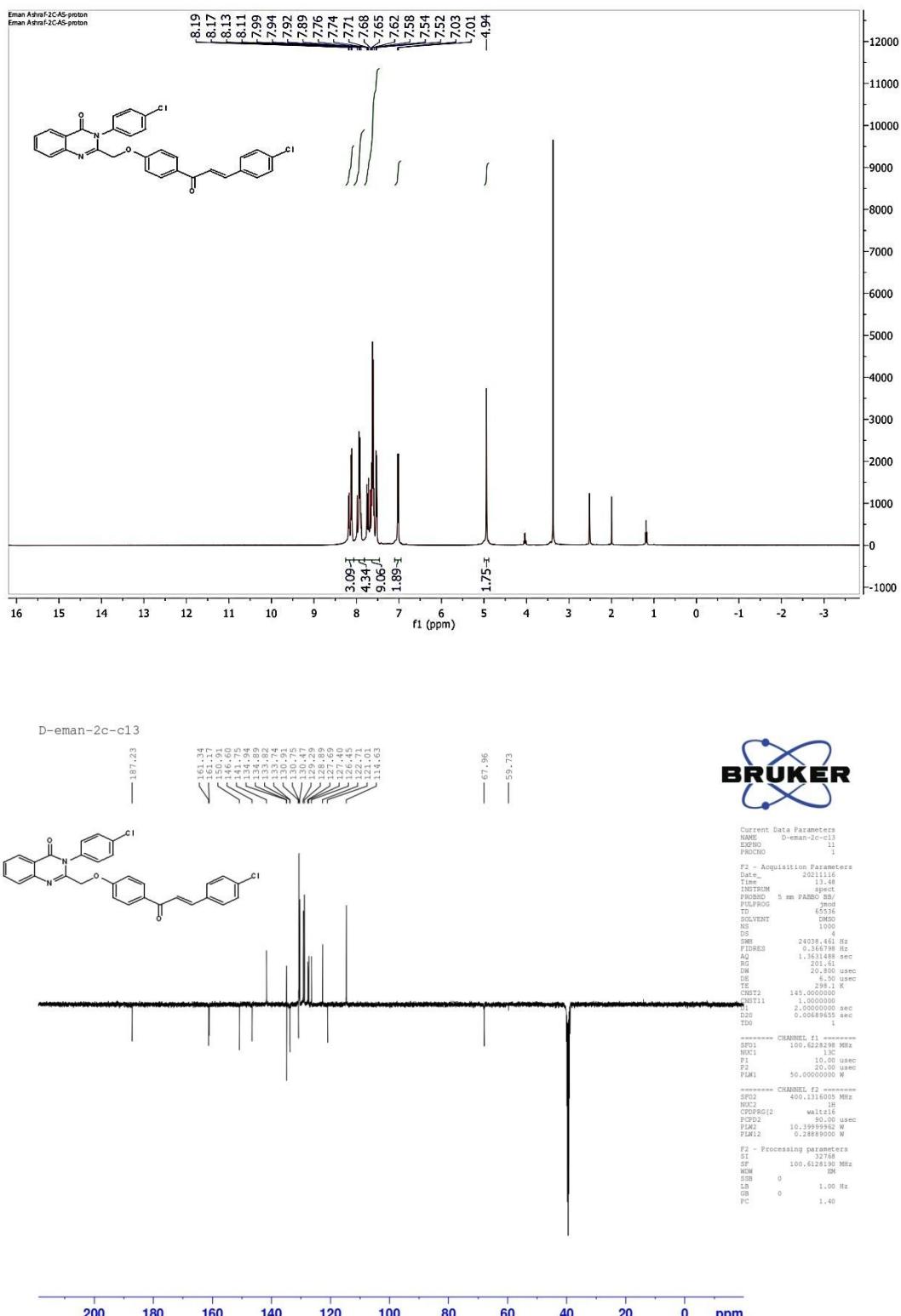


Mass Table
Line#:1 R.Time:5.1(Scan#:615)
MassPeaks:432
RawMode:Single 5.1(615) BasePeak:269(1489914)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	92734	6.22	4	53.00	15207	1.02	7	56.05	1400	0.09
2	51.00	144671	9.71	5	54.05	2462	0.17	8	57.10	2260	0.15
3	52.00	26276	1.76	6	55.00	12166	0.82	9	57.95	1046	0.07

1 / 4

**(E)-3-(4-Chlorophenyl)-2-((4-(3-(4-chlorophenyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one
(27).**



21-Jan-07 15:01:37

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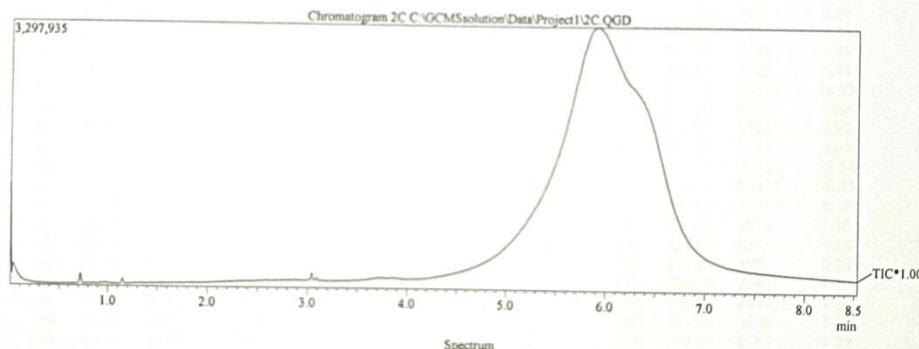
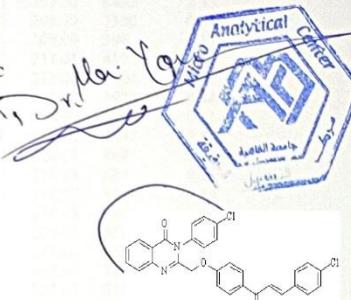
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 02:51:46
Sample Name : 2C
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project1\2C.QGD
Org Data File : C:\GCMSsolution\Project1\2C.QGD
Method File : C:\GCMSsolution\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qgt
\$End\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 03:00:22

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

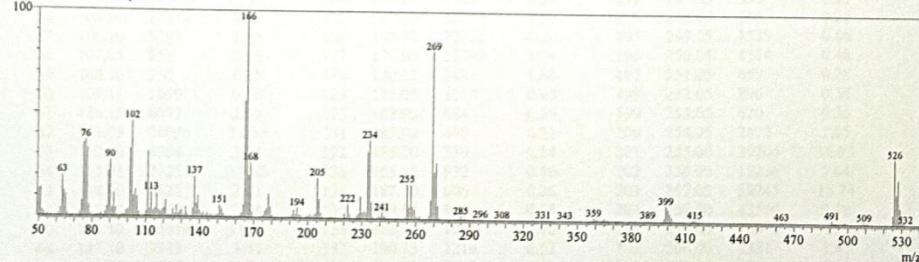
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Project1\2C.QGD



Spectrum

Line# 1 R.Time:5.9(Scan#:713)
MassPeaks:336
RawMode:Single 5.9(713) BasePeak:166(234482)
BG Mode:None Group 1 - Event 1

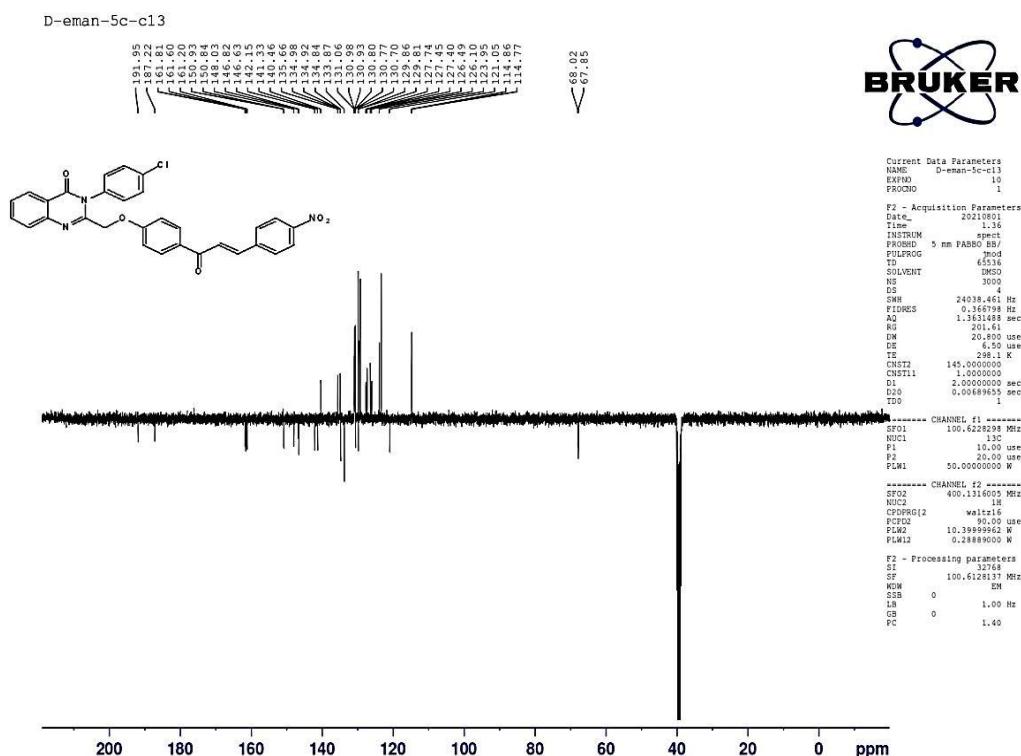
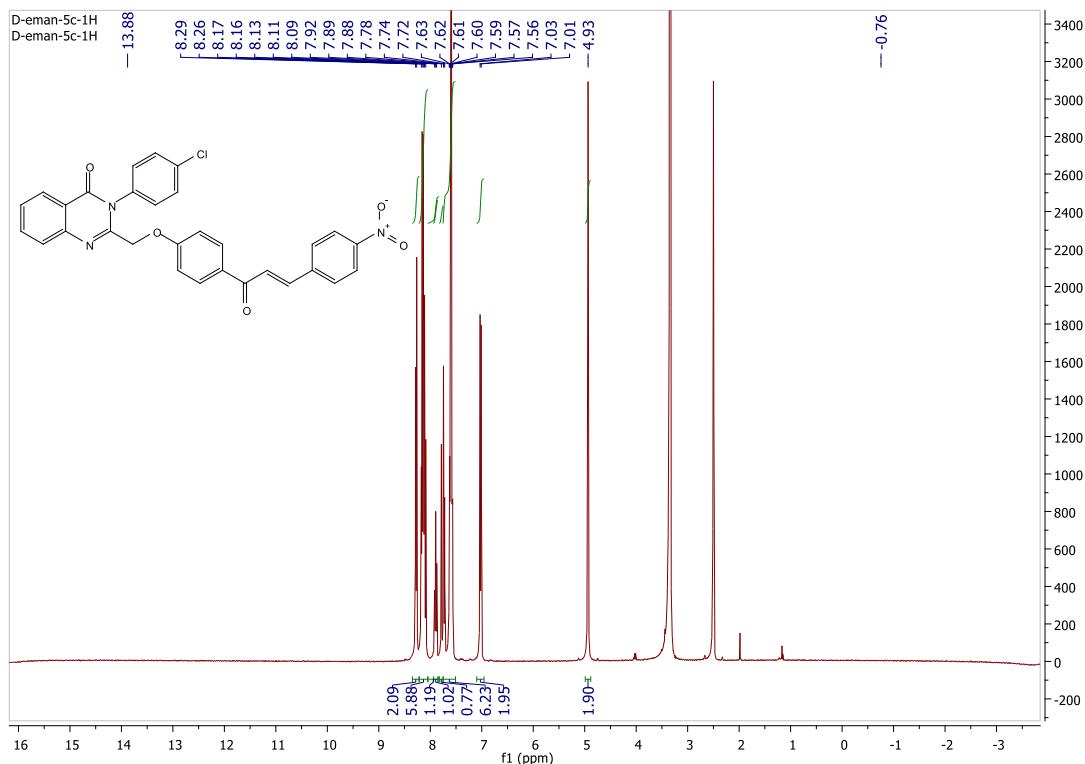


Mass Table

Line#:1 R.Time:5.9(Scan#:713)
MassPeaks:336
RawMode:Single 5.9(713) BasePeak:166(234482)
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	31209	13.31	4	53.00	4252	1.81	7	56.10	706	0.30
2	51.00	32023	13.66	5	54.05	878	0.37	8	57.05	1317	0.56
3	52.00	6662	2.84	6	55.00	2596	1.11	9	58.15	428	0.18

(E)-3-(4-Chlorophenyl)-2-((4-(3-(4-nitrophenyl)acryloyl)phenoxy)methyl)qui-nazolin-4(3H)-one (28).



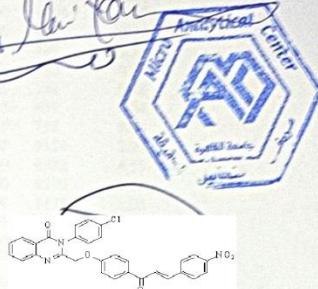
21-Jan-07 15:47:07

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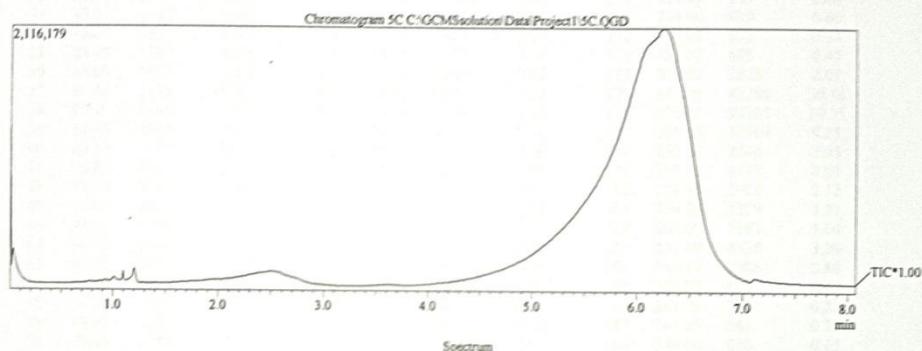
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 03:38:21
Sample Name : 5C
Sample ID :
Customer Name : Dr. Eman Adrafi - Pharmacy - Zagazik
Data File : C:\GCMS\solution\Project1\5C.QGD
Org Data File : C:\GCMS\solution\Project1\5C.QGD
Method File : C:\GCMS\solution\Project1\High Temperature Op
Org Method File : C:\GCMS\solution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMS\solution\System\Tune1\default.oga
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 03:46:29

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

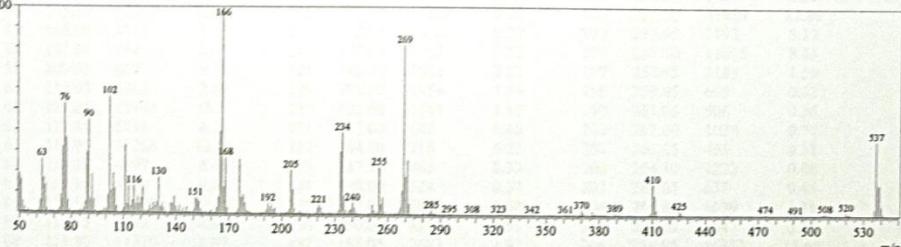


C:\GCMS\solution\Project1\5C.QGD



Spectrum

Line# 1 R.Time:6.3(Scan#:752)
MassPeaks:288
RawMode:Single 6.3(752) BasePeak:166(140206)
BG Mode:None Group 1 - Event 1

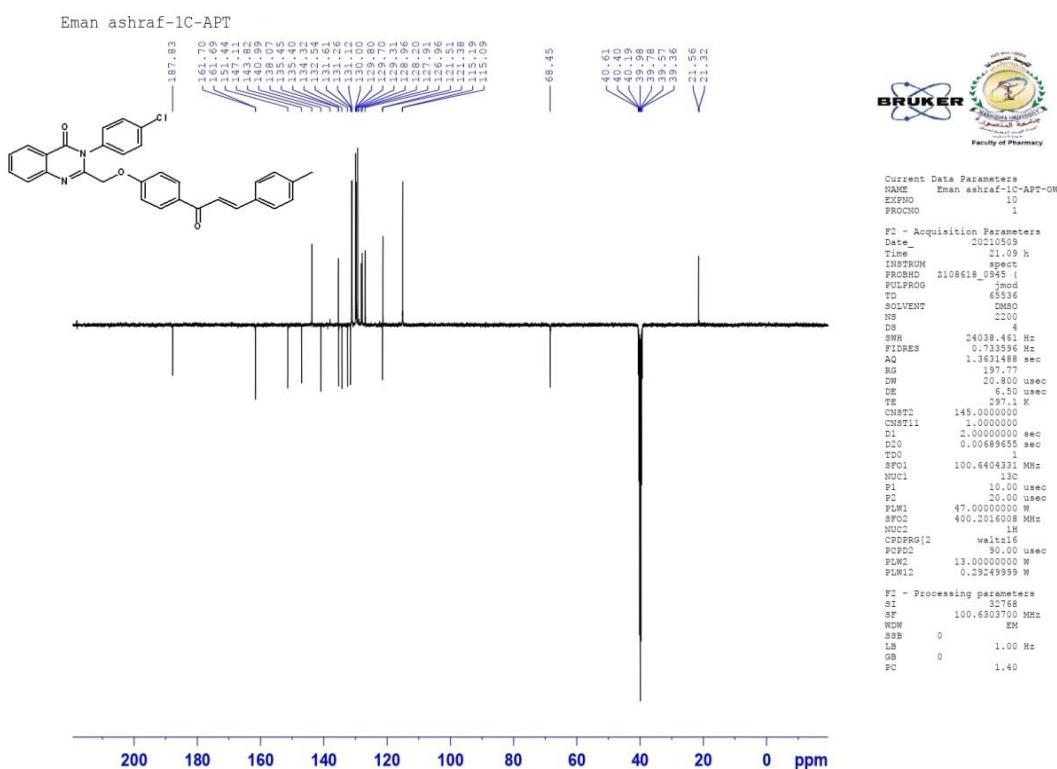
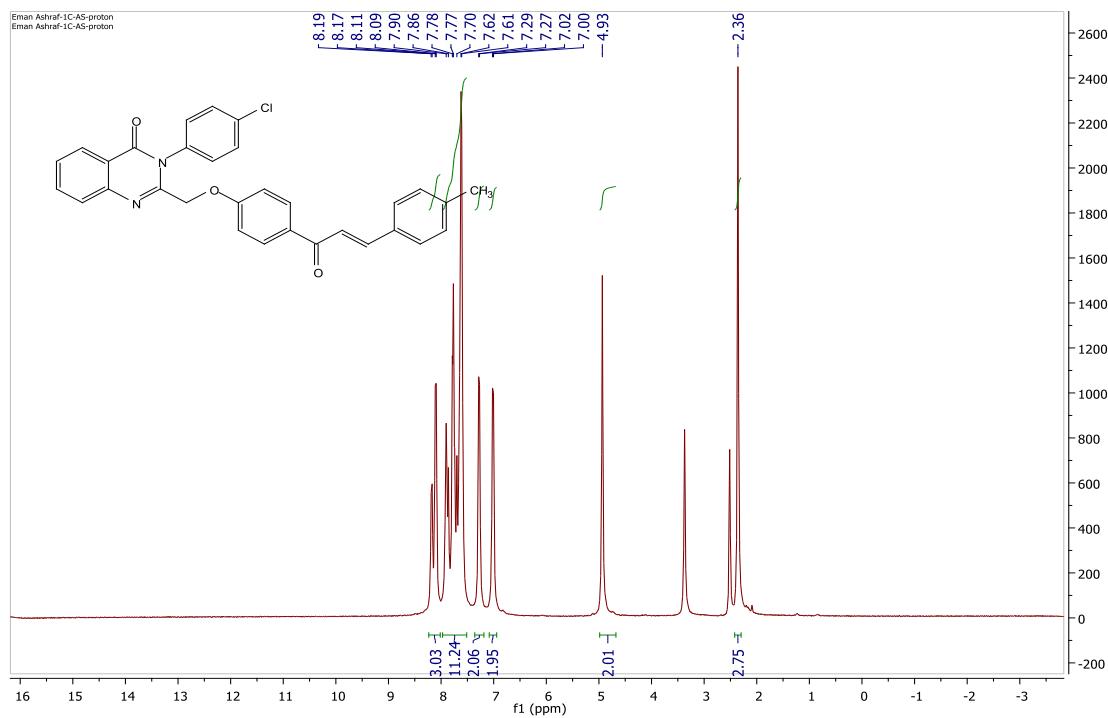


Mass Table

Line# 1 R.Time:6.3(Scan#:752)
MassPeaks:288
RawMode:Single 6.3(752) BasePeak:166(140206)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.
1	50.00	26487	18.89	4	53.00	3479	2.48	7	56.05	608	0.43
2	51.00	22759	16.23	5	54.05	821	0.59	8	57.00	1023	0.73
3	52.05	7780	5.55	6	55.05	2161	1.54	9	58.00	340	0.24

(E)-3-(4-Chlorophenyl)-2-((4-(3-(ptolyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one (29).



21-Jan-07 14:43:31

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DI Analysis
Shimadzu QP-2010 Plus

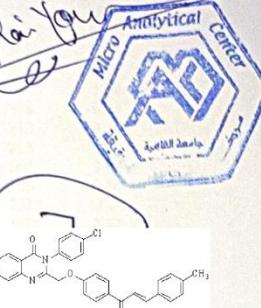
Sample Information

Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 02:32:20
Sample Name : 1C
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Dataproject\1C.QGD
Org Data File : C:\GCMSsolution\Dataproject\1C.QGD
Method File : C:\GCMSsolution\Dataproject\High Temperature Op
Org Method File : C:\GCMSsolution\Dataproject\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qzt
\$End/IS Modified by : Dr. Mai Younis
Modified : 21/01/2007 02:40:52

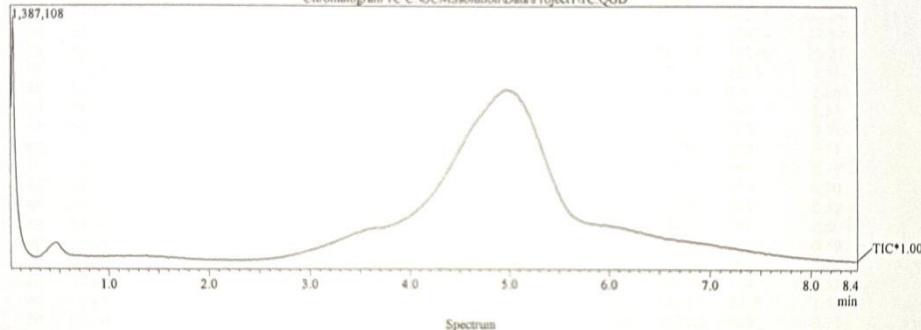
Method

— 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\Dataproject\1C.QGD

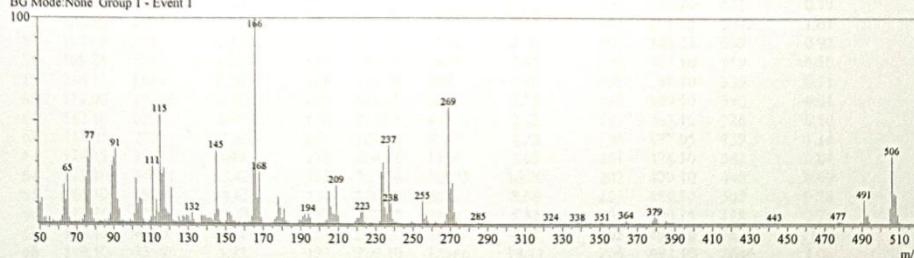


Chromatogram 1C C:\GCMSsolution\Dataproject\1C.QGD



Spectrum

Line#:1 R.Time:5.1(Scan#:610)
MassPeaks:214
RawMode:Single 5.1(610) BasePeak:166(64825)
BG Mode:None Group 1 - Event 1

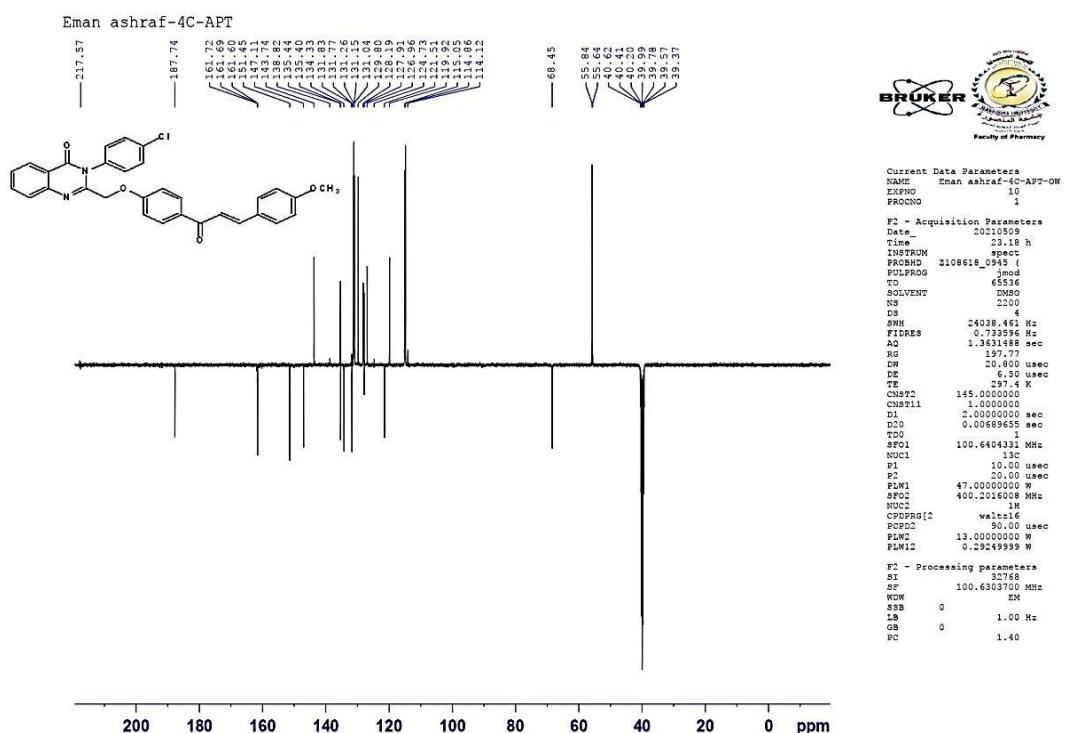
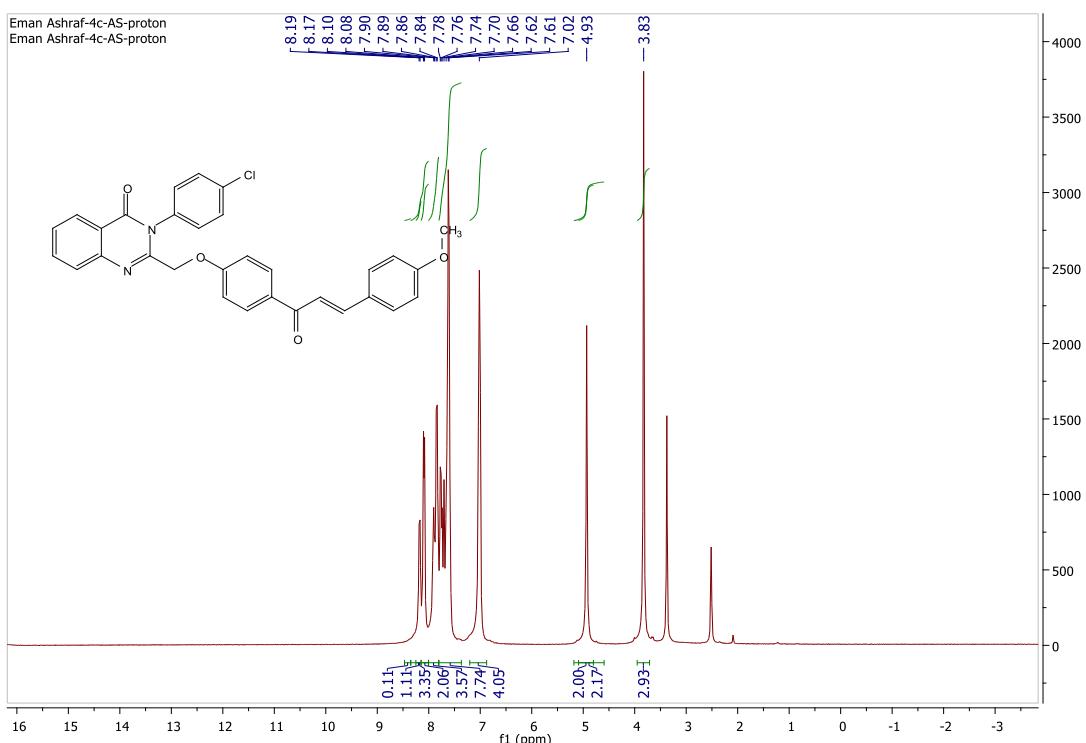


Mass Table

Line#:1 R.Time:5.1(Scan#:610)
MassPeaks:214
RawMode:Single 5.1(610) BasePeak:166(64825)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.
1	50.00	6569	10.13	4	53.05	2065	3.19	7	56.10	351	0.54
2	51.00	8039	12.40	5	54.00	377	0.58	8	57.10	1100	1.70
3	52.05	1722	2.66	6	55.05	1942	3.00	9	58.10	375	0.58

(E)-3-(4-Chlorophenyl)-2-((4-(3-(4-methoxyphenyl)acryloyl)phenoxy)methyl) quinazolin-4(3H)-one
(30).



21-Jan-07 15:30:52

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DI Analysis
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Sample Information

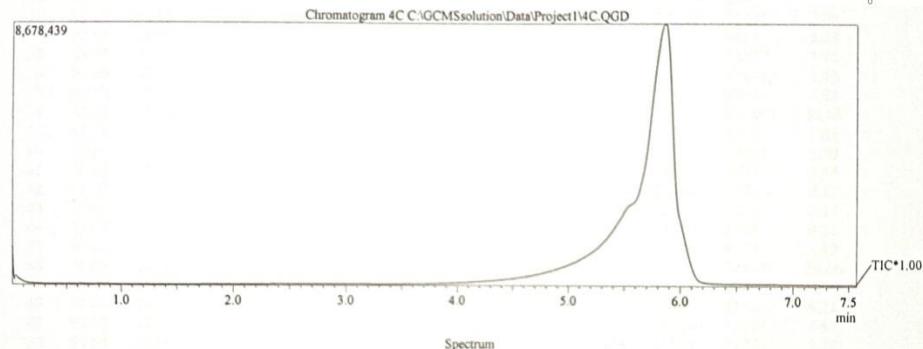
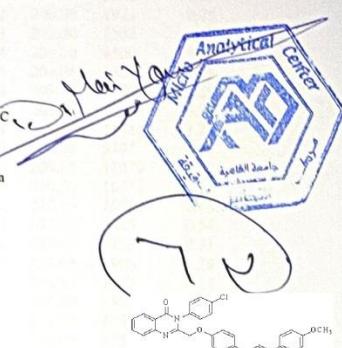
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 03:21:41
Sample Name : 4C
Sample ID :
Customer Name : Dr.Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project1\4C.QGD
Org Data File : C:\GCMSsolution\Project1\4C.QGD
Method File : C:\GCMSsolution\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
\$End/\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 03:29:18

Method

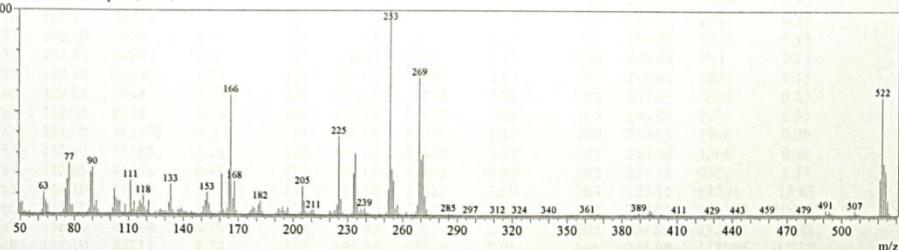
———— Analytical Line 1 ———
IonSourceTemp : 250.00 °C
[MS Table]
—Group 1 - Event 1—
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Project1\4C.QGD



Line#:1 R.Time:5.8(Scan#:700)
MassPeaks:419
RawMode:Single 5.8(700) BasePeak:253(683733)
BG Mode:None Group 1 - Event 1

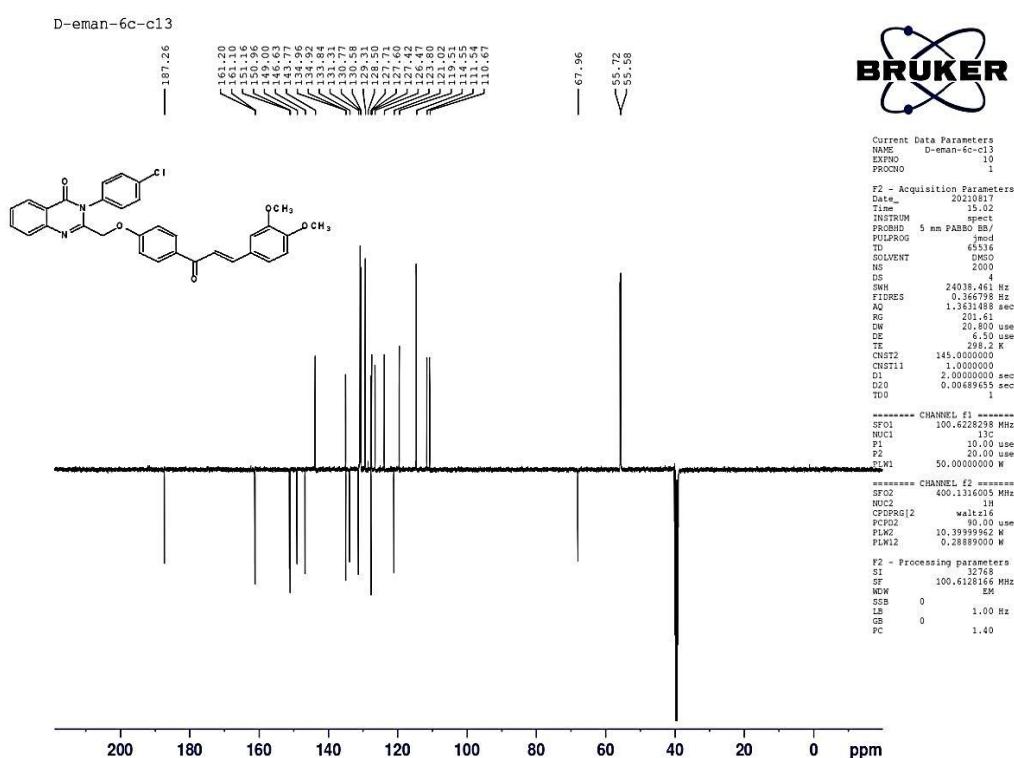
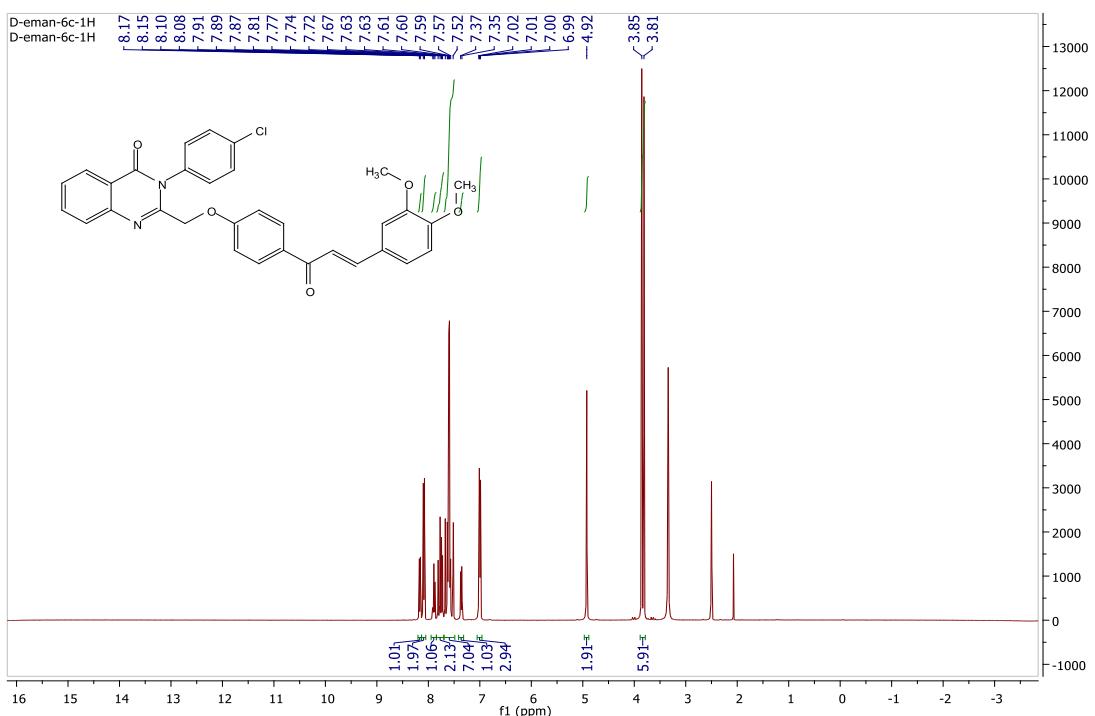


Mass Table

Line#:1 R.Time:5.8(Scan#:700)
MassPeaks:419
RawMode:Single 5.8(700) BasePeak:253(683733)
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	39106	5.72	4	53.00	8422	1.23	7	56.00	1270	0.19
2	51.00	39983	5.85	5	54.05	1726	0.25	8	57.00	2228	0.33
3	52.05	8953	1.31	6	55.00	9764	1.43	9	58.05	673	0.10

(E)-3-(4-Chlorophenyl)-2-((4-(3-(3,4-dimethoxyphenyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one (31).



21-Jan-07 16:05:24

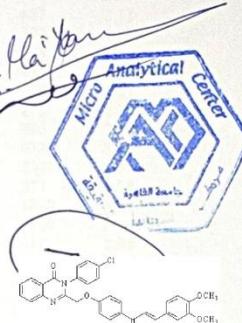
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DI Analysis
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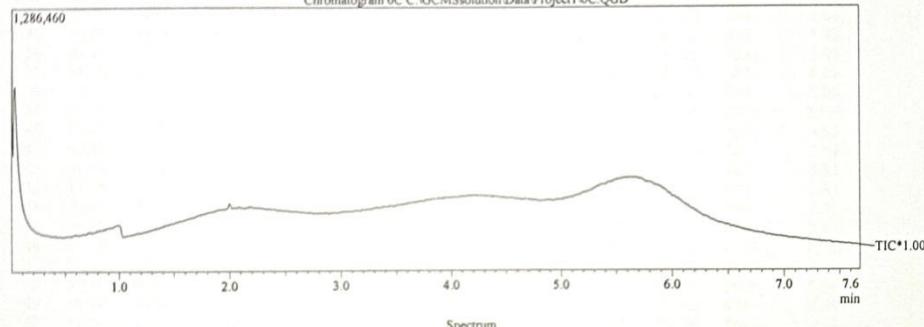
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 03:55:41
Sample Name : 6C
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project1\6C.QGD
Org Data File : C:\GCMSsolution\Project1\6C.QGD
Method File : C:\GCMSsolution\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 04:03:26

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

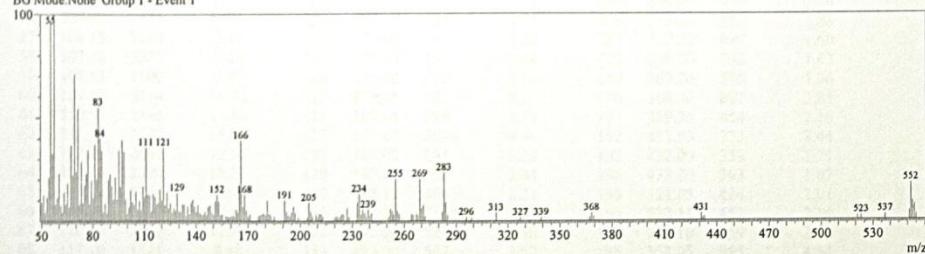
C:\GCMSsolution\Project1\6C.QGD



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



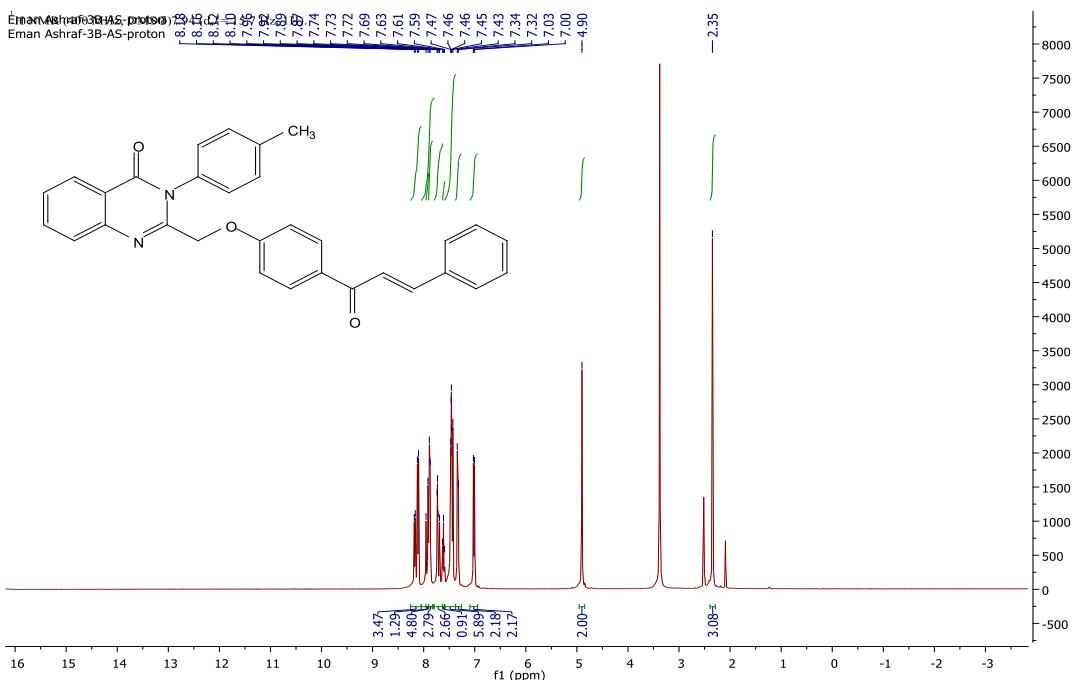
Line#:1 R.Time:5.6(Scan#:675)
MassPeaks:202
RawMode:Single 5.6(675) BasePeak:57(21045)
BG Mode:None Group 1 - Event 1



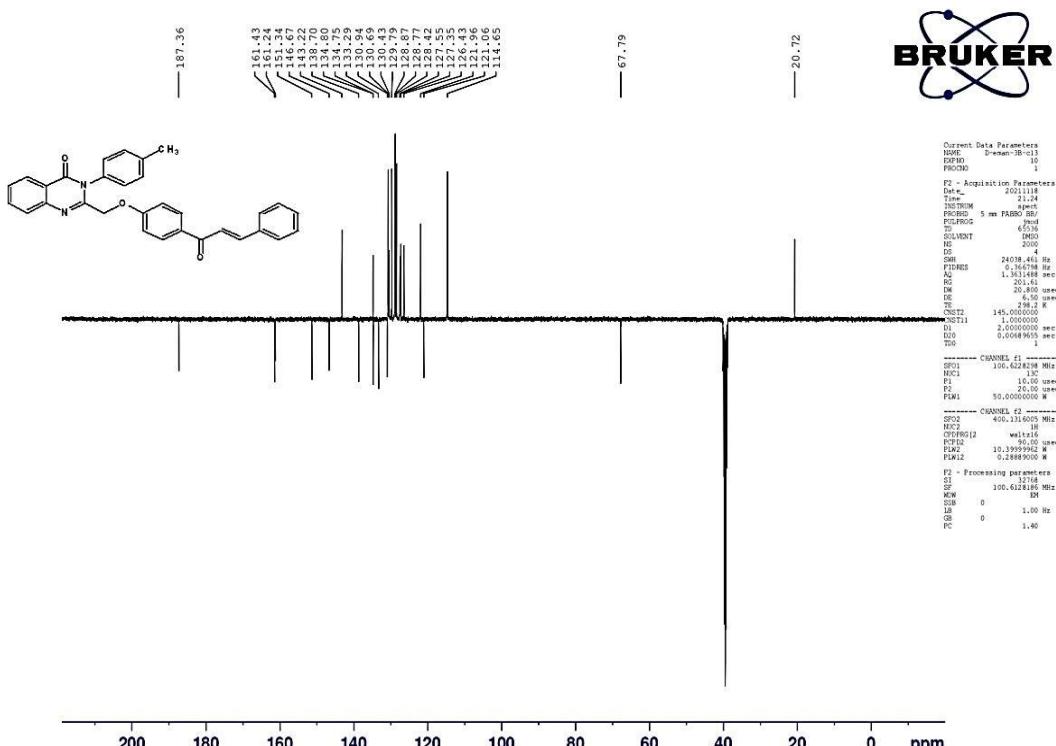
Mass Table
Line#:1 R.Time:5.6(Scan#:675)
MassPeaks:202
RawMode:Single 5.6(675) BasePeak:57(21045)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	1879	8.93	4	53.05	2419	11.49	7	56.10	6863	32.61
2	51.00	2689	12.78	5	54.05	4439	21.09	8	57.05	21045	100.00
3	52.00	862	4.10	6	55.05	20436	97.11	9	58.05	1702	8.09

*(E)-2-((4-Cinnamoylphenoxy)methyl)-3-(*p*-tolyl)quinazolin-4(3*H*)-one (32).*



D-eman-3B-c13



21-Jan-07 13:40:22

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DI Analysis
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Sample Information

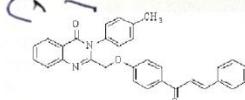
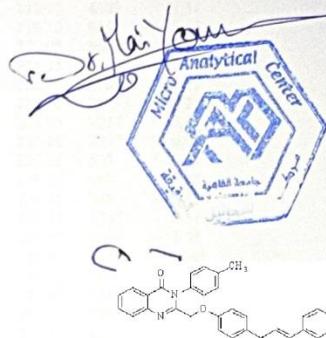
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 01:31:51
Sample Name : 3B
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Datas\Project1\3B.QGD
Org Data File : C:\GCMSSolution\Datas\Project1\3B.QGD
Method File : C:\GCMSSolution\Datas\Project1\High Temperature Op
Org Method File : C:\GCMSSolution\Datas\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1_\default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 01:38:57

Method

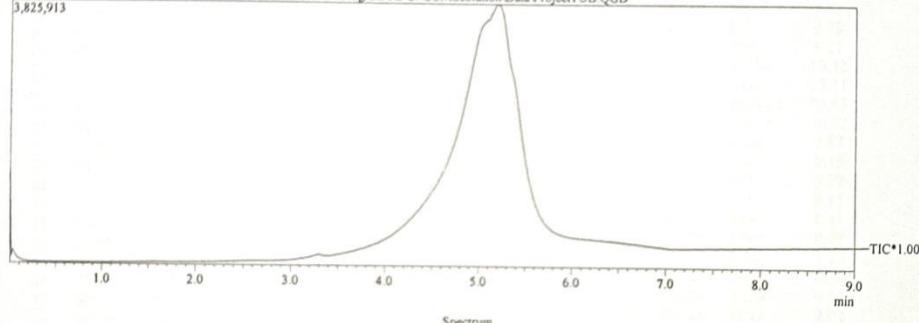
— Analytical Line 1 —
IonSourceTemp : 250.00 °C
[MS Table]
—Group 1 - Event 1—
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSSolution\Datas\Project1\3B.QGD

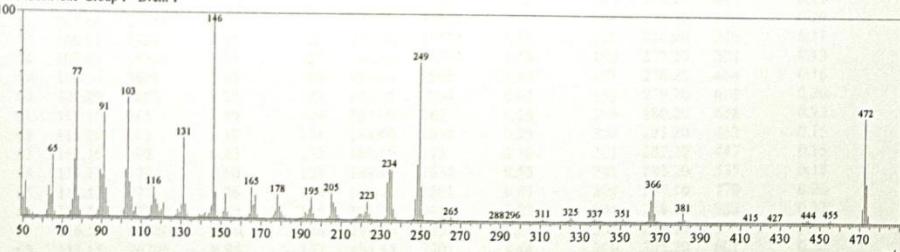


Chromatogram 3B C:\GCMSSolution\Datas\Project1\3B.QGD



Spectrum

Line# 1 R.Time: 5.2(Scan#:626)
MassPeaks:279
RawMode:Single 5.2(626) BasePeak:146(299257)
BG Mode:None Group 1 - Event 1

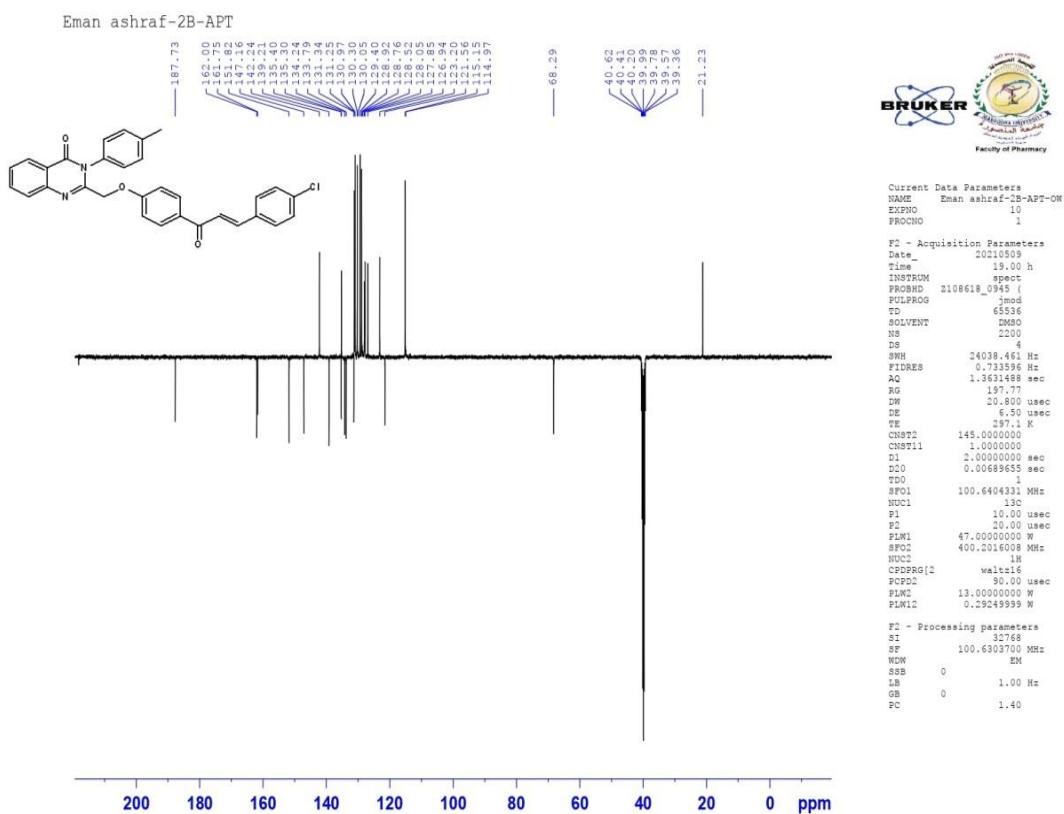
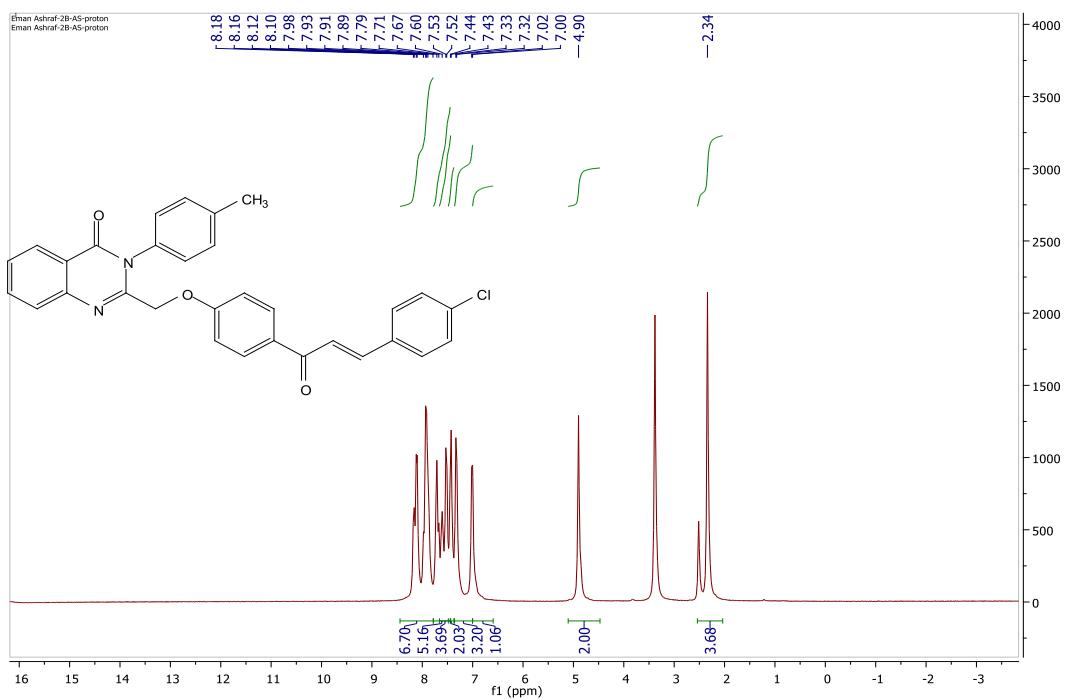


Mass Table
Line#1 R.Time:5.2(Scan#:626)
MassPeaks:279

RawMode:Single 5.2(626) BasePeak:146(299257)
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	50.05	26963	9.01	4	53.05	8608	2.88	7	56.05	916	0.31
2	51.05	51134	17.09	5	54.05	1472	0.49	8	57.10	1906	0.64
3	52.05	11959	4.00	6	55.05	5146	1.72	9	58.05	395	0.13

(E)-2-((4-(3-(4-Chlorophenyl)acryloyl)phenoxy)methyl)-3-(*p*-tolyl)quinazolin-4(3*H*)-one (33).



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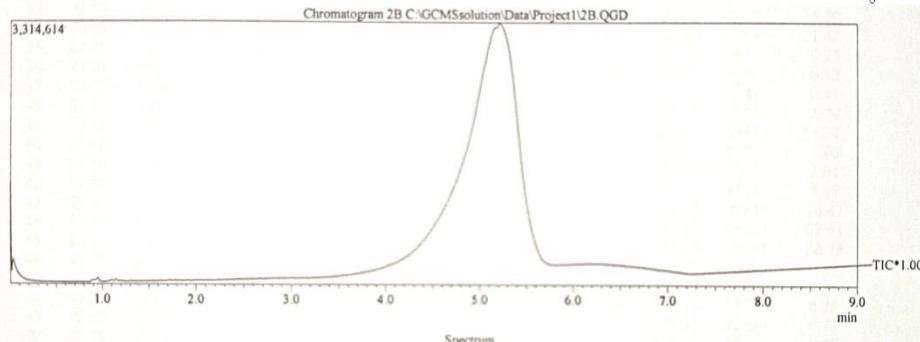
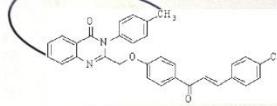
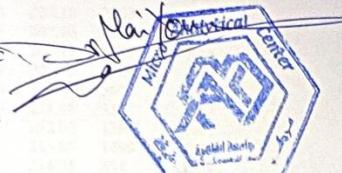
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 01:18:19
Sample Name : 2B
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Datap\Project1\2B.QGD
Org Data File : C:\GCMSSolution\Datap\Project1\2B.QGD
Method File : C:\GCMSSolution\Datap\Project1\High Temperature Op
Org Method File : C:\GCMSSolution\Datap\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1_default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 01:25:36

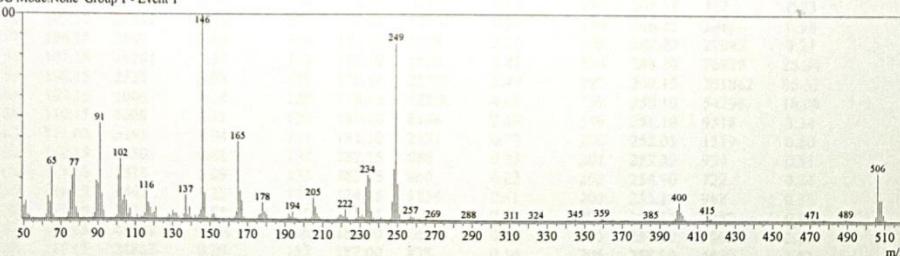
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
Group 1 - Event 1 -
Start Time : 0:00min
End Time : 10:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSSolution\Datap\Project1\2B.QGD



Line#:1 R.Time:5.2(Scan#:622)
MassPeaks:318
RawMode:Single 5.2(622) BasePeak:146(303353)
BG Mode:None Group 1 - Event 1

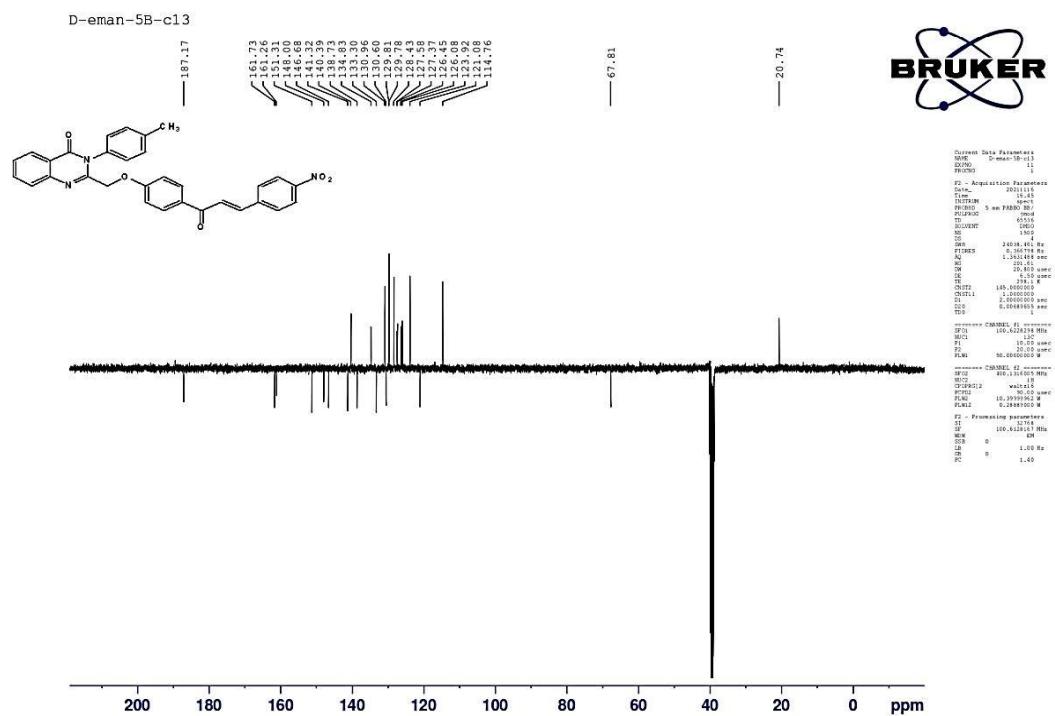
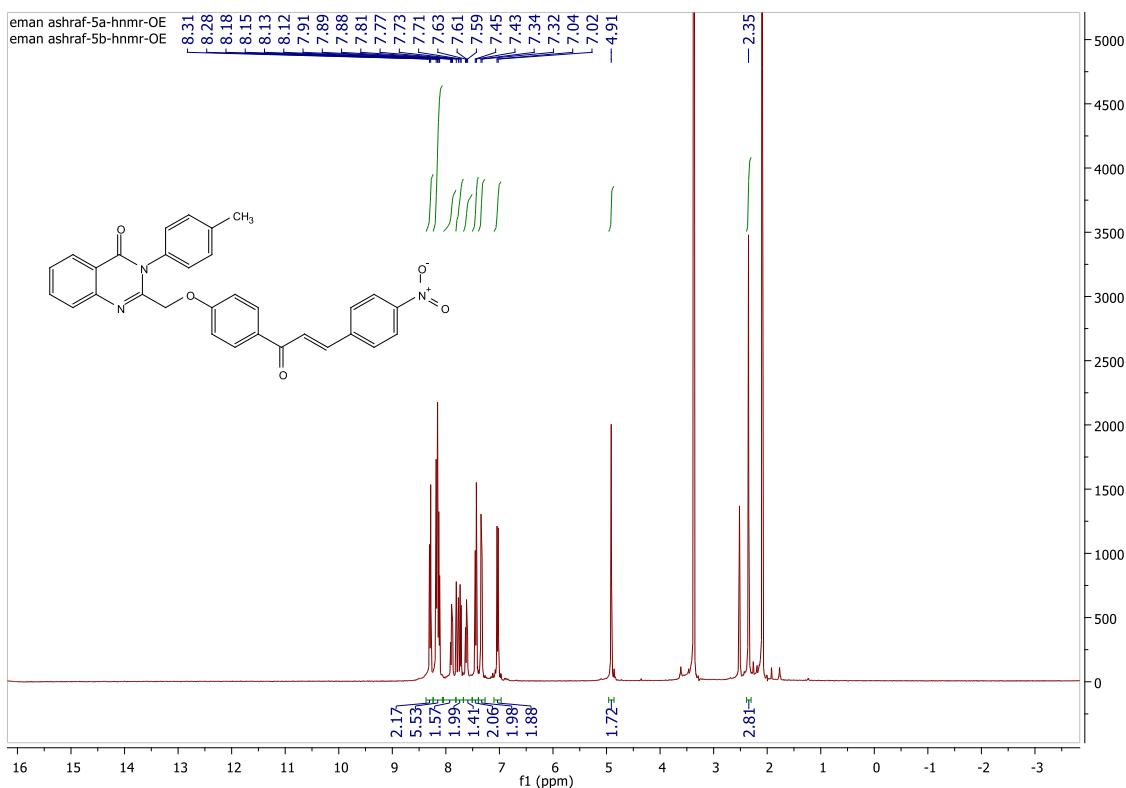


Mass Table

Line#:1 R.Time:5.2(Scan#:622)
MassPeaks:318
RawMode:Single 5.2(622) BasePeak:146(303353)
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	20220	6.67	4	53.05	5500	1.81	7	56.10	799	0.26
2	51.00	27562	9.09	5	54.10	1177	0.39	8	57.05	1611	0.53
3	52.05	7366	2.43	6	55.05	2701	0.89	9	58.05	346	0.11

*(E)-2-((4-(3-(4-Nitrophenyl)acryloyl)phenoxy)methyl)-3-(*p*-tolyl)quinazolin-4(3*H*)-one* (34).



21-Jan-07 14:12:40

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DI Analysis
Shimadzu QP-2010 Plus

Sample Information

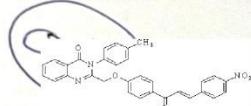
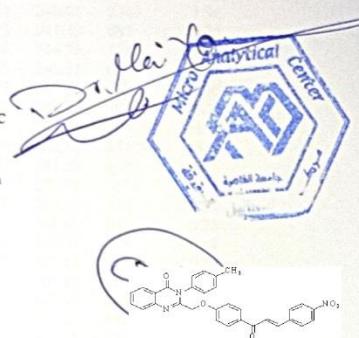
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 02:02:13
Sample Name : 5B
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Project1\5B.QGD
Org Data File : C:\GCMSSolution\Project1\5B.QGD
Method File : C:\GCMSSolution\Project1\High Temperature Op
Org Method File : C:\GCMSSolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1_default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 02:10:43

Method

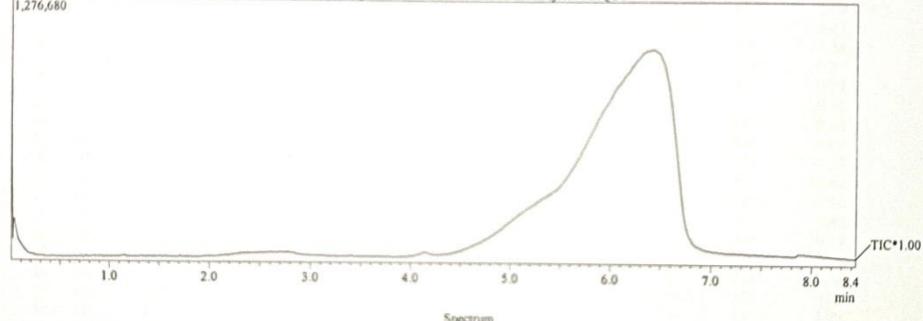
— Analytical Line 1 —
IonSourceTemp : 250.00 °C
[MS Table]
— Group 1 - Event 1 —
Start Time : 0:00min
End Time : 10:00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSSolution\Project1\5B.QGD

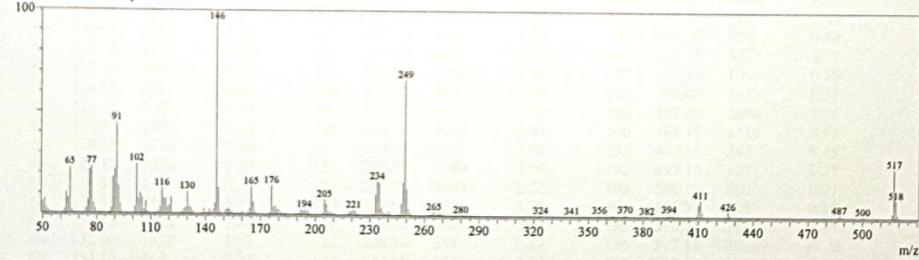


Chromatogram 5B C:\GCMSSolution\Project1\5B.QGD



Spectrum

Line#1 R.Time:6.5(Scan#:777)
MassPeaks:199
RawMode:Single 6.5(777) BasePeak:146(120556)
BG Mode:None Group 1 - Event 1



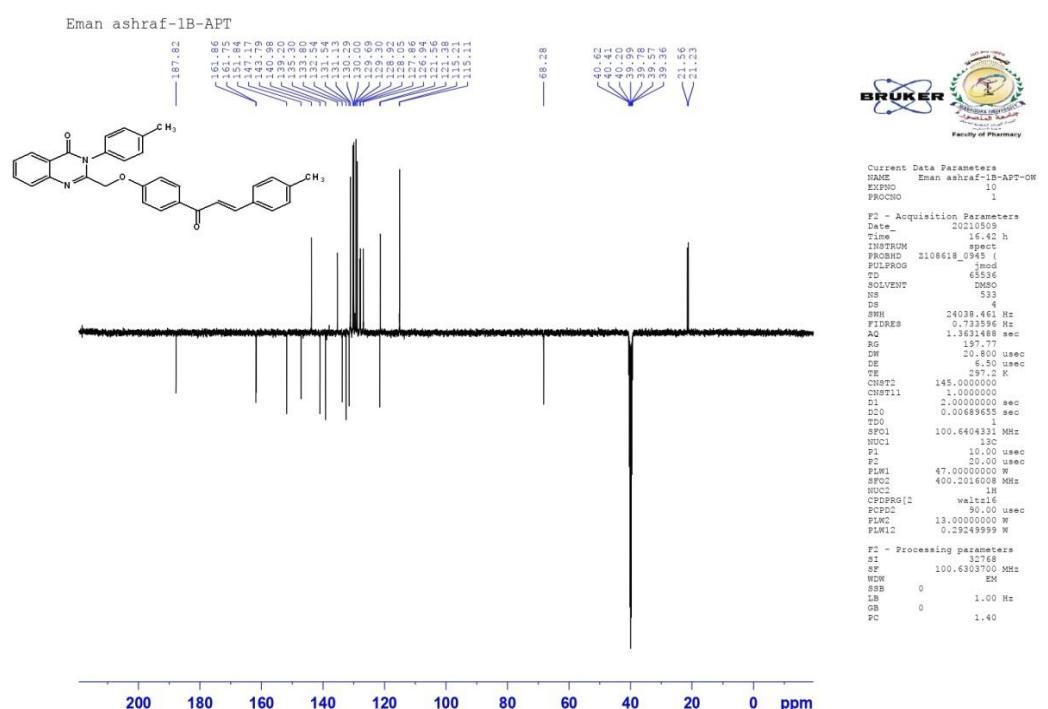
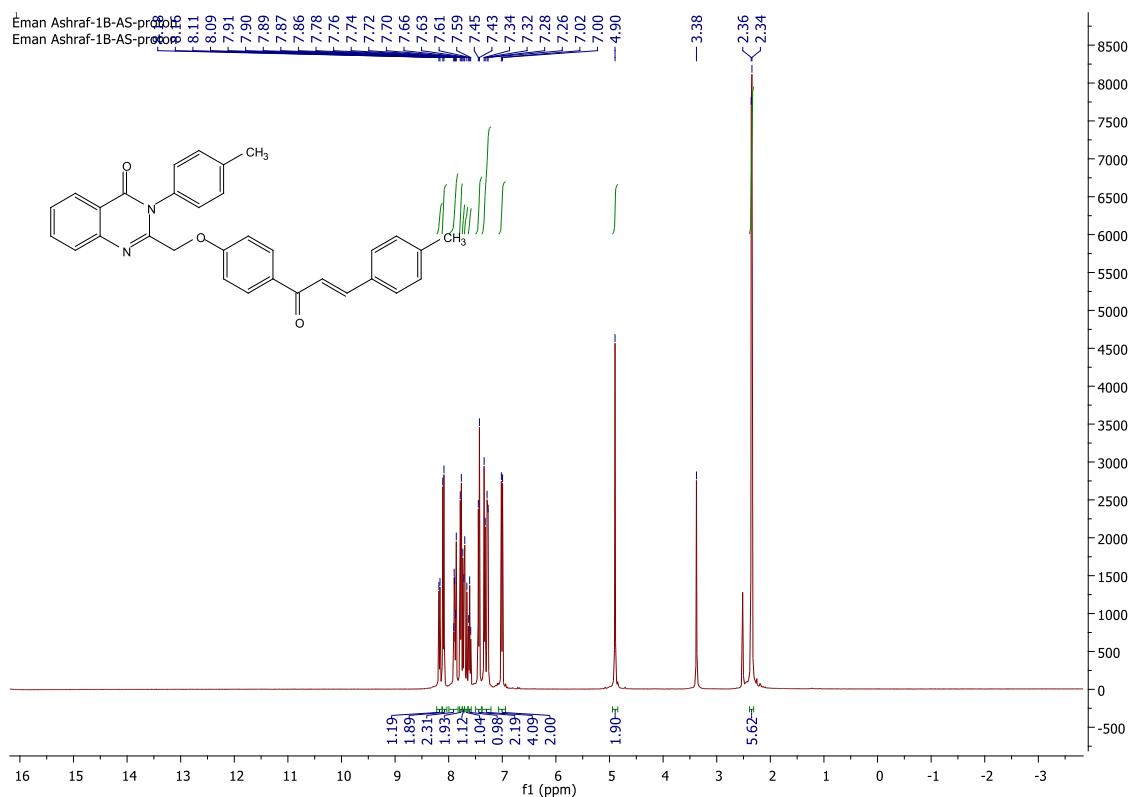
Mass Table

Line#1 R.Time:6.5(Scan#:777)
MassPeaks:199
RawMode:Single 6.5(777) BasePeak:146(120556)

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	7015	5.82	4	53.05	2162	1.79	7	57.05	595	0.49
2	51.00	8663	7.19	5	54.05	534	0.44	8	61.15	395	0.33
3	52.05	3510	2.91	6	55.00	1039	0.86	9	62.15	2519	2.09

(E)-3-(*p*-Tolyl)-2-((4-(3-(*p*-tolyl)acryloyl)phenoxy)methyl)quinazolin-4(3*H*)-one (35).



21-Jan-07 13:12:43

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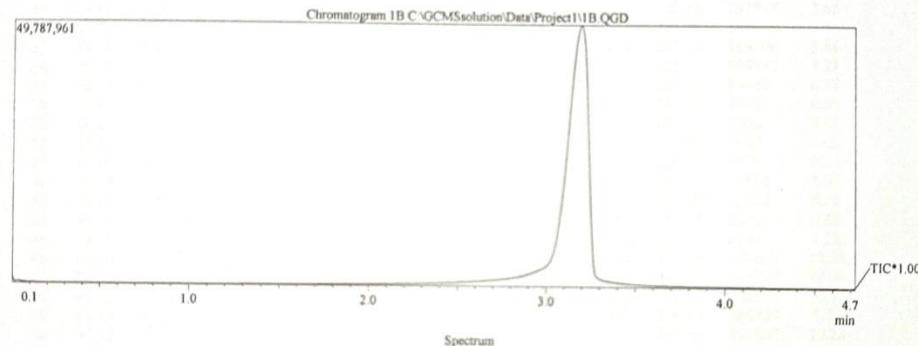
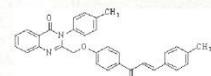
DT Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 01:06:30
Sample Name : 1B
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Dataproject1\1B.QGD
Org Data File : C:\GCMSSolution\Dataproject1\1B.QGD
Method File : C:\GCMSSolution\Dataproject1\High Temperature Op
Org Method File : C:\GCMSSolution\Dataproject1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1\default.qgt
\$EndIf%Modified by : Dr. Mai Younis
Modified : 21/01/2007 01:11:16

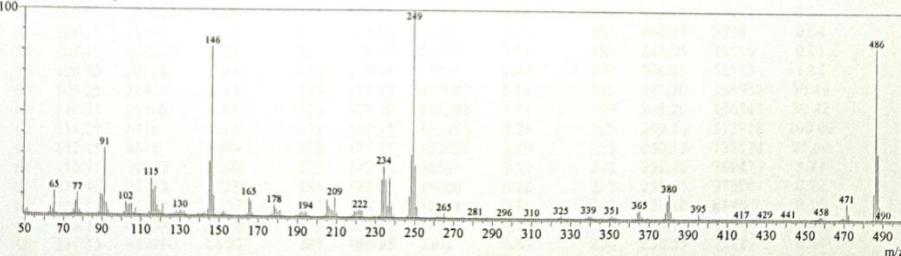
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
Group 1 - Event 1-
Start Time : 0:00min
End Time : 10:00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSSolution\Dataproject1\1B.QGD



Line#:1 R.Time:3.2(Scan#:384)
MassPeaks:441
RawMode:Single 3.2(384) BasePeak:249(5139186)
BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.2(Scan#:384)

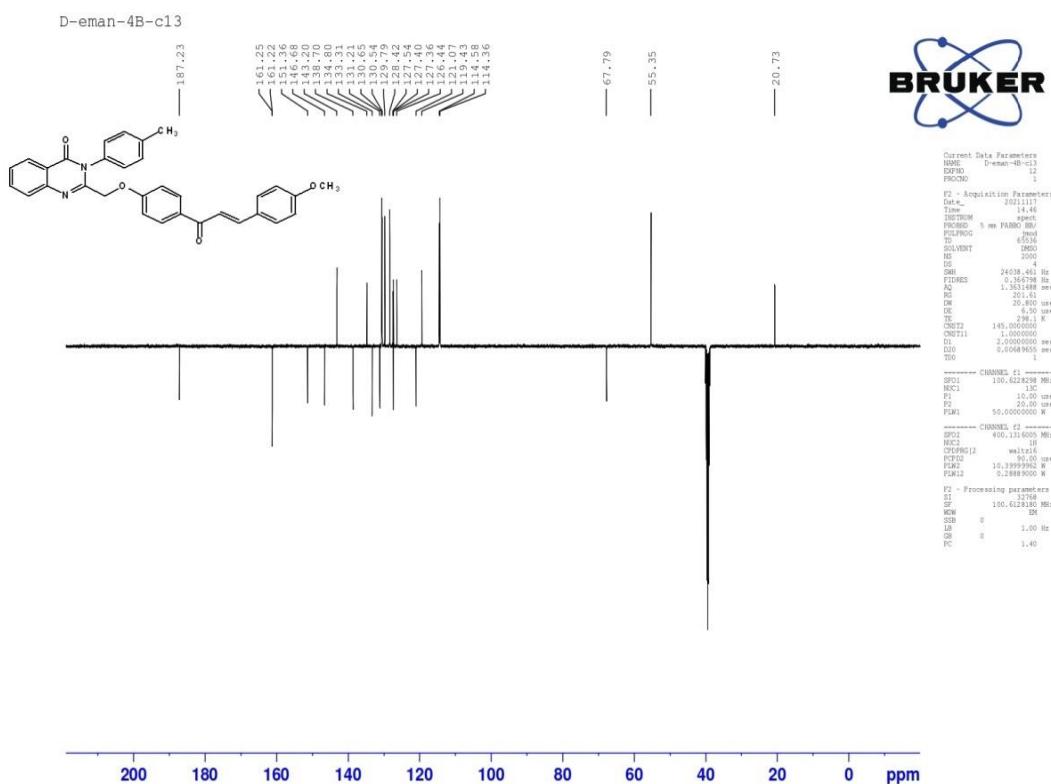
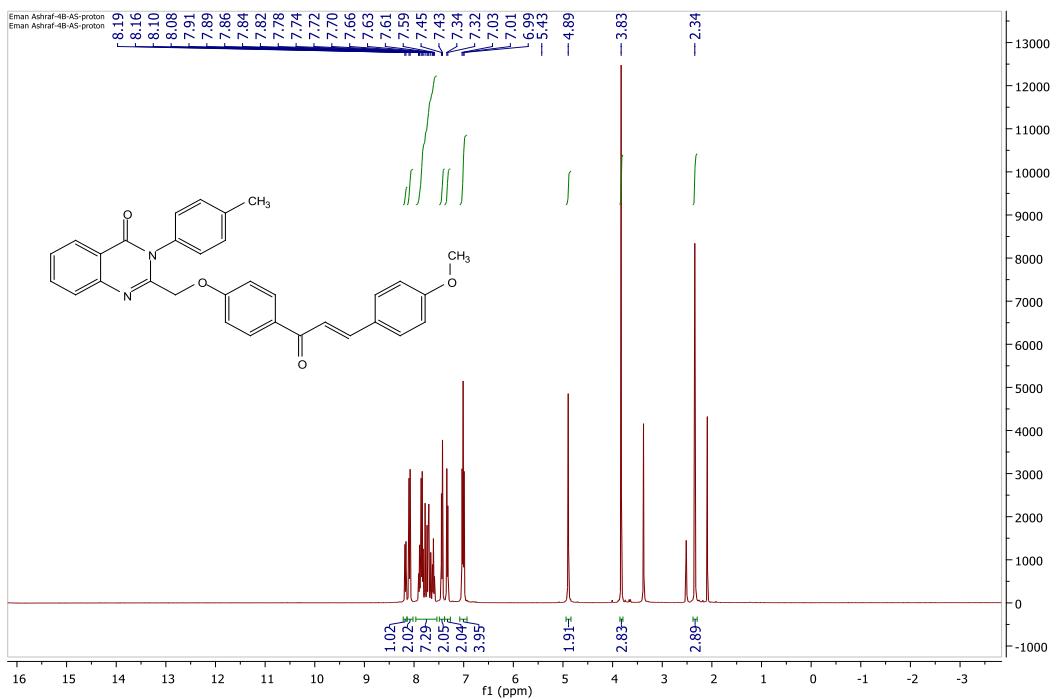
MassPeaks:441

RawMode:Single 3.2(384) BasePeak:249(5139186)

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	50.05	99629	1.94	4	53.05	44022	0.86	7	56.10	5001	0.10
2	51.05	151574	2.95	5	54.05	7639	0.15	8	57.10	11057	0.22
3	52.05	43799	0.85	6	55.05	29070	0.57	9	58.05	2922	0.06

(E)-2-((4-(3-(4-Methoxyphenyl)acryloyl)phenoxy)methyl)-3-(*p*-tolyl)quinazolin-4(3*H*)-one (36).



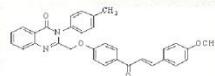
21-Jan-07 13:57:09

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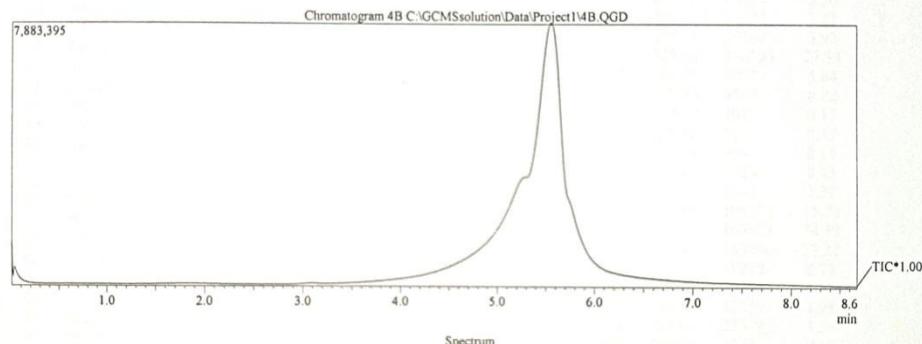
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 01:46:31
Sample Name : 4B
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Dat\Project1\4B.QGD
Org Data File : C:\GCMSsolution\Dat\Project1\4B.QGD
Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Dat\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qgt
\$End\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 01:55:15

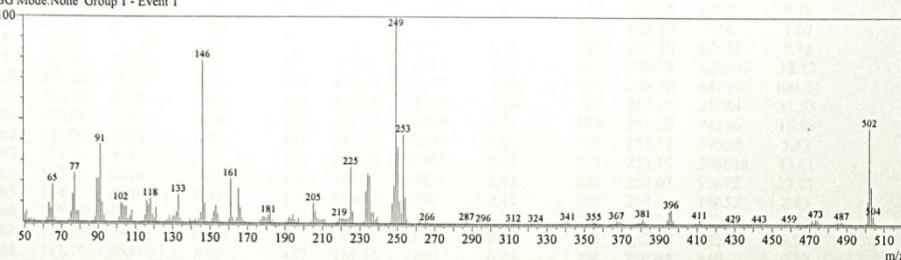
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
Group 1 - Event 1-
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSsolution\Dat\Project1\4B.QGD



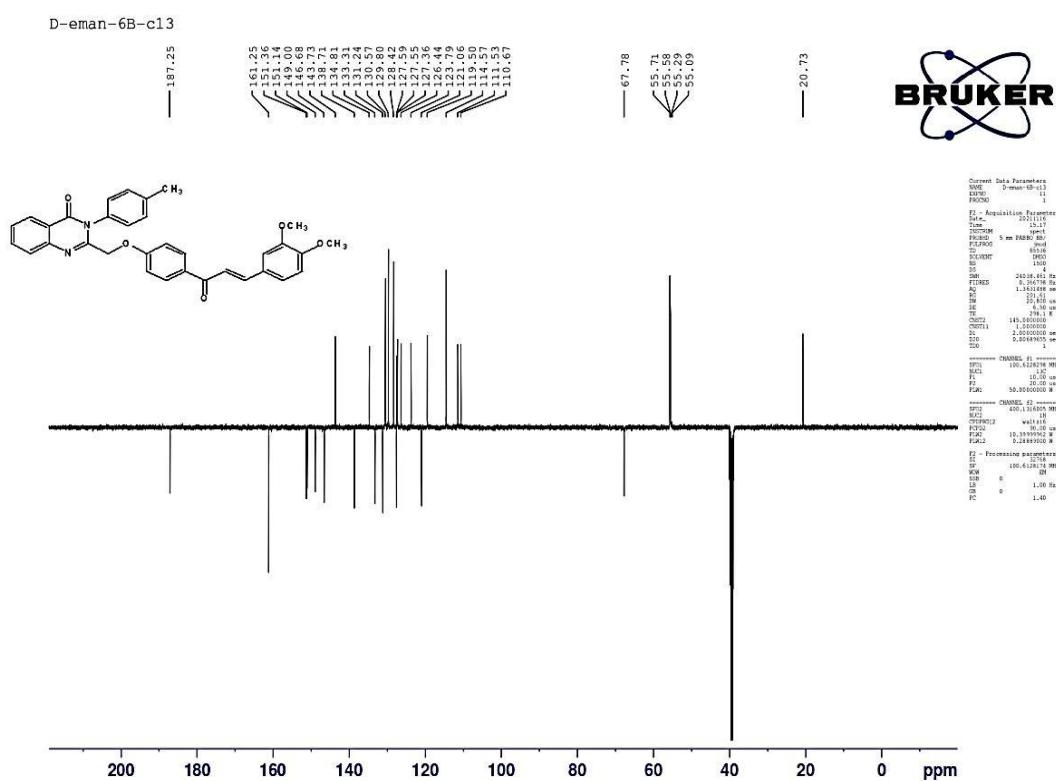
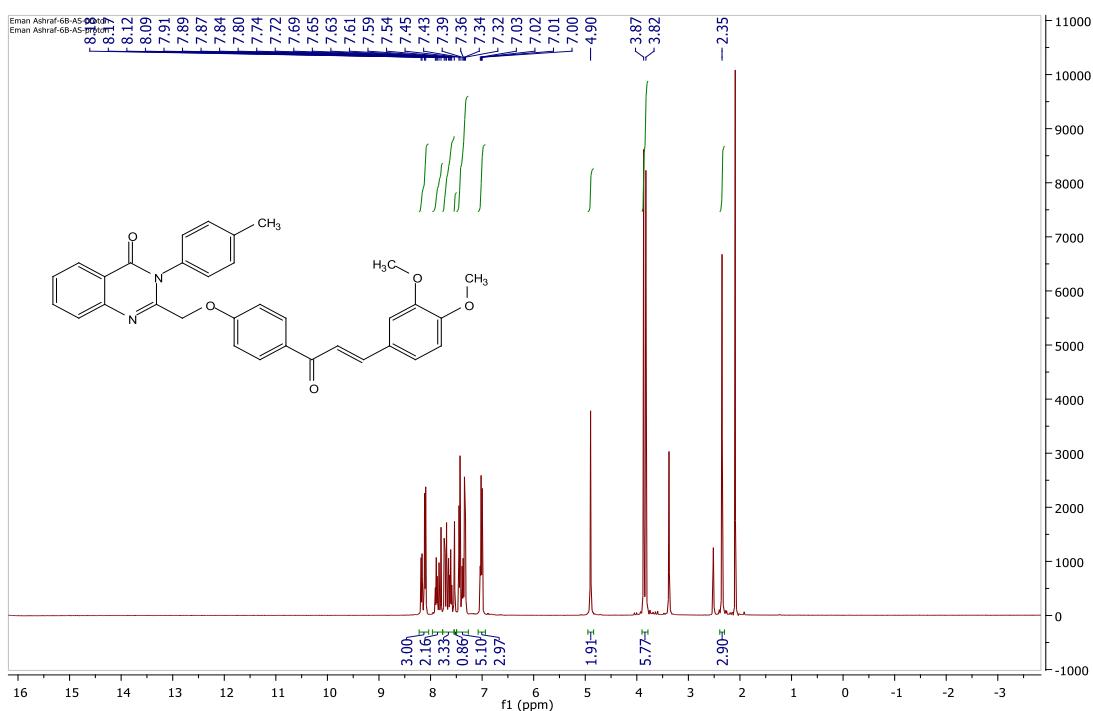
Line#1 R.Time:5.5(Scan#:665)
MassPeaks:363
RawMode:Single 5.5(665) BasePeak:249(685198)
BG Mode:None Group 1 - Event 1



Mass Table

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	27503	4.01	4	53.05	11994	1.75	7	56.05	1622	0.24
2	51.00	37098	5.41	5	54.05	2334	0.34	8	57.05	2558	0.37
3	52.05	11223	1.64	6	55.00	9356	1.37	9	58.05	571	0.08

(E)-2-((4-(3,4-Dimethoxyphenyl)acryloyl)phenoxy)methyl)-3-(*p*-tolyl)quin-azolin-4(3*H*)-one (37).



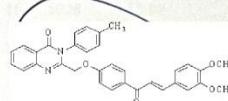
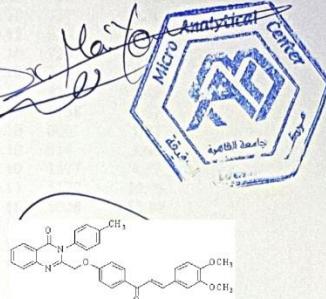
21-Jan-07 14:26:14

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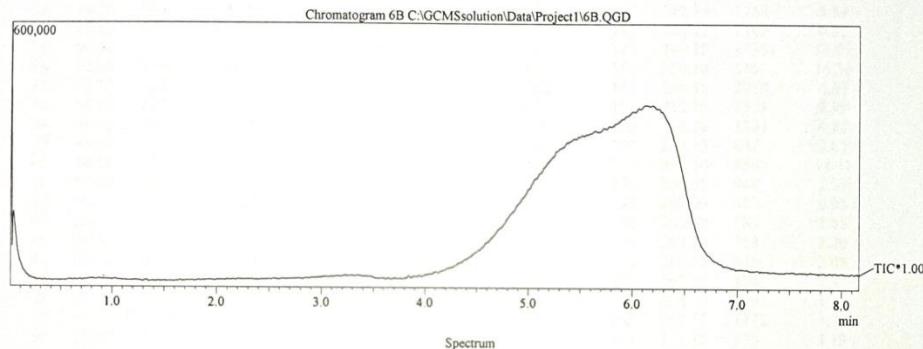
DT Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 02:16:59
Sample Name : 6B
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Dataproject1\6B.QGD
Org Data File : C:\GCMSSolution\Dataproject1\6B.QGD
Method File : C:\GCMSSolution\Dataproject1\High Temperature Op
Org Method File : C:\GCMSSolution\Dataproject1\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1_default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 02:25:13

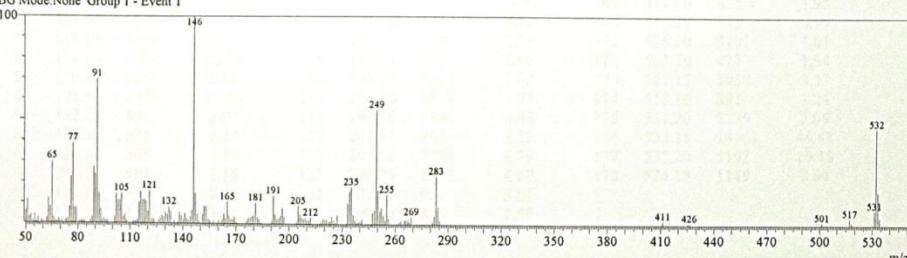
Method
Analytical Line 1
IonSourceTemp : 250.00 °C
[MS Table]
—Group 1 - Event 1—
Start Time : 0:00min
End Time : 10:00min
ACQ Mode : Scan
Event Time : 0:50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00
Electron Voltage : 70 eV
Ionization Mode : EI



C:\GCMSSolution\Dataproject1\6B.QGD



Line#:1 R.Time:5.8(Scan#:702)
MassPeaks:178
RawMode:Single 5.8(702) BasePeak:146(31542)
BG Mode:None Group 1 - Event 1

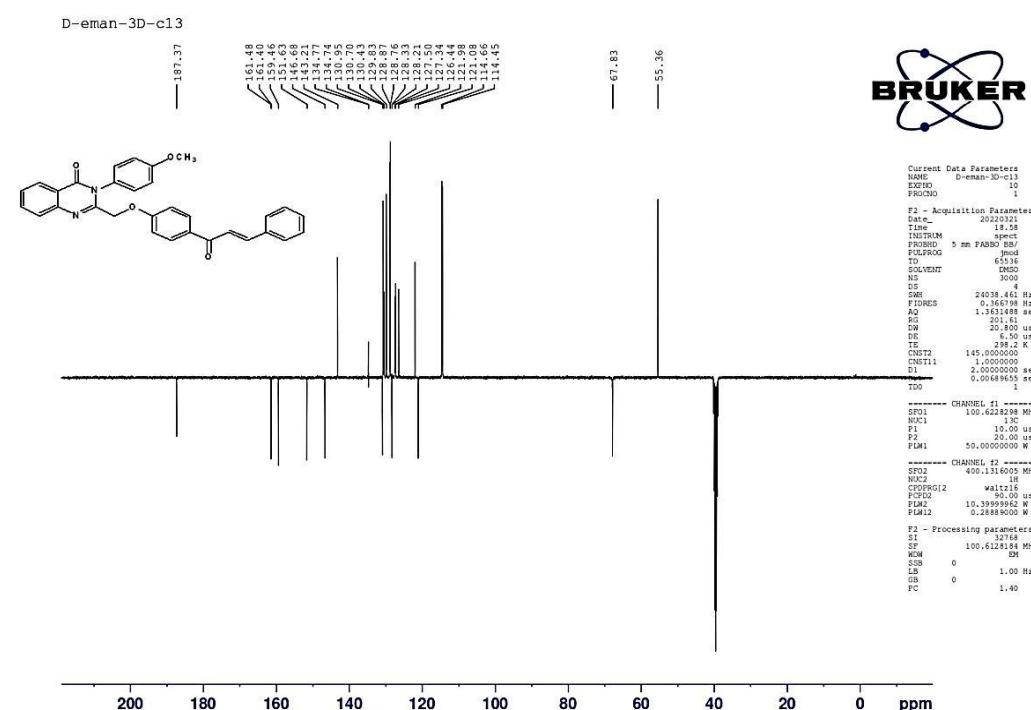
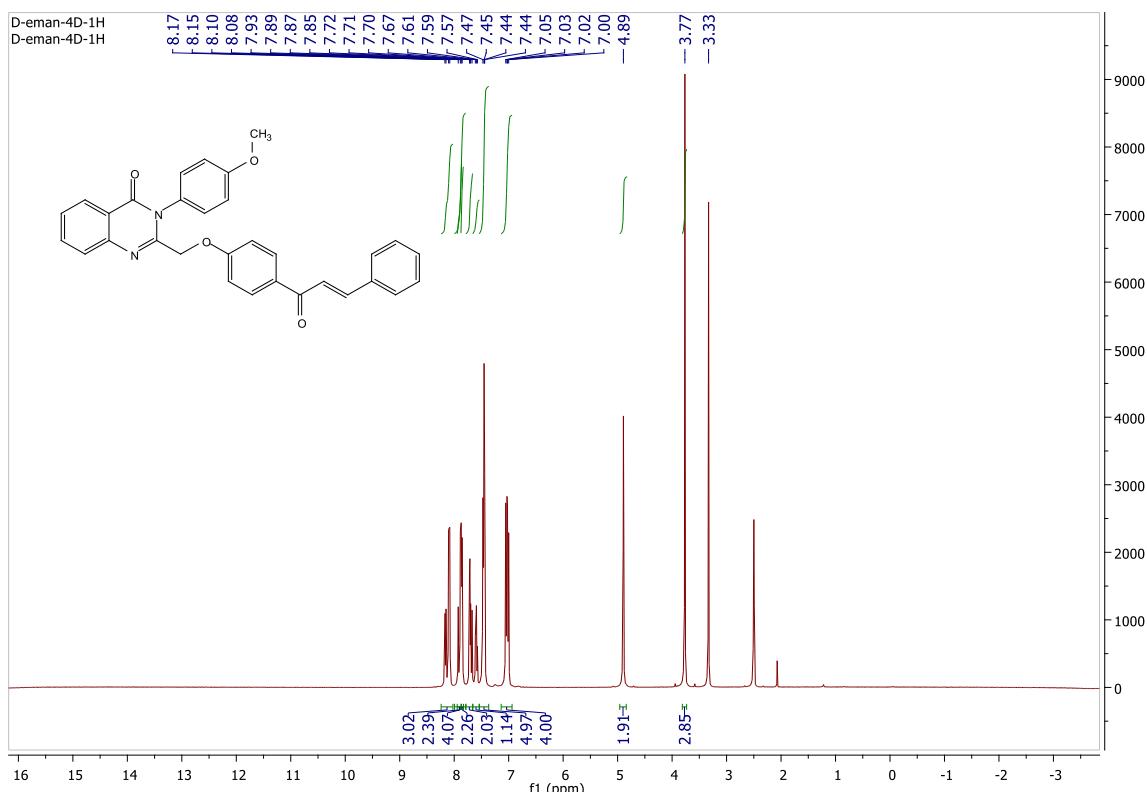


Mass Table

Line#:1 R.Time:5.8(Scan#:702)
MassPeaks:178
RawMode:Single 5.8(702) BasePeak:146(31542)
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	50.05	1996	6.33	4	53.00	1231	3.90	7	56.05	393	1.25
2	51.00	3610	11.45	5	54.10	394	1.25	8	57.00	910	2.89
3	52.00	996	3.16	6	55.05	1353	4.29	9	59.05	488	1.55

(E)-2-((4-Cinnamoylphenoxy)methyl)-3-(4-methoxyphenyl)quinazolin-4(3H)-one (38).



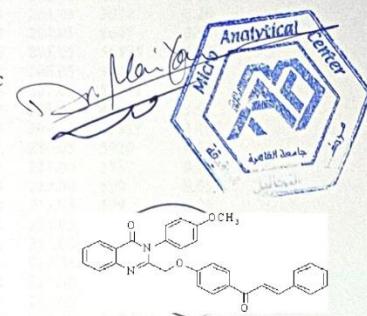
21-Jan-07 16:29:54

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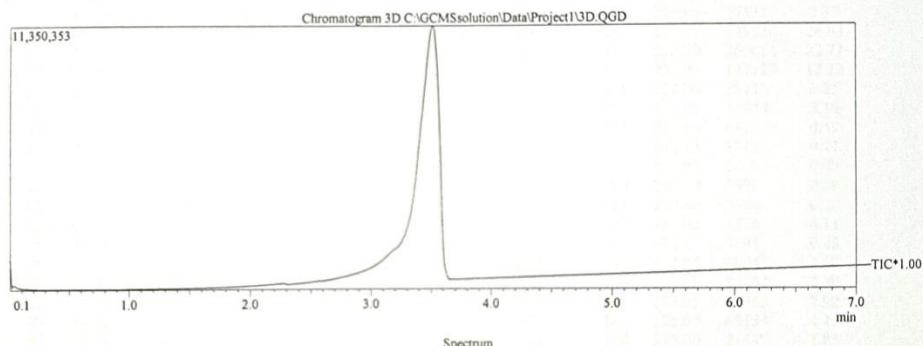
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 04:25:25
Sample Name : 3D
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Project\3D.QGD
Org Data File : C:\GCMSSolution\Project\3D.QGD
Method File : C:\GCMSSolution\Project\High Temperature Op
Org Method File : C:\GCMSSolution\Project\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1_default.qgt
SEnd/SModified by : Dr. Mai Younis
Modified : 21/01/2007 04:29:07

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

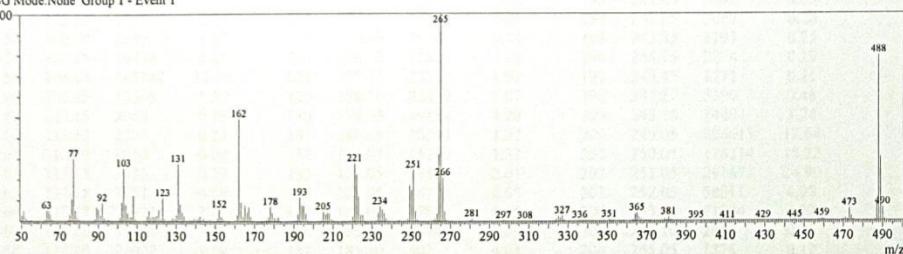


C:\GCMSSolution\Project\3D.QGD



Spectrum

Line#:1 R.Time:3.5(Scan#:423)
MassPeaks:376
RawMode:Single 3.5(423) BasePeak:265(1171271)
BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.5(Scan#:423)

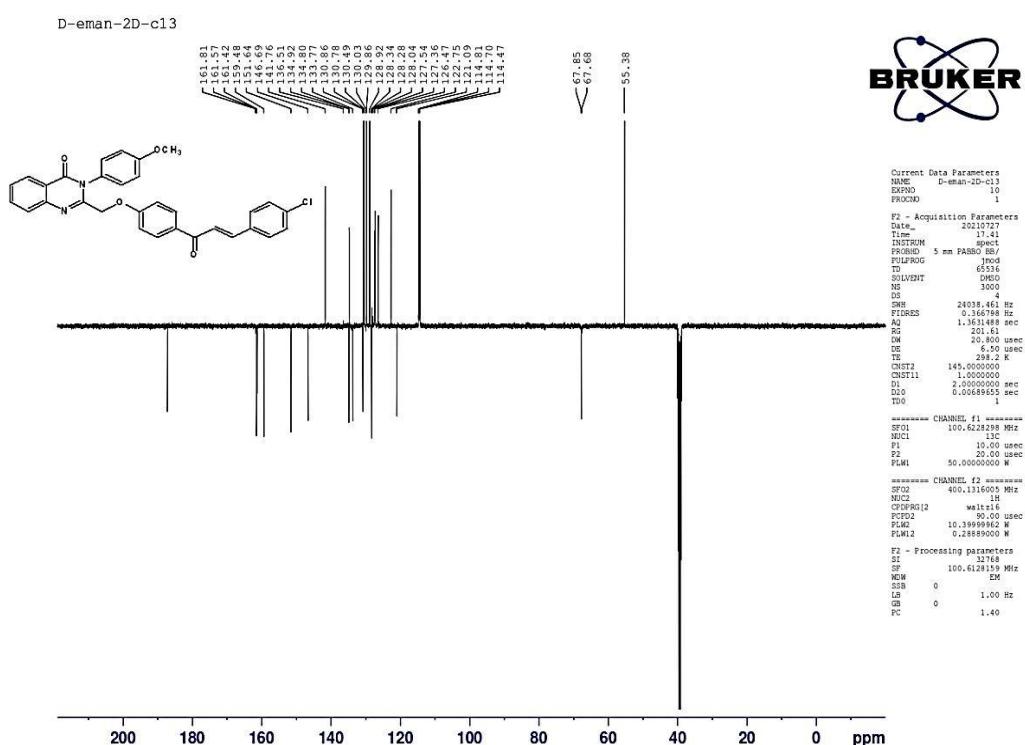
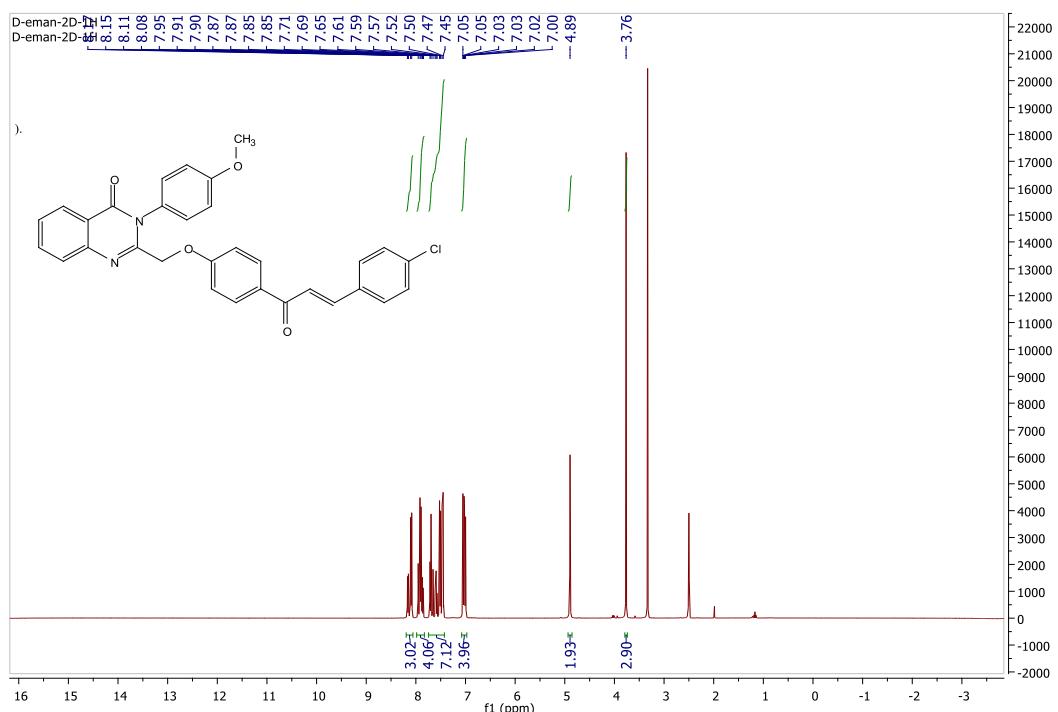
MassPeaks:376

RawMode:Single 3.5(423) BasePeak:265(1171271)

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	50.05	32494	2.77	4	53.00	10962	0.94	7	56.00	1378	0.12
2	51.00	60498	5.17	5	54.05	2500	0.21	8	57.05	2777	0.24
3	52.05	17808	1.52	6	55.00	9049	0.77	9	58.05	666	0.06

(E)-2-((4-(4-Chlorophenyl)acryloyl)phenoxy)methyl-3-(4-methoxyphenyl) quinazolin-4(3H)-one
(39).



21-Jan-07 16:24:17

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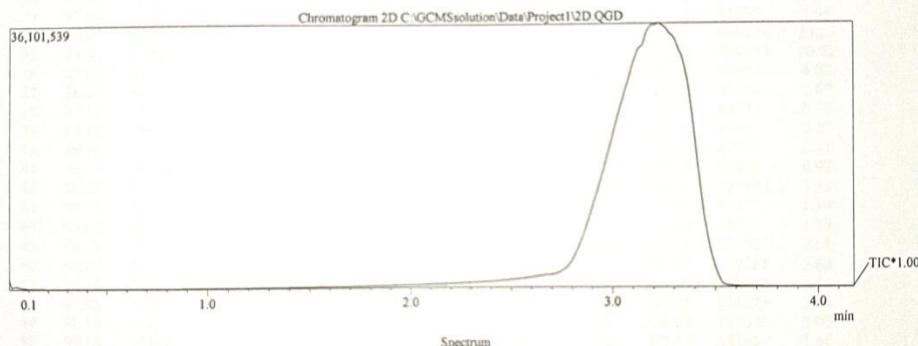
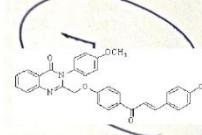
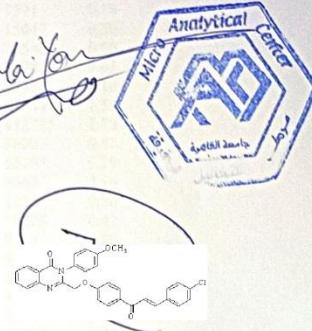
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 04:19:18
Sample Name : 2D
Sample ID :
Customer Name : Dr. Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSSolution\Project\2D.QGD
Org Data File : C:\GCMSSolution\Project\2D.QGD
Method File : C:\GCMSSolution\Project\High Temperature Op
Org Method File : C:\GCMSSolution\Project\High Temperature Op
Report File :
Tuning File : C:\GCMSSolution\System\Tune1\default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 04:23:31

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

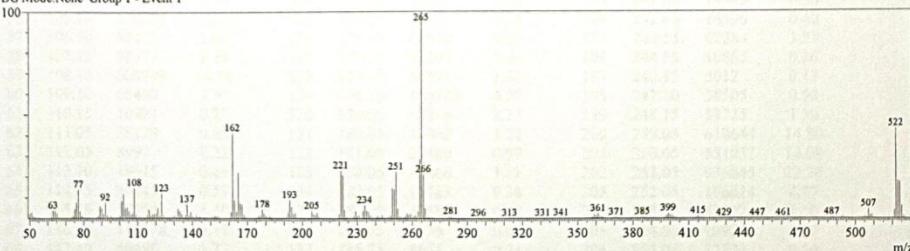
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSSolution\Project\2D.QGD



Spectrum

Line#:1 R.Time:3.2(Scan#:379)
MassPeaks:465
RawMode:Single 3.2(379) BasePeak:265(4125578)
BG Mode:None Group 1 - Event 1

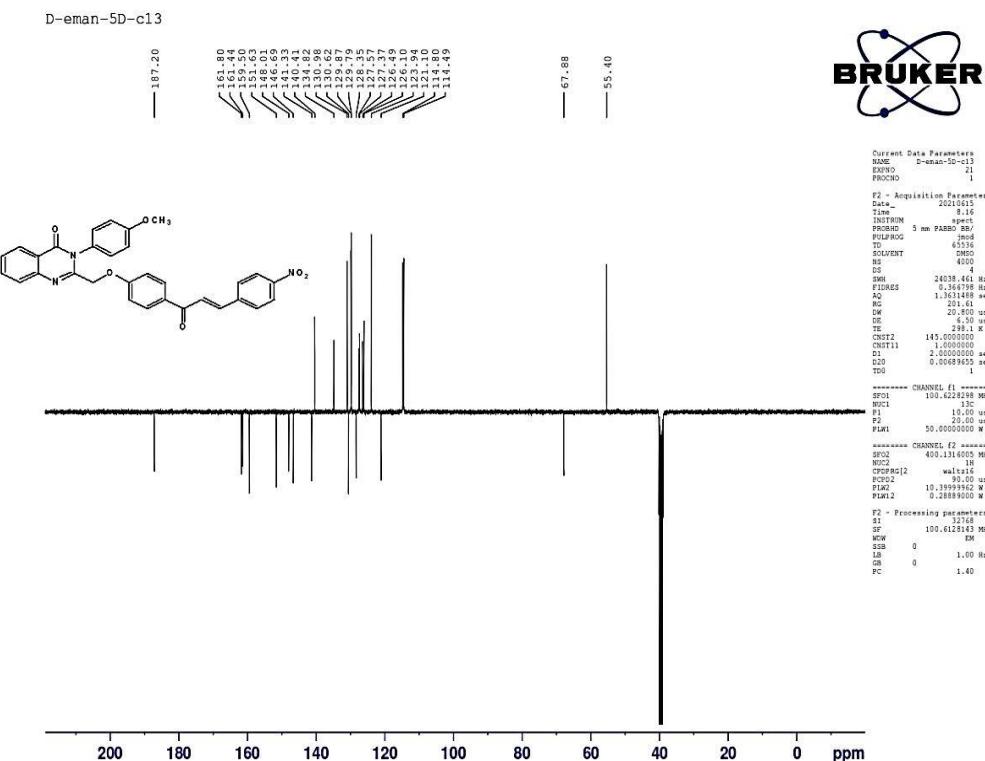
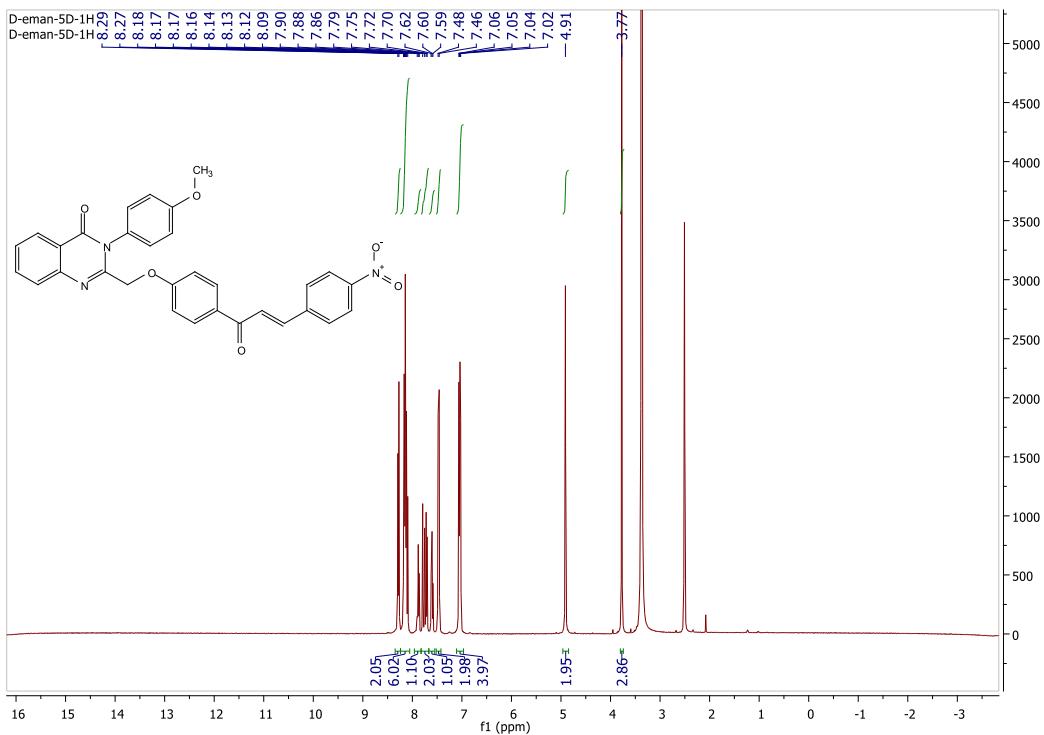


Mass Table
Line#:1 R.Time:3.2(Scan#:379)
MassPeaks:465
RawMode:Single 3.2(379) BasePeak:265(4125578)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In.	Rel. Int.	#	m/z	Abs. In.	Rel. Int.	#	m/z	Abs. In.	Rel. Int.
1	50.05	90645	2.20	4	53.00	26644	0.65	7	56.05	4192	0.10
2	51.00	121642	2.95	5	54.05	6728	0.16	8	57.05	8185	0.20
3	52.05	40970	0.99	6	55.00	17474	0.42	9	58.05	1848	0.04

1 / 4

(E)-3-(4-Methoxyphenyl)-2-((4-(3-(4-nitrophenyl)acryloyl)phenoxy)methyl)quinazolin-4(3H)-one (40).



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**DI Analysis
Shimadzu QP-2010 Plus**

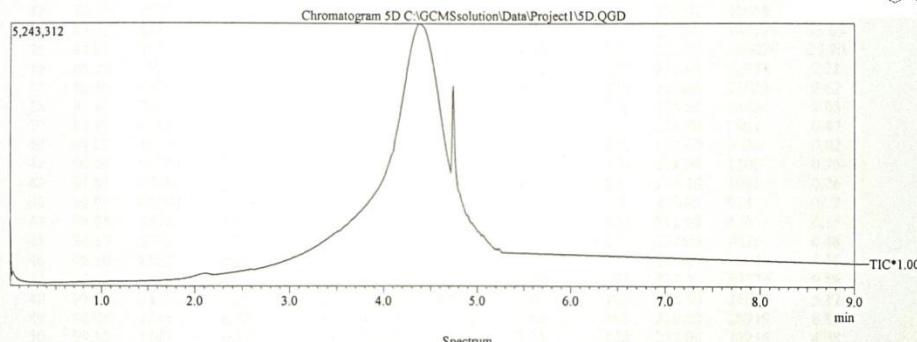
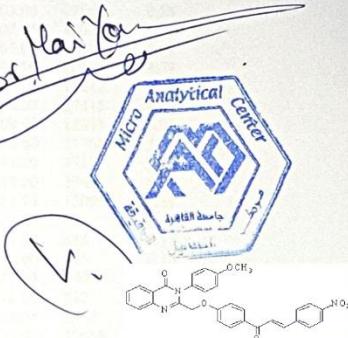
Sample Information

Analyzed by : Dr. Mai Younis
 Analyzed : 21/01/2007 04:46:27
 Sample Name : 5D
 Sample ID :
 Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
 Data File : C:\GCMSsolution\Datap\Project1\5D.QGD
 Org Data File : C:\GCMSsolution\Datap\Project1\5D.QGD
 Method File : C:\GCMSsolution\Datap\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Datap\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1\default.qrt
 \$End/\$Modified by : Dr. Mai Younis
 Modified : 21/01/2007 04:51:47

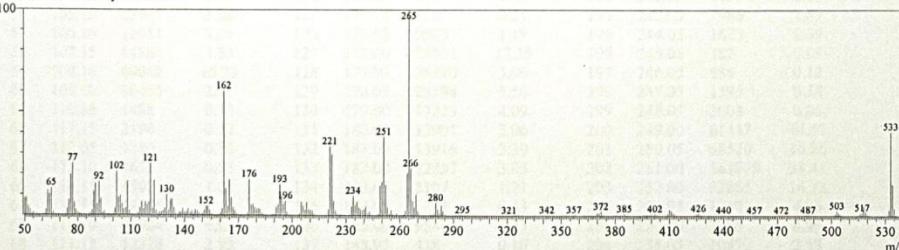
Method

— 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\Datap\Project1\5D.QGD



Line#:1 R.Time:4.4(Scan#:528)
 MassPeaks:385
 RawMode:Single 4.4(528) BasePeak:265(421468)
 BG Mode:None Group 1 - Event 1

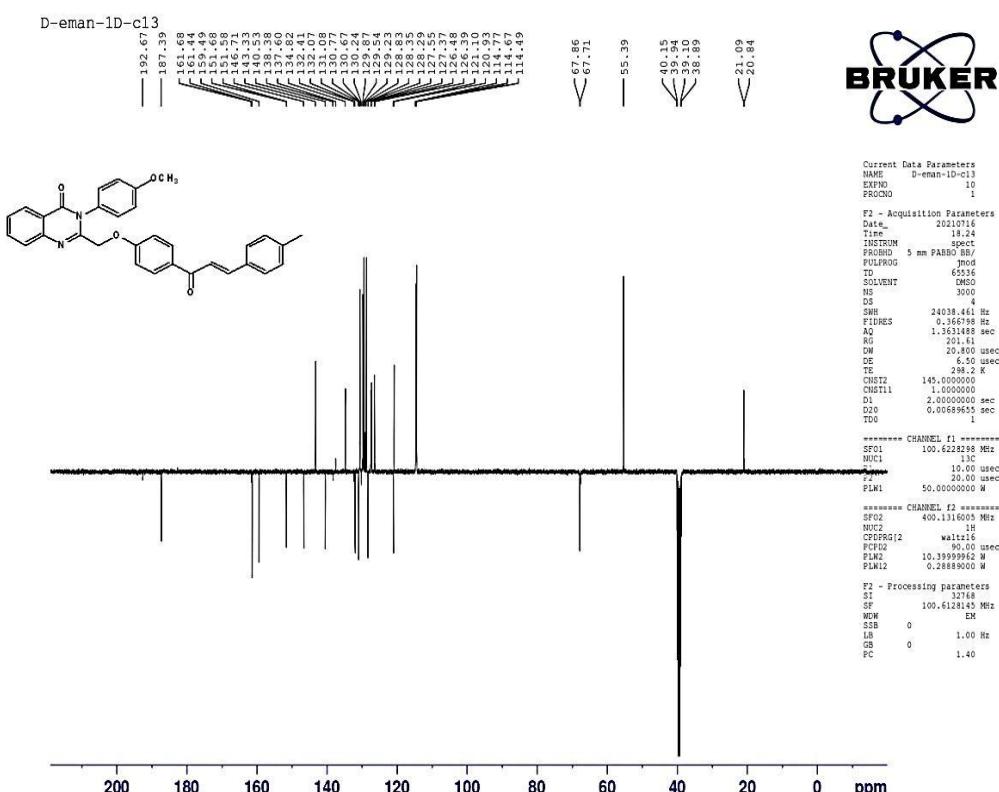
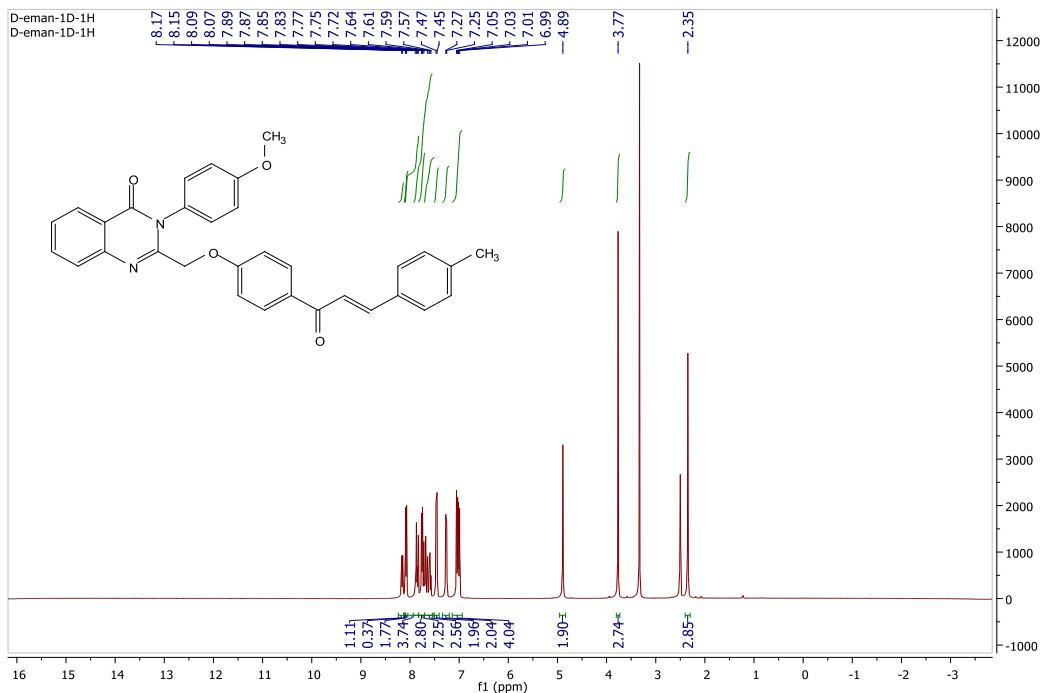


Mass Table
 Line#:1 R.Time:4.4(Scan#:528)

MassPeaks:385
 RawMode:Single 4.4(528) BasePeak:265(421468)
 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	35002	8.30	4	53.00	11956	2.84	7	56.05	1461	0.35
2	51.00	36487	8.66	5	54.05	2721	0.65	8	57.05	2465	0.58
3	52.00	17873	4.24	6	55.00	6169	1.46	9	58.05	717	0.17

*(E)-3-(4-Methoxyphenyl)-2-((4-(3-(*p*-tolyl)acryloyl)phenoxy)methyl)quinazolin-4(3*H*)-one (41).*



21-Jan-07 16:18:16

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DI Analysis
Shimadzu QP-2010 Plus

Sample Information

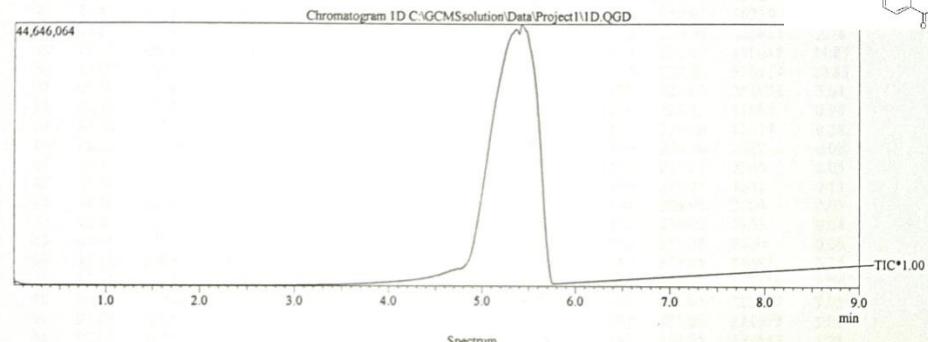
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 04:11:35
Sample Name : 1D
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project\1D.QGD
Org Data File : C:\GCMSsolution\Project\1D.QGD
Method File : C:\GCMSsolution\Project\High Temperature Op
Org Method File : C:\GCMSsolution\Project\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qrt
\$End!\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 04:17:24

Method

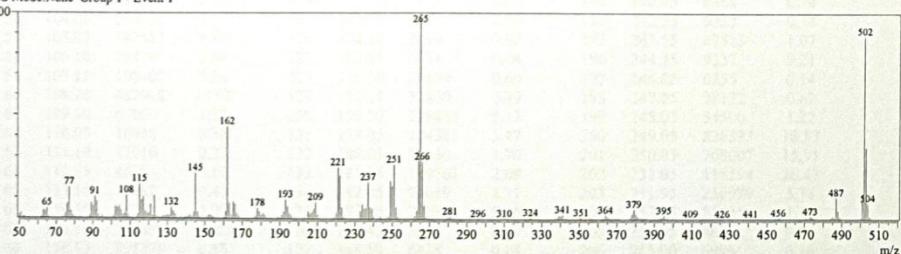
— Analytical Line 1 —
IonSourceTemp : 250.00 °C
[MS Table]
— Group 1 - Event 1 —
Start Time : 0:00min
End Time : 10:00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

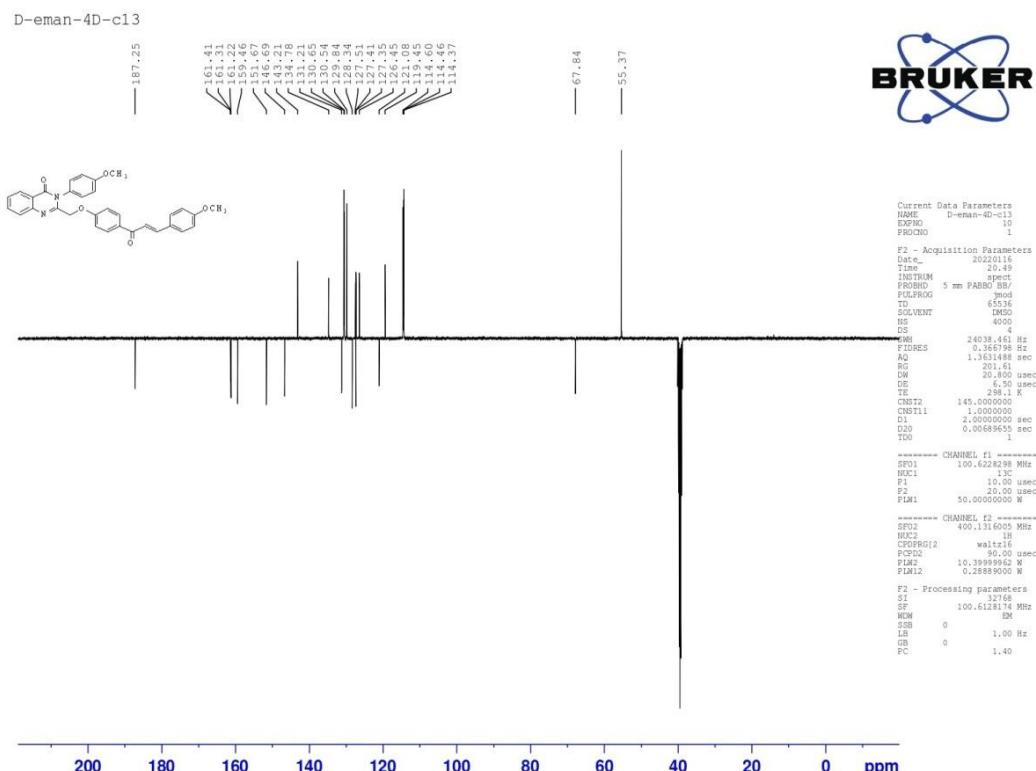
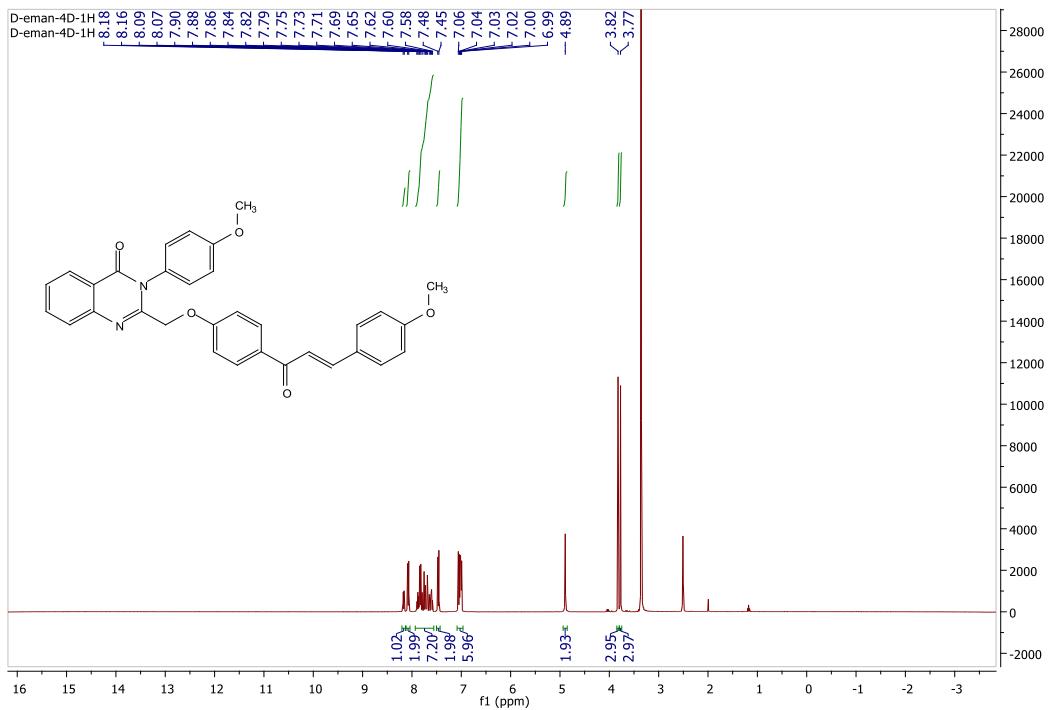
C:\GCMSsolution\Project\1D.QGD



Line#1 R.Time:5.3(Scan#:642)
MassPeaks:440
RawMode:Single 5.3(642) BasePeak:265(4449763)
BG Mode:None Group 1 - Event 1



*(E)-3-(4-Methoxyphenyl)-2-((4-(3-(4-methoxyphenyl)acryloyl)phenoxy)methyl)quinazolin-4(3*H*)-one (42).*



21-Jan-07 16:40:00

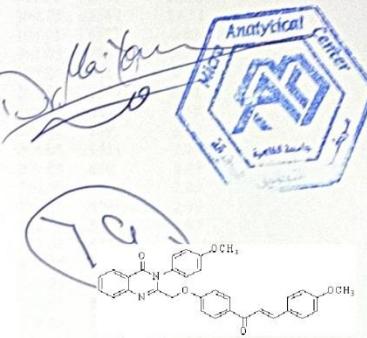
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DI Analysis
Shimadzu QP-2010 Plus

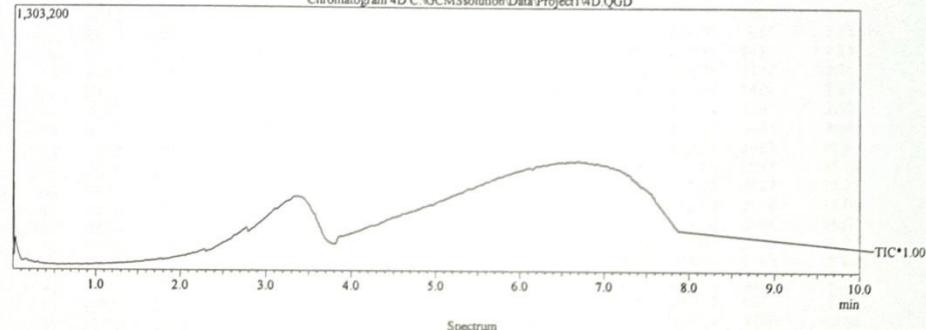
Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 04:31:06
Sample Name : 4D
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Project1\4D.QGD
Org Data File : C:\GCMSsolution\Project1\4D.QGD
Method File : C:\GCMSsolution\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\default.qgt
\$EndIf\$Modified by : Dr. Mai Younis
Modified : 21/01/2007 04:39:02

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\Project1\4D.QGD

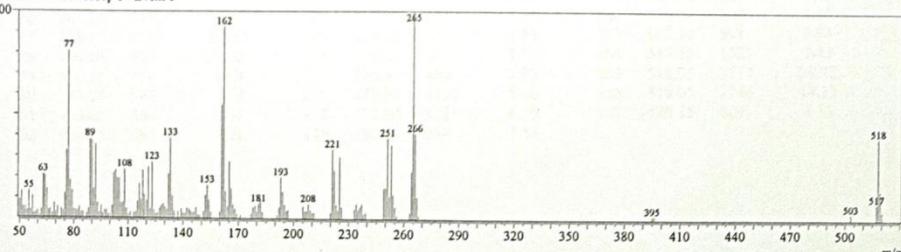


Chromatogram 4D C:\GCMSsolution\Project1\4D.QGD



Spectrum

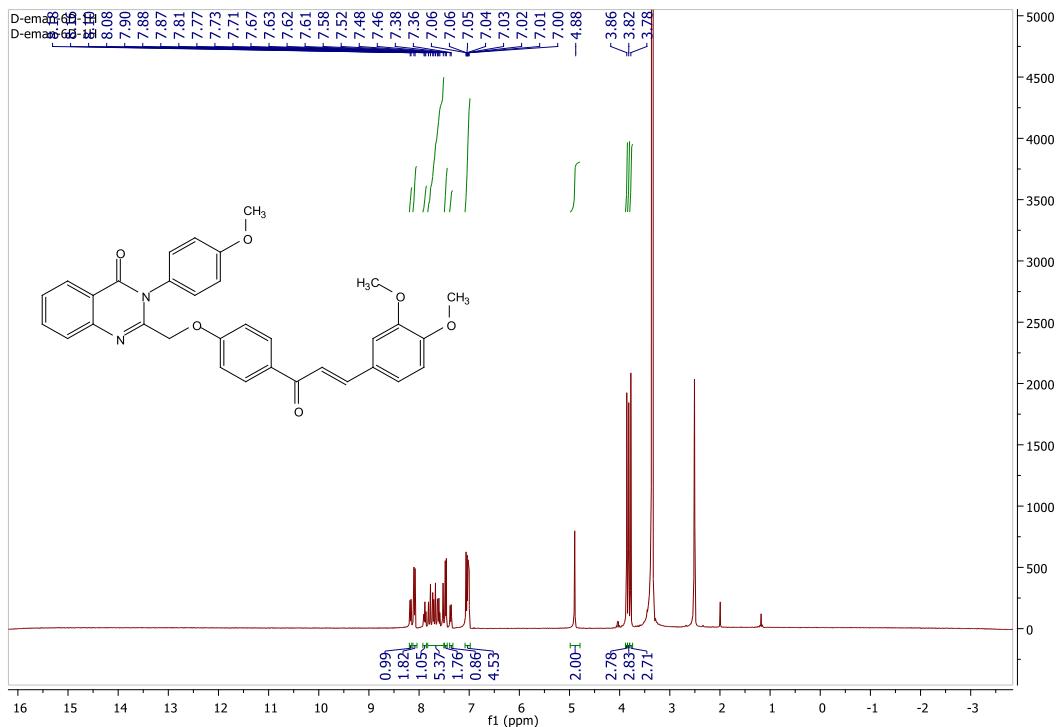
Line#:1 R.Time:3.3(Scan#:399)
MassPeaks:167
RawMode:Single 3.3(399) BasePeak:265(19428)
BG Mode:None Group 1 - Event 1



Mass Table
Line#:1 R.Time:3.3(Scan#:399)
MassPeaks:167
RawMode:Single 3.3(399) BasePeak:265(19428)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.	#	m/z	Abs. Int.	Rel. Int.
1	50.00	1746	8.99	4	53.05	1063	5.47	7	56.10	777	4.00
2	51.00	2519	12.97	5	54.15	687	3.54	8	57.10	2070	10.65
3	52.00	1074	5.53	6	55.05	2536	13.05	9	58.05	437	2.25

(E)-2-((4-(3,4-Dimethoxyphenyl)acryloyl)phenoxy)methyl-3-(4-methoxyphenyl) quinazolin-4(3H)-one (43).



21-Jan-07 17:00:08

Cairo University
Micro Analytical Center

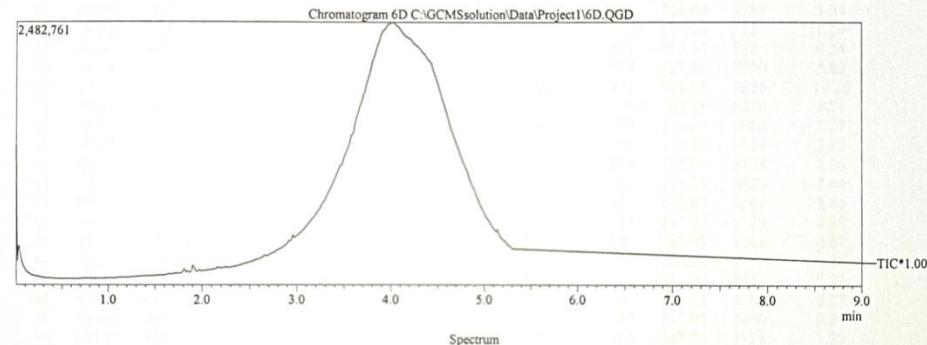
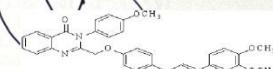
DI Analysis
Shimadzu QP-2010 Plus

Sample Information
Analyzed by : Dr. Mai Younis
Analyzed : 21/01/2007 04:53:53
Sample Name : 6D
Sample ID :
Customer Name : Dr Eman Ashraf - Pharmacy - Zagazik
Data File : C:\GCMSsolution\Datap\Project\6D.QGD
Org Data File : C:\GCMSsolution\Datap\Project\6D.QGD
Method File : C:\GCMSsolution\Datap\Project\High Temperature Op
Org Method File : C:\GCMSsolution\Datap\Project\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
SEndMSModified by : Dr. Mai Younis
Modified : 21/01/2007 04:59:15

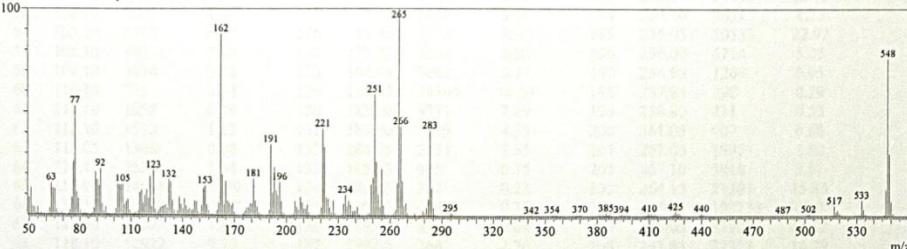
Method
==== Analytical Line 1 =====
IonSourceTemp : 250.00 °C
[MS Table]
-Group 1 - Event 1-
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.50sec
Scan Speed : 1250
Start m/z : 50.00
End m/z : 600.00

Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Datap\Project\6D.QGD



Line#:1 R.Time:4.0(Scan#:478)
MassPeaks:306
RawMode:Single 4.0(478) BasePeak:265(133235)
BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:4.0(Scan#:478)
MassPeaks:306
RawMode:Single 4.0(478) BasePeak:265(133235)
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	11031	8.28	4	53.00	5394	4.05	7	56.00	959	0.72
2	51.00	17745	13.32	5	54.05	1417	1.06	8	57.05	1709	1.28
3	52.00	5809	4.36	6	55.00	5111	3.84	9	58.05	514	0.39