

SUPPORTING INFORMATION

Deep eutectic solvent mediated synthesis of quinazolinones and dihydroquinazolinones: synthesis of natural products and drugs

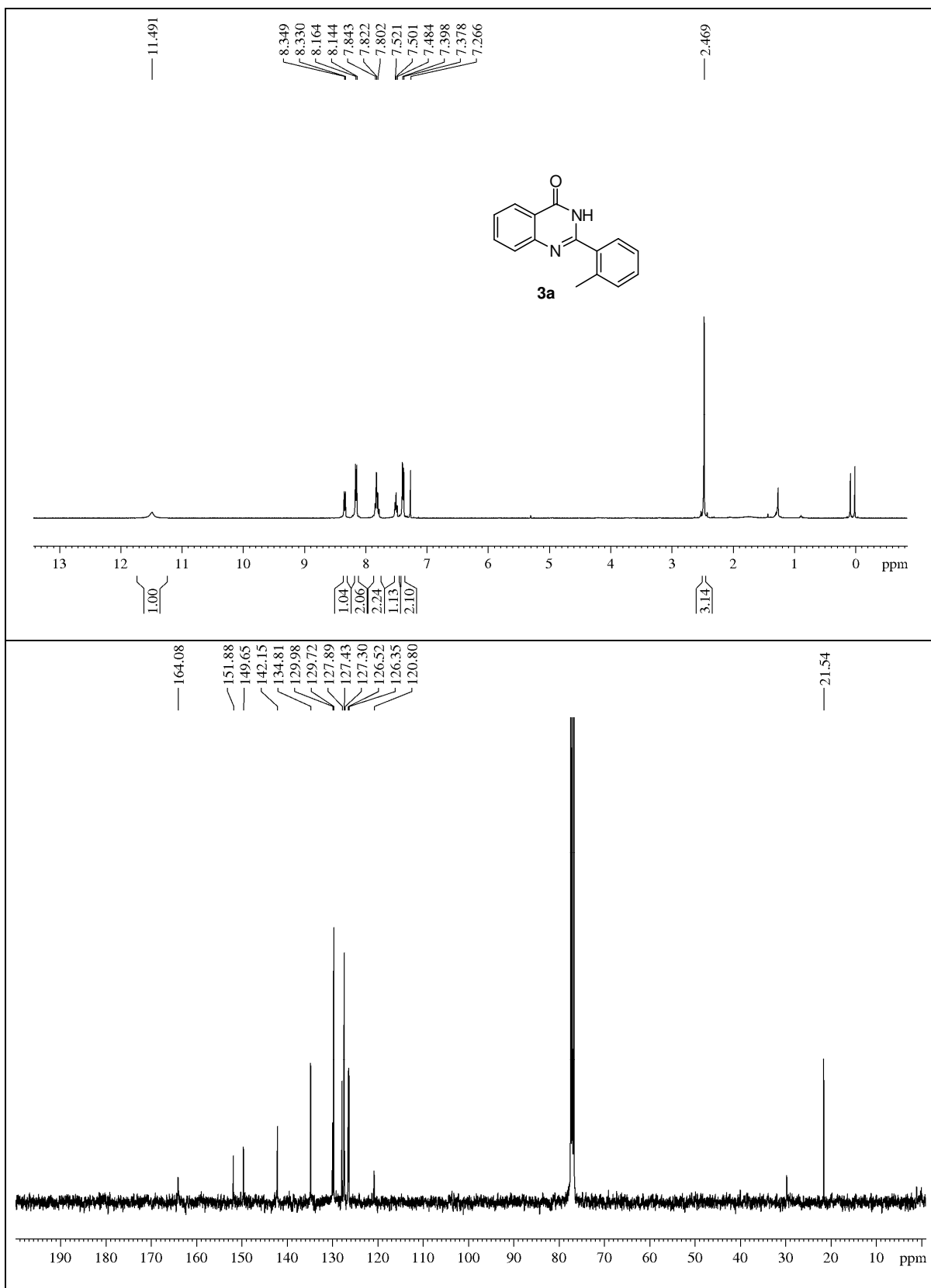
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rsc@uohyd.ernet.in

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^1H , ^{13}C -NMR, HRMS, LCMS & CHN Spectra of compounds 3a- 12f

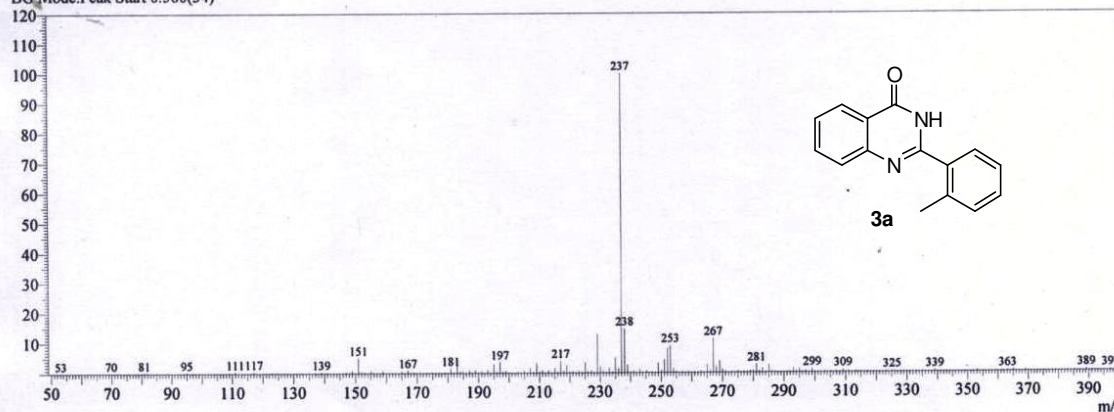


**LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD**

User : Admin
 Sample : SKG-608
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\SKG-608-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

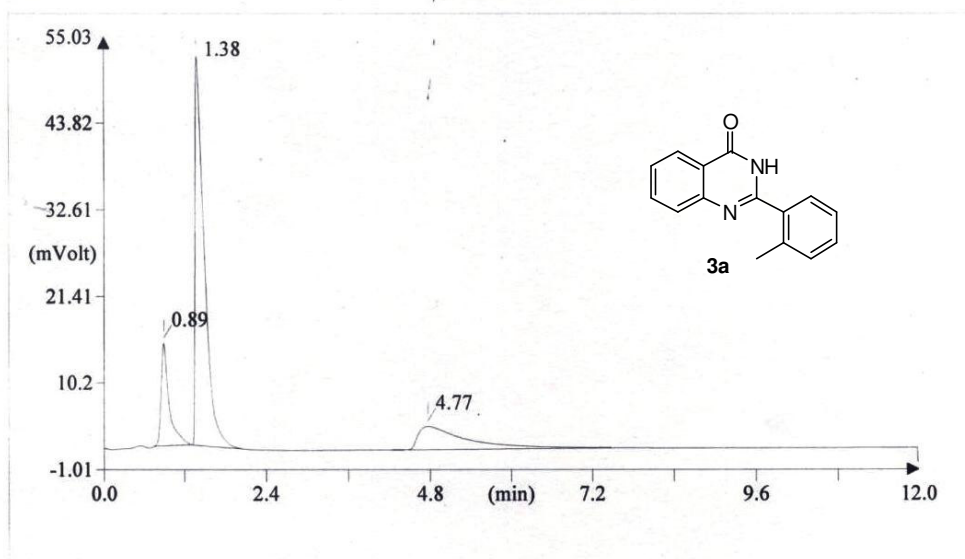
Line#:1 R.Time:0.758(Scan#:46) Positive
 MassPeaks:314 BasePeak:237.05(7483766)
 RawMode:Single 0.758(46)
 BG_Mode:Peak Start 0.560(34)



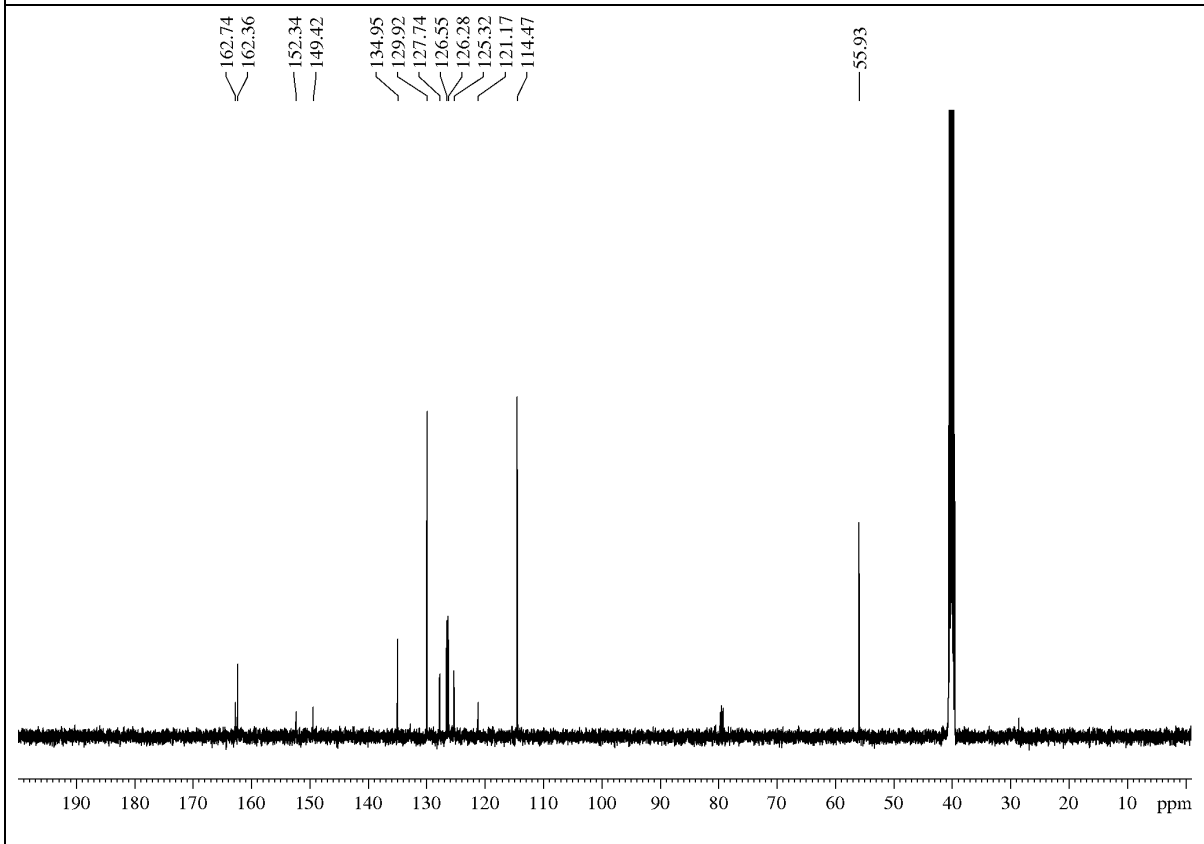
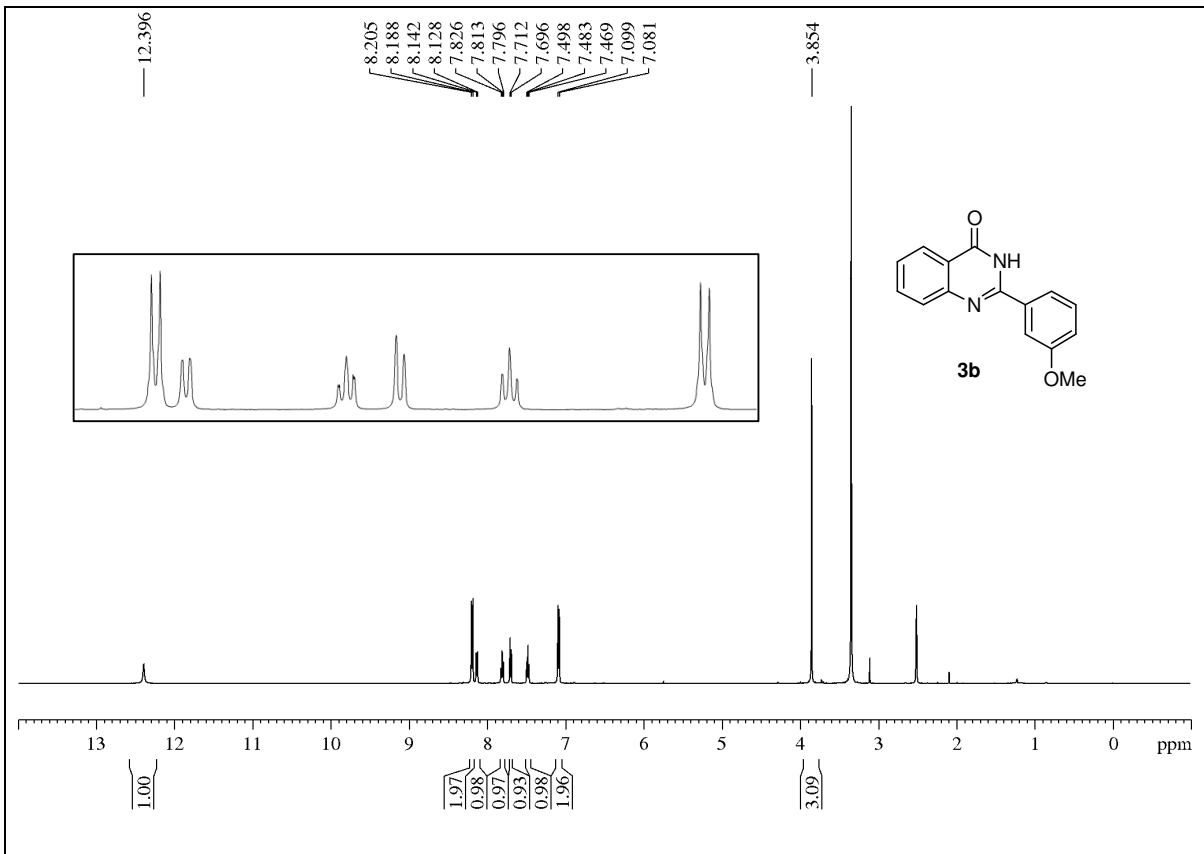
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.758	0.560	1.043	280005070	24556967	11.40		100.00		237.05	7483766
				280005070	24556967			100.00			

FLASH EA 1112 SERIES CHN REPORT
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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-608 (# 142)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-2.dat
Sample weight: 1.206



Element Name	Element %	Ret. Time
Nitrogen	11.96	0.89
Carbon	76.12	1.38
Hydrogen	5.18	4.77

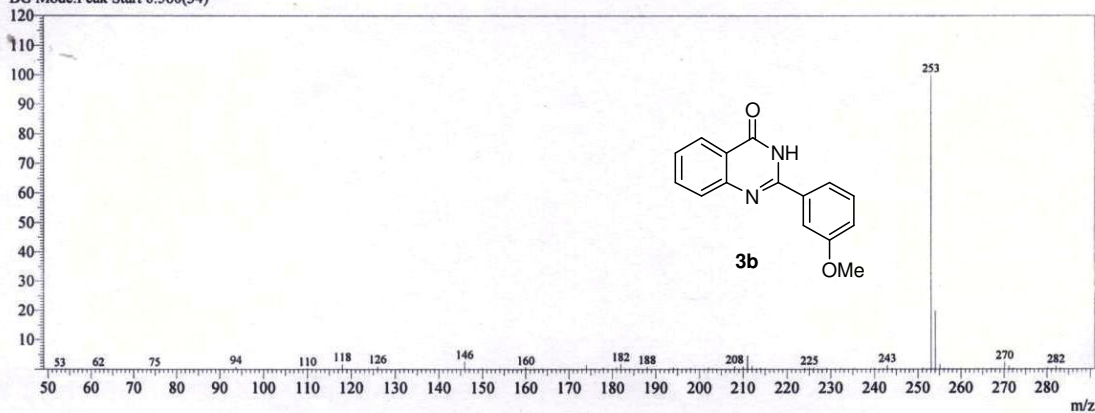


**LCMS-2010A DATA REPORT
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User : Admin
Sample : SKG-452-I
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-452-I-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.759(Scan#:46) Positive
MassPeaks:172 BasePeak:253.05(6921410)
RawMode:Single 0.759(46)
BG Mode:Peak Start 0.560(34)

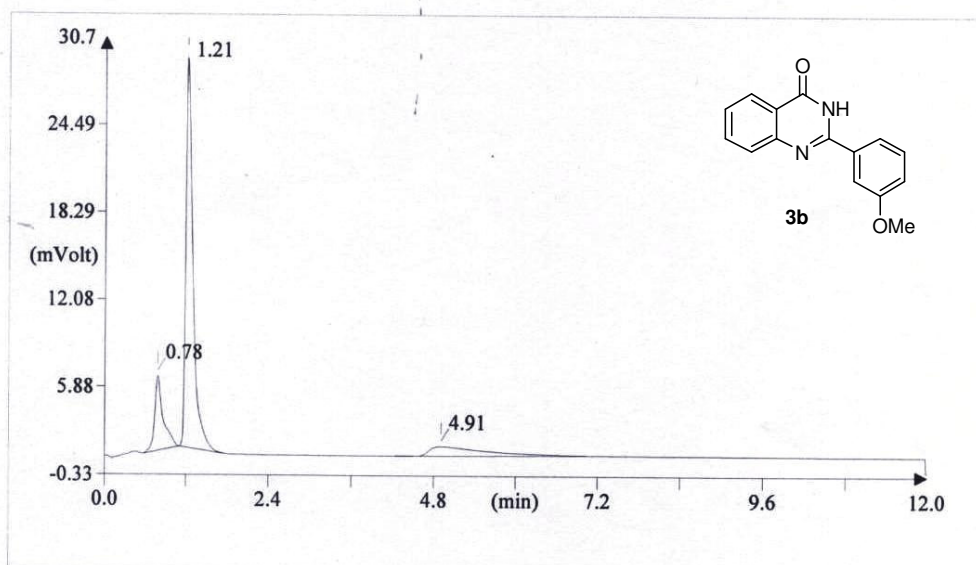


MS Peak Table

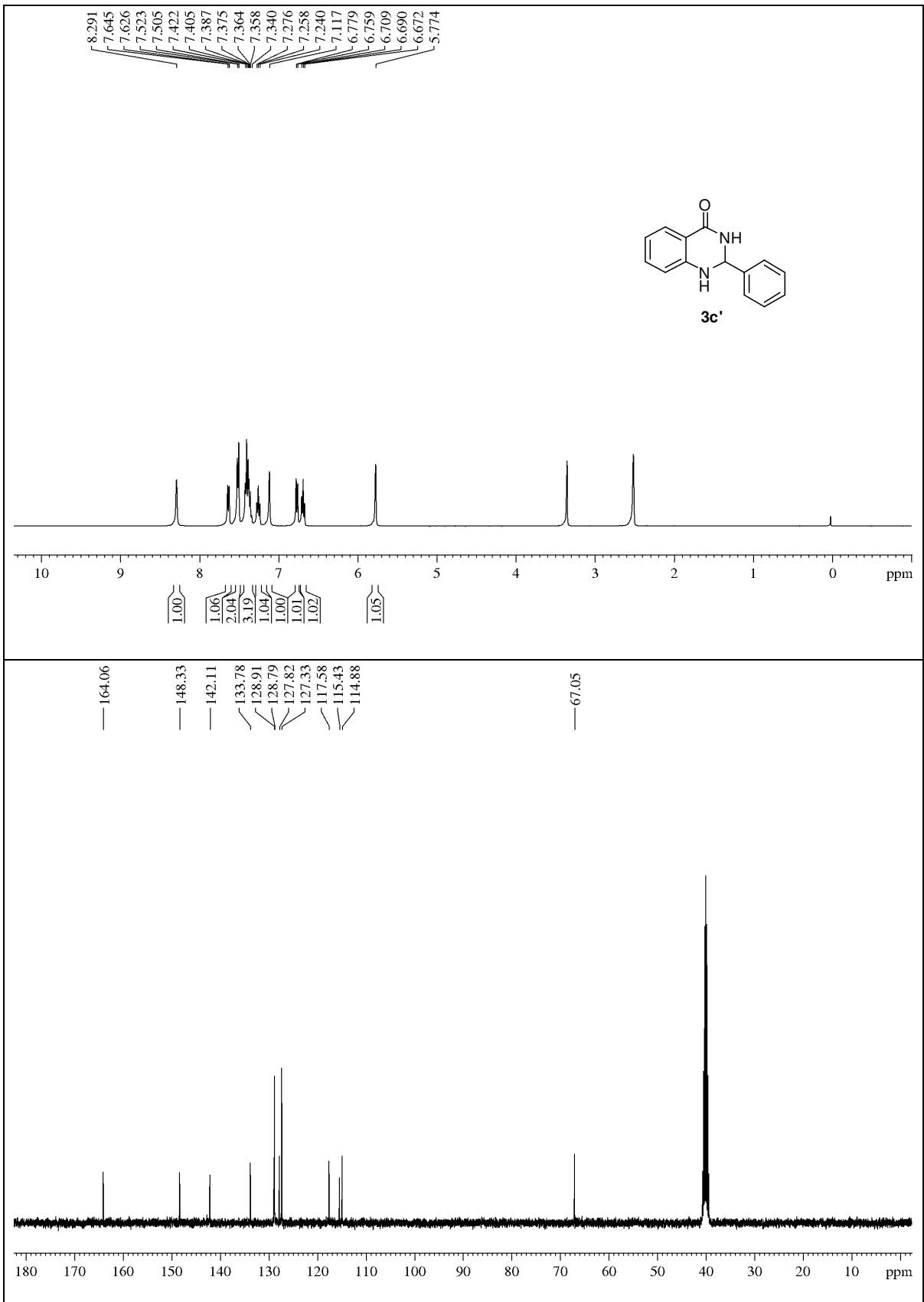
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.759	0.560	1.043	171035756	15606881	10.95		100.00		253.05	6921410
				171035756	15606881			100.00			

FLASH EA 1112 SERIES CHN REPORT
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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-452-I (# 155)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-15.dat
Sample weight: 1.106



Element Name	Element %	Ret. Time
Nitrogen	11.26	0.78
Carbon	71.57	1.21
Hydrogen	4.71	4.91

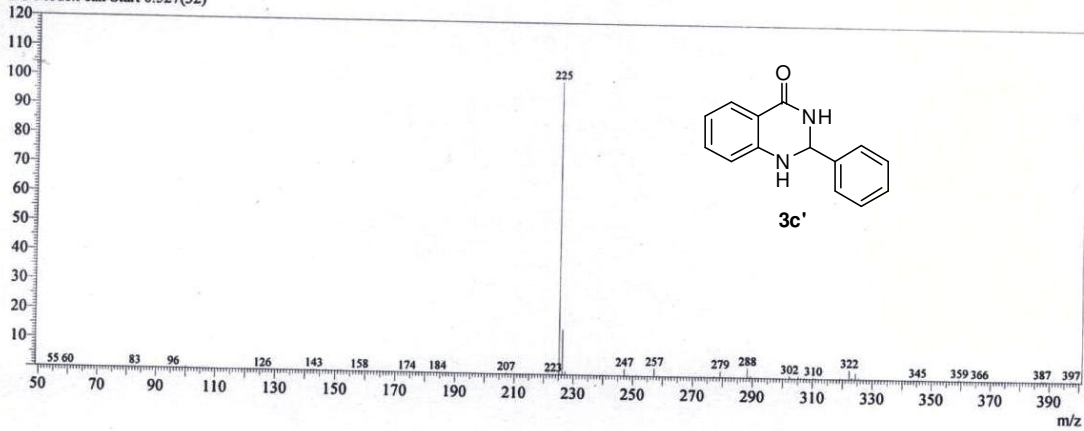


LCMS-2010A DATA REPORT
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User : Admin
Sample : SKG-493-II
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-493-II-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#1 R.Time:0.773(Scan#:47) Positive
MassPeaks:268 BasePeak:225.20(8313275)
RawMode:Single 0.773(47)
BG Mode:Peak Start 0.527(32)

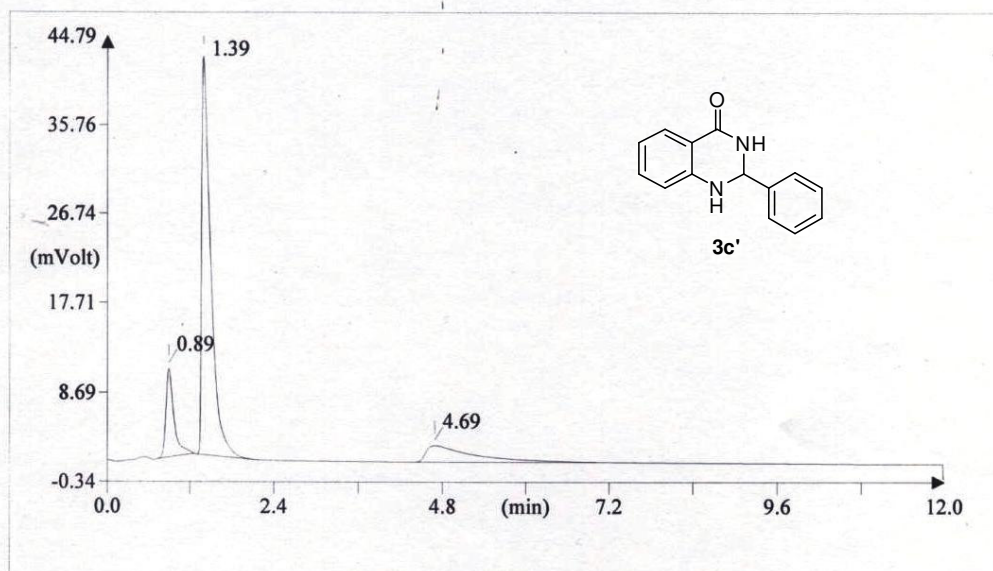


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.773	0.527	1.043	246029086	18431530	13.34		100.00	
				246029086	18431530			100.00	

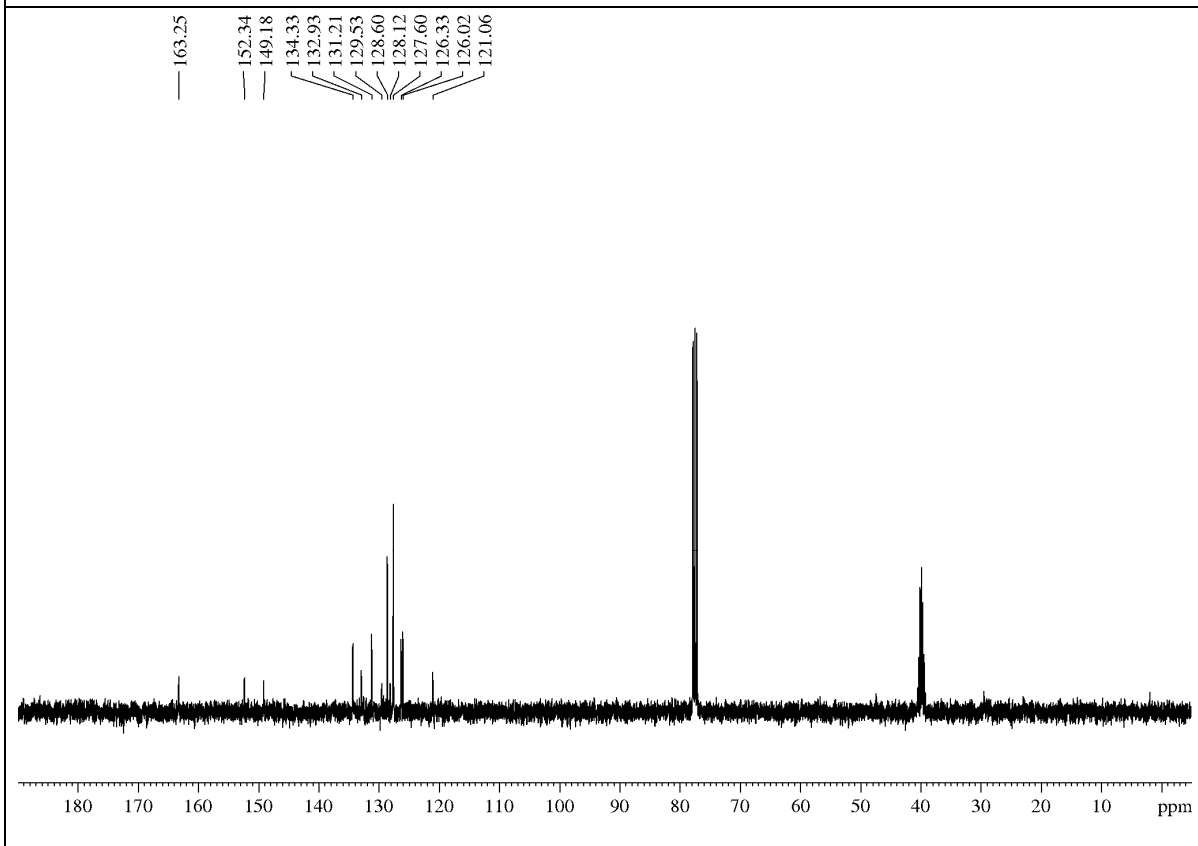
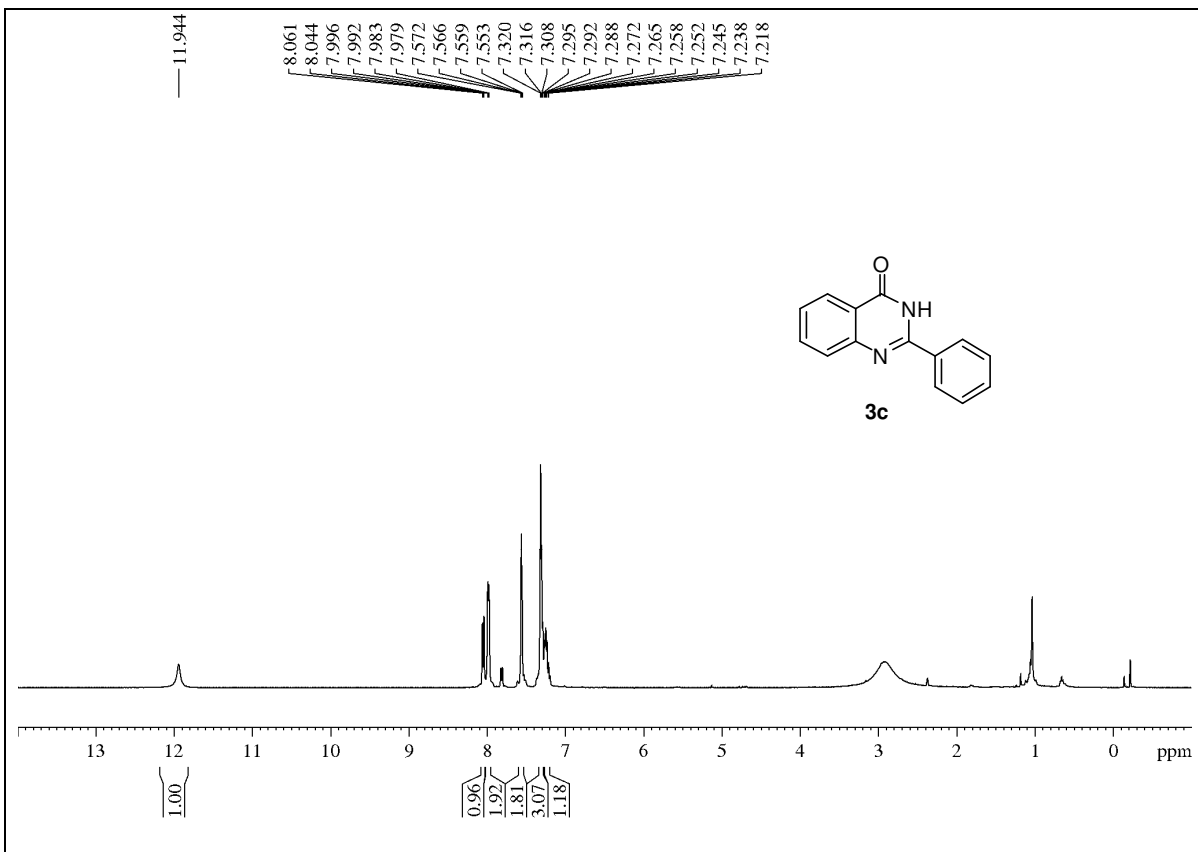
Base m/z Base Int.
225.20 8313275

FLASH EA 1112 SERIES CHN REPORT
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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-493-II (# 156)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-16.dat
Sample weight: 1.141



Element Name	Element %	Ret. Time
Nitrogen	12.56	0.89
Carbon	74.82	1.39
Hydrogen	5.45	4.69

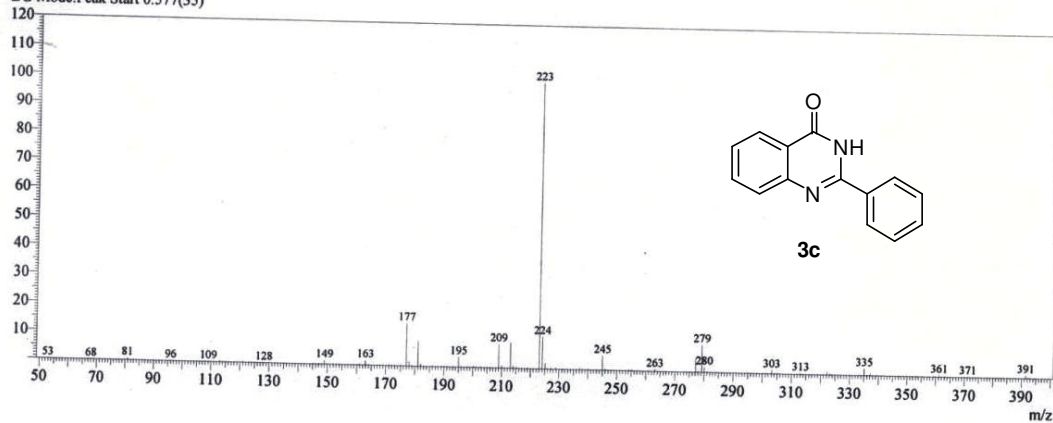


LCMS-2010A DATA REPORT
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User : Admin
Sample : SKG-493-I
Inj. Volume : 5.000
Data Name : C:\LCMSSolution\User\Data\SKG-493-I-APCI-POS1.qld
Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.782(Scan#:47) Positive
MassPeaks:257 BasePeak:223.10(8019945)
RawMode:Single 0.782(47)
BG Mode:Peak Start 0.577(35)

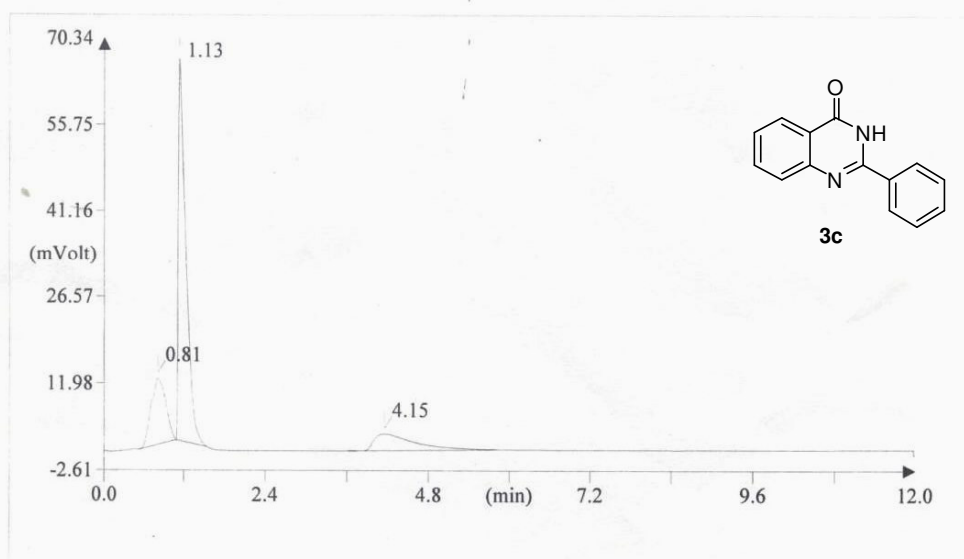


MS Peak Table

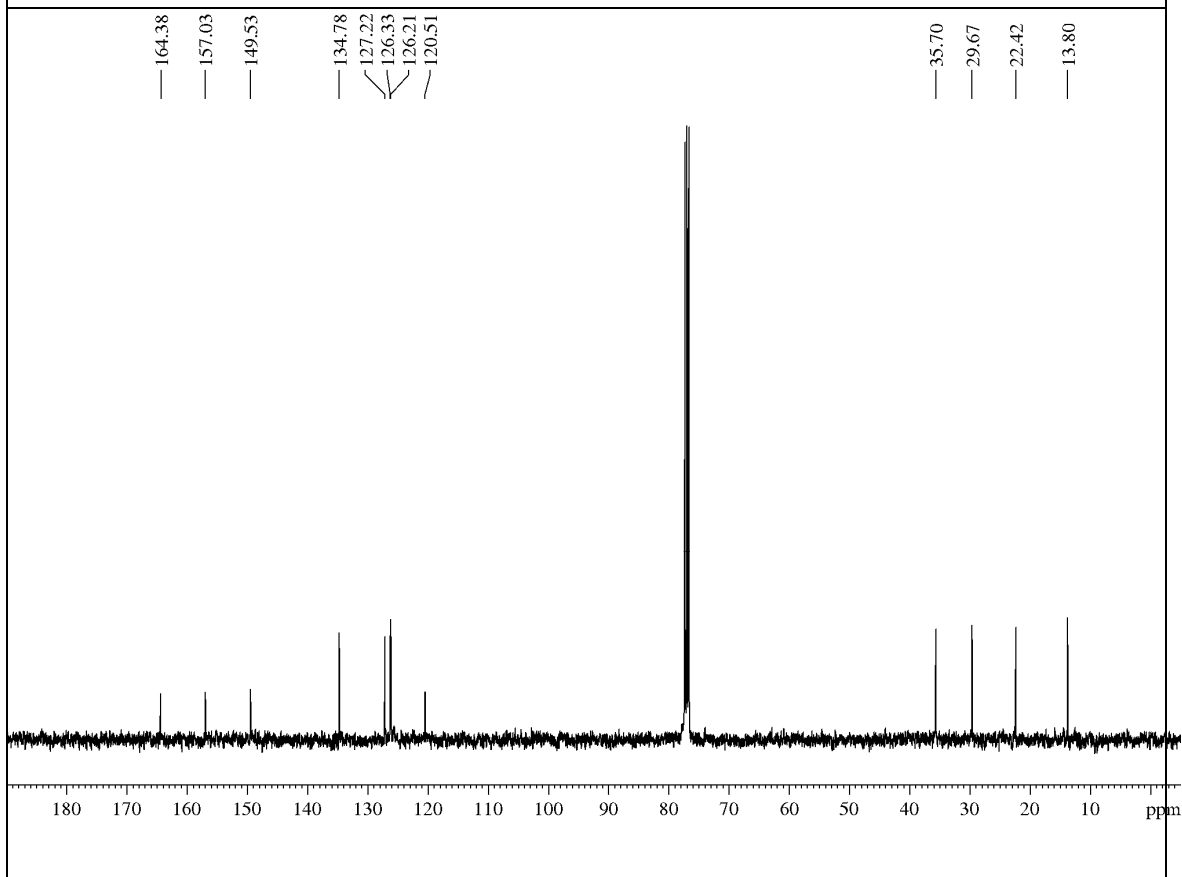
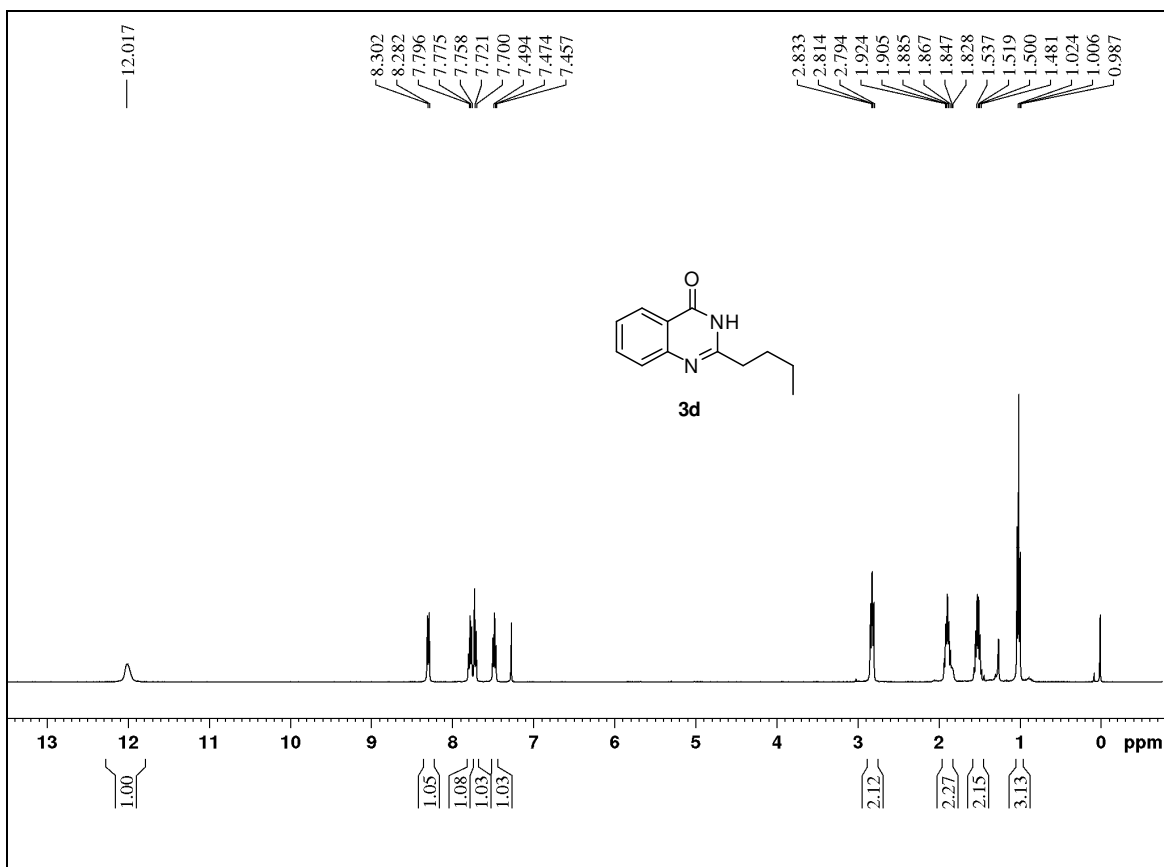
Peak#	R. Time	I. Time	F. Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.782	0.577	1.043	200722973	16822675	11.93		100.00		223.10	8019945
				200722973	16822675			100.00			

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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-493-I (# 141)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-1.dat
Sample weight: 1.496



Element Name	Element %	Ret. Time
Nitrogen	12.53	0.81
Carbon	75.81	1.13
Hydrogen	4.51	4.15



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Analysis Info

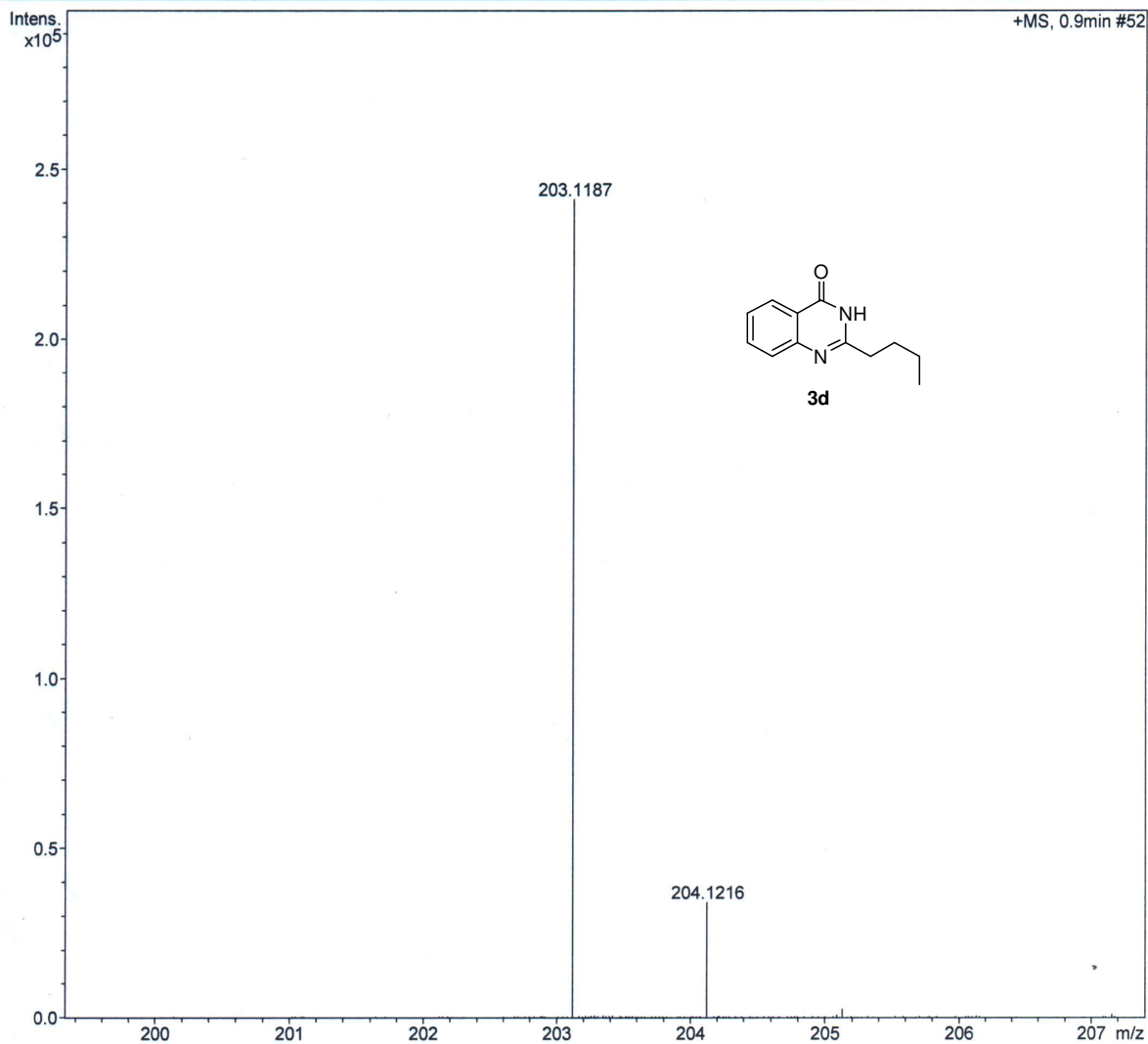
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-613-IIR.d
Method tune_low.m
Sample Name SKG-613-II-DCM-MEOH
Comment

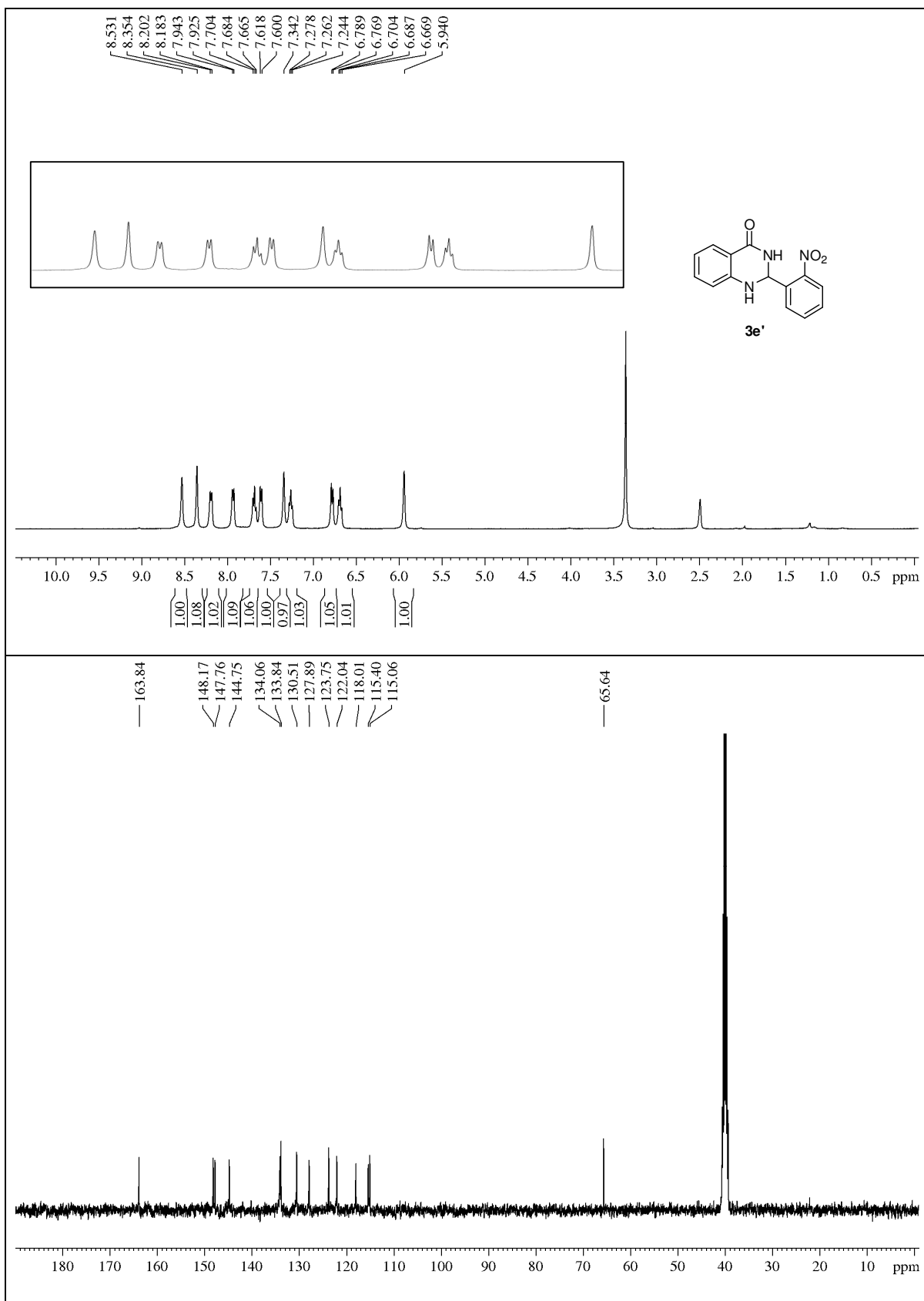
Acquisition Date 8/19/2015 11:51:01 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





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Analysis Info

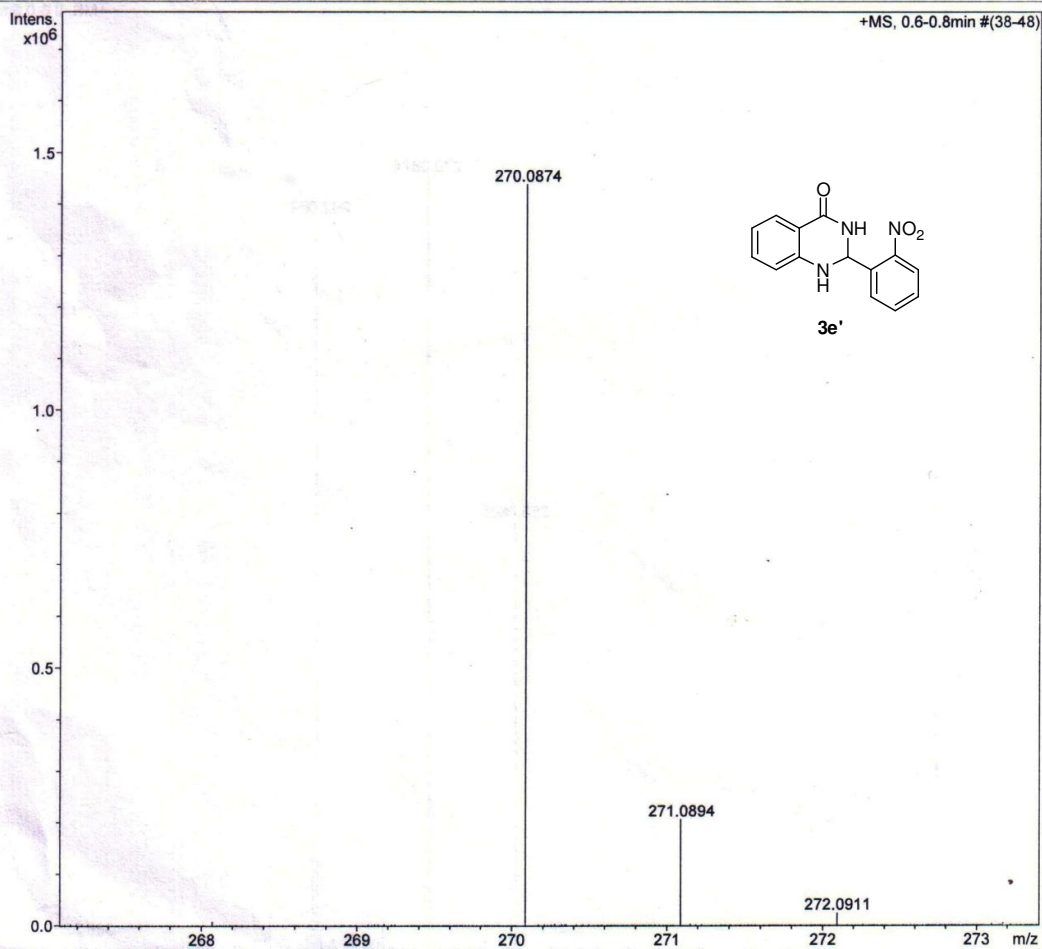
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Method tune_low_Pos.m
Sample Name SKG-503-DCM-MEOH
Comment

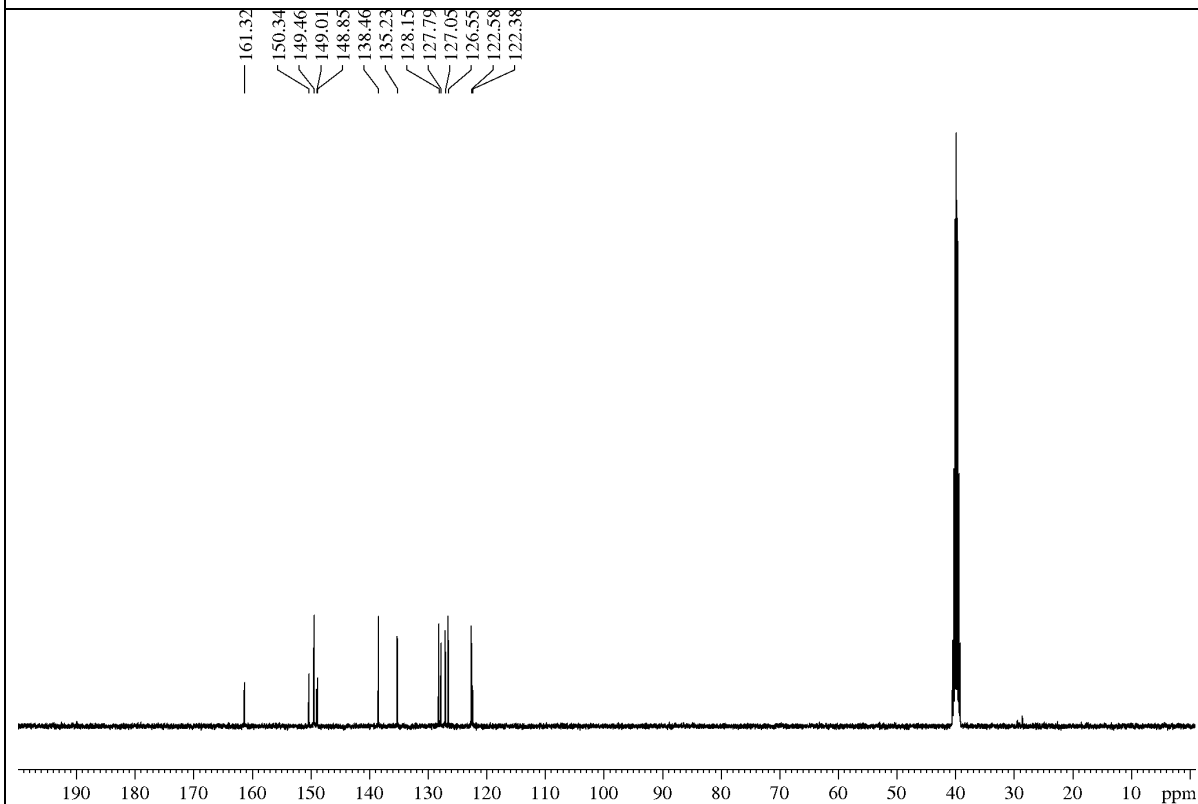
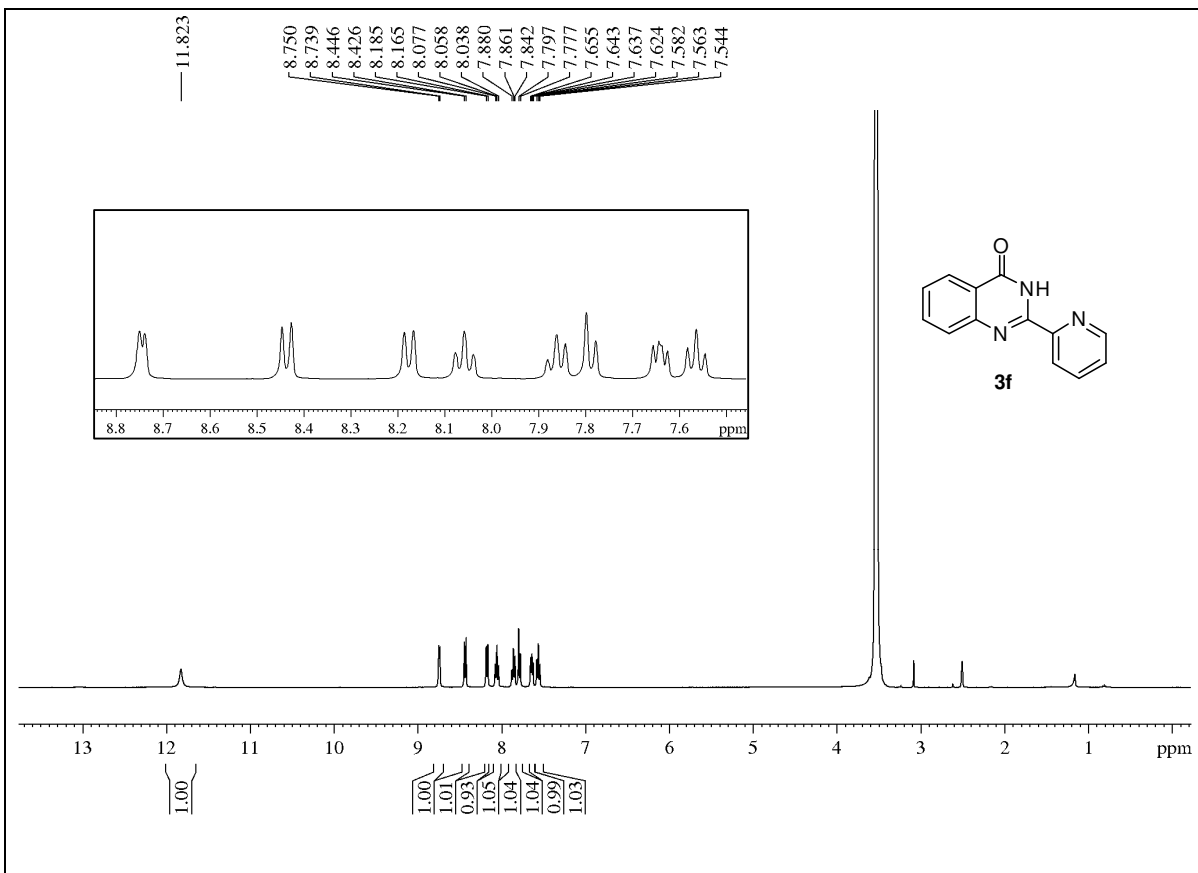
Acquisition Date 4/16/2014 12:13:15 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



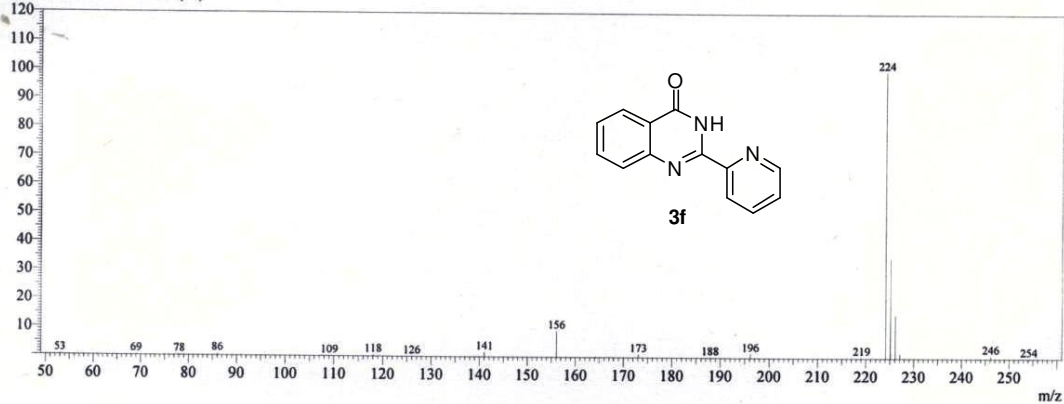


**LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
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User : Admin
Sample : SKG-533
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-533-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.786(Scan#:48) Positive
MassPeaks:84 BasePeak:224.10(13443212)
RawMode:Single 0.786(48)
BG Mode:Peak Start 0.527(32)

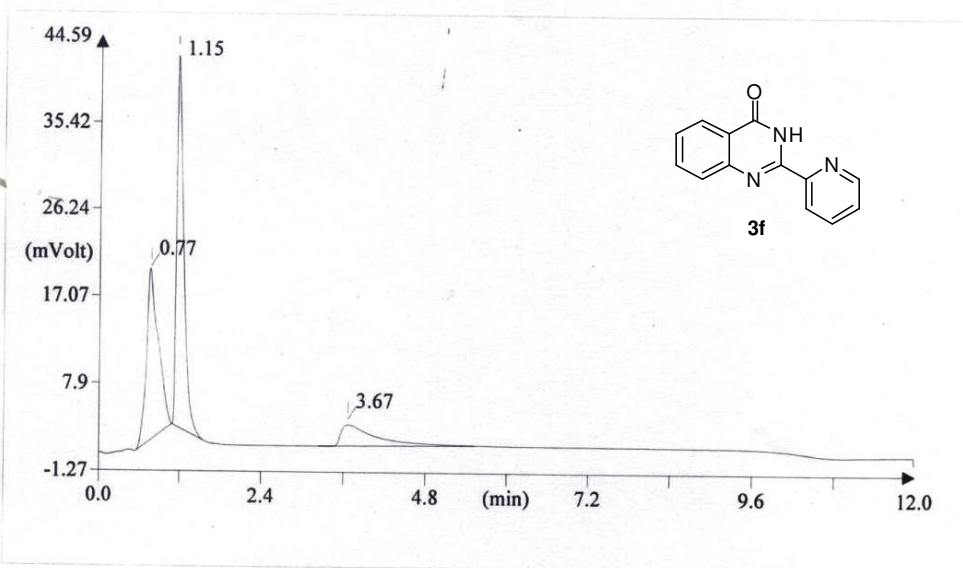


MS Peak Table

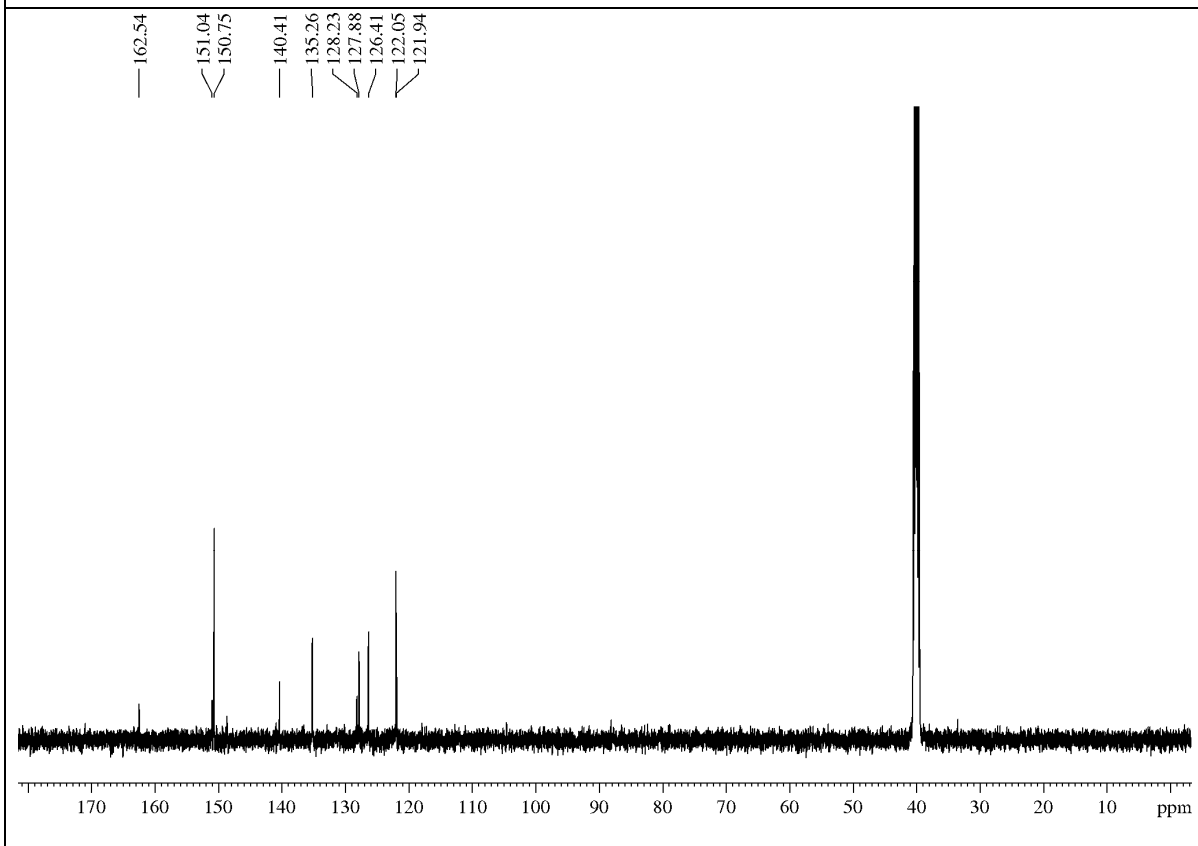
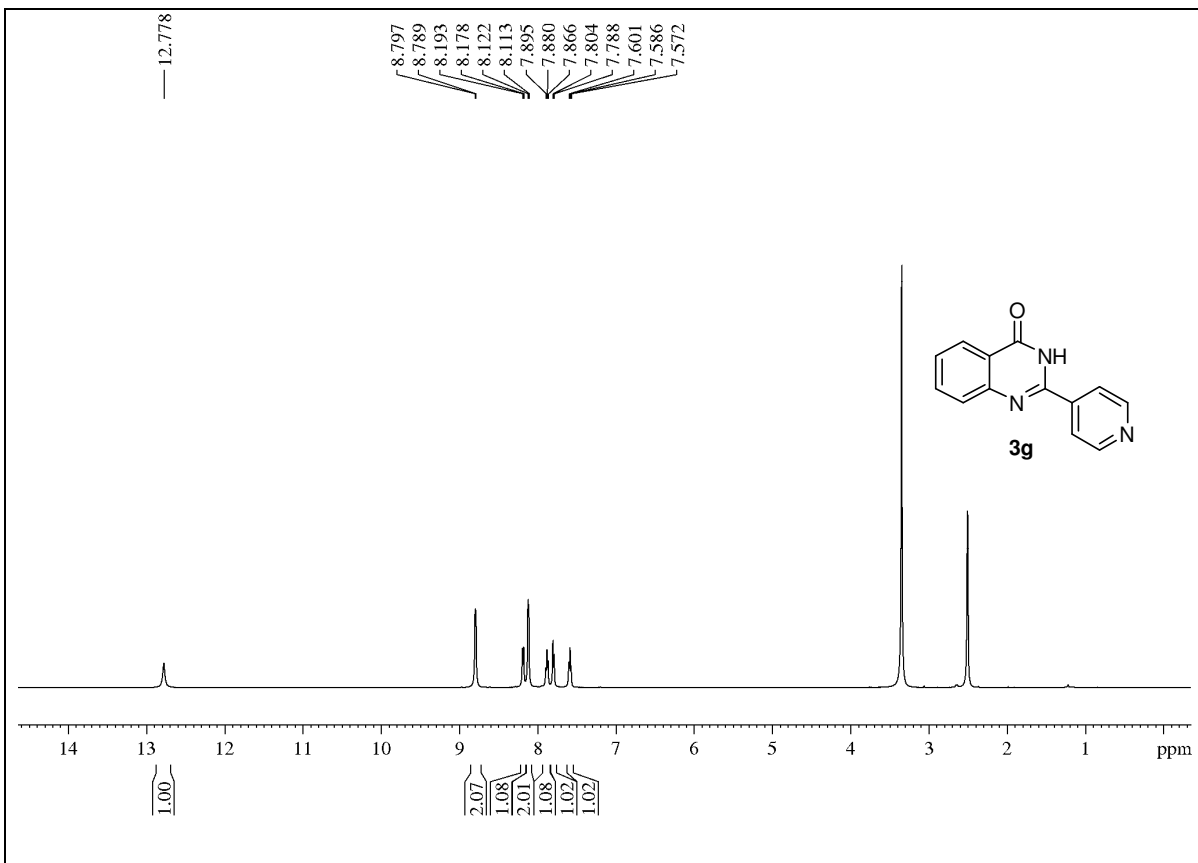
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.786	0.527	1.043	293076473	19476036	15.04		100.00		224.10	13443212
				293076473	19476036			100.00			

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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-533 (# 164)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-24.dat
Sample weight: 1.146



Element Name	Element %	Ret. Time
Nitrogen	18.75	0.77
Carbon	69.86	1.15
Hydrogen	4.15	3.67



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Analysis Info

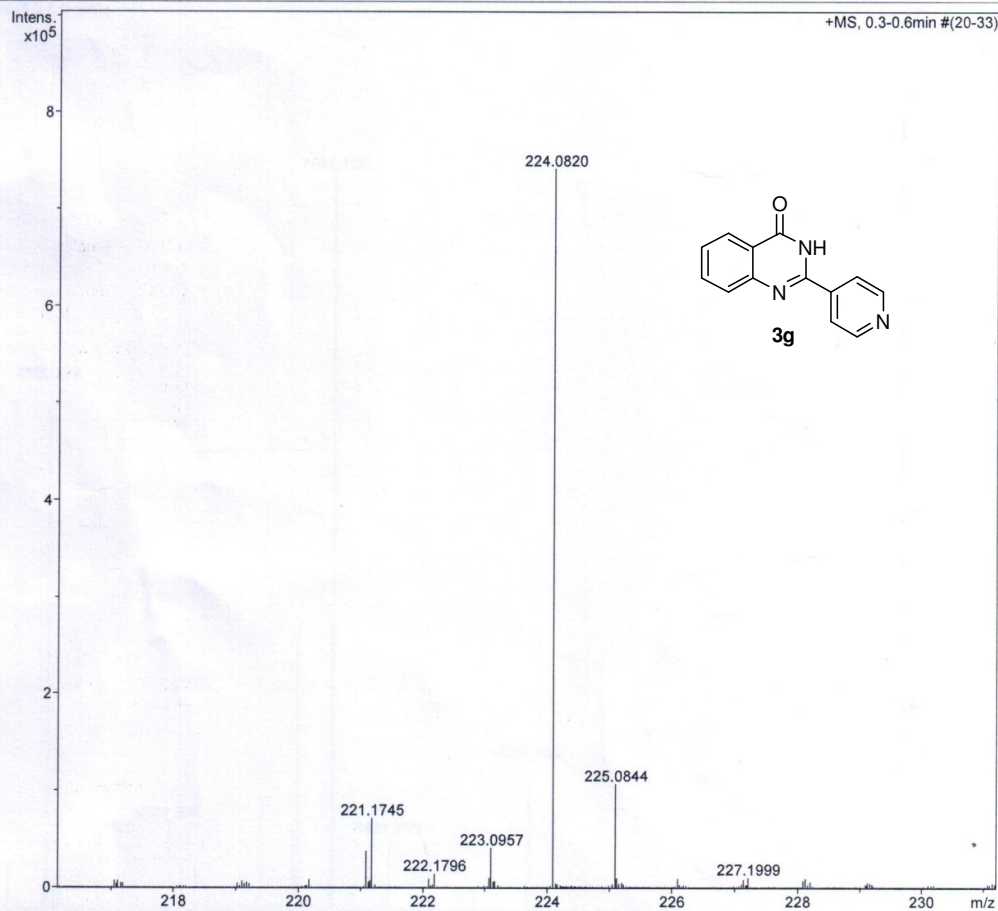
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-766R2.d
Method tune_low_Pos.m
Sample Name SKG-766-DCM-MEOH
Comment

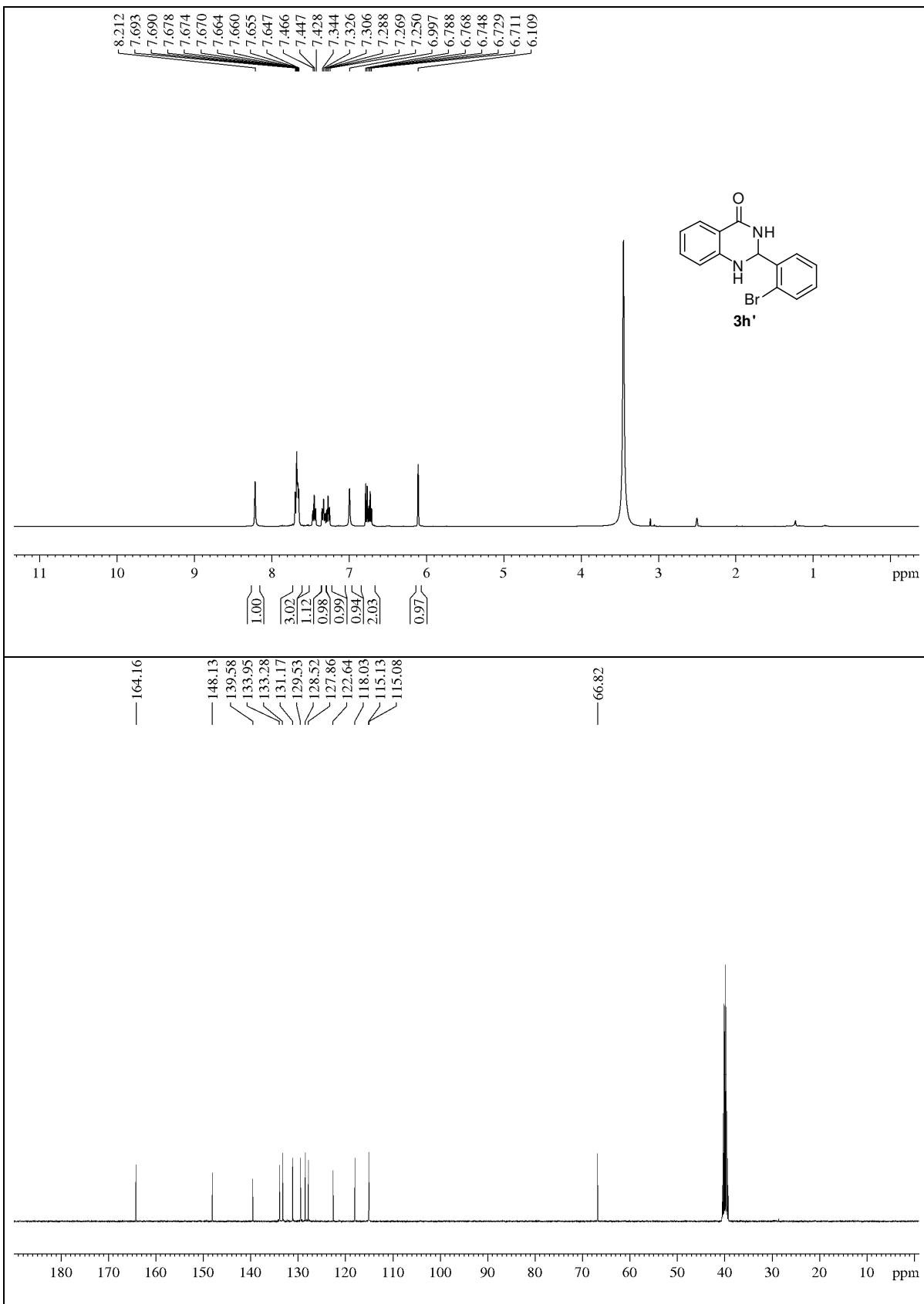
Acquisition Date 7/20/2015 12:15:37 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	6.0 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

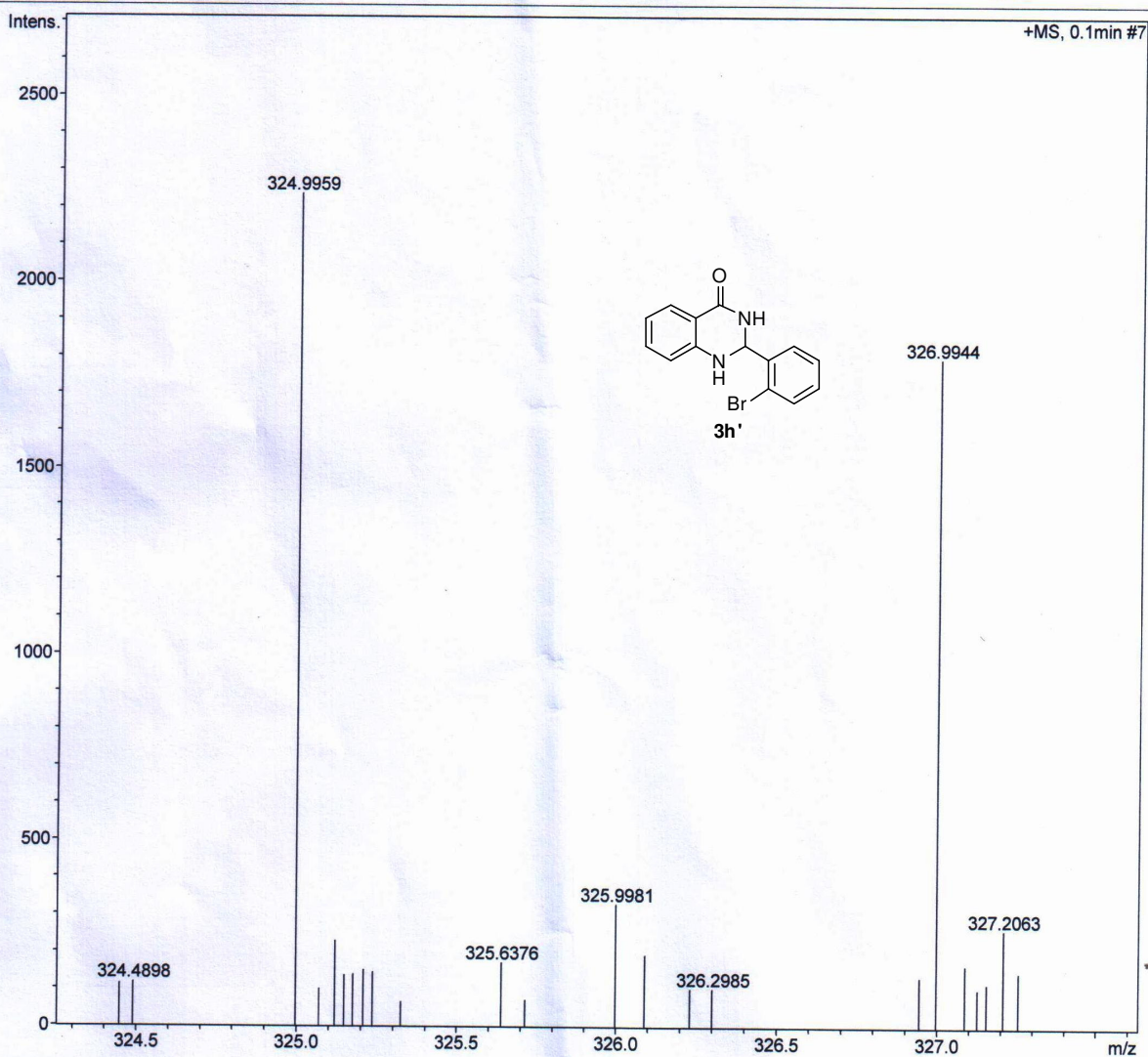
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-605R1.d
Method TL-P.m
Sample Name SKG-605-DCM-MEOH
Comment

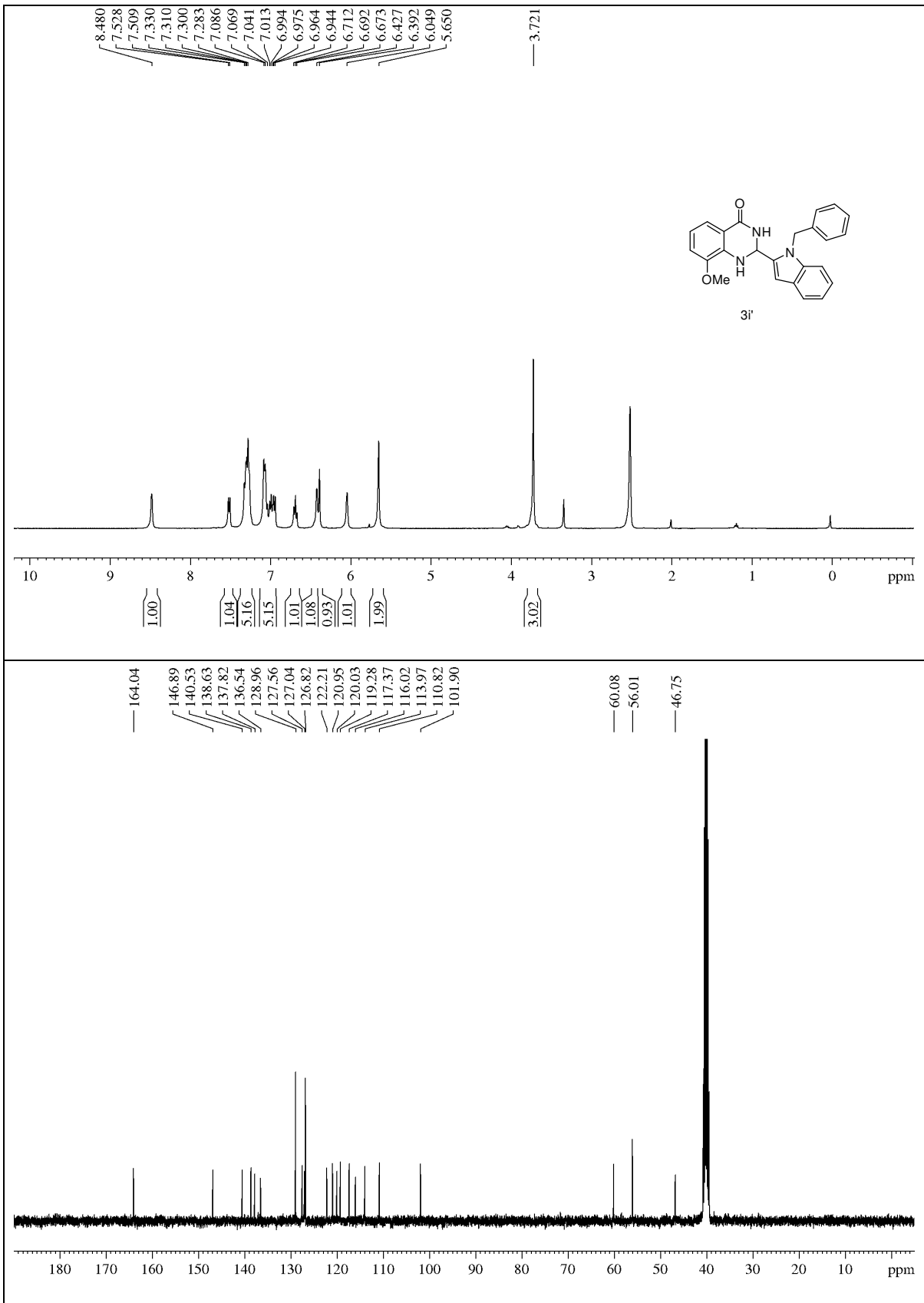
Acquisition Date 7/2/2015 12:37:42 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

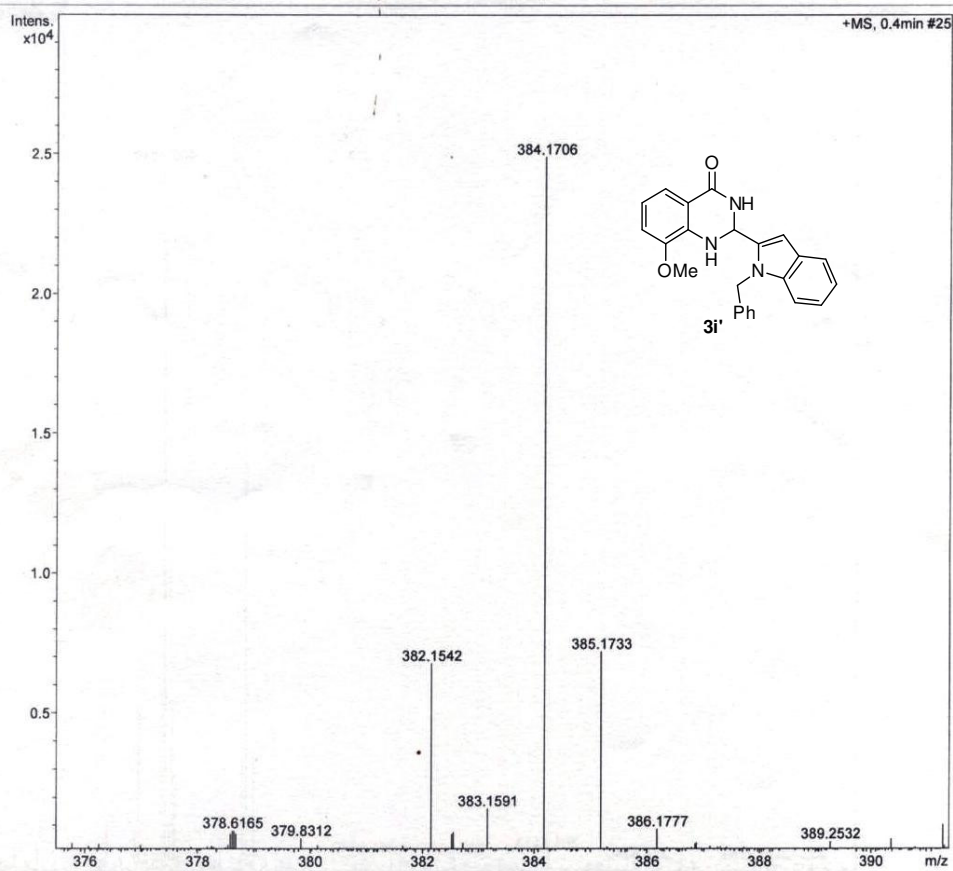
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Method tune_low_Pos.m
Sample Name SKG-564-DCM-MEOH
Comment

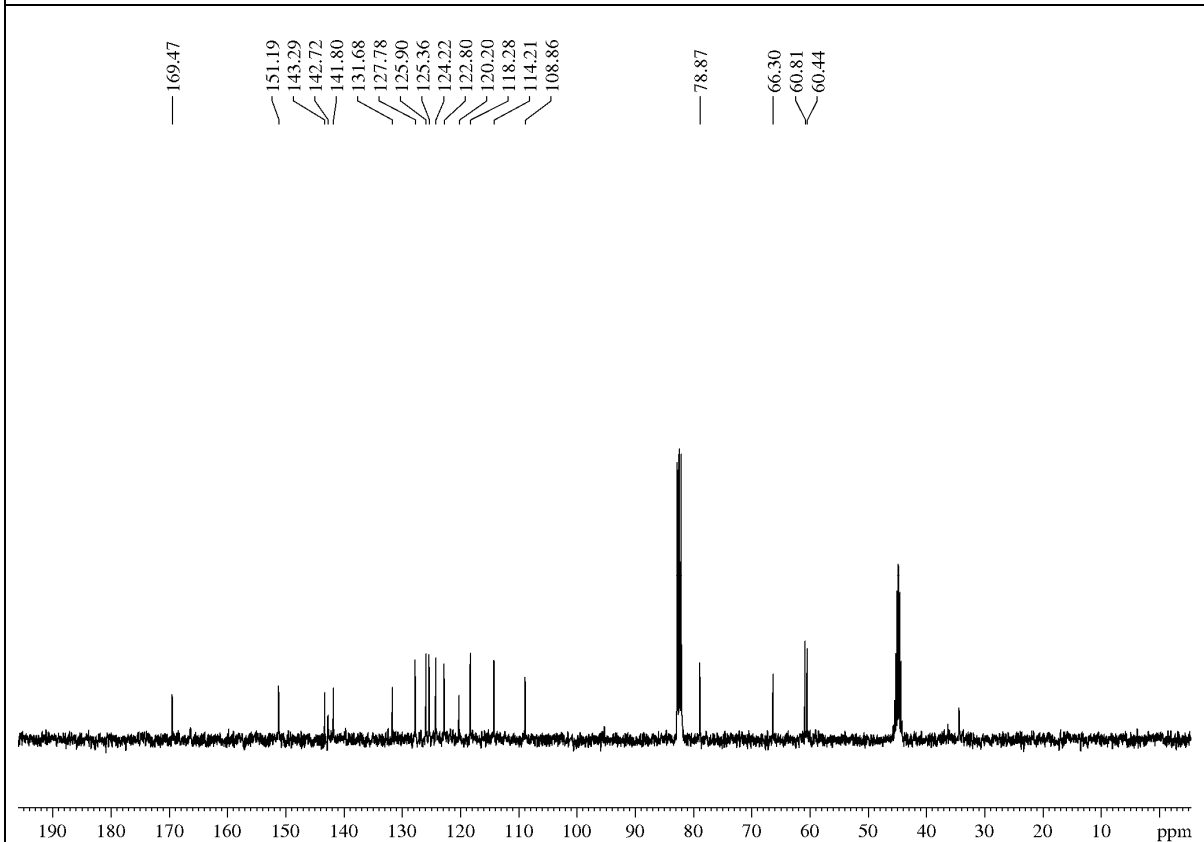
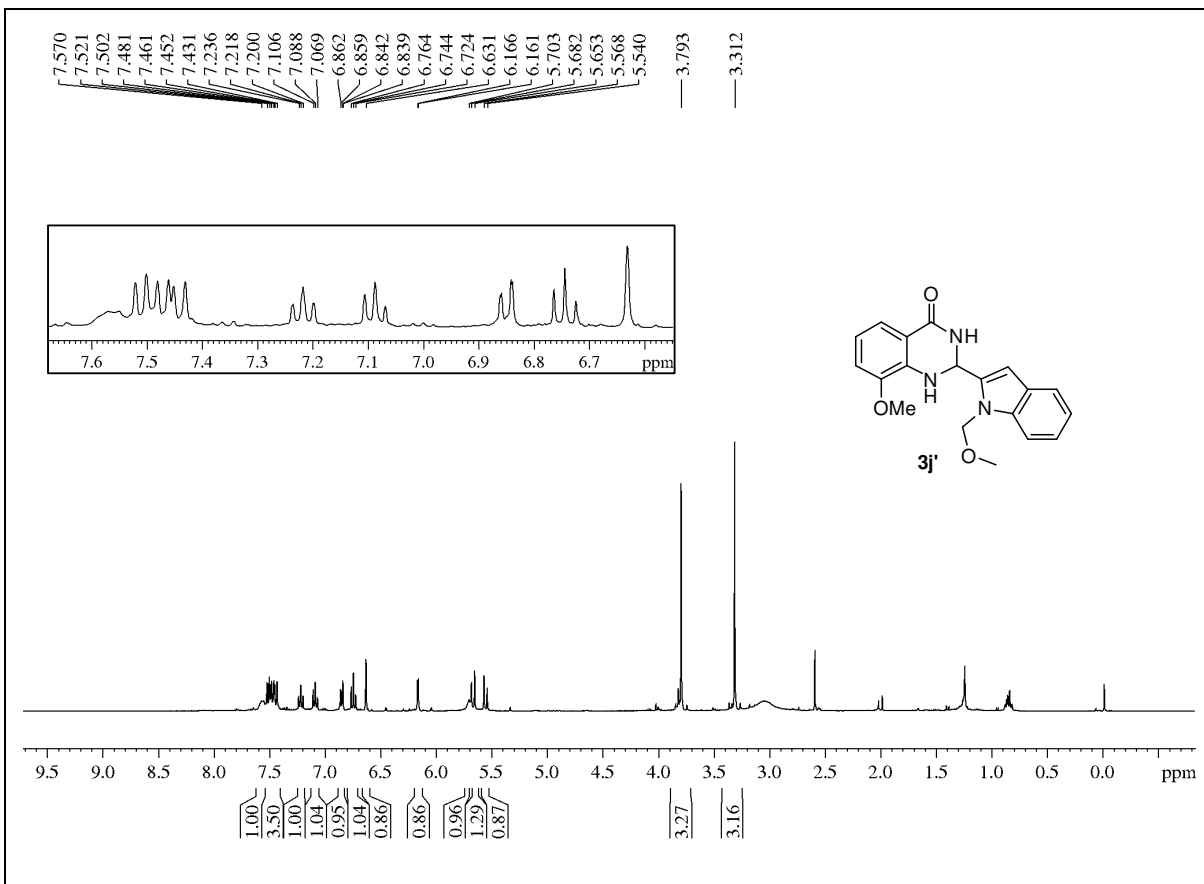
Acquisition Date 2/23/2015 1:34:03 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active	Set Capillary	4400 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



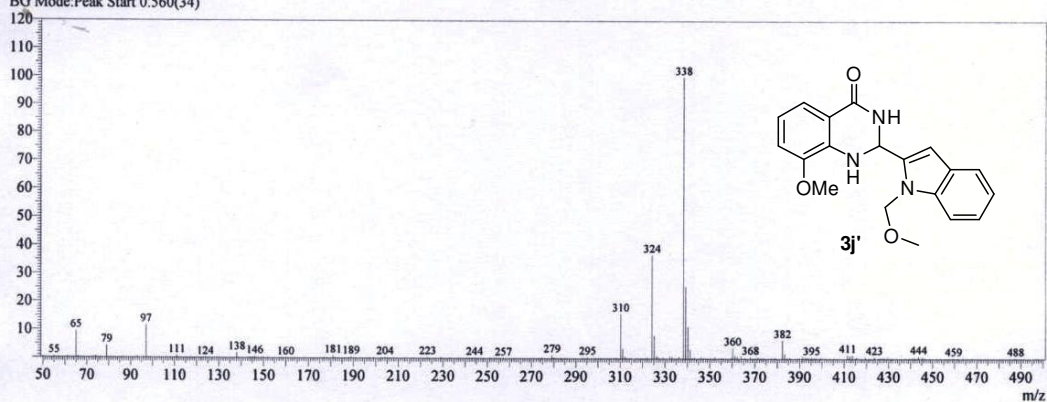


**LCMS-2010A DATA REPORT
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User : Admin
 Sample : SKG-622
 Inj. Volume : 5.000
 Data Name : C:\LCMSSolution\User\Data\SKG-622-APCI-POS1.qld
 Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.788(Scan#:48) Positive
 MassPeaks:350 BasePeak:338.20(2051111)
 RawMode:Single 0.788(48)
 BG Mode:Peak Start 0.560(34)

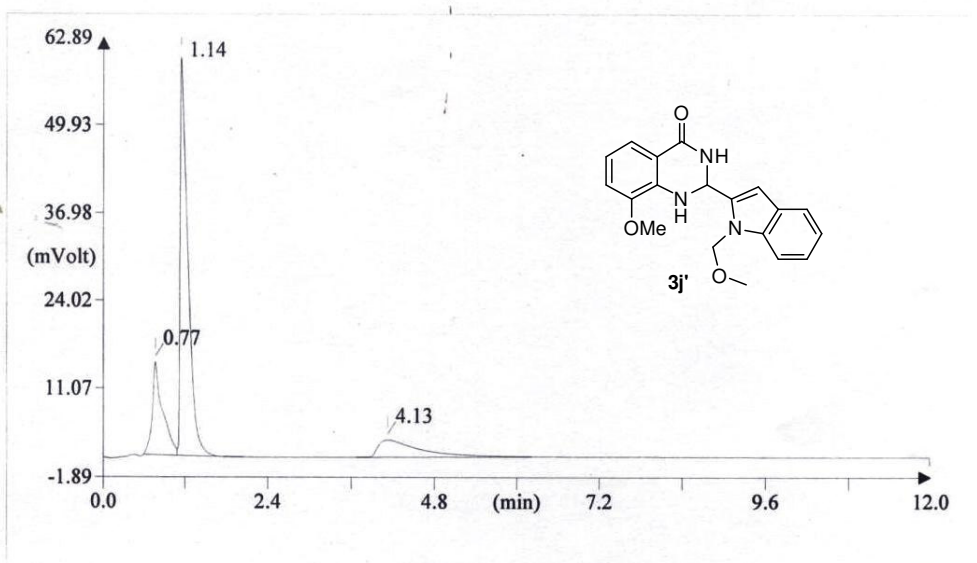


MS Peak Table

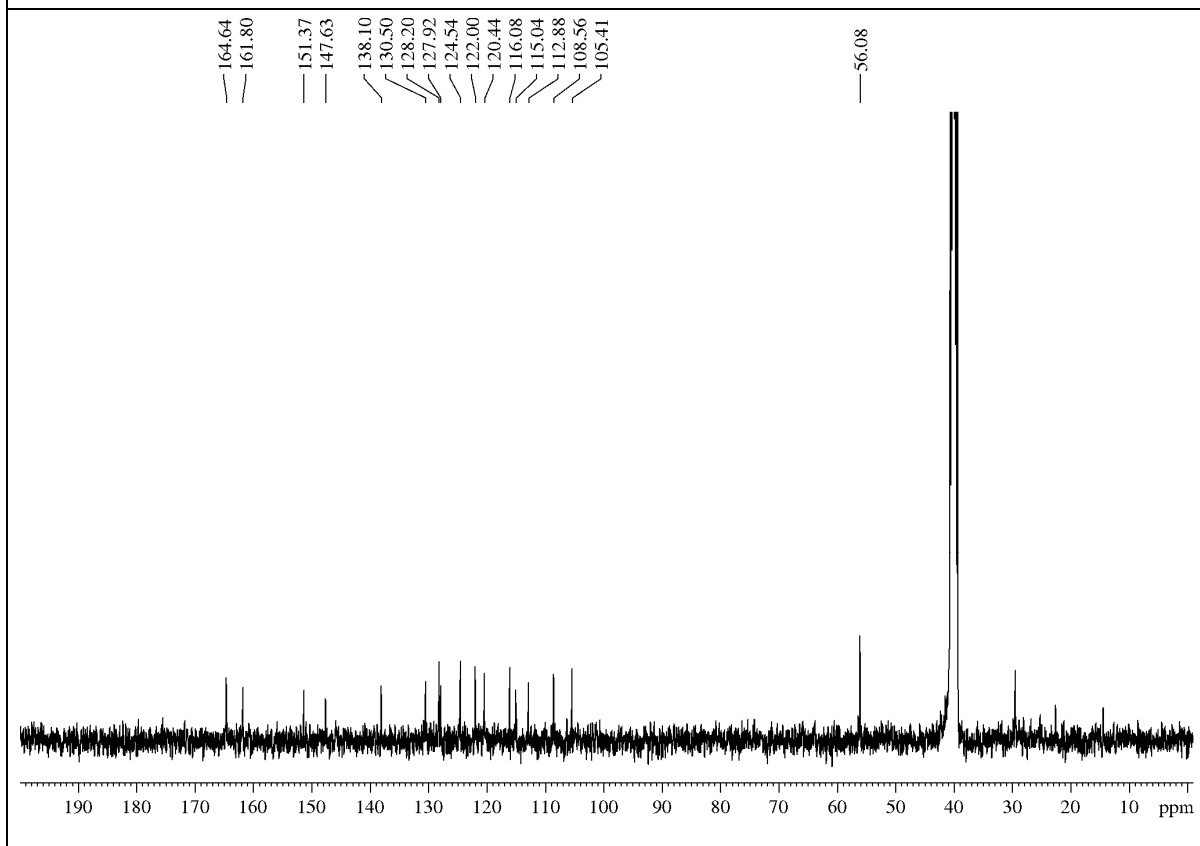
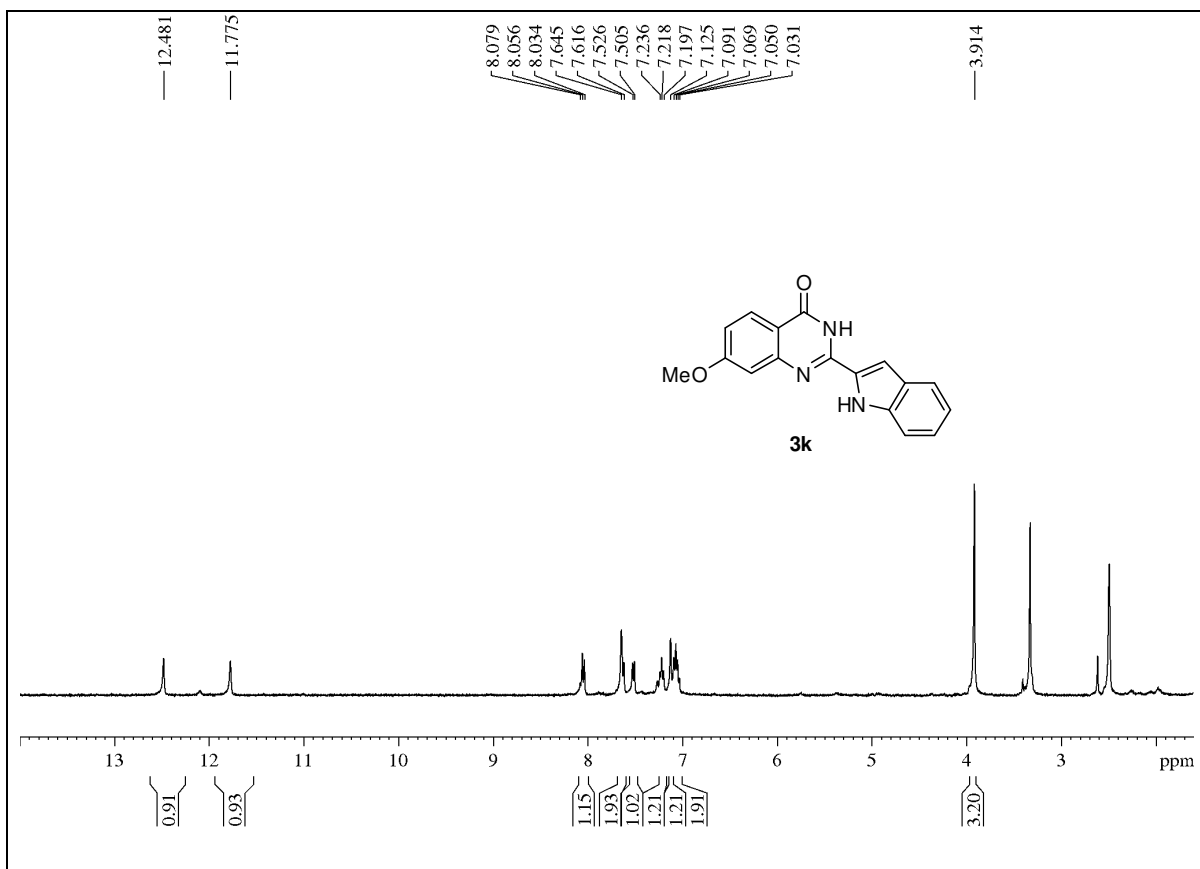
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.788	0.560	1.043	73767456	5944592	12.40		100.00		338.20	2051111
				73767456	5944592			100.00			

FLASH EA 1112 SERIES CHN REPORT
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Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-622 (# 143)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-3.dat
Sample weight: 1.341



Element Name	Element %	Ret. Time
Nitrogen	12.38	0.77
Carbon	67.49	1.14
Hydrogen	5.73	4.13



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Analysis Info

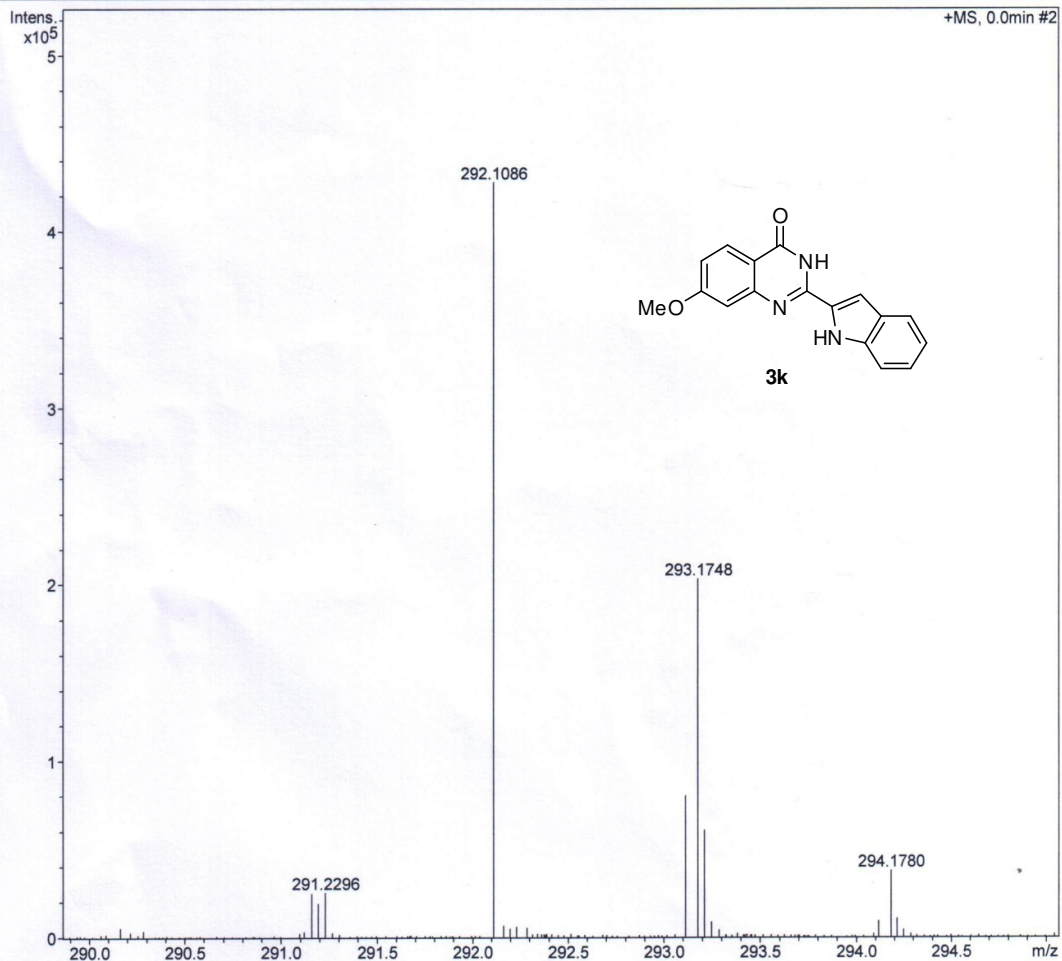
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-401.d
Method TL-P.m
Sample Name SKG-401-DCM-MEOH
Comment

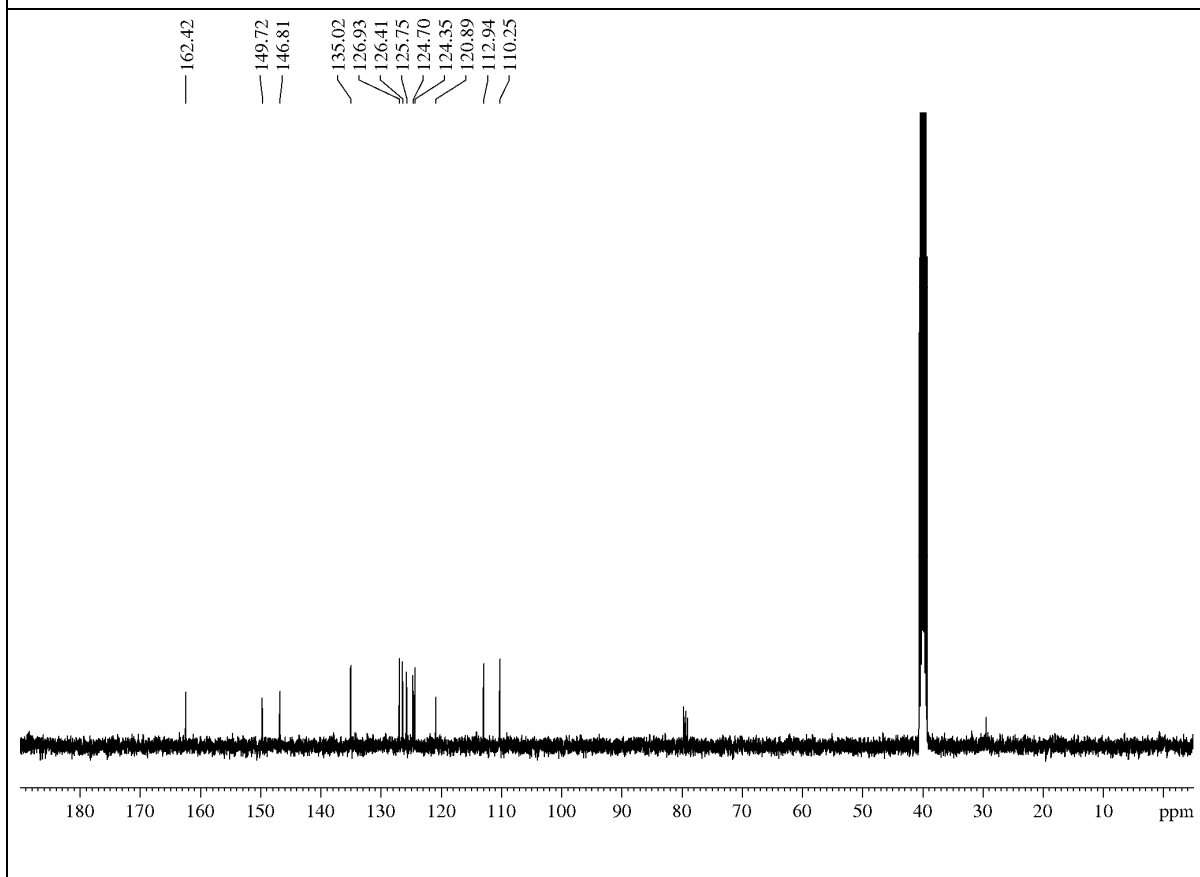
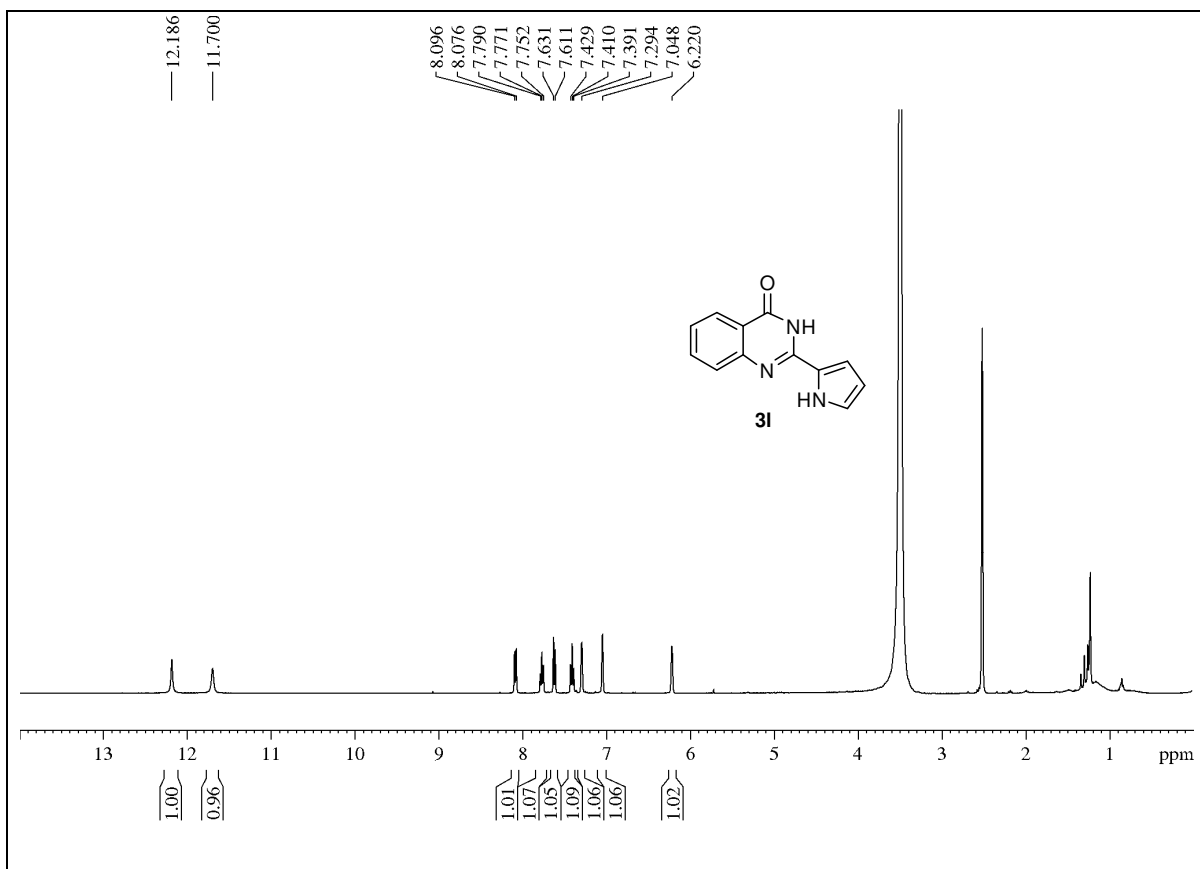
Acquisition Date 7/2/2015 12:02:43 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



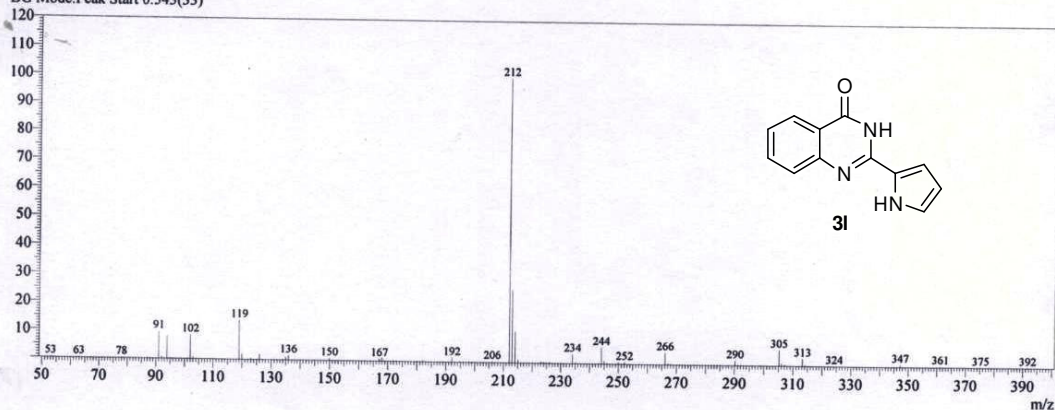


LCMS-2010A DATA REPORT
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User : Admin
Sample : SKG-321
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-321-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.799(Scan#:48) Positive
MassPeaks:249 BasePeak:212.05(14257197)
RawMode:Single 0.799(48)
BG Mode:Peak Start 0.543(33)



MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.799	0.543	1.010	344634718	26479198	13.01		100.00		212.05	14257197
				344634718	26479198			100.00			

FLASH EA 1112 SERIES CHN REPORT
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Method filename:

Sample ID:

Analysis type:

Chromatogram filename:

Sample weight:

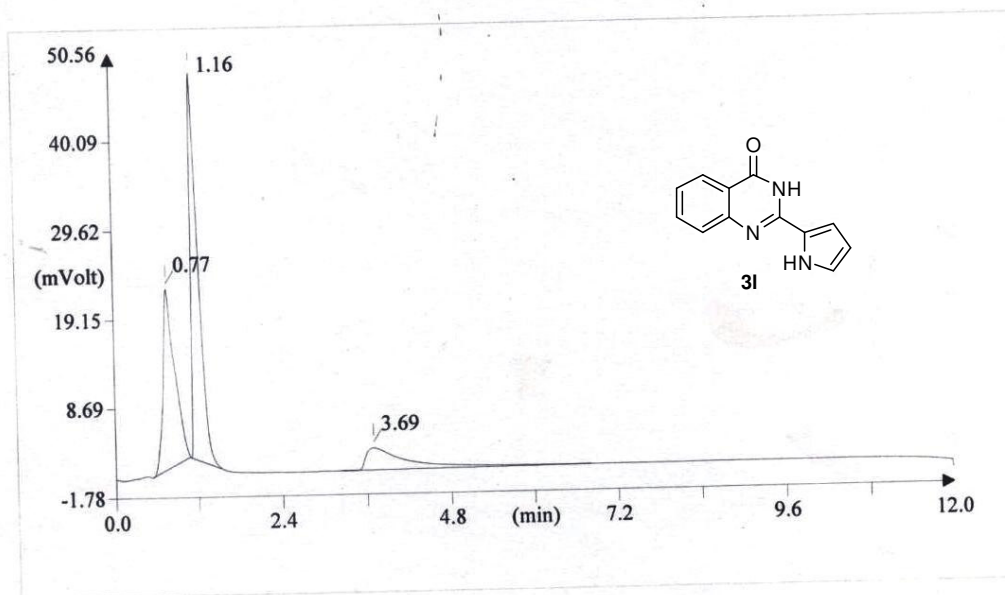
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SKG-321 (# 163)

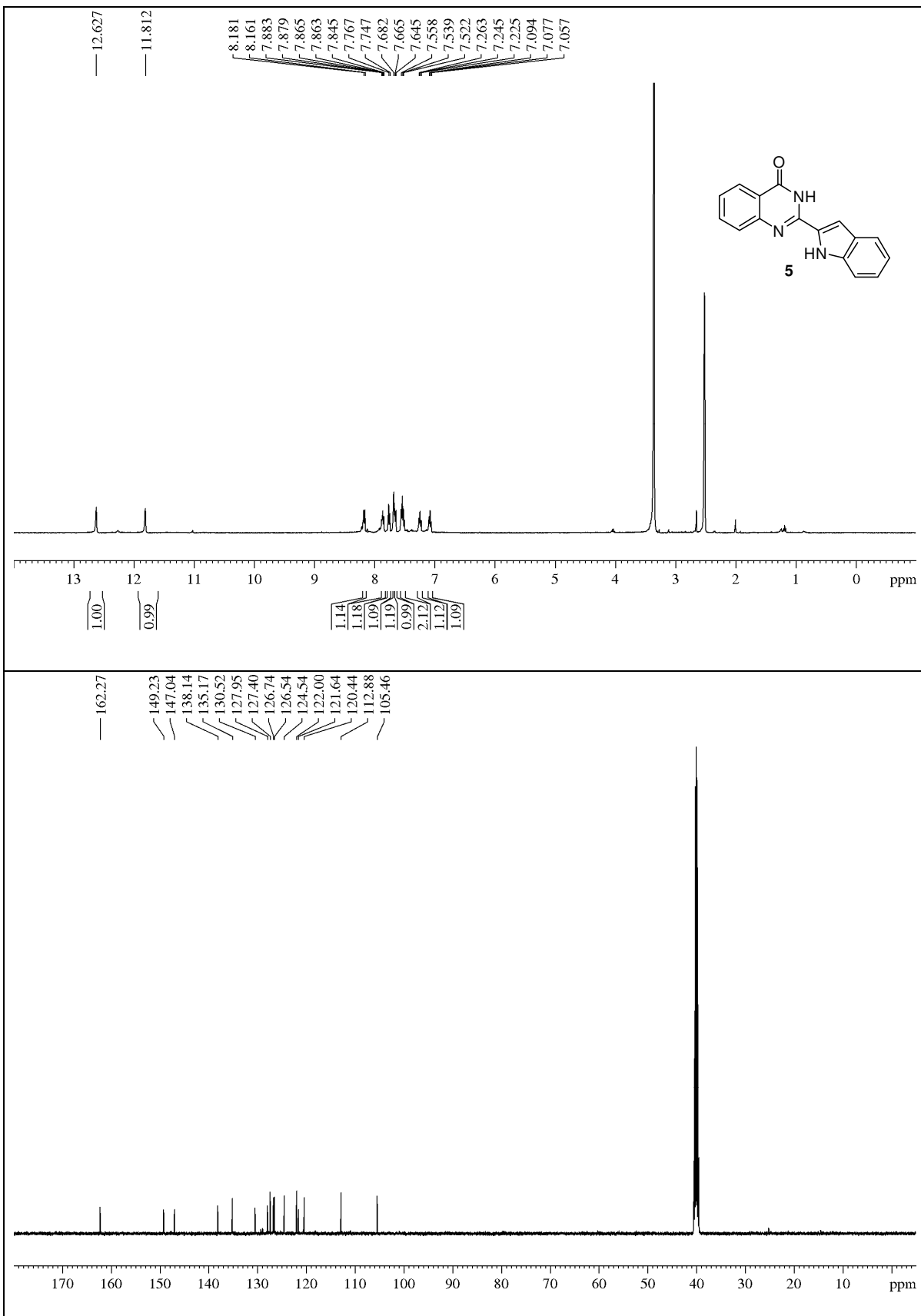
UnkNown

UNK-18022015-23.dat

1.153



Element Name	Element %	Ret. Time
Nitrogen	19.78	0.77
Carbon	68.15	1.16
Hydrogen	4.36	3.69



BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

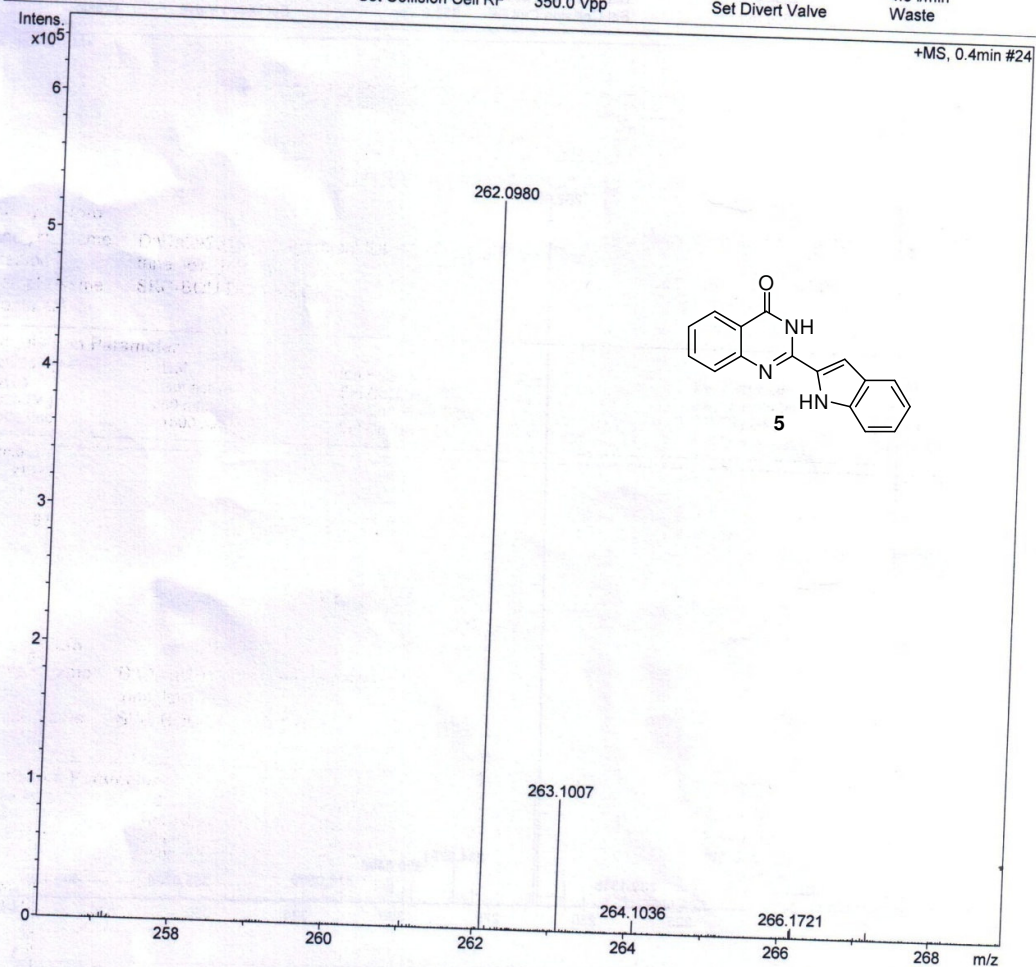
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-BOU-R.d
Method tune_low_Pos.m
Sample Name SKG-BOU-DCM-MEOH
Comment

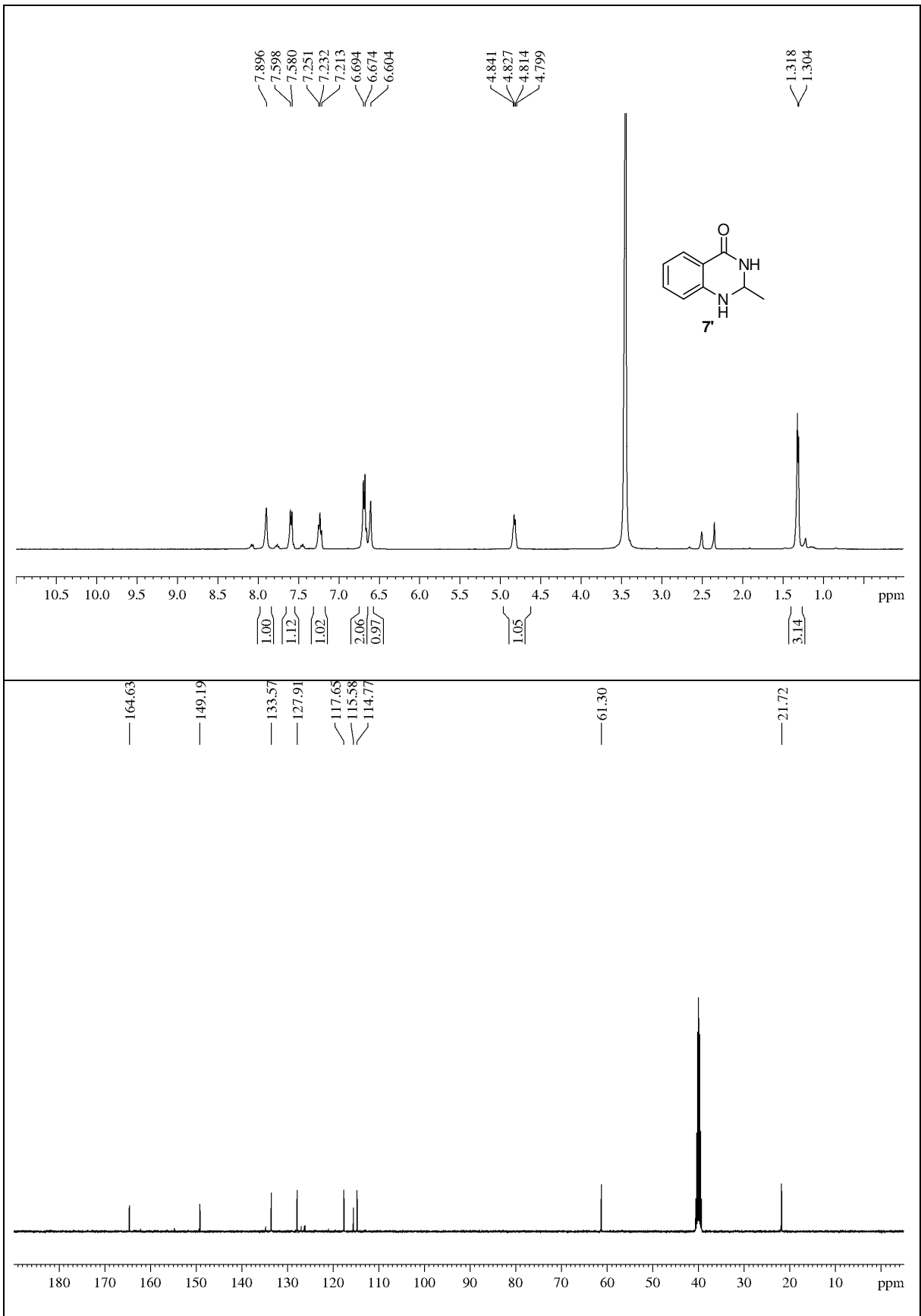
Acquisition Date 7/20/2015 12:29:37 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

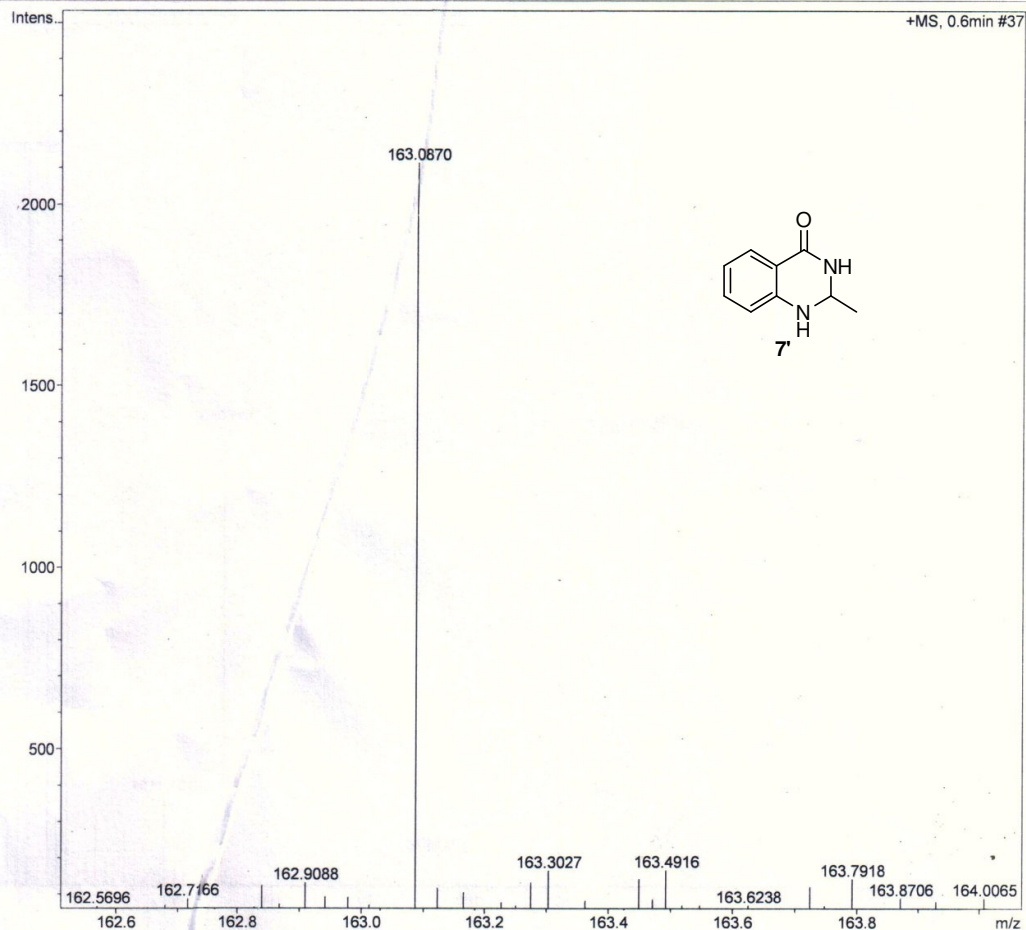
Analysis Name D:\Data\2015\DrNagarajan\mar\SKG-614.d
Method tune_low_Pos.m
Sample Name SKG-614DCM-MEOH
Comment

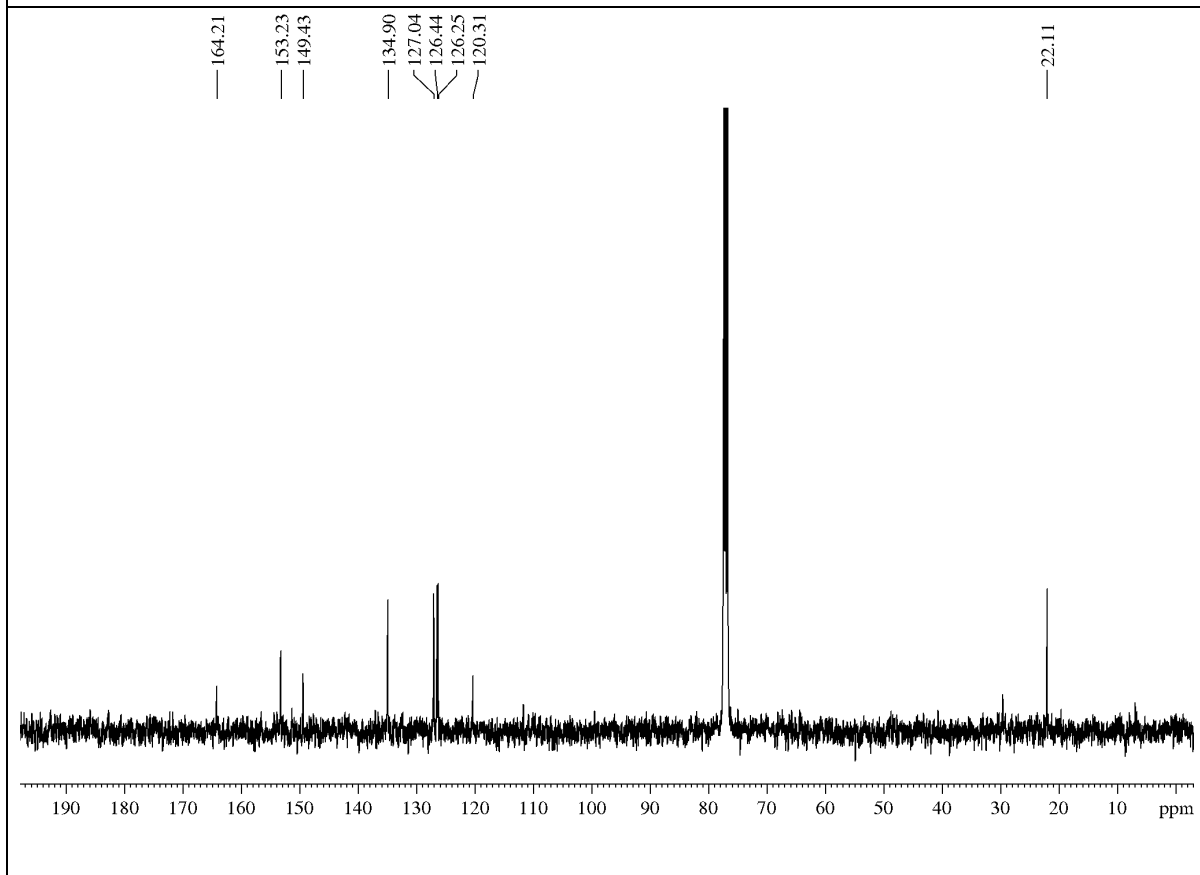
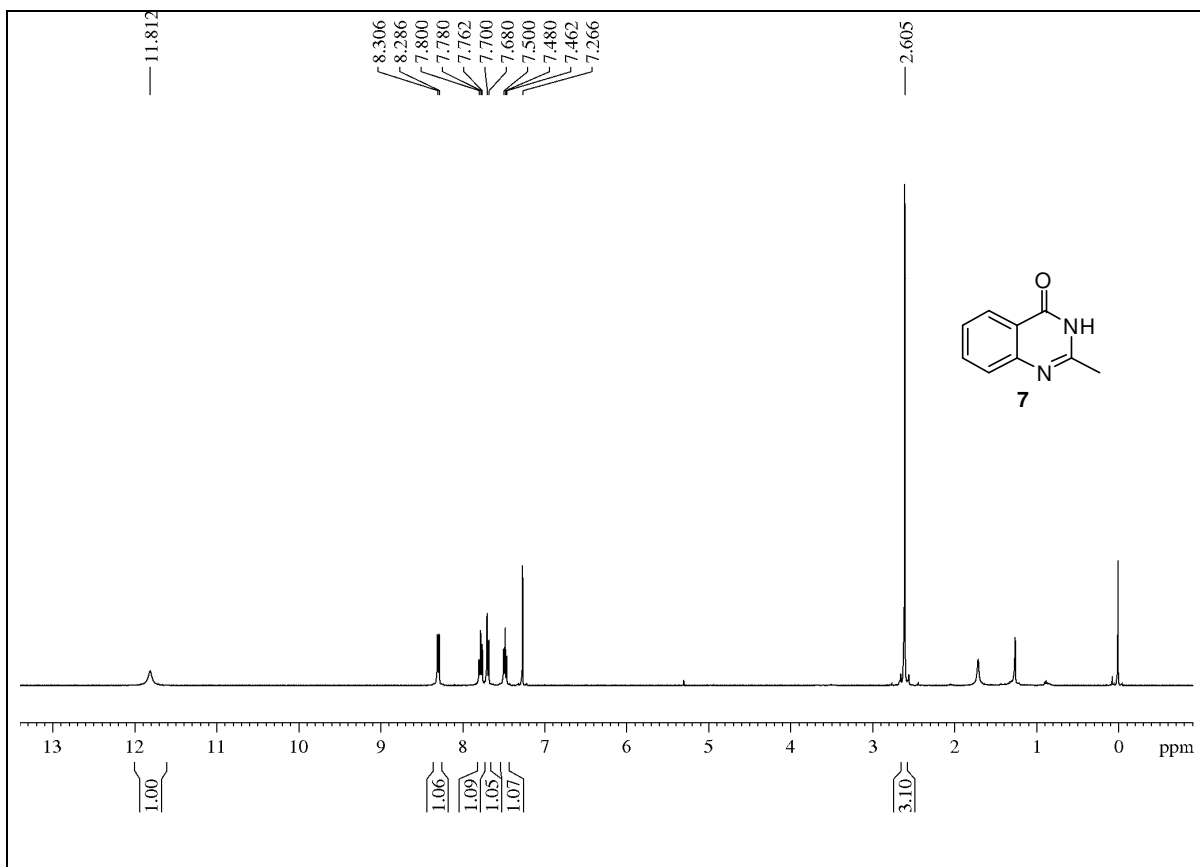
Acquisition Date 3/5/2015 11:02:02 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	10.0 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	10.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

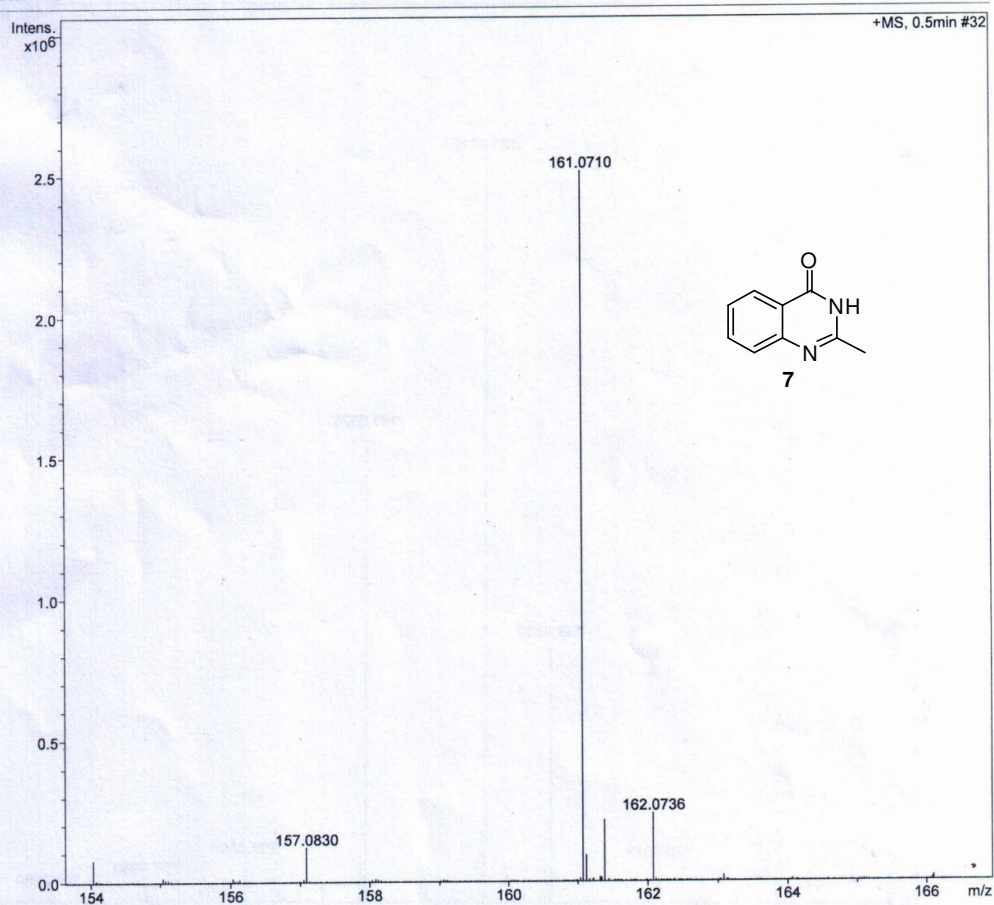
Analysis Name D:\Data\2015\DrNagarajan\mar\SKG-625.d
Method tune_low_Pos.m
Sample Name SKG-625-DCM-MEOH
Comment

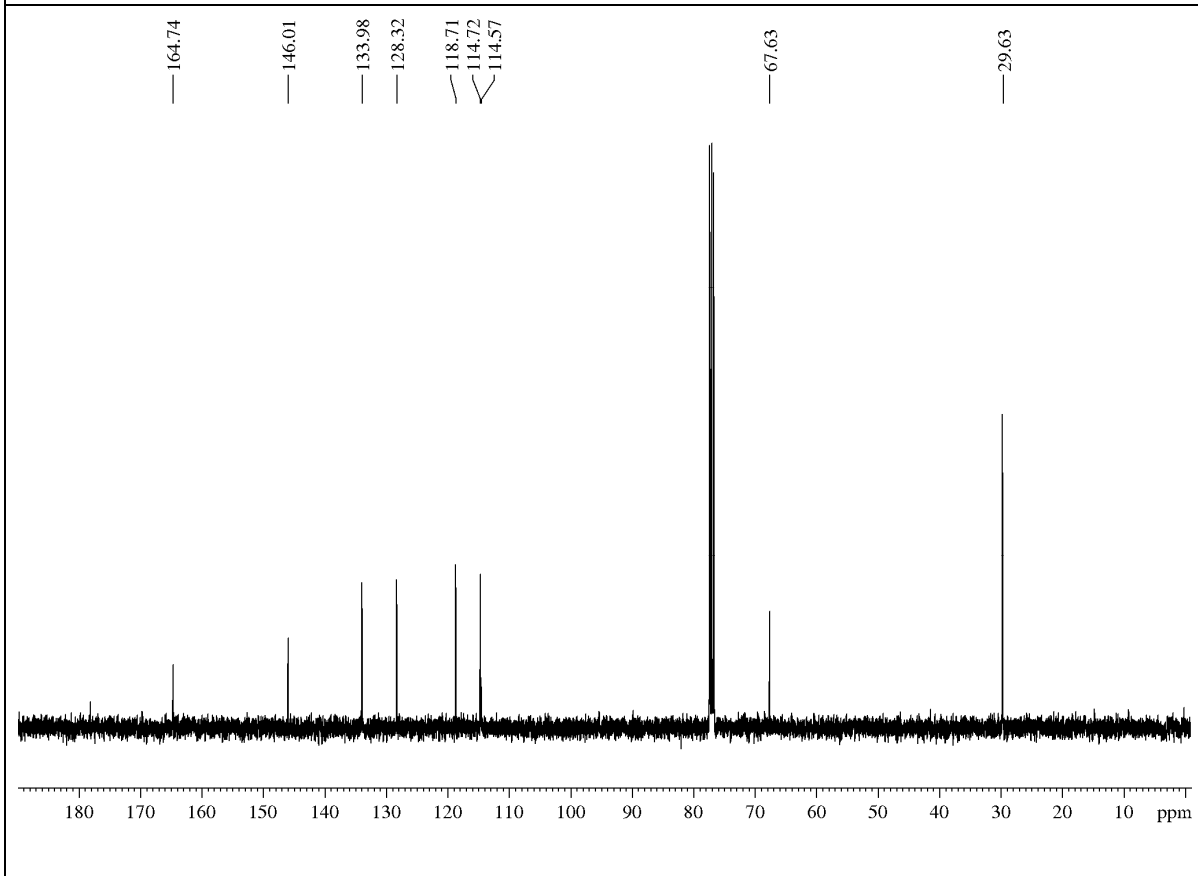
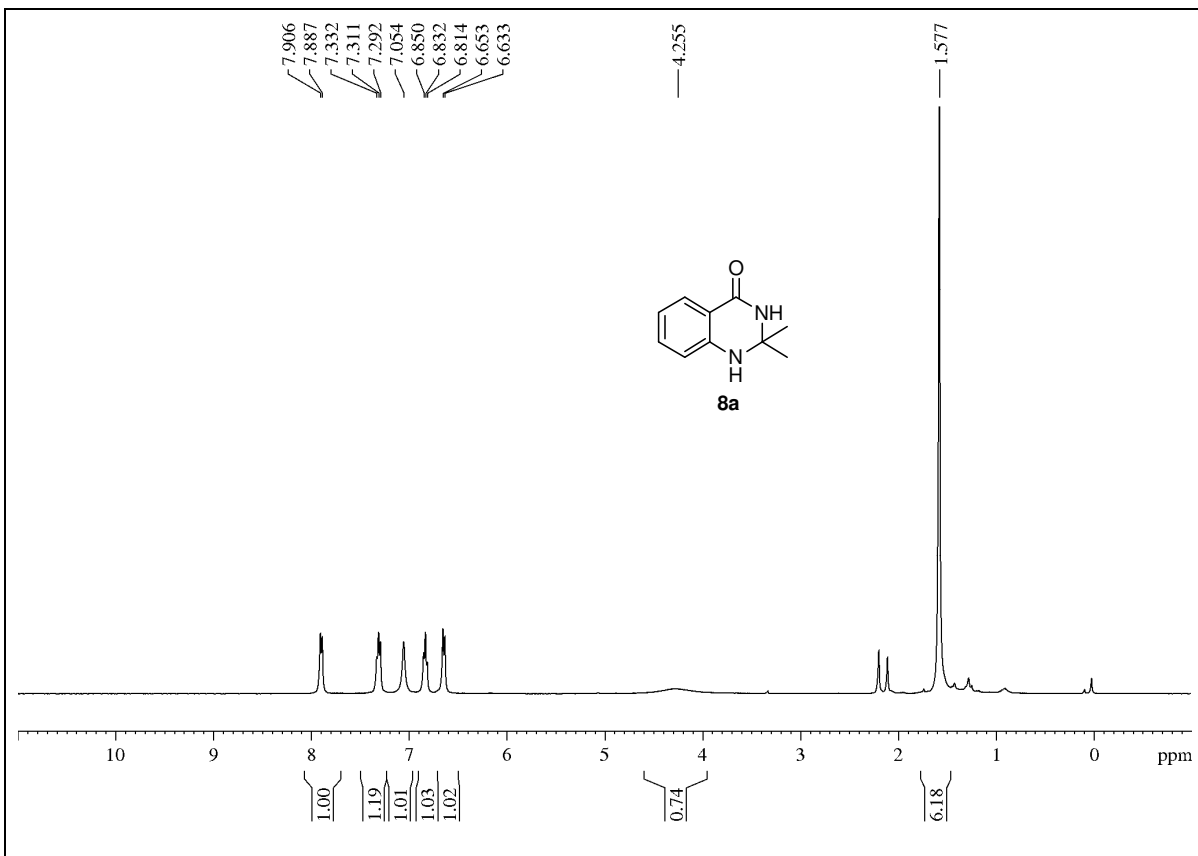
Acquisition Date 3/5/2015 10:52:18 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	6.0 psi
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



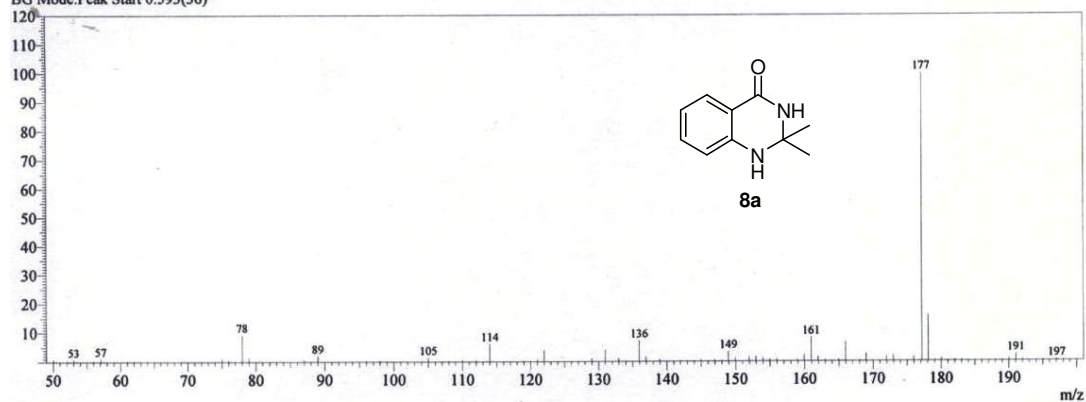


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-676
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-676-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#: 1 R.Time: 0.782(Scan#: 47) Positive
MassPeaks: 85 BasePeak: 177.15(31741)
RawMode: Single 0.782(47)
BG Mode: Peak Start 0.593(36)



Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.782	0.593	0.943	2487266	253416	9.81		100.00		177.15	31741
				2487266	253416			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename:

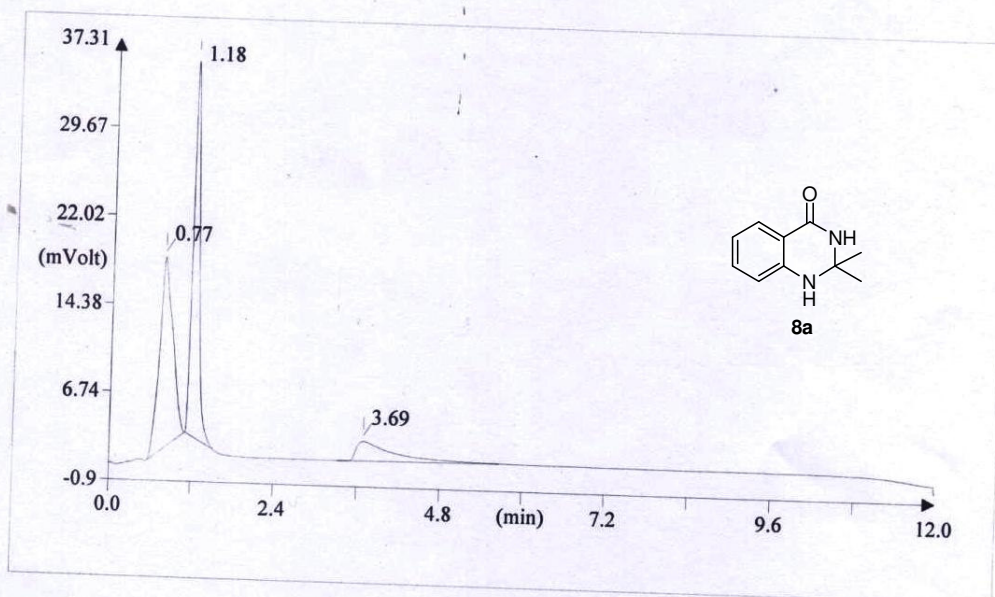
Sample ID:

Analysis type:

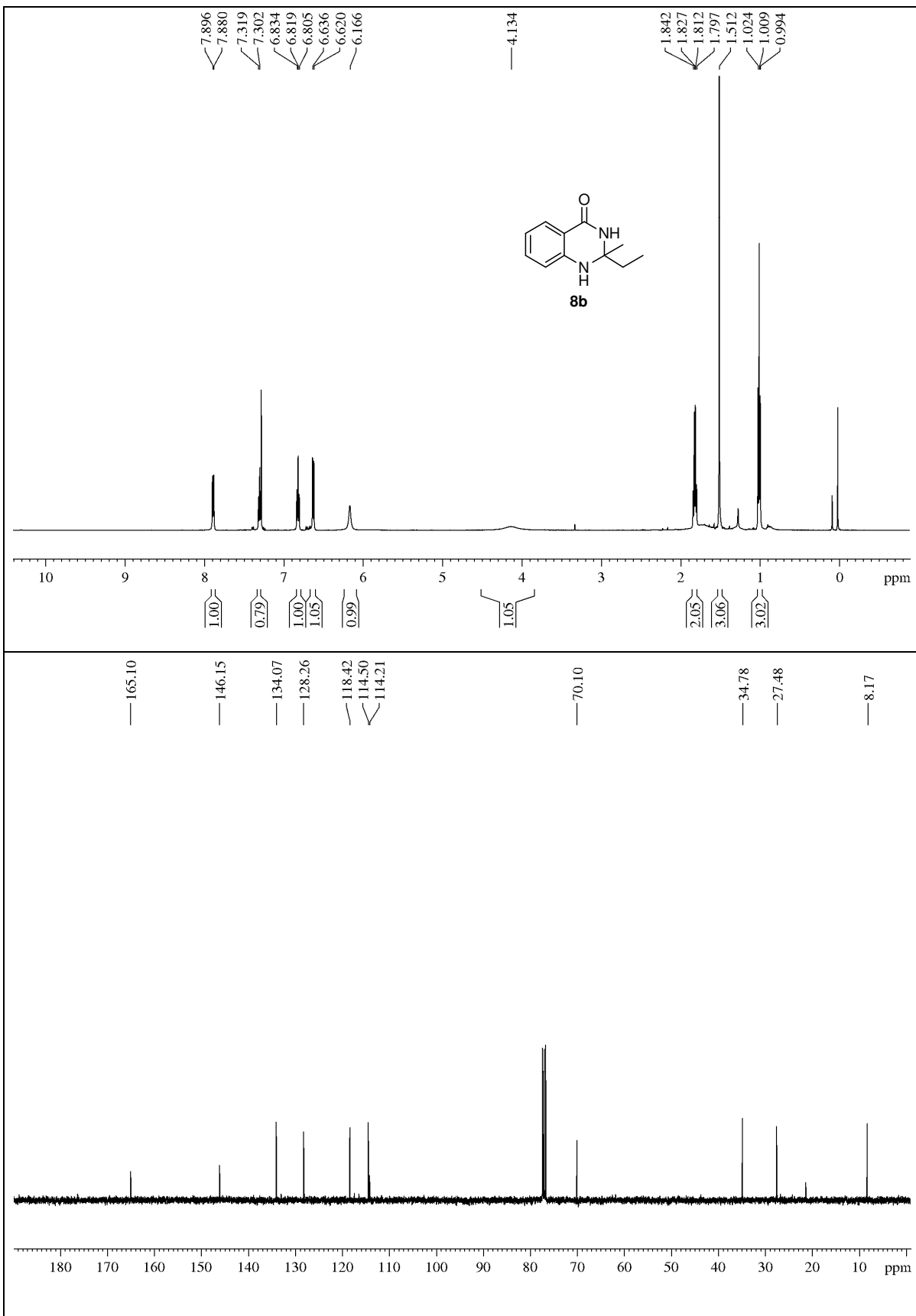
Chromatogram filename:

Sample weight:

C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
SKG-676 (# 162)
UnkNown
UNK-18022015-22.dat
1.119



Element Name	Element %	Ret. Time
Nitrogen	15.82	0.77
Carbon	68.26	1.18
Hydrogen	6.81	3.69

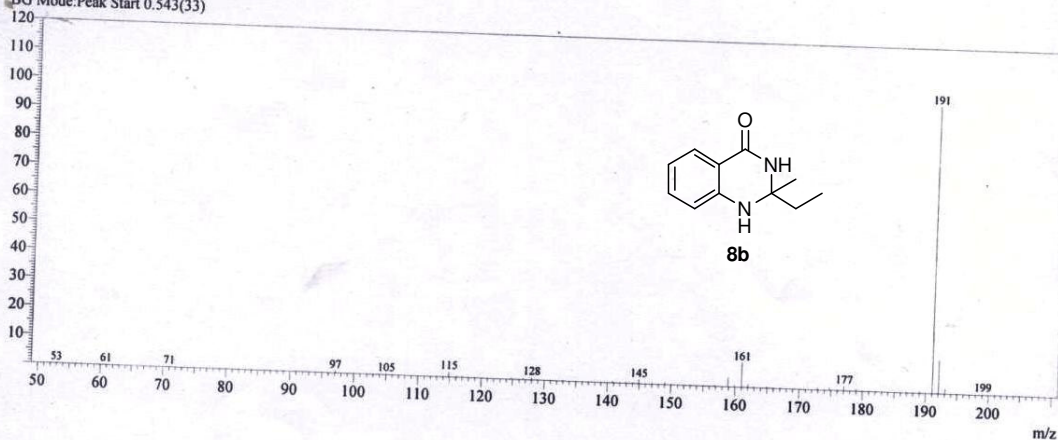


LCMS-2010A DATA REPORT SCHOOL OF CHEMISTRY UNIVERSITY OF HYDERABAD

User : Admin
 Sample : SKG-675
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\SKG-675-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

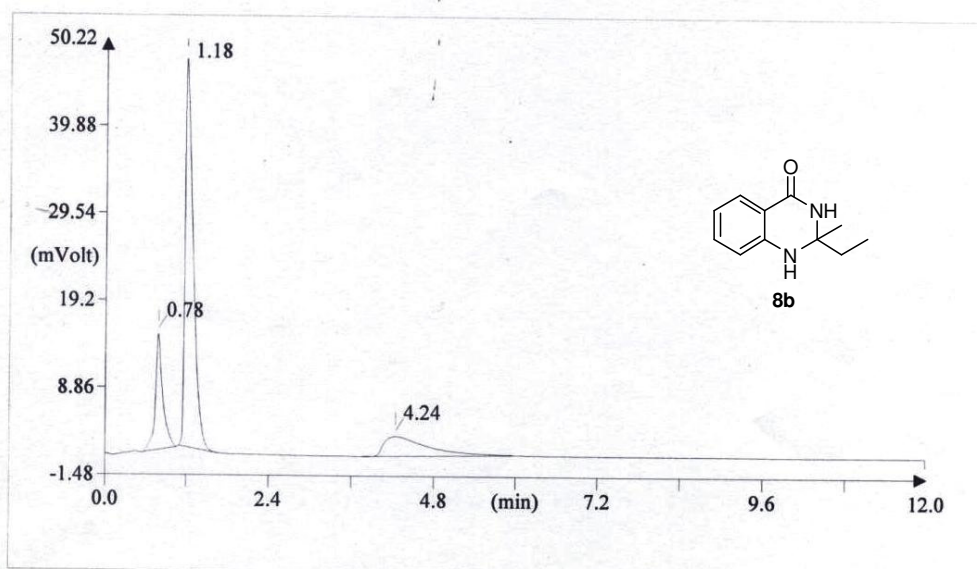
Line#:1 R.Time:0.780(Scan#:47) Positive
 MassPeaks:108 BasePeak:191.05(10128940)
 RawMode:Single 0.780(47)
 BG Mode:Peak Start 0.543(33)



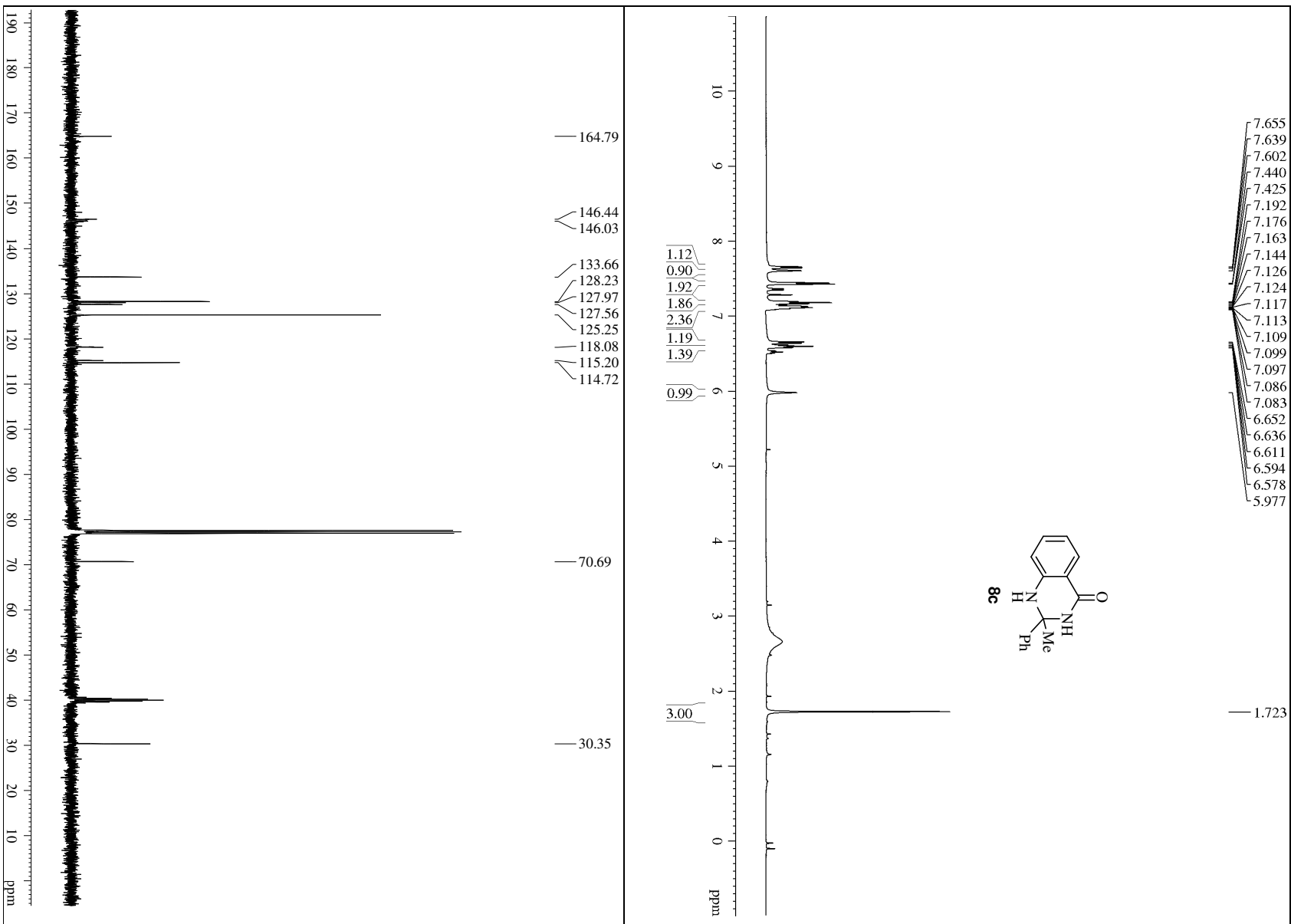
Peak#	R. Time	I. Time	F. Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.780	0.543	1.043	240182538	19357889	12.40		100.00		191.05	10128940
				240182538	19357889			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-675 (#161)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-21.dat
Sample weight: 1.241



Element Name	Element %	Ret. Time
Nitrogen	14.62	0.78
Carbon	69.56	1.18
Hydrogen	7.35	4.24



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Analysis Info

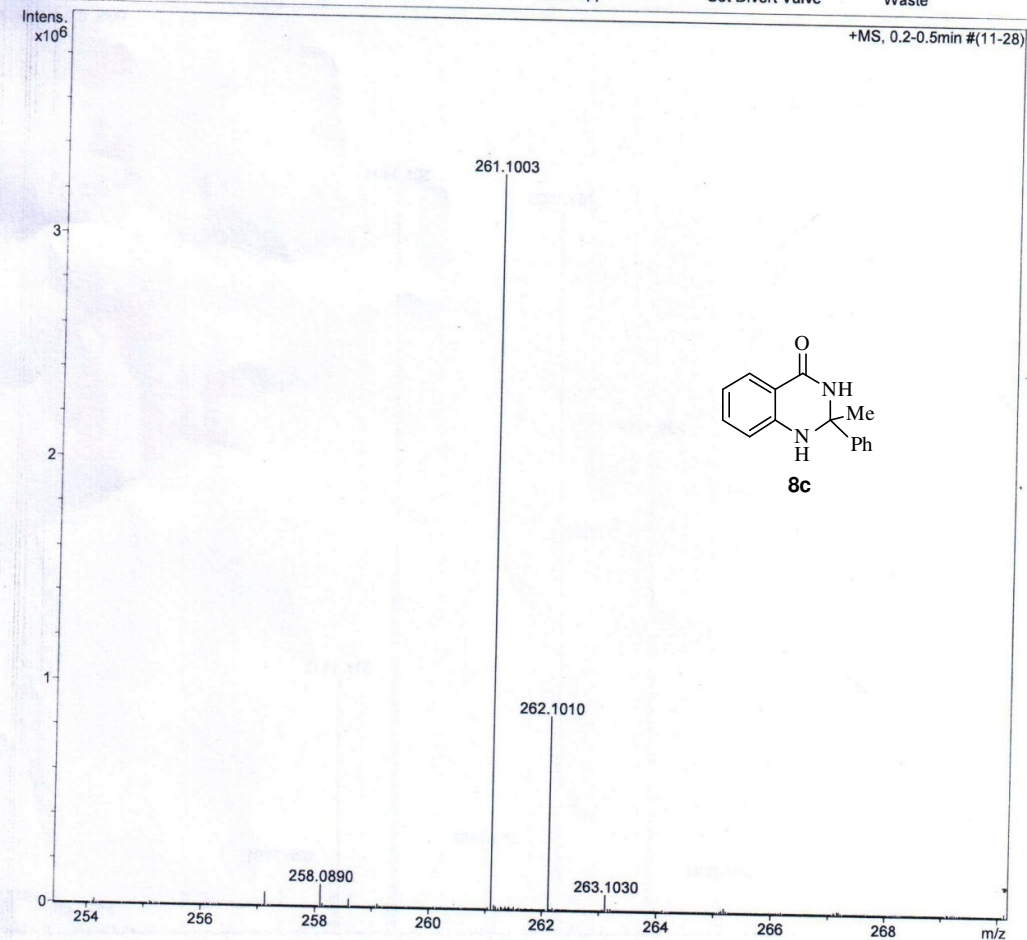
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-724.d
Method tune_low.m
Sample Name SKG-724-DCM-MEOH
Comment

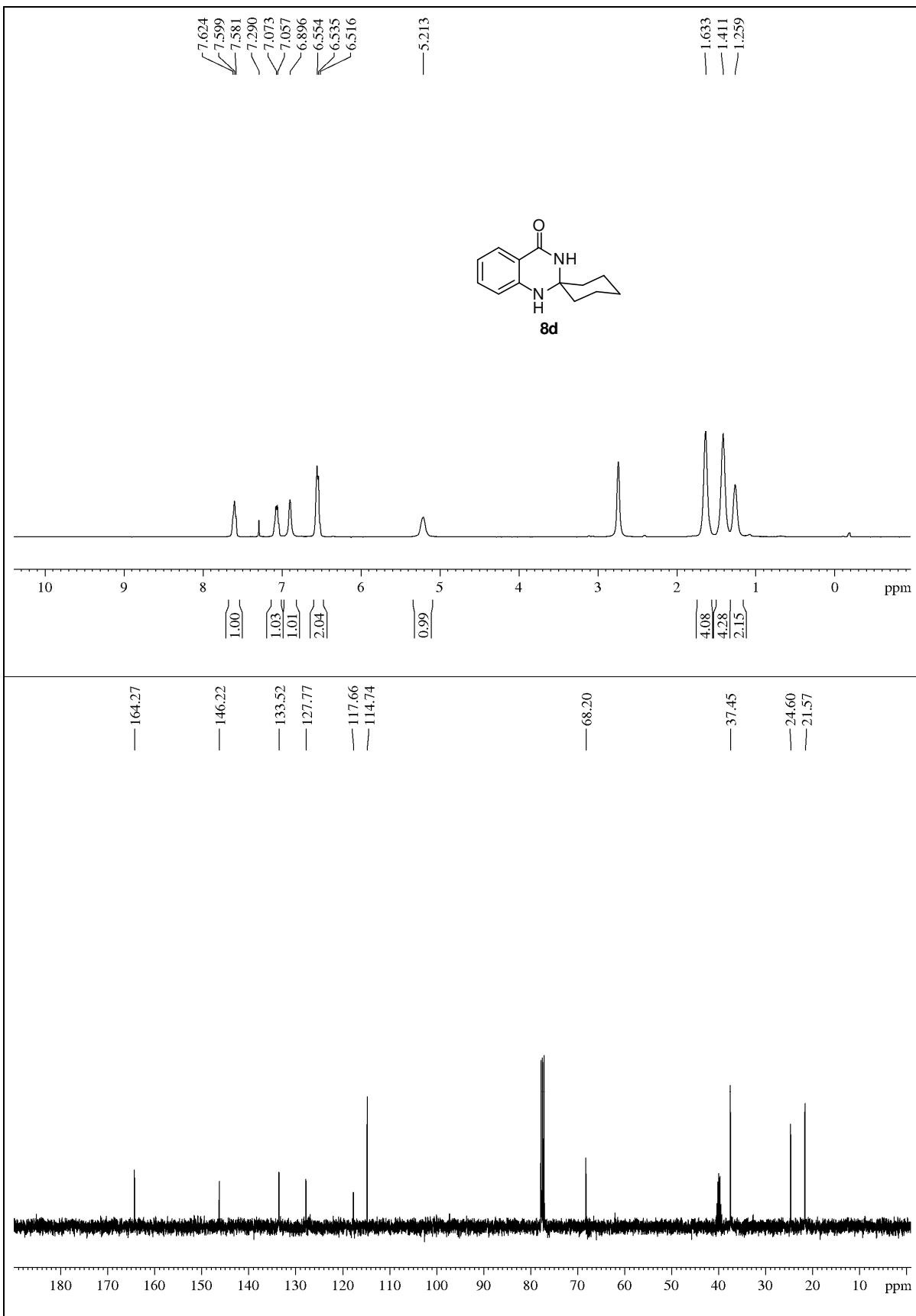
Acquisition Date 7/2/2015 11:48:30 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	6.0 psi
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



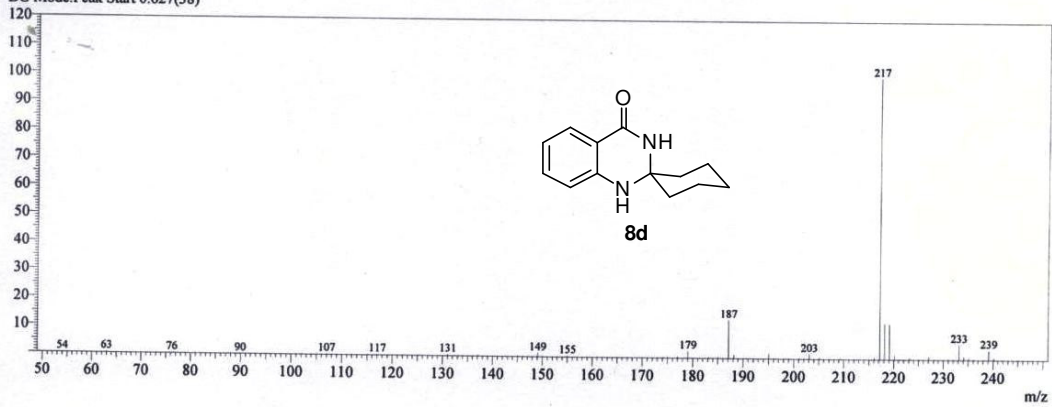


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-679
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-679-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

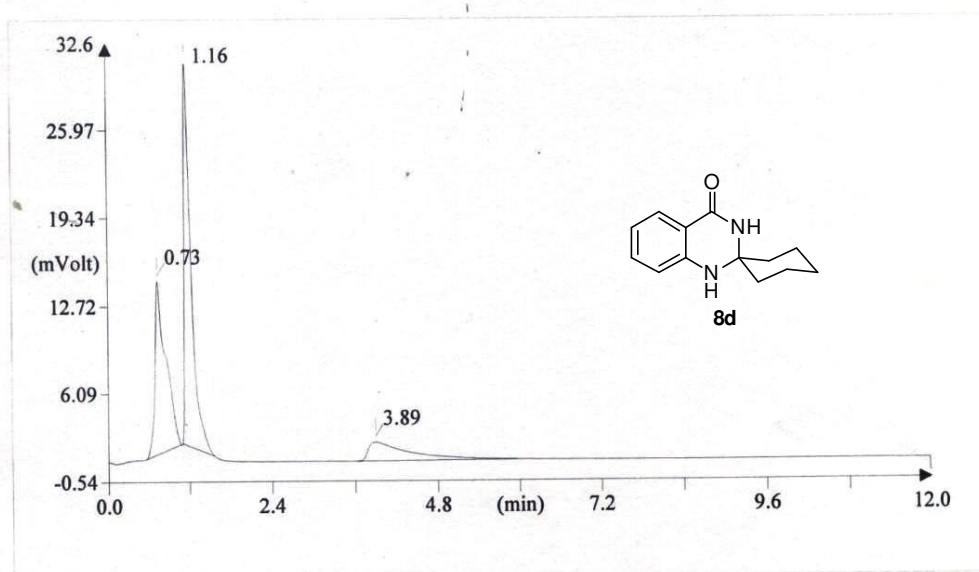
Line#: 1 R.Time: 0.845(Scan#: 51) Positive
MassPeaks: 99 BasePeak: 217.15(3171594)
RawMode: Single 0.845(51)
BG Mode: Peak Start 0.627(38)



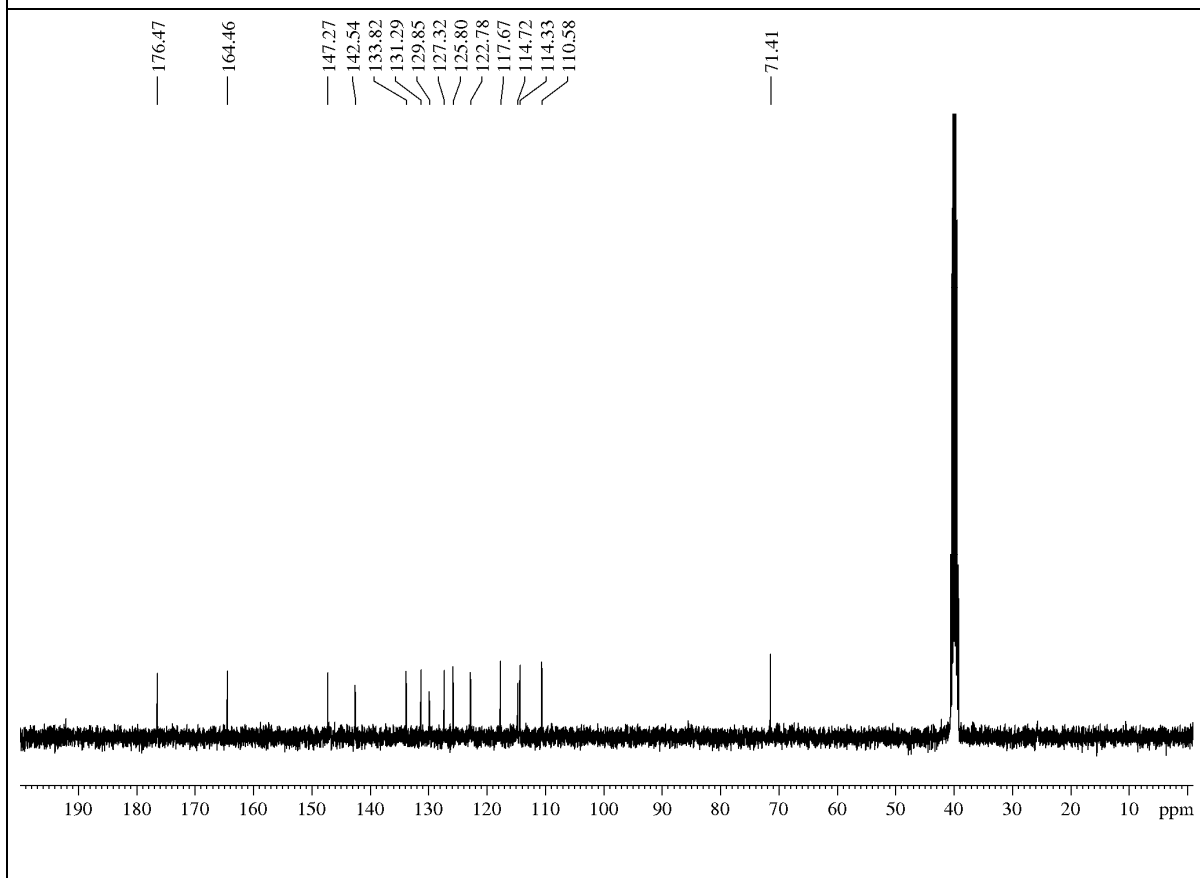
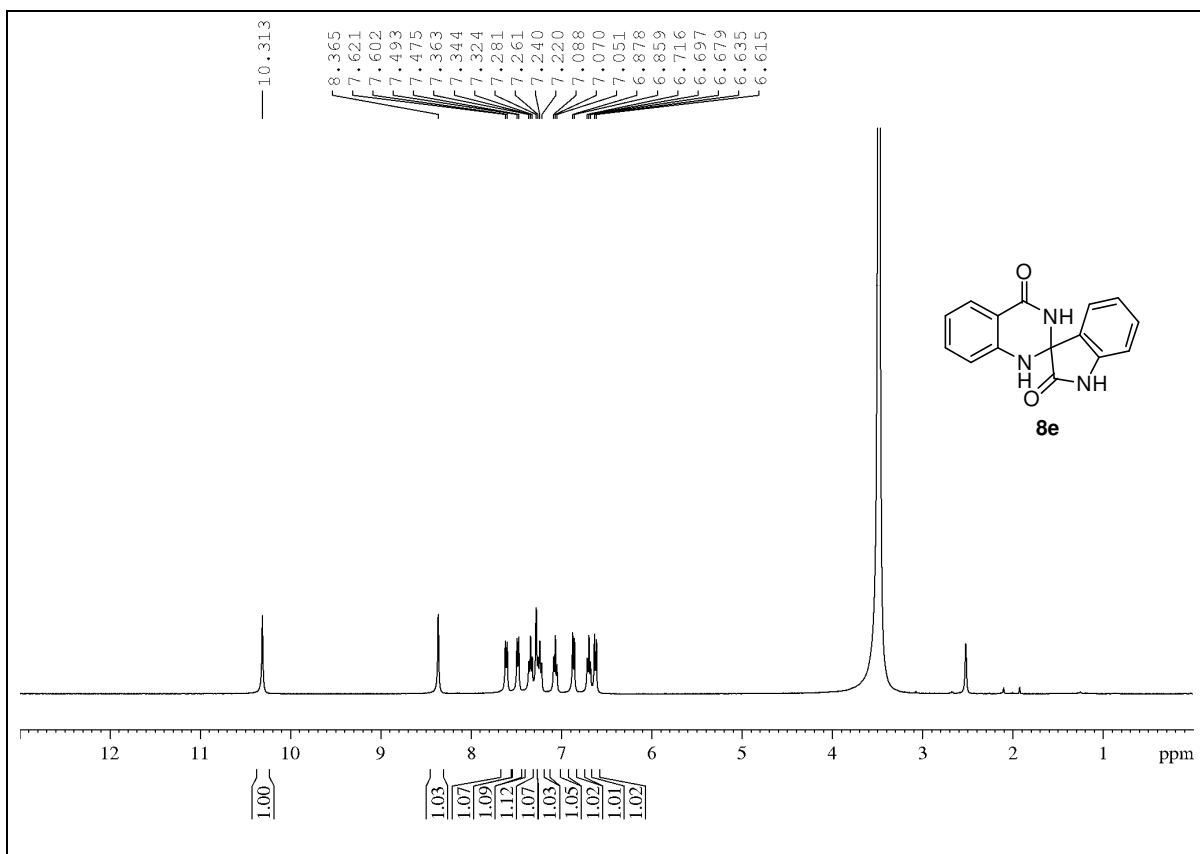
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.845	0.627	1.143	120622280	10580566	11.40		100.00		217.15	3171594
				120622280	10580566			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-679 (# 146)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-6.dat
Sample weight: 1.112



Element Name	Element %	Ret. Time
Nitrogen	13.07	0.73
Carbon	72.25	1.16
Hydrogen	7.41	3.89

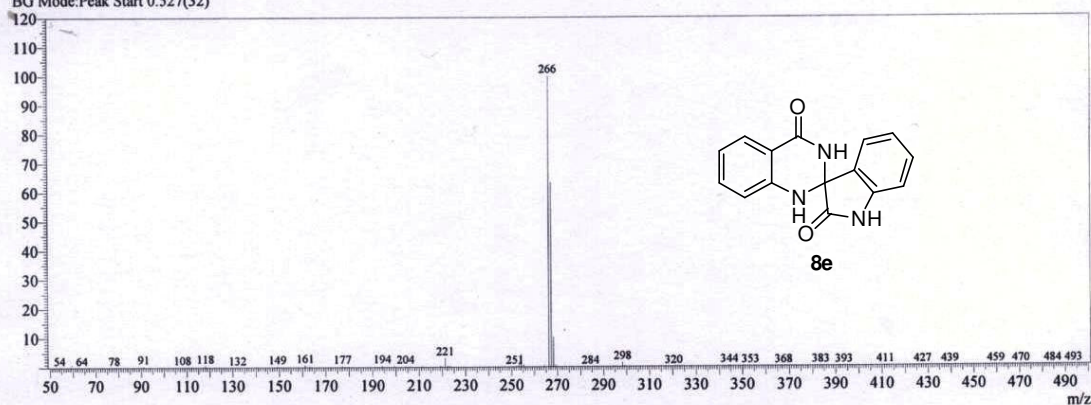


**LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD**

User : Admin
Sample : SKG-678
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-678-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.964(Scan#:58) Positive
MassPeaks:181 BasePeak:266.25(14363291)
RawMode:Single 0.964(58)
BG Mode:Peak Start 0.527(32)



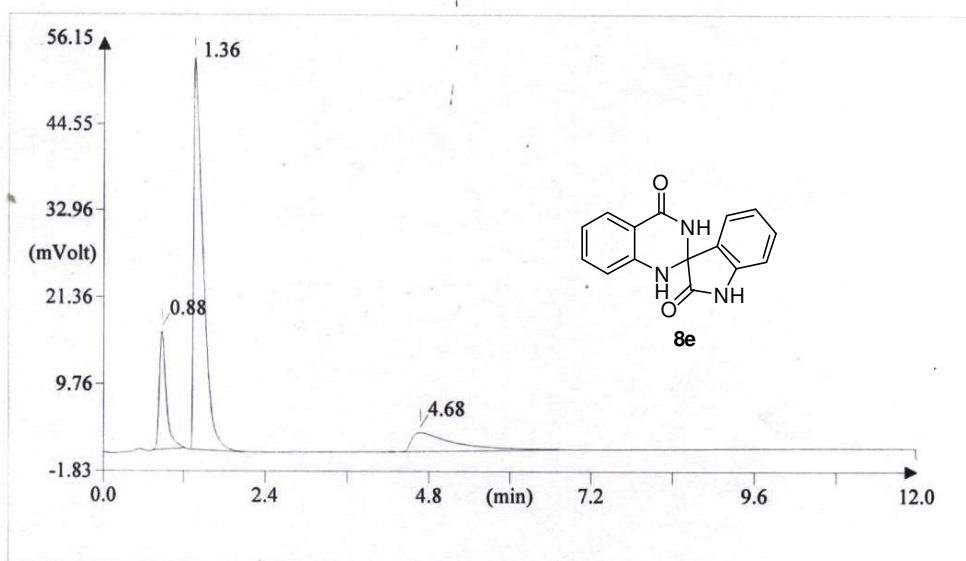
MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.964	0.527	1.143	226437874	7121250	31.79		100.00	
				226437874	7121250			100.00	

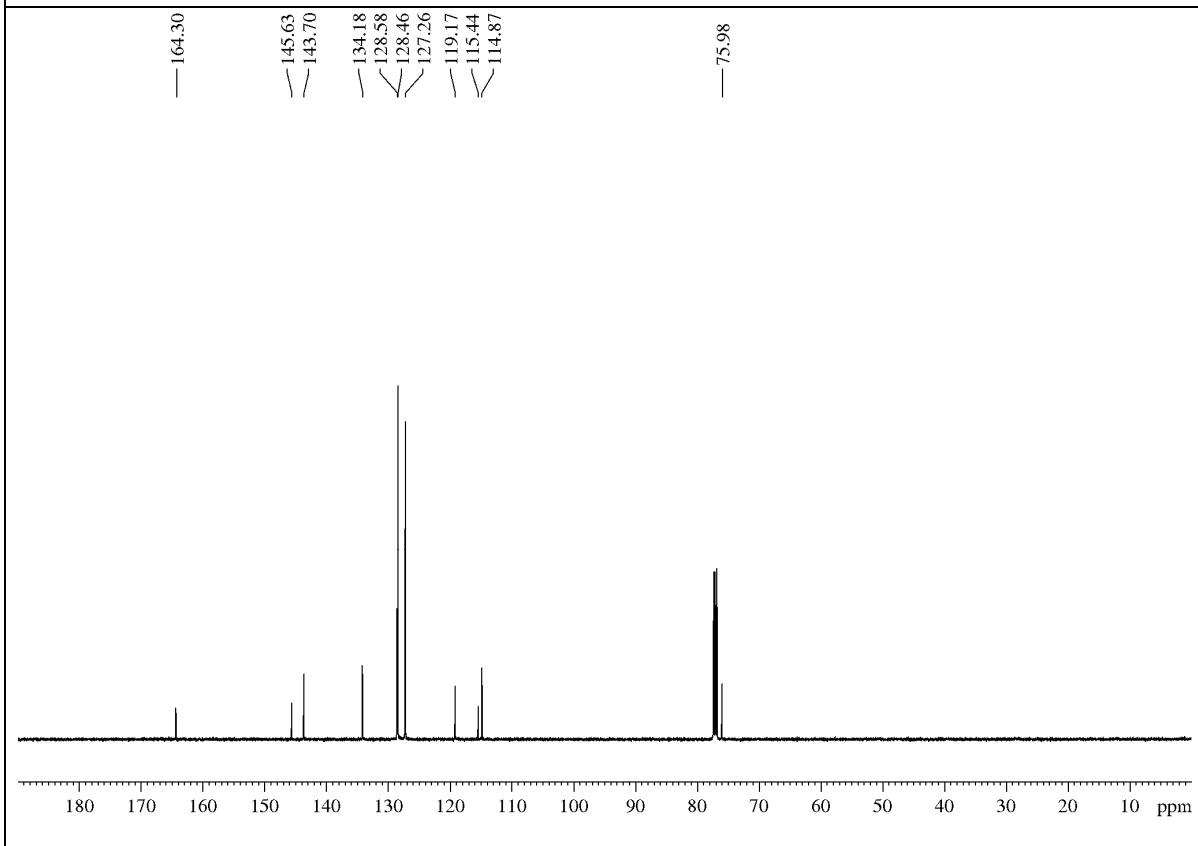
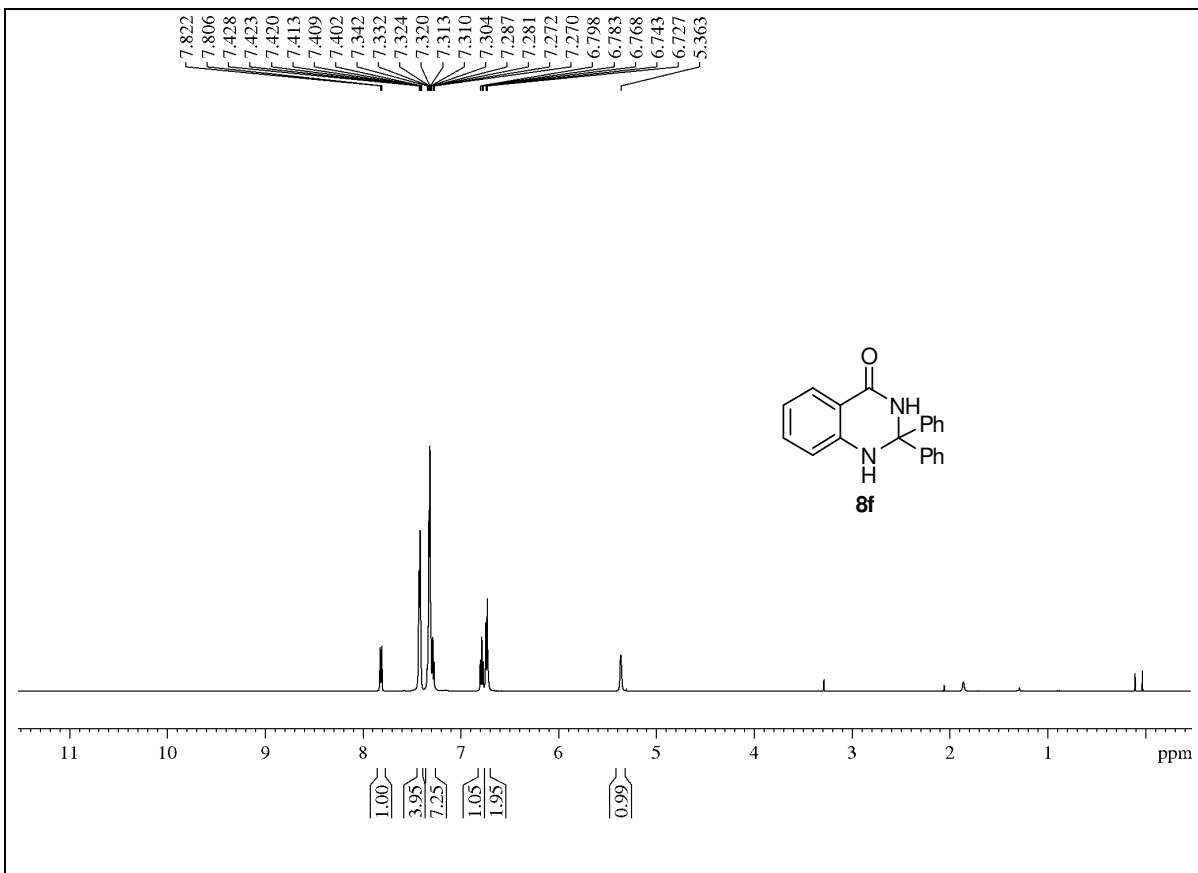
Base m/z Base Int.
266.25 14363291

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-678 (# 158)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-18.dat
Sample weight: 1.263



Element Name	Element %	Ret. Time
Nitrogen	15.76	0.88
Carbon	67.85	1.36
Hydrogen	4.12	4.68



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Analysis Info

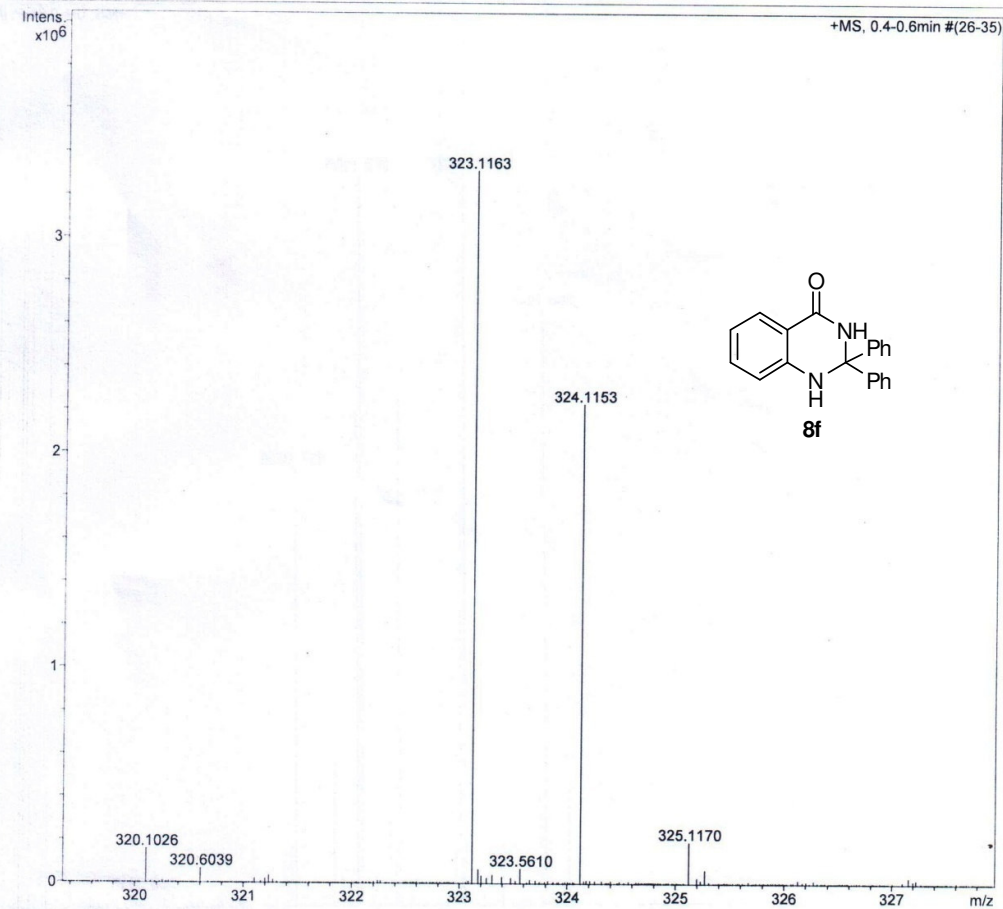
Analysis Name D:\Data\2015\DrNagarajan\JULY\SKG-726R1.d
Method tune_low.m
Sample Name SKG-726-DCM-MEOH
Comment

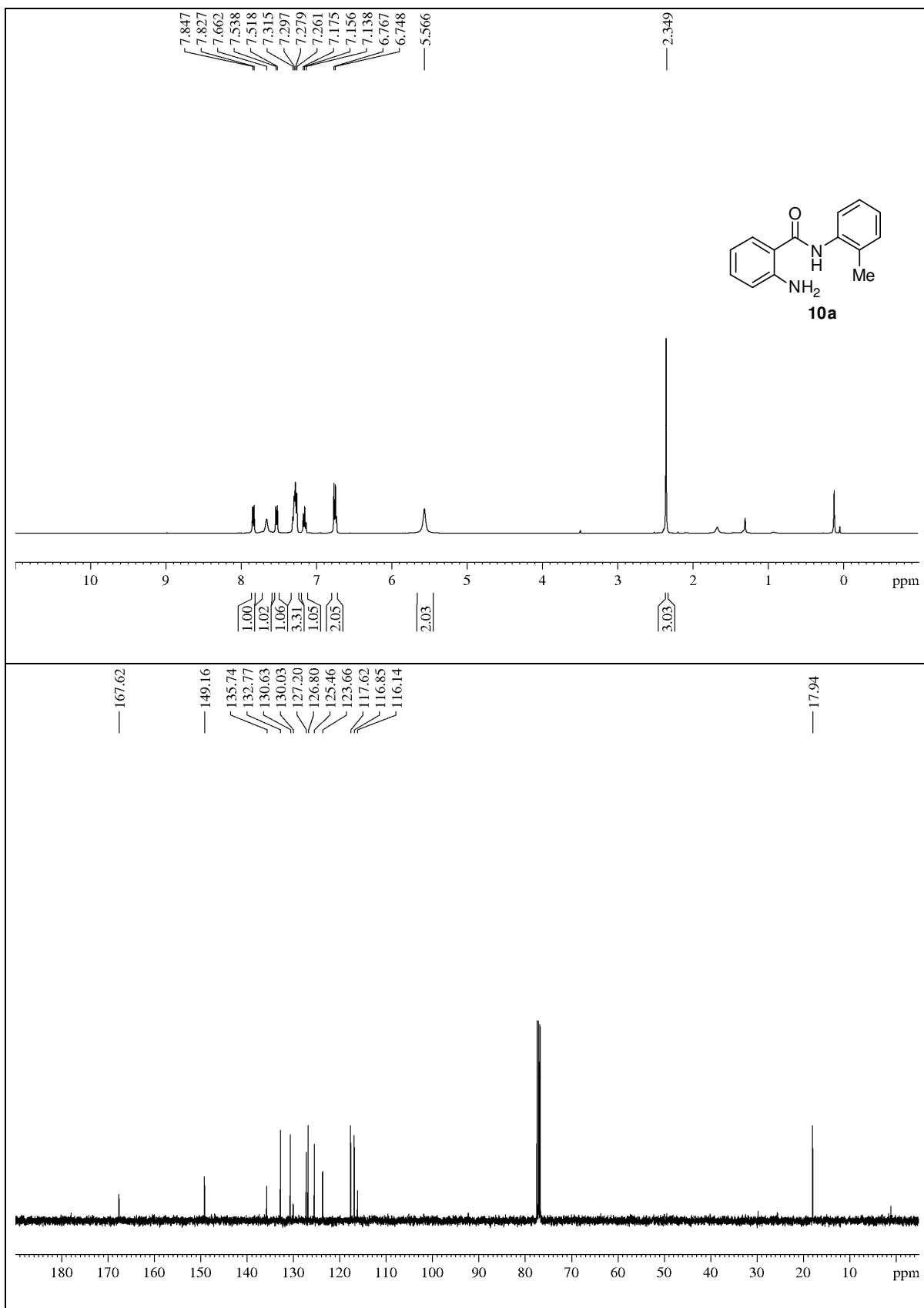
Acquisition Date 7/2/2015 12:15:13 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

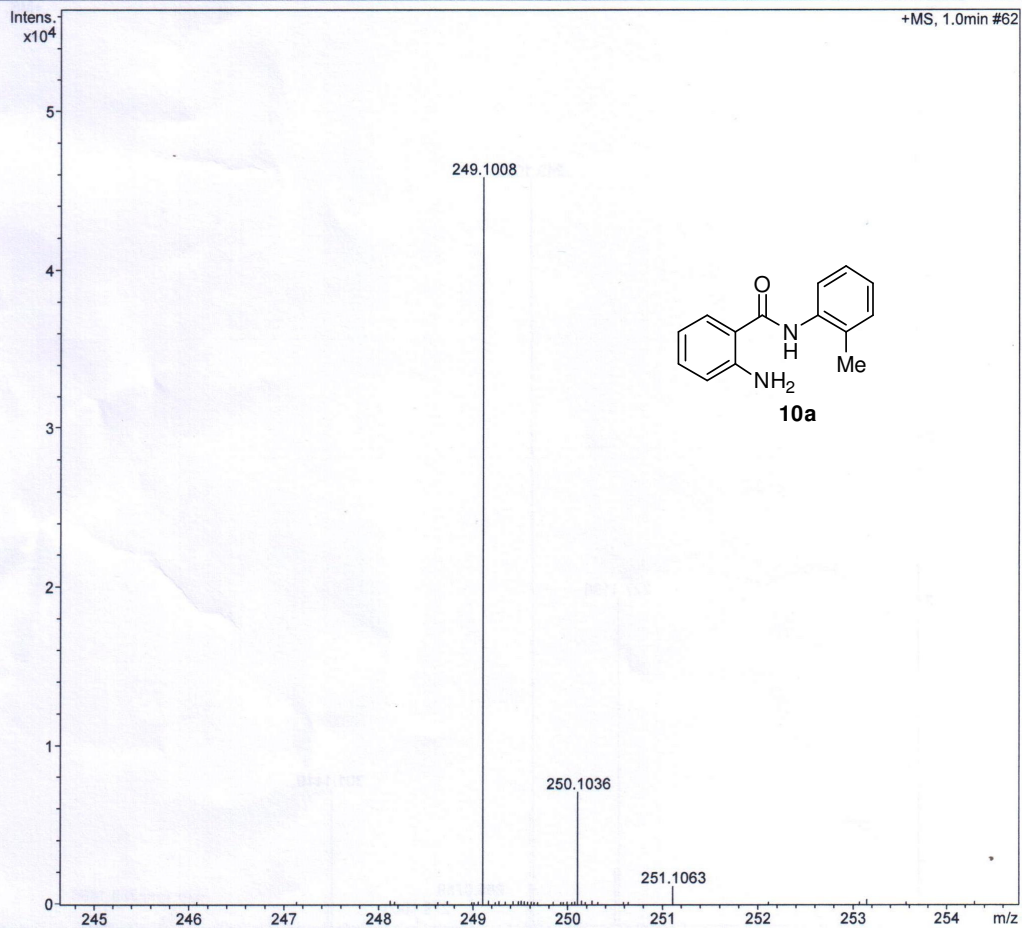
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-644.d
Method tune_low.m
Sample Name SKG-644-DCM-MEOH
Comment

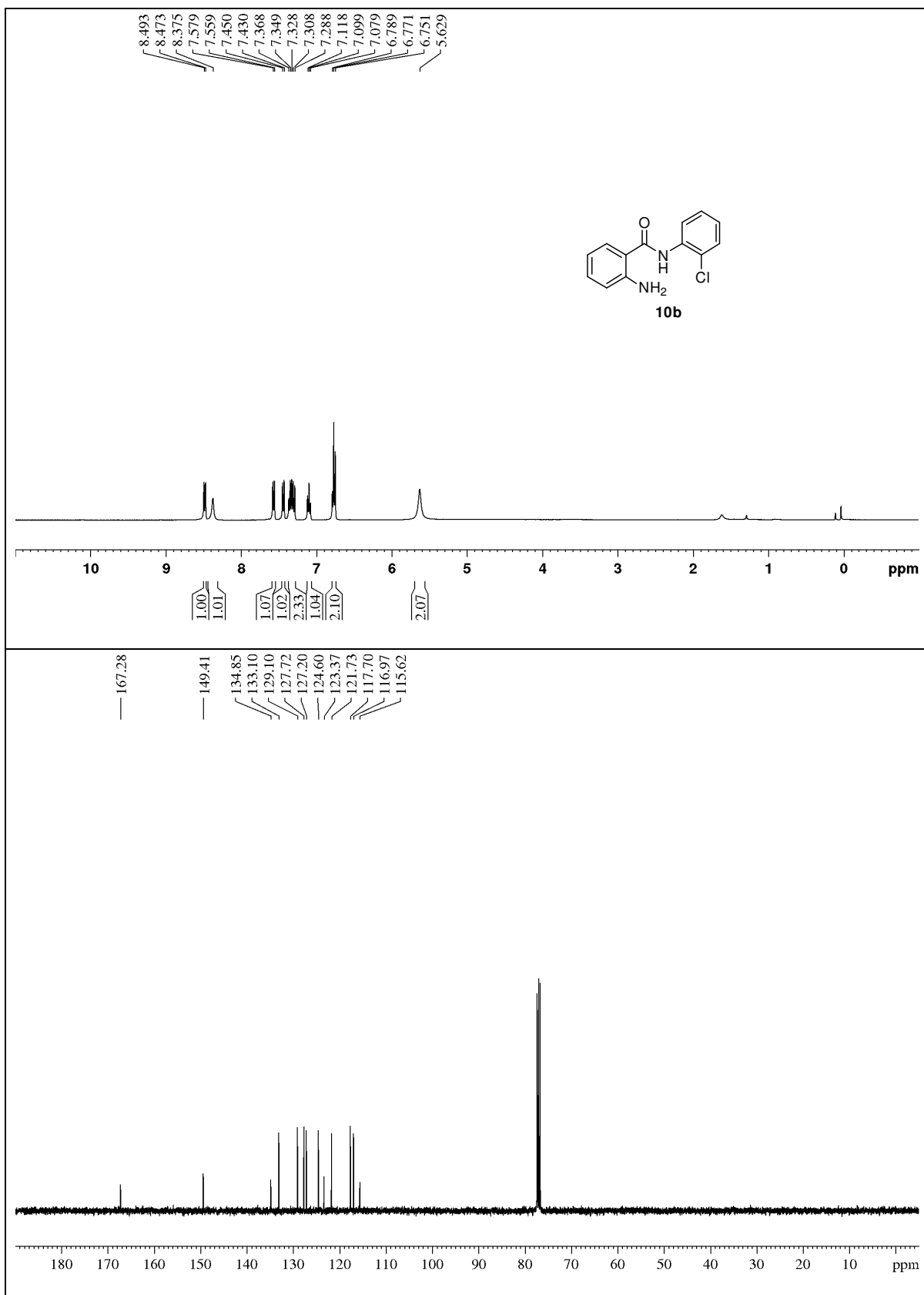
Acquisition Date 8/5/2015 12:13:15 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





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Analysis Info

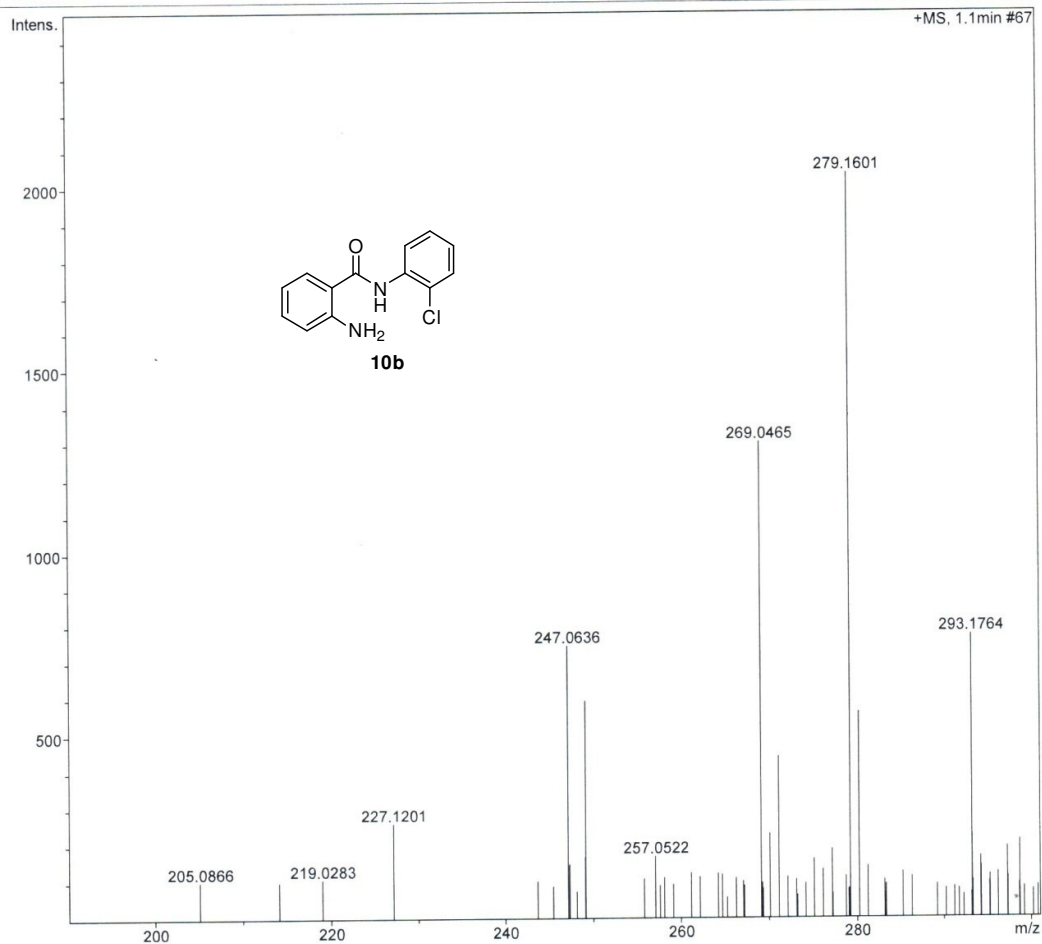
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-656.d
Method tune_low.m
Sample Name SKG-656-DCM-MEOH
Comment

Acquisition Date 8/5/2015 12:26:16 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





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Analysis Info

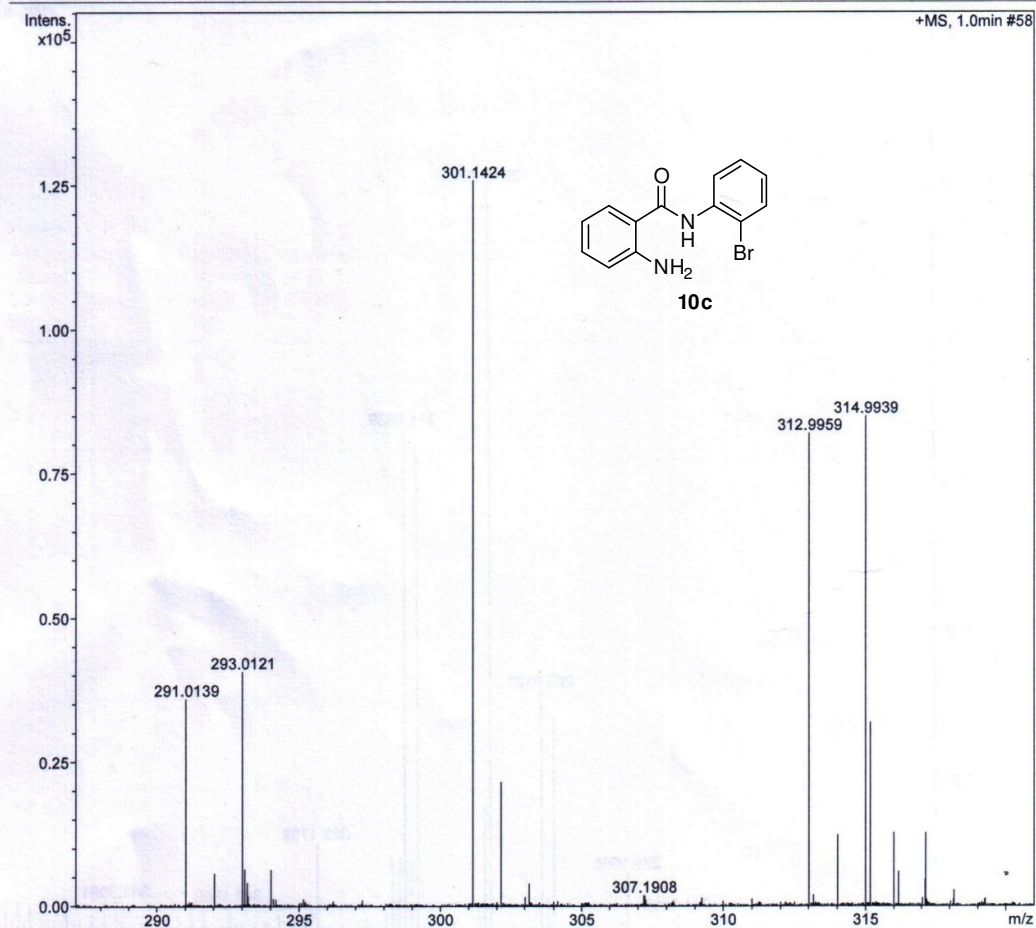
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-665R.d
Method tune_low.m
Sample Name SKG-665-DCM-MEOH
Comment

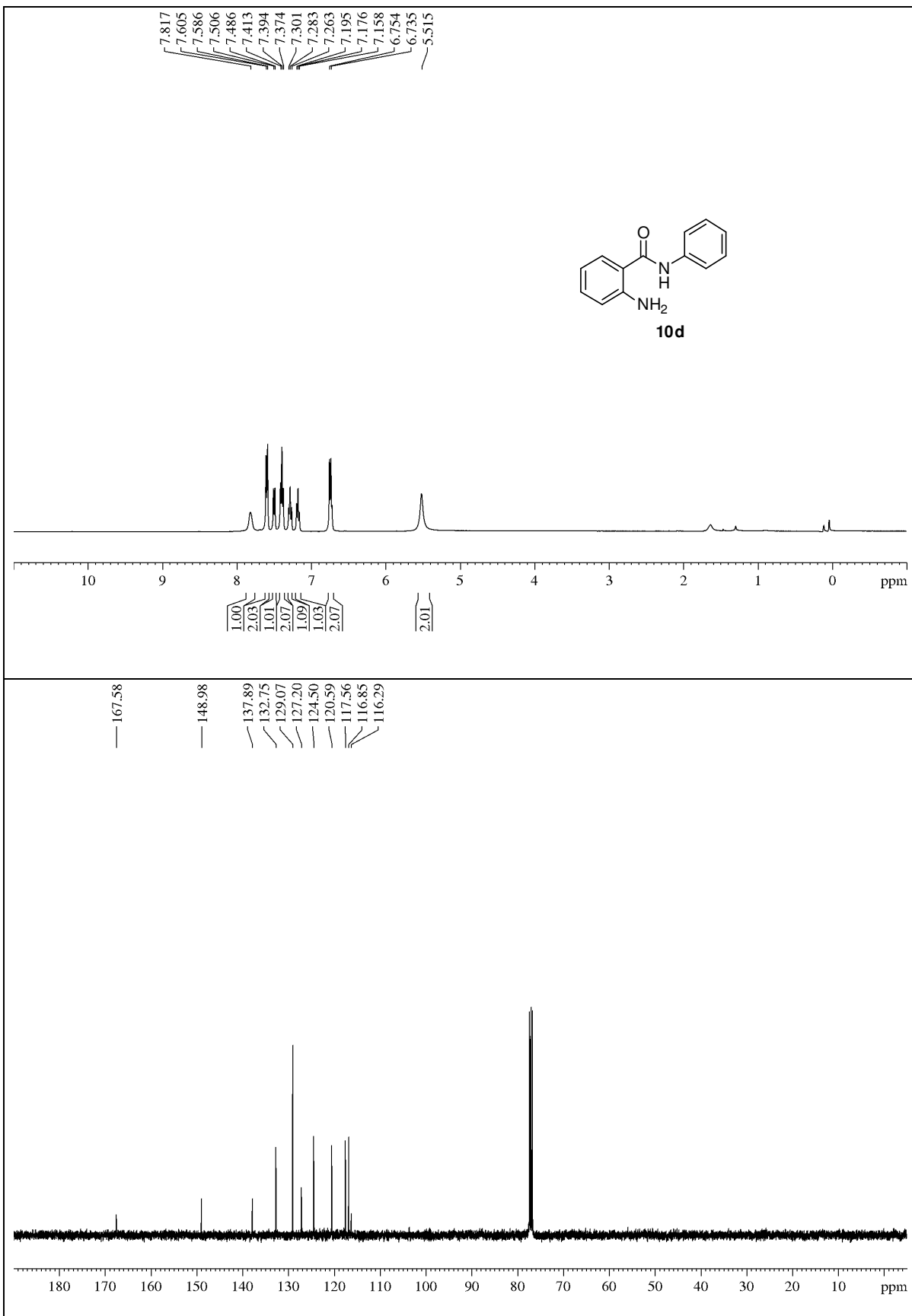
Acquisition Date 8/5/2015 1:08:23 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

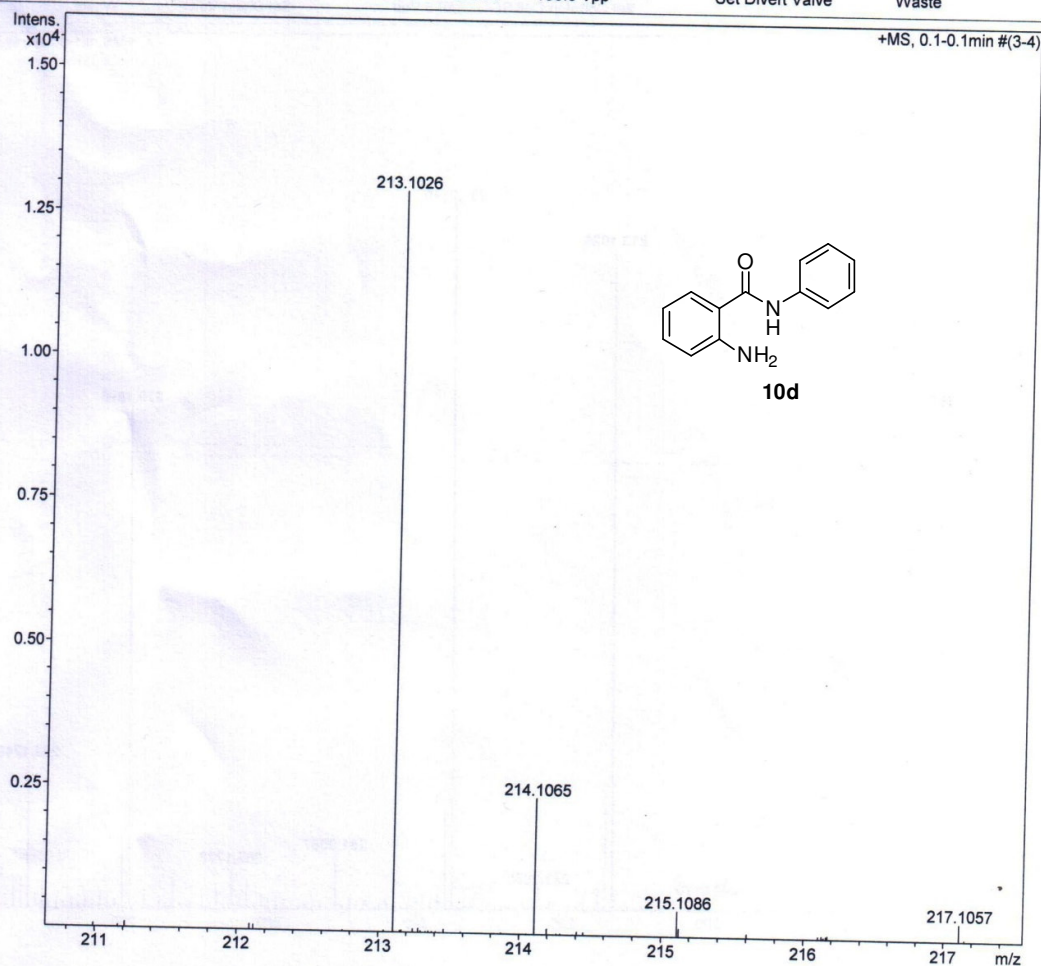
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-654.d
Method tune_low.m
Sample Name SKG-654-DCM-MEOH
Comment

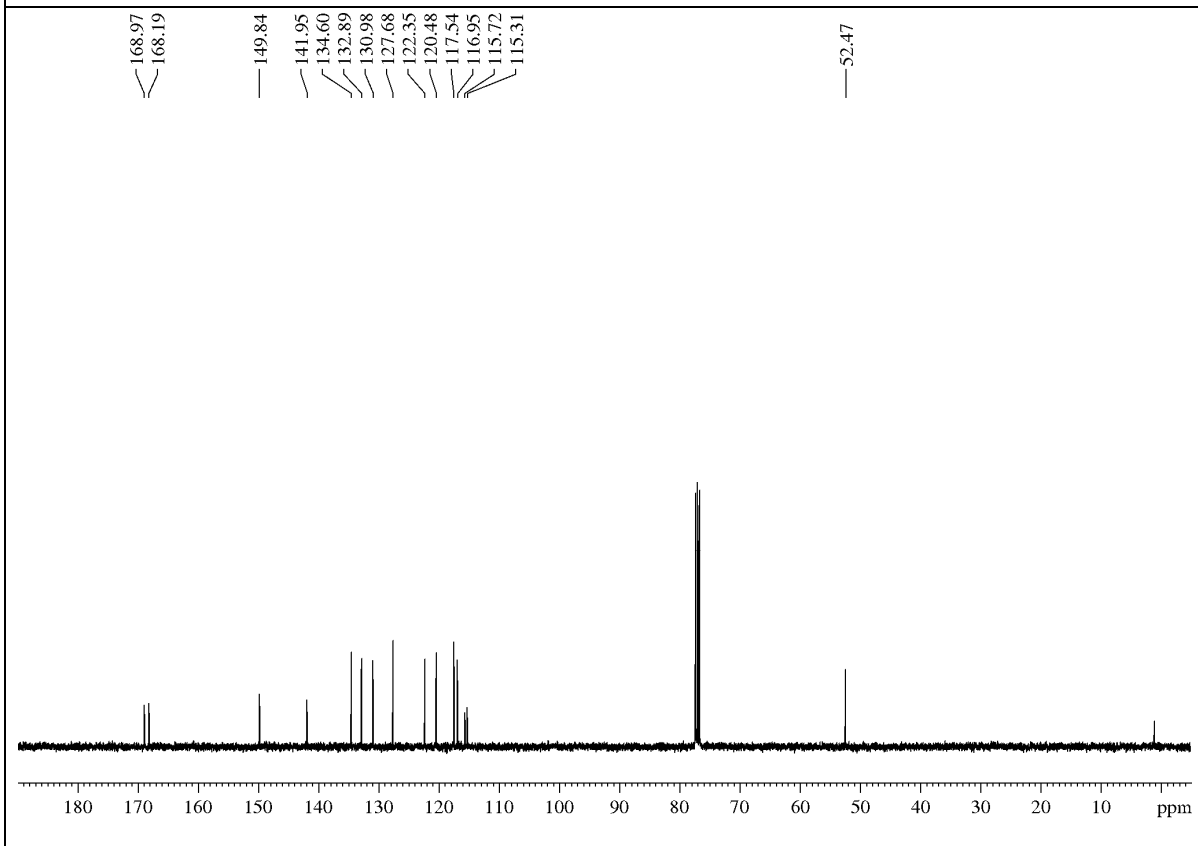
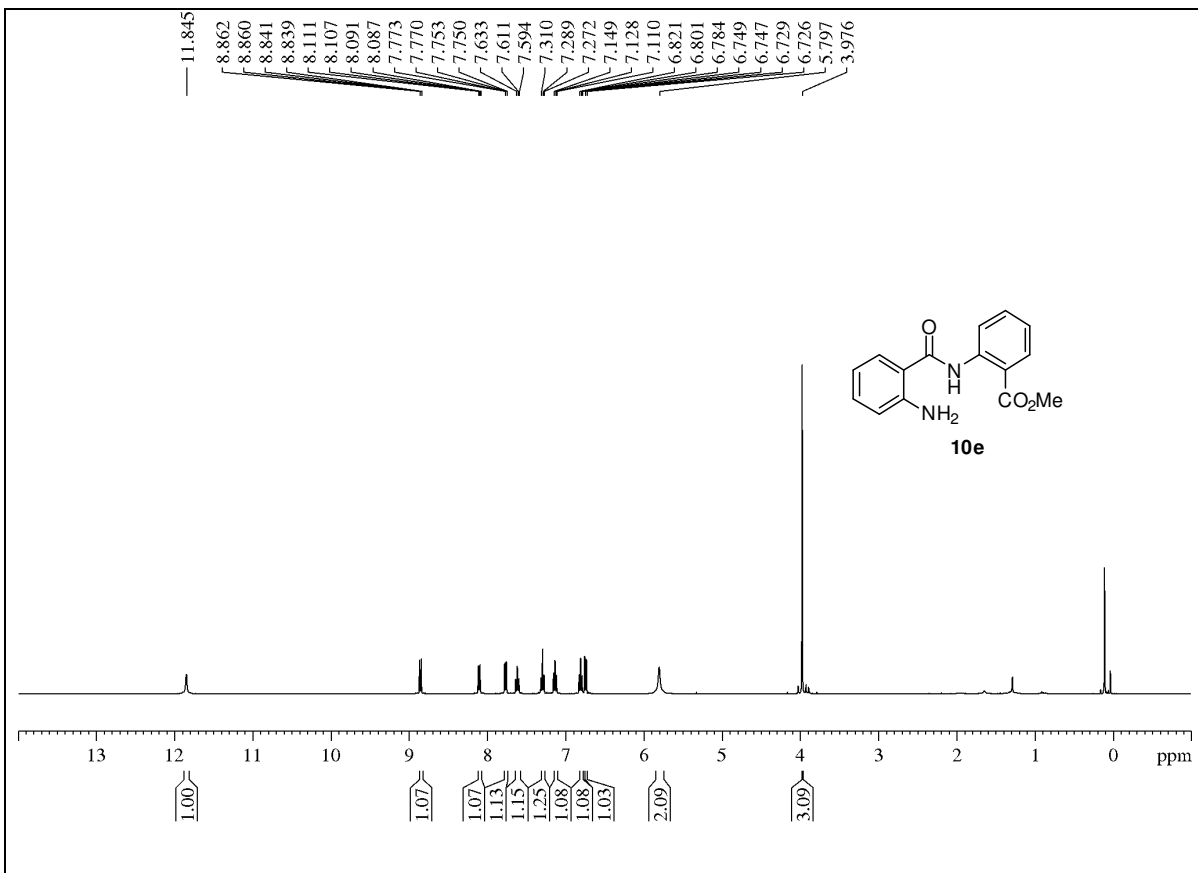
Acquisition Date 8/5/2015 12:00:24 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





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Analysis Info

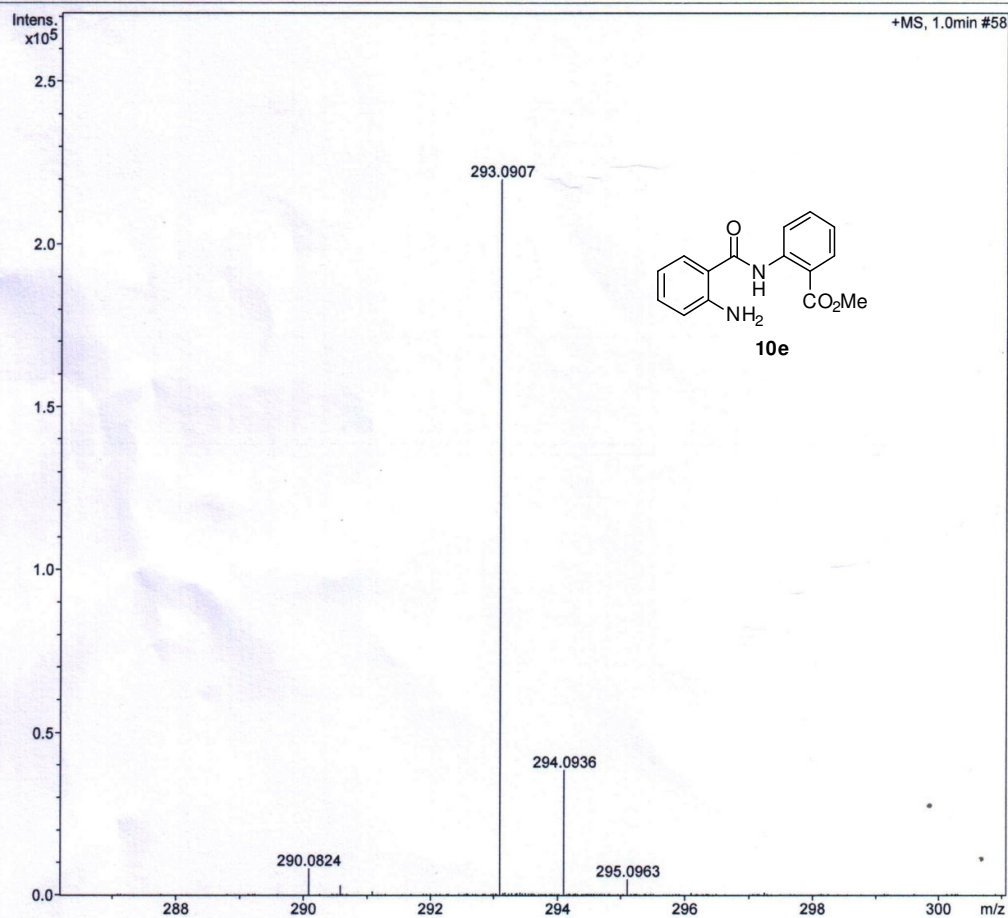
Analysis Name D:\Data\2015\DrNagarajan\AUG\SKG-659R.d
Method tune_low.m
Sample Name SKG-659-DCM-MEOH
Comment

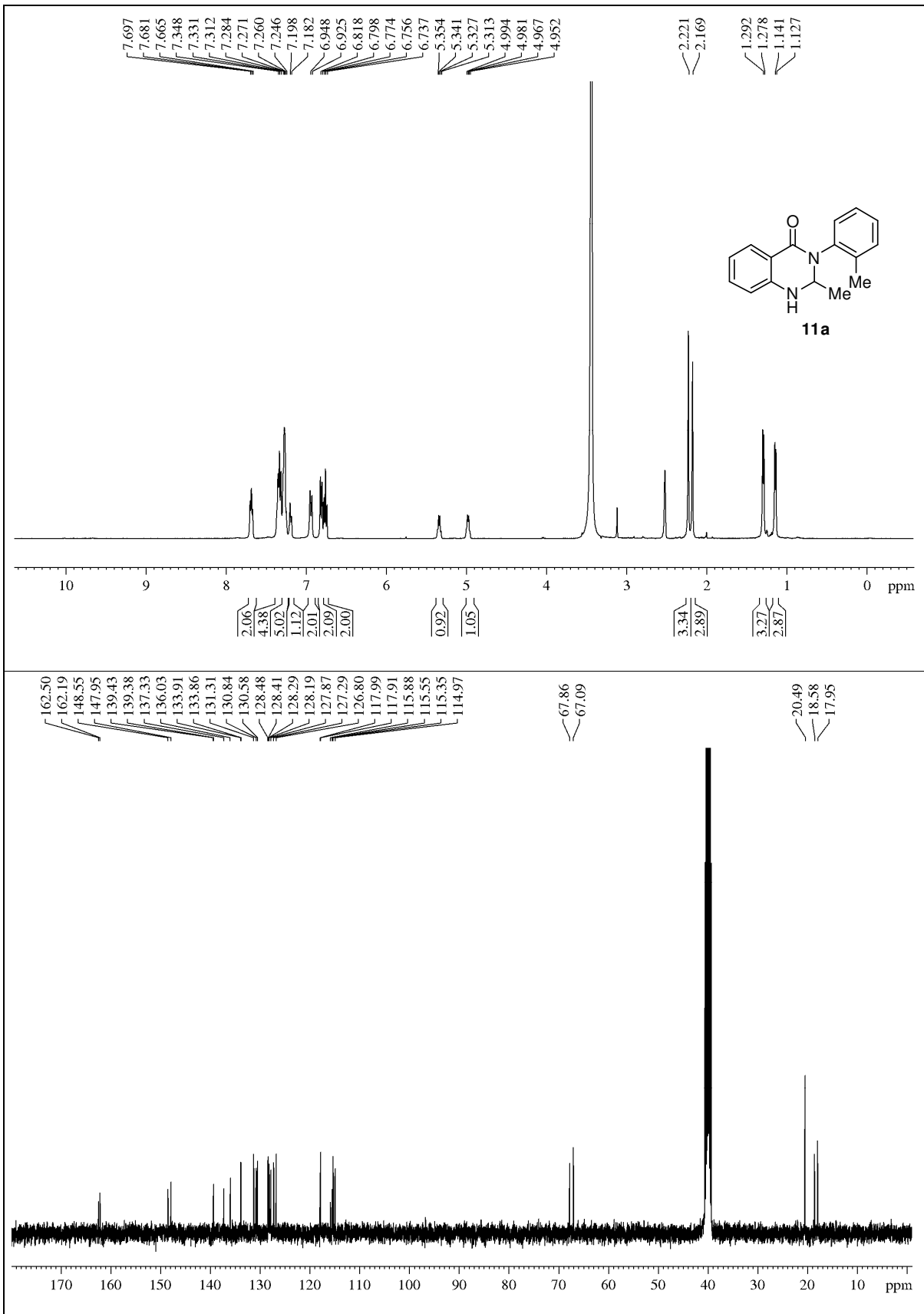
Acquisition Date 8/5/2015 12:42:20 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



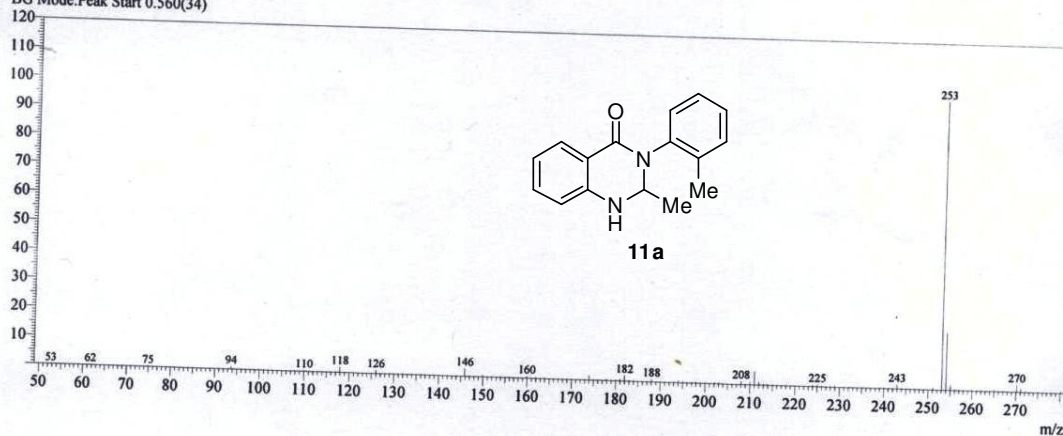


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-696
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-696-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line# 1 R.Time:0.759(Scan#:46) Positive
MassPeaks:169 BasePeak:253.05(6921410)
RawMode:Single 0.759(46)
BG Mode:Peak Start 0.560(34)

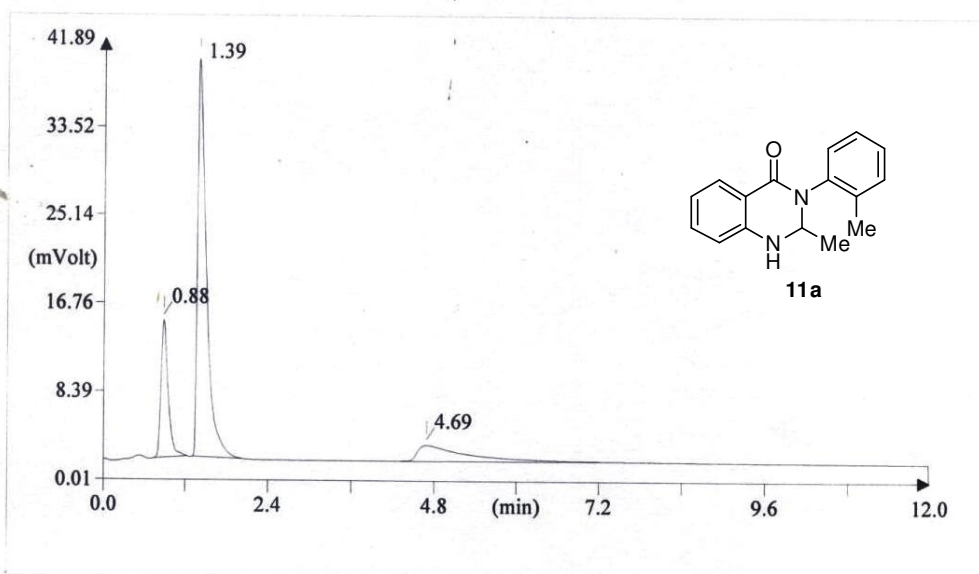


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.759	0.560	0.943	137998589	14374840	9.60		100.00	
				137998589	14374840			100.00	

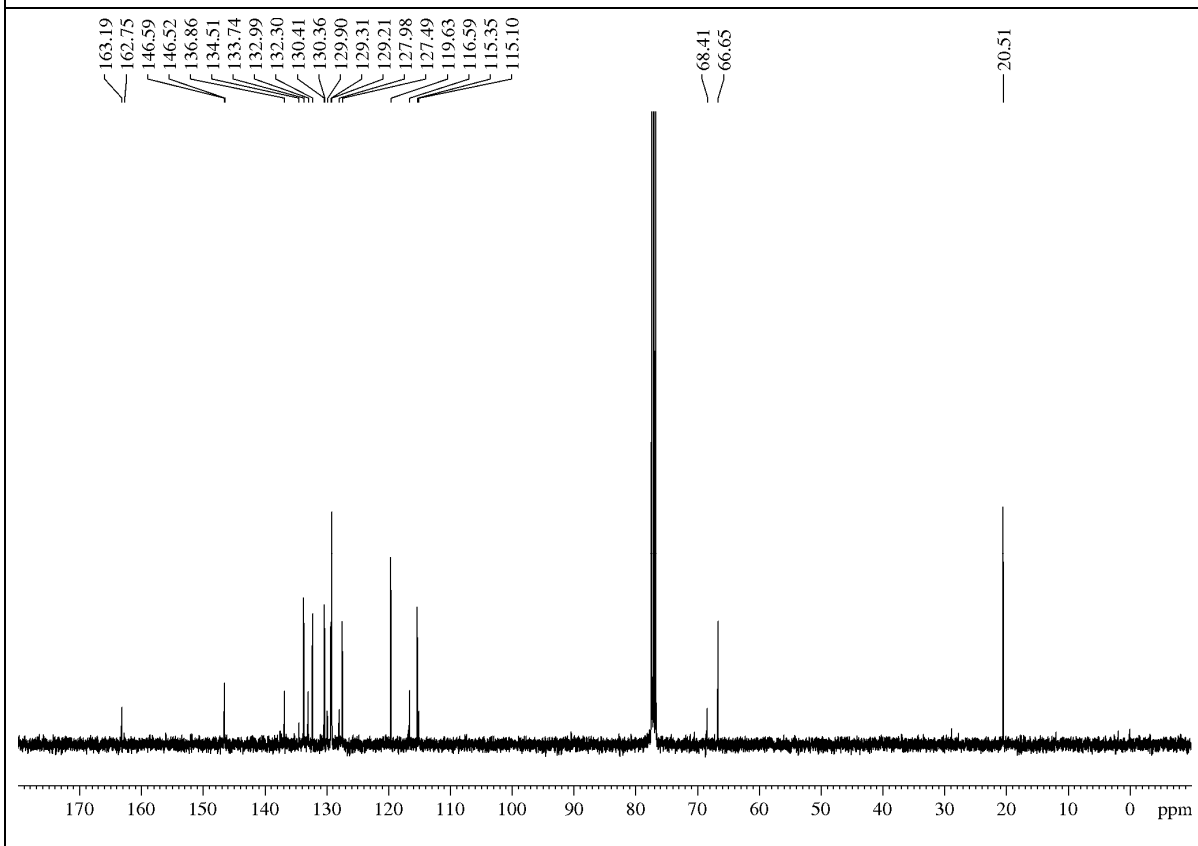
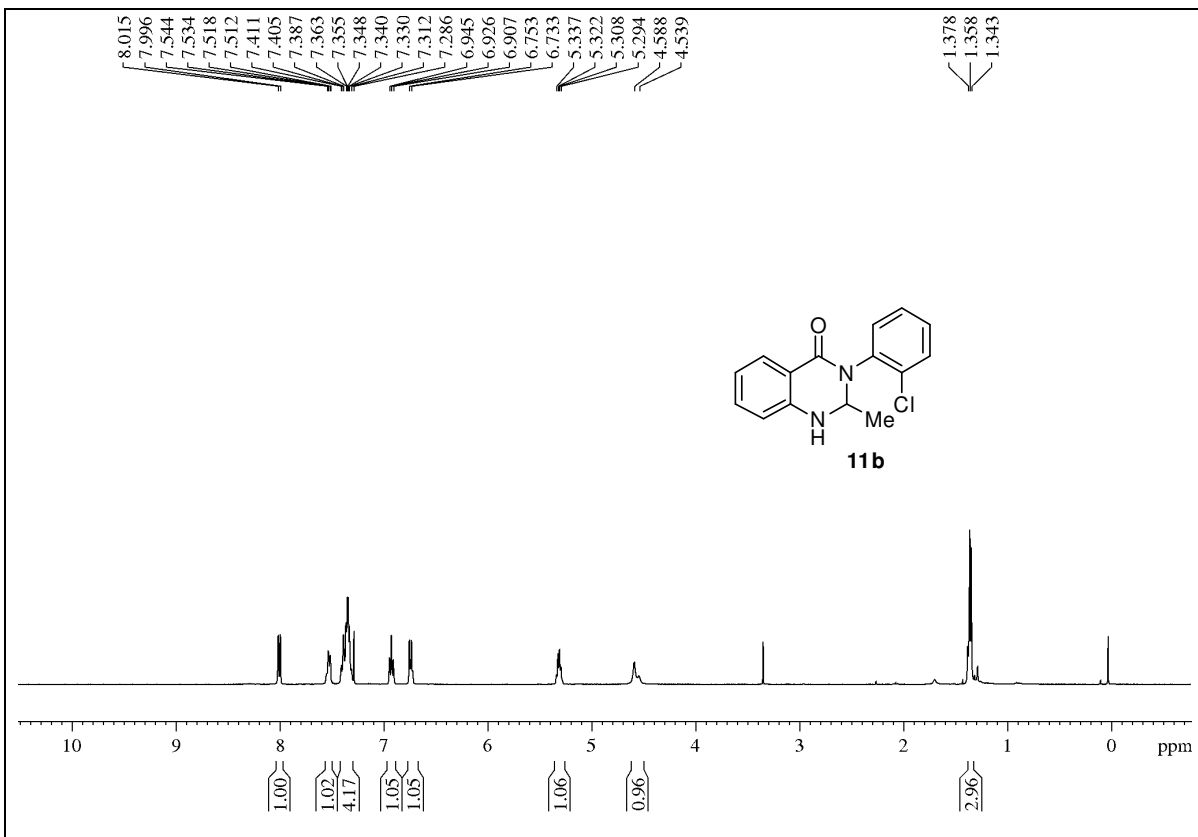
Base m/z Base Int.
253.05 6921410

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-696 (# 149)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-9.dat
Sample weight: 1.132



Element Name	Element %	Ret. Time
Nitrogen	11.18	0.88
Carbon	76.31	1.39
Hydrogen	6.31	4.69

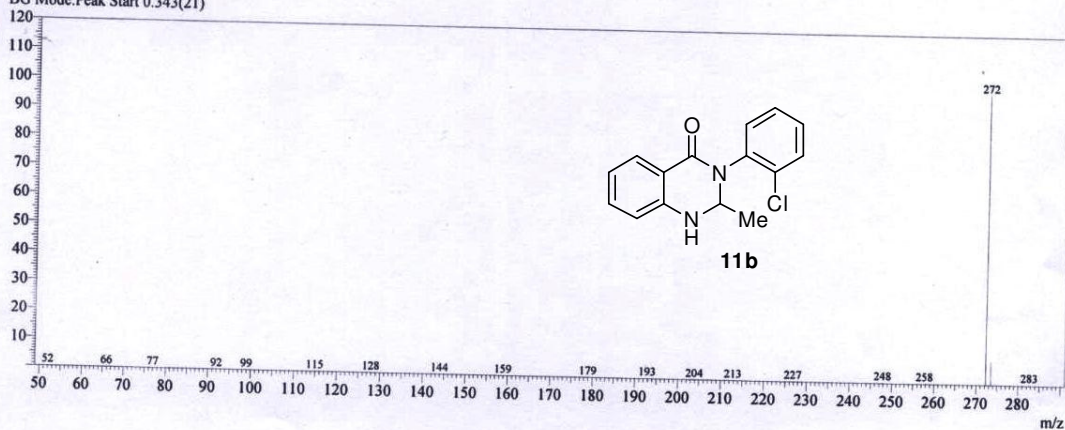


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-658
Inj. Volume : 5.000
Data Name : G:\LCMSsolution\User\Data\SKG-658-ESI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\Copy of JAY-4-APCI.qlm

MS Spectrum

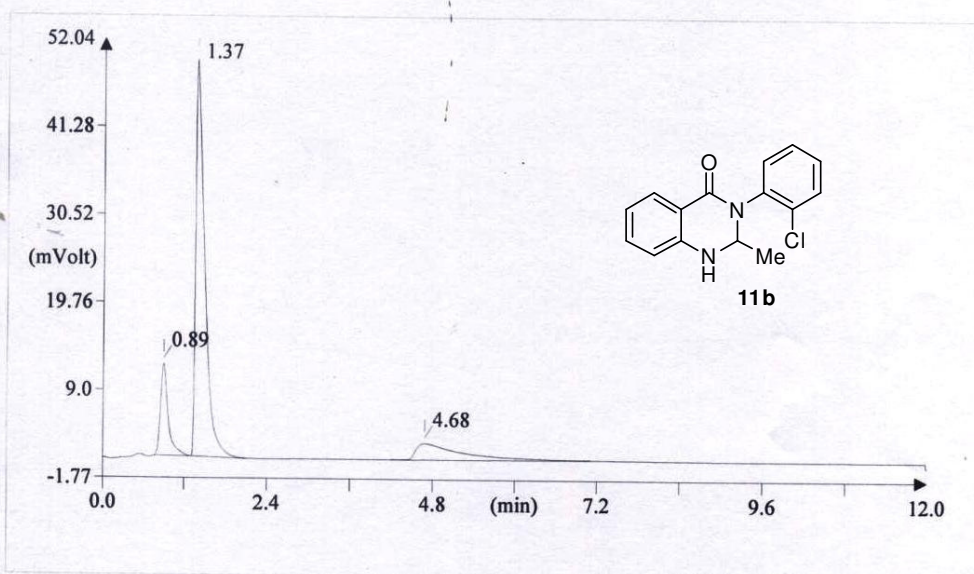
Line# 1 R.Time: 0.621 (Scan#: 38) Positive
MassPeaks: 74 BasePeak: 272.25 (351872)
RawMode: Single 0.621 (38)
BG Mode: Peak Start 0.343 (21)



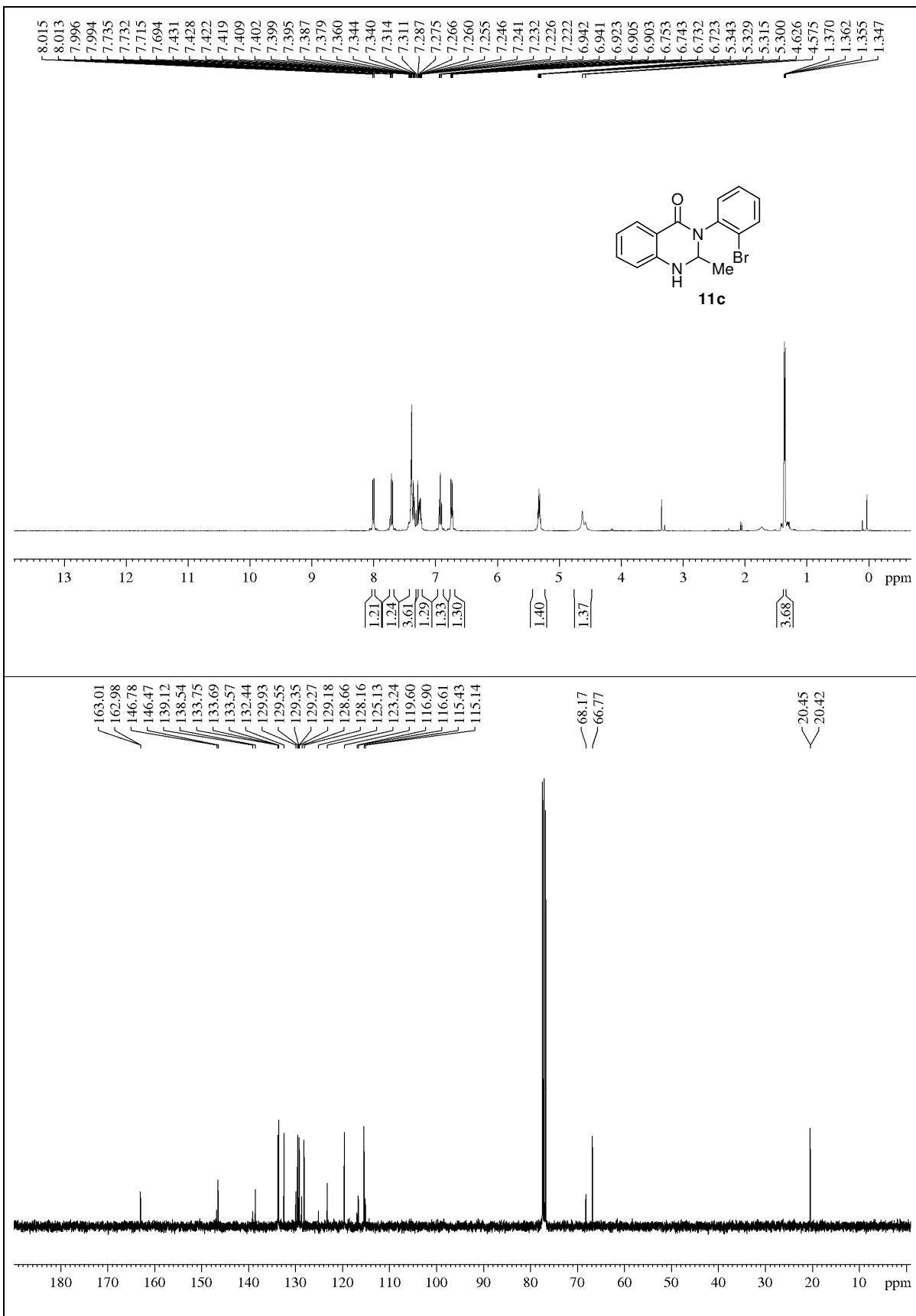
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.621	0.343	1.043	26945307	1624710	16.58		100.00		272.25	351872
				26945307	1624710			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-658 (# 144)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-4.dat
Sample weight: 1.307



Element Name	Element %	Ret. Time
Nitrogen	10.36	0.89
Carbon	66.15	1.37
Hydrogen	4.73	4.68



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Analysis Info

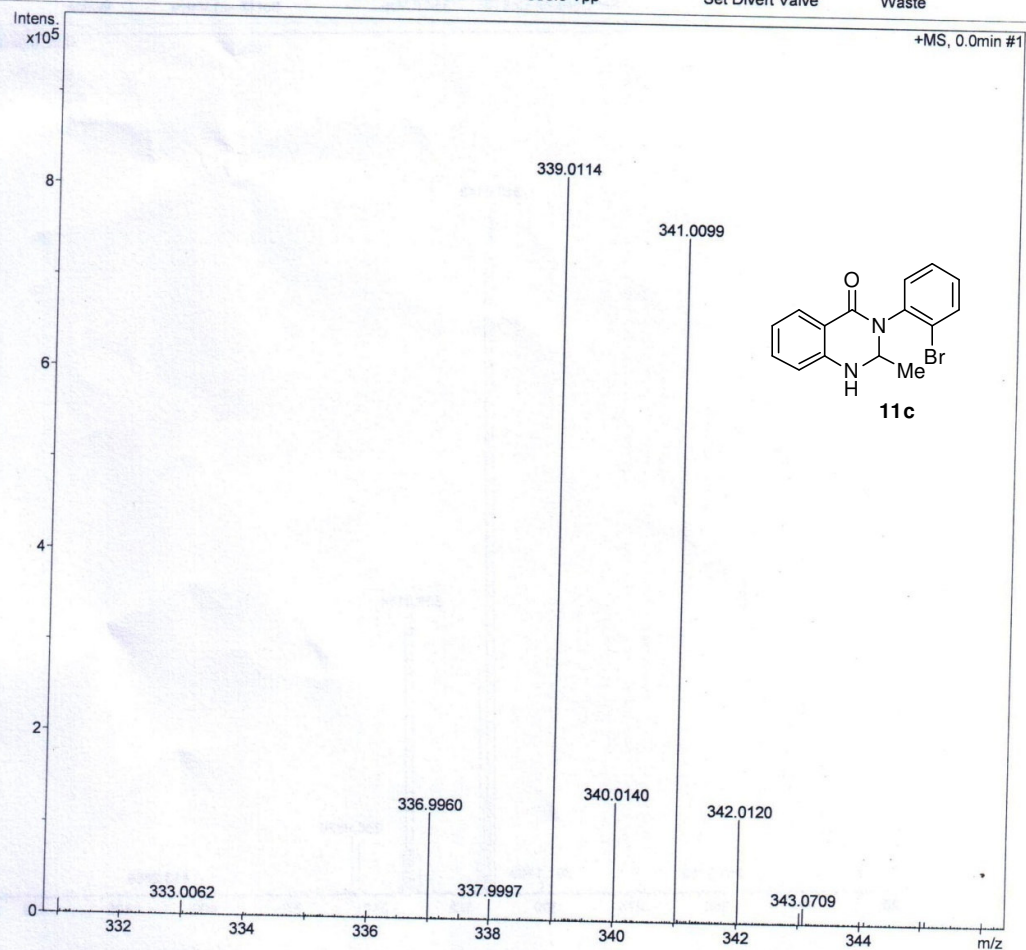
Analysis Name D:\Data\2015\DrNagarajan\mar\SKG-667.d
Method TL-P.m
Sample Name SKG-667-DCM-MEOH
Comment

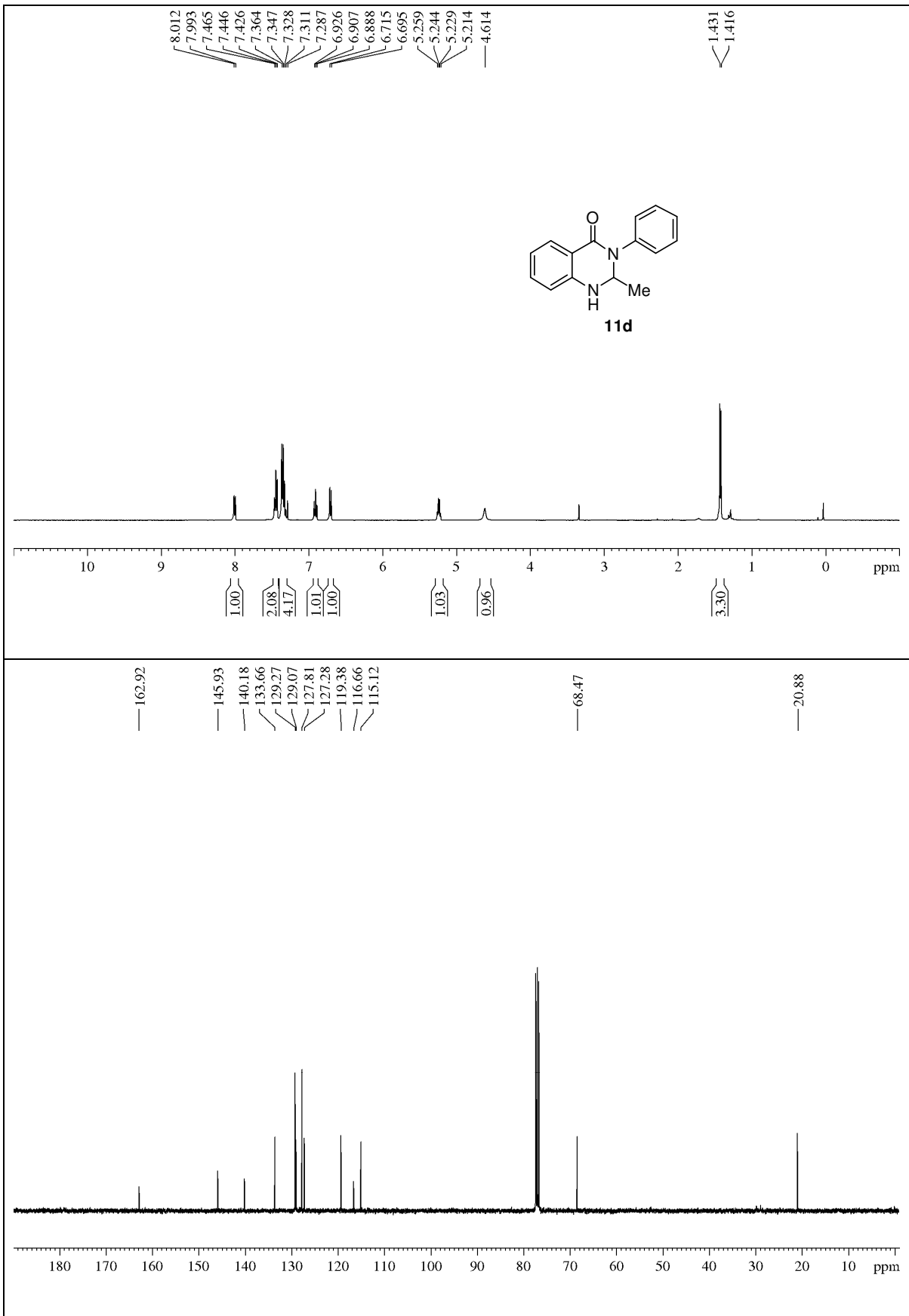
Acquisition Date 3/18/2015 1:16:10 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



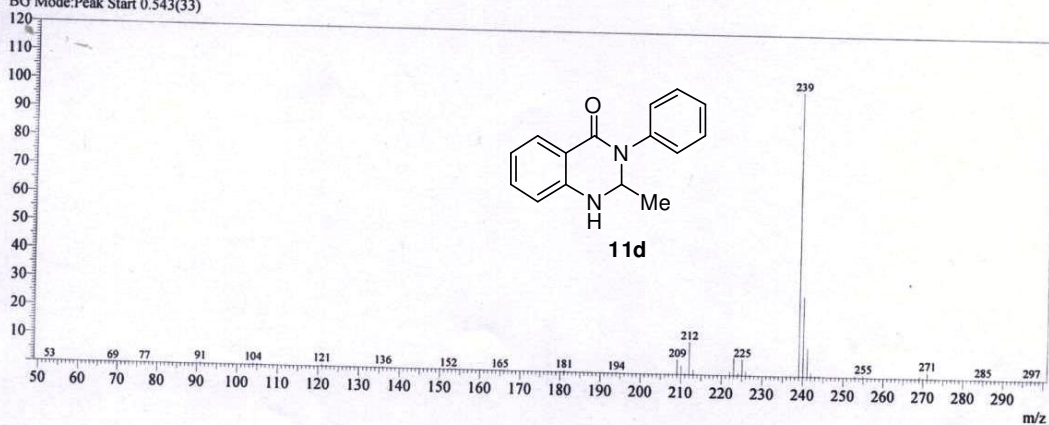


**LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD**

User : Admin
 Sample : SKG-657
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\SKG-657-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

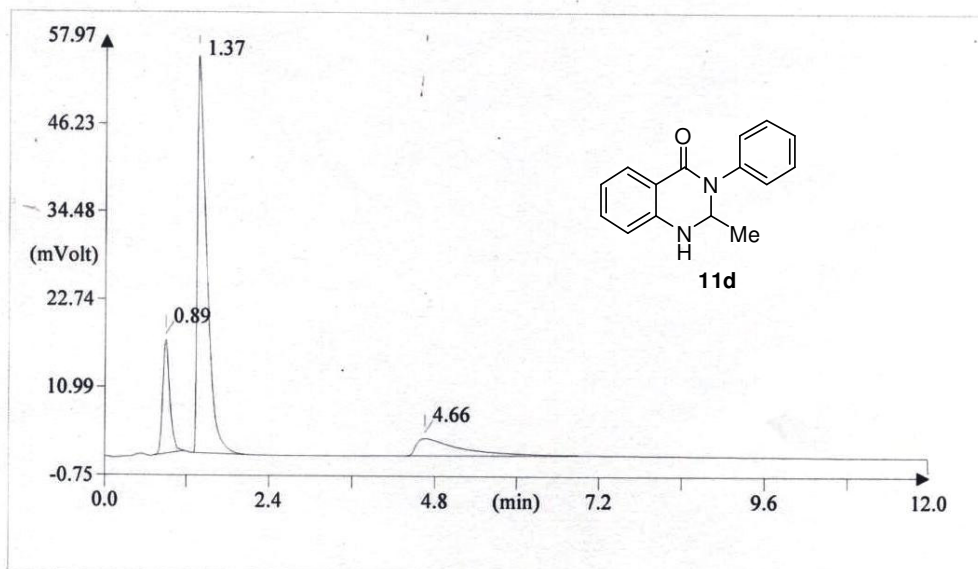
Line#:1 R.Time:0.786(Scan#:48) Positive
 MassPeaks:175 BasePeak:239.00(10605560)
 RawMode:Single 0.786(48)
 BG Mode:Peak Start 0.543(33)



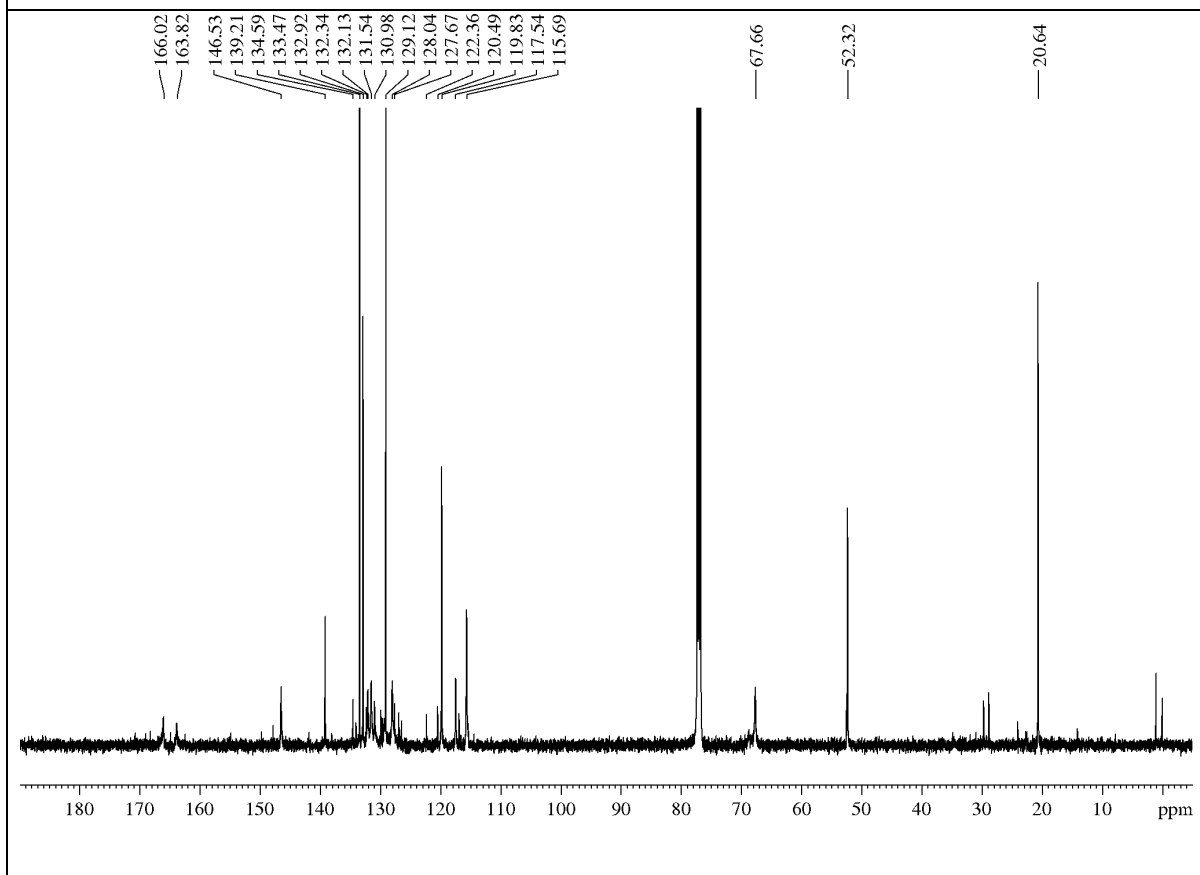
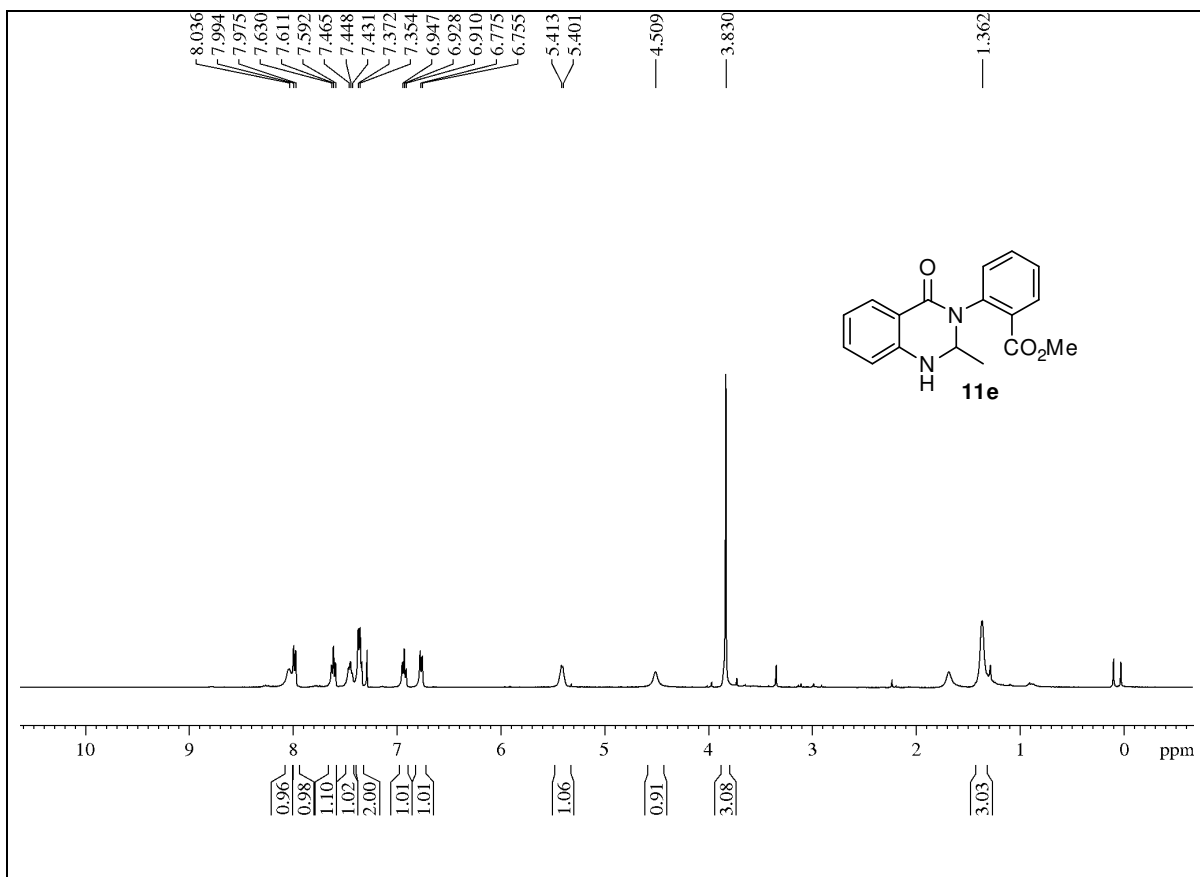
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.786	0.543	1.043	542626652	40162806	13.51		100.00		239.00	10605560
				542626652	40162806			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-657 (# 157)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-17.dat
Sample weight: 1.226



Element Name	Element %	Ret. Time
Nitrogen	11.65	0.89
Carbon	75.52	1.37
Hydrogen	6.07	4.66



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Analysis Info

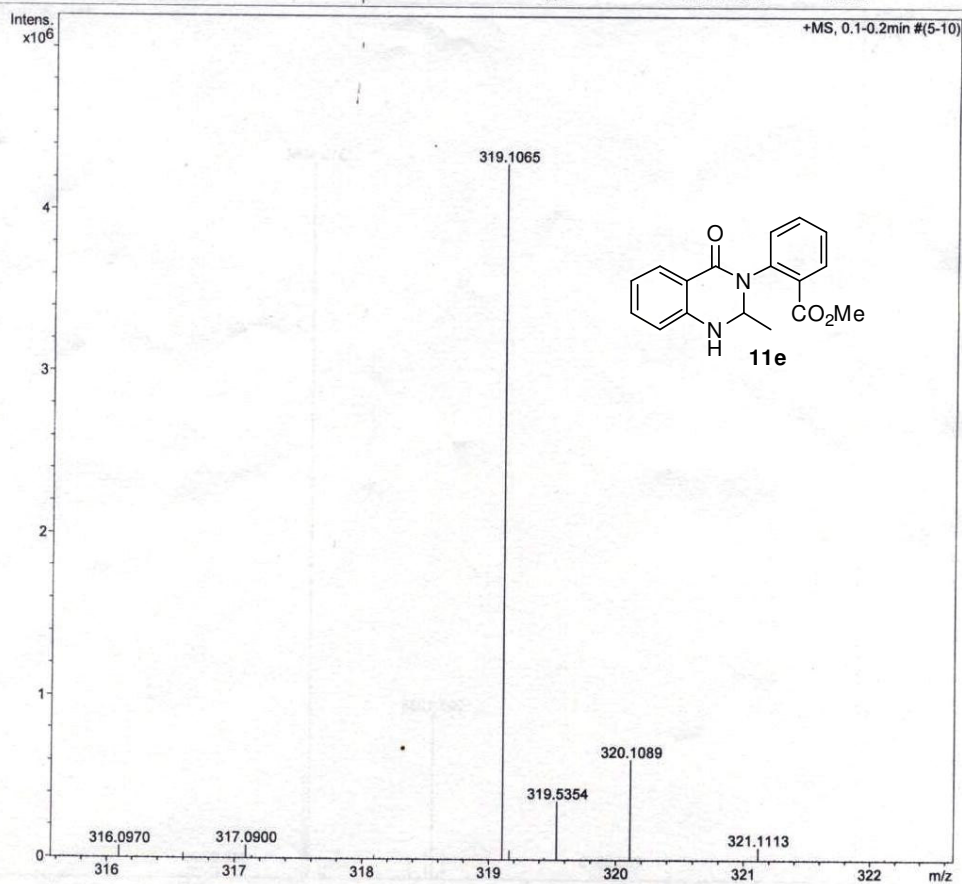
Analysis Name D:\Data\2015\DrNagarajan\FEB\SKG-688.d
Method TL-P.m
Sample Name SKG-688-DCM-MEOH
Comment

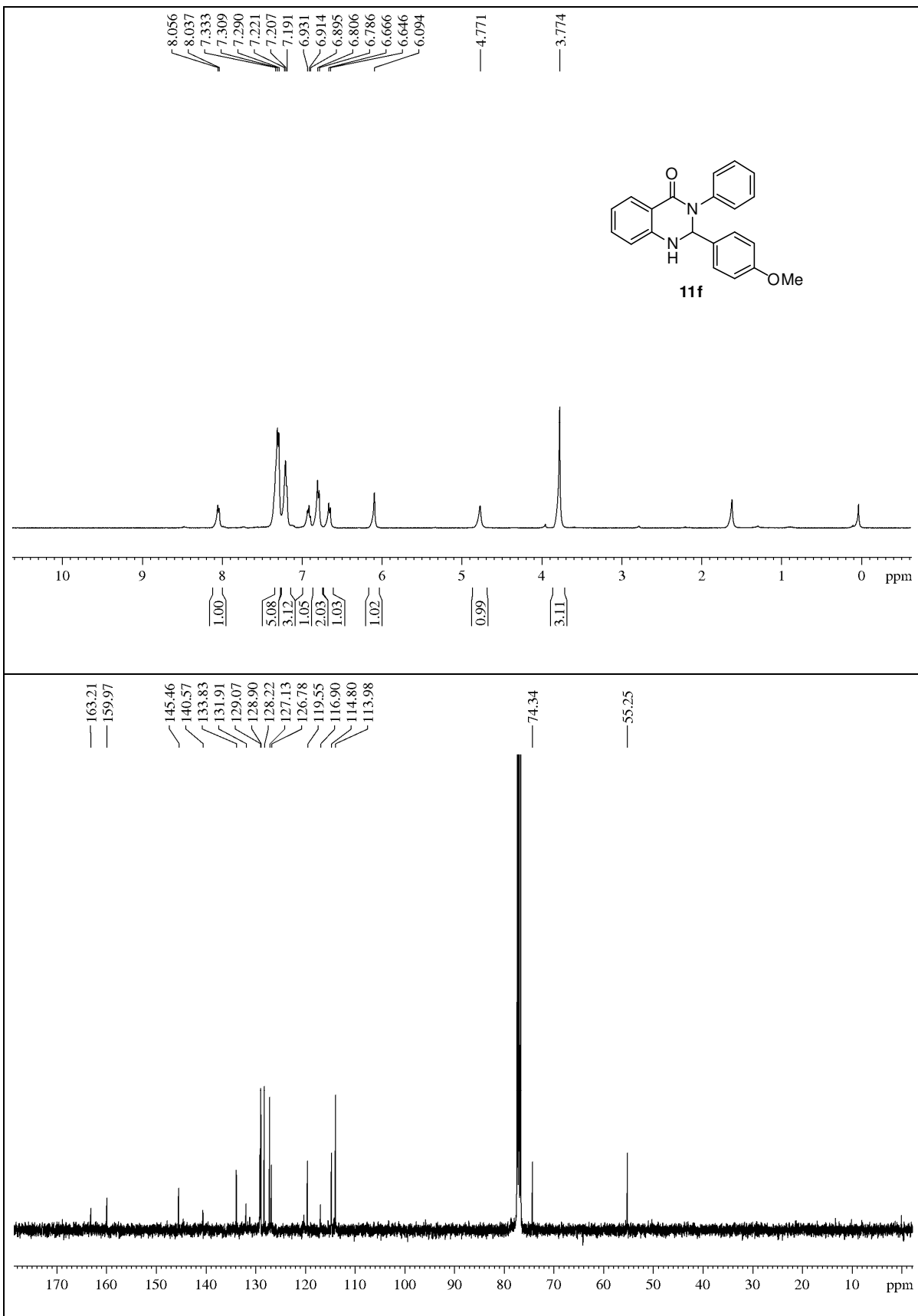
Acquisition Date 2/23/2015 12:39:19 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



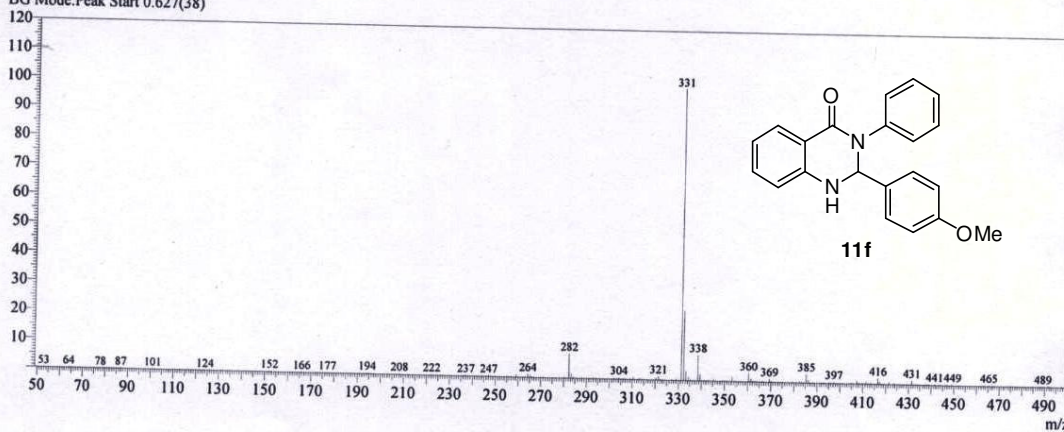


**LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD**

User : Admin
 Sample : SKG-670
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\SKG-670-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.828(Scan#:50) Positive
 MassPeaks:318 BasePeak:331.25(6821119)
 RawMode:Single 0.828(50)
 BG Mode:Peak Start 0.627(38)

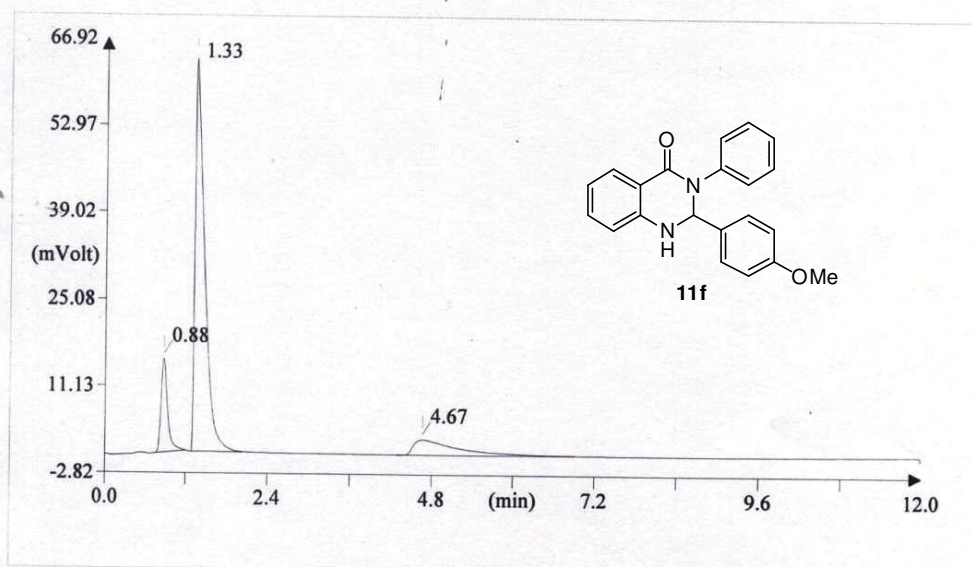


Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.828	0.627	1.093	118182453	10608738	11.14		100.00	

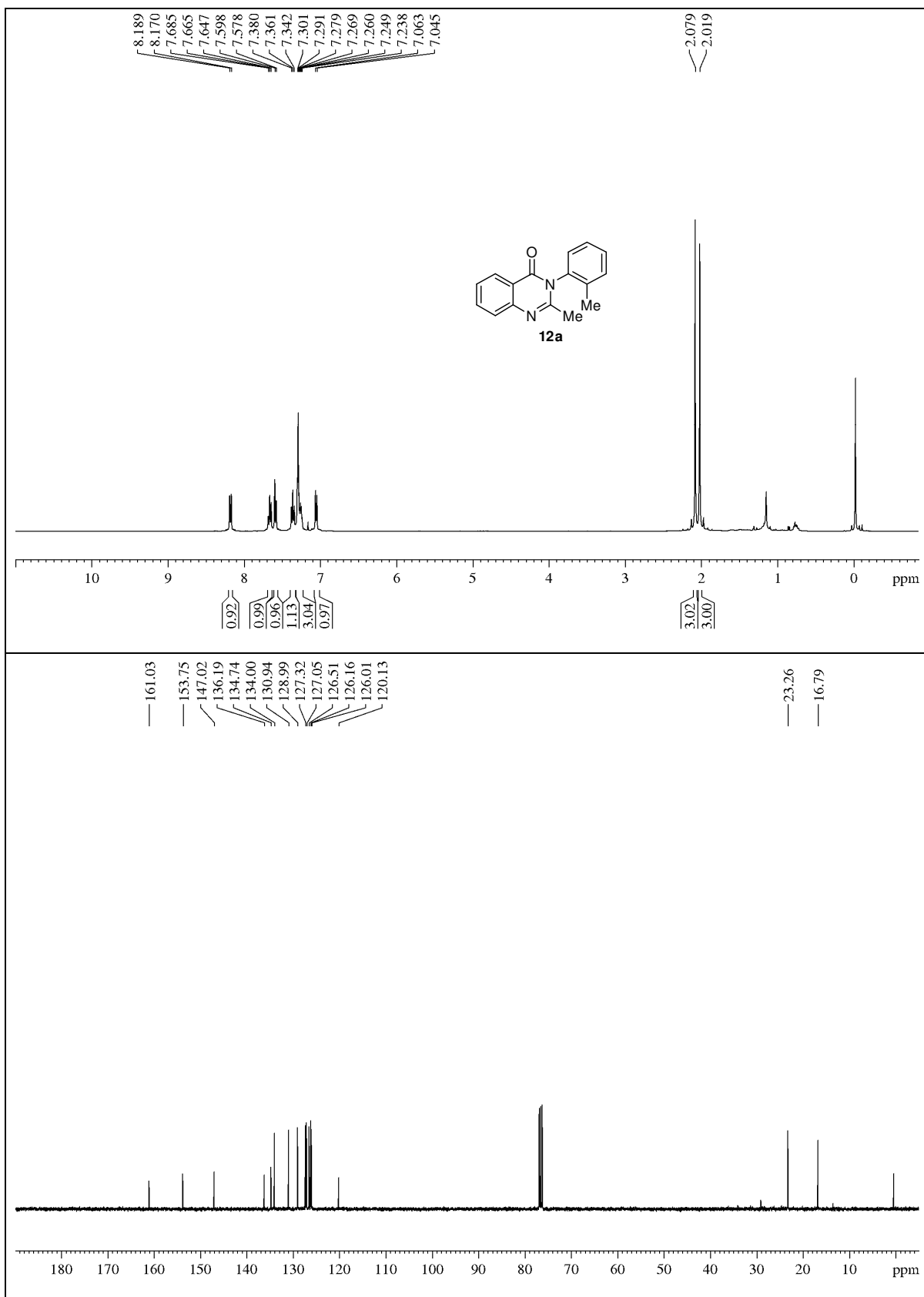
Base m/z Base Int.
 331.25 6821119

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-670 (# 150)
Analysis type: UnkNown
Chromatogram filename: UNK-18022015-10.dat
Sample weight: 1.483



Element Name	Element %	Ret. Time
Nitrogen	8.56	0.88
Carbon	76.25	1.33
Hydrogen	5.41	4.67



BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

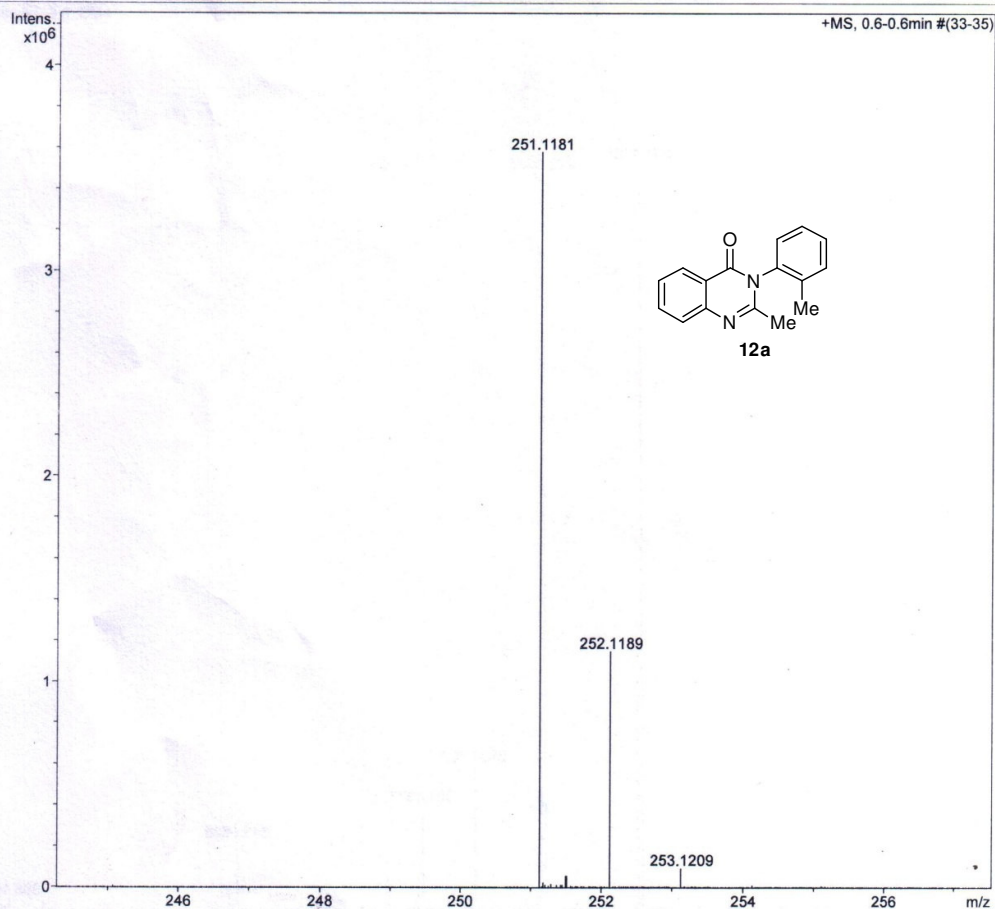
Analysis Name D:\Data\2015\DrNagarajan\mar\SKG-698R.d
Method tune_low_Pos.m
Sample Name SKG-698-DCM-MEOH
Comment

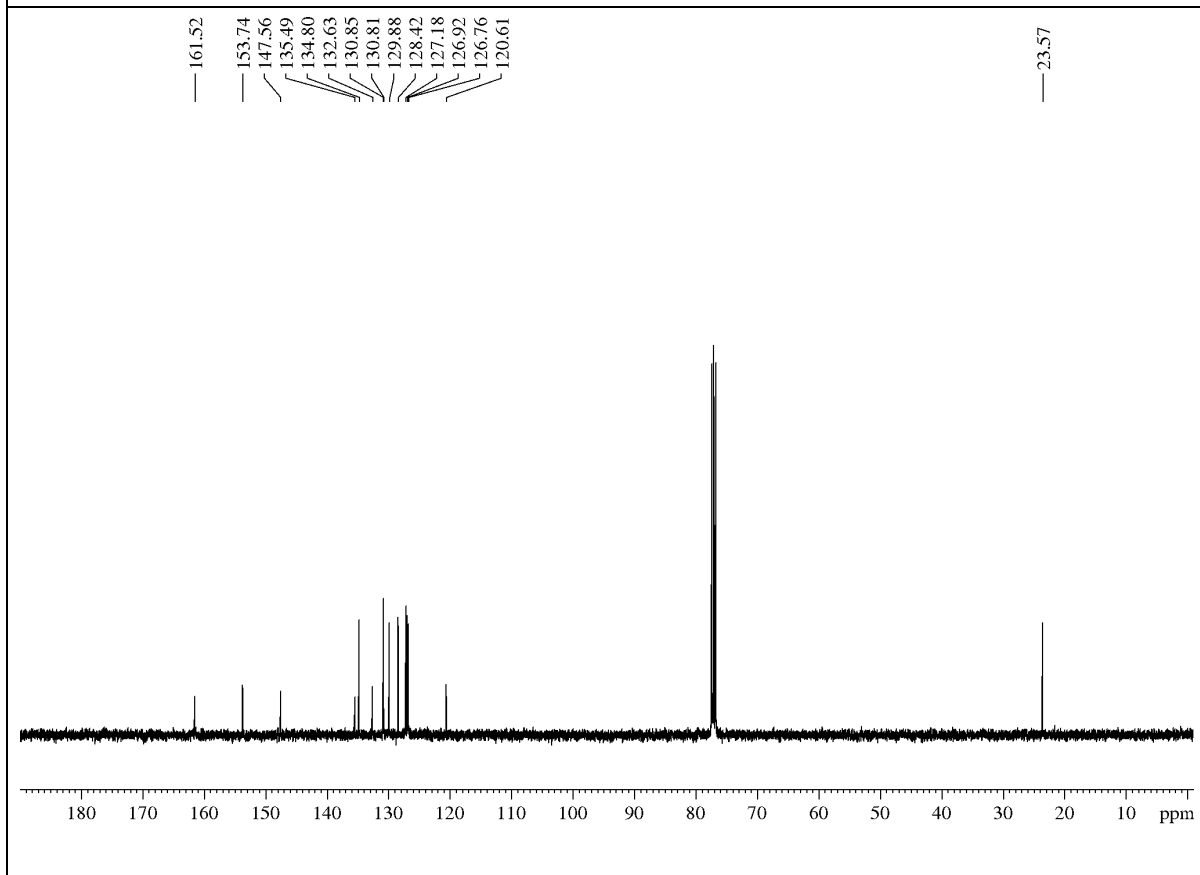
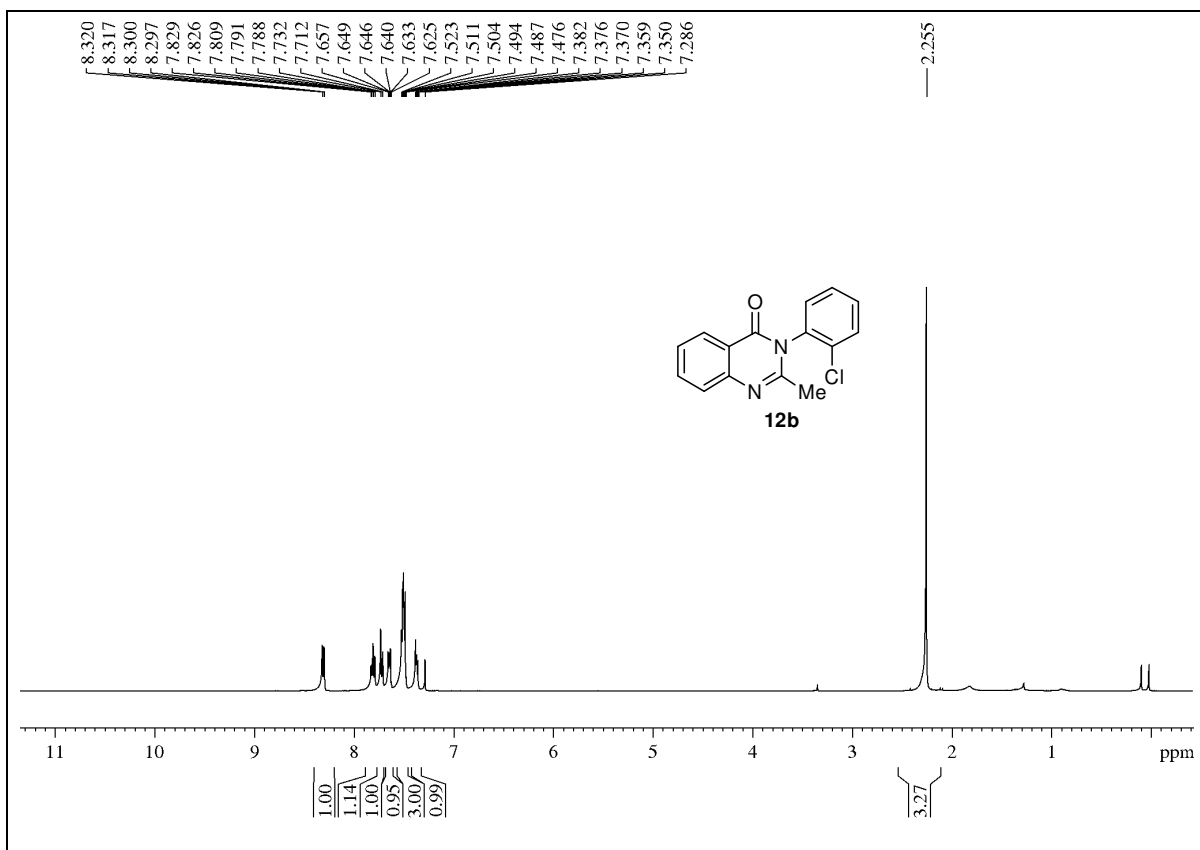
Acquisition Date 3/18/2015 1:06:21 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



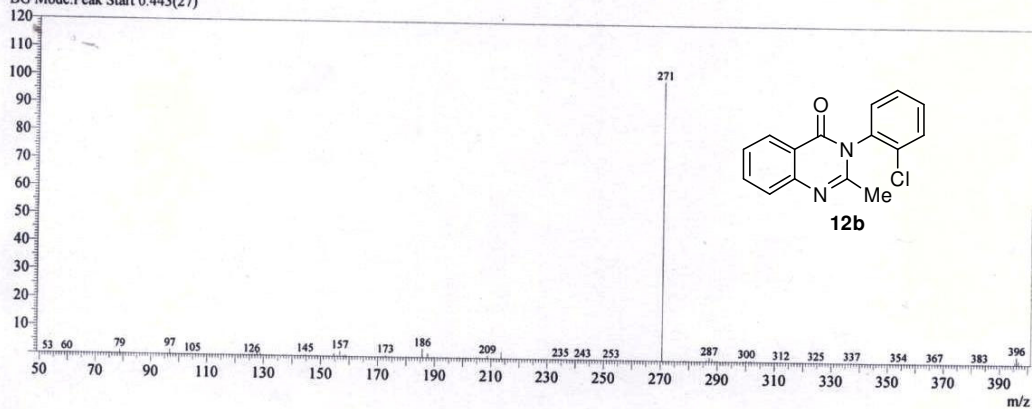


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-663
Inj. Volume : 5.000
Data Name : G:\LCMSSolution\User\Data\SKG-663-APCI-POS1.qld
Method Name : C:\LCMSSolution\User\Method\Copy of JAY-4-APCI.qlm

MS Spectrum

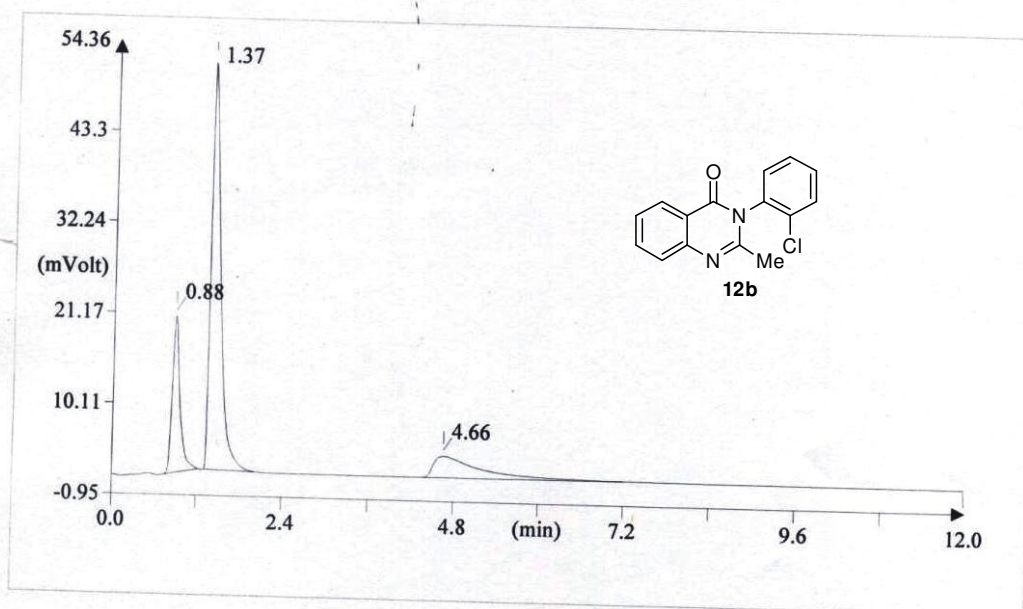
Line#:1 R.Time:0.638(Scan#:39) Positive
MassPeaks:269 BasePeak:270.60(6372491)
RawMode:Single 0.638(39)
BG Mode:Peak Start 0.443(27)



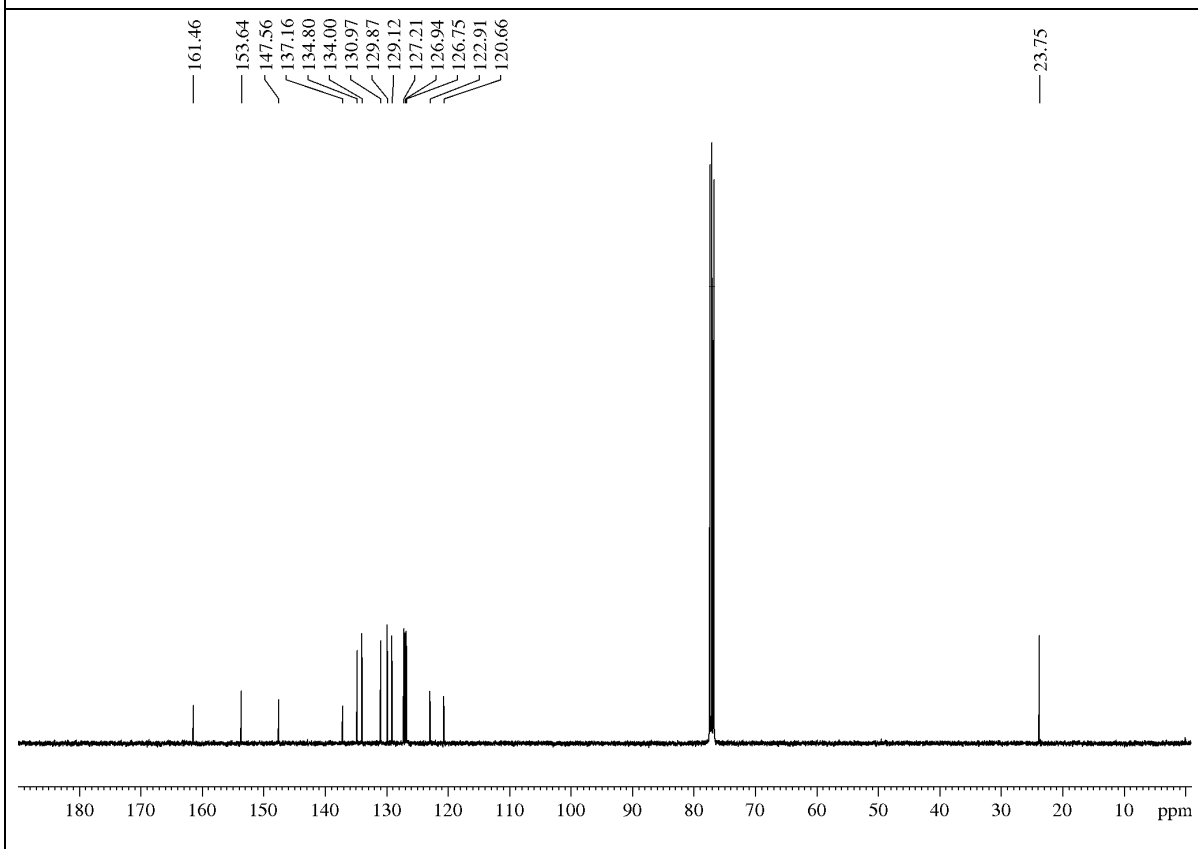
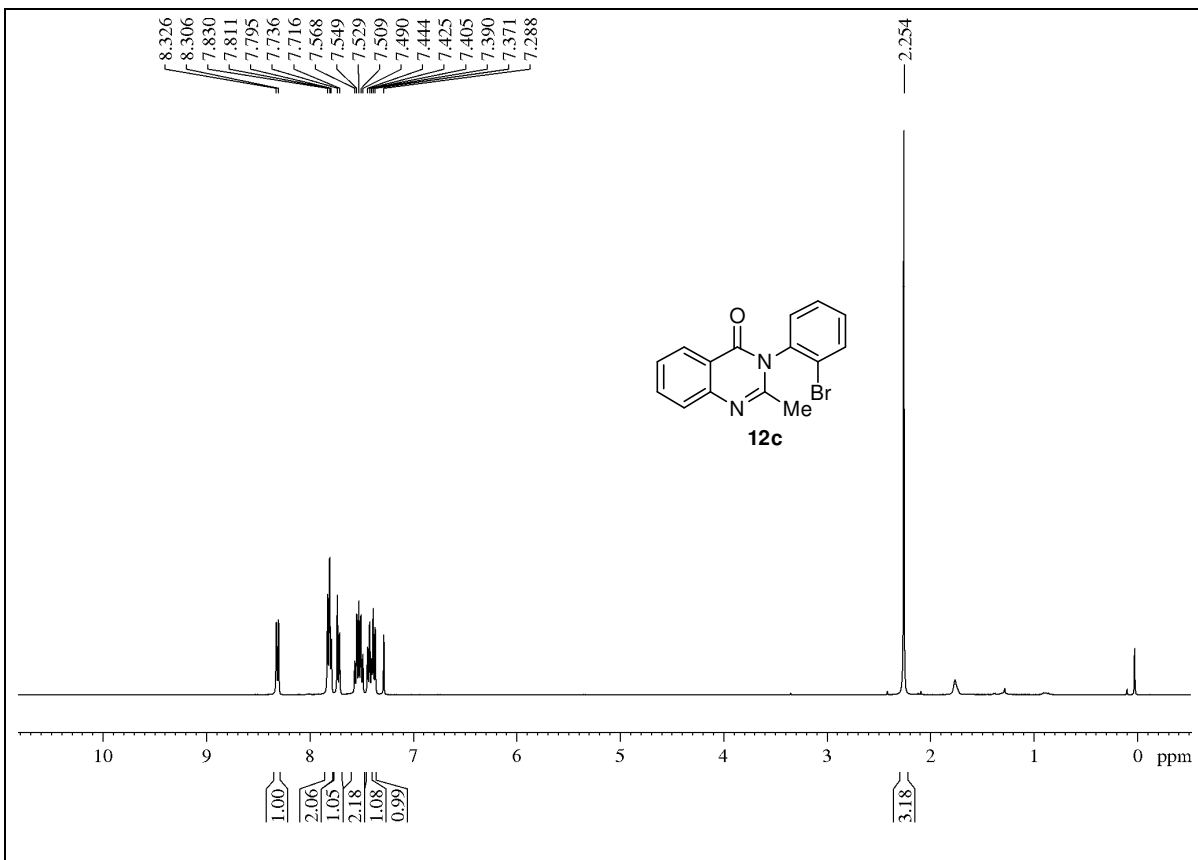
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.638	0.443	0.793	91618087	9861805	9.29		100.00		270.60	6372491
				91618087	9861805			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: SKG-663 (# 154)
Analysis type: UnkNqwn
Chromatogram filename: UNK-18022015-14.dat
Sample weight: 1.316



Element Name	Element %	Ret. Time
Nitrogen	10.26	0.88
Carbon	66.42	1.37
Hydrogen	4.18	4.66



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University of Hyderabad

Analysis Info

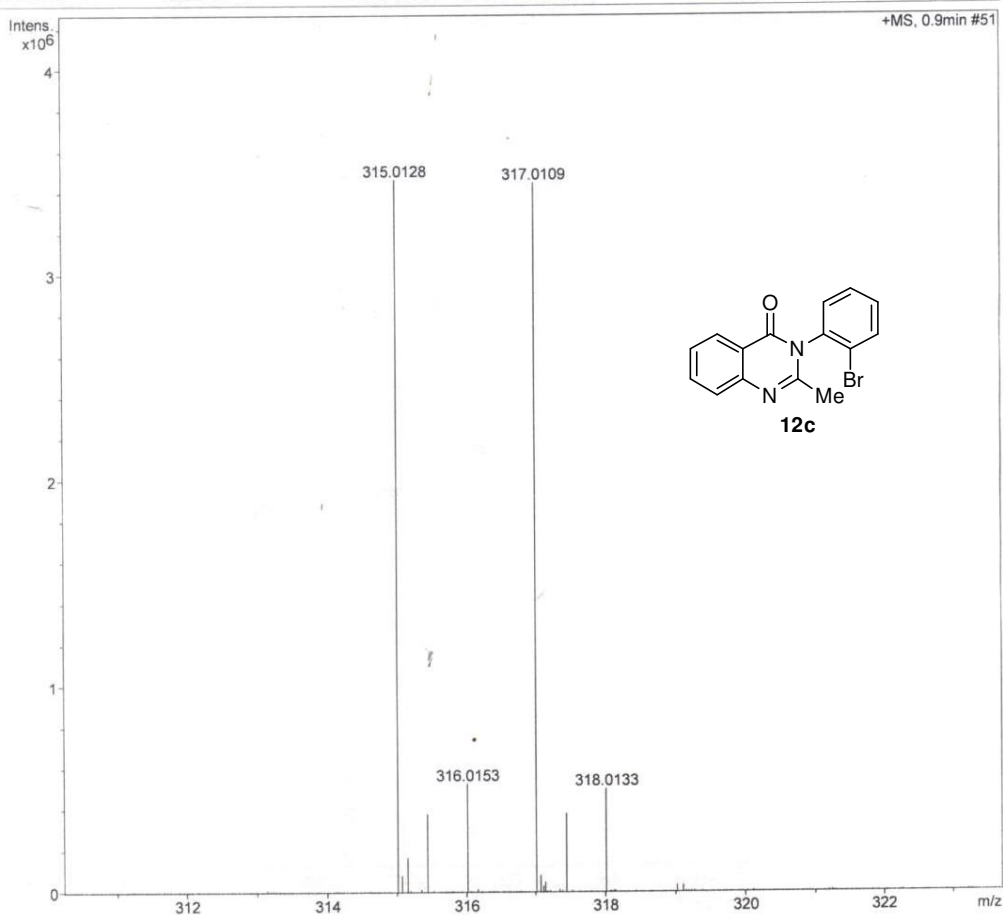
Analysis Name D:\Data\2015\DrNagarajan\FEB\SKG-668.d
Method tune_low_Pos.m
Sample Name SKG-668-DCM-MEOH
Comment

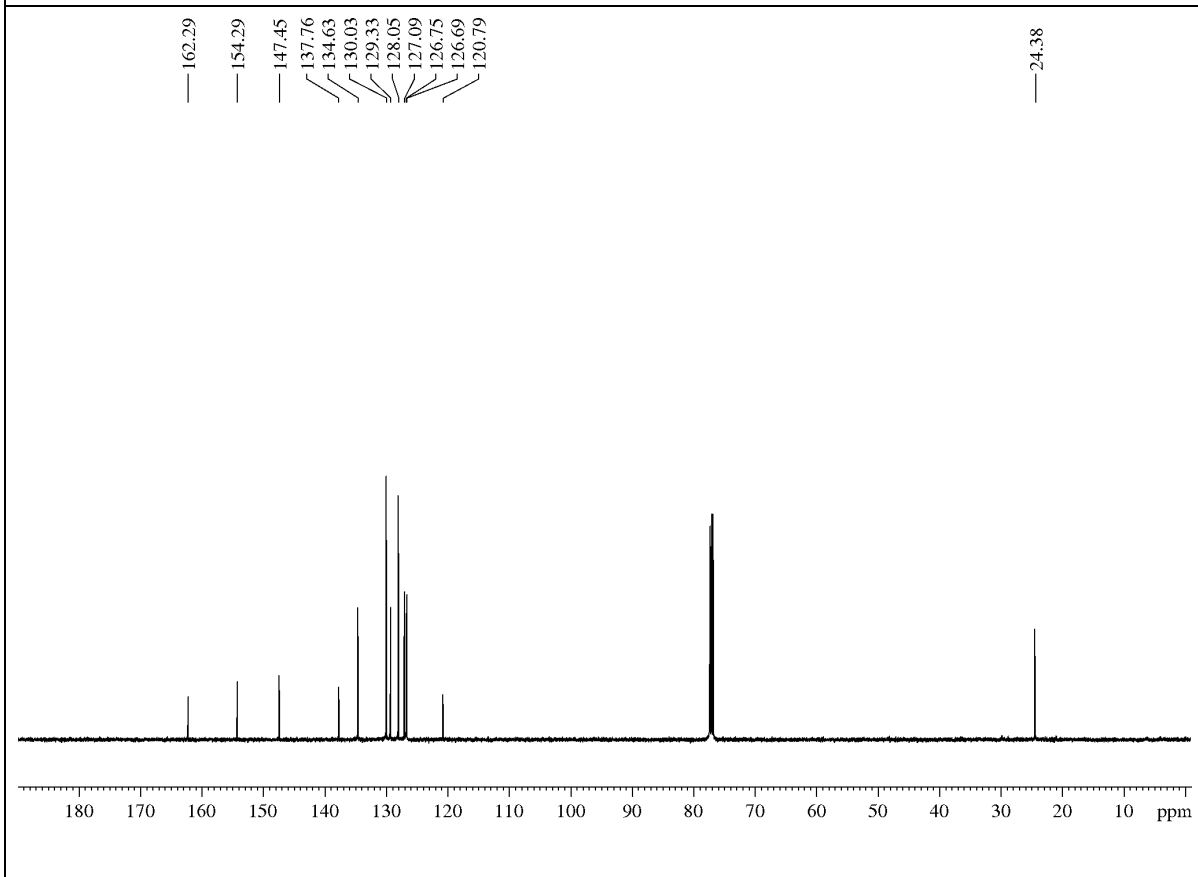
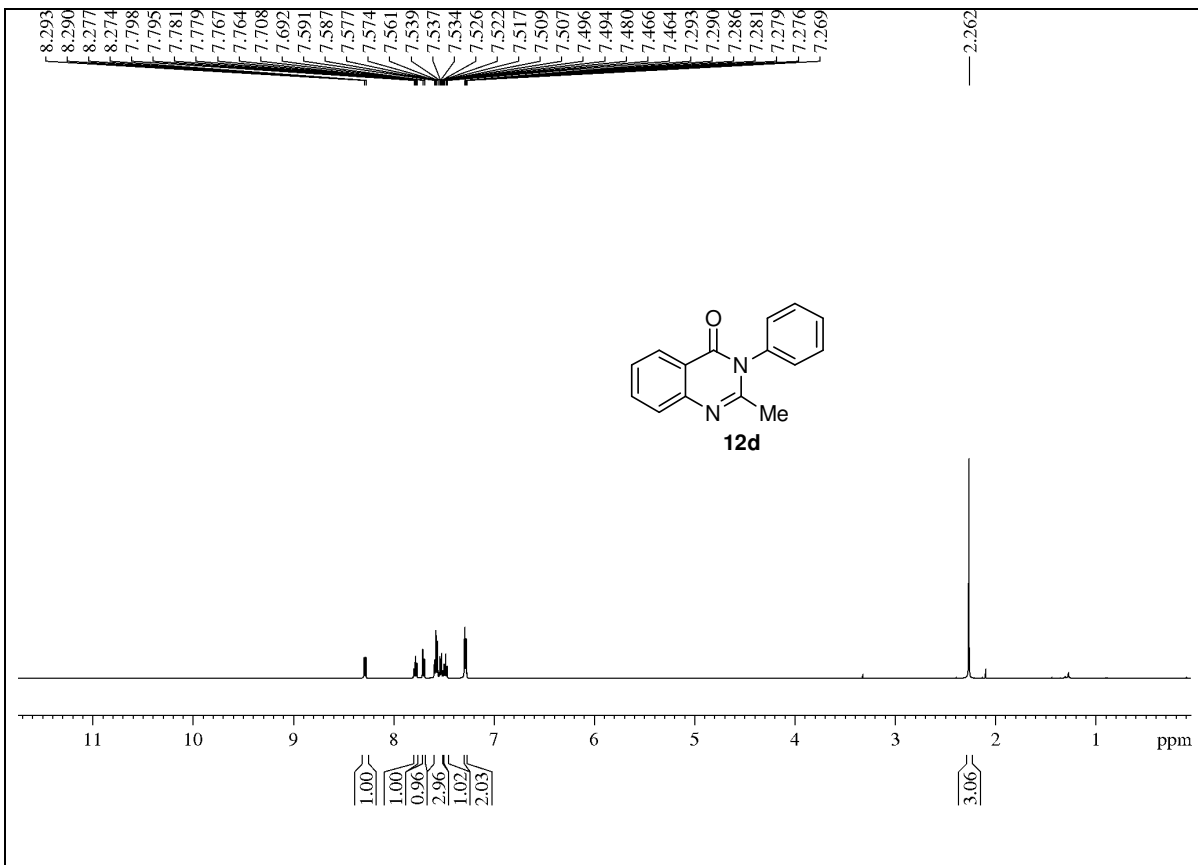
Acquisition Date 2/23/2015 1:16:47 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.6 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

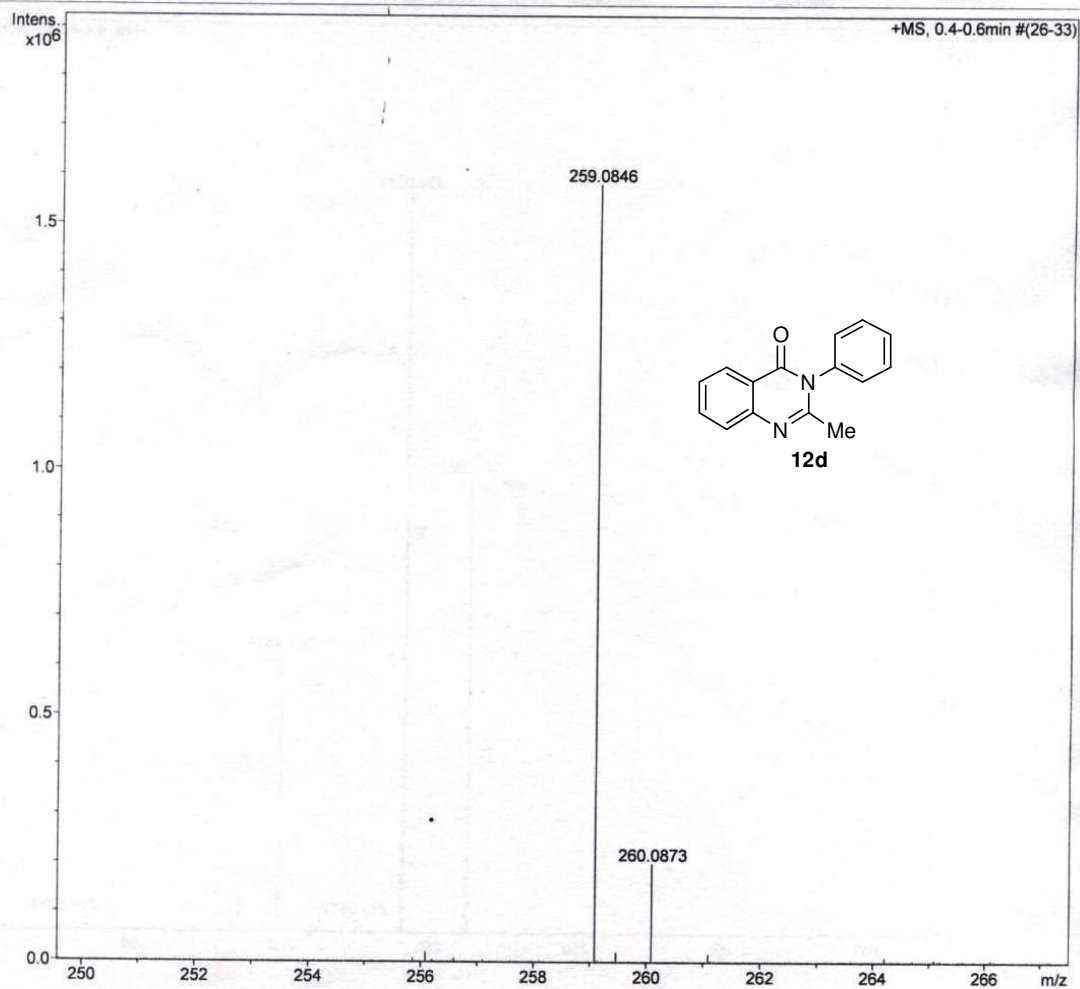
Analysis Name D:\Data\2015\DrNagarajan\FEB\SKG-660.d
Method TL-P.m
Sample Name SKG-660-DCM-MEOH
Comment

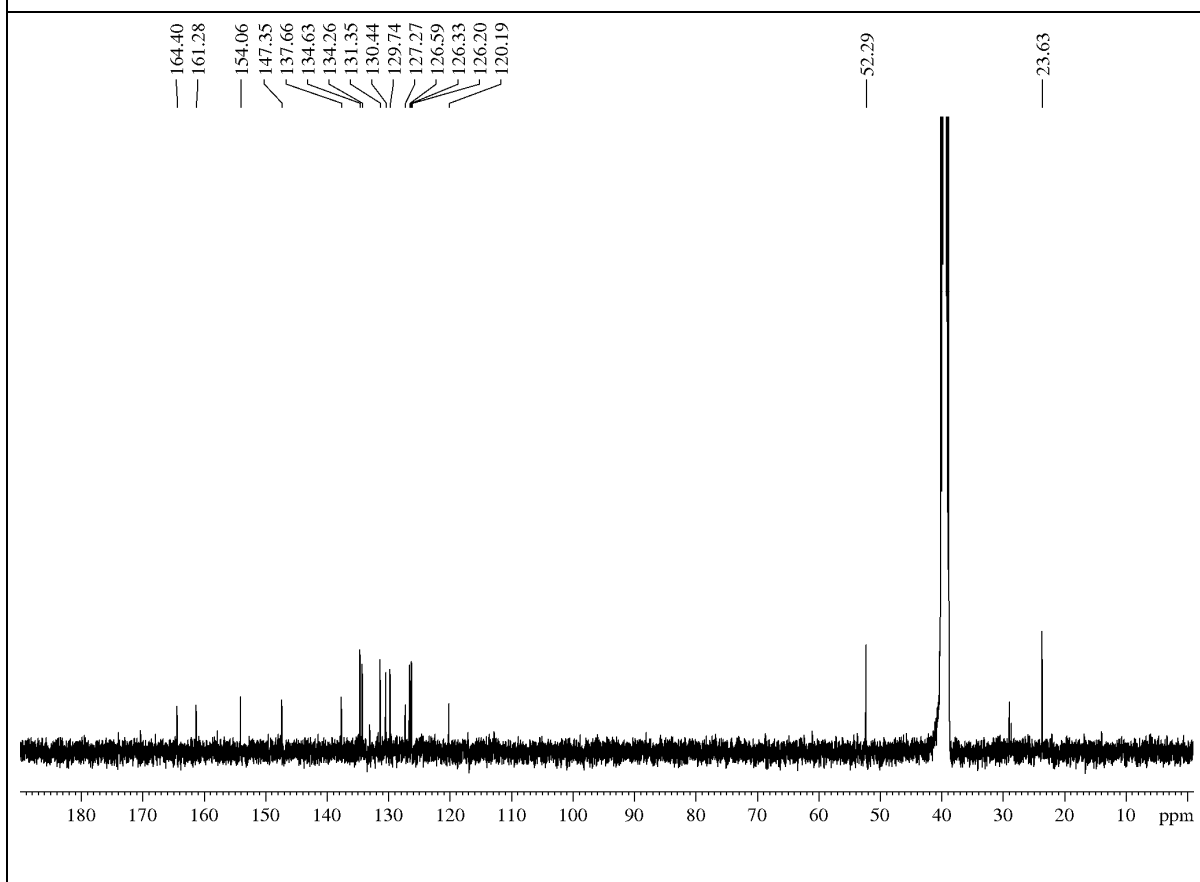
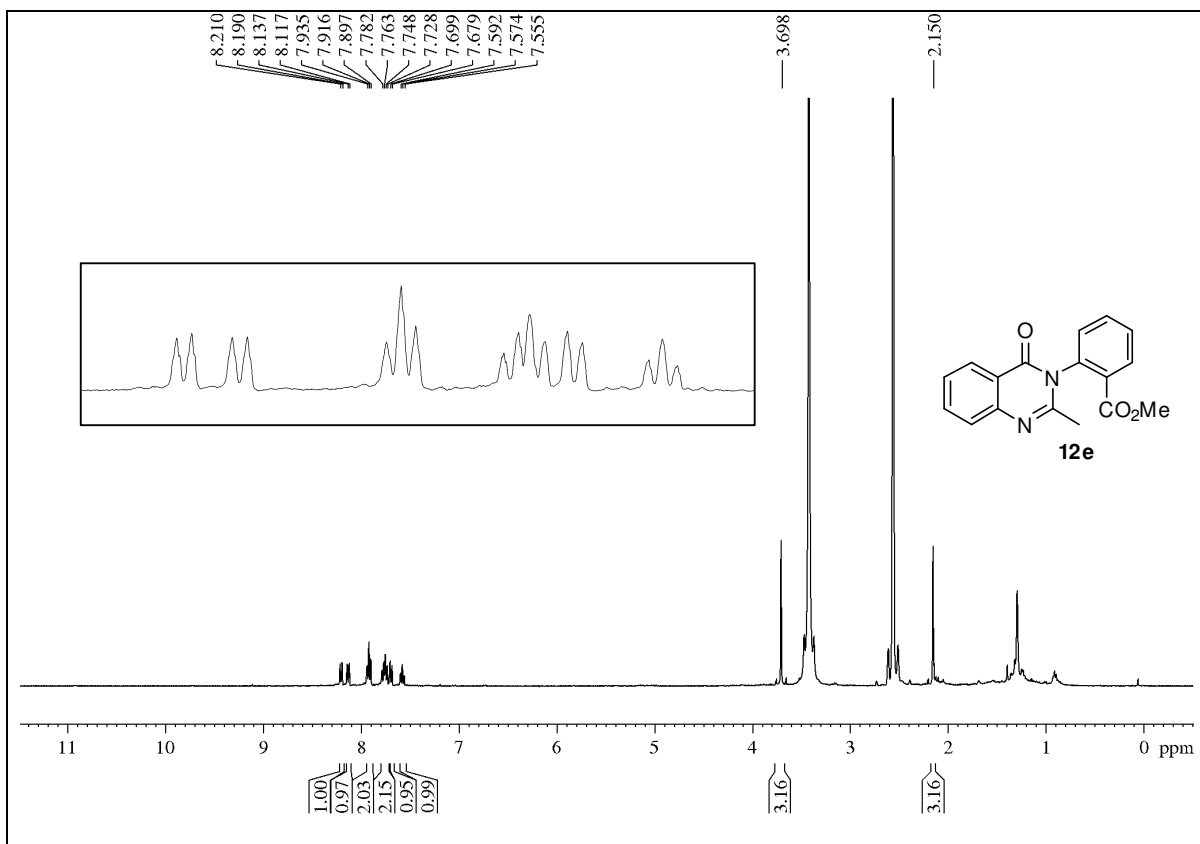
Acquisition Date 2/23/2015 11:21:17 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	600 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





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Analysis Info

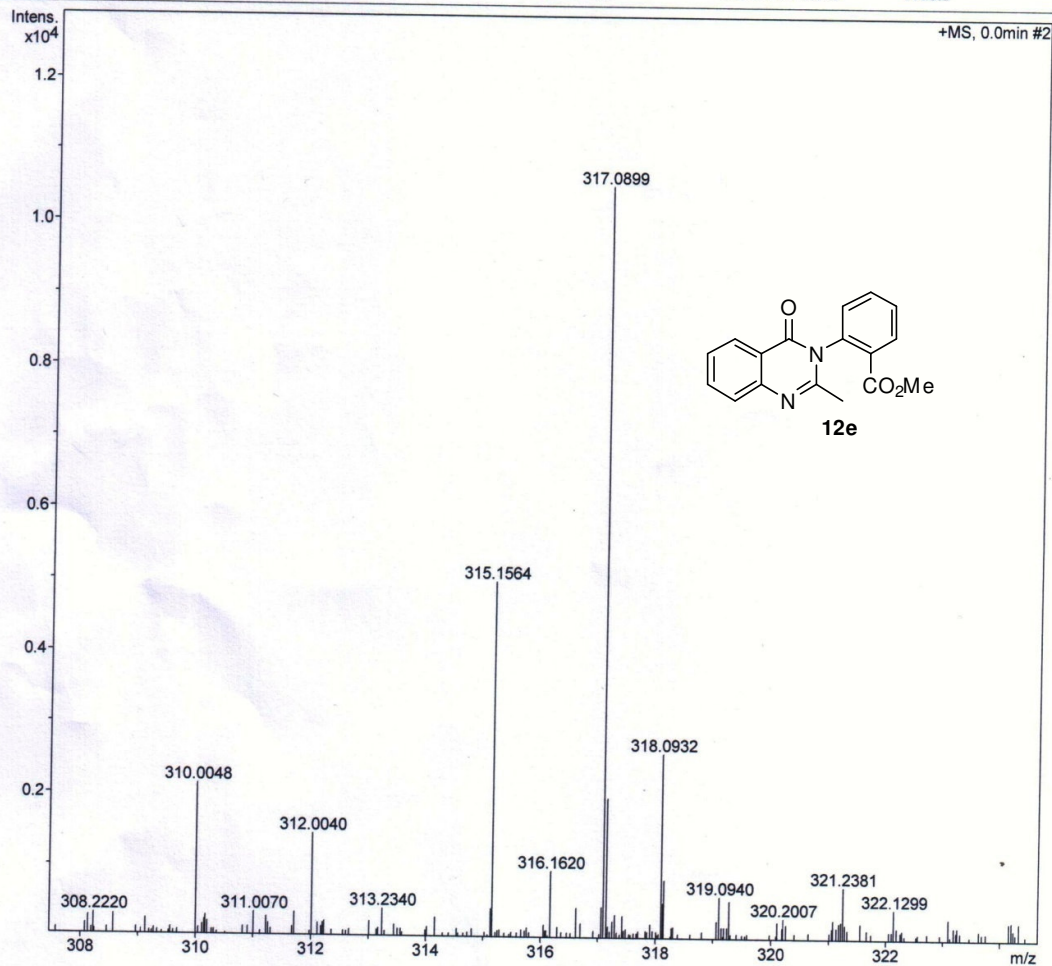
Analysis Name D:\Data\2015\DrNagarajan\JUNE\SKG-701.d
Method tune_low.m
Sample Name SKG-701-DCM-MEOH
Comment

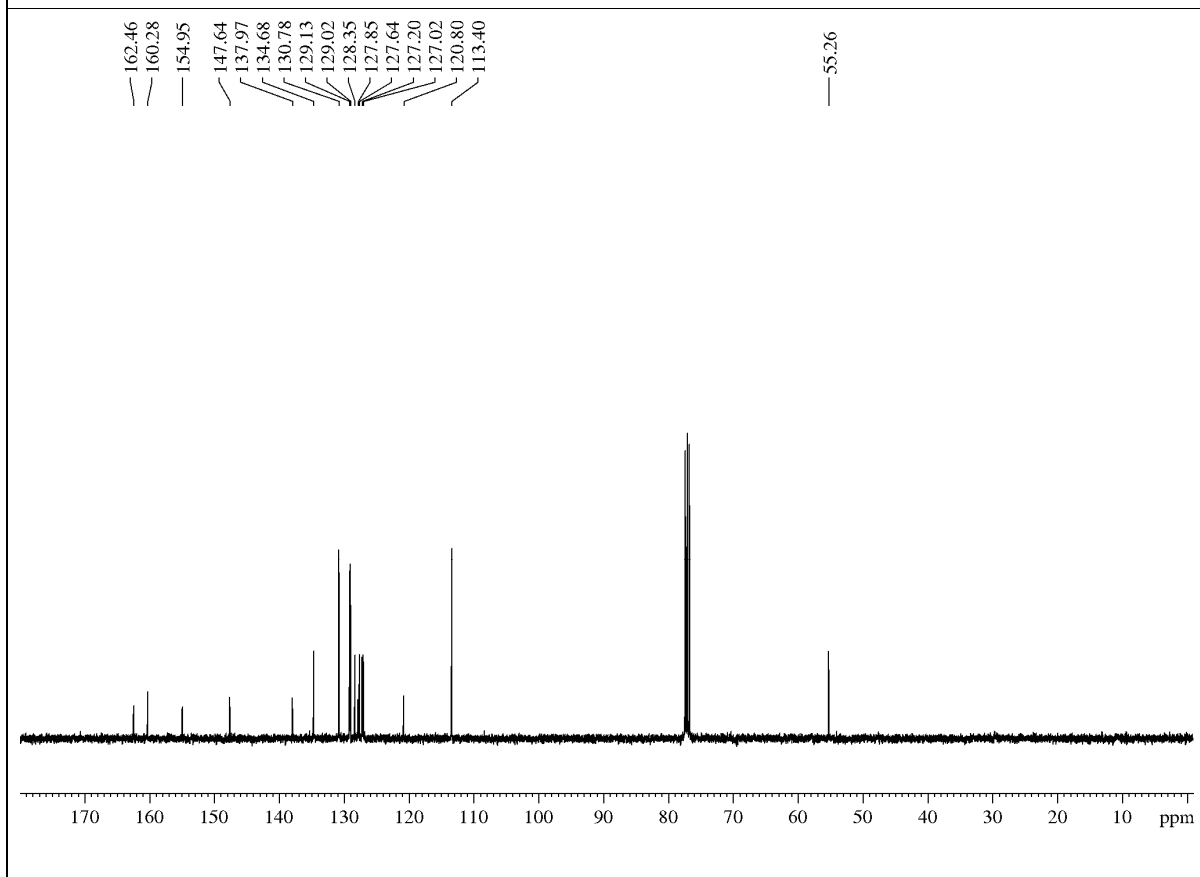
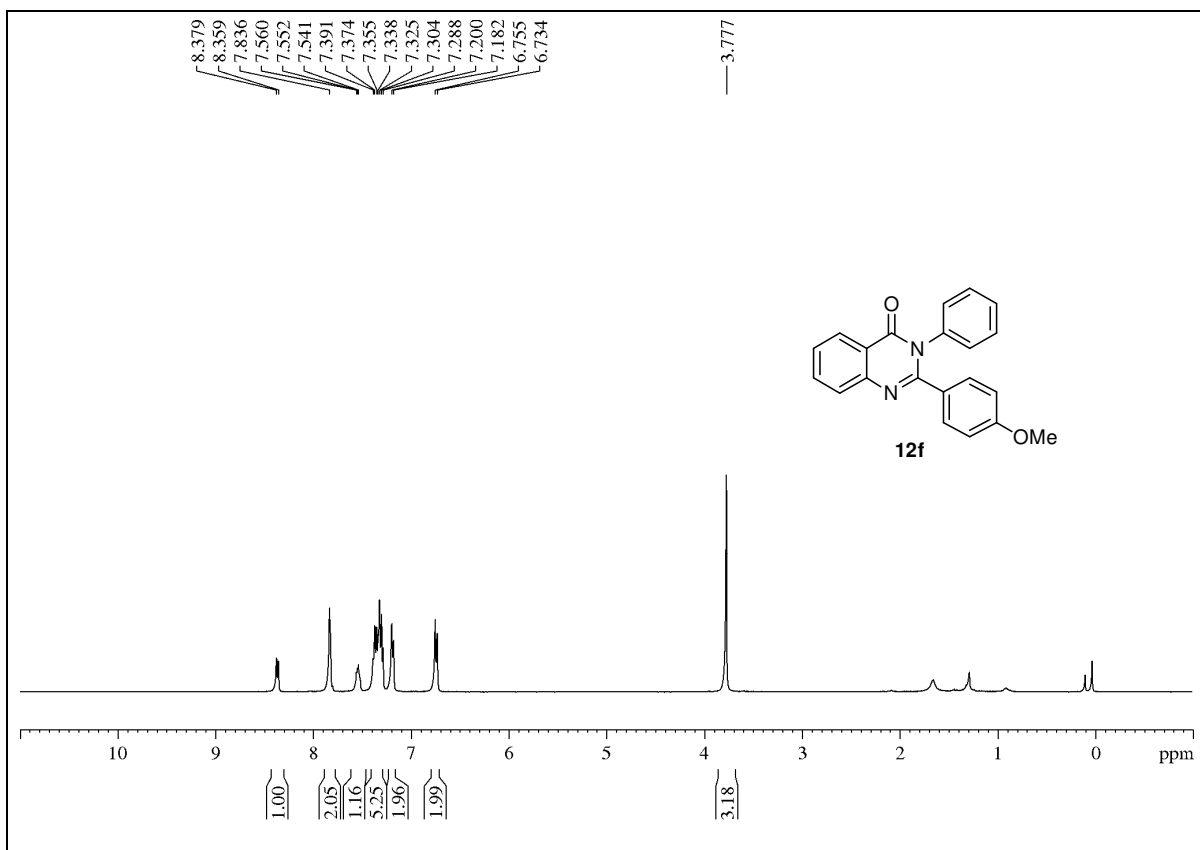
Acquisition Date 6/29/2015 1:02:12 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



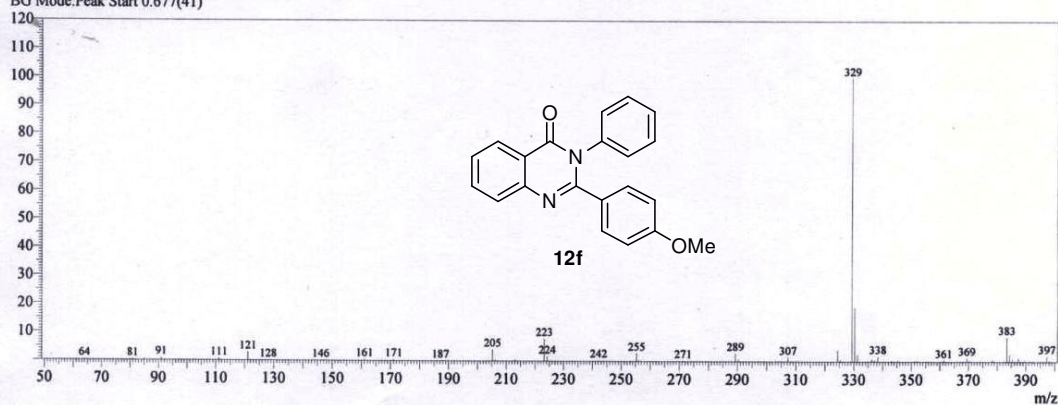


LCMS-2010A DATA REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

User : Admin
Sample : SKG-673
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\SKG-673-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#: 1 R.Time: 0.831(Scan#: 50) Positive
MassPeaks: 154 BasePeak: 329.35(5409029)
RawMode: Single 0.831(50)
BG Mode: Peak Start 0.677(41)

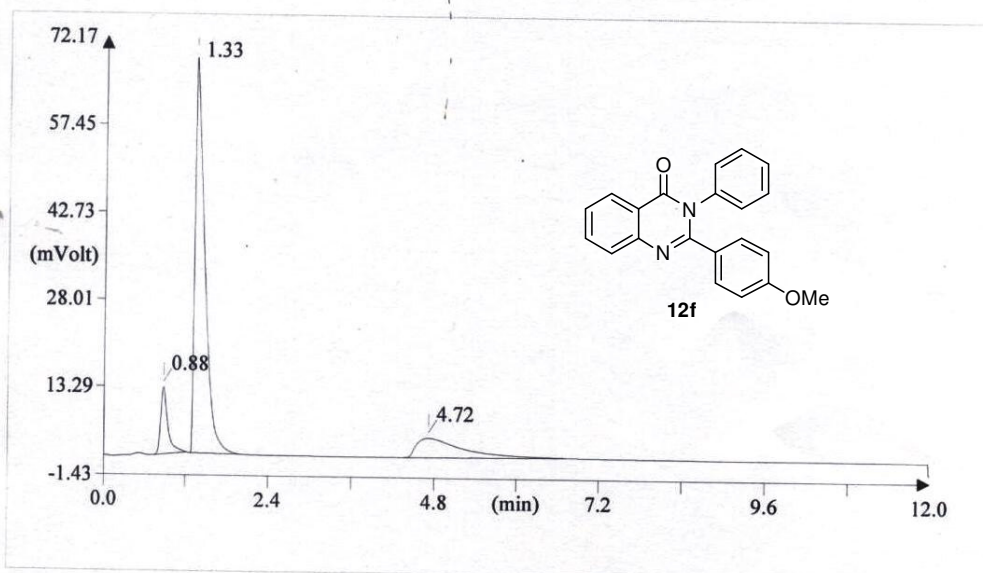


MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.831	0.677	1.043	82279782	7660294	10.74		100.00		329.35	5409029
				82279782	7660294			100.00			

FLASH EA 1112 SERIES CHN REPORT
SCHOOL OF CHEMISTRY
UNIVERSITY OF HYDERABAD

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
 Sample ID: SKG-673 (# 151)
 Analysis type: UnkNown
 Chromatogram filename: UNK-18022015-11.dat
 Sample weight: 1512



Element Name	Element %	Ret. Time
Nitrogen	8.45	0.88
Carbon	76.95	1.33
Hydrogen	5.07	4.72