

NIS Mediated Regioselective Amidation of Indole with Quinazolinone and Pyrimidone

Suman Kr Ghosh and Rajagopal Nagarajan*

School of Chemistry, University of Hyderabad, Hyderabad-500 046, INDIA

E-mail: rpsc@uohyd.ernet.in

Supporting Information

Table of contentspage number

X-Ray Data2-3

¹H, ¹³C, NMR spectra and HRMS data 4-89

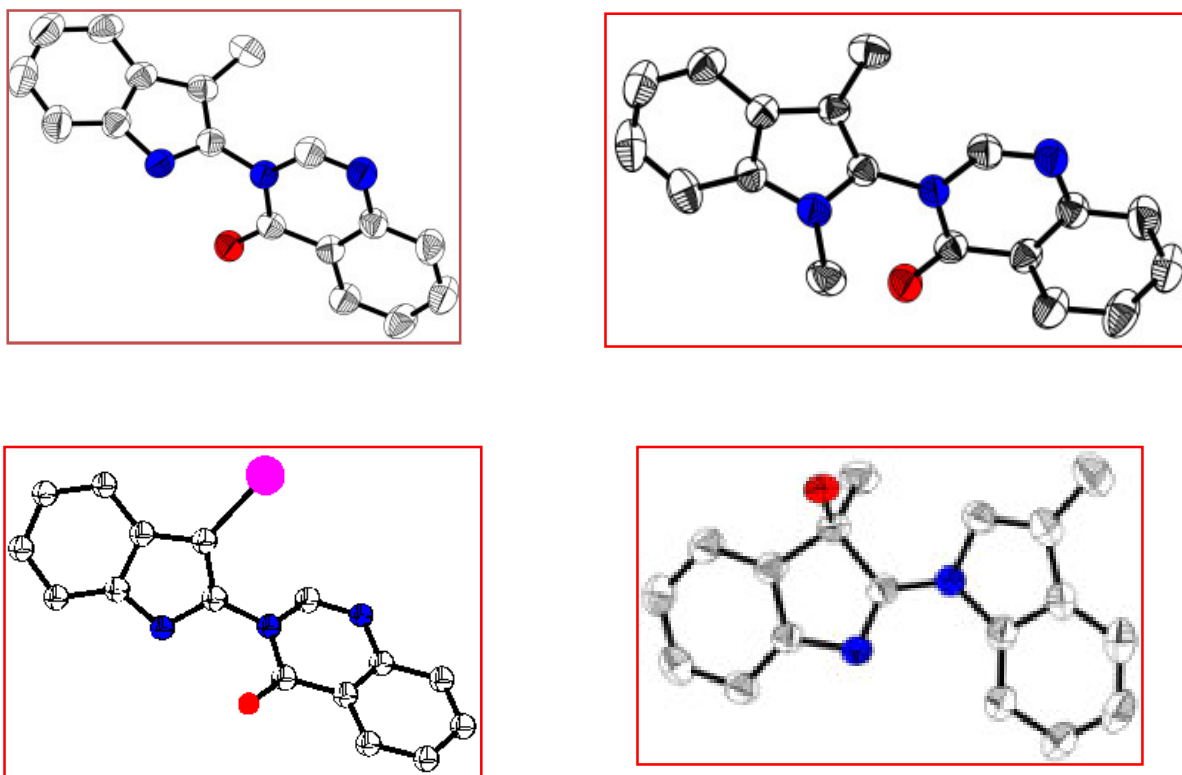


Figure 1 : ORTEP of Compound 3a, 3i, 5aa, 9 (Hydrogens are removed for clarity)

Molecular formula: $C_{17}H_{13}N_3O_1$, unit cell parameters: $a=10.830(3)$, $b=12.205(3)$, $c=12.209(3)\text{\AA}$, $\alpha=102.677(4)^\circ$, $\beta=106.686(4)^\circ$, $\gamma=110.923(4)^\circ$ and space group $P -1$. CCDC 956412 contains the supplementary crystallographic data for compound **3a** of this paper.

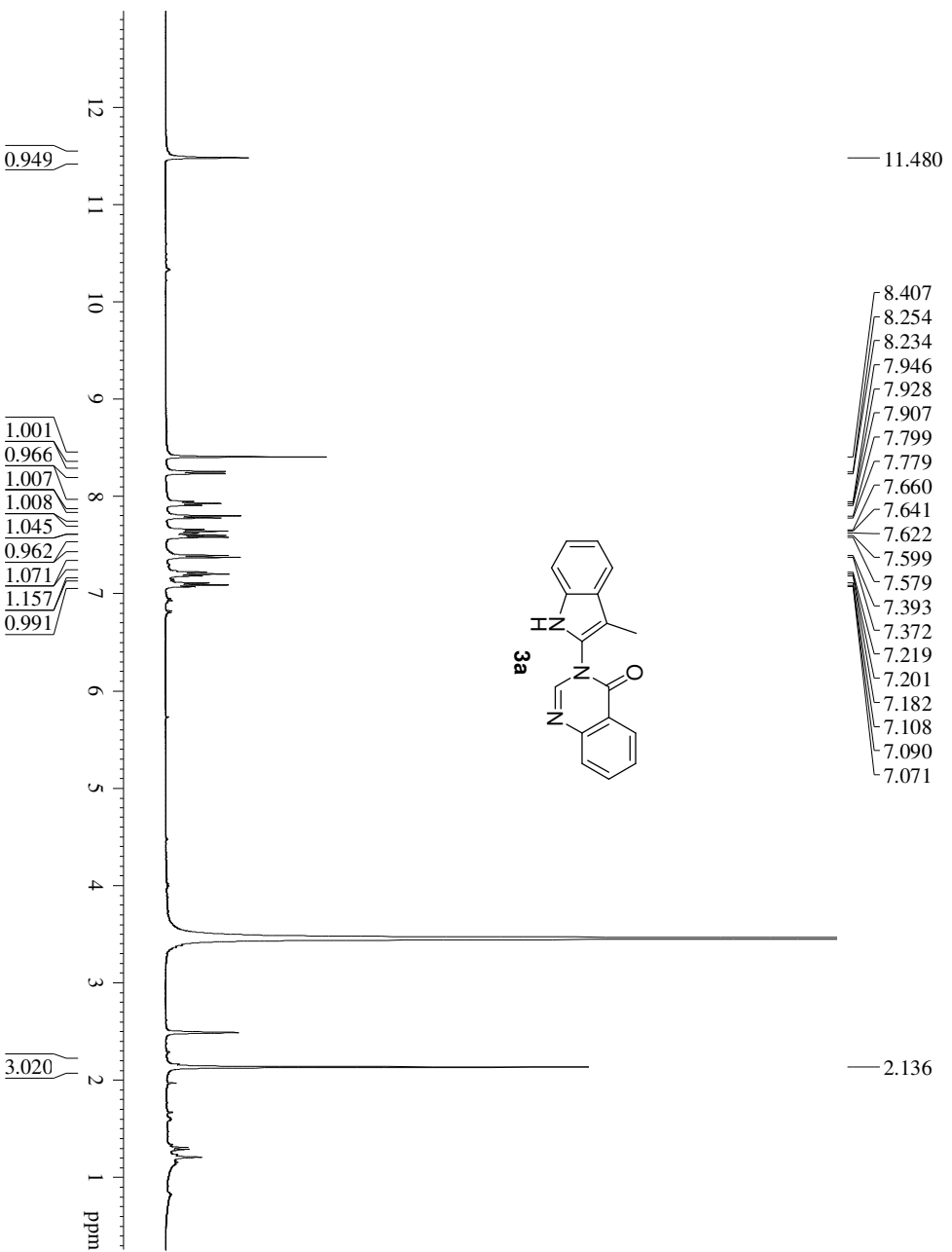
Molecular formula: $C_{18}H_{15}N_3O_1$, unit cell parameters: $a=8.3989(18)$, $b=12.9656(14)$, $c=13.6993(18)\text{\AA}$, $\beta=101.702(16)^\circ$ and space group $P 21/n$. CCDC 956410 contains the supplementary crystallographic data for compound **3i** of this paper.

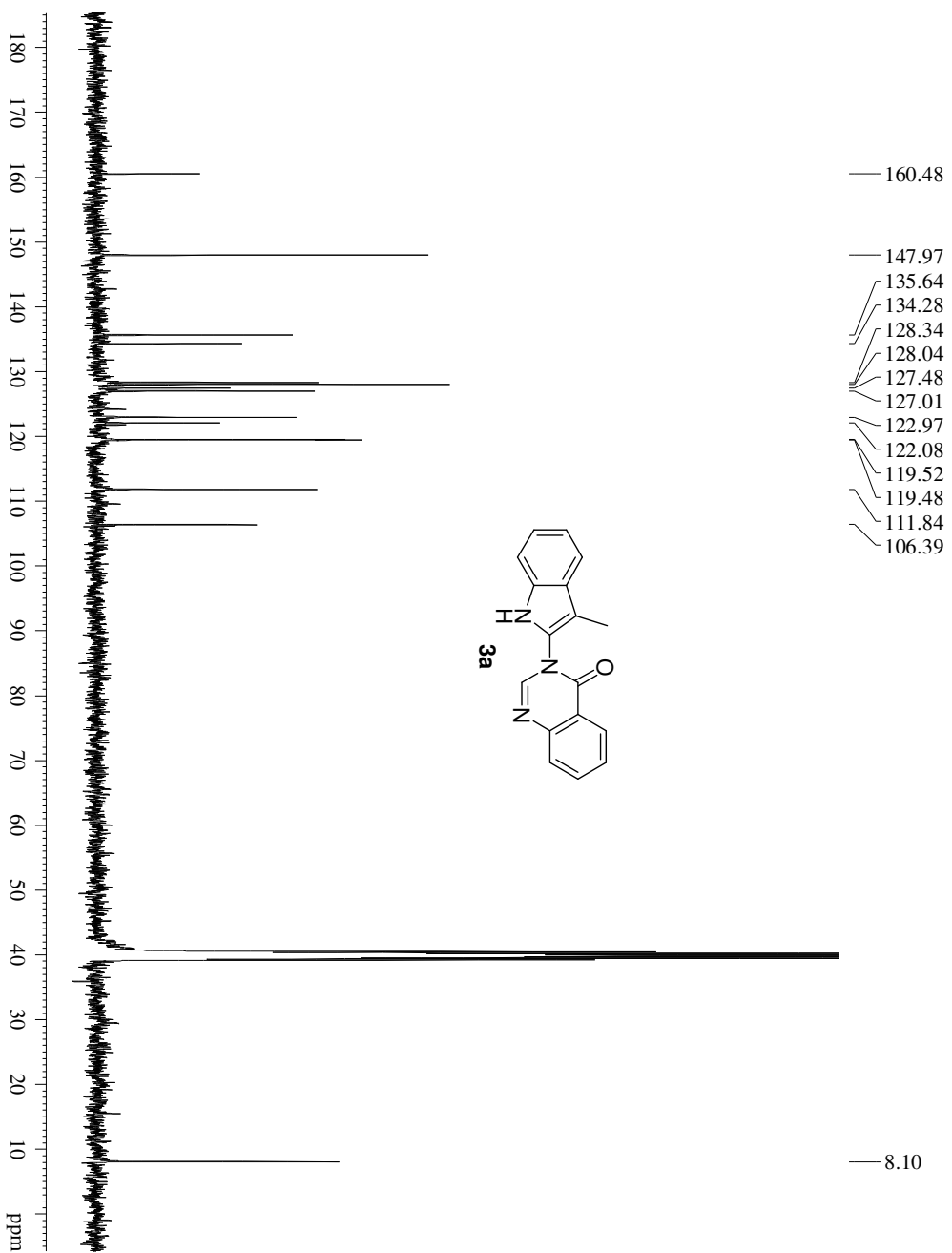
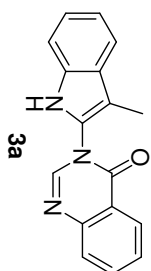
Molecular formula: $C_{16}H_{10}I_1N_3O_1$, unit cell parameters: $a=13.0741(18)$, $b=4.2988(4)$, $c=24.974(3)\text{\AA}$, $\beta=100.040(11)^\circ$ and space group $P 21/n$. CCDC 956409 contains the supplementary crystallographic data for compound **5aa** of this paper.

Molecular formula: $C_{18}H_{16}N_2O_1$, unit cell parameters: $a=10.8278(7)$, $b=11.3669(8)$, $c=13.0687(6)\text{\AA}$, $\alpha=100.716(5)^\circ$, $\beta=106.227(5)^\circ$, $\gamma=104.477(6)^\circ$ and space group P -1. CCDC 956411 contains the supplementary crystallographic data for compound **9** of this paper.

These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

¹H, ¹³C NMR, HRMS Spectral Data of Compounds





BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

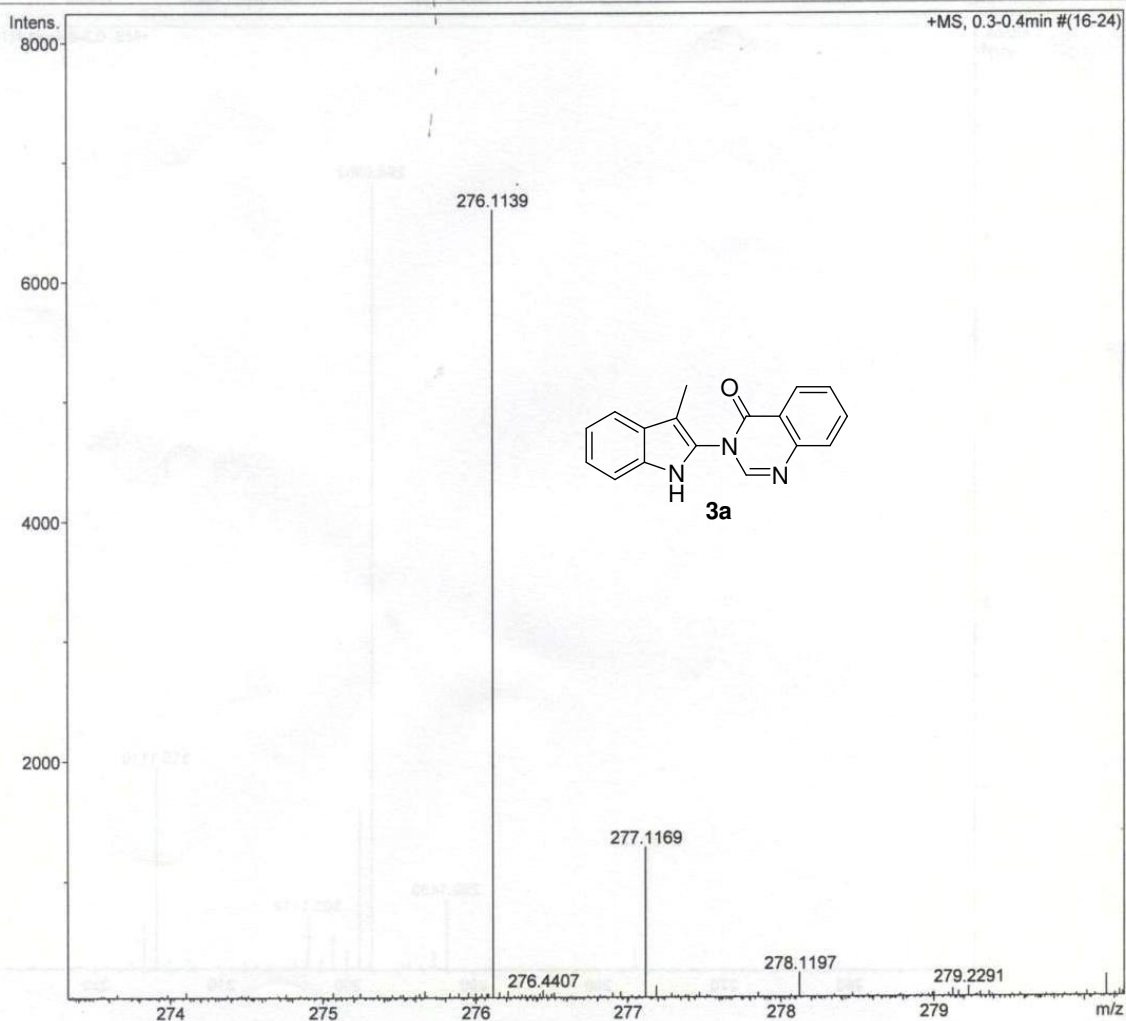
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-54.d
Method tune_low_PosR.m
Sample Name SKG-54--DCM-MEOH
Comment

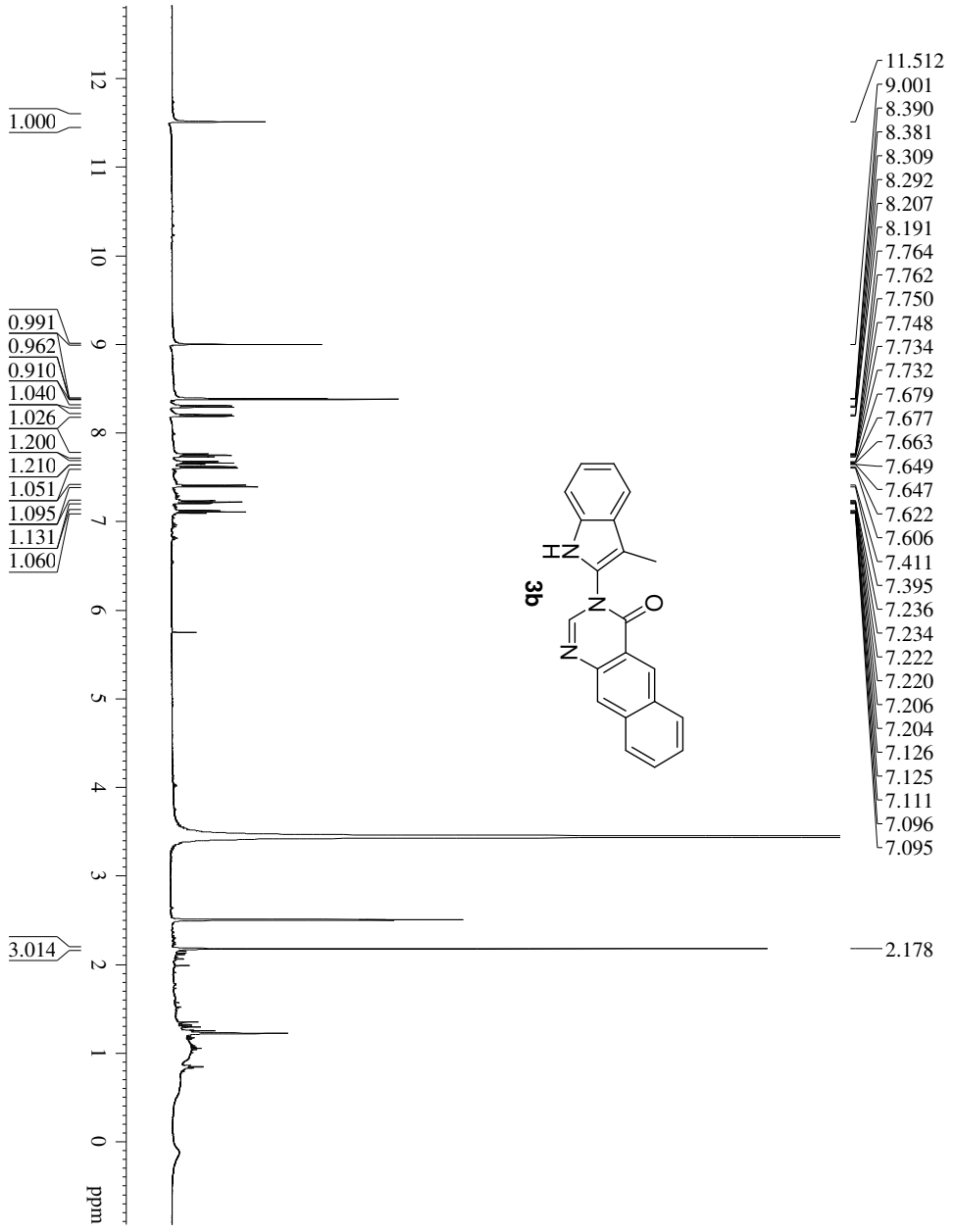
Acquisition Date 7/26/2013 2:10:38 PM

Operator Ramu Sridhar
Instrument maXis 10138

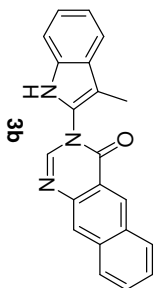
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





160.94
146.97
143.26
136.73
134.30
131.89
129.90
129.52
128.80
128.46
128.22
127.55
127.37
125.83
122.92
120.87
119.50
119.45
111.85
106.44



—8.17

BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

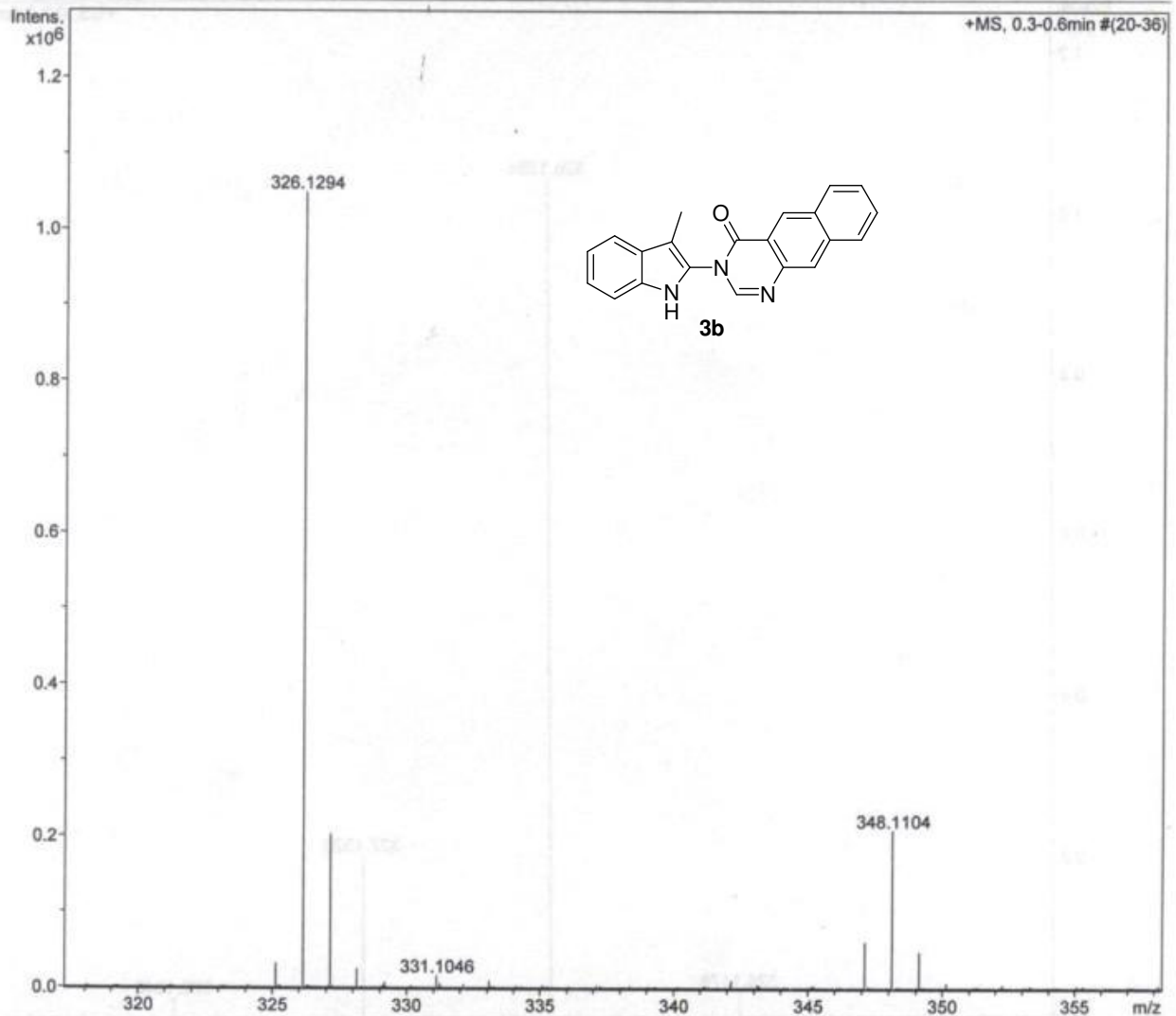
Analysis Info

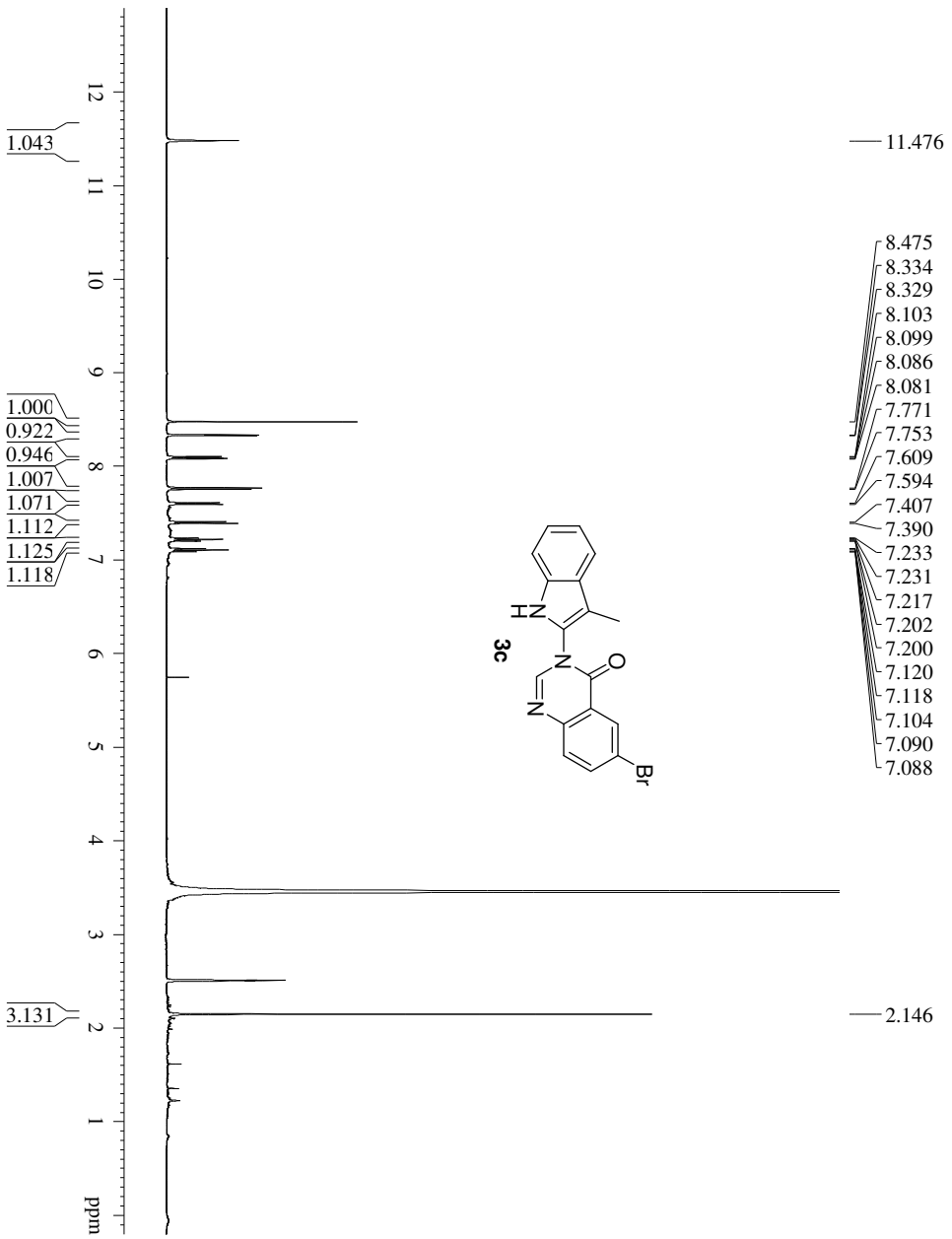
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JUNE\SKG-108.d
Method tune_low_Pos.m
Sample Name SKG-108-DCM-MEOH
Comment

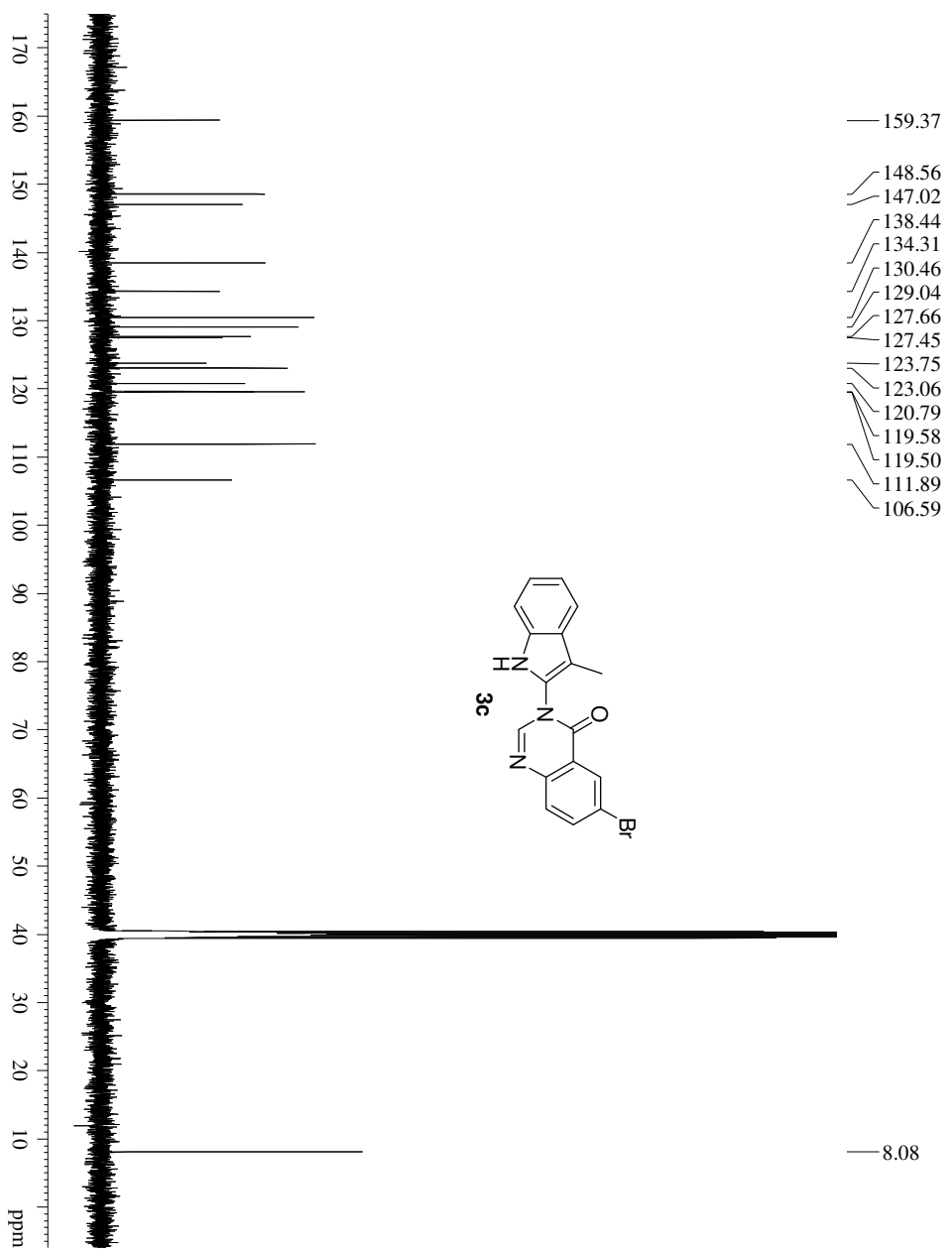
Acquisition Date 6/4/2013 11:57:28 AM
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

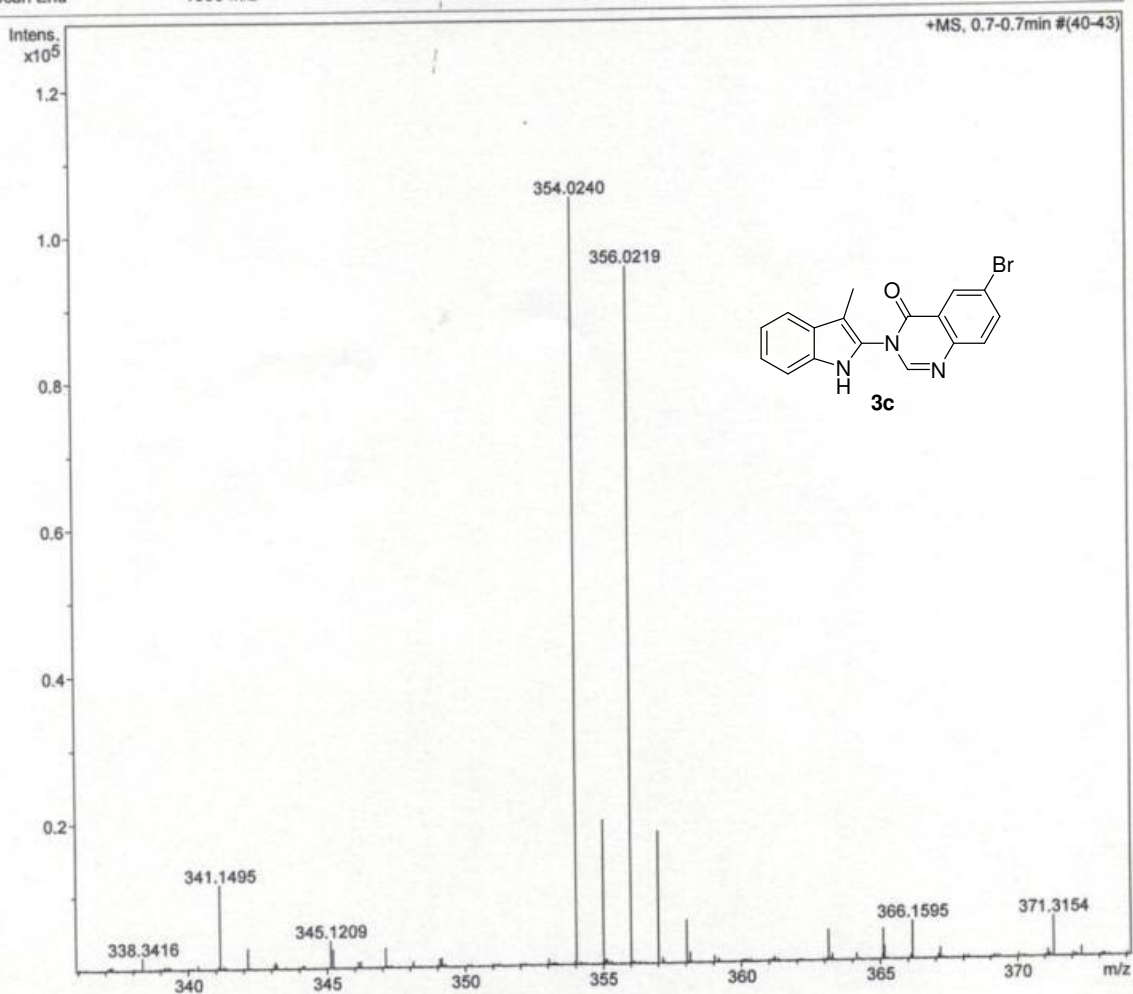
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JUNE\SKG-102.d
Method tune_low_Pos.m
Sample Name SKG-102-DCM-MEOH
Comment

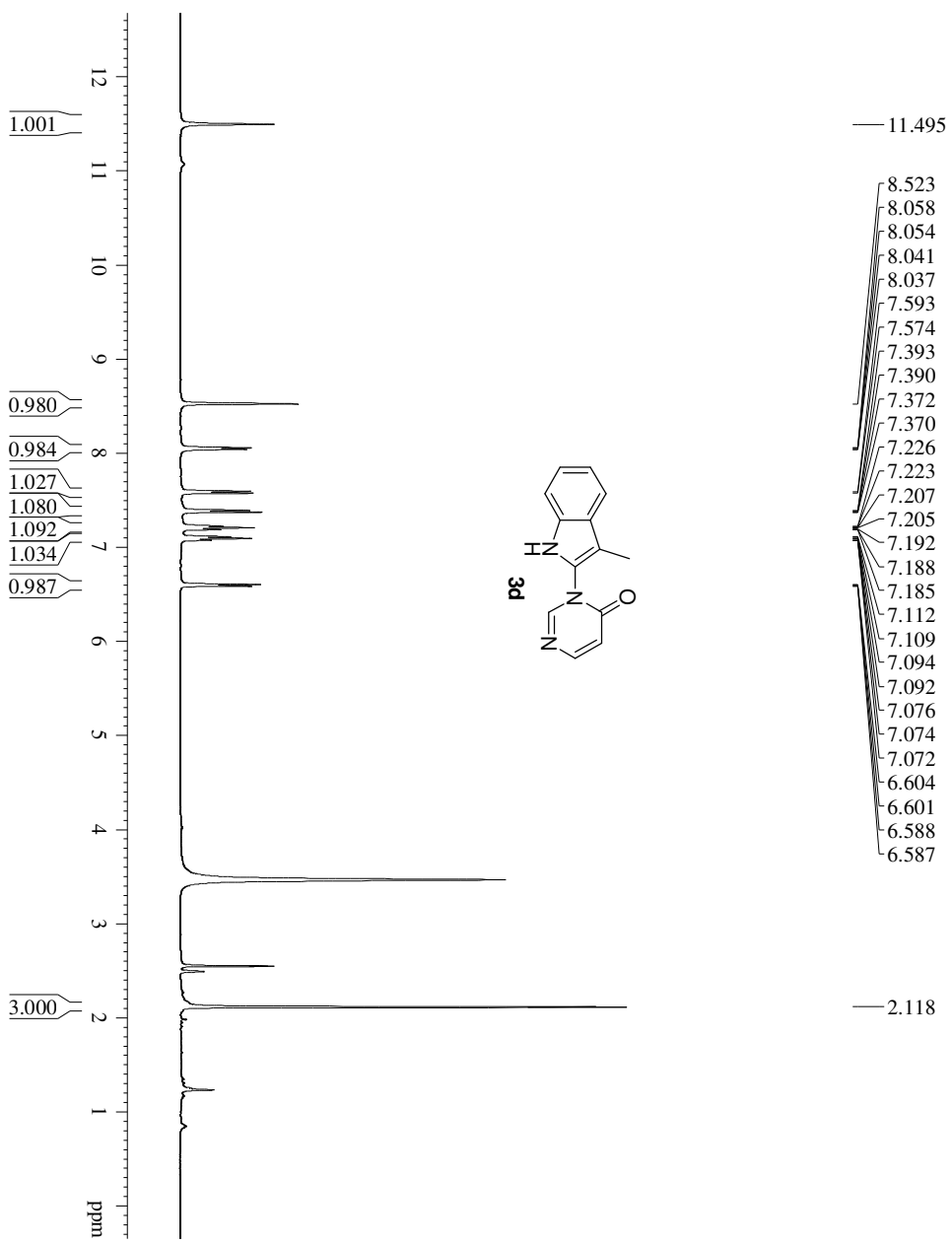
Acquisition Date 6/4/2013 12:08:16 PM

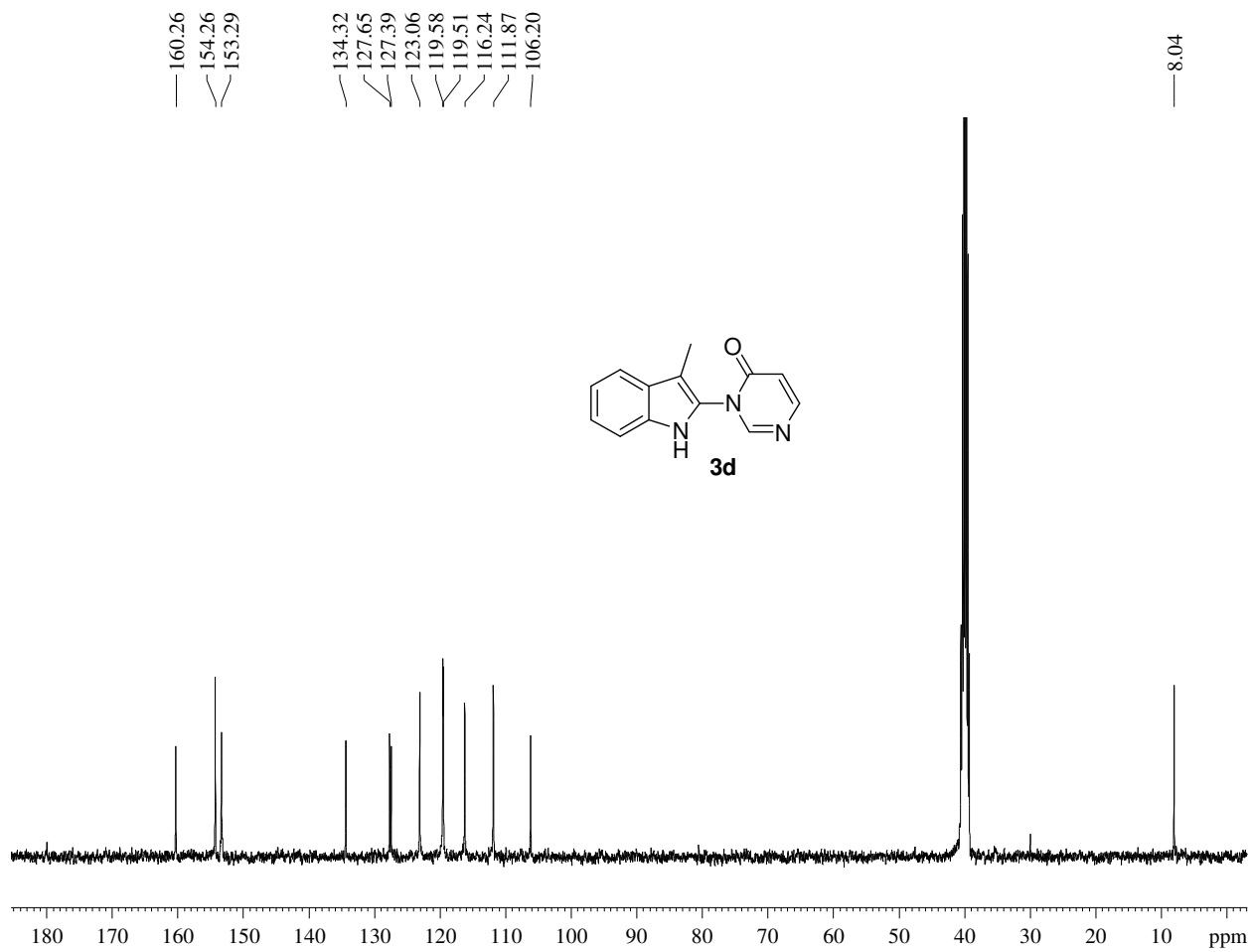
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

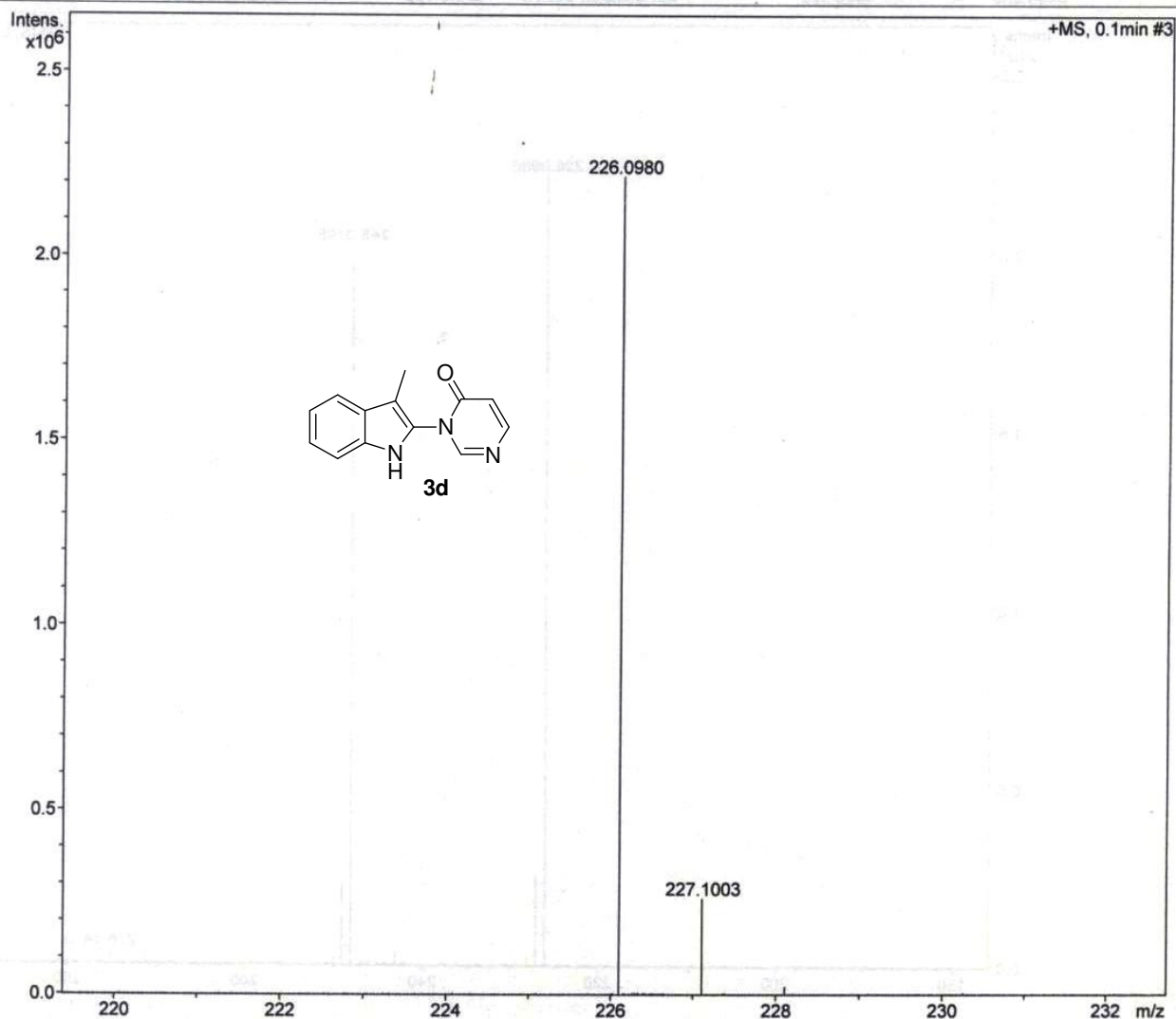
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-180.d
Method tune_low.m
Sample Name SKG-180-DCM-MEOH
Comment

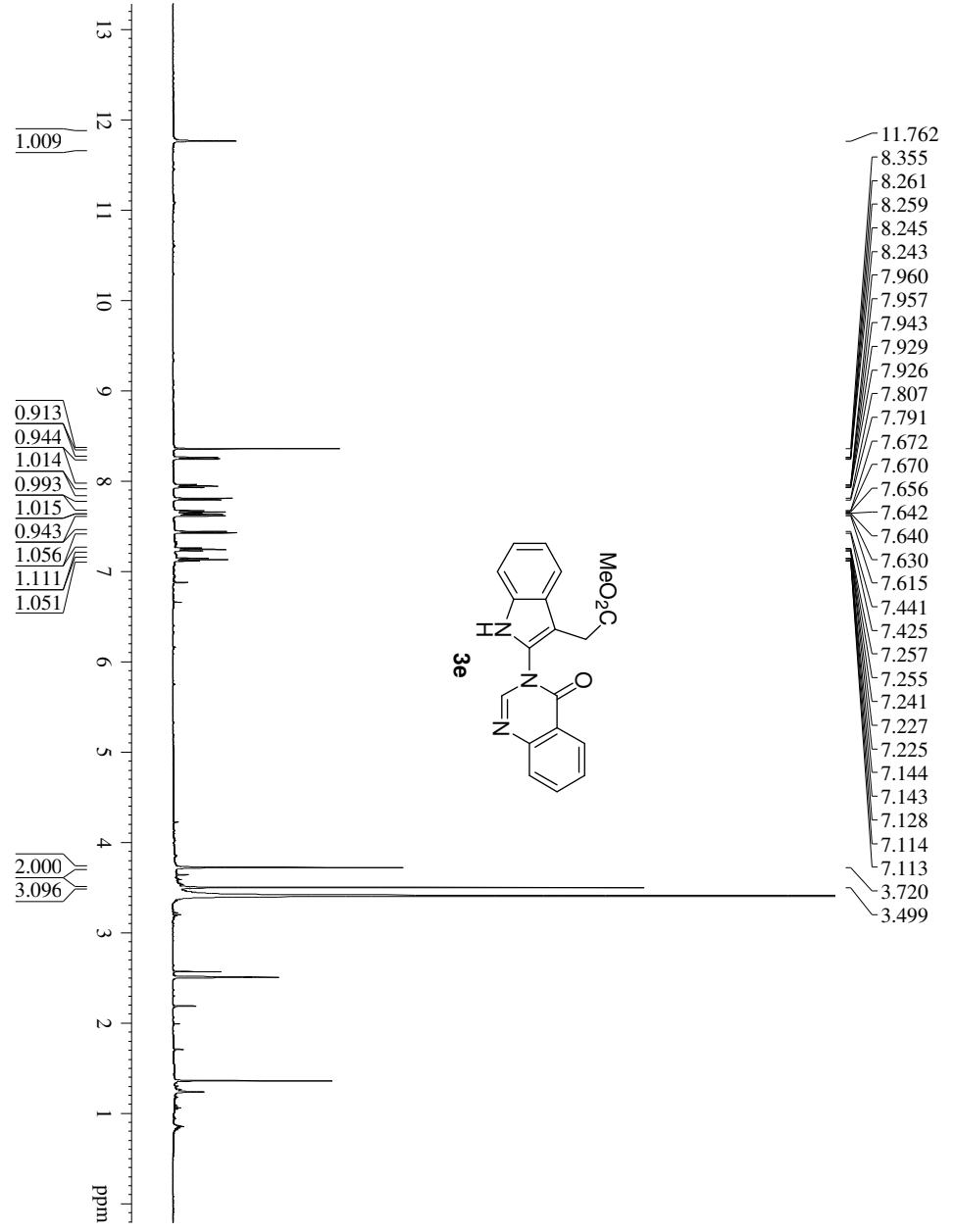
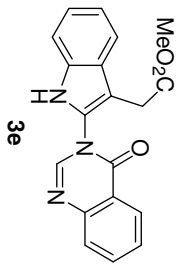
Acquisition Date 5/23/2013 12:32:43 PM

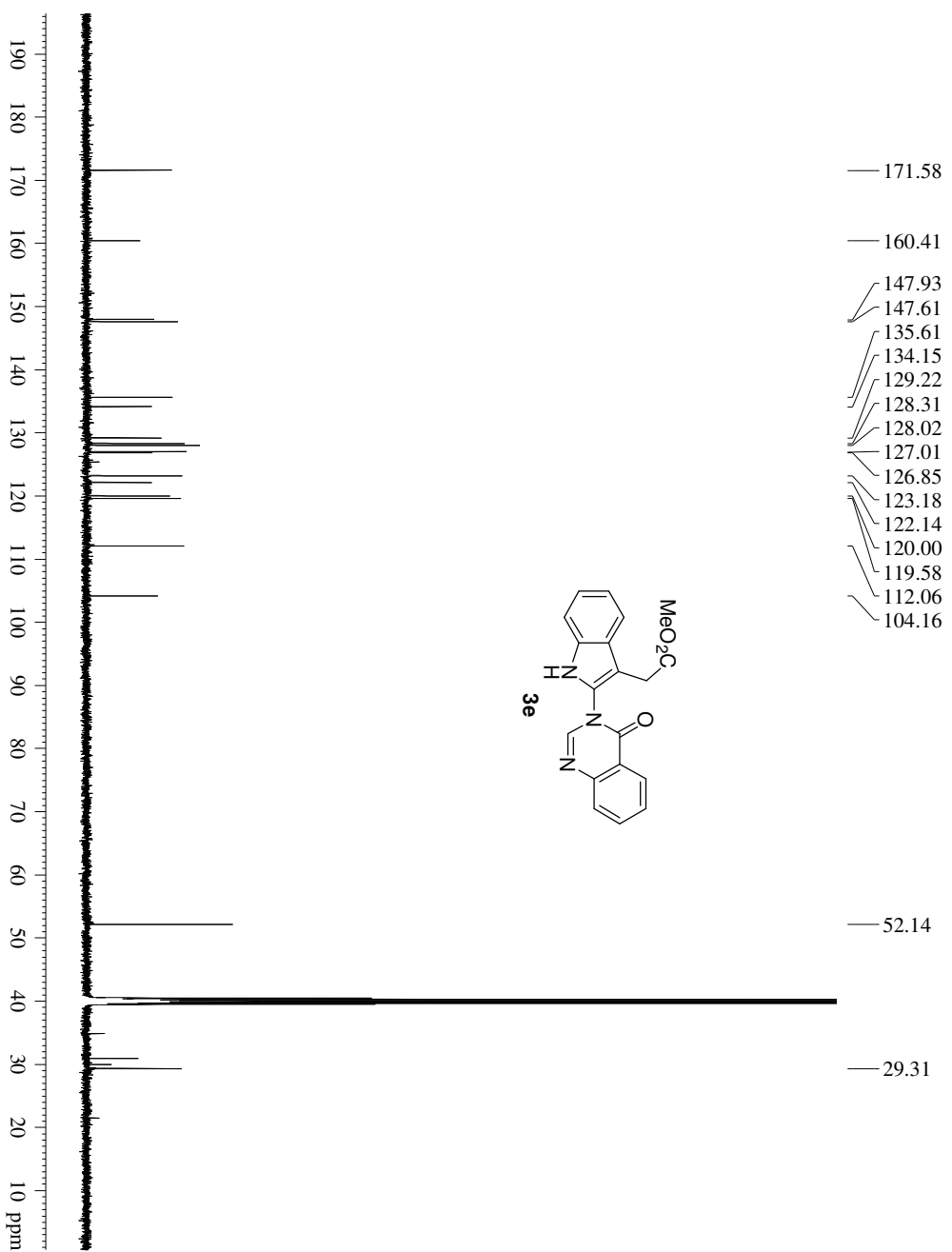
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

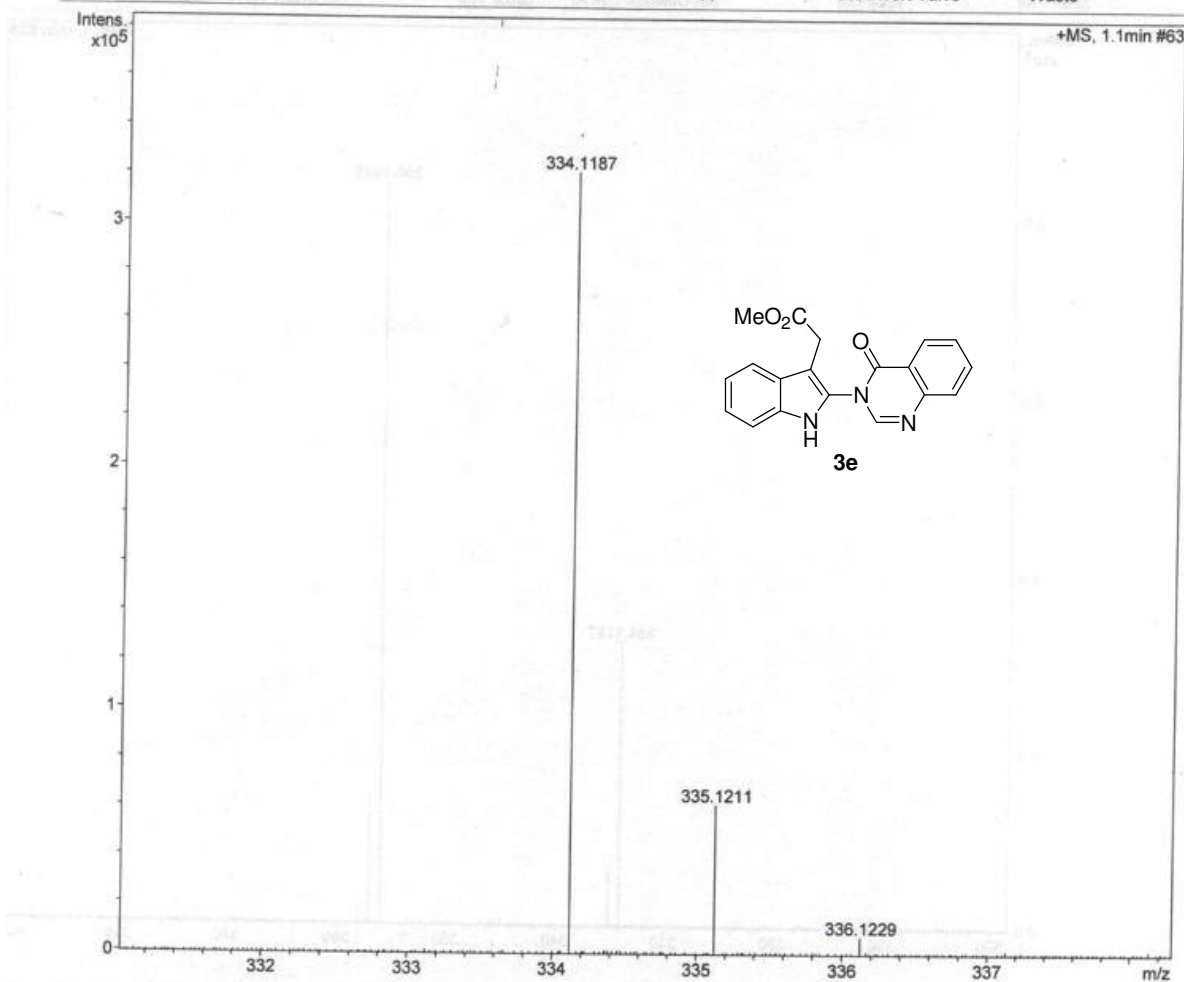
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-113.d
Method tune_low.m
Sample Name SKG-113-DCM-MEOH
Comment

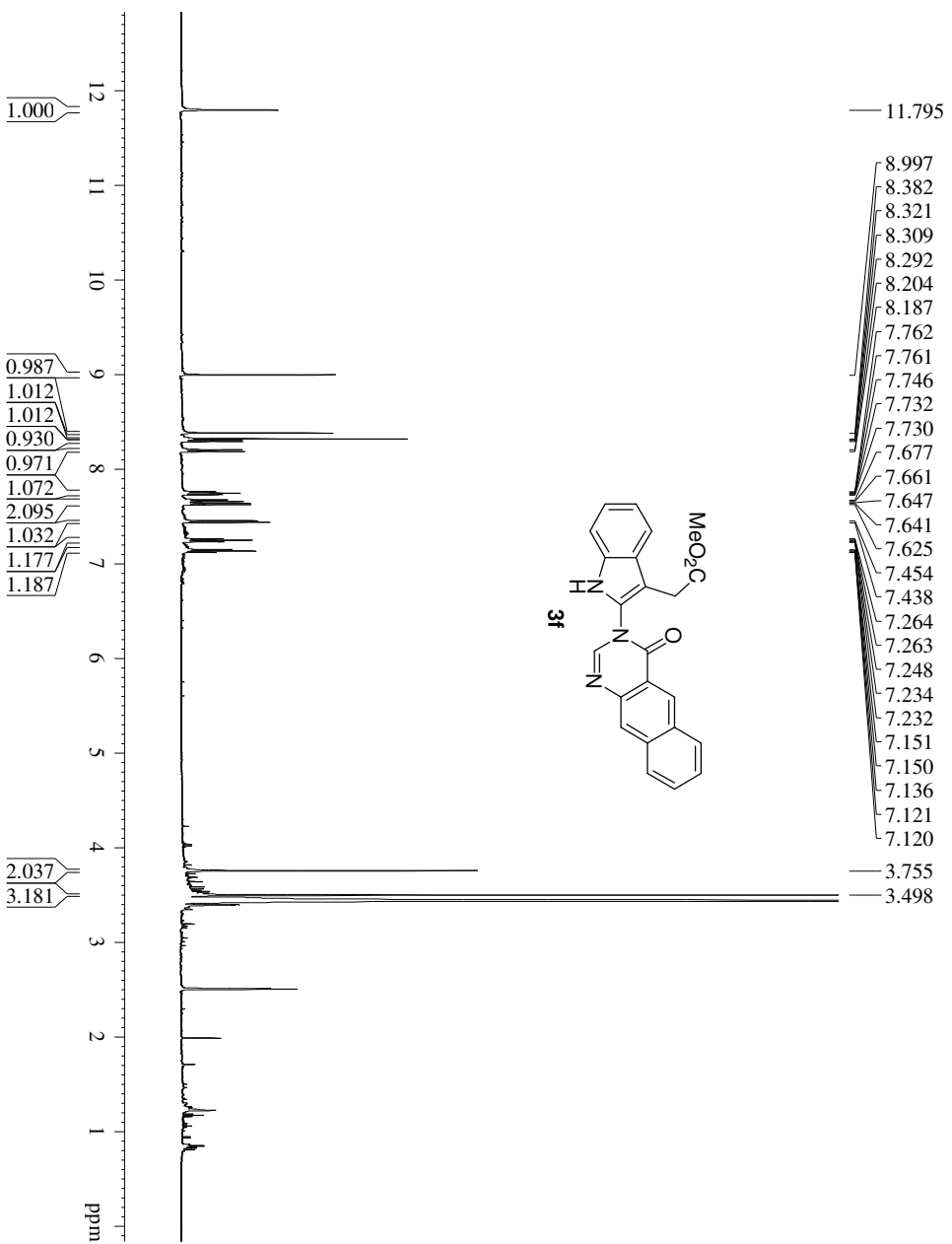
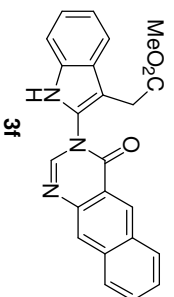
Acquisition Date 5/23/2013 1:01:49 PM

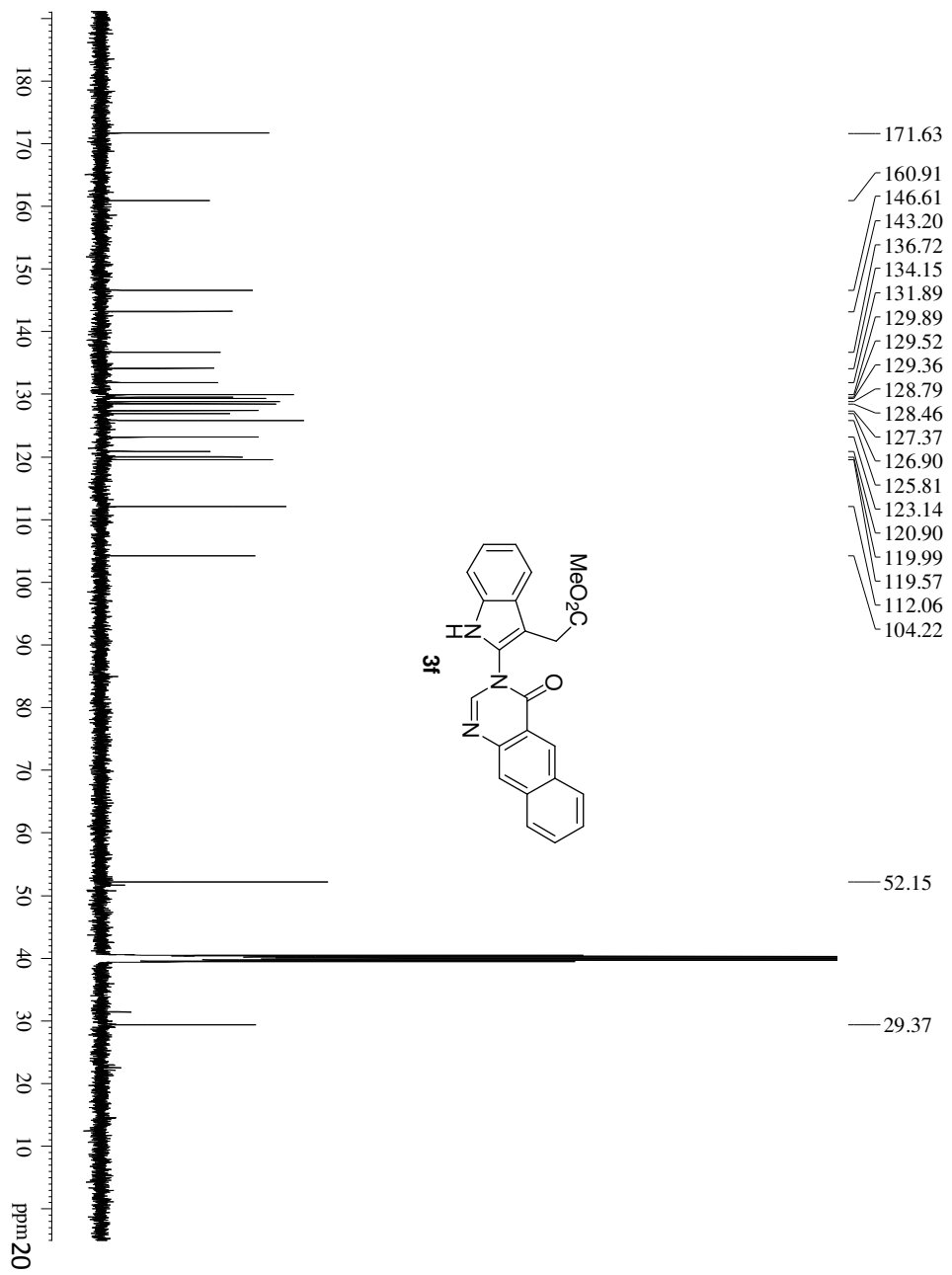
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

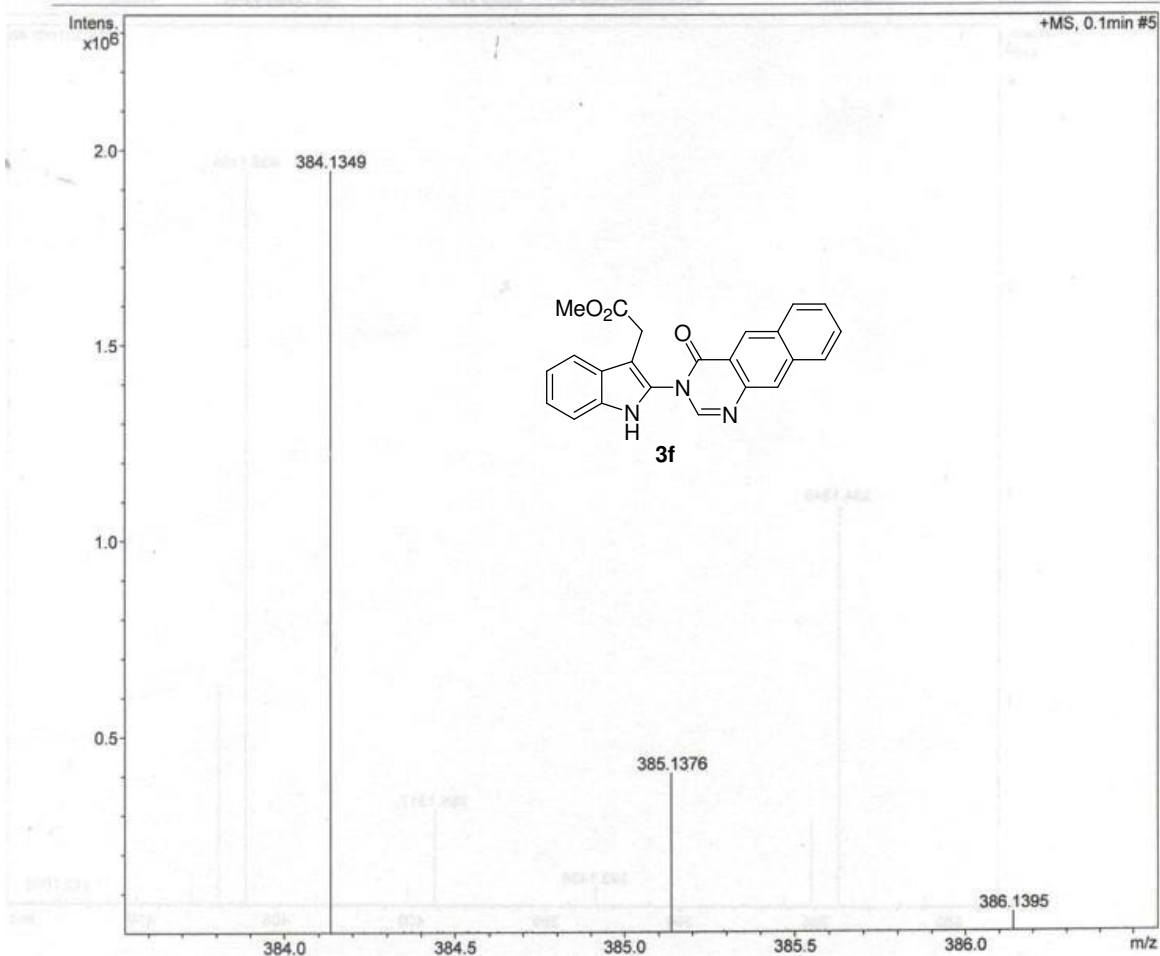
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-114R.d
Method tune_low_Pos.m
Sample Name SKG-114-DCM-MEOH
Comment

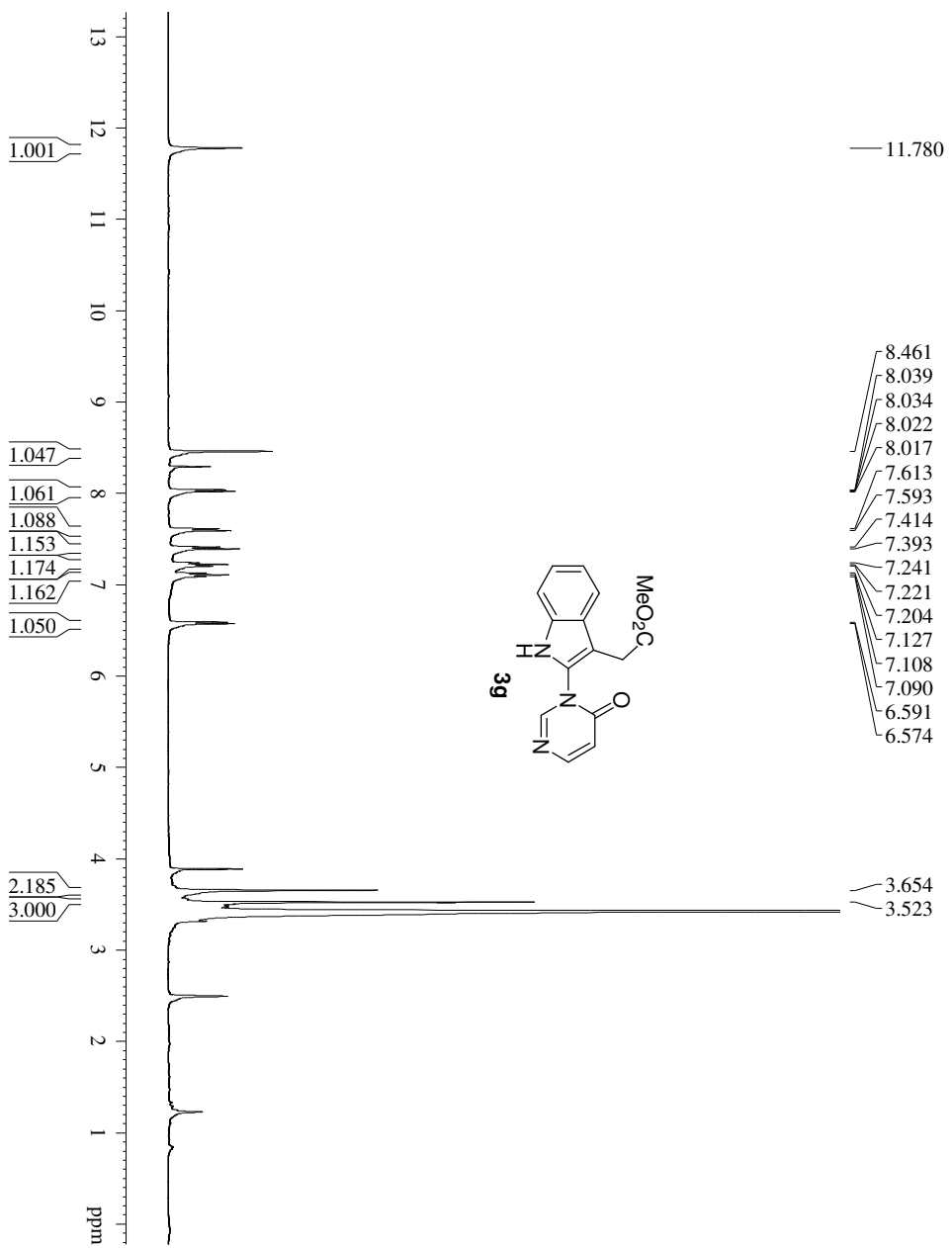
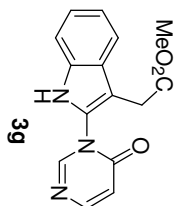
Acquisition Date 5/23/2013 1:14:06 PM

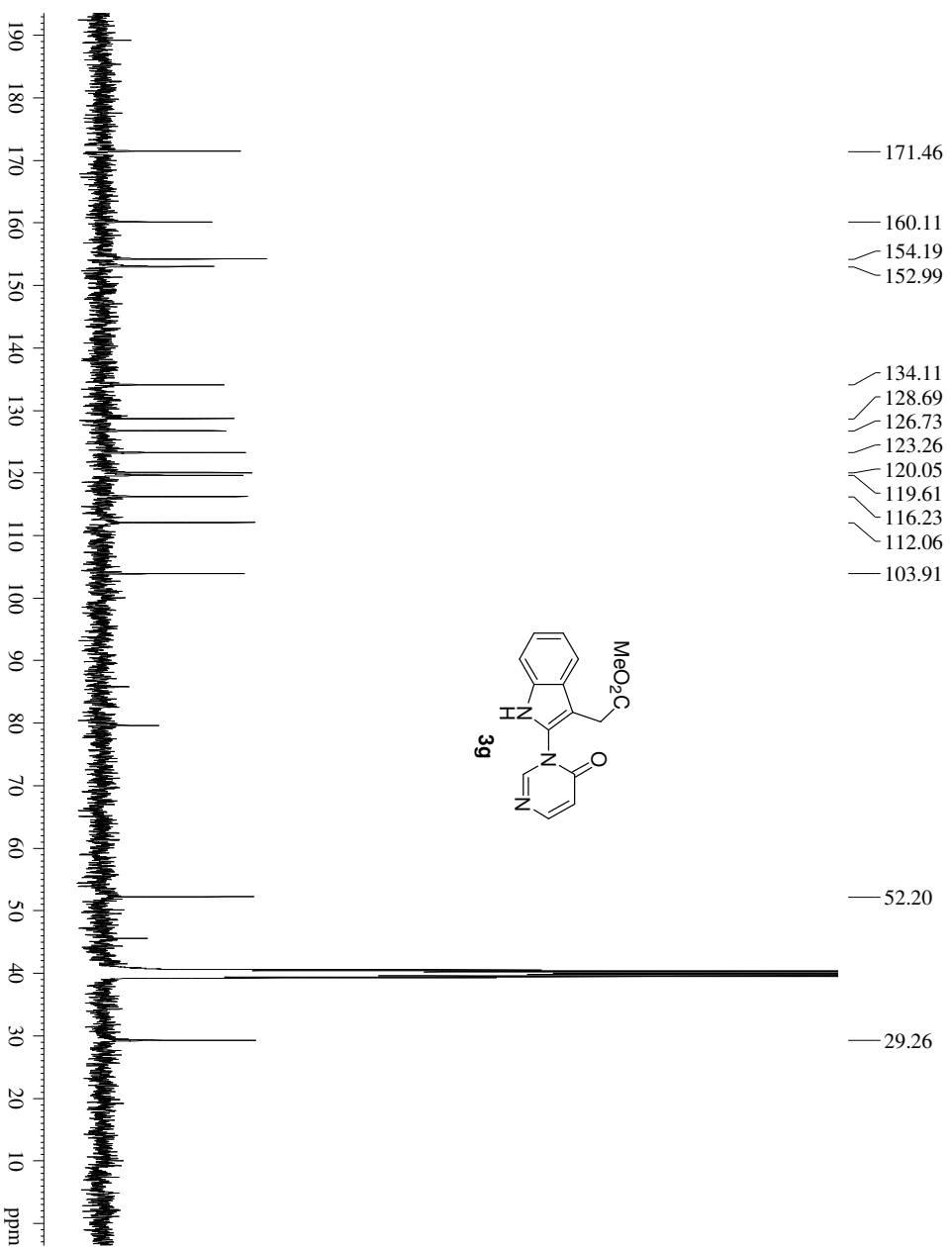
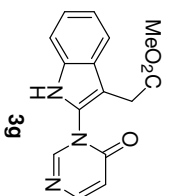
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

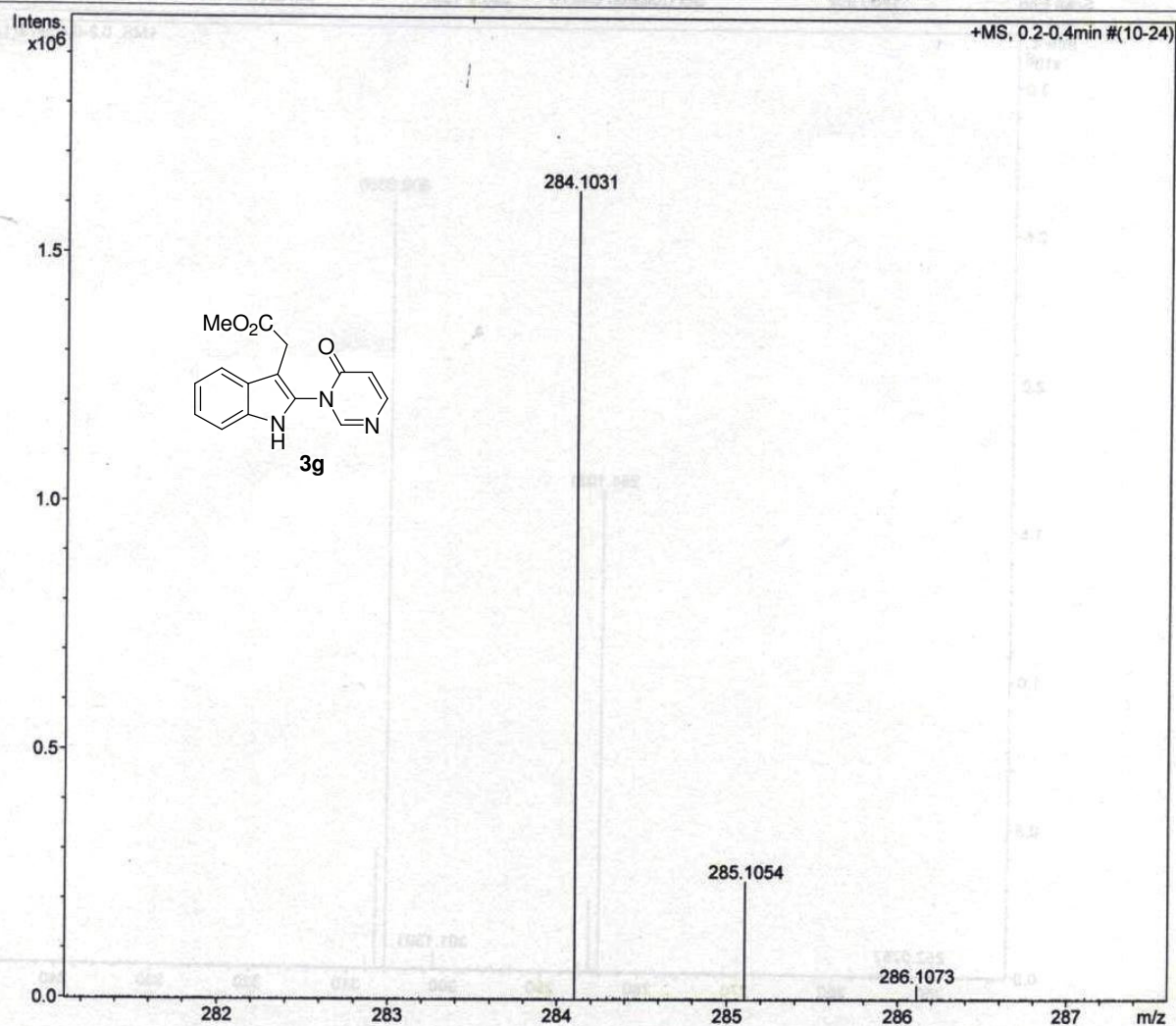
Analysis Name D:\Data\2013\Dr.NAGARAJANMAYISKG-184.d
Method tune_low.m
Sample Name SKG-184-DCM-MEOH
Comment

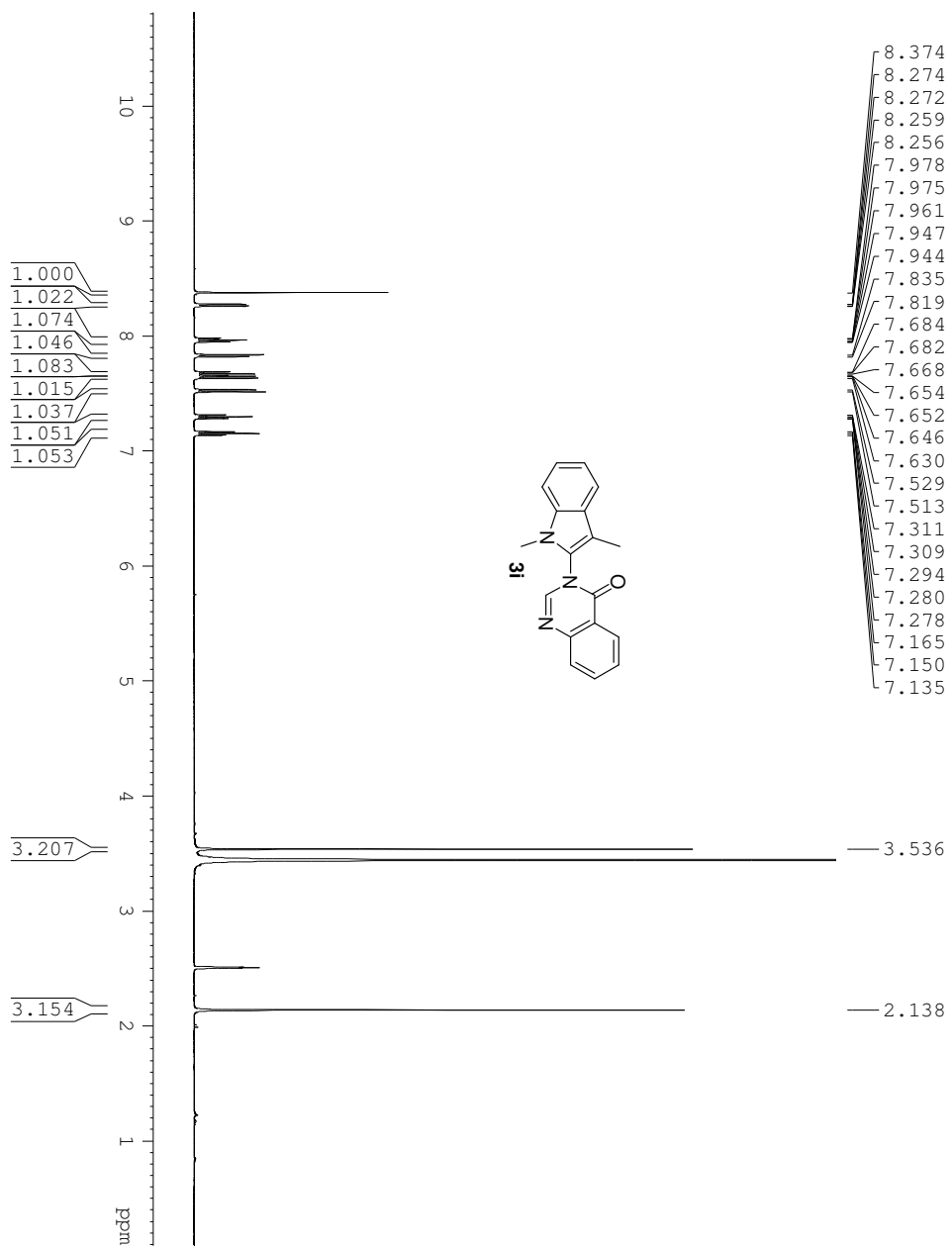
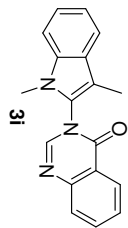
Acquisition Date 5/23/2013 12:43:19 PM

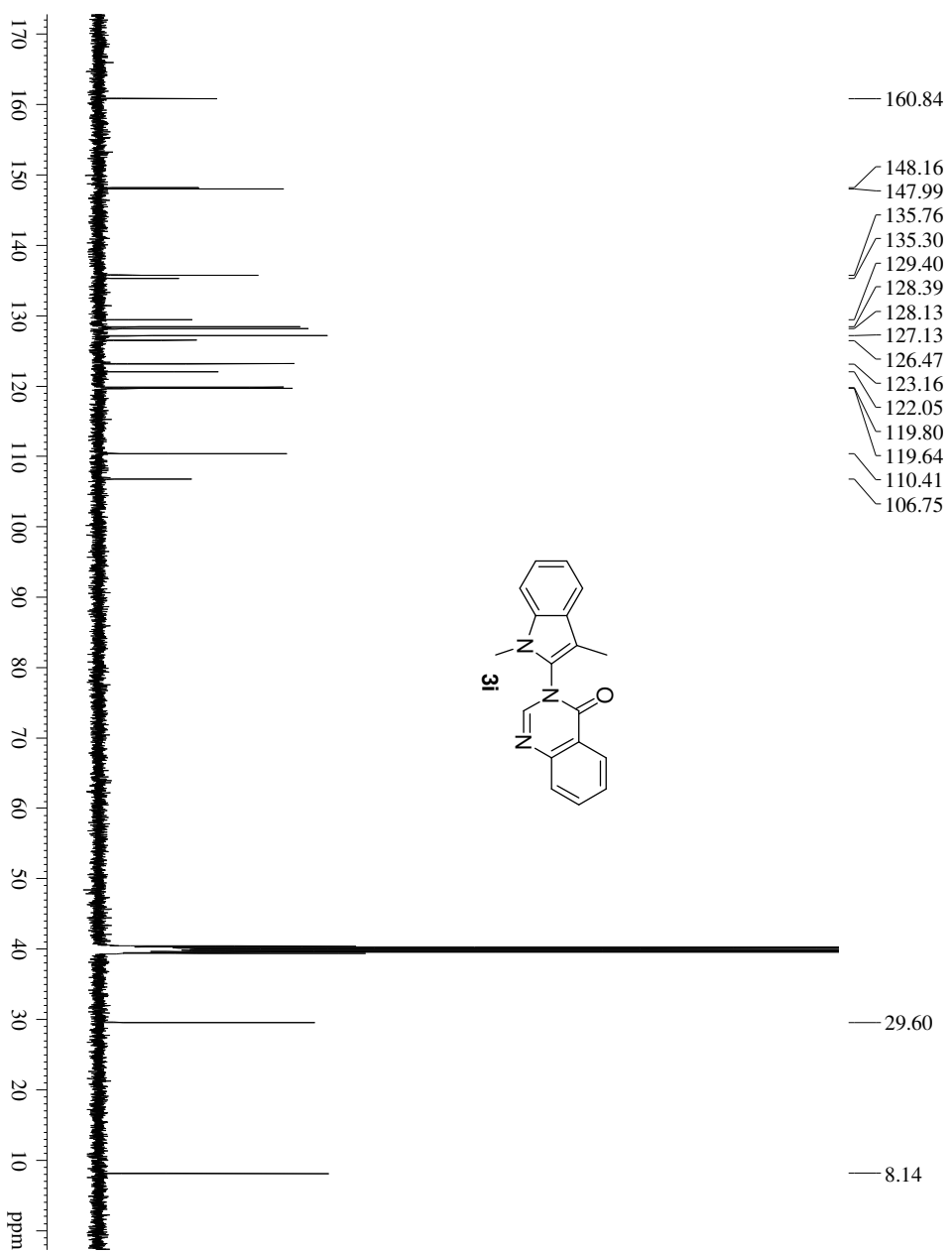
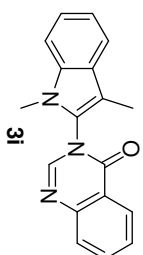
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

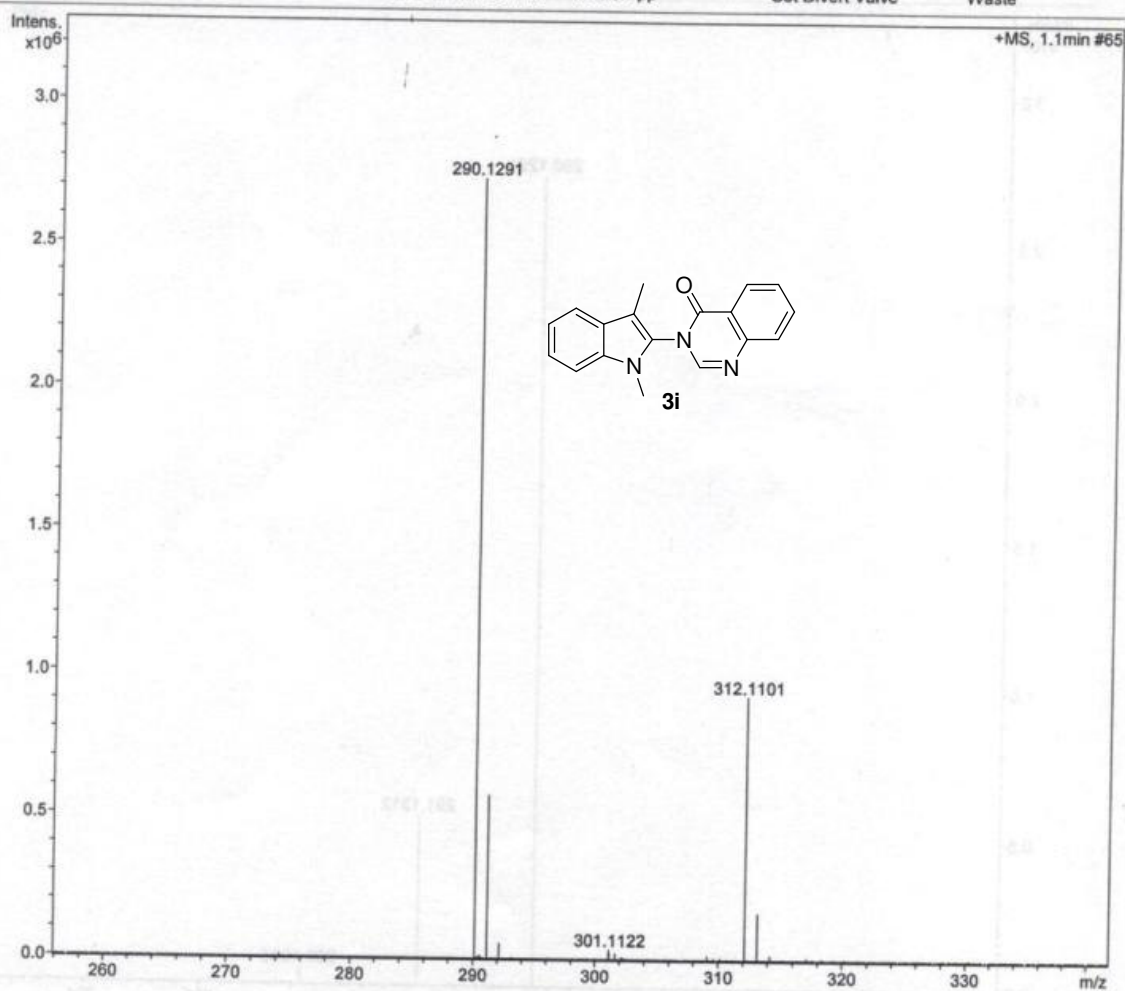
Analysis Info

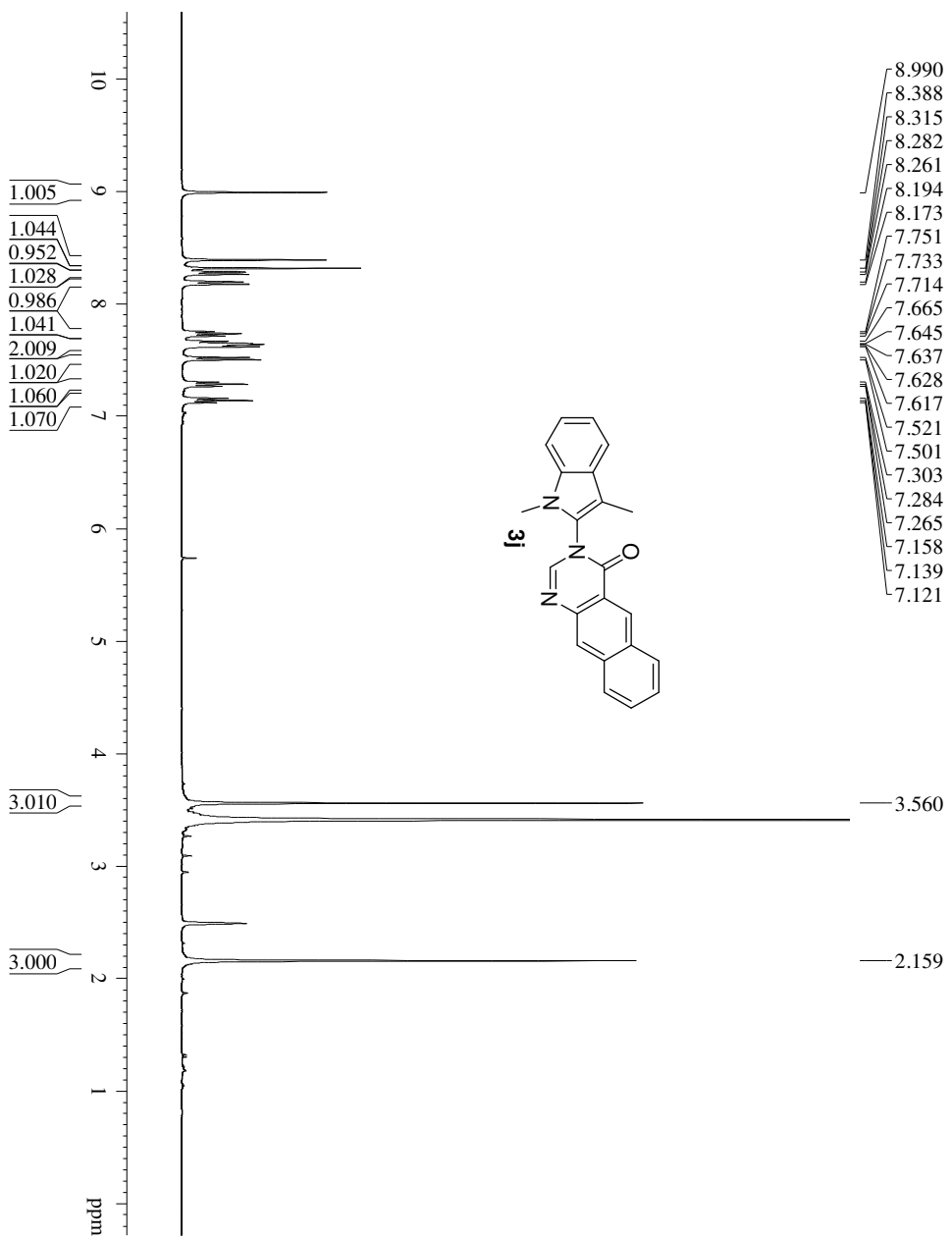
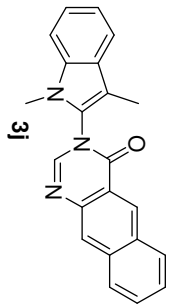
Analysis Name D:\Data\2013\Dr.NAGARAJANJUNE\SKG-92.d
Method tune_low.m
Sample Name SKG-92-DCM-MEOH
Comment

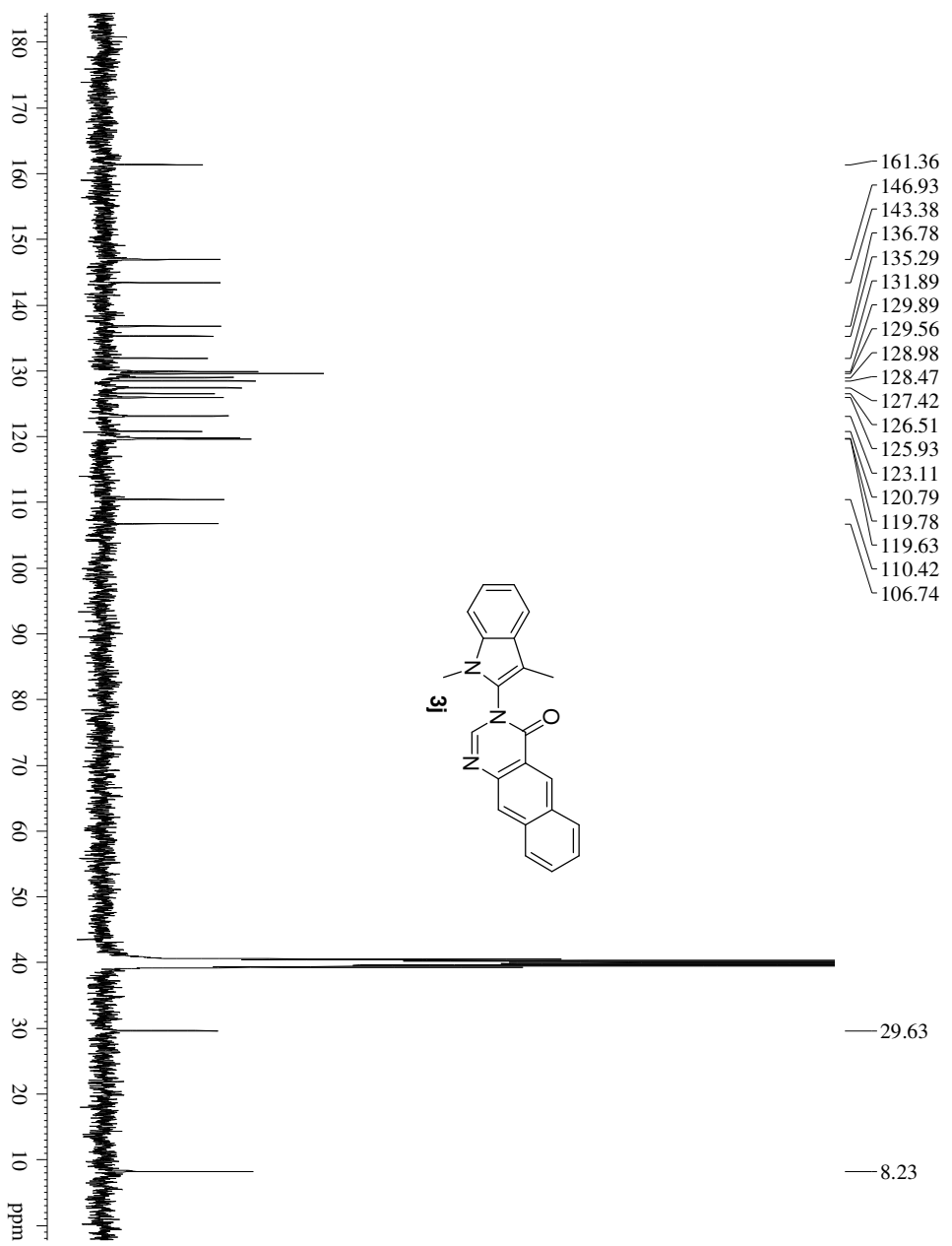
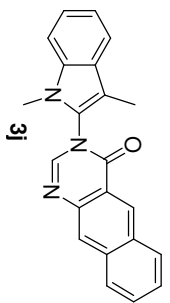
Acquisition Date 6/4/2013 11:45:32 AM
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

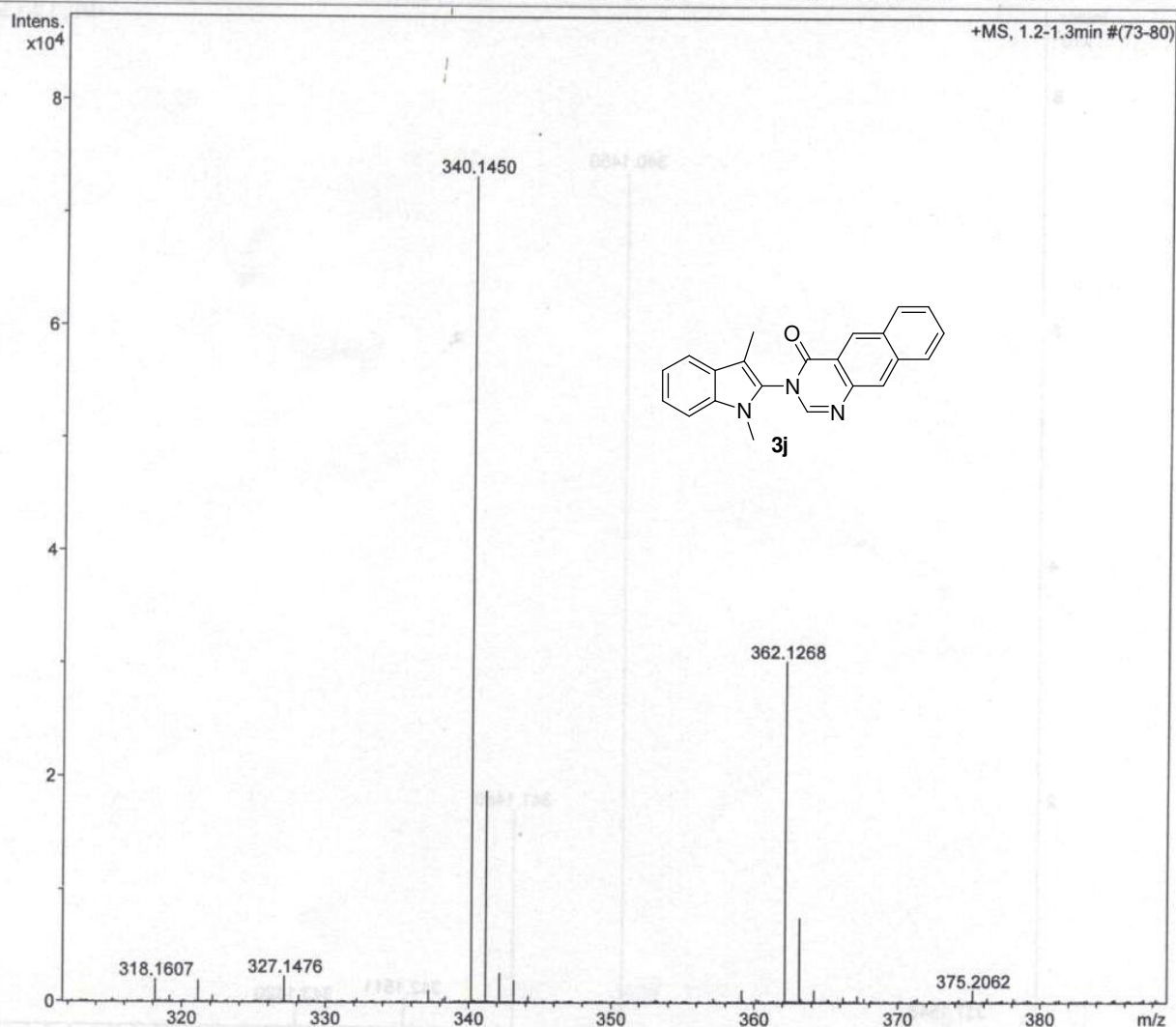
Analysis Info

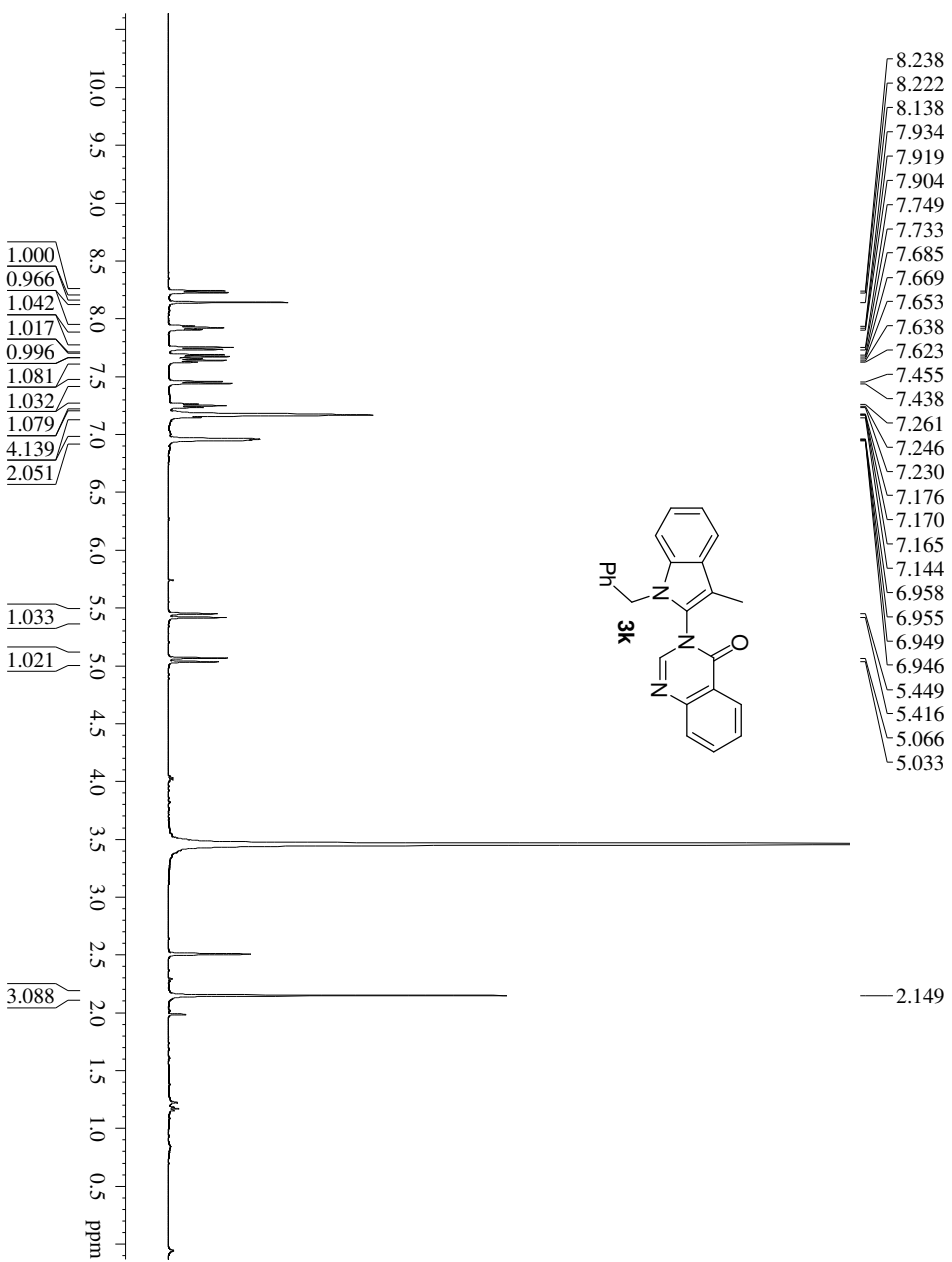
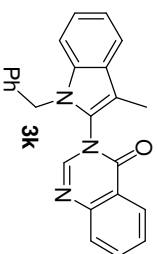
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JUNE\SKG-122.d
Method tune_low_Pos.m
Sample Name SKG-122--DCM-MEOH
Comment

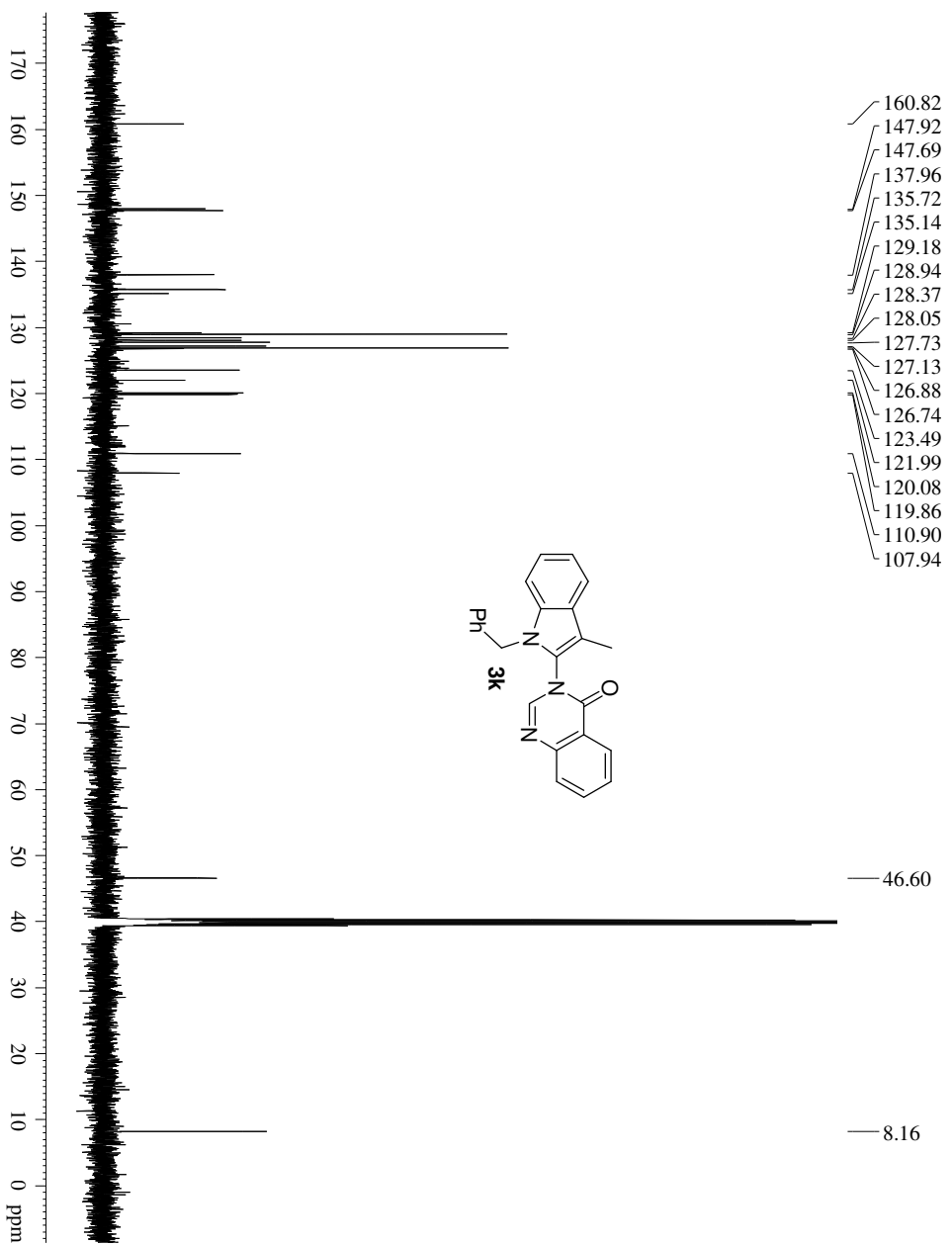
Acquisition Date 6/4/2013 12:57:09 PM
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

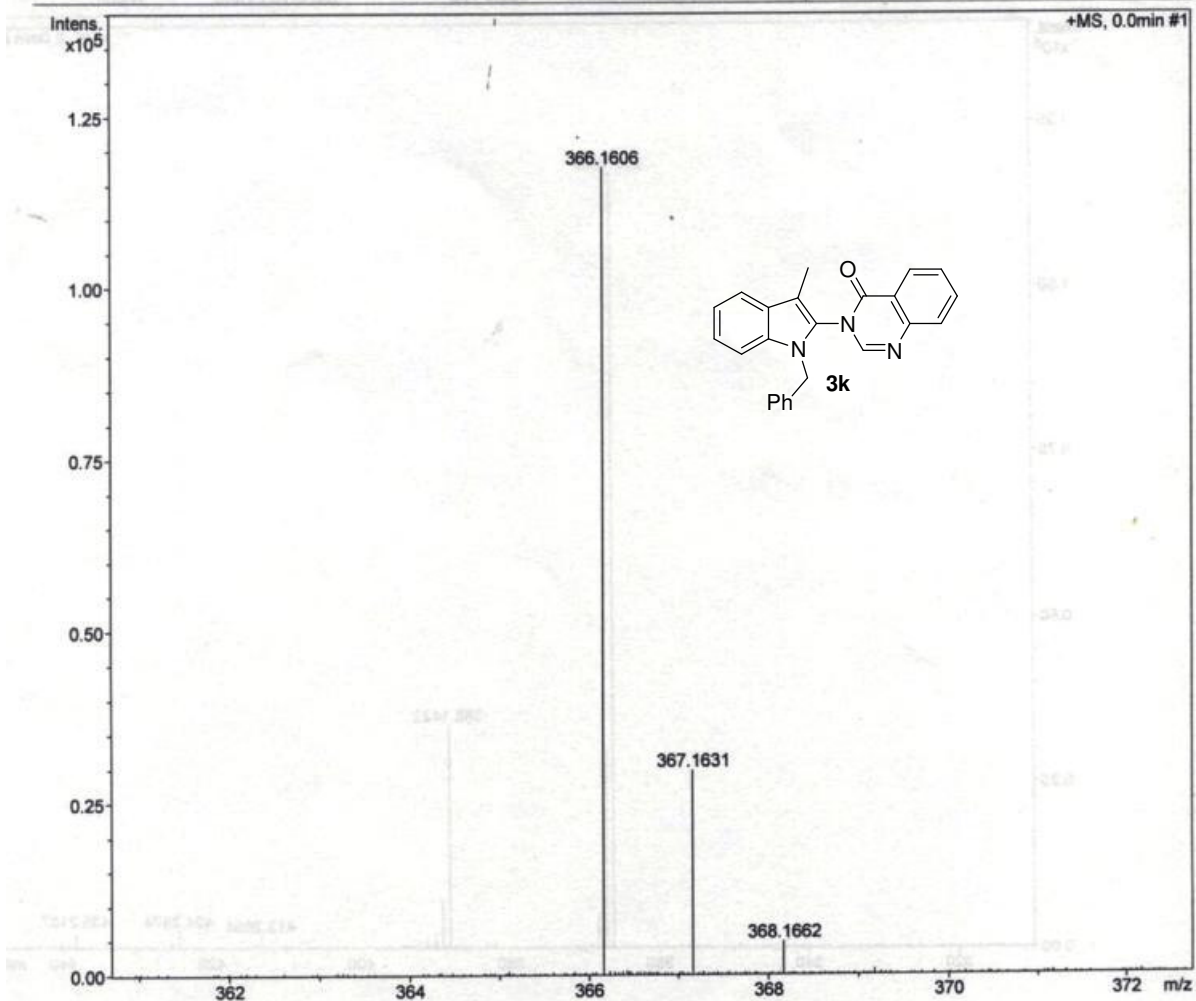
Analysis Name D:\Data\2013\Dr.NAGARAJANJUNE\SKG-101.d
Method tune_low_Pos.m
Sample Name SKG-101-DCM-MEOH
Comment

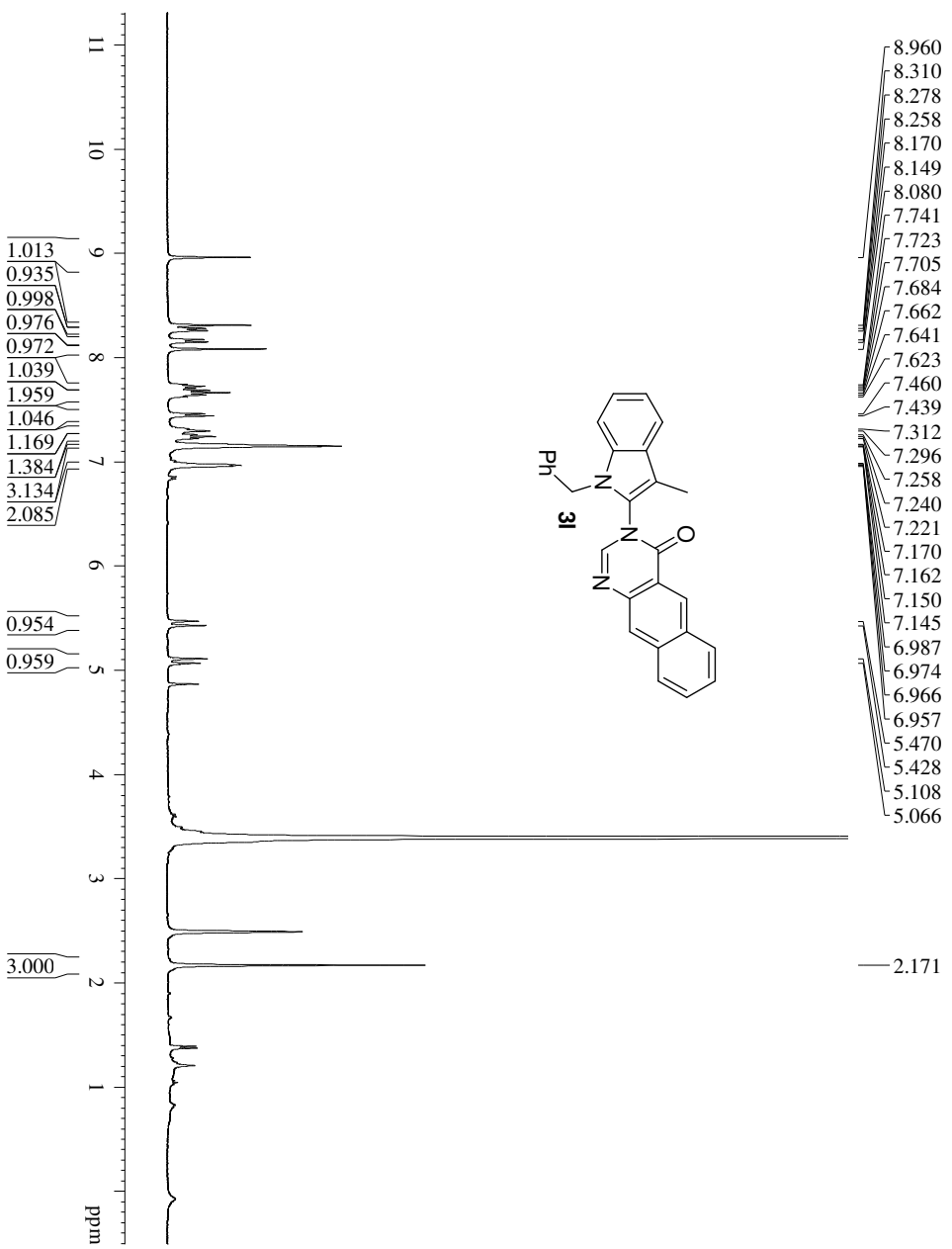
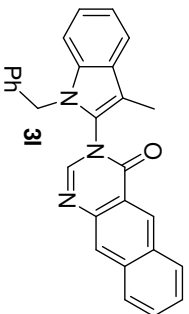
Acquisition Date 6/4/2013 12:17:18 PM

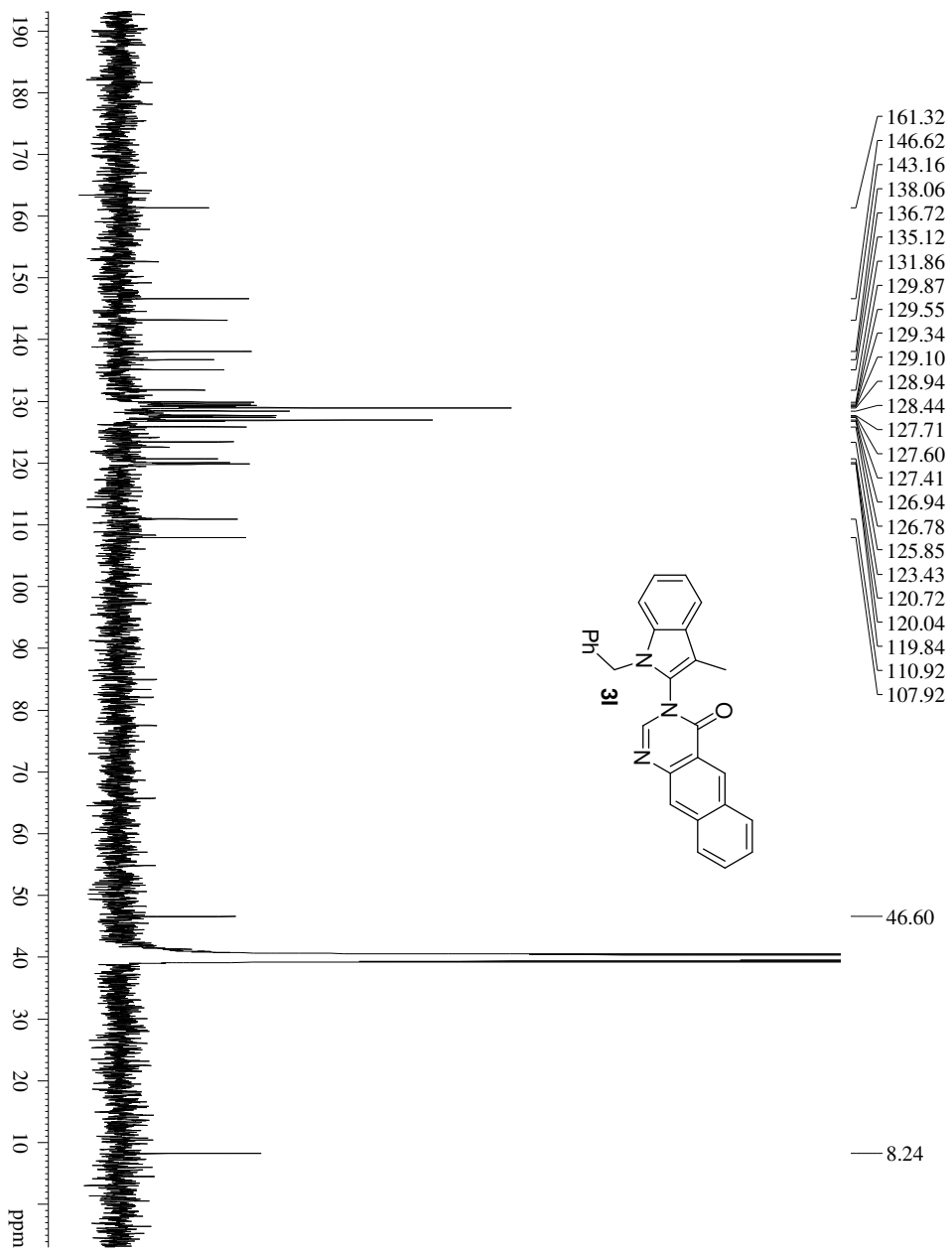
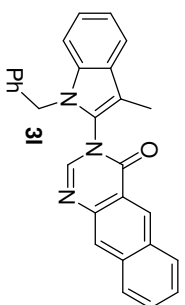
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

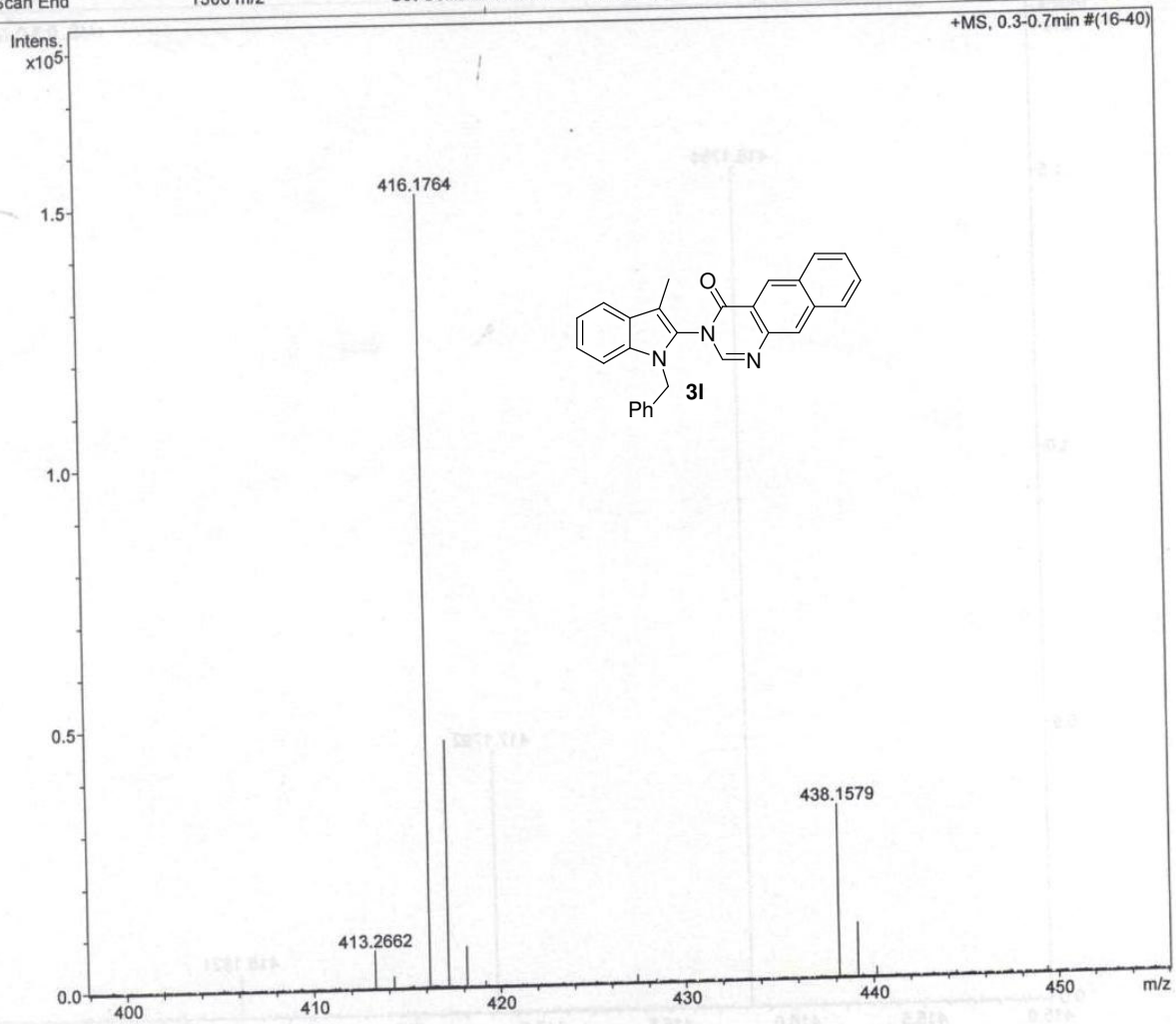
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JUNE\SKG-123.d
Method tune_low_Pos.m
Sample Name SKG-123--DCM-MEOH
Comment

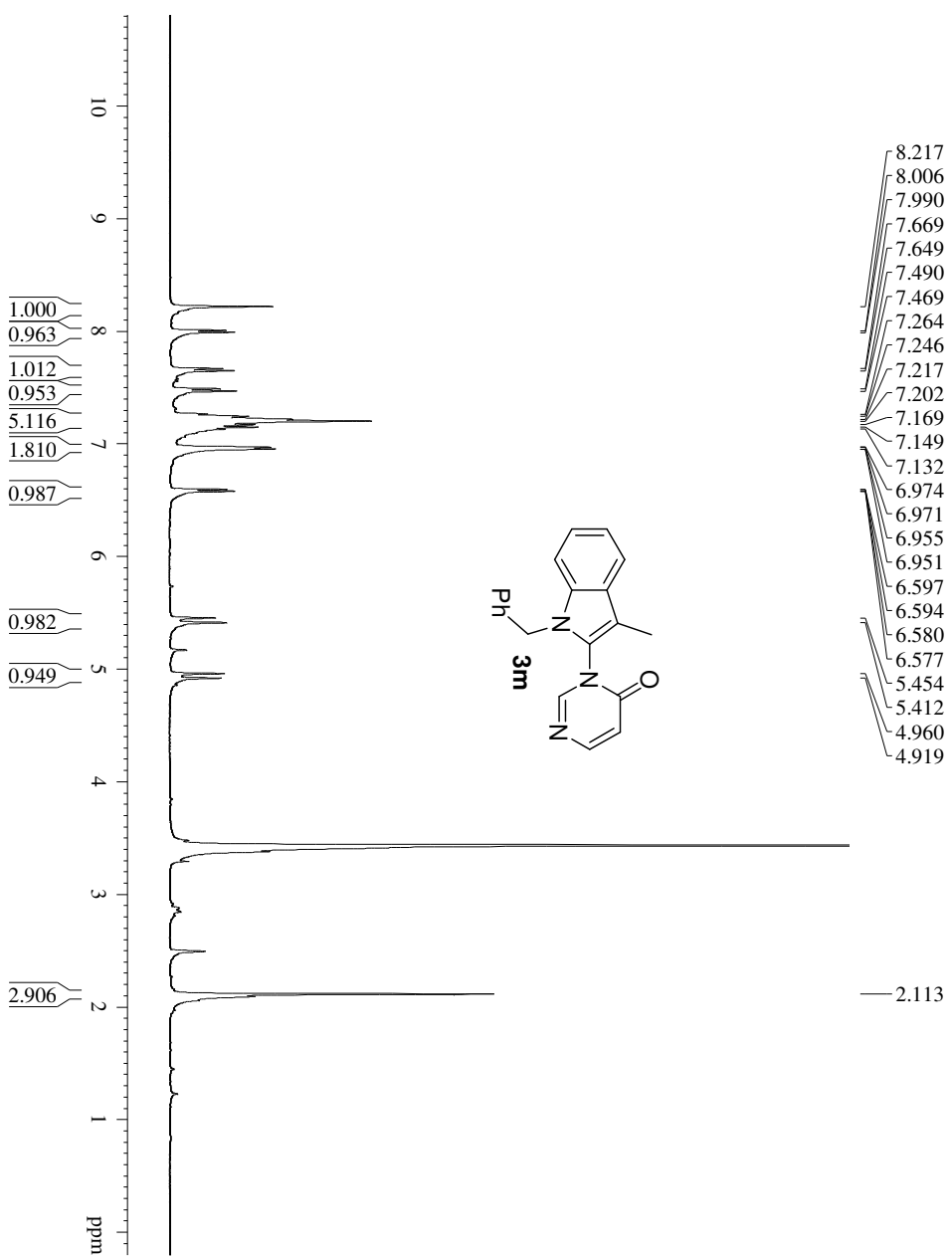
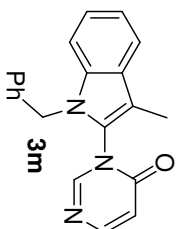
Acquisition Date 6/4/2013 12:33:41 PM

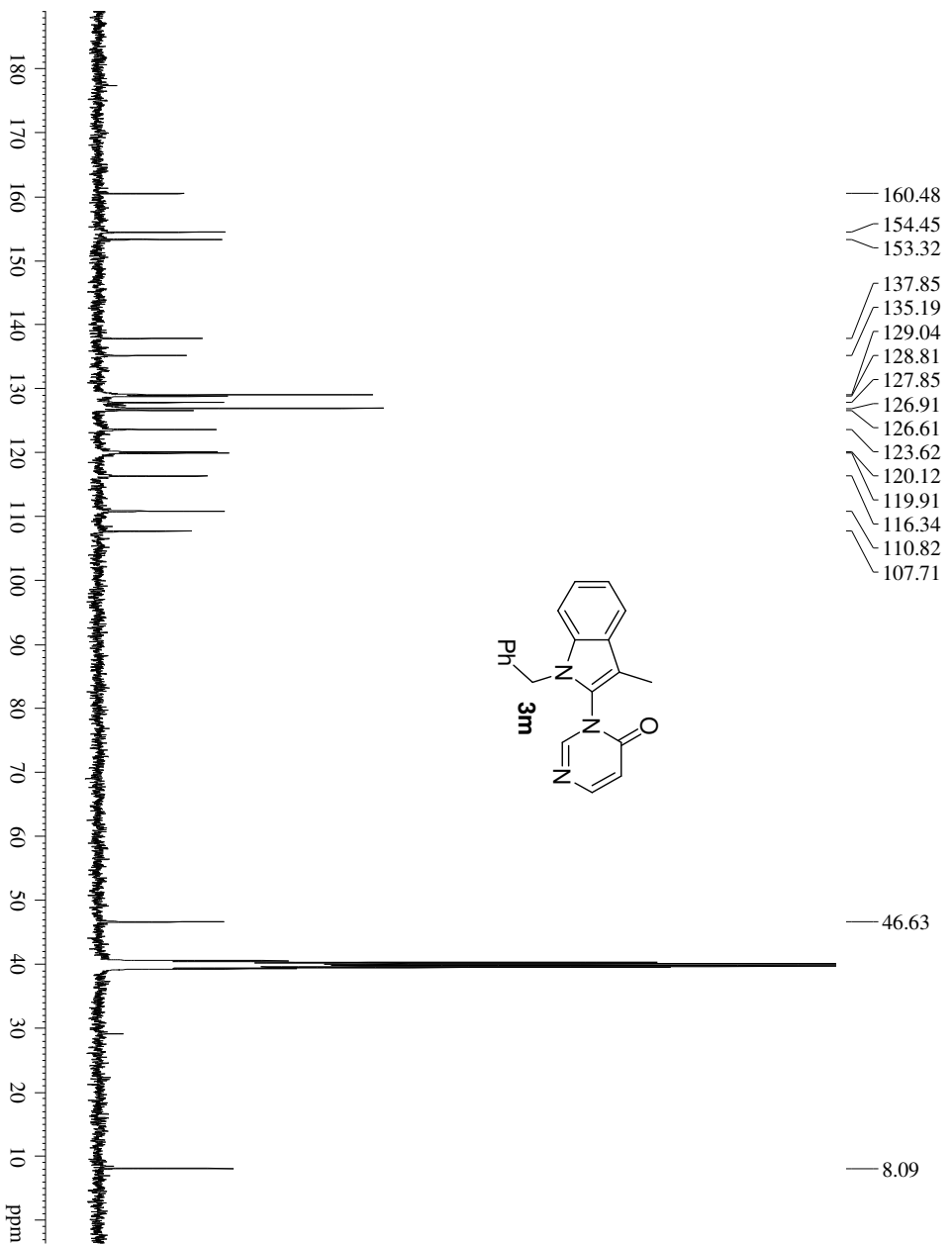
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

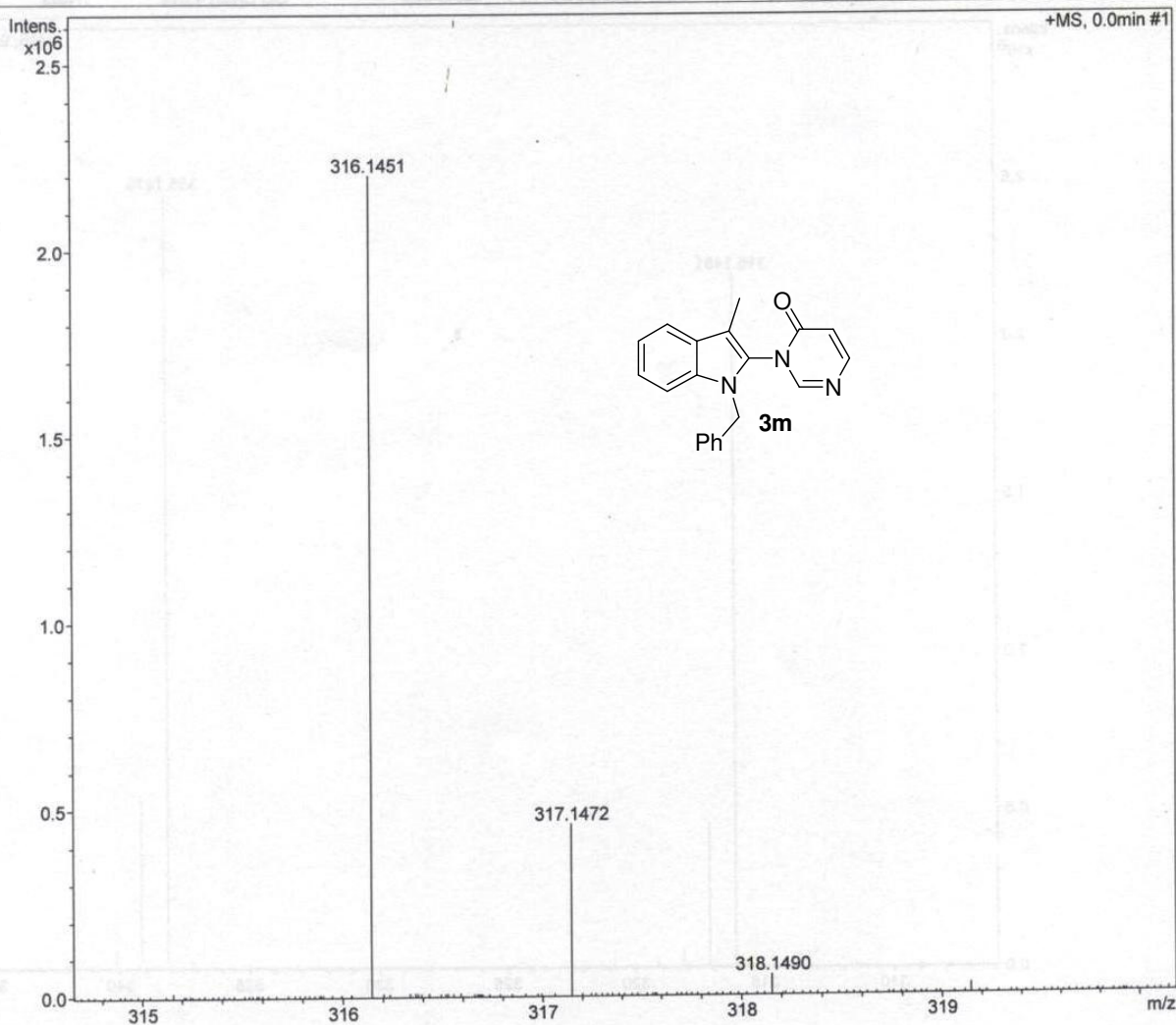
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-183.d
Method tune_low.m
Sample Name SKG-183-DCM-MEOH
Comment

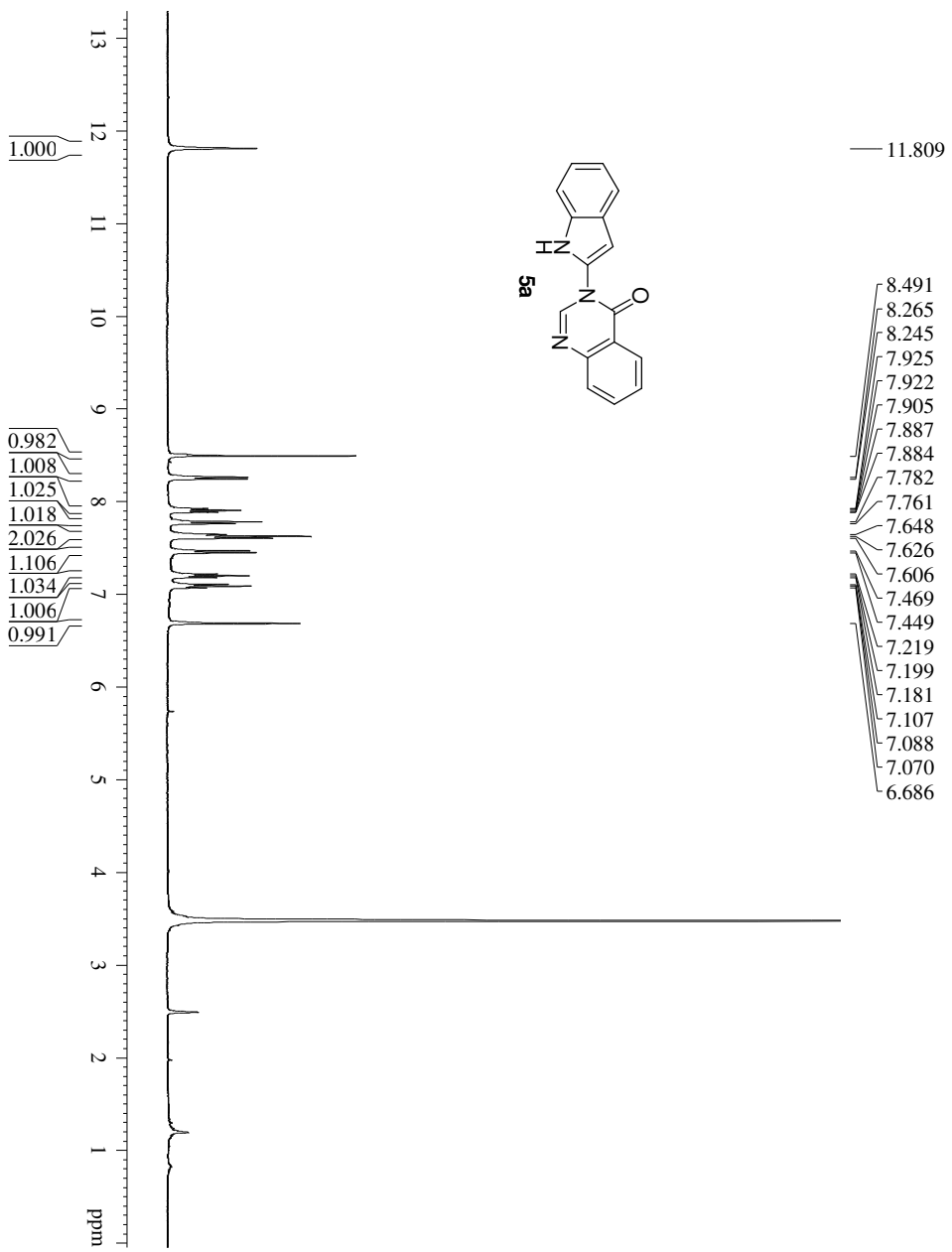
Acquisition Date 5/23/2013 12:52:31 PM

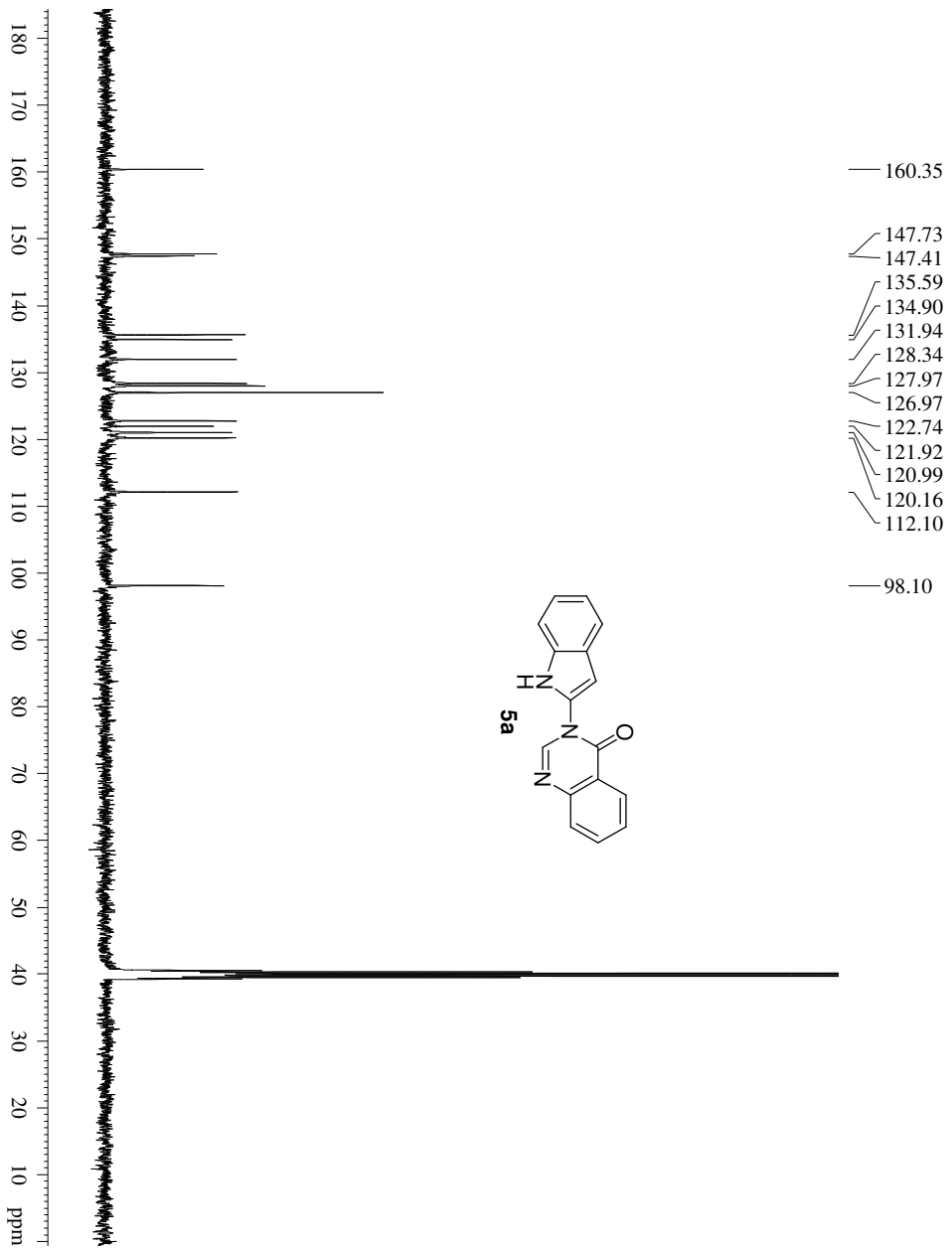
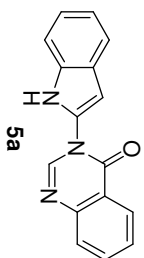
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

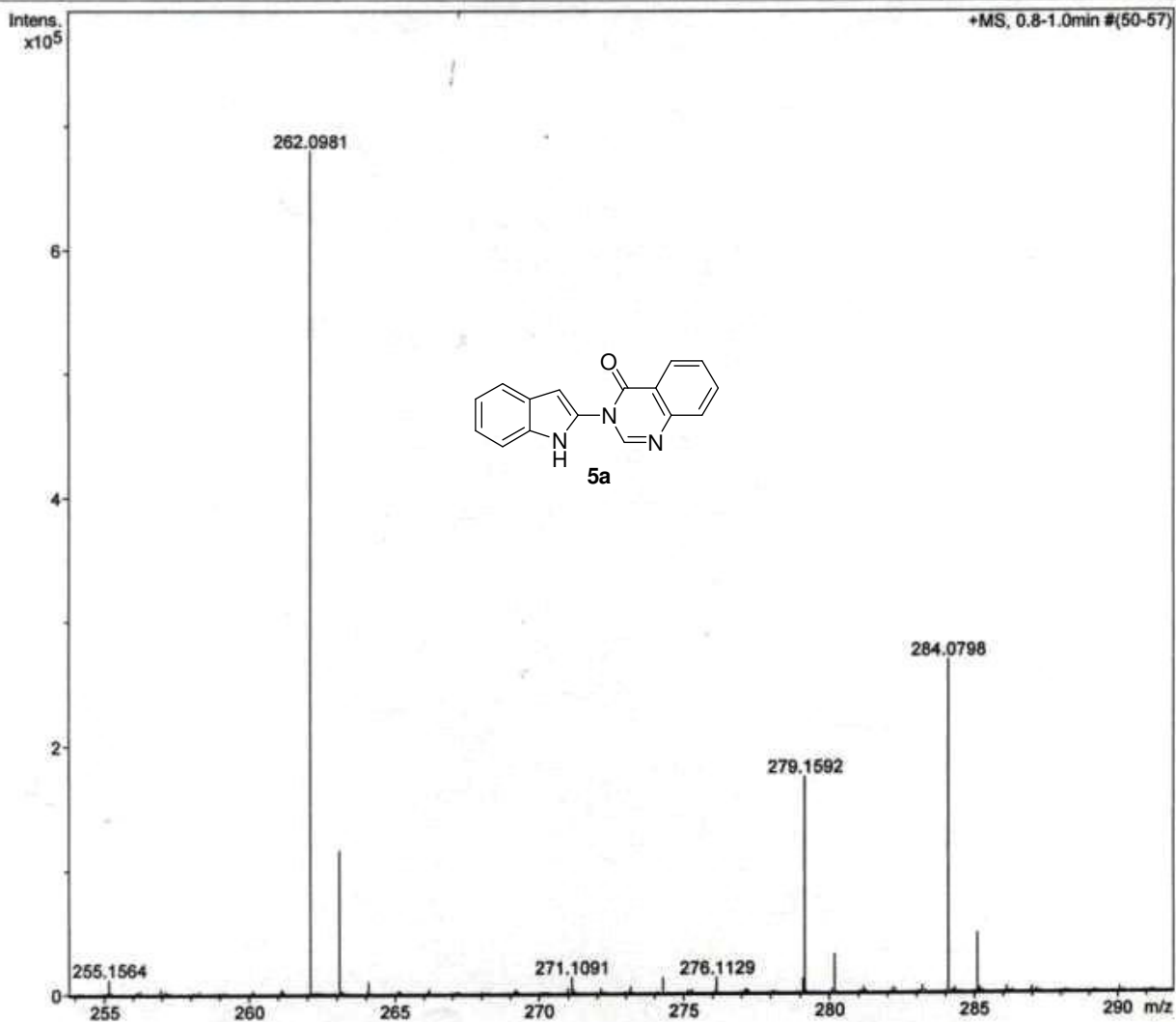
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-191.d
Method tune_low_Pos.m
Sample Name SKG-191-DCM-MEOH
Comment

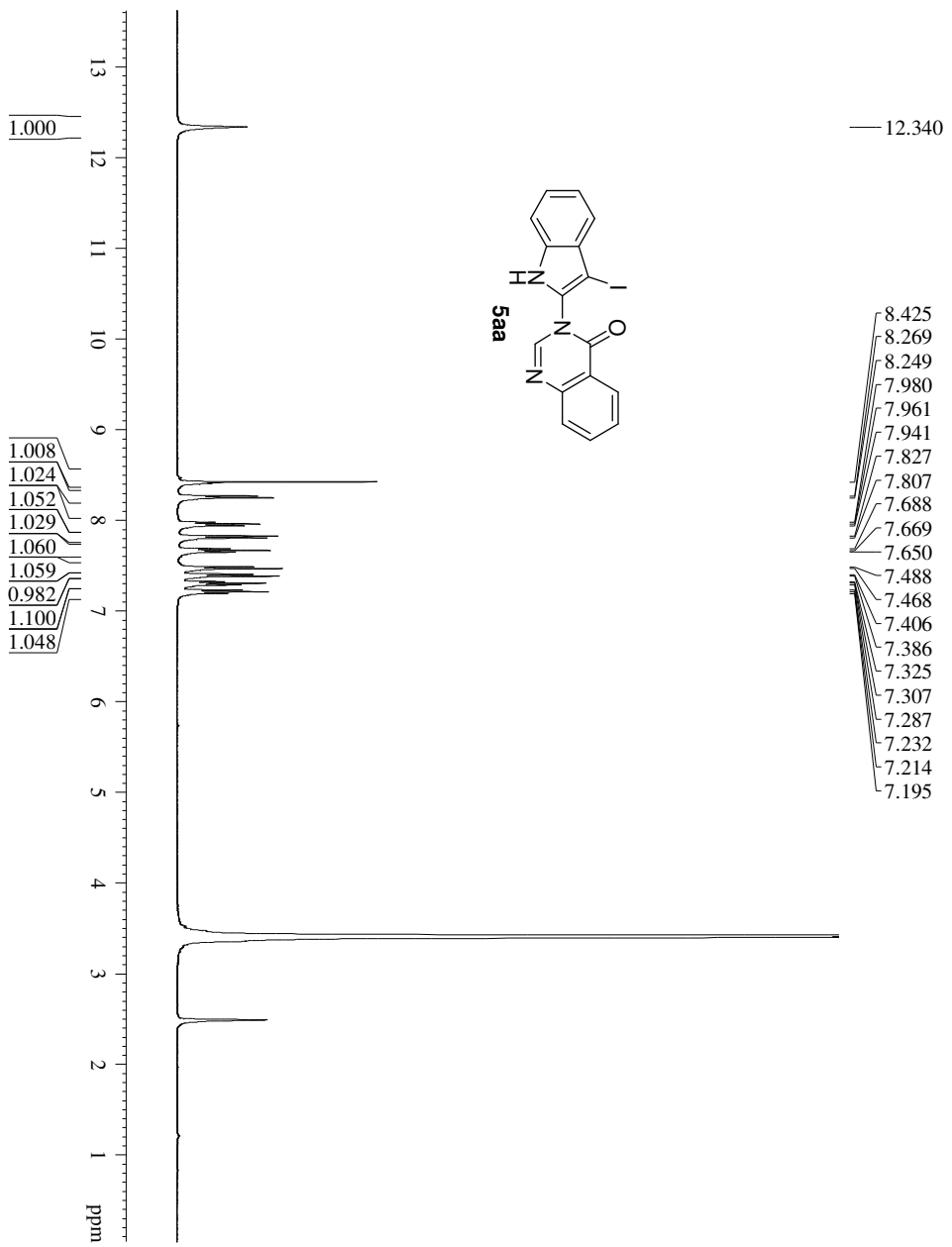
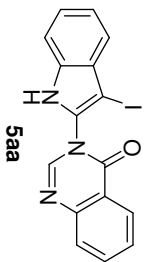
Acquisition Date 5/27/2013 5:00:43 PM

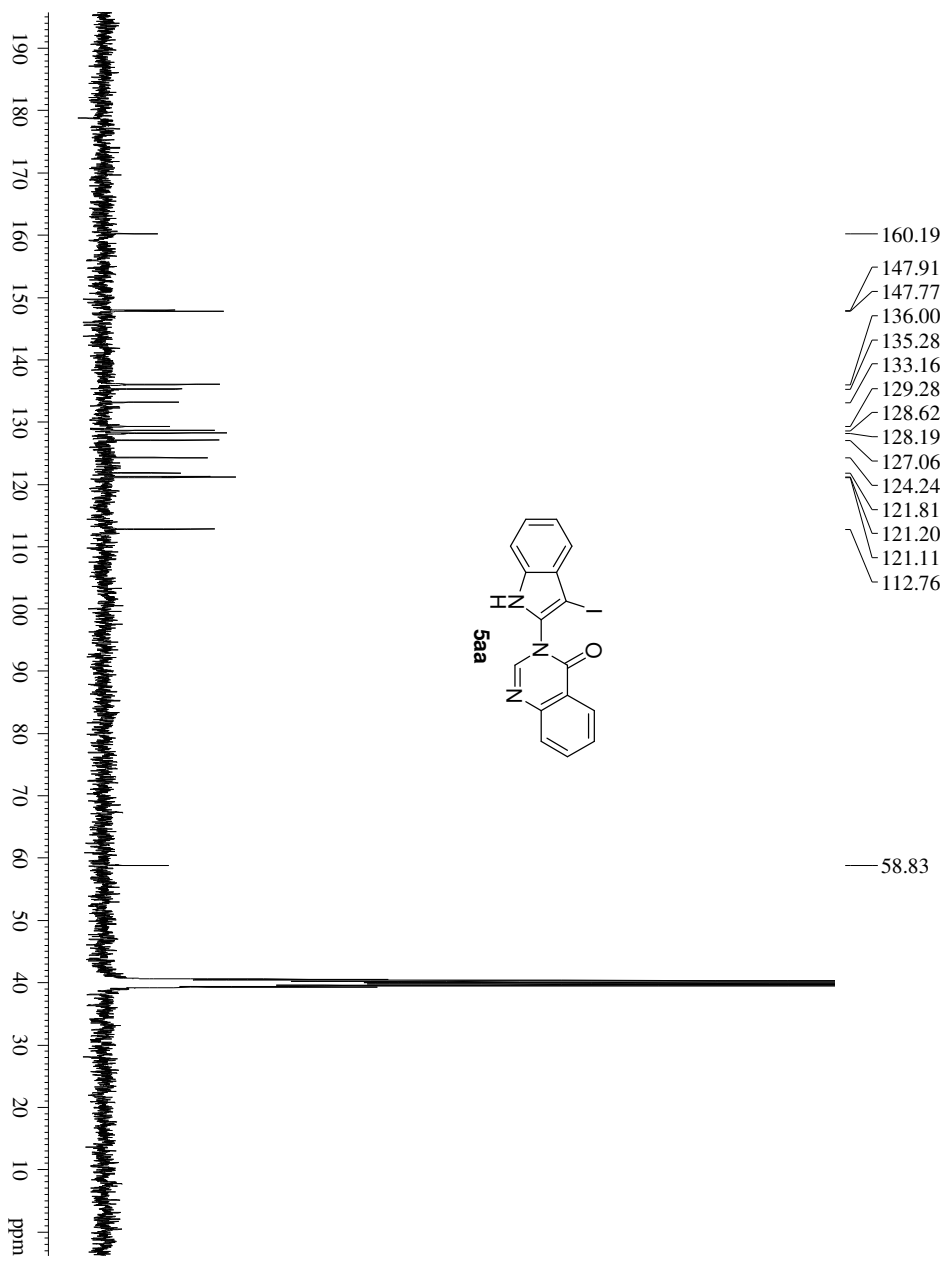
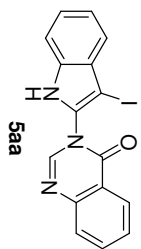
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4400 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

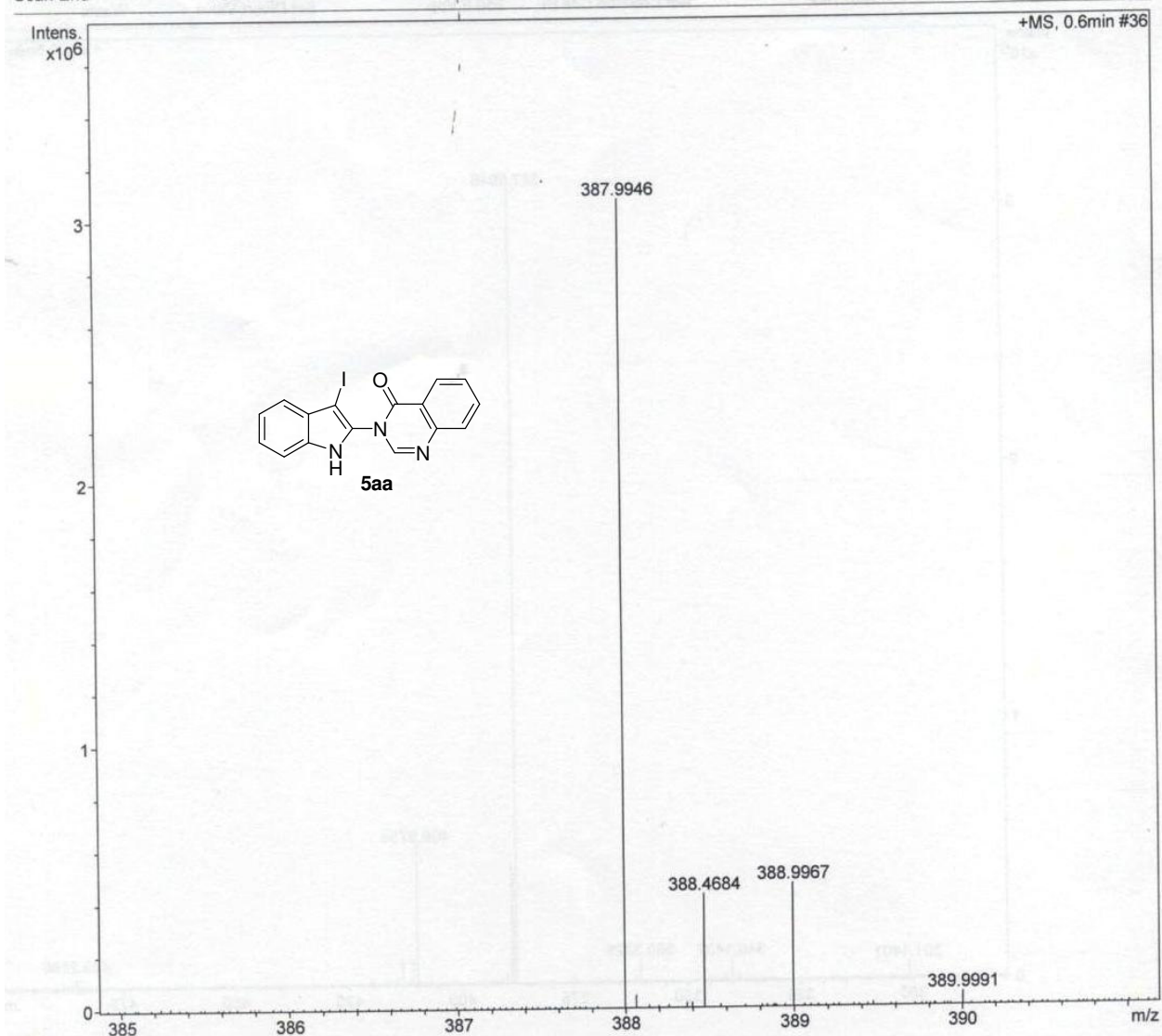
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-127..d
Method tune_low_Pos.m
Sample Name SKG-127--DCM-MEOH
Comment

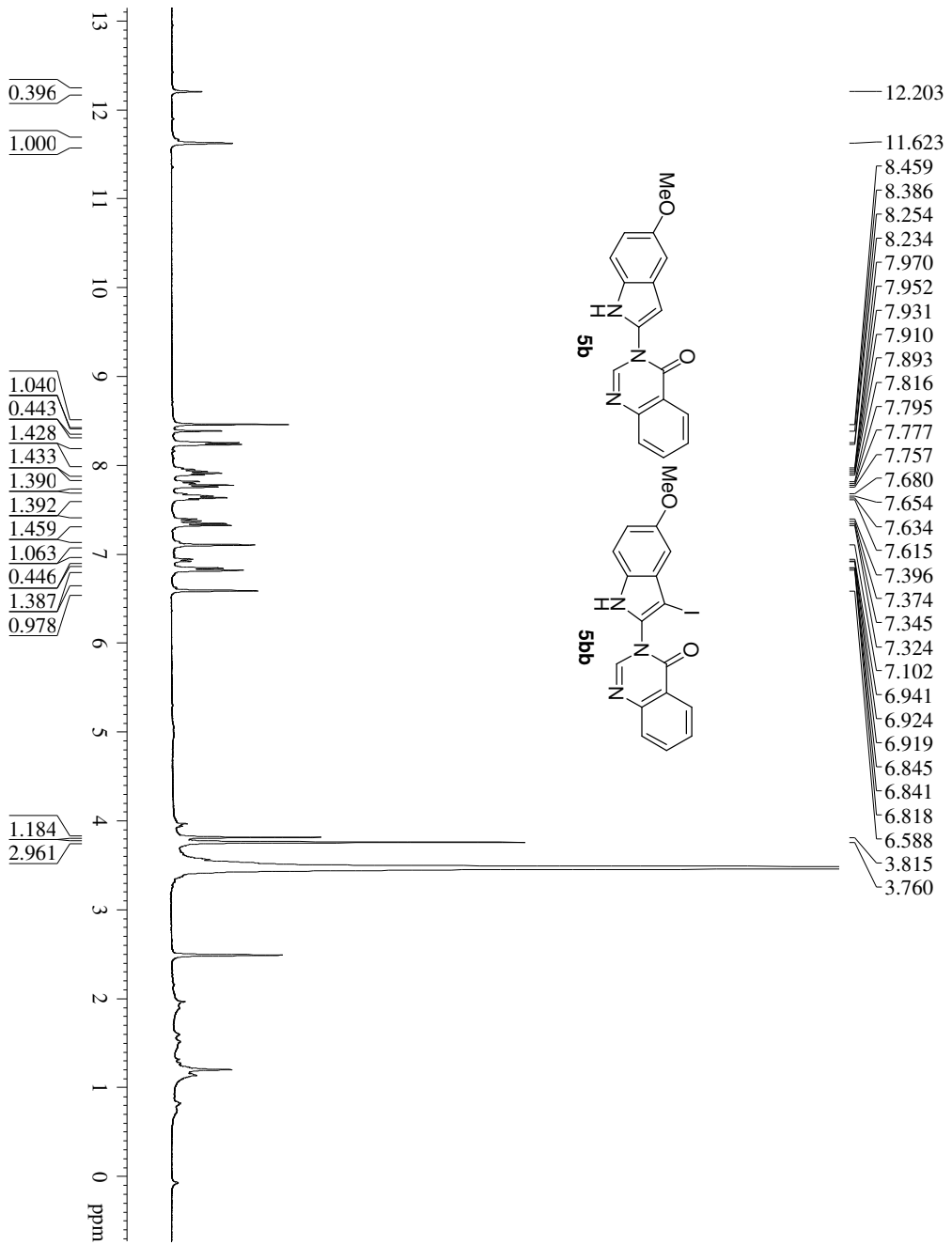
Acquisition Date 7/29/2013 11:21:49 AM

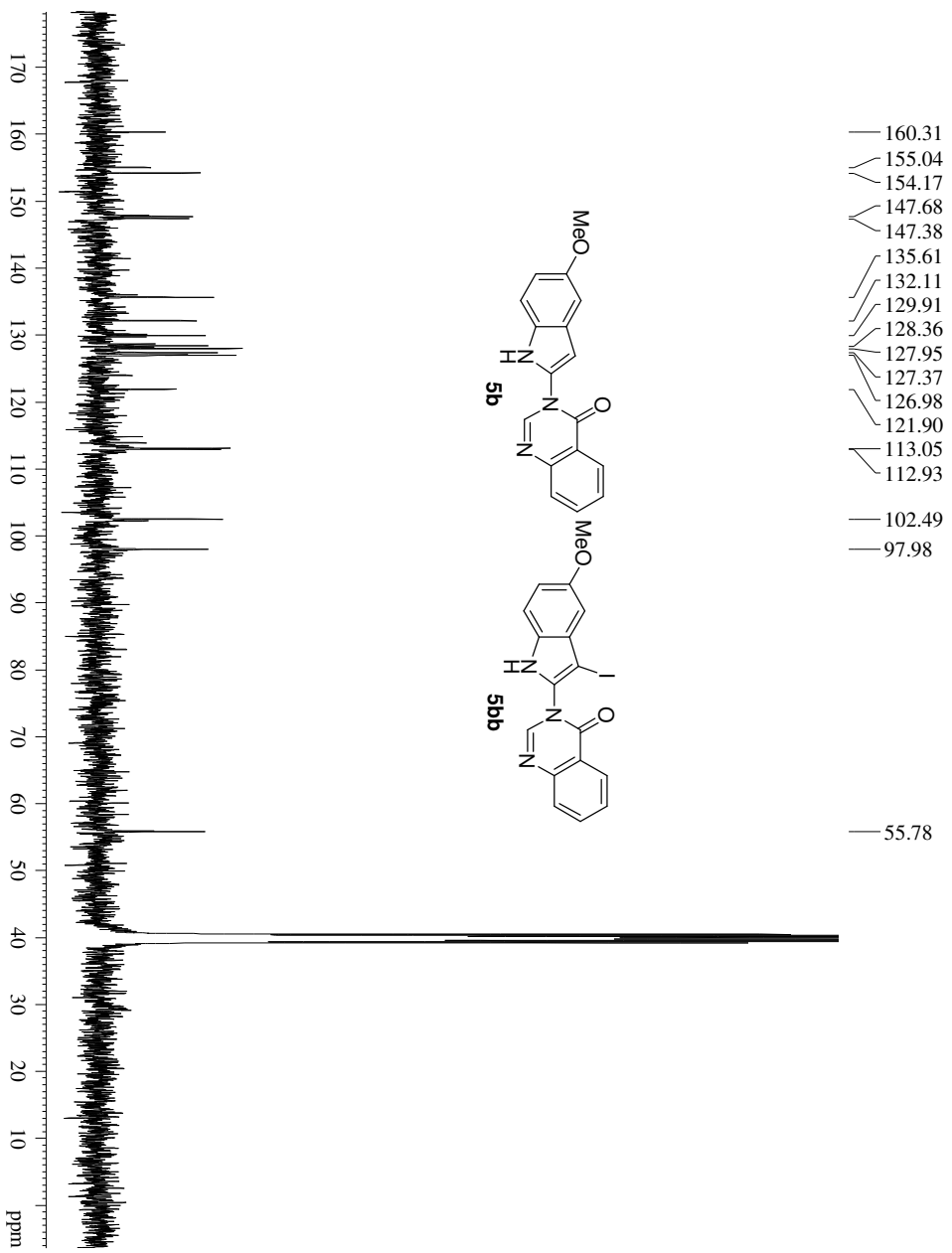
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

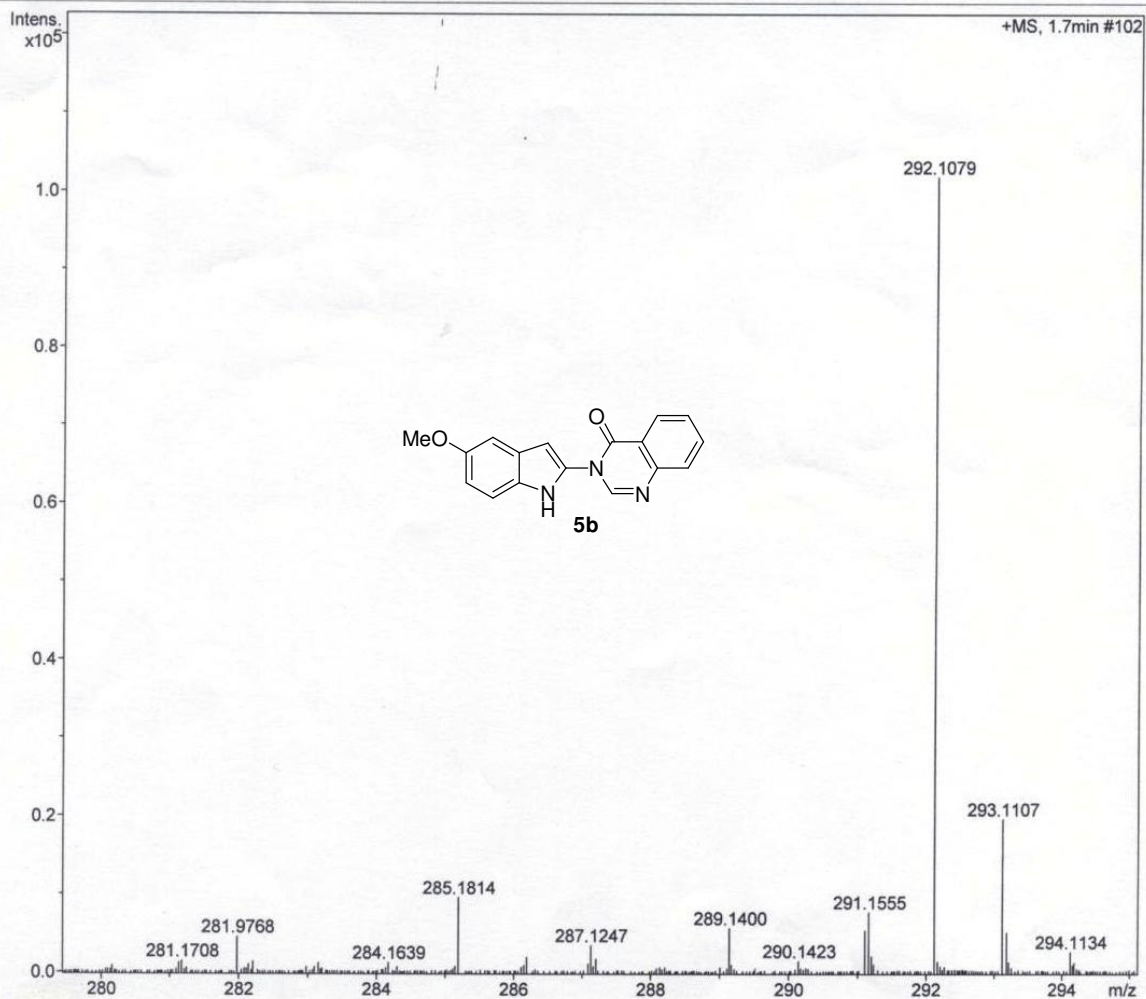
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-133.d
Method tune_low.m
Sample Name SKG-133-DCM-MEOH
Comment

Acquisition Date 5/28/2013 3:55:37 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	3500 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



BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

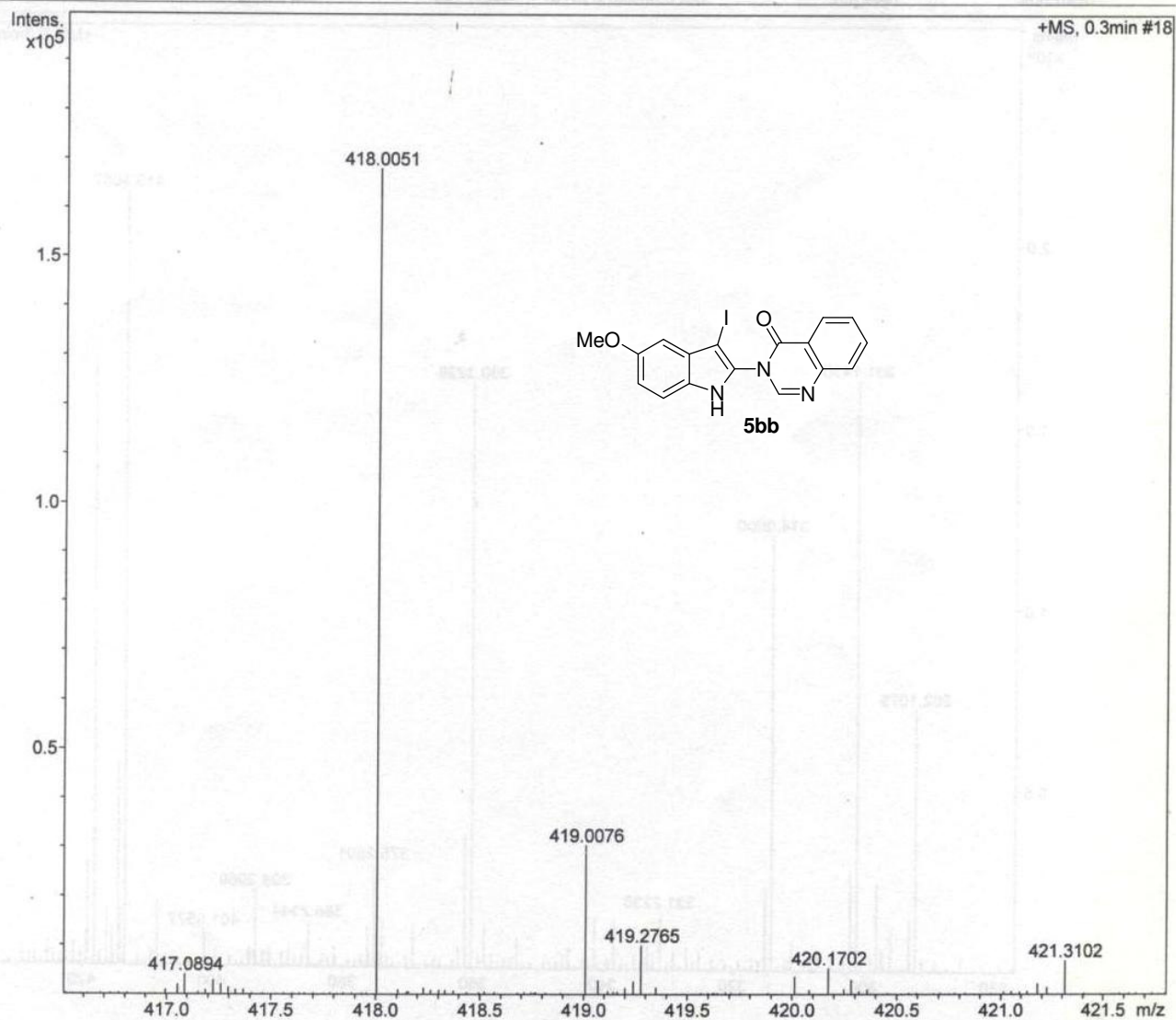
Analysis Name D:\Data\2013\Dr.NAGARAJANMAYSKG-133.d
Method tune_low.m
Sample Name SKG-133-DCM-MEOH
Comment

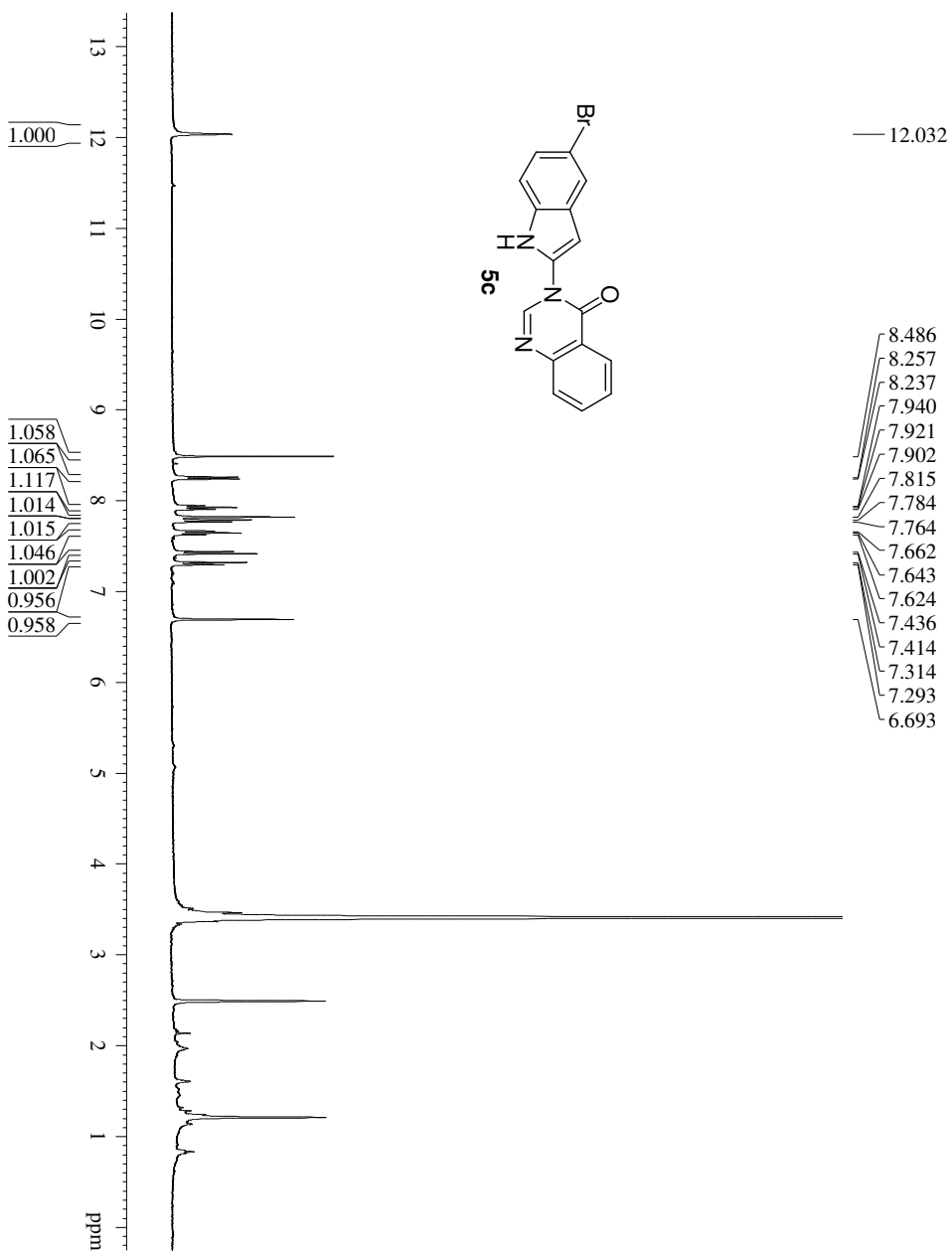
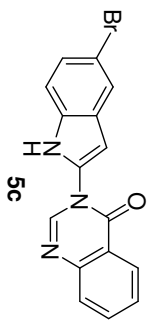
Acquisition Date 5/28/2013 3:55:37 PM

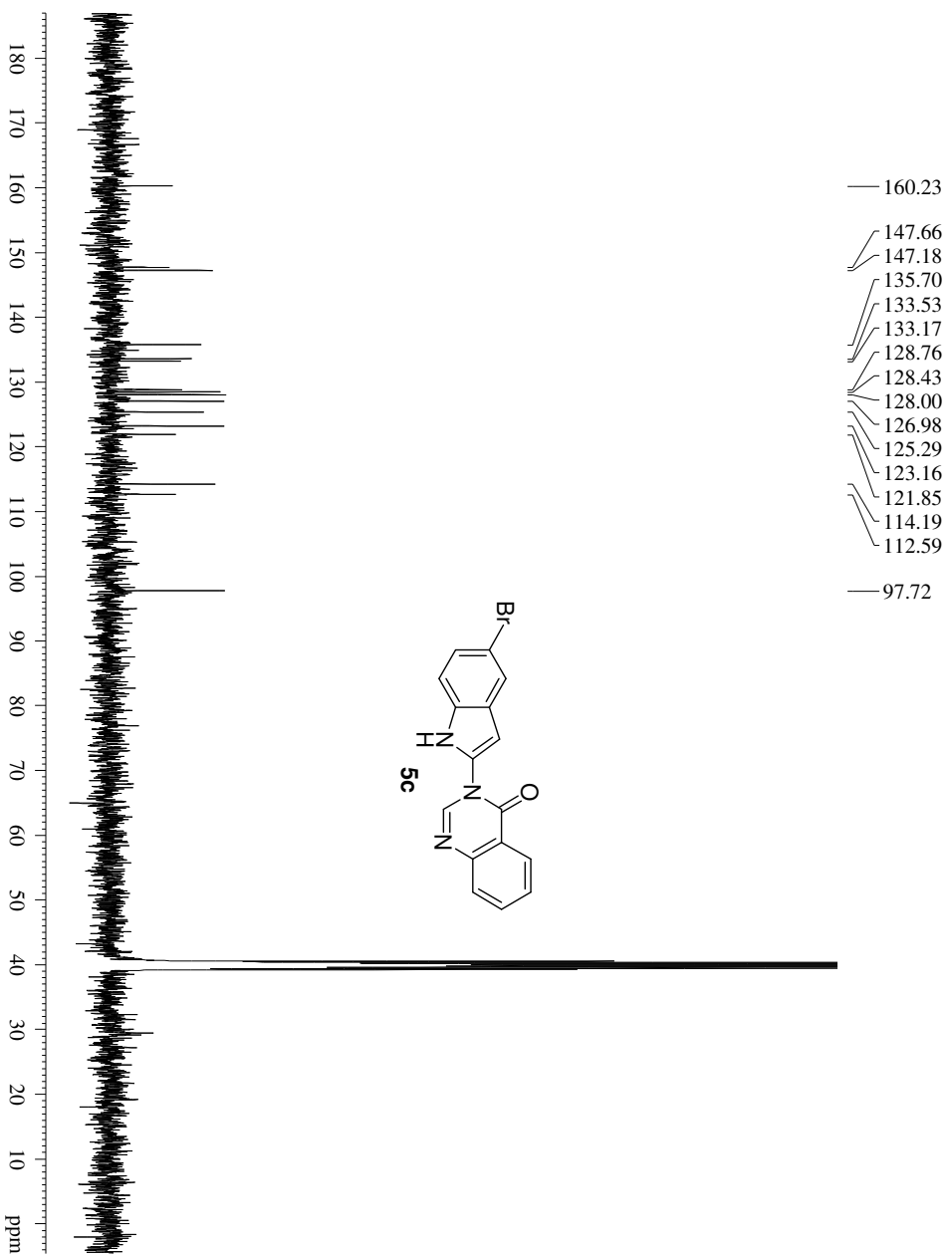
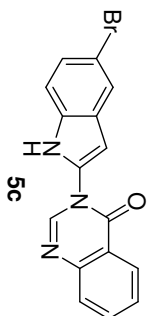
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

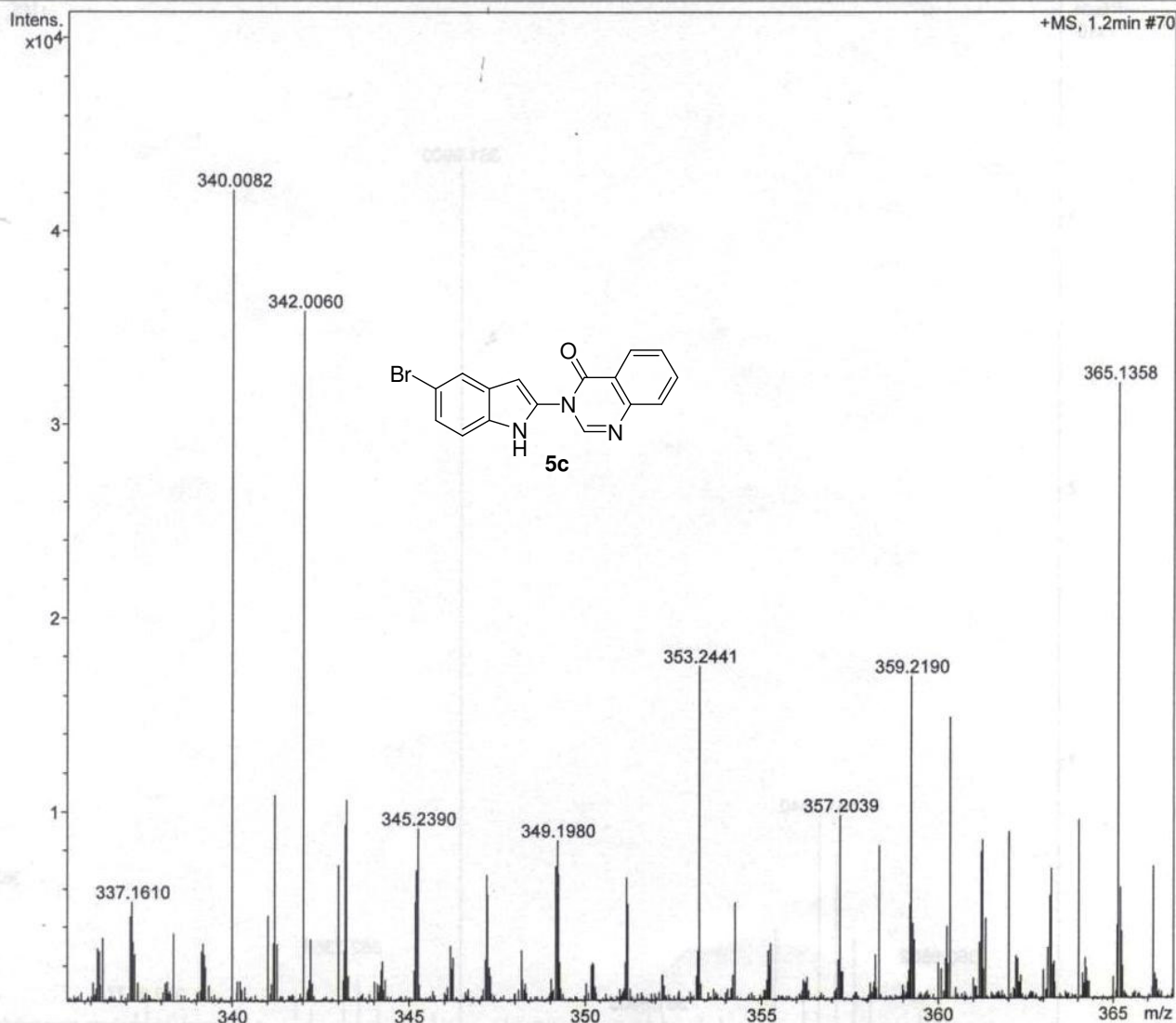
Analysis Name D:\Data\2013\Dr.NAGARAJAN\MAY\SKG-132-I.d
Method tune_low.m
Sample Name SKG-132-I-DCM-MEOH
Comment

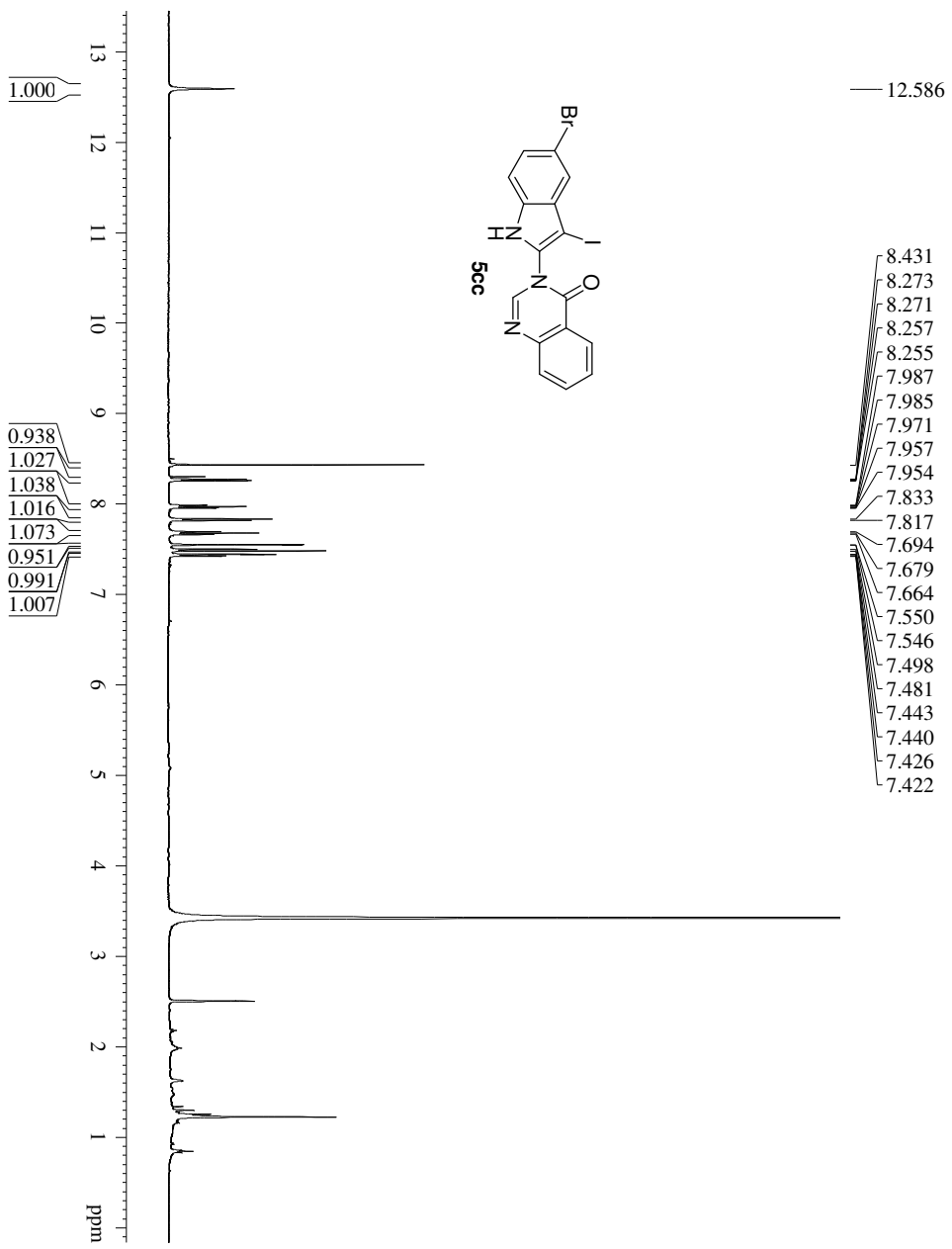
Acquisition Date 5/28/2013 4:10:46 PM

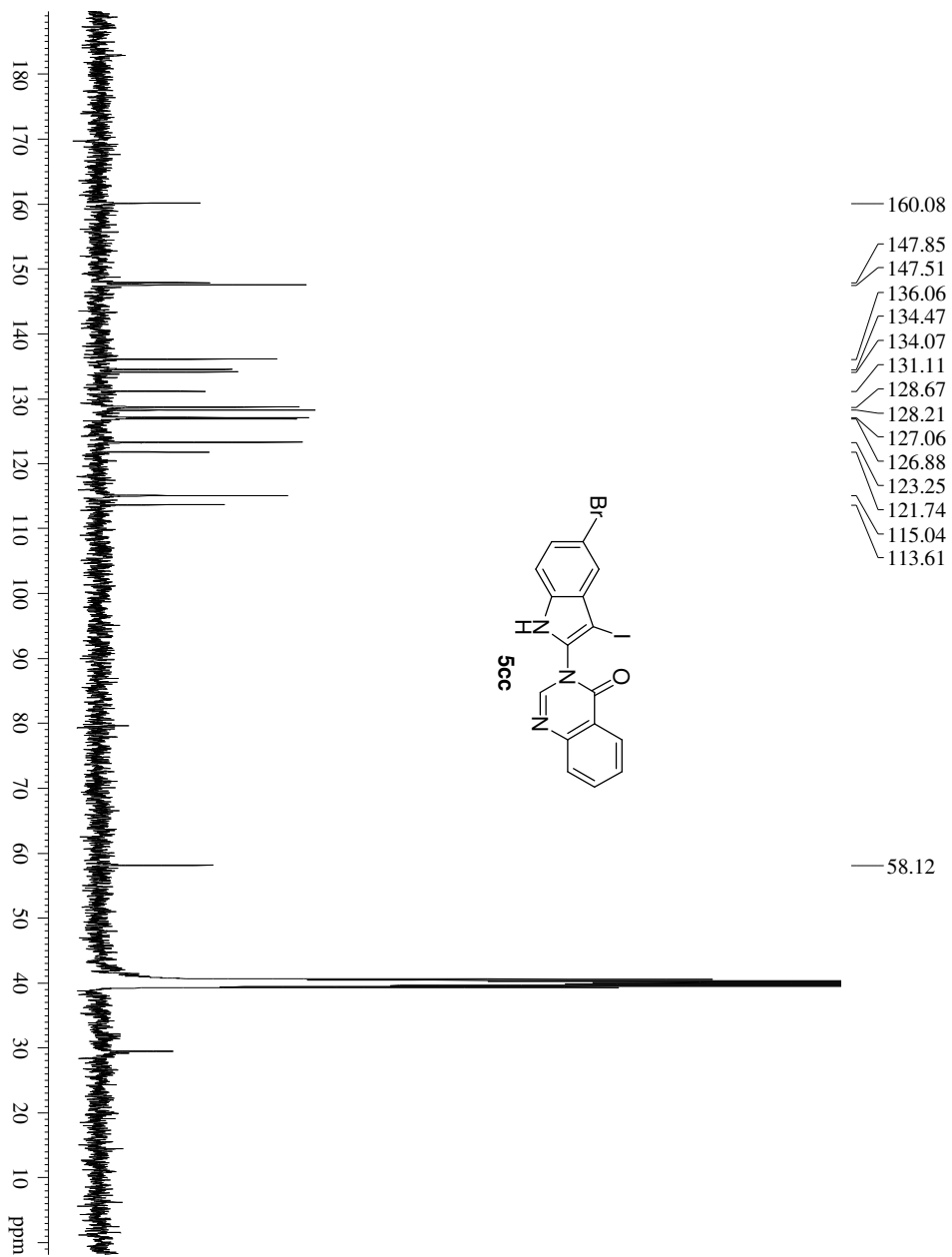
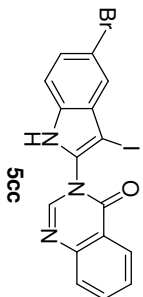
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

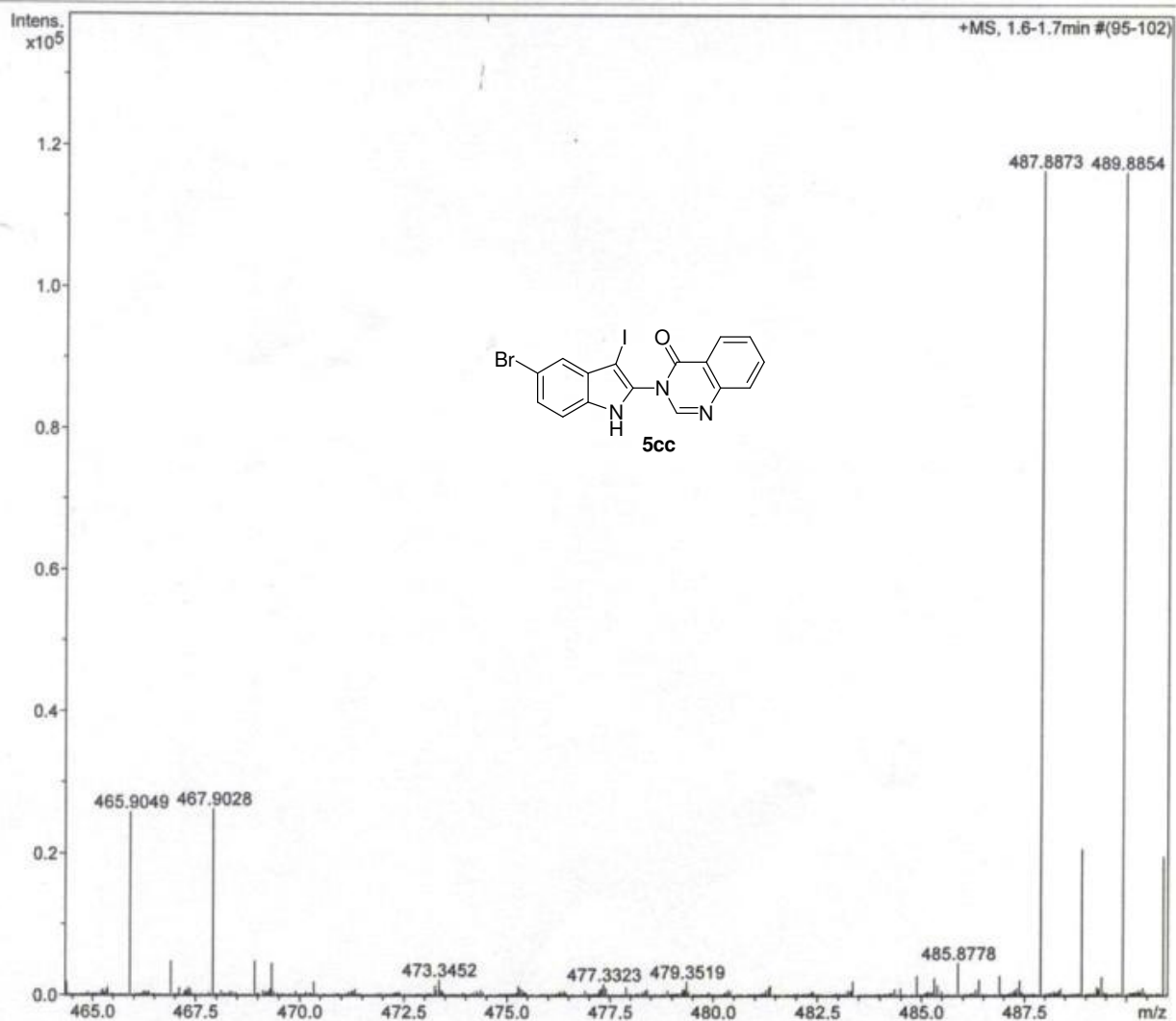
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-132-II.d
Method tune_low.m
Sample Name SKG-132-II-DCM-MEOH
Comment

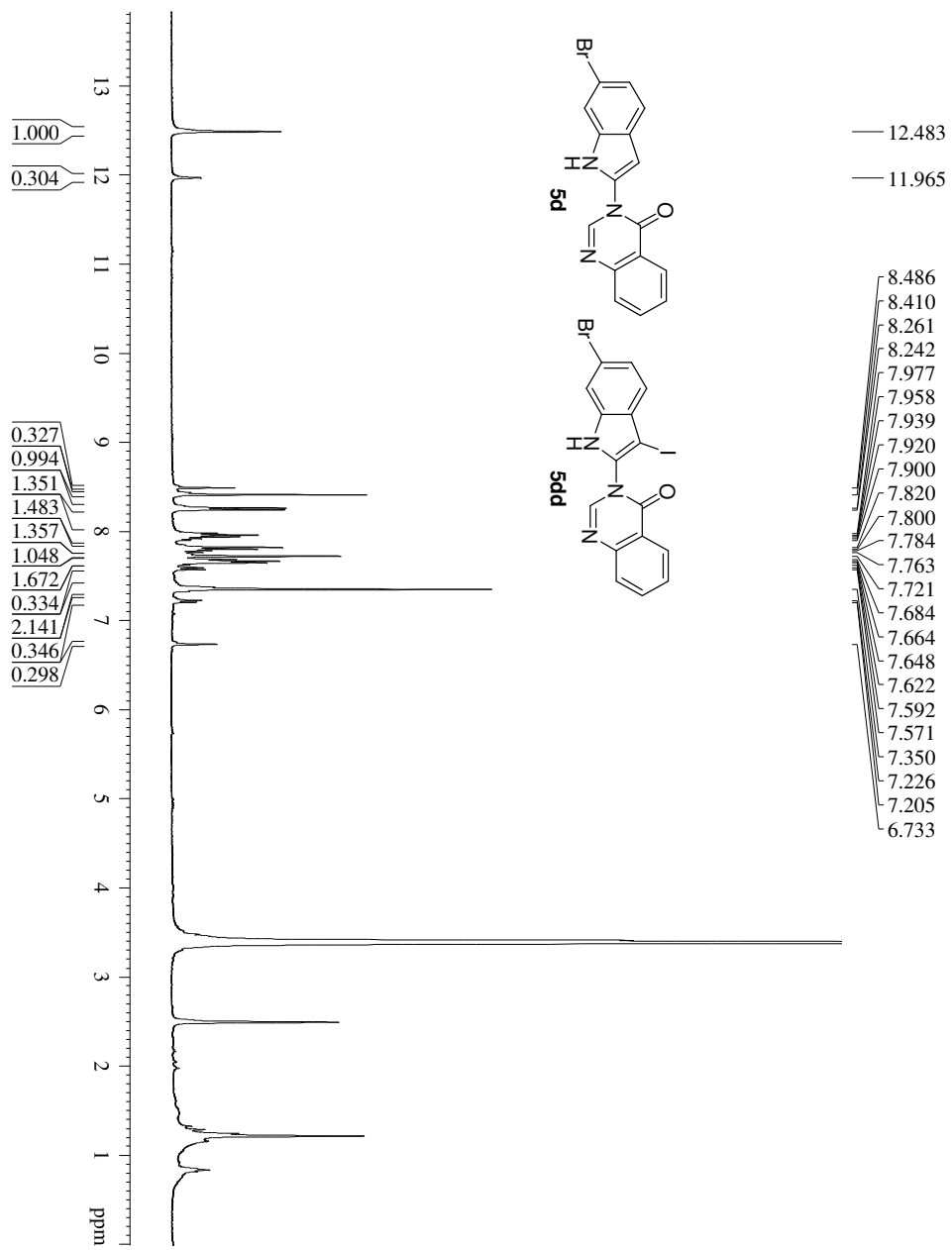
Acquisition Date 5/28/2013 4:23:44 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

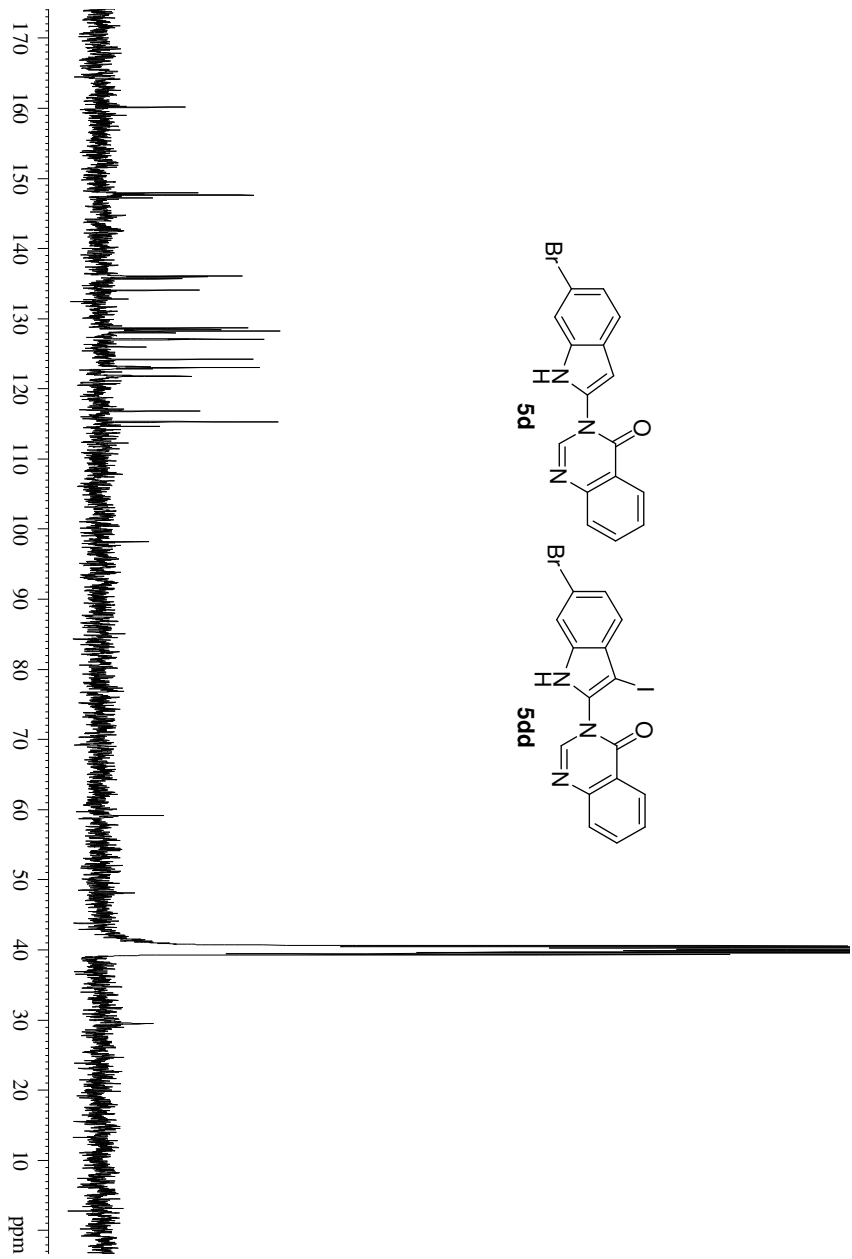
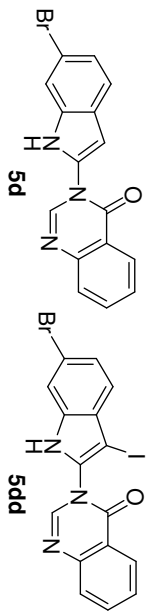
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste





160.10
147.86
147.55
147.19
136.03
135.92
135.67
134.03
128.64
128.43
128.20
127.99
127.05
125.95
124.18
123.00
121.76
116.78
115.27
114.63
98.17

59.15



BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

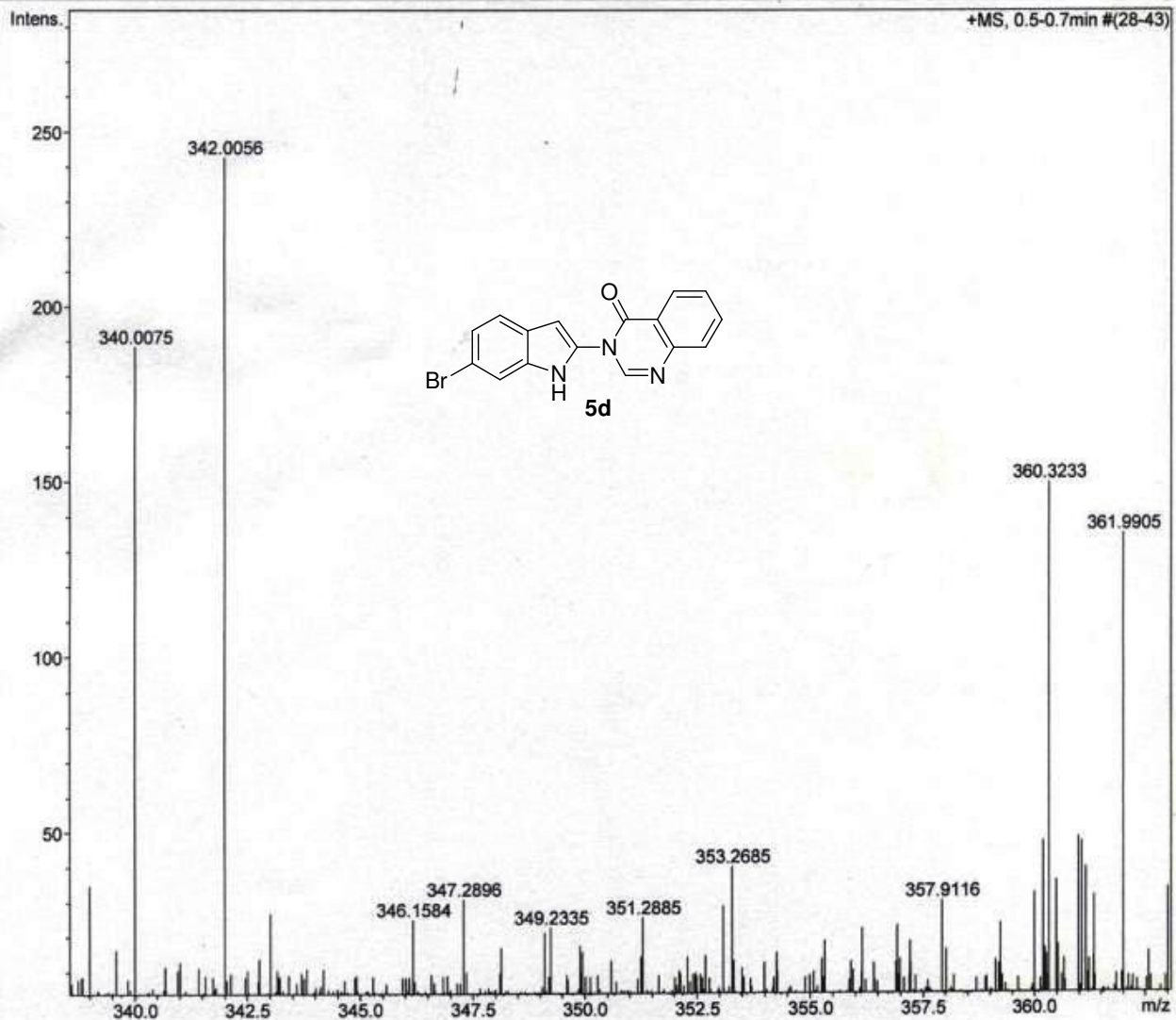
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-177R.d
Method tune_low.m
Sample Name SKG-177-DCM-MEOH
Comment

Acquisition Date 5/28/2013 4:49:06 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	3500 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



BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

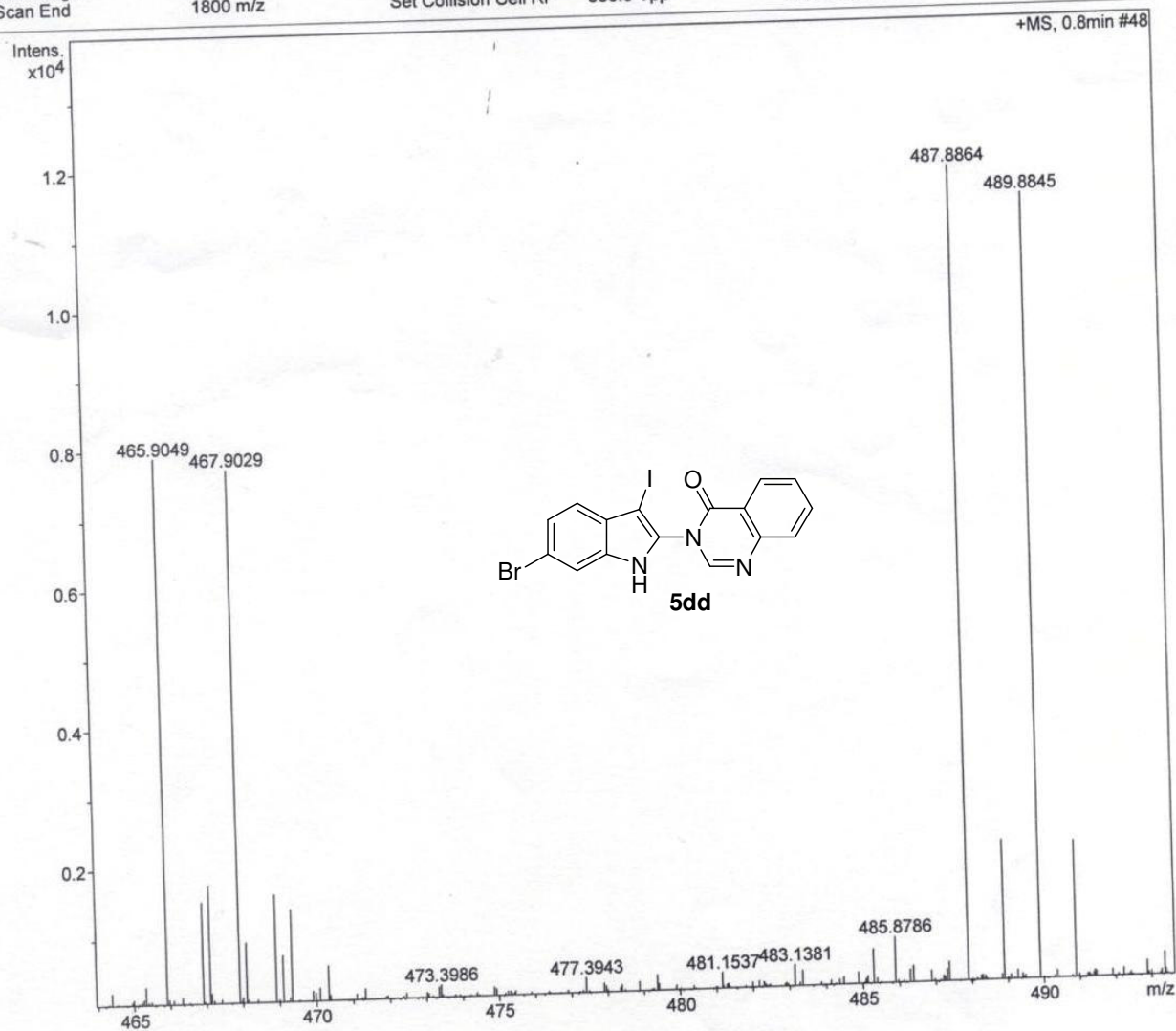
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-177R.d
Method tune_low.m
Sample Name SKG-177-DCM-MEOH
Comment

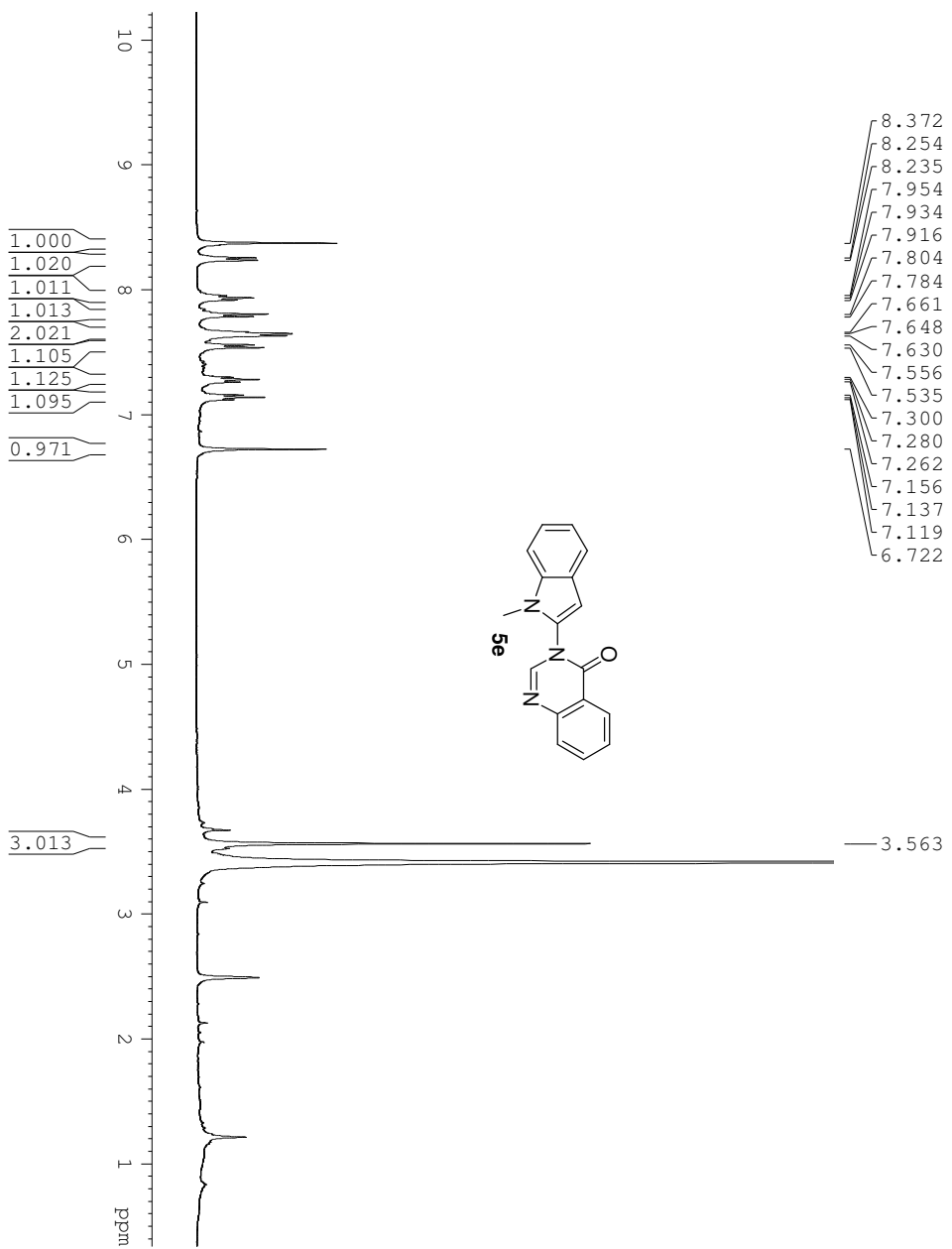
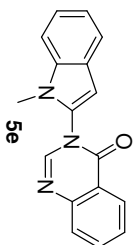
Acquisition Date 5/28/2013 4:49:06 PM

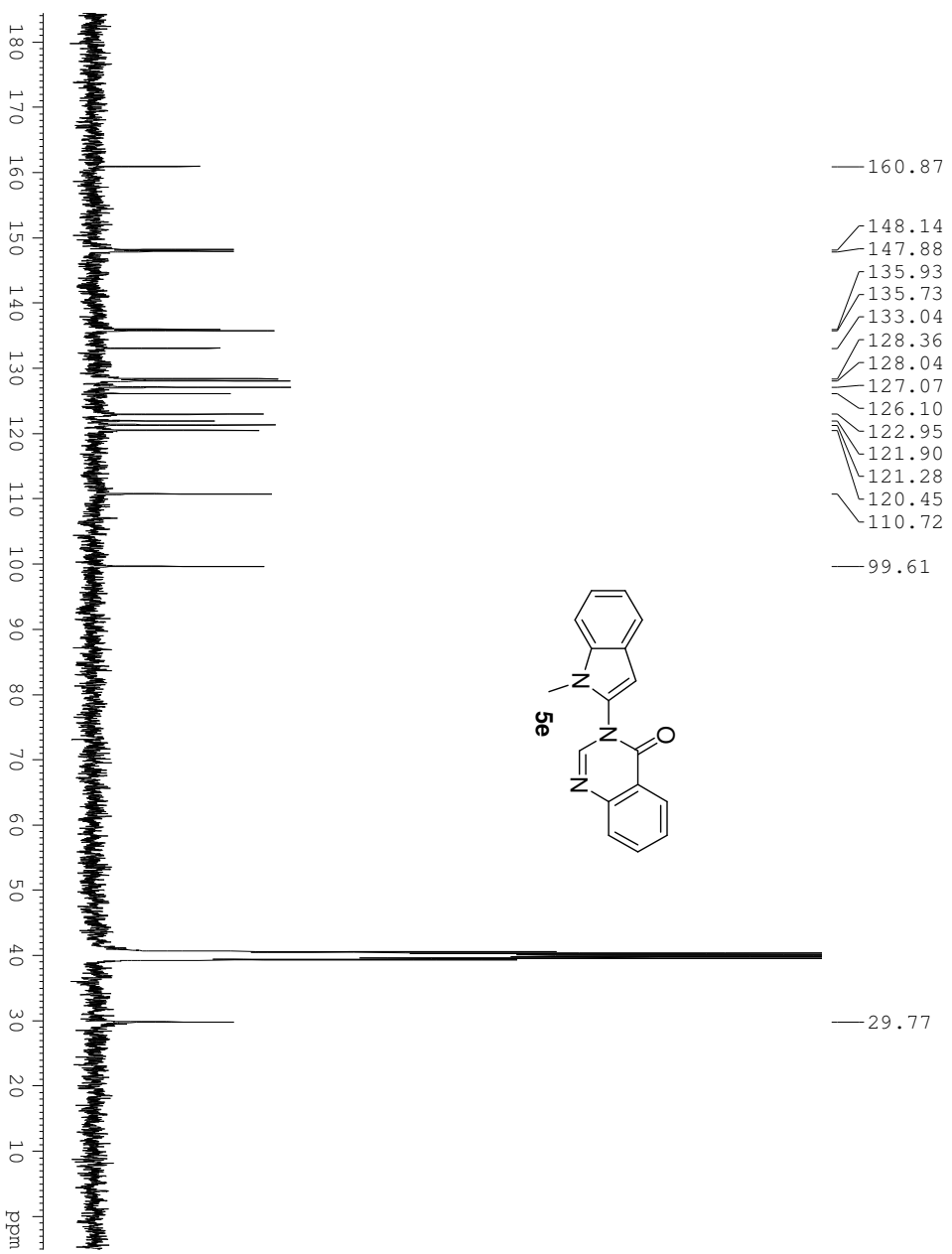
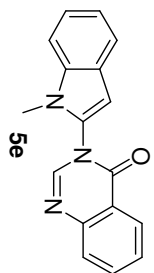
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

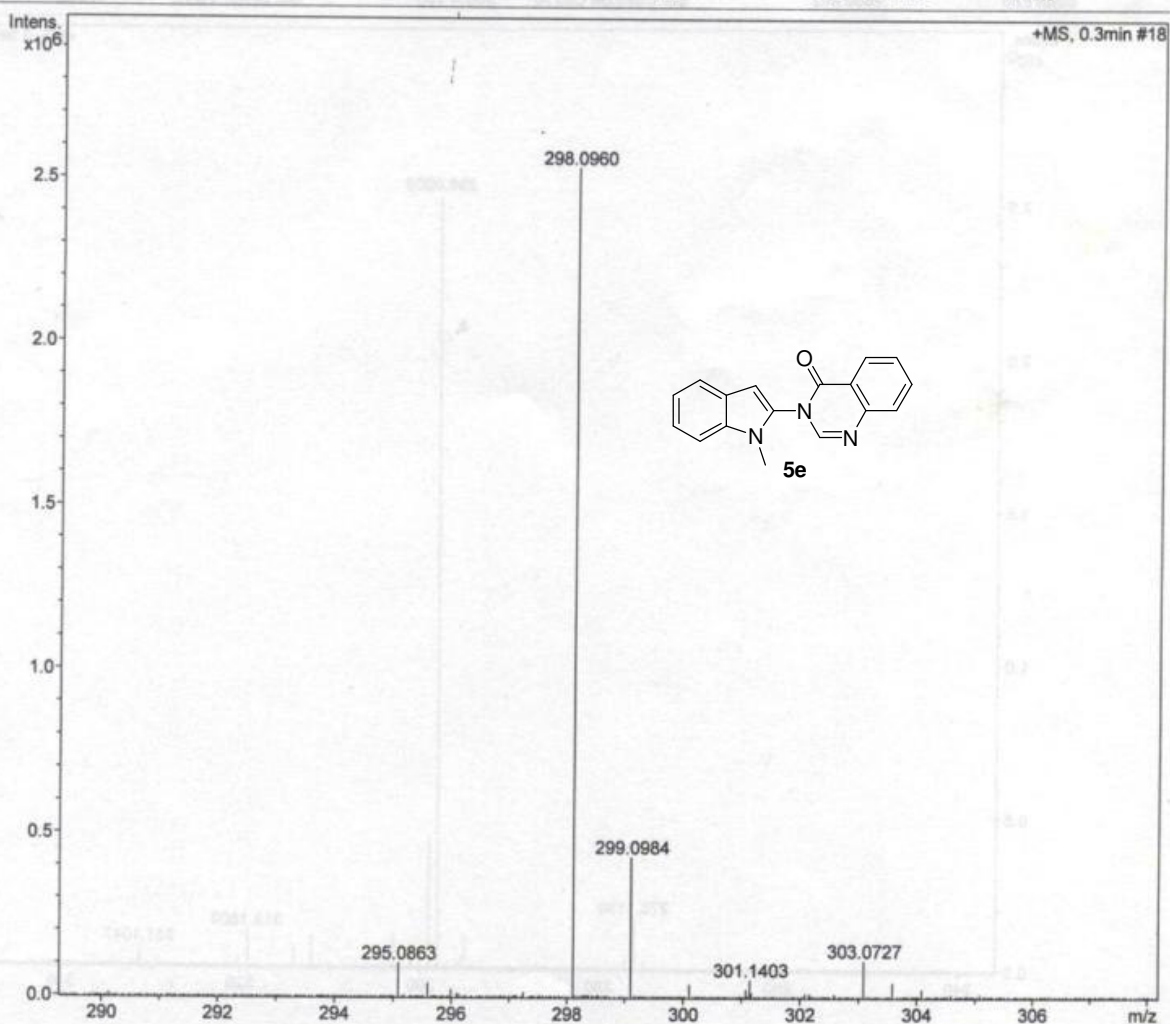
Analysis Name D:\Data\2013\Dr.NAGARAJANMAY\SKG-137R.d
Method tune_low.m
Sample Name SKG-137-DCM-MEOH
Comment

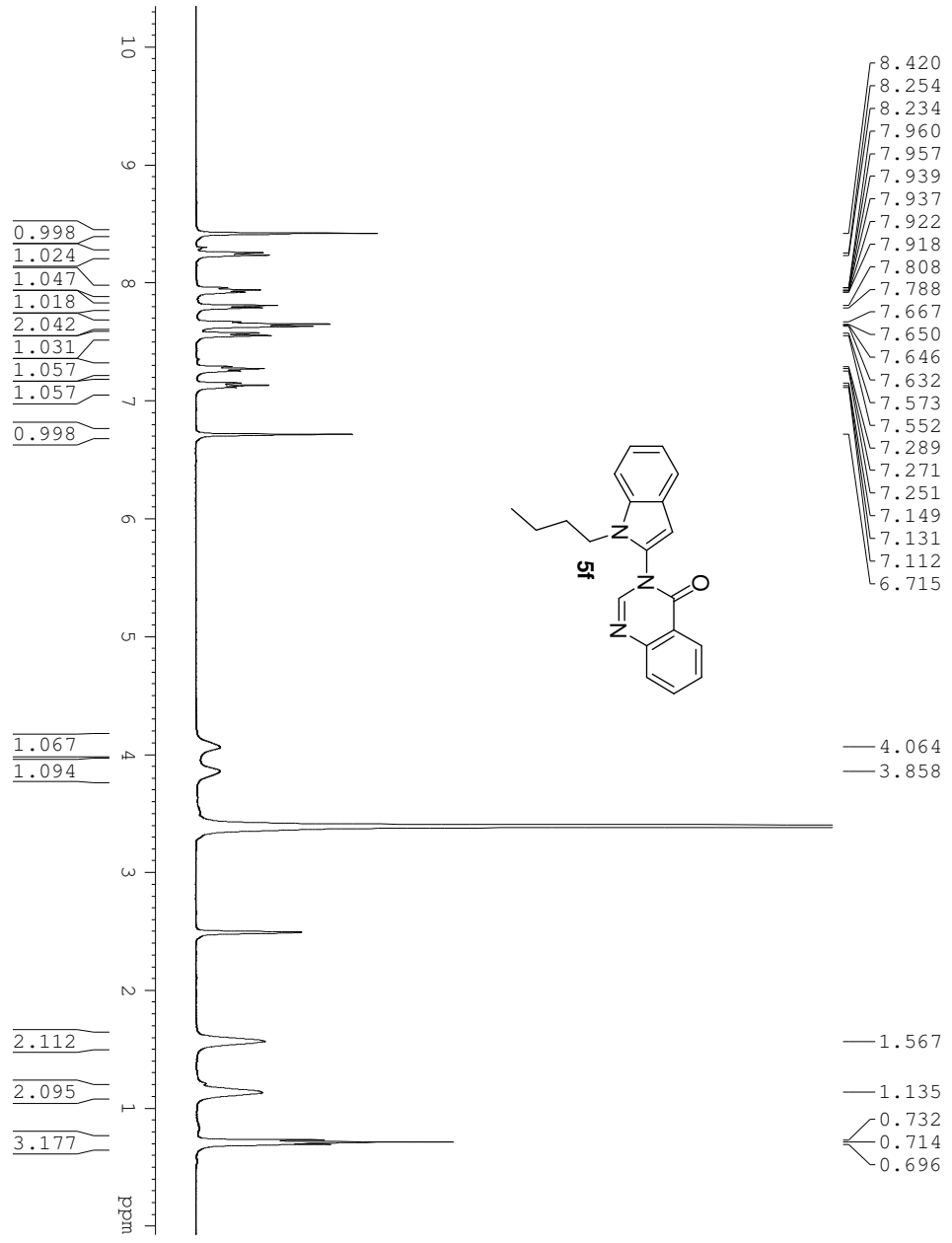
Acquisition Date 5/28/2013 3:40:42 PM

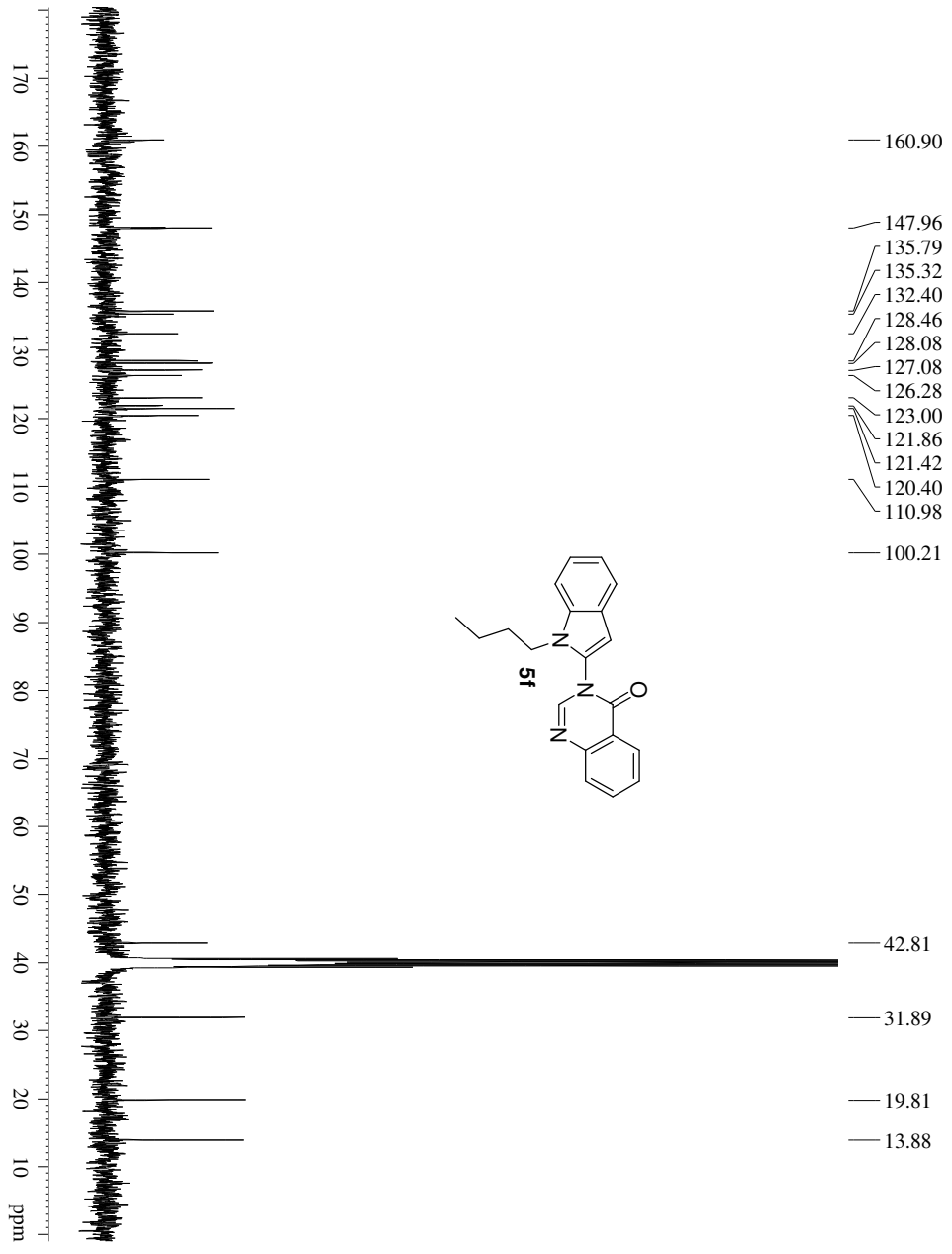
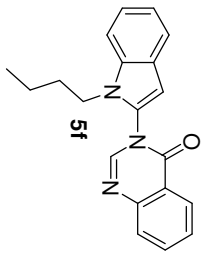
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

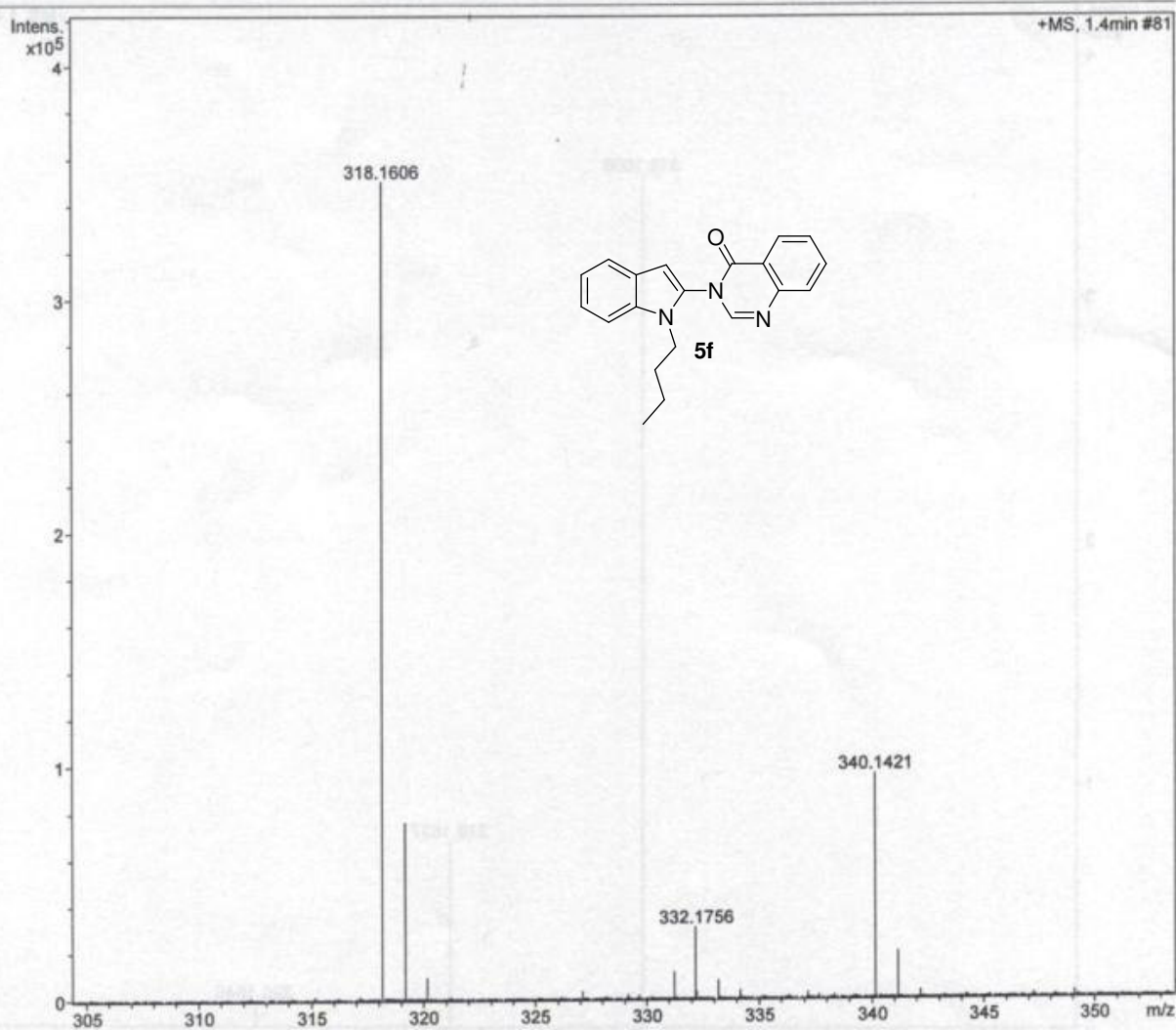
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JUNE\SKG-138.d
Method tune_low_Pos.m
Sample Name SKG-138—DCM-MEOH
Comment

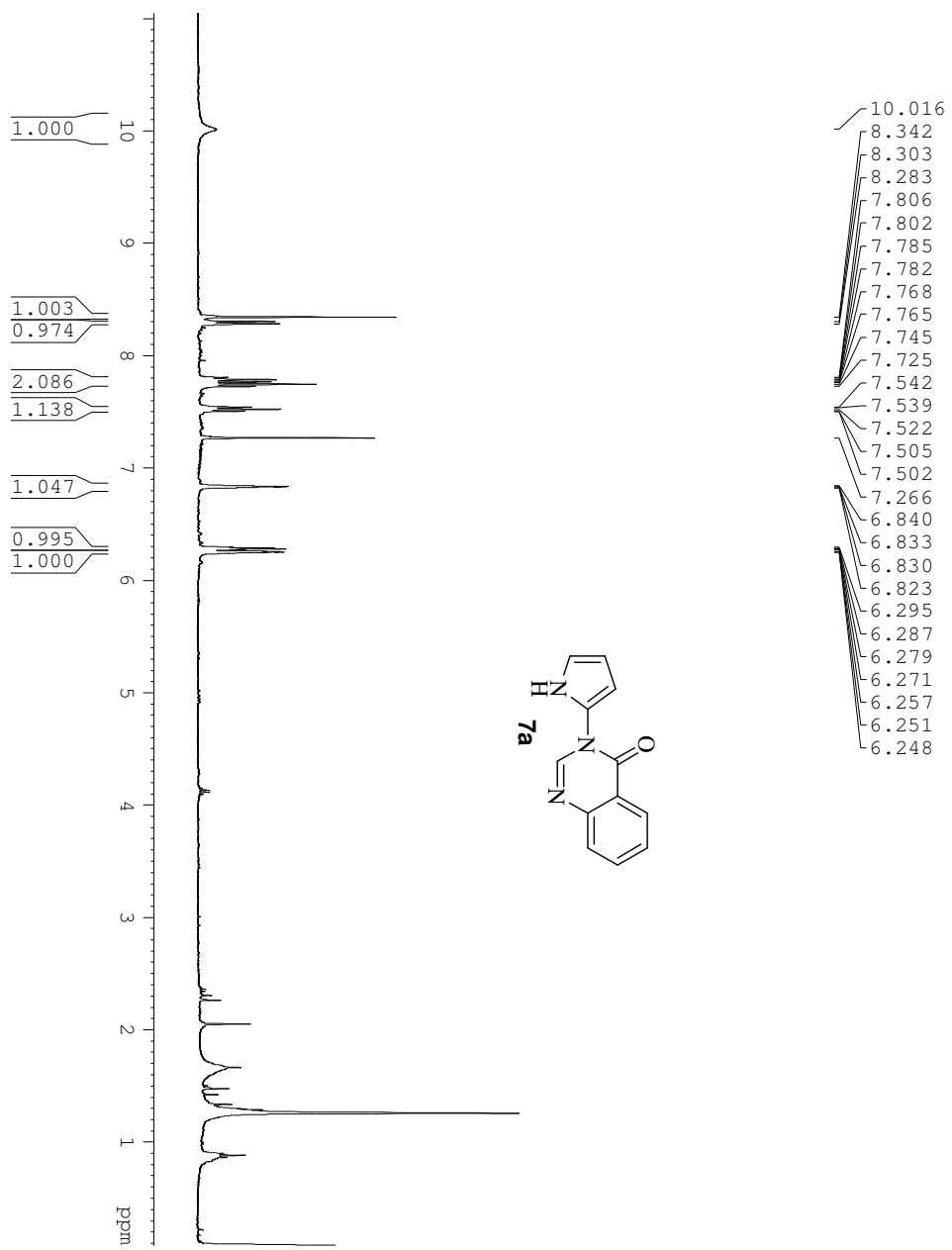
Acquisition Date 6/4/2013 12:47:53 PM

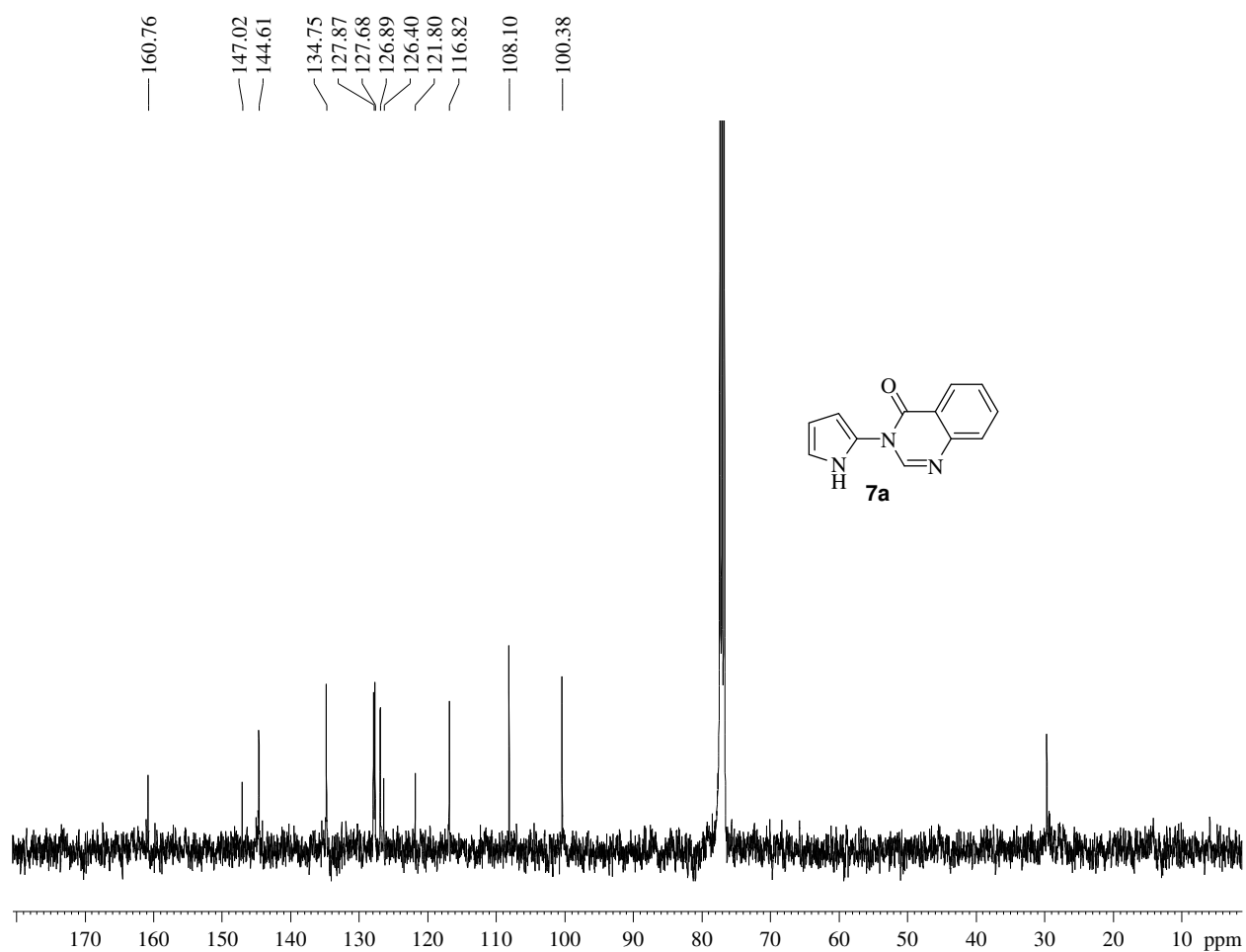
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

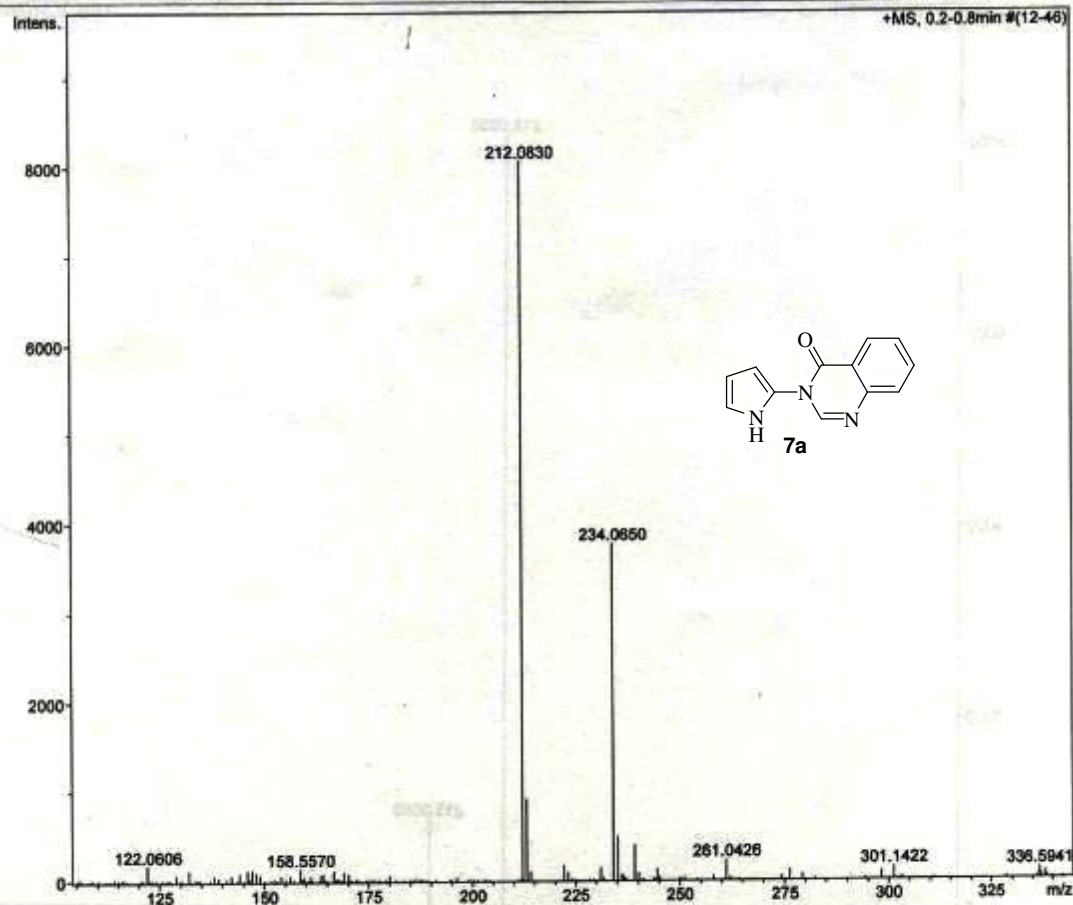
Analysis Name D:\Data\2013\Dr.NAGARAJAN\MARCH\SKG-86.d
Method tune_low_PosR.m
Sample Name SKG-86-DCM-MEOH
Comment

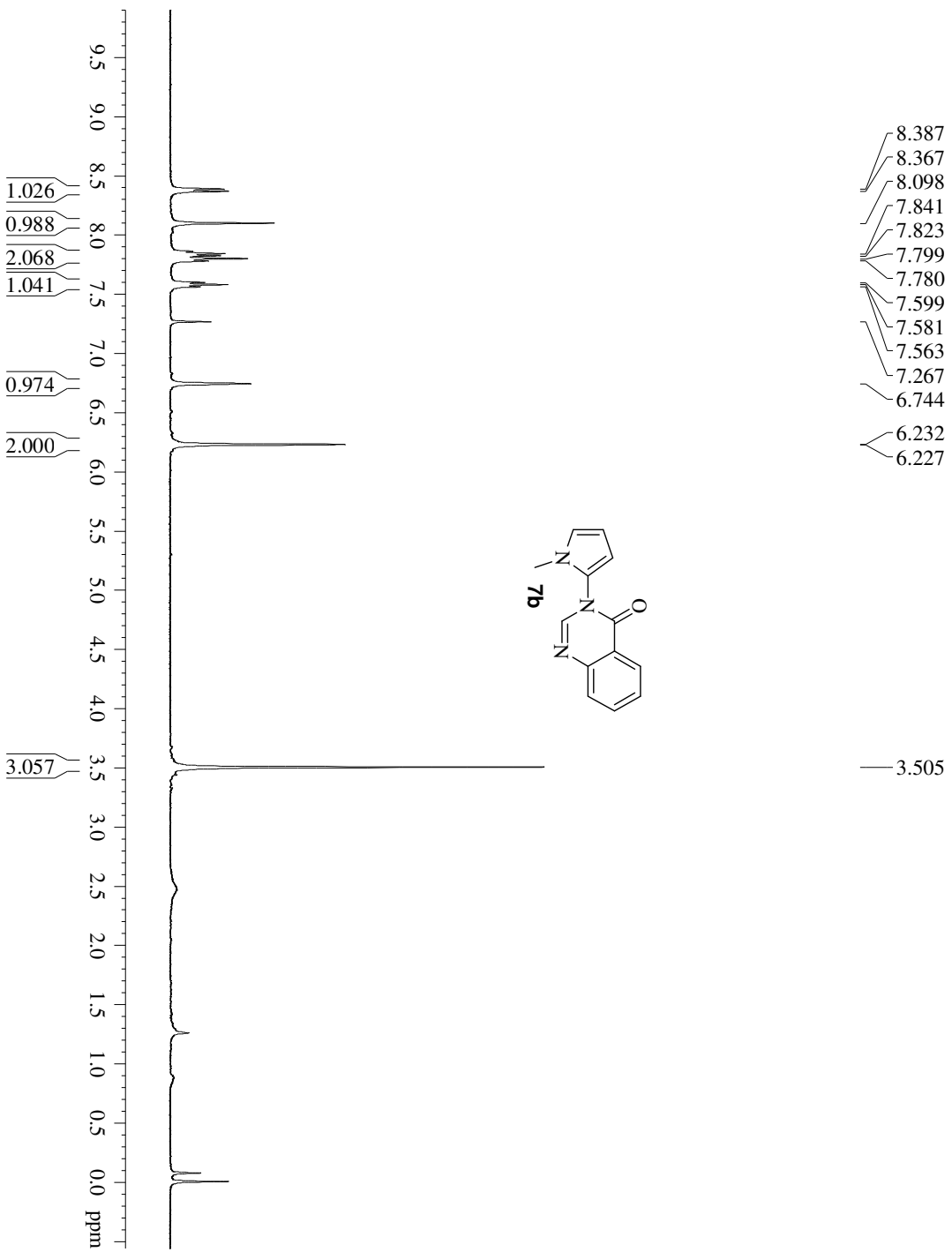
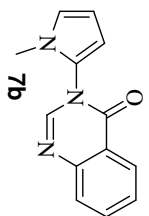
Acquisition Date 3/11/2013 12:42:10 PM

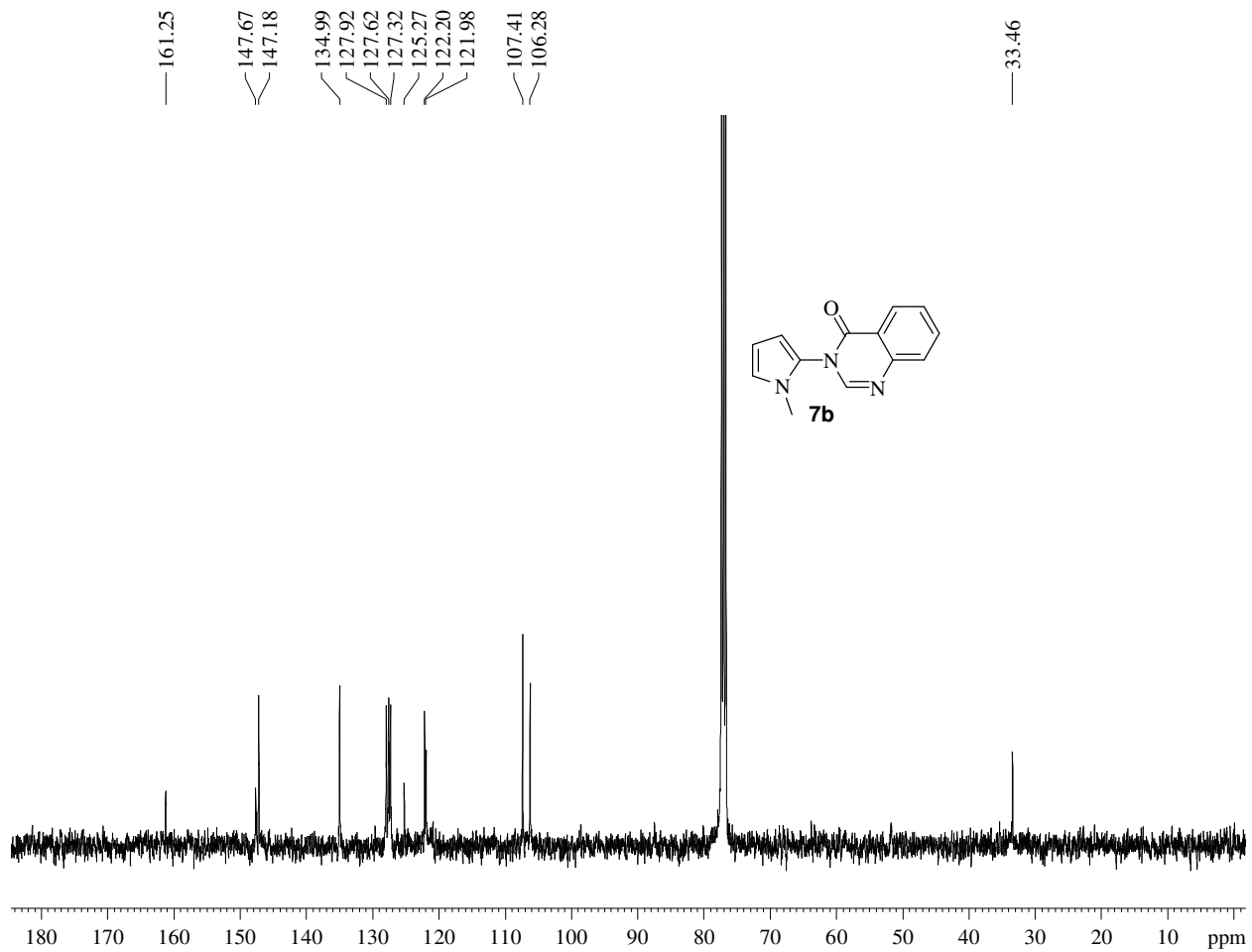
Operator Rajesh Vashisth
Instrument maXis 10138

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	1000 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

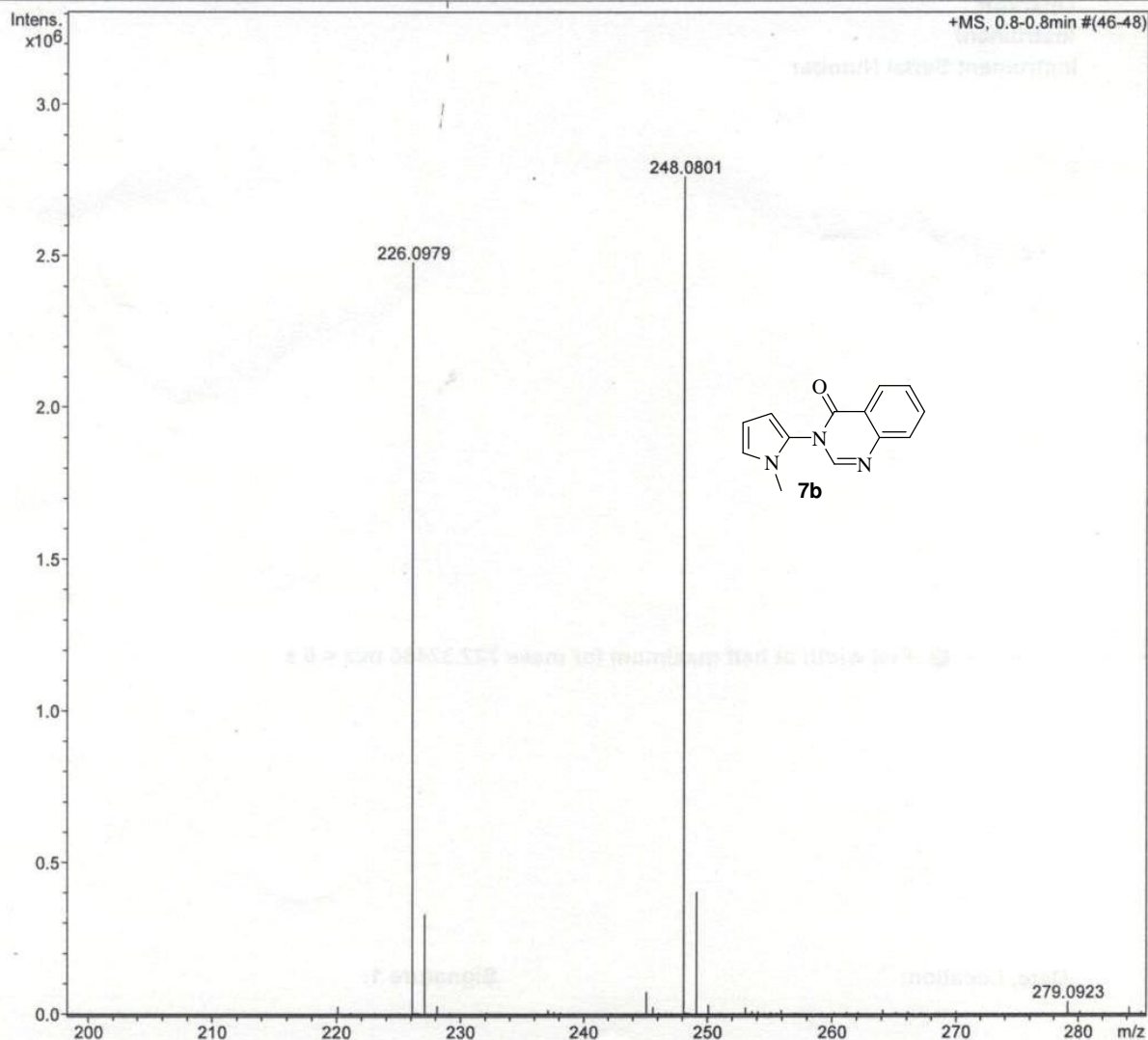
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-200.d
Method tune_low_Pos.m
Sample Name SKG-200-DCM-MEOH
Comment

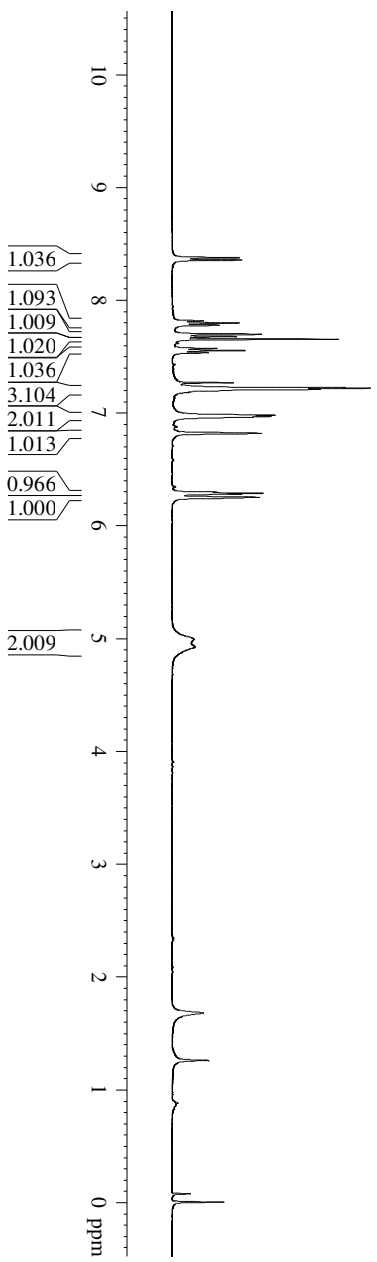
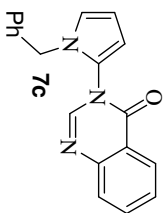
Acquisition Date 7/23/2013 11:45:11 AM

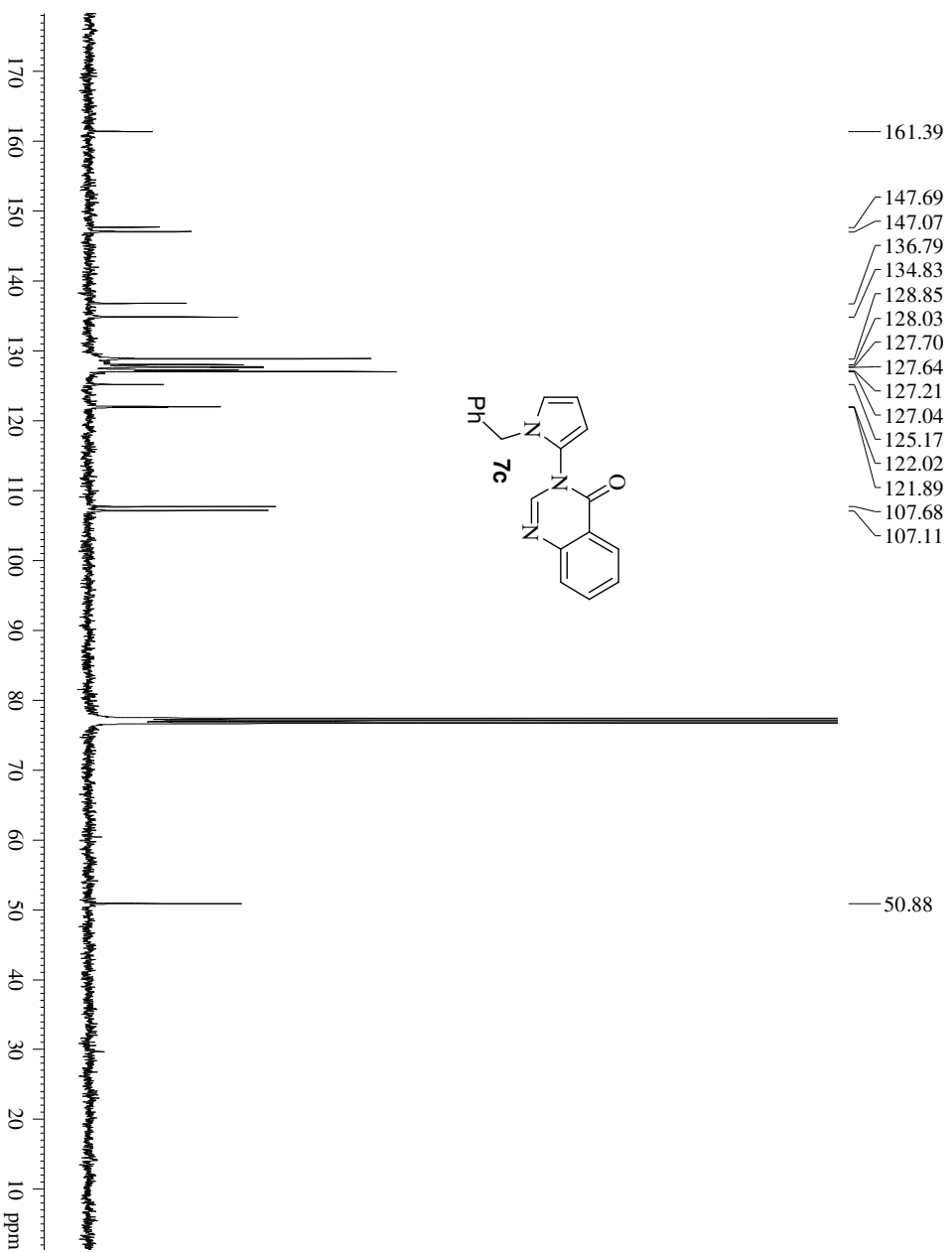
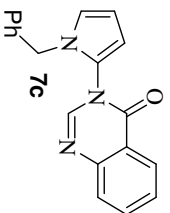
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

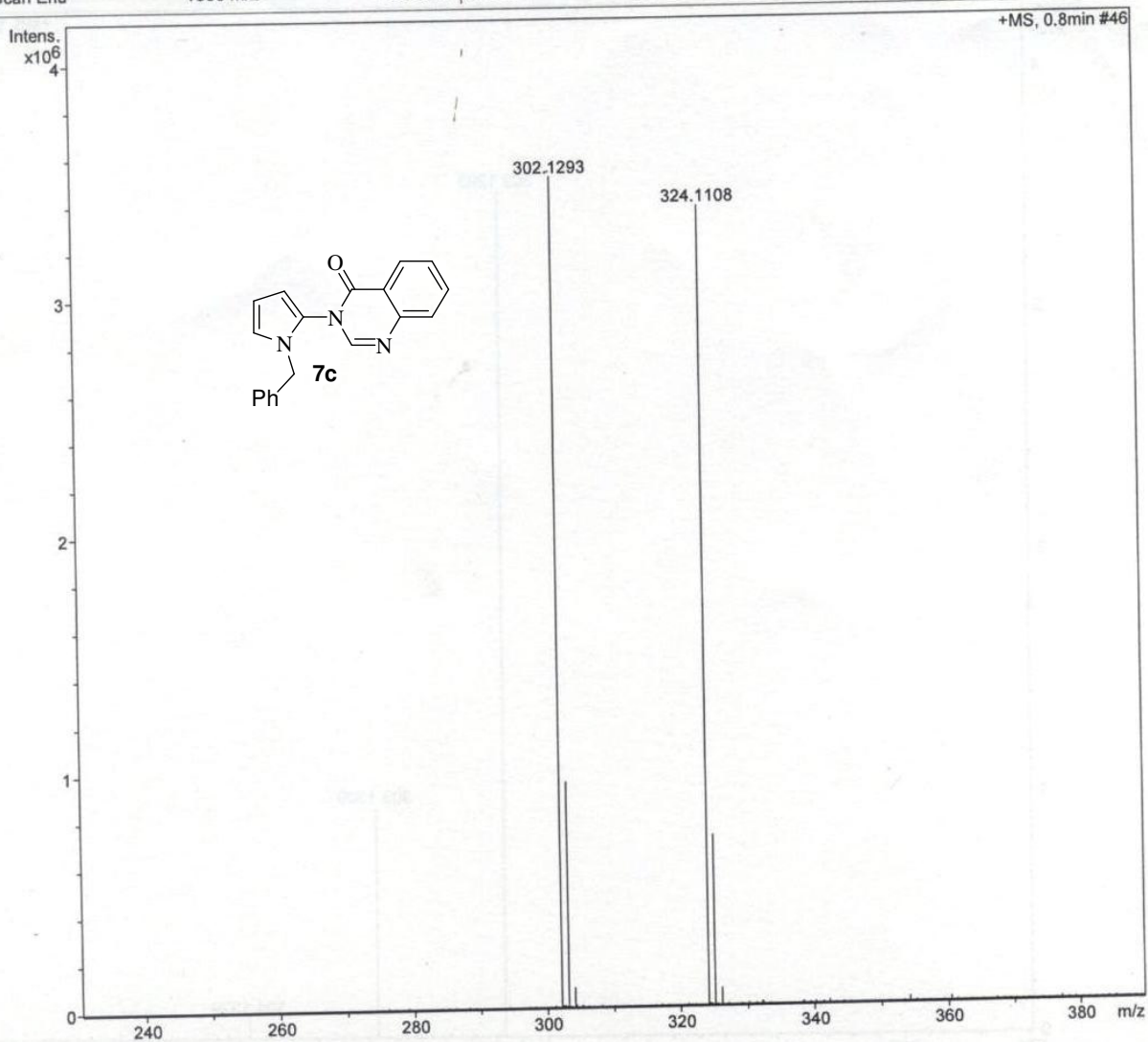
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-188.d
Method tune_low_Pos.m
Sample Name SKG-188-DCM-MEOH
Comment

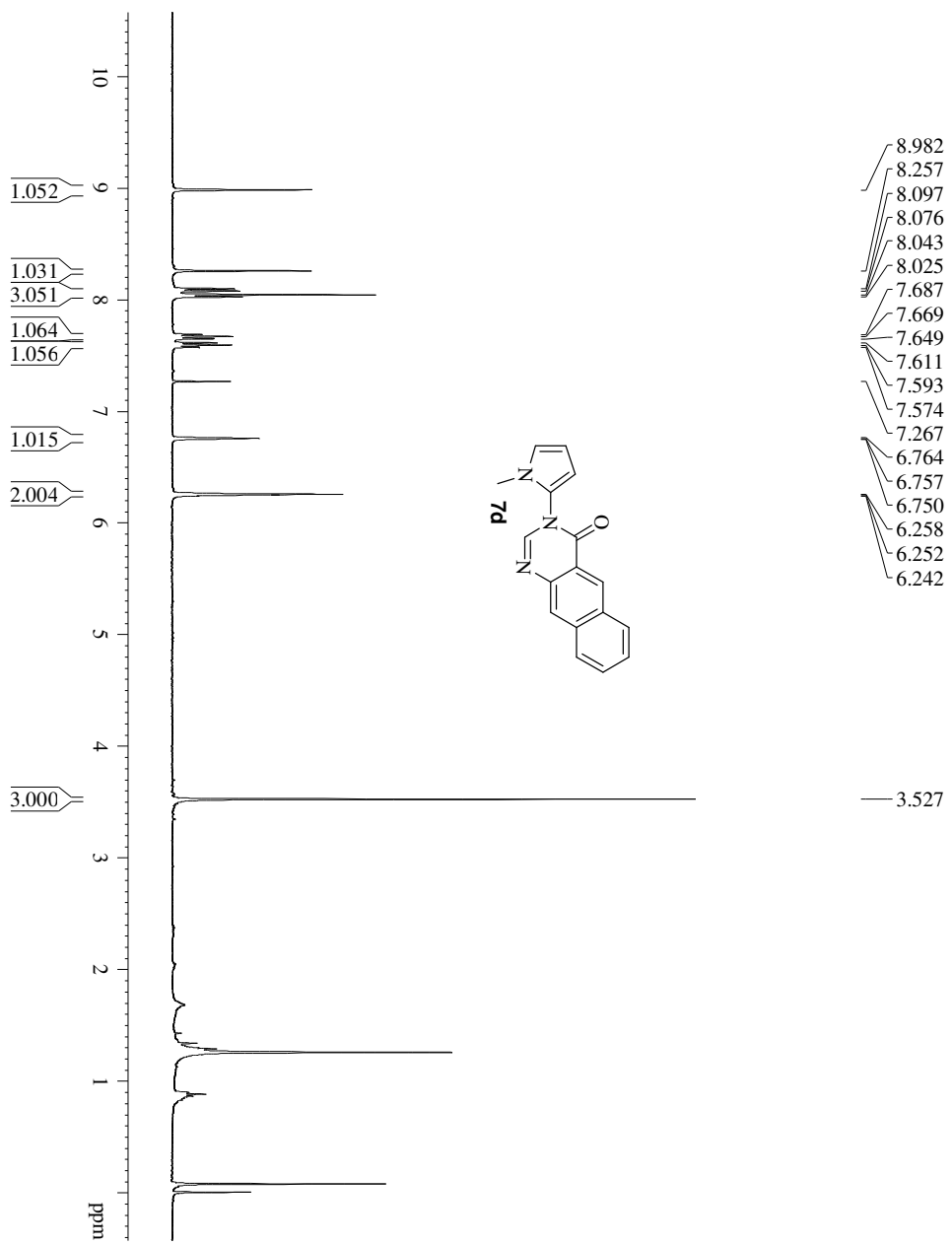
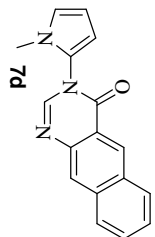
Acquisition Date 7/23/2013 12:10:46 PM

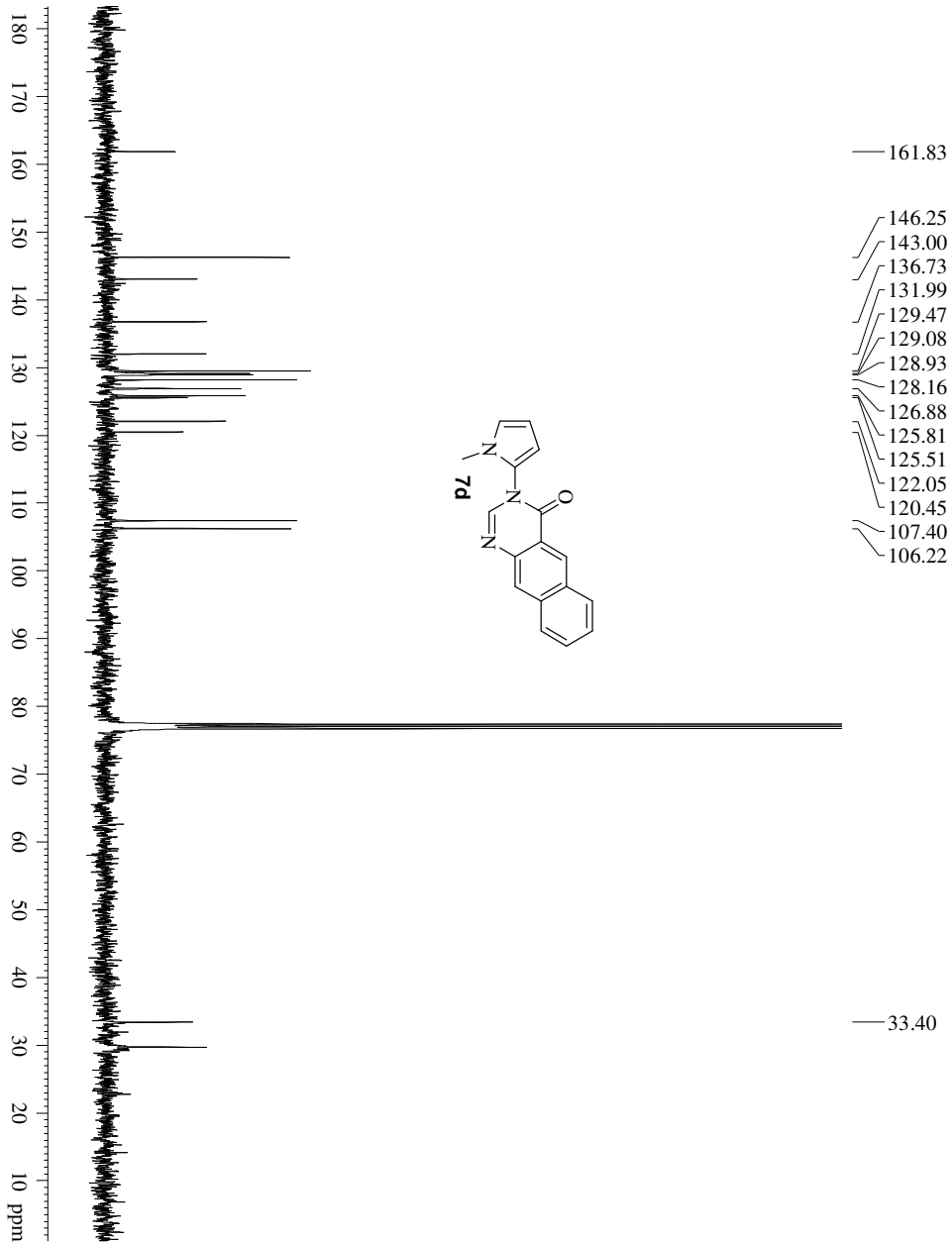
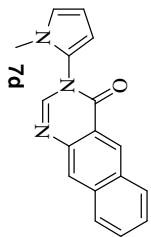
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4200 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

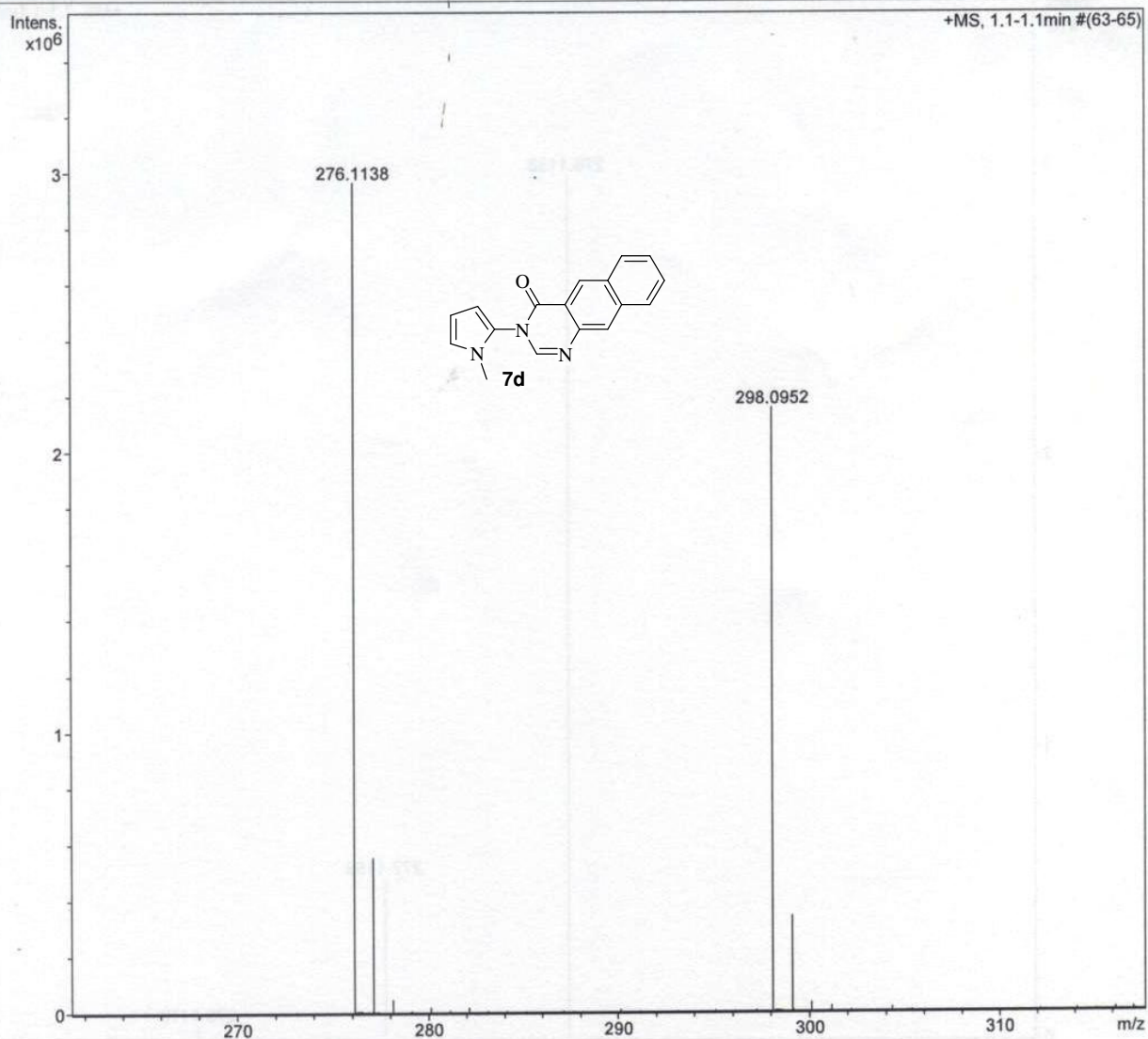
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-201.d
Method tune_low_Pos.m
Sample Name SKG-201-DCM-MEOH
Comment

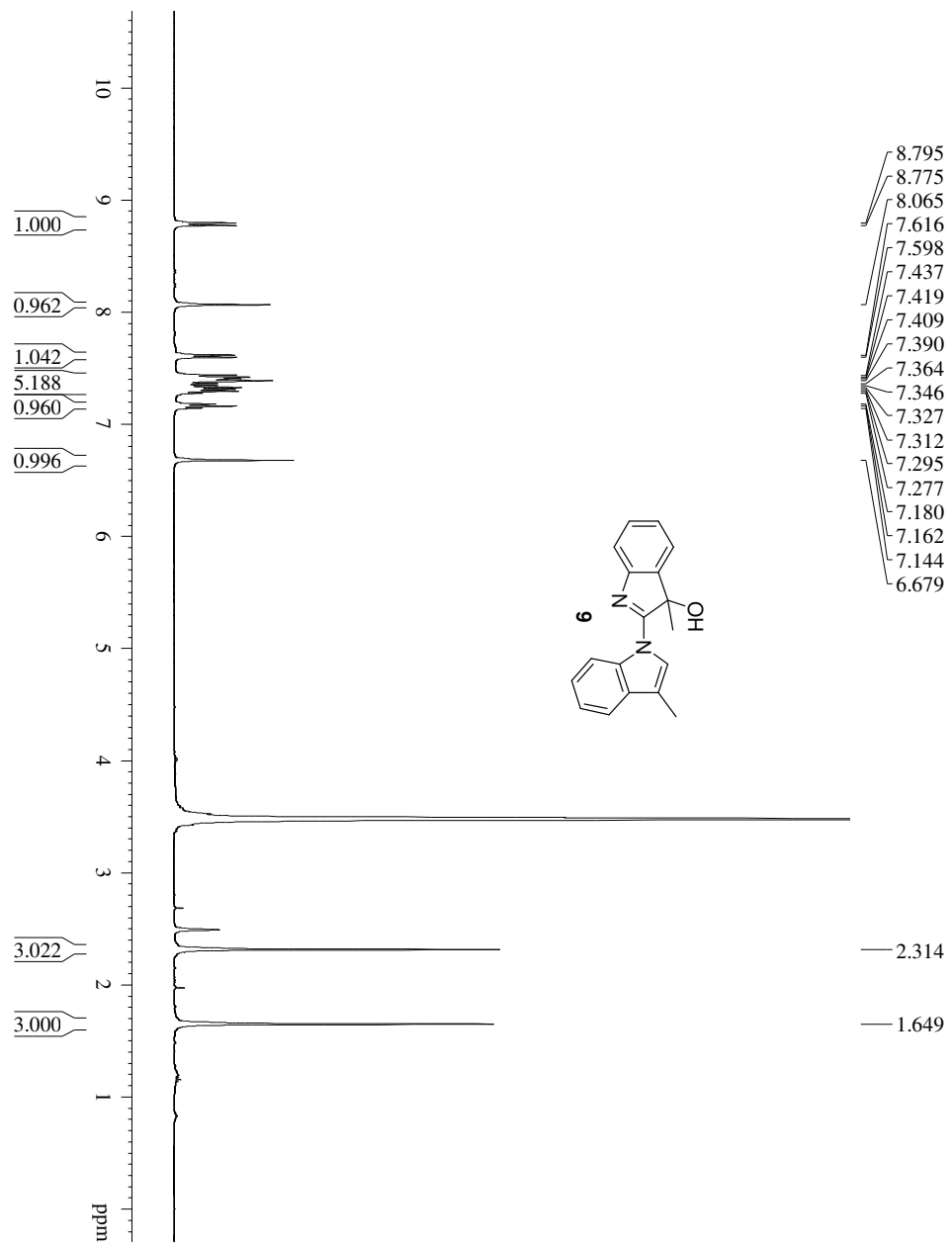
Acquisition Date 7/23/2013 12:00:10 PM

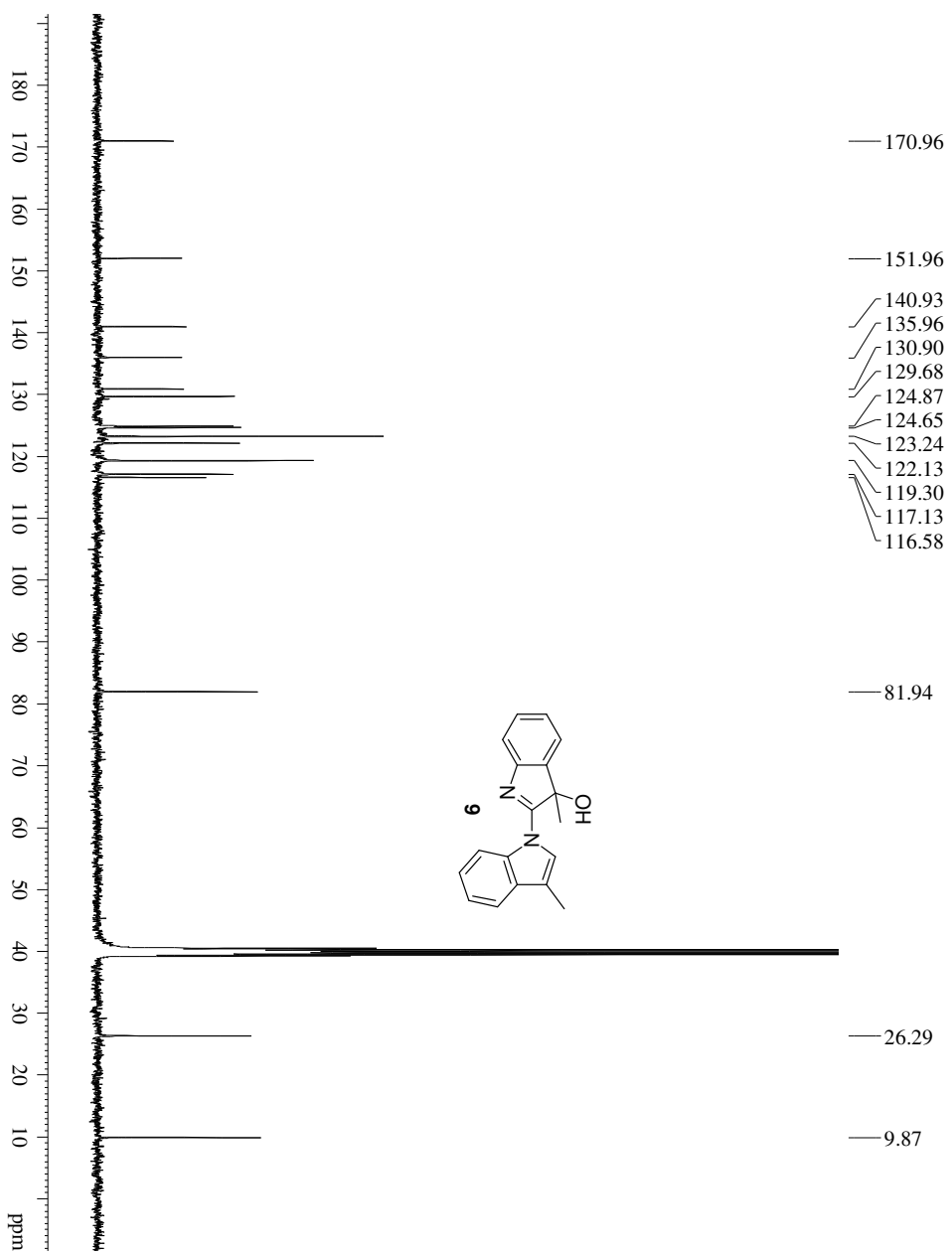
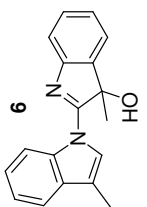
Operator Ramu Sridhar
Instrument maXis 10138

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	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

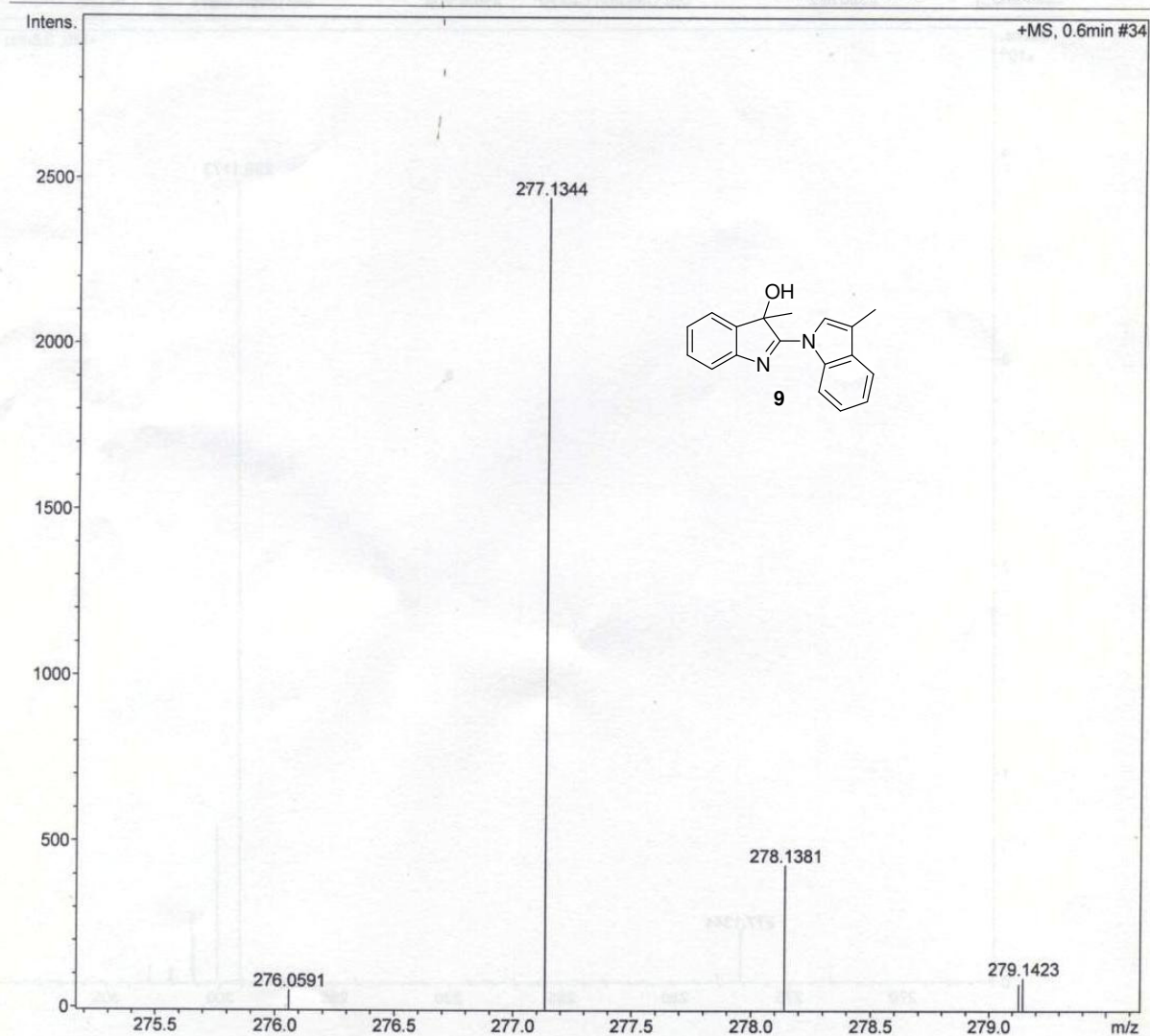
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-69.d
Method tune_low_Pos-R2.m
Sample Name SKG-69--DCM-MEOH
Comment

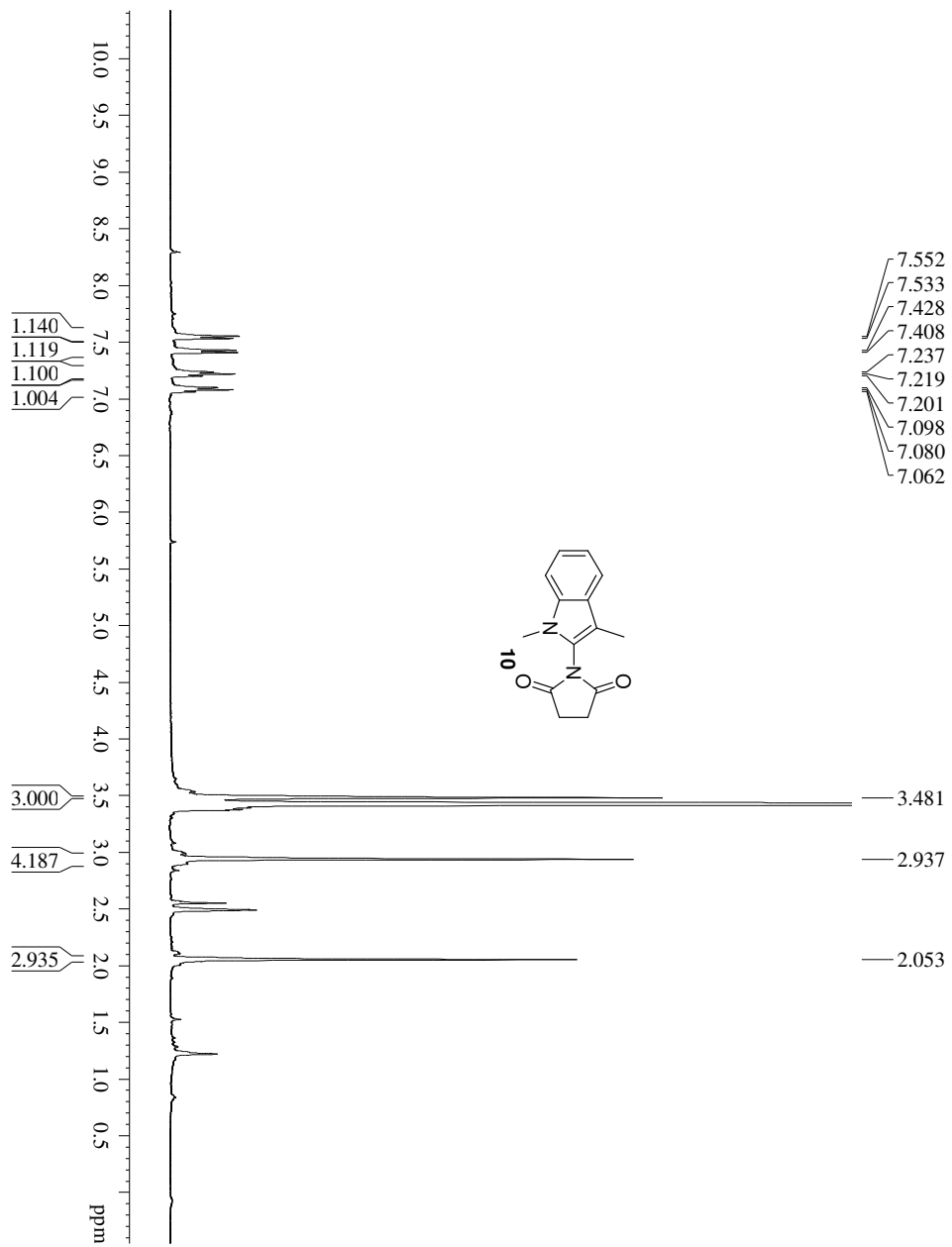
Acquisition Date 7/26/2013 2:53:34 PM

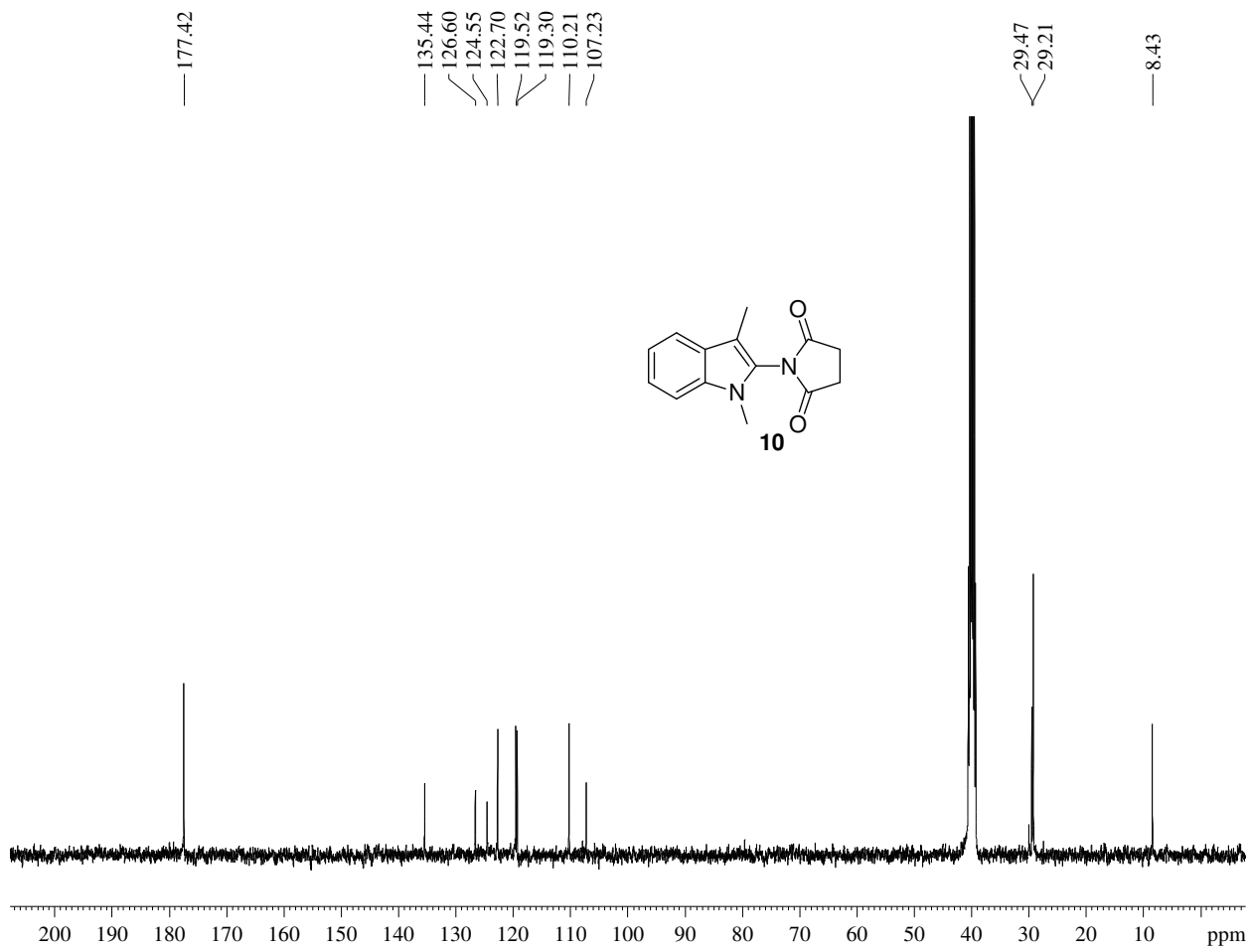
Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2400 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	2580 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

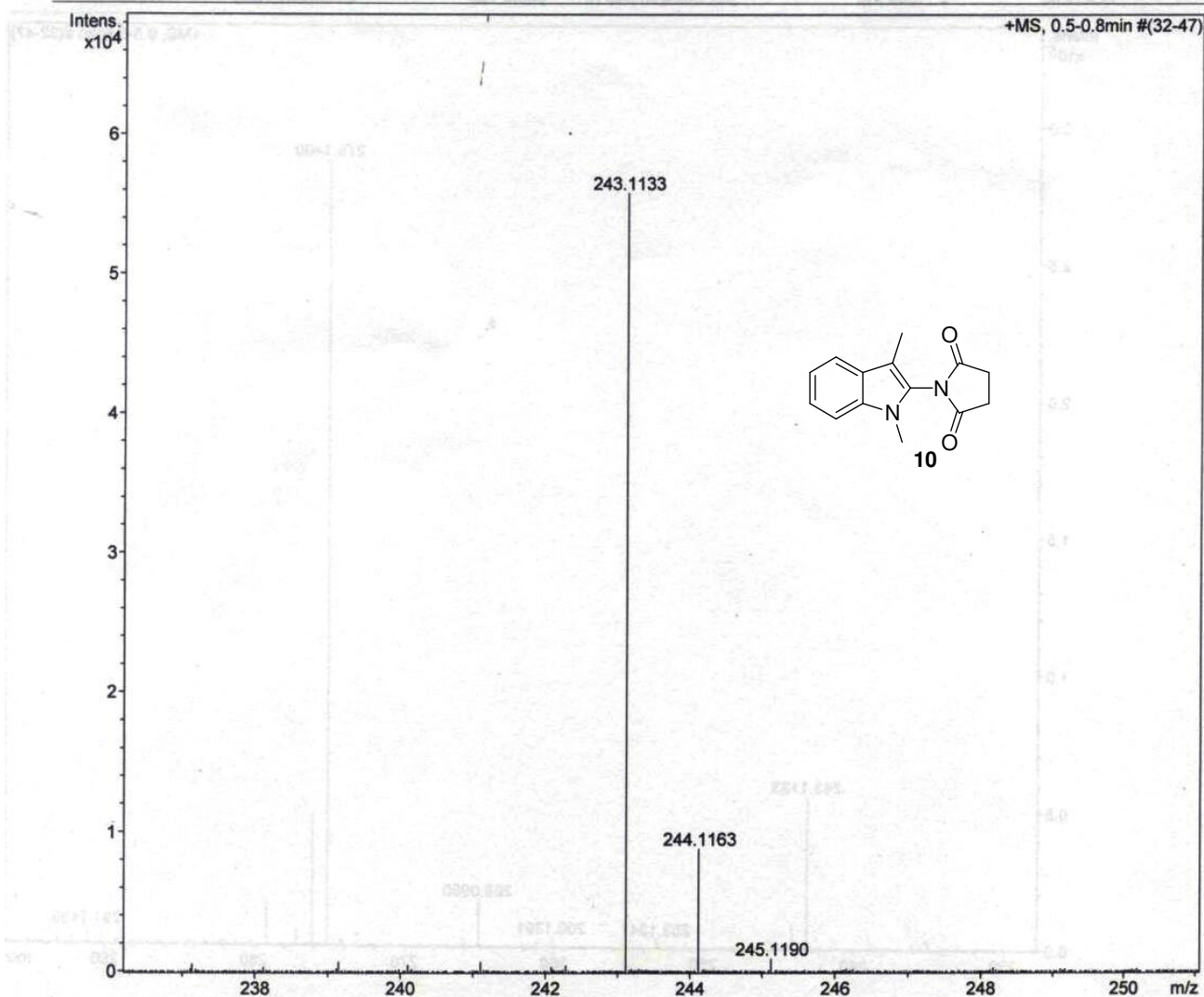
Analysis Name D:\Data\2013\Dr.NAGARAJANMAYISKG-195R.d
Method tune_low_Pos.m
Sample Name SKG-195-DCM-MEOH
Comment

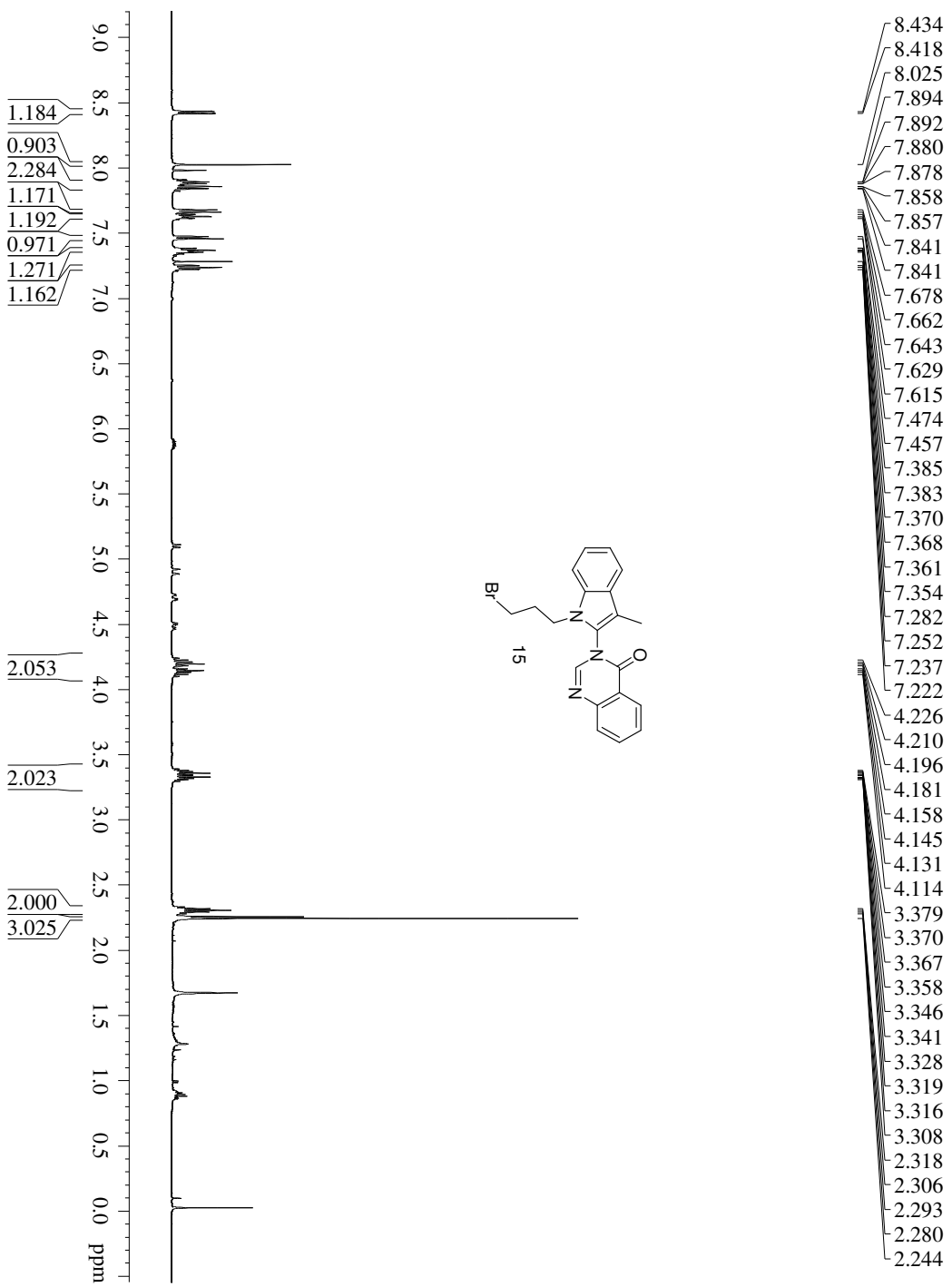
Acquisition Date 5/31/2013 4:10:34 PM

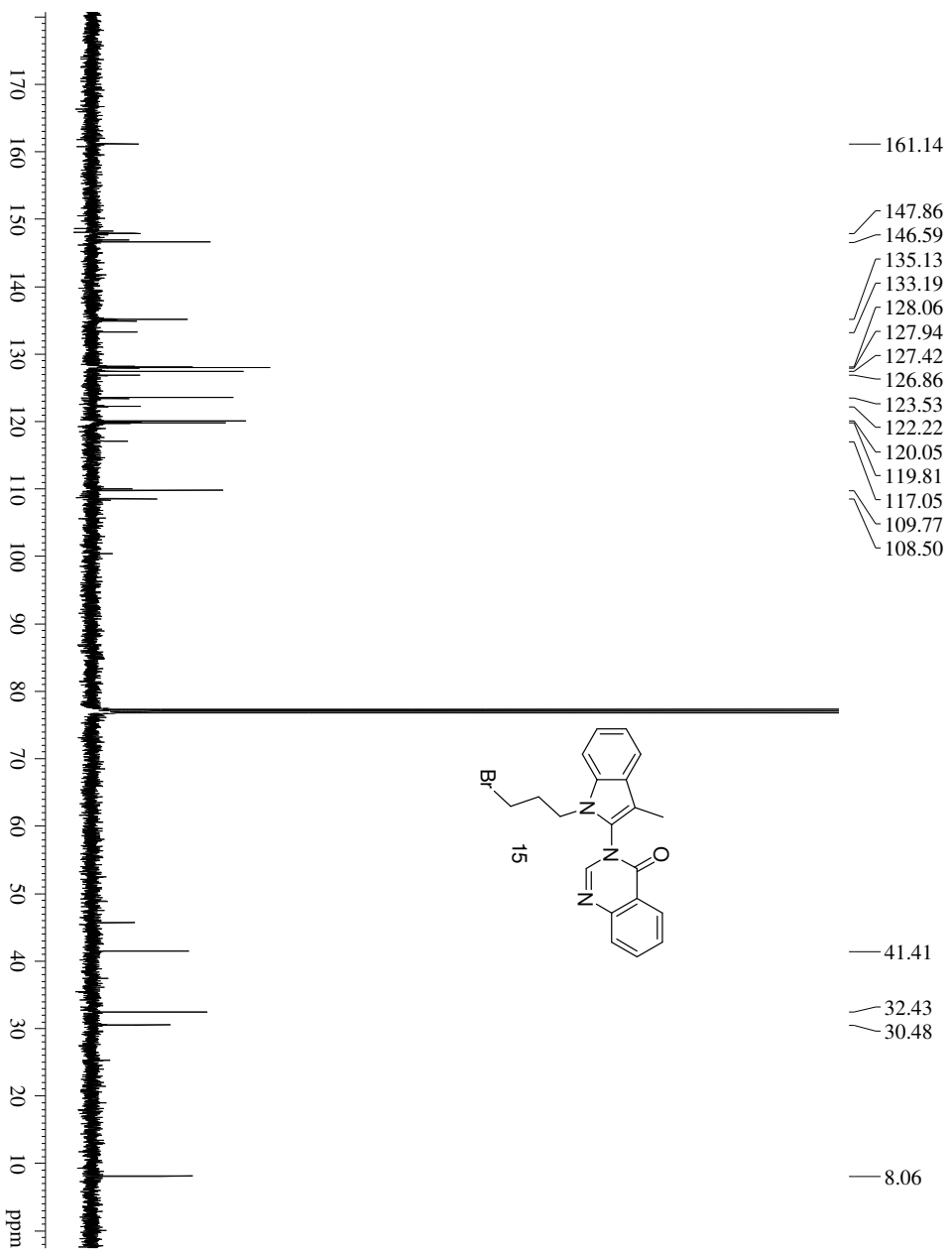
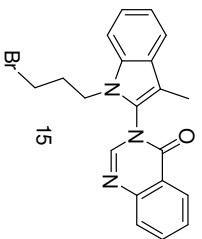
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT
School of Chemistry
University of Hyderabad

Analysis Info

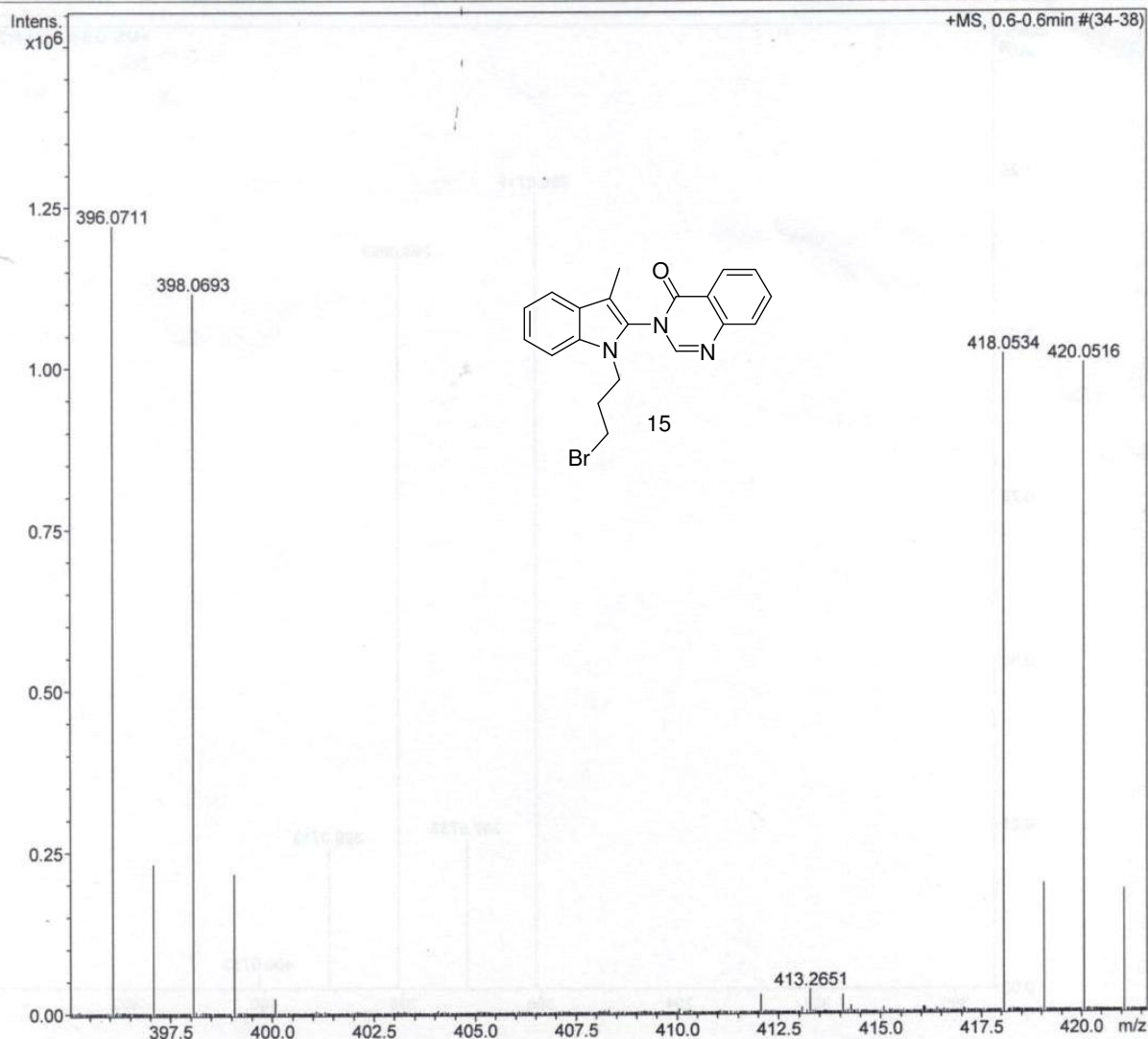
Analysis Name D:\Data\2013\Dr.NAGARAJAN\JULY\SKG-251-I.d
Method tune_low_Pos.m
Sample Name SKG-251-I-DCM-MEOH
Comment

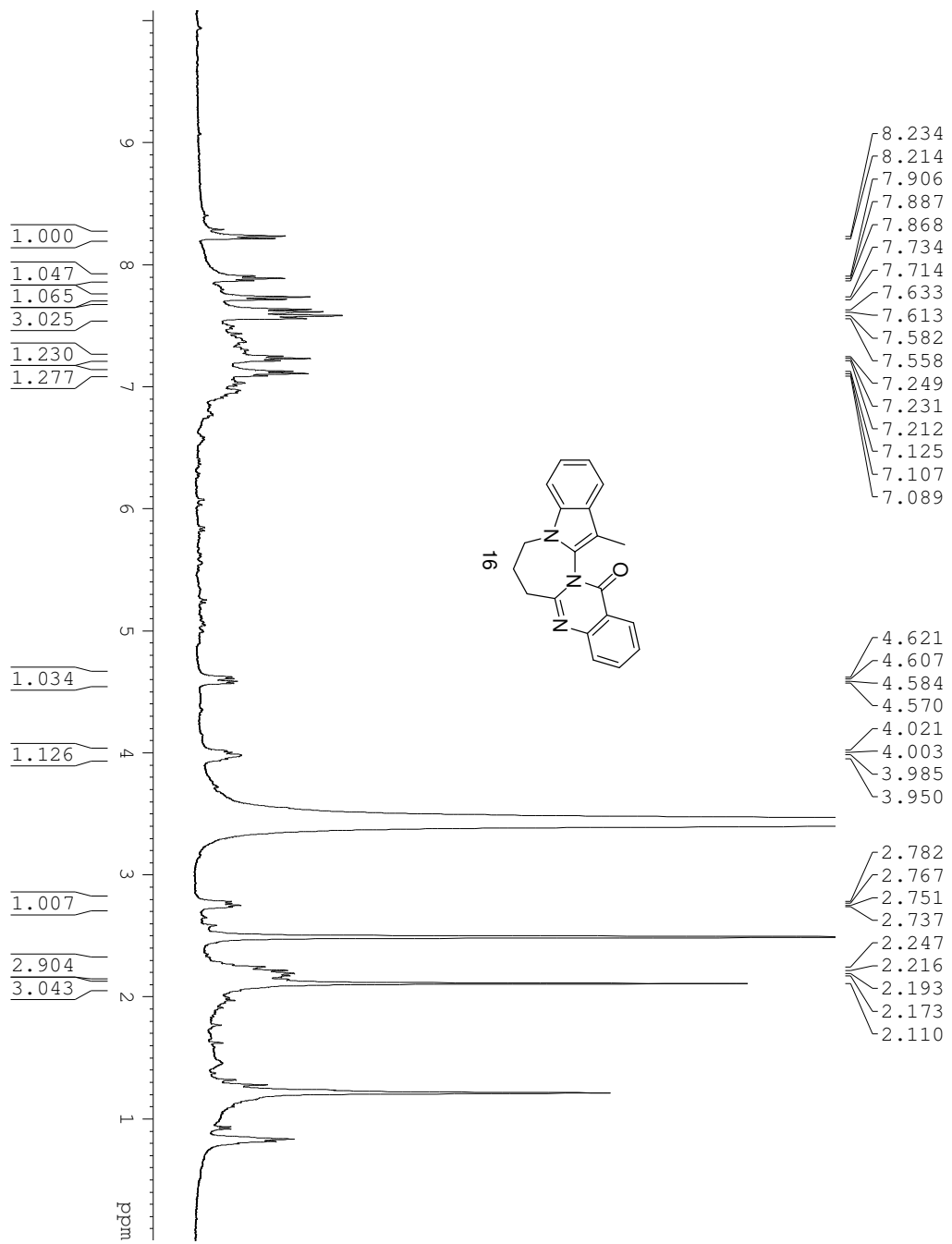
Acquisition Date 7/23/2013 12:27:45 PM

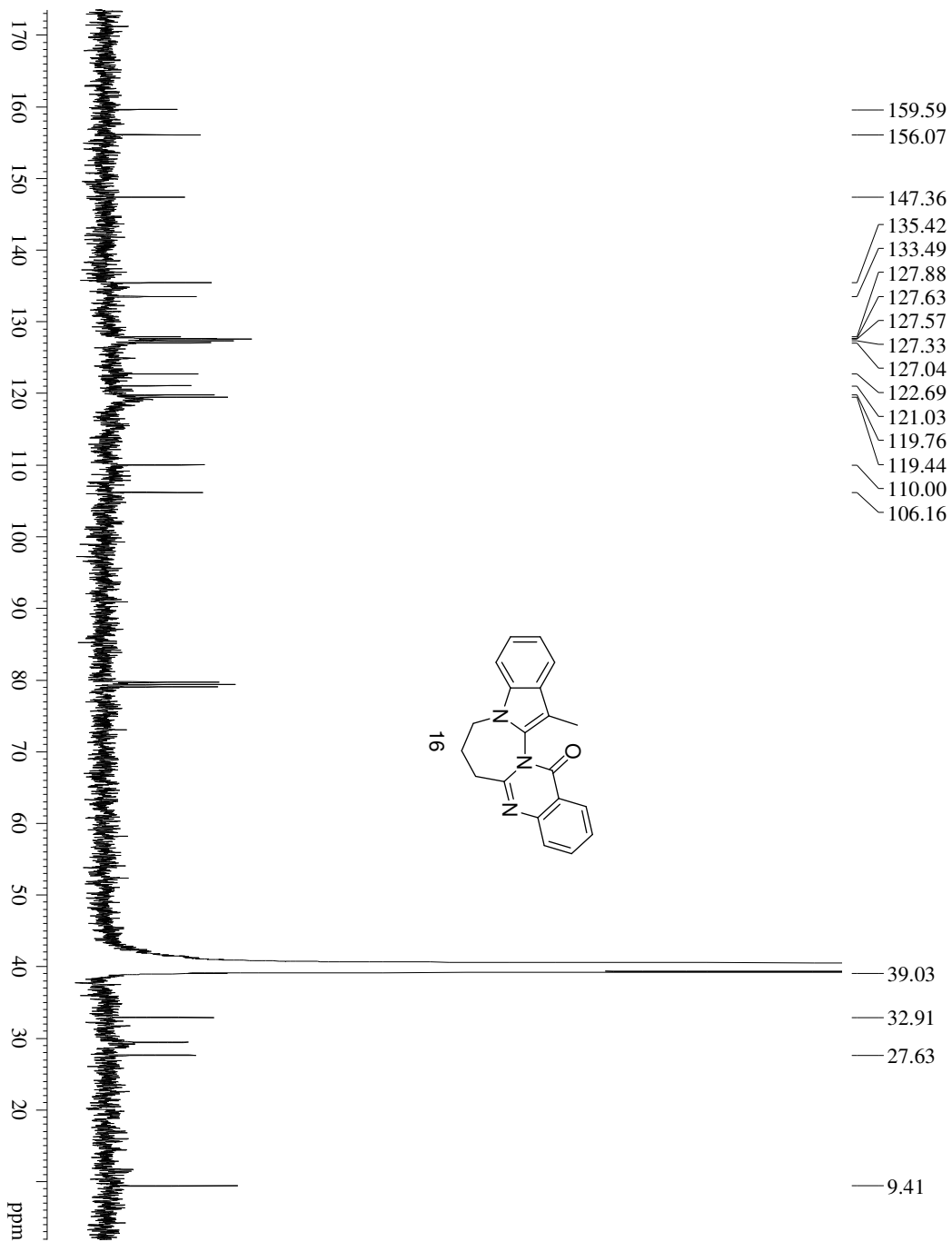
Operator Ramu Sridhar
Instrument maXis 10138

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







BRUKER MAXIS HRMS REPORT

School of Chemistry
University of Hyderabad

Analysis Info

Analysis Name D:\Data\2013\Dr.NAGARAJAN\AUG\SKG-265.d
Method tune_low_Pos.m
Sample Name SKG-265-DCM-MEOH
Comment

Acquisition Date 8/12/2013 12:50:19 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 3800 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste

