

Friedel-Crafts Alkylations of Electron-rich Aromatics with 3-Hydroxy-2-oxindoles: Scopes and Limitations[†]

Lakshmana K. Kinthada, Santanu Ghosh, K. Naresh Babu, Mohd. Sharique, Soumava Biswas, and Alakesh Bisai*

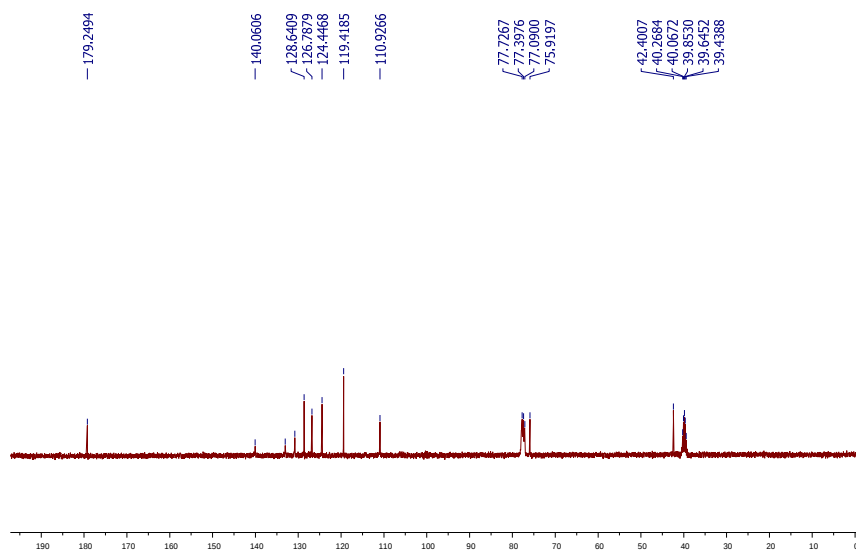
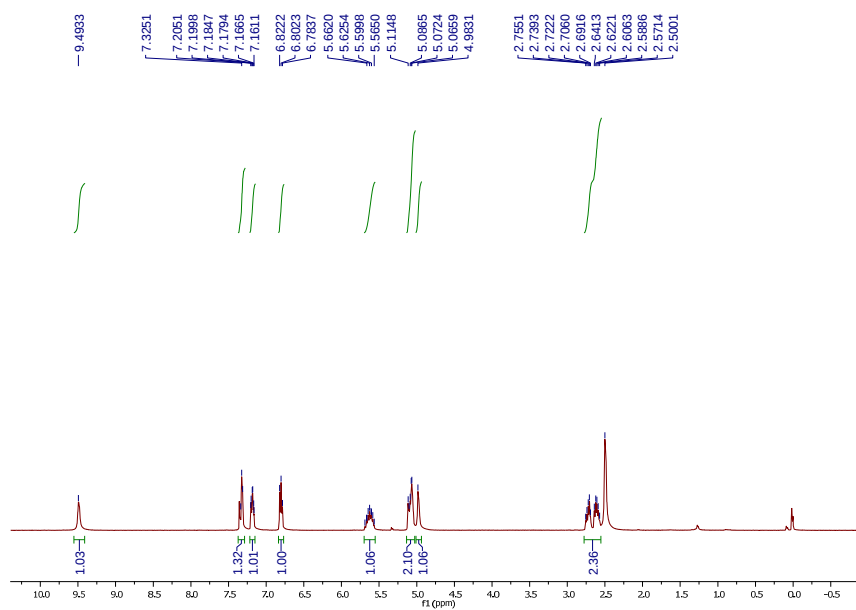
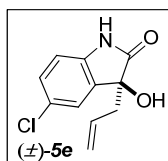
Department of Chemistry, Indian Institute of Science Education and Research Bhopal, Bhopal, M.P.-462 066, India.

Corresponding author: alakesh@iiserb.ac.in

Spectral Graphics and HRMS data

S2-S117

Spectral graphic



Display Report

Analysis Info

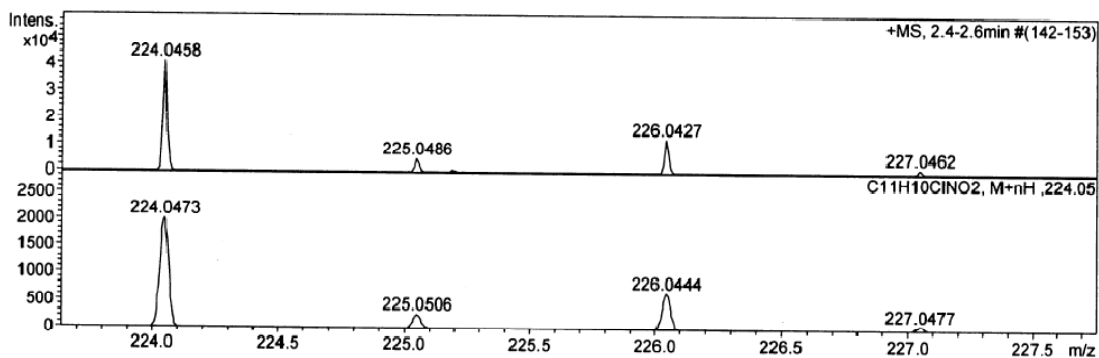
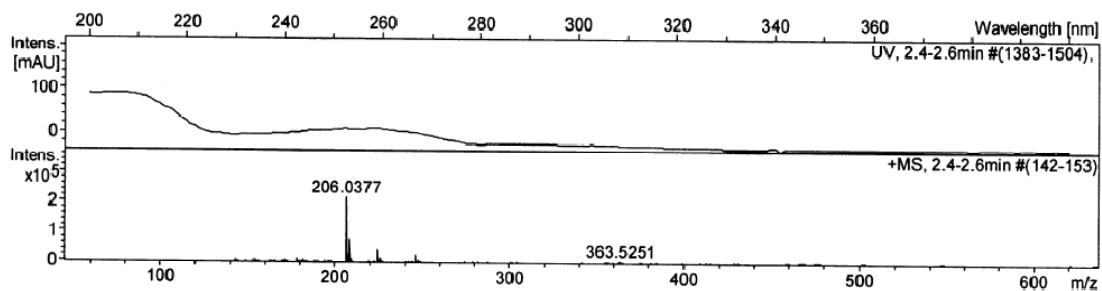
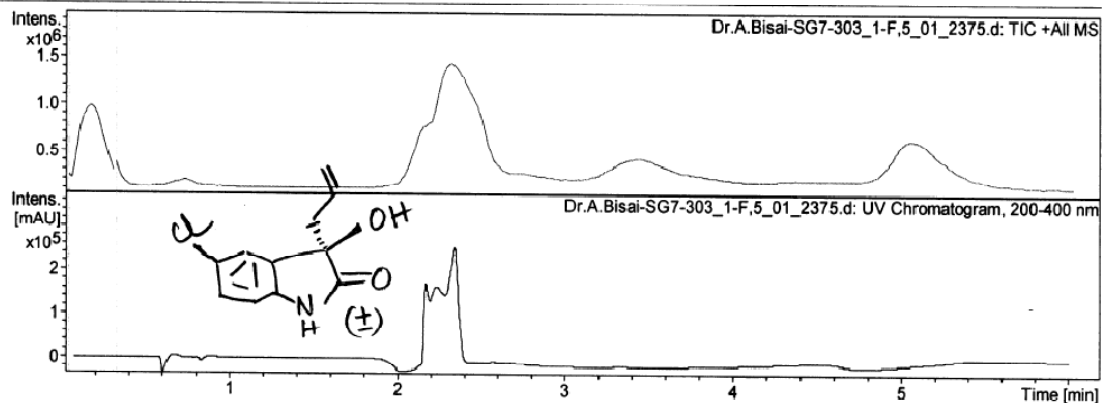
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Method HRLCMS-20 Sept.m
Sample Name Dr.A.Bisai-SG7-303
Comment

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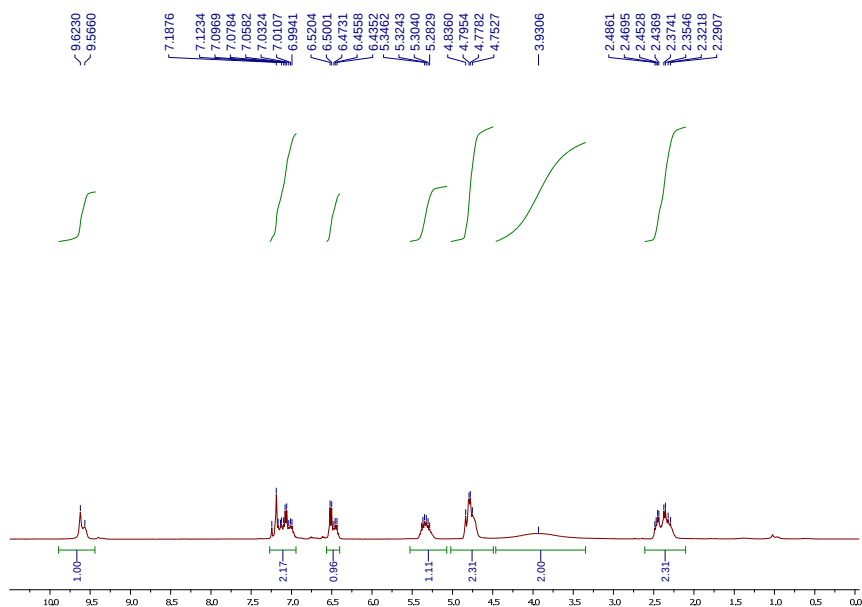
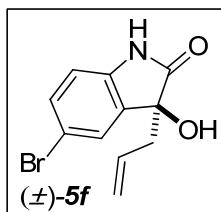
Operator Amit
Instrument micrOTOF-Q II 10330

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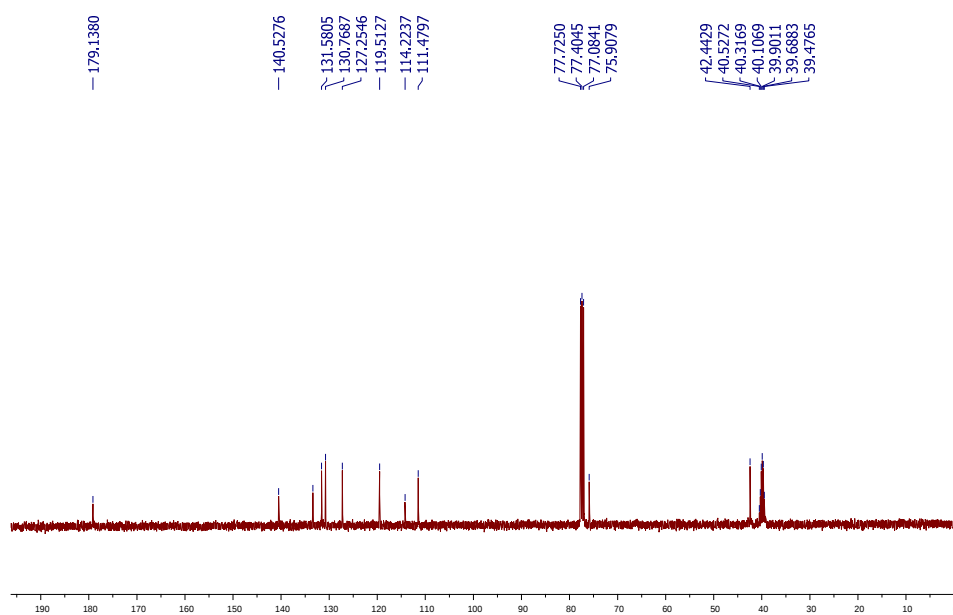
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-5e



^1H NMR (400 MHz, 0.4 mL CDCl_3 , 0.1 mL DMSO-D_6) of compound (±)-5f



^{13}C NMR (100 MHz, 0.4 mL CDCl_3 , 0.1 mL DMSO-D_6) of compound (±)-5f

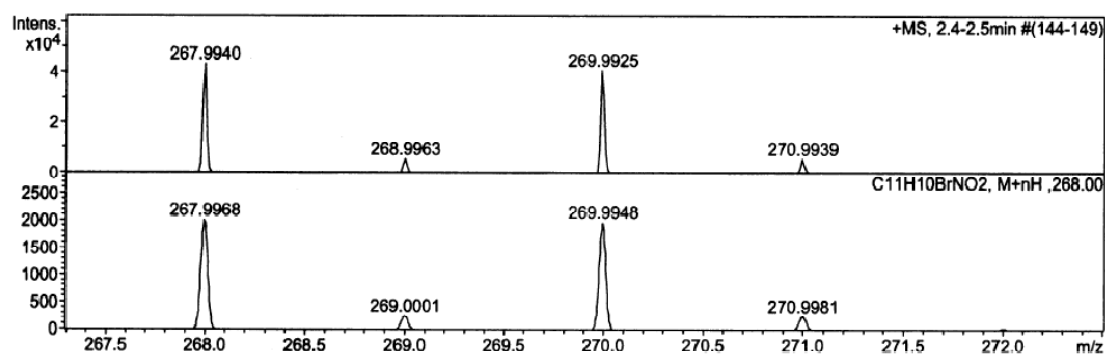
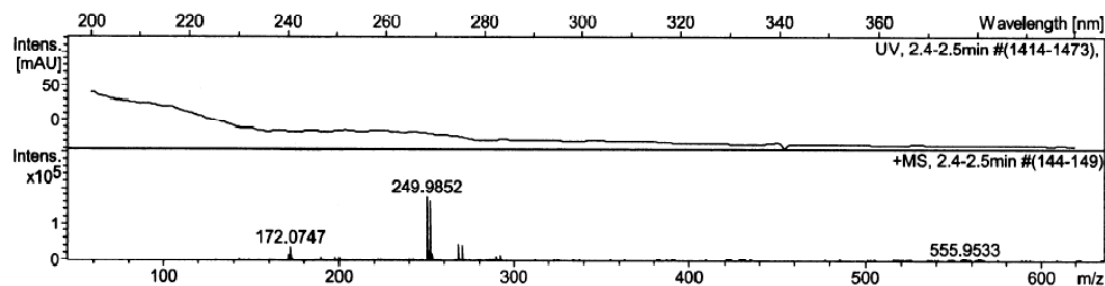
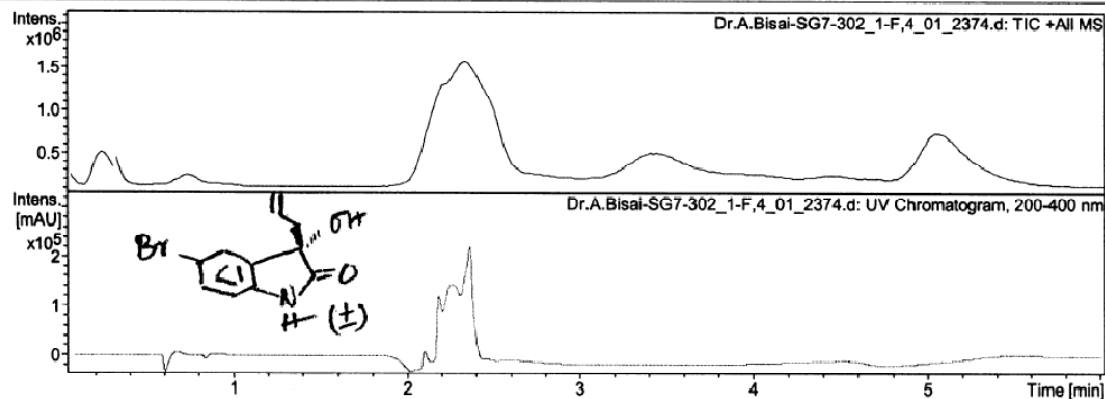
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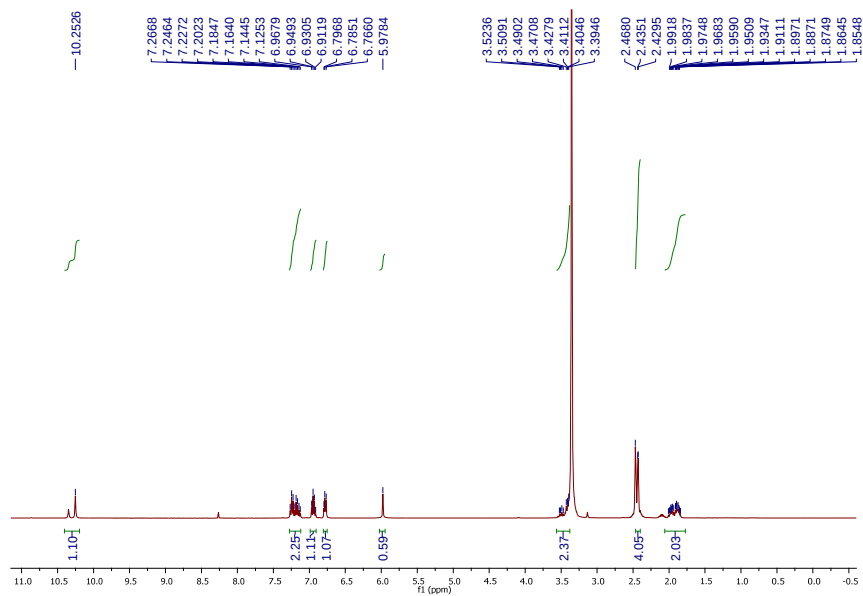
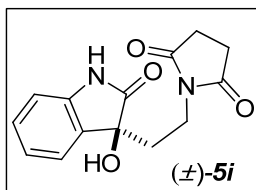
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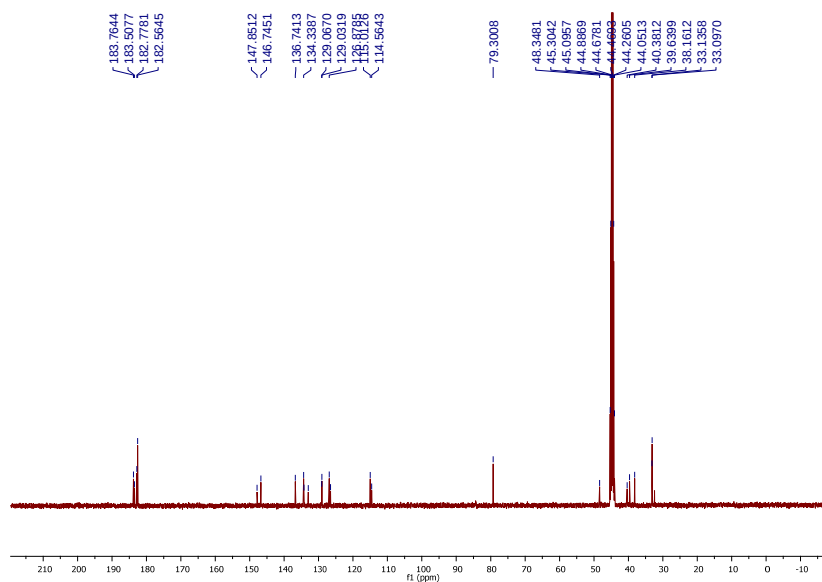
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		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-5f



¹H NMR (400 MHz, DMSO-d₆) of compound (±)-**5i**



¹³C NMR (100 MHz, DMSO-D₆) of compound (±)-**5i**

Display Report

Analysis Info

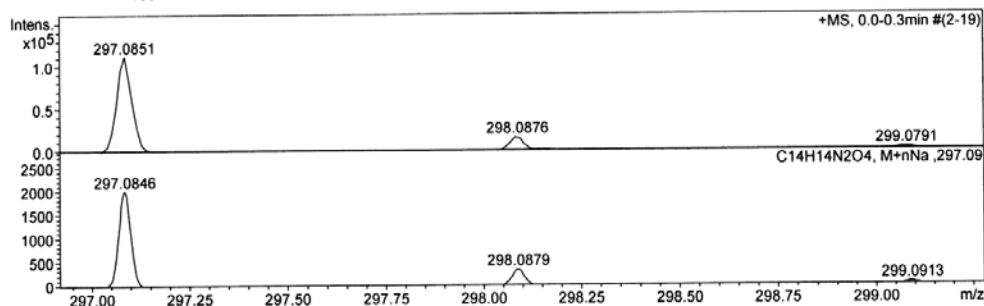
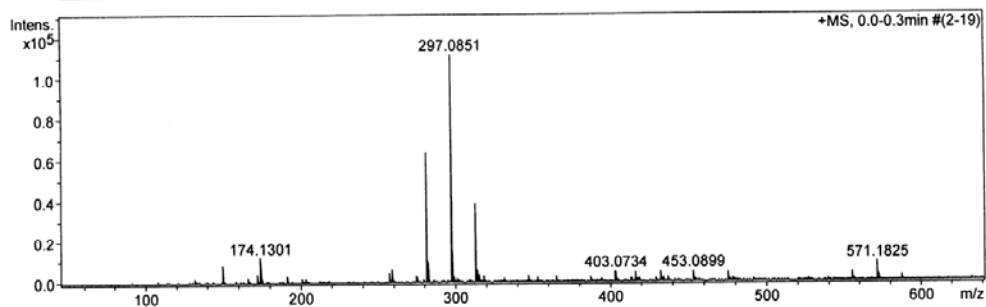
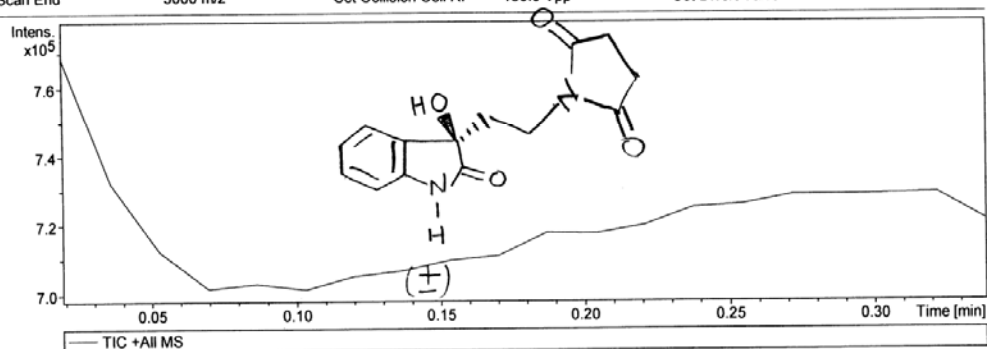
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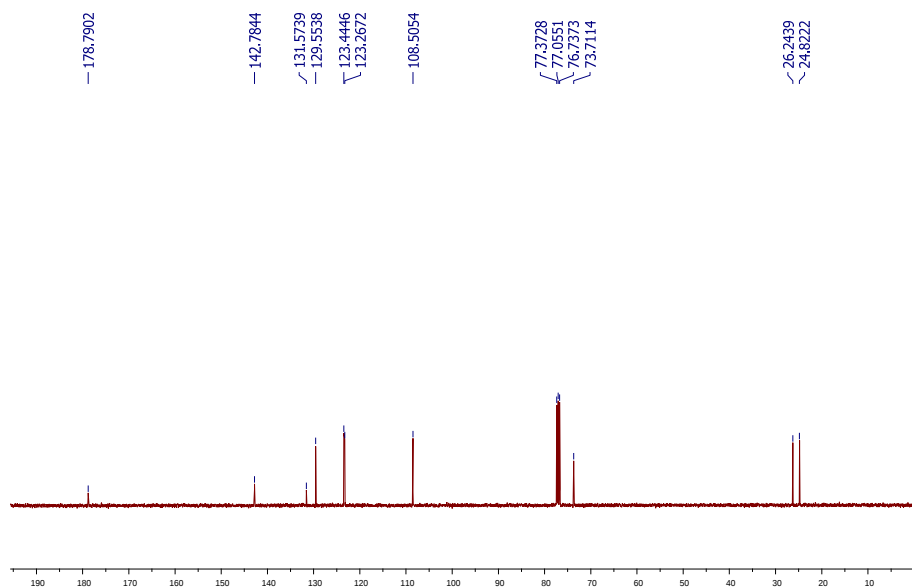
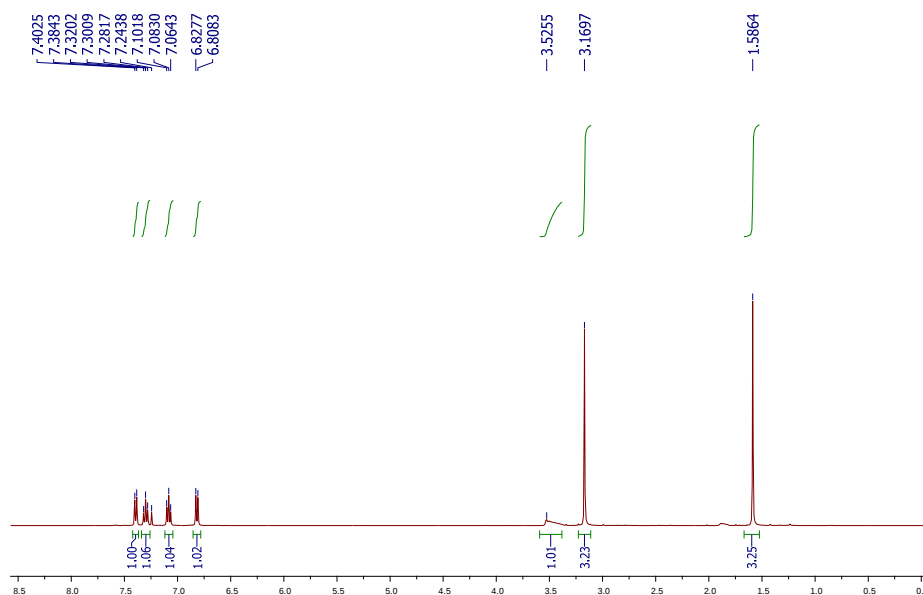
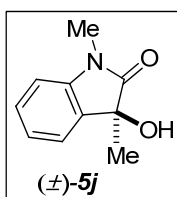
Operator Amit
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-5i



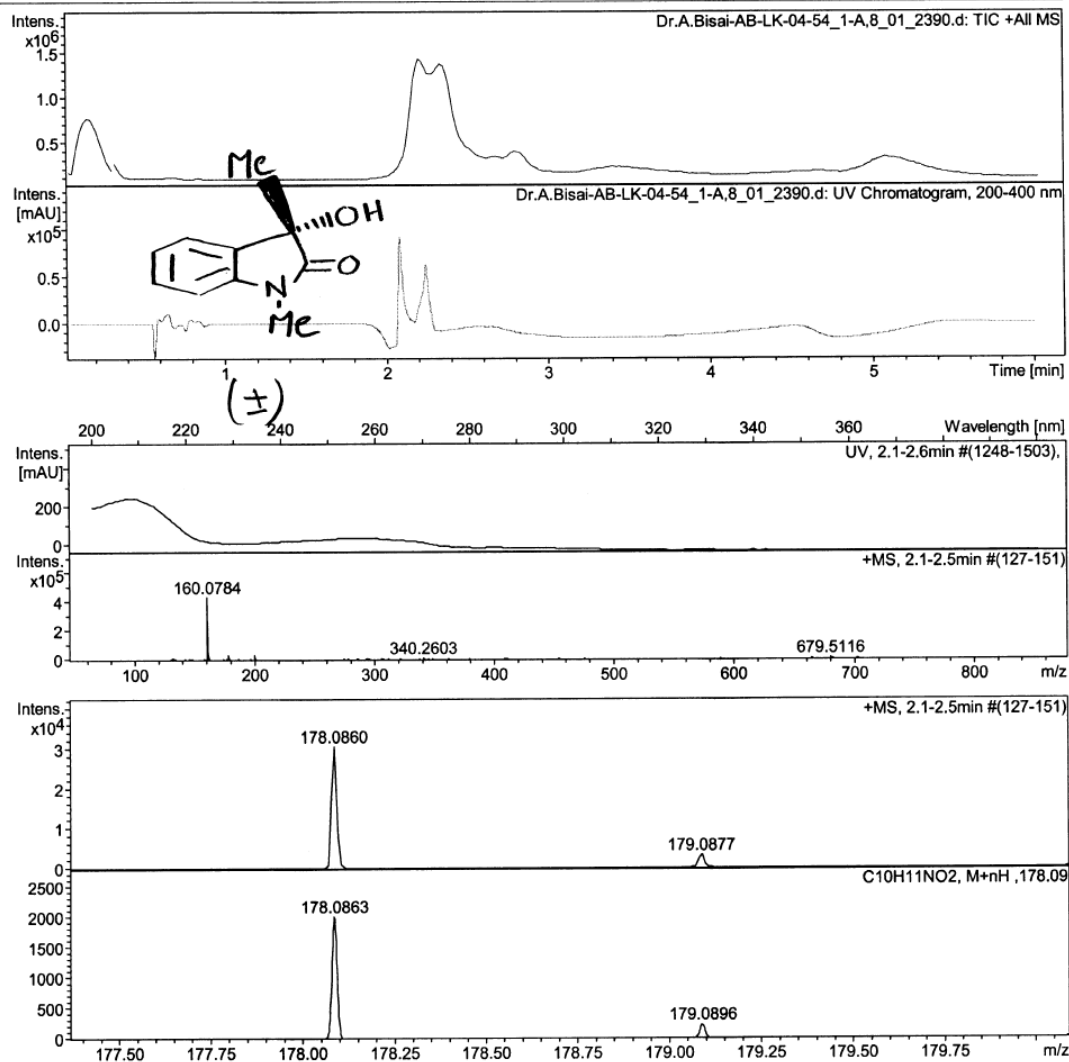
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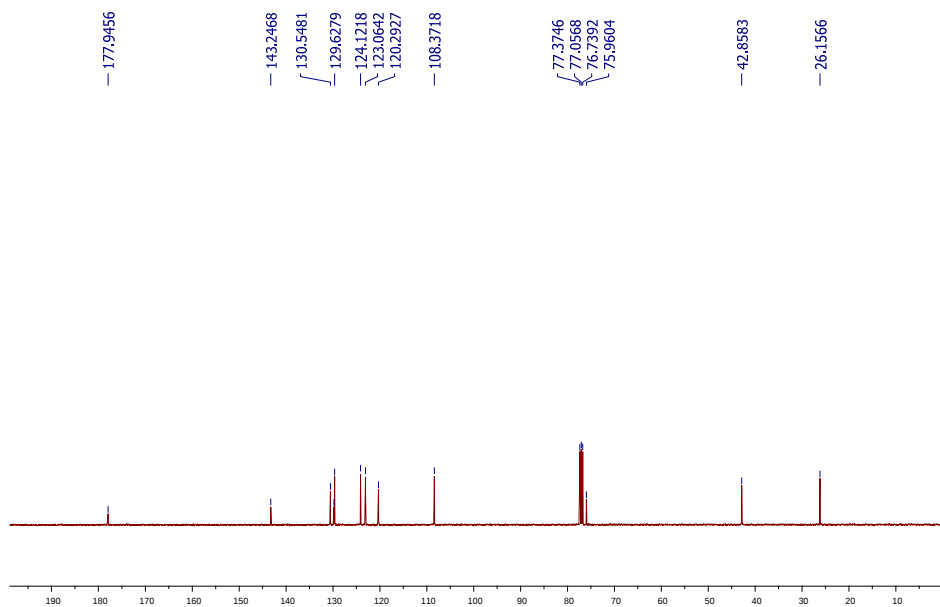
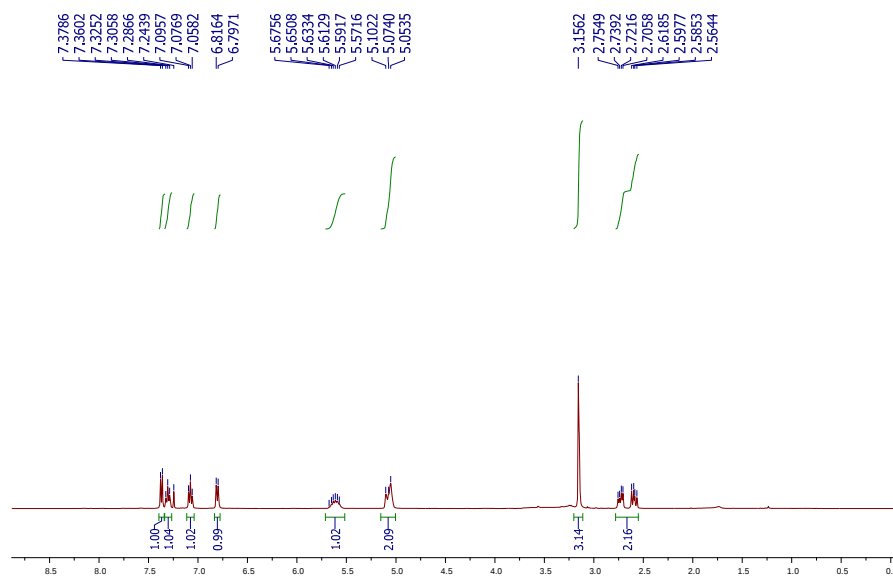
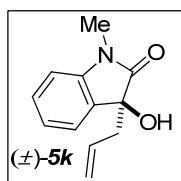
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Comment			

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
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		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-5j



Display Report

Analysis Info

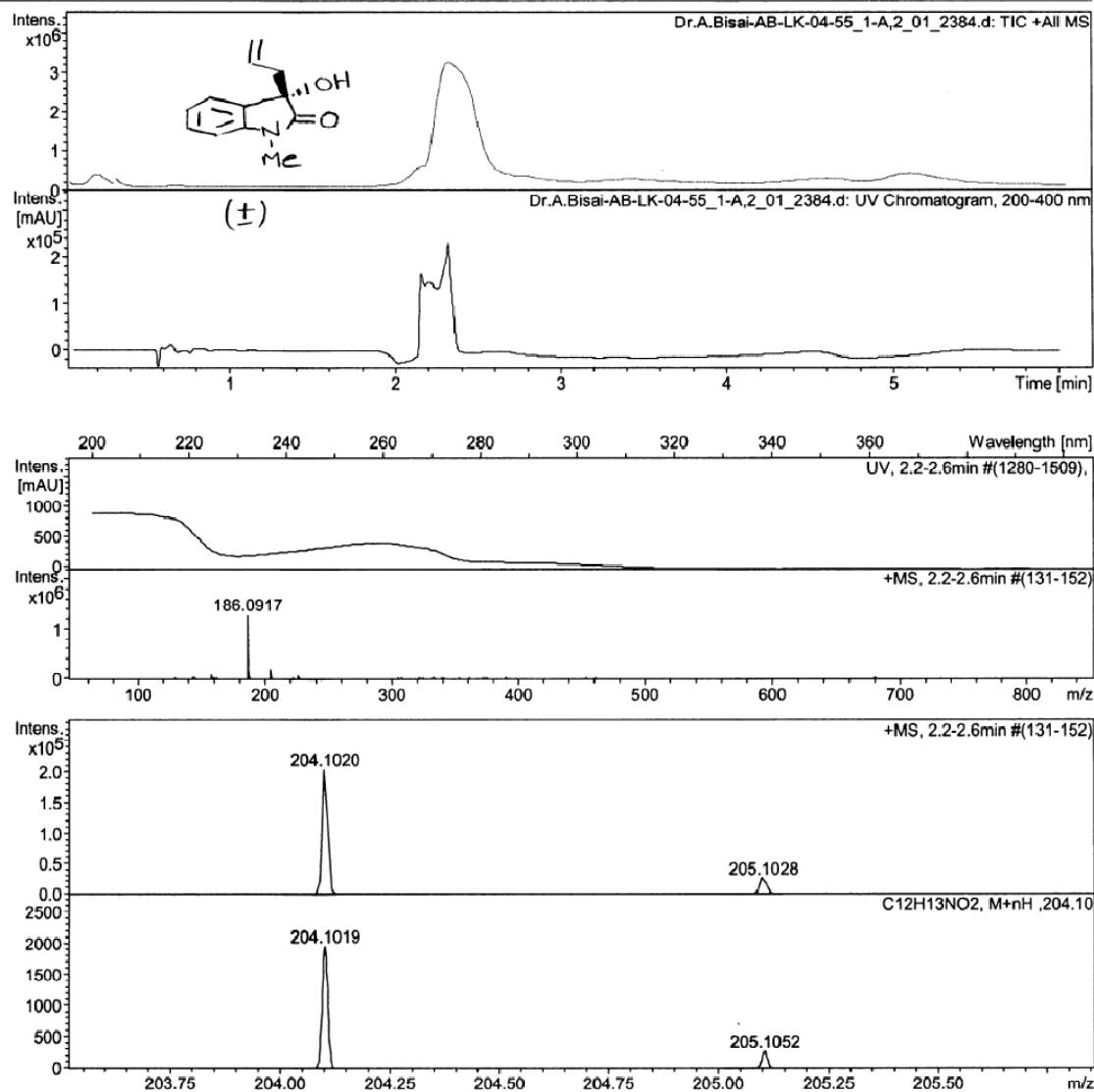
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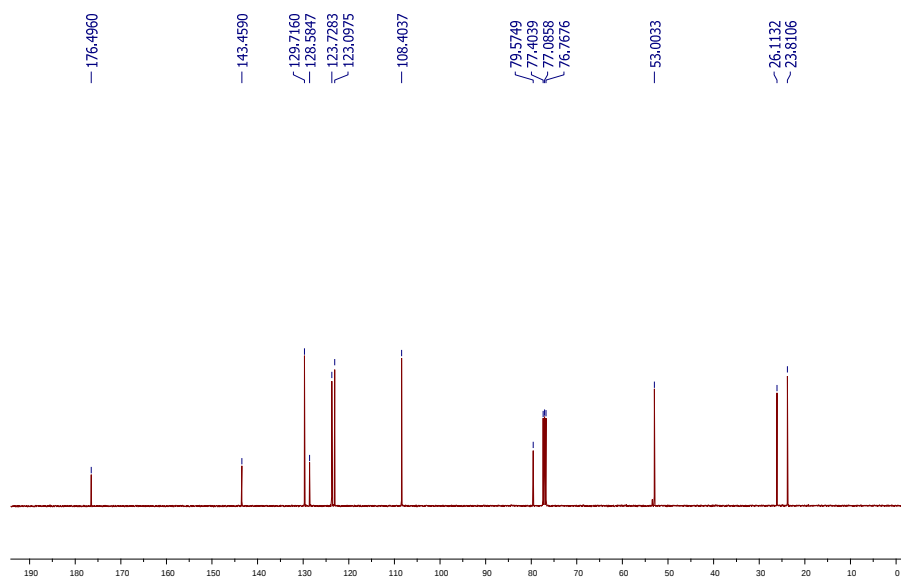
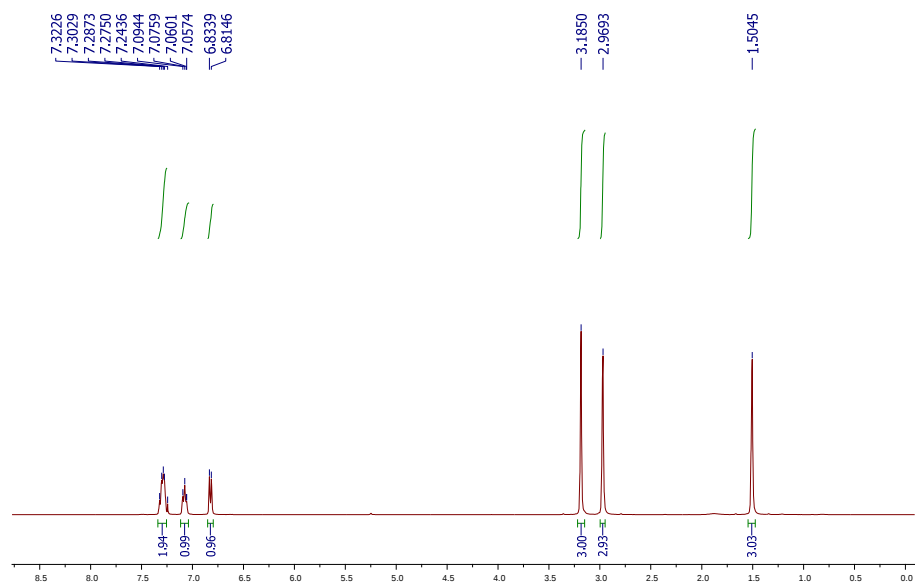
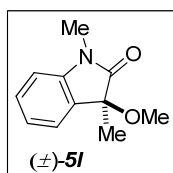
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Scanned copy of mass spectrum of ($\pm$)-5k



Display Report

Analysis Info

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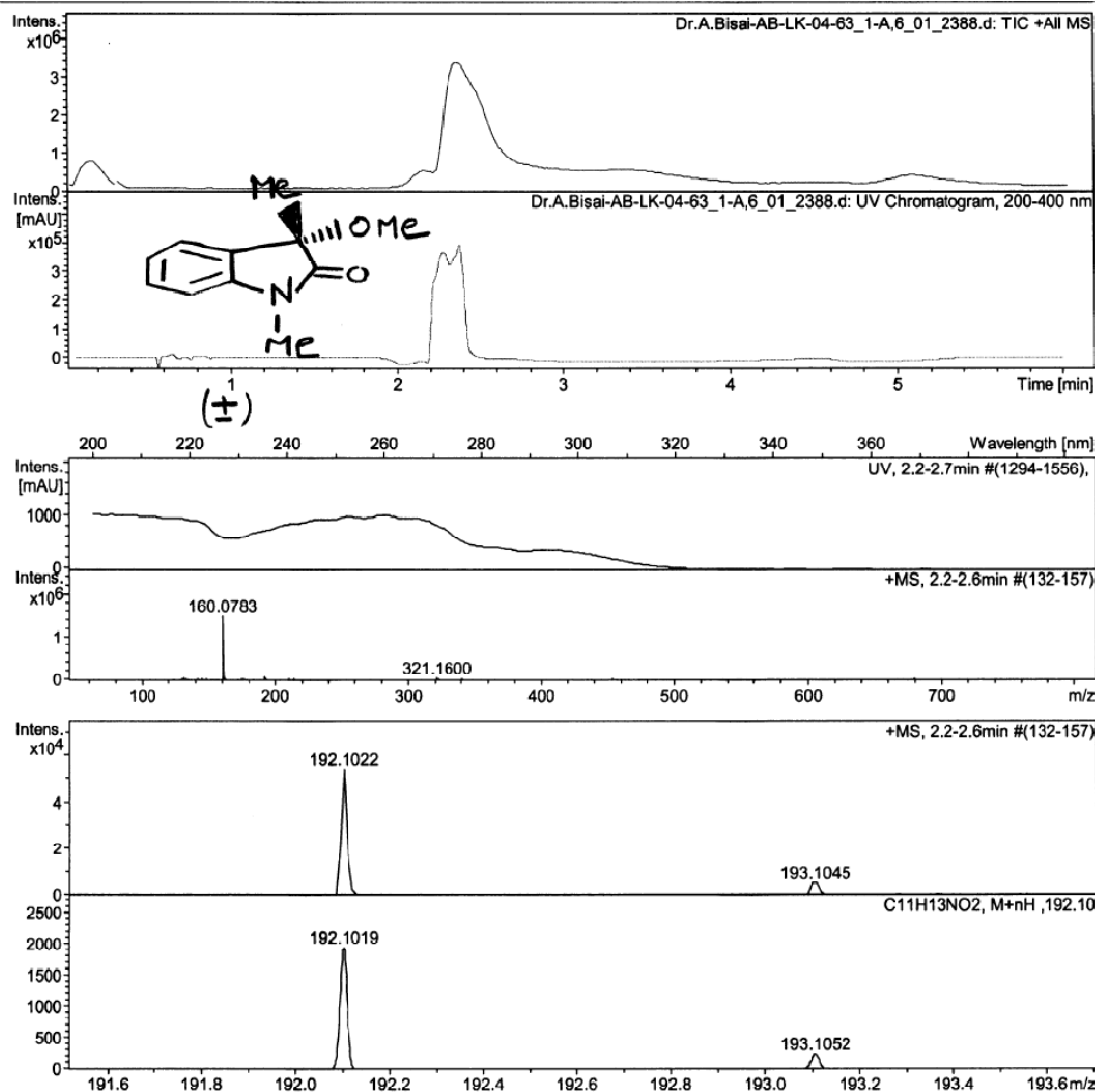
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Operator: Amit

Instrument: micrOTOF-Q II 10330

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

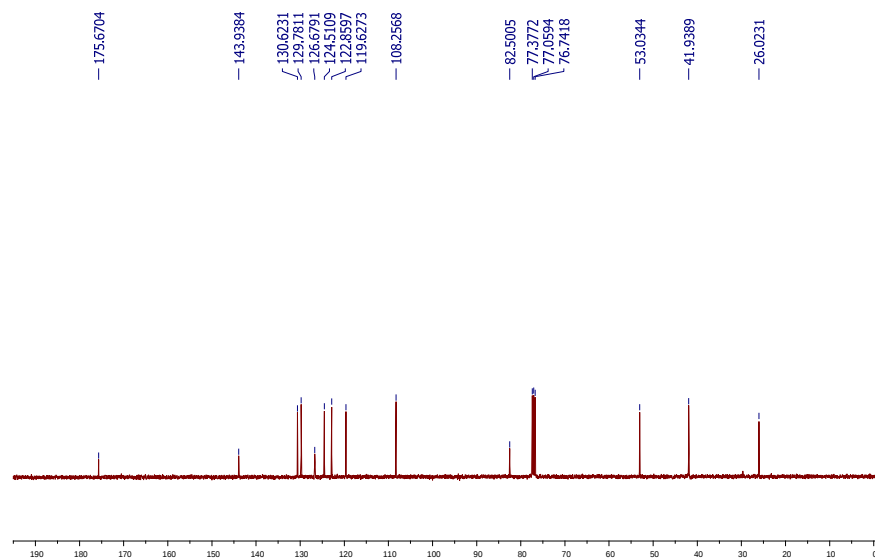
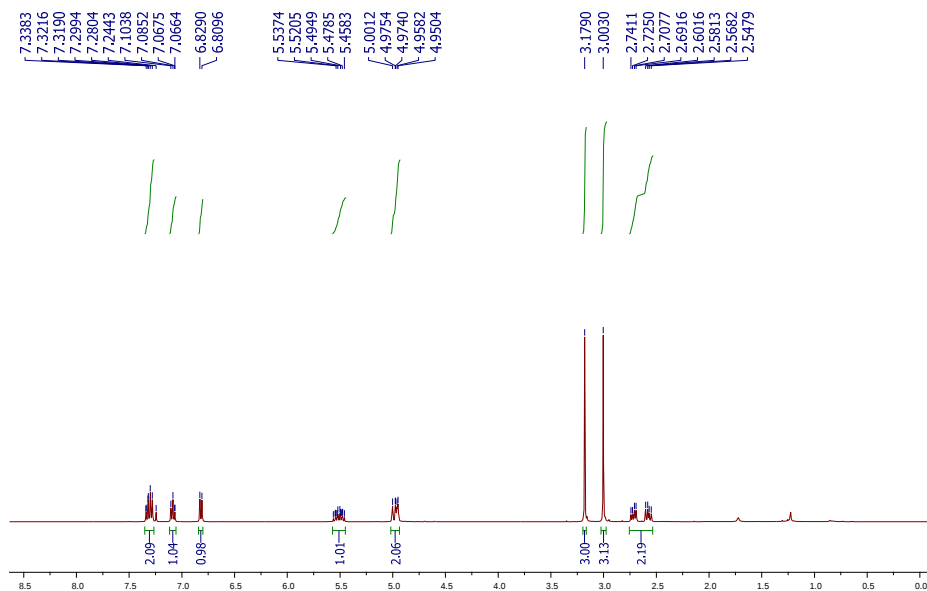
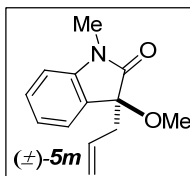


Bruker Compass DataAnalysis 4.0

printed: 4/29/2014 9:56:26 PM

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Scanned copy of mass spectrum of (±)-51



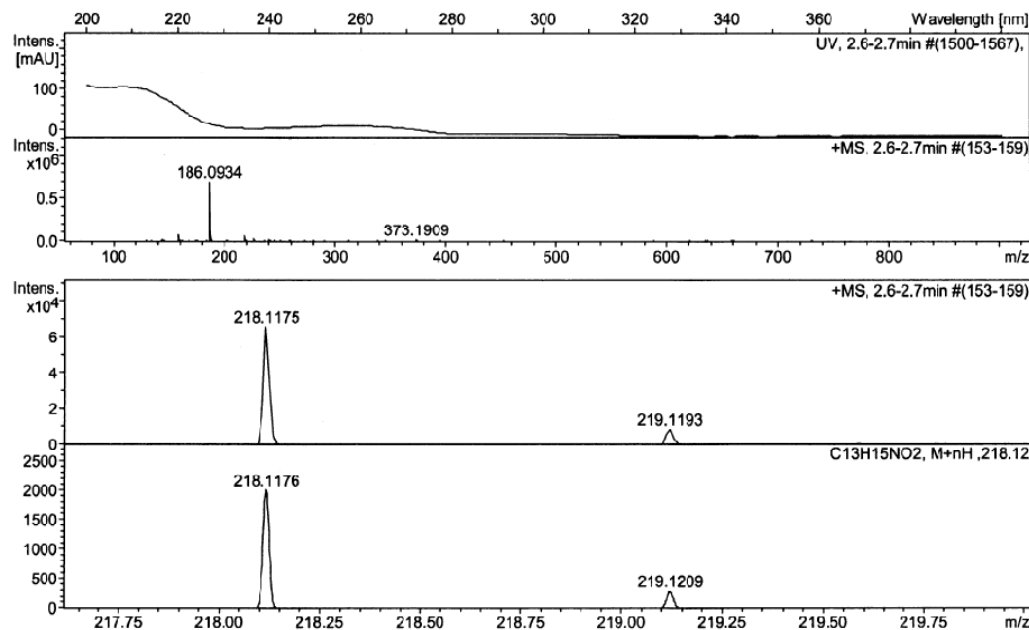
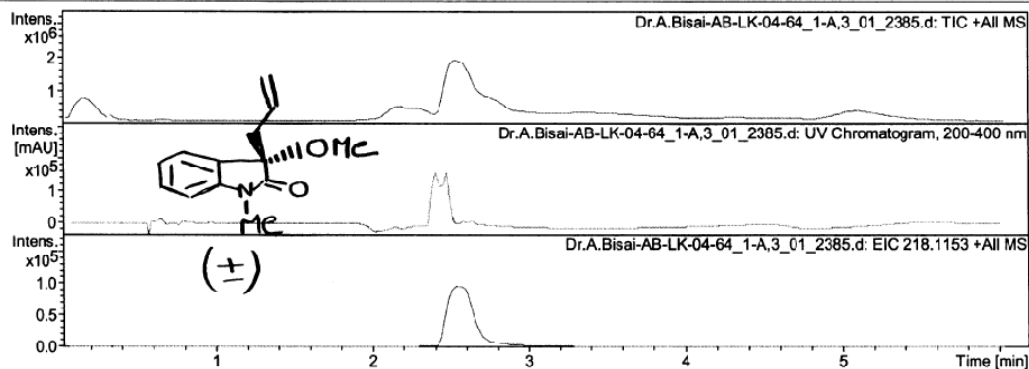
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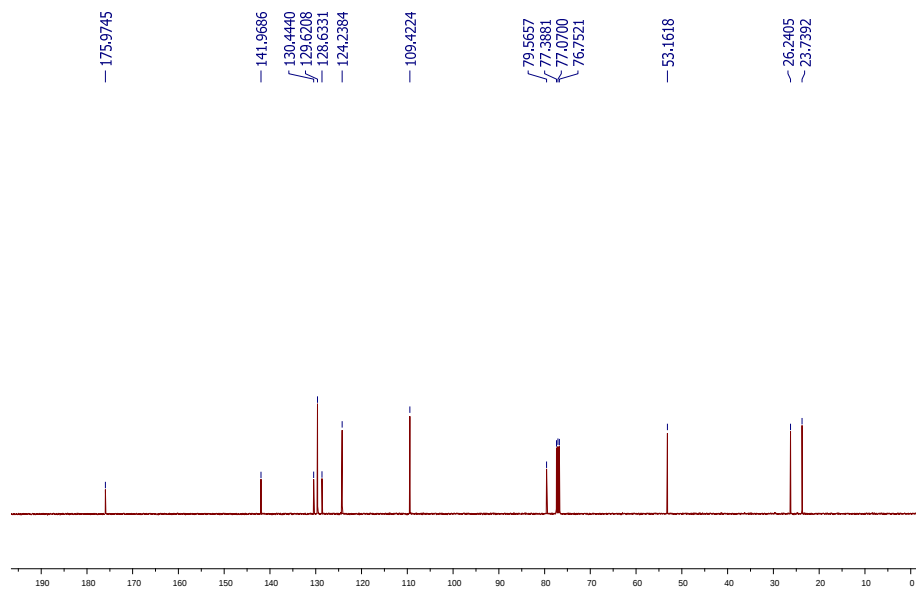
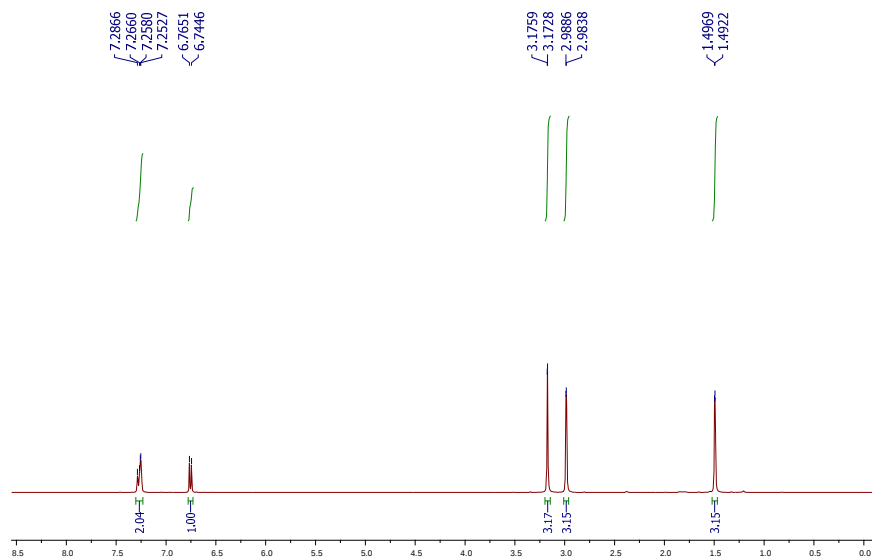
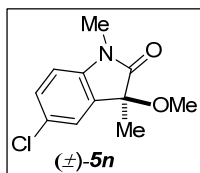
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Operator	Amit
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

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		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-5m



Display Report

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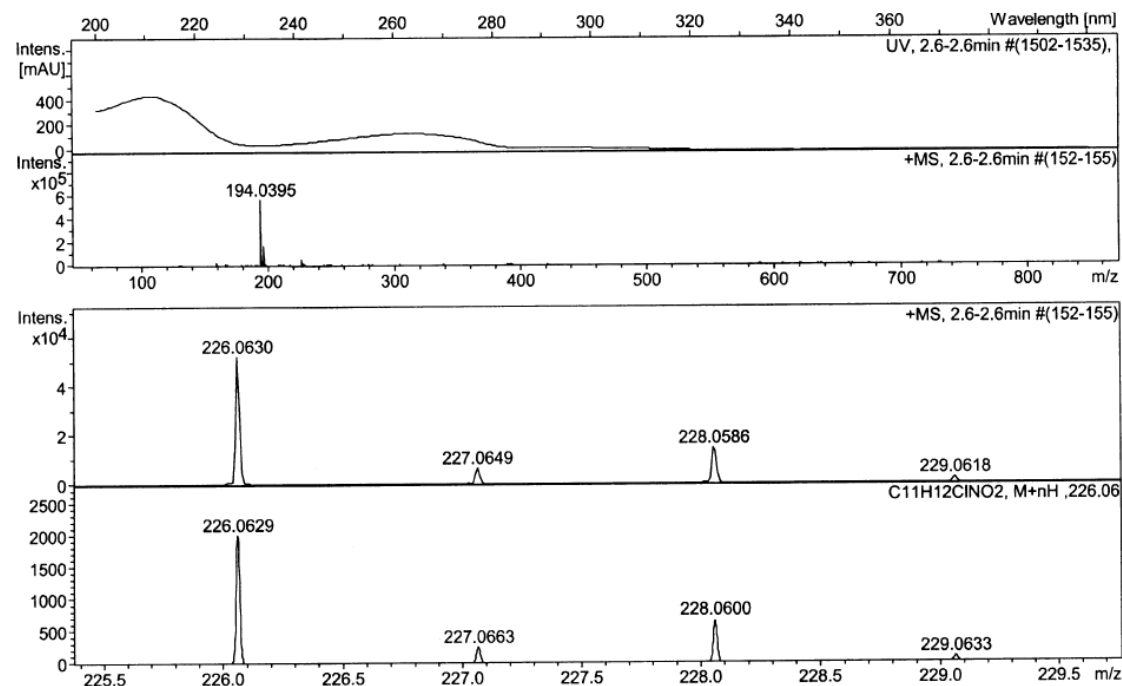
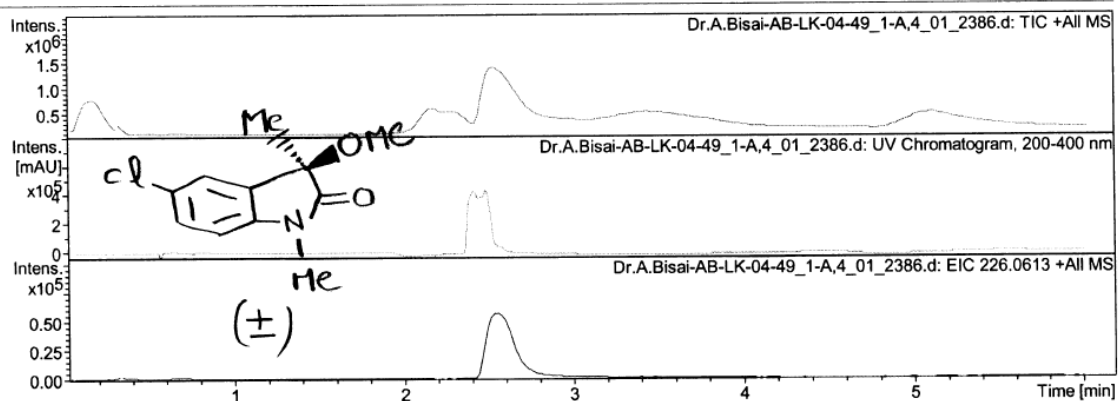
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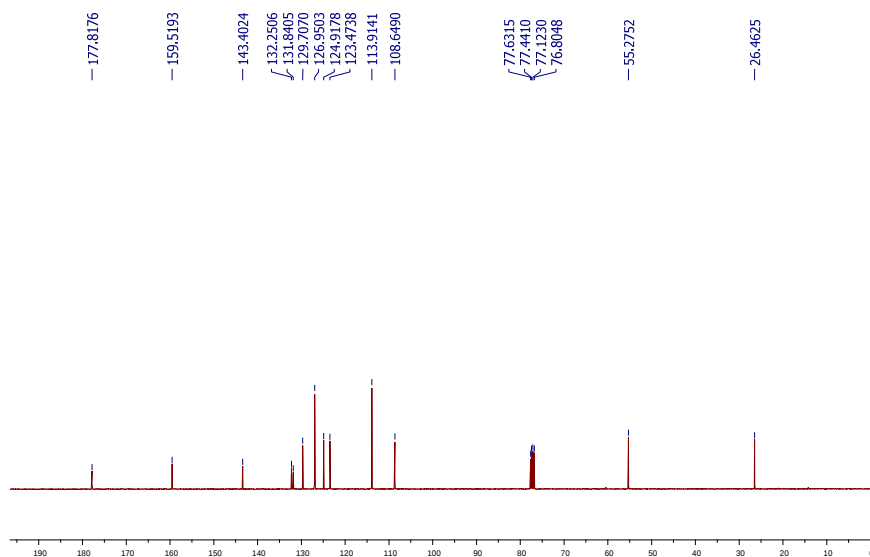
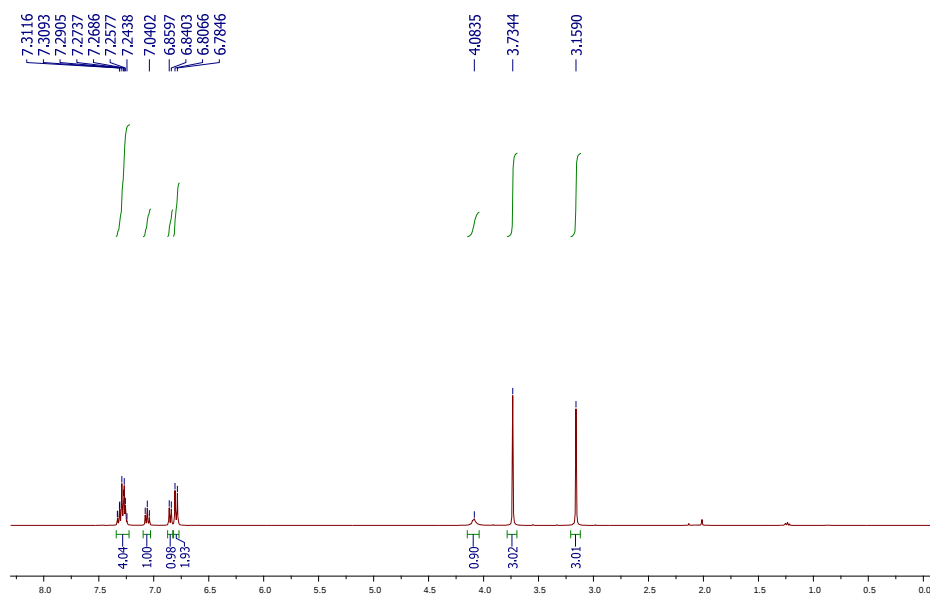
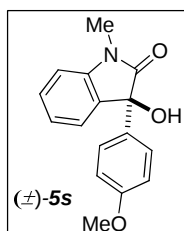
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Scanned copy of mass spectrum of (±)-5n



Display Report

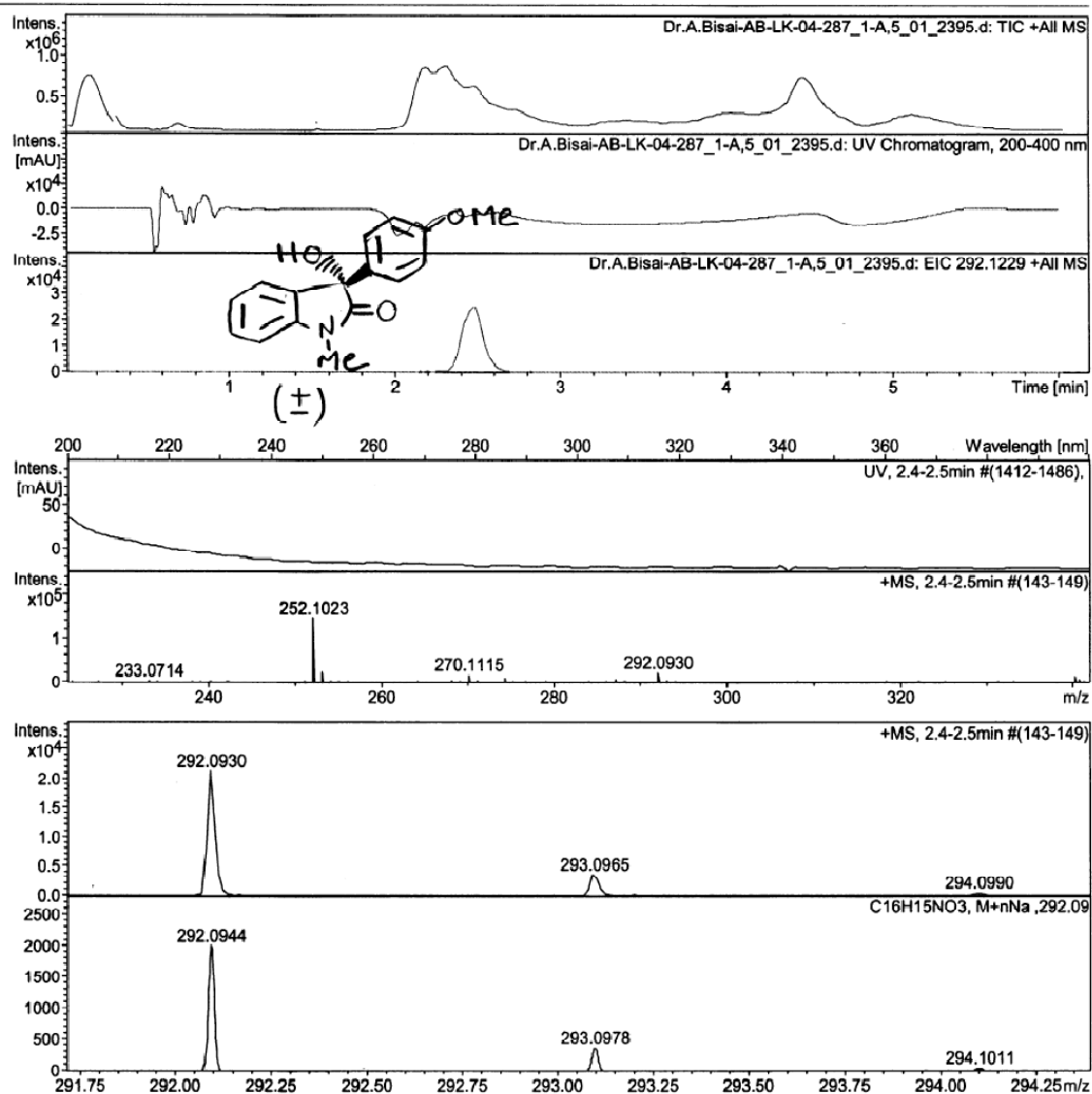
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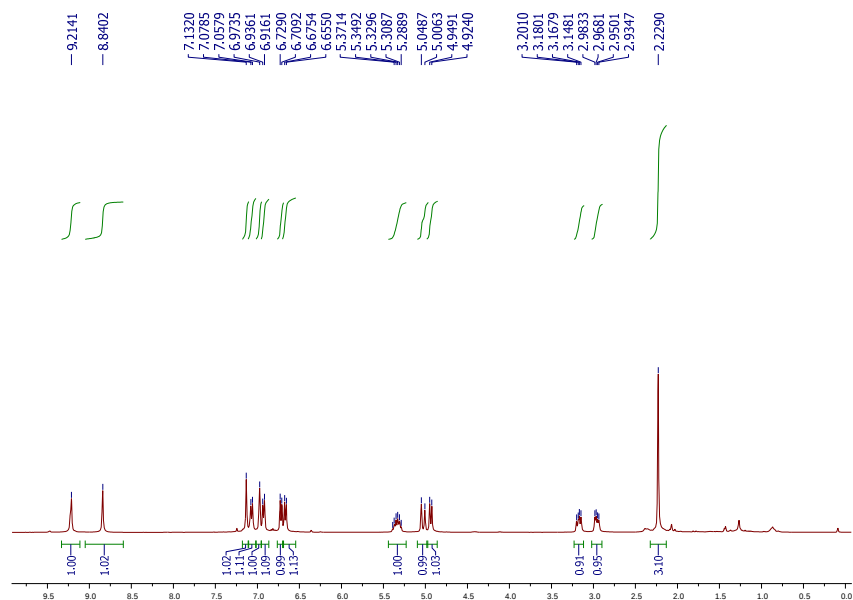
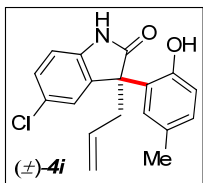
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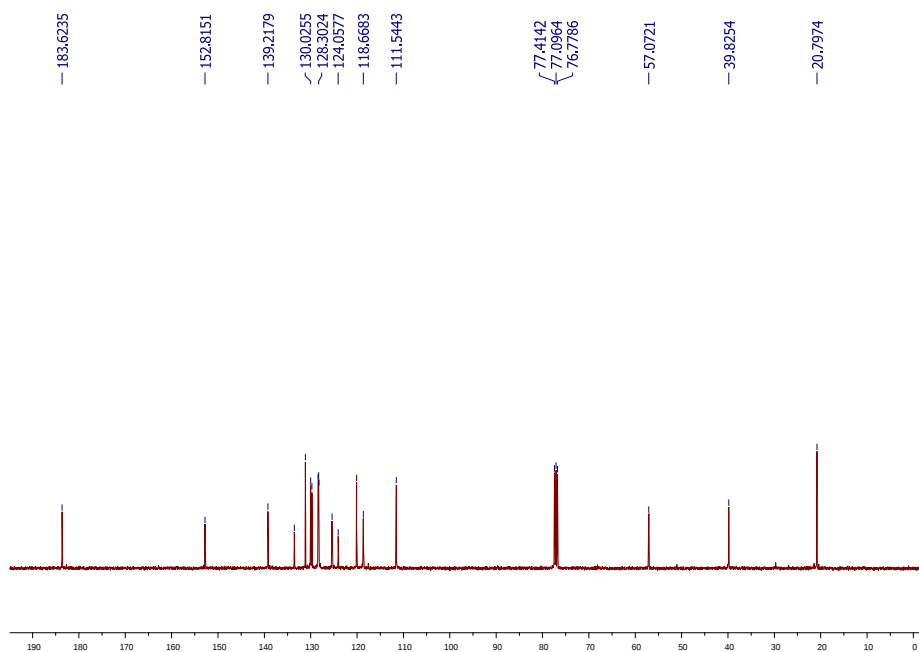
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Scanned copy of mass spectrum of (±)-5s



¹H NMR (400 MHz, CDCl₃) of compound (±)-4i



¹³C NMR (100 MHz, CDCl₃) of compound (±)-4i

Display Report

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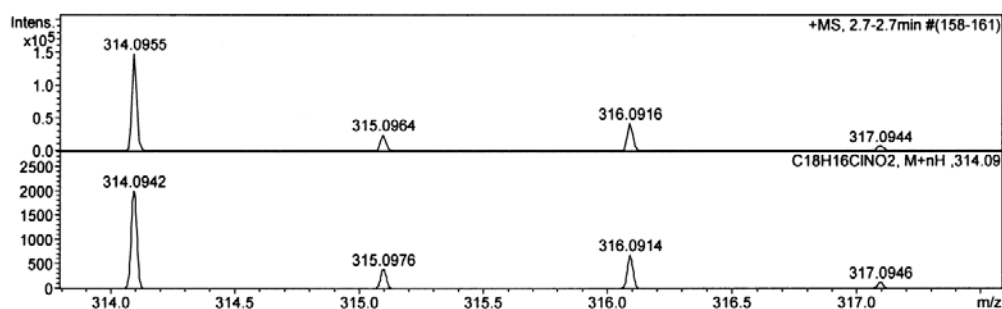
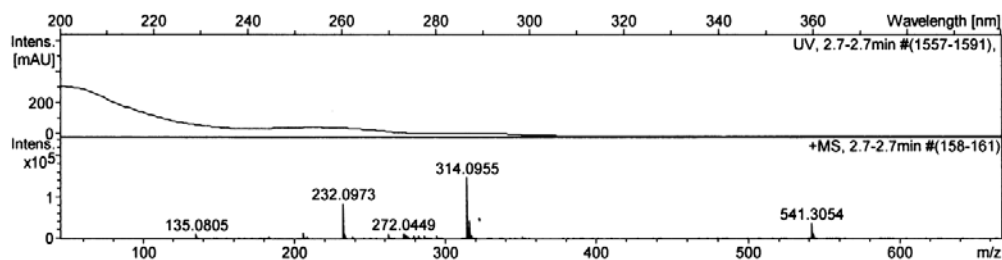
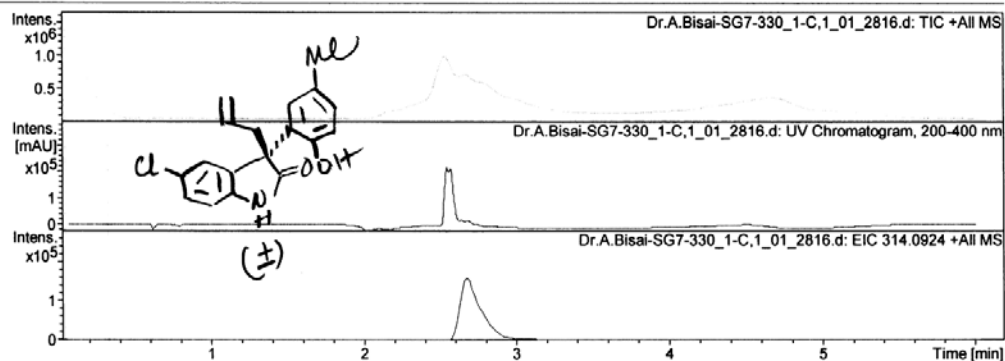
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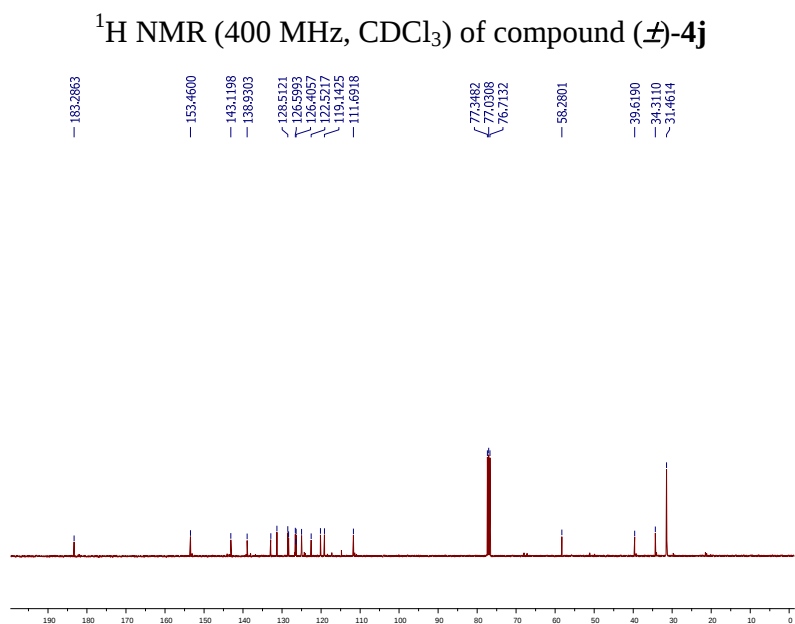
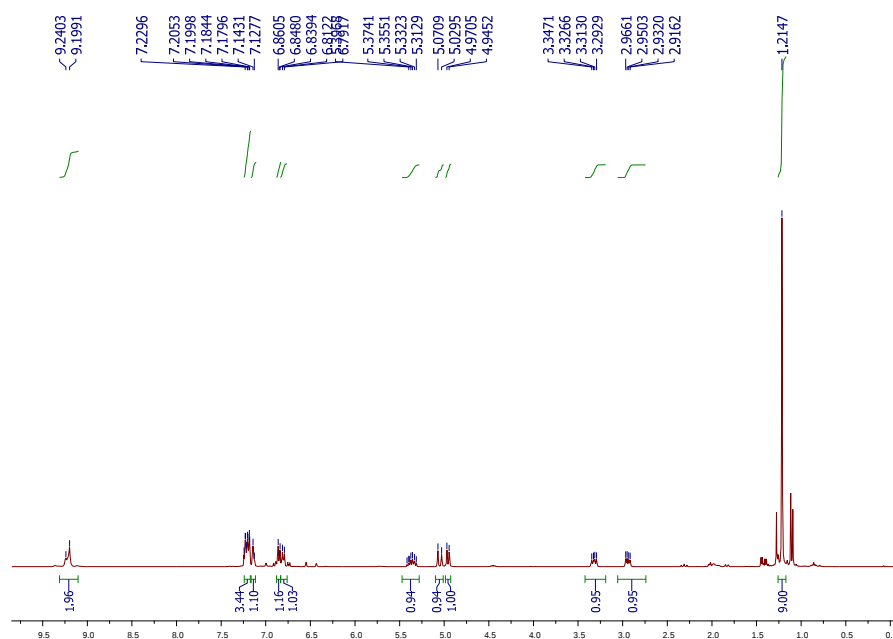
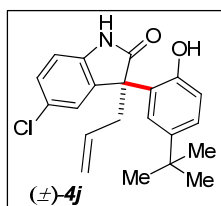
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Scanned copy of mass spectrum of (±)-4i



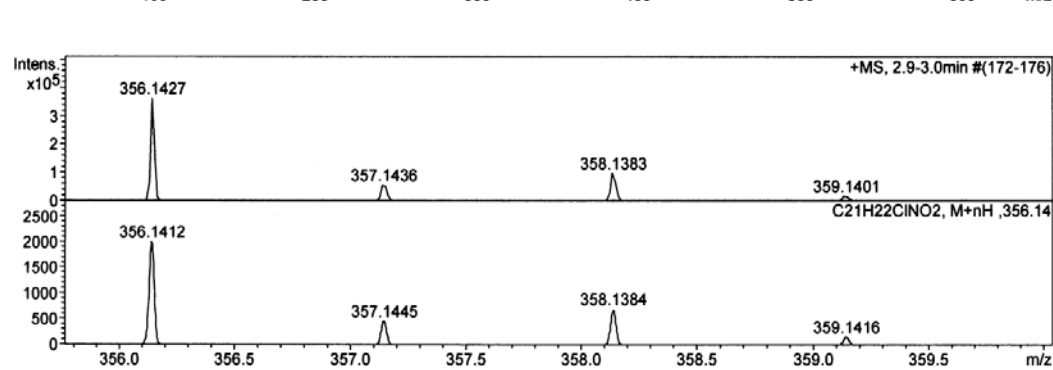
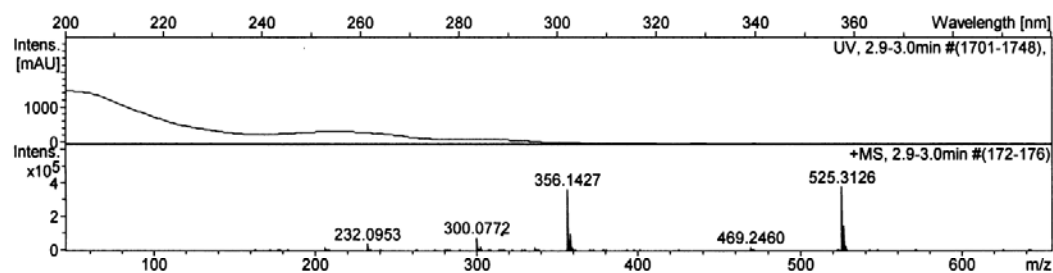
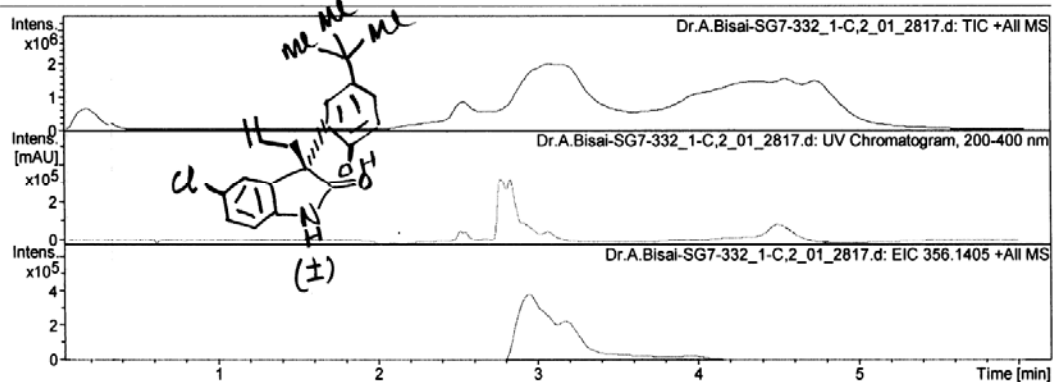
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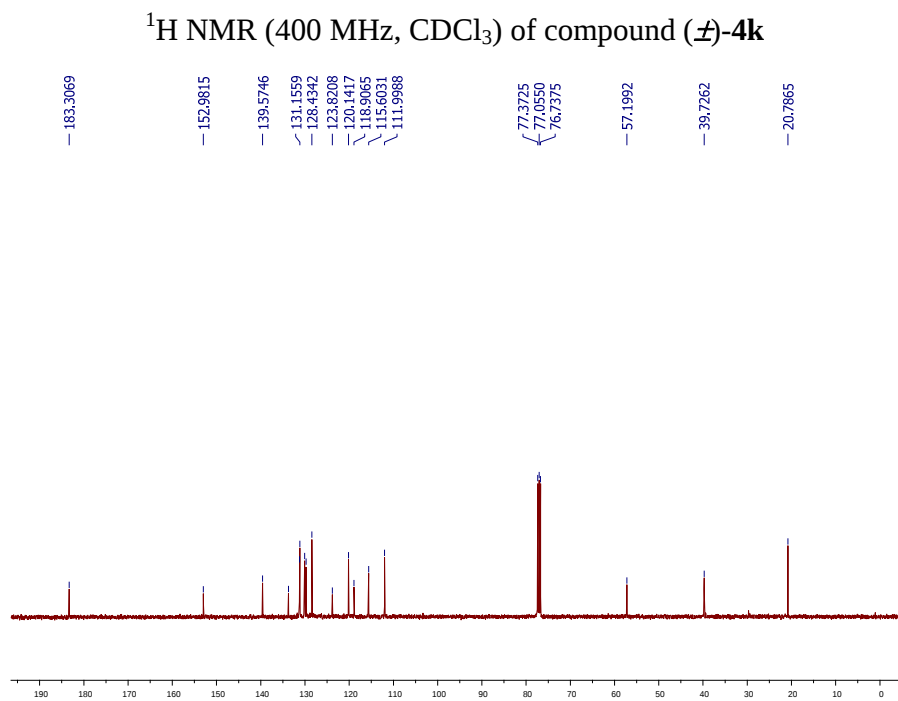
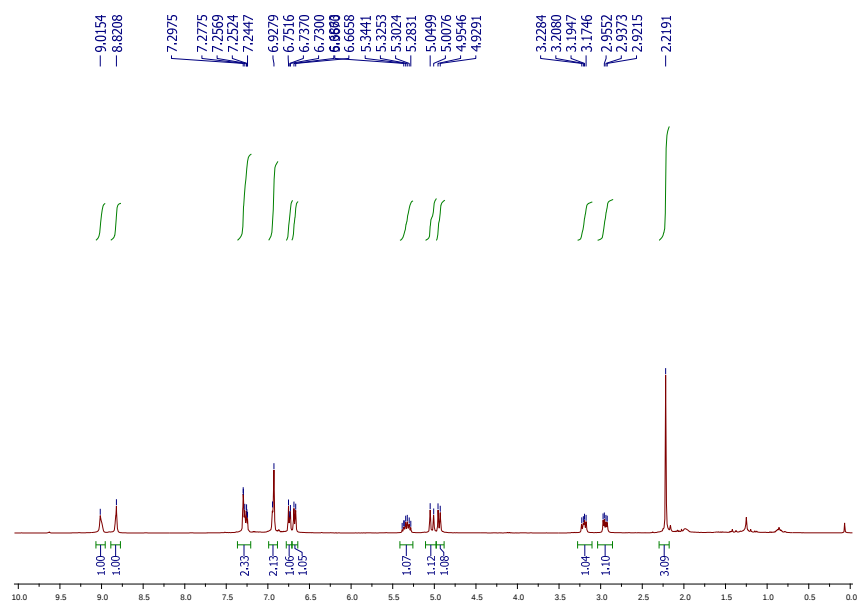
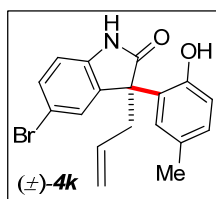
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Comment			

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		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-4j



Display Report

Analysis Info

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 Method HRLCMS-20 Sept.m
 Sample Name Dr.A.Bisai-SG7-324
 Comment

Acquisition Date 6/9/2014 3:11:38 AM

Operator

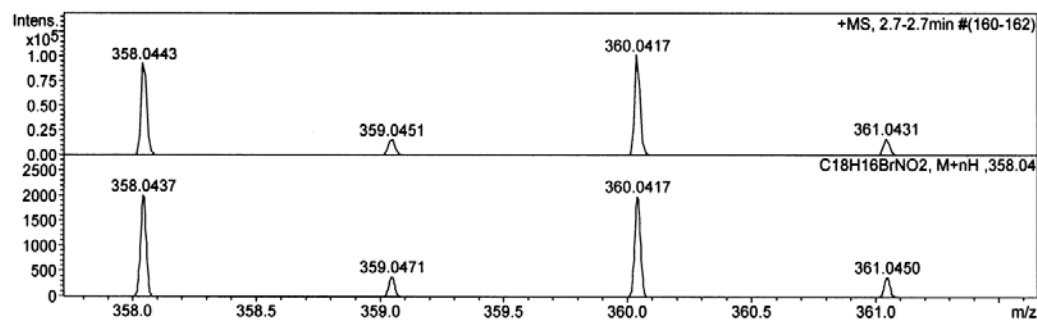
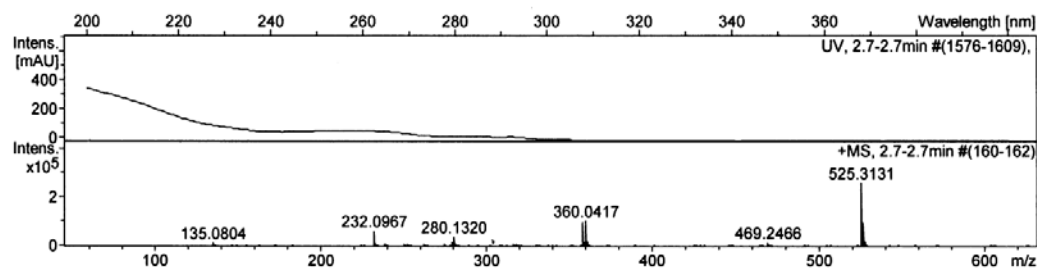
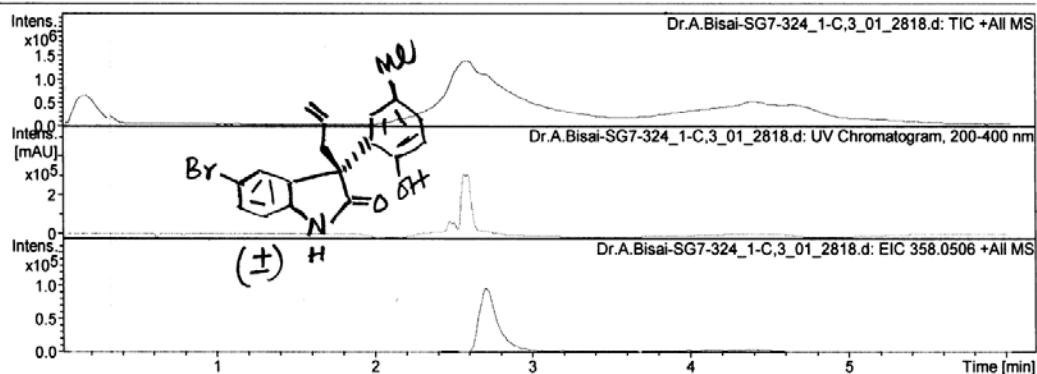
Ravindra

Instrument

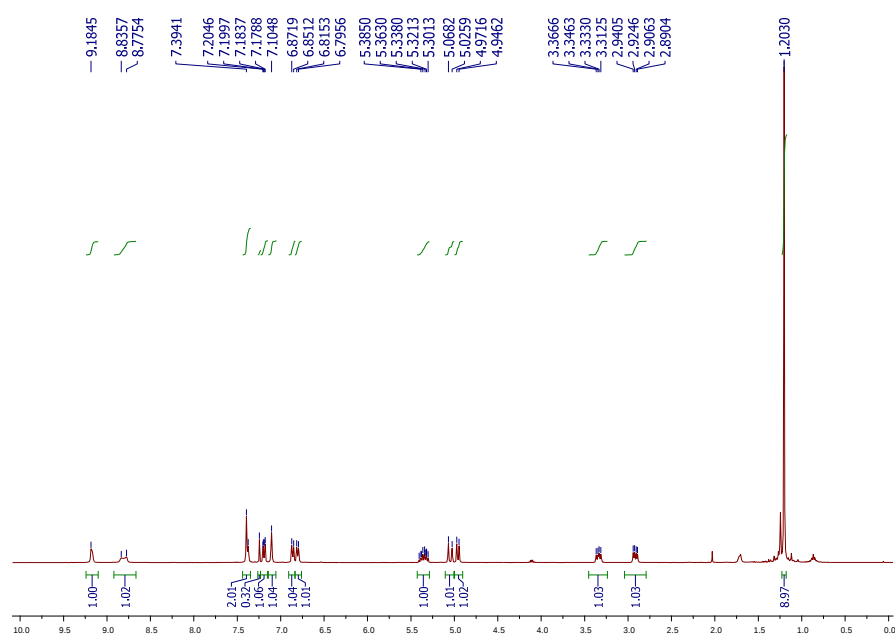
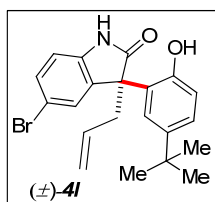
micrOTOF-Q II 10330

Acquisition Parameter

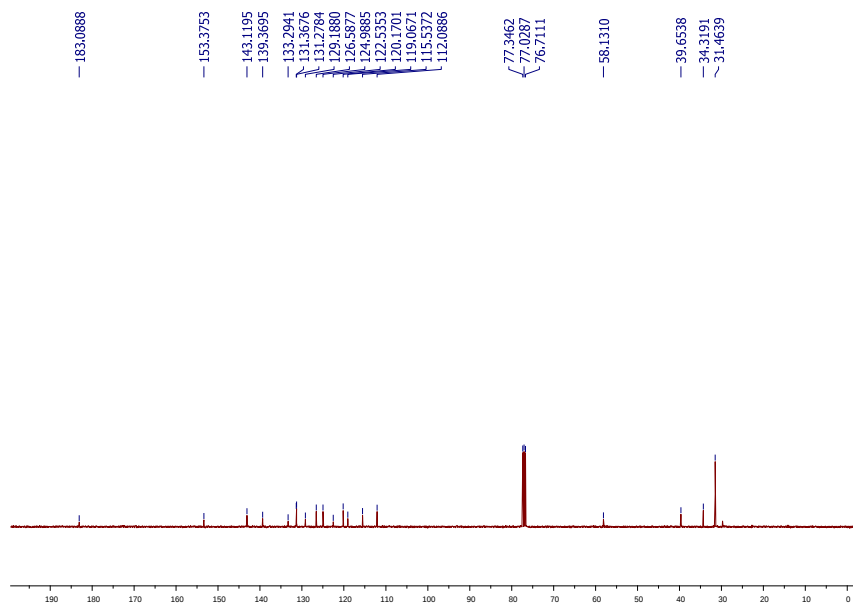
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-4k



¹H NMR (400 MHz, CDCl₃) of compound (±)-**4I**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**4I**

Display Report

Analysis Info

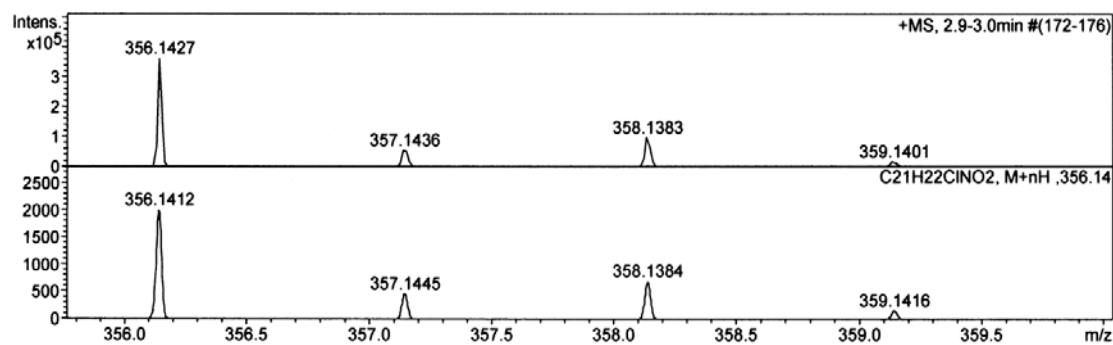
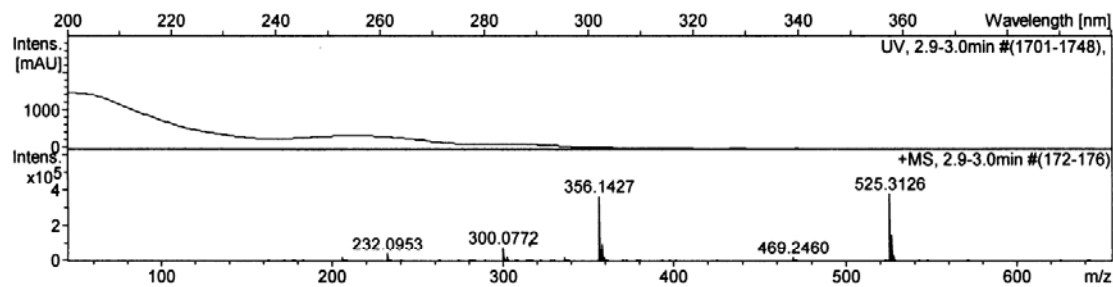
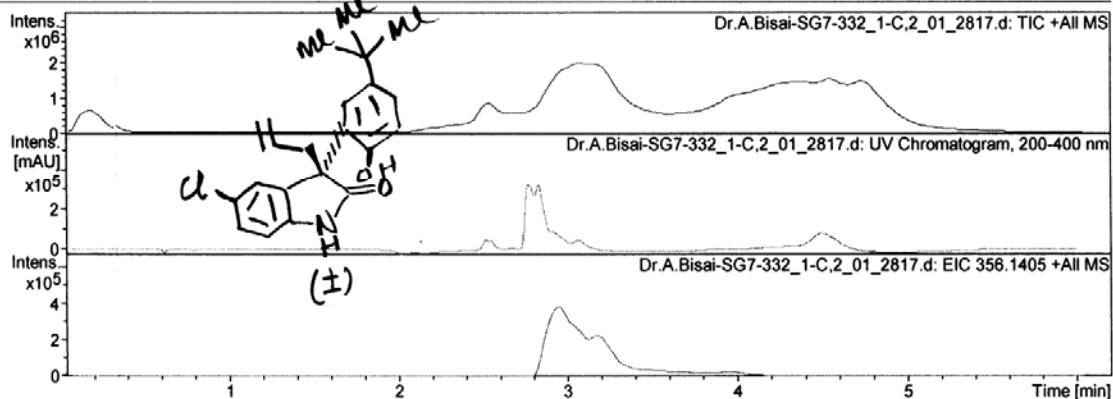
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 Sample Name: Dr.A.Bisai-SG7-332
 Comment:

Acquisition Date: 6/9/2014 3:04:29 AM

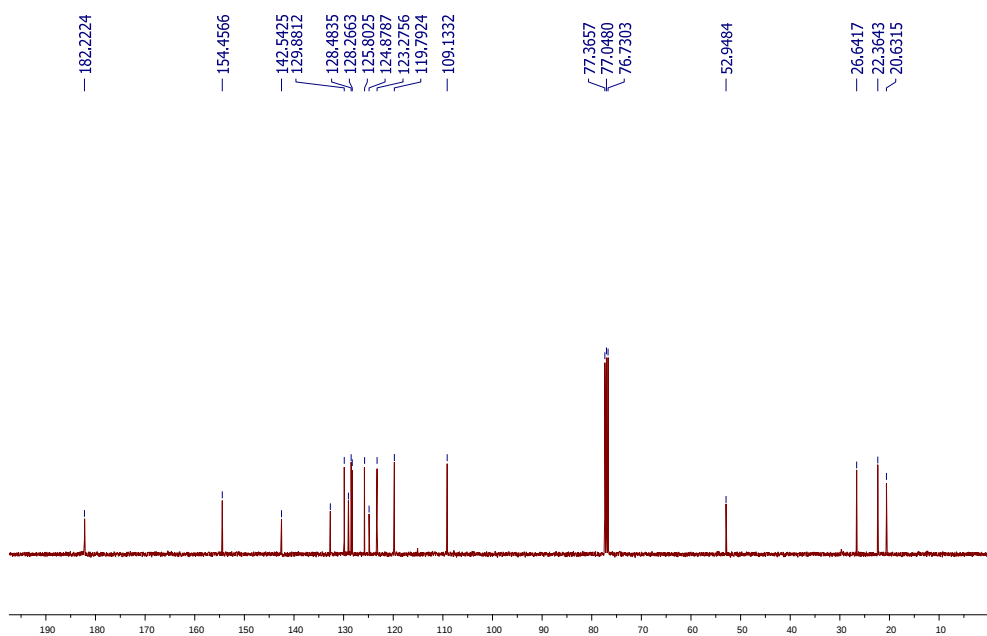
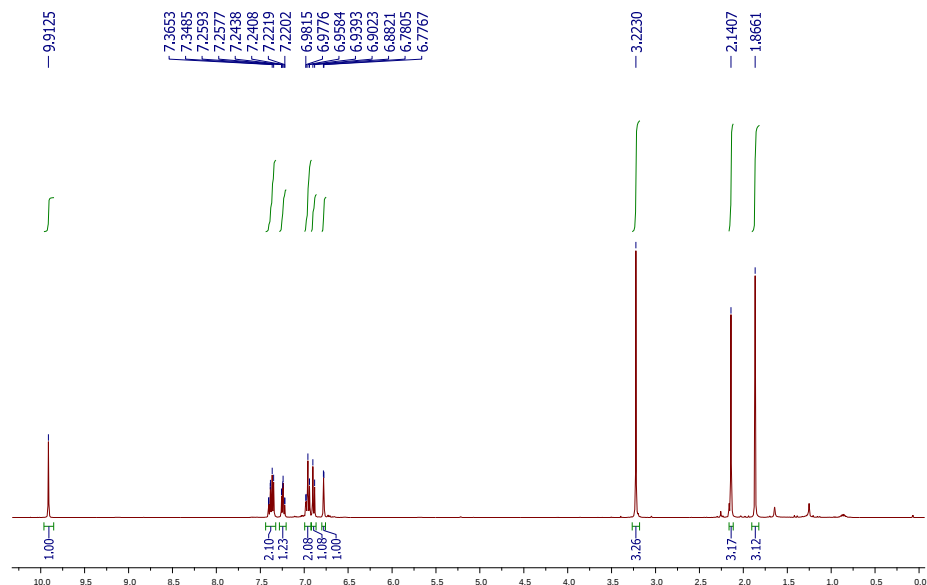
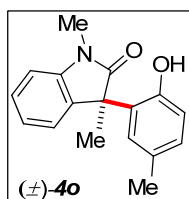
Operator: Ravindra
 Instrument: micrOTOF-Q II 10330

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-41



Display Report

Analysis Info

Analysis Name	D:\Data\user data\2014\APRIL\25 APR\Dr.A.Bisai-SG7-348_1-E,5_01_2360.d
Method	HRLCMS-20 Sept.m
Sample Name	Dr.A.Bisai-SG7-348
Comment	

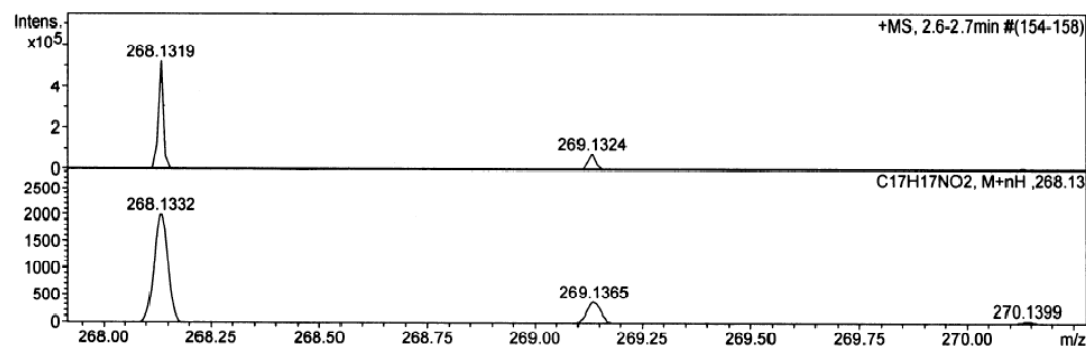
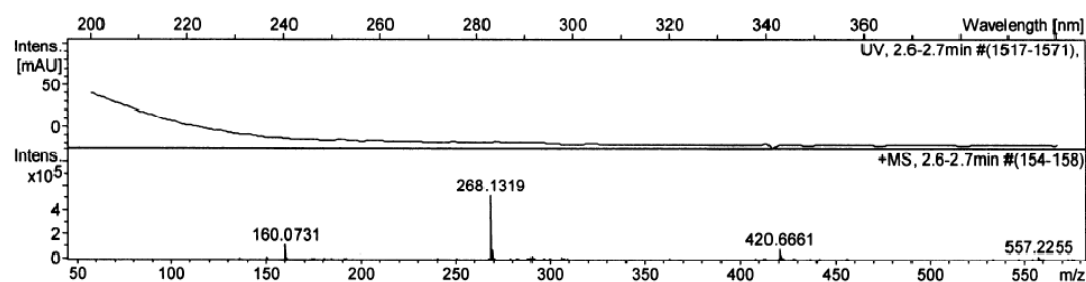
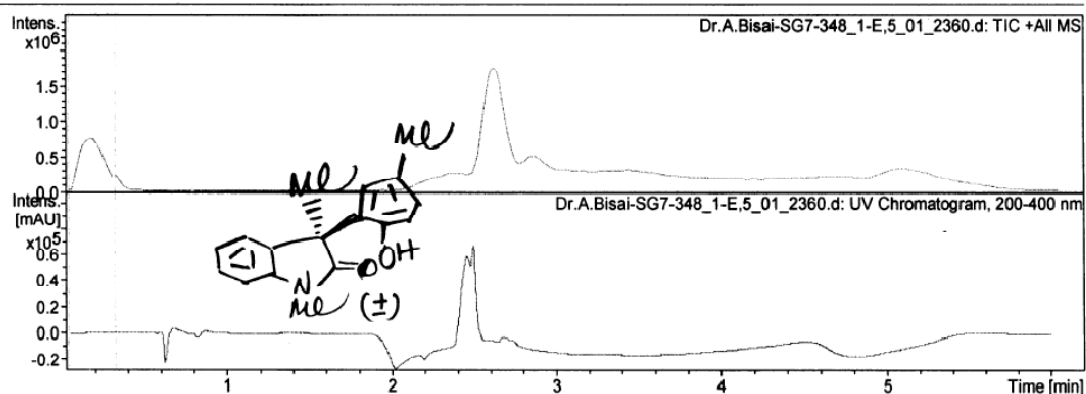
Acquisition Date 4/26/2014 1:01:25 AM

Operator Amit

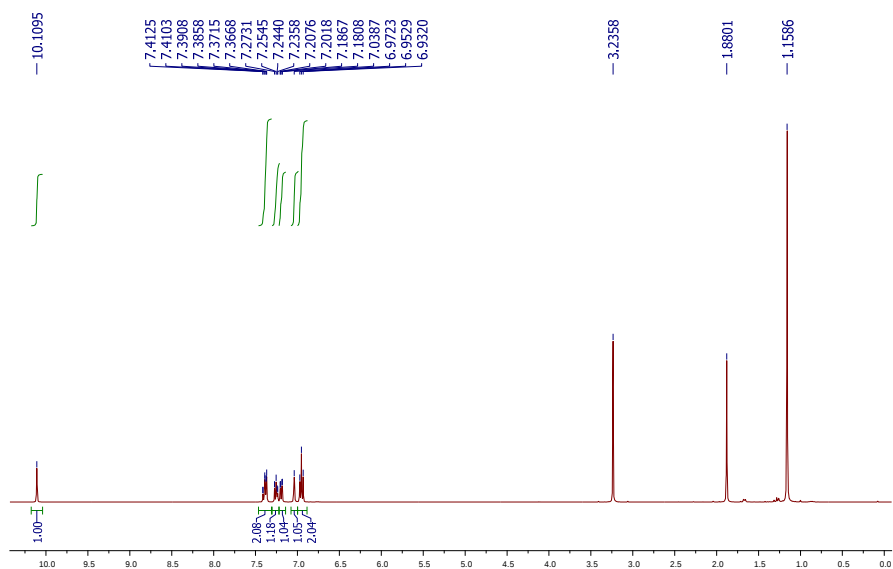
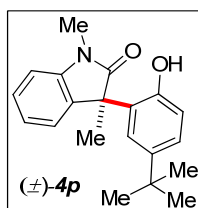
Instrument micrOTOF-Q II 10330

Acquisition Parameter

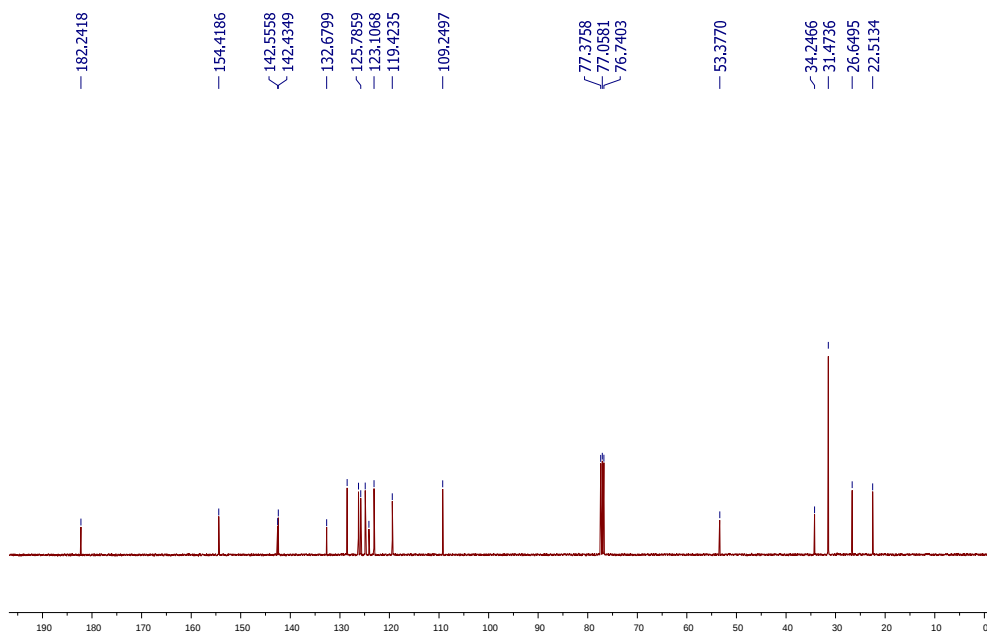
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-40



^1H NMR (400 MHz, CDCl_3) of compound **(±)-4p**



^{13}C NMR (100 MHz, CDCl_3) of compound **(±)-4p**

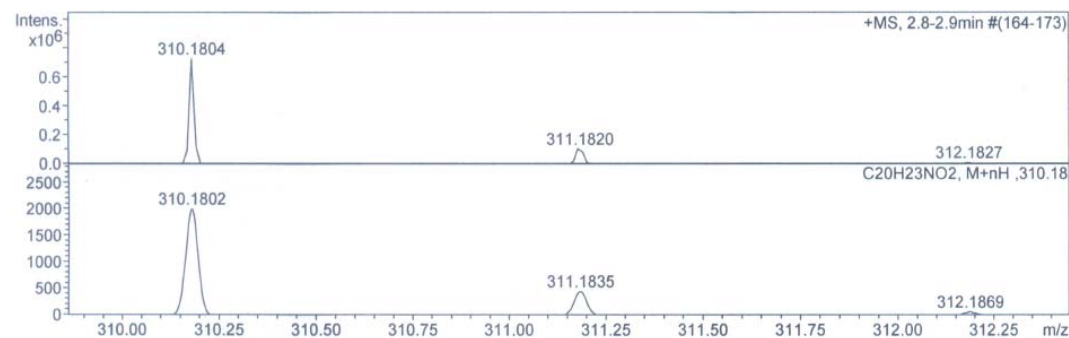
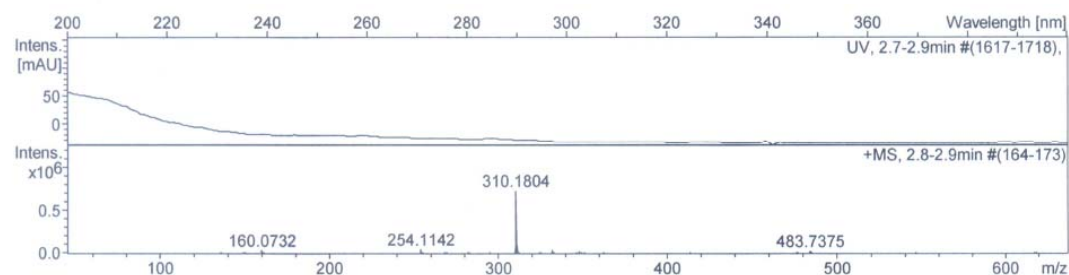
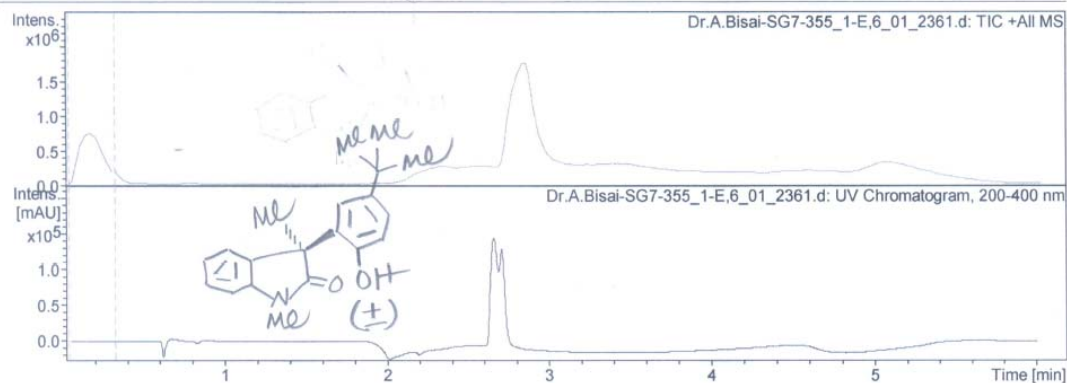
Display Report

Analysis Info

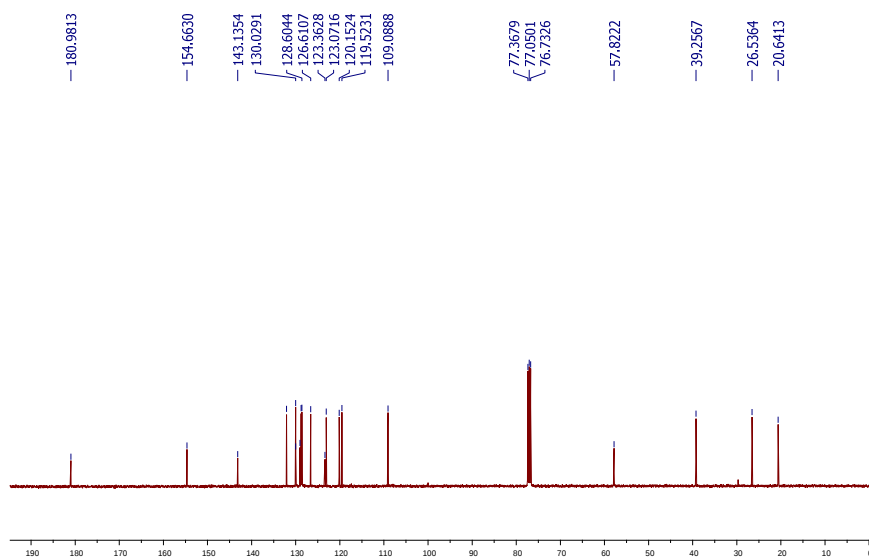
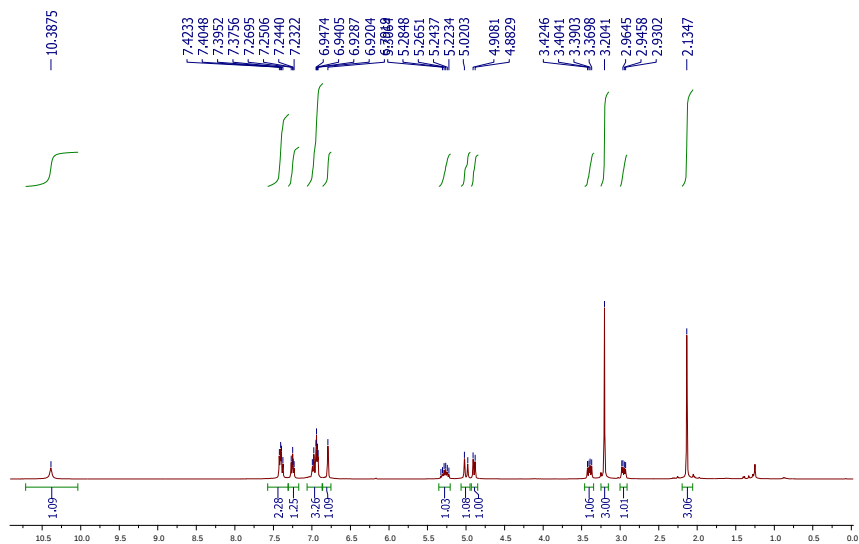
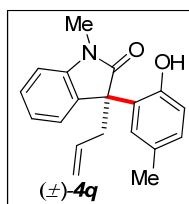
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Sample Name	Dr.A.Bisai-SG7-355
Comment	
Acquisition Date	4/26/2014 1:08:36 AM
Operator	Amit
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-4p



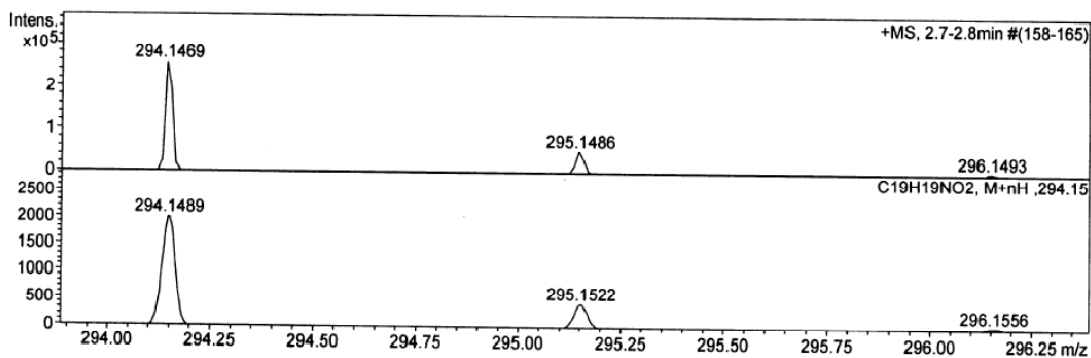
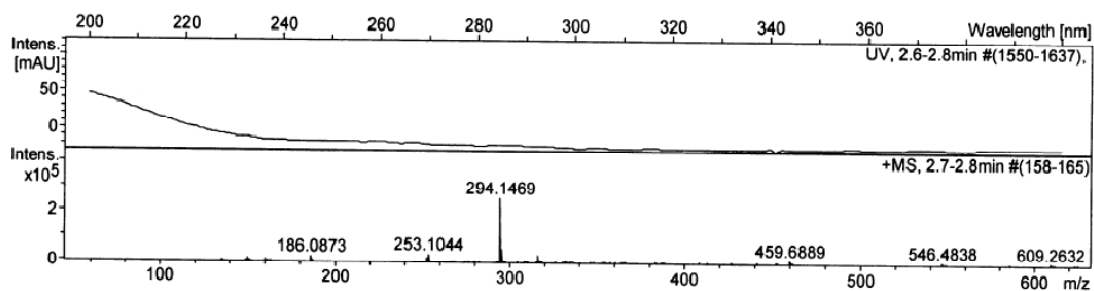
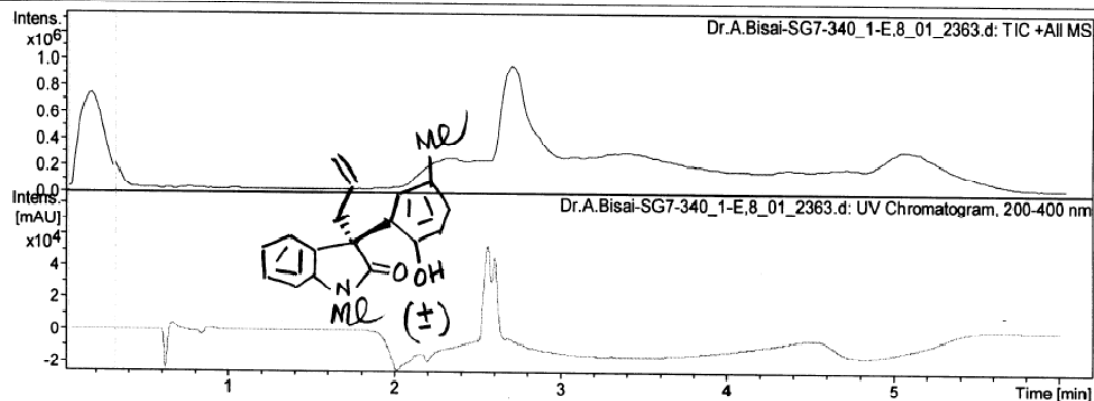
Display Report

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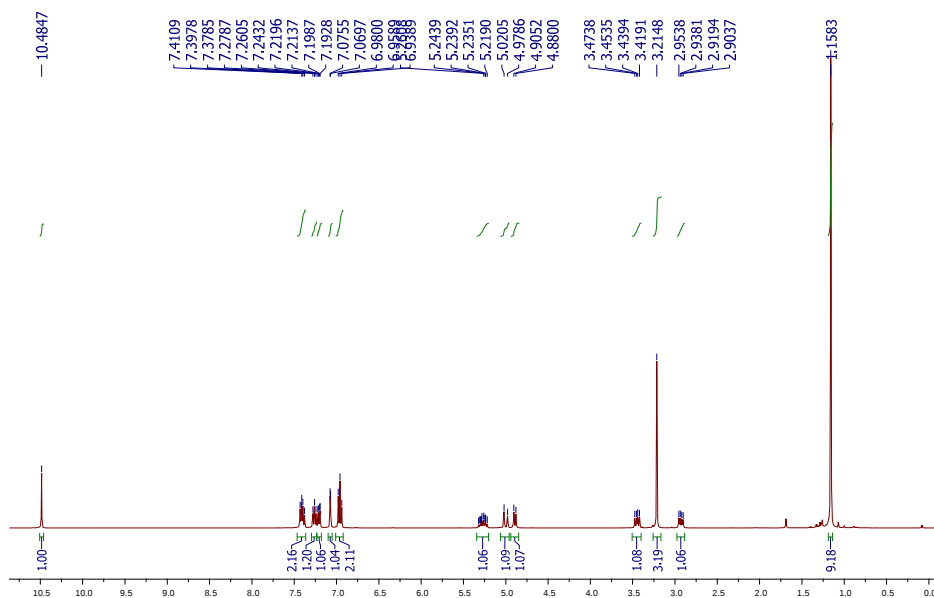
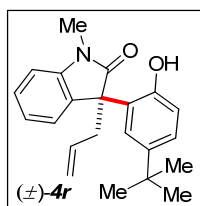
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Comment	
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Operator	Amit
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

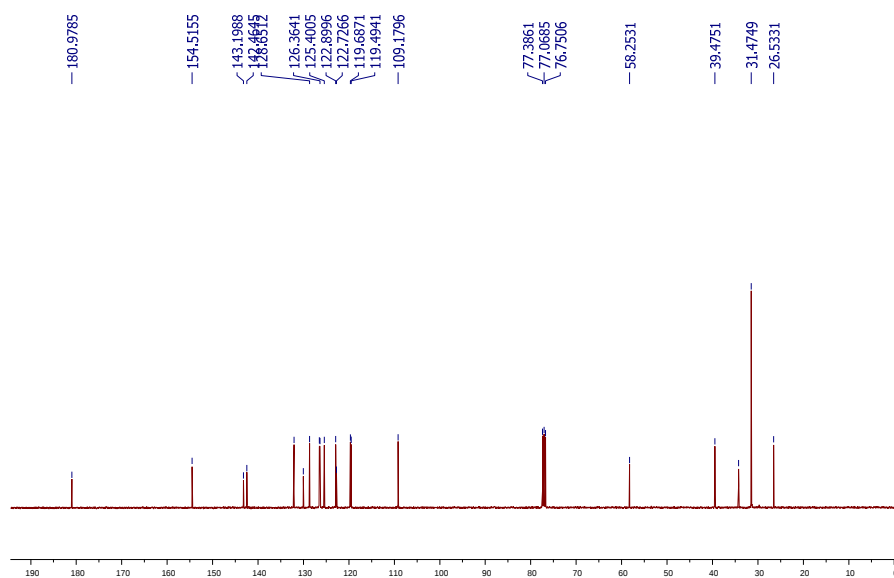
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-4q



¹H NMR (400 MHz, CDCl₃) of compound (±)-**4r**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**4r**

Display Report

Analysis Info

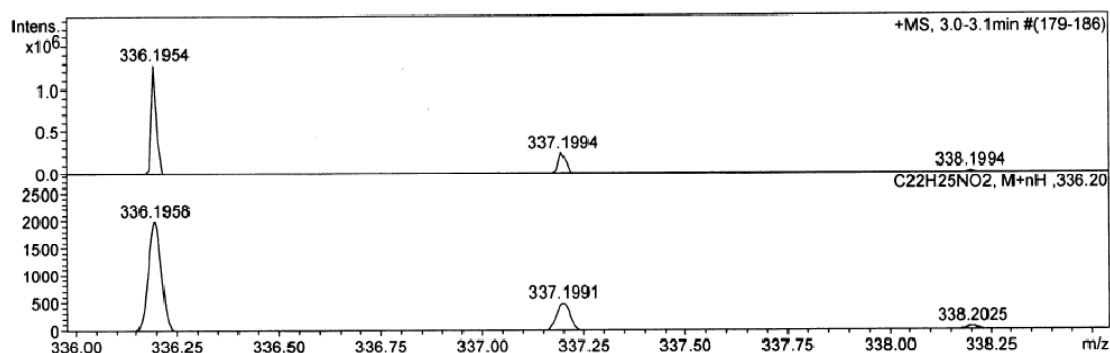
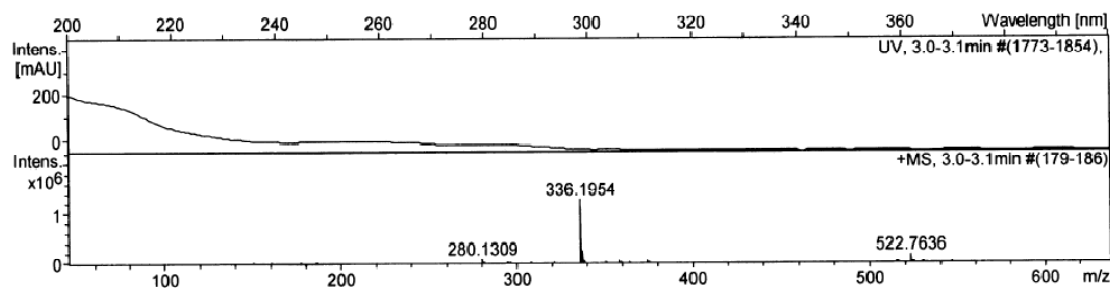
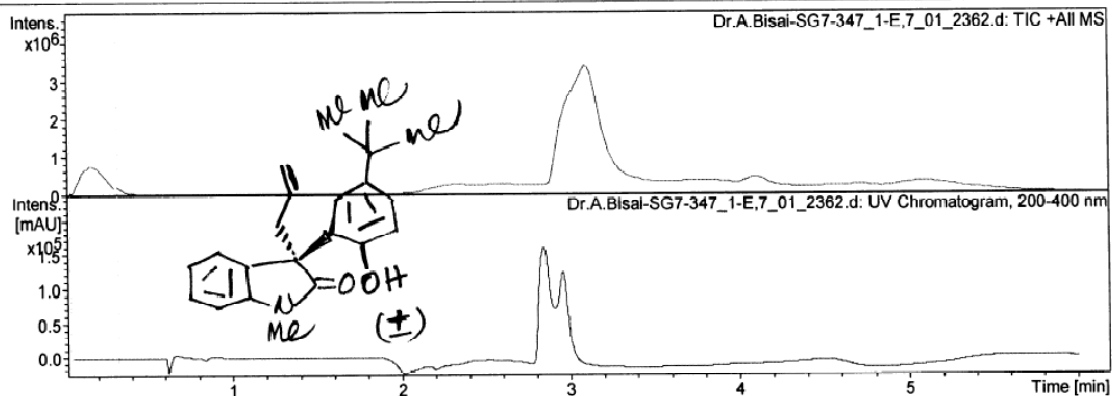
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 Comment:

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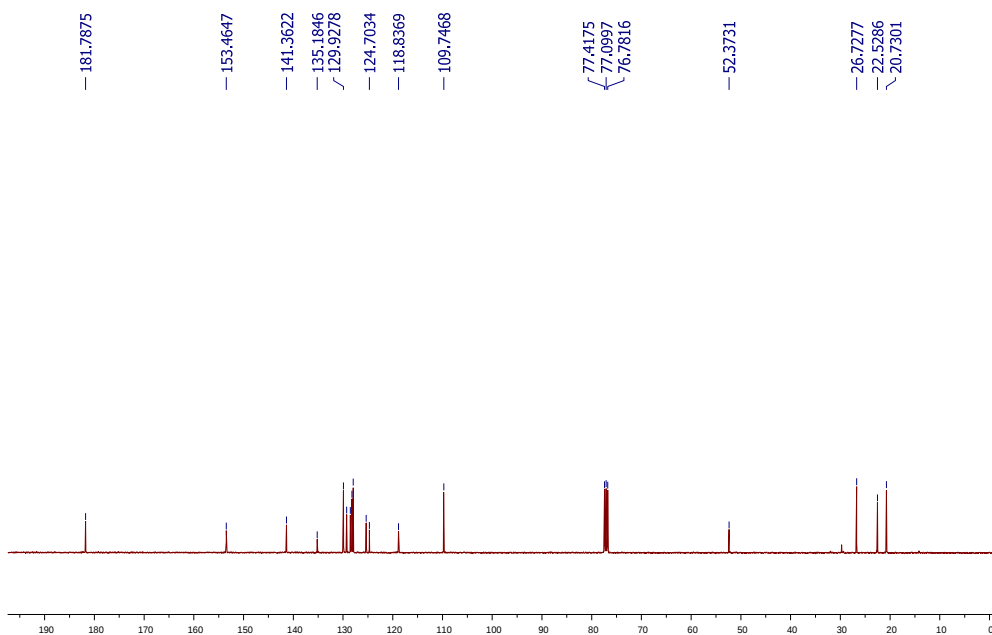
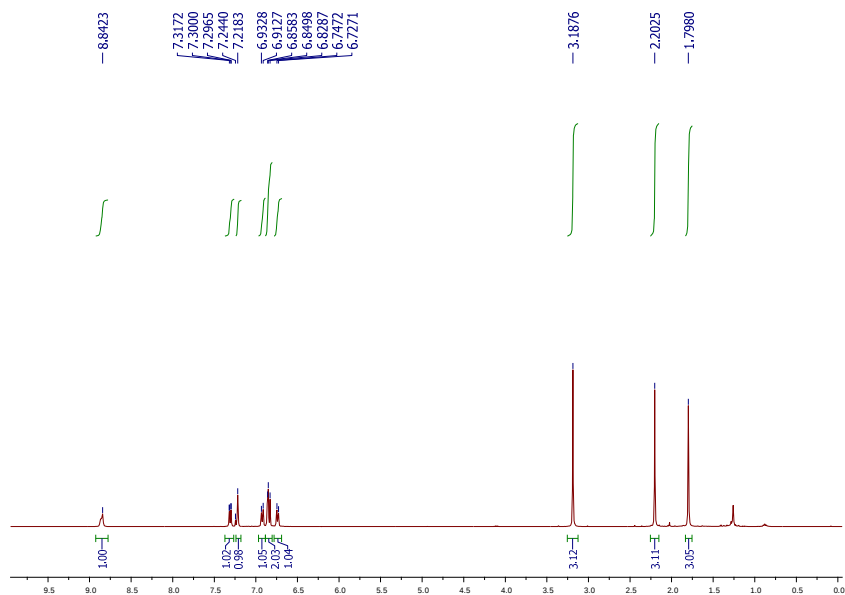
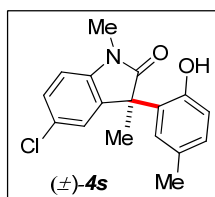
Operator: Amit
 Instrument: micrOTOF-Q II 10330

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of ($\pm$)-4r



Display Report

Analysis Info

Analysis Name: D:\Data\user data\2014\APRIL\28 APR\Dr.A Bisai-SG8-28_1-F_6_01_2376.d
 Method: HRLCMS-20 Sept.m
 Sample Name: Dr.A Bisai-SG8-28
 Comment:

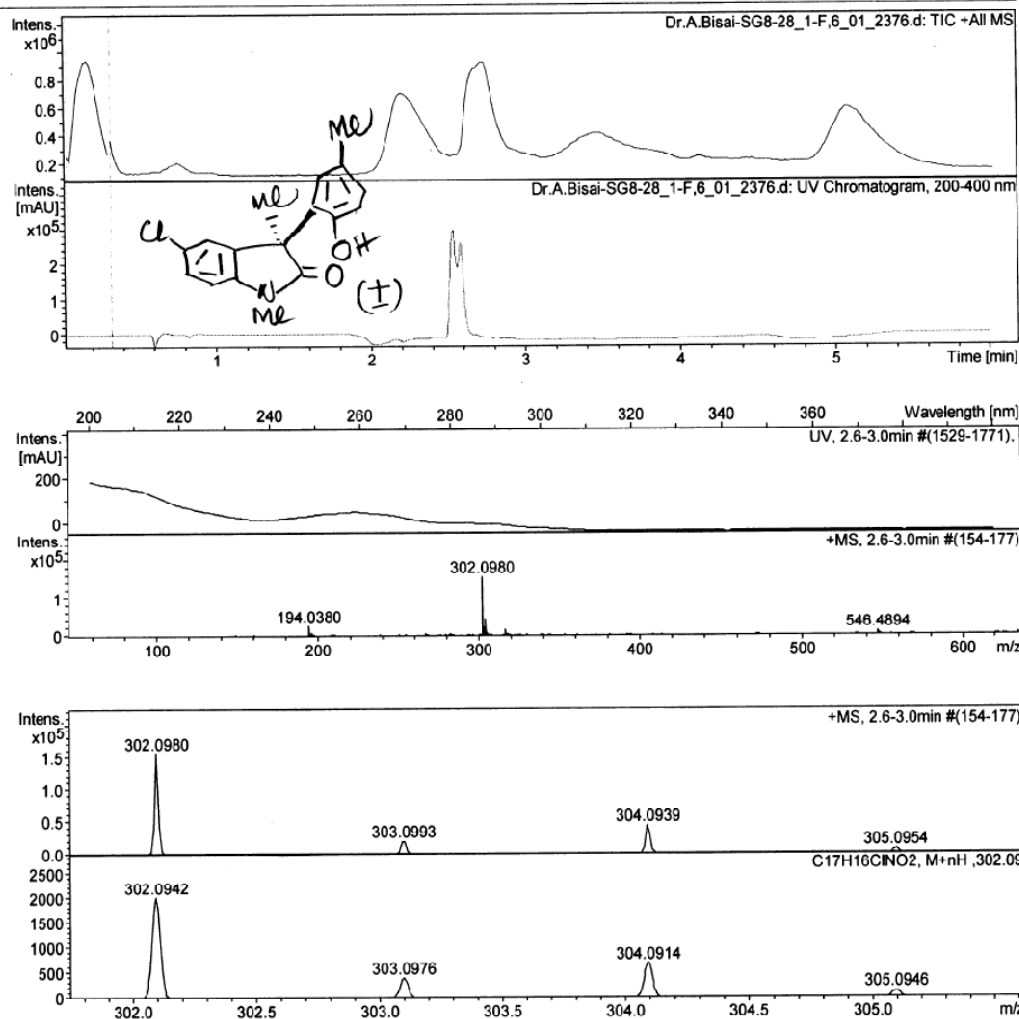
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Operator: Amit

Instrument: micrOTOF-Q II 10330

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

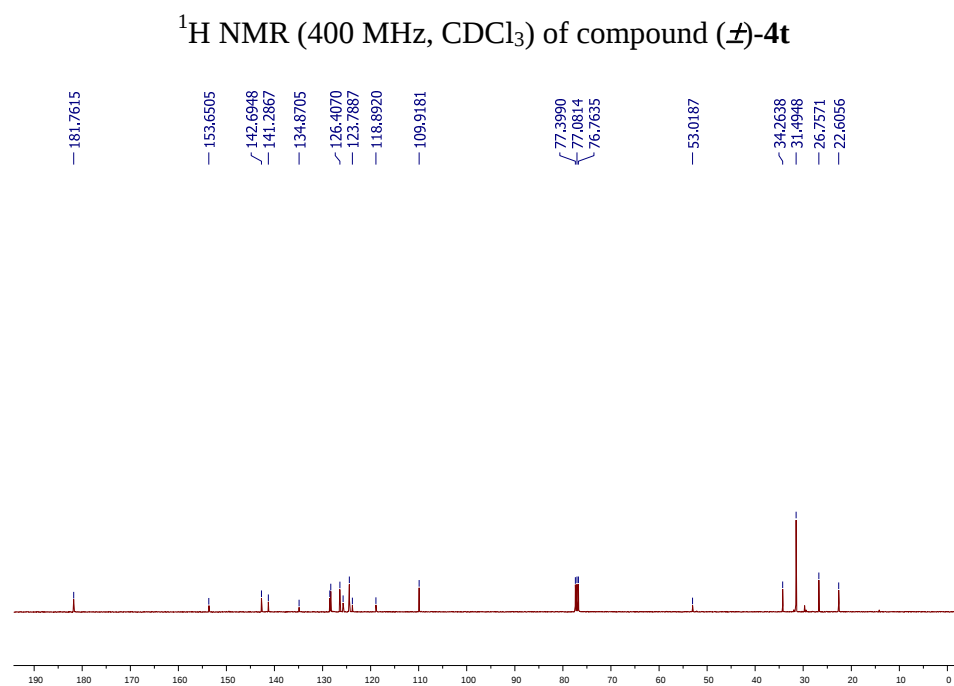
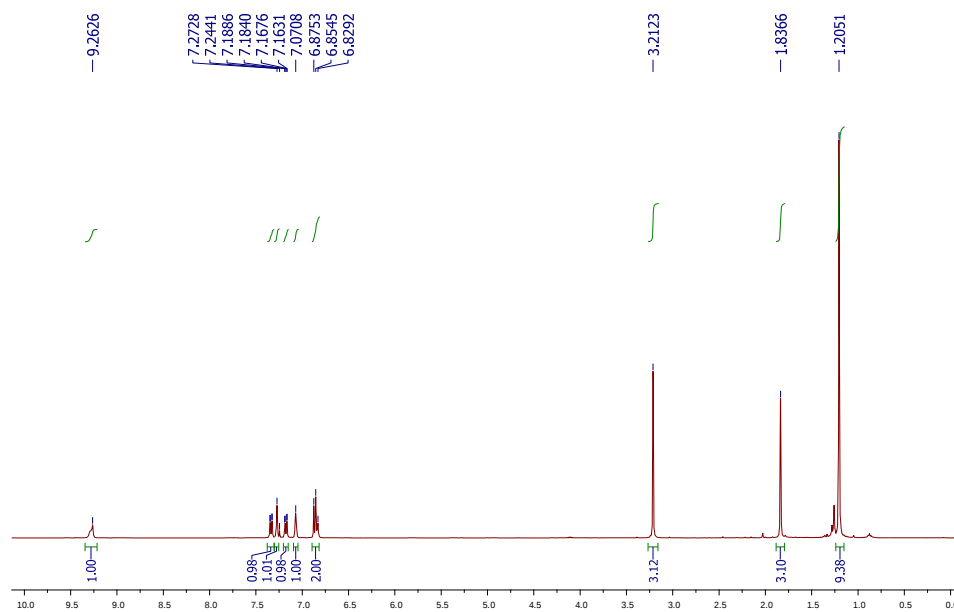
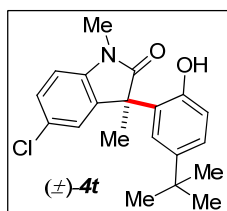


Bruker Compass DataAnalysis 4.0

printed: 4/29/2014 4:38:14 AM

Page 1 of 1

Scanned copy of mass spectrum of (±)-4s



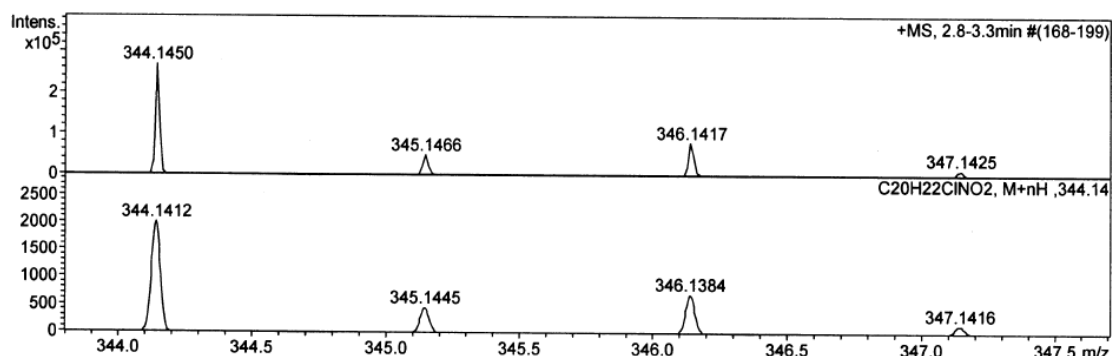
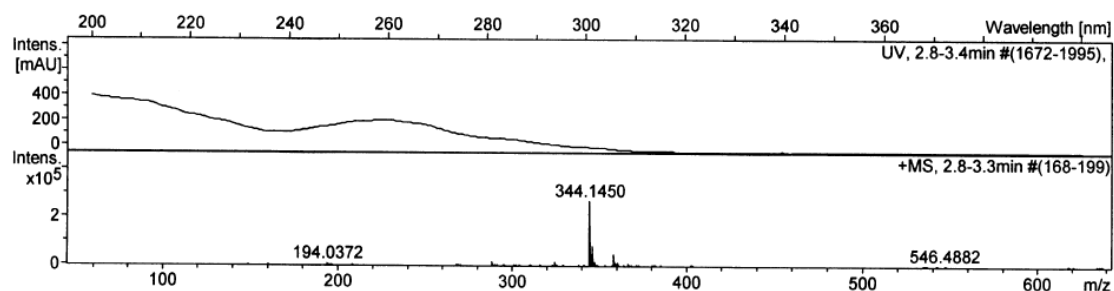
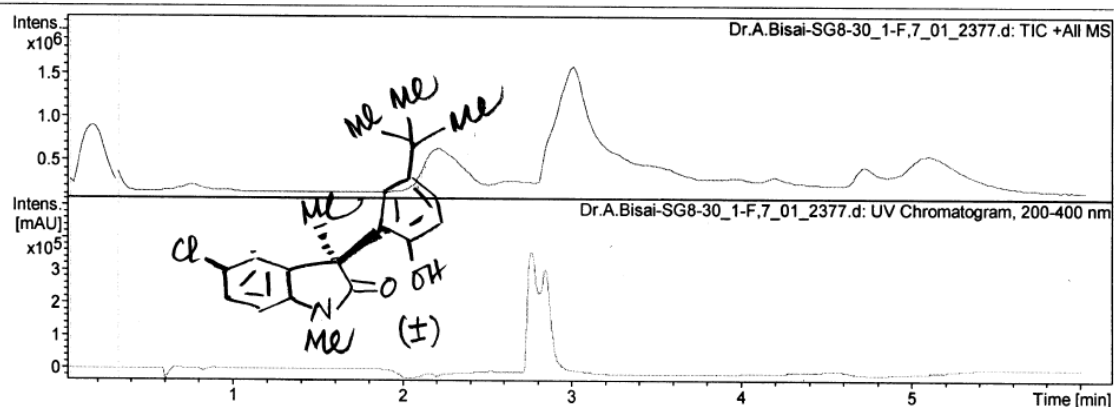
Display Report

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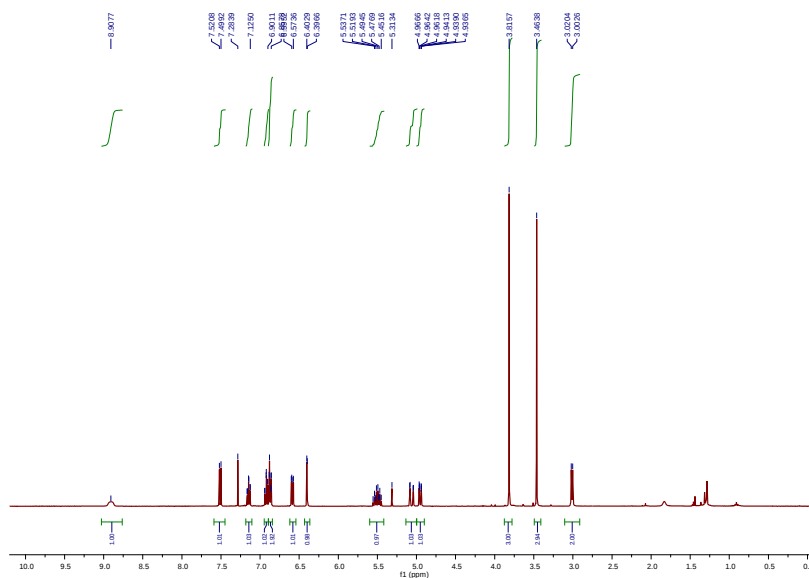
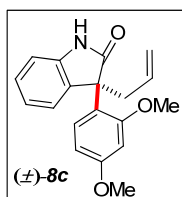
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Method	HRLCMS-20 Sept.m	Operator	Amit
Sample Name	Dr.A.Bisai-SG8-30	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
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Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-4t



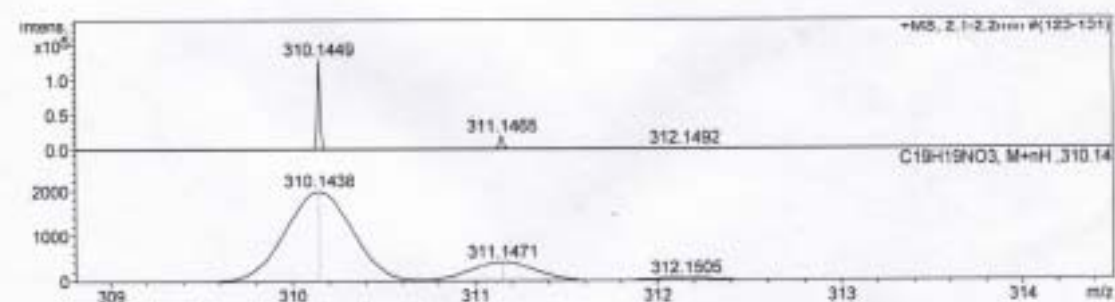
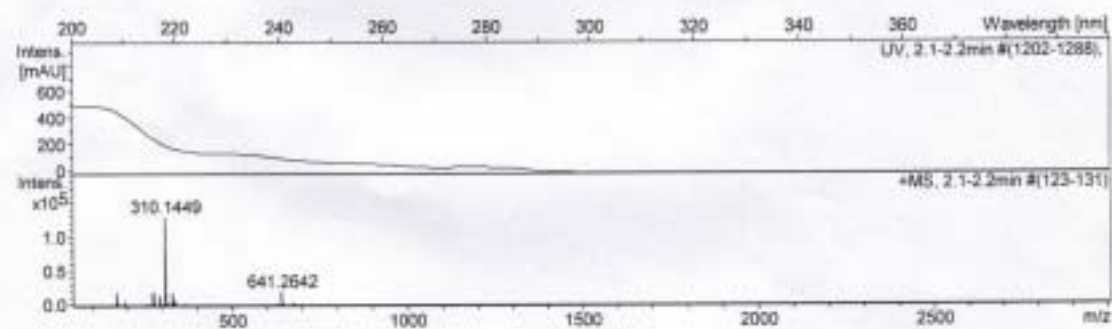
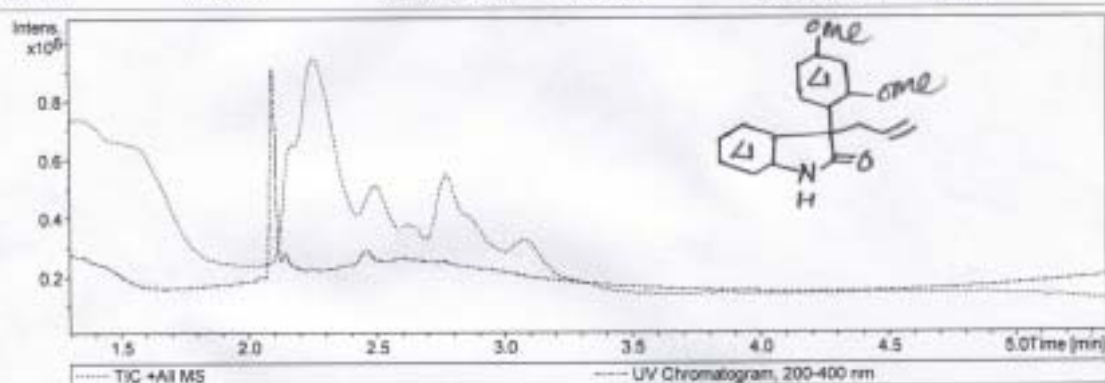
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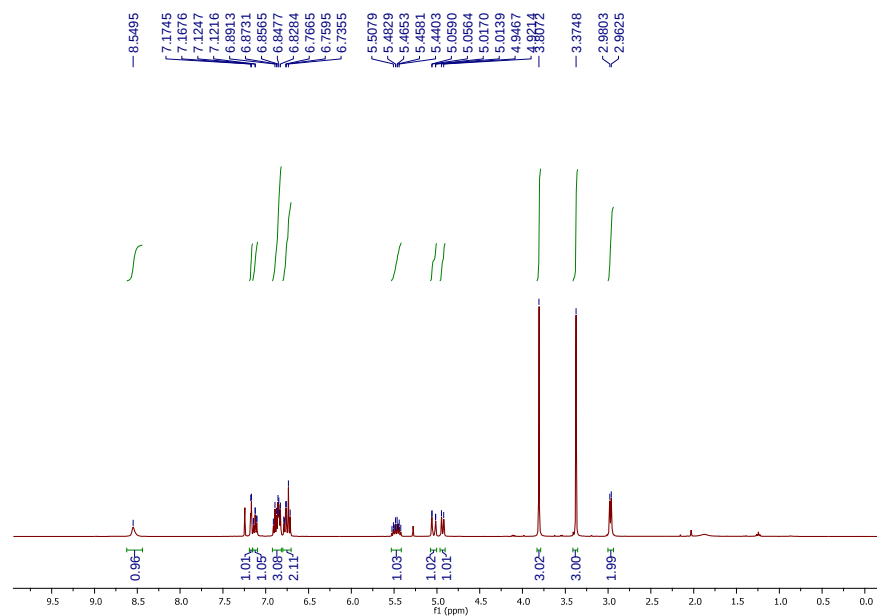
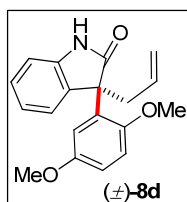
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Sample Name	Dr. A. Bisai- SG2-352 R	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

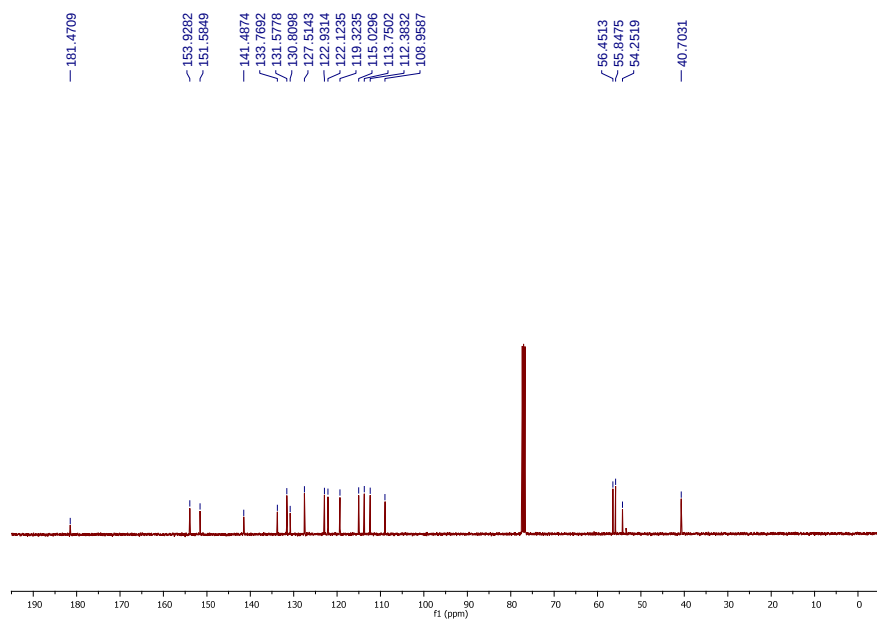
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (*±*)-8c



¹H NMR (400 MHz, CDCl₃) of compound (±)-8d



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8d

Display Report

Analysis Info

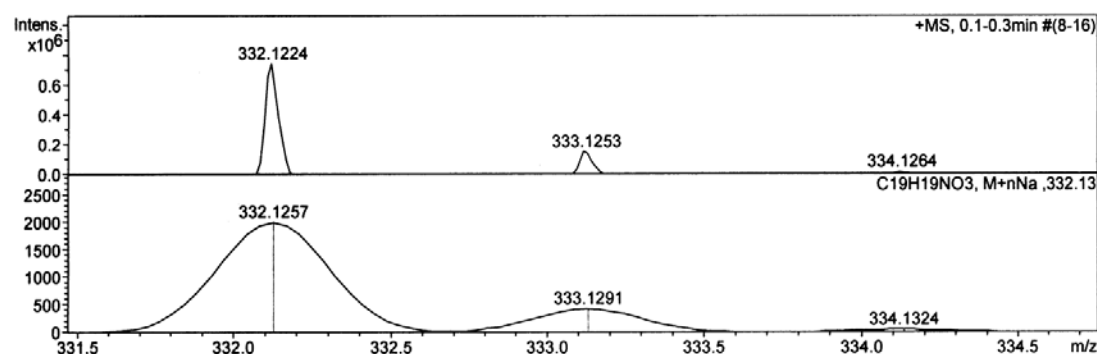
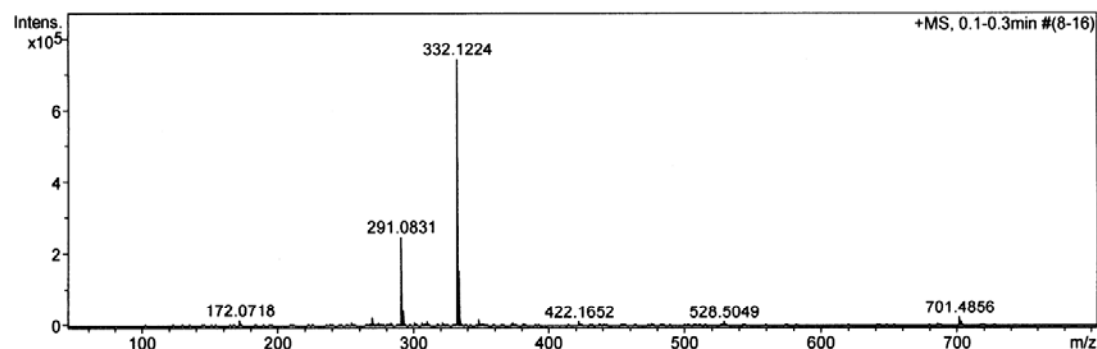
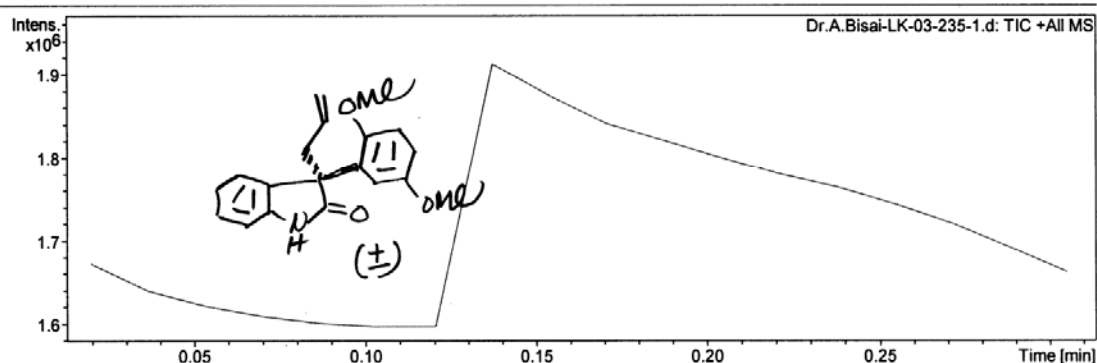
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 Comment

Acquisition Date 12/20/2013 3:41:29 PM

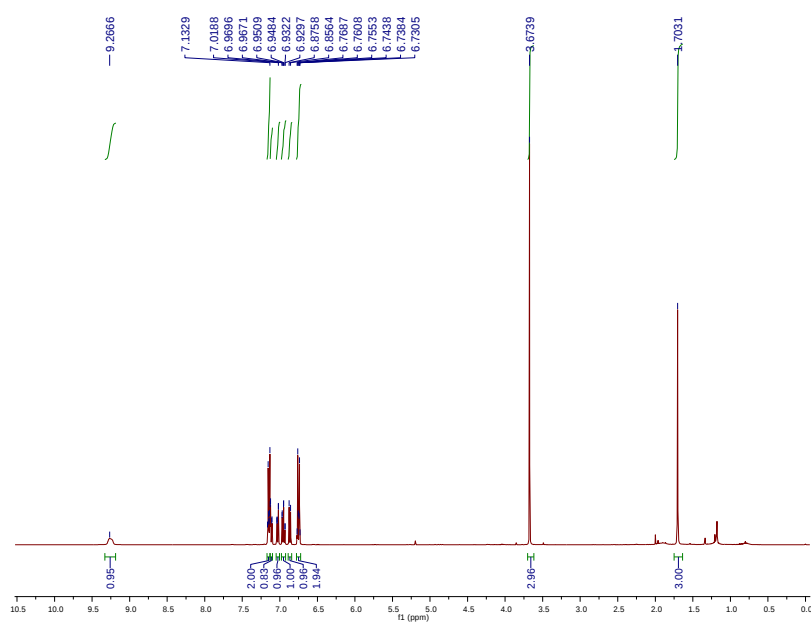
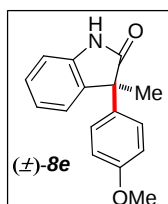
Operator Amit
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

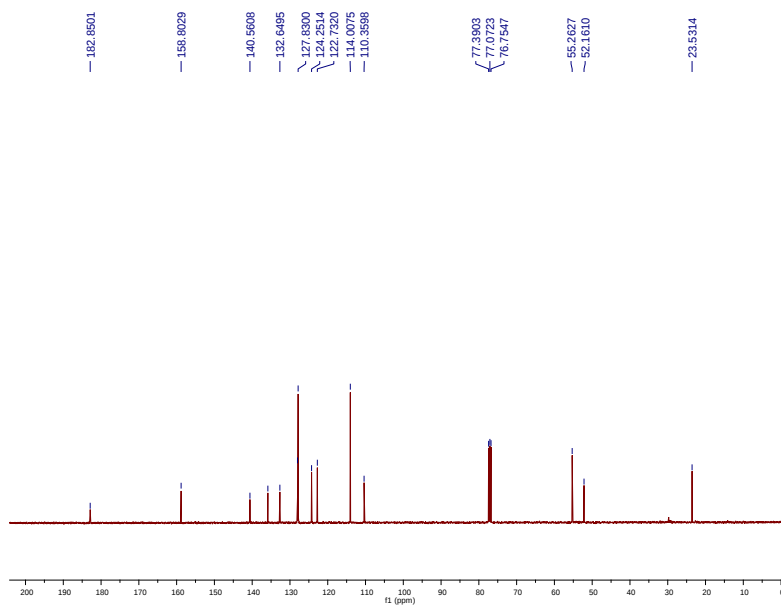
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-8d



¹H NMR (400 MHz, CDCl₃) of compound (±)-**8e**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**8e**



Display Report

Analysis Info

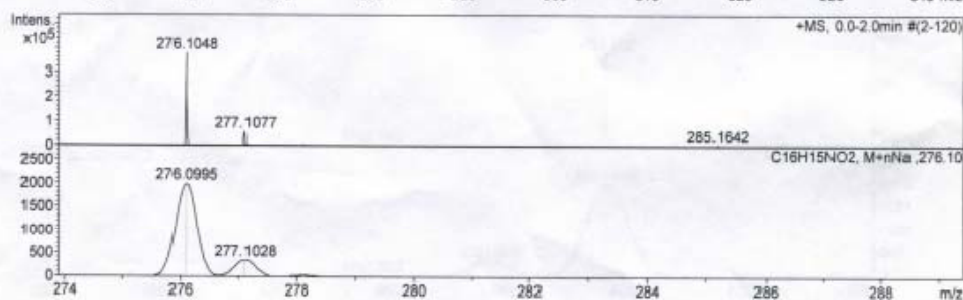
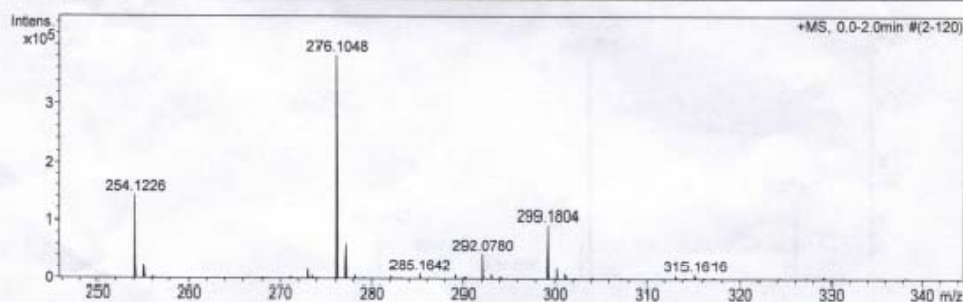
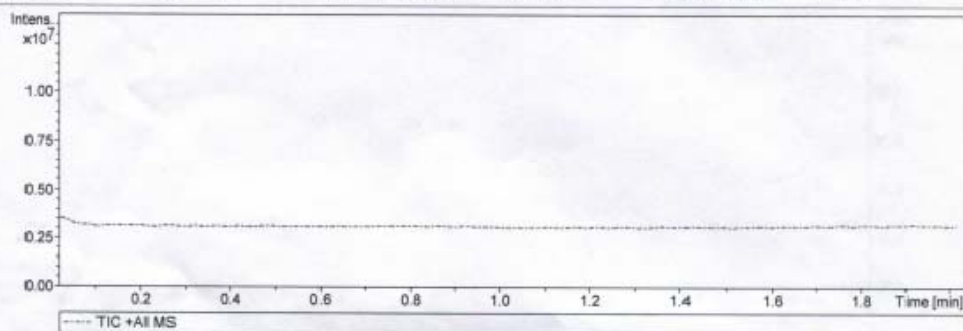
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 Sample Name AB-SG-2-380
 Comment

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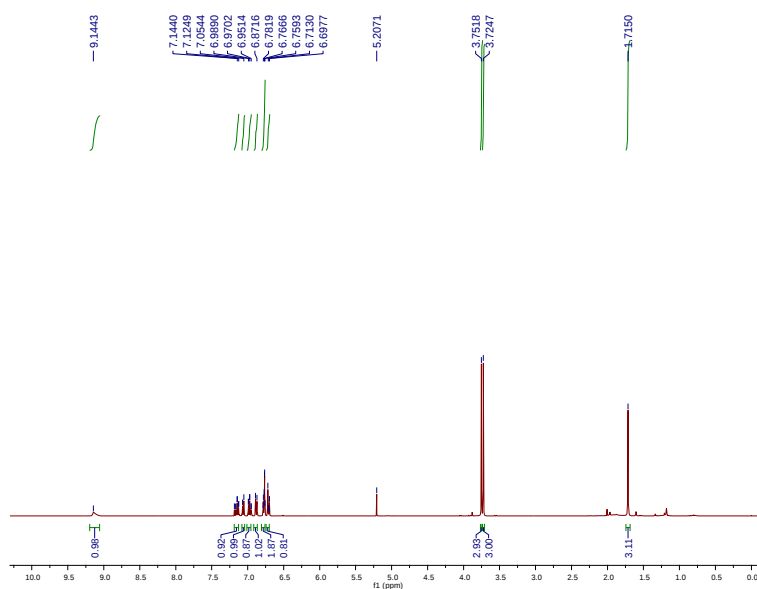
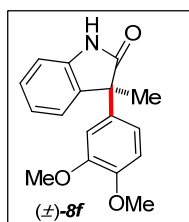
Operator RAMSUKUMARI
 Instrument microTOF-Q II 10330

Acquisition Parameter

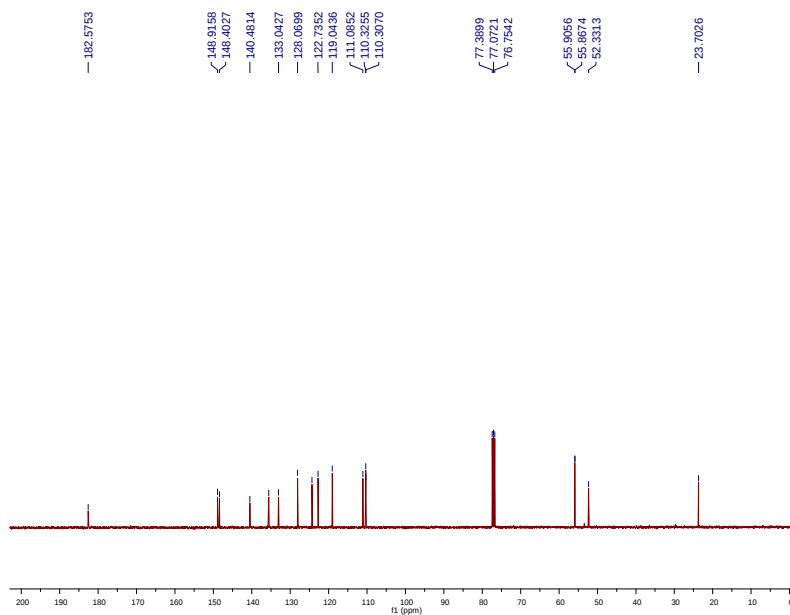
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Scan End	1500 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



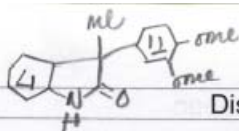
Scanned copy of mass spectrum of ($\pm$)-8e



¹H NMR (400 MHz, CDCl₃) of compound (±)-8f



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8f



Display Report

Analysis Info

Analysis Name D:\Data\user data\JULY 18\Akesh Bisai-SG-2-382.d
 Method tune_low.m
 Sample Name AB-SG-2-382
 Comment

Acquisition Date 7/18/2011 12:37:38 PM

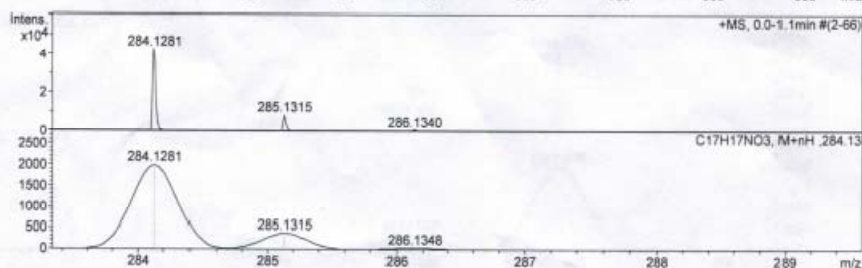
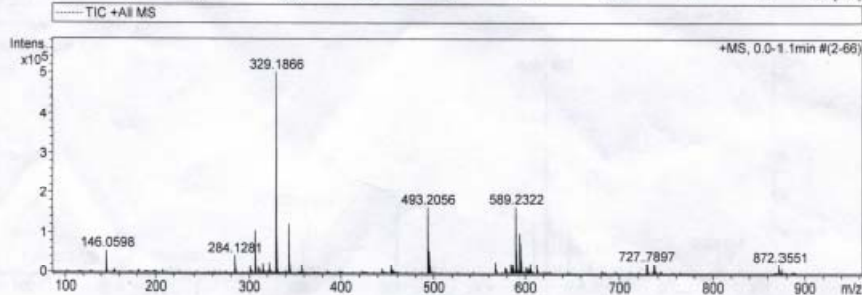
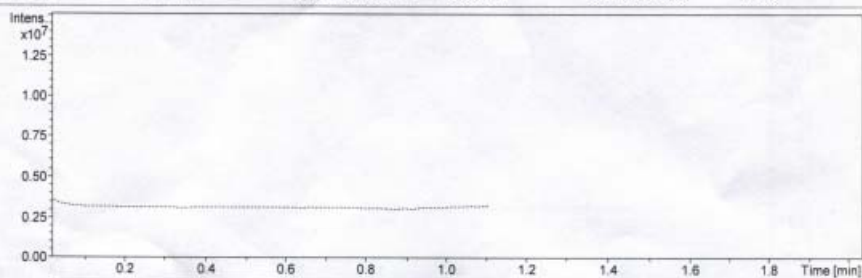
Operator *Meena Sharma*

Instrument RAMSUKUMARI

micrOTOF-Q II 10330

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	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	130.0 Vpp	Set Divert Valve	Waste



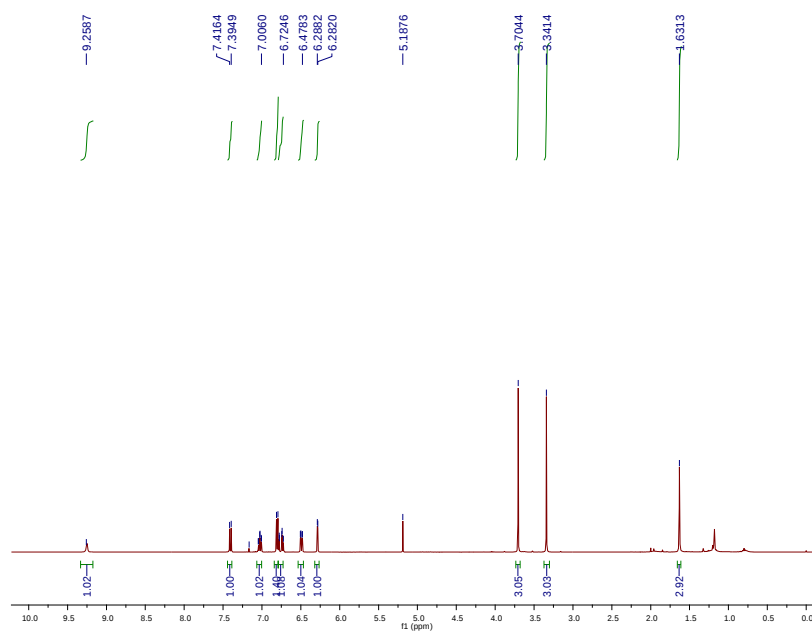
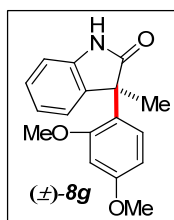
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printed: 7/18/2011 1:00:04 PM

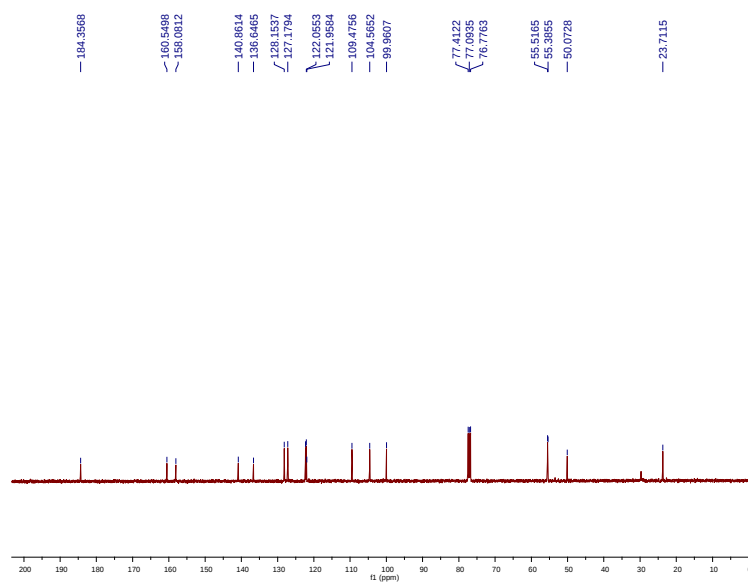
Page 1 of 1

M.W. = 283.1208

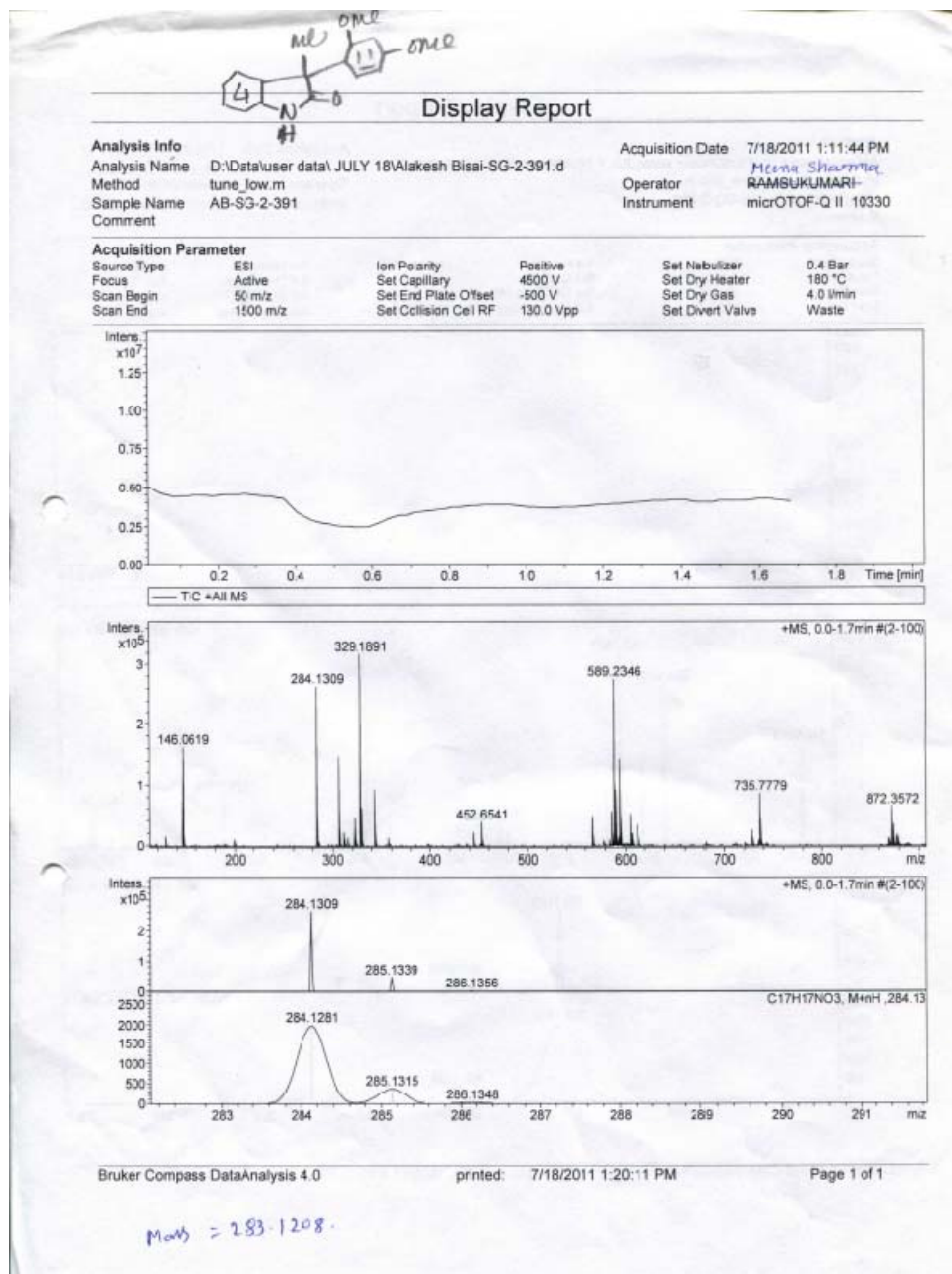
Scanned copy of mass spectrum of ($\pm$)-8f



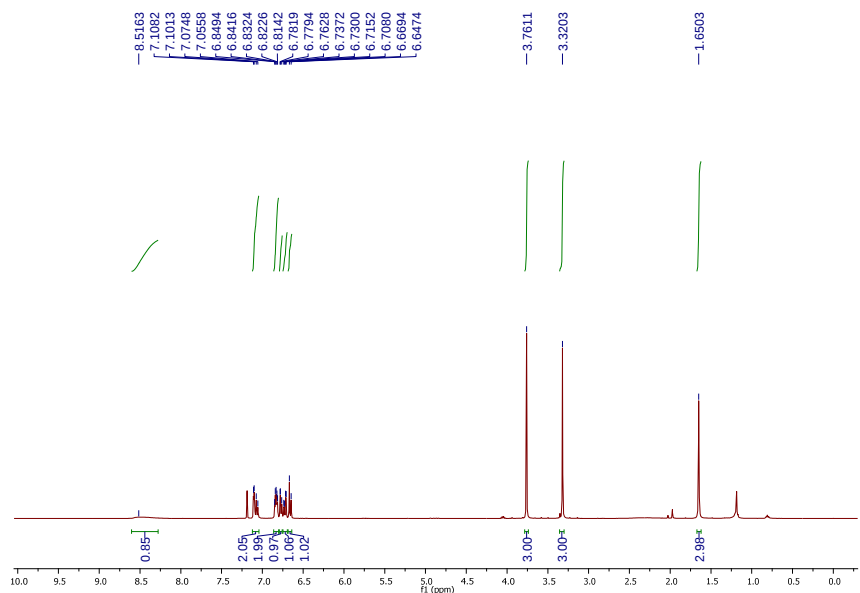
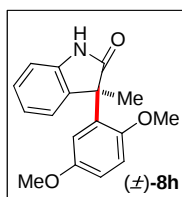
¹H NMR (400 MHz, CDCl₃) of compound (±)-8g



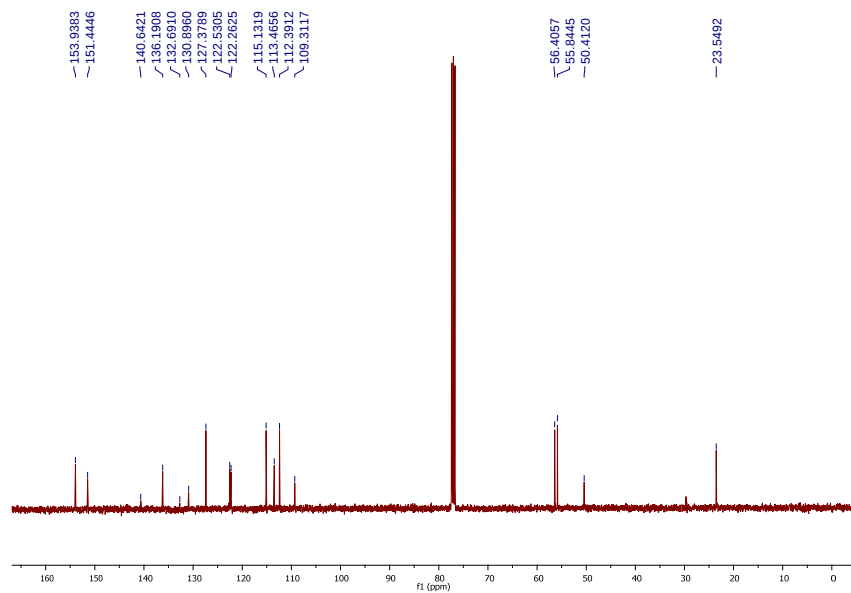
¹³C NMR (100 MHz, CDCl₃) of compound (±)-8g



Scanned copy of mass spectrum of ($\pm$)-8g



¹H NMR (400 MHz, CDCl₃) of compound (±)-8h



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8h

Display Report

Analysis Info

Analysis Name D:\Data\user data\2013\DEC\20 dec\Dr.A.Bisai-LK-03-239.d
 Method tune_low.m
 Sample Name LK-03-239
 Comment

Acquisition Date 12/20/2013 3:34:50 PM

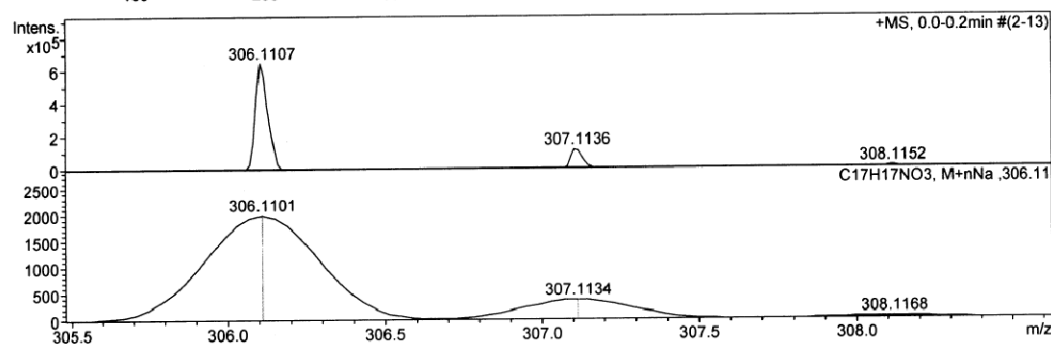
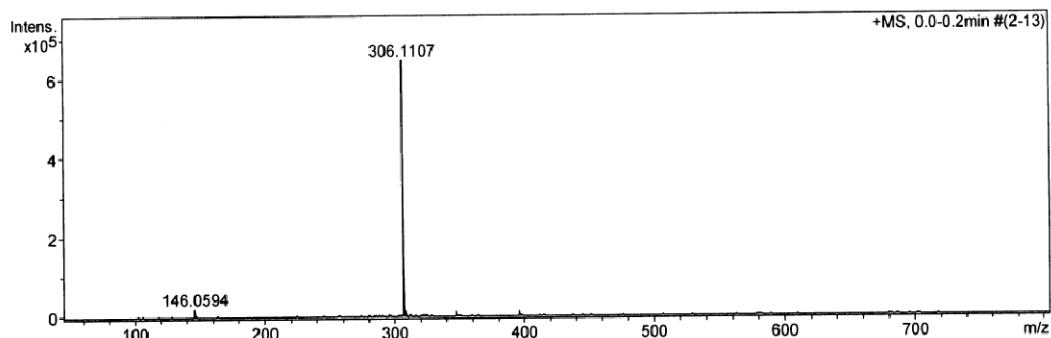
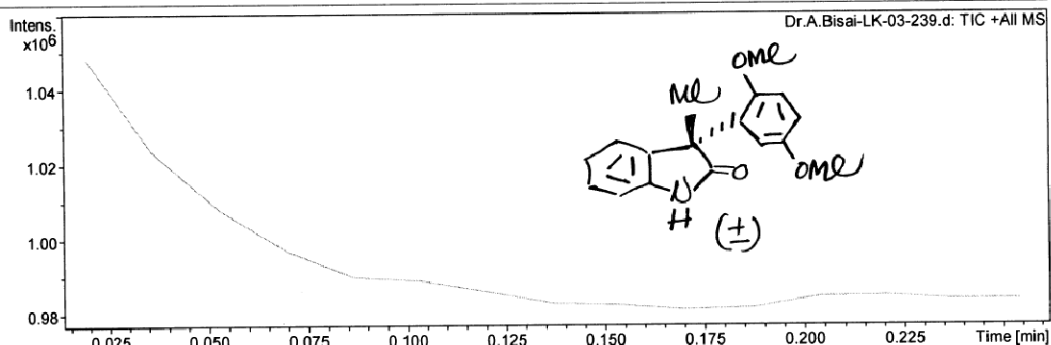
Operator Amit
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

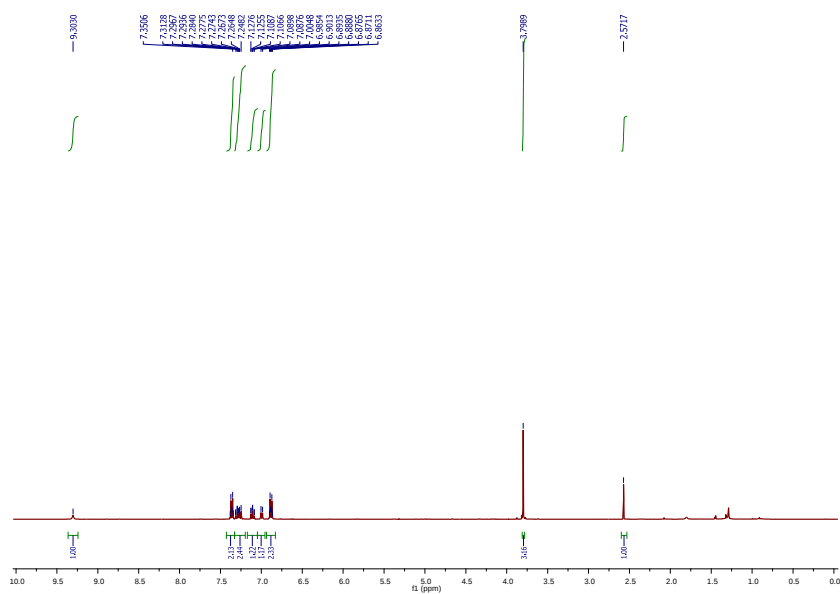
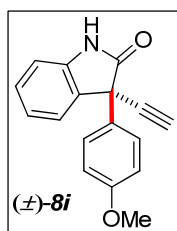
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 Focus Not active
 Scan Begin 50 m/z
 Scan End 3000 m/z

Ion Polarity Positive
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 Set End Plate Offset -500 V
 Set Collision Cell RF 130.0 Vpp

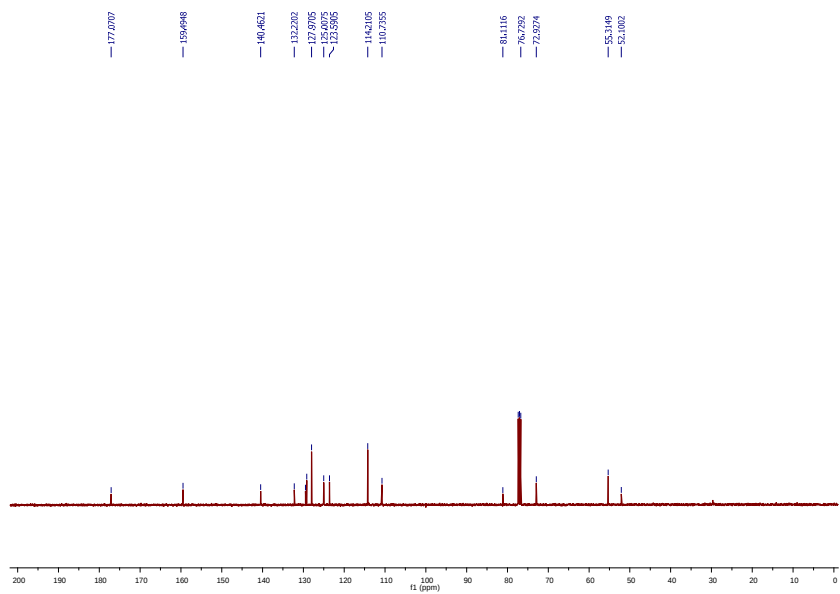
Set Nebulizer 0.4 Bar
 Set Dry Heater 180 °C
 Set Dry Gas 4.0 l/min
 Set Divert Valve Waste



Scanned copy of mass spectrum of (±)-8h



¹H NMR (400 MHz, CDCl₃) of compound (±)-8i



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8i

Display Report

Analysis Info

Analysis Name D:\Data\user data\may2012\25 may\Dr.A.Bisai-SG2-372_1-A_8_01_2370.d
 Method HRLCMS-20 Sept.m
 Sample Name Dr.A.Bisai-SG2-372
 Comment

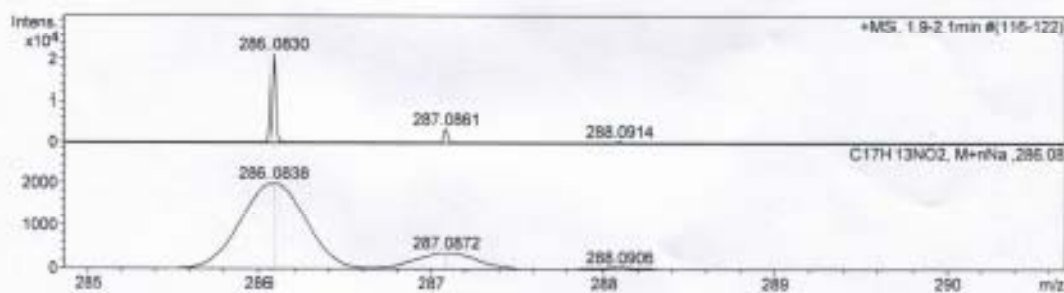
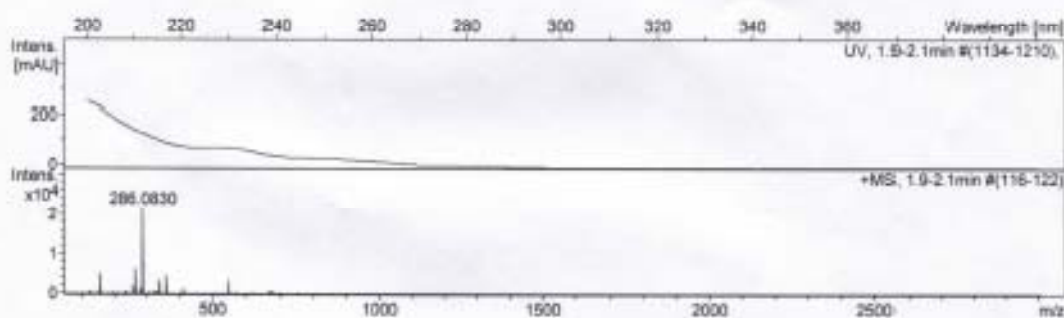
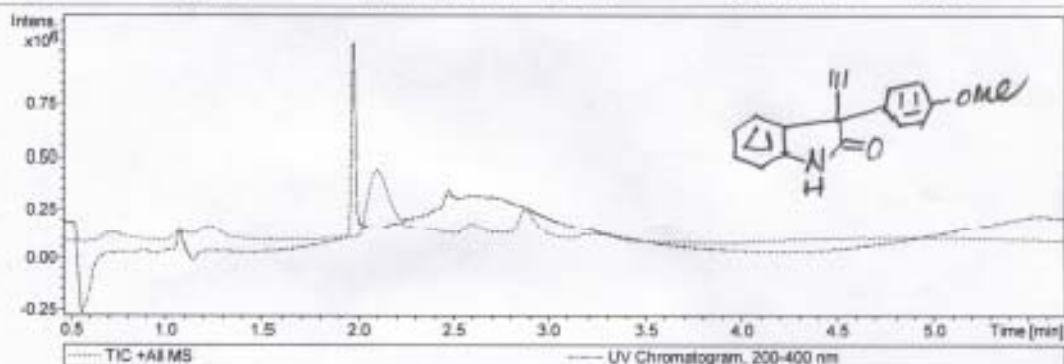
Acquisition Date 5/25/2012 1:29:29 PM

Operator Meena Sharma

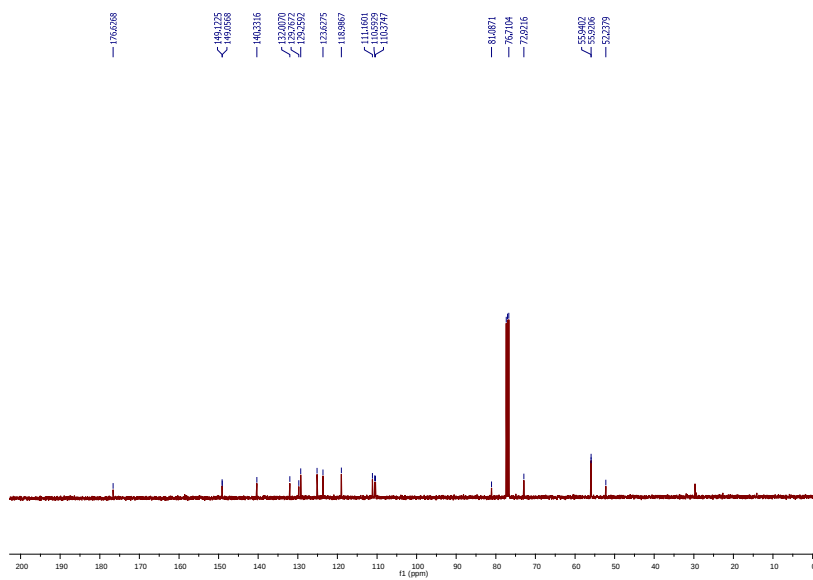
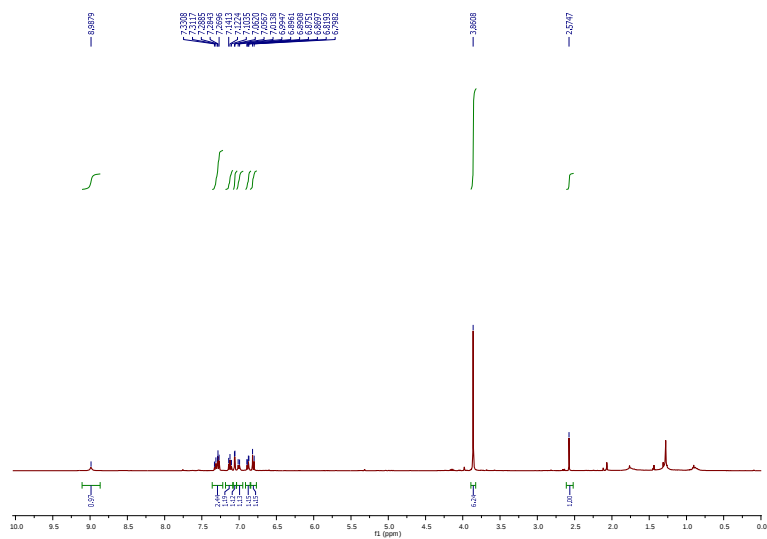
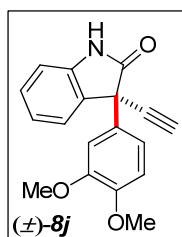
Instrument micrOTOF-Q II 10330

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of ($\pm$)-**8i**



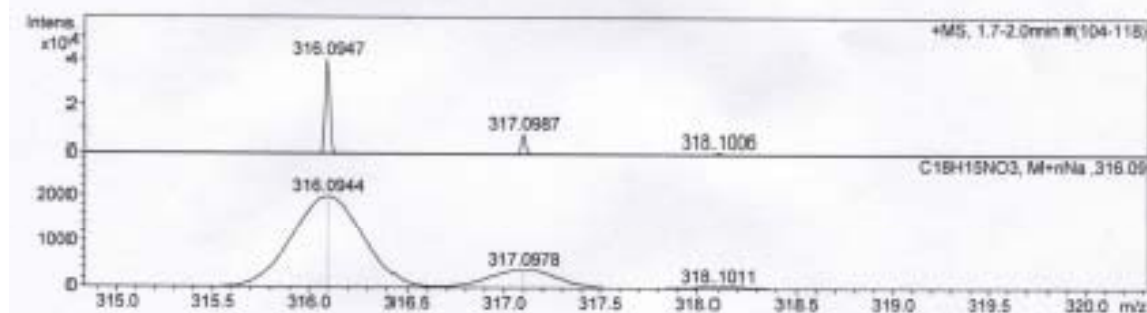
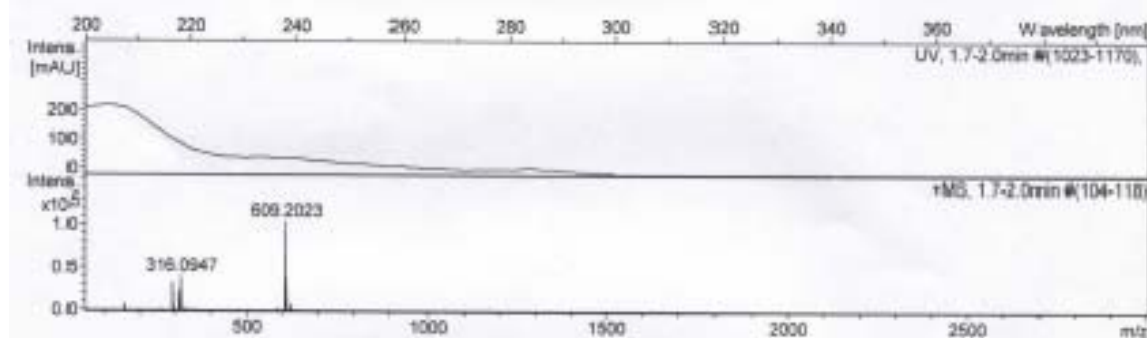
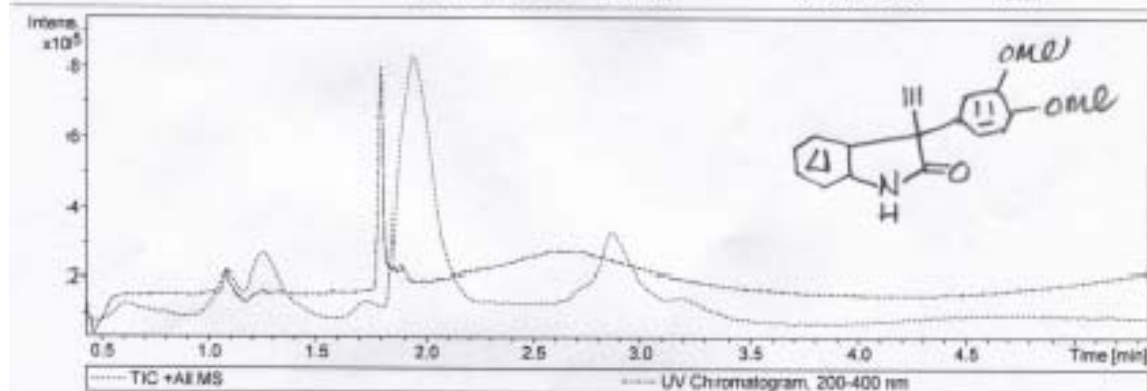
Display Report

Analysis Info

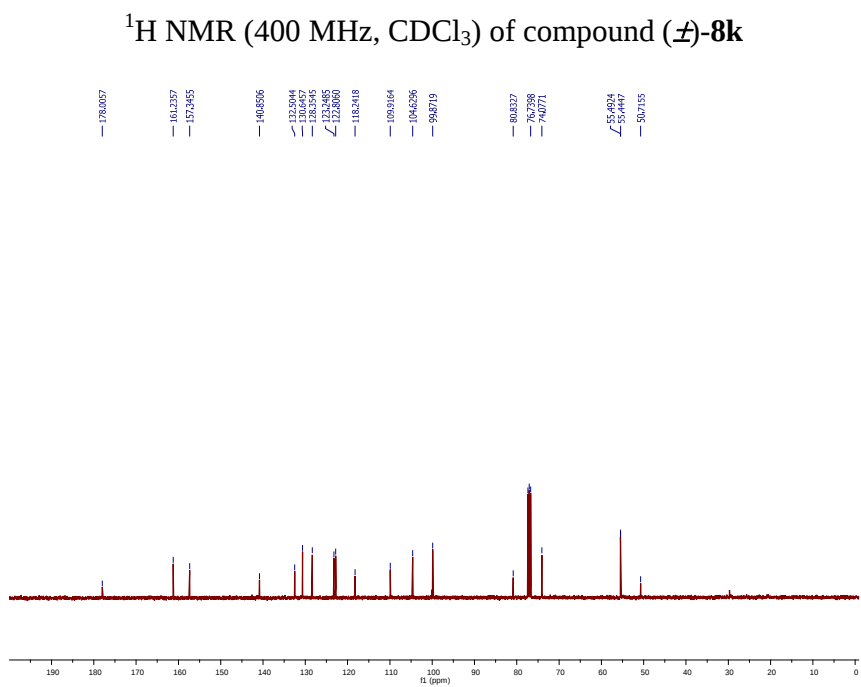
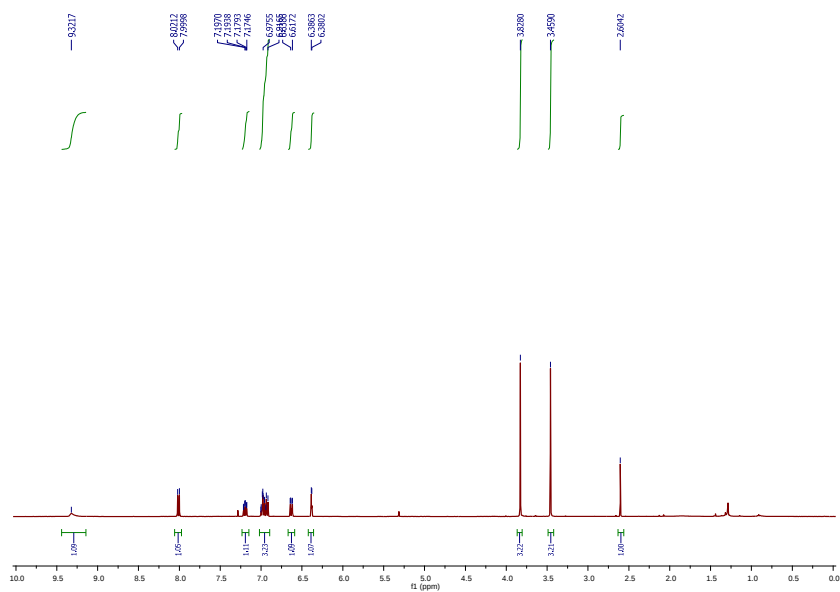
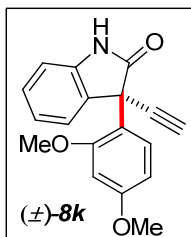
Analysis Name	D:\Data\user data\may2012\25 may\Dr.A.Bisai-SG2-367(R)_1-A.6_01_2368.d	Acquisition Date	5/26/2012 1:05:37 PM
Method	HPLCMS-20 Sept.m	Operator	Meena Sharma
Sample Name	Dr.A.Bisai-SG2-367(R)	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	305 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-8j



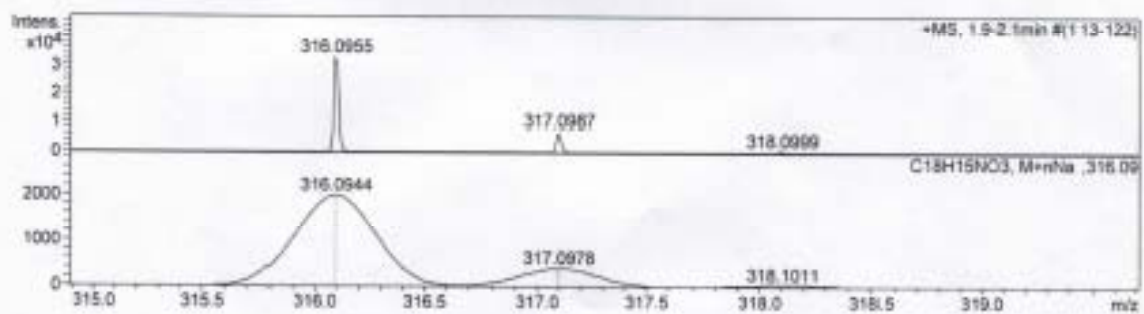
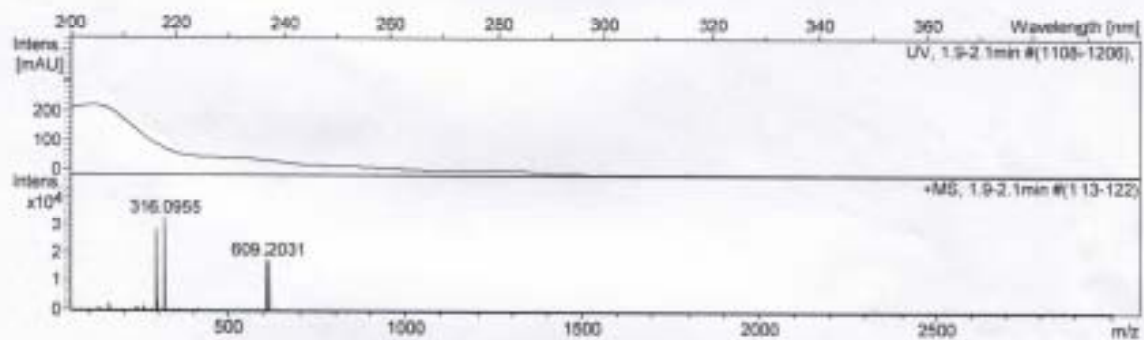
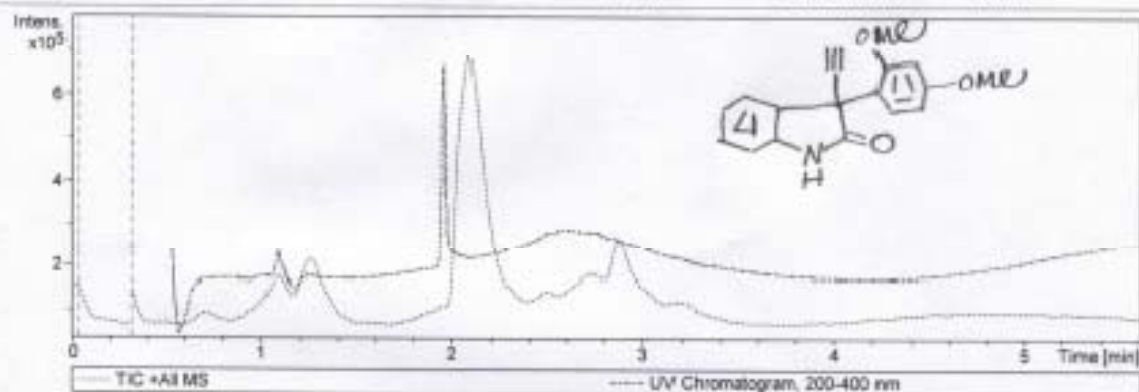
Display Report

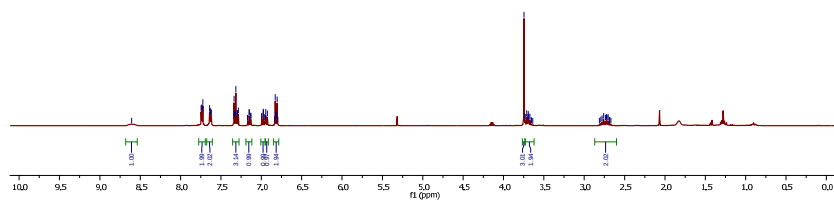
Analysis Info

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Method	HPLCMS-20 Sept.m
Sample Name	Dr.A.Bisai-SG2-371(R)
Comment	
Acquisition Date	5/26/2012 12:53:43 PM
Operator	Meena Sharma
Instrument	microTOF-Q II 10330

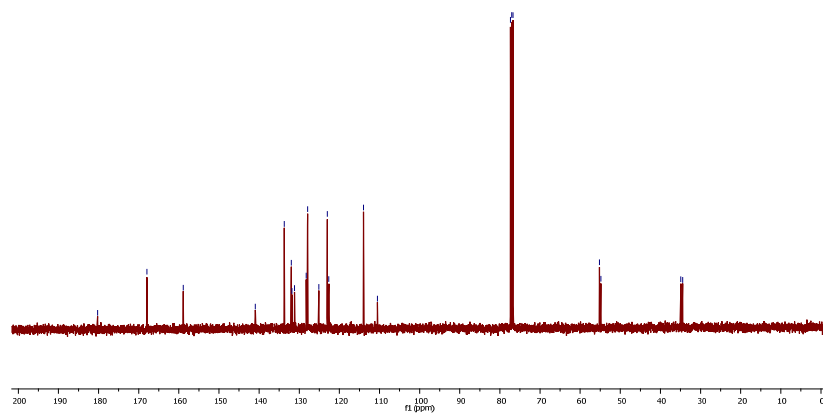
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
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Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste

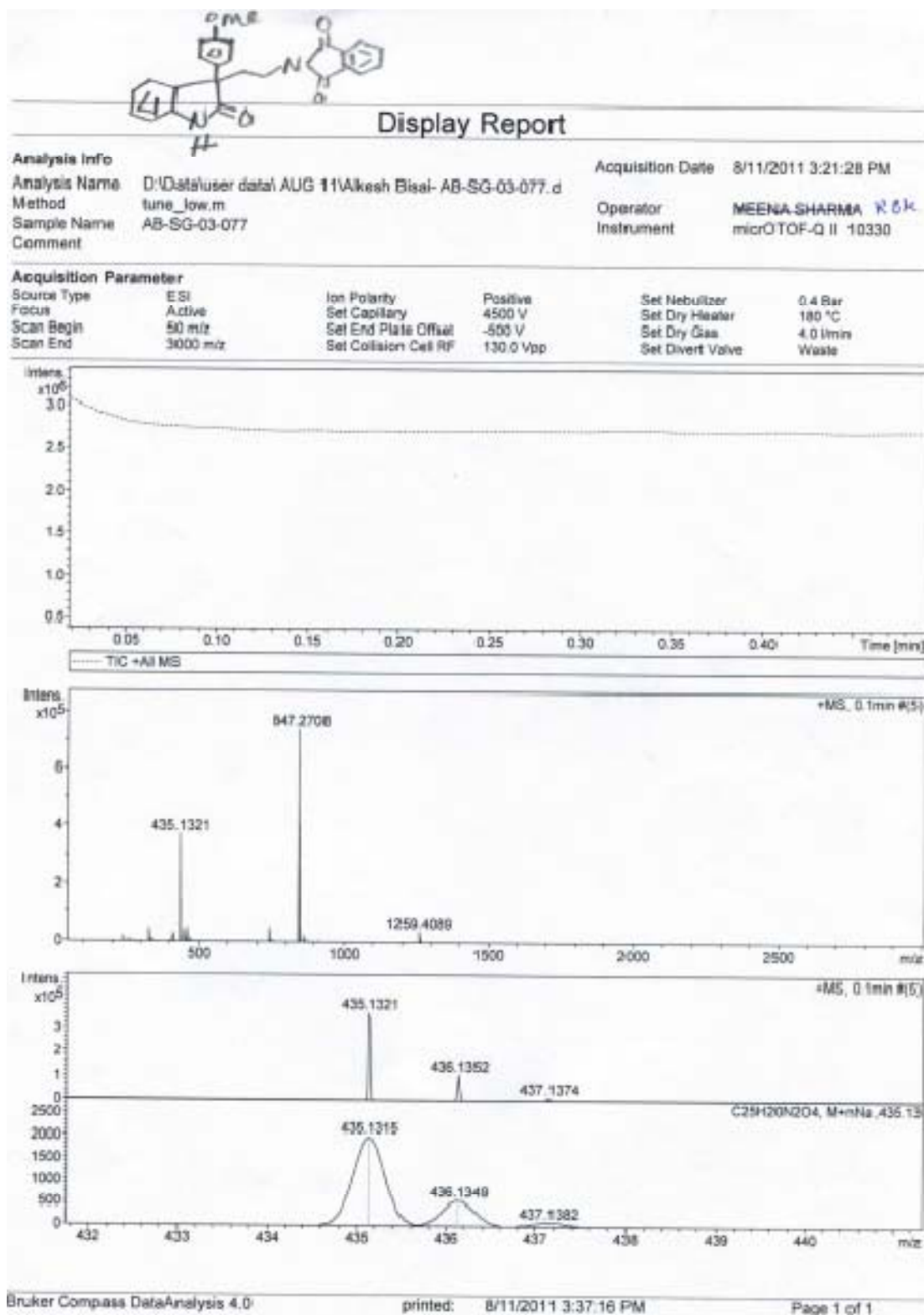




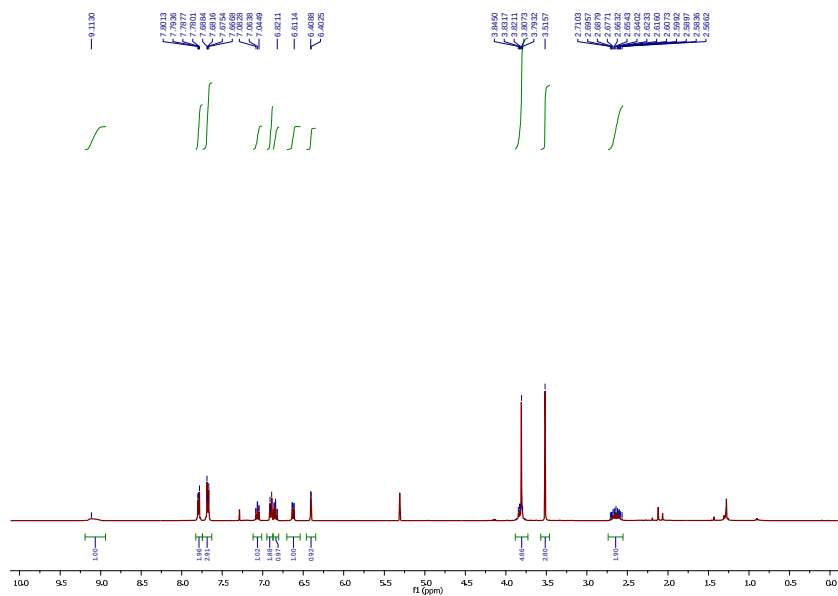
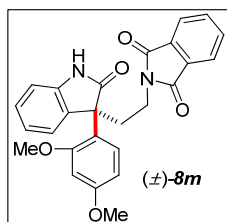
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— 167.9575
— 158.8850
— 140.9342
— 133.7411
— 131.8050
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— 127.9265
— 125.1044
— 123.0101
— 122.6200
— 113.9767
— 110.5052
77.3512
77.0333
76.7157
55.2112
54.8206
34.9112
34.4007



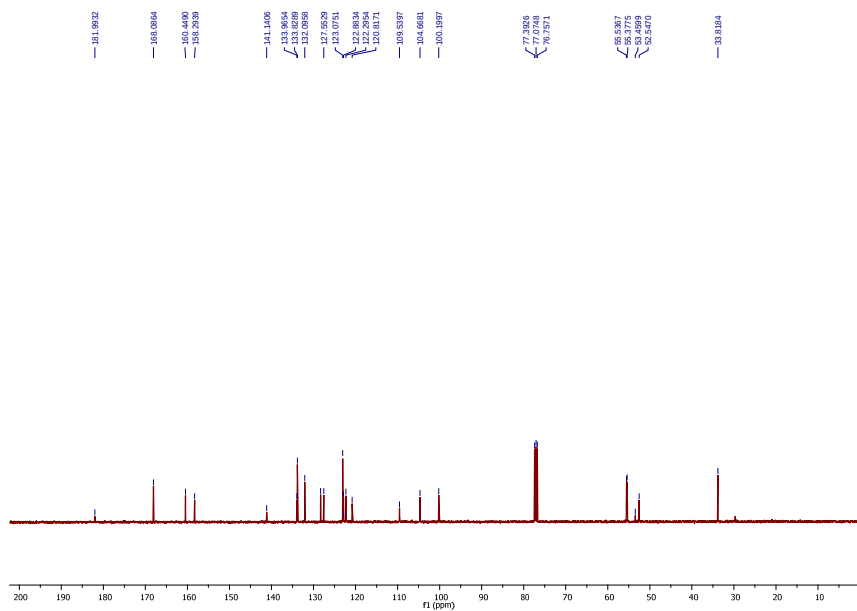
S58



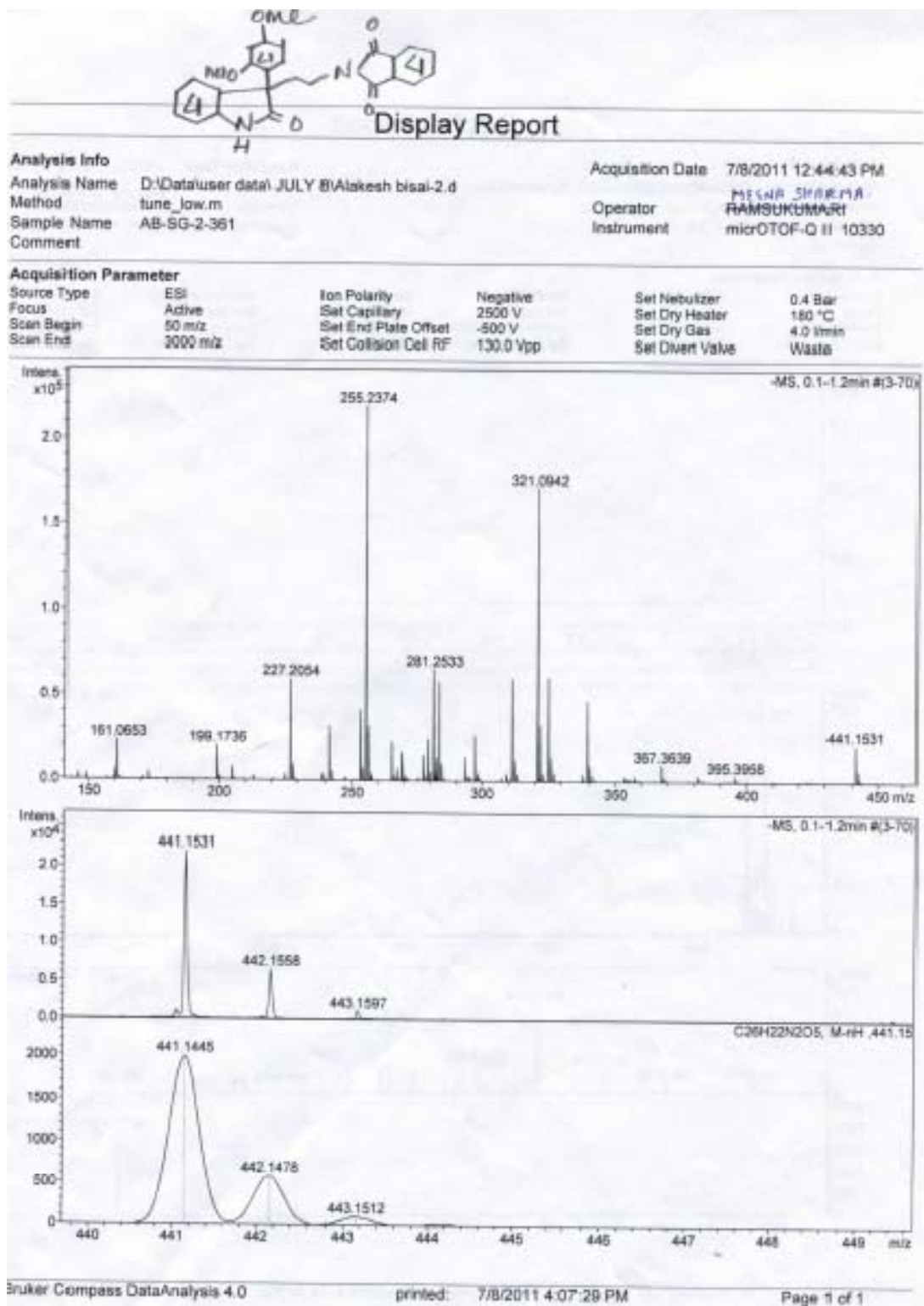
Scanned copy of mass spectrum of (*±*)-**8l**



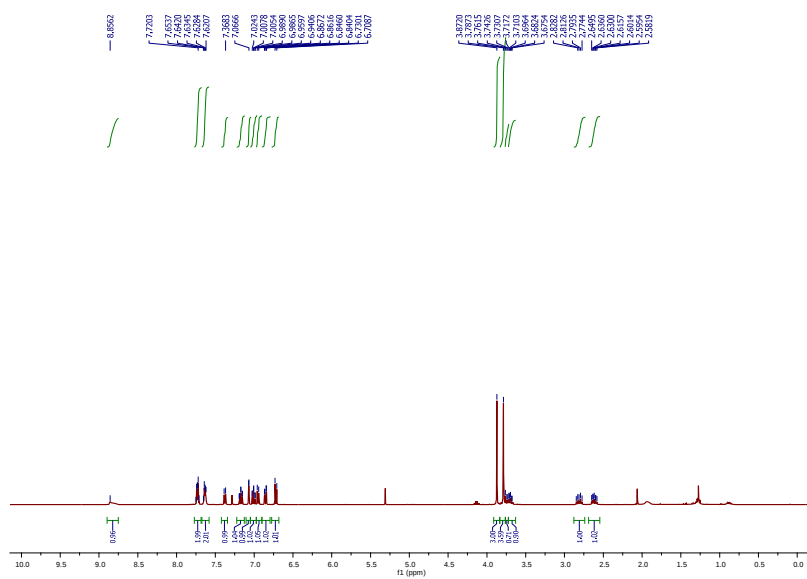
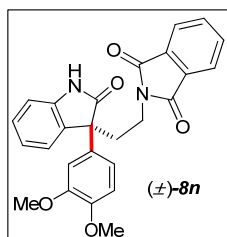
¹H NMR (400 MHz, CDCl₃) of compound (±)-**8m**

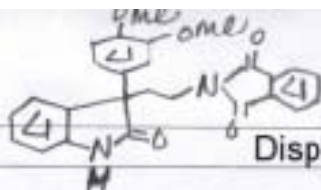


¹³C NMR (100 MHz, CDCl₃) of compound (±)-**8m**



Scanned copy of mass spectrum of ($\pm$)-8m





Display Report

Analysis Info

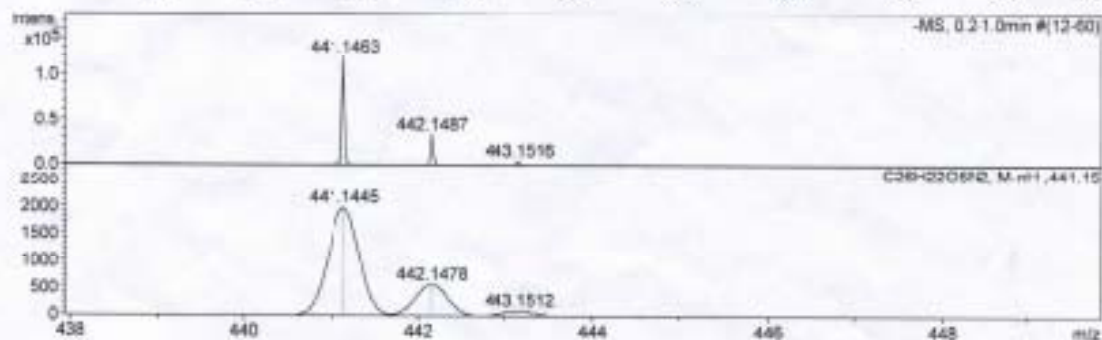
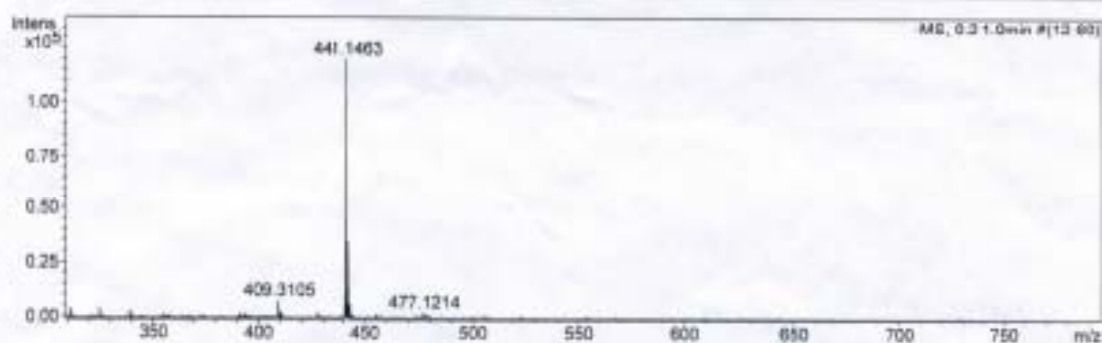
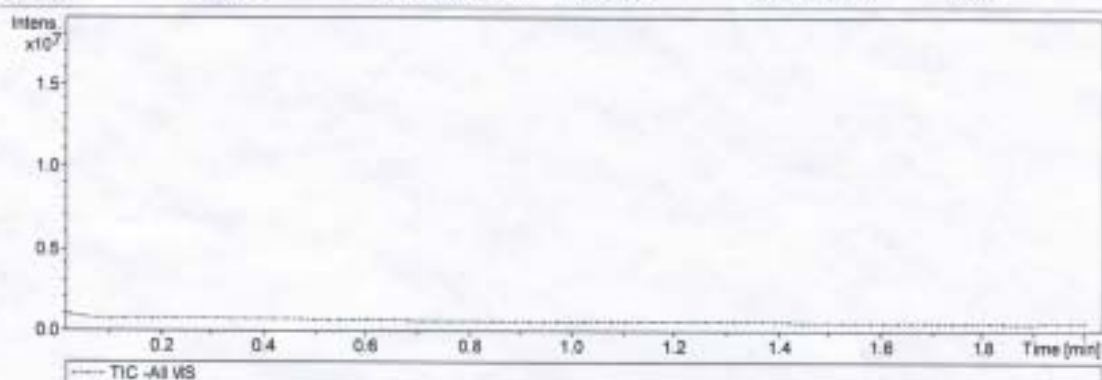
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 Method tune_low.m
 Sample Name AB-SG-2-362
 Comment

Acquisition Date 7/8/2011 2:51:34 PM

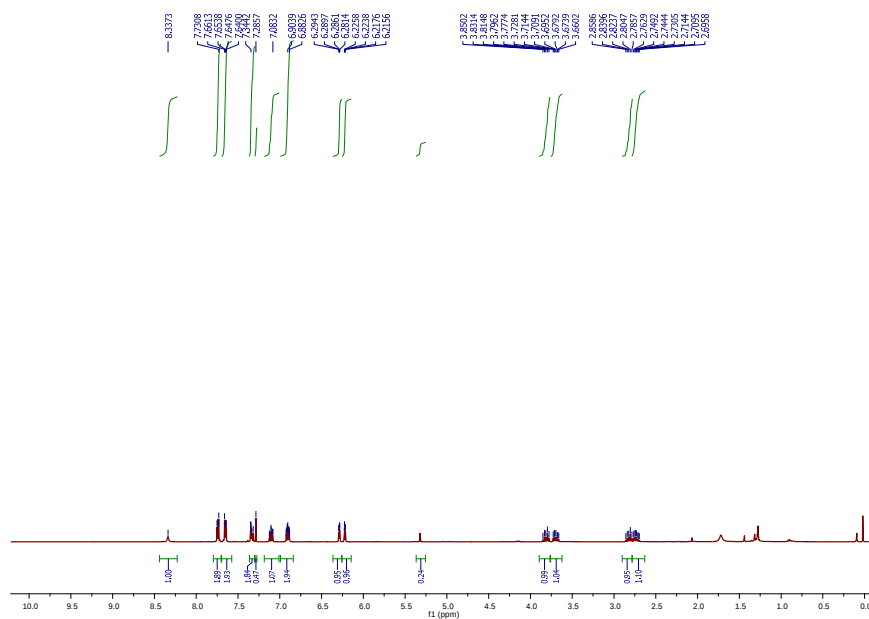
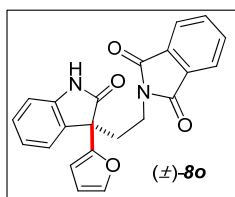
Operator RAMSUKUMARI
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

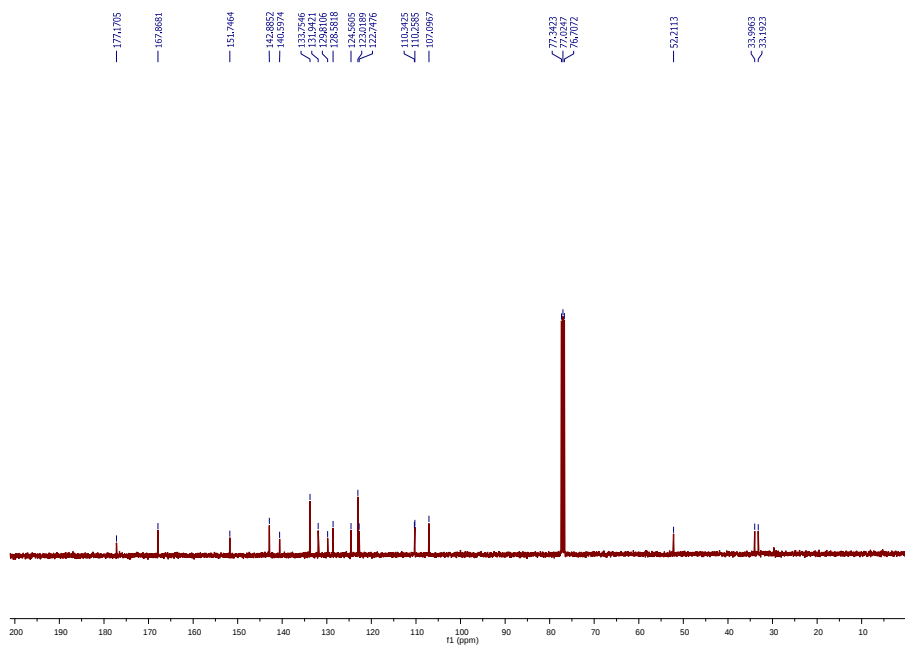
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



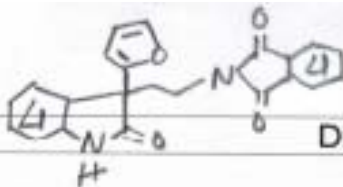
Scanned copy of mass spectrum of ($\pm$)-8n



¹H NMR (400 MHz, CDCl₃) of compound (±)-**8o**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**8o**



Display Report

Analysis Info

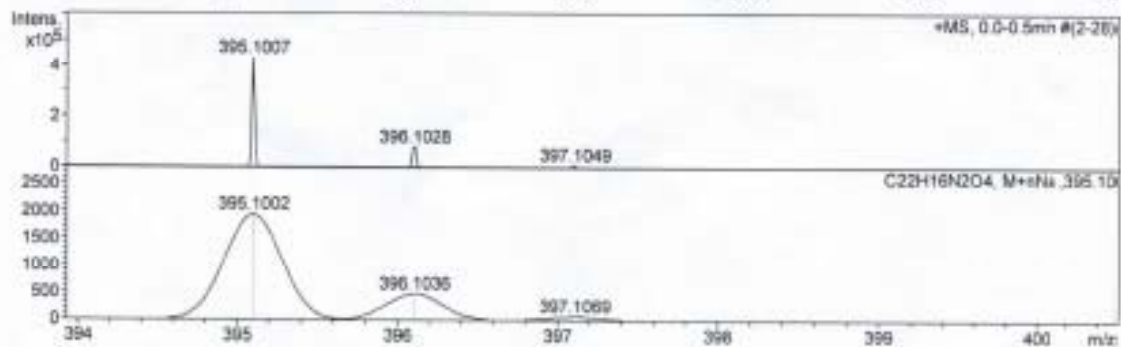
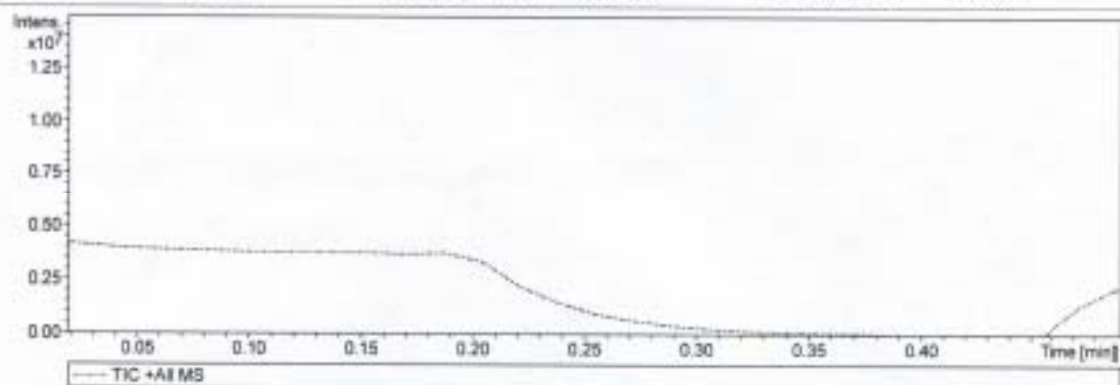
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 Comment:

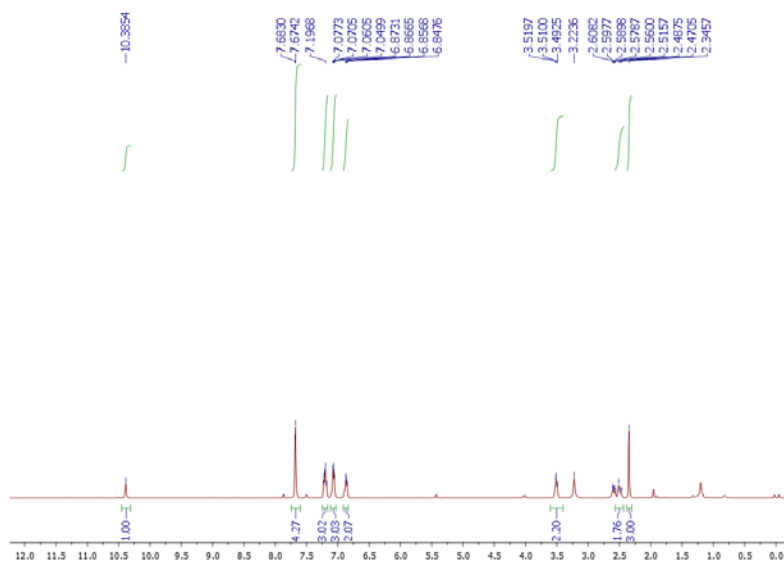
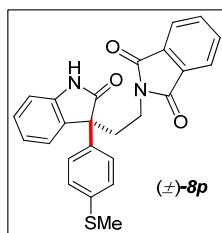
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Operator: MEENA SHARMA
 Instrument: micrOTOF-Q II 10330

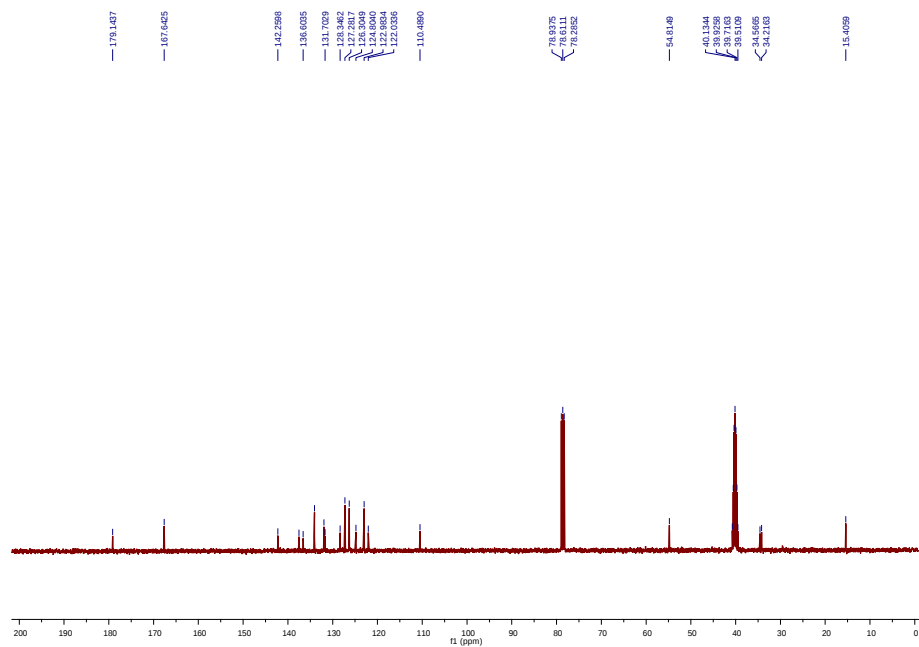
Acquisition Parameter

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Focus	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	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste





¹H NMR (400 MHz, CDCl₃) of compound (±)-**8p**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**8p**

Display Report

Analysis Info

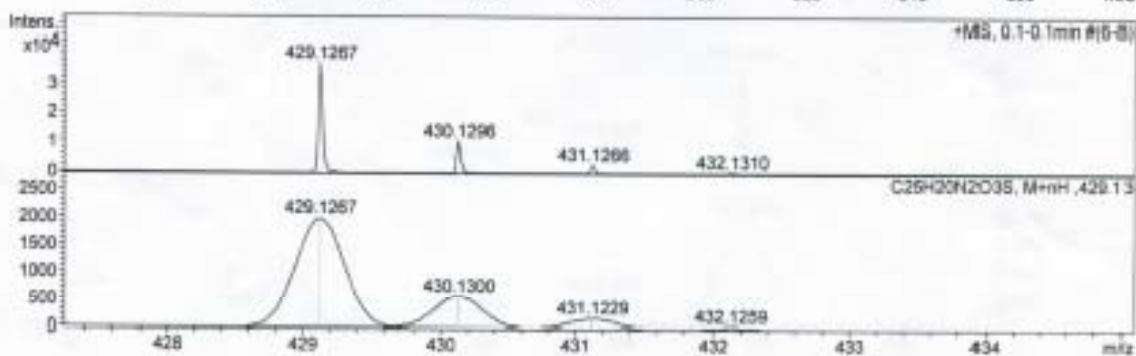
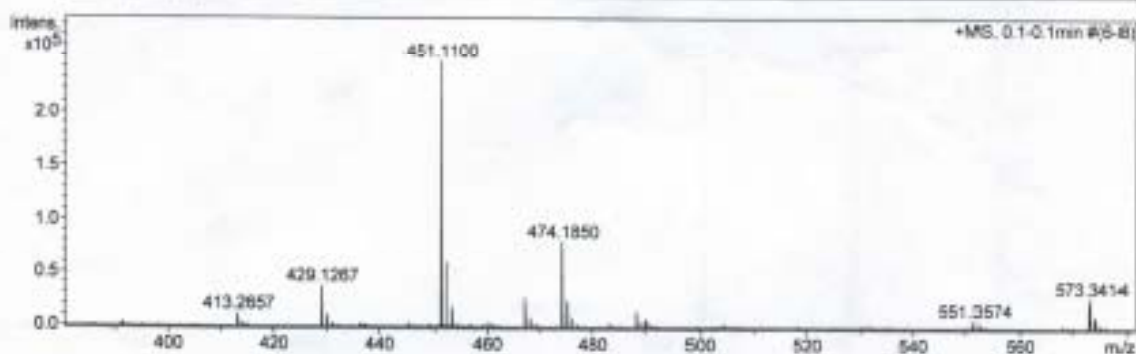
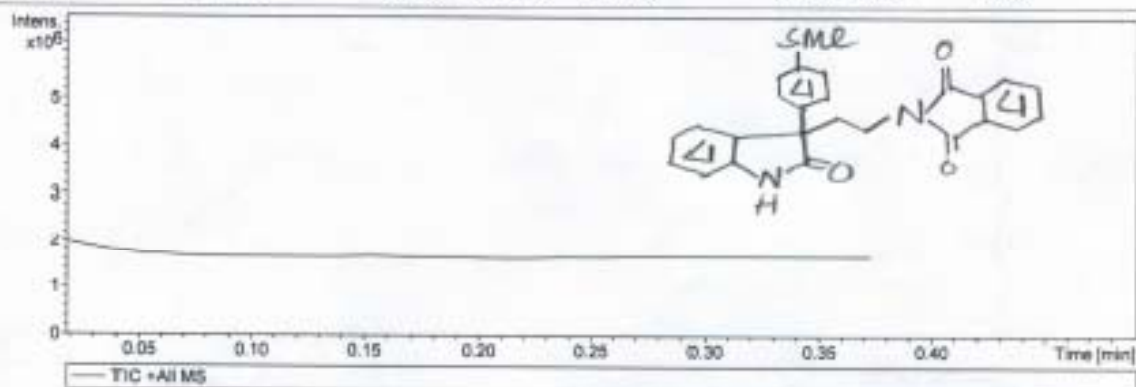
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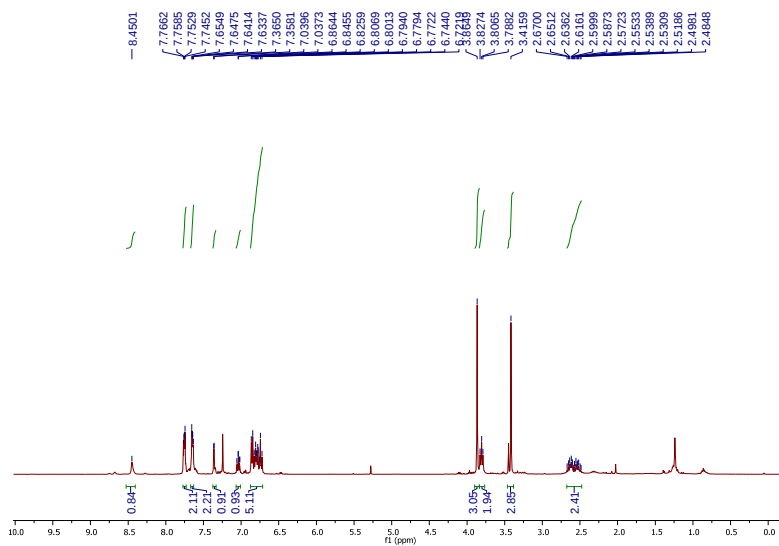
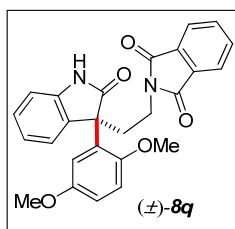
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 Instrument: micrOTOF-Q II 10330

Acquisition Parameter

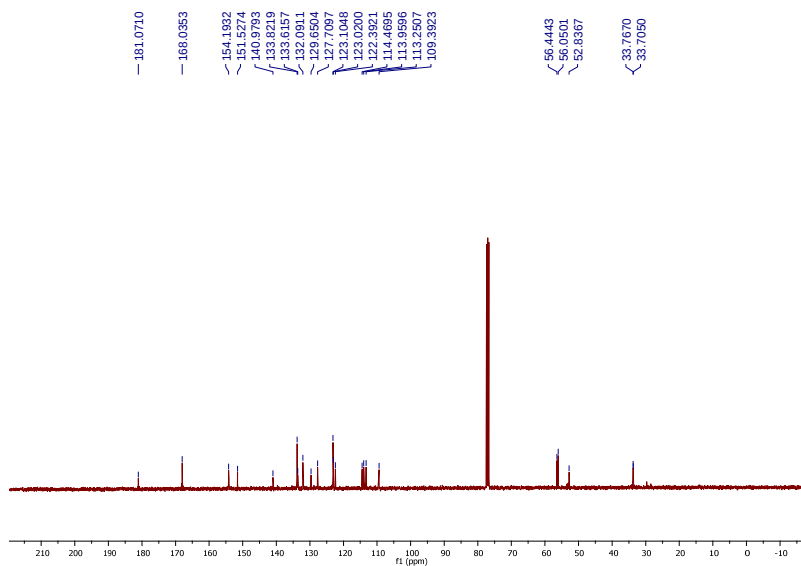
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of ($\pm$)-8p



¹H NMR (400 MHz, CDCl₃) of compound (±)-8q



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8q

Display Report

Analysis Info

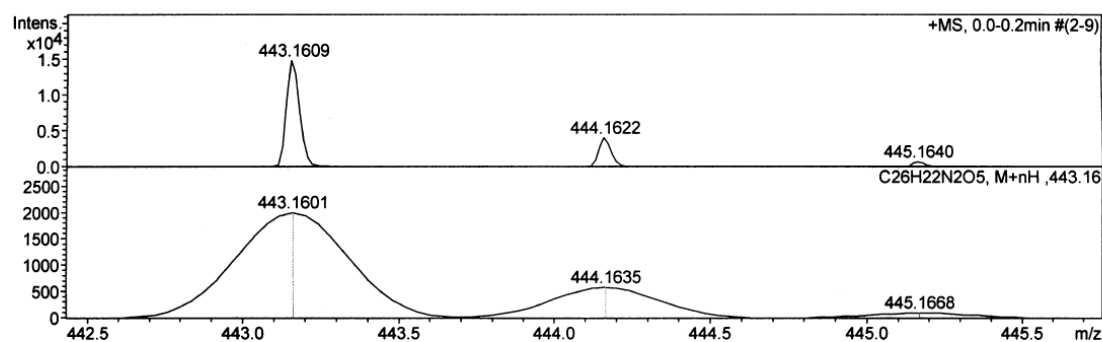
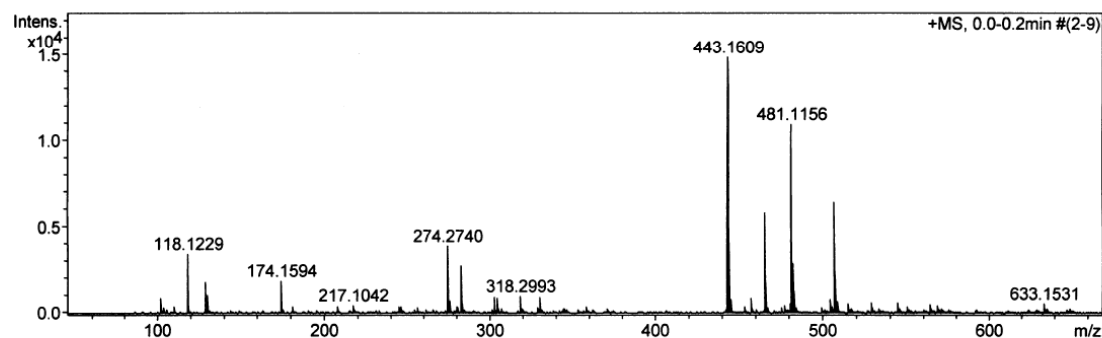
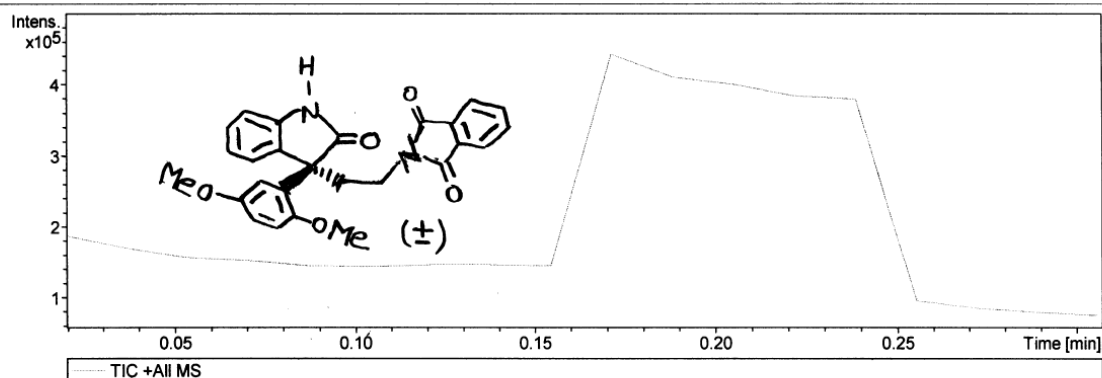
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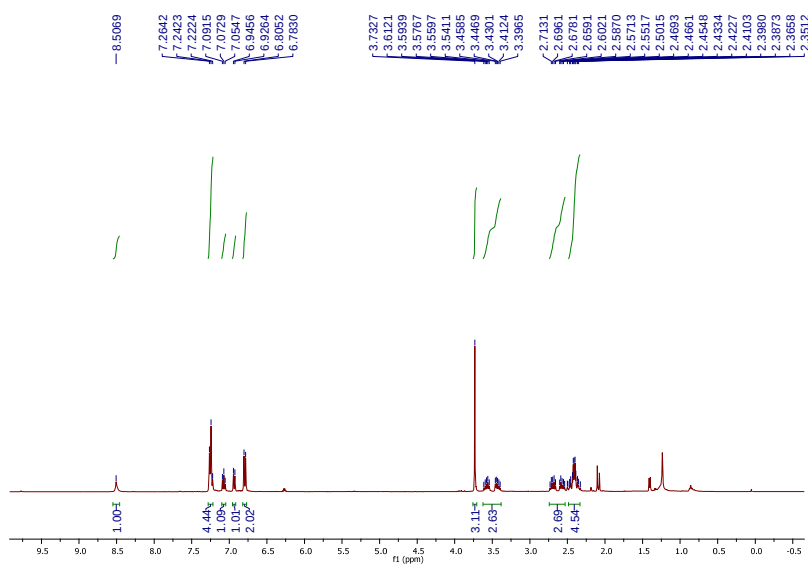
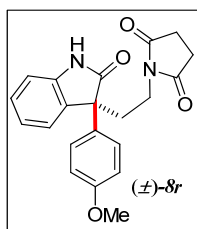
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Operator Amit
 Instrument micrOTOF-Q II 10330

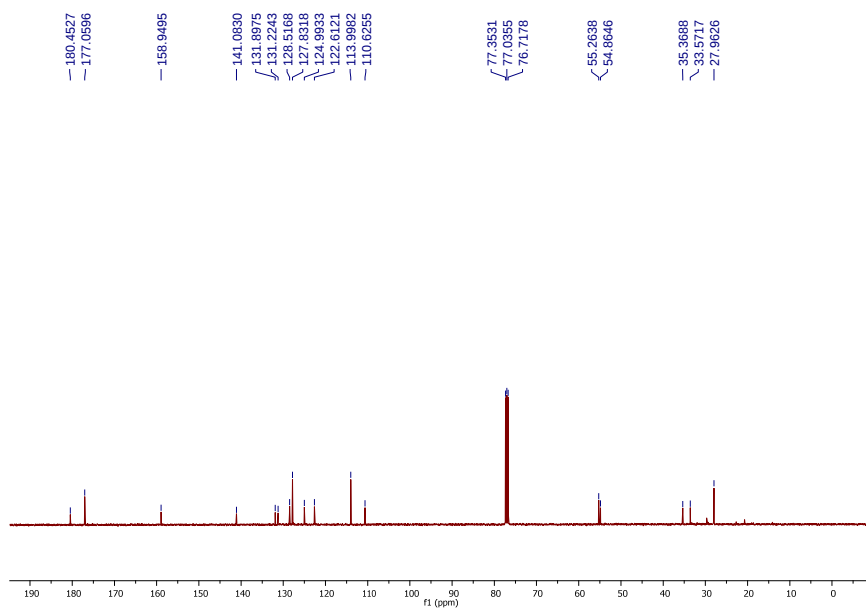
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste





¹H NMR (400 MHz, CDCl₃) of compound (±)-**8r**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**8r**

Display Report

Analysis Info

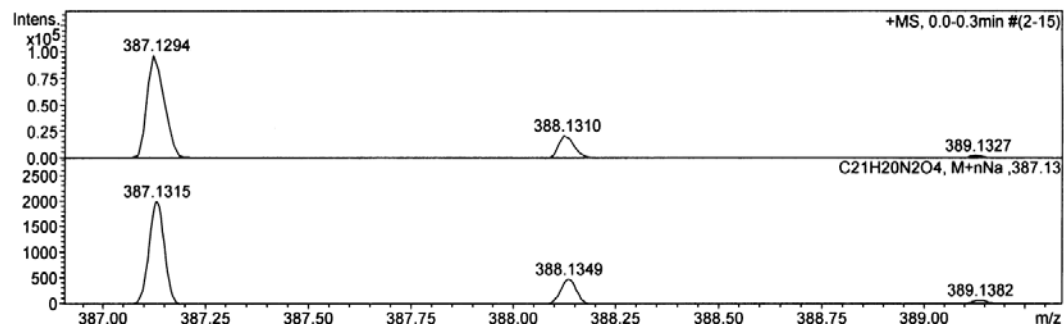
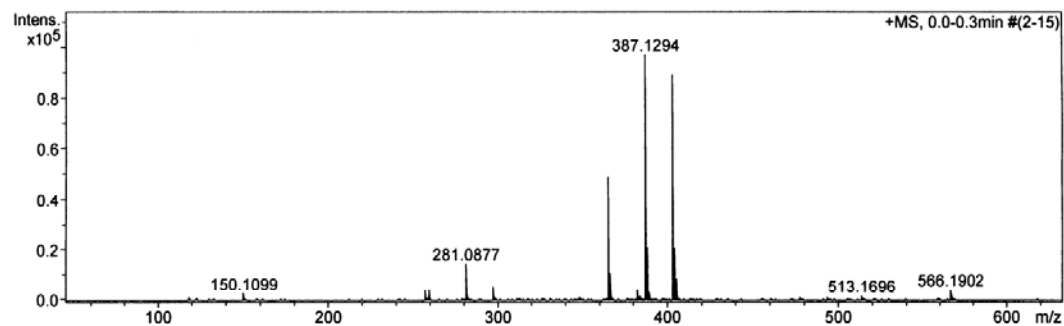
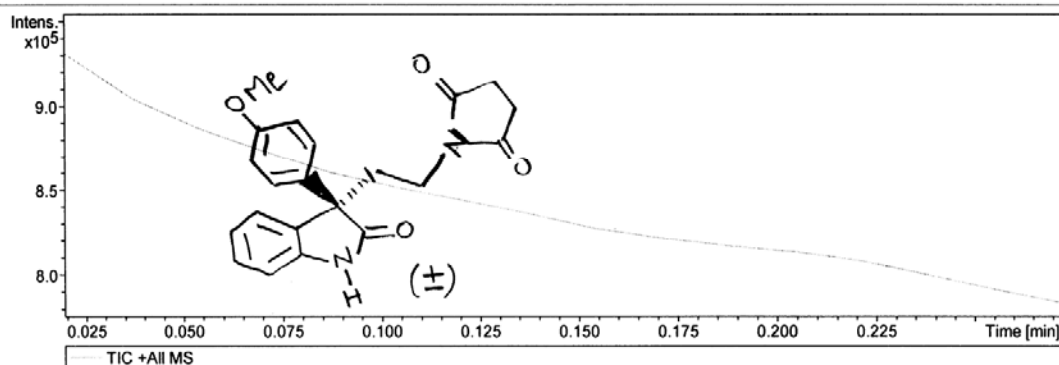
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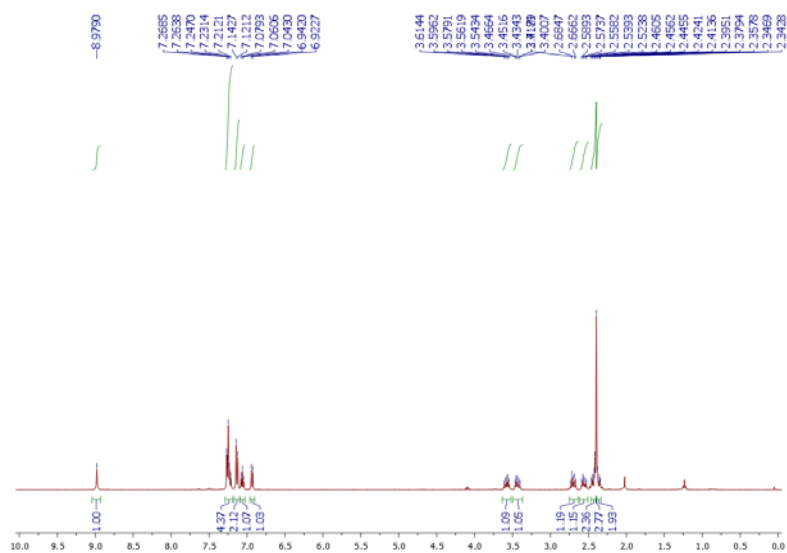
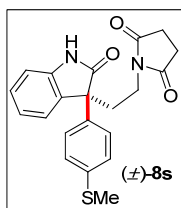
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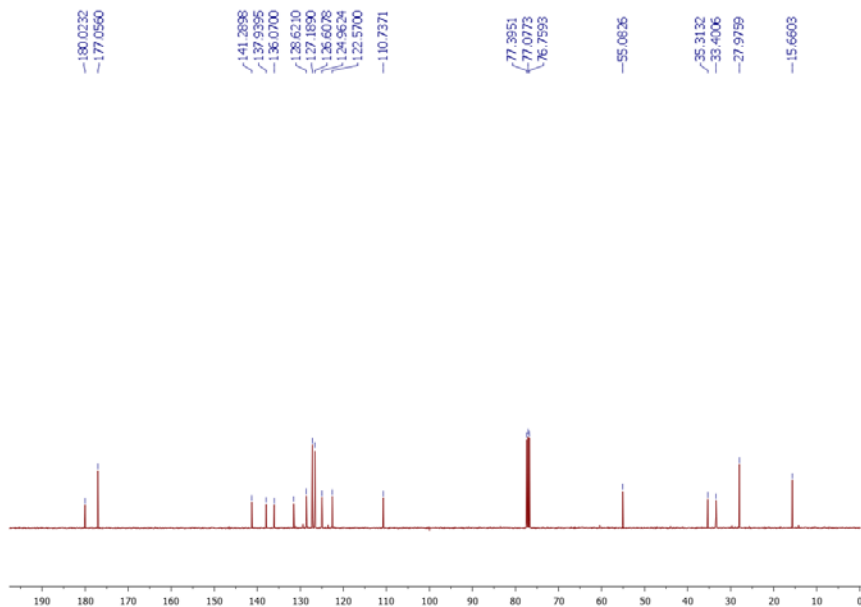
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of $(\pm)$ -8r



¹H NMR (400 MHz, CDCl₃) of compound (±)-8s



¹³C NMR (100 MHz, CDCl₃) of compound (±)-8s

Display Report

Analysis Info

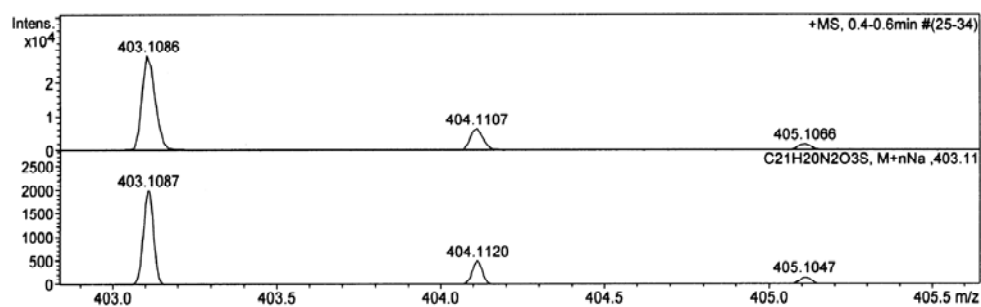
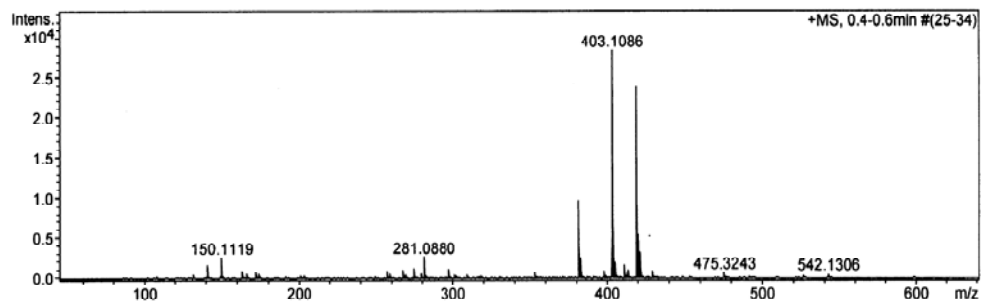
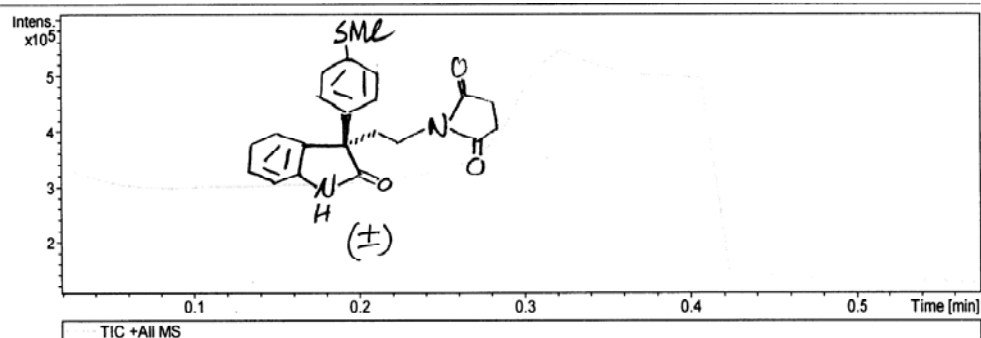
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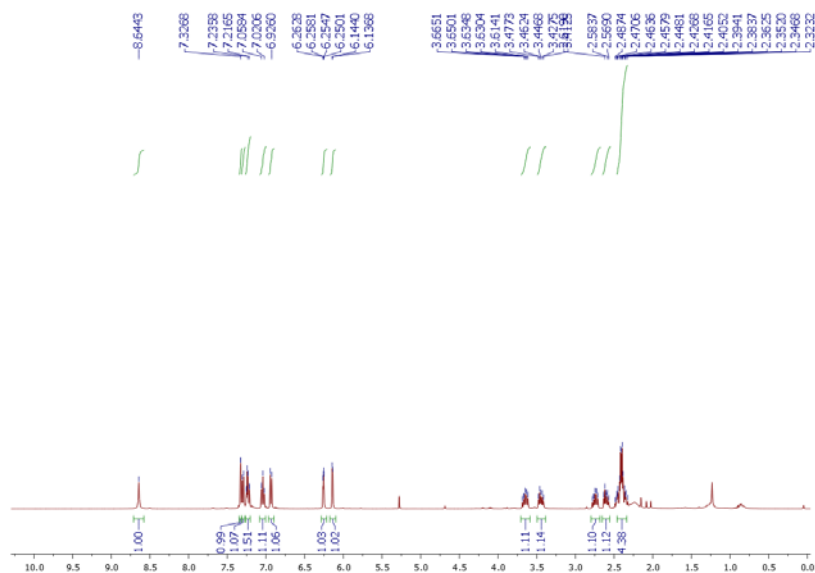
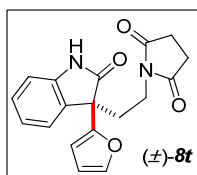
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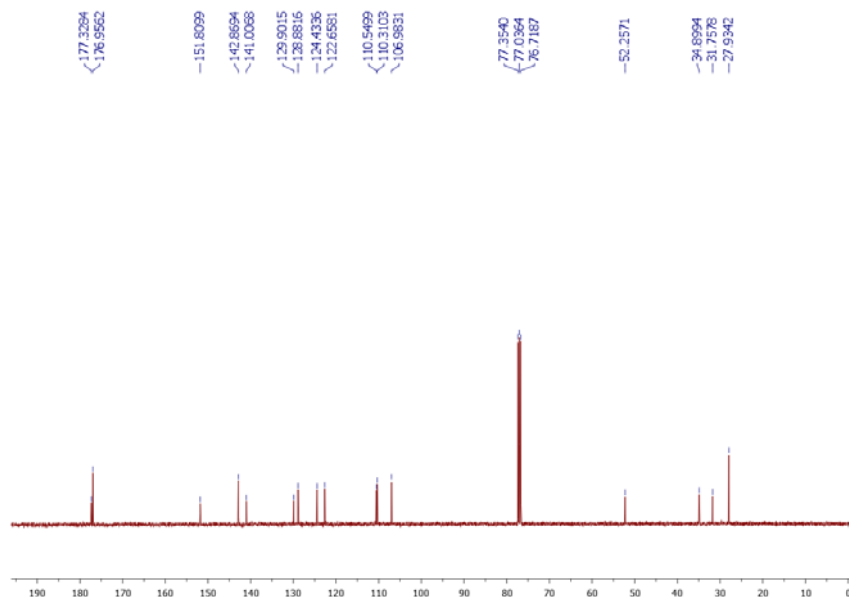
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-8s



^1H NMR (400 MHz, CDCl_3) of compound (±)-**8t**



^{13}C NMR (100 MHz, CDCl_3) of compound (±)-**8t**

Display Report

Analysis Info

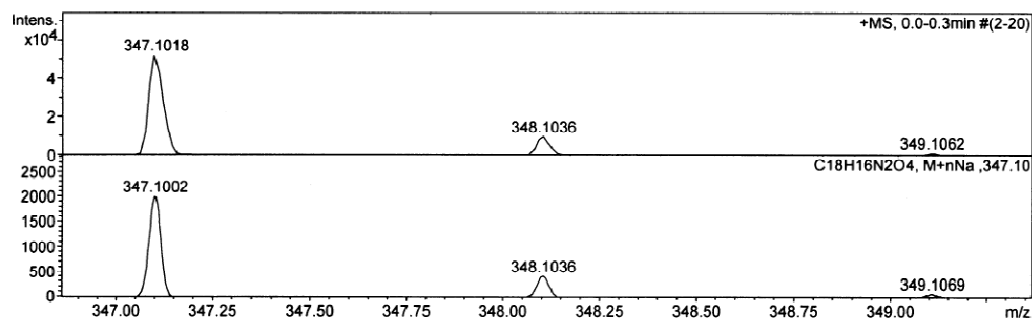
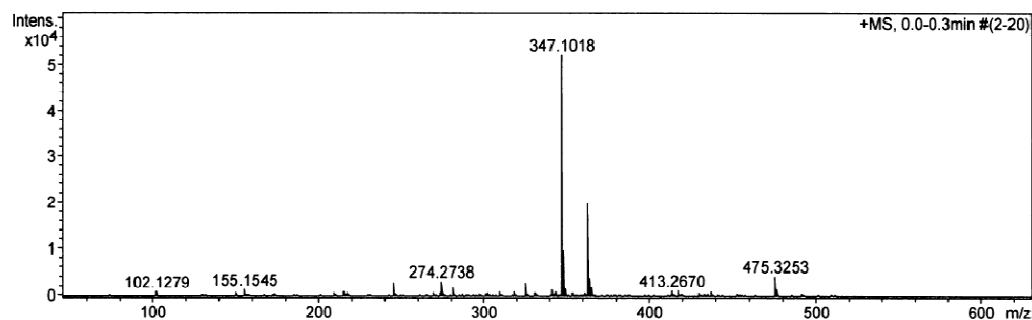
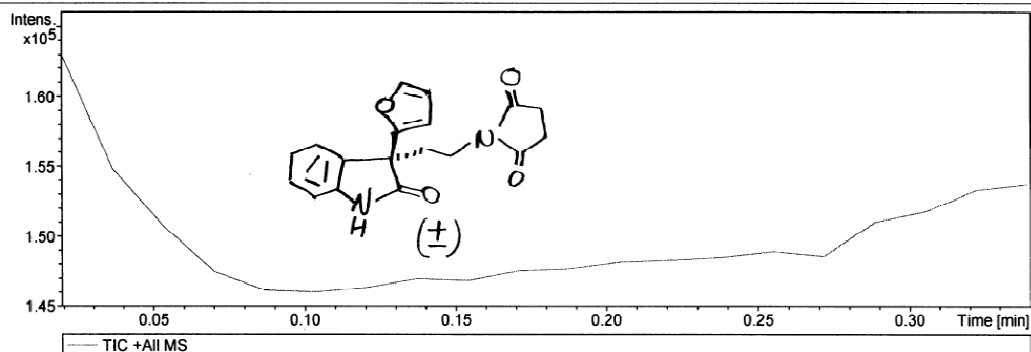
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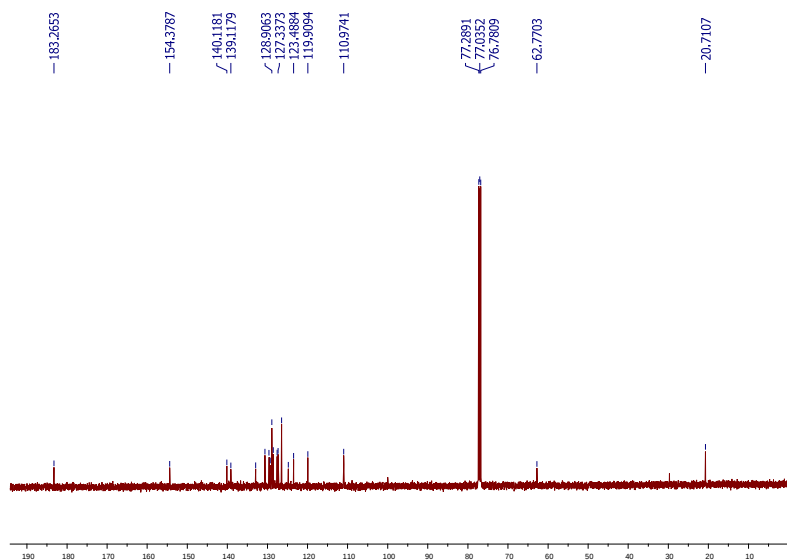
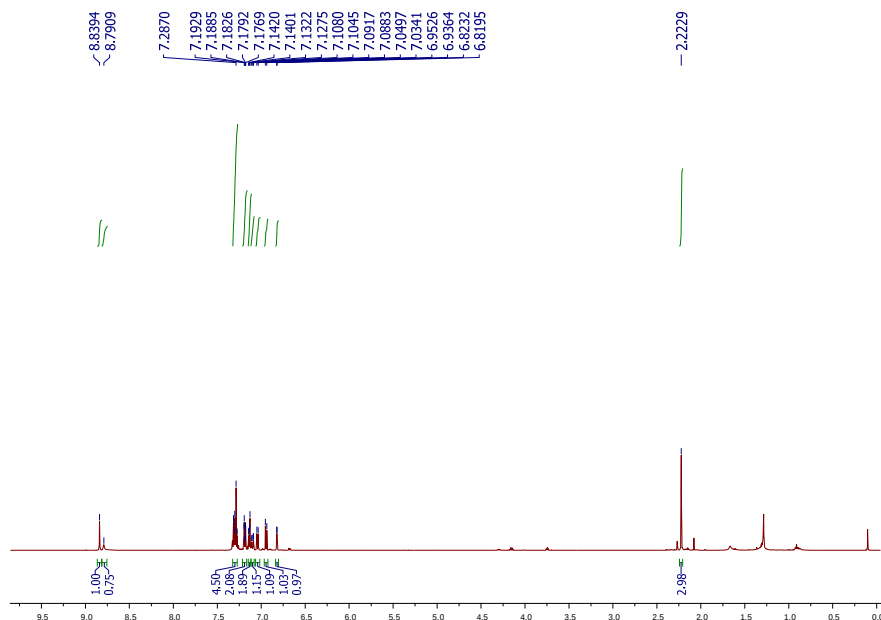
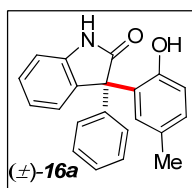
Operator Amit
Instrument micrOTOF-Q II 10330

Acquisition Parameter

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Scanned copy of mass spectrum of (±)-8t



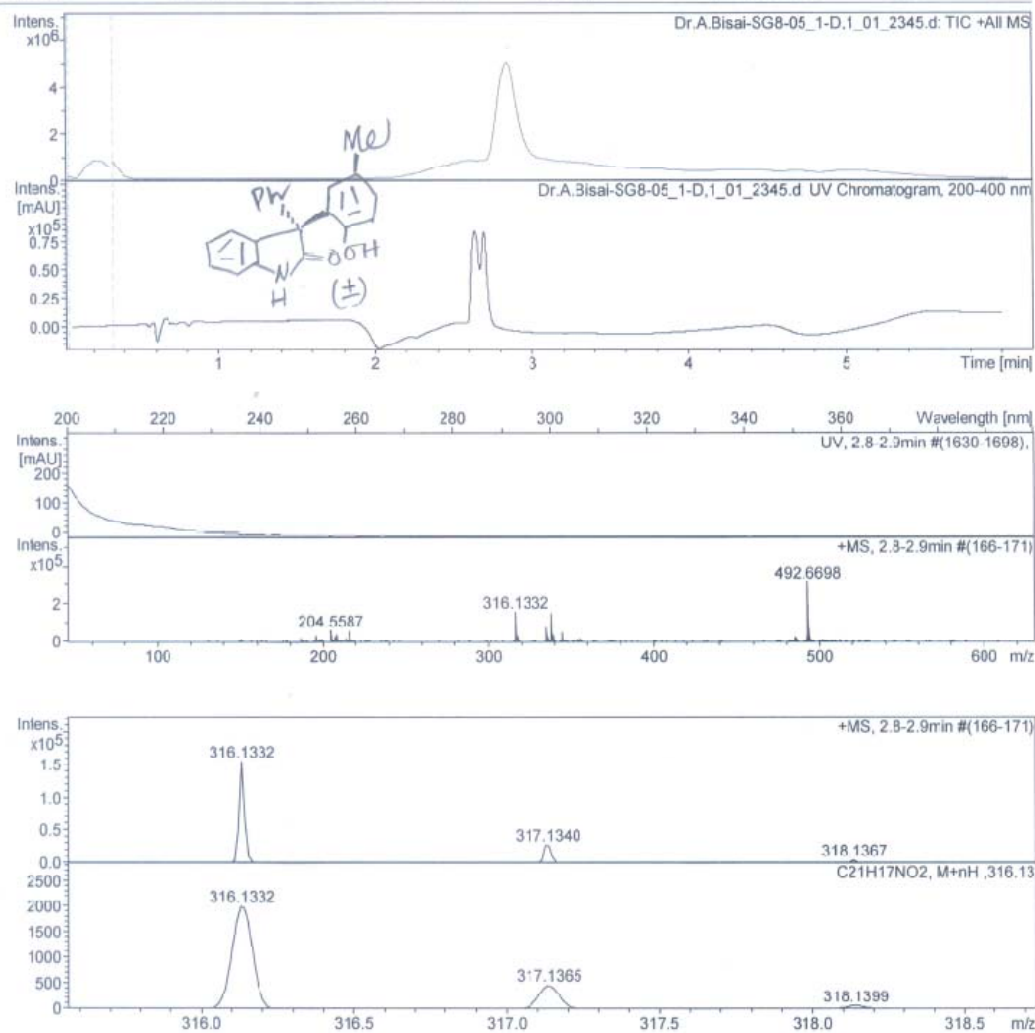
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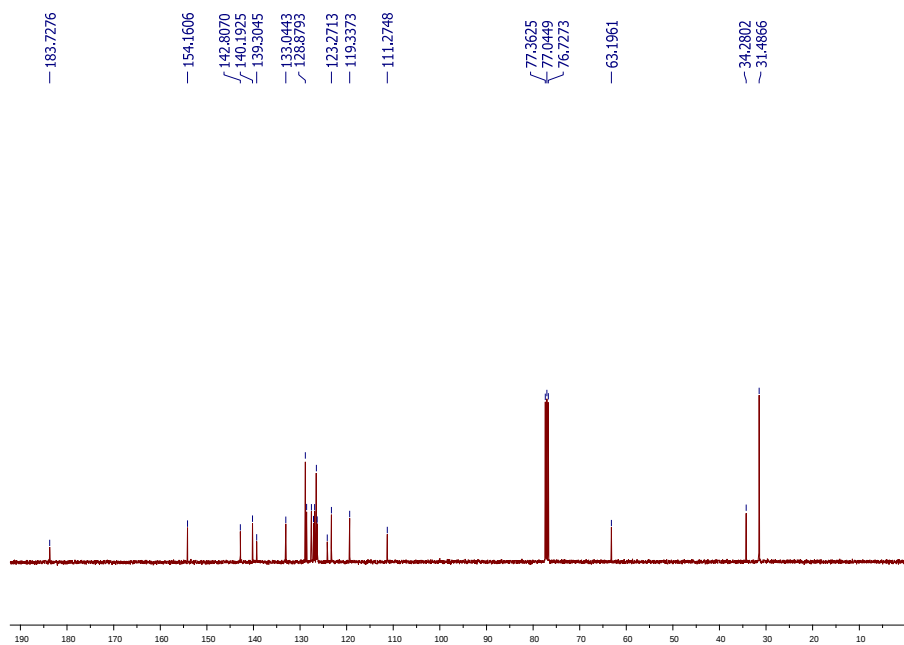
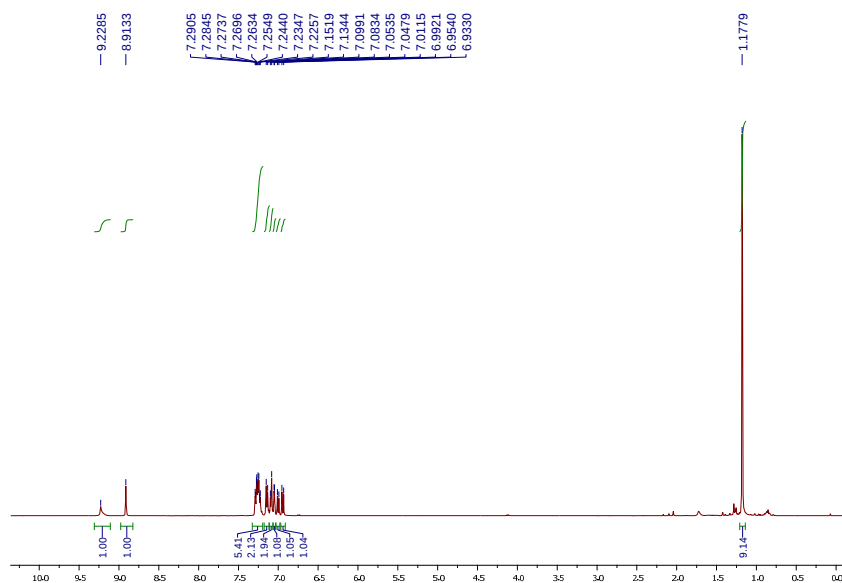
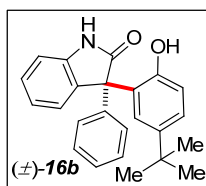
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Sample Name	Dr.A.Bisai-SG8-05
Comment	
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Operator	Amit
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16a



Display Report

Analysis Info

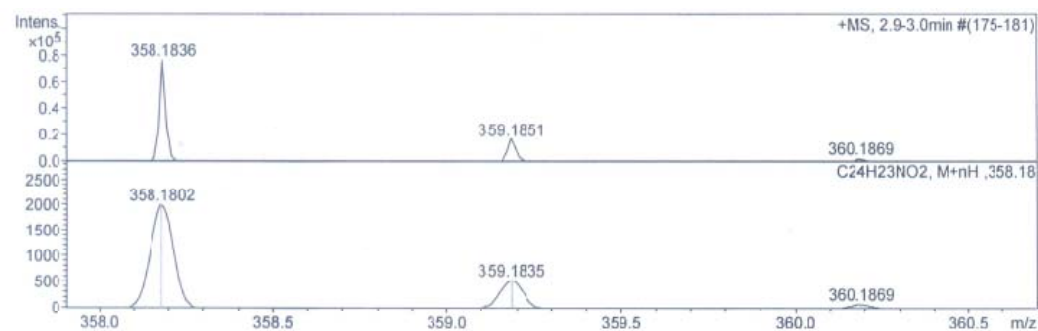
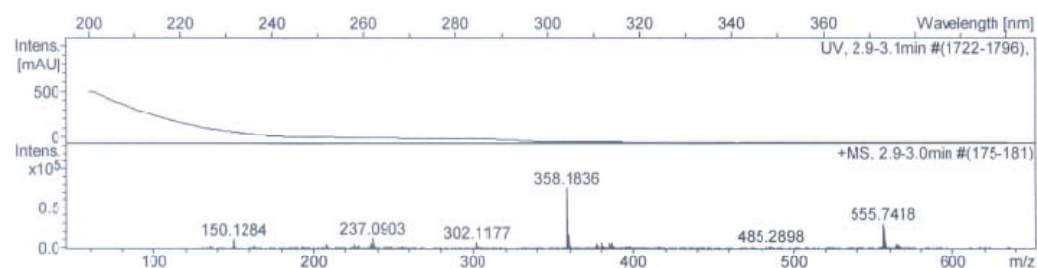
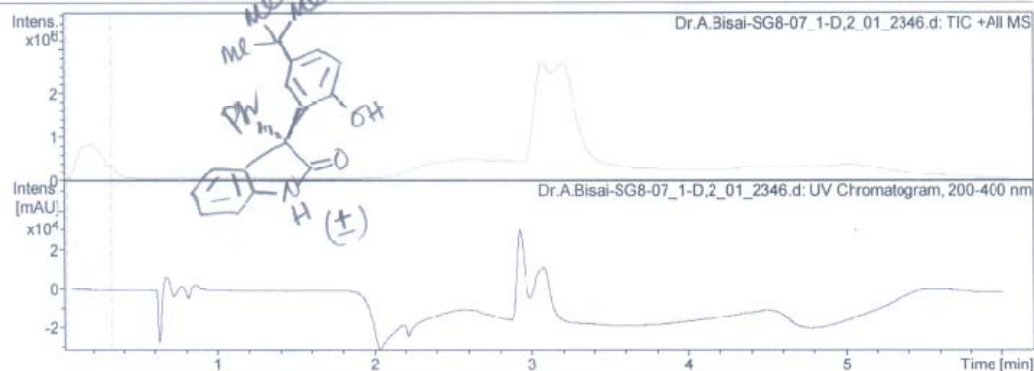
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 Sample Name Dr.A.Bisai-SG8-07
 Comment

Acquisition Date 4/25/2014 2:03:08 AM

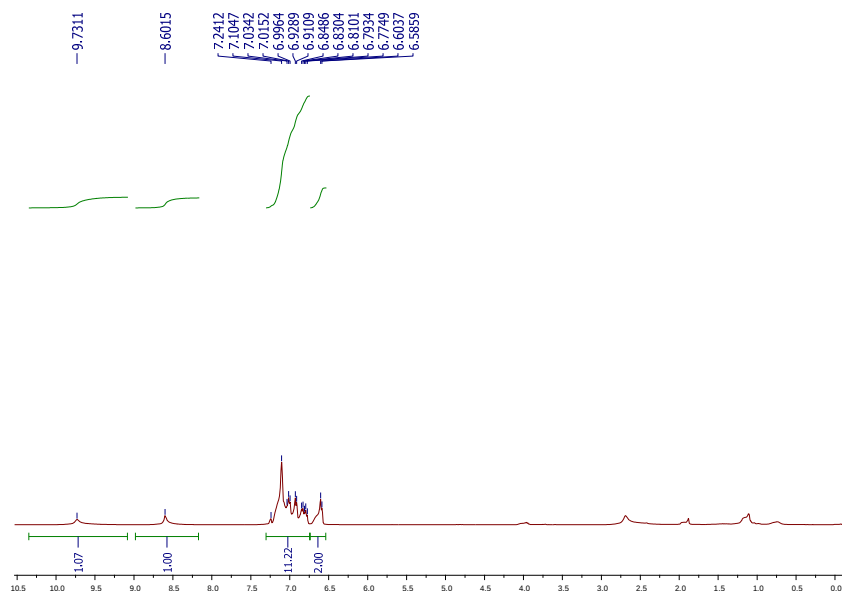
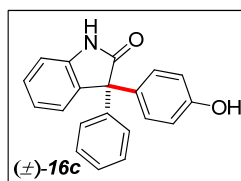
Operator Amit
 Instrument micrCTOF-Q II 10330

Acquisition Parameter

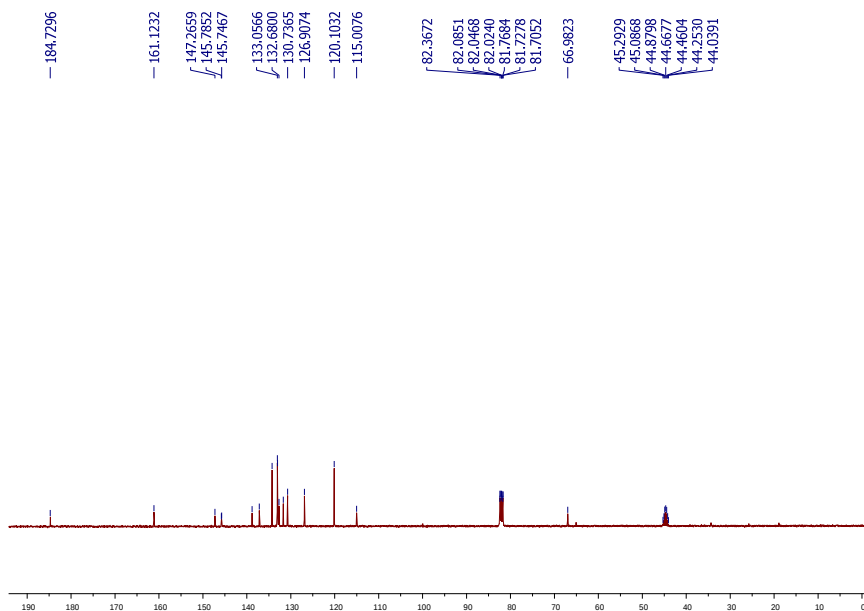
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16b



¹H NMR (400 MHz, 0.4 mL CDCl₃, 0.1 mL DMSO-D₆) of compound (±)-16c



¹³C NMR (100 MHz, 0.4 mL CDCl₃, 0.1 mL DMSO-D₆) of compound (±)-16c

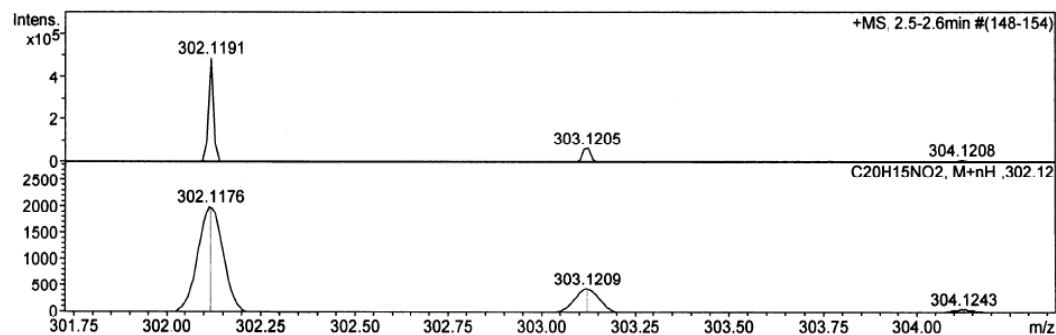
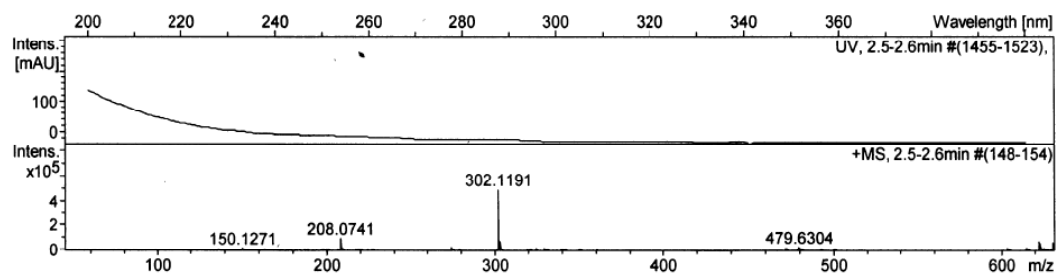
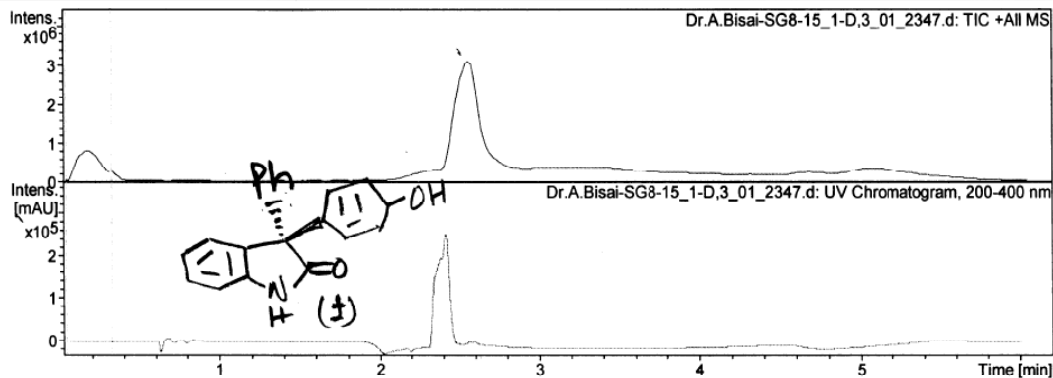
Display Report

Analysis Info

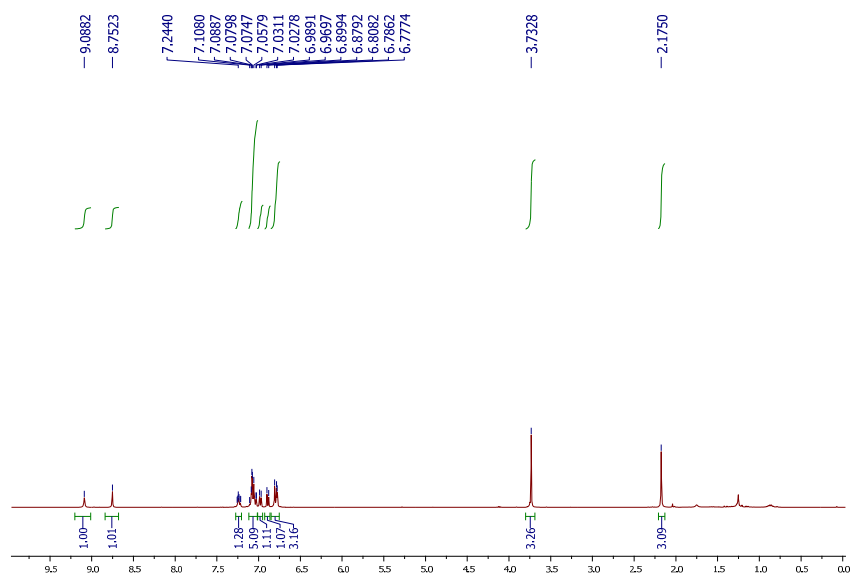
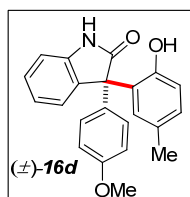
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Sample Name	Dr.A.Bisai-SG8-15	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

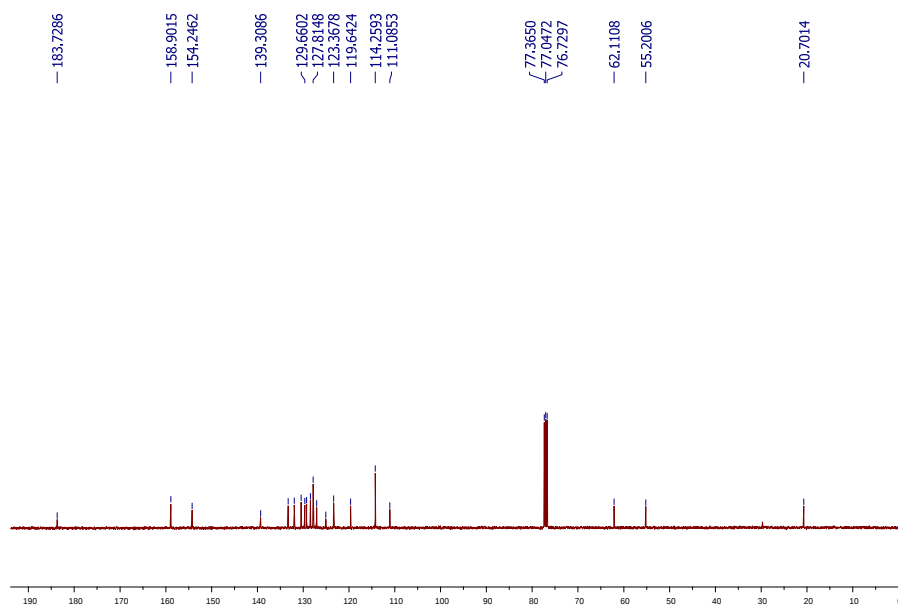
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Scan End	3000 m/z	Set End Plate Offset	-500 V
		Set Collision Cell RF	130.0 Vpp
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16c



^1H NMR (400 MHz, CDCl_3) of compound (±)-16d



^{13}C NMR (100 MHz, CDCl_3) of compound (±)-16d

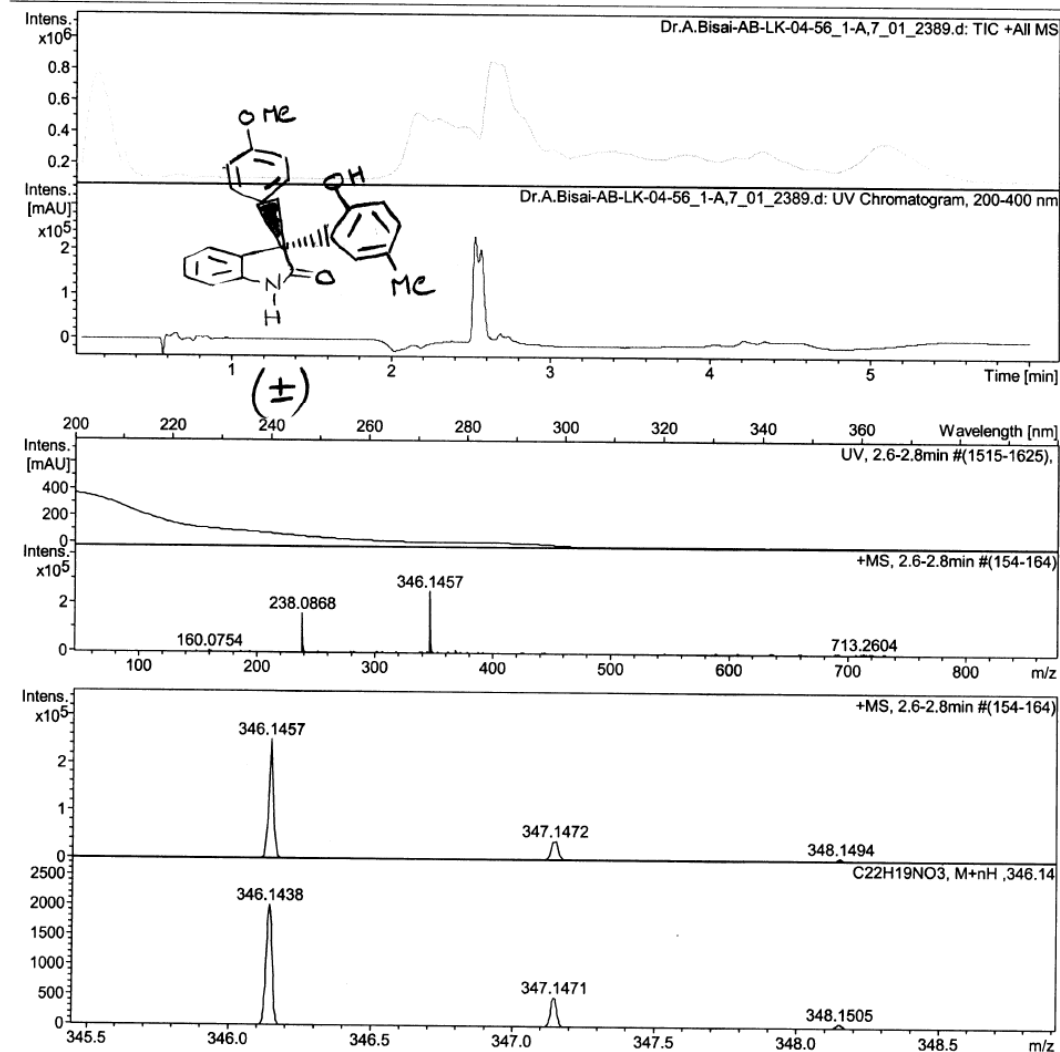
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Comment	
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Operator	Amit
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

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		Set Divert Valve	Waste

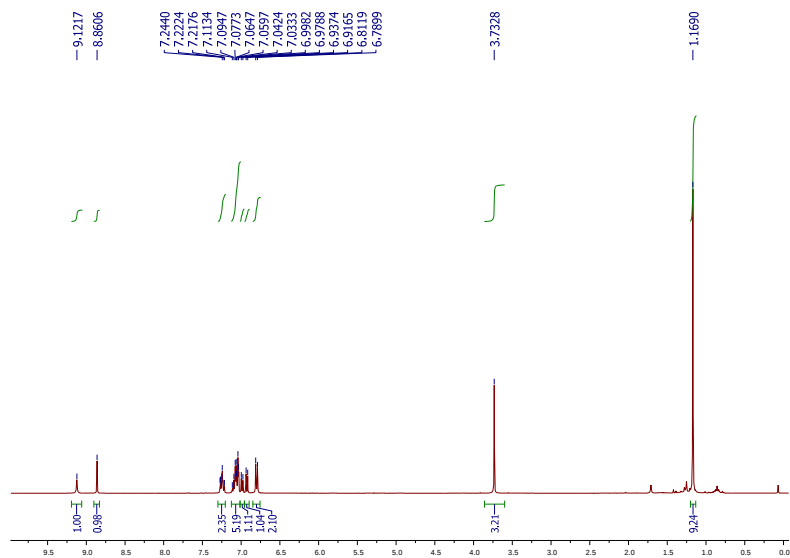
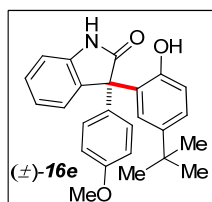


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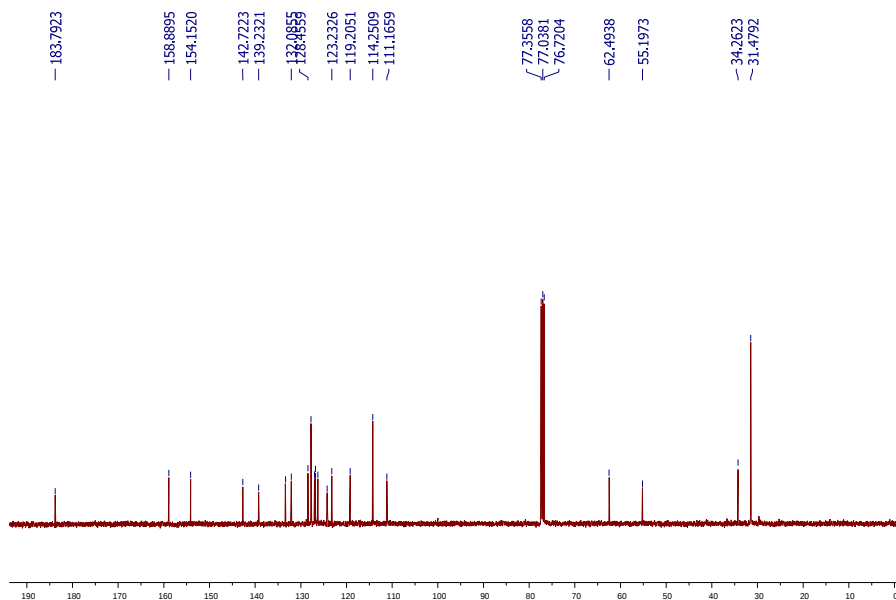
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Page 1 of 1

Scanned copy of mass spectrum of (±)-16d



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16e**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16e**

Display Report

Analysis Info

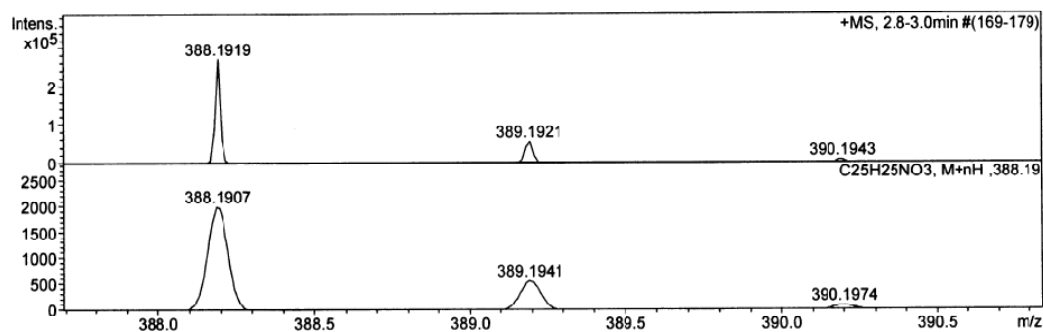
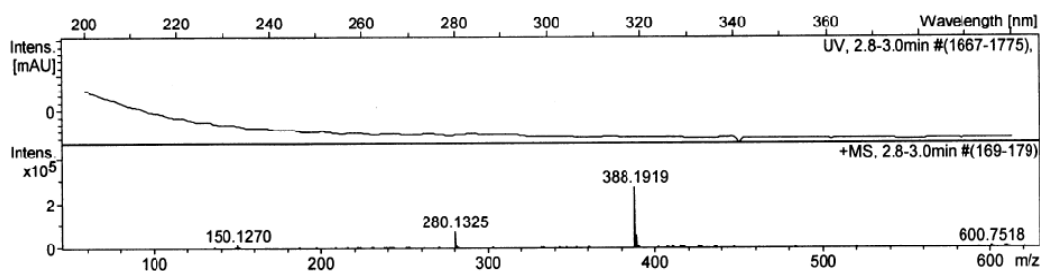
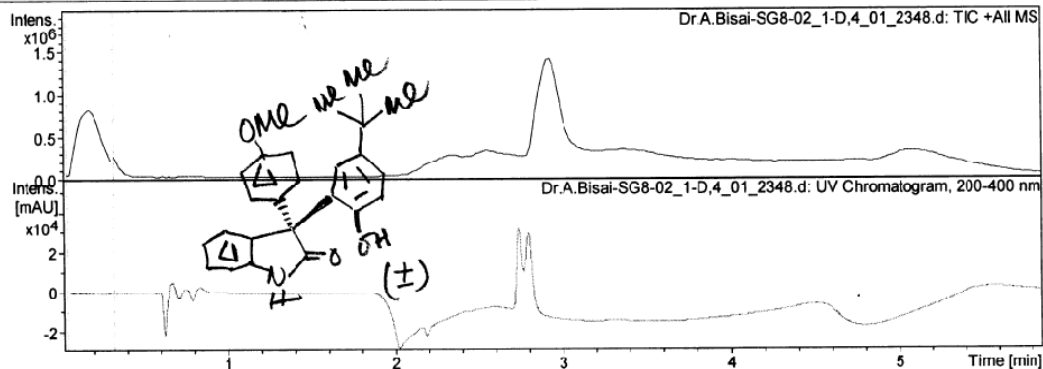
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 Comment

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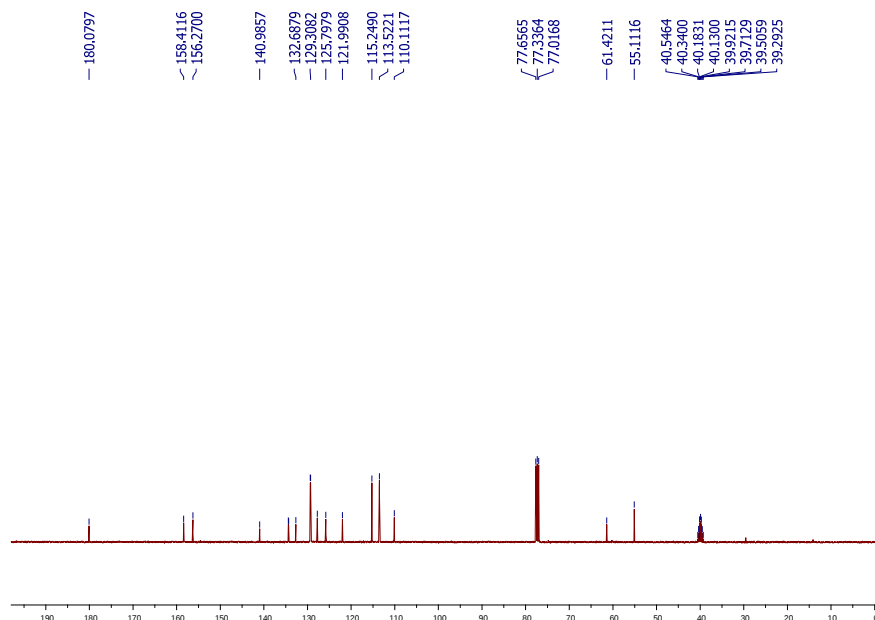
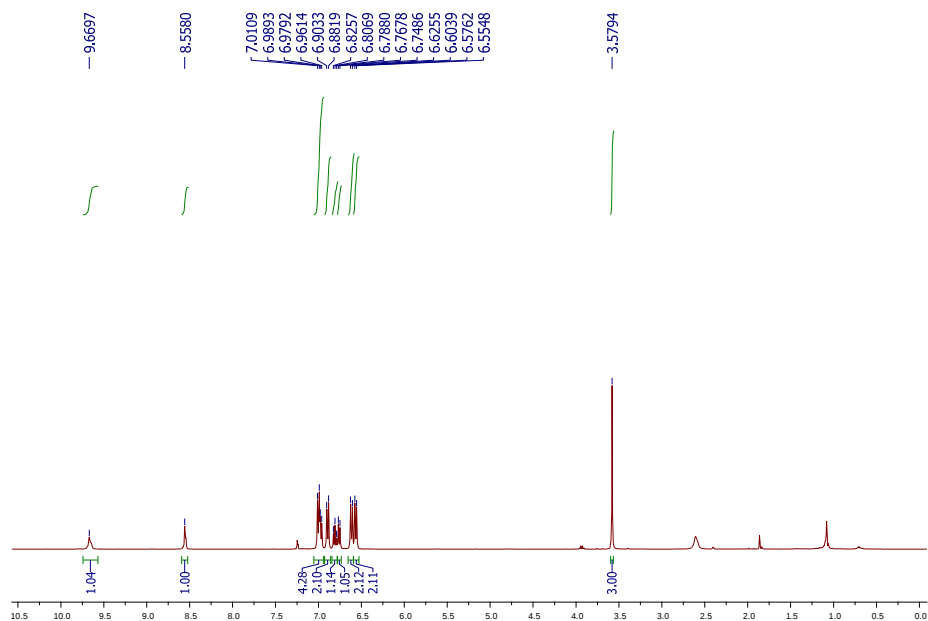
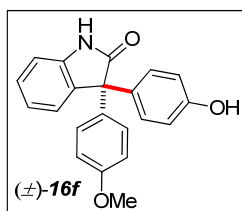
Operator Amit
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16e



Display Report

Analysis Info

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Method HRLCMS-20 Sept.m
Sample Name Dr.A.Bisai-SG8-03
Comment

Acquisition Date 4/26/2014 12:25:35 AM

Operator Amit

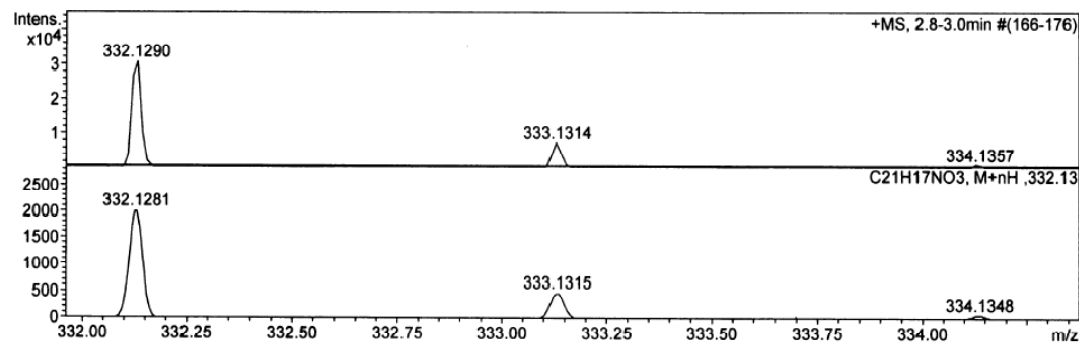
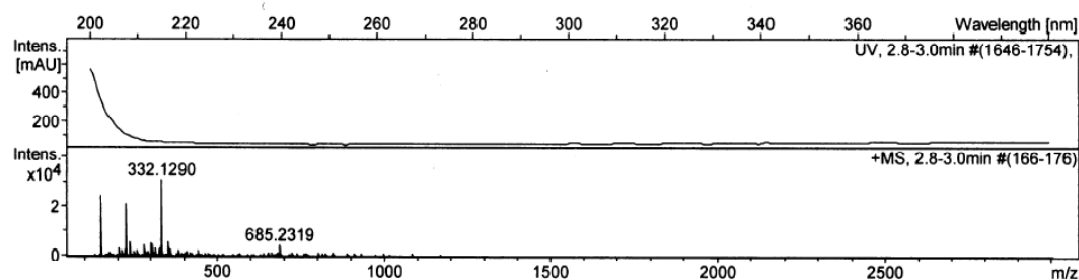
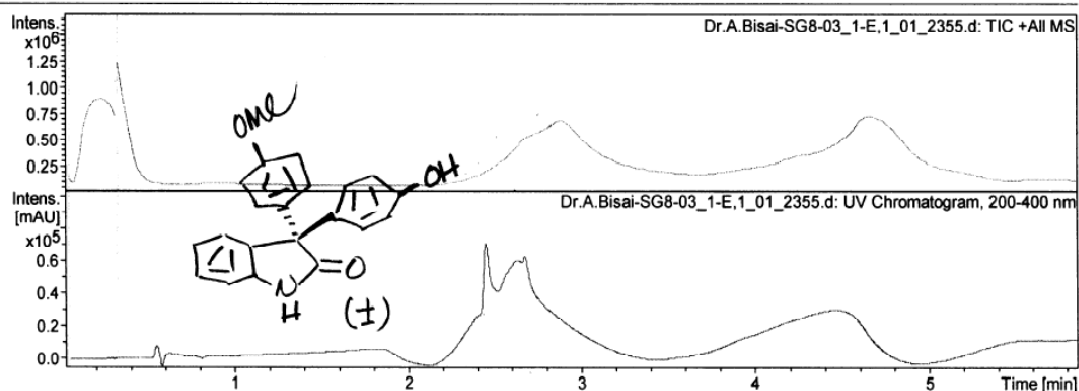
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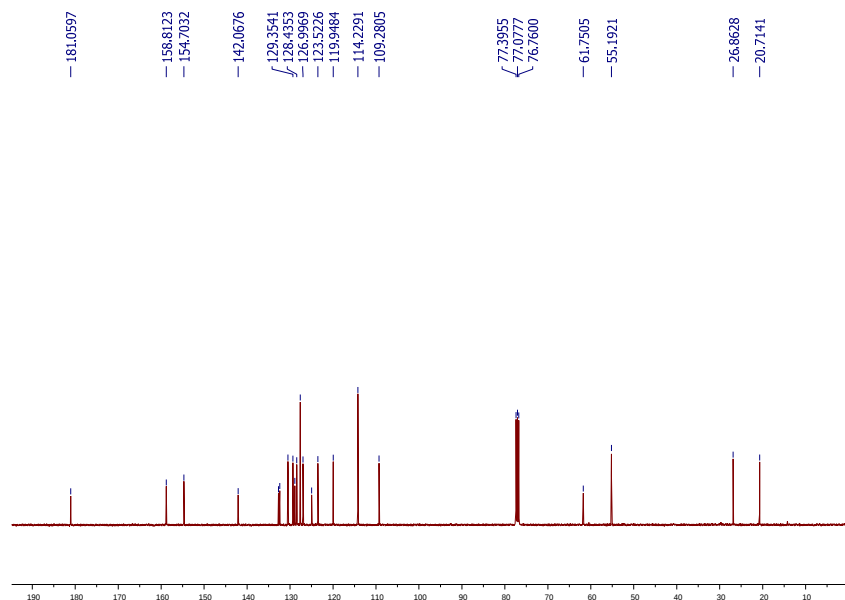
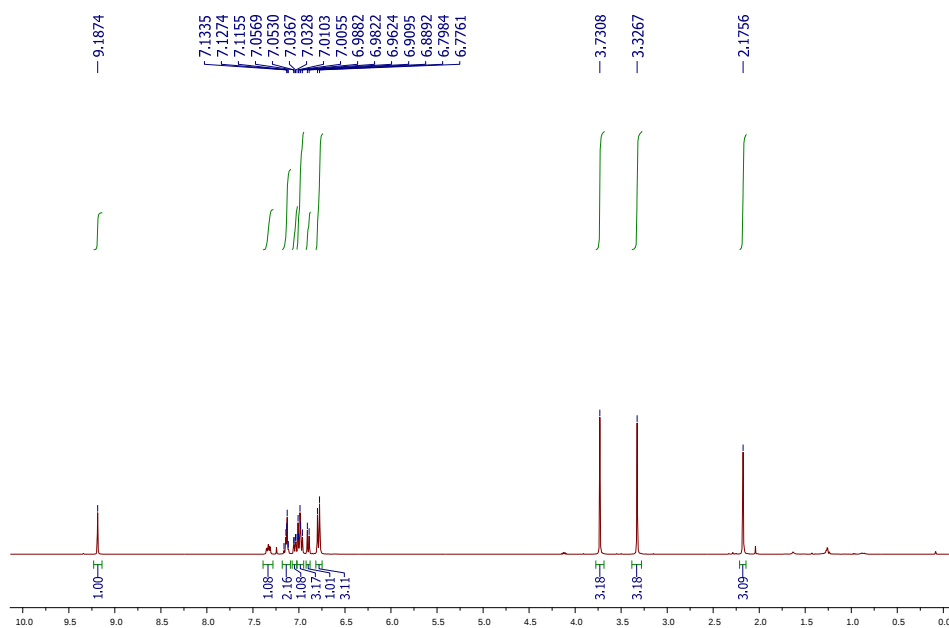
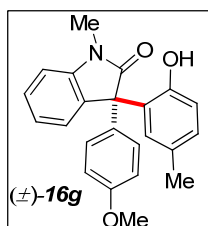
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Scan End 3000 m/z

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Set Collision Cell RF 130.0 Vpp

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Set Divert Valve Waste



Scanned copy of mass spectrum of (±)-16f



Display Report

Analysis Info

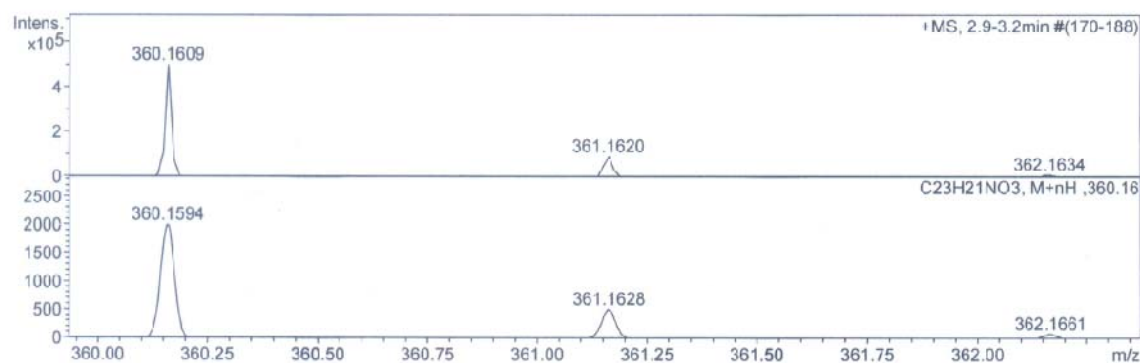
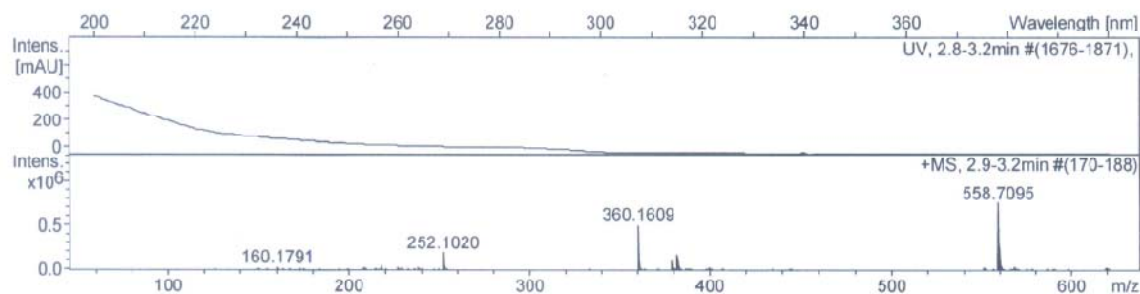
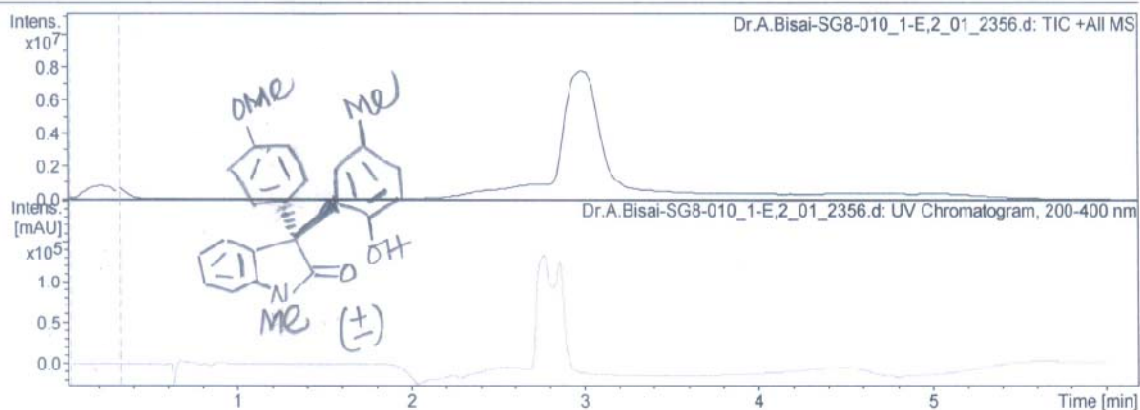
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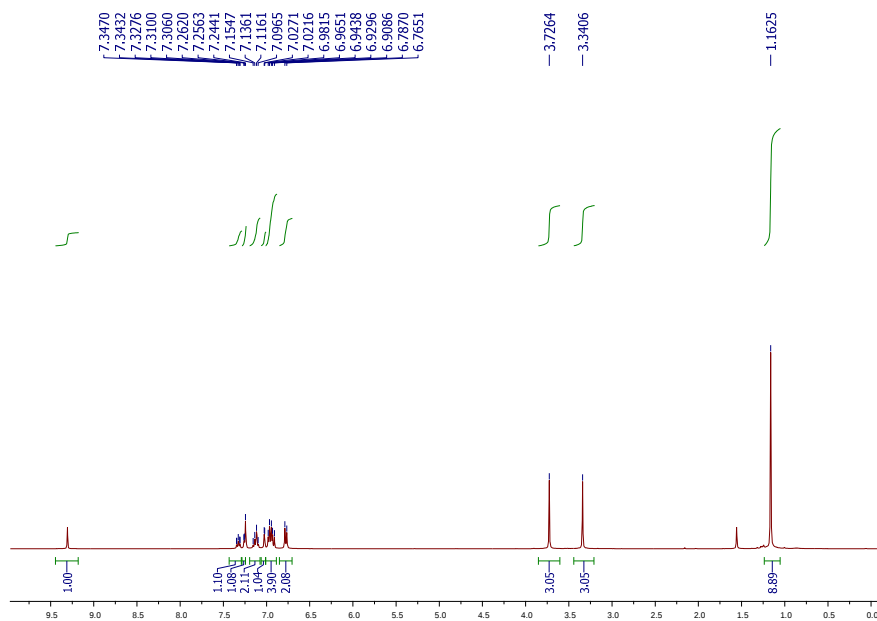
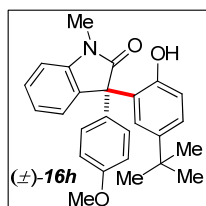
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Instrument micrOTOF-Q II 10330

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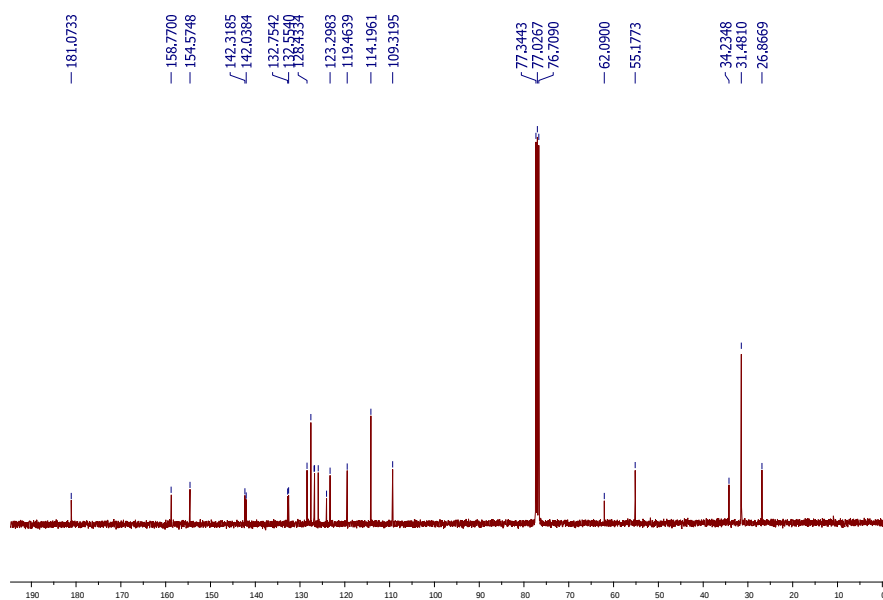
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16g



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16h**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16h**

Display Report

Analysis Info

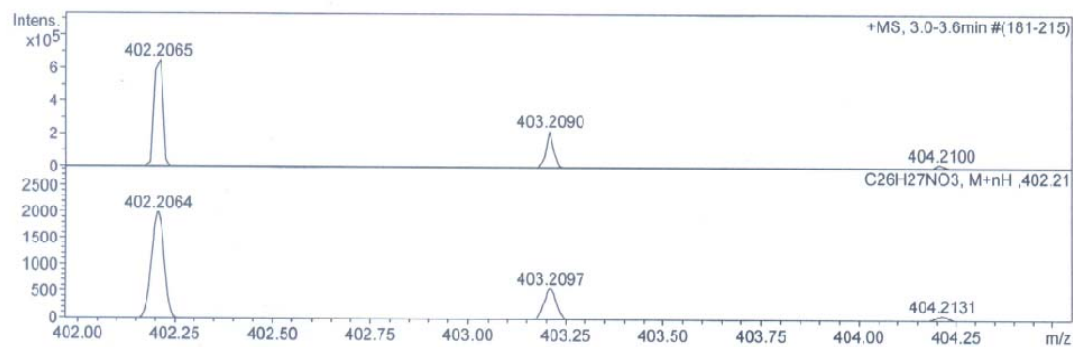
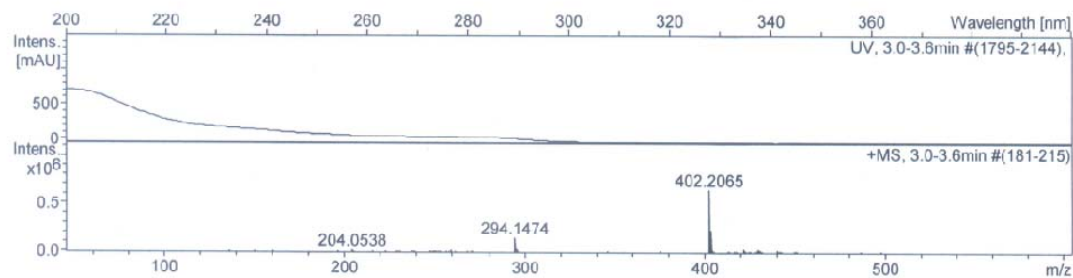
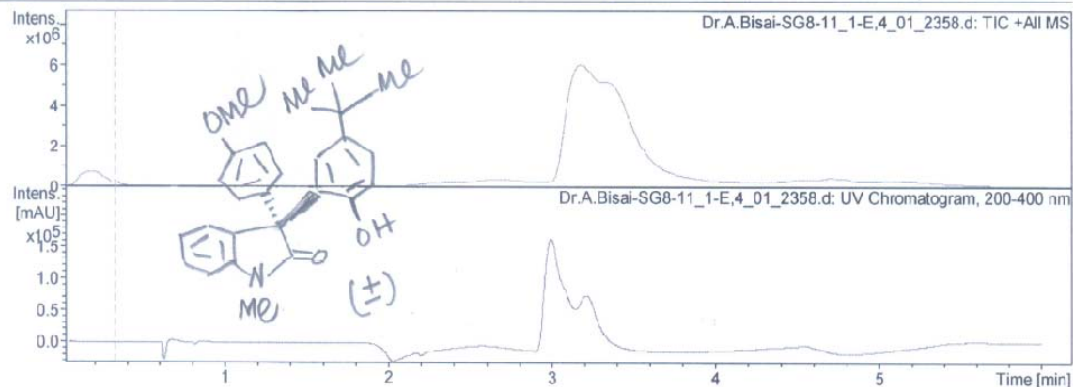
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 Method HPLCMS-20 Sept m
 Sample Name Dr.A.Bisai-SG8-11
 Comment

Acquisition Date 4/26/2014 12:47:02 AM

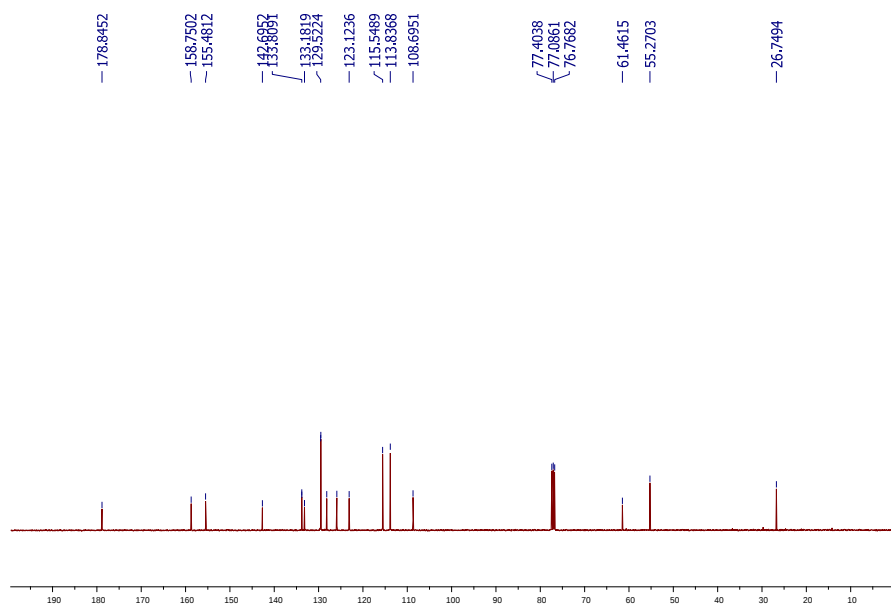
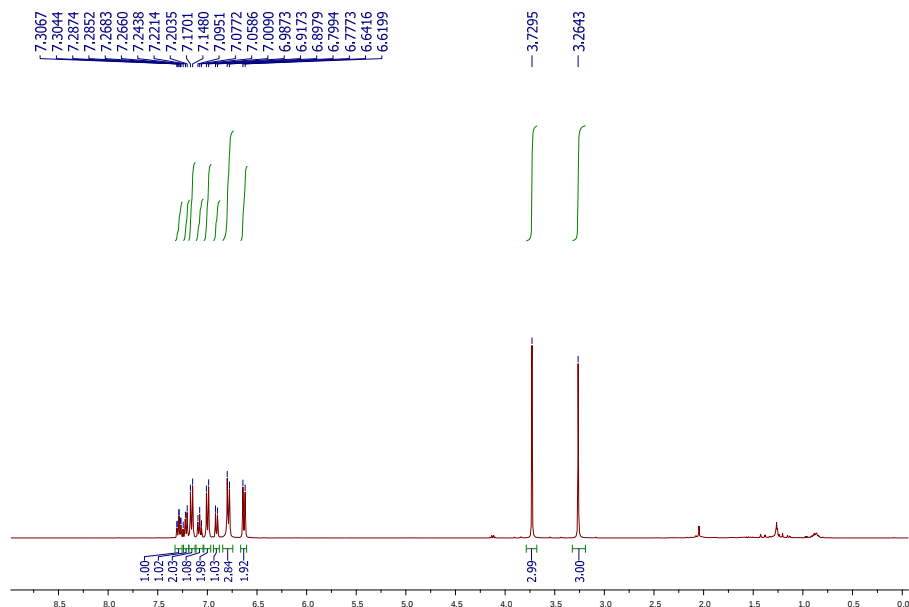
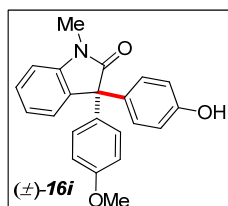
Operator Amit
 Instrument microTOF-Q II 10330

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16h



Display Report

Analysis Info

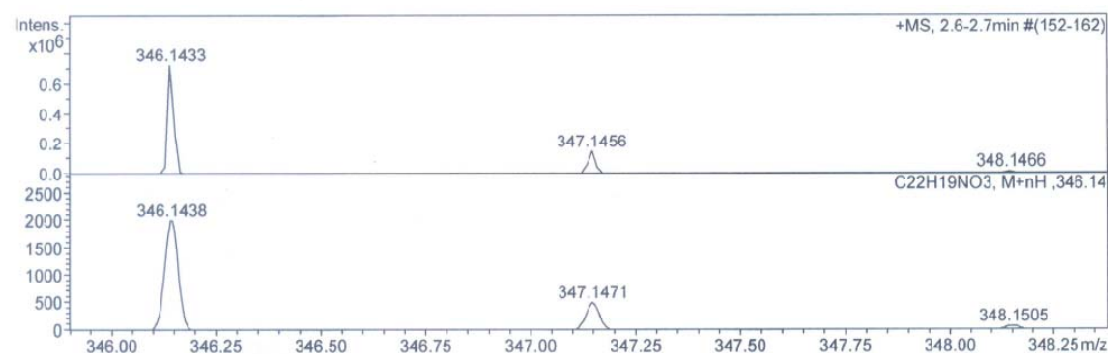
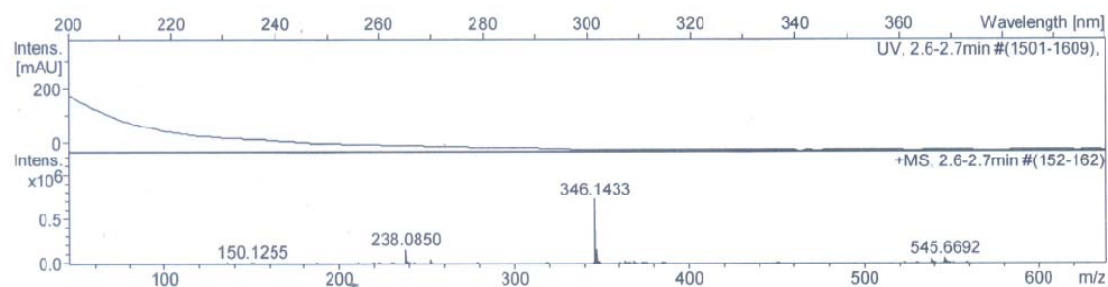
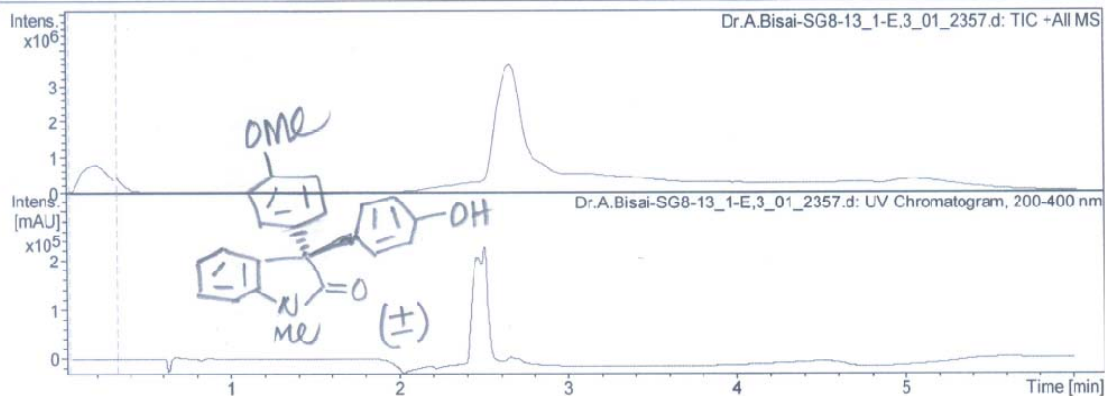
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 Sample Name Dr.A.Bisai-SG8-13
 Comment

Acquisition Date 4/26/2014 12:39:54 AM

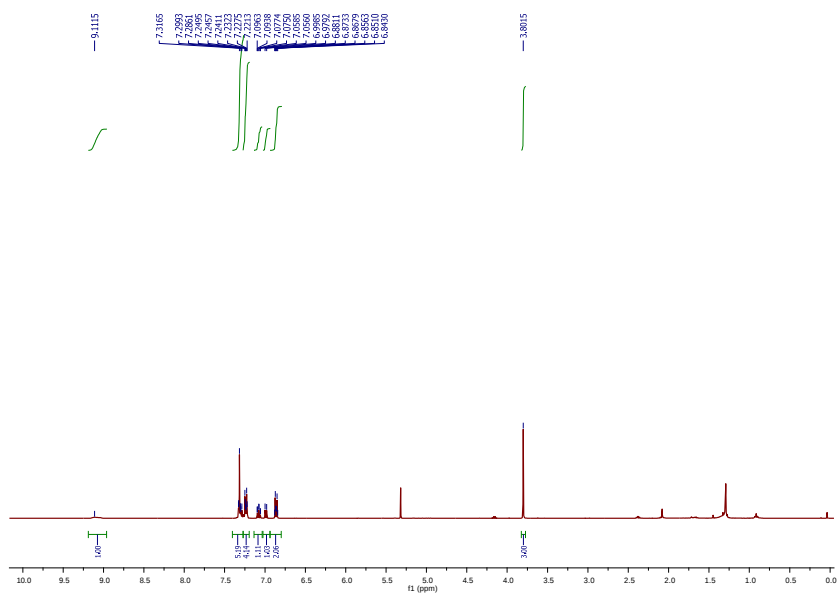
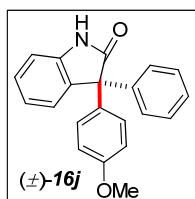
Operator Amit
 Instrument microTOF-Q II 10330

Acquisition Parameter

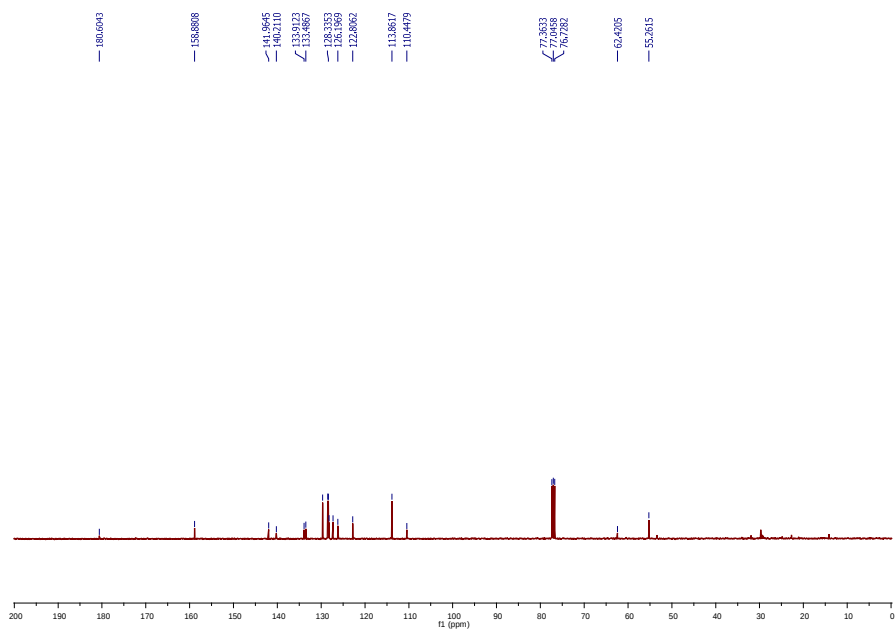
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



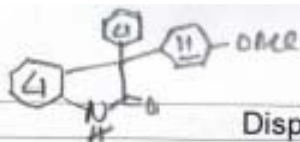
Scanned copy of mass spectrum of (±)-16i



¹H NMR (400 MHz, CDCl₃) of compound (±)-16j



¹³C NMR (100 MHz, CDCl₃) of compound (±)-16j



Display Report

Analysis Info

Analysis Name D:\Data\user data\ JULY 25\Aakash Bisai-SG-03-010.d
 Method tune_low.m
 Sample Name AB-SG-03-010
 Comment

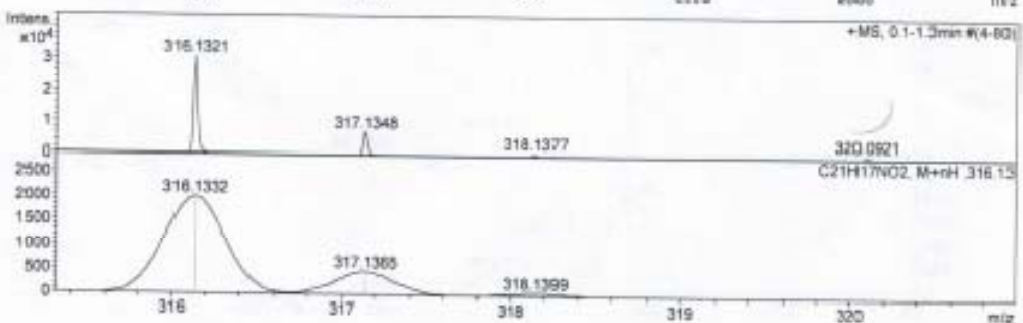
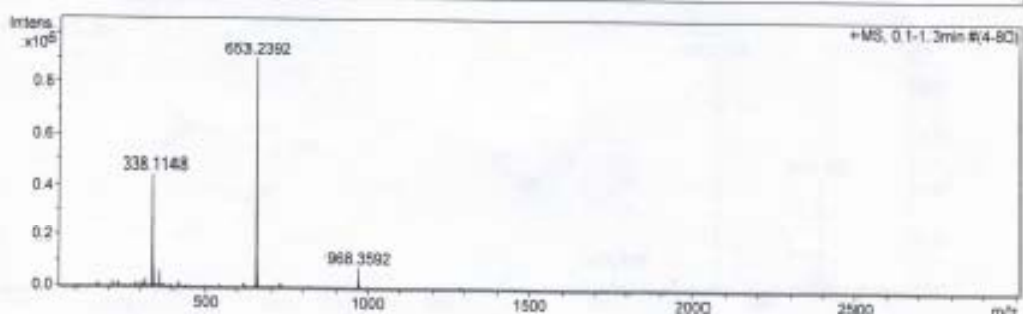
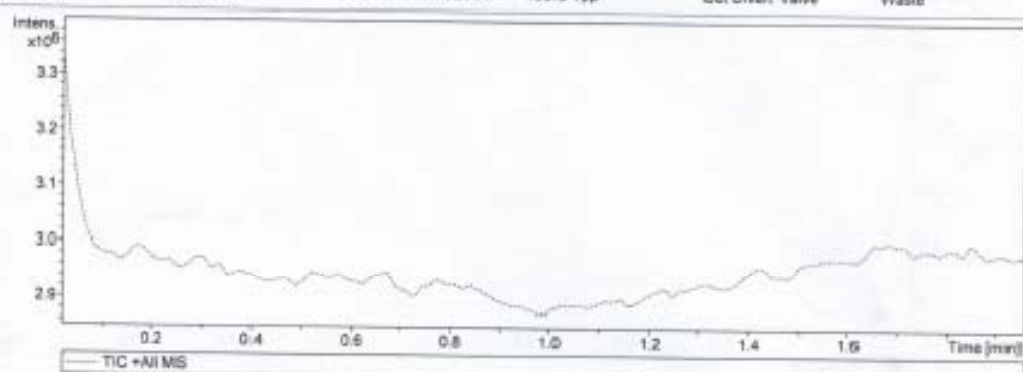
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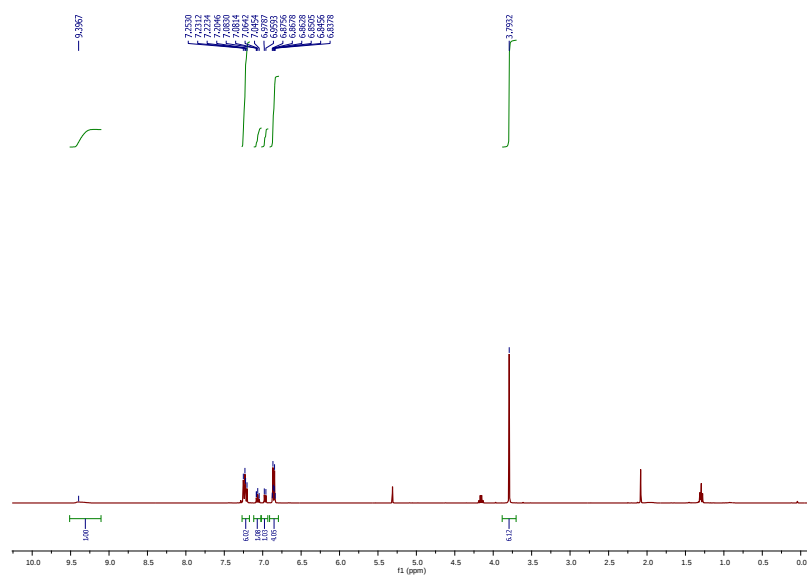
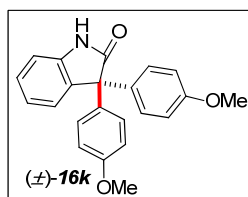
Operator MEENA SHARMA

Instrument micrOTOF-Q II 10330

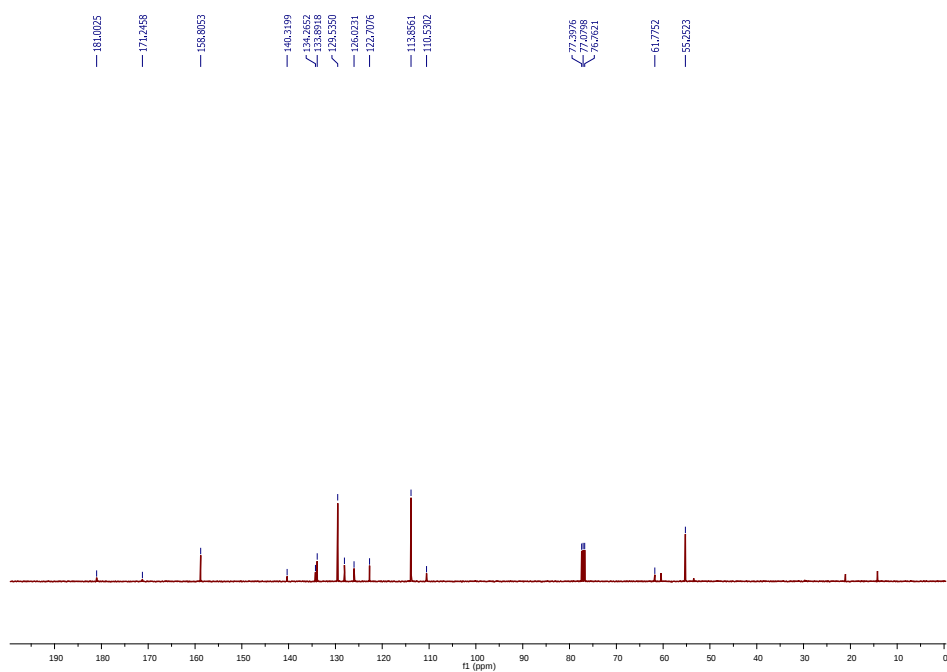
Acquisition Parameter

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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

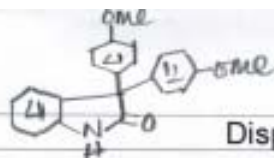




¹H NMR (400 MHz, CDCl₃) of compound (±)-16k



¹³C NMR (100 MHz, CDCl₃) of compound (±)-16k



Display Report

Analysis Info

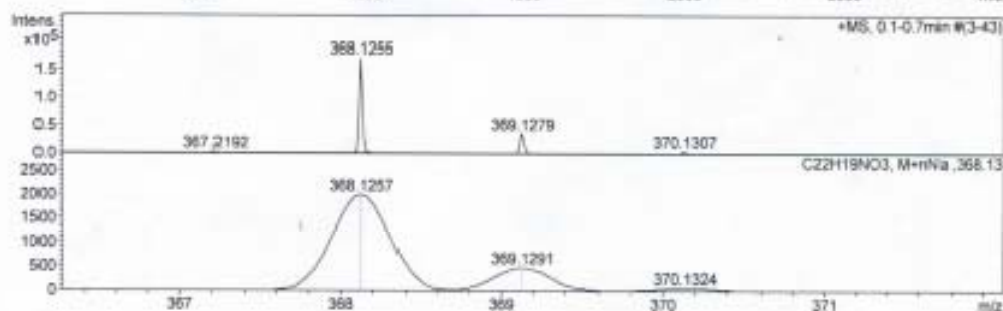
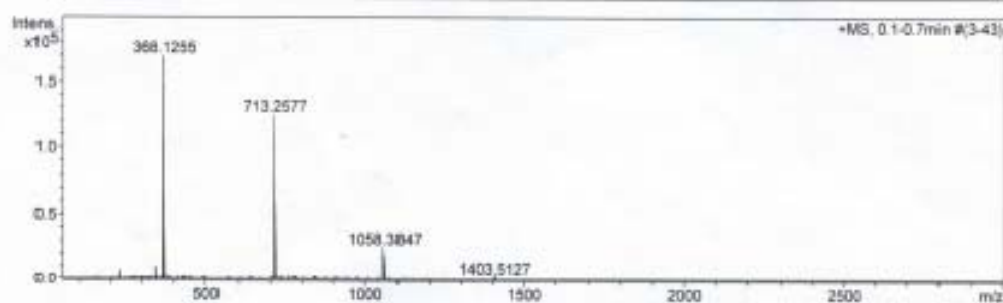
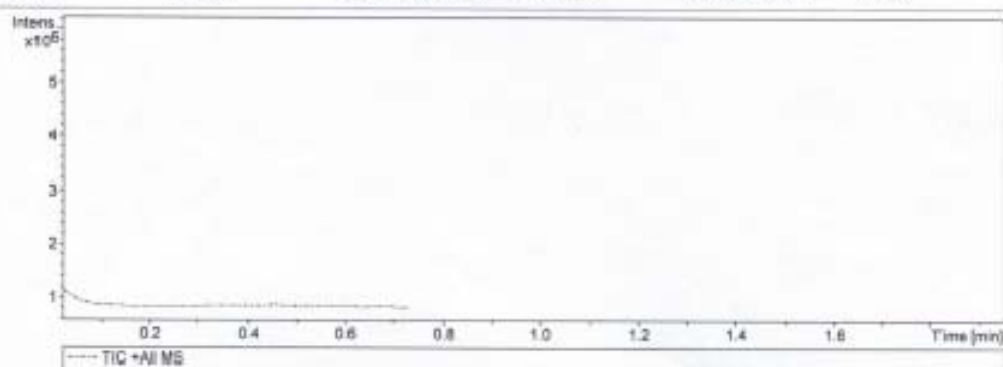
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 Method tune_low.m
 Sample Name AB-SG-03-001
 Comment

Acquisition Date 7/25/2011 12:25:05 PM

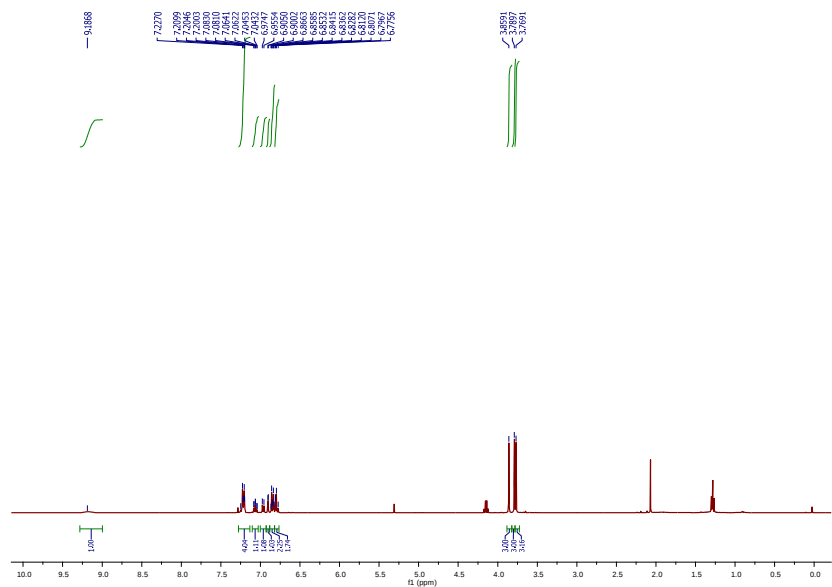
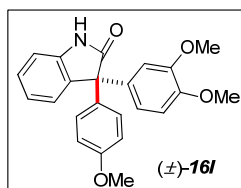
Operator MEENA SHARMA
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

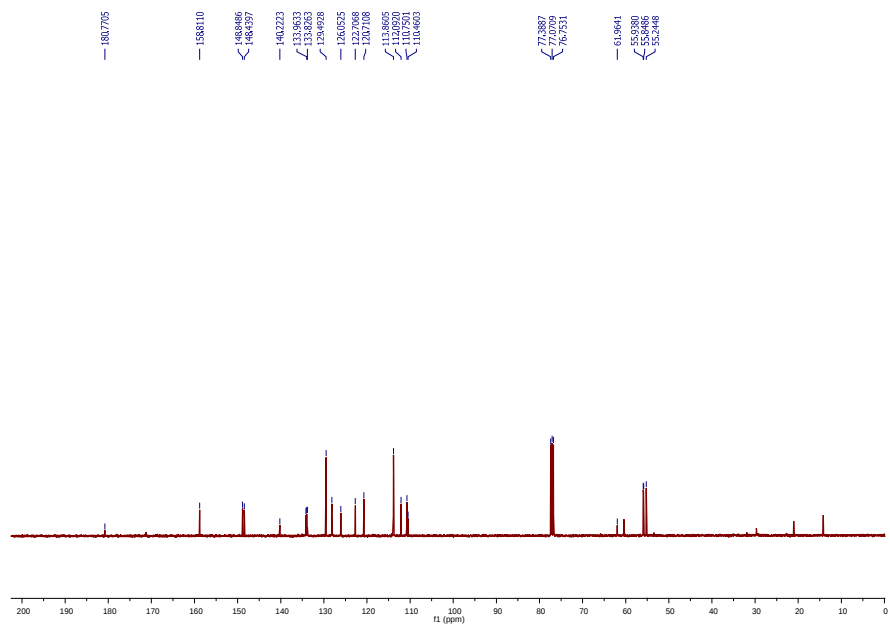
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End: Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision: Cell RF	130.0 Vpp	Set Divert: Valve	Waste



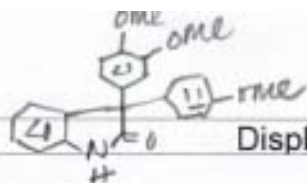
Scanned copy of mass spectrum of ($\pm$)-16k



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16I**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16I**



Display Report

Analysis Info

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 Method: tune_low.m
 Sample Name: AB-SG-03-013
 Comment:

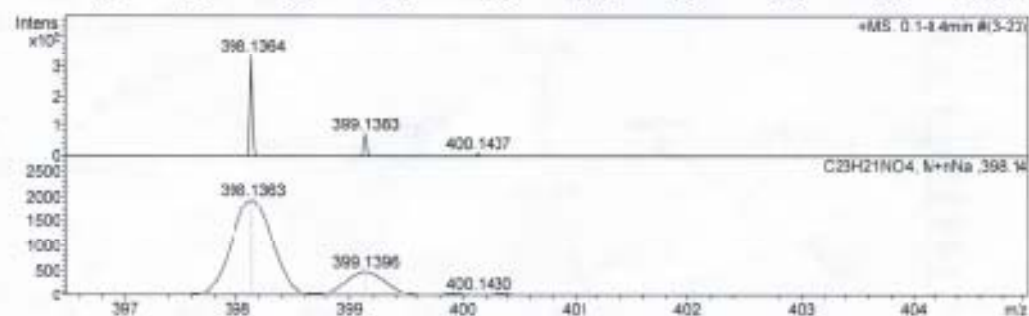
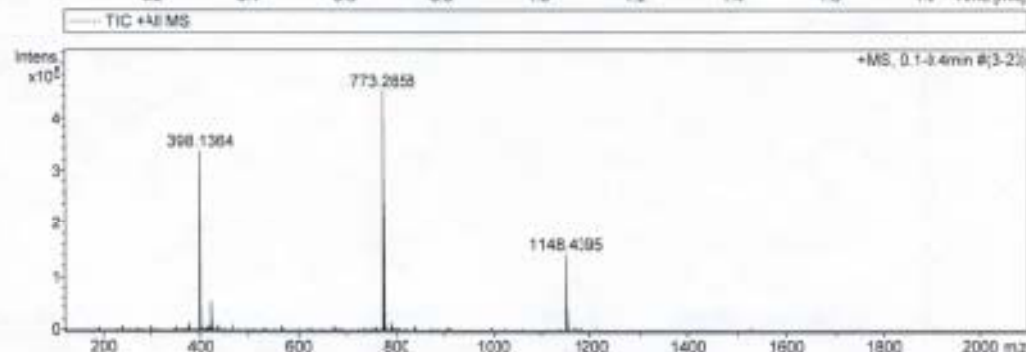
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Operator: MEENA SHARMA

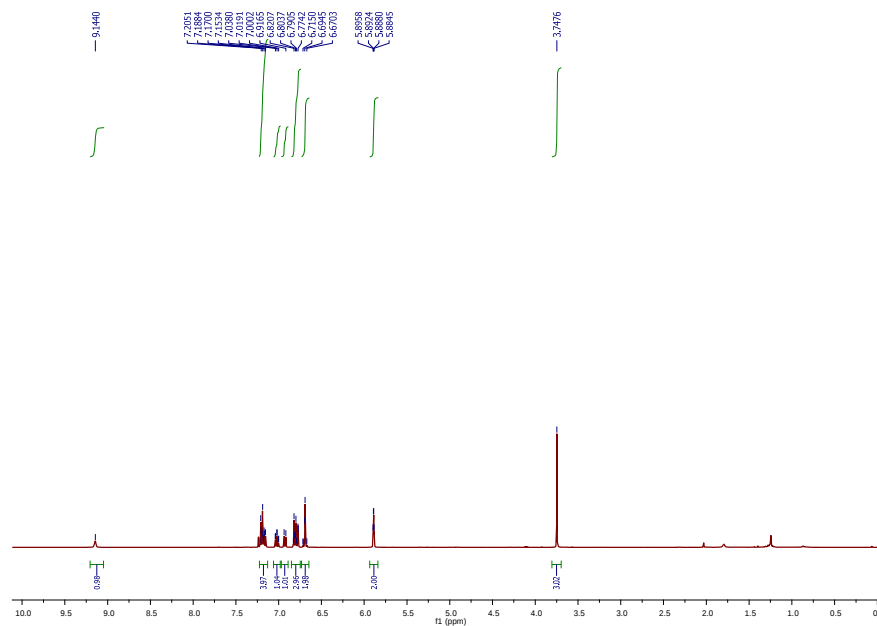
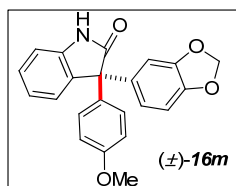
Instrument: micrOTOF-Q II 10330

Acquisition Parameter

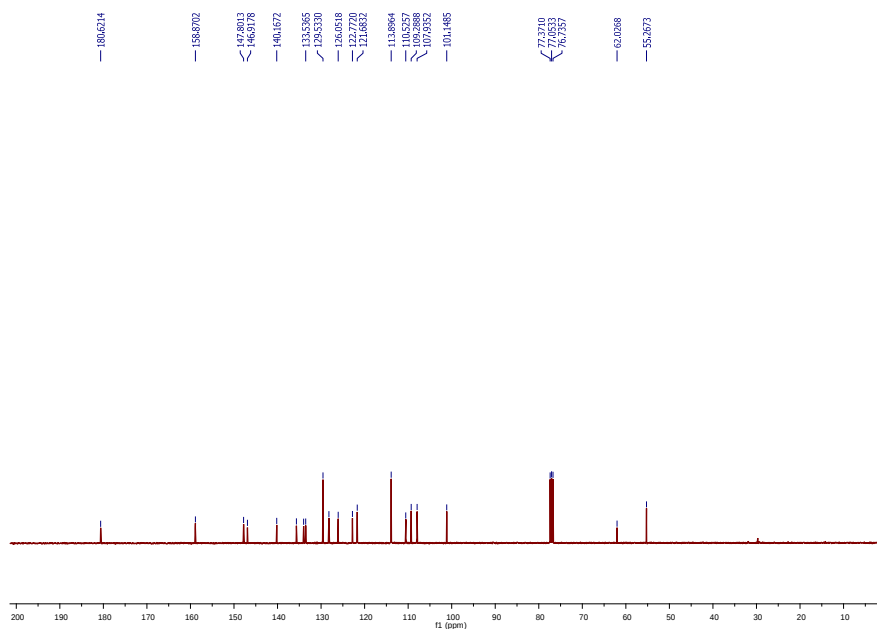
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



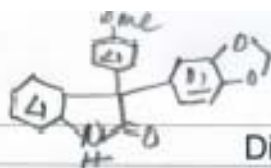
Scanned copy of mass spectrum of ($\pm$)-161



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16m**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16m**



Display Report

Analysis Info:

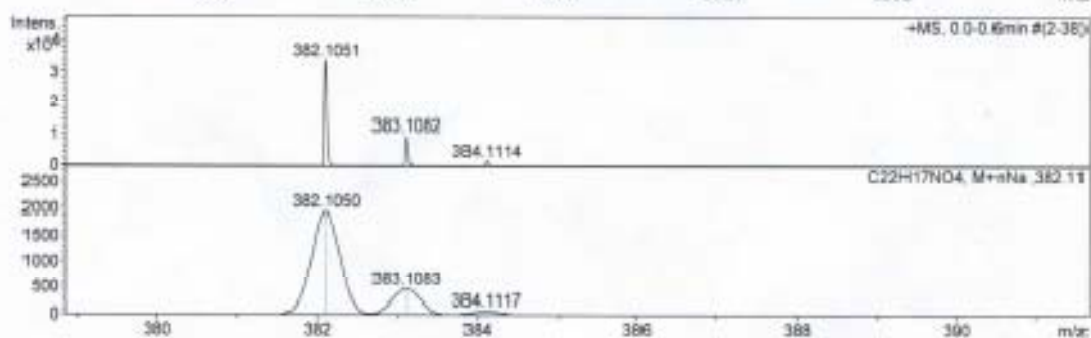
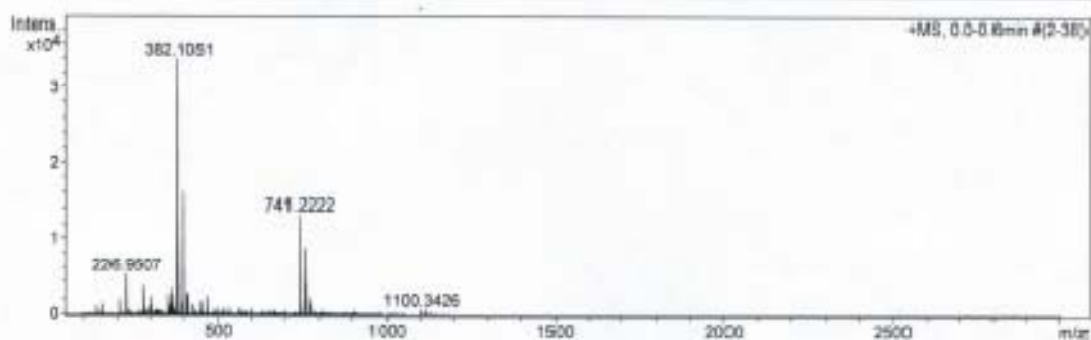
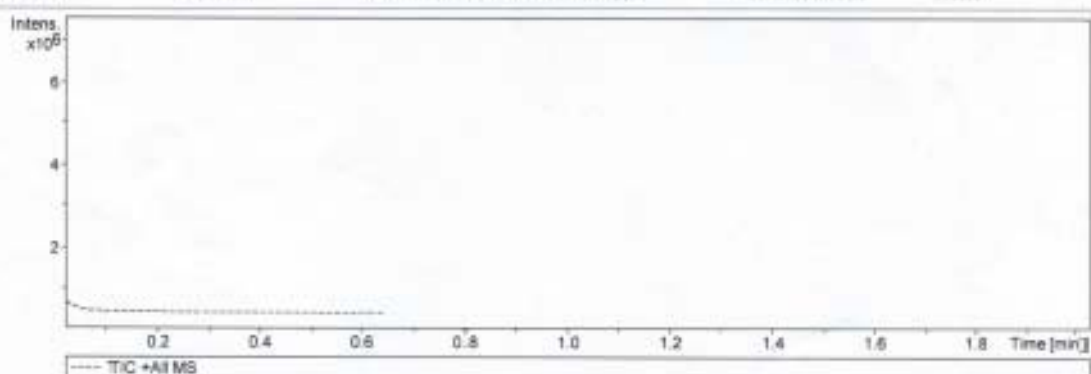
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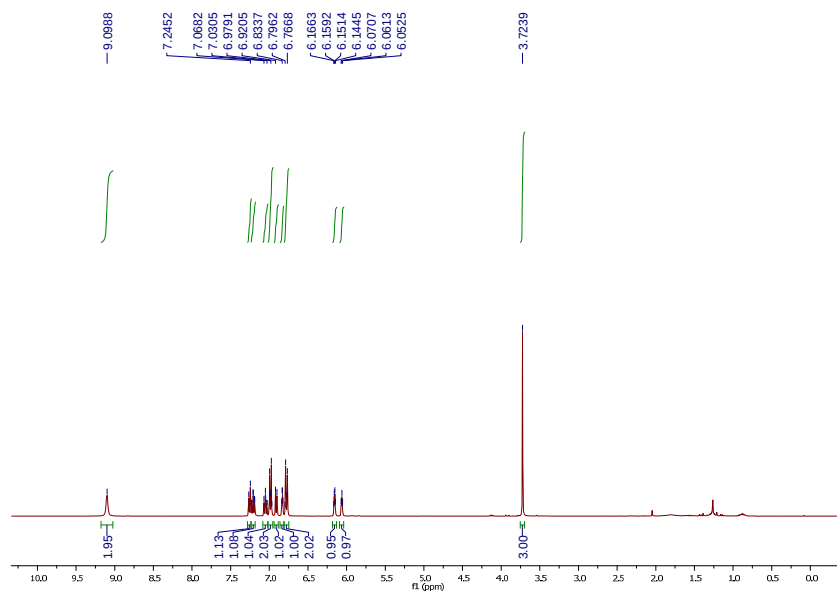
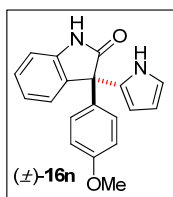
Operator: MEENA SHARMA
 Instrument: micrOTOF-Q II 10330

Acquisition Parameter

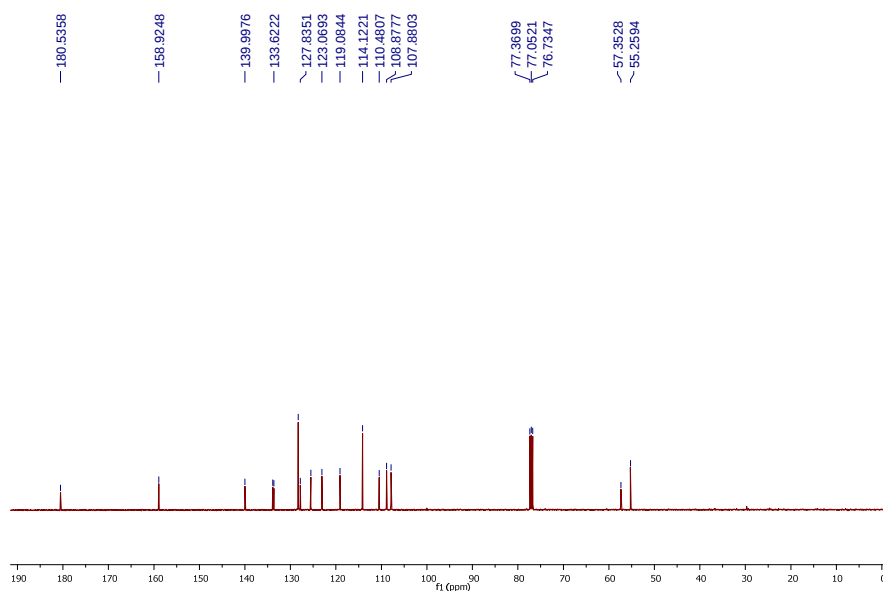
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of ($\pm$)-16m



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16n**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16n**

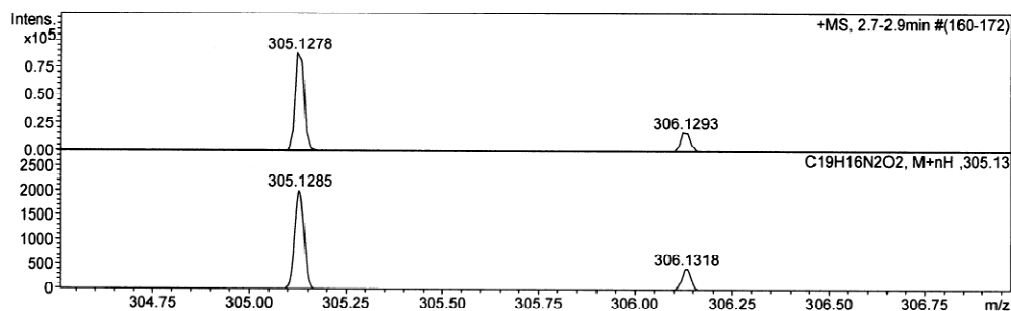
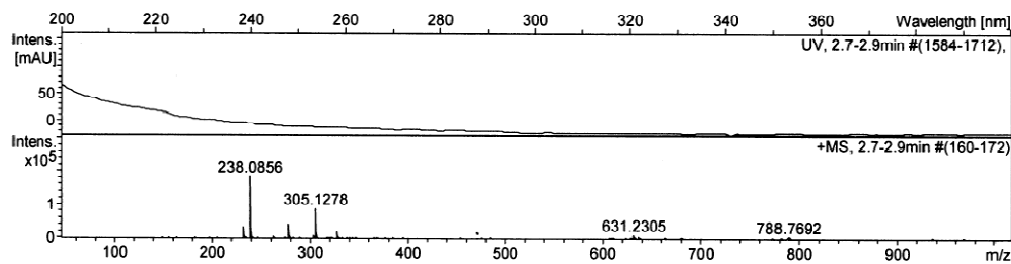
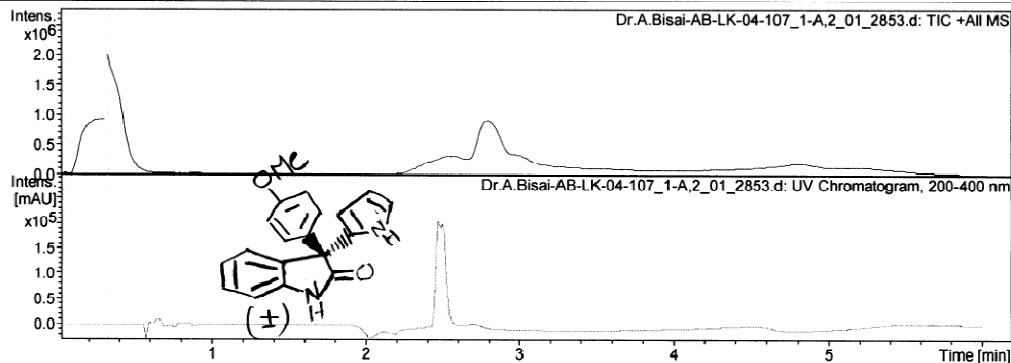
Display Report

Analysis Info

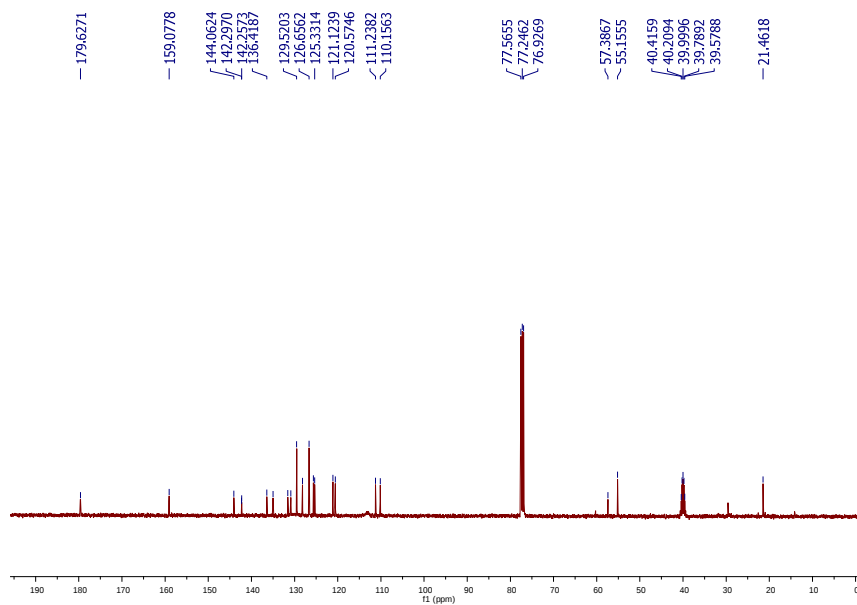
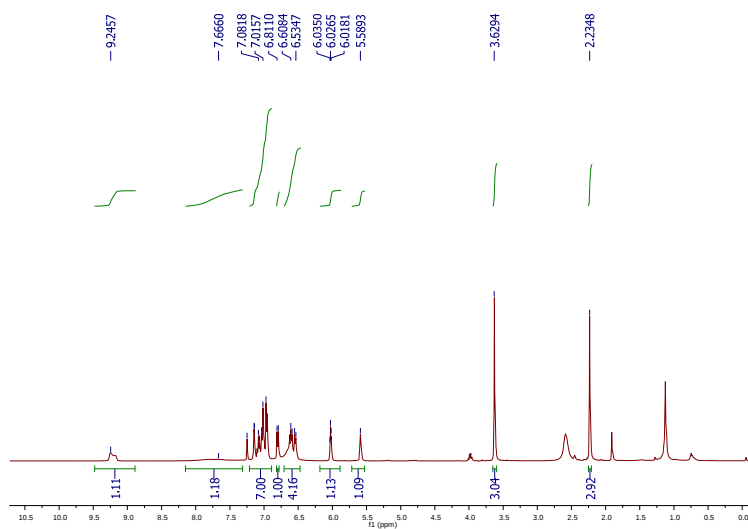
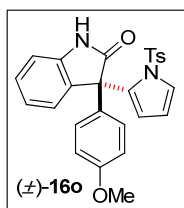
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Method	HRLCMS-20 Sept.m	Operator	Ravindra
Sample Name	Dr.A.Bisai-AB-LK-04-107	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Active	Set Capillary	4500 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16n



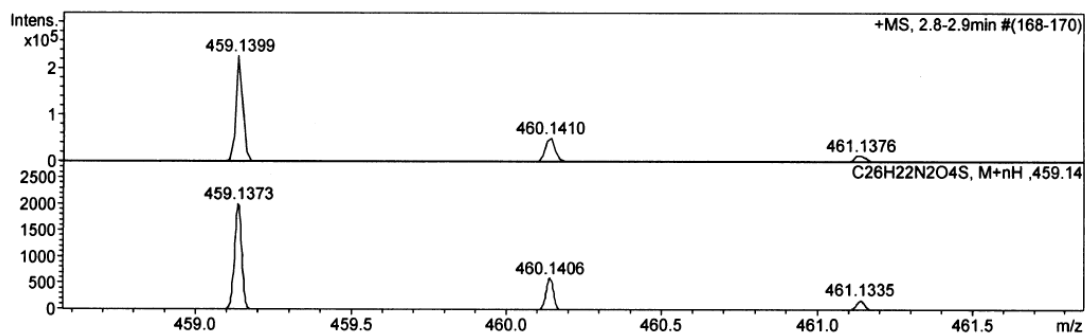
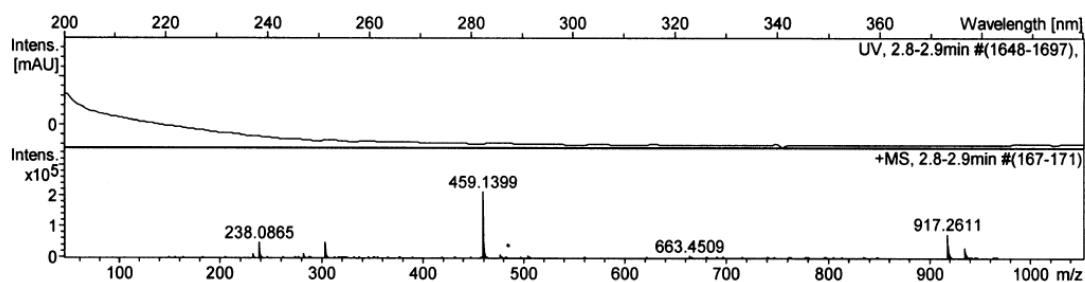
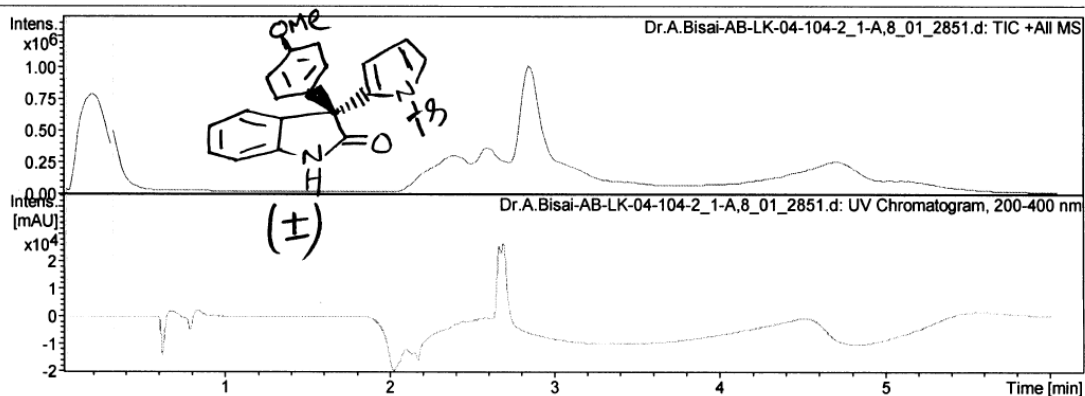
Display Report

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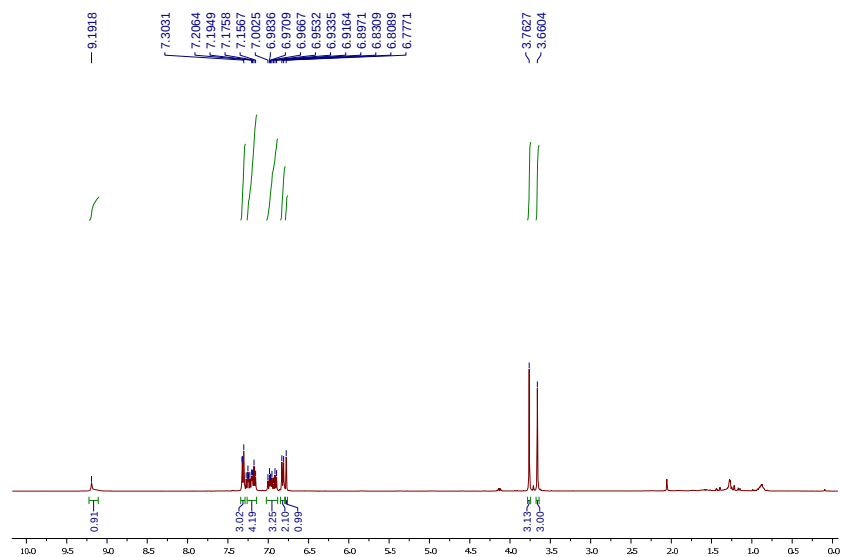
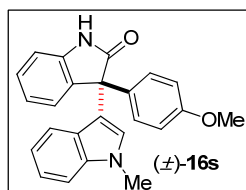
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Method	HRLCMS-20 Sept.m
Sample Name	Dr.A.Bisai-AB-LK-04-104-2
Comment	
Acquisition Date	6/13/2014 4:12:45 AM
Operator	Ravindra
Instrument	micrOTOF-Q II 10330

Acquisition Parameter

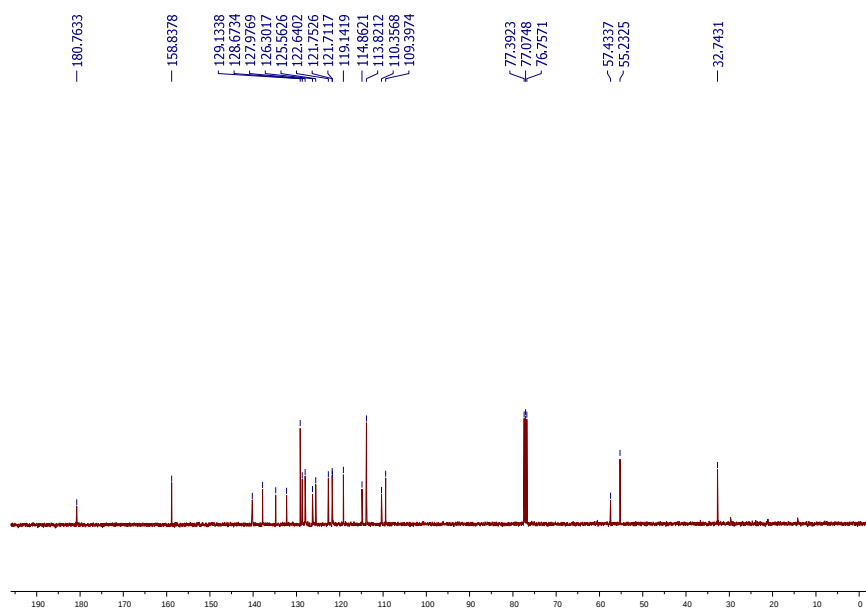
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp
		Set Nebulizer	1.2 Bar
		Set Dry Heater	200 °C
		Set Dry Gas	7.0 l/min
		Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16o



¹H NMR (400 MHz, CDCl₃) of compound (±)-**16s**



¹³C NMR (100 MHz, CDCl₃) of compound (±)-**16s**

Display Report

Analysis Info

Analysis Name D:\Data\user data\2014\JUNE\13 JUN\Dr.A.Bisai-AB-LK-04-105_1-A,5_01_2845.d
 Method HRLCMS-20 Sept.m
 Sample Name Dr.A.Bisai-AB-LK-04-105
 Comment

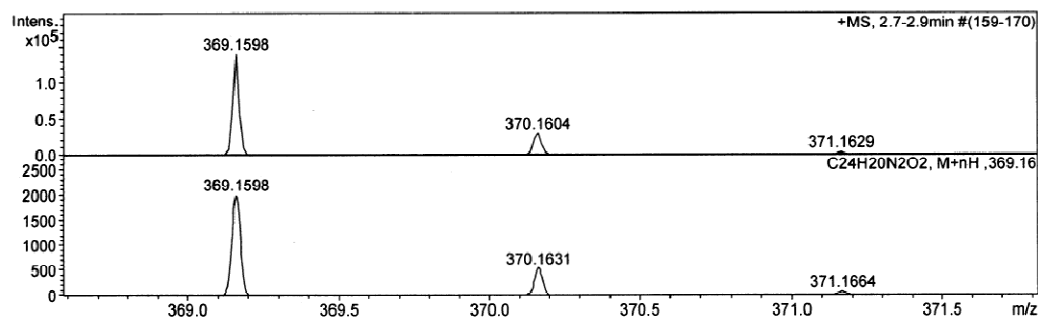
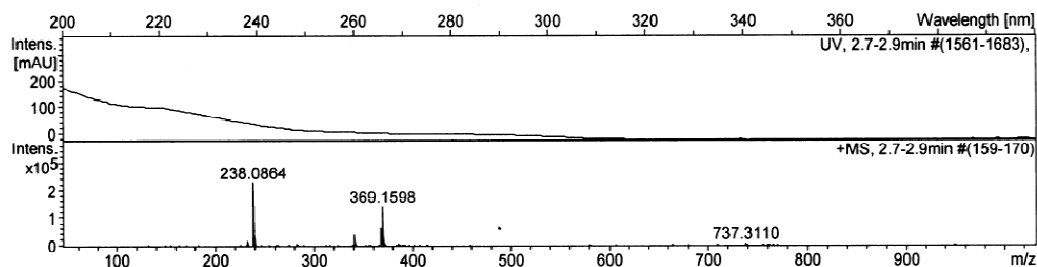
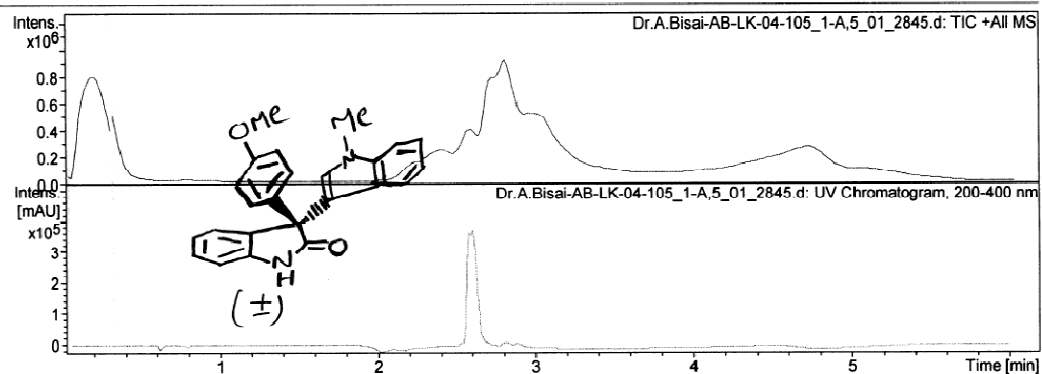
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Operator Ravindra

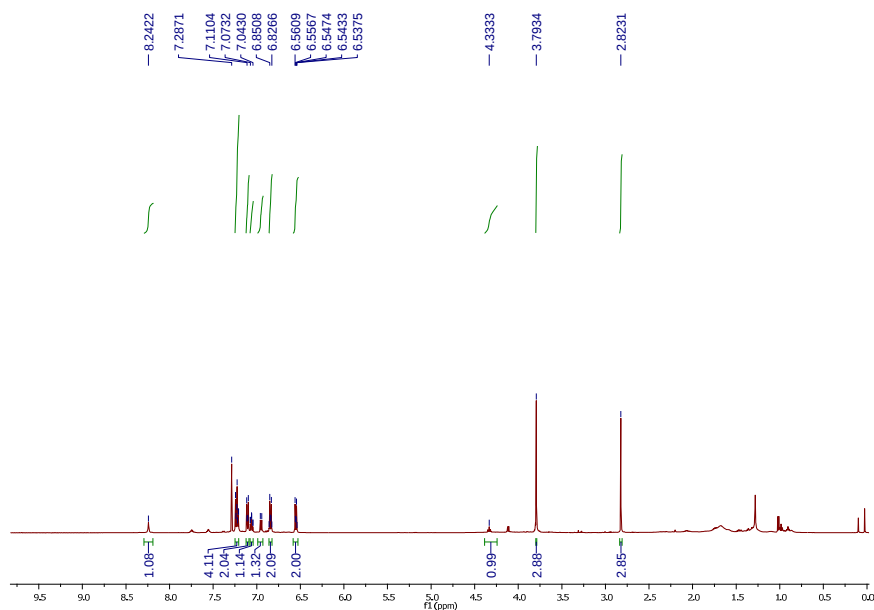
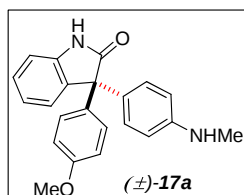
Instrument micrOTOF-Q II 10330

Acquisition Parameter

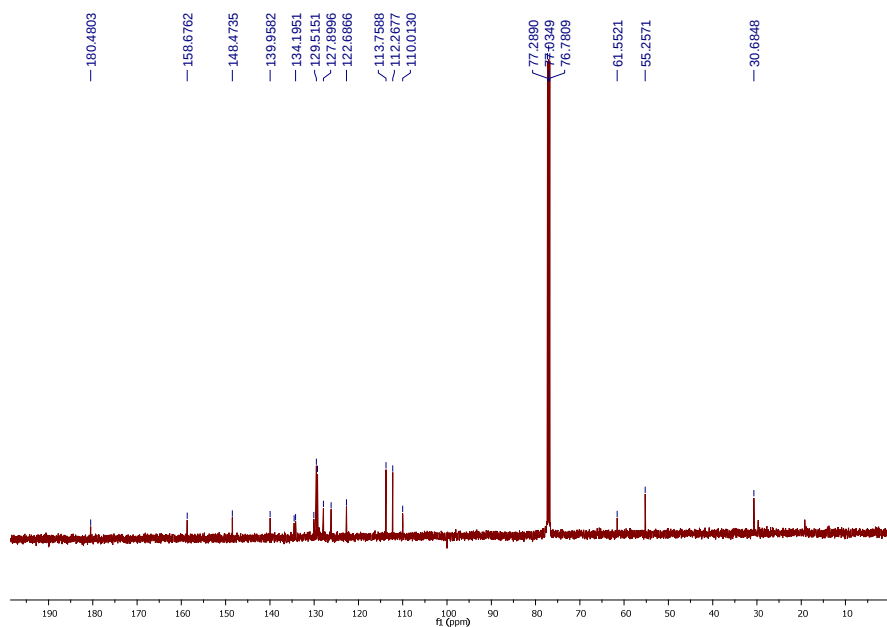
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-16s



¹H NMR (500 MHz, CDCl₃) of compound (±)-17a



¹³C NMR (125 MHz, CDCl₃) of compound (±)-17a

Display Report

Analysis Info

Analysis Name D:\Data\user data\2014\JULY31 july\Dr.A.Bisai-AB-SG8-123.d
 Method tune_low.m
 Sample Name AB-SG8-123
 Comment

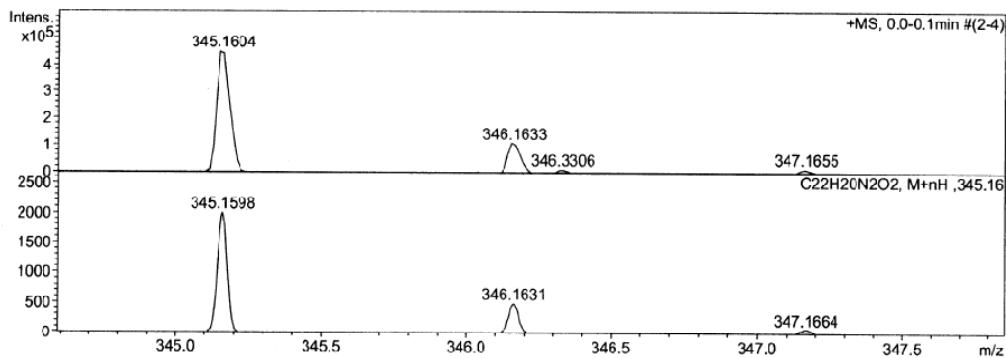
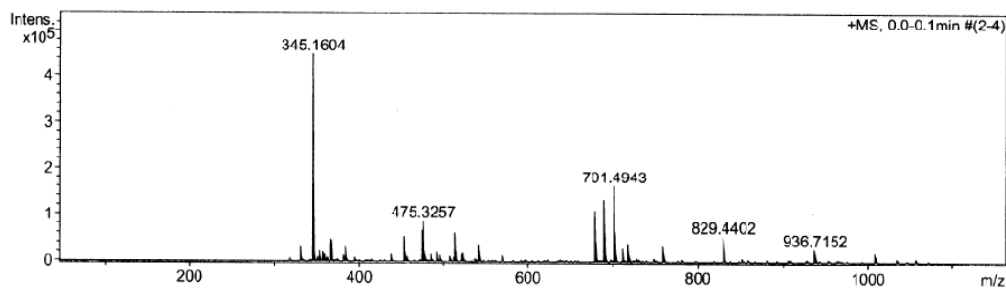
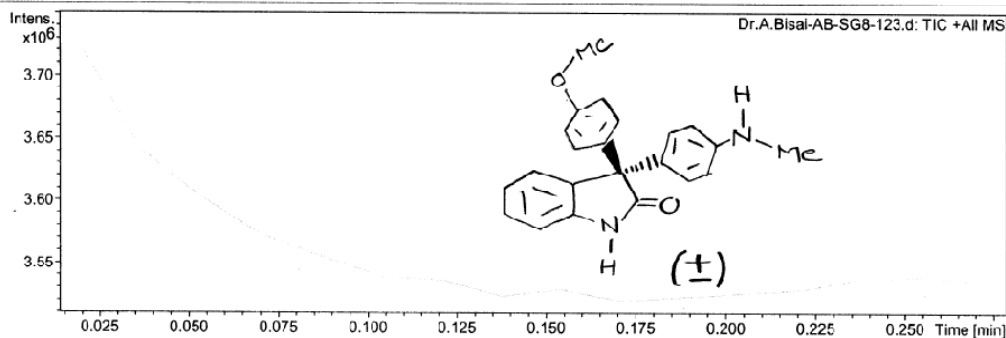
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Operator Ravindra

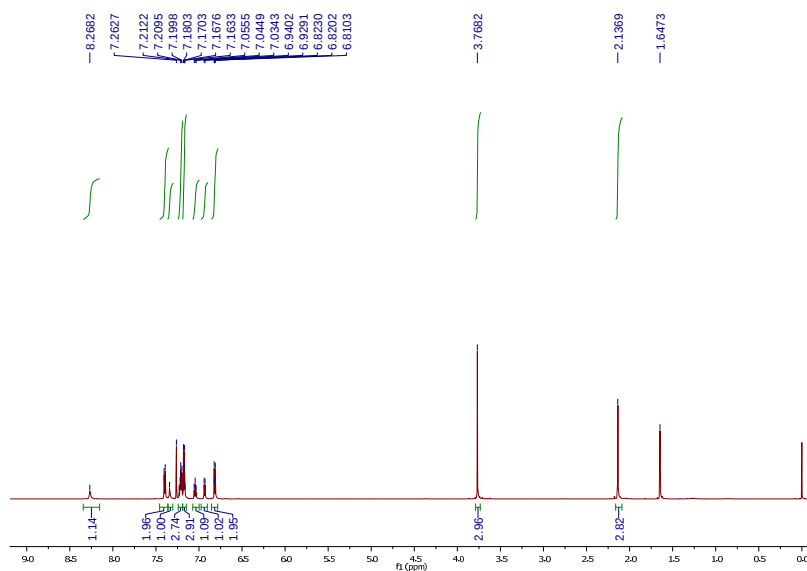
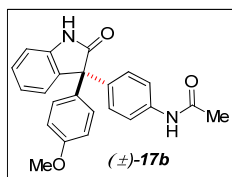
Instrument micrOTOF-Q II 10330 -

Acquisition Parameter

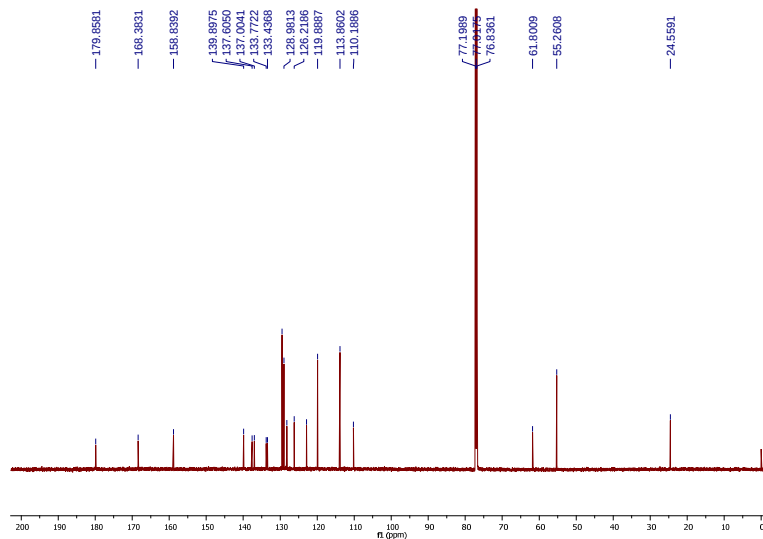
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	630.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (+)-17a



¹H NMR (700 MHz, CDCl₃) of compound (±)-17b [H₂O peak at 1.64]



¹³C NMR (175 MHz, CDCl₃) of compound (±)-17b

Display Report

Analysis Info

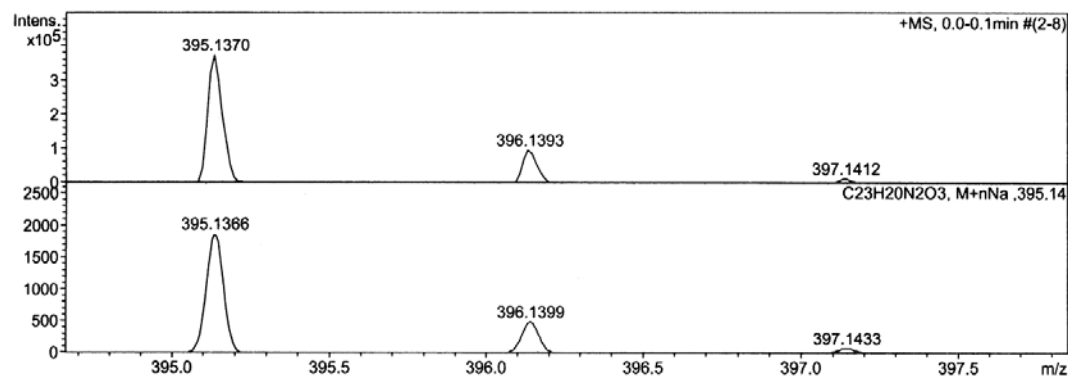
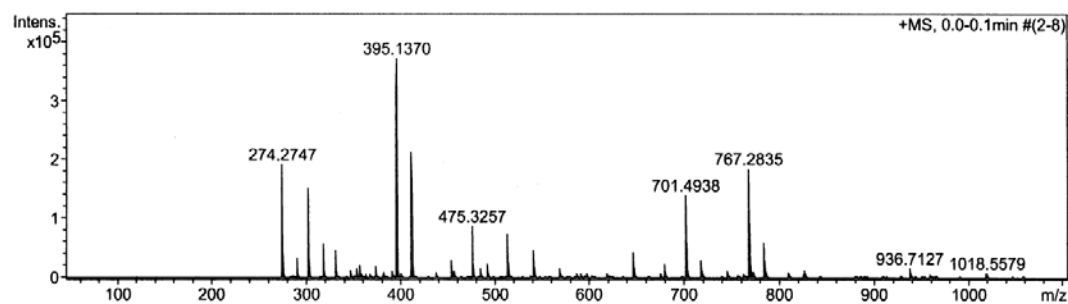
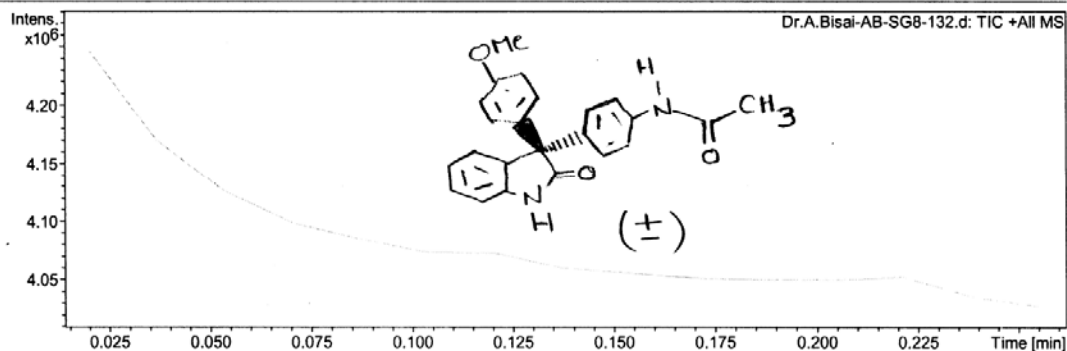
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 Comment

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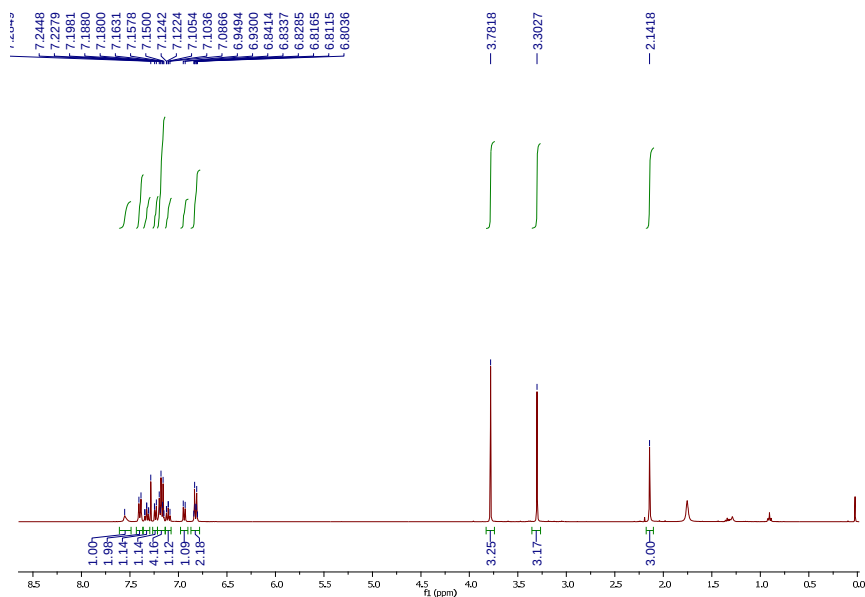
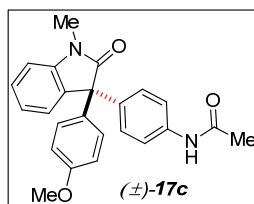
Operator Ravindra
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

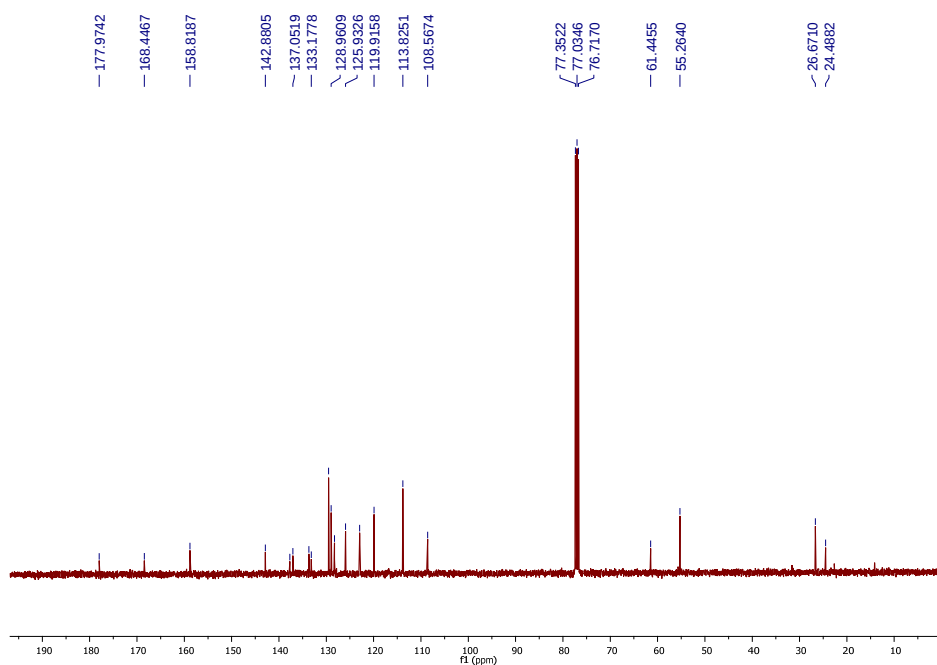
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	530.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-17b



¹H NMR (500 MHz, CDCl₃) of compound (±)-17c



¹³C NMR (125 MHz, CDCl₃) of compound (±)-17c

Display Report

Analysis Info

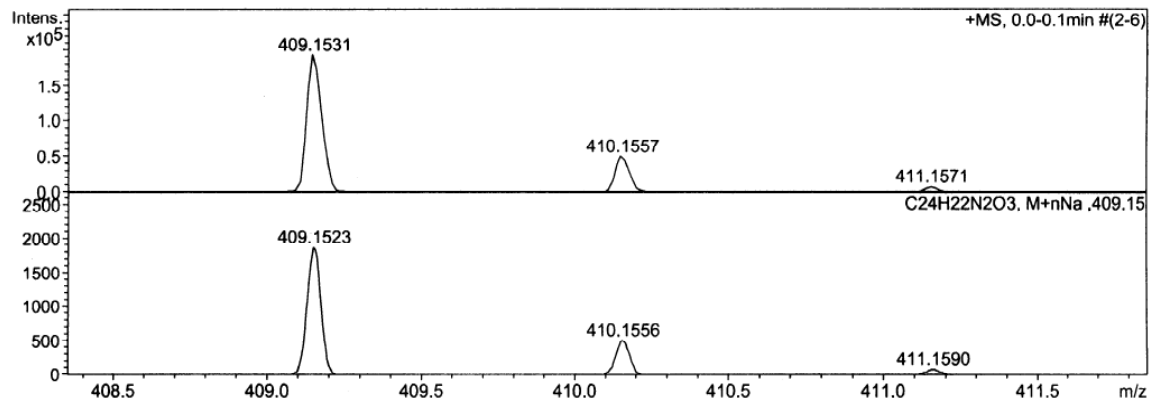
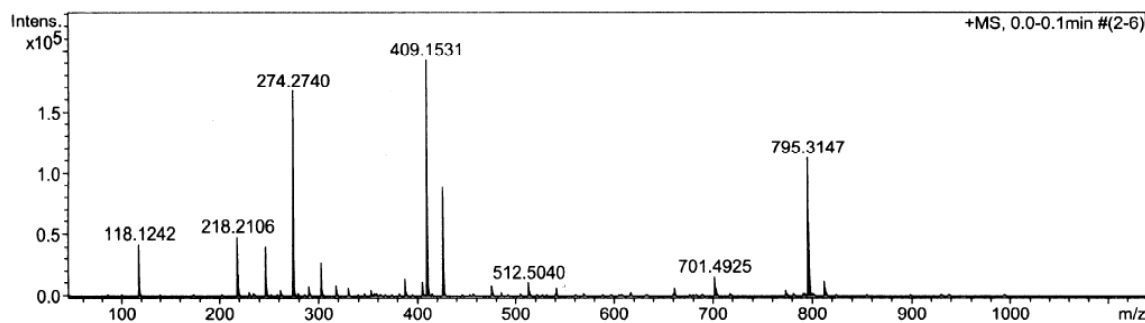
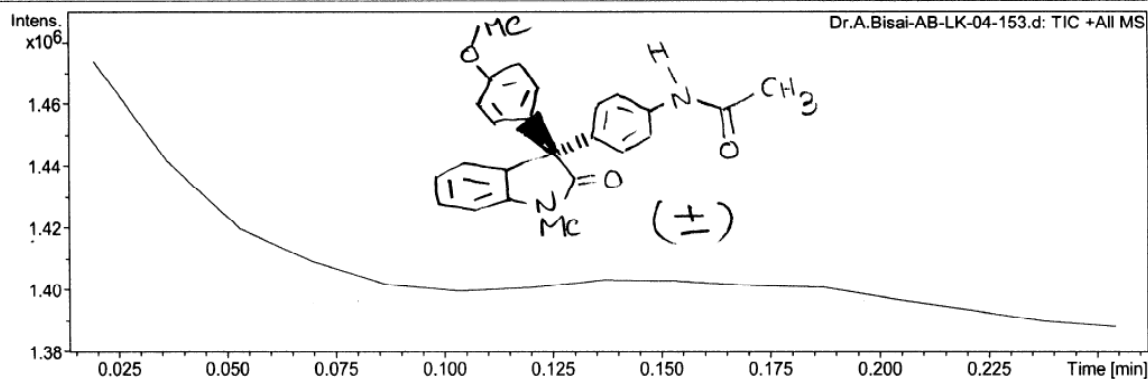
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Acquisition Date 7/31/2014 1:34:17 AM

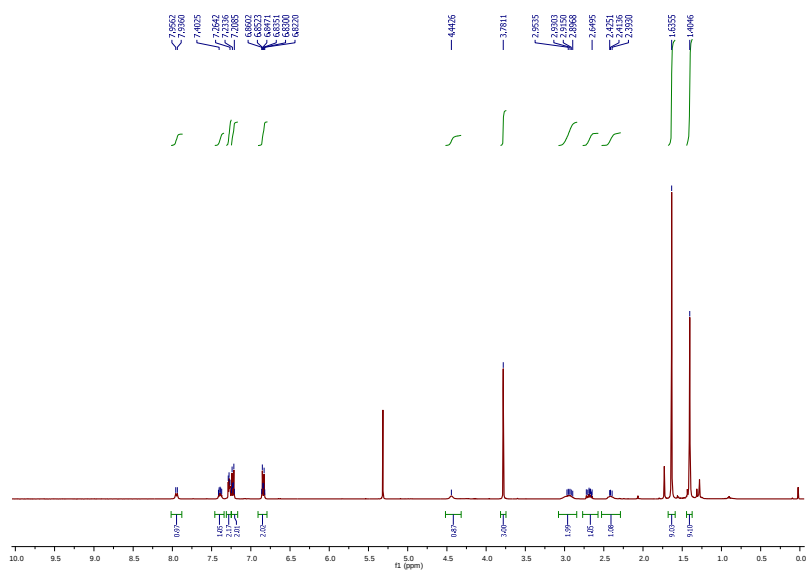
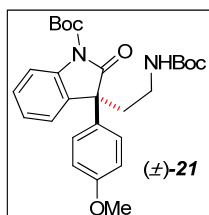
Operator Ravindra
 Instrument micrOTOF-Q II 10330

Acquisition Parameter

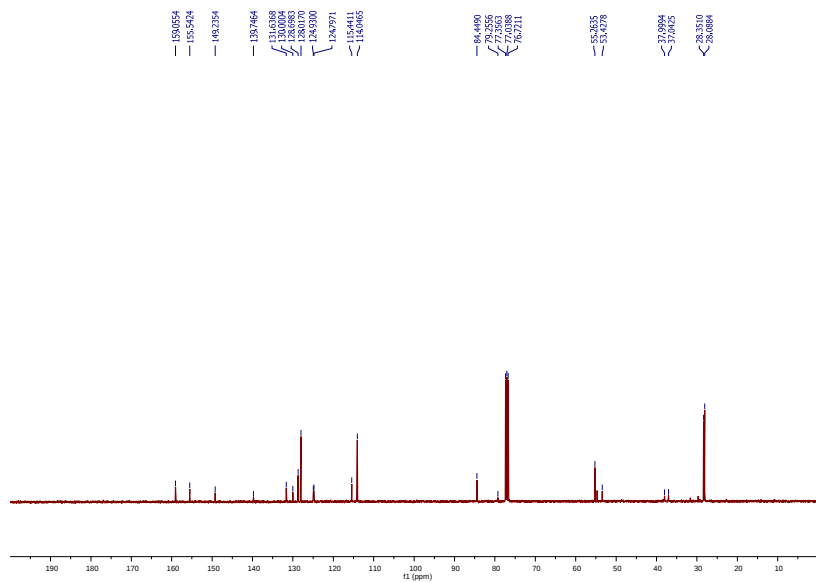
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum of (±)-17c



¹H NMR (400 MHz, CDCl₃) of compound (±)-21



¹³C NMR (100 MHz, CDCl₃) of compound (±)-21

Display Report

Analysis Info

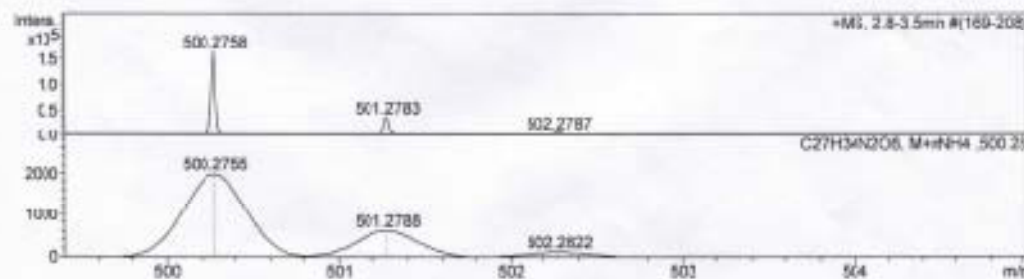
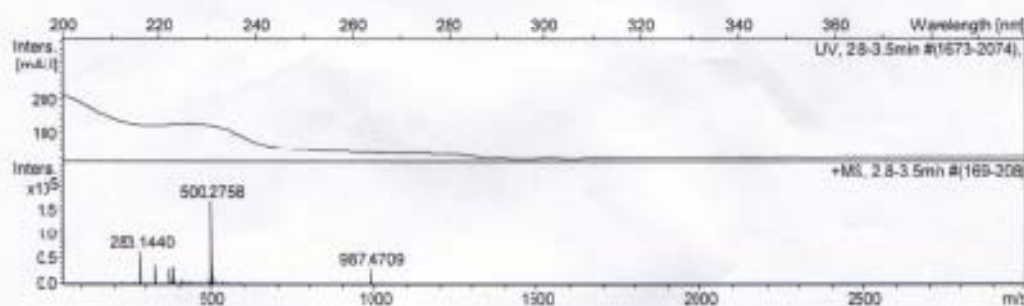
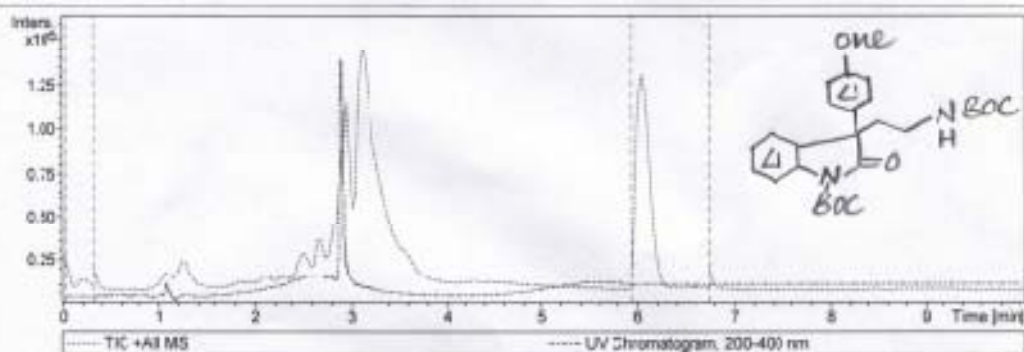
Analysis Name: D:\Data\user data\may2012\25 may\Dr. A. Bisai-SB-80 PS(R)_1-A_5_01_2385.d
 Method: HPLCMS-20 Septm
 Sample Name: Dr. A. Bisai-SB-80 PS(R)
 Comment: 54-2-80PSR

Acquisition Date: 6/26/2012 12:31:23 PM

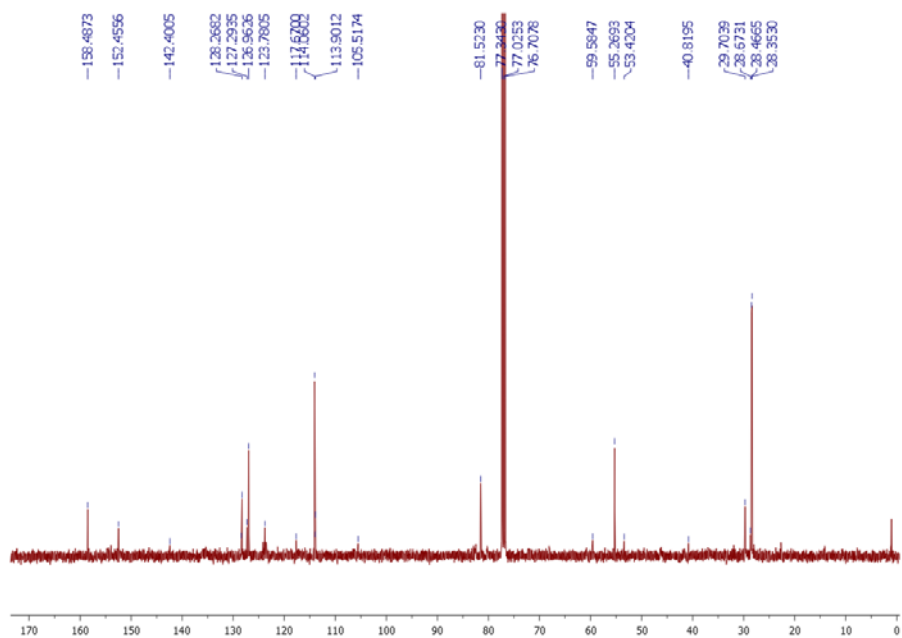
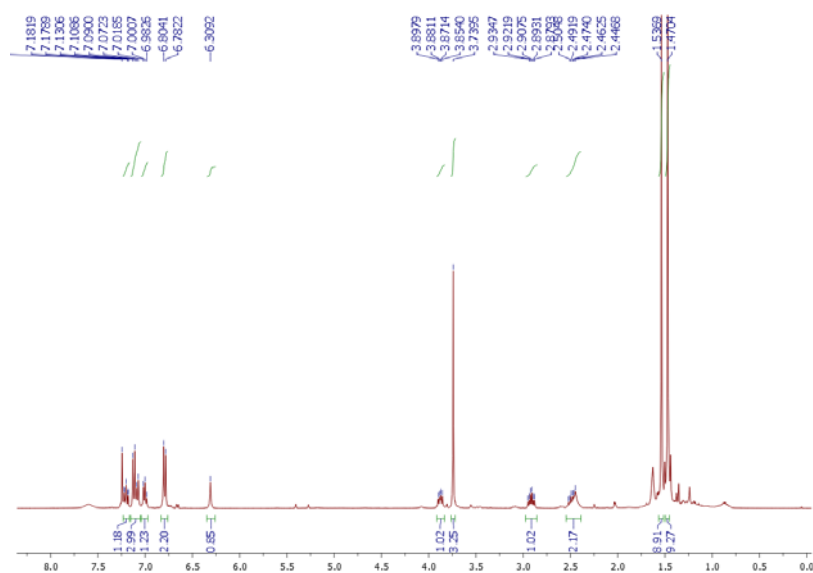
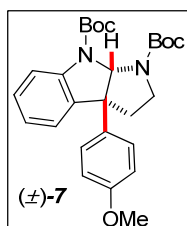
Operator: Meena Sharma
 Instrument: micrOTOF-Q II 10330

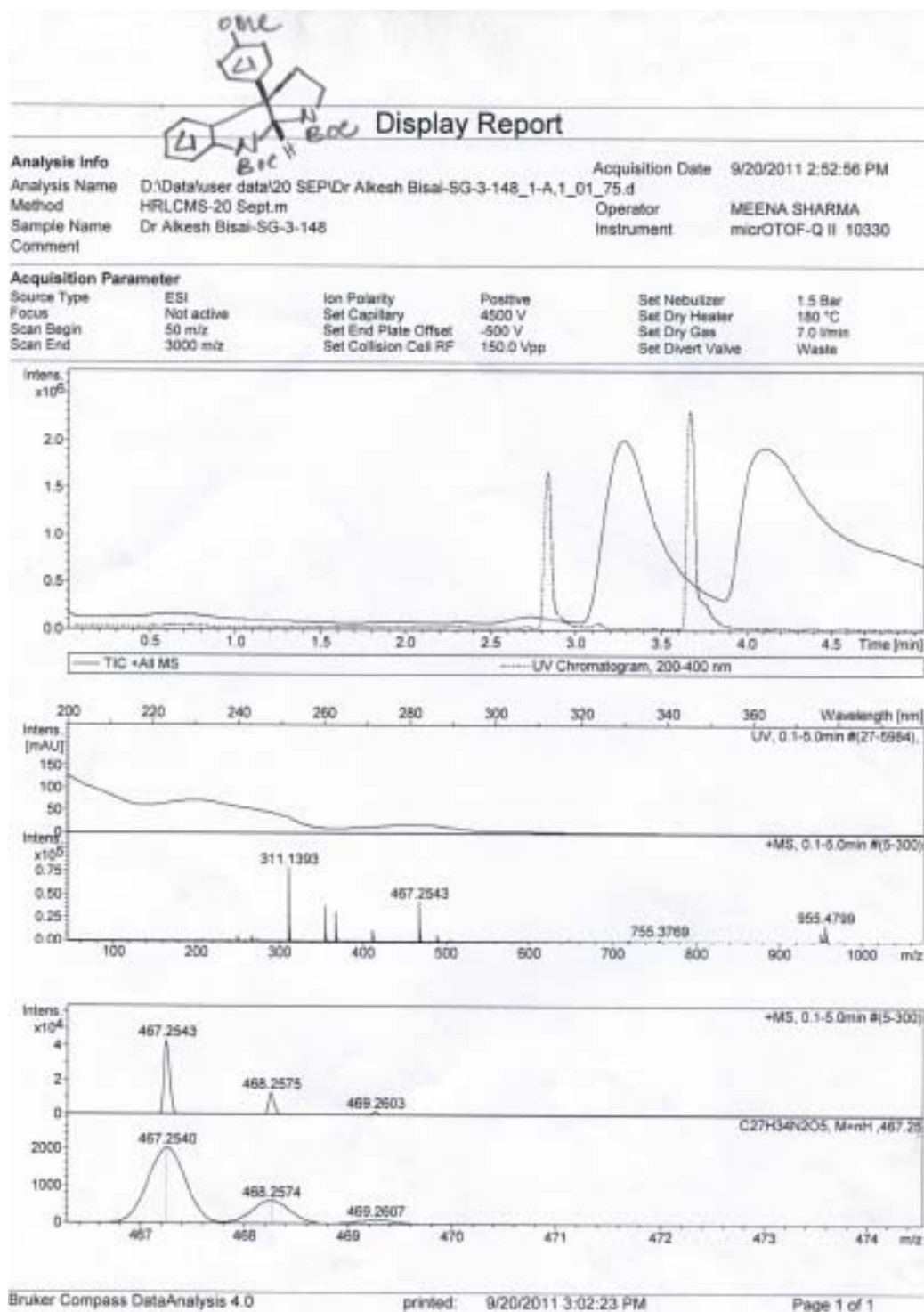
Acquisition Parameter

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Scan End	3000 m/z	Se: Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



Scanned copy of mass spectrum (±)-21





Scanned copy of mass spectrum of ($\pm$)-7