

# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

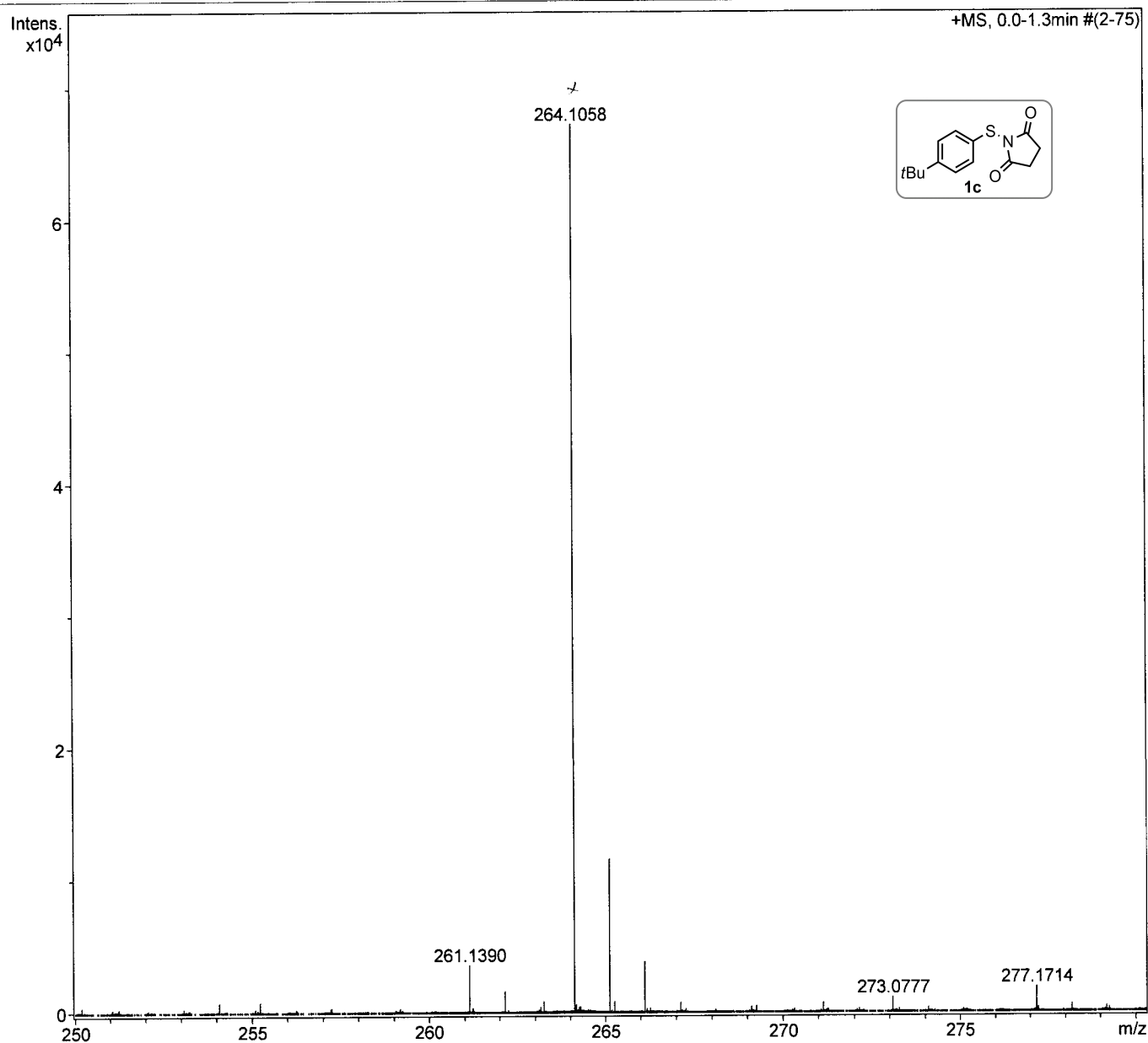
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-SM-tBu.d  
Method tune\_low\_Pos.m  
Sample Name ERA-SM-tBu  
Comment

Acquisition Date 12/10/2015 4:06:04 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

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## Analysis Info

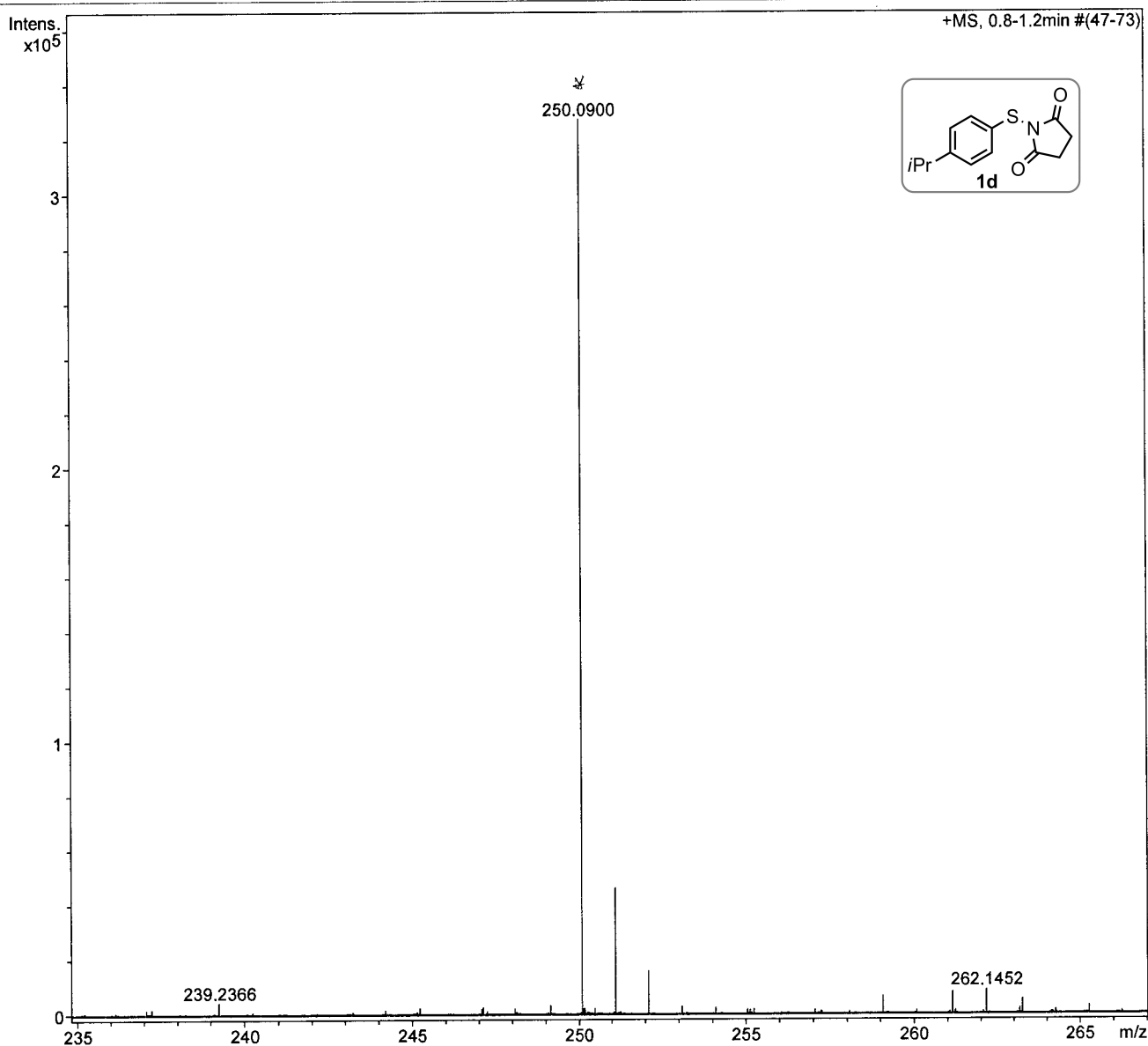
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-SM-ipr.d  
Method tune\_low\_Pos.m  
Sample Name ERA-SM-ipr  
Comment

Acquisition Date 12/10/2015 3:23:12 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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

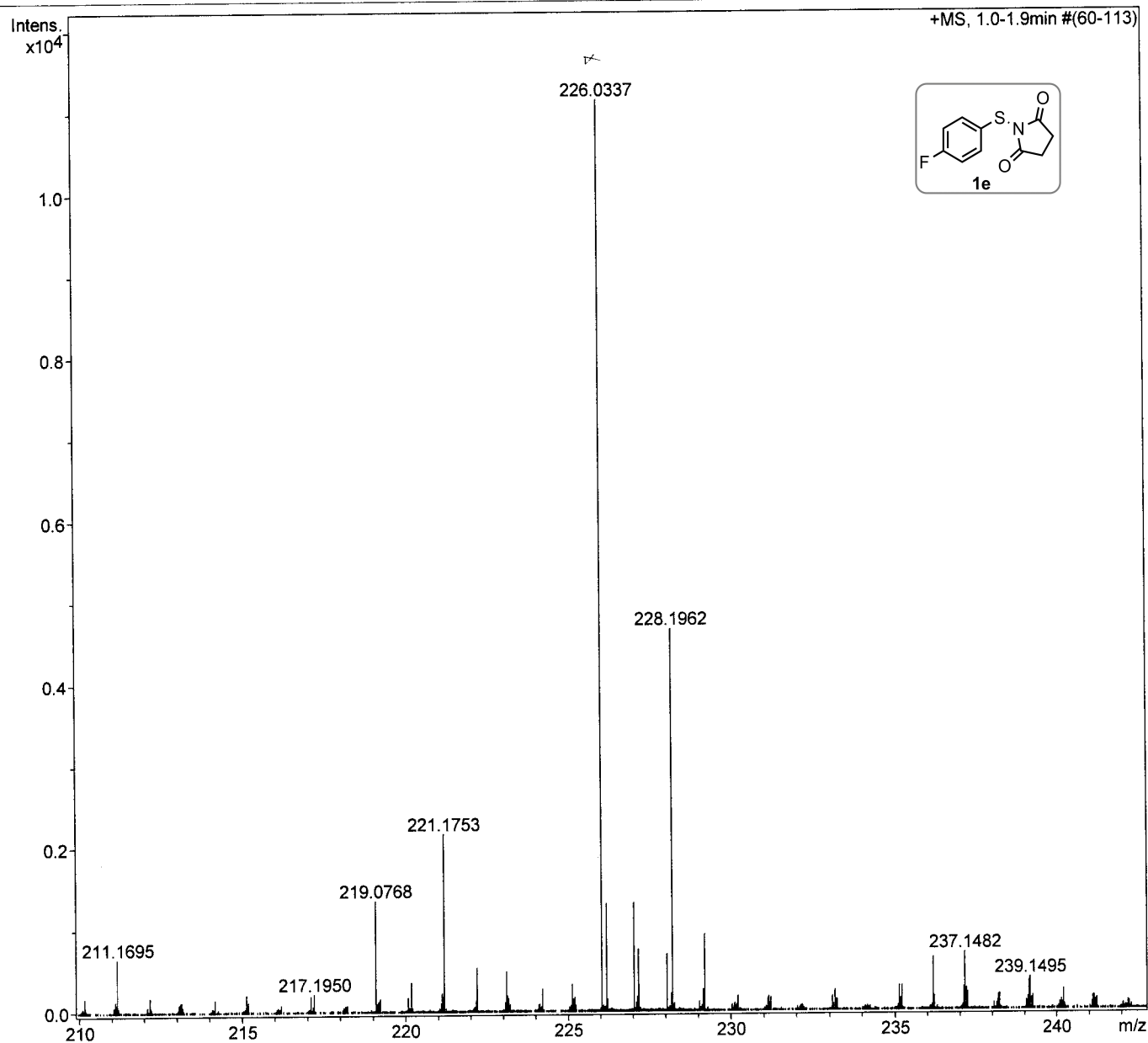
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-SM-P-F.d  
Method tune\_low\_Pos.m  
Sample Name ERA-SM-P-F  
Comment

Acquisition Date 12/10/2015 3:51:00 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

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## Analysis Info

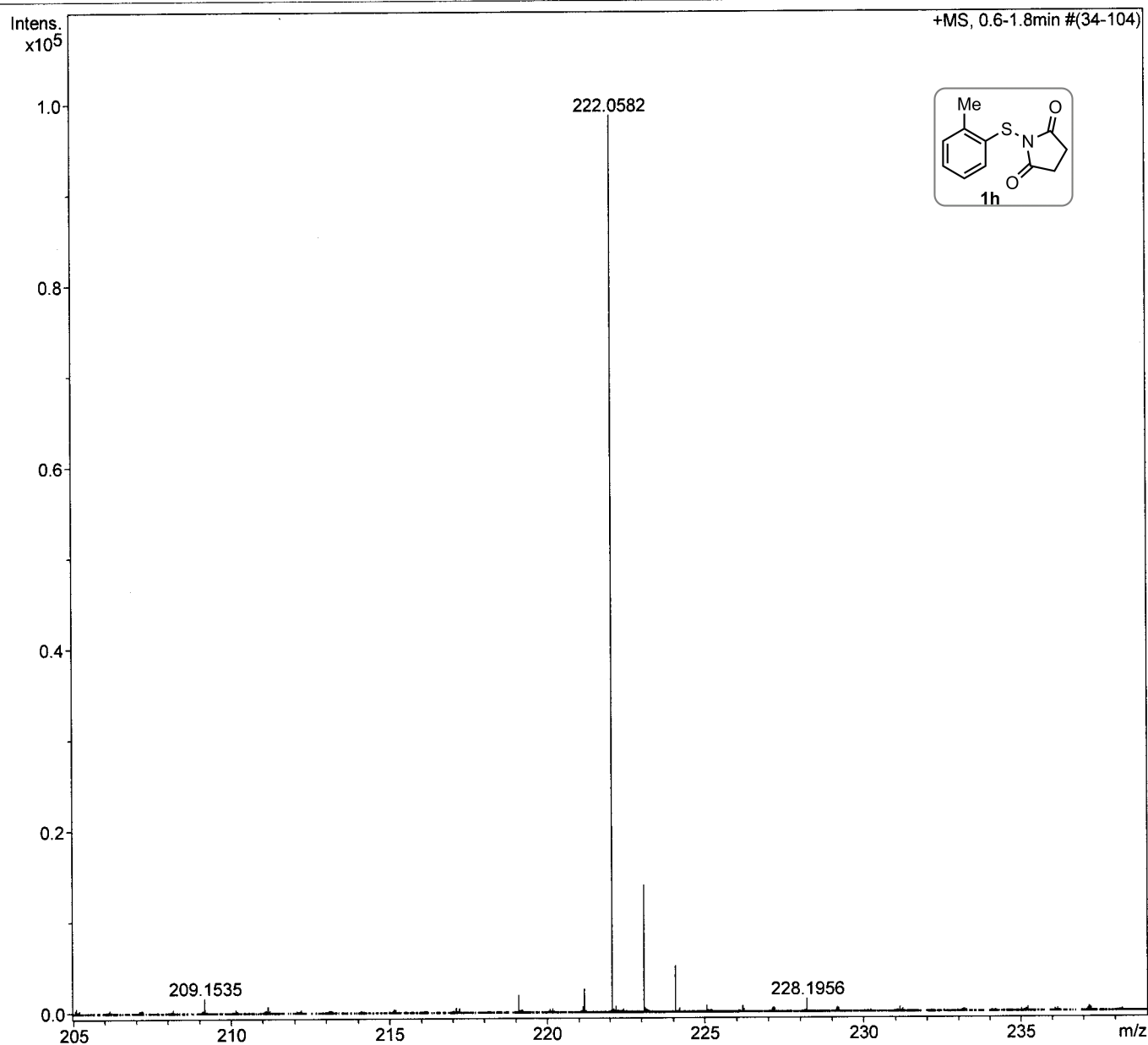
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-SM-OR-ME.d  
Method tune\_low\_Pos.m  
Sample Name ERA-SM-OR-ME  
Comment

Acquisition Date 12/10/2015 3:57:48 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  
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## Analysis Info

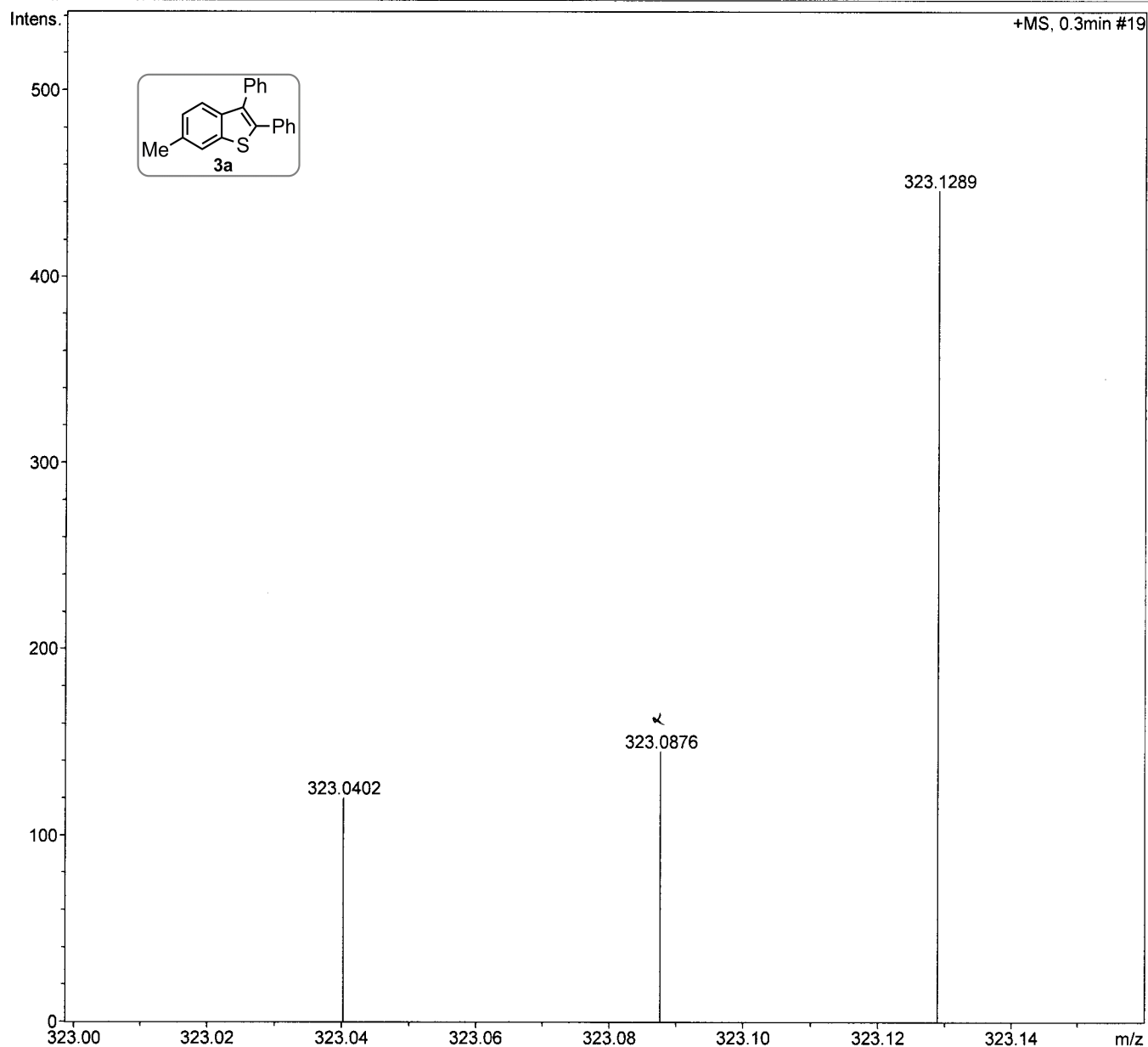
Analysis Name D:\Data\2015\DR.AK.SAHOO\AUG\ERA-P-ME-R1.d  
Method tune\_low.m  
Sample Name ERA-P-ME  
Comment

Acquisition Date 8/3/2015 12:26:32 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 4.4 psi   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# Display Report

## Analysis Info

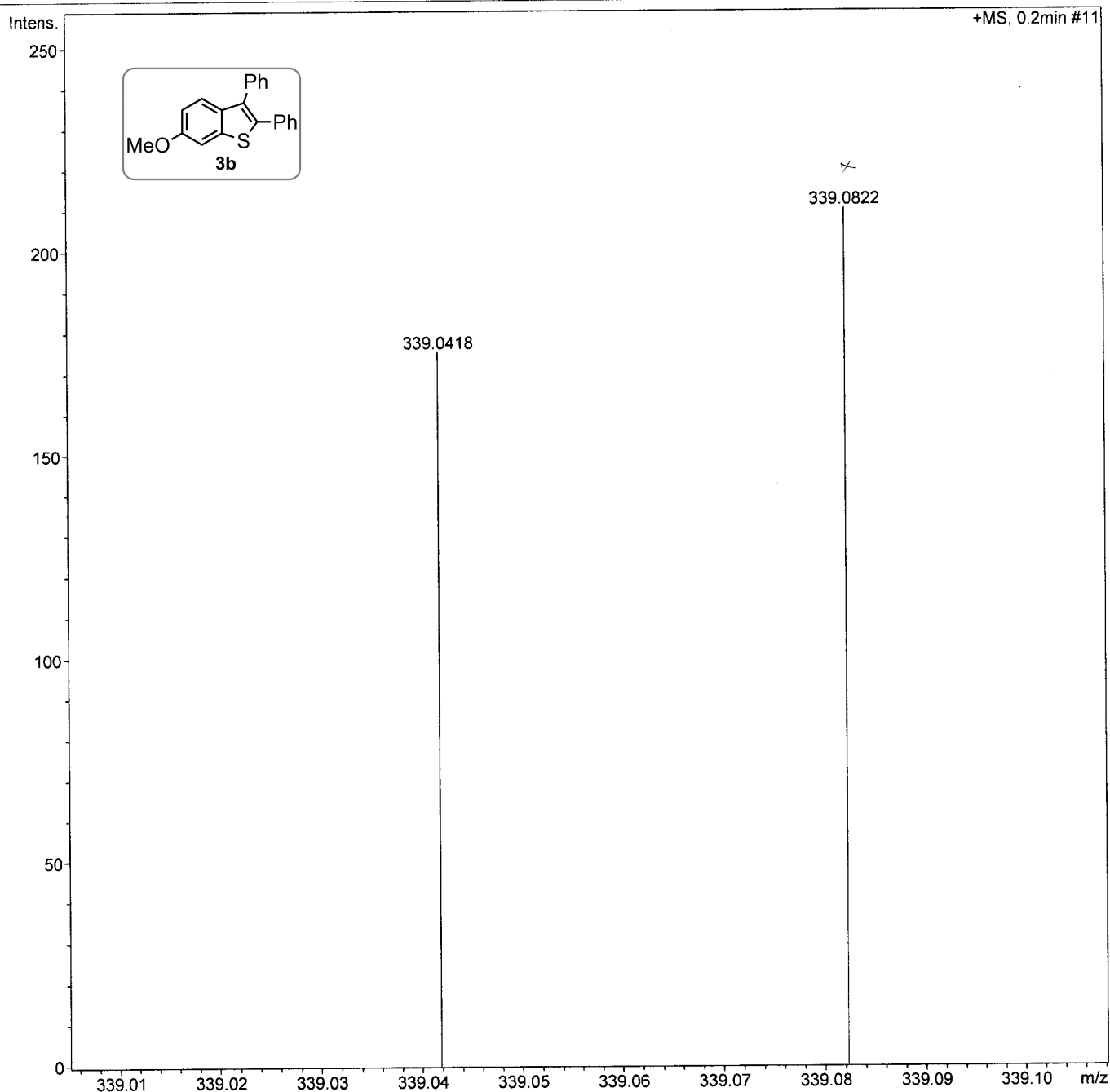
Analysis Name F:\Data\2015\DR.AK.SAHOOAUG\ERA-P-OME.d  
Method tune\_low\_Pos.m  
Sample Name ERA-P-OME-CHCL3-ACN  
Comment

Acquisition Date 8/3/2015 12:48:10 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  
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## Analysis Info

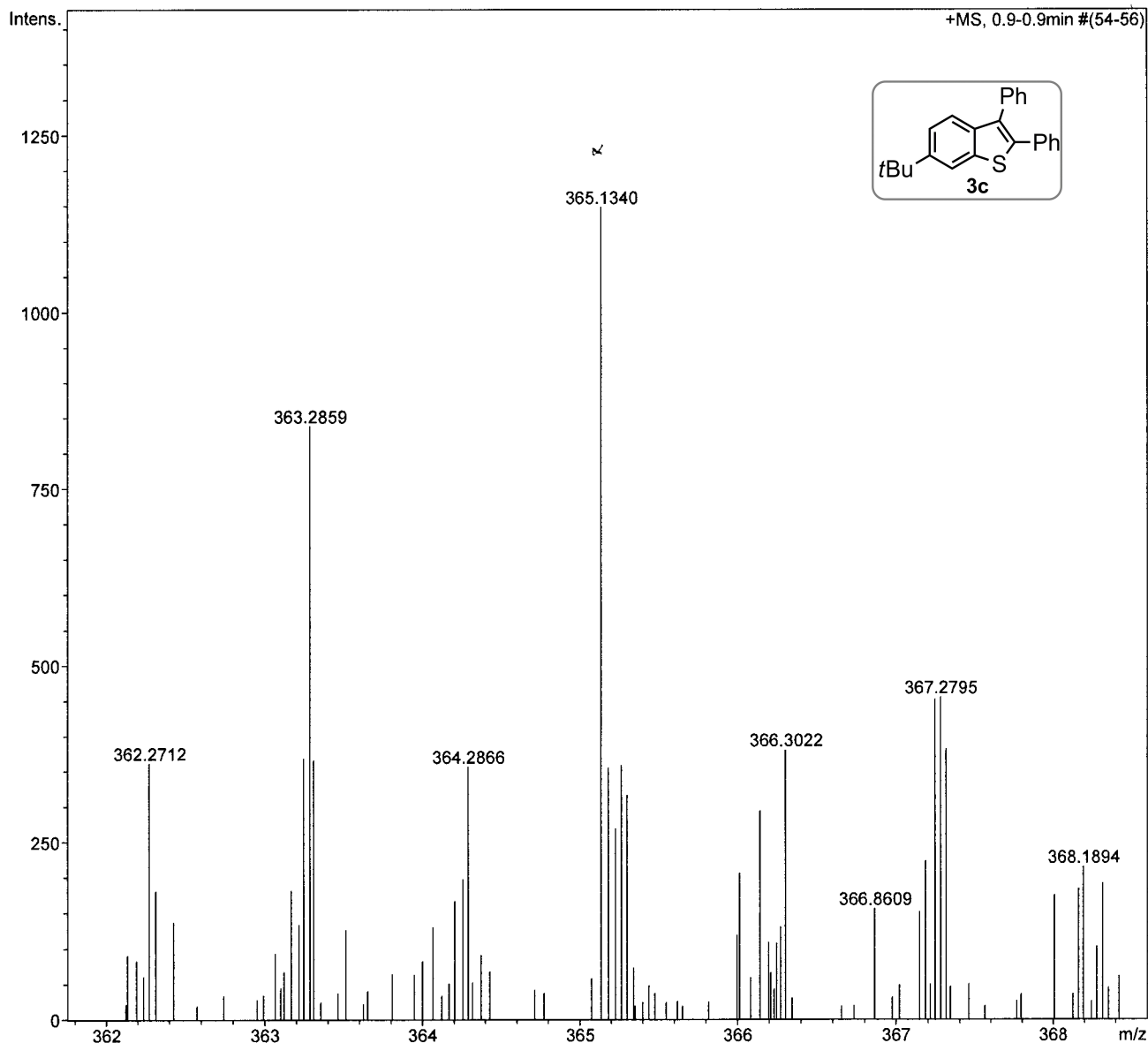
Analysis Name D:\Data\2015\DR.AK.SAHOO\AUG\ERA-6-178R.d  
Method tune\_low\_Pos-R2.m  
Sample Name ERA-6-178-CHCL3-ACN  
Comment

Acquisition Date 8/3/2015 1:19:04 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    | 2580 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

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## Analysis Info

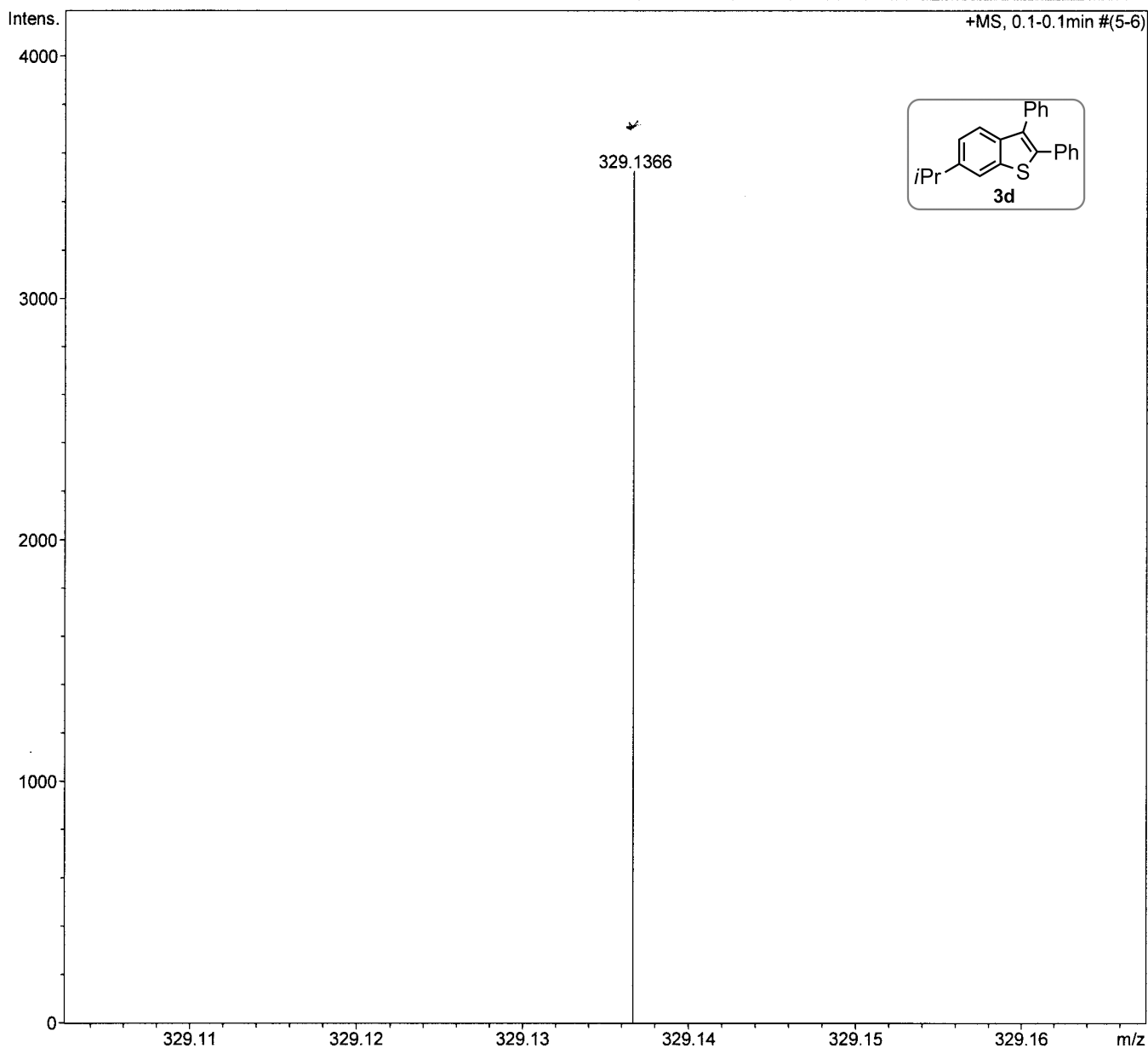
Analysis Name D:\Data\2015\DR.AK.SAHOOAUG\ERA-6-175R.d  
Method tune\_low\_Pos.m  
Sample Name ERA-6-175-CHCL3-ACN  
Comment

Acquisition Date 8/3/2015 1:08:31 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         | 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  
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## Analysis Info

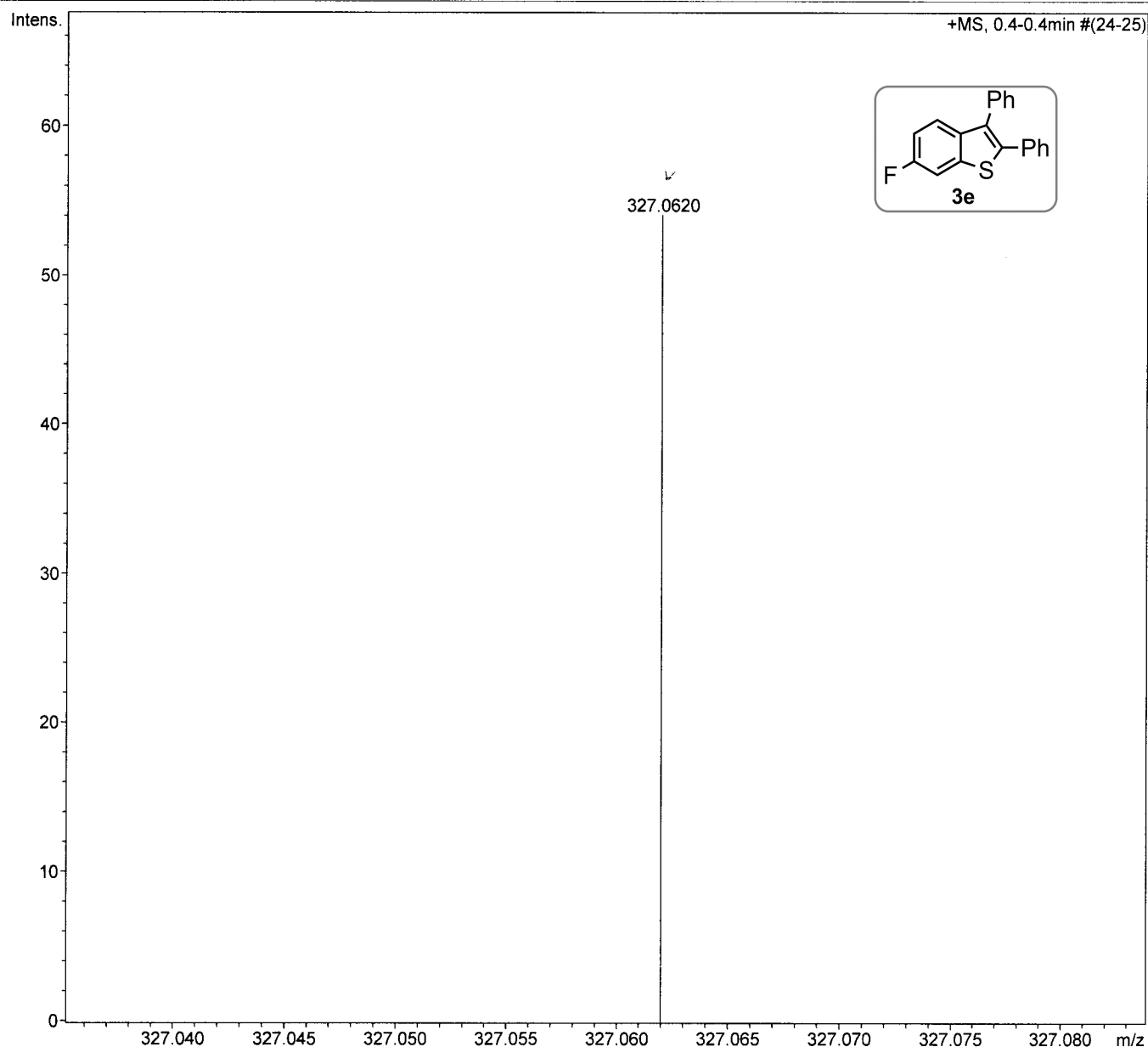
Analysis Name D:\Data\2015\DR.AK.SAHOOWJULY\ERA-7-25R1.d  
Method tune\_low.m  
Sample Name ERA-7-25R1-CHCL3-ACN  
Comment

Acquisition Date 7/27/2015 3:24:02 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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



# BRUKER MAXIS HRMS REPORT

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## Analysis Info

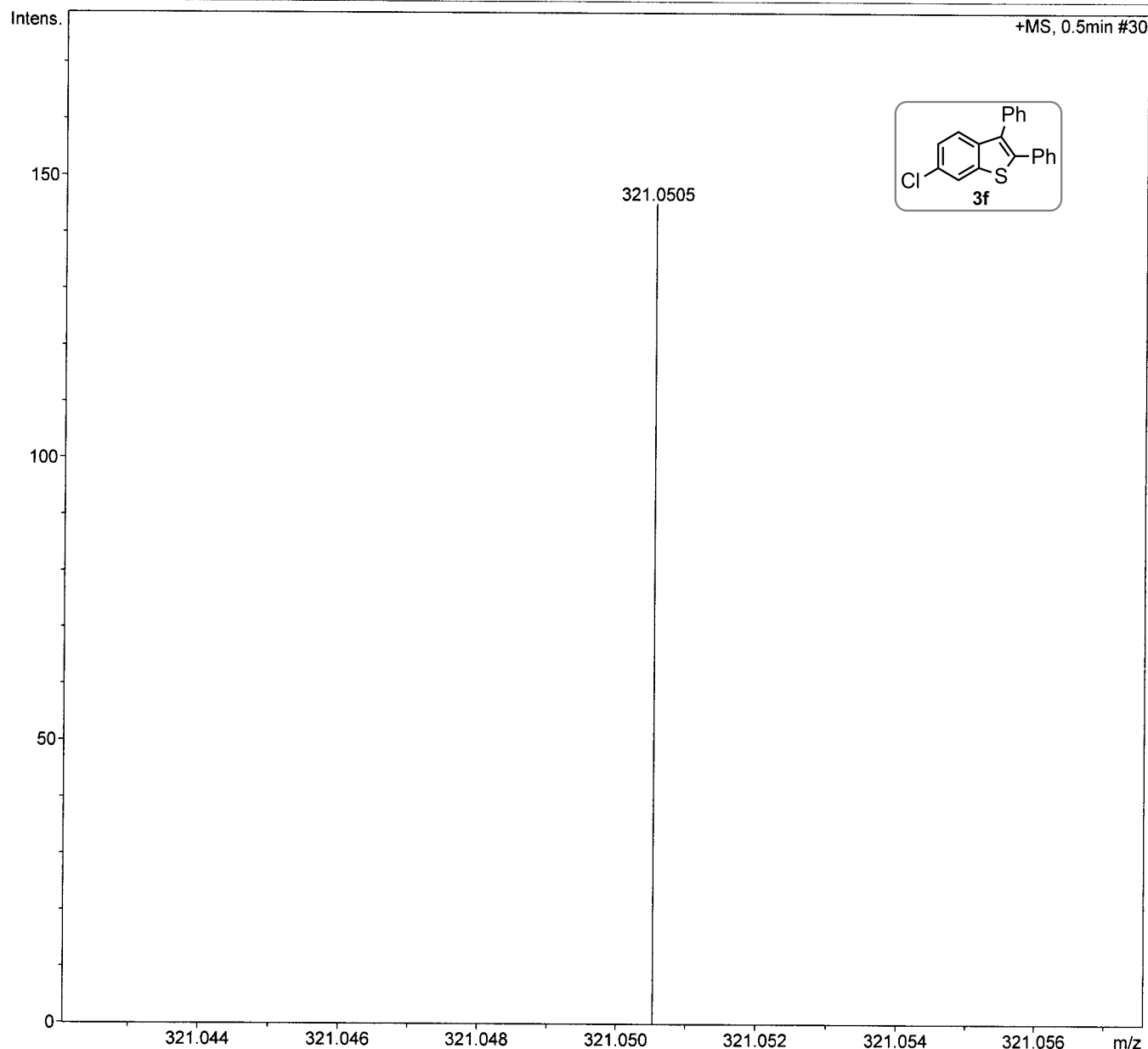
Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\ERA-7-70.d  
Method tune\_low.m  
Sample Name ERA-7-70-CHCL3-ACN  
Comment

Acquisition Date 7/27/2015 3:52:11 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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



# BRUKER MAXIS HRMS REPORT

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## Analysis Info

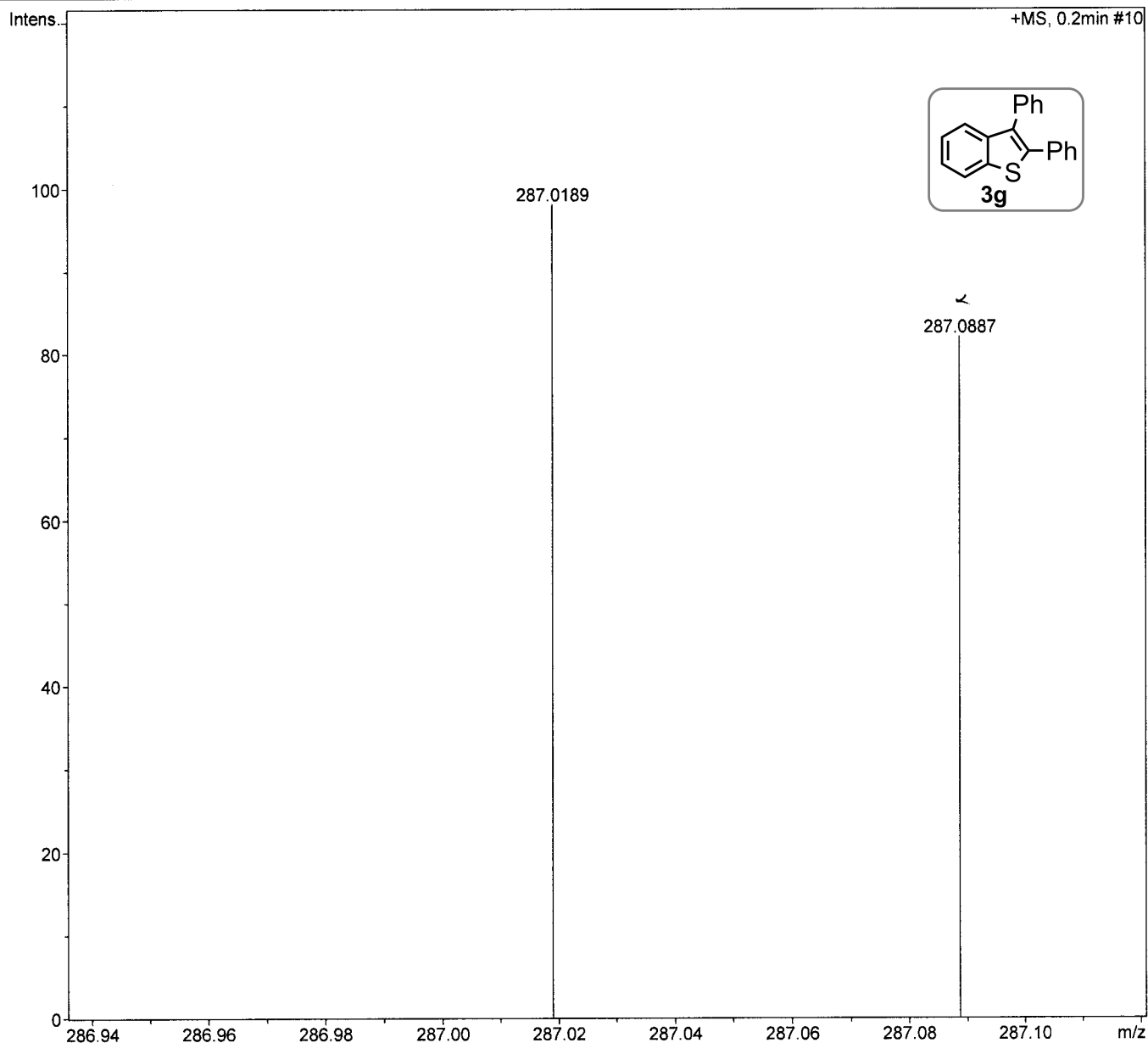
Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\ERA-PH.d  
Method tune\_low\_Pos-R2.m  
Sample Name ERA-PH-CHCL3-ACN  
Comment

Acquisition Date 7/31/2015 4:13:09 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    | 2580 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



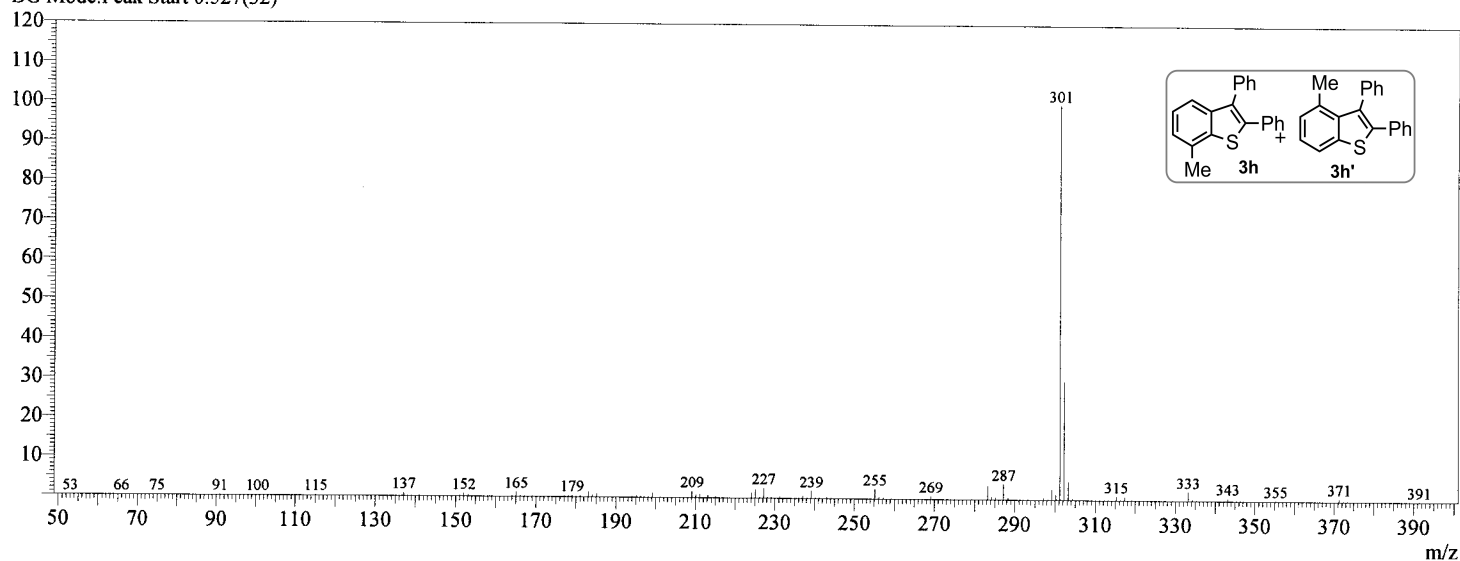
# LCMS-2010A DATA REPORT

## SHIMADZU

User : Admin  
Sample : ERA-7-31  
Inj. Volume : 5.000  
Data Name : E:\Data\ERA-7-31-APCI-POS1.qld  
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.774(Scan#:47) Positive  
MassPeaks:313 BasePeak:301.20(10321524)  
RawMode:Single 0.774(47)  
BG Mode:Peak Start 0.527(32)



MS Peak Table

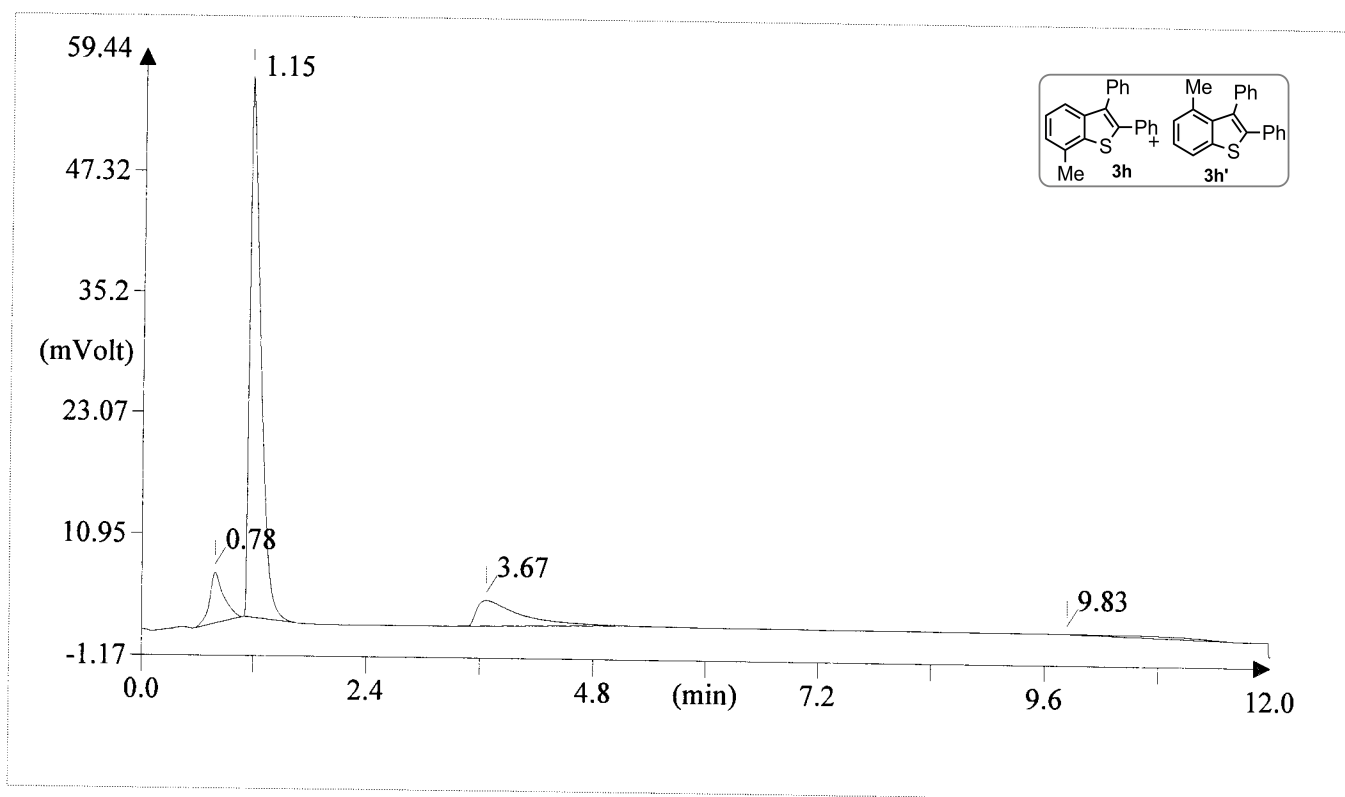
| Peak# | R.Time | I.Time | F.Time | Area      | Height   | A/H   | Mark | %Total | Name |
|-------|--------|--------|--------|-----------|----------|-------|------|--------|------|
| 1     | 0.774  | 0.527  | 1.043  | 279024402 | 20922606 | 13.33 |      | 100.00 |      |
|       |        |        |        | 279024402 | 20922606 |       |      | 100.00 |      |

Base m/z Base Int.  
301.20 10321524

# FLASH EA 1112 SERIES CHNS REPORT

## THERMO FINNIGAN

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys\_data\_ex  
 Sample ID: ERA-7-31 (# 196)  
 Analysis type: UnkNown  
 Chromatogram filename: UNK-25022016-6.dat  
 Sample weight: .986



| Element Name | Element % | Ret. Time |
|--------------|-----------|-----------|
| Nitrogen     | 0. 07     | 0. 78     |
| Carbon       | 83. 85    | 1. 15     |
| Hydrogen     | 5. 41     | 3. 67     |
| Sulphur      | 10. 56    | 9. 83     |

# UOH -SCHOOL OF CHEMISTRY -HRMS

## Analysis Info

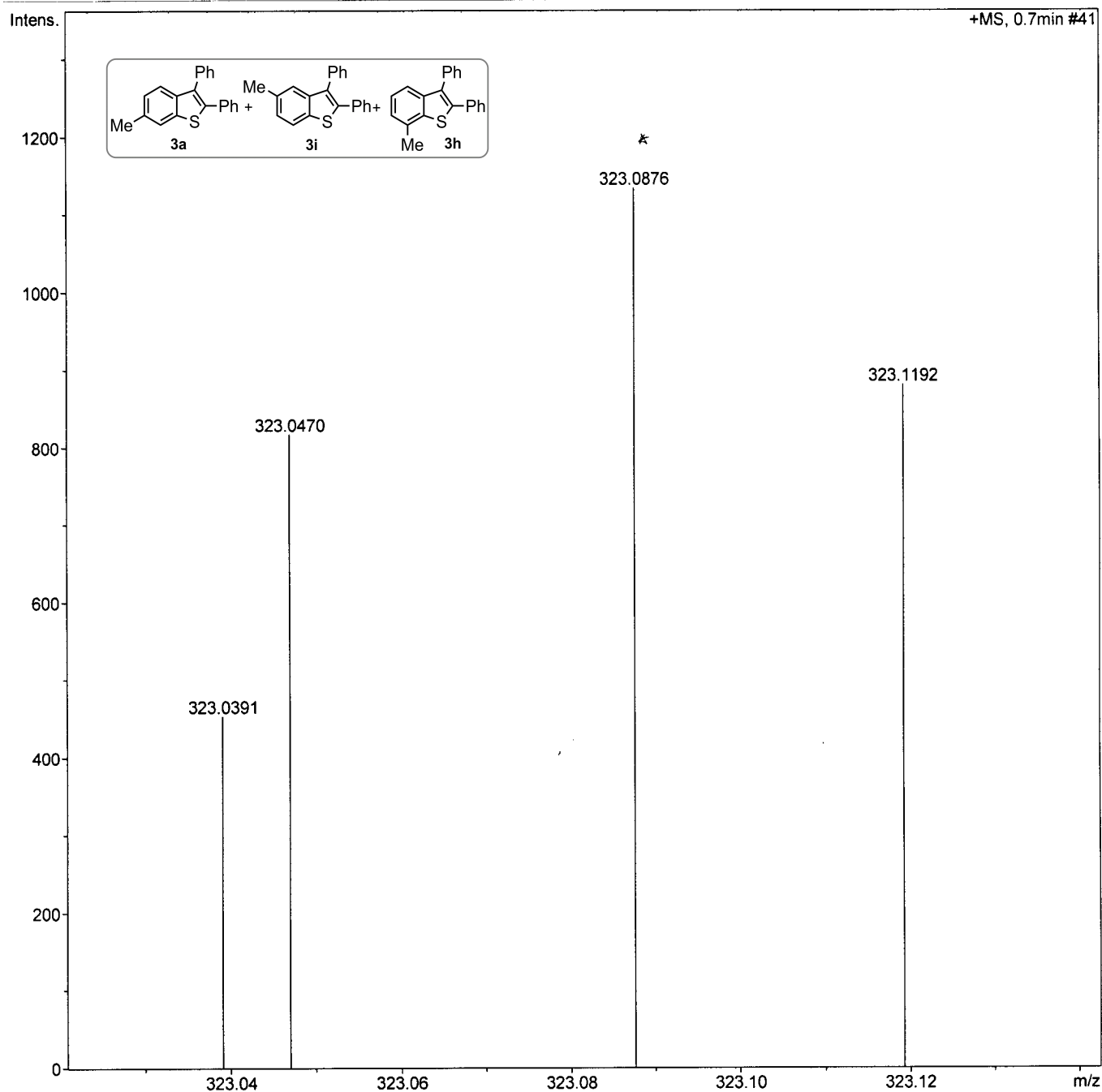
Analysis Name D:\Data\2016\DR.A.K.SAHOO\MARCH\ERA-7-89.d  
 Method tune\_low.m  
 Sample Name ERA-7-89-DCM-MEOH  
 Comment

Acquisition Date 3/31/2016 10:54:06 AM

Operator Rajesh Vashisth  
 Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1500 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
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## Analysis Info

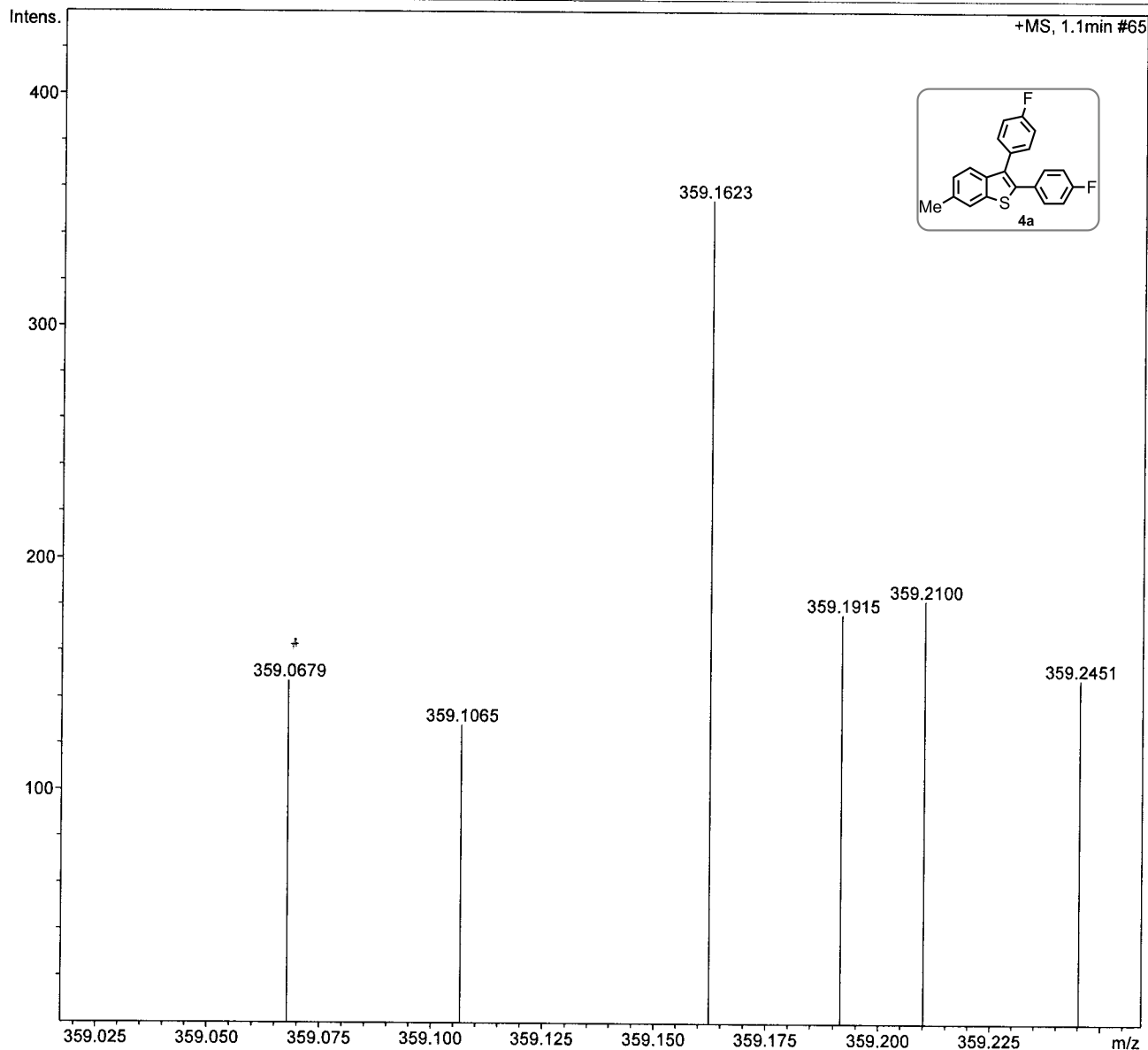
Analysis Name D:\Data\2015\DR.AK.SAHOOWJULY\ERA-7-49.d  
Method tune\_low.m  
Sample Name ERA-7-49-CHCL3-ACN  
Comment

Acquisition Date 7/27/2015 4:14:08 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 4.4 psi   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

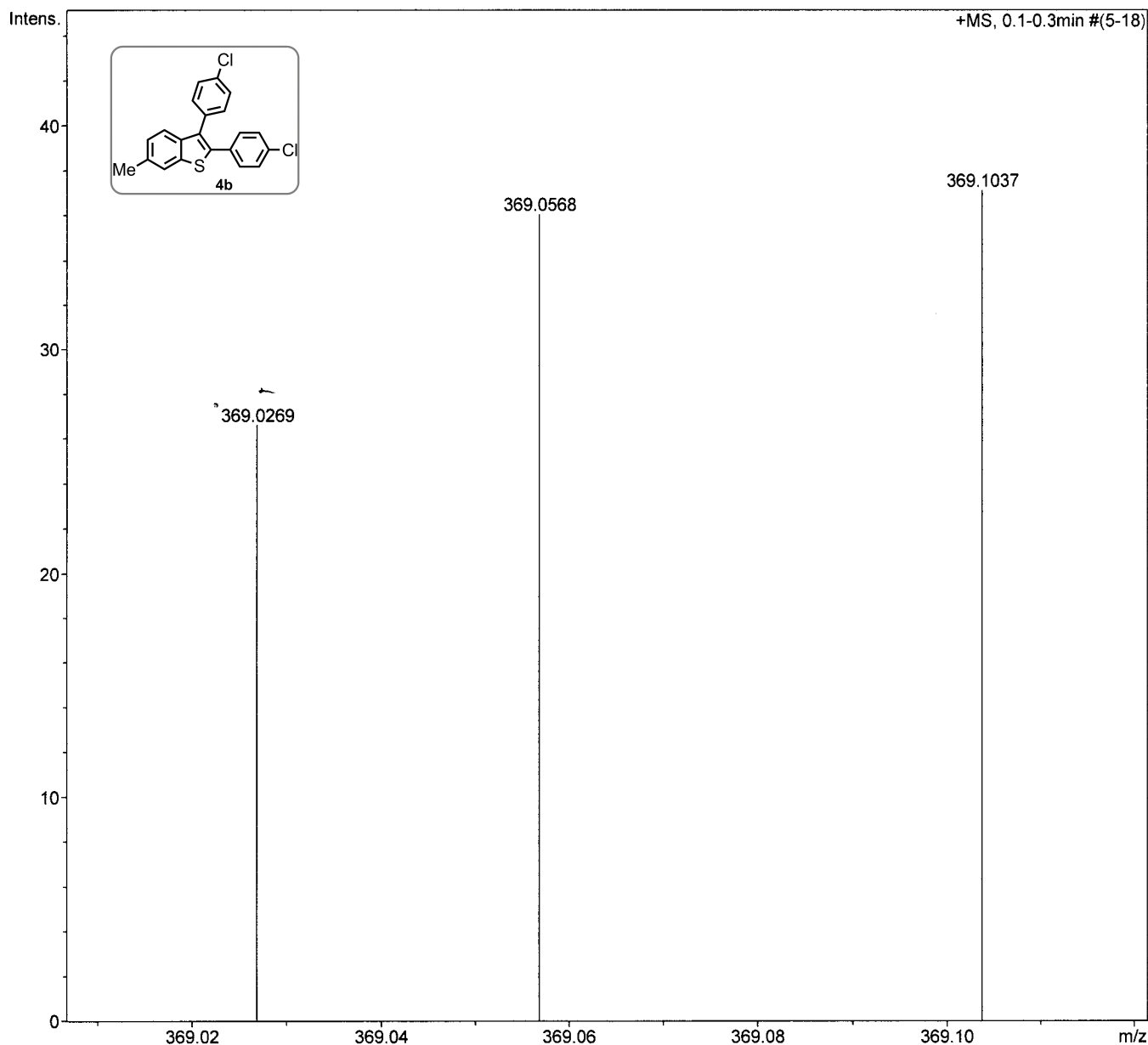
Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\ERA-7-50.d  
Method tune\_low.m  
Sample Name ERA-7-50-CHCL3-ACN  
Comment

Acquisition Date 7/27/2015 4:30:33 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 4.4 psi   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |





# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

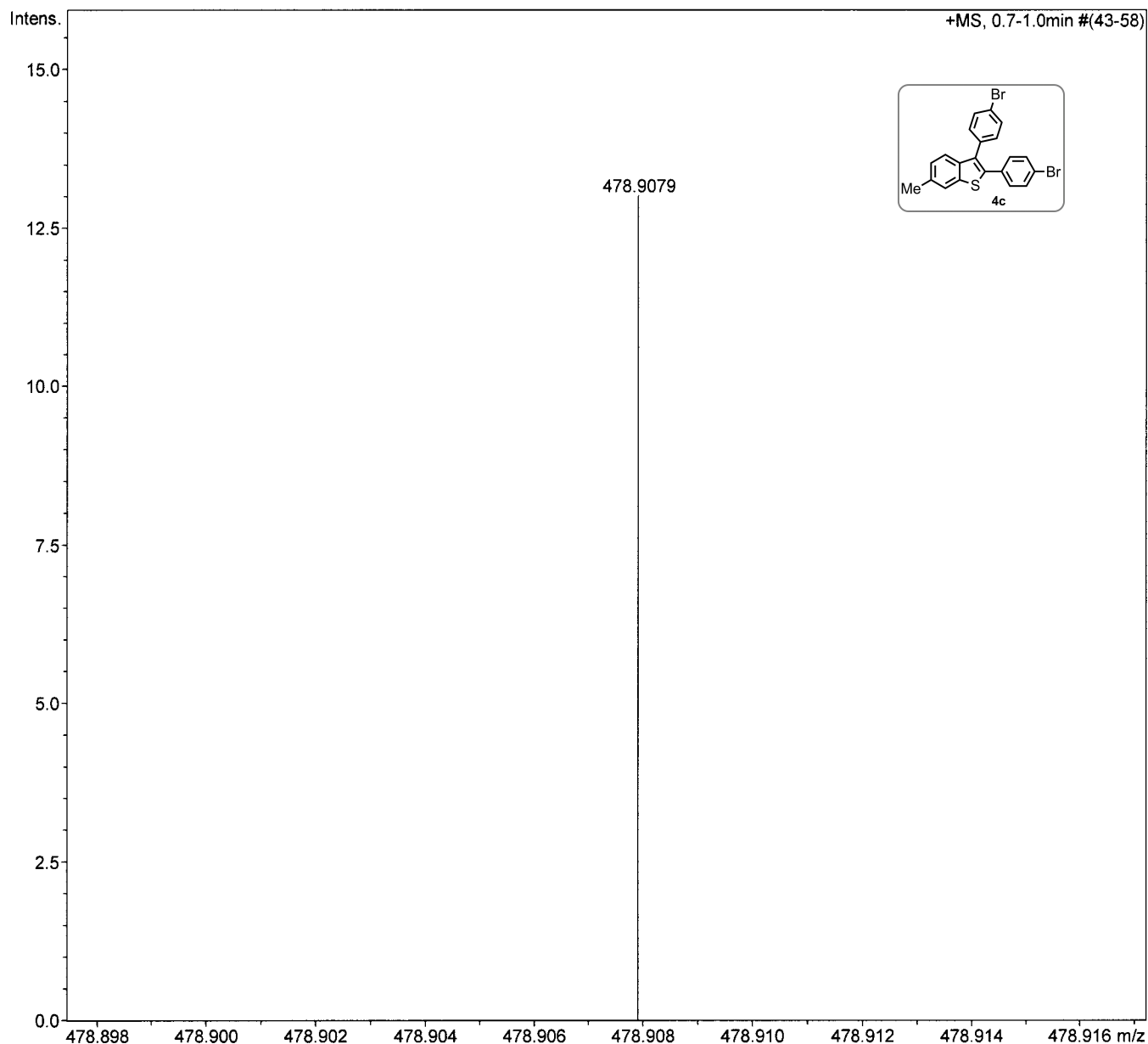
Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\ERA-7-69.d  
Method tune\_low.m  
Sample Name ERA-7-69-CHCL3-ACN  
Comment

Acquisition Date 7/27/2015 4:52:49 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         | 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    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# Display Report

## Analysis Info

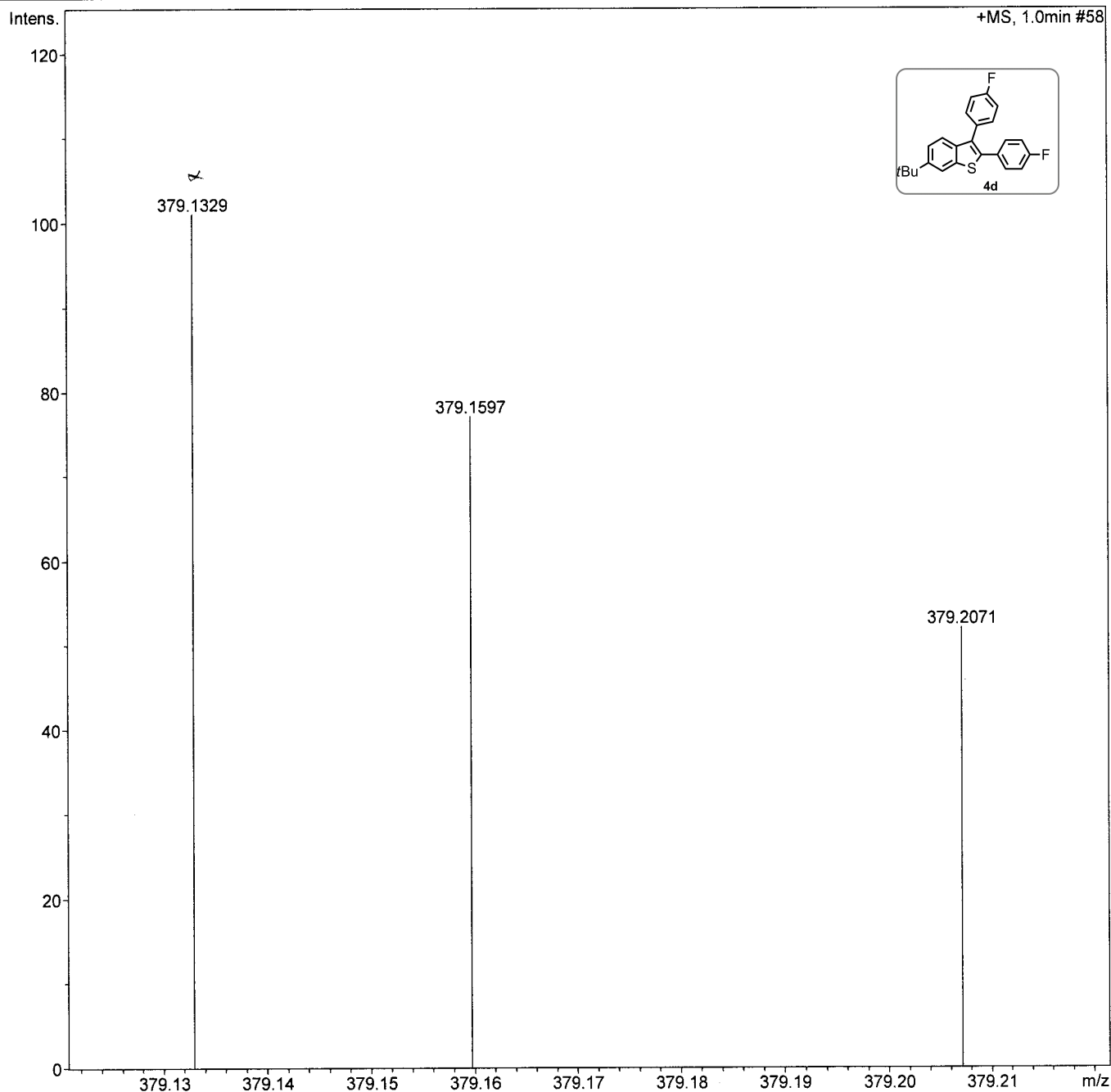
Analysis Name F:\Data\2015\DR.AK.SAHOO\NOVERA-7-54.d  
Method tune\_low\_Pos-R2.m  
Sample Name ERA-7-54-chcl3-acn  
Comment

Acquisition Date 11/12/2015 4:18:35 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    | 2580 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# UOH -SCHOOL OF CHEMISTRY -HRMS

## Analysis Info

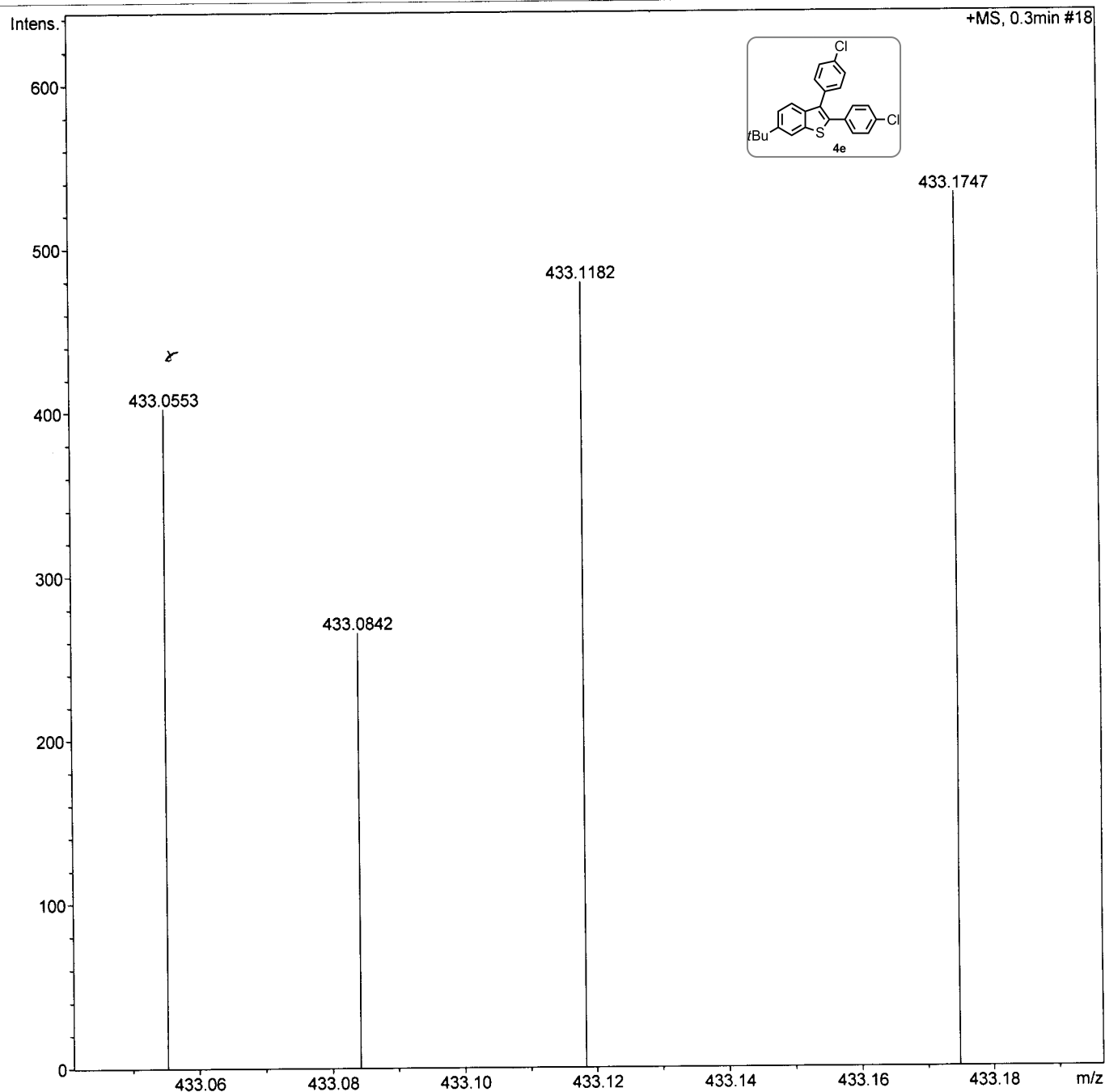
Analysis Name D:\Data\2016\DR.A.K.SAHOO\MARCH\ERA-7--55R.d  
 Method tune\_low\_Pos.m  
 Sample Name ERA-7-55-DCM-MEOH  
 Comment

Acquisition Date 3/31/2016 12:04:53 PM

Operator Rajesh Vashisth  
 Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| 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  
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## Analysis Info

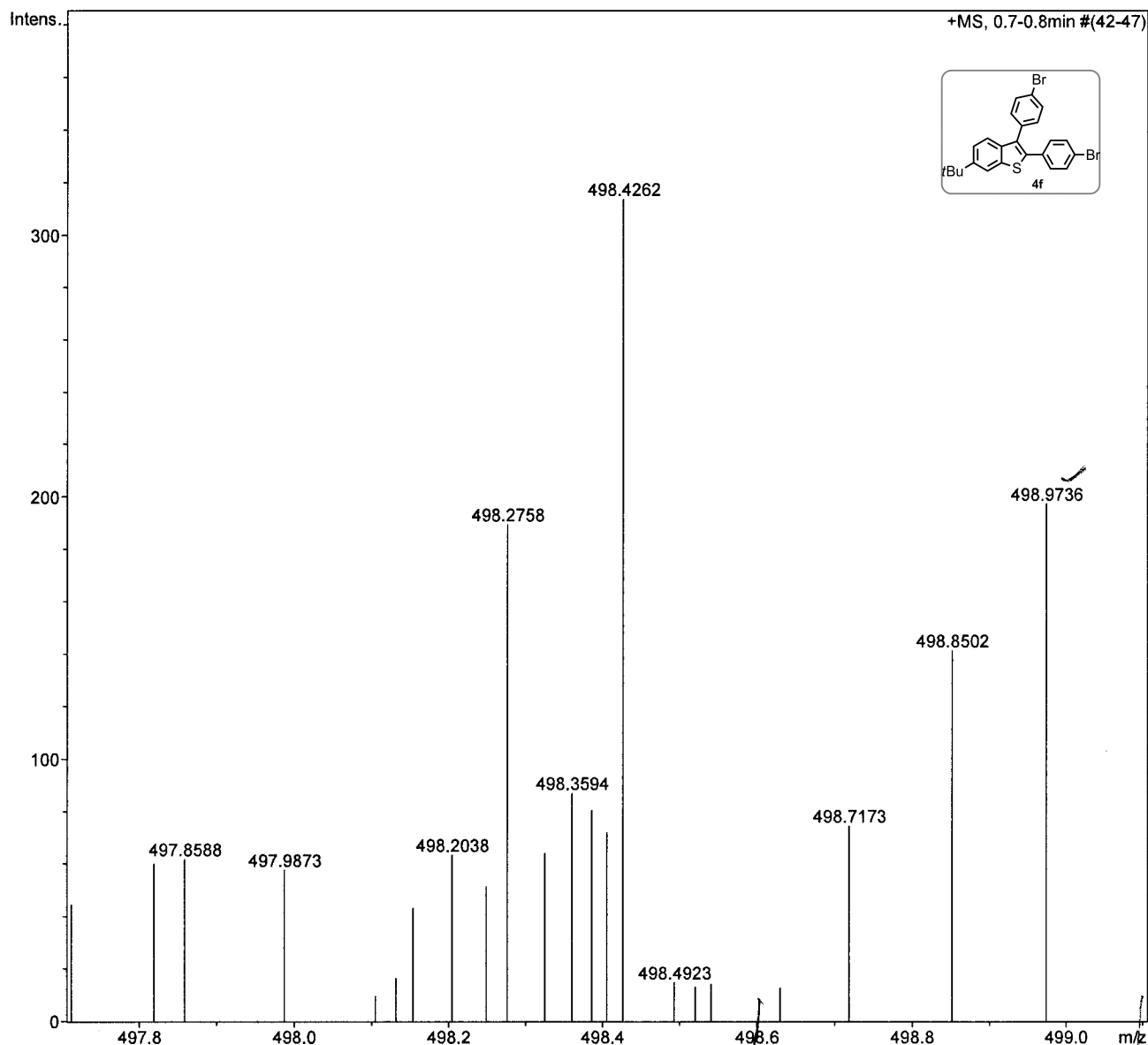
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\ERA-7-20.d  
Method tune\_low\_Pos-R2.m  
Sample Name ERA-7-20-chcl3-acn  
Comment

Acquisition Date 11/12/2015 4:55:01 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    | 2580 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



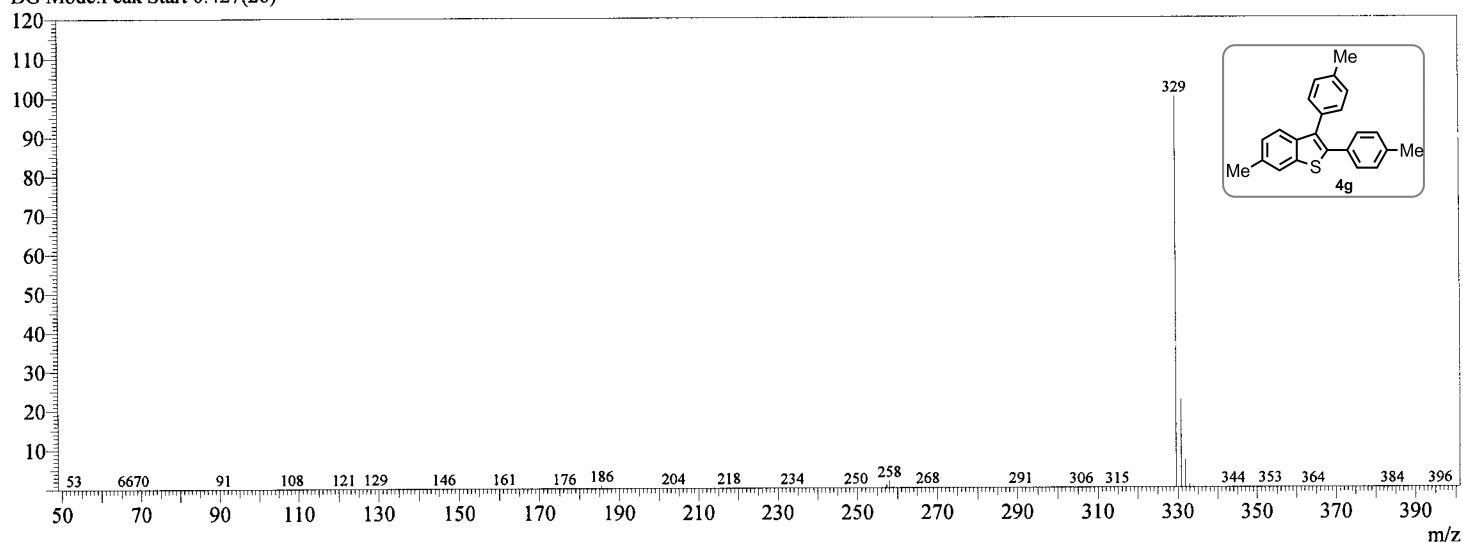
# LCMS-2010A DATA REPORT

## SHIMADZU

User : Admin  
Sample : ERA-7-90  
Inj. Volume : 5.000  
Data Name : G:\LCMSsolution\User\Data\ERA-7-90-APCI-POS1.qld  
Method Name : C:\LCMSsolution\User\Method\Copy of JAY-4-APCI.qlm

### MS Spectrum

Line#:1 R.Time:0.607(Scan#:37) Positive  
MassPeaks:188 BasePeak:329.55(4595101)  
RawMode:Single 0.607(37)  
BG Mode:Peak Start 0.427(26)



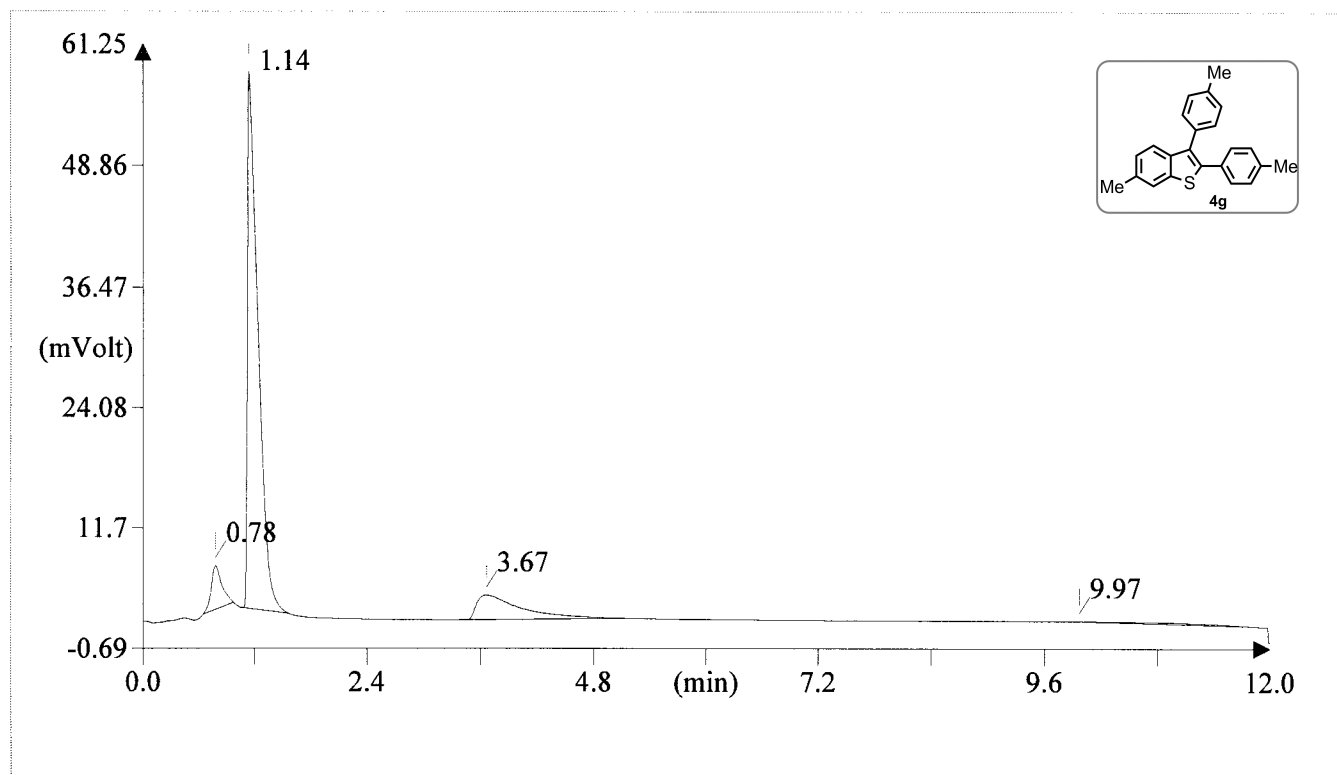
| MS Peak Table |        |        |        |          |         |          |
|---------------|--------|--------|--------|----------|---------|----------|
| Peak#         | R.Time | I.Time | F.Time | Area     | Height  | A/H Mark |
| 1             | 0.607  | 0.427  | 0.843  | 65344746 | 6069219 | 10.76    |
|               |        |        |        | 65344746 | 6069219 | 100.00   |

Base m/z Base Int.  
329.55 4595101

# FLASH EA 1112 SERIES CHNS REPORT

## THERMO FINNIGAN

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys\_data\_ex  
 Sample ID: ERA-7-90 (# 102)  
 Analysis type: UnkNown  
 Chromatogram filename: UNK-13022016-2.dat  
 Sample weight: 1.223



| Element Name | Element % | Ret. Time |
|--------------|-----------|-----------|
| Nitrogen     | 0.08      | 0.78      |
| Carbon       | 84.17     | 1.14      |
| Hydrogen     | 6.18      | 3.67      |
| Sulphur      | 9.69      | 9.97      |

# Display Report

## Analysis Info

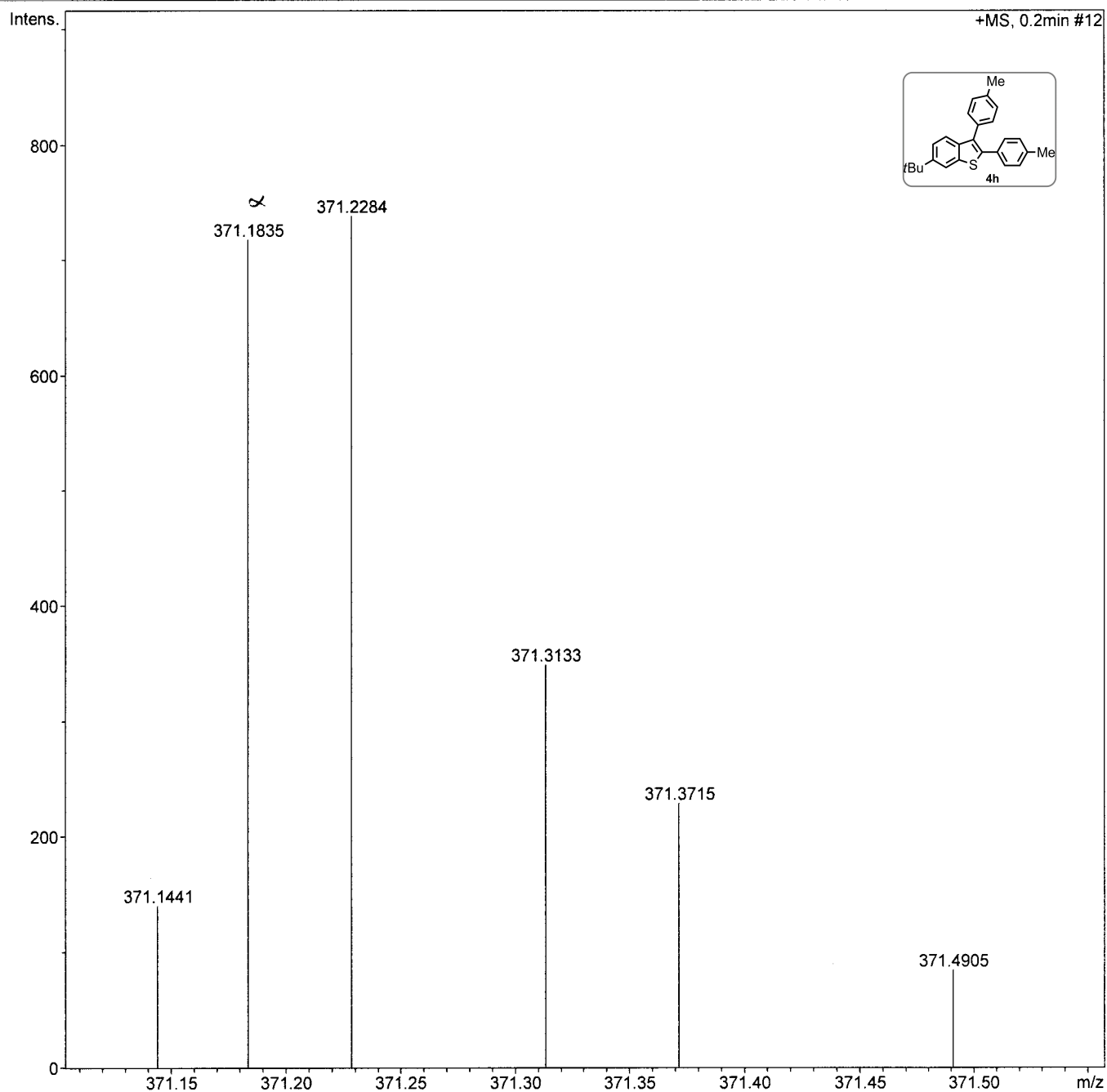
Analysis Name F:\Data\2015\DR.AK.SAHOO\NOVERA-7-37R.d  
Method tune\_low\_Pos-R2.m  
Sample Name ERA-7-37-chcl3-acn  
Comment

Acquisition Date 11/12/2015 3:47:59 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    | 2580 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# Display Report

## Analysis Info

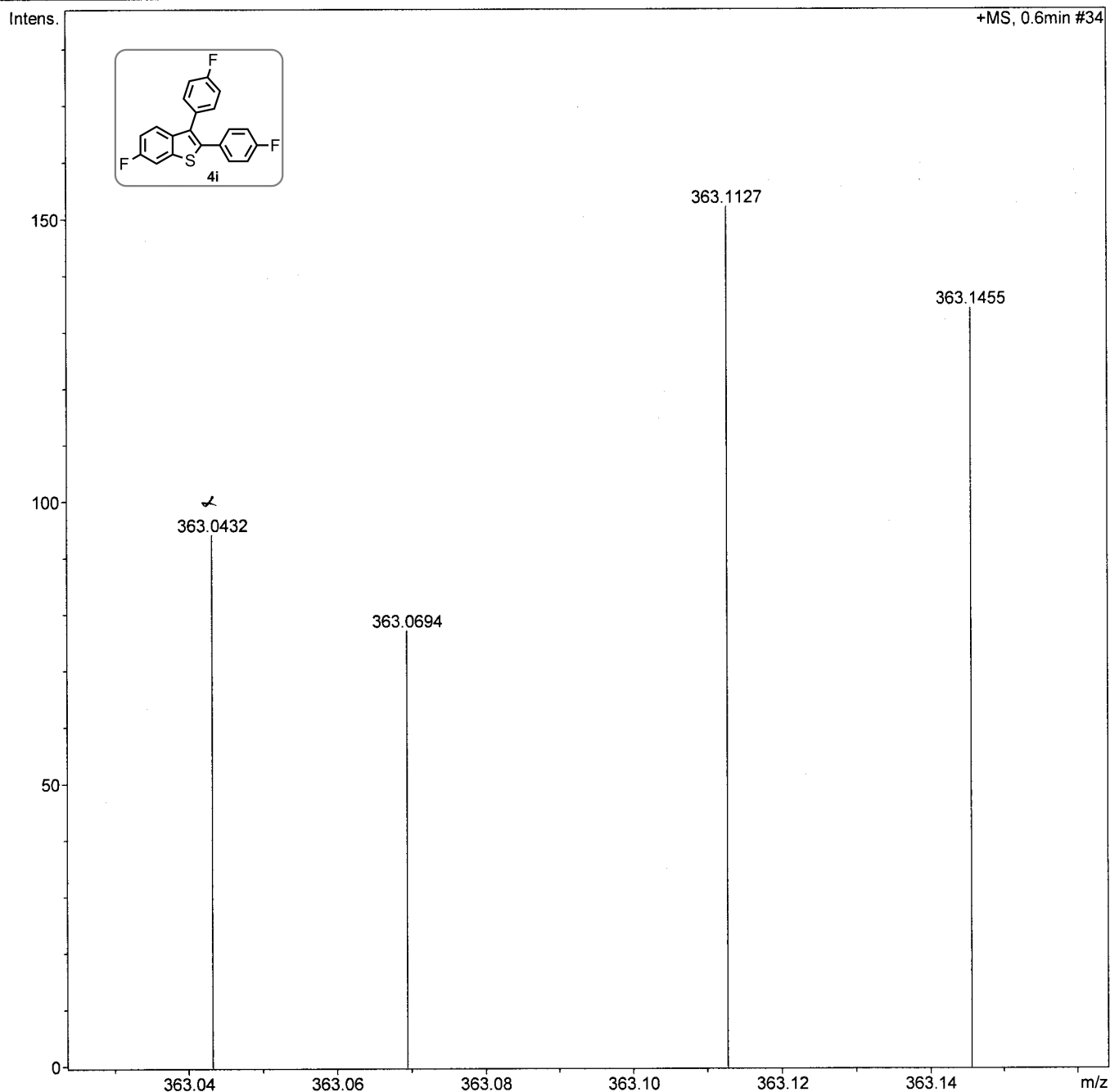
Analysis Name F:\Data\2015\DR.AK.SAHOOAUG\ERA-NA-14.d  
Method tune\_low.m  
Sample Name ERA-NA-14-MEOH  
Comment

Acquisition Date 8/10/2015 4:12:41 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         | 3200 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |





# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

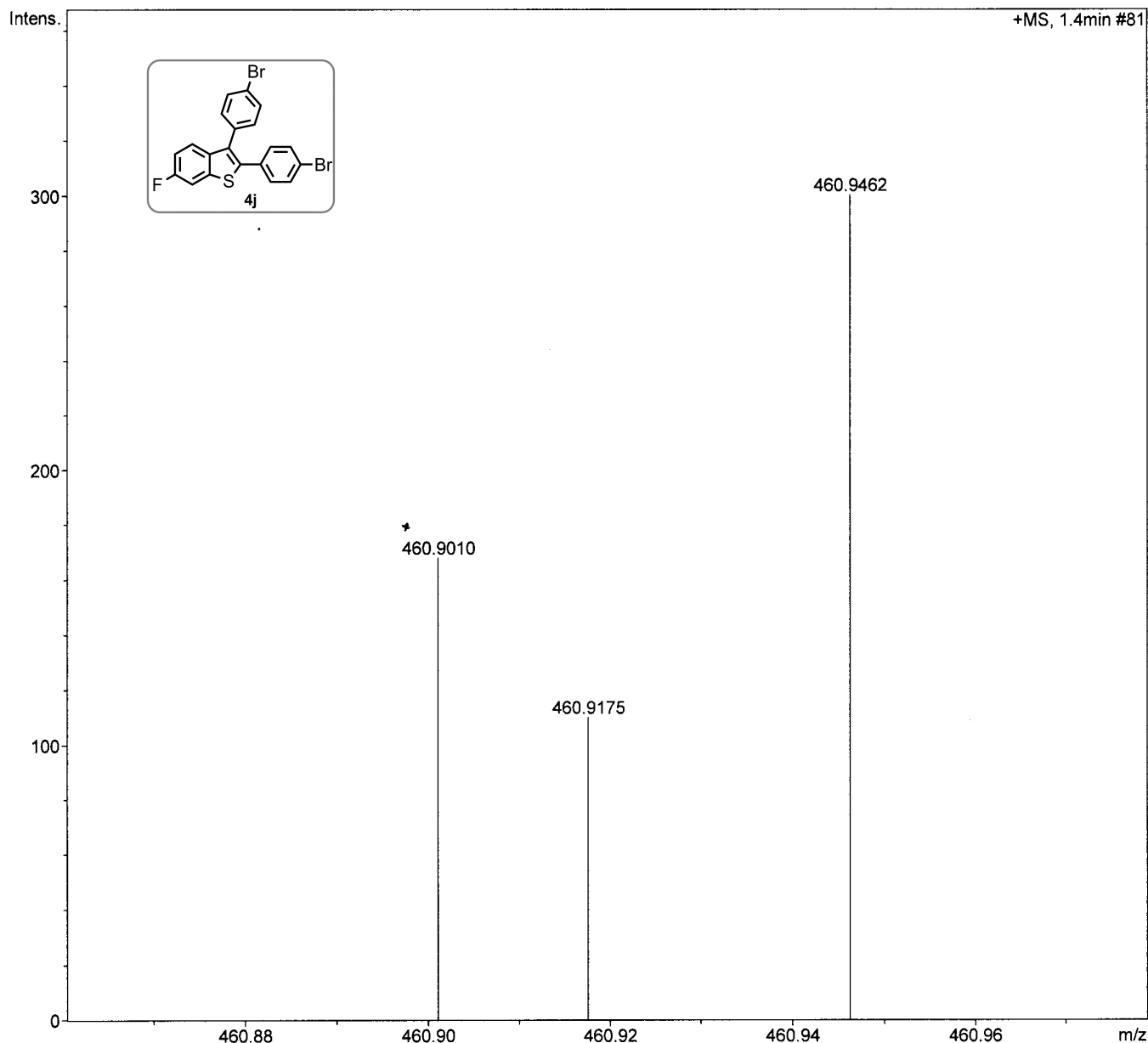
Analysis Name D:\Data\2015\DR.AK.SAHOOAUG\ERA-7-124R.d  
Method tune\_low.m  
Sample Name ERA-7-124-MEOH  
Comment

Acquisition Date 8/12/2015 11:53:48 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         | 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    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

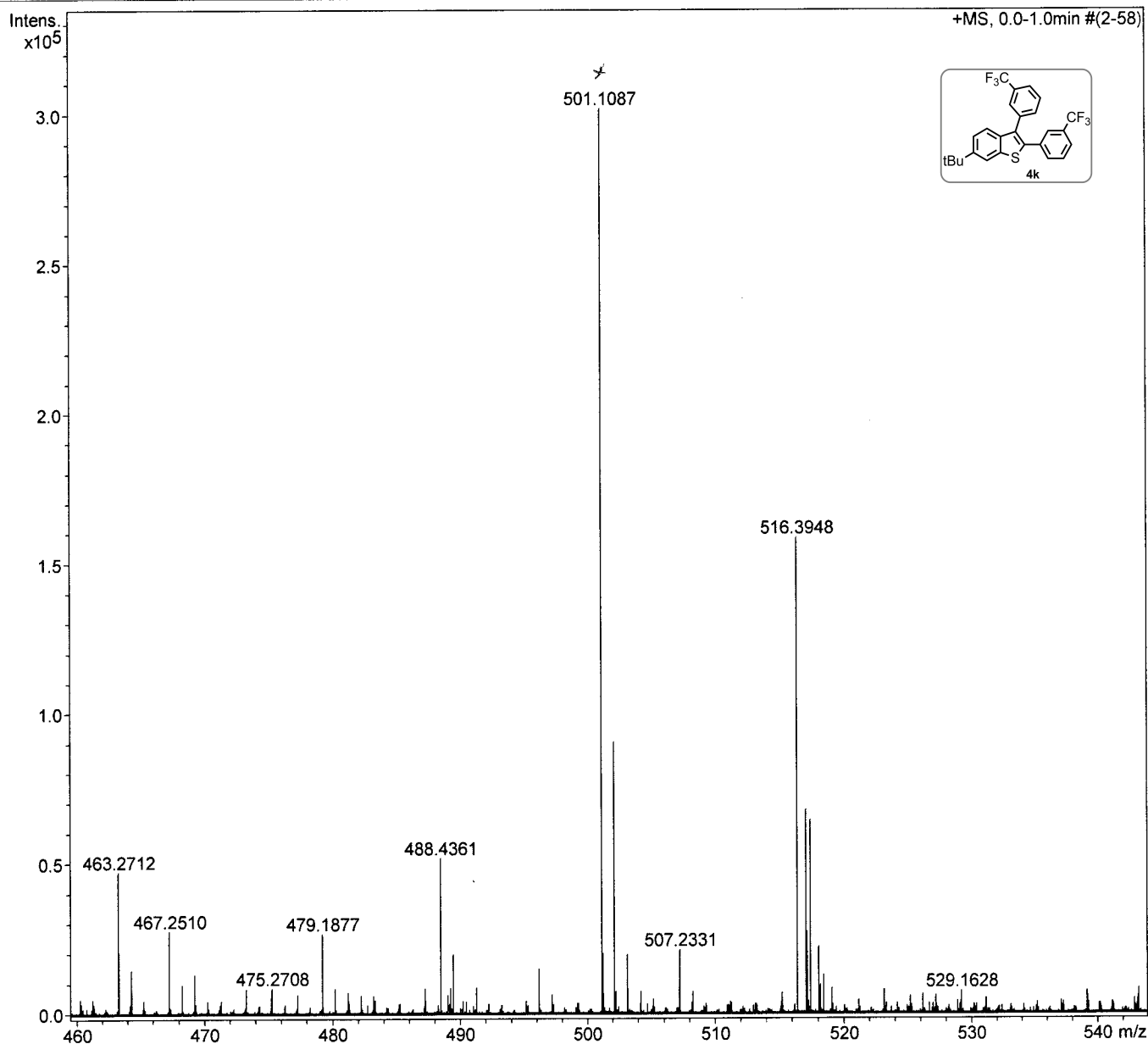
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\ERA-7-107.d  
Method tune\_low.m  
Sample Name ERA-7-107  
Comment

Acquisition Date 11/20/2015 3:00:05 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

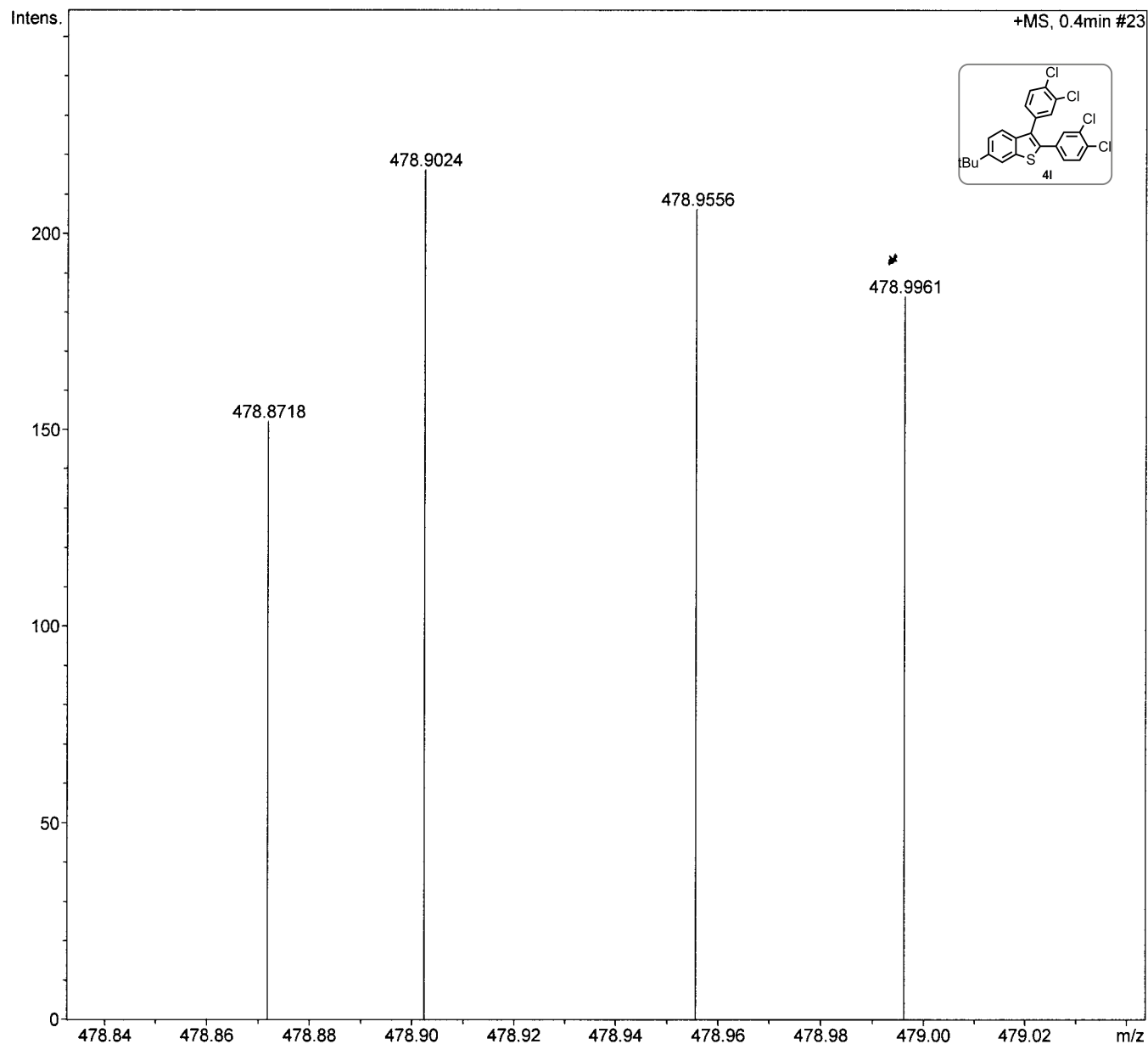
Analysis Name D:\Data\2015\DR.AK.SAHOO\AUG\ERA-7-67.d  
Method tune\_low.m  
Sample Name ERA-7-67-MEOH  
Comment

Acquisition Date 8/12/2015 12:11:46 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   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

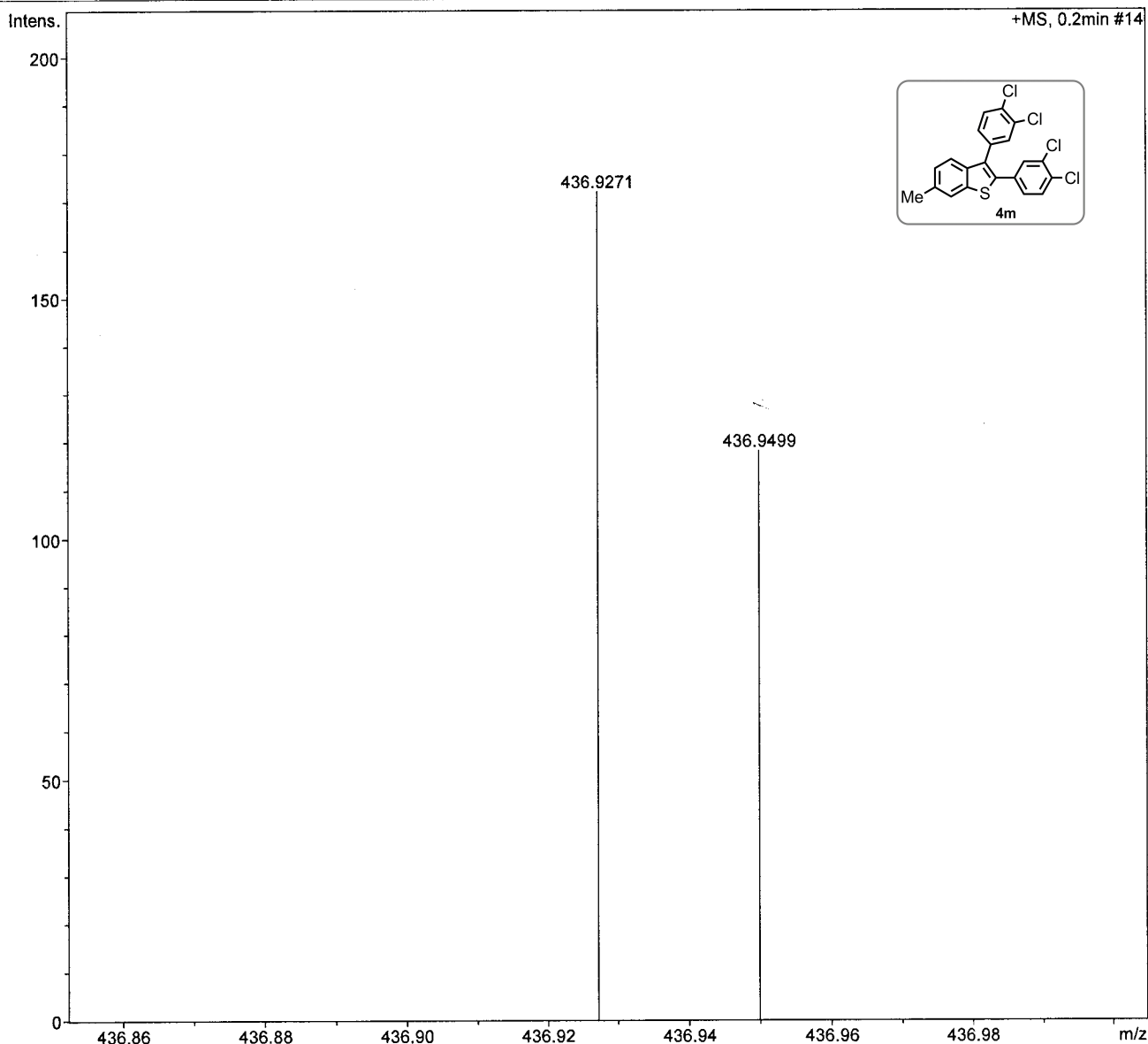
Analysis Name D:\Data\2015\DR.AK.SAHOO\AUG\ERA-7-74-RI.d  
Method tune\_low.m  
Sample Name ERA-7-74-RI-MEOH  
Comment

Acquisition Date 8/12/2015 11:37:13 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         | 3000 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1700 m/z   | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

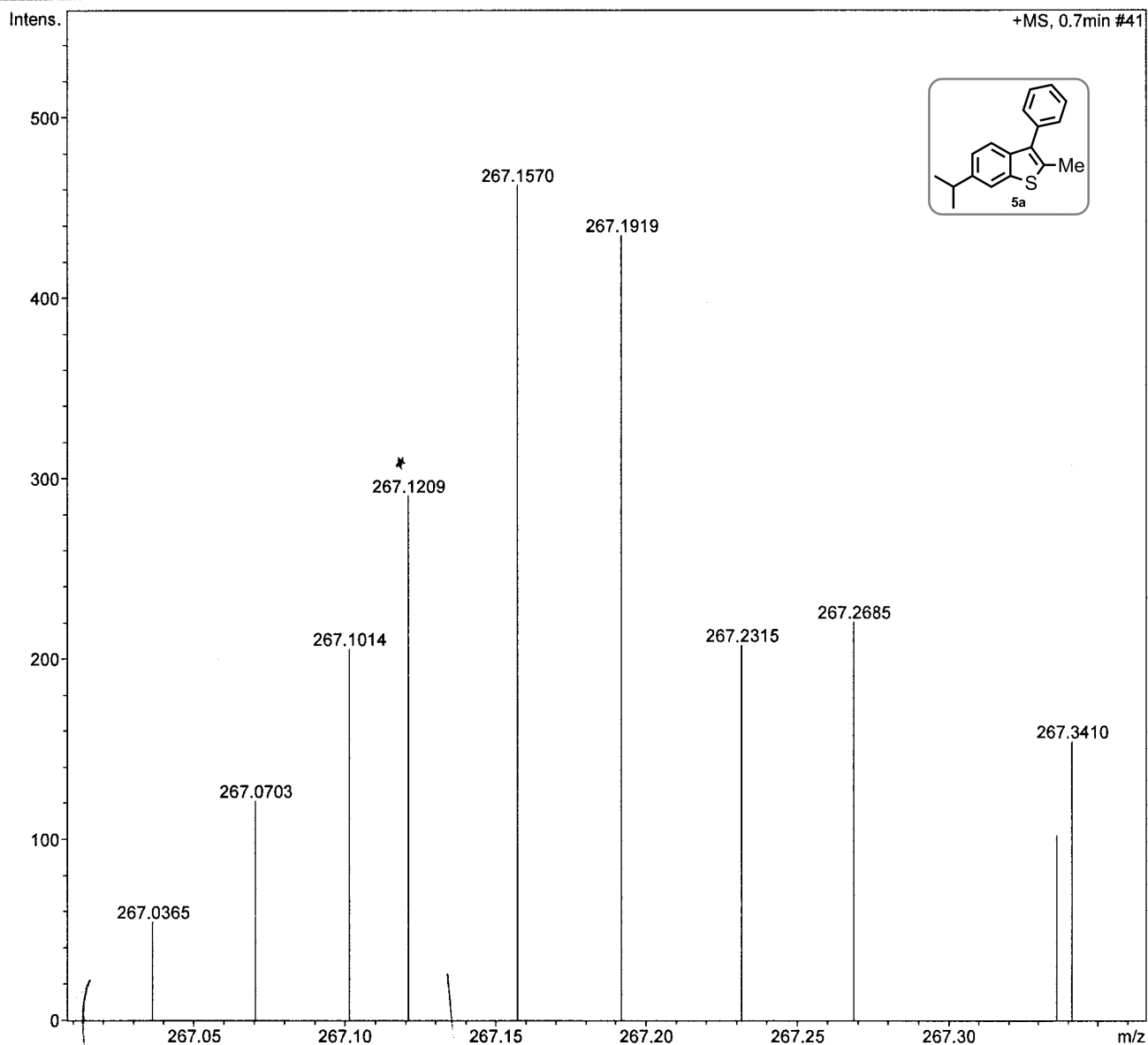
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\SD-NA-157.d  
Method tune\_low.m  
Sample Name SD-NA-157-CHCL3-ACN  
Comment

Acquisition Date 11/17/2015 10:43:02 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         | 4500 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1500 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# UOH -SCHOOL OF CHEMISTRY -HRMS

## Analysis Info

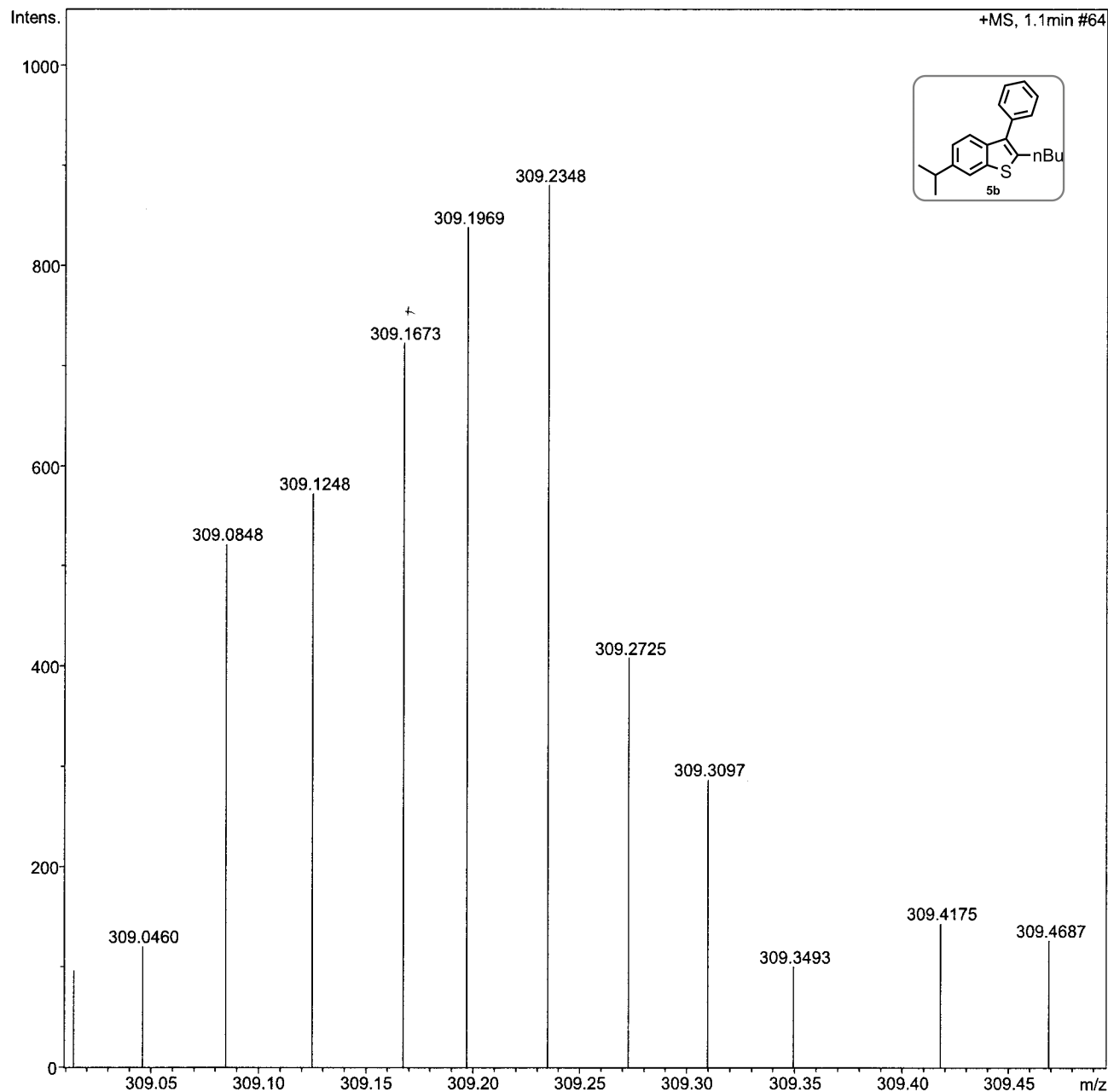
Analysis Name D:\Data\2016\DR.A.K.SAHOO\MARCH\ERA-NA-158R.d  
 Method tune\_low.m  
 Sample Name ERA-NA-158-DCM-MEOH  
 Comment

Acquisition Date 3/31/2016 11:14:17 AM

Operator Rajesh Vashisth  
 Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 200 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1800 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

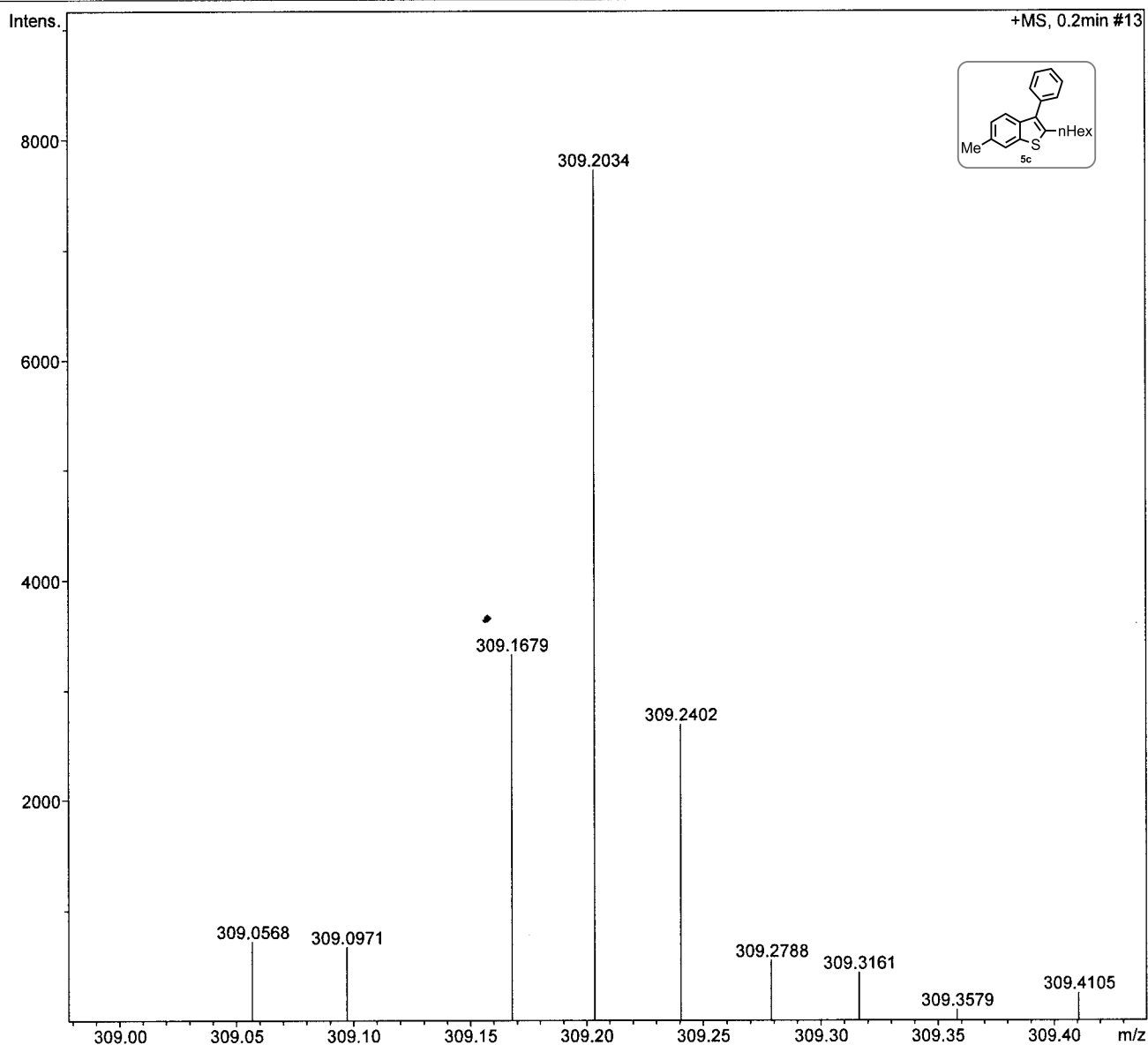
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\SD-NA-168R.d  
Method TL-P.m  
Sample Name SD-NA-168-CHCL3-ACN  
Comment

Acquisition Date 11/17/2015 11:02:41 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    | 600 m/z    | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

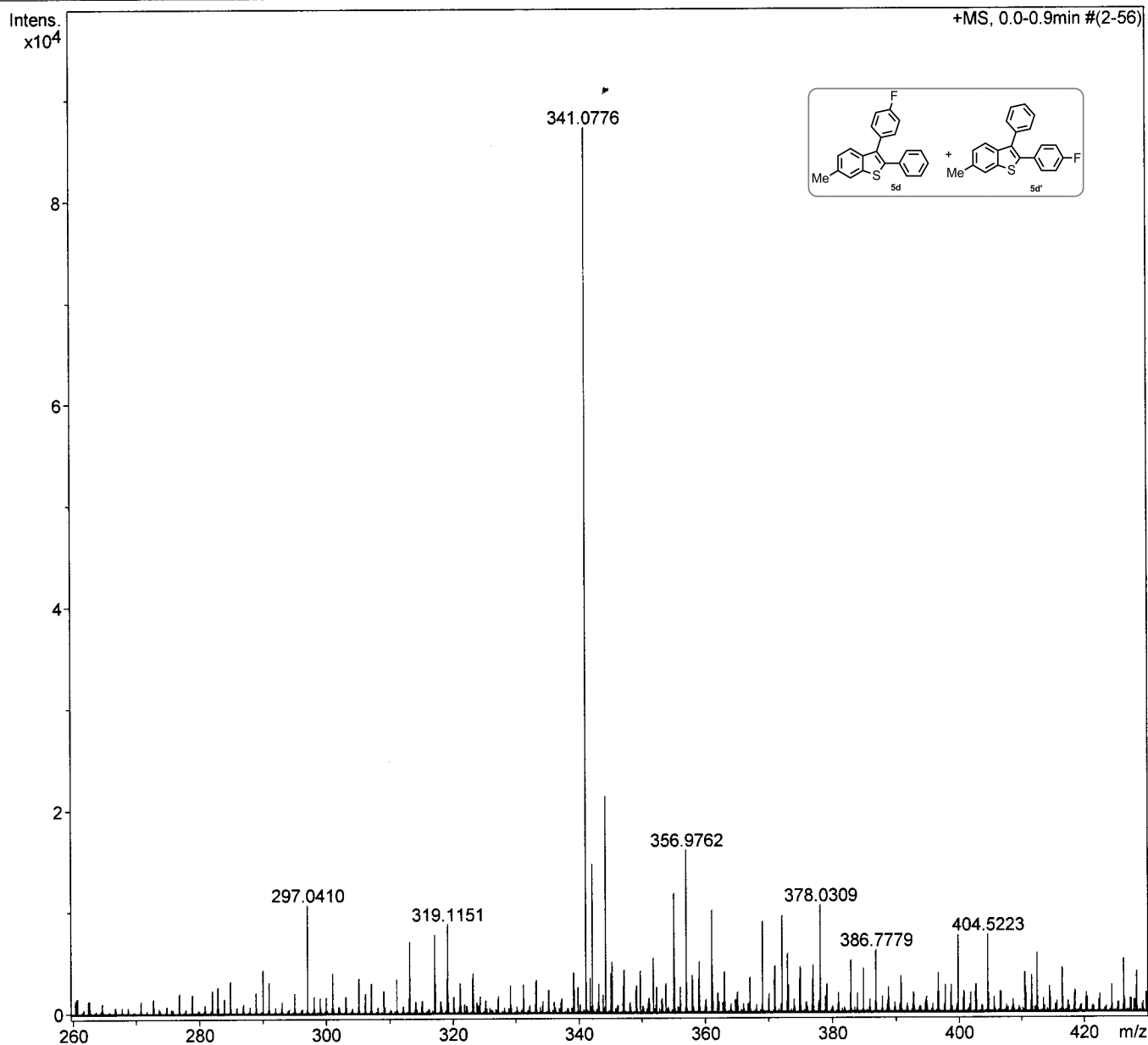
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\ERA-NA-97.d  
Method tune\_low.m  
Sample Name ERA-NA-97  
Comment

Acquisition Date 11/20/2015 3:12:32 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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





# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

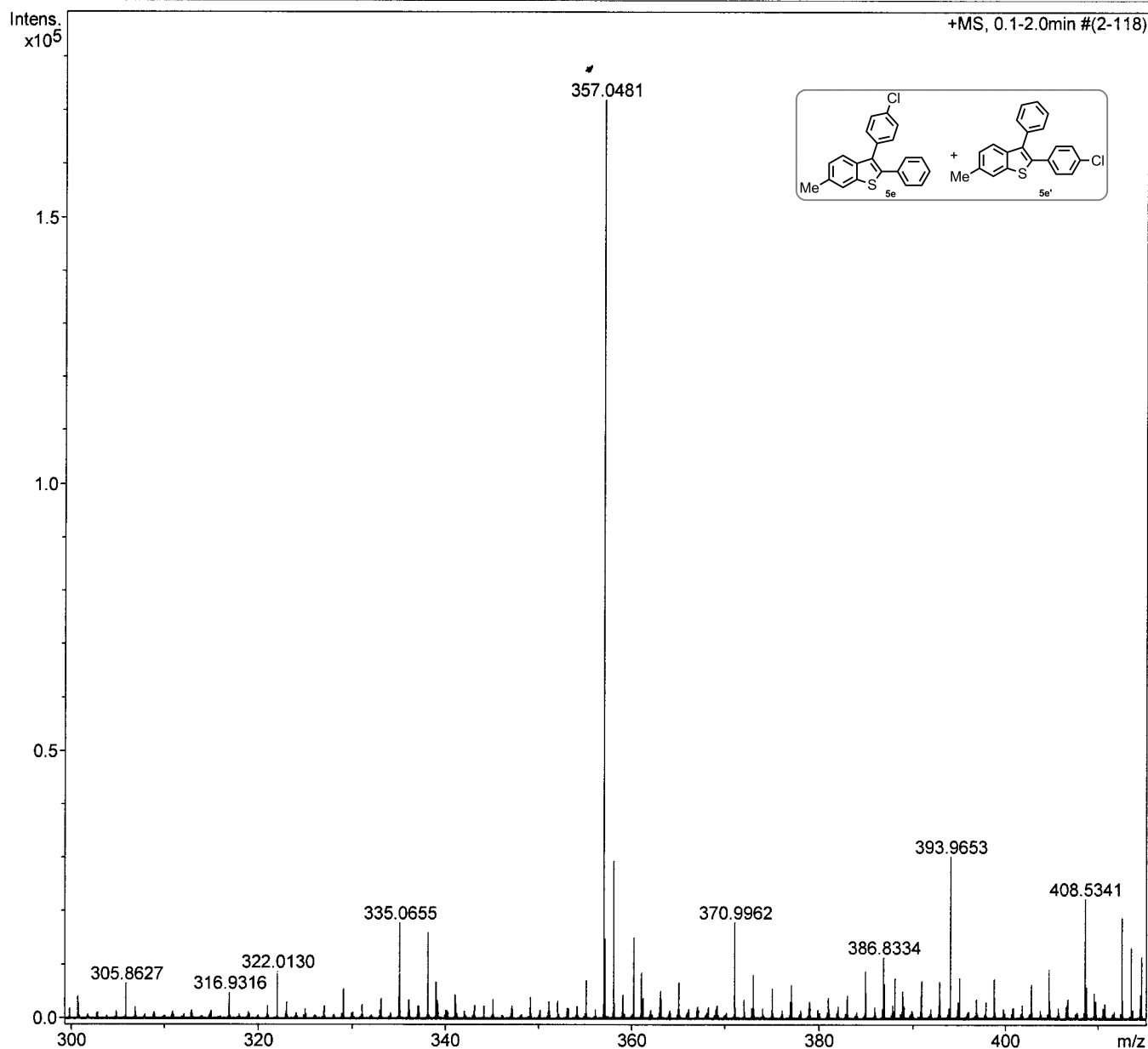
Analysis Name D:\Data\2015\DR.AK.SAHOO\NOV\ERA-NA-98.d  
Method tune\_low.m  
Sample Name ERA-NA-98  
Comment

Acquisition Date 11/20/2015 3:18:18 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         | 4500 V    | Set Dry Heater   | 200 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1800 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



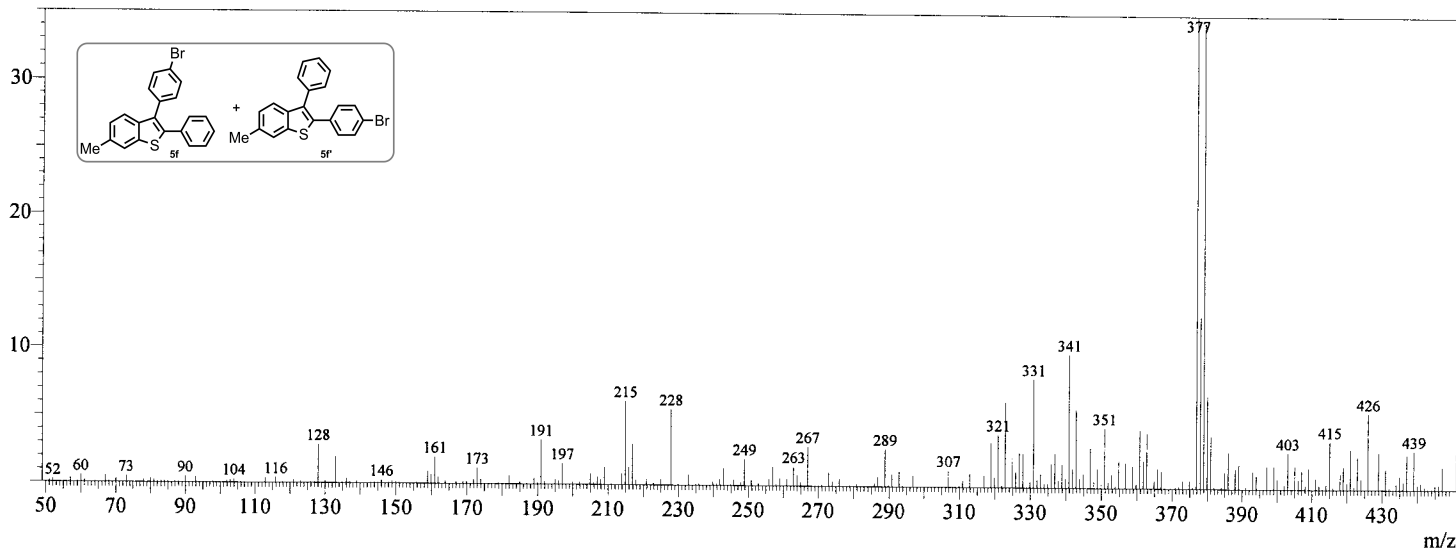
# LCMS-2010A DATA REPORT

## SHIMADZU

User : Admin  
 Sample : ERA-NA-124  
 Inj. Volume : 5.000  
 Data Name : E:\Data\ERA-NA-124-APCI-NEG1.qld  
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

### MS Spectrum

Line#:1 R.Time:0.715(Scan#:43) Negative  
 MassPeaks:255 BasePeak:376.85(52735)  
 RawMode:Single 0.715(43)  
 BG Mode:Peak Start 0.277(17)



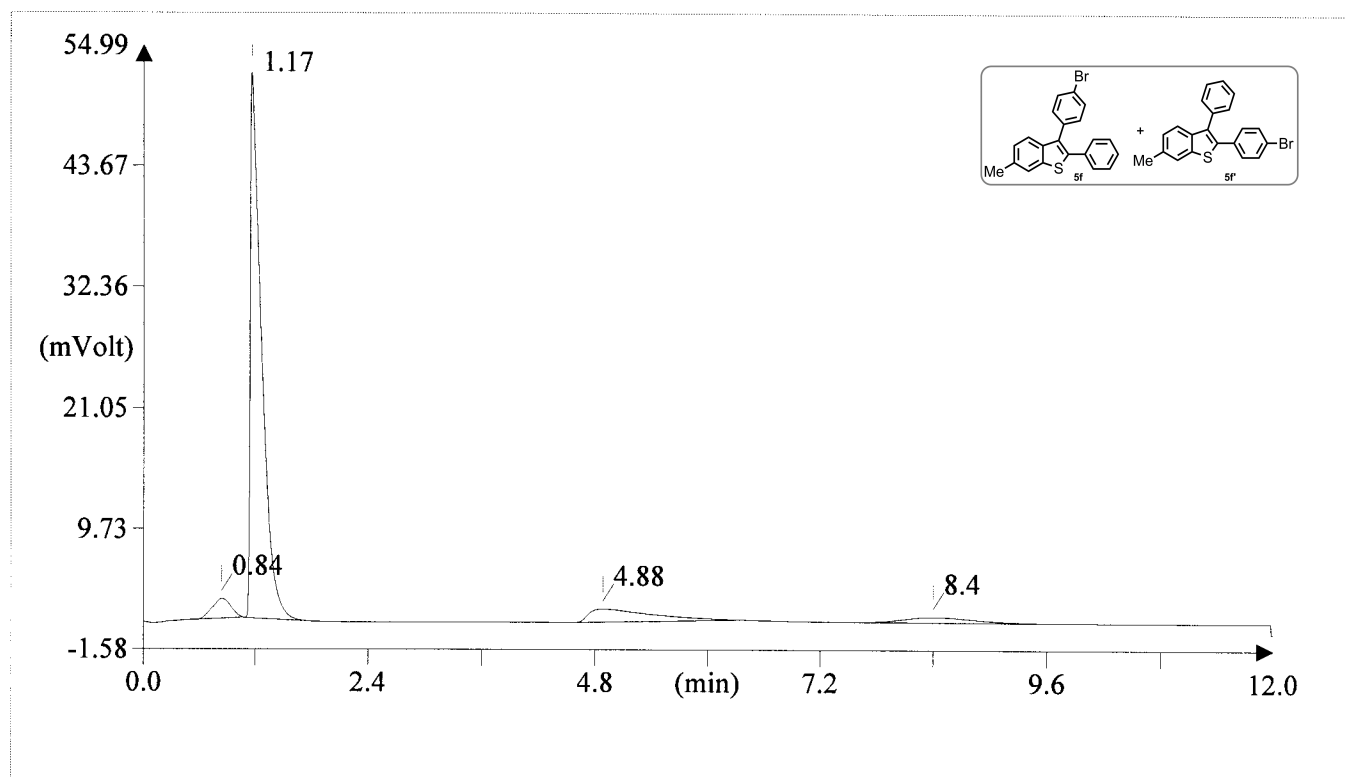
### MS Peak Table

| Peak# | R.Time | I.Time | F.Time | Area     | Height | A/H   | Mark | %Total | Name | Base m/z | Base Int. |
|-------|--------|--------|--------|----------|--------|-------|------|--------|------|----------|-----------|
| 1     | 0.715  | 0.277  | 1.660  | 40499071 | 926613 | 43.70 |      | 100.00 |      | 376.85   | 52735     |
|       |        |        |        | 40499071 | 926613 |       |      | 100.00 |      |          |           |

# FLASH EA 1112 SERIES CHNS REPORT

## THERMO FINNIGAN

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys\_data\_ex  
 Sample ID: ERA-NA-124 (# 197)  
 Analysis type: UnkNown  
 Chromatogram filename: UNK-25022016-7.dat  
 Sample weight: 1.131



| Element Name | Element % | Ret. Time |
|--------------|-----------|-----------|
| Nitrogen     | 0. 04     | 0. 84     |
| Carbon       | 66. 42    | 1. 17     |
| Hydrogen     | 3. 91     | 4. 88     |
| Sulphur      | 8. 38     | 8. 40     |

# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

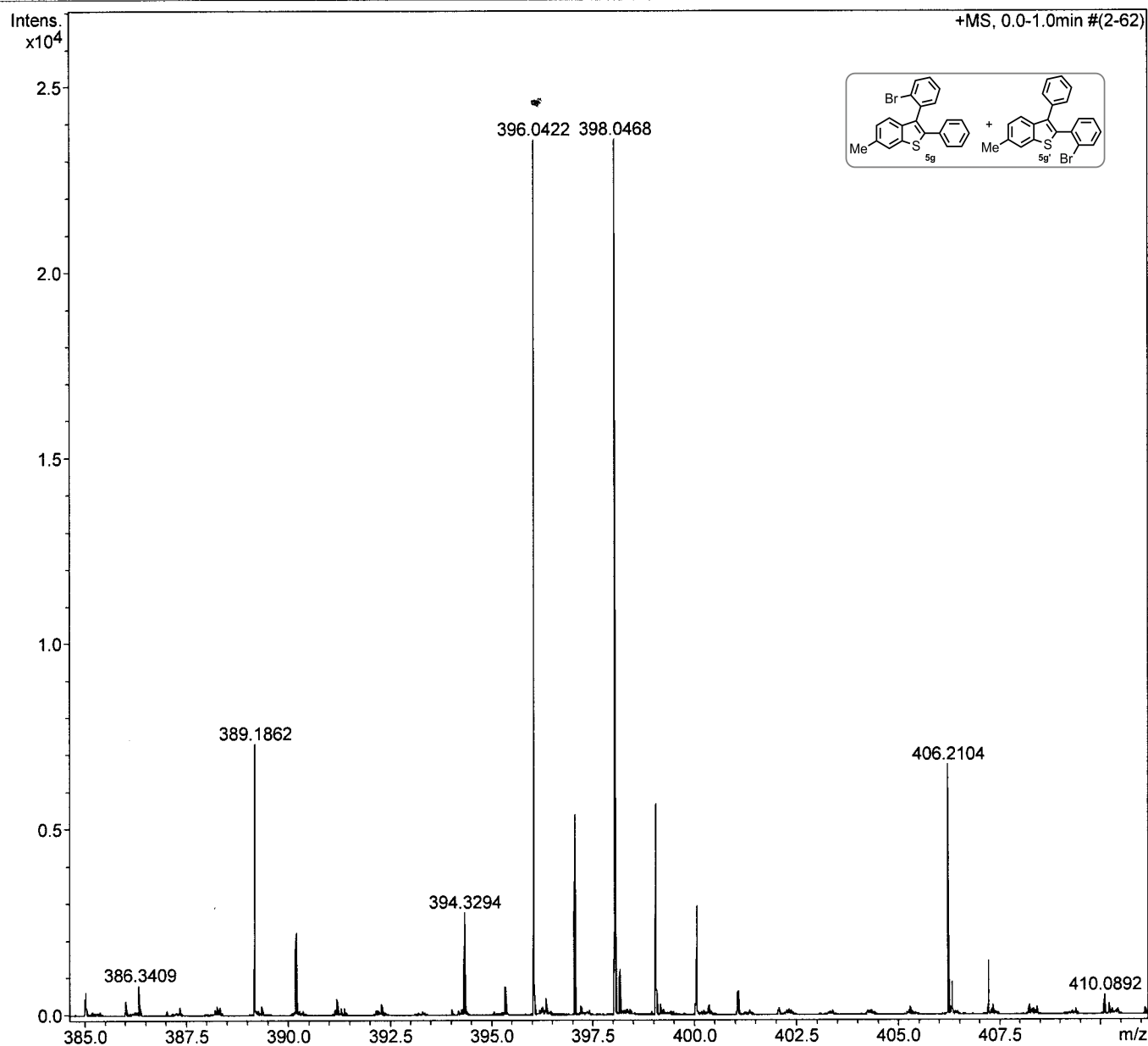
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-NA-153.d  
Method tune\_low.m  
Sample Name ERA-NA-153  
Comment

Acquisition Date 12/30/2015 3:55:22 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 200 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1800 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

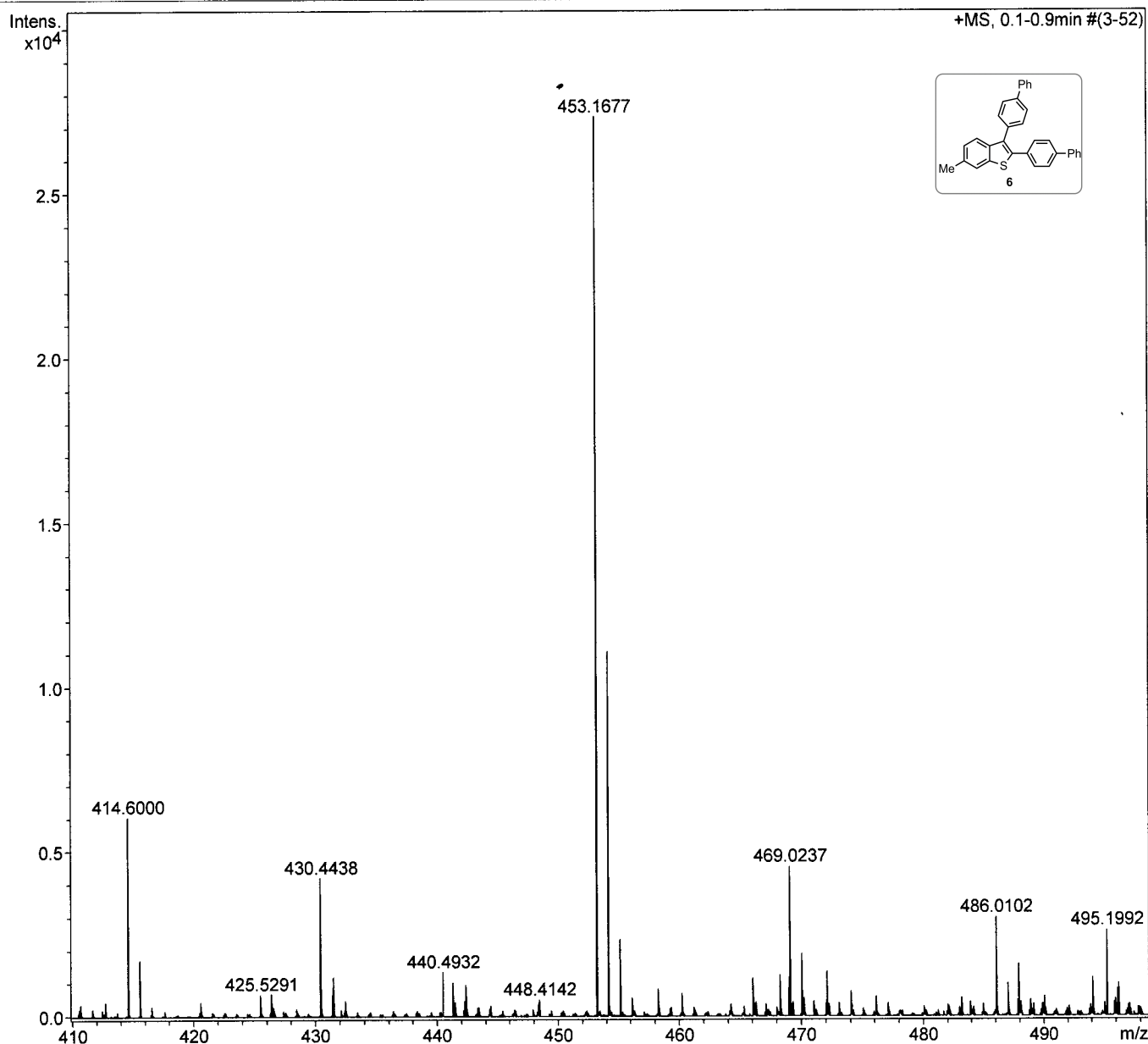
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-NA-136.d  
Method tune\_low.m  
Sample Name ERA-NA-136  
Comment

Acquisition Date 12/30/2015 3:45:27 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 200 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1800 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

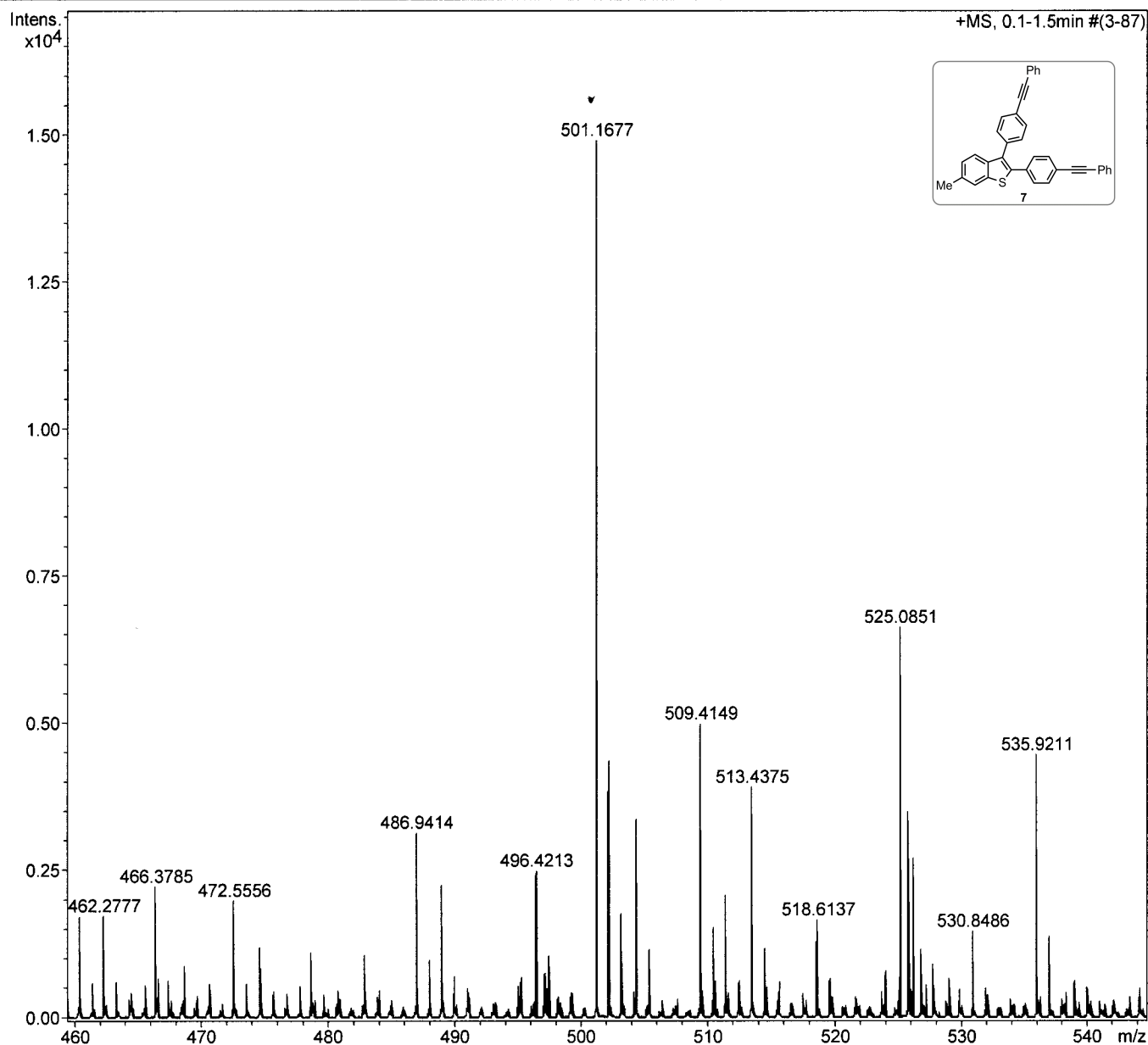
Analysis Name D:\Data\2015\DR.AK.SAHOO\DEC\ERA-NA-139.d  
Method tune\_low.m  
Sample Name ERA-NA-139  
Comment

Acquisition Date 12/30/2015 3:50:01 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 4500 V    | Set Dry Heater   | 200 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 1800 m/z   | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |



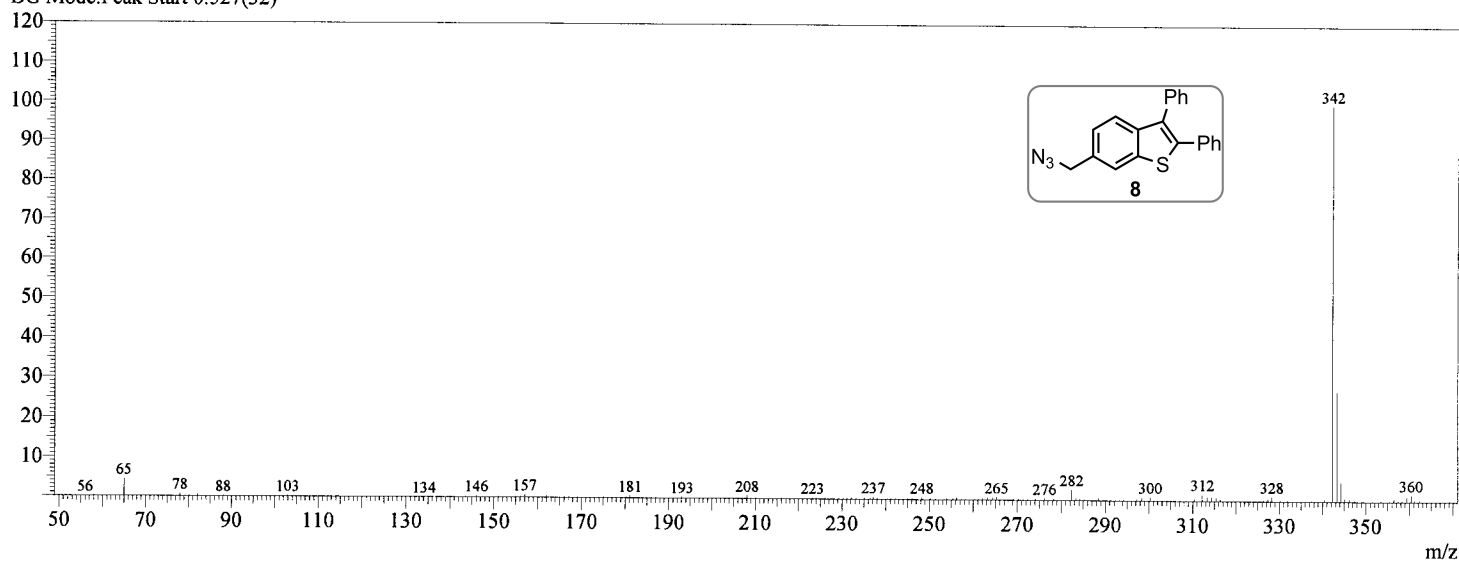
# LCMS-2010A DATA REPORT

## SHIMADZU

User : Admin  
Sample : ERA-SD-3  
Inj. Volume : 5.000  
Data Name : E:\Data\ERA-SD-3-APCI-POS1.qld  
Method Name : C:\LCMSsolution\User\Method\esi.qlm

### MS Spectrum

Line#:1 R.Time:0.779(Scan#:47) Positive  
MassPeaks:181 BasePeak:342.30(3765285)  
RawMode:Single 0.779(47)  
BG Mode:Peak Start 0.527(32)



### MS Peak Table

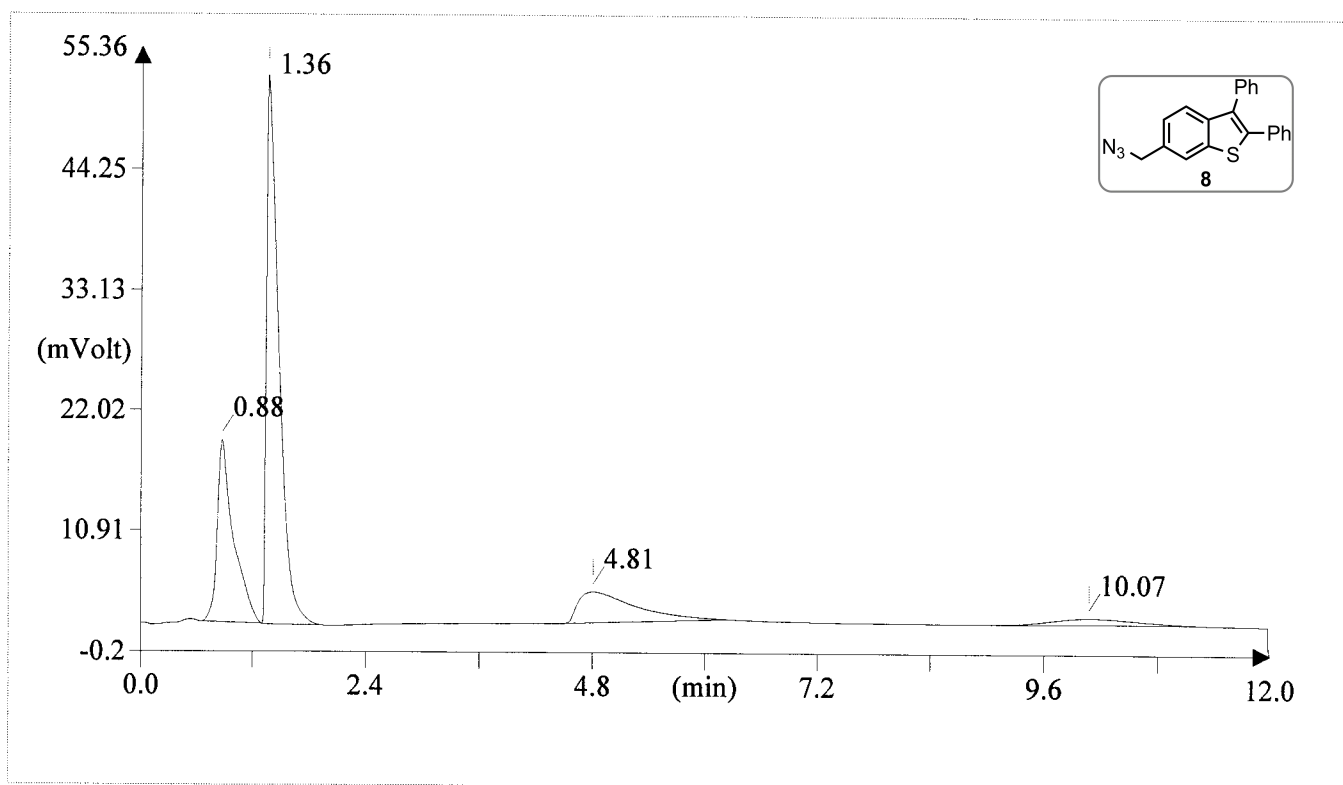
| Peak# | R.Time | I.Time | F.Time | Area     | Height  | A/H   | Mark | %Total | Name |
|-------|--------|--------|--------|----------|---------|-------|------|--------|------|
| 1     | 0.779  | 0.527  | 1.060  | 55846893 | 3495512 | 15.97 |      | 100.00 |      |
|       |        |        |        | 55846893 | 3495512 |       |      | 100.00 |      |

Base m/z Base Int.  
342.30 3765285

# FLASH EA 1112 SERIES CHNS REPORT

## THERMO FINNIGAN

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys\_data\_ex  
 Sample ID: ERA-SD-3 (# 198)  
 Analysis type: UnkNown  
 Chromatogram filename: UNK-25022016-8.dat  
 Sample weight: 1.125



| Element Name | Element % | Ret. Time |
|--------------|-----------|-----------|
| Nitrogen     | 12. 25    | 0. 88     |
| Carbon       | 73. 96    | 1. 36     |
| Hydrogen     | 4. 38     | 4. 81     |
| Sulphur      | 9. 25     | 10. 07    |



# BRUKER MAXIS HRMS REPORT

School of Chemistry  
University of Hyderabad

## Analysis Info

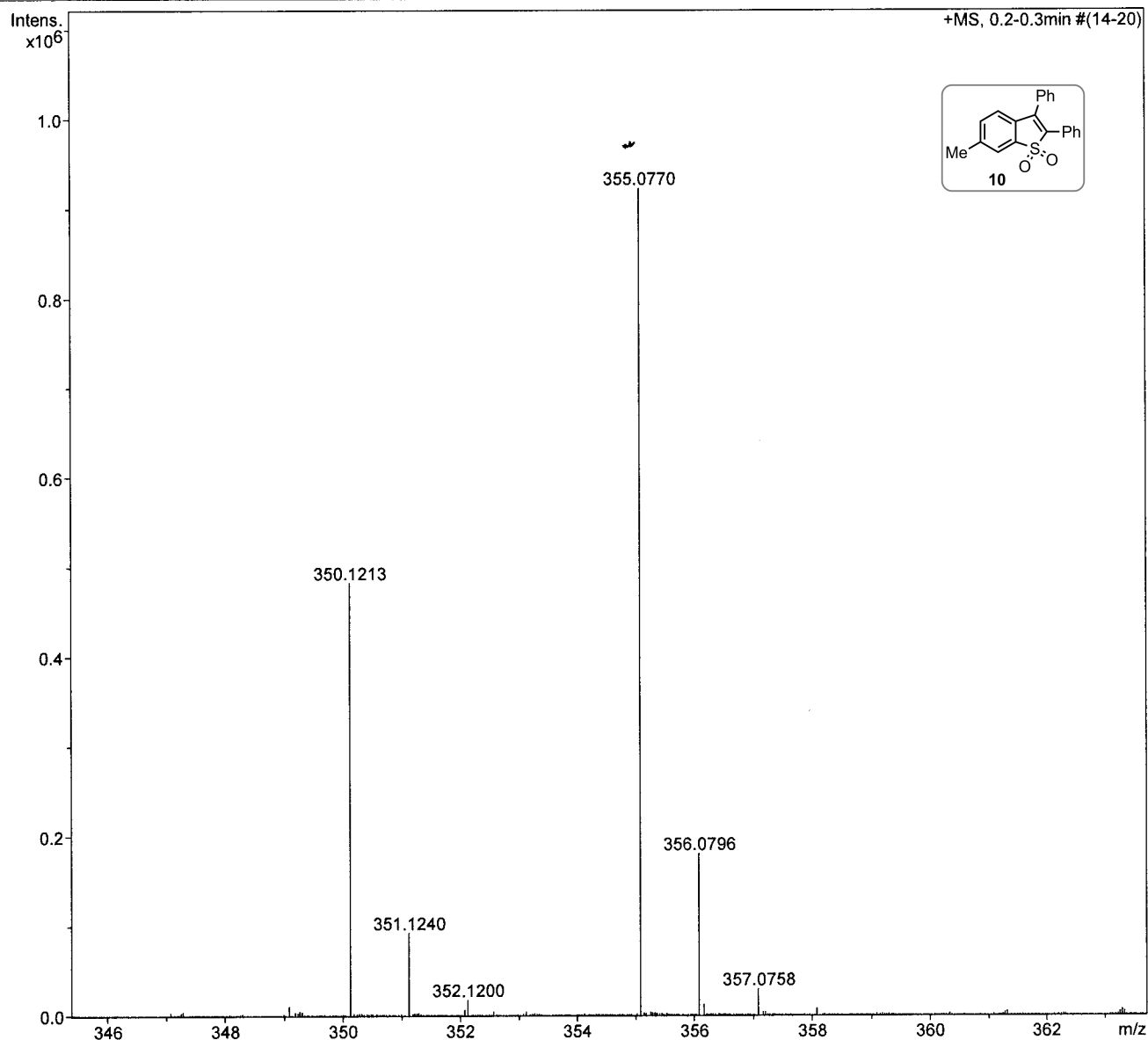
Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\MSD-T-503.d  
Method tune\_low.m  
Sample Name MSD-T-503-DCM-MEOH  
Comment

Acquisition Date 7/27/2015 1:14:03 PM

Operator Ramu Sridhar  
Instrument maXis 10138

## Acquisition Parameter

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



# UOH -SCHOOL OF CHEMISTRY -HRMS

## Analysis Info

Analysis Name D:\Data\2016\DR.A.K.SAHOO\MARCH\ERA-8-42.d  
Method TL-P.m  
Sample Name ERA-8-42-DCM-MEOH  
Comment

Acquisition Date 3/31/2016 12:28:17 PM

Operator Rajesh Vashisth  
Instrument maXis 10138

## Acquisition Parameter

|             |            |                       |           |                  |           |
|-------------|------------|-----------------------|-----------|------------------|-----------|
| Source Type | ESI        | Ion Polarity          | Positive  | Set Nebulizer    | 0.3 Bar   |
| Focus       | Not active | Set Capillary         | 3800 V    | Set Dry Heater   | 180 °C    |
| Scan Begin  | 50 m/z     | Set End Plate Offset  | -500 V    | Set Dry Gas      | 4.0 l/min |
| Scan End    | 700 m/z    | Set Collision Cell RF | 350.0 Vpp | Set Divert Valve | Waste     |

