

Harnessing Sulfur and Nitrogen in the Cobalt (III)-Catalyzed Unsymmetrical Double Annulation of Thioamides: Probing the Origin of Chemo- and Regioselectivity

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SUPPORTING INFORMATION

HRMS Data

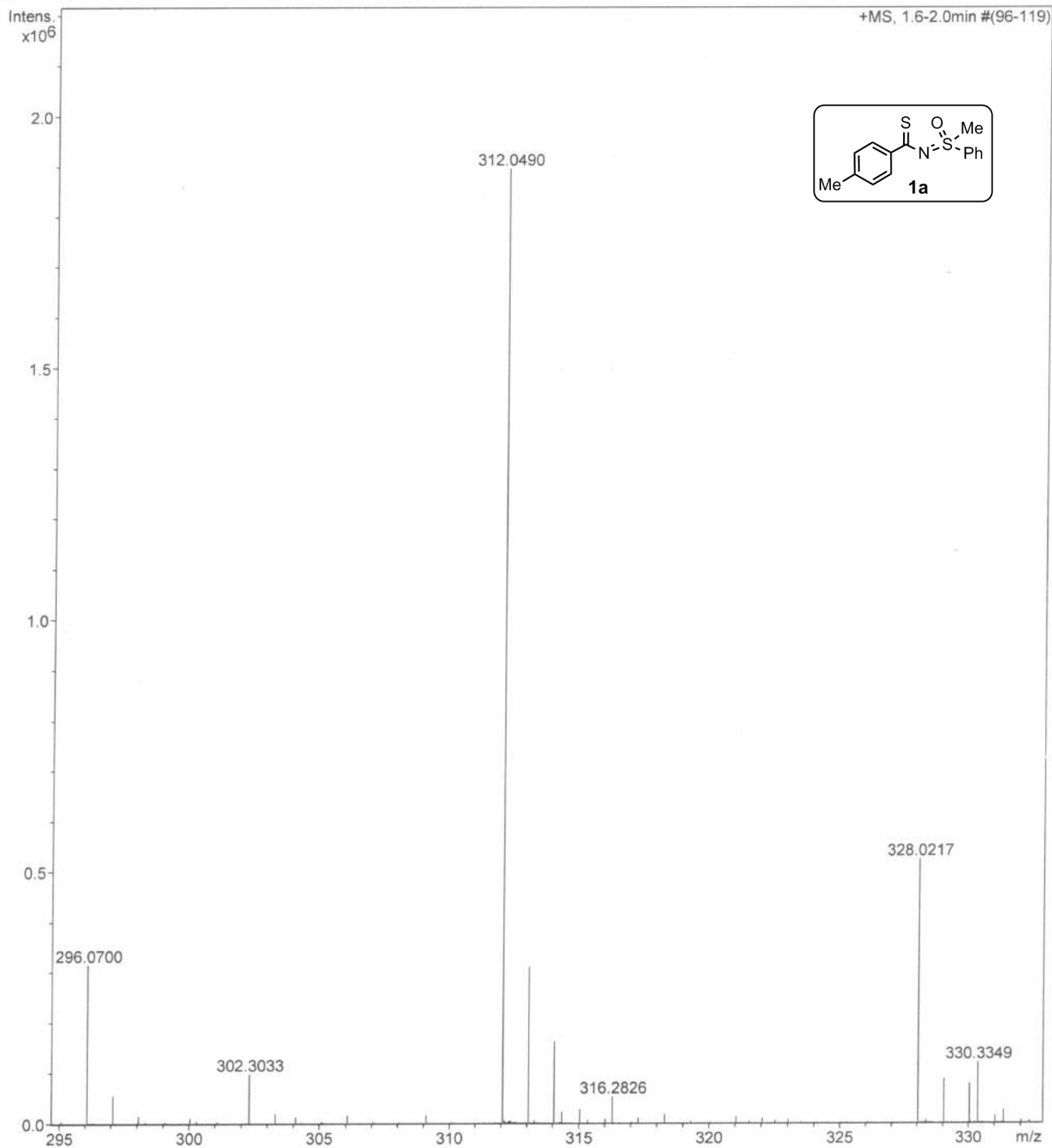
Generic Display Report

Analysis Info

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Method tune_low.m
Sample Name MJ-05-14
Comment

Acquisition Date 3/21/2018 4:11:53 AM

Operator Rajesh Vashisth
Instrument maXis



MJ-5-385

UNIVERSITY OF HYDERABAD

ACRHEM

XEVO-G2XSQTOF#YEA1155

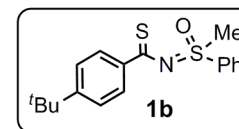
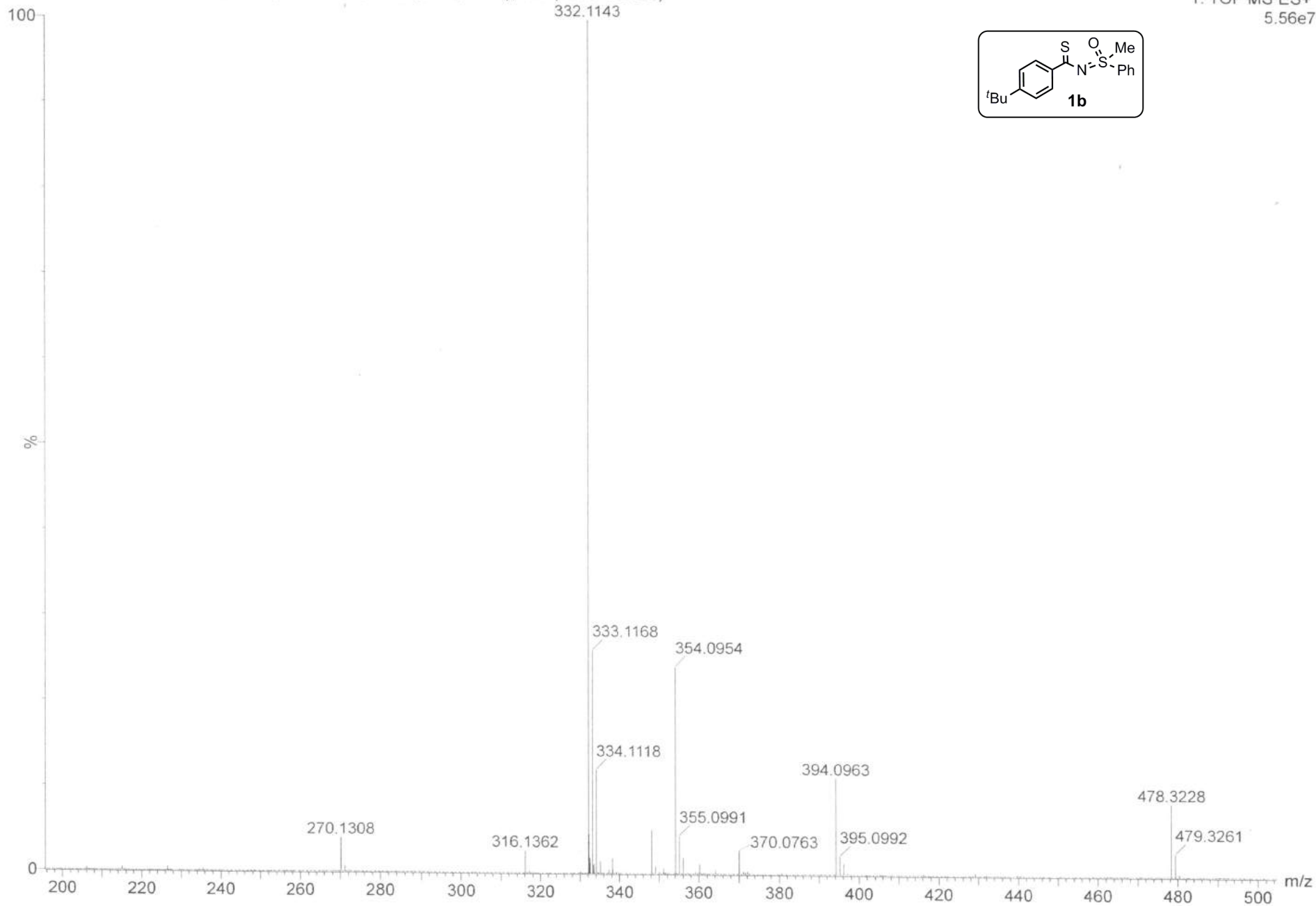
18-Nov-2020

12:20:29

18112020_14 +VE 16 (0.174) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (16:19-75:120)

1: TOF MS ES+

5.56e7



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

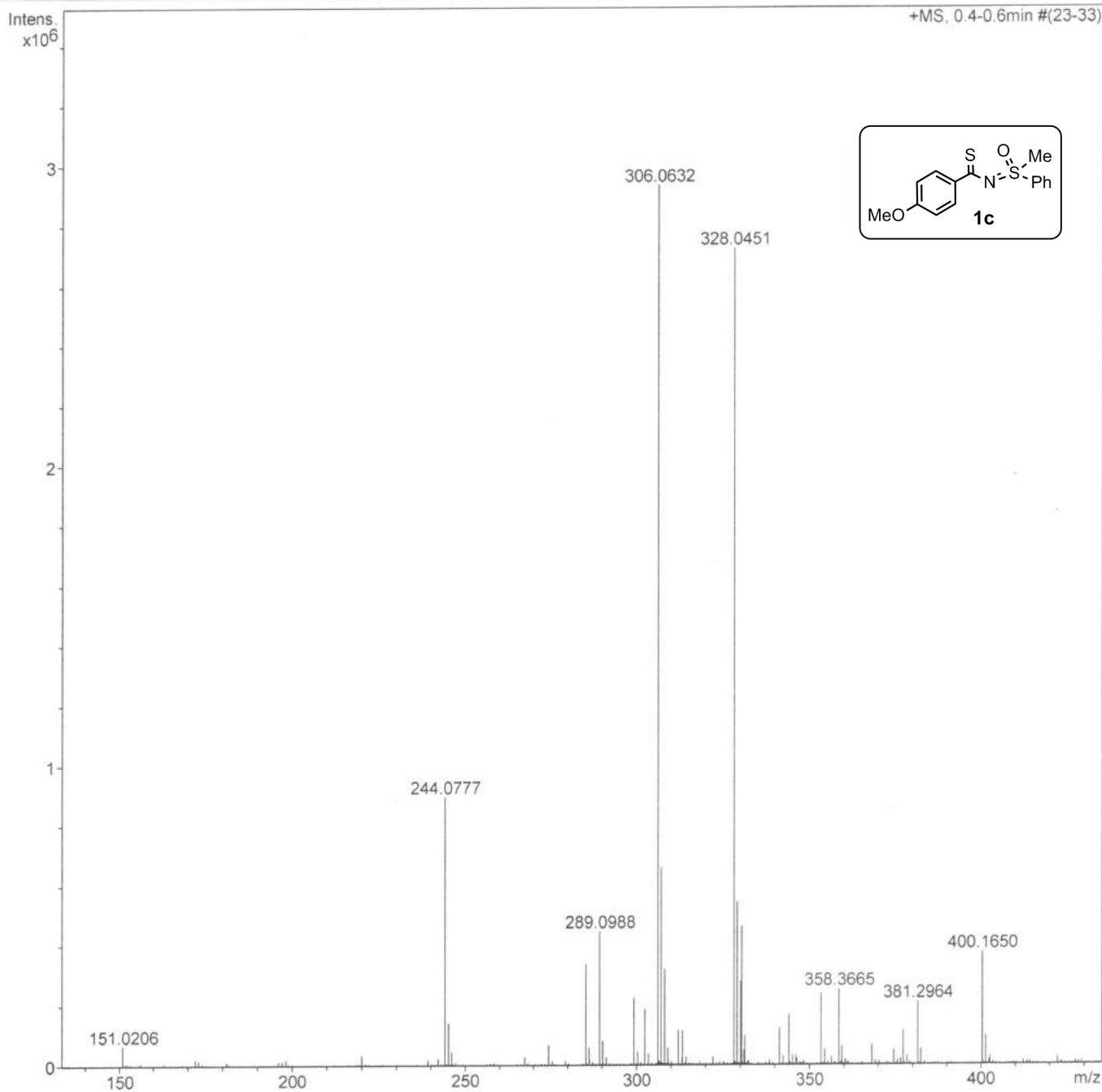
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Sample Name AS-22-DCM-MEOH
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Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
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UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

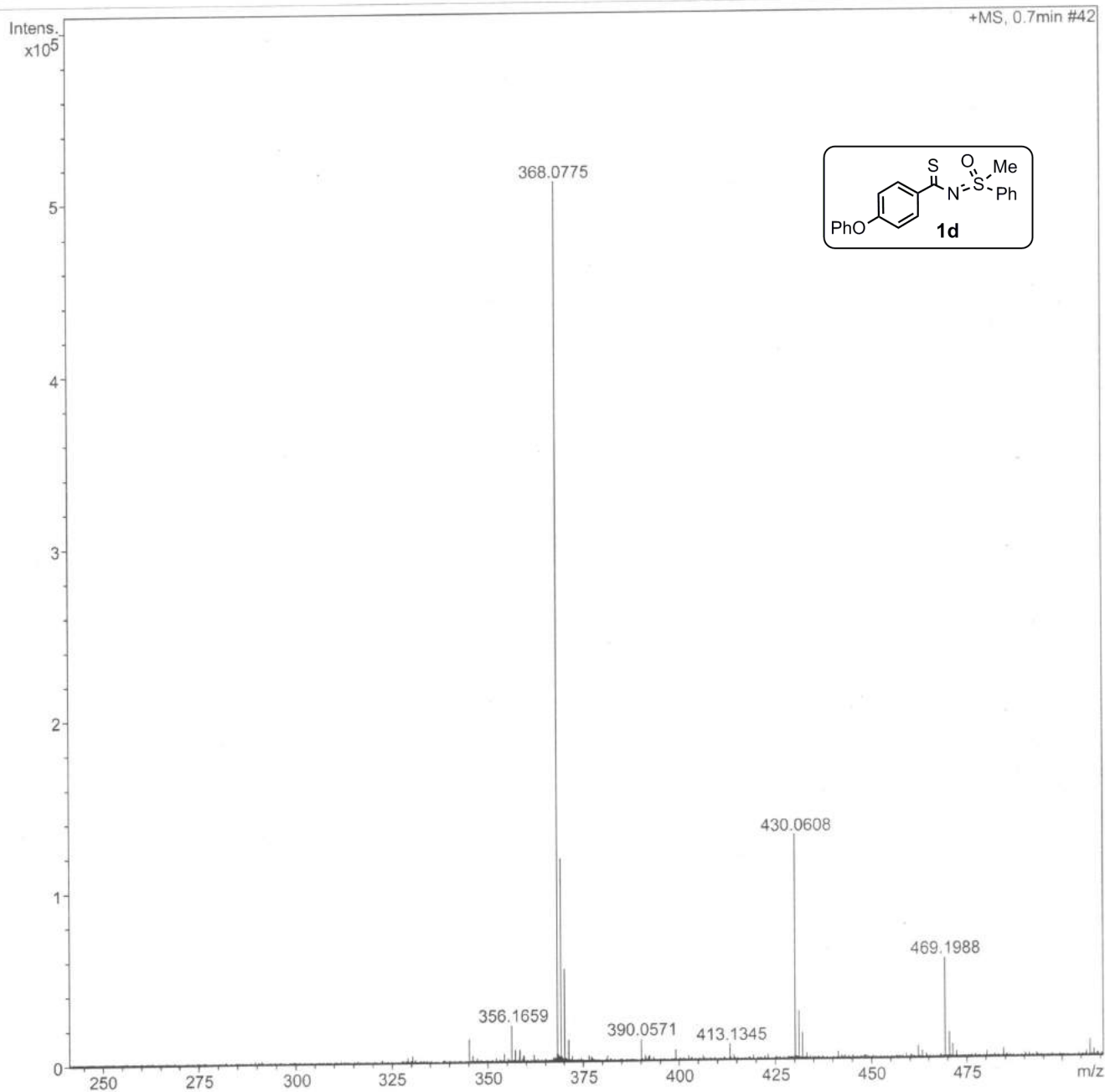
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 Sample Name AS-38-DCM-MEOH
 Comment

Acquisition Date 12/24/2018 12:36:42 PM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

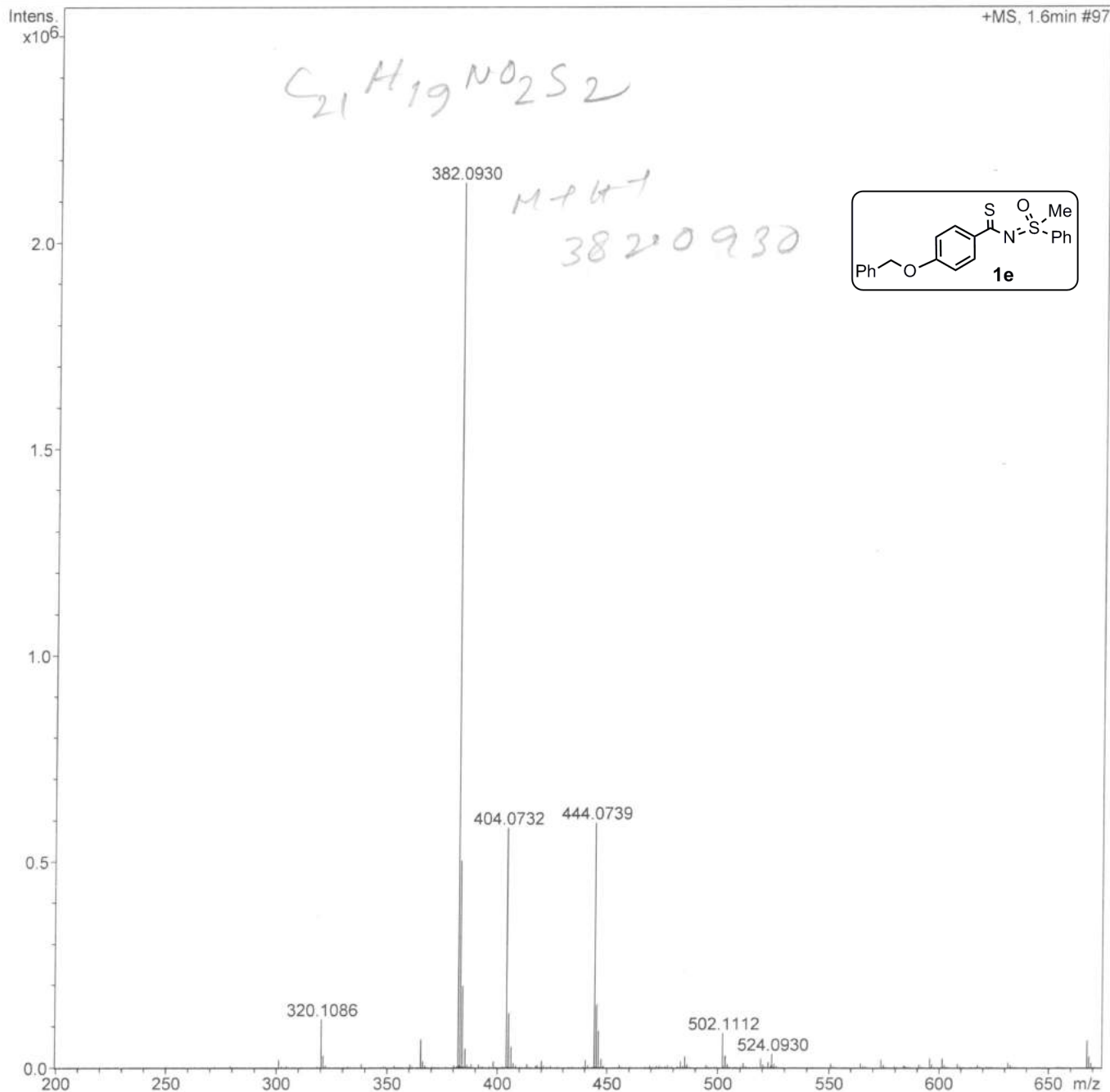
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Method TL-P.m
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Acquisition Date 10/28/2019 2:43:01 AM

Operator UOH-Chemistry
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
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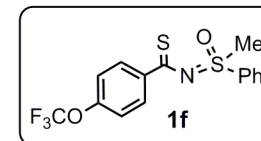
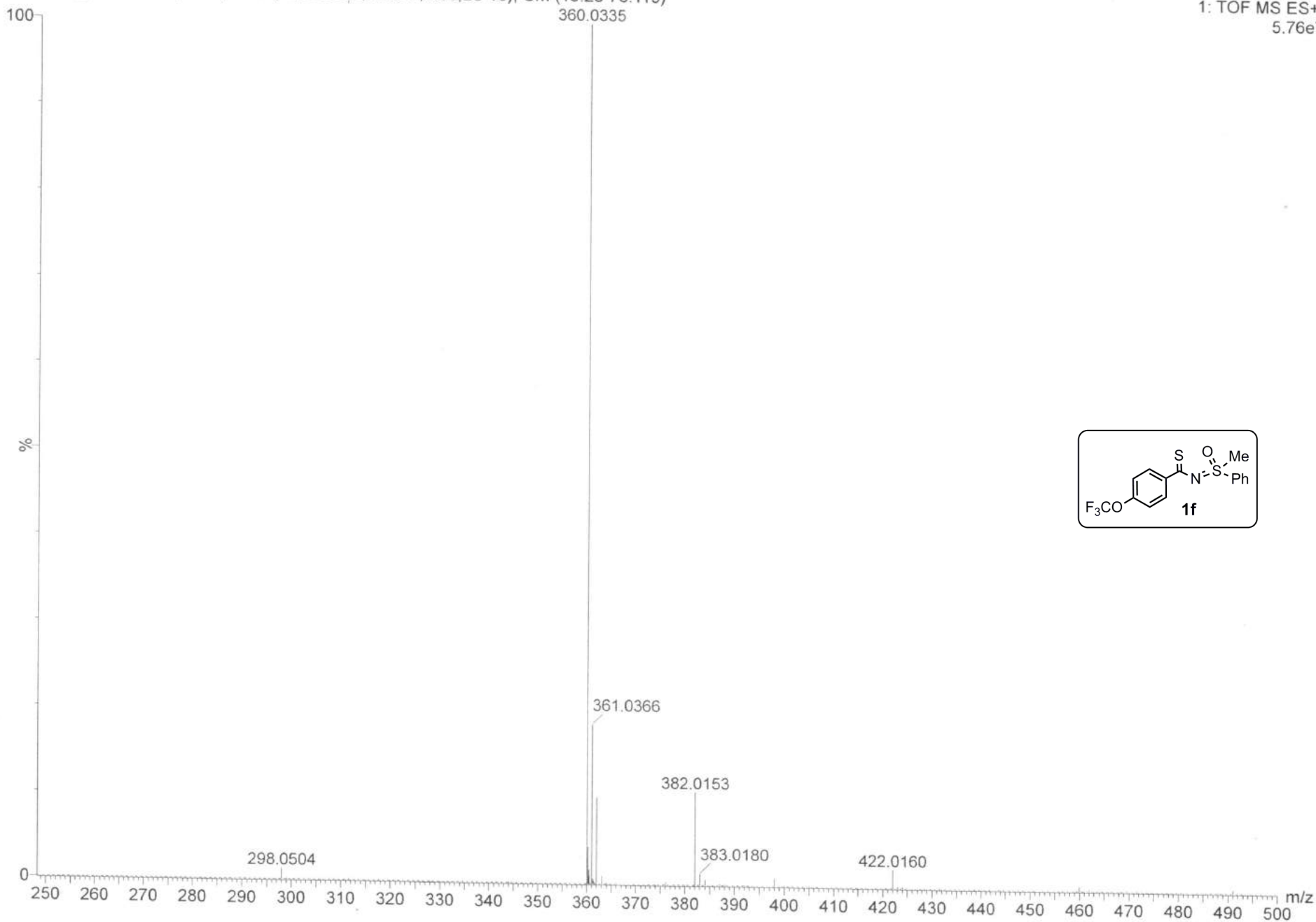
MJ-611

UNIVERSITY OF HYDERABAD
ACRHEM
XEVO-G2XSQTOF#YEA1155

10-Nov-2020
15:35:08

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1: TOF MS ES+
5.76e7



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

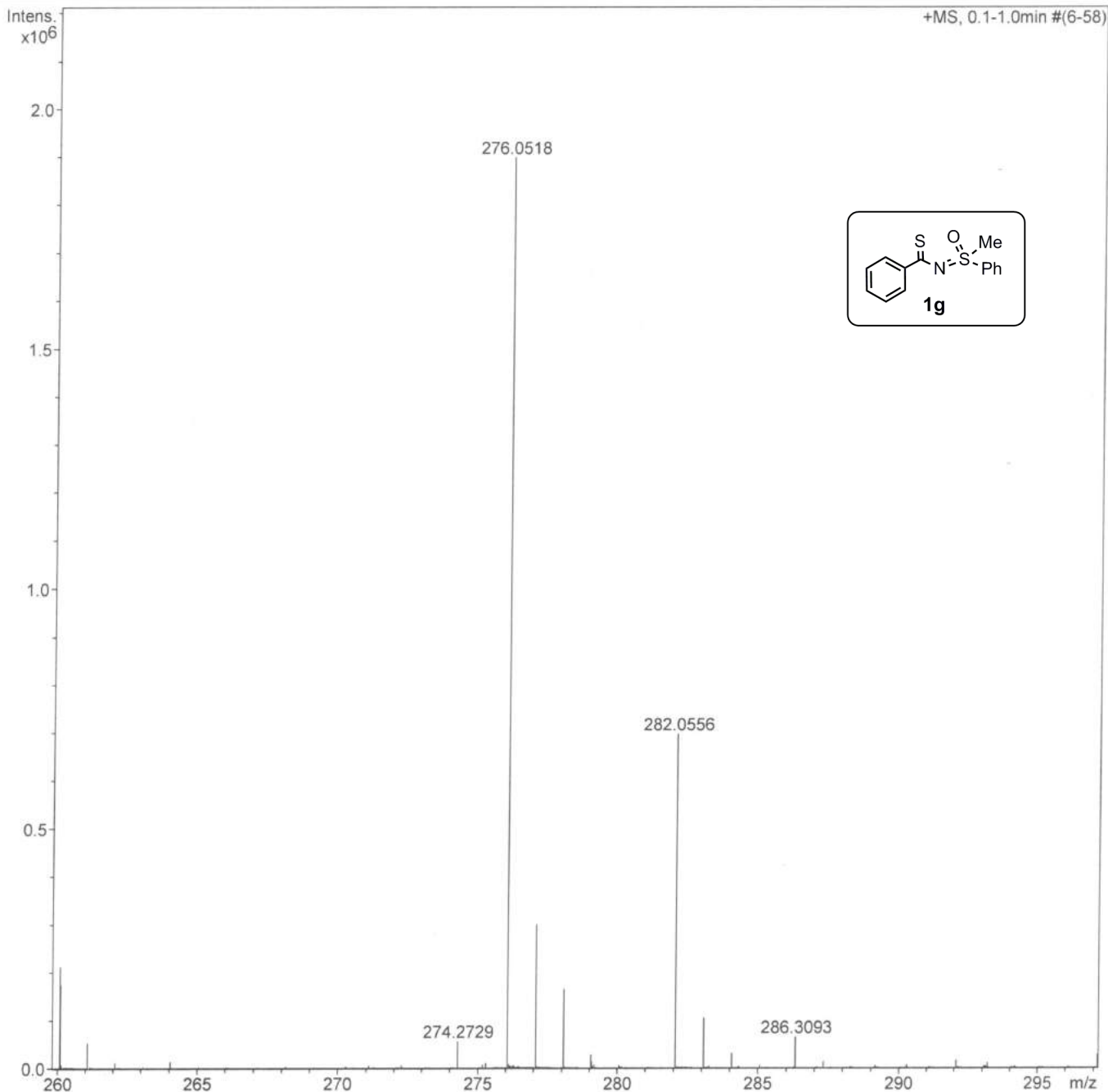
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 Comment

Acquisition Date 3/21/2018 3:43:22 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	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
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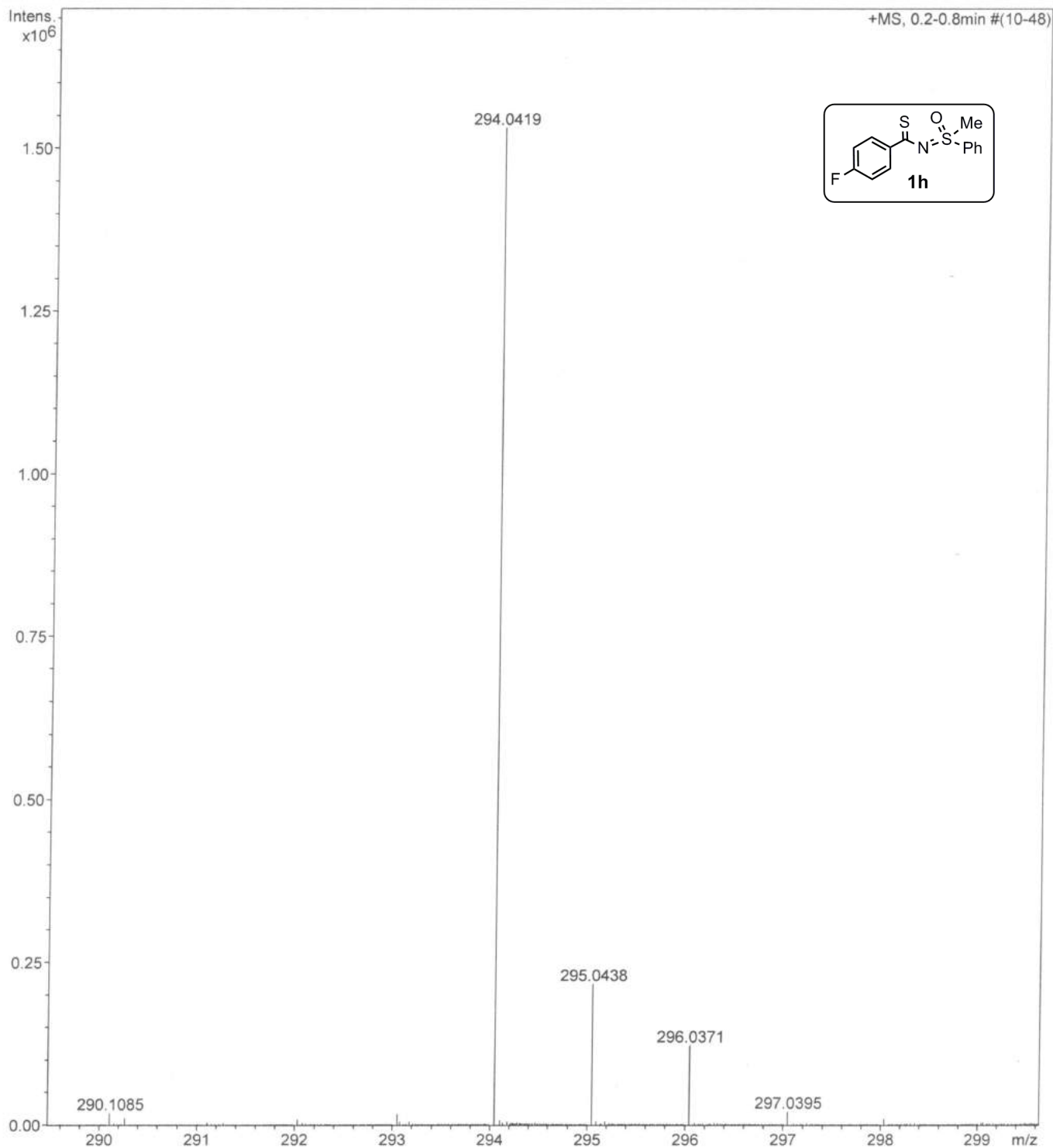
Generic Display Report

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Comment

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Operator Rajesh Vashisth
Instrument maXis



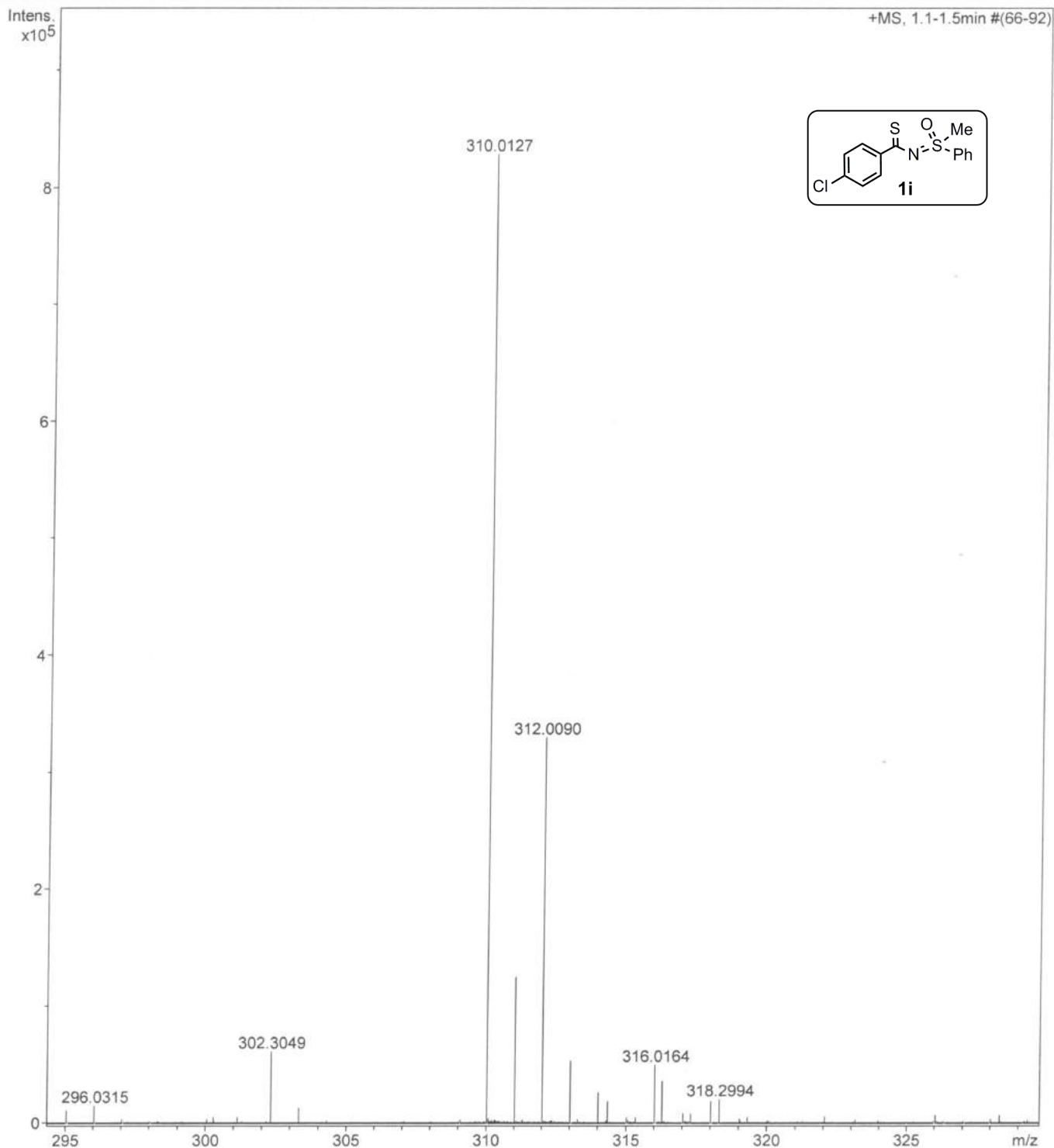
Generic Display Report

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Acquisition Date 3/21/2018 3:52:43 AM

Operator Rajesh Vashisth
Instrument maXis



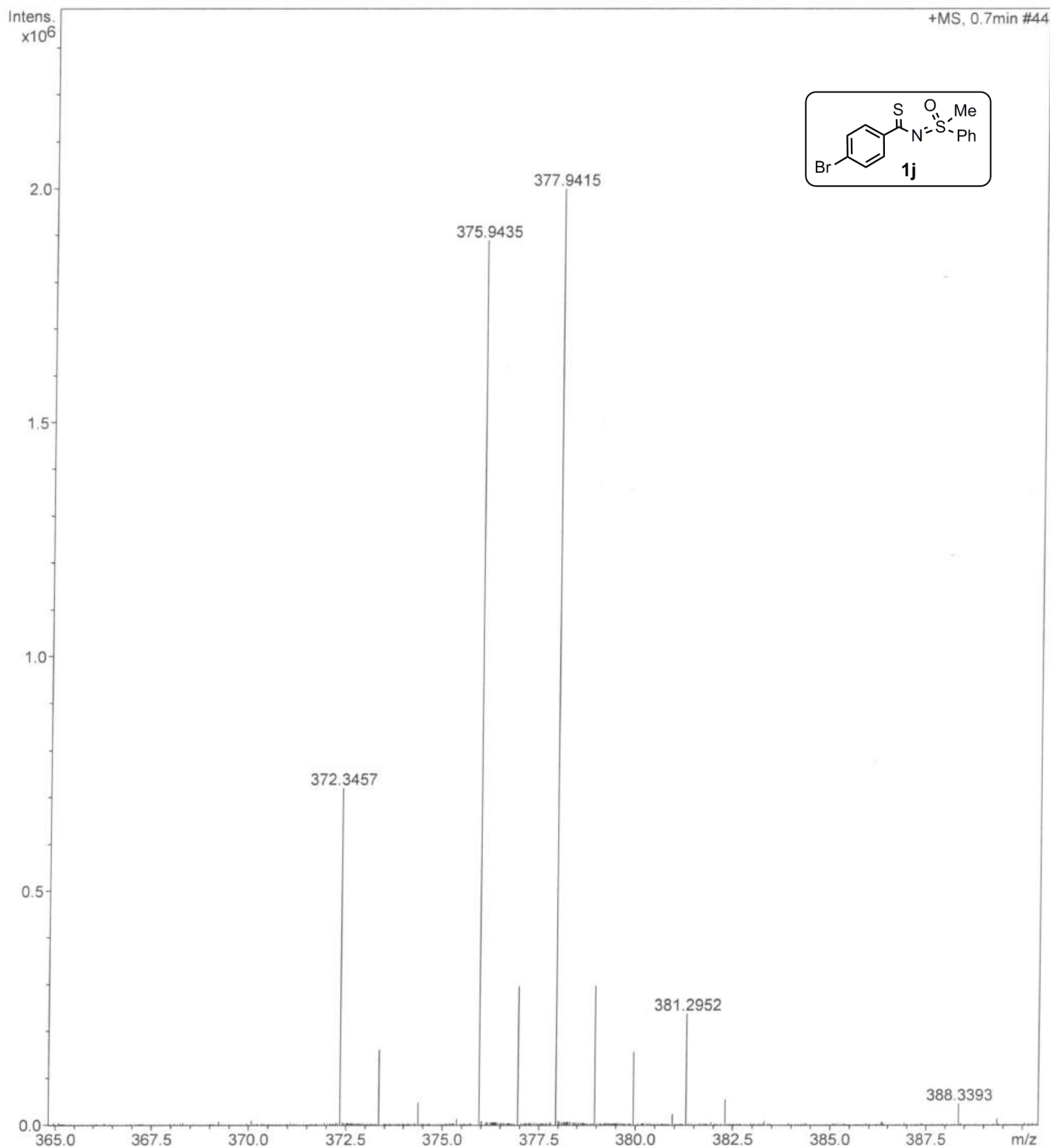
Generic Display Report

Analysis Info

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Method tune_low.m
Sample Name MJ-11-14
Comment

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Operator Rajesh Vashisth
Instrument maXis



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

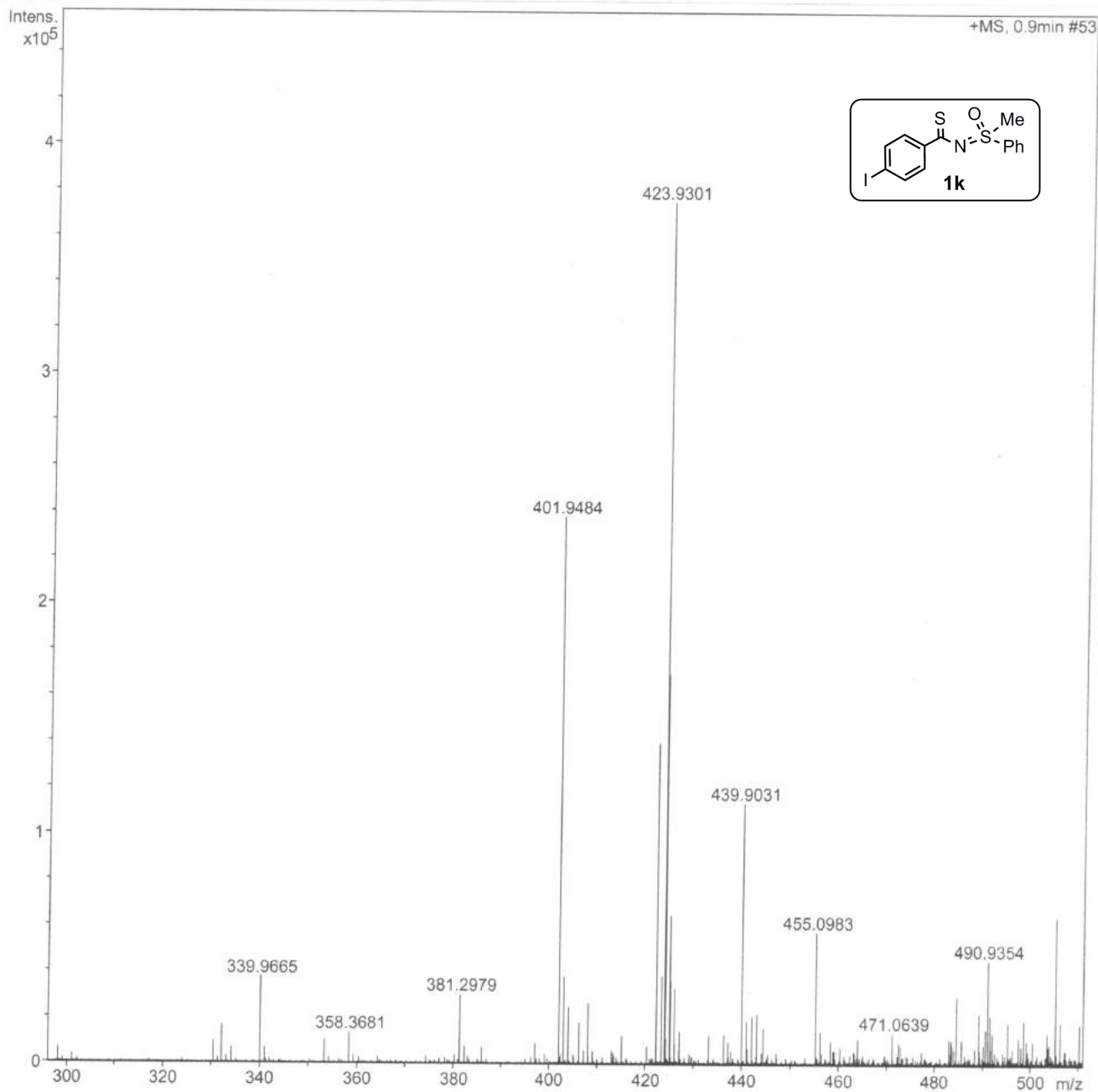
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 Sample Name S-1-124-DCM-MEOH
 Comment

Acquisition Date 12/13/2018 11:49:06 AM

Operator UOH-Chemistry
 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	6.0 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

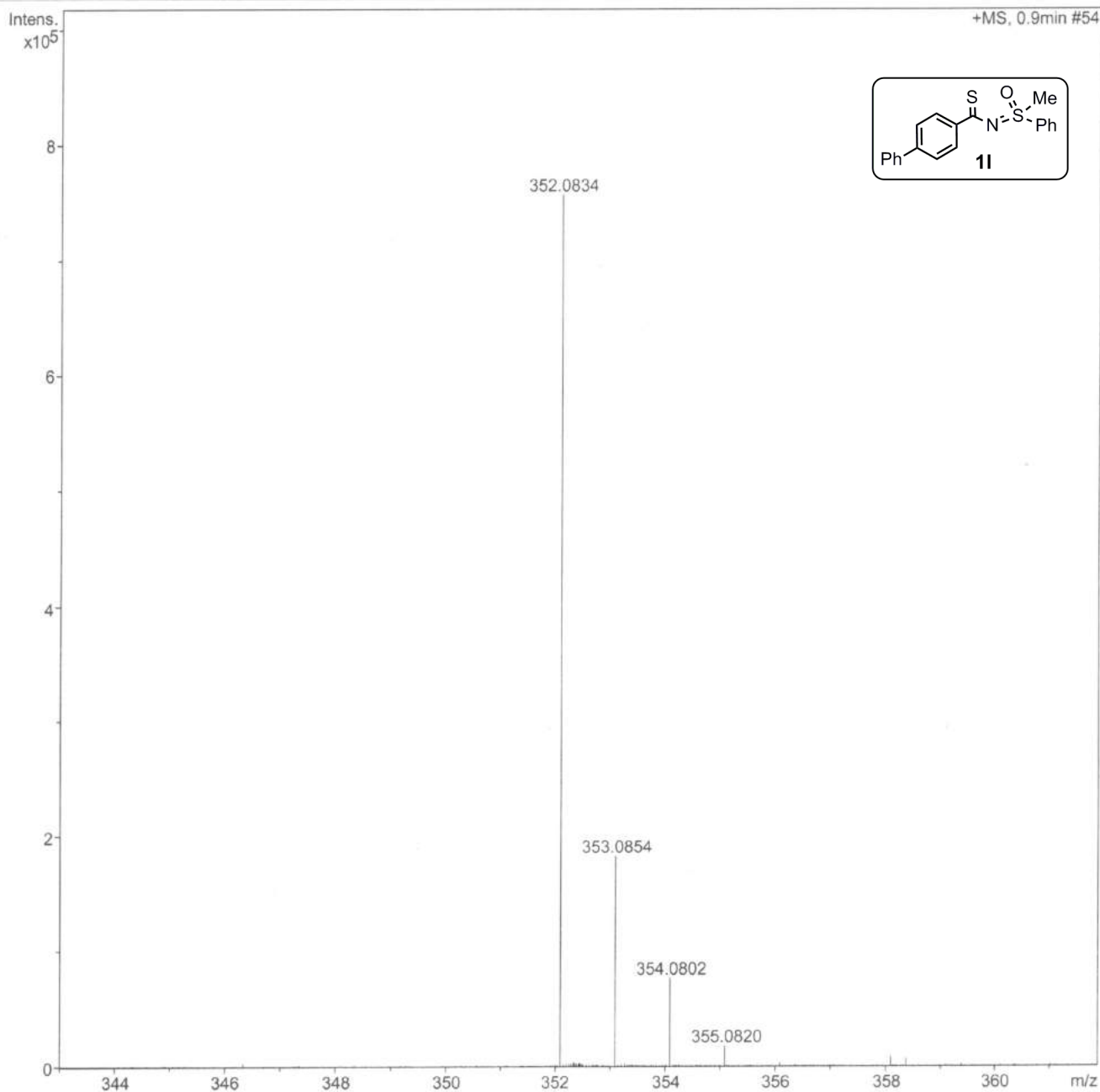
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Sample Name MJ-48-15-B-dcm-meoh
Comment

Acquisition Date 1/16/2019 11:36:22 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3900 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	200.0 Vpp	Set Divert Valve	Waste



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

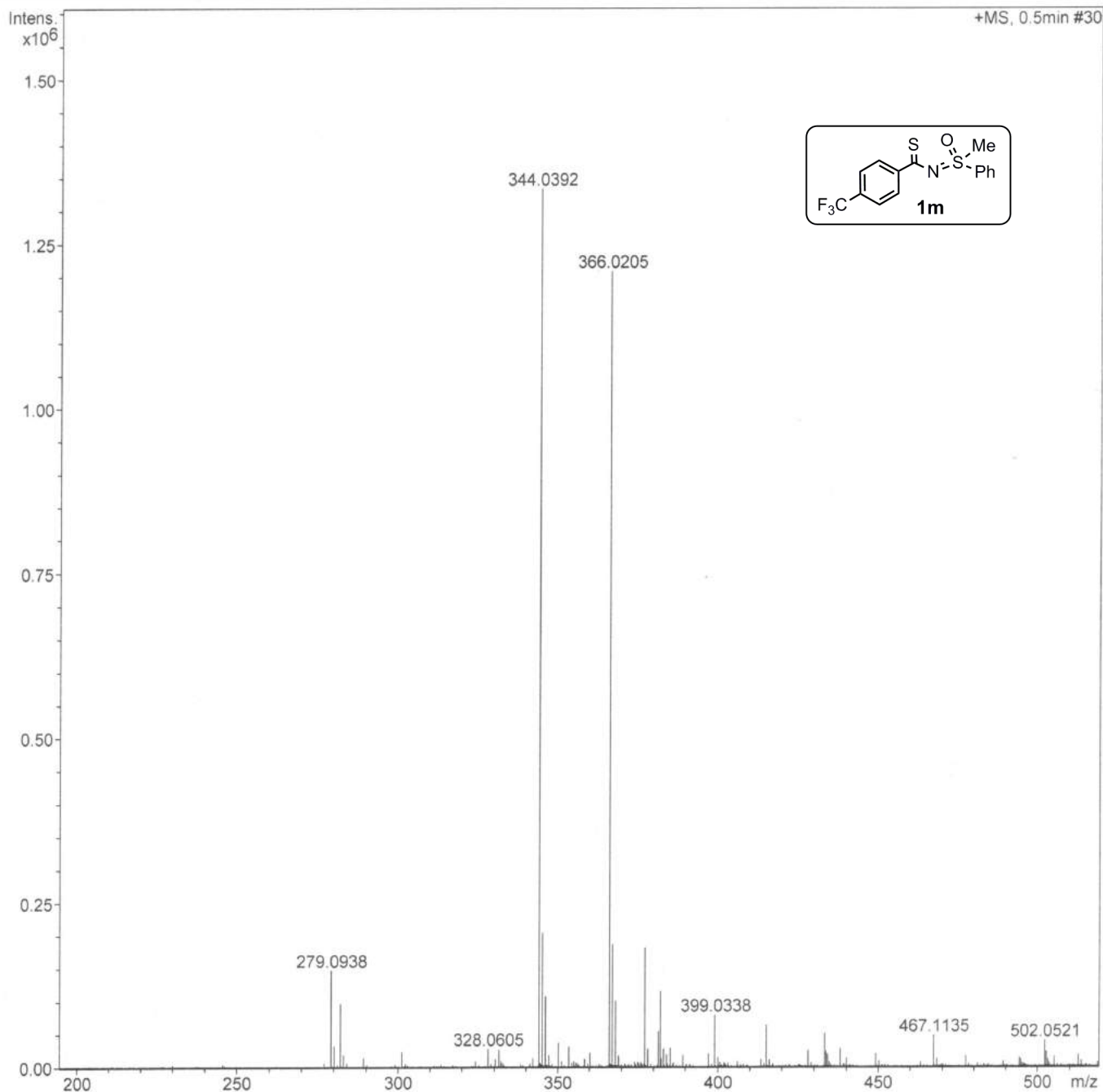
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 Sample Name S-1-94-DCM-MEOH
 Comment

Acquisition Date 12/13/2018 10:40:07 AM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 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

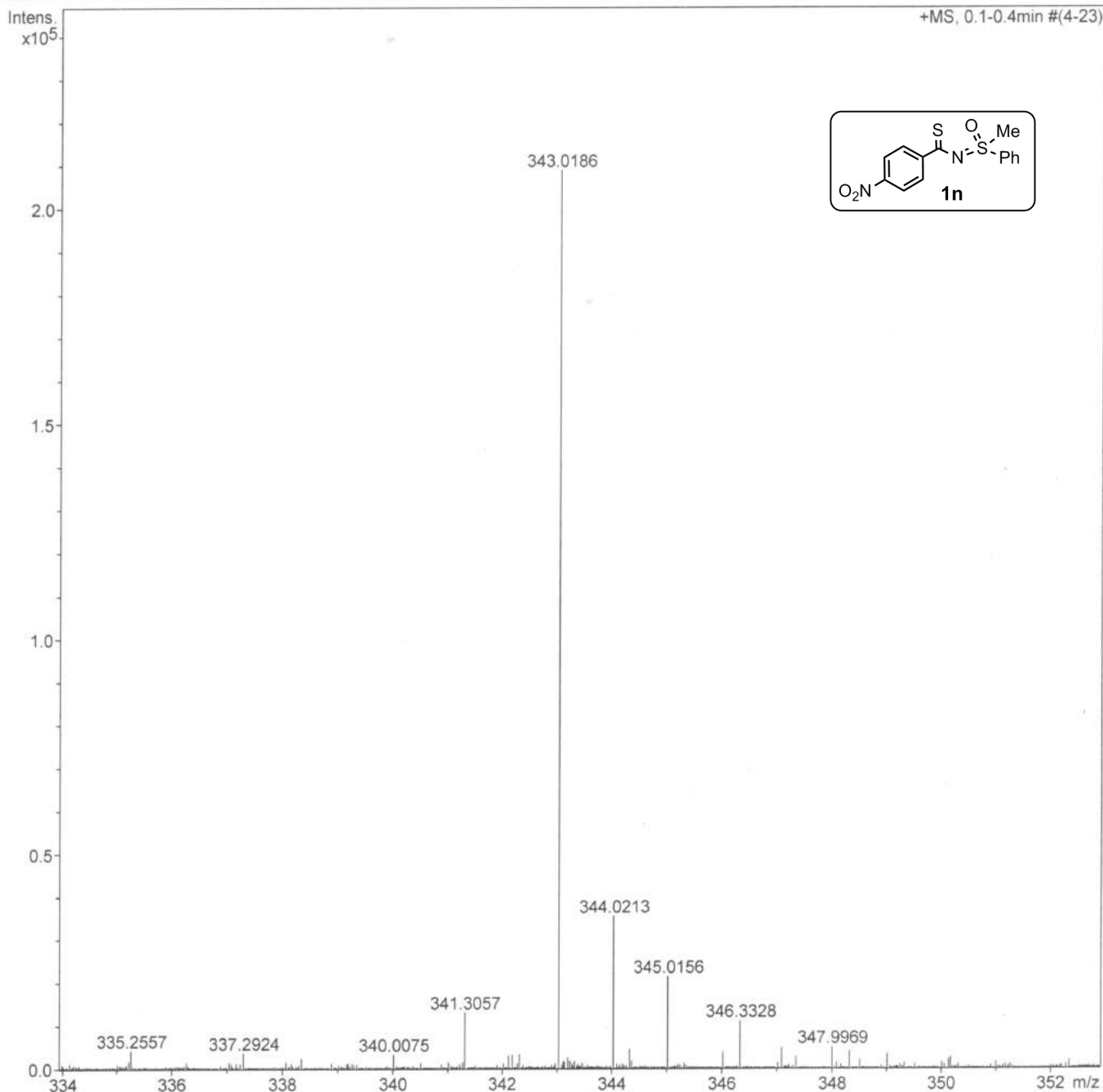
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 Sample Name MJ-25-15
 Comment

Acquisition Date 12/17/2018 6:07:20 PM

Operator UOH-Chemistry
 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
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UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

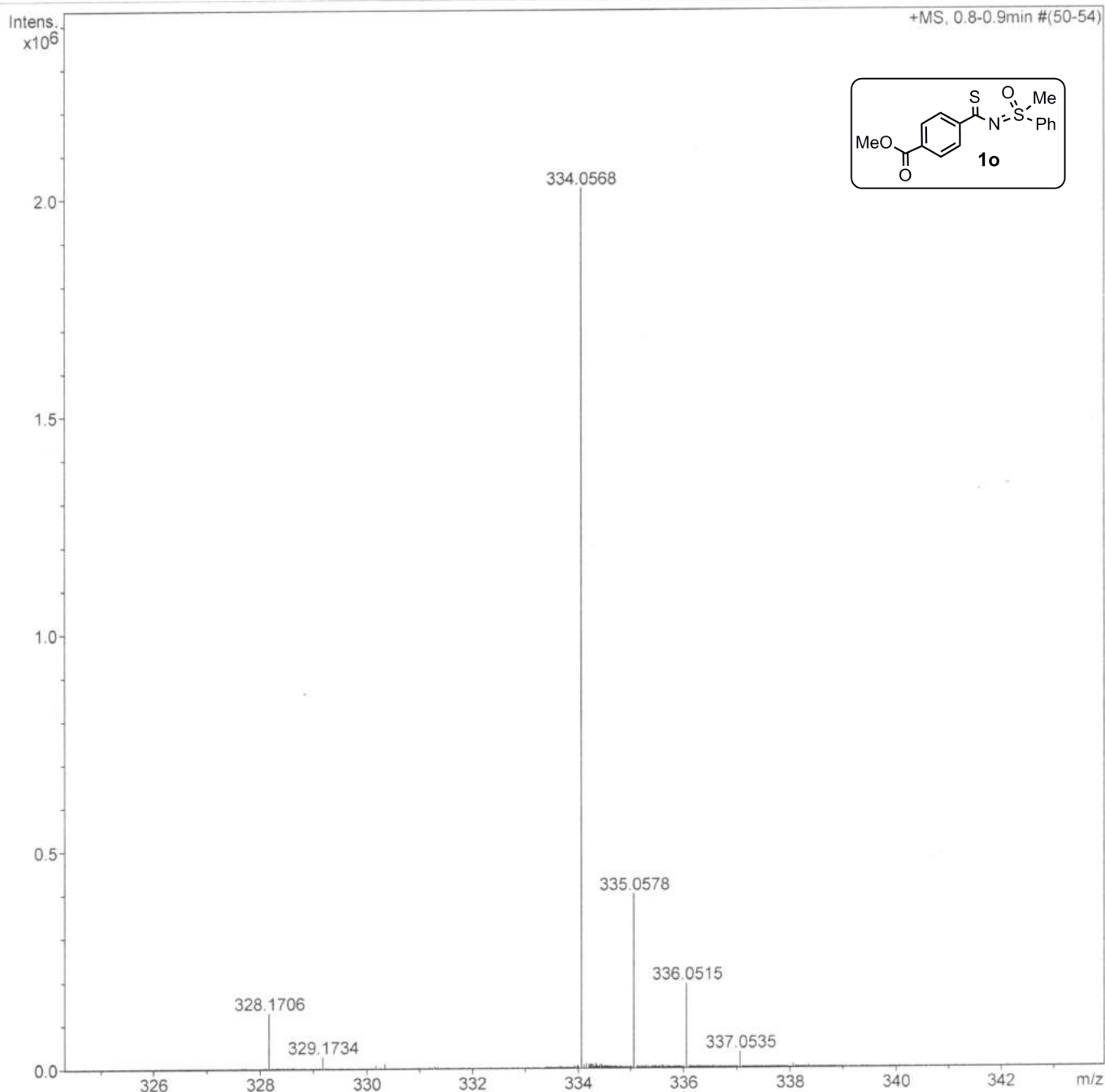
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Acquisition Date 12/24/2018 11:49:11 AM

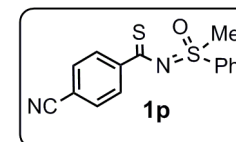
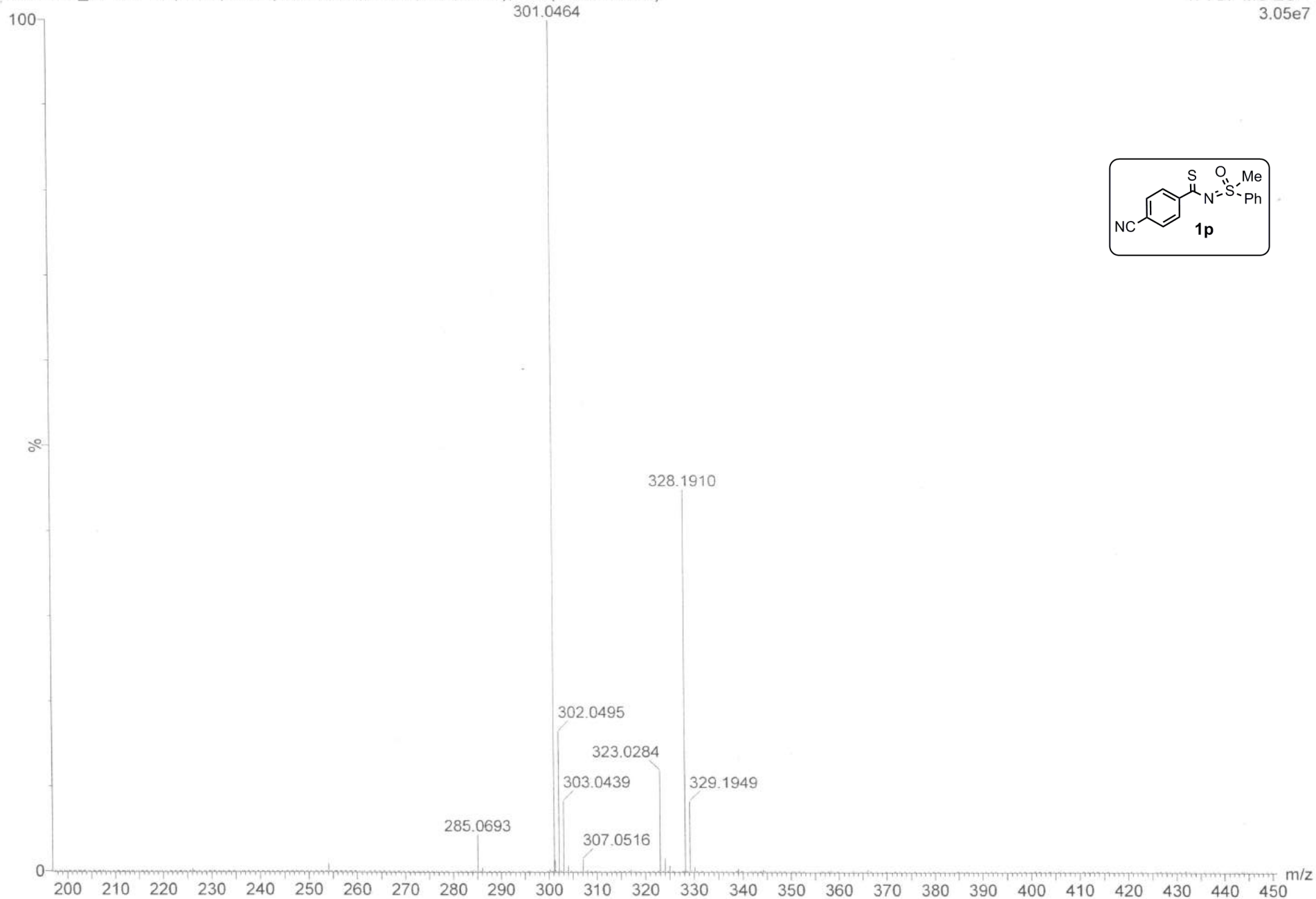
Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

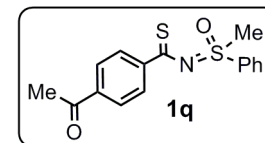
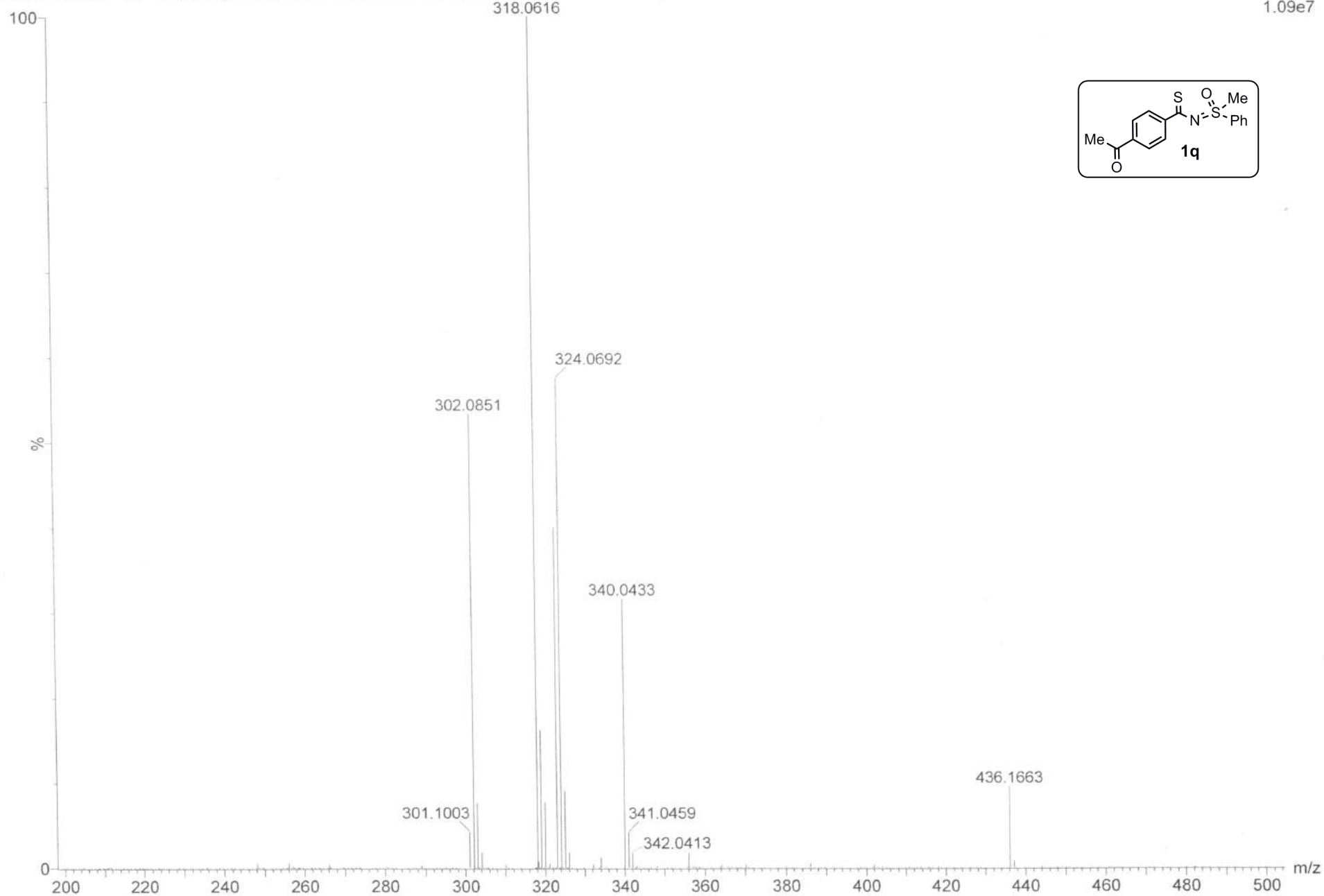
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Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



04112020_11 +VE 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:27-73:125)

1: TOF MS ES+
3.05e7

21102020_16 +VE 18 (0.191) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (18:23-71:137)

1: TOF MS ES+
1.09e7

MJ-17-153

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XEVO-G2XSQTOF#YEA1155

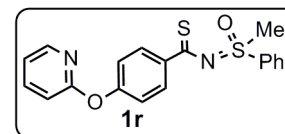
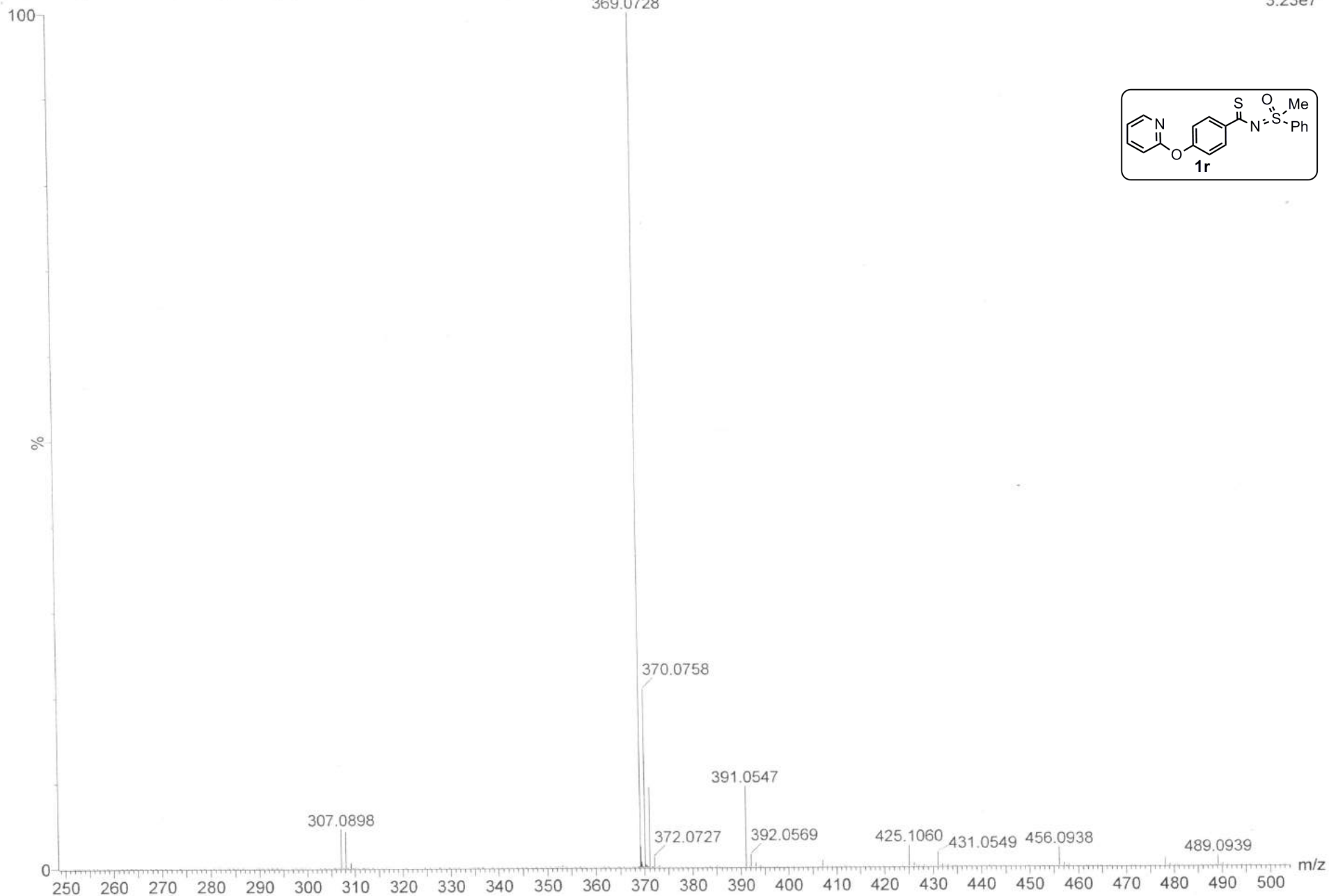
21-Oct-2020

15:19:25

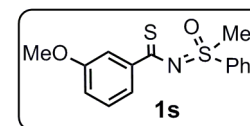
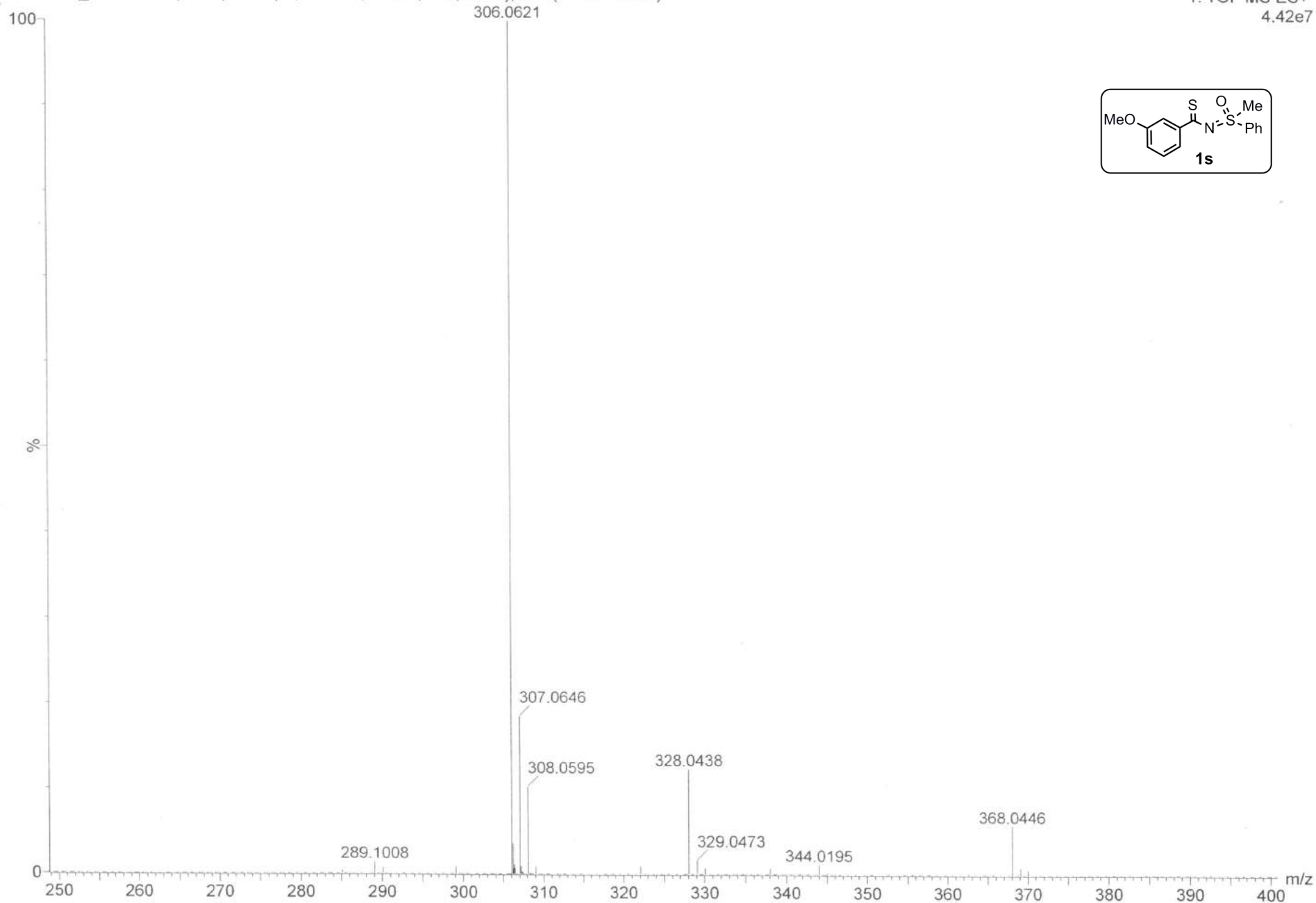
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1: TOF MS ES+

3.23e7



04112020_12 +VE 17 (0.182) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (17:22-73:117)

1: TOF MS ES+
4.42e7

UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

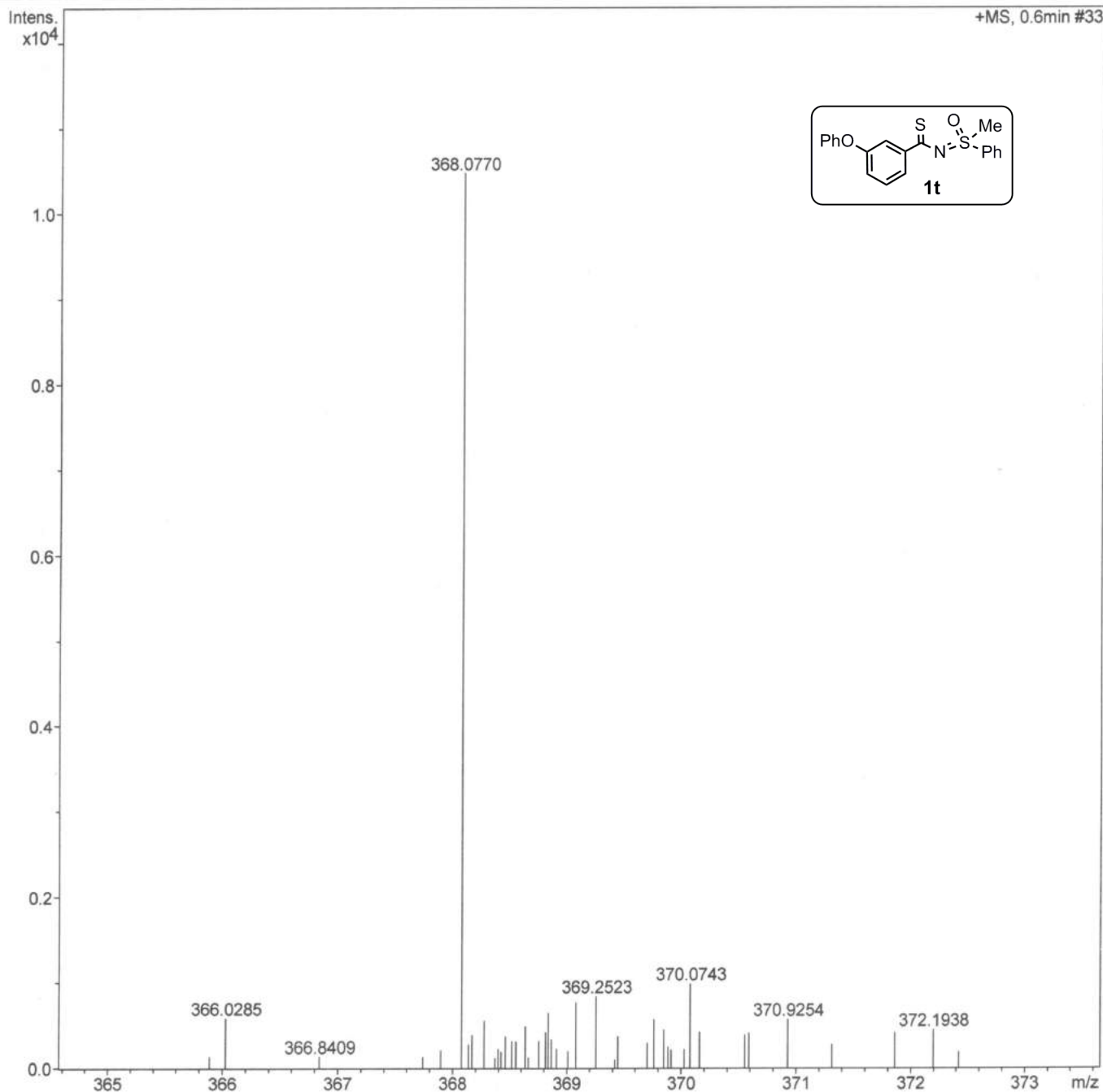
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 Sample Name MJ-10715-DCM-MEOH
 Comment

Acquisition Date 11/16/2018 12:34:20 PM

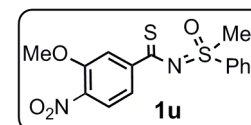
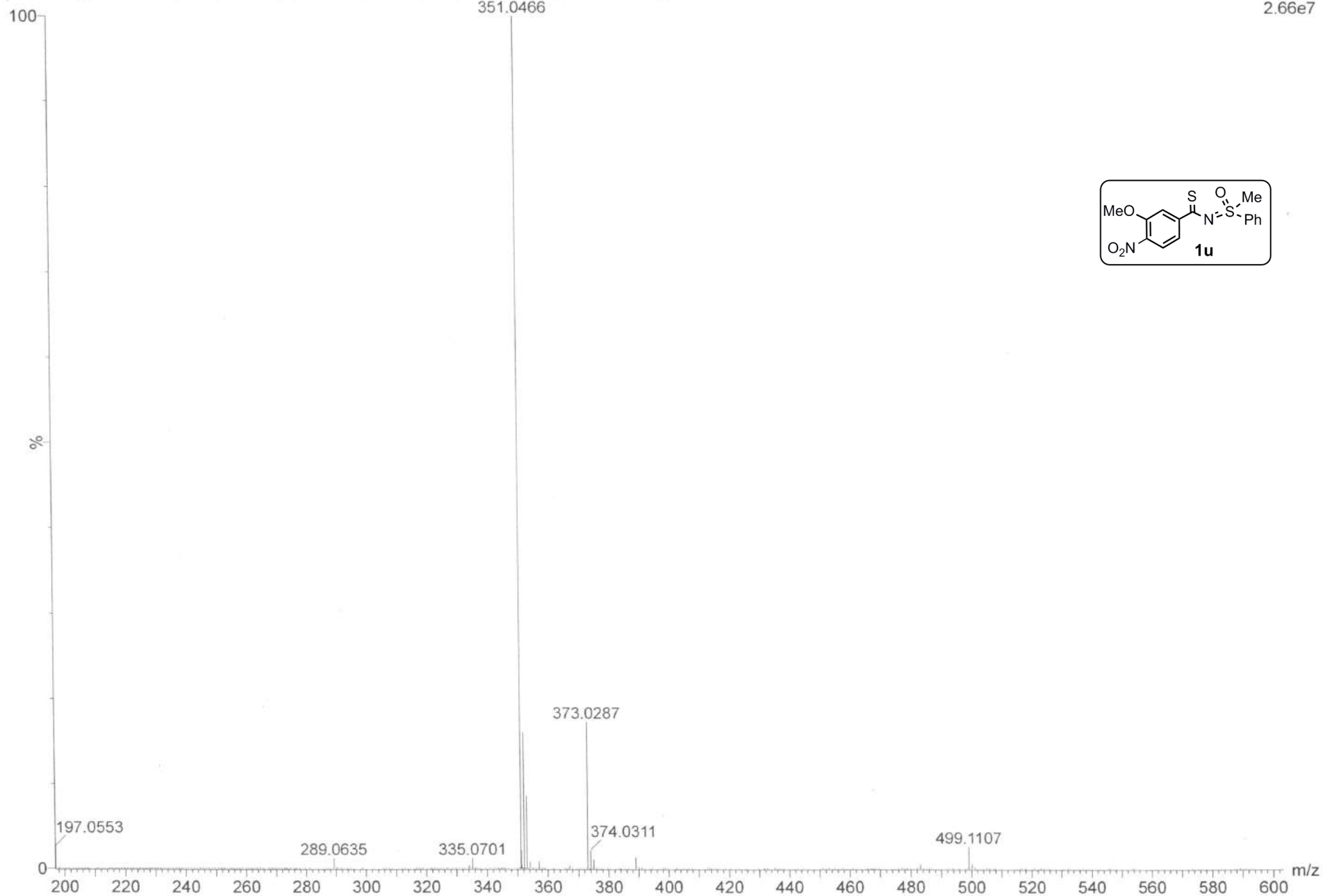
Operator UOH-Chemistry
 Instrument maXis 10138

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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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2.66e7

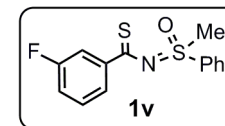
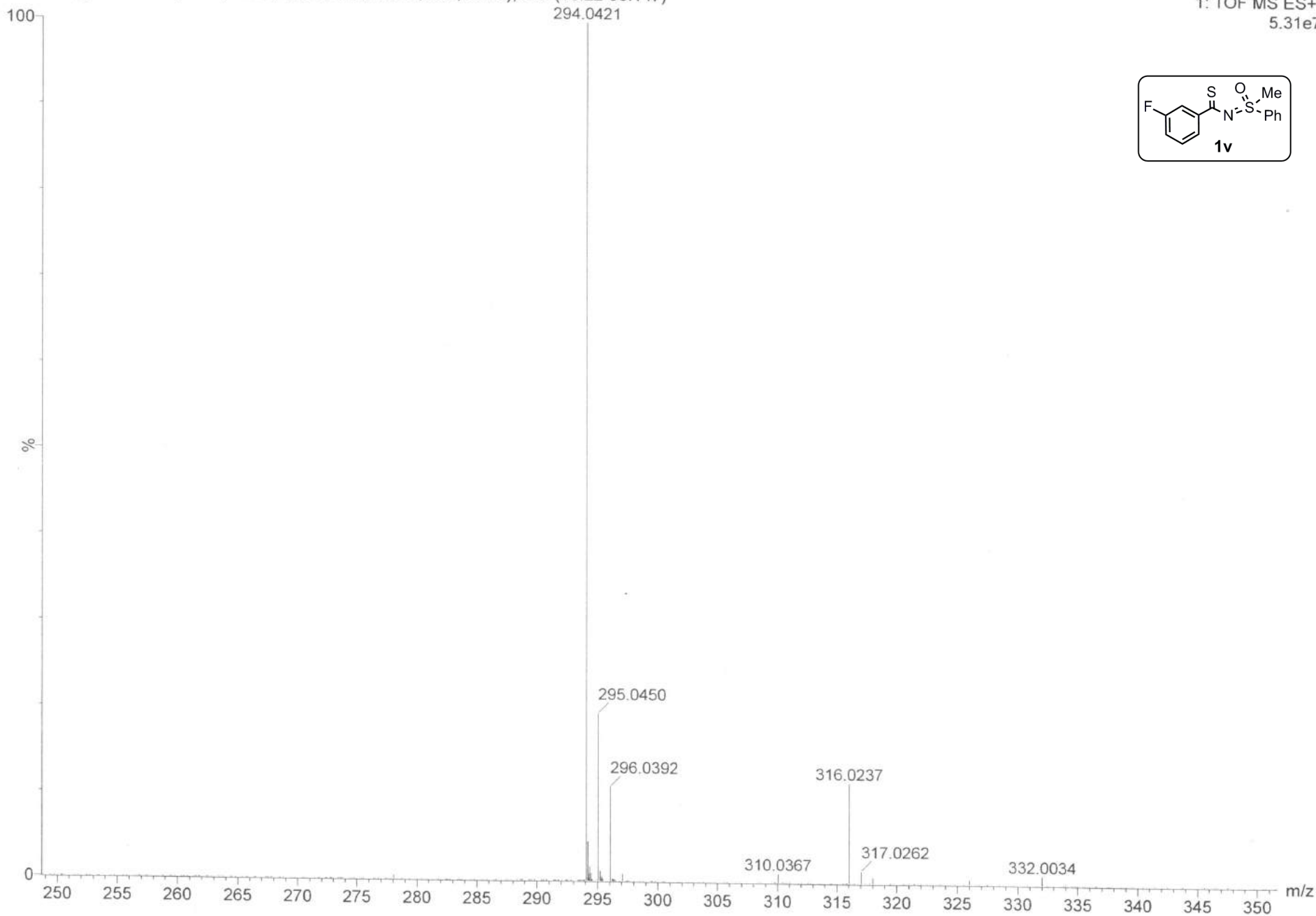
MJ-17-281

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XEVO-G2XSQTOF#YEA1155

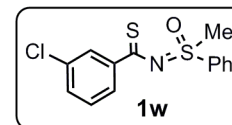
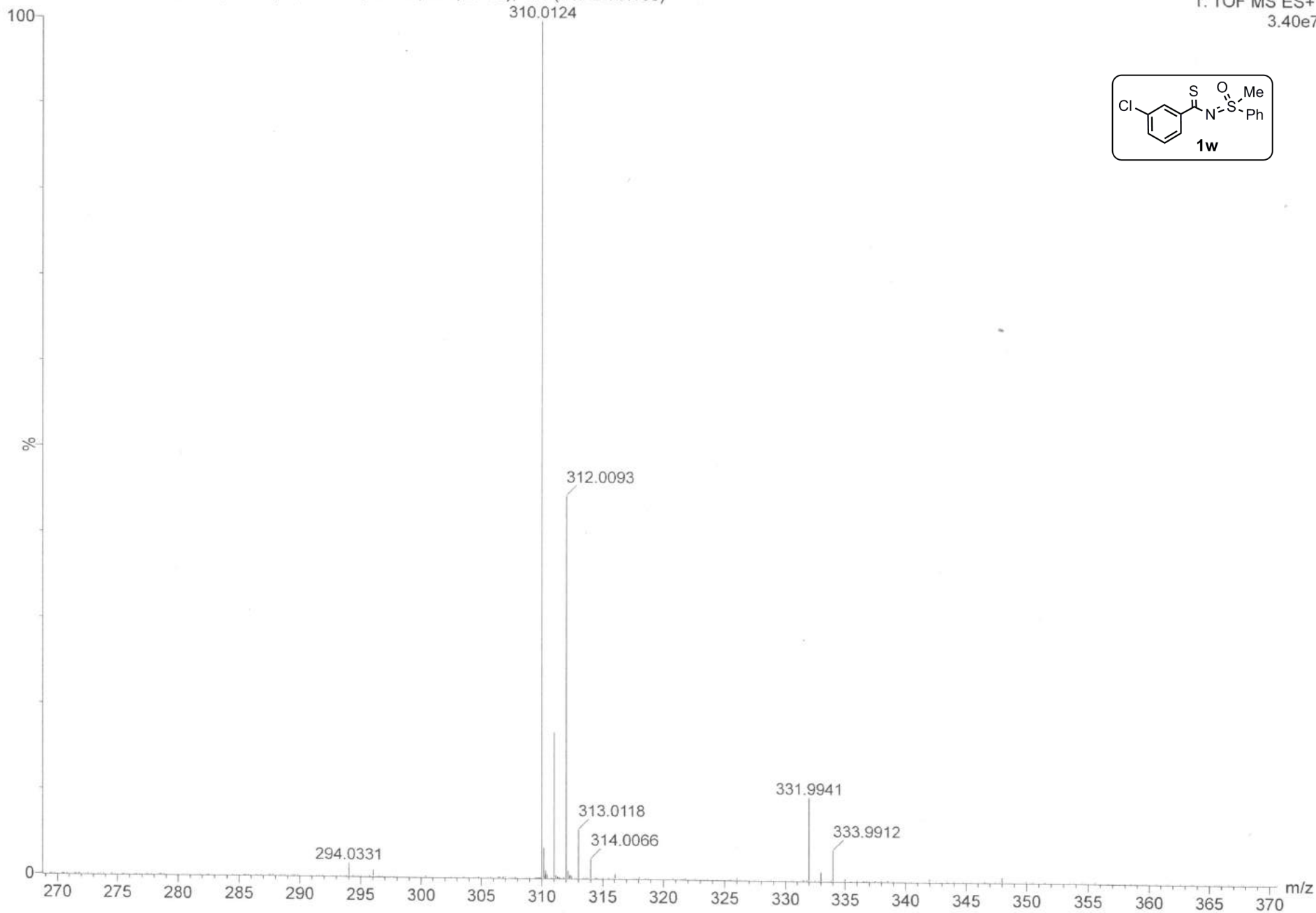
04-Nov-2020
12:02:19

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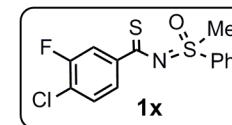
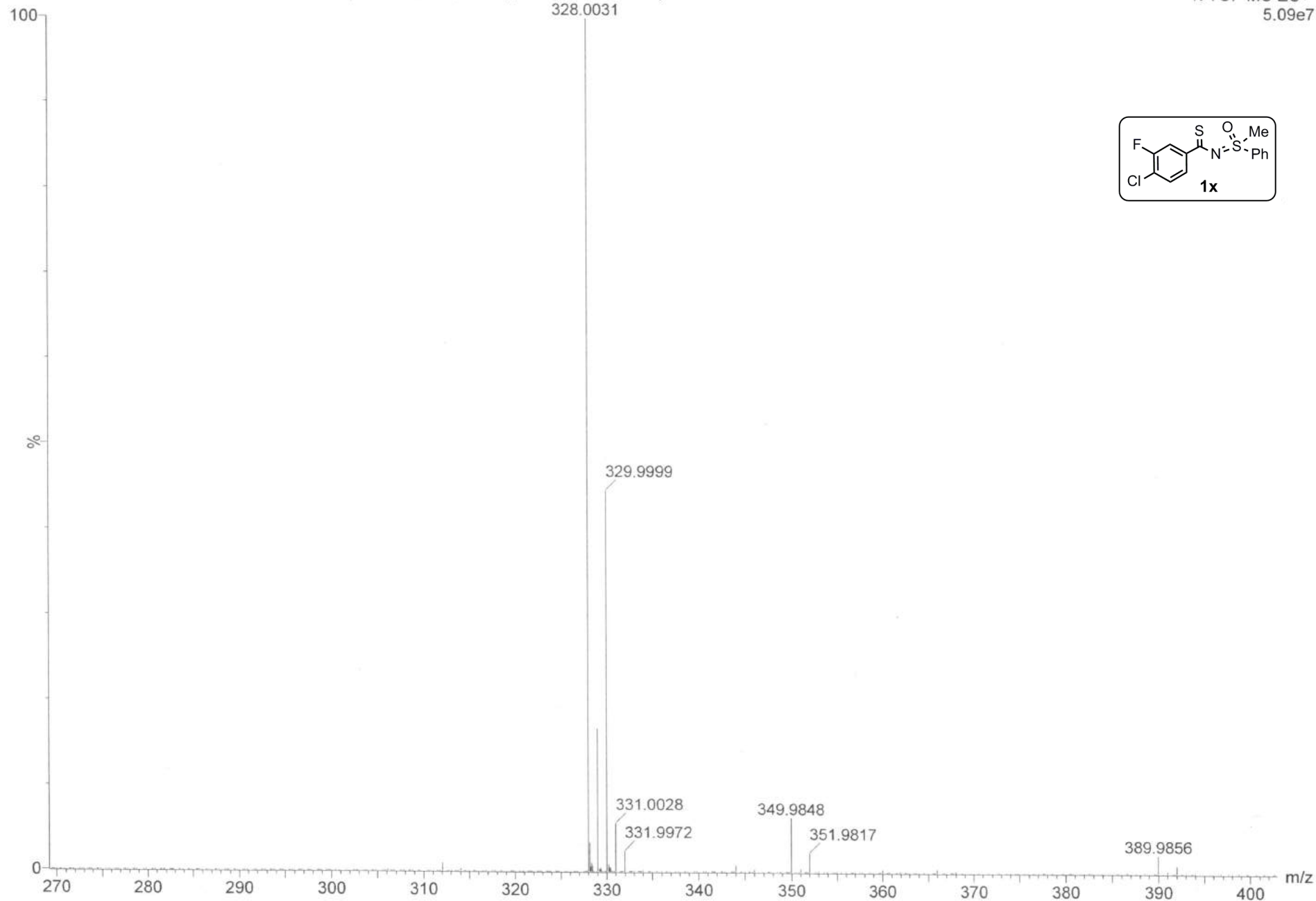
1: TOF MS ES+
5.31e7



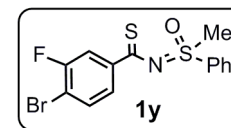
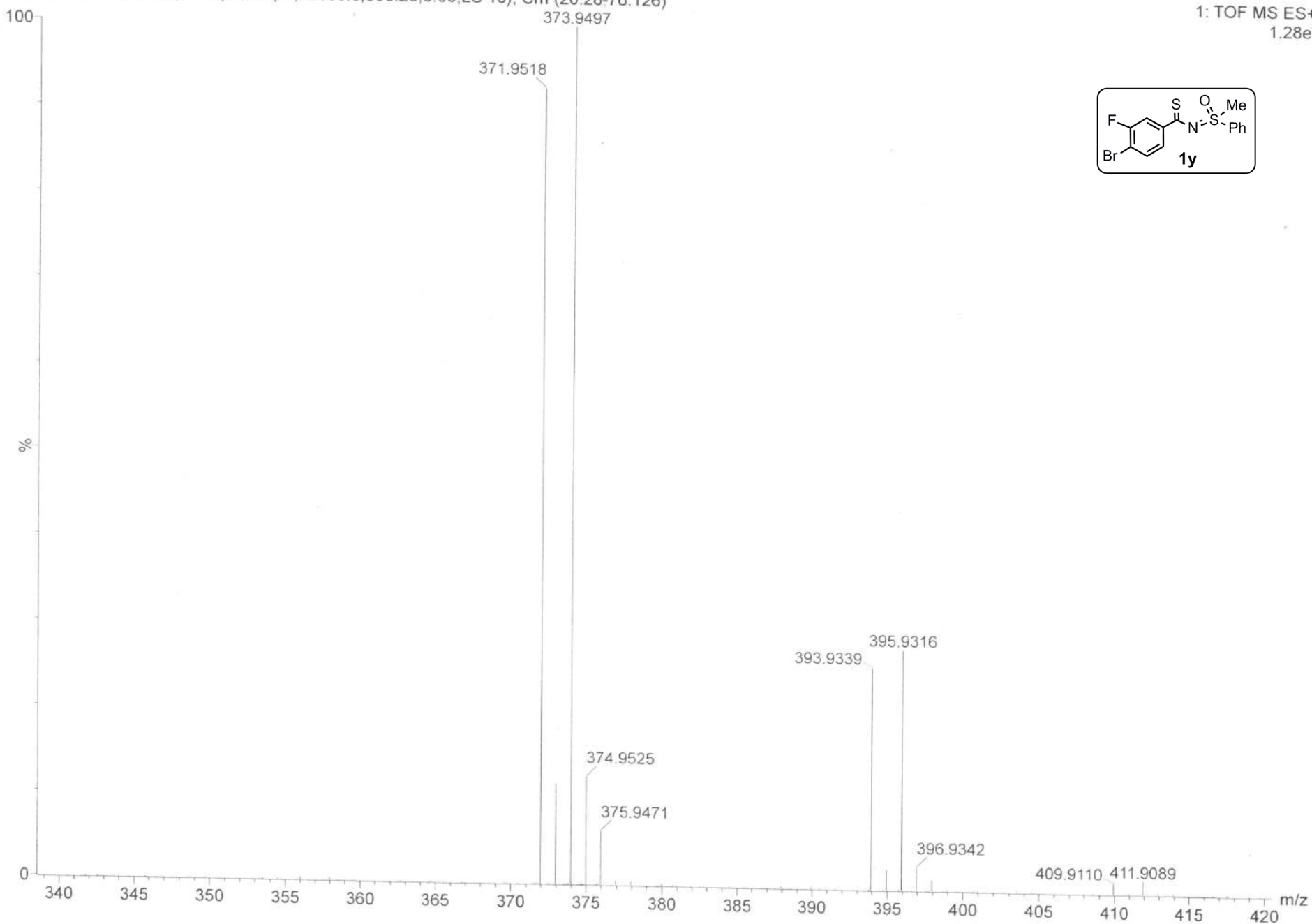
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1: TOF MS ES+
3.40e7

04112020_15 +VE 17 (0.182) AM2 (Ar,22000,0,556.28,0.00,LS 10); Cm (17:23-73:121)

1: TOF MS ES+
5.09e7

06112020_09 +VE 20 (0.228) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (20:28-76:126)

1: TOF MS ES+
1.28e7

UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

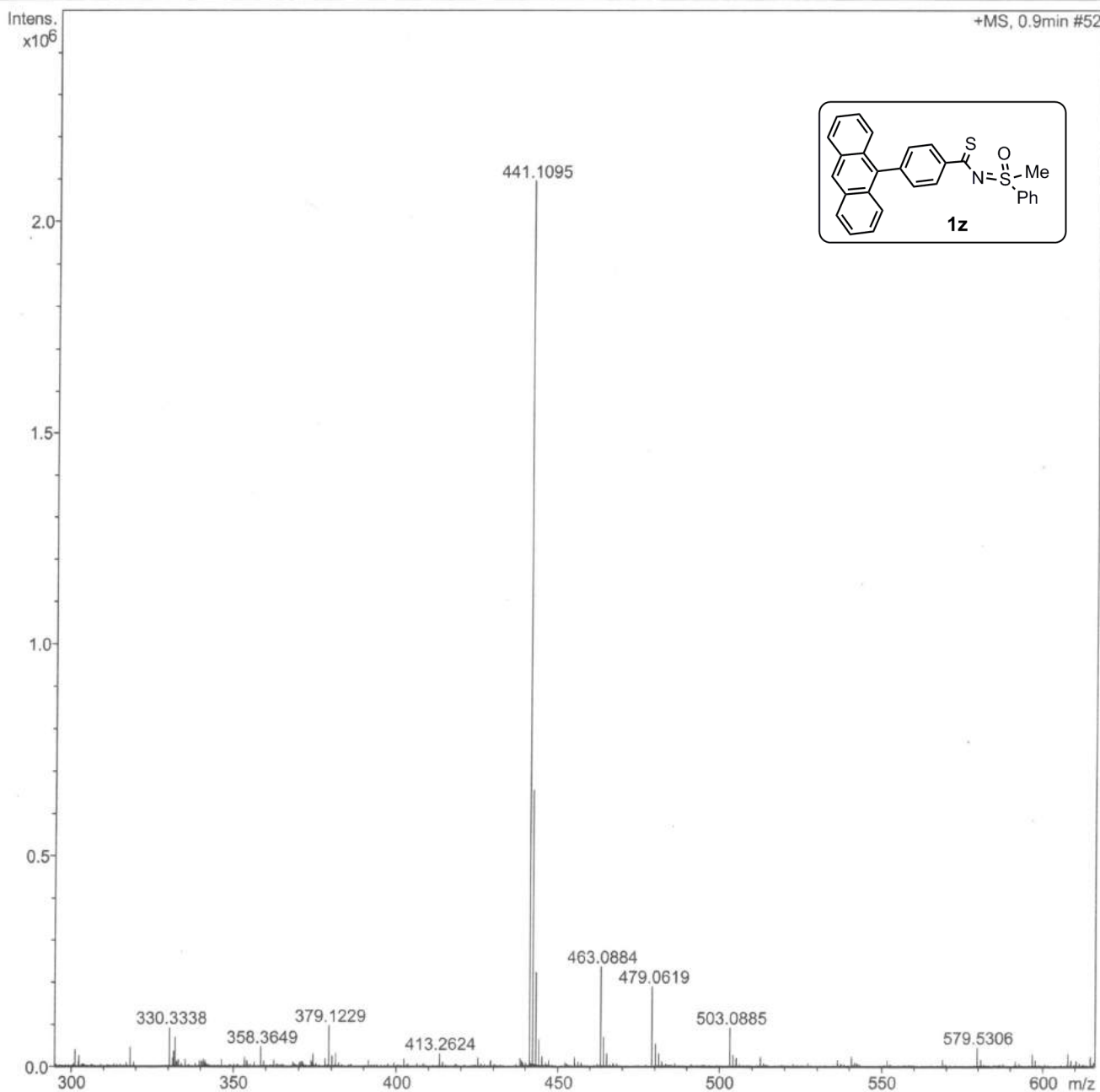
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 Comment

Acquisition Date 1/21/2019 11:29:45 AM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

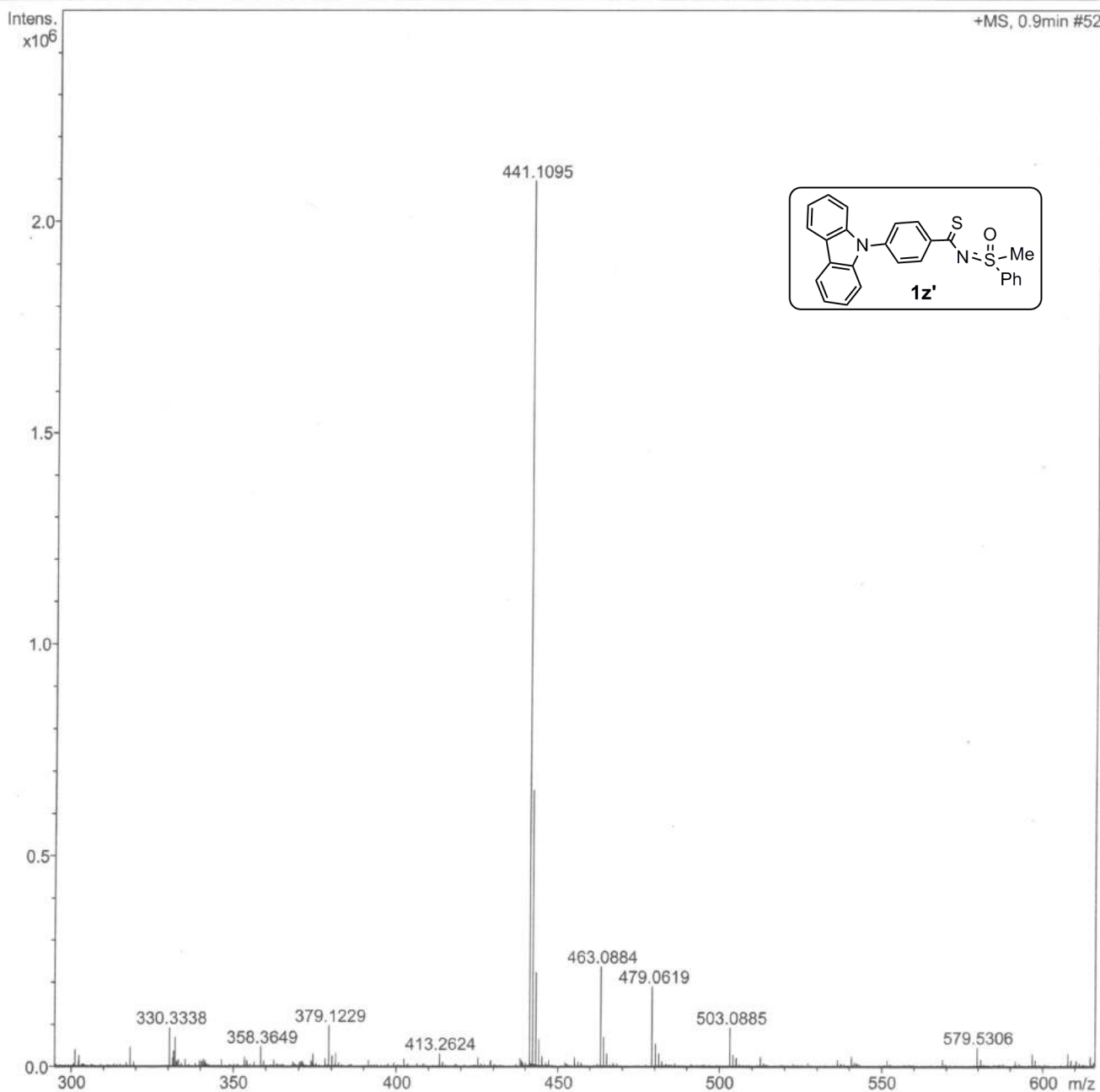
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 Comment

Acquisition Date 1/21/2019 11:29:45 AM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
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Scan End	2500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



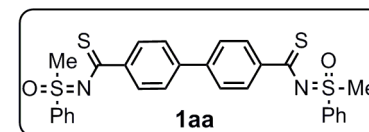
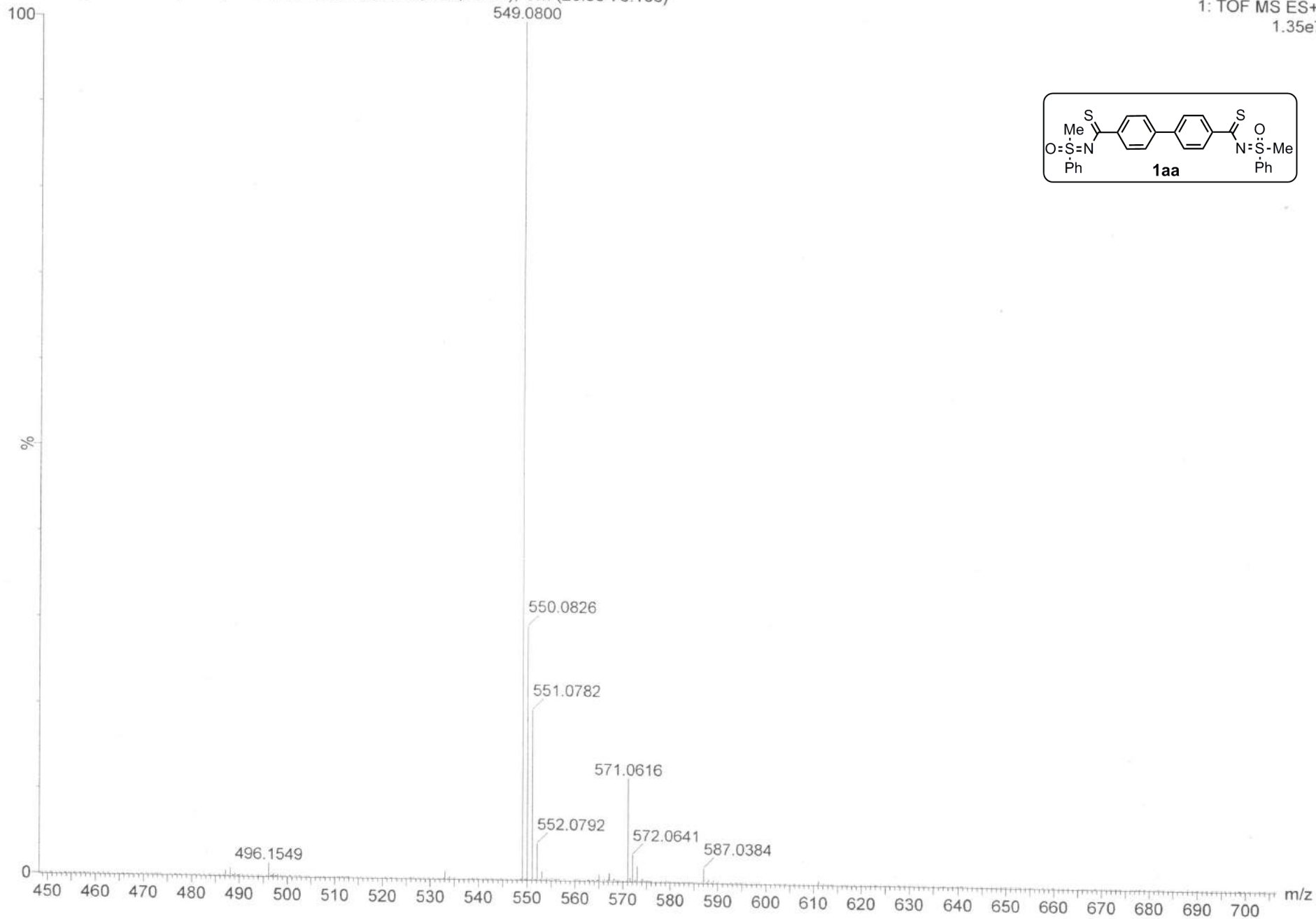
MJ-Bi

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XEVO-G2XSQTOF#YEA1155

10-Nov-2020
15:32:27

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1: TOF MS ES+
1.35e7



Display Report

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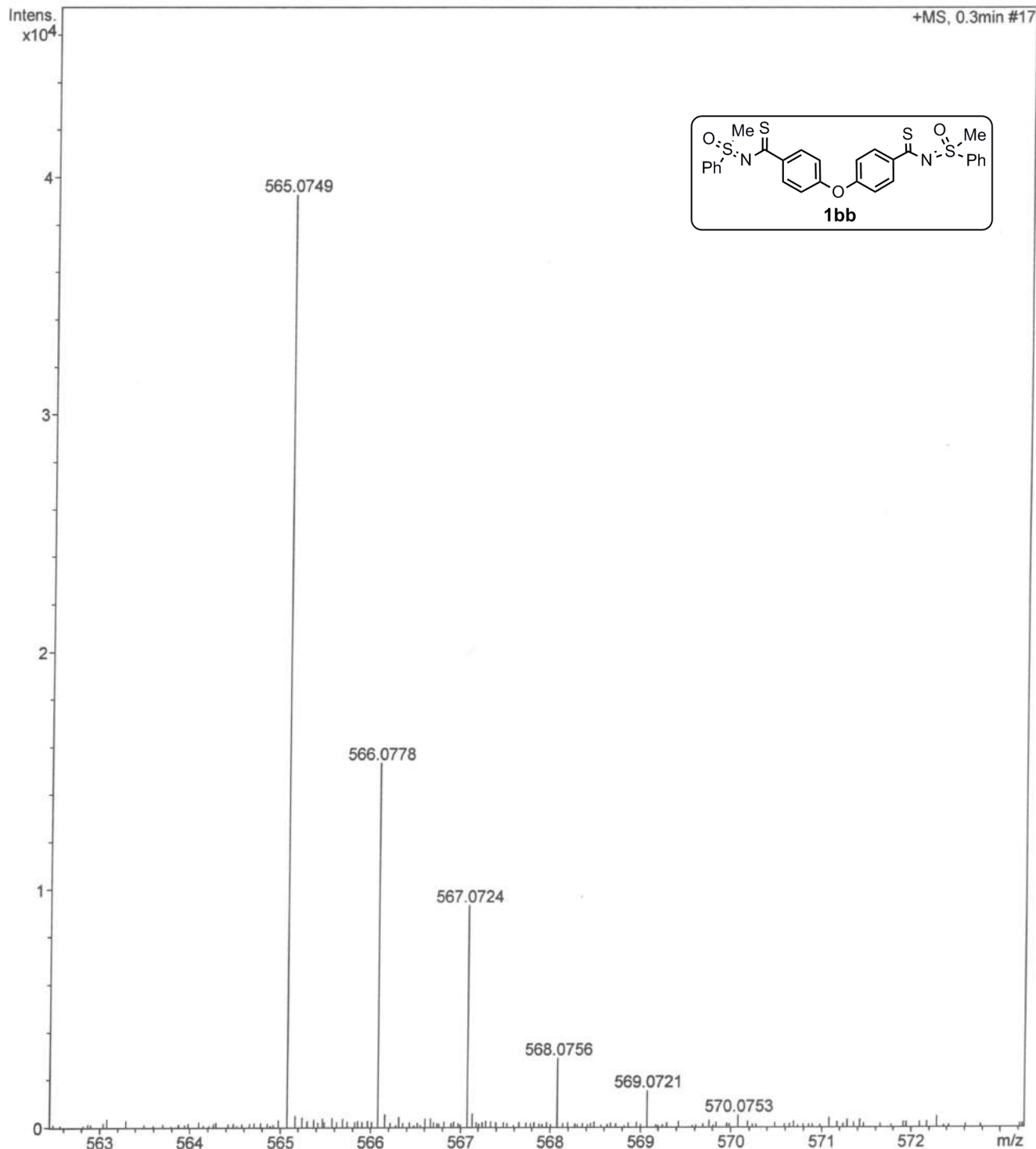
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Sample Name MJ-17-DIMPS
Comment

Acquisition Date 3/19/2020 12:20:27 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

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Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
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Display Report

Analysis Info

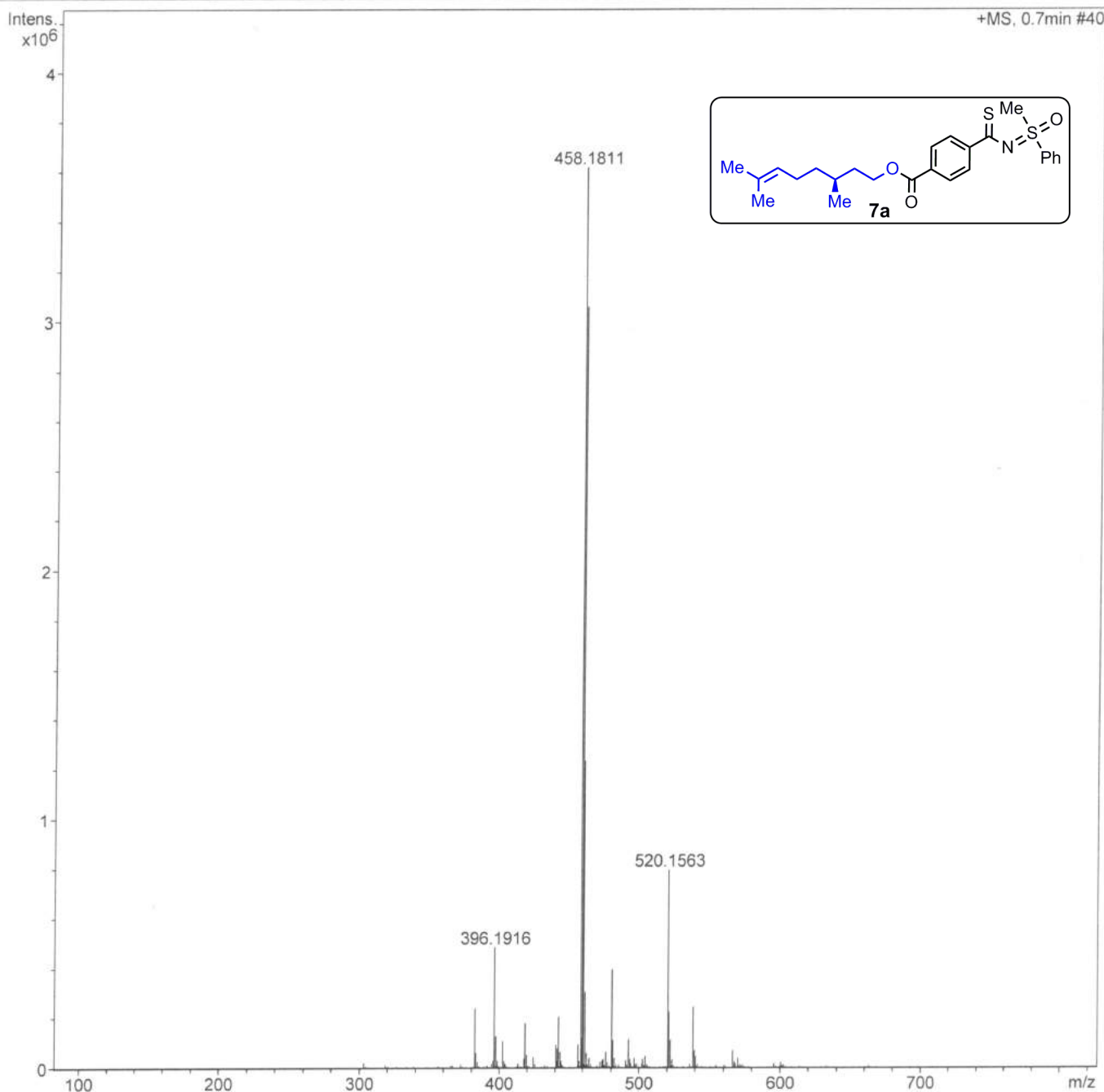
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Sample Name AS-384-MEOH
Comment

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Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

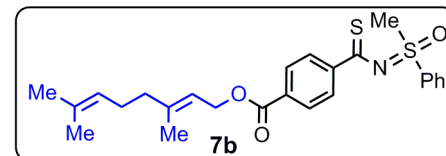
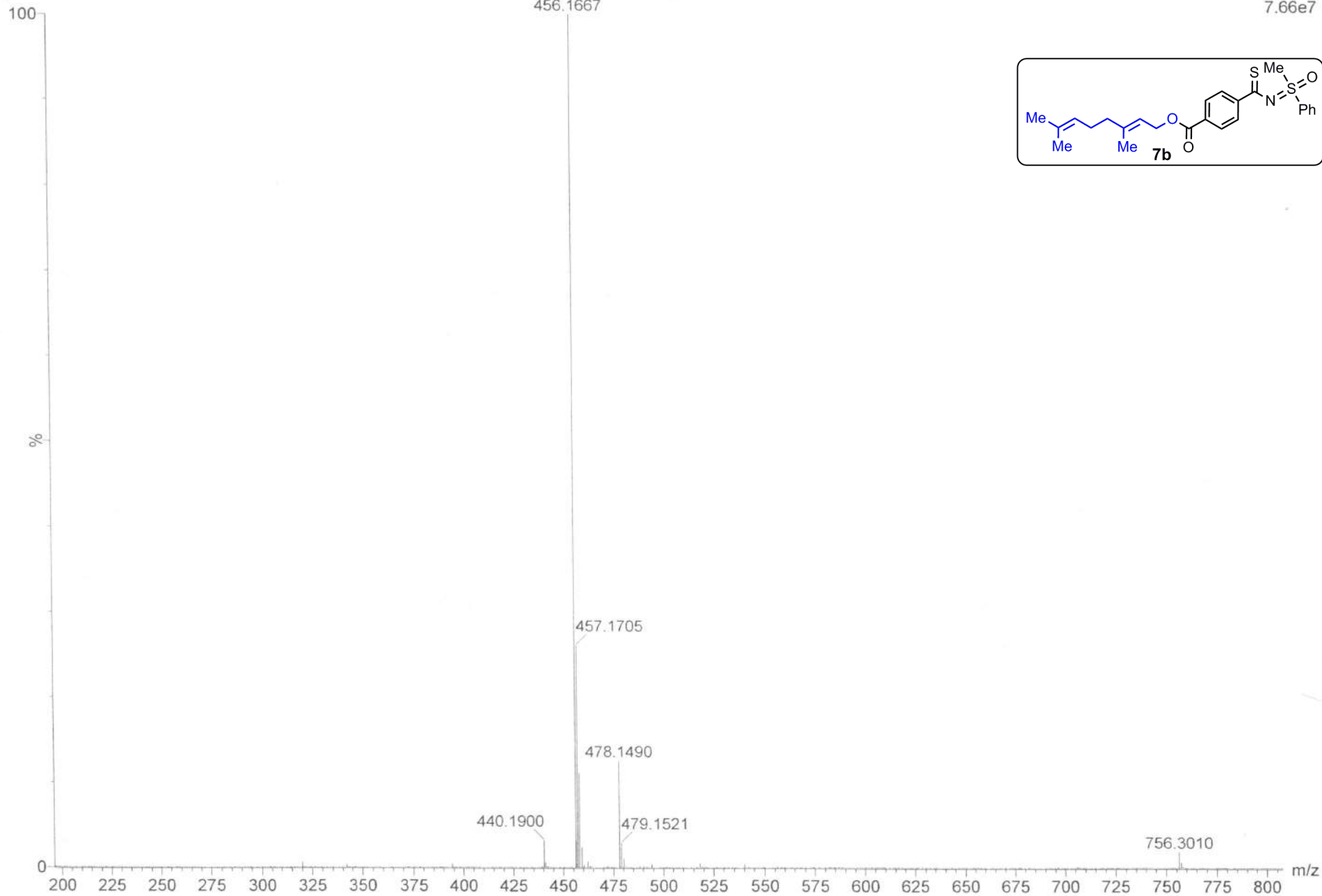
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



22102020_03 +VE 28 (0.296) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (28:36-101:140)

1: TOF MS ES+

7.66e7



Display Report

Analysis Info

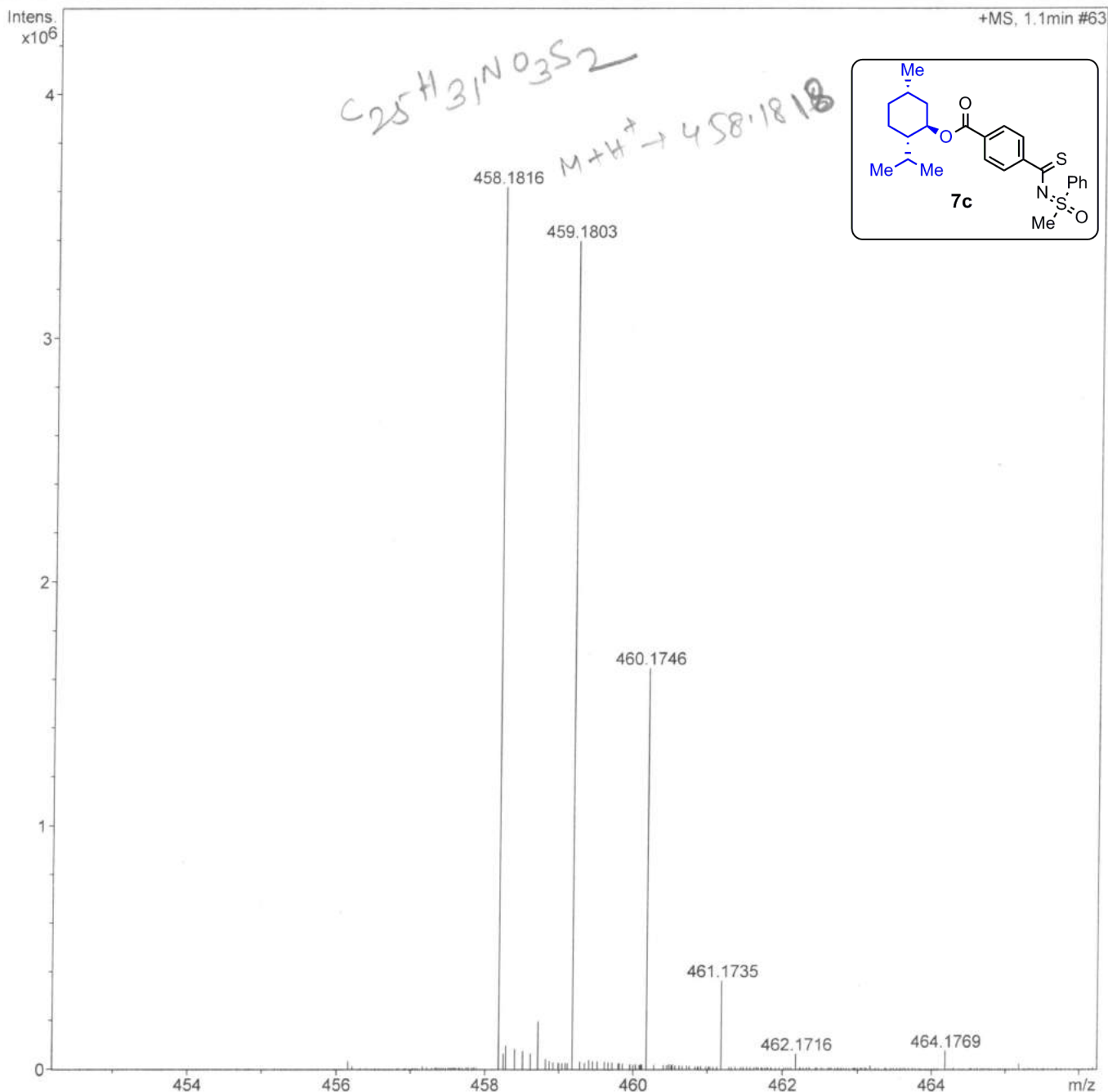
Analysis Name D:\Data\2019\PROF. AKS\OCT\AS-379.d
Method tune_low_Pos.m
Sample Name AS-379-MEOH
Comment

Acquisition Date 10/28/2019 2:58:02 AM

Operator UOH-Chemistry
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	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

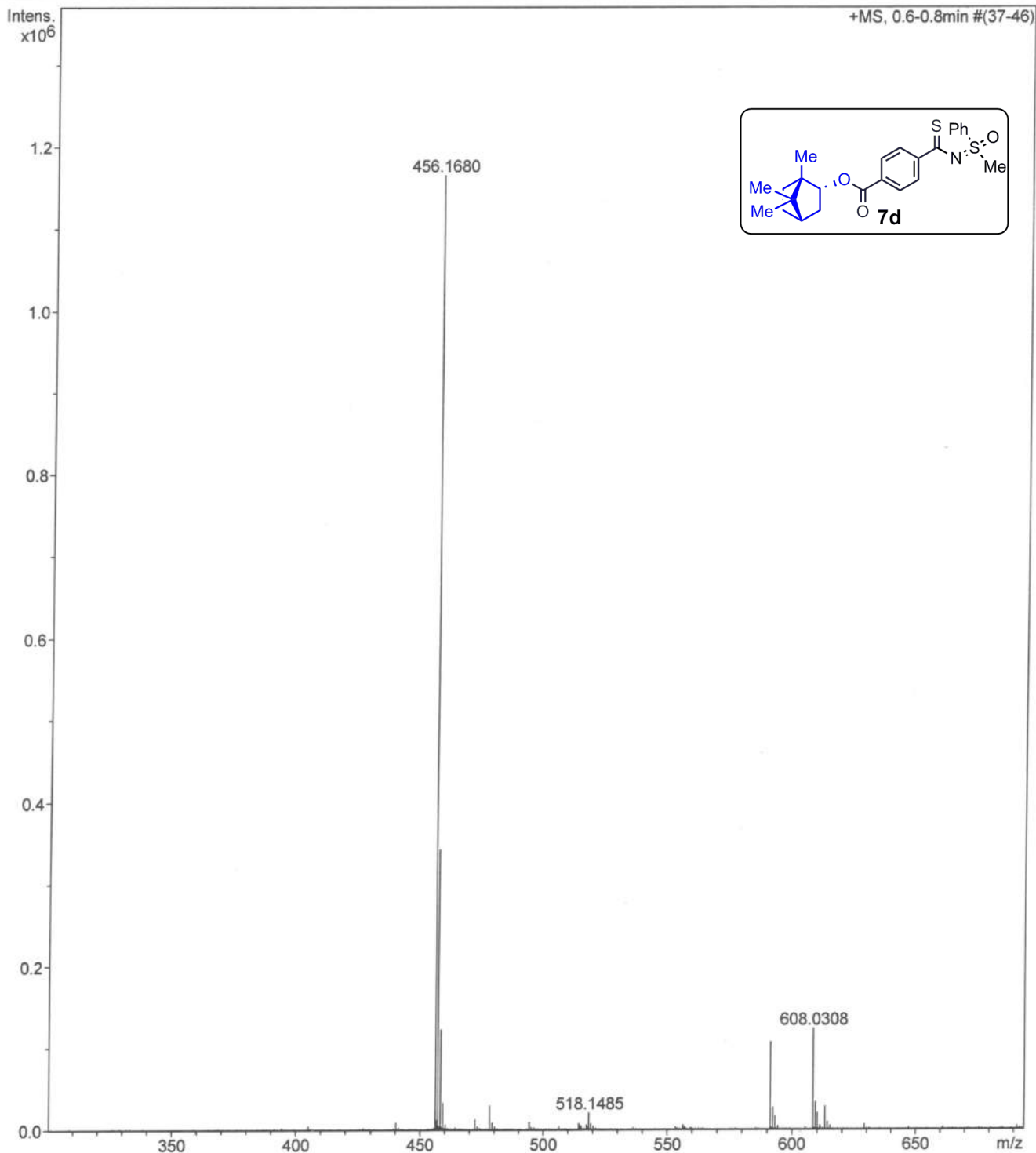
Analysis Name D:\Data\2020\PROF.AKS\MAR\SRS-8-24.d
Method tune_low_Pos-R2.m
Sample Name SRS-8-24
Comment

Acquisition Date 3/18/2020 4:47:36 PM

Operator UOH-Chemistry
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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



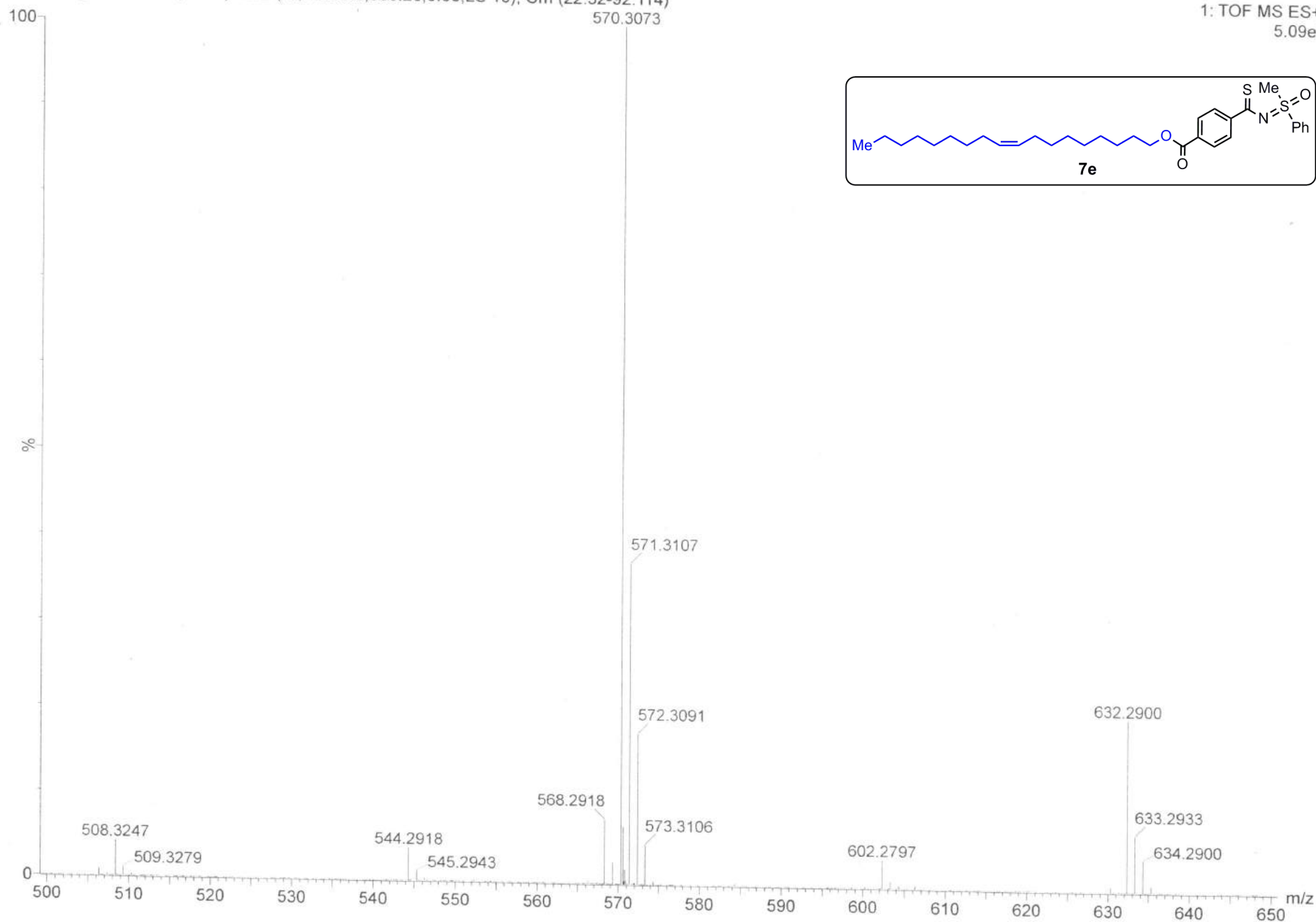
MJ-496

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ACRHEM
XEVO-G2XSQTOF#YEA1155

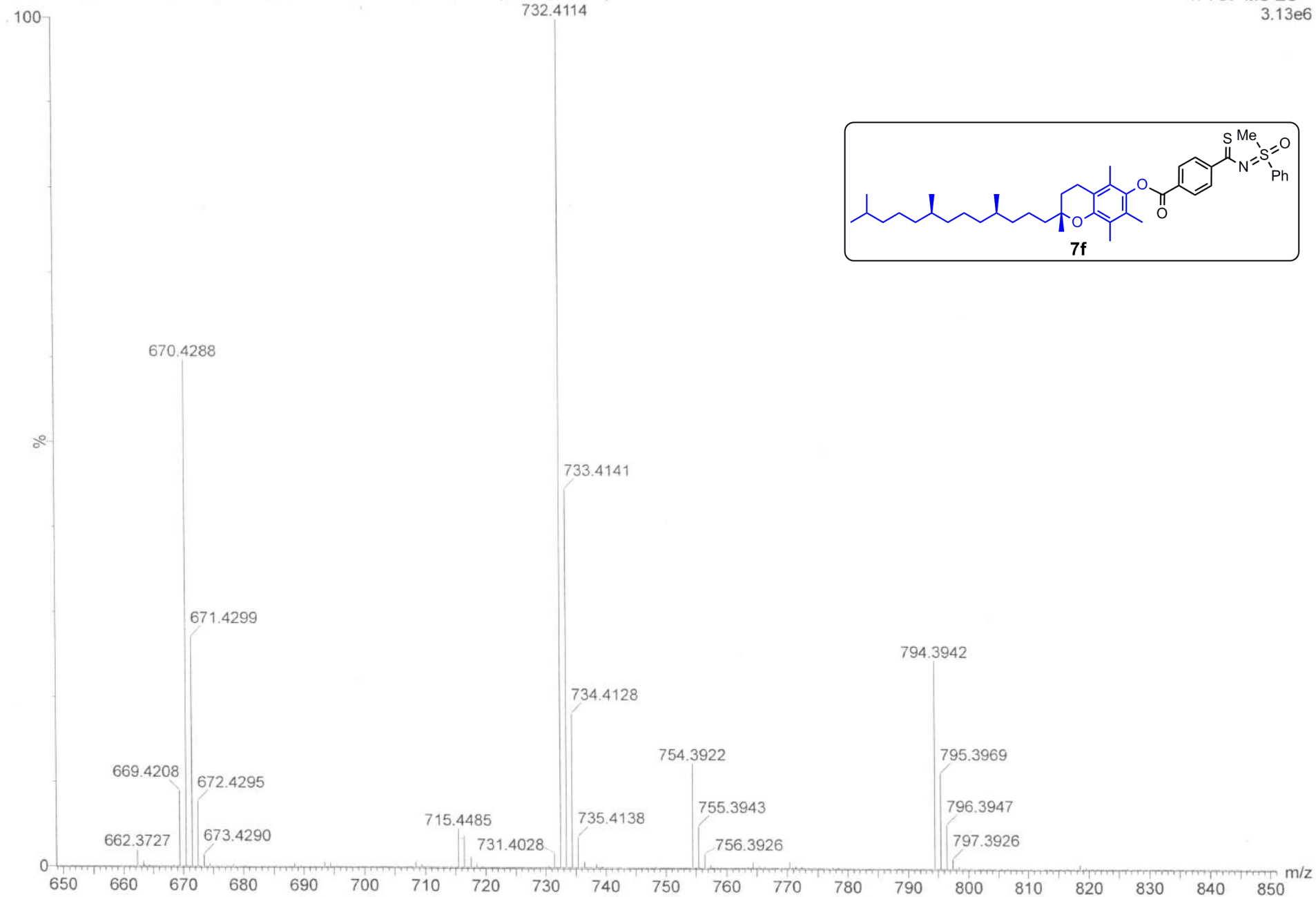
10-Nov-2020
15:27:13

10112020_23 +VE 22 (0.245) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (22:32-92:114)

1: TOF MS ES+
5.09e7



22102020_05 +VE 8 (0.105) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (4:8-1:4)

1: TOF MS ES+
3.13e6

Display Report

Analysis Info

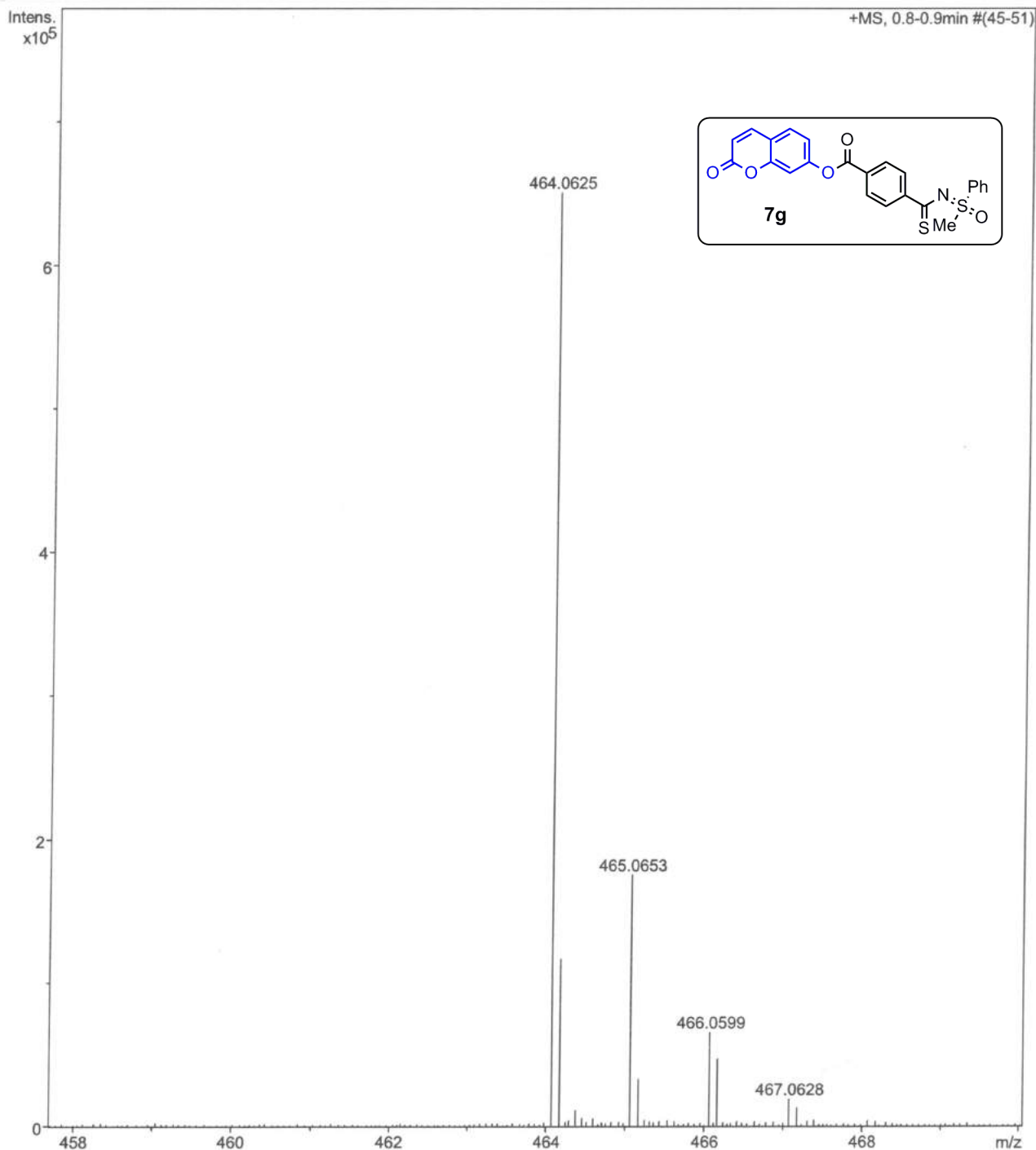
Analysis Name D:\Data\2020\PROF.AKS\MAR\SRS-8-9.d
Method tune_low_Pos-R2.m
Sample Name SRS-8-9
Comment

Acquisition Date 3/18/2020 4:37:14 PM

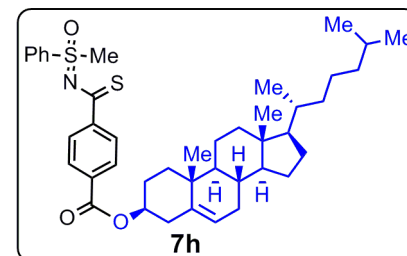
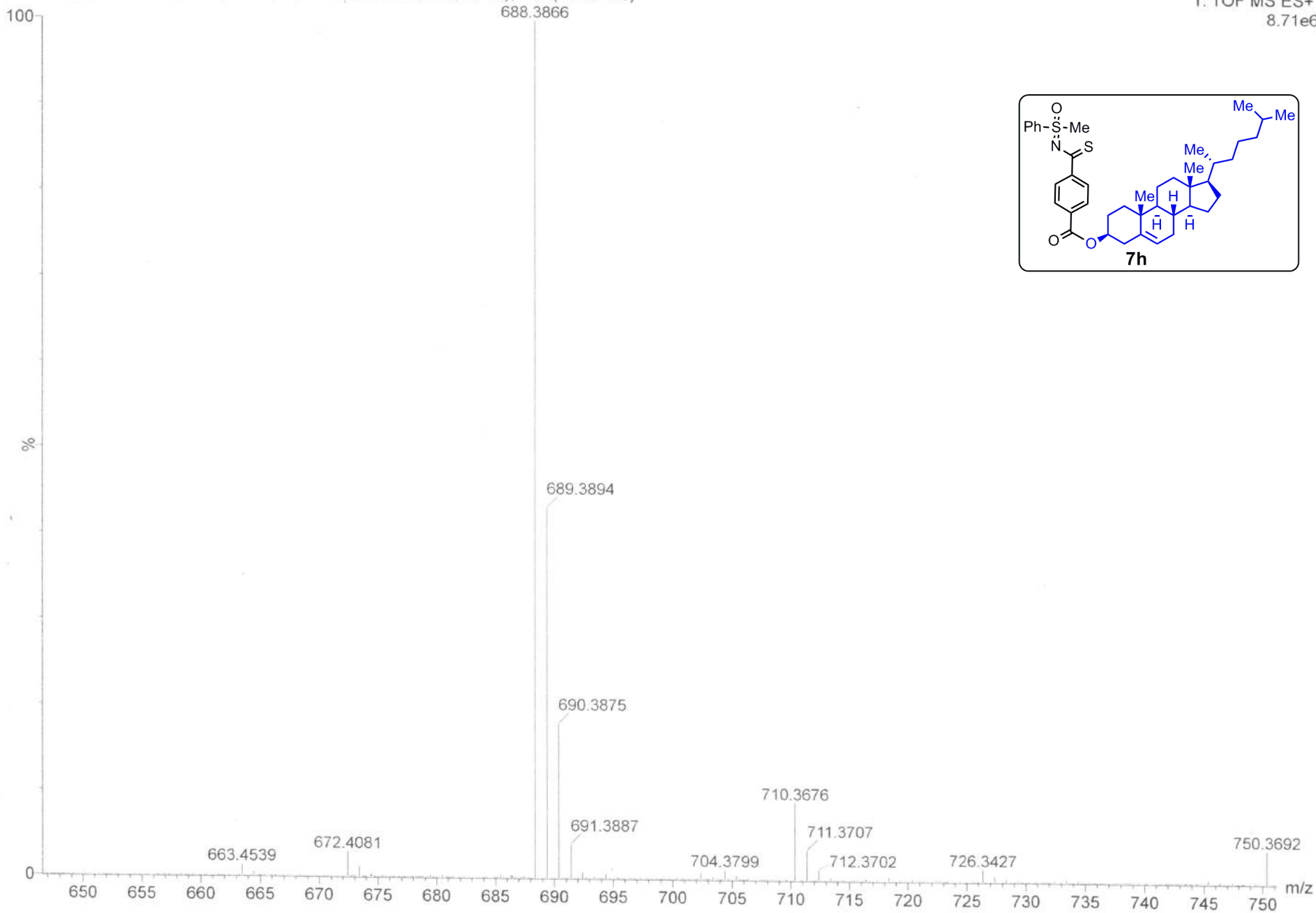
Operator UOH-Chemistry
Instrument maXis 10138

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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



10112020_24 +VE 15 (0.165) AM2 (Ar,22000,0,556.28,0.00,LS 10); Cm (15:19-1:5)

1: TOF MS ES+
8.71e6

Display Report

Analysis Info

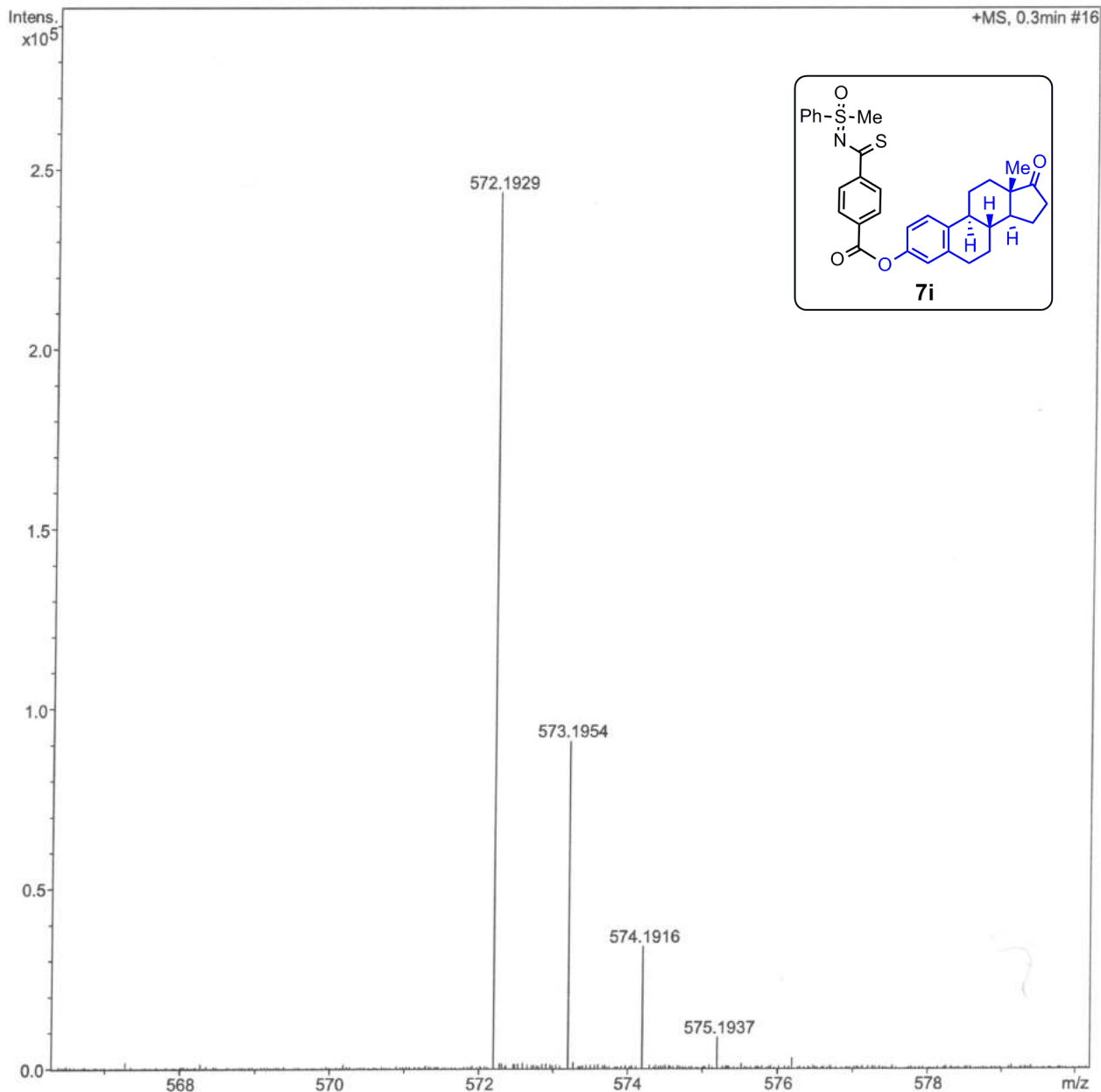
Analysis Name D:\Data\2020\PROF.AKS\MAR\SRS-8-85R.d
Method tune_low_Pos-R2.m
Sample Name SRS-8-85
Comment

Acquisition Date 3/16/2020 4:06:24 PM

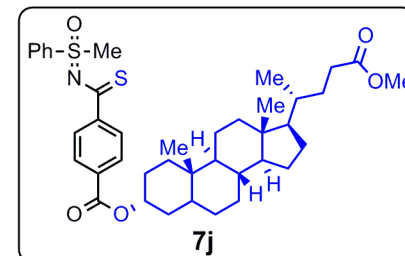
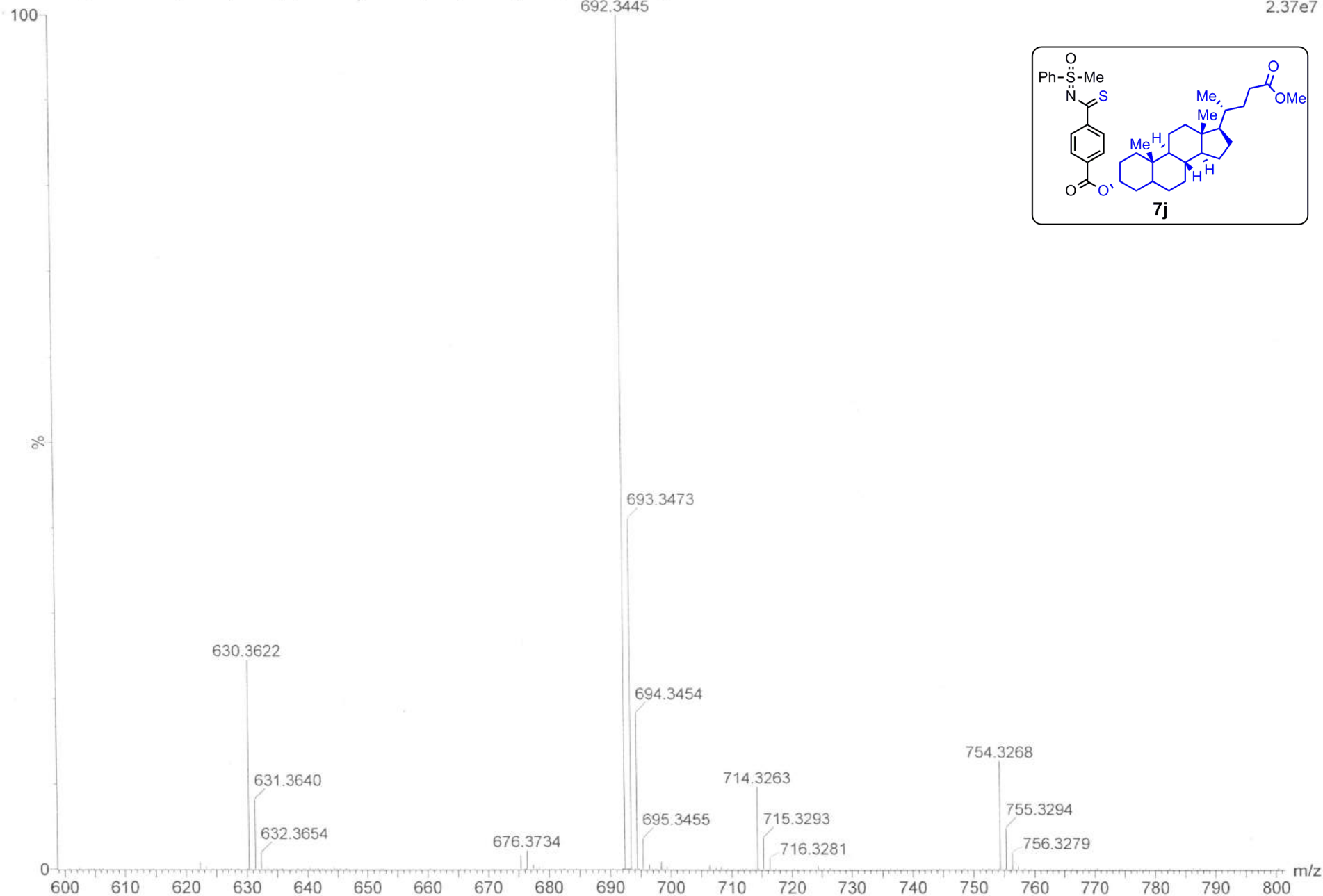
Operator UOH-Chemistry
Instrument maXis 10138

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	2580 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



22102020_04 +VE 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:30-96:145)

1: TOF MS ES+
2.37e7

Display Report

Analysis Info

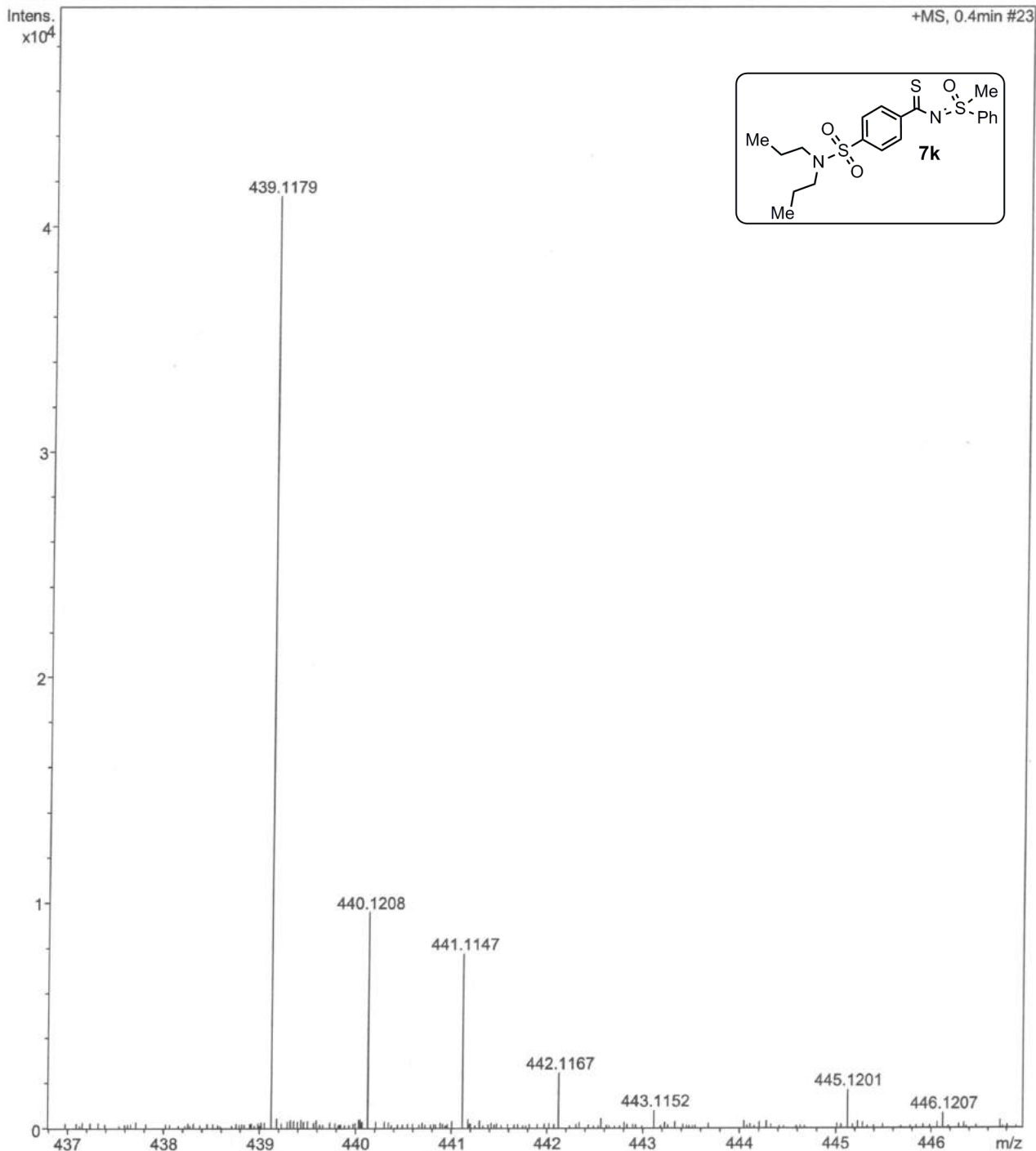
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-PROBIN-R.d
Method tune_low.m
Sample Name MJ-17-PROBIN
Comment

Acquisition Date 3/19/2020 12:15:27 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	10.2 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

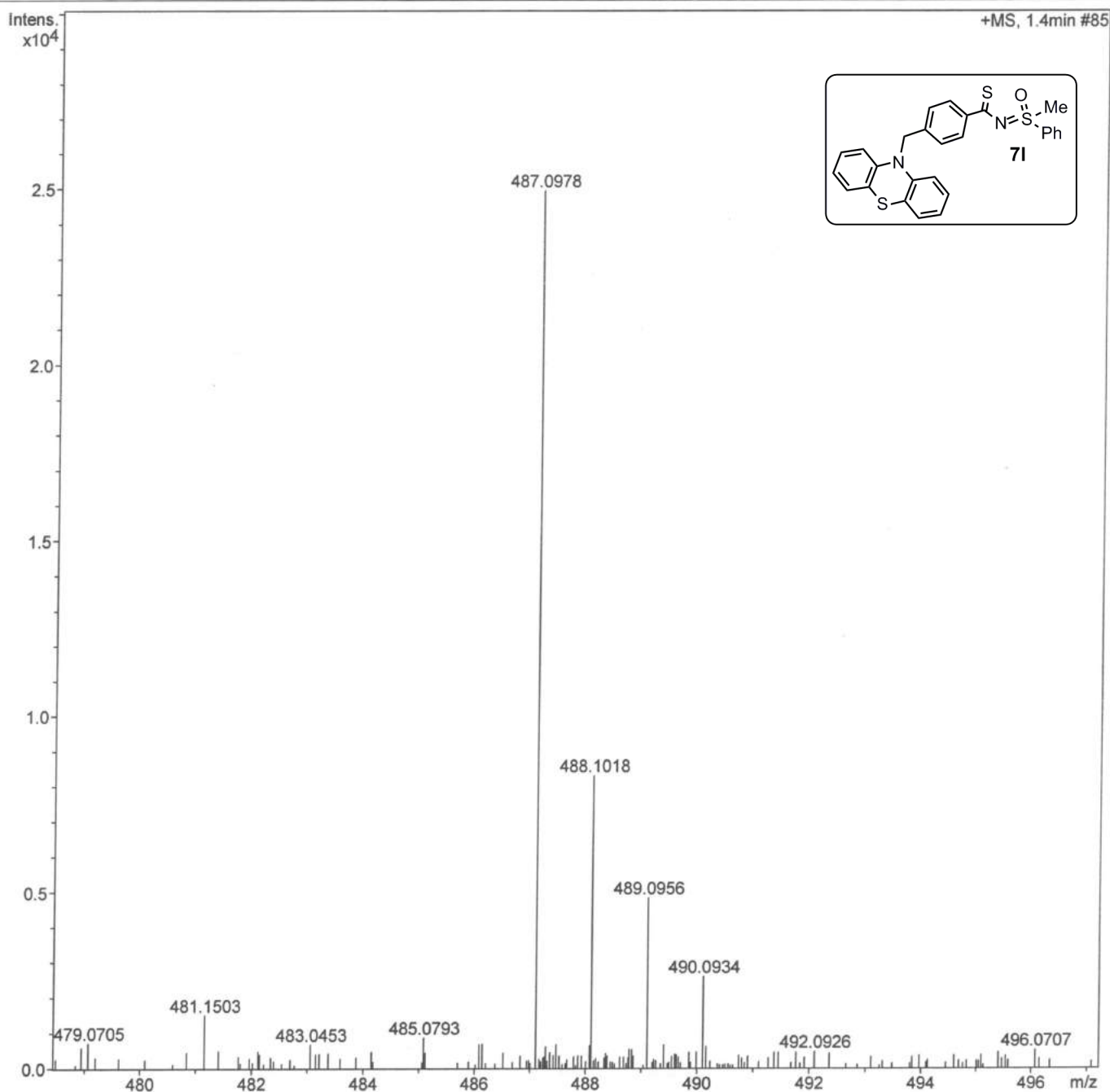
Analysis Name D:\Data\2020\PROF.AKS\MAR\SRS-8-92R.d
Method tune_low.m
Sample Name SRS-8-92
Comment

Acquisition Date 3/16/2020 3:43:10 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

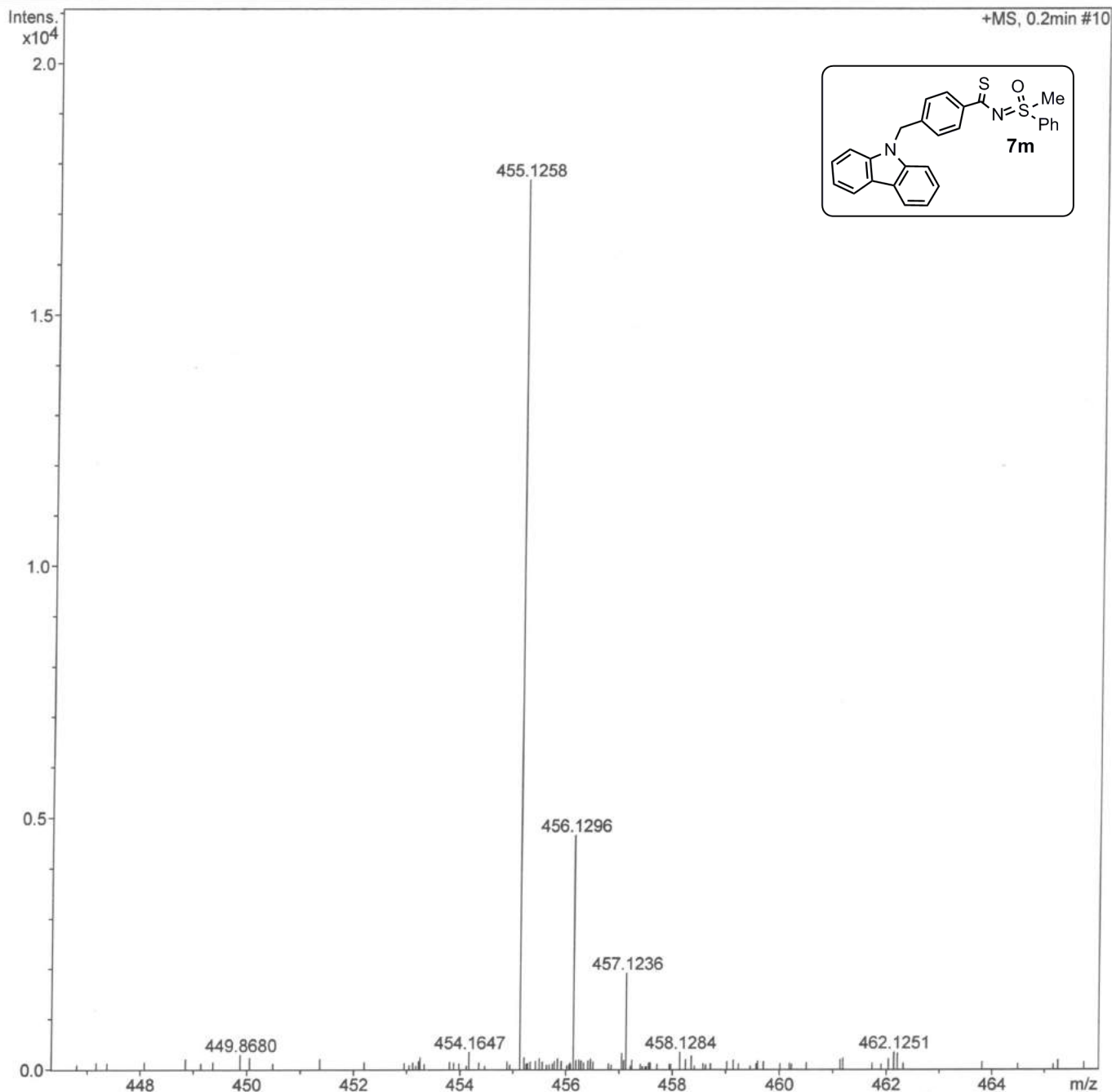
Analysis Name D:\Data\2020\PROF.AKS\MAR\8-90.d
Method tune_low.m
Sample Name 8-90
Comment

Acquisition Date 3/16/2020 3:31:43 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\OCTAS-179R.d
Method tune_low_Pos.m
Sample Name AS-179
Comment

Acquisition Date 10/30/2019 12:20:55 AM

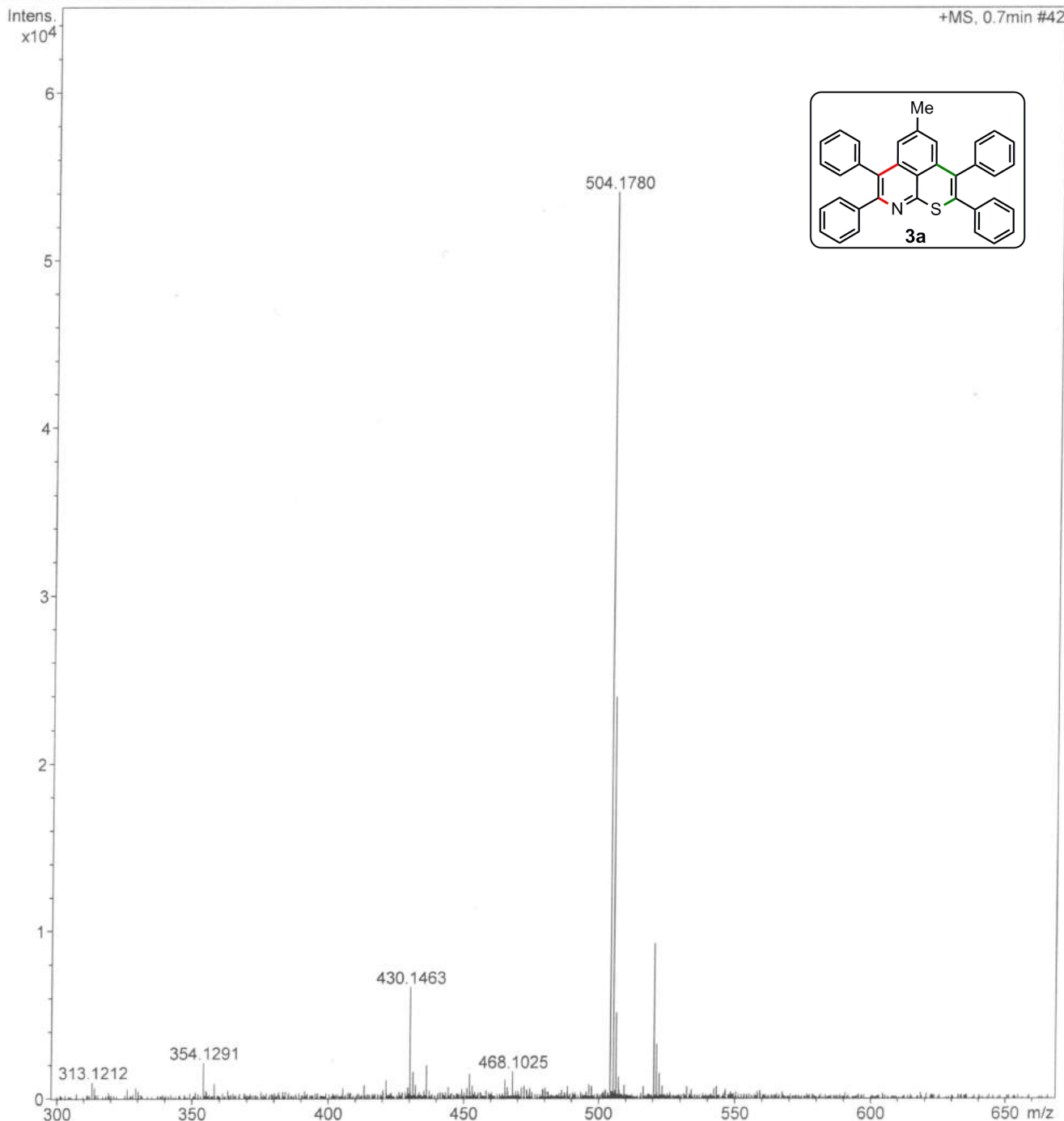
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

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

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste



Display Report

Analysis Info

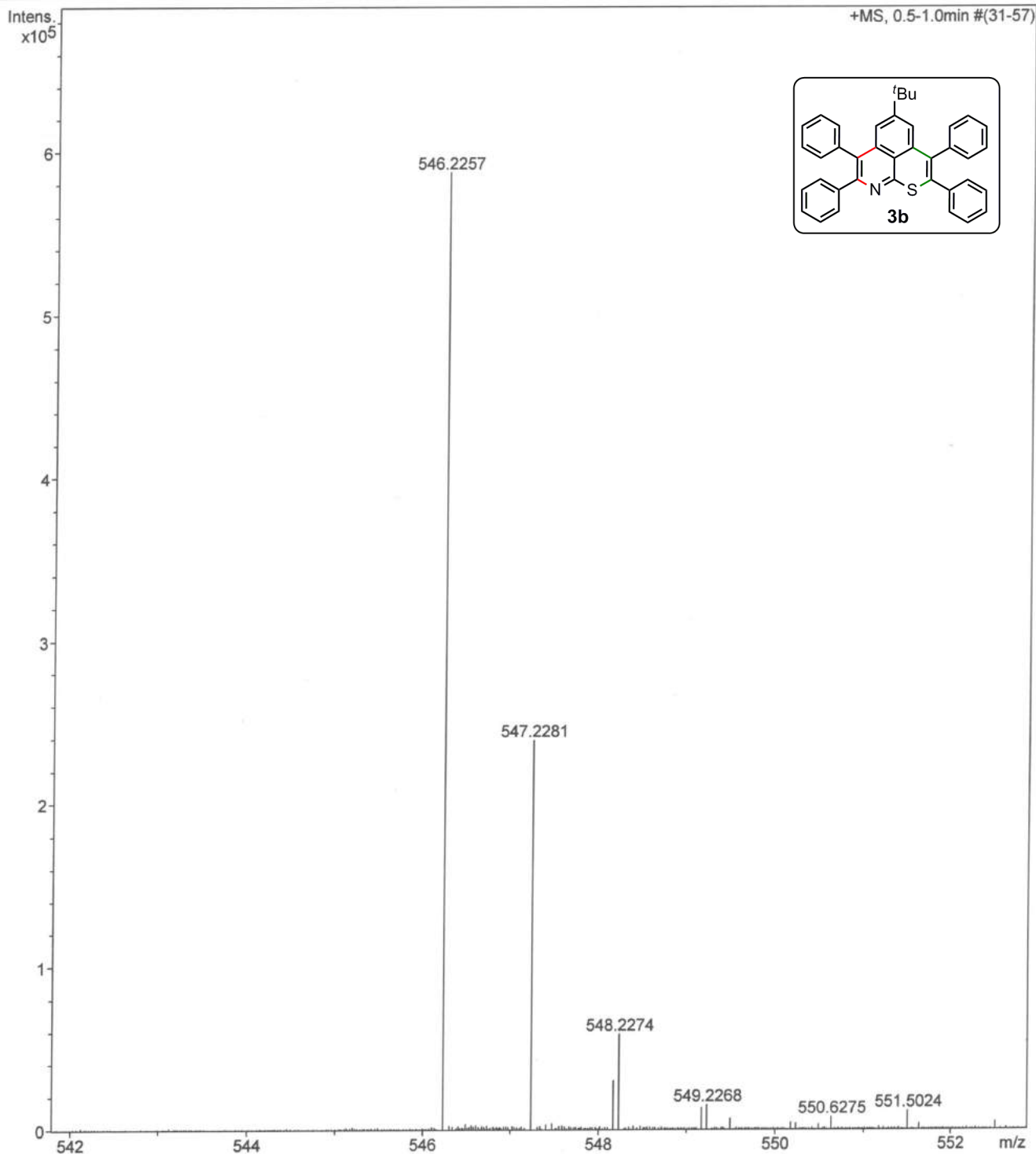
Analysis Name D:\Data\2019\PROF. AKS\OCT\SRS-1-378.d
Method tune_low.m
Sample Name SRS-1-378-DCM-MEOH
Comment

Acquisition Date 10/9/2019 4:16:53 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\NOVAS-320R1.d
Method TL-P.m
Sample Name AS-320
Comment

Acquisition Date 11/8/2019 3:52:17 AM

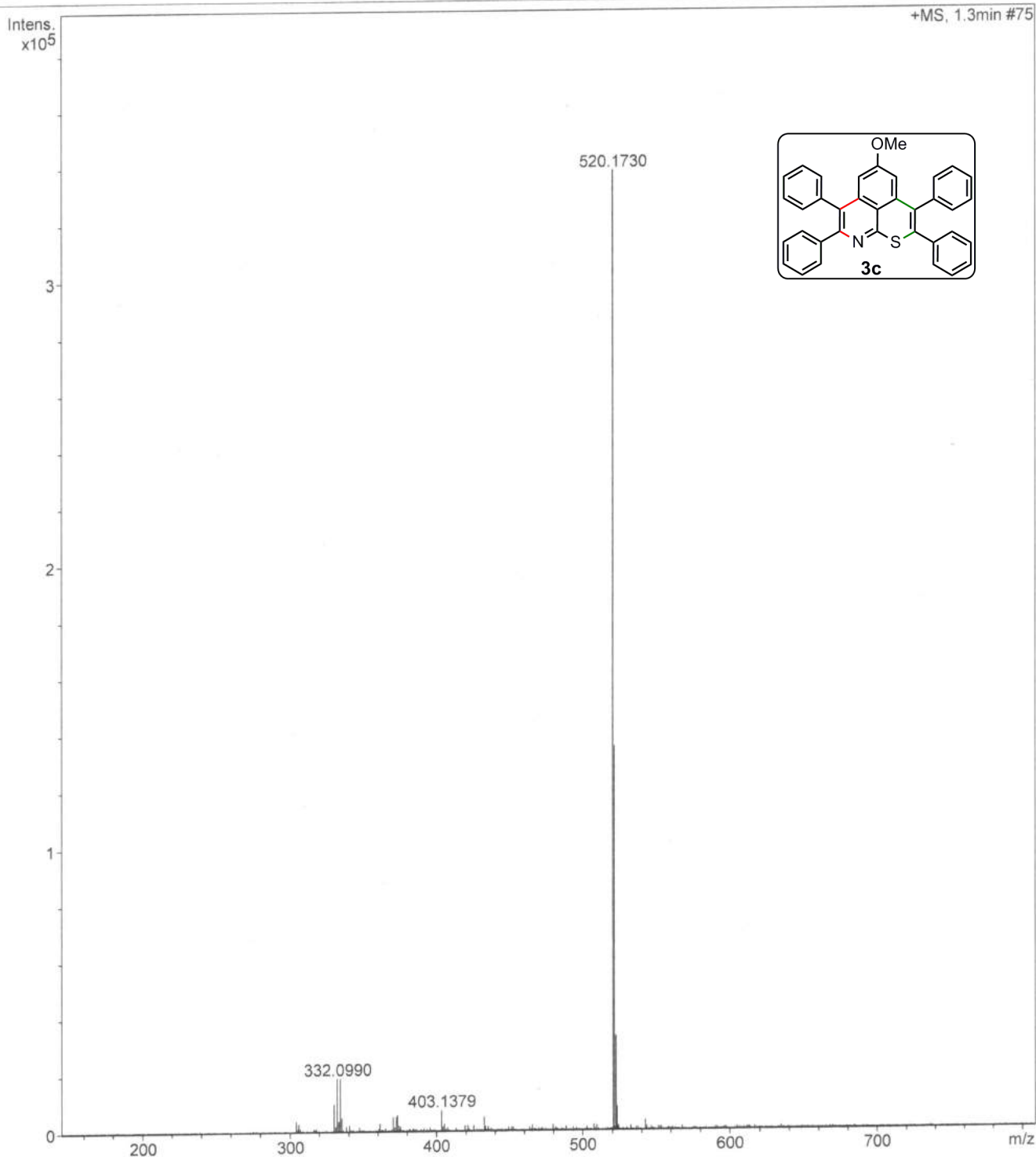
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 900 m/z

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

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\OCTAS-216R.d
Method TL-P.m
Sample Name AS-216
Comment

Acquisition Date 10/30/2019 1:32:05 AM

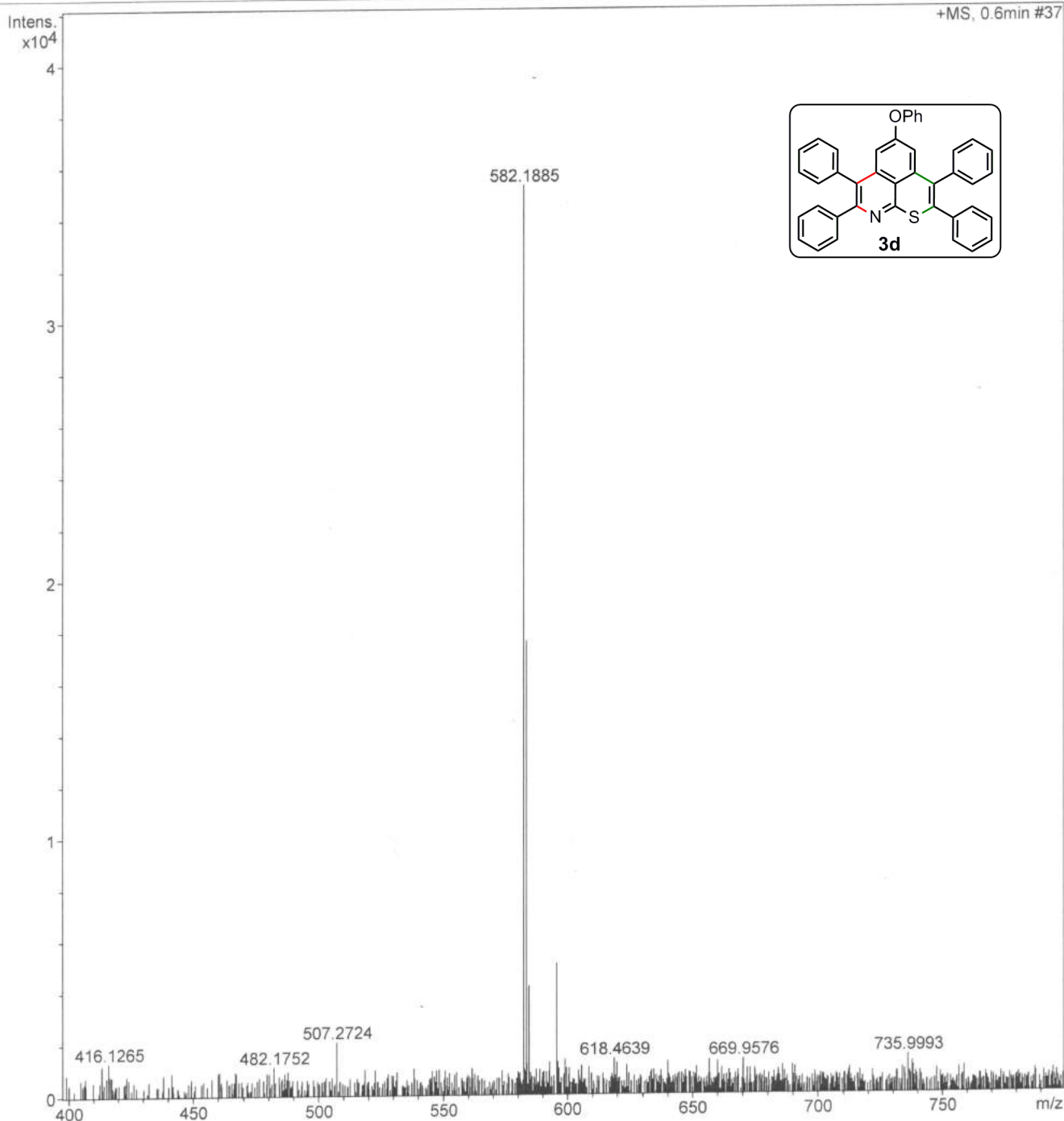
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 800 m/z

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

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



Display Report

Analysis Info

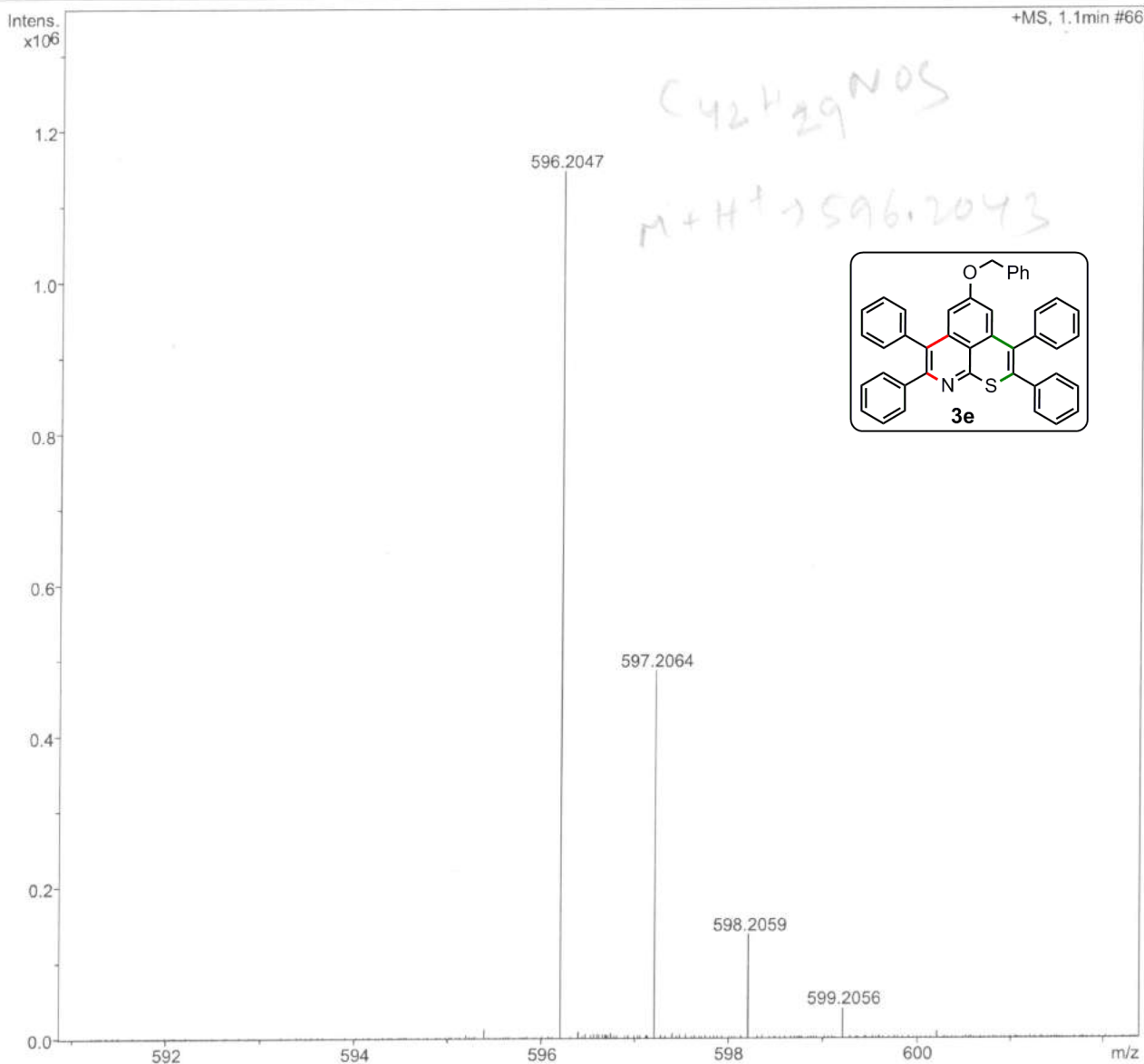
Analysis Name D:\Data\2019\PROF. AKS\OCT\As-324R.d
Method tune_low_PosR.m
Sample Name AS-324
Comment

Acquisition Date 10/28/2019 11:14:35 PM

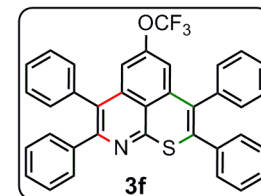
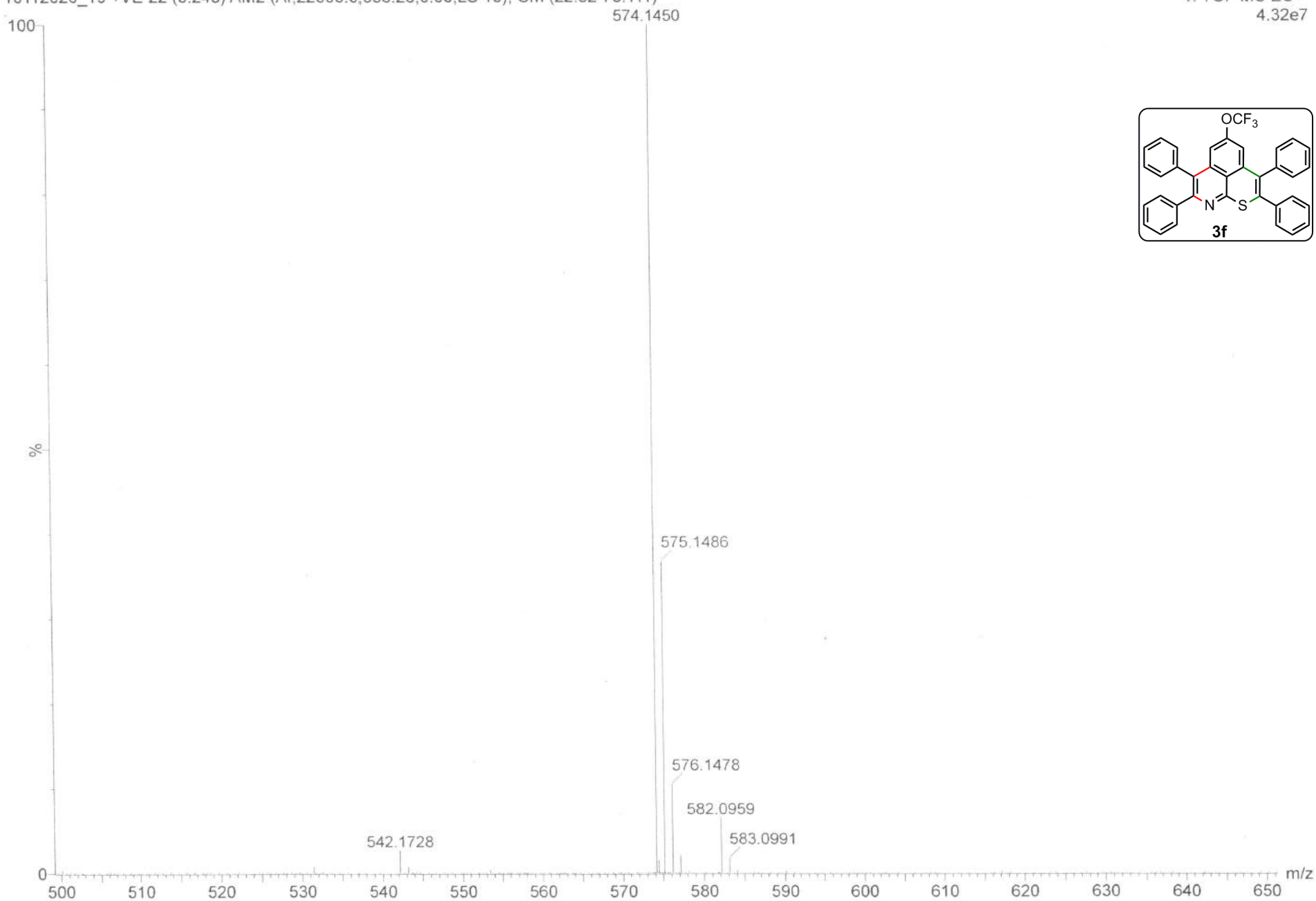
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



10112020_19 +VE 22 (0.245) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (22:32-73:111)

1: TOF MS ES+
4.32e7

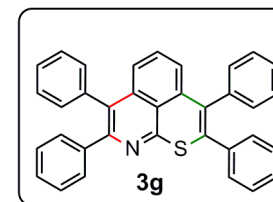
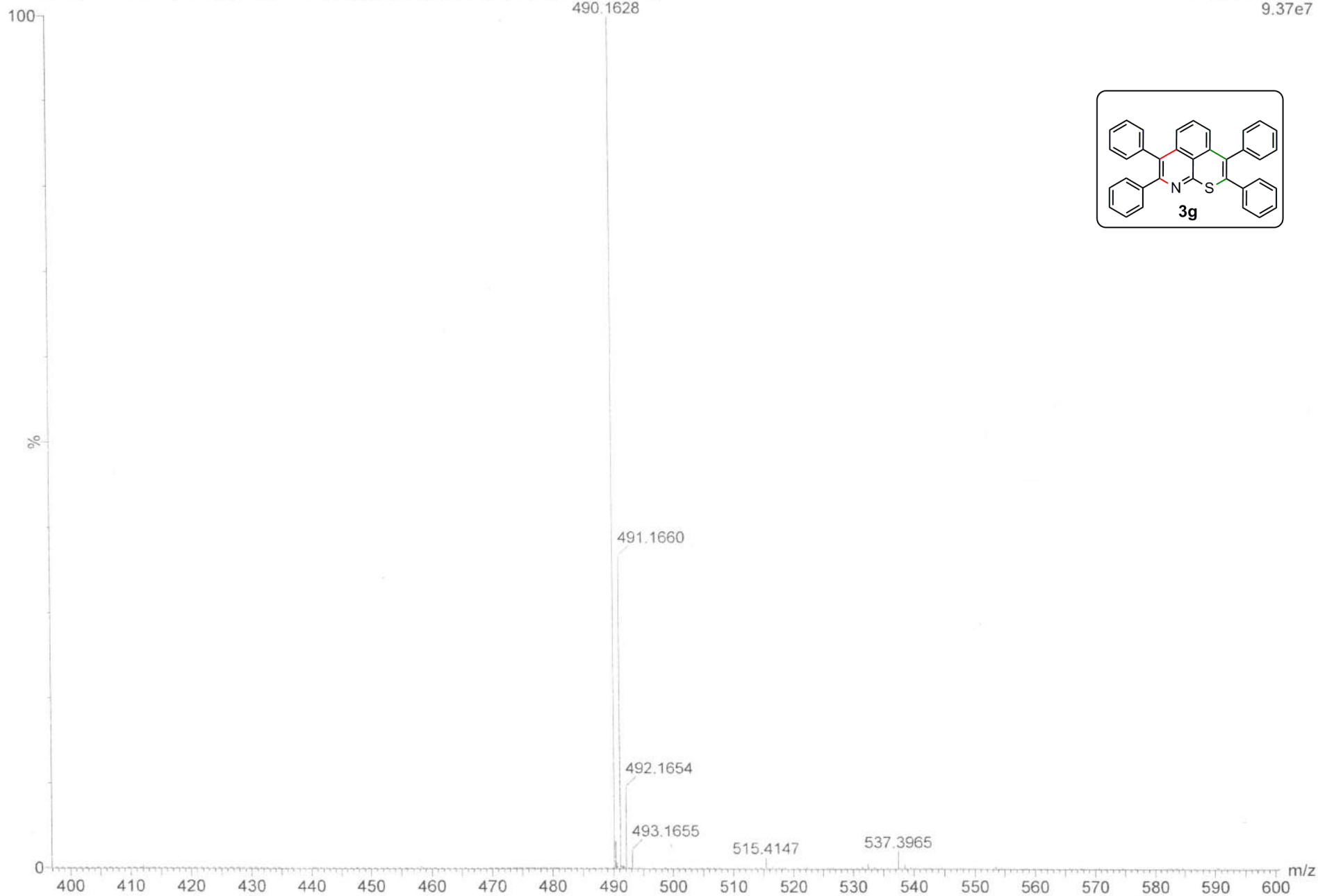
MJ-510

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ACRHEM
XEVO-G2XSQTOF#YEA1155

10-Nov-2020
15:24:32

10112020_22 +VE 21 (0.236) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (21:32-85:122)

1: TOF MS ES+
9.37e7



Display Report

Analysis Info

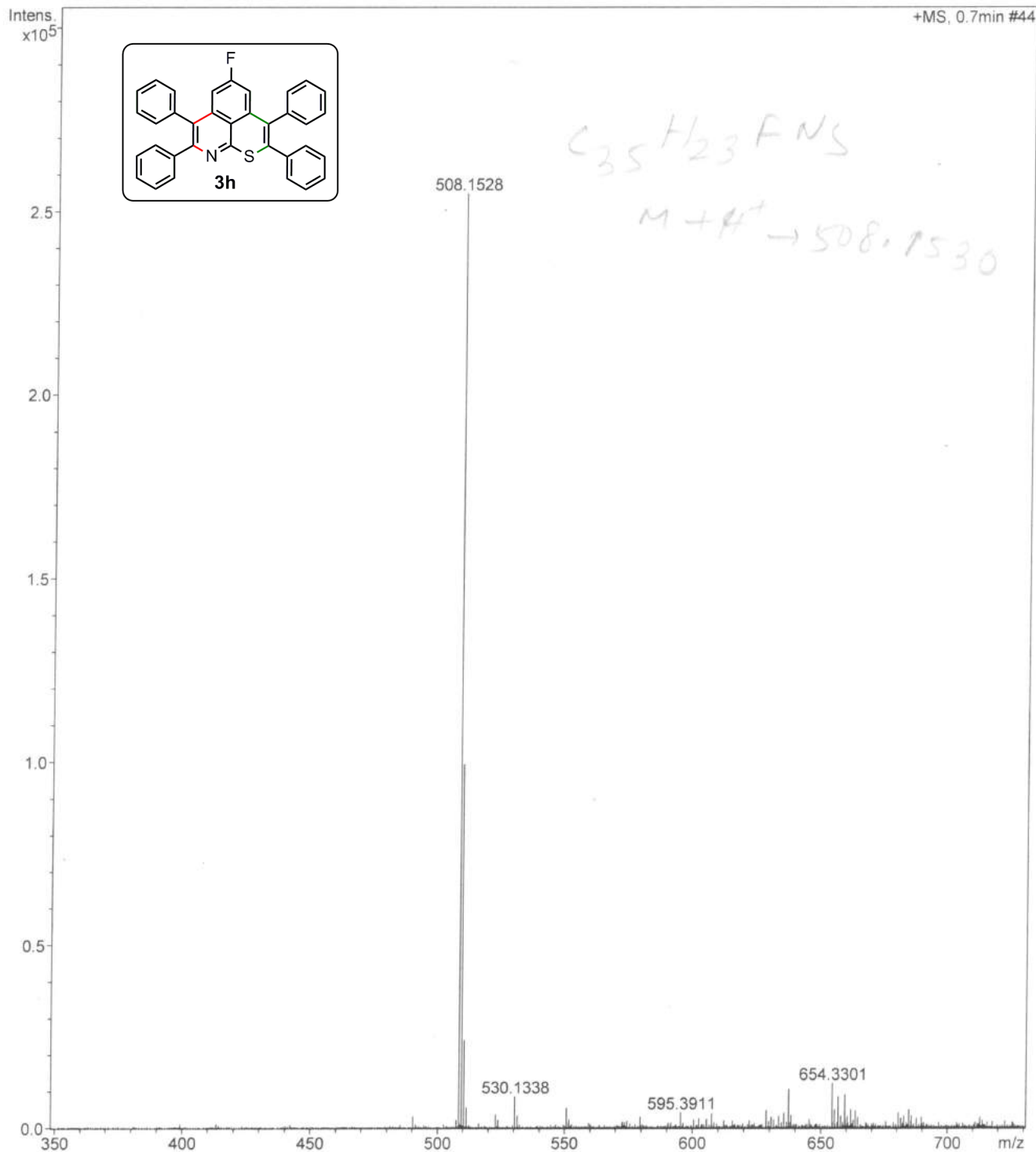
Analysis Name D:\Data\2019\PROF. AKS\NOVAS-322.d
Method tune_low.m
Sample Name AS-322
Comment

Acquisition Date 11/5/2019 12:10:24 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\OCTAS-217R.d
Method tune_low_Pos.m
Sample Name AS-217
Comment

Acquisition Date 10/30/2019 12:51:49 AM

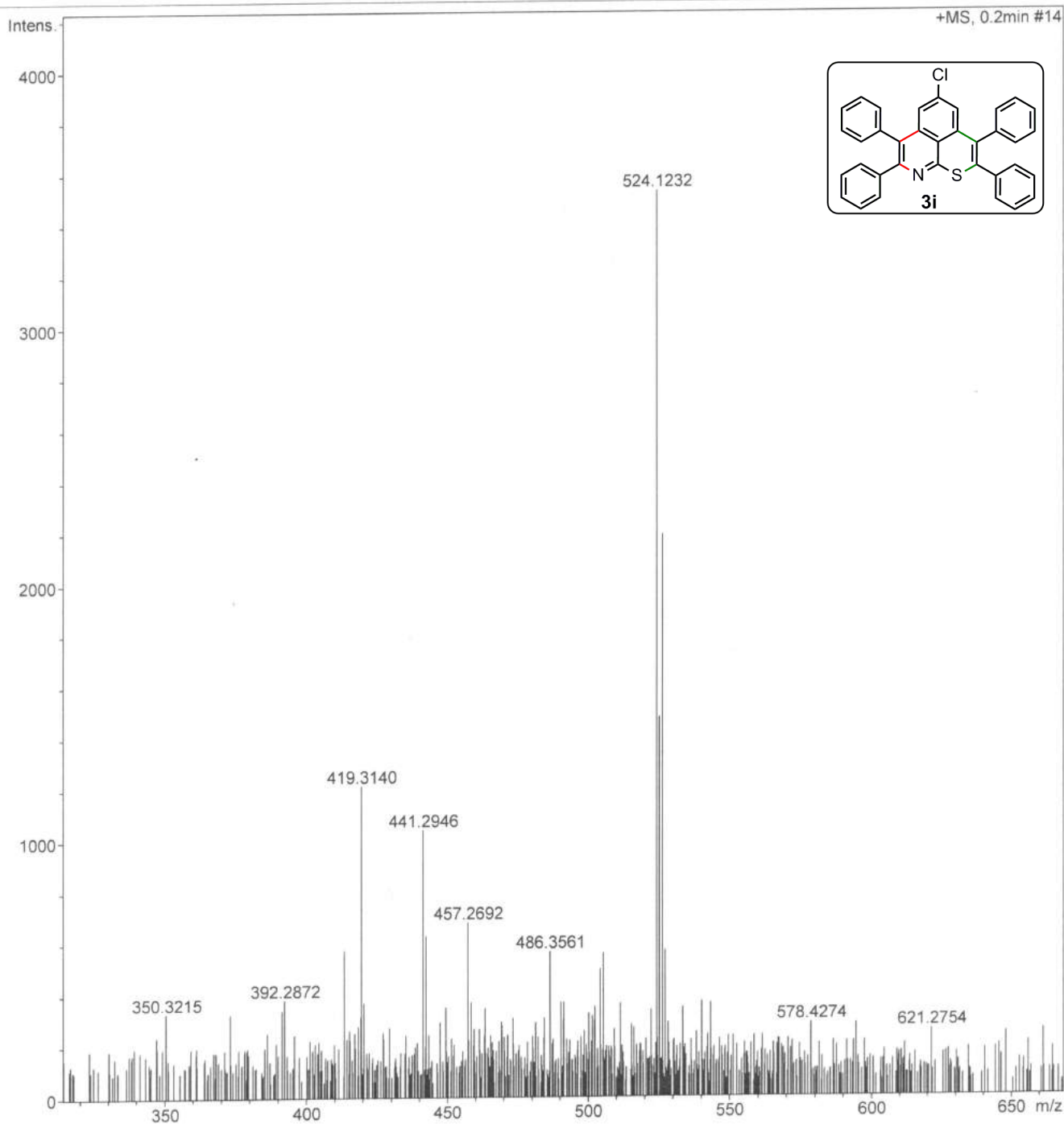
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

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

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\NOVAS-319r.d
Method TL-P.m
Sample Name AS-321
Comment

Acquisition Date 11/8/2019 4:11:59 AM

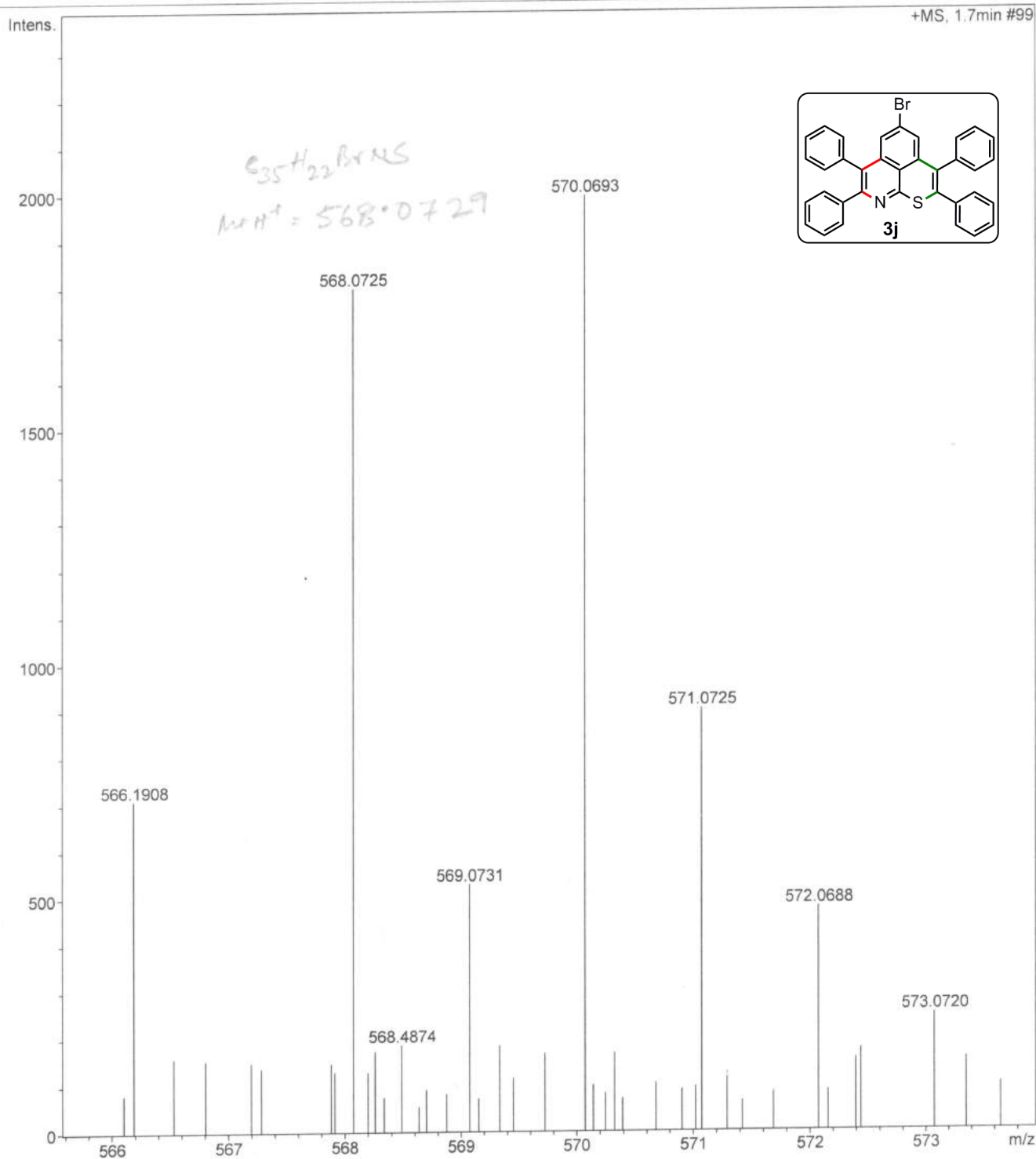
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

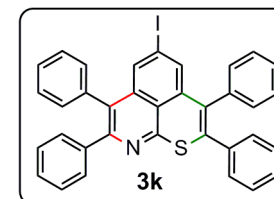
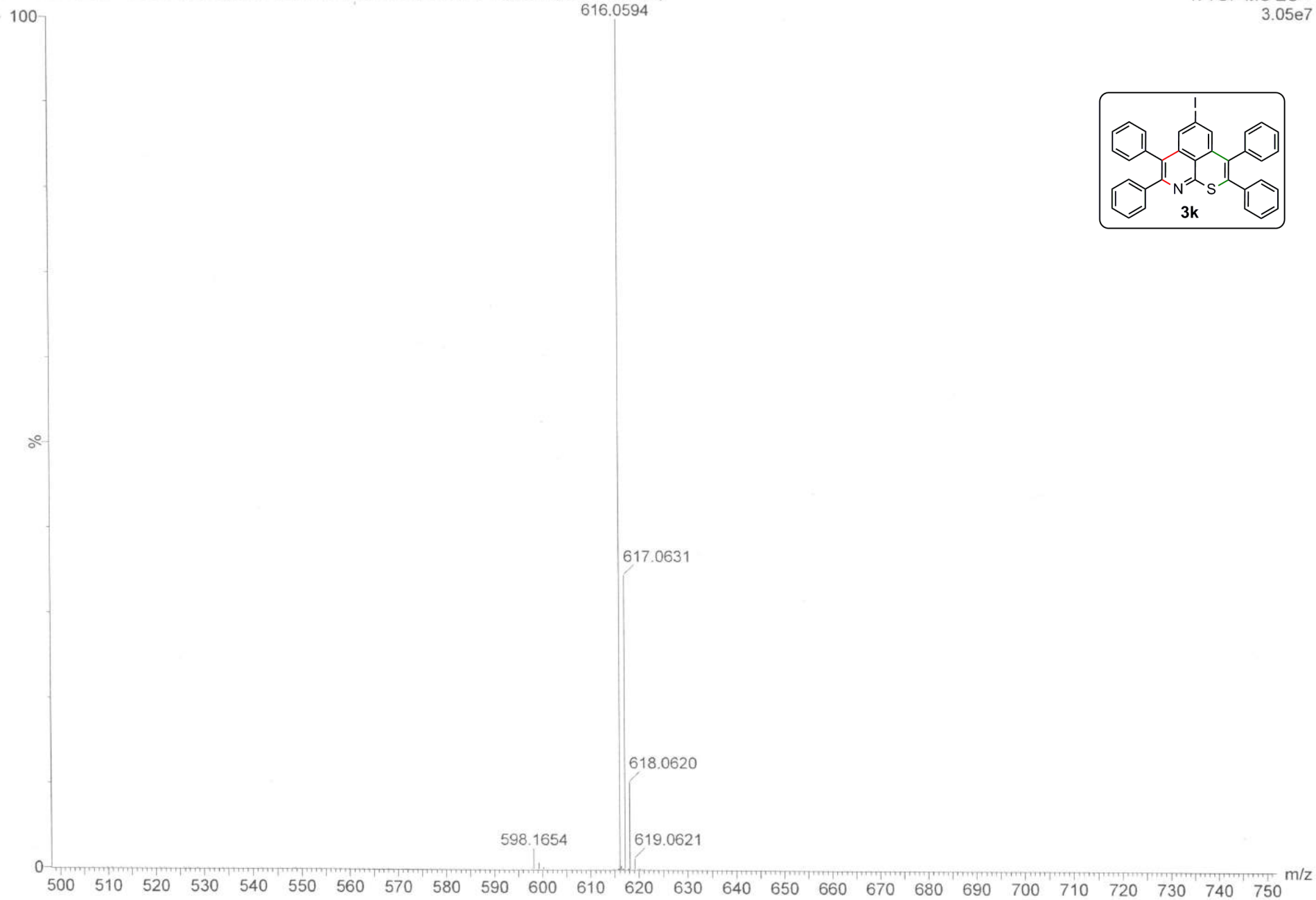
Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 900 m/z

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



20102020_30 +VE 36 (0.365) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (36:49-96:155)

1: TOF MS ES+
3.05e7

Display Report

Analysis Info

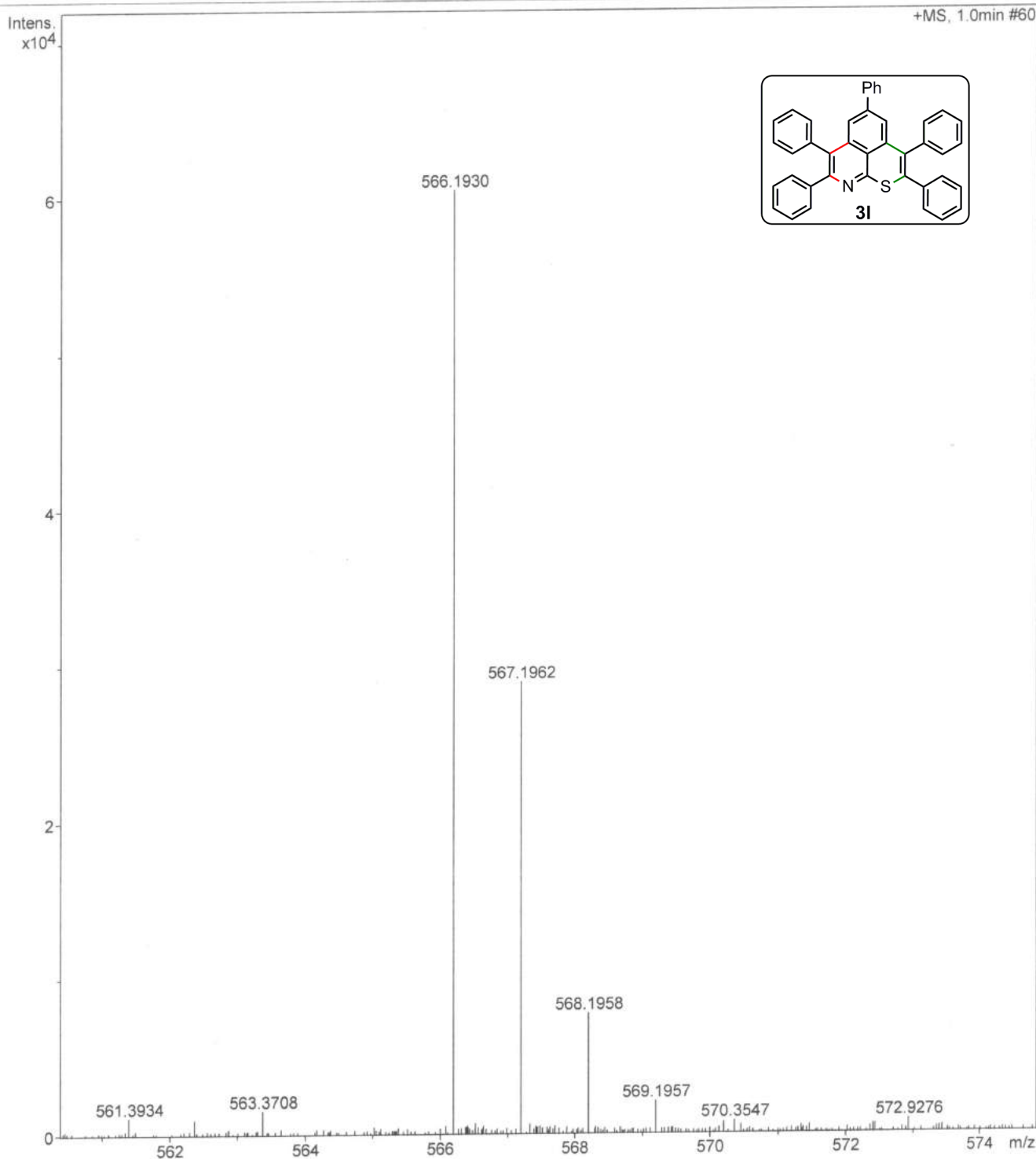
Analysis Name D:\Data\2019\PROF. AKS\NOVAS-321R.d
Method TL-P.m
Sample Name AS-321
Comment

Acquisition Date 11/8/2019 4:01:56 AM

Operator UOH-Chemistry
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	900 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Analysis Info

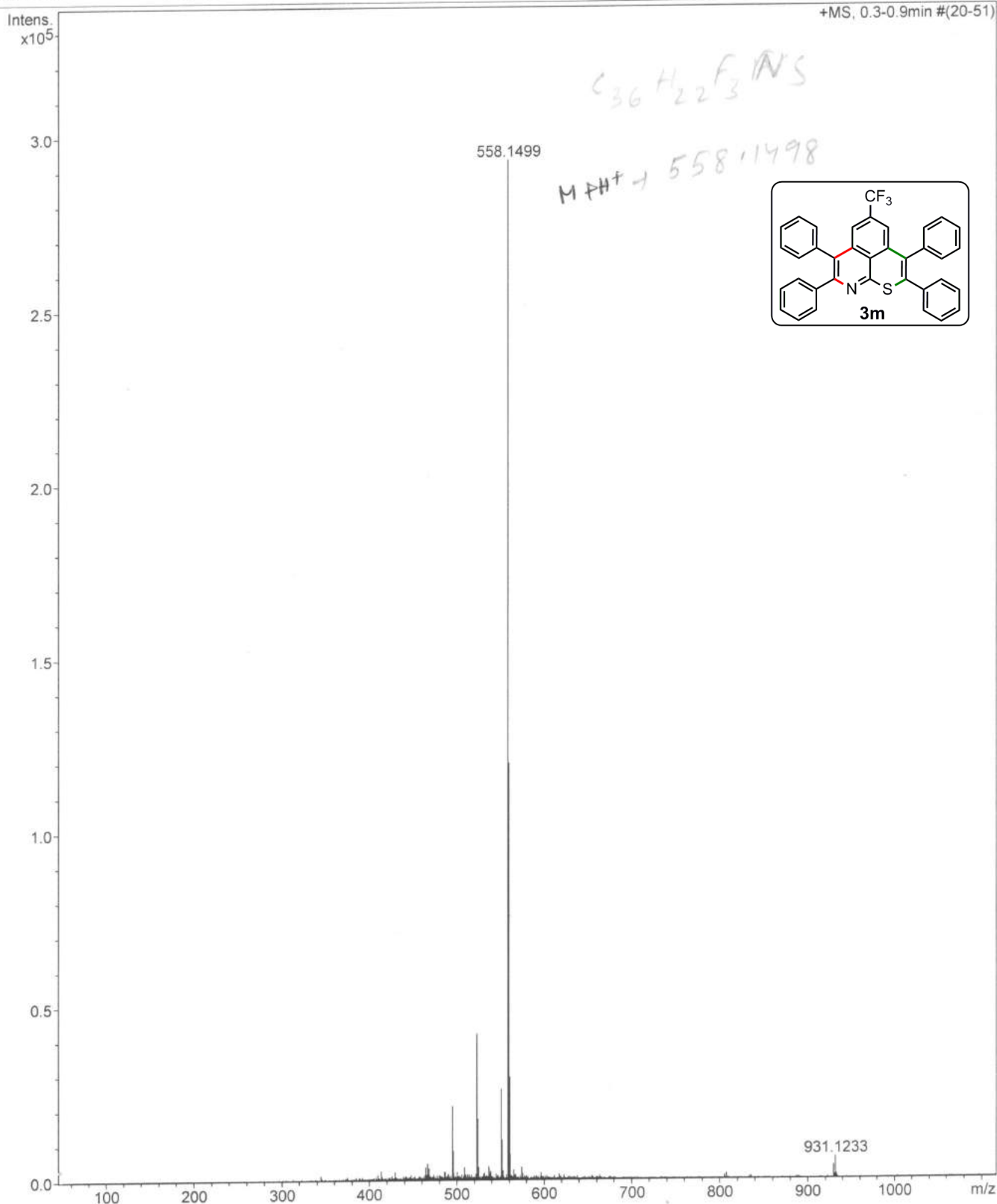
Analysis Name D:\Data\2019\PROF. AKS\OCTAS-170-2.d
 Method tune_low.m
 Sample Name AS-170
 Comment

Acquisition Date 10/30/2019 6:23:50 AM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\OCTAS-169R.d
Method tune_low_Pos.m
Sample Name AS-169
Comment

Acquisition Date 10/30/2019 1:01:19 AM

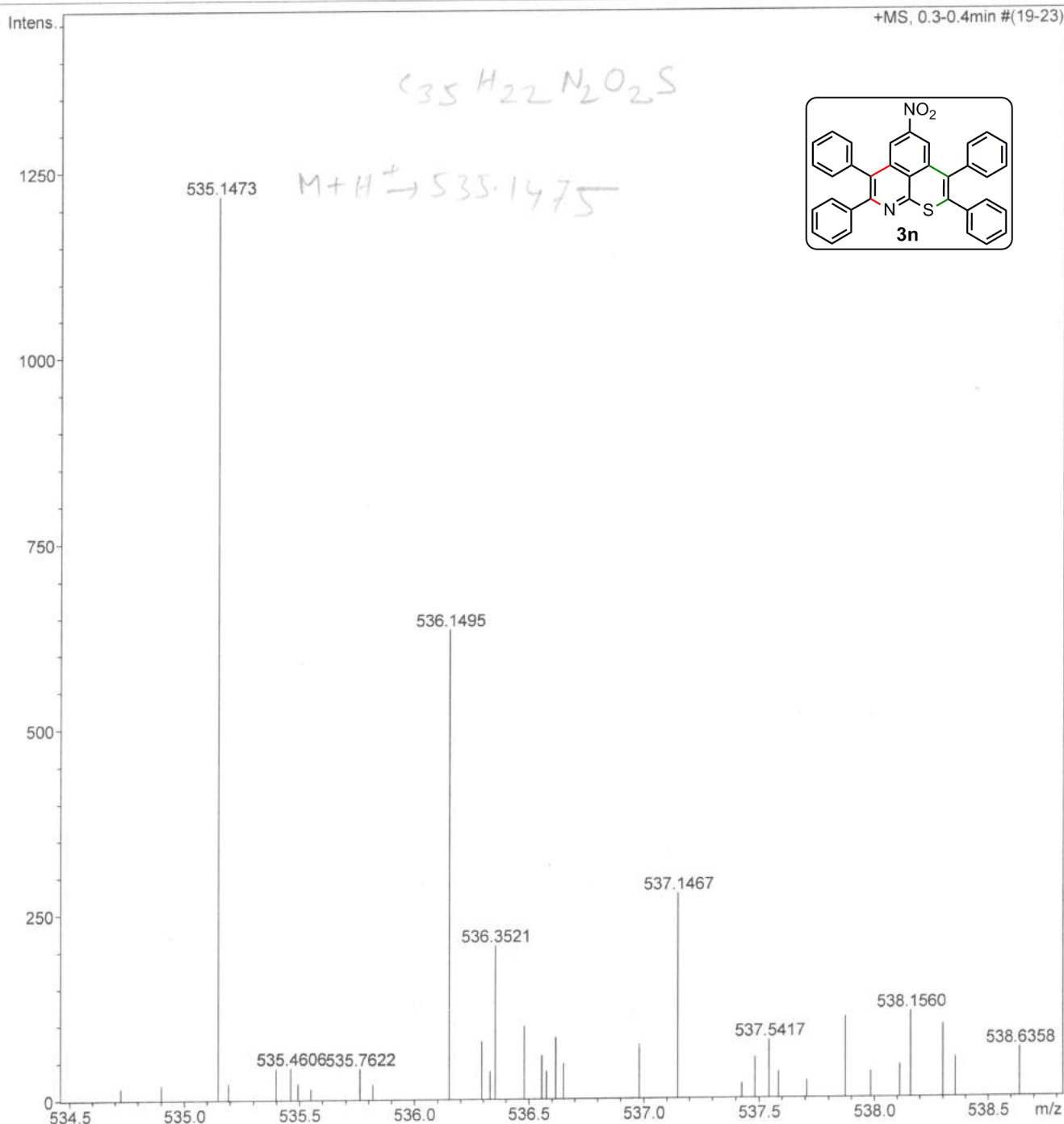
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

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

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 6.0 l/min
Set Divert Valve Waste



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

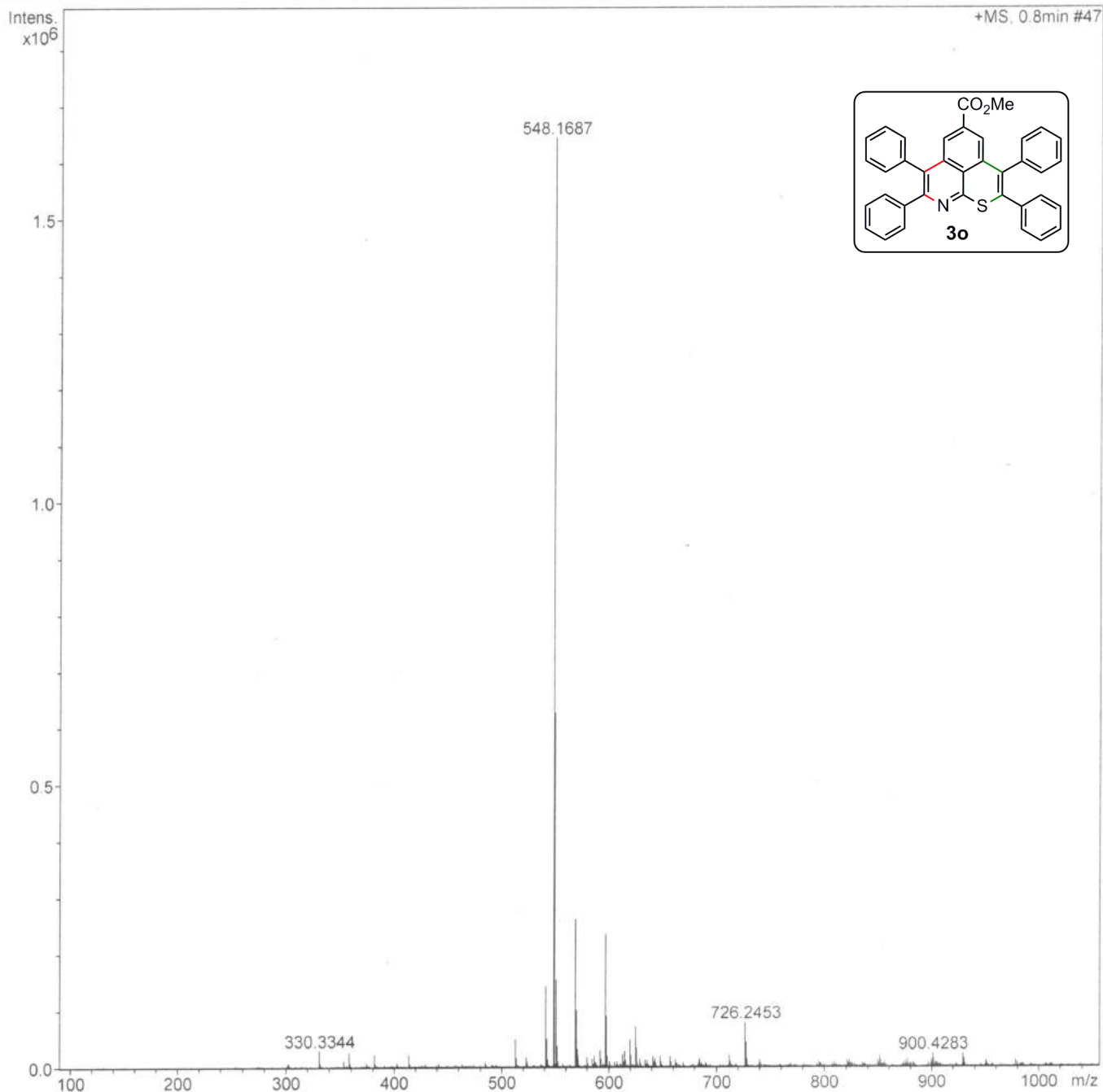
Analysis Name D:\Data\2019\PROF.TJ\JAN\AG-3-113.d
 Method tune_low.m
 Sample Name AG-3-113
 Comment

Acquisition Date 1/8/2019 5:02:17 PM

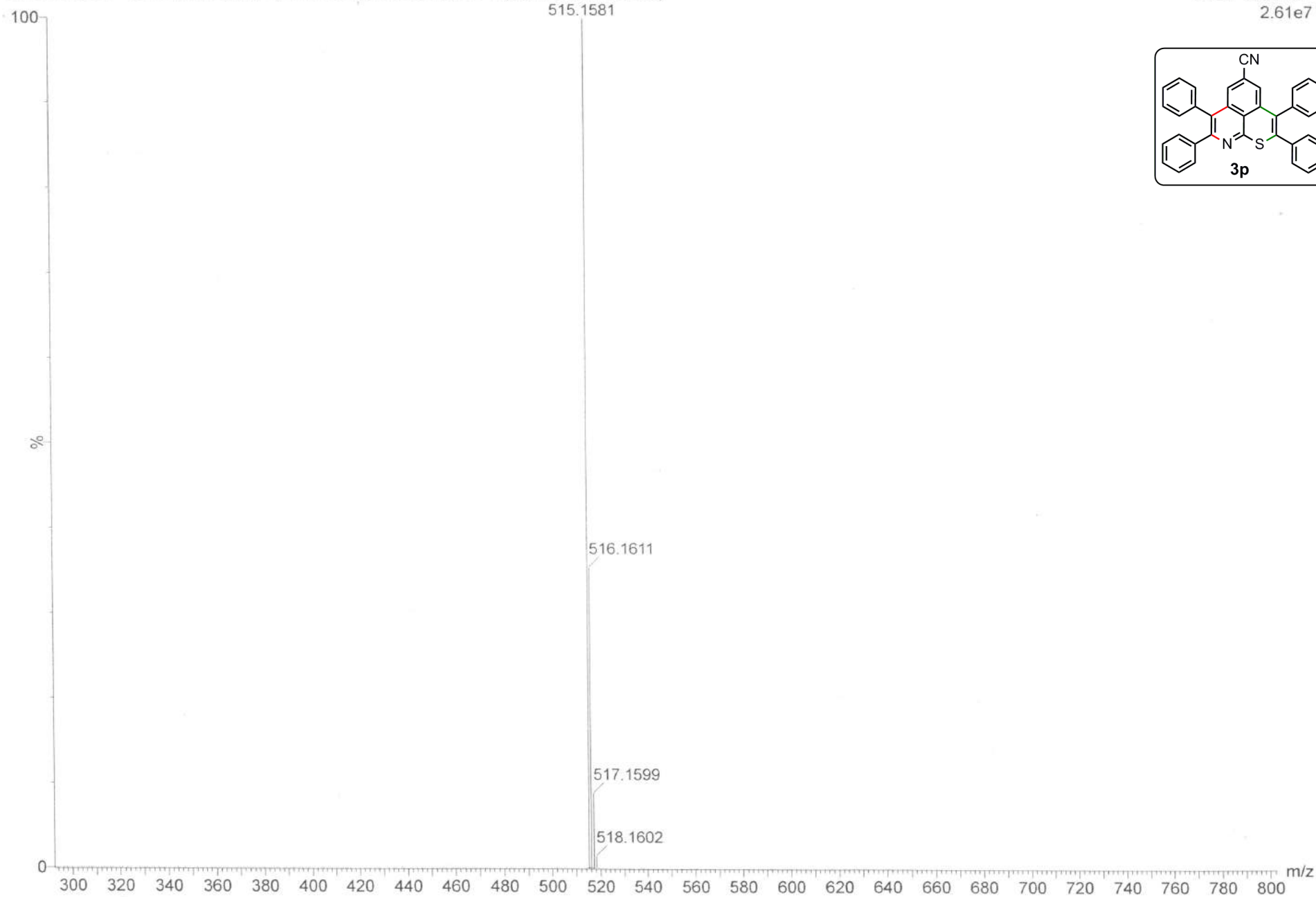
Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



21102020_13 +VE 20 (0.228) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (20:32-75:138)

1: TOF MS ES+
2.61e7

MJ-17-214

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XEVO-G2XSQTOF#YEA1155

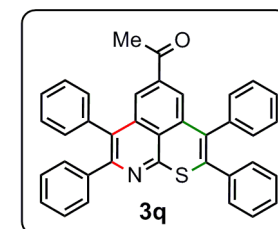
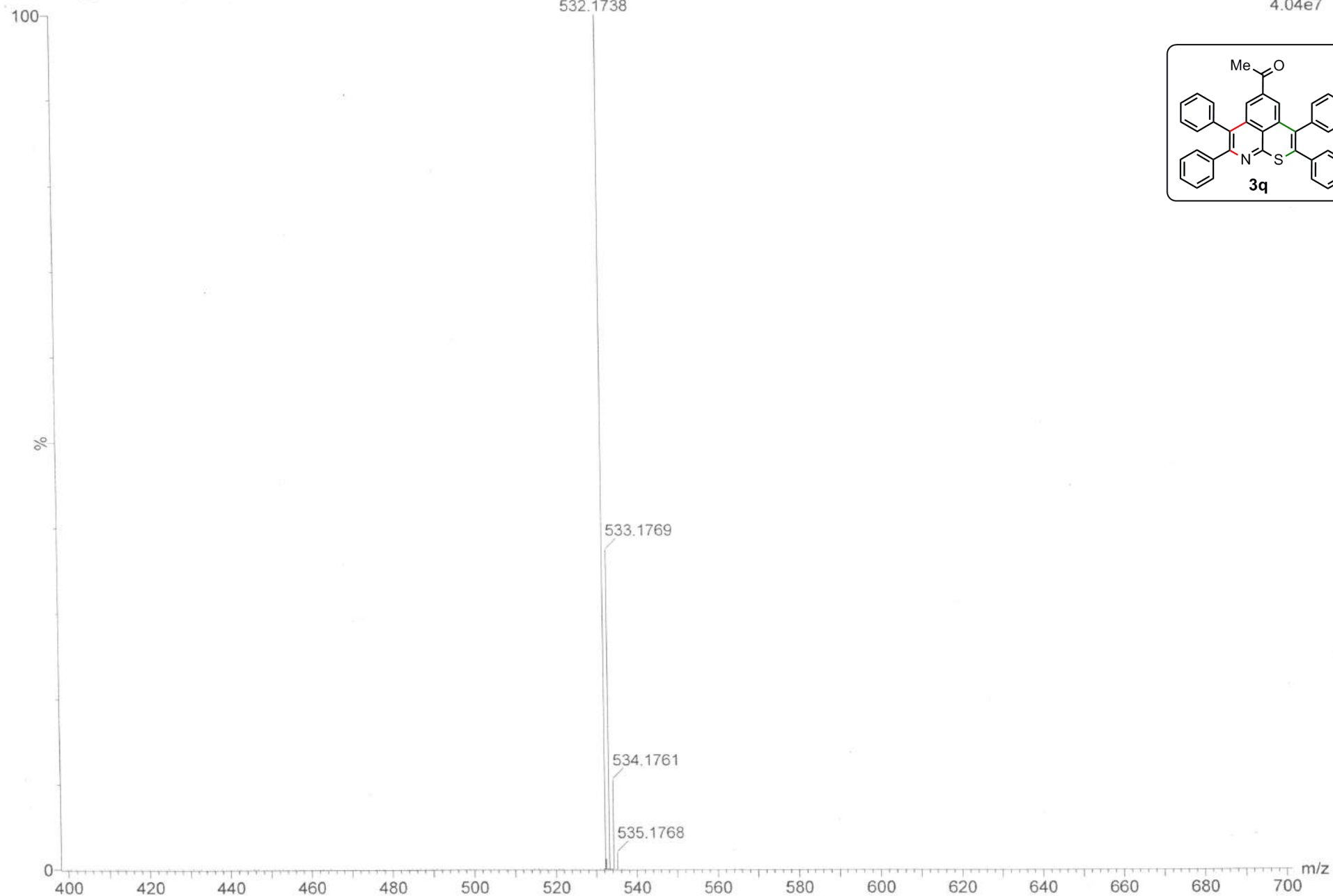
20-Oct-2020

15:15:11

20102020_31 +VE 27 (0.288) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (27:38-83:143)

1: TOF MS ES+

4.04e7



MJ-17-160

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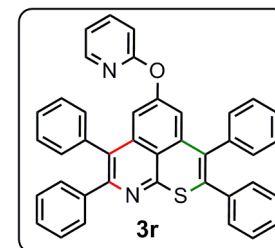
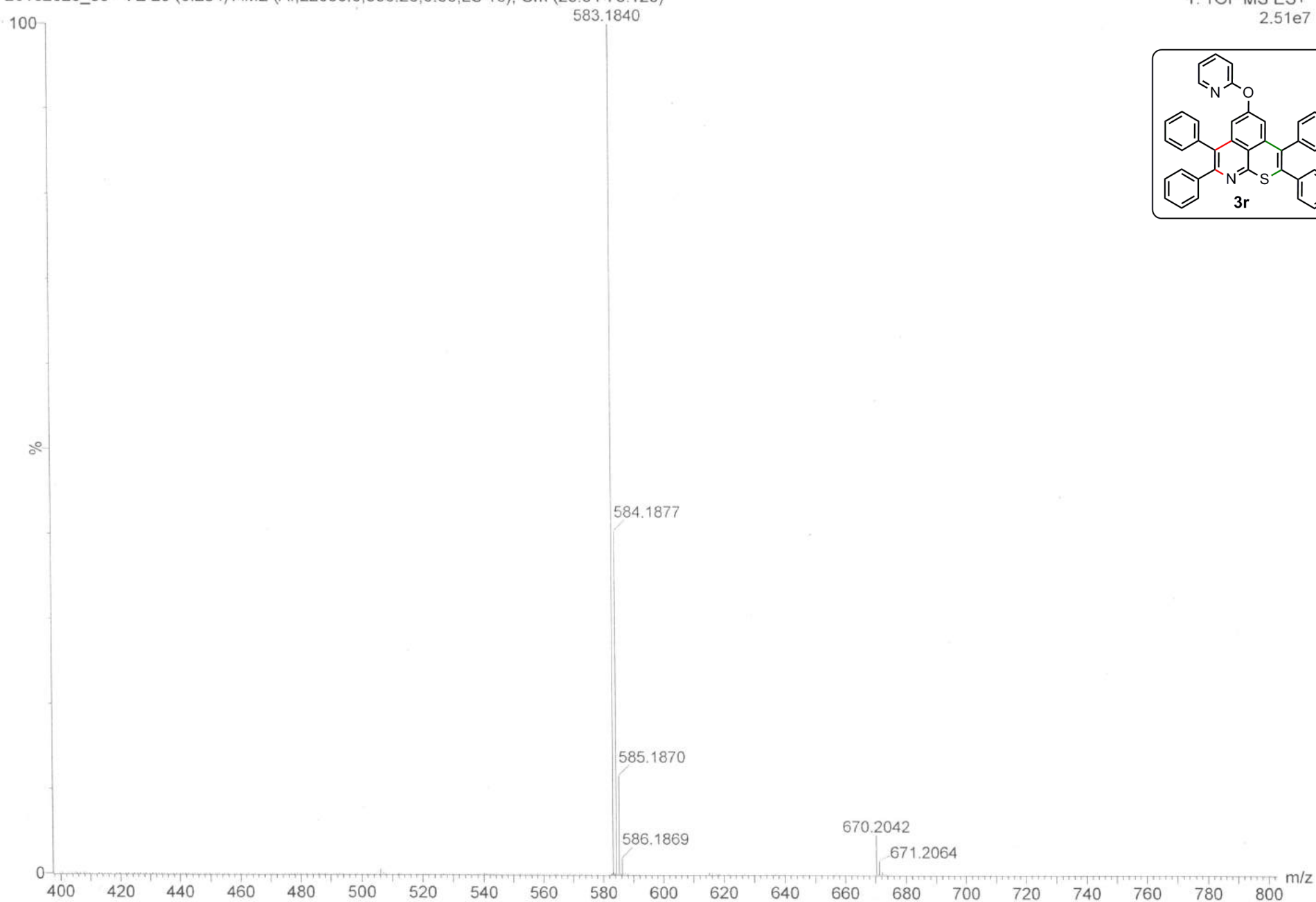
XEVO-G2XSQTOF#YEA1155

20-Oct-2020

15:25:57

20102020_35 +VE 23 (0.254) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (23:34-73:120)

1: TOF MS ES+
2.51e7



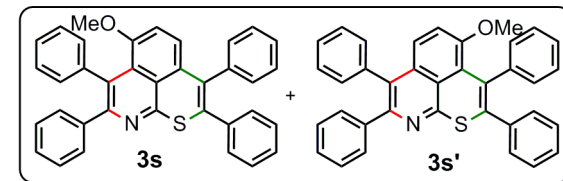
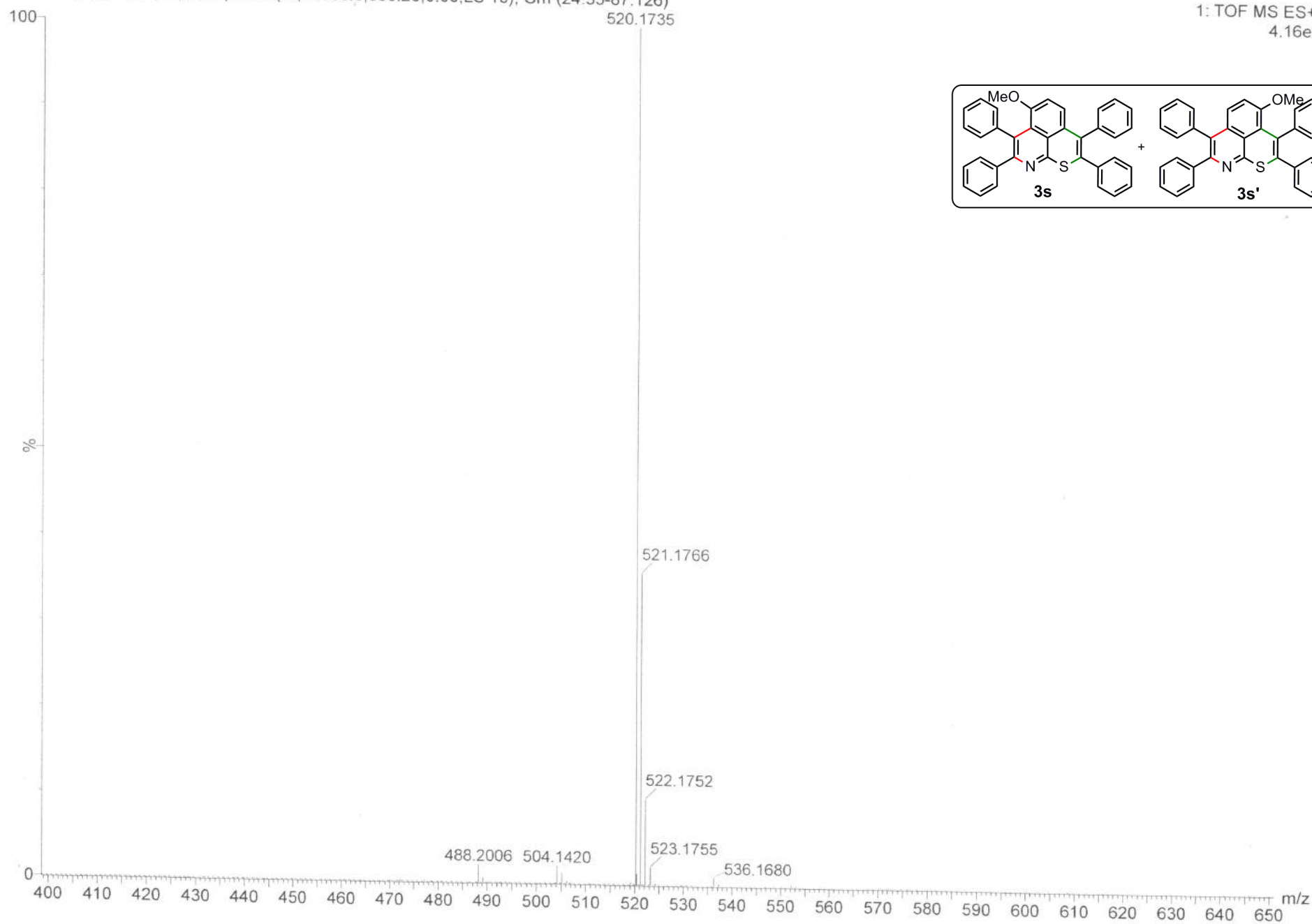
MJ-17-271

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ACRHEM
XEVO-G2XSQTOF#YEA1155

04-Nov-2020
11:47:32

04112020_09 +VE 24 (0.262) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (24:35-87:126)

1: TOF MS ES+
4.16e7



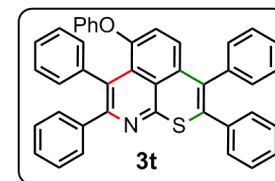
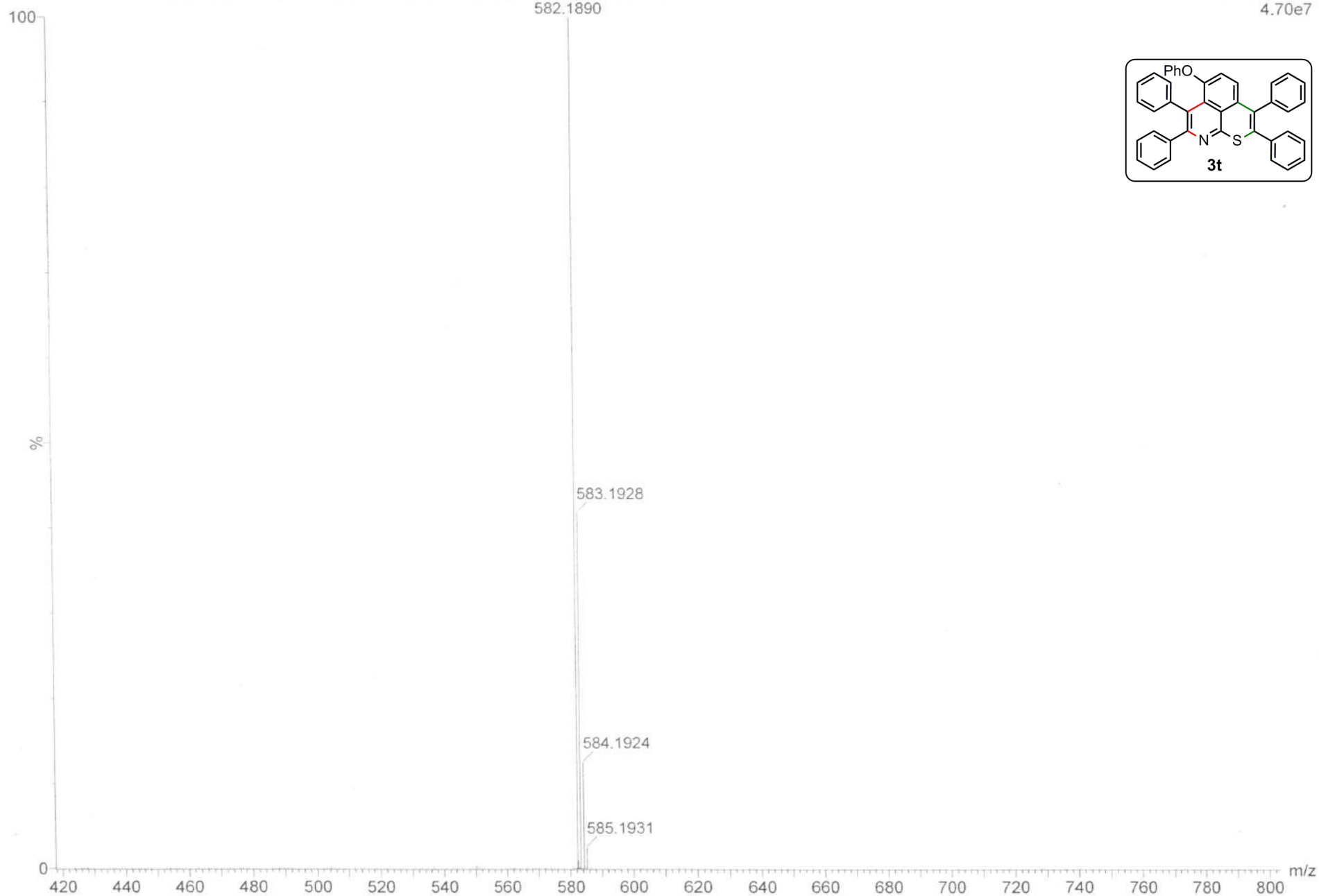
MJ-17-272

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XEVO-G2XSQTOF#YEA1155

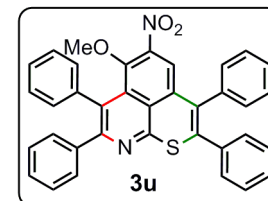
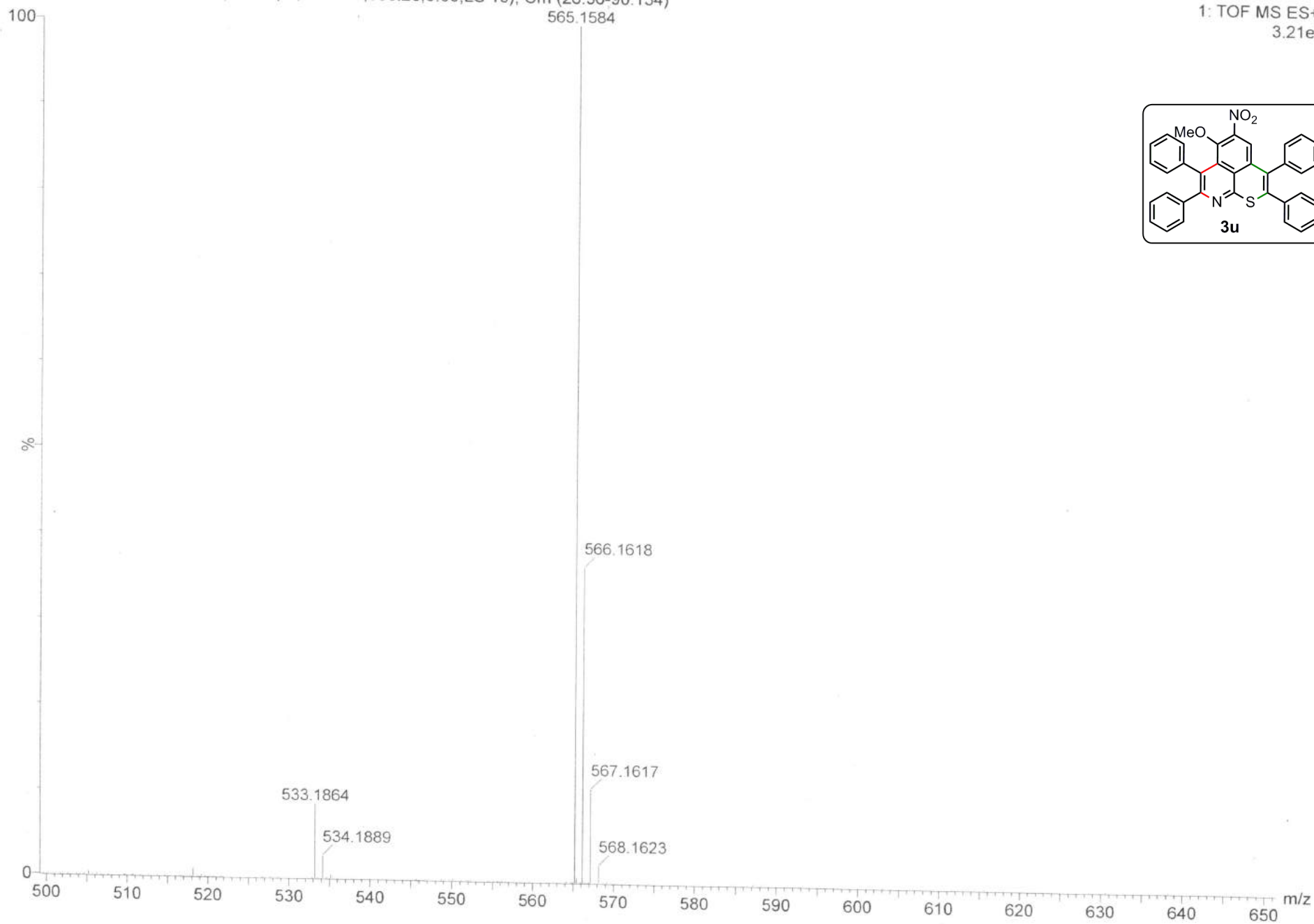
04-Nov-2020
11:44:54

04112020_08 +VE 34 (0.348) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (34:51-91:137)

1: TOF MS ES+
4.70e7



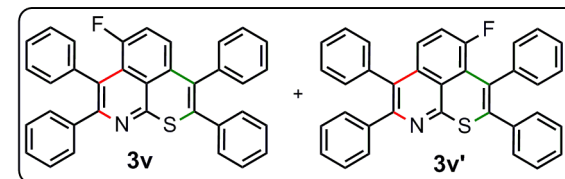
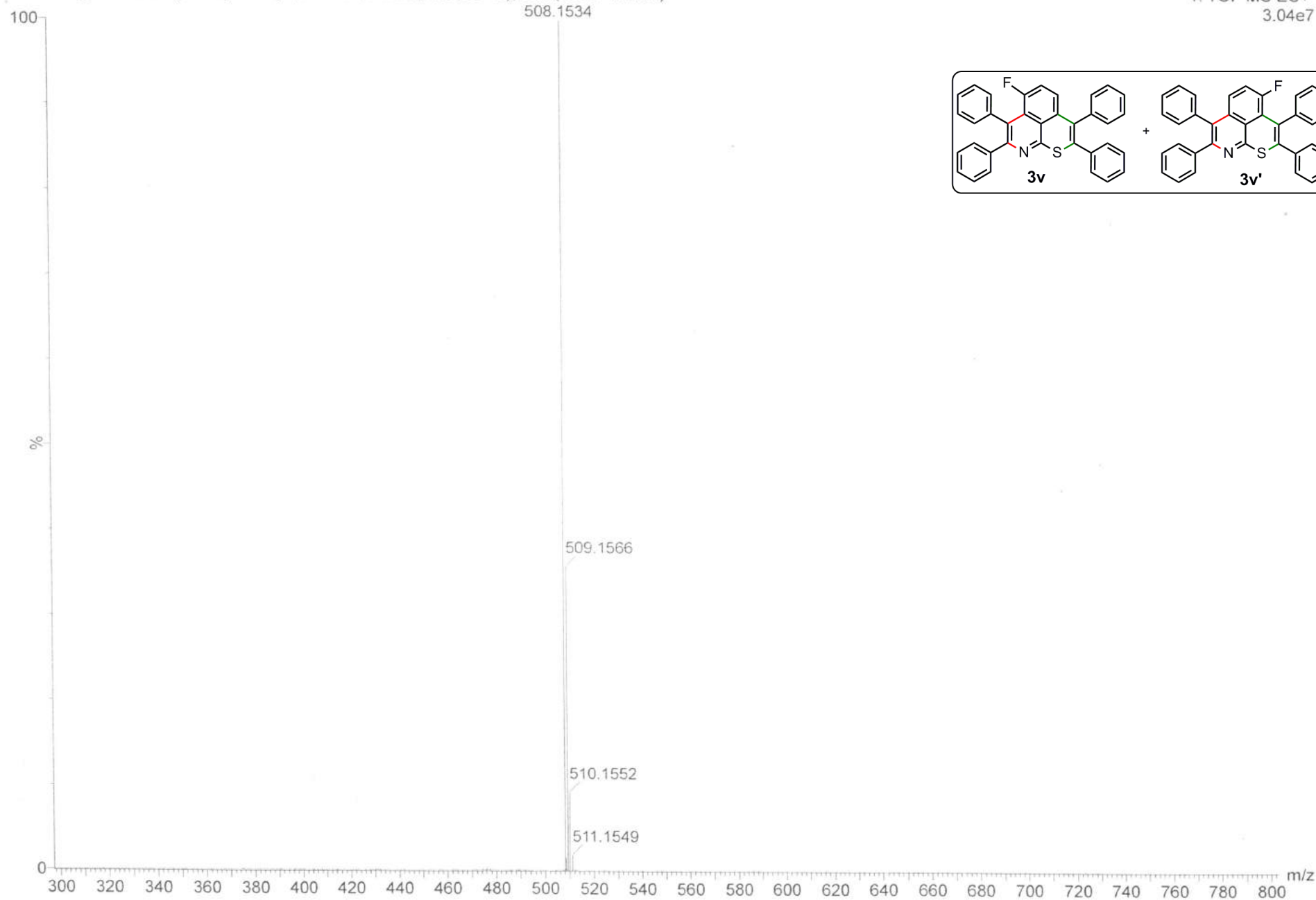
06112020_10 +VE 26 (0.279) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (26:36-90:134)

1: TOF MS ES+
3.21e7

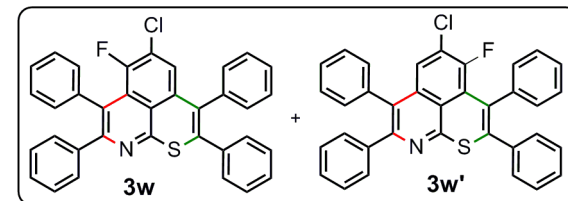
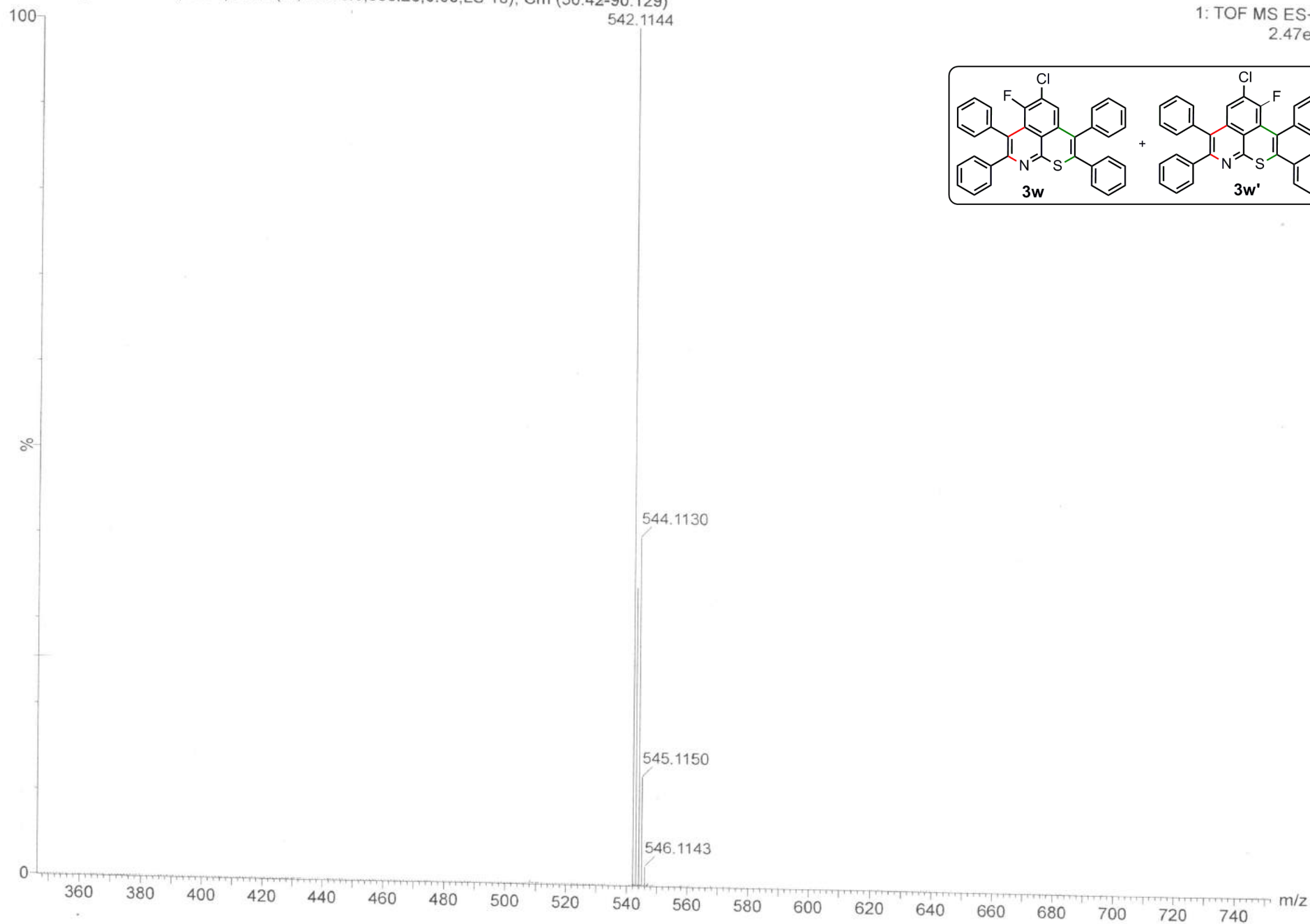
03112020_34 +VE 28 (0.296) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (28:37-72:108)

1: TOF MS ES+

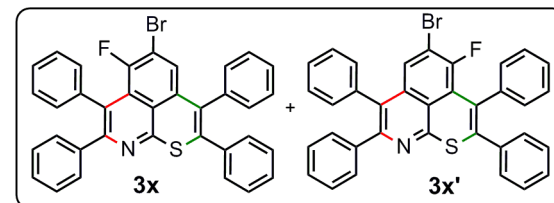
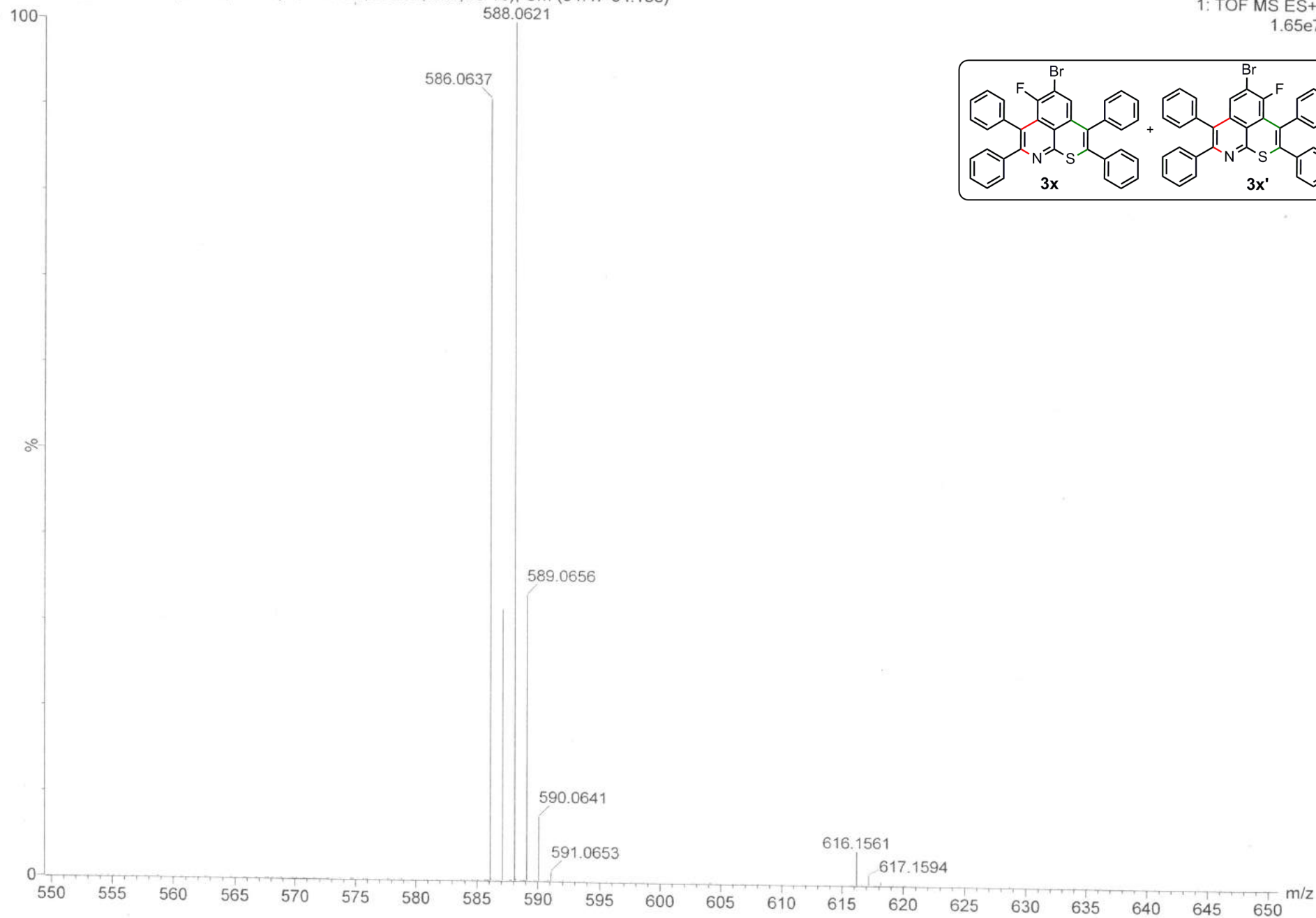
3.04e7



03112020_29 +VE 30 (0.314) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (30:42-90:129)

1: TOF MS ES+
2.47e7

03112020_28 +VE 34 (0.348) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (34:47-94:133)

1: TOF MS ES+
1.65e7

Display Report

Analysis Info

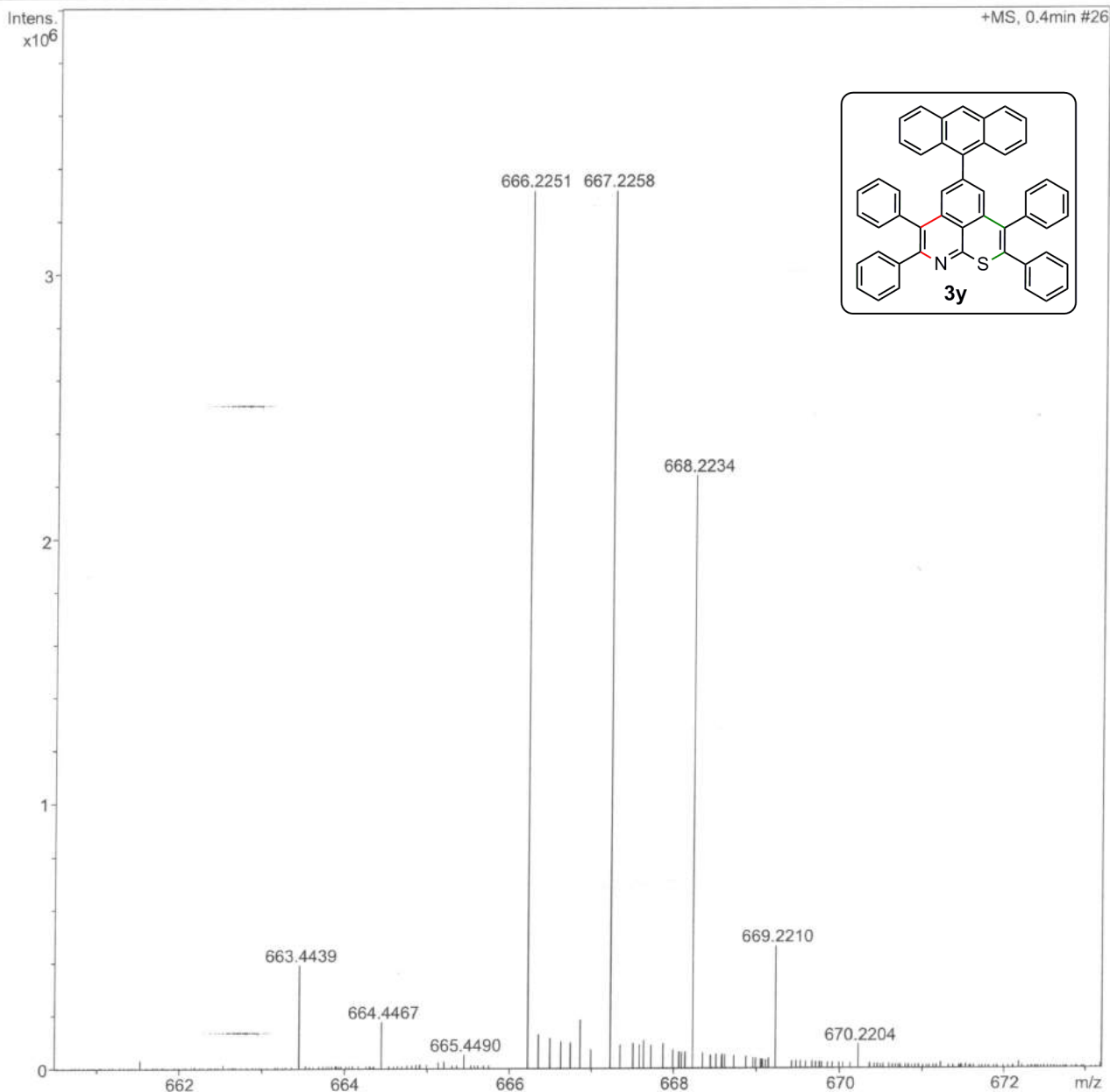
Analysis Name D:\Data\2019\PROF. AKS\july\MJ-16-12.d
Method tune_low.m
Sample Name MJ-16-12-DCM-MEOH
Comment

Acquisition Date 7/15/2019 4:35:24 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

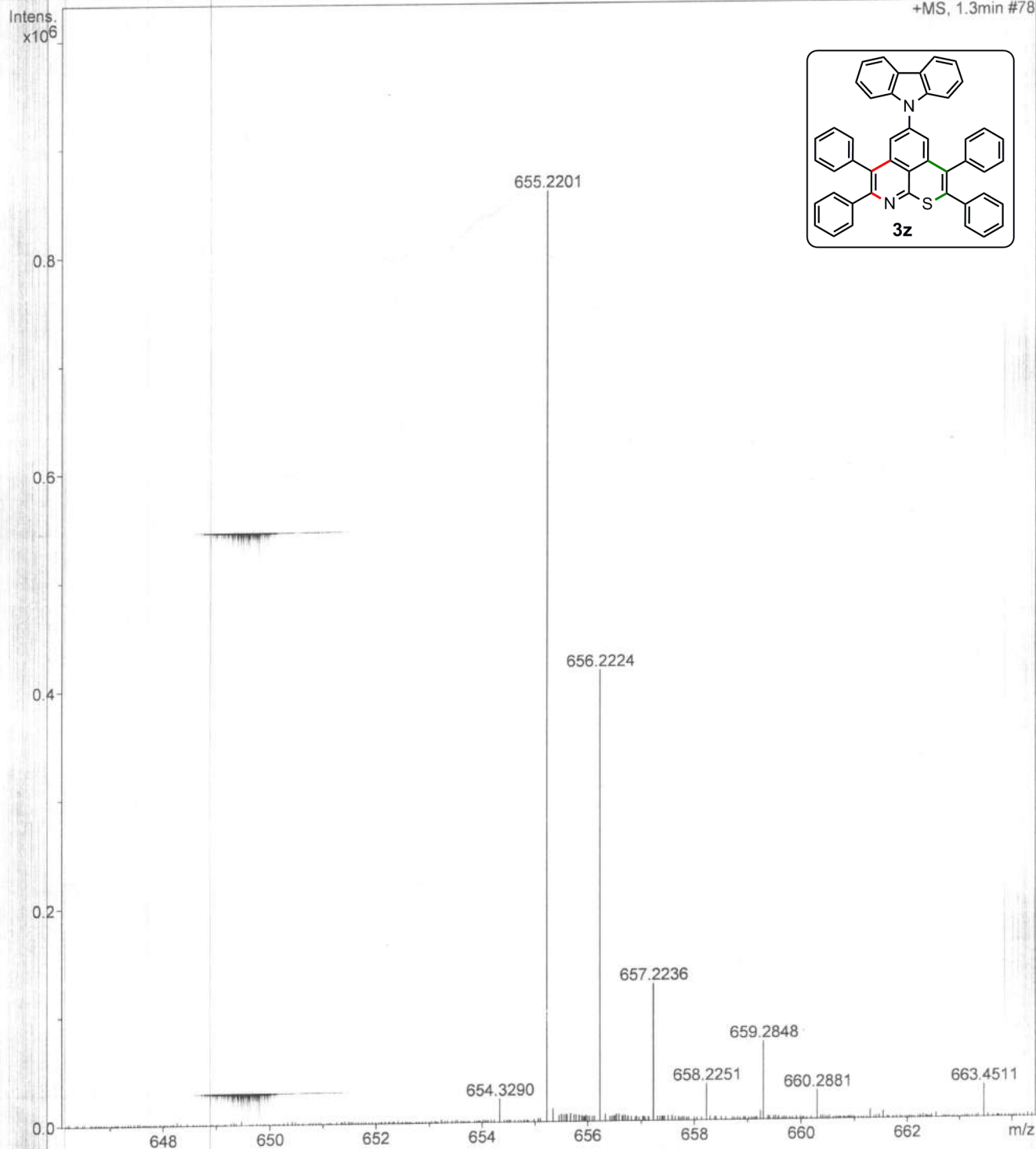
Analysis Name D:\Data\2019\PROF. AKS\OCT\SRS-1-376.d
Method tune_low.m
Sample Name SRS-1-376-DCM-MEOH
Comment

Acquisition Date 10/9/2019 4:26:55 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

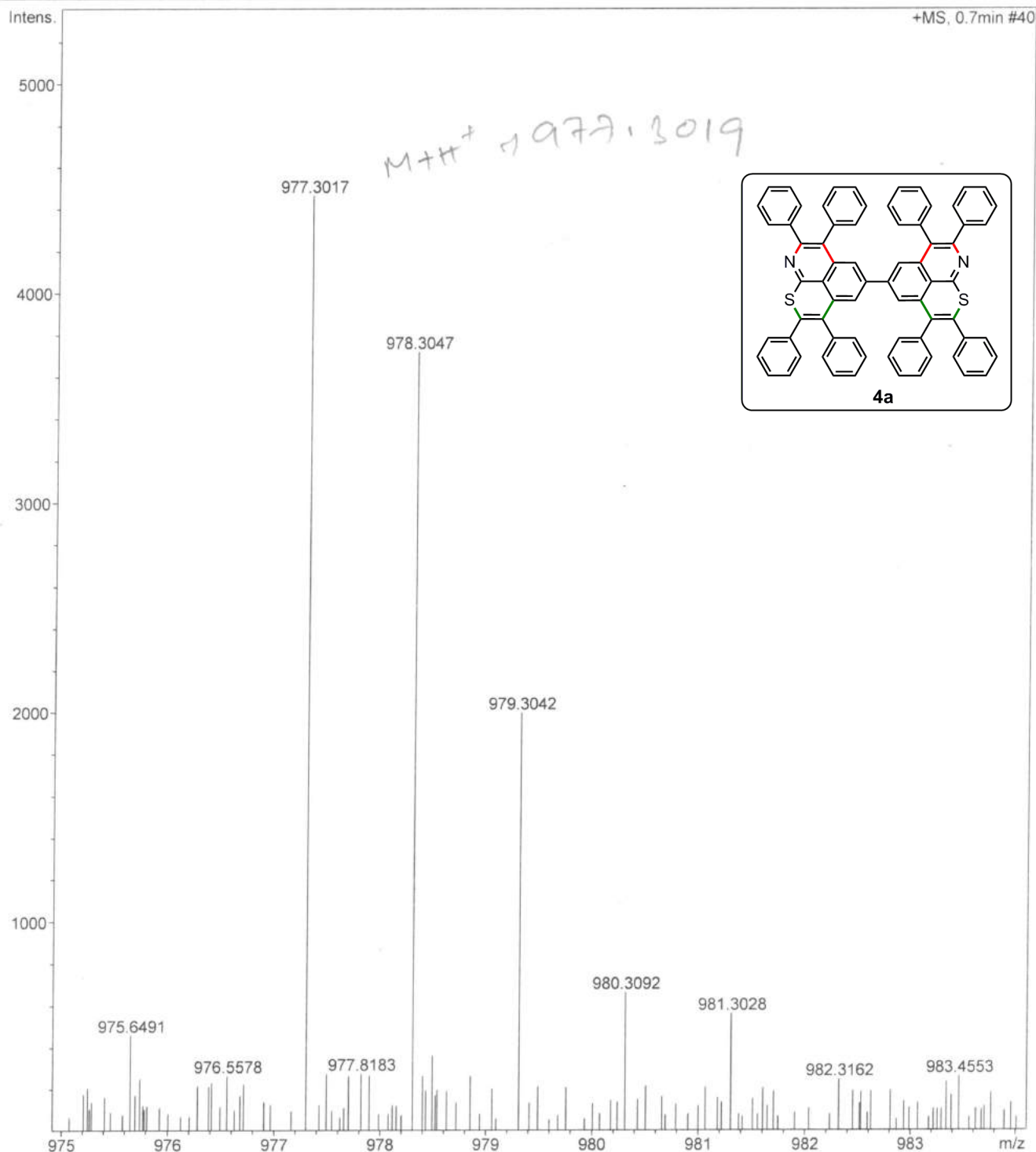
Analysis Name D:\Data\2019\PROF. AKS\NOVAS-325.d
Method tune_low_Pos.m
Sample Name AS-325
Comment

Acquisition Date 11/5/2019 12:55:10 AM

Operator UOH-Chemistry
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	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



MJ-17-36R

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XEVO-G2XSQTOF#YEA1155

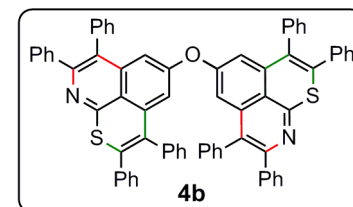
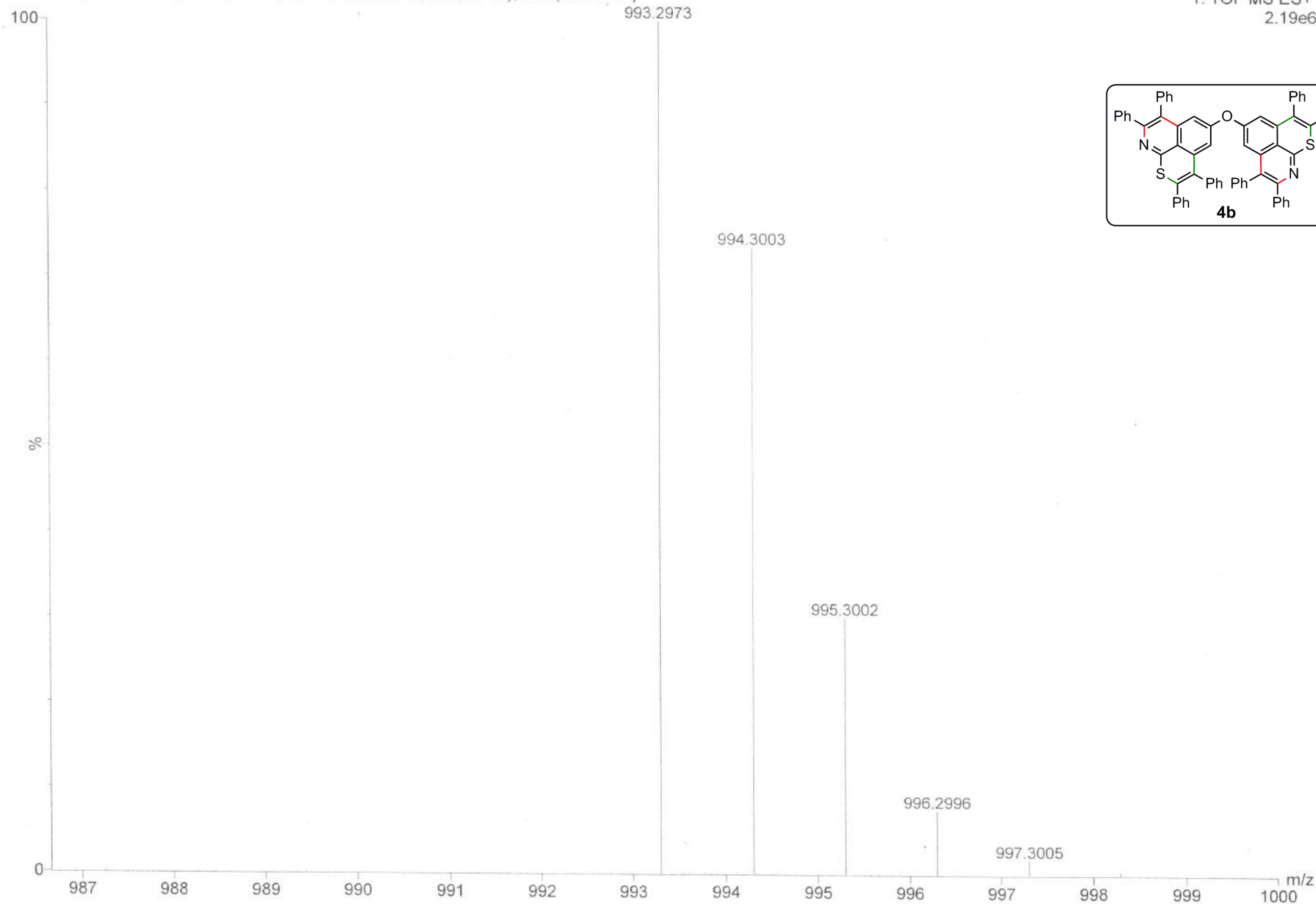
06-Nov-2020

12:27:25

06112020_13 +VE 15 (0.165) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (15:20-1:5)

1: TOF MS ES+

2.19e6



Display Report

Analysis Info

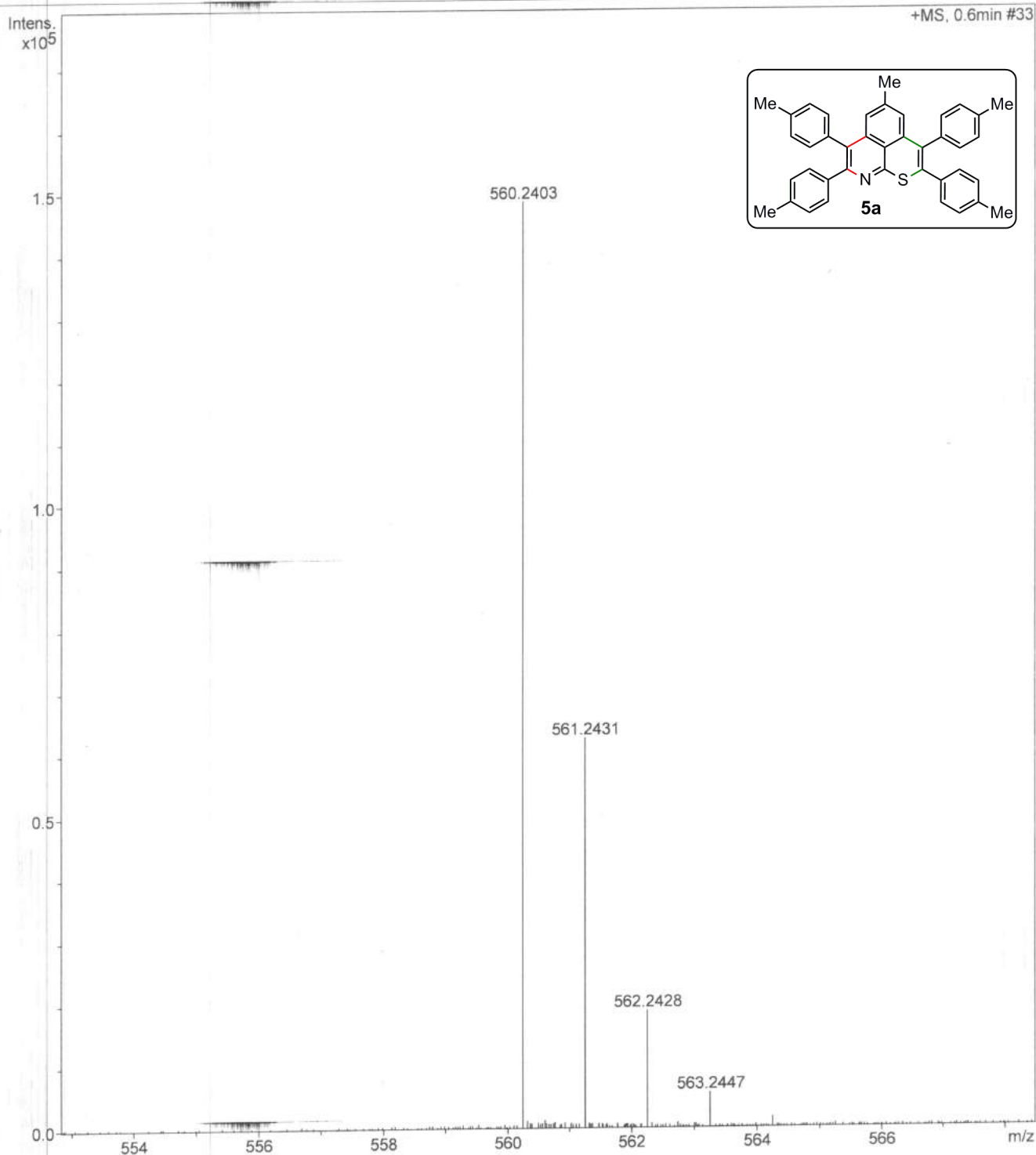
Analysis Name D:\Data\2019\PROF. AKS\SEP\AG-3-203.d
Method tune_low_Pos.m
Sample Name AG-3-203-DCM-MEOH
Comment

Acquisition Date 9/27/2019 12:39:31 AM

Operator UOH-Chemistry
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



Display Report

Analysis Info

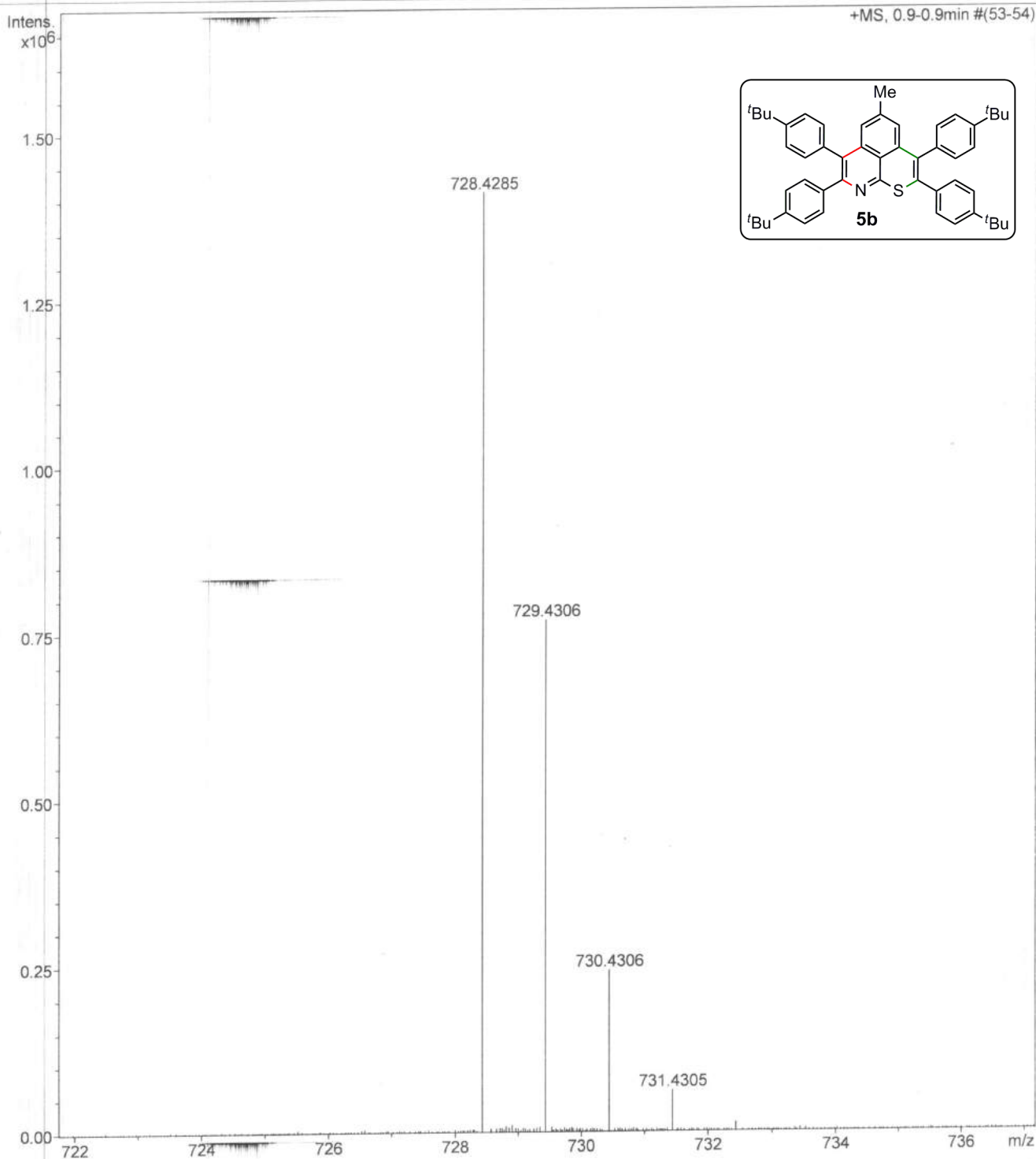
Analysis Name D:\Data\2019\PROF. AKS\SEP\AG-4-71.d
Method tune_low_Pos.m
Sample Name AG-4-71-DCM-MEOH
Comment

Acquisition Date 9/27/2019 1:01:05 AM

Operator UOH-Chemistry
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	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\SEPVAG-3-205.d
Method tune_low_Pos.m
Sample Name AG-3-205-DCM-MEOH
Comment

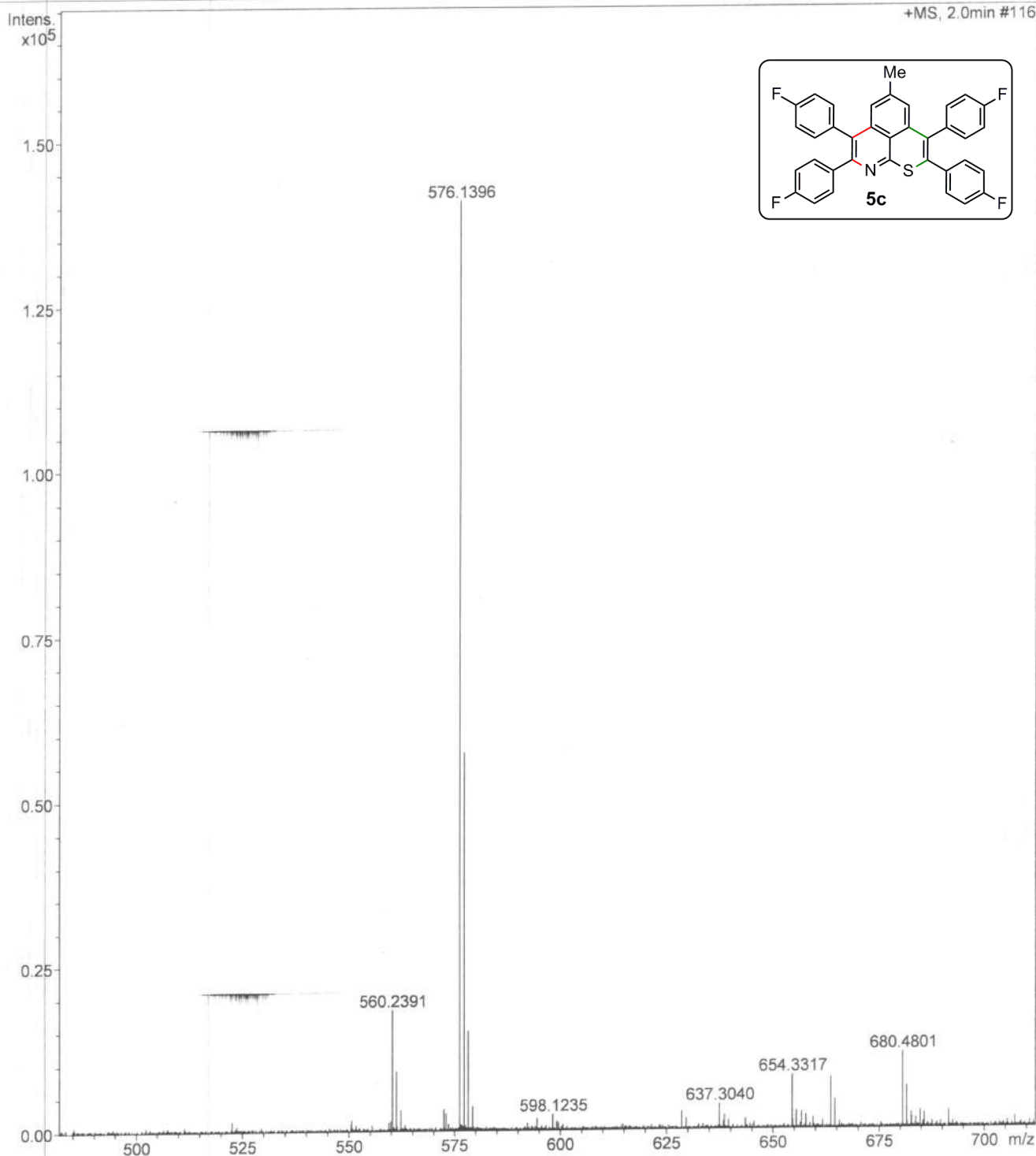
Acquisition Date 9/27/2019 12:52:32 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	4200 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp

Set Nebulizer	0.3 Bar
Set Dry Heater	180 °C
Set Dry Gas	4.0 l/min
Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\SEP\AG-4-74.d
Method tune_low_Pos.m
Sample Name AG-4-74-DCM-MEOH
Comment

Acquisition Date 9/27/2019 12:35:55 AM

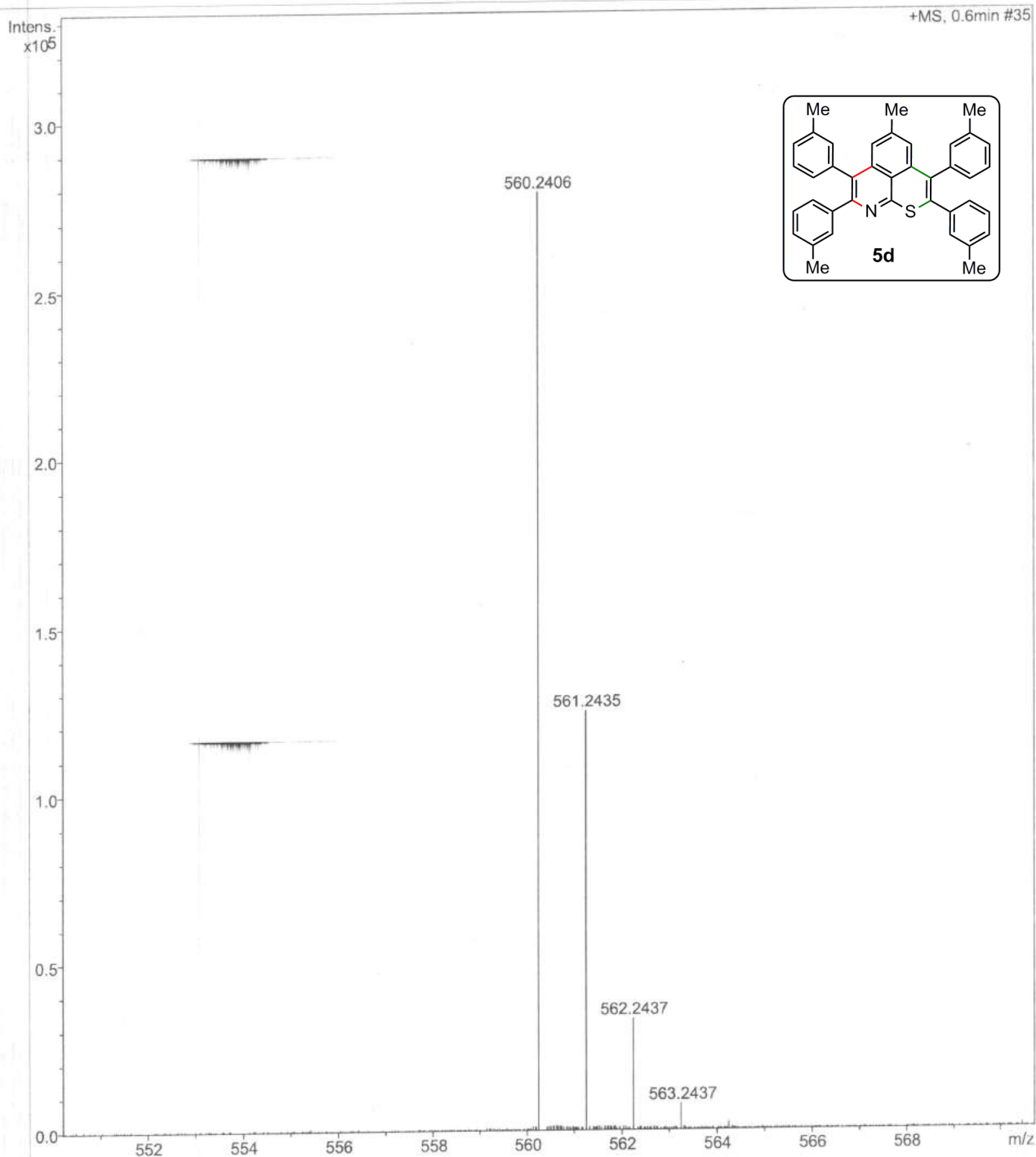
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

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

Ion Polarity Positive
Set Capillary 4200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste



Display Report

Analysis Info

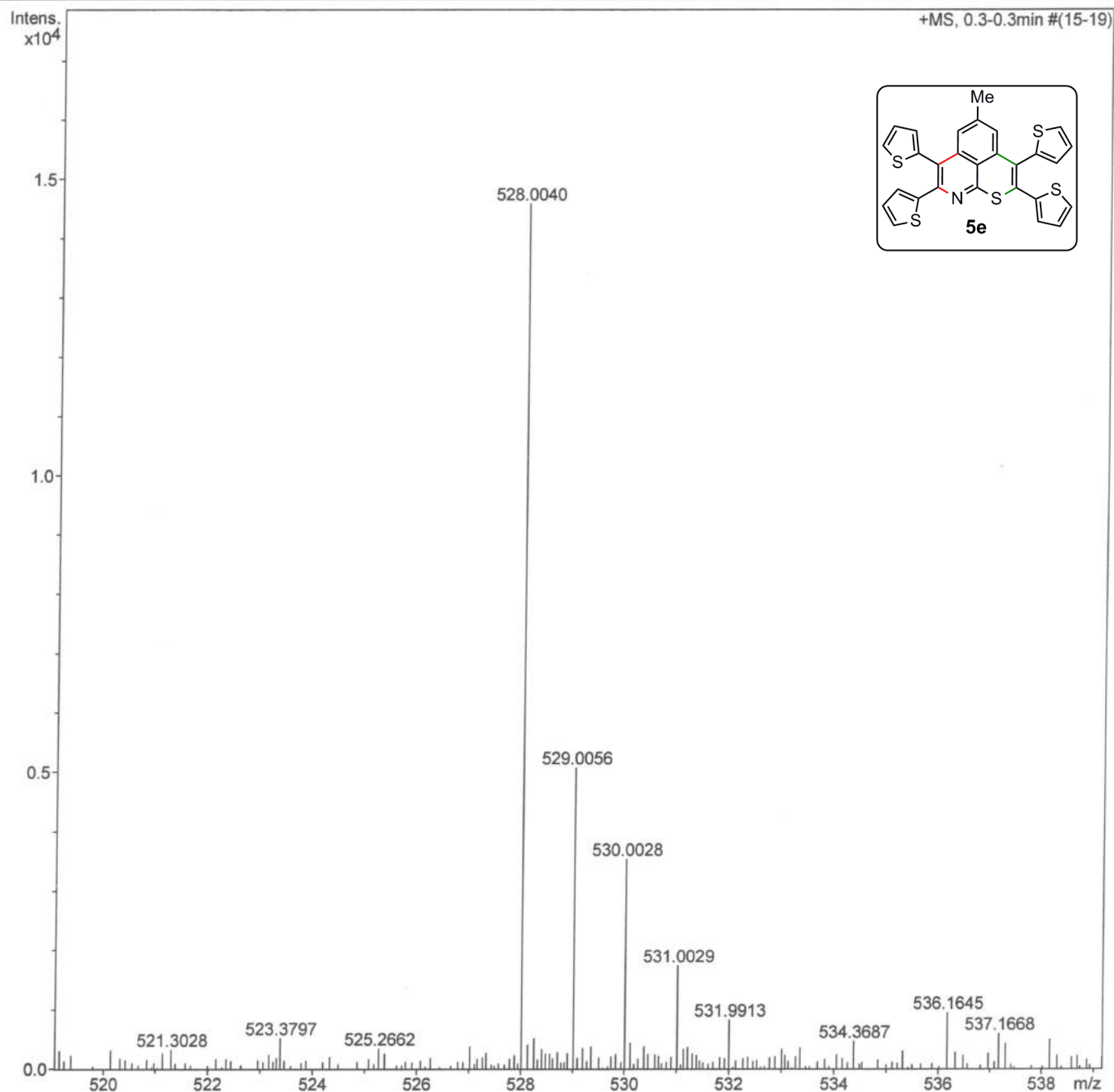
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-16-28R.d
Method tune_low.m
Sample Name MJ-16-28
Comment

Acquisition Date 3/5/2020 2:45:36 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	2800 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



Display Report

Analysis Info

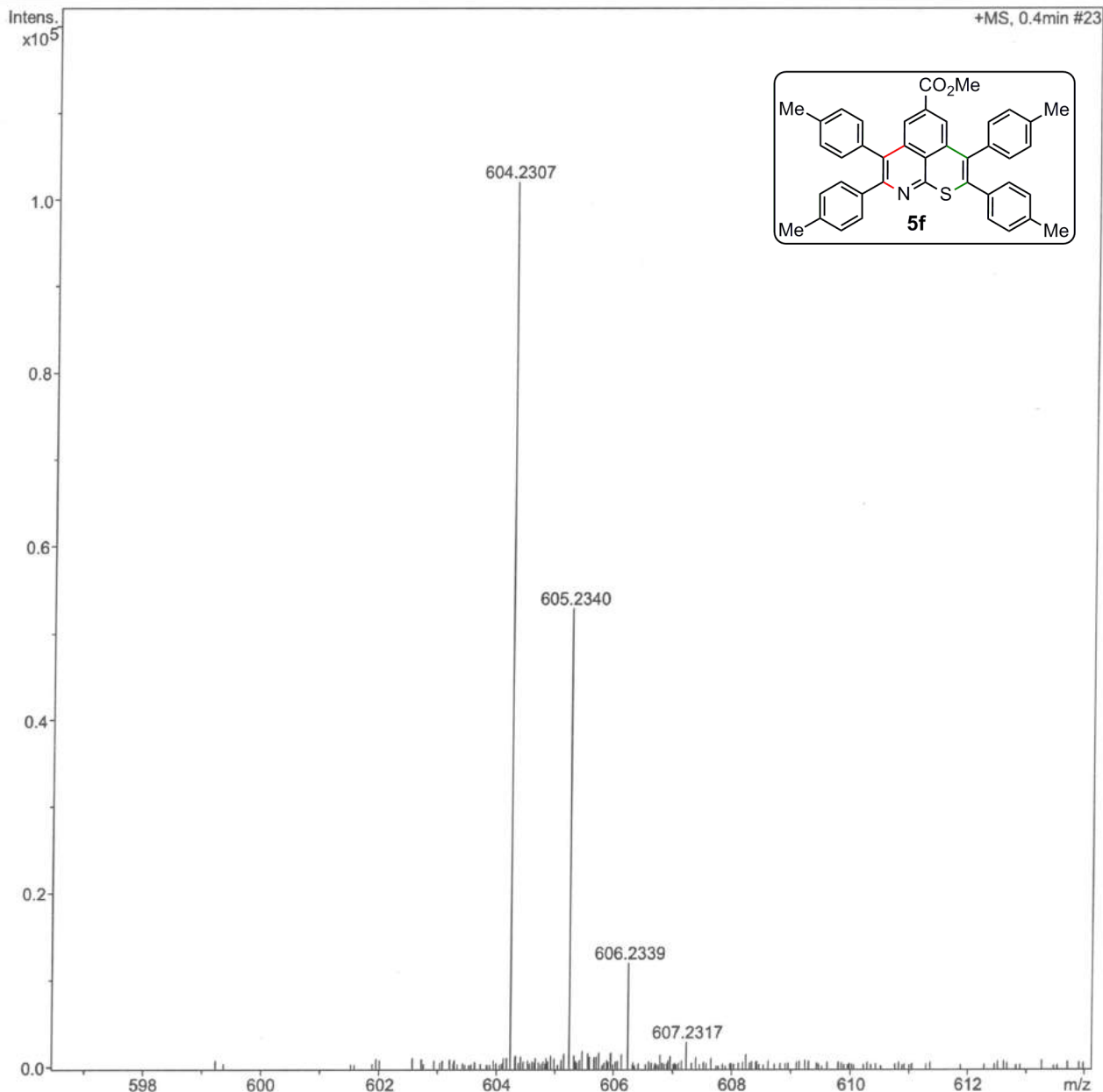
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-72.d
Method tune_low_PosR.m
Sample Name MJ-17-72
Comment

Acquisition Date 3/5/2020 3:00:29 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



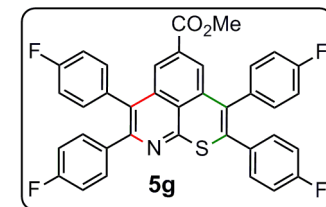
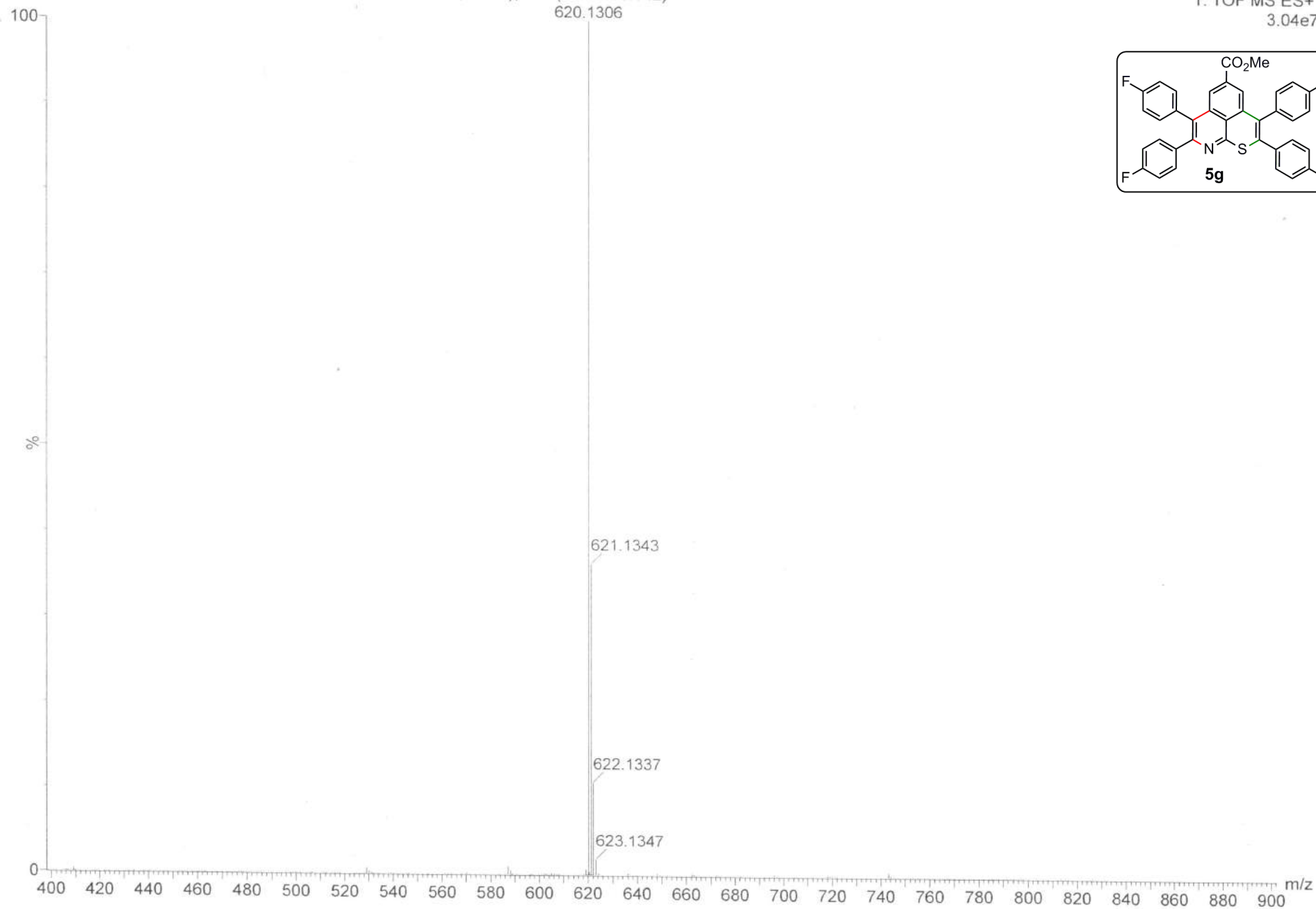
MJ-17-248

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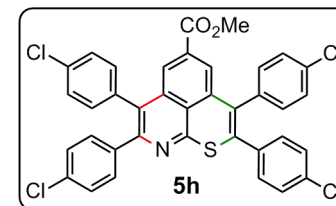
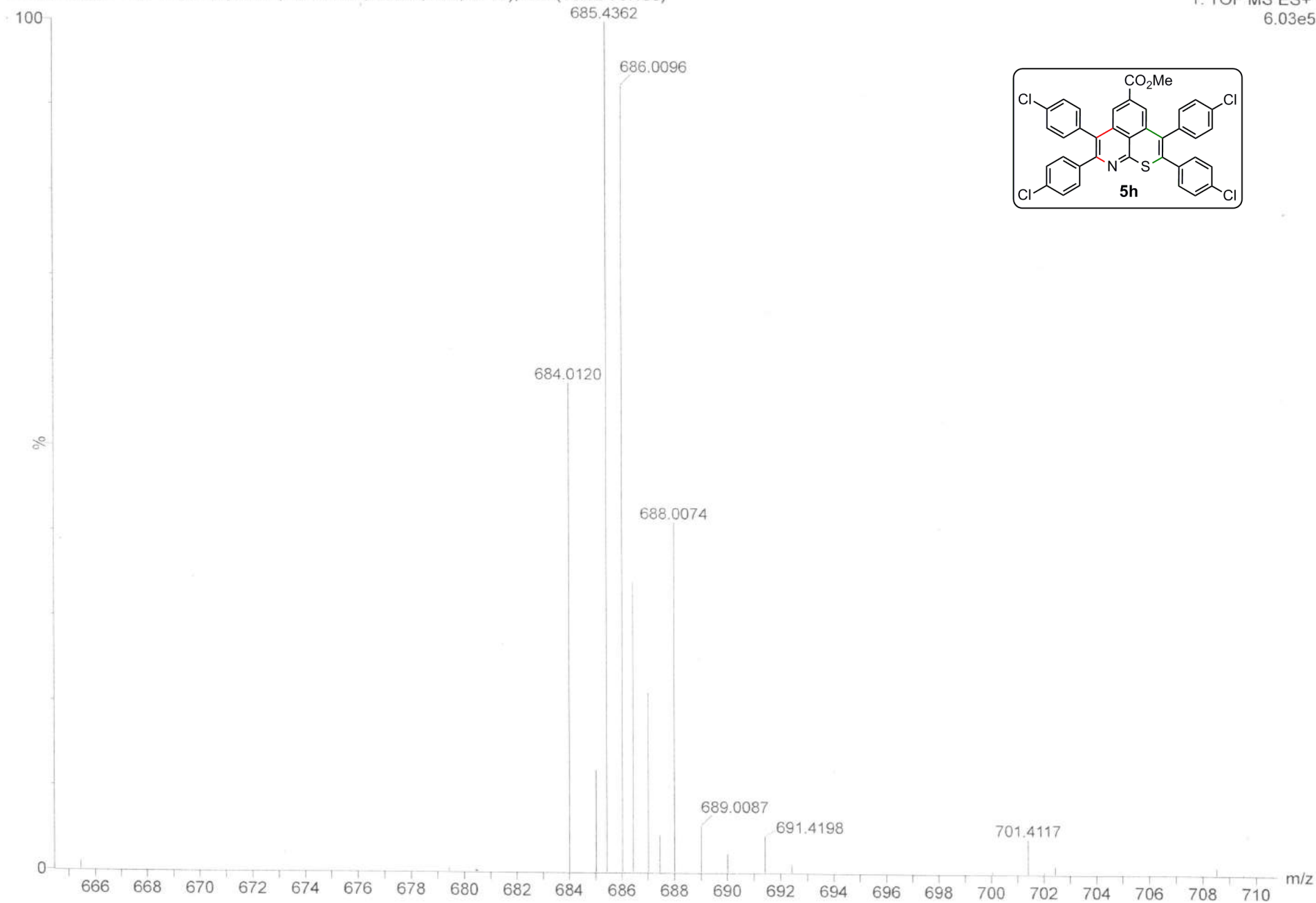
03-Nov-2020
16:04:20

03112020_31 +VE 24 (0.262) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (24:36-88:142)

1: TOF MS ES+
3.04e7



23112020_07 +VE 11 (0.131) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (10:12-75:135)

1: TOF MS ES+
6.03e5

Display Report

Analysis Info

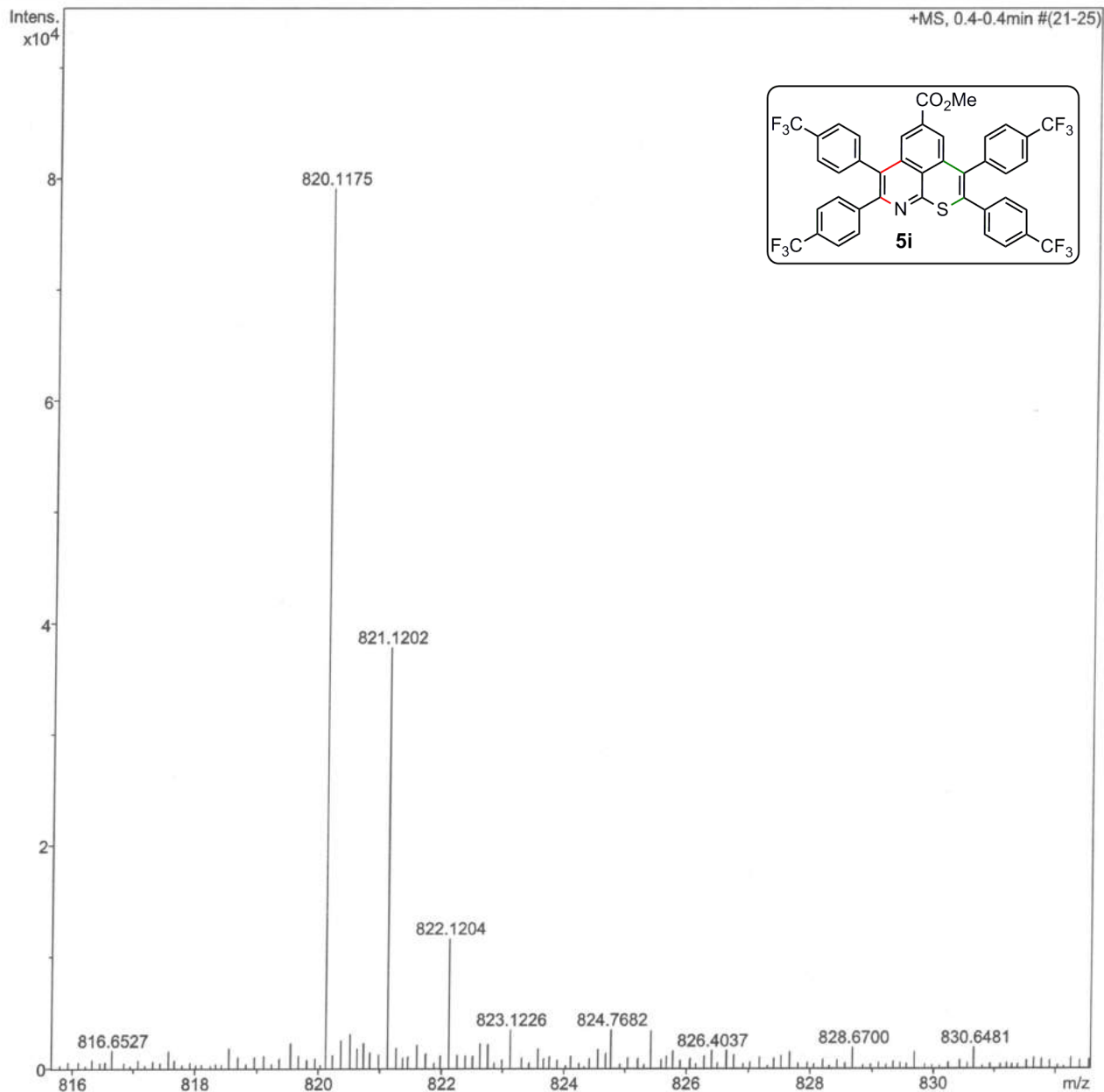
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-74.d
Method tune_low.m
Sample Name MJ-17-74
Comment

Acquisition Date 3/13/2020 3:44:26 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



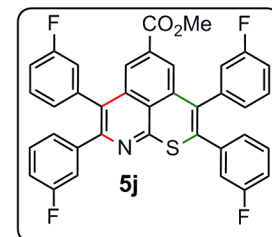
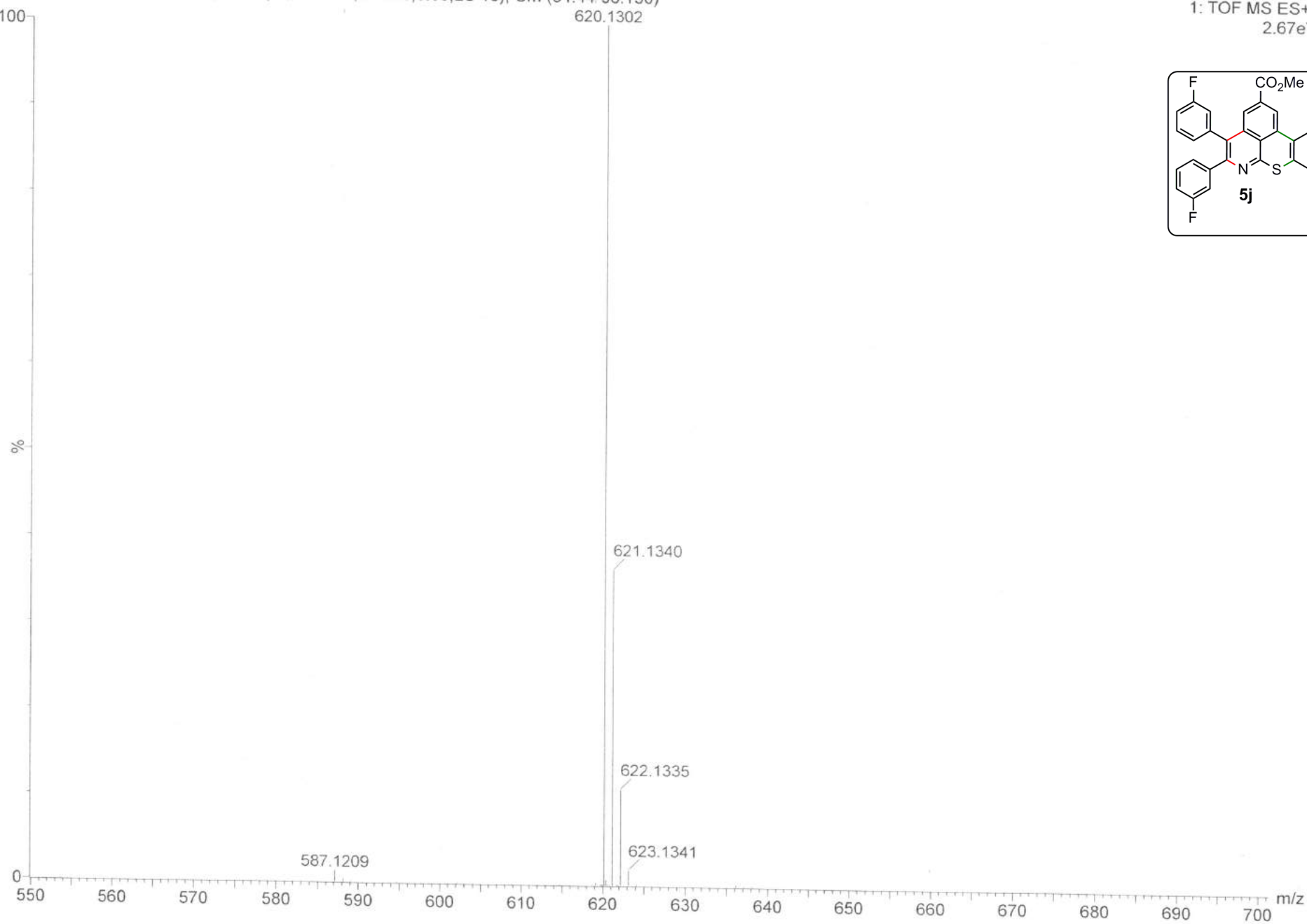
MJ-17-246

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XEVO-G2XSQTOF#YEA1155

03-Nov-2020
16:01:42

03112020_30 +VE 34 (0.348) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (34:44-96:150)

1: TOF MS ES+
2.67e7



Display Report

Analysis Info

Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-101.d
Method tune_low_PosR.m
Sample Name MJ-17-101
Comment

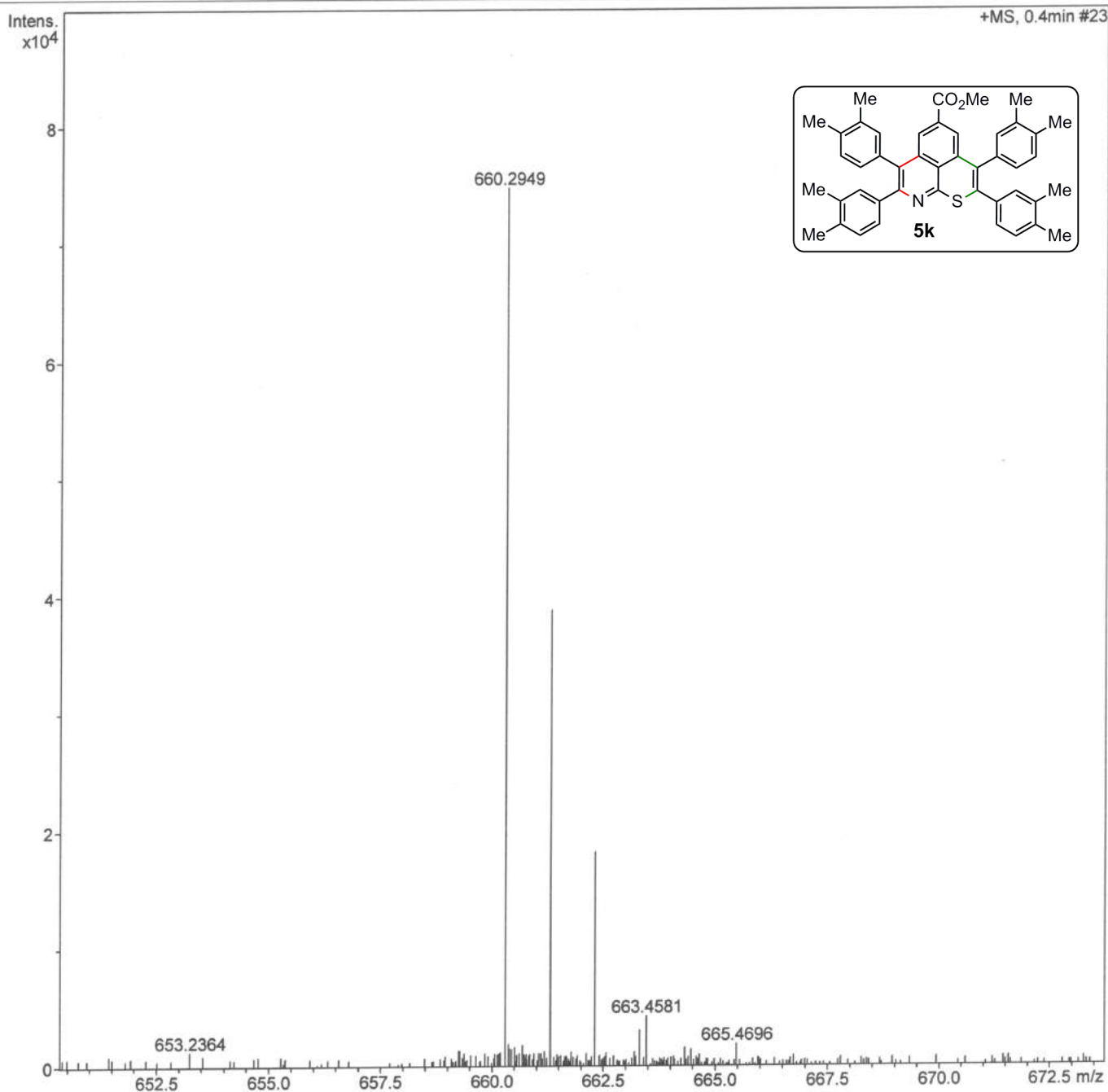
Acquisition Date 3/13/2020 12:50:05 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

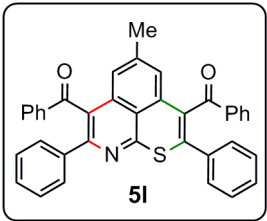
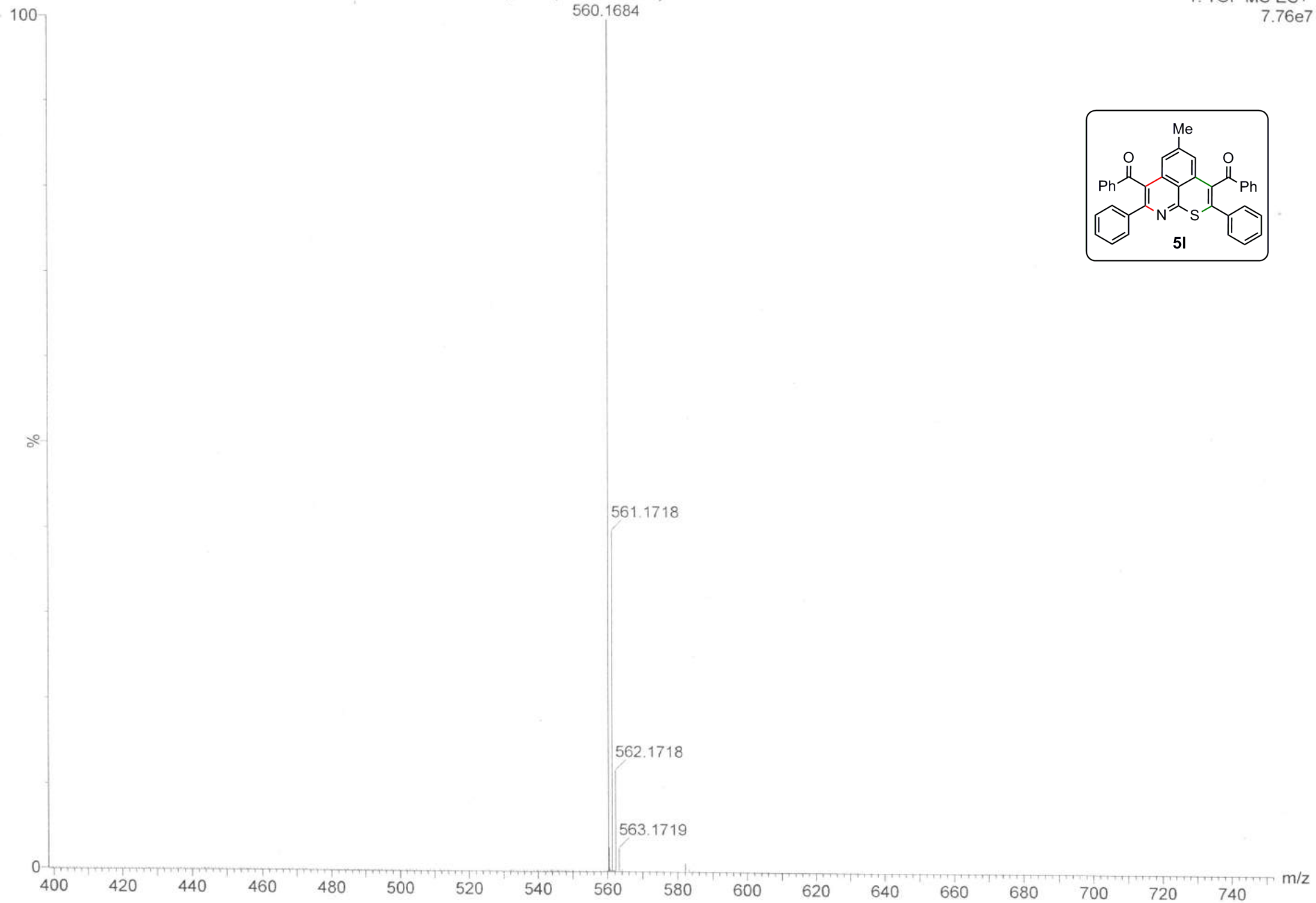
Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	2600 V
Scan Begin	200 m/z	Set End Plate Offset	-500 V
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp

Set Nebulizer	4.4 psi
Set Dry Heater	250 °C
Set Dry Gas	5.0 l/min
Set Divert Valve	Waste



23112020_08 +VE 26 (0.279) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (26:38-83:147)

1: TOF MS ES+
7.76e7



Display Report

Analysis Info

Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-102.d
Method tune_low_PosR.m
Sample Name MJ-17-102
Comment

Acquisition Date 3/12/2020 4:47:01 PM

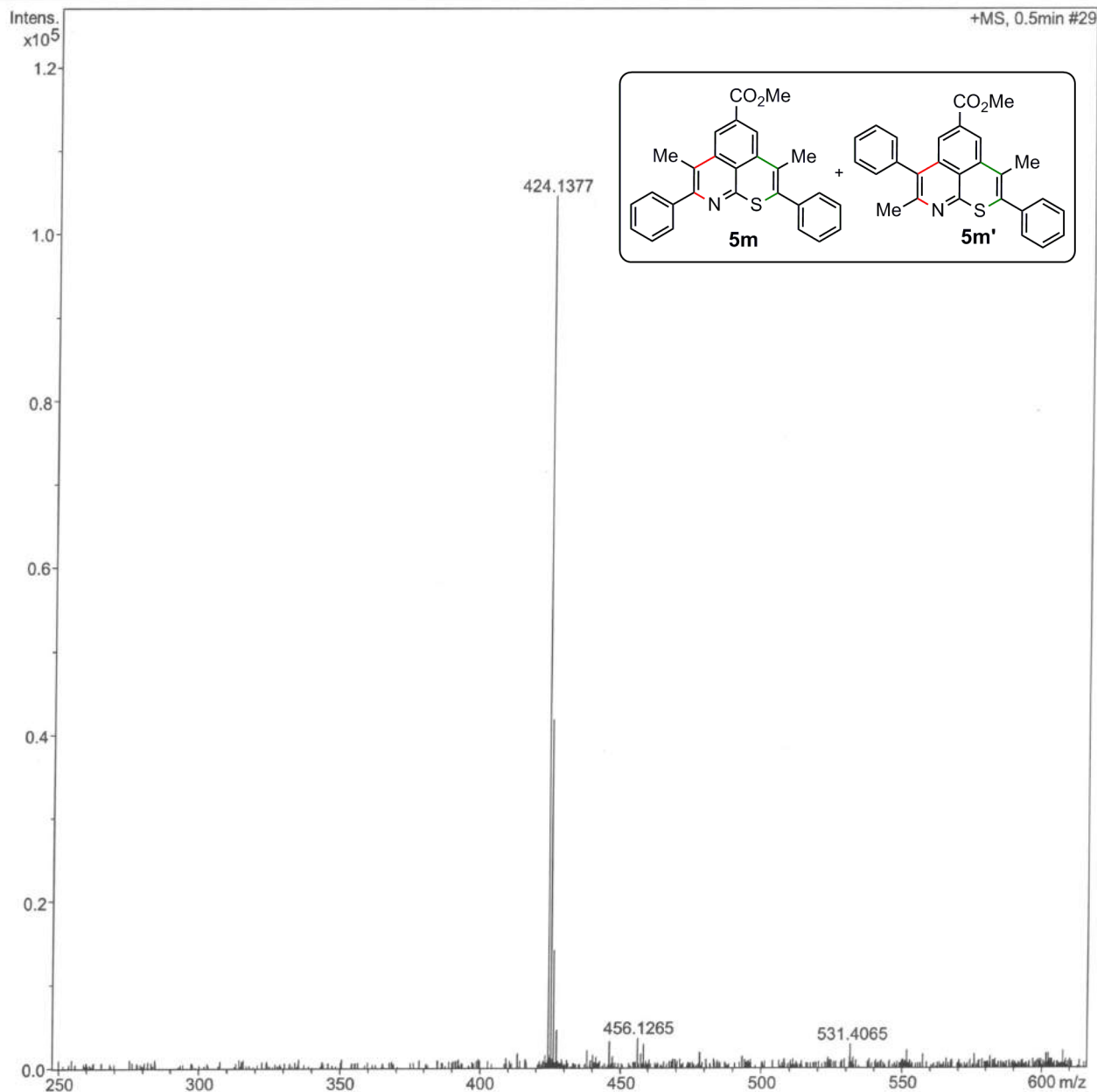
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

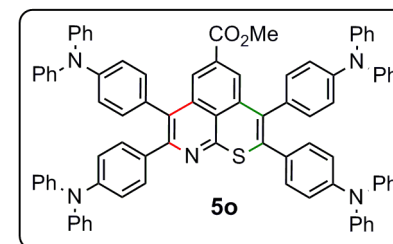
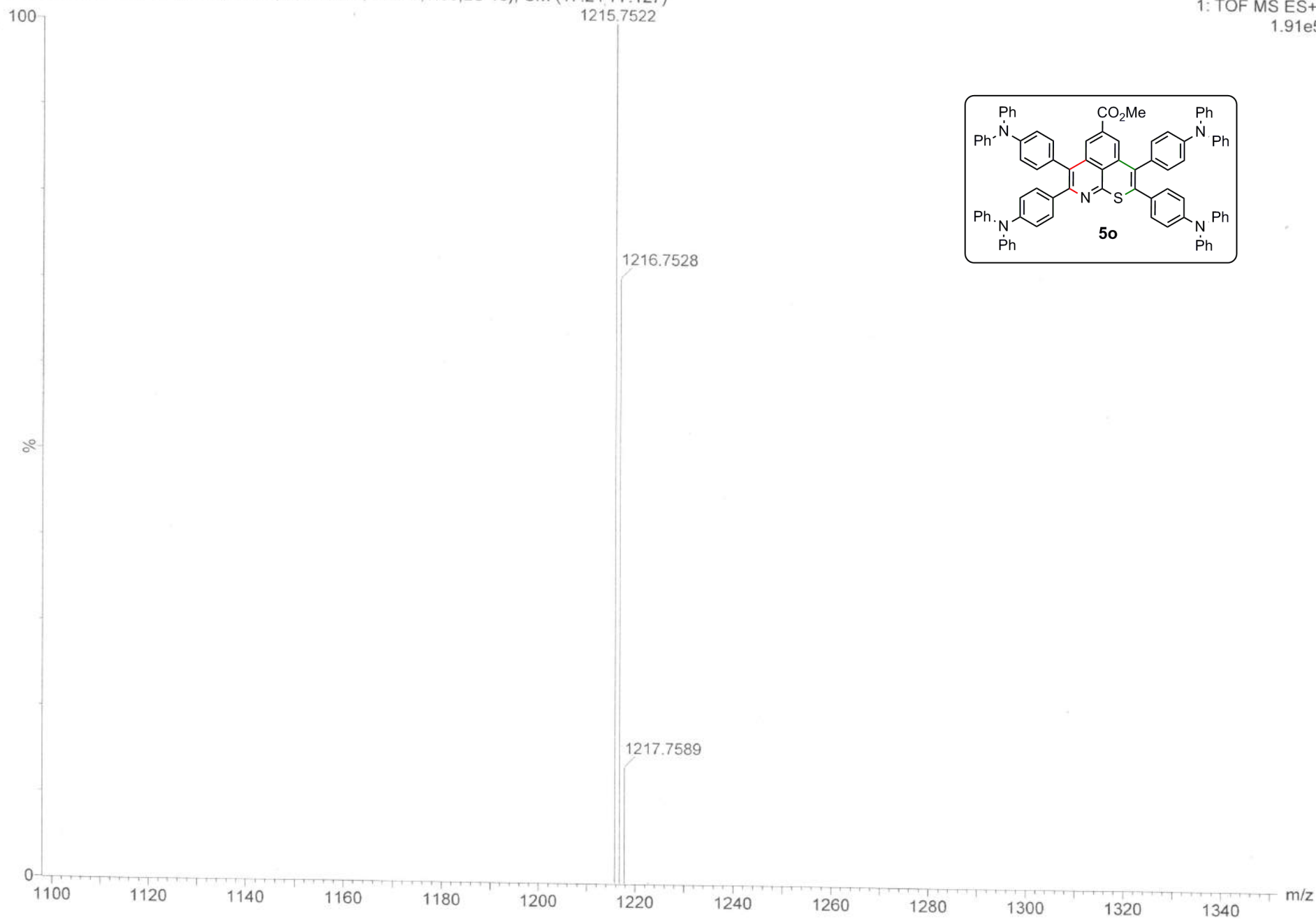
Source Type ESI
Focus Not active
Scan Begin 100 m/z
Scan End 2500 m/z

Ion Polarity Positive
Set Capillary 3200 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp

Set Nebulizer 4.4 psi
Set Dry Heater 250 °C
Set Dry Gas 5.0 l/min
Set Divert Valve Waste



23112020_17 +VE 17 (0.182) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (17:24-77:127)

1: TOF MS ES+
1.91e5

Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF SKD\JULY\MJ-16-13--R5.d
Method tune_low_Pos.m
Sample Name MJ-16-13--R5-MEOH
Comment

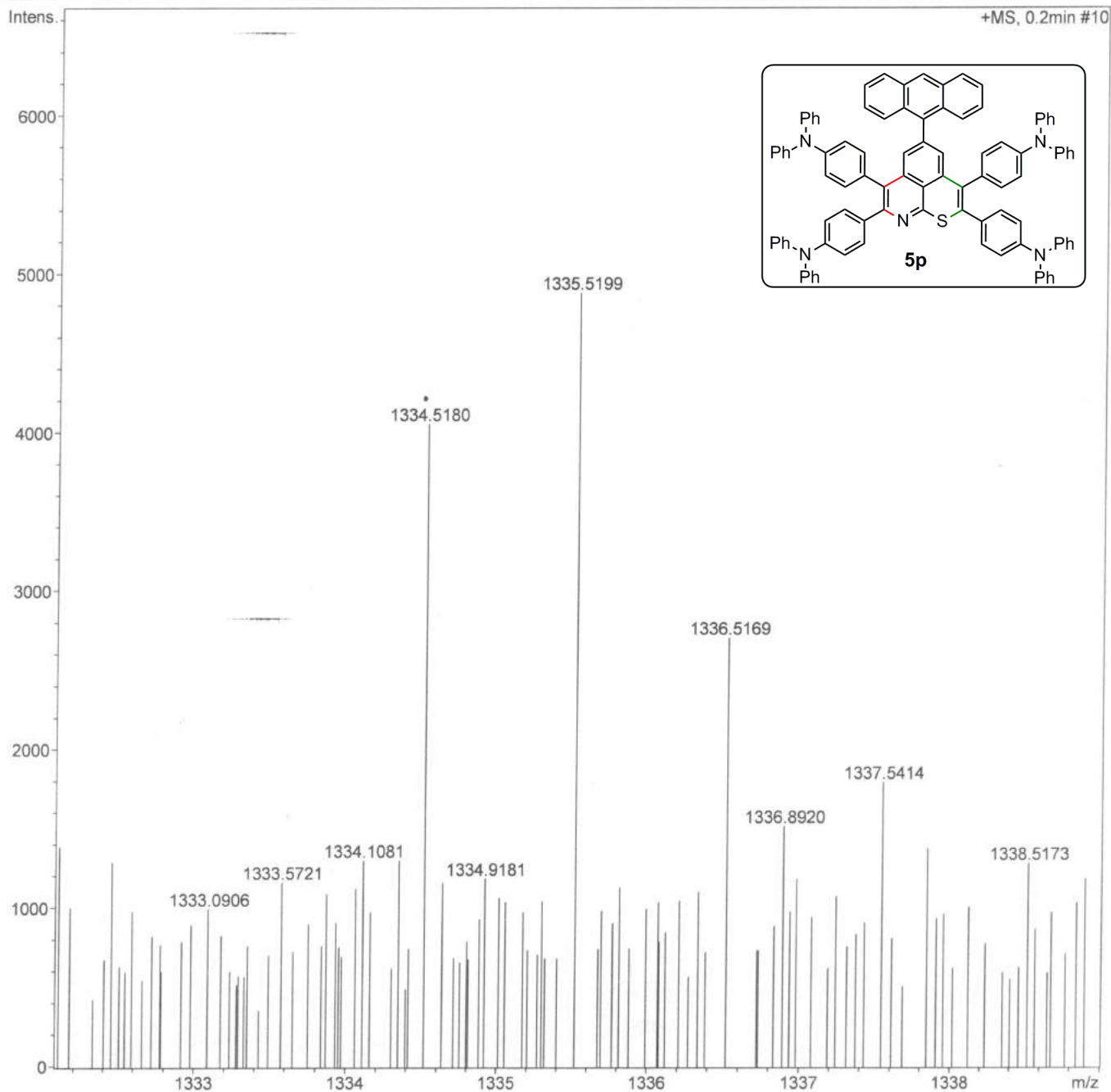
Acquisition Date 7/16/2019 11:20:35 AM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	4200 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp

Set Nebulizer	0.3 Bar
Set Dry Heater	180 °C
Set Dry Gas	6.0 l/min
Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name	D:\Data\2019\PROF. AKS\SEP\SRS-4-244.d
Method	tune_low.m
Sample Name	SRS-4-244-MEOH
Comment	

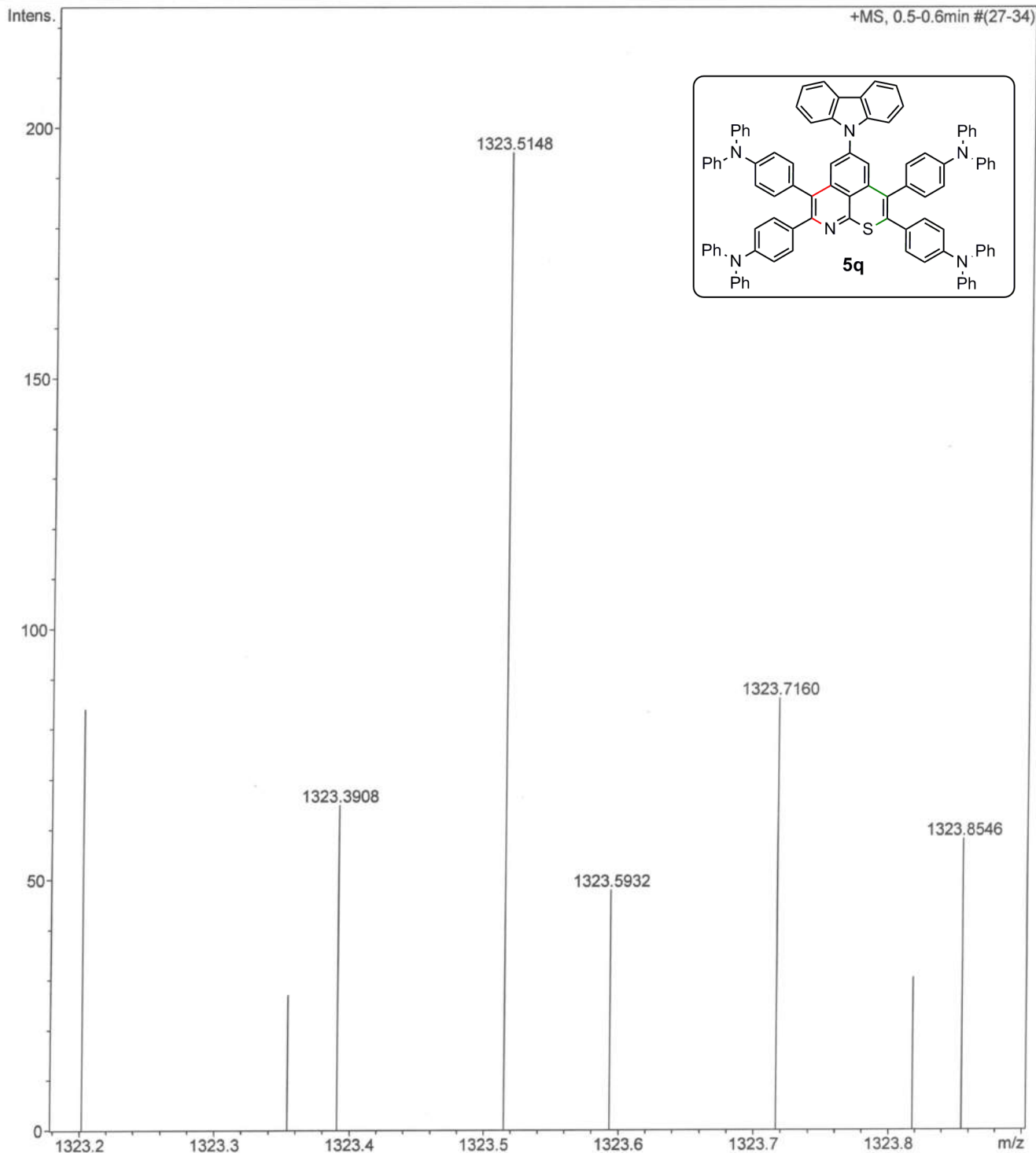
Acquisition Date 9/28/2019 3:20:06 AM

Operator	UOH-Chemistry	
Instrument	maXis	10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	3800 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp

Set Nebulizer	0.4 Bar
Set Dry Heater	200 °C
Set Dry Gas	6.0 l/min
Set Divert Valve	Waste



Display Report

Analysis Info

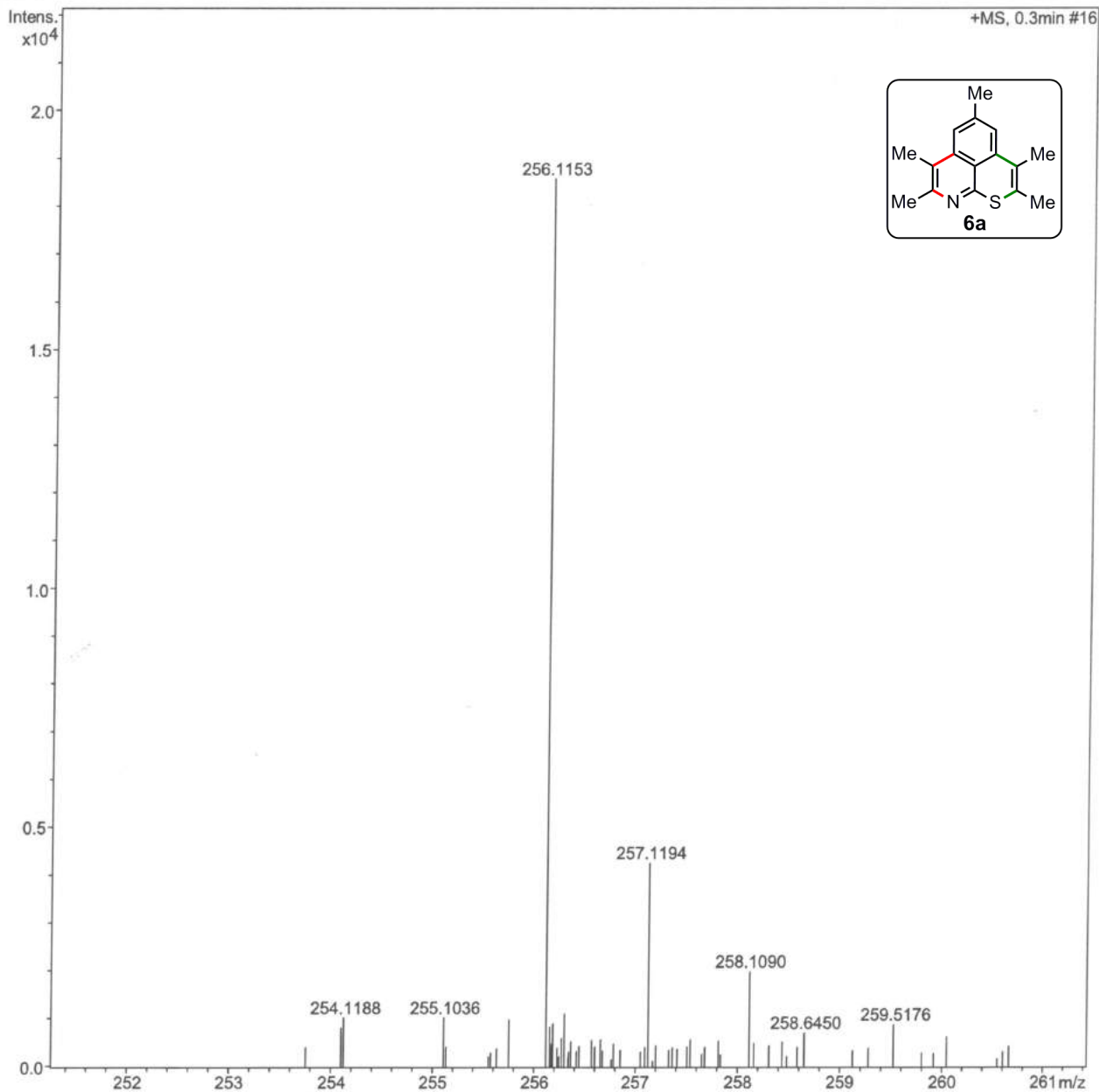
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-105R.d
Method tune_low_PosR.m
Sample Name MJ-17-105
Comment

Acquisition Date 3/5/2020 12:59:12 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name D:\Data\2019\PROF. AKS\july\MJ-16-18R.d
Method tune_low_Pos.m
Sample Name MJ-16-18-DCM-MEOH
Comment

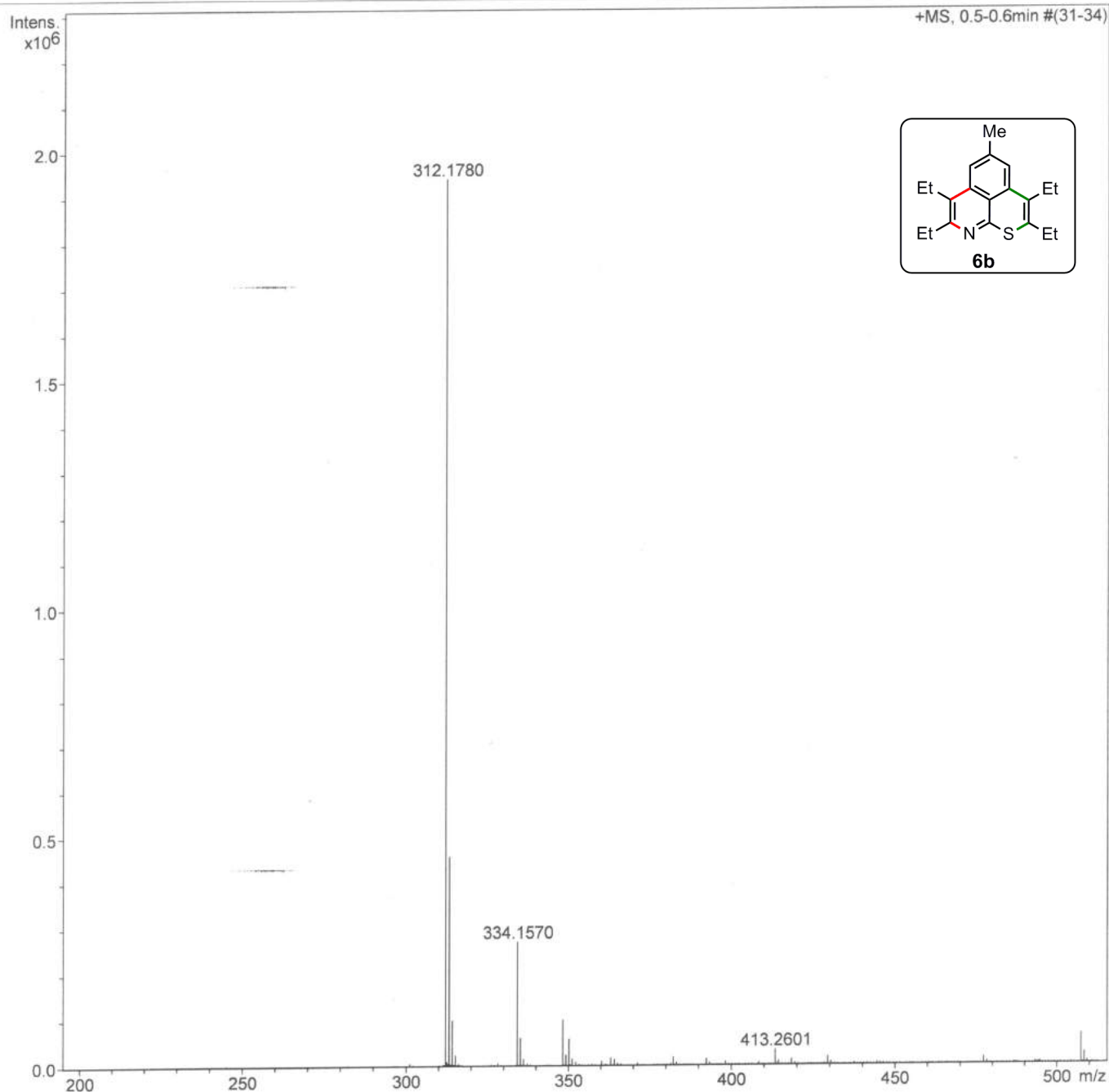
Acquisition Date 7/15/2019 3:45:53 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Focus	Not active	Set Capillary	3600 V
Scan Begin	50 m/z	Set End Plate Offset	-500 V
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp

Set Nebulizer	0.3 Bar
Set Dry Heater	180 °C
Set Dry Gas	4.0 l/min
Set Divert Valve	Waste



Display Report

Analysis Info

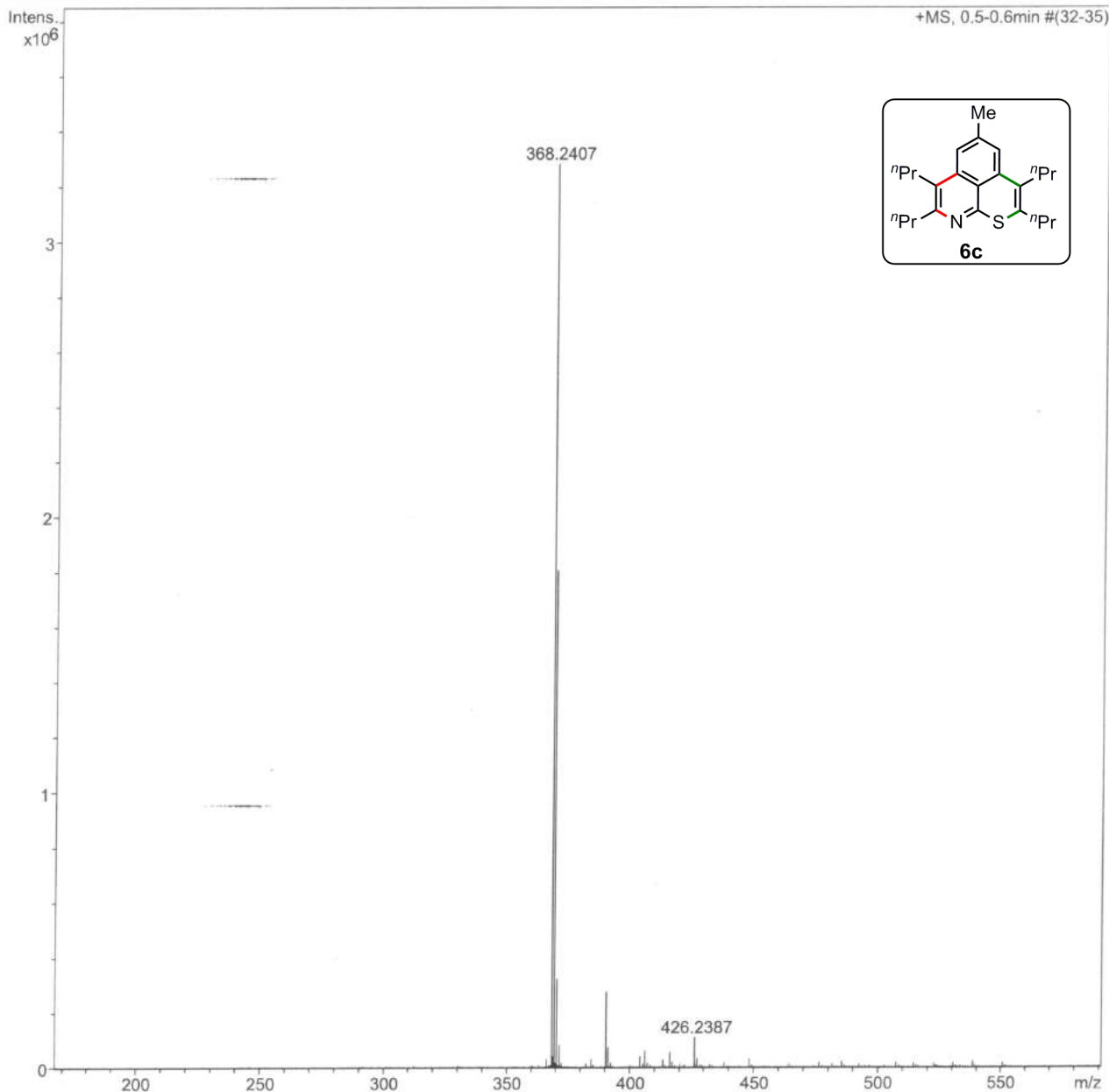
Analysis Name D:\Data\2019\PROF. AKS\july\MJ-16-19.d
Method tune_low.m
Sample Name MJ-16-19-DCM-MEOH
Comment

Acquisition Date 7/15/2019 3:57:19 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

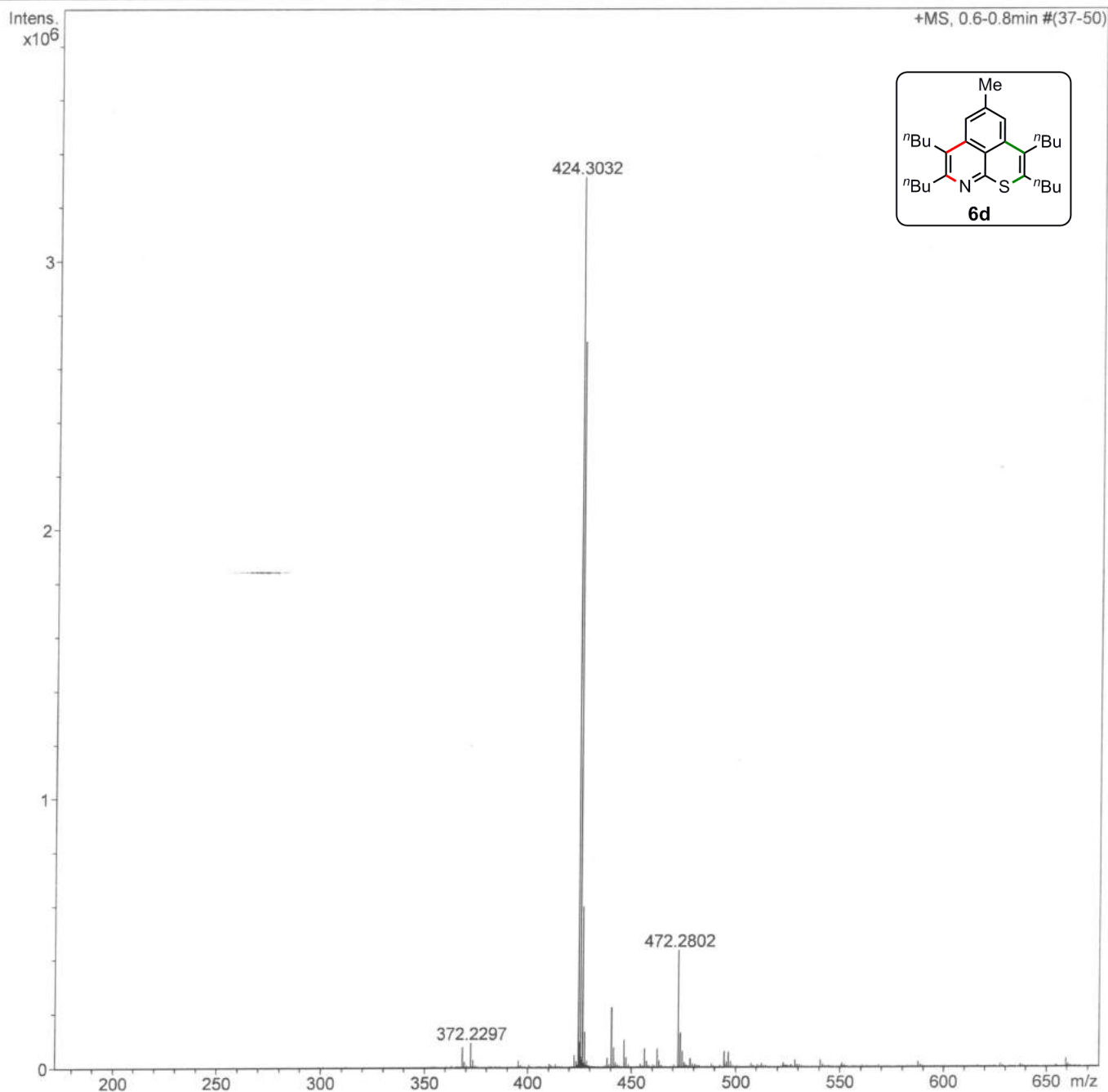
Analysis Name D:\Data\2019\PROF. AKS\july\MJ-16-20.d
Method tune_low.m
Sample Name MJ-16-20-DCM-MEOH
Comment

Acquisition Date 7/15/2019 4:07:55 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 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

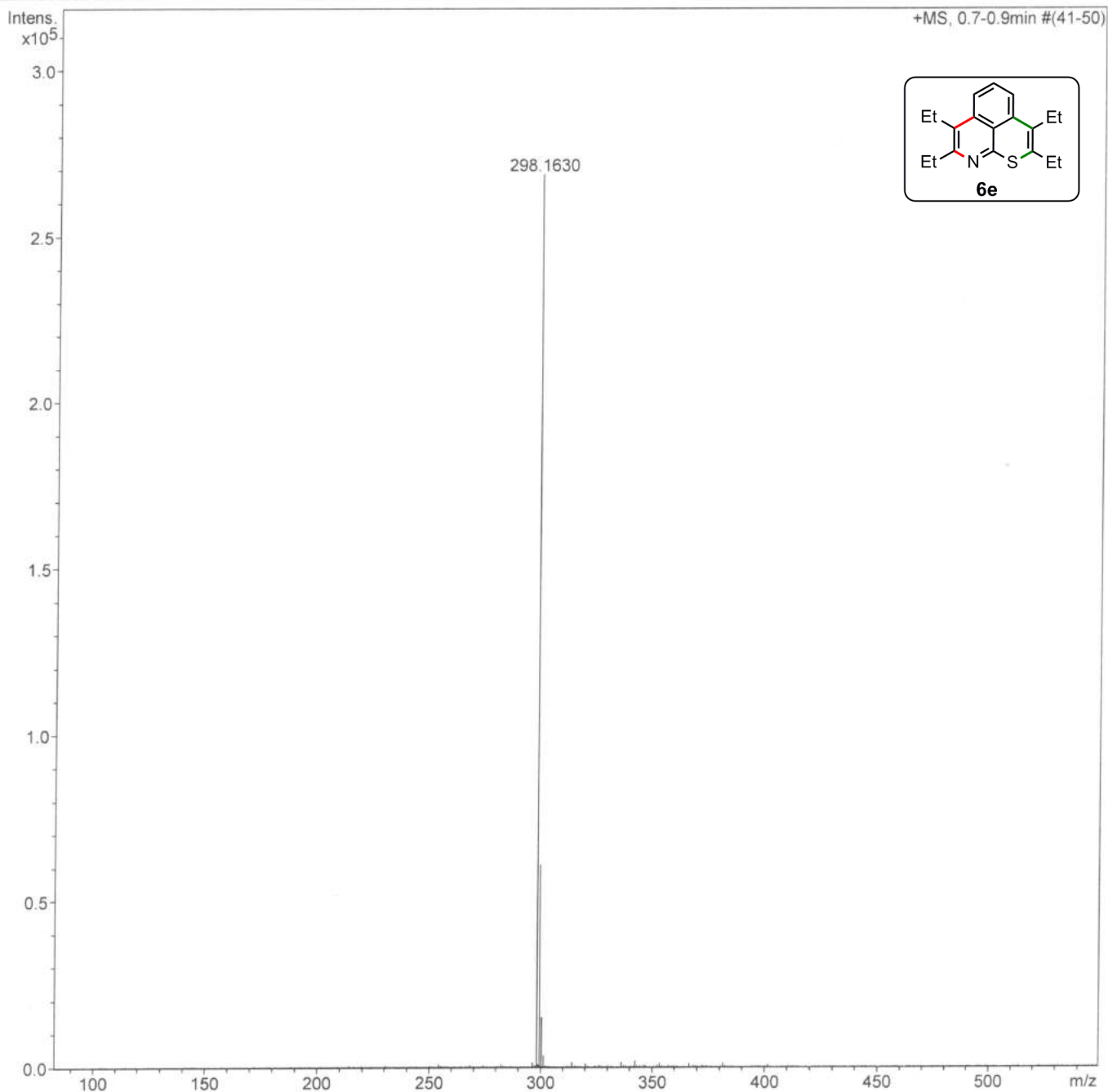
Analysis Name D:\Data\2018\prof aks\march\mj-23-14.d
 Method tune_low.m
 Sample Name mj-23-14
 Comment

Acquisition Date 2/21/2018 7:49:16 AM

Operator Rajesh Vashisth
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 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

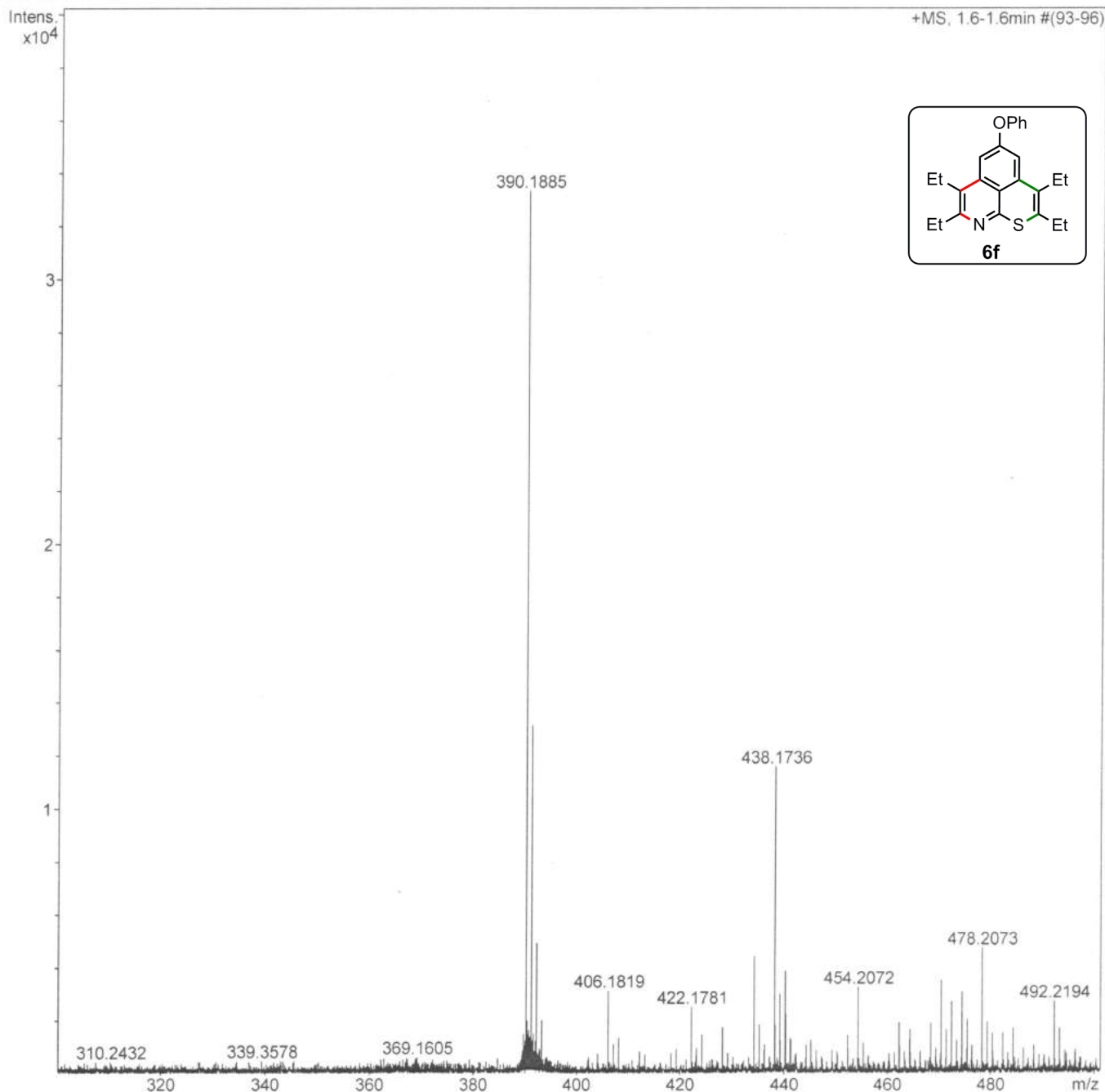
Analysis Name D:\Data\2018\prof aks\DEC\AS-40.d
 Method tune_low_PosR.m
 Sample Name AS-40-DCM-MEOH
 Comment

Acquisition Date 12/24/2018 12:44:09 PM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



MJ-17-566

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ACRHEM

XEVO-G2XSQTOF#YEA1155

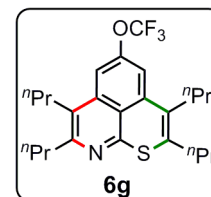
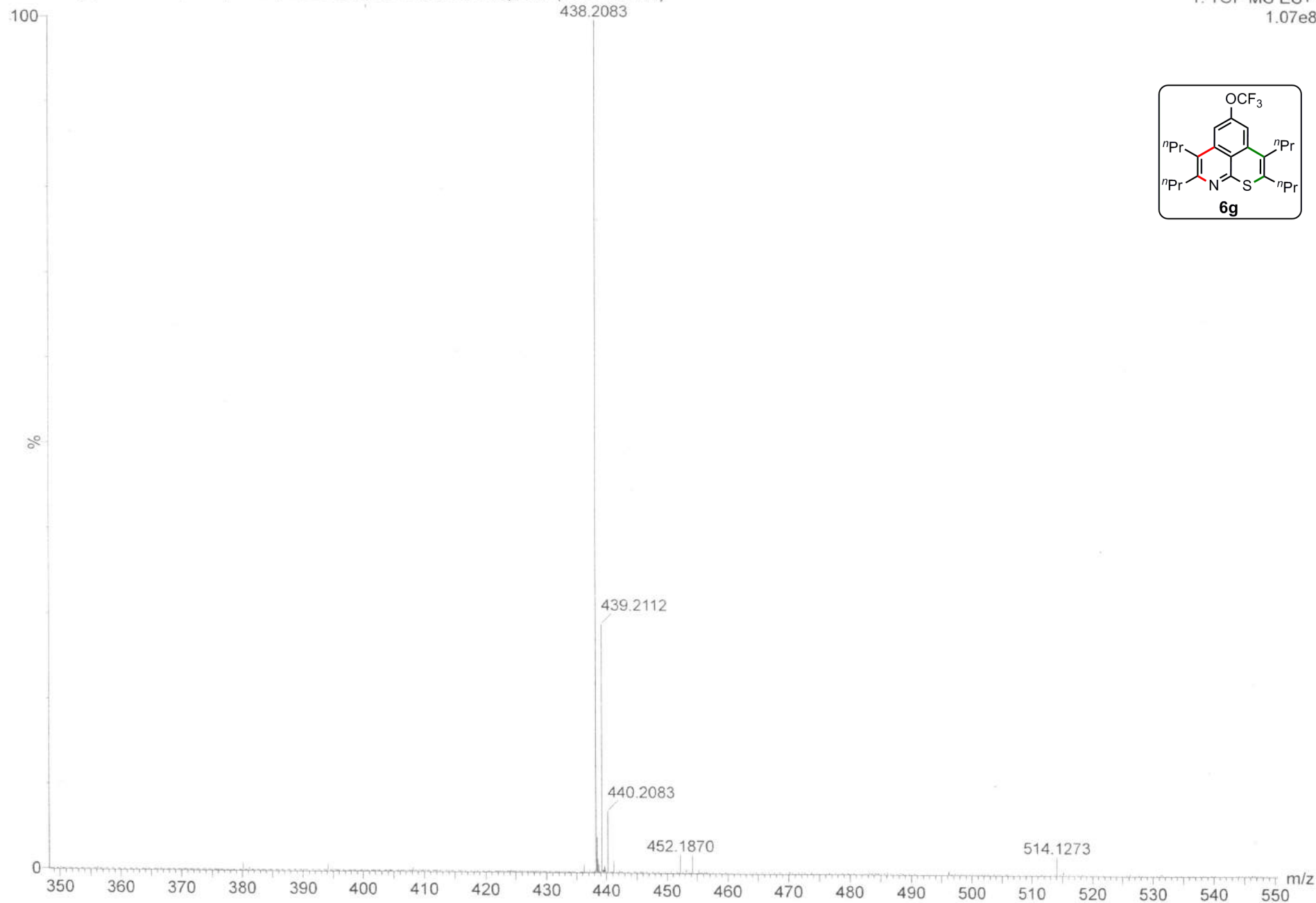
10-Nov-2020

14:47:26

10112020_18 +VE 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:26-77:114)

1: TOF MS ES+

1.07e8



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

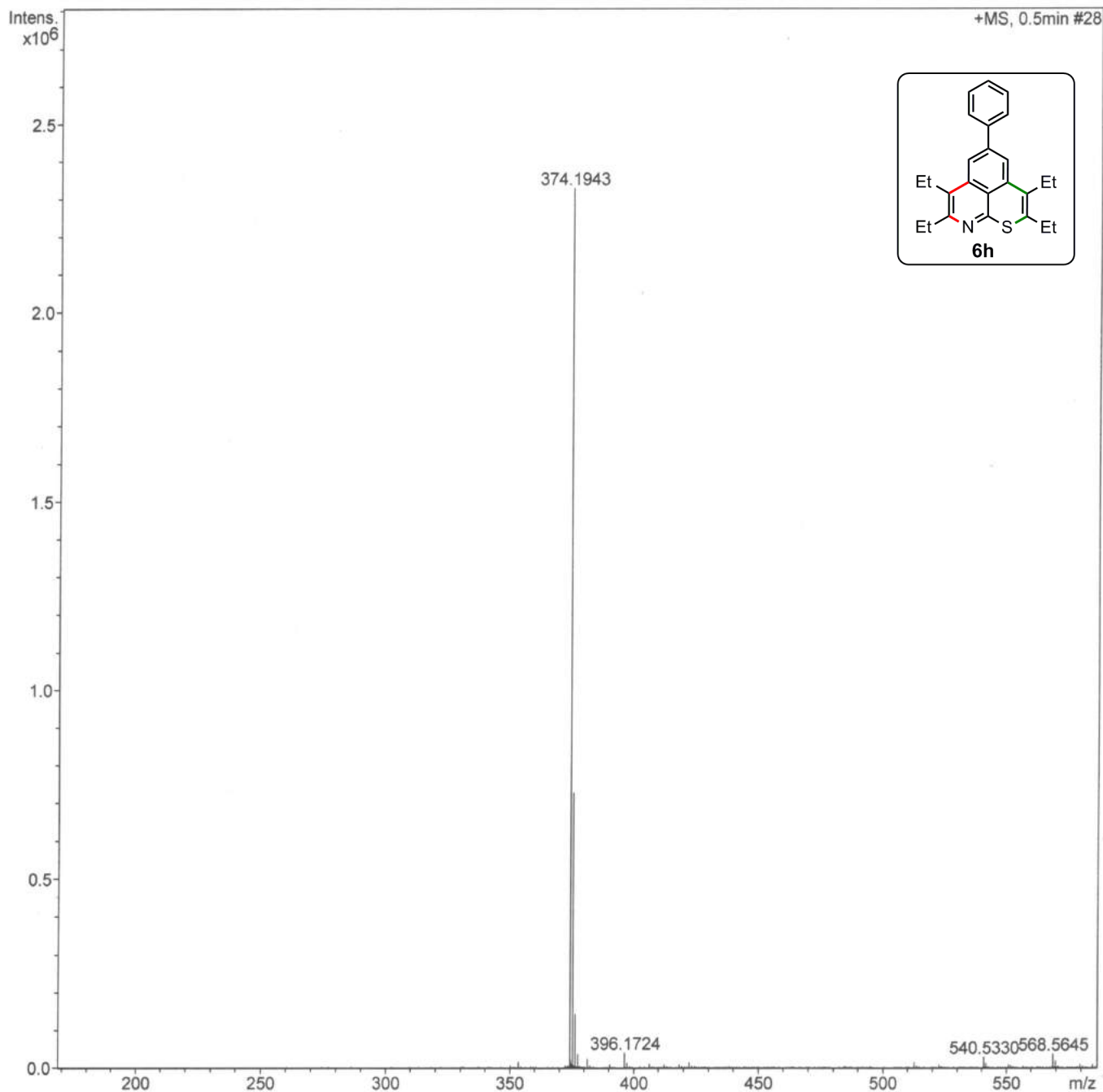
Analysis Name D:\Data\2018\prof aks\NOVMJ-56-15.d
 Method tune_low.m
 Sample Name MJ-56-15-dcm-meoh
 Comment

Acquisition Date 11/12/2018 12:40:02 PM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

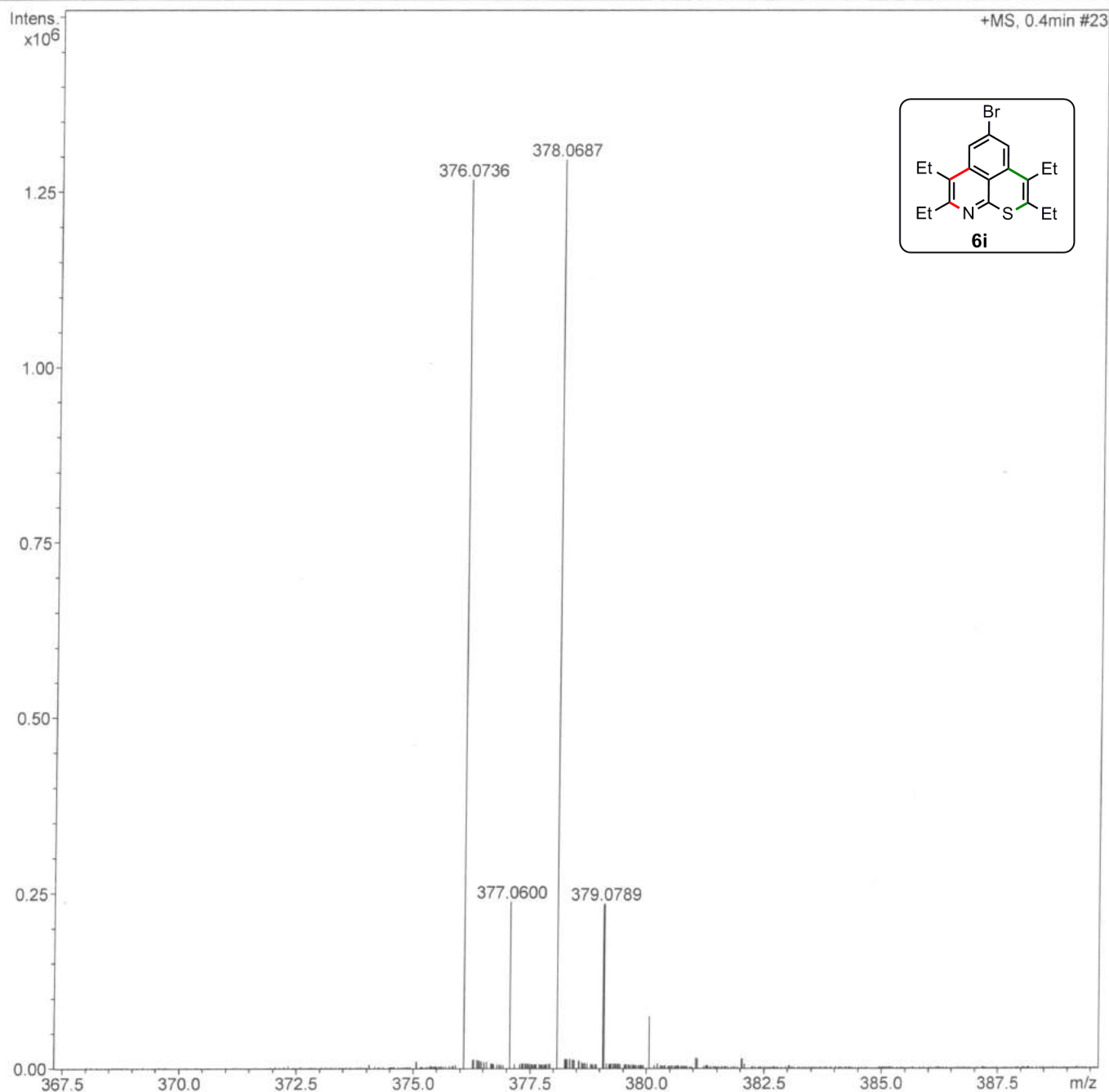
Analysis Name D:\Data\2018\prof aks\march\MJ-17-14.d
Method tune_low.m
Sample Name MJ-17-14
Comment

Acquisition Date 2/22/2018 4:13:37 AM

Operator Rajesh Vashisth
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 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

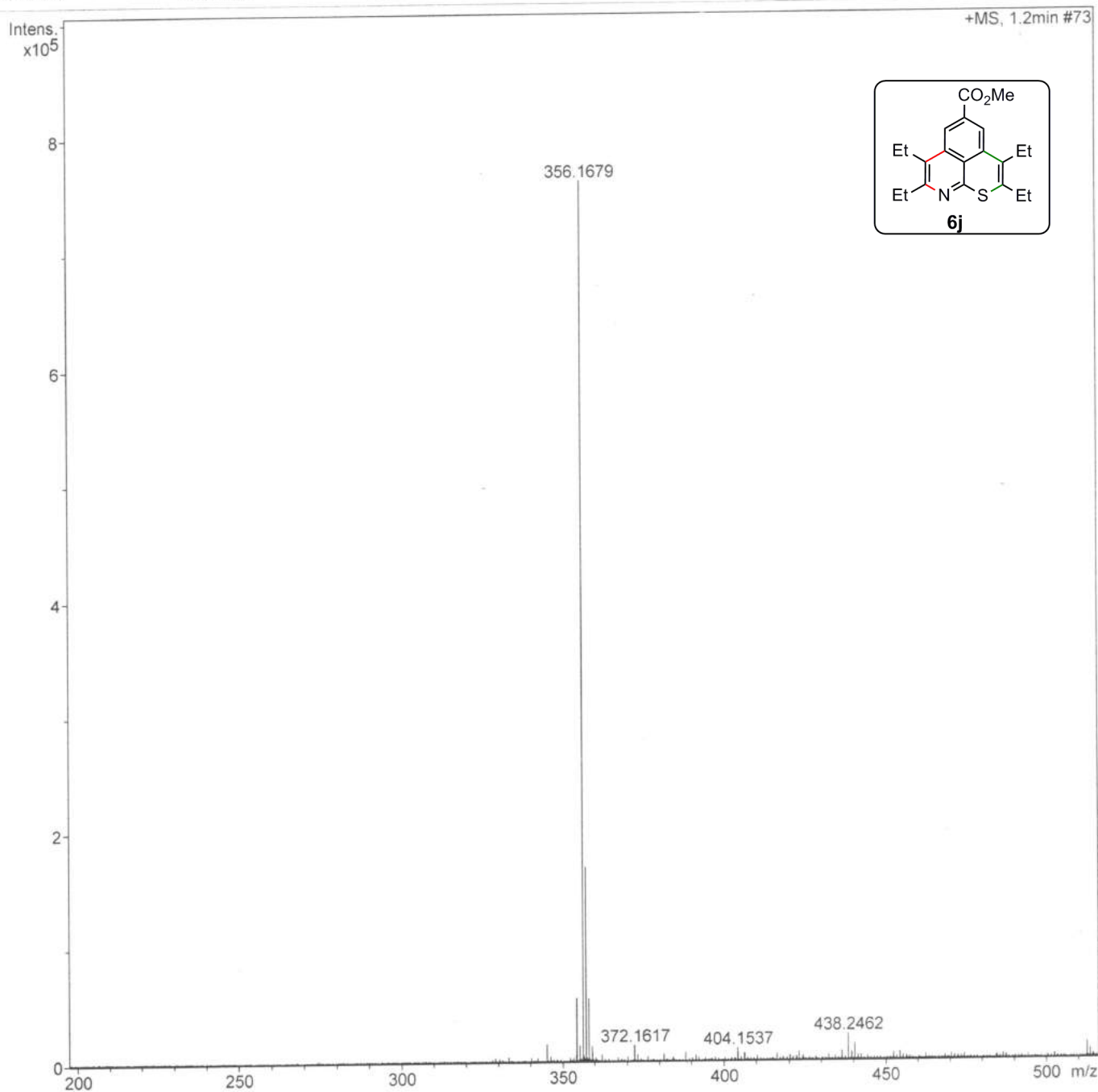
Analysis Name D:\Data\2018\prof aks\DEC\AS-41.d
 Method tune_low_PosR.m
 Sample Name AS-41-DCM-MEOH
 Comment

Acquisition Date 12/24/2018 12:25:39 PM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

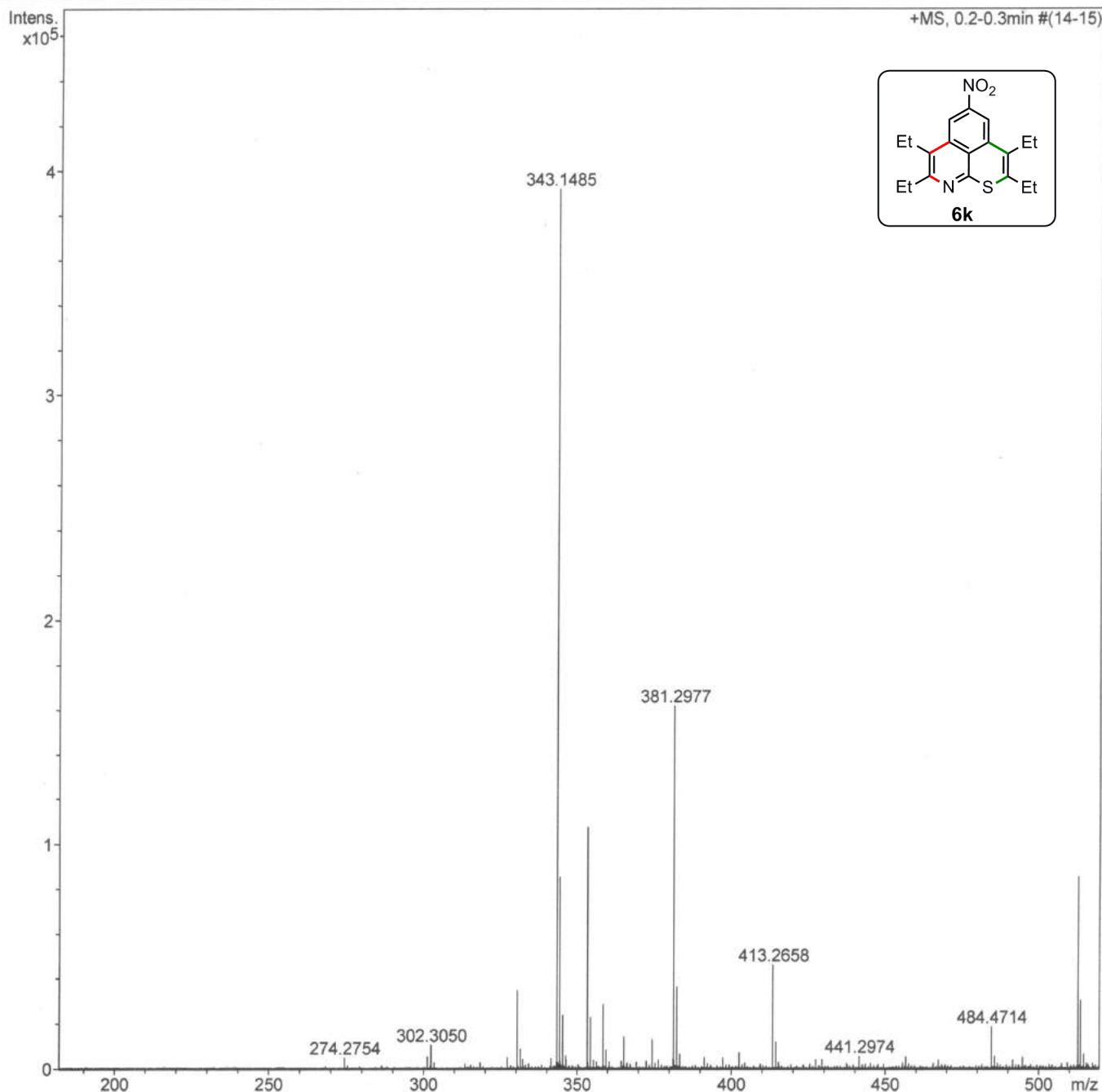
Analysis Name D:\Data\2018\prof aks\NOV\MJ-28-15r.d
 Method tune_low.m
 Sample Name MJ-28-15-DCM-MEOH
 Comment

Acquisition Date 11/5/2018 10:37:24 AM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	2800 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	200.0 Vpp	Set Divert Valve	Waste



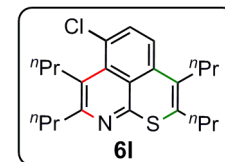
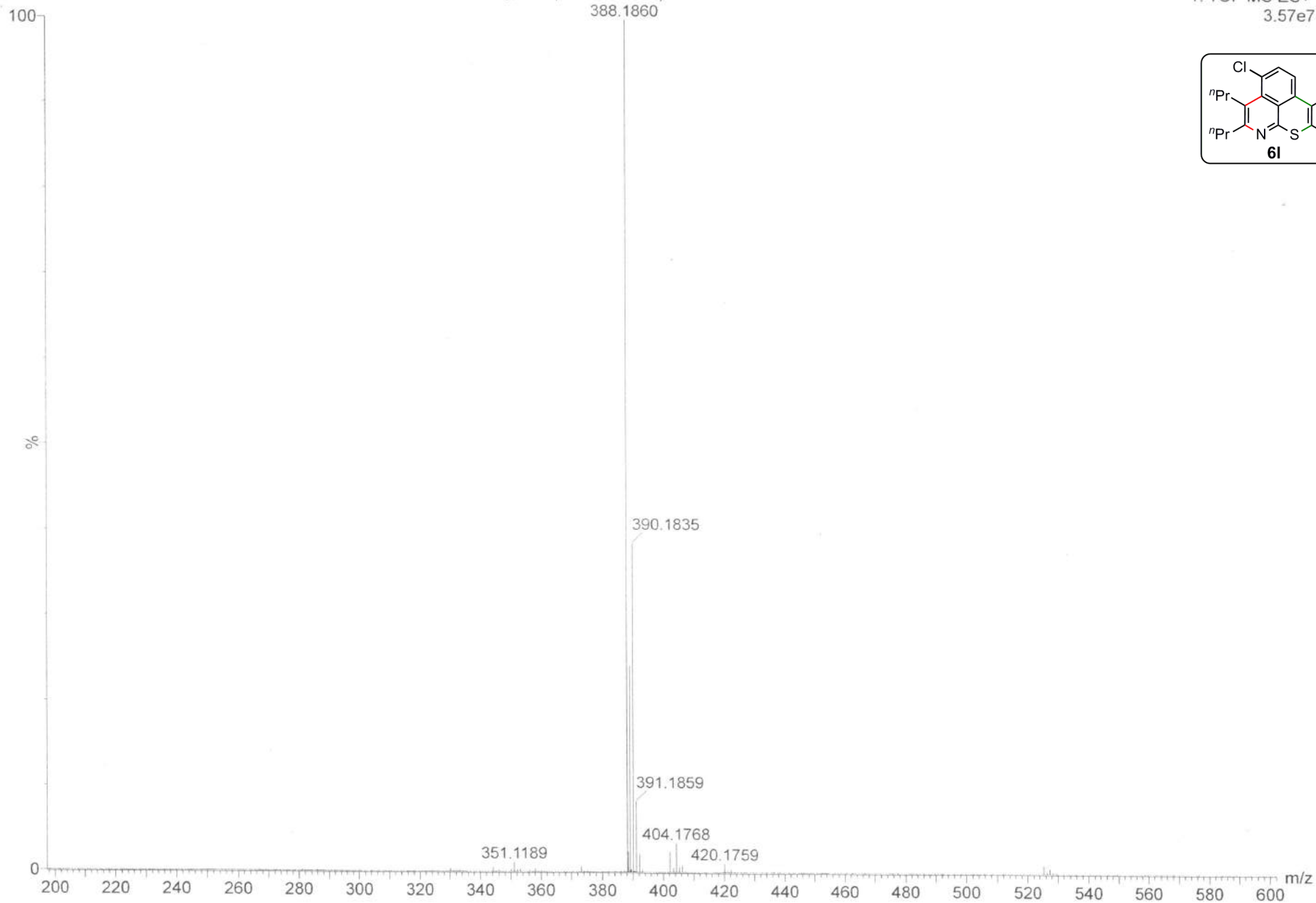
MJ-17-256

UNIVERSITY OF HYDERABAD
ACRHEM
XEVO-G2XSQTOF#YEA1155

18-Nov-2020
12:25:52

18112020_16 +VE 18 (0.191) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (18:24-82:124)

1: TOF MS ES+
3.57e7



UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

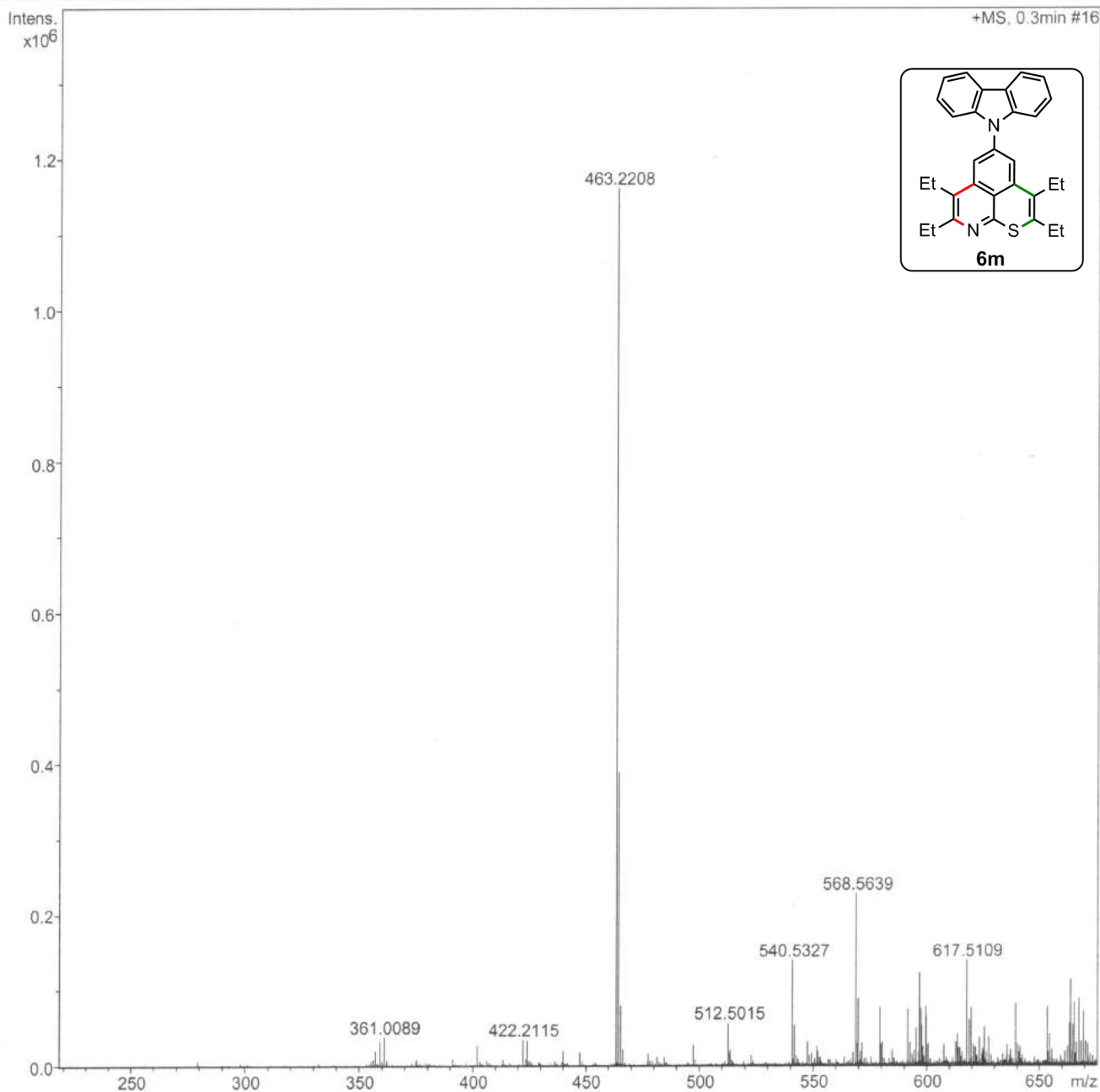
Analysis Name D:\Data\2018\prof aks\DEC\S-1-129.d
 Method tune_low_Pos.m
 Sample Name S-1-129-DCM-MEOH
 Comment

Acquisition Date 12/13/2018 12:01:21 PM

Operator UOH-Chemistry
 Instrument maXis 10138

Acquisition Parameter

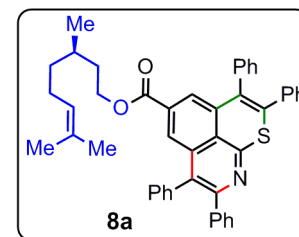
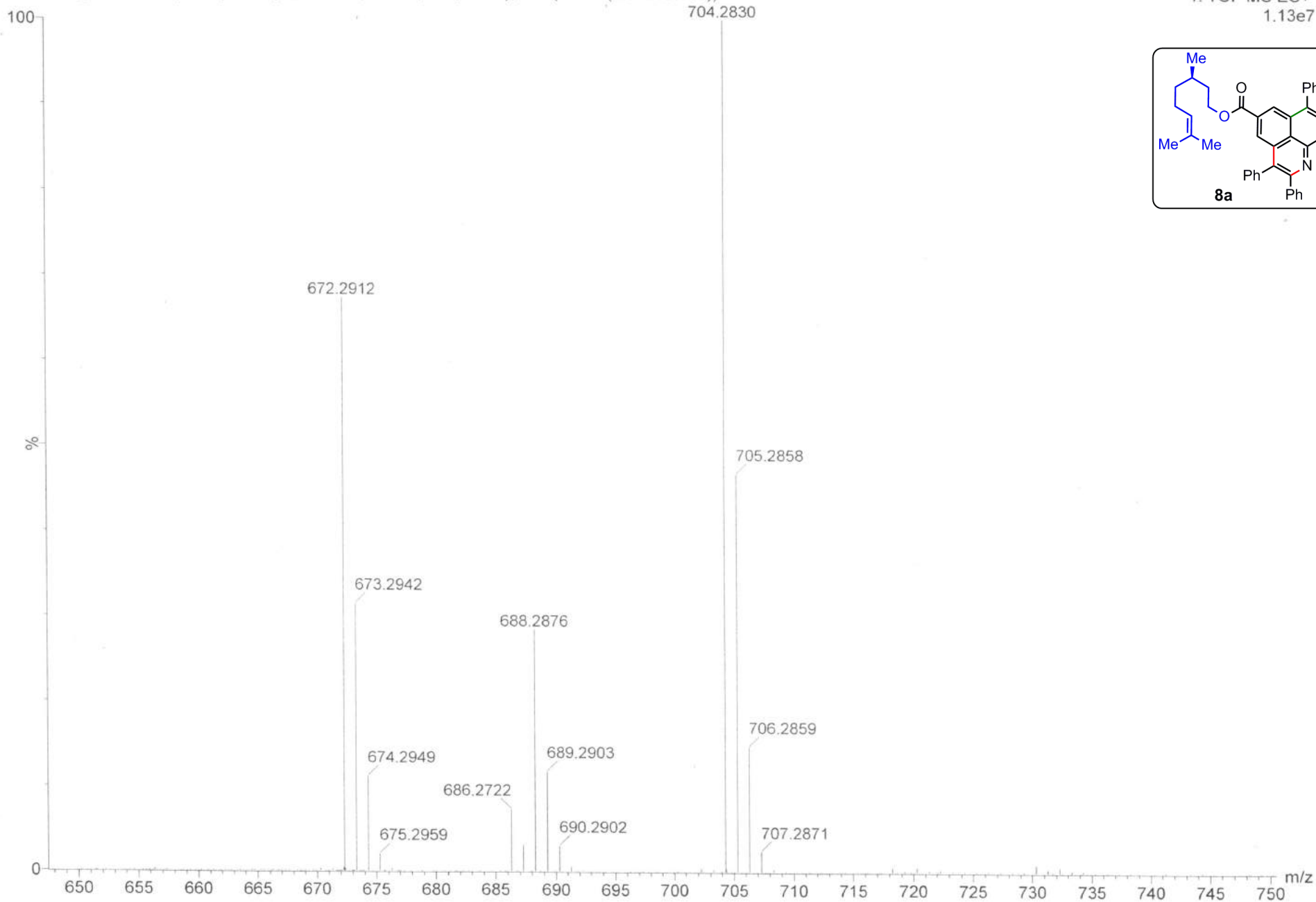
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



10112020_16 +VE 45 (0.462) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (45:54-(1:5+145:166))

1: TOF MS ES+

1.13e7



MJ-17-213R

UNIVERSITY OF HYDERABAD

ACRHEM

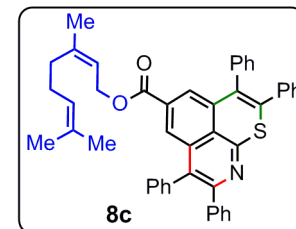
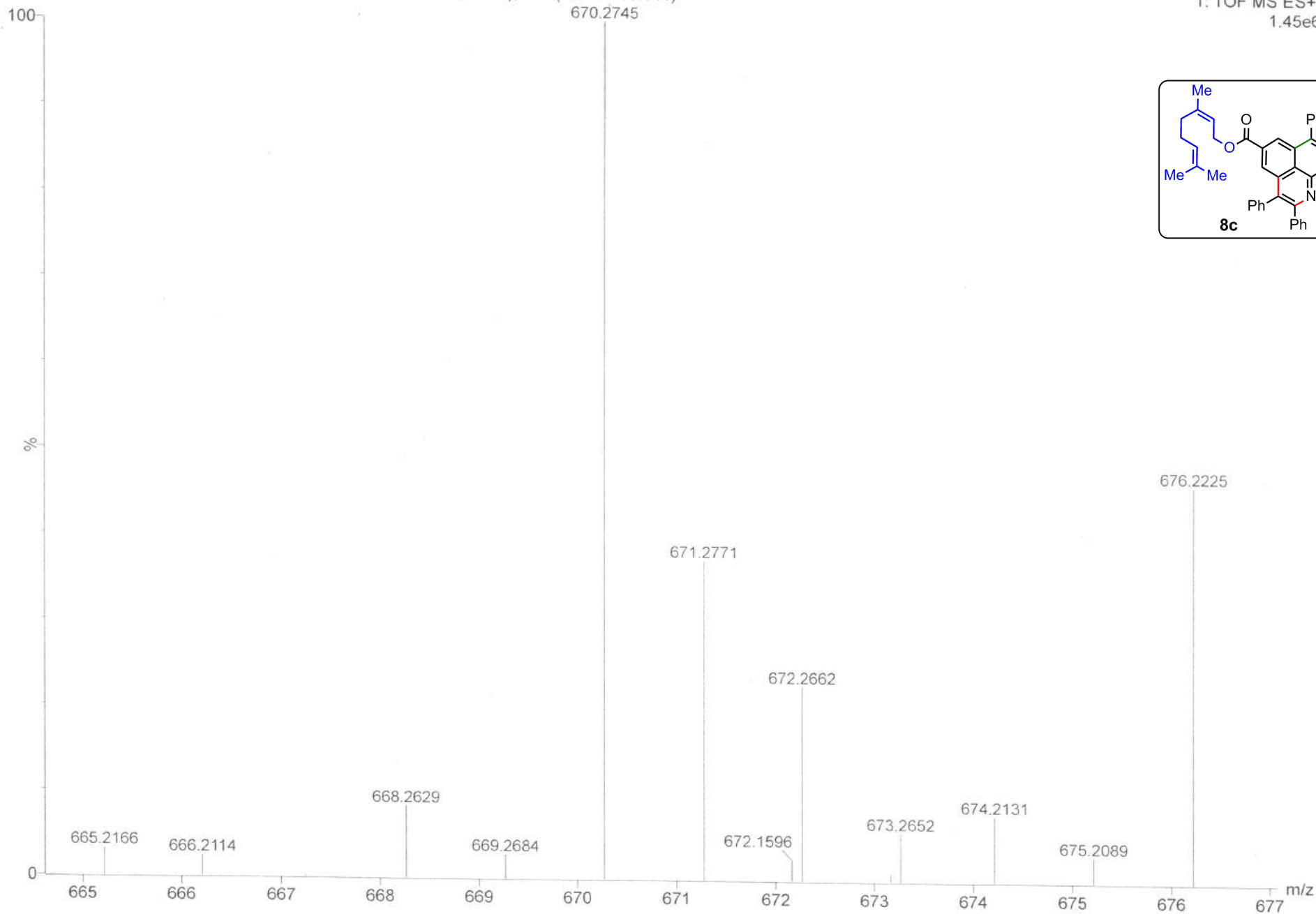
XEVO-G2XSQTOF#YEA1155

06-Nov-2020

12:30:06

06112020_14 +VE 26 (0.279) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (26:36-103:141)

1: TOF MS ES+
1.45e6



AS 405

Display Report

Analysis Info

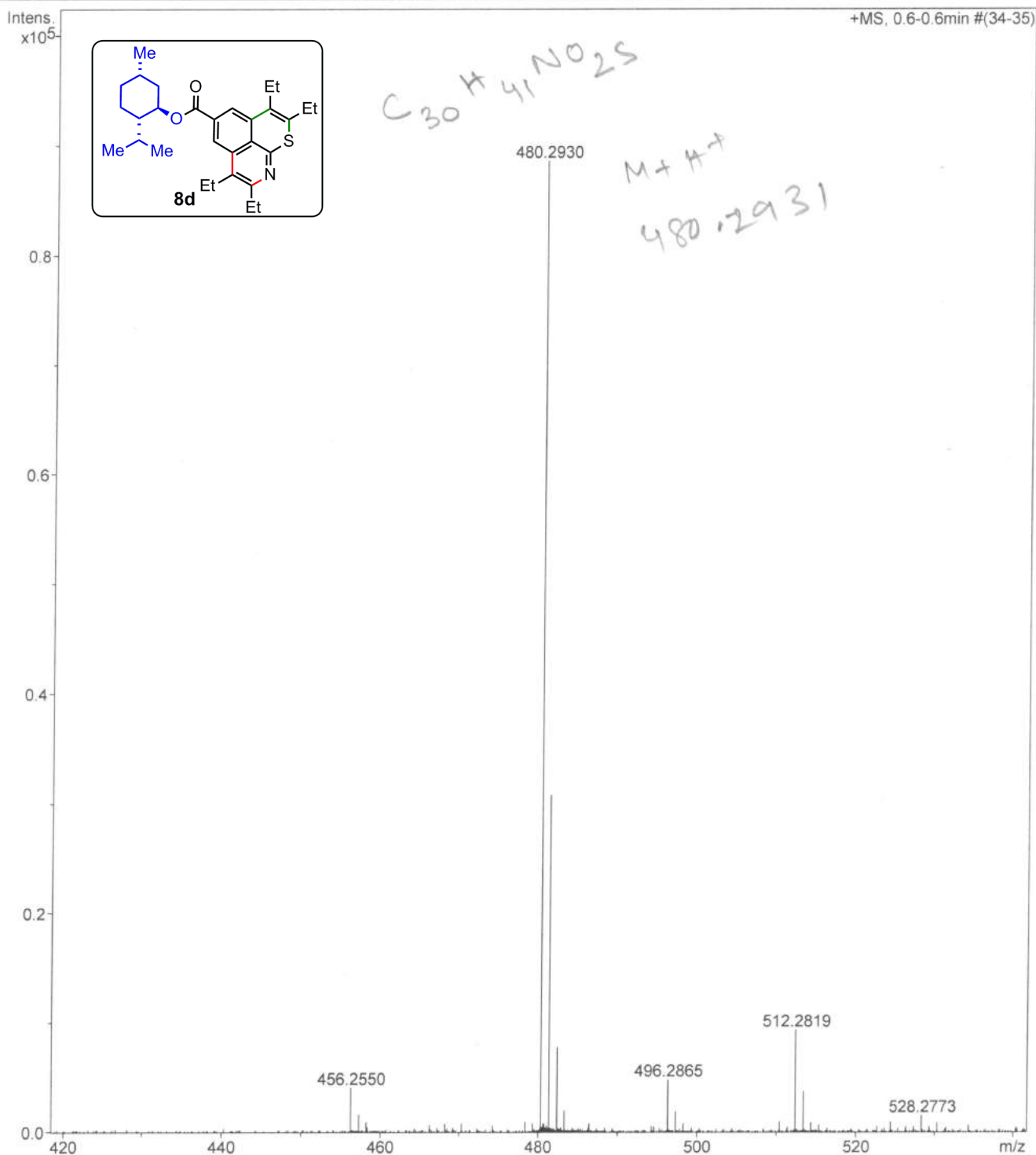
Analysis Name D:\Data\2019\PROF. AKS\OCT\SD-17-25-1.d
Method tune_low_Pos-R2.m
Sample Name SD-17-25
Comment

Acquisition Date 10/29/2019 3:59:47 AM

Operator UOH-Chemistry
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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



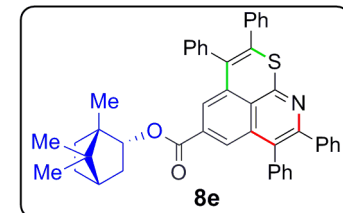
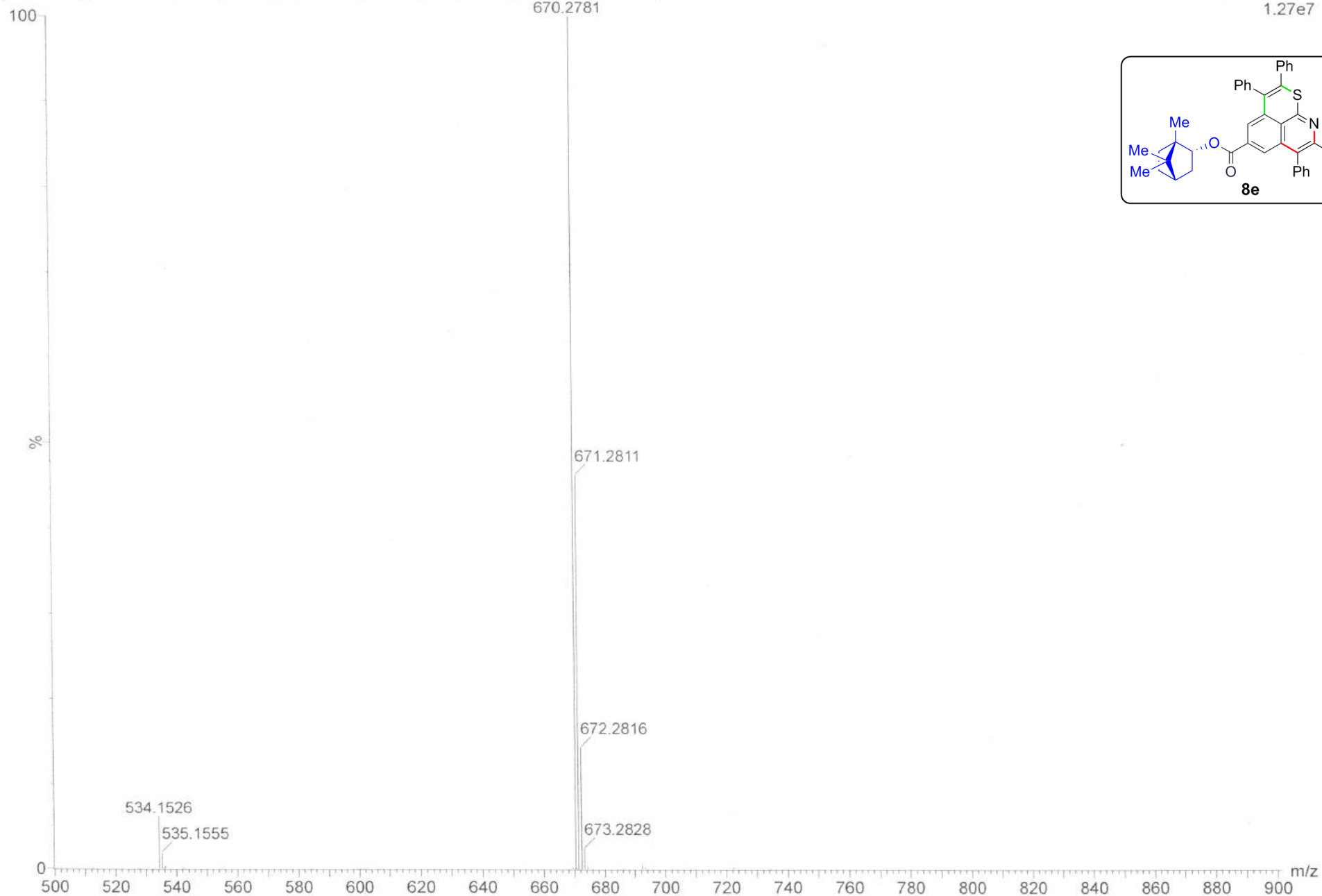
MJ-8-48

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ACRHEM
XEVO-G2XSQTOF#YEA1155

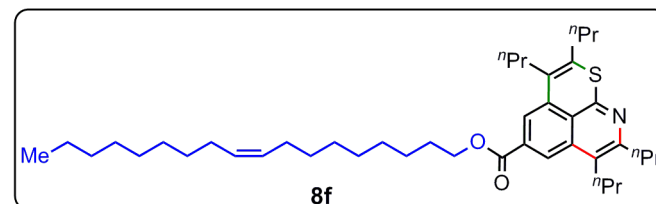
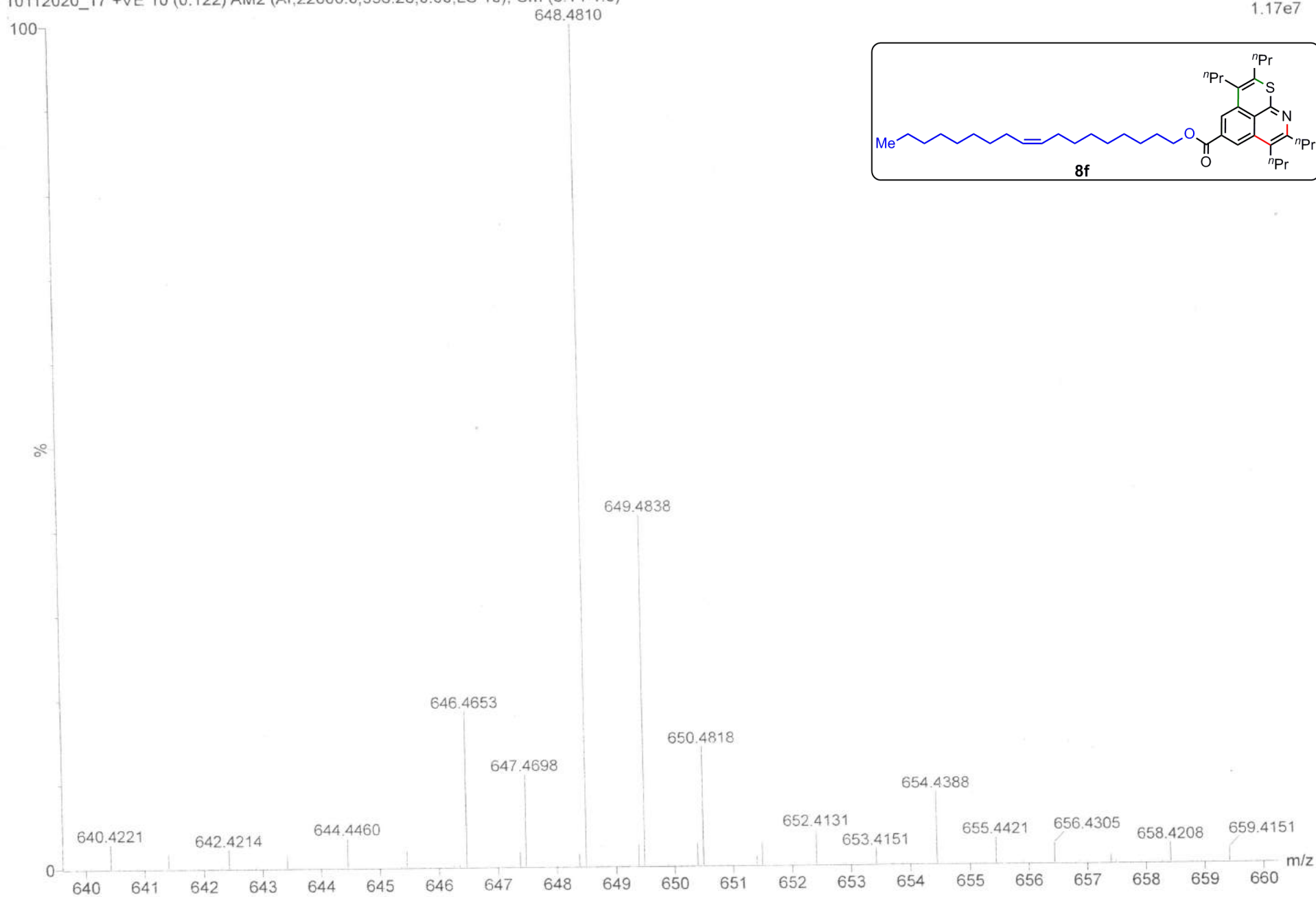
18-Nov-2020
12:28:34

18112020_17 +VE 19 (0.219) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (19:26-70:143)

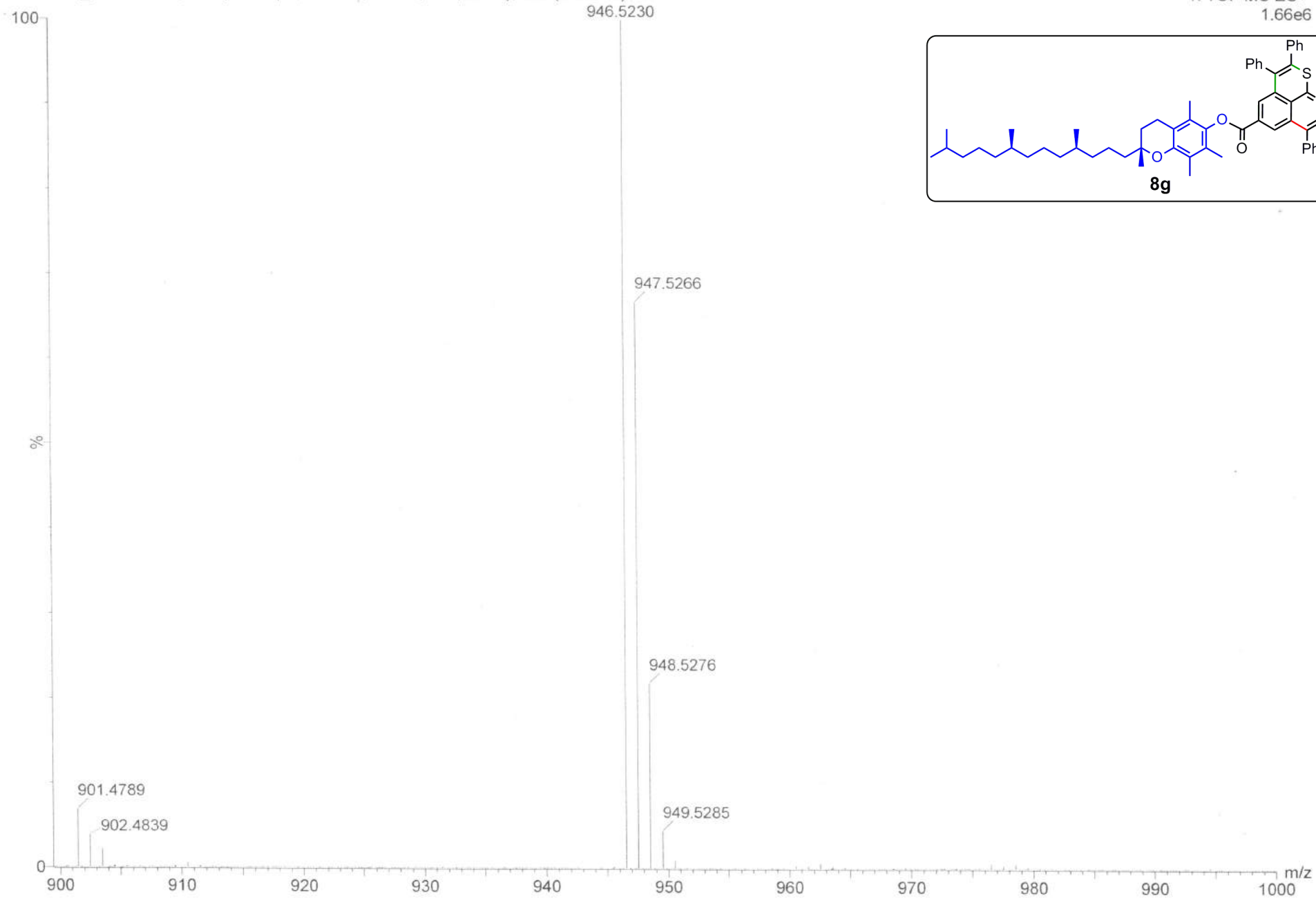
1: TOF MS ES+
1.27e7



10112020_17 +VE 10 (0.122) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (8:14-1:5)



06112020_12 +VE 10 (0.122) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (8:12-1:5)

1: TOF MS ES+
1.66e6

Display Report

Analysis Info

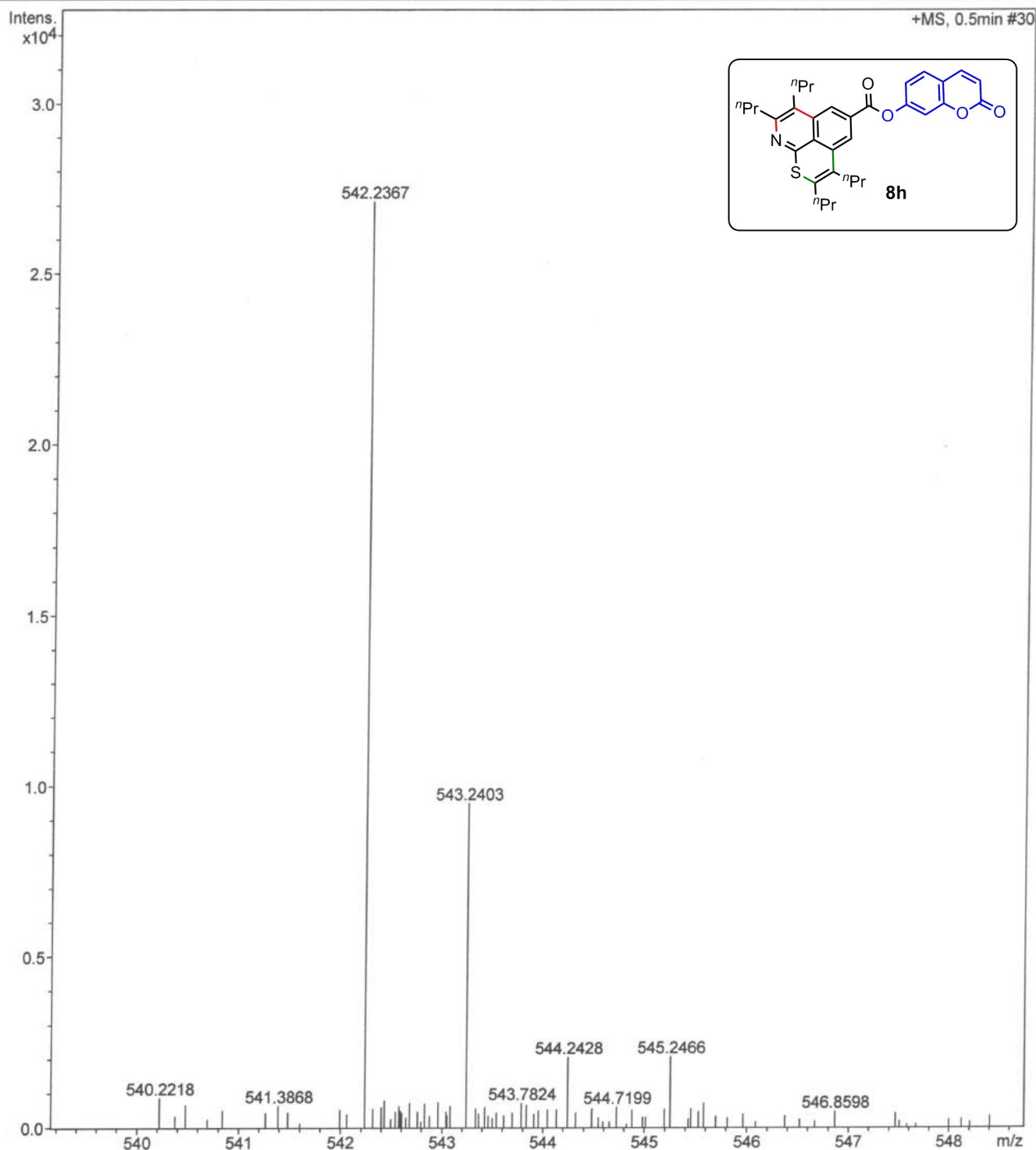
Analysis Name D:\Data\2020\PROF.AKS\MAR\SRS-8-10R.d
Method tune_low_PosR.m
Sample Name SRS-8-10
Comment

Acquisition Date 3/19/2020 11:54:23 AM

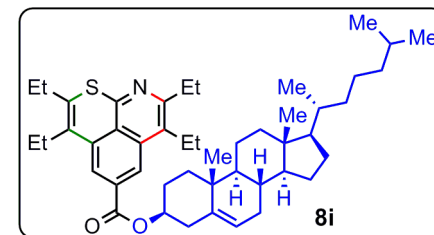
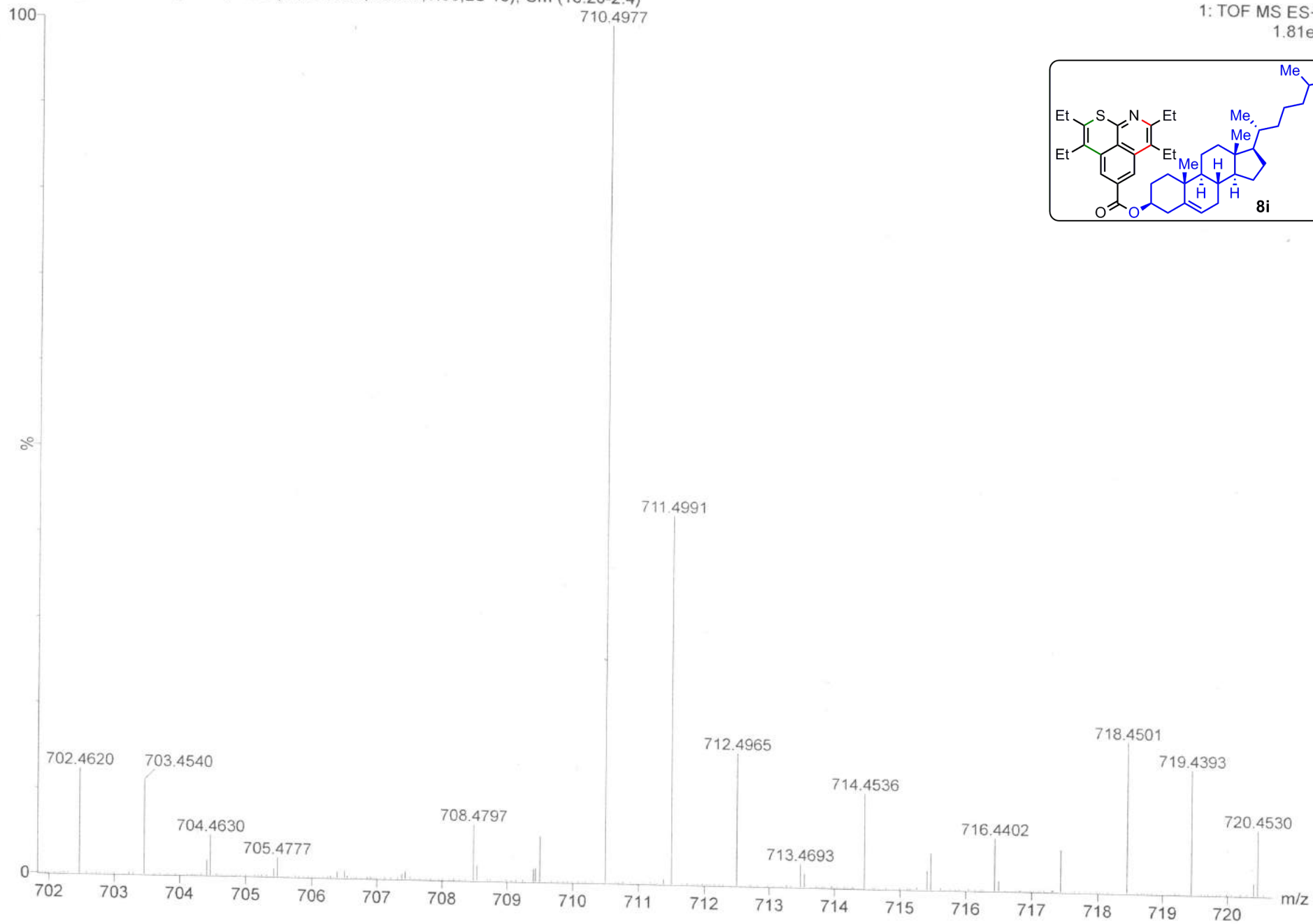
Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2600 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



10112020_15 +VE 18 (0.191) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (18:20-2:4)

1: TOF MS ES+
1.81e5

Display Report

Analysis Info

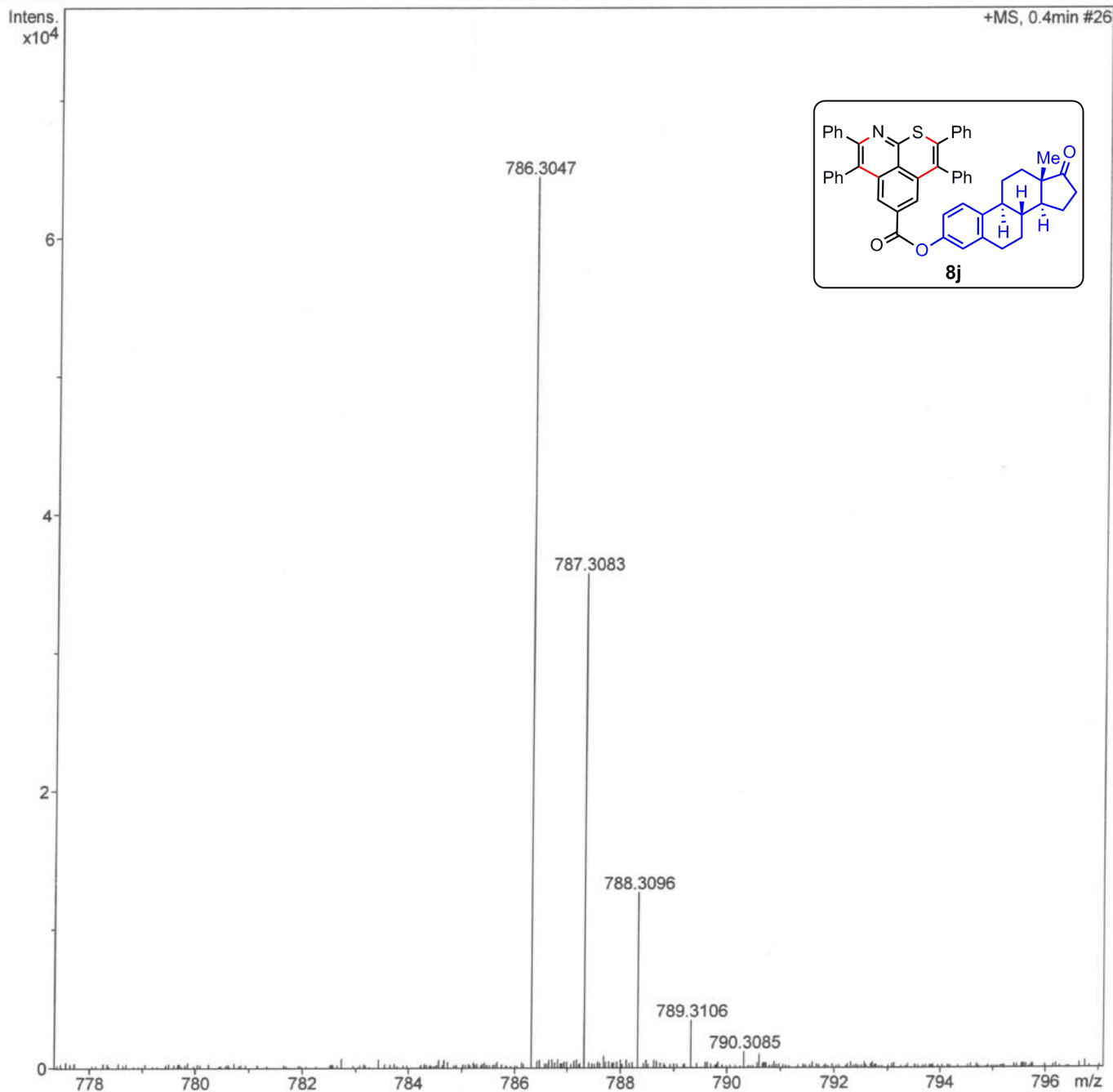
Analysis Name	D:\Data\2020\PROF.AKS\MAR\SRS-8-88.d
Method	tune_low_Pos-R2.m
Sample Name	SRS-8-88
Comment	

Acquisition Date 3/16/2020 4:11:49 PM

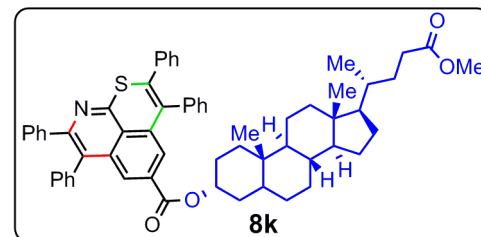
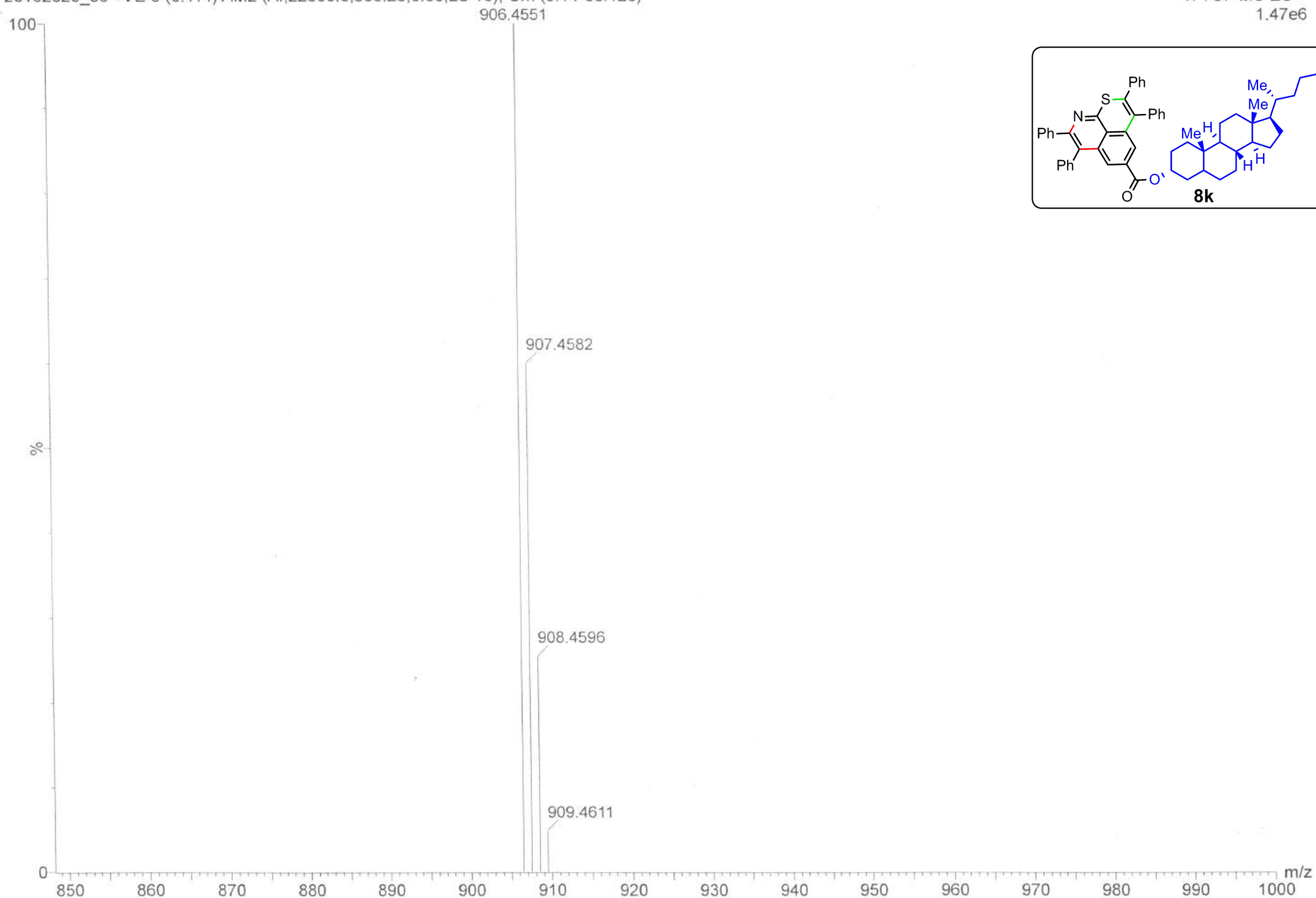
Operator	UOH-Chemistry
Instrument	maXis 10138

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	2580 m/z	Set Collision Cell RF	300.0 Vpp	Set Divert Valve	Waste



20102020_36 +VE 9 (0.114) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (9:14-88:126)

1: TOF MS ES+
1.47e6

Display Report

Analysis Info

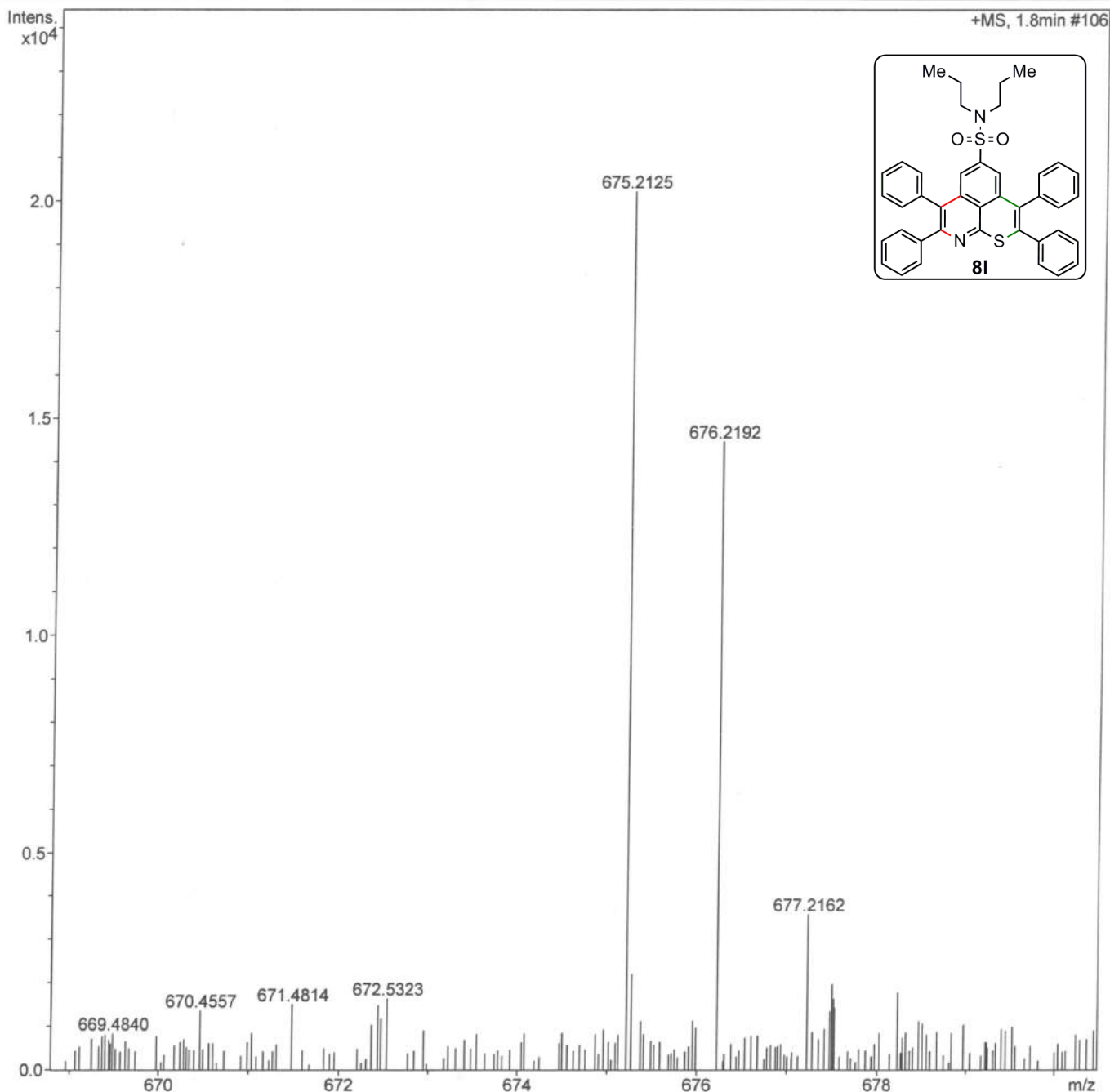
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-98.d
Method tune_low_PosR.m
Sample Name MJ-17-98
Comment

Acquisition Date 3/13/2020 12:41:32 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



MJ-17-97R

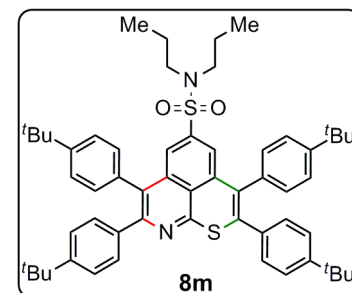
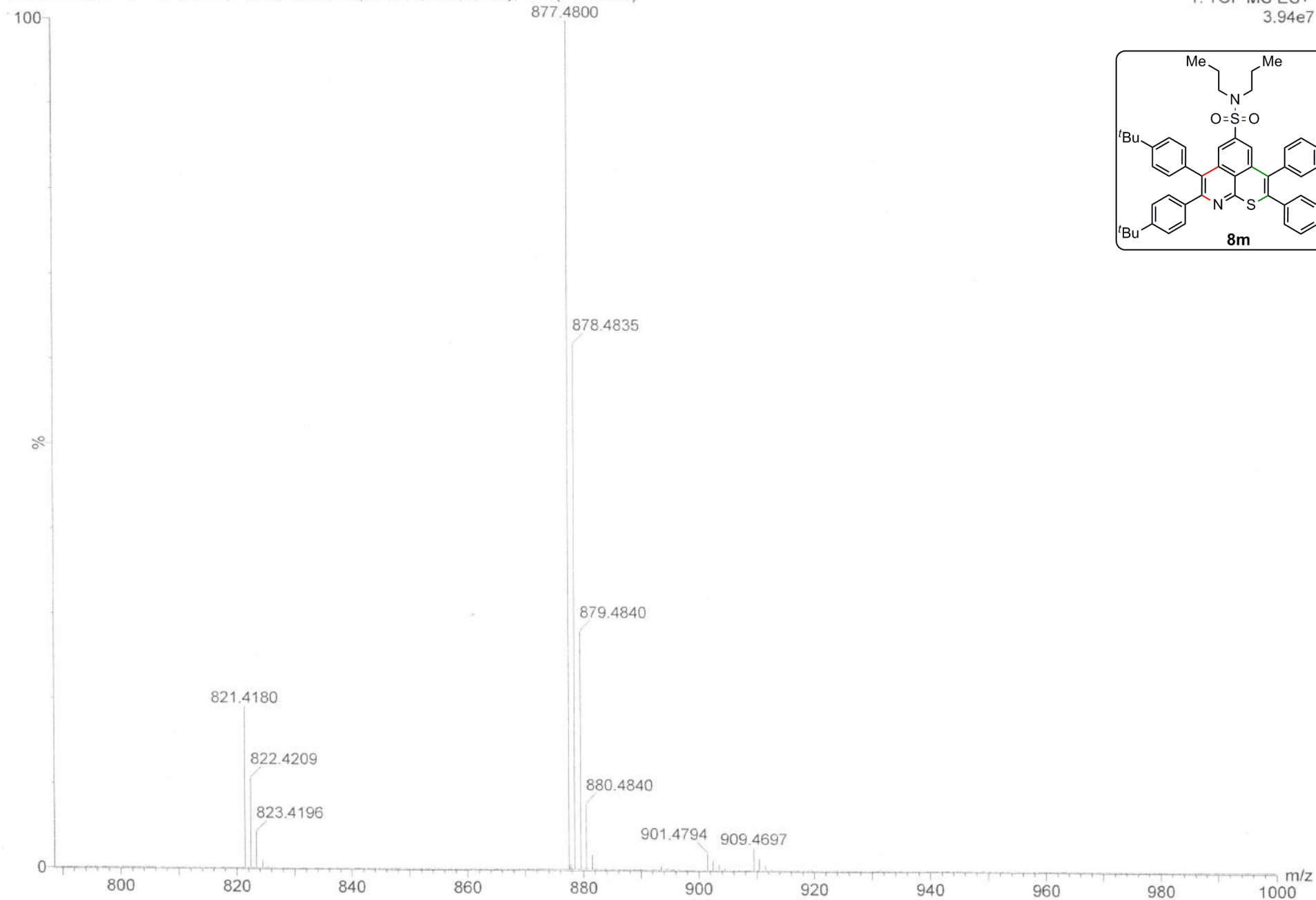
UNIVERSITY OF HYDERABAD
ACRHEM
XEVO-G2XSQTOF#YEA1155

06-Nov-2020

12:22:11

06112020_11 +VE 14 (0.157) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (14:22-1:5)

1: TOF MS ES+
3.94e7



Display Report

Analysis Info

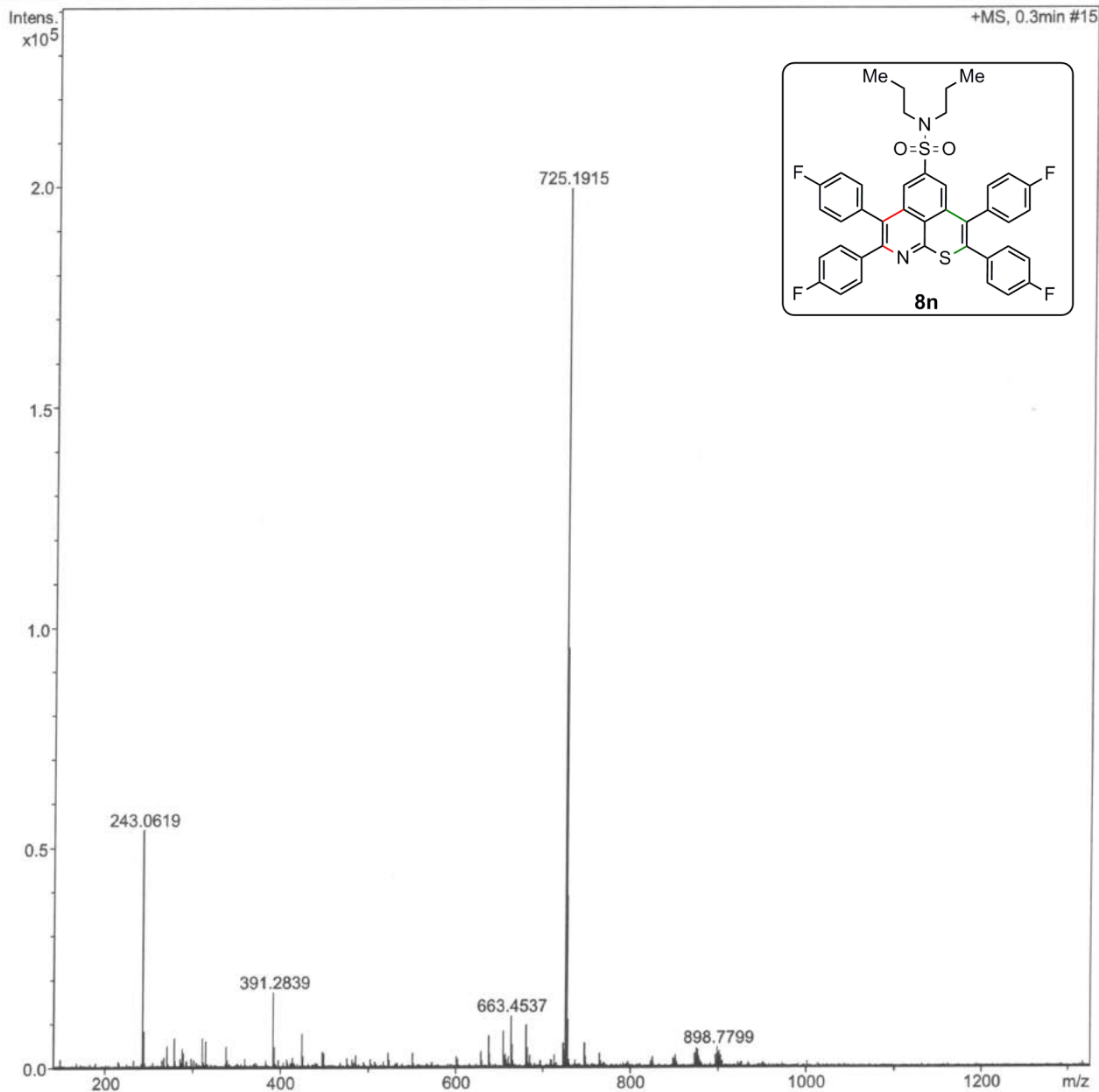
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-93.d
Method tune_low.m
Sample Name MJ-17-93
Comment

Acquisition Date 3/13/2020 3:37:11 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

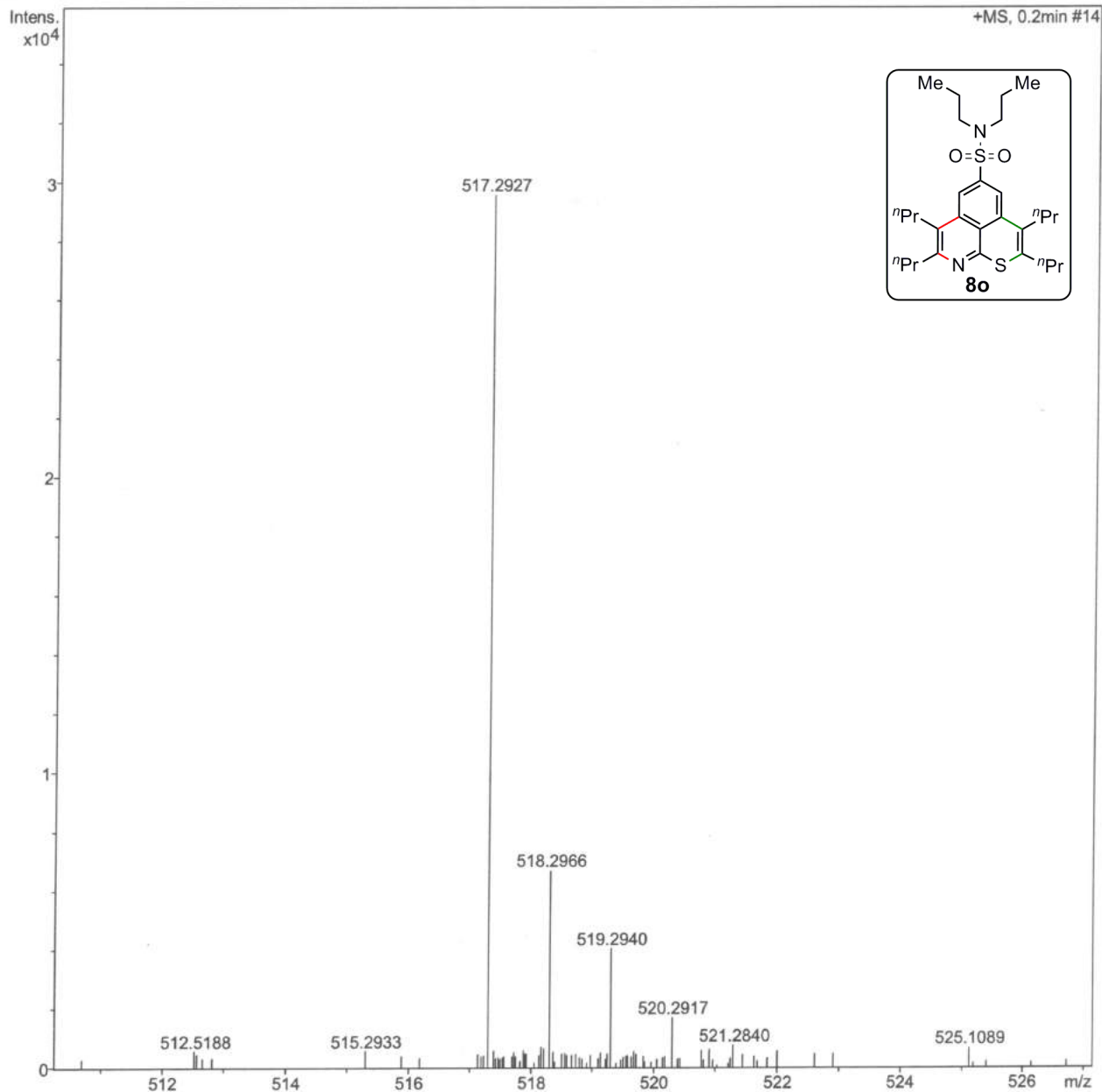
Analysis Name D:\Data\2020\PROF.AKS\MAR\MJ-17-94R.d
Method tune_low_PosR.m
Sample Name MJ-17-94
Comment

Acquisition Date 3/12/2020 4:54:31 PM

Operator UOH-Chemistry
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	2800 V	Set Dry Heater	250 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

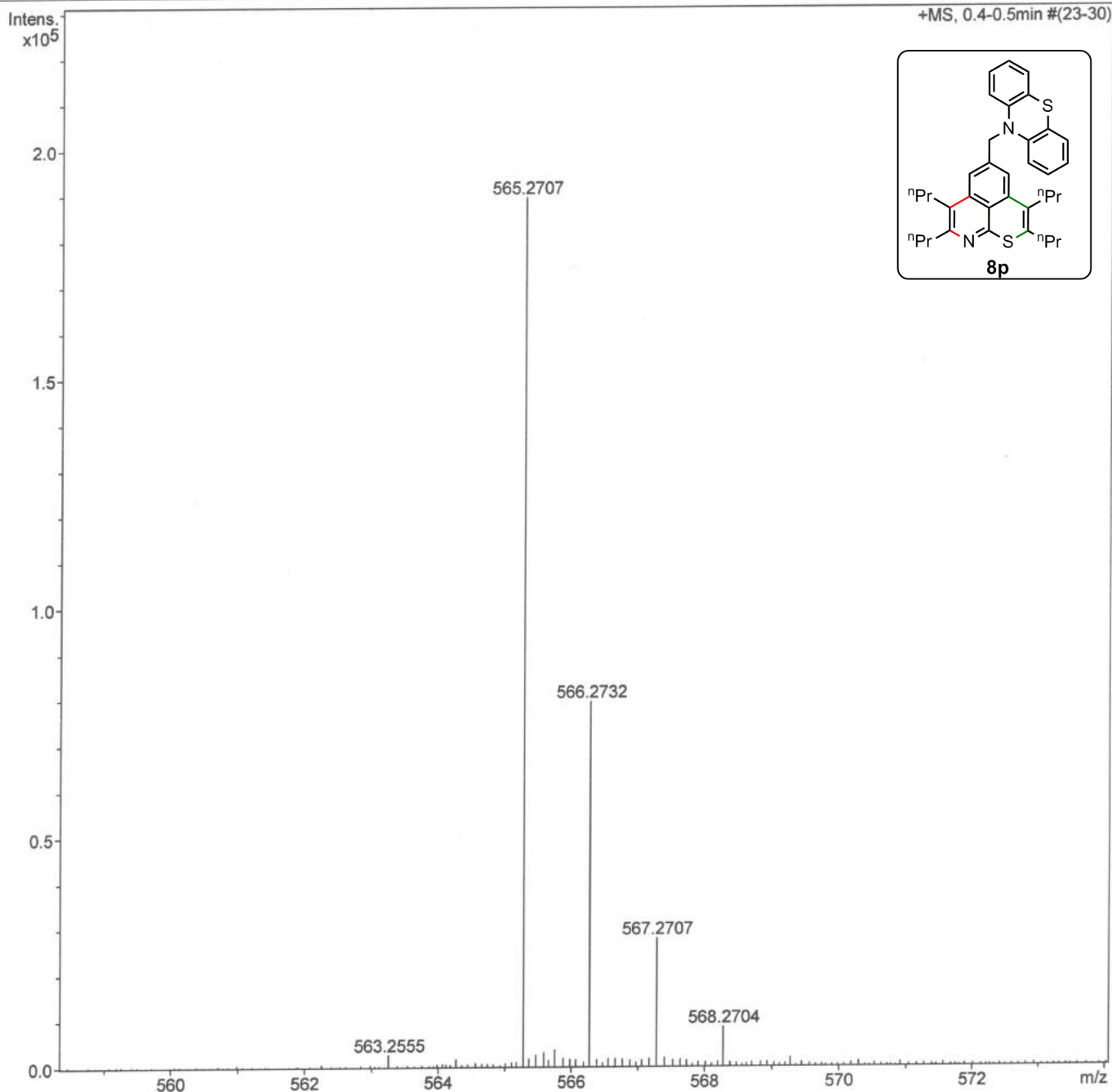
Analysis Name D:\Data\2020\PROF.AKSMAR\SRS-8-93.d
Method tune_low_Pos-R2.m
Sample Name SRS-8-93
Comment

Acquisition Date 3/16/2020 3:57:31 PM

Operator UOH-Chemistry
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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Display Report

Analysis Info

Analysis Name	D:\Data\2020\PROF.AKS\MAR\SRS-8-91.d
Method	tune_low.m
Sample Name	SRS-8-91
Comment	

Acquisition Date 3/16/2020 3:50:59 PM

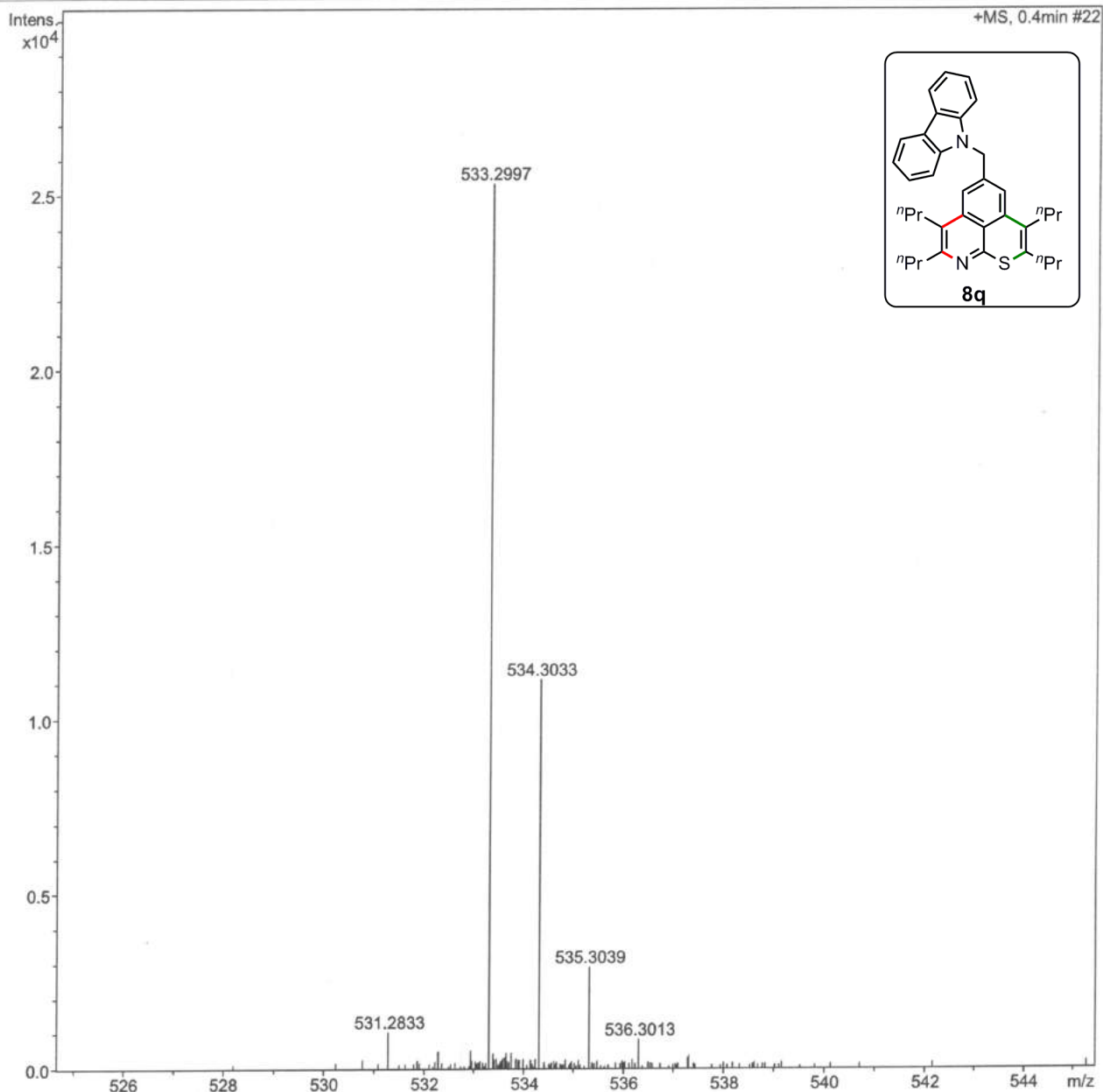
Operator	UOH-Chemistry
Instrument	maXis 10138

Acquisition Parameter

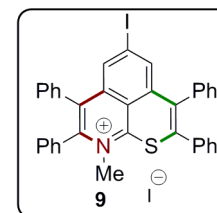
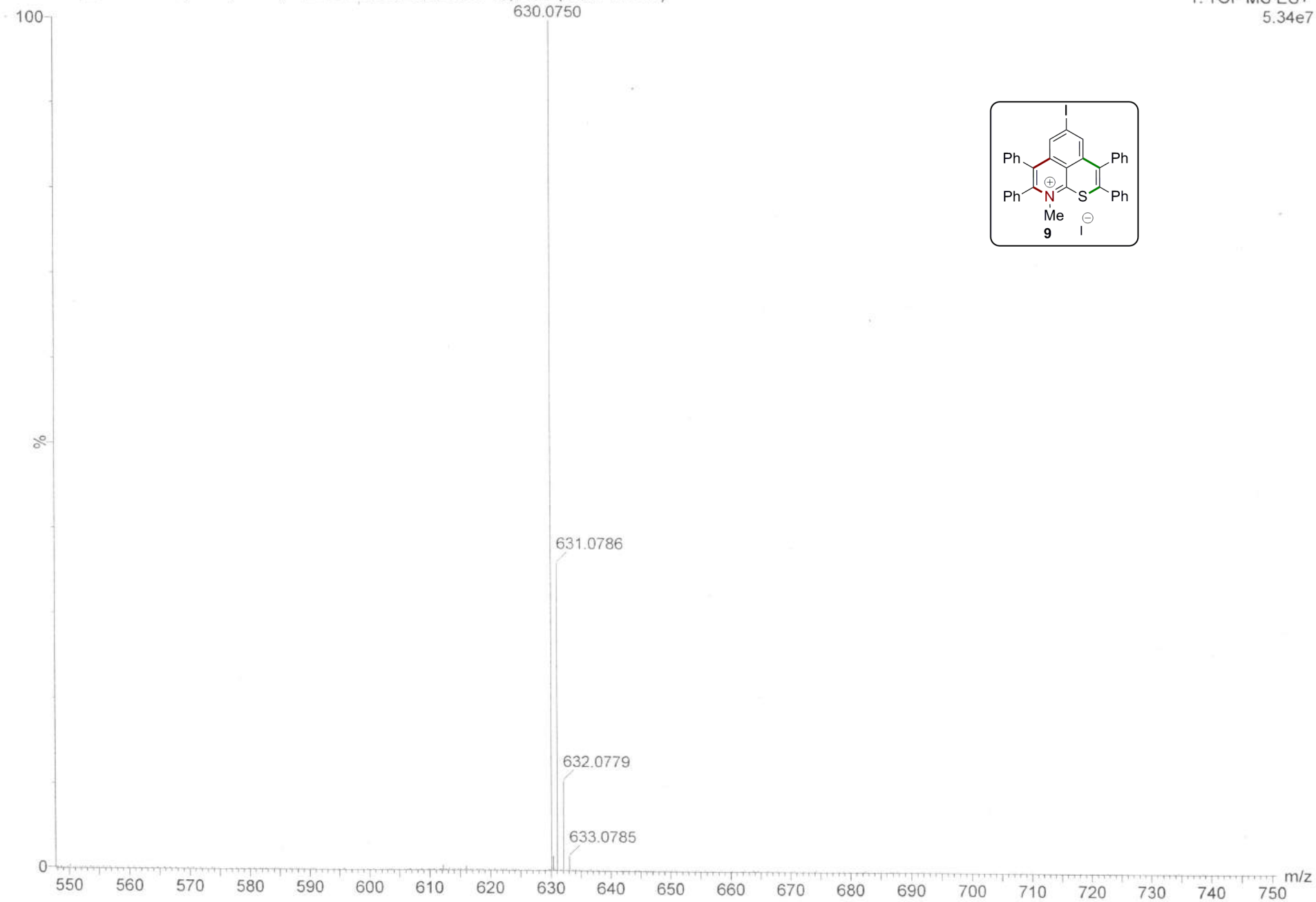
Source Type	ESI
Focus	Not active
Scan Begin	50 m/z
Scan End	1800 m/z

Ion Polarity	Positive
Set Capillary	2600 V
Set End Plate Offset	-500 V
Set Collision Cell RF	200.0 Vpp

Set Nebulizer	5.8 psi
Set Dry Heater	200 °C
Set Dry Gas	4.0 l/min
Set Divert Valve	Waste



23112020_09 +VE 20 (0.228) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (20:31-81:117)

1: TOF MS ES+
5.34e7

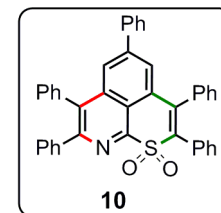
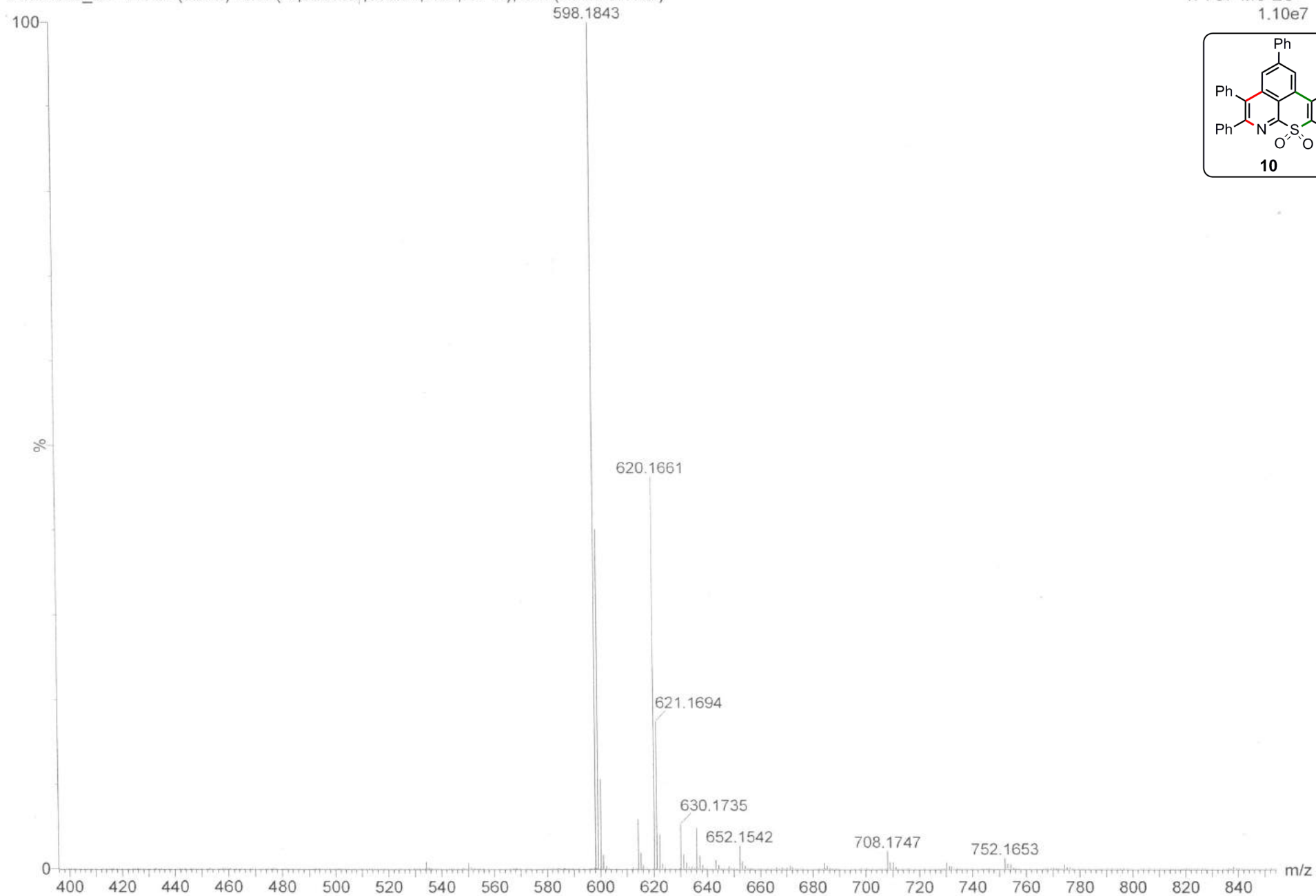
MJ-17-224

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ACRHEM
XEVO-G2XSQTOF#YEA1155

20-Oct-2020
15:17:52

20102020_32 +VE 24 (0.262) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (24:33-83:126)

1: TOF MS ES+
1.10e7



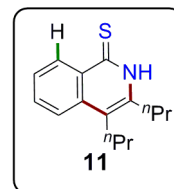
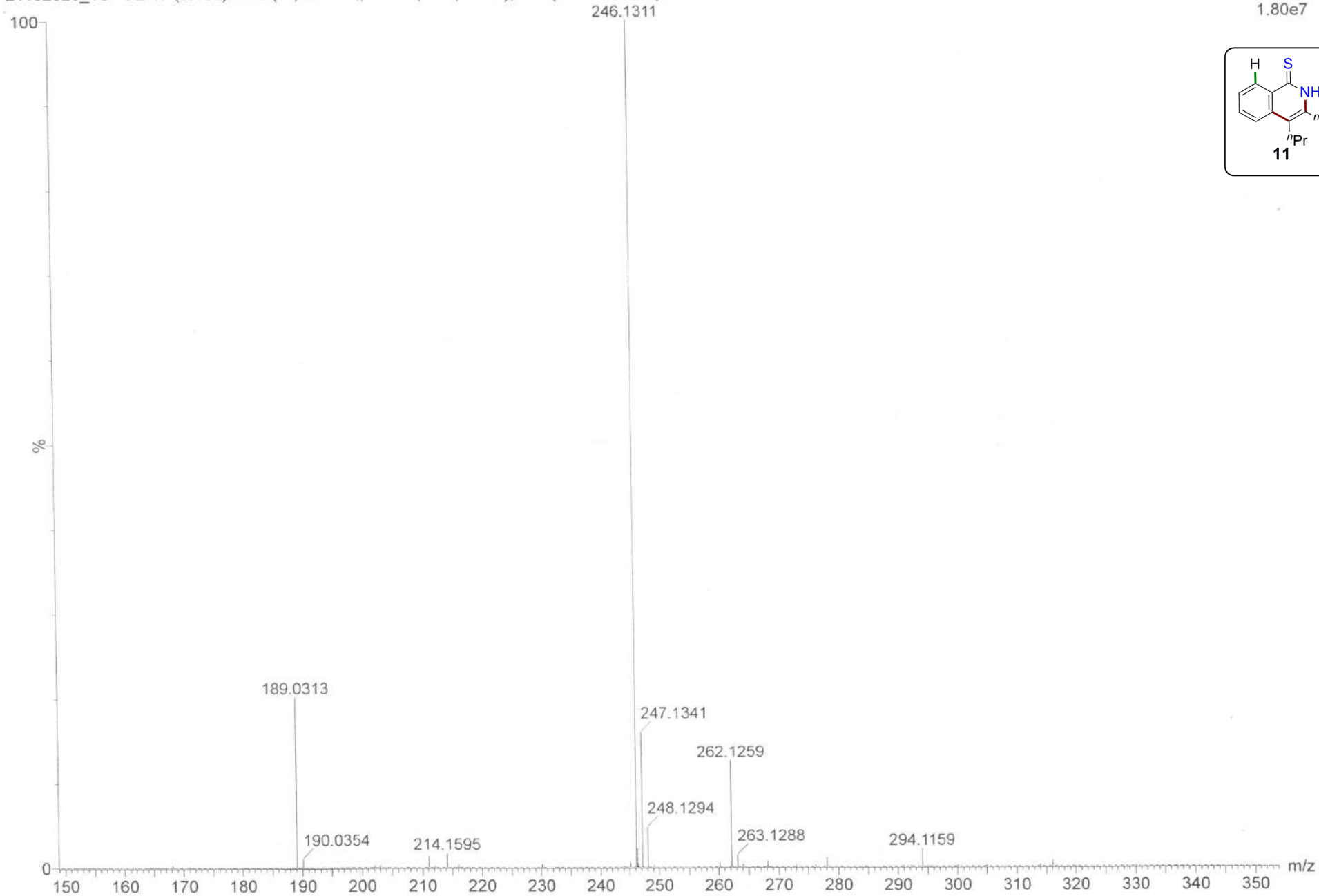
MJ-17-MONO

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ACRHEM
XEVO-G2XSQTOF#YEA1155

21-Oct-2020
15:22:03

21102020_18 +VE 17 (0.182) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (17:24-71:109)

1: TOF MS ES+
1.80e7



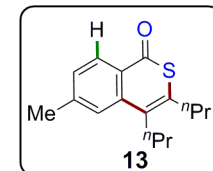
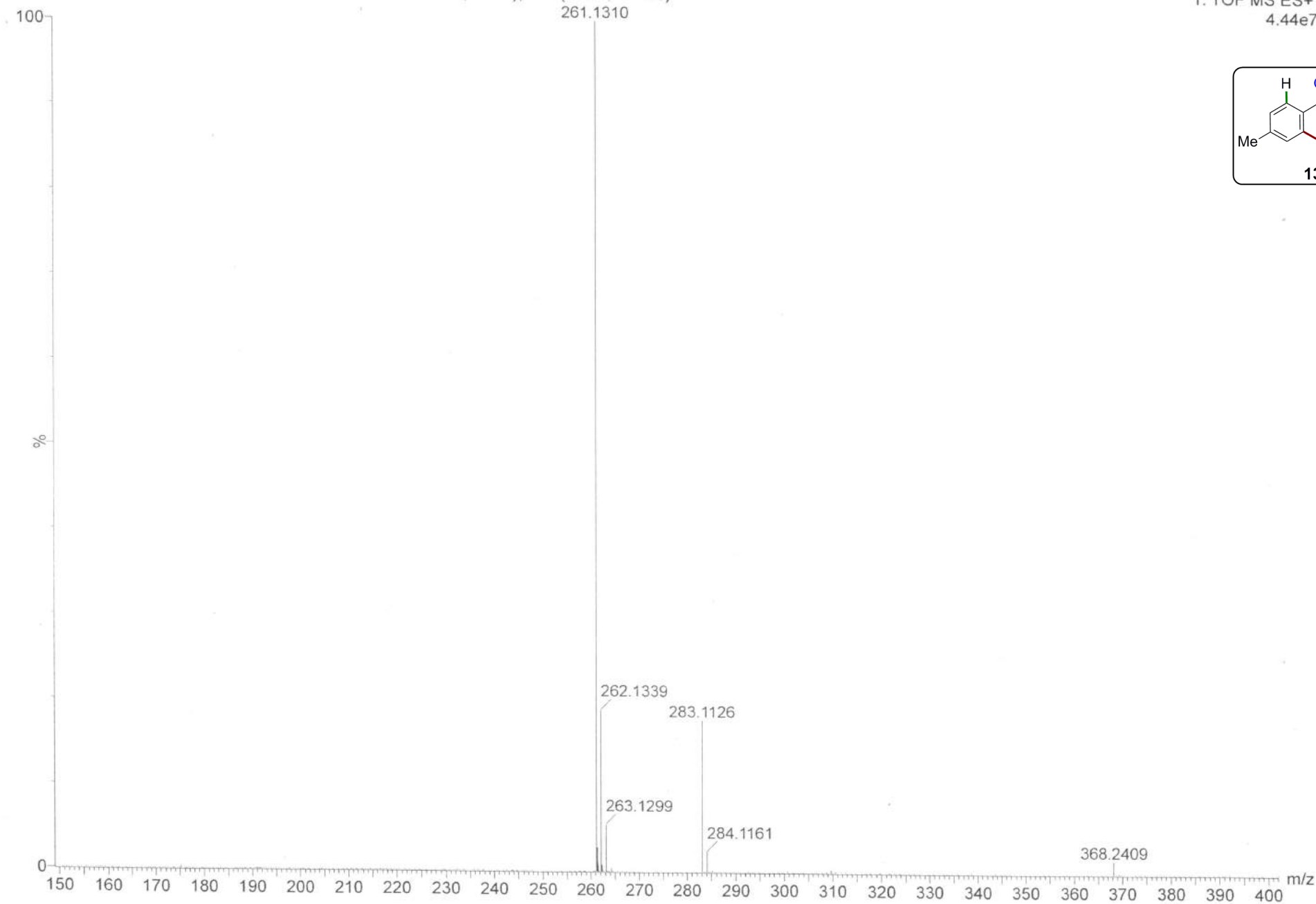
MJ-17-249

UNIVERSITY OF HYDERABAD
ACRHEM
XEVO-G2XSQTOF#YEA1155

20-Oct-2020
15:20:35

20102020_33 +VE 17 (0.182) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (17:24-71:136)

1: TOF MS ES+
4.44e7



04112020_10 +VE 18 (0.191) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (18:23-84:130)

1: TOF MS ES+
5.49e7