

Triphenylphosphine Promoted Regio and Stereoselective α - Halogenation of Ynamides

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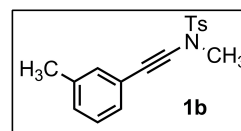
SUPPORTING INFORMATION

LCMS-2010A DATA REPORT

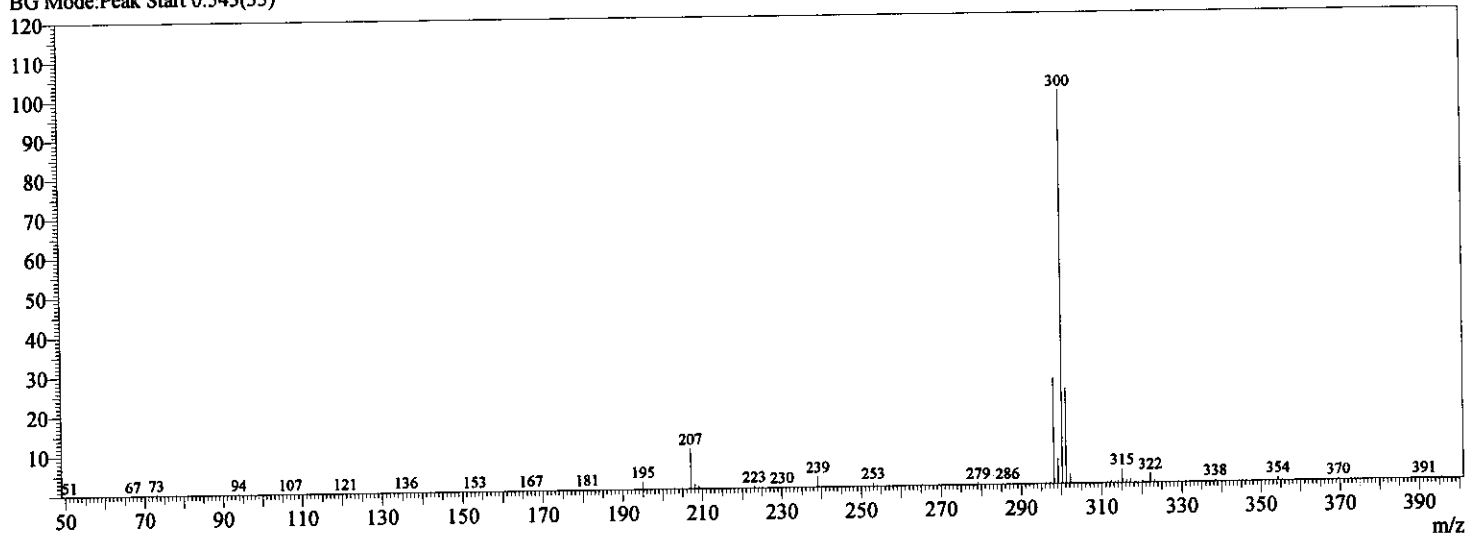
SHIMADZU

User : Admin
 Sample : RKM-3-224
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\RKM-3-224-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.787(Scan#:48) Positive
 MassPeaks:226 BasePeak:300.20(3771367)
 RawMode:Single 0.787(48)
 BG Mode:Peak Start 0.543(33)



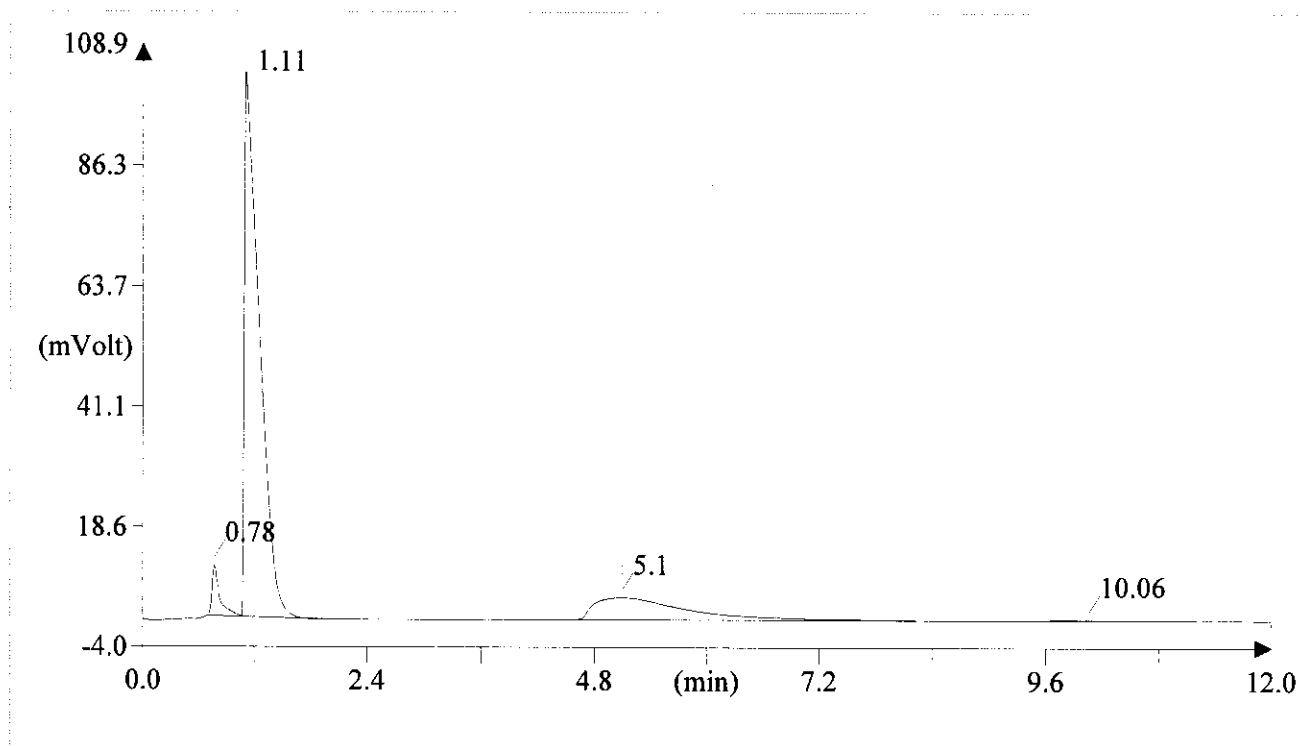
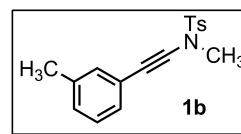
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.787	0.543	1.043	94799964	7832291	12.10		100.00	
				94799964	7832291			100.00	

Base m/z Base Int.
 300.20 3771367

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: RKM-3-224 (# 162)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-2.dat
 Sample weight: 2.815



Element Name	Element %	Ret. Time
Nitrogen	4.61	0.78
Carbon	68.35	1.11
Hydrogen	5.75	5.10
Sulphur	10.62	10.06

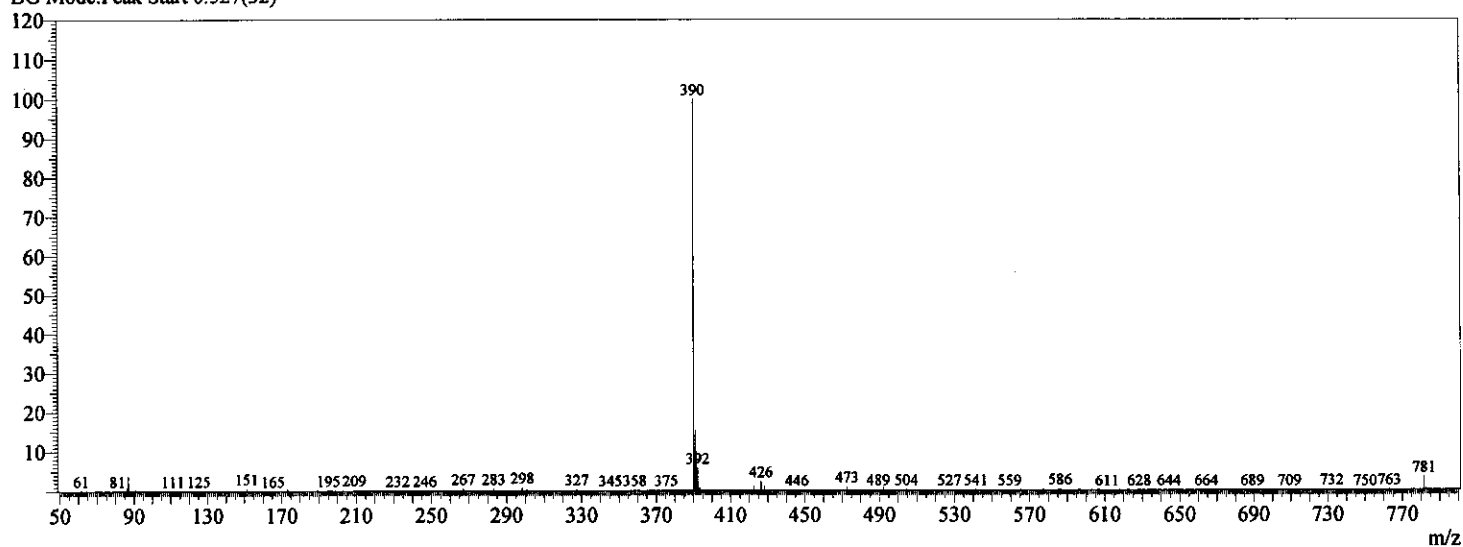
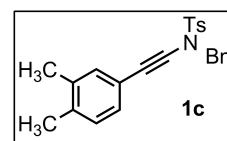
LCMS-2010A DATA REPORT

SHIMADZU

User : Admin
 Sample : RP-3-72
 Inj. Volume : 5.000
 Data Name : C:\LCMSSolution\User\Data\RP-3-72-ESI-POS1.qld
 Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.773(Scan#:47)
 MassPeaks:341 BasePeak:390.25(1616089)
 RawMode:Single 0.773(47)
 BG Mode:Peak Start 0.527(32)



MS Peak Table

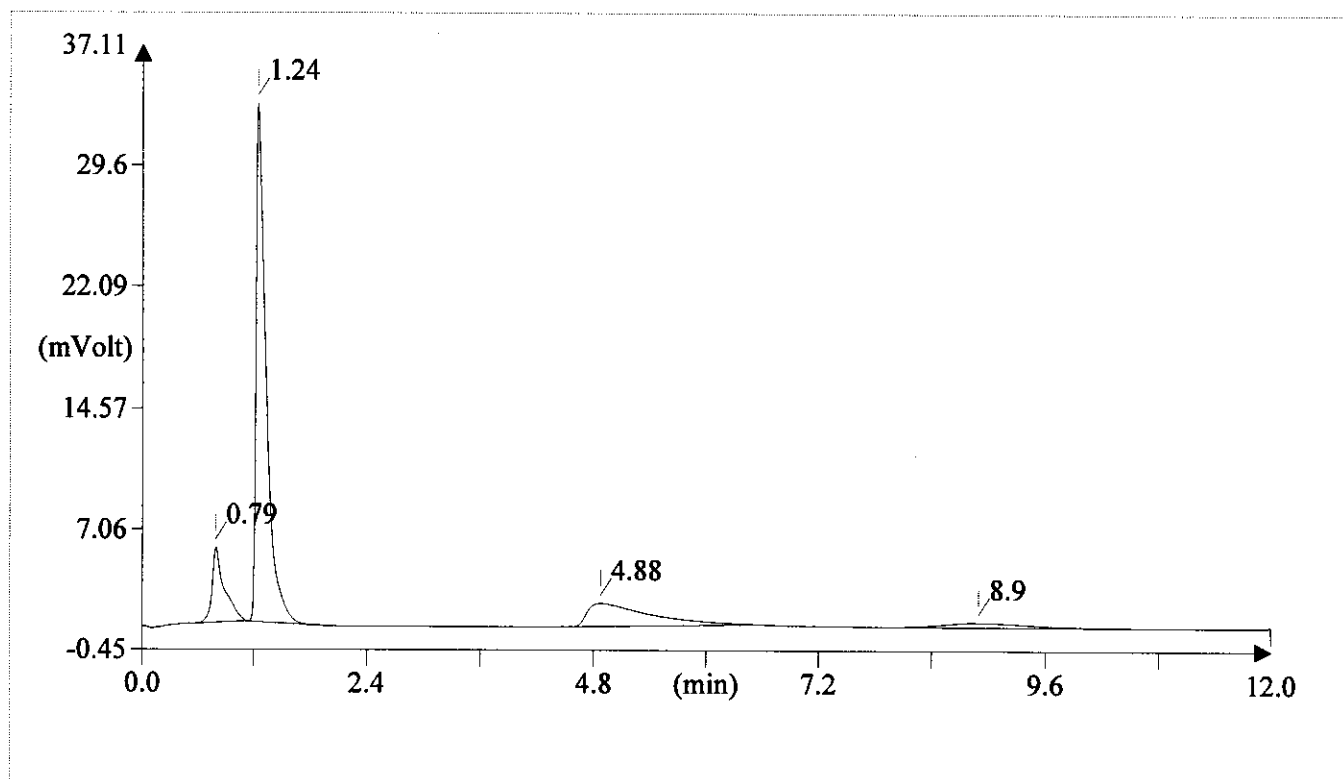
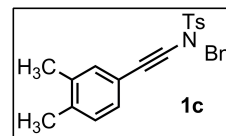
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.773	0.527	1.043	24597640	1726918	14.24		100.00	
				24597640	1726918			100.00	

Base m/z : 390.25
 Base Int. : 1616089

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: RP-3-72 (# 168)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-8.dat
 Sample weight: 1.103



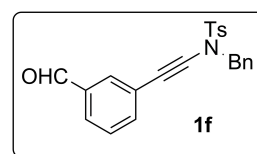
Element Name	Element %	Ret. Time
Nitrogen	3.65	0.79
Carbon	74.15	1.24
Hydrogen	5.98	4.88
Sulphur	8.31	8.90

LCMS-2010A DATA REPORT

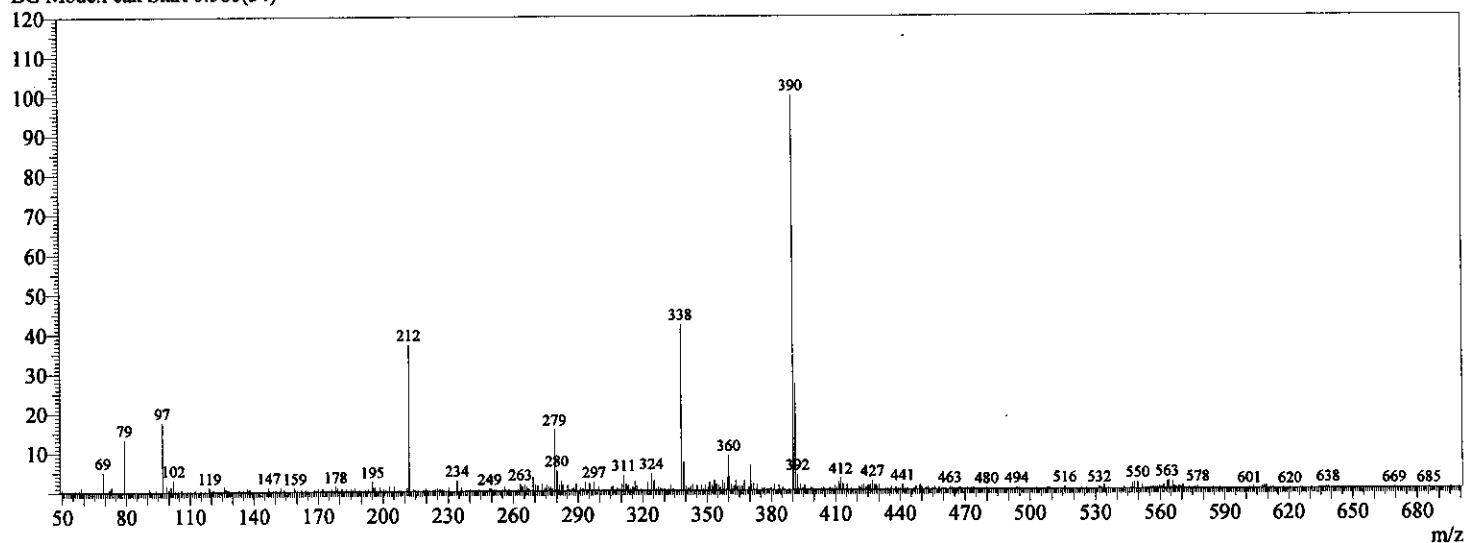
SHIMADZU

User : Admin
 Sample : PB-8-47
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\PB-8-47-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.777(Scan#:47) Positive
 MassPeaks:472 BasePeak:390.30(522653)
 RawMode:Single 0.777(47)
 BG Mode:Peak Start 0.560(34)



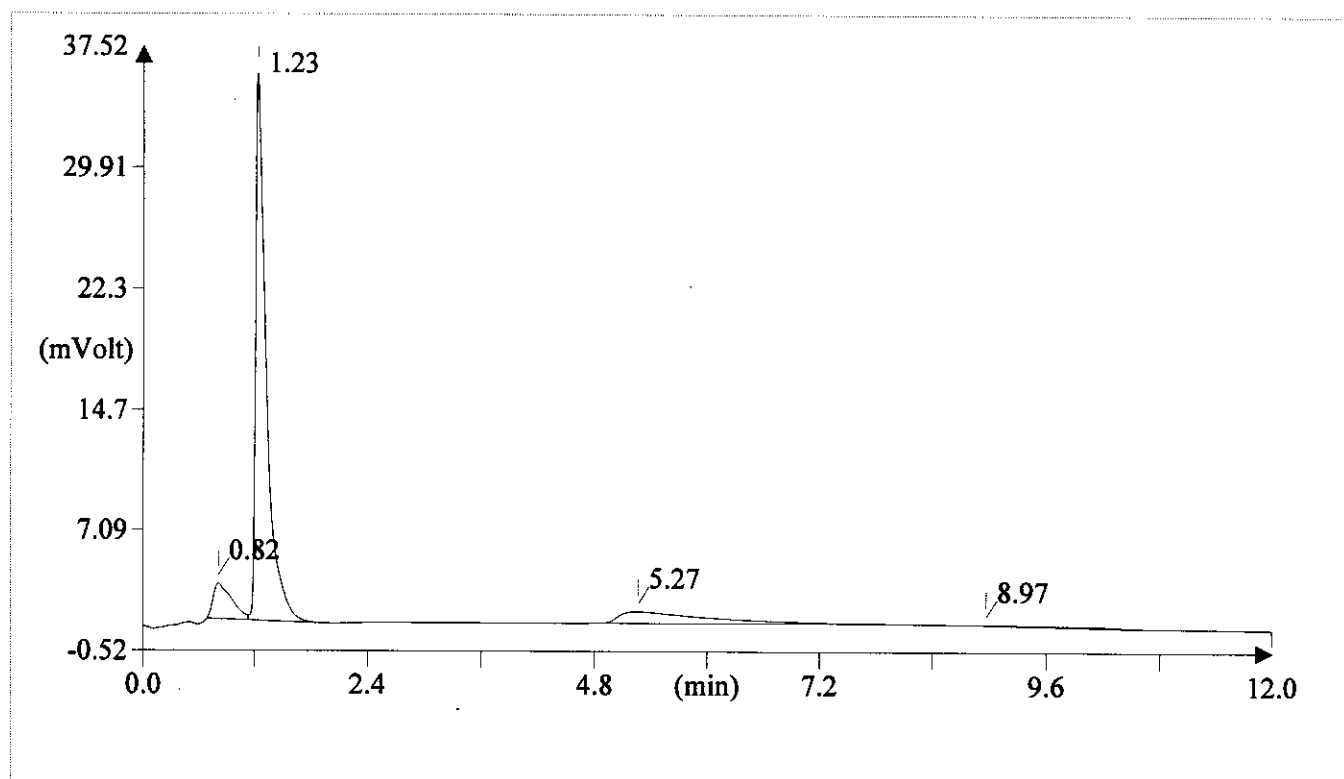
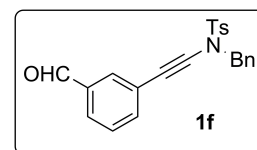
MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.777	0.560	1.060	29133753	1735894	16.78		100.00		390.30	522653
				29133753	1735894			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: PB-8-47 (# 166)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-6.dat
 Sample weight: 1.123



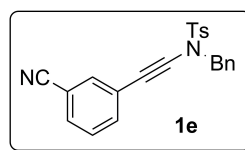
Element Name	Element %	Ret. Time
Nitrogen	3.56	0.82
Carbon	70.85	1.23
Hydrogen	4.88	5.27
Sulphur	8.31	8.97

LCMS-2010A DATA REPORT

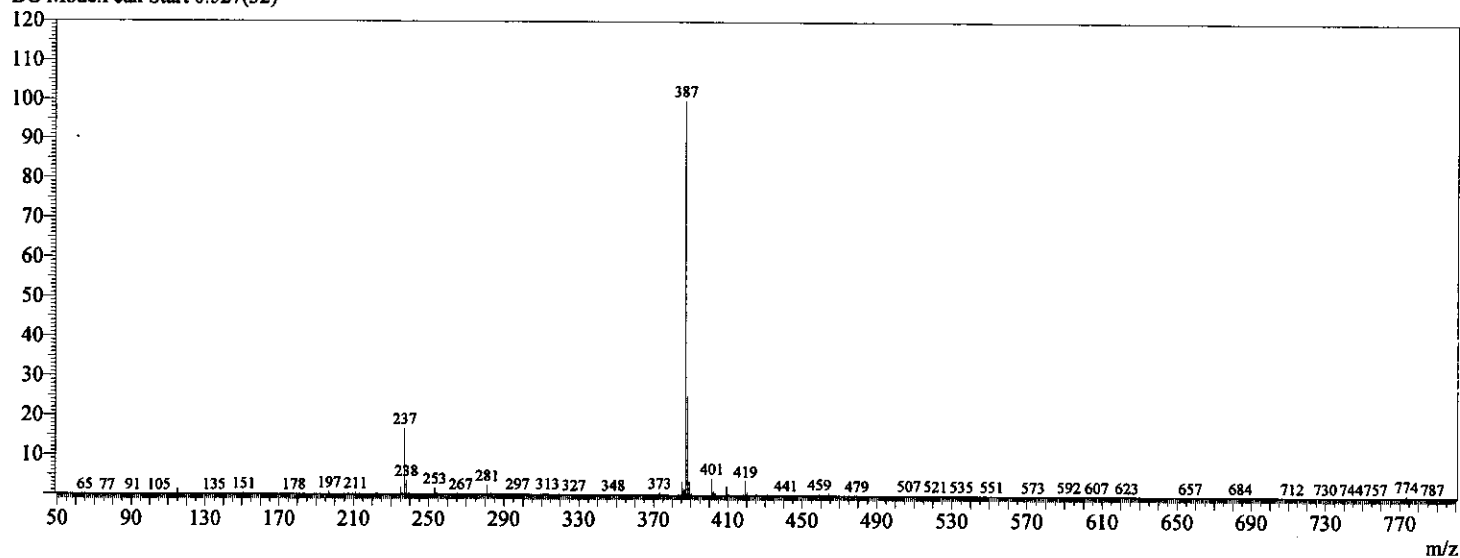
SHIMADZU

User : Admin
 Sample : PB-8-49
 Inj. Volume : 5.000
 Data Name : C:\LCMSSolution\User\Data\PB-8-49-APCI-POS1.qld
 Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.775(Scan#:47) Positive
 MassPeaks:555 BasePeak:387.25(5233916)
 RawMode:Single 0.775(47)
 BG Mode:Peak Start 0.527(32)



MS Peak Table

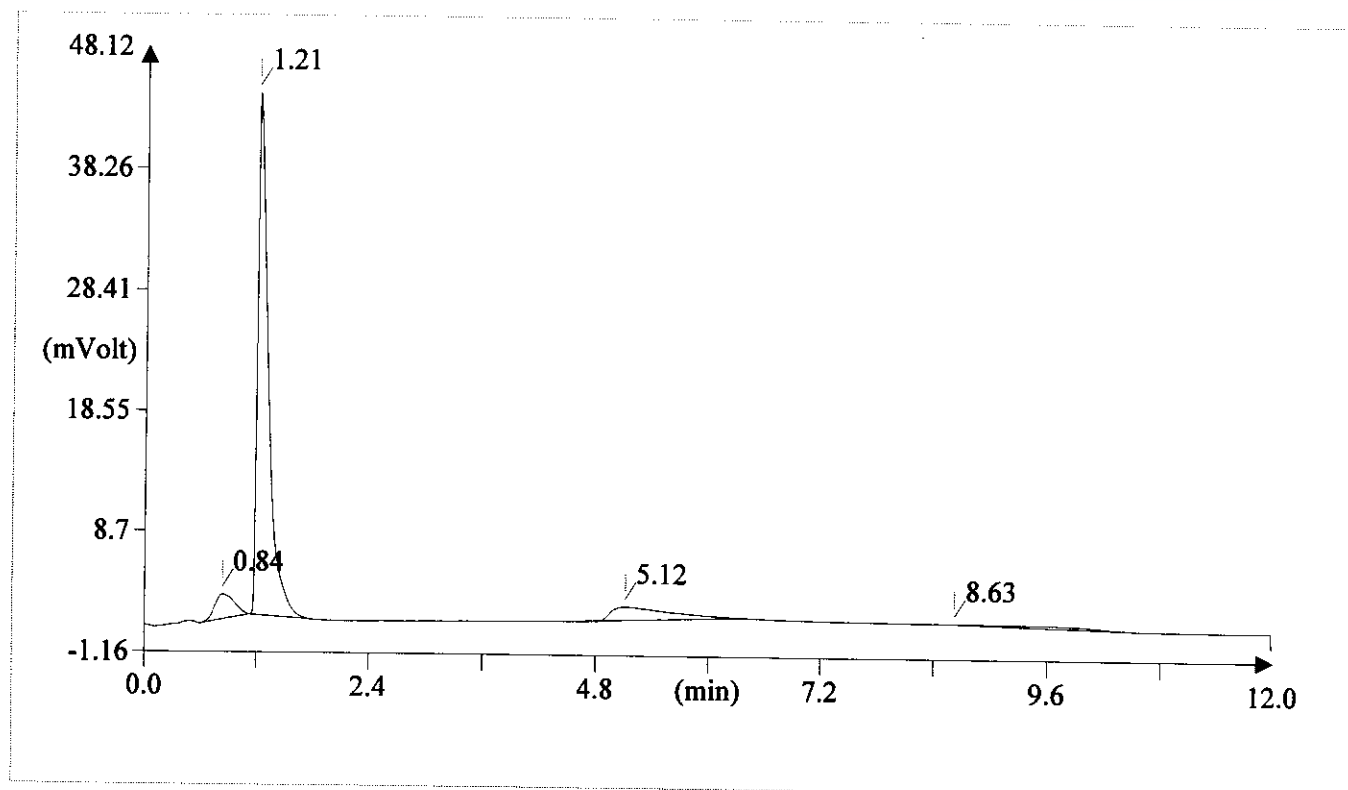
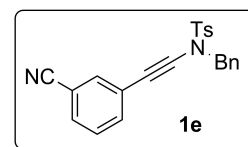
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.775	0.527	1.043	120562790	10353029	11.64		100.00	
				120562790	10353029			100.00	

Base m/z Base Int.
 387.25 5233916

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: PB-8-49 (# 174)
 Analysis type: UnkNown
 Chromatogram filename: UNK-20092015-14.dat
 Sample weight: 1.106



Element Name	Element %	Ret. Time
Nitrogen	7.32	0.84
Carbon	71.56	1.21
Hydrogen	4.61	5.12
Sulphur	8.38	8.63

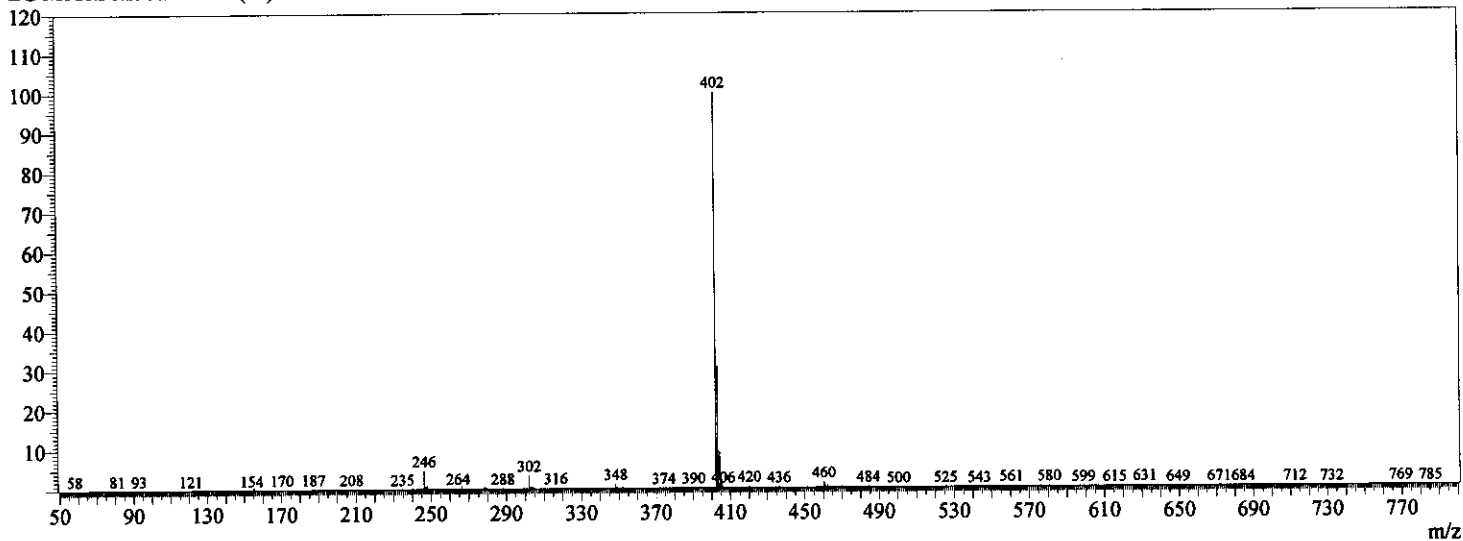
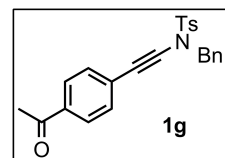
LCMS-2010A DATA REPORT

SHIMADZU

User : Admin
Sample : PB-8-R2G
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\PB-8-R2G-APCI-NEG1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.762(Scan#:46) Negative
MassPeaks:508 BasePeak:402.25(4430766)
RawMode:Single 0.762(46)
BG Mode:Peak Start 0.527(32)



MS Peak Table

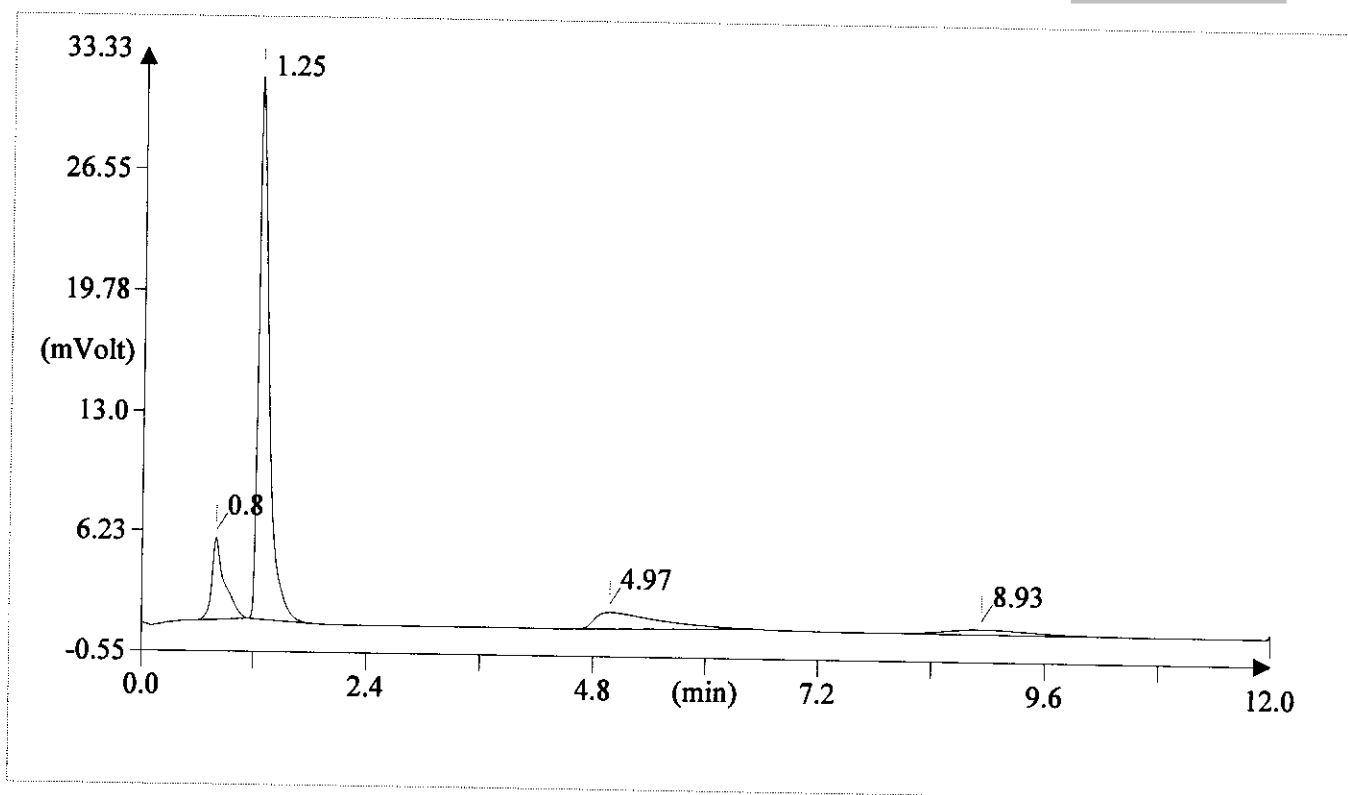
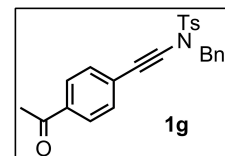
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.762	0.527	1.043	112292509	7576090	14.82		100.00	
				112292509	7576090			100.00	

Base m/z Base Int.
402.25 4430766

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: PB-8-R2G (# 164)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-4.dat
 Sample weight: 1.106



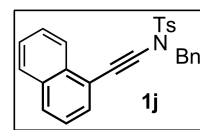
Element Name	Element %	Ret. Time
Nitrogen	3.52	0.80
Carbon	71.35	1.25
Hydrogen	5.28	4.97
Sulphur	7.89	8.93

LCMS-2010A DATA REPORT

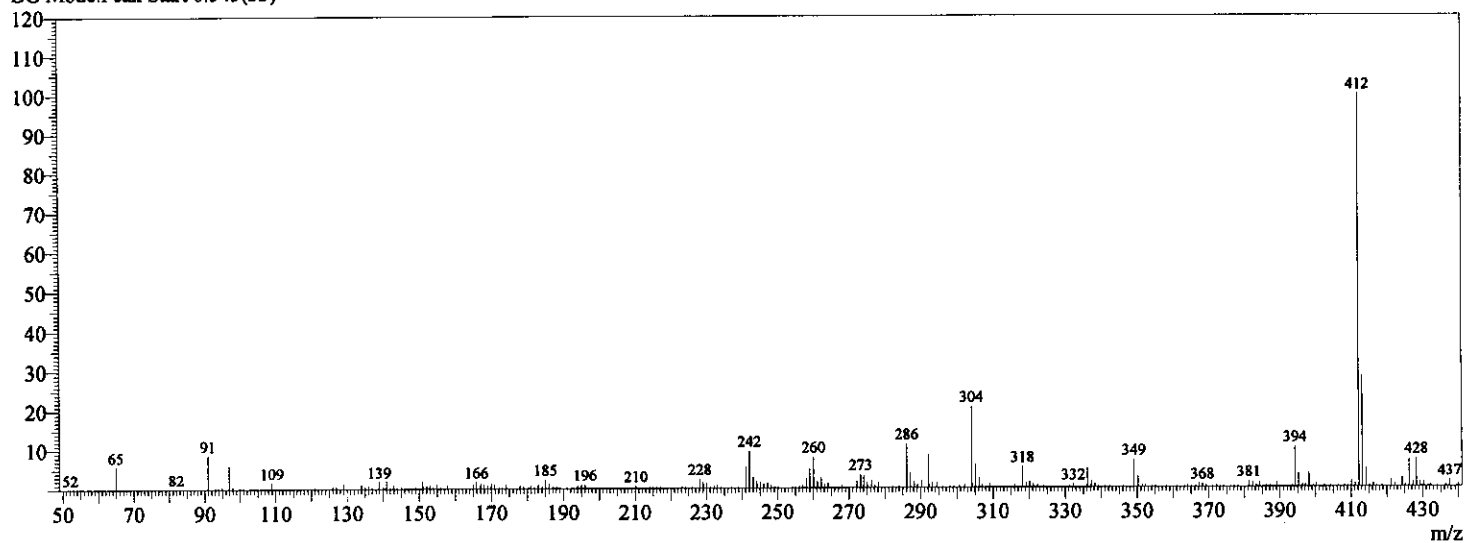
SHIMADZU

User : Admin
 Sample : RP-3-68
 Inj. Volume : 5.000
 Data Name : C:\LCMSSolution\User\Data\RP-3-68-APCI-POS1.qld
 Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.763(Scan#:46) Positive
 MassPeaks:304 BasePeak:412.25(2291233)
 RawMode:Single 0.763(46)
 BG Mode:Peak Start 0.543(33)



MS Peak Table

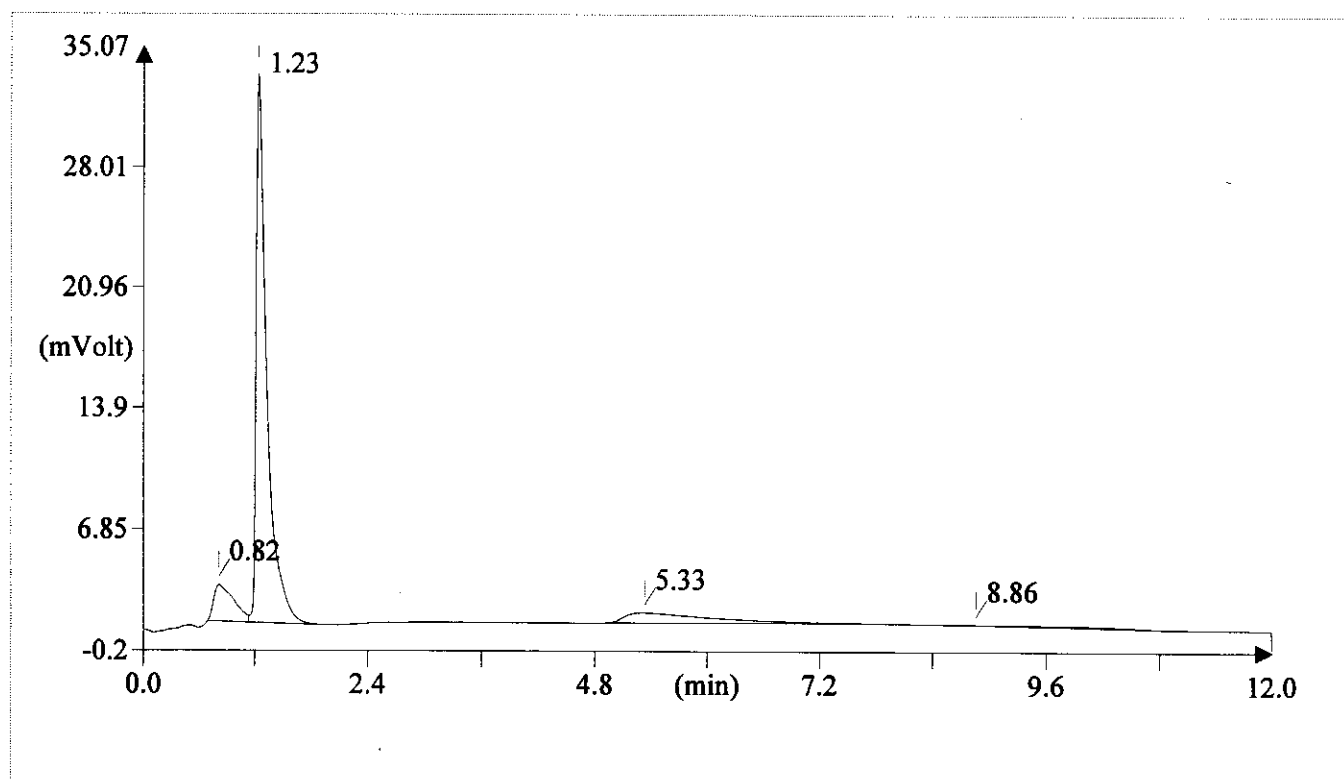
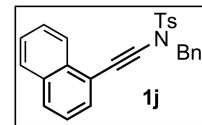
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.763	0.543	1.043	217299993	15742563	13.80		100.00	
				217299993	15742563			100.00	

Base m/z Base Int.
 412.25 2291233

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: RP-3-68 (# 167)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-7.dat
 Sample weight: 1.109



Element Name	Element %	Ret. Time
Nitrogen	3.46	0.82
Carbon	75.73	1.23
Hydrogen	5.18	5.33
Sulphur	7.71	8.86

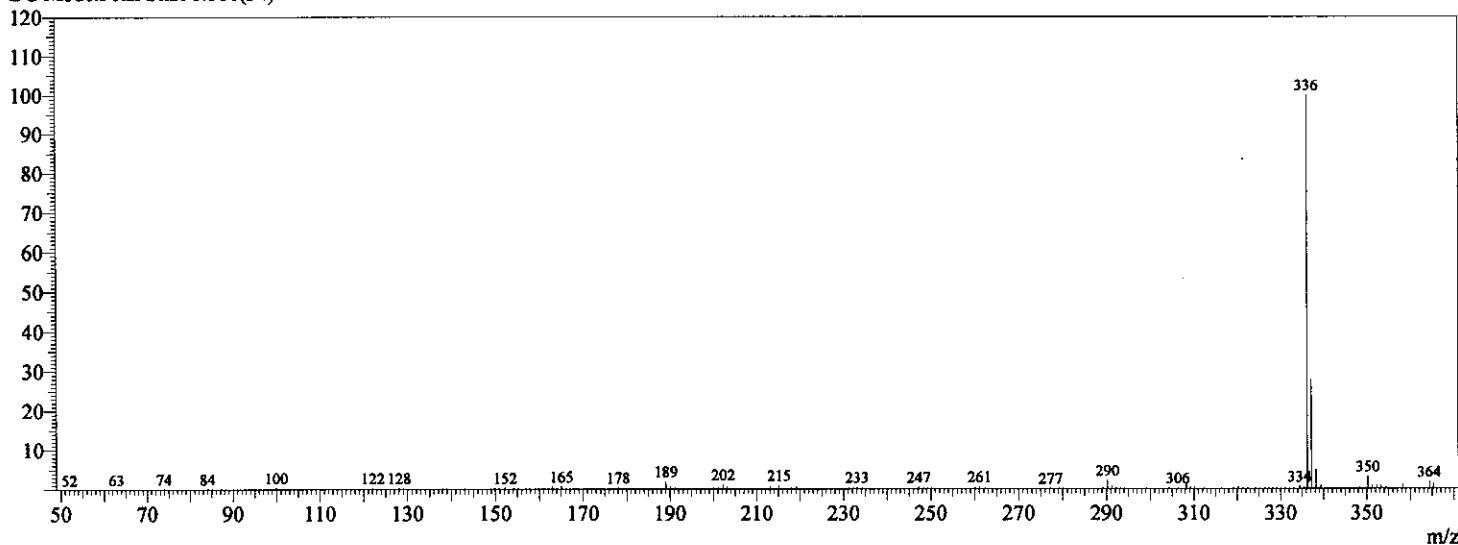
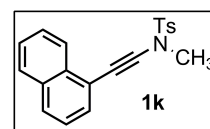
LCMS-2010A DATA REPORT

SHIMADZU

User : Admin
Sample : RP-3-76
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\RP-3-76-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.763(Scan#:46) Positive
MassPeaks:283 BasePeak:336.25(10788256)
RawMode:Single 0.763(46)
BG Mode:Peak Start 0.560(34)



MS Peak Table

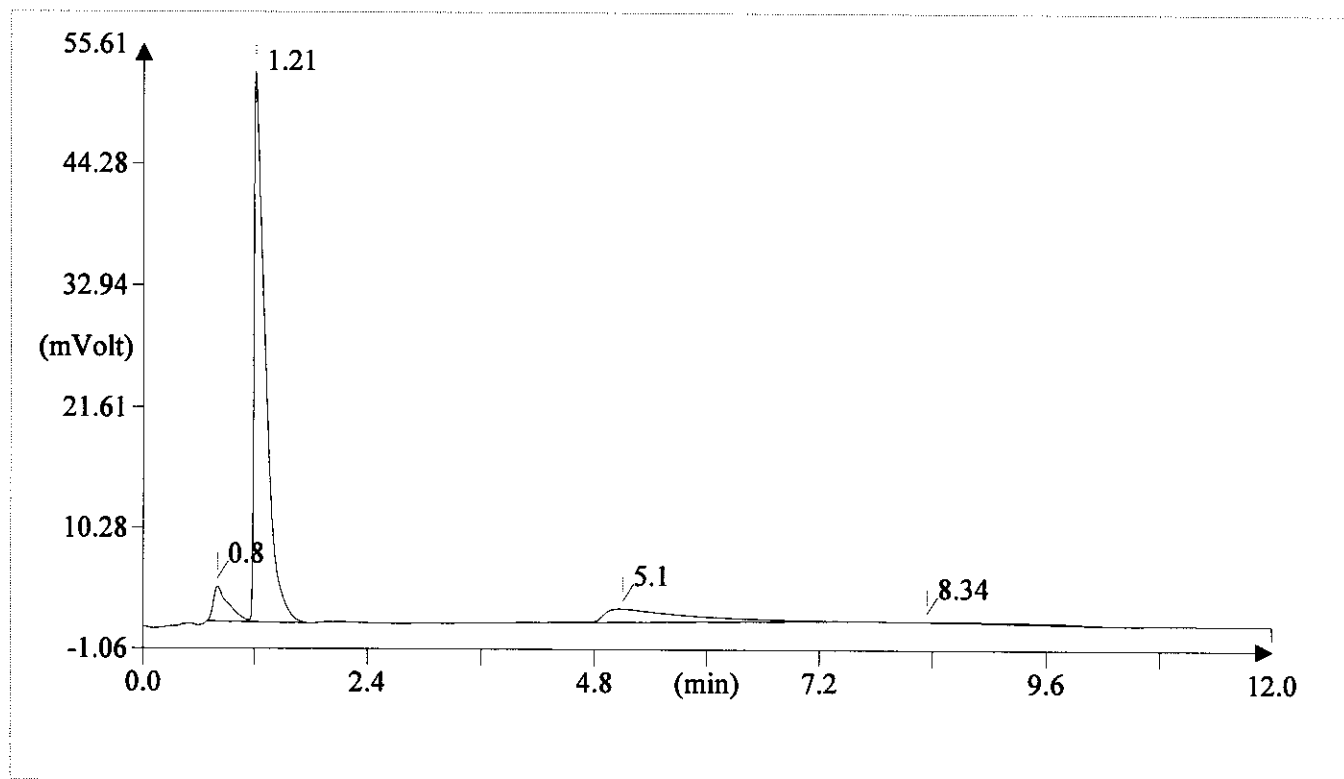
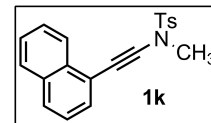
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.763	0.560	1.043	583294479	42218331	13.81		100.00	
				583294479	42218331			100.00	

Base m/z Base Int.
336.25 10788256

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: RP-3-76 (# 170)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-10.dat
 Sample weight: 1.263



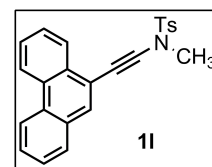
Element Name	Element %	Ret. Time
Nitrogen	4.23	0.80
Carbon	71.56	1.21
Hydrogen	5.18	5.10
Sulphur	9.49	8.34

LCMS-2010A DATA REPORT

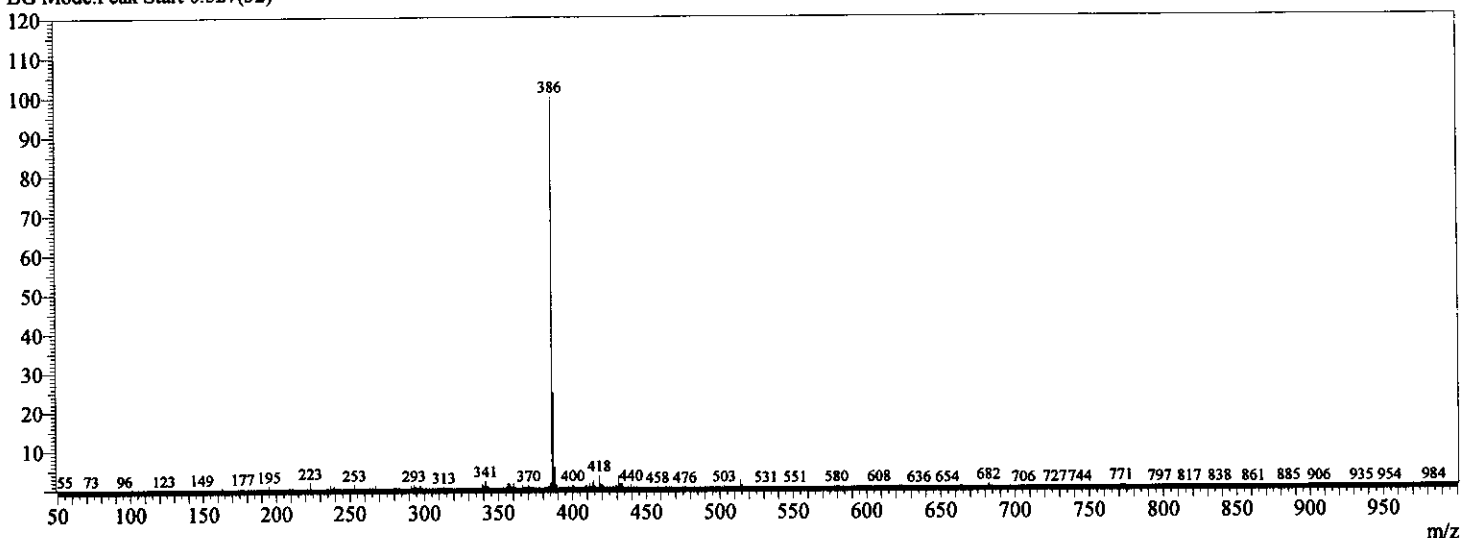
SHIMADZU

User : Admin
 Sample : RKM-3-226
 Inj. Volume : 5.000
 Data Name : C:\LCMSsolution\User\Data\RKM-3-226-APCI-POS1.qld
 Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.733(Scan#:44) Positive
 MassPeaks:765 BasePeak:386.25(3677271)
 RawMode:Single 0.733(44)
 BG Mode:Peak Start 0.527(32)



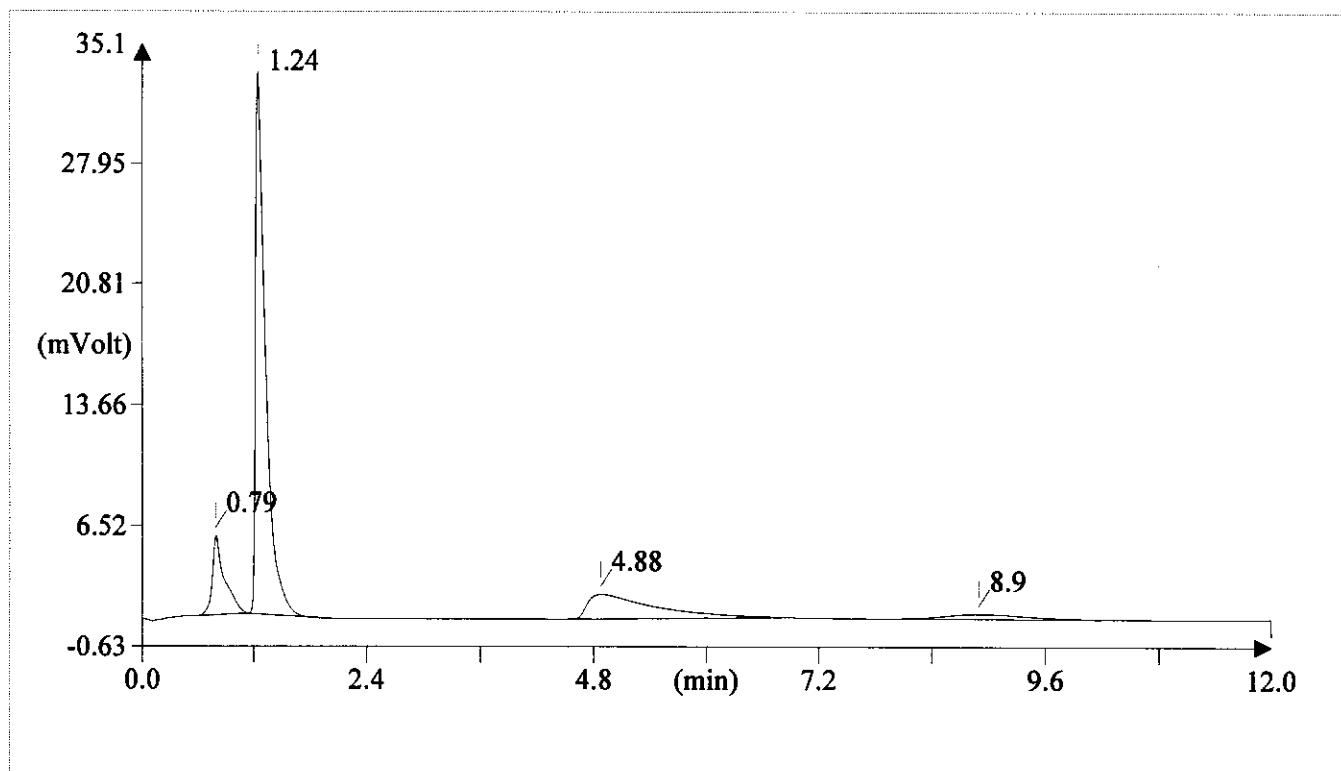
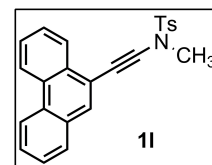
MS Peak Table									
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name
1	0.733	0.527	1.043	102388604	8868688	11.54		100.00	
				102388604	8868688			100.00	

Base m/z Base Int.
 386.25 3677271

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: RKM-3-226 (# 163)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-3.dat
 Sample weight: 1.113



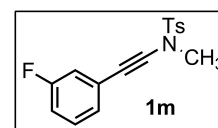
Element Name	Element %	Ret. Time
Nitrogen	3.72	0.79
Carbon	74.65	1.24
Hydrogen	4.91	4.88
Sulphur	8.38	8.90

LCMS-2010A DATA REPORT

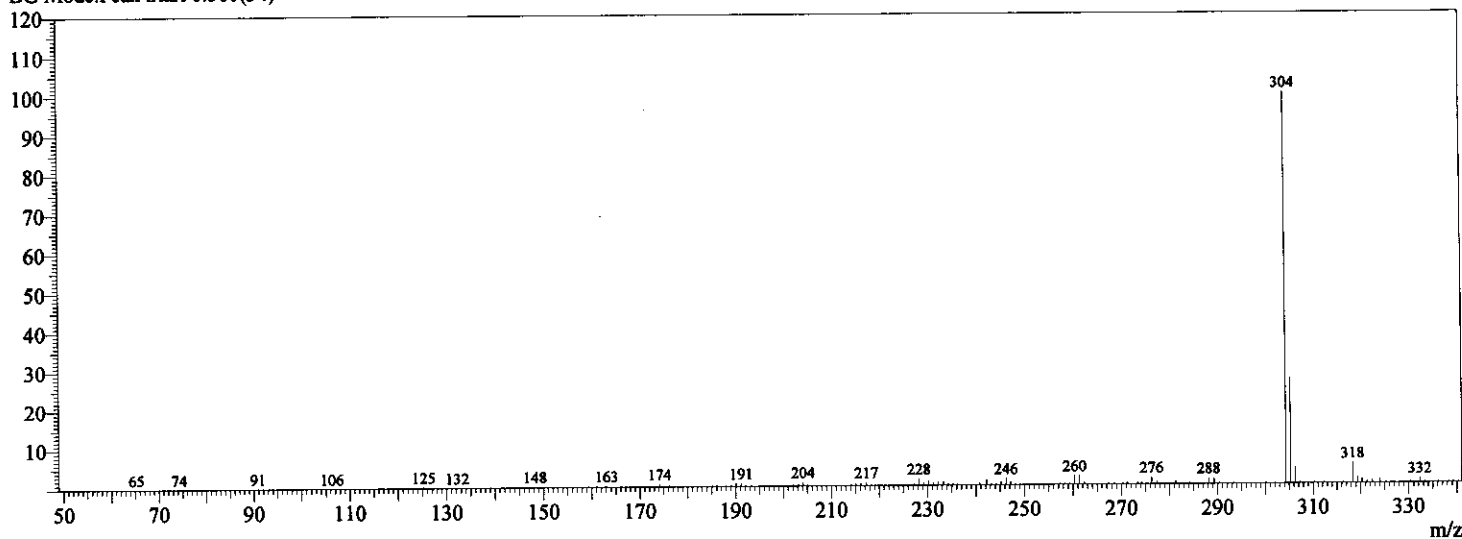
SHIMADZU

User : Admin
Sample : PB-8-45
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\PB-8-45-ESI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.767(Scan#:46) Positive
MassPeaks:182 BasePeak:304.30(3928511)
RawMode:Single 0.767(46)
BG Mode:Peak Start 0.560(34)



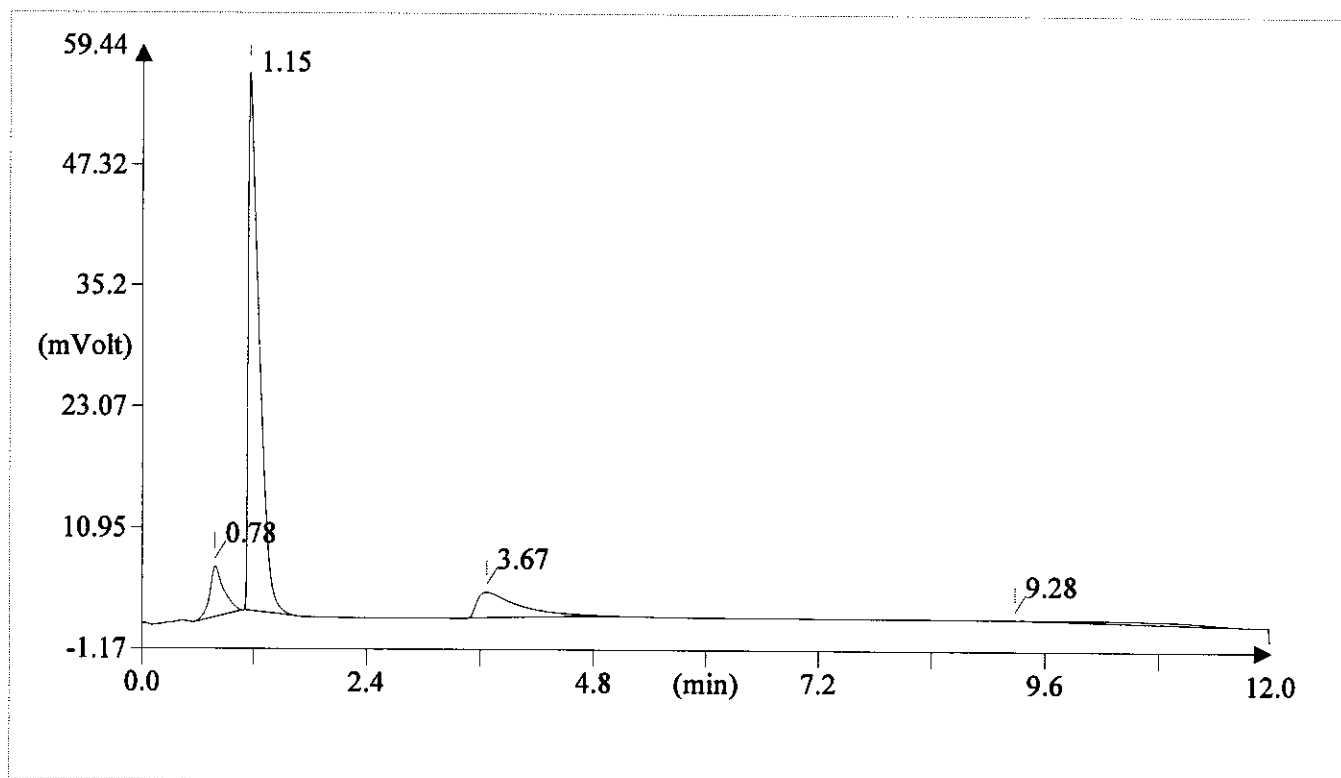
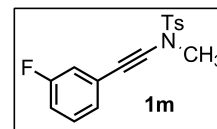
MS Peak Table							
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark
1	0.767	0.560	1.043	135562407	10068569	13.46	
				135562407	10068569		

Base m/z Base Int.
304.30 3928511

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: PB-8-45 (# 165)
 Analysis type: UnkNown
 Chromatogram filename: UNK-30012015-9.dat
 Sample weight: 1.315



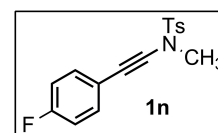
Element Name	Element %	Ret. Time
Nitrogen	4.56	0.78
Carbon	63.41	1.15
Hydrogen	4.58	3.67
Sulphur	10.45	9.28

LCMS-2010A DATA REPORT

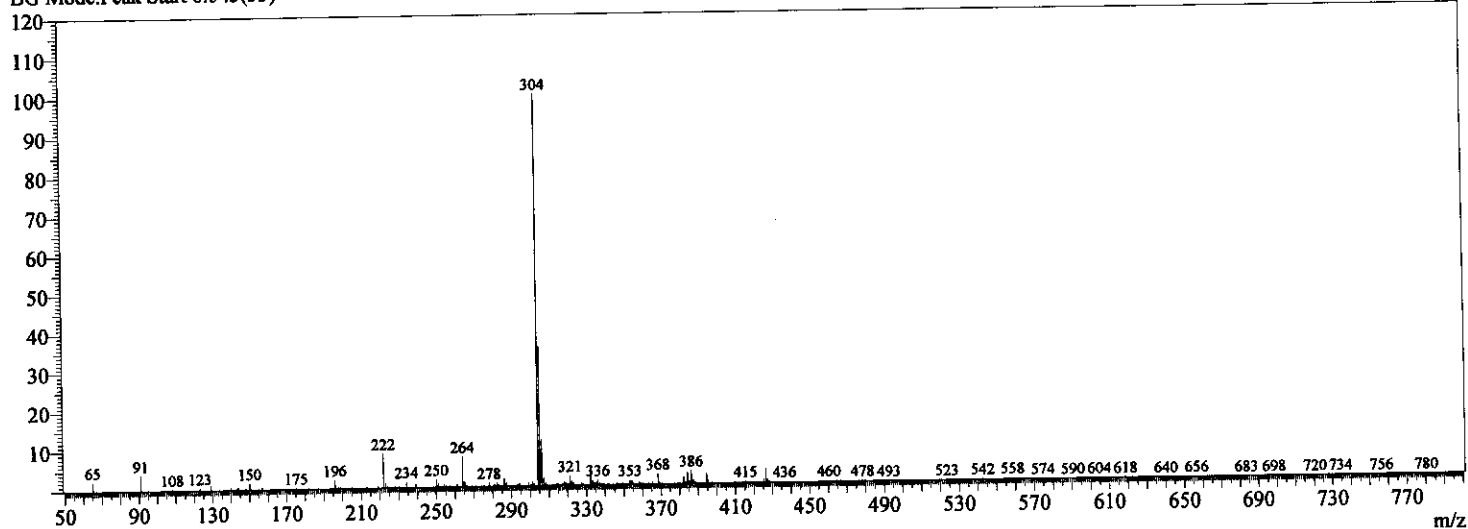
SHIMADZU

User : Admin
Sample : RKM-3-223
Inj. Volume : 5.000
Data Name : C:\LCMSSolution\User\Data\RKM-3-223-APCI-POS1.qld
Method Name : C:\LCMSSolution\User\Method\esi.qlm

MS Spectrum



Line#:1 R.Time:0.762(Scan#:46) Positive
MassPeaks:621 BasePeak:304.15(11631373)
RawMode:Single 0.762(46)
BG Mode:Peak Start 0.543(33)



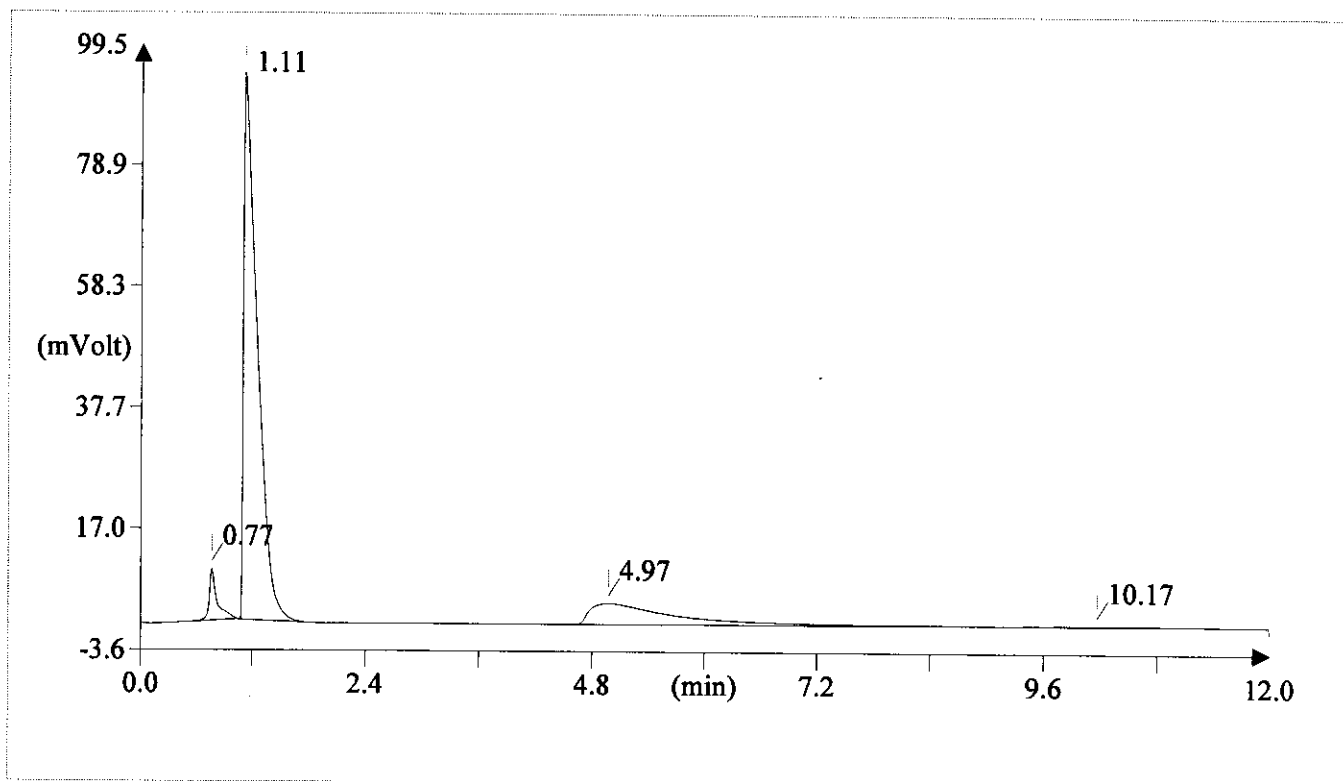
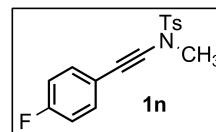
MS Peak Table						
Peak#	R.Time	I.Time	F.Time	Area	Height	A/H Mark
1	0.762	0.543	1.027	372191128	30657746	12.14
				372191128	30657746	

Base m/z Base Int.
304.15 11631373

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: RKM-3-223 (# 161)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-1.dat
 Sample weight: 2.612



Element Name	Element %	Ret. Time
Nitrogen	4.58	0.77
Carbon	63.26	1.11
Hydrogen	4.69	4.97
Sulphur	10.45	10.17

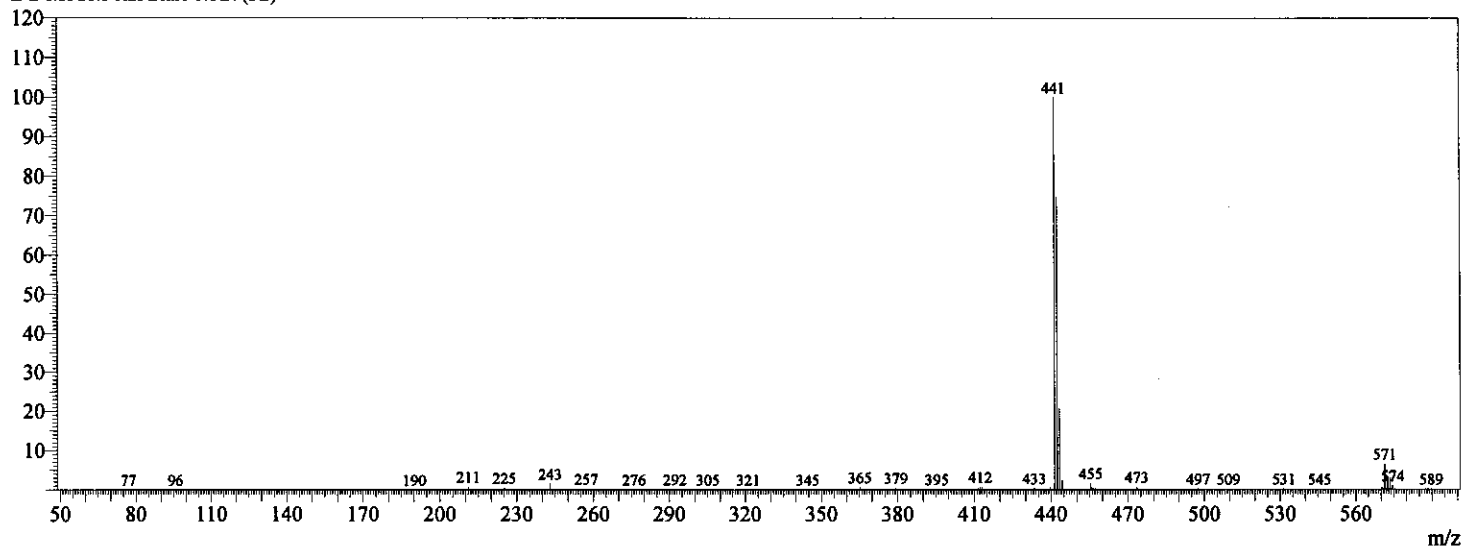
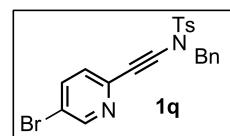
LCMS-2010A DATA REPORT

SHIMADZU

User : Admin
Sample : RP-3-73
Inj. Volume : 5.000
Data Name : C:\LCMSsolution\User\Data\RP-3-73-APCI-POS1.qld
Method Name : C:\LCMSsolution\User\Method\esi.qlm

MS Spectrum

Line#:1 R.Time:0.793(Scan#:48) Positive
MassPeaks:249 BasePeak:441.35(15965070)
RawMode:Single 0.793(48)
BG Mode:Peak Start 0.527(32)



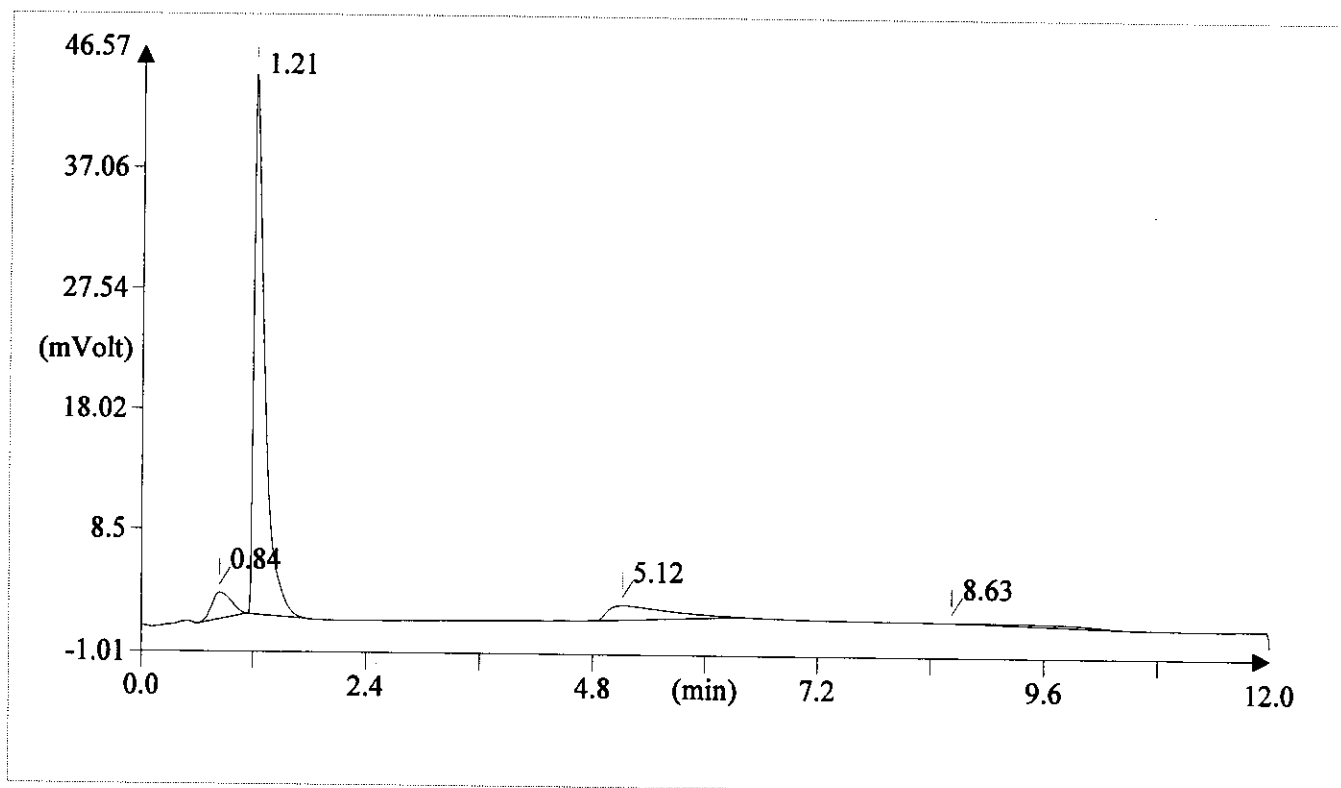
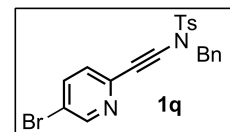
MS Peak Table

Peak#	R.Time	I.Time	F.Time	Area	Height	A/H	Mark	%Total	Name	Base m/z	Base Int.
1	0.793	0.527	1.043	487050737	27566979	17.66		100.00		441.35	15965070
				487050737	27566979			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: RP-3-73 (# 169)
 Analysis type: UnkNown
 Chromatogram filename: UNK-29092015-9.dat
 Sample weight: 1.215



Element Name	Element %	Ret. Time
Nitrogen	6.29	0.84
Carbon	57.23	1.21
Hydrogen	3.82	5.12
Sulphur	7.32	8.63

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Analysis Info

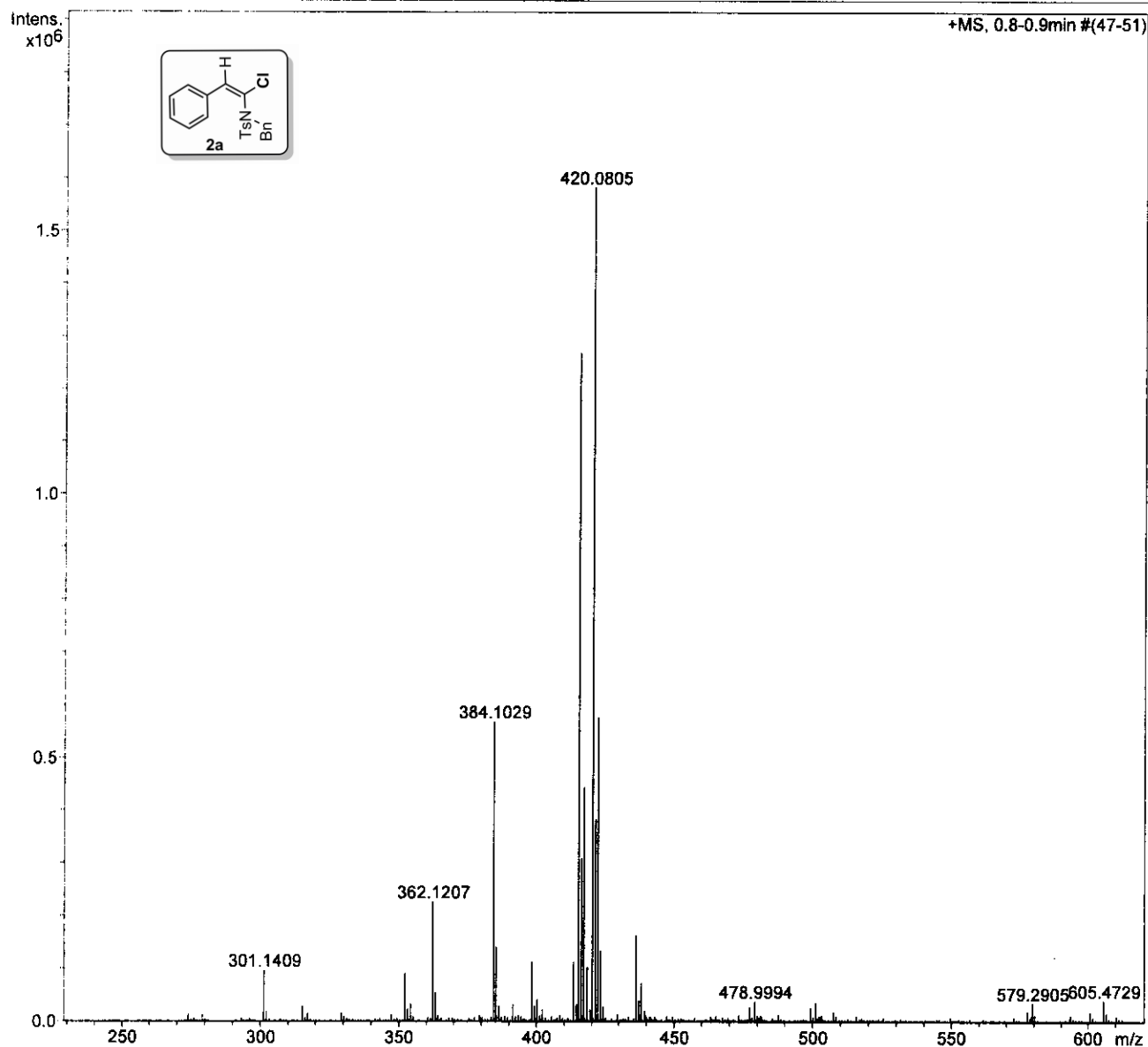
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Method tune_low_Pos.m
Sample Name PB-6-150-BN-MEOH
Comment

Acquisition Date 6/4/2015 12:43:10 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	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



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Analysis Info

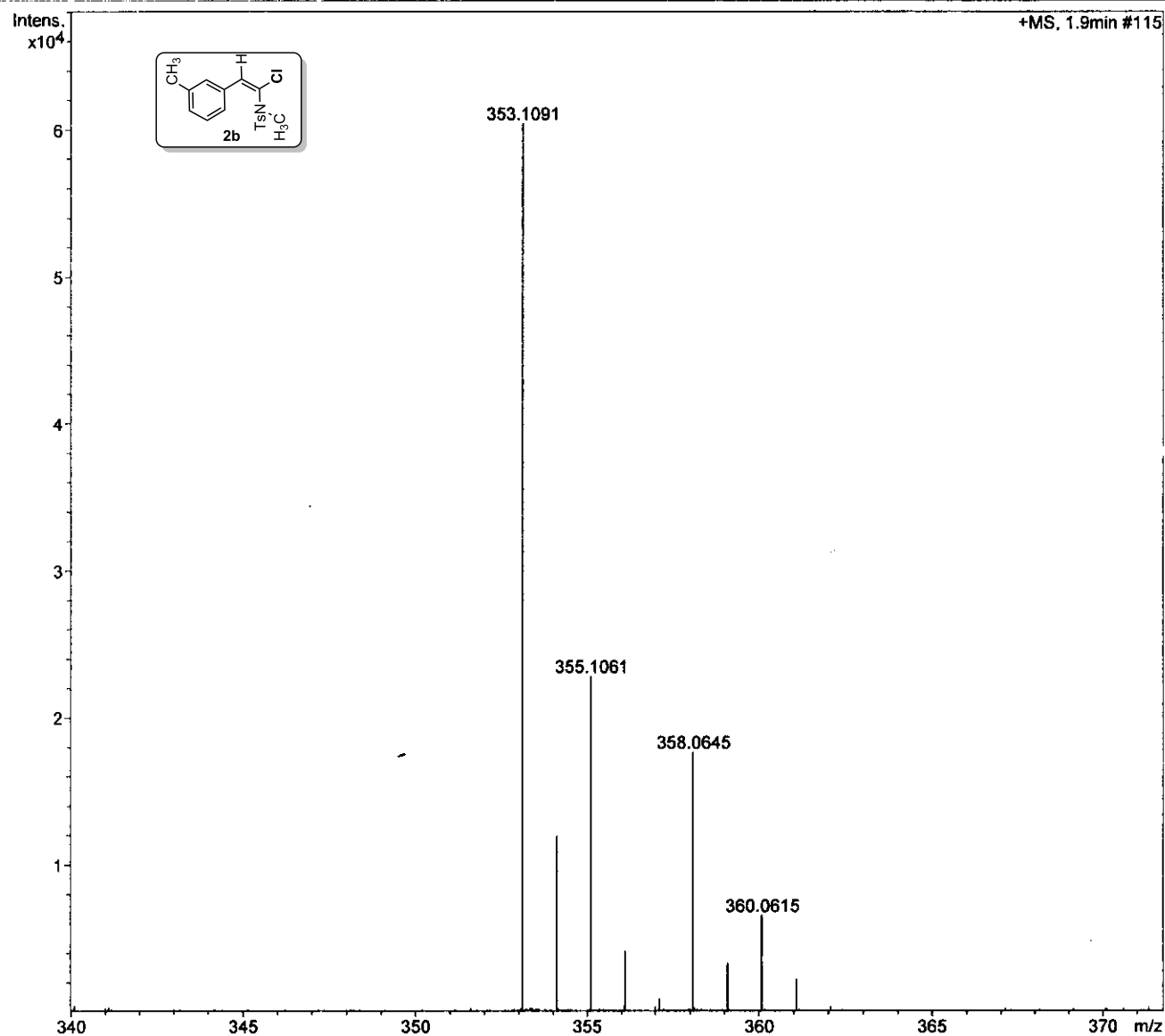
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Method tune_low.m
Sample Name RKM-2-117
Comment

Acquisition Date 3/20/2015 4:25:09 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	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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Analysis Info

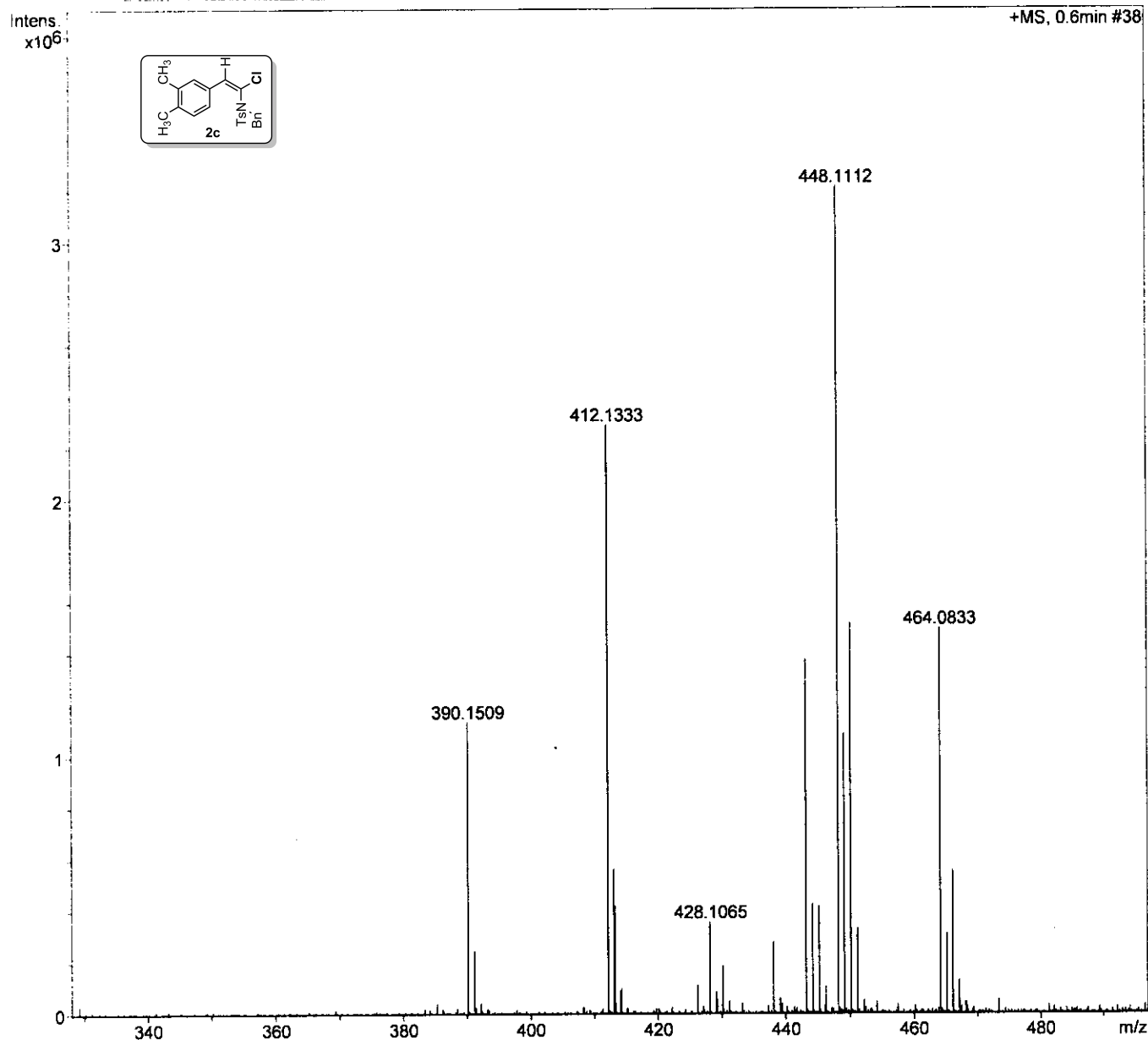
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Method tune_low.m
Sample Name RP-2-10-MEOH
Comment

Acquisition Date 5/11/2015 11:56:36 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	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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Analysis Info

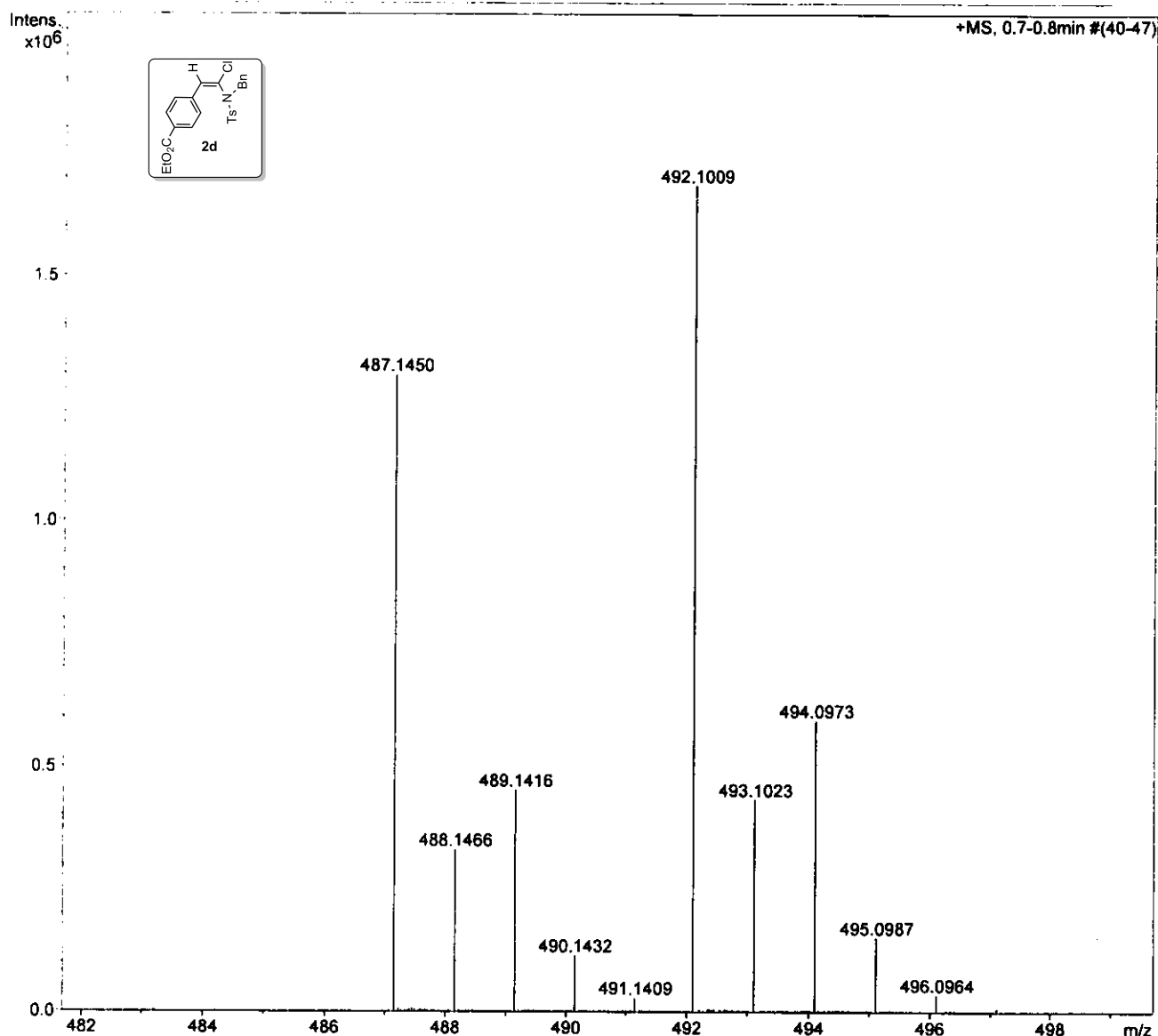
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Method tune_low_Pos-R2.m
Sample Name RKM-3-70-DCM-MEOH
Comment

Acquisition Date 6/8/2015 1:14:59 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



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Analysis Info

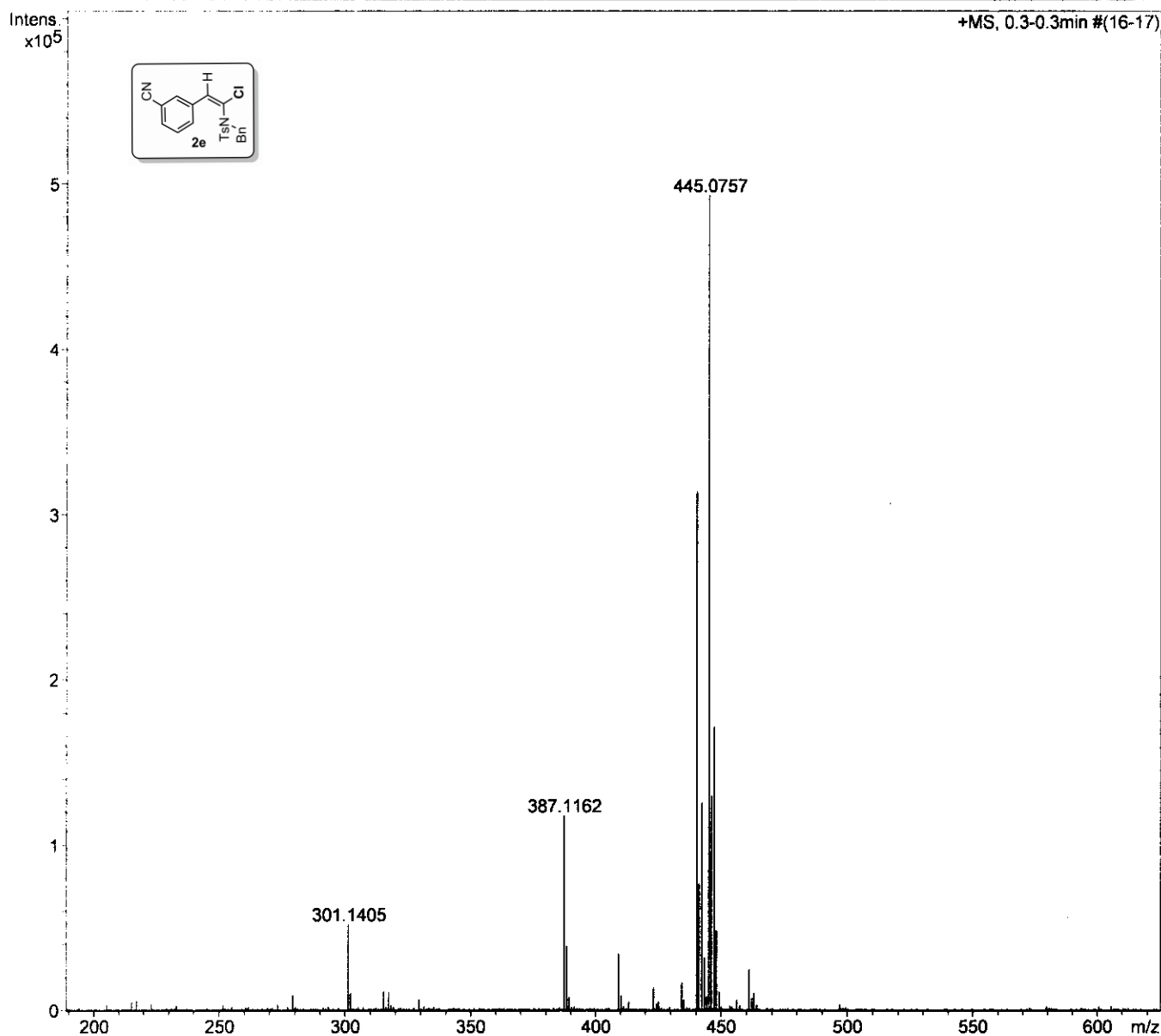
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Method tune_low.m
Sample Name RKM-3-73-DCM-MEOH
Comment

Acquisition Date 6/8/2015 12:33:33 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



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Analysis Info

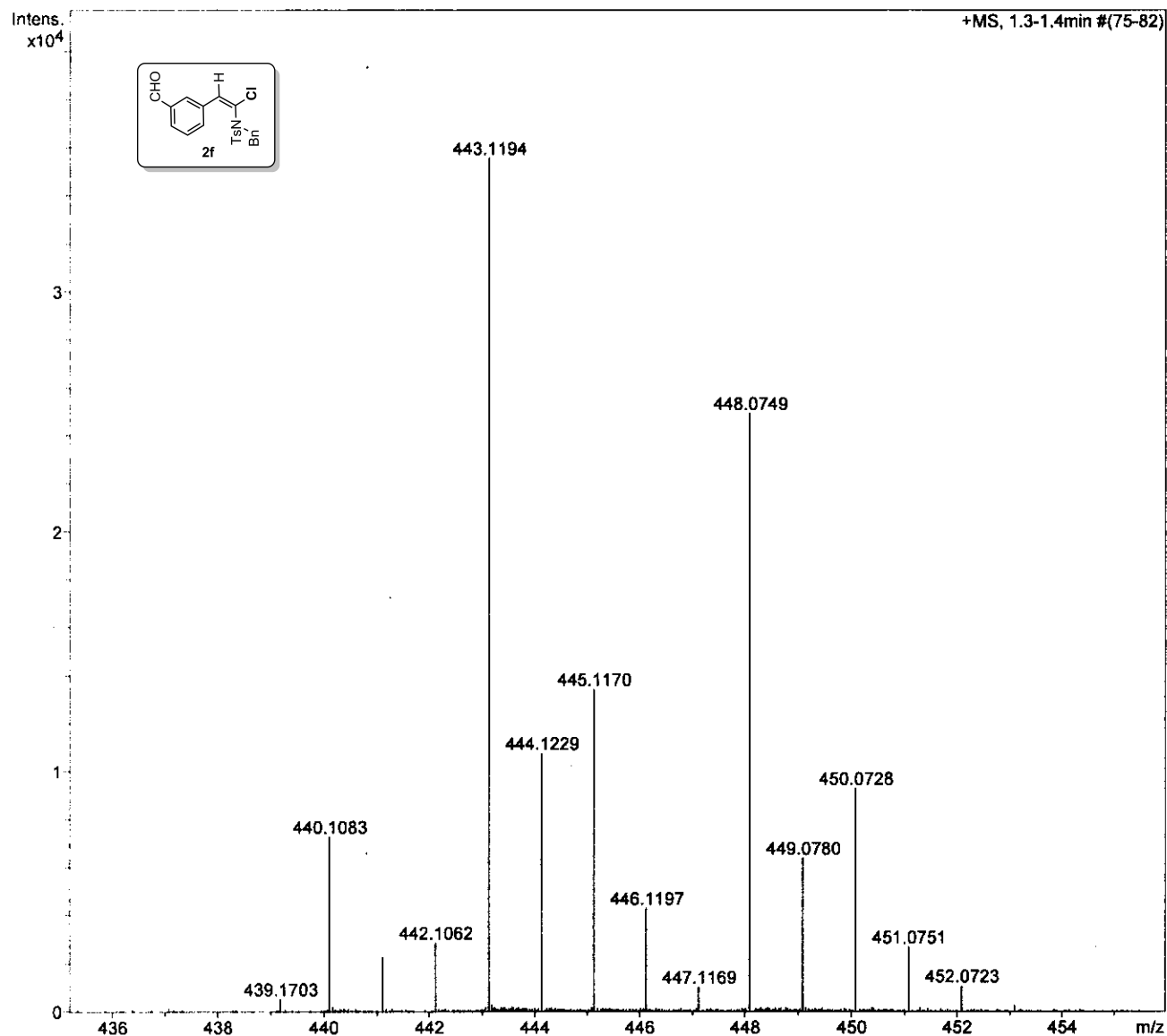
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Method tune_low.m
Sample Name RKM-3-74-DCM-MEOH
Comment

Acquisition Date 6/8/2015 12:45:05 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	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



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Analysis Info

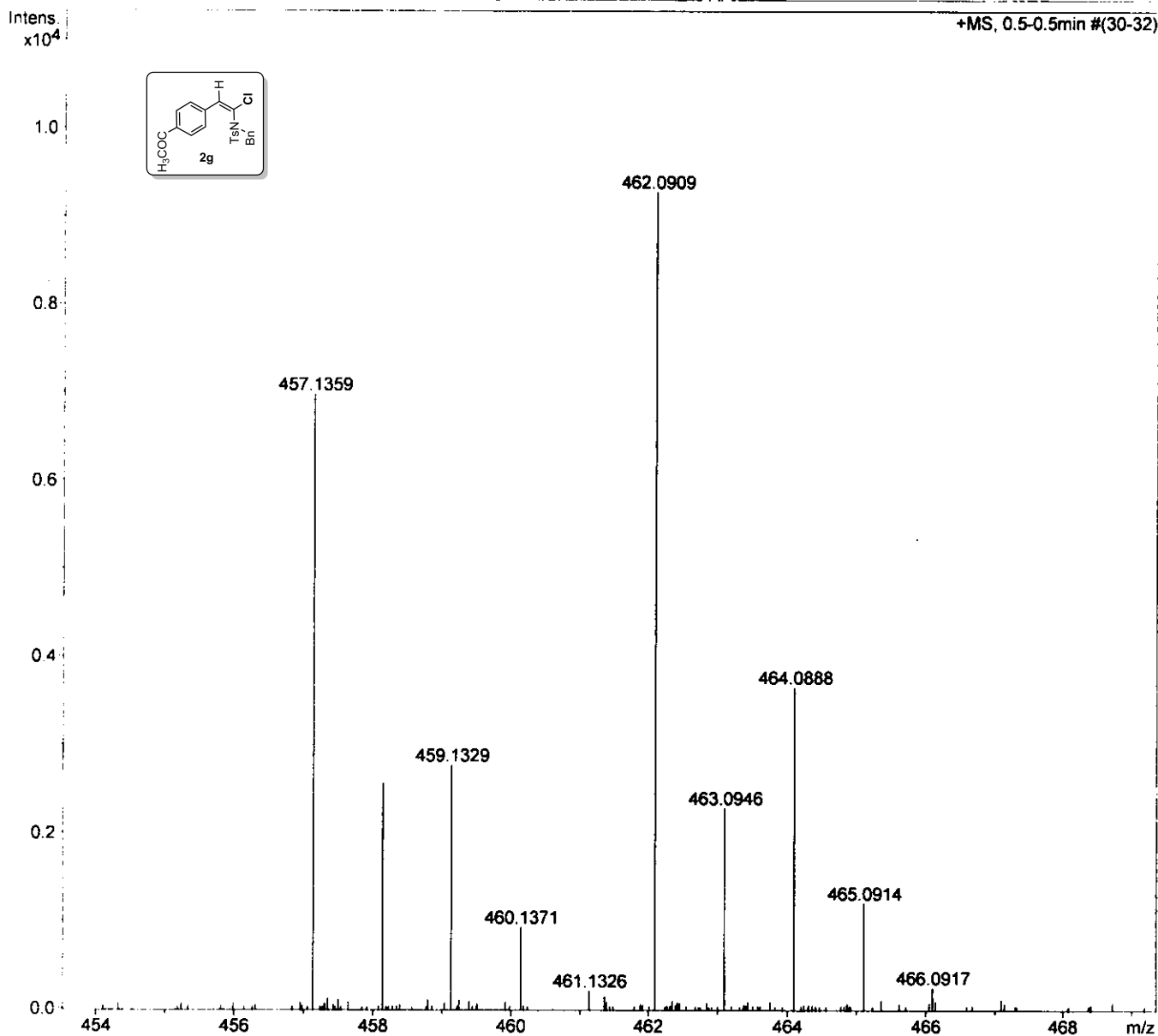
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Method tune_low.m
Sample Name RKM-3-69-DCM-MEOH
Comment

Acquisition Date 6/8/2015 12:54:20 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

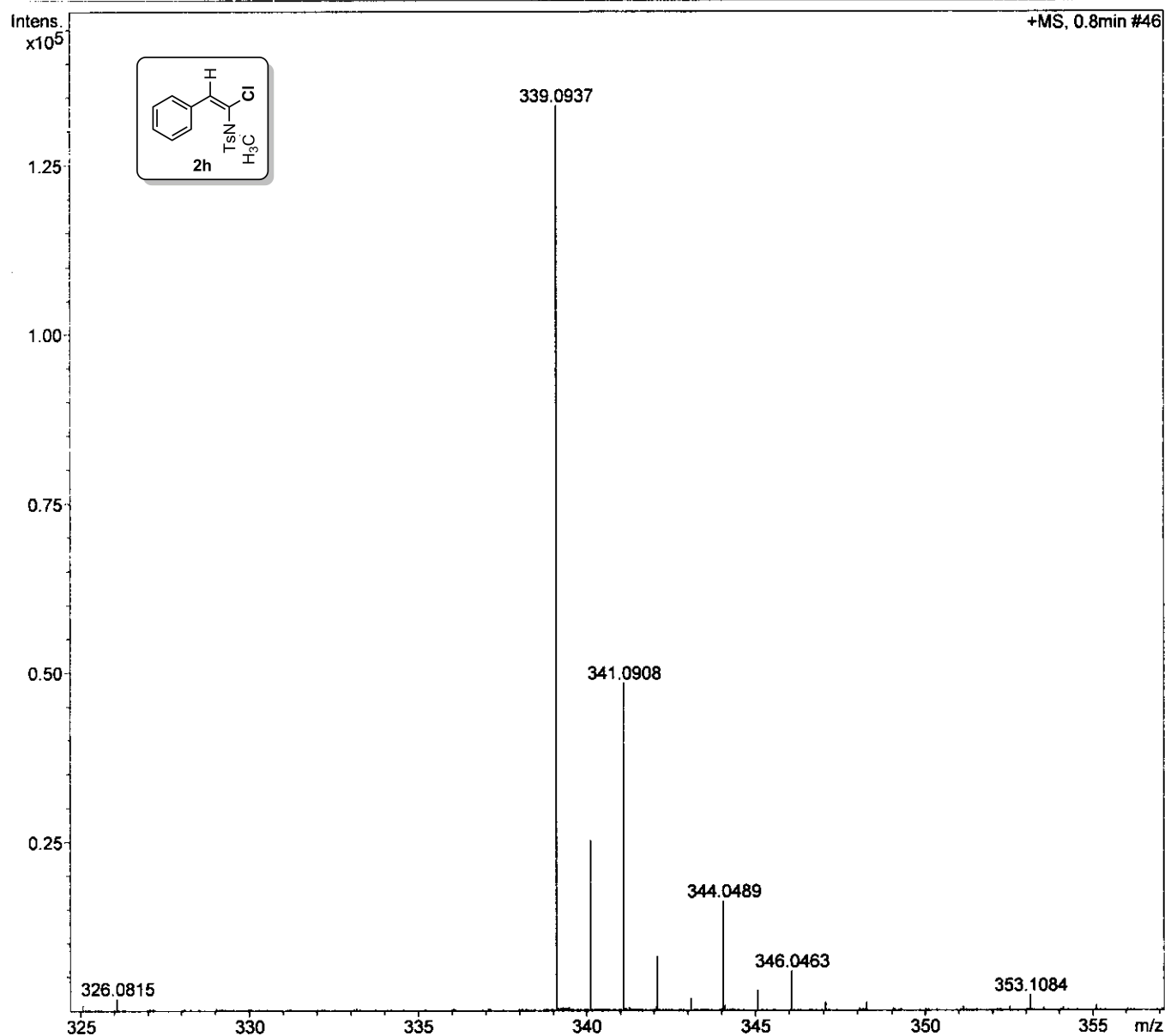
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Sample Name RKM-2-103
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Acquisition Date 3/20/2015 3:41:23 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

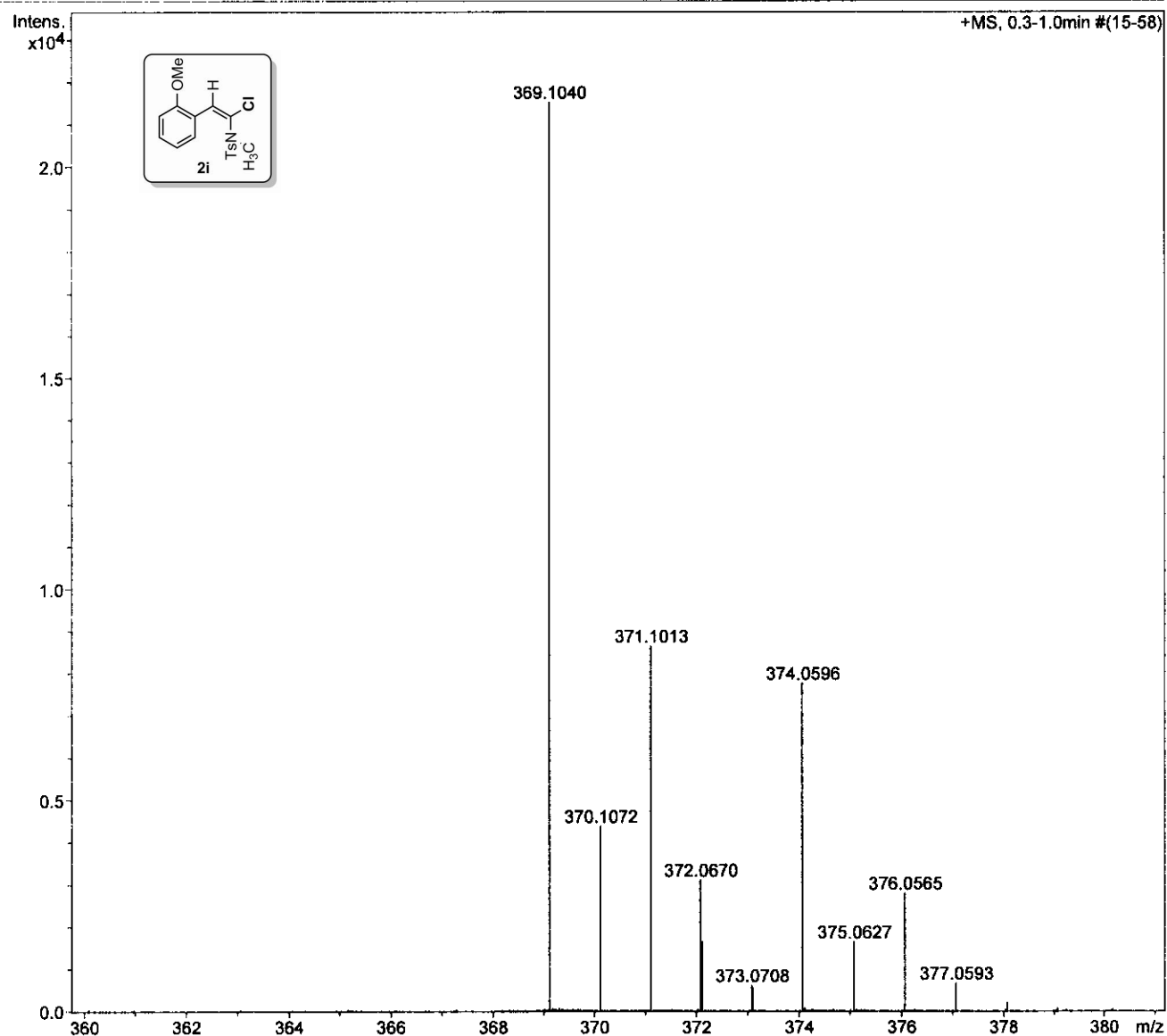
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Sample Name RKM-2-135
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Acquisition Date 3/20/2015 1:54:00 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

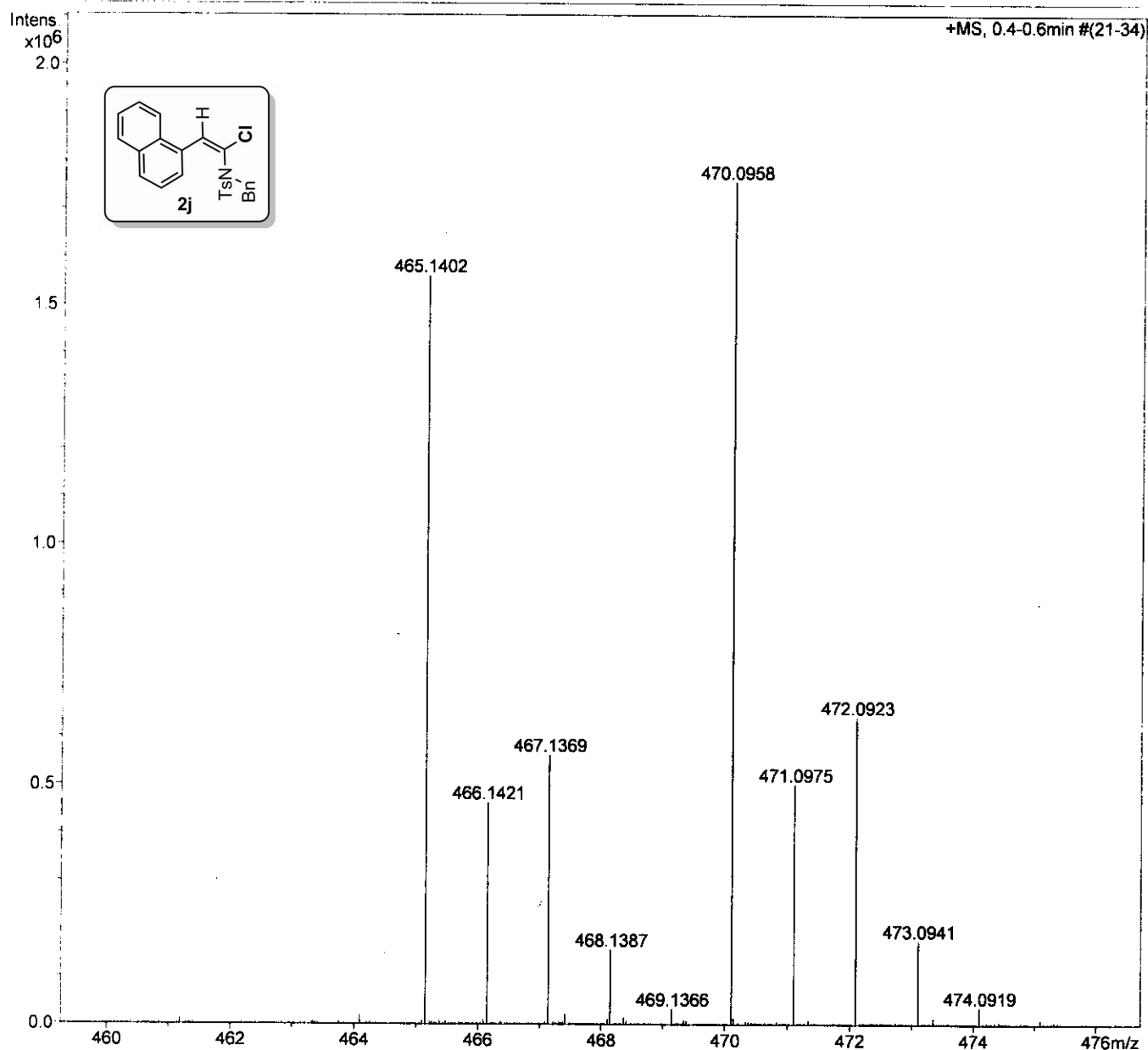
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Method tune_low_Pos.m
Sample Name RP-2-18-MEOH
Comment

Acquisition Date 5/11/2015 12:06:04 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	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



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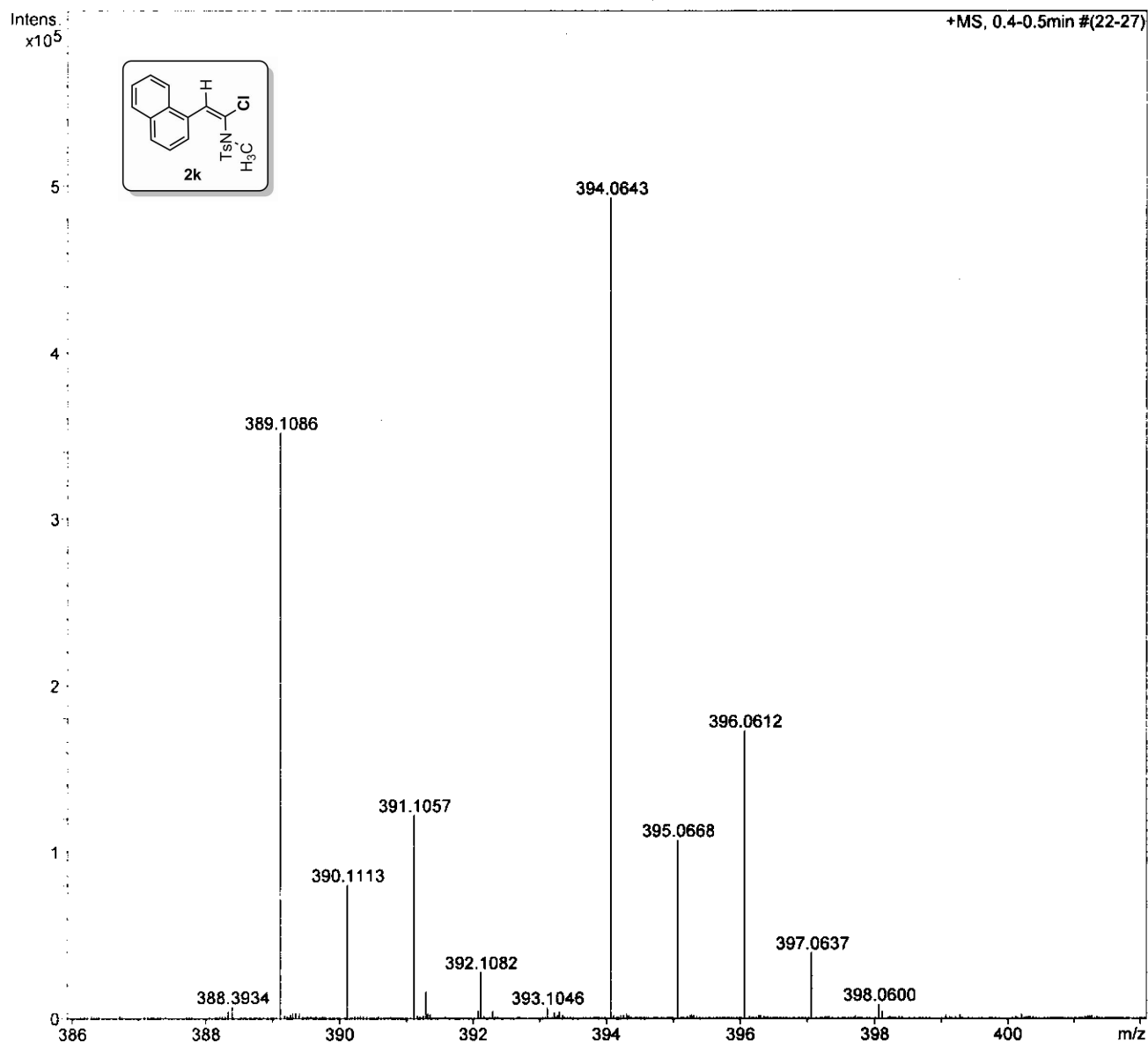
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Sample Name RP-2-21-MEOH
Comment

Acquisition Date 5/8/2015 4:22:18 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	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



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Analysis Info

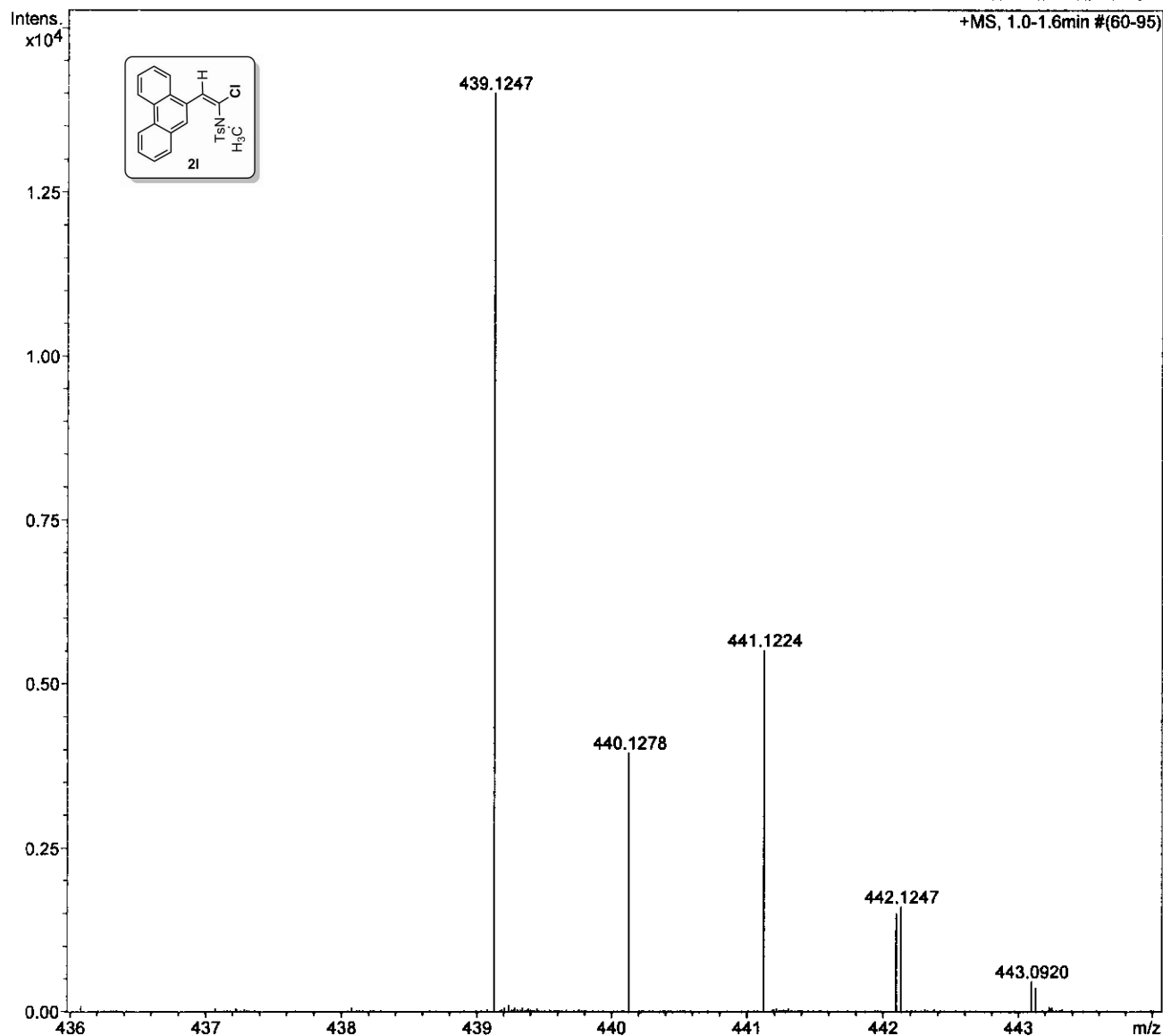
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Method tune_low.m
Sample Name RKM-2-144
Comment

Acquisition Date 3/20/2015 2:04:57 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

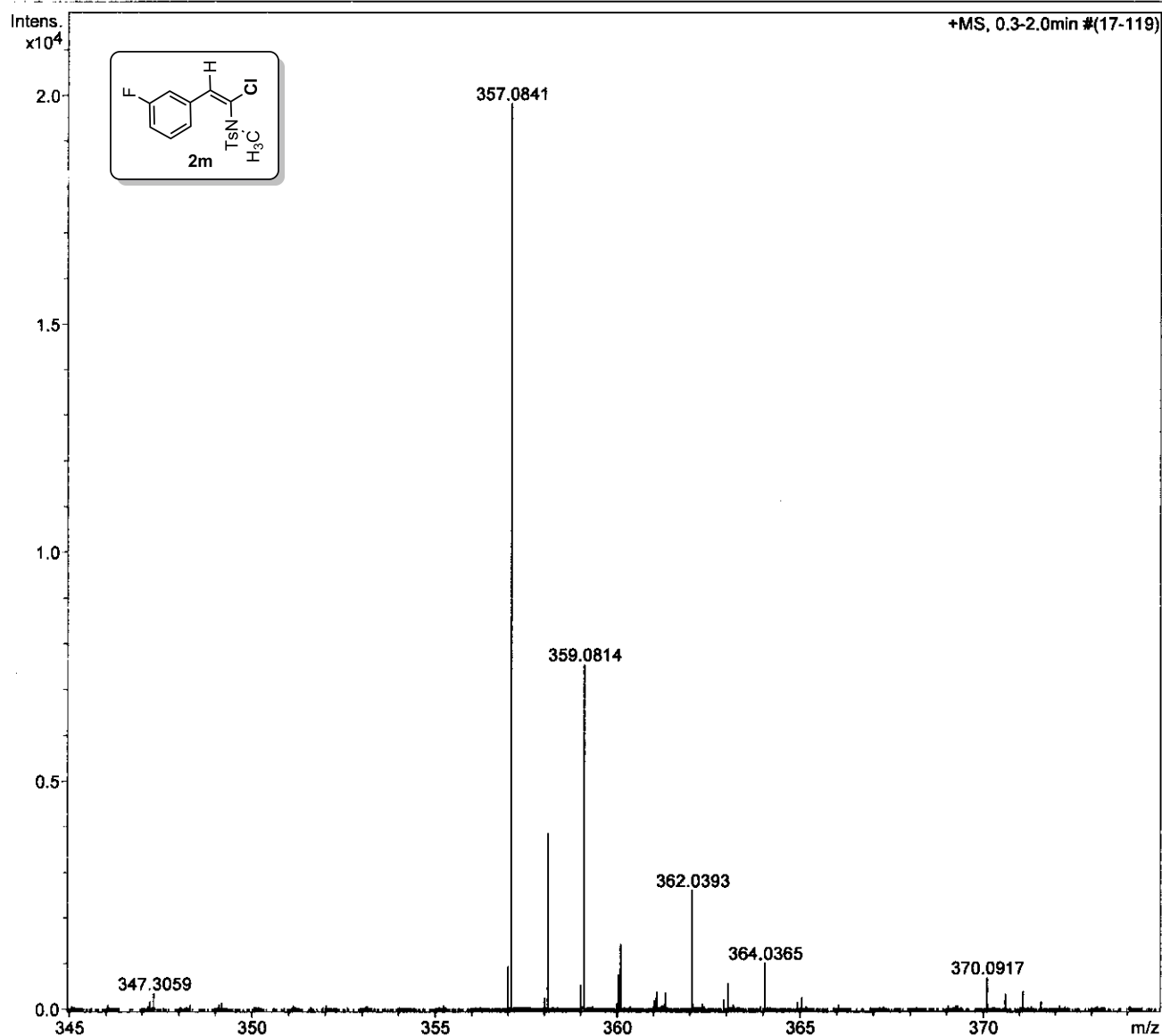
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Sample Name RKM-2-116
Comment

Acquisition Date 3/20/2015 4:11:29 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

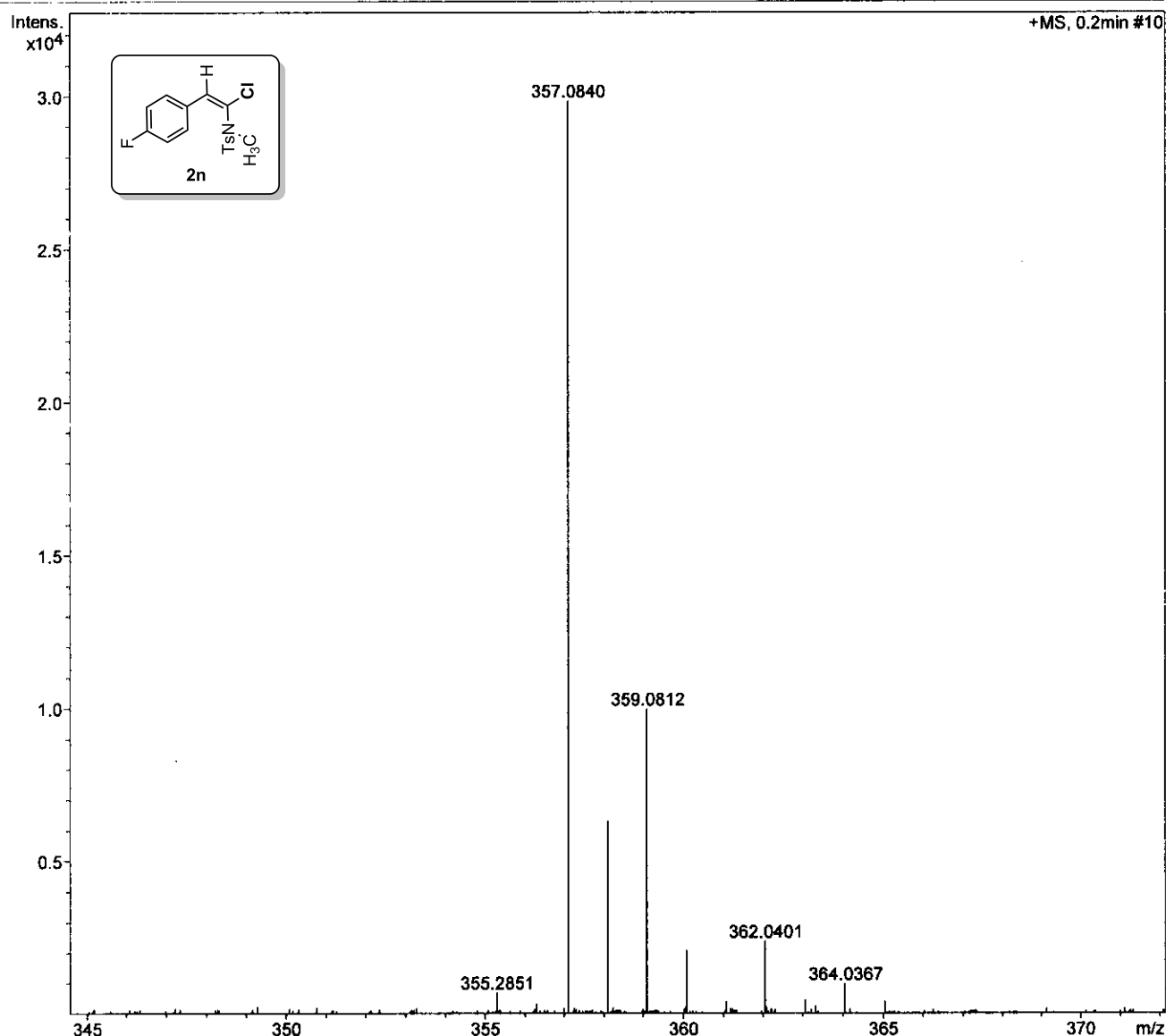
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Sample Name RKM-2-115
Comment

Acquisition Date 3/20/2015 3:57:25 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

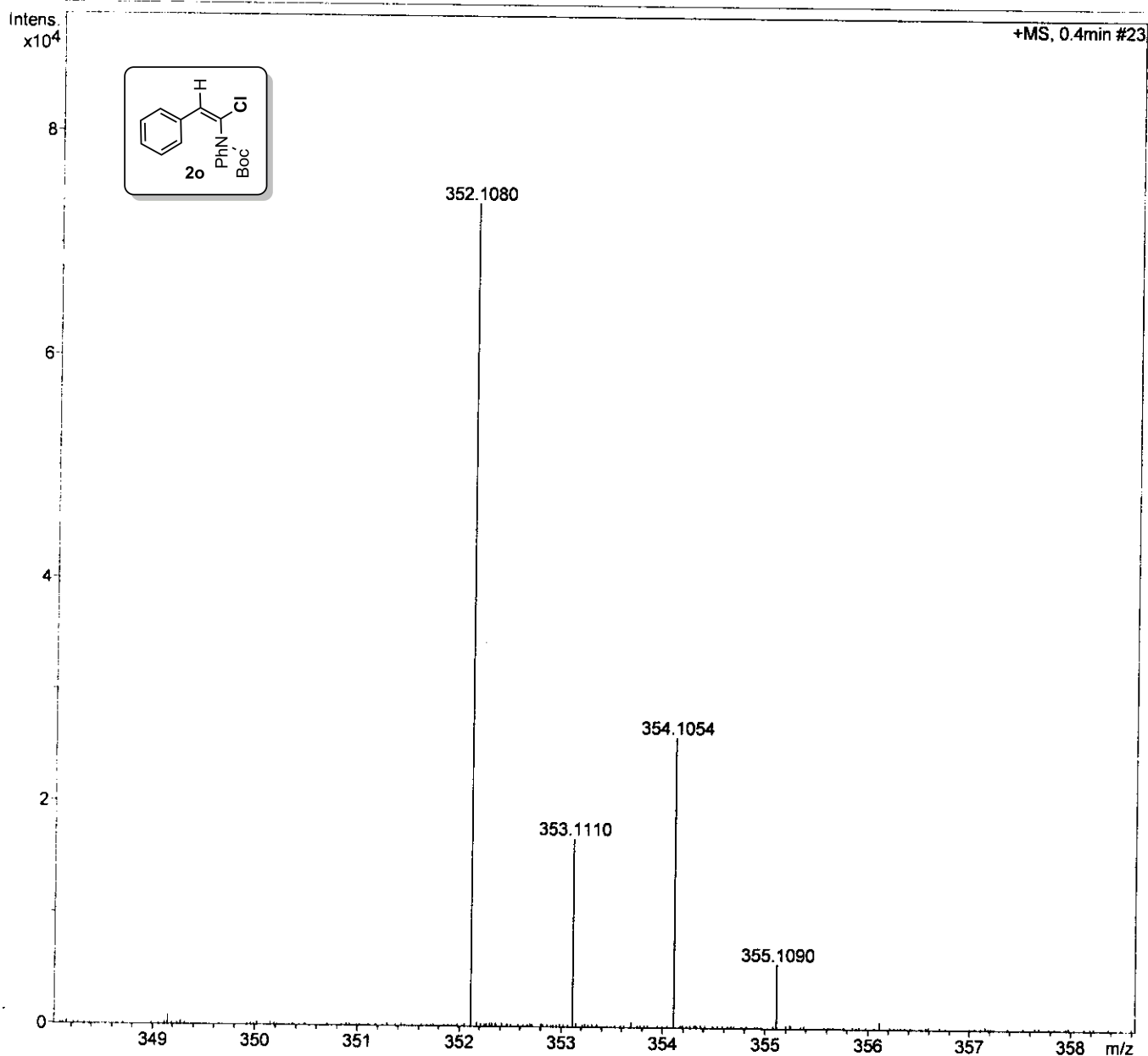
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Method tune_low_Pos.m
Sample Name PB-6-150-MEOH
Comment

Acquisition Date 6/4/2015 12:33:07 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

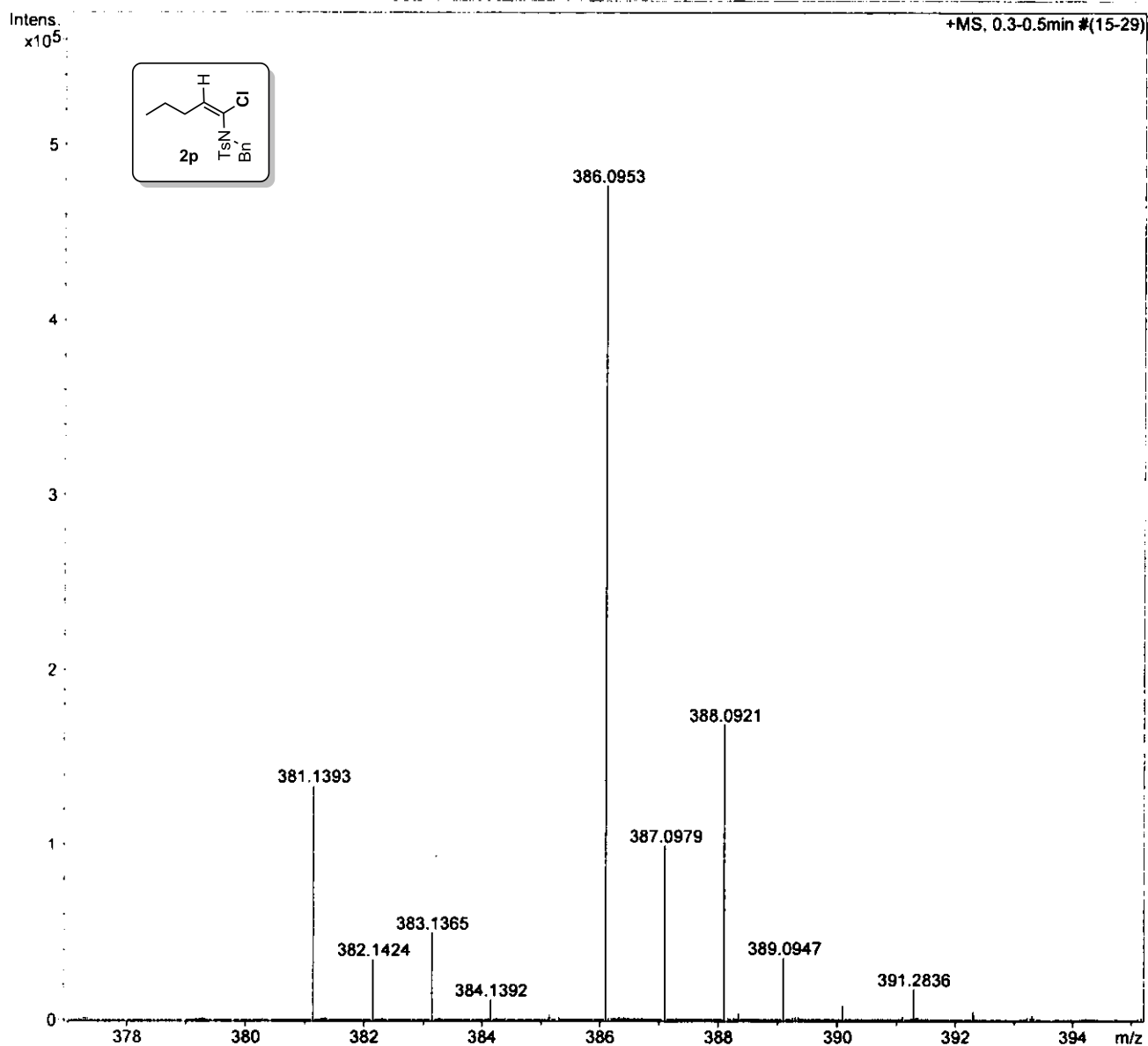
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Method tune_low.m
Sample Name RP-2-77-MEOH
Comment

Acquisition Date 6/4/2015 10:56:46 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



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Analysis Info

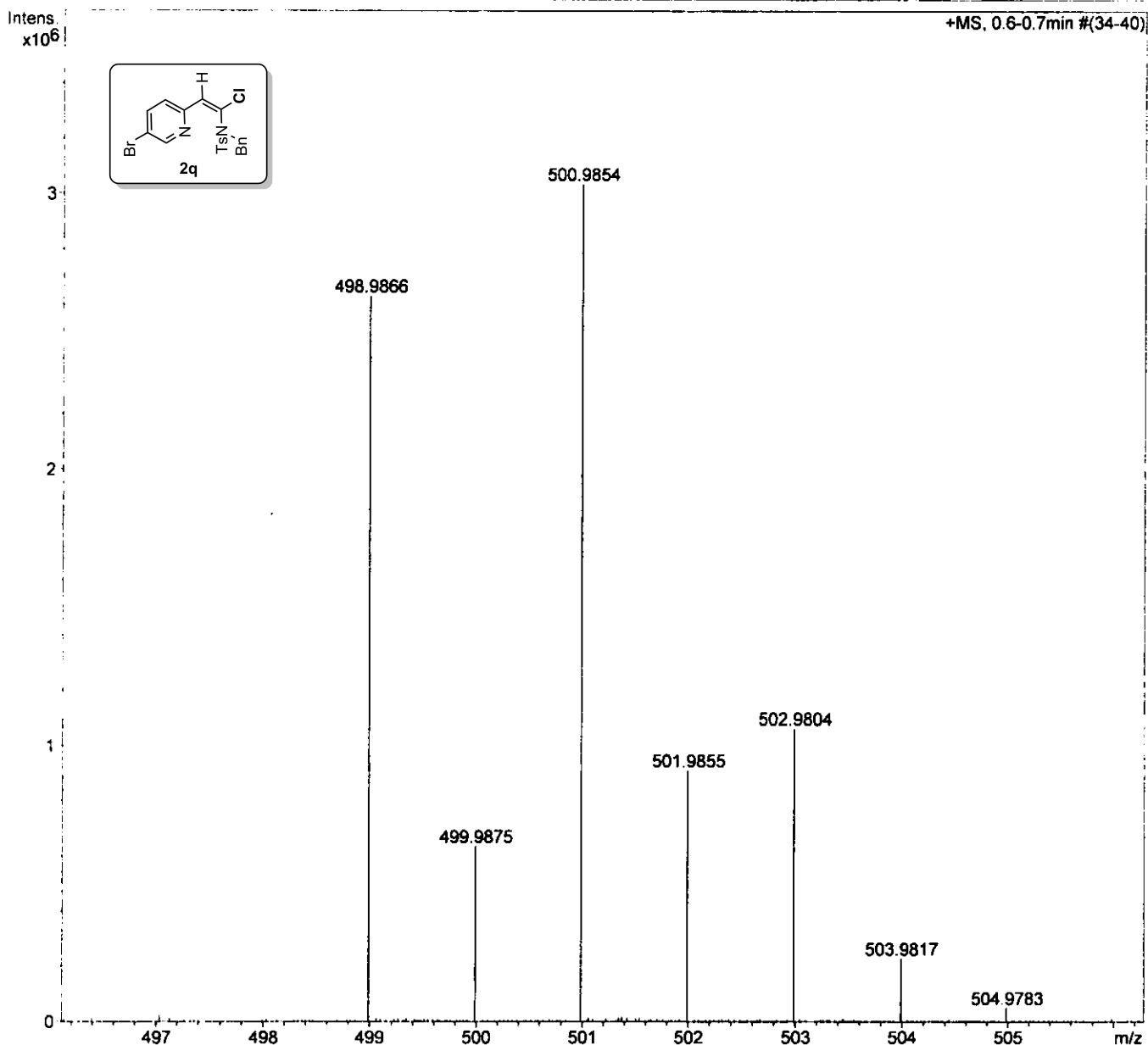
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Comment

Acquisition Date 6/4/2015 12:04:17 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



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Analysis Info

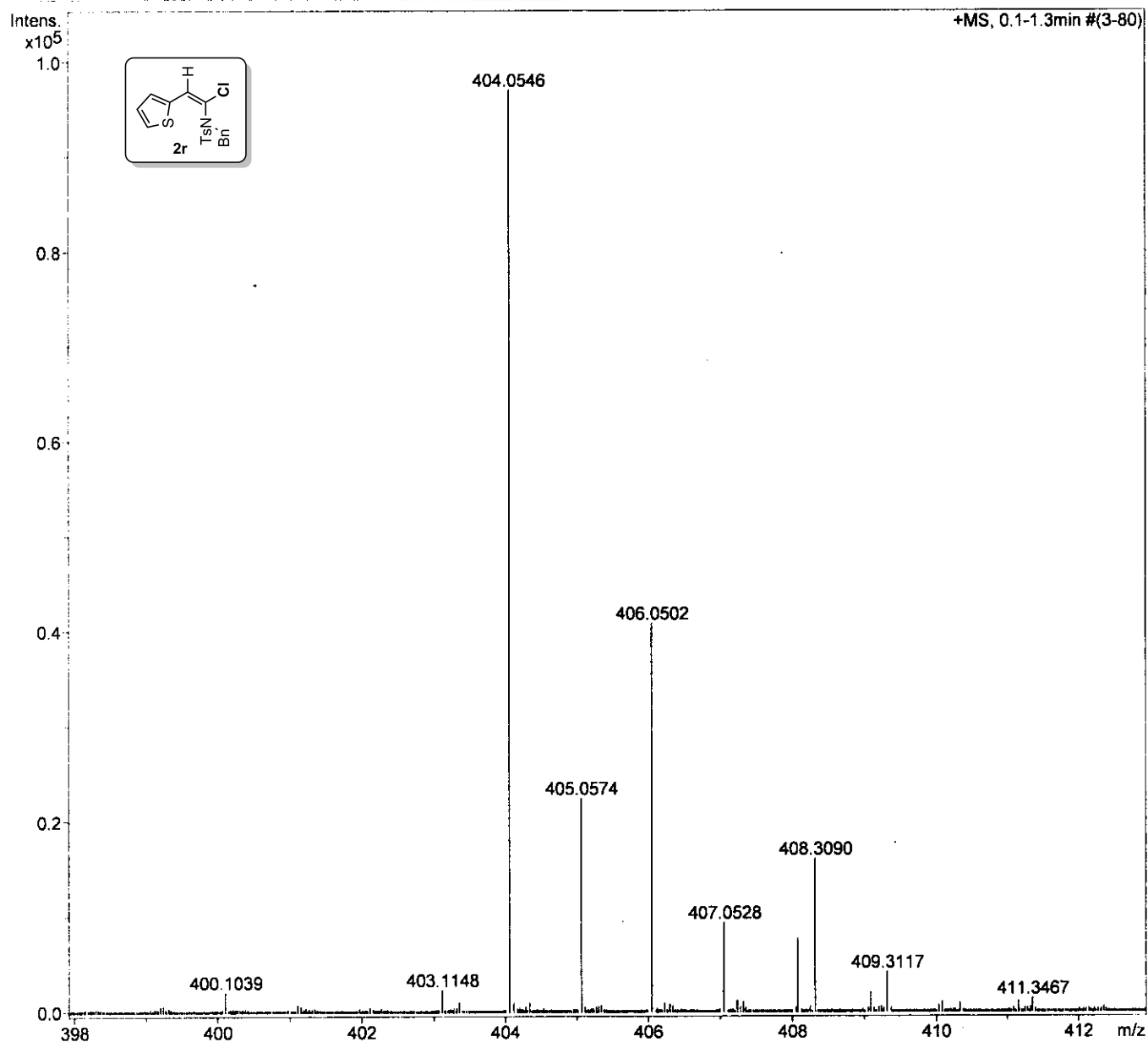
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Sample Name RP-2-98
Comment

Acquisition Date 6/18/2015 3:56:37 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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Analysis Info

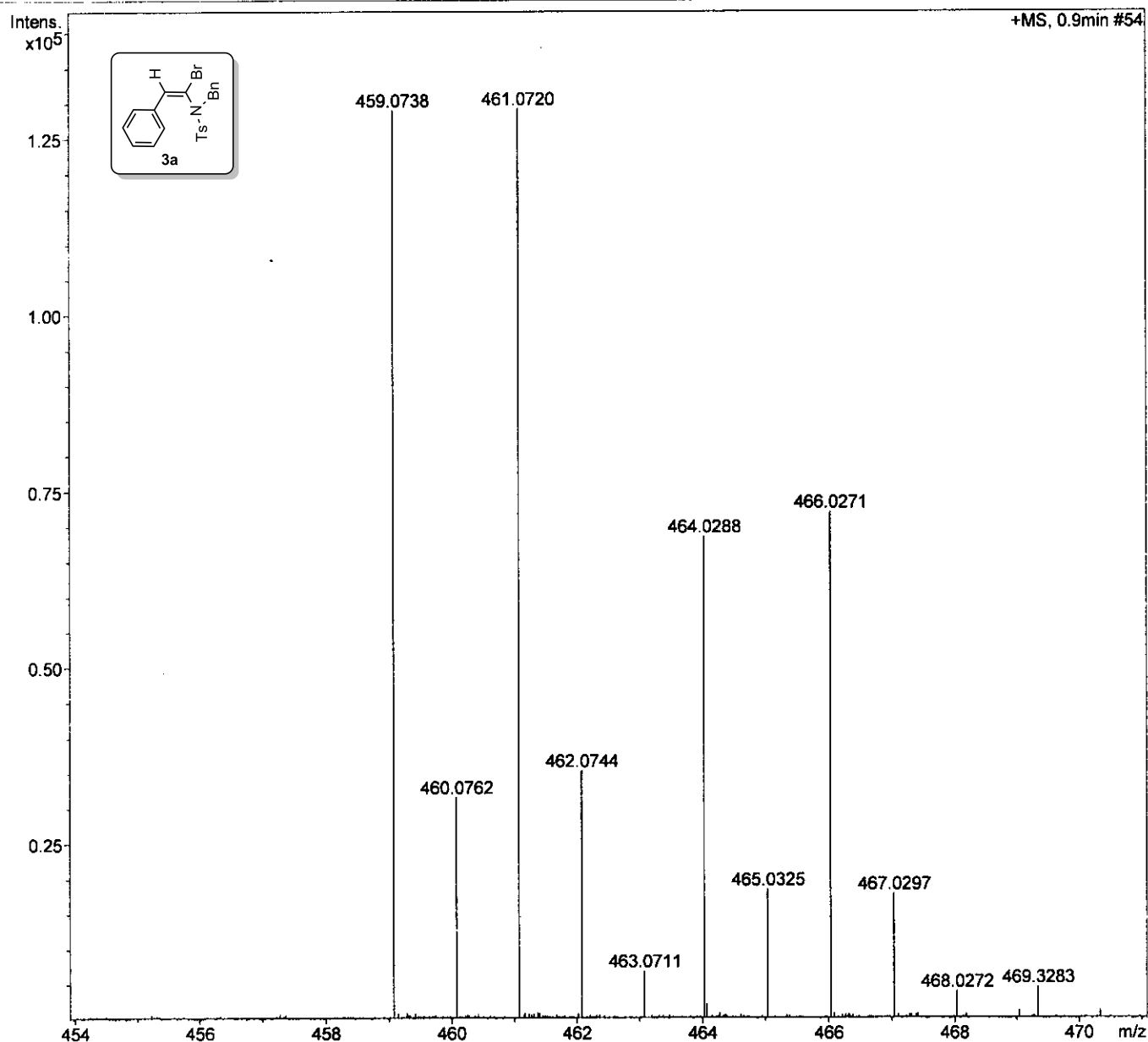
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Comment

Acquisition Date 2/27/2015 5:03:57 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
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Analysis Info

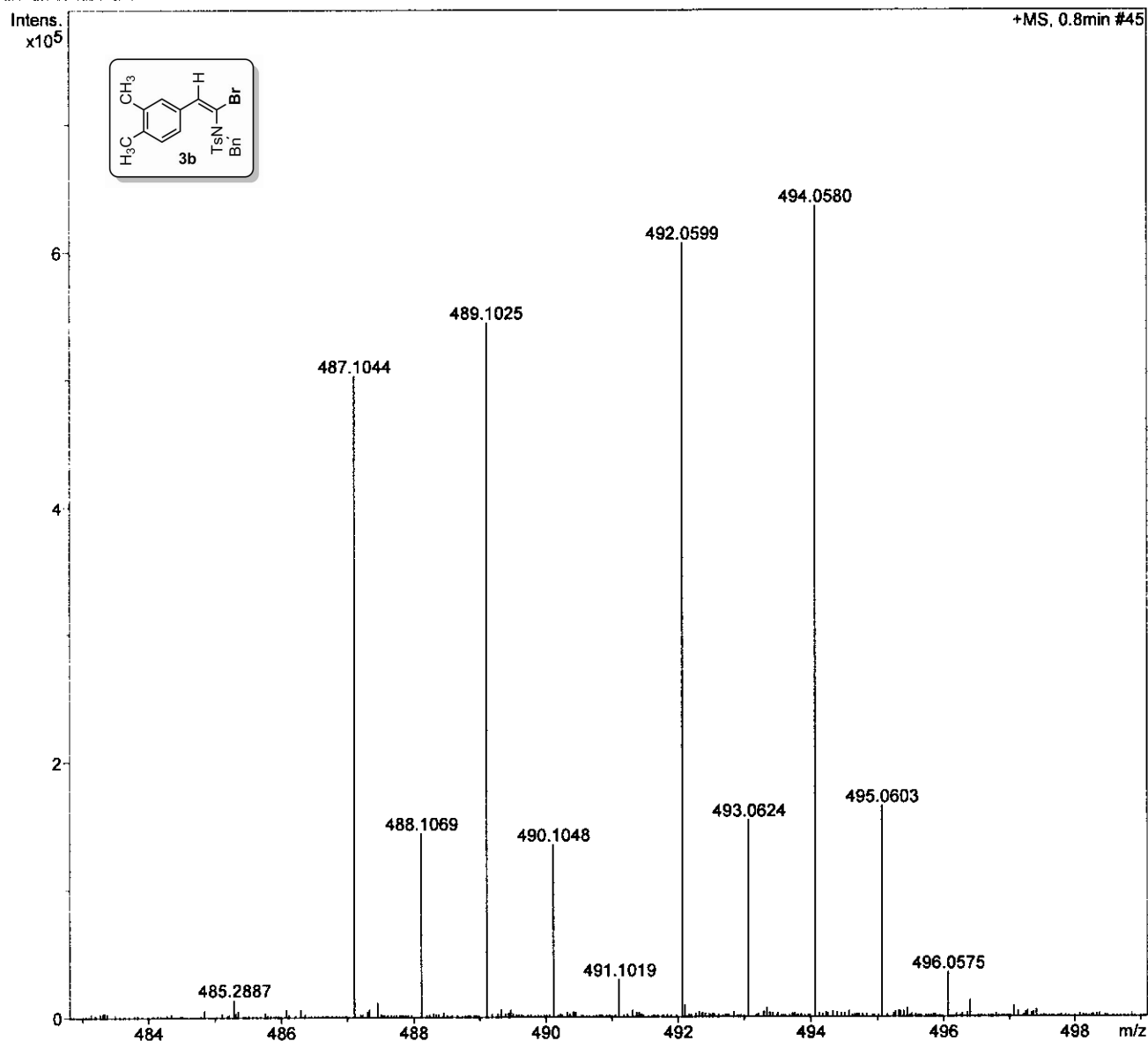
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Method TL-P.m
Sample Name RP-2-8-MEOH
Comment

Acquisition Date 5/11/2015 12:26:12 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	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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Analysis Info

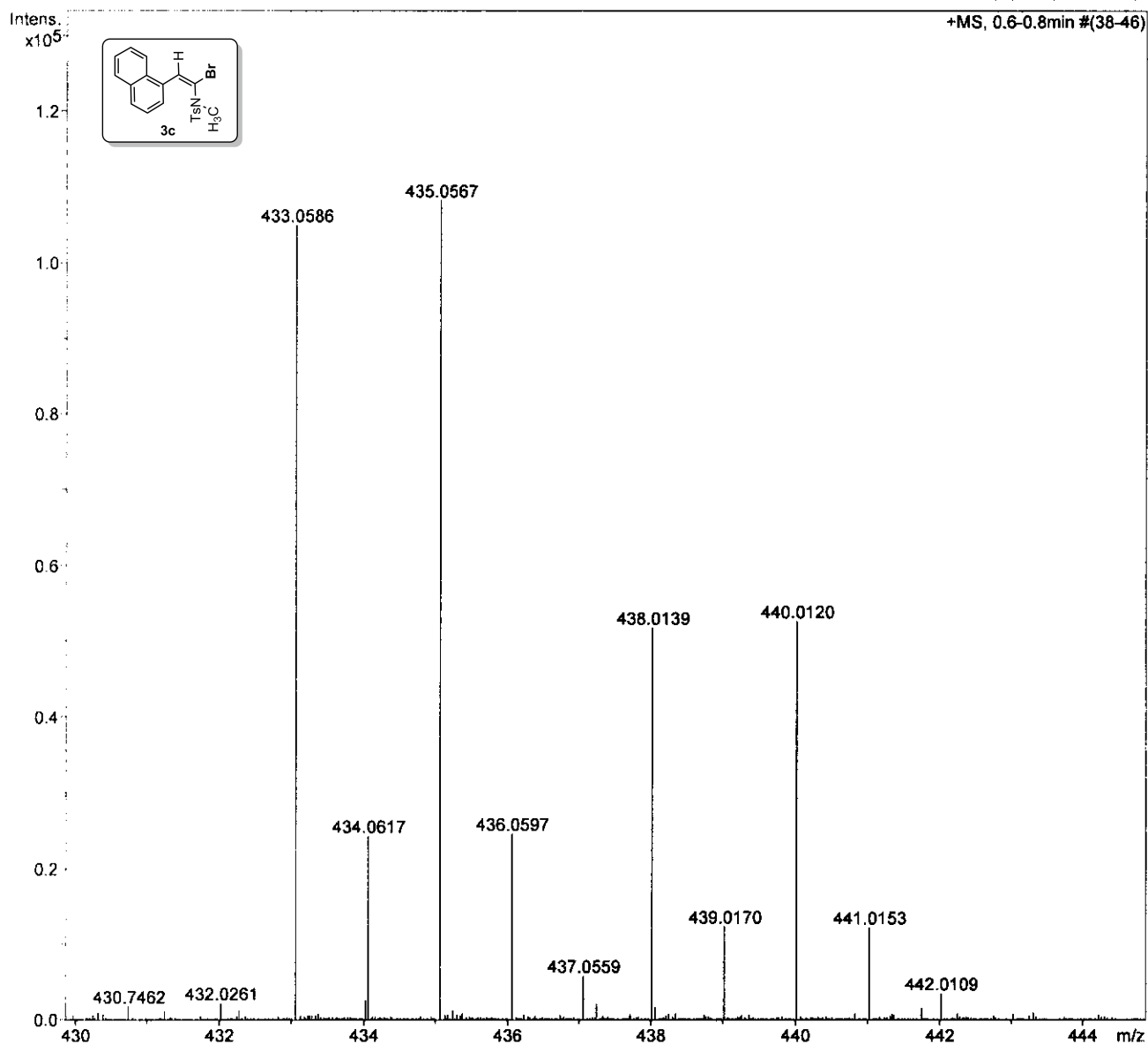
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Method tune_low.m
Sample Name RP-2-19-MEOH
Comment

Acquisition Date 5/8/2015 4:32:37 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
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Analysis Info

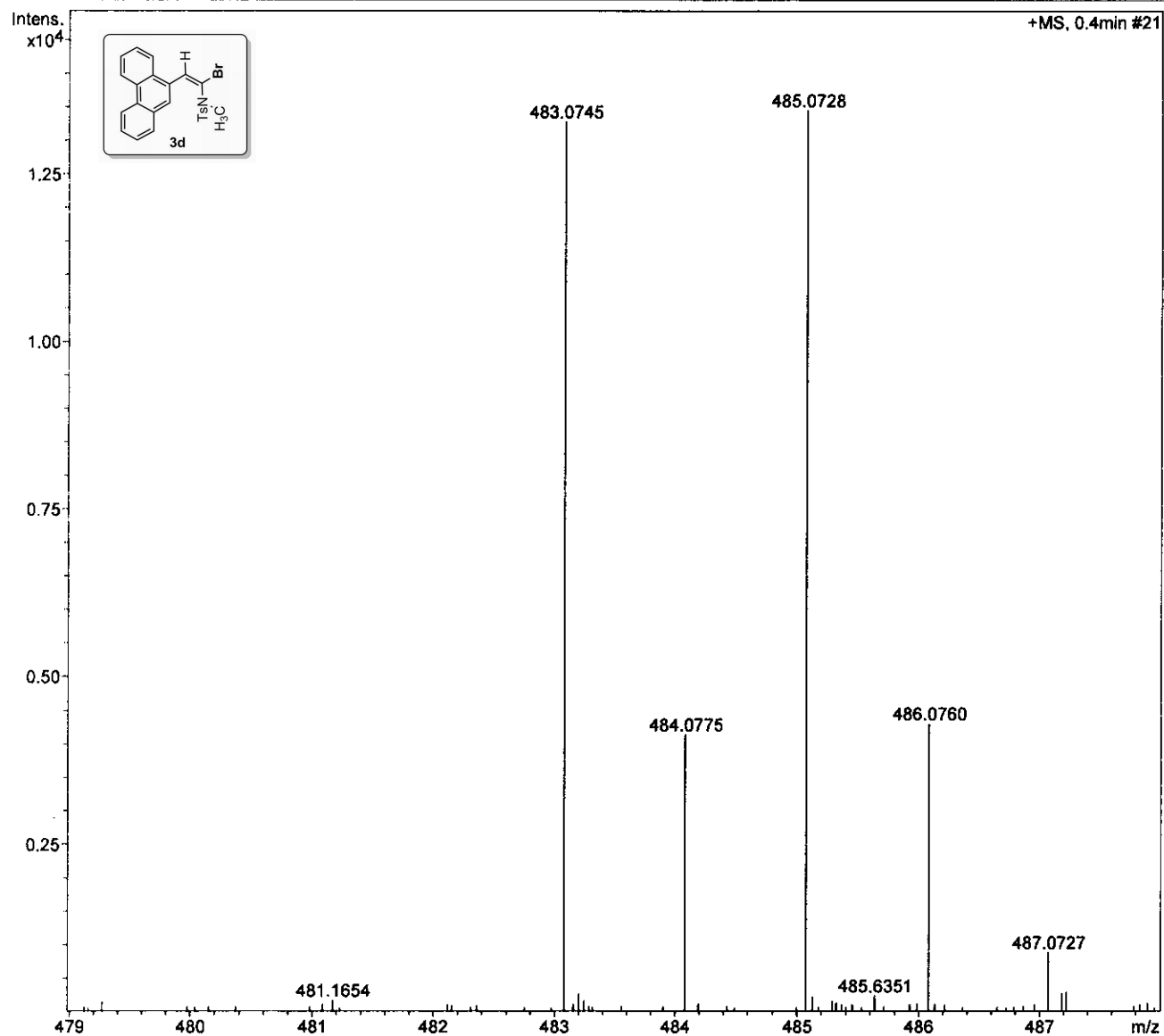
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Method tune_low.m
Sample Name RKM-2-145
Comment

Acquisition Date 3/20/2015 2:17:26 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

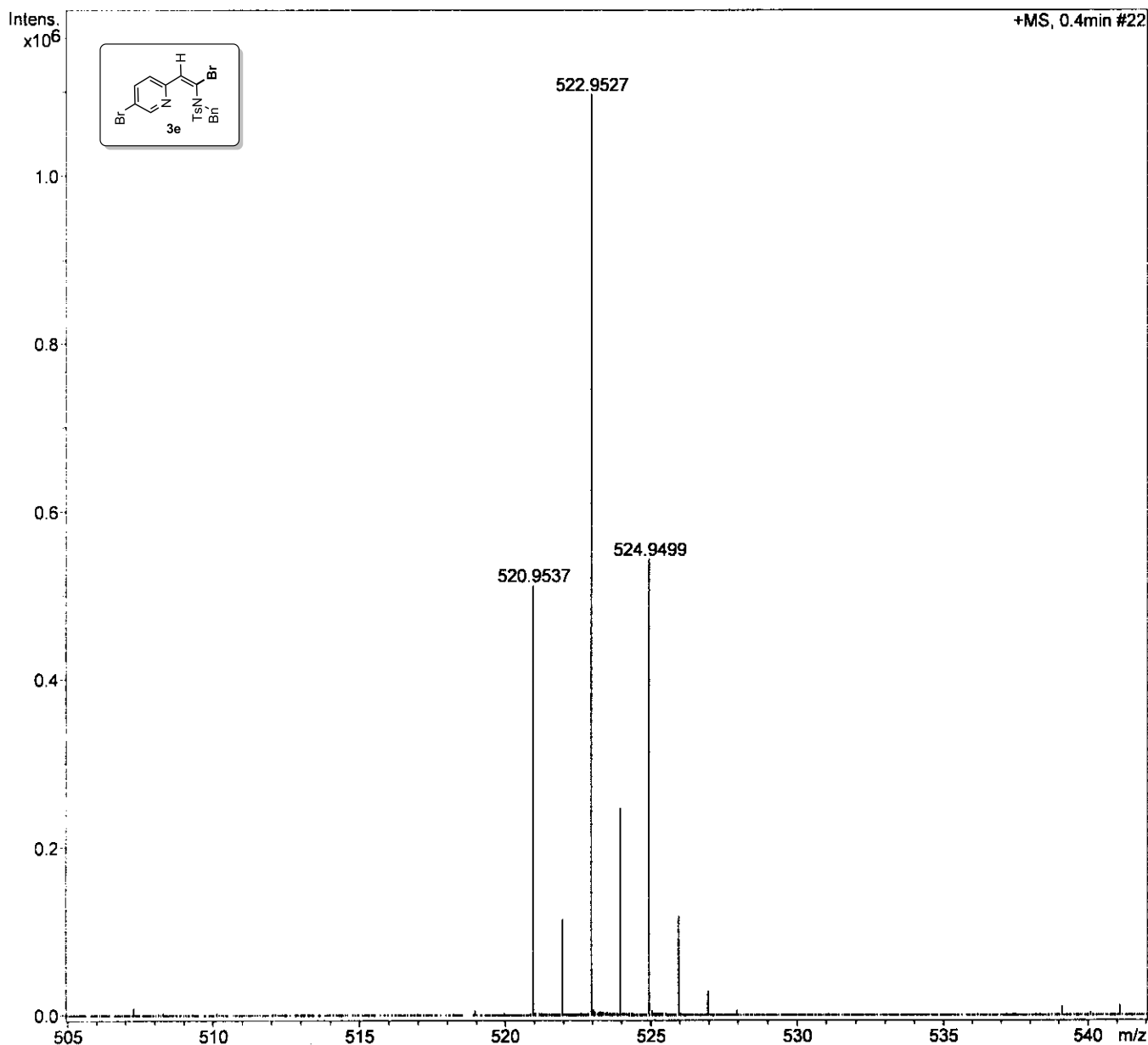
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Method tune_low.m
Sample Name RP-2-33
Comment

Acquisition Date 6/18/2015 3:30:56 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
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Analysis Info

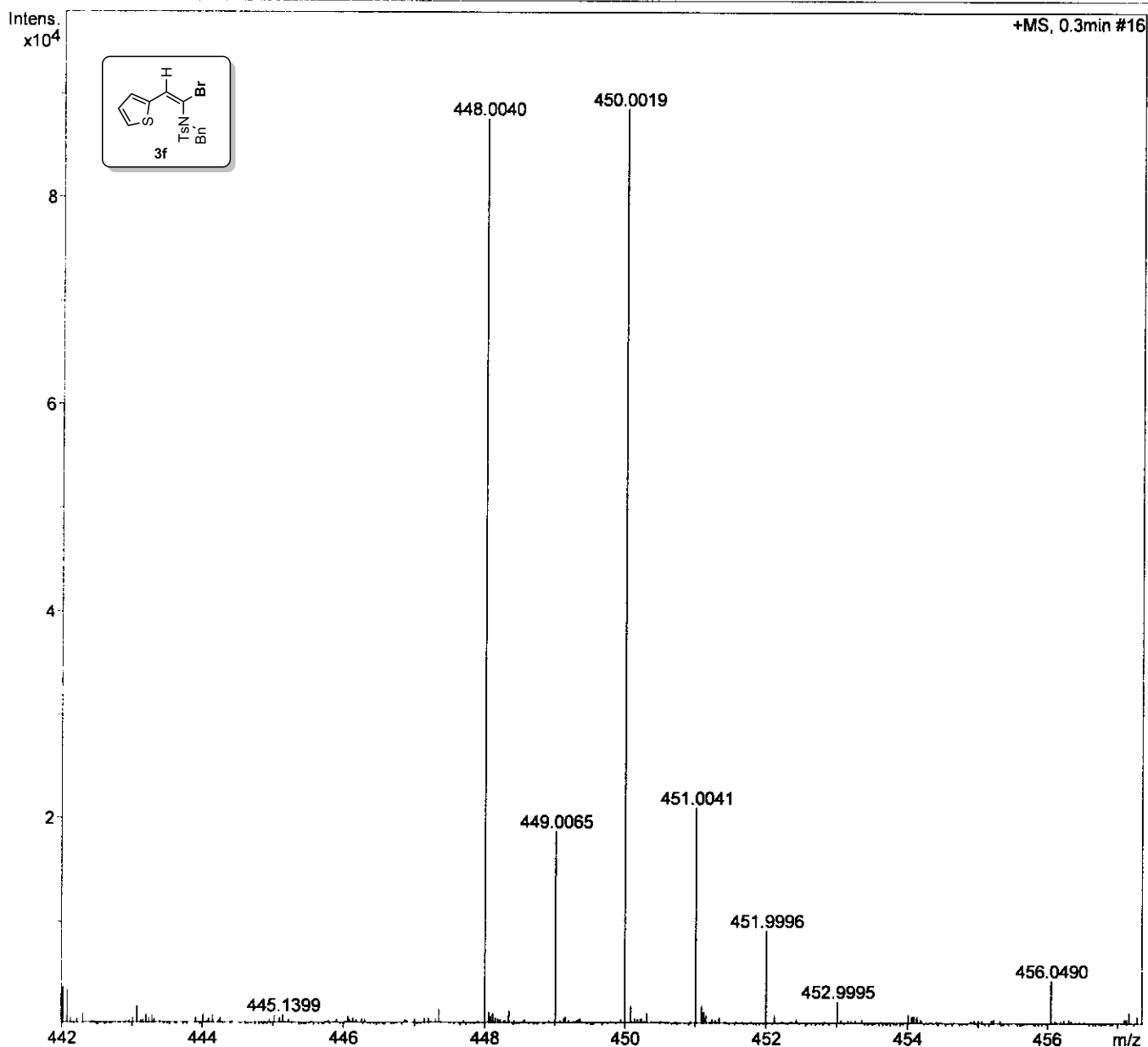
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Method tune_low.m
Sample Name RP-2-99
Comment

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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
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Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste

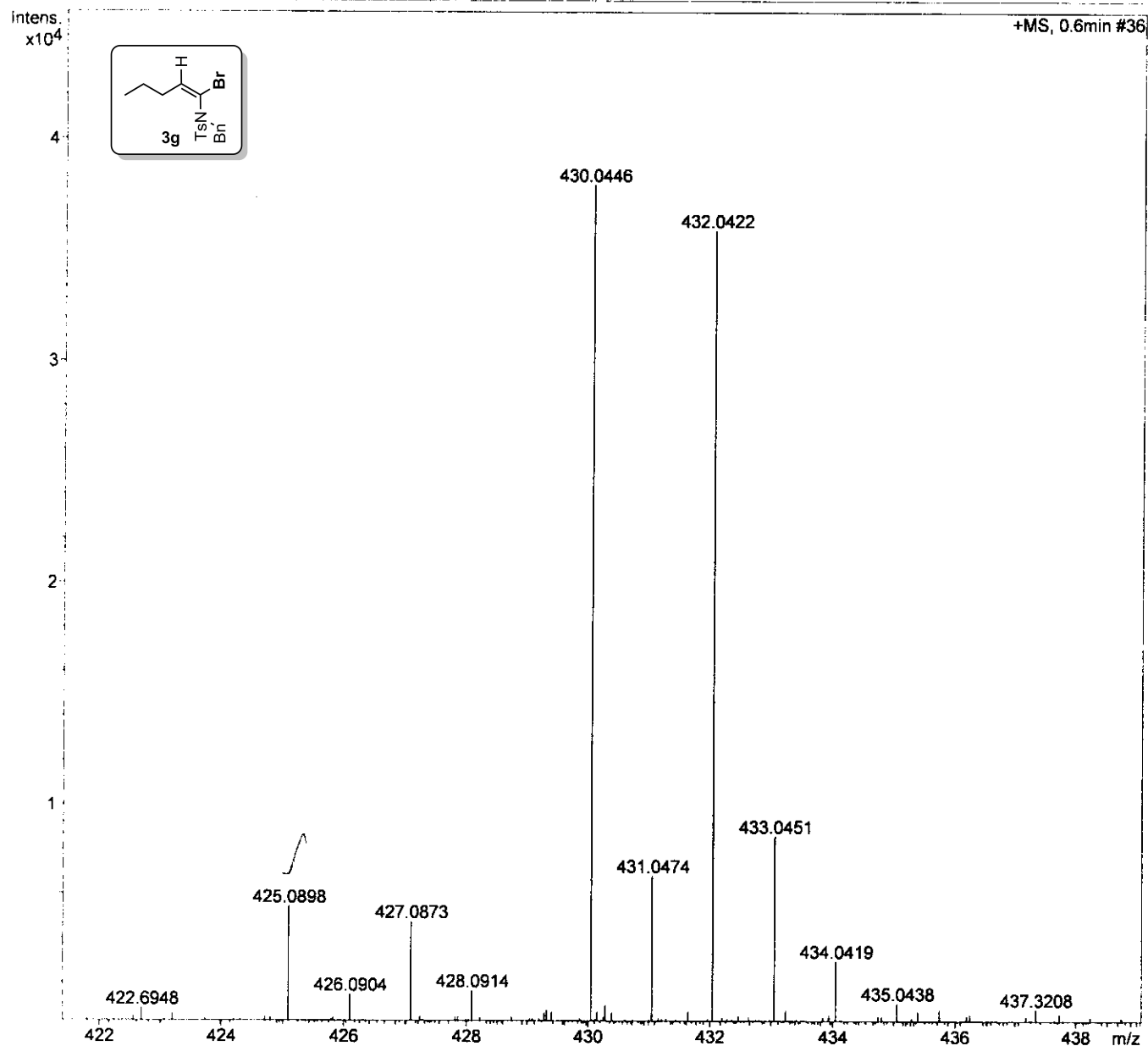


School of Chemistry
University of Hyderabad

Analysis Name	D:\Data\2015\DR.AK.SAHOO\JUNE\RP-2-76.d
Method	tune_low.m
Sample Name	RP-2-76-MEOH
Comment	

Operator	Ramu Sridhar	
Instrument	maXis	10138

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



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Analysis Info

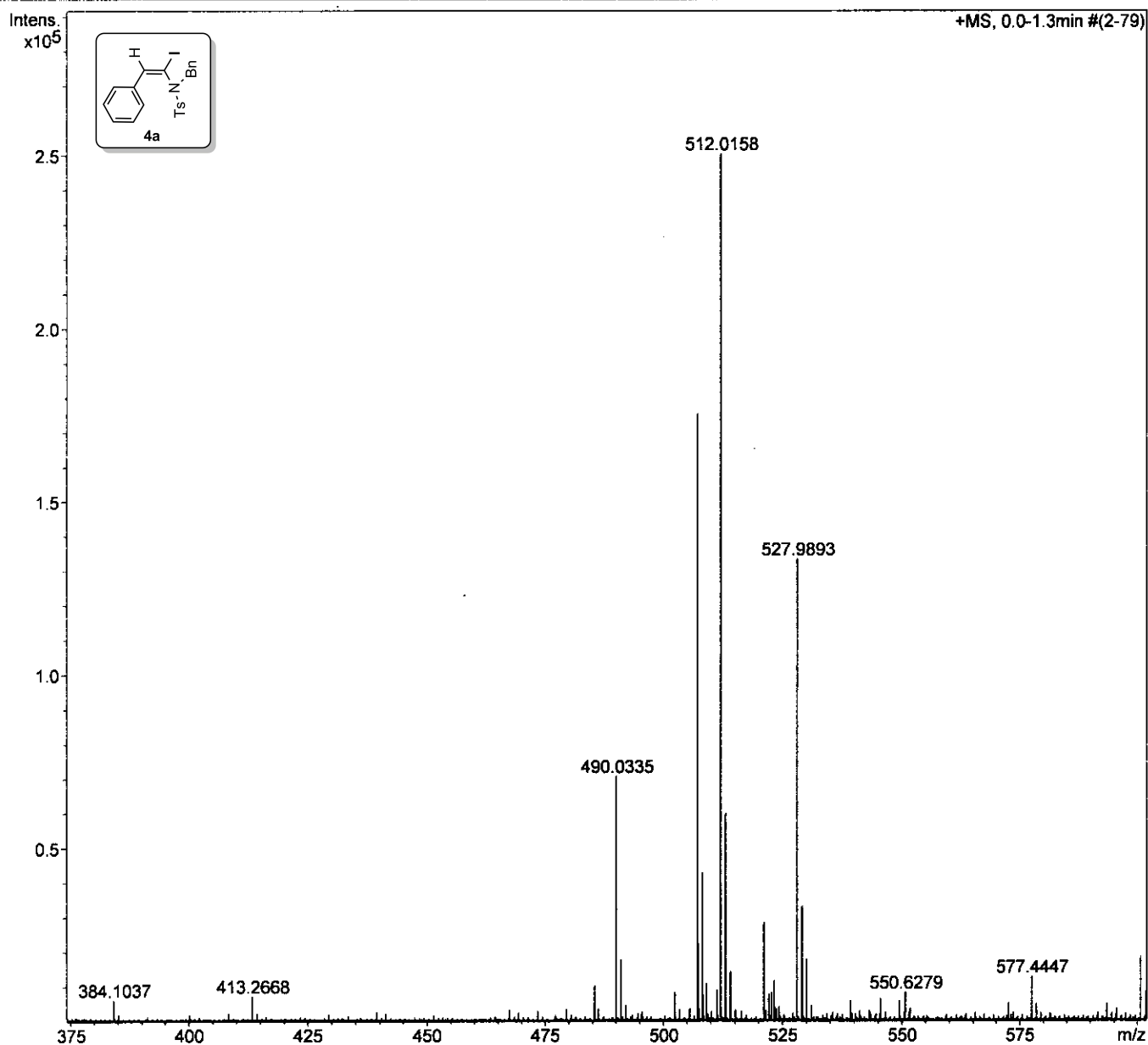
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Method tune_low.m
Sample Name RP-1-170
Comment

Acquisition Date 2/27/2015 5:13:56 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

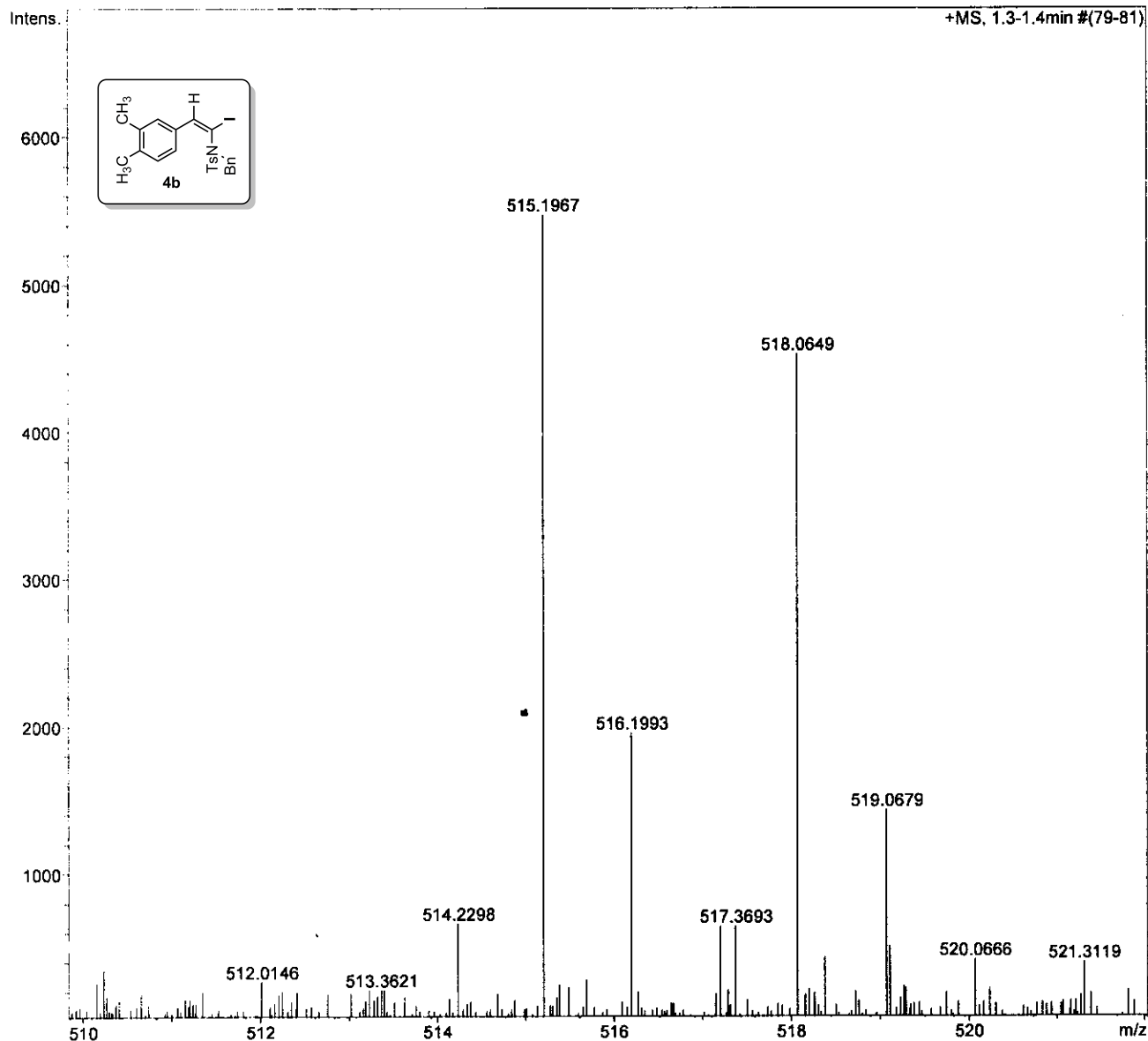
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Method tune_low.m
Sample Name RP-2-9-MEOH
Comment

Acquisition Date 6/29/2015 3:30:15 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.0 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	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



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Analysis Info

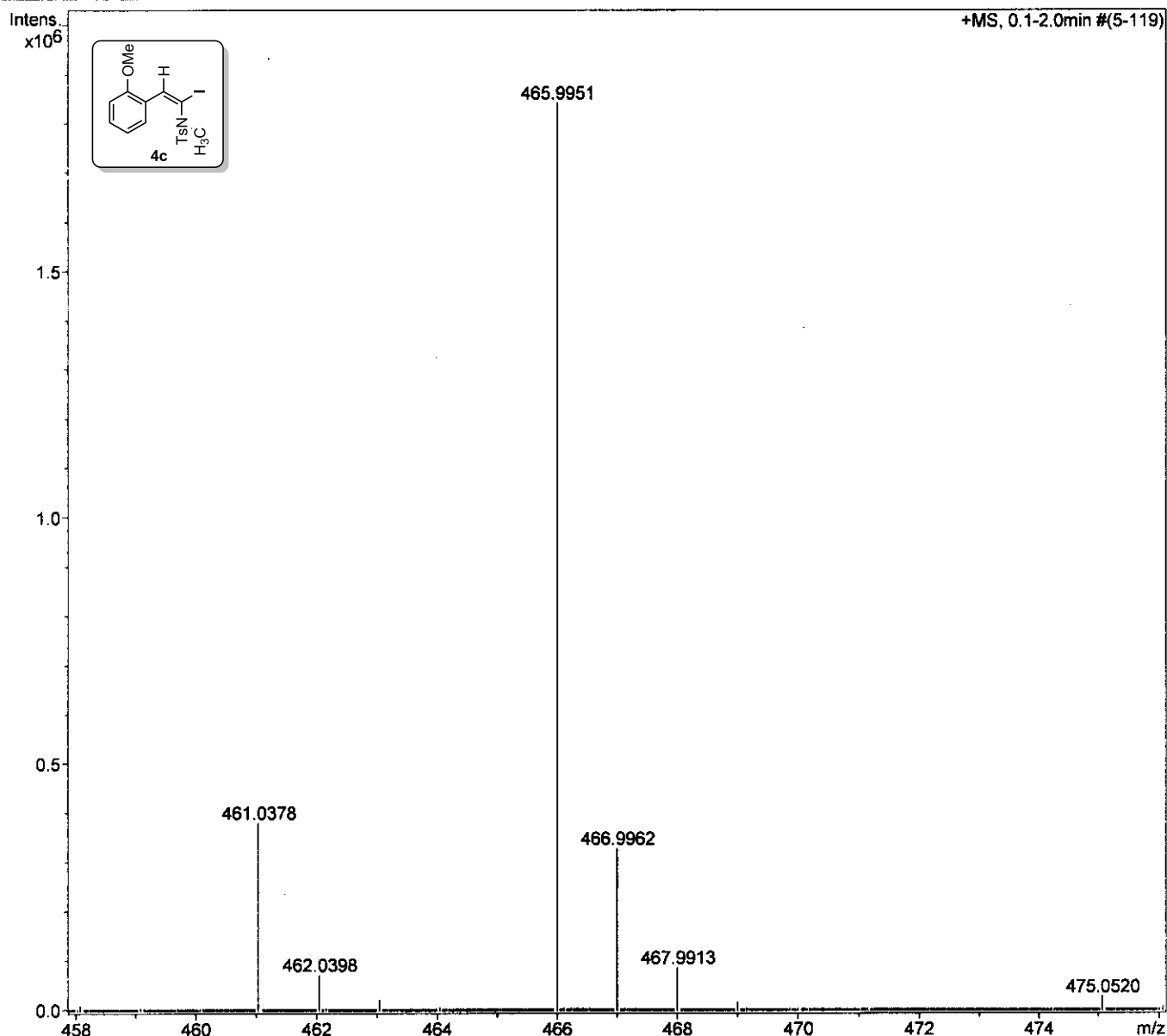
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Method tune_low_Pos-R2.m
Sample Name RKM-2-151
Comment

Acquisition Date 3/20/2015 2:53:10 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	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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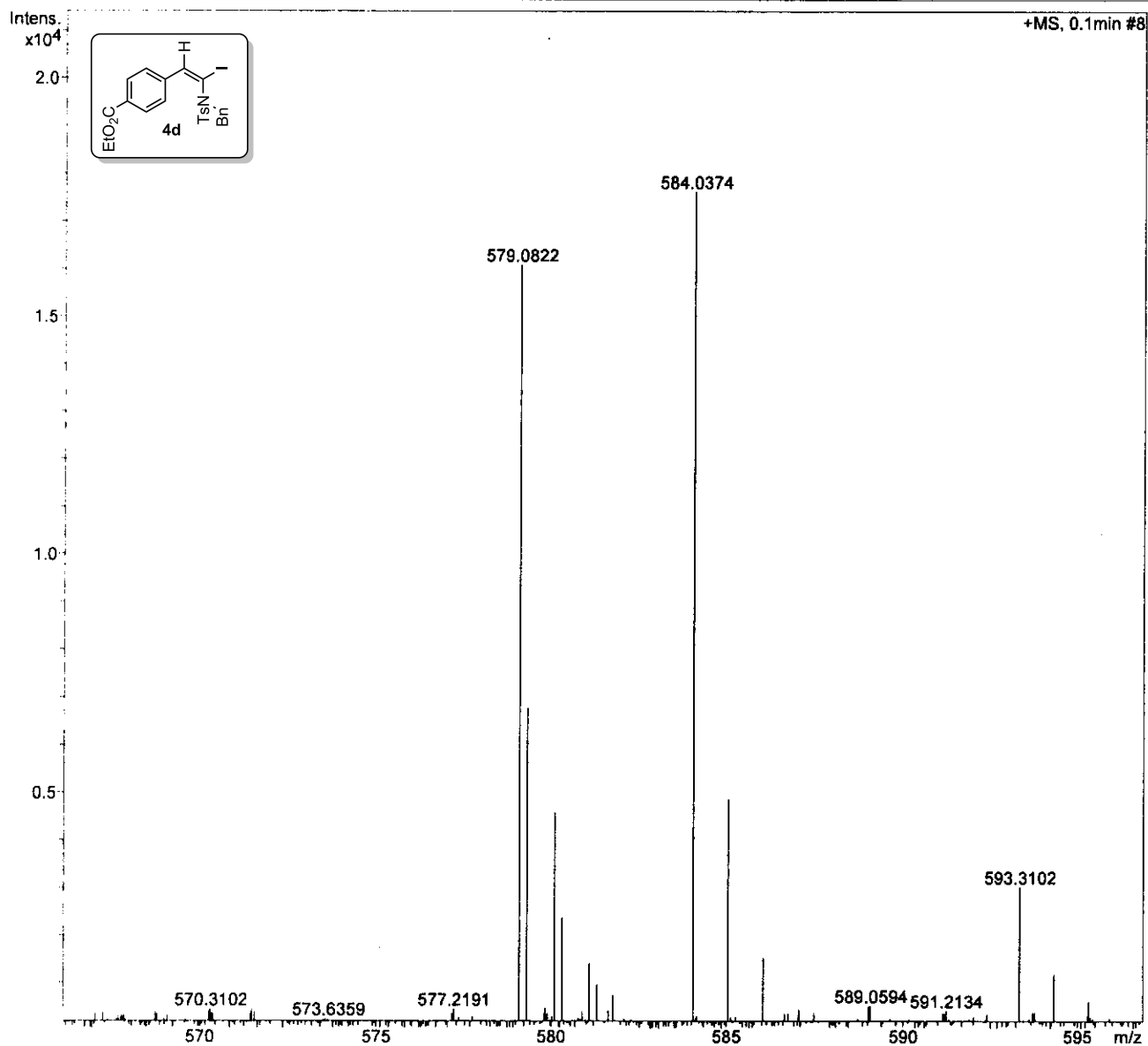
Analysis Info

Analysis Name D:\Data\2015\DR.AK.SAHOO\JULY\PB-7-70.d
Method tune_low.m
Sample Name PB-7-70-MEOH
Comment

Acquisition Date 7/6/2015 4:07:59 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	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



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Analysis Info

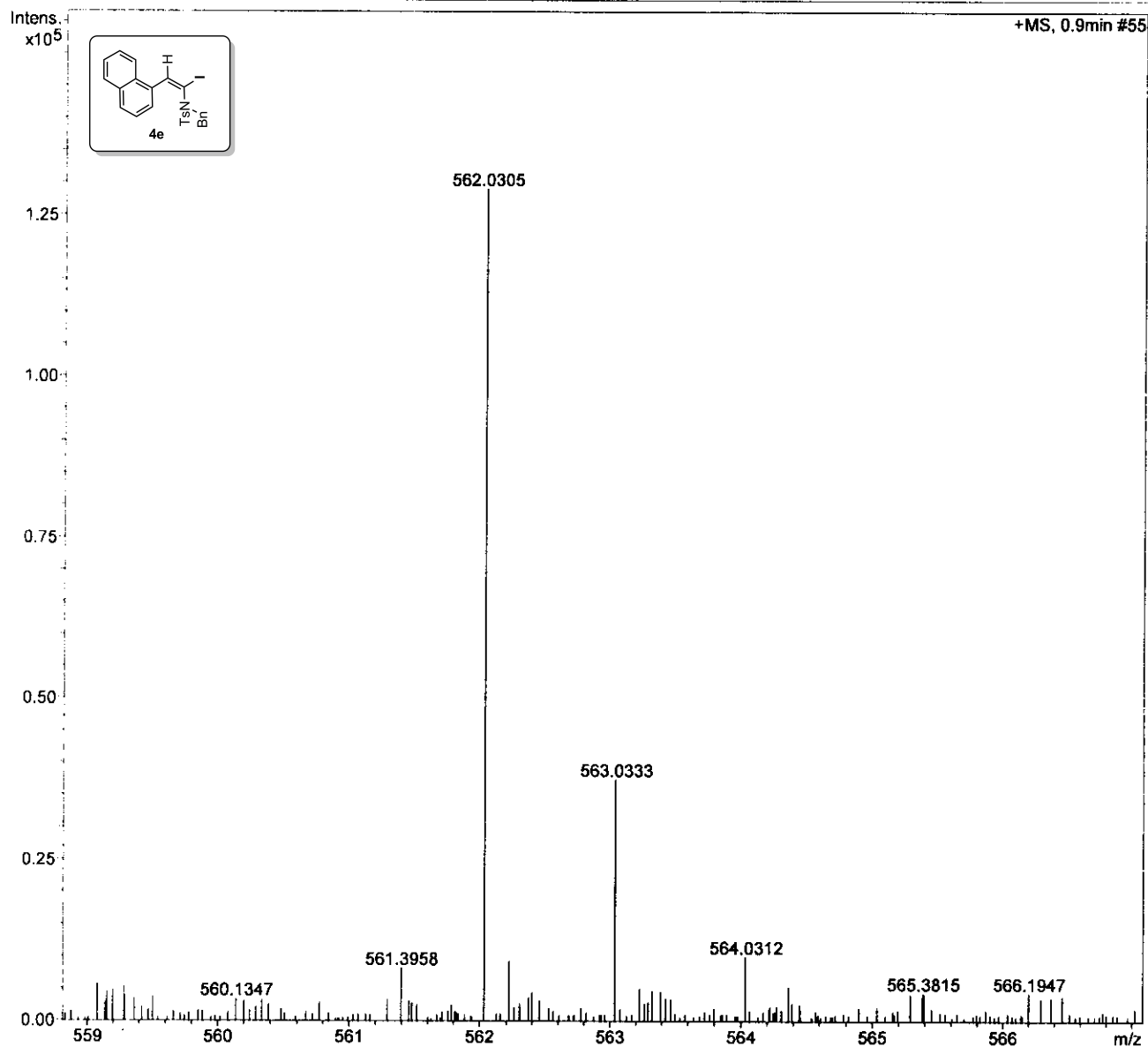
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Method TL-P.m
Sample Name RP-2-17-MEOH
Comment

Acquisition Date 5/11/2015 1:00:34 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	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	700 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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Analysis Info

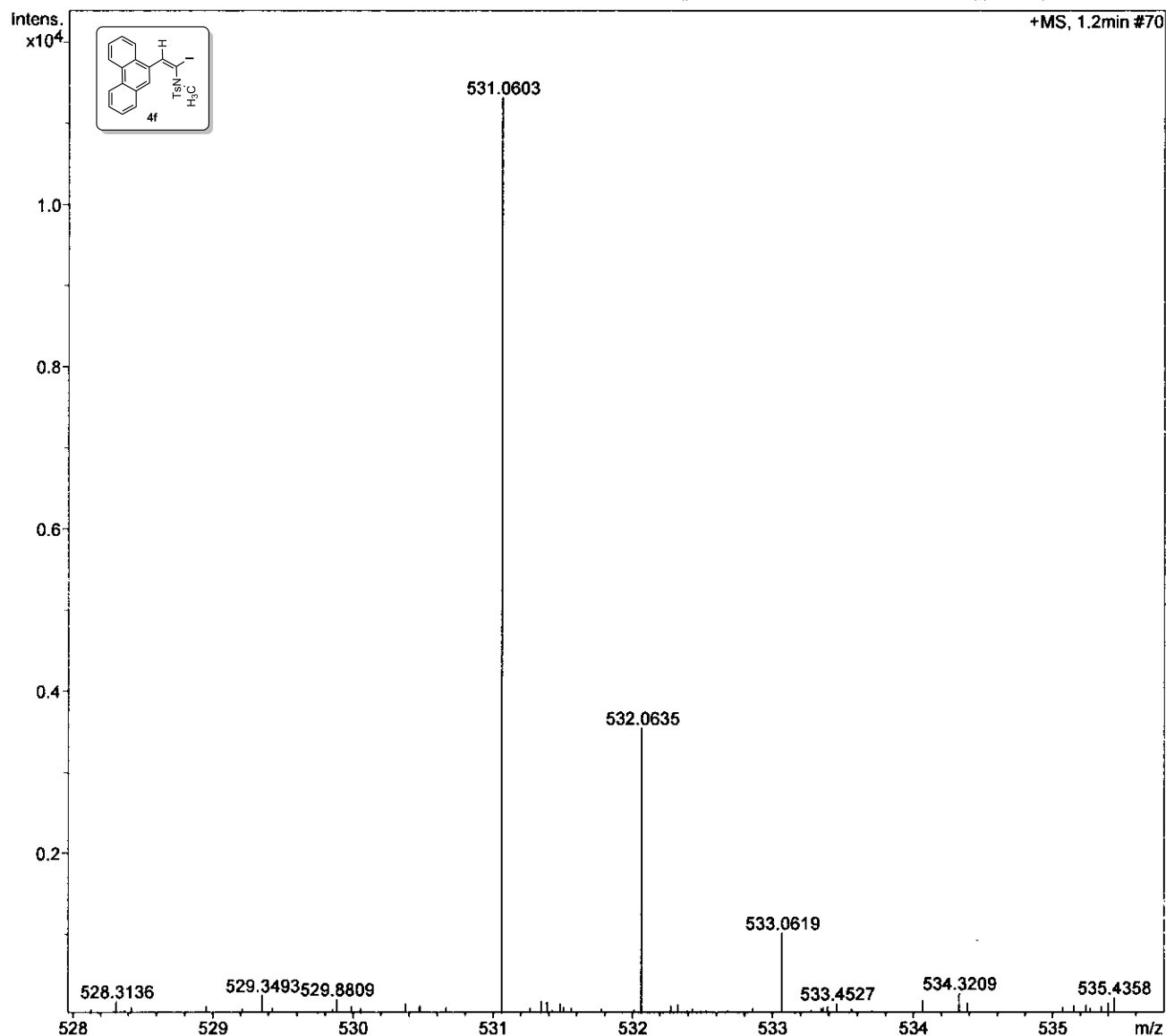
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Method tune_low.m
Sample Name RKM-2-146
Comment

Acquisition Date 3/20/2015 2:28:34 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

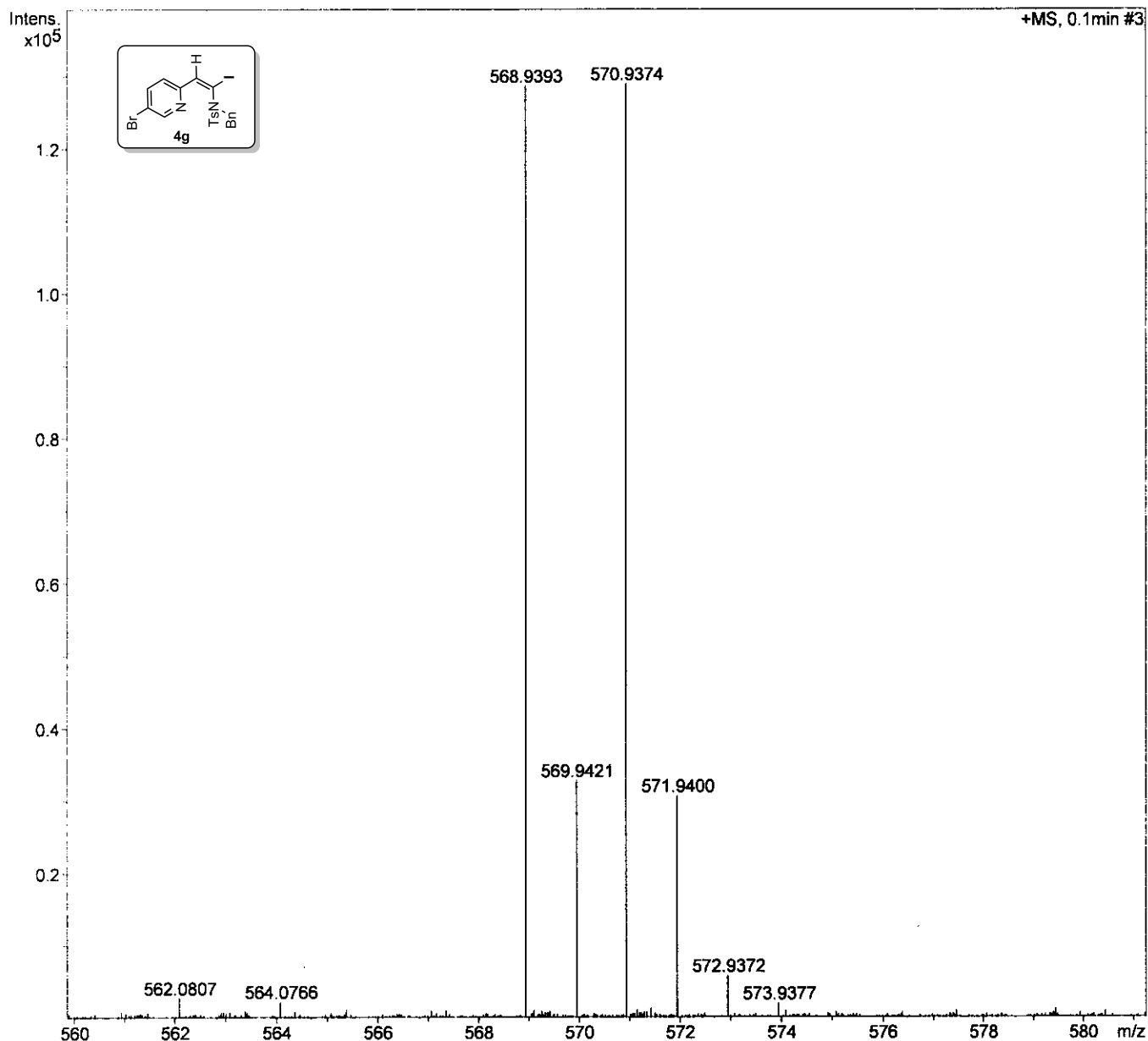
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Method tune_low_Pos.m
Sample Name RP-2-34
Comment

Acquisition Date 6/18/2015 3:38:12 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	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



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Analysis Info

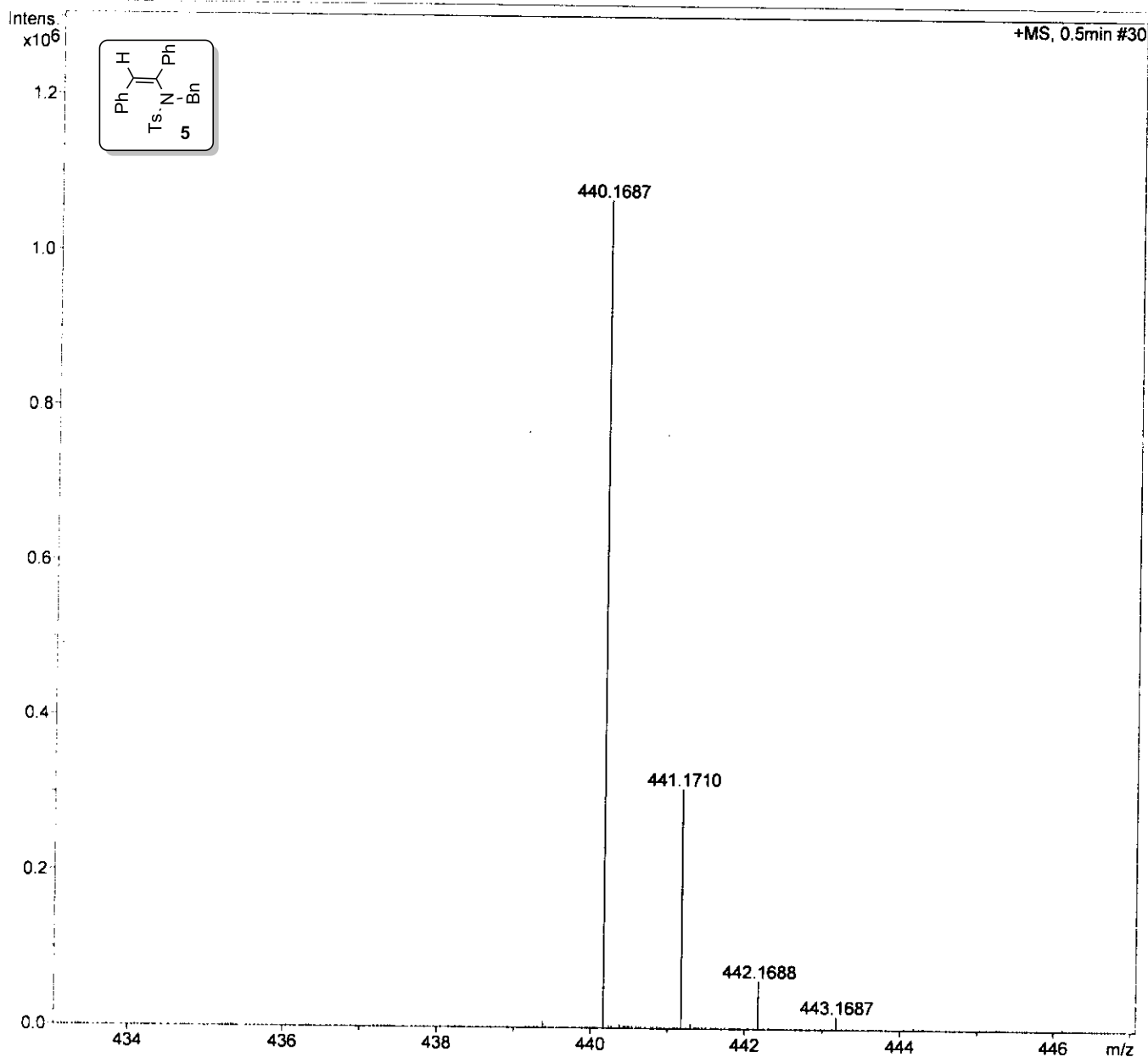
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Method tune_low_Pos.m
Sample Name PB-6-90--MEOH
Comment

Acquisition Date 6/4/2015 12:59:10 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	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



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Analysis Info

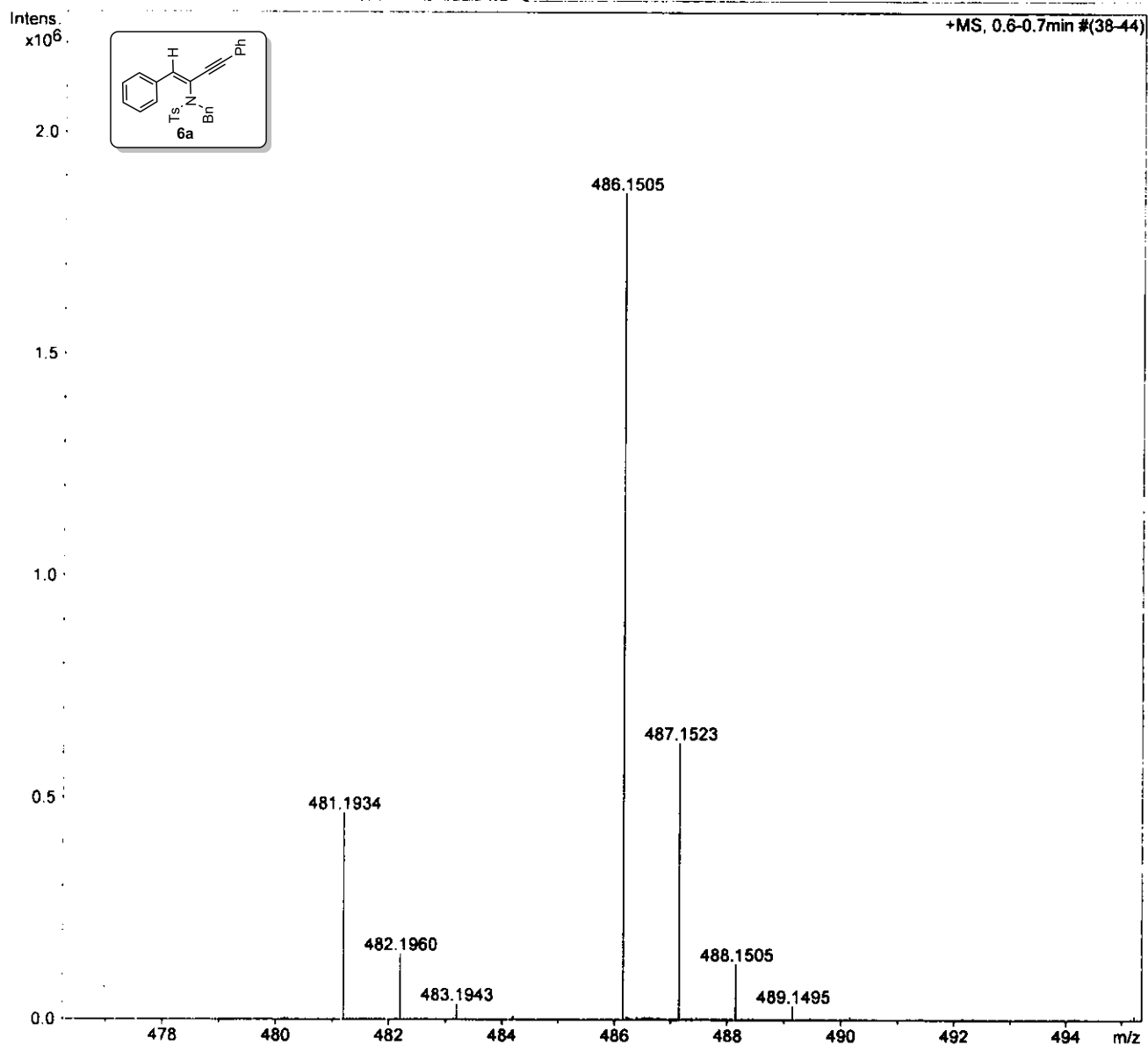
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Method tune_low_Pos.m
Sample Name PB-6-92-MEOH
Comment

Acquisition Date 6/4/2015 1:14:31 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



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Analysis Info

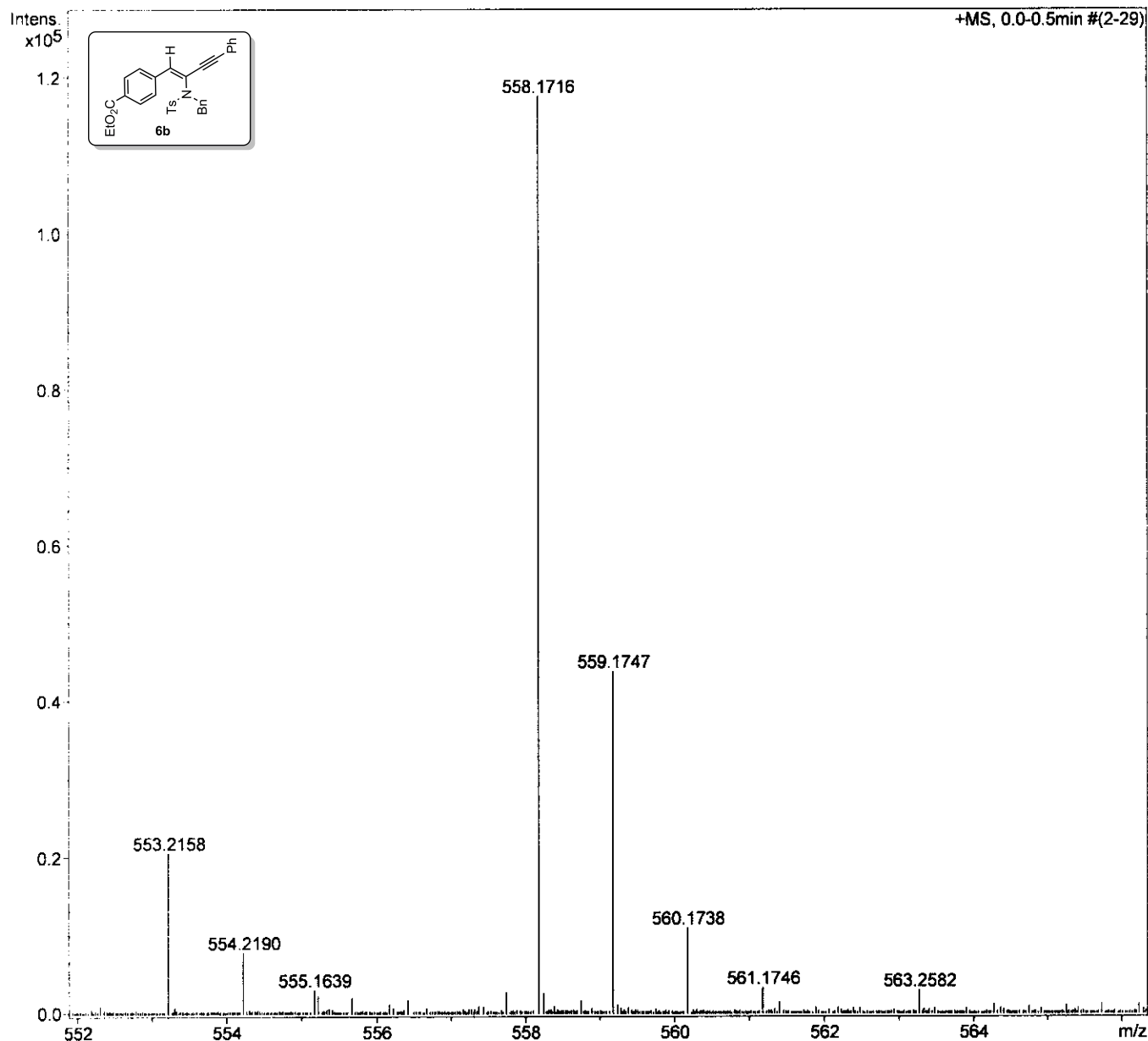
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Method tune_low.m
Sample Name PB-7-44-MEOH
Comment

Acquisition Date 6/17/2015 11:22:41 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	3200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1700 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



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Analysis Info

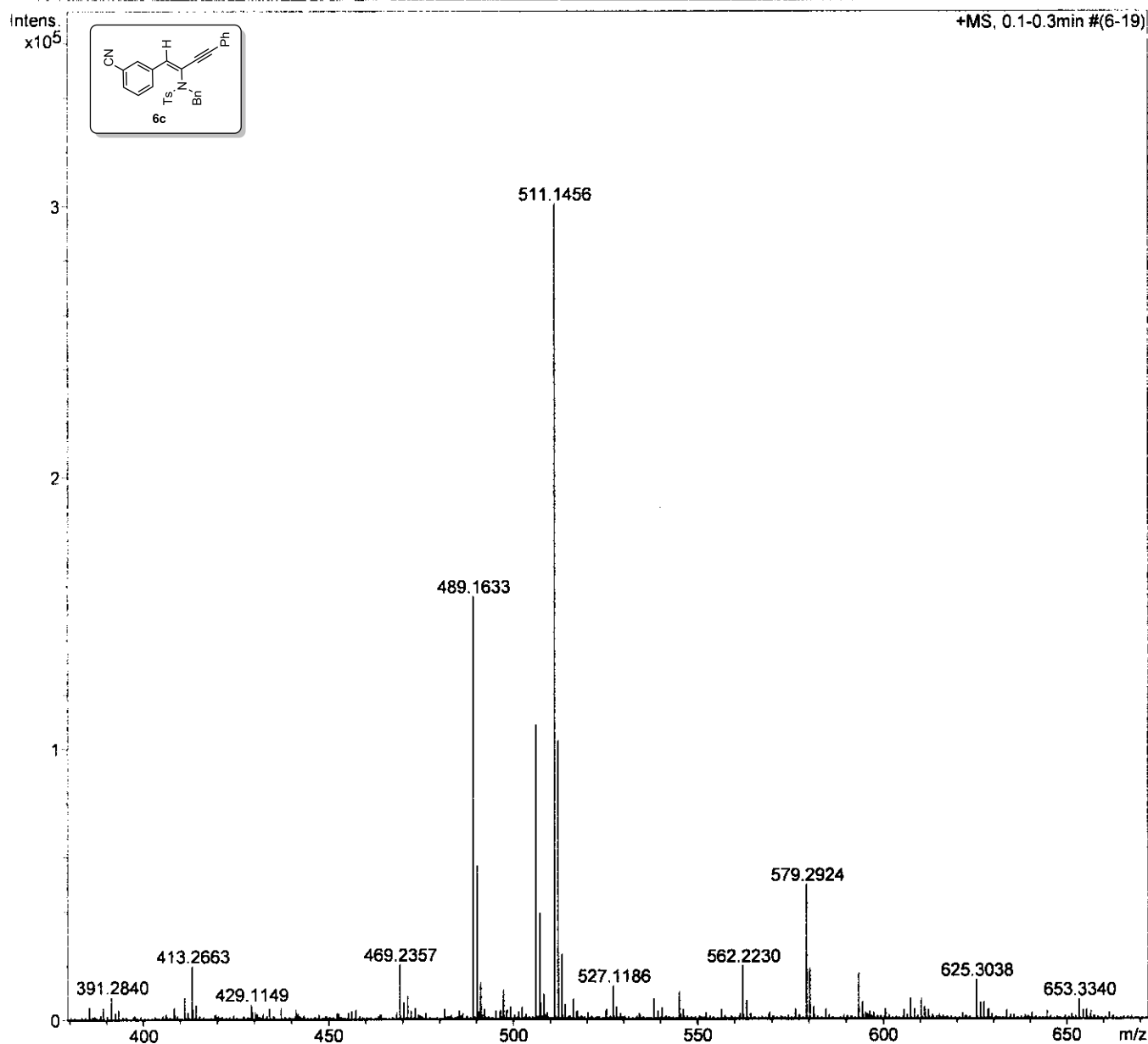
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Method tune_low.m
Sample Name PB-7-48-MEOH
Comment

Acquisition Date 6/17/2015 11:12:55 AM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

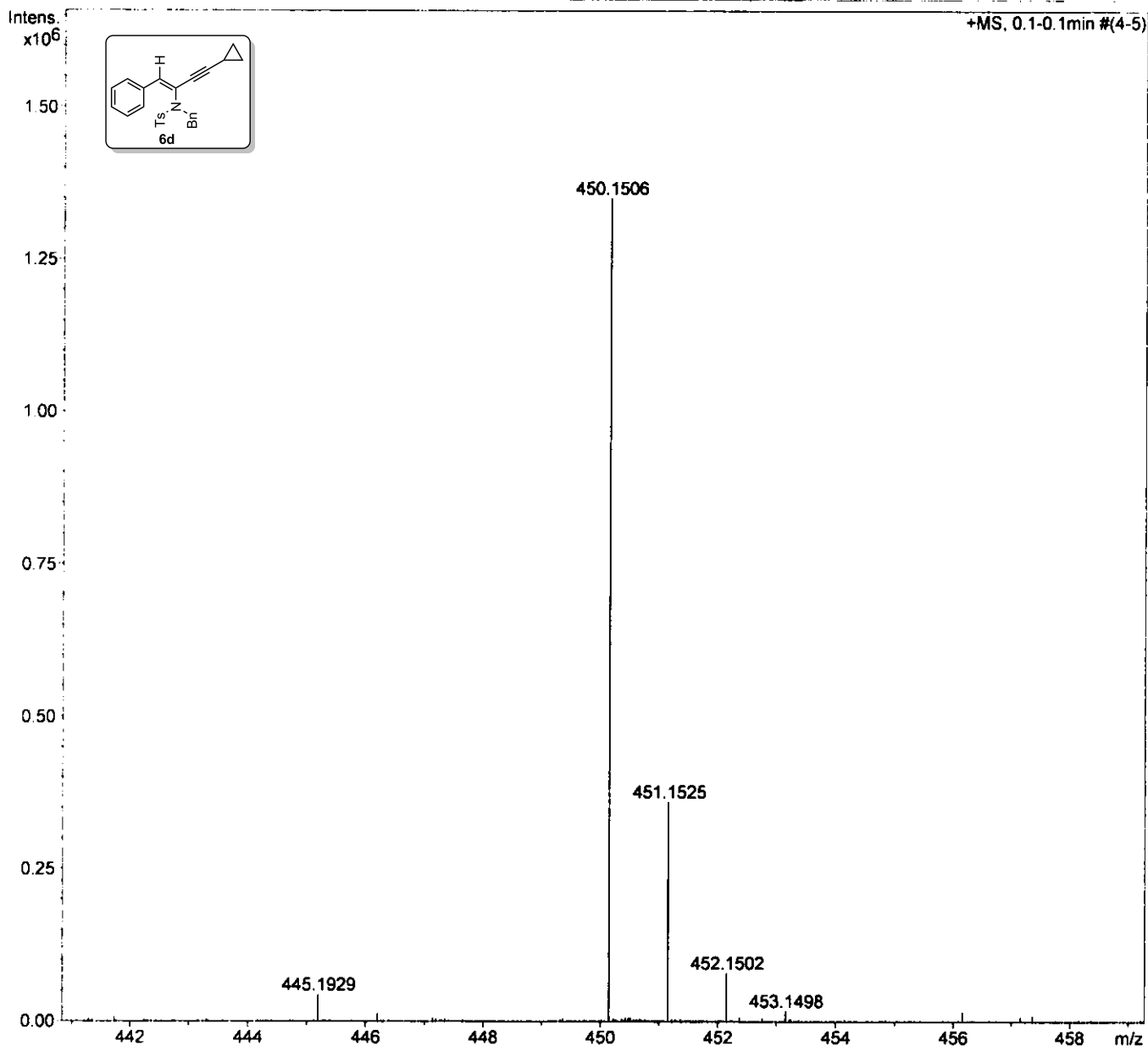
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Method tune_low.m
Sample Name PB-7-40-MEOH
Comment

Acquisition Date 6/16/2015 1:19:30 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

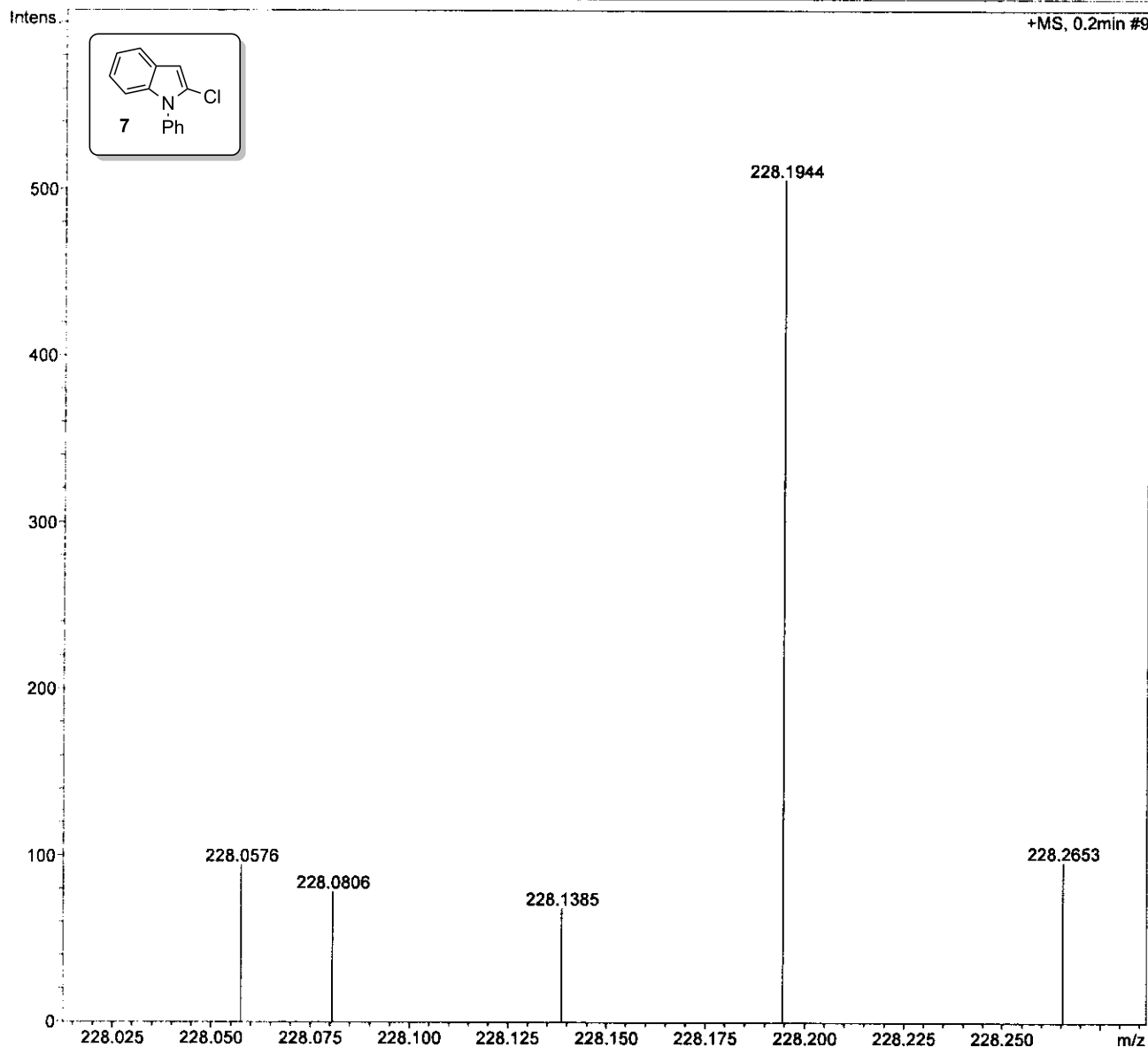
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Sample Name PB-B-163-ACN
Comment

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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



228.0576

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Analysis Info

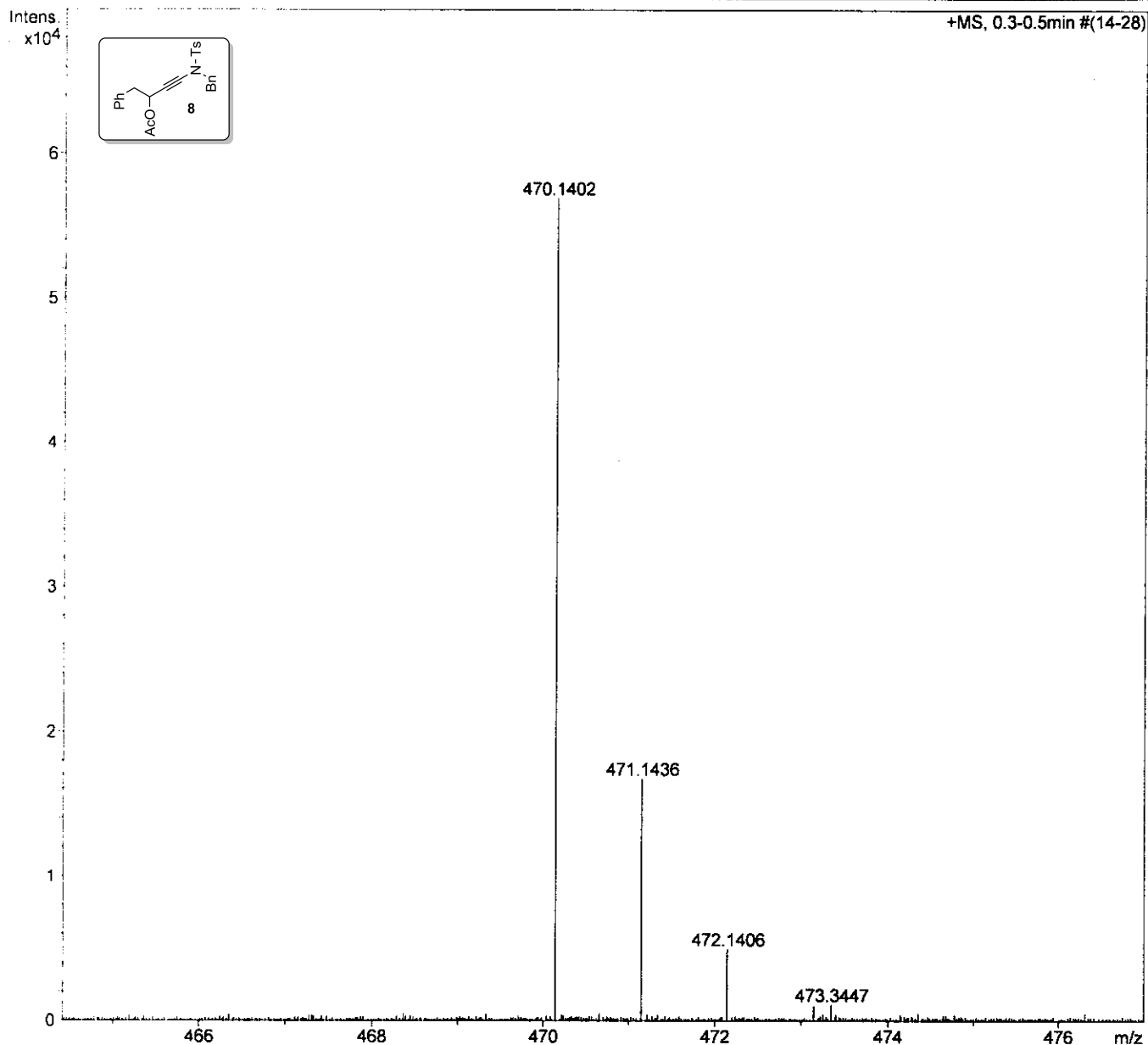
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Method tune_low.m
Sample Name PB-7-54-MEOH
Comment

Acquisition Date 7/6/2015 3:58:25 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

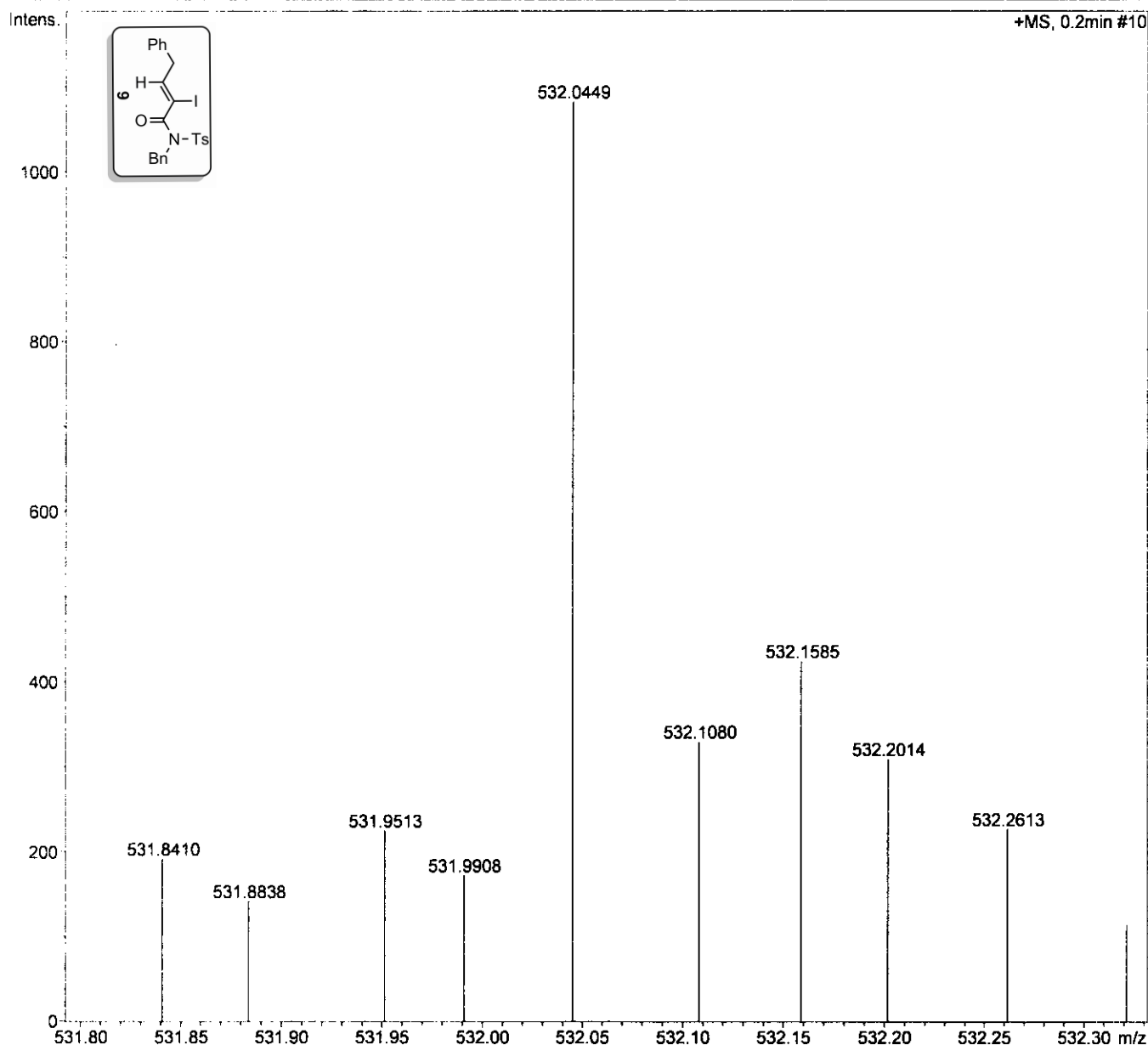
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Acquisition Date 6/26/2015 4:03:22 PM

Operator Ramu Sridhar
Instrument maXis 10138

Acquisition Parameter

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



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Analysis Info

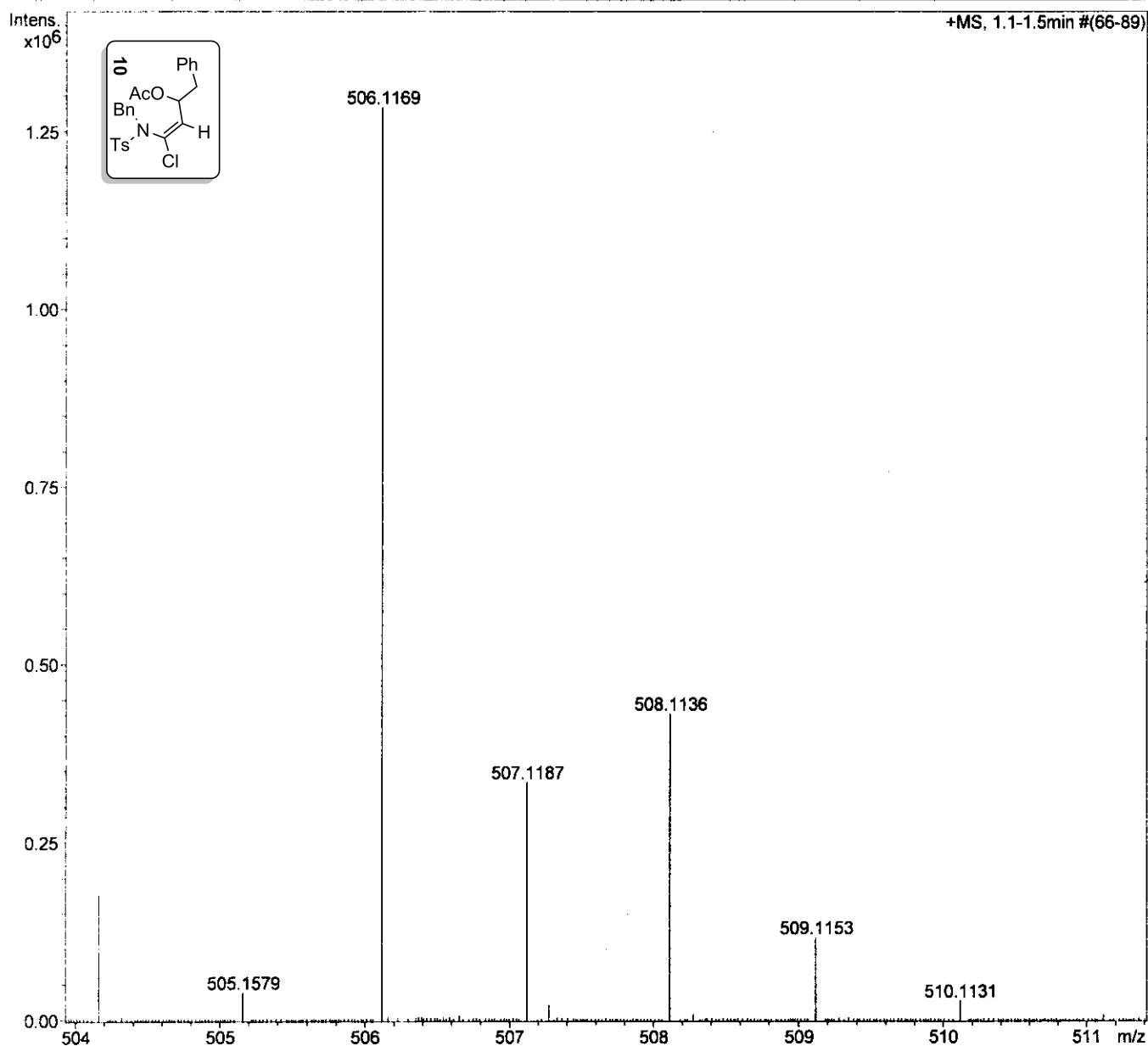
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Method tune_low_Pos-R2.m
Sample Name PB-07-60
Comment

Acquisition Date 6/18/2015 4:02:55 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



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Analysis Info

Analysis Name D:\Data\2015\DR.AK.SAHOO\JUNE\PB-6-55.d
Method tune_low_Pos.m
Sample Name PB-6-55-MEOH
Comment 7-55

Acquisition Date 6/16/2015 1:09:35 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	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	400.0 Vpp	Set Divert Valve	Waste

