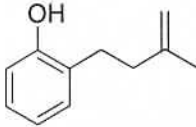


**U of M****University of Minnesota Department of Chemistry****Mass Spectrometry Service Laboratory**

email: chmmslab@umn.edu

**Submit Sample To:** Mass Spectrometry Facility  
207 Pleasant St. SE  
Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX : (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13																			
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N																			
P.I./Advisor: Chris Douglas		U of M Budget # 5190022																					
Company/University:		P.O.# (For non-U of M Clients)																					
Shipping Address:		Billing Address:																					
Sample Label: 6a		Molecular Weight: 162.2283																					
 6a		Molecular Formula: C <sub>11</sub> H <sub>14</sub> O																					
		Melting/Boiling Point: N/A																					
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA																					
		Thermal Stability: Yes																					
		Toxicity: NO																					
Reactivity: acidic proton																							
<b>Chromatography Conditions:</b>		<b>Analysis Requested</b>																					
		<table border="1"><thead><tr><th></th><th>EI</th><th>CI</th><th>MALDI</th><th>ESI</th></tr></thead><tbody><tr><td>Low Resolution Nominal Mass</td><td></td><td></td><td></td><td></td></tr><tr><td>High Resolution Accurate Mass</td><td></td><td></td><td></td><td>✓</td></tr></tbody></table>					EI	CI	MALDI	ESI	Low Resolution Nominal Mass					High Resolution Accurate Mass				✓			
			EI	CI	MALDI	ESI																	
		Low Resolution Nominal Mass																					
High Resolution Accurate Mass				✓																			
<b>Special Sample Considerations:</b>																							
<table border="1"><tbody><tr><td>+Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>-Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>GCMS</td><td></td><td></td><td></td><td></td></tr><tr><td>LCMS</td><td></td><td></td><td></td><td></td></tr></tbody></table>				+Ve					-Ve					GCMS					LCMS				
+Ve																							
-Ve																							
GCMS																							
LCMS																							
<b>Instrument Used</b>		<b>Conditions Used</b>		<b>Operator Comments</b>																			
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Bruker Reflex III		Acc. Voltage:																					
Bruker BioTOF II		Resolution:																					
Waters Triple Quad		Scan Range:																					
Waters Synapt G2		Gas Used:																					
Log #:	Analyst:	Analysis Date:		Analyses Run:	Total Cost:																		

100643

6a

chresi

Kyle Kalstabakken

3/12/2013 12:58:35 PM

# Display Report

## Analysis Info

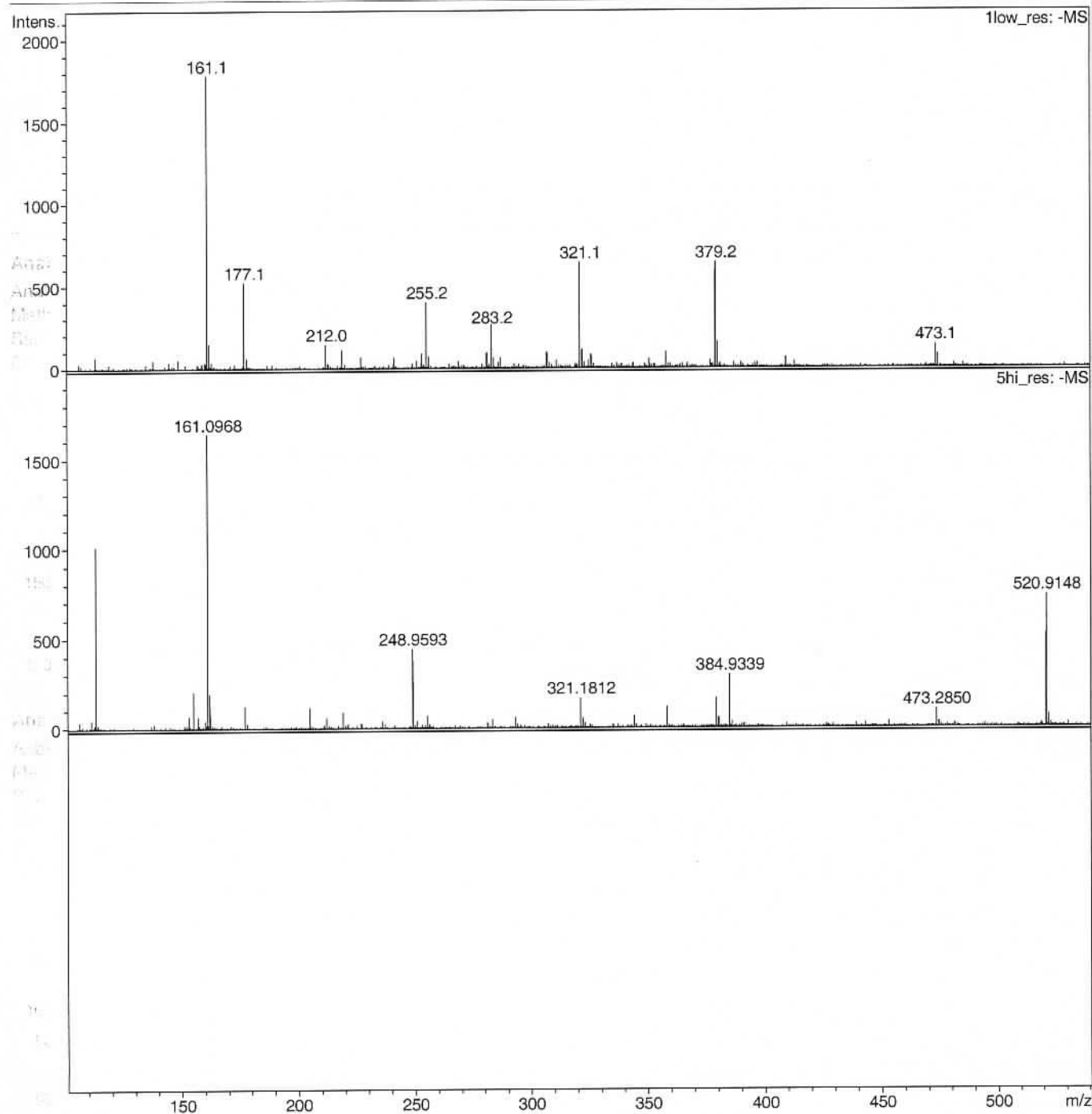
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Method negative\_041013.tofpar  
Sample Name 100643  
Comment

Acquisition Date 4/12/2013 10:58:01 AM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

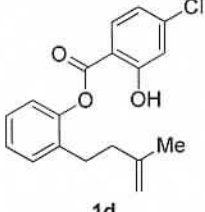
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a



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Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX: (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13																					
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N																					
P.I./Advisor: Chris Douglas		U of M Budget # 5190022																							
Company/University:		P.O.# (For non-U of M Clients)																							
Shipping Address:		Billing Address:																							
Sample Label: 1d		Molecular Weight: 316.7788																							
 1d		Molecular Formula: C <sub>18</sub> H <sub>17</sub> ClO <sub>3</sub>																							
		Melting/Boiling Point: N/A																							
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA																							
		Thermal Stability: Yes																							
		Toxicity: NO																							
Reactivity: acidic proton																									
<b>Chromatography Conditions:</b>		<b>Analysis Requested</b>																							
		<table border="1"><thead><tr><th></th><th>EI</th><th>CI</th><th>MALDI</th><th>ESI</th></tr></thead><tbody><tr><td>Low Resolution Nominal Mass</td><td></td><td></td><td></td><td></td></tr><tr><td>High Resolution Accurate Mass</td><td></td><td></td><td></td><td>✓</td></tr></tbody></table>					EI	CI	MALDI	ESI	Low Resolution Nominal Mass					High Resolution Accurate Mass				✓					
	EI	CI	MALDI	ESI																					
Low Resolution Nominal Mass																									
High Resolution Accurate Mass				✓																					
<b>Special Sample Considerations:</b>																									
		<table border="1"><tbody><tr><td>+Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>-Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>GCMS</td><td></td><td></td><td></td><td></td></tr><tr><td>LCMS</td><td></td><td></td><td></td><td></td></tr></tbody></table>				+Ve					-Ve					GCMS					LCMS				
+Ve																									
-Ve																									
GCMS																									
LCMS																									
<b>Instrument Used</b>		<b>Conditions Used</b>		<b>Operator Comments</b>																					
Finnigan MAT 95		Source Temp:		[M-H] <sup>-</sup> : 315.0794																					
Bruker Reflex III		Acc. Voltage:																							
Bruker BioTOF II		Resolution:																							
Waters Triple Quad		Scan Range:																							
Waters Synapt G2		Gas Used:																							
Log #:	Analyst:	Analysis Date:		Analyses Run:	Total Cost:																				

100644

1d

chresi

Kyle Kalstabakken

3/12/2013 12:59:38 PM

# Display Report

## Analysis Info

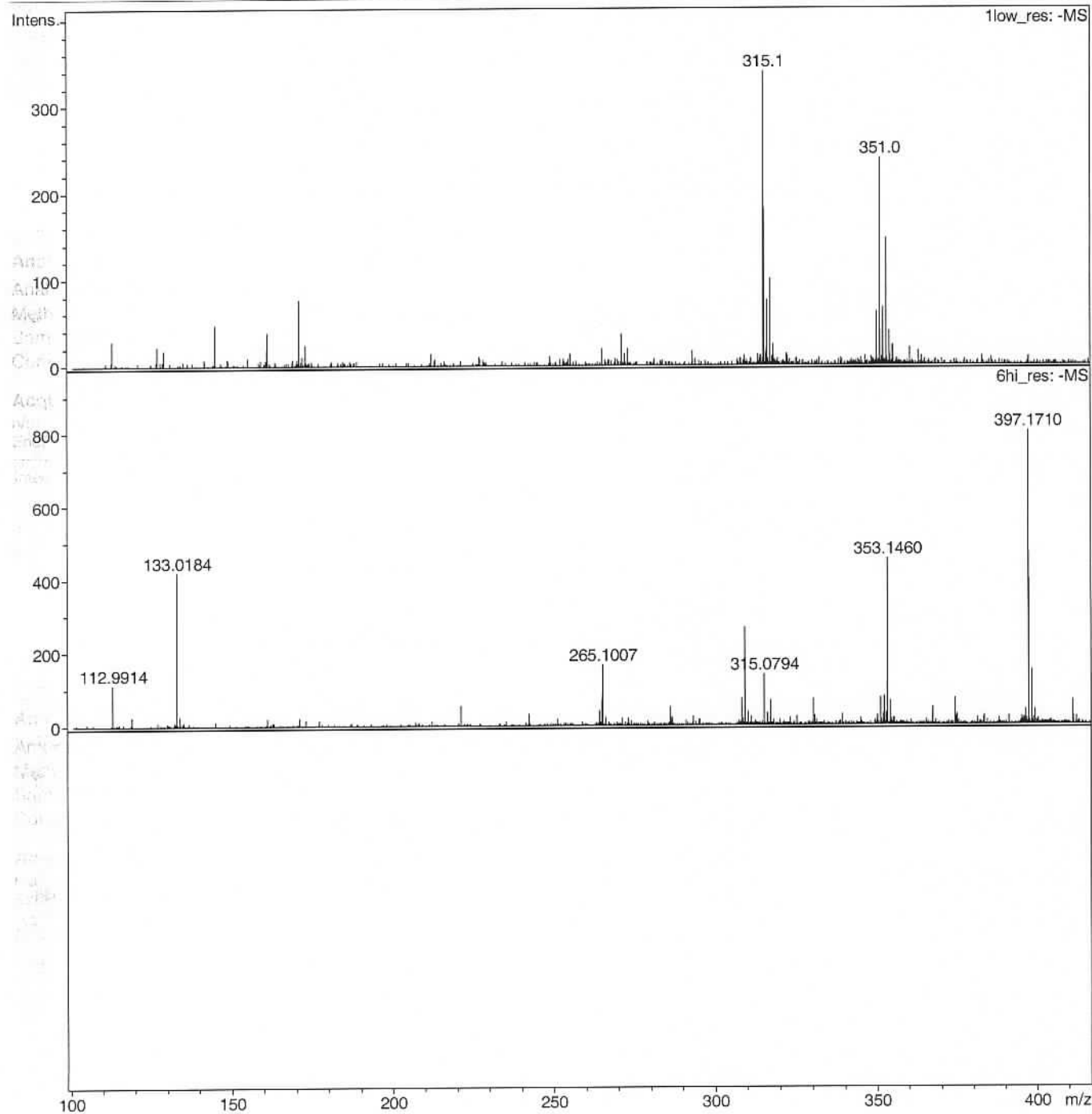
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Method negative\_041013.tofpar  
Sample Name 100644  
Comment

Acquisition Date 4/11/2013 5:19:07 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

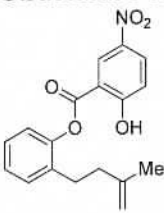
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a



**U of M****University of Minnesota Department of Chemistry****Mass Spectrometry Service Laboratory**

email: chmmslab@umn.edu

**Submit Sample To:** Mass Spectrometry Facility  
207 Pleasant St. SE  
Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX : (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13																			
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N																			
P.I./Advisor: Chris Douglas		U of M Budget # 5190022																					
Company/University:		P.O.# (For non-U of M Clients)																					
Shipping Address:		Billing Address:																					
Sample Label: 1h		Molecular Weight: 327.3313																					
 1h		Molecular Formula: C <sub>18</sub> H <sub>17</sub> NO <sub>5</sub>																					
		Melting/Boiling Point: N/A																					
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA																					
		Thermal Stability: Yes																					
		Toxicity: NO																					
Reactivity: acidic proton																							
<b>Chromatography Conditions:</b>		<b>Analysis Requested</b>																					
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			EI	CI	MALDI	ESI																	
		Low Resolution Nominal Mass																					
High Resolution Accurate Mass				✓																			
<b>Special Sample Considerations:</b>																							
<table border="1"><tbody><tr><td>+Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>-Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>GCMS</td><td></td><td></td><td></td><td></td></tr><tr><td>LCMS</td><td></td><td></td><td></td><td></td></tr></tbody></table>				+Ve					-Ve					GCMS					LCMS				
+Ve																							
-Ve																							
GCMS																							
LCMS																							
<b>Instrument Used</b>		<b>Conditions Used</b>		<b>Operator Comments</b>																			
Finnigan MAT 95		Source Temp:		[M-H] <sup>-</sup> : 326.1027																			
Bruker Reflex III		Acc. Voltage:																					
Bruker BioTOF II		Resolution:																					
Waters Triple Quad		Scan Range:																					
Waters Synapt G2		Gas Used:																					
Log #:		Analyst:		Analysis Date:																			
				Analyses Run:																			
				Total Cost:																			

100645

1h

chresi

Kyle Kalstabakken

3/12/2013 1:00:35 PM

# Display Report

## Analysis Info

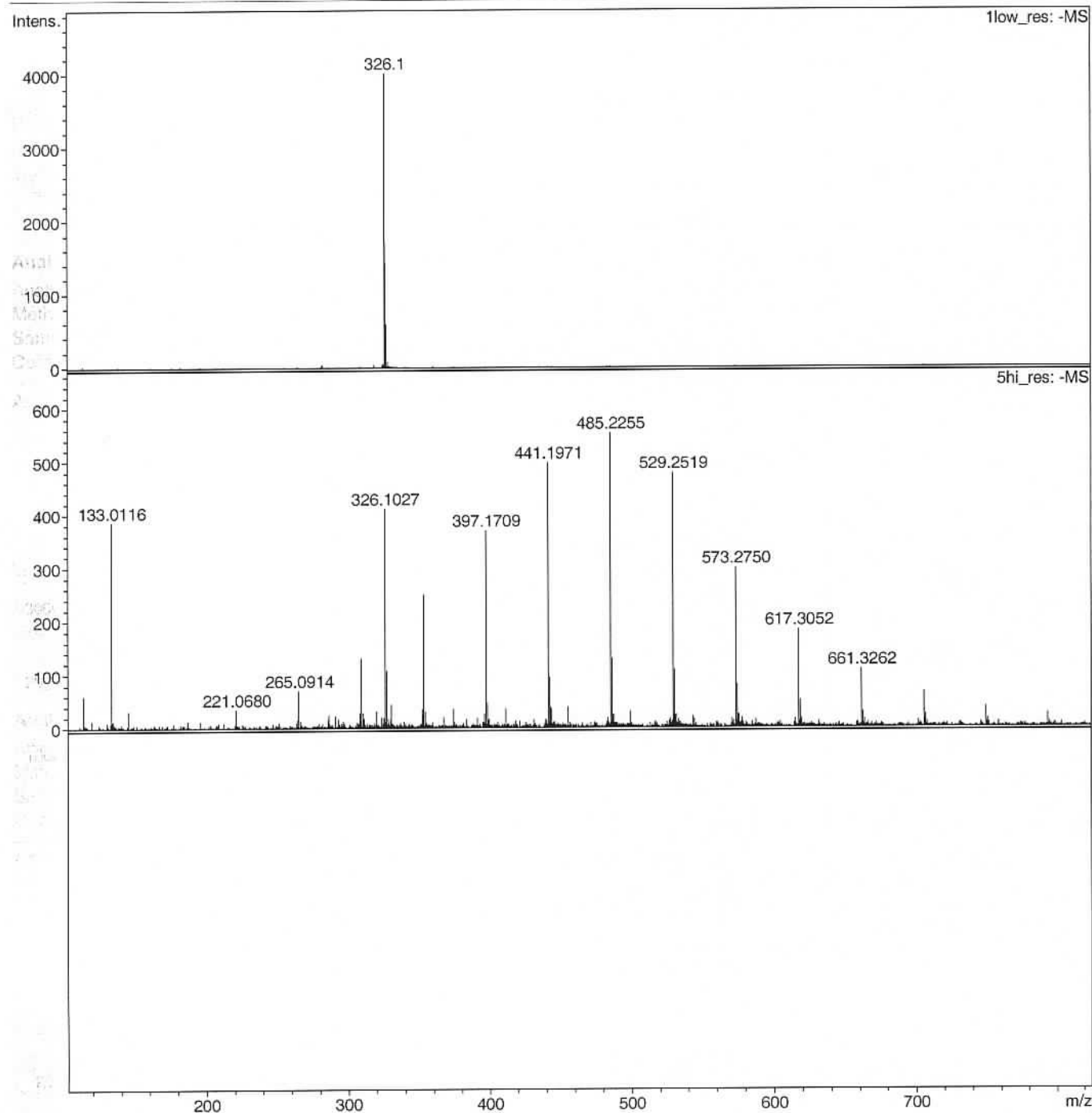
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Method negative\_041013.tofpar  
Sample Name 100645  
Comment

Acquisition Date 4/11/2013 5:28:57 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

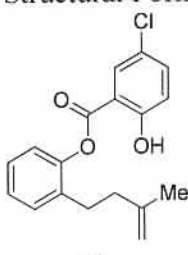
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a



**U of M****University of Minnesota Department of Chemistry****Mass Spectrometry Service Laboratory**

email: chmmslab@umn.edu

**Submit Sample To:** Mass Spectrometry Facility  
207 Pleasant St. SE  
Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX : (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13																					
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N																					
P.I./Advisor: Chris Douglas		U of M Budget # 5190022																							
Company/University:		P.O.# (For non-U of M Clients)																							
Shipping Address:		Billing Address:																							
Sample Label: 1i		Molecular Weight: 316.7788																							
 1i		Molecular Formula: C <sub>18</sub> H <sub>17</sub> ClO <sub>3</sub>																							
		Melting/Boiling Point: N/A																							
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA																							
		Thermal Stability: Yes																							
		Toxicity: NO																							
Reactivity: acidic proton																									
<b>Chromatography Conditions:</b>		<b>Analysis Requested</b>																							
		<table border="1"><thead><tr><th></th><th>EI</th><th>CI</th><th>MALDI</th><th>ESI</th></tr></thead><tbody><tr><td>Low Resolution Nominal Mass</td><td></td><td></td><td></td><td></td></tr><tr><td>High Resolution Accurate Mass</td><td></td><td></td><td></td><td>✓</td></tr></tbody></table>					EI	CI	MALDI	ESI	Low Resolution Nominal Mass					High Resolution Accurate Mass				✓					
	EI	CI	MALDI	ESI																					
Low Resolution Nominal Mass																									
High Resolution Accurate Mass				✓																					
<b>Special Sample Considerations:</b>		<table border="1"><tbody><tr><td>+Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>-Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>GCMS</td><td></td><td></td><td></td><td></td></tr><tr><td>LCMS</td><td></td><td></td><td></td><td></td></tr></tbody></table>				+Ve					-Ve					GCMS					LCMS				
+Ve																									
-Ve																									
GCMS																									
LCMS																									
<b>Instrument Used</b>		<b>Conditions Used</b>		<b>Operator Comments</b>																					
Finnigan MAT 95		Source Temp:		[M-H] <sup>-</sup> : 315.0784																					
Bruker Reflex III		Acc. Voltage:																							
Bruker BioTOF II		Resolution:																							
Waters Triple Quad		Scan Range:																							
Waters Synapt G2		Gas Used:																							
Log #:	Analyst:	Analysis Date:		Analyses Run:	Total Cost:																				

100646

1i

chresi

Kyle Kalstabakken

3/12/2013 1:01:35 PM

# Display Report

## Analysis Info

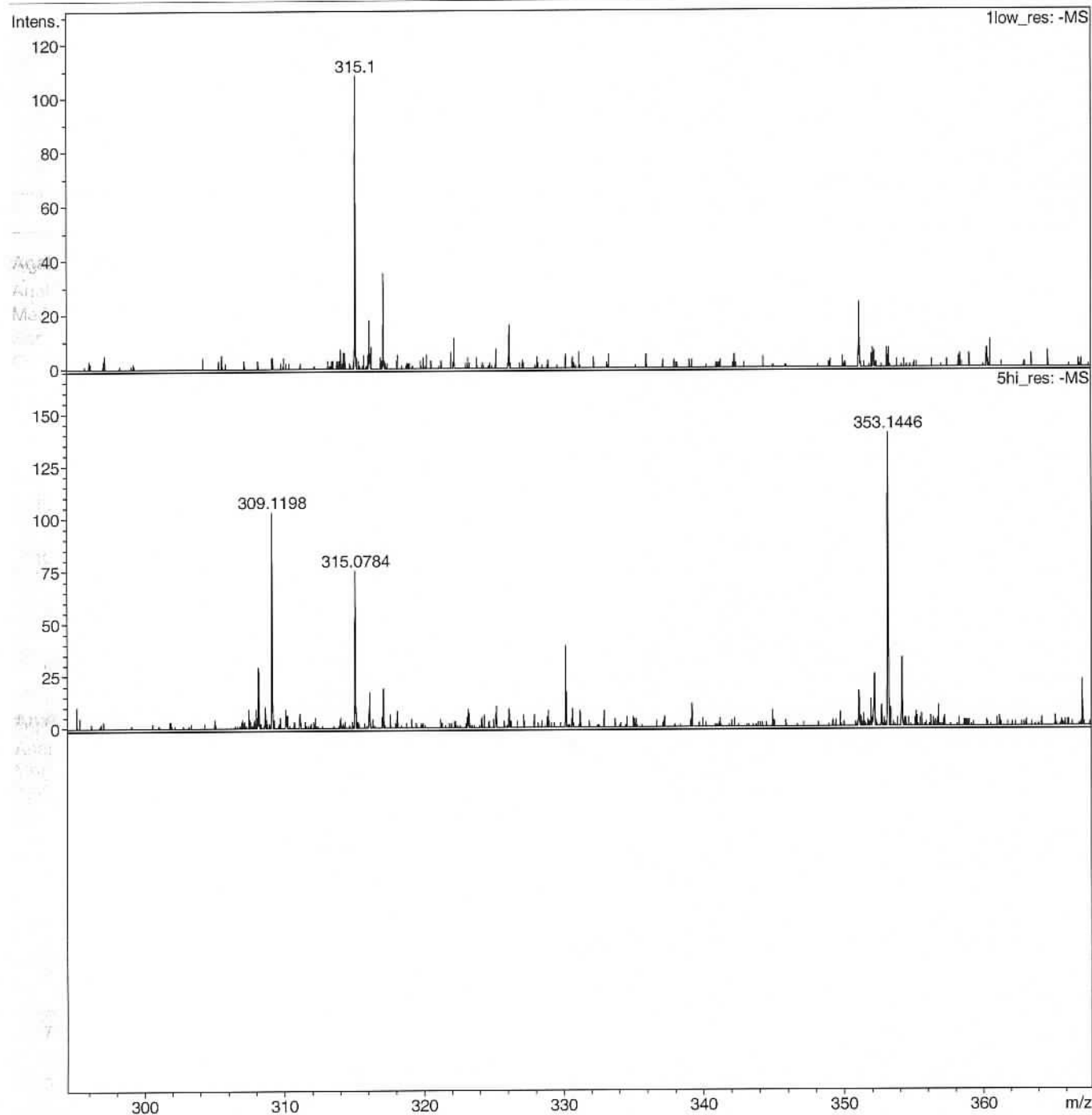
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Method negative\_041013.tofpar  
Sample Name 100646  
Comment

Acquisition Date 4/11/2013 5:37:13 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

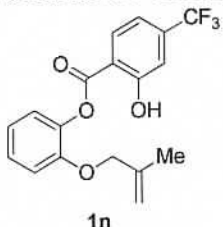
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a





**University of Minnesota Department of Chemistry**  
**Mass Spectrometry Service Laboratory**  
 email: [chmmmslab@umn.edu](mailto:chmmmslab@umn.edu)

**Submit Sample To:** Mass Spectrometry Facility  
207 Pleasant St. SE  
Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX : (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13		
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N		
P.I./Advisor: Chris Douglas		U of M Budget # 5190022				
Company/University:		P.O.# (For non-U of M Clients)				
Shipping Address:		Billing Address:				
Sample Label: 1n		Molecular Weight: 352.3045				
Structural Formula or Sample Composition: 		Molecular Formula: C <sub>18</sub> H <sub>15</sub> F <sub>3</sub> O <sub>4</sub>				
		Melting/Boiling Point: N/A				
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA				
		Thermal Stability: Yes				
		Toxicity: NO				
		Reactivity: acidic proton				
Chromatography Conditions:		Analysis Requested				
			EI	CI	MALDI	ESI
		Low Resolution Nominal Mass				
		High Resolution Accurate Mass				✓
Special Sample Considerations:		+Ve				
		-Ve				
		GCMS				
		LCMS				
Instrument Used		Conditions Used		Operator Comments  [M-4] <sup>-</sup> : 351.0849		
Finnigan MAT 95		Source Temp:				
Bruker Reflex III		Acc. Voltage:				
Bruker BioTOF II		Resolution:				
Waters Triple Quad		Scan Range:				
Waters Synapt G2		Gas Used:				
Log #:		Analyst:		Analysis Date:		
				Analyses Run:		
				Total Cost:		

100647  
1n  
chresi  
Kyle Kalstabakken  
3/12/2013 1:02:39 PM

# Display Report

## Analysis Info

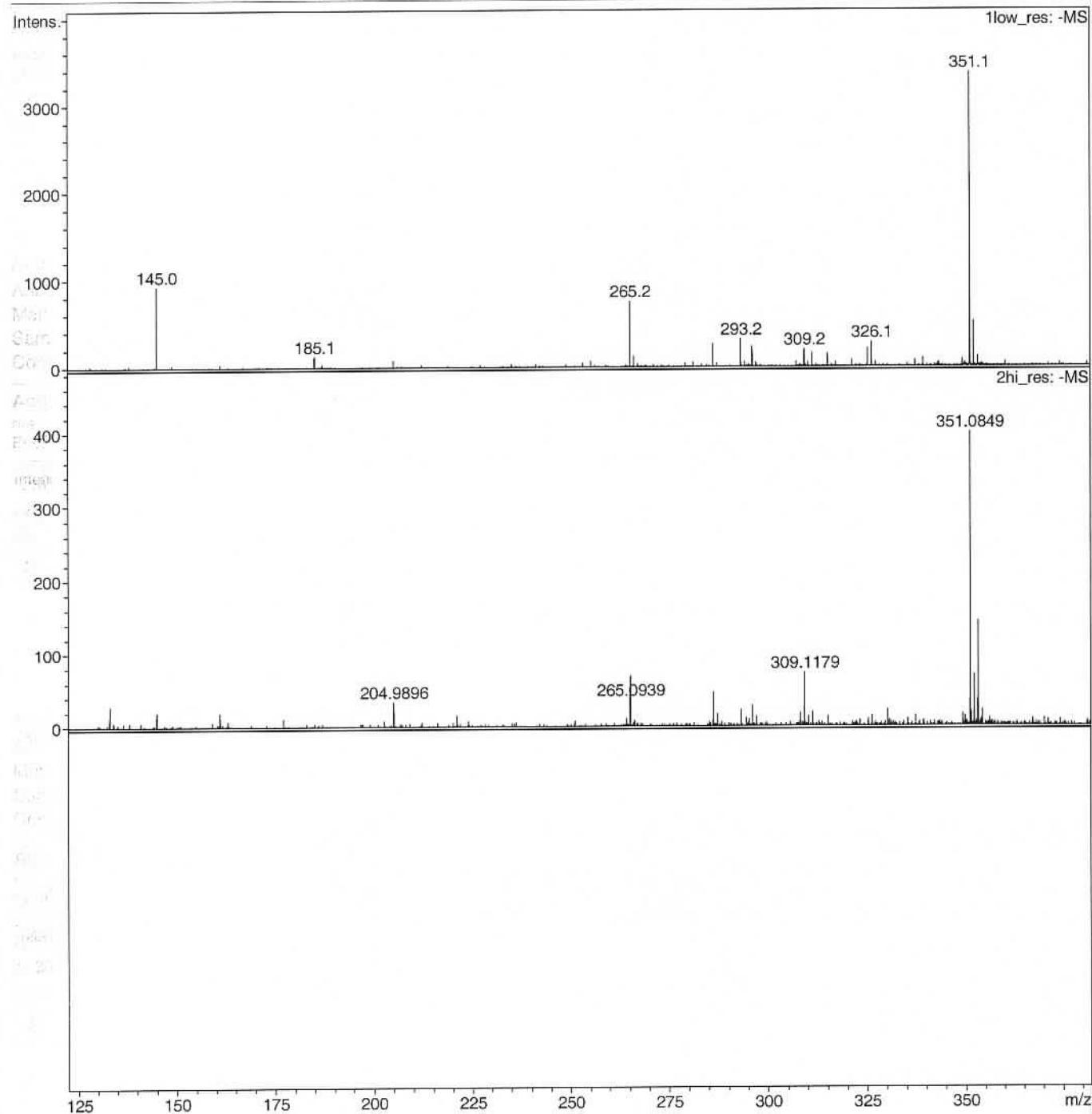
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Method negative\_041013.tofpar  
Sample Name 100647  
Comment

Acquisition Date 4/11/2013 5:42:54 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

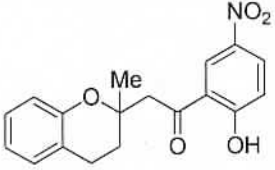
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a



**U of M****University of Minnesota Department of Chemistry****Mass Spectrometry Service Laboratory**

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FAX: (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13																			
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N																			
P.I./Advisor: Chris Douglas		U of M Budget # 5190022																					
Company/University:		P.O.# (For non-U of M Clients)																					
Shipping Address:		Billing Address:																					
Sample Label: 2h		Molecular Weight: 327.3313																					
<div>Structural Formula or Sample Composition:</div>  <p>2h</p>		Molecular Formula: C <sub>18</sub> H <sub>17</sub> NO <sub>5</sub>																					
		Melting/Boiling Point: N/A																					
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA																					
		Thermal Stability: Yes																					
		Toxicity: NO																					
<div>Chromatography Conditions:</div>		<div>Analysis Requested</div>																					
		<table border="1"><thead><tr><th></th><th>EI</th><th>CI</th><th>MALDI</th><th>ESI</th></tr></thead><tbody><tr><td>Low Resolution Nominal Mass</td><td></td><td></td><td></td><td></td></tr><tr><td>High Resolution Accurate Mass</td><td></td><td></td><td></td><td>✓</td></tr></tbody></table>					EI	CI	MALDI	ESI	Low Resolution Nominal Mass					High Resolution Accurate Mass				✓			
			EI	CI	MALDI	ESI																	
		Low Resolution Nominal Mass																					
		High Resolution Accurate Mass				✓																	
<div>Special Sample Considerations:</div>																							
<table border="1"><tbody><tr><td>+Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>-Ve</td><td></td><td></td><td></td><td></td></tr><tr><td>GCMS</td><td></td><td></td><td></td><td></td></tr><tr><td>LCMS</td><td></td><td></td><td></td><td></td></tr></tbody></table>				+Ve					-Ve					GCMS					LCMS				
+Ve																							
-Ve																							
GCMS																							
LCMS																							
<div>Instrument Used</div>		<div>Conditions Used</div>		<div>Operator Comments</div>																			
Finnigan MAT 95		Source Temp:		[M-H] <sup>-</sup> : 326.1034																			
Bruker Reflex III		Acc. Voltage:																					
Bruker BioTOF II		Resolution:																					
Waters Triple Quad		Scan Range:																					
Waters Synapt G2		Gas Used:																					
Log #:	Analyst:	Analysis Date:		Analyses Run:	Total Cost:																		

100648

2h

chresi

Kyle Kalstabakken

3/12/2013 1:03:28 PM

# Display Report

## Analysis Info

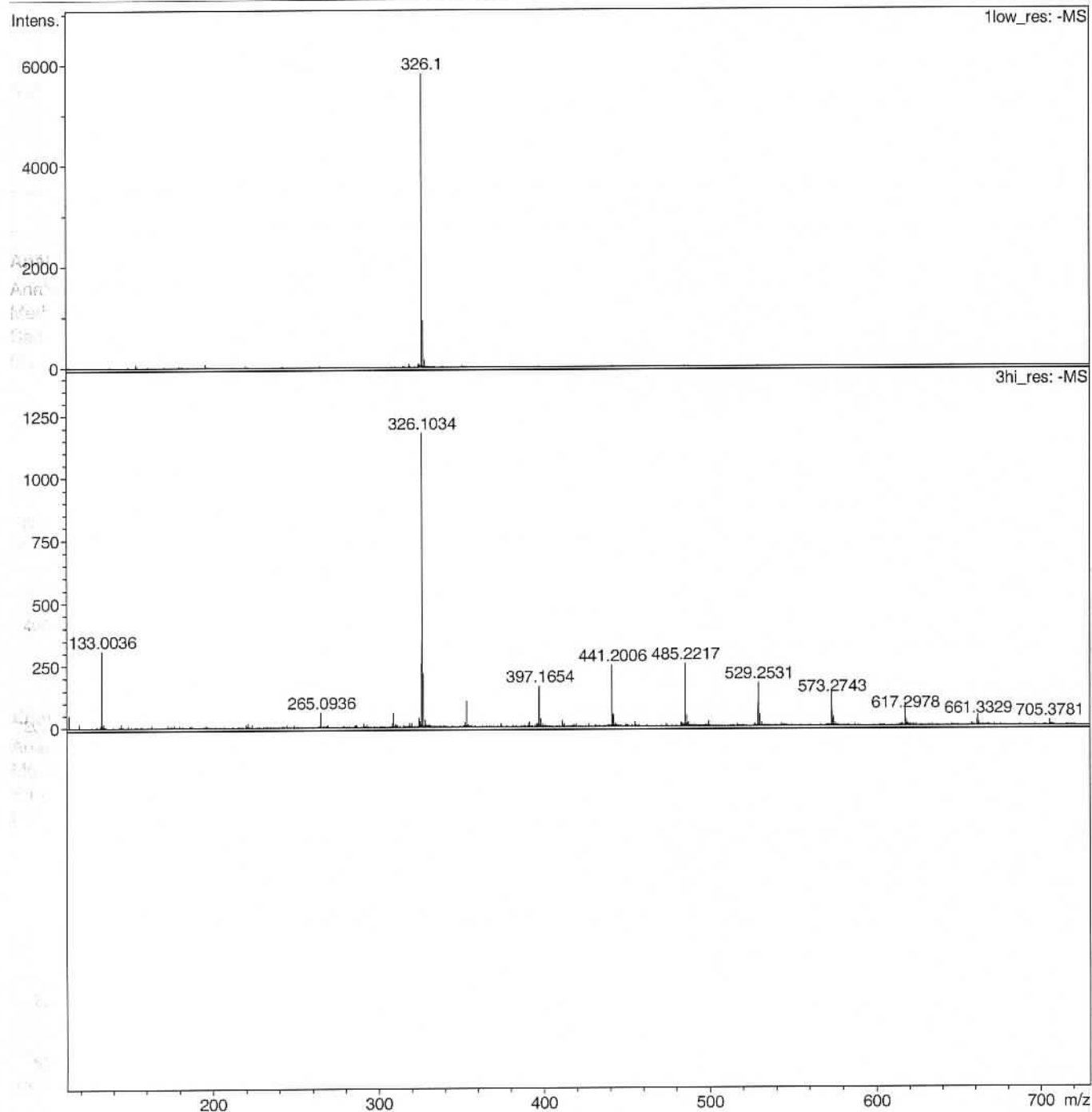
Analysis Name Z:\mslab\100648\3hi\_res  
Method negative\_041013.tofpar  
Sample Name 100648  
Comment

Acquisition Date 4/11/2013 5:53:24 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

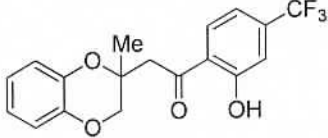
n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a



**U of M****University of Minnesota Department of Chemistry****Mass Spectrometry Service Laboratory**

email: chmmslab@umn.edu

**Submit Sample To:** Mass Spectrometry Facility  
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Minneapolis, MN 55455  
Phone: (612)-625-8099  
FAX: (612)-626-7541

Name: Zhongda Pan		Phone: 612 481 7665		Date: 03/04/13					
Email: panxx160@umn.edu		Email Results? Yes		FAX: FAX Results? Y / N					
P.I./Advisor: Chris Douglas		U of M Budget # 5190022							
Company/University:		P.O.# (For non-U of M Clients)							
Shipping Address:		Billing Address:							
Sample Label: 2n		Molecular Weight: 352.3045							
 2n		Molecular Formula: C <sub>18</sub> H <sub>15</sub> F <sub>3</sub> O <sub>4</sub>							
		Melting/Boiling Point: N/A							
		Solubility: DCM, CH <sub>3</sub> CN, MeOH, EA							
		Thermal Stability: Yes							
		Toxicity: NO							
		Reactivity: acidic proton							
<b>Chromatography Conditions:</b>		<b>Analysis Requested</b>							
		EI		CI	MALDI	ESI			
		Low Resolution Nominal Mass							
		High Resolution Accurate Mass				✓			
<b>Special Sample Considerations:</b>		+Ve							
		-Ve							
		GCMS							
		LCMS							
<b>Instrument Used</b>		<b>Conditions Used</b>		<b>Operator Comments</b>					
Finnigan MAT 95		Source Temp:		[M-H] <sup>-</sup> : 351.0837					
Bruker Reflex III		Acc. Voltage:							
Bruker BioTOF II		Resolution:							
Waters Triple Quad		Scan Range:							
Waters Synapt G2		Gas Used:							
Log #:		Analyst:		Analysis Date:		Analyses Run:		Total Cost:	

100649

2n

chresi

Kyle Kalstabakken

3/12/2013 1:04:23 PM

# Display Report

## Analysis Info

Analysis Name Z:\mslab\100649\4hi\_res  
Method negative\_041013.tofpar  
Sample Name 100649  
Comment

Acquisition Date 4/11/2013 6:04:25 PM

Operator operator name  
Instrument BioTOF II

## Acquisition Parameter

n/a	n/a	n/a	n/a	detbias	1800 V
EndP	3000 V	n/a	n/a	n/a	n/a

