

Diastereoselective Synthesis of Novel Spiro Indanone Fused Pyrano[3,2-*c*]Chromene Derivatives following Hetero-Diels-Alder reaction and In Vitro Anticancer Studies

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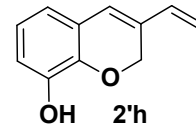
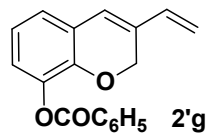
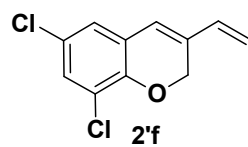
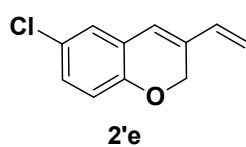
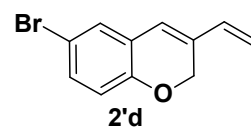
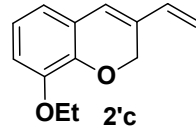
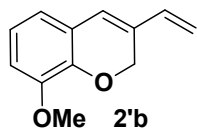
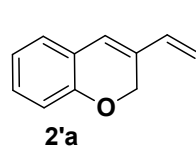
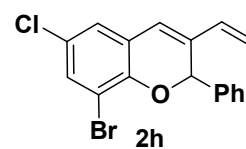
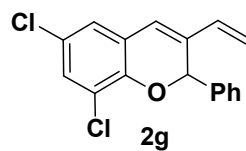
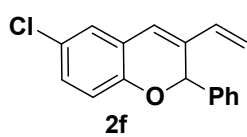
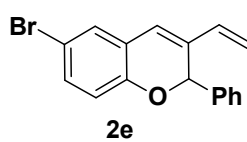
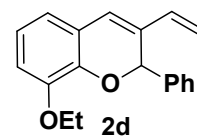
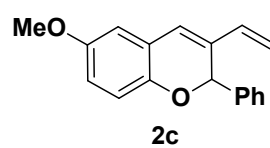
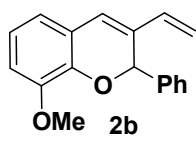
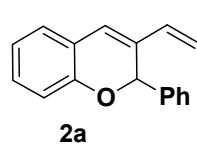
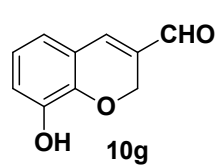
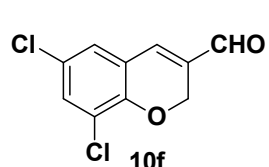
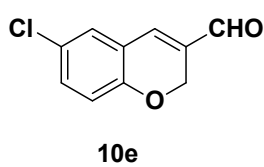
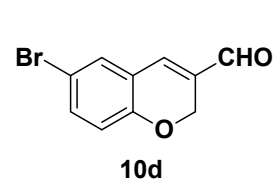
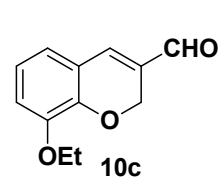
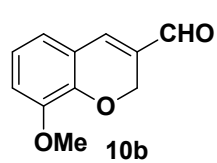
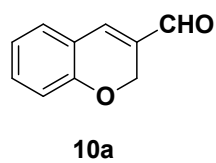
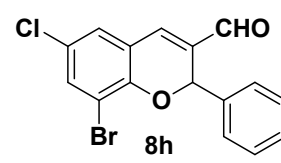
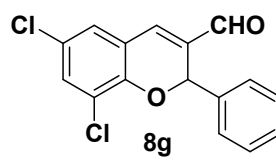
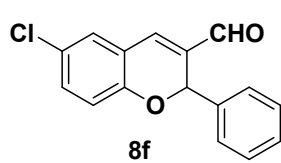
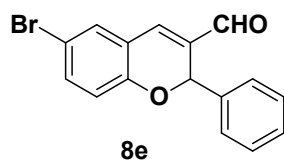
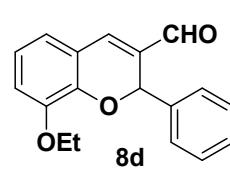
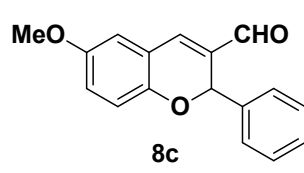
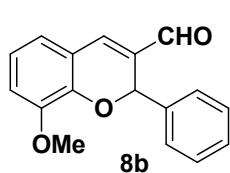
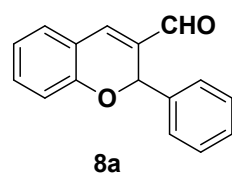
Mass spectra for 10g	
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Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2c	44-45
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2d	45-46
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 2e	47-49
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 2f	50-52
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2g	53-54
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2h	54-55
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2'a	56-57
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2'b	58-60
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2'c	60-61
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 2'd	62-64
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 2'e	65-66
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 2'f	66-68
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Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3c	88-90
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3d	91-93
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3e	94-96
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3f	97-100
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3g	101-104

Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3h	105-107
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3'a	108-110
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Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3'd	118-120
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3'e	121-123
Copies of ^1H (400 MHz), ^{13}C NMR, IR, Mass spectra for 3'f	124-126
Copies of ^1H (400 MHz), ^{13}C NMR, IR spectra for 3'g	127-128

Experimental Section

General remarks:

^1H NMR spectra were recorded on 400 MHz (100 MHz for ^{13}C NMR) JEOL NMR spectrometer with CDCl_3 as solvent and tetramethylsilane (TMS) as internal standard. Chemical shifts were reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl_3 at 7.26 ppm (for ^1H NMR) or 77.0 ppm (for ^{13}C NMR). Melting points are uncorrected and were determined with SMP10 digital melting point apparatus using open capillary tubes. All reagents and solvents used in this study were commercially available (from Sigma-Aldrich) and were used without further purification.



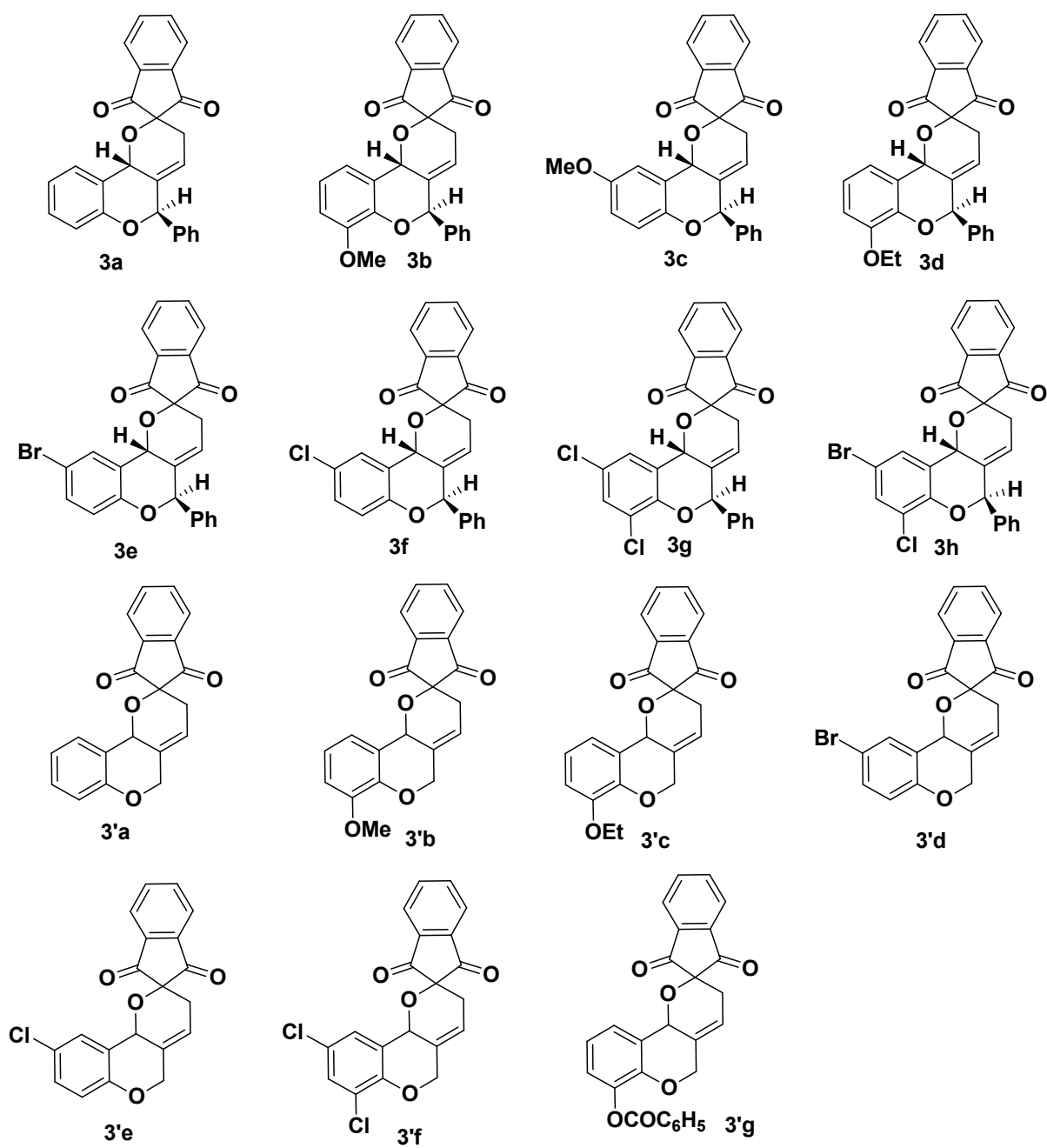
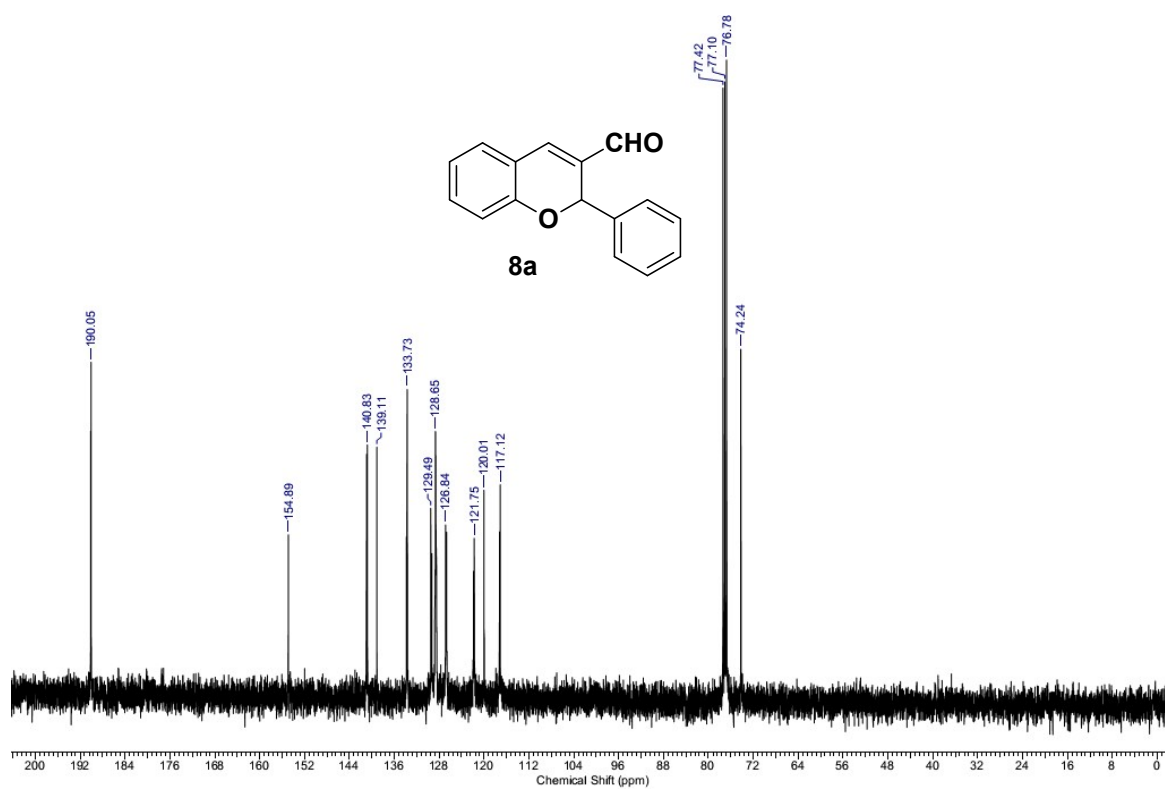
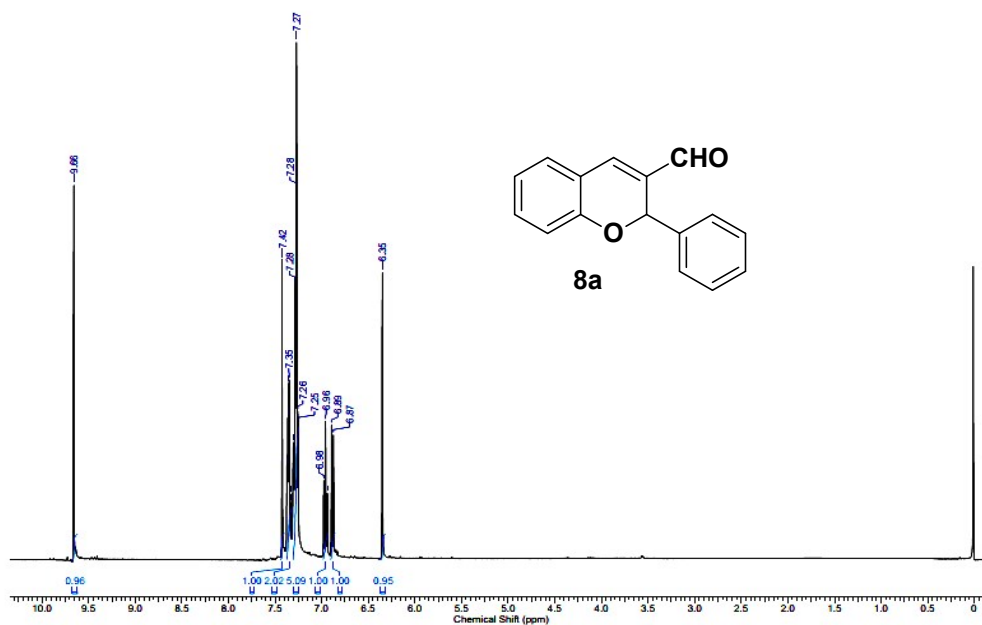
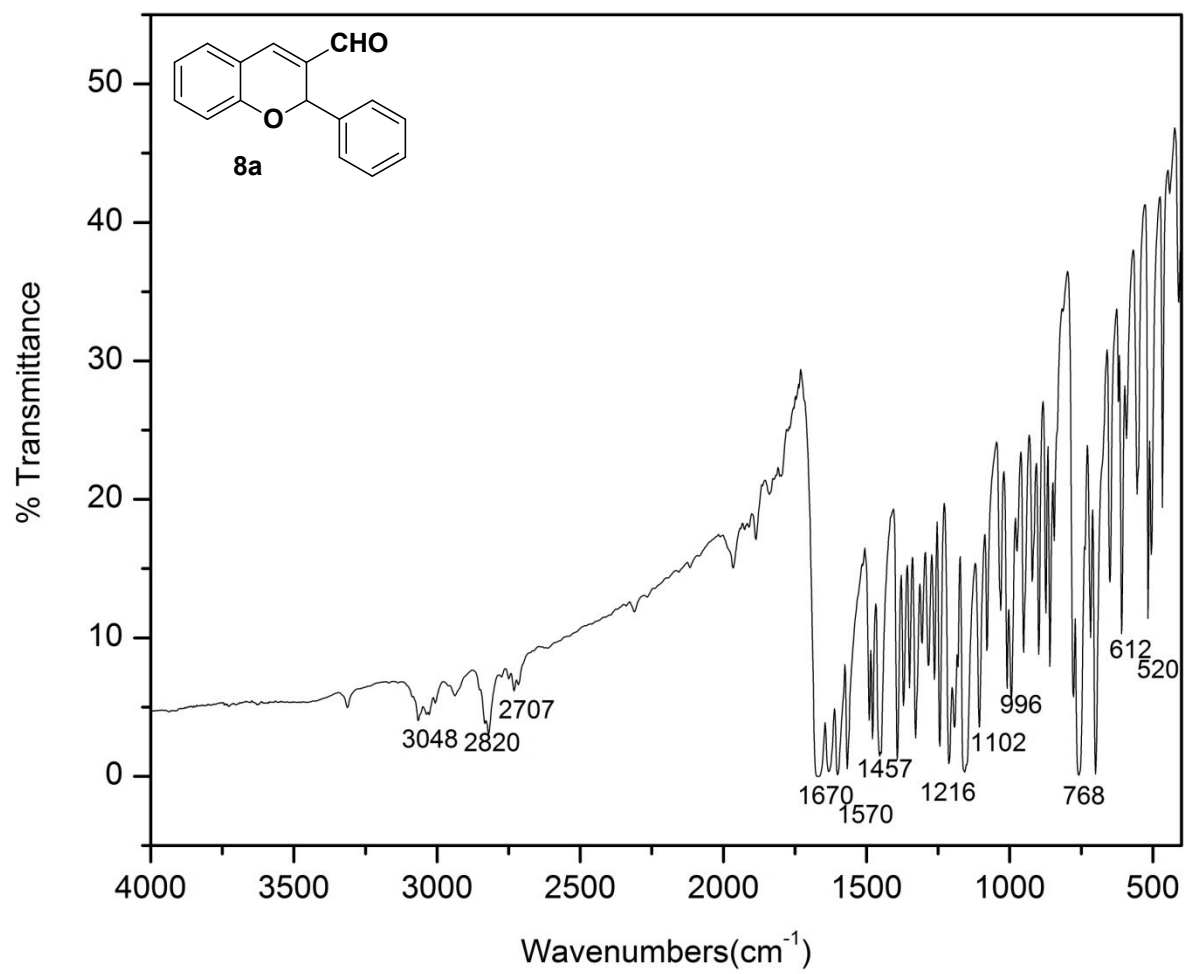


FIGURE 1: Structure of all products





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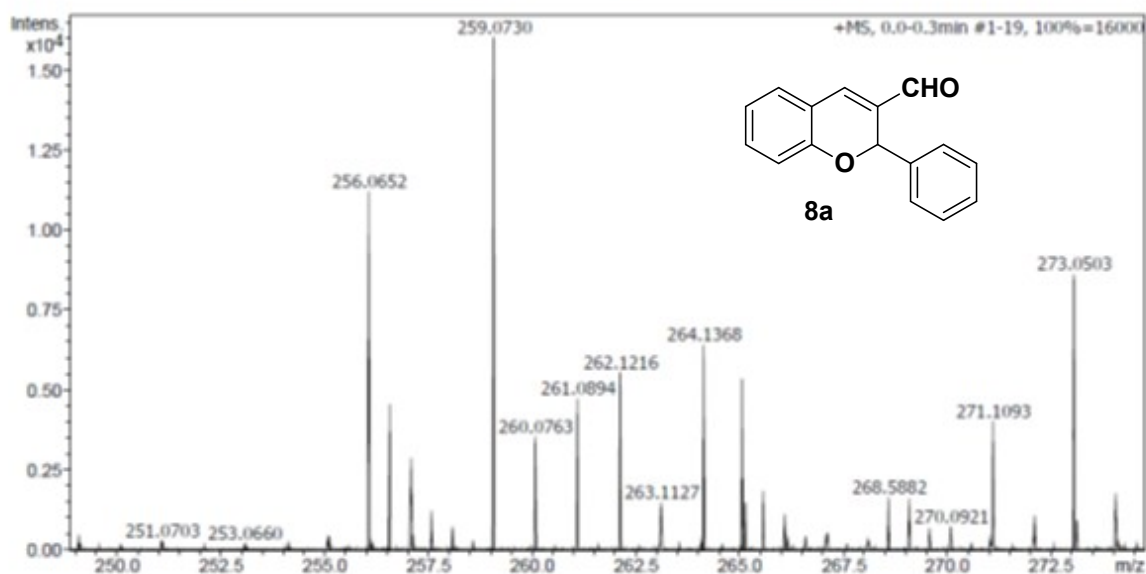
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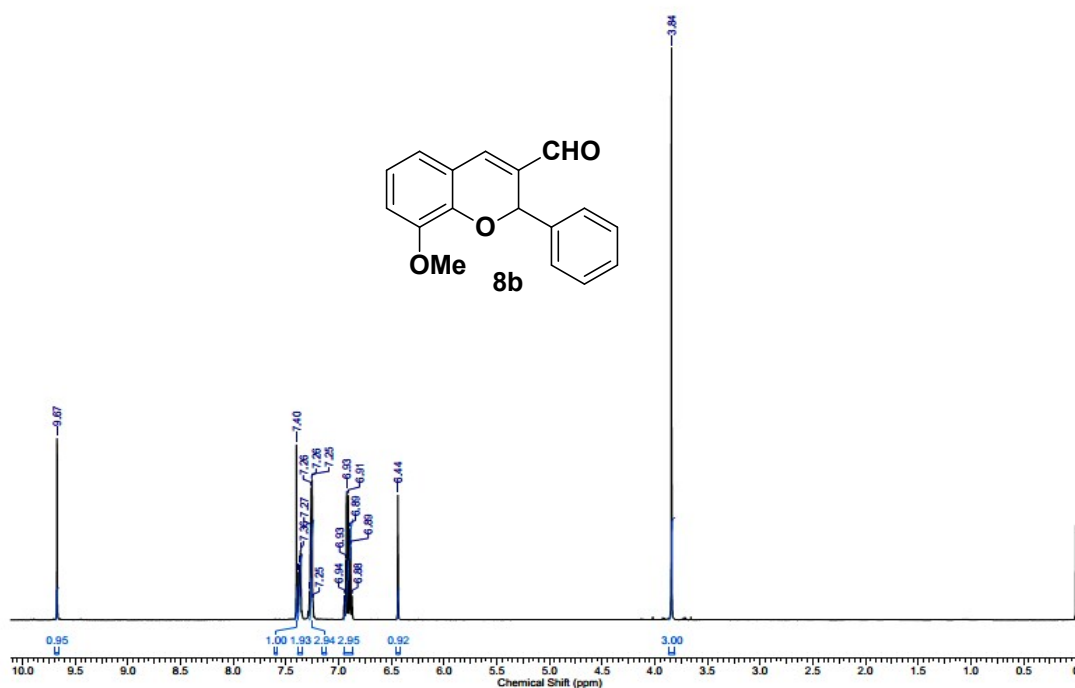
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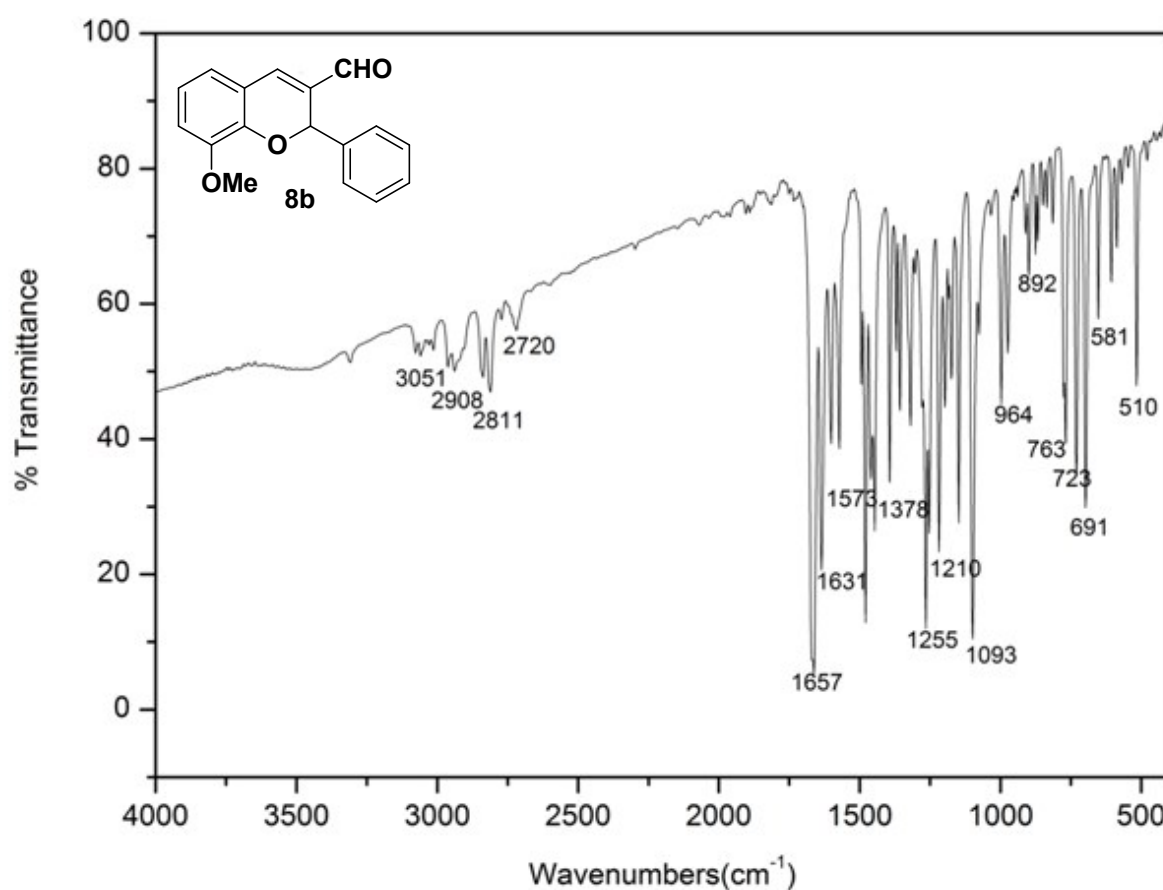
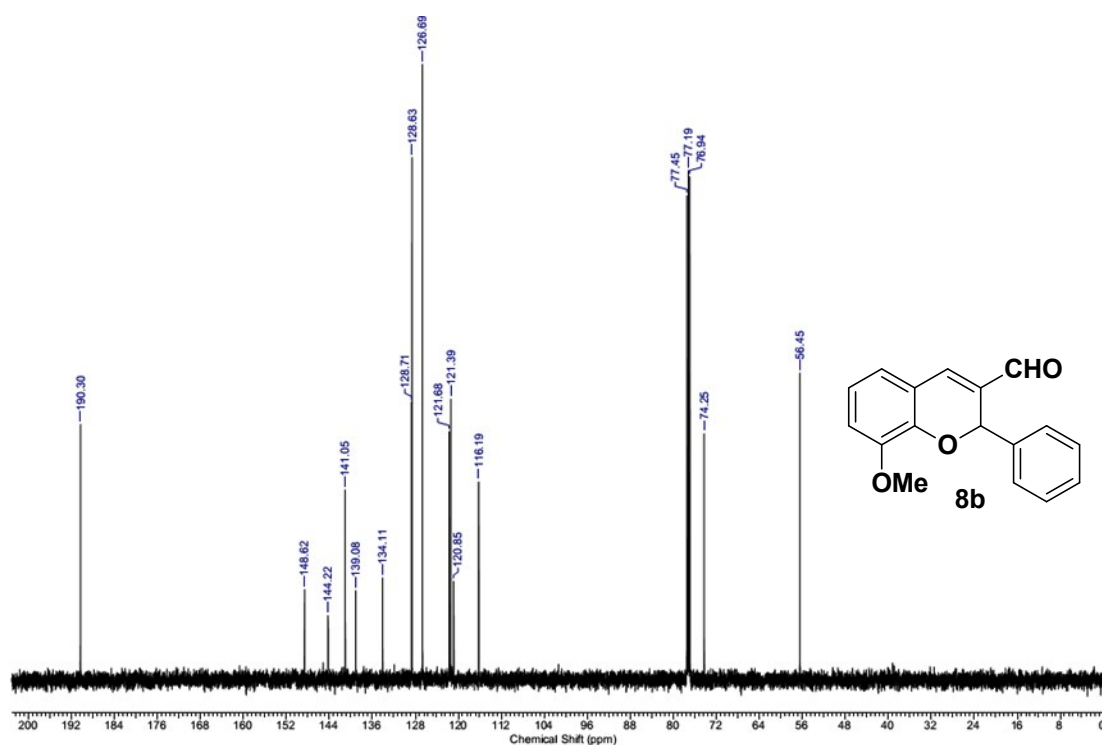
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Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
259.0730	1	C16H12NaO2	259.0730	-0.0	28.8	1	100.00	10.5	even	ok





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Analysis Info

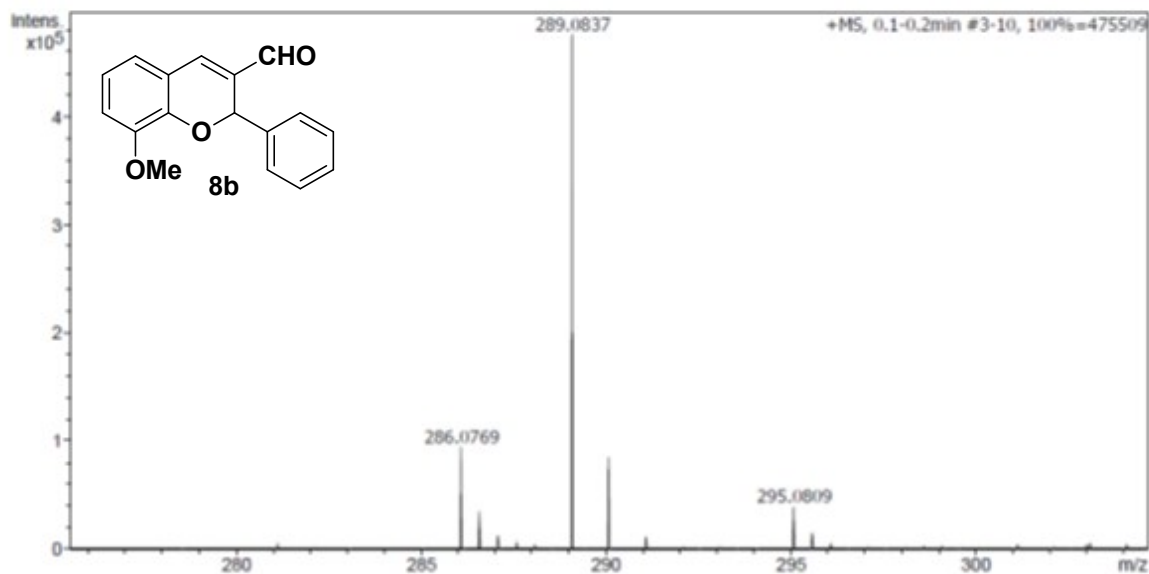
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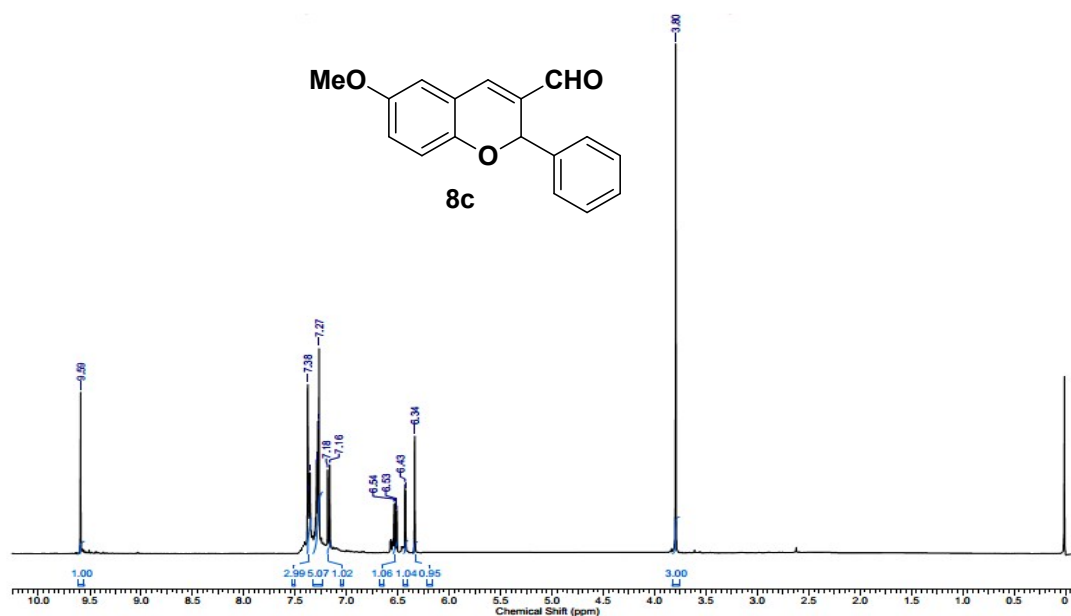
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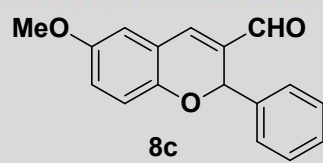
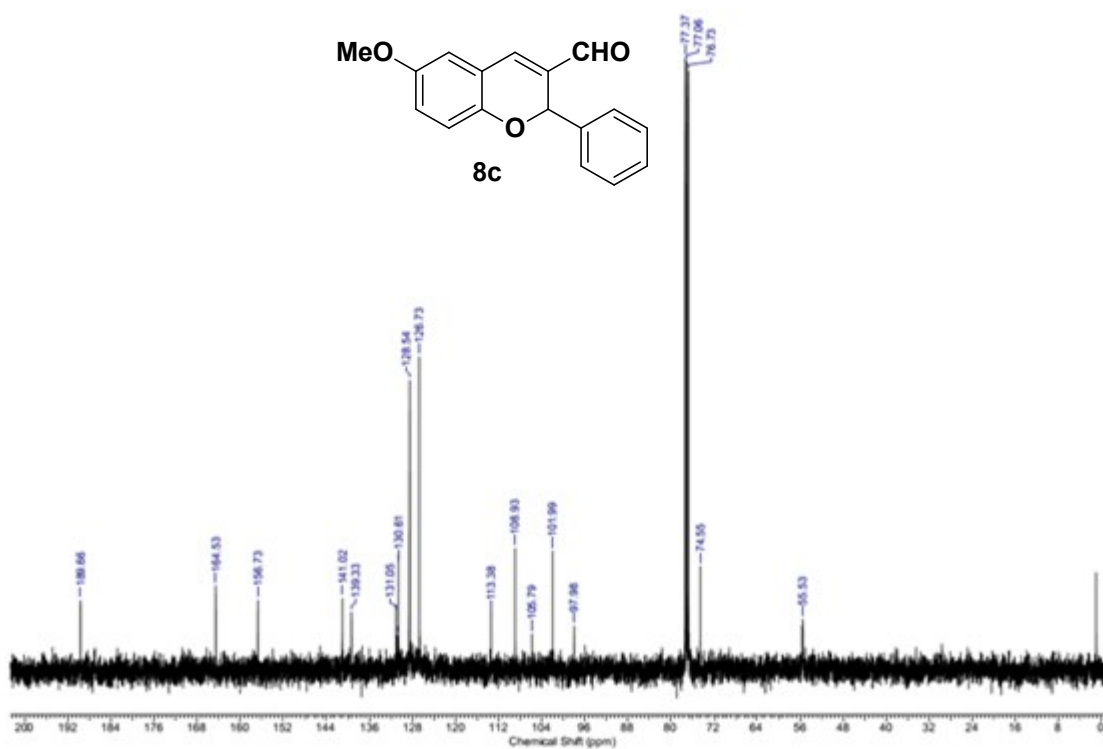
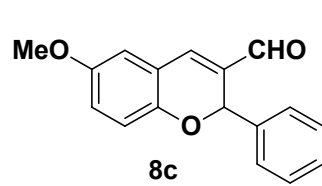
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
289.0837	1	C17H14NaO3	289.0835	0.7	4.8	1	100.00	10.5	even	ok





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Analysis Info

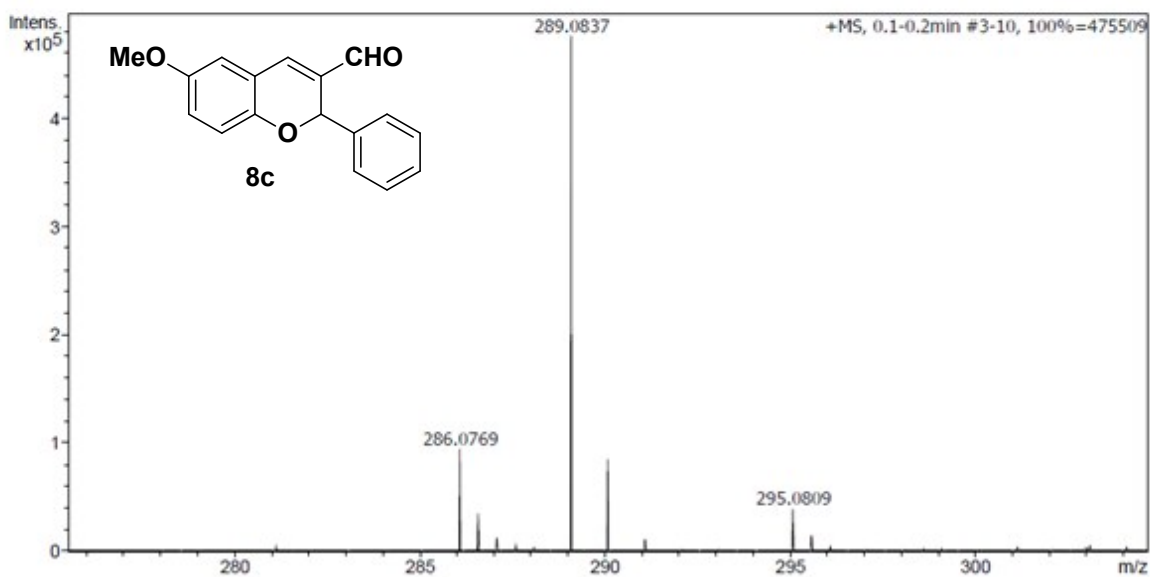
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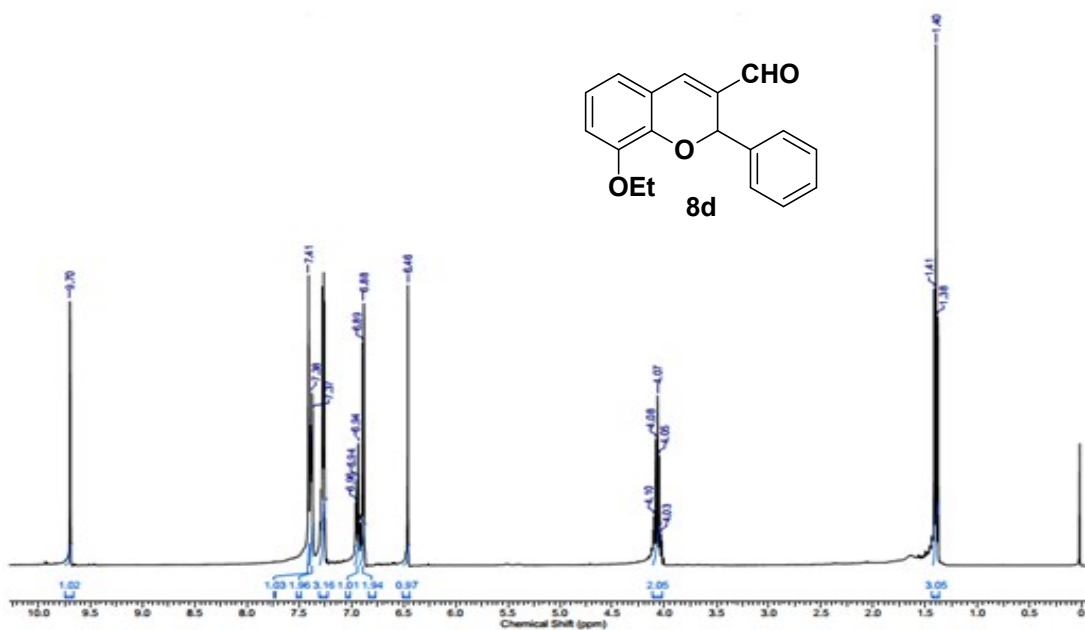
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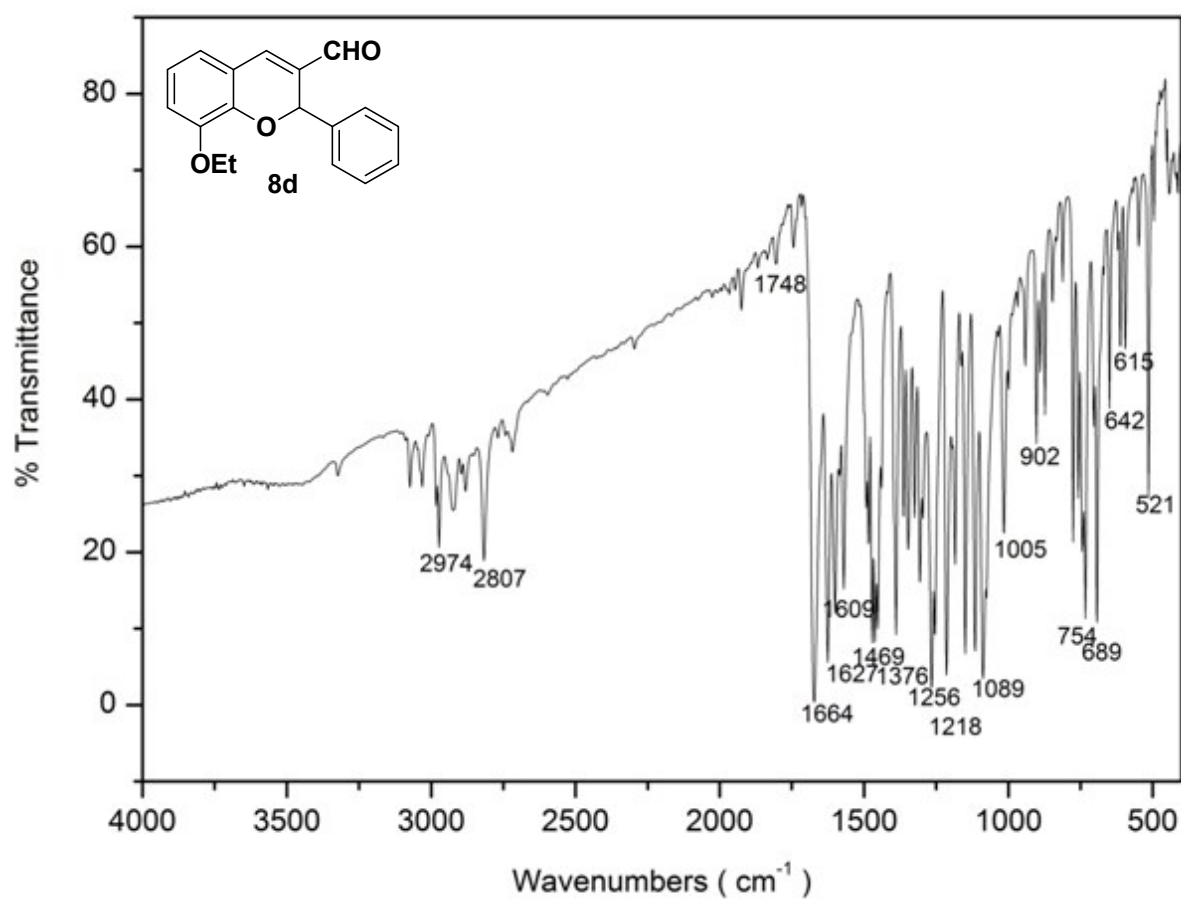
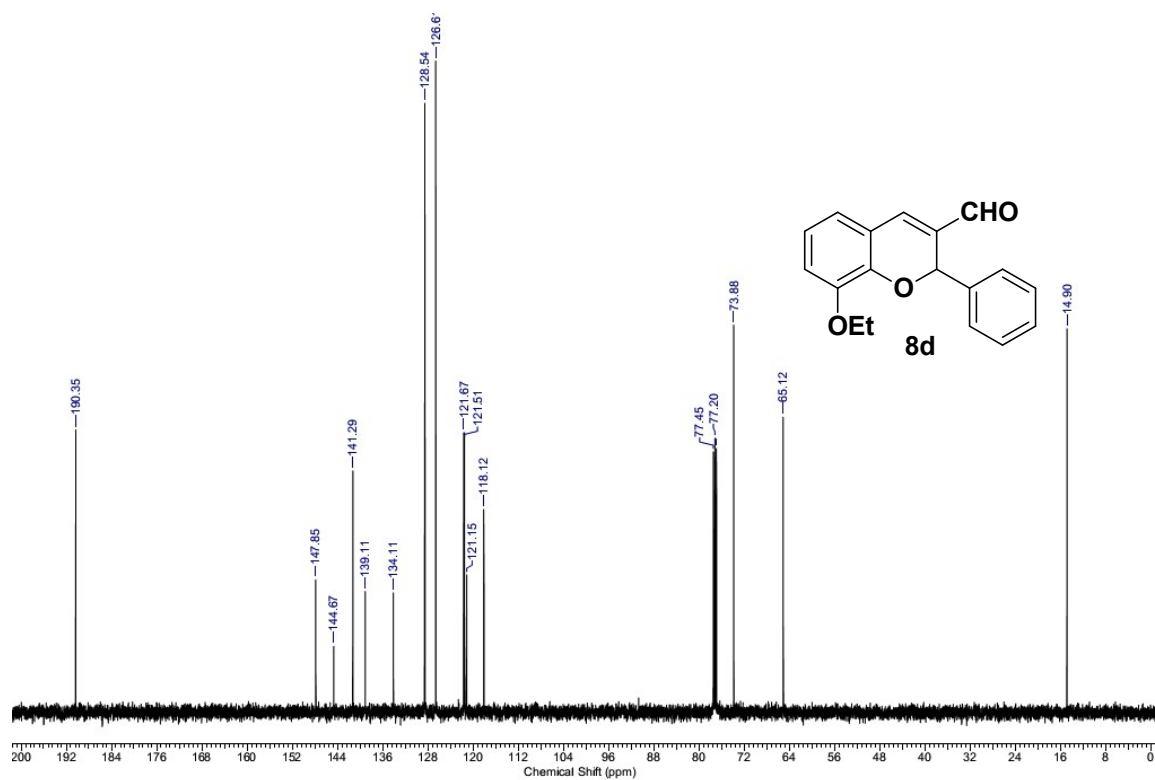
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Scan End	1000 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
289.0837	1	C17H14NaO3	289.0835	0.7	4.8	1	100.00	10.5	even	ok





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Analysis Info

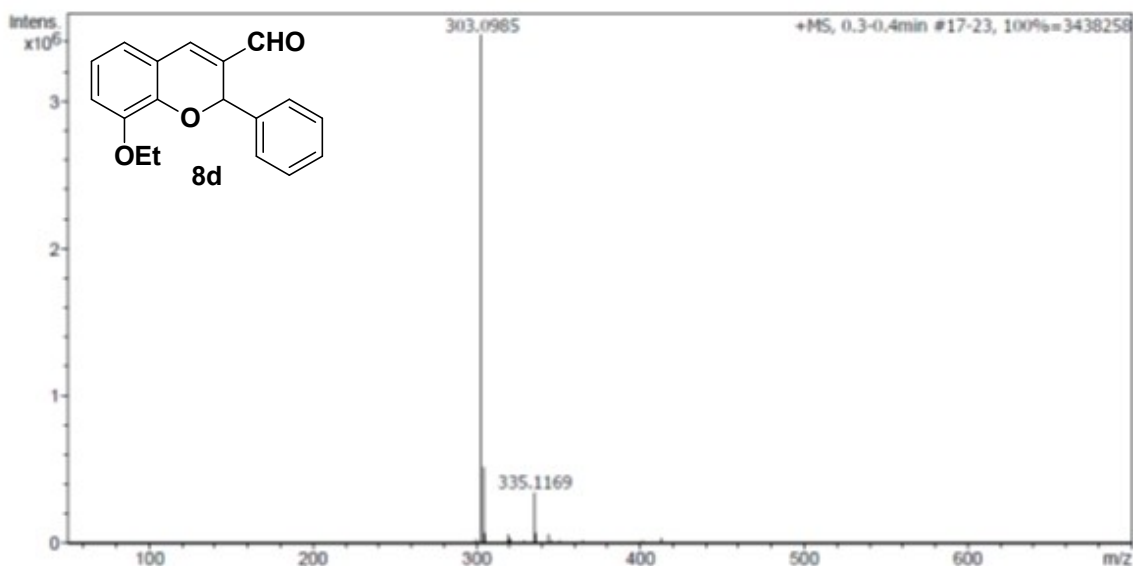
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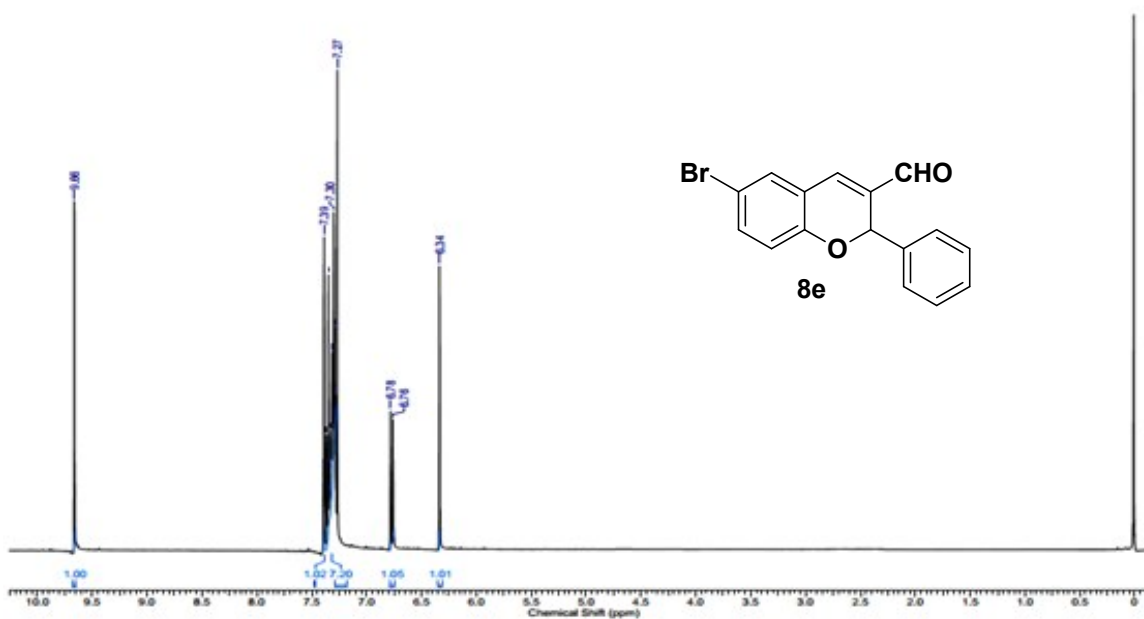
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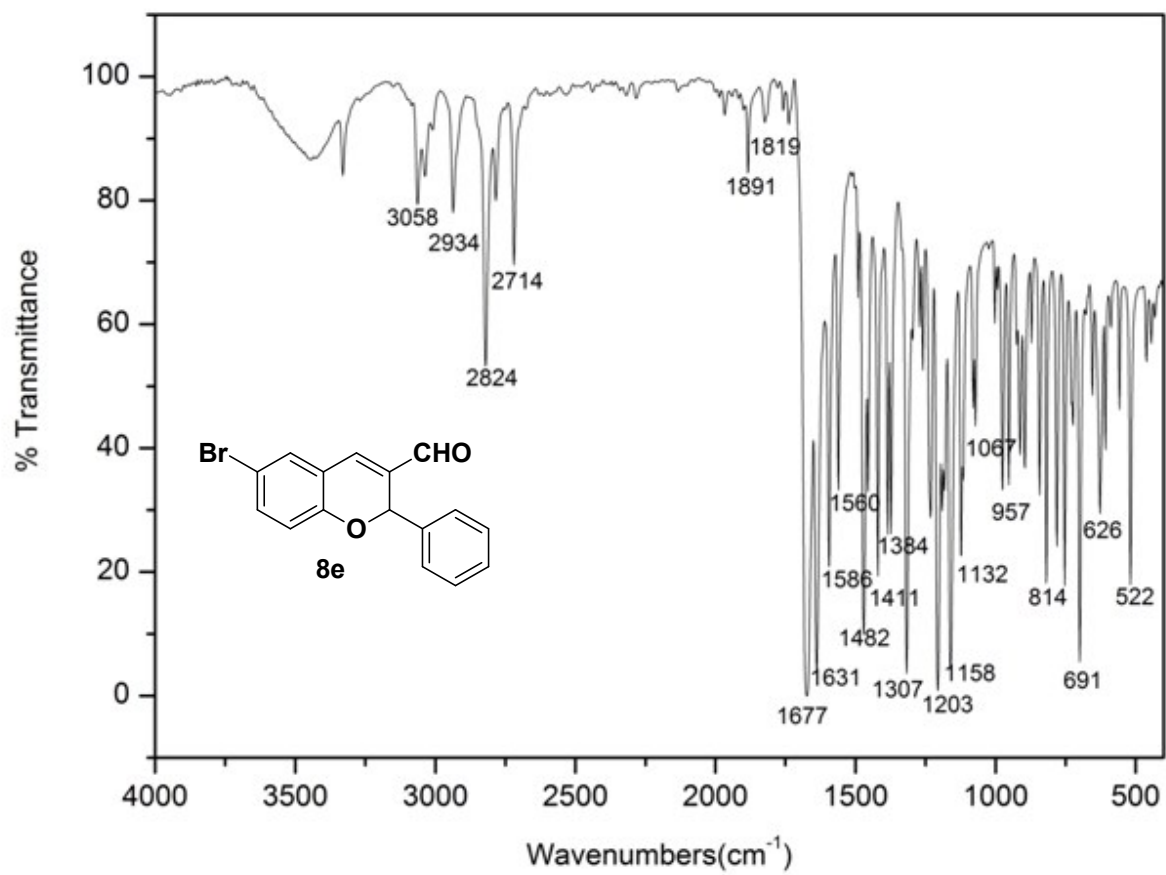
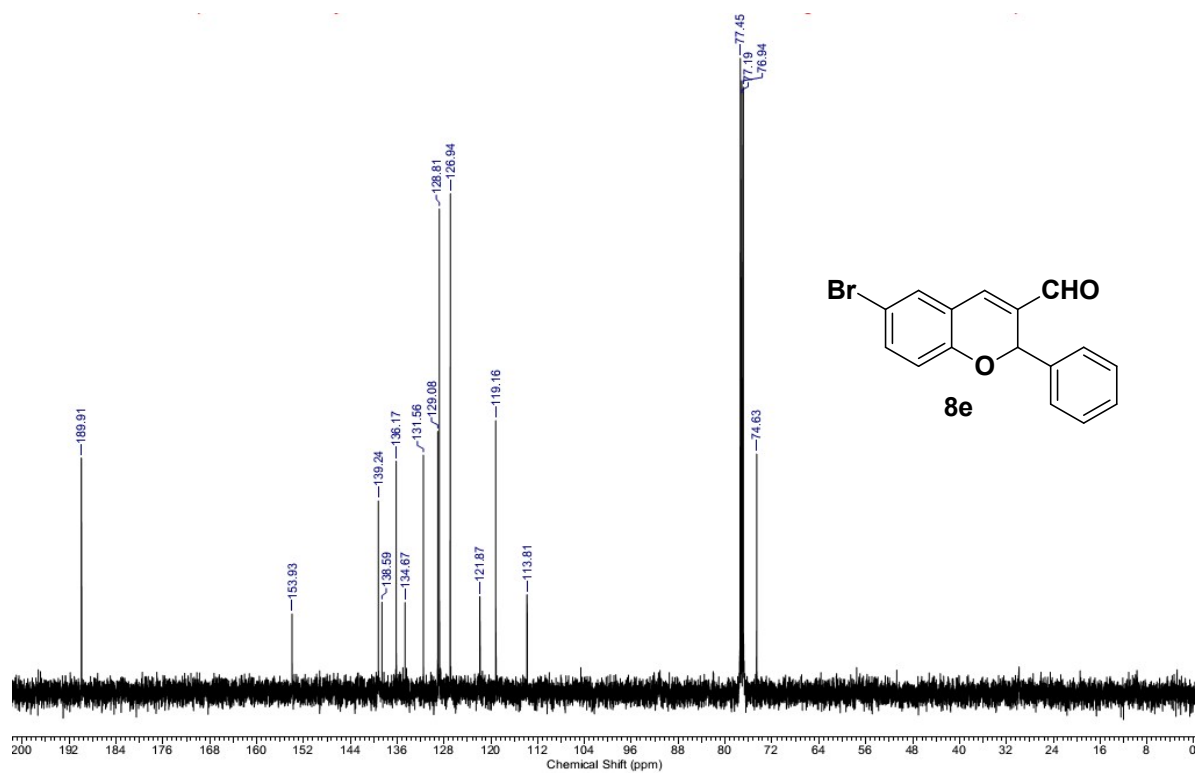
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Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
303.0985	1	C18H16NaO3	303.0992	-2.2	28.4	1	100.00	10.5	even	ok





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Analysis Info

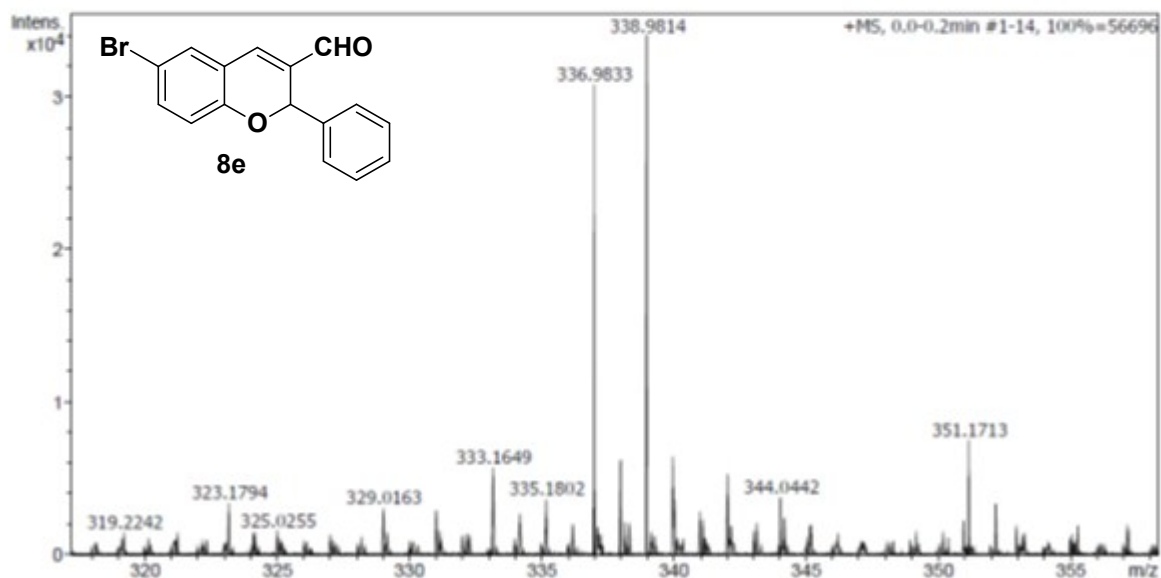
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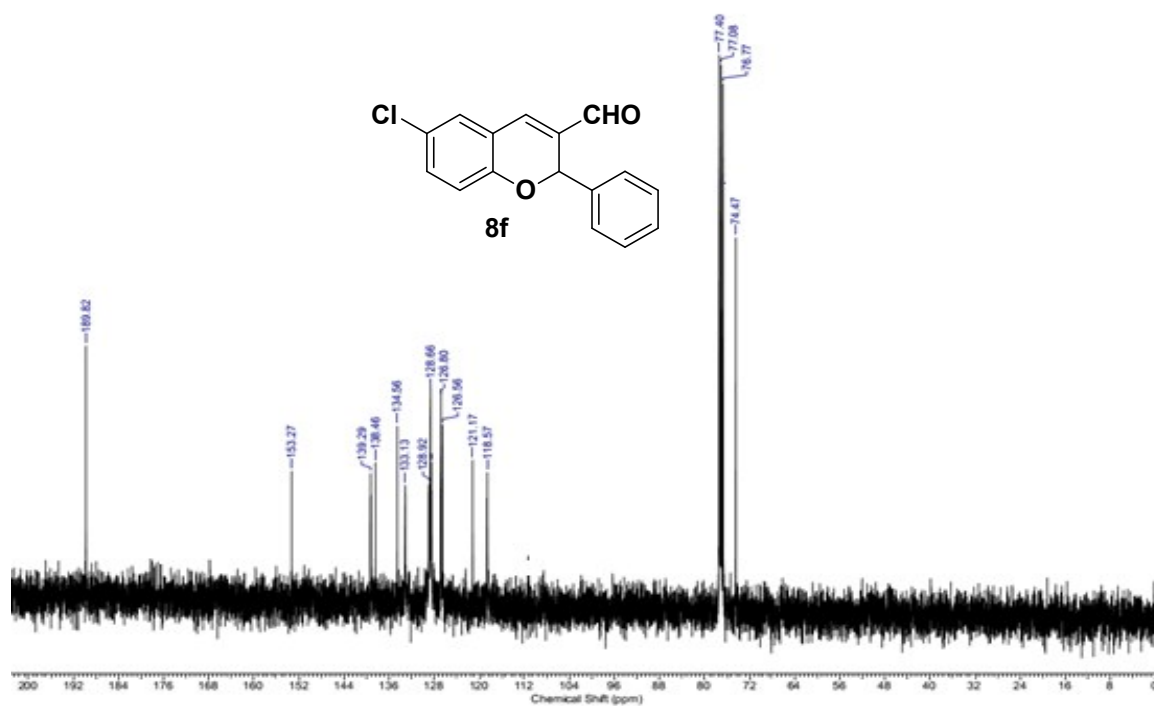
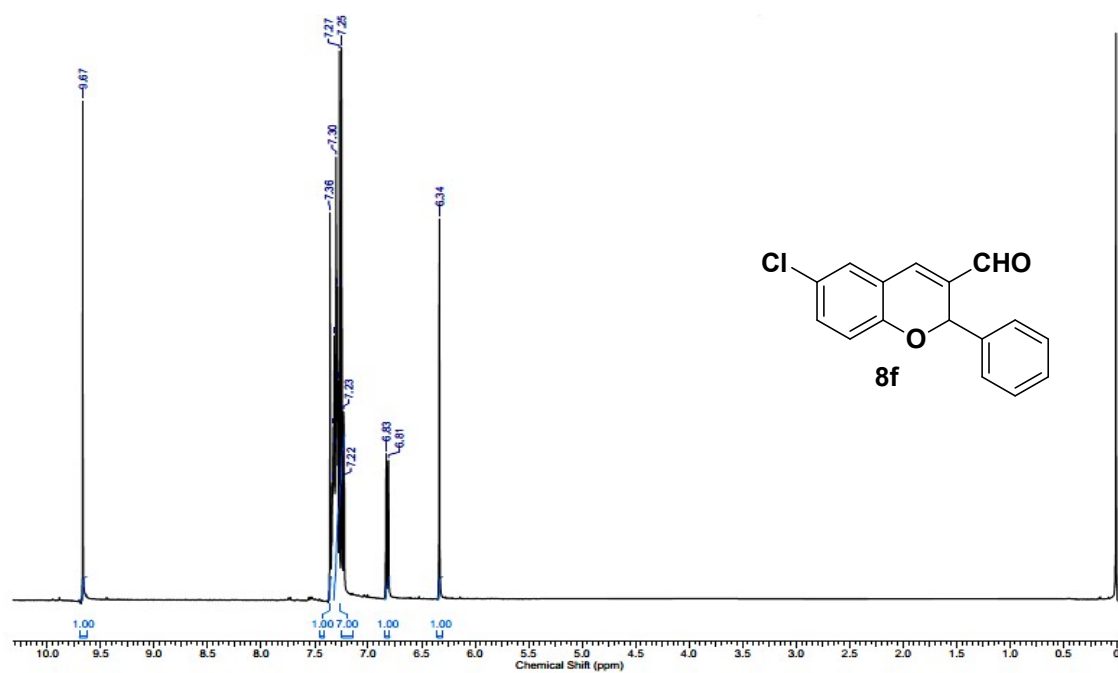
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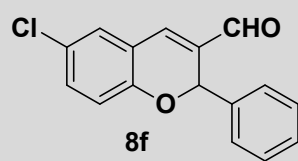
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Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
336.9833	1	C16H11BrNaO2	336.9835	0.4	52.2	1	100.00	10.5	even	ok





DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

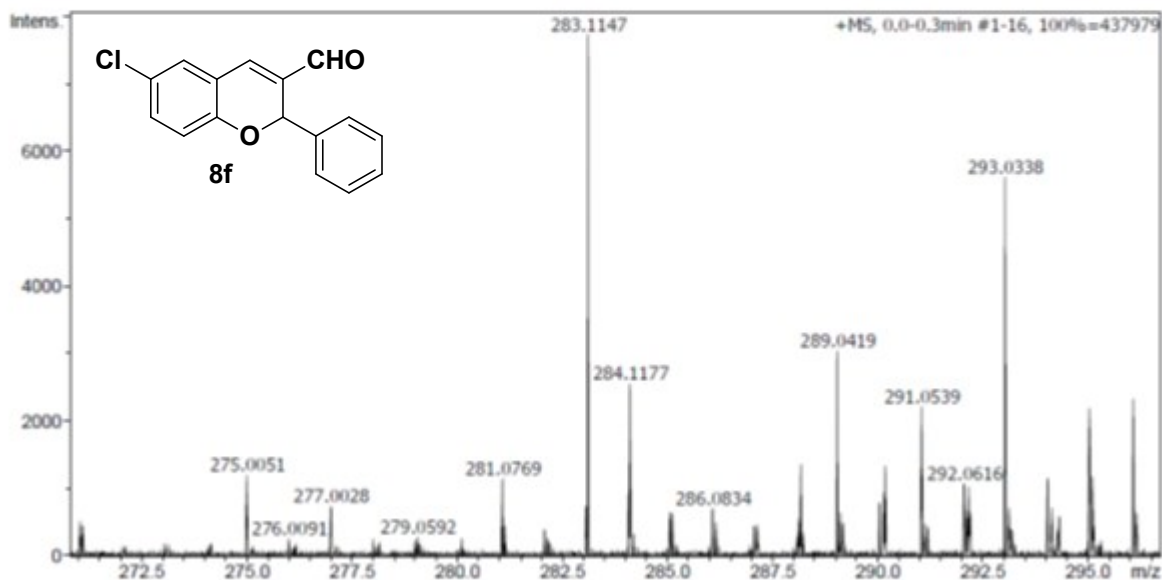
Analysis Name D:\Data\SEPT-2016\INN-SP-SLB-CA 5.d
 Method Tune_pos_NAICSI-500A.m
 Sample Name INN-SP-SLB-CA 5
 Comment C16H11ClO2

Acquisition Date 9/10/2016 7:32:11 PM

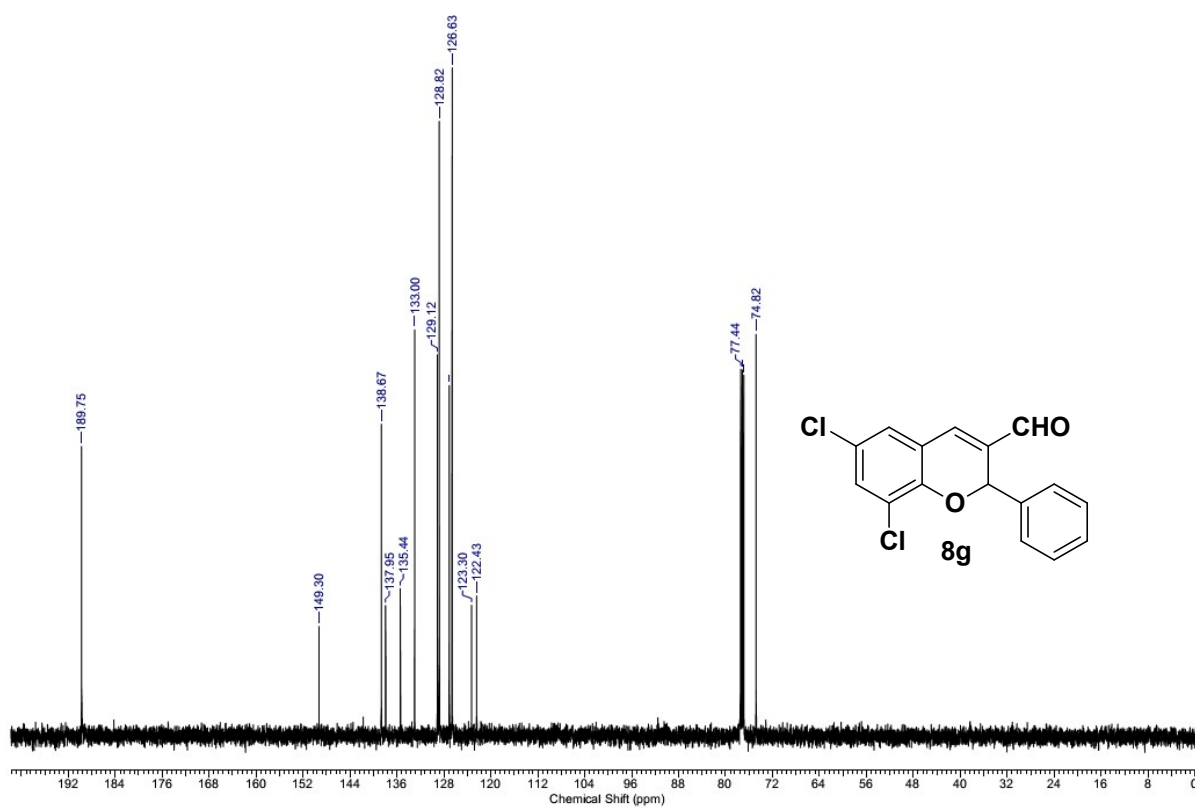
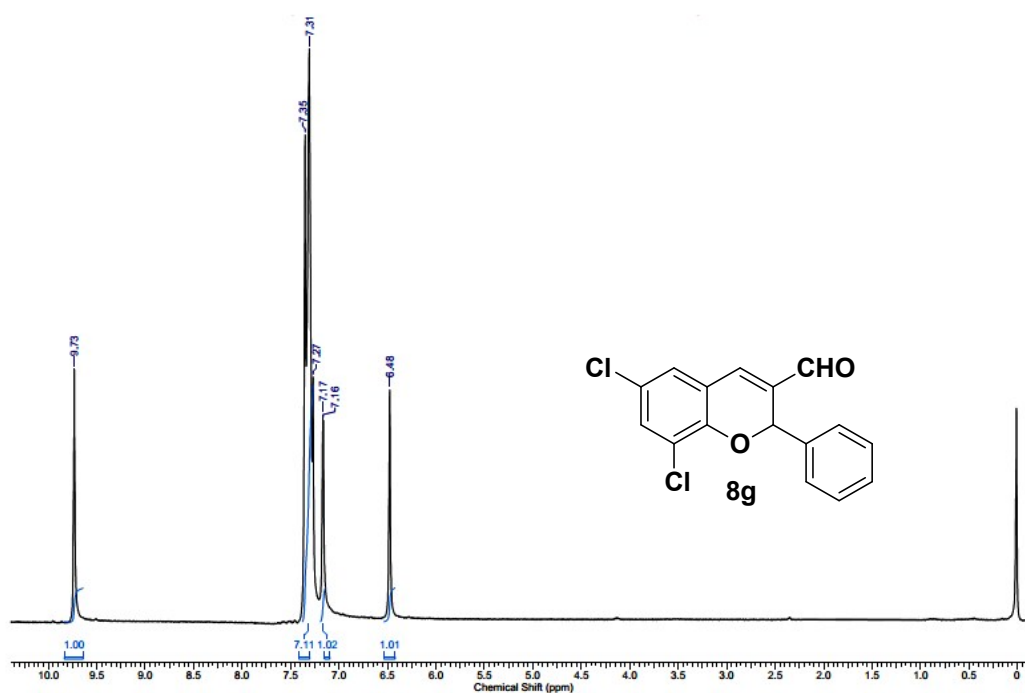
Operator SJG IN
 Instrument maXis impact 282001.00081

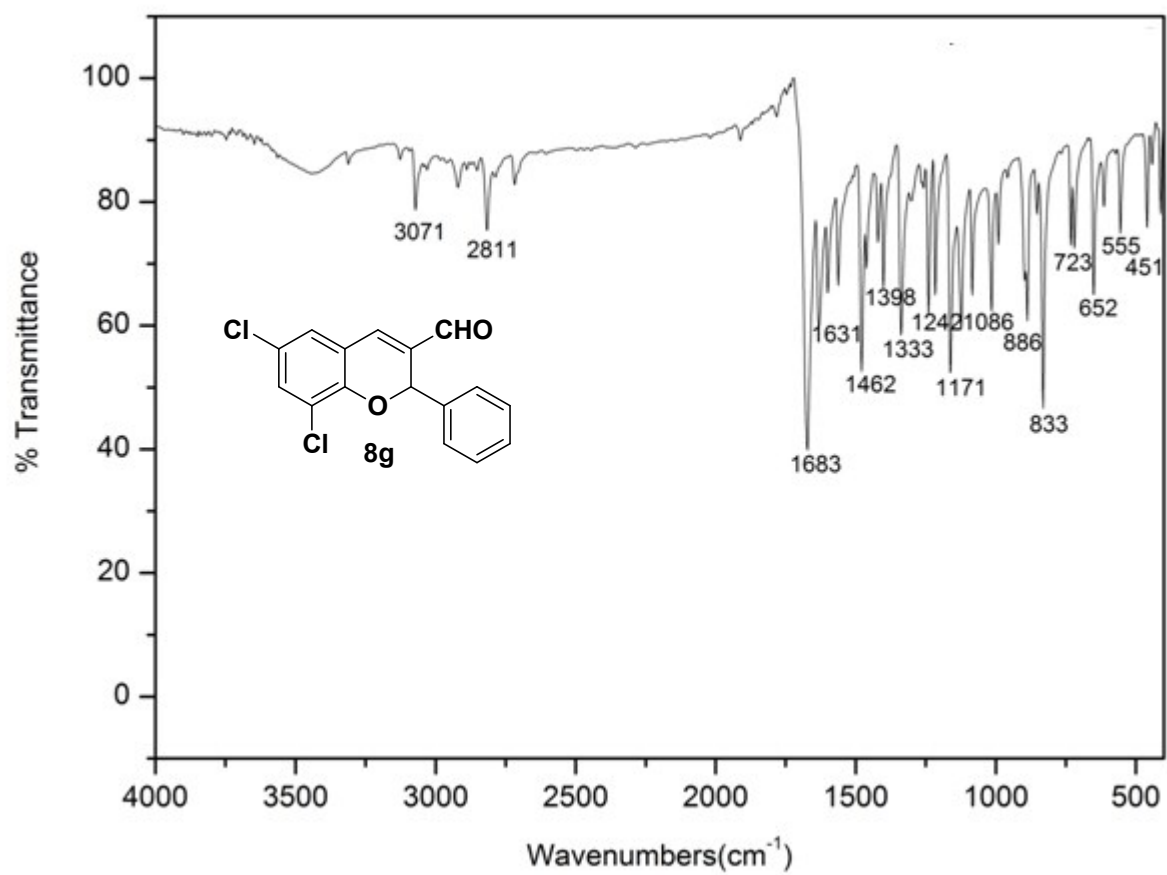
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 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	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
293.0338	1	C16H11ClNaO2	293.0340	-0.6	37.0	1	100.00	10.5	even	ok





DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

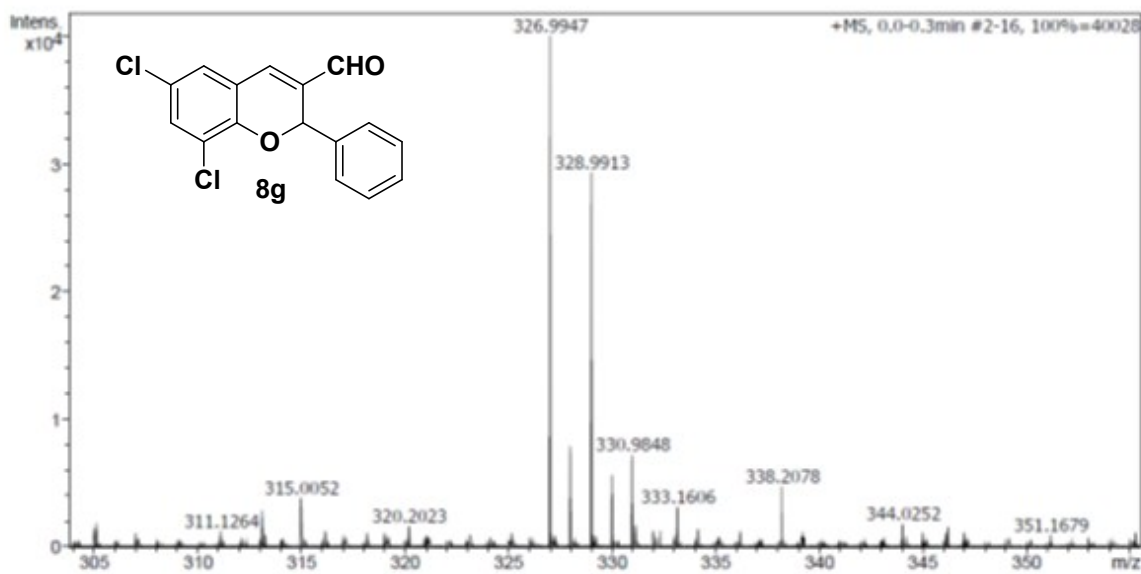
Analysis Name D:\Data\SEPT-2016\INN-SP-SLB-CA 4.d
 Method Tune_pos_NAICSI-500A.m
 Sample Name INN-SP-SLB-CA 4
 Comment C16H10Cl2O2

Acquisition Date 9/10/2016 7:11:42 PM

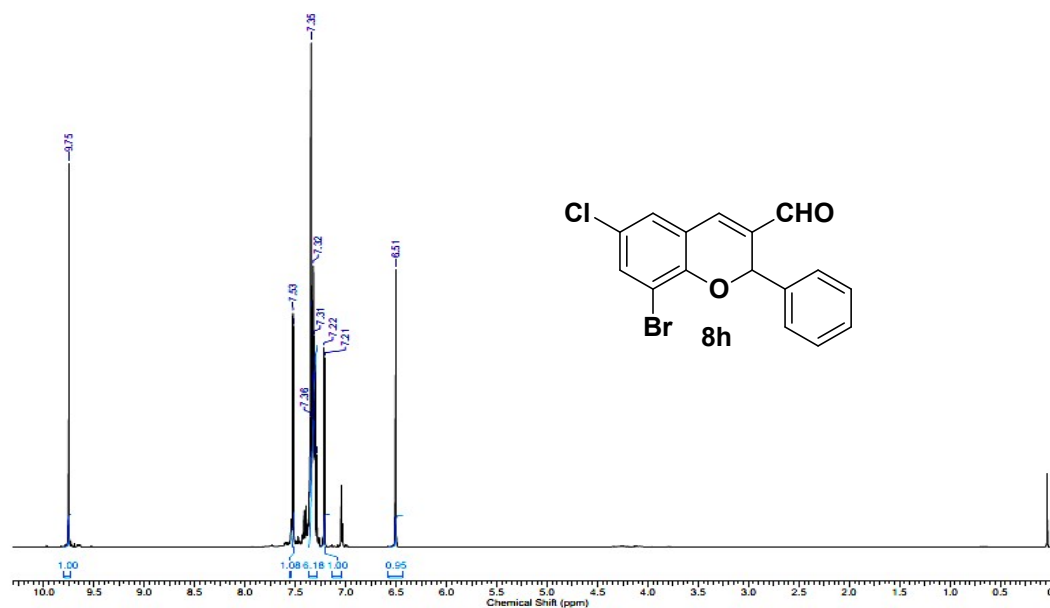
Operator SJG IN
 Instrument maXis impact 282001.00081

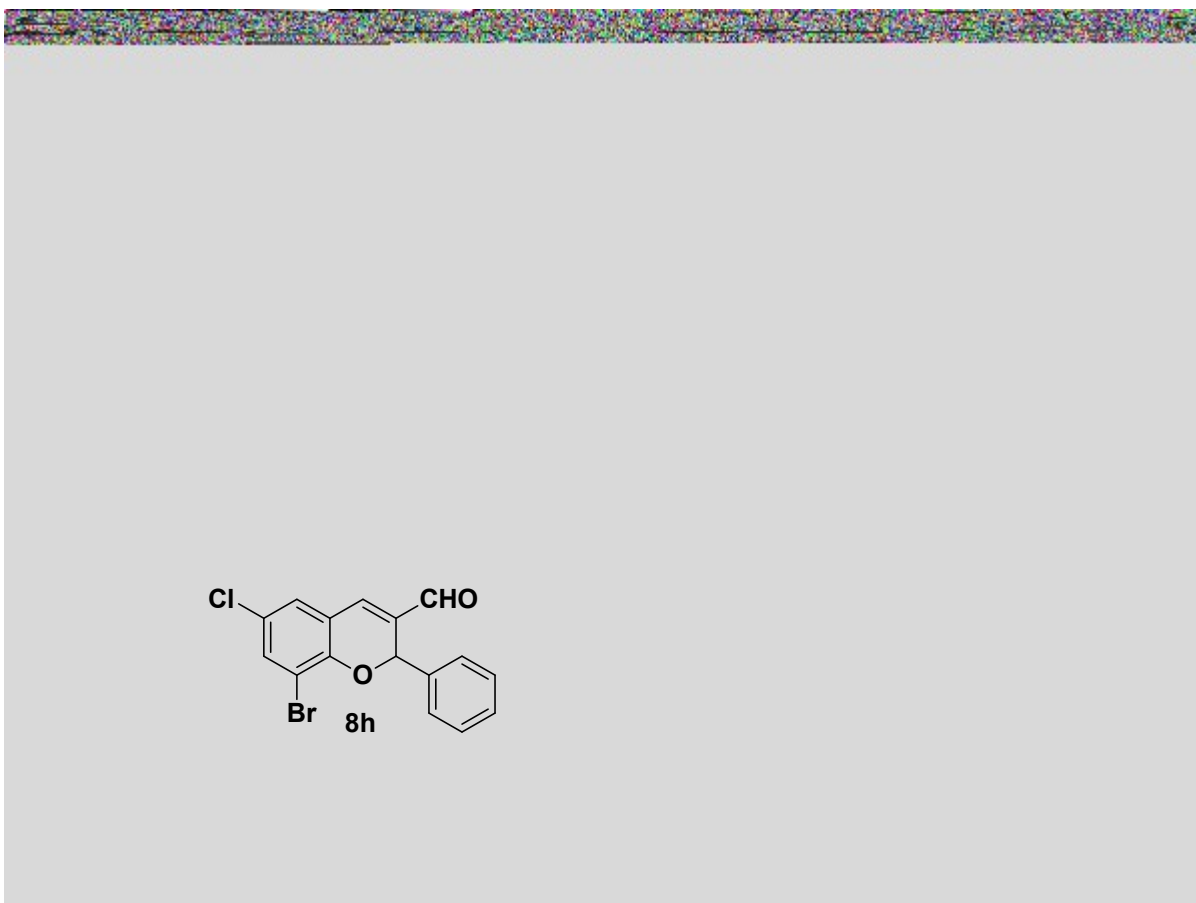
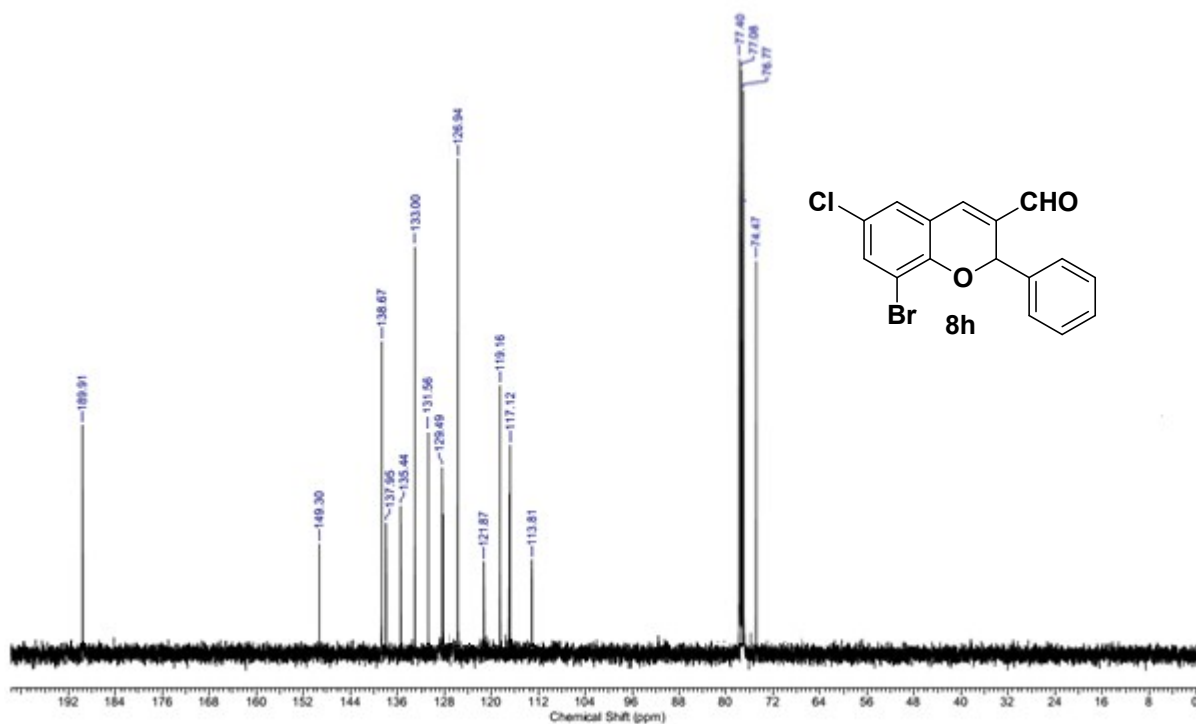
Acquisition Parameter

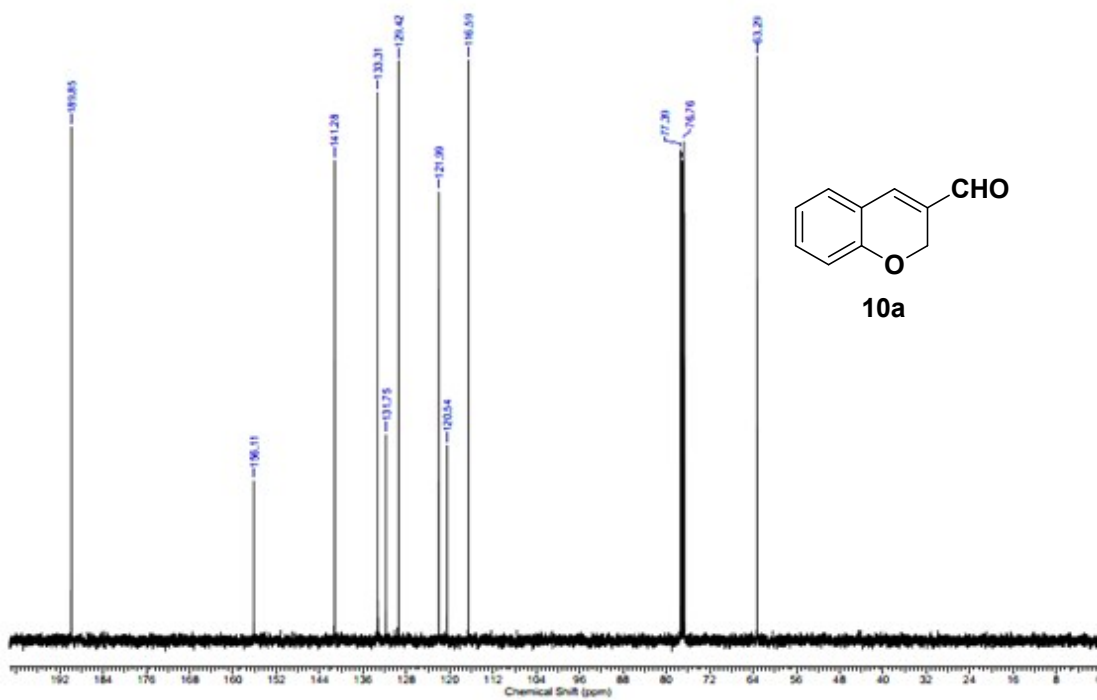
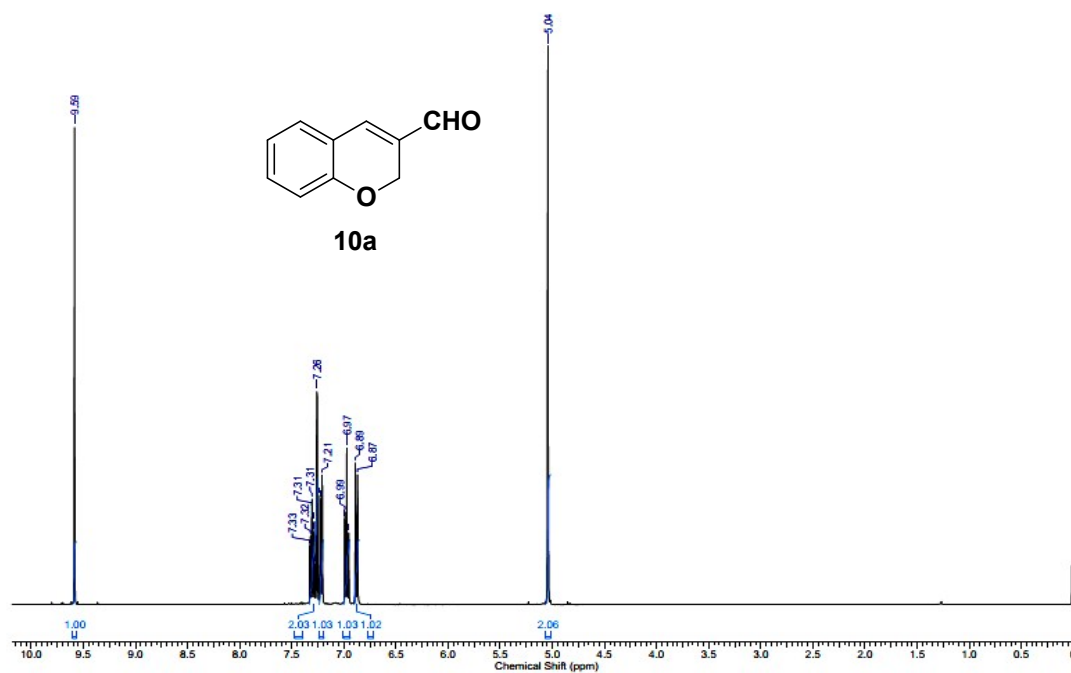
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source

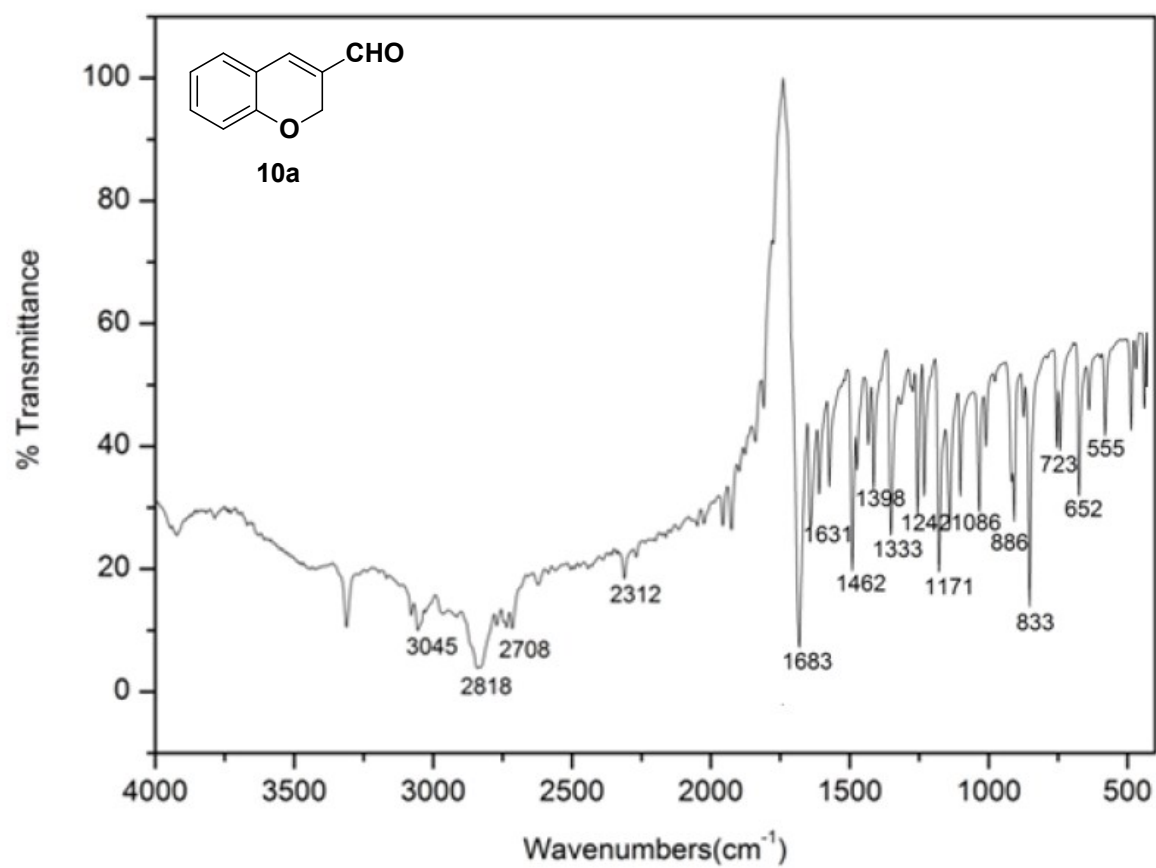


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
326.9947	1	C16H10Cl2NaO2	326.9950	1.1	43.1	1	100.00	10.5	even	ok









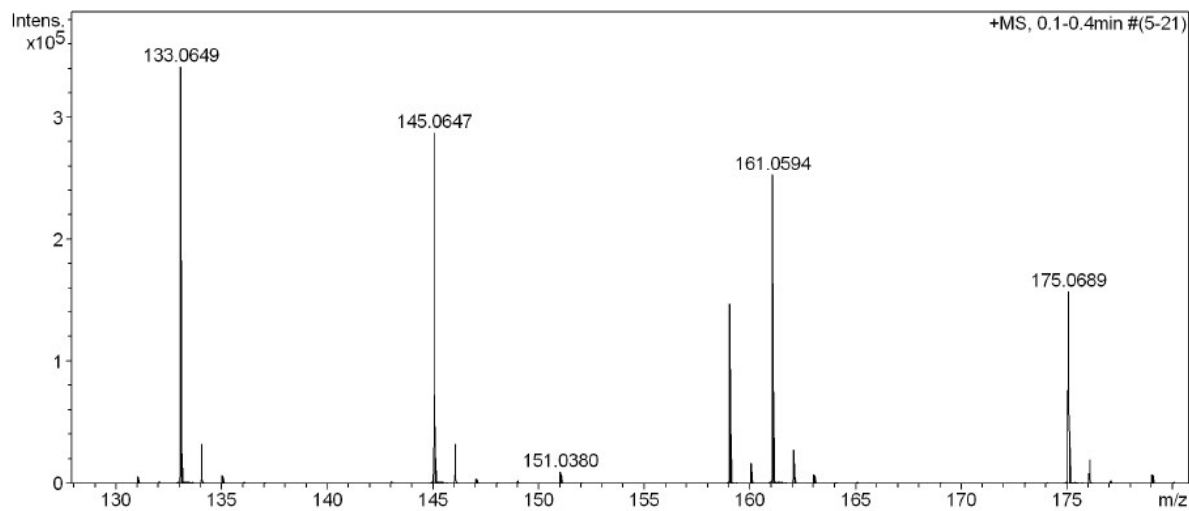
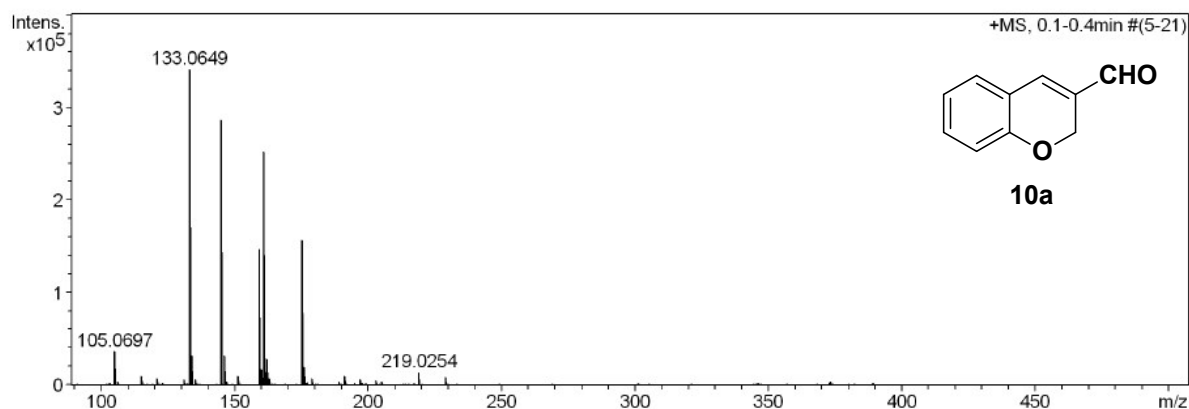
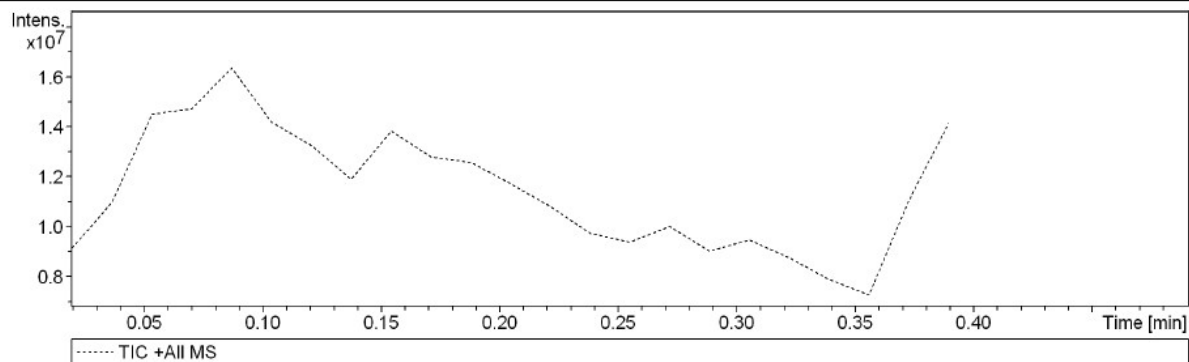
Generic Display Report

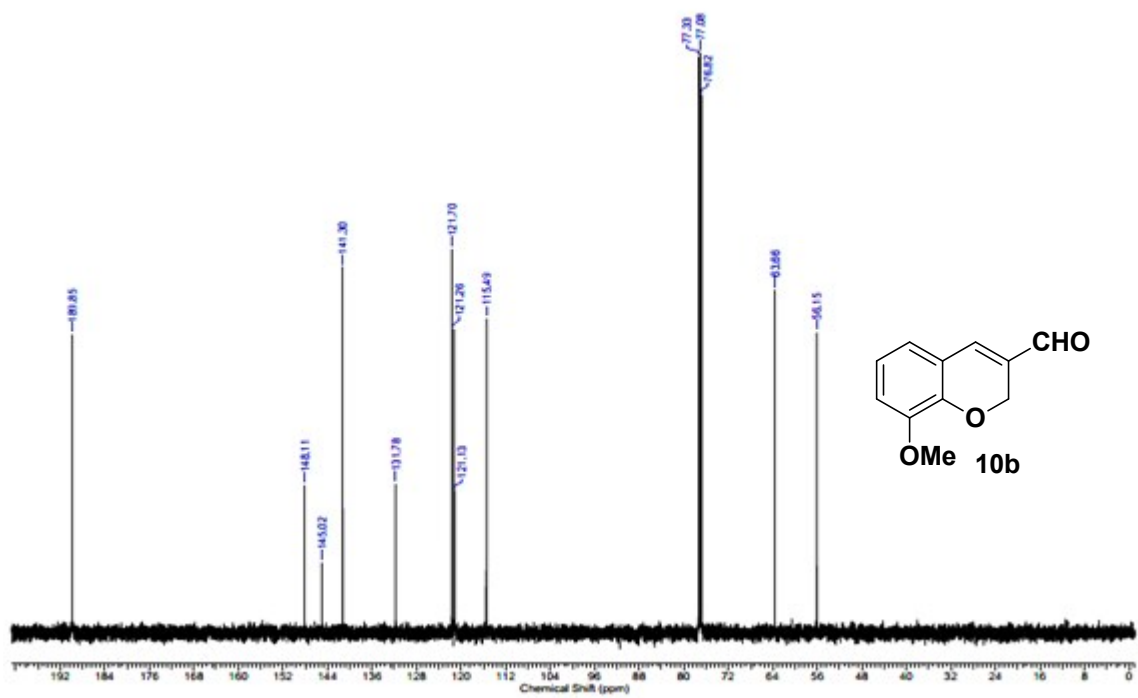
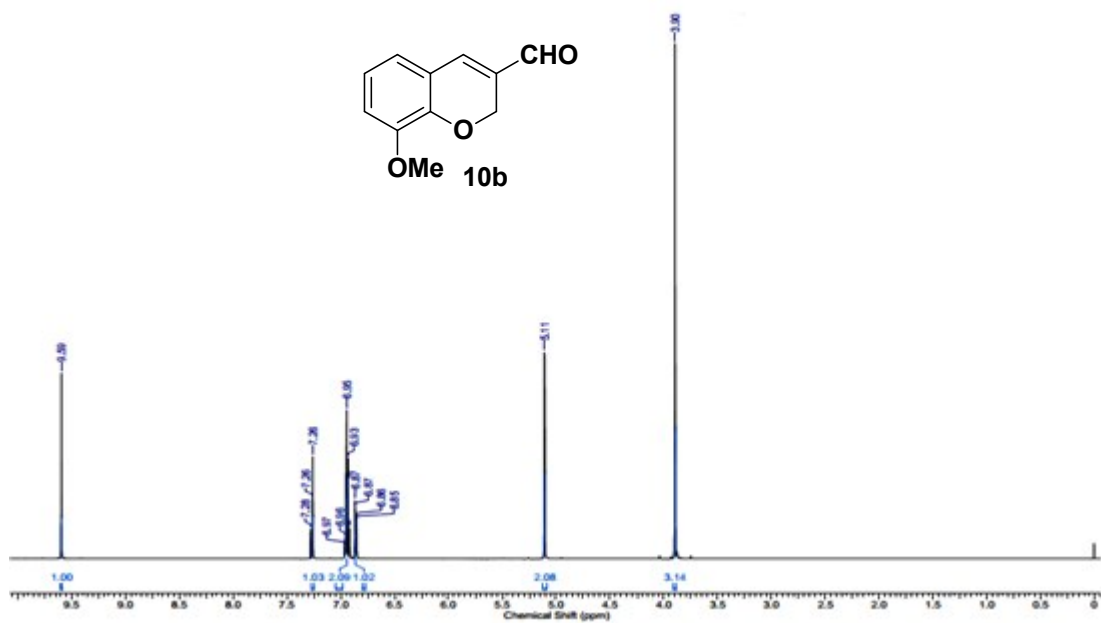
Analysis Info

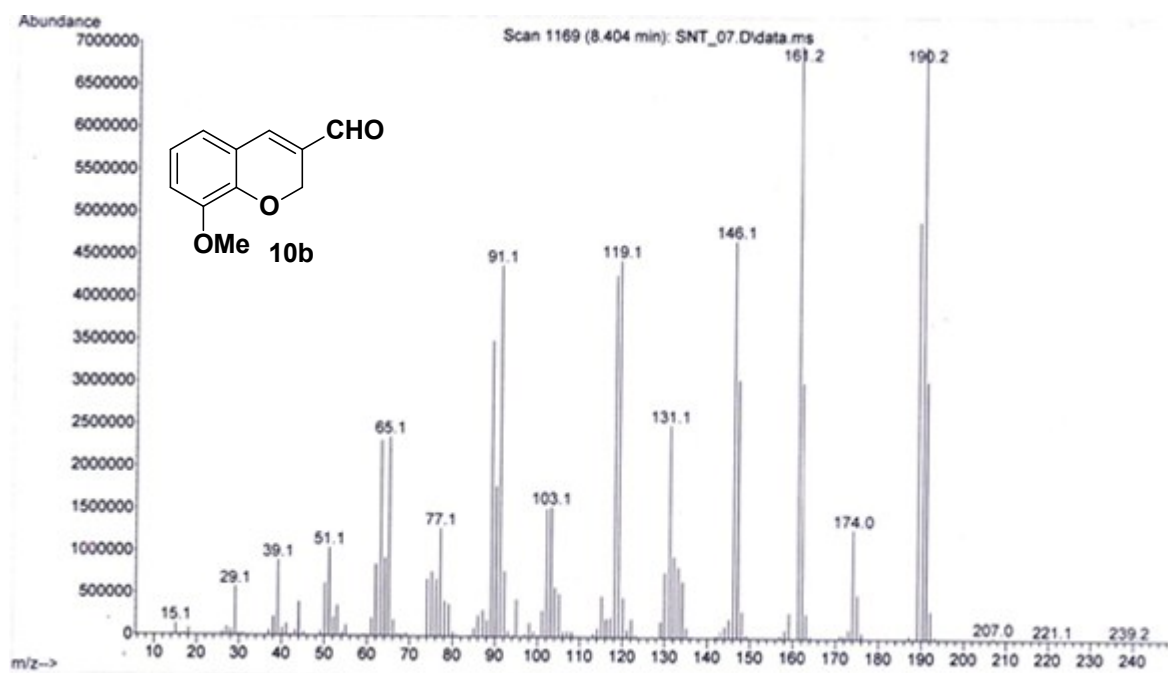
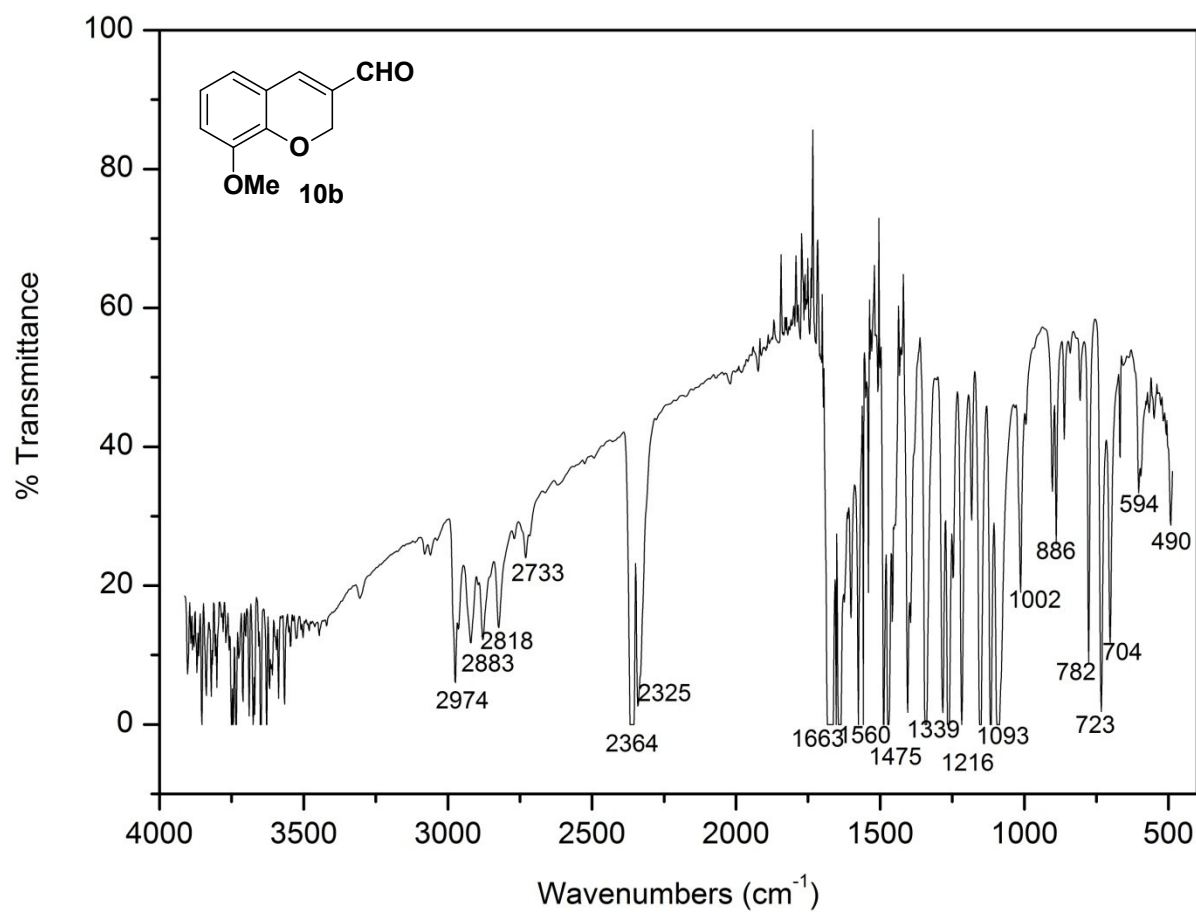
Analysis Name D:\Data\AUG-2016\CSP\31082016_CSP_SDP_SNT_01.d
Method Pos_tune_low.m
Sample Name Bruker micro TOF -Q II
Comment

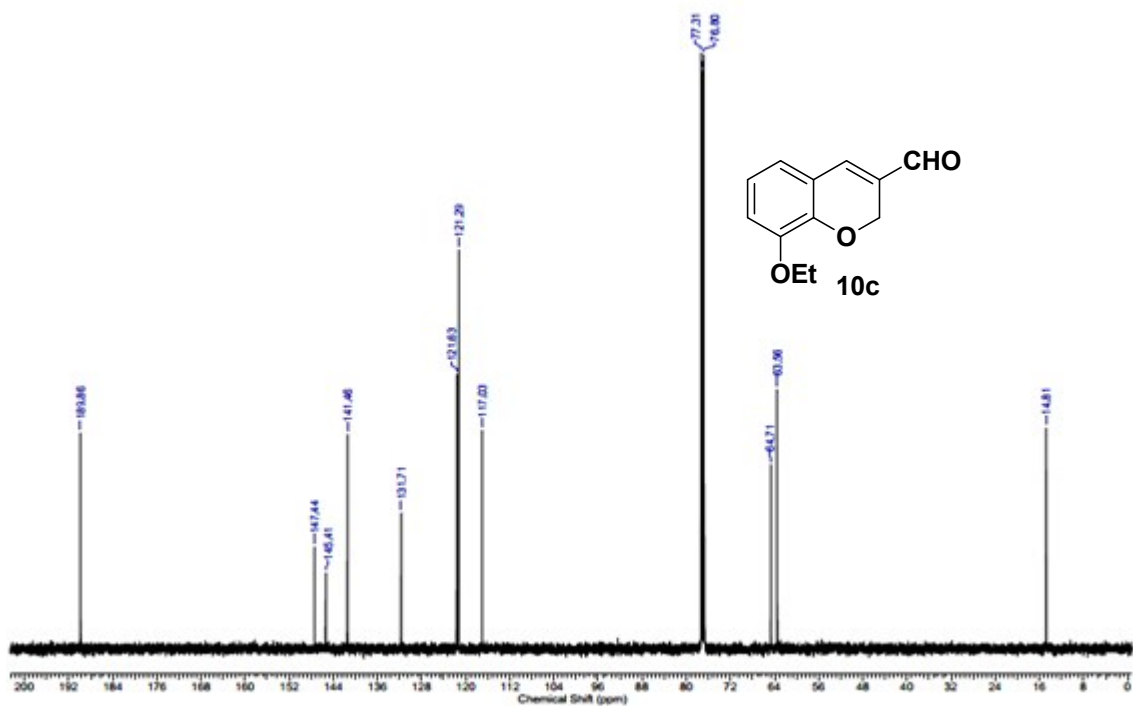
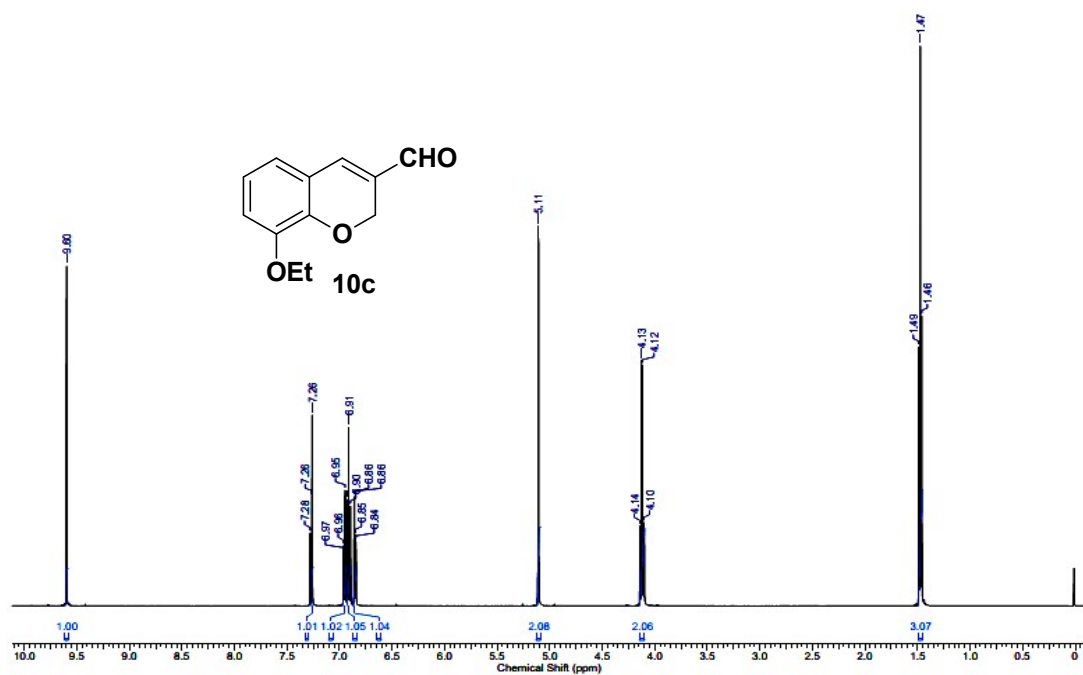
Acquisition Date 8/31/2016 7:39:12 PM

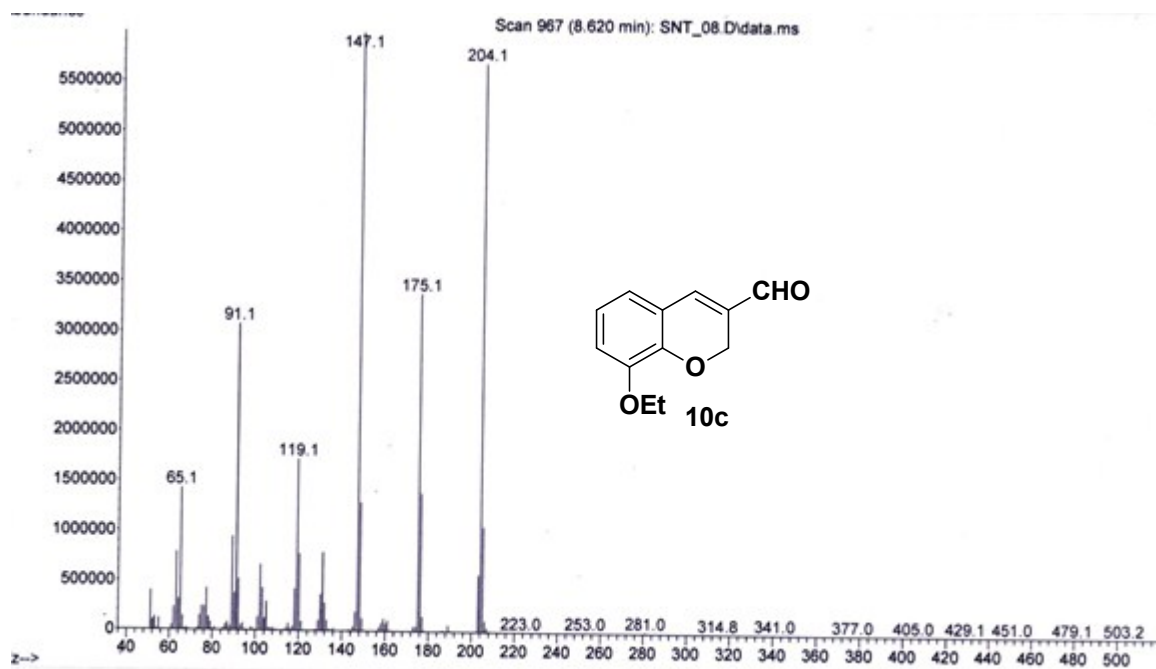
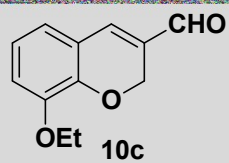
Operator Amit S.Sahu
Instrument microTOF-Q II

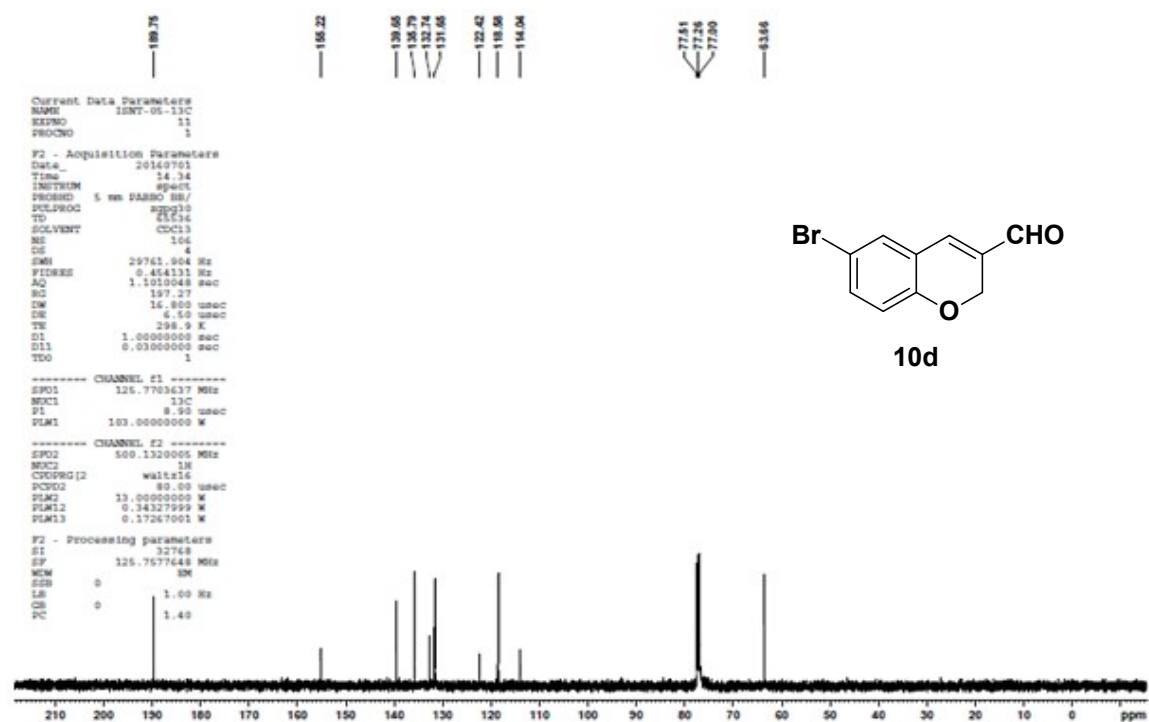
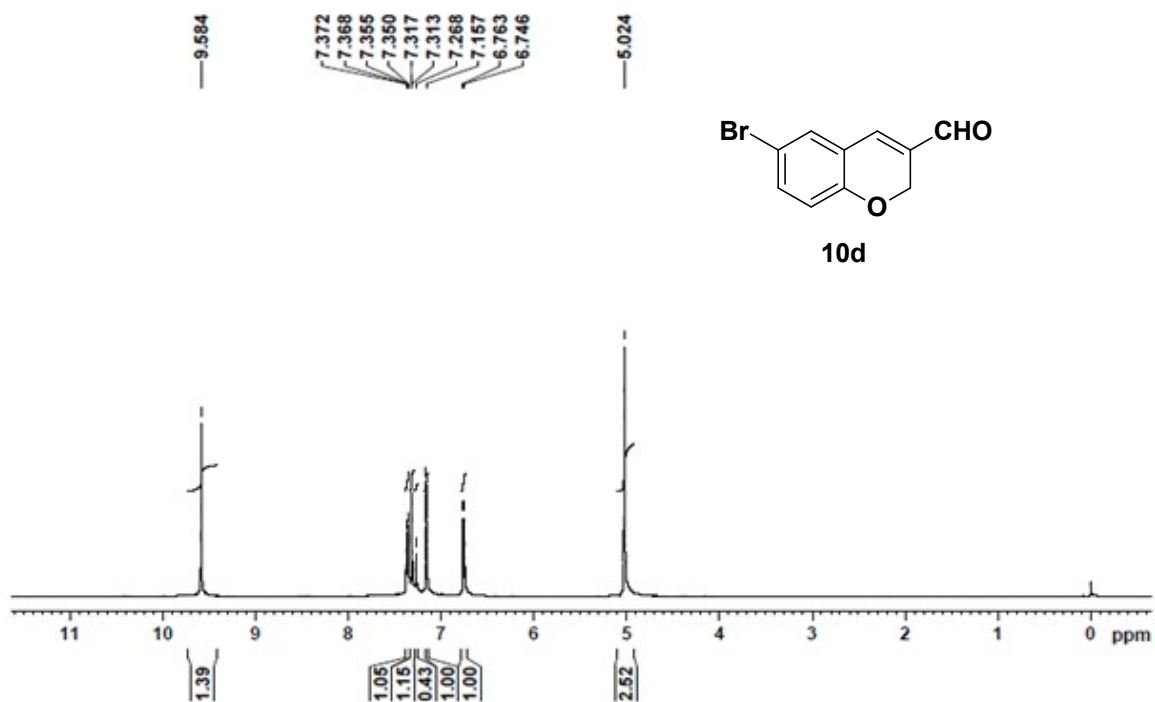


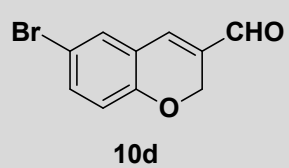












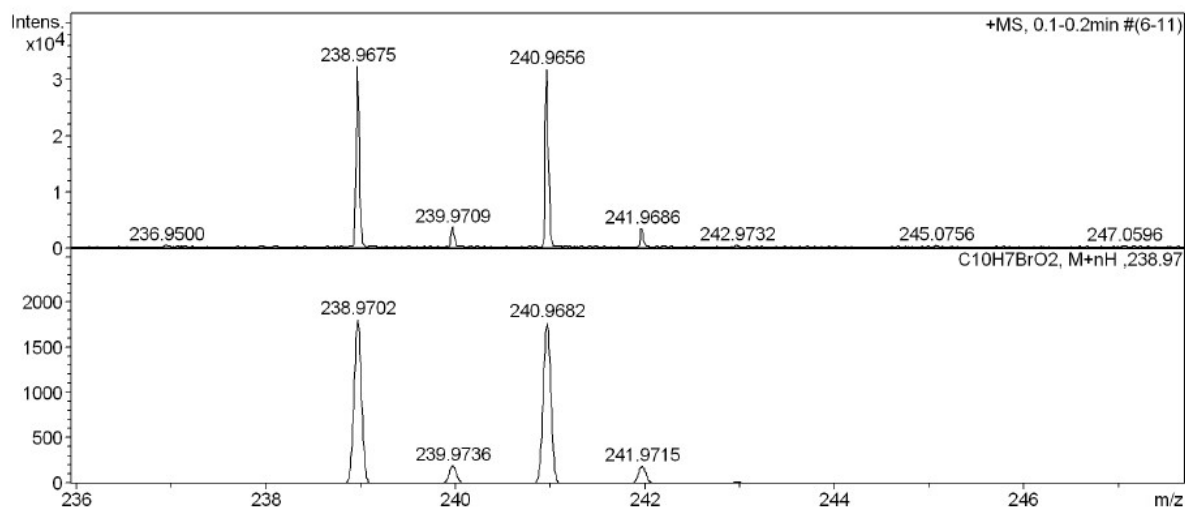
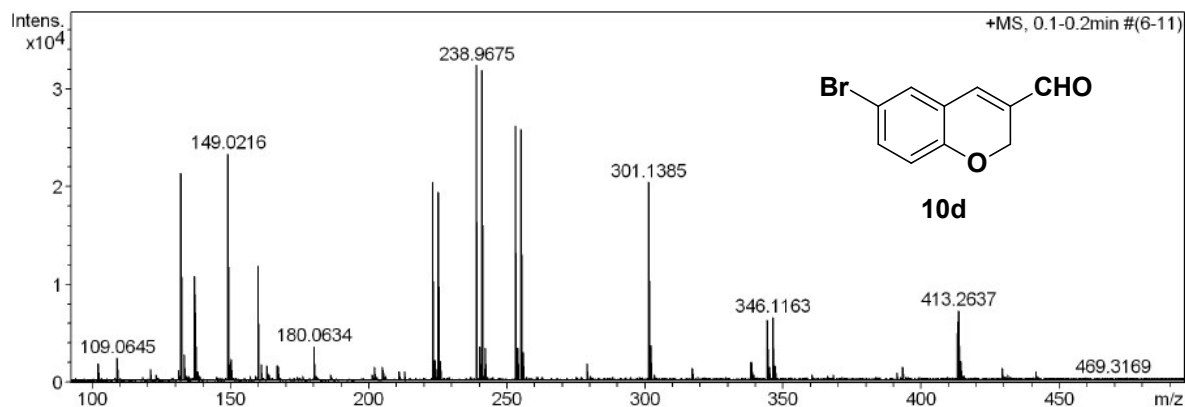
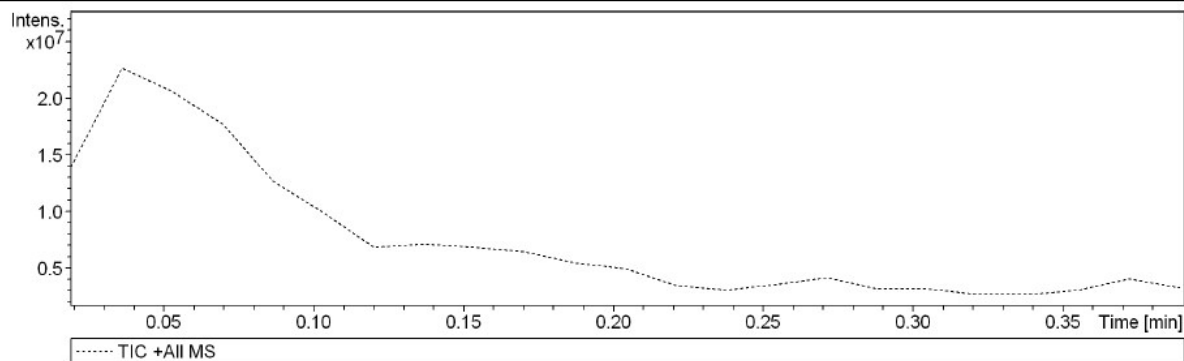
Generic Display Report

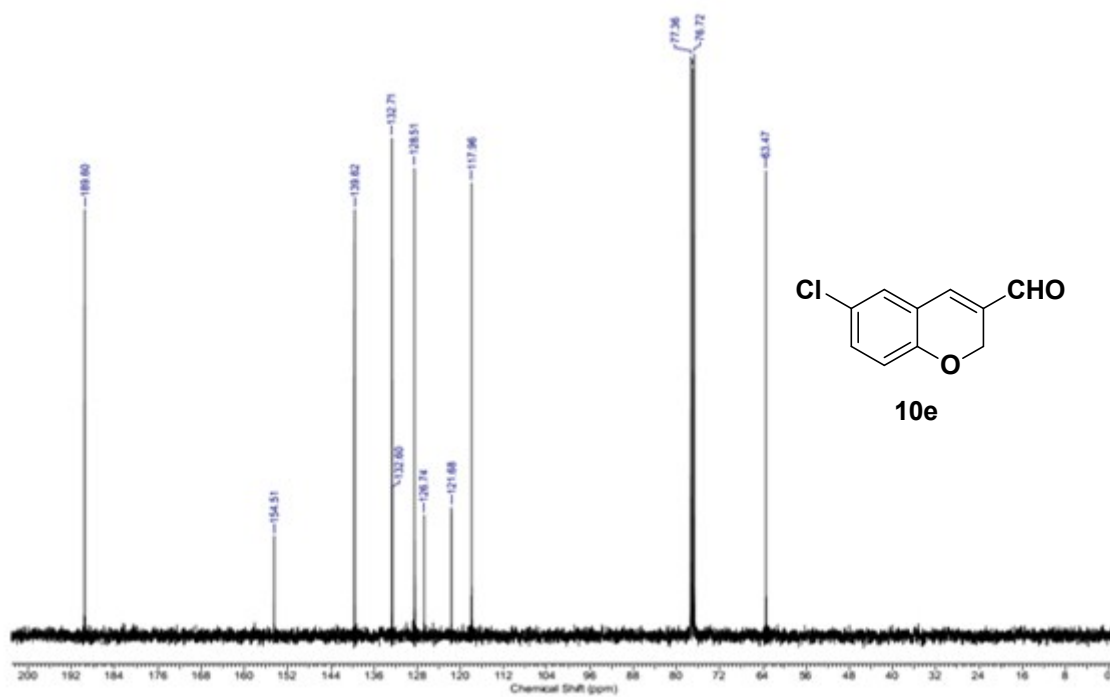
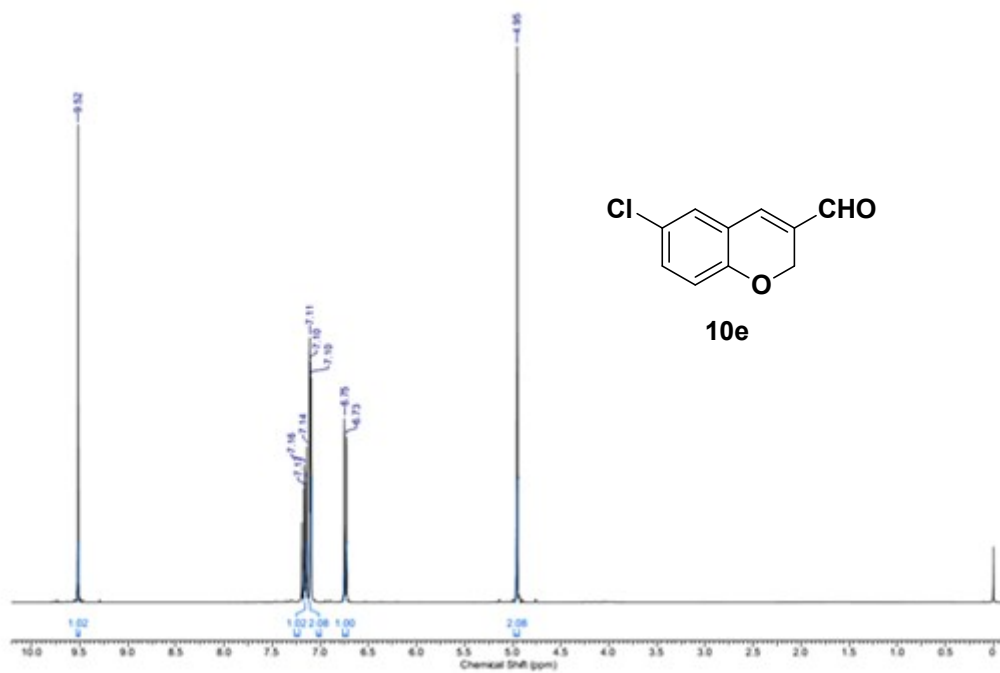
Analysis Info

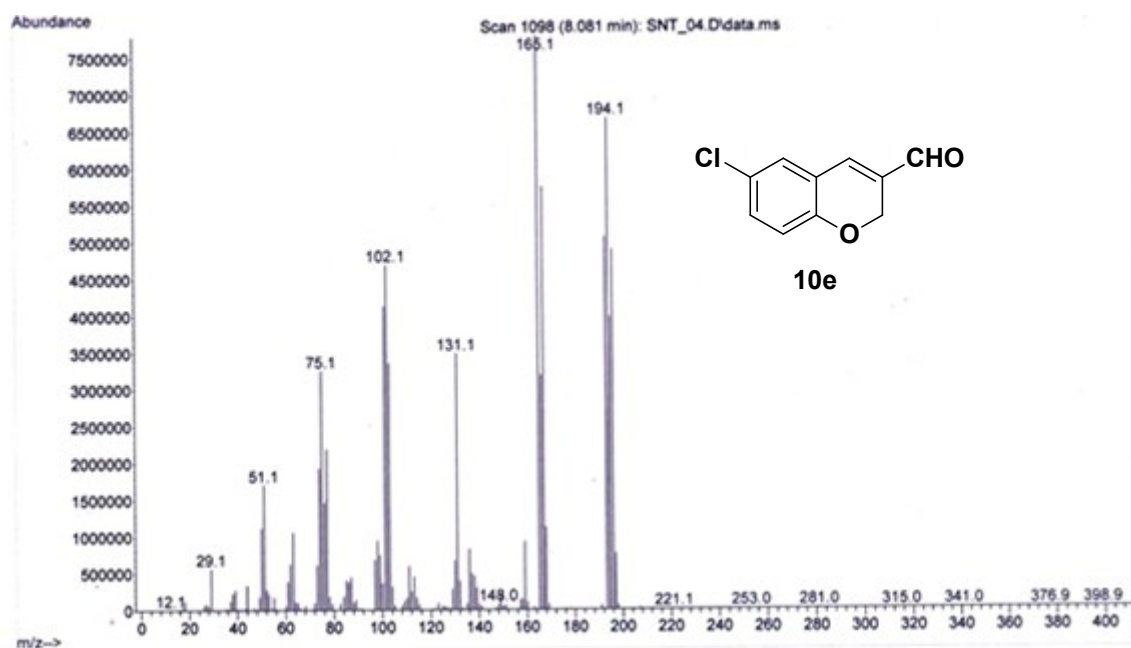
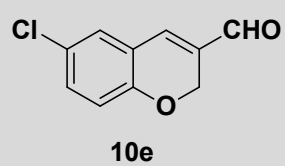
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Method Pos_tune_low.m
Sample Name Bruker micro TOF -Q II
Comment

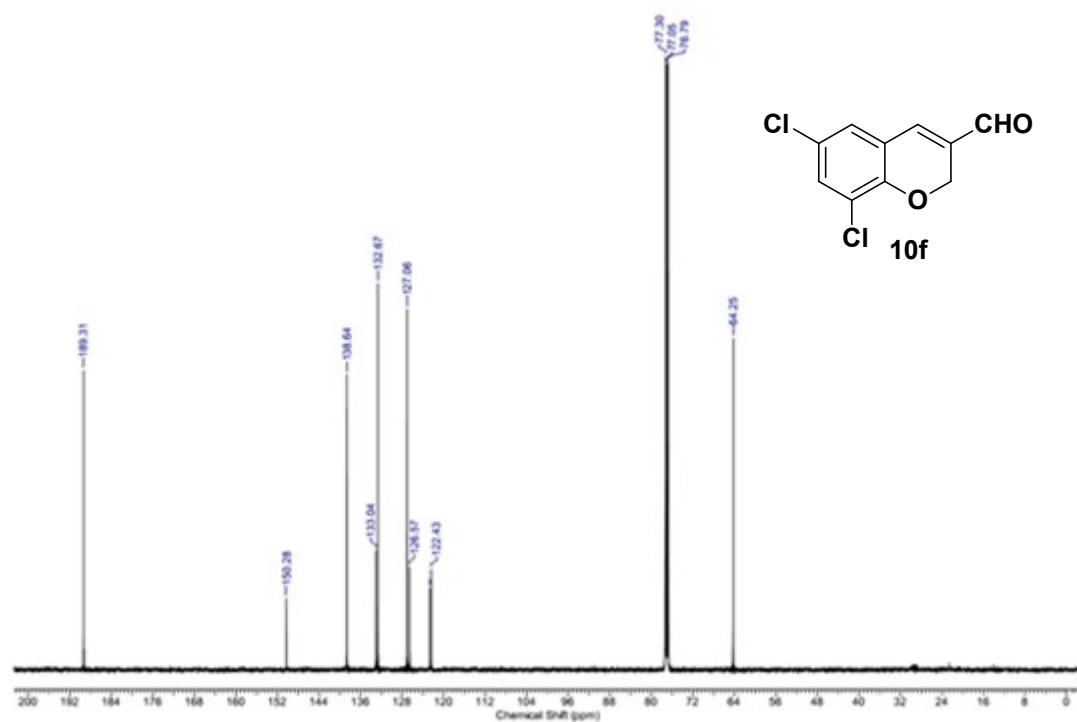
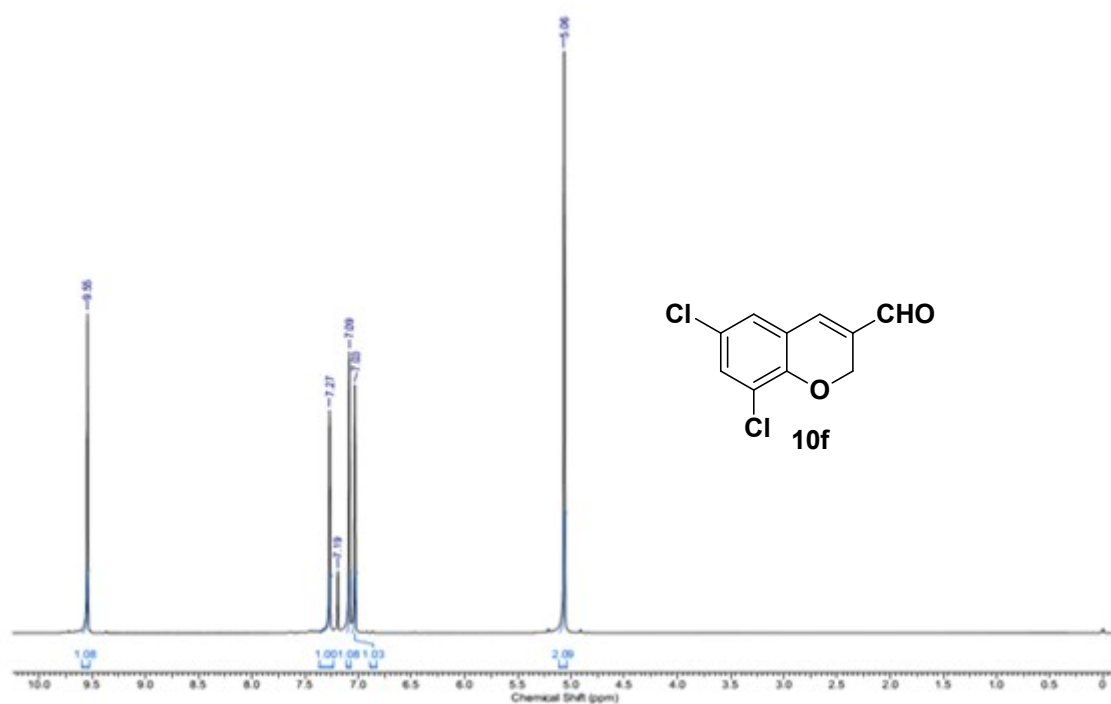
Acquisition Date 8/31/2016 7:01:01 PM

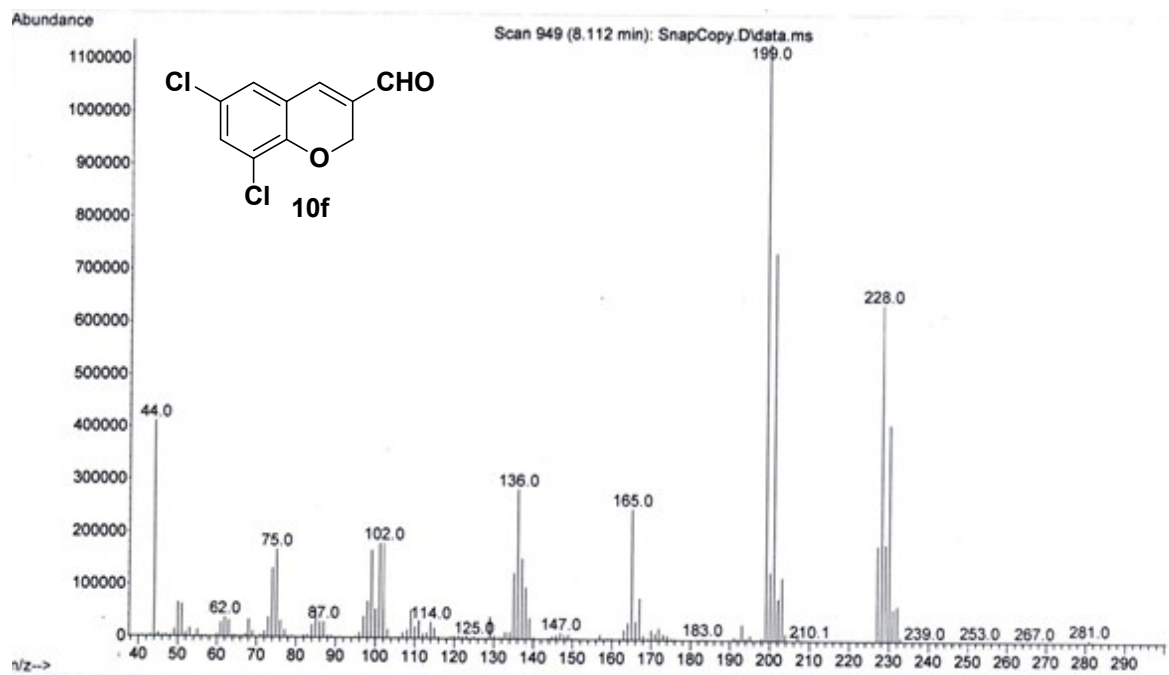
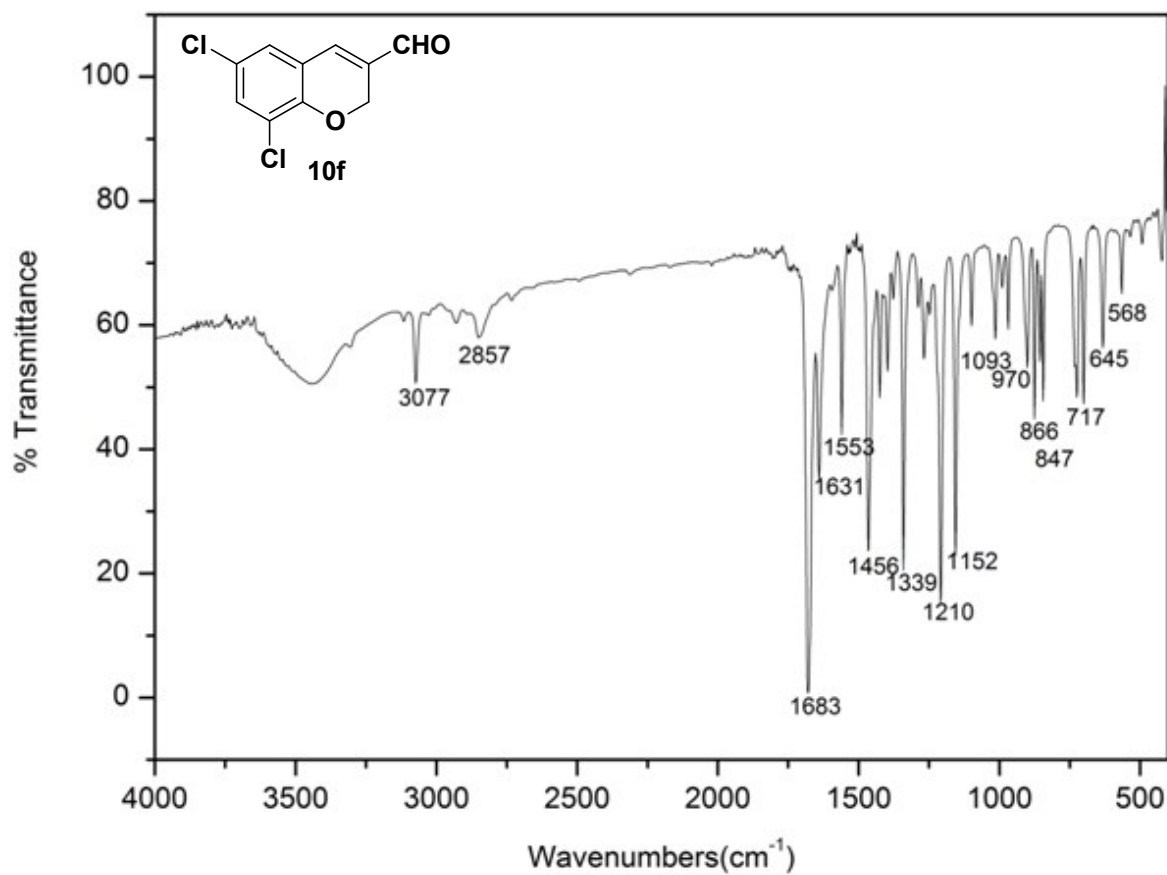
Operator Amit S.Sahu
Instrument microTOF-Q II

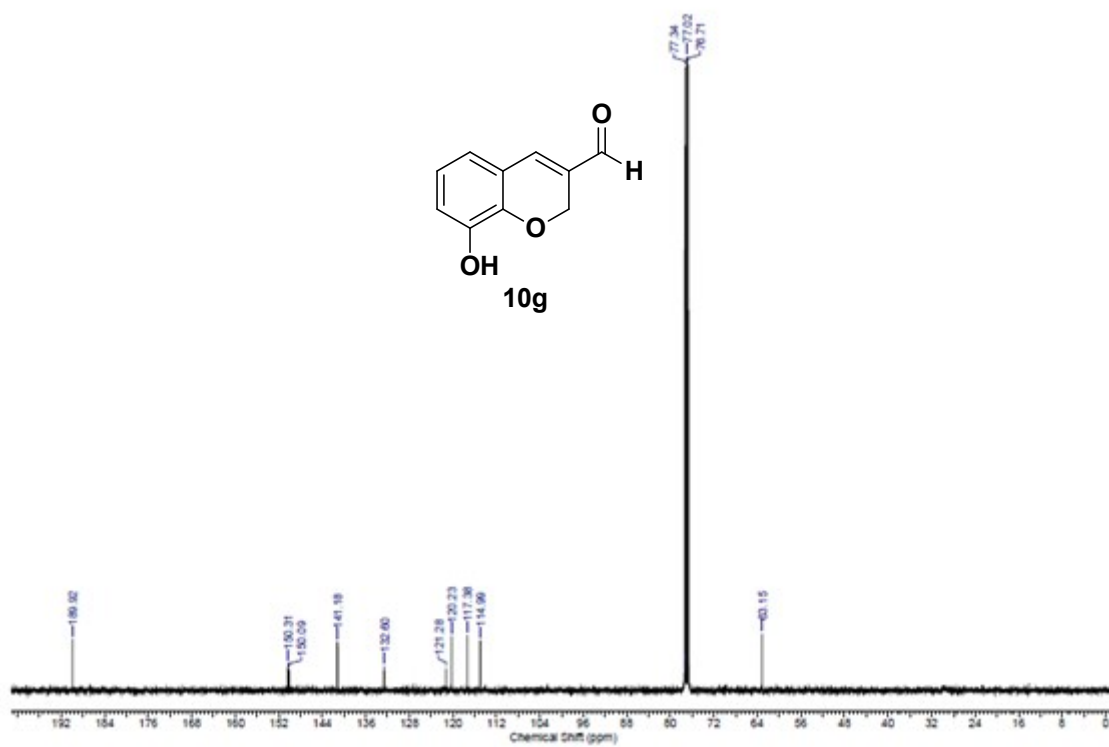
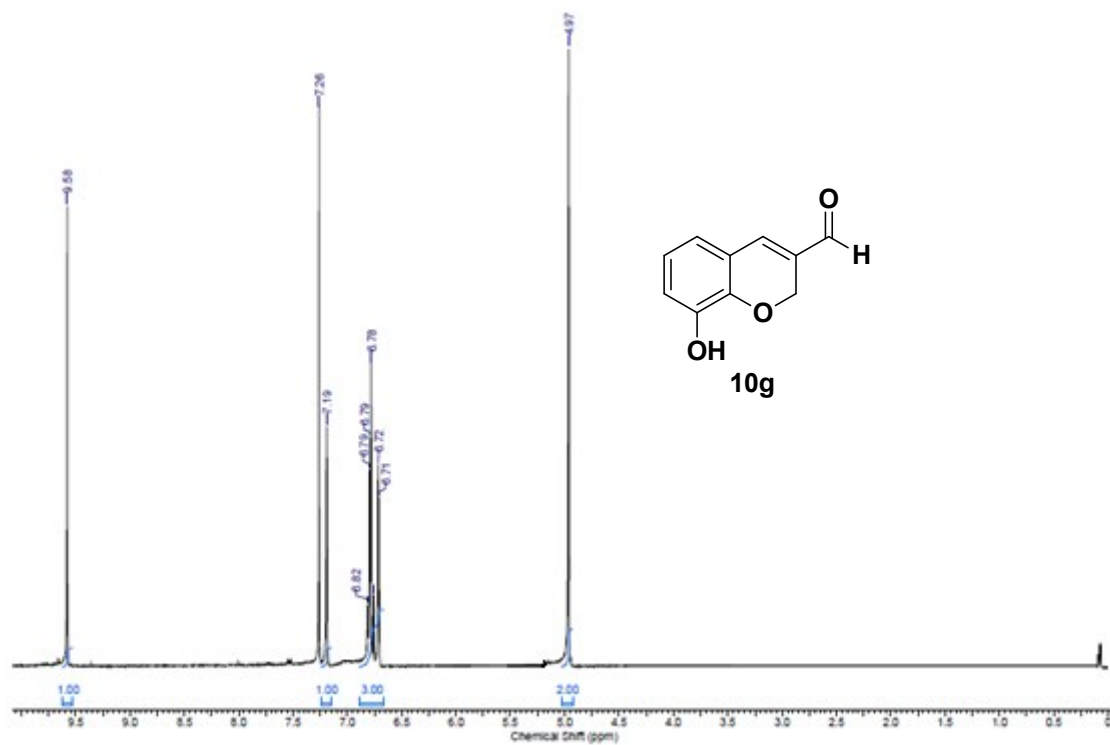


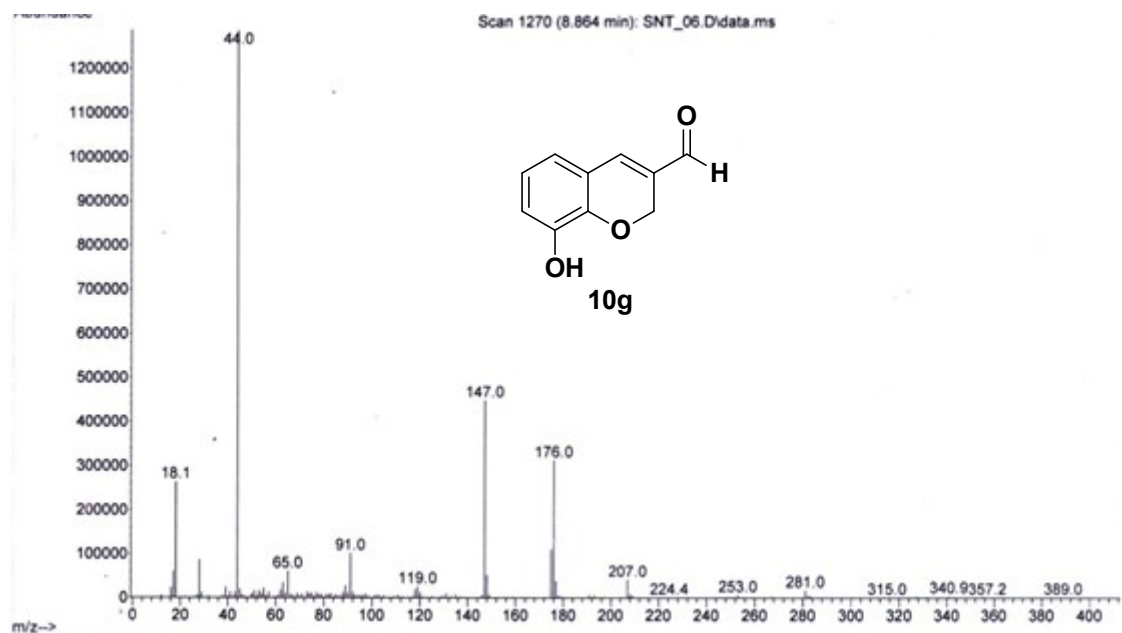
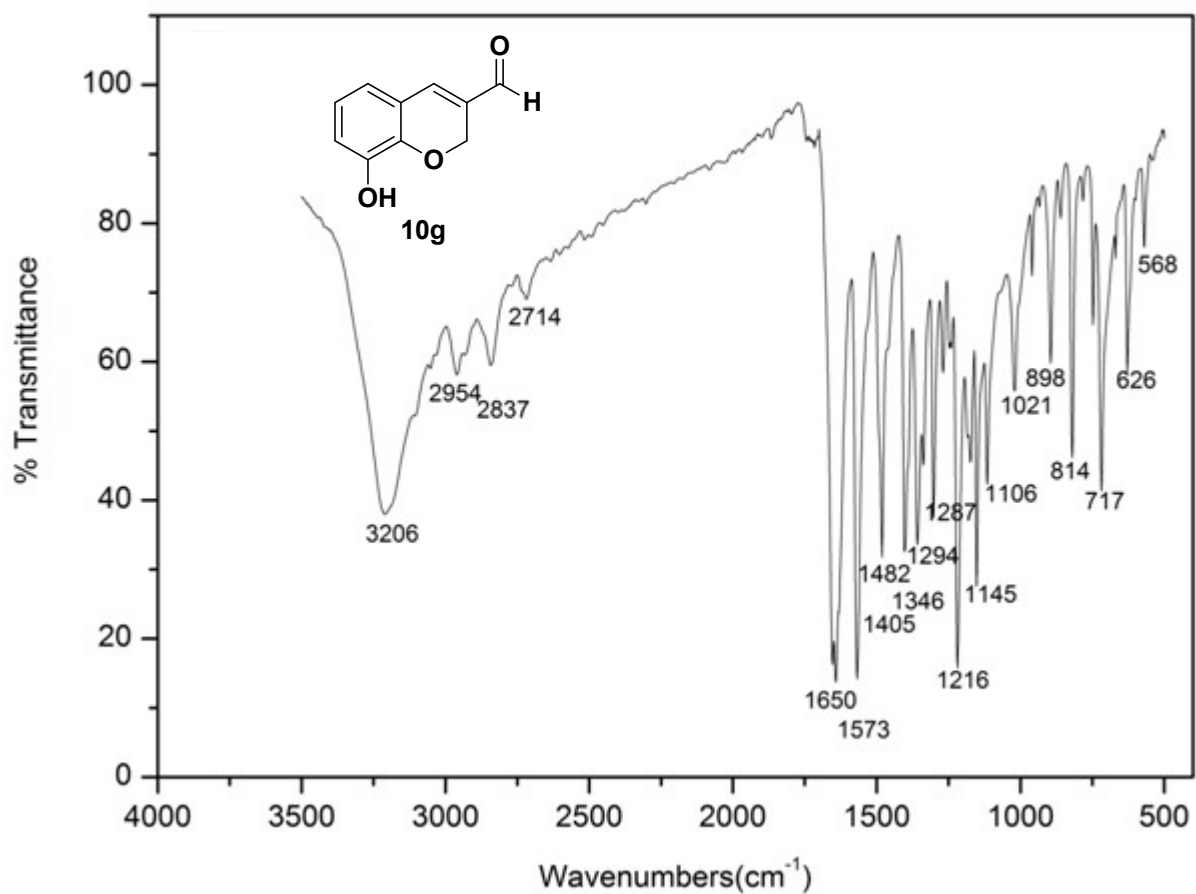




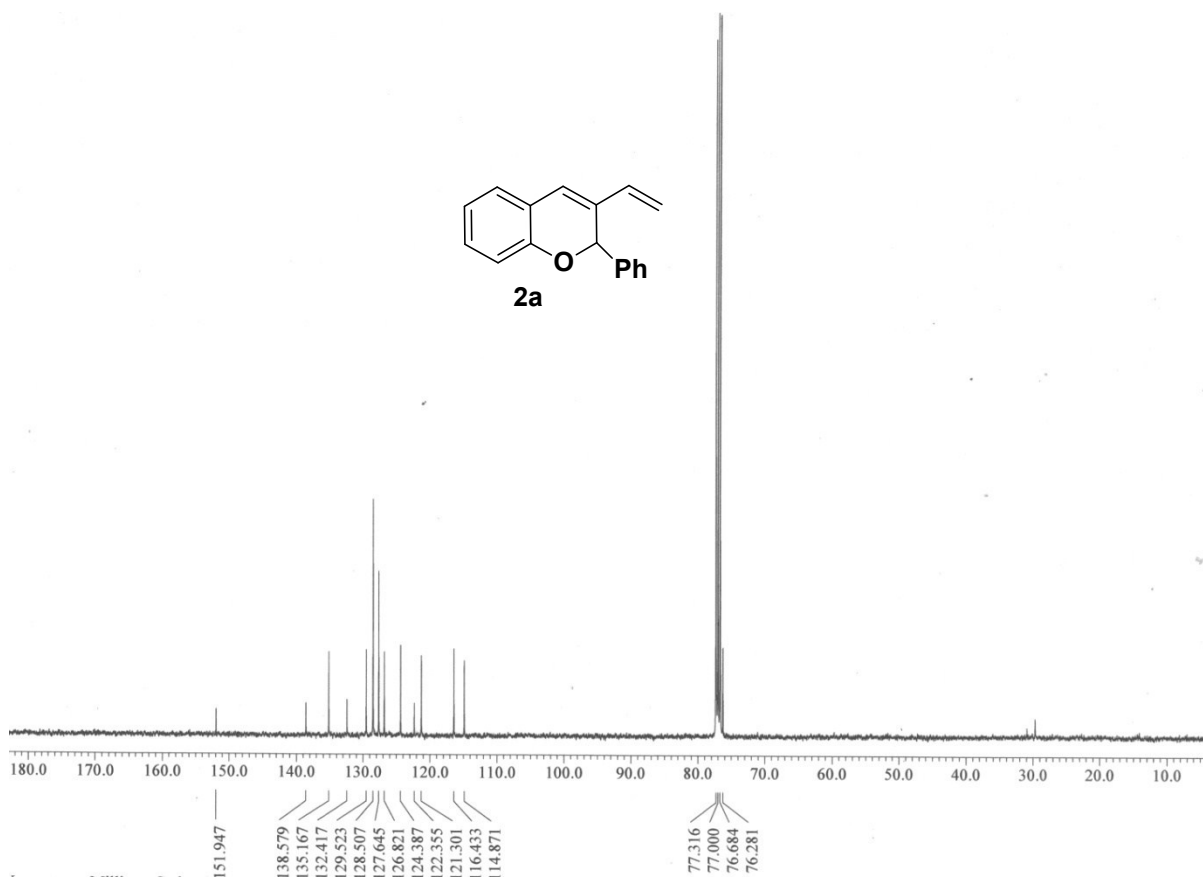
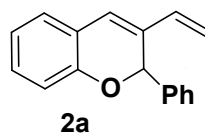
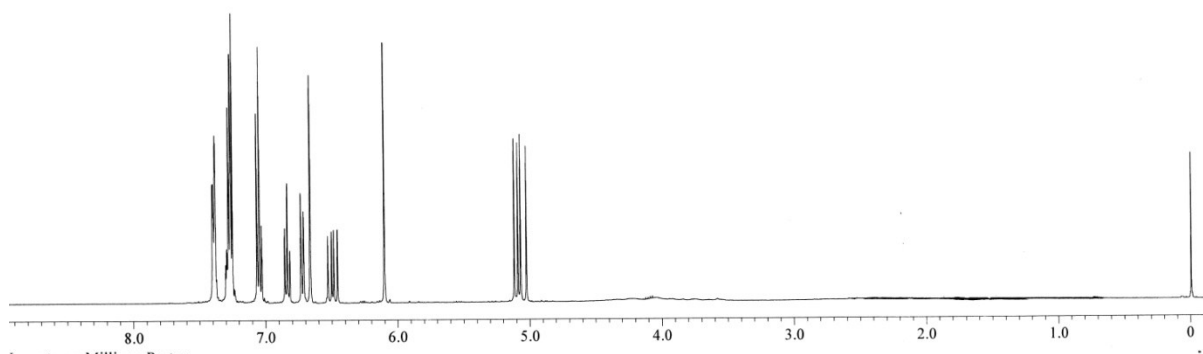
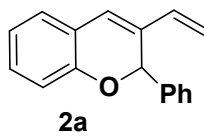


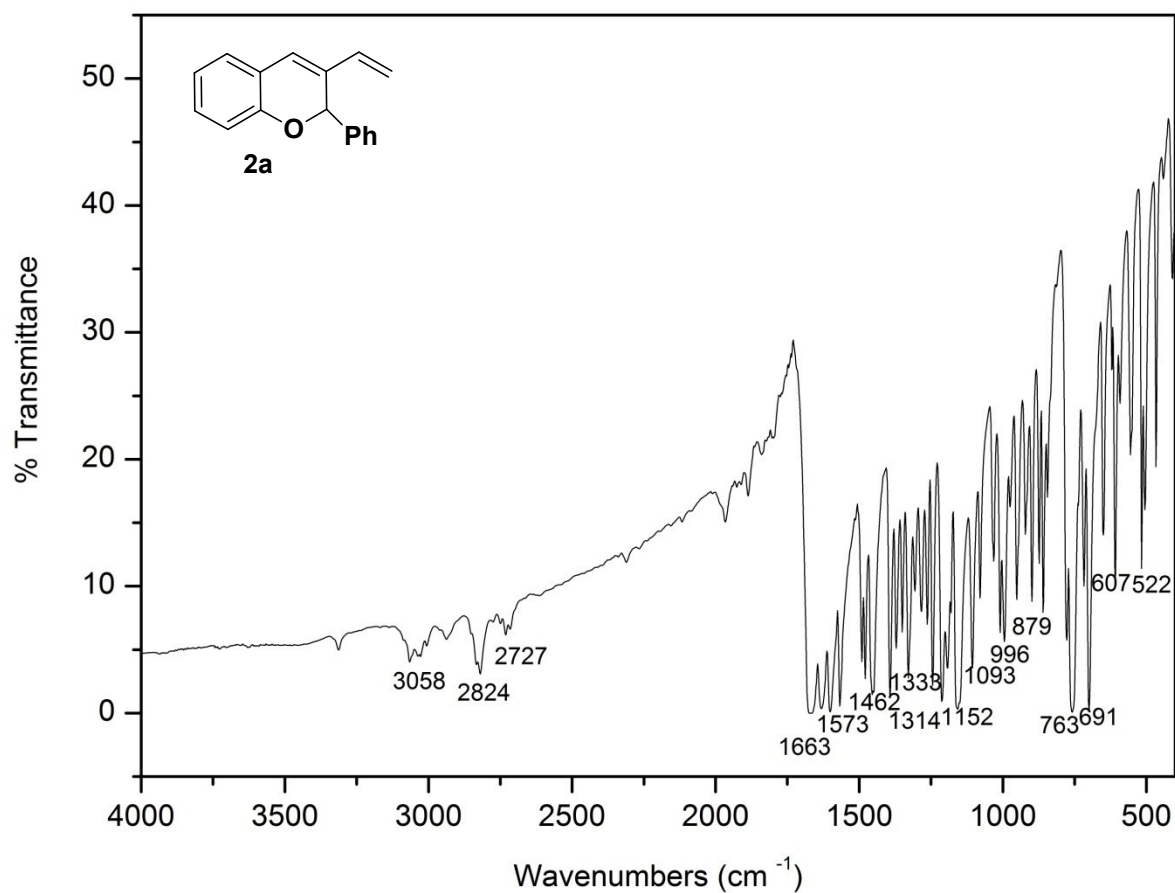






2.04 3.75 2.11 3.05 2.87 0.93 1.00 2.15



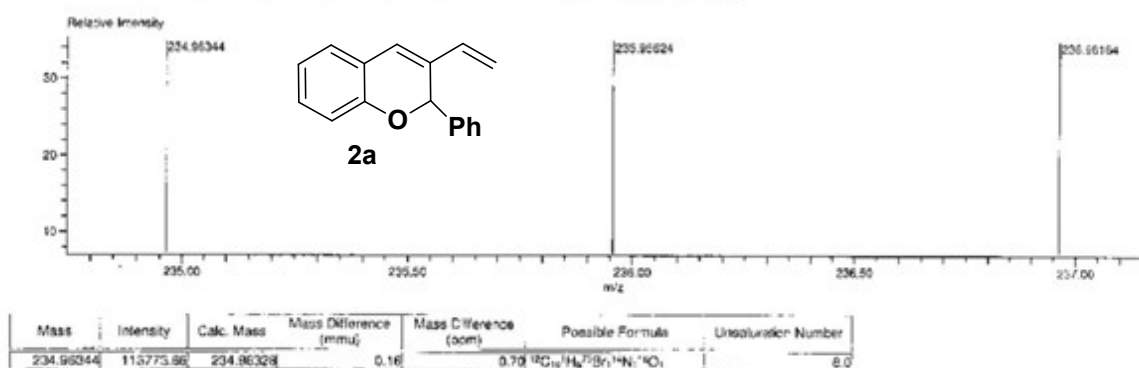


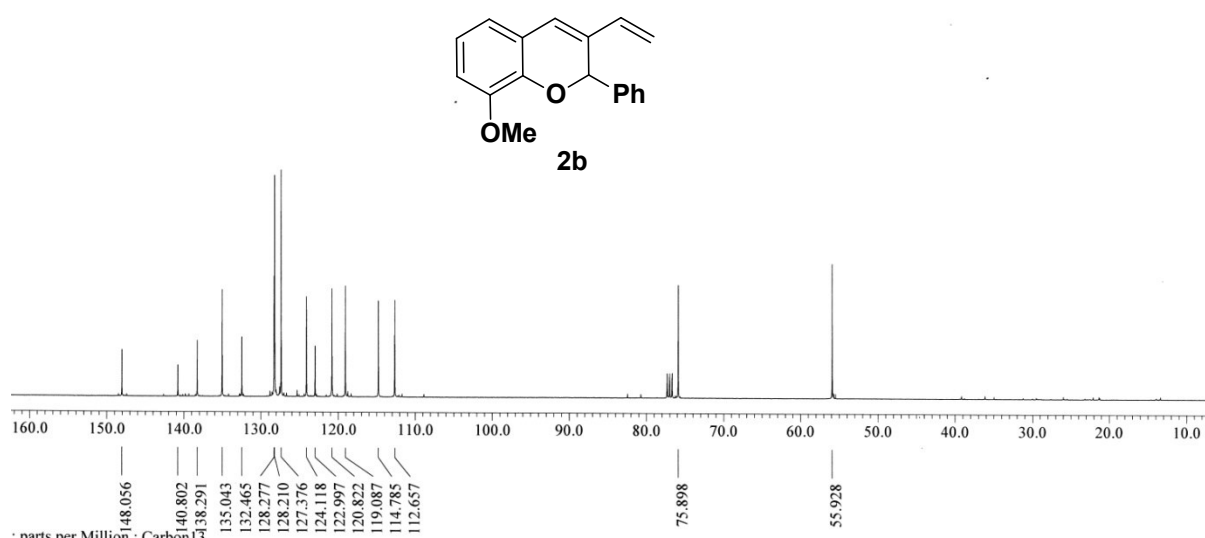
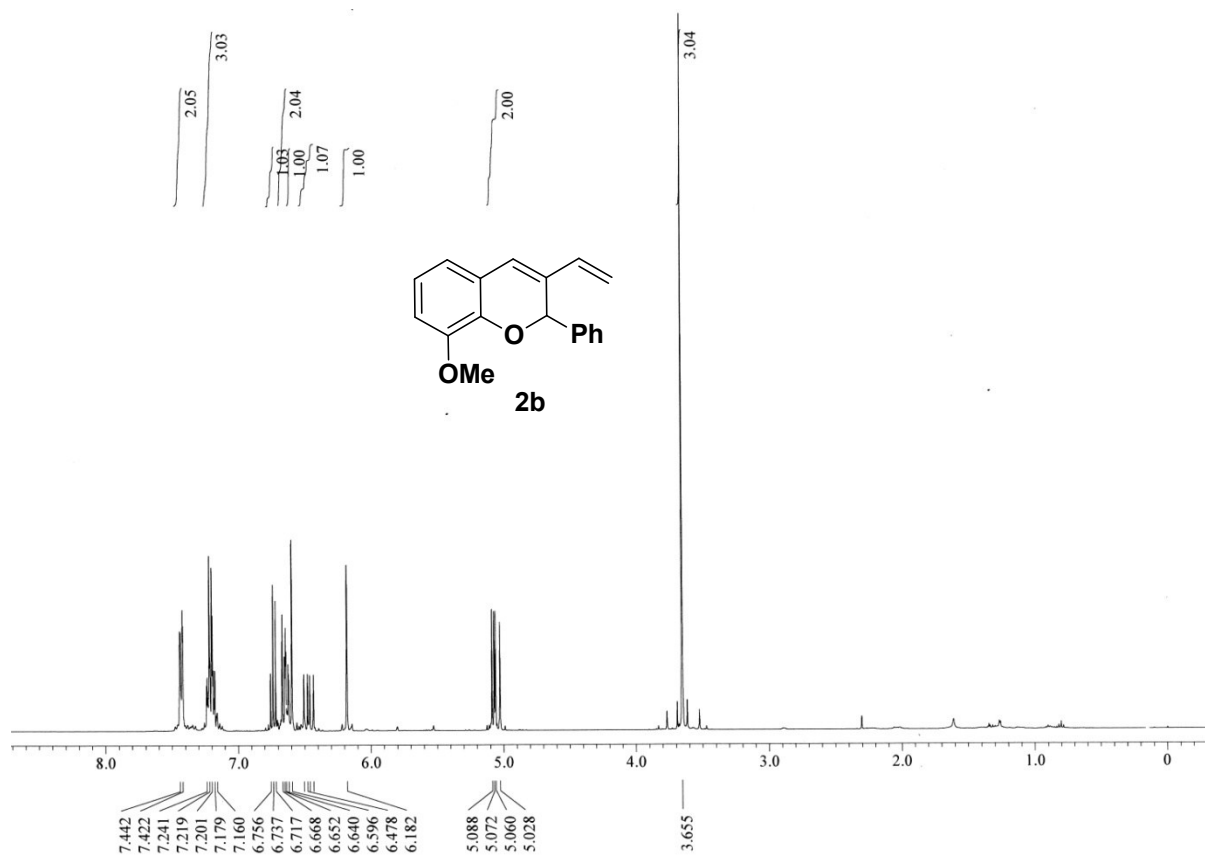
Data: DKM-RZ-1-HR
 Sample Name: DKM-RZ-1-HR, Y BHARATH. EI-HR-MS-DIP-300
 Description:
 Ionization Mode: EI+
 History: Determine m/z [Peak Detect (Centroid, 1 Area), Smooth (5), Correct Base, Smooth (3), Average (MS (1) 0.42, 1.20)]

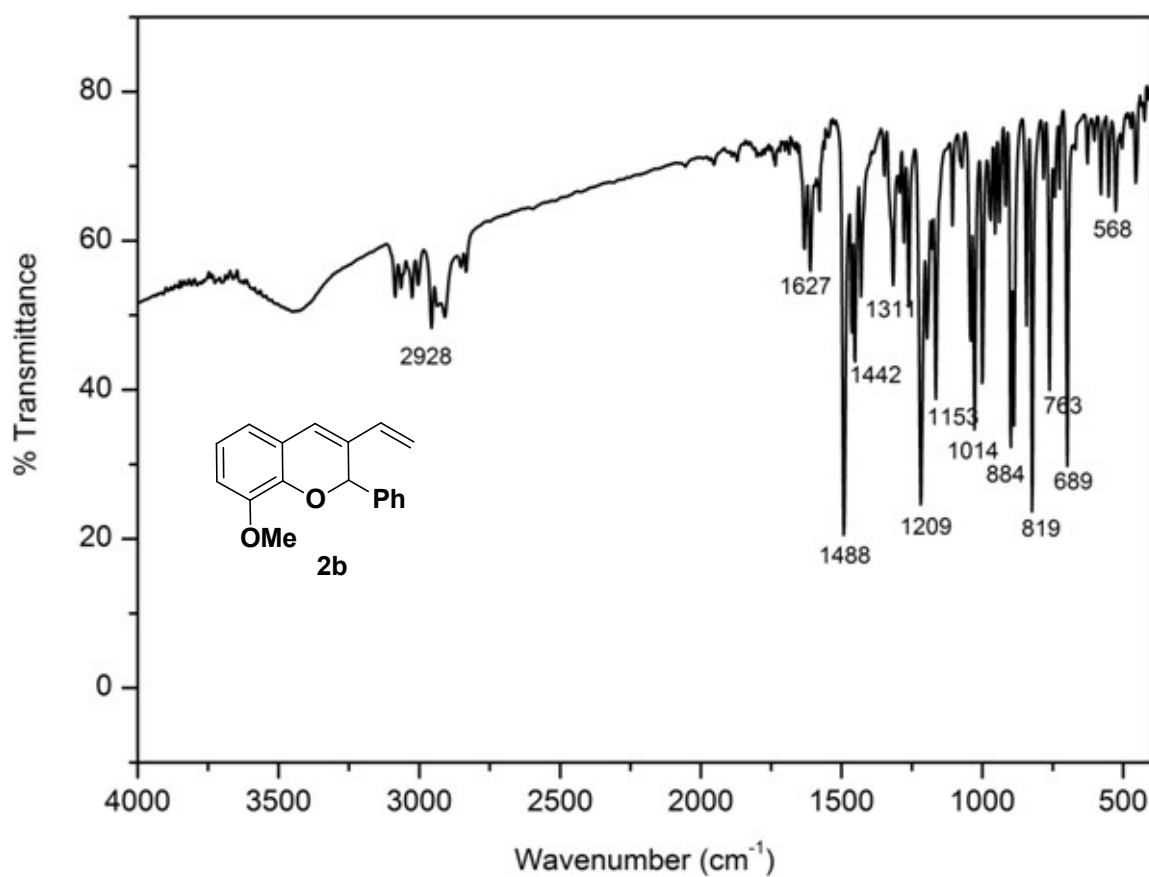
Charge number: 1
 Tolerance: 2000.00 (ppm)
 Elements: ^1H : 0.10, ^1H : 0.06, ^{79}Br : 0.11, ^{81}Br : 0.09, ^{12}C : 0.00, ^{13}C : 0.00, ^{14}N : 0.00, ^{15}N : 0.00, ^{16}O : 0.00, ^{17}O : 0.00, ^{18}O : 0.00, ^{35}Cl : 0.00, ^{37}Cl : 0.00

Acquired: 25-08-2014 11:34:22
 Operator: JEOL
 Mass Calibration date: EI/POSCAL7112012
 Created: 25-08-2014 11:39:20
 Created by: JEOL

Unsaturation Number: 1.5 .. 59.6 (Fraction Both)





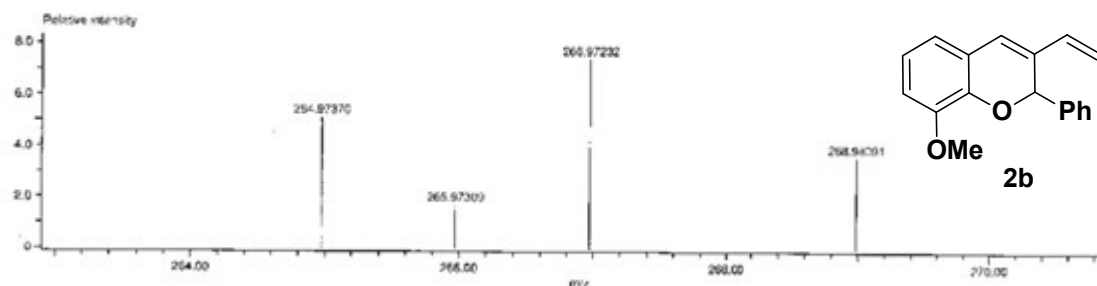


Data: DKM-NB-03-HR
 Sample Name: DKM-NB-03-HR, Y. BHARATHI [E]-HR-MS-DIP-300
 Description:
 Ionization Mode: ESI-
 History: Determine m/z [Peak Detect (Centroid, 1 Area), Smooth (3), Convex: Base (3), Smooth (3), Average (MS (1) 0.72, 0.98)]

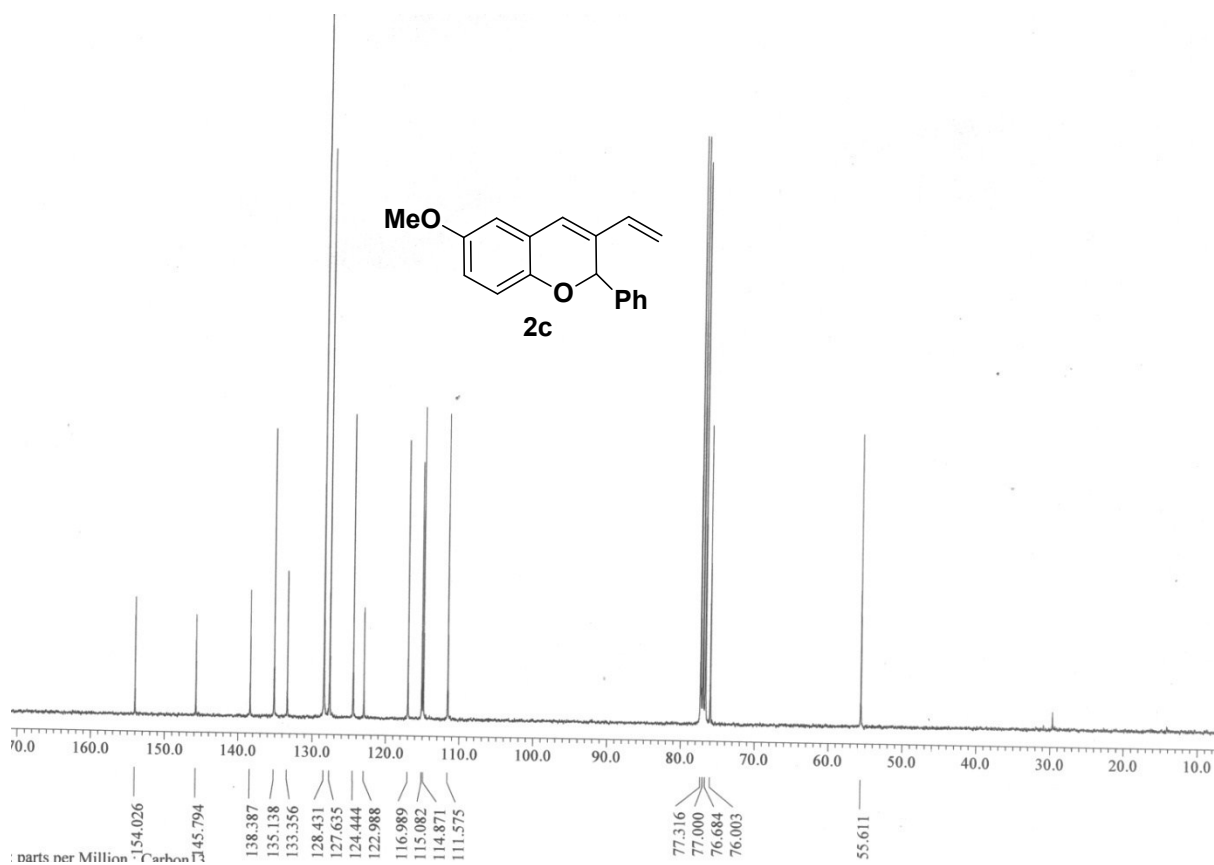
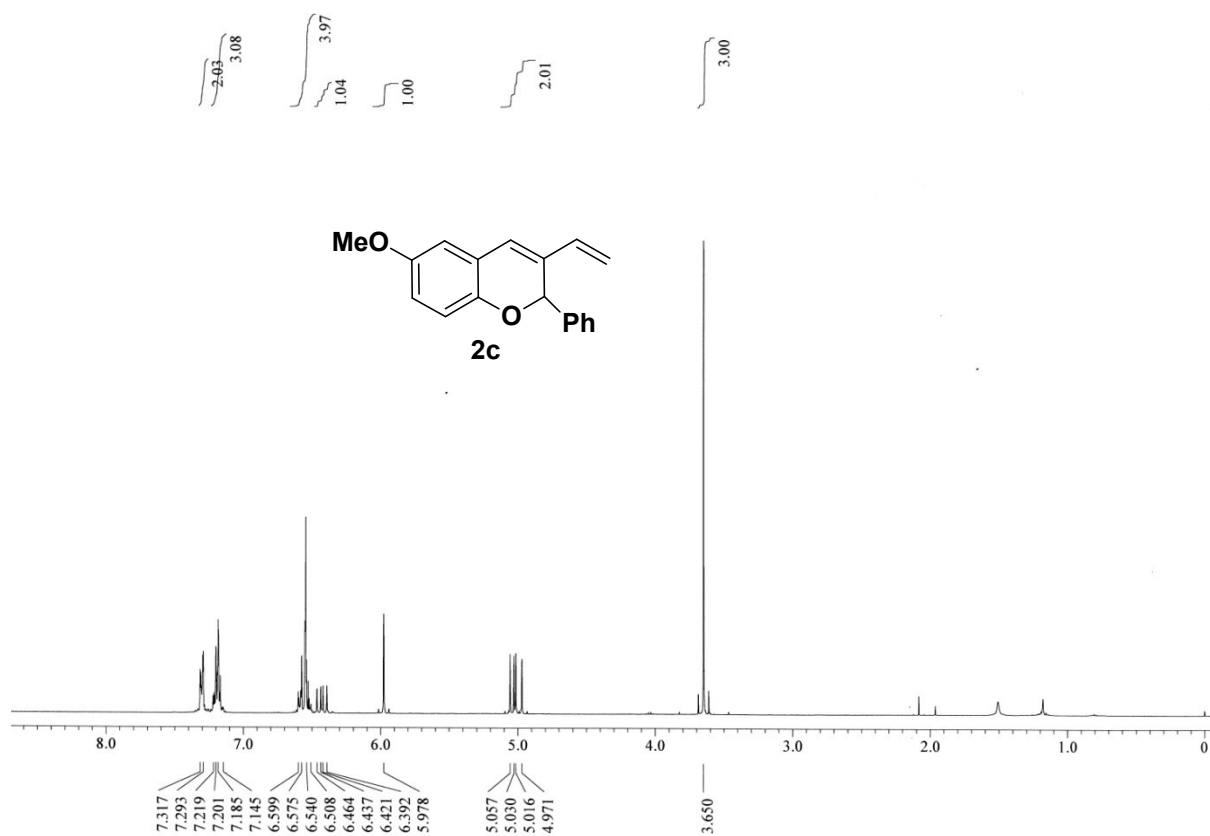
Acquired: 26-06-2014 14:30:06
 Operator: JIEOL
 Mass Calibration data: EIPDS/CAL711/2012
 Created: 26-06-2014 14:35:25
 Created by: JIEOL

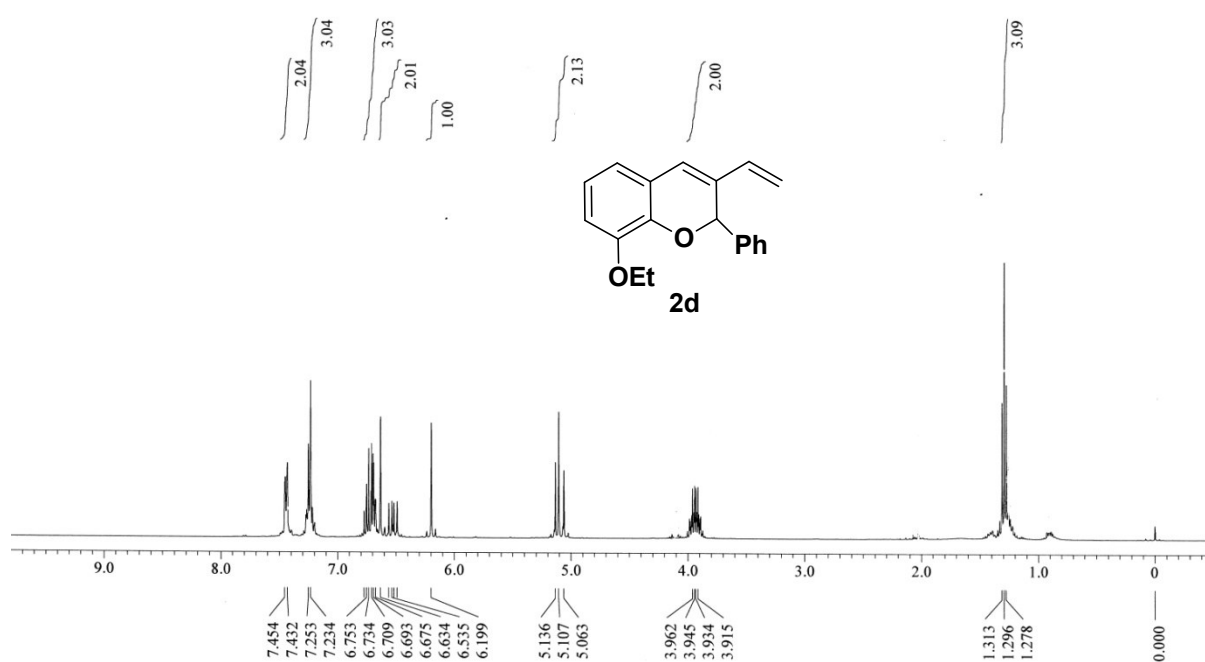
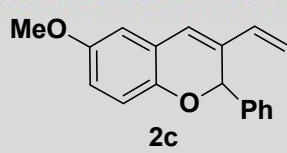
Charge number: 1
 Tolerance: 2000.00 (ppm)
 Element: ¹²C: 11, ¹H: 0, ⁸Br: 0, ¹F: 0, ¹⁹F: 0, ¹⁶O: 0, ¹⁸O: 0, ¹⁴N: 0, ¹⁵N: 0, ¹³C: 0, ²S: 0, ³¹P: 0, ³³S: 0

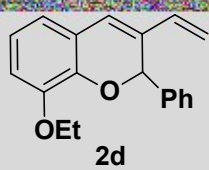
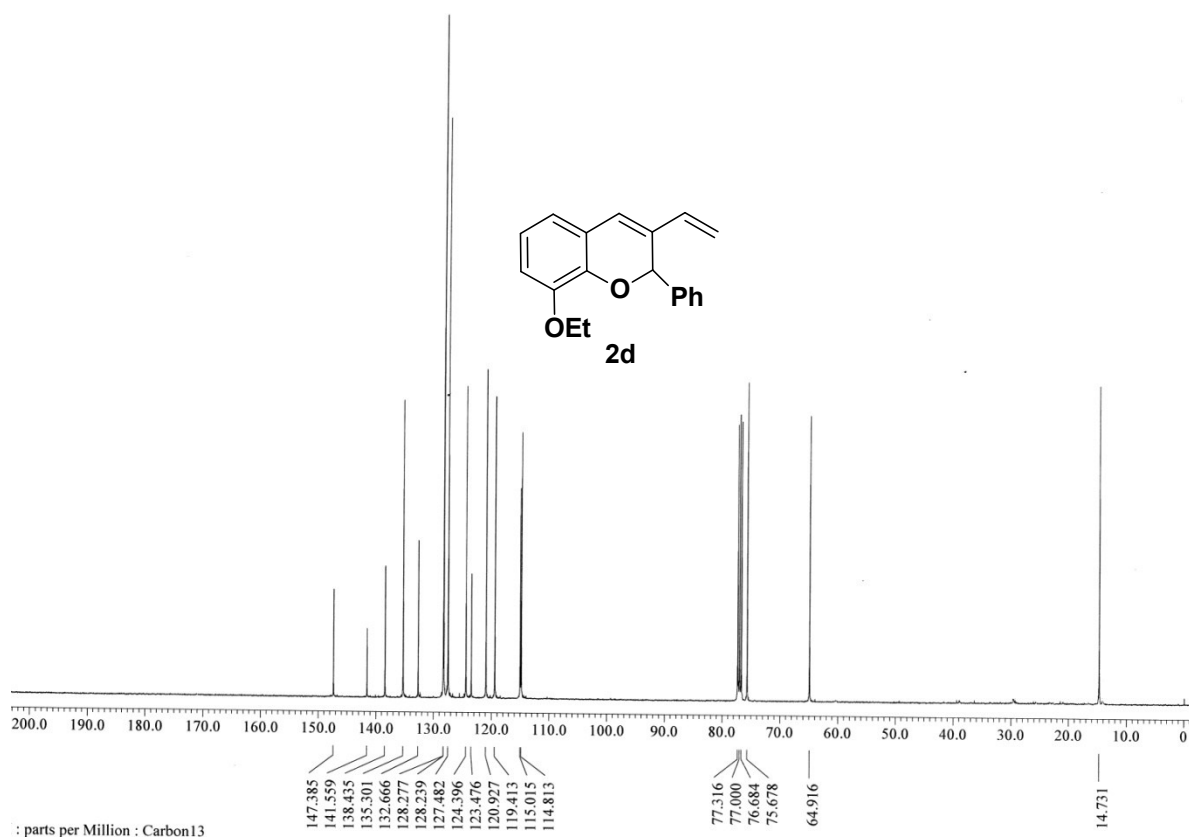
Unsaturation Number: 1.5 .. 60.0 (Fraction Both)

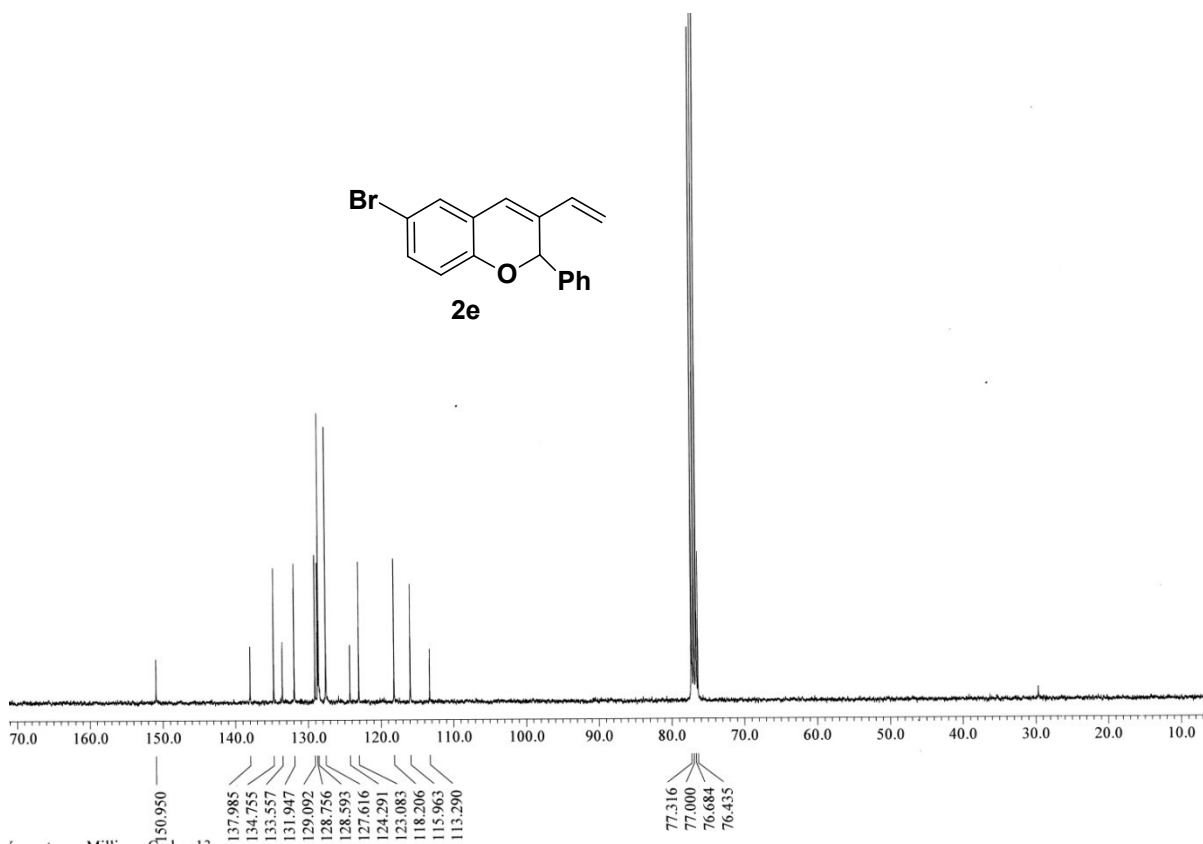
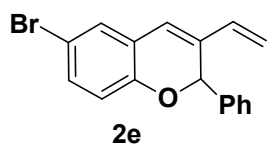
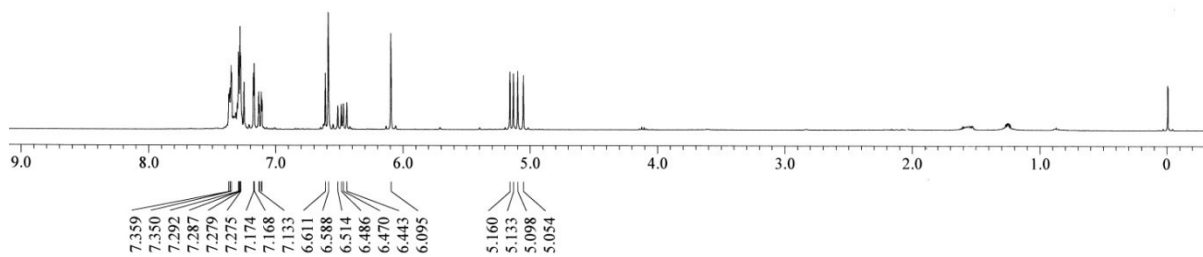
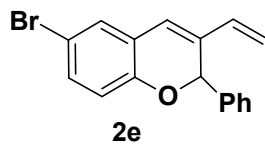
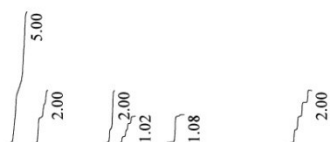


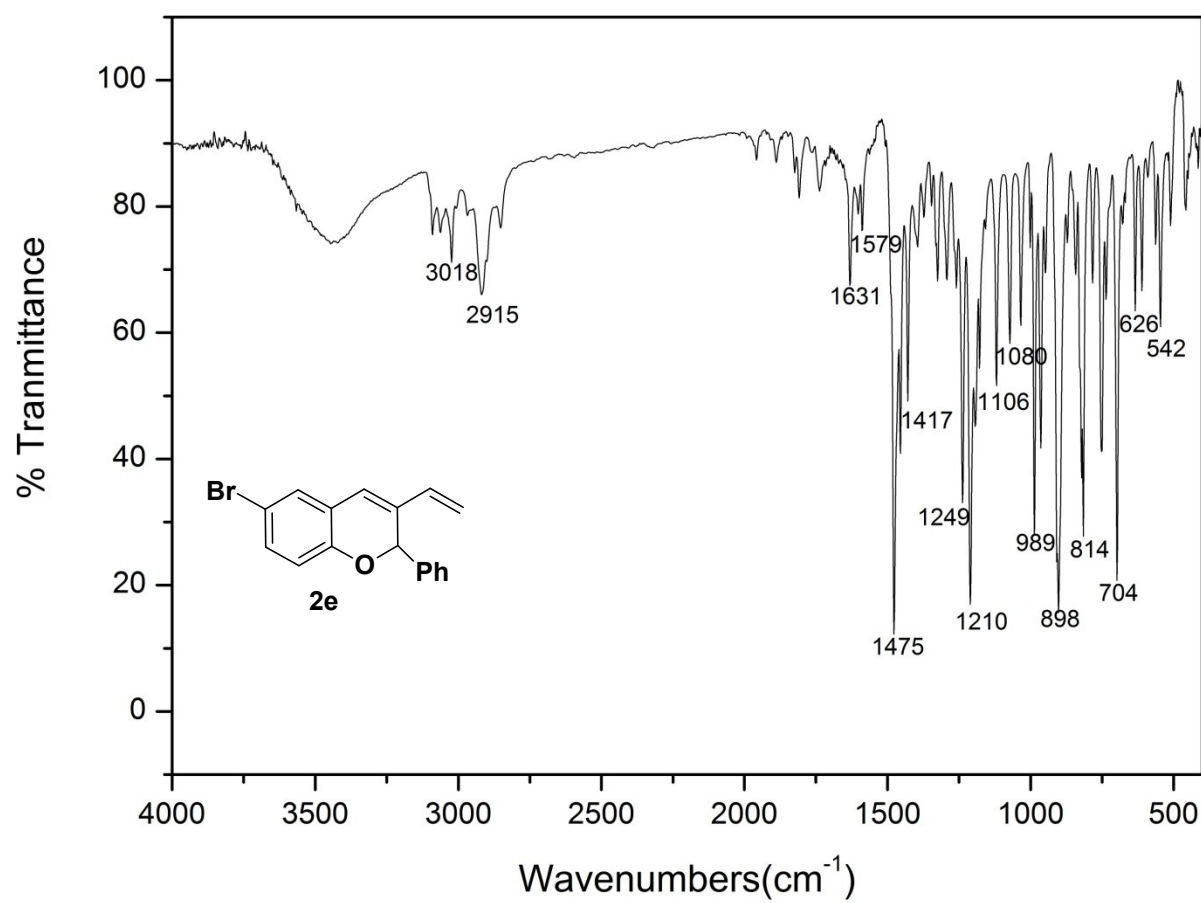
Mass	Intensity	Calc. Mass	Mass Difference (m/z)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
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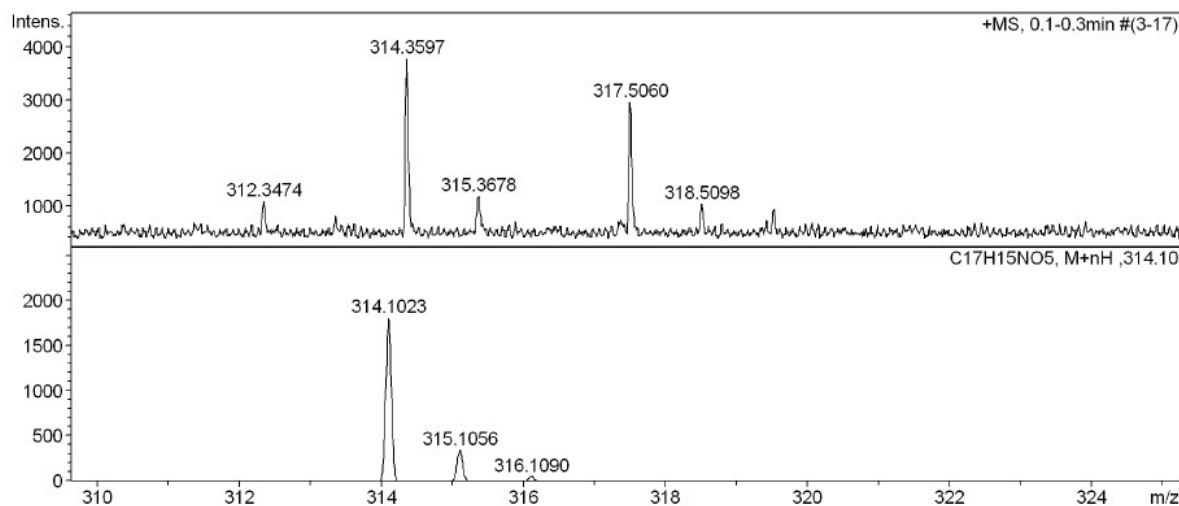
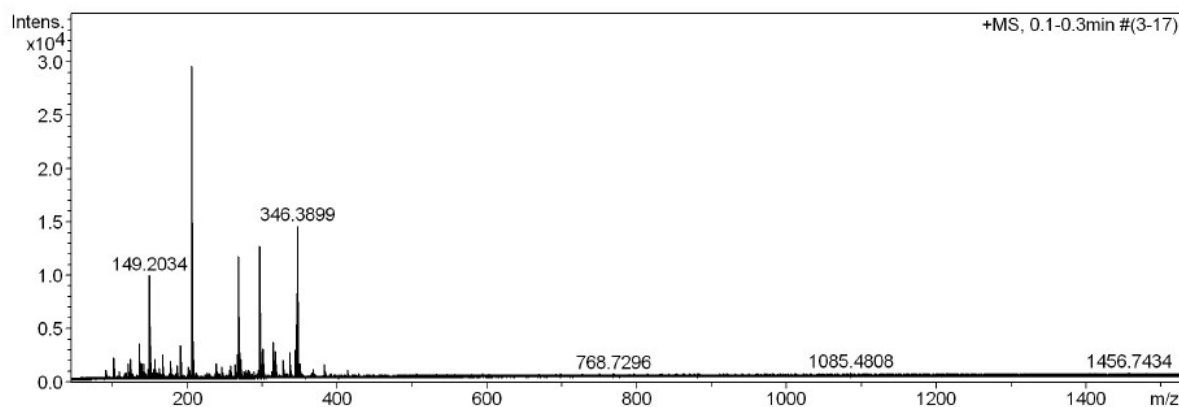
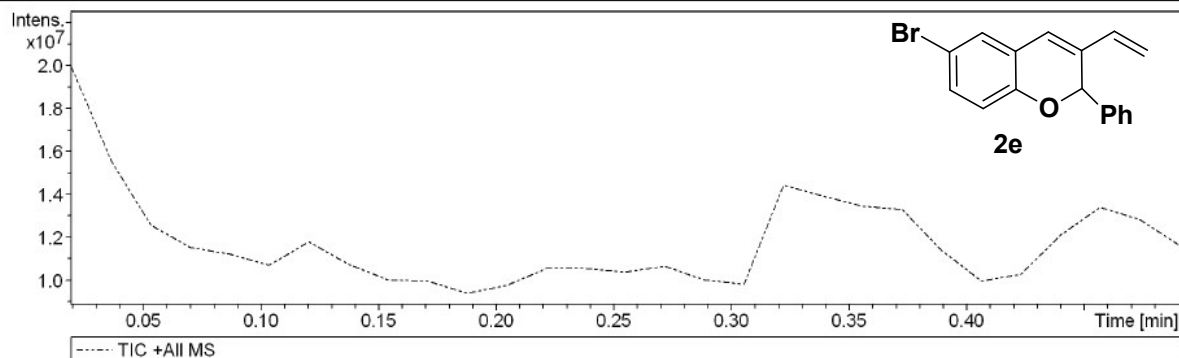
Generic Display Report

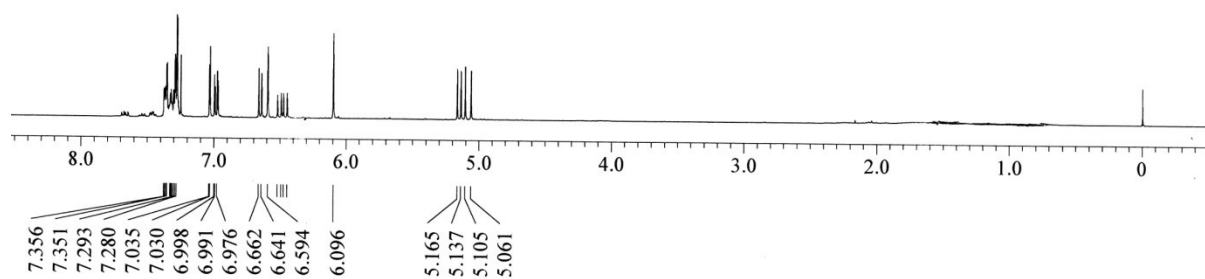
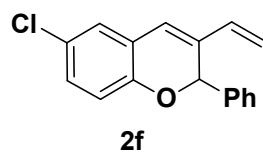
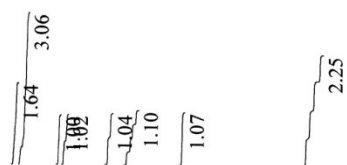
Analysis Info

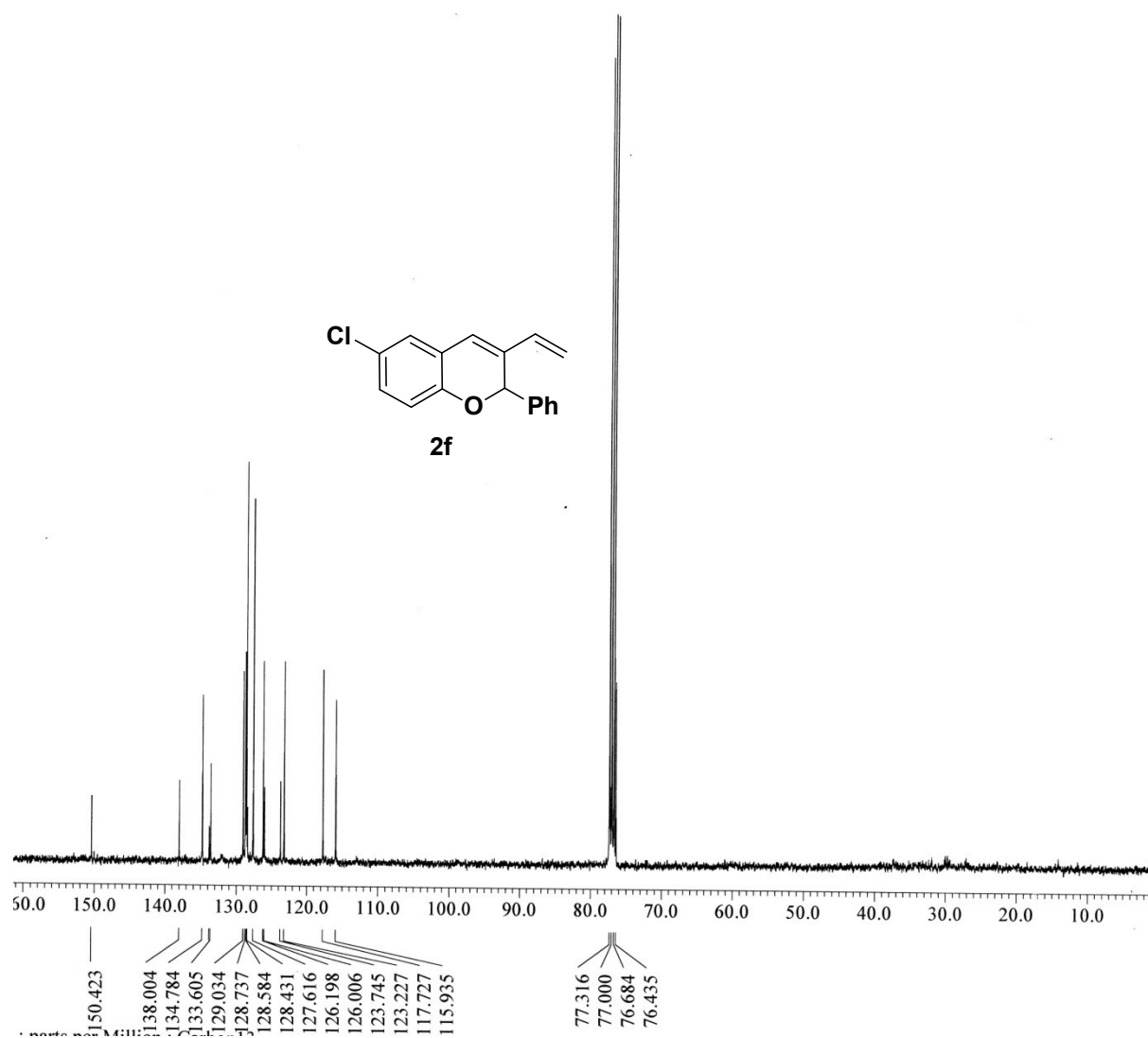
Analysis Name D:\Data\AUG-2016\CSP\31082016_CSP_SDP_S_17.d
Method Pos_tune_low.m
Sample Name Bruker micro TOF -Q II
Comment

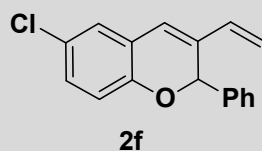
Acquisition Date 8/31/2016 2:44:51 PM

Operator Amit S.Sahu
Instrument micrOTOF-Q II









Data:DKM-SIJ-A16

Sample Name:DKM-SIJ-A16, Y BHARATH, EI-HR-MS

Description:

Ionization Mode:EI+

History:Date:mine m/z[Peak Detect[Centroid,1 Area],Smooth[6]],Correct Base[1],Smooth[3],Average[MS[1] 0.35,0.51]

Acquired:23-07-2014 14:01:48

Operator:J.EOL

Mass Calibration data:EIPOSICAL7112012

Created:23-07-2014 14:12:28

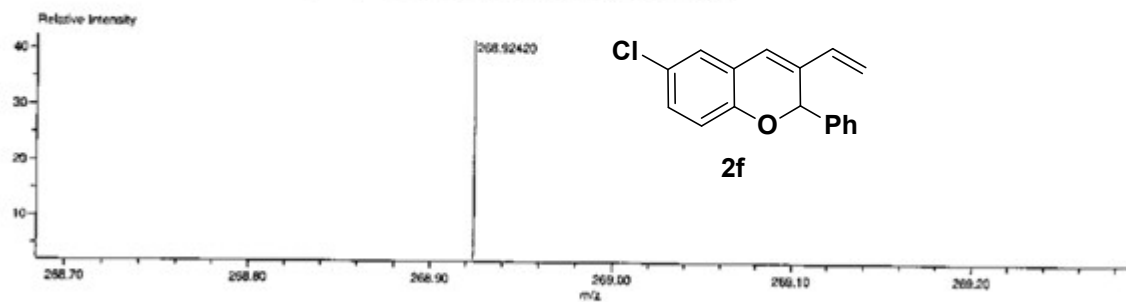
Created by:J.EOL

Charge number:1

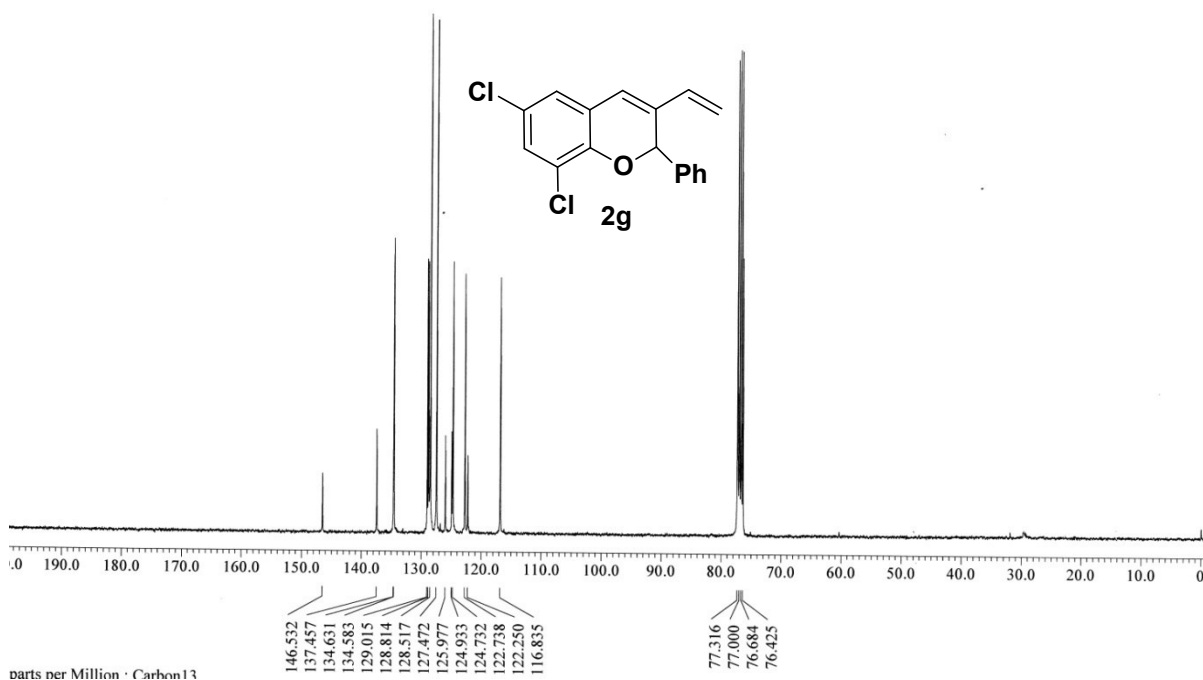
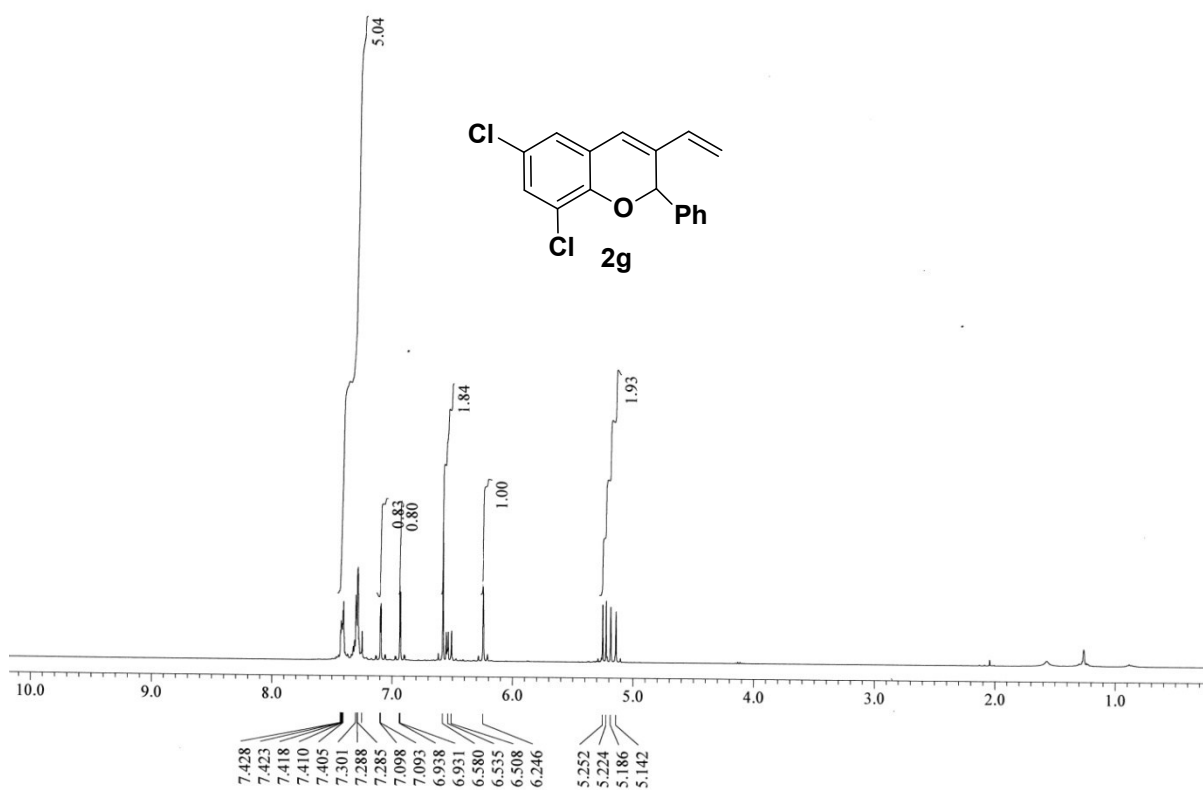
Tolerance:5.00(ppm)

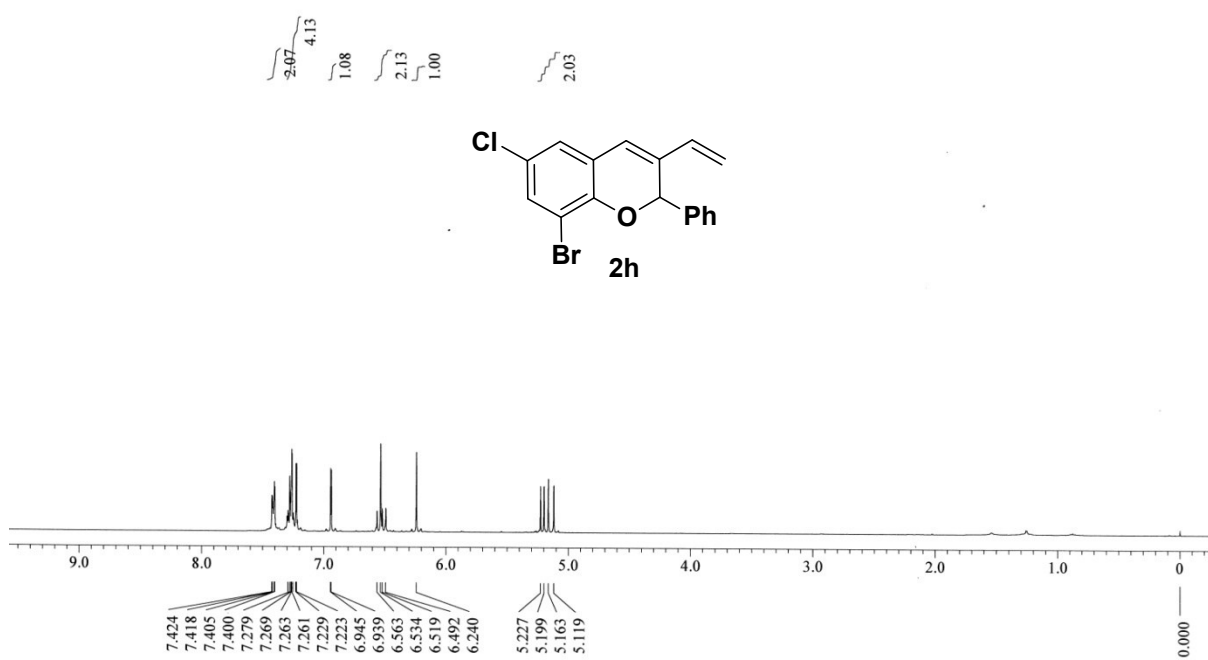
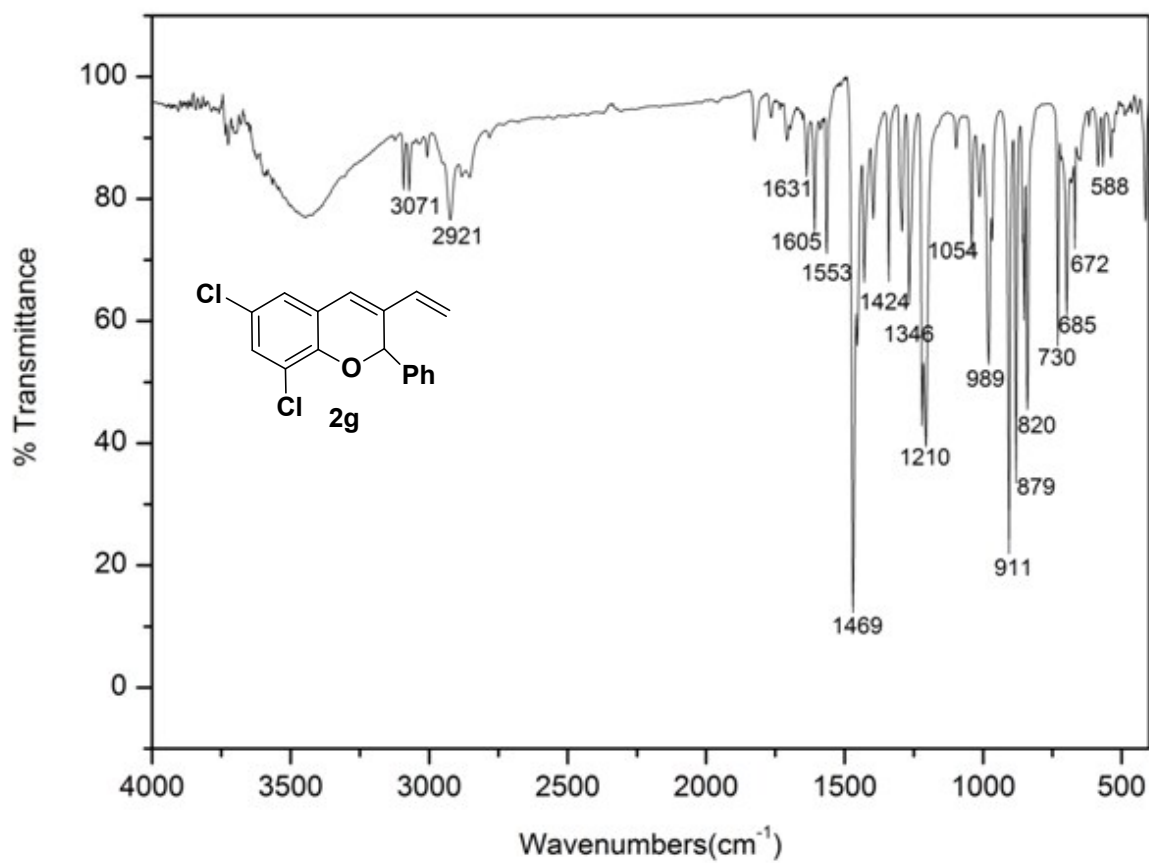
Unsaturation Number:-1.5 ~ 50.0 (Fraction:Both)

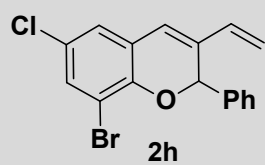
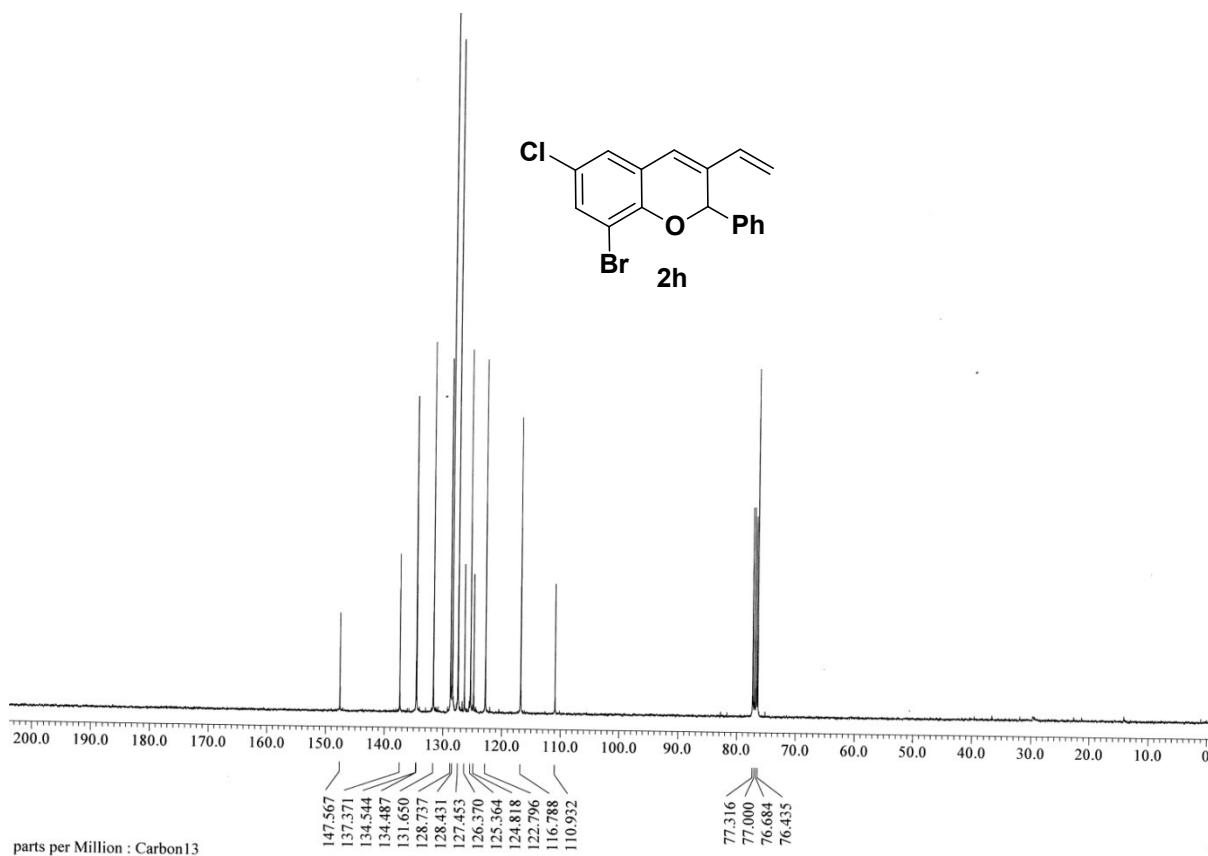
Element:¹²C:0 ~ 12, ¹H:0 ~ 10, ¹⁸O:0 ~ 1, ³⁵Cl:0 ~ 1, ¹⁹F:0 ~ 0, ³¹P:0 ~ 0, ¹⁴N:0 ~ 1, ¹⁶O:0 ~ 1, ³³S:0 ~ 0, ⁸¹Br:0 ~ 0

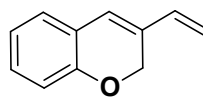


Mass	Intensity	Calc. Mass	Mass Difference (amu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
268.92420	72976.64	268.92420	-0.10	-0.37	C ₁₉ H ₁₅ ClO	5.0

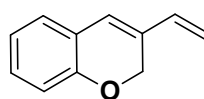
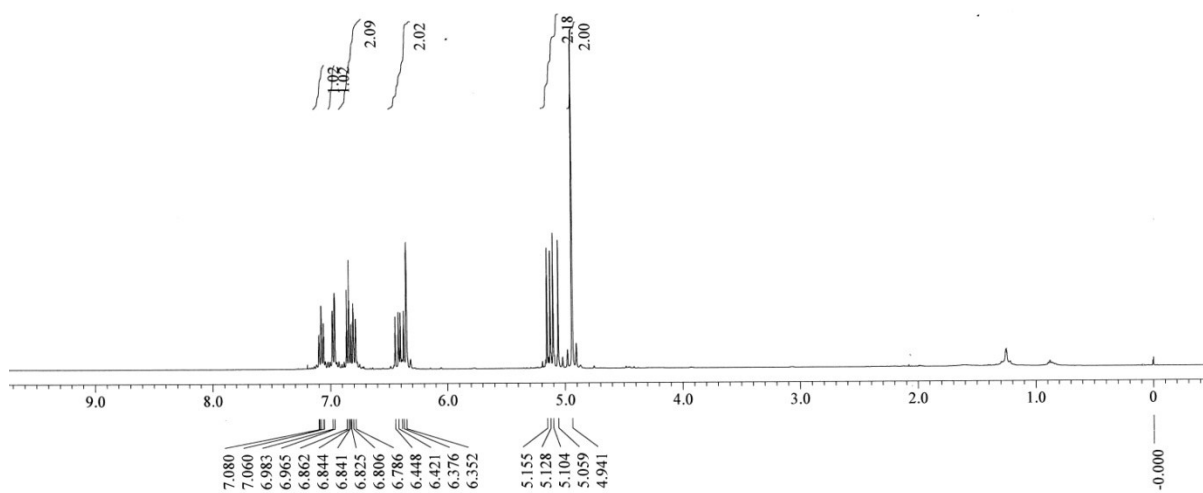




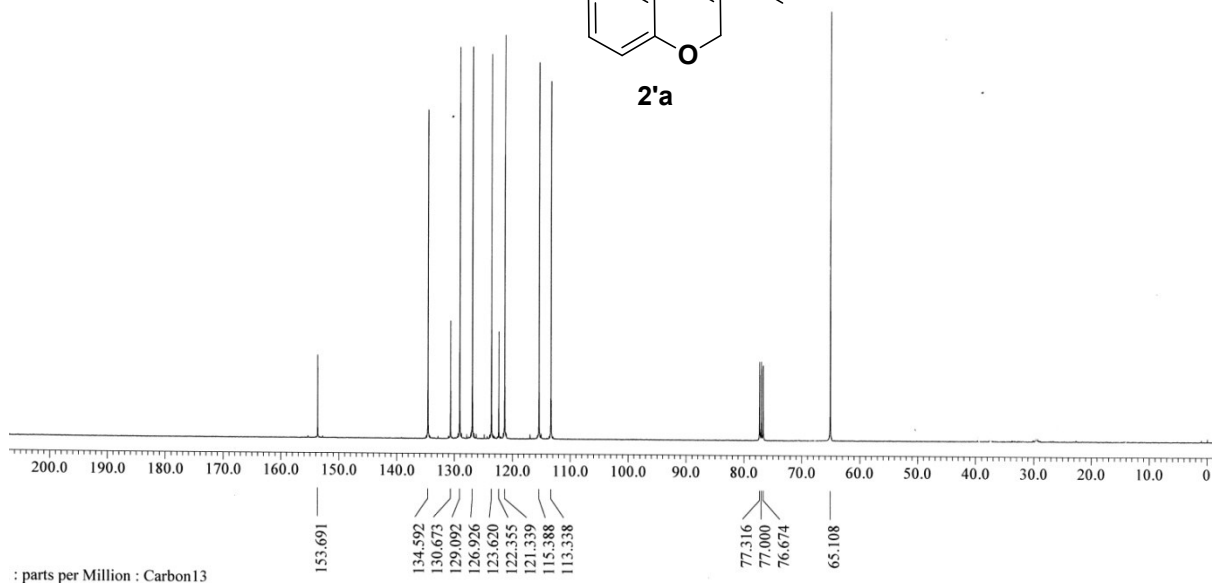


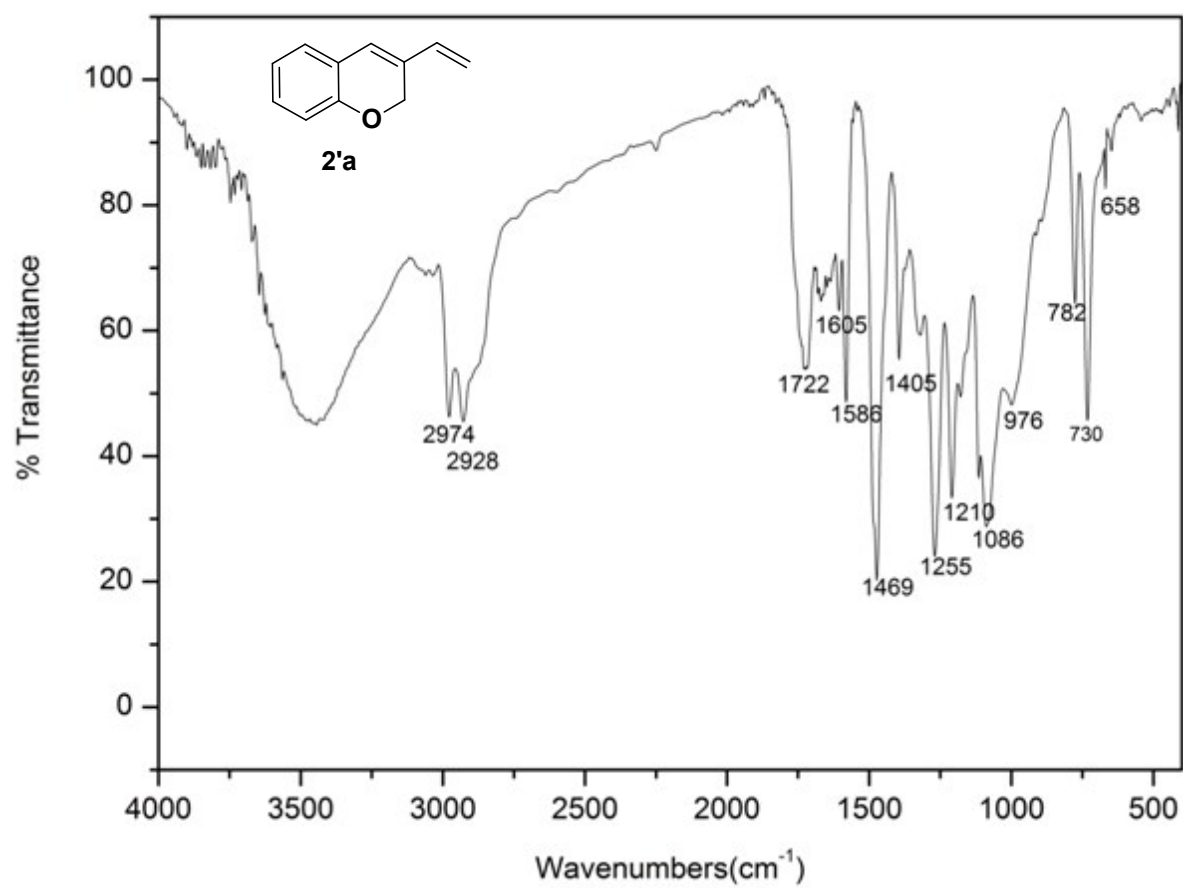


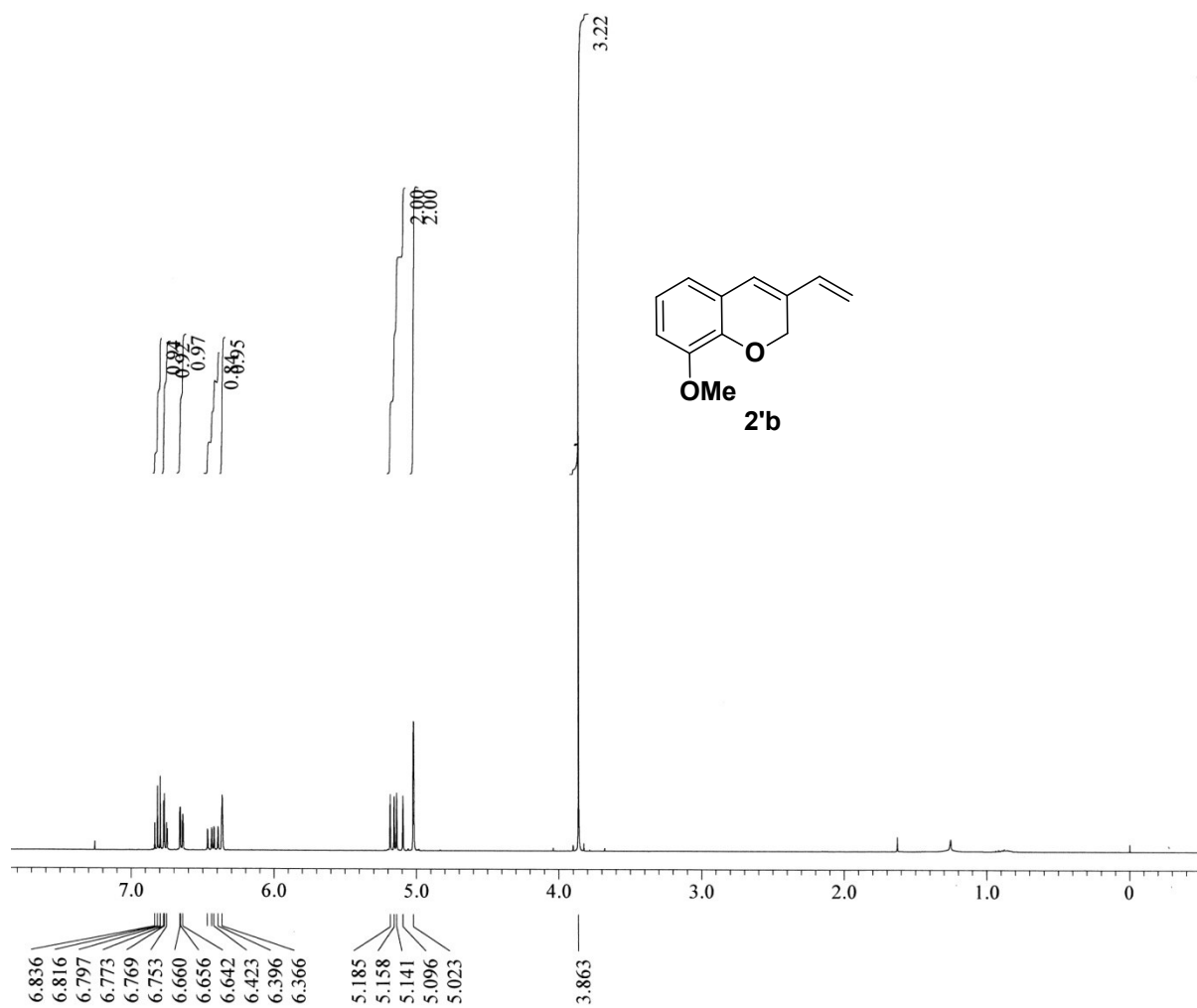
2'a

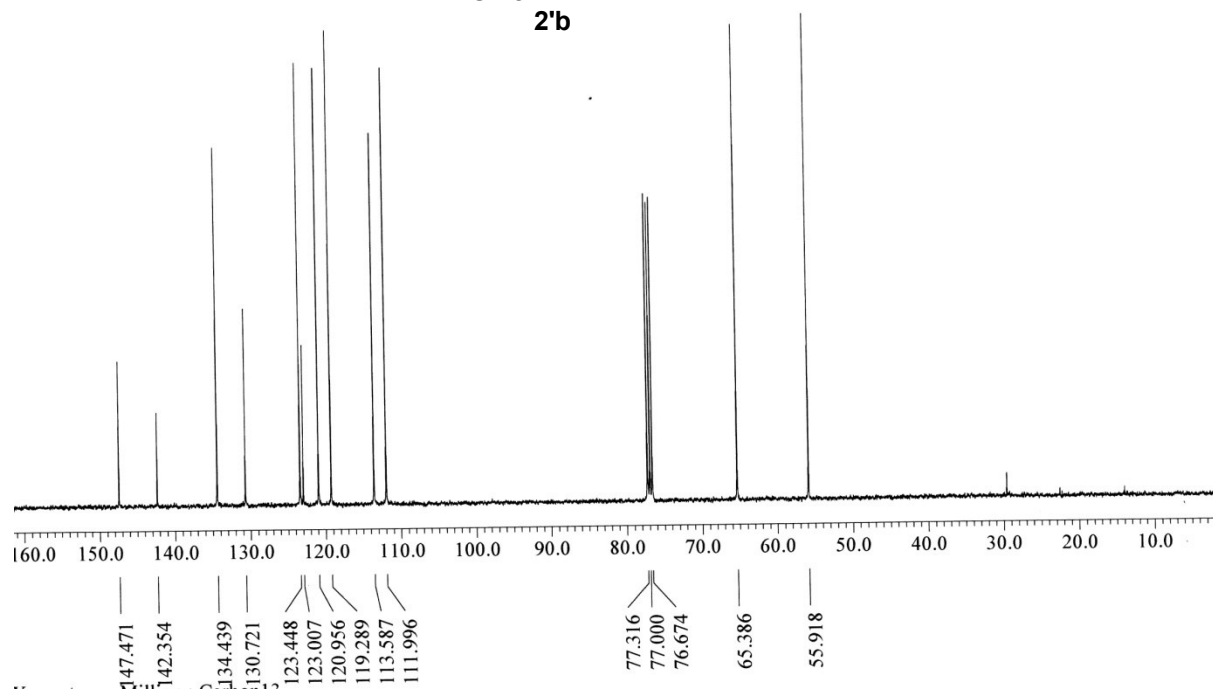
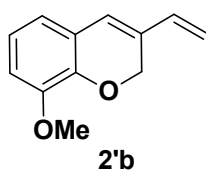


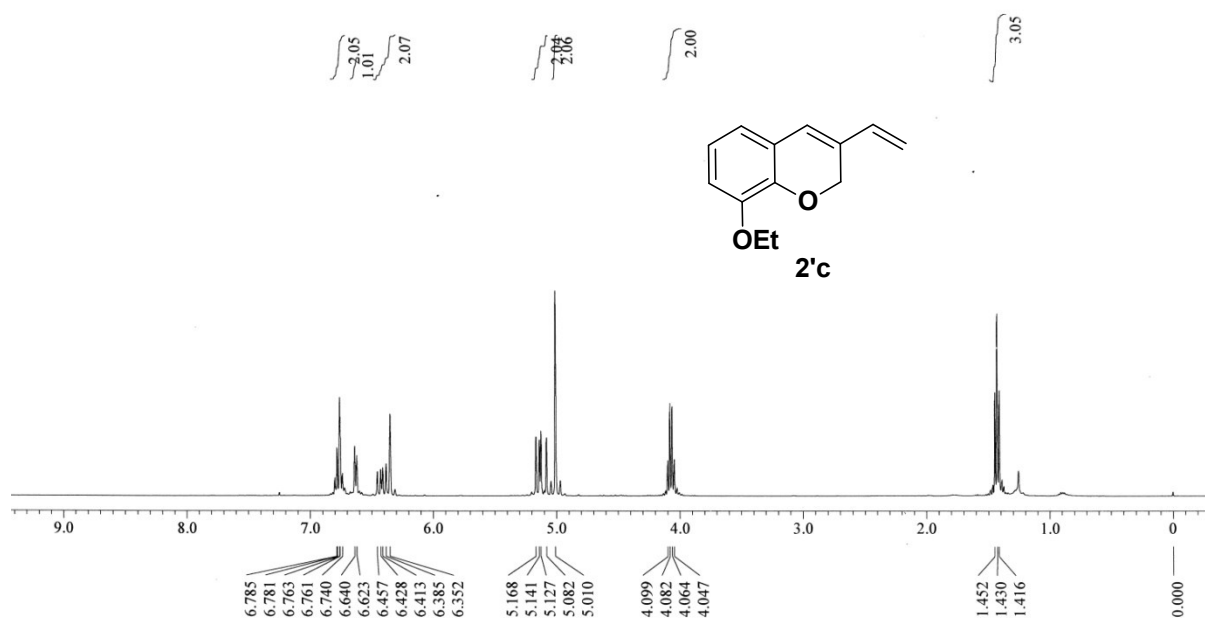
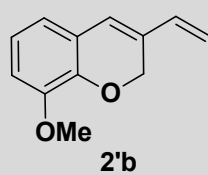
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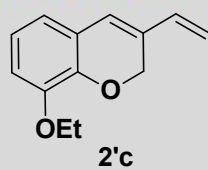
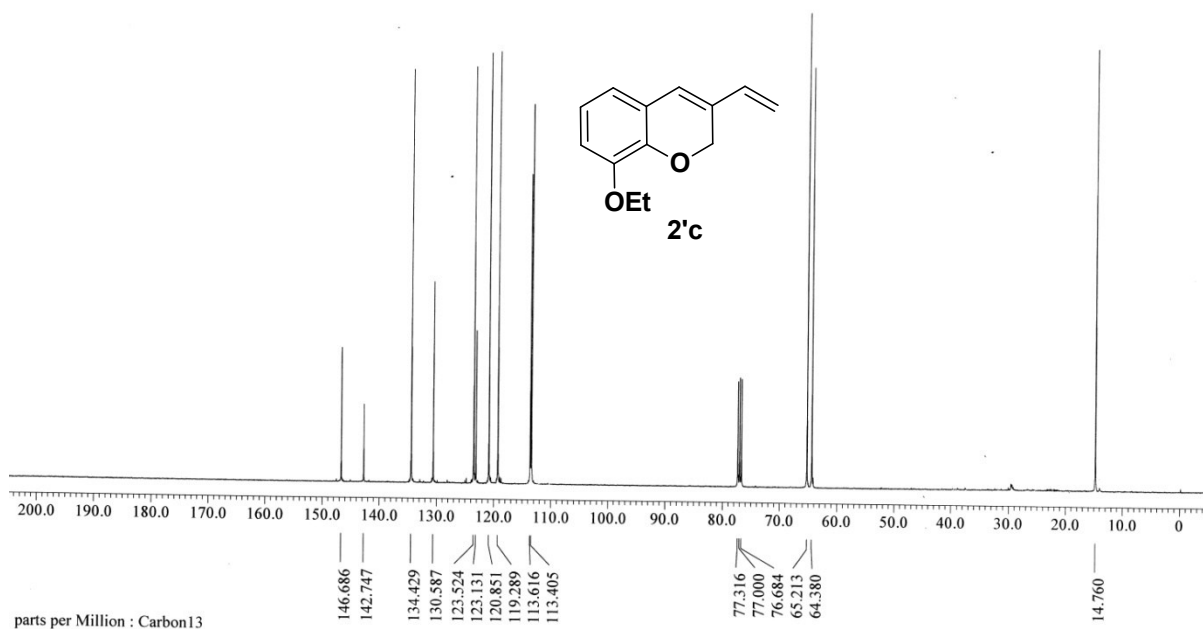


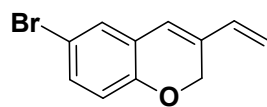
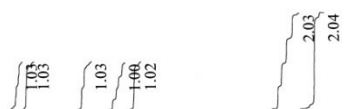




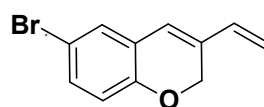
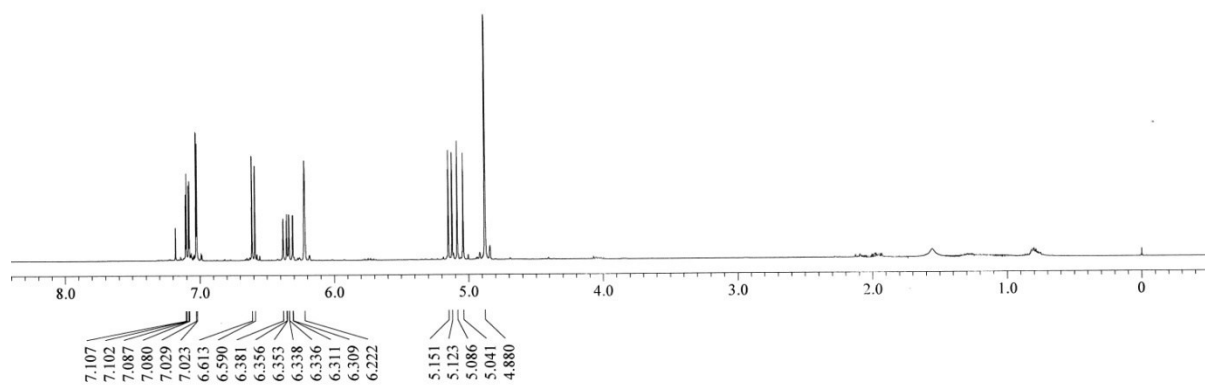




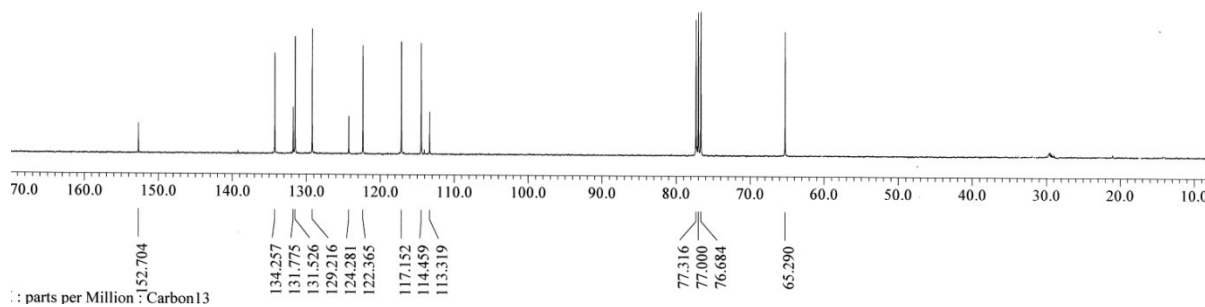


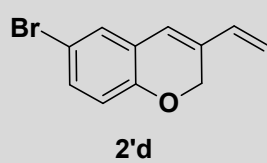


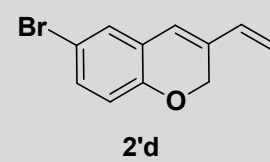
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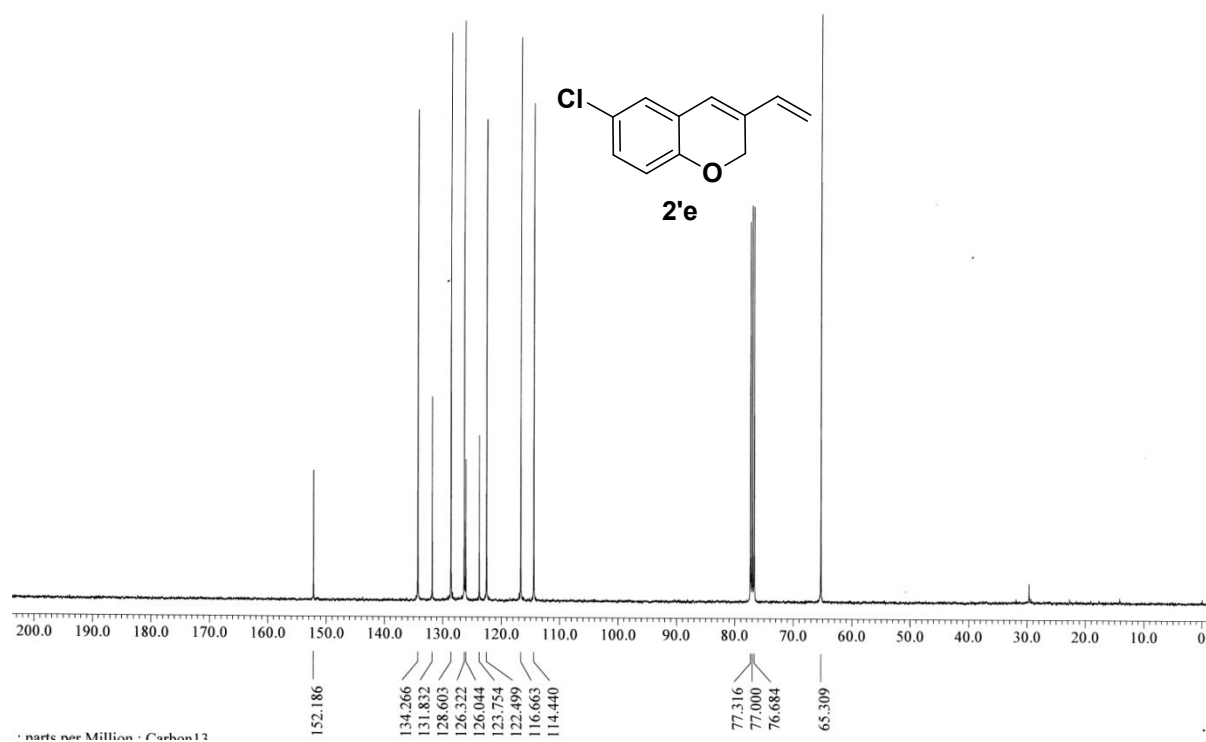
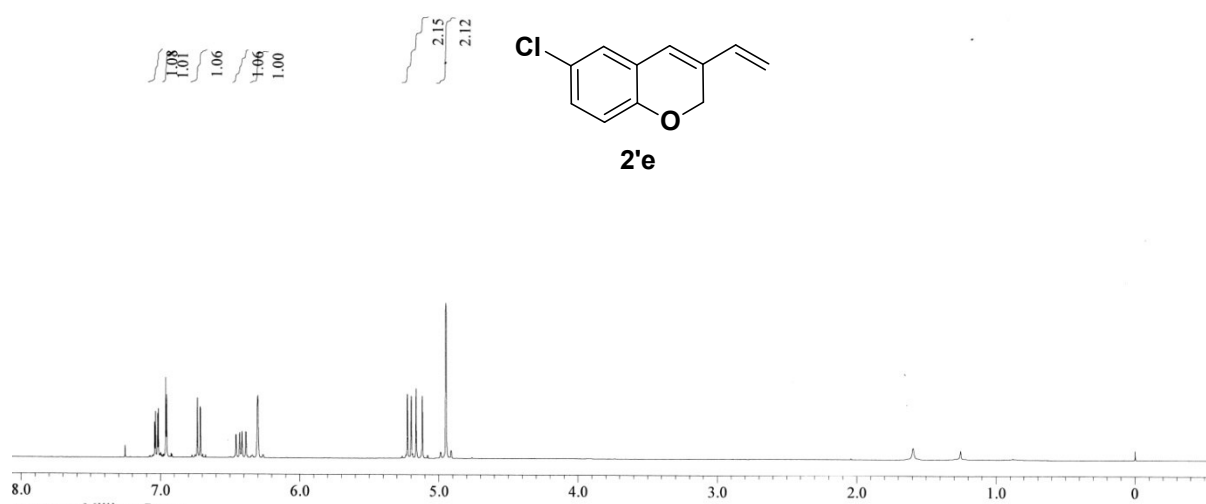


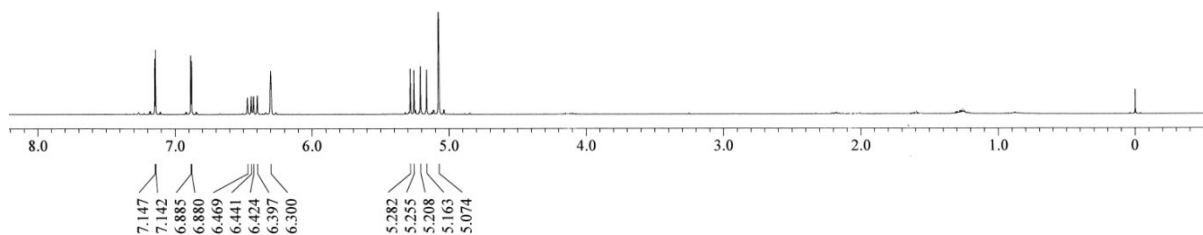
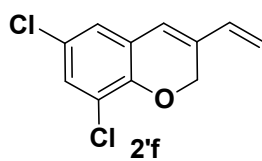
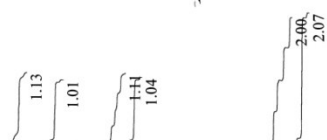
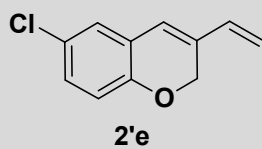
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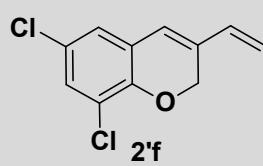
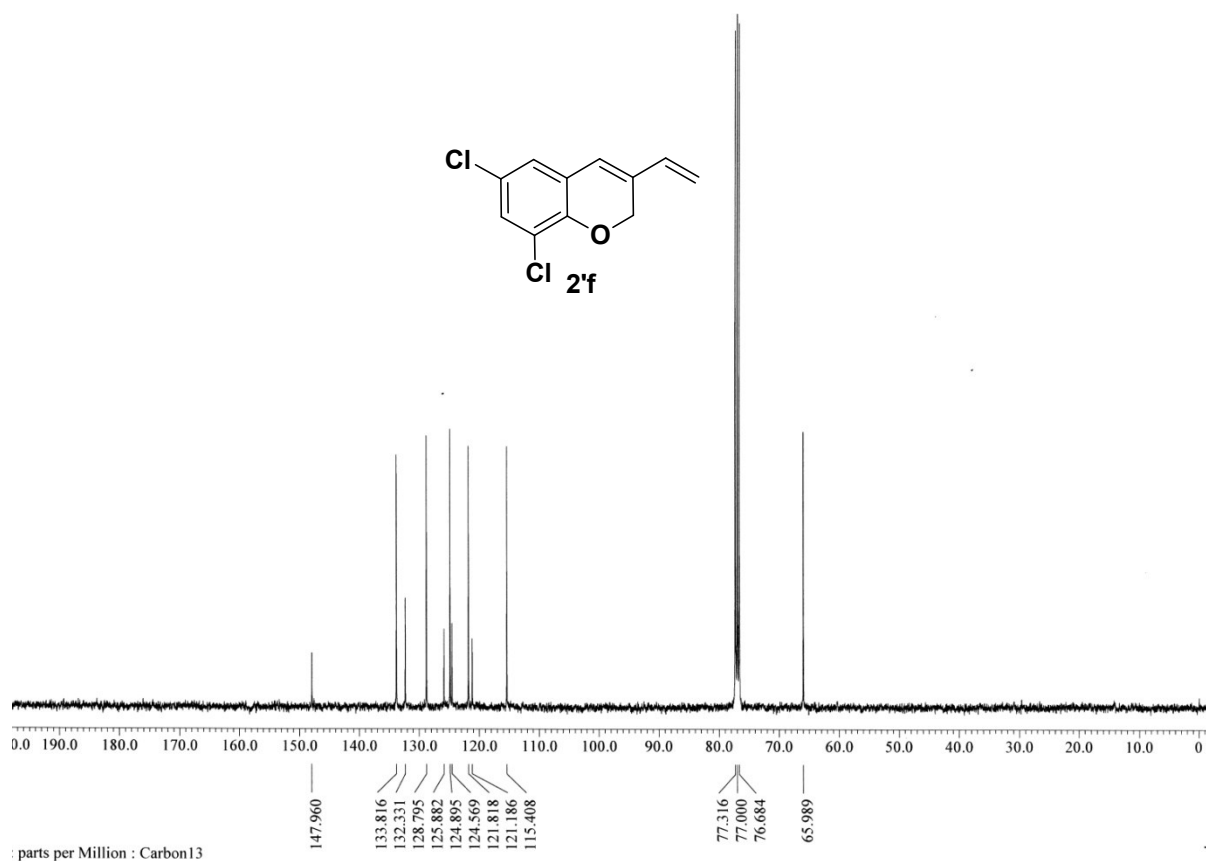


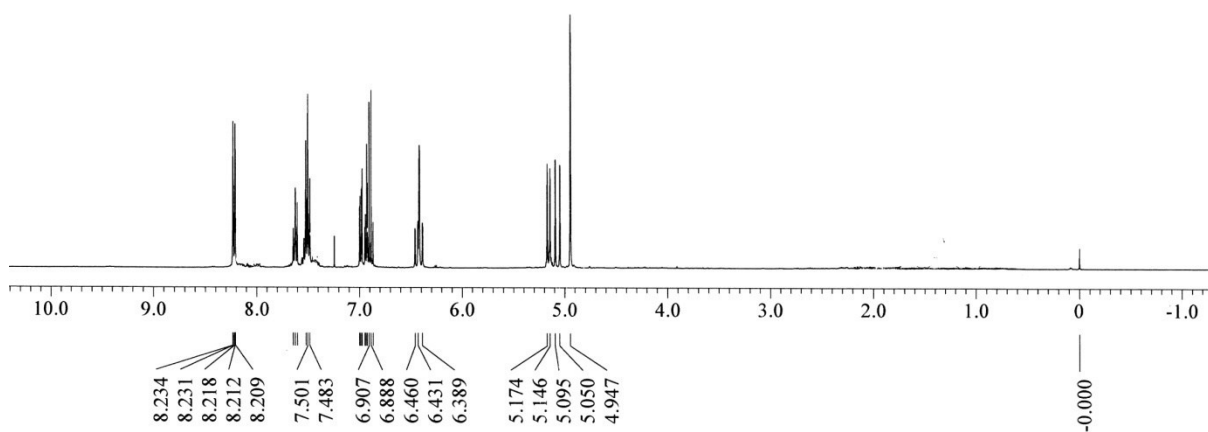
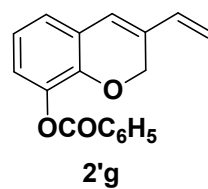
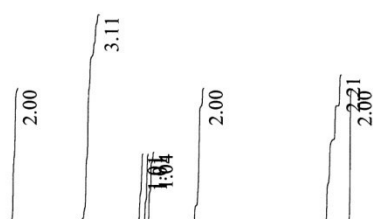
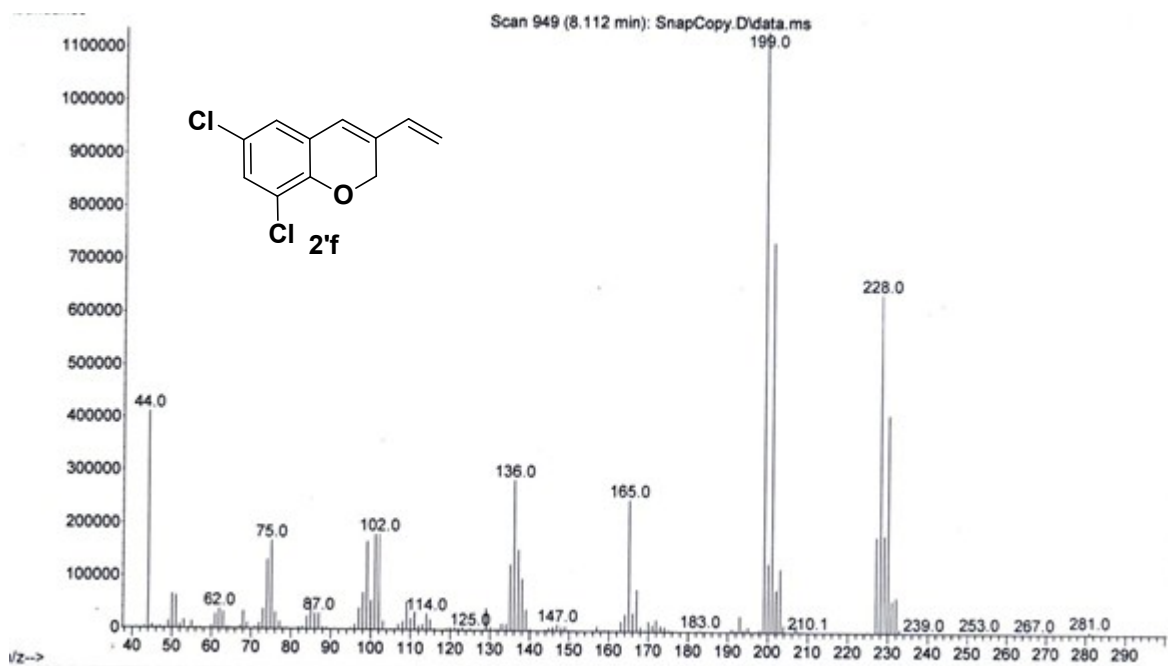


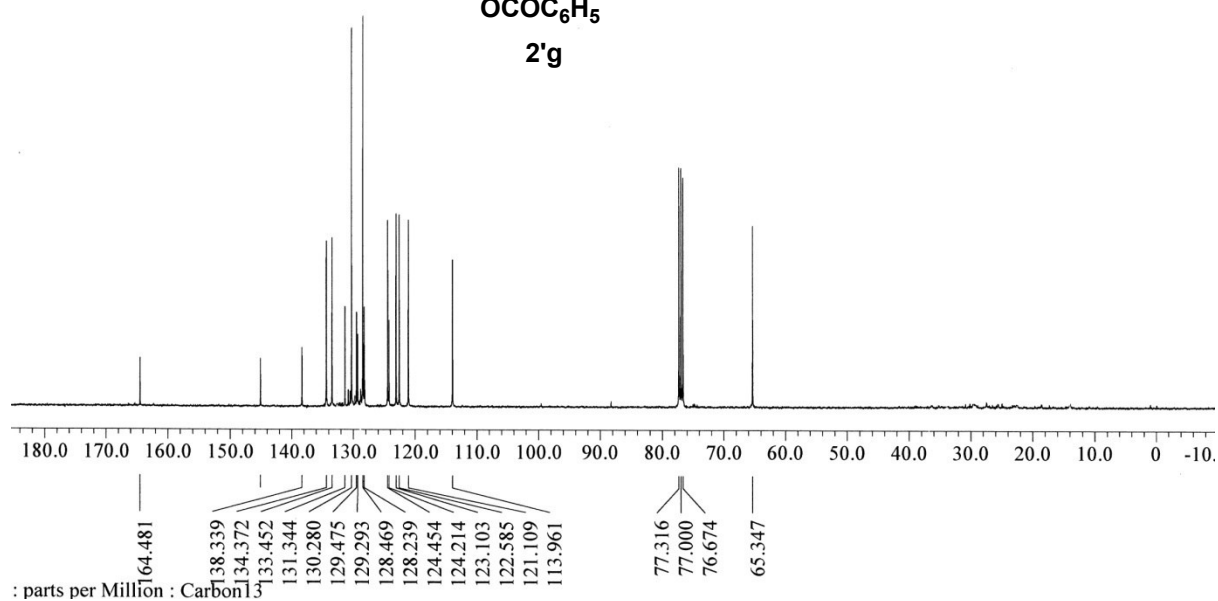
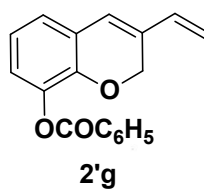


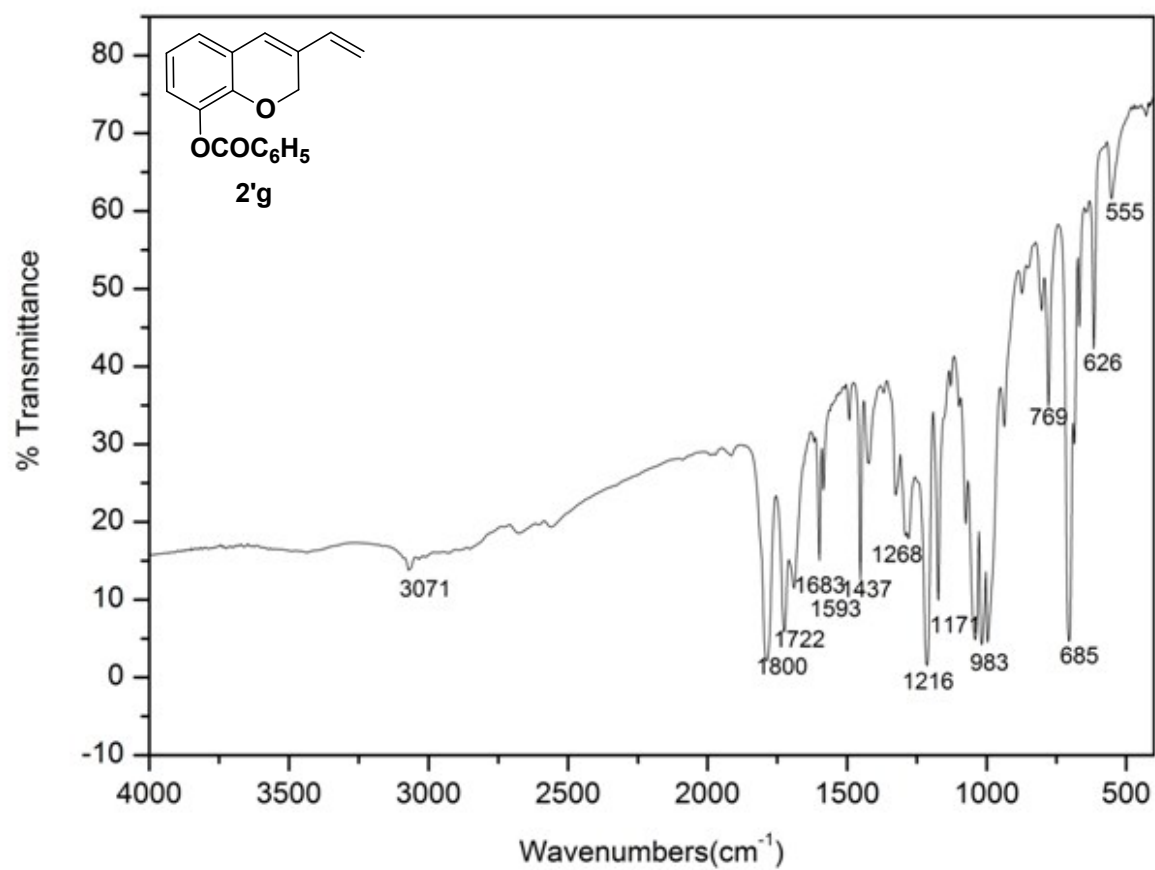


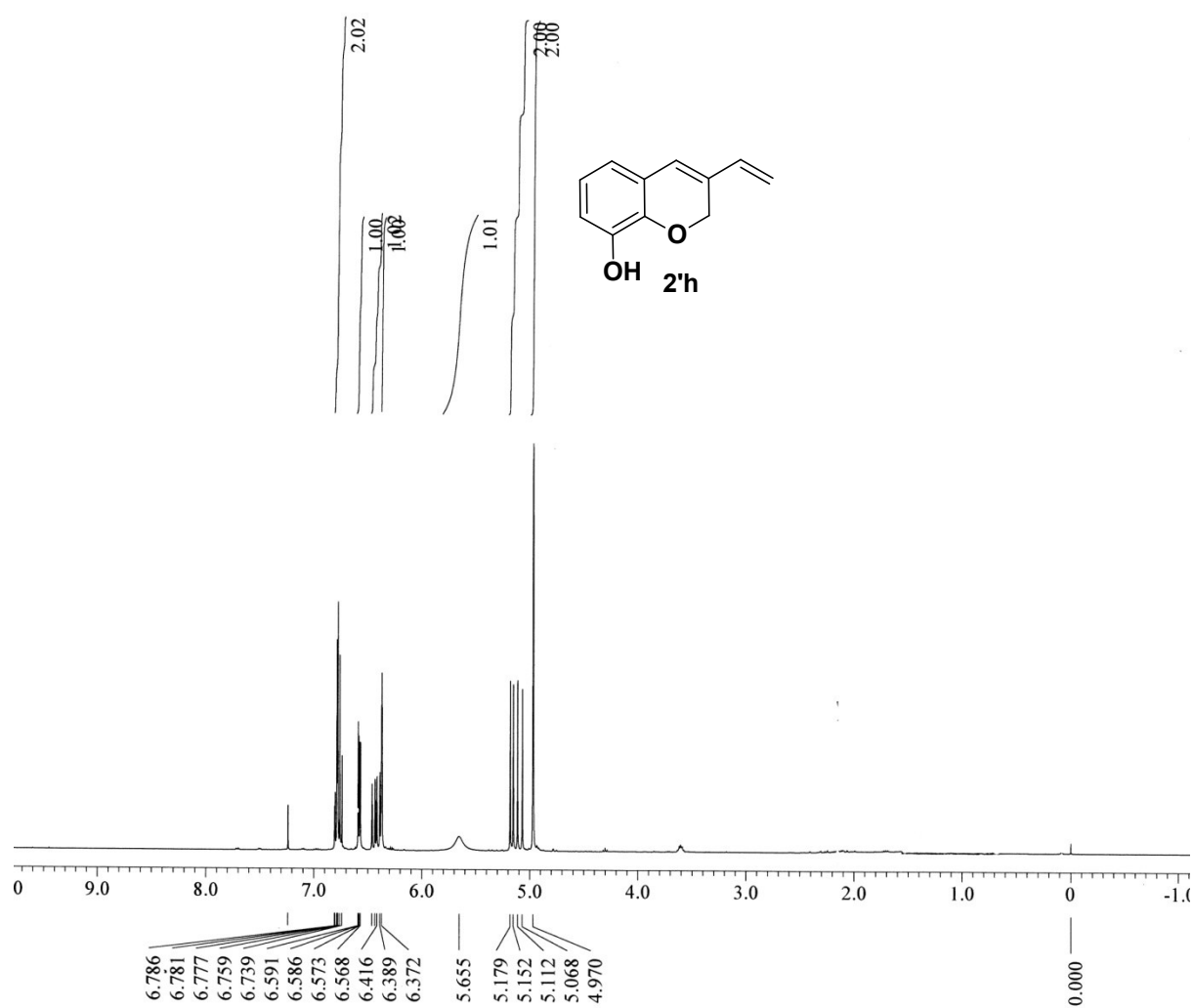


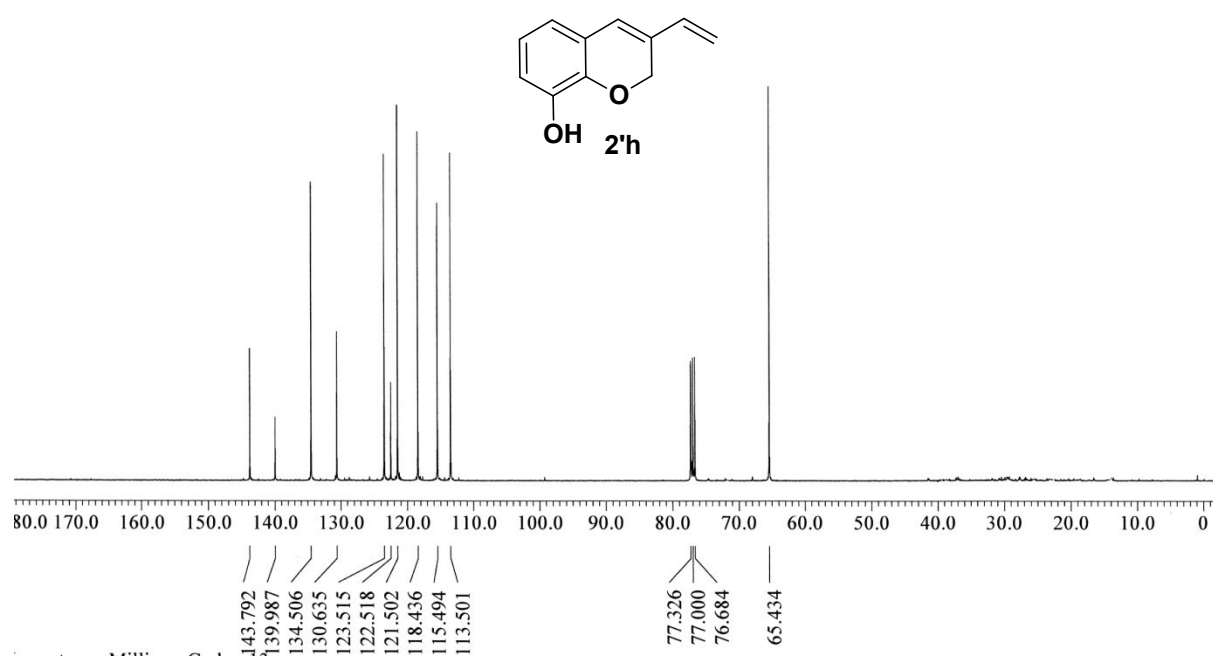


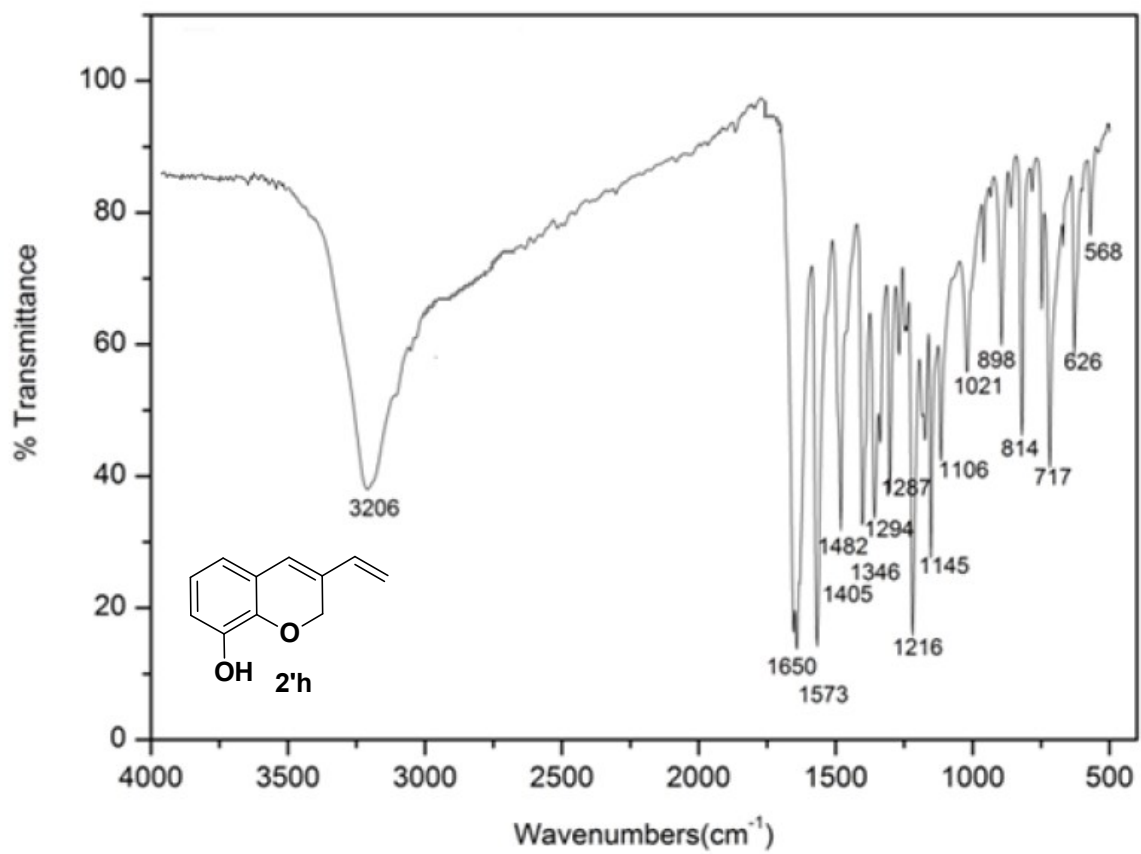


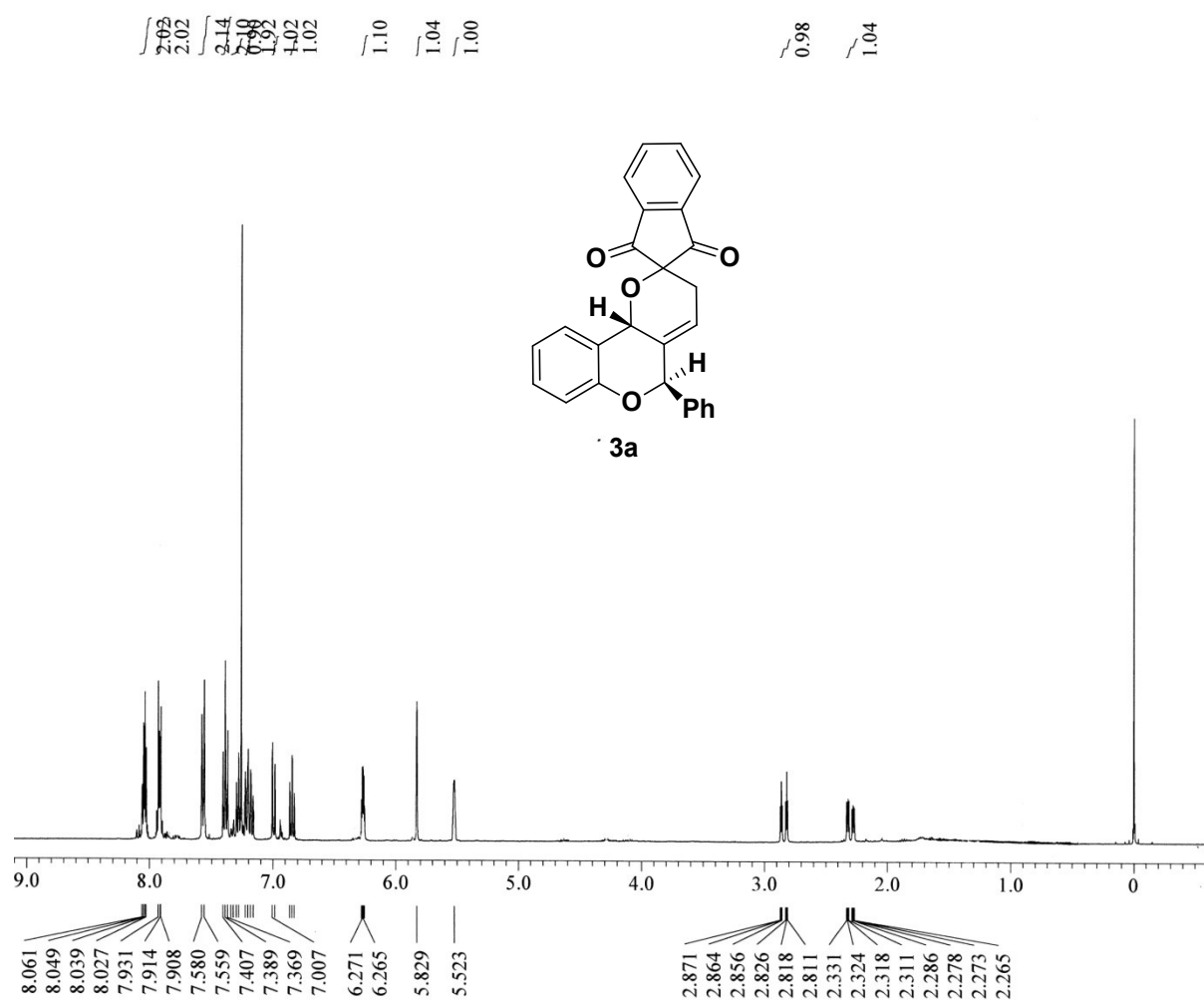


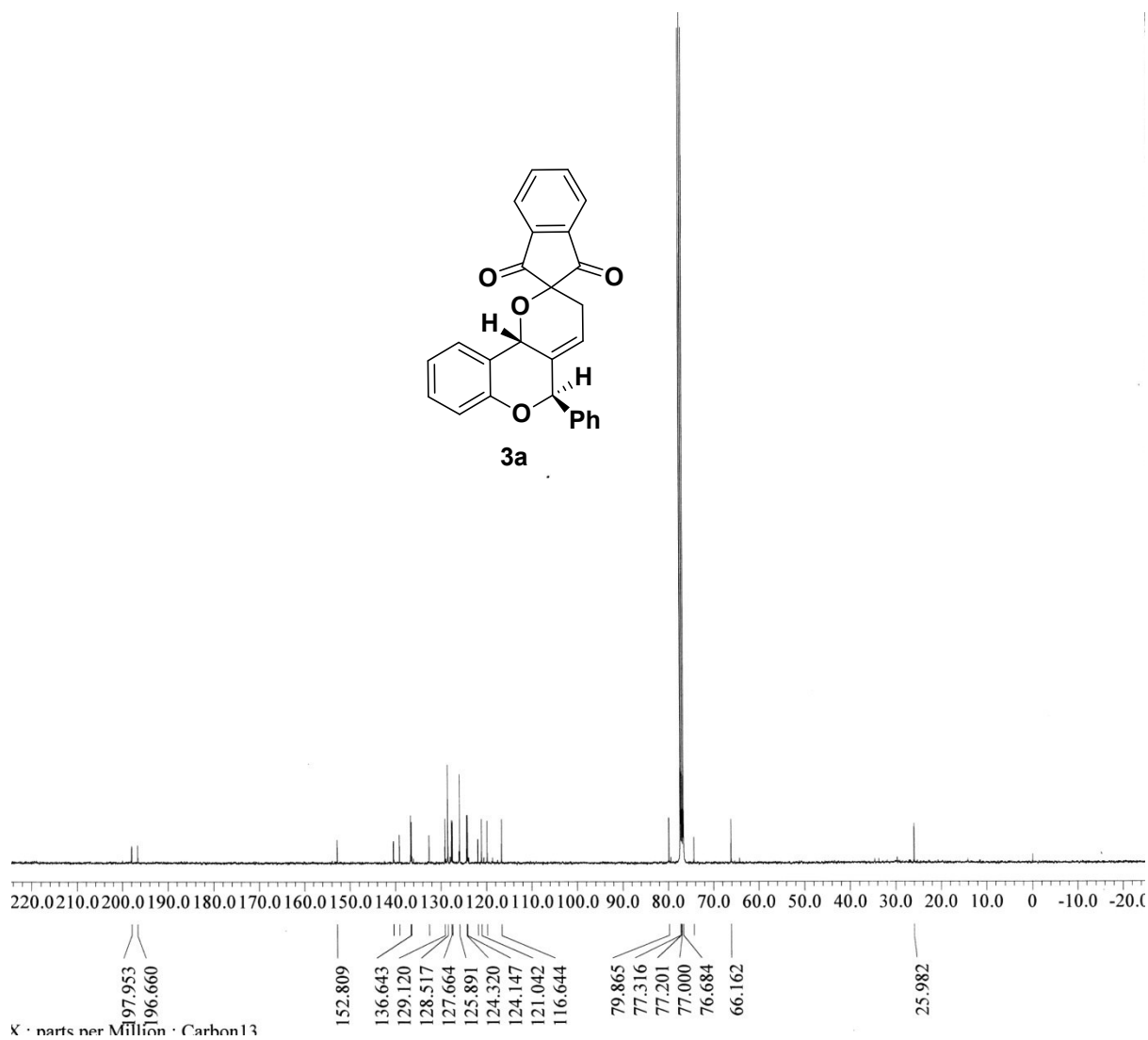
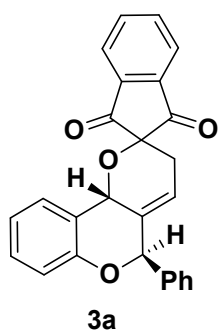


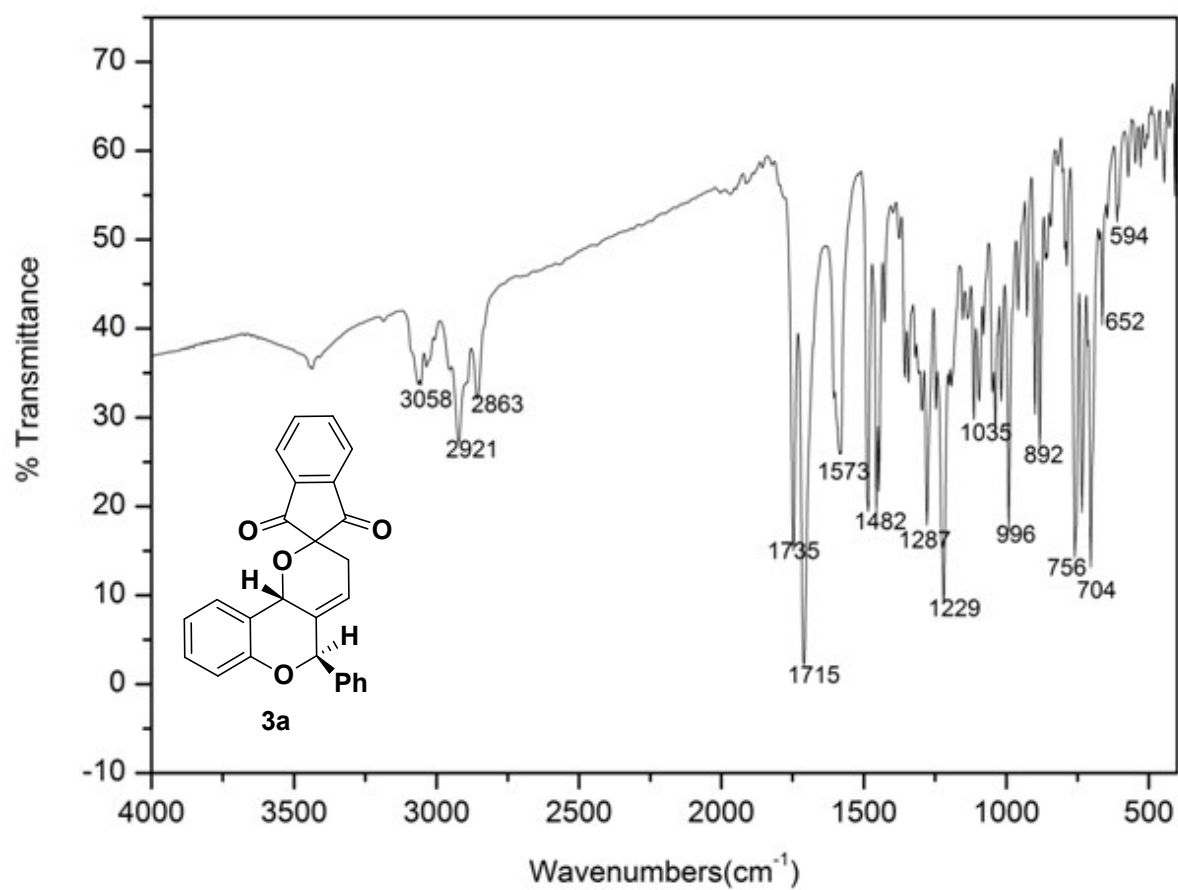












Display Report

Analysis Info

Analysis Name D:\Data\DEC-2016\NKS\GC\11102017_NKS_GC-PRA_67.d
Method Wash.pos tune_low_22092017.m
Sample Name ESI-MS
Comment

Acquisition Date 10/12/2017 8:06:21 PM

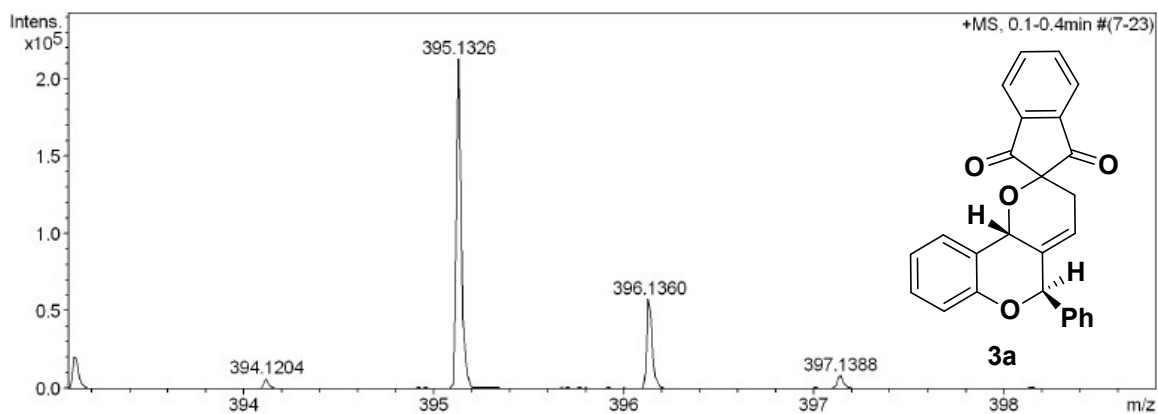
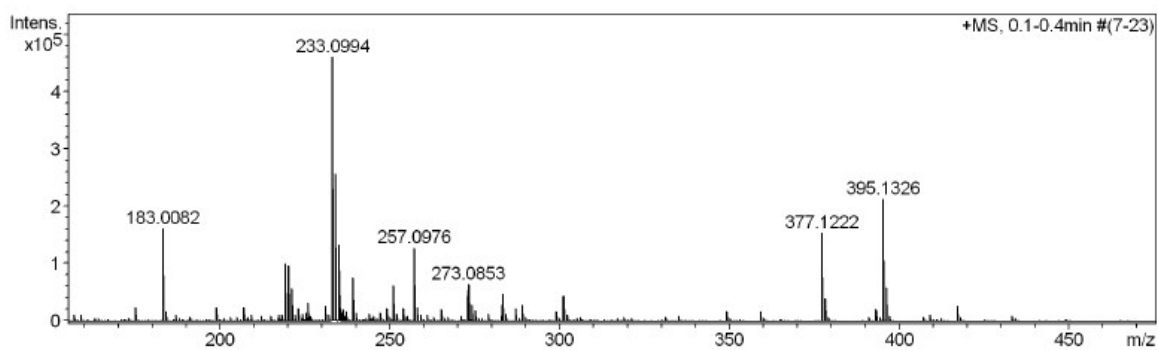
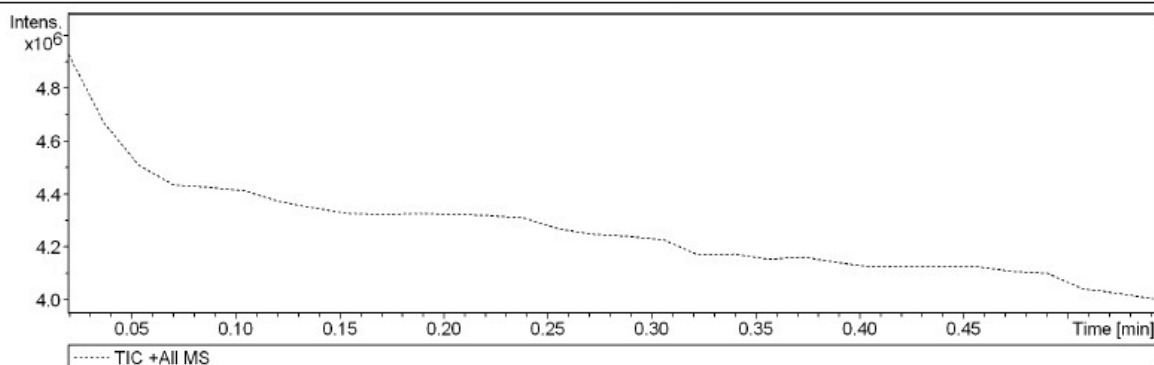
Operator G.CREDDY
Instrument microTOF-Q II 10337

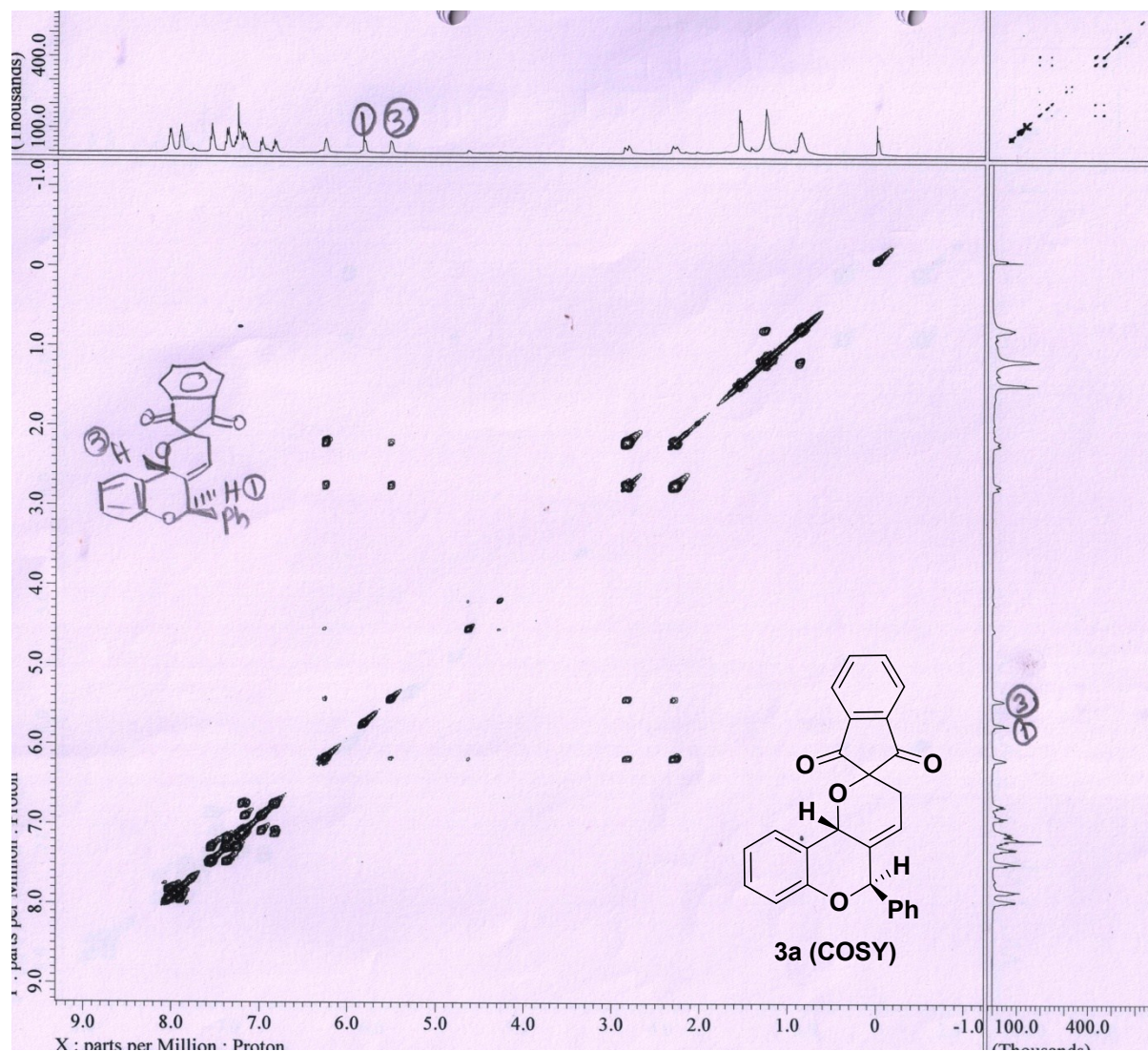
Acquisition Parameter

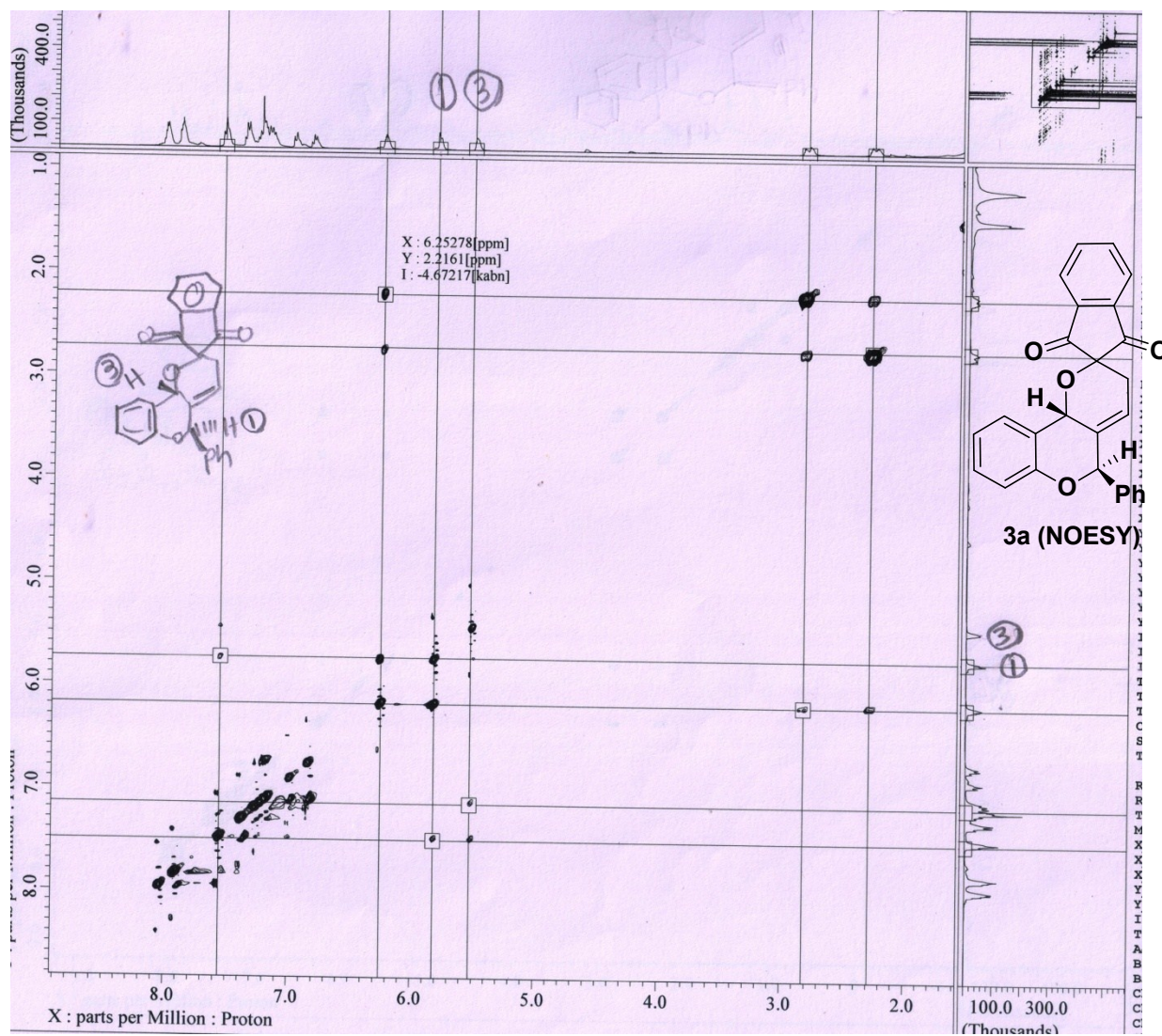
Source Type ESI
Focus Active
Scan Begin 50 m/z
Scan End 3000 m/z

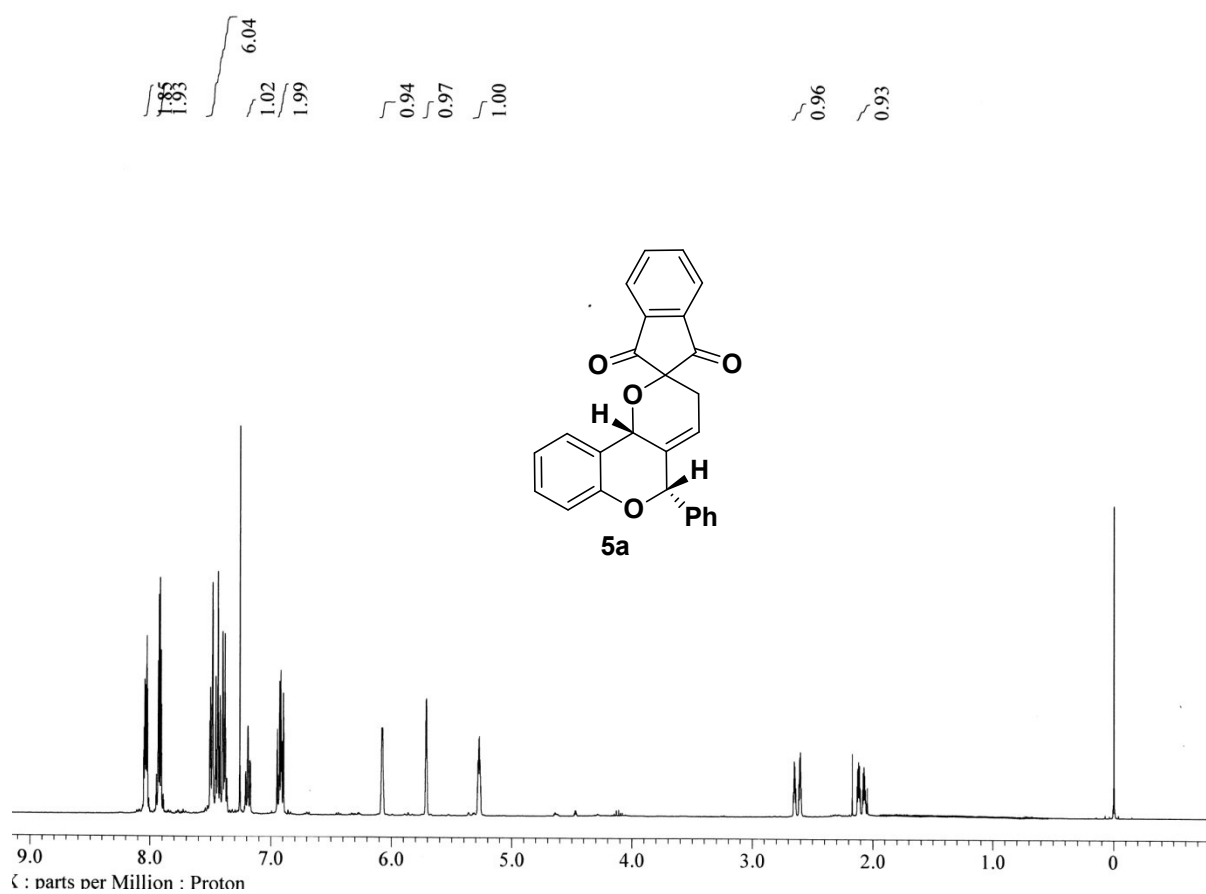
Ion Polarity Positive
Set Capillary 4500 V
Set End Plate Offset -500 V
Set Collision Cell RF 200.0 Vpp

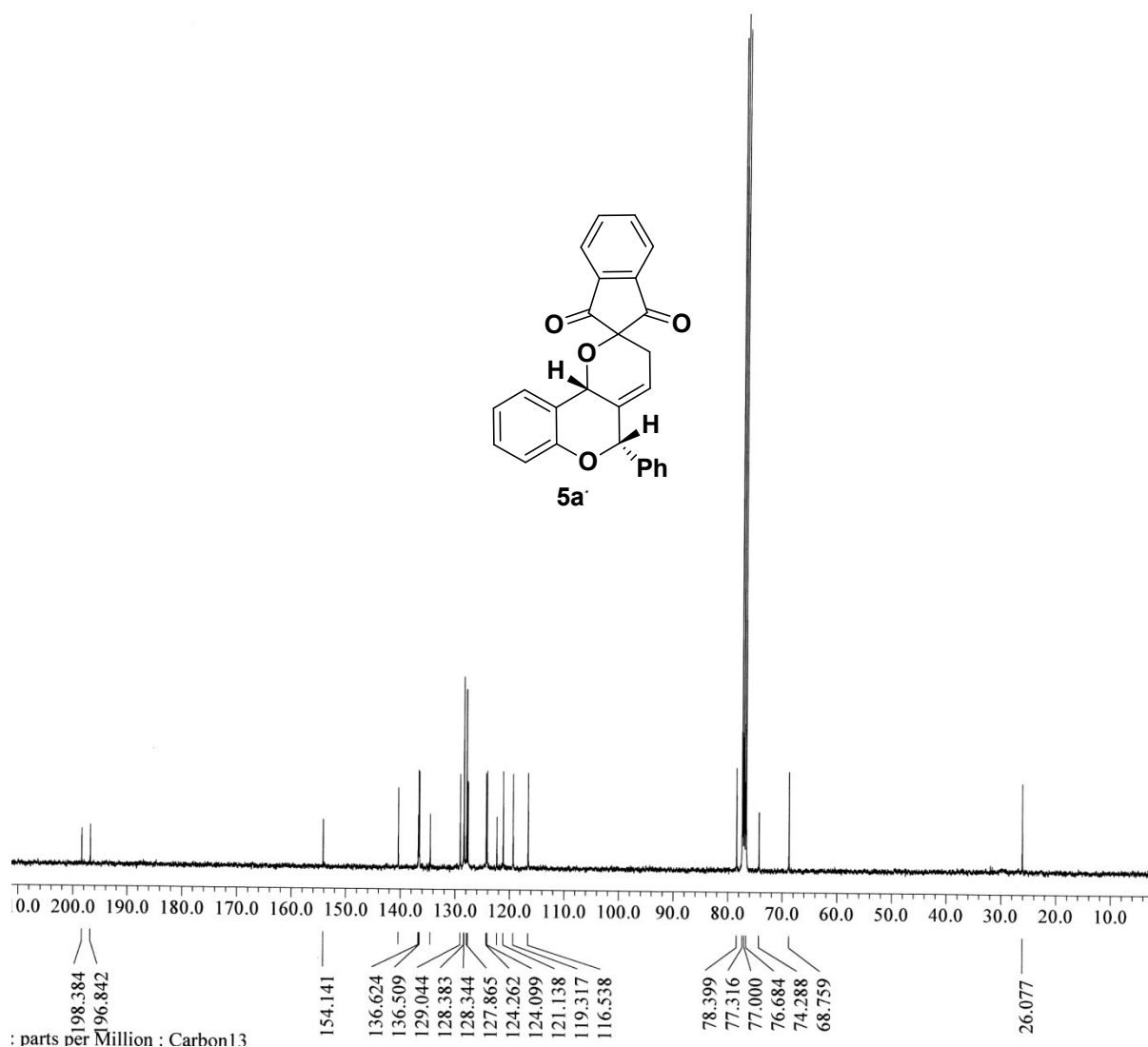
Set Nebulizer 0.4 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Source

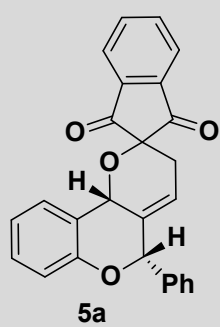


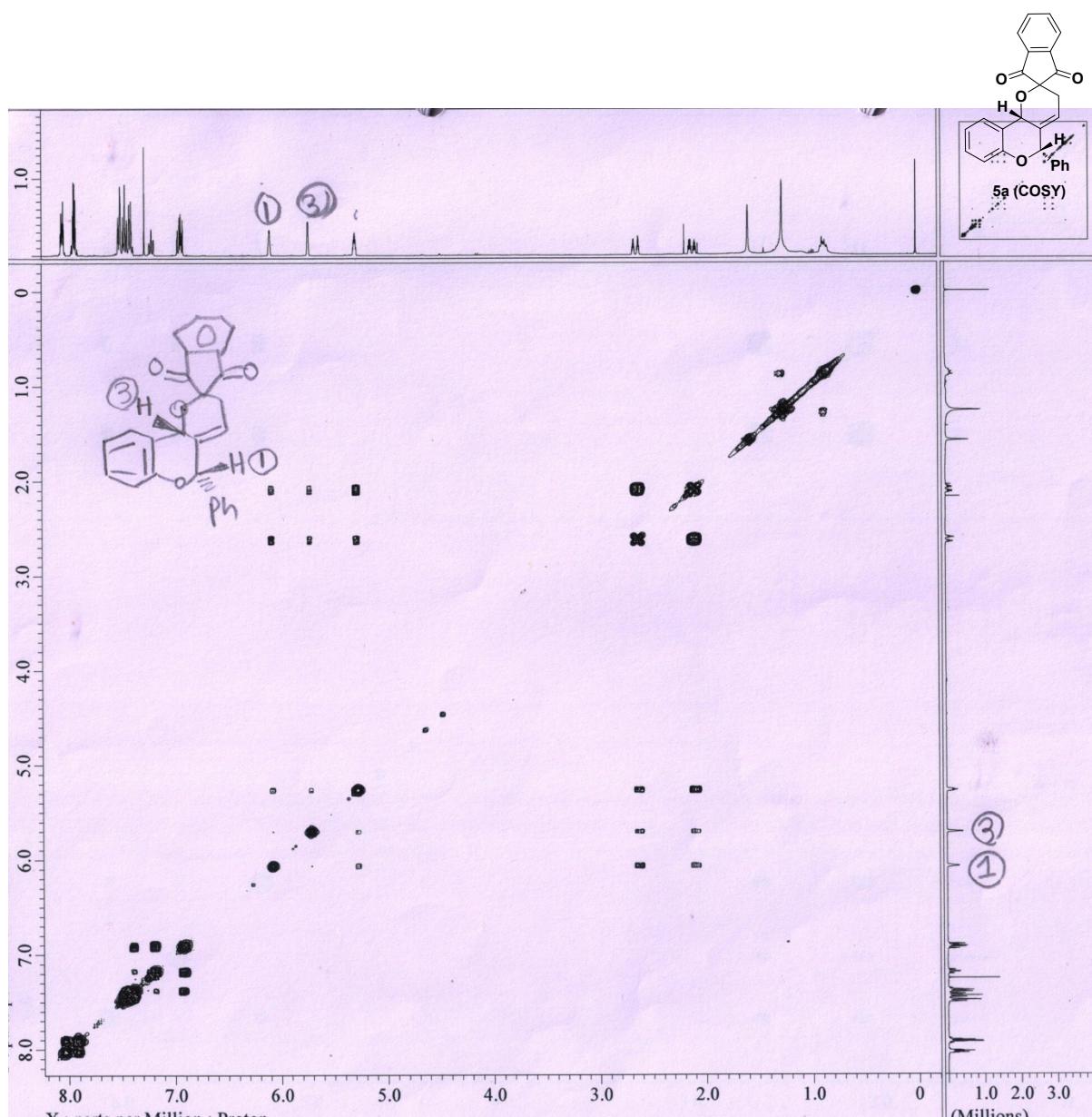


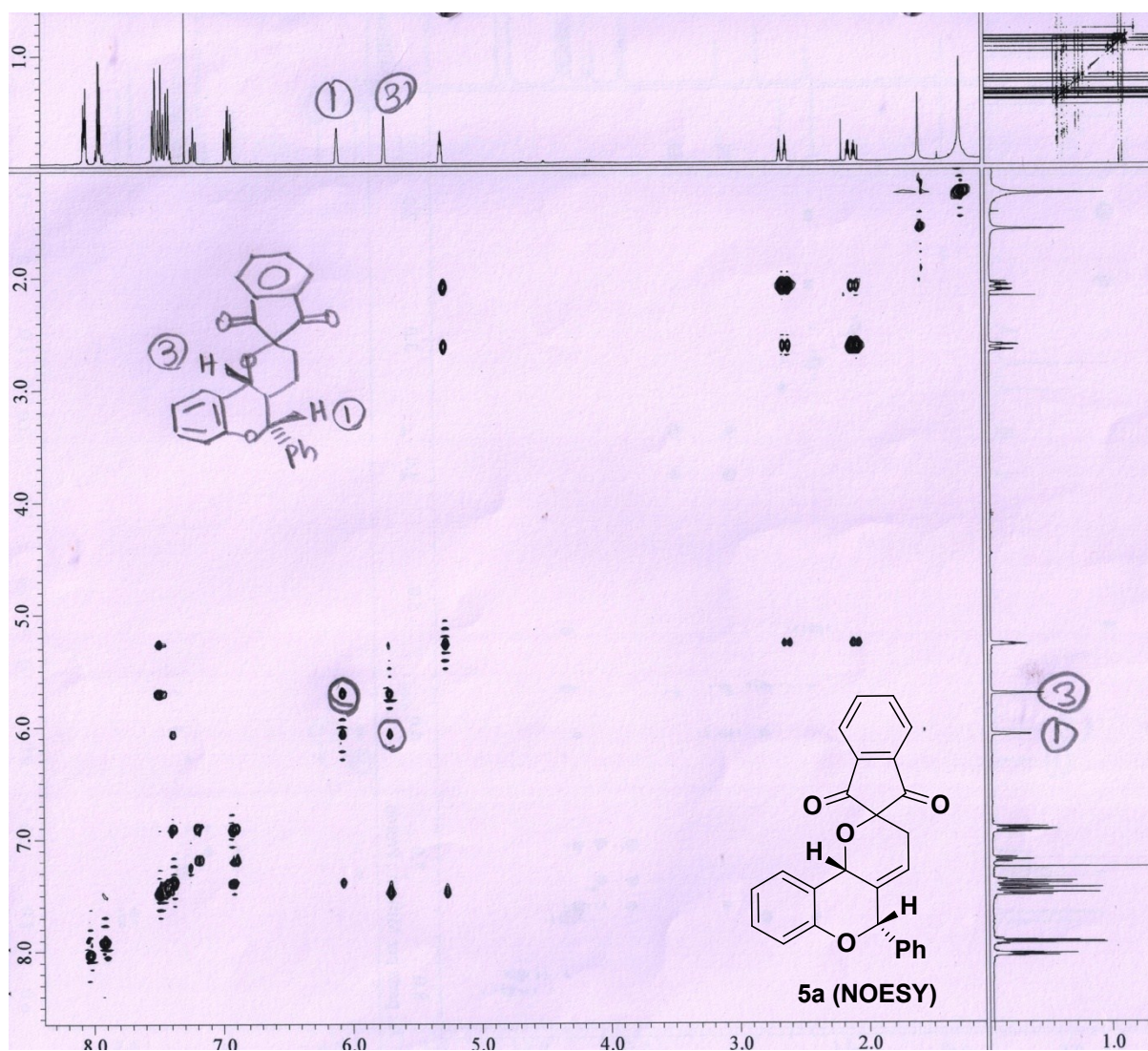


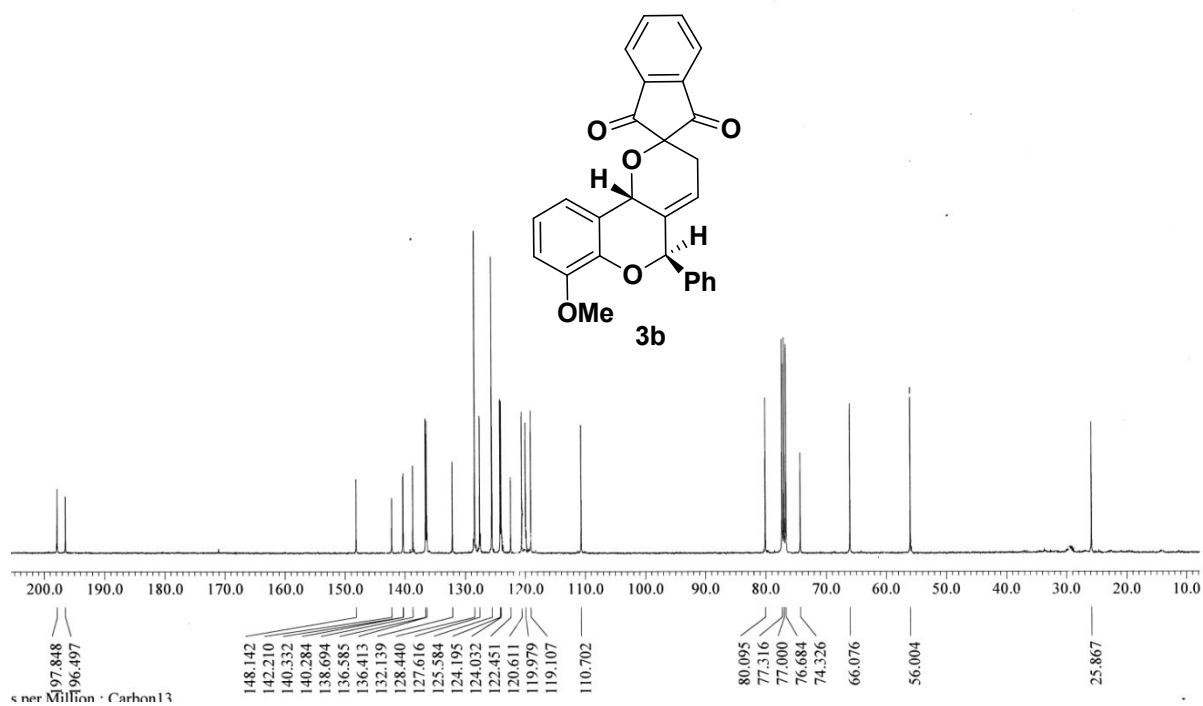
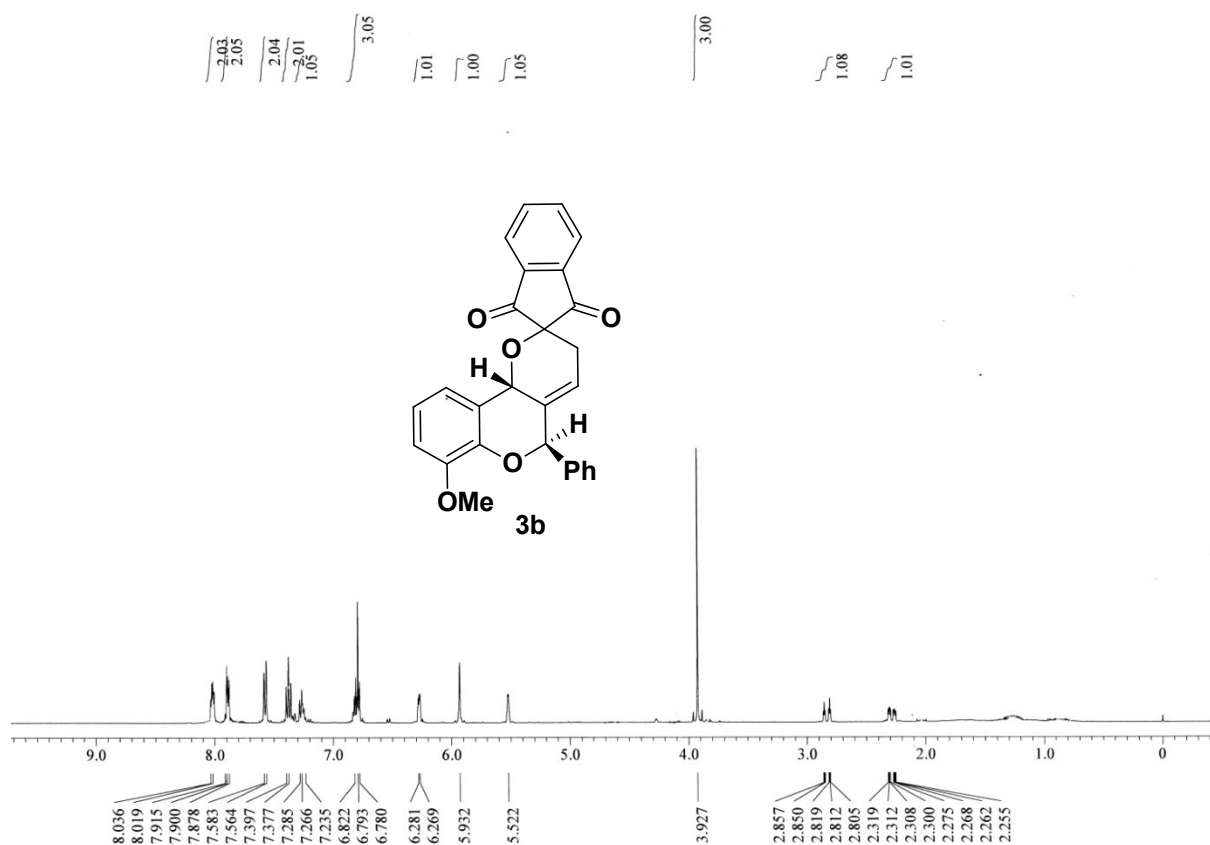


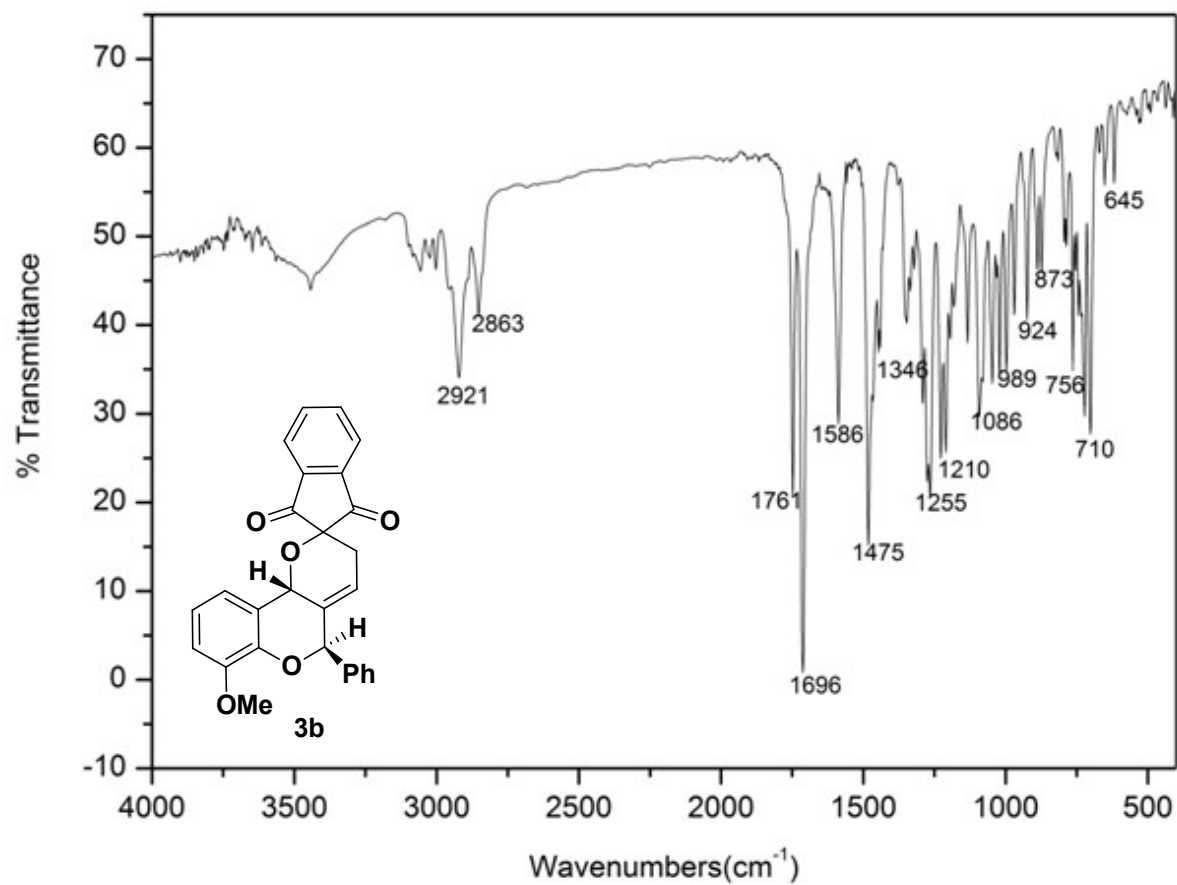












Display Report

Analysis Info

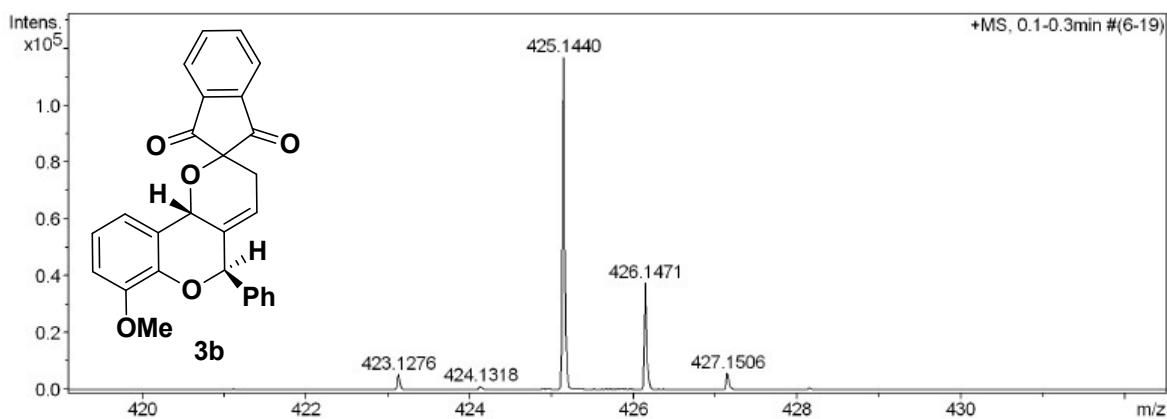
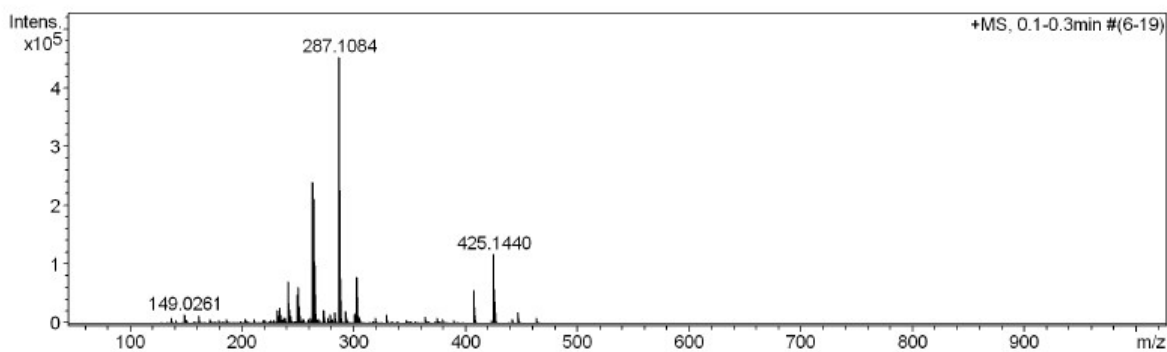
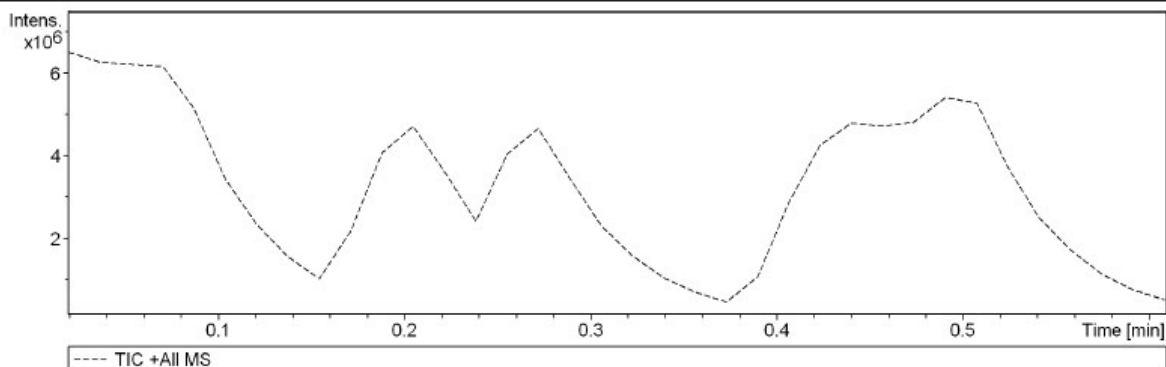
Analysis Name D:\Data\DEC-2016\NKS\GC\11102017_NKS_GC-PRA_149.d
Method Wash.pos tune_low_22092017.m
Sample Name ESI-MS
Comment

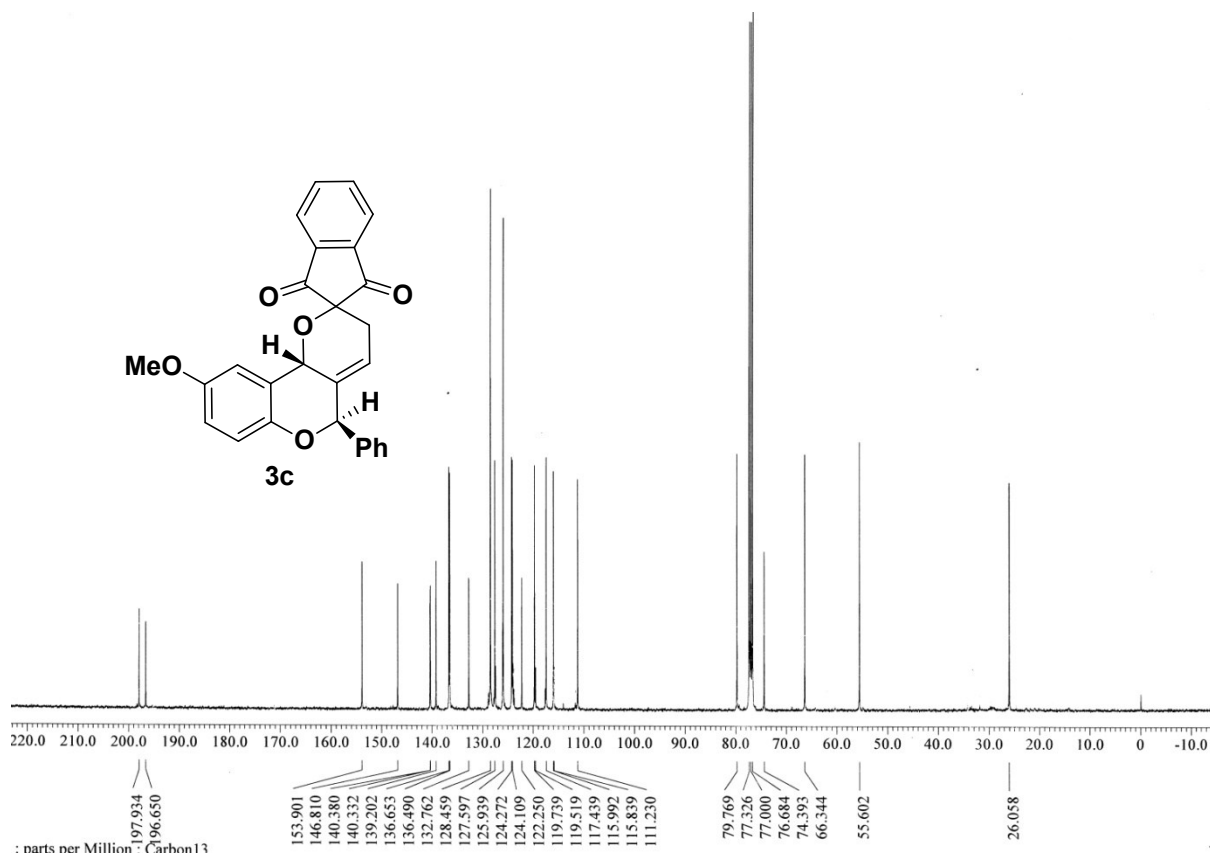
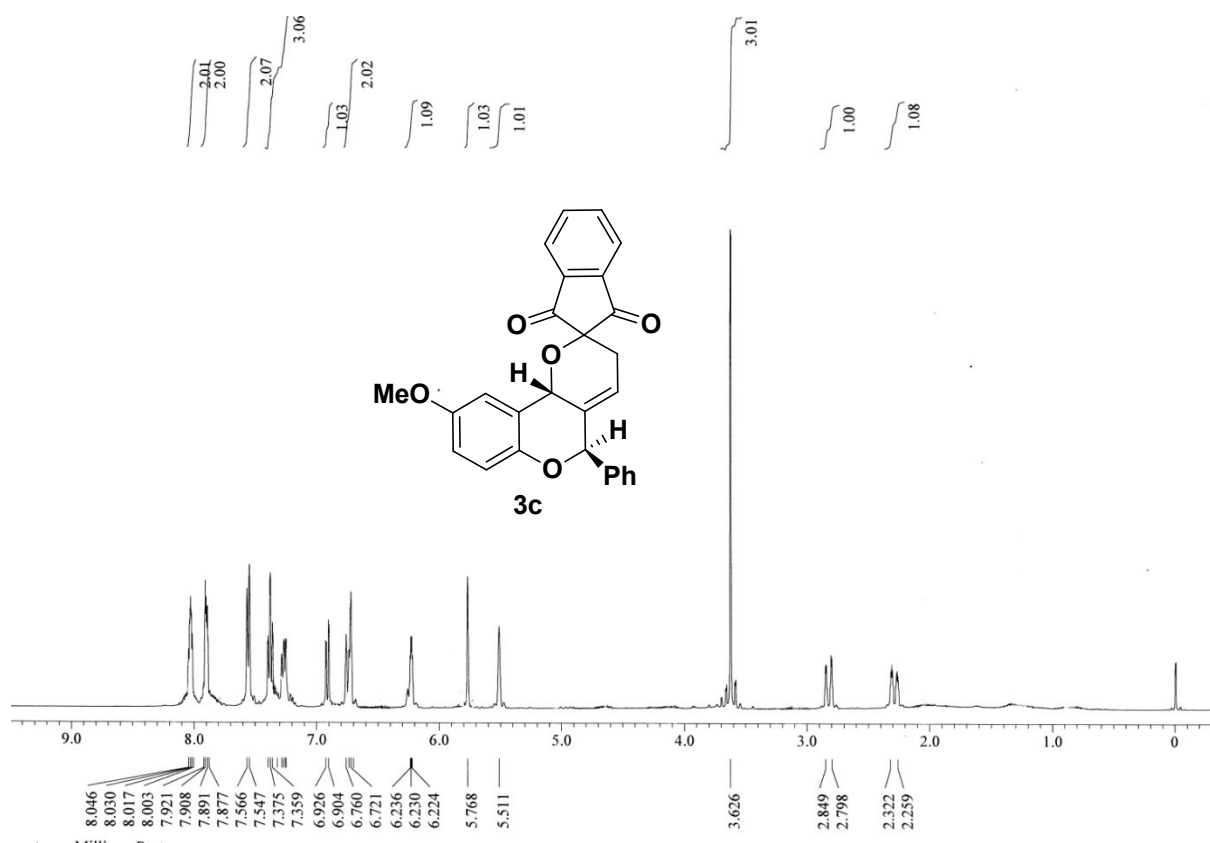
Acquisition Date 10/12/2017 8:14:01 PM

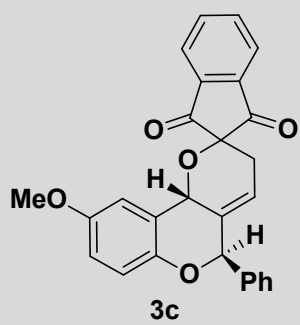
Operator G.CREDDY
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source







Display Report

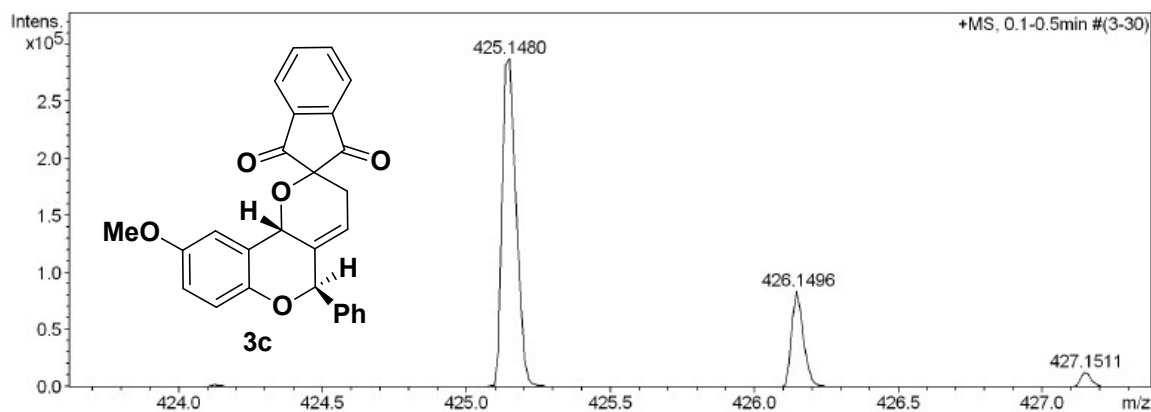
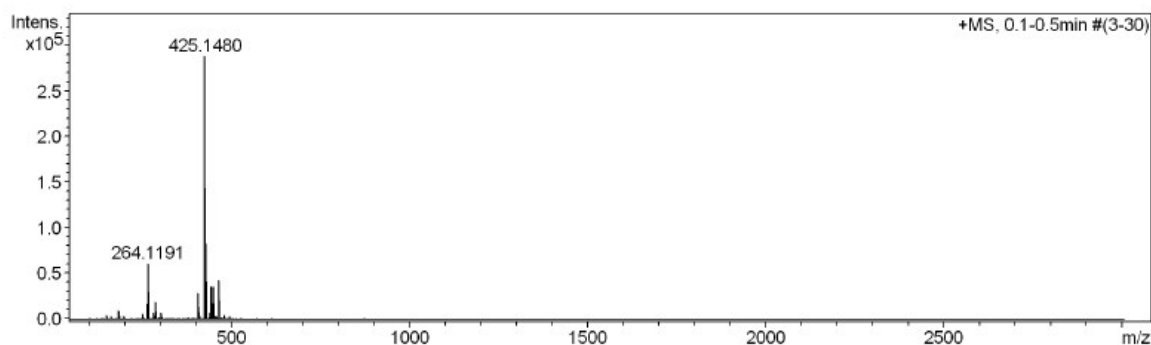
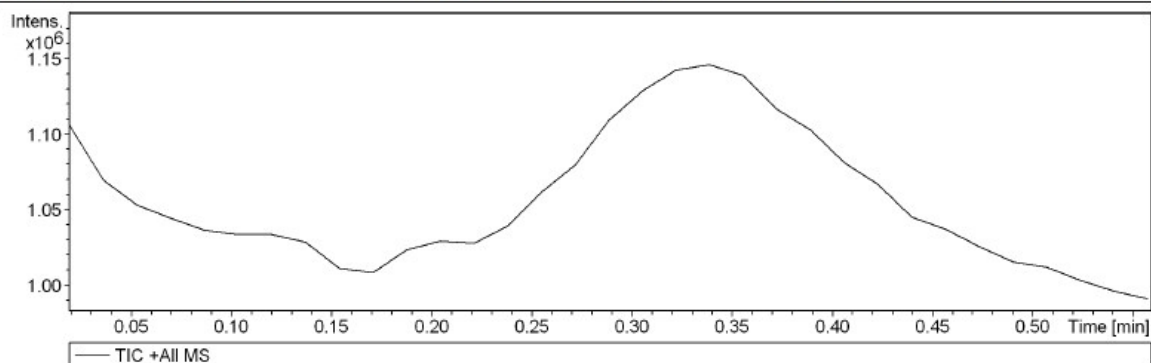
Analysis Info

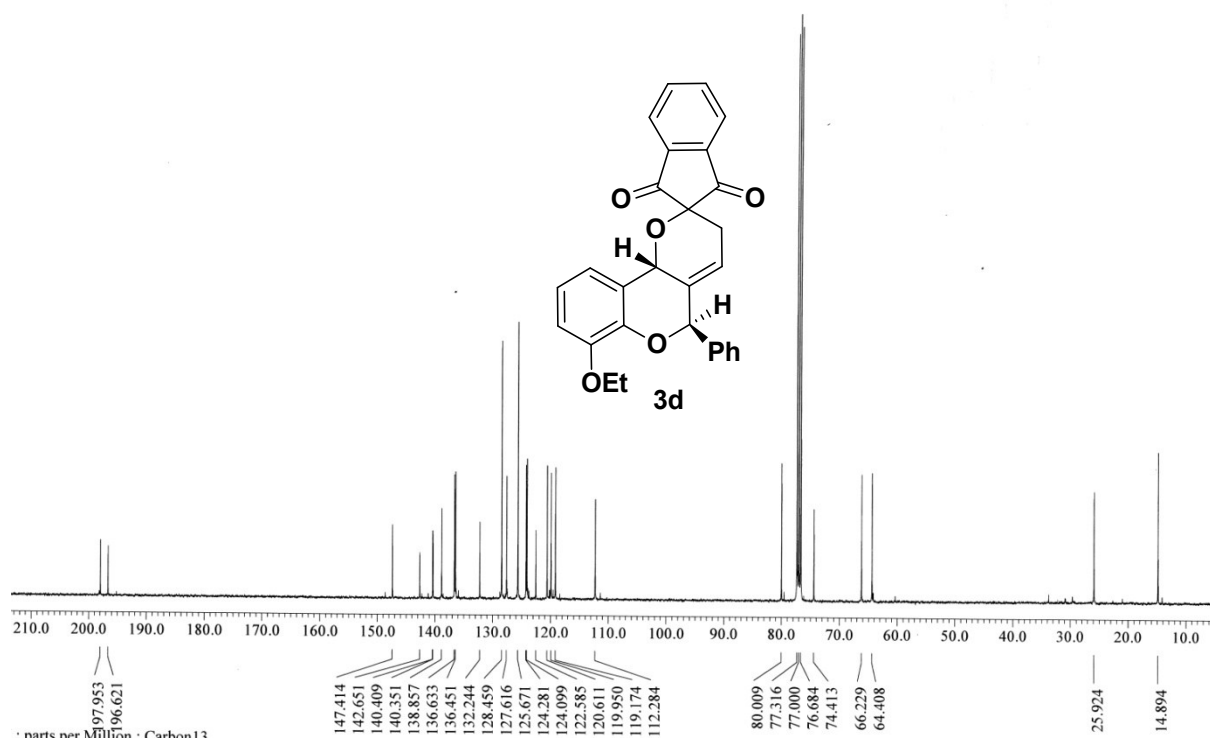
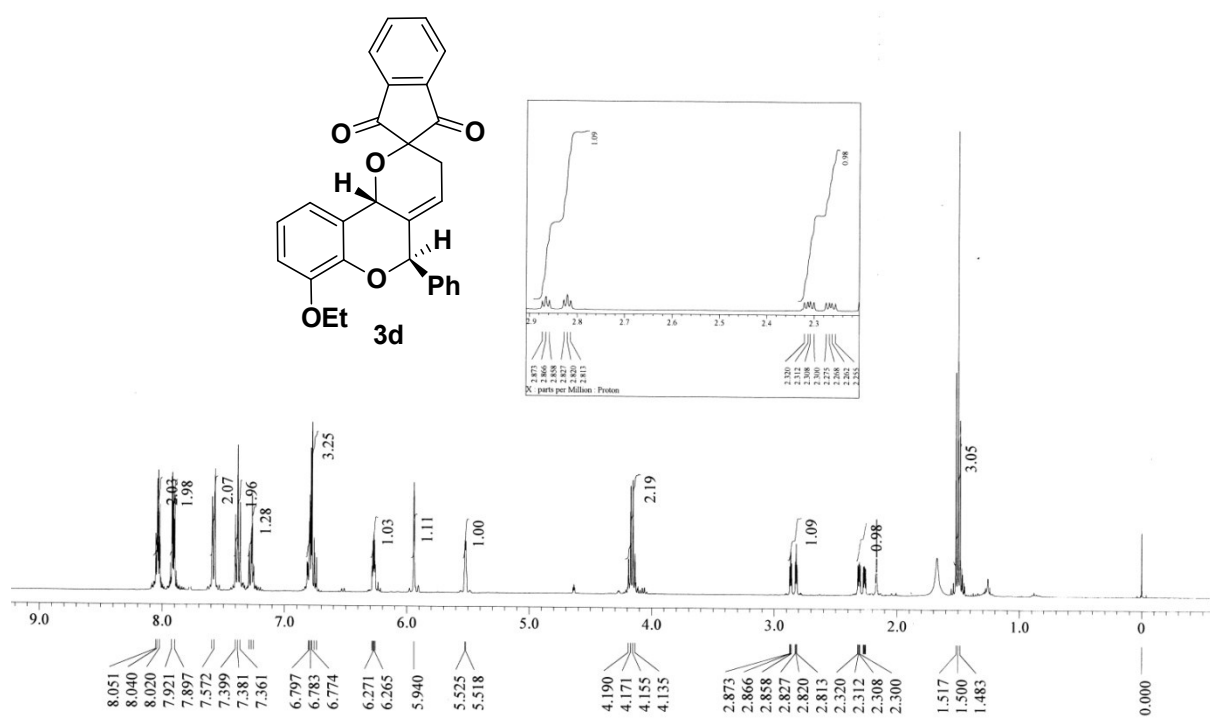
Analysis Name D:\Data\DEC-2016\NKS\GC\05092017_NKS_GC-PRA-153.d
Method Pos_tune_low.m
Sample Name 05092017_NKS_GC-stp
Comment

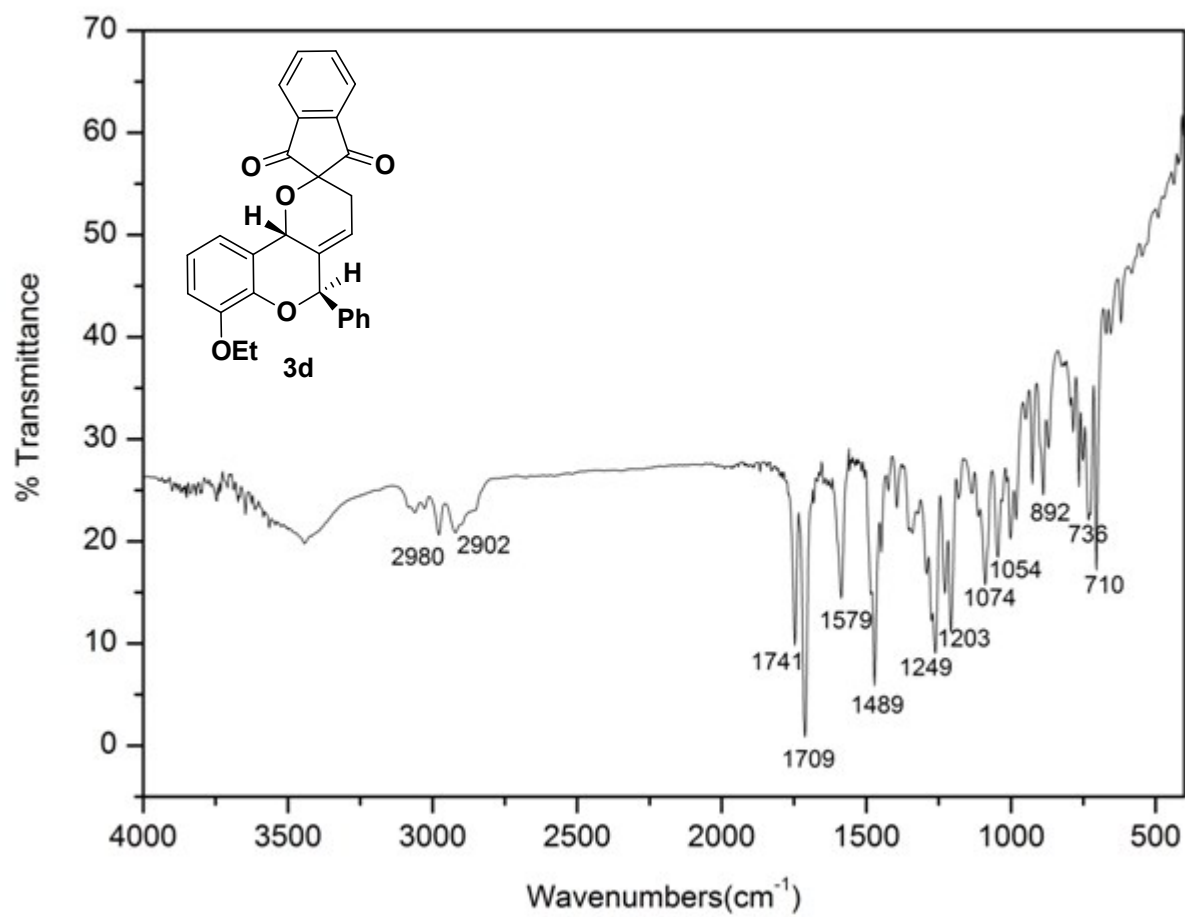
Acquisition Date 9/5/2017 7:58:34 PM
Operator G.C.S.Reddy
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste







Display Report

Analysis Info

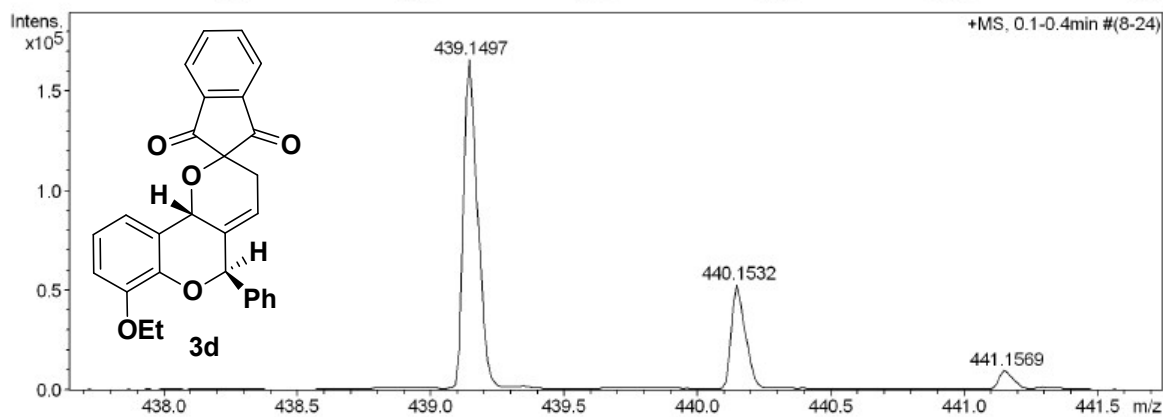
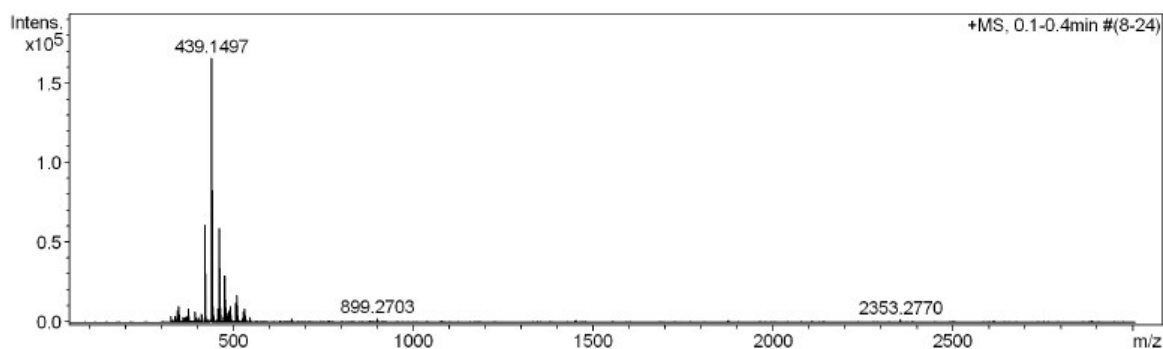
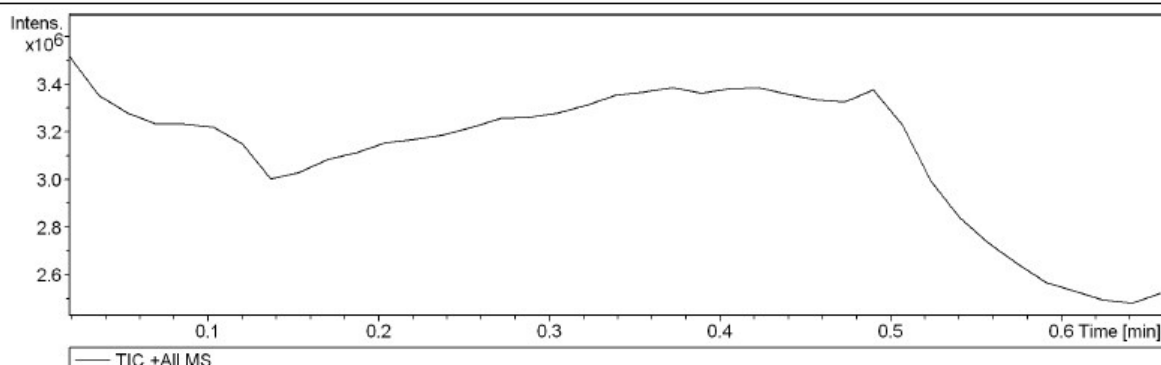
Analysis Name D:\Data\DEC-2016\NKS\GC\11102017_NKS_GC-PRA-169.d
Method pos tune_wide.m
Sample Name ESI-MS
Comment

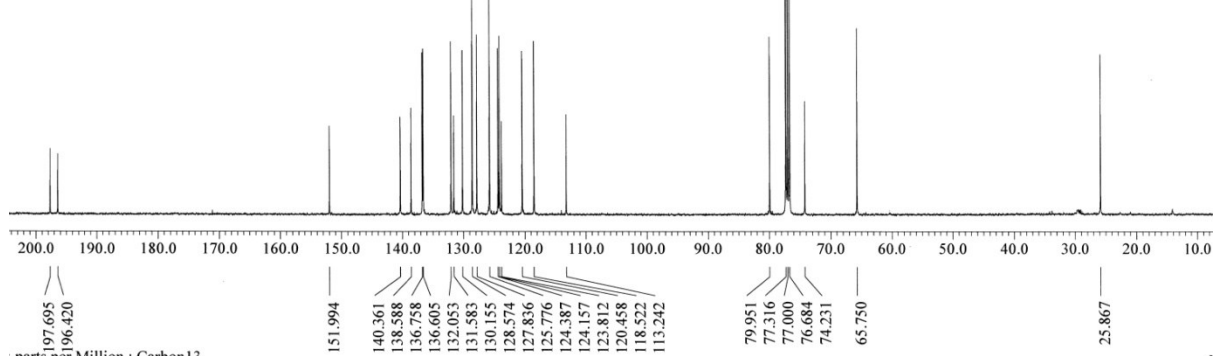
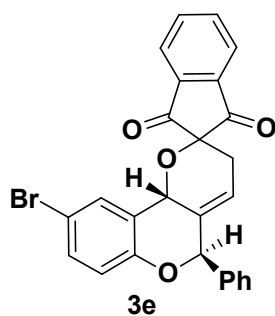
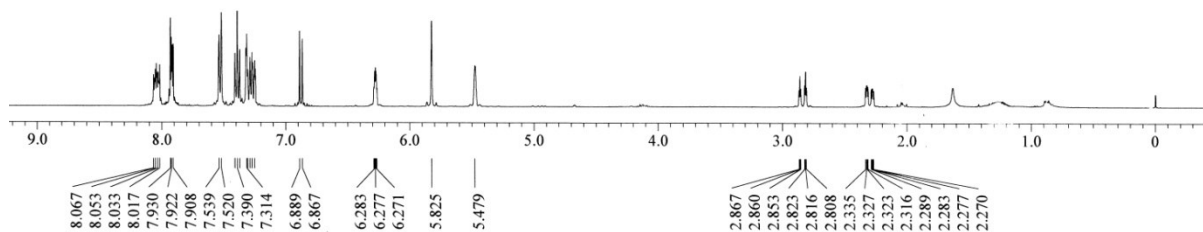
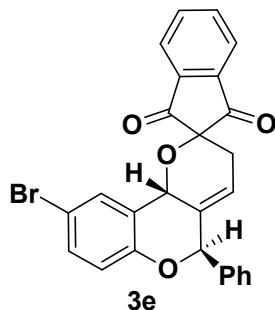
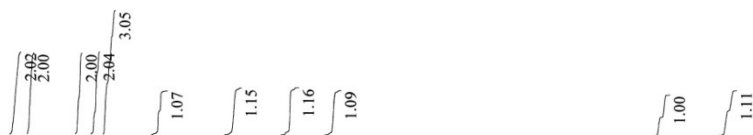
Acquisition Date 10/13/2017 8:26:43 PM

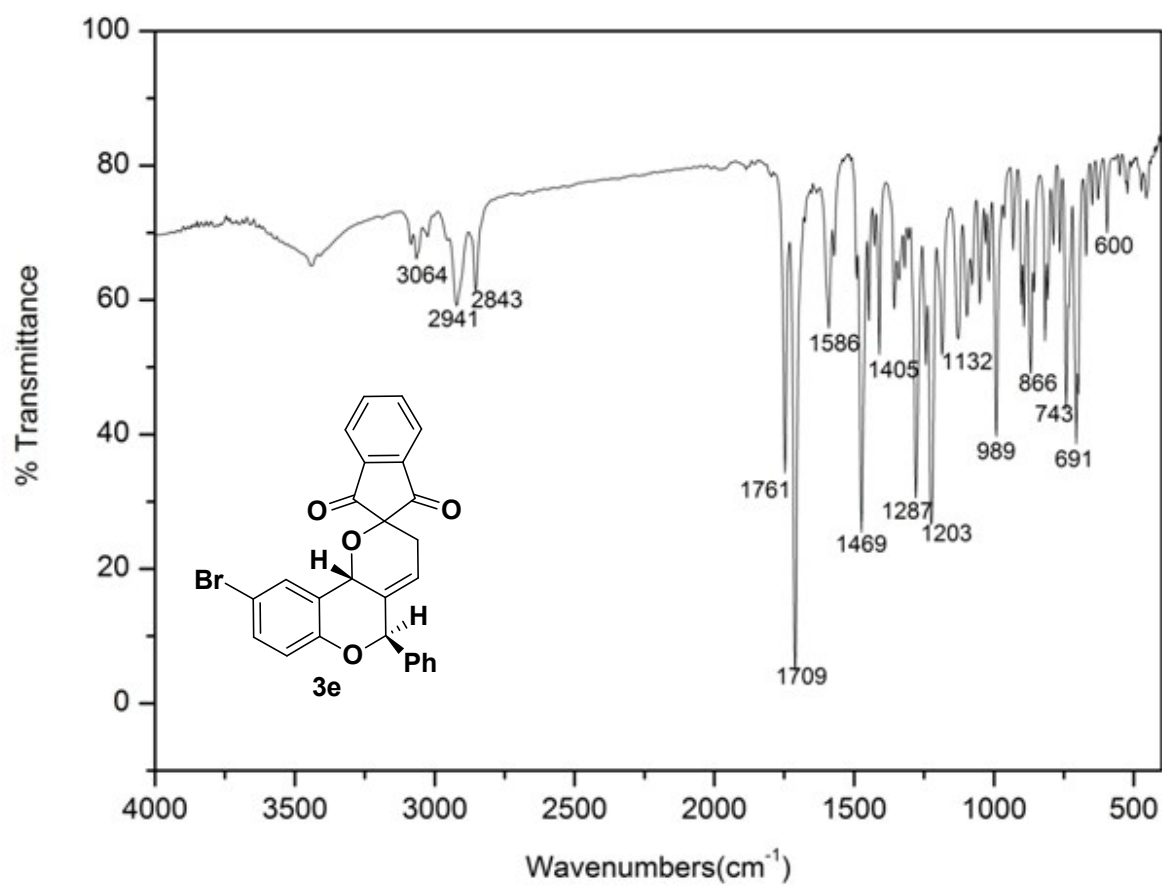
Operator G.CREDDY
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







Display Report

Analysis Info

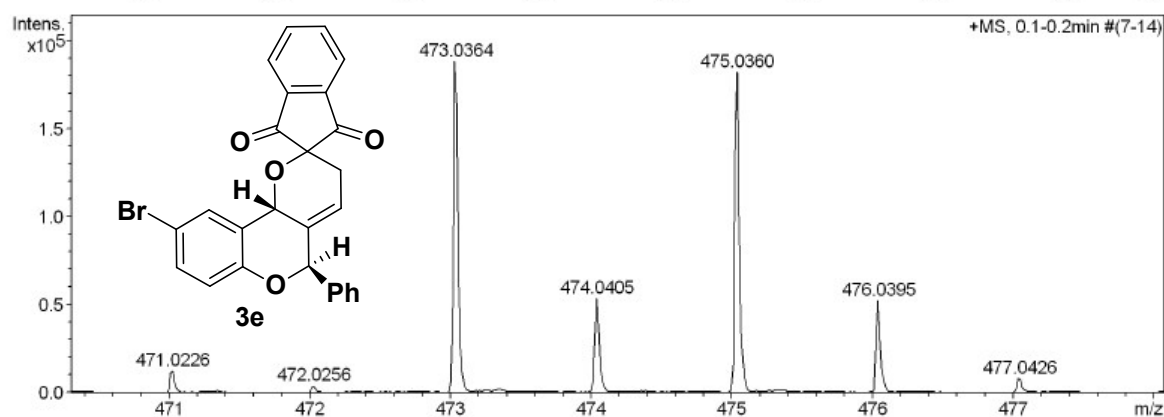
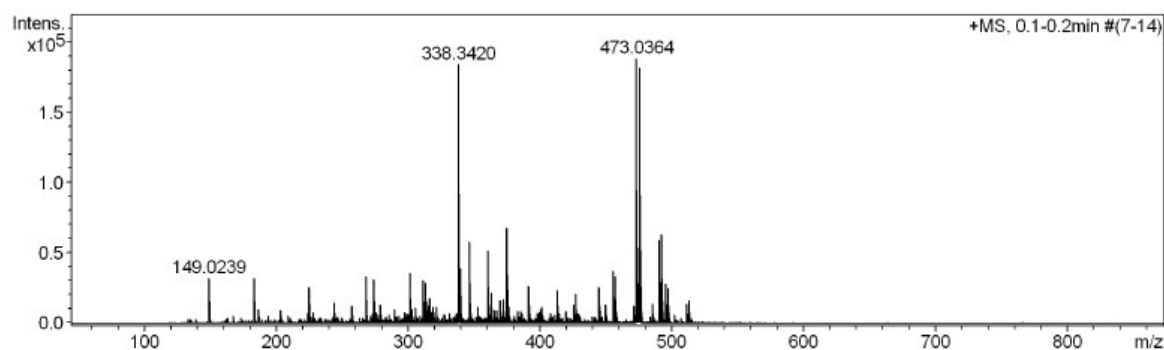
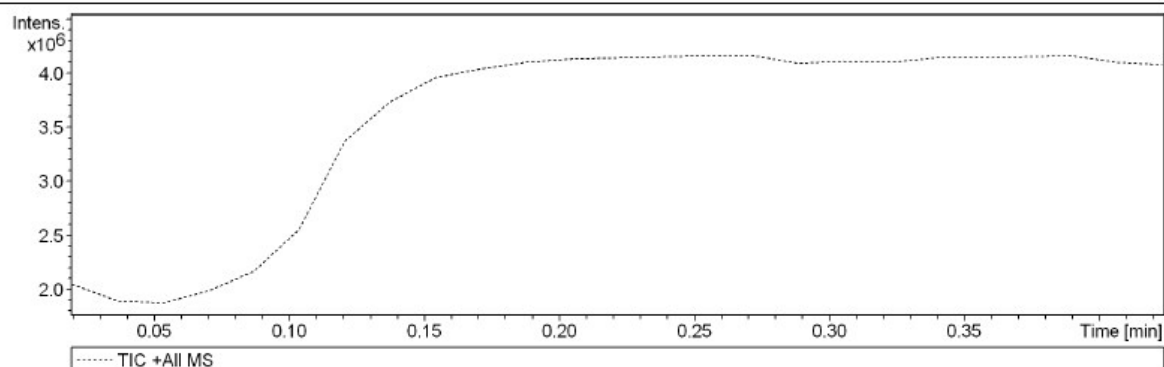
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Method Wash_pos tune_low_22092017.m
Sample Name ESI-MS
Comment

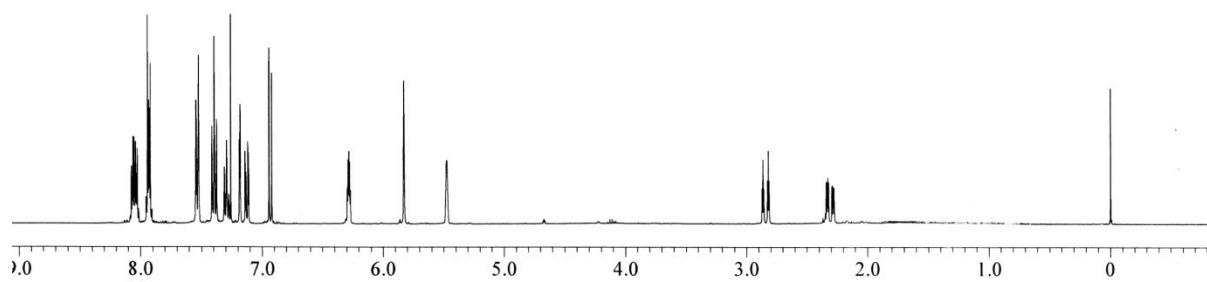
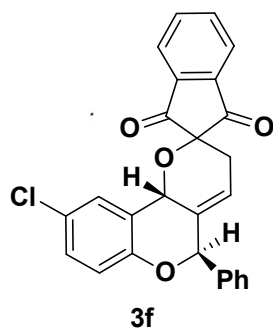
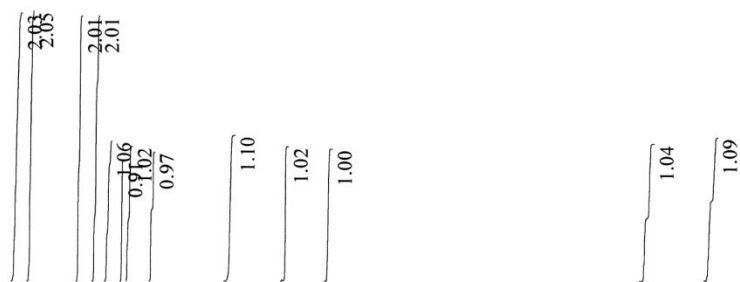
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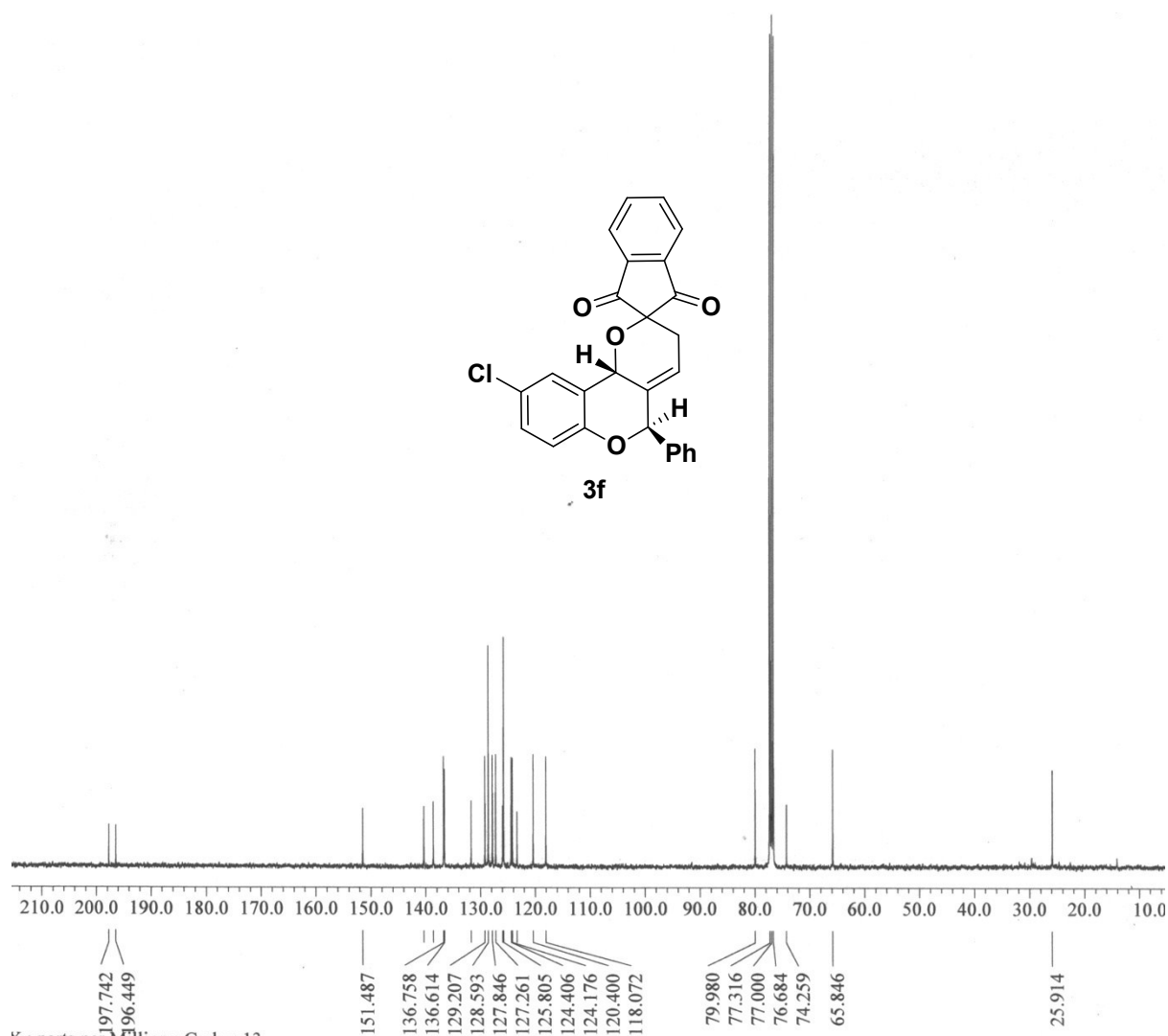
Operator G.CREDDY
Instrument microTOF-Q II 10337

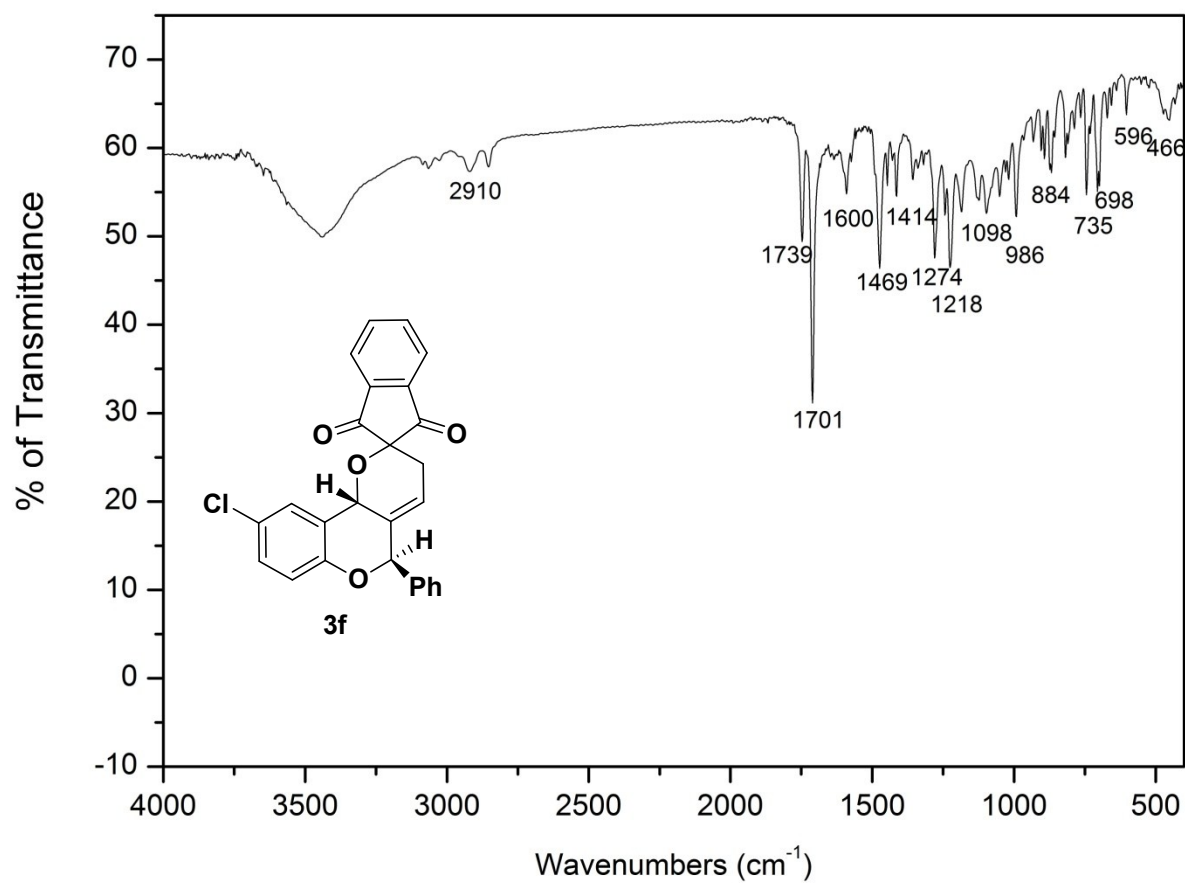
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source









Display Report

Analysis Info

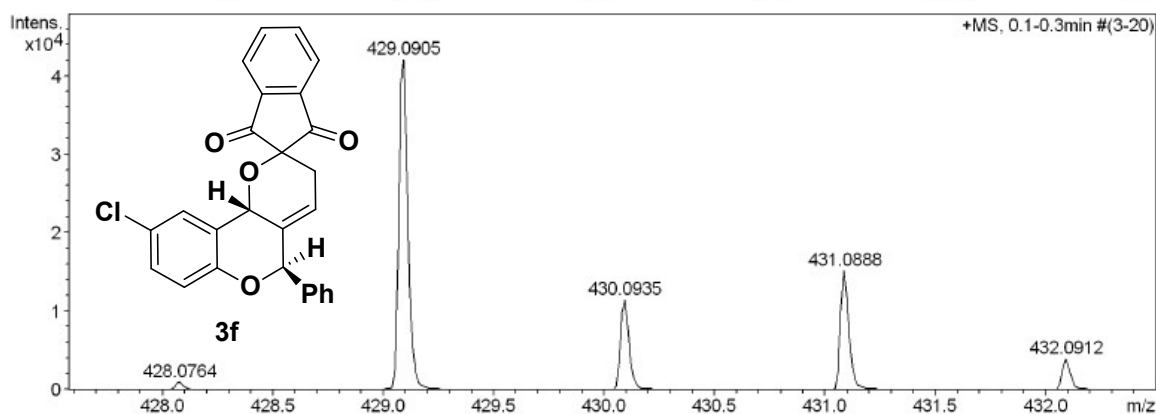
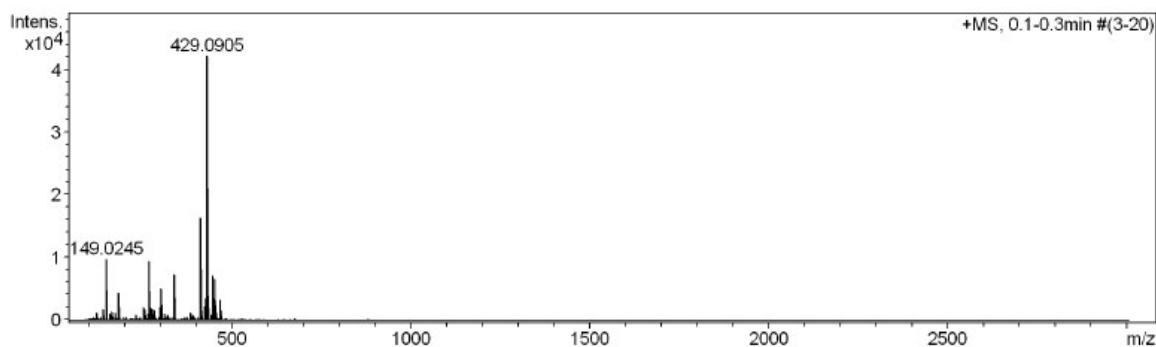
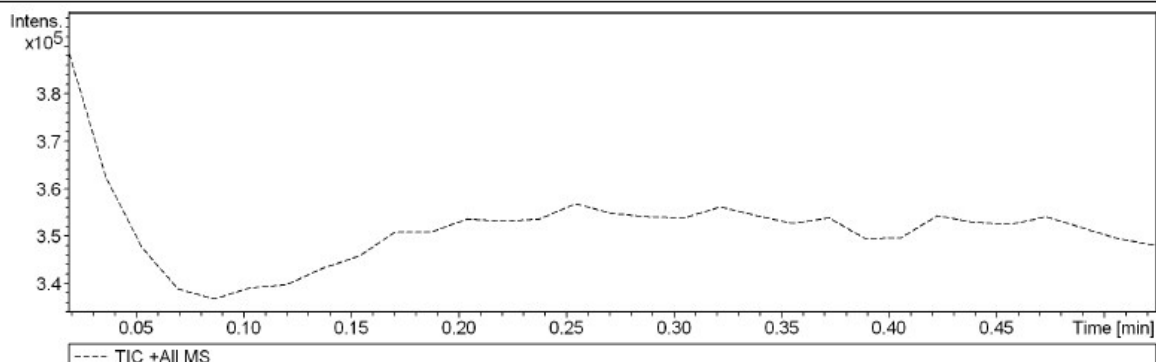
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Method Pos_tune_low.m
Sample Name 05092017_NKS_GC-stp
Comment

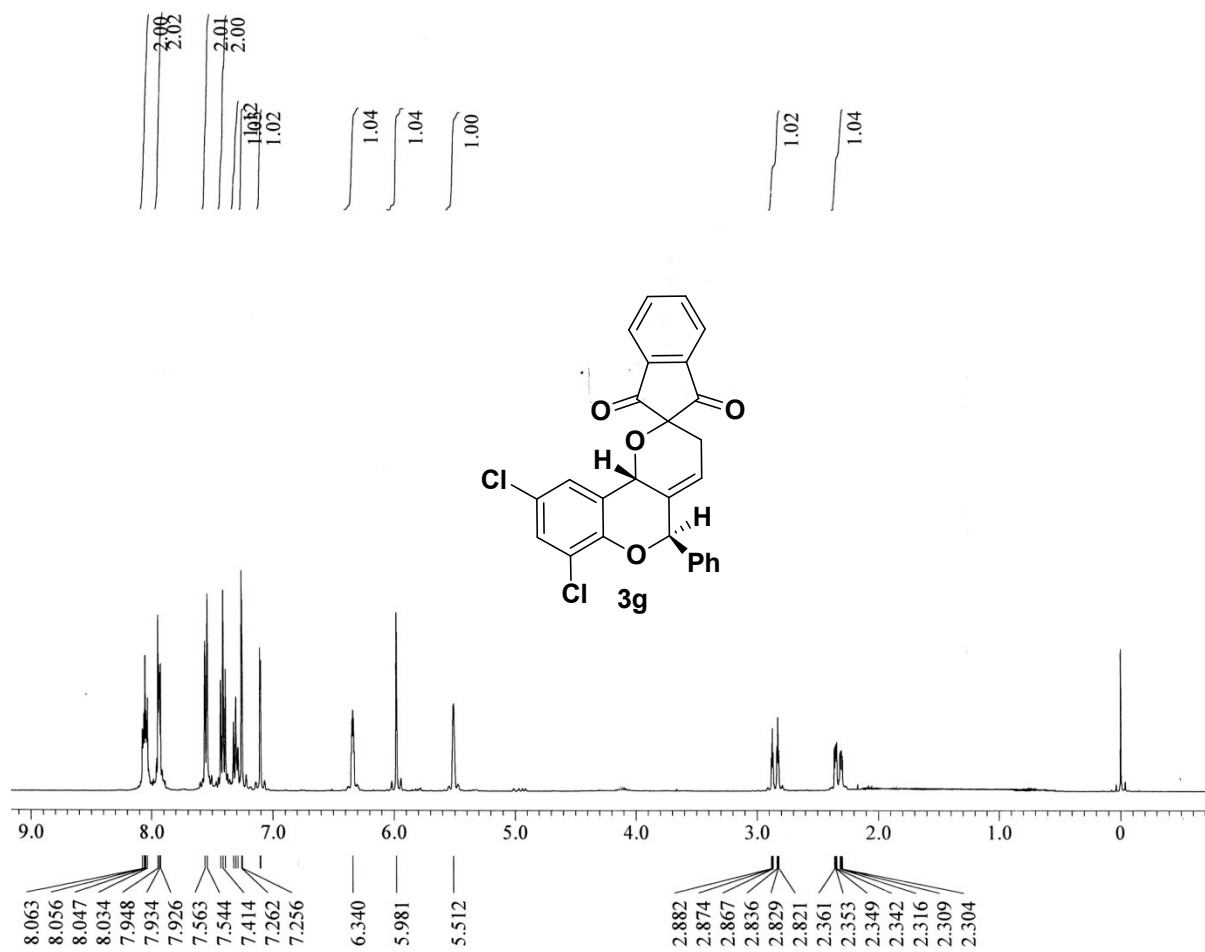
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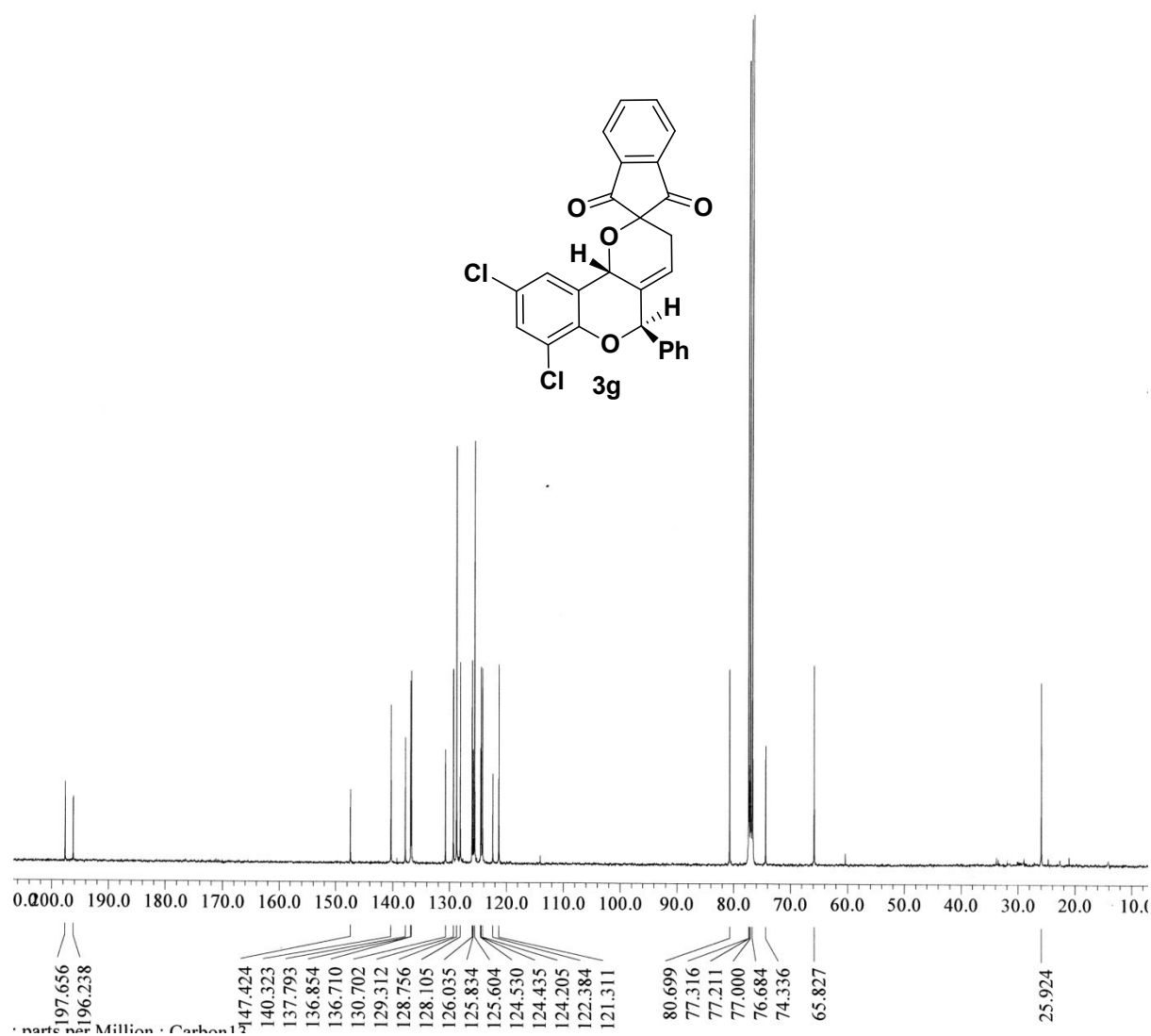
Operator G.C.S.Reddy
Instrument micrOTOF-Q II 10337

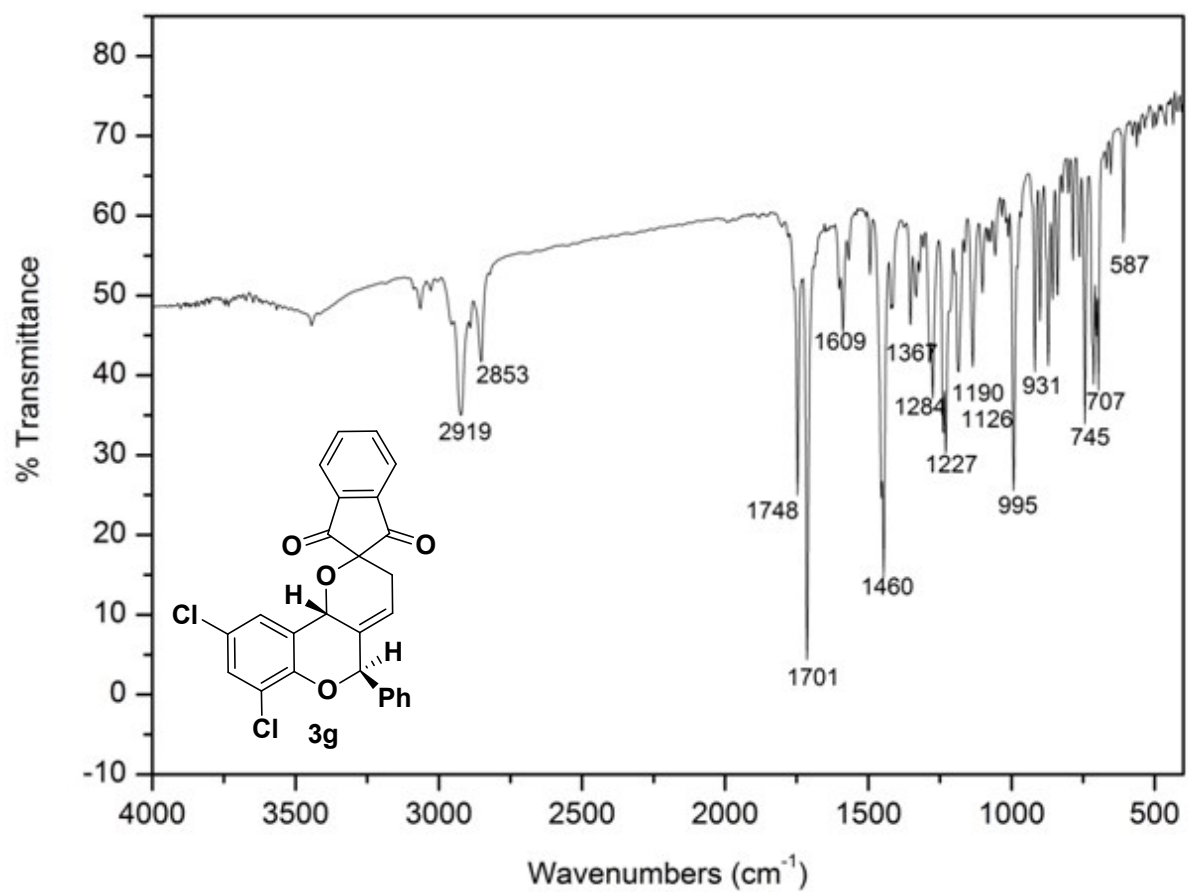
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste









Display Report

Analysis Info

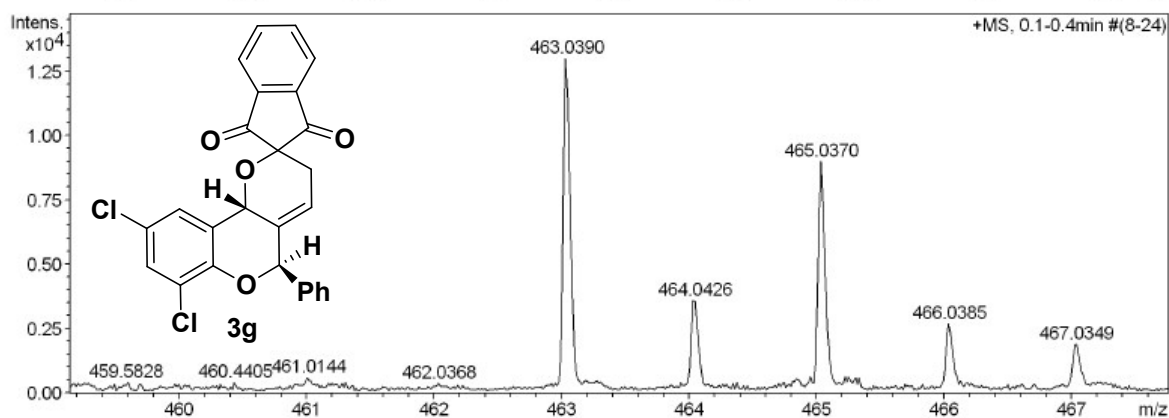
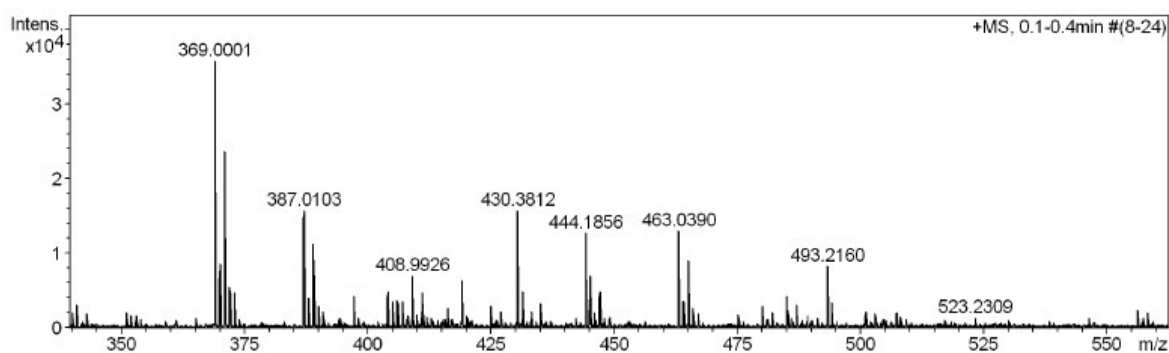
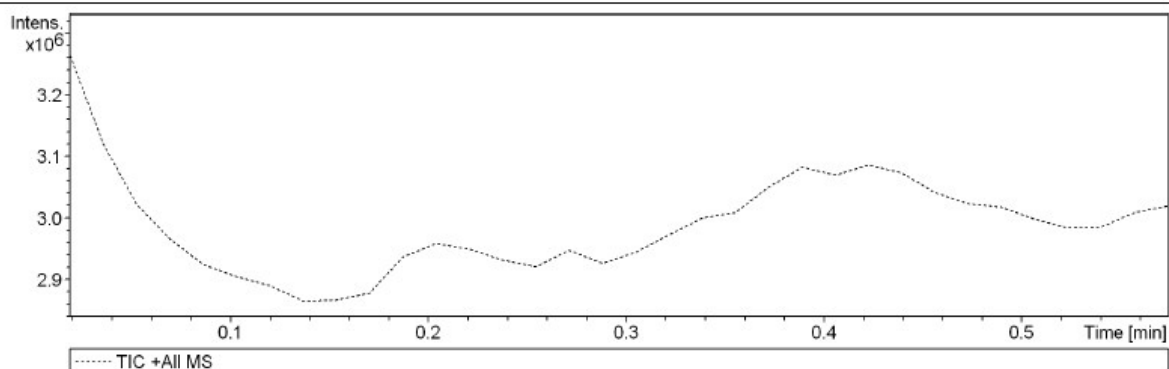
Analysis Name D:\Data\DEC-2016\NKS\GC\06102017_NKS_GC_PRA-160.d
Method Pso_tune_wide.m
Sample Name ESI-MS
Comment

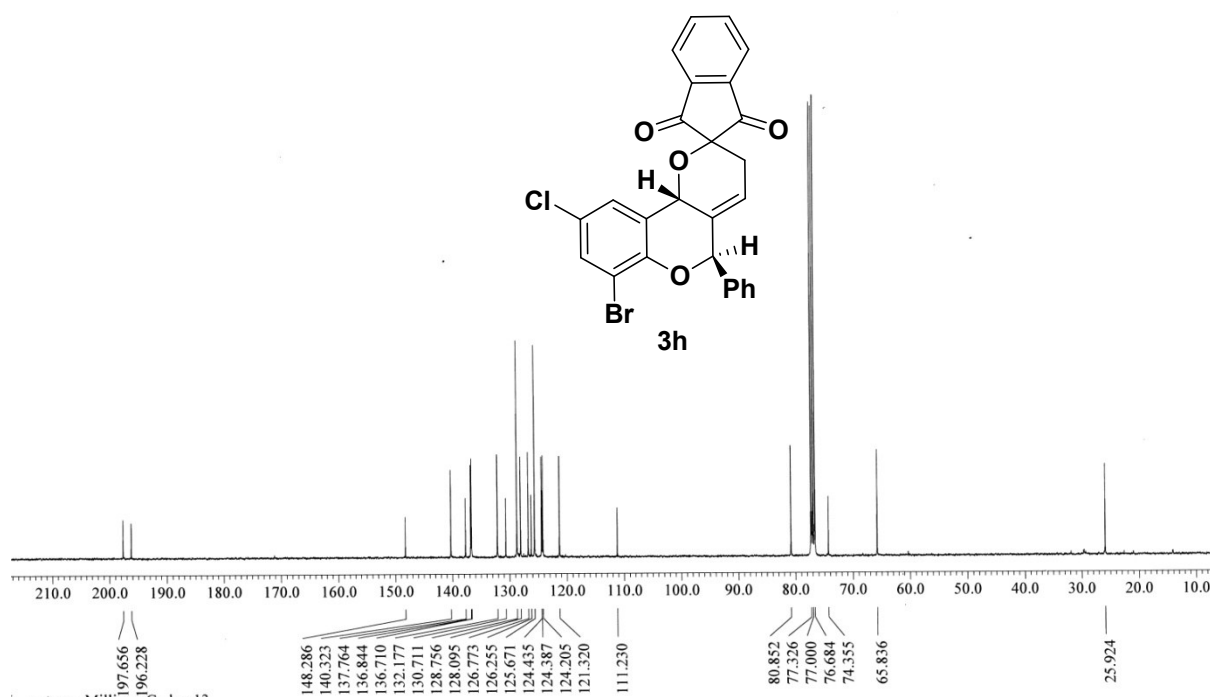
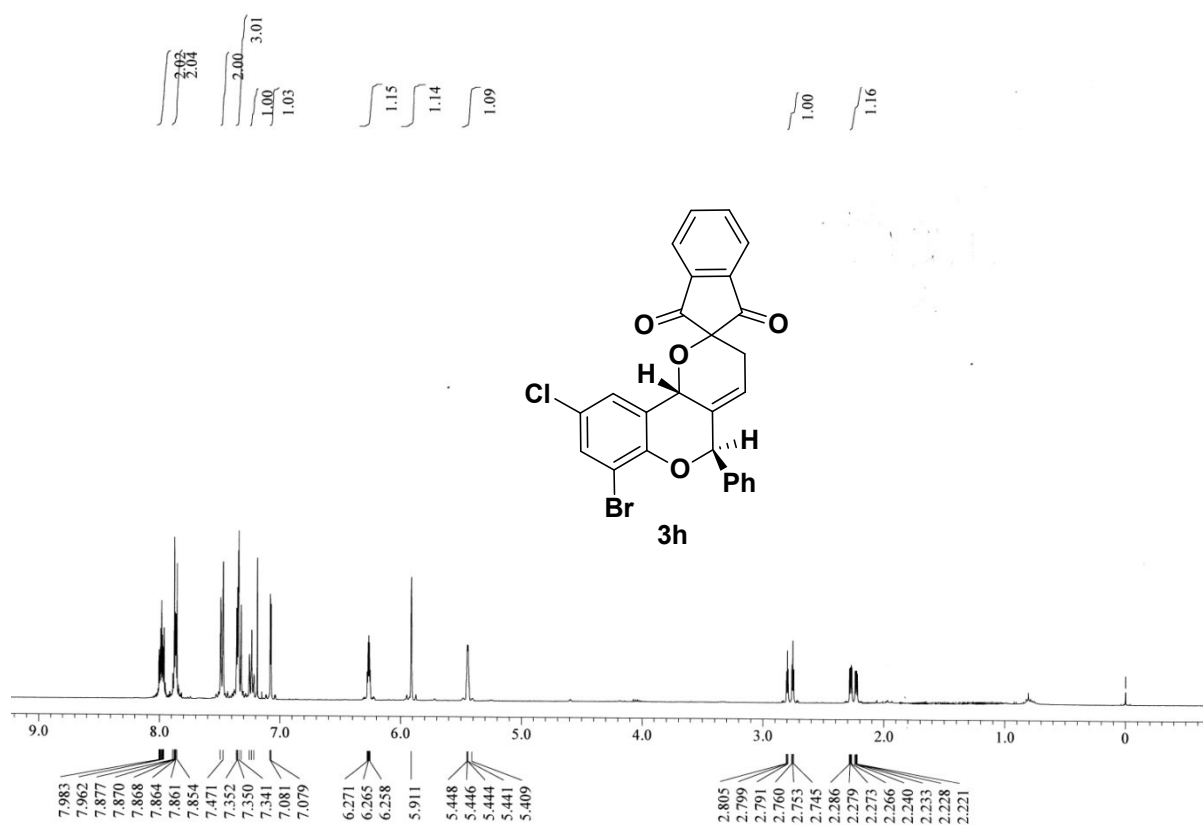
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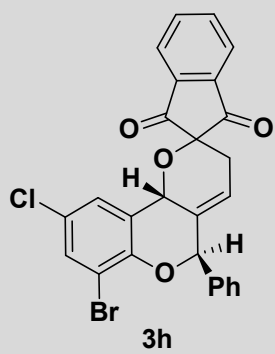
Operator Amit S.Sahu
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







Display Report

Analysis Info

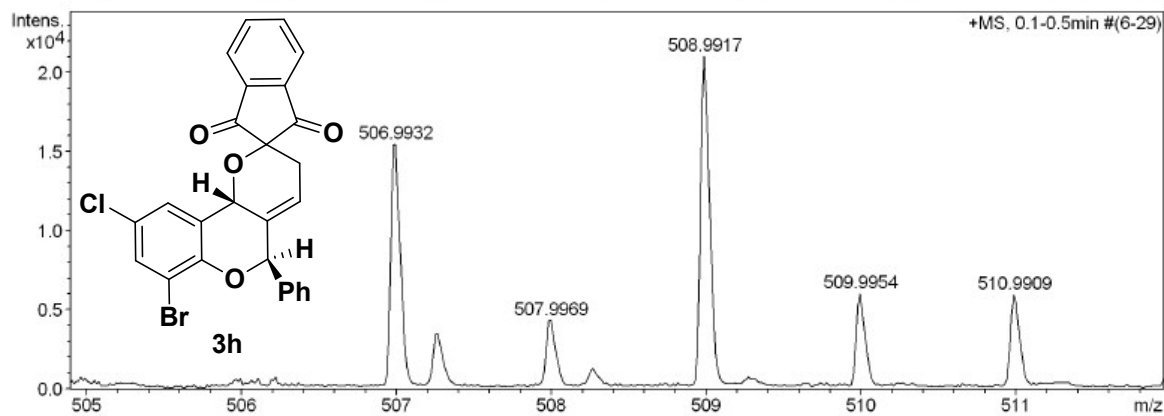
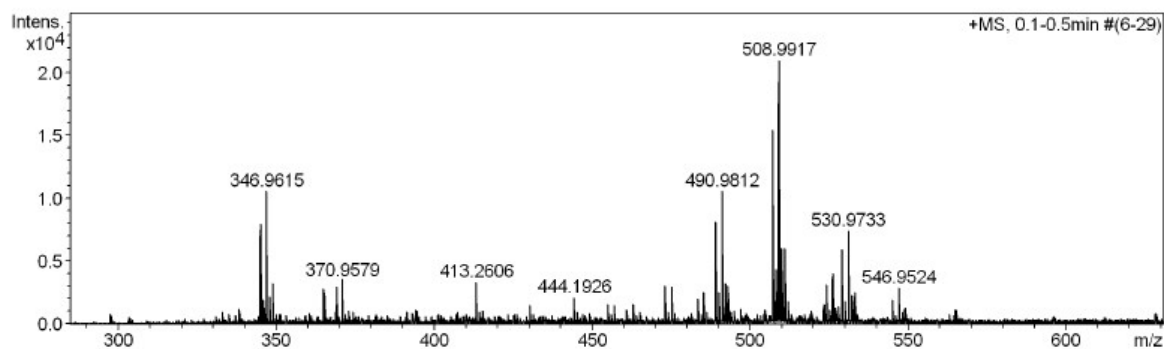
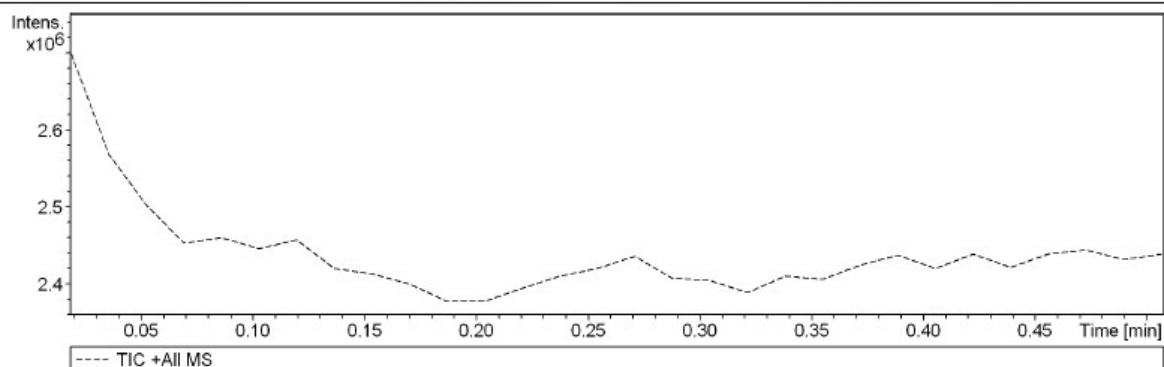
Analysis Name D:\Data\DEC-2016\NKS\GC\11102017_NKS_GC-PRA-166.d
Method pos tune_wide.m
Sample Name ESI-MS
Comment

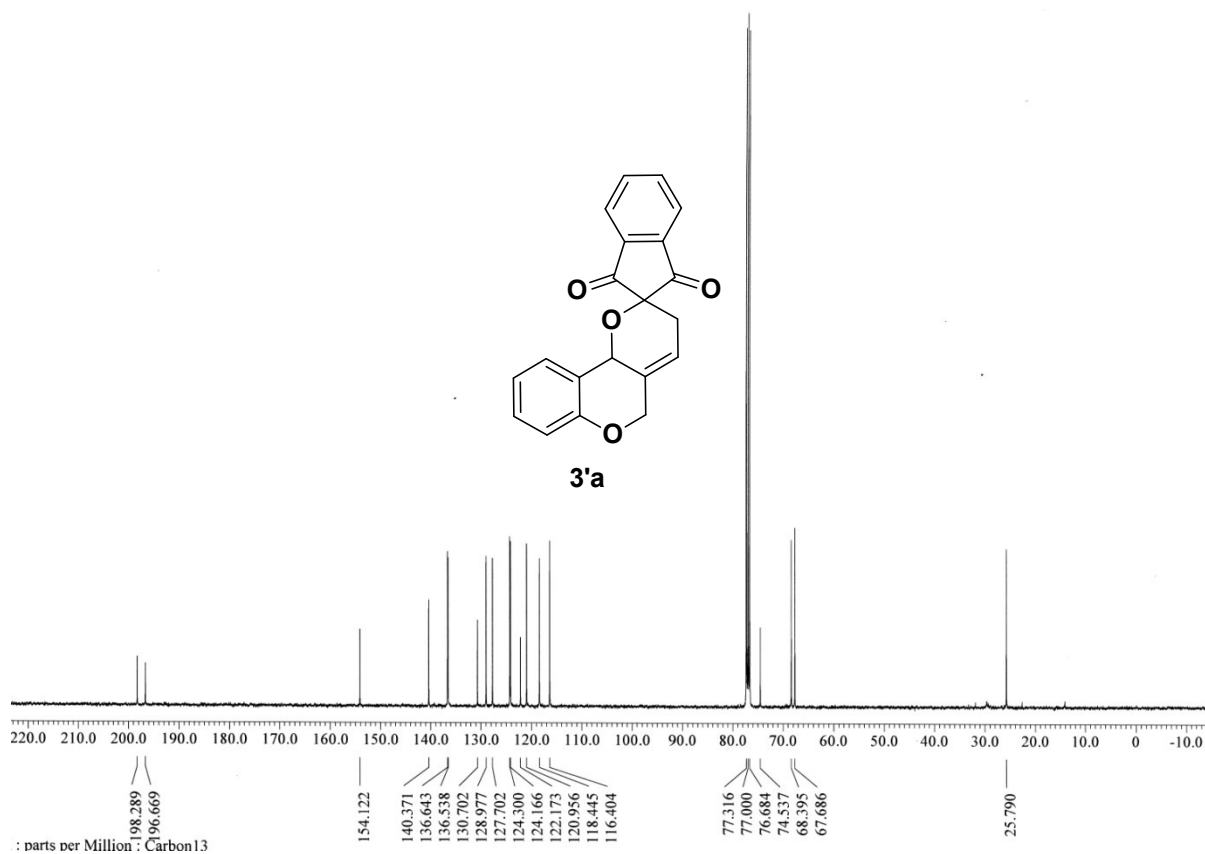
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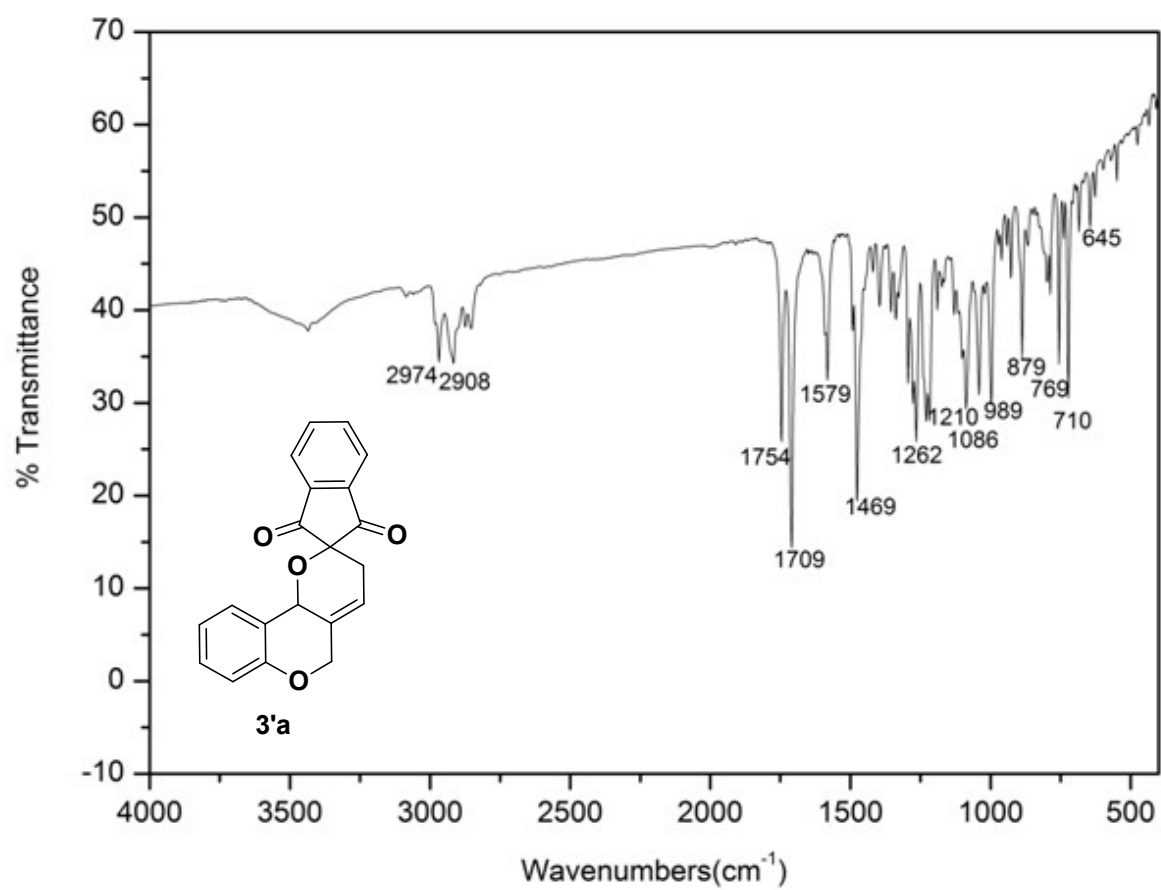
Operator G.CREDDY
Instrument micrOTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







Display Report

Analysis Info

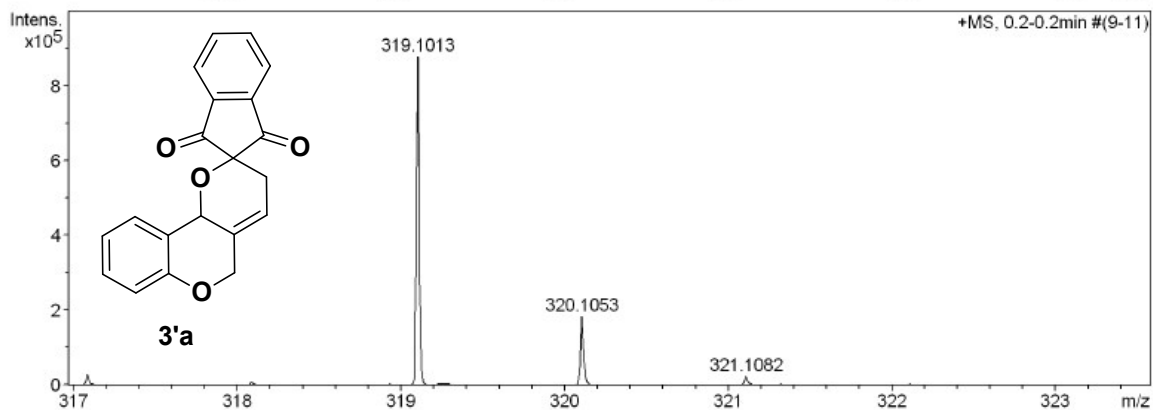
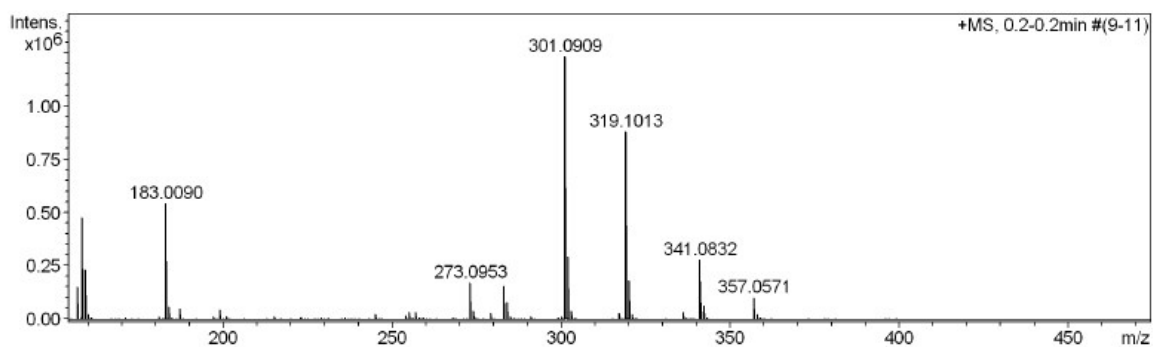
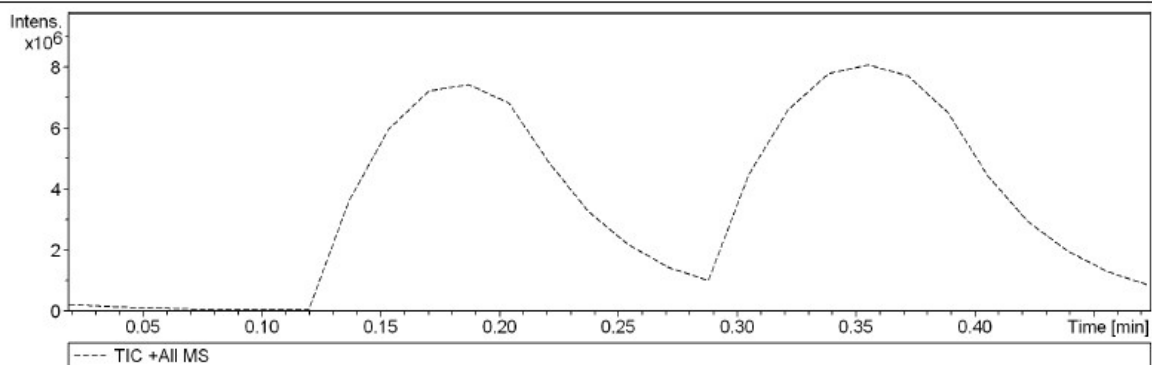
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Method Wash.pos tune_low_22092017.m
Sample Name ESI-MS
Comment

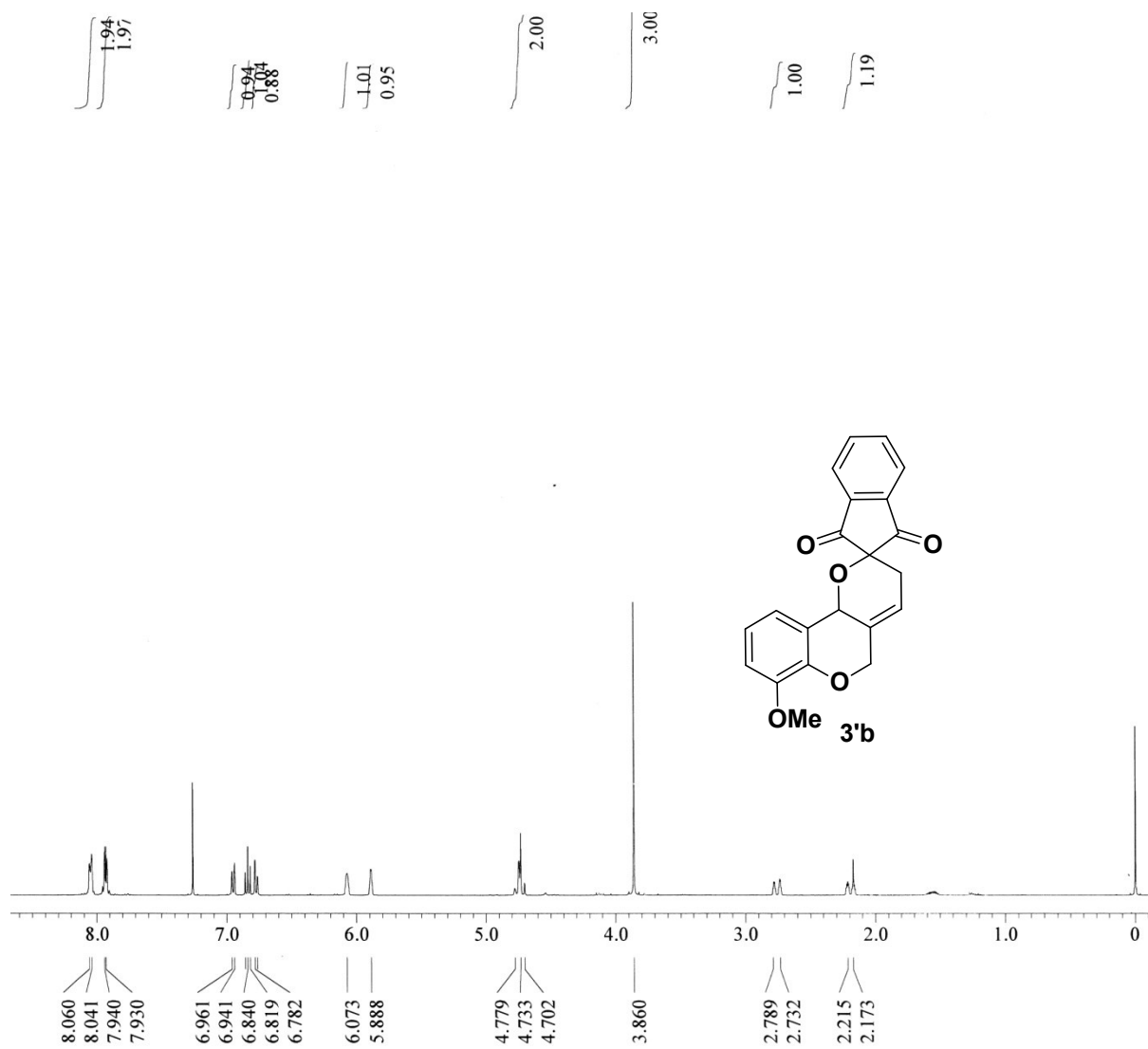
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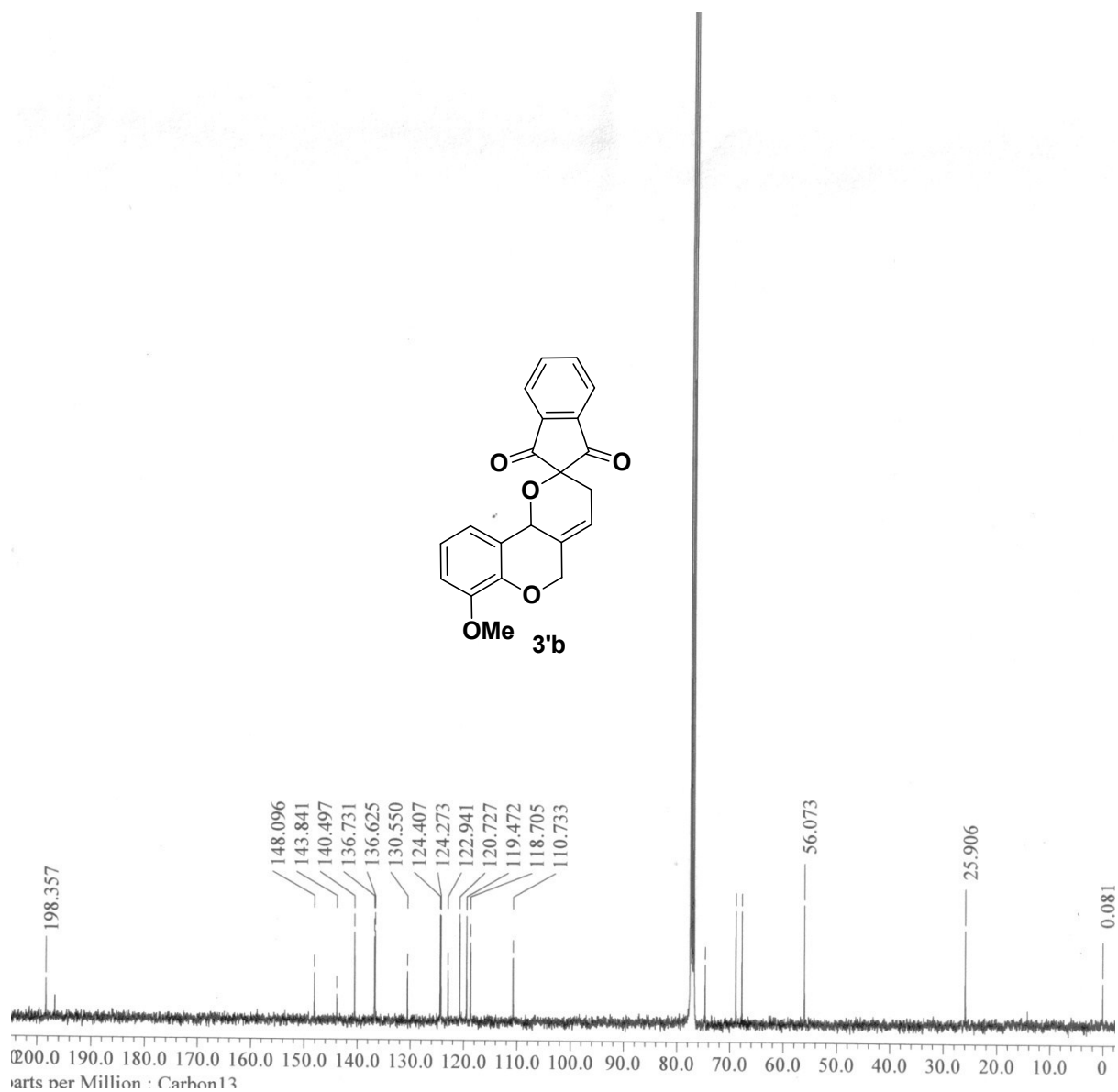
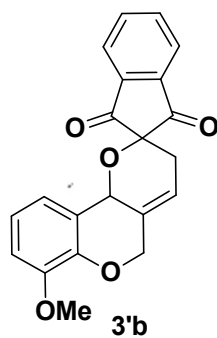
Operator Amit S.Sahu
Instrument microTOF-Q II 10337

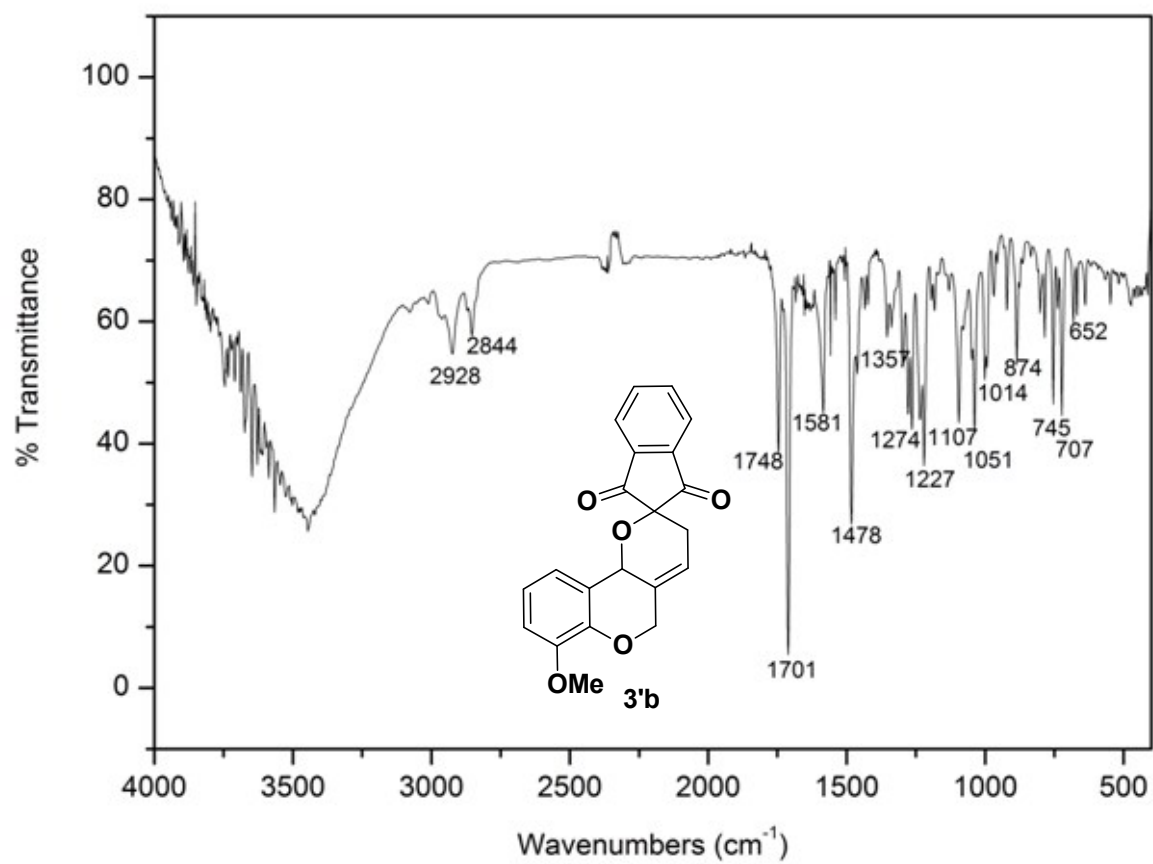
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source









Display Report

Analysis Info

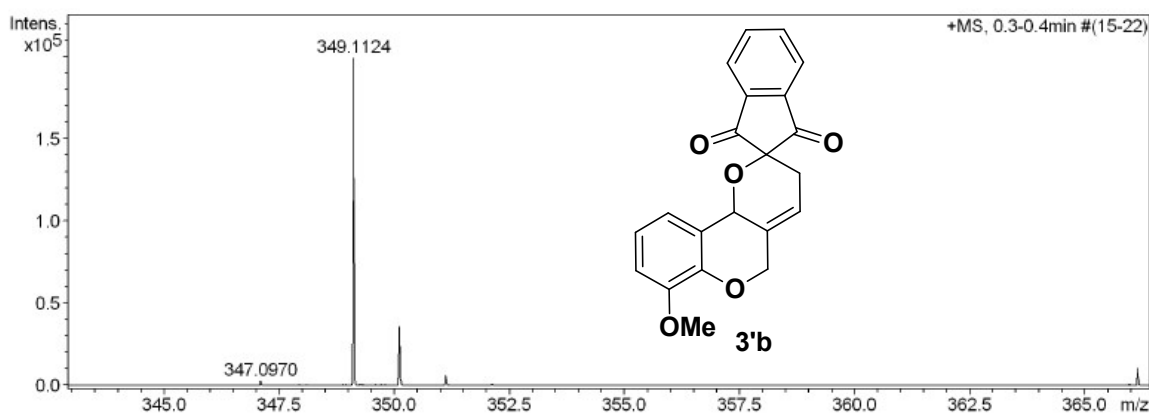
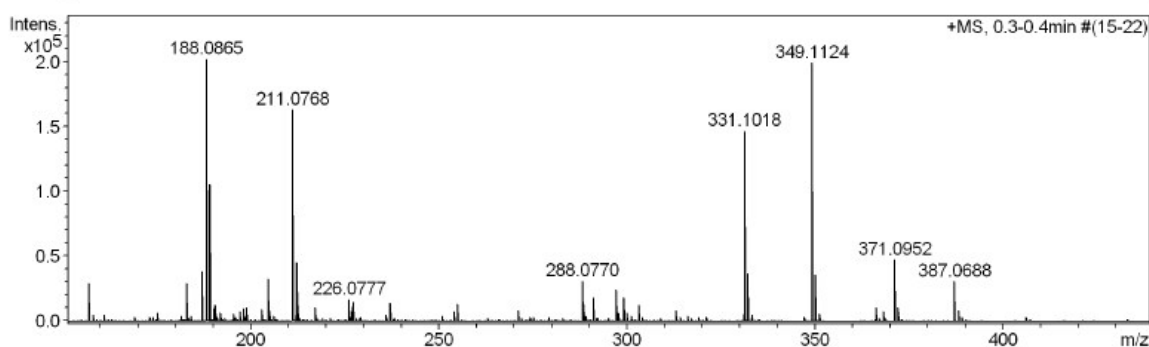
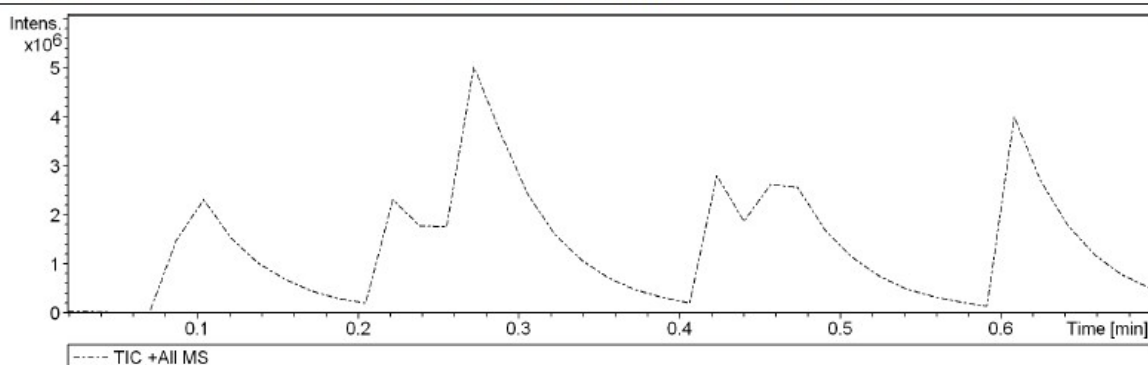
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Method Wash.pos tune_low_22092017.m
Sample Name ESI-MS
Comment

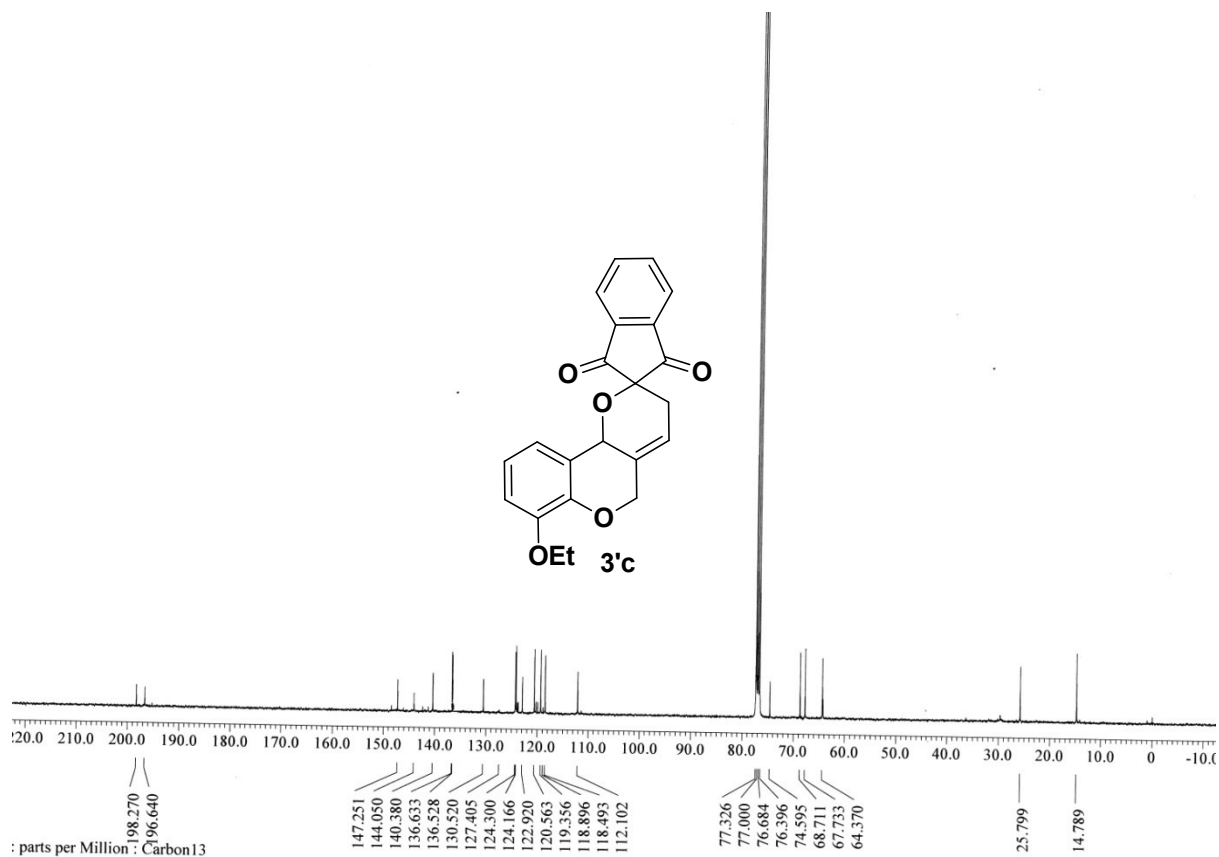
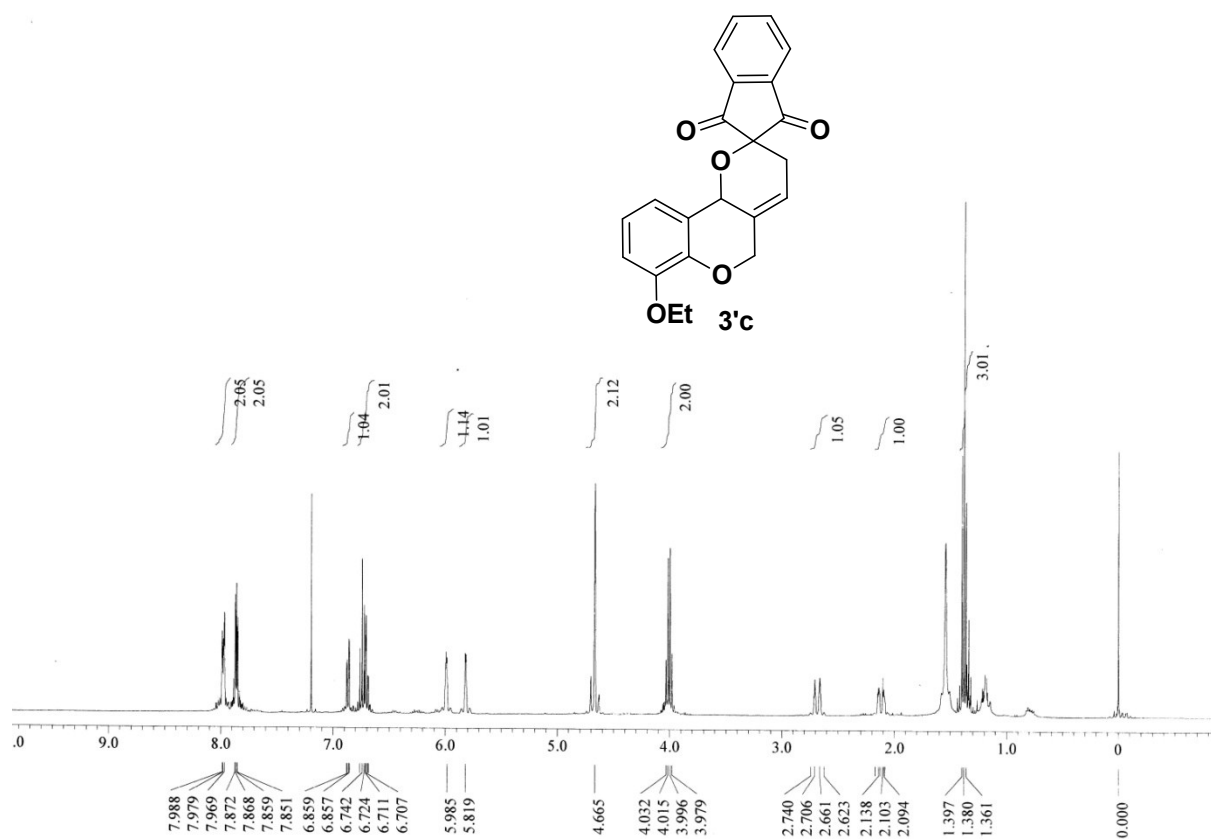
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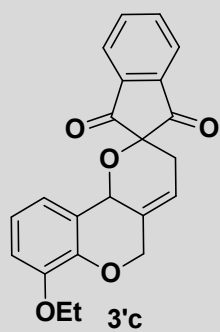
Operator G.CREDDY
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source







Display Report

Analysis Info

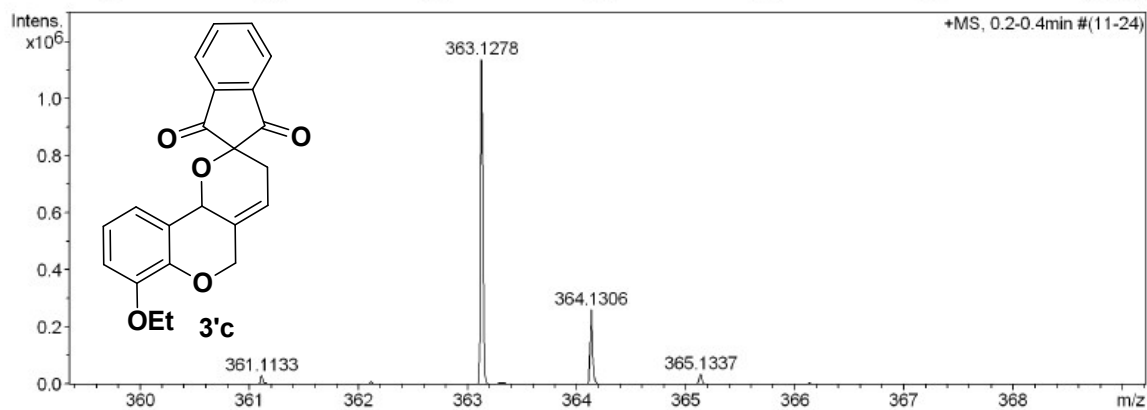
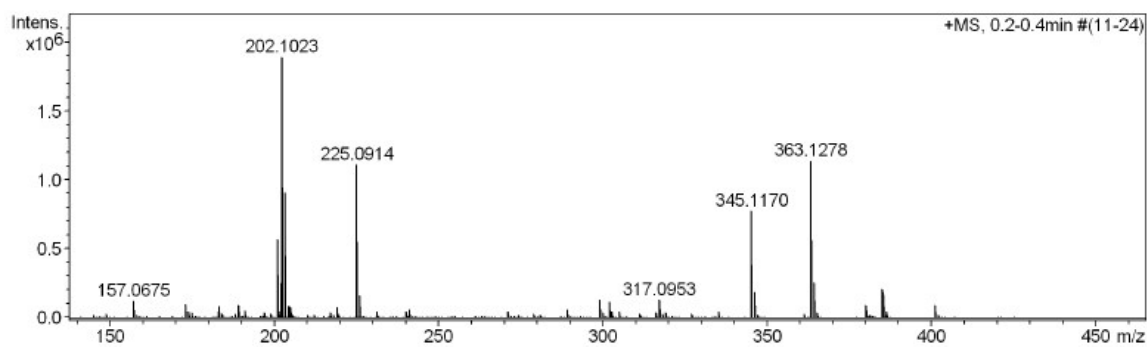
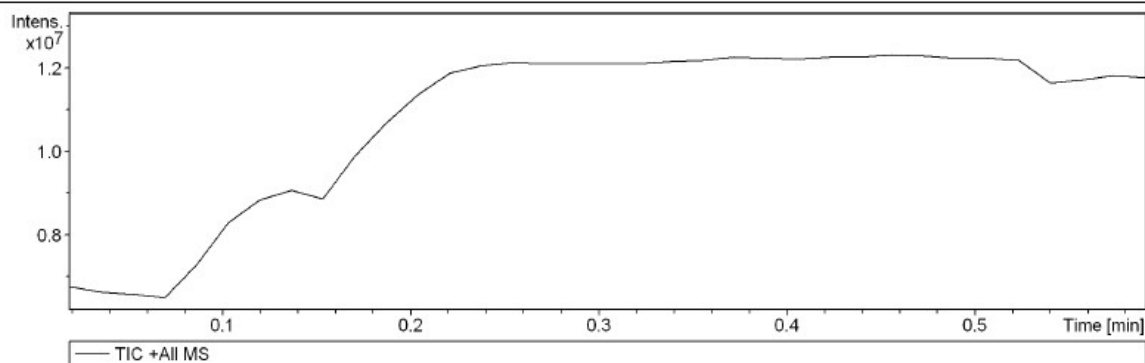
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Method Wash.pos tune_low_22092017.m
Sample Name ESI-MS
Comment

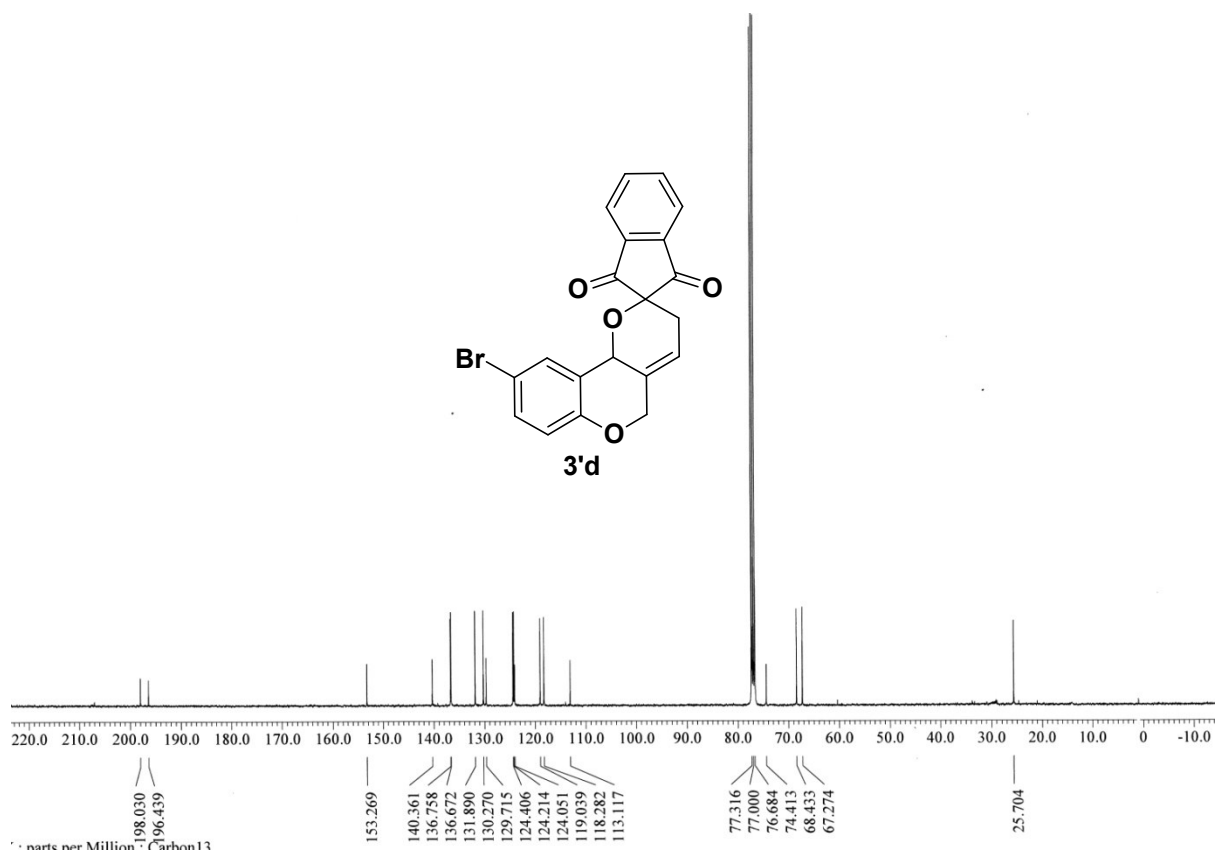
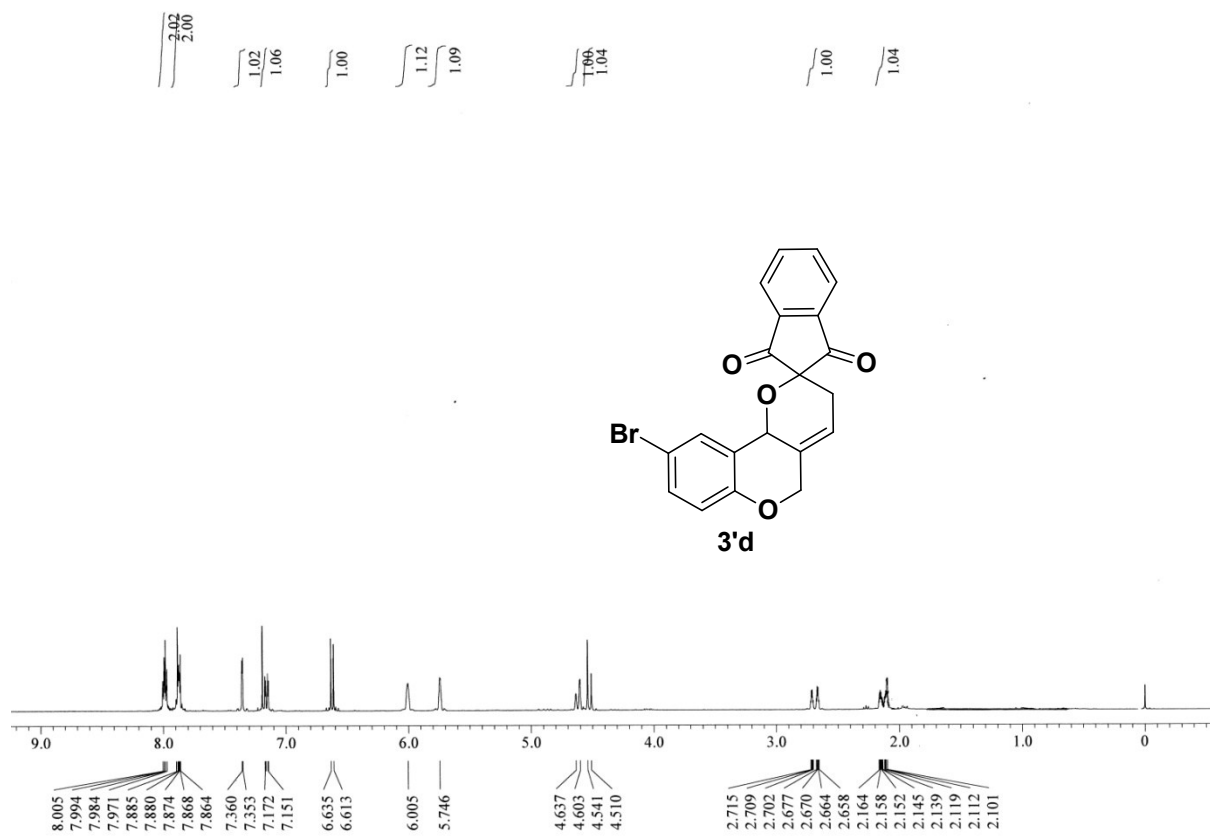
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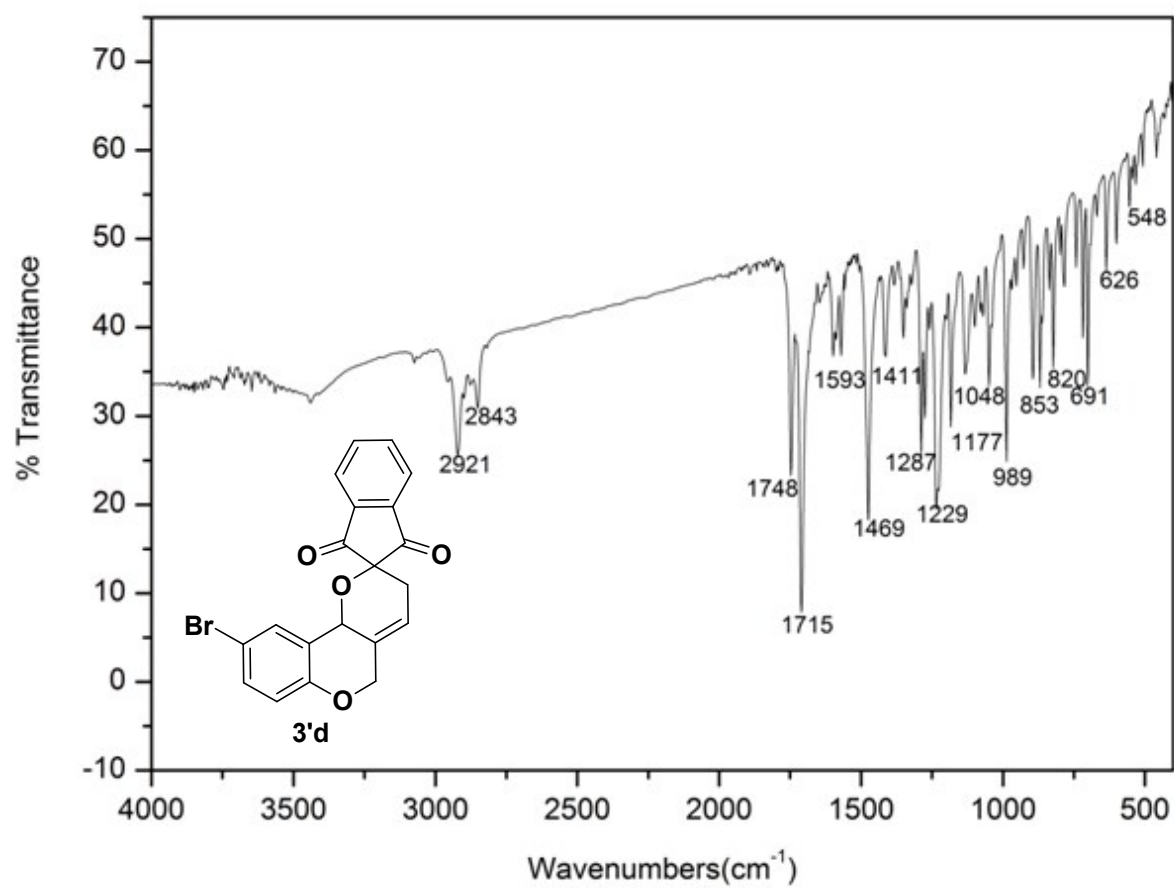
Operator G.CREDDY
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	200.0 Vpp	Set Divert Valve	Source







Display Report

Analysis Info

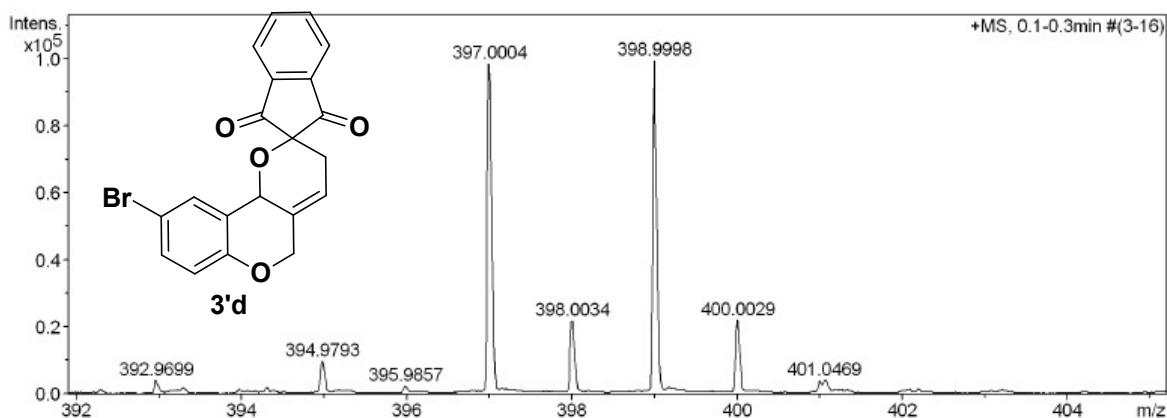
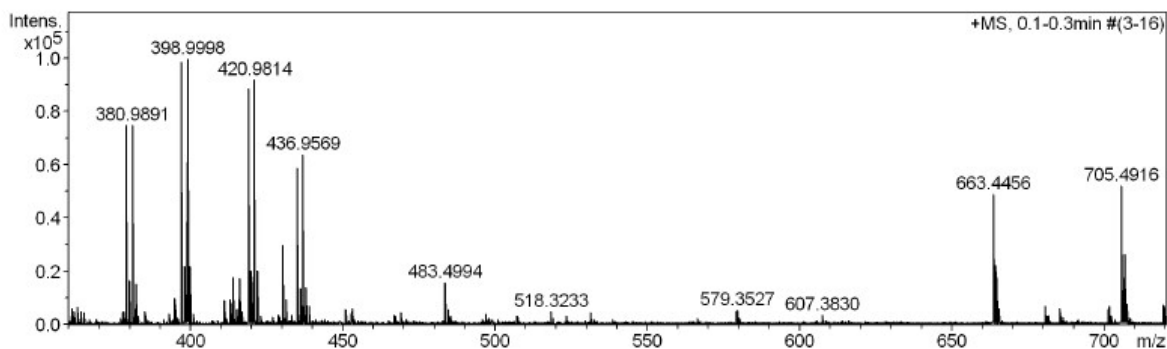
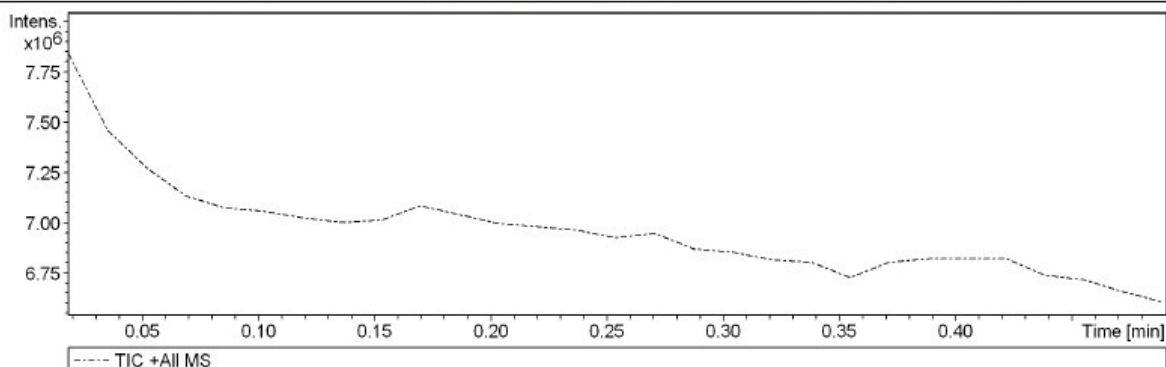
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Method pos tune_wide.m
Sample Name ESI-MS
Comment

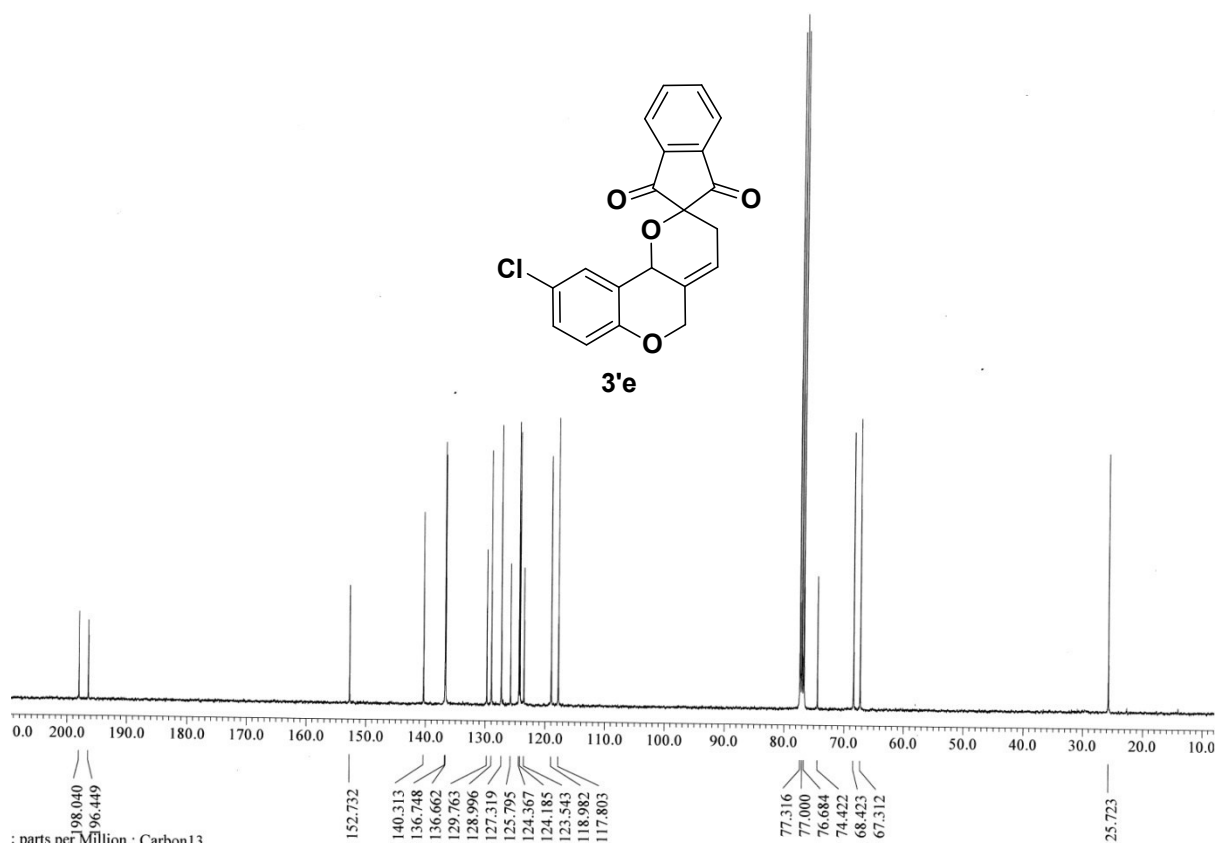
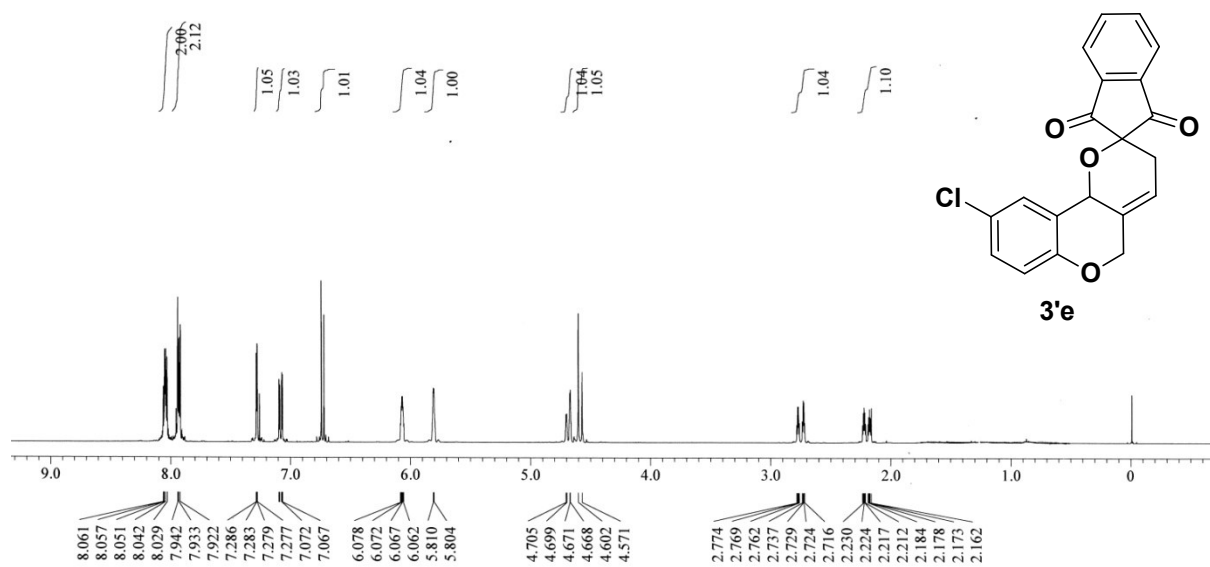
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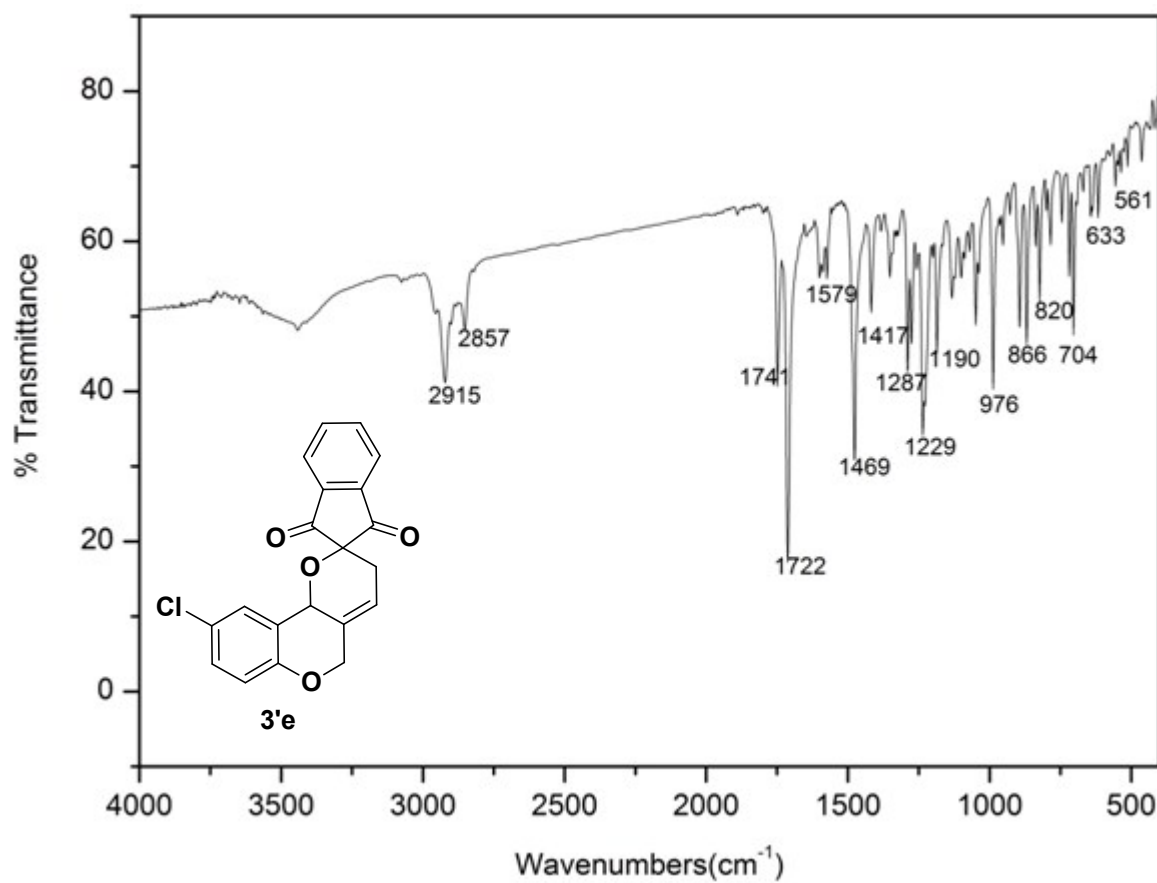
Operator G.CREDDY
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste







Display Report

Analysis Info

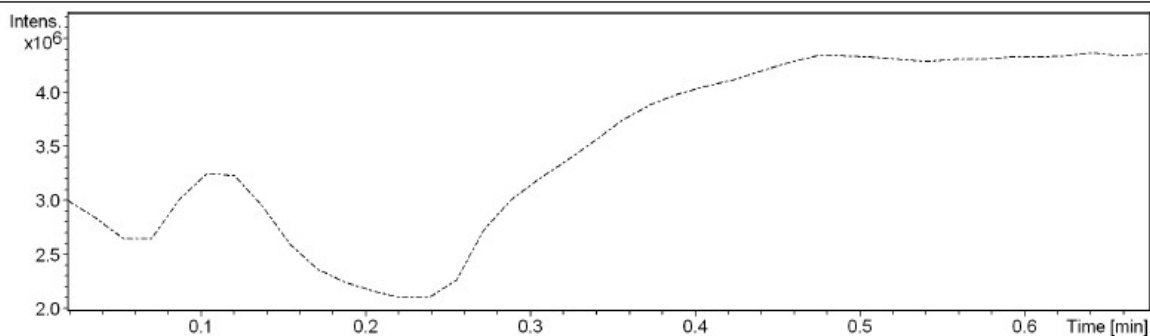
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Method Pso_tune_wide.m
Sample Name ESI-MS
Comment

Acquisition Date 10/8/2017 7:16:03 PM

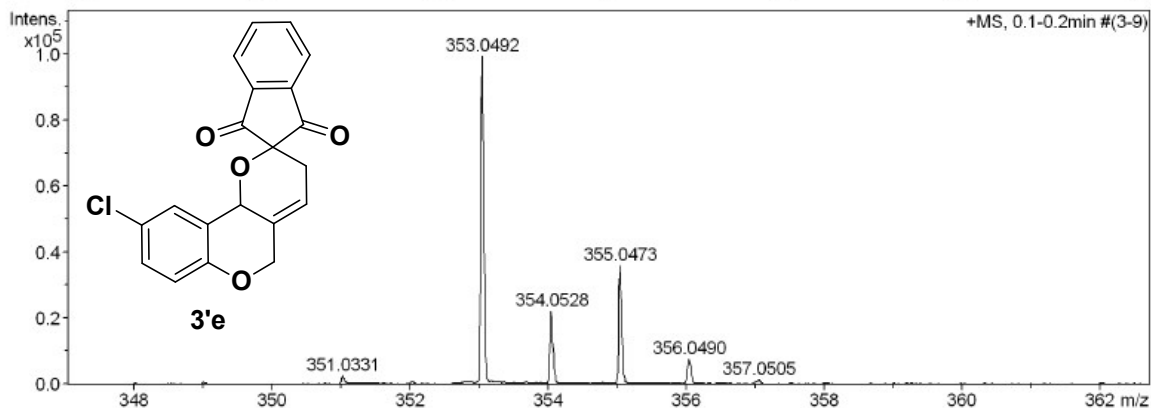
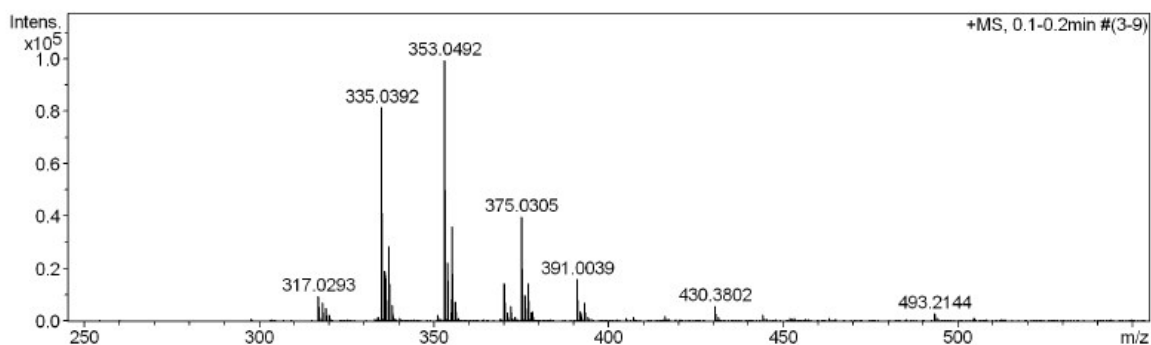
Operator Amit S.Sahu
Instrument microTOF-Q II 10337

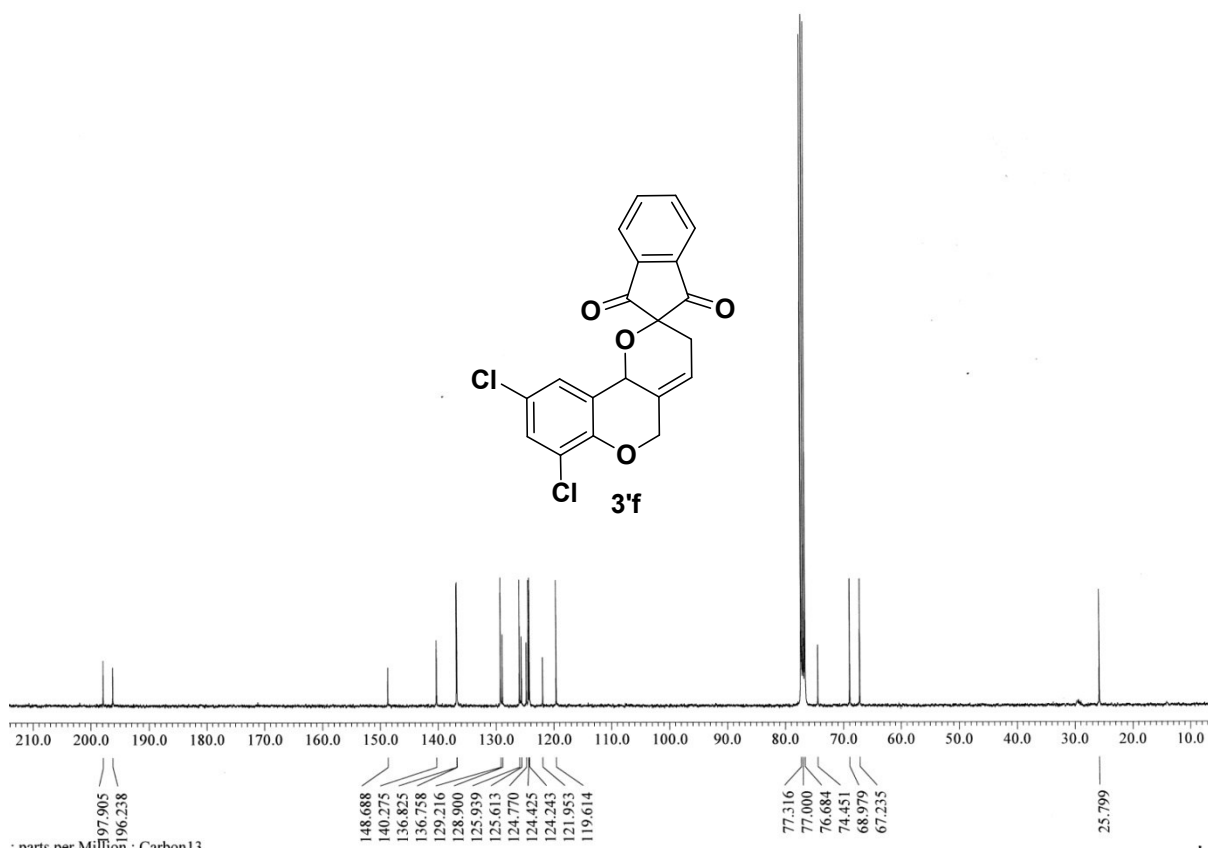
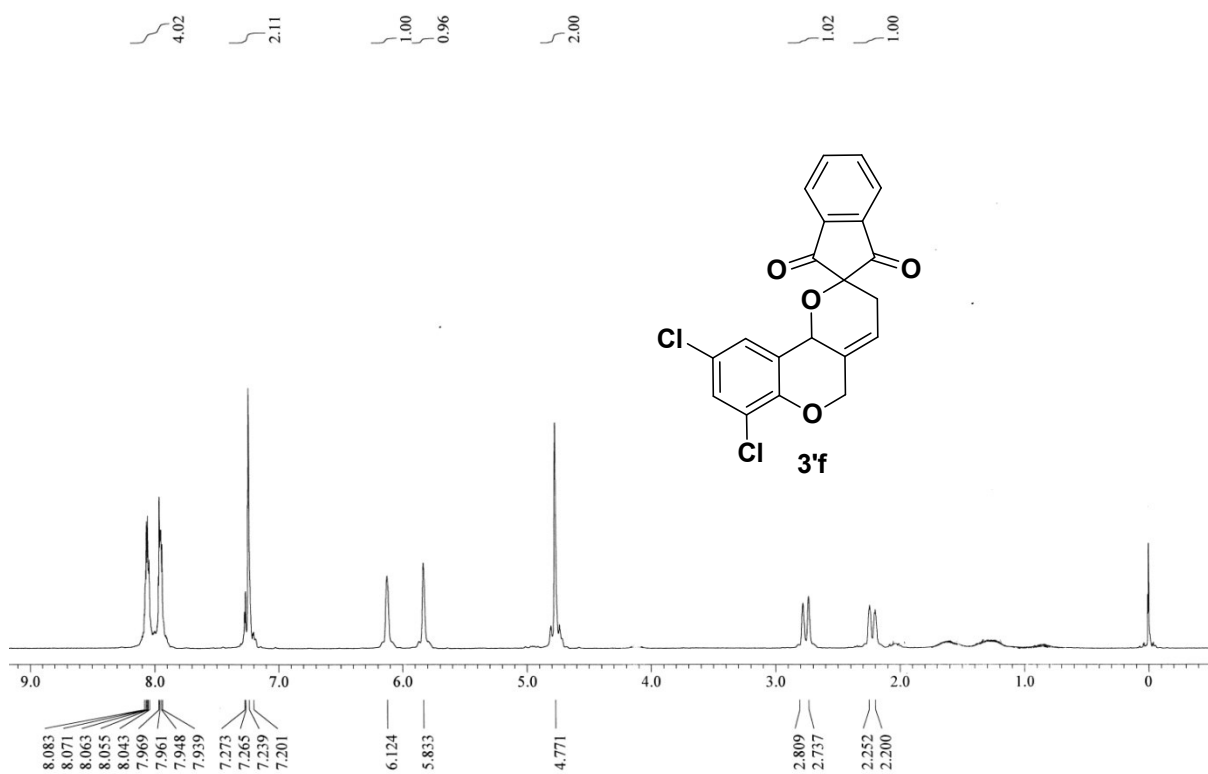
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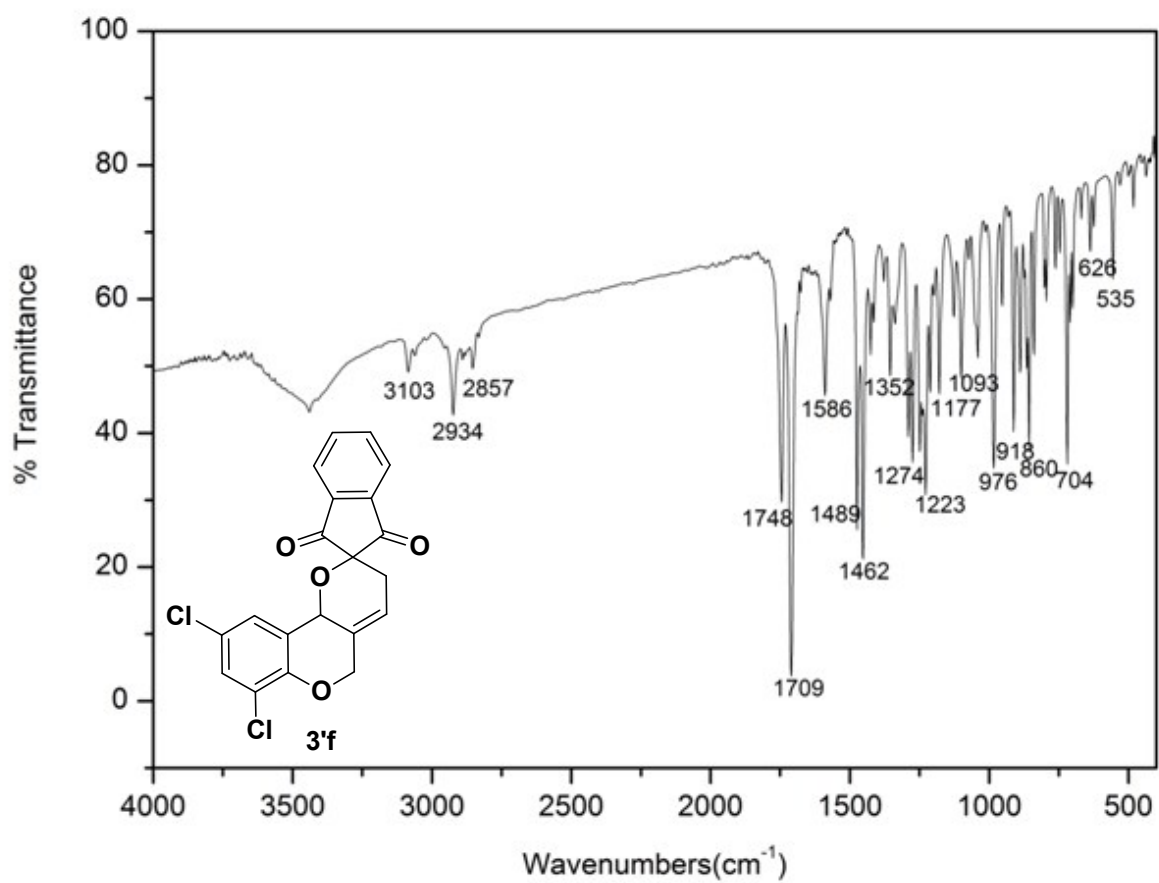
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste



----- TIC +All MS







Display Report

Analysis Info

Analysis Name D:\Data\DEC-2016\NKS\GC\06102017_NKS_GC_PRA-155.d
Method Pso_tune_wide.m
Sample Name ESI-MS
Comment

Acquisition Date 10/8/2017 6:58:02 PM

Operator Amit S.Sahu
Instrument microTOF-Q II 10337

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste

