

## **Supporting Information**

### **Two-Pot Synthesis and Photophysical Studies of 1,6-disubstituted 5-Aza-Indoles from Succinaldehyde and N-Aryl Propargylic-Imines**

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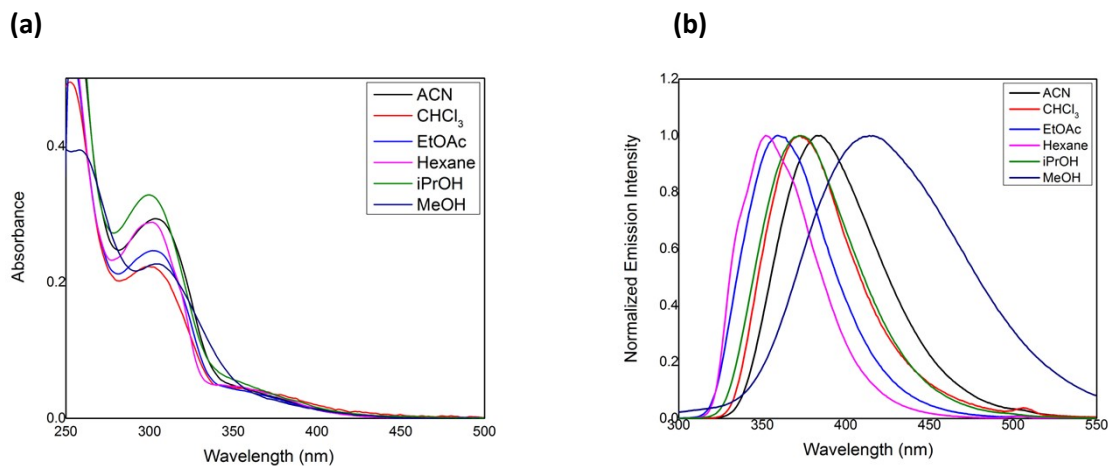
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## Supporting data for the photophysical study

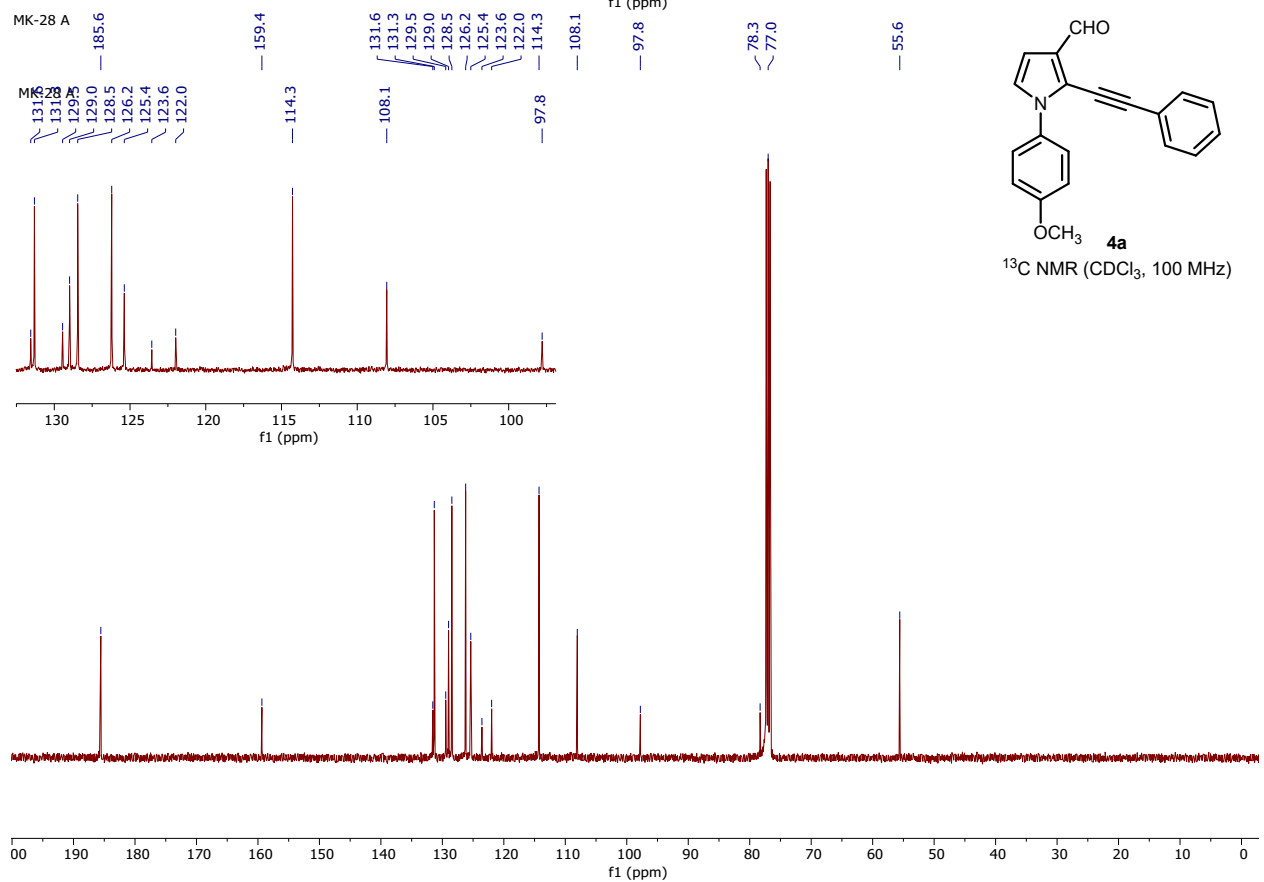
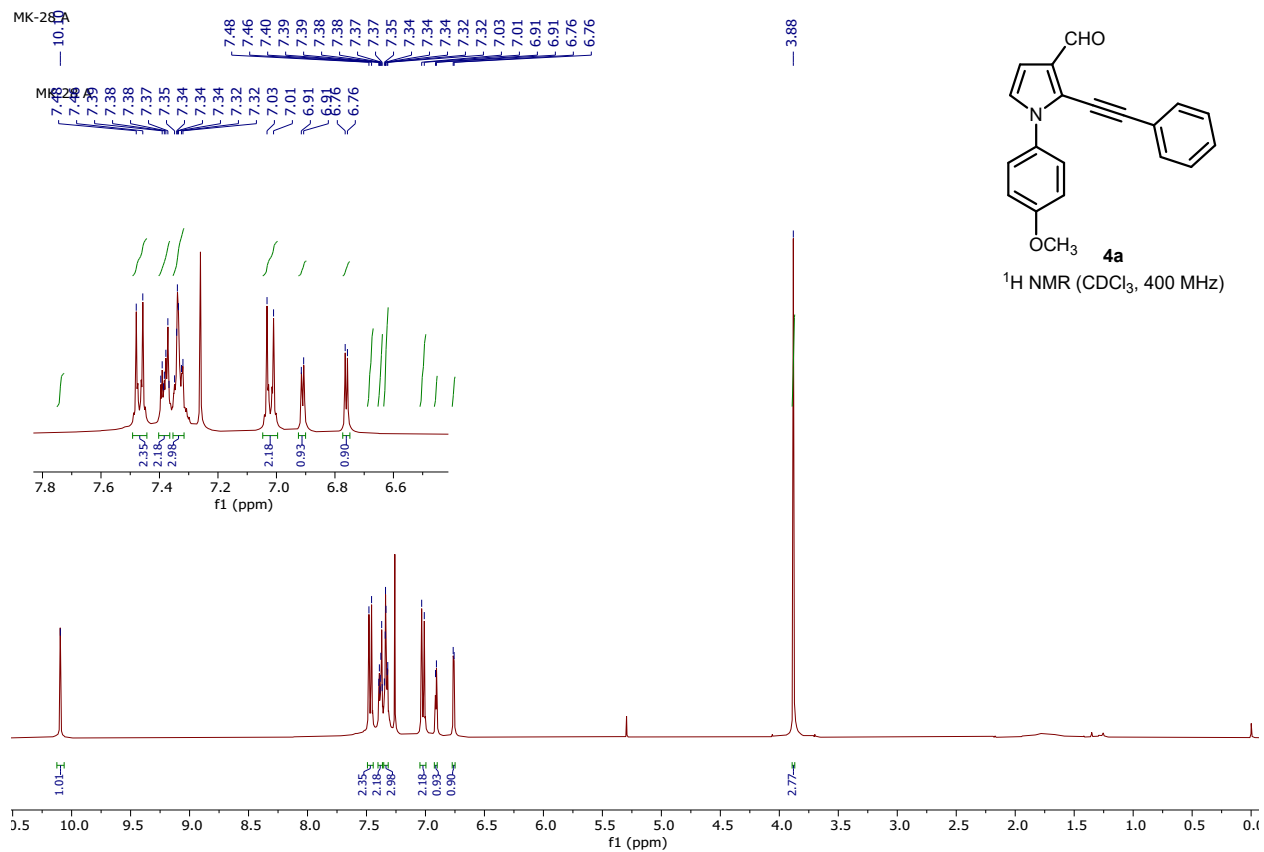
**Figure-S1:** (a) Normalized UV/Vis absorption, (b) normalized fluorescent emission of compound **5a** ( $c = 10^{-4}$  M) in different solvents at  $T = 298$  K.



**Table-S1:** Photophysical data for 1-(4-Methoxyphenyl)-6-phenyl-1*H*-pyrrolo[3,2-*c*]pyridine (**5a**) in different solvents<sup>[a]</sup>

Solvent	Absorbance <sup>[b]</sup> $\lambda_{\max}$ (nm)	Emission $\lambda_{\max}$ (nm)	Stokes Shift $\nu$ (cm <sup>-1</sup> )	$\epsilon$ (M <sup>-1</sup> CM <sup>-1</sup> )
Hexane	301	350	4651	28722
Chloroform	301	372	6677	22351
2-Propanol	301	377	06340	33293
Ethyl acetate	304	369	5794	24888
Acetonitrile	305	383	6697	29351
Methanol	306	464	11128	22962

[a] Measured in solvent ( $c = 1 \times 10^{-4}$  M) at 298 K. [b] Excited at 300 nm



# Compound Report

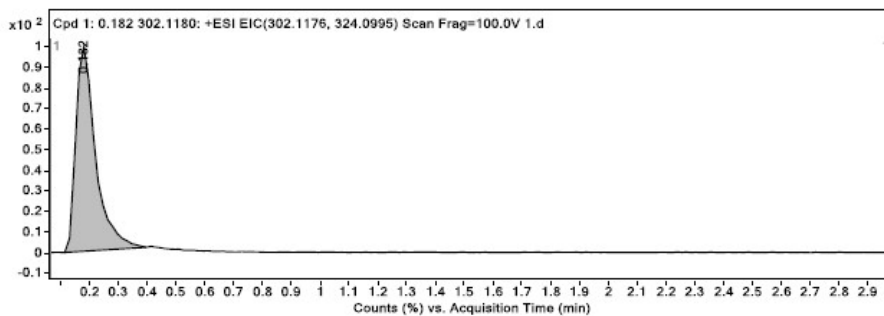
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		Version	Q-TOF B.06.01 (B6172 SP1)

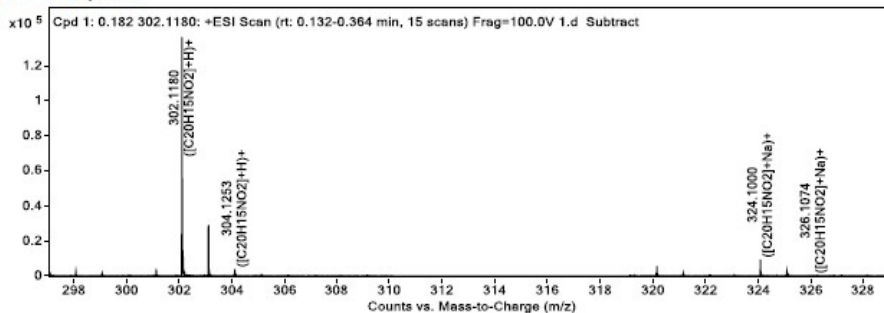
## Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.182 302.1180	0.182	301.1108	136512	C20 H15 N O2	301.1103	1.63

Compound Label	m/z	RT	Algorithm	Mass
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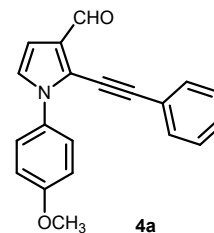


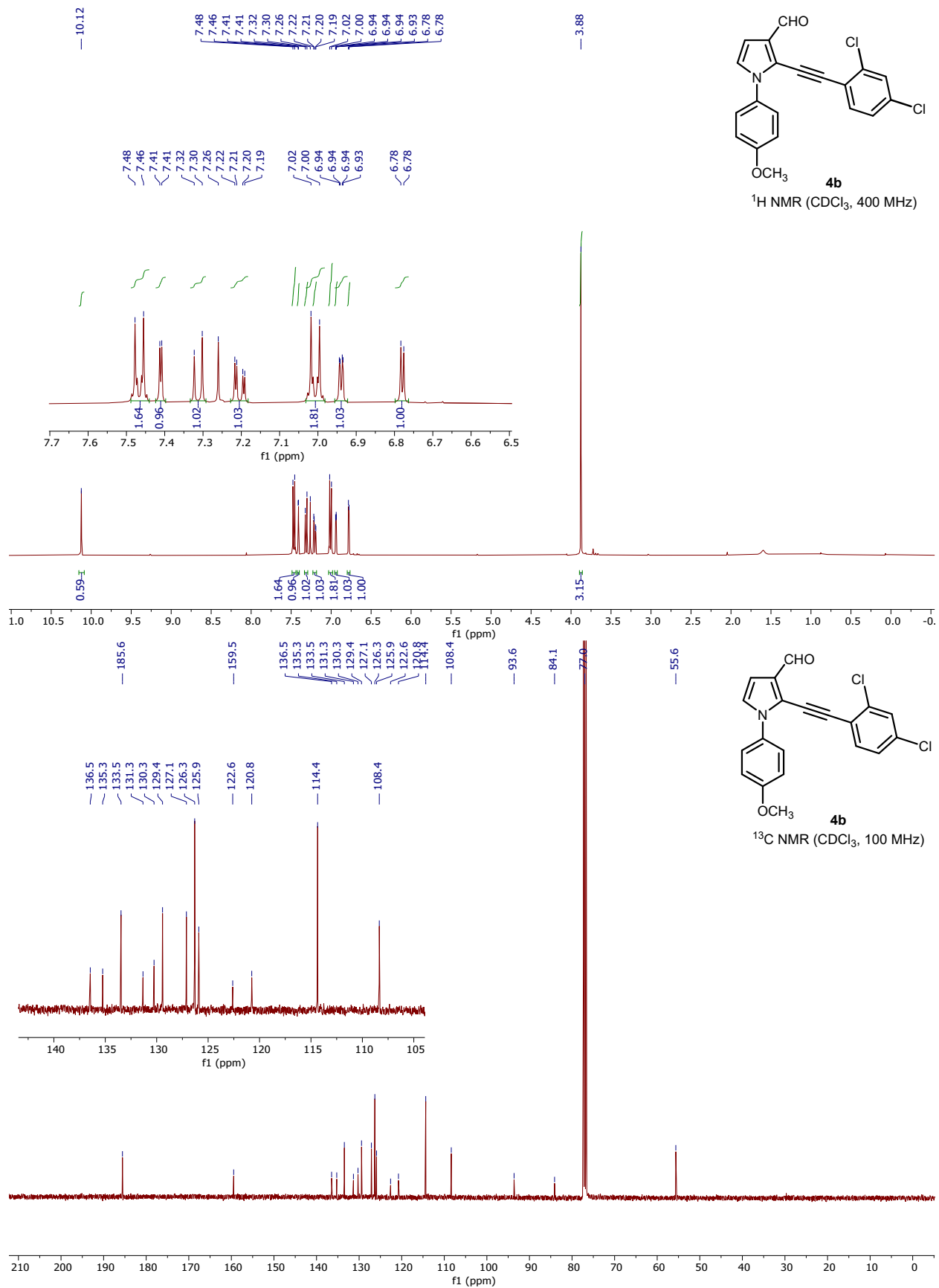
## MS Zoomed Spectrum



## MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
302.118	302.1176	-1.43	1	136512.07	C20H15NO2	(M+H)+
303.1214	303.1208	-1.83	1	29337.21	C20H15NO2	(M+H)+
304.1253	304.1238	-5.12	1	3788.84	C20H15NO2	(M+H)+
305.1308	305.1265	-14.01	1	412.62	C20H15NO2	(M+H)+
324.1	324.0995	-1.7	1	9347.34	C20H15NO2	(M+Na)+
325.103	325.1028	-0.68	1	2101.16	C20H15NO2	(M+Na)+
326.1074	326.1057	-5.26	1	299.08	C20H15NO2	(M+Na)+





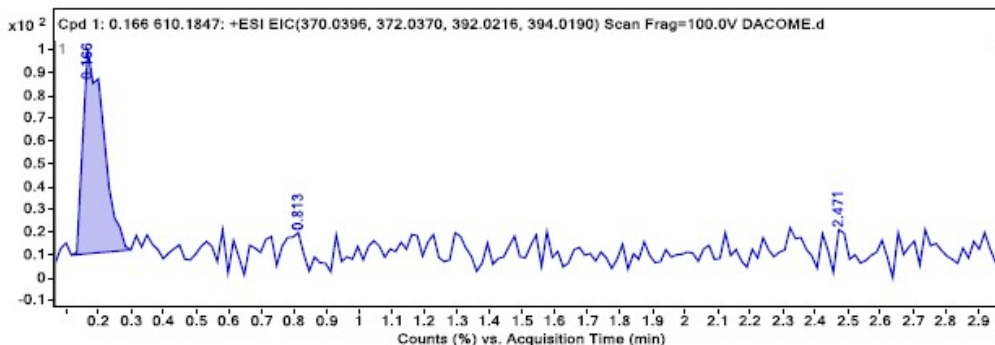
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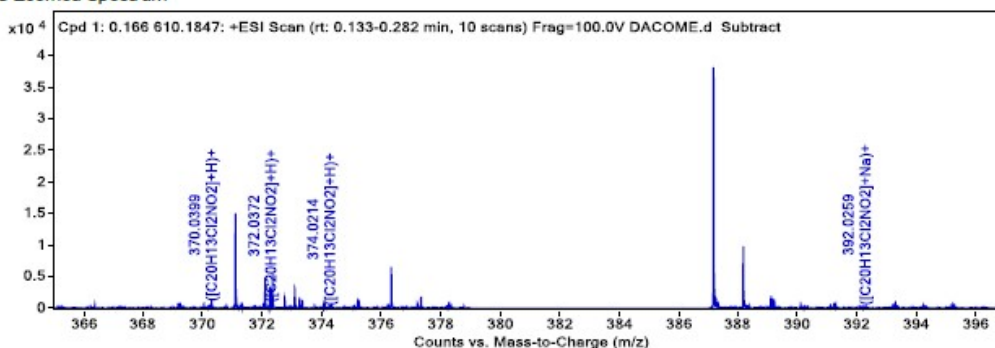
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.166 610.1847	0.166	369.0326	732	C20 H13 Cl2 N O2	369.0323	0.84

Compound Label	m/z	RT	Algorithm	Mass
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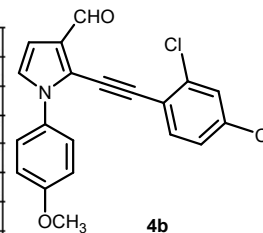


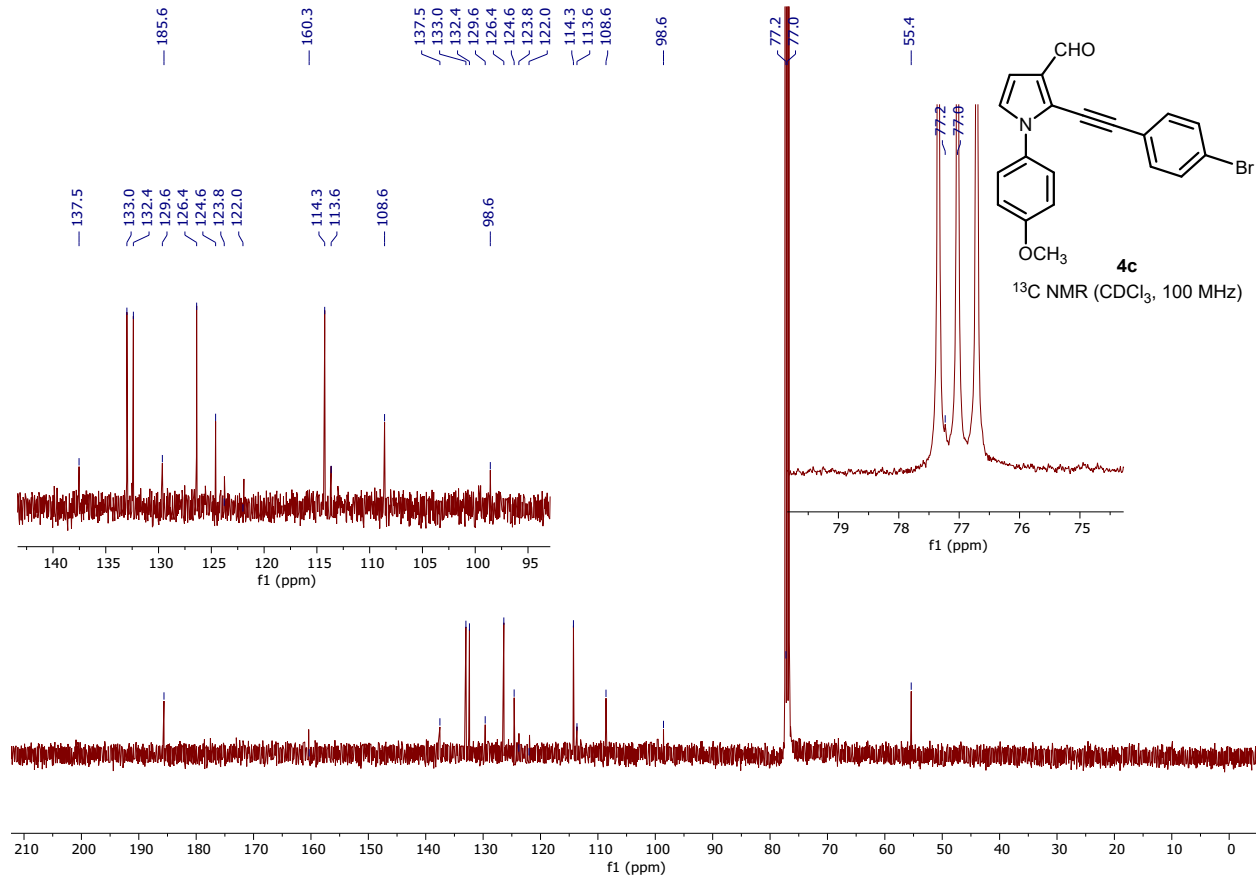
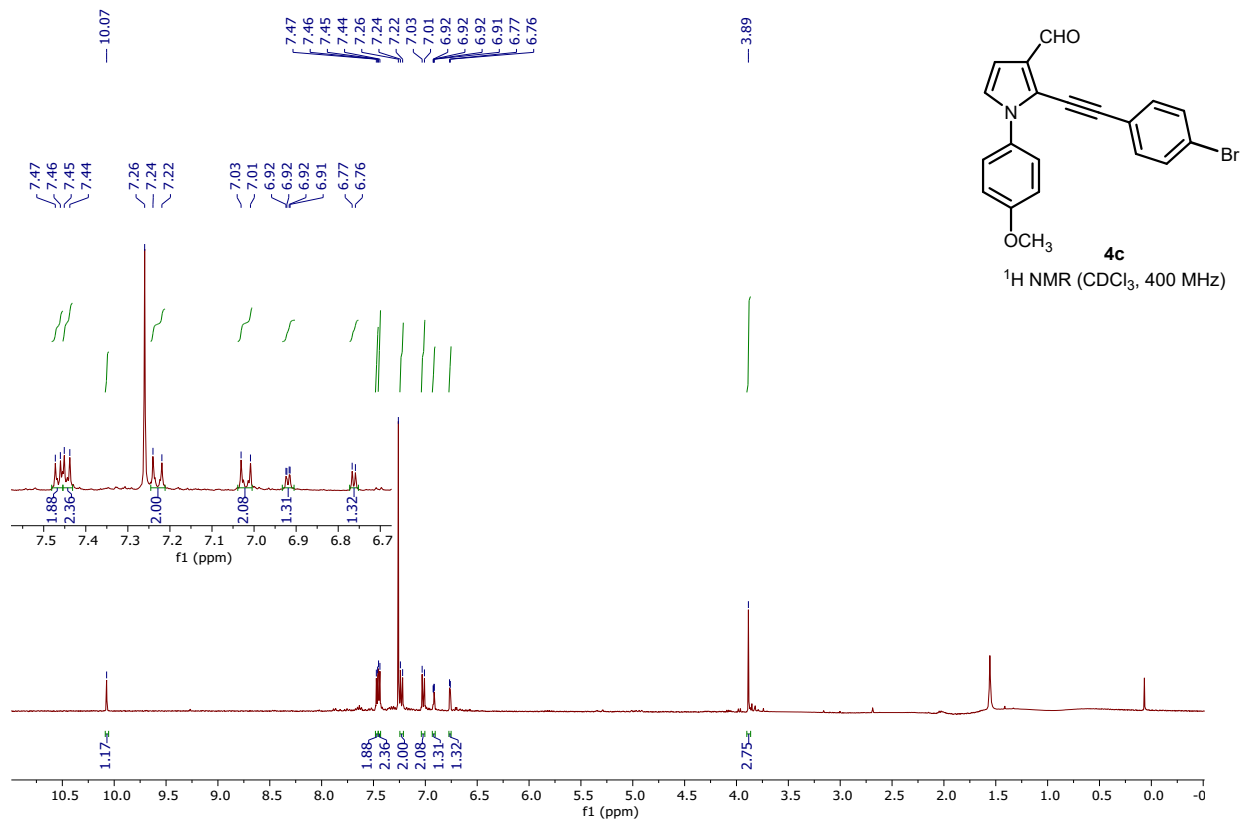
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
370.0399	370.0396	-0.84	1	731.9	C20H13Cl2NO2	(M+H)+
371.0463	371.0429	-9.33	1	247.46	C20H13Cl2NO2	(M+H)+
372.0372	372.037	-0.43	1	597.72	C20H13Cl2NO2	(M+H)+
373.0394	373.0401	1.73	1	212.29	C20H13Cl2NO2	(M+H)+
374.0214	374.0351	36.55	1	71.2	C20H13Cl2NO2	(M+H)+
392.0259	392.0216	-11.13	1	125.64	C20H13Cl2NO2	(M+Na)+





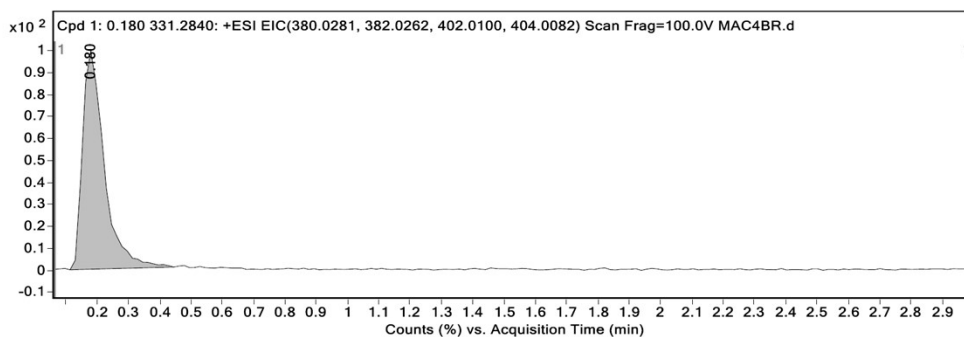
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<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

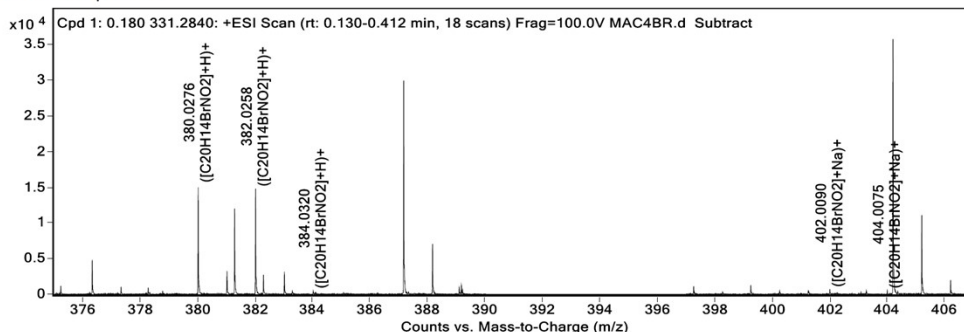
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.180 331.2840	0.18	379.0203	15341	C20 H14 Br N O2	379.0208	-1.25

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.180 331.2840	380.0276	0.18	Find By Formula	379.0203

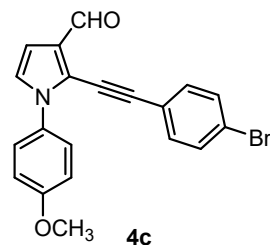


### MS Zoomed Spectrum

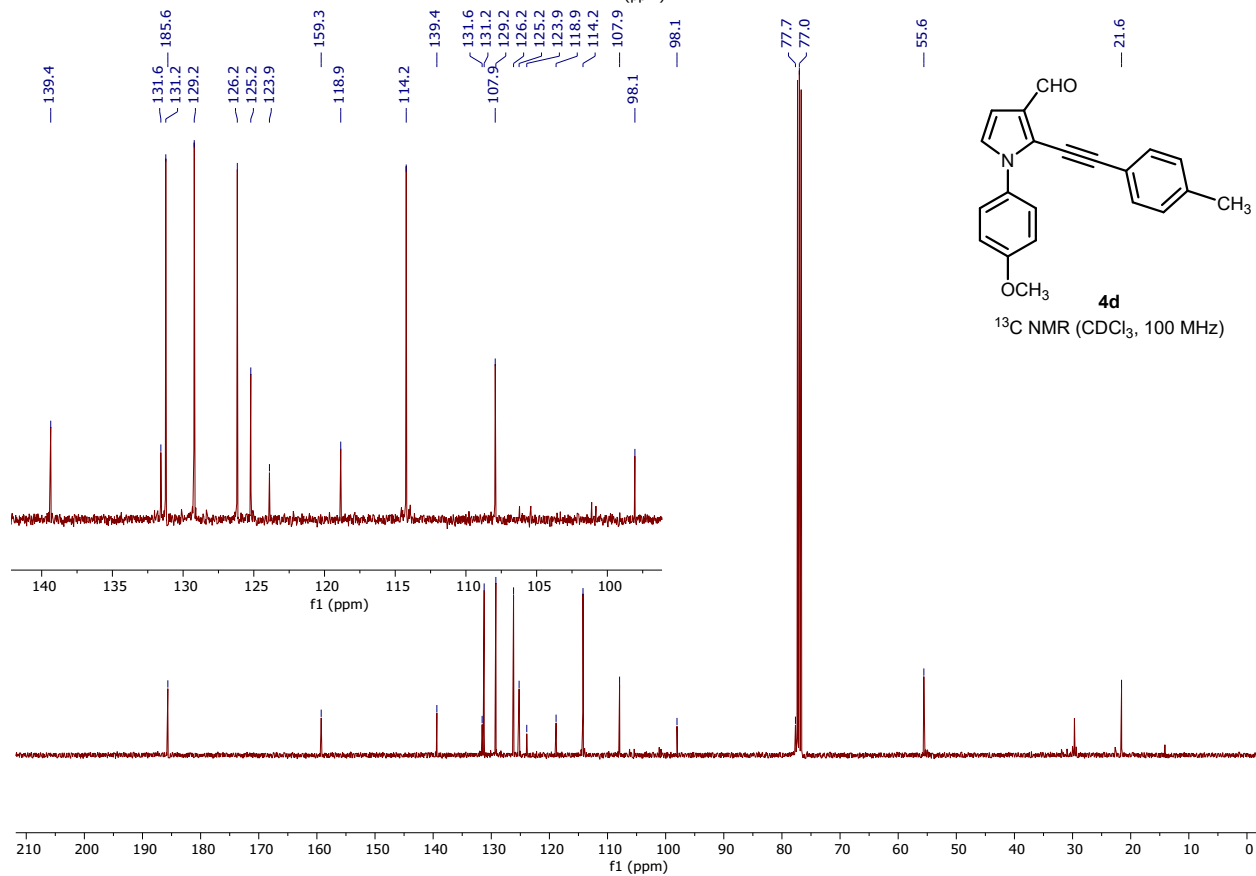
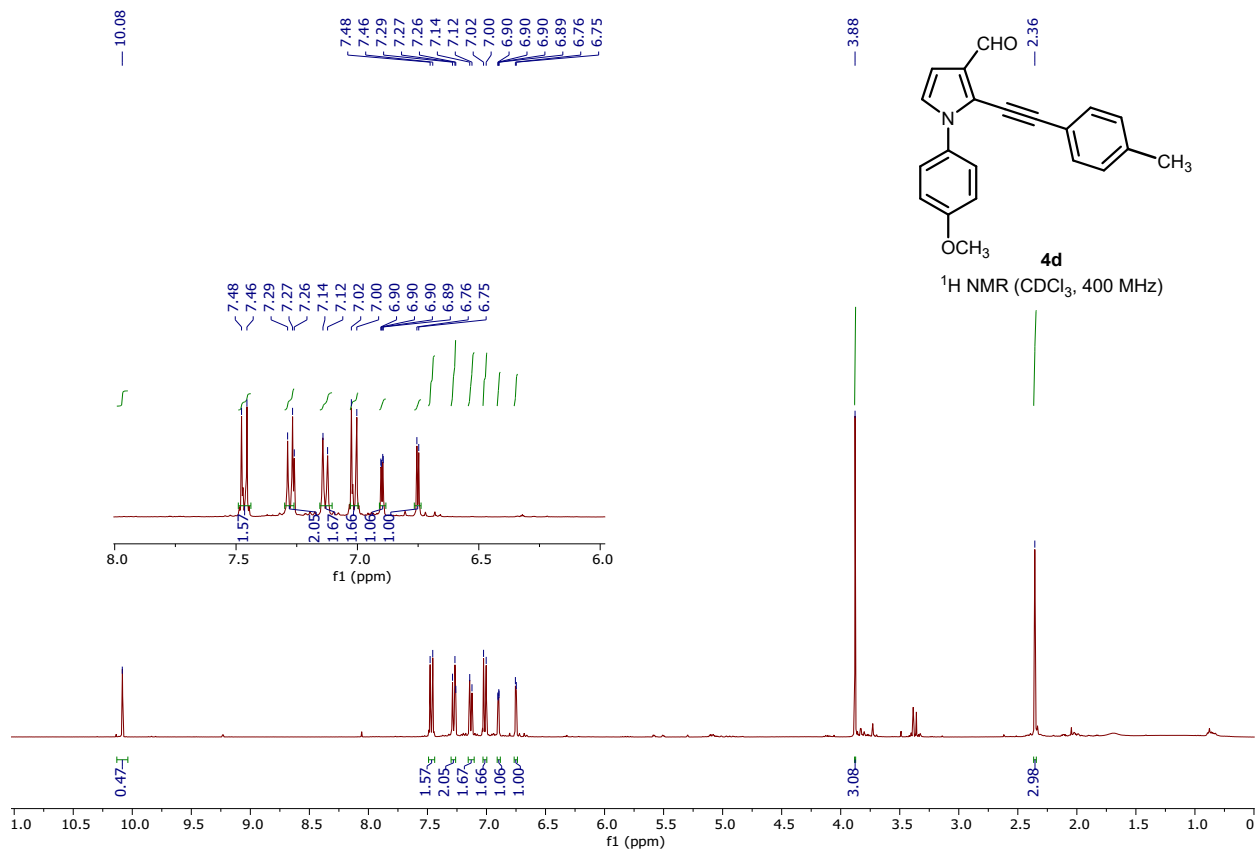


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
380.0276	380.0281	1.33	1	15341.27	C20H14BrNO2	(M+H)+
381.0312	381.0313	0.38	1	3314.55	C20H14BrNO2	(M+H)+
382.0258	382.0262	1.19	1	14791.64	C20H14BrNO2	(M+H)+
383.0291	383.0294	0.74	1	3153.12	C20H14BrNO2	(M+H)+
384.032	384.0323	0.63	1	506.2	C20H14BrNO2	(M+H)+
385.0324	385.035	6.8	1	72.76	C20H14BrNO2	(M+H)+
402.009	402.01	2.43	1	710.08	C20H14BrNO2	(M+Na)+
403.0116	403.0133	4.13	1	159.41	C20H14BrNO2	(M+Na)+
404.0075	404.0082	1.67	1	516.49	C20H14BrNO2	(M+Na)+
404.9993	405.0113	29.8	1	58.03	C20H14BrNO2	(M+Na)+







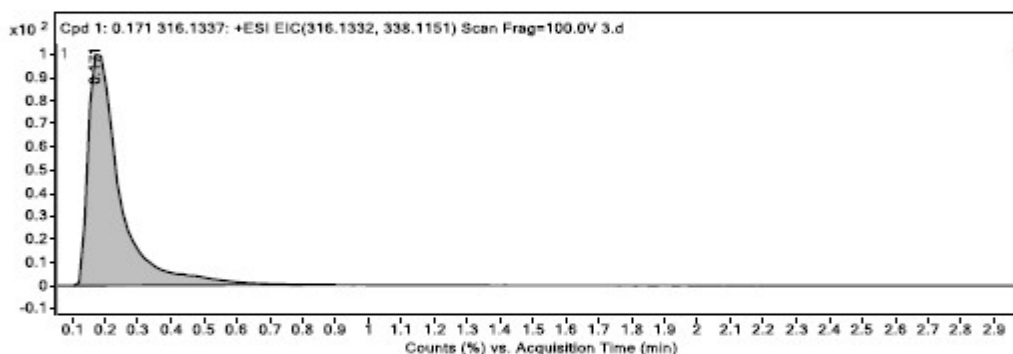
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Sample Group		Info.	
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		Version	Q-TOF B.06.01 (B6172 SP1)

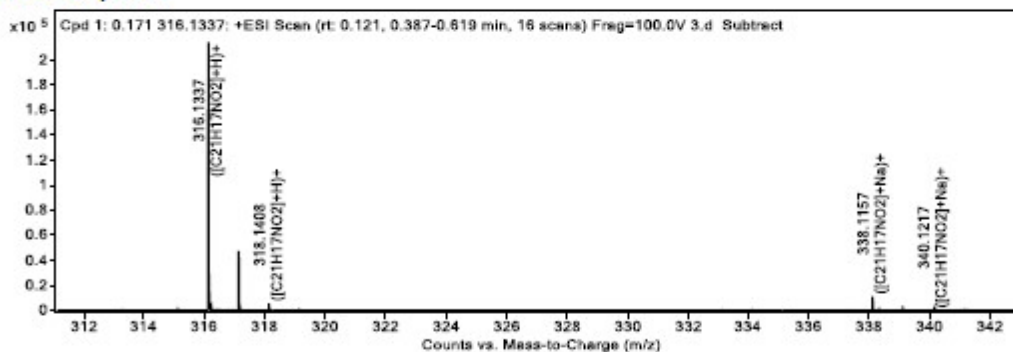
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.171 316.1337	0.171	315.1265	11328	C21 H17 N O2	315.1259	1.79

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.171 316.1337	338.1157	0.171	Find By Formula	315.1265

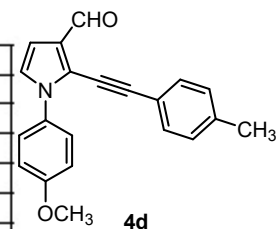


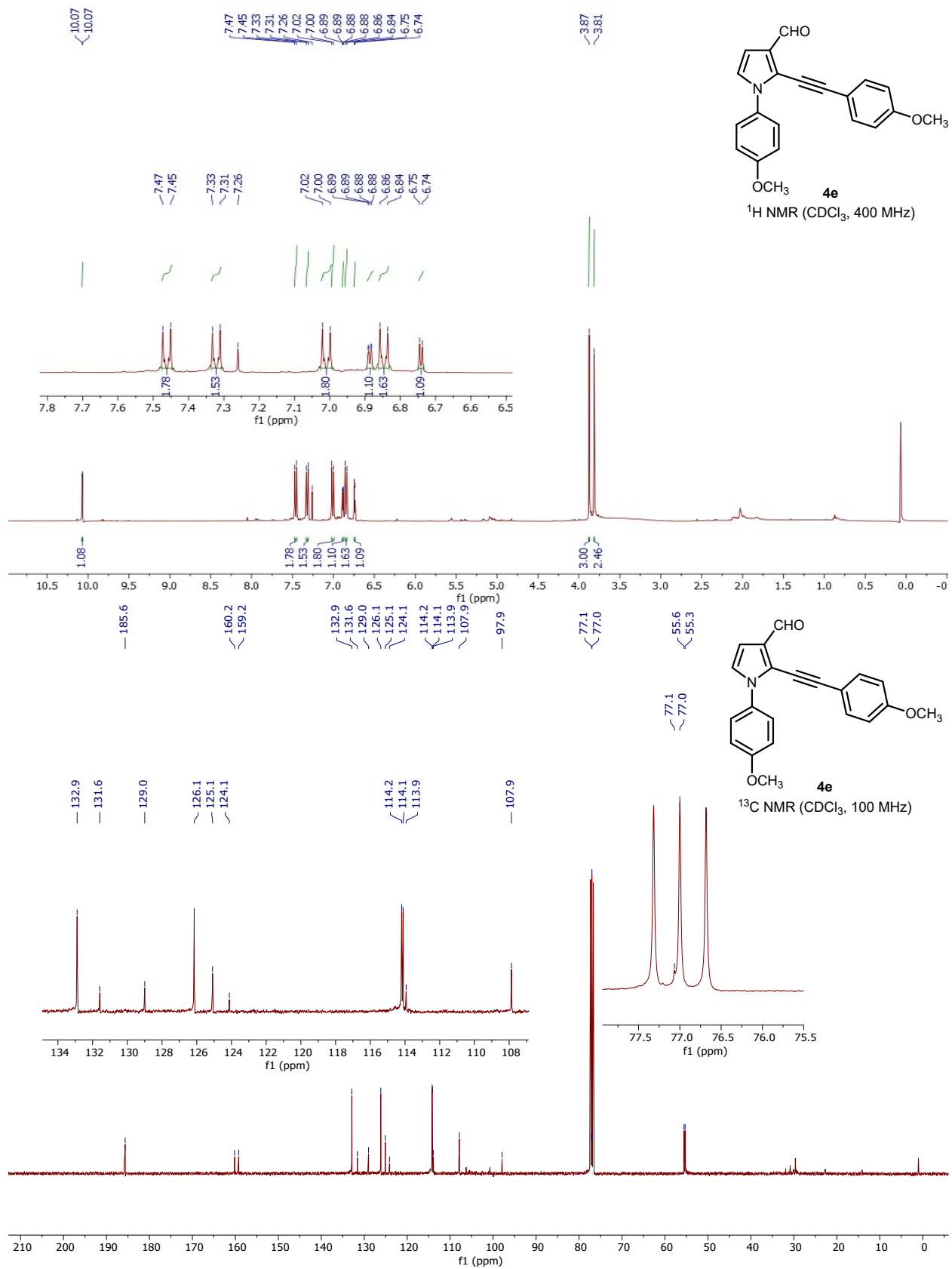
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
316.1337	316.1332	-1.68	1	214712.72	C21H17NO2	(M+H)+
317.1371	317.1365	-1.93	1	47966.8	C21H17NO2	(M+H)+
318.1408	318.1395	-4.2	1	5779.13	C21H17NO2	(M+H)+
319.1435	319.1423	-3.92	1	587.35	C21H17NO2	(M+H)+
338.1157	338.1151	-1.55	1	11328.28	C21H17NO2	(M+Na)+
339.1191	339.1184	-1.86	1	2628.92	C21H17NO2	(M+Na)+
340.1217	340.1214	-1.01	1	322.06	C21H17NO2	(M+Na)+





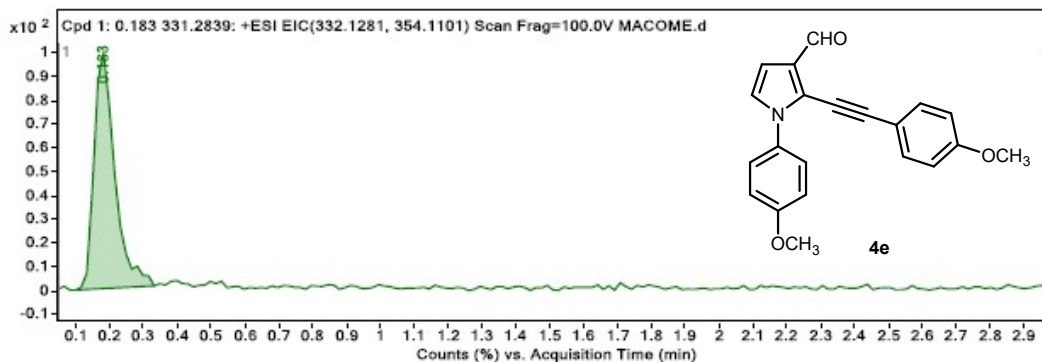
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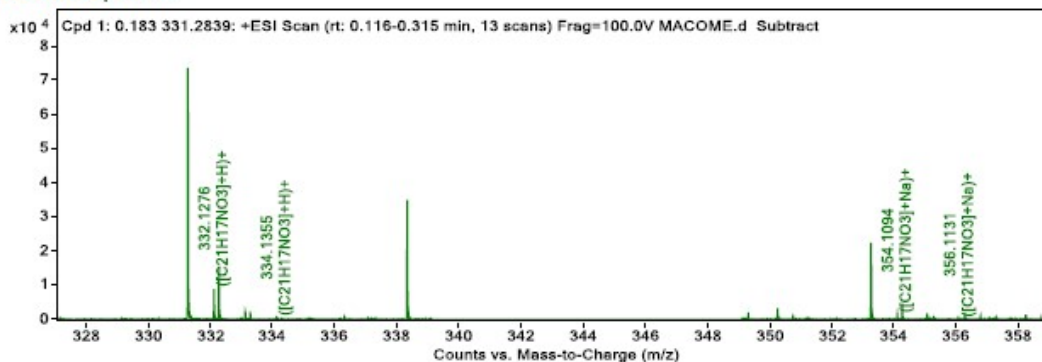
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.183 331.2839	0.183	331.1204	8926	C21 H17 N O3	331.1208	-1.38

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.183 331.2839	332.1276	0.183	Find By Formula	331.1204

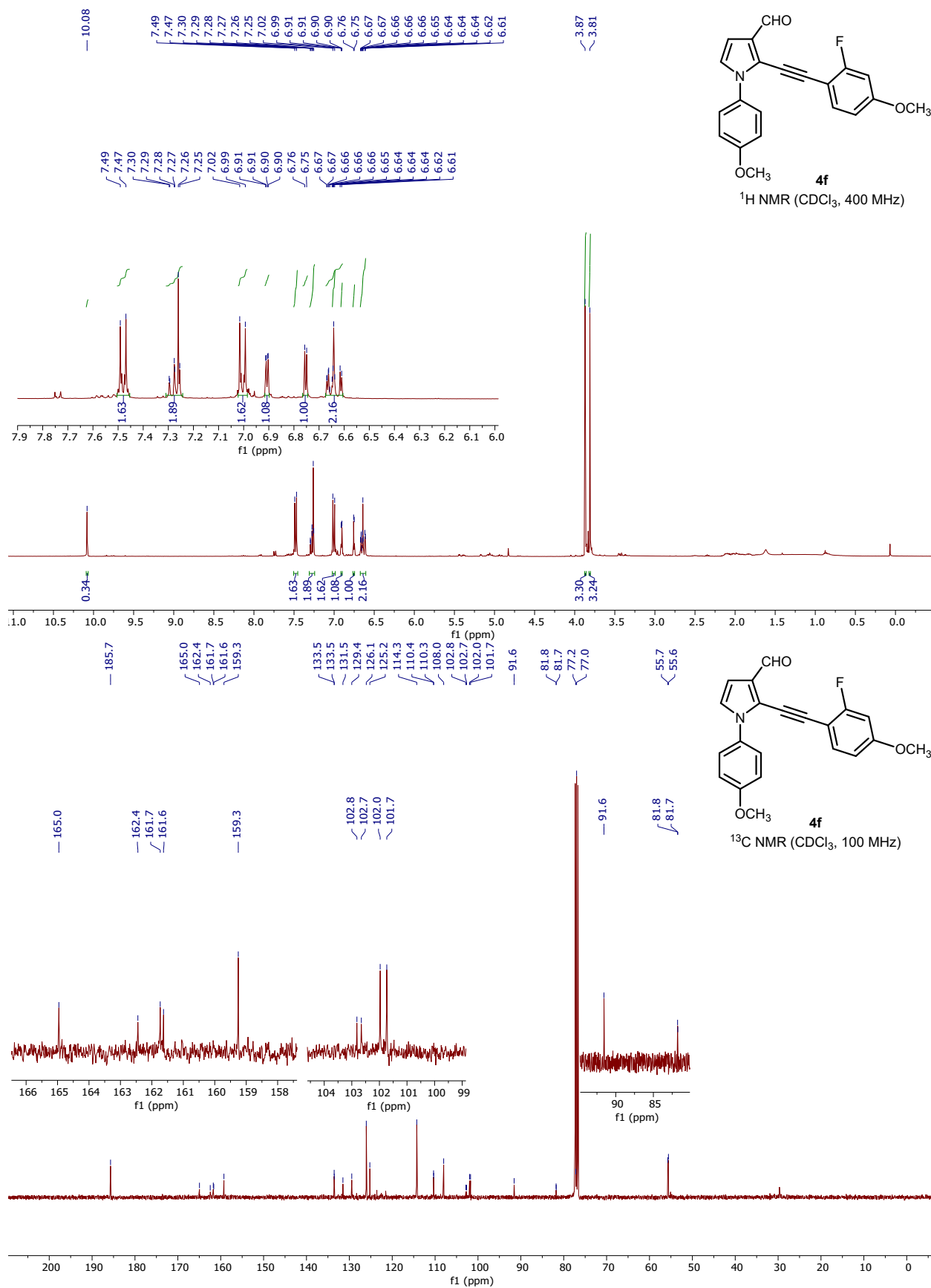


### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
332.1276	332.1281	1.49	1	8925.76	C21H17NO3	(M+H)+
333.1307	333.1314	2.1	1	2130.65	C21H17NO3	(M+H)+
334.1355	334.1342	-3.85	1	425.85	C21H17NO3	(M+H)+
354.1094	354.1101	1.79	1	1308.26	C21H17NO3	(M+Na)+
355.1141	355.1133	-2.22	1	394.72	C21H17NO3	(M+Na)+
356.1131	356.1162	8.55	1	52.77	C21H17NO3	(M+Na)+



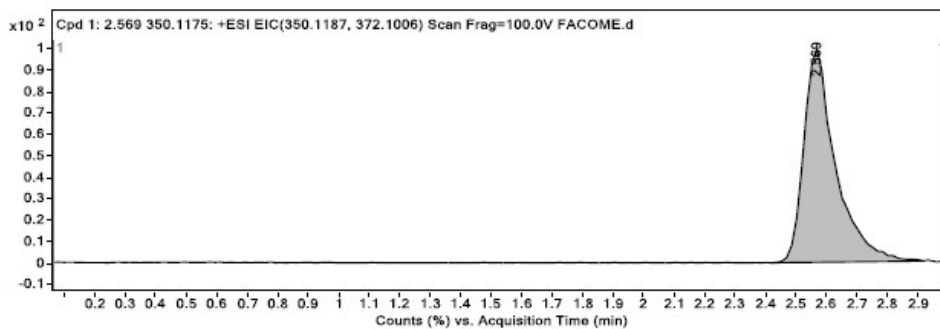
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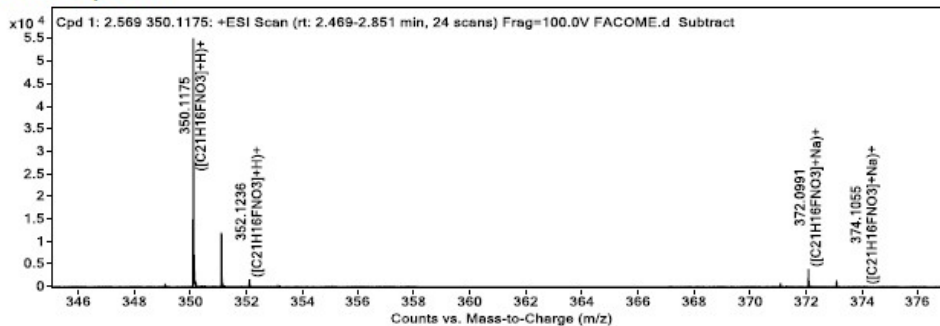
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 2.569 350.1175	2.569	349.1102	55324	C21 H16 F N O3	349.1114	-3.51

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 2.569 350.1175	350.1175	2.569	Find By Formula	349.1102

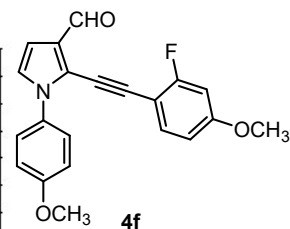


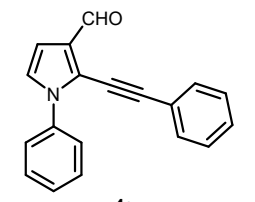
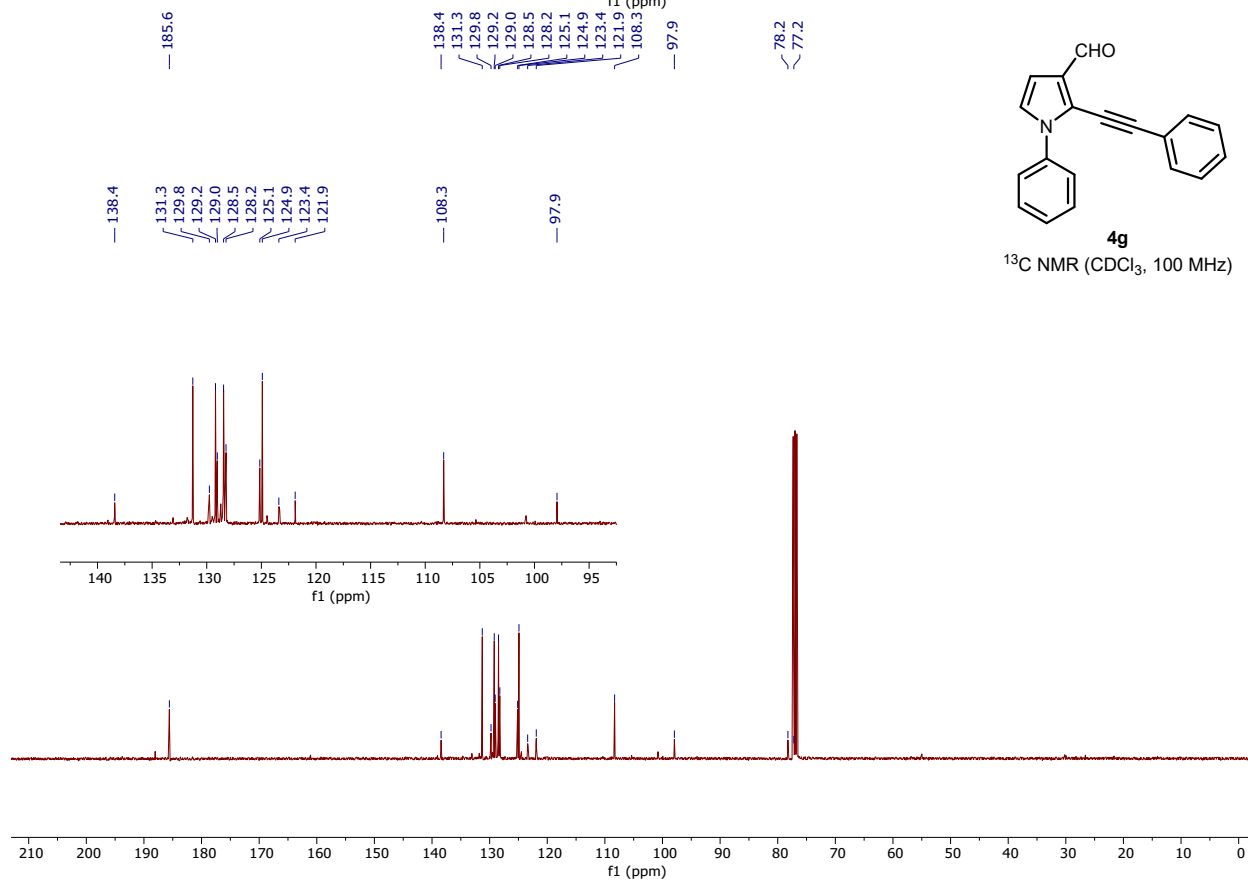
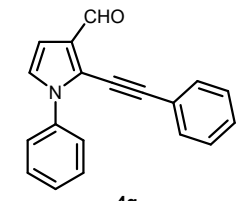
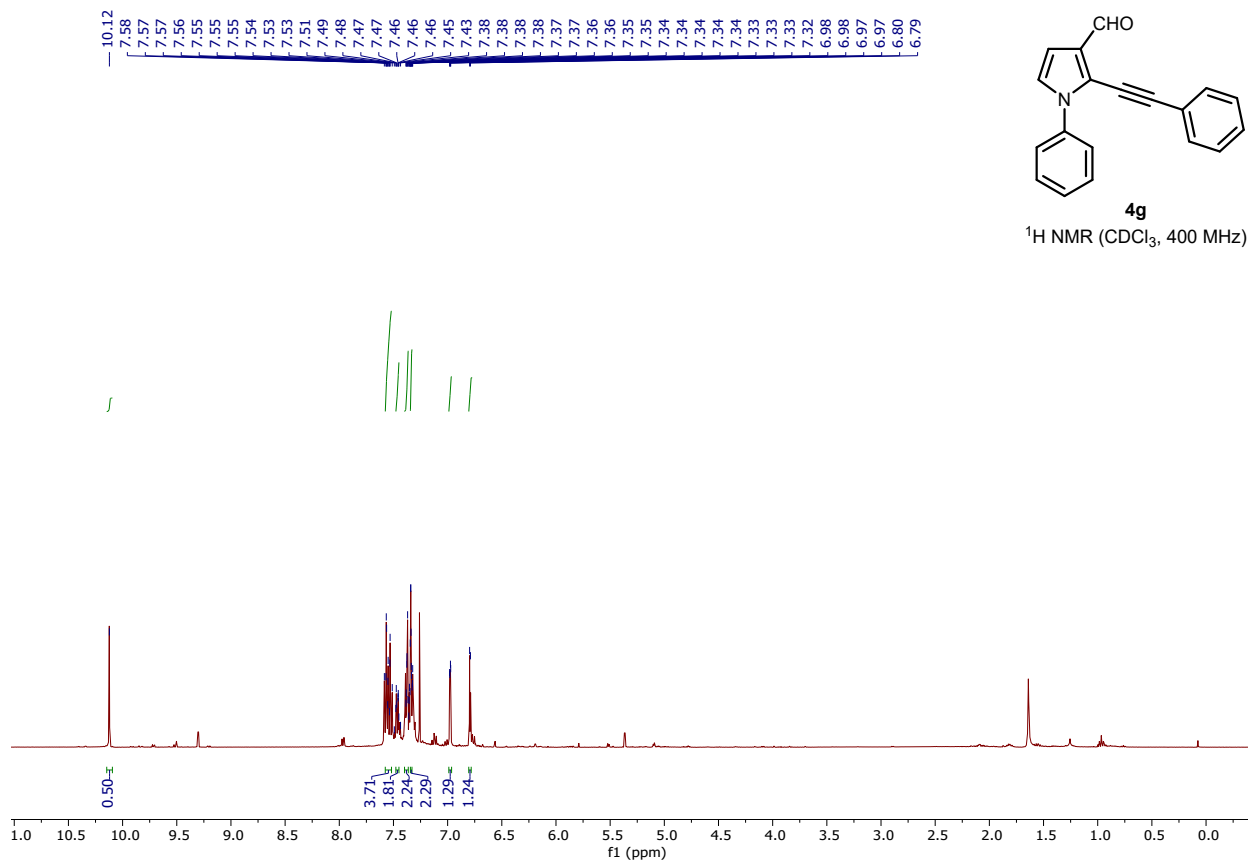
#### MS Zoomed Spectrum



#### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
350.1175	350.1187	3.5	1	55324.09	C21H16FNO3	(M+H)+
351.1209	351.122	3.17	1	12154.92	C21H16FNO3	(M+H)+
352.1236	352.1248	3.48	1	1623.58	C21H16FNO3	(M+H)+
353.1268	353.1275	2.01	1	176.22	C21H16FNO3	(M+H)+
372.0991	372.1006	4.04	1	3963.76	C21H16FNO3	(M+Na)+
373.1023	373.1039	4.46	1	1005	C21H16FNO3	(M+Na)+
374.1055	374.1068	3.32	1	98.82	C21H16FNO3	(M+Na)+





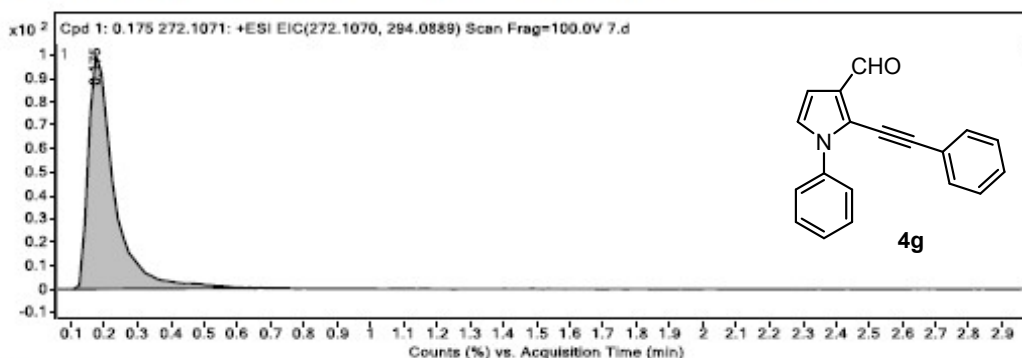
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Sample Group		Info.	
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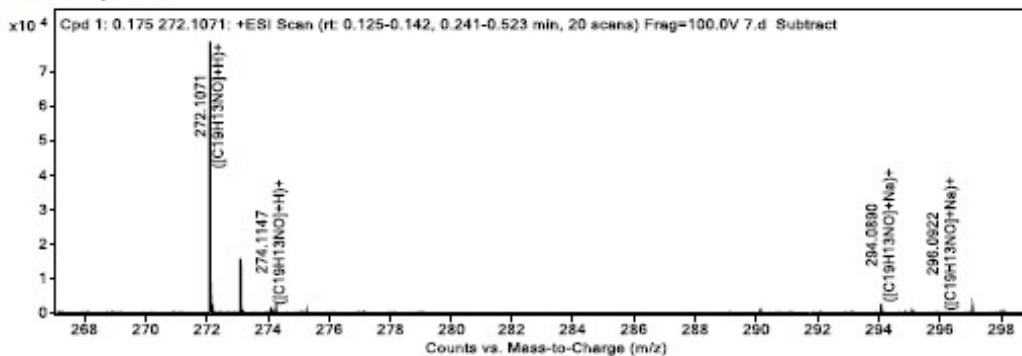
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.175 272.1071	0.175	271.0999	79040	C19 H13 N O	271.0997	0.59

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.175 272.1071	272.1071	0.175	Find By Formula	271.0999



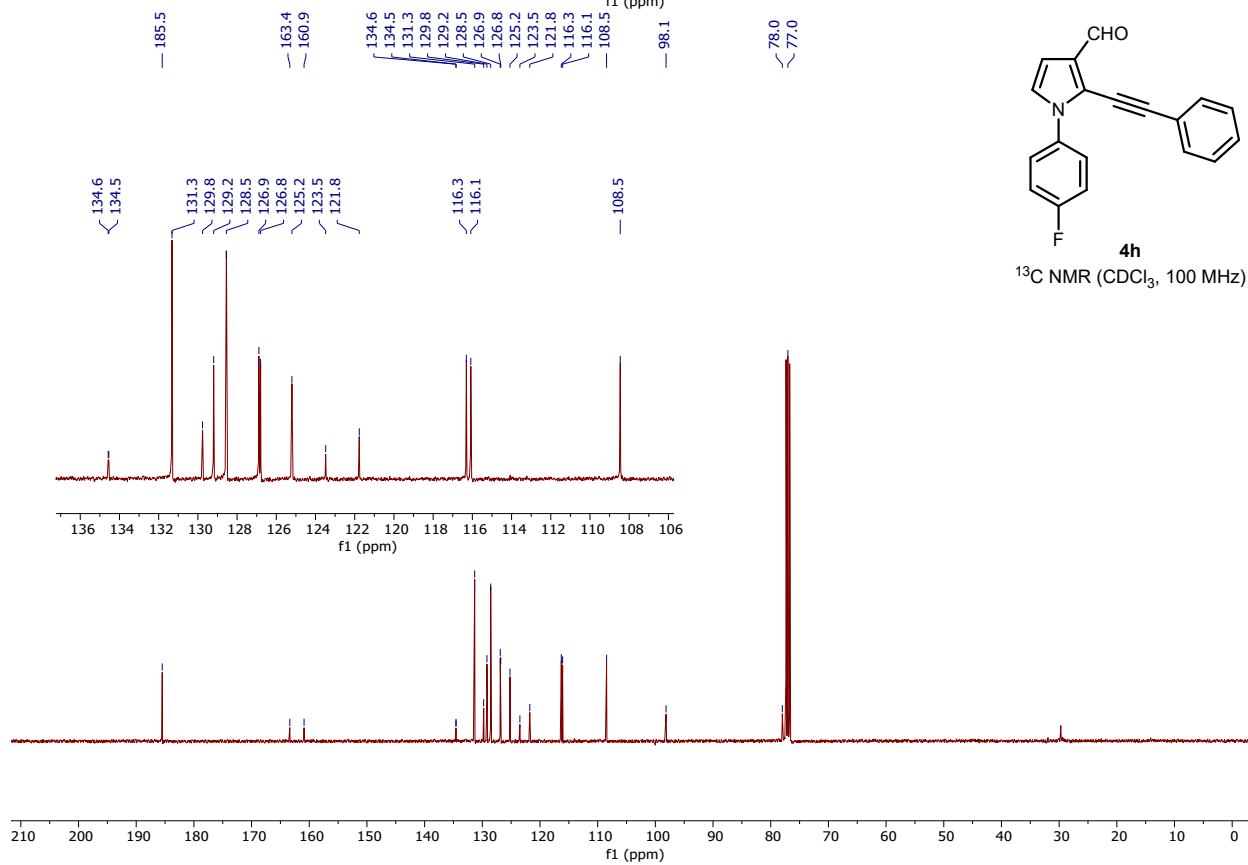
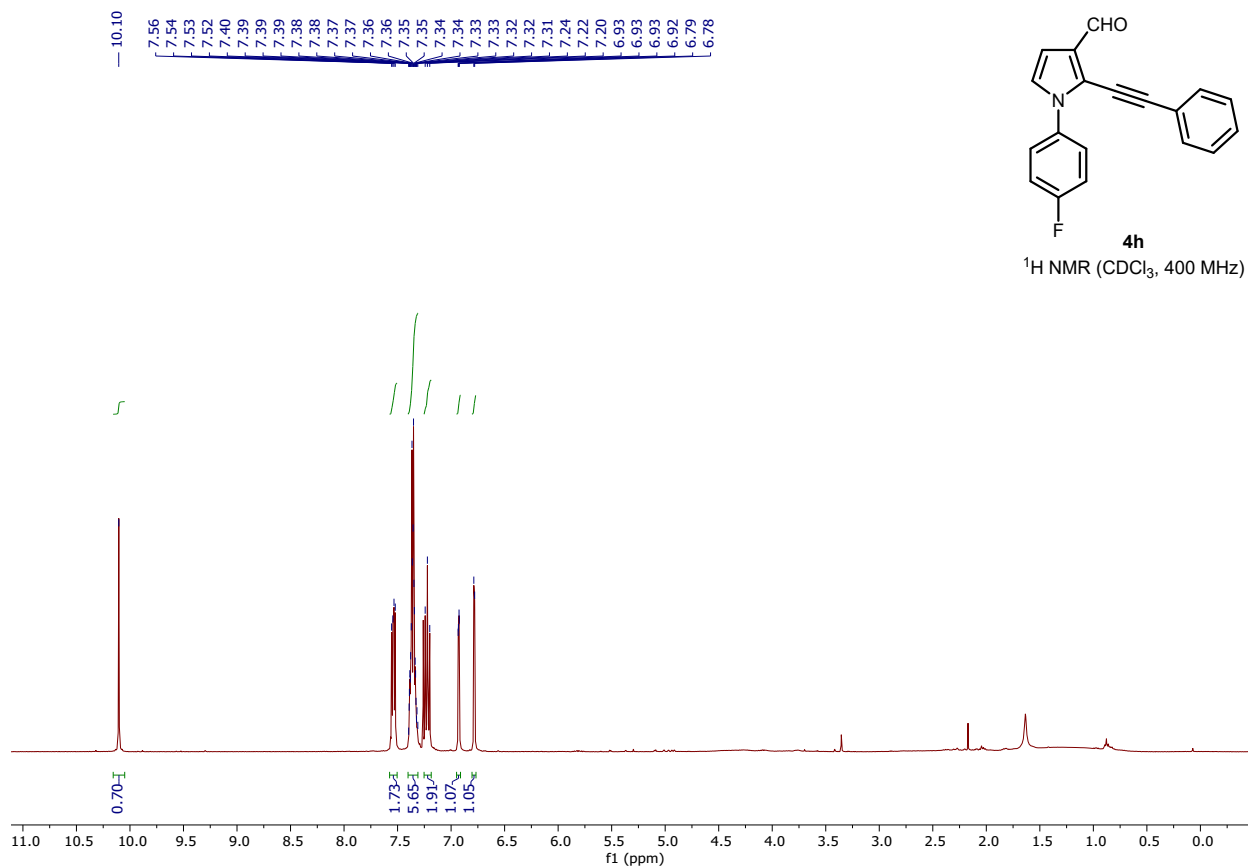
### MS Zoomed Spectrum



### MS Spectrum Peak List

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272.1071	272.107	-0.46	1	79039.51	C19H13NO	(M+H)+
273.1105	273.1103	-0.83	1	16345.5	C19H13NO	(M+H)+
274.1147	274.1133	-5.1	1	1785.17	C19H13NO	(M+H)+
294.089	294.0889	-0.11	1	2558.93	C19H13NO	(M+Na)+
295.0925	295.0922	-0.88	1	545.98	C19H13NO	(M+Na)+
296.0922	296.0953	10.27	1	85.37	C19H13NO	(M+Na)+





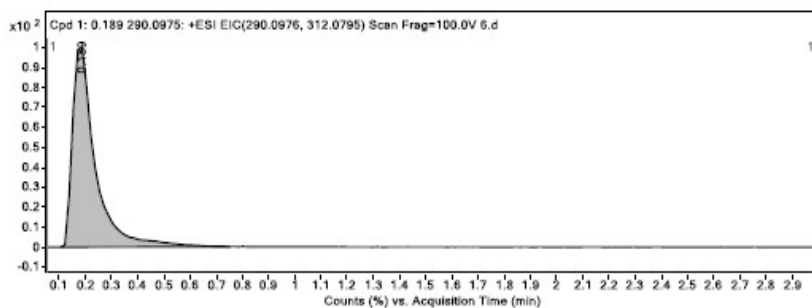
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IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

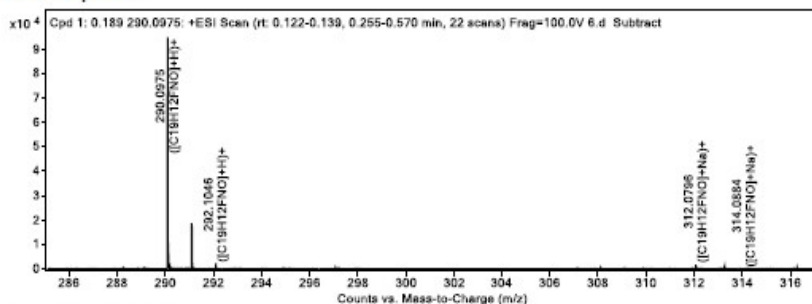
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.189 290.0975	0.189	289.0902	95219	C19 H12 F N O	289.0903	-0.18

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.189 290.0975	290.0975	0.189	Find By Formula	289.0902

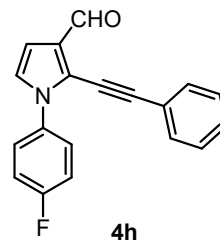


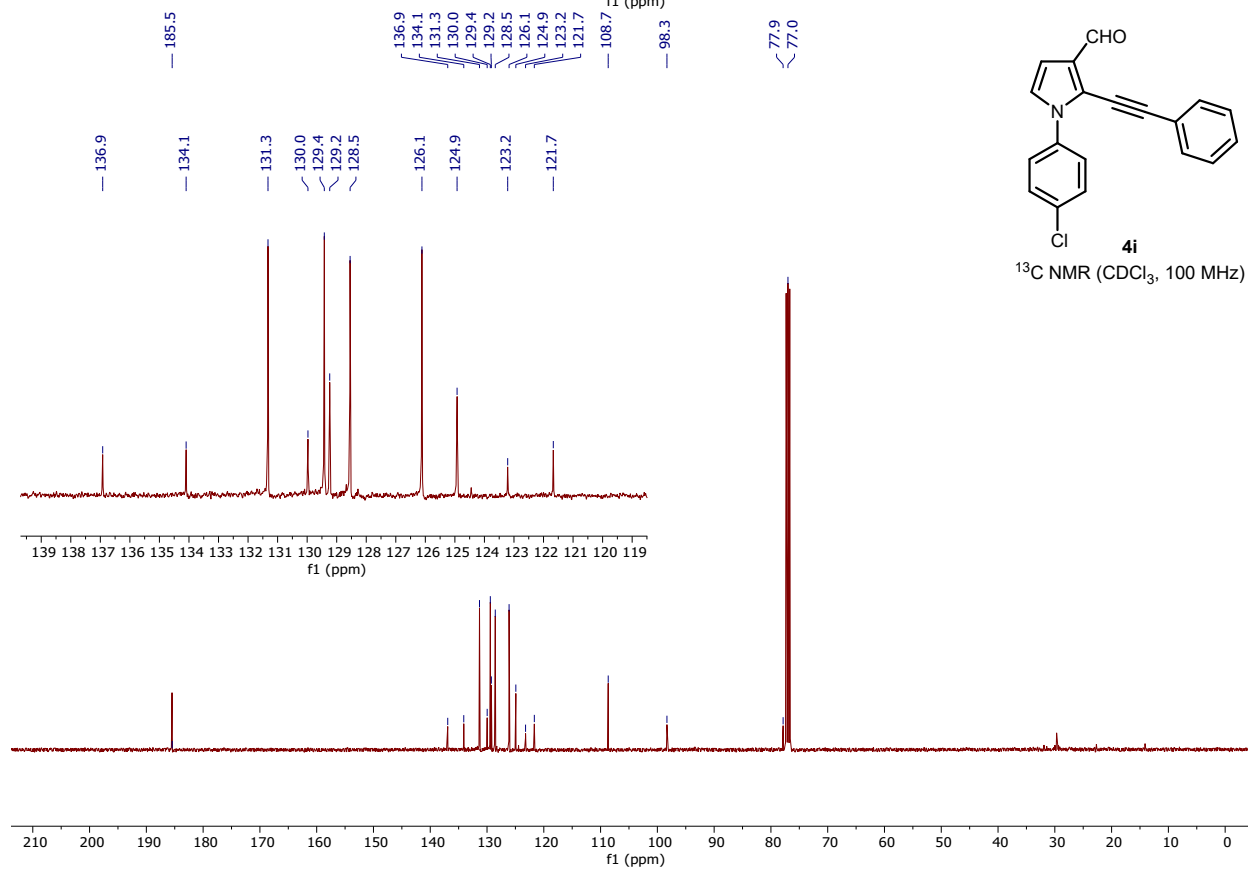
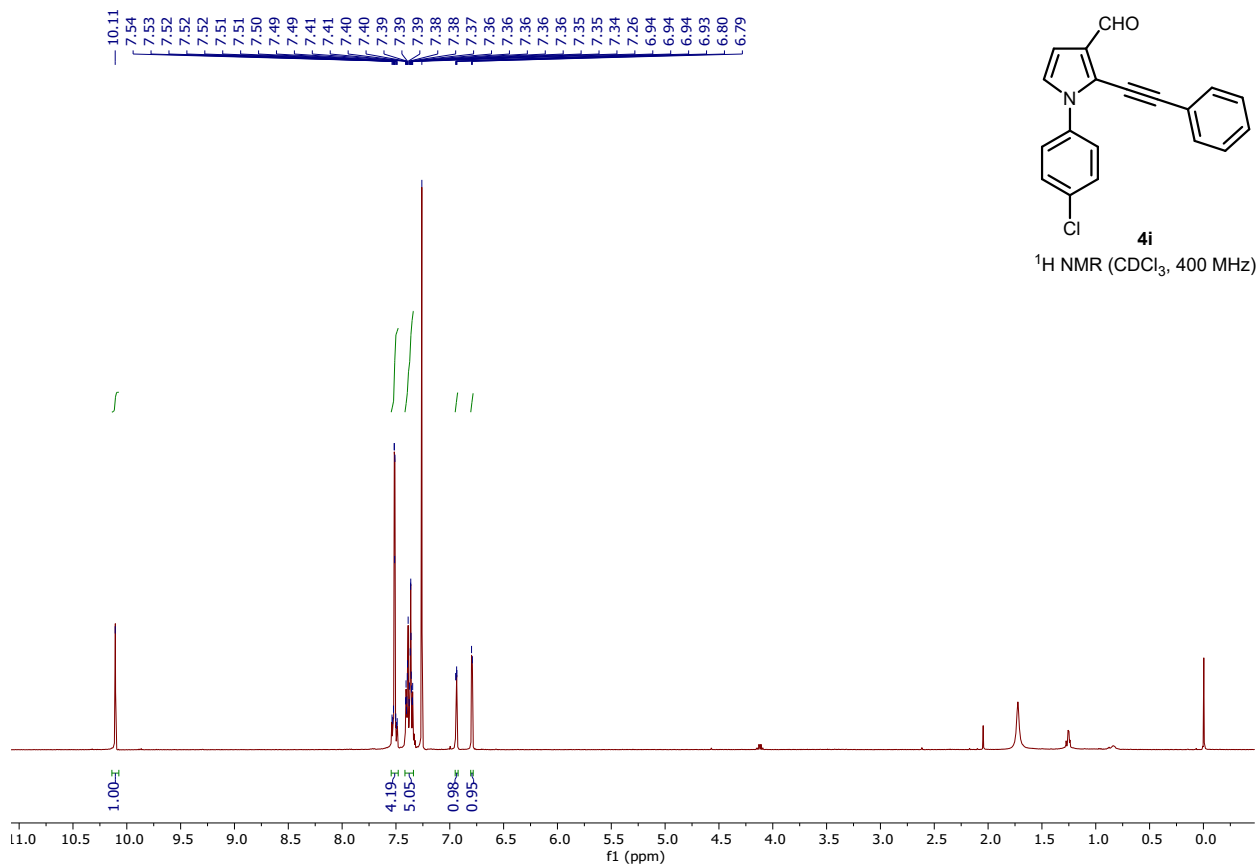
#### MS Zoomed Spectrum



#### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
290.0975	290.0976	0.3	1	95218.65	C19H12FNO	(M+H)+
291.1008	291.1008	0.04	1	19580.29	C19H12FNO	(M+H)+
292.1046	292.1039	-2.51	1	2083.31	C19H12FNO	(M+H)+
293.1098	293.1068	-10.27	1	186.08	C19H12FNO	(M+H)+
312.0796	312.0795	-0.15	1	1826.96	C19H12FNO	(M+Na)+
313.083	313.0828	-0.69	1	265.86	C19H12FNO	(M+Na)+
314.0884	314.0858	-8.03	1	63.35	C19H12FNO	(M+Na)+





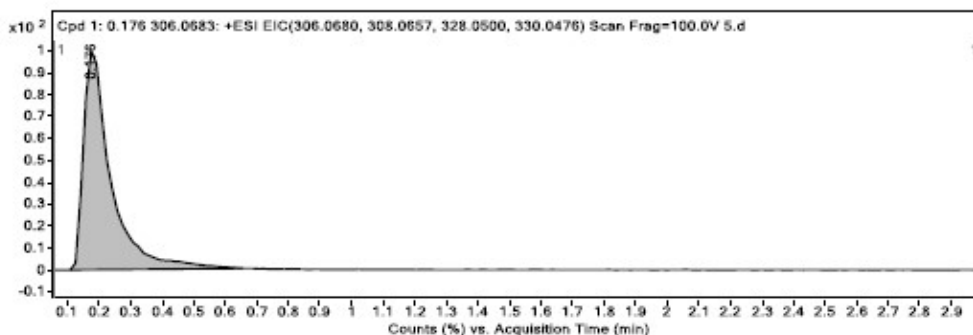
Data File	5.d	Sample Name	5
Sample Type	Sample	Position	P1-B5
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/7/2019 6:40:58 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

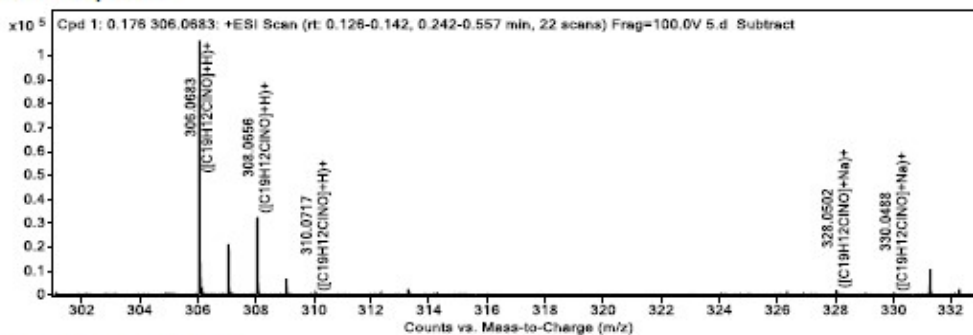
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.176 306.0683	0.176	305.061	106459	C19 H12 Cl N O	305.0607	0.7

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.176 306.0683	306.0683	0.176	Find By Formula	305.061

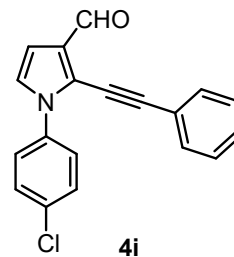


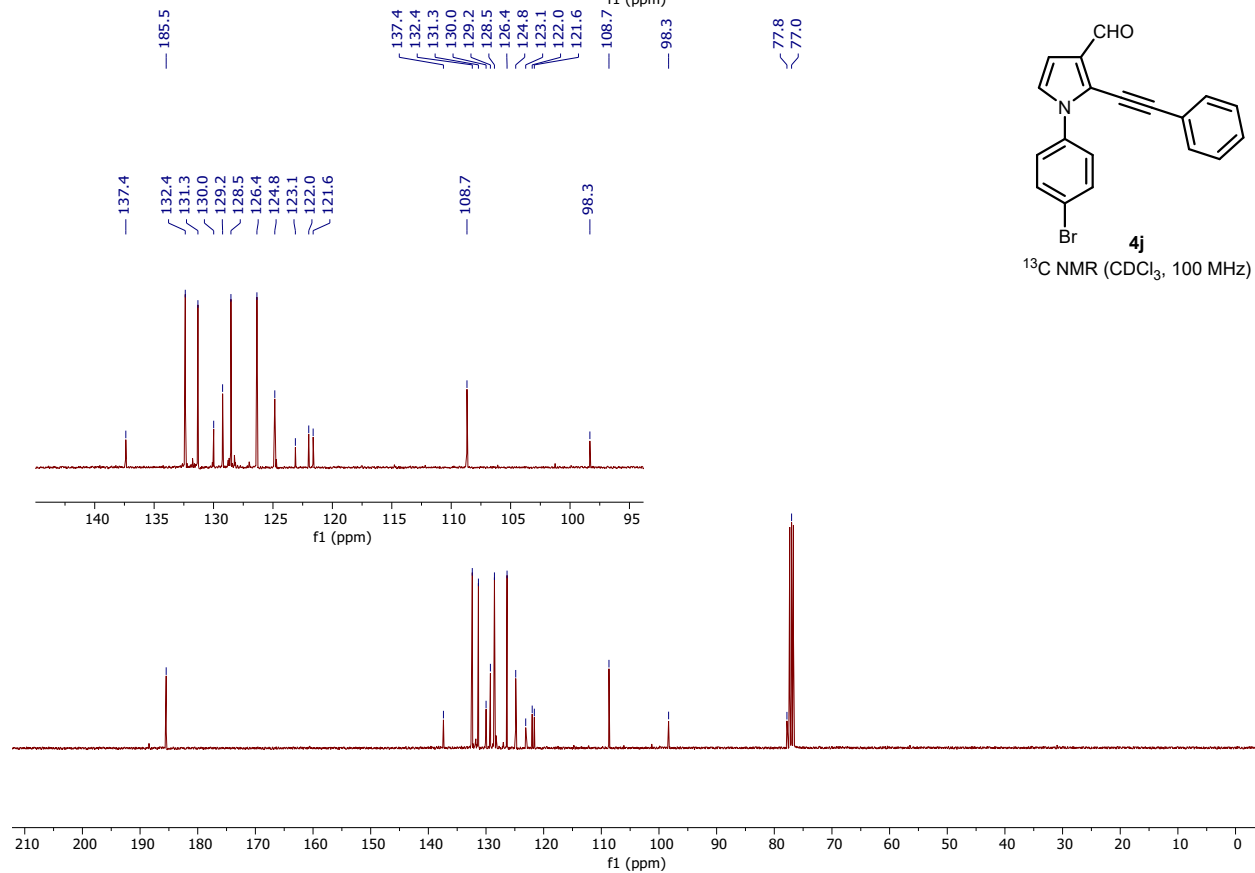
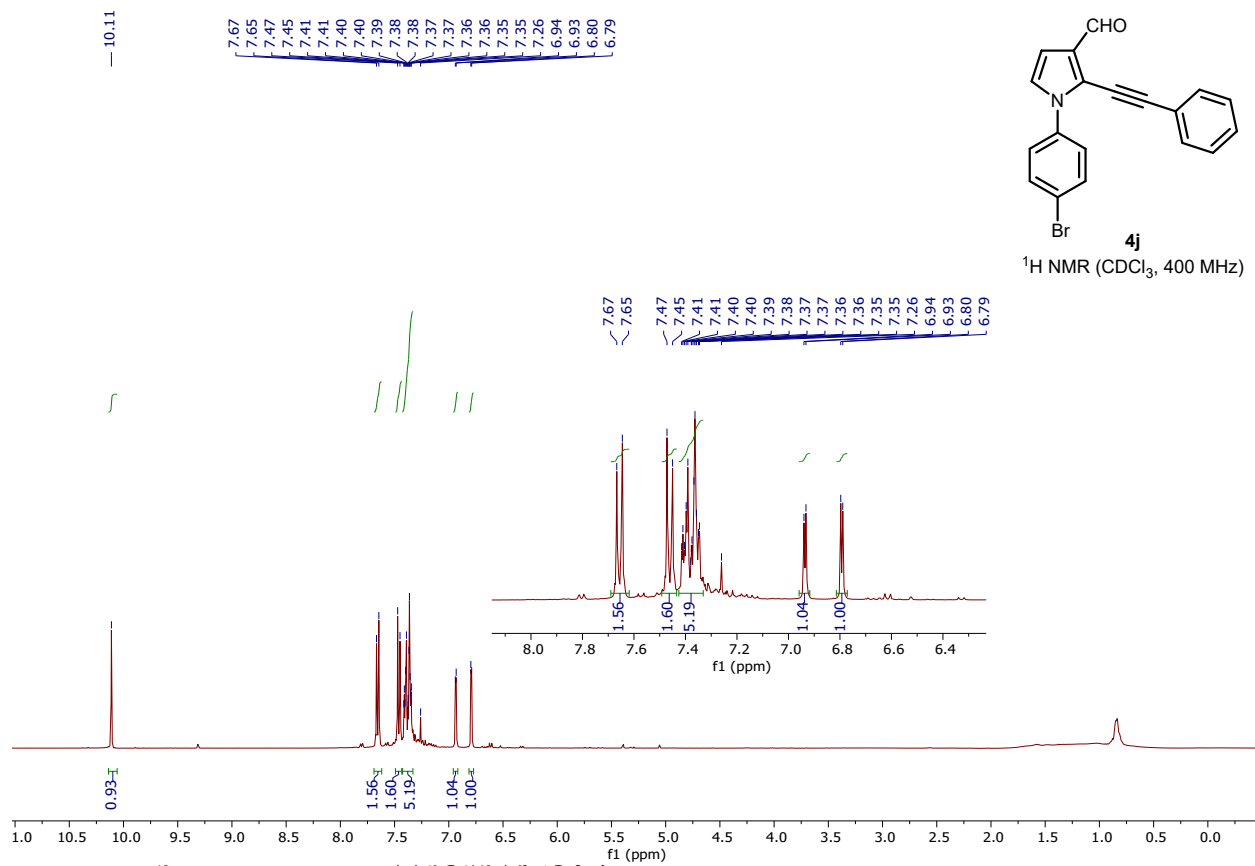
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
306.0683	306.068	-0.9	1	106459.45	C19H12ClNO	(M+H)+
307.0716	307.0713	-1.11	1	21651.07	C19H12ClNO	(M+H)+
308.0656	308.0657	0.2	1	33304.6	C19H12ClNO	(M+H)+
309.0687	309.0686	-0.31	1	6765.33	C19H12ClNO	(M+H)+
310.0717	310.0715	-0.73	1	728.4	C19H12ClNO	(M+H)+
311.0759	311.0744	-4.99	1	90.88	C19H12ClNO	(M+H)+
328.0502	328.05	-0.66	1	2027.2	C19H12ClNO	(M+Na)+
329.0537	329.0532	-1.51	1	462.68	C19H12ClNO	(M+Na)+
330.0488	330.0476	-3.42	1	673.53	C19H12ClNO	(M+Na)+
331.0486	331.0505	5.81	1	161.11	C19H12ClNO	(M+Na)+





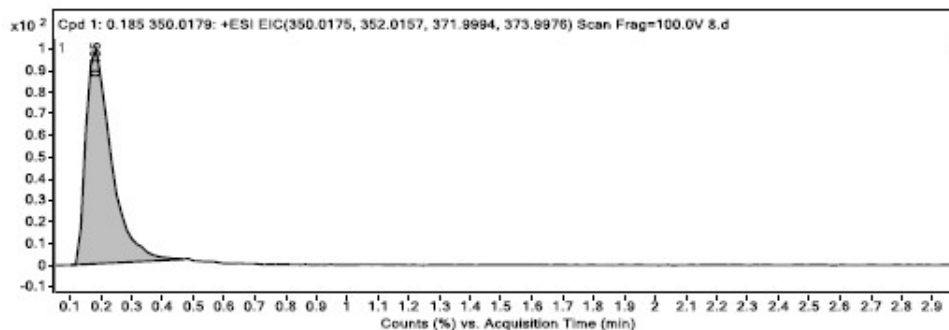
Data File	8.d	Sample Name	8
Sample Type	Sample	Position	P1-B8
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/7/2019 7:05:59 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

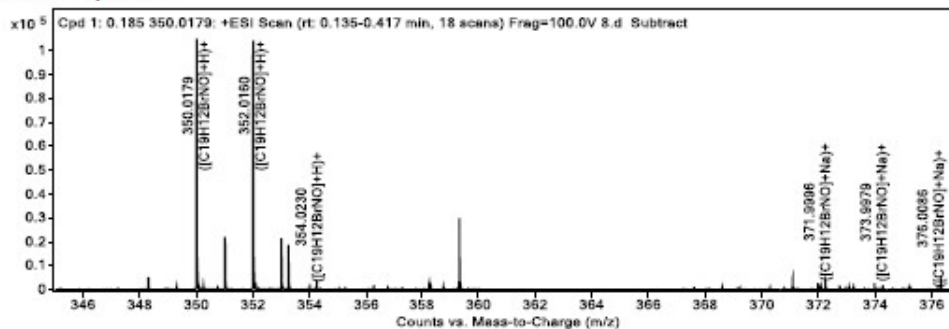
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.185 350.0179	0.185	349.0106	106647	C19H12BrNO	349.0102	1.16

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.185 350.0179	350.0179	0.185	Find By Formula	349.0106

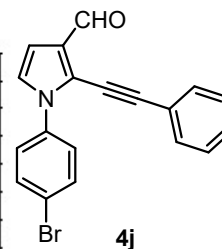


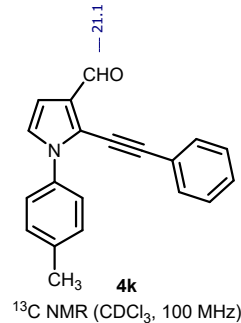
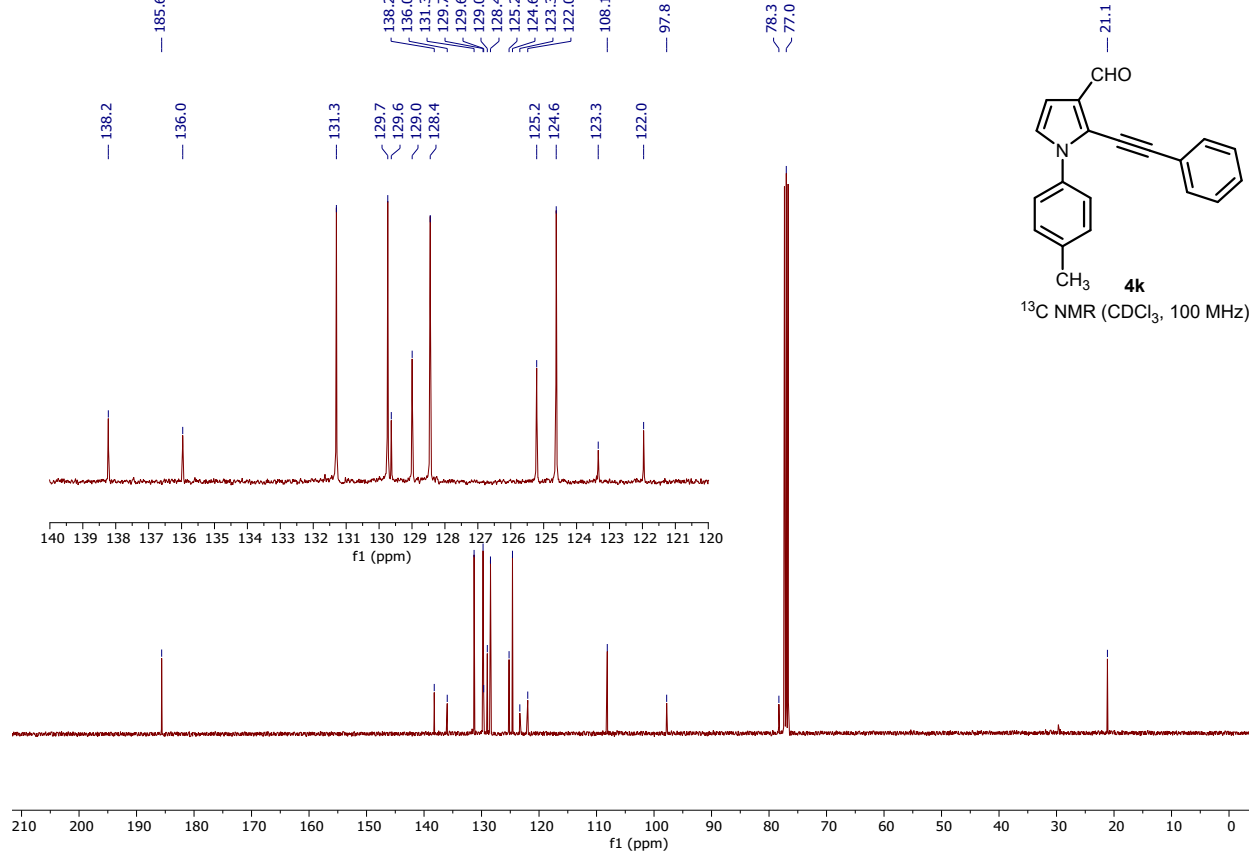
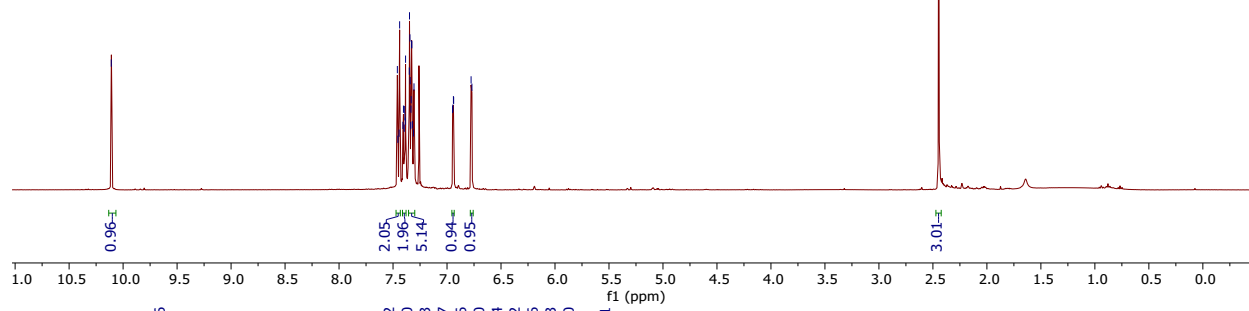
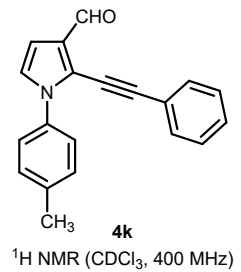
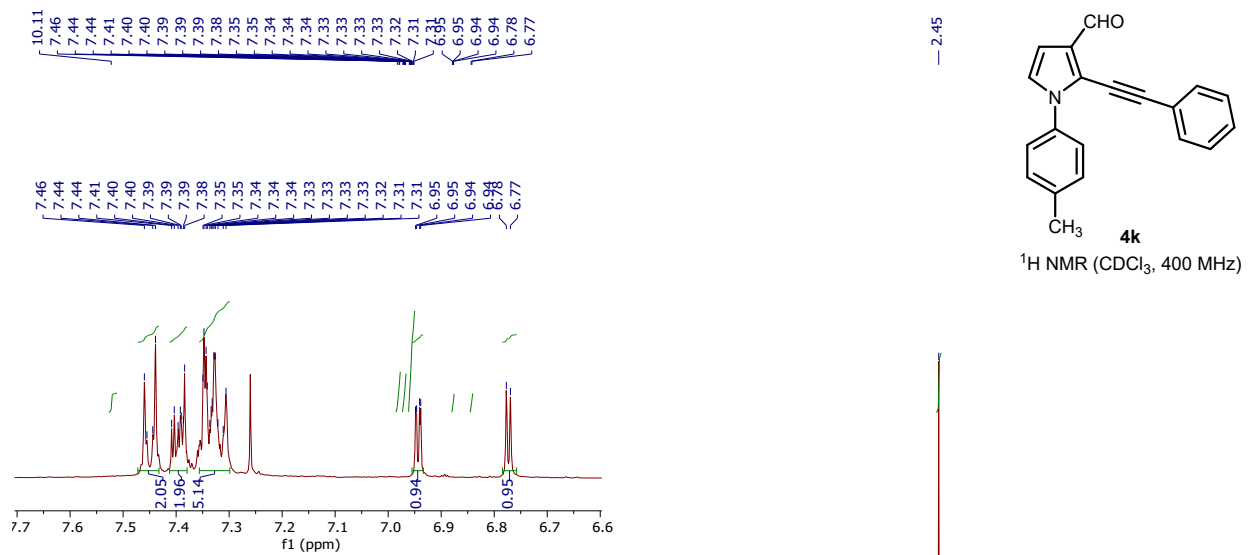
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
350.0179	350.0175	-1.12	1	106646.78	C19H12BrNO	(M+H)+
351.0213	351.0208	-1.57	1	22226.58	C19H12BrNO	(M+H)+
352.016	352.0157	-0.99	1	104488.75	C19H12BrNO	(M+H)+
353.0193	353.0188	-1.39	1	21638.8	C19H12BrNO	(M+H)+
354.023	354.0218	-3.36	1	2303.98	C19H12BrNO	(M+H)+
355.0262	355.0247	-4.21	1	219.97	C19H12BrNO	(M+H)+
371.9996	371.9994	-0.4	1	2852.54	C19H12BrNO	(M+Na)+
373.003	373.0027	-0.73	1	588.91	C19H12BrNO	(M+Na)+
373.9979	373.9976	-0.83	1	2706.39	C19H12BrNO	(M+Na)+
375.0018	375.0007	-2.85	1	582.05	C19H12BrNO	(M+Na)+
376.0086	376.0038	-12.95	1	116.3	C19H12BrNO	(M+Na)+





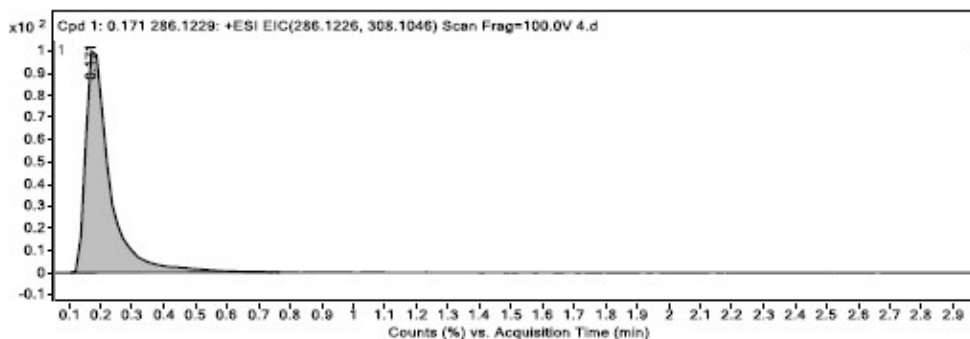
Data File	4.d	Sample Name	4
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/7/2019 6:32:37 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

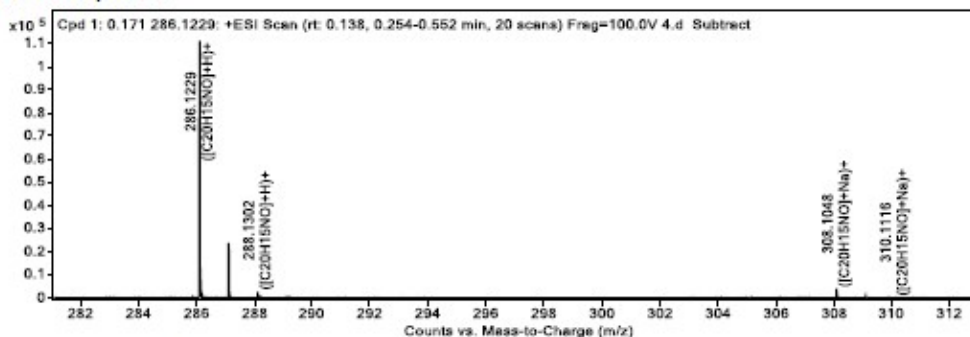
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.171 286.1229	0.171	285.1156	114136	C20 H15 N O	285.1154	0.94

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.171 286.1229	286.1229	0.171	Find By Formula	285.1156

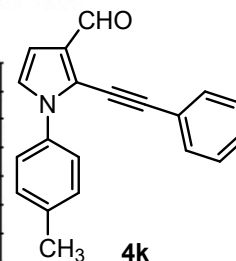


### MS Zoomed Spectrum

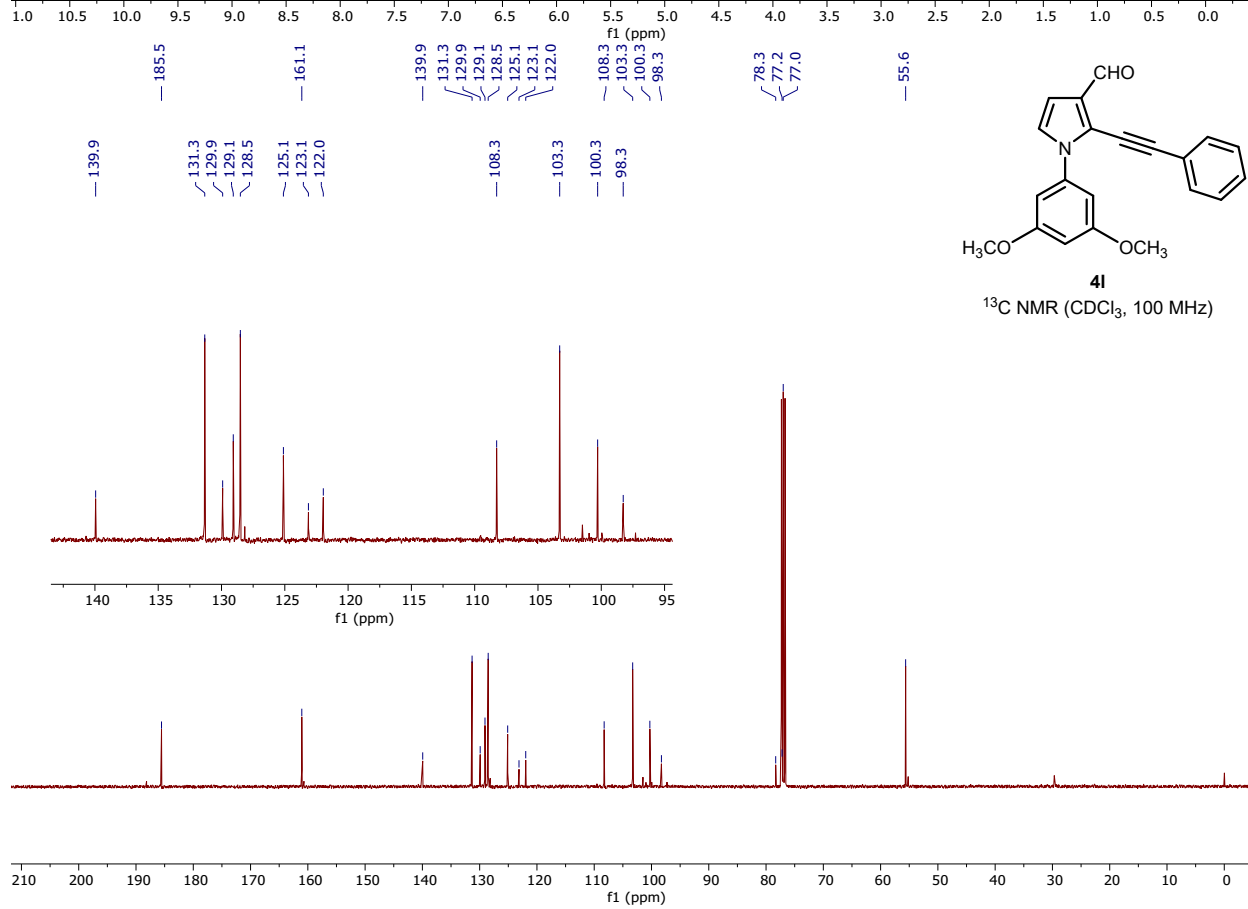
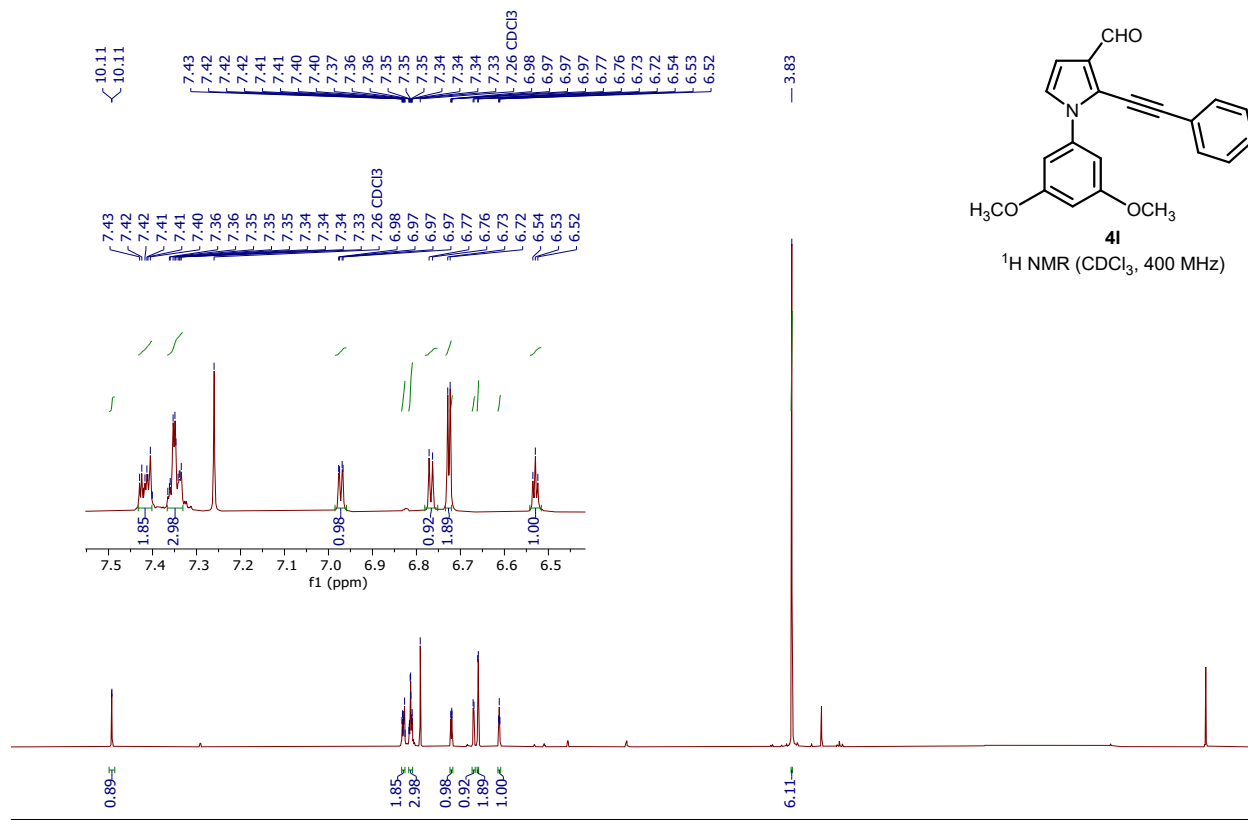


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
286.1229	286.1226	-0.82	1	114135.98	C20H15NO	(M+H) <sup>+</sup>
287.1262	287.1259	-1.02	1	24646.46	C20H15NO	(M+H) <sup>+</sup>
288.1302	288.129	-4.2	1	2670.58	C20H15NO	(M+H) <sup>+</sup>
289.1361	289.1319	-14.24	1	267.9	C20H15NO	(M+H) <sup>+</sup>
308.1048	308.1046	-0.75	1	3832.11	C20H15NO	(M+Na) <sup>+</sup>
309.1077	309.1079	0.65	1	805.7	C20H15NO	(M+Na) <sup>+</sup>
310.1116	310.1109	-2.1	1	98.95	C20H15NO	(M+Na) <sup>+</sup>







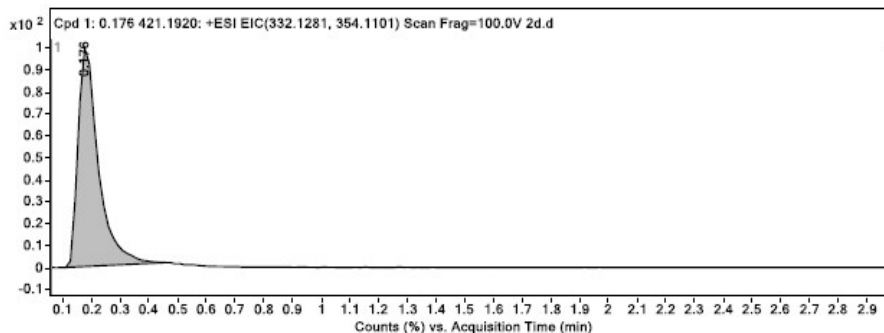
Data File	2d.d	Sample Name	2
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/7/2019 6:15:57 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

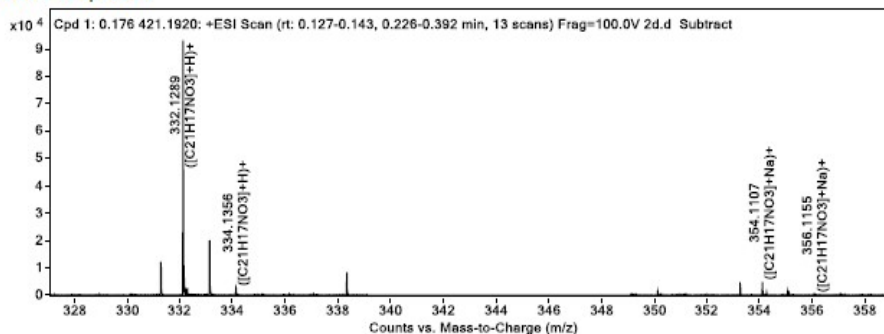
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.176 421.1920	0.176	331.1216	93626	C21 H17 N O3	331.1208	2.35

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.176 421.1920	332.1289	0.176	Find By Formula	331.1216

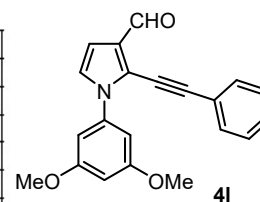


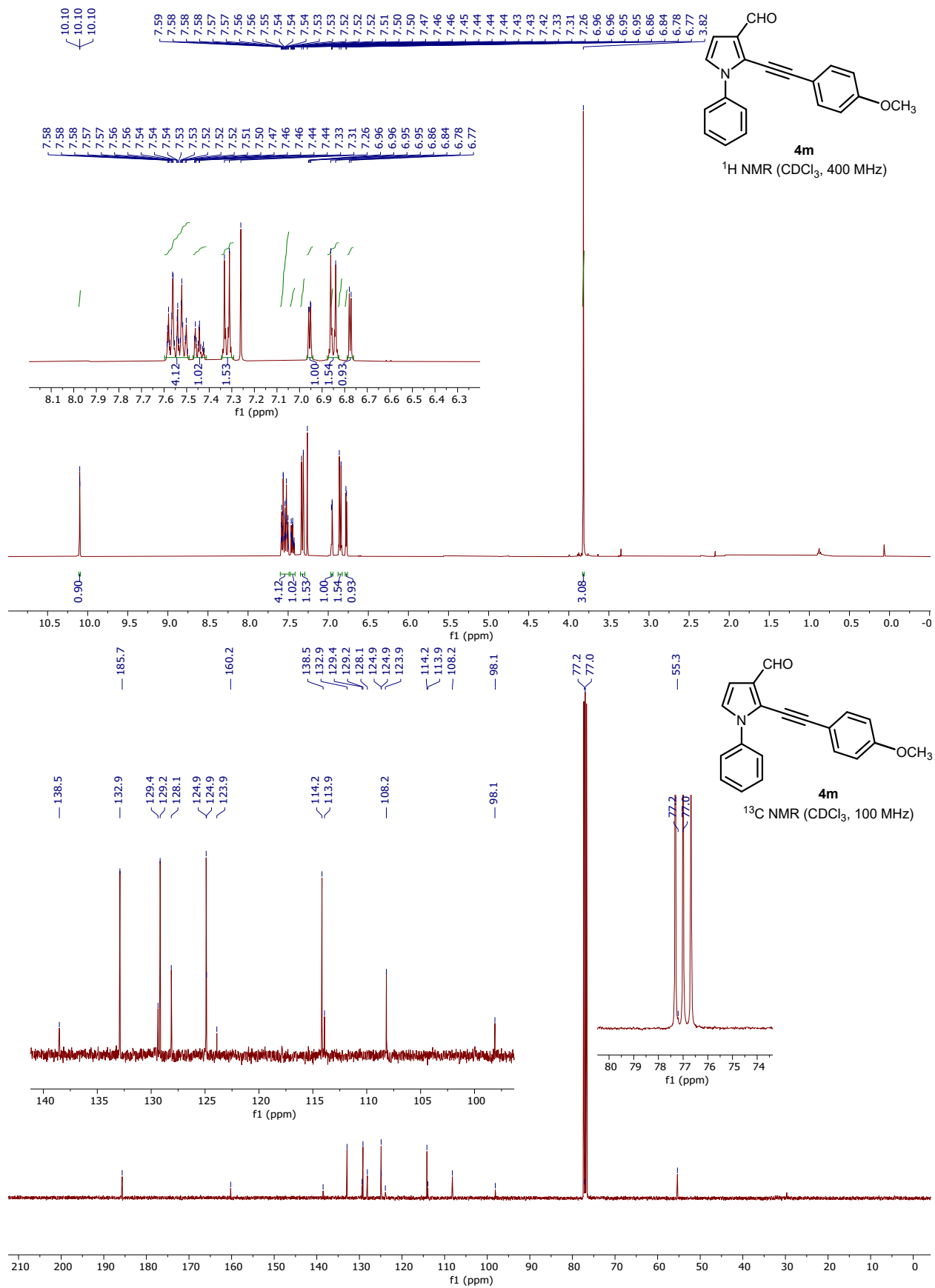
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
332.1289	332.1281	-2.32	1	93625.55	C21H17NO3	(M+H)+
333.1322	333.1314	-2.45	1	20901.31	C21H17NO3	(M+H)+
334.1356	334.1342	-3.92	1	2648.44	C21H17NO3	(M+H)+
354.1107	354.1101	-1.91	1	4846.8	C21H17NO3	(M+Na)+
355.1136	355.1133	-0.84	1	1261.62	C21H17NO3	(M+Na)+
356.1155	356.1162	1.83	1	267.14	C21H17NO3	(M+Na)+





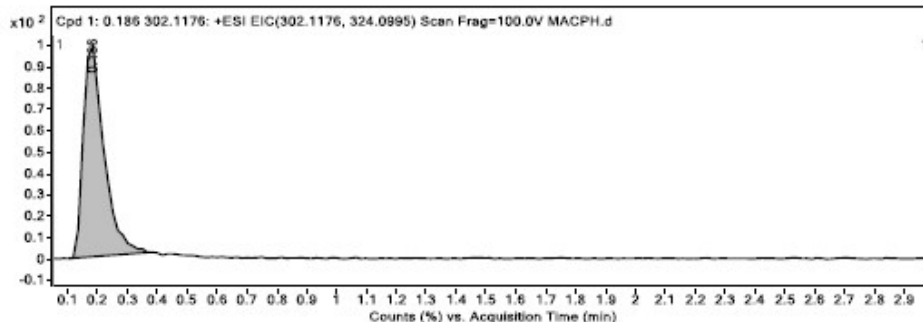
Data File	MACPH.d	Sample Name	MACPH
Sample Type	Sample	Position	P1-C8
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/8/2019 5:55:53 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

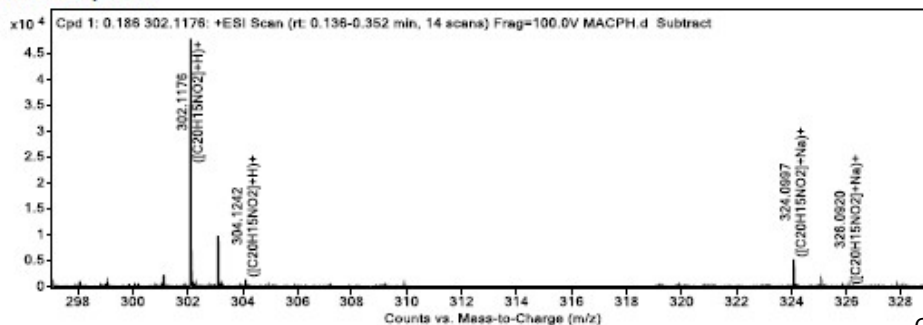
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.186 302.1176	0.186	301.1104	47992	C20 H15 N O2	301.1103	0.32

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.186 302.1176	302.1176	0.186	Find By Formula	301.1104

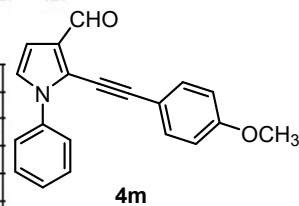


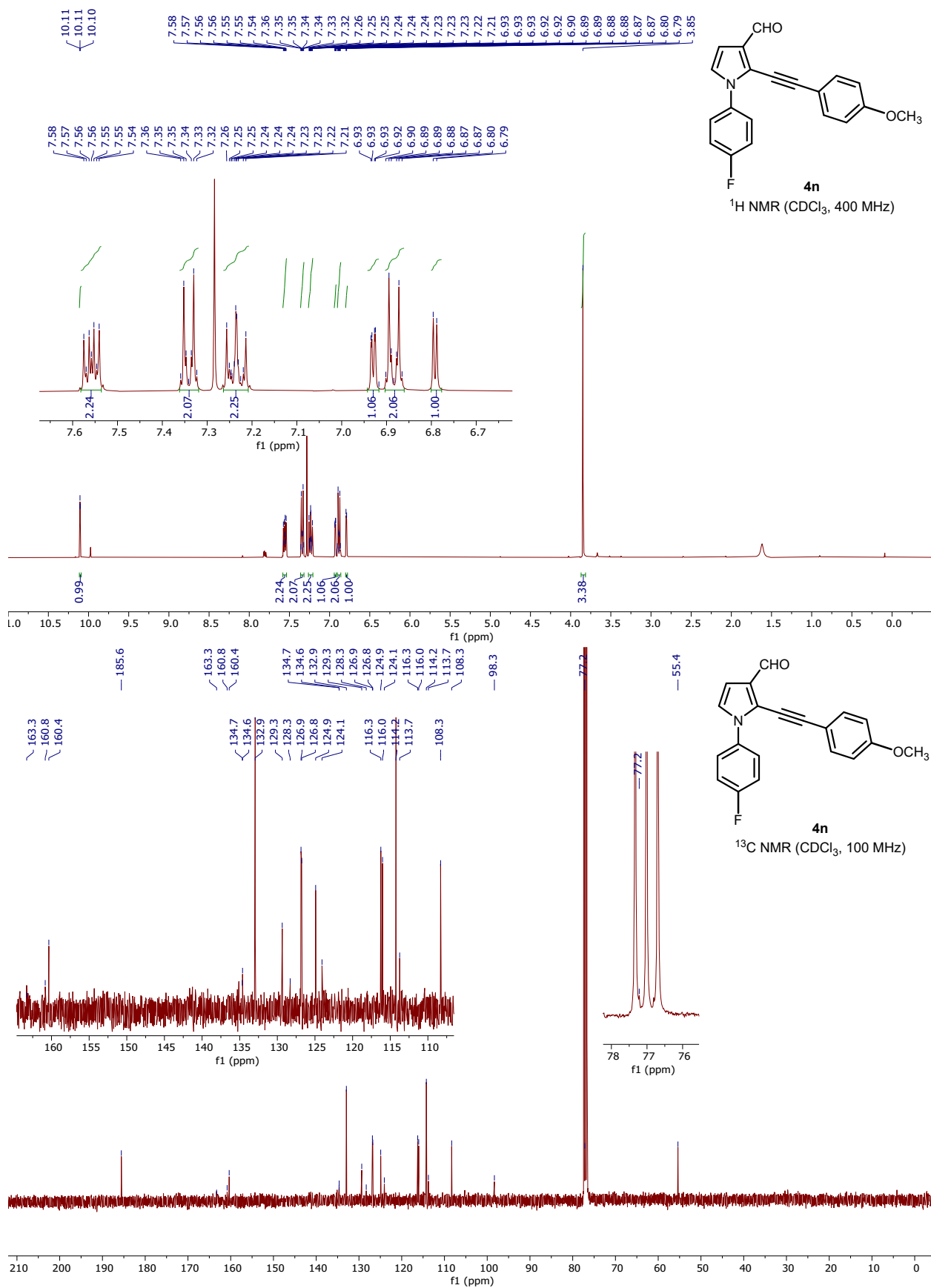
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
302.1176	302.1176	-0.13	1	47991.99	C20H15NO2	(M+H)+
303.1212	303.1208	-1.21	1	9806.79	C20H15NO2	(M+H)+
304.1242	304.1238	-1.31	1	1438.42	C20H15NO2	(M+H)+
305.1209	305.1265	18.41	1	96.44	C20H15NO2	(M+H)+
324.0997	324.0995	-0.68	1	5312.54	C20H15NO2	(M+Na)+
325.1029	325.1028	-0.41	1	1088.06	C20H15NO2	(M+Na)+
326.092	326.1057	41.98	1	32.34	C20H15NO2	(M+Na)+





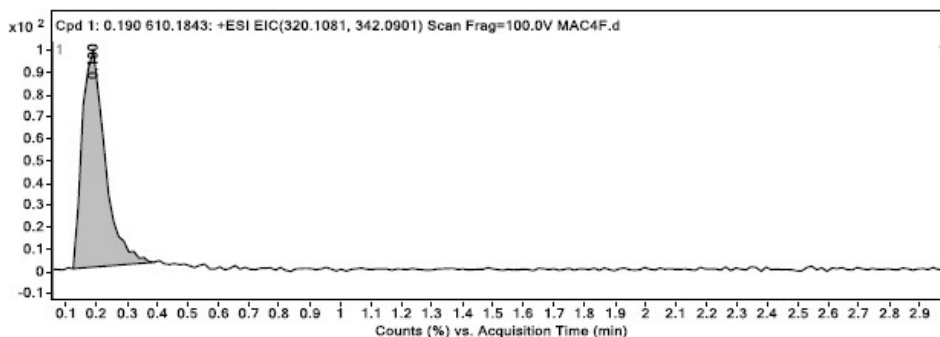
Data File	MAC4F.d	Sample Name	MAC4F
Sample Type	Sample	Position	P1-C5
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/8/2019 6:12:33 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

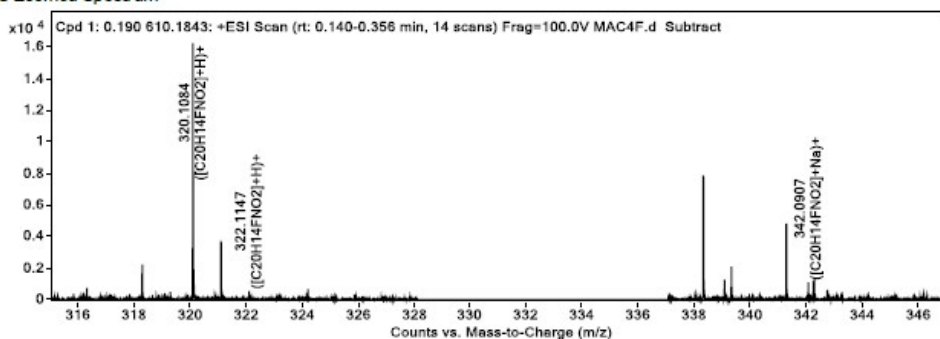
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.190 610.1843	0.19	319.1011	16276	C20 H14 F N O2	319.1009	0.91

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.190 610.1843	320.1084	0.19	Find By Formula	319.1011

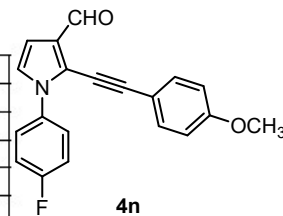


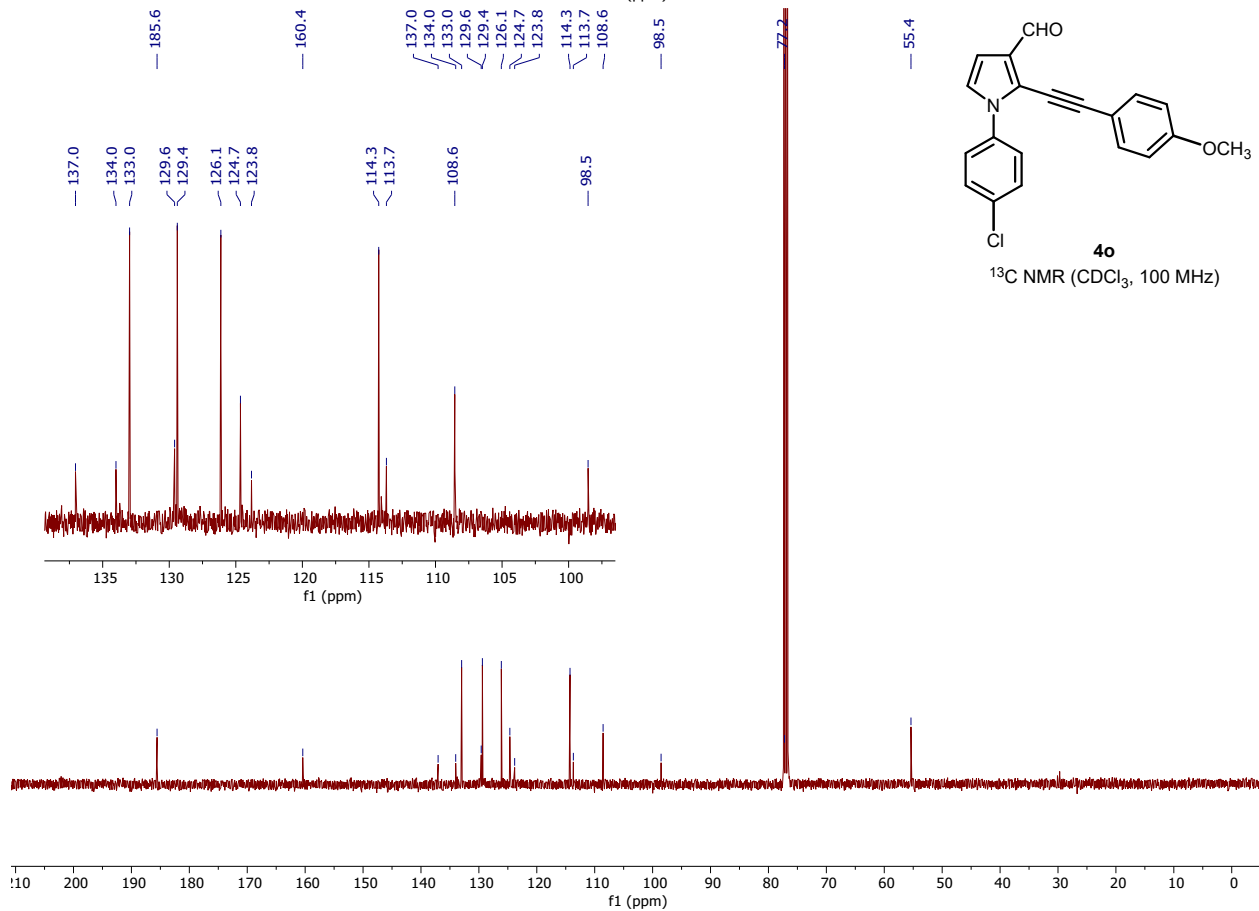
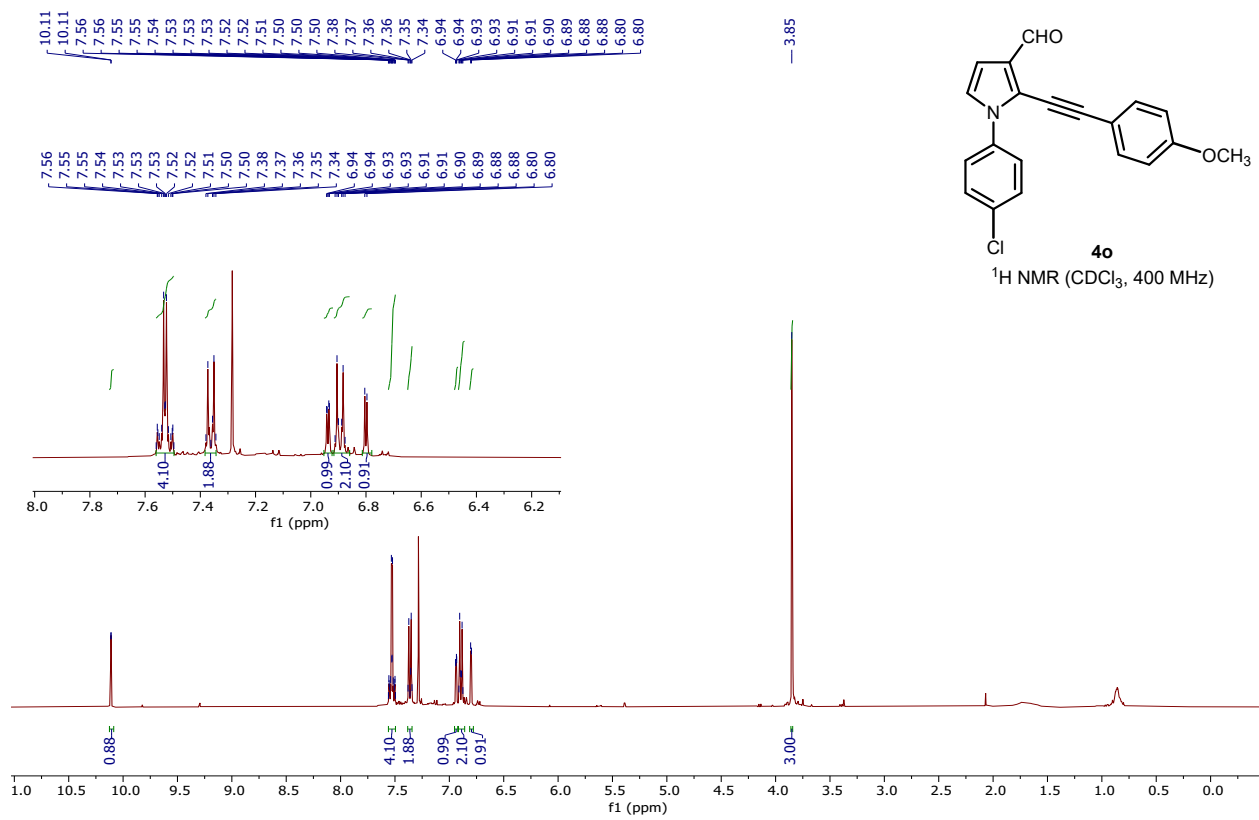
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
320.1084	320.1081	-0.91	1	16276.14	C20H14FNO2	(M+H)+
321.1116	321.1114	-0.48	1	3749.48	C20H14FNO2	(M+H)+
322.1147	322.1143	-1.2	1	531.62	C20H14FNO2	(M+H)+
323.1203	323.1171	-9.75	1	63.83	C20H14FNO2	(M+H)+
342.0907	342.0901	-1.76	1	1093.72	C20H14FNO2	(M+Na)+
343.0932	343.0934	0.33	1	212.11	C20H14FNO2	(M+Na)+





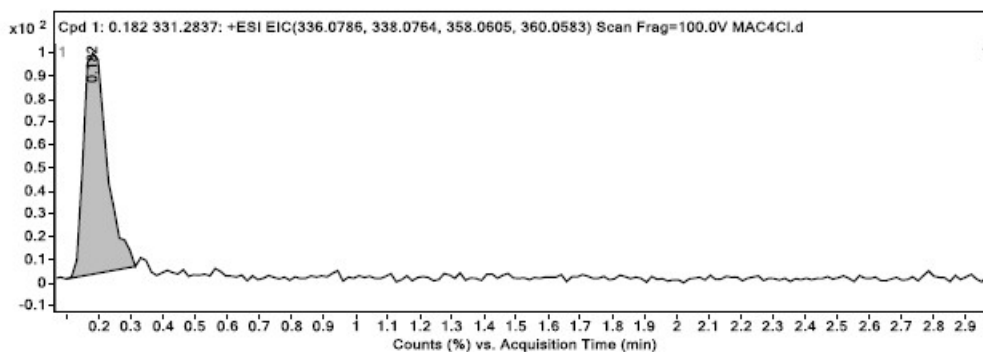
Data File	MAC4Cl.d	Sample Name	MAC4Cl
Sample Type	Sample	Position	P1-B11
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/8/2019 5:30:51 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

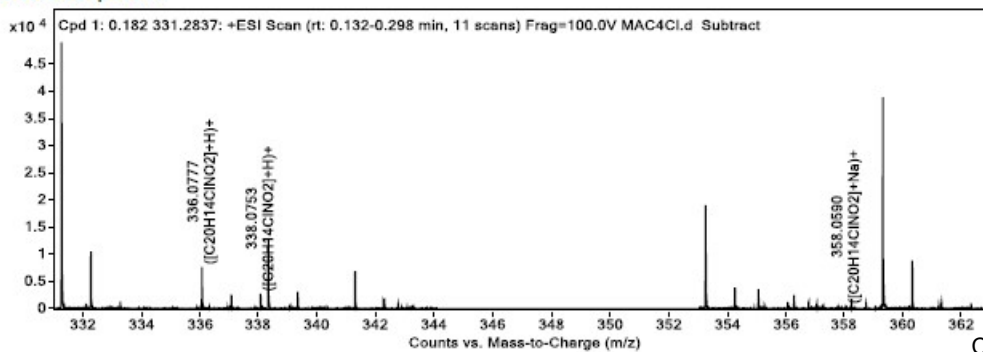
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.182 331.2837	0.182	335.07	7726	C20 H14 Cl N O2	335.0713	-3.84

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.182 331.2837	336.0777	0.182	Find By Formula	335.07

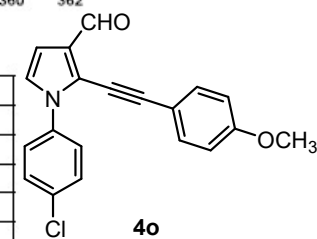


### MS Zoomed Spectrum

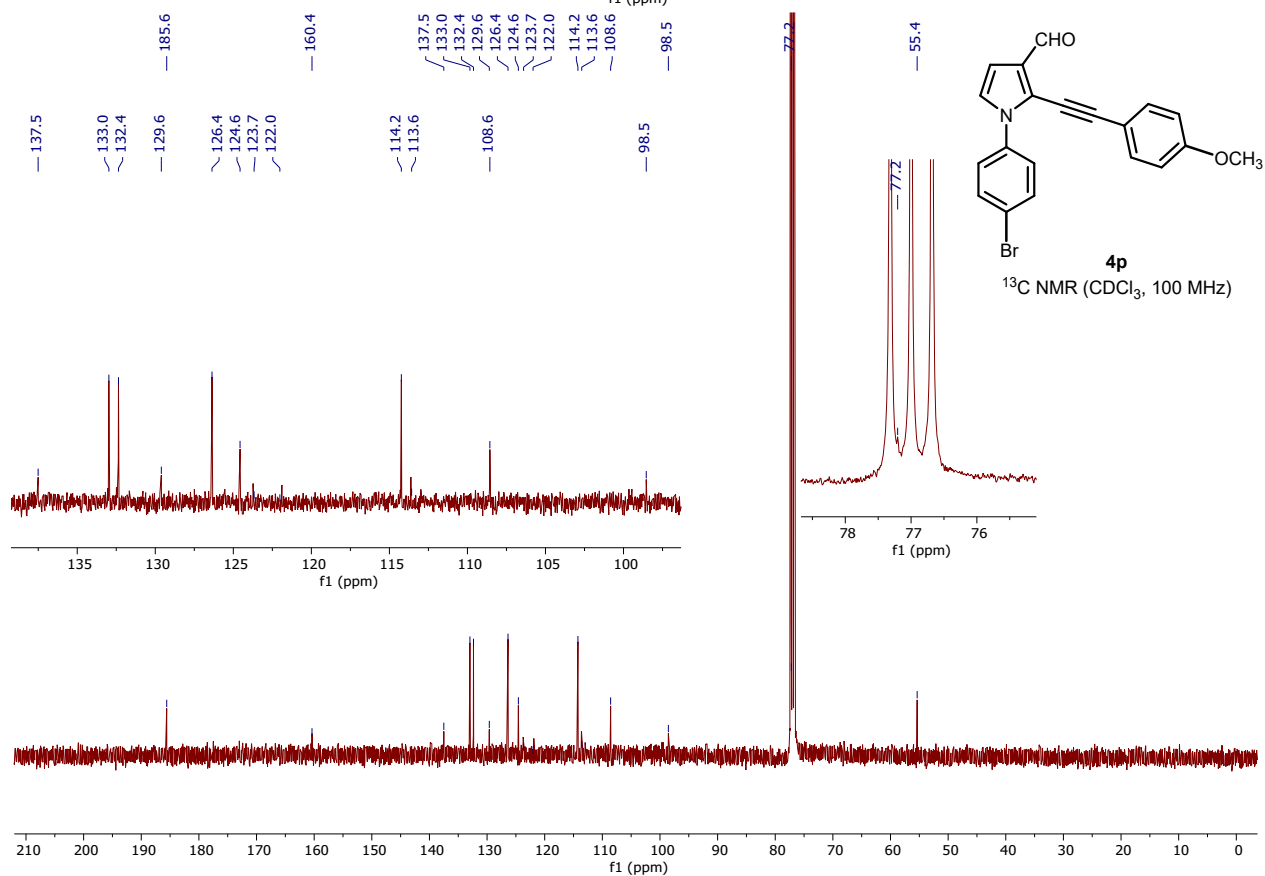
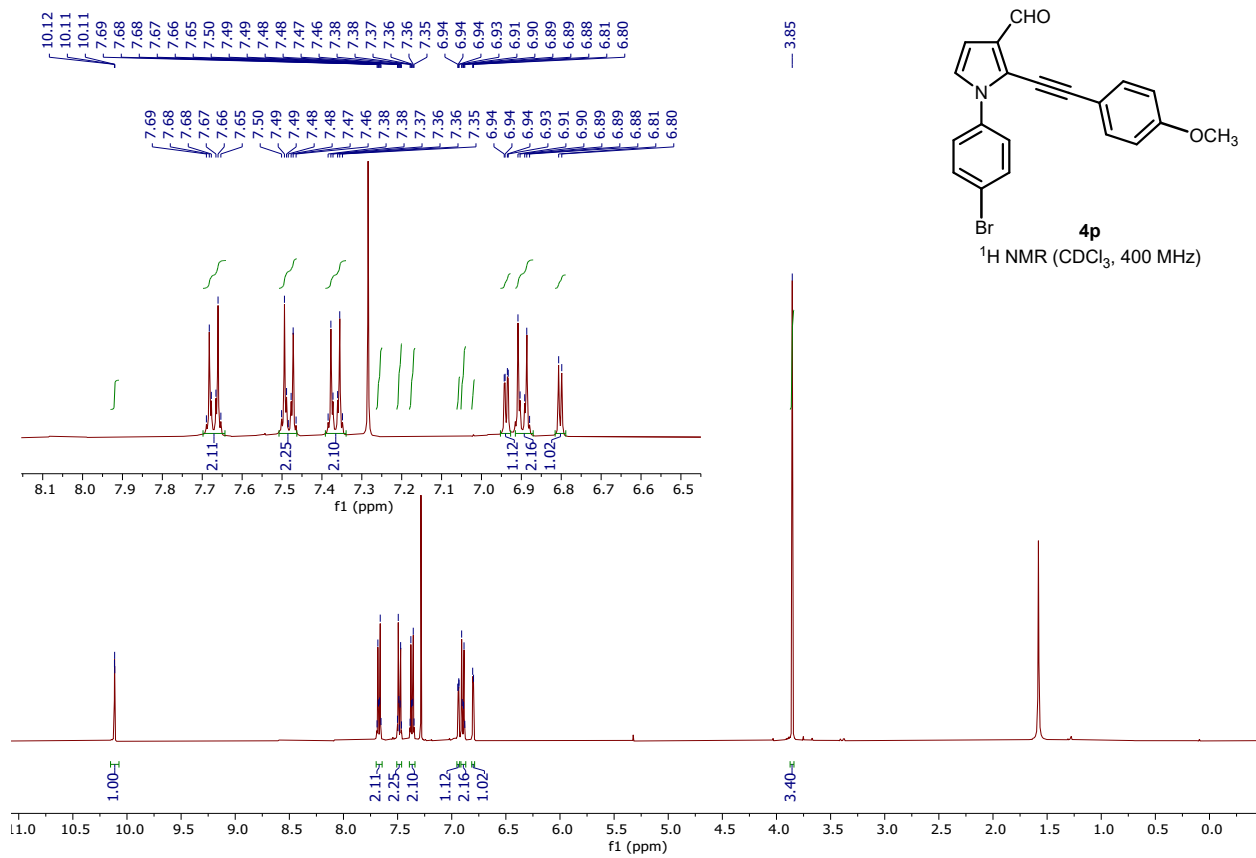


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
336.0777	336.0786	2.77	1	7725.93	C20H14ClNO2	(M+H)+
337.0778	337.0819	11.97	1	2585.17	C20H14ClNO2	(M+H)+
338.0753	338.0764	3.02	1	2800.21	C20H14ClNO2	(M+H)+
339.084	339.0792	-14.29	1	610.56	C20H14ClNO2	(M+H)+
358.059	358.0605	4.19	1	504.92	C20H14ClNO2	(M+Na)+







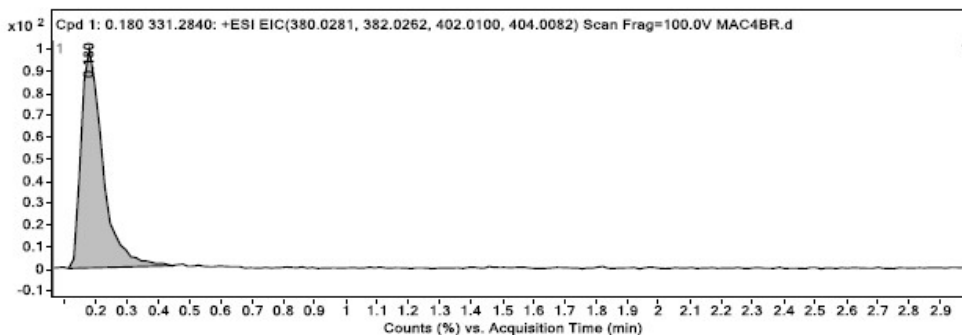
Data File	MAC4BR.d	Sample Name	MAC4BR
Sample Type	Sample	Position	P1-C6
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/8/2019 5:39:10 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

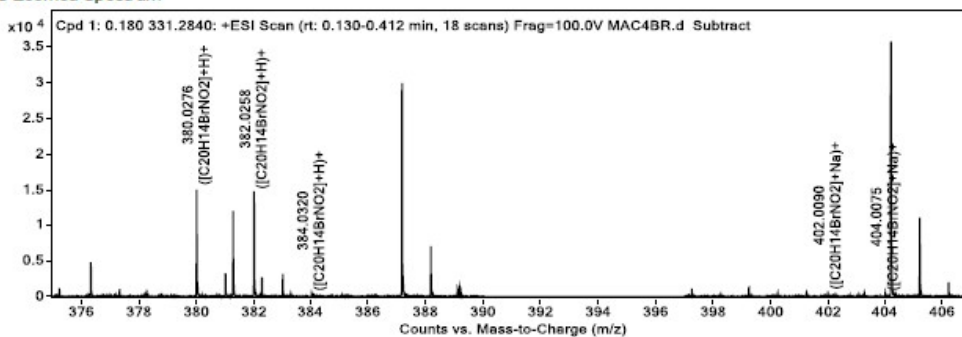
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.180 331.2840	0.18	379.0203	15341	C20 H14 Br N O2	379.0208	-1.25

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.180 331.2840	380.0276	0.18	Find By Formula	379.0203

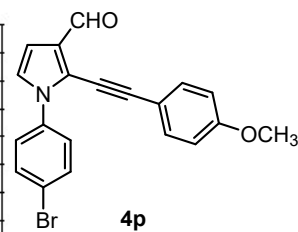


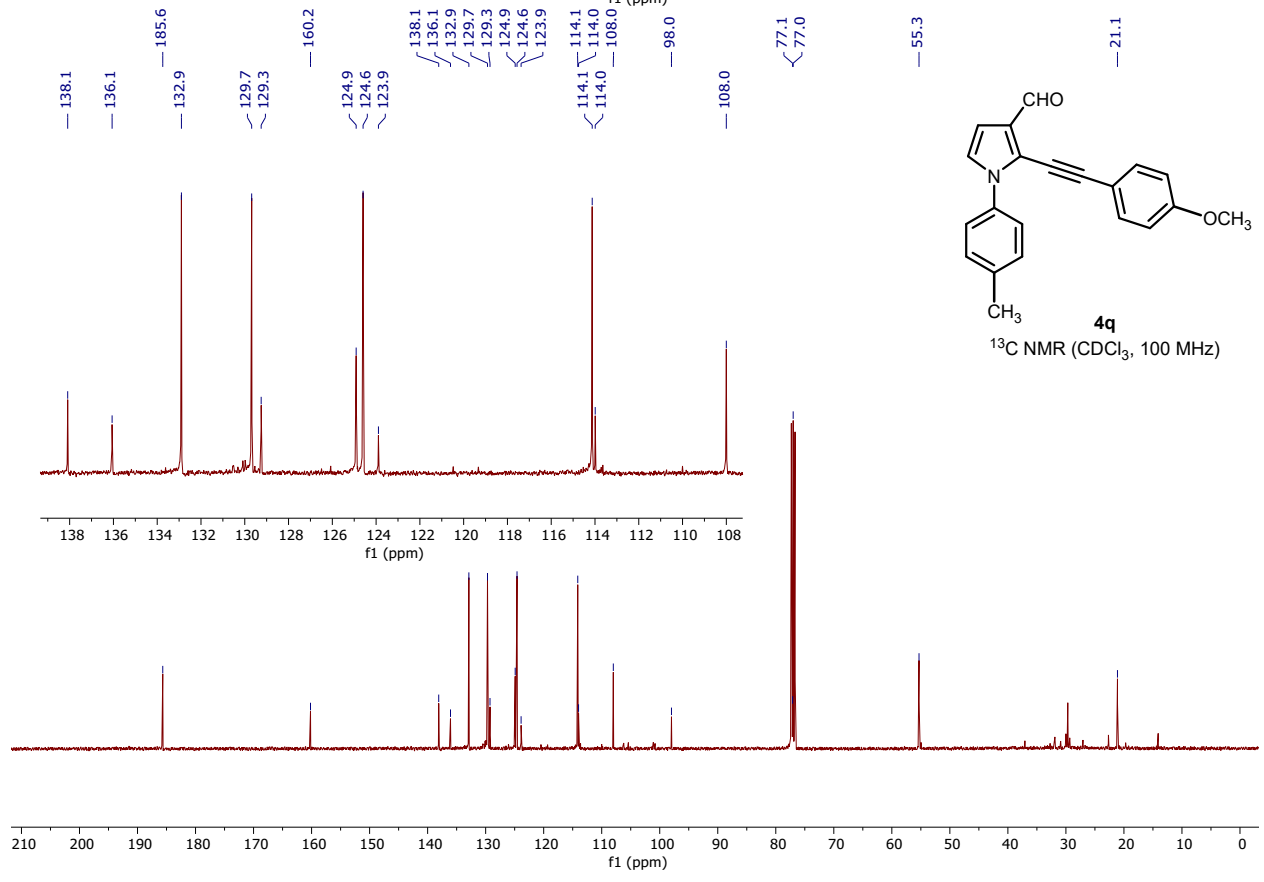
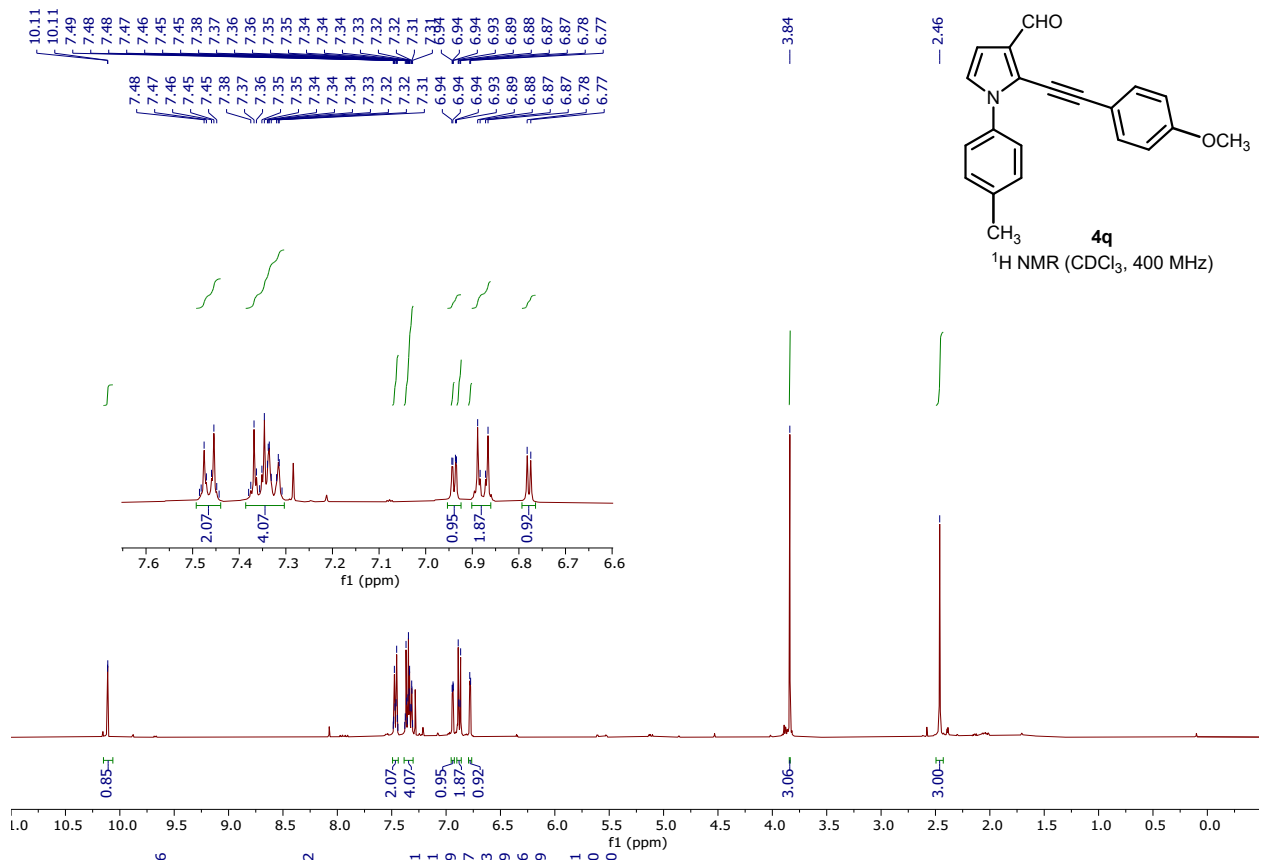
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
380.0276	380.0281	1.33	1	15341.27	C20H14BrNO2	(M+H)+
381.0312	381.0313	0.38	1	3314.55	C20H14BrNO2	(M+H)+
382.0258	382.0262	1.19	1	14791.64	C20H14BrNO2	(M+H)+
383.0291	383.0294	0.74	1	3153.12	C20H14BrNO2	(M+H)+
384.032	384.0323	0.63	1	506.2	C20H14BrNO2	(M+H)+
385.0324	385.035	6.8	1	72.76	C20H14BrNO2	(M+H)+
402.009	402.01	2.43	1	710.08	C20H14BrNO2	(M+Na)+
403.0116	403.0133	4.13	1	159.41	C20H14BrNO2	(M+Na)+
404.0075	404.0082	1.67	1	516.49	C20H14BrNO2	(M+Na)+
404.9993	405.0113	29.8	1	58.03	C20H14BrNO2	(M+Na)+





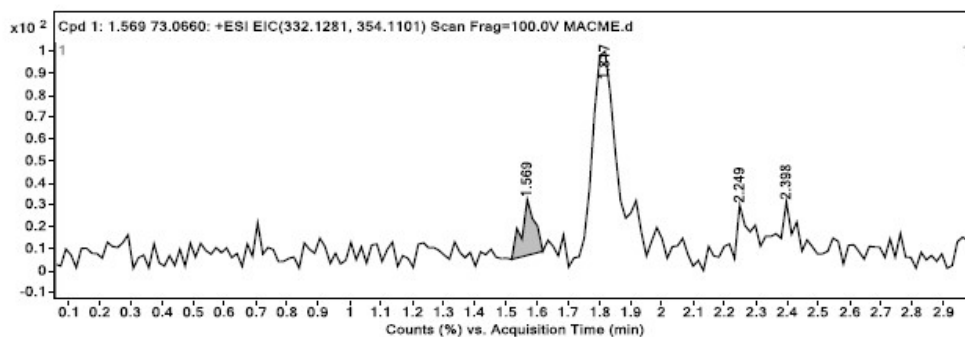
Data File	MACME.d	Sample Name	MACME
Sample Type	Sample	Position	P2-A6
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.bintu.m	Acquired Time	6/21/2019 5:25:37 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

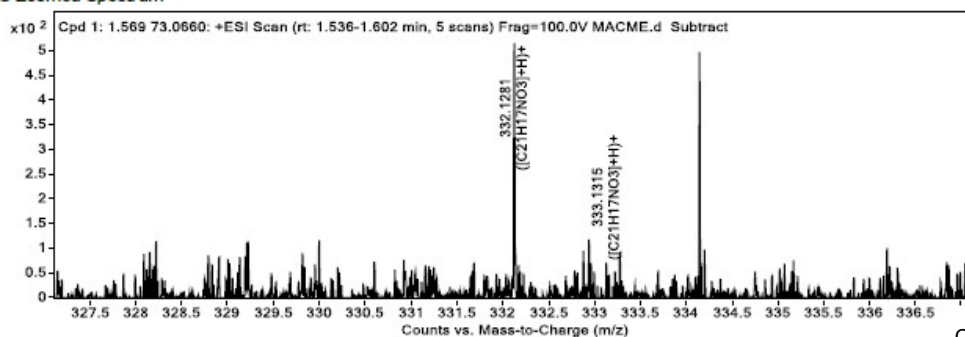
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 1.569 73.0660	1.569	331.1208	528	C21 H17 N O3	331.1208	-0.14

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 1.569 73.0660	332.1281	1.569	Find By Formula	331.1208

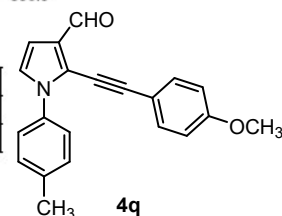


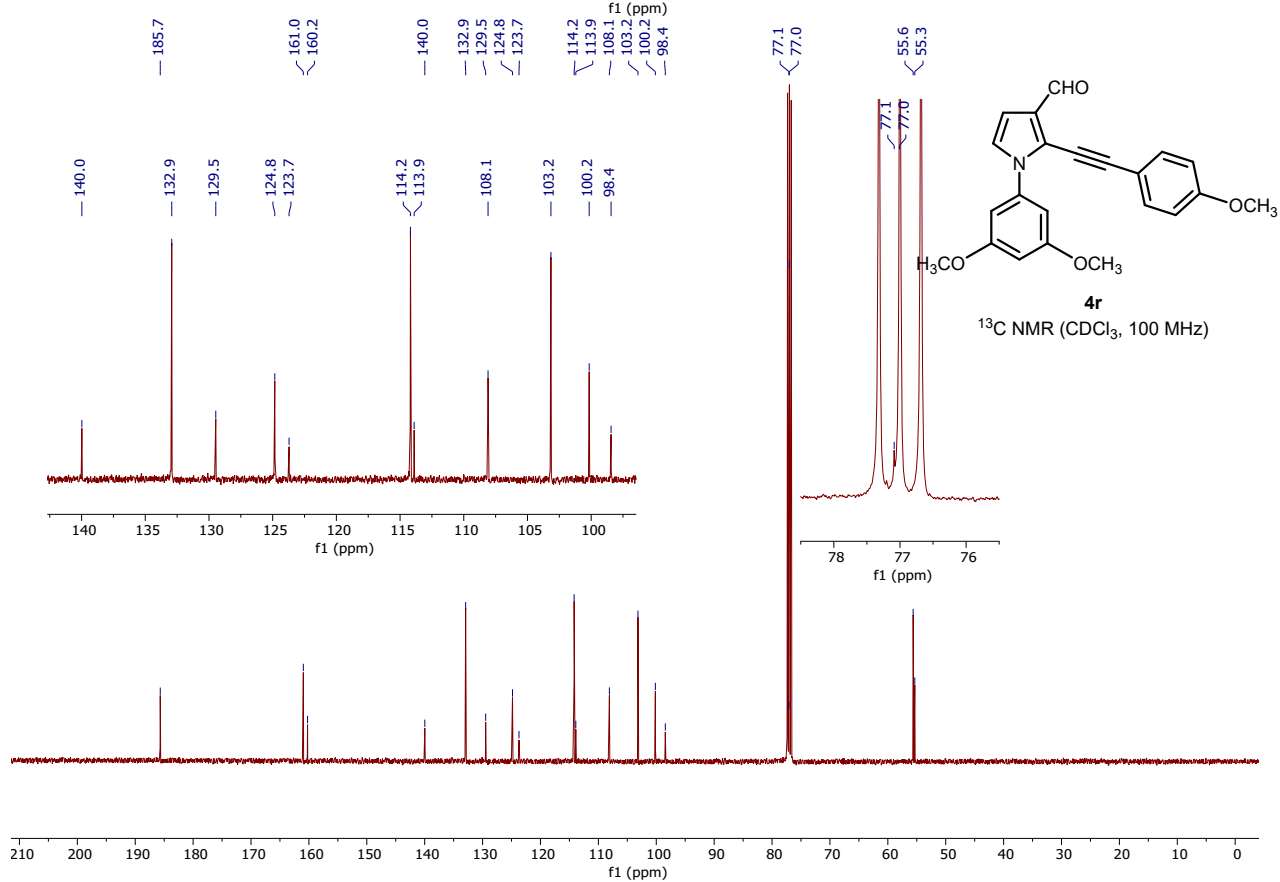
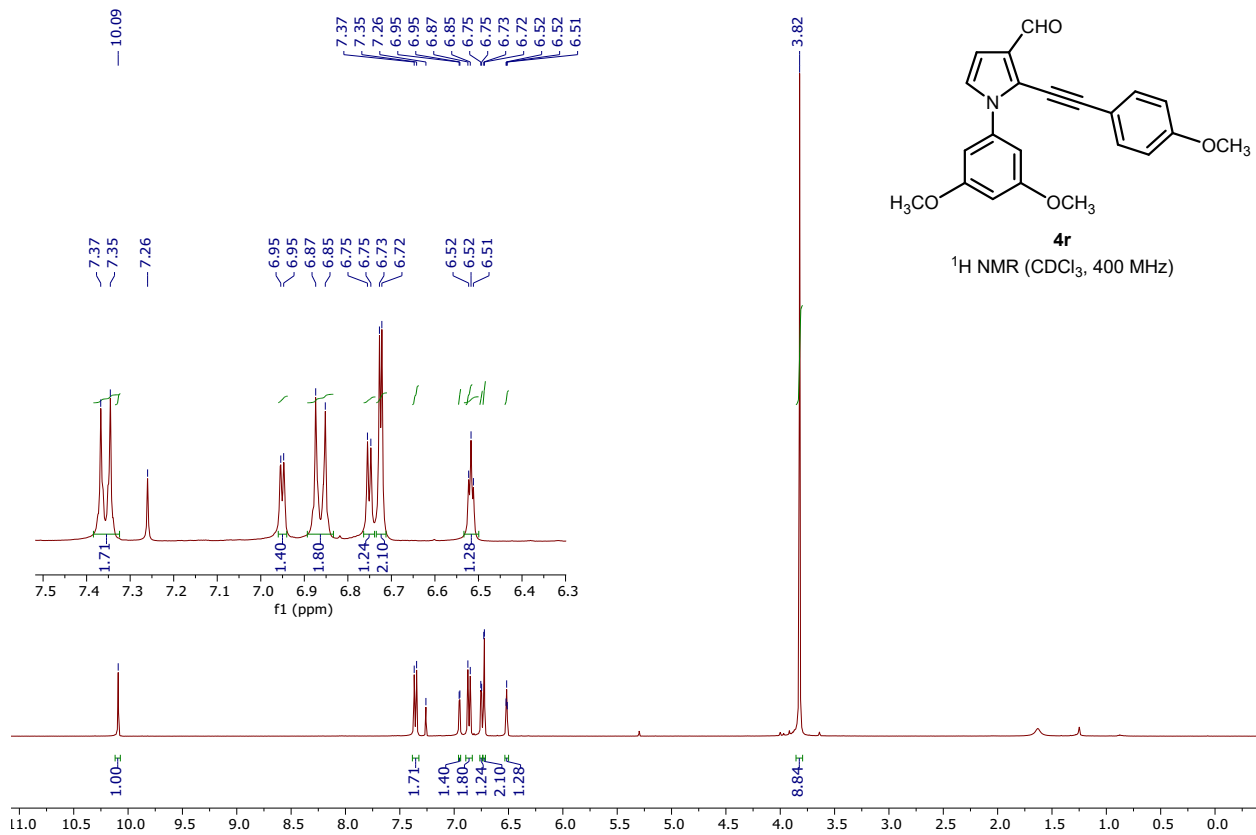
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
332.1281	332.1281	0.2	1	528.12	C21H17NO3	(M+H)+
333.1315	333.1314	-0.3	1	71.35	C21H17NO3	(M+H)+





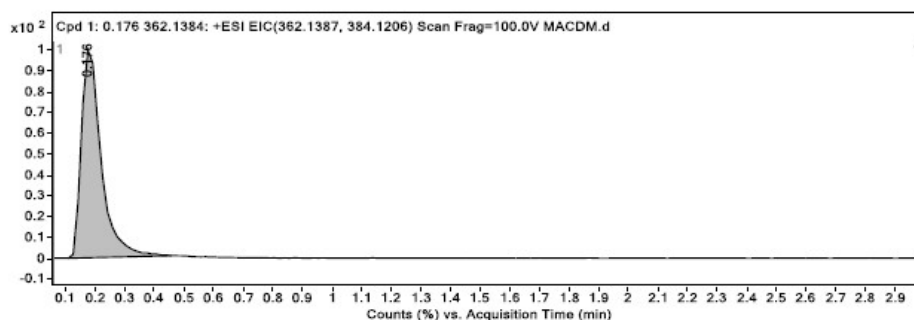
<b>Data File</b>	MACDM.d	<b>Sample Name</b>	MACDM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-C7
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	5/8/2019 5:47:32 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

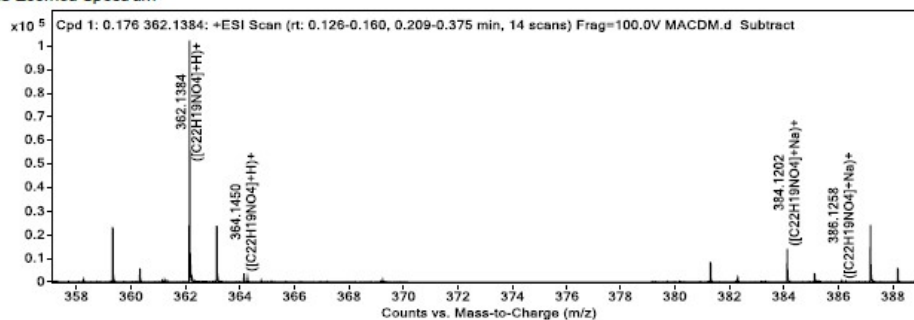
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.176 362.1384	0.176	361.1311	105491	C22 H19 N O4	361.1314	-0.96

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.176 362.1384	362.1384	0.176	Find By Formula	361.1311

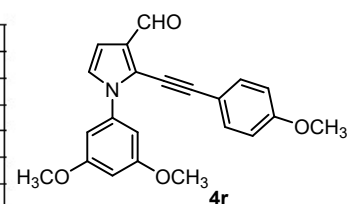


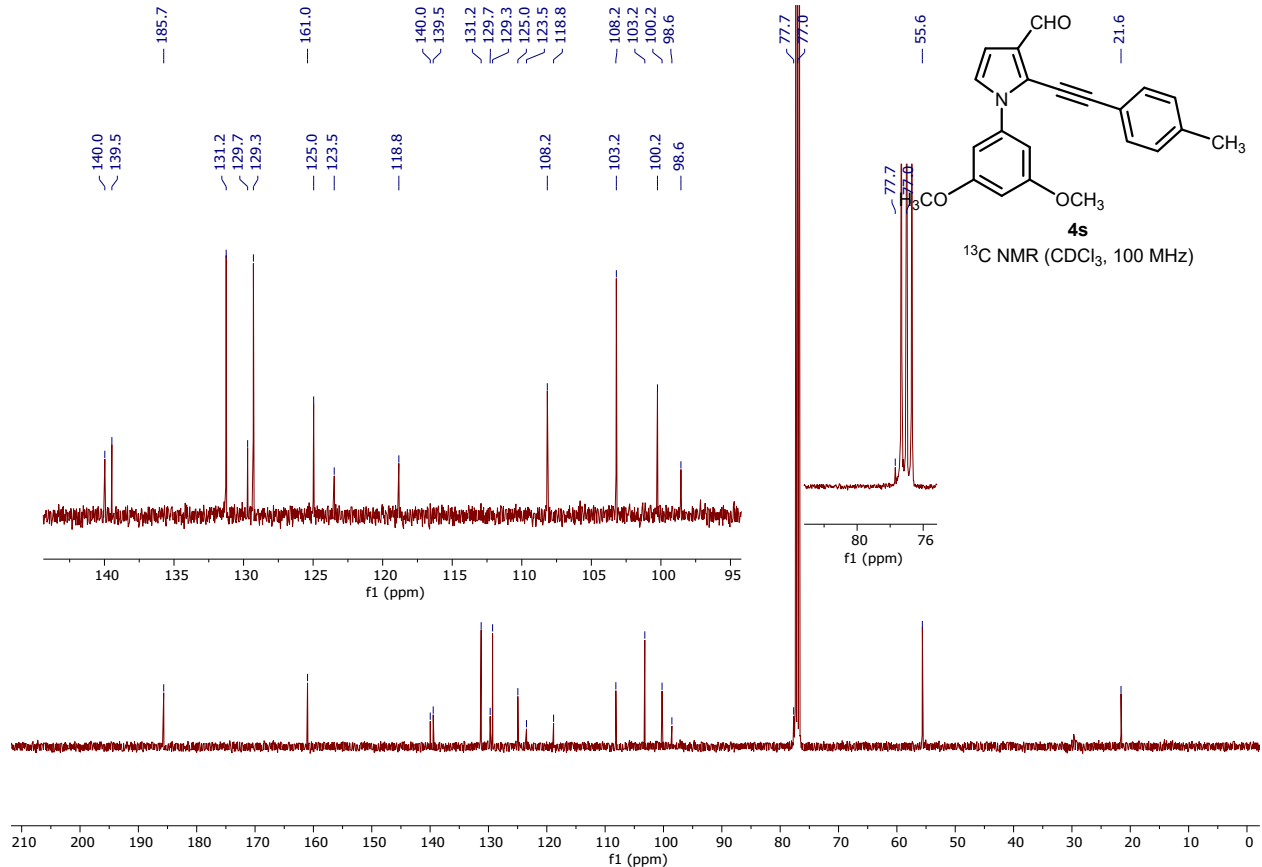
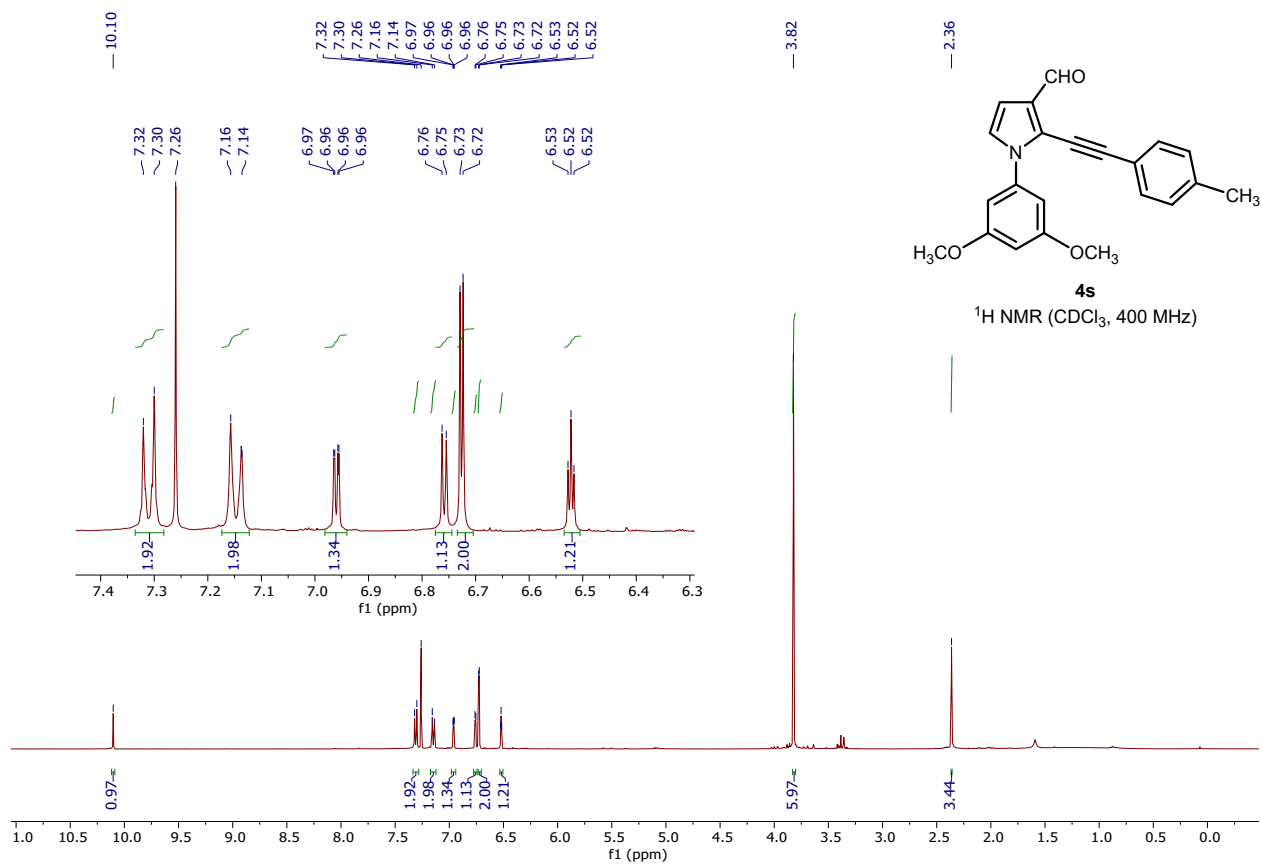
#### MS Zoomed Spectrum



#### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
362.1384	362.1387	0.92	1	105491	C22H19NO4	(M+H)+
363.1416	363.142	1.08	1	24772.92	C22H19NO4	(M+H)+
364.145	364.1447	-0.56	1	3598.46	C22H19NO4	(M+H)+
365.1476	365.1474	-0.33	1	461.07	C22H19NO4	(M+H)+
384.1202	384.1206	1.21	1	14413.23	C22H19NO4	(M+Na)+
385.1235	385.1239	1.17	1	3533.77	C22H19NO4	(M+Na)+
386.1258	386.1267	2.3	1	570.28	C22H19NO4	(M+Na)+









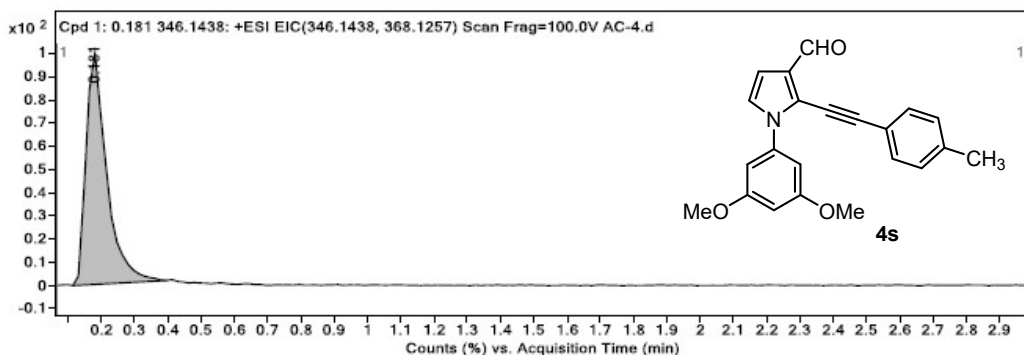
Data File	AC-4.d	Sample Name	AC-4
Sample Type	Sample	Position	P1-B9
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	5/8/2019 5:14:05 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

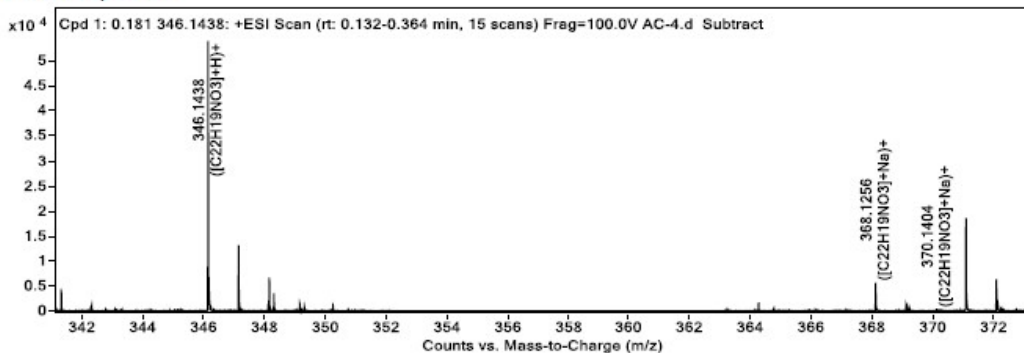
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.181 346.1438	0.181	345.1366	5654	C22 H19 N O3	345.1365	0.23

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.181 346.1438	368.1256	0.181	Find By Formula	345.1366

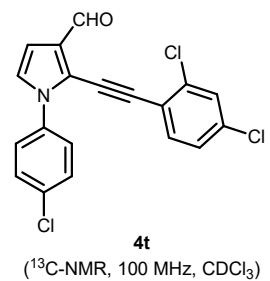
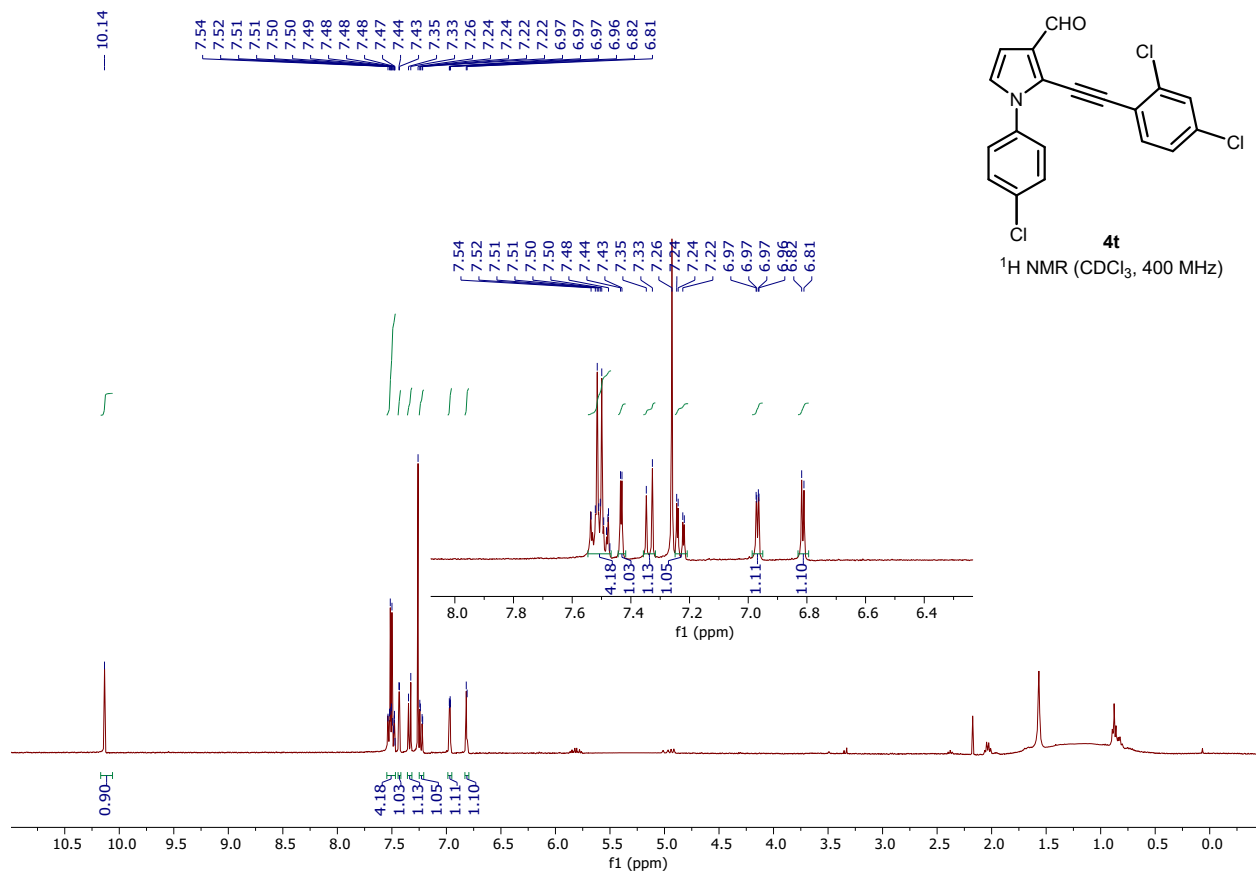


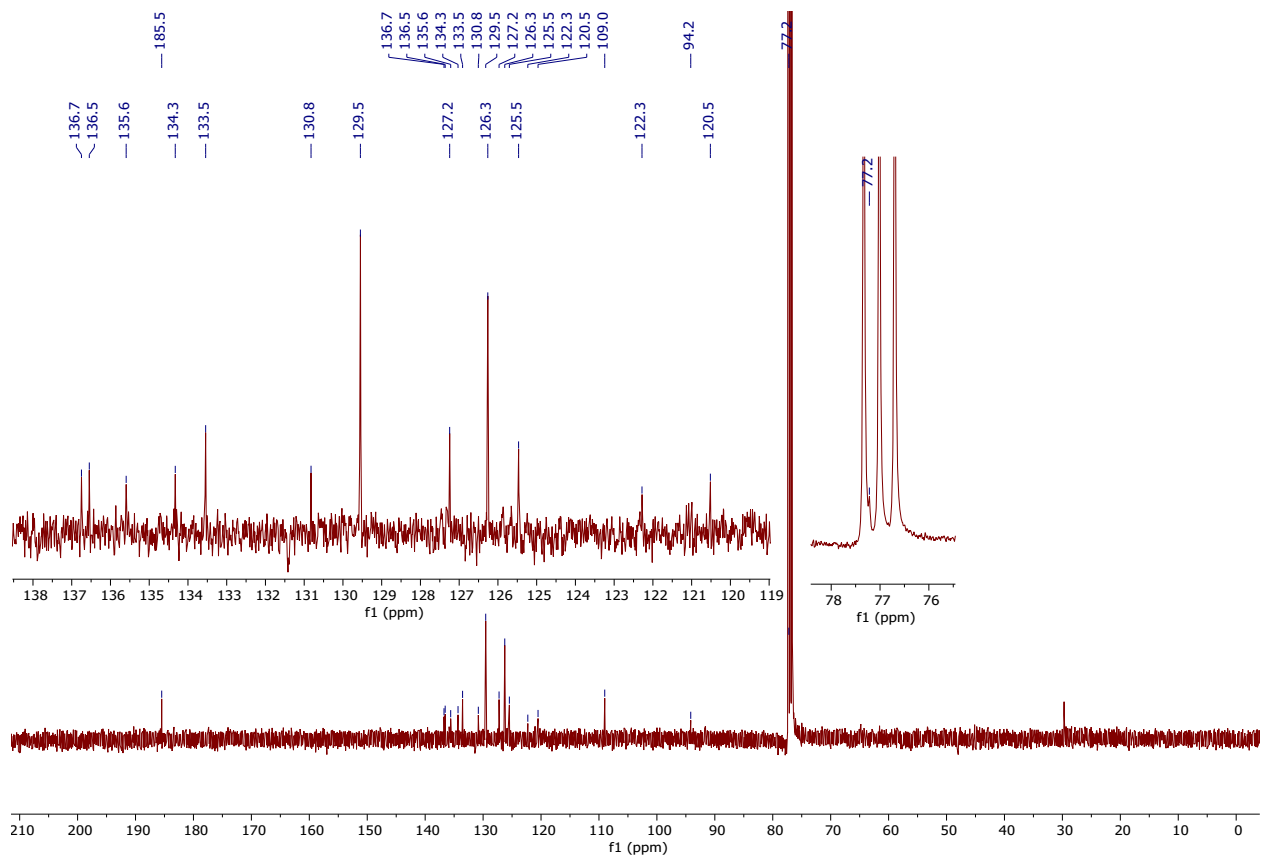
### MS Zoomed Spectrum

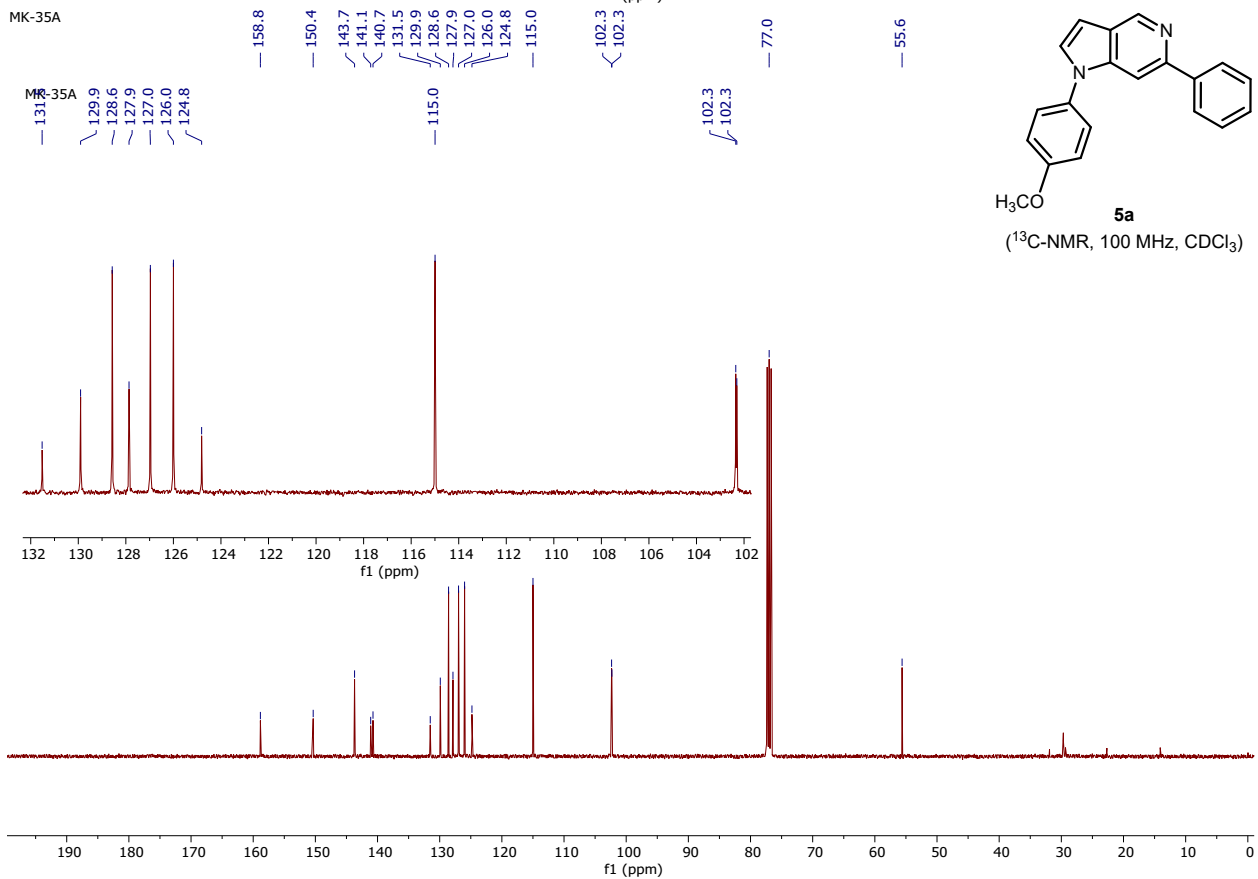
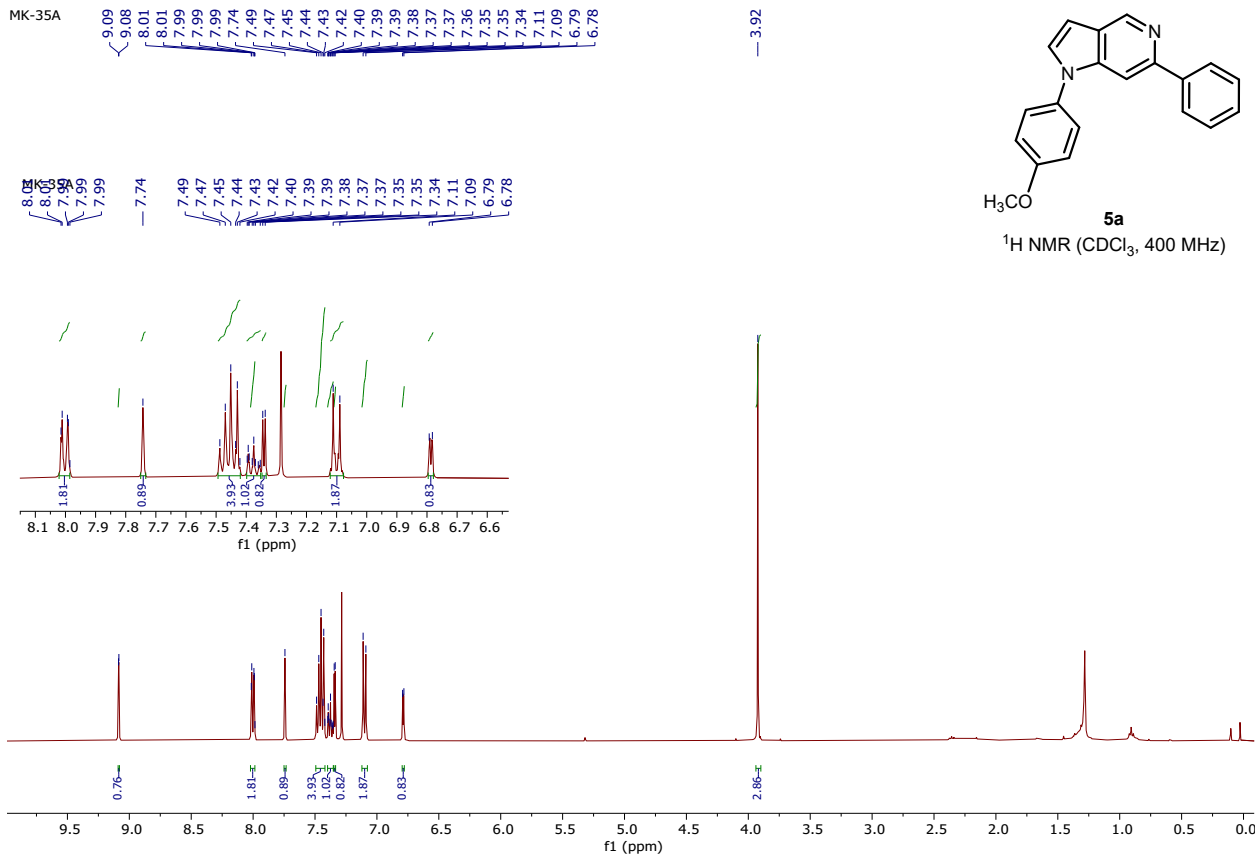


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
346.1438	346.1438	-0.16	1	54563.42	C22H19NO3	(M+H)+
347.1471	347.1471	-0.25	1	13207.87	C22H19NO3	(M+H)+
368.1256	368.1257	0.3	1	5653.64	C22H19NO3	(M+Na)+
369.1286	369.129	1.14	1	1387.26	C22H19NO3	(M+Na)+
370.1404	370.1319	-23.03	1	352.6	C22H19NO3	(M+Na)+







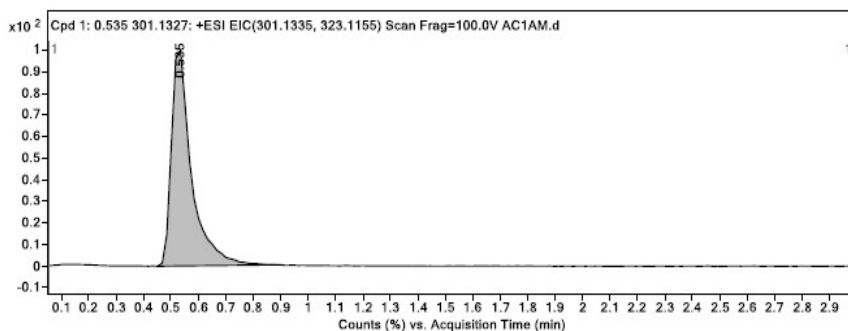
Data File	AC1AM.d	Sample Name	AC1AM
Sample Type	Sample	Position	P2-A8
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.bintu.m	Acquired Time	6/21/2019 5:42:15 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

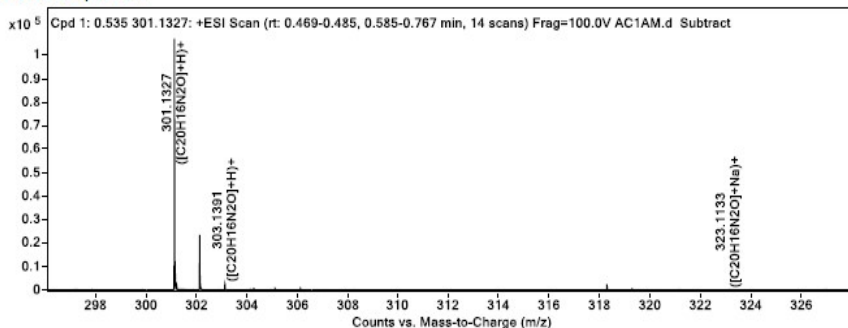
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.535 301.1327	0.535	300.1254	109002	C20 H16 N2 O	300.1263	-2.8

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.535 301.1327	301.1327	0.535	Find By Formula	300.1254

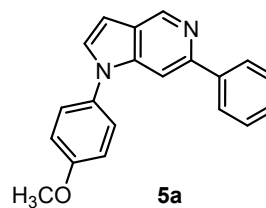


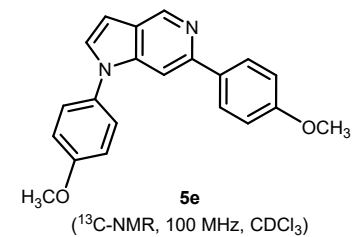
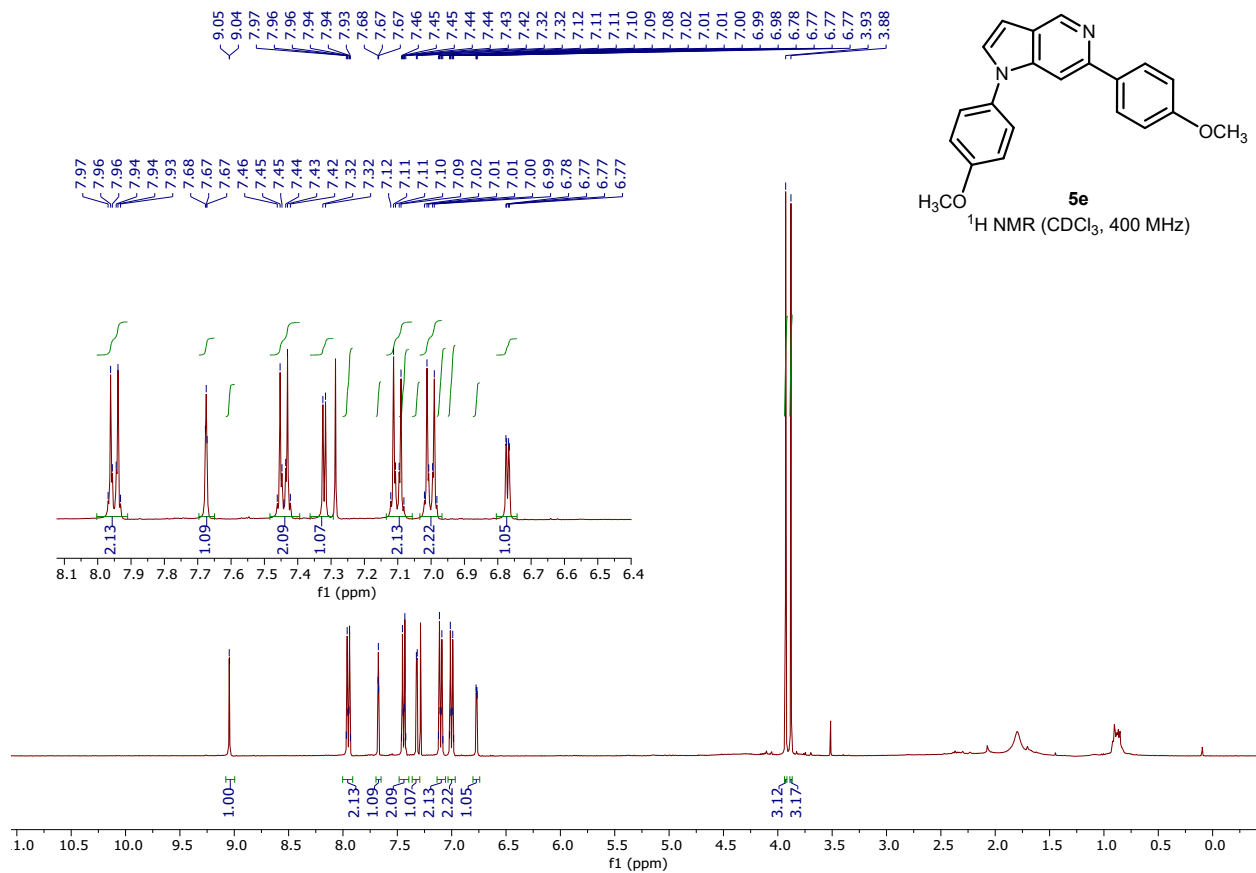
### MS Zoomed Spectrum

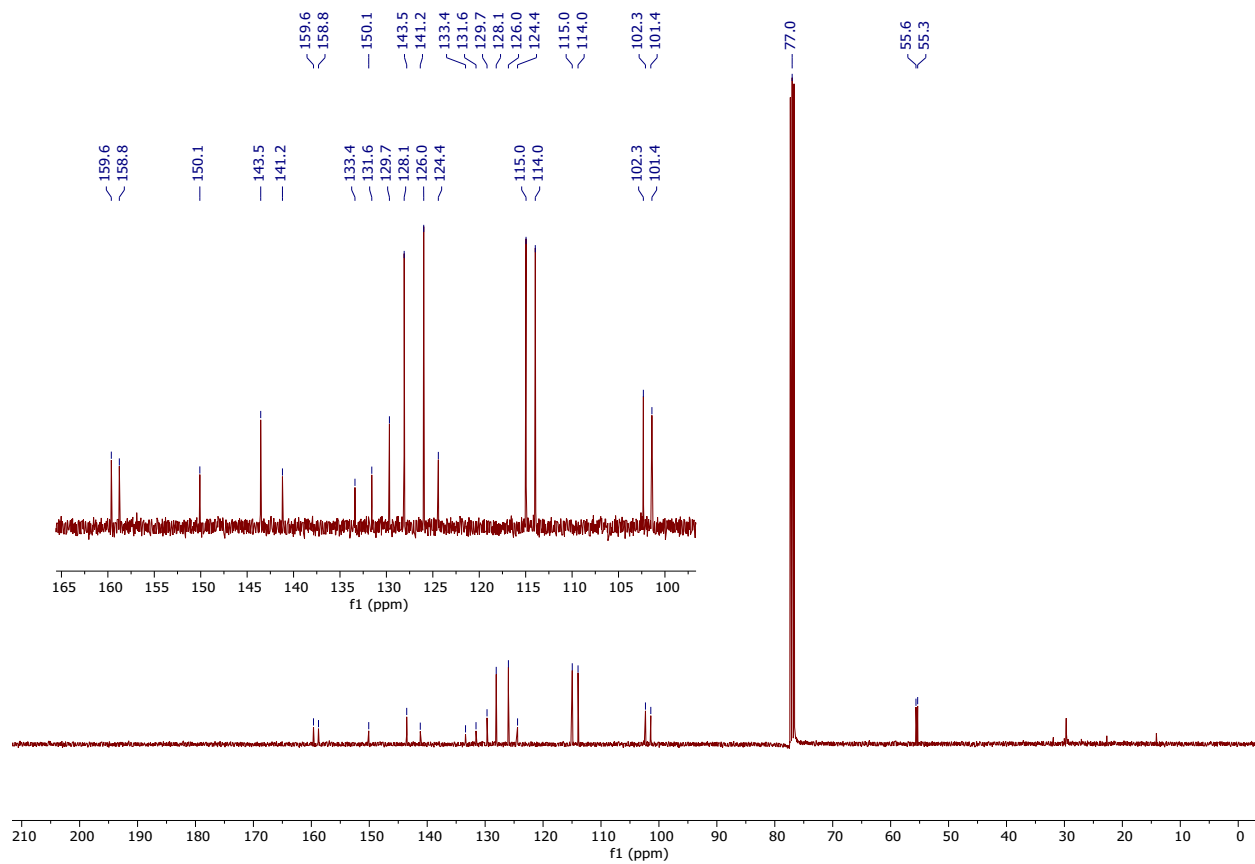


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
301.1327	301.1335	2.79	1	109001.56	C20H16N2O	(M+H)+
302.1359	302.1367	2.84	1	24236.32	C20H16N2O	(M+H)+
303.1391	303.1397	2.2	1	2619.28	C20H16N2O	(M+H)+
304.1418	304.1426	2.62	1	248.62	C20H16N2O	(M+H)+
323.1133	323.1155	6.78	1	110.54	C20H16N2O	(M+Na)+







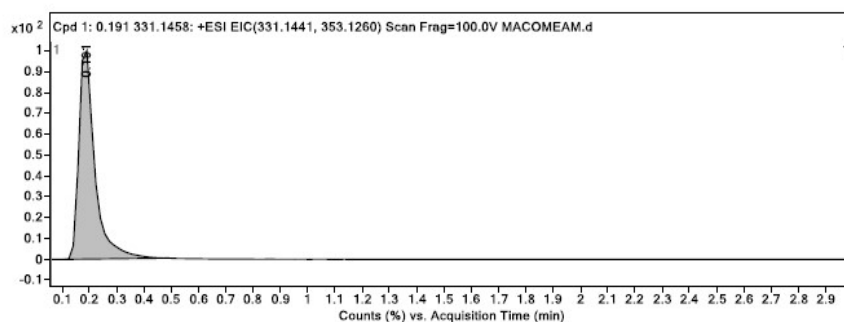
Data File	MACOMEAM.d	Sample Name	MACOMEAM
Sample Type	Sample	Position	P1-E8
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	6/24/2019 1:09:50 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

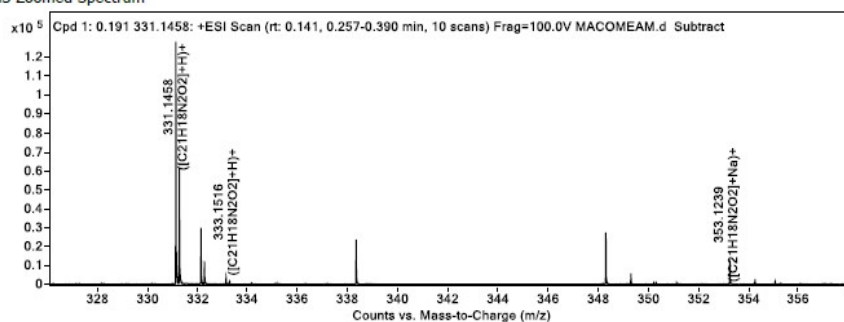
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.191 331.1458	0.191	330.1386	128784	C21 H18 N2 O2	330.1368	5.31

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.191 331.1458	331.1458	0.191	Find By Formula	330.1386

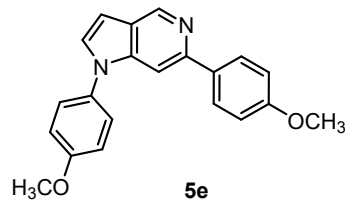


#### MS Zoomed Spectrum

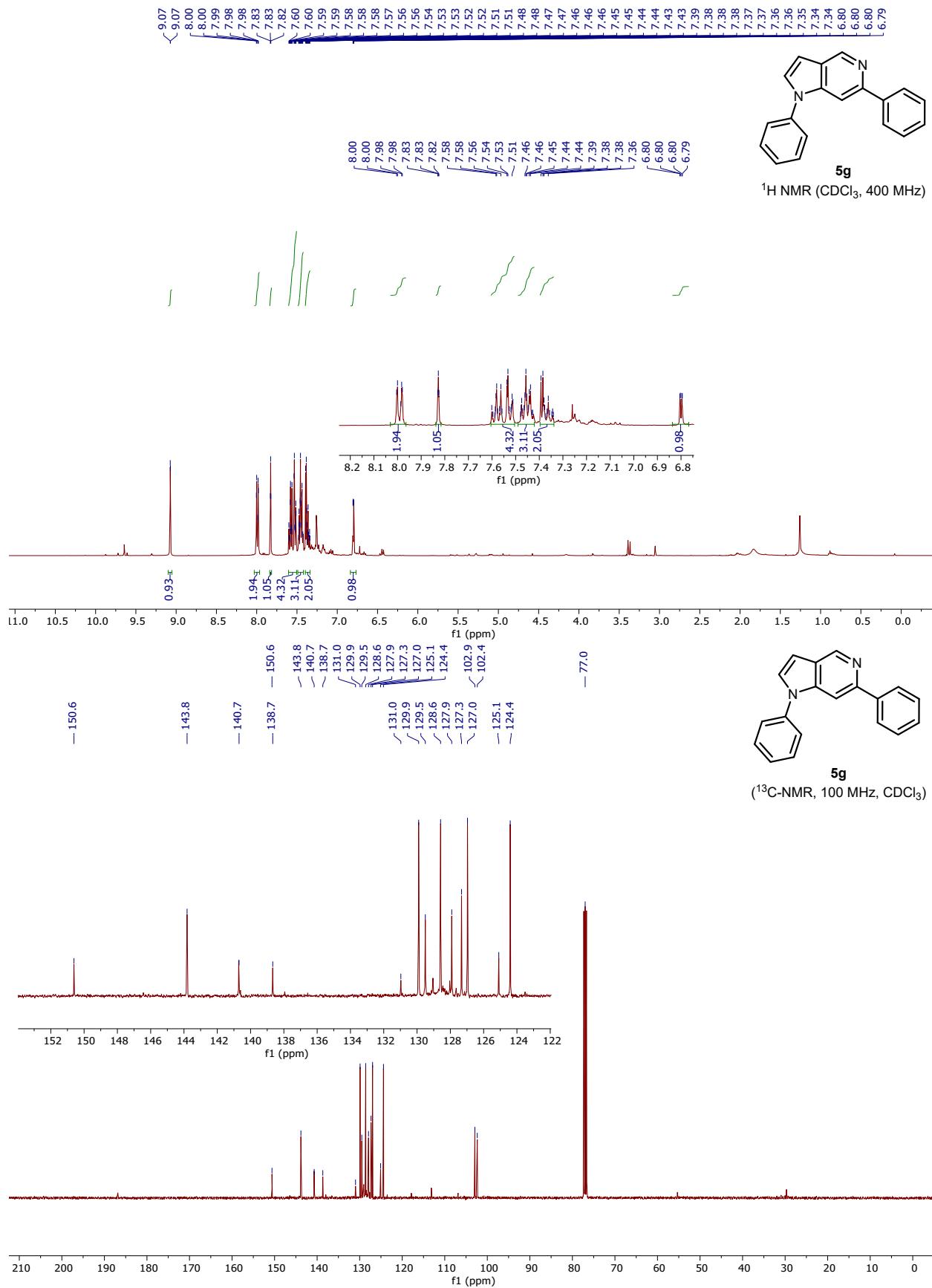


#### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
331.1458	331.1441	-5.24	1	128783.57	C21H18N2O2	(M+H)+
332.1492	332.1473	-5.67	1	29913.06	C21H18N2O2	(M+H)+
333.1516	333.1502	-4.35	1	3601.38	C21H18N2O2	(M+H)+
334.155	334.1529	-6.15	1	388.43	C21H18N2O2	(M+H)+
353.1239	353.126	6.2	1	159.86	C21H18N2O2	(M+Na)+







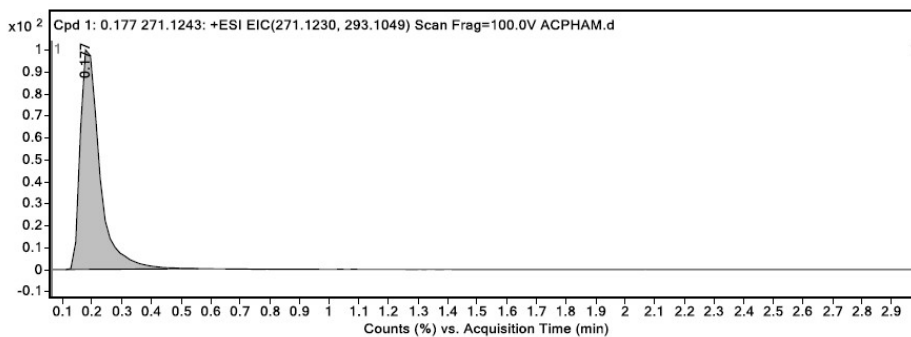
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<b>Sample Type</b>	Sample	<b>Position</b>	P1-E4
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 12:44:47 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW</b>	6200 series TOF/6500 series
		<b>Version</b>	Q-TOF B.06.01 (B6172 SP1)

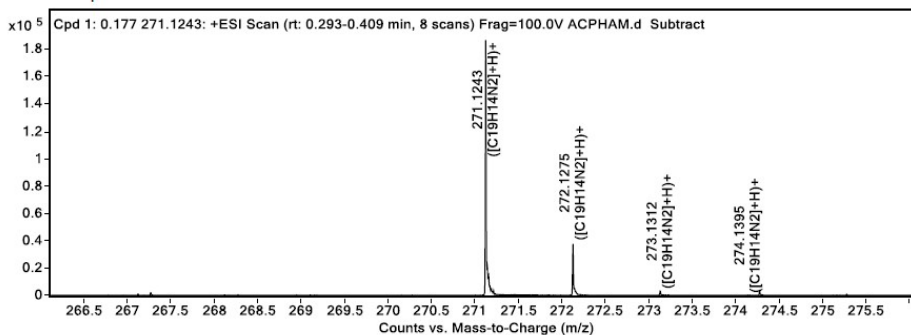
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.177 271.1243	0.177	270.117	189624	C19H14N2	270.1157	4.83

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.177 271.1243	271.1243	0.177	Find By Formula	270.117

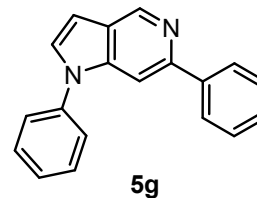


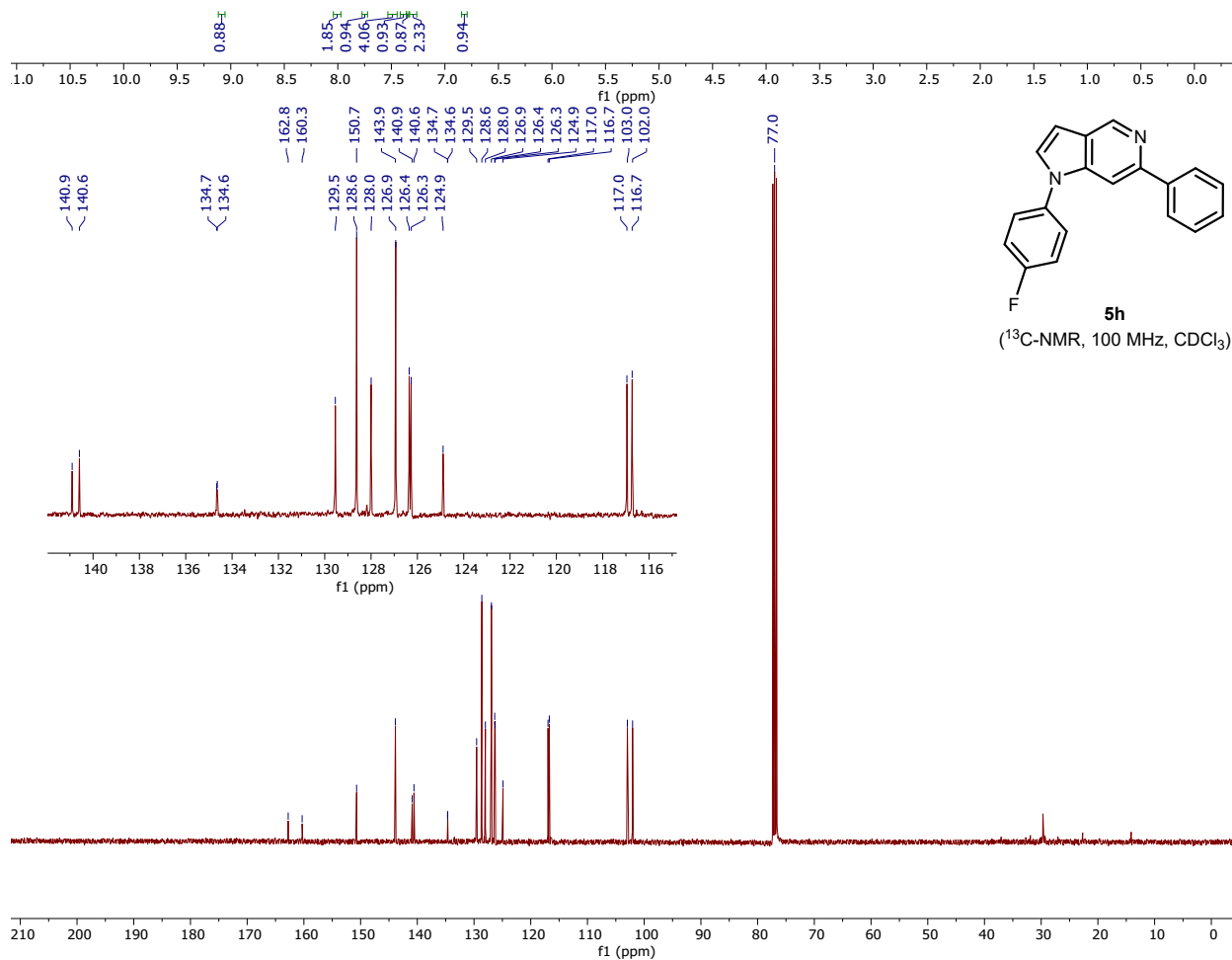
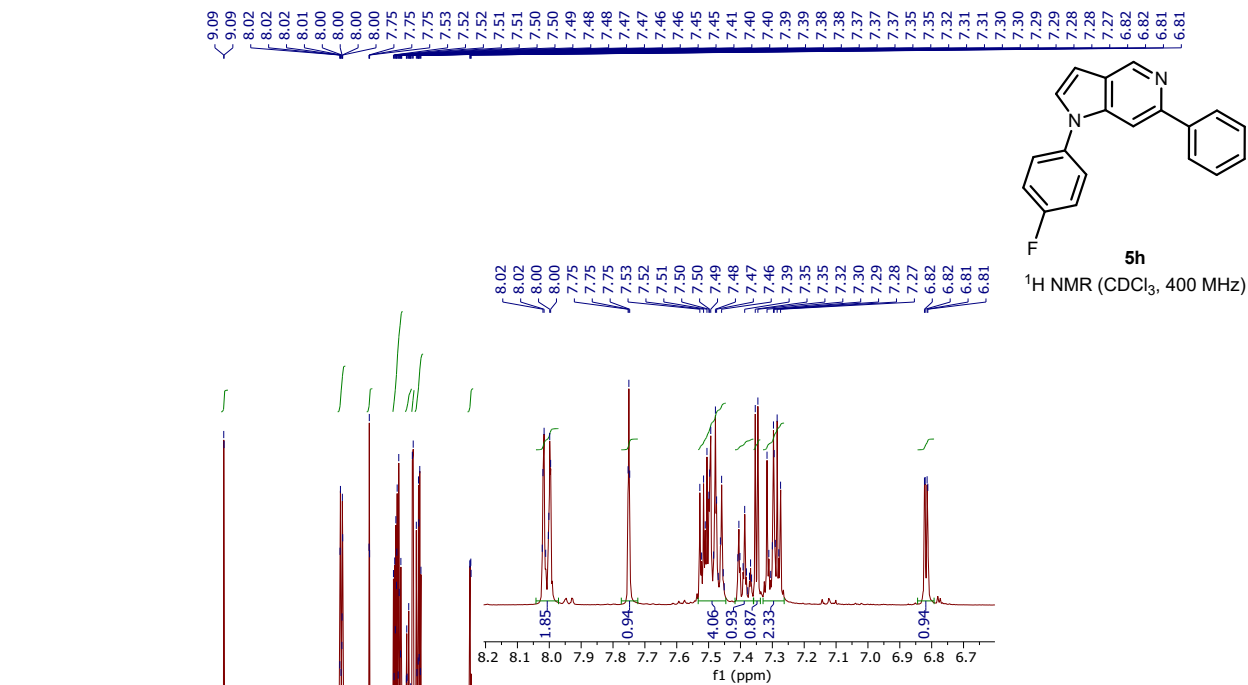
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
271.1243	271.123	-4.72	1	189624.17	C19H14N2	(M+H) <sup>+</sup>
272.1275	272.1261	-4.92	1	38635	C19H14N2	(M+H) <sup>+</sup>
273.1312	273.1293	-7.17	1	3255.94	C19H14N2	(M+H) <sup>+</sup>
274.1395	274.1324	-25.73	1	191.39	C19H14N2	(M+H) <sup>+</sup>





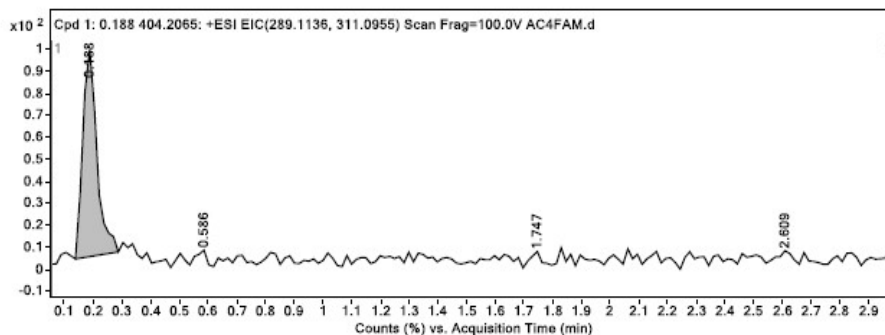
Data File	AC4FAM.d	Sample Name	AC4FAM
Sample Type	Sample	Position	P1-E2
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.m	Acquired Time	6/24/2019 12:28:03 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

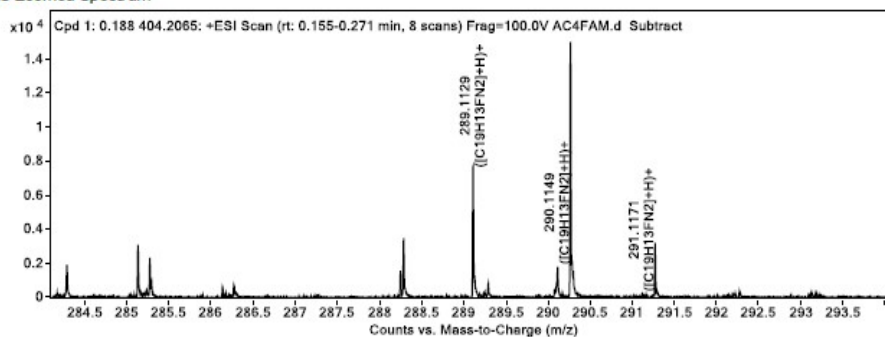
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.188 404.2065	0.188	288.1054	7995	C19 H13 F N2	288.1063	-2.99

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.188 404.2065	289.1129	0.188	Find By Formula	288.1054

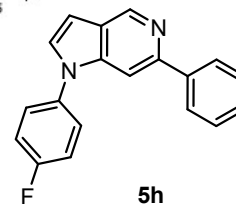


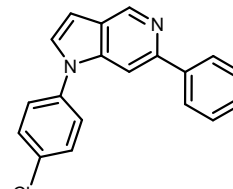
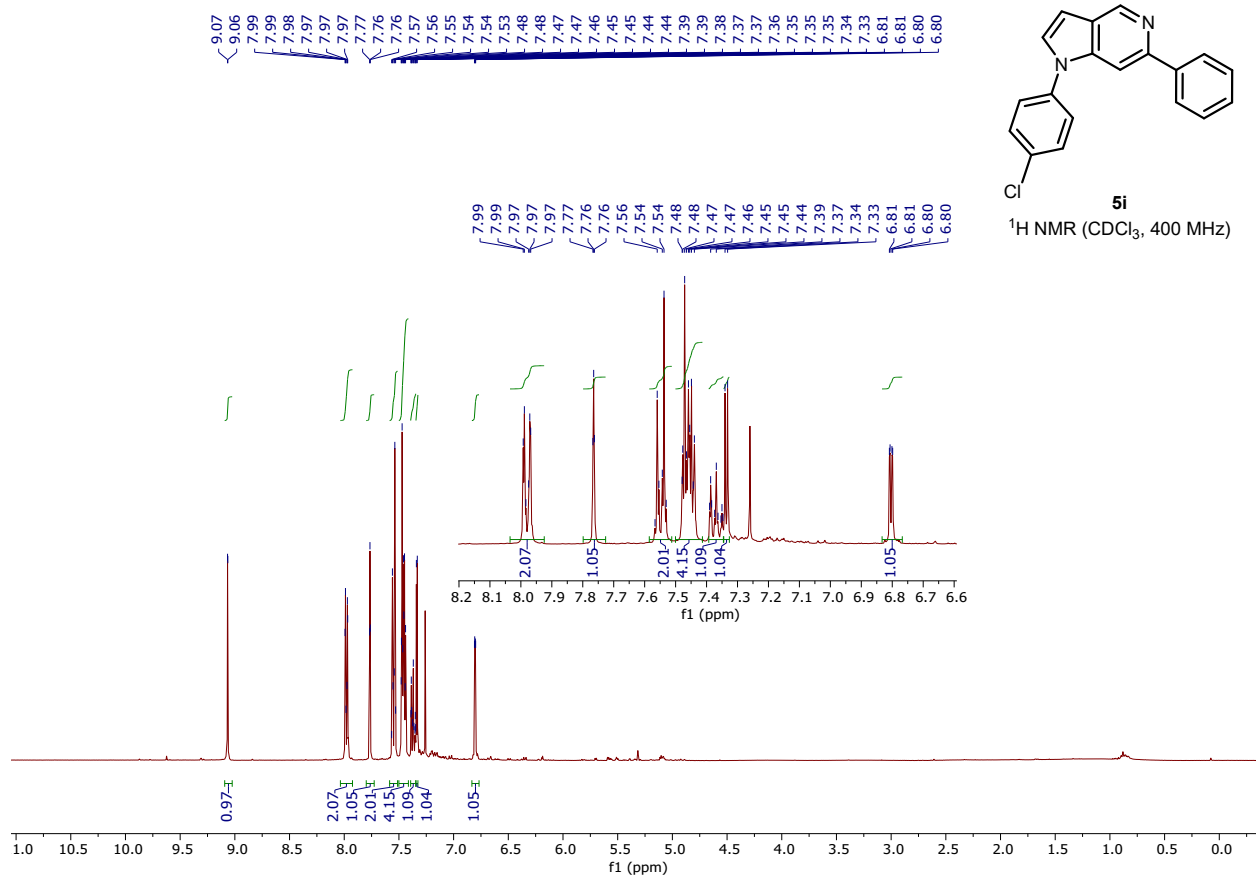
#### MS Zoomed Spectrum



#### MS Spectrum Peak List

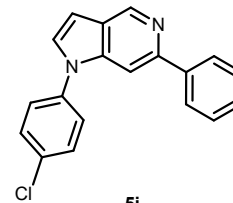
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
289.1129	289.1136	2.09	1	7995.41	C19H13FN2	(M+H)+
290.1149	290.1167	6.09	1	1805.73	C19H13FN2	(M+H)+
291.1171	291.1199	9.53	1	218.33	C19H13FN2	(M+H)+





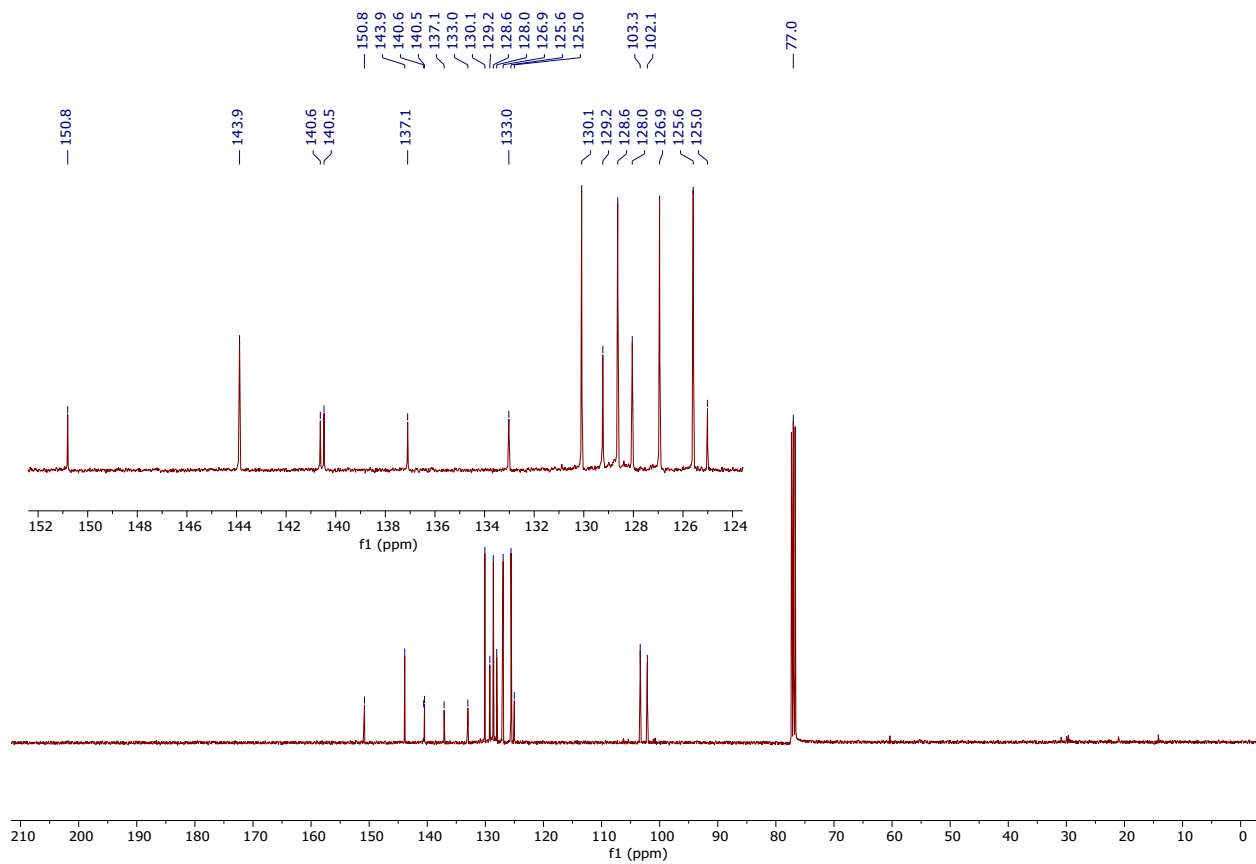
**5i**

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz)



**5i**

(<sup>13</sup>C-NMR, 100 MHz, CDCl<sub>3</sub>)



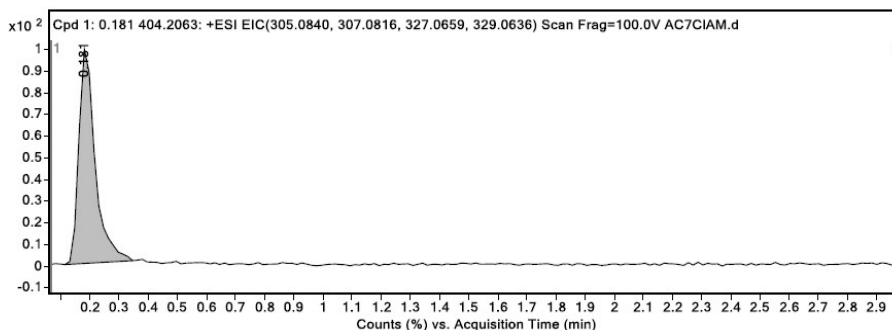
<b>Data File</b>	AC7CIAM.d	<b>Sample Name</b>	AC7CIAM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-E3
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 12:36:25 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

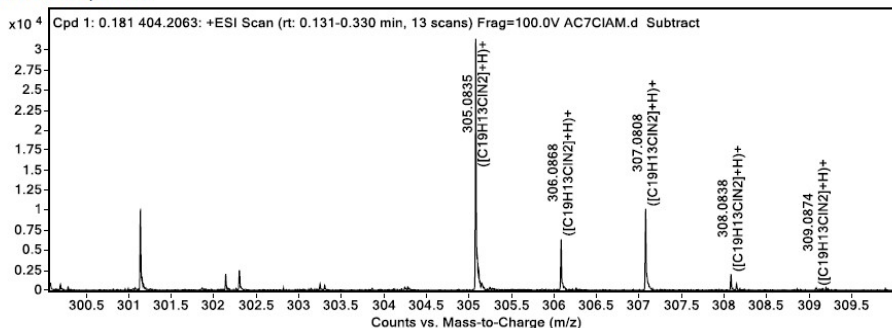
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.181 404.2063	0.181	304.0762	32457	C19 H13 Cl N2	304.0767	-1.83

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.181 404.2063	305.0835	0.181	Find By Formula	304.0762

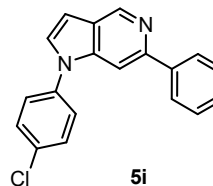


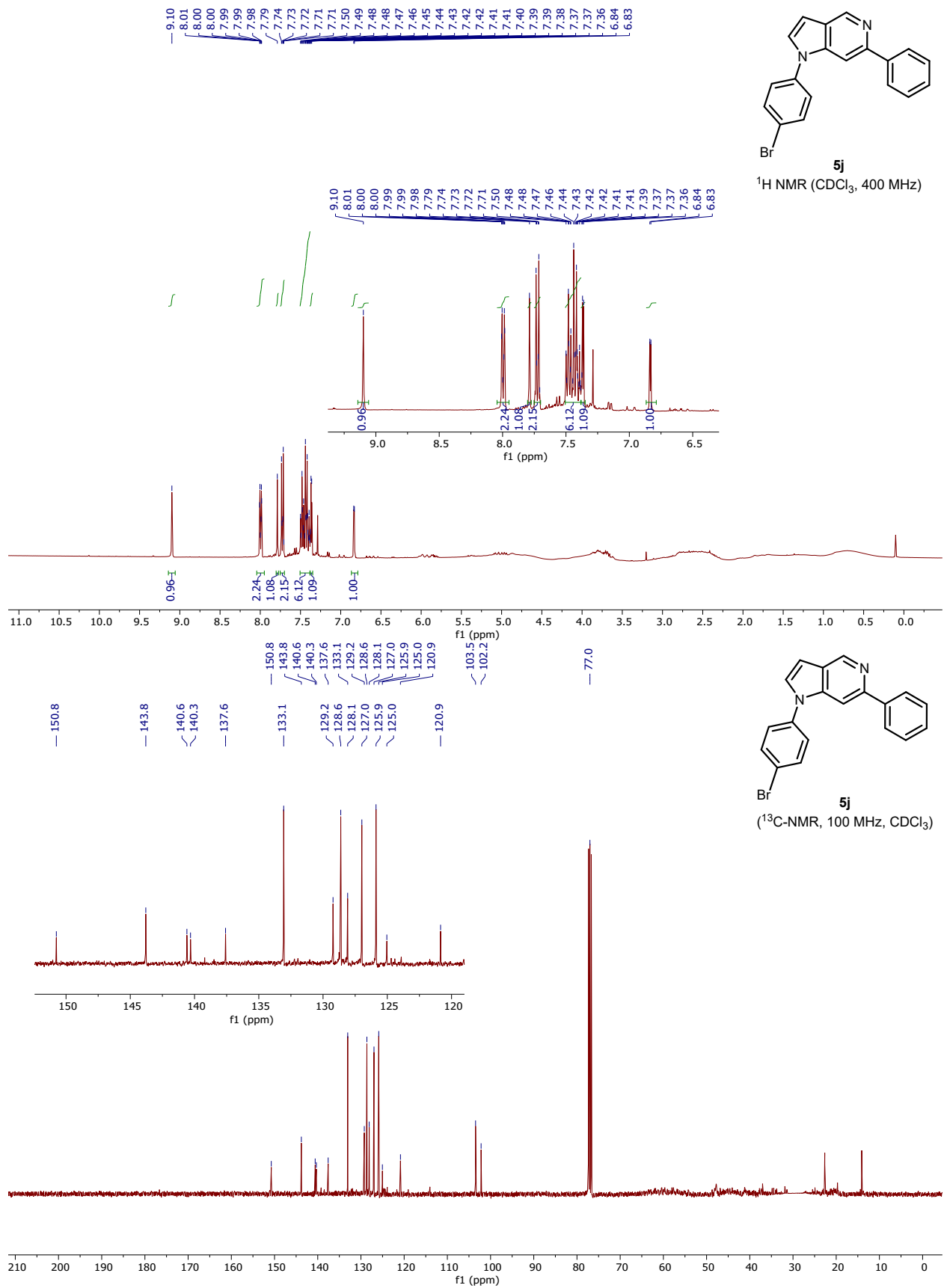
### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
305.0835	305.084	1.7	1	32456.55	C19H13ClN2	(M+H)+
306.0868	306.0872	1.14	1	6498.44	C19H13ClN2	(M+H)+
307.0808	307.0816	2.66	1	10217.14	C19H13ClN2	(M+H)+
308.0838	308.0844	1.97	1	2032.82	C19H13ClN2	(M+H)+
309.0874	309.0874	0.2	1	298.57	C19H13ClN2	(M+H)+









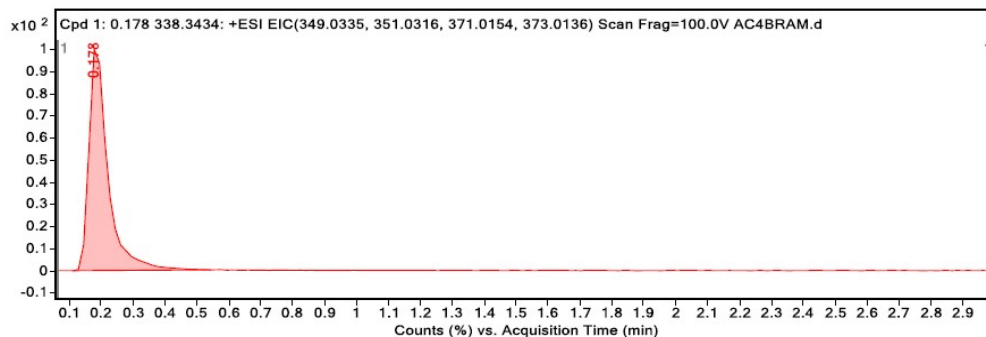
<b>Data File</b>	AC4BRAM.d	<b>Sample Name</b>	AC4BRAM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-E10
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 1:34:50 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

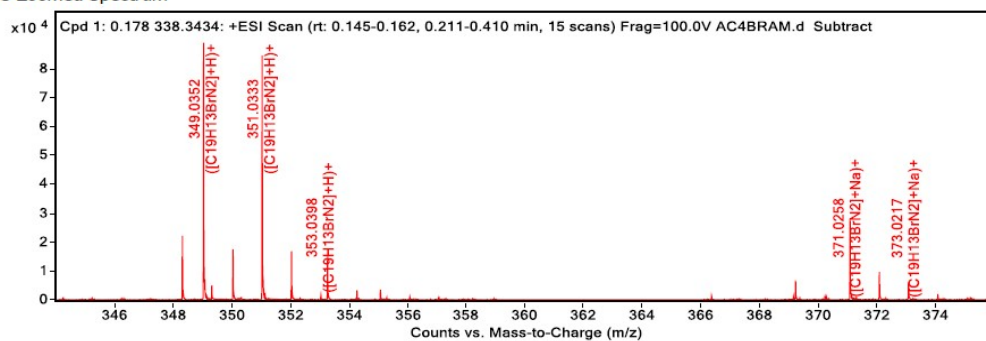
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.178 338.3434	0.178	348.028	89197	C19 H13 Br N2	348.0262	5.06

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.178 338.3434	349.0352	0.178	Find By Formula	348.028

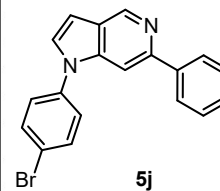


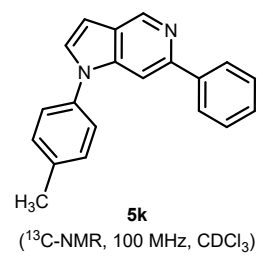
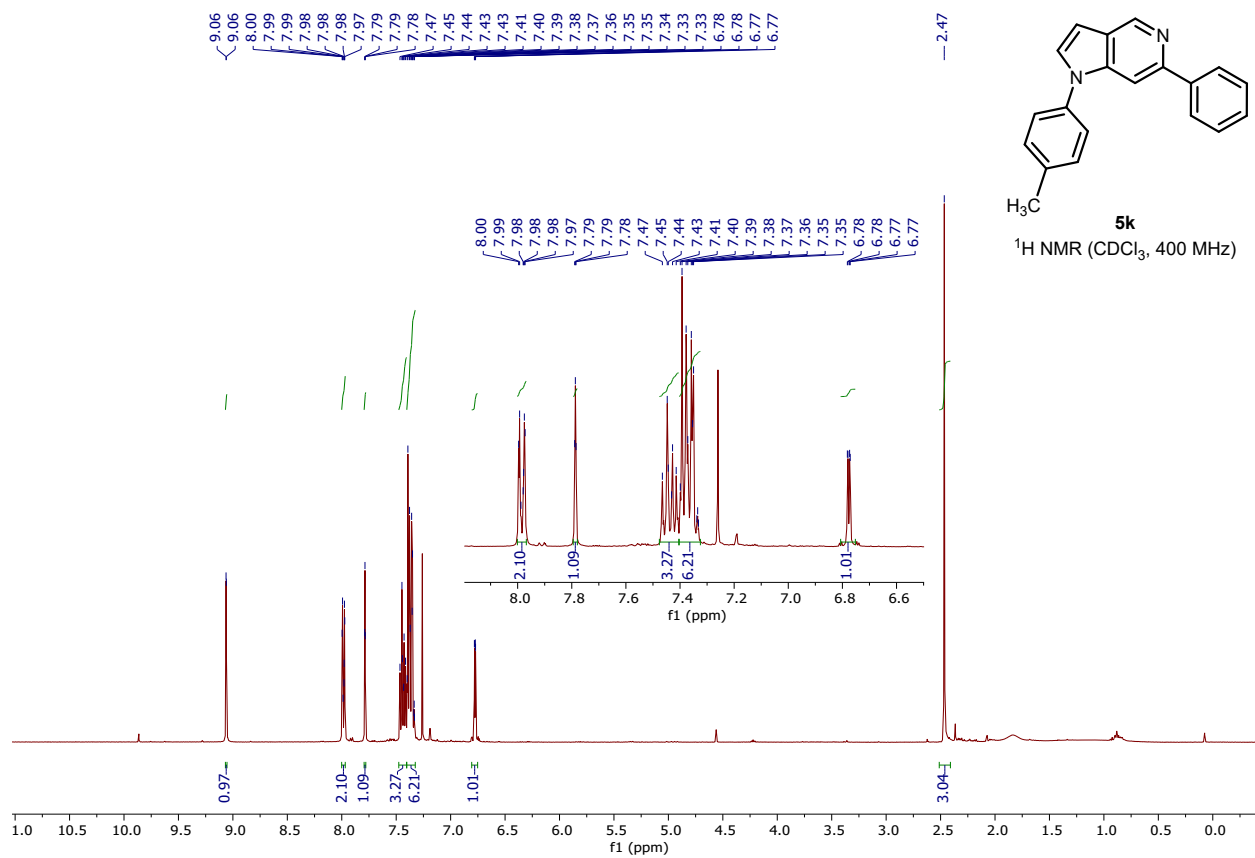
### MS Zoomed Spectrum

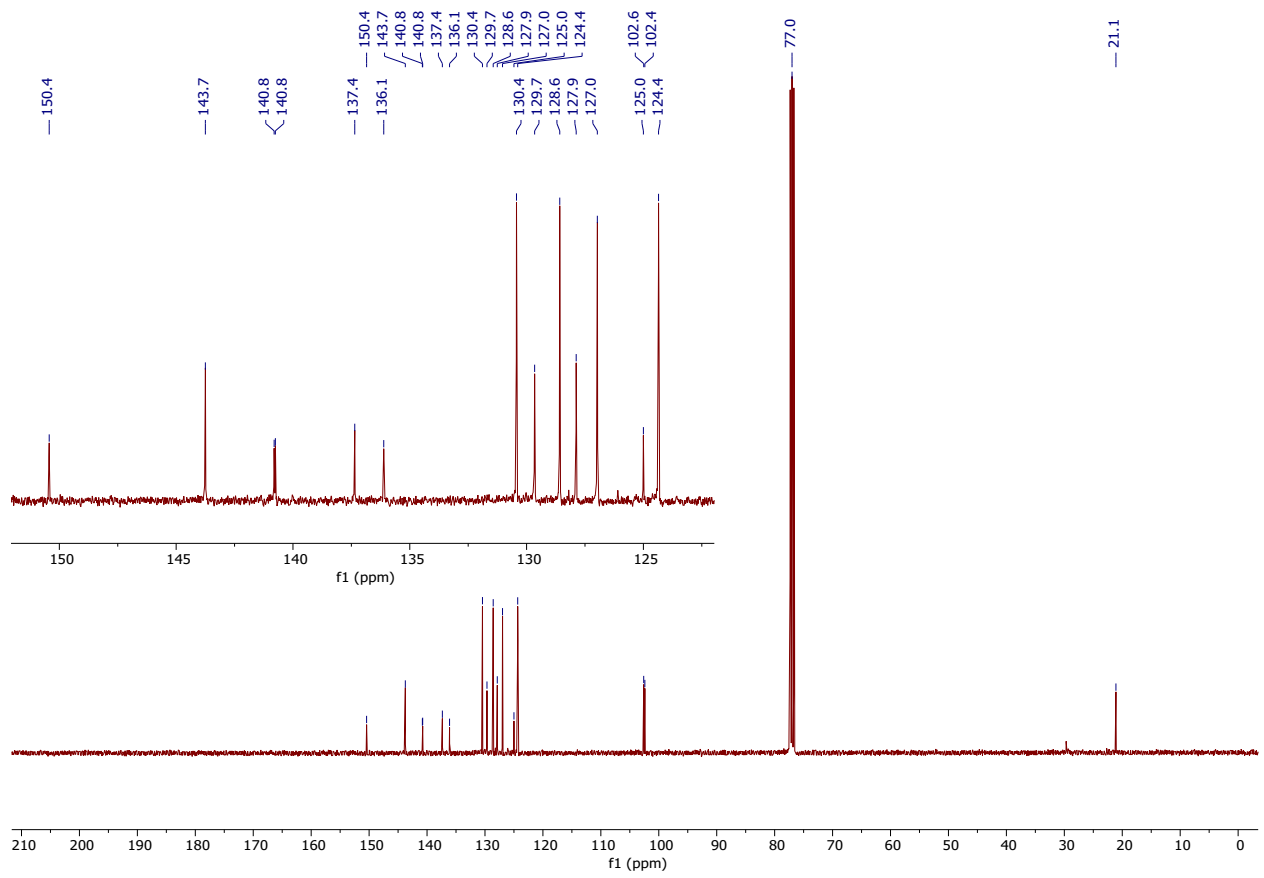


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
349.0352	349.0335	-5.04	1	89196.89	C19H13BrN2	(M+H)+
350.0384	350.0366	-4.95	1	17865.1	C19H13BrN2	(M+H)+
351.0333	351.0316	-4.91	1	84592.49	C19H13BrN2	(M+H)+
352.0365	352.0347	-5.12	1	17224	C19H13BrN2	(M+H)+
353.0398	353.0378	-5.6	1	1702.3	C19H13BrN2	(M+H)+
354.0433	354.0409	-6.87	1	118.15	C19H13BrN2	(M+H)+
371.0258	371.0154	-27.85	1	201.65	C19H13BrN2	(M+Na)+
372.0301	372.0186	-30.92	1	64.59	C19H13BrN2	(M+Na)+
373.0217	373.0136	-21.92	1	73.54	C19H13BrN2	(M+Na)+







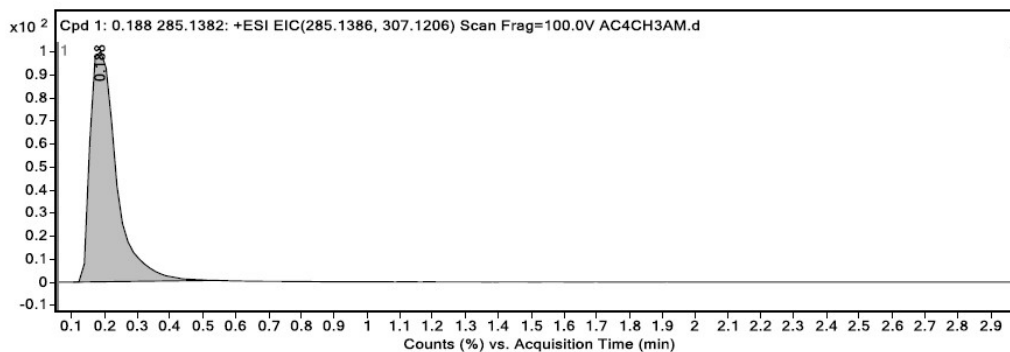
<b>Data File</b>	AC4CH3AM.d	<b>Sample Name</b>	AC4CH3AM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-E1
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 12:19:43 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW</b>	6200 series TOF/6500 series
		<b>Version</b>	Q-TOF B.06.01 (B6172 SP1)

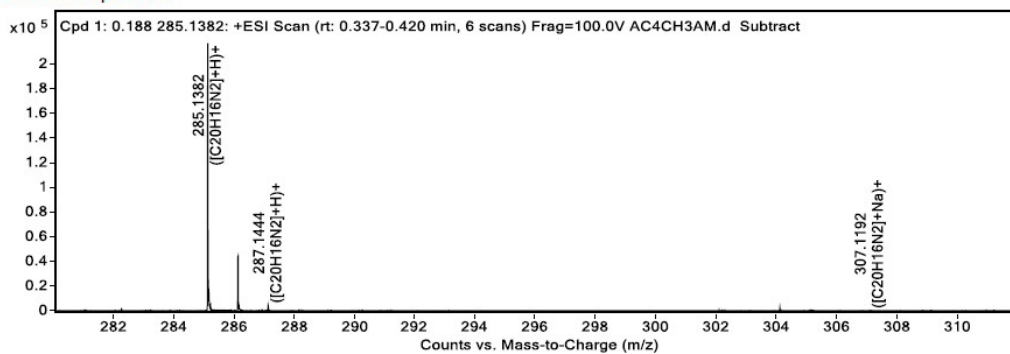
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.188 285.1382	0.188	284.1309	216885	C20 H16 N2	284.1313	-1.42

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.188 285.1382	285.1382	0.188	Find By Formula	284.1309

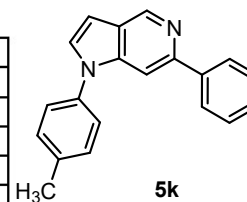


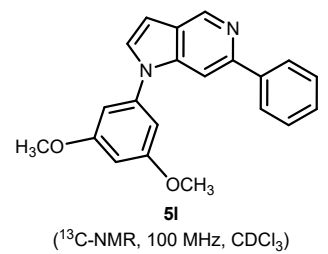
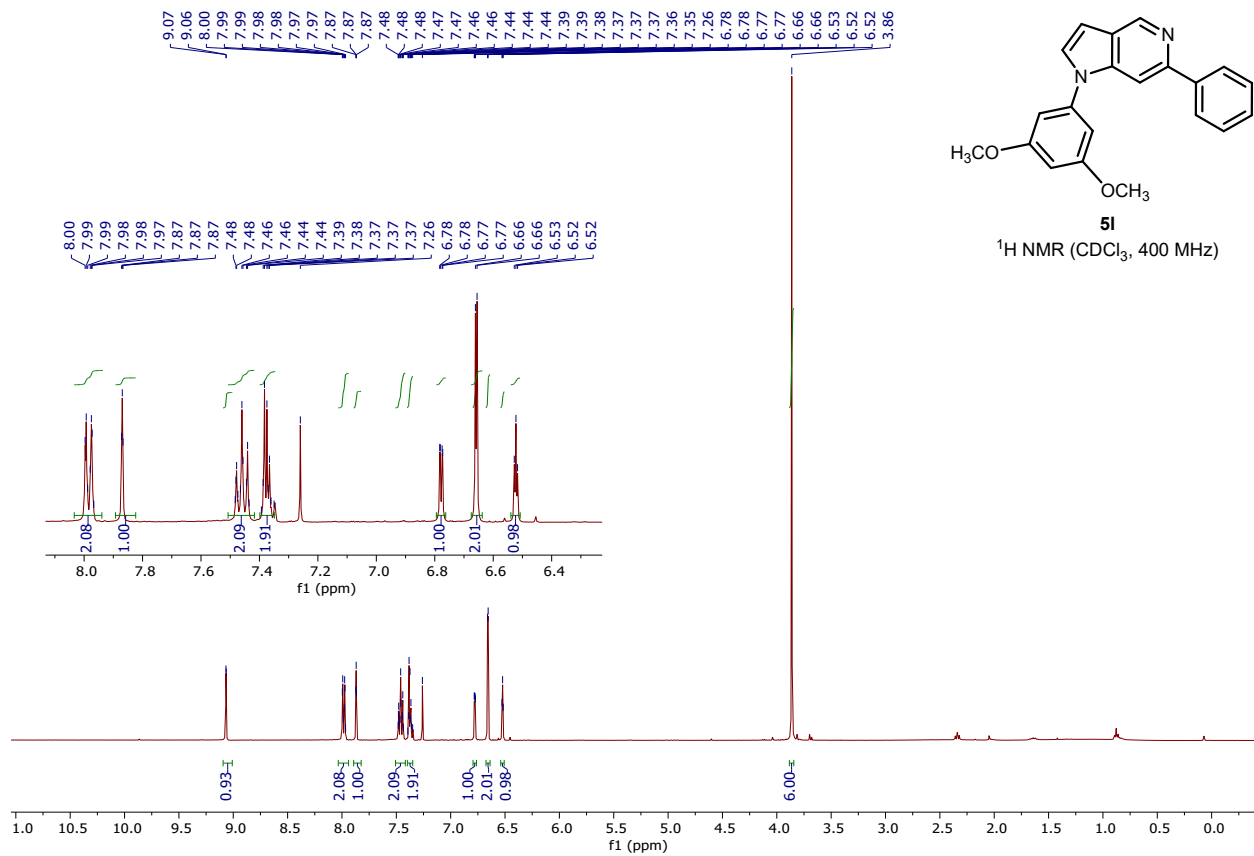
### MS Zoomed Spectrum

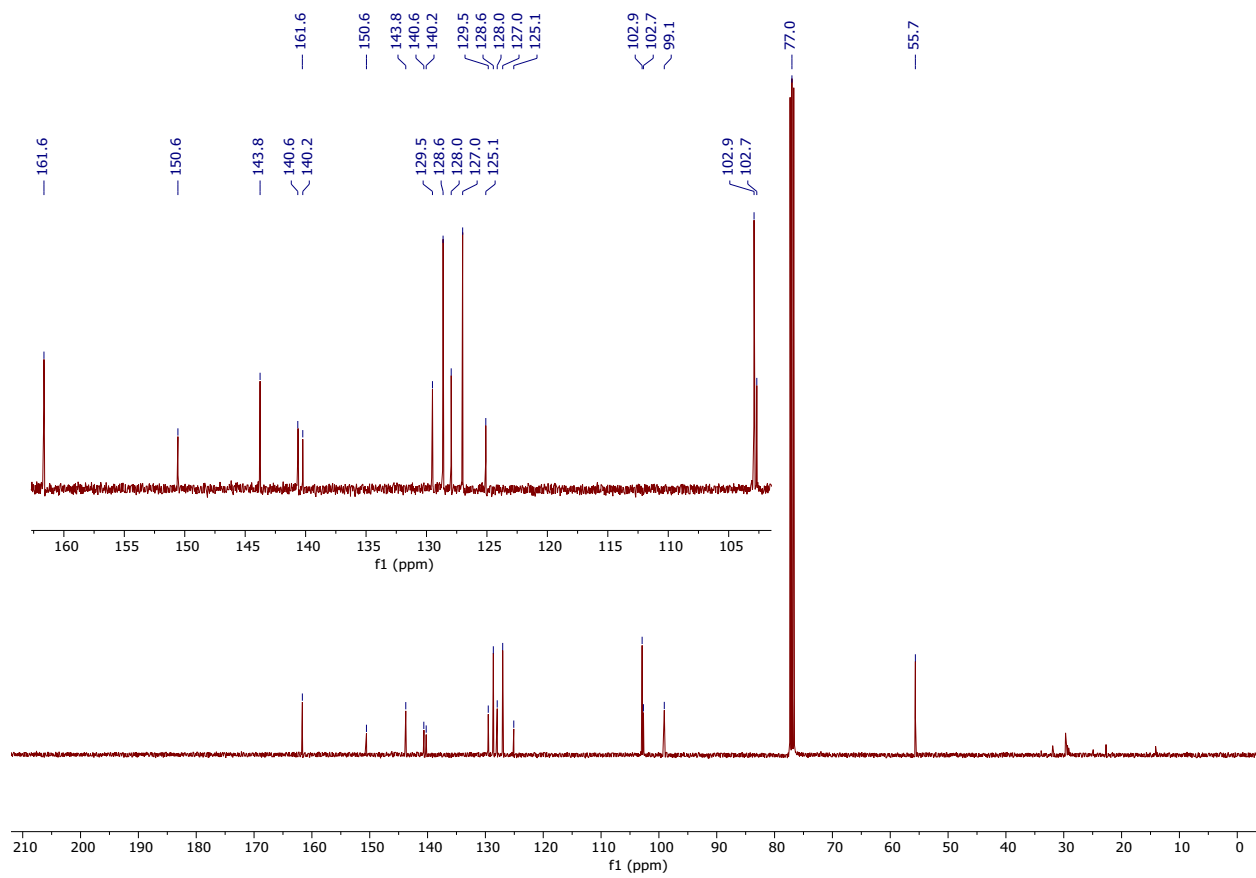


### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
285.1382	285.1386	1.51	1	216885.44	C20H16N2	(M+H)+
286.1415	286.1418	0.94	1	45441.02	C20H16N2	(M+H)+
287.1444	287.145	1.97	1	4364.42	C20H16N2	(M+H)+
288.1508	288.1481	-9.36	1	301.94	C20H16N2	(M+H)+
307.1192	307.1206	4.48	1	177.97	C20H16N2	(M+Na)+







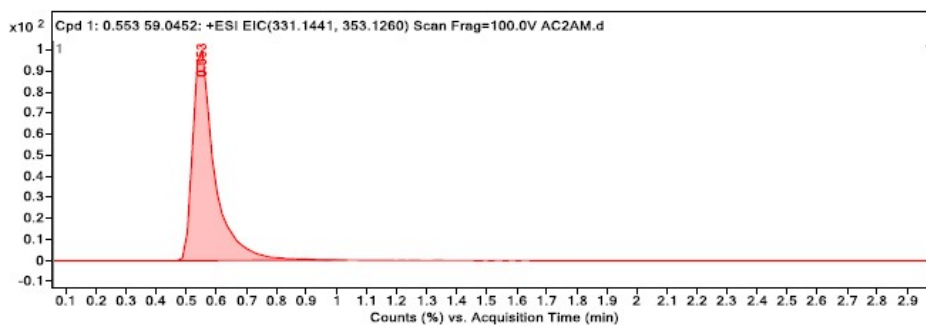
Data File	AC2AM.d	Sample Name	AC2AM
Sample Type	Sample	Position	P2-A7
Instrument Name	Instrument 1	User Name	
Acq Method	ChB60ChD40_isocratic_esi_positive_3min.bintu.m	Acquired Time	6/21/2019 5:33:54 PM
IRM Calibration Status	Success	DA Method	PROCESSNEW.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

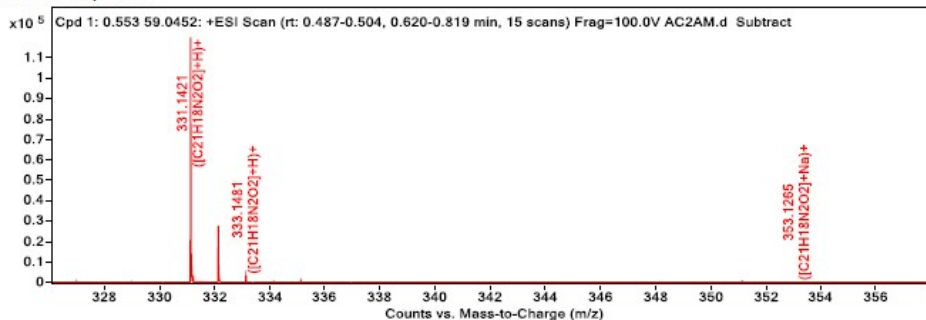
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.553 59.0452	0.553	330.1348	120877	C21 H18 N2 O2	330.1368	-6.13

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.553 59.0452	331.1421	0.553	Find By Formula	330.1348

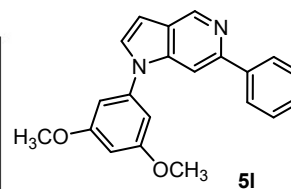


### MS Zoomed Spectrum

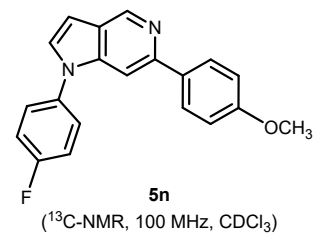
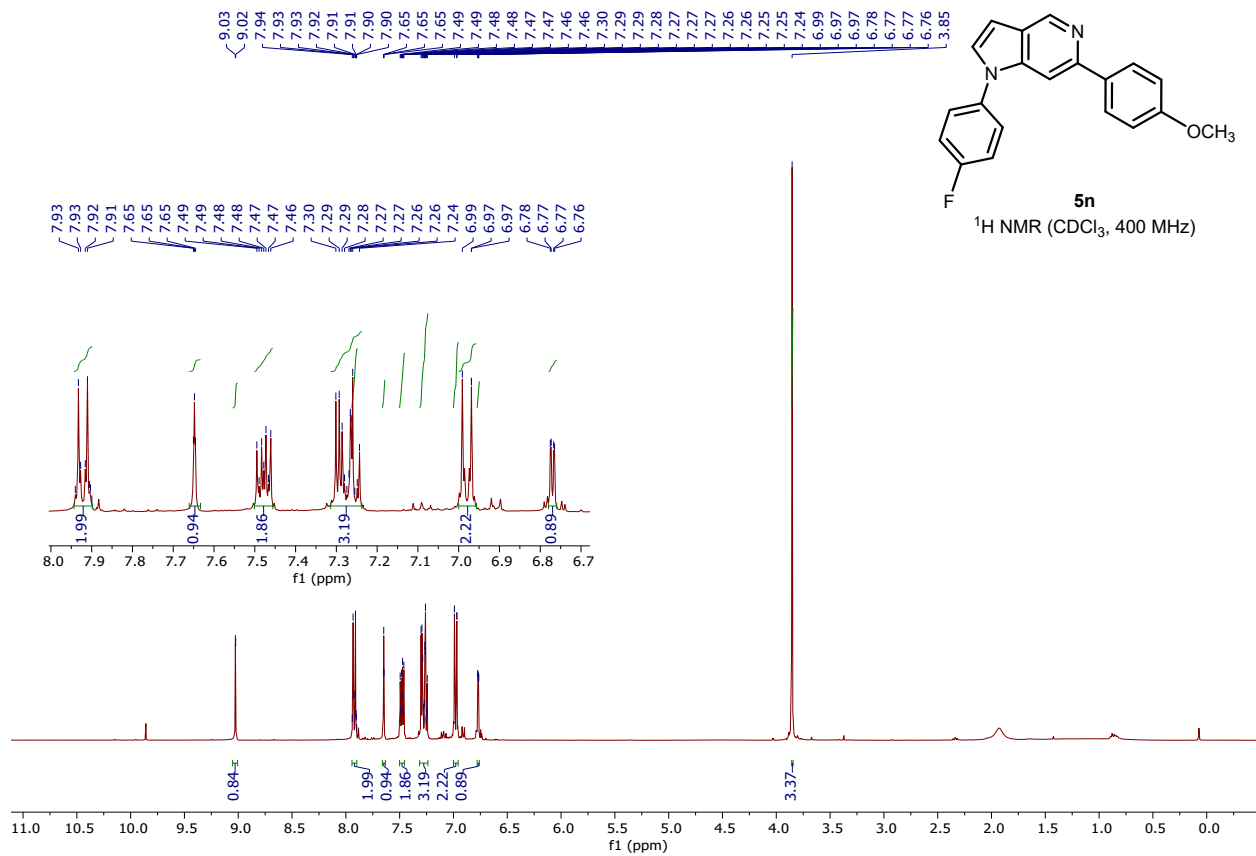


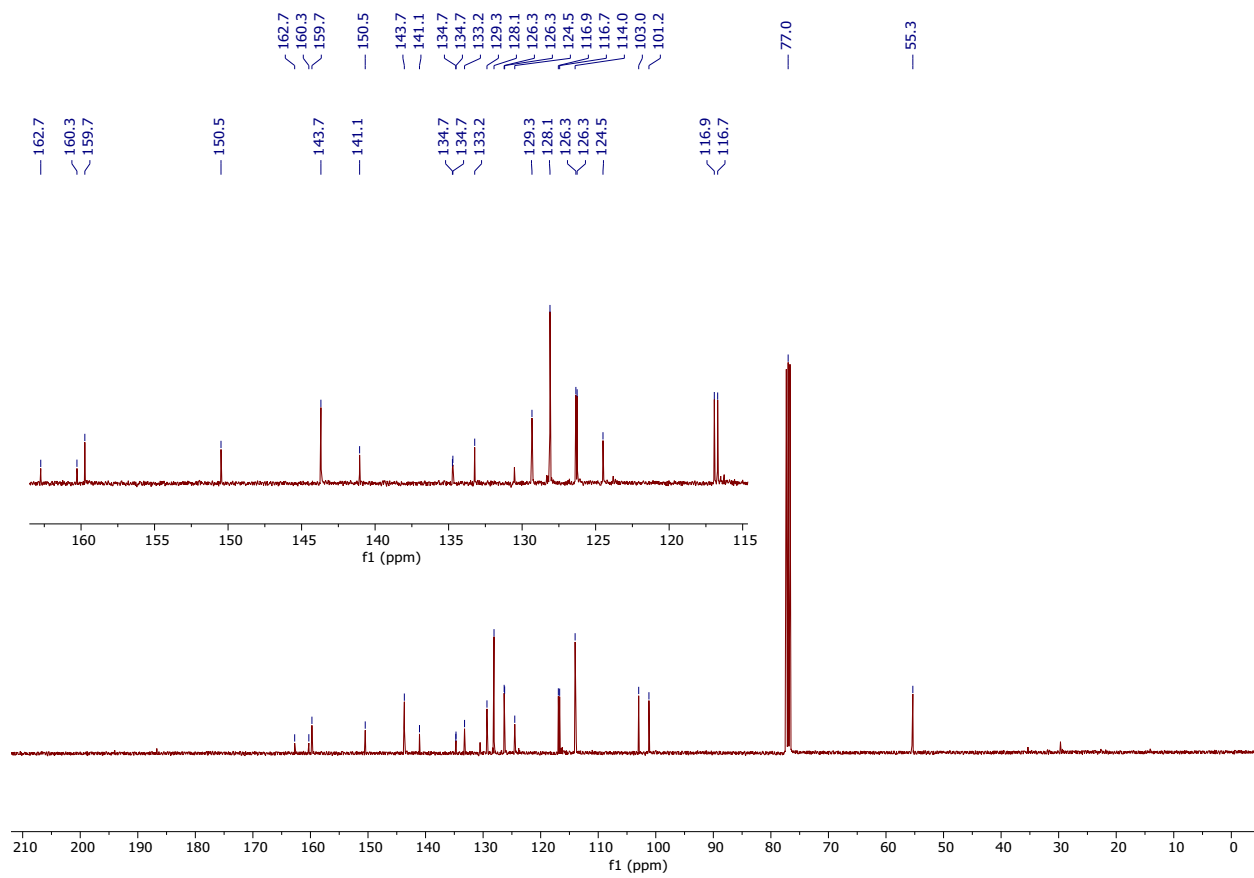
### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
331.1421	331.1441	6.17	1	120876.95	C21H18N2O2	(M+H)+
332.1454	332.1473	5.82	1	27796.15	C21H18N2O2	(M+H)+
333.1481	333.1502	6.16	1	3211.98	C21H18N2O2	(M+H)+
334.1505	334.1529	7.16	1	403.58	C21H18N2O2	(M+H)+
353.1265	353.126	-1.17	1	79.85	C21H18N2O2	(M+Na)+









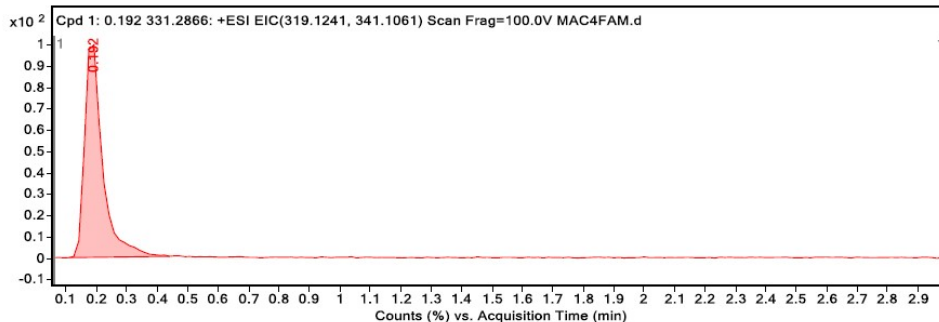
<b>Data File</b>	MAC4FAM.d	<b>Sample Name</b>	MAC4FAM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-E9
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 1:18:10 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW Version</b>	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

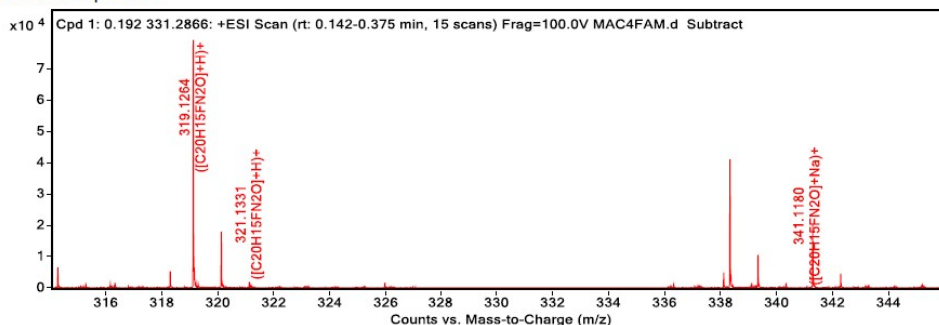
#### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.192 331.2866	0.192	318.1191	79417	C20 H15 F N2 O	318.1168	7.1

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.192 331.2866	319.1264	0.192	Find By Formula	318.1191

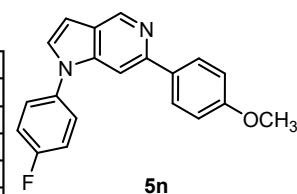


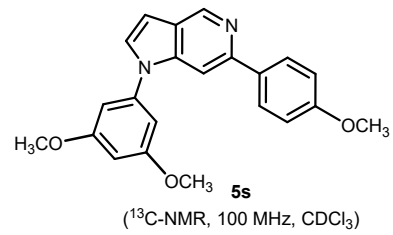
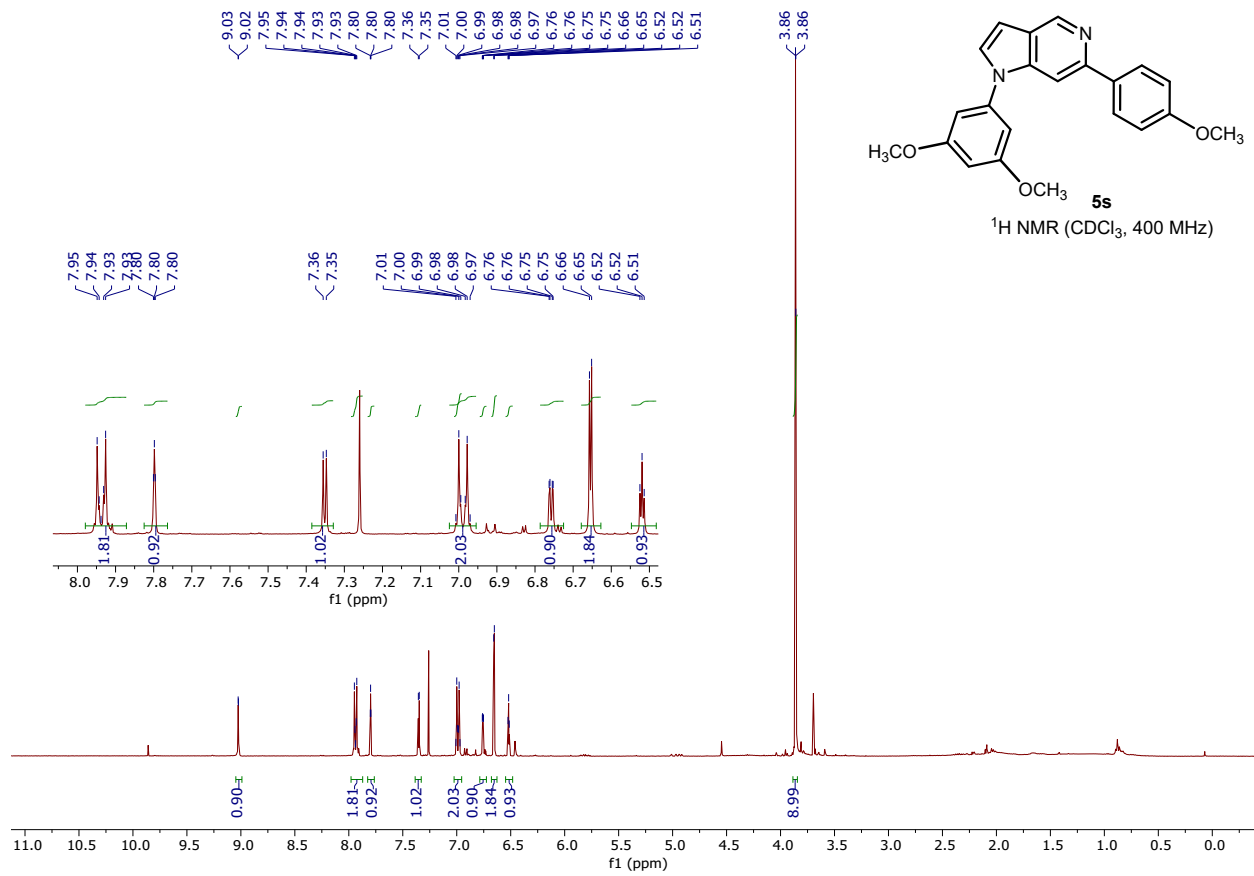
#### MS Zoomed Spectrum

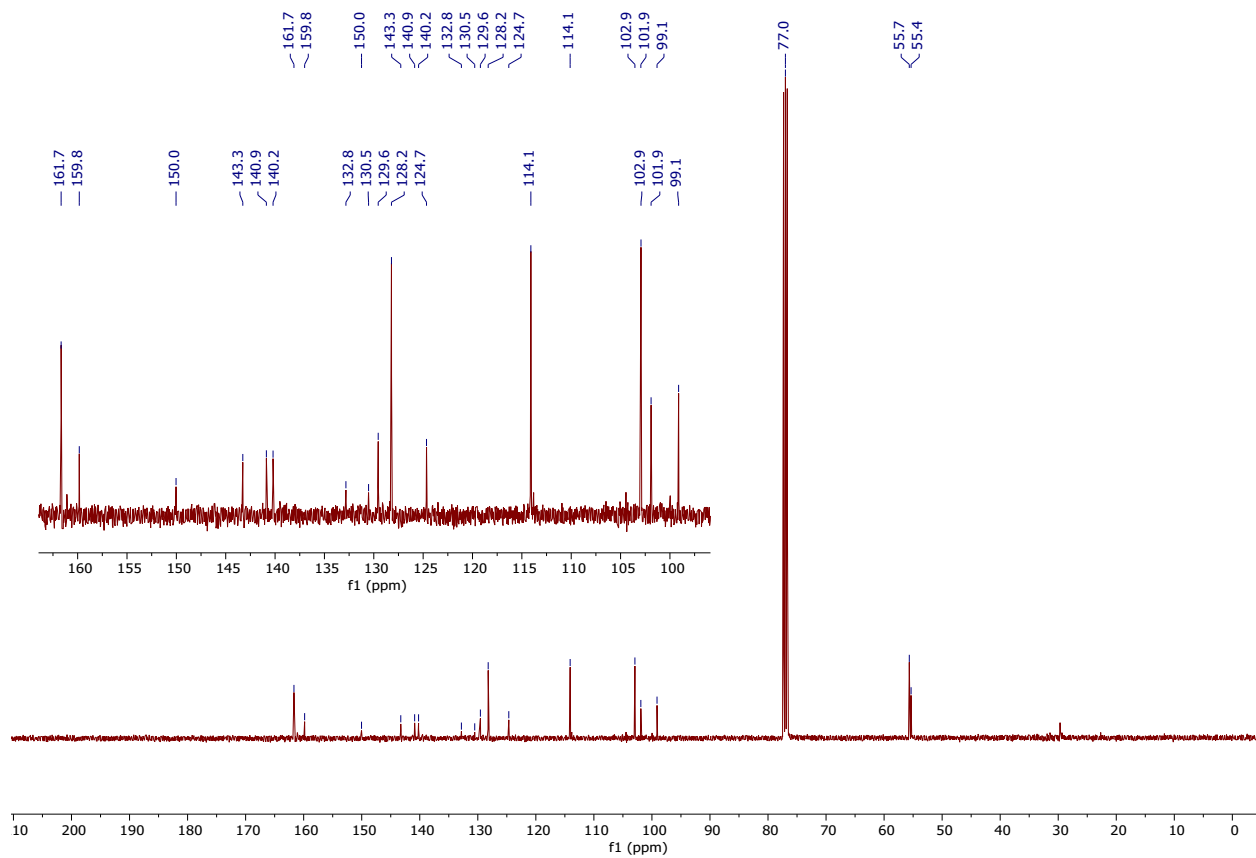


#### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
319.1264	319.1241	-7.07	1	79417.44	C20H15FN2O	(M+H)+
320.1295	320.1273	-6.77	1	17944.06	C20H15FN2O	(M+H)+
321.1331	321.1303	-8.62	1	1947.11	C20H15FN2O	(M+H)+
322.1319	322.1332	3.77	1	100.01	C20H15FN2O	(M+H)+
341.118	341.1061	-34.89	1	148.68	C20H15FN2O	(M+Na)+







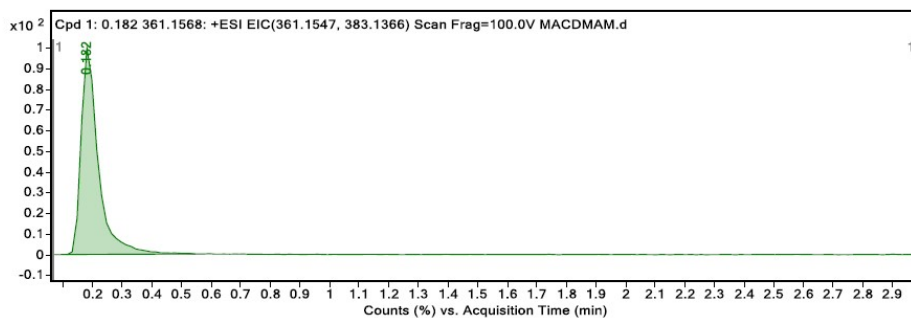
<b>Data File</b>	MACDMAM.d	<b>Sample Name</b>	MACDMAM
<b>Sample Type</b>	Sample	<b>Position</b>	P1-E6
<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Acq Method</b>	ChB60ChD40_isocratic_esi_positive_3min.m	<b>Acquired Time</b>	6/24/2019 1:26:32 PM
<b>IRM Calibration Status</b>	Success	<b>DA Method</b>	PROCESSNEW.m
<b>Comment</b>			

<b>Sample Group</b>		<b>Info.</b>	
<b>Stream Name</b>	LC 1	<b>Acquisition SW</b>	6200 series TOF/6500 series
		<b>Version</b>	Q-TOF B.06.01 (B6172 SP1)

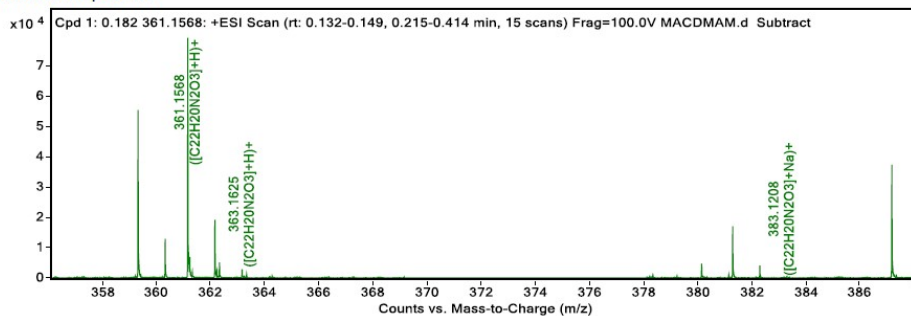
### Compound Table

Compound Label	RT	Mass	Abund	Formula	Tgt Mass	Diff (ppm)
Cpd 1: 0.182 361.1568	0.182	360.1495	79262	C22 H20 N2 O3	360.1474	5.88

Compound Label	m/z	RT	Algorithm	Mass
Cpd 1: 0.182 361.1568	361.1568	0.182	Find By Formula	360.1495

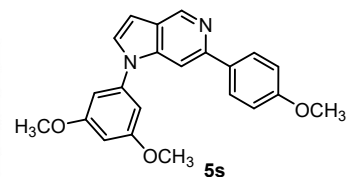


### MS Zoomed Spectrum



### MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
361.1568	361.1547	-5.84	1	79262.38	C22H20N2O3	(M+H)+
362.1601	362.1579	-6.26	1	19321.79	C22H20N2O3	(M+H)+
363.1625	363.1607	-4.84	1	2887.92	C22H20N2O3	(M+H)+
364.1658	364.1634	-6.59	1	378.85	C22H20N2O3	(M+H)+
383.1208	383.1366	41.3	1	70.45	C22H20N2O3	(M+Na)+



## DFT Computational study of frontier orbitals

### DFT settings:

Program: ORCA 4.2

Functional: B3LYP

Basis set: def2-TZVP

Auxiliary basis set: def2/J

Additional settings to speed up the calculation: RIJCOSX

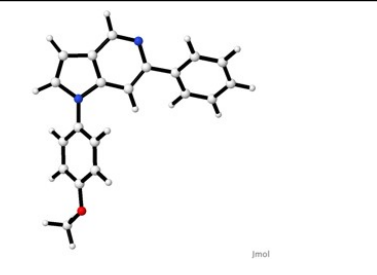
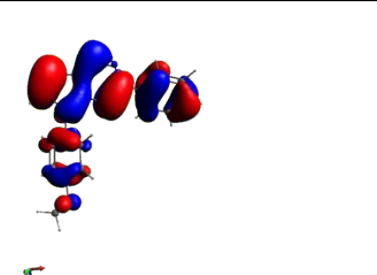
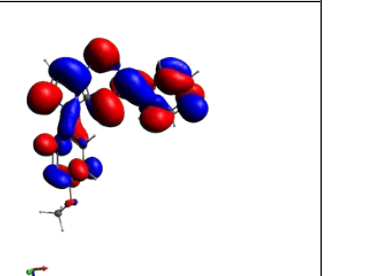
Dispersion correction: D3BJ

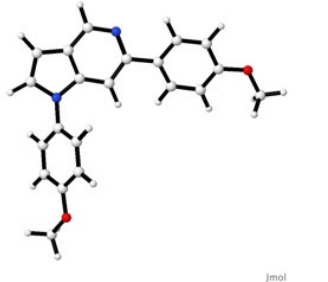
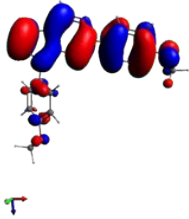
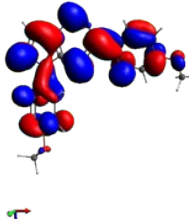
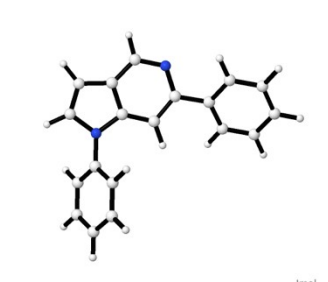
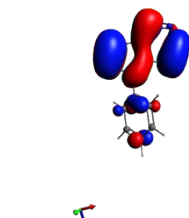
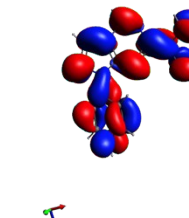
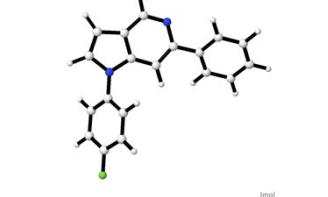
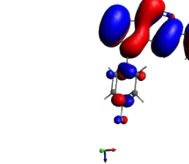
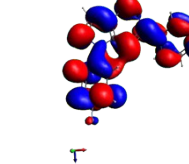
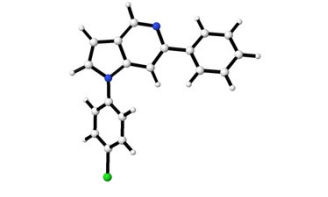
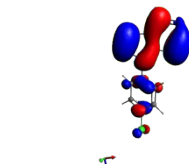
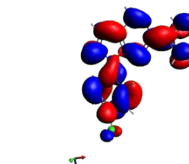
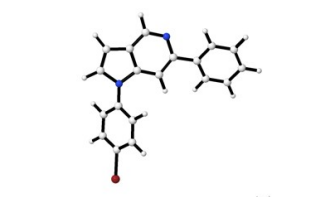
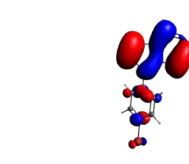
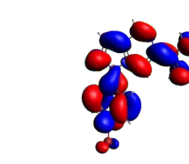
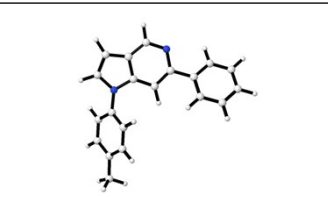
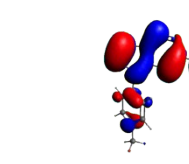
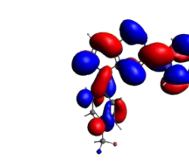
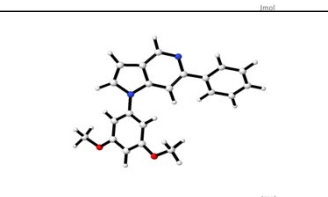
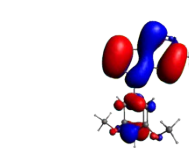
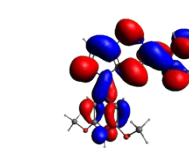
Integration accuracy and grid: IntAccX: 5,5,5; GridX: 3,3,4

### HOMO-LUMO Energies

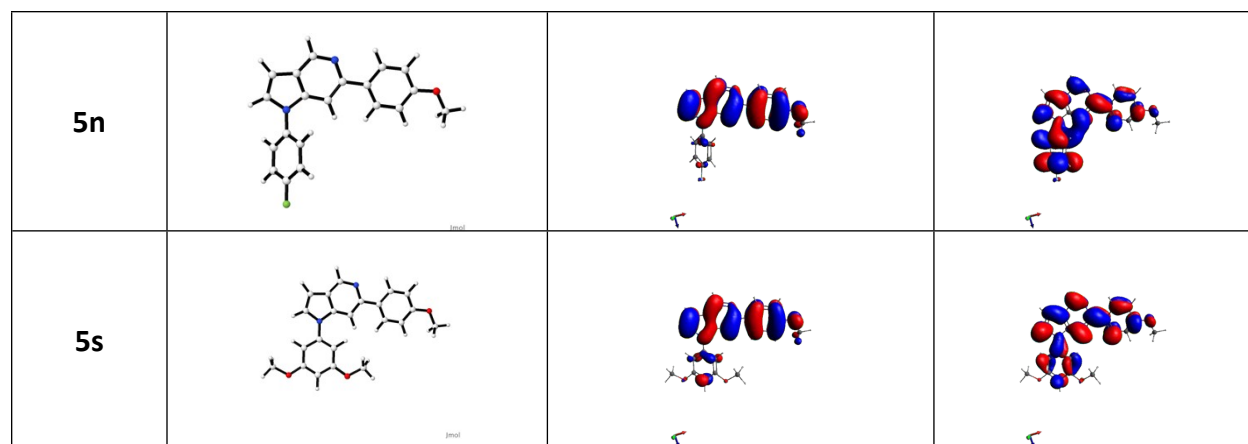
Compound	HOMO (eV)	LUMO (eV)	E_gap (eV)
5a	-5.5965	-0.9836	4.6129
5e	-5.3189	-0.9119	4.407
5g	-5.698	-1.1255	4.5725
5h	-5.7756	-1.1795	4.5961
5i	-5.8044	-1.3412	4.4632
5j	-5.7942	-1.3541	4.4401
5k	-5.6345	-1.1351	4.4994
5l	-5.6841	-1.1016	4.5825
5n	-5.4255	-1.1516	4.2739
5s	-5.3987	-1.1702	4.2285

### Structure and images of HOMO and LUMO orbitals

Structure	3D view	HOMO	LUMO
5a			

5e			
5g			
5h			
5i			
5j			
5k			
5l			





### XYZ coordinates

#### Compound-5a

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**FINAL SINGLE POINT ENERGY -956.342094142865 Eh**  
 -----

H	-1.84133953298016	3.53455345505027	0.26381365351168
C	-2.67427526539721	3.09814269741260	-0.27032158646731
C	-3.86379225276380	2.86098539609940	0.42434599832909
C	-4.95582249162972	2.31670327473898	-0.24867698784897
H	-5.88573926971814	2.12242174889781	0.26426595932919
C	-4.84311848160570	1.98821218535706	-1.59775186062206
H	-5.67952802797279	1.53299539141359	-2.11181766781534
C	-3.65923789681002	2.21735437594412	-2.28498675130066
C	-2.57755385260765	2.79106607819429	-1.61268104415136
H	-1.66366284512989	2.99819192289287	-2.15151043643008
C	-0.45829201000611	-0.00076663806740	-4.53462365479298
N	-0.62764399317094	-0.01203331202100	-5.87739192784165
C	-1.71212351368462	0.53606027119078	-6.40188543586829
C	-2.69236675768037	1.16076708001361	-5.62459730625454
C	-1.36334187399932	0.59607867355966	-3.66198120135001
C	-2.47922060112983	1.19963203816089	-4.22649193376136
C	-3.93383118147491	1.83127856352129	-5.87802631925287
C	-4.41017127626165	2.25197513948293	-4.67173832354849
H	-1.81360031459375	0.48174319737824	-7.48204903246715
H	-1.17903389359791	0.61181460008418	-2.59855463185379
H	-4.40200044159750	1.99545056266134	-6.83408871702910
H	-5.29553738632372	2.81501932032330	-4.43035545395870
N	-3.53545338630538	1.87863999863757	-3.65582142092621
C	0.77657778265298	-0.62183497245916	-4.00532502873020

C	0.77730465780754	-1.30148286599214	-2.78463989464407
H	-0.15308950281088	-1.43696955730086	-2.24778960802434
C	1.95069951455368	-1.83340789390836	-2.26772269809612
H	1.93082037463066	-2.36382153950832	-1.32414536758982
C	3.14617836707476	-1.68899103672802	-2.96219303551404
H	4.06352453198885	-2.09537500245983	-2.55489665679716
C	3.15340917792093	-1.02722657938728	-4.18571934637777
H	4.08060265959543	-0.91159950126991	-4.73328974480209
C	1.97848575351763	-0.50635944885357	-4.70857063033451
H	1.97640122619893	0.00384838041148	-5.66201563233057
O	-3.85105368634082	3.19079570989163	1.74196809691442
C	-5.01466370837973	2.95918532772369	2.51755356391801
H	-5.85980080469588	3.55042557971529	2.15226972615561
H	-5.29025668815947	1.90004303234413	2.52218916571205
H	-4.76239310911348	3.27139434685482	3.52807317291172

### Compound-5e

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**FINAL SINGLE POINT ENERGY -1070.860004685996 Eh**  
 -----

H	-1.72666773962377	3.41657526439265	0.25907585891902
C	-2.57948141233272	3.00231659957403	-0.26126426736671
C	-3.74797452492281	2.75293882401368	0.46368735022328
C	-4.86388568304139	2.23606443631717	-0.19076416565372
H	-5.77799446880245	2.02998081557358	0.34561353490499
C	-4.79680688104040	1.95218226539688	-1.55287169545844
H	-5.65290063998094	1.51946464305334	-2.05357416766227
C	-3.63560849118551	2.19898570650913	-2.27277440346492
C	-2.52809168513491	2.74064314909679	-1.61619876278458
H	-1.63140062086125	2.96391312331543	-2.17687630309154
C	-0.53018559717947	0.09444460077074	-4.77980533554369
N	-0.79416516698529	0.10942502724951	-6.10864612588444
C	-1.91252677383910	0.66253711394350	-6.54773783669214
C	-2.84772481348491	1.25539029715347	-5.69467366221325
C	-1.38418931852848	0.66676039046315	-3.83901428935552
C	-2.54340504054429	1.26469735860900	-4.31290681638286
C	-4.11000463090210	1.91606643220688	-5.85323827463701
C	-4.51266007669390	2.30147833881492	-4.60924484393640
H	-2.08223038987696	0.63793820071225	-7.62058280898518
H	-1.13278399416115	0.66948355585859	-2.78985258392263
H	-4.63884543129253	2.09767674540218	-6.77373240095461
H	-5.38676255931551	2.84741036747344	-4.29783528037578
N	-3.56940459472212	1.91743712495608	-3.65954973383448
C	0.74351322739070	-0.52402592013242	-4.35319502089986

C	0.90383066817274	-1.06556097371414	-3.07911758888129
H	0.06005629642839	-1.11334945495002	-2.40325730839870
C	2.11997590278751	-1.58327293110876	-2.65037604830590
H	2.19487747331286	-1.99696253738044	-1.65587053999793
C	3.21743175418274	-1.57008380621512	-3.50807156132746
C	3.06822102058539	-1.05547831029815	-4.79848111966699
H	3.92598753154609	-1.05556903977014	-5.45850126968142
C	1.85162291739190	-0.54621294850094	-5.21053179228110
H	1.73991169746013	-0.14326454870292	-6.20758257936165
O	-3.69290971794088	3.04600619555453	1.78923468634916
C	-4.83612181901346	2.81121962572164	2.59309007707544
H	-5.68505818319263	3.41793453405050	2.26393166961659
H	-5.12334063557155	1.75508121724617	2.58576709871283
H	-4.55145462713977	3.10098659977611	3.60180747478154
C	4.65500173345040	-2.52540598577114	-1.86386724533048
H	5.69268647992528	-2.84774070598265	-1.81335613262337
H	4.48216133568762	-1.73777103970746	-1.12384299378961
H	4.00328809450474	-3.37588377435117	-1.64337120282586
O	4.45292938448383	-2.04250657661998	-3.18224158901083

### Compound-5g

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**FINAL SINGLE POINT ENERGY -841.825637059253 Eh**  
 -----

H	-1.69825699245798	3.38025120330746	0.45510695441316
C	-2.55602649774231	2.98032279753769	-0.06988231039646
C	-3.75498658431732	2.77755219400936	0.60503695128719
H	-3.83356694110776	3.01338400775754	1.65822998597653
C	-4.85456962373030	2.27599376844467	-0.08141664465393
H	-5.78955487486792	2.11005395750380	0.43789131889889
C	-4.75627245368248	1.96472684382356	-1.43143047197615
H	-5.60001062298840	1.54544584163666	-1.96291895649819
C	-3.55366994649676	2.17004540002076	-2.10477723207116
C	-2.45372309120735	2.68848268310531	-1.42323425063595
H	-1.53341175764889	2.87645441577457	-1.95789623700150
C	-0.42496830099291	-0.01253780120536	-4.53036253964226
N	-0.67112710873137	-0.02423810171150	-5.86120209276496
C	-1.77926023508384	0.52954421937795	-6.32437279747082
C	-2.71272560736756	1.15512568482295	-5.49335391288632
C	-1.27891417623016	0.58851312053513	-3.60883809922921
C	-2.42349771595035	1.19405421766484	-4.10903185639614
C	-3.96901096937856	1.81902117837916	-5.68206666891373
C	-4.38625559057188	2.23170888440003	-4.45293050421488
H	-1.94200667402385	0.47686934217557	-7.39707242354028

H	-1.03588720699740	0.60252520070358	-2.55758817623368
H	-4.48420270332833	1.98443038252790	-6.61322221876145
H	-5.26126896472065	2.78875050457551	-4.16533771791386
N	-3.45520545666903	1.86643910744838	-3.48311700586502
C	0.83791936833520	-0.63572400801200	-4.07507861581081
C	0.93531682314210	-1.24952124935412	-2.82332154736769
H	0.05514857624939	-1.34036942905728	-2.19984968553197
C	2.14102890310984	-1.77489178282017	-2.38076130629456
H	2.19525341925135	-2.25010769608306	-1.40952904199566
C	3.27418831072610	-1.69725841771628	-3.18184681702168
H	4.21597617403134	-2.10044312600189	-2.83141104243582
C	3.18316992448386	-1.10883128992969	-4.43871446596110
H	4.05856869222849	-1.04872733029500	-5.07345975209024
C	1.97655685472440	-0.58815848483643	-4.88374081402747
H	1.89925305001151	-0.13012623850970	-5.86011000497223

### Compound-5h

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**FINAL SINGLE POINT ENERGY -941.075265664758 Eh**  
 -----

H	-1.70927784575081	3.44888433038818	0.42616193929109
C	-2.54892072888388	3.02396211694963	-0.10594634707816
C	-3.74341325876961	2.80461528612899	0.55783559451800
F	-3.83040030799592	3.12013801412020	1.86660974783472
C	-4.84983636736684	2.27215218458995	-0.07962579915249
H	-5.76233181929177	2.10545557615274	0.47575353818094
C	-4.75066210396596	1.93852566951932	-1.42438350558847
H	-5.59289512100005	1.49321218043186	-1.93634627389601
C	-3.56096410696044	2.15583249454898	-2.11667341028541
C	-2.46474630298474	2.70736721508255	-1.45458446467120
H	-1.55222608087761	2.90118888338651	-1.99992332102672
C	-0.42147224897756	-0.01435952914003	-4.53425221719216
N	-0.65847283070119	-0.01611509507308	-5.86674847109674
C	-1.76894811608422	0.53063053187158	-6.33266554389783
C	-2.71408338731814	1.13952524338891	-5.50227707479491
C	-1.28623782289371	0.57141416427843	-3.61301183009493
C	-2.43285117935682	1.17082301077866	-4.11622222761495
C	-3.97323801433690	1.79733332453822	-5.69364819810830
C	-4.39810004659638	2.20290196170012	-4.46477527451964
H	-1.92323217174738	0.48702535850760	-7.40700323670439
H	-1.04908193920087	0.57876178891550	-2.56005771300150
H	-4.48542872193233	1.96320290874307	-6.62639159158978
H	-5.27712810742569	2.75460660013526	-4.17880915032282
N	-3.47061507868273	1.83493331018729	-3.49187012951257

C	0.84212866041725	-0.63351155762459	-4.07586818813397
C	0.92452574567160	-1.28650820609157	-2.84312907758402
H	0.03416633741831	-1.40606325198947	-2.23910018030155
C	2.12781038595932	-1.81598845598675	-2.39812522490857
H	2.17057530358676	-2.32456628378538	-1.44344887338338
C	3.27302394739252	-1.69900315360981	-3.17707024596594
H	4.21313842083315	-2.10442490528737	-2.82470429331256
C	3.19792133547130	-1.06700385756348	-4.41386988063897
H	4.08411774966714	-0.97450792680151	-5.02940772801639
C	1.99335496510550	-0.54532842558149	-4.86295964266904
H	1.92779085757871	-0.05636150580907	-5.82508170476134

### Compound-5i

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**FINAL SINGLE POINT ENERGY -1301.391295272537 Eh**  
 -----

H	-2.06766452225201	2.73635072572289	0.88523526267165
C	-2.86221706536994	2.52125764115939	0.18459792786077
C	-4.17046922756865	2.39913014803874	0.63452318417801
Cl	-4.53635987350508	2.59295625331053	2.32907760979887
C	-5.19825553698951	2.12693168424962	-0.25808674589983
H	-6.21201030040437	2.02067686908848	0.10091695428531
C	-4.91237691272111	1.97178406688488	-1.60473548185336
H	-5.70756364472684	1.72450202523614	-2.29408927832957
C	-3.60607665833983	2.10937632382726	-2.07491084517673
C	-2.58427586304743	2.39232105143715	-1.16990285436346
H	-1.57420640030757	2.53602780258252	-1.52521333114088
C	-0.30738085506778	0.11753971074732	-4.52744891738325
N	-0.54422912461090	0.14440767291683	-5.85939708038168
C	-1.62429513083134	0.75140173884220	-6.31773654179090
C	-2.54104917457854	1.38560624518459	-5.47811478839229
C	-1.18217215537764	0.66996821820001	-3.59131412747959
C	-2.30207738002994	1.33221966489949	-4.08349611555612
C	-3.76588228116720	2.09978914132460	-5.67889553849805
C	-4.22720138236046	2.44302032112896	-4.44722842331432
H	-1.77797816889051	0.73814931479236	-7.39300327203572
H	-0.99551630340533	0.55815906891378	-2.53445697035262
H	-4.23001452032397	2.34280190673860	-6.61987664239807
H	-5.09751478516619	3.01006471660168	-4.16689115648165
N	-3.35435600847188	1.98563343191079	-3.45853733341327
C	0.95325403685801	-0.53402924248283	-4.10480689384460
C	1.62605622407815	-0.13584652113626	-2.94564112573279
H	1.23647789711404	0.67948539071334	-2.34997339233306
C	2.81767113617916	-0.74366056070138	-2.57221186431131

H	3.33403432781355	-0.40818890492079	-1.68156539979229
C	3.35573436723439	-1.76522734143715	-3.34643083221102
H	4.28453052938485	-2.23771250751507	-3.05275307860958
C	2.70025580917980	-2.16264701581289	-4.50782938182807
H	3.11819351894635	-2.94917319903032	-5.12374815465760
C	1.51331136907873	-1.55050873845197	-4.88484216653461
H	1.00560405964723	-1.84383710296368	-5.79278320469774

### Compound-5j

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**FINAL SINGLE POINT ENERGY -3415.272314522263 Eh**  
 -----

H	-1.82330750089460	3.02766744475728	0.65983429693481
C	-2.66274037955122	2.73758587493110	0.04412288887146
C	-3.92826851002322	2.60606335167408	0.60010819693577
C	-5.01344452090269	2.24799792092050	-0.18757546632652
H	-5.99498418293314	2.14198496029073	0.25148417464191
C	-4.82501232605363	2.00247914408592	-1.53927960123133
H	-5.66106744576900	1.68861864259482	-2.14903164869106
C	-3.56133277131963	2.13432354363404	-2.11351603513135
C	-2.48384715537647	2.51468248181287	-1.31486135007255
H	-1.50866179105881	2.65859349278655	-1.75768776766964
C	-0.40321332216478	-0.05269370237234	-4.54730395179379
N	-0.65805989191087	-0.06161625879477	-5.87635368991860
C	-1.74917746067359	0.52368231520043	-6.33761089810136
C	-2.65797173191629	1.18134794488299	-5.50556790482389
C	-1.24813764209597	0.56004259469012	-3.62236166758310
C	-2.37720712683625	1.19882869184988	-4.11878474538427
C	-3.88628027083561	1.89192426465087	-5.70244390426427
C	-4.30307226360095	2.30708031682382	-4.47597877878454
H	-1.91758874118982	0.47278379743626	-7.40952810263445
H	-1.00752227972748	0.55858644885527	-2.57109380751233
H	-4.38101728357565	2.08731691832769	-6.63889026797104
H	-5.16002537881979	2.89485730335543	-4.19643671150896
N	-3.39683559612762	1.90001421079079	-3.49592861440883
C	0.86858900925826	-0.67594306215716	-4.11388840169743
C	1.04863763760259	-1.16286519873102	-2.81554743849551
H	0.21853610422462	-1.17392188141141	-2.12144570998084
C	2.27708832744998	-1.66195980670966	-2.40668247845760
H	2.39619701684558	-2.03373610358294	-1.39682694377714
C	3.34978850982187	-1.69307471622909	-3.28989334149372
H	4.30891777049029	-2.07752883933979	-2.96694336608944
C	3.17373023977135	-1.24119149254094	-4.59345605923409
H	3.99989684039026	-1.27036398821579	-5.29295379329788

C	1.94626698996392	-0.74059722439851	-5.00227155961074
H	1.80376862935062	-0.38032890944641	-6.01122169974652
Br	-4.18886150181221	2.92610951957838	2.46235614830893

**Compound-5k**

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**FINAL SINGLE POINT ENERGY -881.132717171891 Eh**  
 -----

H	-1.81418142080905	3.00116893562939	0.62701590906781
C	-2.66166710792769	2.75036046922224	-0.00024261767570
C	-3.90574140191310	2.51706473268148	0.58889164097540
C	-4.97878876739834	2.22970654438753	-0.25047452504393
H	-5.95784940335254	2.05464717010754	0.17870250203579
C	-4.81375478093722	2.12263471572991	-1.62550078743287
H	-5.64899830325676	1.84469715932966	-2.25430064522199
C	-3.55929042577374	2.32305006184327	-2.19235613891447
C	-2.48764965359782	2.67310832208478	-1.37220005170214
H	-1.52368307323591	2.88275047445790	-1.81310562410204
C	-0.38468766395089	0.12665042483871	-4.51970884839519
N	-0.63691168397942	0.04099175282928	-5.84650656367187
C	-1.71035383669597	0.62933524490475	-6.34699158575054
C	-2.60310657307829	1.36304975609728	-5.55988100066383
C	-1.23853145778941	0.77489513706700	-3.63124899650280
C	-2.34418050514487	1.41997103870893	-4.17030526098349
C	-3.82185569065002	2.08094860818443	-5.79250603328327
C	-4.25477982322576	2.52929112801026	-4.58122211557752
H	-1.87857888029812	0.51491773225867	-7.41402964804128
H	-1.04999021554485	0.75145496959012	-2.56980993004741
H	-4.30311187265773	2.25610477829647	-6.74004400548109
H	-5.11586813547102	3.12348207932122	-4.32772589581706
N	-3.36760793660875	2.13973120942985	-3.58108372124426
C	0.86357926327787	-0.50339633029887	-4.03452159214623
C	1.52259083467392	-0.01753367751670	-2.90015826991802
H	1.13489080509486	0.85132225951531	-2.38434681910508
C	2.69366875142667	-0.60934733384804	-2.44870072030946
H	3.19585267379332	-0.20825117692701	-1.57709471850581
C	3.23115336793664	-1.69885938874687	-3.12462997592154
H	4.14441900093874	-2.16085522352484	-2.77157393575973
C	2.59263666935454	-2.18174720554027	-4.26277250147230
H	3.01074854287082	-3.02319167204526	-4.80099282593988
C	1.42361575533829	-1.58710654527155	-4.71651700047306
H	0.92742951226859	-1.94931561939385	-5.60591001108734
C	-4.05936615193940	2.55536130978174	2.08332905432134
H	-5.08152618740730	2.32550950378190	2.38479231738813

H	-3.39911542832866	1.82803008601167	2.56078226414169
H	-3.79567879600140	3.53751856901187	2.48389867826141

### Compound-5l

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**FINAL SINGLE POINT ENERGY -1070.861327176153 Eh**  
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O	-1.42257856233832	3.15847438276048	0.93650511304911
C	-2.44003717488994	2.79622669134724	0.11577768859617
C	-3.67609297492702	2.62551272704794	0.73069342947127
C	-4.78883943326677	2.29615293612125	-0.03305938358620
H	-3.77384179095733	2.77108598728593	1.79689137293337
C	-4.67124662725500	2.10237909087824	-1.41131380803989
H	-5.50958318191147	1.79686691736875	-2.01650829428403
C	-3.42410393695233	2.26872872680296	-2.00488142268117
C	-2.30224524729502	2.62450597265002	-1.26337465002028
H	-1.36496188003019	2.79531155463514	-1.76712414671708
C	-0.47403669537886	-0.01450065513229	-4.58213073099557
N	-0.69318704935372	0.11753108100876	-5.91112038959797
C	-1.72881116445159	0.82339737285968	-6.33342878985927
C	-2.60661193654185	1.46878497738758	-5.45892977726074
C	-1.26757570199235	0.60398318857566	-3.61827330620264
C	-2.33674964397113	1.36646747529506	-4.07321829100340
C	-3.78529500240517	2.27037744135822	-5.60442538820005
C	-4.17934146132144	2.62356187949728	-4.34917600861748
H	-1.87632412777915	0.88584376079634	-7.40796065623762
H	-1.04057908064082	0.50579907567884	-2.56769599123902
H	-4.26505184823041	2.56124018125033	-6.52378801286067
H	-4.99872954469601	3.24068450142359	-4.02334222372562
N	-3.30478958384770	2.09171098824888	-3.40487299155536
C	0.69366005345147	-0.83127653433530	-4.17883518131696
C	0.68049501254643	-1.59030331645013	-3.00451116671389
H	-0.22112336111664	-1.63967105852102	-2.40750298282304
C	1.80040188440362	-2.31174719640590	-2.61257591551083
H	1.7685555907017	-2.90209147806247	-1.70567366754945
C	2.95439391931795	-2.28644422309432	-3.38680742599708
H	3.82937099182624	-2.84315735831651	-3.07567658962132
C	2.97147763087699	-1.55091199532331	-4.56859923105999
H	3.86303740997617	-1.53176028577462	-5.18304580442646
C	1.84903386879810	-0.83810574109339	-4.96556629057767
H	1.85232283981703	-0.27005360930596	-5.88566081983741
O	-5.95753701515441	2.17045892448344	0.64789748749064
C	-7.15439484452515	1.98952530919400	-0.09213341253010
H	-7.28945946401364	2.78756329464565	-0.82727466528937



H	-7.17007185297955	1.02192783632785	-0.60306952575270
H	-7.96128482545296	2.02642792749335	0.63602097817185
C	-0.13301449811314	3.36533488528805	0.37869021882556
H	0.25313744586599	2.45140381929006	-0.08165347666763
H	-0.14246749526678	4.16753565073280	-0.36403901817203
H	0.50705039110581	3.65279889408175	1.20887314799213

### Compound-5n

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**FINAL SINGLE POINT ENERGY -1055.592732704585 Eh**  
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O	4.46548004360759	-0.54470959964814	-2.10956328495435
C	-3.90995298178229	3.19571667315633	-0.26952497224207
C	-5.07476322933566	2.71211167928416	0.29919573079152
C	-5.93296844802415	1.87393428196803	-0.38995437206114
F	-5.38364376167291	3.07607658932124	1.56100216243931
C	-5.60853651701995	1.50337555509440	-1.68894224719495
H	-6.25576491229166	0.83386299472695	-2.23919808556846
C	-4.44777870420500	1.98708322561782	-2.28833196721236
C	-3.60206881788790	2.83401606066444	-1.57264910927992
H	-2.71347579448006	3.22589891069648	-2.04644397786279
C	-0.60222229387261	0.71160825404281	-4.28197820509697
N	-0.67415322595724	0.70083281483340	-5.63506066415572
C	-1.82483128080638	0.94909728758438	-6.23688714548561
C	-2.99440755046979	1.24913464769293	-5.53240560773721
C	-1.69896244578154	1.02593454659403	-3.48061133766516
C	-2.89500087345664	1.31099547250828	-4.12325378652696
C	-4.35451223576549	1.54962683285338	-5.87398168811457
C	-5.01478404376622	1.77992130562976	-4.70499265837918
H	-1.82563849153465	0.91189813087605	-7.32253392766607
H	-1.62071436447066	1.05588740969426	-2.40524350611577
H	-4.78379999068500	1.59931931608193	-6.86068795879613
H	-6.03636313813672	2.07012785033801	-4.52743416221601
N	-4.13947350217116	1.65045510791617	-3.62741147766807
C	0.70975187094106	0.38130975497062	-3.68348561984972
C	0.83640063898788	0.02614526308629	-2.34120474437081
H	-0.03938794018993	-0.04094290562181	-1.71047646940808
C	2.06754454778541	-0.28299142213252	-1.77720742323556
H	2.11222671287582	-0.56752288843223	-0.73661944244865
C	3.21755163060080	-0.24448546753025	-2.56273861242625
H	-3.26745826823426	3.85419307685101	0.29846511474085
C	3.11164646688475	0.11010906626286	-3.91018280713374
H	4.01103100695211	0.13940142866152	-4.51133607279852

C	1.87877059724886	0.40868313162126	-4.45778088211575
H	1.79767129951162	0.67412081232718	-5.50231430398293
H	-6.83050922263707	1.51026362923201	0.09064266383594
C	4.59799926221012	-0.95874515103874	-0.75883892506176
H	4.00290877758370	-1.85415032711503	-0.55592044749522
H	4.29801910393612	-0.16440884823926	-0.06891727218441
H	5.65155007550915	-1.18596450043005	-0.61258250729663

### Compound-5s

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**FINAL SINGLE POINT ENERGY -1185.376417852070 Eh**  
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O	4.59198340967297	-0.21538593542813	-2.22566799799689
C	-3.88470400555329	2.66026077995141	-0.10877029863568
C	-5.20516346719660	2.53907626533382	0.30608087740916
C	-6.16525047942670	2.10770695789825	-0.60005396969459
C	-5.80965145202219	1.73911293578406	-1.89776394095045
H	-6.54402134262076	1.34048660502886	-2.57767963421565
C	-4.48005575537633	1.86570406713107	-2.29916442543321
C	-3.51300081111049	2.34721299919031	-1.41788107106503
H	-2.51177306243212	2.52827811031995	-1.76482860438164
C	-0.60409929204406	0.53779882430252	-4.32920366776211
N	-0.69182019480548	0.51937691996671	-5.67944210374220
C	-1.85205315666595	0.76779987099372	-6.26224573218489
C	-3.00182291320228	1.09602596614513	-5.54225934073834
C	-1.69746895117285	0.82772164959061	-3.51218935407715
C	-2.89812232177358	1.15117595078549	-4.13100963958948
C	-4.34731135425938	1.44681592519730	-5.88543311151301
C	-4.99608671872976	1.70541165693957	-4.71942827128377
H	-1.87552685760953	0.71644741715007	-7.34712158463203
H	-1.60314932675573	0.81539356485016	-2.44067532093641
H	-4.77142867065925	1.51809670029695	-6.87312606521023
H	-6.00262768234810	2.04564125924086	-4.55637049881459
N	-4.13292937561627	1.54403062143549	-3.63319176600138
C	0.73528664946299	0.28812193386021	-3.74905401843133
C	0.92464831485811	0.06808334372069	-2.38542582846037
H	0.07629053940283	0.01519250409736	-1.71690855301197
C	2.18922069009403	-0.10955761641175	-1.83822372622561
H	2.28291901039444	-0.28656106340116	-0.77722875365004
C	3.31153889065915	-0.06776704913439	-2.66336850345172
O	-3.01473134712574	3.12417013742730	0.82600676558242
C	3.14206912384774	0.13491738294712	-4.03496487183369
H	4.01966305798856	0.15988140320656	-4.66770086988729

C	1.87727917405474	0.30482534296860	-4.56425132422375
H	1.74798201283483	0.46631255542153	-5.62492316389986
O	-7.44109820169456	2.06294772214422	-0.13346260832454
C	4.79829959518040	-0.44400605138954	-0.84241291122213
H	4.30214262873478	-1.36143951047482	-0.51131392814434
H	4.43496957969183	0.39569088611591	-0.24262998177641
H	5.87279326930411	-0.54690022399270	-0.70836032864021
H	-5.48857571506107	2.81194684957755	1.31214085721489
C	-1.65413956459339	3.29312173222382	0.46398806593257
H	-1.19810415758384	2.34276992785937	0.17161256778275
H	-1.54153437302357	4.01256327386383	-0.35147094876688
H	-1.15579892301833	3.67779559413071	1.35027821372447
C	-8.50185822706449	1.94868627082001	-1.06907404556603
H	-8.41614614595197	2.70452147534104	-1.85506019613105
H	-8.53488836960946	0.95561980860173	-1.52760486746158
H	-9.41568373007426	2.11430425837250	-0.50275151967853