

## Supporting information

# Base-Induced Regioselective Radical Arylation of 3-Aminochromones with Arayl hydrazine

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## Supporting Information

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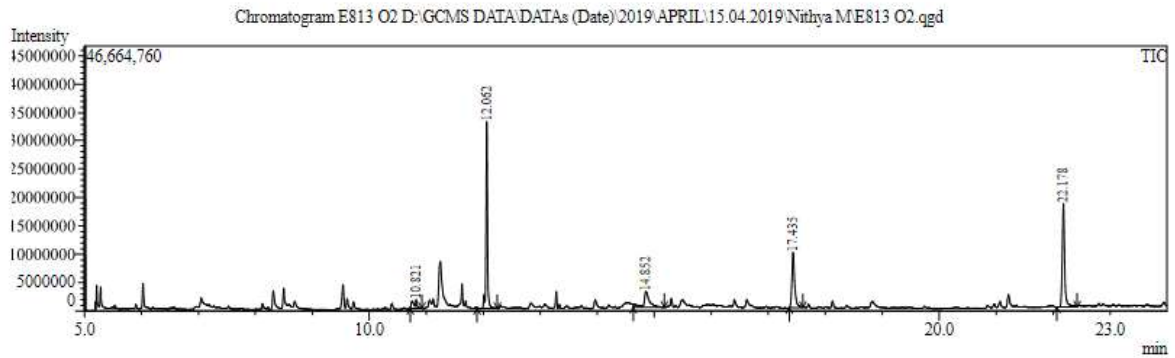
I.	GC-MS chromatogram of optimized conditions	S-1
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### GC-MS Analysis:

GC-MS data shown here is respect to reactant (3-amino-8-methoxy-2-phenyl-4H-chromen-4-one) irrespective of phenyl hydrazine, since we used 2.5 equivalent of Phenyl hydrazine.

## Supporting information

### GC-MS chromatogram of optimized conditions:

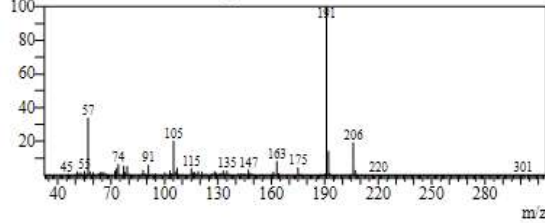


Line#:1 R.Time:10.820(Scan#:1163)

MassPeaks:118

RawMode:Averaged 10.815-10.825(1164-1166) BasePeak:191.00(430189)

BG Mode:Calc. from Peak Group 1 - Event 1

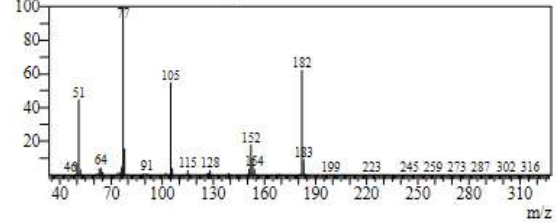


Line#:2 R.Time:12.060(Scan#:1413)

MassPeaks:127

RawMode:Averaged 12.055-12.065(1412-1414) BasePeak:77.05(8239592)

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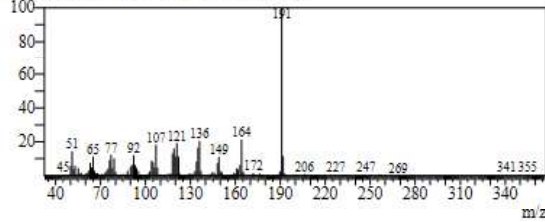


Line#:3 R.Time:14.850(Scan#:1971)

MassPeaks:171

RawMode:Averaged 14.845-14.855(1970-1972) BasePeak:190.95(458019)

BG Mode:Calc. from Peak Group 1 - Event 1

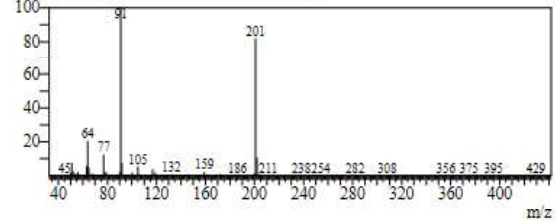


Line#:4 R.Time:17.435(Scan#:2488)

MassPeaks:176

RawMode:Averaged 17.430-17.440(2487-2489) BasePeak:91.00(3190384)

BG Mode:Calc. from Peak Group 1 - Event 1

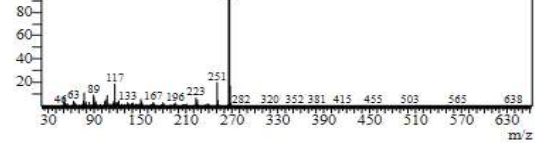


Line#:5 R.Time:22.180(Scan#:3437)

MassPeaks:286

RawMode:Averaged 22.175-22.185(3436-3438) BasePeak:266.90(3662248)

BG Mode:Calc. from Peak Group 1 - Event 1

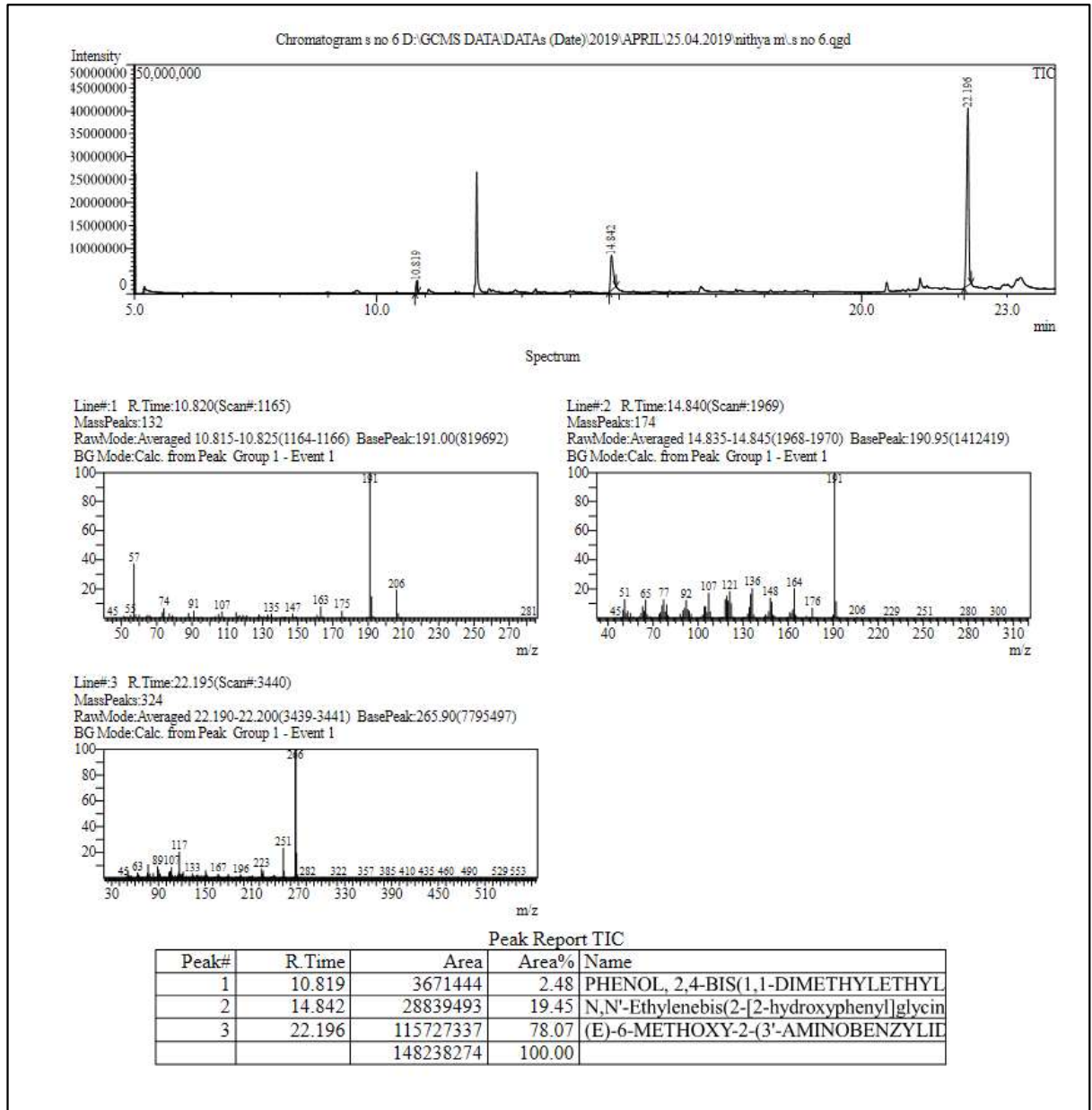


Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	10.821	7245381	4.21	Phenol, 2,4-bis(1,1-dimethylethyl)-
2	12.062	60971807	35.45	Diazene, diphenyl- (CAS)
3	14.852	18281227	10.63	N,N'-Ethylenebis(2-[2-hydroxyphenyl]glycin
4	17.435	32318015	18.79	Butanenitrile, 2-(4-methylphenylhydrazono)-
5	22.178	53164261	30.91	(E)-6-METHOXY-2-(3'-AMINO BENZYLID
		171980691	100.00	

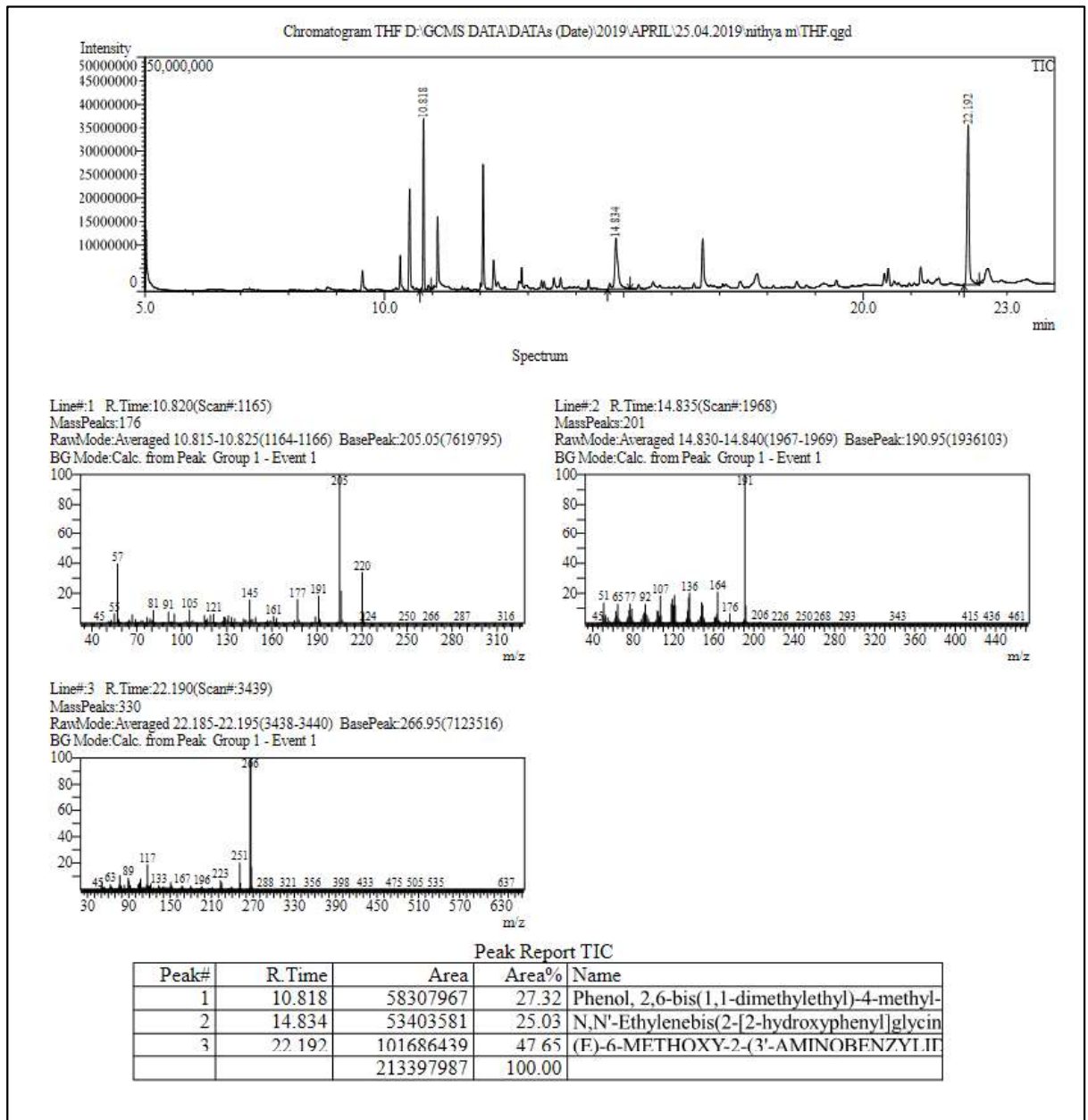
GC-MS chromatogram data for entry 1 in table 1

## Supporting information



GC-MS chromatogram data for entry 2 in table 1

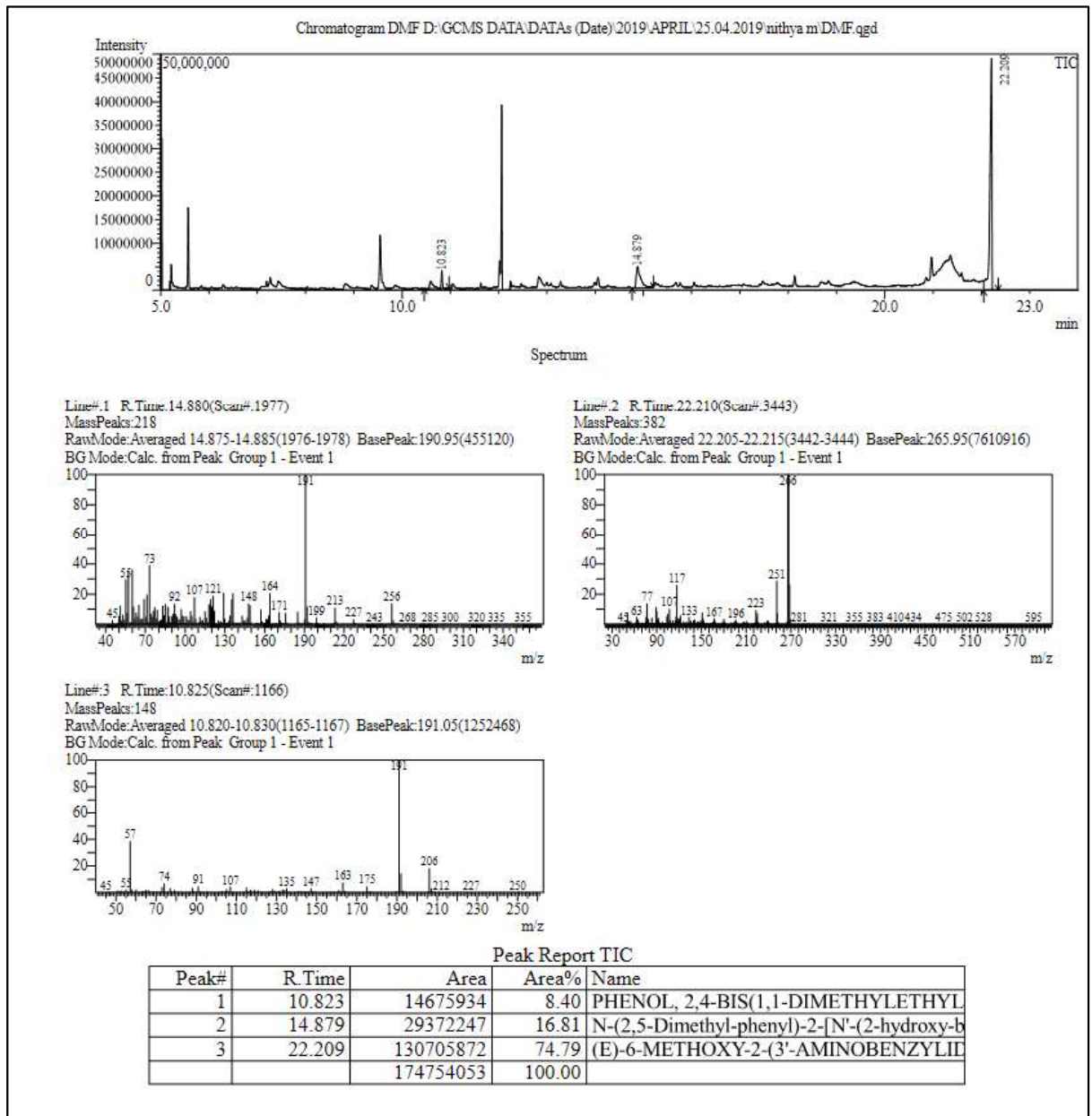
## Supporting information



GC-MS chromatogram of entry 3 in table 1

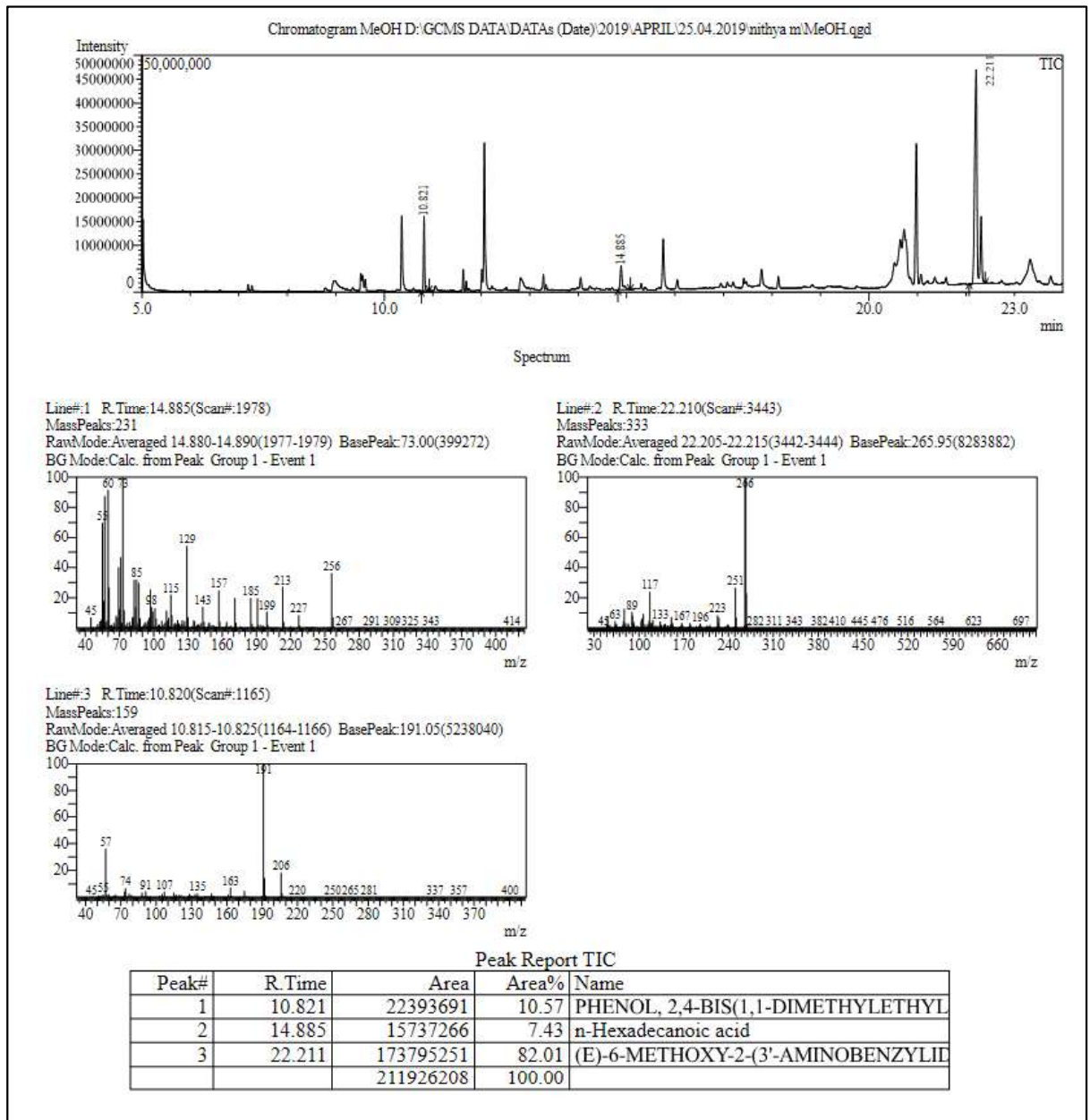


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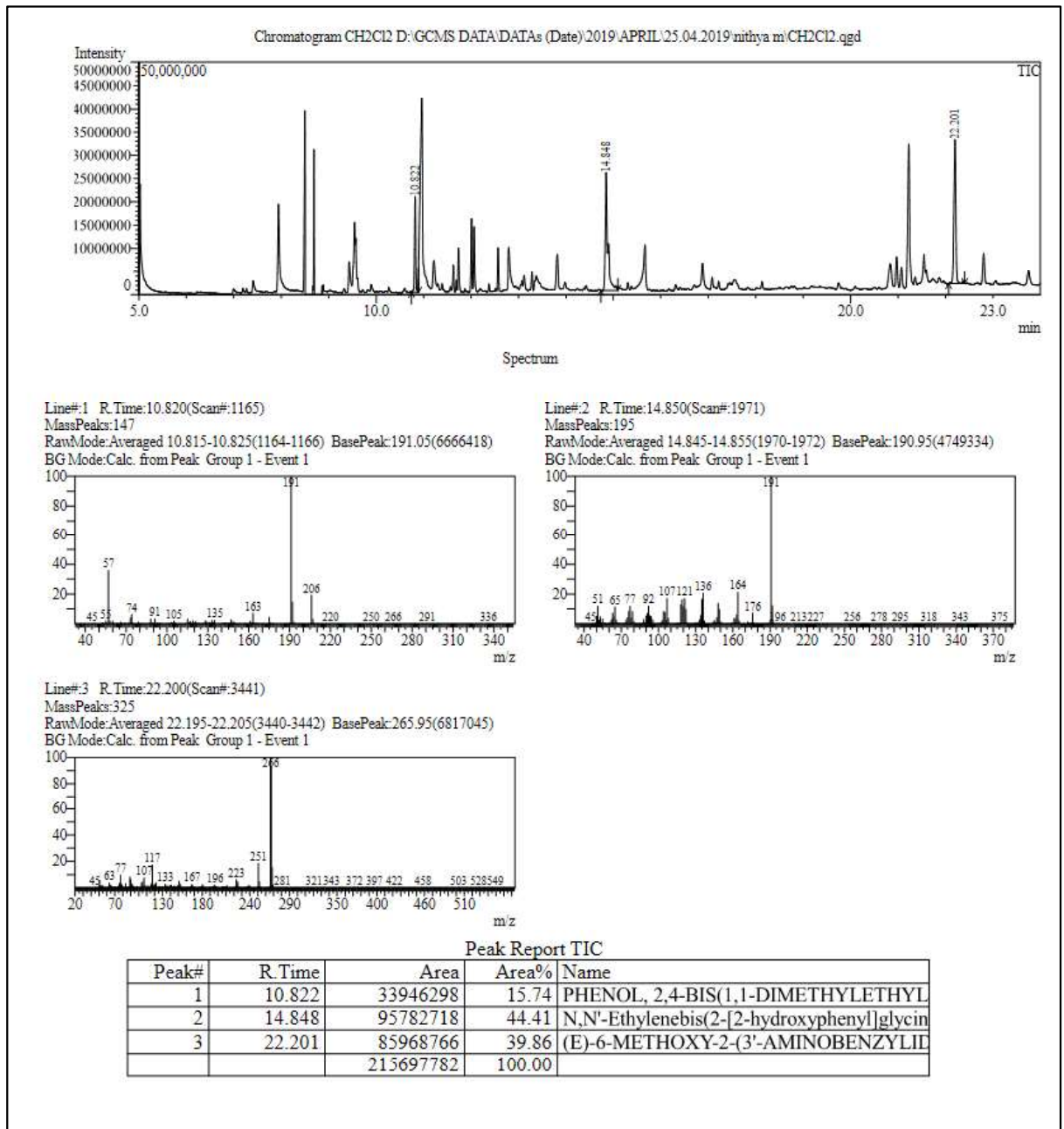
GC-MS chromatogram of entry 4 in table 1

## Supporting information



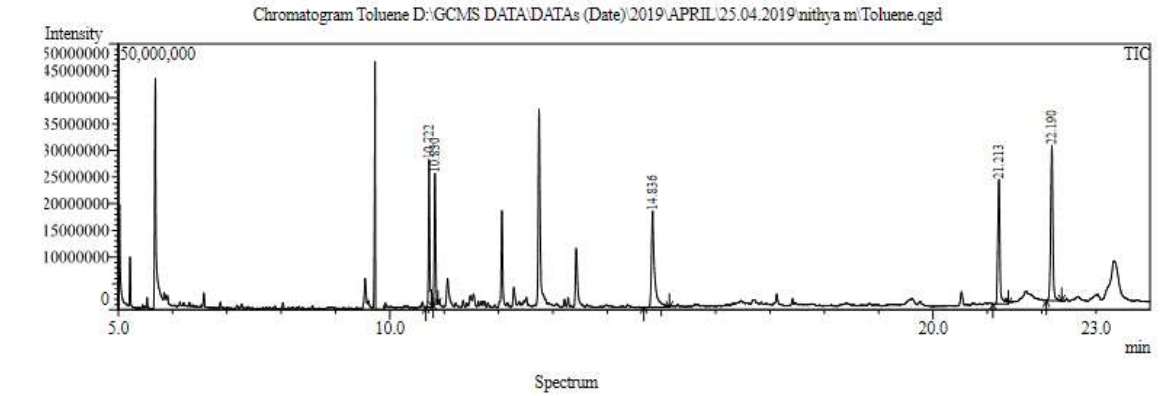
GC-MS chromatogram of entry 5 table 1

## Supporting information

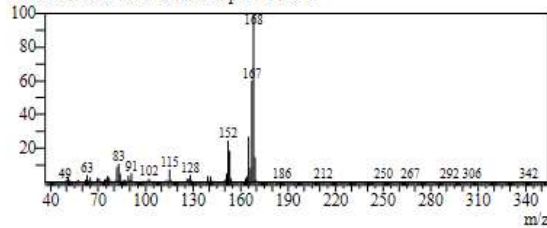


GC-MS chromatogram of entry 6 in table 1

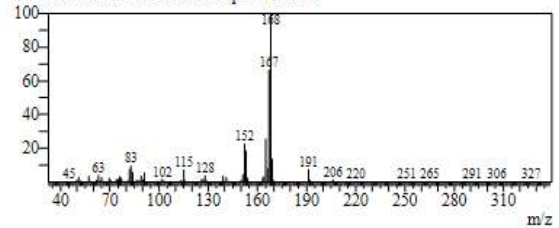
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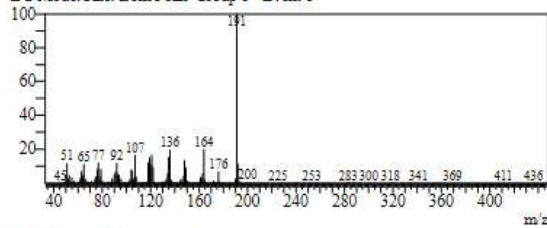
Line#:1 R.Time:10.720(Scan#:1145)  
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BG Mode:Calc. from Peak Group 1 - Event 1



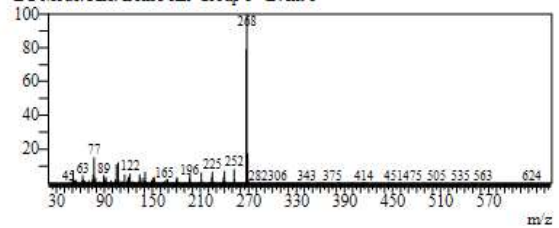
Line#:2 R.Time:10.830(Scan#:1167)  
MassPeaks:152  
RawMode:Averaged 10.825-10.835(1166-1168) BasePeak:168.05(5939495)  
BG Mode:Calc. from Peak Group 1 - Event 1



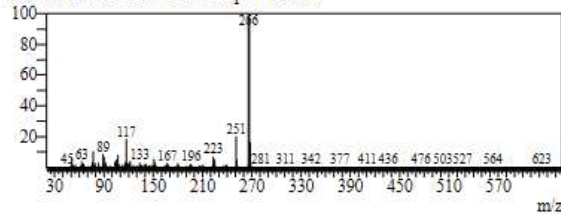
Line#:3 R.Time:14.835(Scan#:1968)  
MassPeaks:219  
RawMode:Averaged 14.830-14.840(1967-1969) BasePeak:190.95(3535176)  
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:4 R.Time:21.215(Scan#:3244)  
MassPeaks:355  
RawMode:Averaged 21.210-21.220(3243-3245) BasePeak:267.95(5081668)  
BG Mode:Calc. from Peak Group 1 - Event 1



Line#:5 R.Time:22.190(Scan#:3439)  
MassPeaks:323  
RawMode:Averaged 22.185-22.195(3438-3440) BasePeak:265.95(6114649)  
BG Mode:Calc. from Peak Group 1 - Event 1



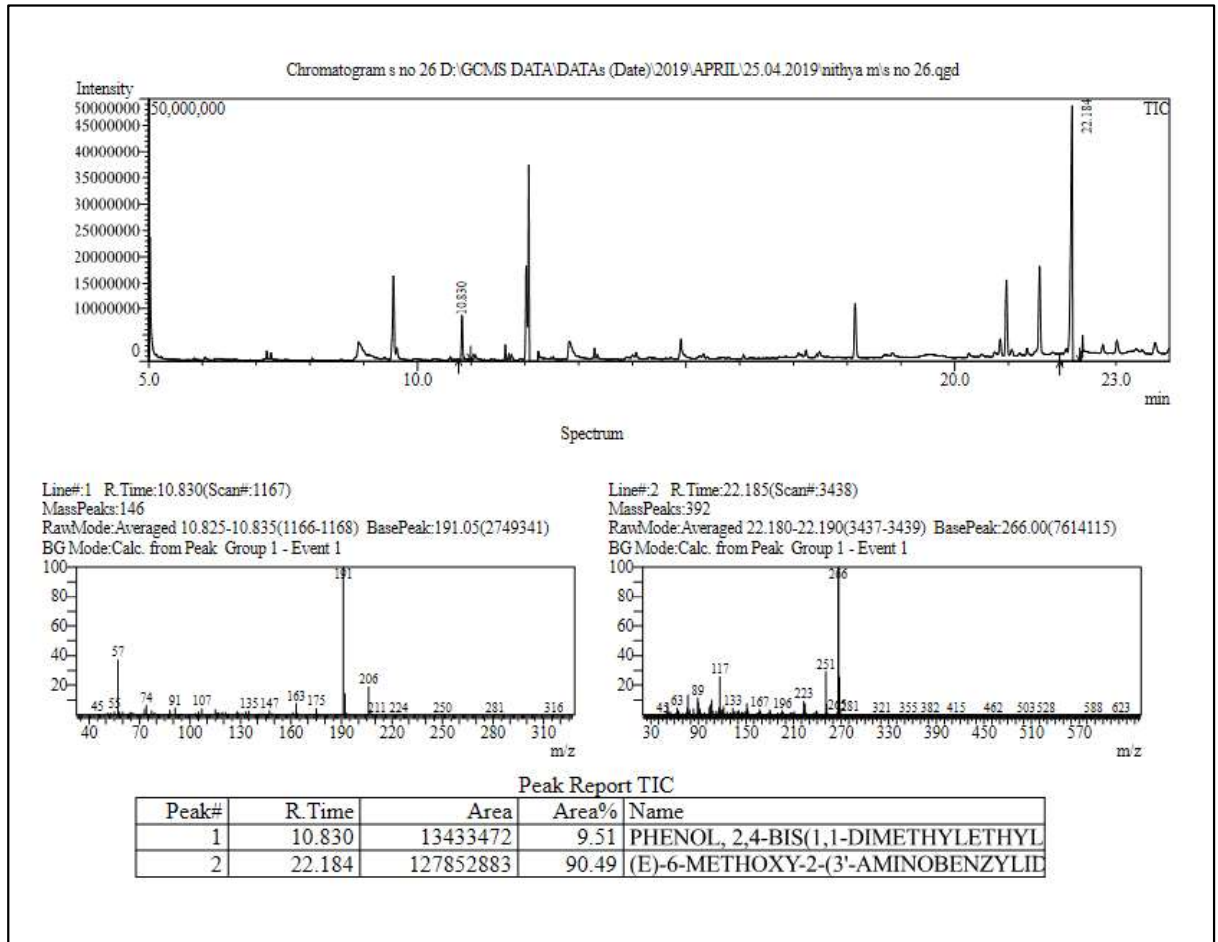
Peak Report TIC

Peak#	R.Time	Area	Area%	Name
1	10.722	48863415	16.03	1,1'-Biphenyl, 4-methyl-
2	10.830	40007743	13.13	1,1'-Biphenyl, 4-methyl-
3	14.836	72523074	23.79	N,N'-Ethylencbis(2-[2-hydroxyphenyl]glycin
4	21.213	62767858	20.59	4H-1-Benzopyran-4-one, 3-hydroxy-7-metho
5	22.190	80638448	26.46	(E)-6-METHOXY-2-(3'-AMINO BENZYL)IE

GC-

GC-MS chromatogram of entry 7 table 1

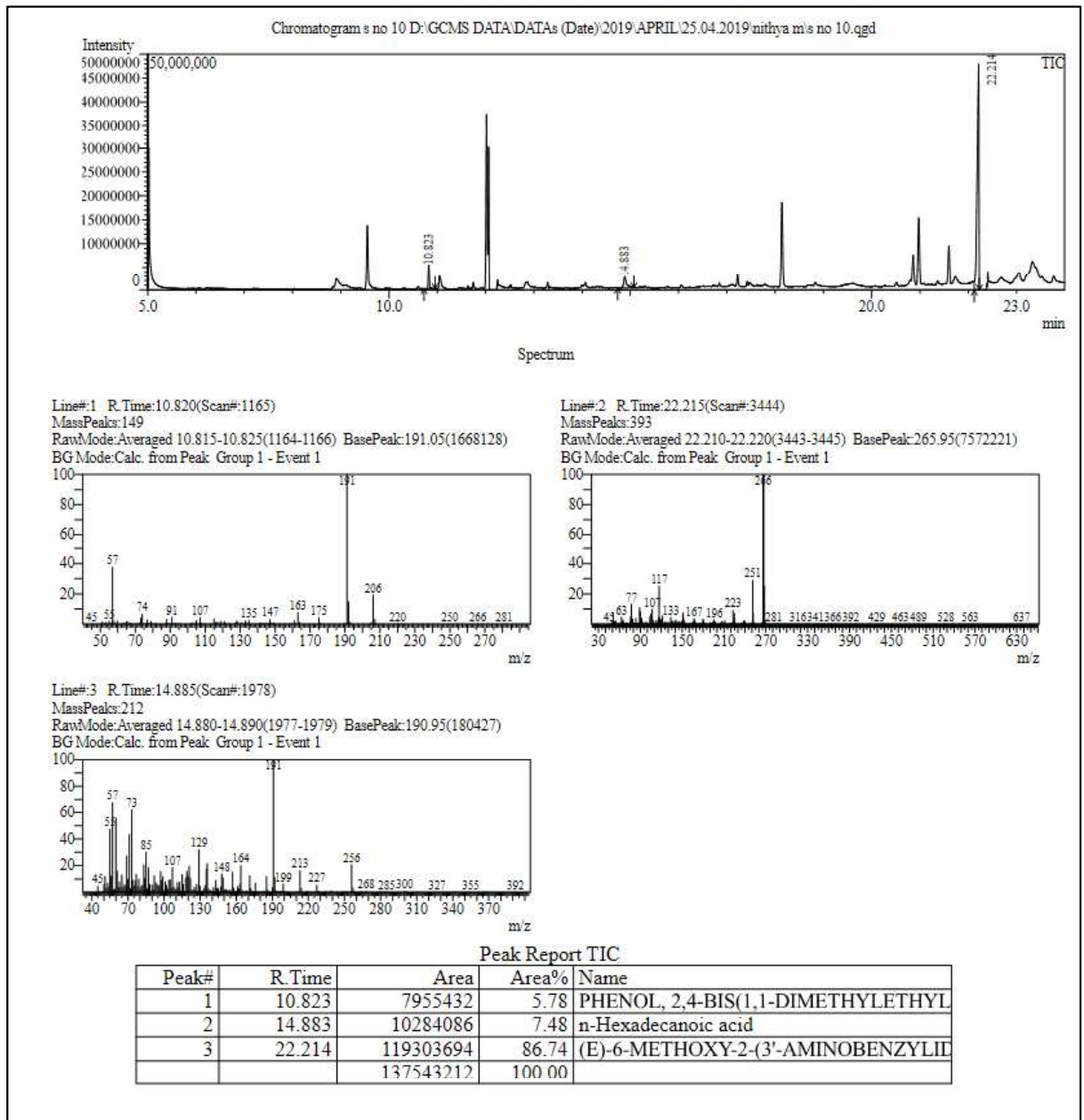
## Supporting information



GC-MS chromatogram of entry 8 in table 1



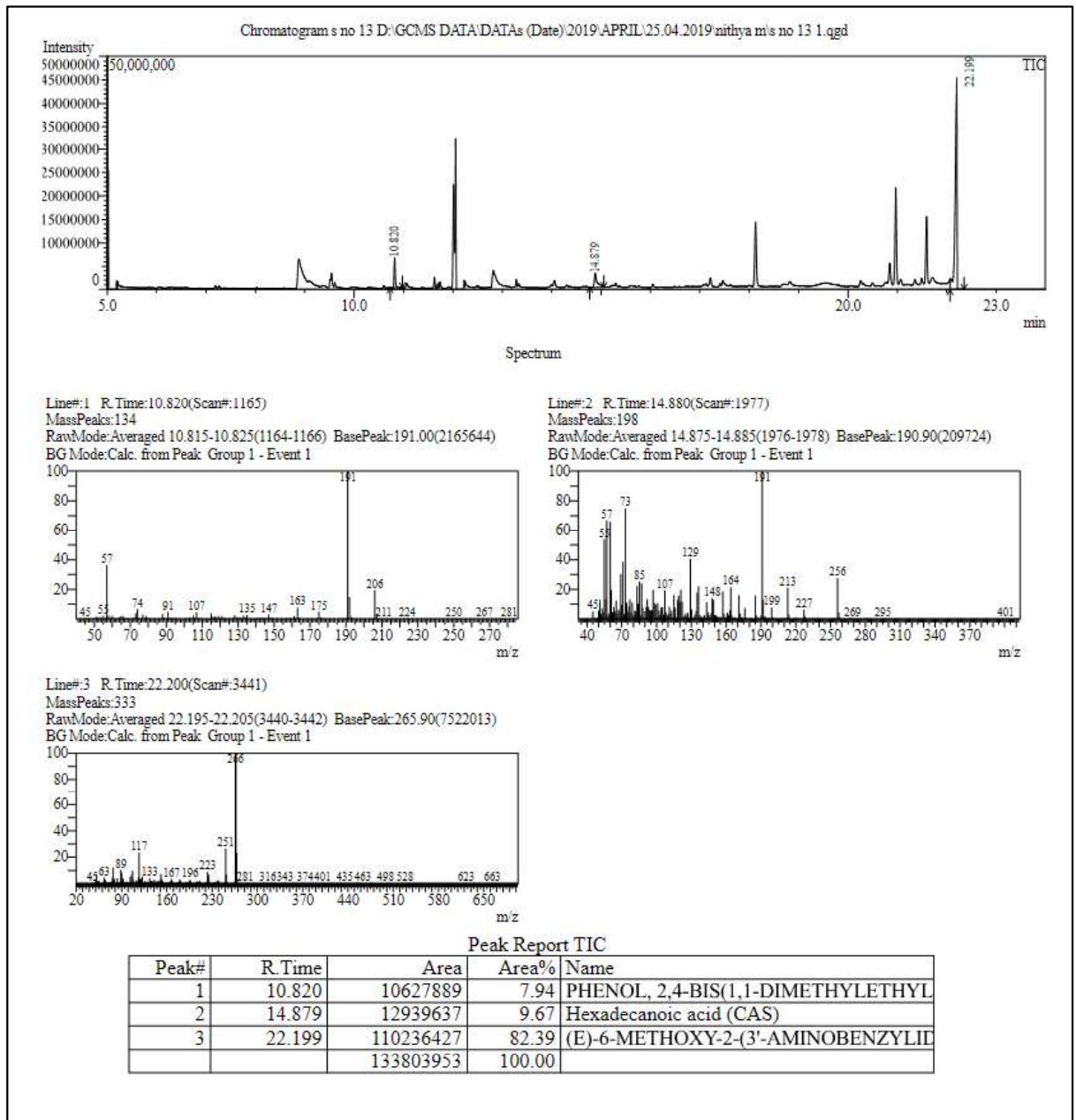
## Supporting information



GC-MS chromatogram of entry 9 in table 1

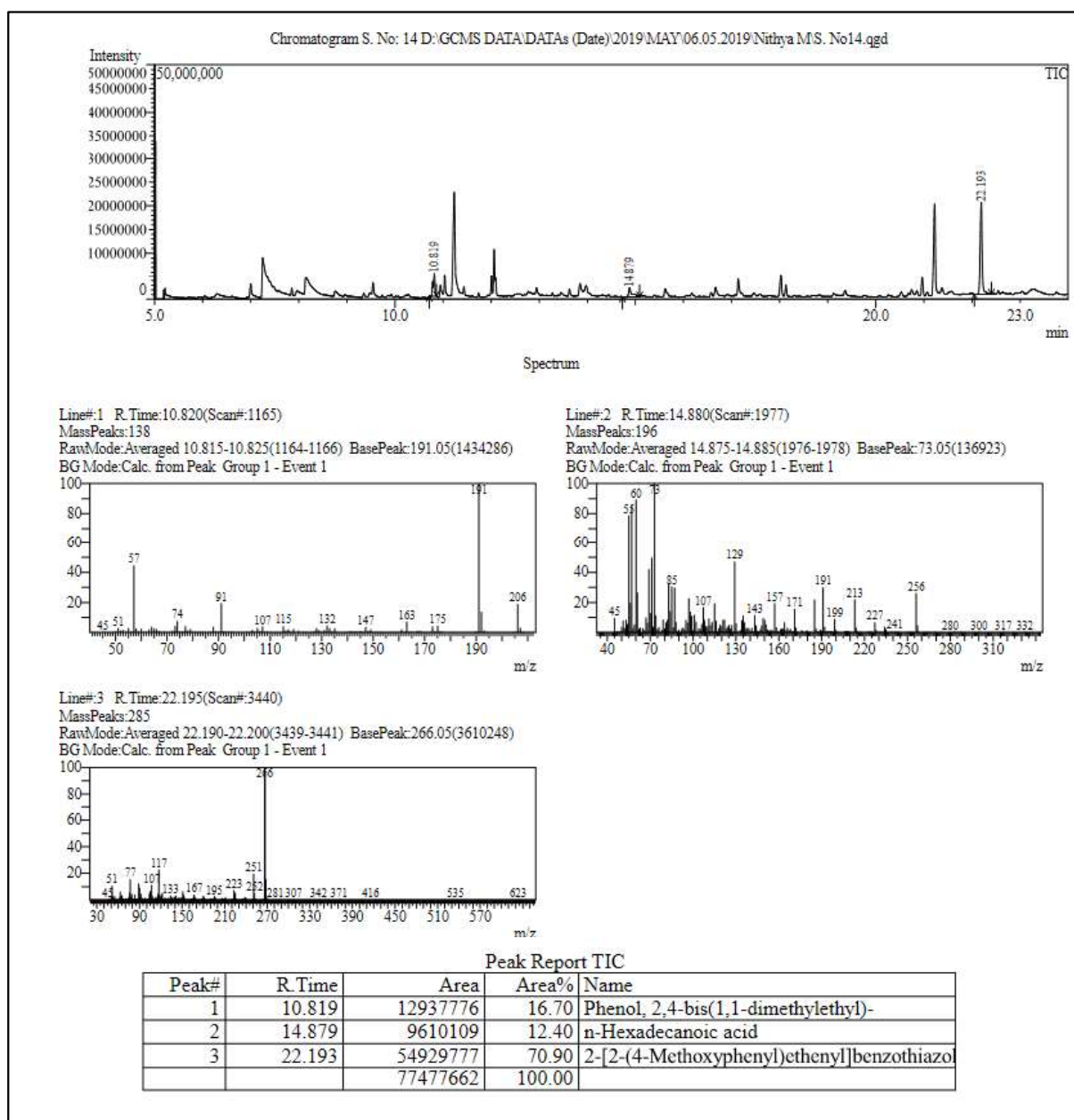


## Supporting information



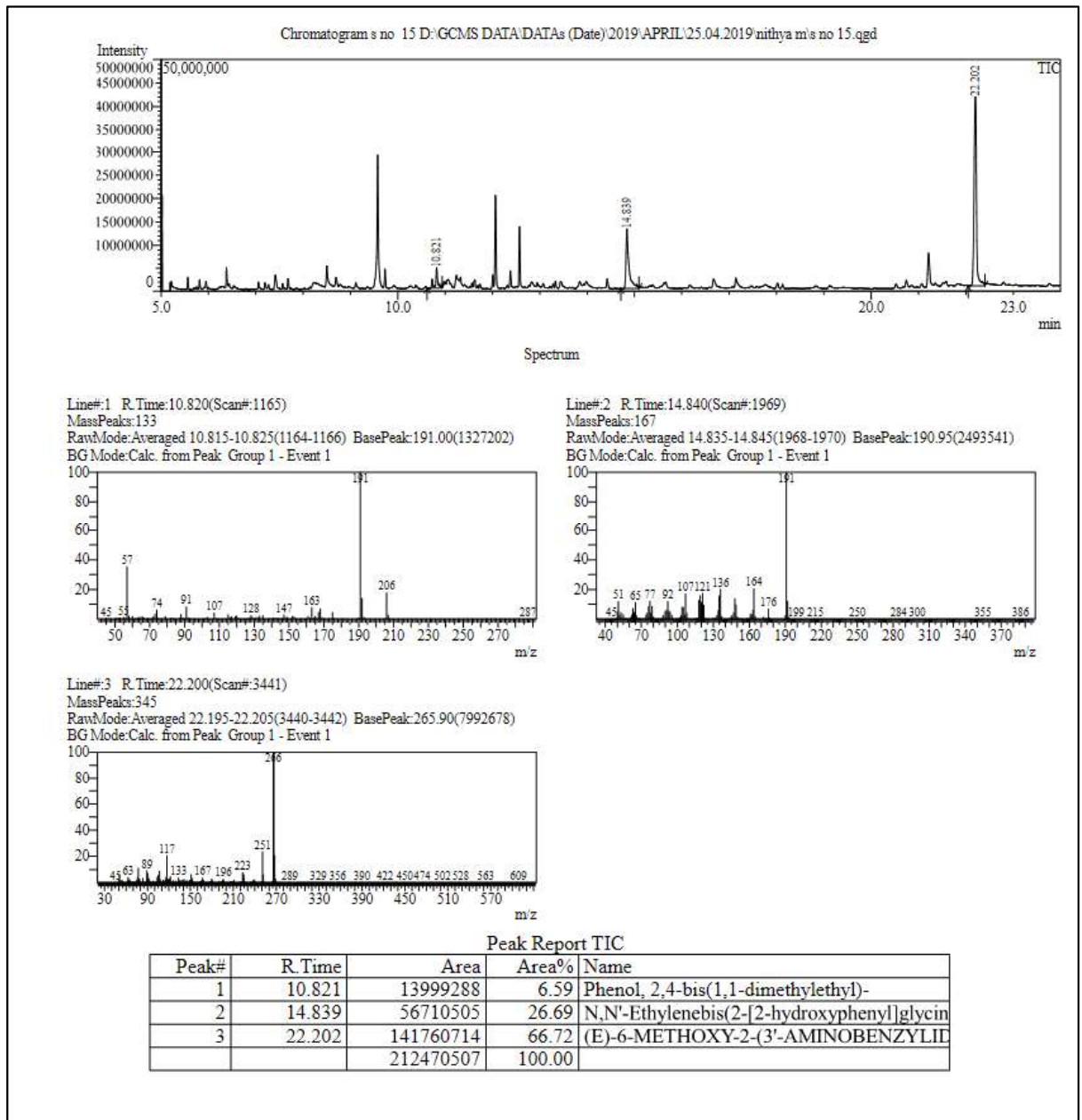
GC-MS chromatogram of entry 10 in table 1

## Supporting information



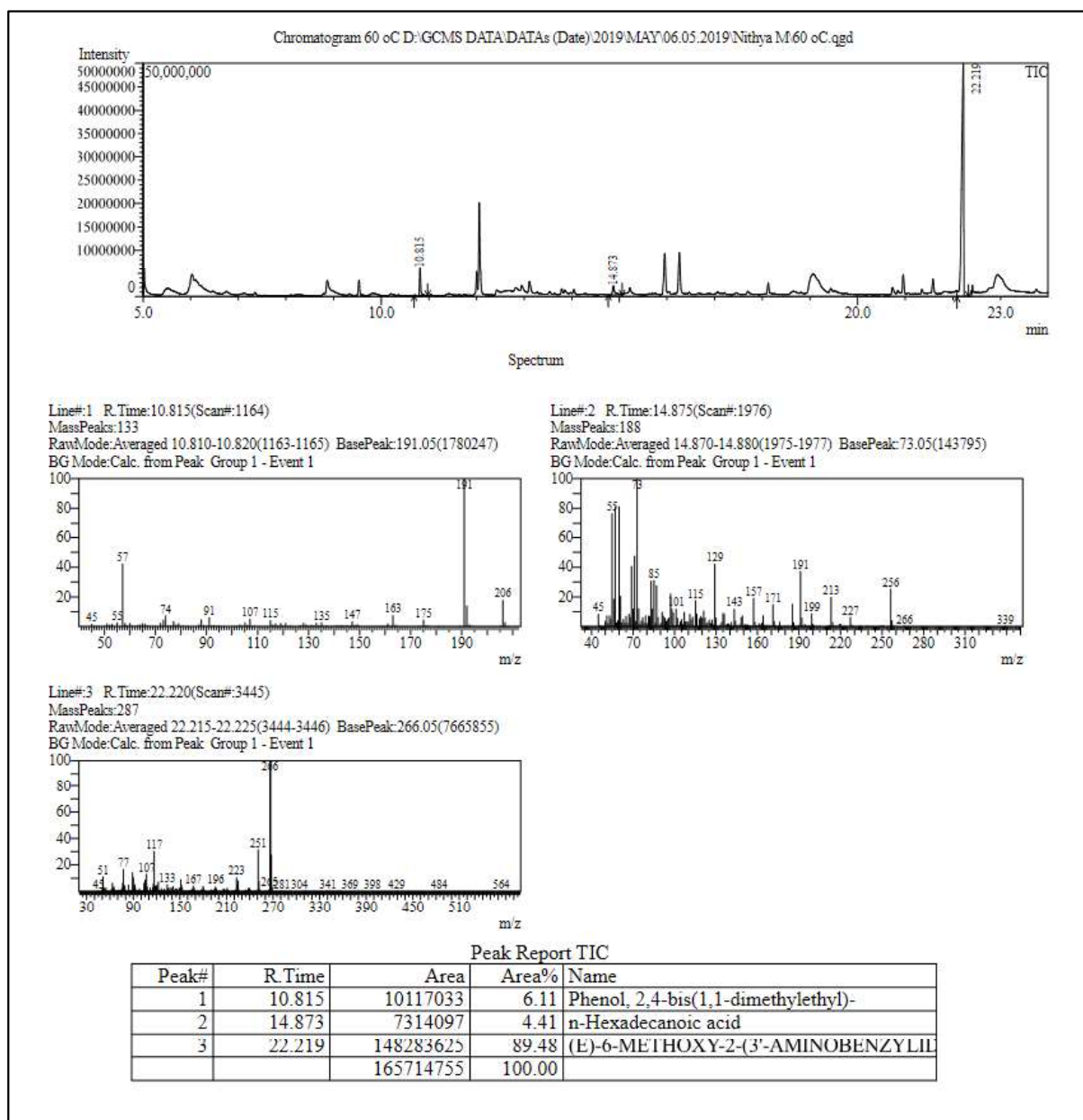
GC-MS chromatogram of entry 11 in table 1

## Supporting information



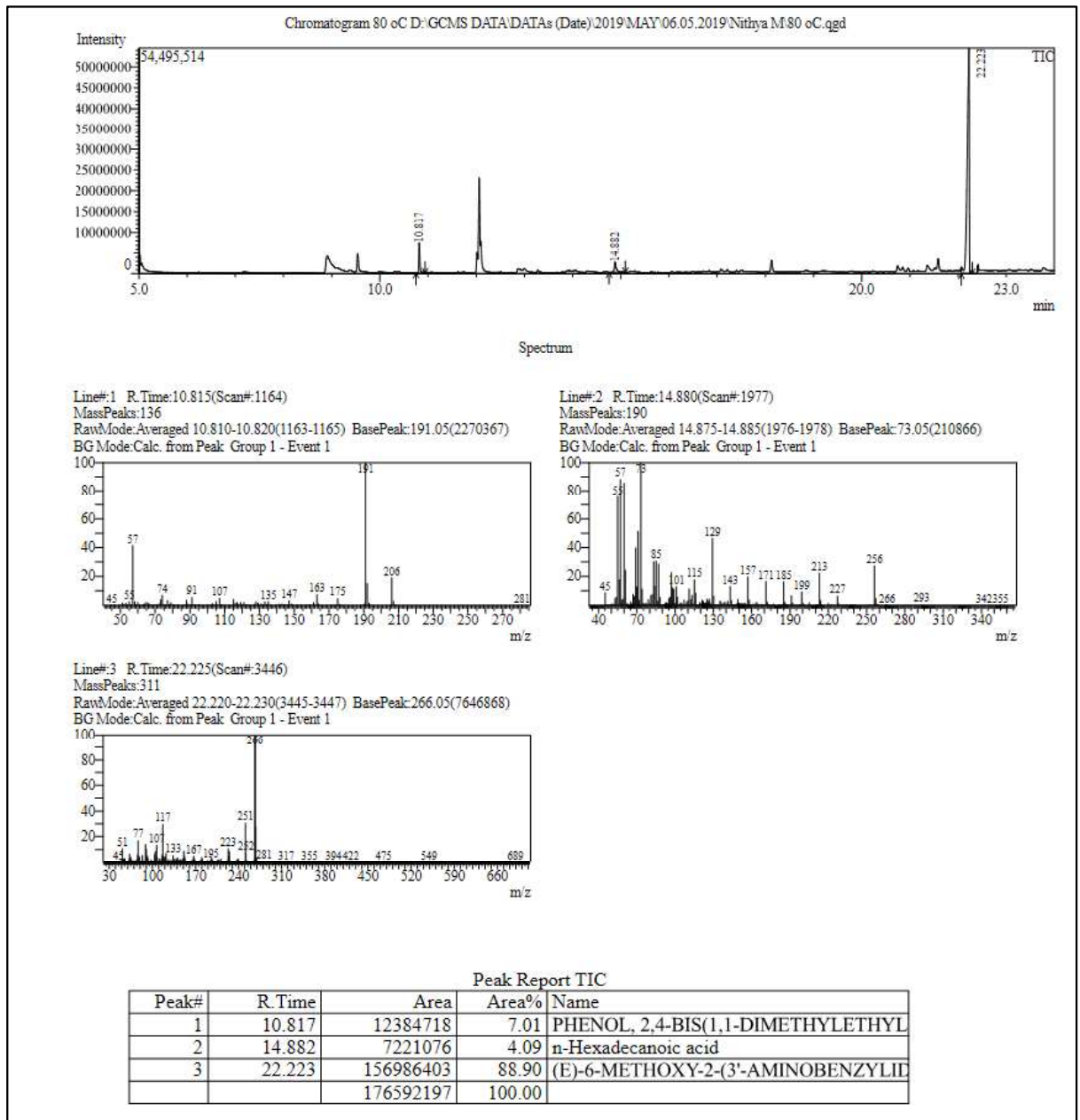
GC-MS chromatogram of entry 12 in table 1

## Supporting information



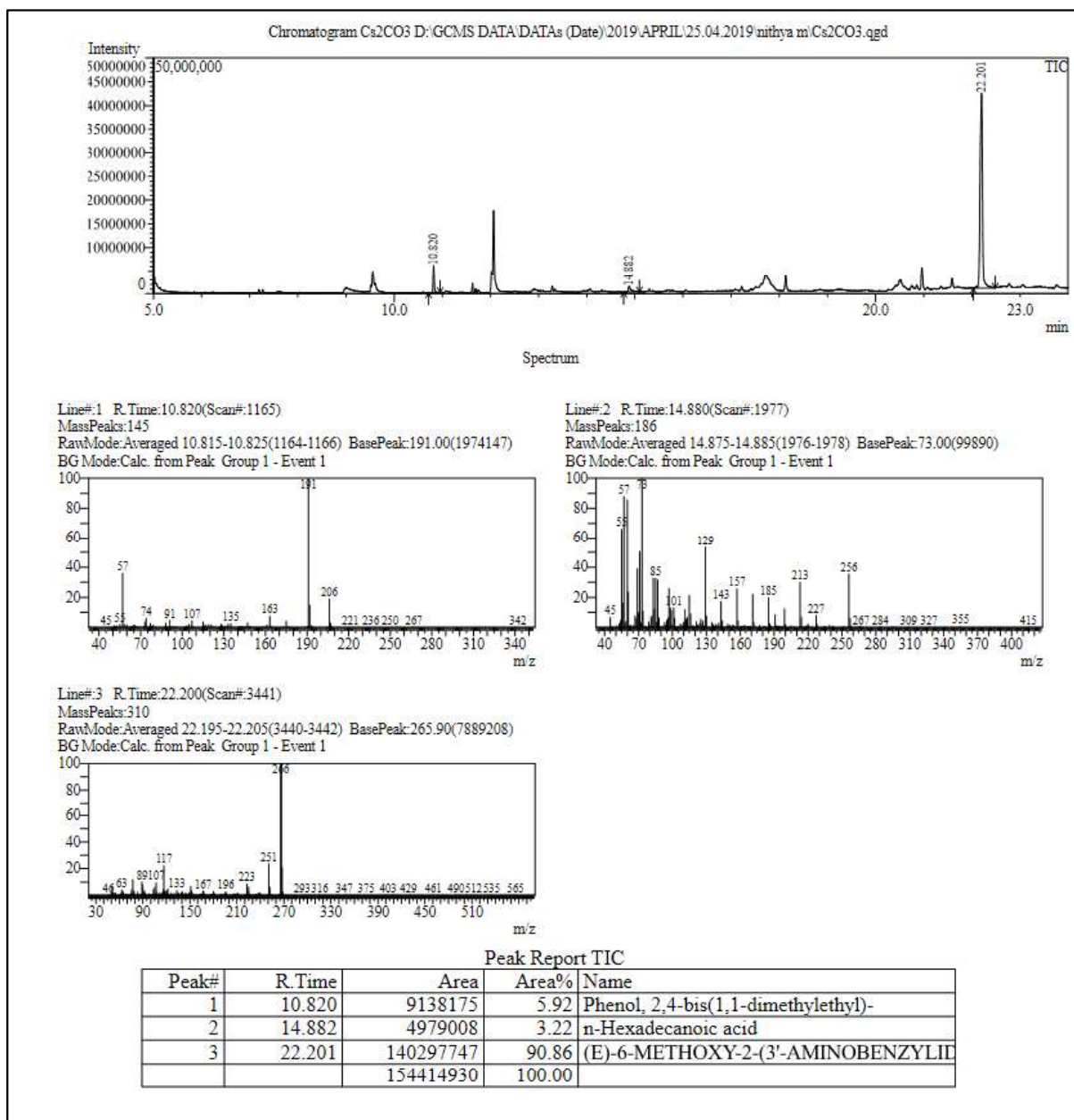
GC-MS chromatogram of entry 13 in table 1

## Supporting information



GC-MS chromatogram of entry 14 in table 1

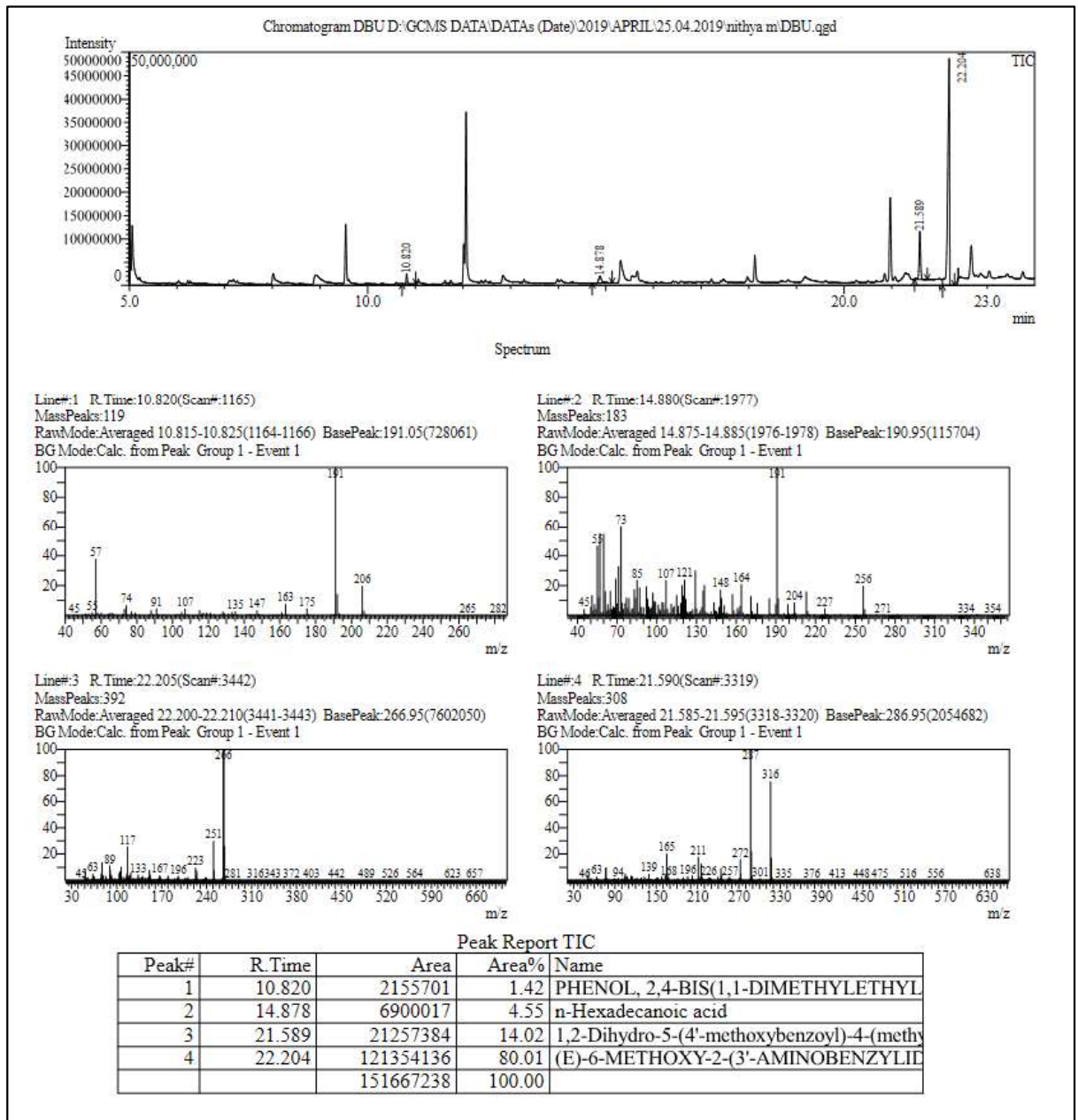
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GC-MS chromatogram of entry 15 in table 1

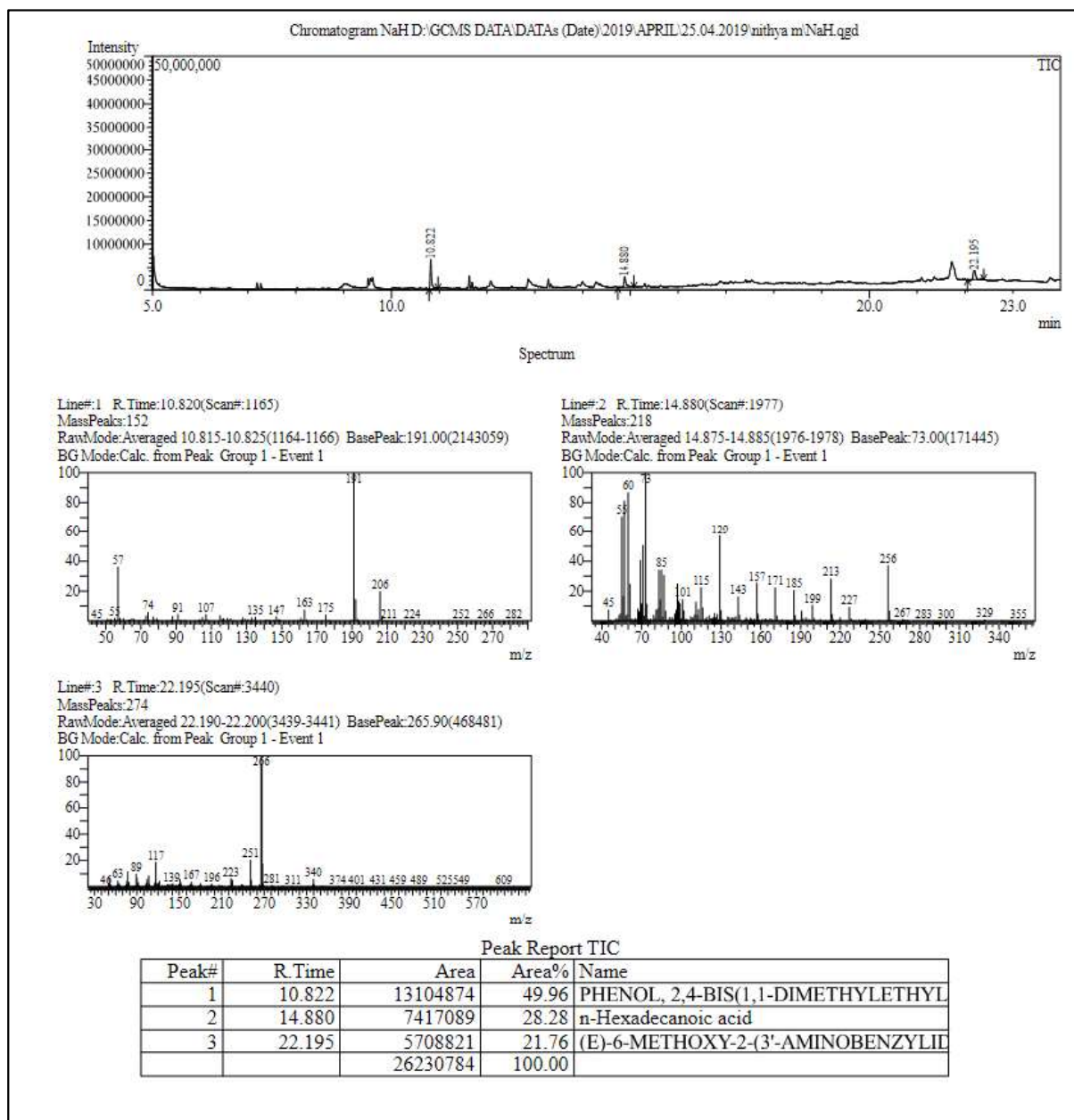


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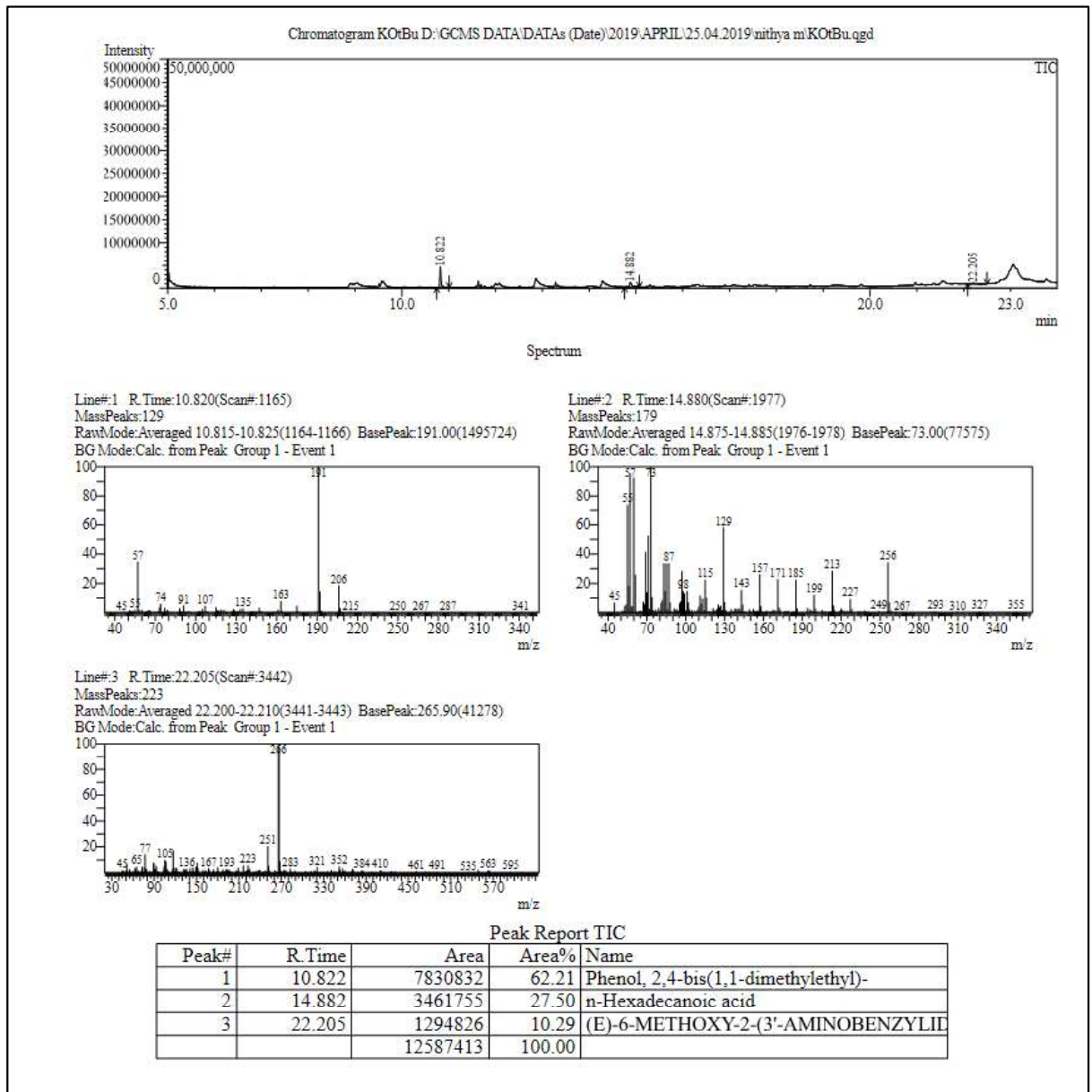
GC-MS chromatogram of entry 16 in table 1

## Supporting information



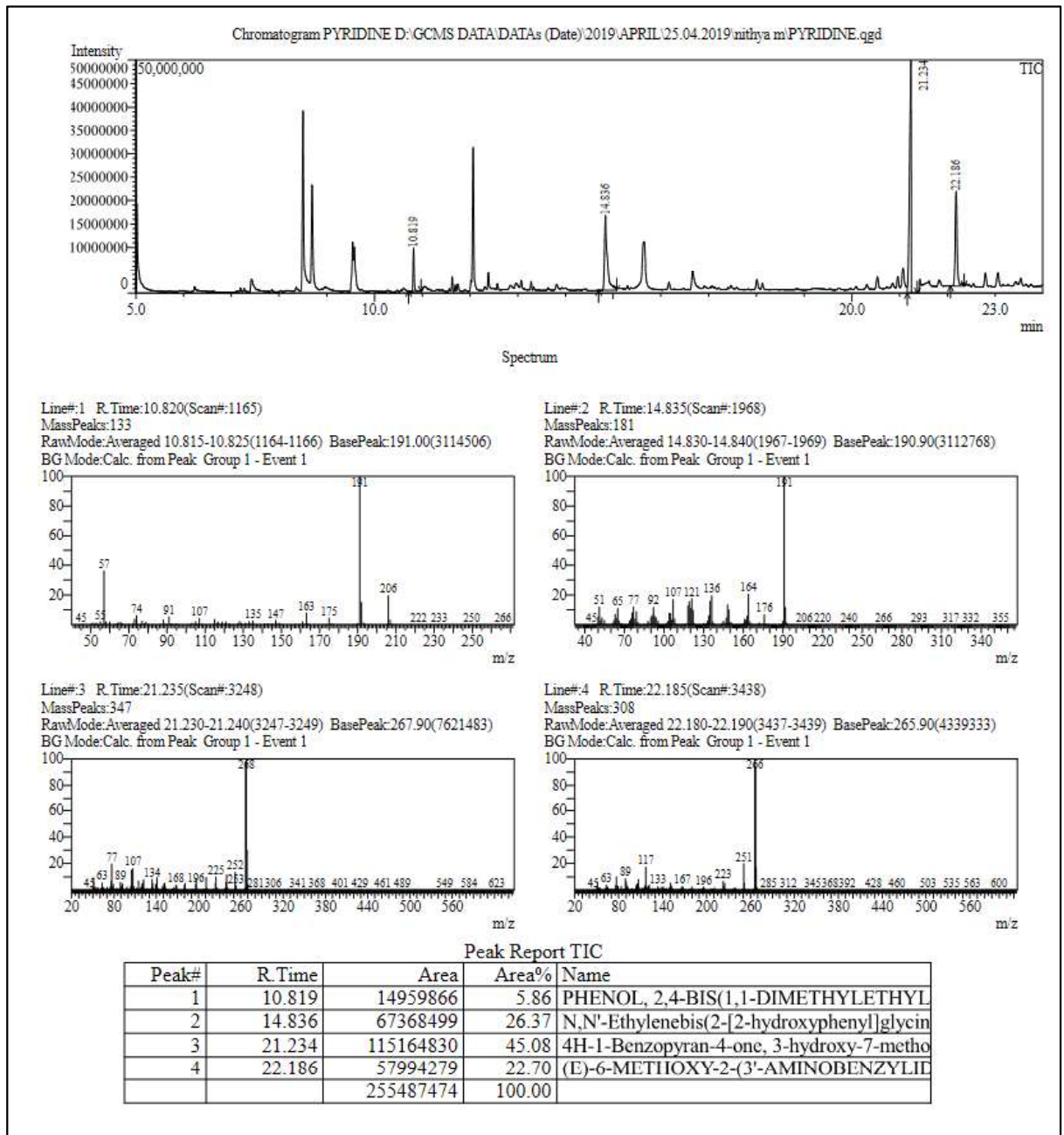
GC-MS chromatogram of entry 17 in table 1

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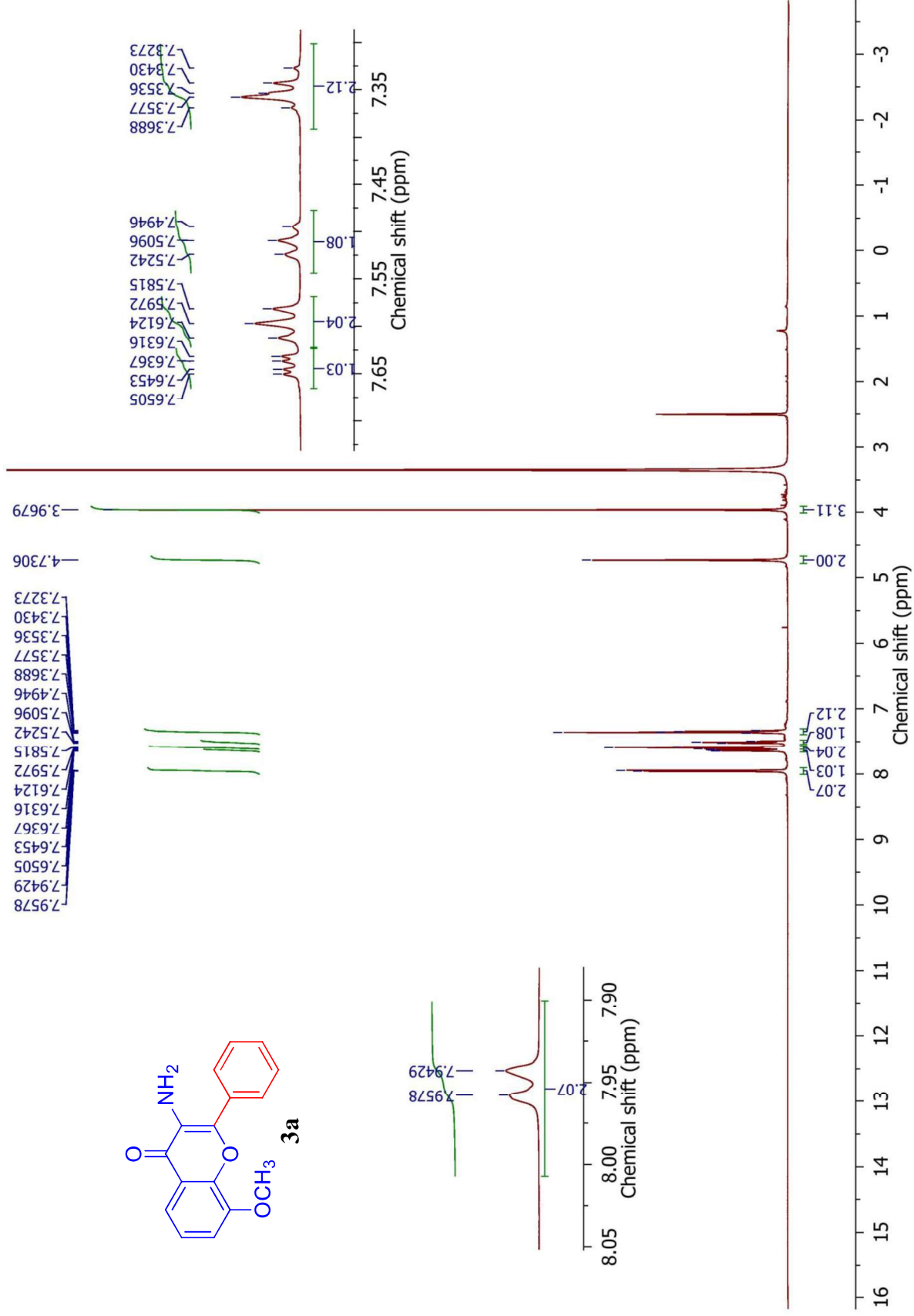
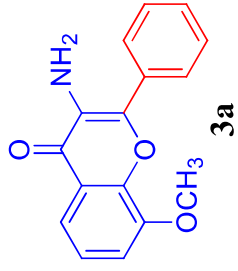


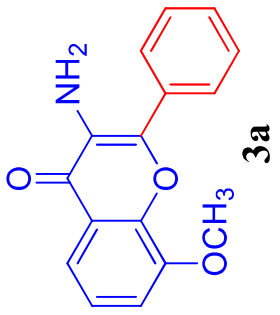
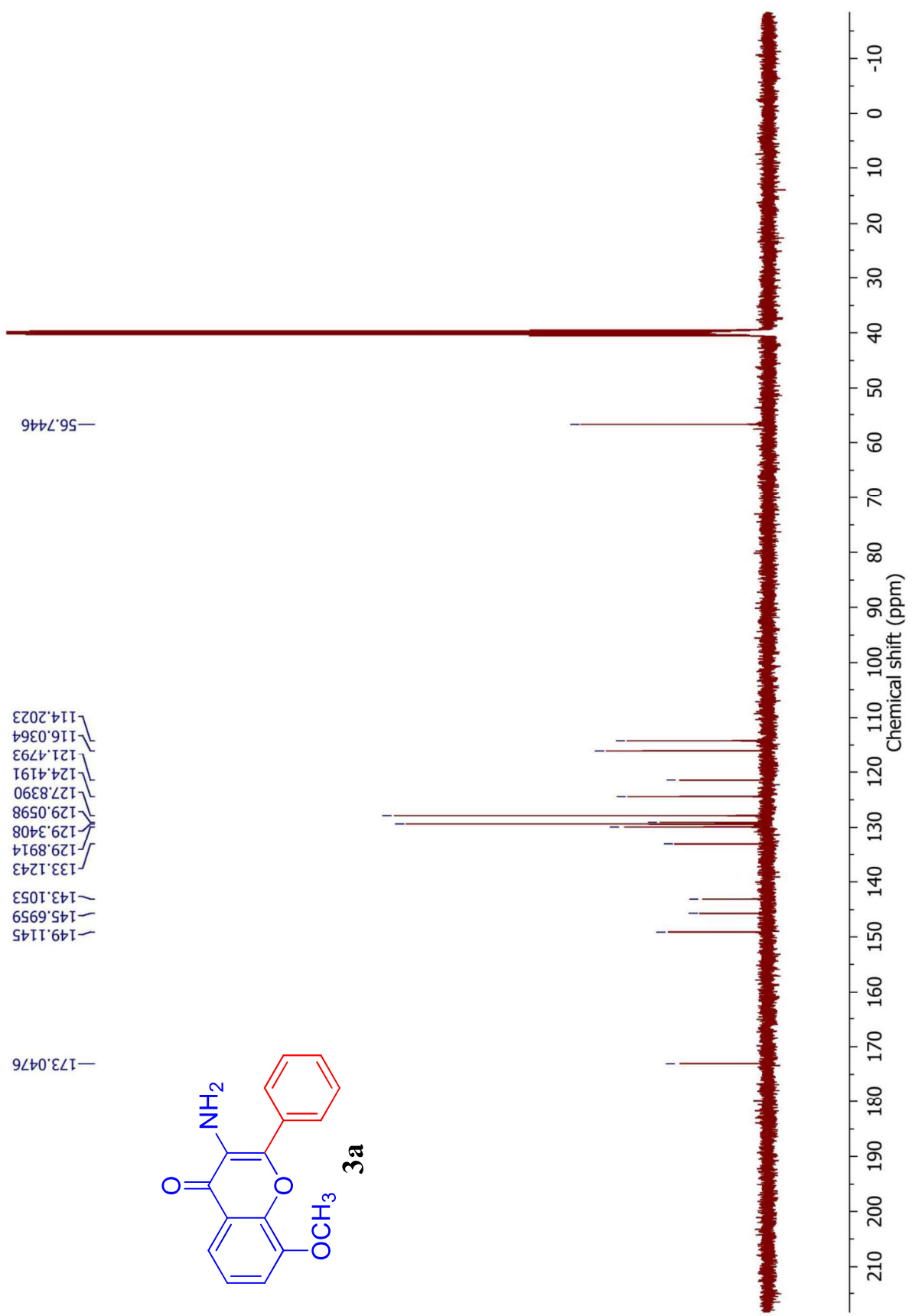
GC-MS chromatogram of entry 18 in table 1

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GC-MS chromatogram of entry 19 in table 1



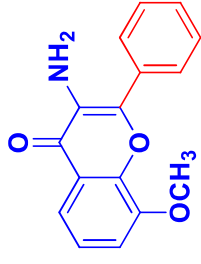




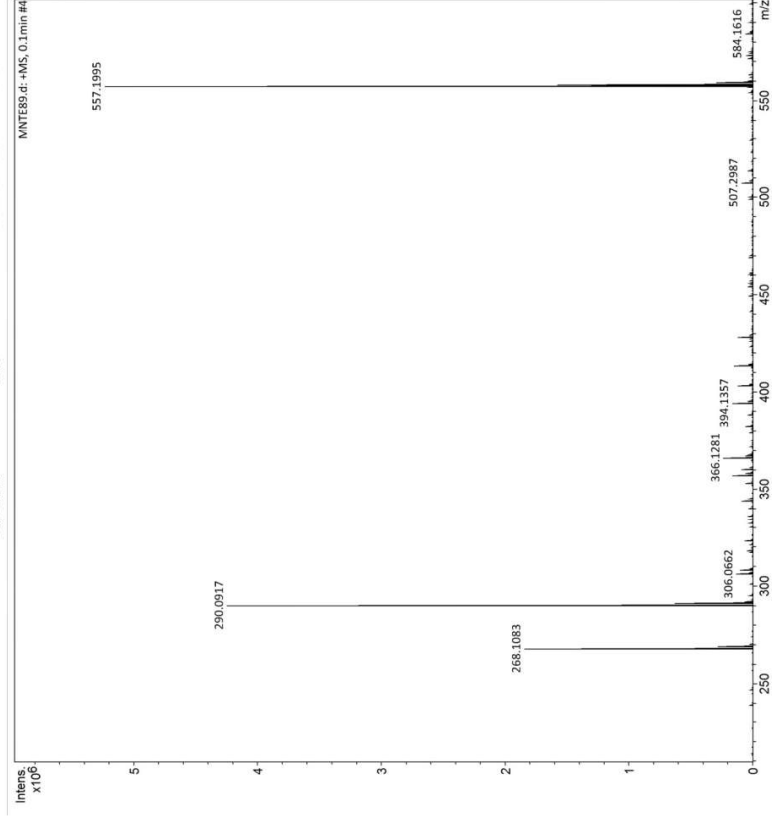
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Comment  
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Operator HRMS  
Instrument maxis impact 1819696.00160

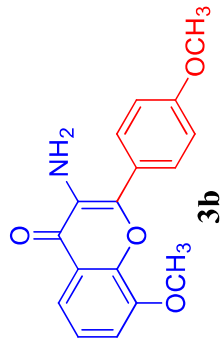
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Set End Plate Offset -500 V  
Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.5 Bar  
Set Dry Gas 200 °C  
Set Divert Valve 4.0 l/min  
Set APCI Heater 0 °C



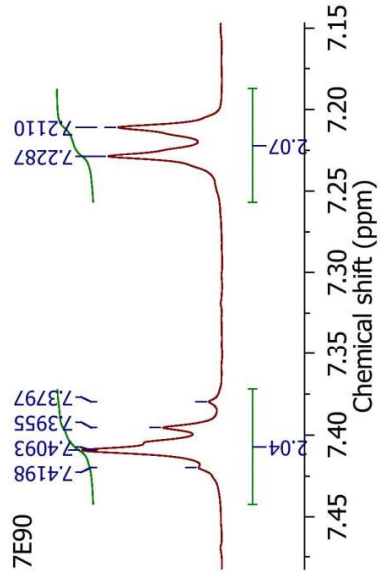
3a



7E90

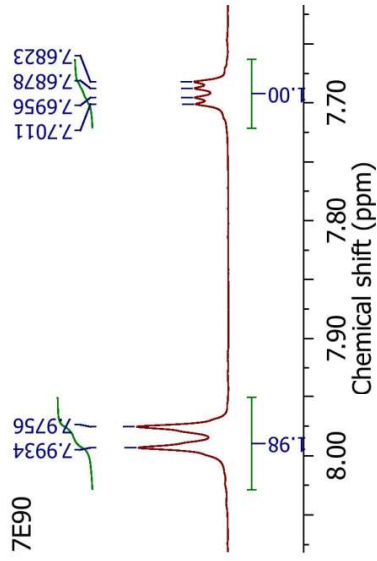


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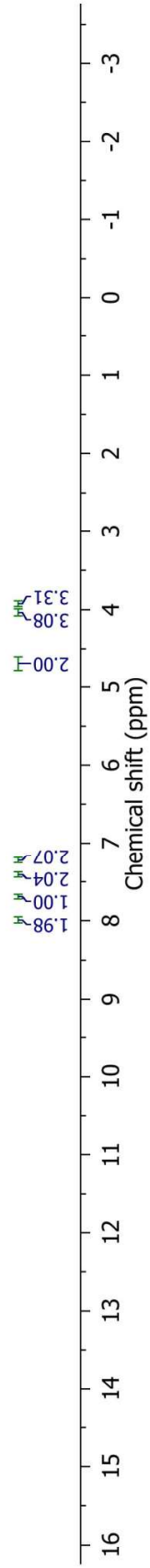


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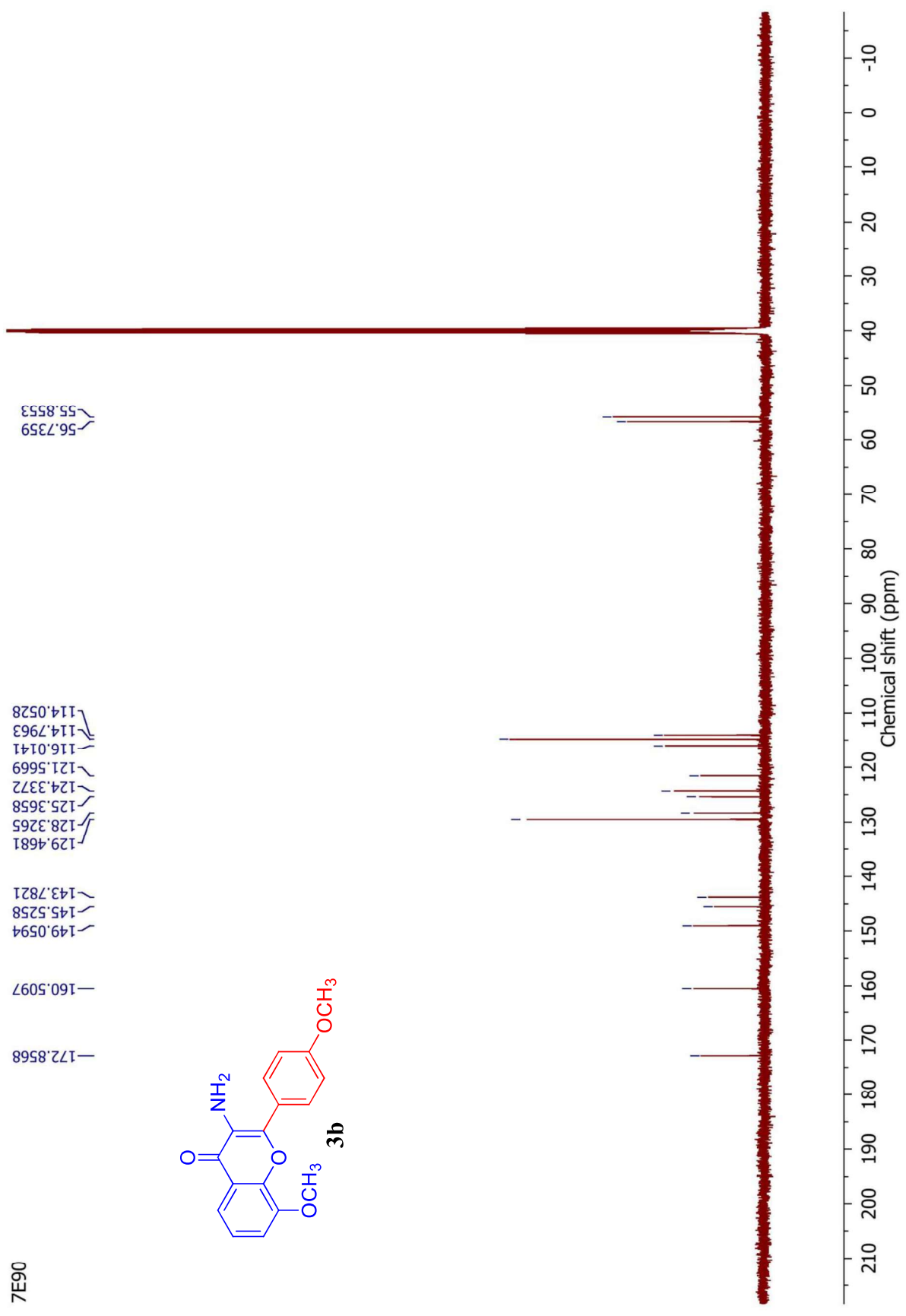


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Chemical shift (ppm)

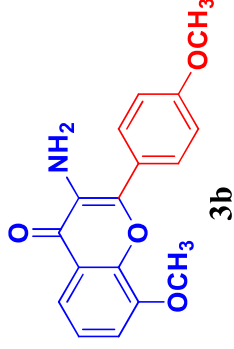
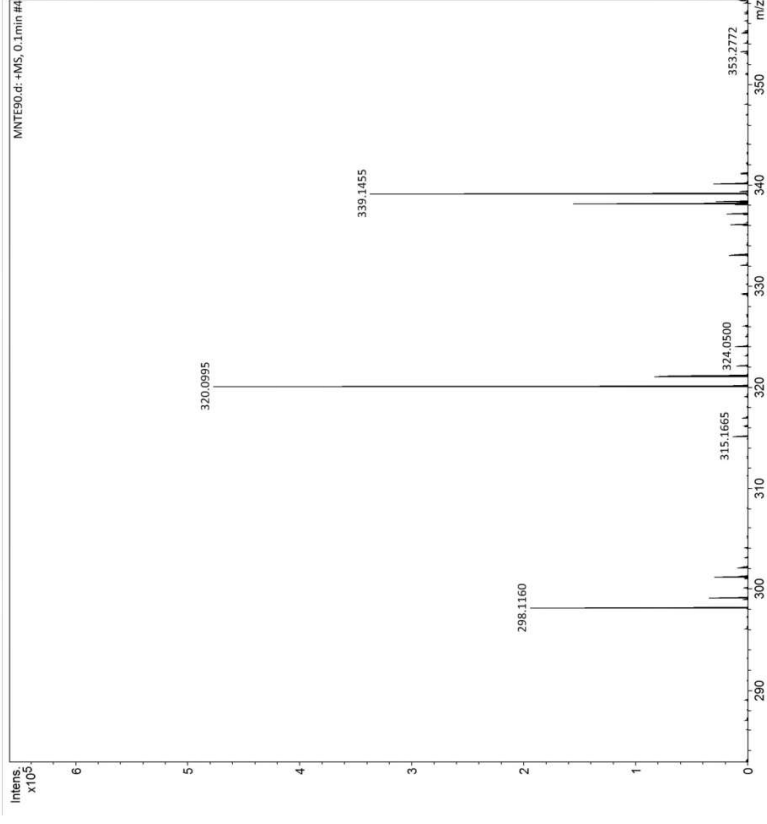


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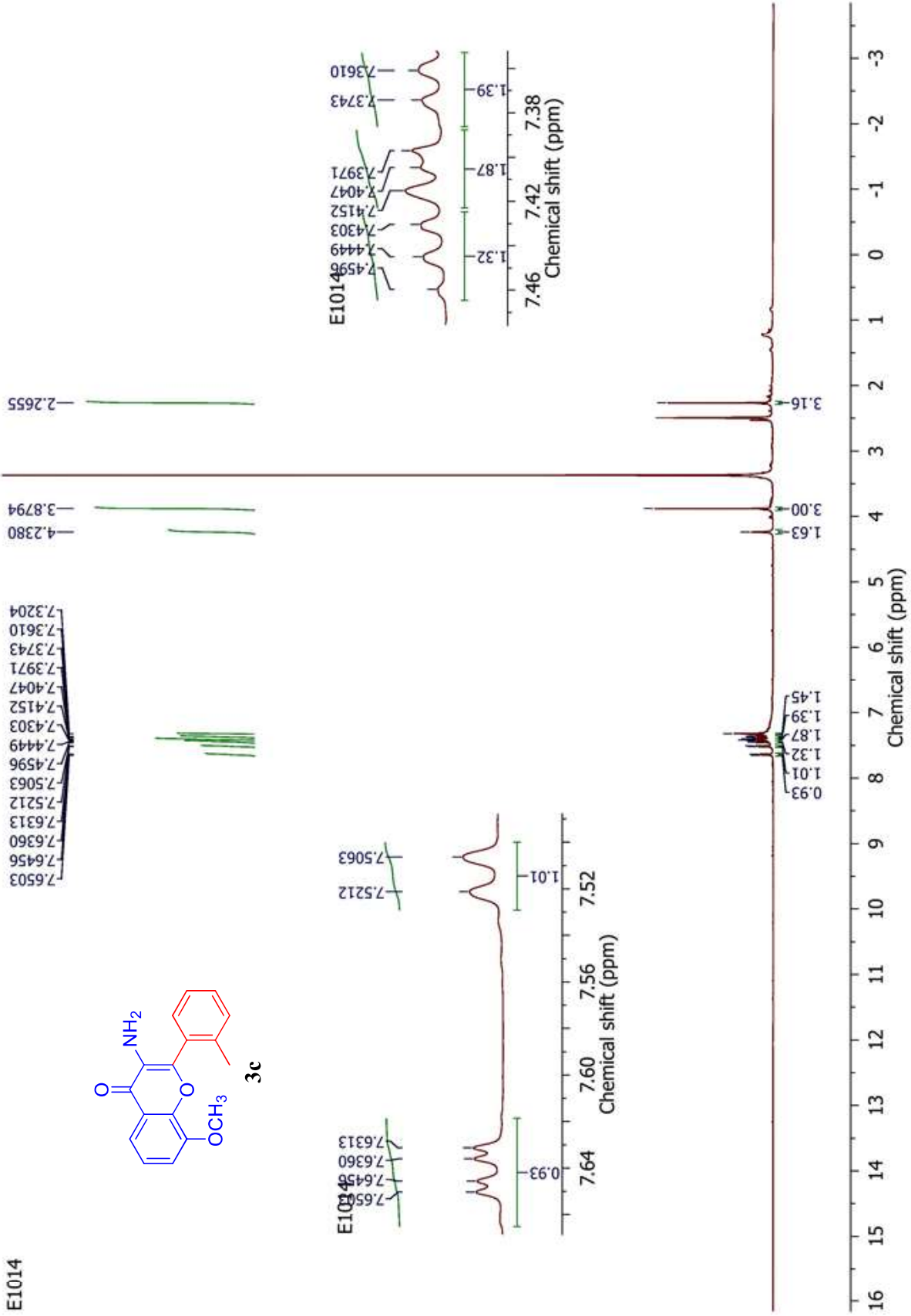
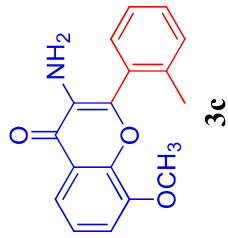
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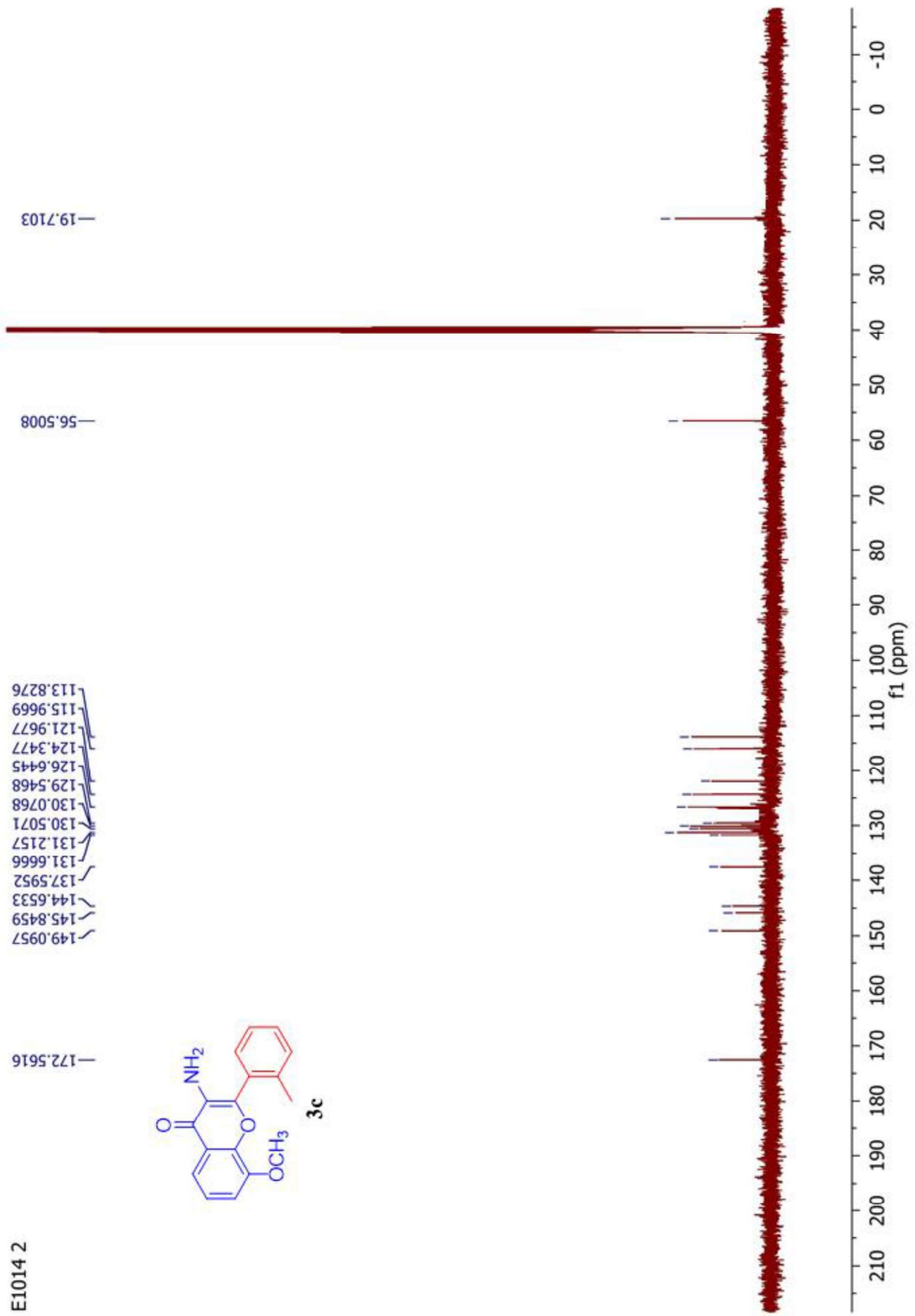
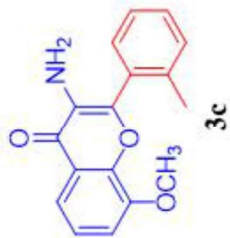
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Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.5 Bar  
Set Dry Gas Heater 200 °C  
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Set Divert Valve Source  
Set APCI Heater 0 °C



E1014

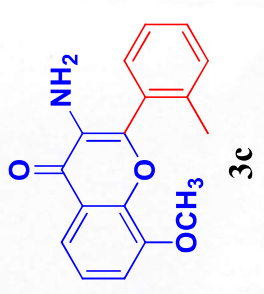
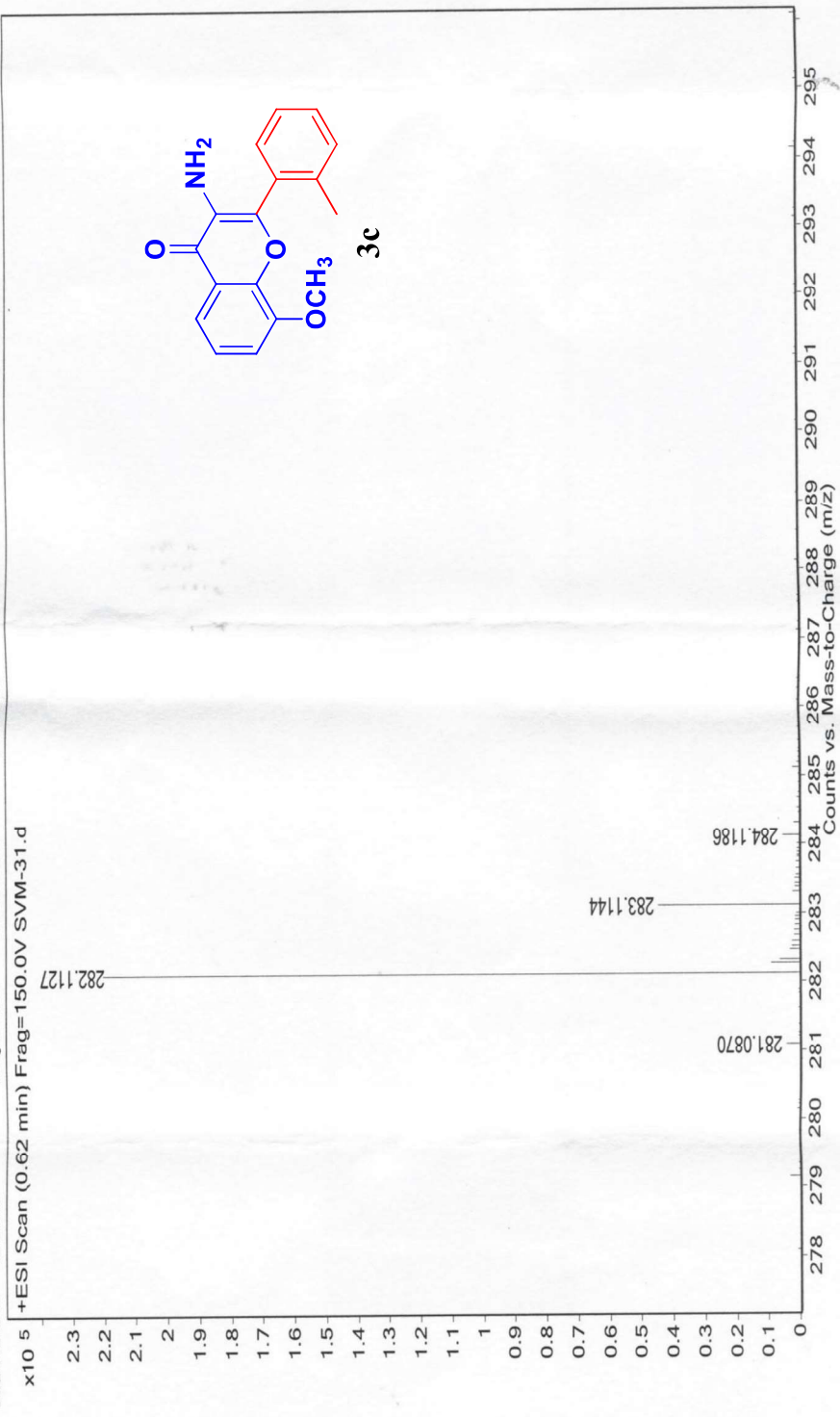


E1014 2

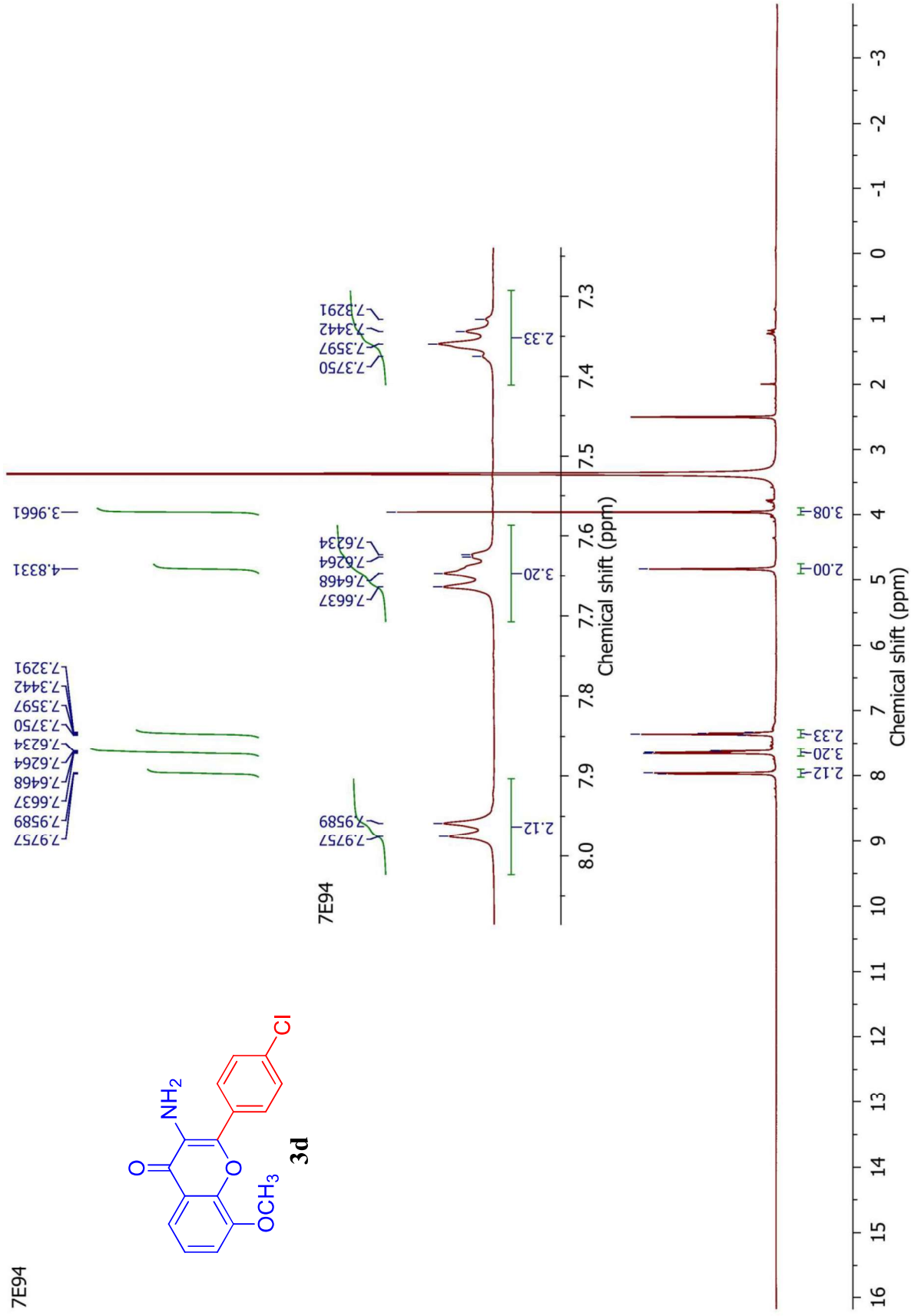
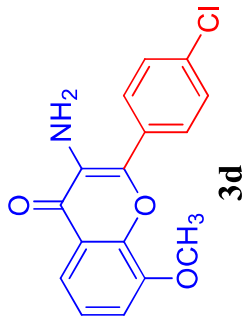




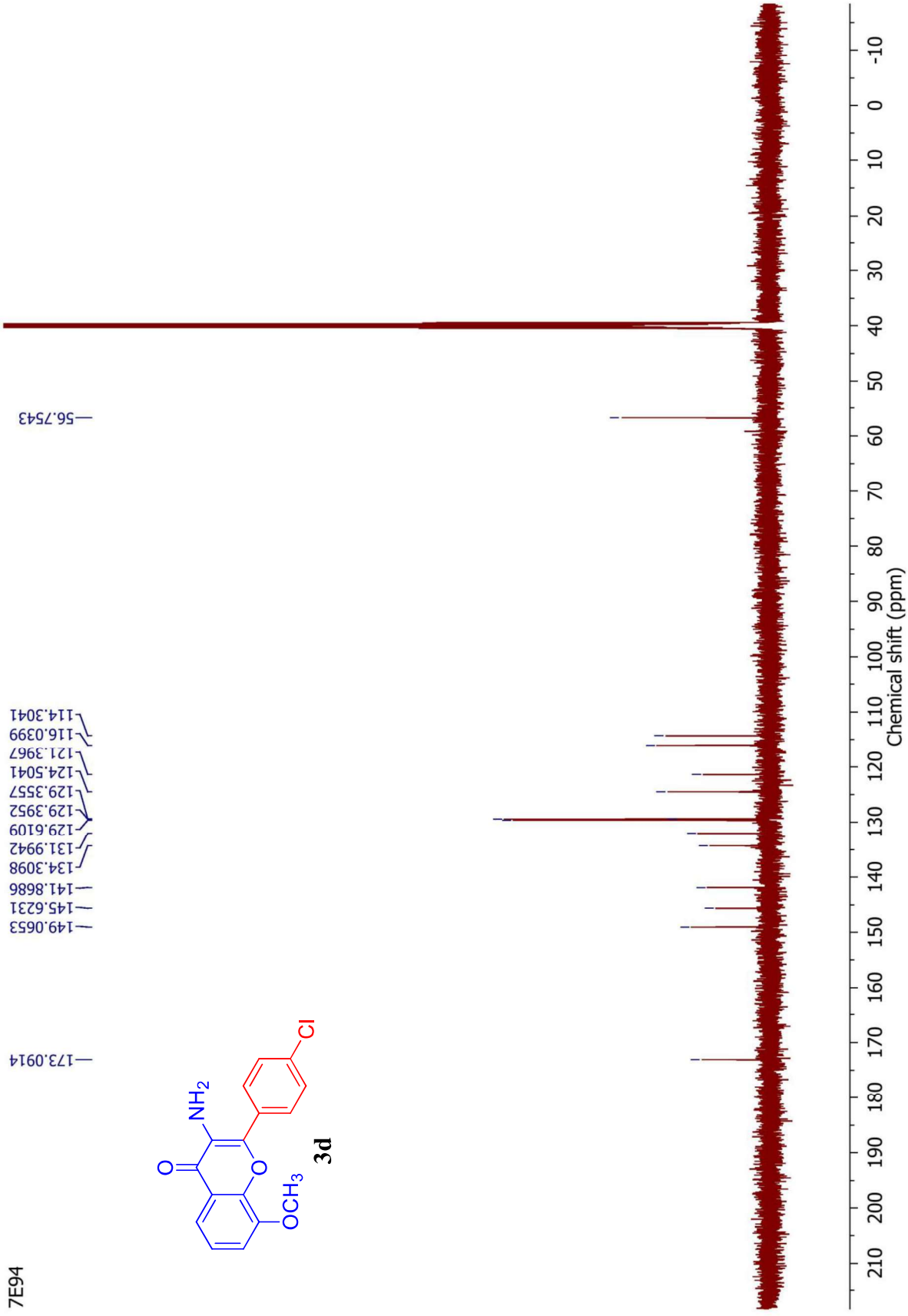
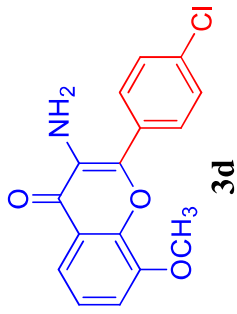
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7E94



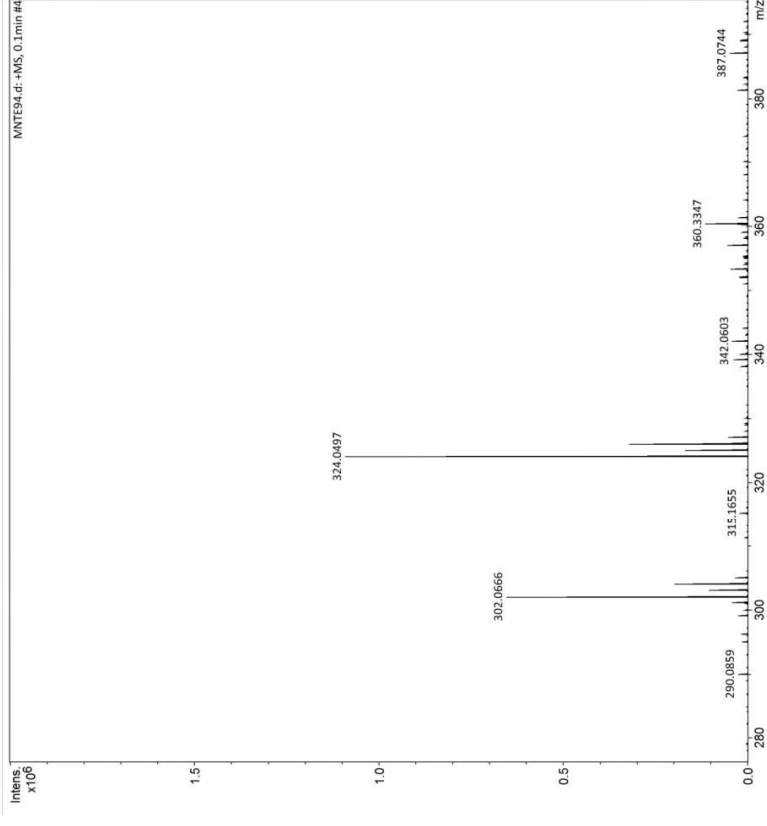
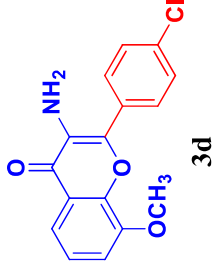
7E94



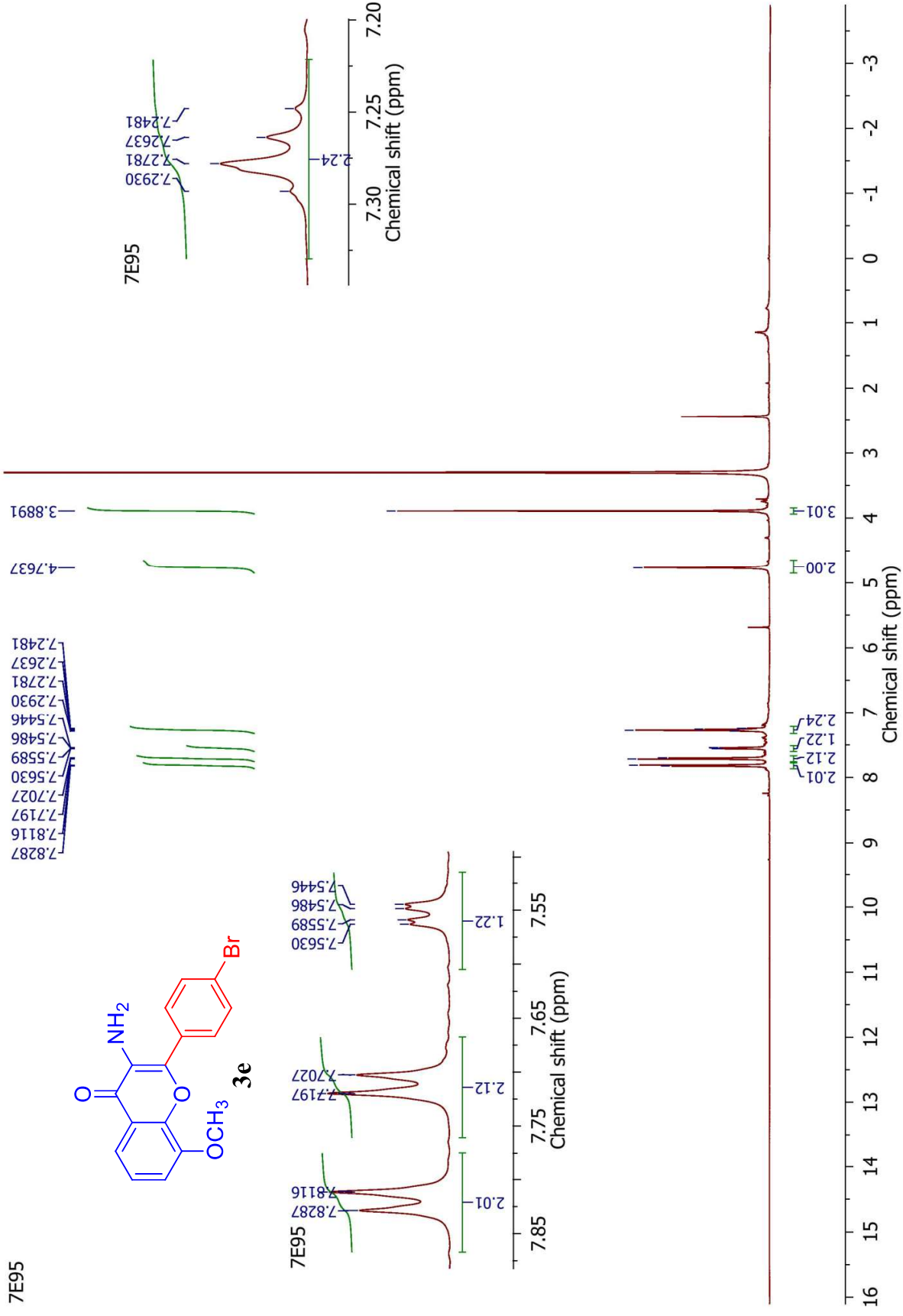
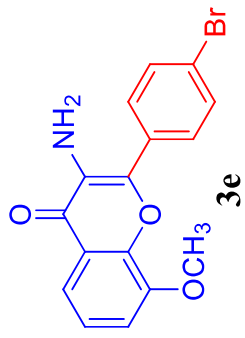
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Operator HRMS  
Instrument maxis impact 1819696.00160

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Set End Plate Offset -500 V  
Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.5 Bar  
Set Dry Gas Heater 200 °C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Source  
Set APCI Heater 0 °C

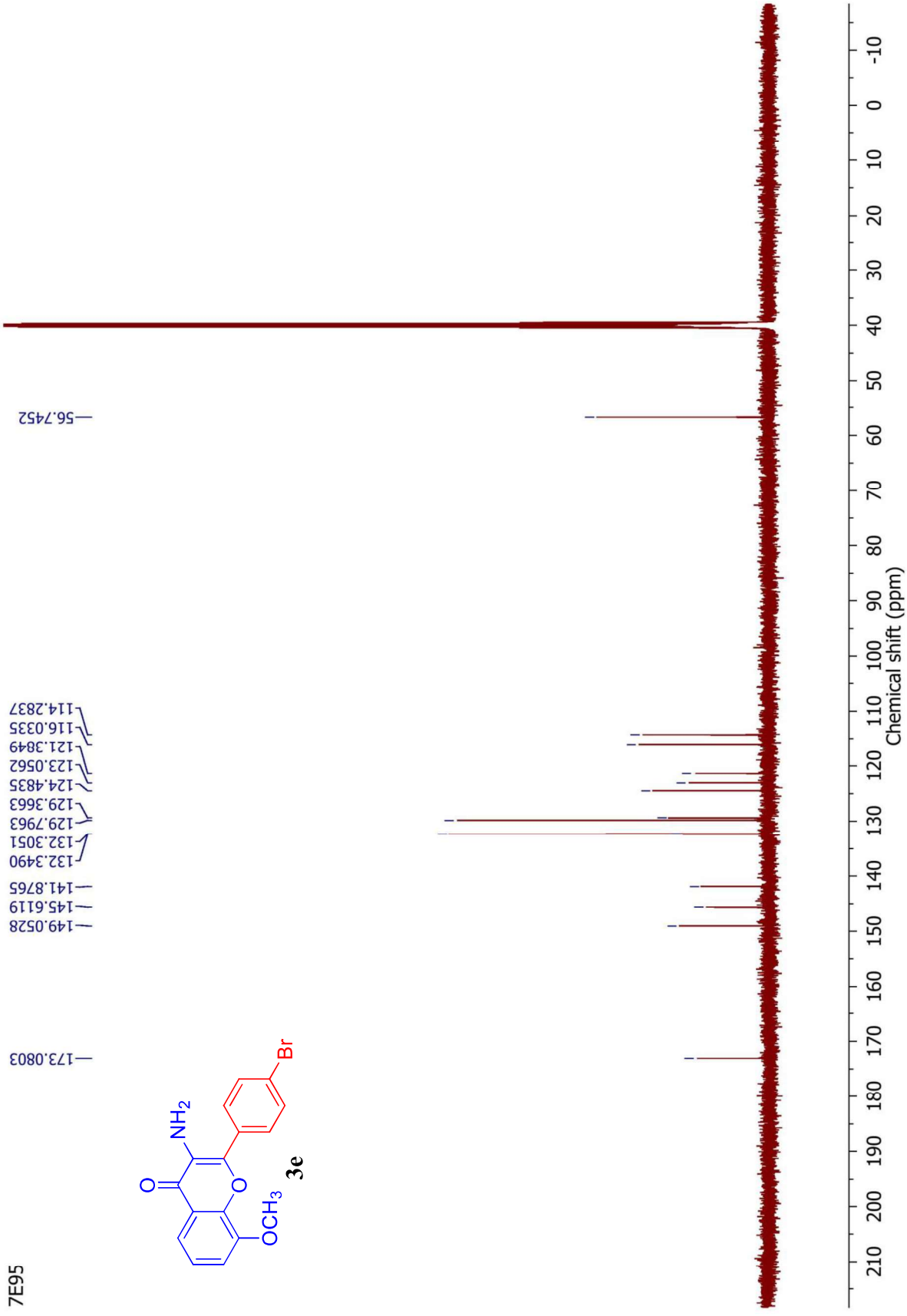
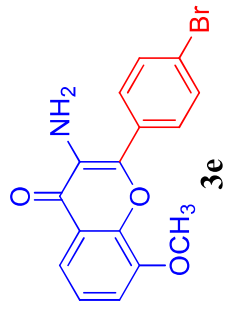


7E95





7E95



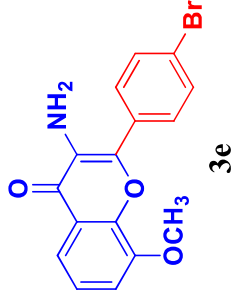
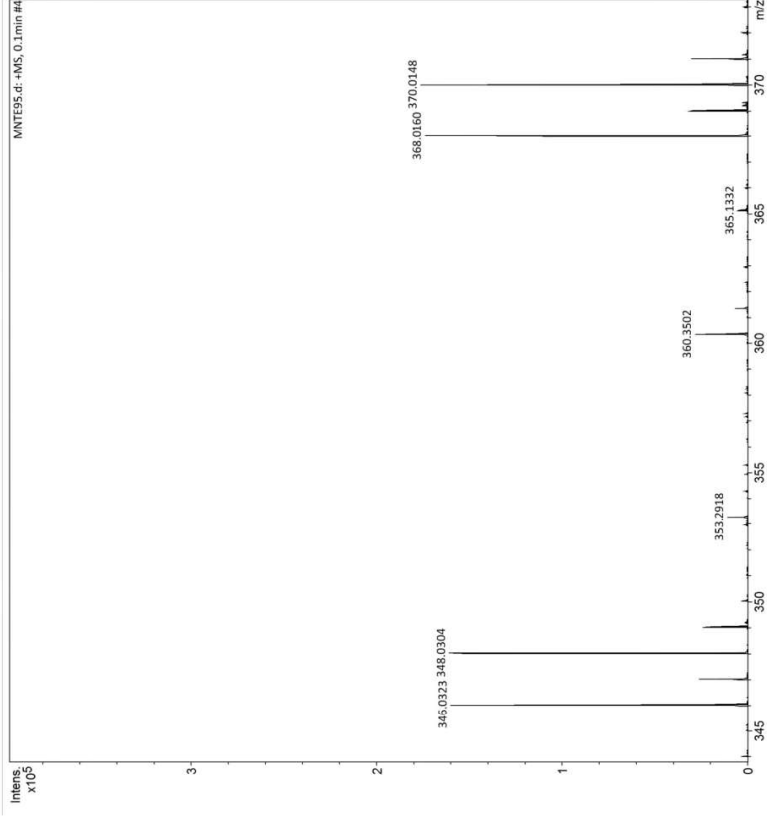
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Sample Name MEOH  
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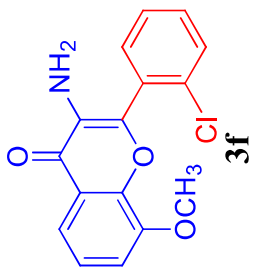
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Operator HRMS  
Instrument maxis impact 1819696.00160

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E932

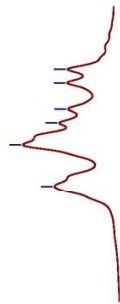


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7.6017  
7.5948  
7.5873  
7.5629  
7.5480  
7.5330  
7.3782  
7.3748  
7.3624  
7.3591  
7.3473  
7.3318

3.8982  
2.8045  
2.8018

E932

7.6996  
7.6847  
7.6769  
7.6719  
7.6626  
7.6578



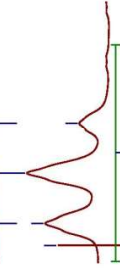
E932

7.6177  
7.6017  
7.5948  
7.5873  
7.5629  
7.5480  
7.5330



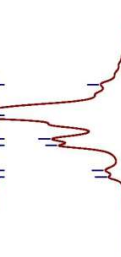
E932

7.5629  
7.5480  
7.5330



E932

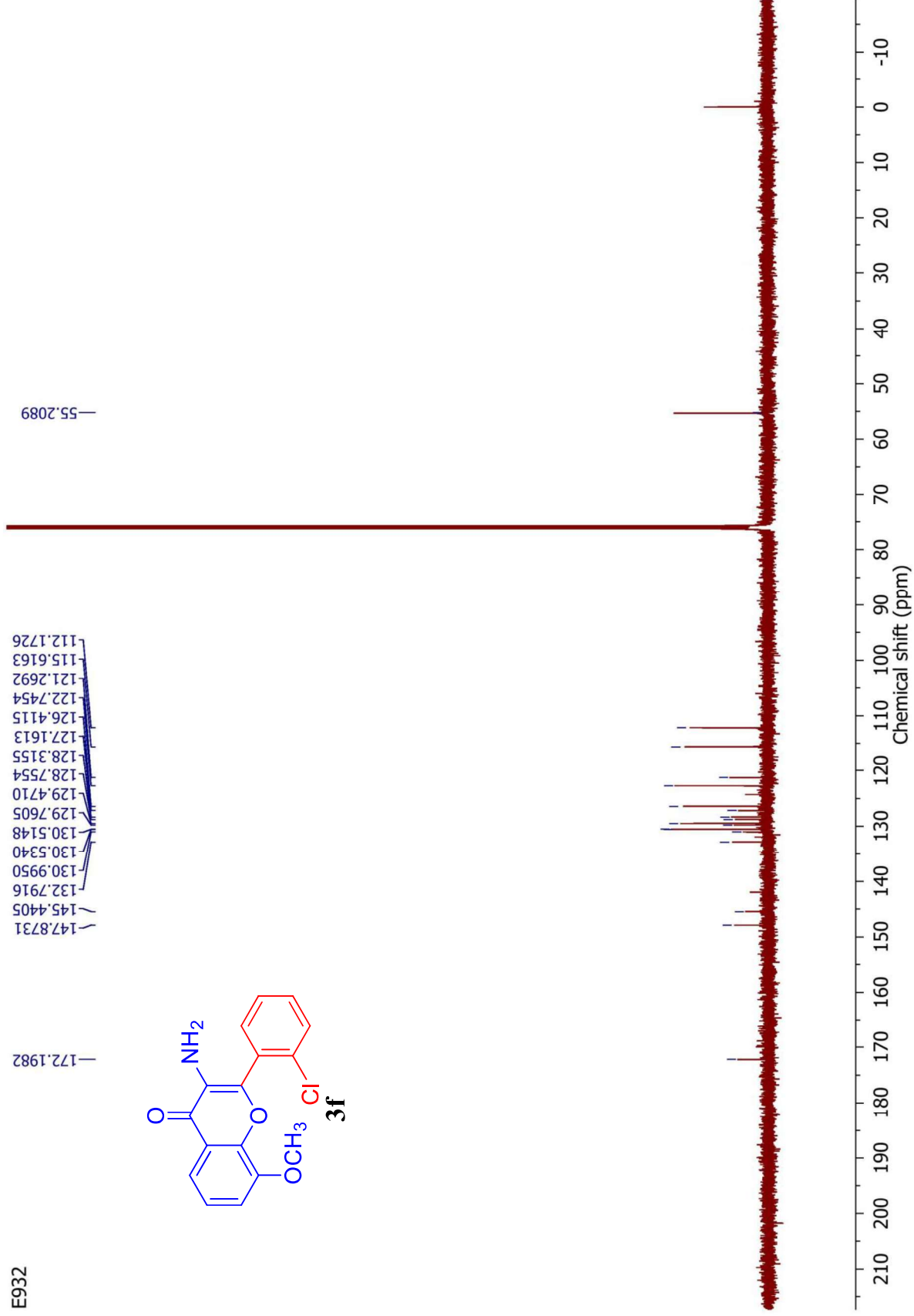
7.3782  
7.3748  
7.3624  
7.3591  
7.3473  
7.3318



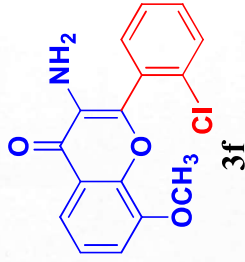
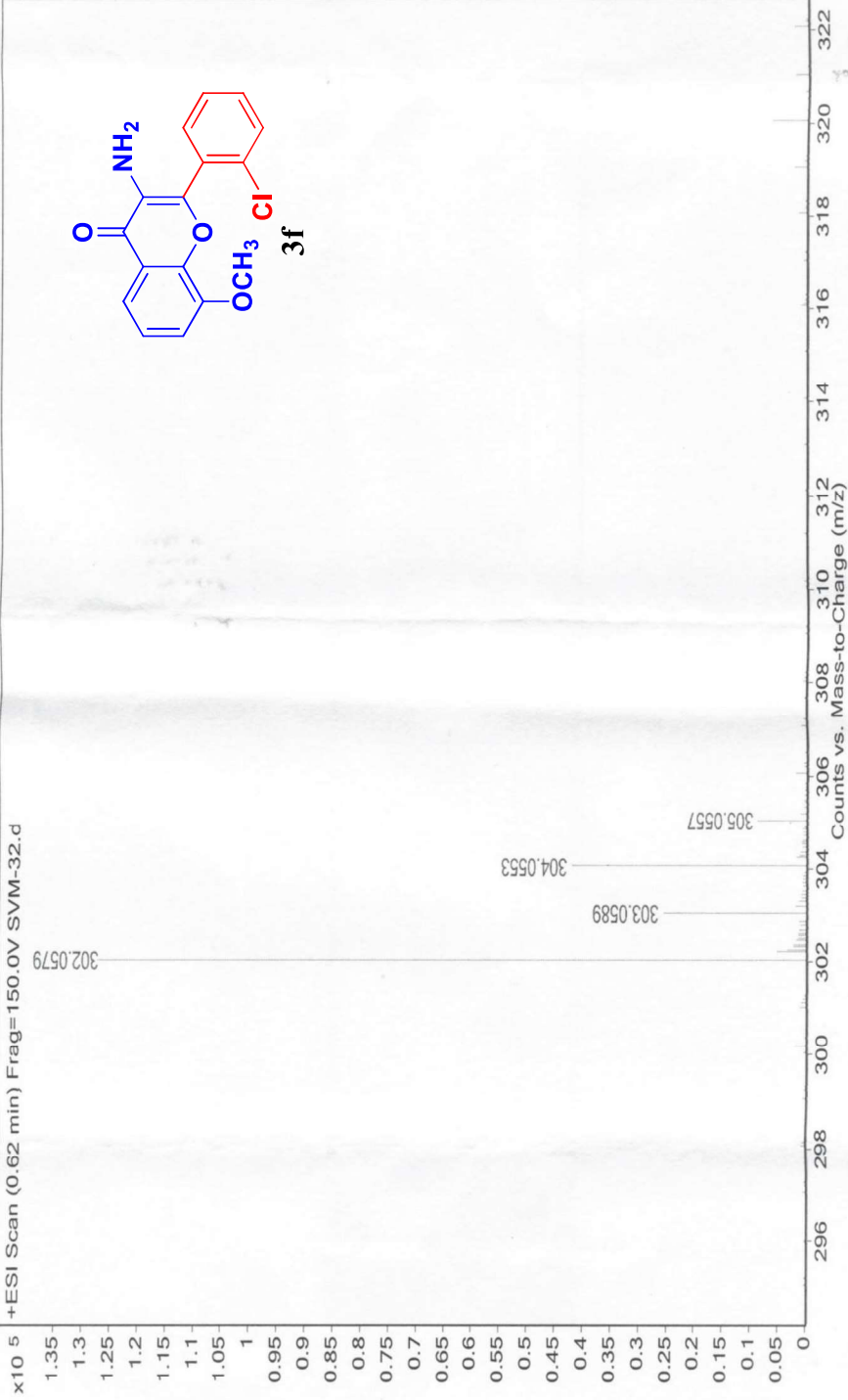
3.10  
1.84  
1.22  
1.95

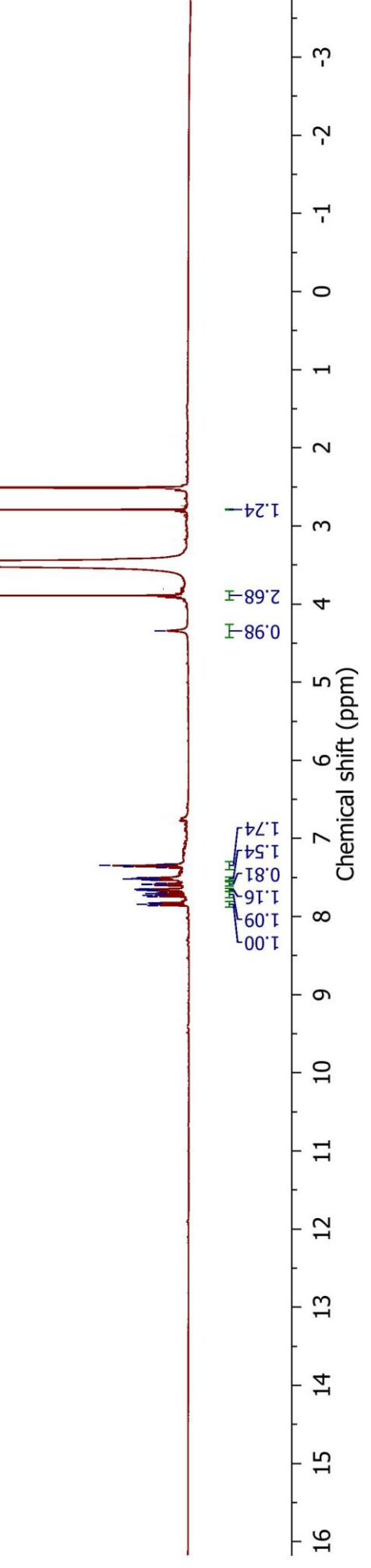
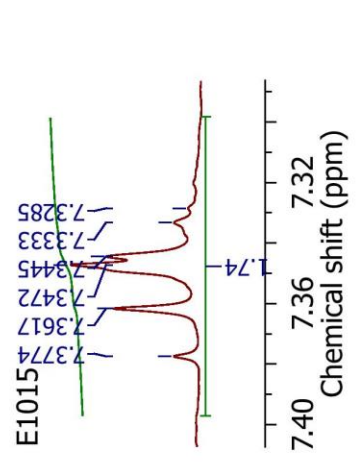
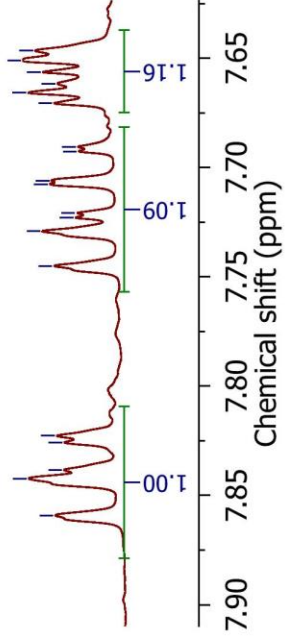
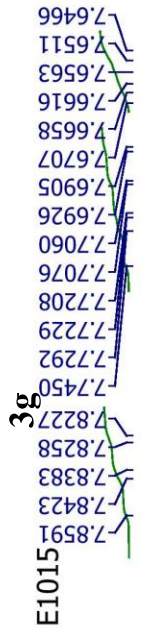
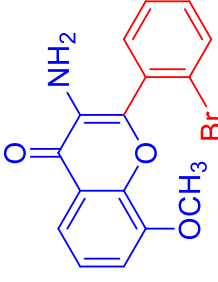
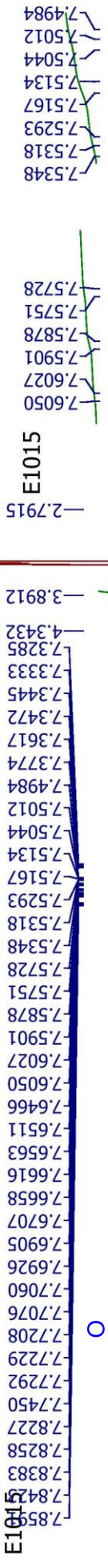
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3

Chemical shift (ppm)



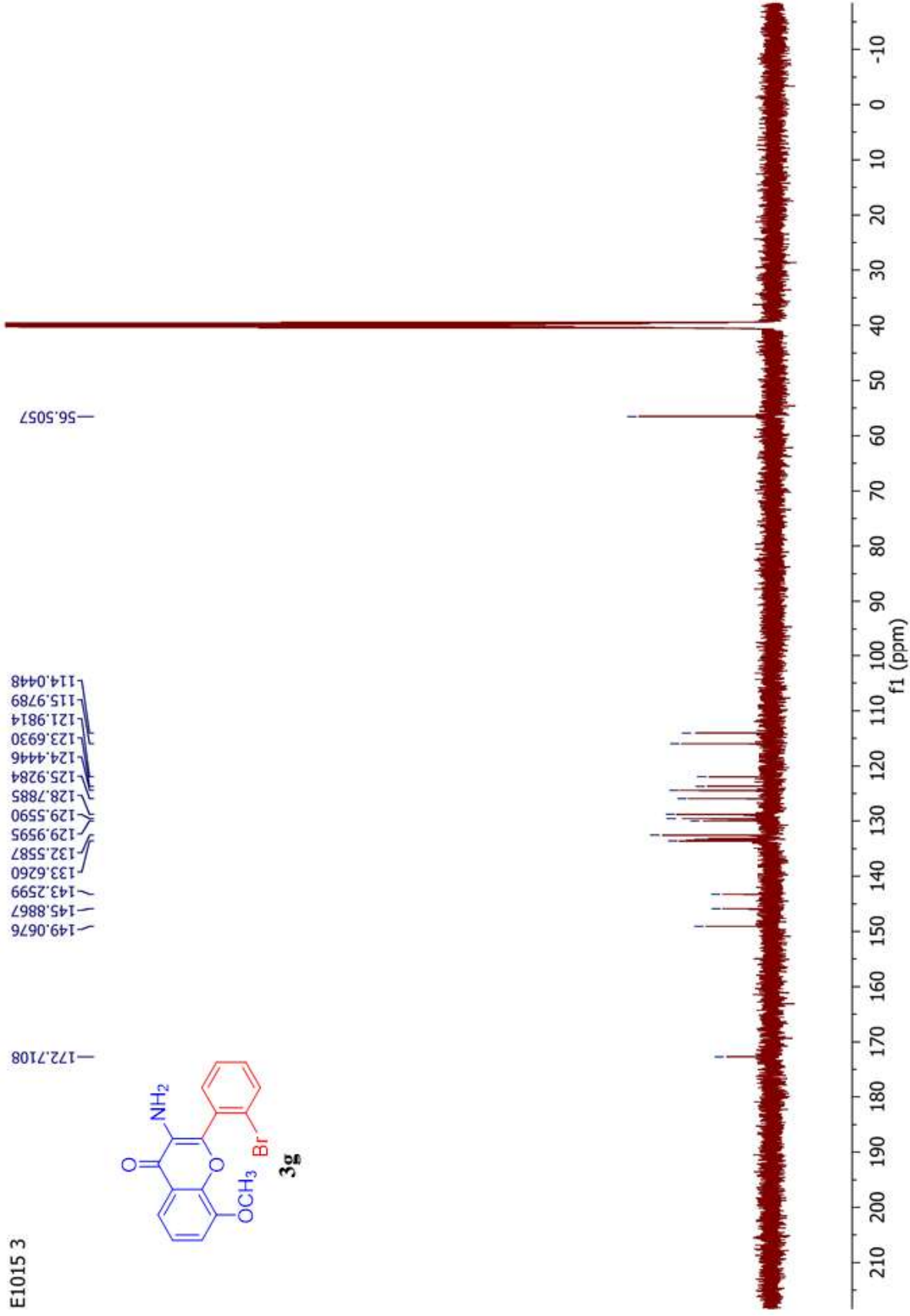
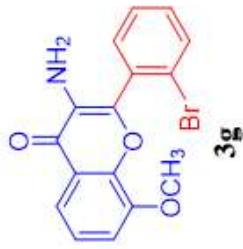
Sample Name: Seenivasan (1113)    Position: InjPosition    Instrument Name: Instrument 1    User Name: Success  
Inj Vol: 1    ACQ Method: SVM-32.d    SampleType: Sample    IRM Calibration Status: 12/6/2019 1:32:40 PM  
Data Filename: SVM-32.d    Method: ISOCRATIC.m    Comment:    Acquired Time: 12/6/2019 1:32:40 PM



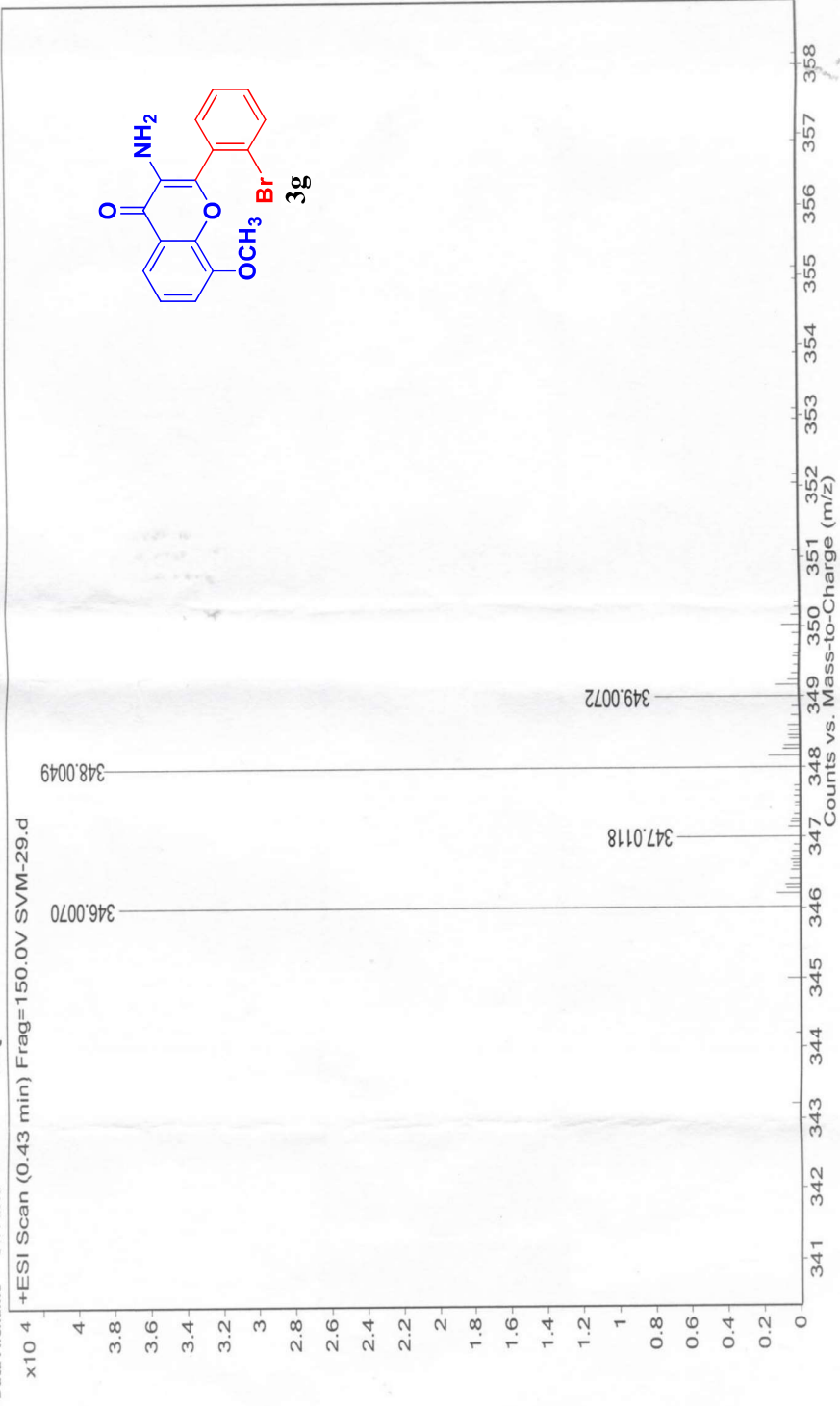




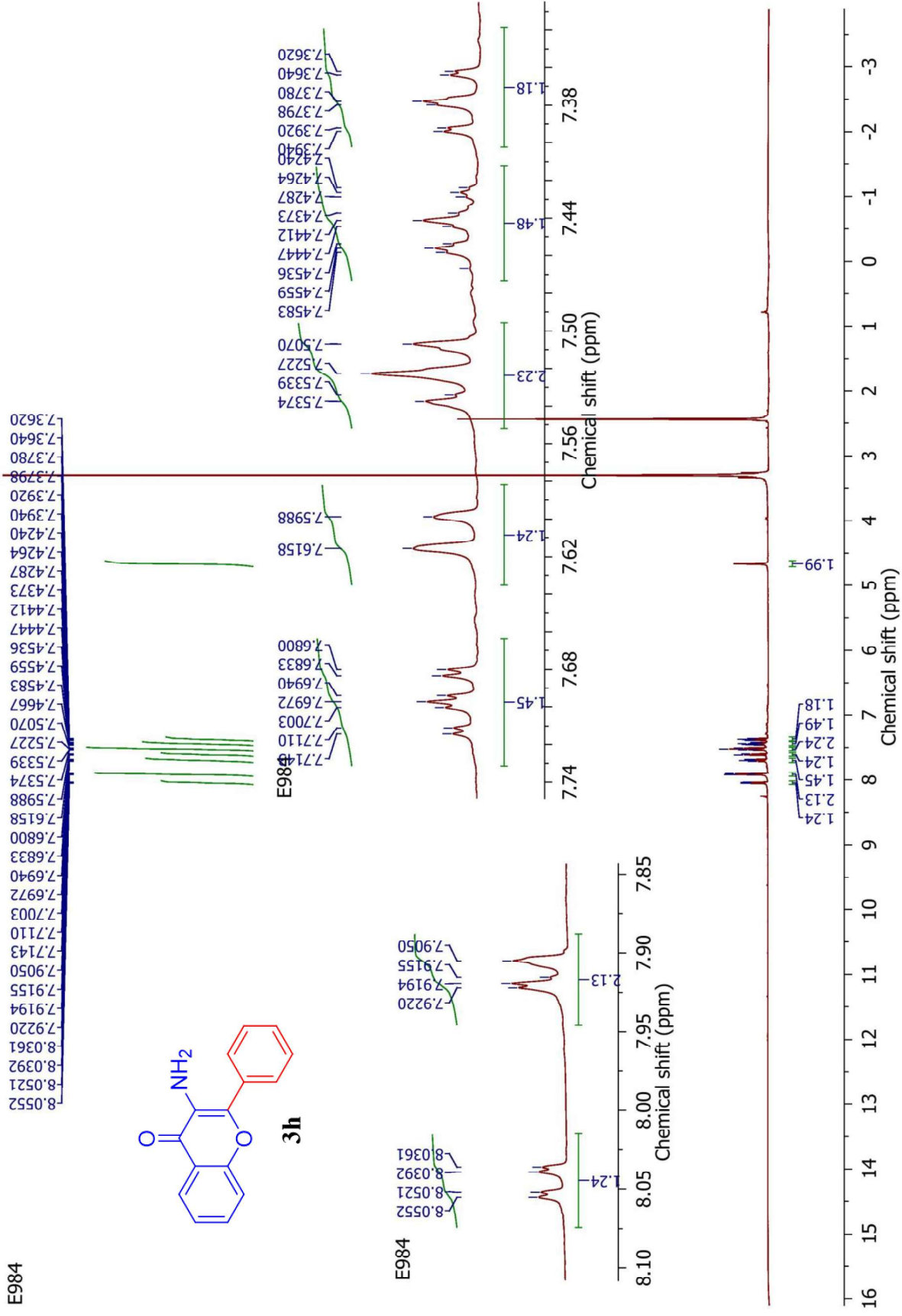
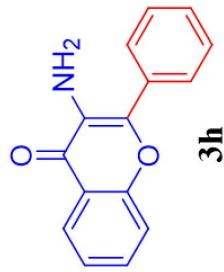
E1015 3



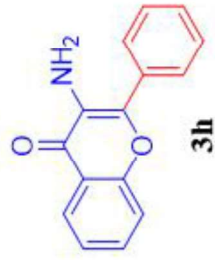
Sample Name: Seenivasan (1113)  
Inj Vol: 1  
Data Filename: SVM-29.d  
Position: InjPosition  
ACQ Method: ISOCRATIC.m  
Vial: 35  
Instrument Name: Instrument 1  
SampleType: Sample  
Comment:  
User Name: Success  
IRM Calibration Status: Success  
Acquired Time: 12/6/2019 1:21:44 PM



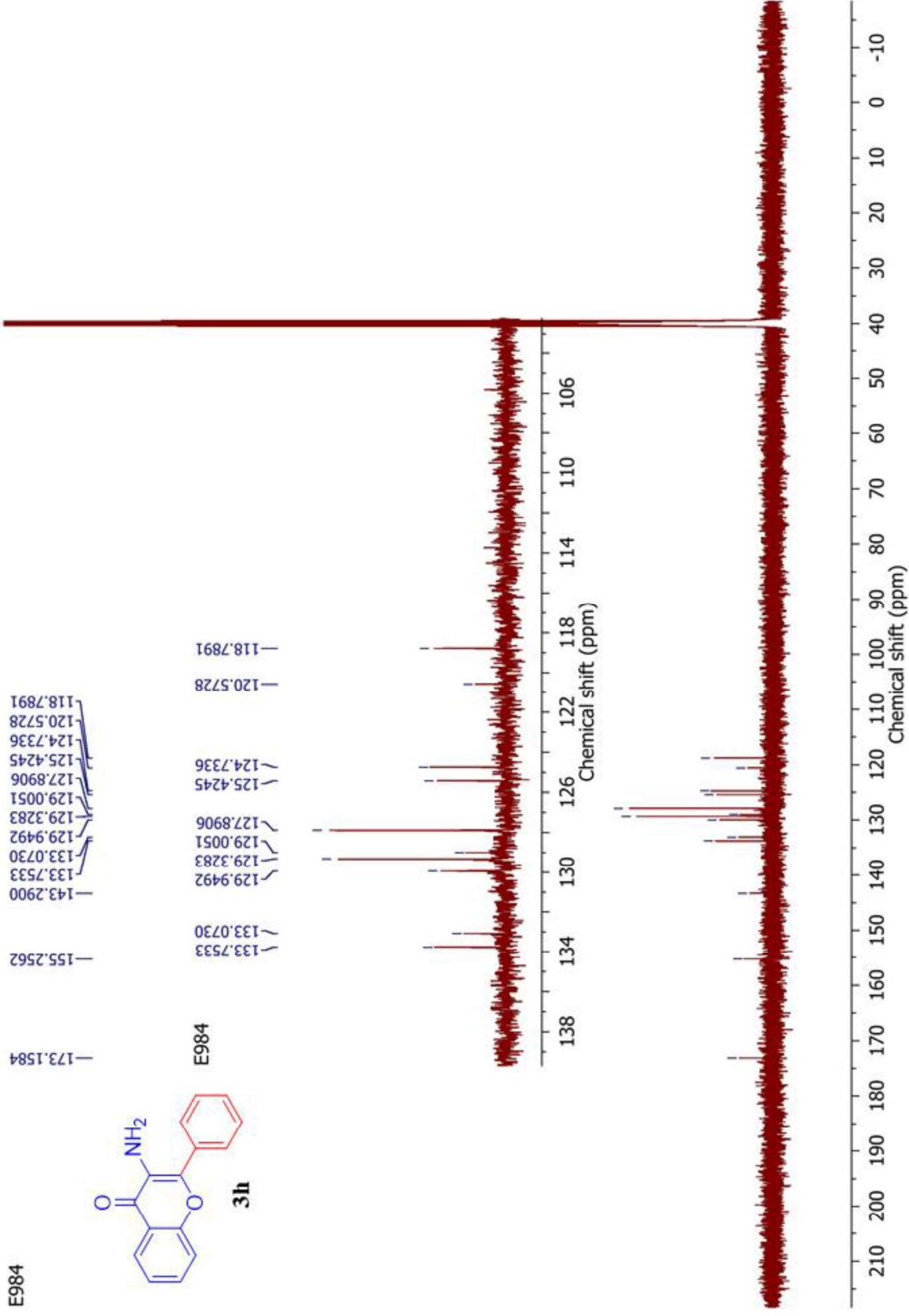
E984



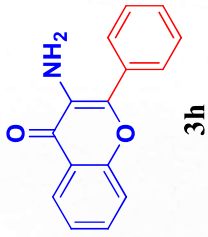
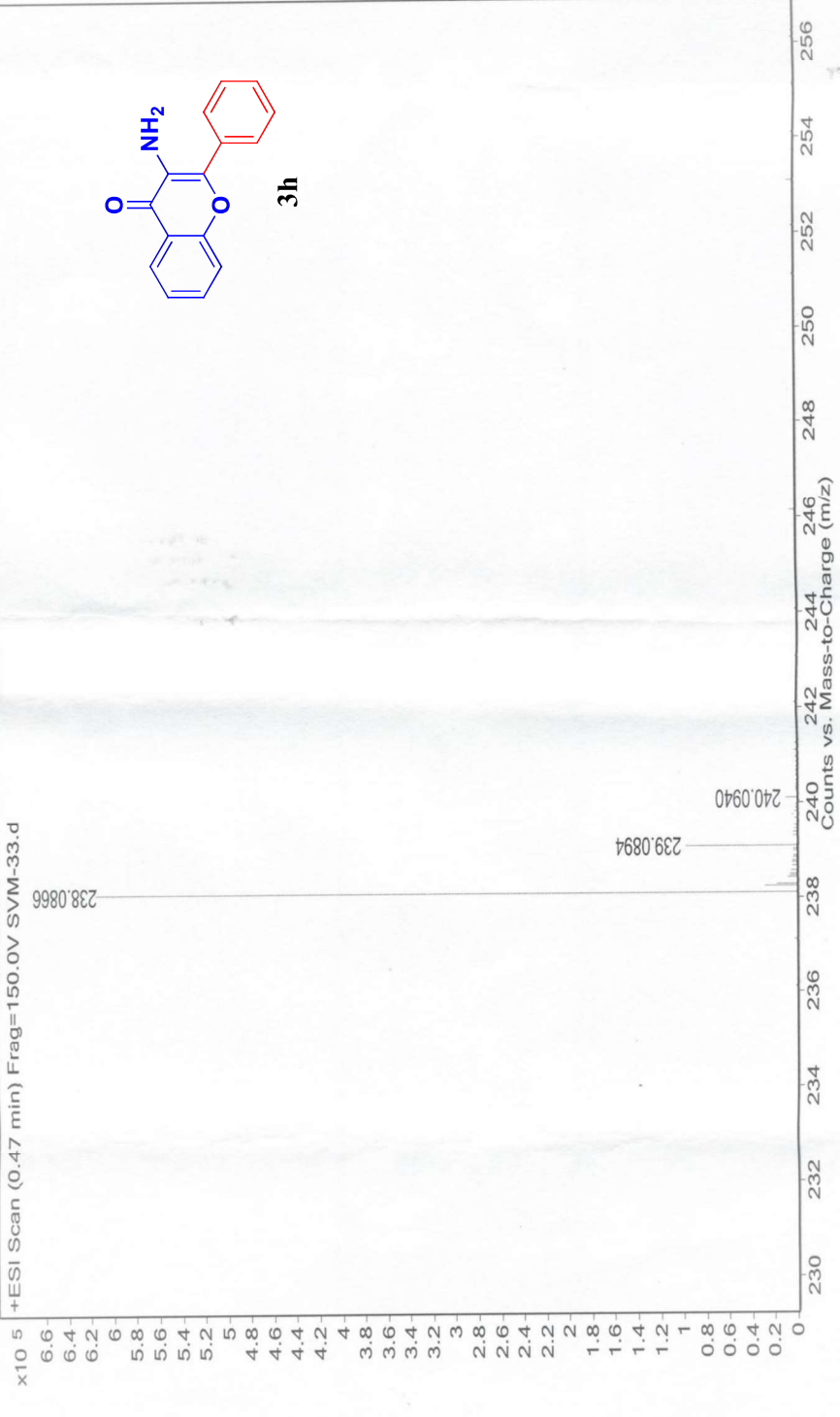
E984

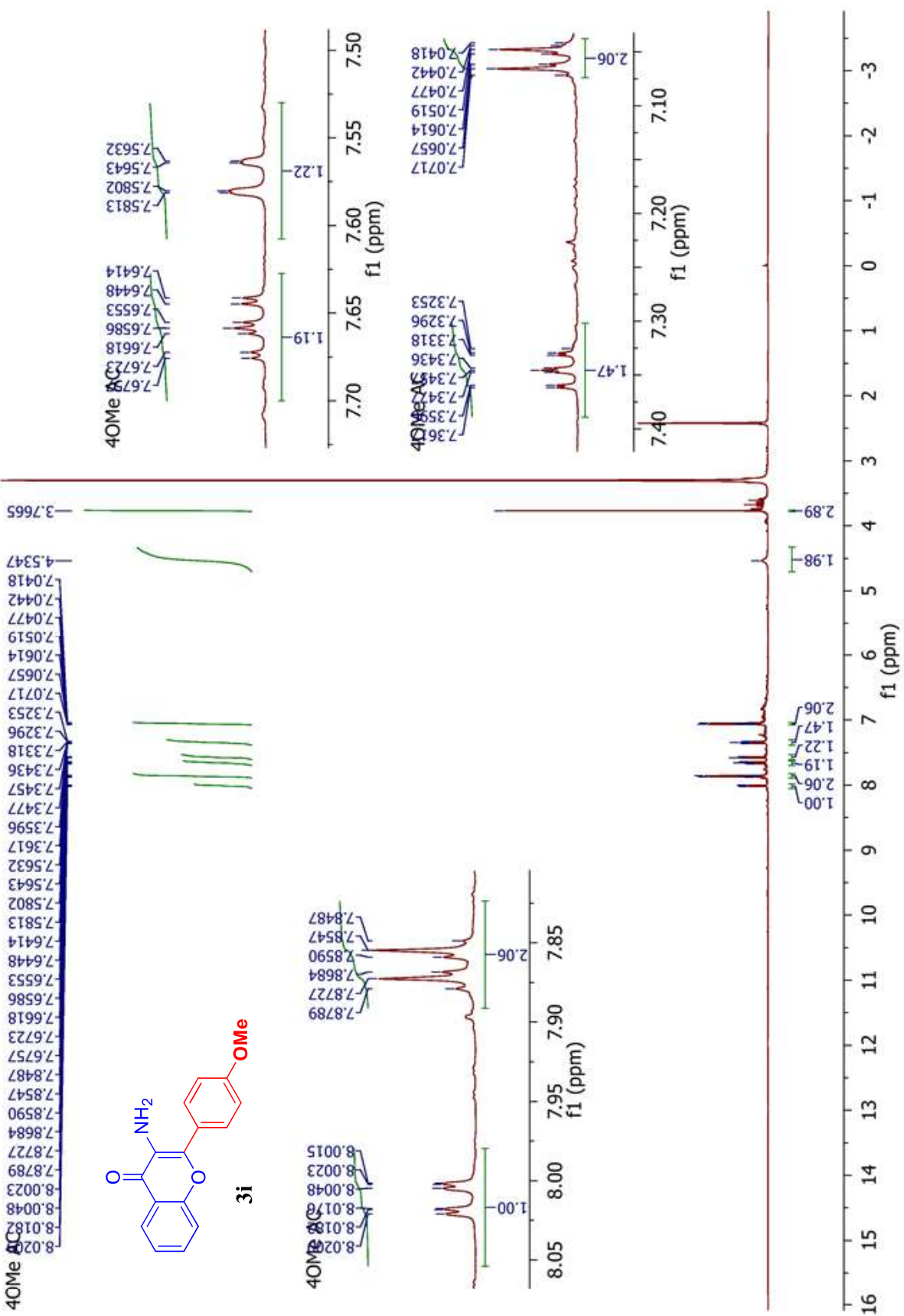
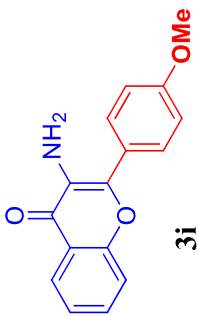


E984



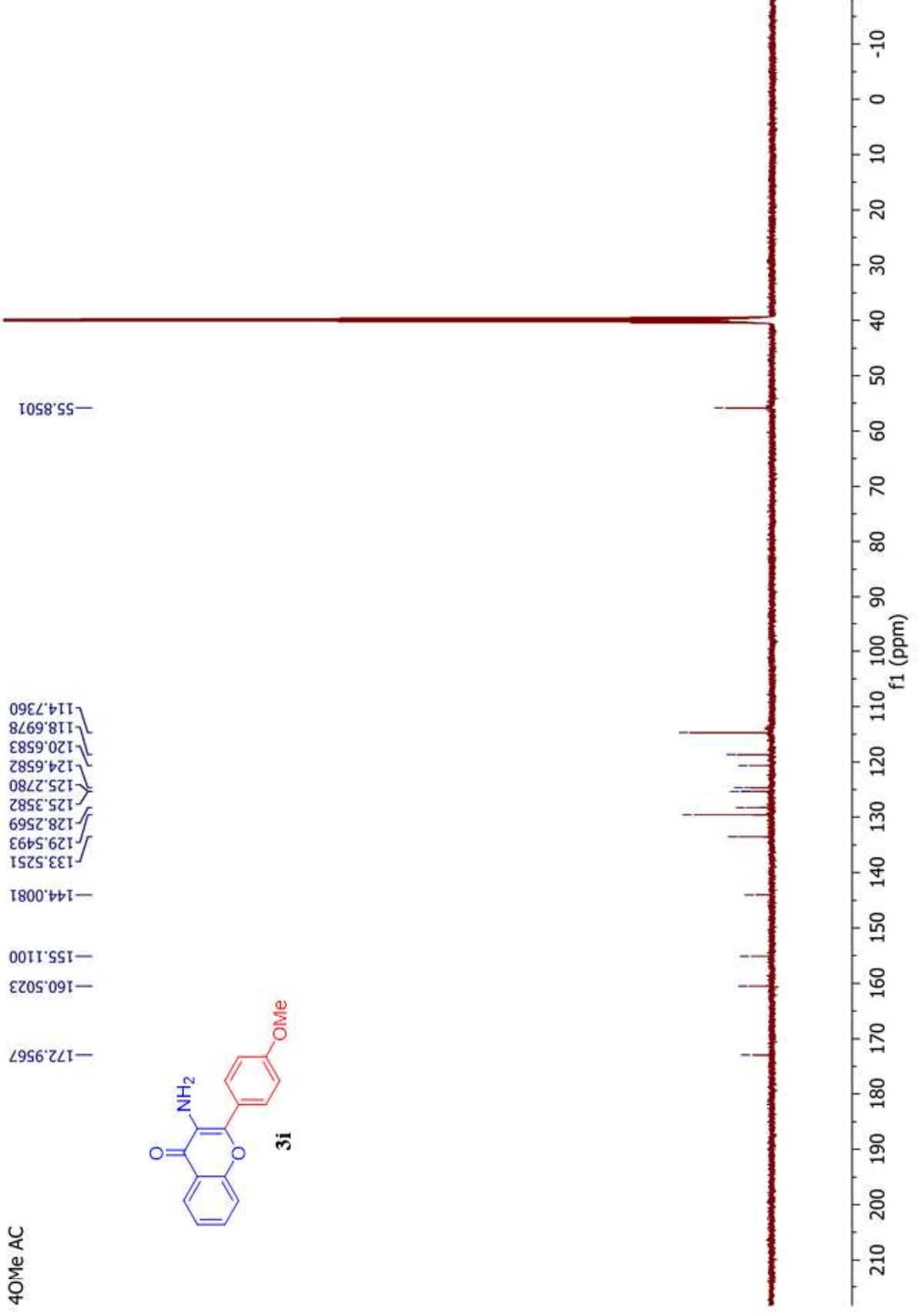
Sample Name: Seenivasan (1113)    Vial 39    Instrument Name: Instrument 1    User Name: Success  
Inj Vol: 1    InjPosition: Vial 39    SampleType: Sample    IRM Calibration Status: Success  
Data Filename: SVM-33.d    ACQ Method: ISOCRATIC.m    Comment:    Acquired Time: 12/6/2019 1:36:21 PM



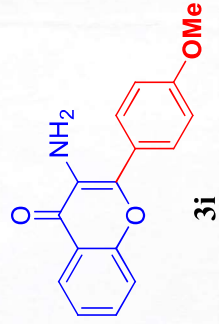
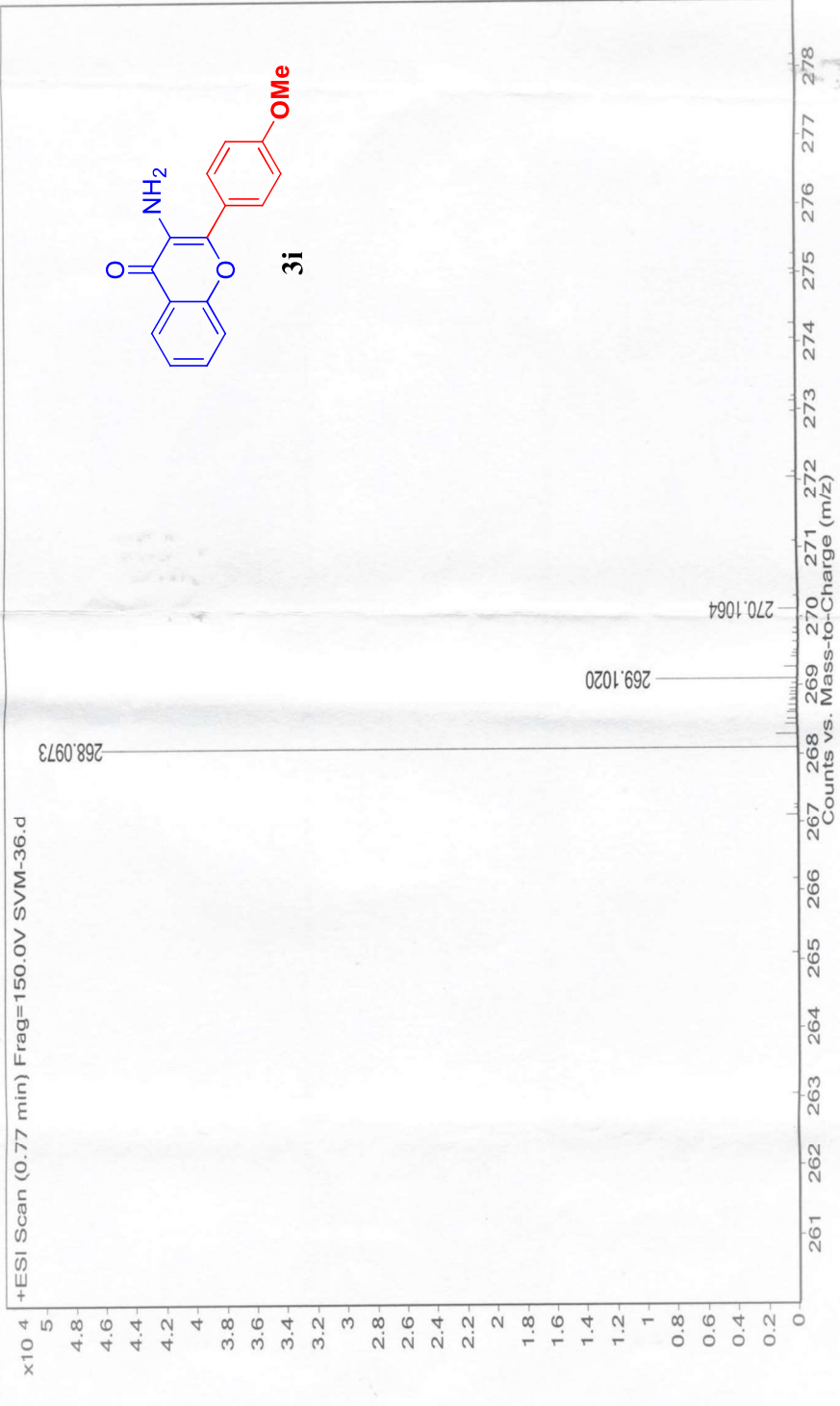




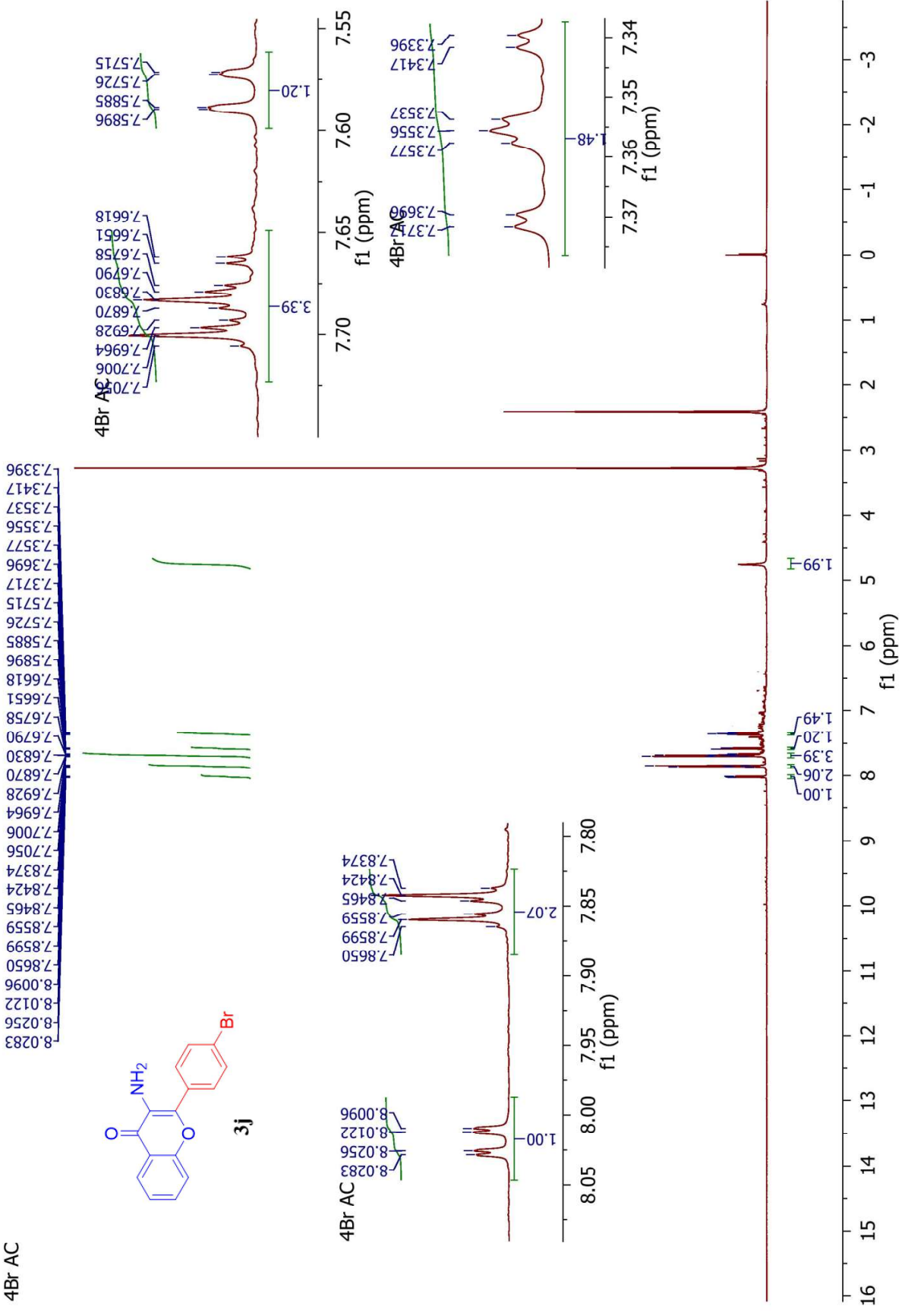
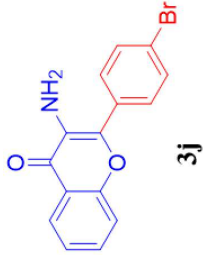
40Me AC



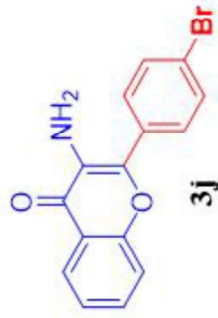
Sample Name Seenuvasan (1113) Position Vial 43 Instrument Name Instrument 1 User Name Success  
Inj Vol 1 InjPosition ISOCRATIC.m Sample Sample 12/6/2019 1:50:51 PM  
Data Filename SVM-36.d ACQ Method ISOCRATIC.m Comment Comment IRM Calibration Status  
+ESI Scan (0.77 min) Frag=150.0V SVM-36.d



4Br AC



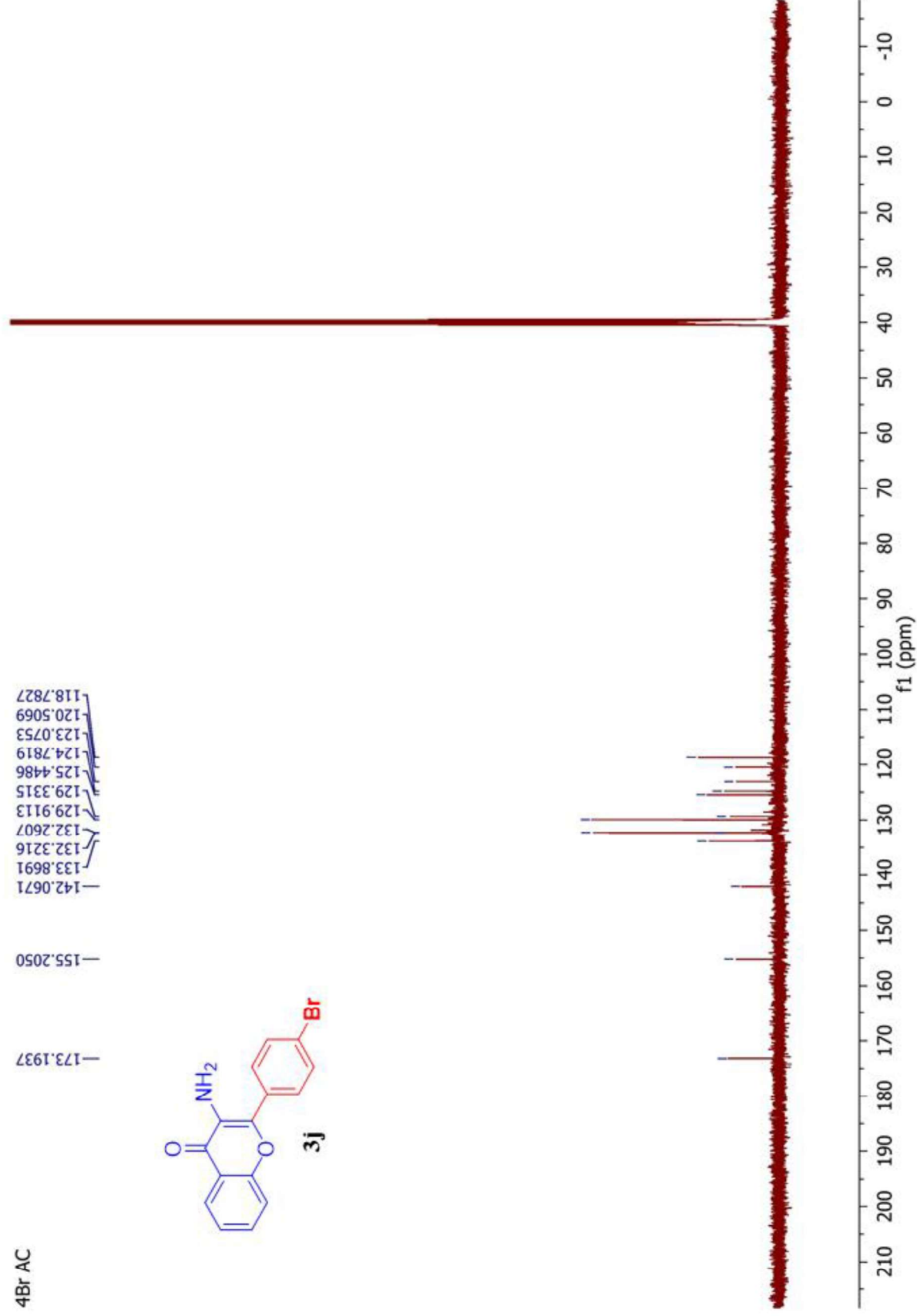
4Br AC



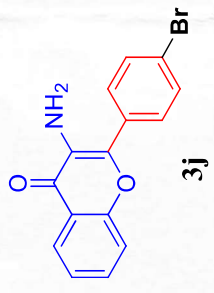
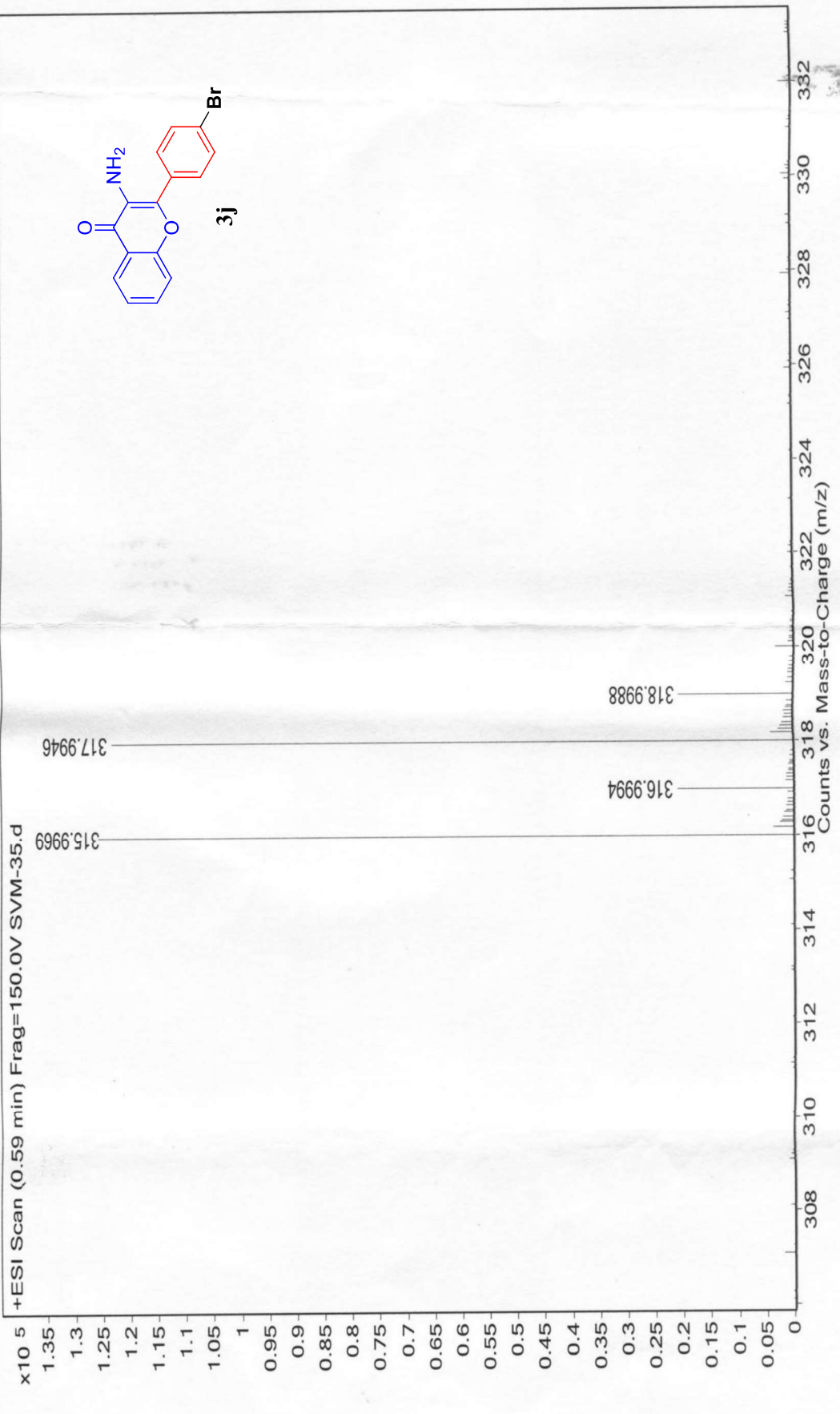
142.0671  
133.8691  
132.3216  
132.2607  
129.9113  
129.3315  
125.4486  
124.7819  
123.0753  
120.5069  
118.7827

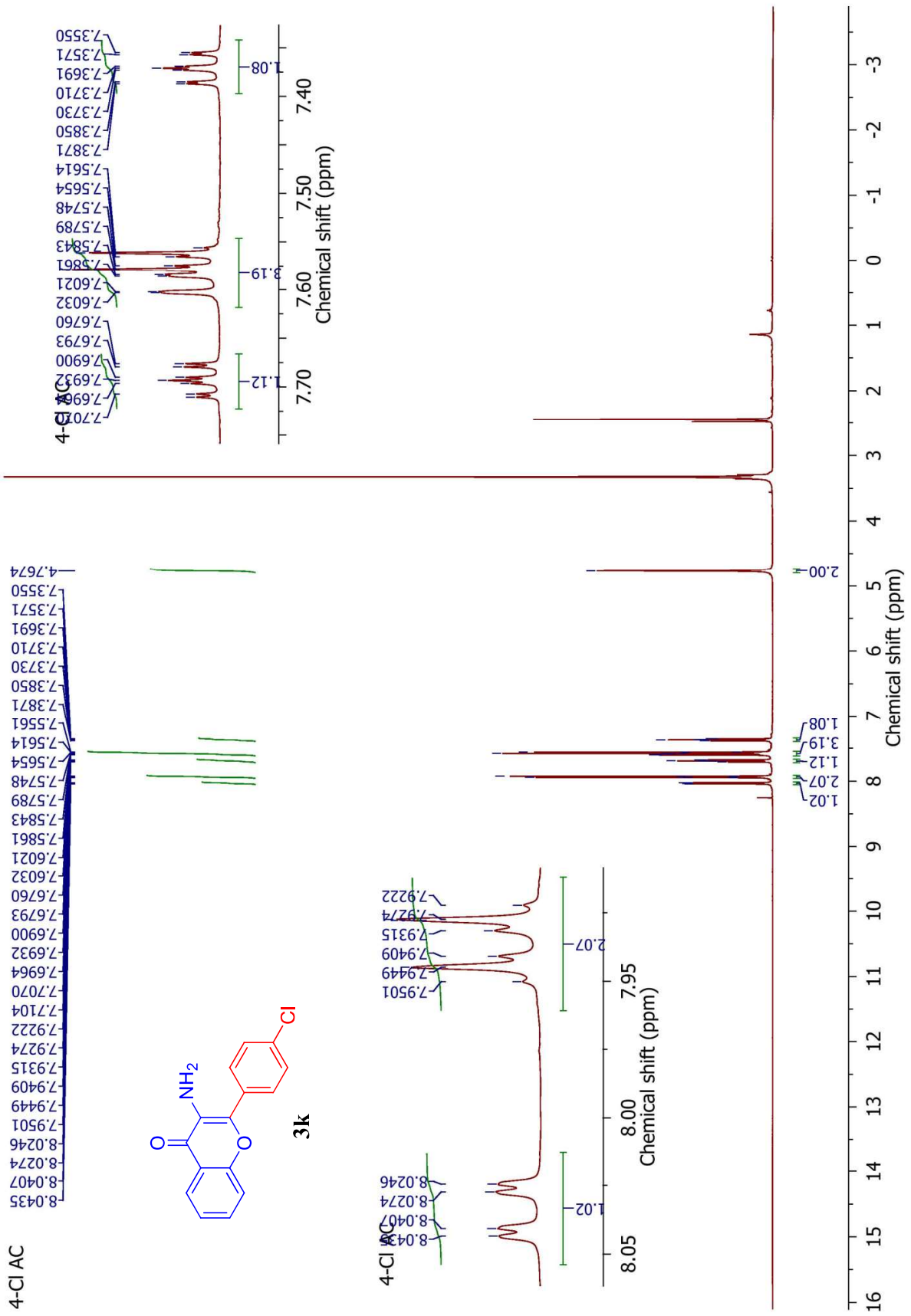
155.2050

173.1937



**Sample Name** Seenuvasan (1113) **Position** Vial 42 **User Name** Success  
**Inj Vol** 1 **InjPosition** ISOCRATIC.m **IRM Calibration Status** 12/6/2019 1:47:14 PM  
**Data Filename** SVM-35.d **ACQ Method** ISOCRATIC.m **SampleType** Sample **Acquired Time**





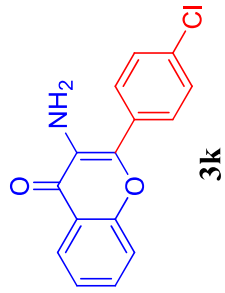


4Cl AC

—173.1940

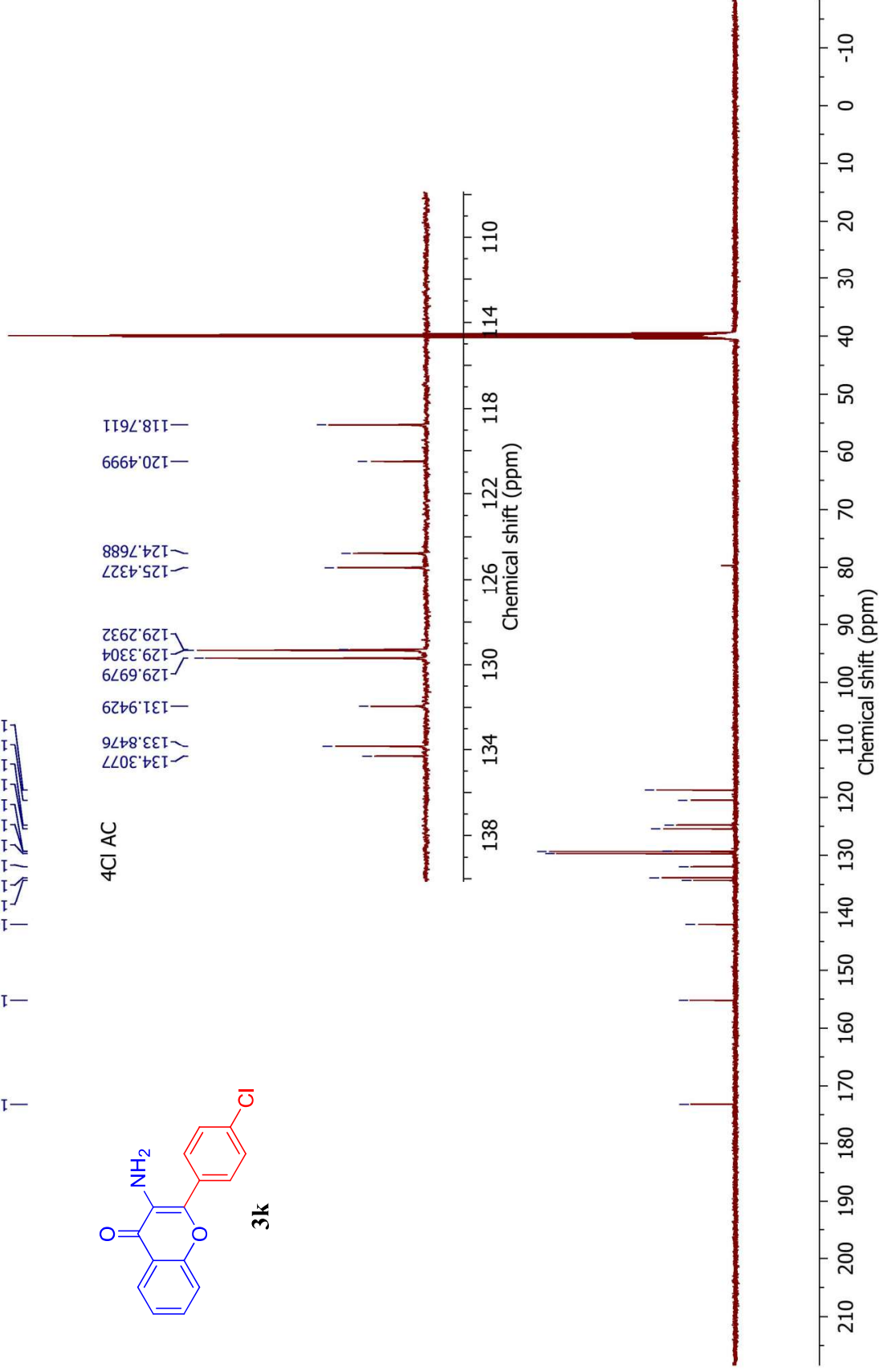
—155.1950

—142.0583  
—134.3077  
—133.8476  
—131.9429  
—129.6979  
—129.3304  
—129.2932  
—125.4327  
—124.7688  
—120.4999  
—118.7611

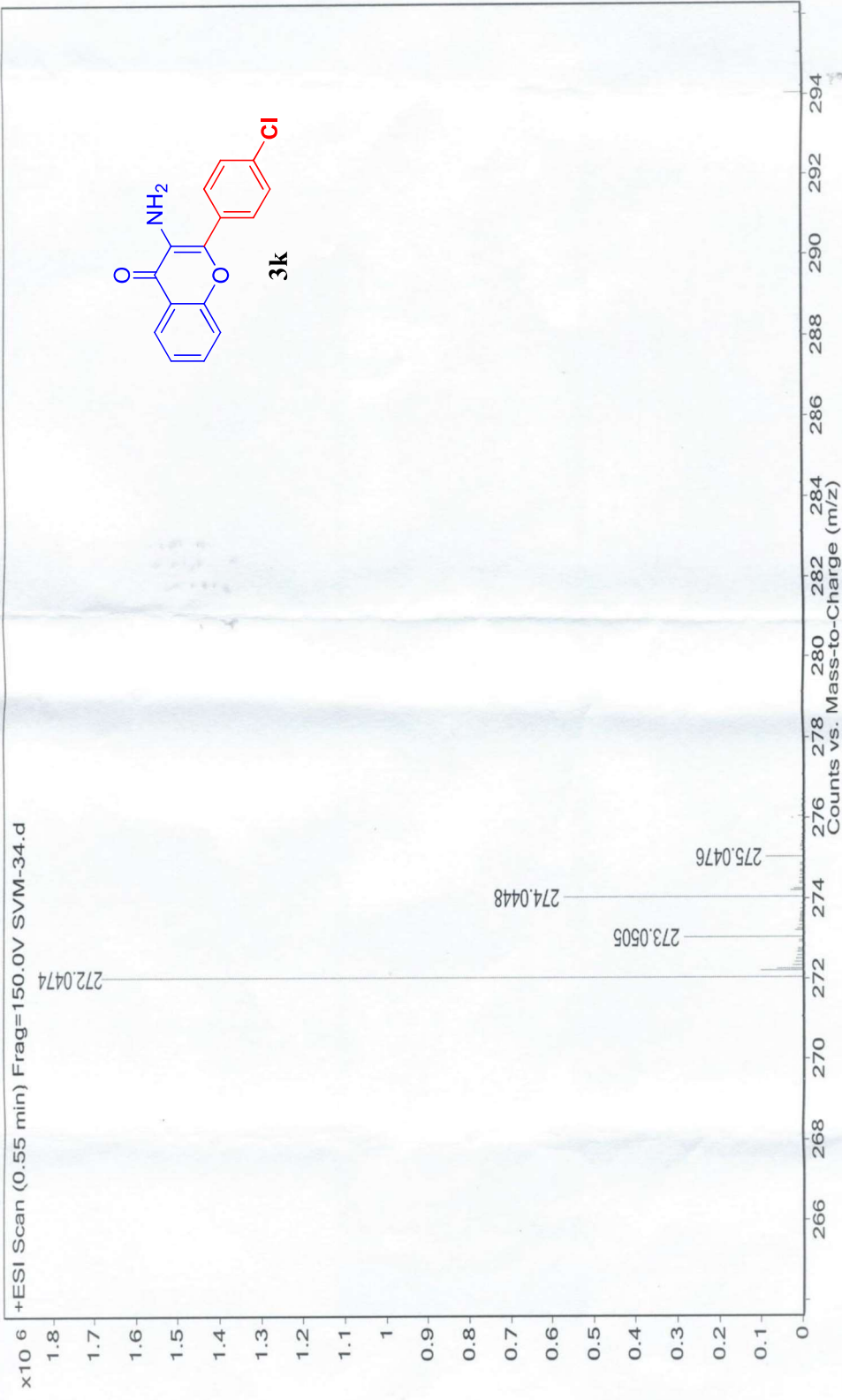


4Cl AC

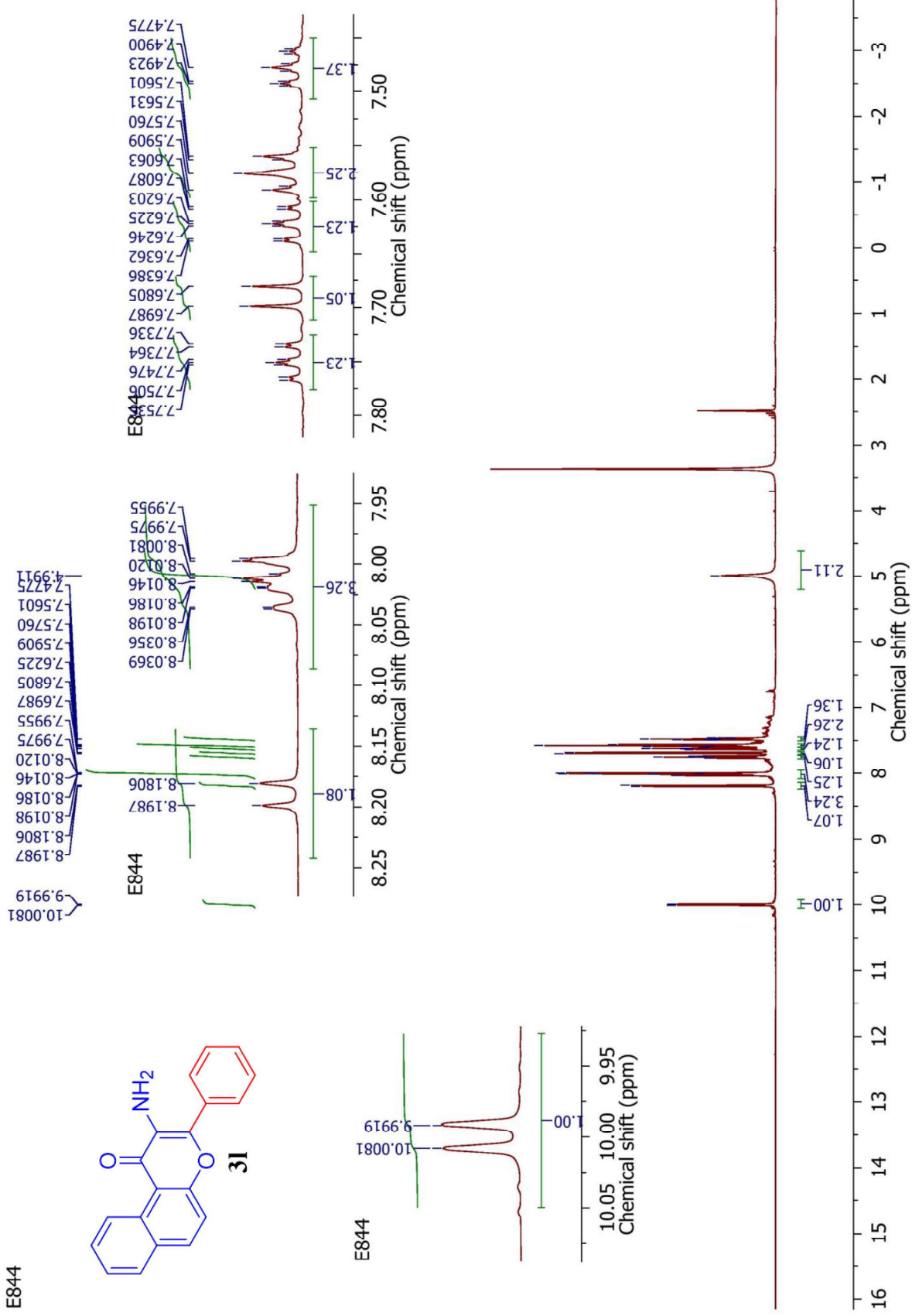
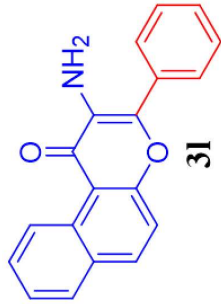
—134.3077  
—133.8476  
—131.9429  
—129.6979  
—129.3304  
—129.2932  
—125.4327  
—124.7688  
—120.4999  
—118.7611



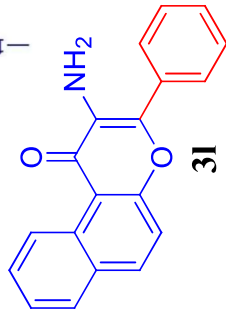
Sample Name Seenuvasan (1113) Position Vial 40 Instrument Name Instrument 1 User Name Success  
Inj Vol 1 InjPosition ACQ Method ISOCRATIC.m Sample Comment Sample 12/6/2019 1:40:06 PM  
Data Filename SVM-34.d +ESI Scan (0.55 min) Frag=150.0V SVM-34.d



E844

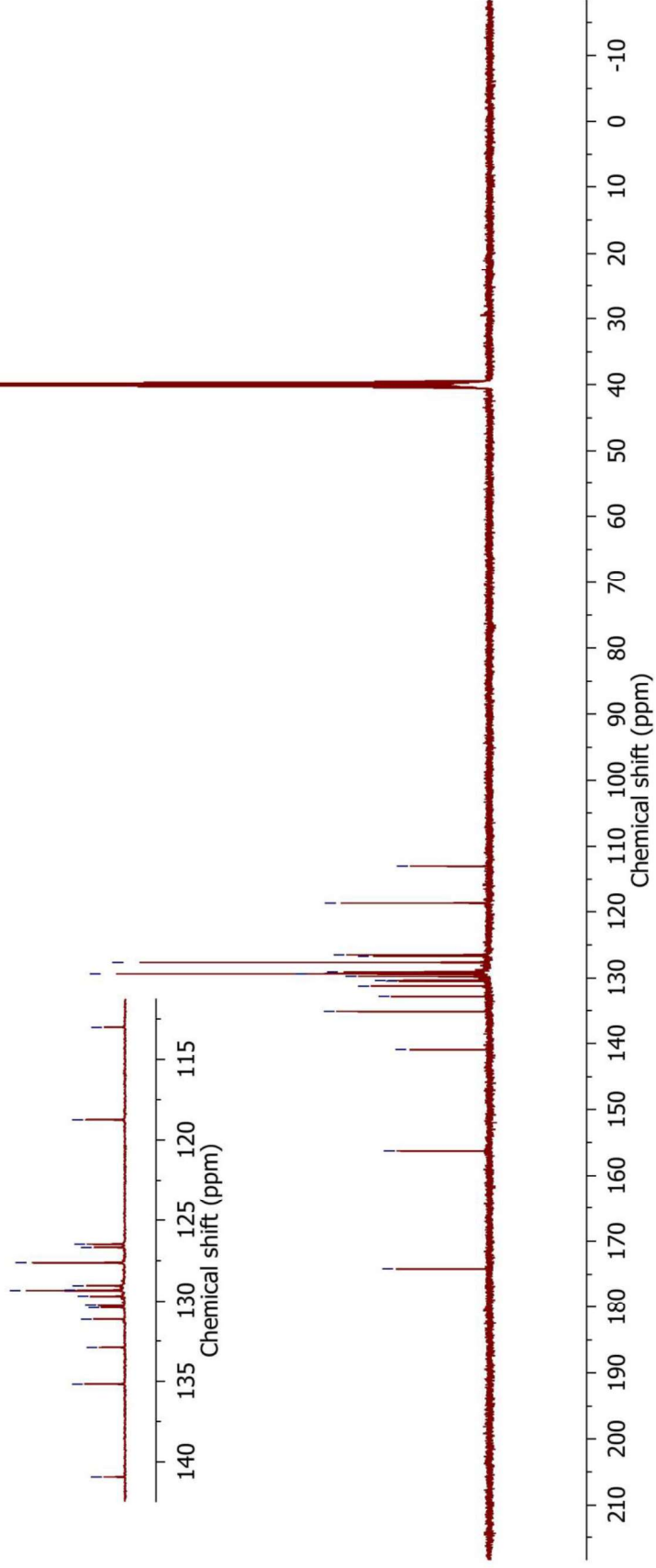


E844

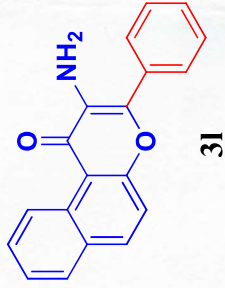
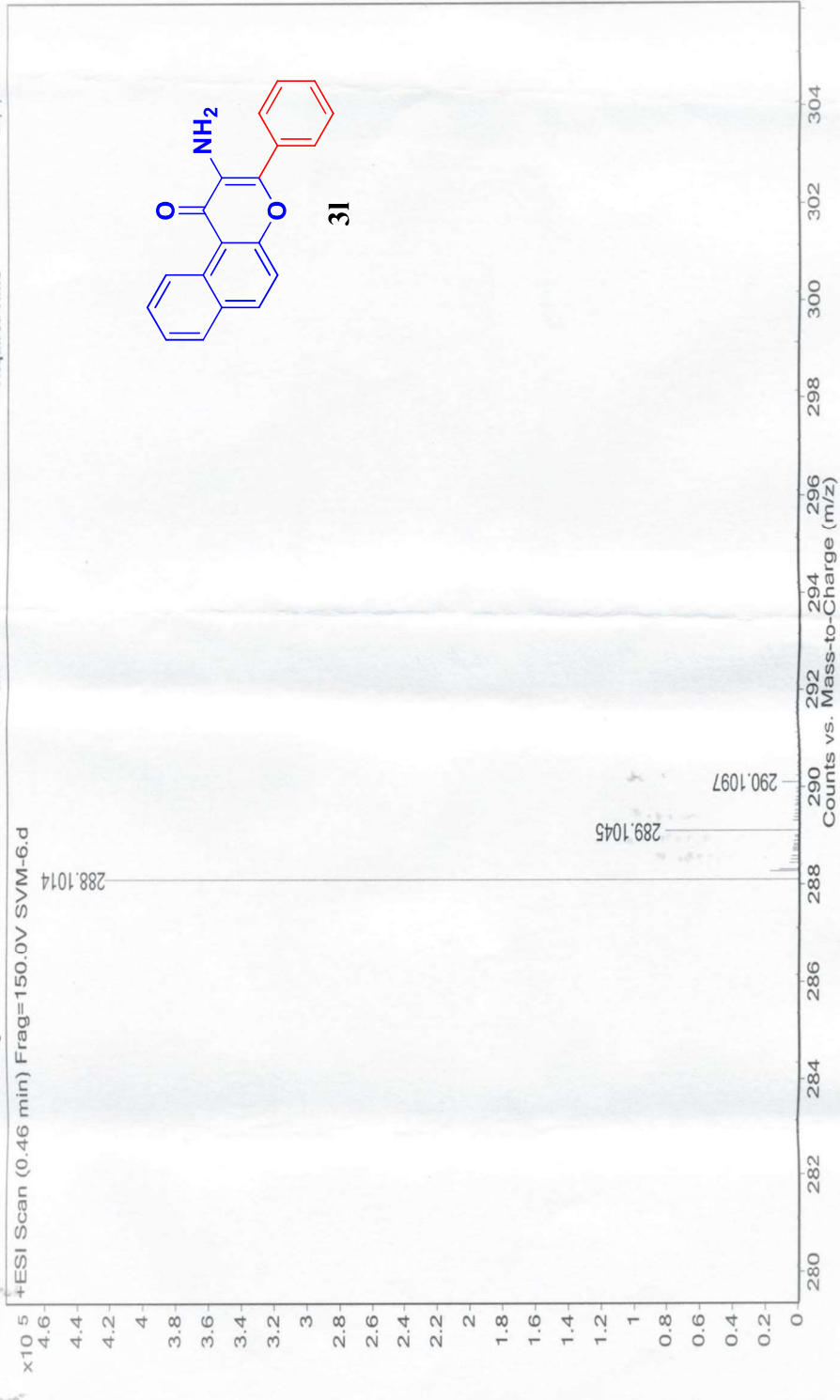


174.1728  
156.2676  
135.1716  
131.1571  
130.3111  
129.6940  
129.3390  
129.3165  
129.0393  
127.6273  
126.6812  
126.4914  
113.0098

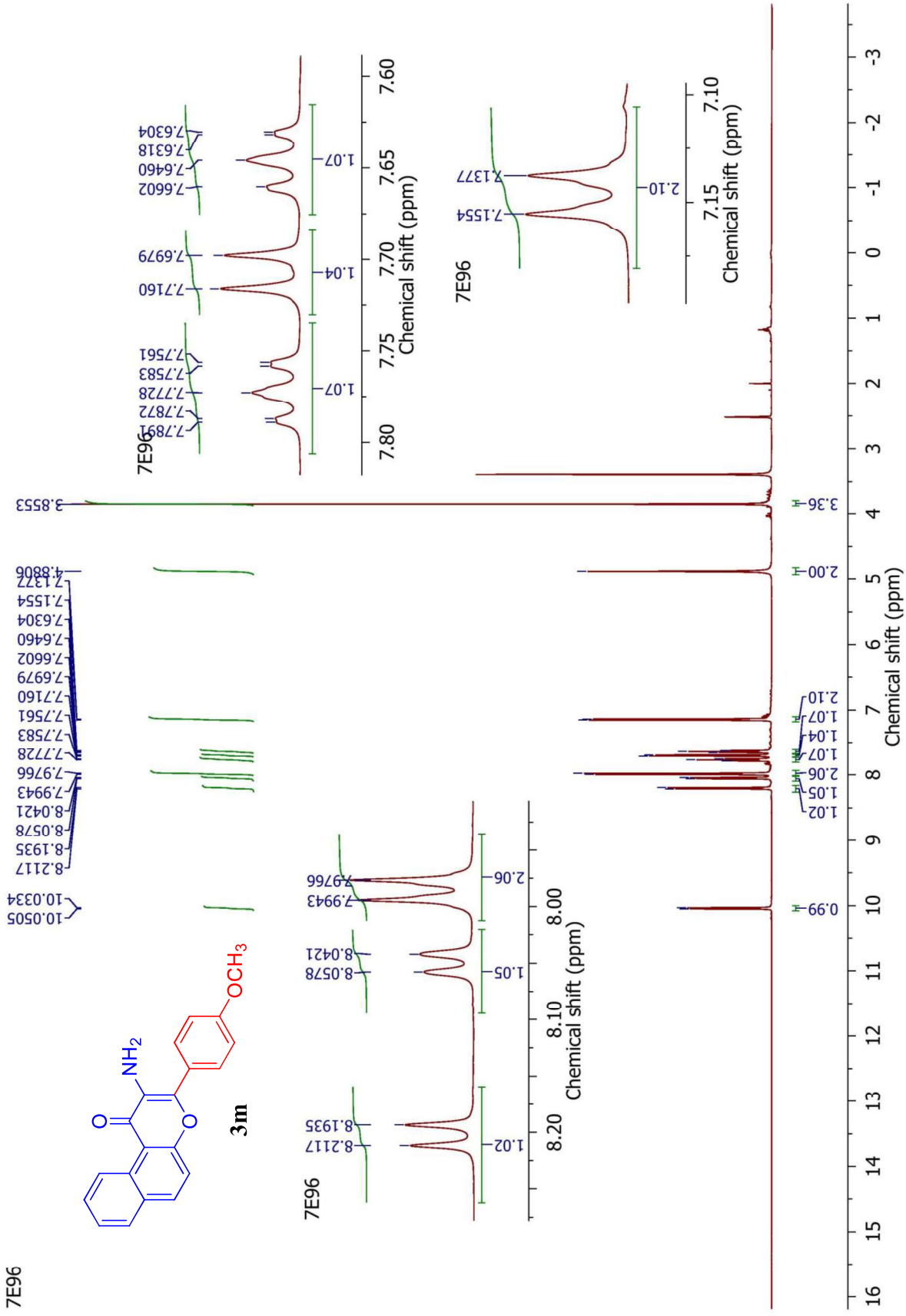
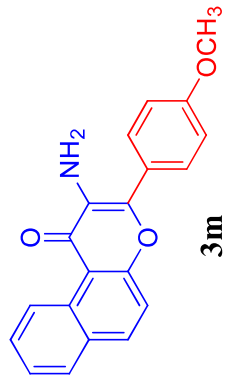
E844  
140.9389  
135.1716  
132.9078  
131.1571  
130.4311  
130.3111  
129.6940  
129.3390  
129.3165  
129.0393  
127.6273  
126.6812  
126.4914  
118.7460  
113.0098



Sample Name Seenuvasan (1113) Position Vial 41 User Name Success  
Inj Vol 1 InjPosition ISOCRATIC.m Instrument 1 IRM Calibration Status 12/6/2019 1:43:41 PM  
Data Filename SVM-6.d SVM-6.d Comment Sample Acquired Time

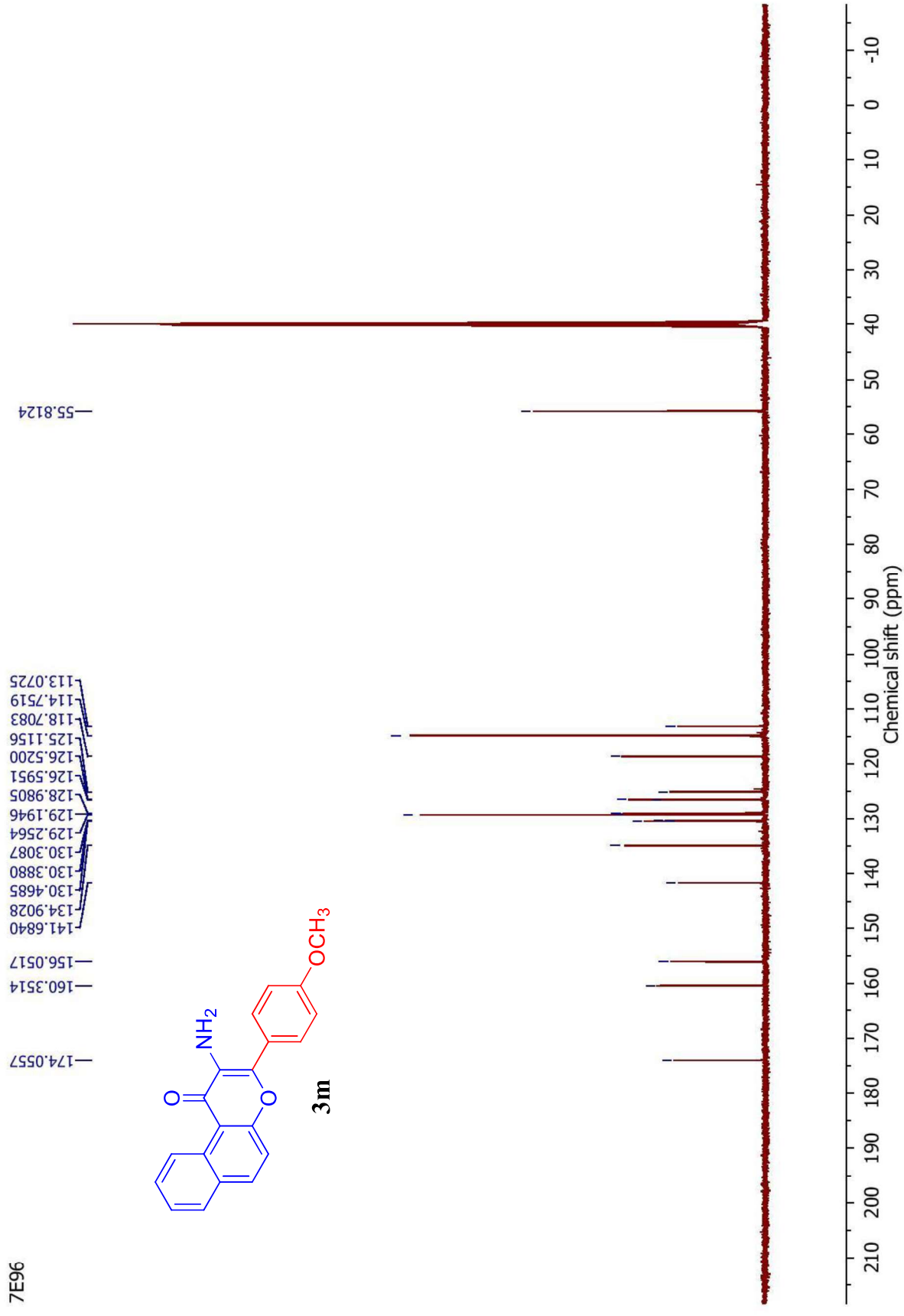
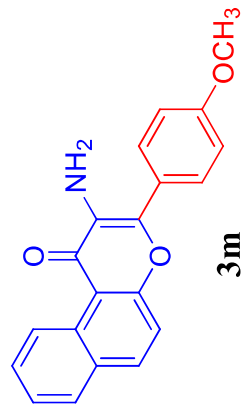


7E96





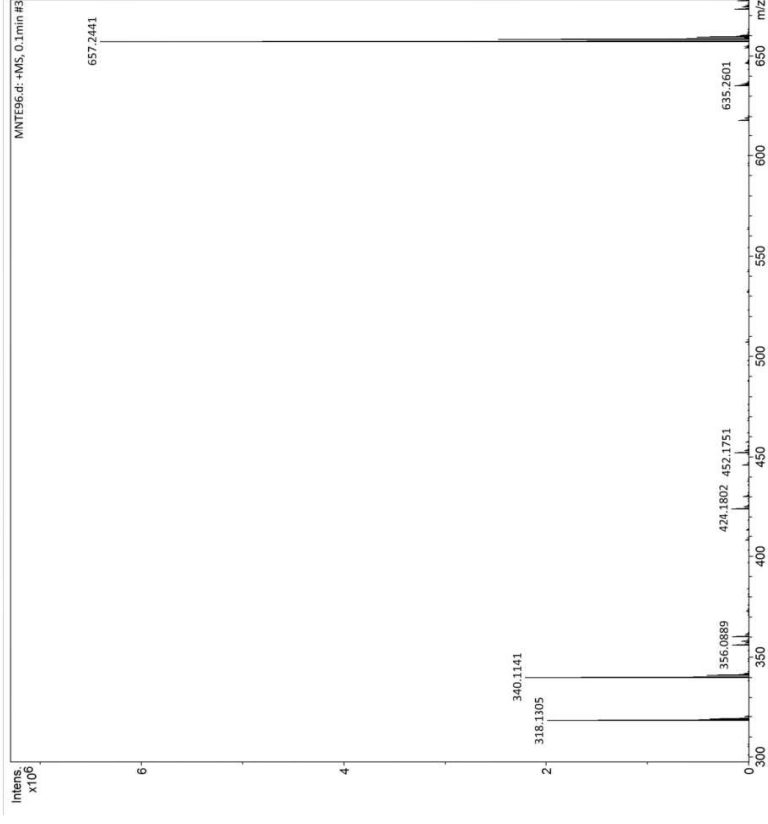
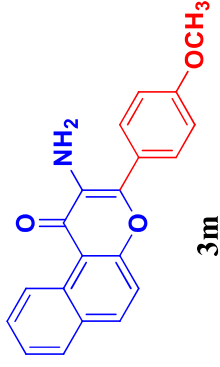
7E96



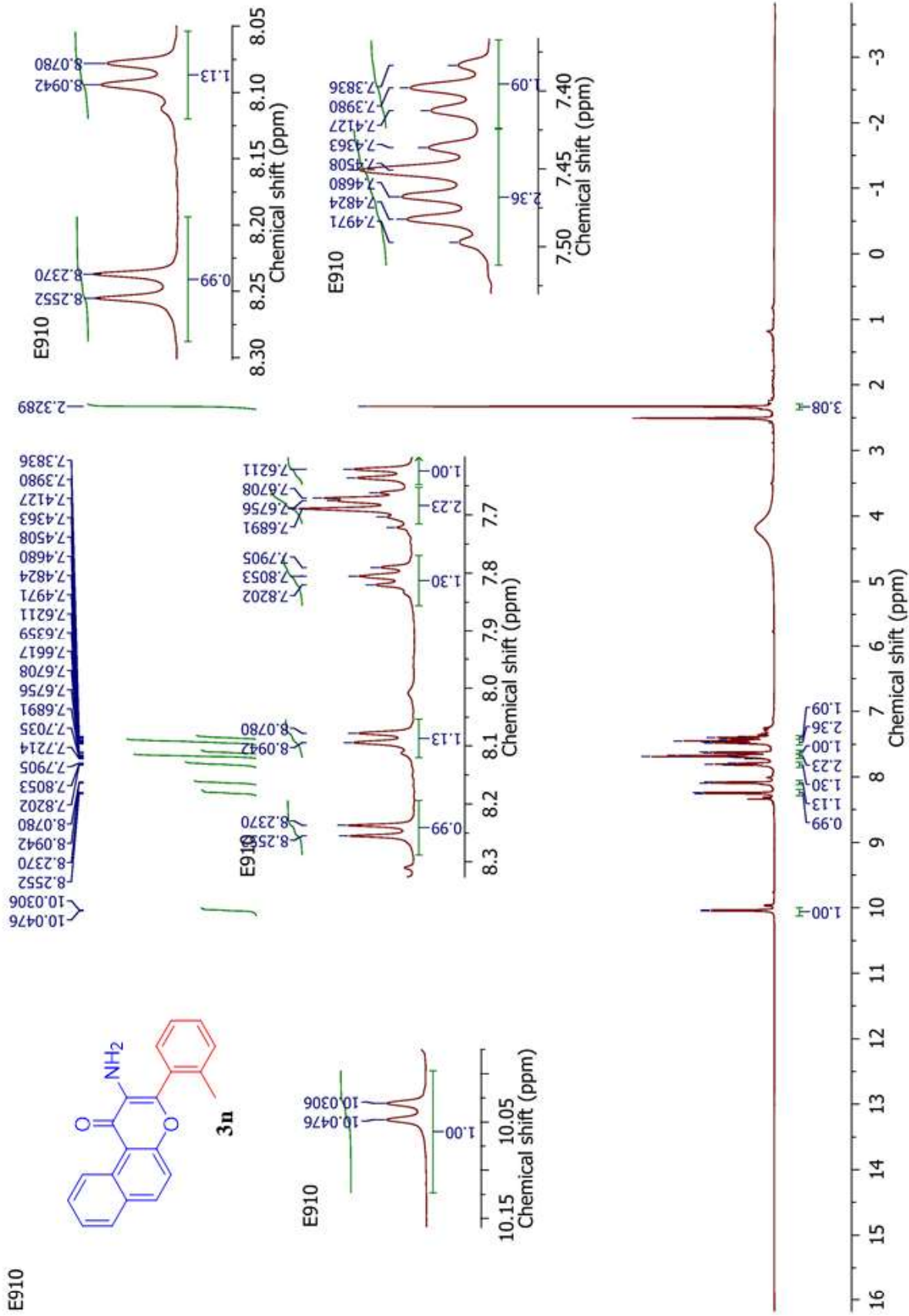
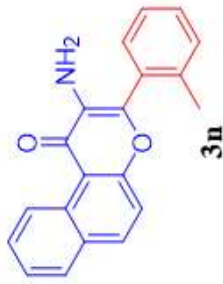
# Display Report

**Analysis Info**  
Analysis Name D:\Data\User Data\Dr. Jerome\MNTE96.d  
Method Tune\_pos\_Standard.m  
Sample Name MEOH  
Comment  
Acquisition Date 7/24/2019 2:40:44 PM  
Operator HRMS  
Instrument maxis impact 1819696.00160

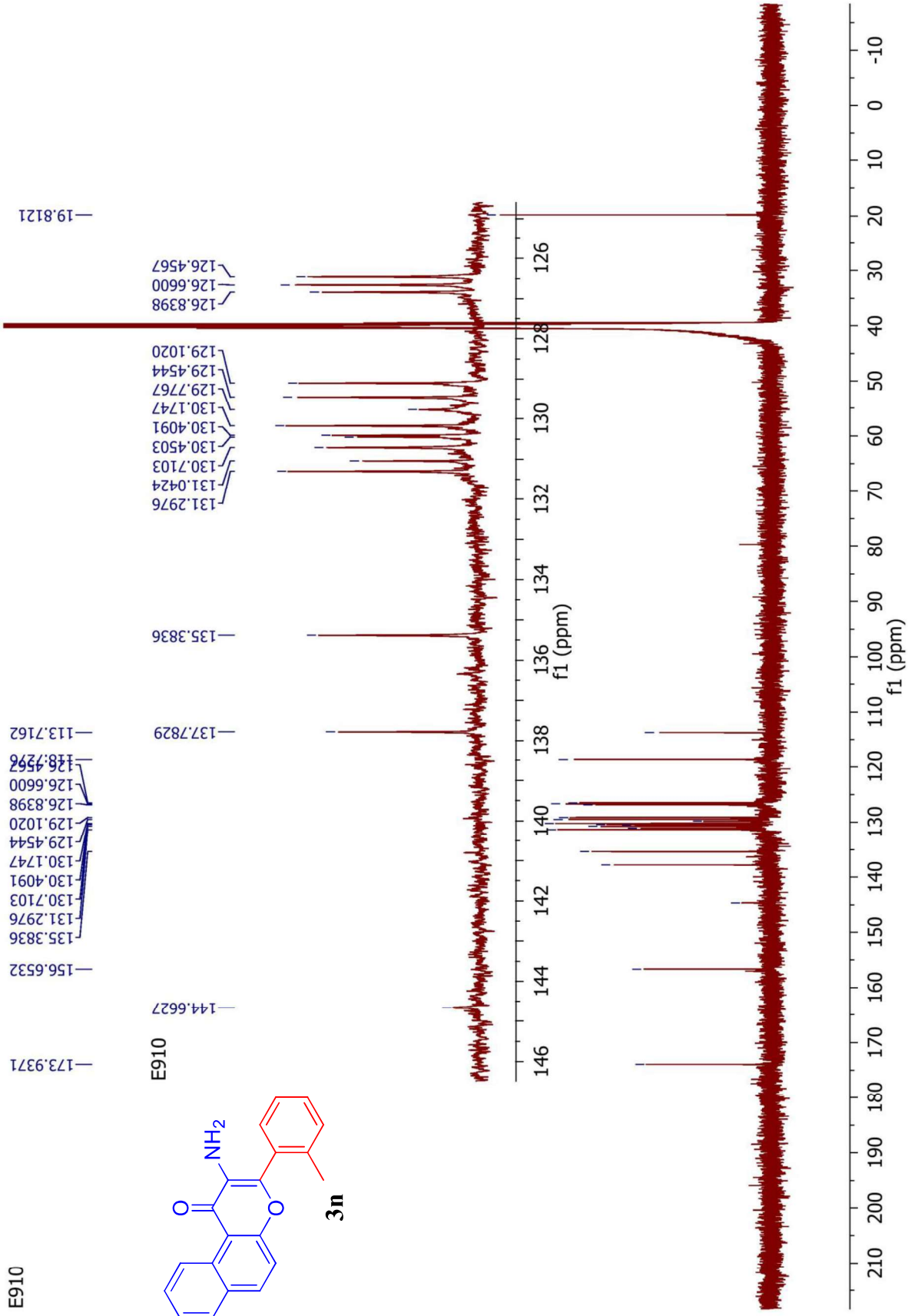
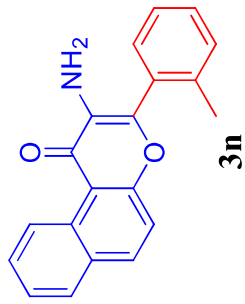
**Acquisition Parameter**  
Source Type ESI  
Polarity Positive  
Scan Range 50 m/z  
Scan End 3000 m/z  
Ion Polarity Positive  
Set Corona 4500 V  
Set End Plate Offset -500 V  
Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.5 Bar  
Set Dry Gas 200 °C  
Set Divert Valve 4.0 l/min  
Set APCI Heater Source 0 °C



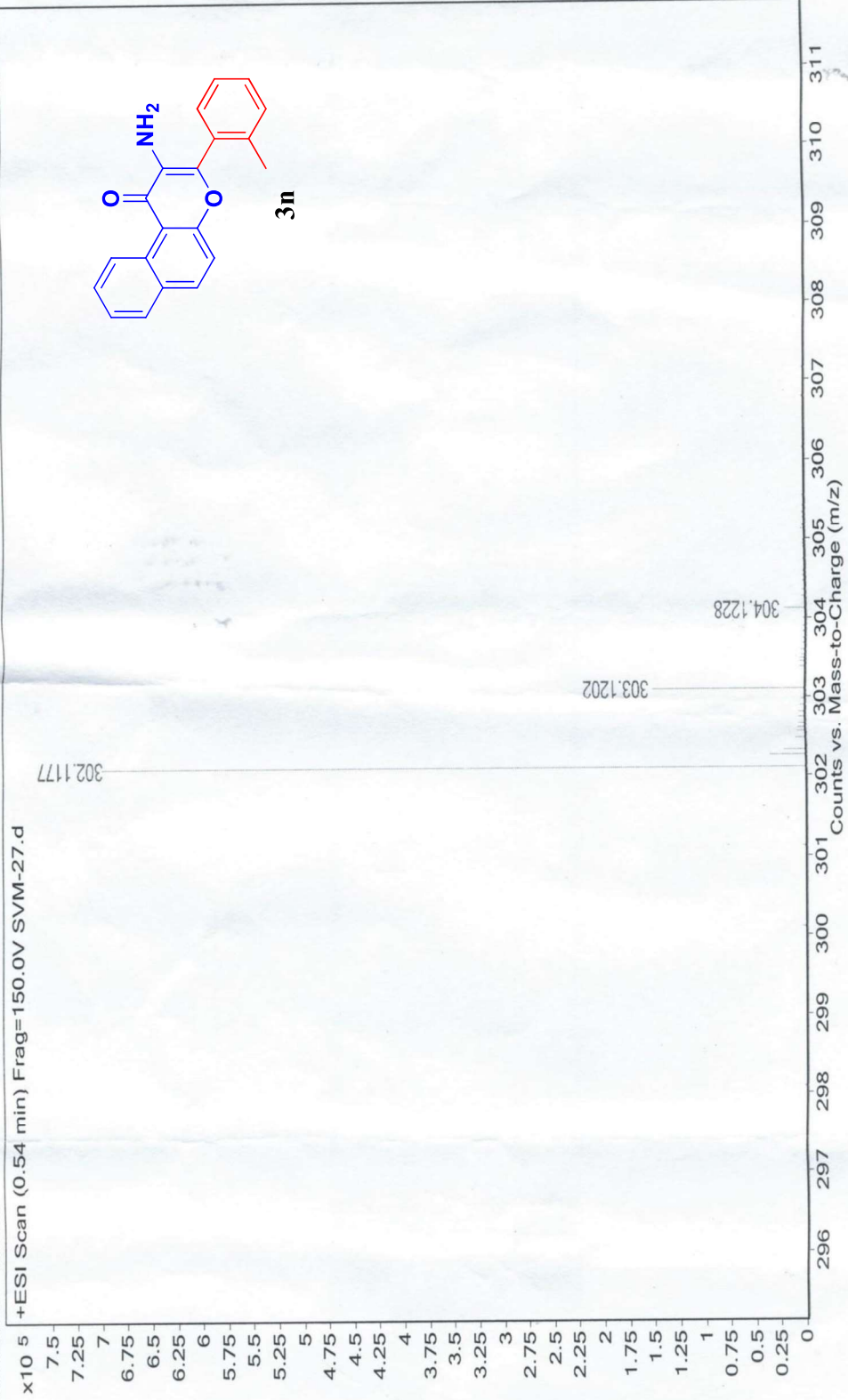
E910



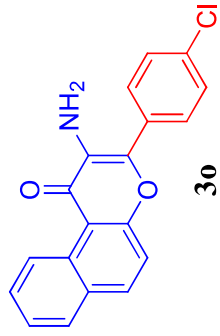
E910



**Sample Name** Seenivasan (1113) **Position** Vial 33 **User Name** Success  
**Inj Vol** 1 **InjPosition** **Instrument 1** Instrument 1  
**Data Filename** SVM-27.d **ACQ Method** ISOCRATIC.m **SampleType** Sample **IRM Calibration Status** Acquired Time  
 12/6/2019 1:14:30 PM

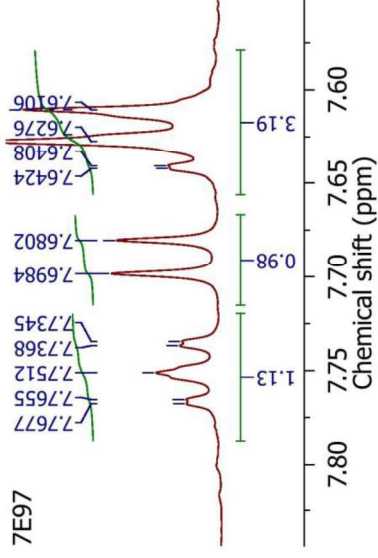


7E97

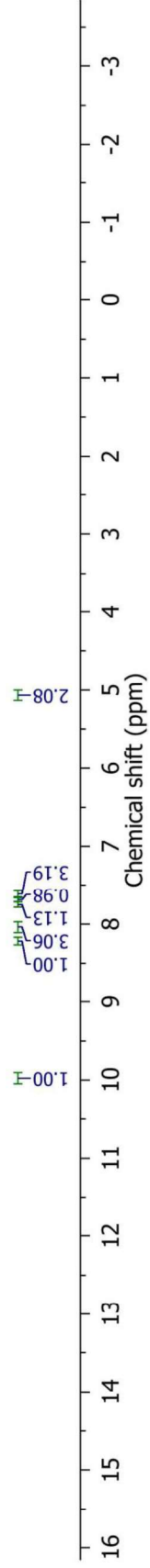
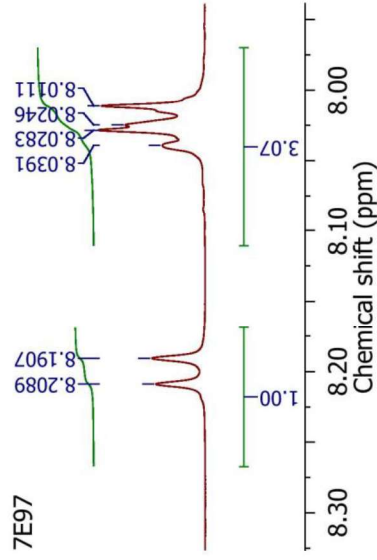


9.9795  
9.9625  
8.2089  
8.1907  
8.0391  
8.0283  
8.0246  
8.0111  
7.7512  
7.7368  
7.7345  
7.6984  
7.6802  
7.6424  
7.6408  
7.6276  
5.0688

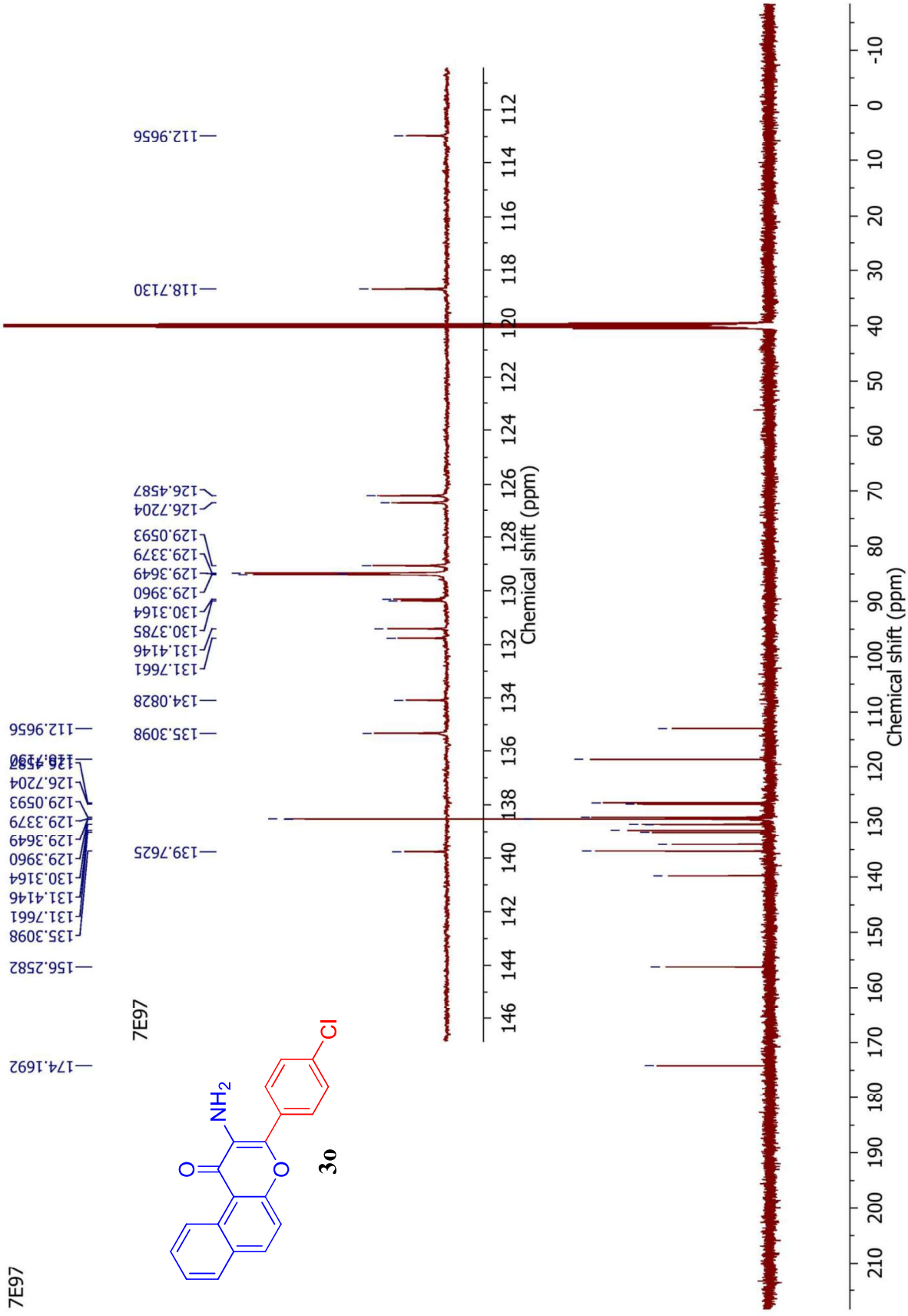
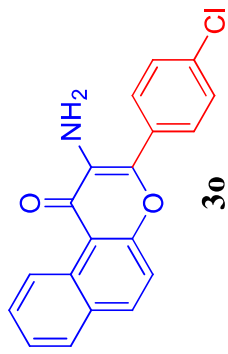
7E97



7E97



7E97

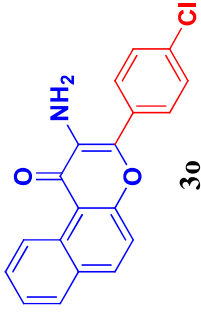
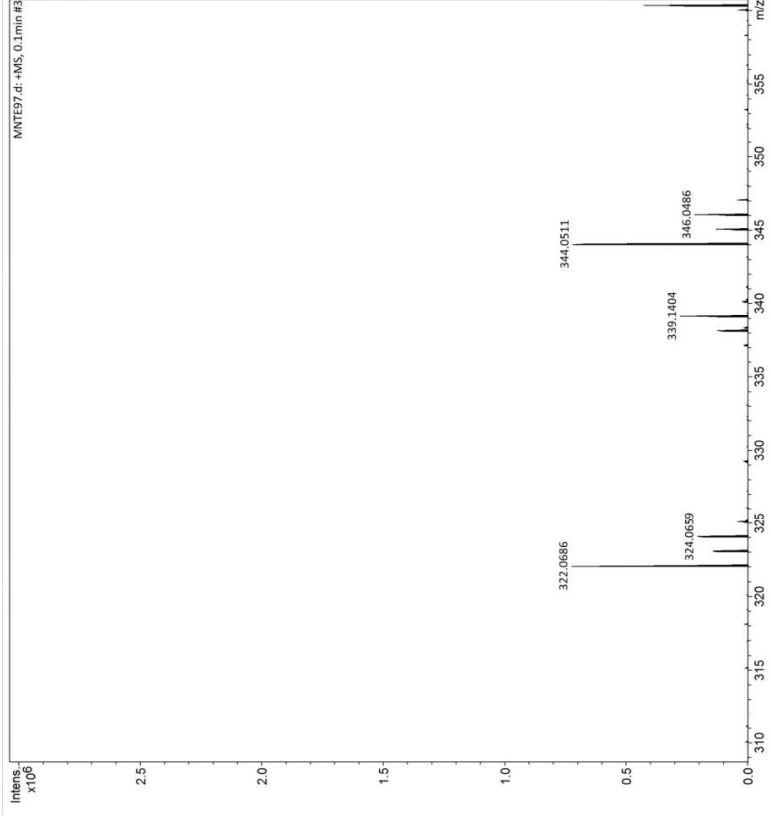


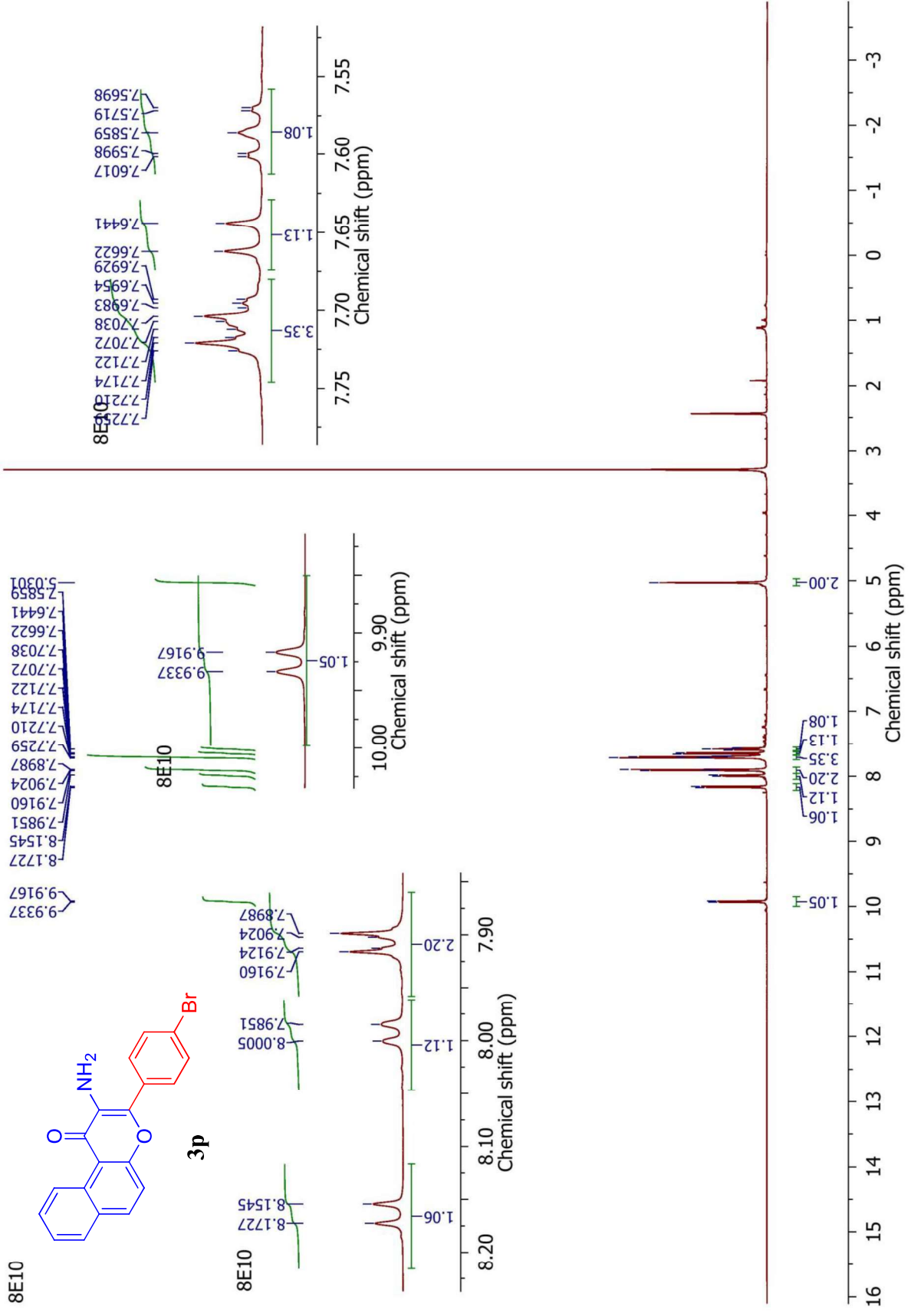


# Display Report

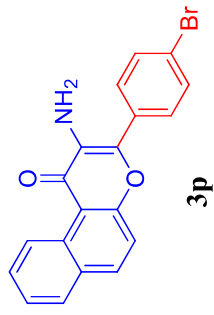
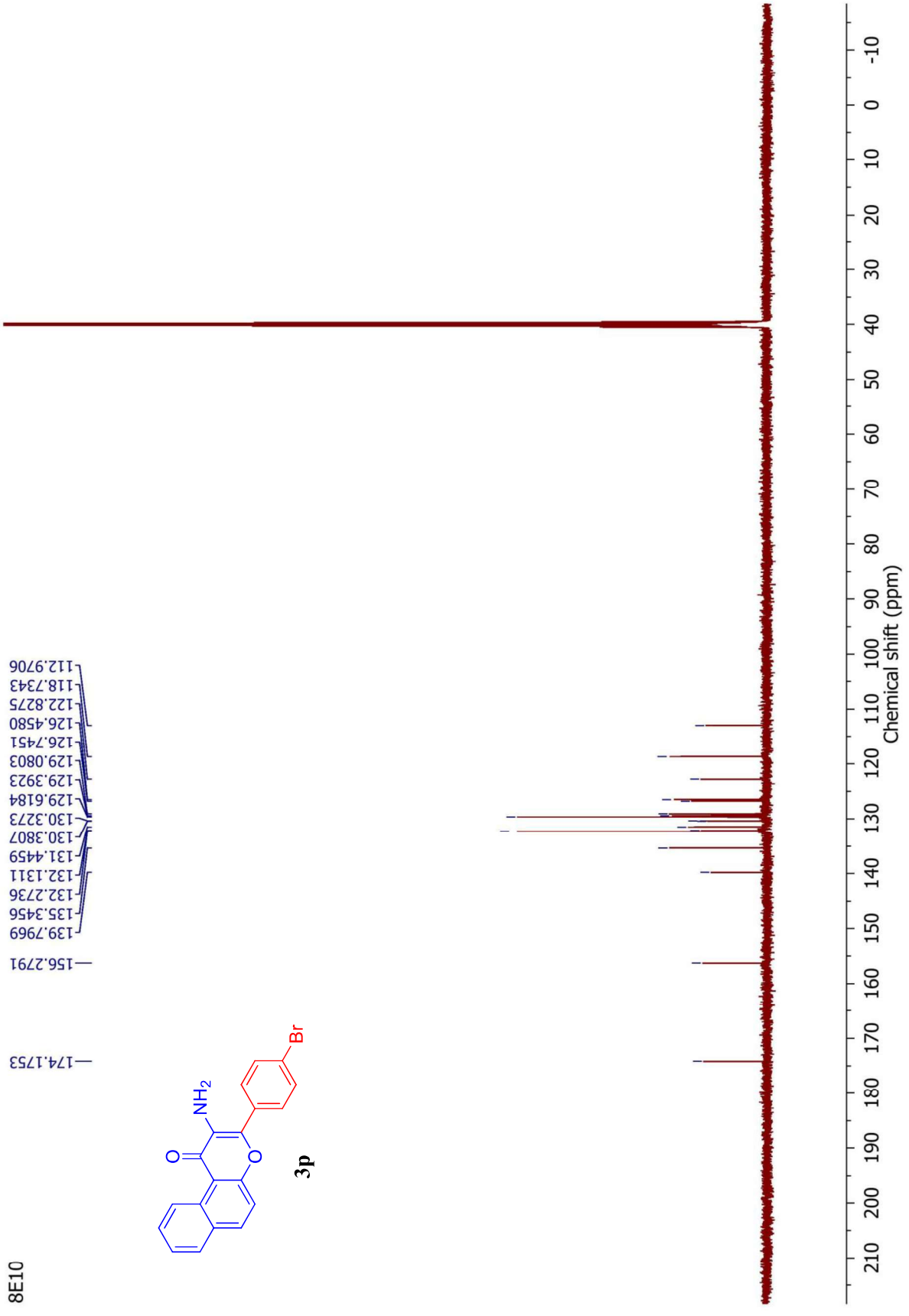
**Analysis Info**  
Analysis Name D:\Data\User Data\Dr. Jerome\MNTE97.d  
Method Tune\_pos\_Standard.m  
Sample Name BLANK  
Comment  
Acquisition Date 7/23/2019 12:13:38 PM  
Operator HRMS  
Instrument maxis impact 1819696.00160

**Acquisition Parameter**  
Source Type ESI  
Pulsed Active  
Scan Begin 50 m/z  
Scan End 3000 m/z  
Ion Polarity Positive  
Set Corona 4500 V  
Set End Plate Offset -500 V  
Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.5 Bar  
Set Dry Heater 200 °C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Source  
Set APCI Heater 0 °C





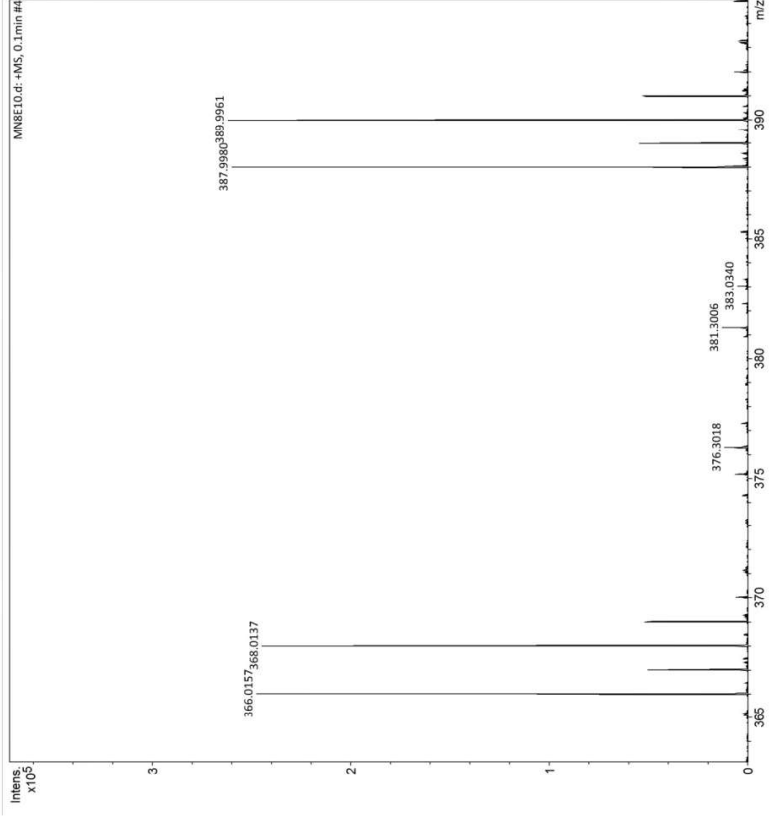
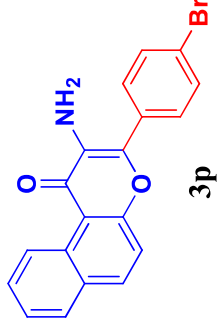
8E10



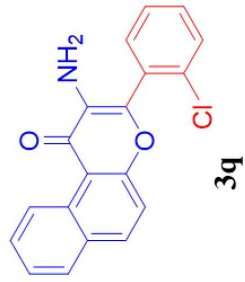
# Display Report

**Analysis Info**  
Analysis Name D:\Data\User Data\Dr.Jerome\MN8E10.d  
Method Tune\_pos\_Mid.m  
Sample Name MEOH  
Comment  
Acquisition Date 7/25/2019 10:57:32 AM  
Operator HRMS  
Instrument maxis impact 1819696.00160

**Acquisition Parameter**  
Source Type ESI  
ESI Active  
Tune\_pos\_Mid.m  
Scan Begin 100 m/z  
Scan End 5000 m/z  
Ion Polarity Positive  
Set Capillary 3500 V  
Set End Plate Offset -500 V  
Set Charging Voltage 2000 V  
Set Corona 0 nA  
Set Nebuliser 0.3 Bar  
Set Dry Heater 200 °C  
Set Dry Gas 4.0 l/min  
Set Divert Valve Source  
Set APCI Heater 0 °C



E934

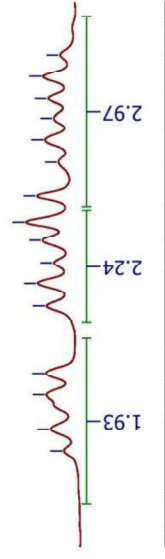


10.0559  
10.0389

8.2443  
8.2261  
8.0958  
8.0800  
7.8068  
7.7832  
7.7682  
7.7222  
7.7065  
7.6773  
7.6646  
7.6469  
7.6084  
7.5933  
7.5795  
7.5647  
4.7035

E934

7.8218  
7.8068  
7.7832  
7.7682  
7.7222  
7.7065  
7.6924  
7.6773  
7.6646  
7.6469  
7.6232  
7.6084  
7.5933  
7.5795  
7.5647  
7.5497



E934

10.0559  
10.0389

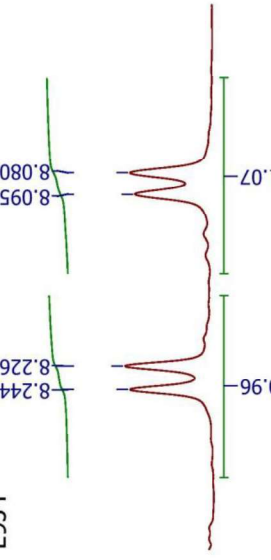
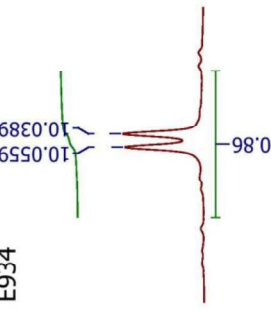
E934

8.0958  
8.0800

7.8068  
7.7832  
7.7682

7.6084  
7.5933

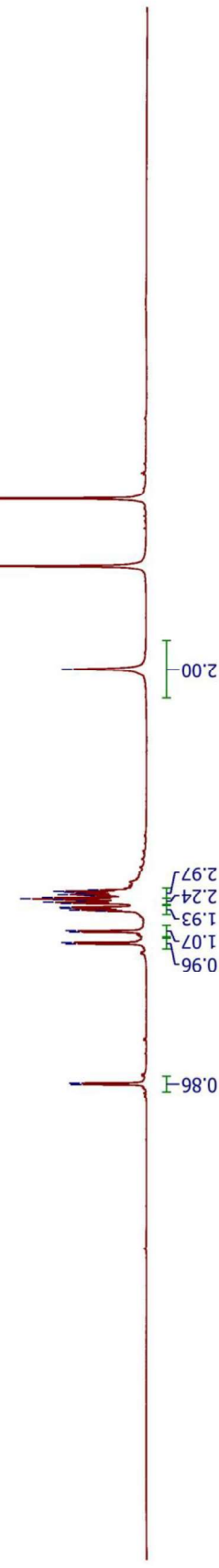
7.5497



10.2 10.1 10.0 9.9  
Chemical shift (ppm)

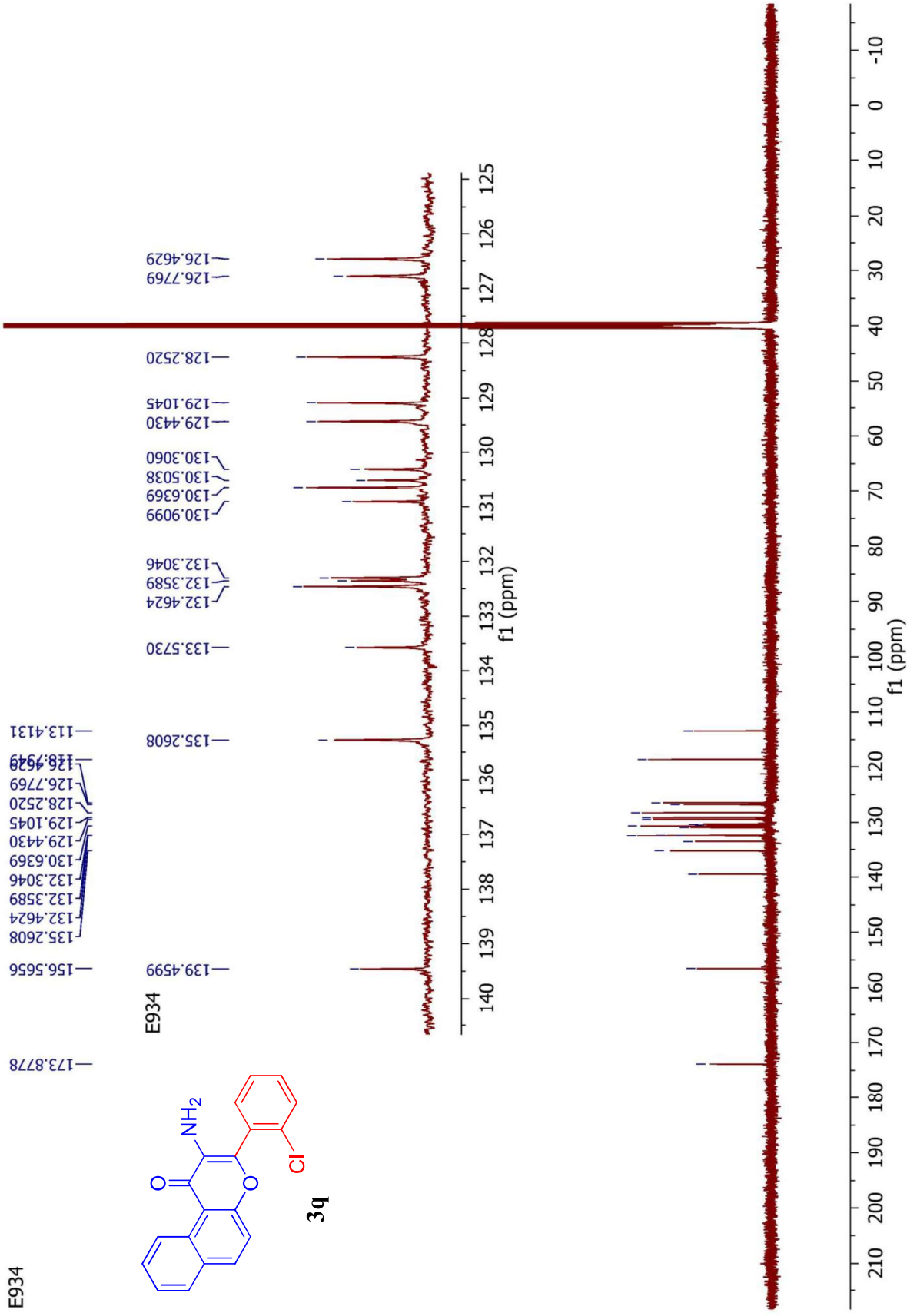
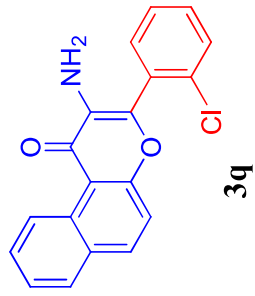
8.35 8.25 8.15 8.05  
Chemical shift (ppm)

7.80 7.70 7.60  
Chemical shift (ppm)

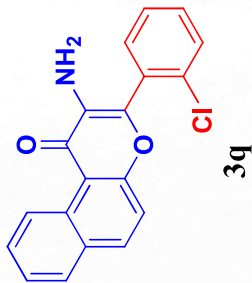
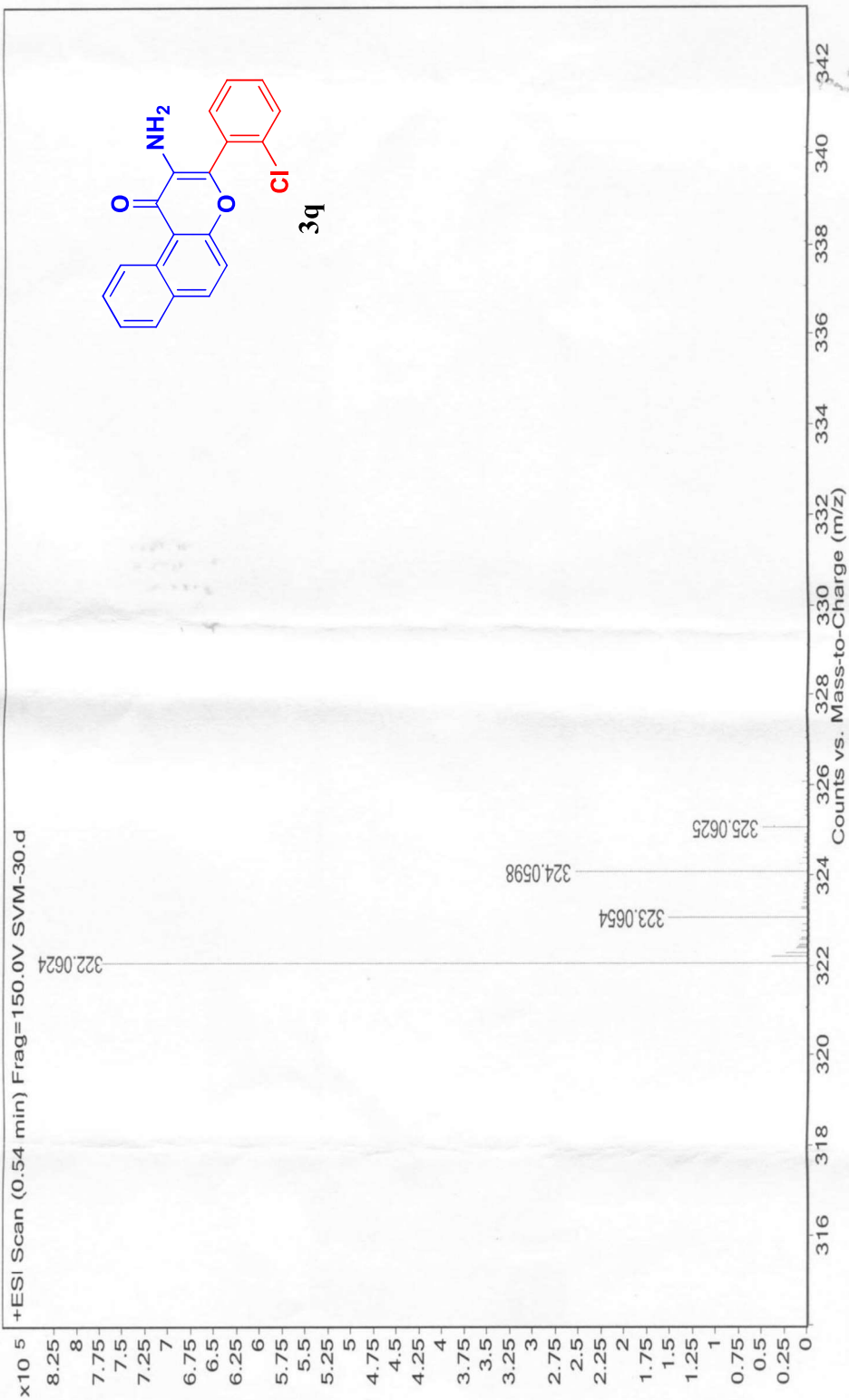


16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3  
Chemical shift (ppm)

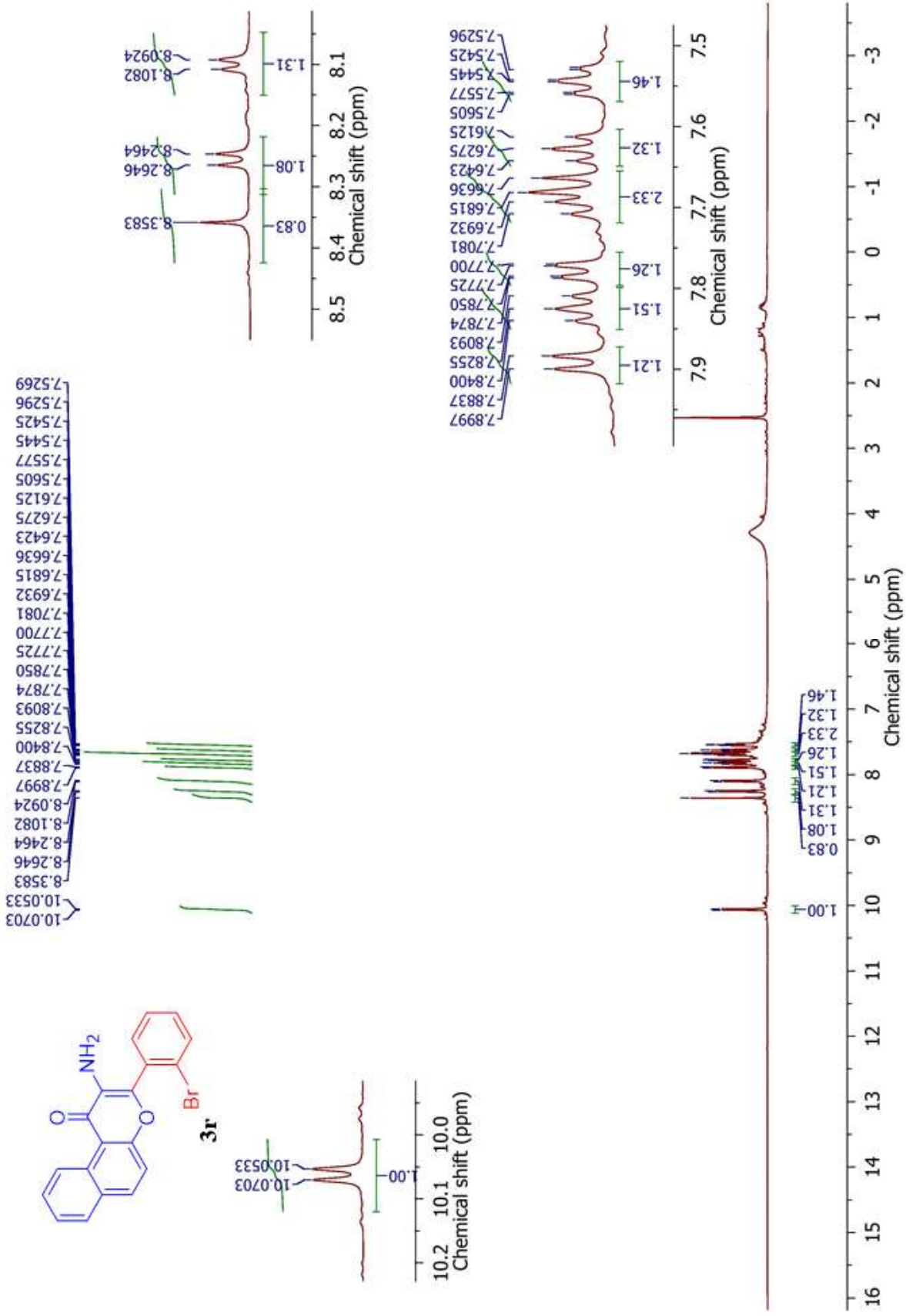
E934

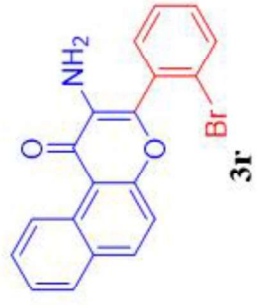
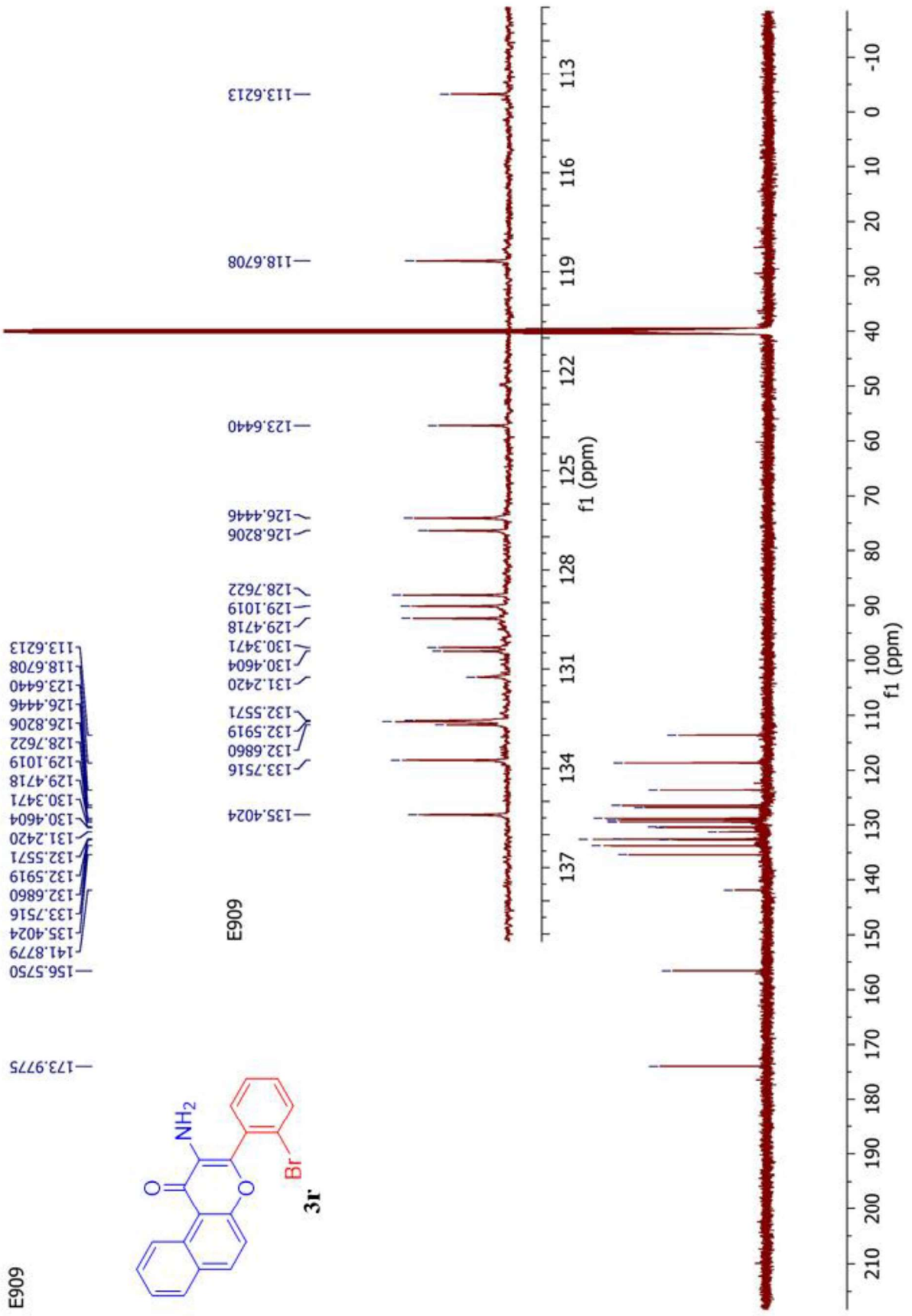


Sample Name Seenuvasan (1113) Position Vial 36 User Name  
Inj Vol 1 InjPosition ACQ Method ISOCRATIC.m Instrument Name  
Data Filename SVM-30.d SVM-30.d Instrument Type Sample IRM Calibration Status Success  
Comment 12/6/2019 1:25:21 PM  
Acquired Time





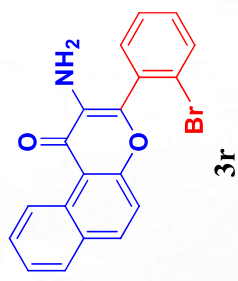
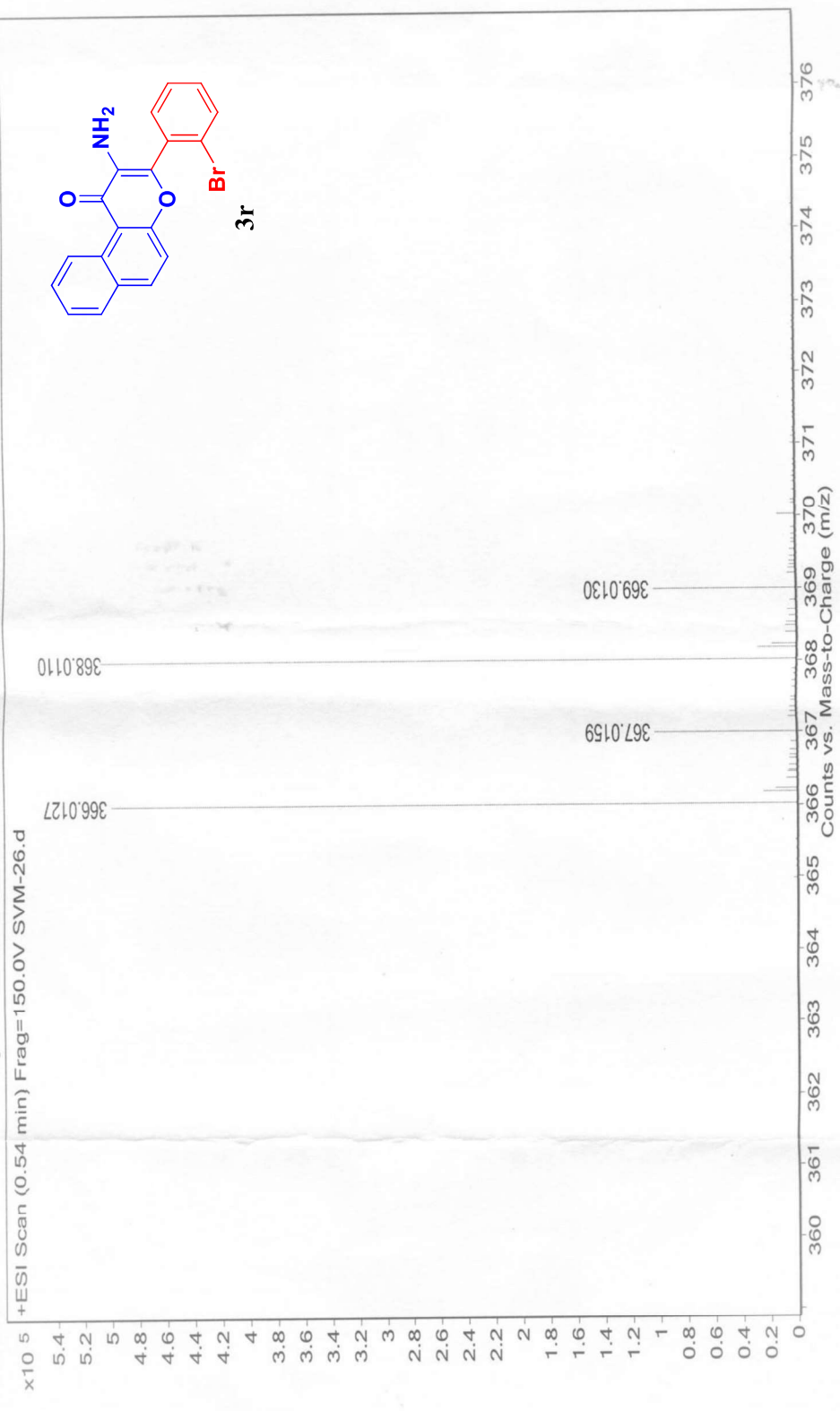




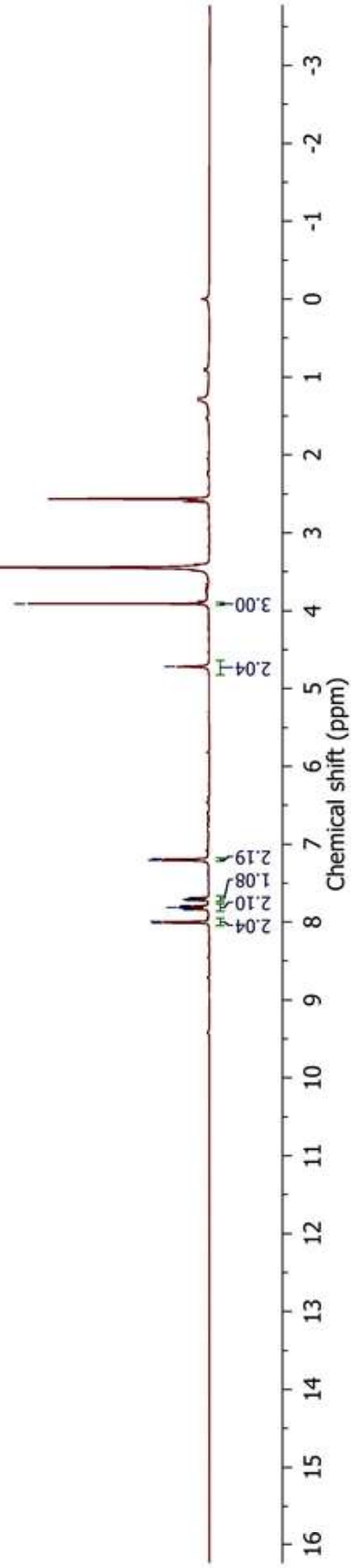
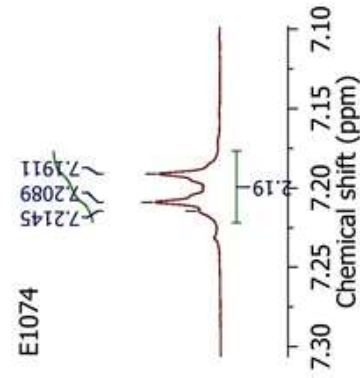
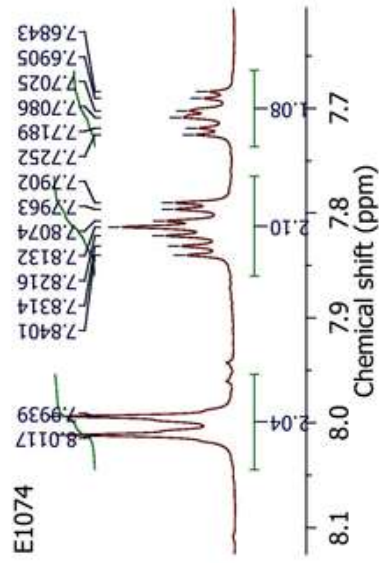
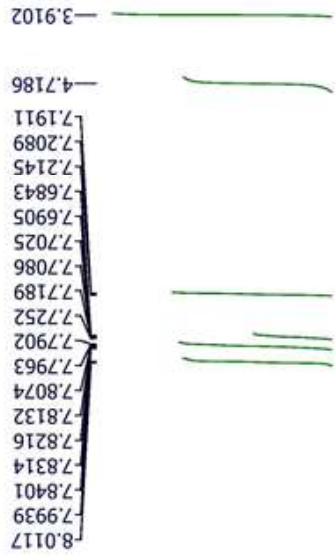
E909

E909

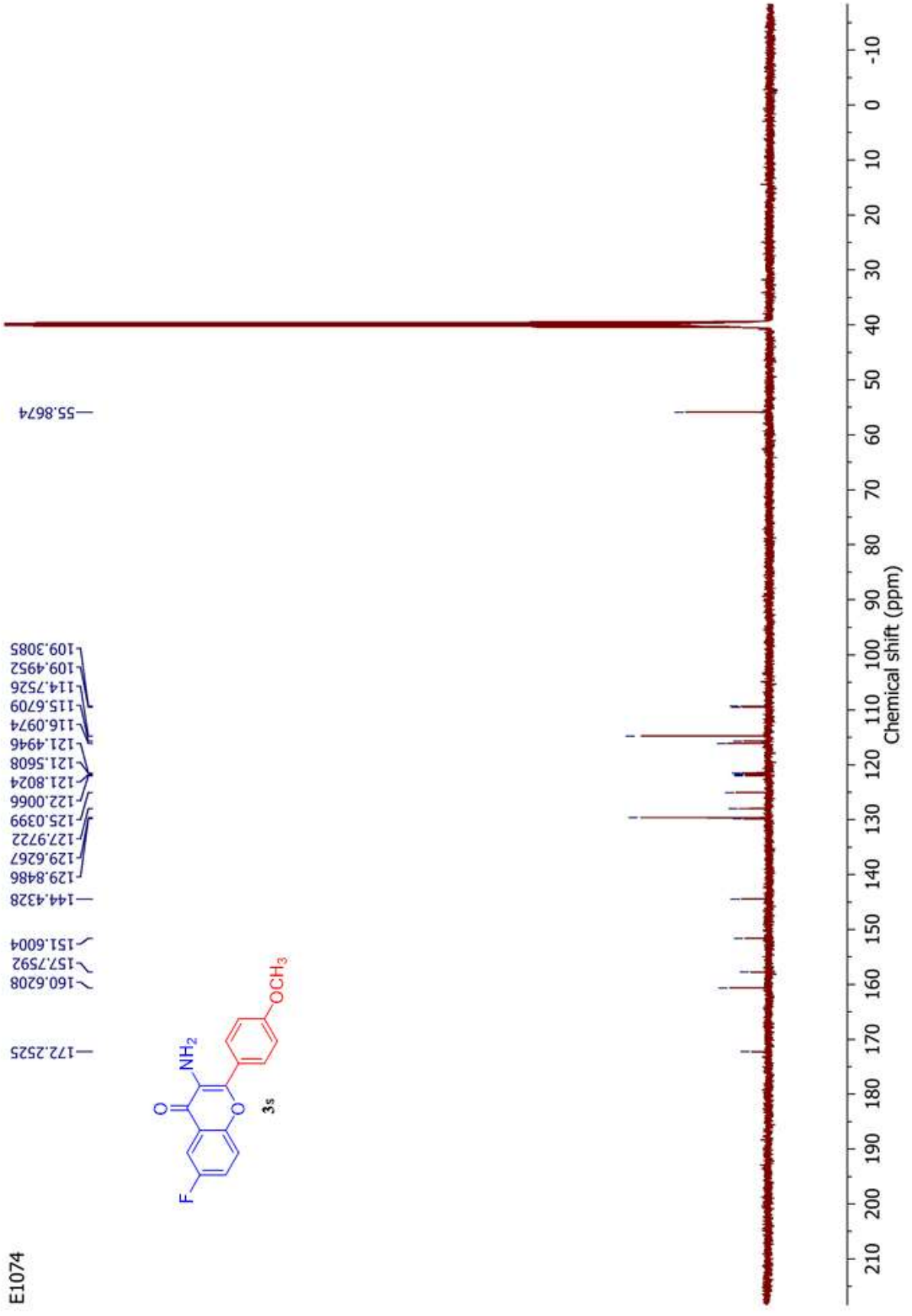
Sample Name: Seenuvasan (1113)    Vial 32    User Name: Success  
 Inj Vol: 1    InjPosition: ISOCRATIC.m    Instrument 1: Sample    IRM Calibration Status: 12/6/2019 1:10:50 PM  
 Data Filename: SVM-26.d    ACQ Method: ISOCRATIC.m    Instrument Name: SampleType    Comment: Acquired Time



E1074



E1074



E991

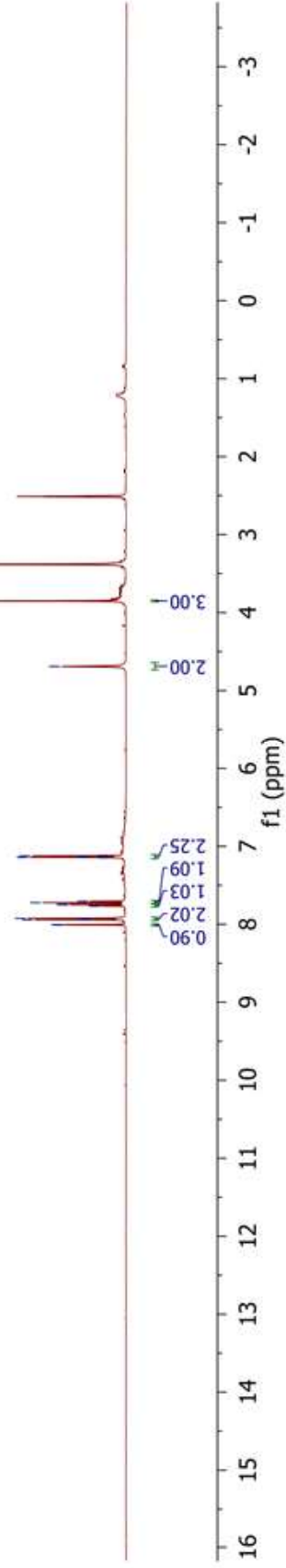
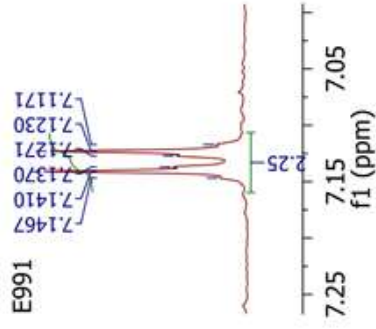
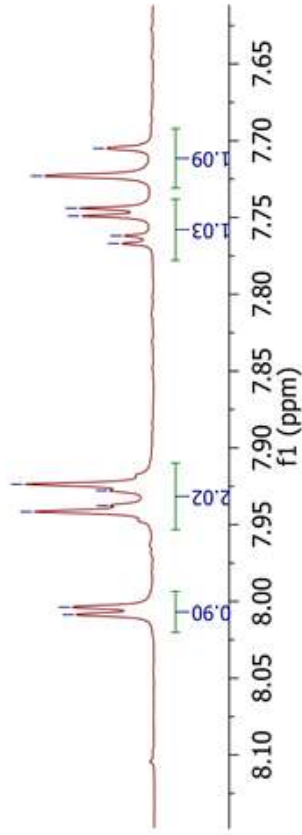


8.0086  
8.0038  
7.9416  
7.9375  
7.9278  
7.9237  
7.7670  
7.7619  
7.7490  
7.7439  
7.7229  
7.7050  
7.1467  
7.1410  
7.1370  
7.1271  
7.1230  
7.1171  
4.6906  
3.8510

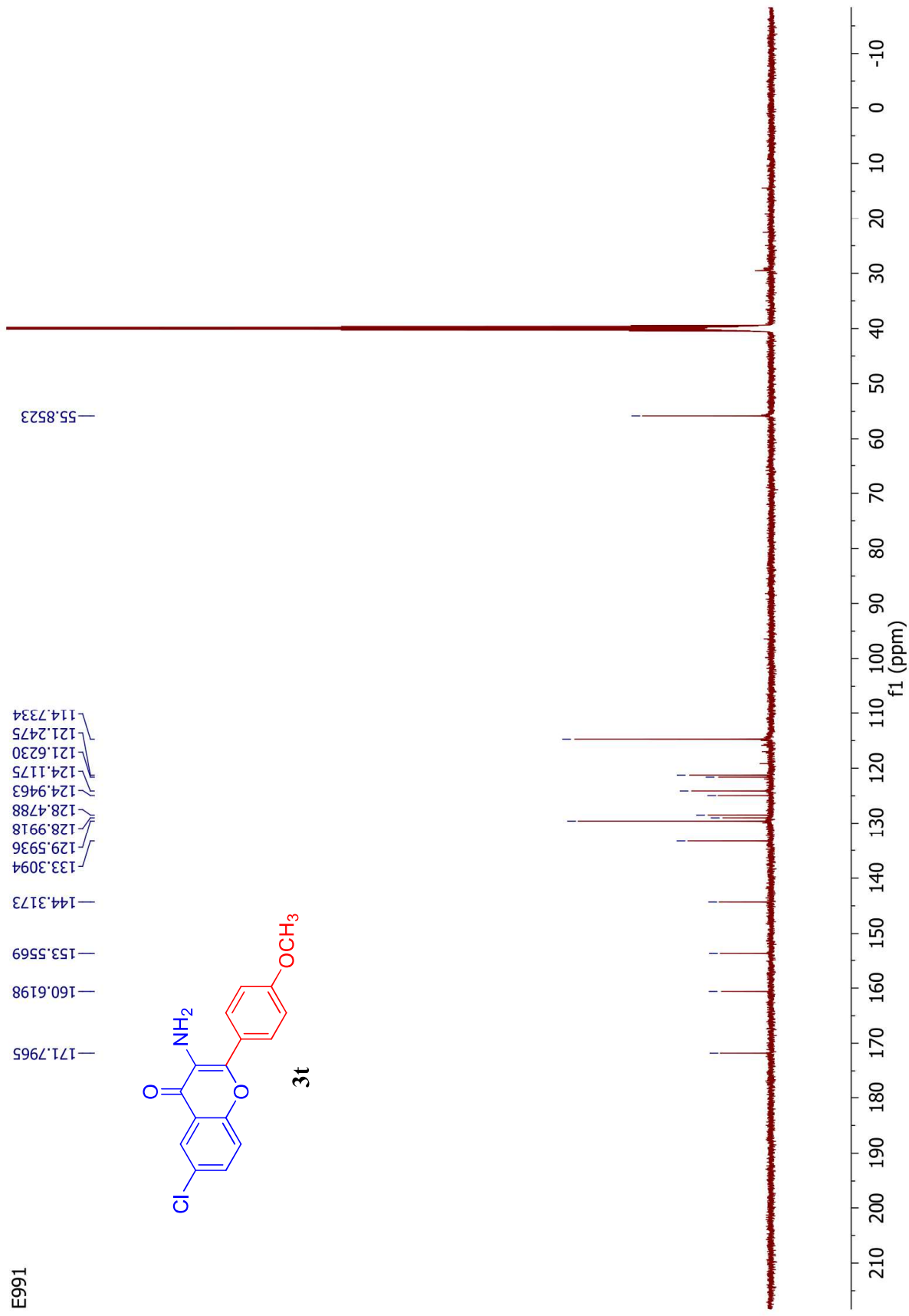
E991

8.0086  
8.0038  
7.9416  
7.9375  
7.9278  
7.9237

7.7670  
7.7619  
7.7490  
7.7439  
7.7229  
7.7050



E991





Sample Name: Seenivasan (1113)    Vial: 45    Instrument Name: Instrument 1    User Name: Success  
 Inj Vol: 1    InjPosition: ISOCRATIC.m    SampleType: Sample    IRM Calibration Status: 12/6/2019 1:58:12 PM  
 Data Filename: SVM-38.d    ACQ Method: ISOCRATIC.m    Comment:    Acquired Time:

