

## Supporting Information

### **Pd(II)-Catalyzed Regioselective Functionalization of C–H Bond of Antipyrenes: Synthesis of Pyrazolono-maleimides and Pyrazolono-quinones**

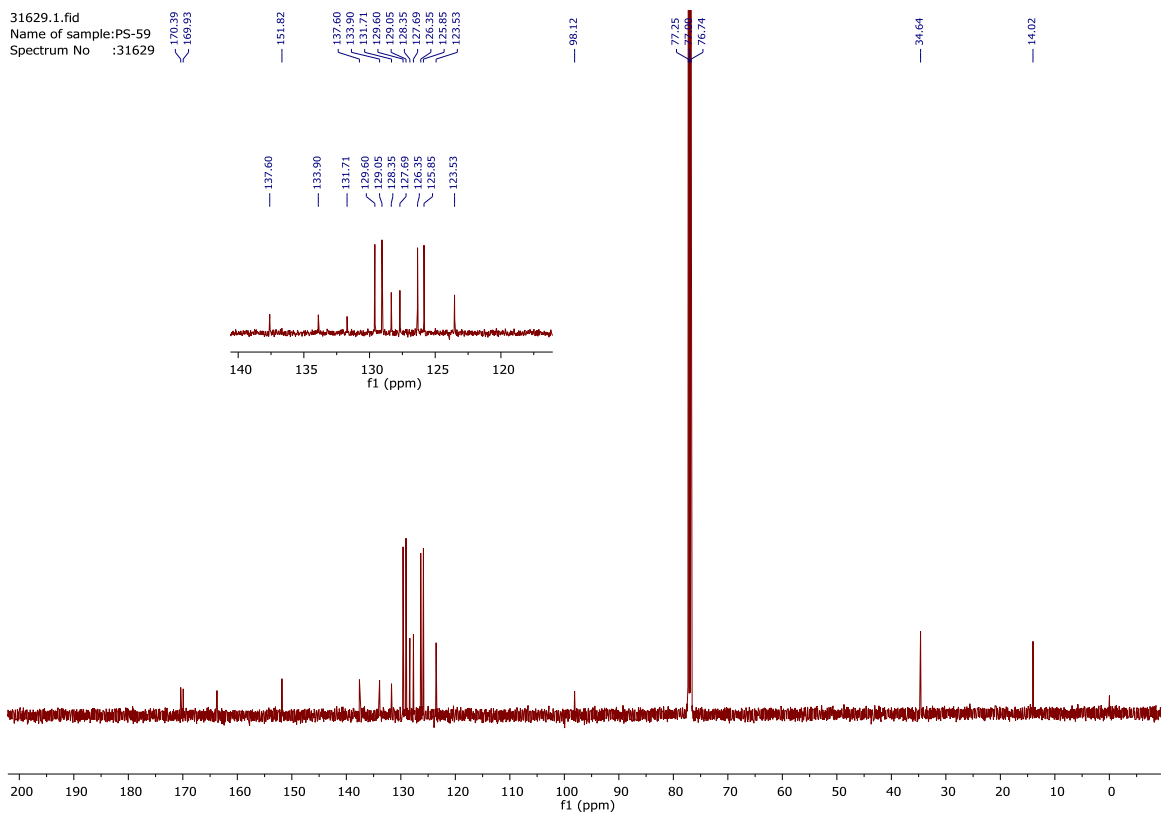
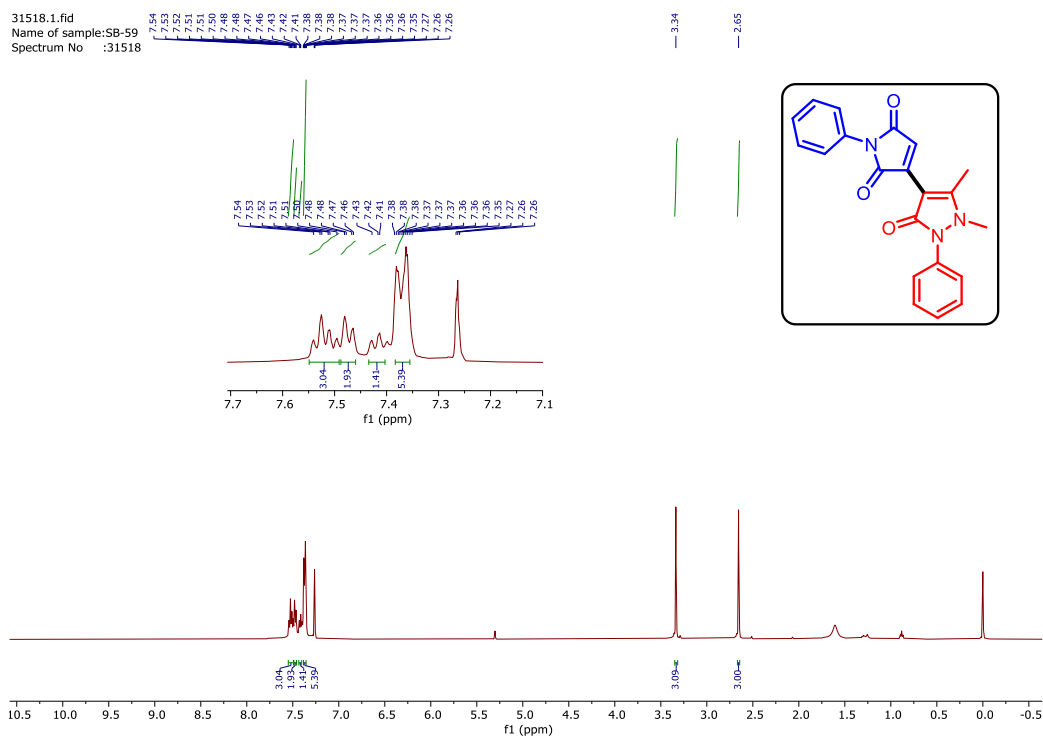
Priya Sonowal, Pratiksha Bhorali, Sabera Sultana, and Sanjib Gogoi\*

Applied Organic Chemistry, Chemical Sciences & Technology Division, CSIR-North East Institute of Science and Technology, Jorhat 785006, AcSIR, Ghaziabad-201002, India. E-mail: skgogoi1@gmail.com; sanjibgogoi@neist.res.in

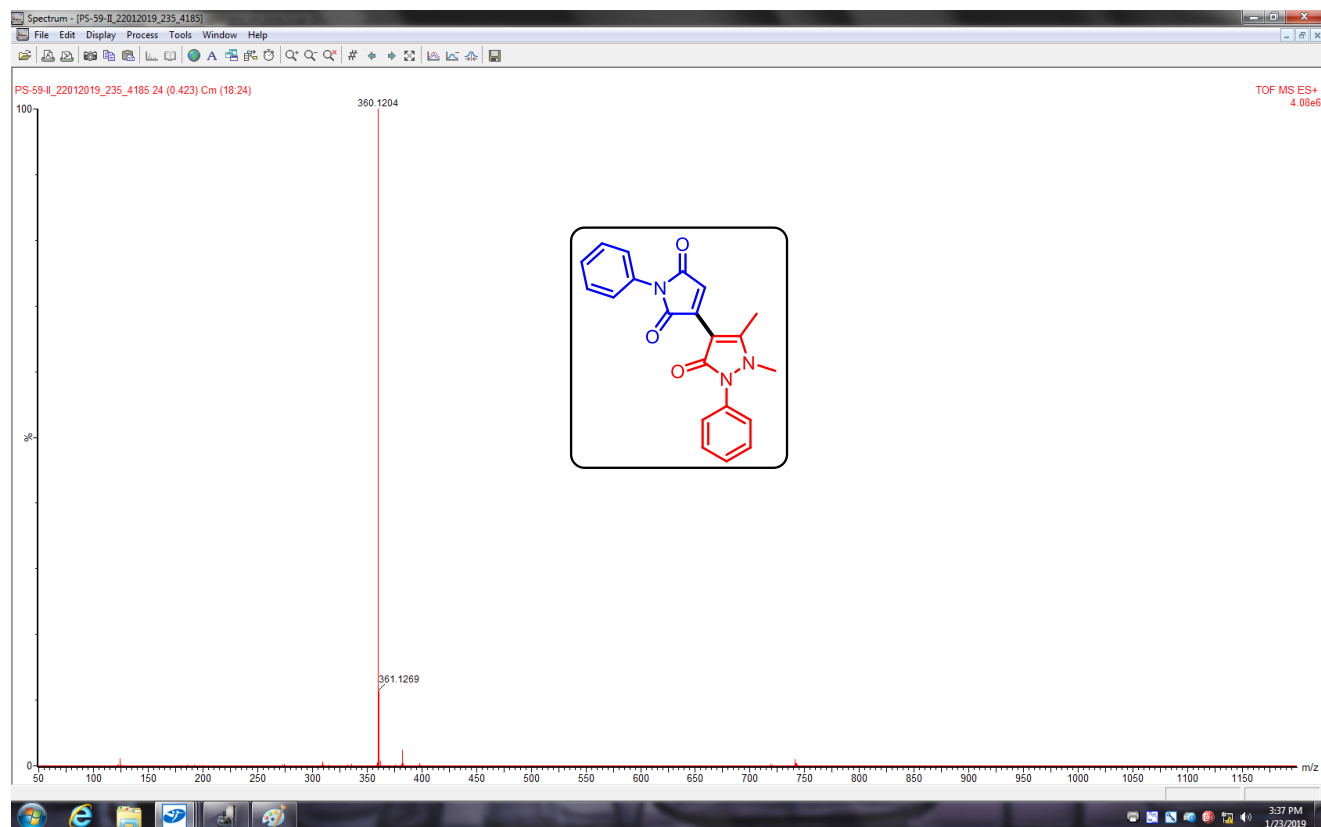
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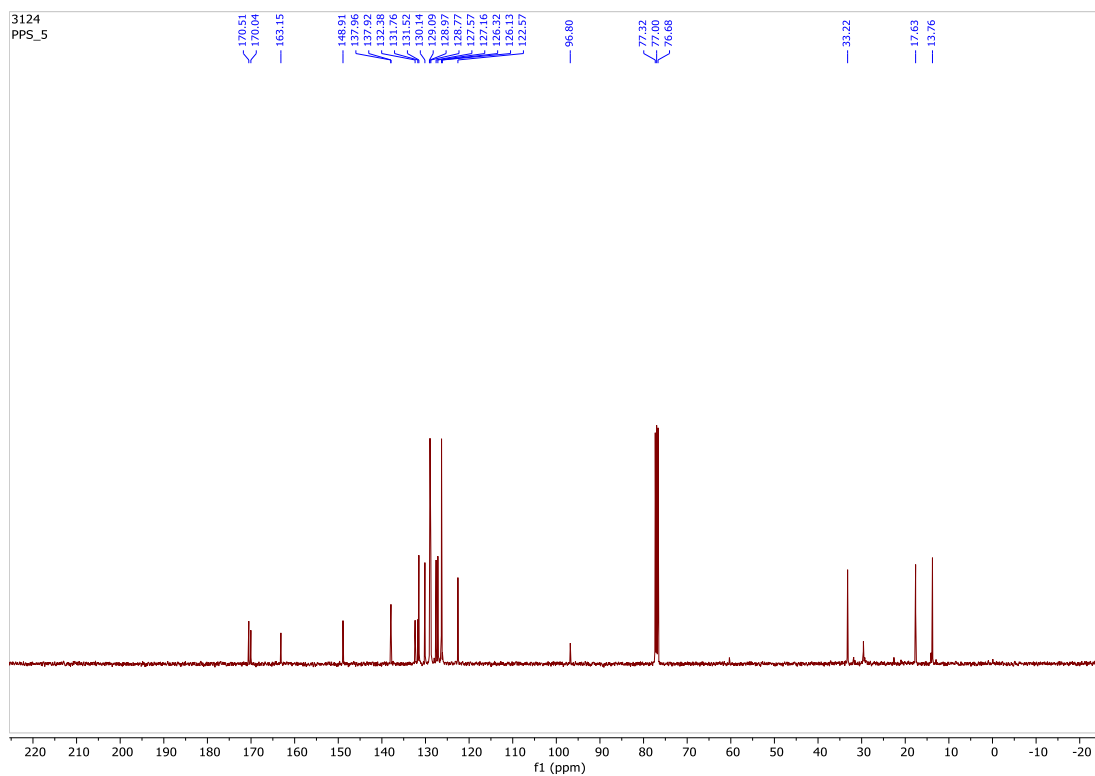
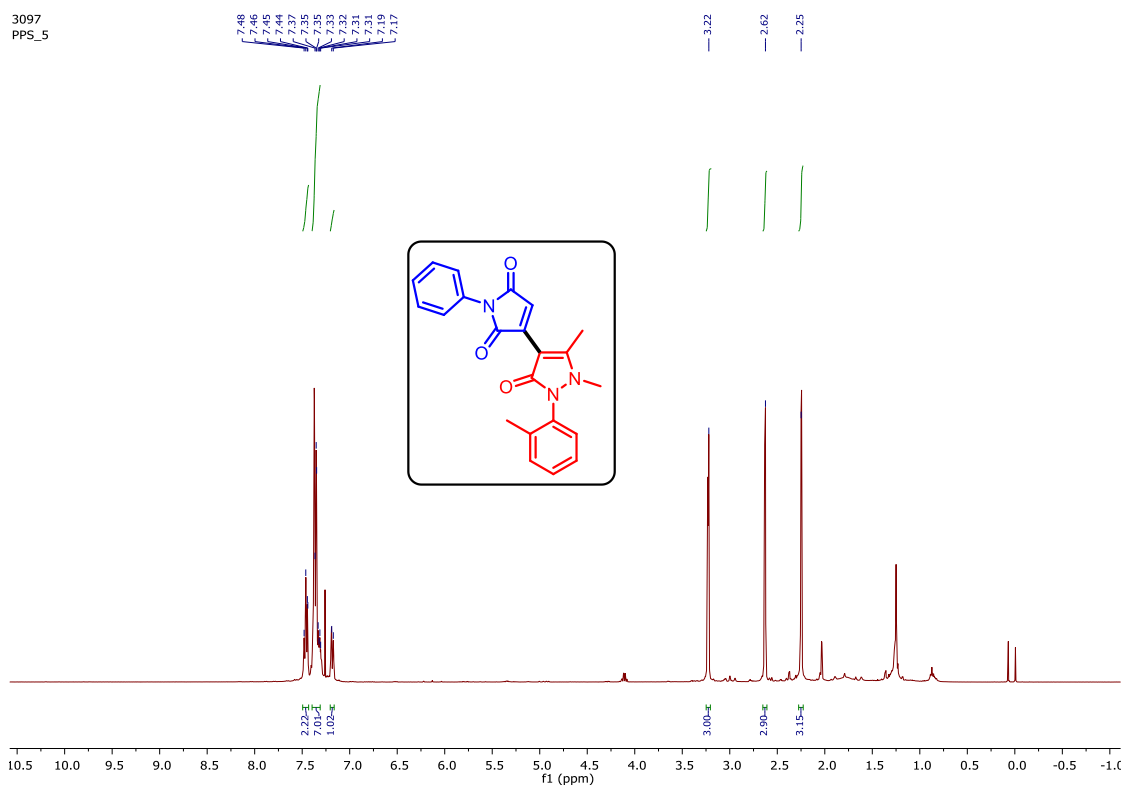
# <sup>1</sup>H and <sup>13</sup>C of Compound 3aa (500 & 125 MHz, CDCl<sub>3</sub>):



## HRMS Spectra of Compound 3aa:

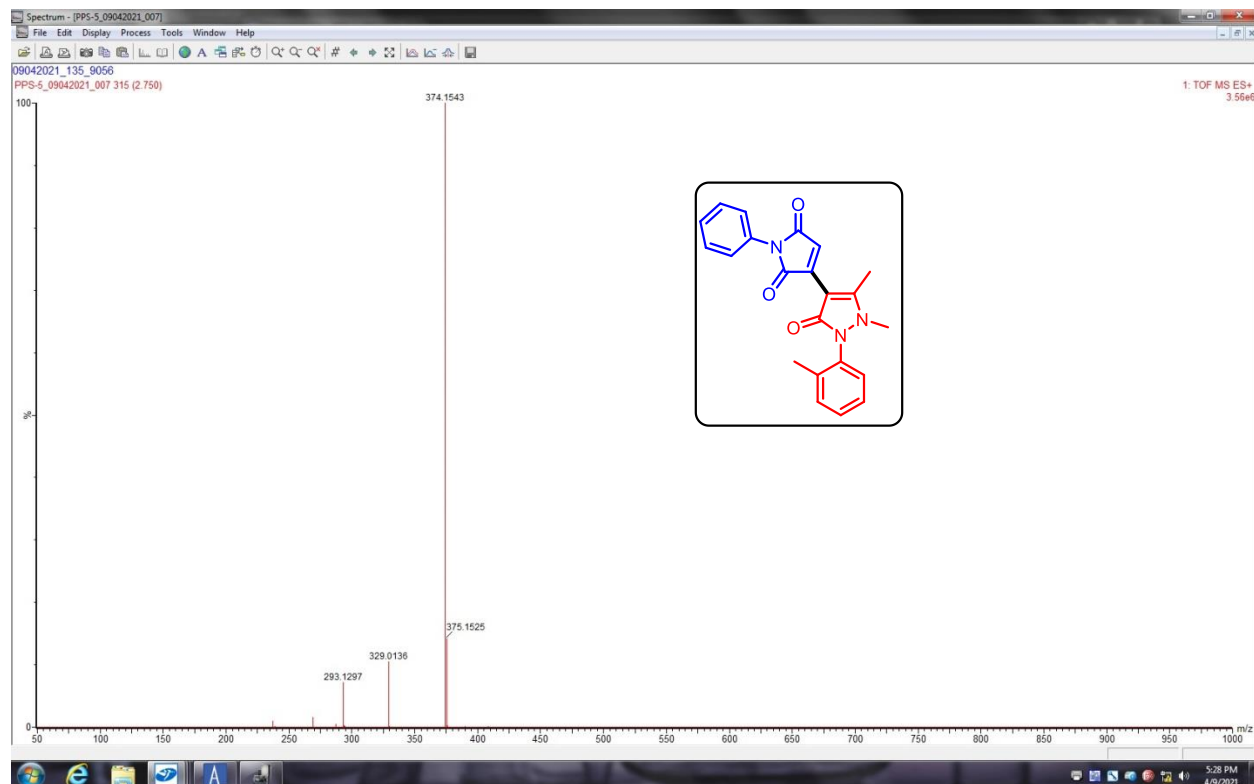


**$^1\text{H}$  and  $^{13}\text{C}$  of Compound 3ba (400 & 100 MHz,  $\text{CDCl}_3$ ):**

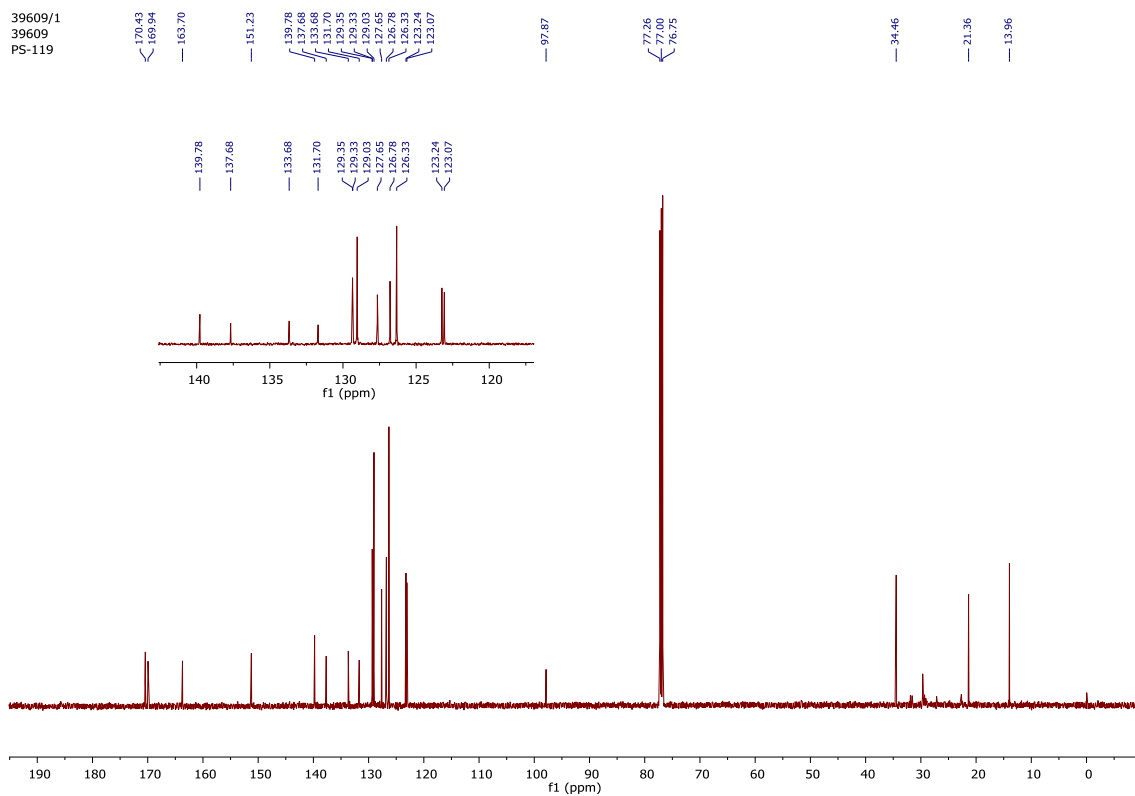
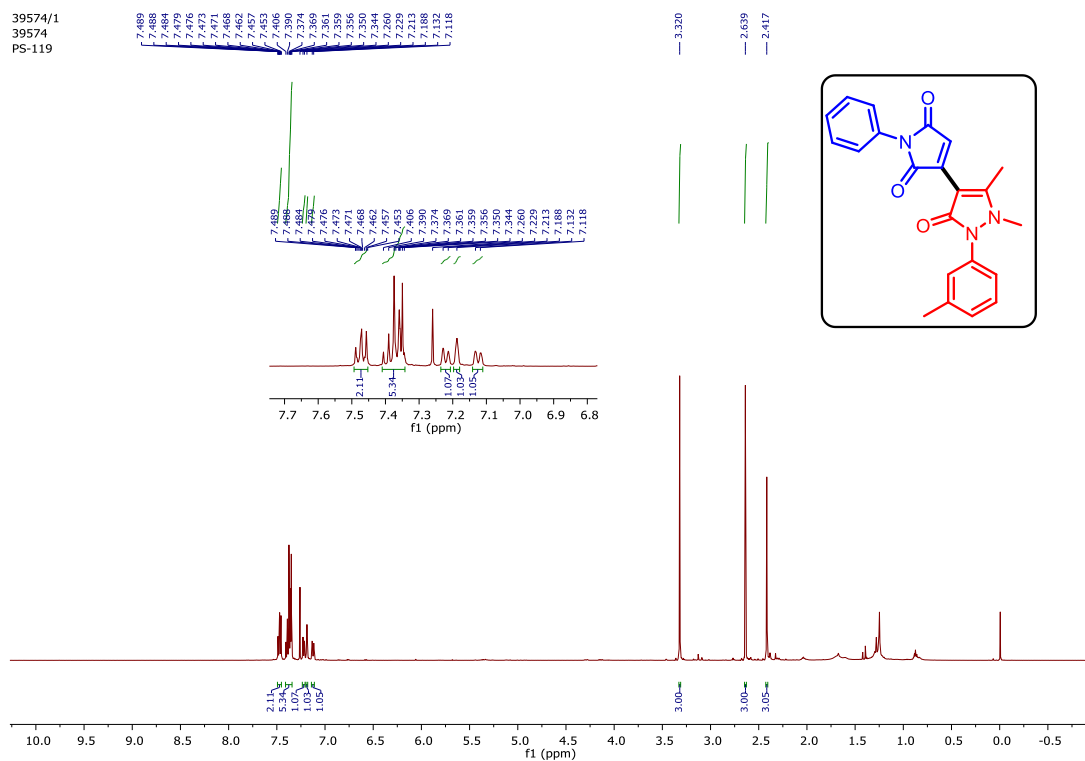




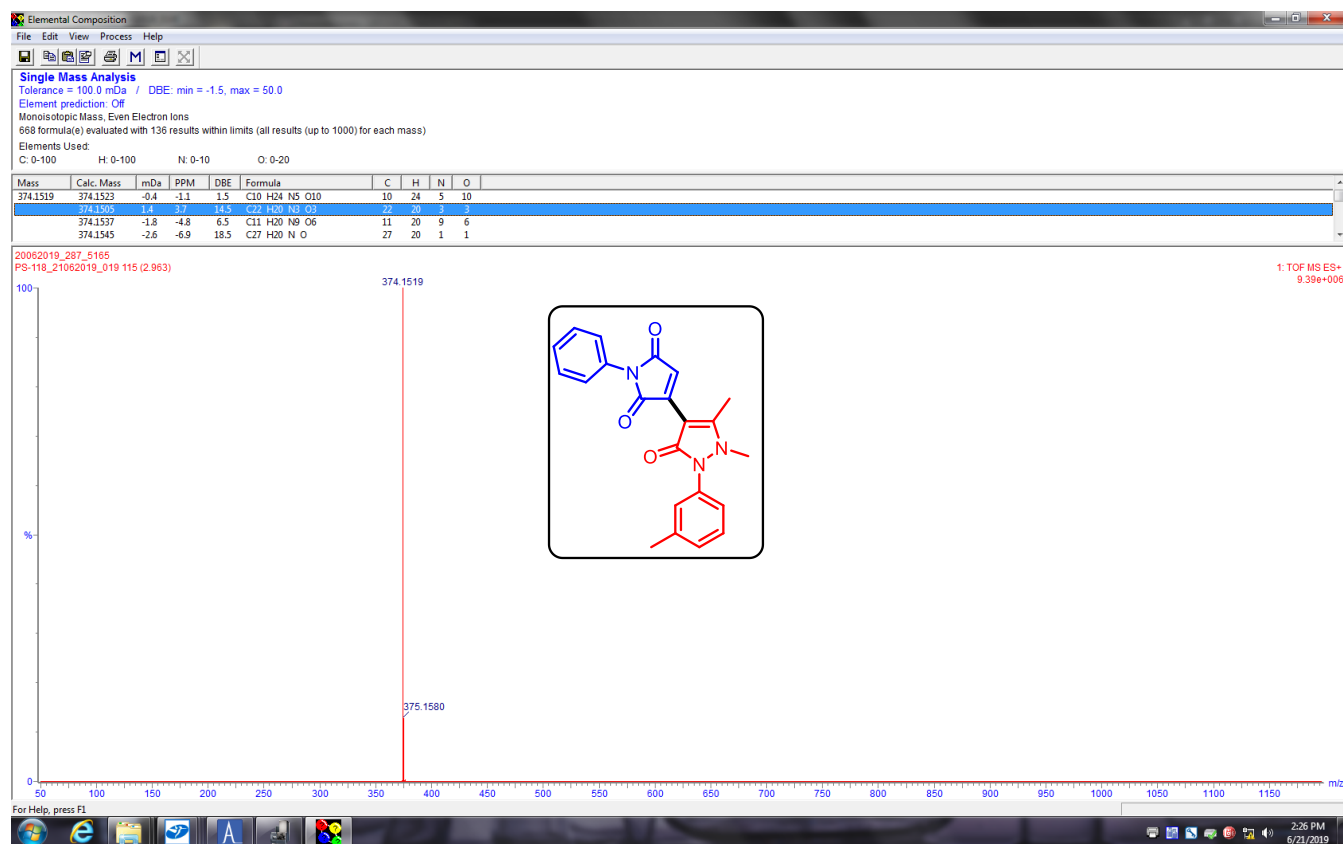
## HRMS Spectra of Compound 3ba:



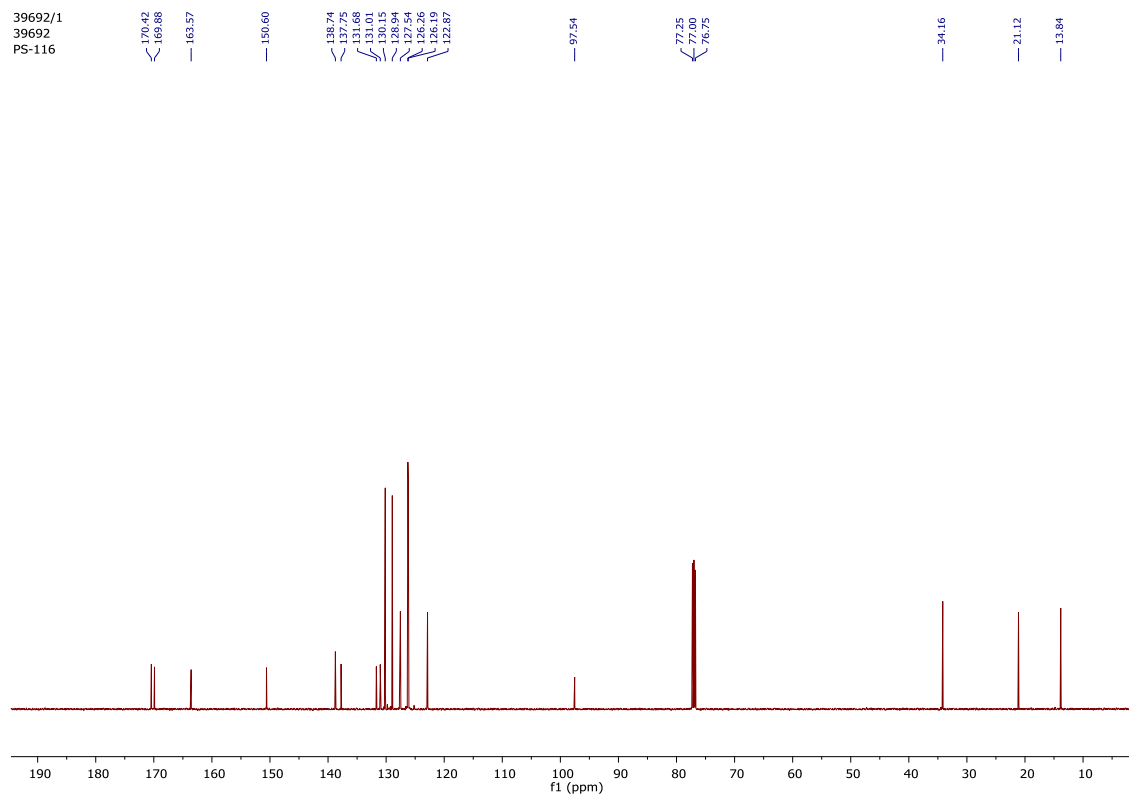
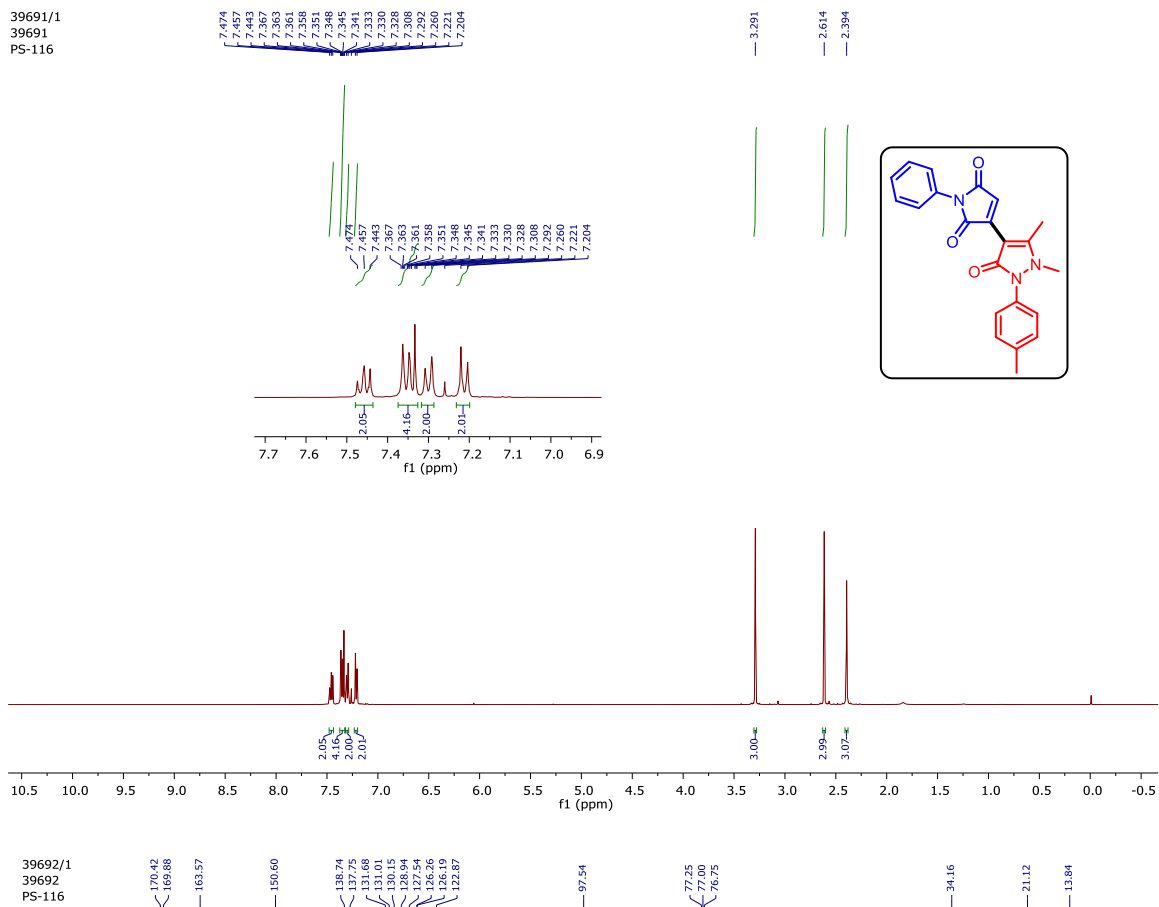
**$^1\text{H}$  and  $^{13}\text{C}$  of Compound 3ca (500 & 125 MHz,  $\text{CDCl}_3$ ):**



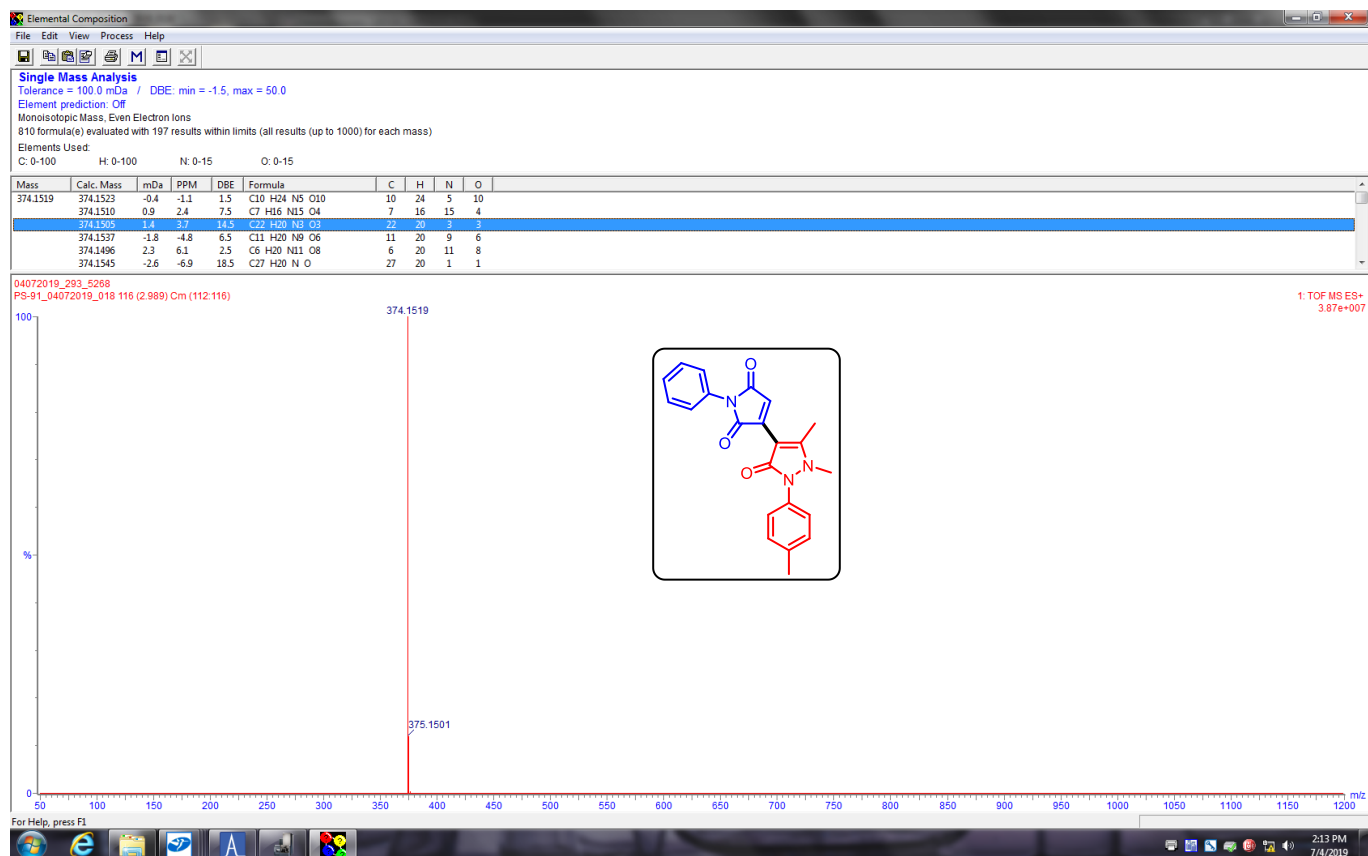
## HRMS Spectra of Compound 3ca:



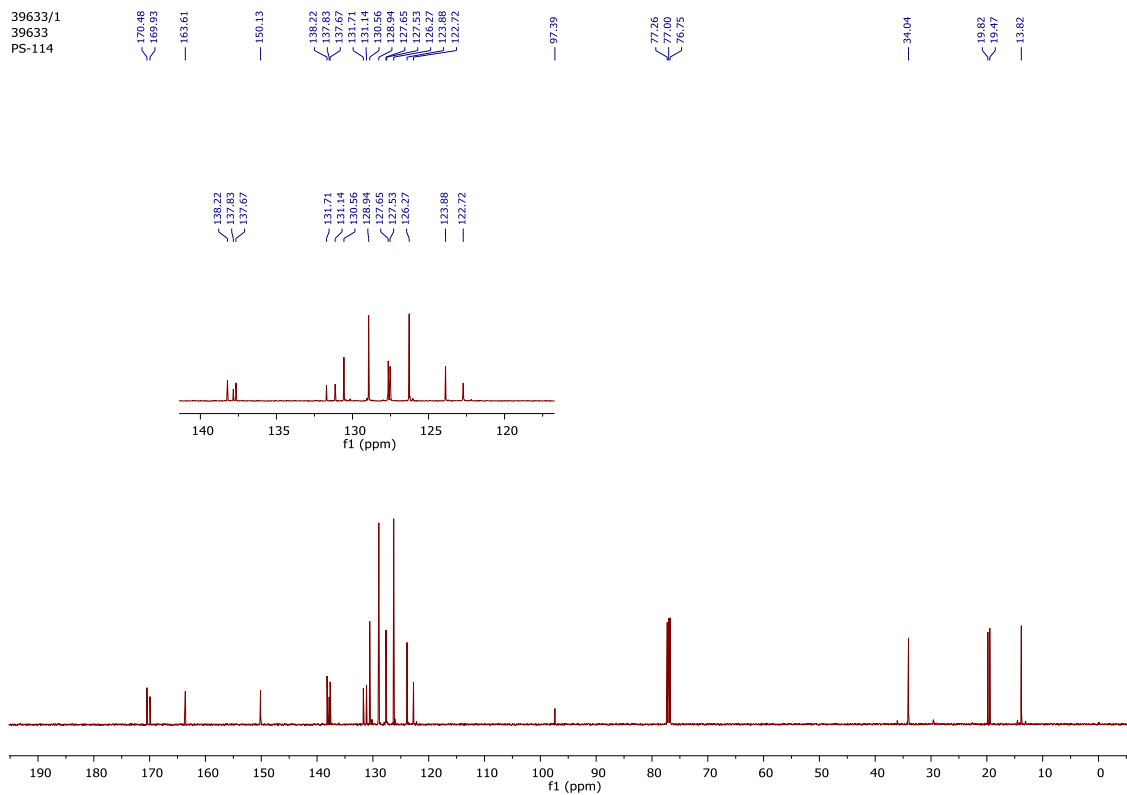
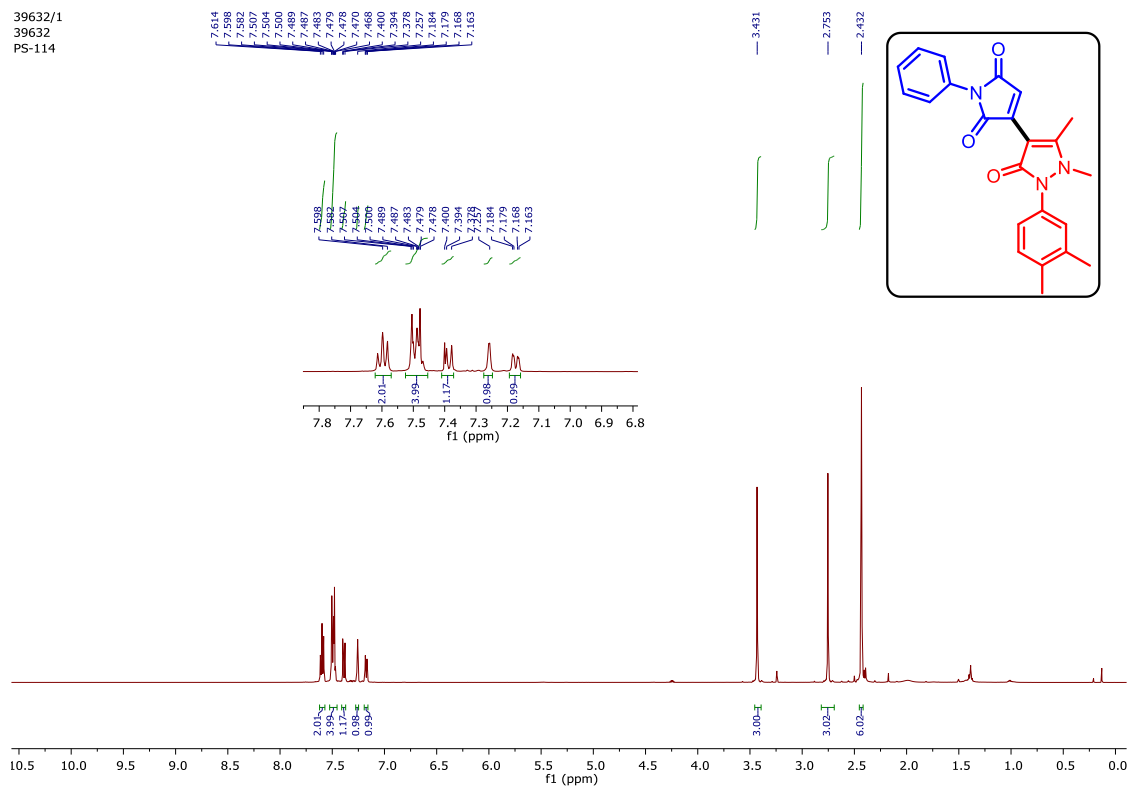
# <sup>1</sup>H and <sup>13</sup>C of Compound 3da (500 & 125 MHz, CDCl<sub>3</sub>):



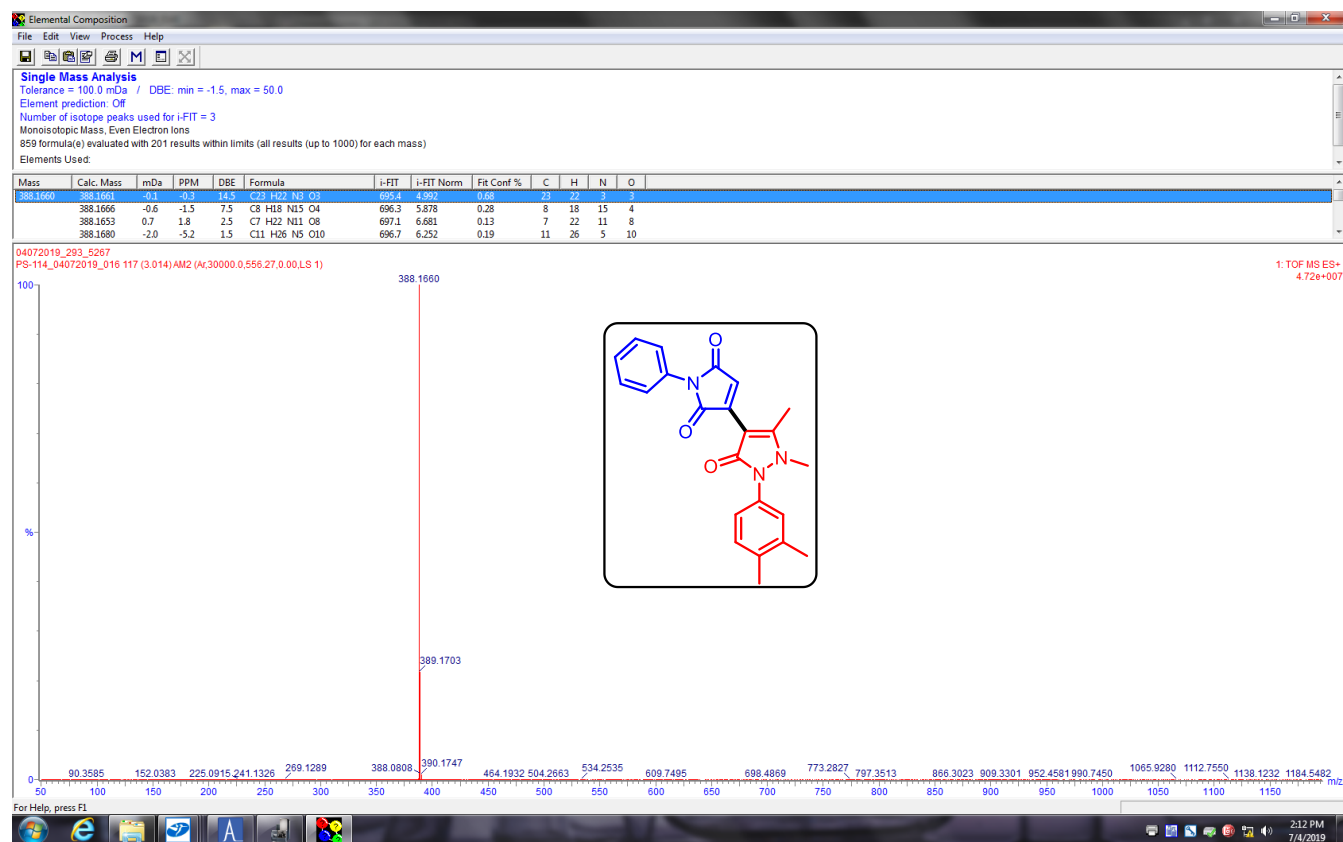
## HRMS Spectra of Compound 3da:



# <sup>1</sup>H and <sup>13</sup>C of Compound 3ea (500 & 125 MHz, CDCl<sub>3</sub>):



## HRMS Spectra of Compound 3ea:



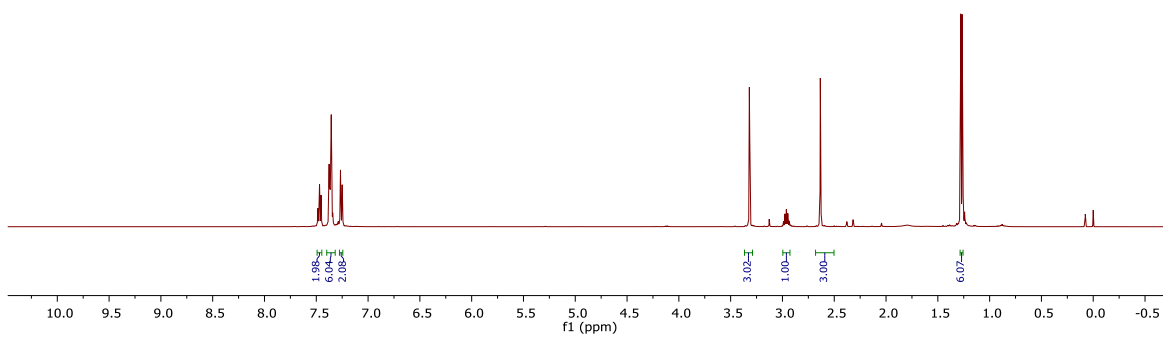
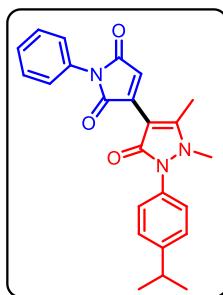
# <sup>1</sup>H and <sup>13</sup>C of Compound 3fa (500 & 125 MHz, CDCl<sub>3</sub>):

39547/1  
39547  
PS-120

7.49  
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7.34  
7.27  
7.25

3.32  
3.29  
2.98  
2.96  
2.95  
2.93  
2.63

1.28  
1.27



39553/1  
39553  
PS-120

170.45  
169.50  
163.58

150.57  
149.48

137.78  
131.69  
131.18

128.94  
128.94  
127.55  
127.55  
126.27  
126.20  
122.89  
122.85

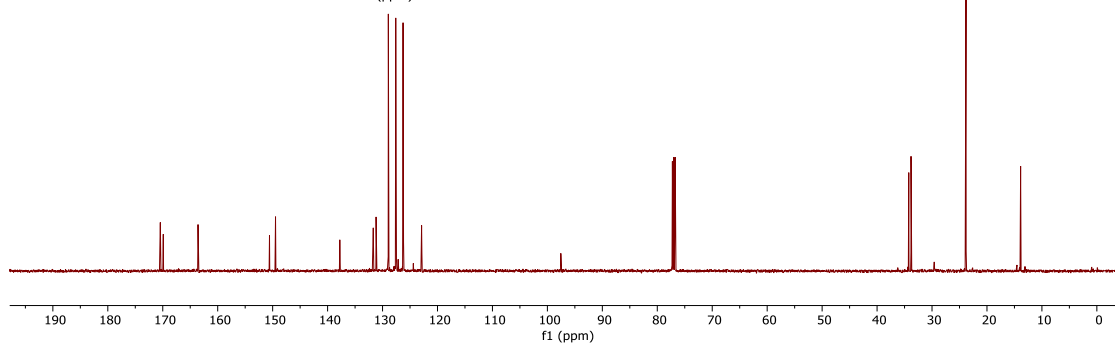
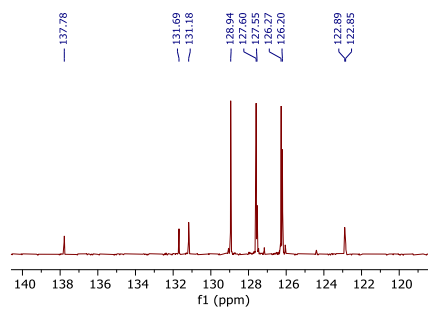
97.55

77.25  
77.00  
76.74

34.23  
33.82

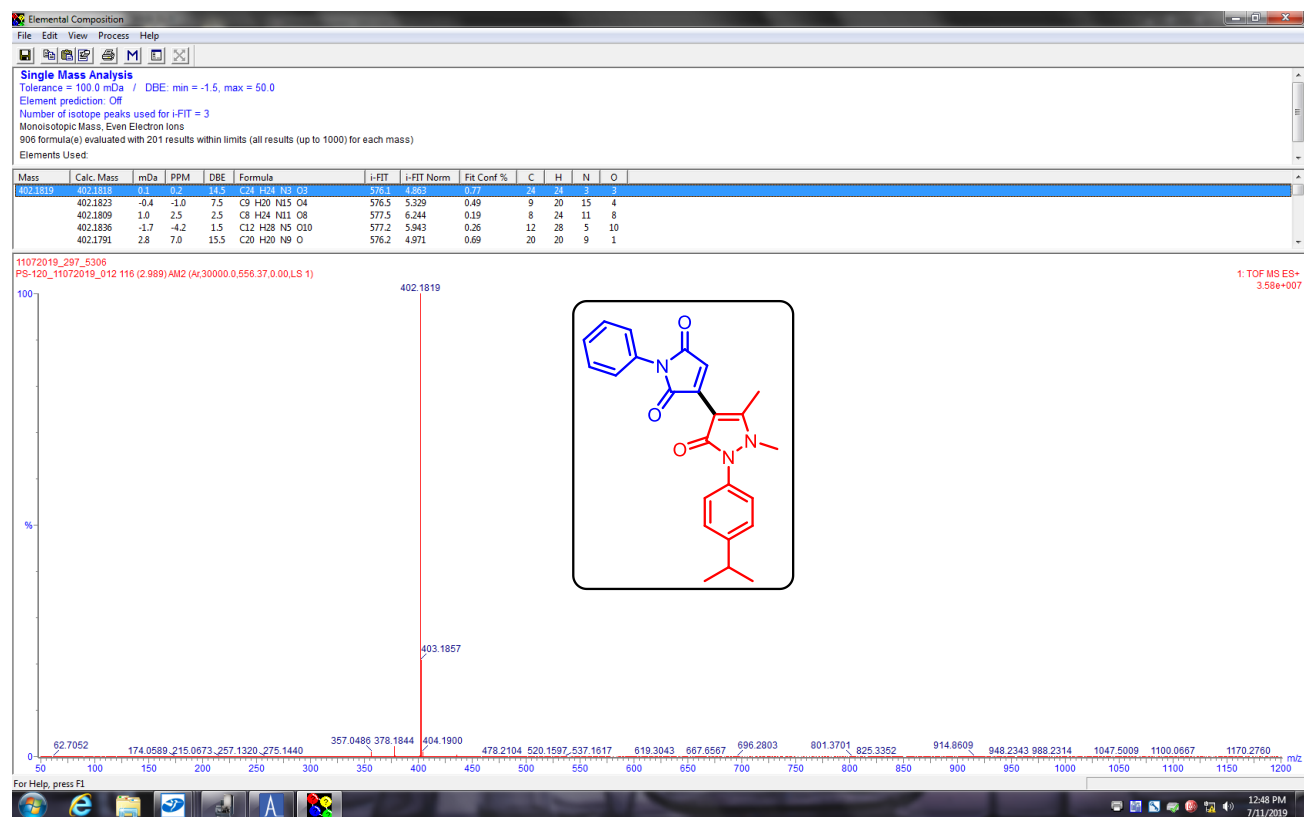
23.81

13.87

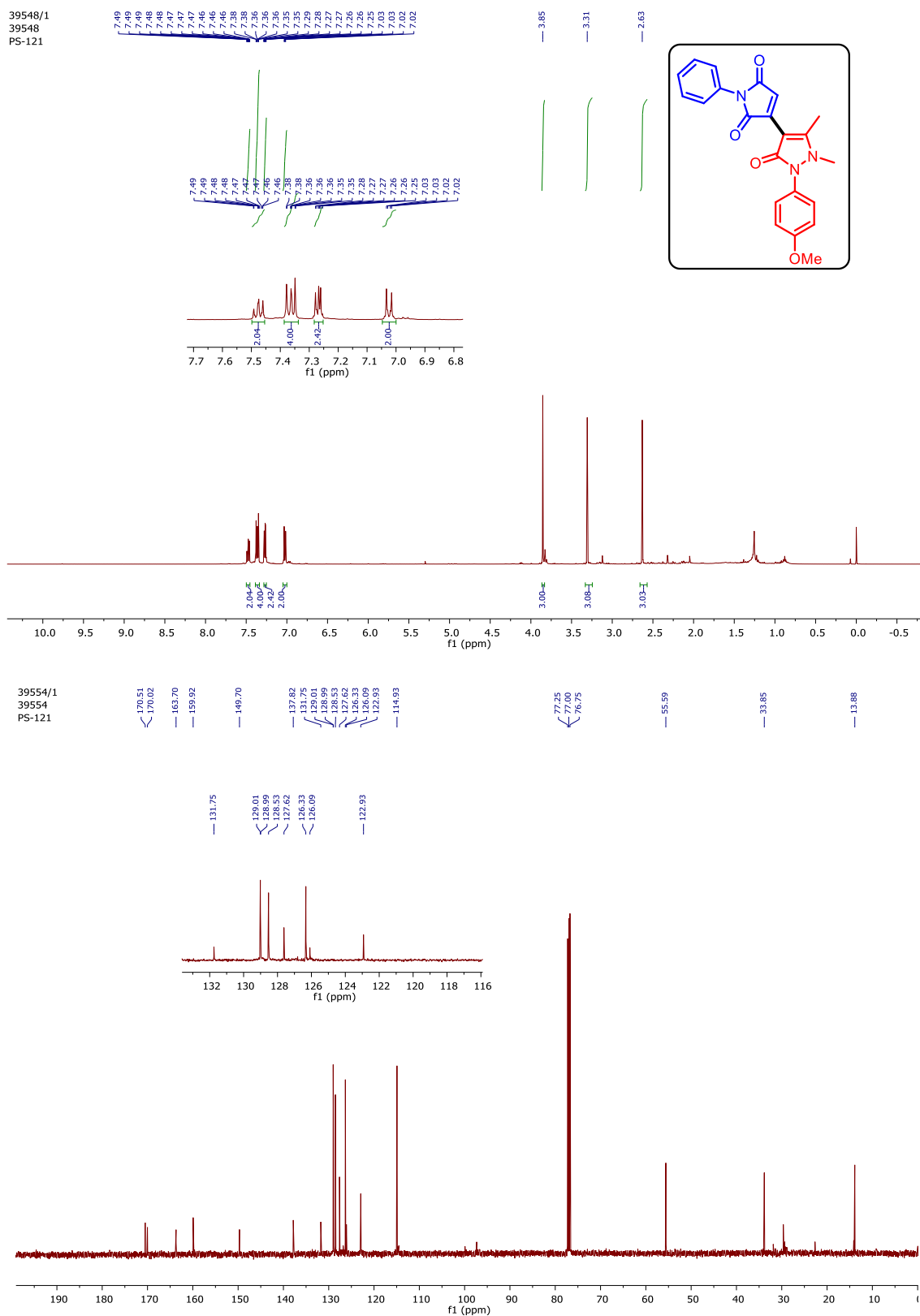




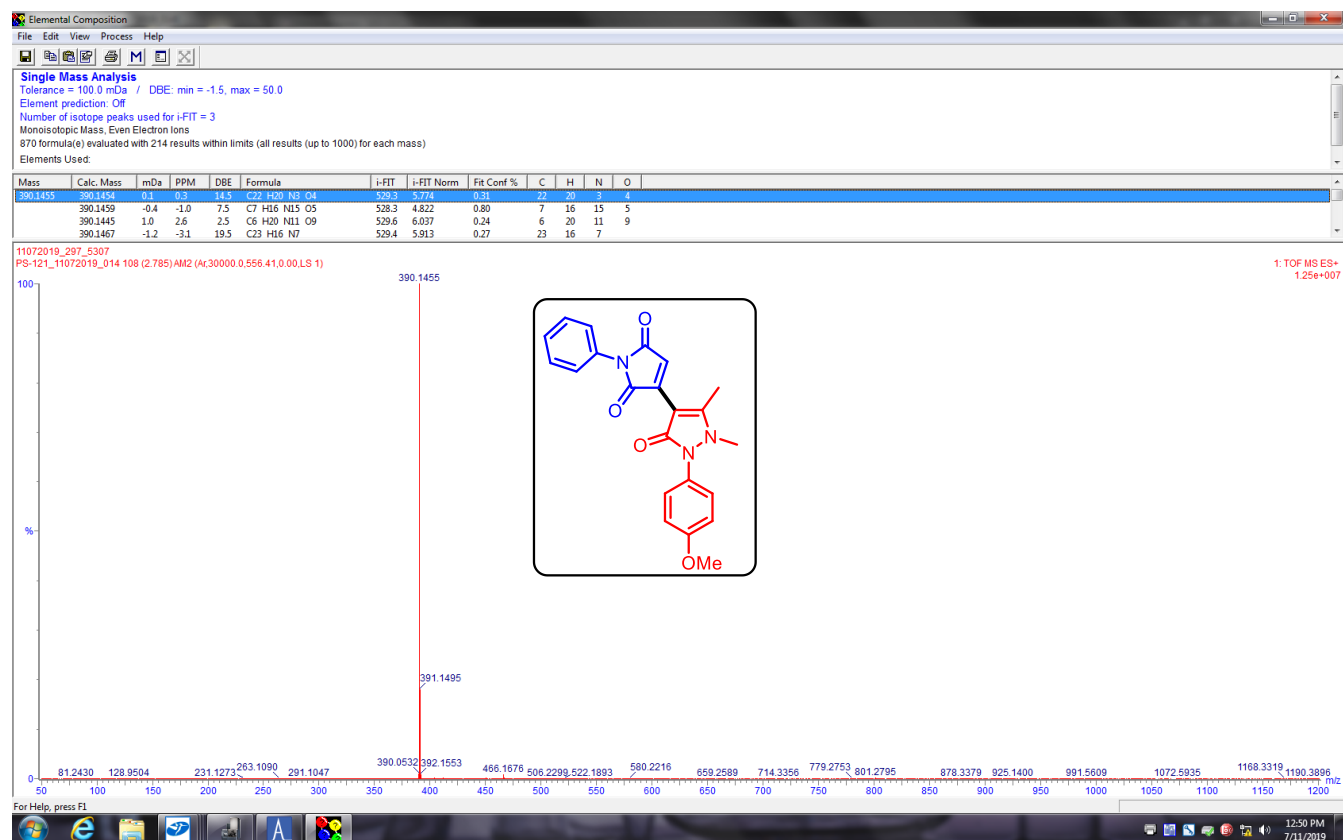
## HRMS Spectra of Compound 3fa:



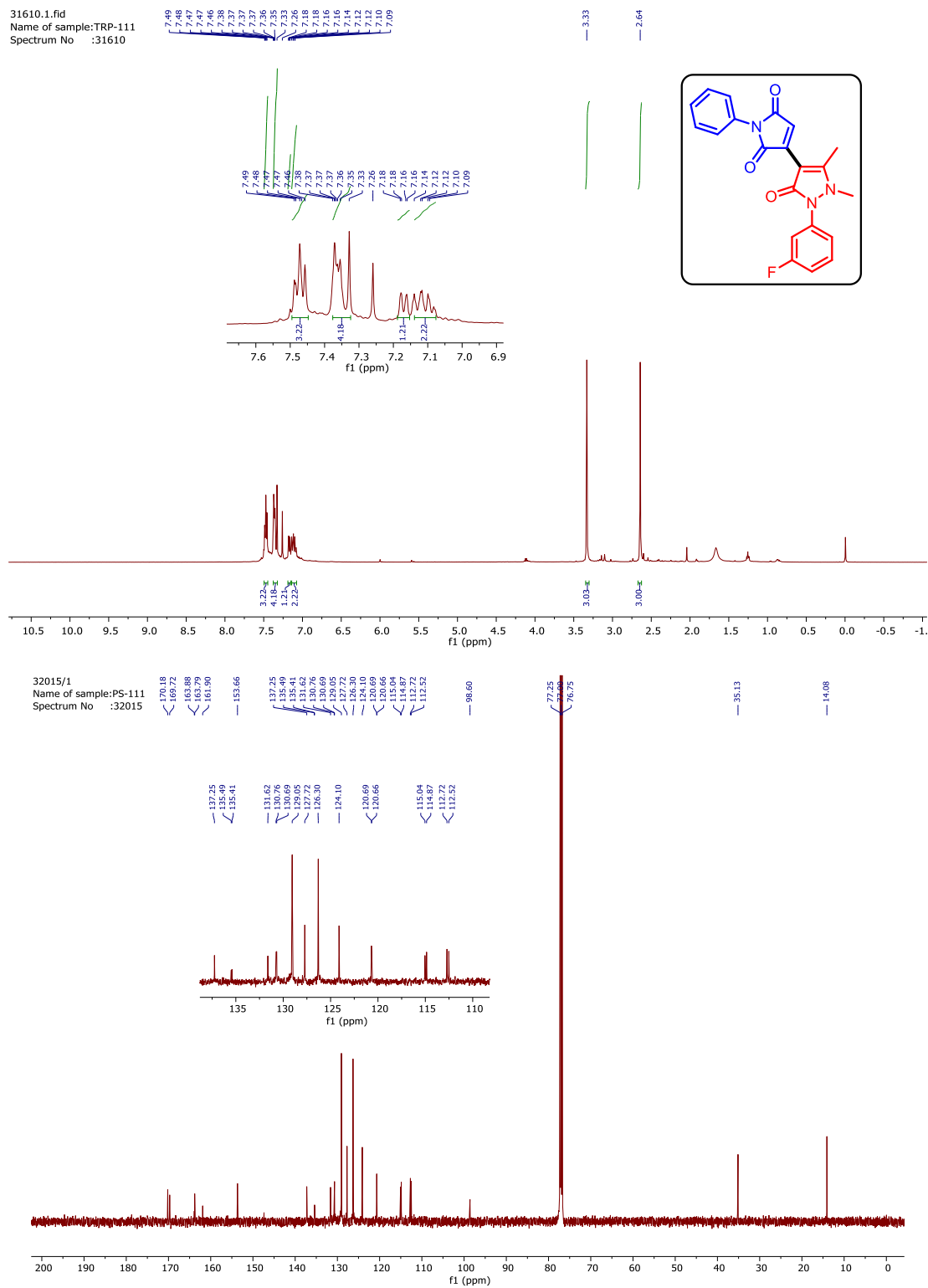
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ga (500 & 125 MHz, CDCl<sub>3</sub>):



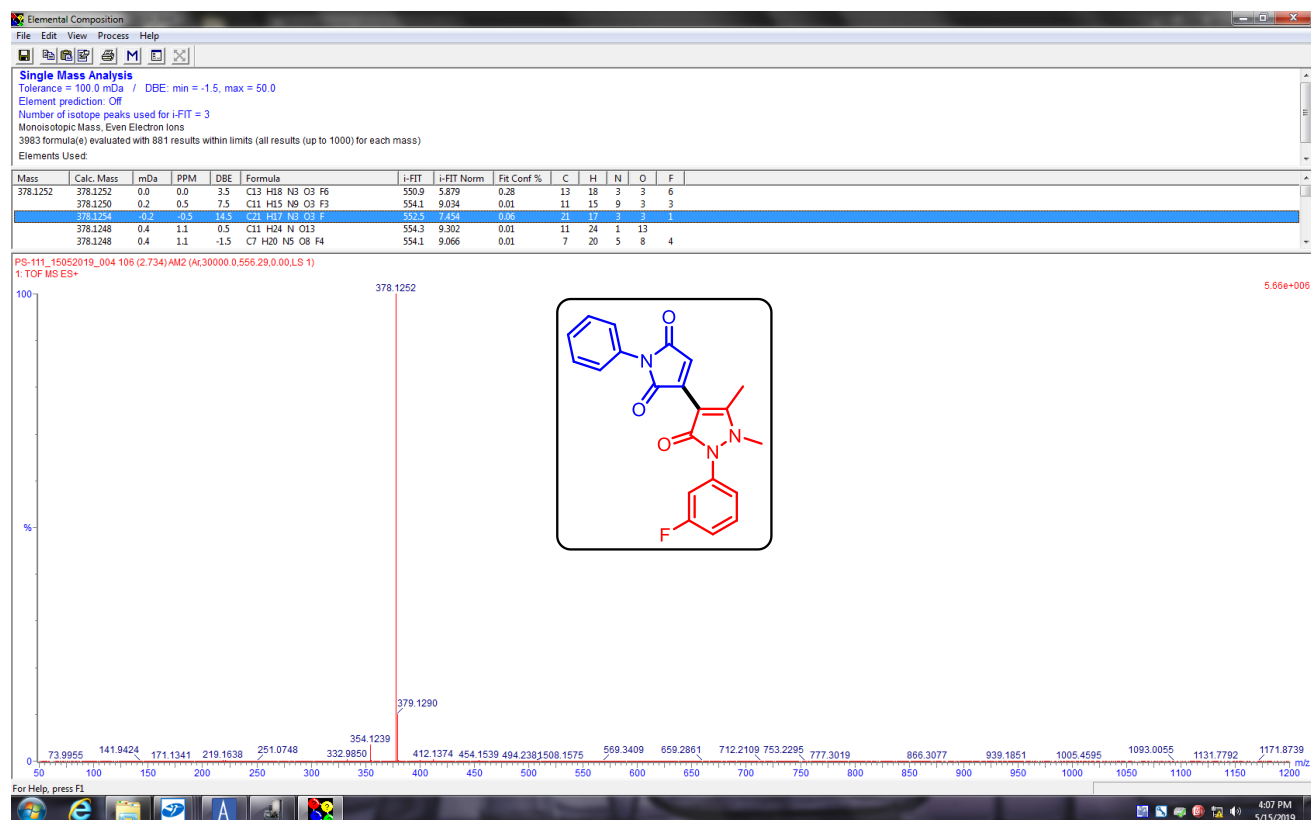
## HRMS Spectra of Compound 3ga:



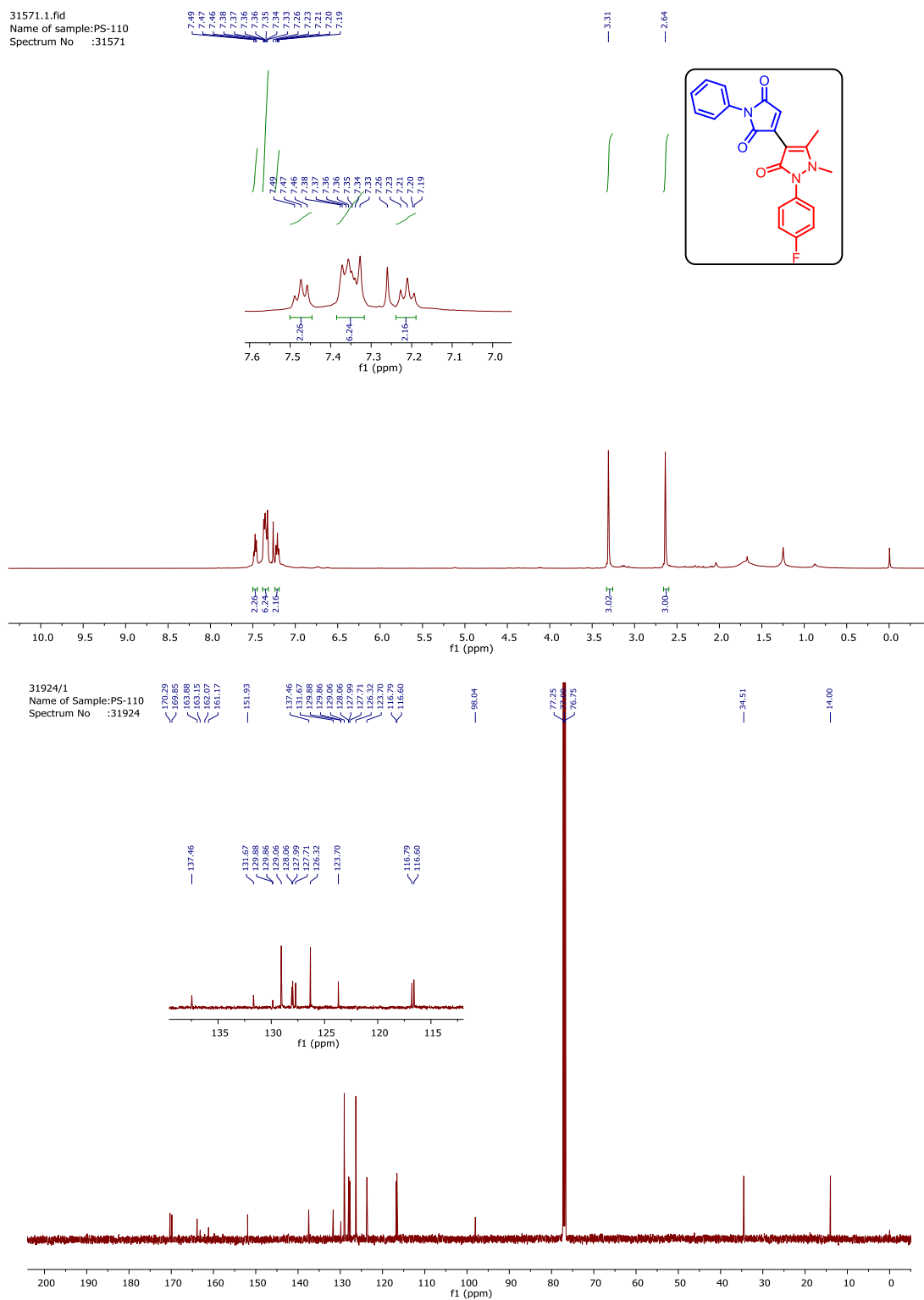
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ha (500 & 125 MHz, CDCl<sub>3</sub>):



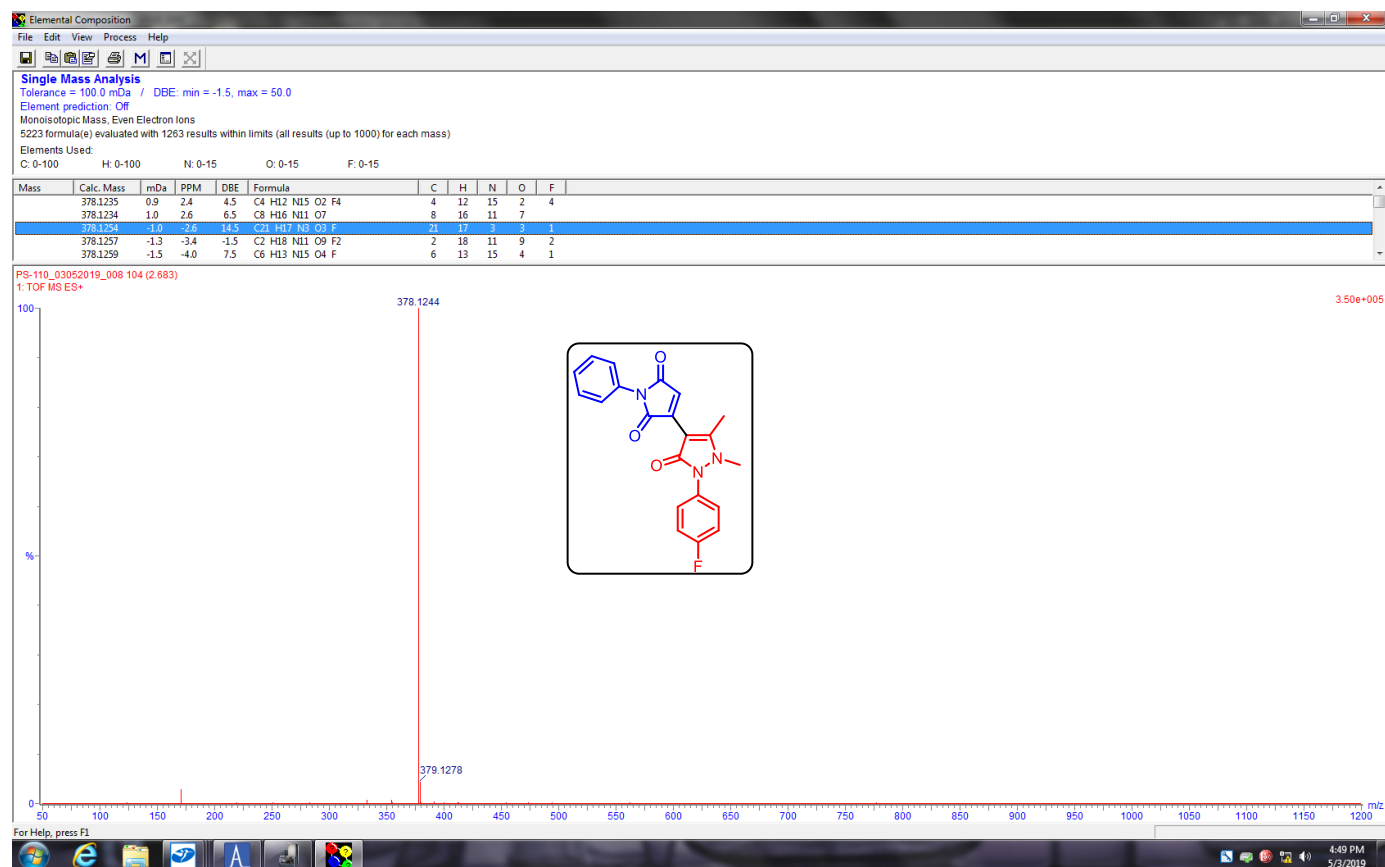
## HRMS Spectra of Compound 3ha:



# <sup>1</sup>H and <sup>13</sup>C of Compound 3ia (500 & 125 MHz, CDCl<sub>3</sub>):



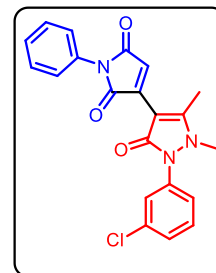
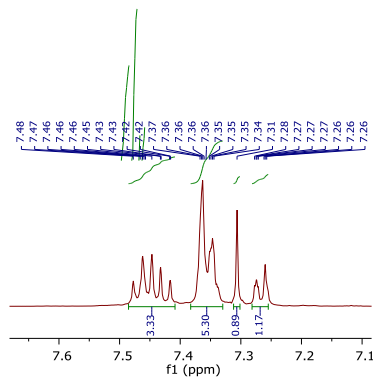
## HRMS Spectra of Compound 3ia:



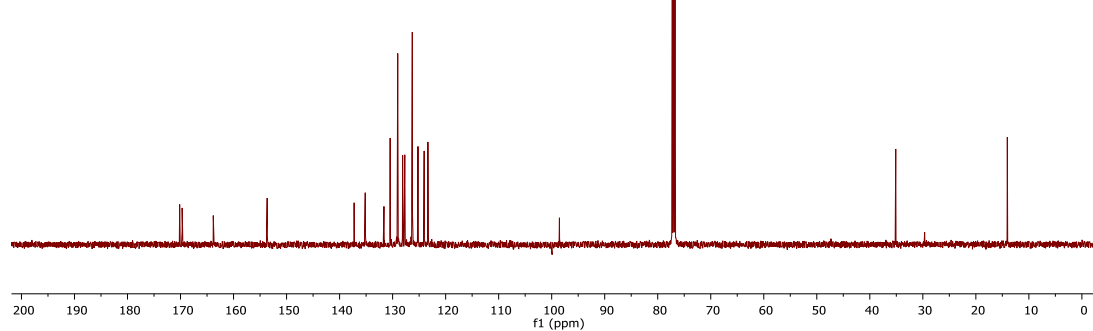
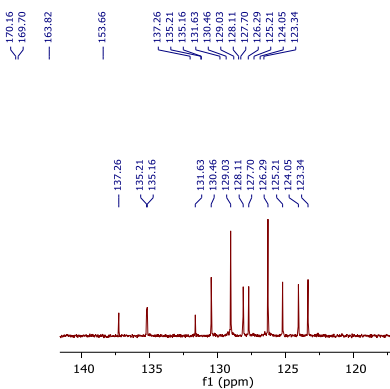
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ja (500 & 125 MHz, CDCl<sub>3</sub>):

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Spec No: 39639  
Sample ID :PS-113

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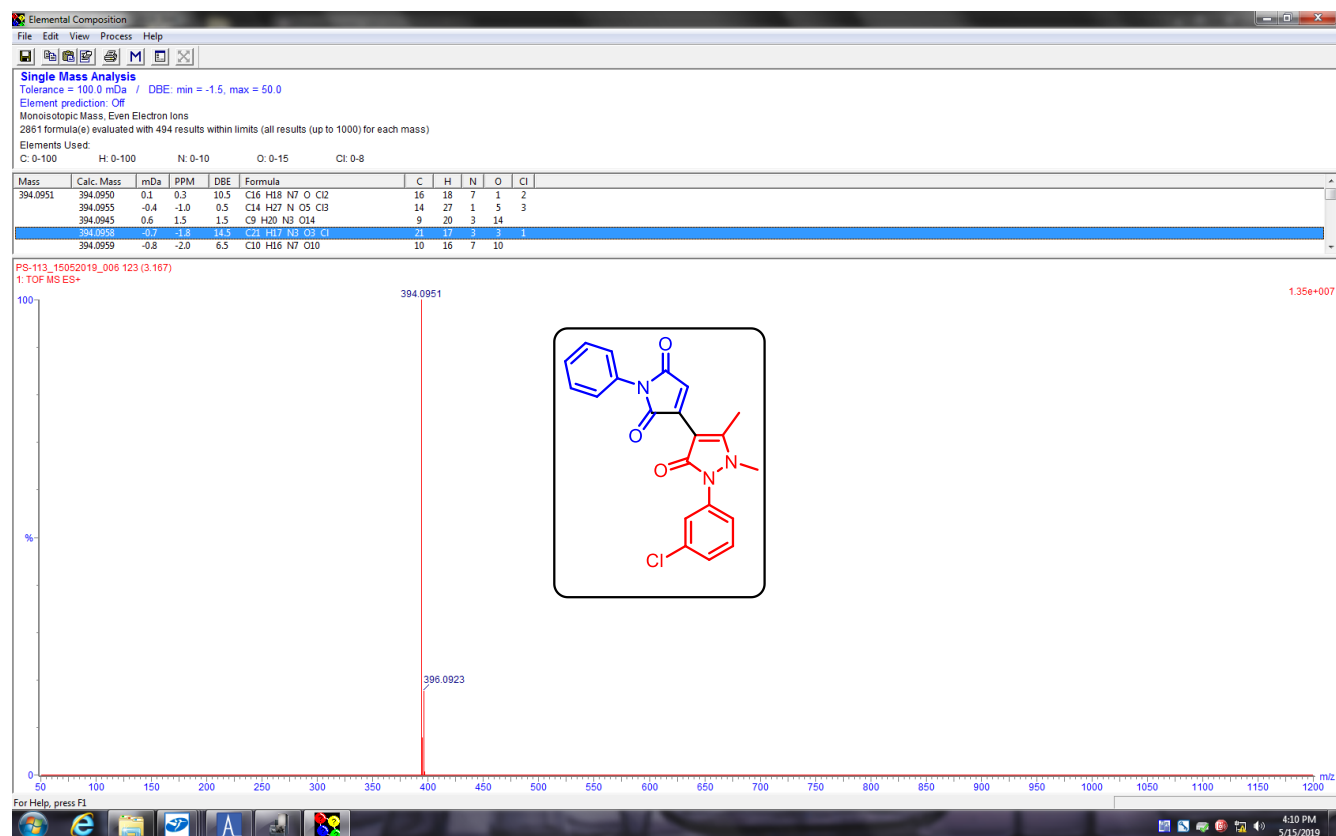


31990/1  
Name of sample:SB-113  
Spectrum No :31990



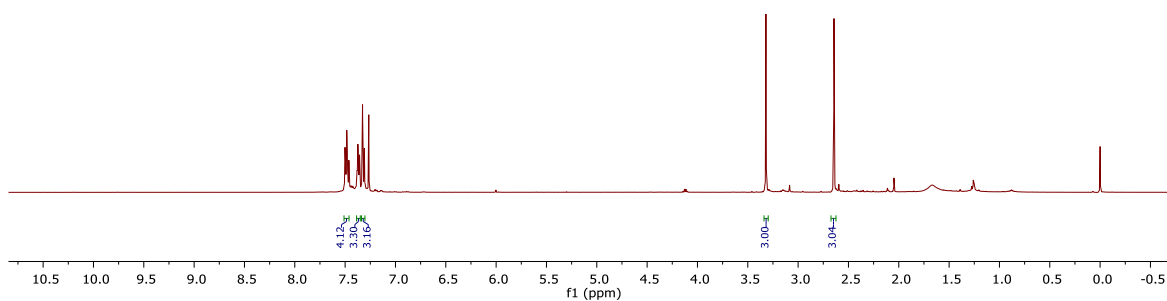
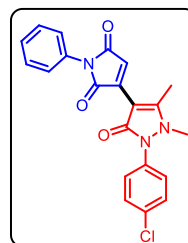
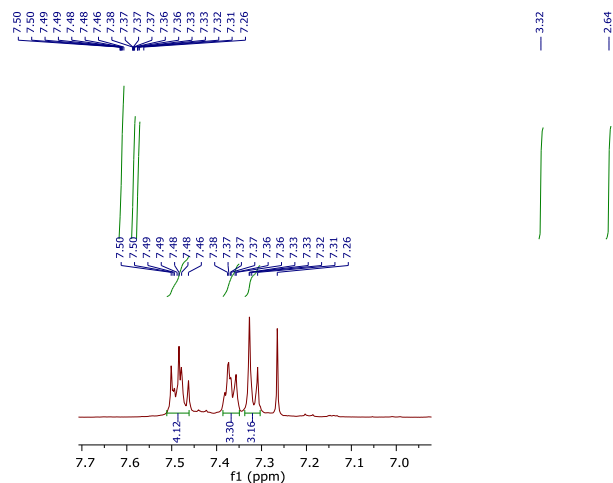


## HRMS Spectra of Compound 3ja:

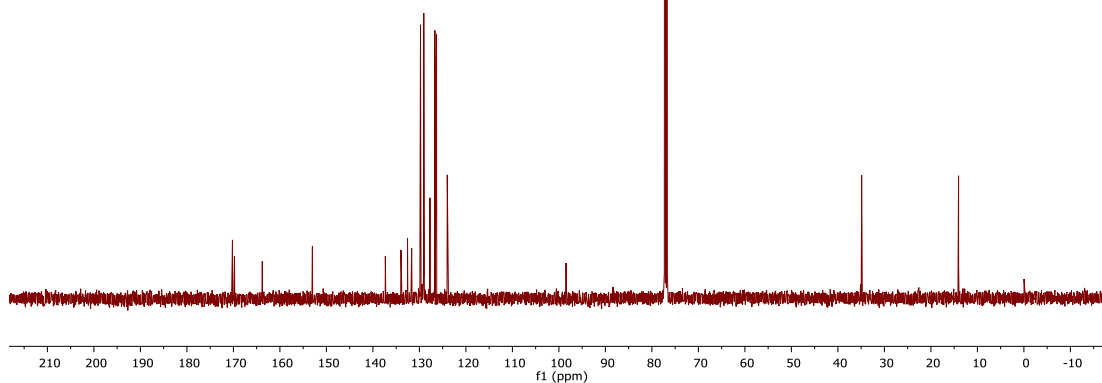
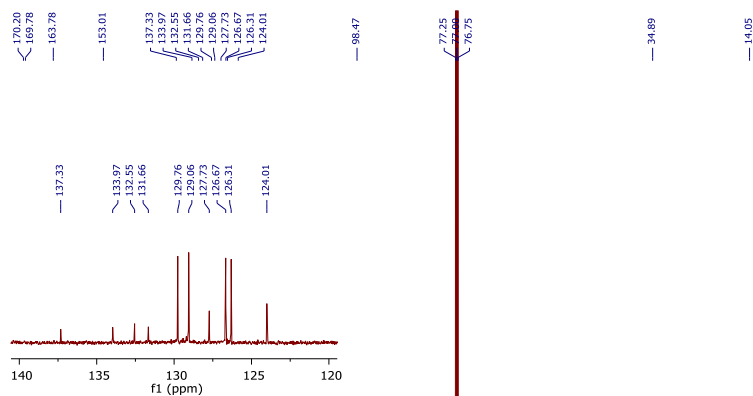


# <sup>1</sup>H and <sup>13</sup>C of Compound 3ka (500 & 125 MHz, CDCl<sub>3</sub>):

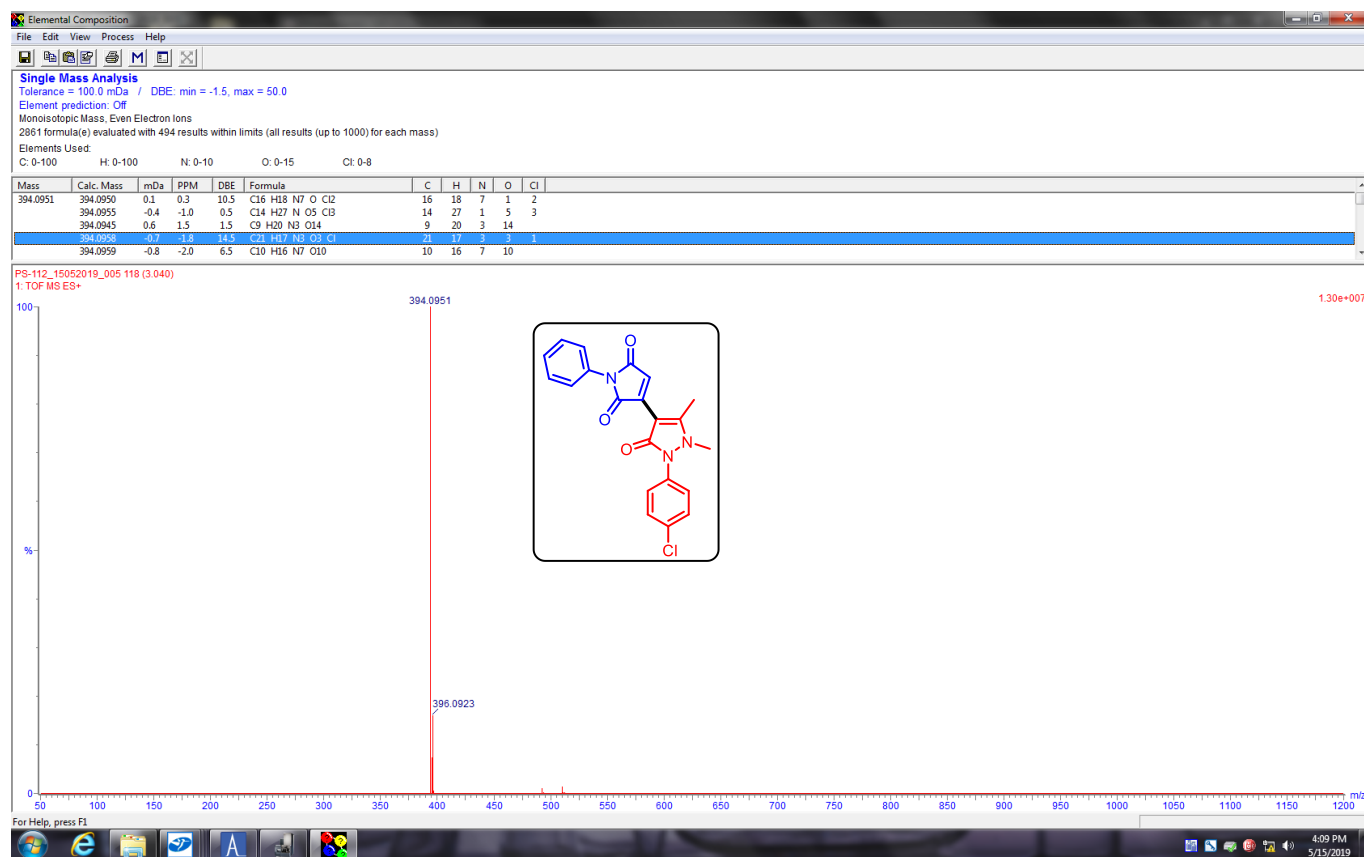
31608.1.fid  
Name of sample:PS-112  
Spectrum No :31608



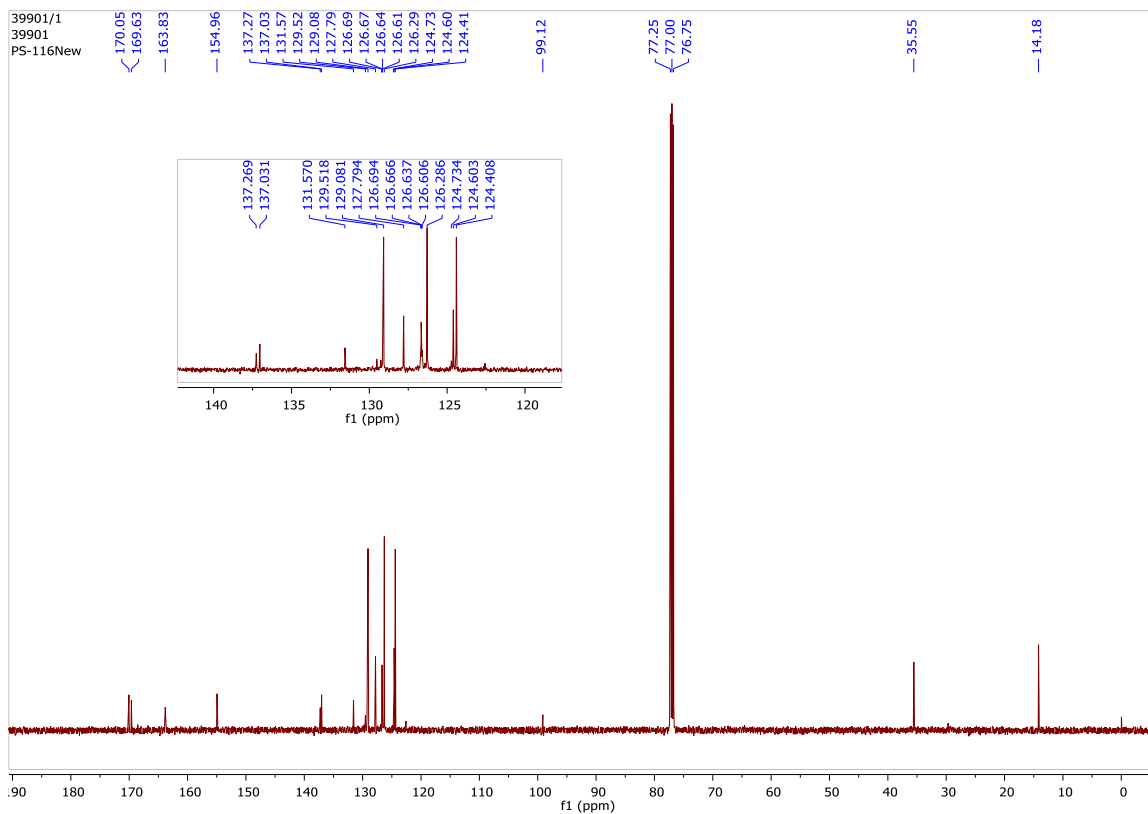
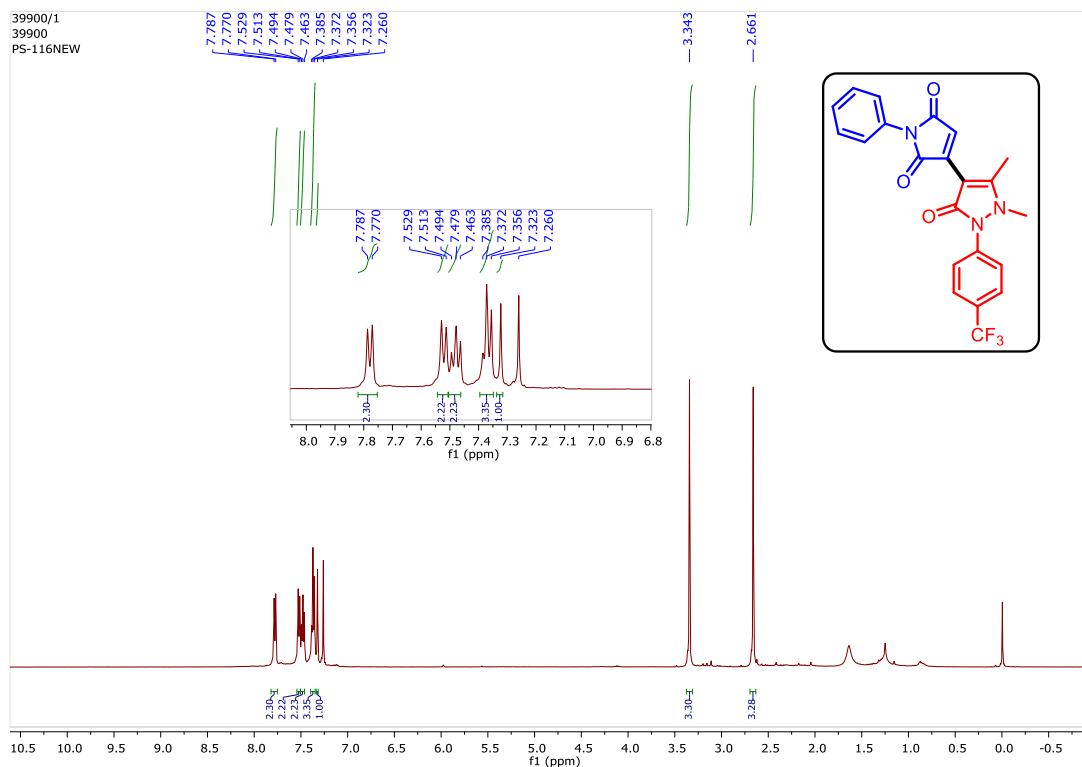
31983/1  
Name of sample:PS-112  
Spectrum No :31983



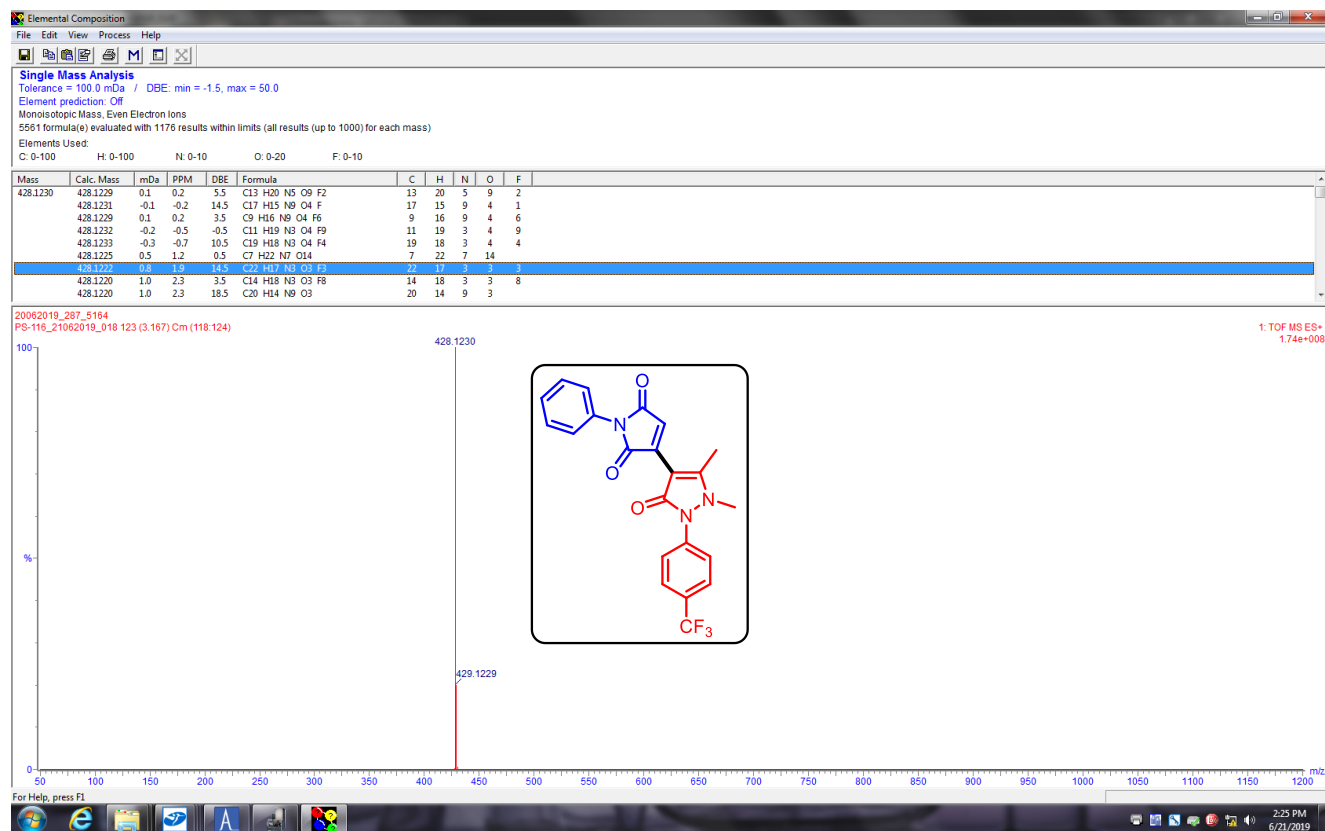
## HRMS Spectra of Compound 3ka:



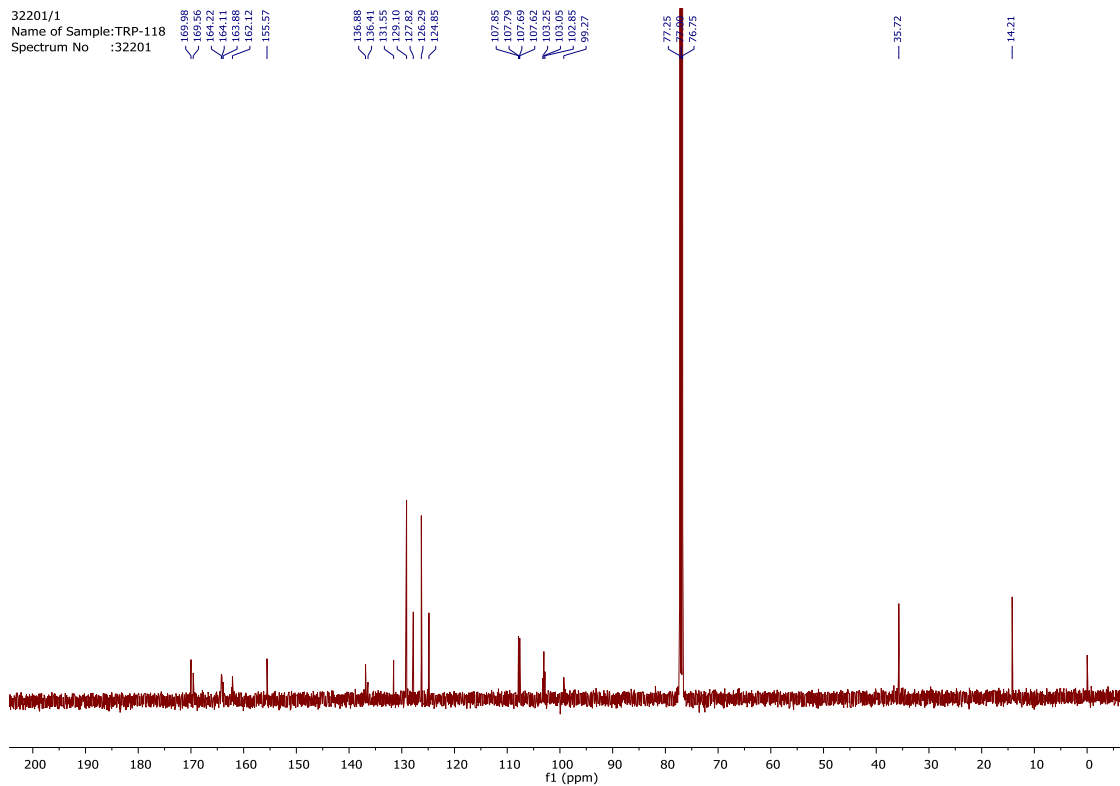
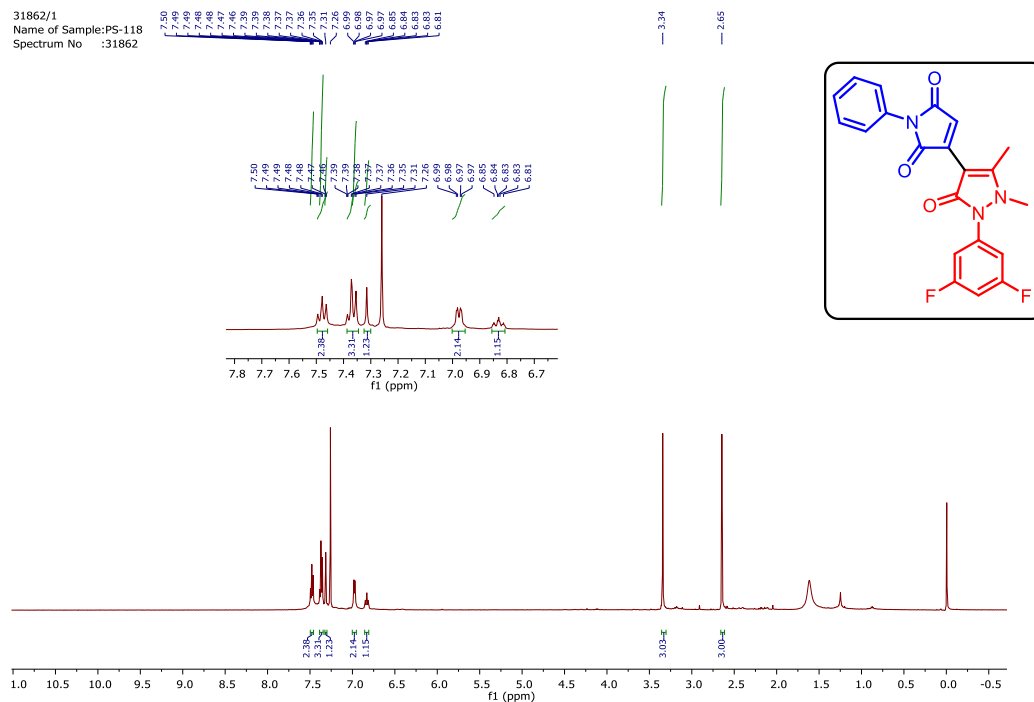
**$^1\text{H}$  and  $^{13}\text{C}$  of Compound 3la (500 & 125 MHz,  $\text{CDCl}_3$ ):**



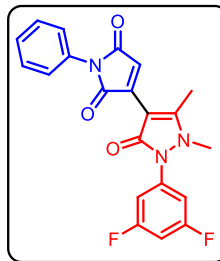
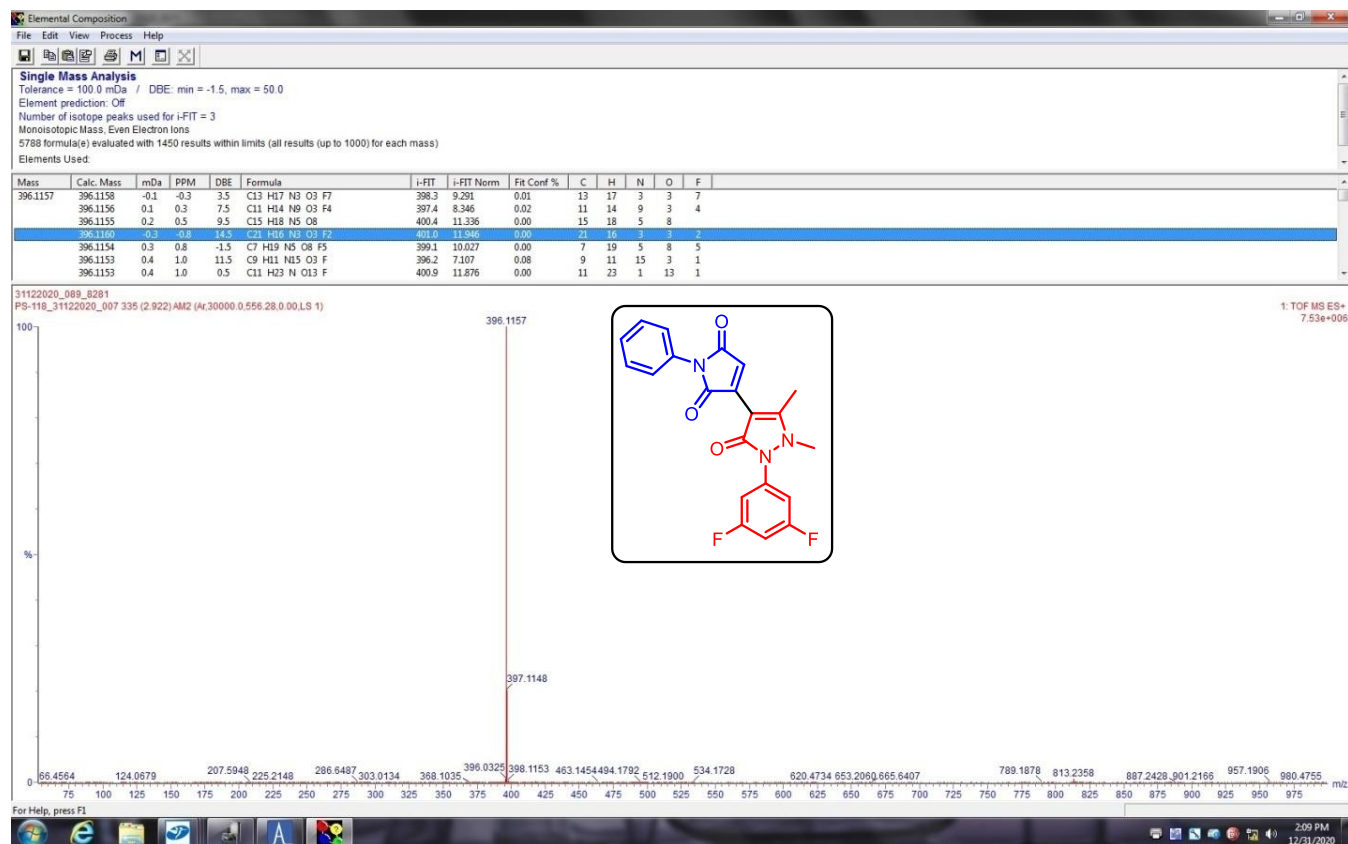
## HRMS Spectra of Compound 3la:



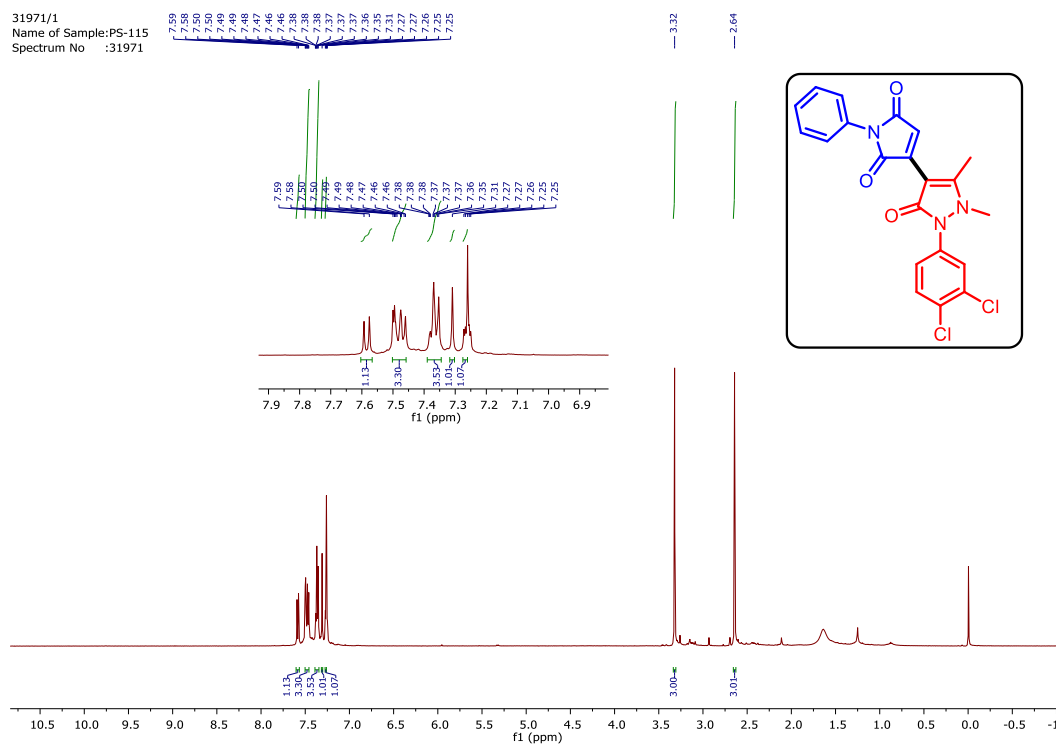
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ma (500 & 125 MHz, CDCl<sub>3</sub>):



## HRMS Spectra of Compound 3ma:

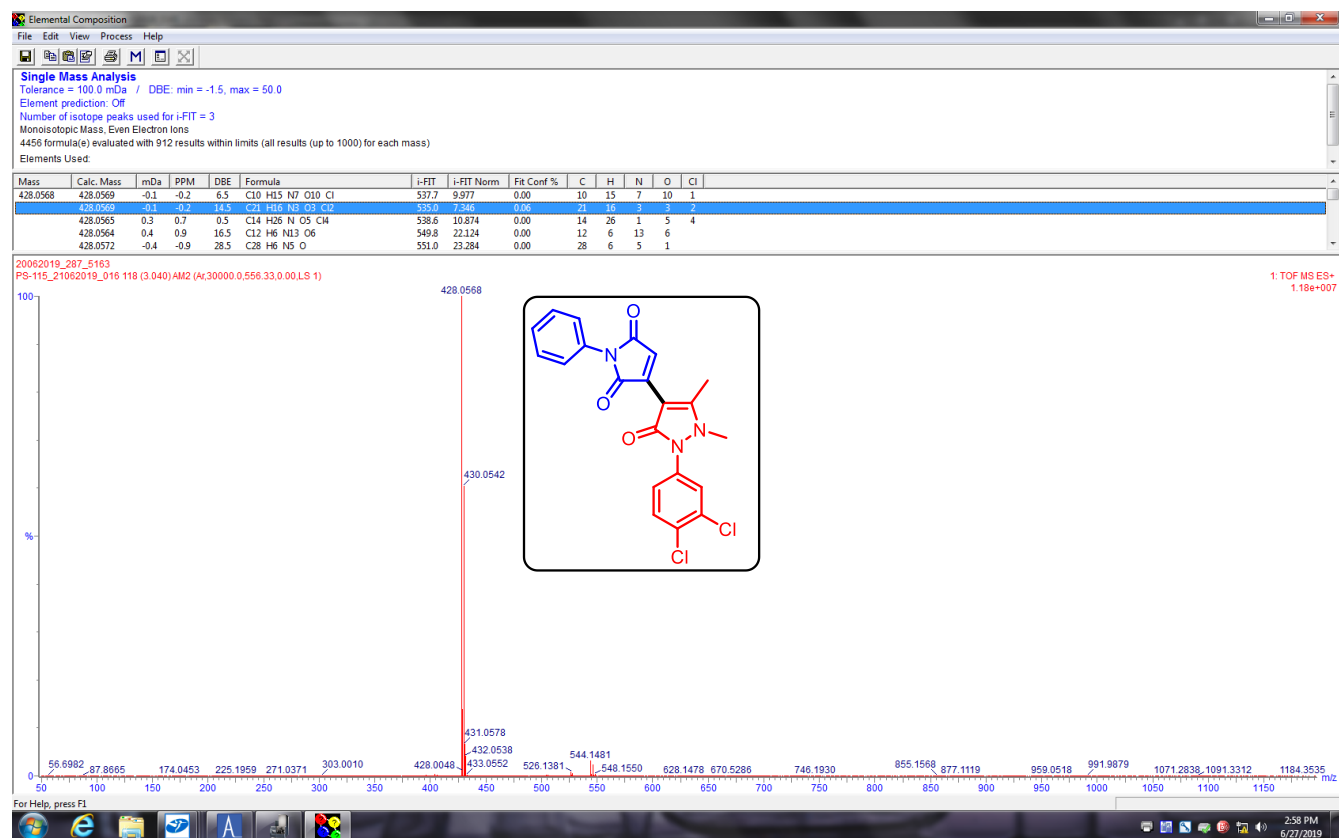


# <sup>1</sup>H and <sup>13</sup>C of Compound 3na (500 & 125 MHz, CDCl<sub>3</sub>):

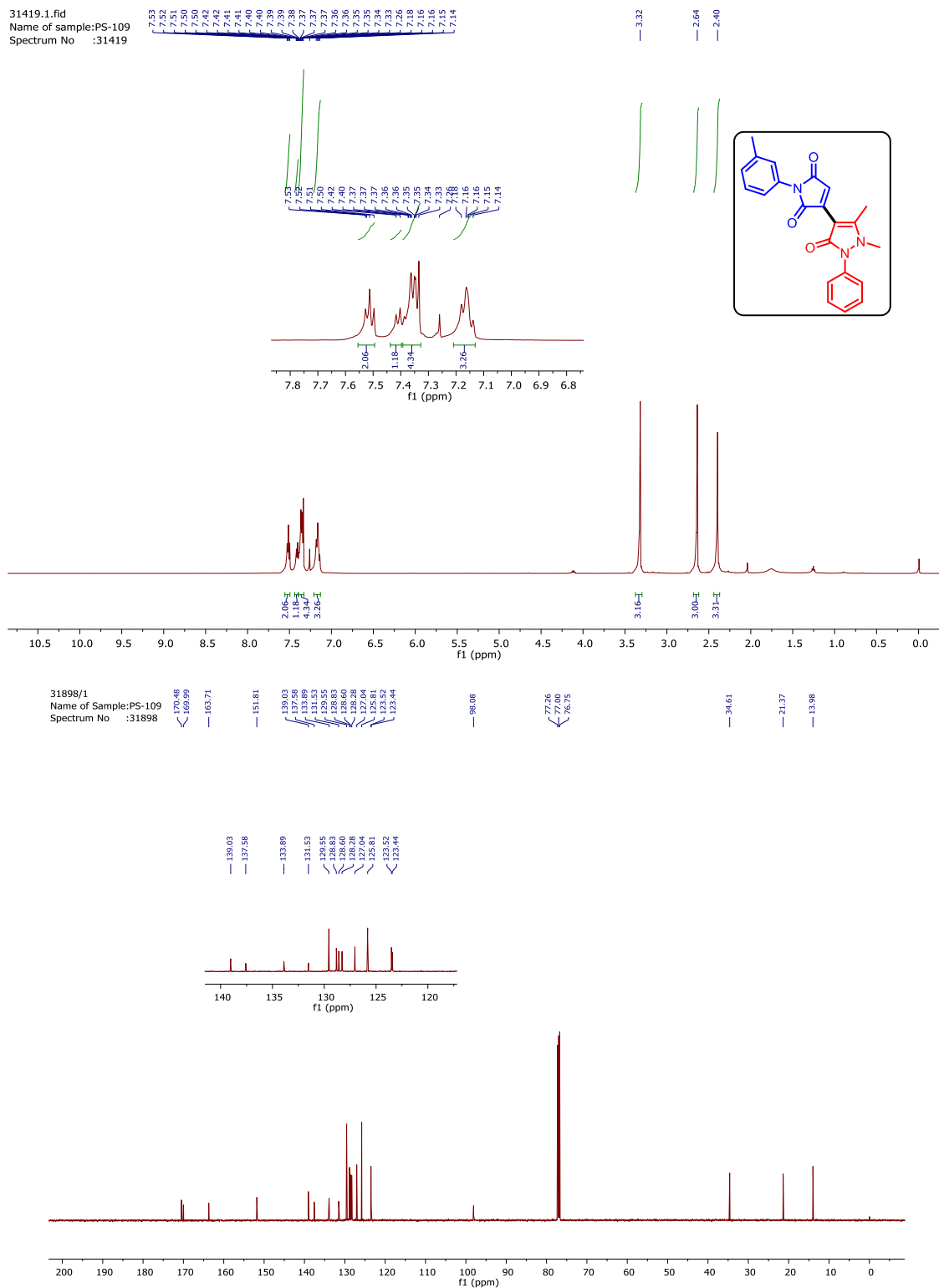




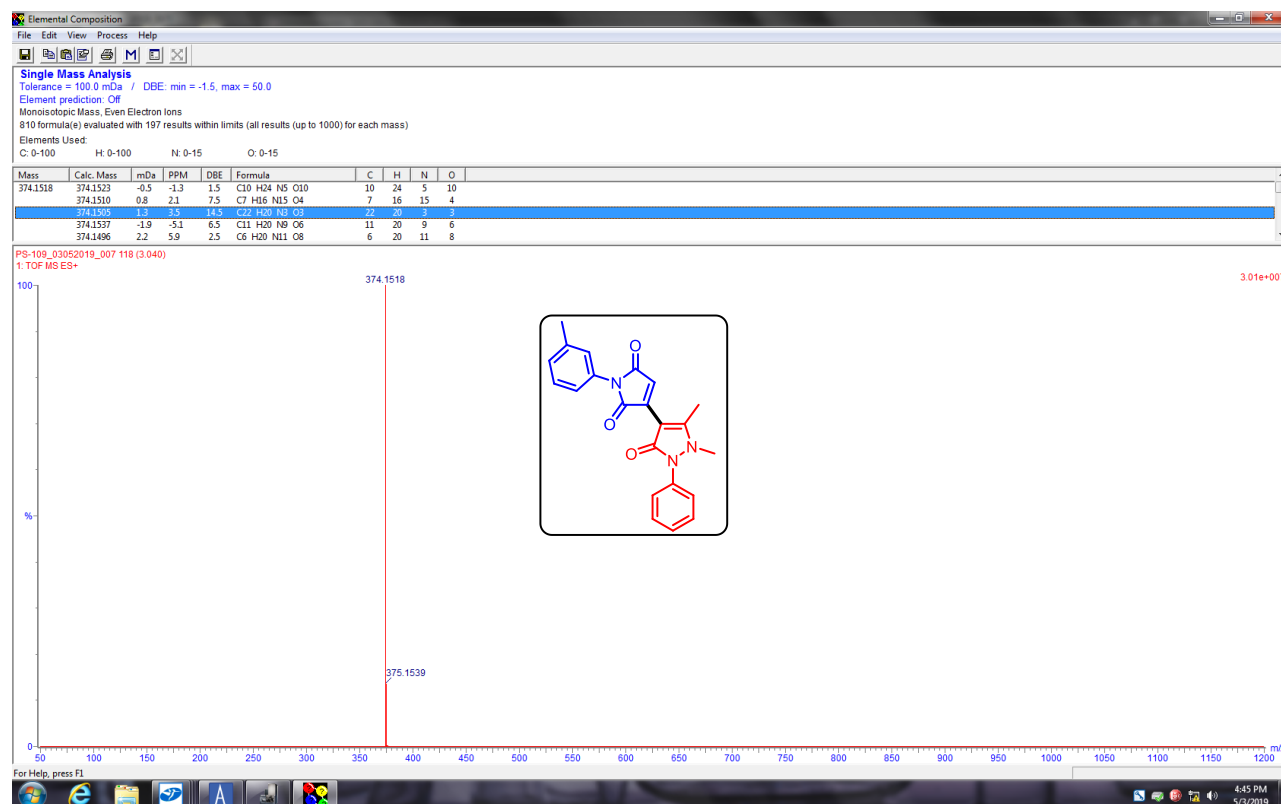
## HRMS Spectra of Compound 3na:



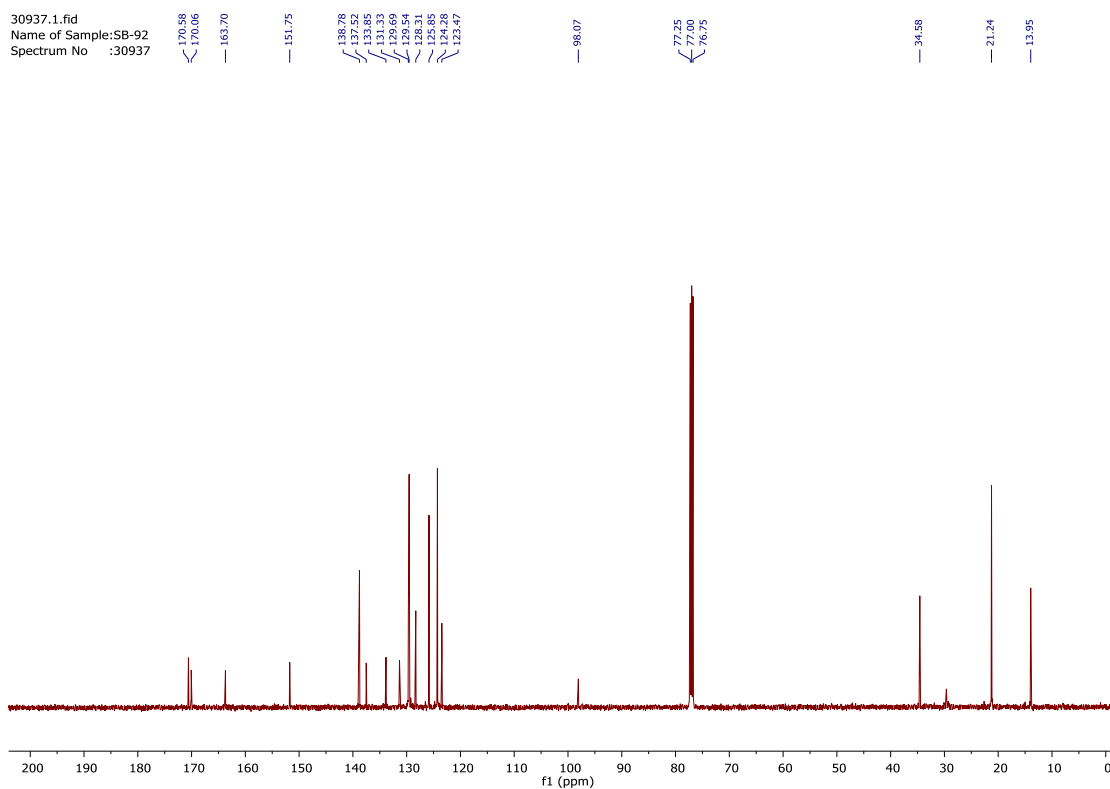
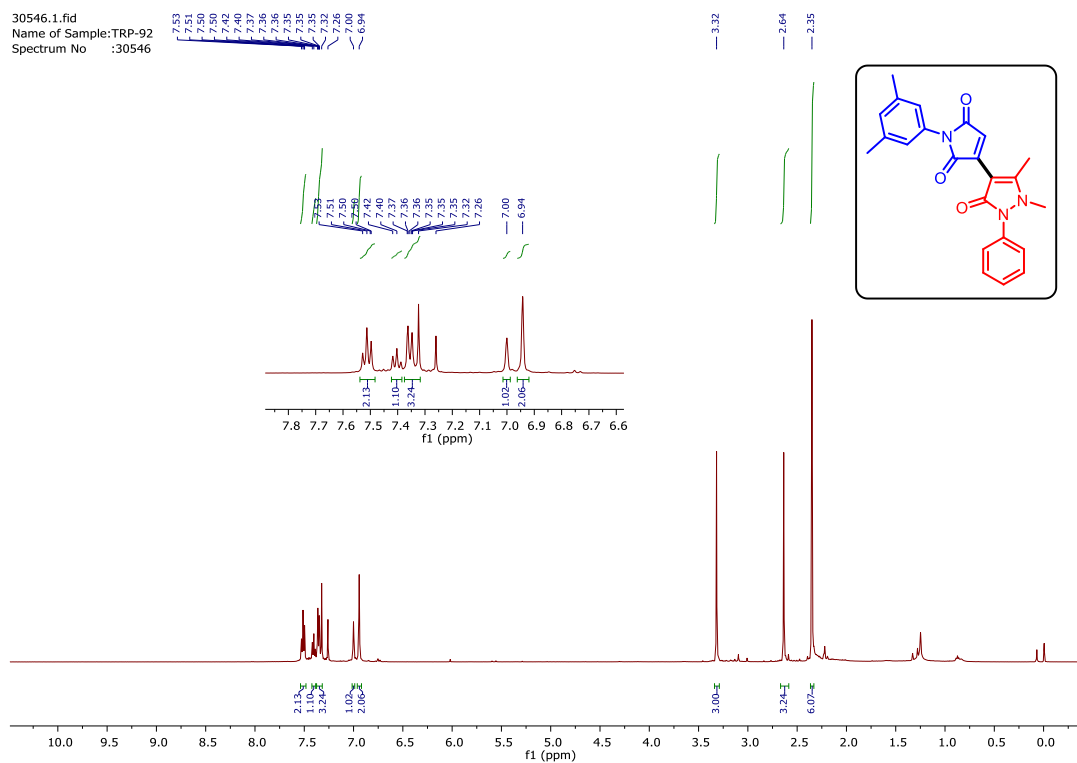
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ab (500 & 125 MHz, CDCl<sub>3</sub>):



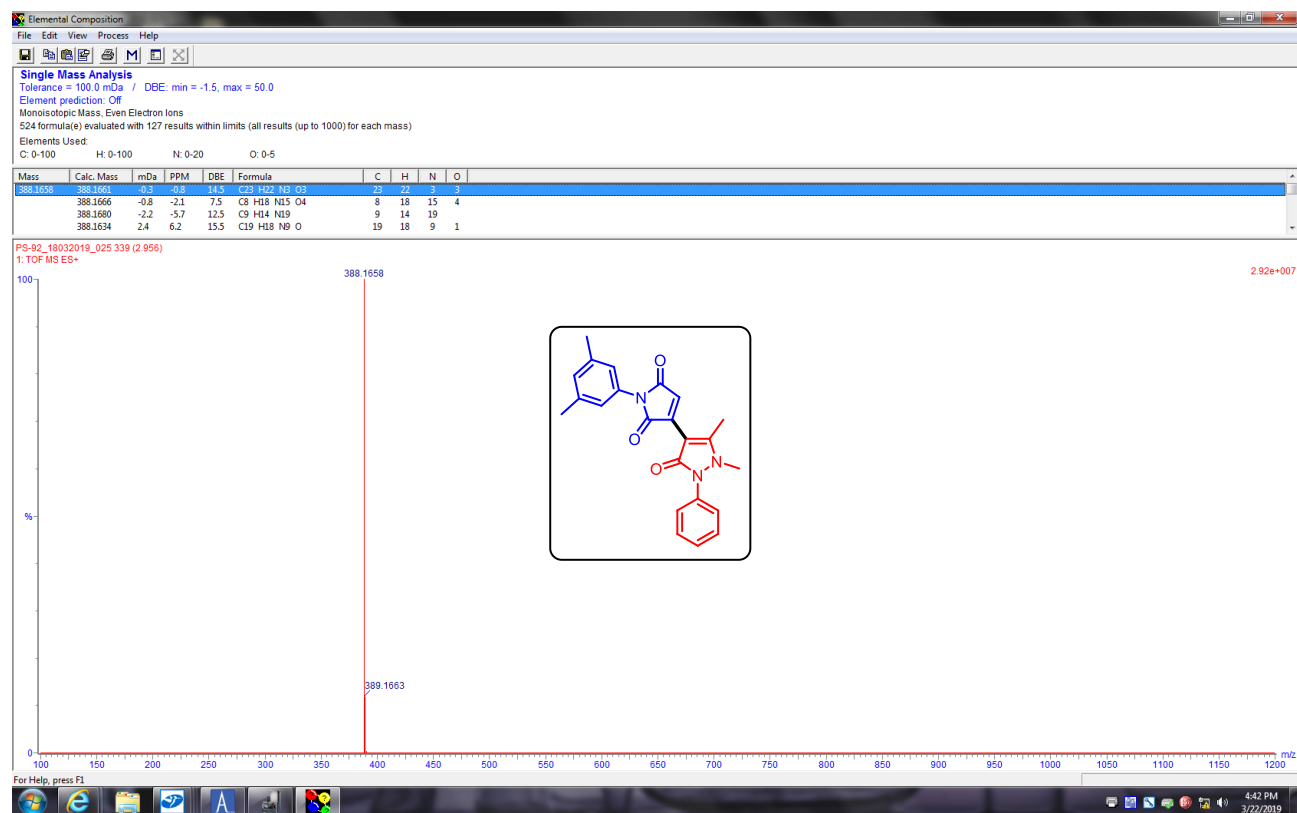
## HRMS Spectra of Compound 3ab:



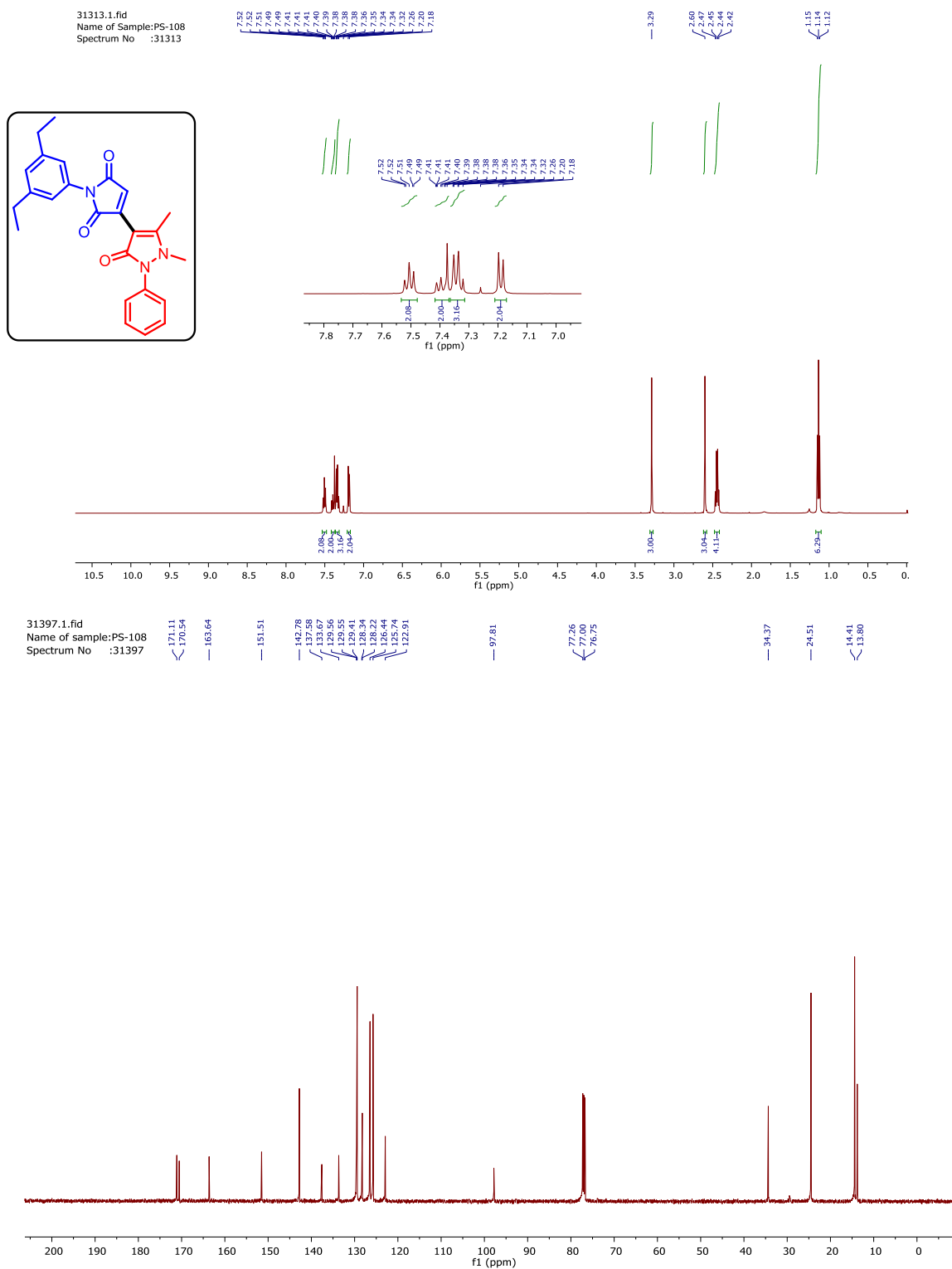
# $^1\text{H}$ and $^{13}\text{C}$ of Compound 3ac (500 & 125 MHz, $\text{CDCl}_3$ ):



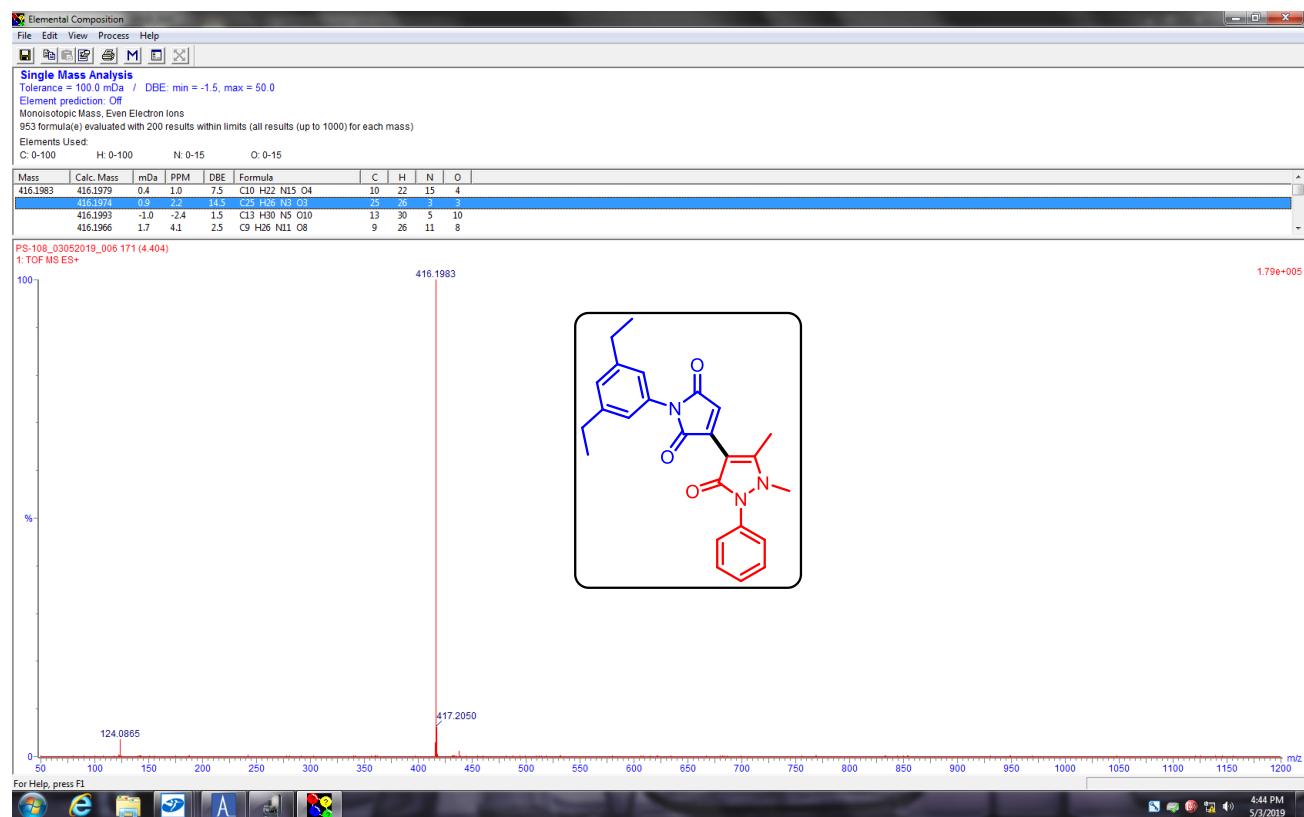
## HRMS Spectra of Compound 3ac:



# <sup>1</sup>H and <sup>13</sup>C of Compound 3ad (500 & 125 MHz, CDCl<sub>3</sub>):

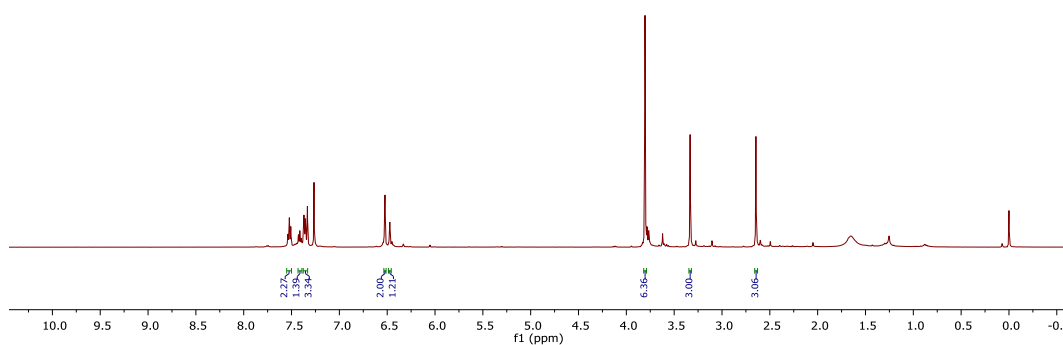
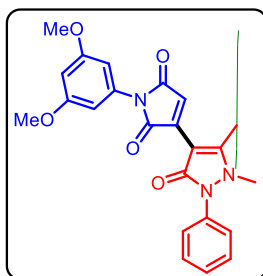


## HRMS Spectra of Compound 3ad:

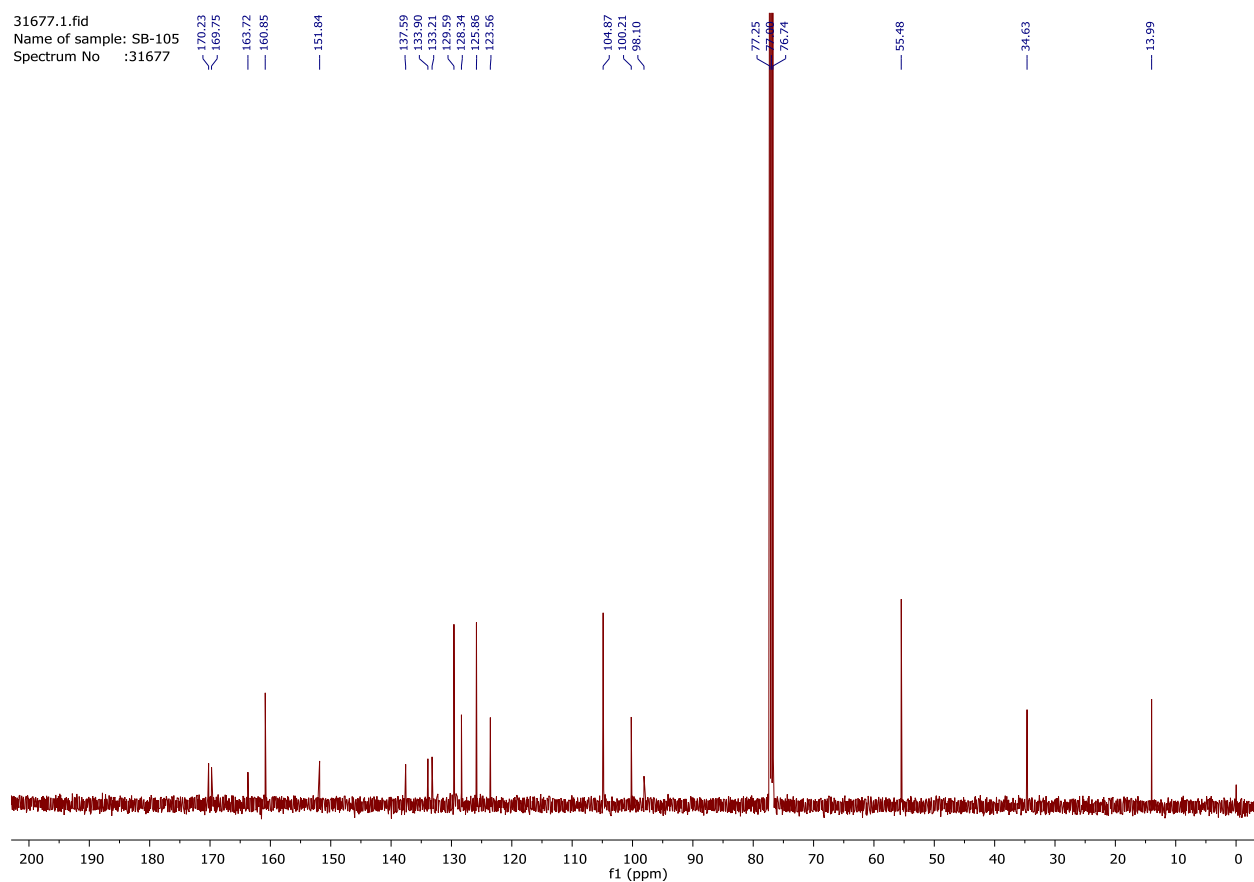


# <sup>1</sup>H and <sup>13</sup>C of Compound 3ae (500 & 125 MHz, CDCl<sub>3</sub>):

31491.1.fid  
Name of sample: SB-105  
Spectrum No : 31491

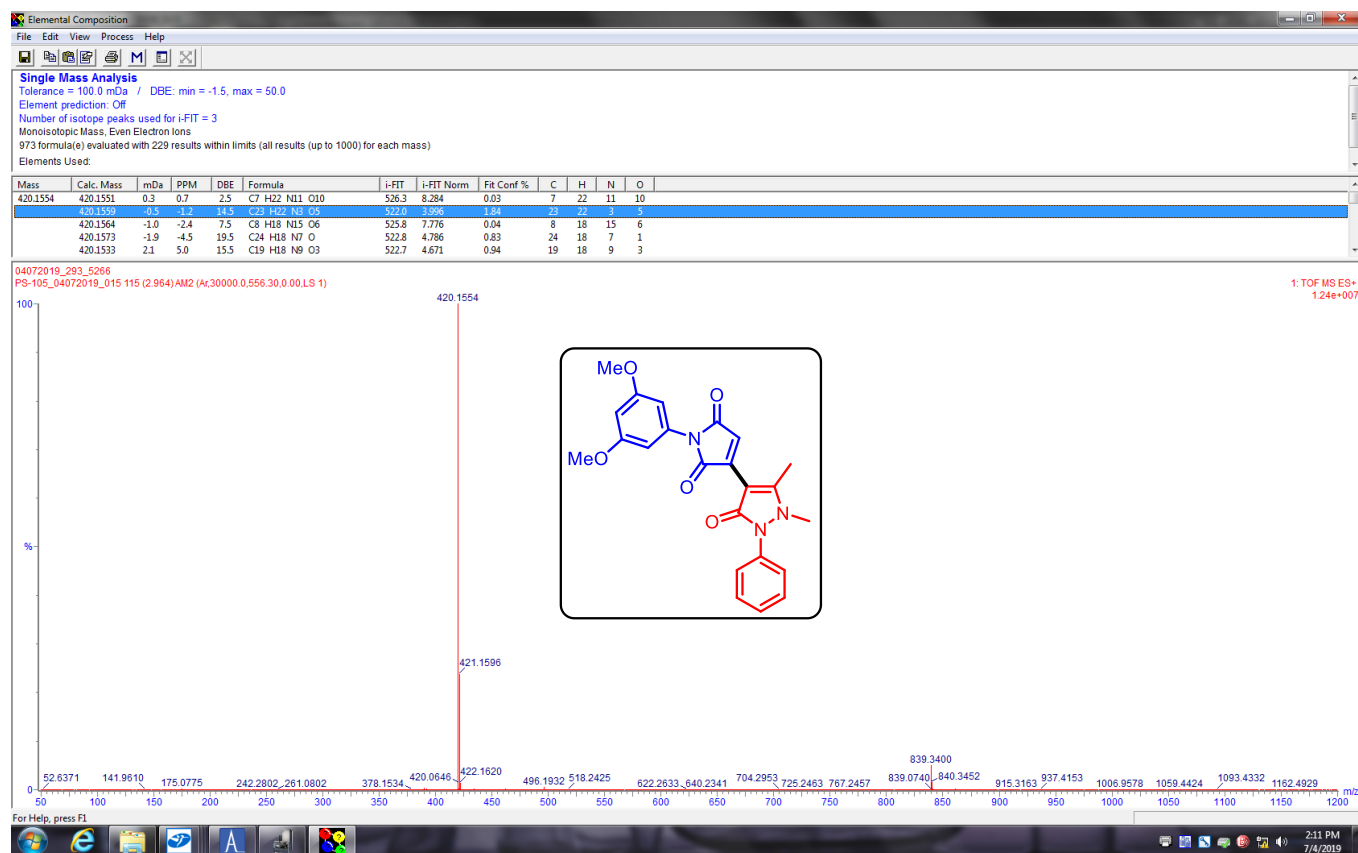


31677.1.fid  
Name of sample: SB-105  
Spectrum No : 31677

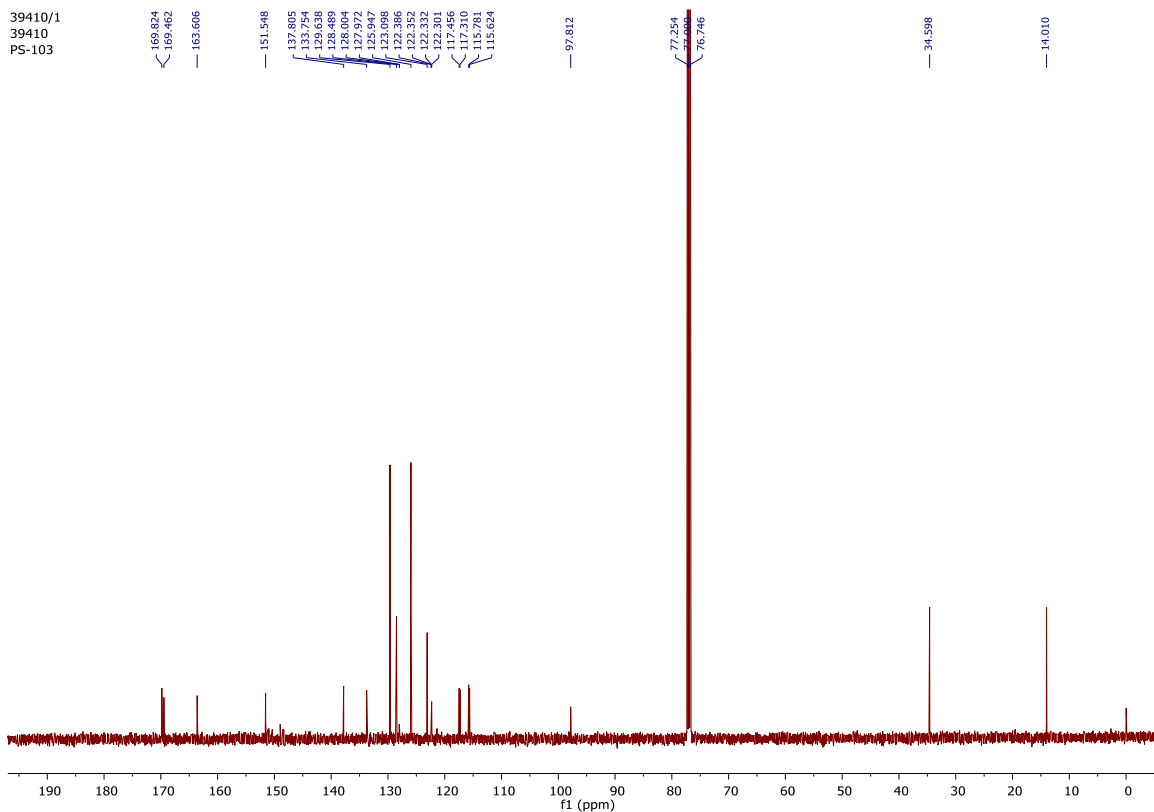
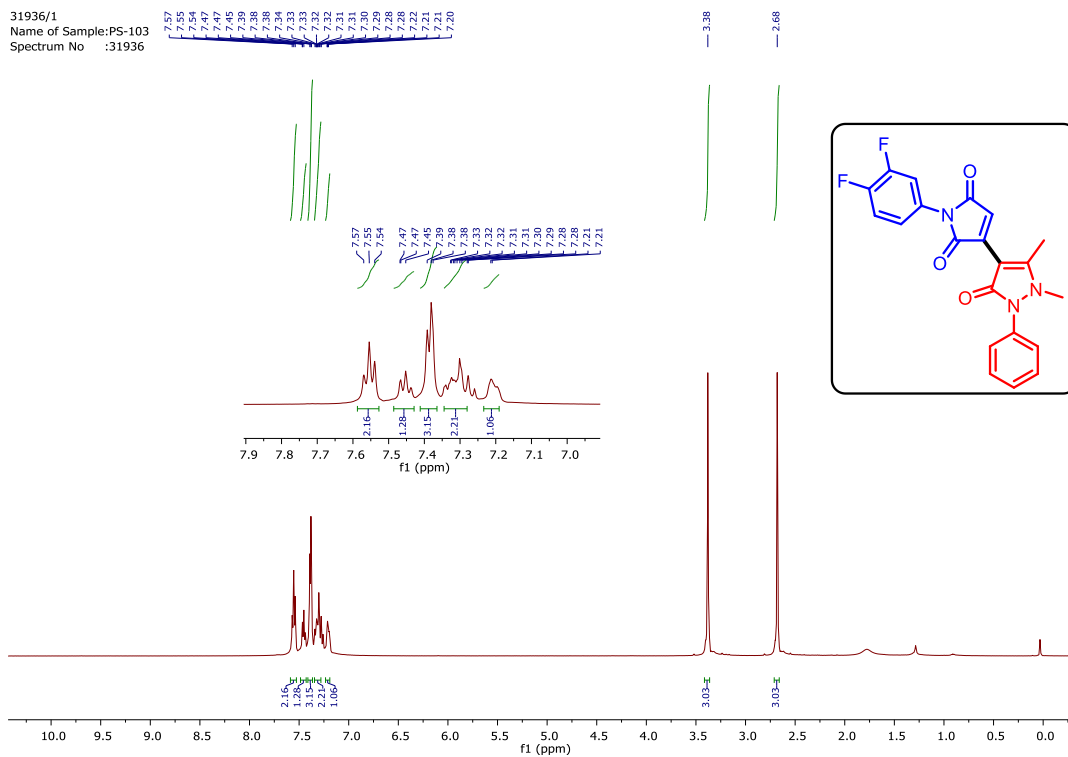




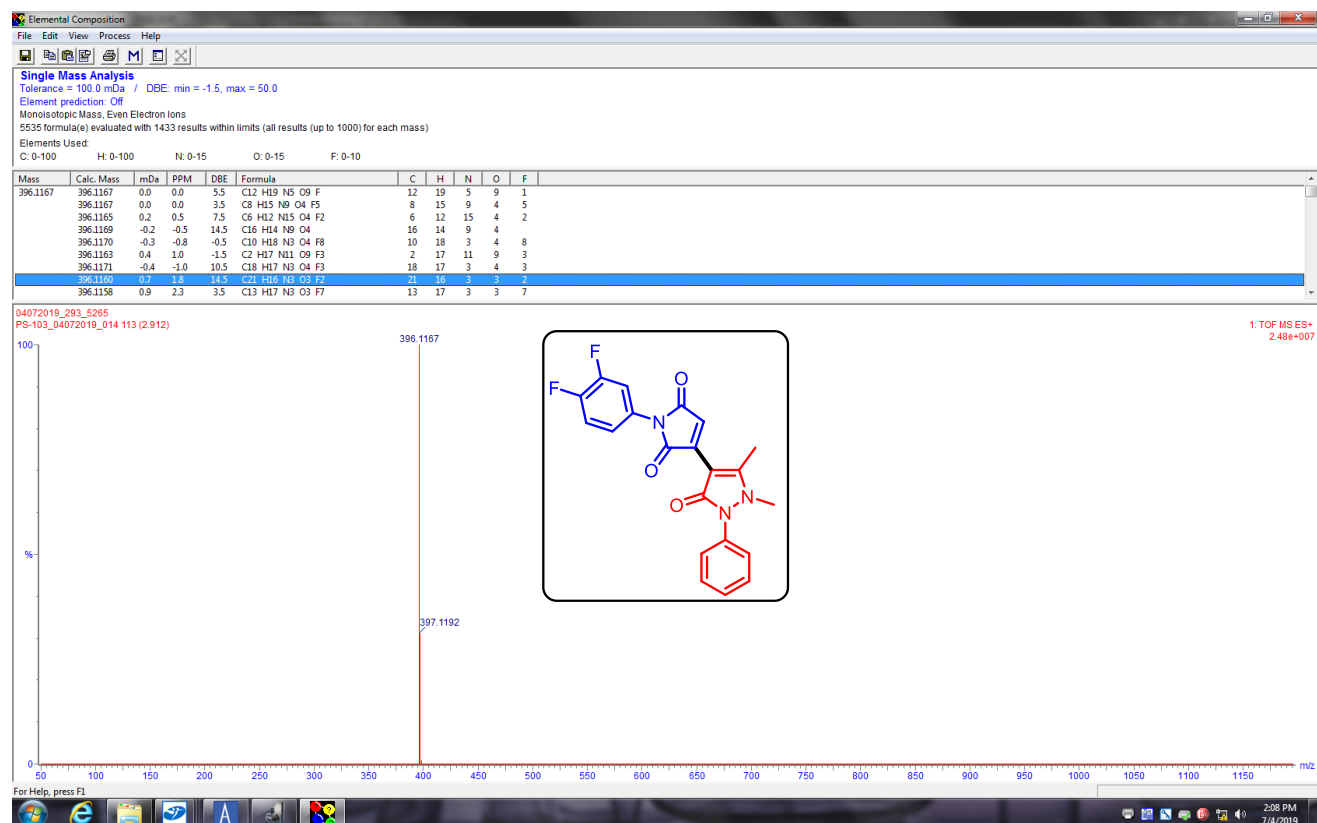
## HRMS Spectra of Compound 3ae:



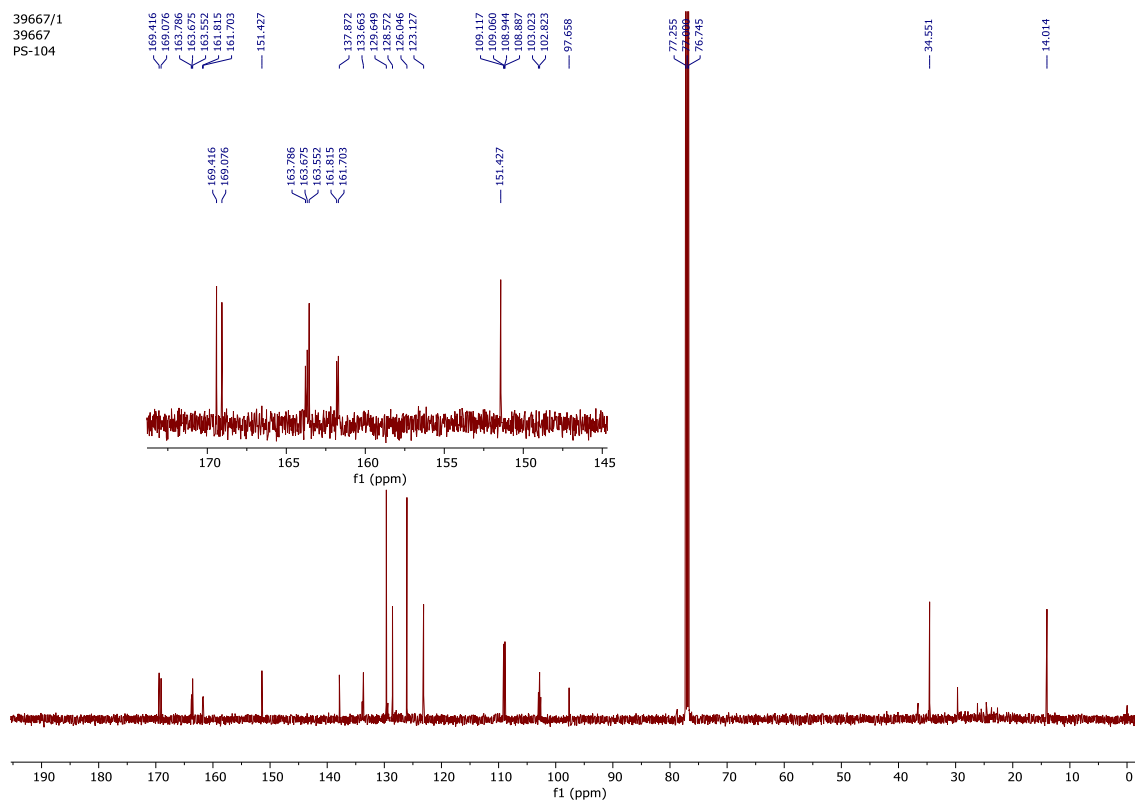
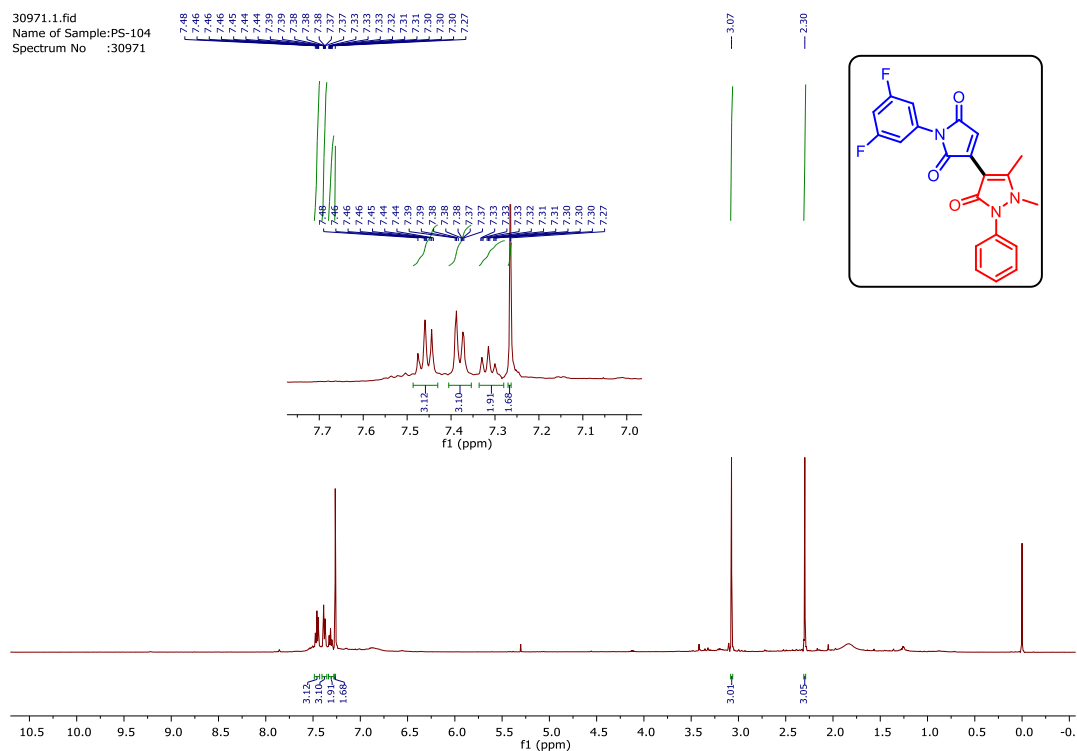
# <sup>1</sup>H and <sup>13</sup>C of Compound 3af (500 & 125 MHz, CDCl<sub>3</sub>):



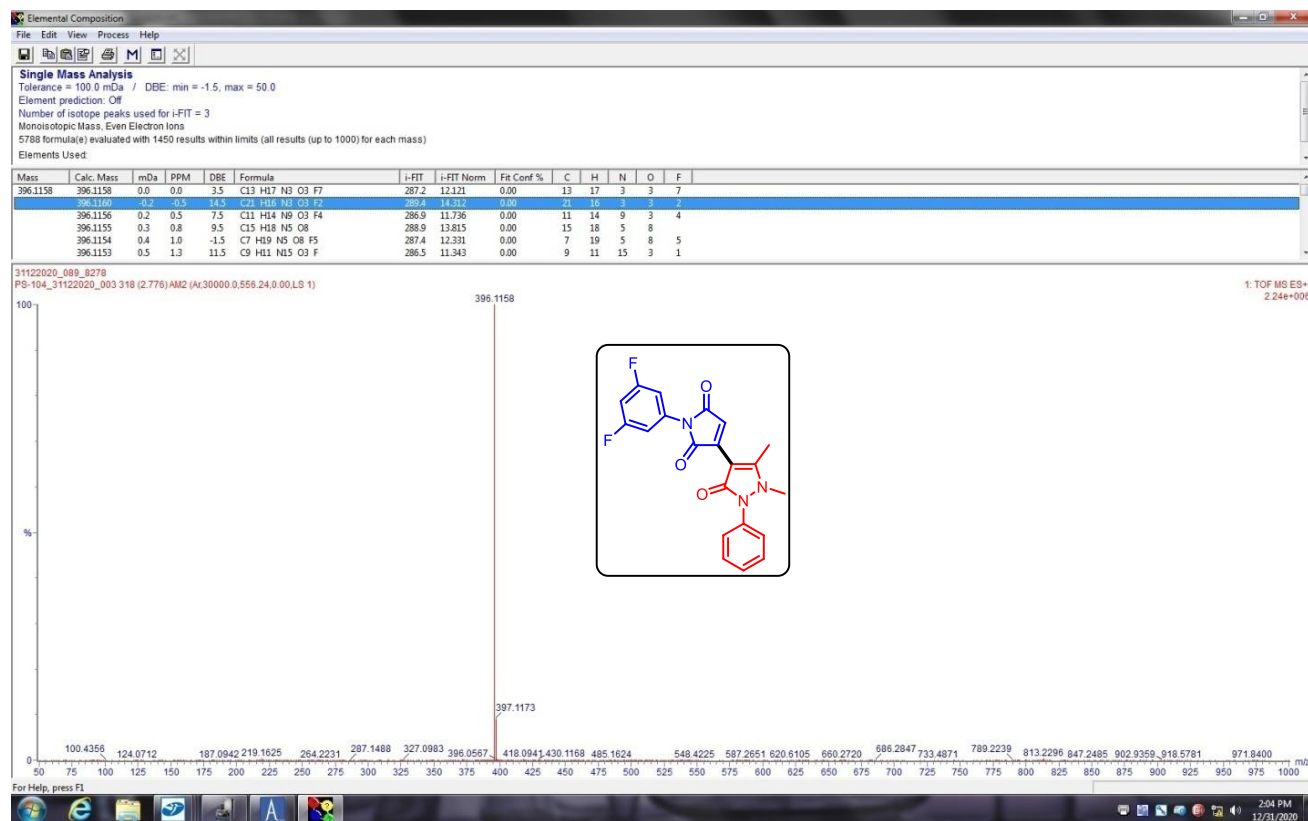
## HRMS Spectra of Compound 3af:



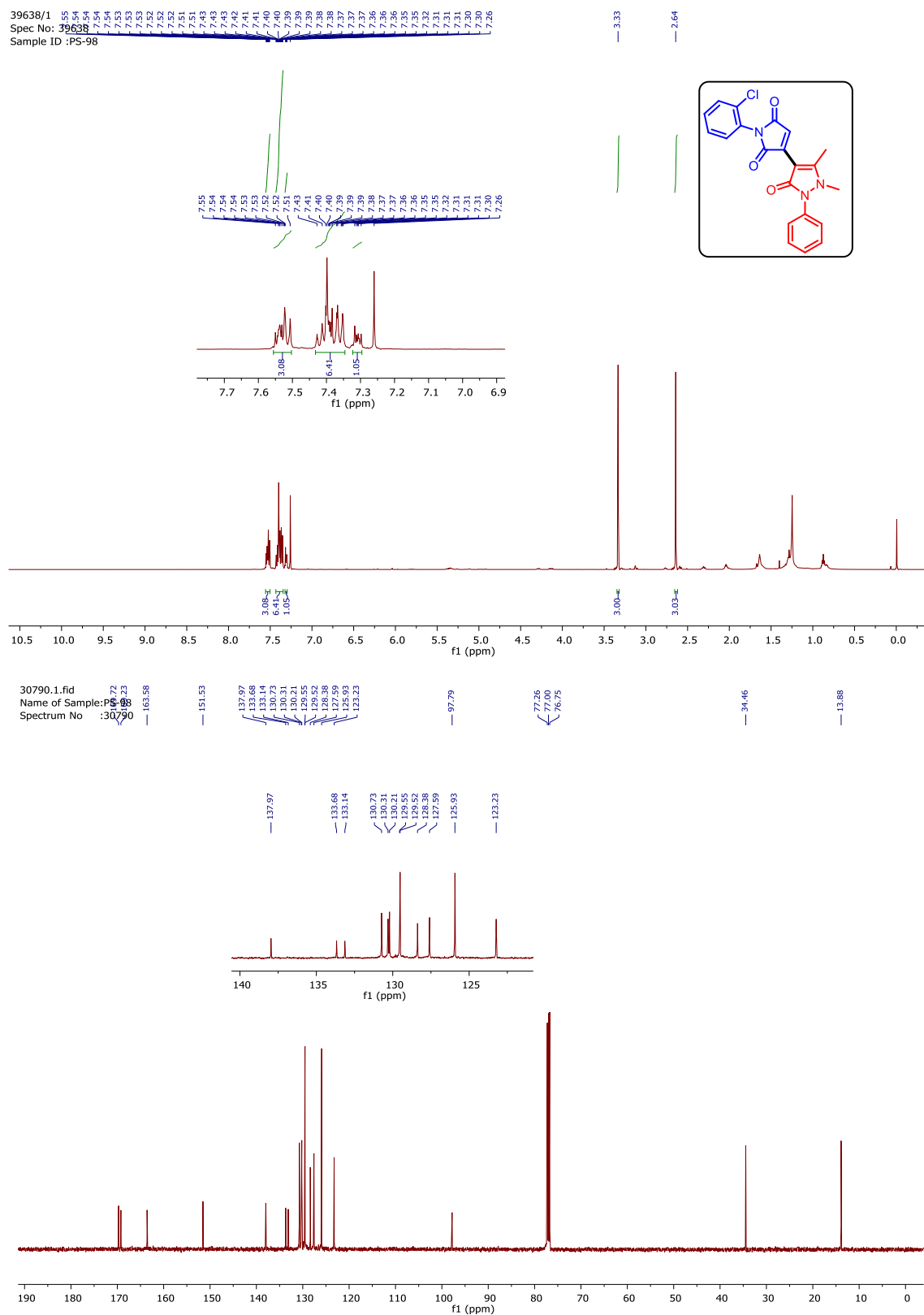
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ag (500 & 125 MHz, CDCl<sub>3</sub>):



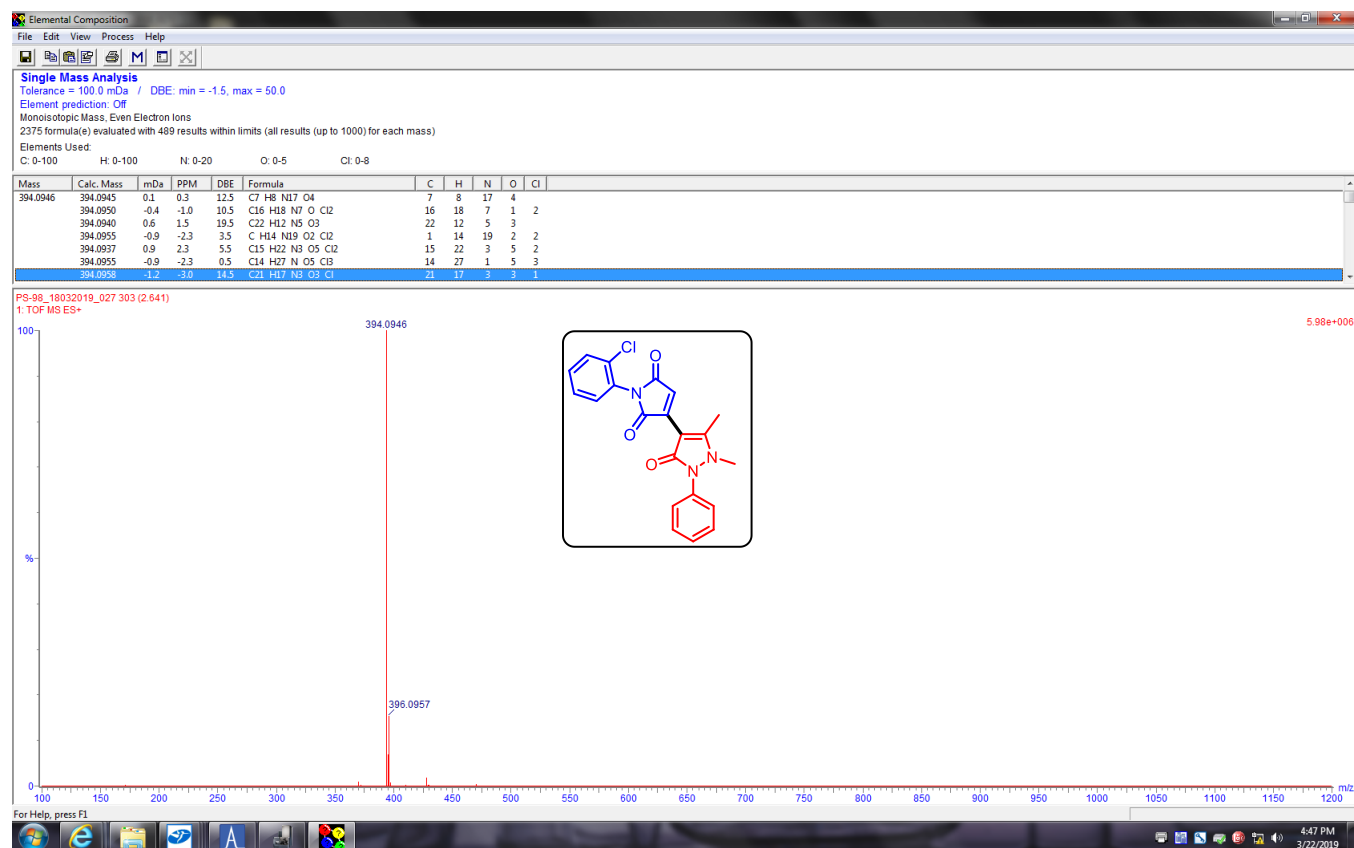
## HRMS Spectra of Compound 3ag:



# <sup>1</sup>H and <sup>13</sup>C of Compound 3ah (500 & 125 MHz, CDCl<sub>3</sub>):



## HRMS Spectra of Compound 3ah:



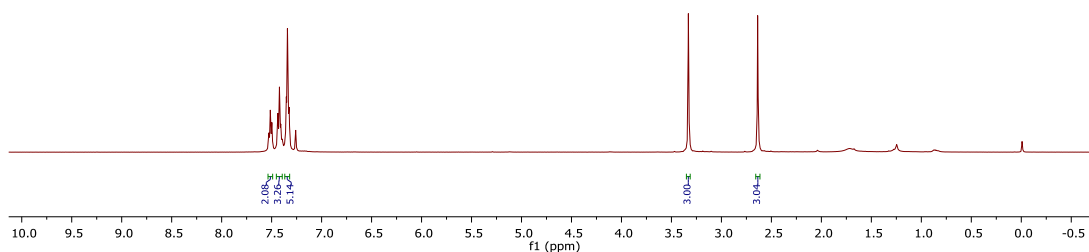
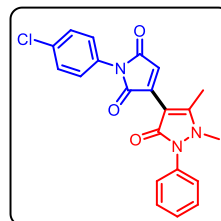
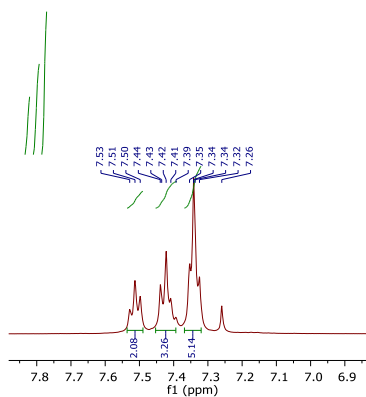
# <sup>1</sup>H and <sup>13</sup>C of Compound 3ai (500 & 125 MHz, CDCl<sub>3</sub>):

30547.1.fid  
Name of Sample:PS-97  
Spectrum No :30547

7.53  
7.51  
7.50  
7.44  
7.43  
7.42  
7.41  
7.39  
7.35  
7.34  
7.34  
7.34  
7.26

3.33

2.64



30932.1.fid  
Name of Sample:PS-97  
Spectrum No :30932

170.02  
169.35  
163.58

151.54

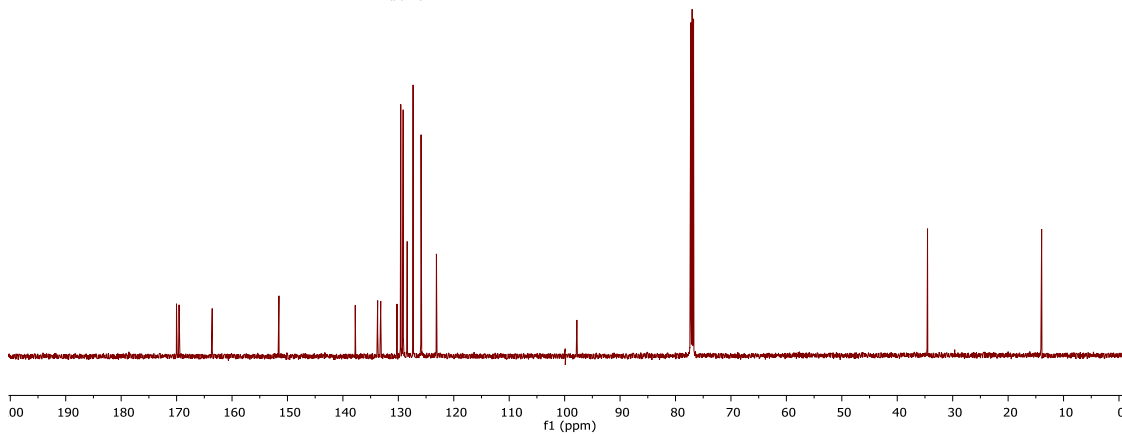
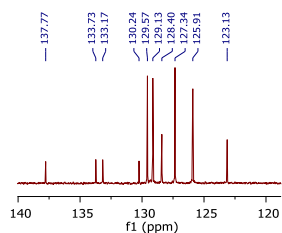
137.77  
133.73  
133.17  
130.24  
129.57  
129.13  
128.40  
127.34  
125.91  
123.13

97.80

77.25  
77.00  
76.75

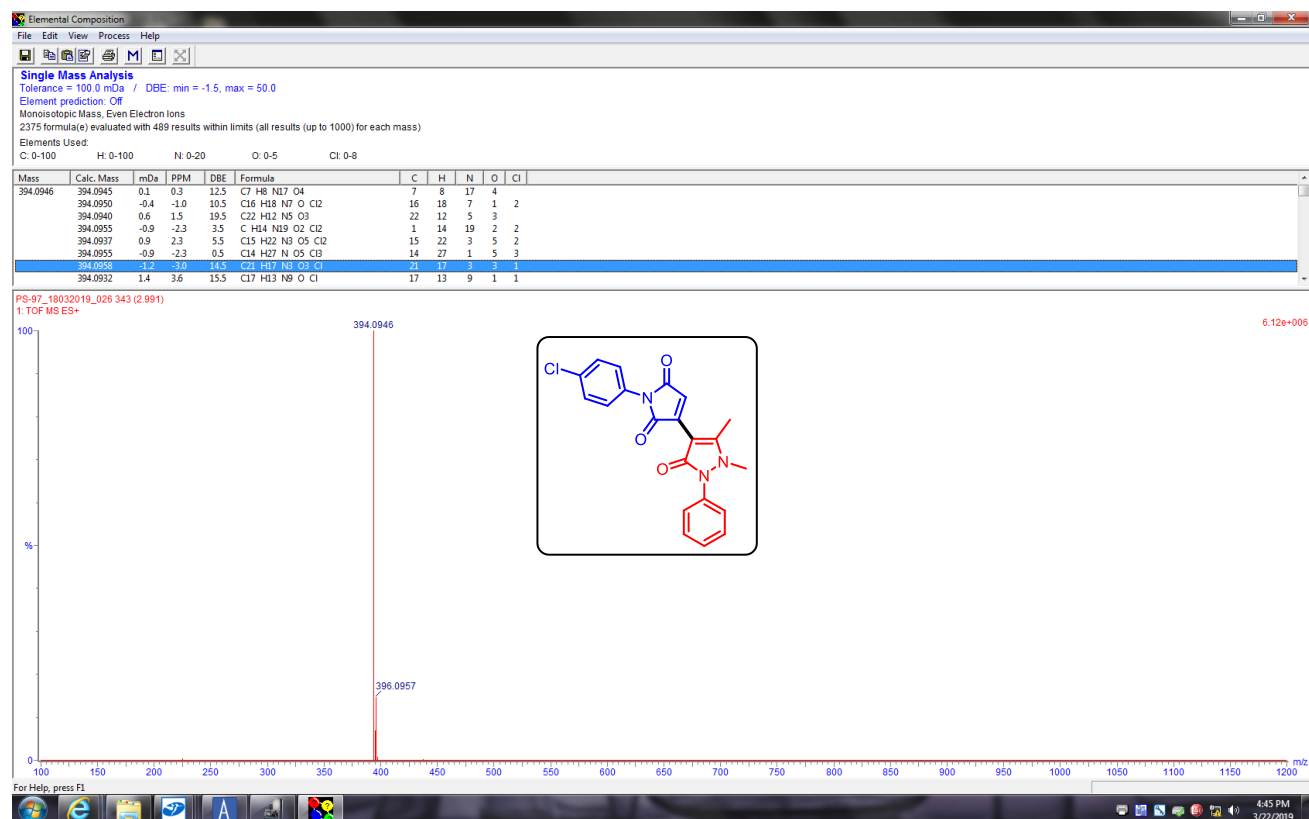
34.54

13.95





## HRMS Spectra of Compound 3ai:



30643.1.fid  
Name of Sample:SB-100  
Spectrum No :30643

7.58  
7.57  
7.52  
7.50  
7.49  
7.49  
7.48  
7.41  
7.36  
7.35  
7.35  
7.26

Chemical structure of compound 30643.1.fid: BrC1=CC=C(C=C1)N2C(=O)C=C(C2[C@H]3C(=O)N(C4=CC=CC=C4)C3)C5=CC=CC=C5

Chemical structure of compound 30783.1.fid: BrC1=CC=C(C=C1)N2C(=O)C=C(C2[C@H]3C(=O)N(C4=CC=CC=C4)C3)C5=CC=CC=C5

30783.1.fid  
Name of Sample:PS-100  
Spectrum No :30783

169.84  
169.42  
163.58

151.49

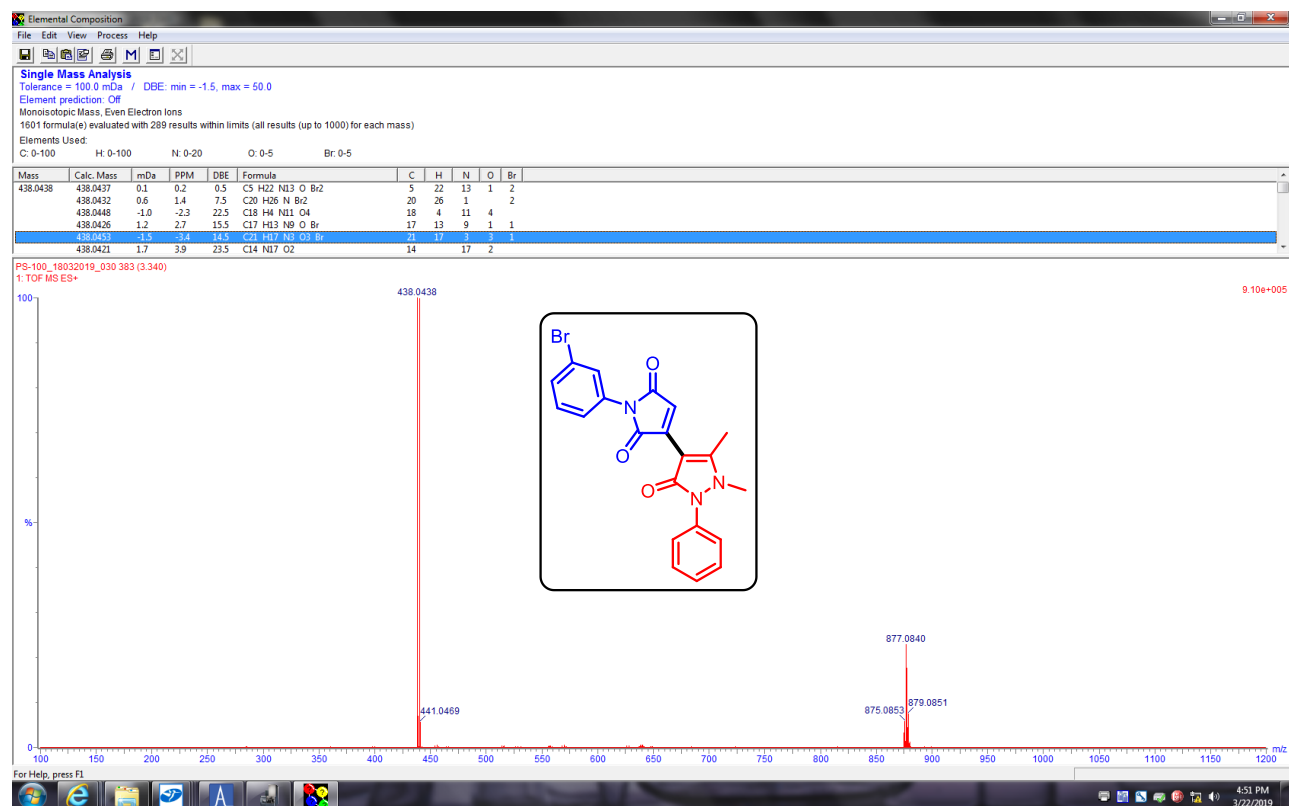
137.76  
137.76  
137.70  
133.97  
130.58  
130.19  
129.61  
129.09  
128.49  
126.00  
126.00  
124.73  
123.19  
122.27

97.78

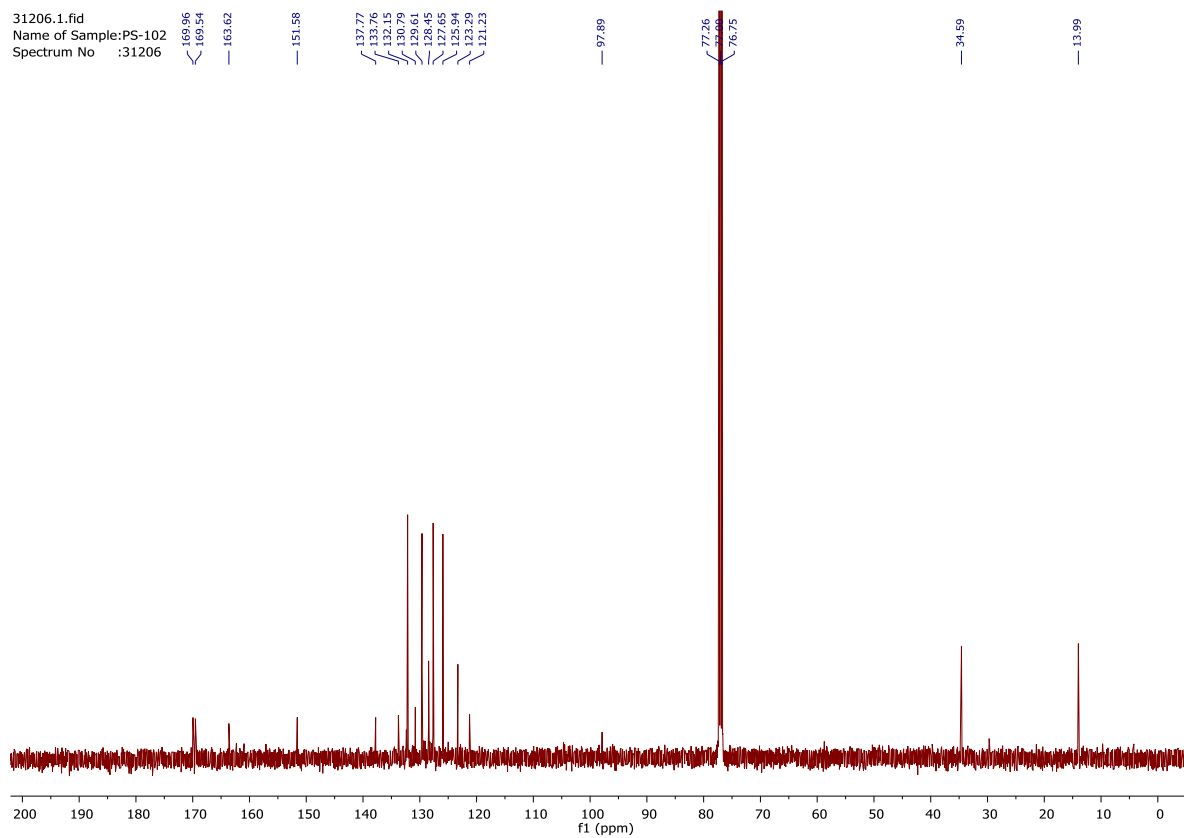
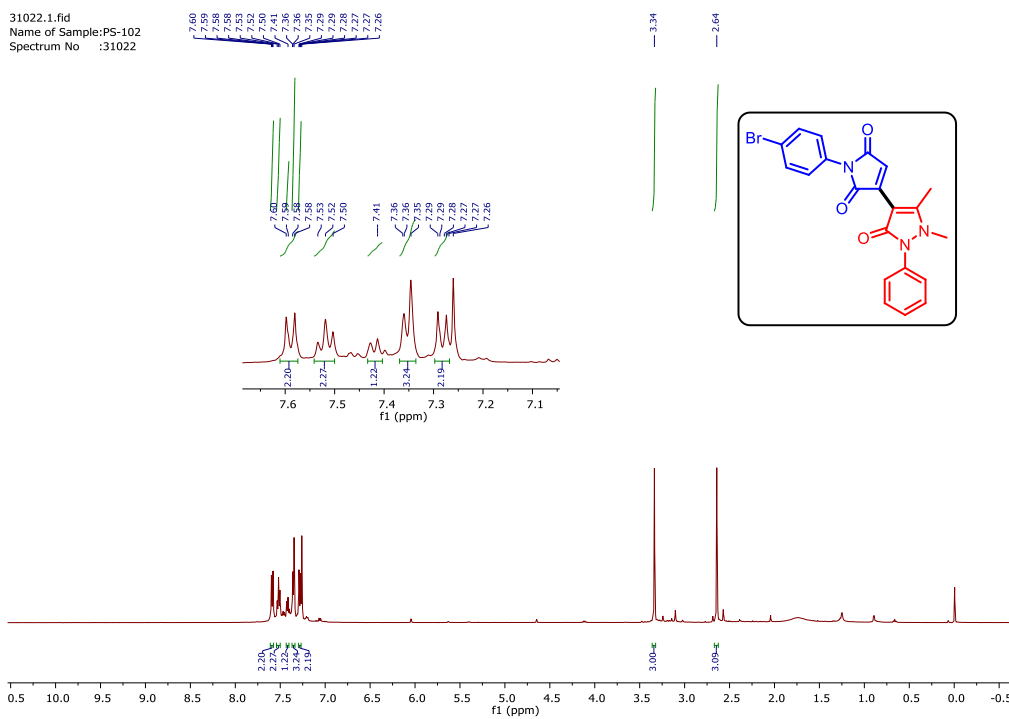
77.25  
76.75

34.54

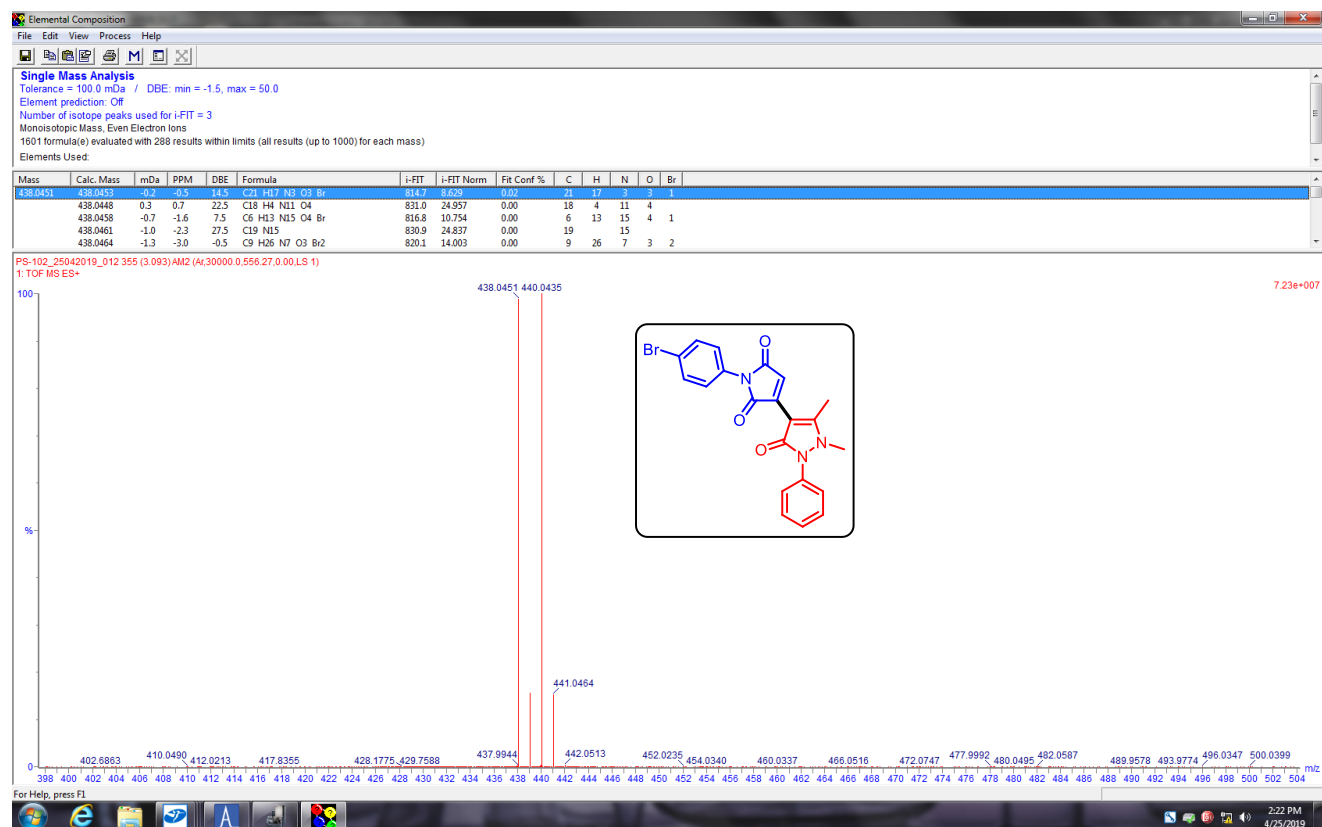
## HRMS Spectra of Compound 3aj:



# <sup>1</sup>H and <sup>13</sup>C of Compound 3ak (500 & 125 MHz, CDCl<sub>3</sub>):



## HRMS Spectra of Compound 3ak:



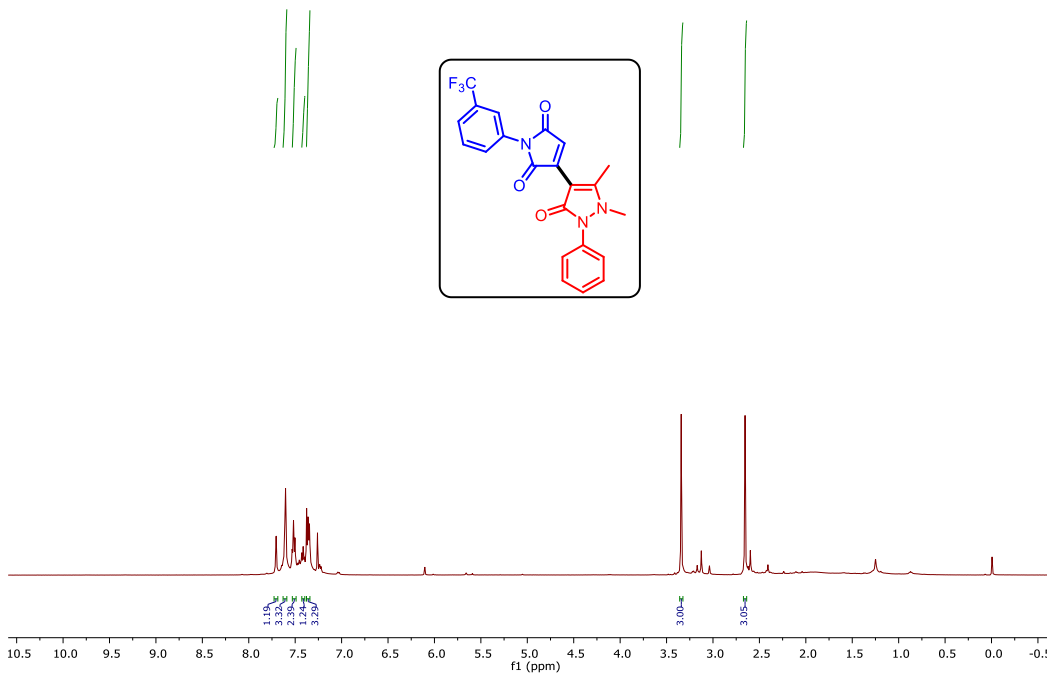
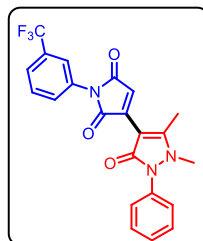
# <sup>1</sup>H and <sup>13</sup>C of Compound 3aI (500 & 125 MHz, CDCl<sub>3</sub>):

31970/1  
Name of Sample:PS-107  
Spectrum No :31970

7.71  
7.62  
7.61  
7.60  
7.58  
7.52  
7.50  
7.44  
7.43  
7.38  
7.36  
7.35  
7.28

3.34

2.65



32130/1  
Name of sample:PS-107  
Spectrum No :32130

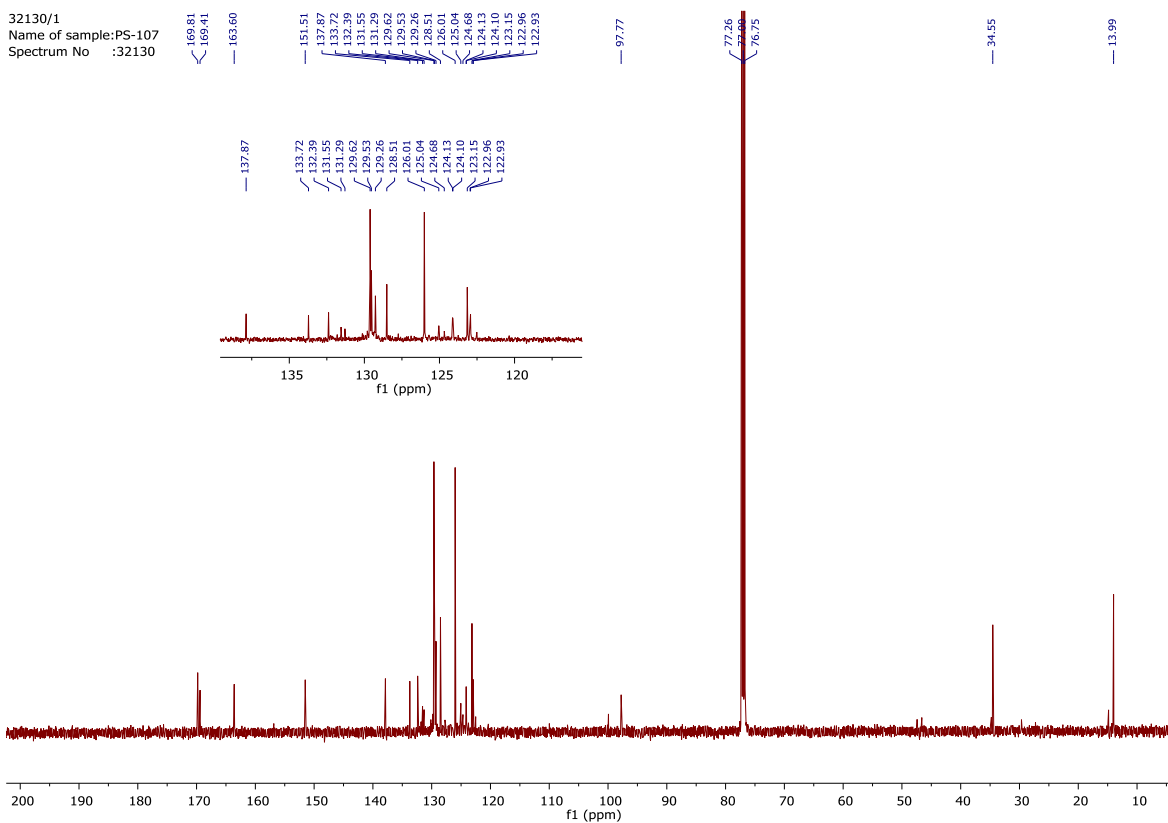
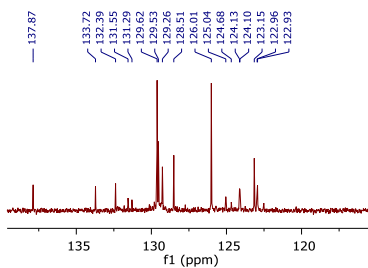
169.81  
169.41  
163.60

151.51  
147.77  
133.72  
132.39  
131.29  
129.52  
129.26  
128.51  
126.01  
125.04  
124.68  
124.13  
123.15  
122.96  
122.93

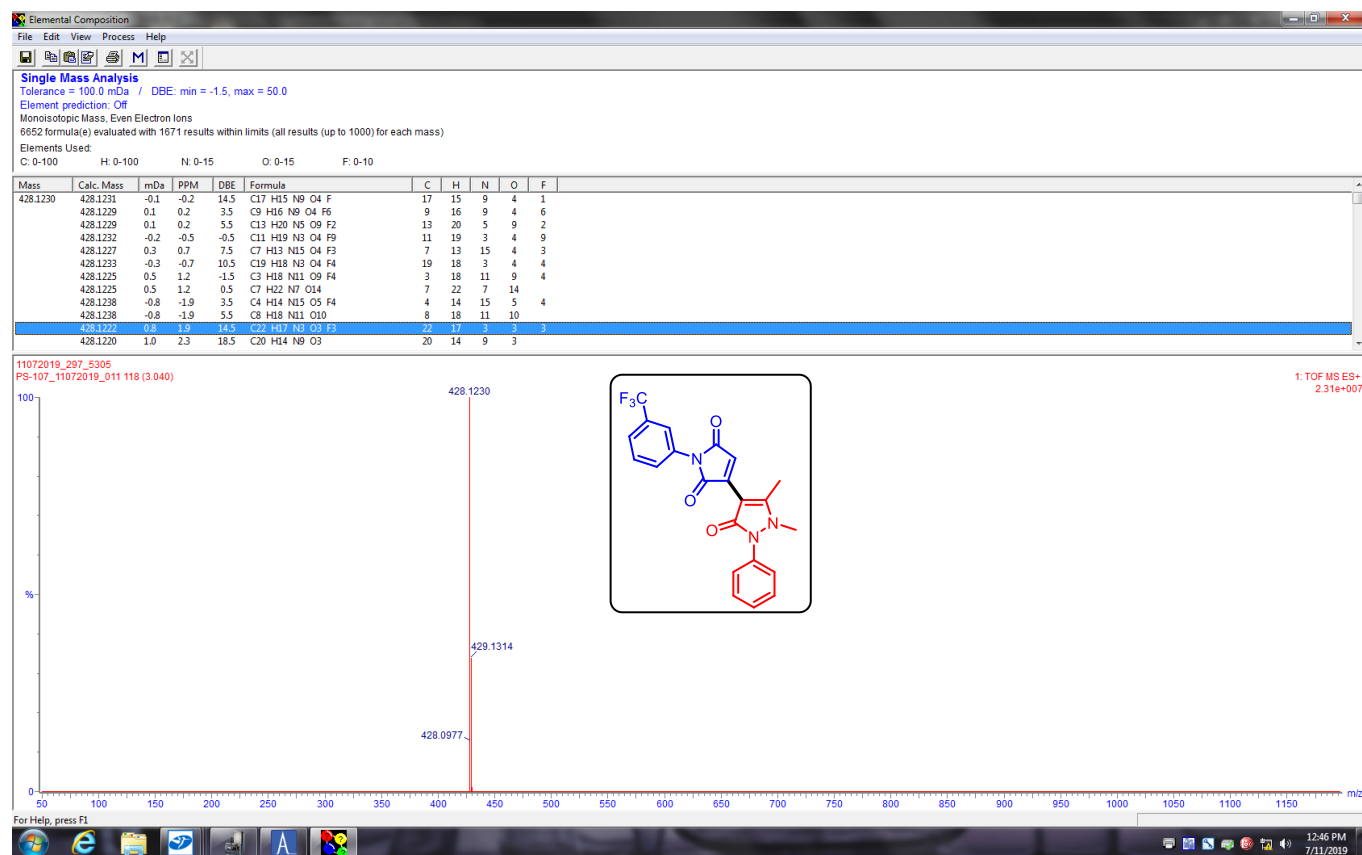
97.77

34.55

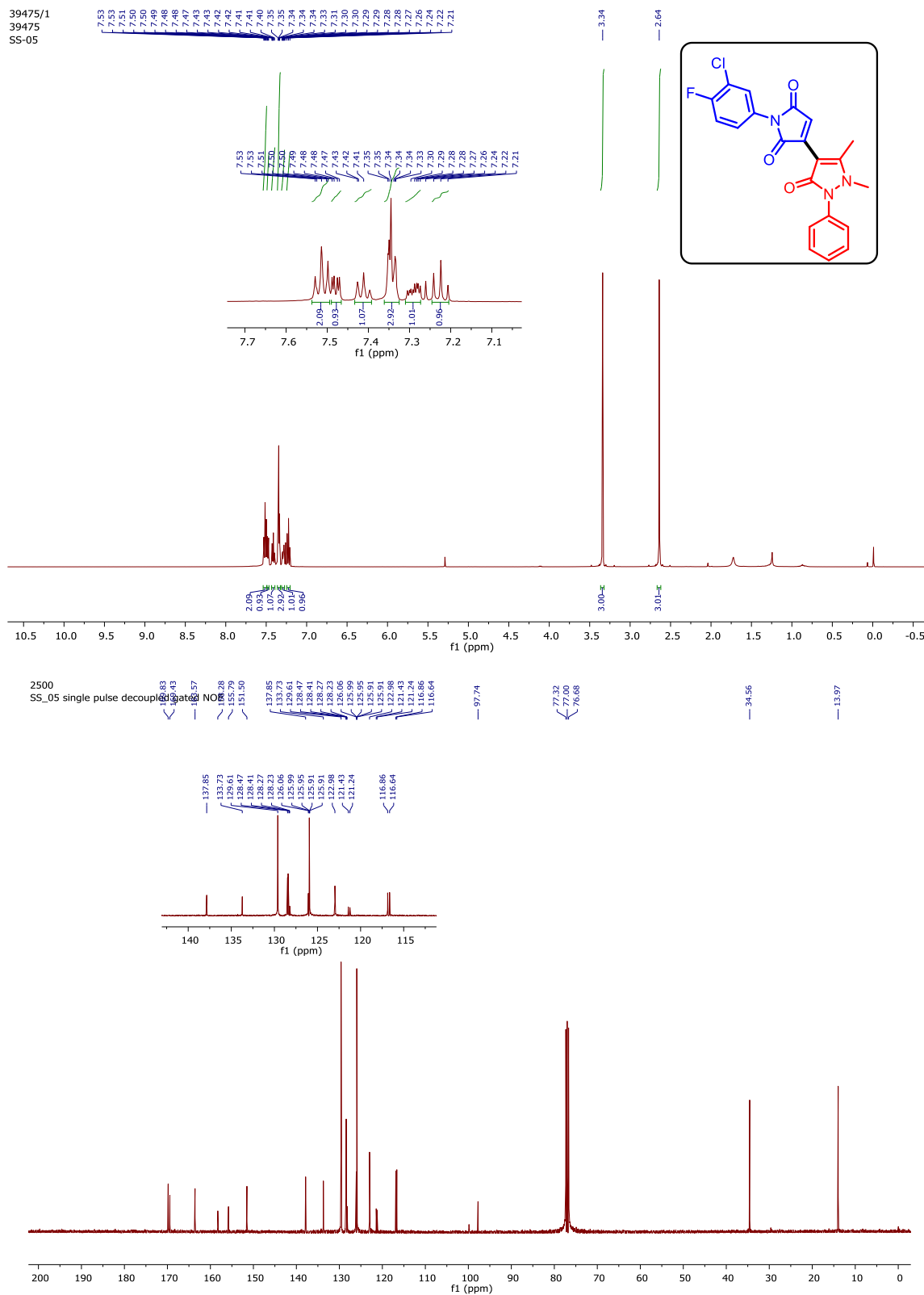
13.99



## HRMS Spectra of Compound 3al:



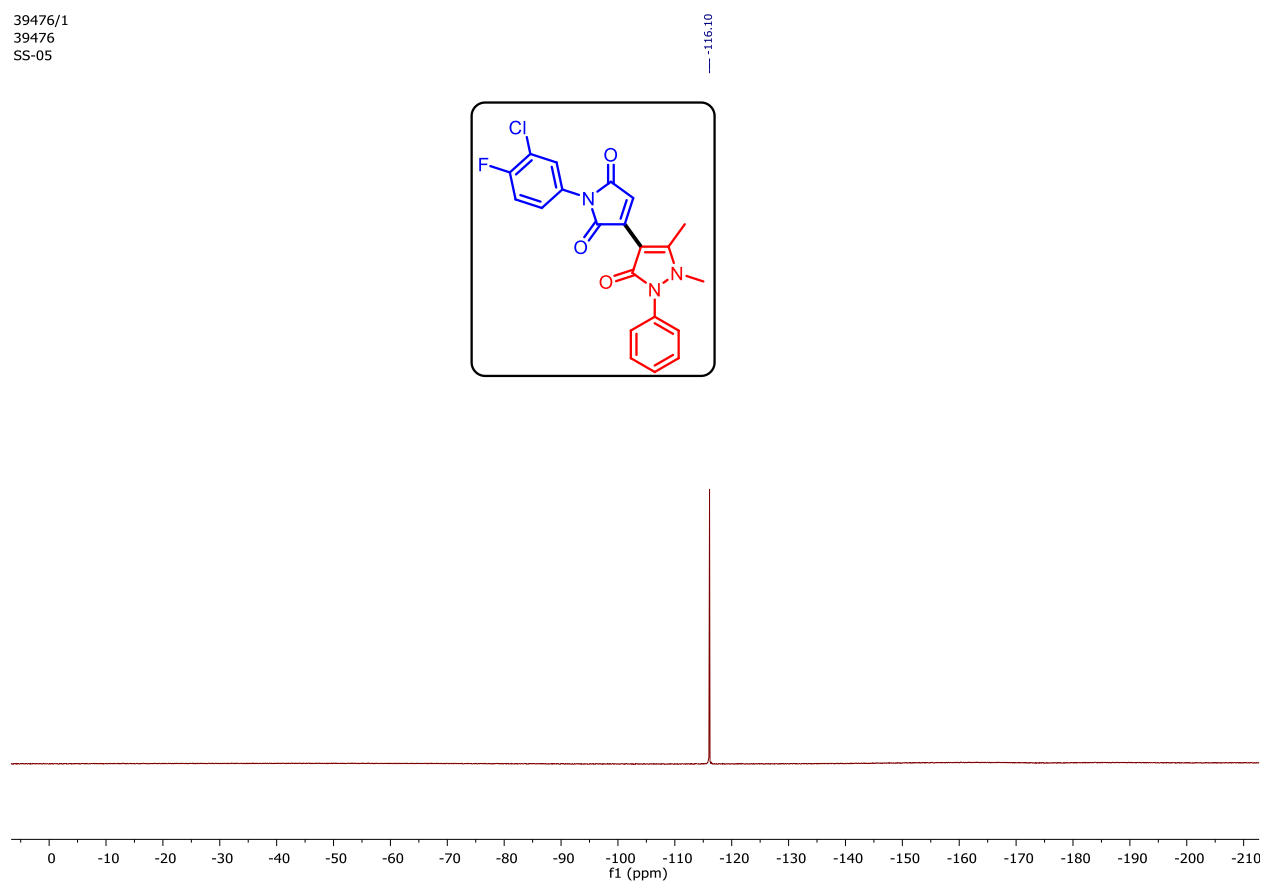
# <sup>1</sup>H and <sup>13</sup>C of Compound 3am (500 & 100 MHz, CDCl<sub>3</sub>):



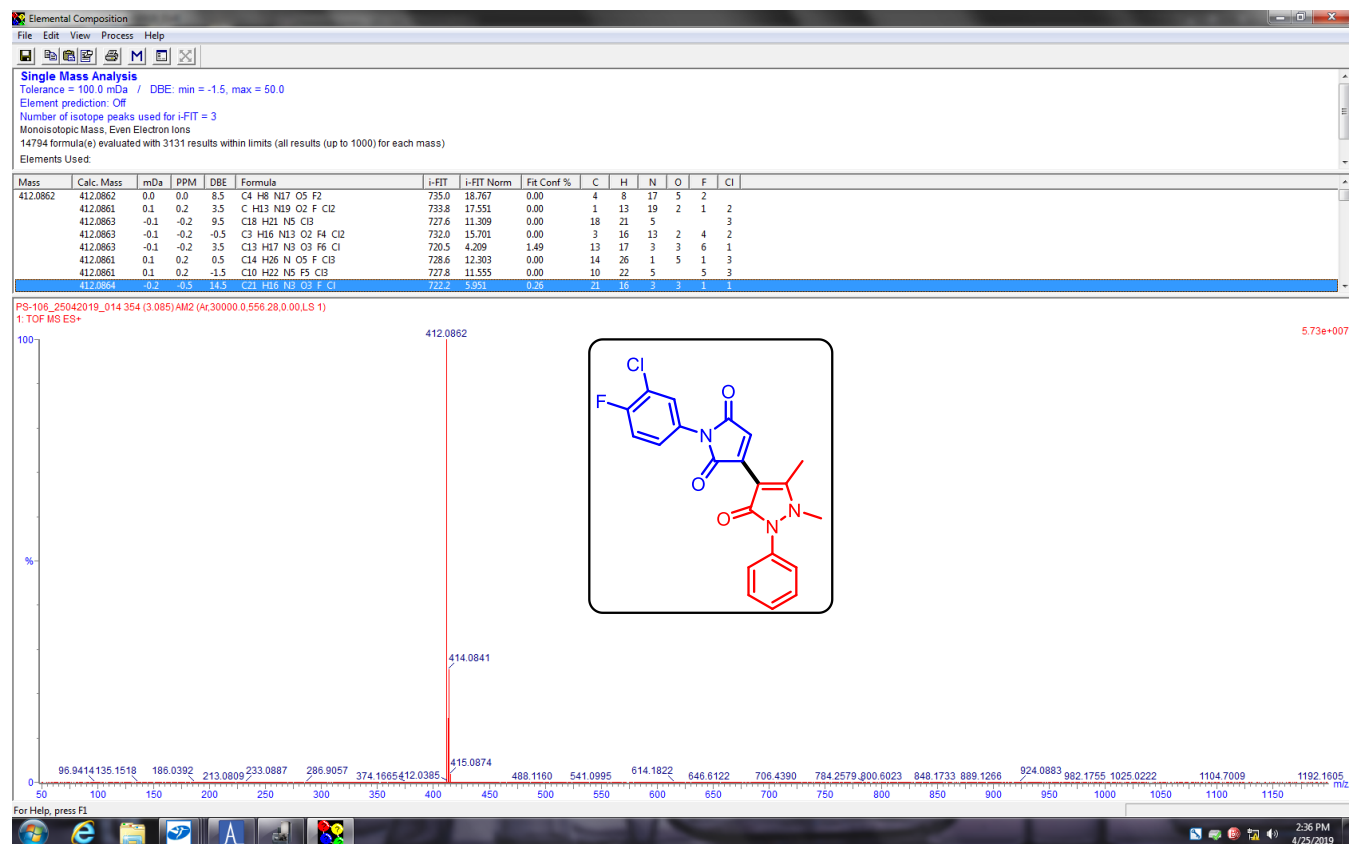


**$^{19}\text{F}$  NMR of Compound 3am (376 MHz,  $\text{CDCl}_3$ ):**

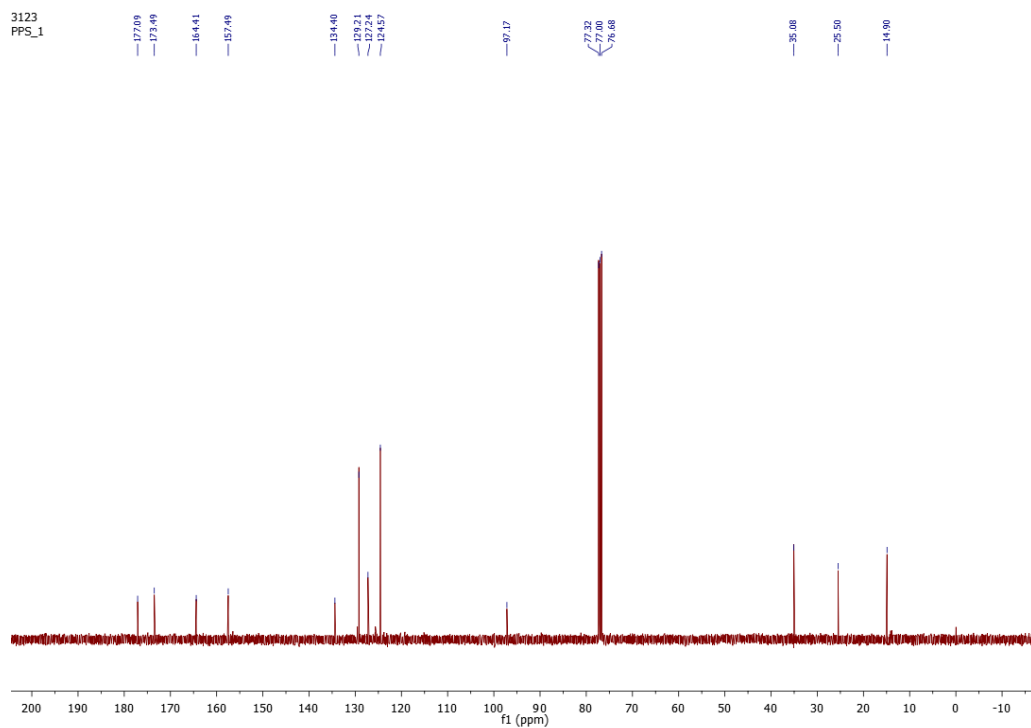
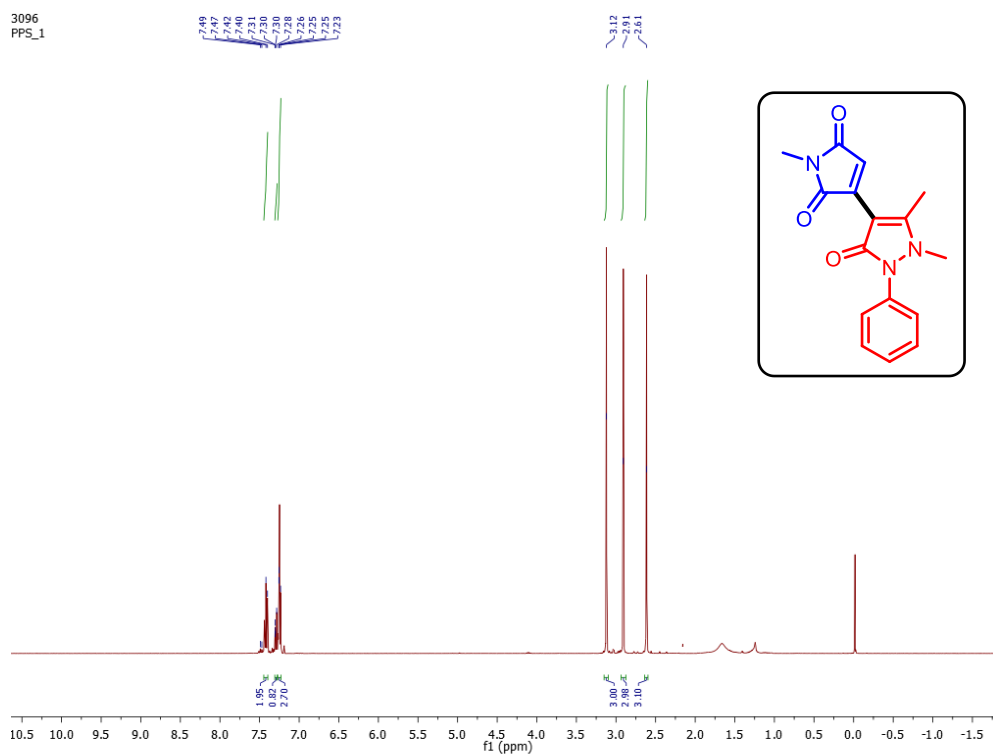
39476/1  
39476  
SS-05



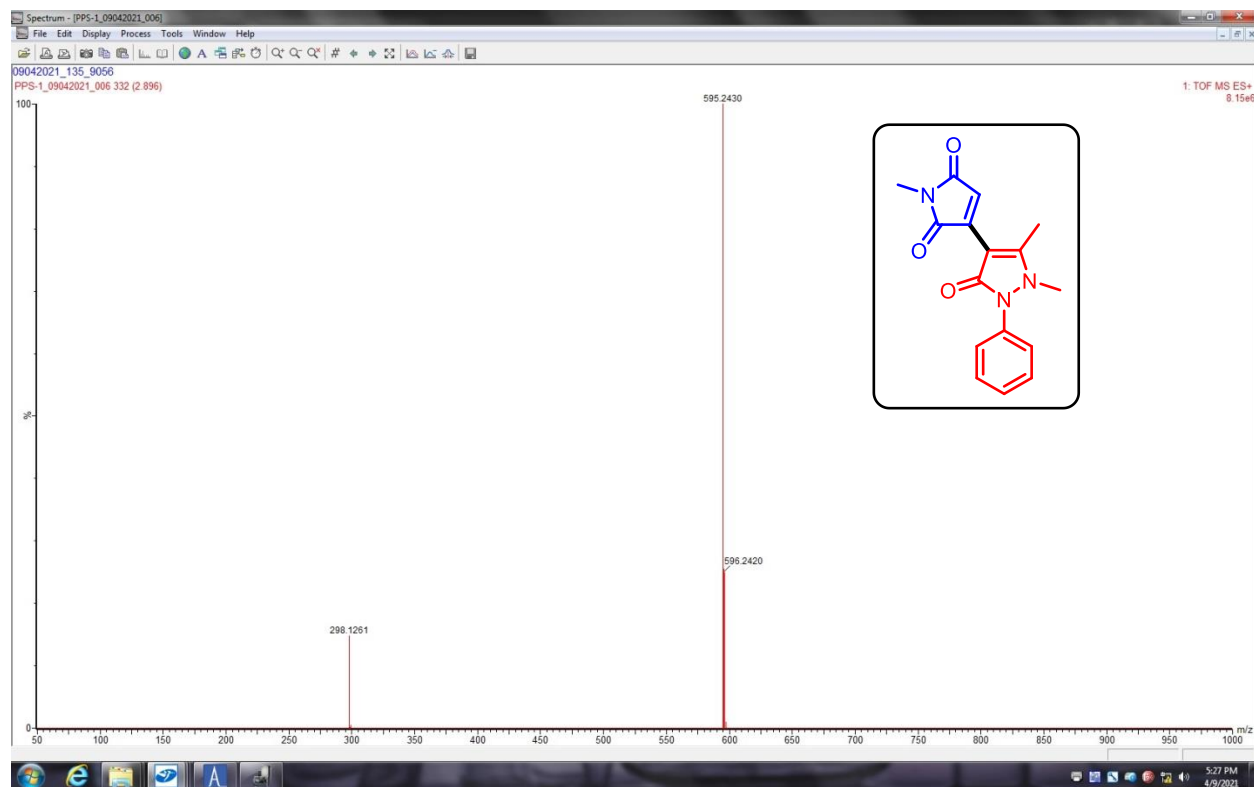
## HRMS Spectra of Compound 3am:



**$^1\text{H}$  and  $^{13}\text{C}$  of Compound 3an (400 & 100 MHz,  $\text{CDCl}_3$ ):**

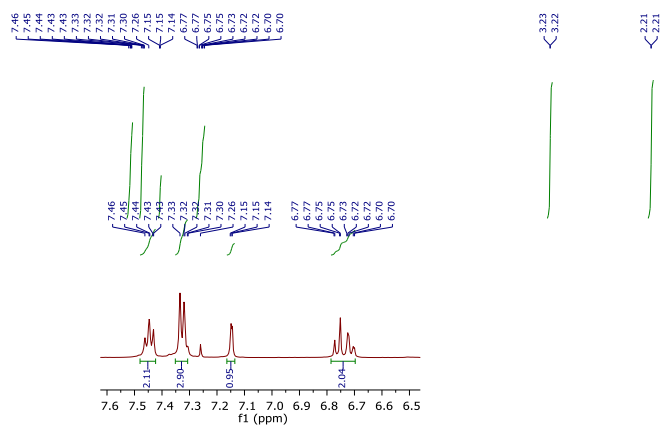


## HRMS Spectra of Compound 3an:

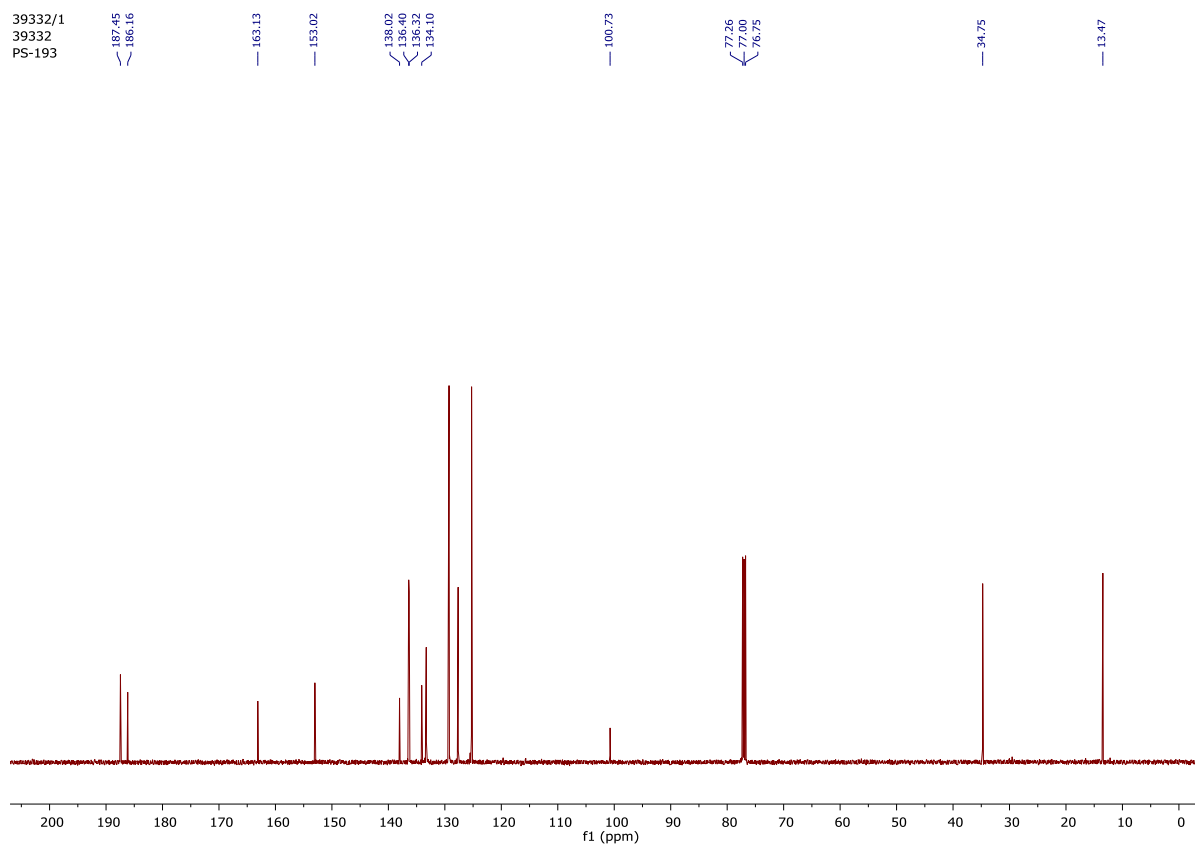


# <sup>1</sup>H and <sup>13</sup>C of Compound 3aa' (500 & 125 MHz, CDCl<sub>3</sub>):

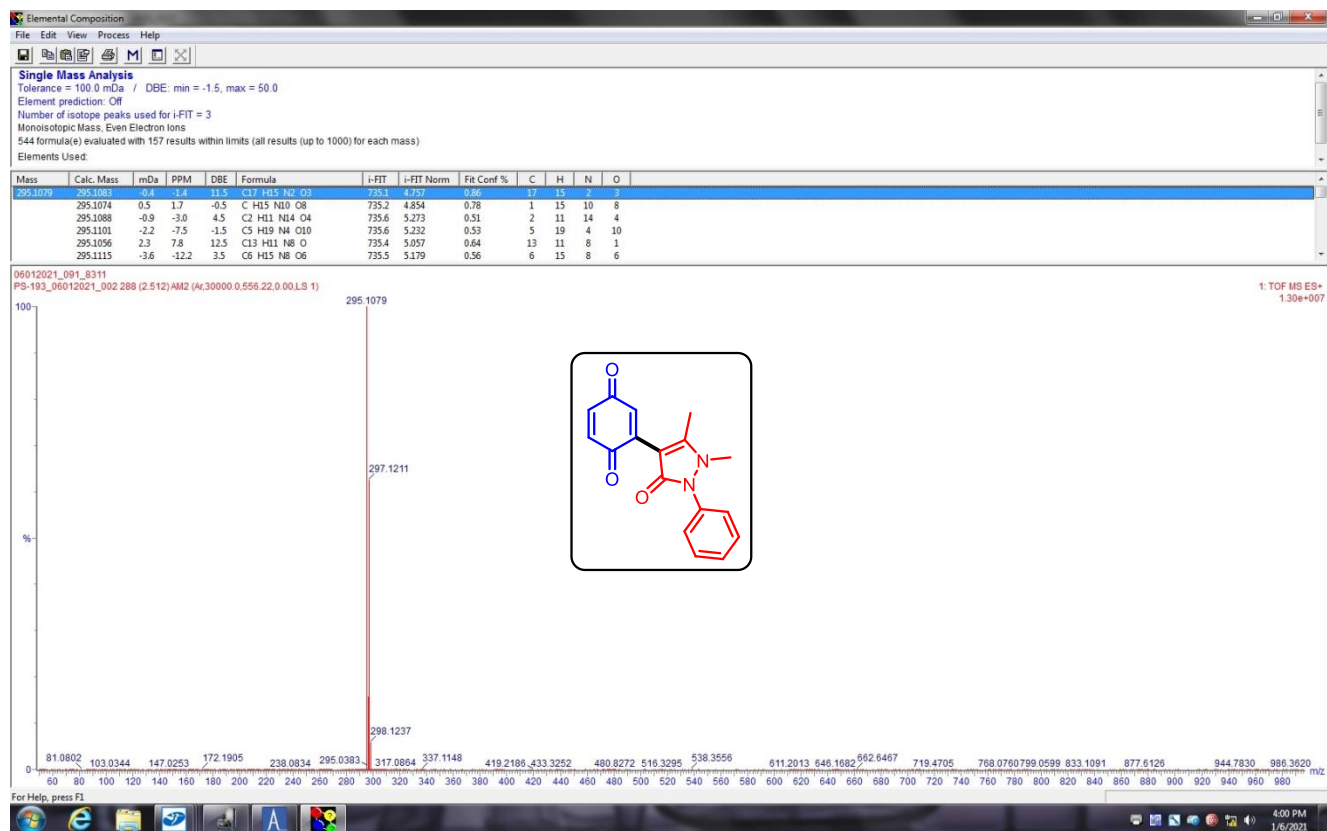
39331/1  
39331  
PS-193



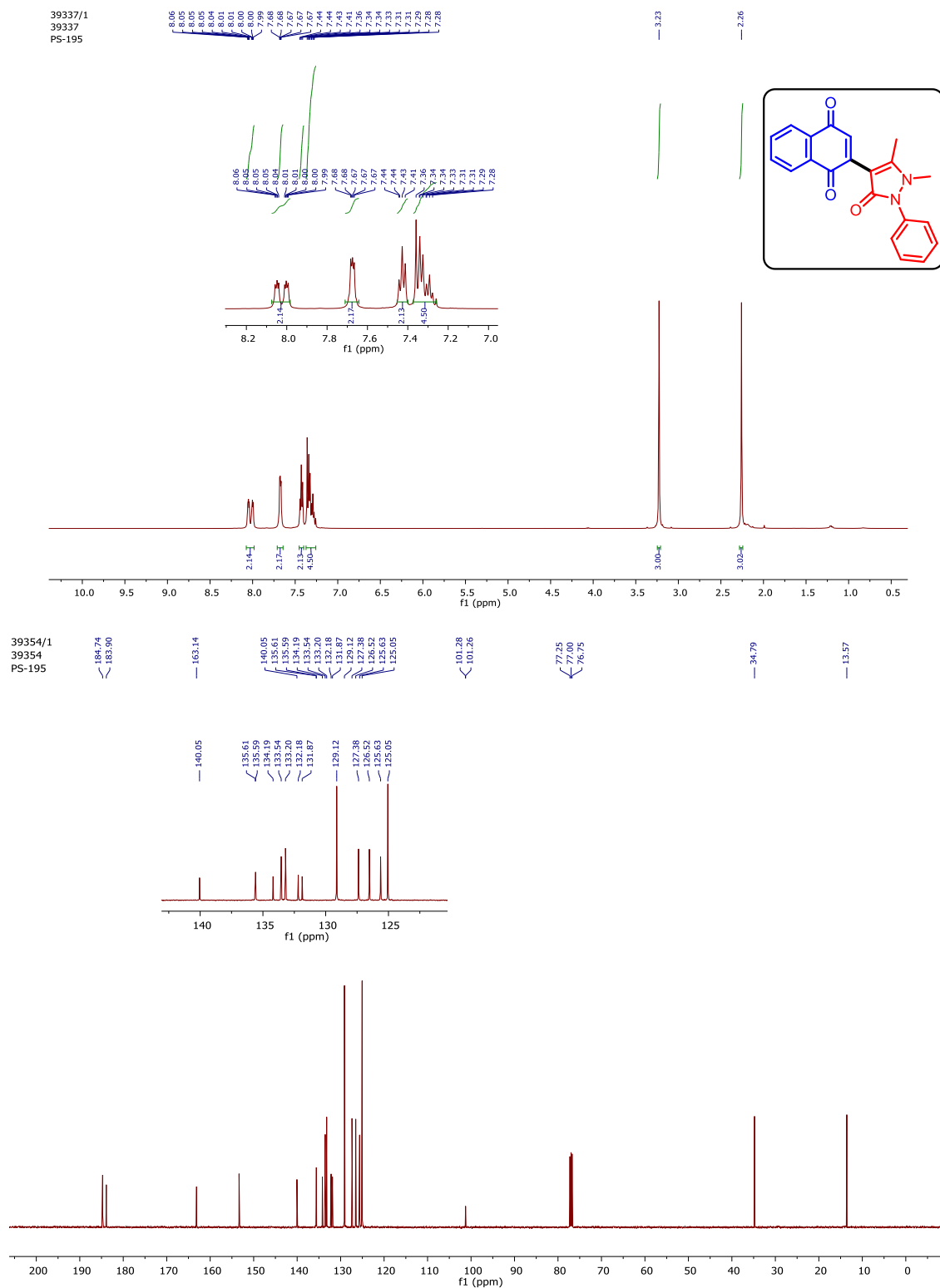
39332/1  
39332  
PS-193



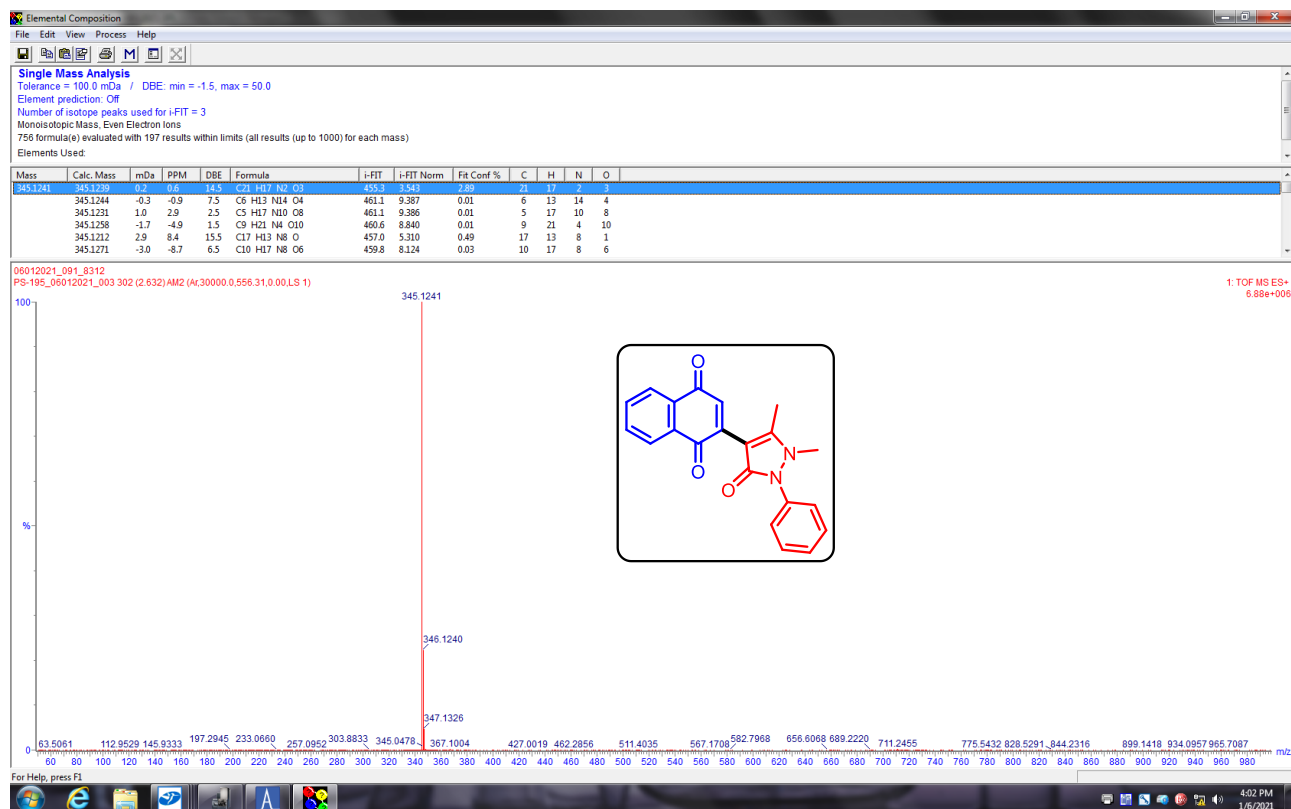
## HRMS Spectra of Compound 3aa:



**$^1\text{H}$  and  $^{13}\text{C}$  of Compound 3ab' (500 & 125 MHz,  $\text{CDCl}_3$ ):**

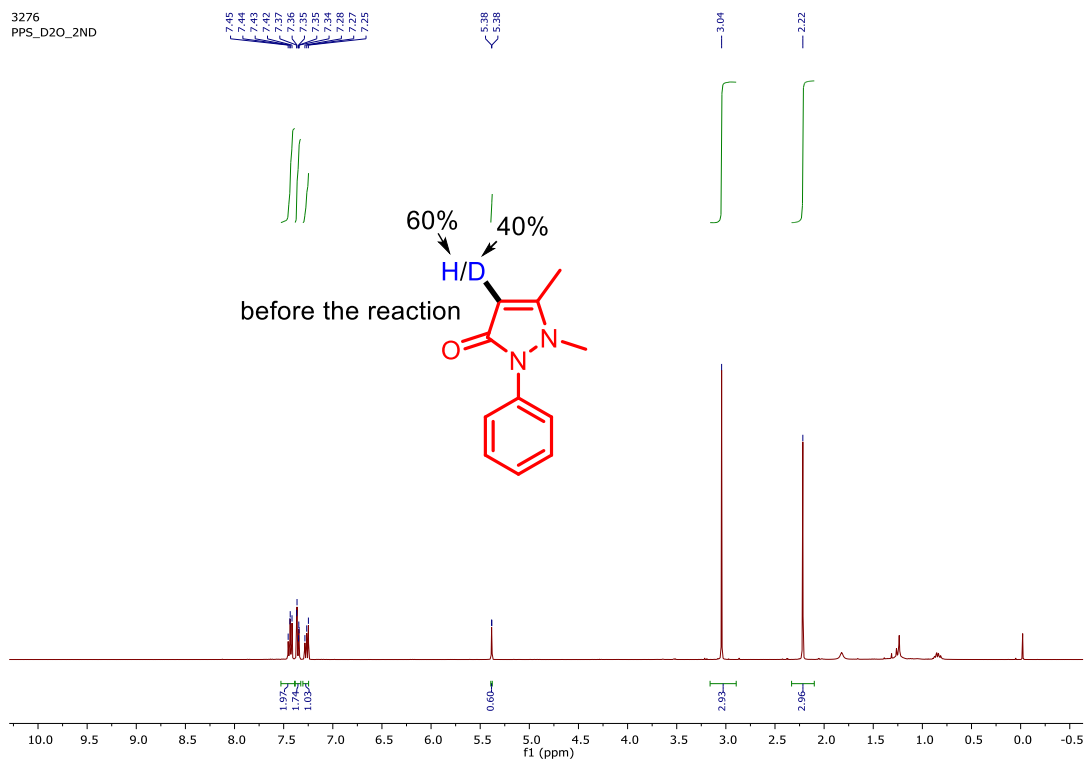


## HRMS Spectra of Compound 3ab'





3276  
PPS\_D2O\_2ND



3236  
PPS\_D2O\_Pd

