

# **An expeditious method to synthesize difluoroboron complexes of $\beta$ -keto amides from $\beta$ -keto nitriles and $\text{BF}_3 \cdot \text{OEt}_2$**

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Beijing University of Chemical Technology, Beijing 100029, P. R. China.*

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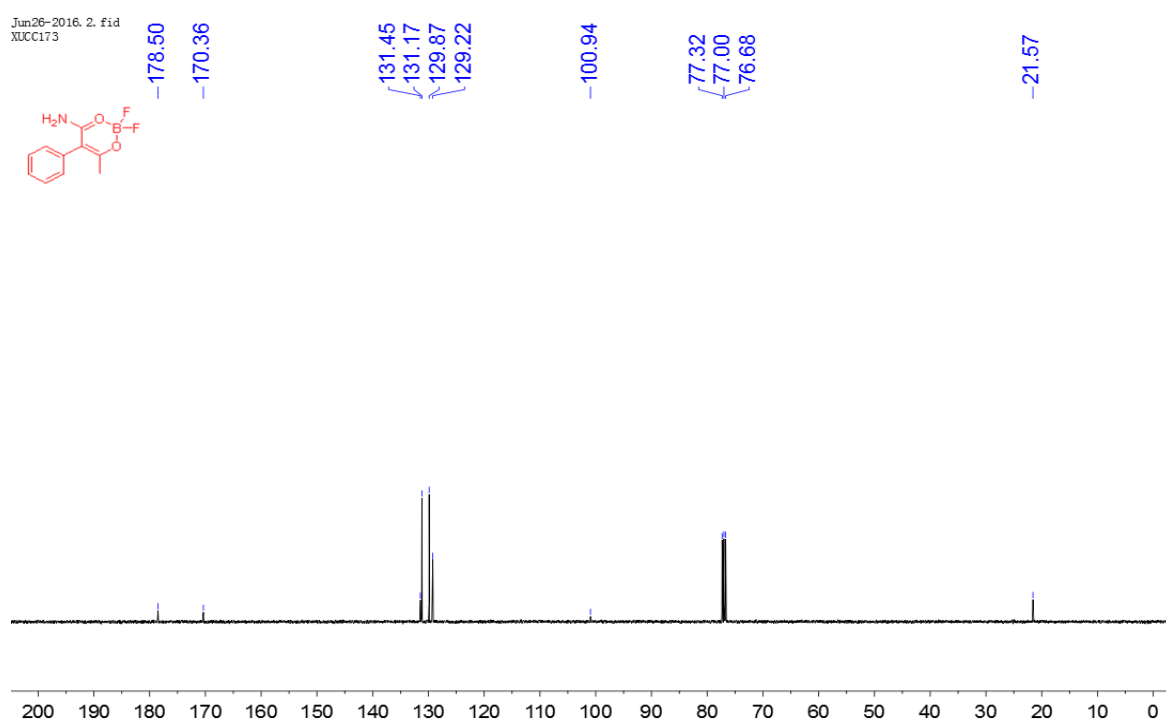
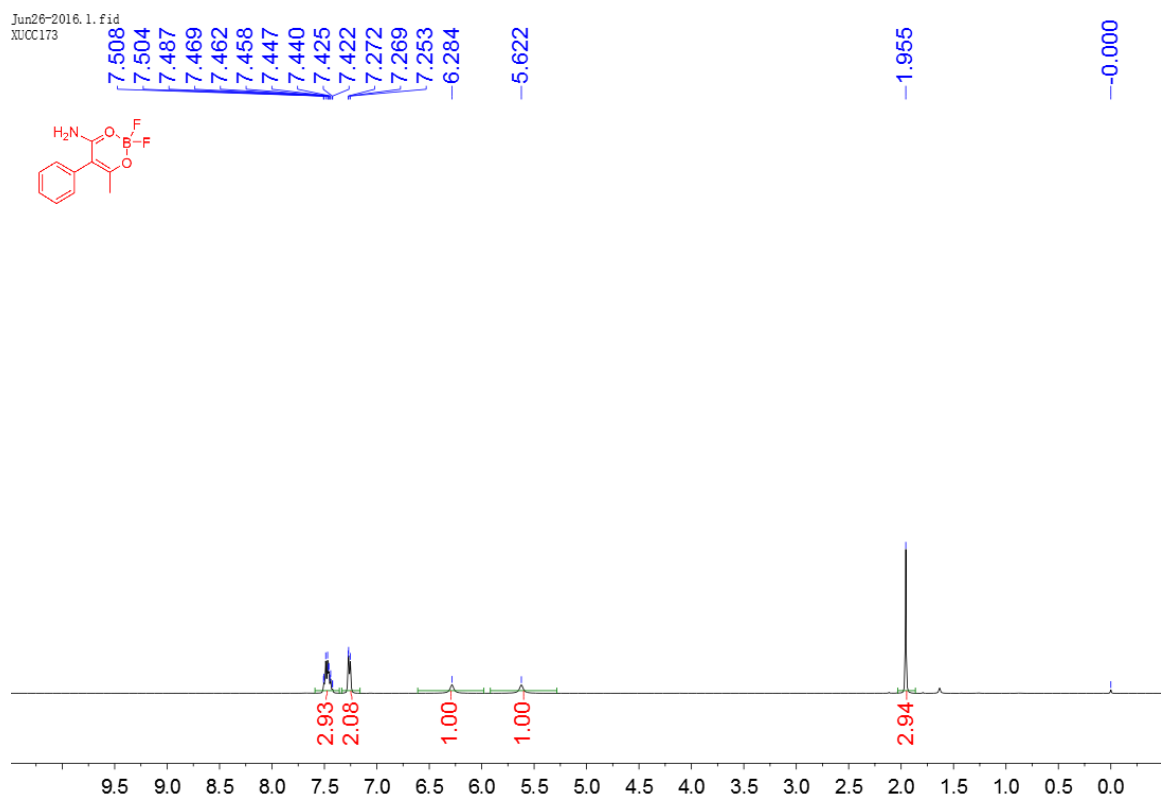
## **Electronic Supplementary Information**

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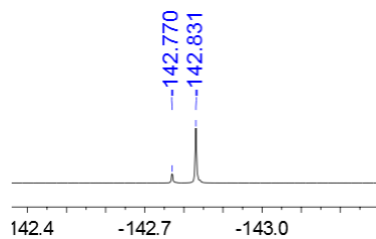
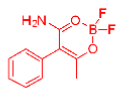
|                                                                                                                              |     |
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# Copies of $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of $\text{BF}_2$ complexes 2

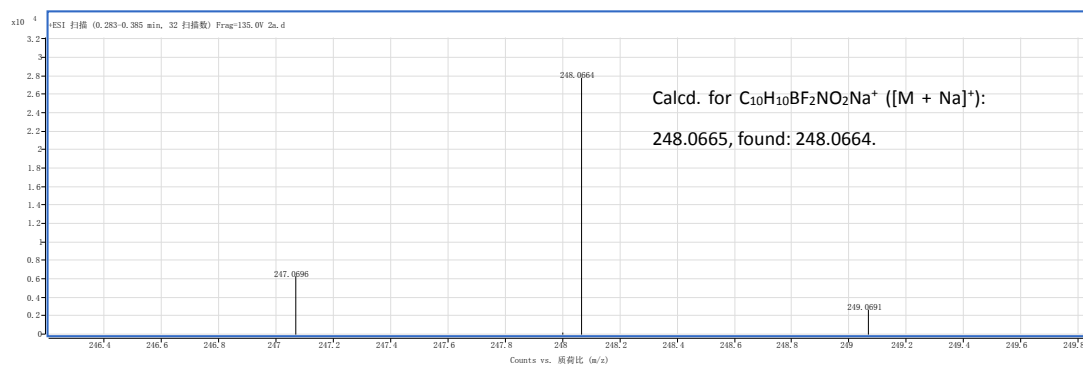
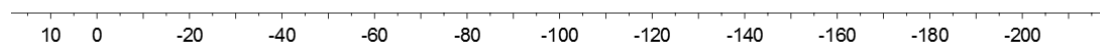
$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2a**



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Xucc-Pr F

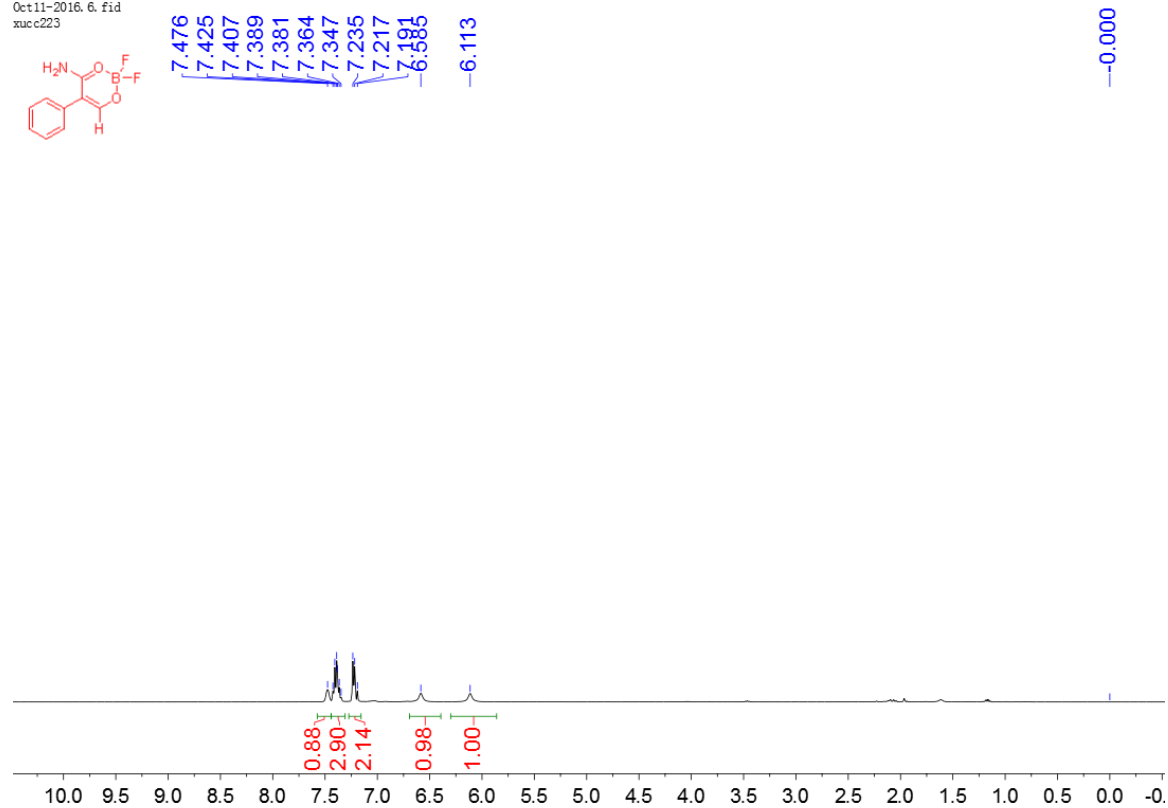
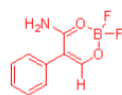


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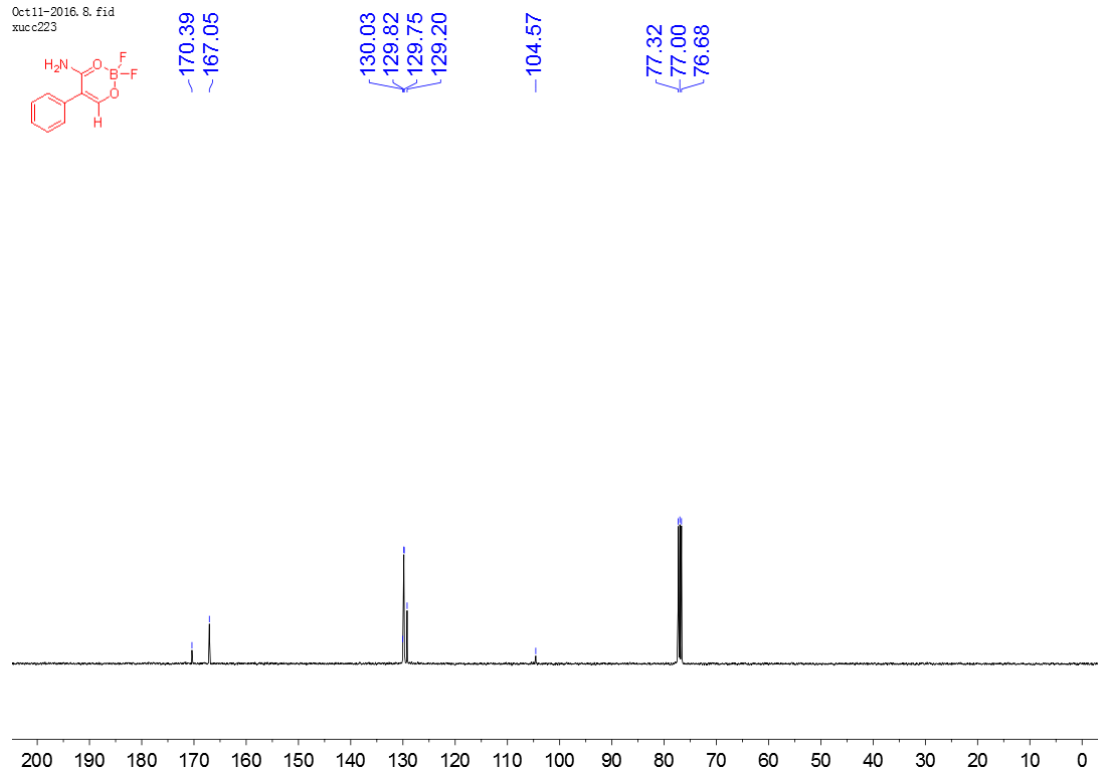
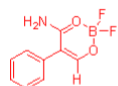


# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2b**

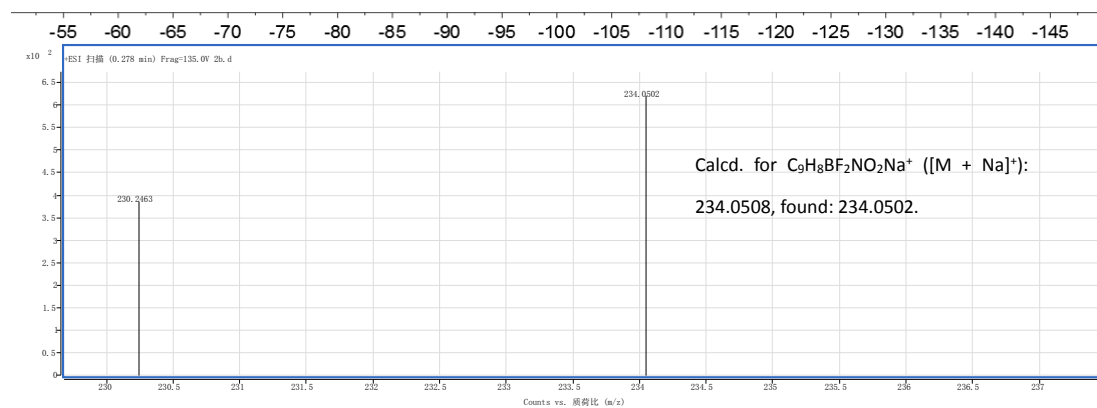
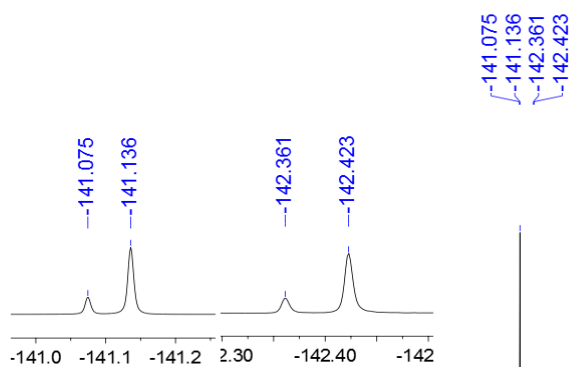
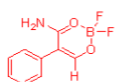
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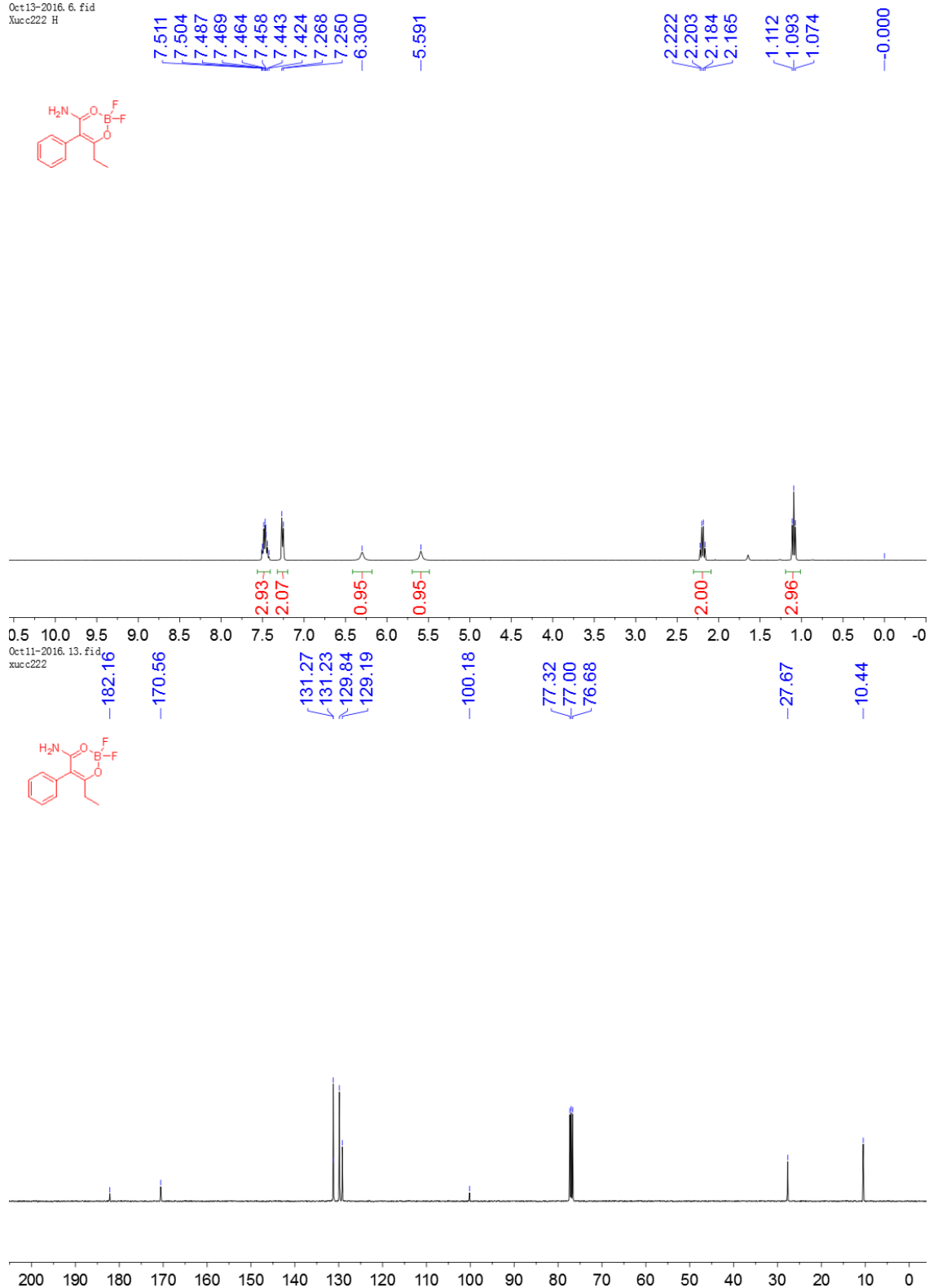


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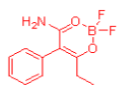


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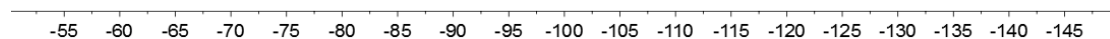
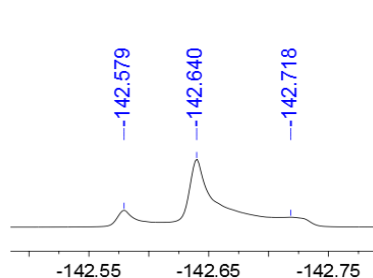
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Xucc222 H



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xuc c222

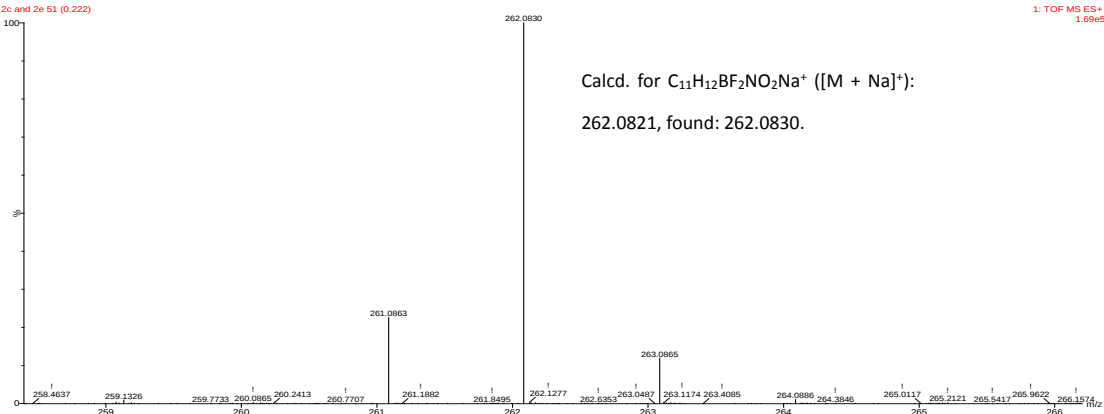


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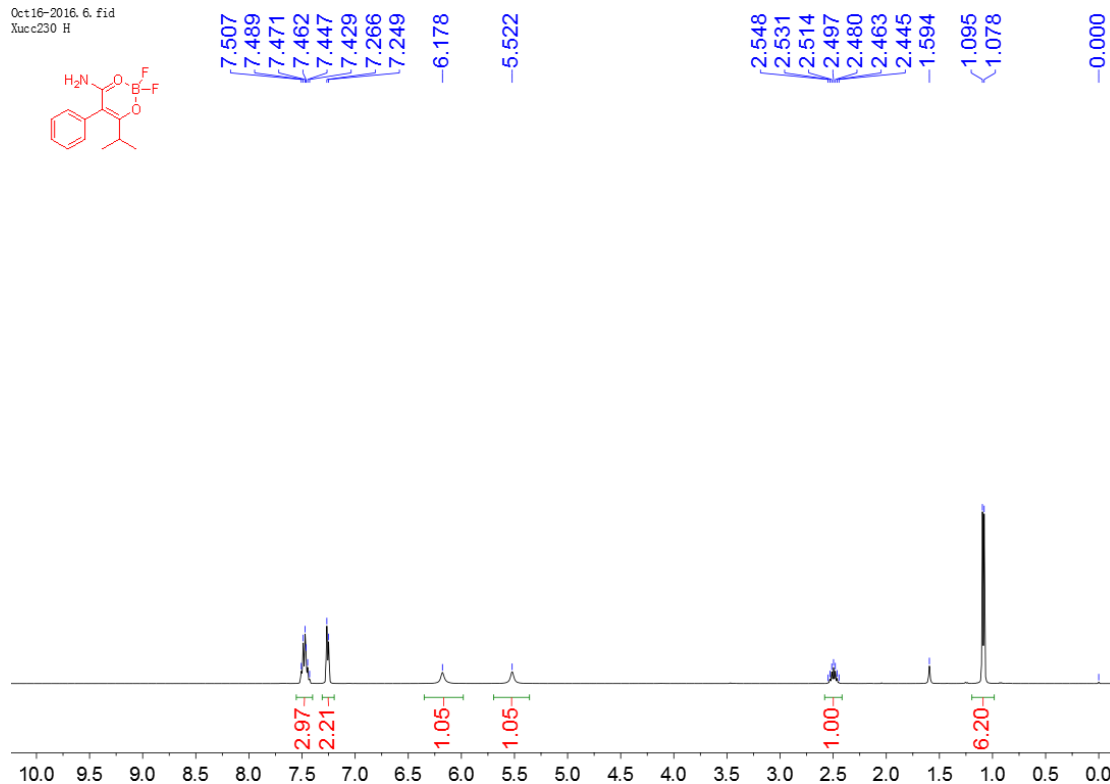
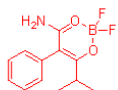
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1: TOF MS ES+  
1.69e5

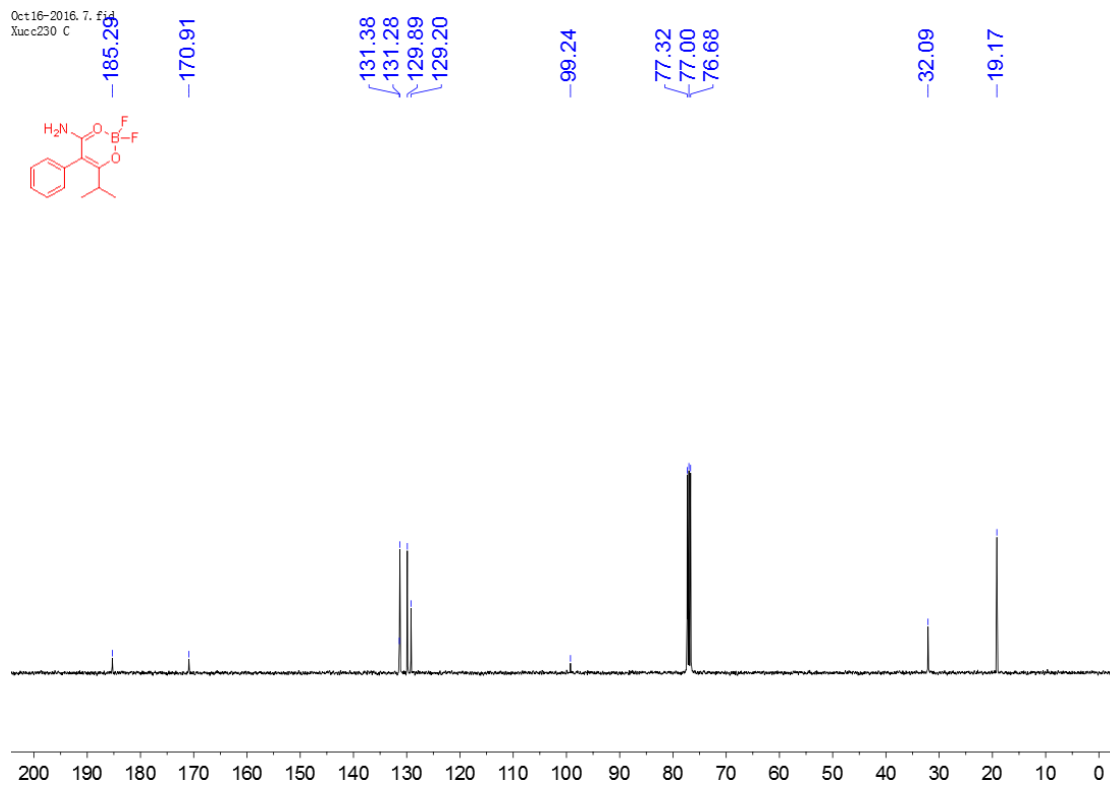
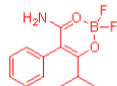


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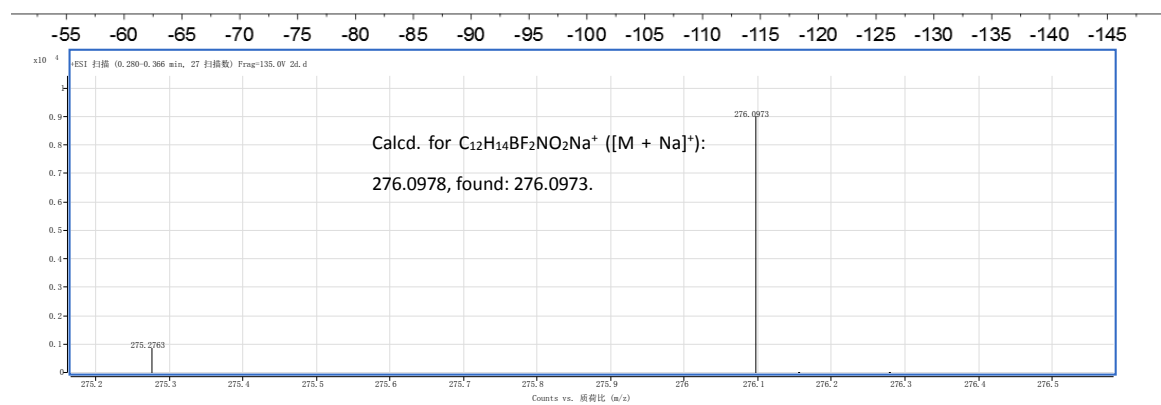
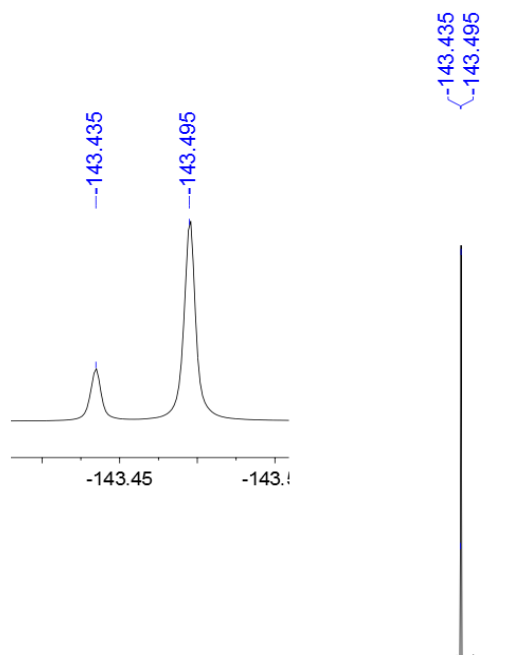
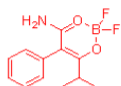
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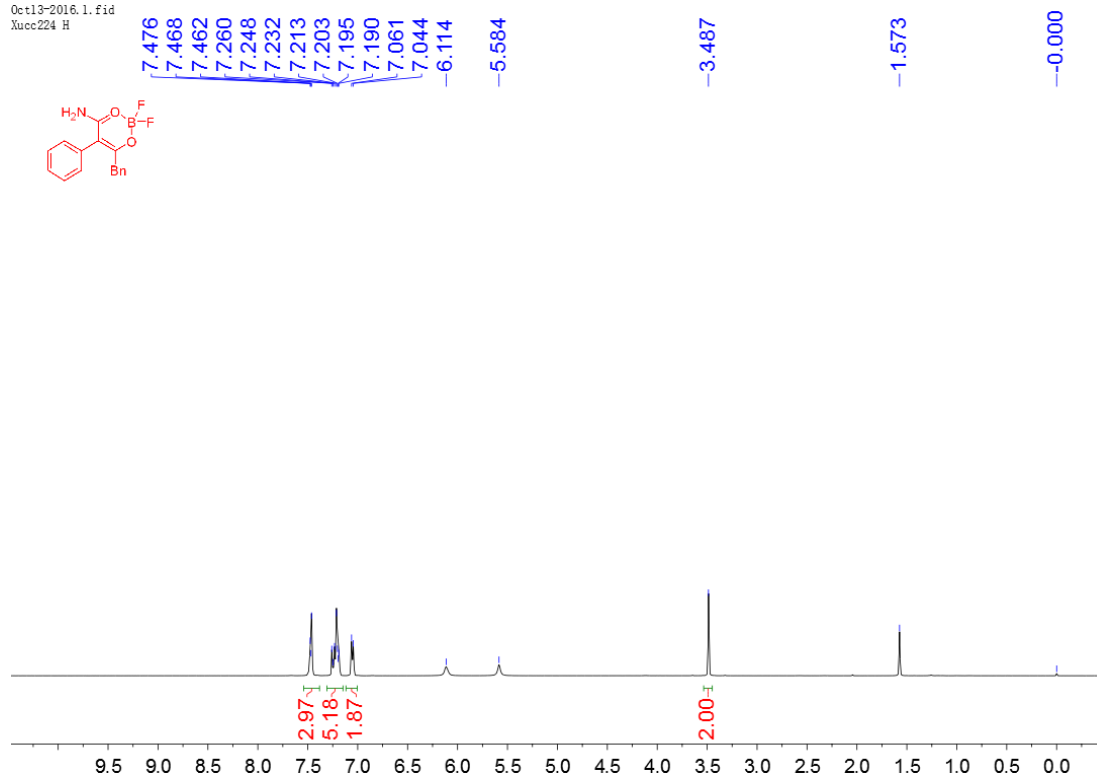


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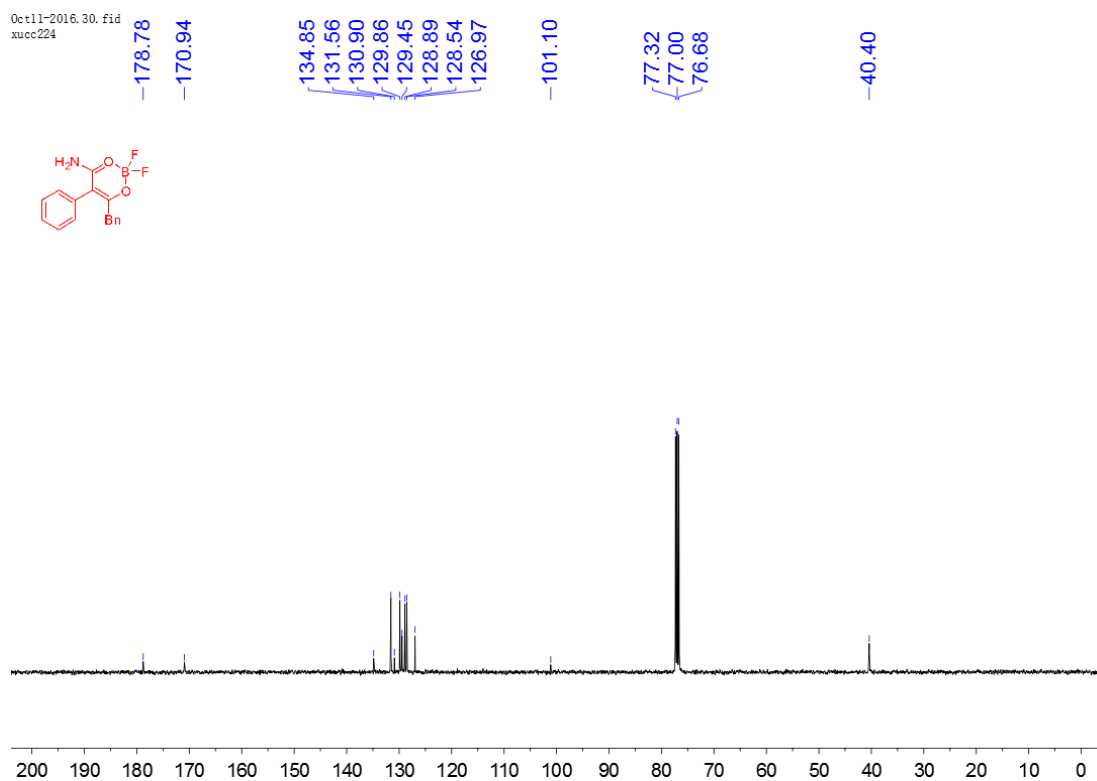


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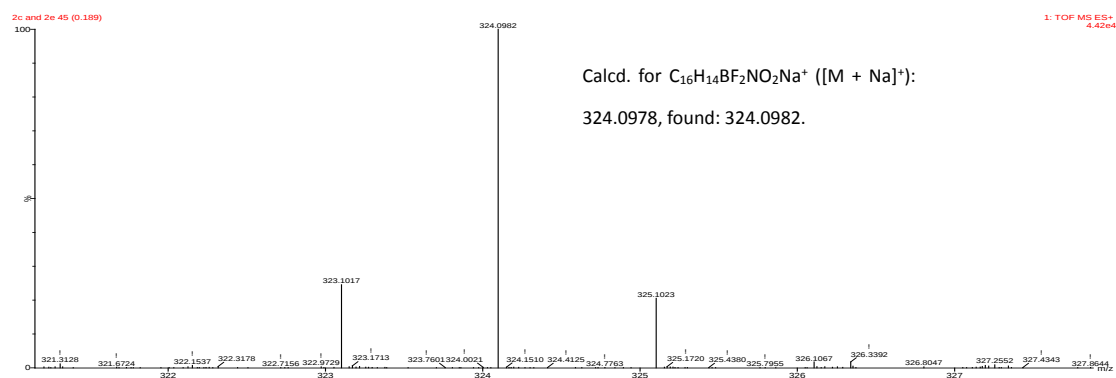
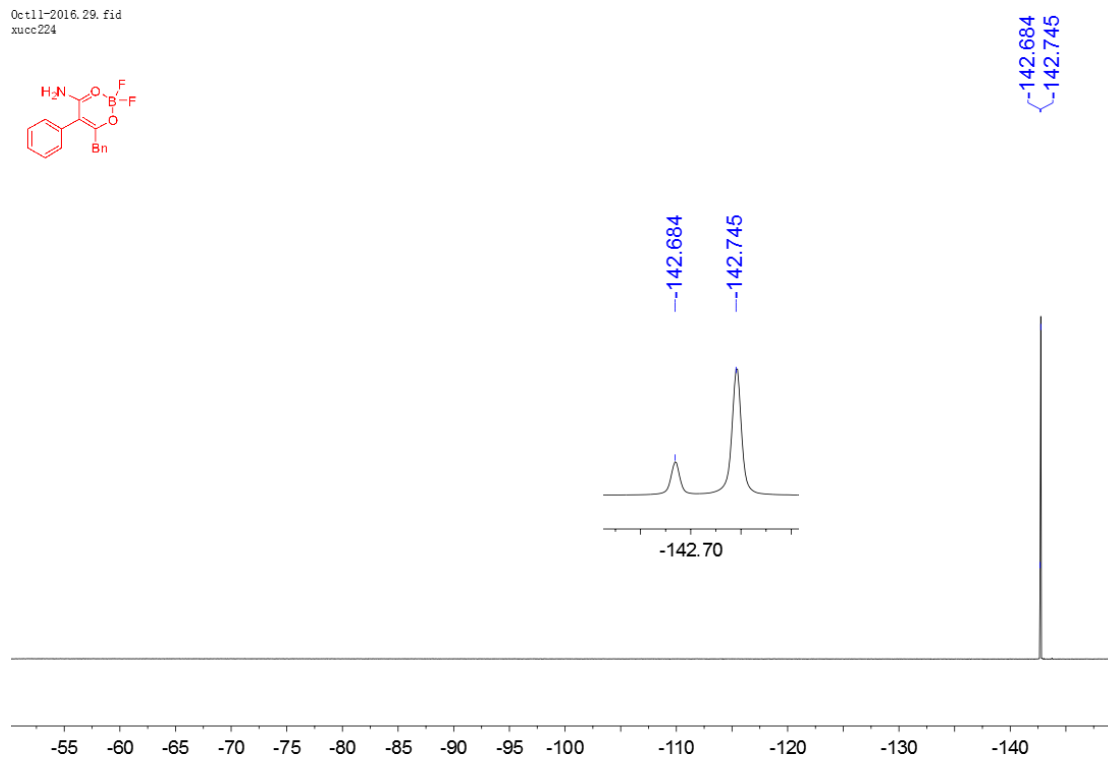
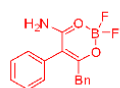
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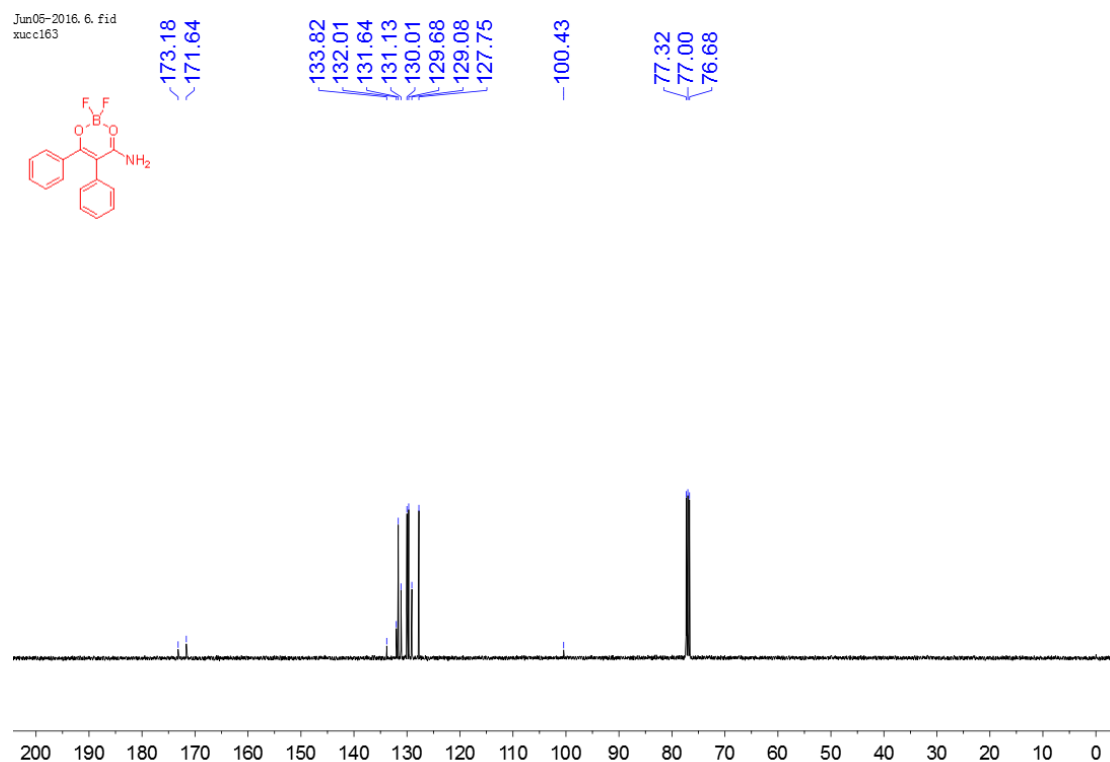
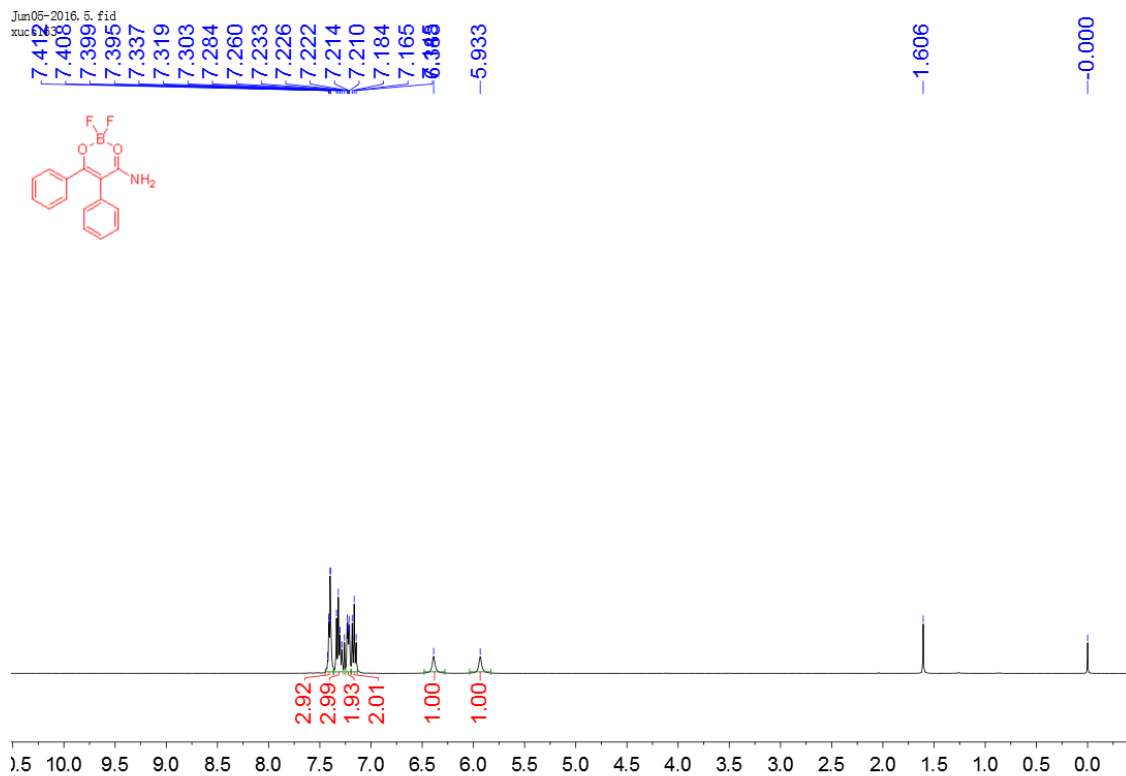
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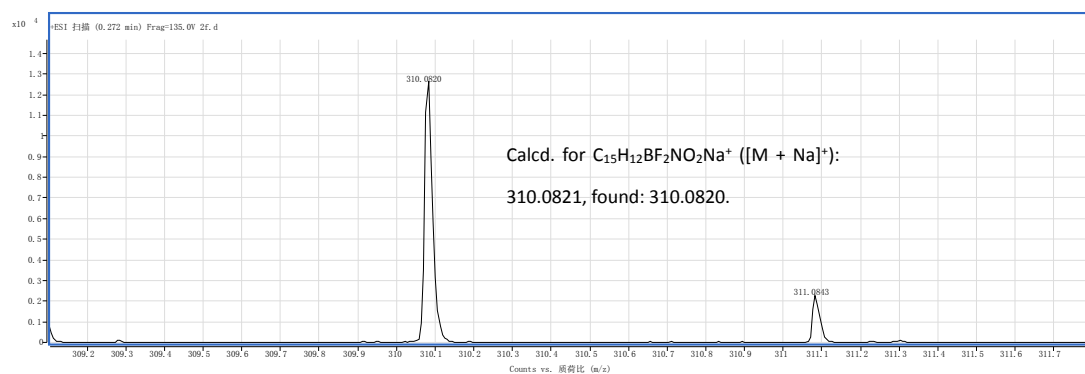
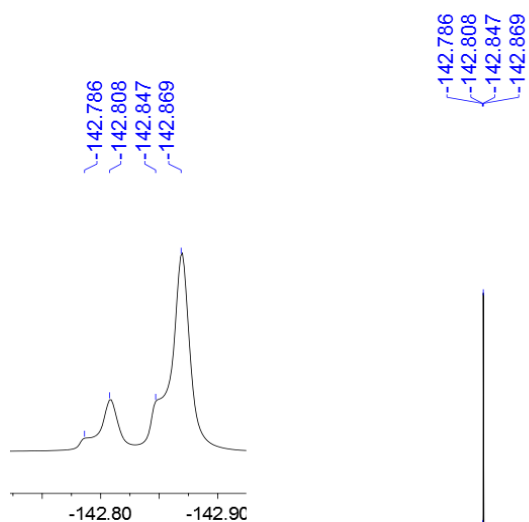
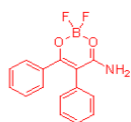


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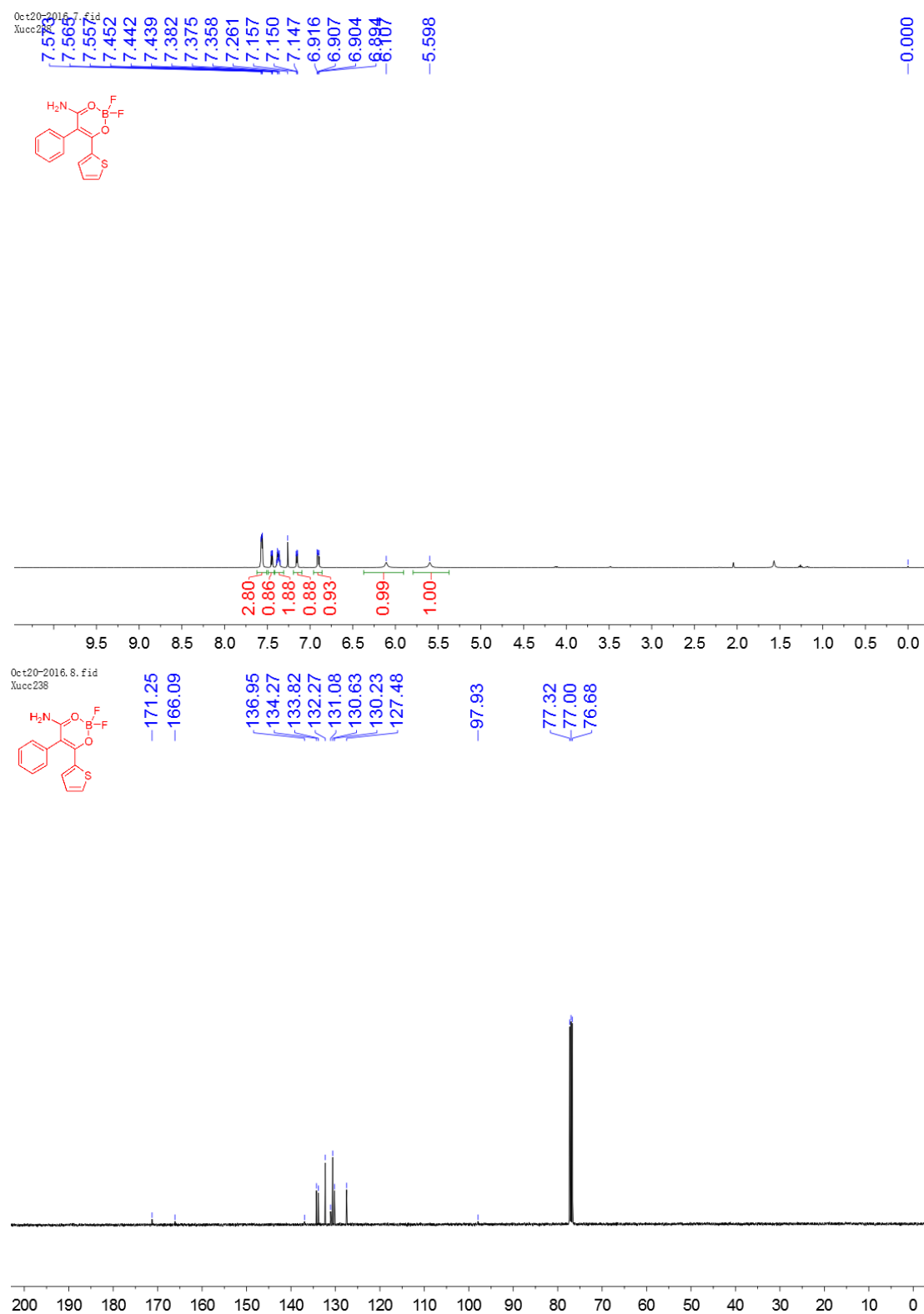


$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2f**

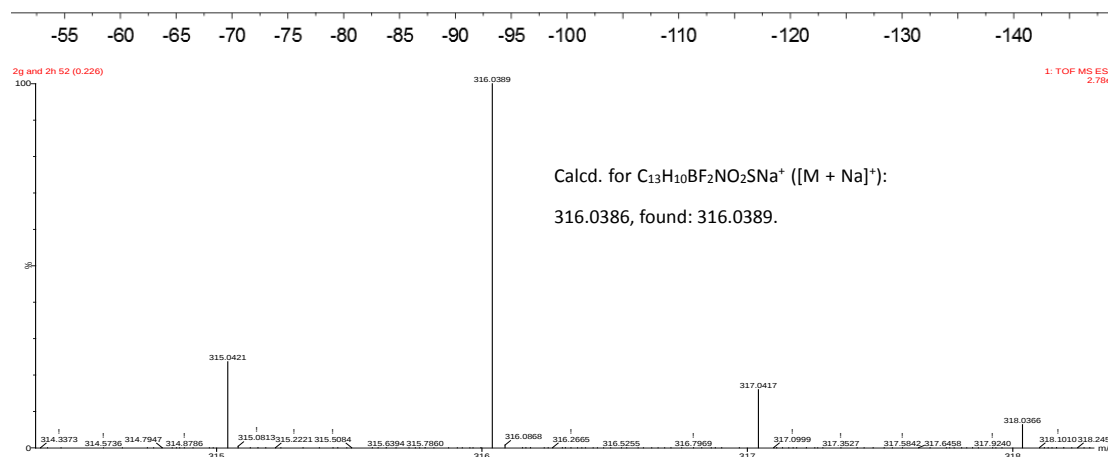
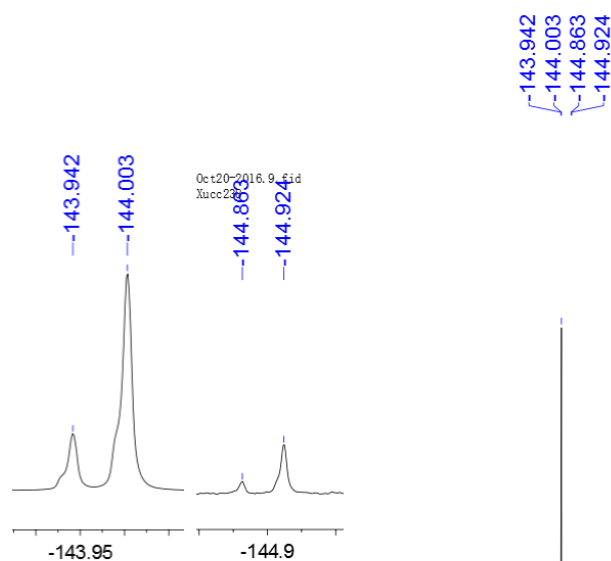
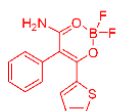




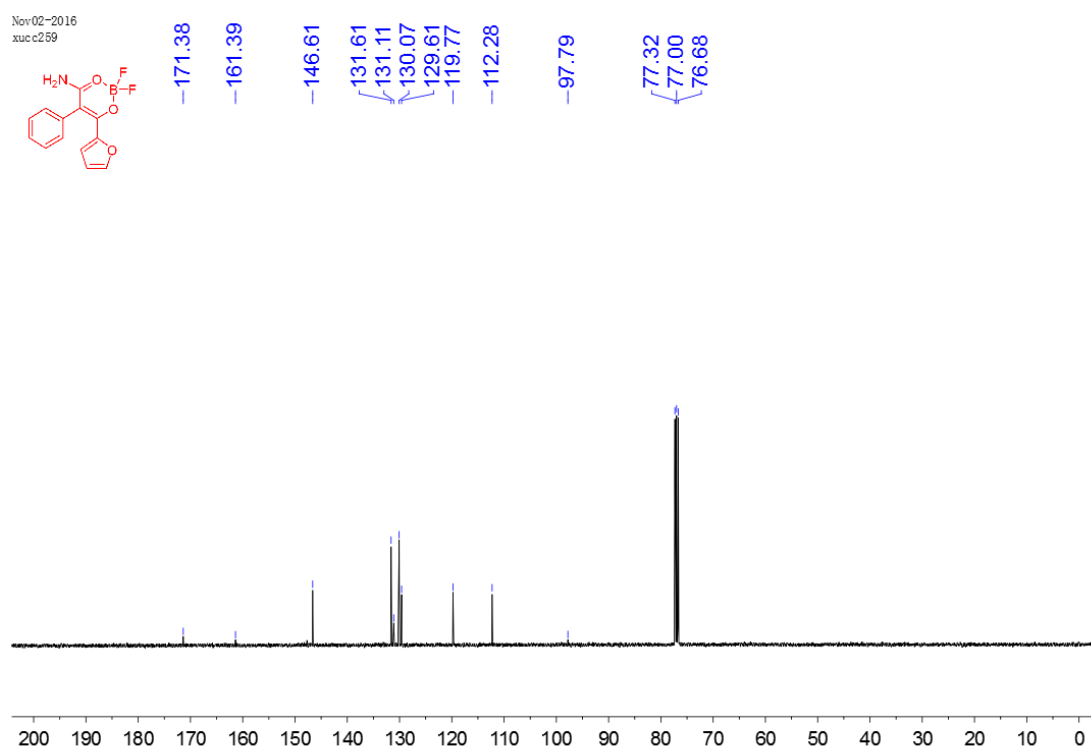
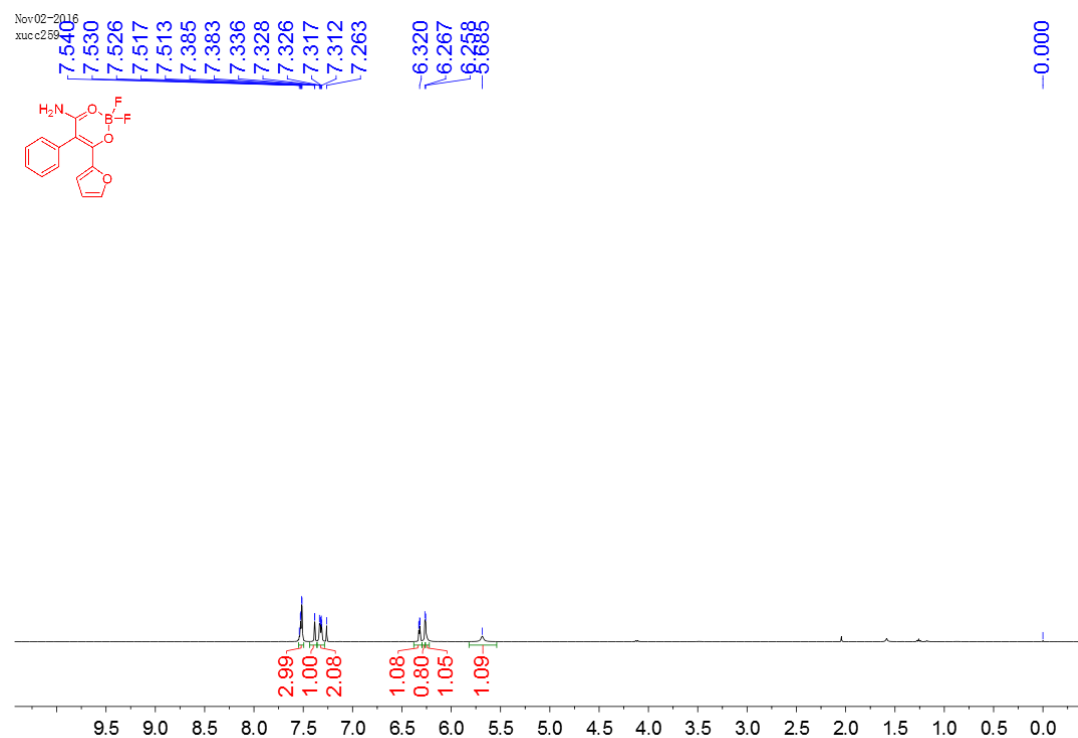
$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2g**



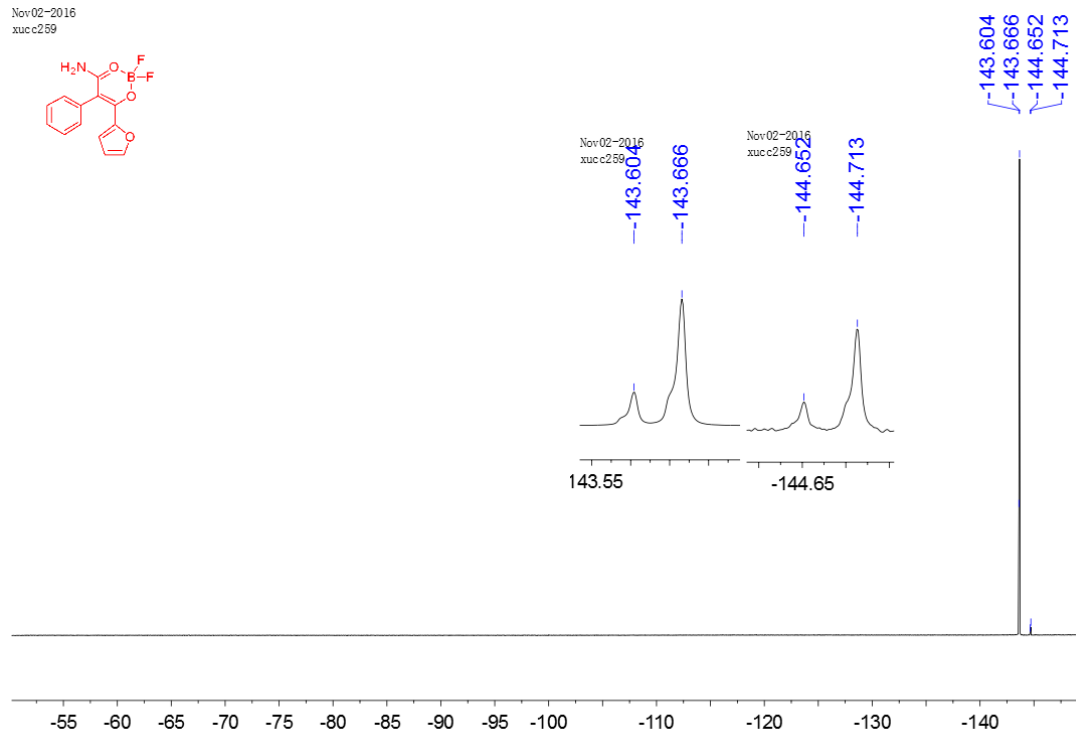
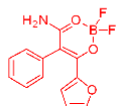
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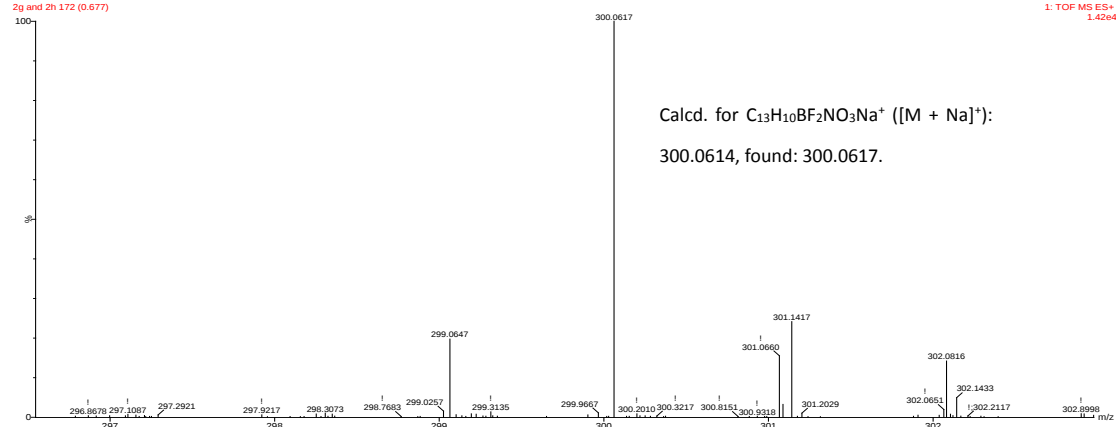
$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2h**



Nov02-2016  
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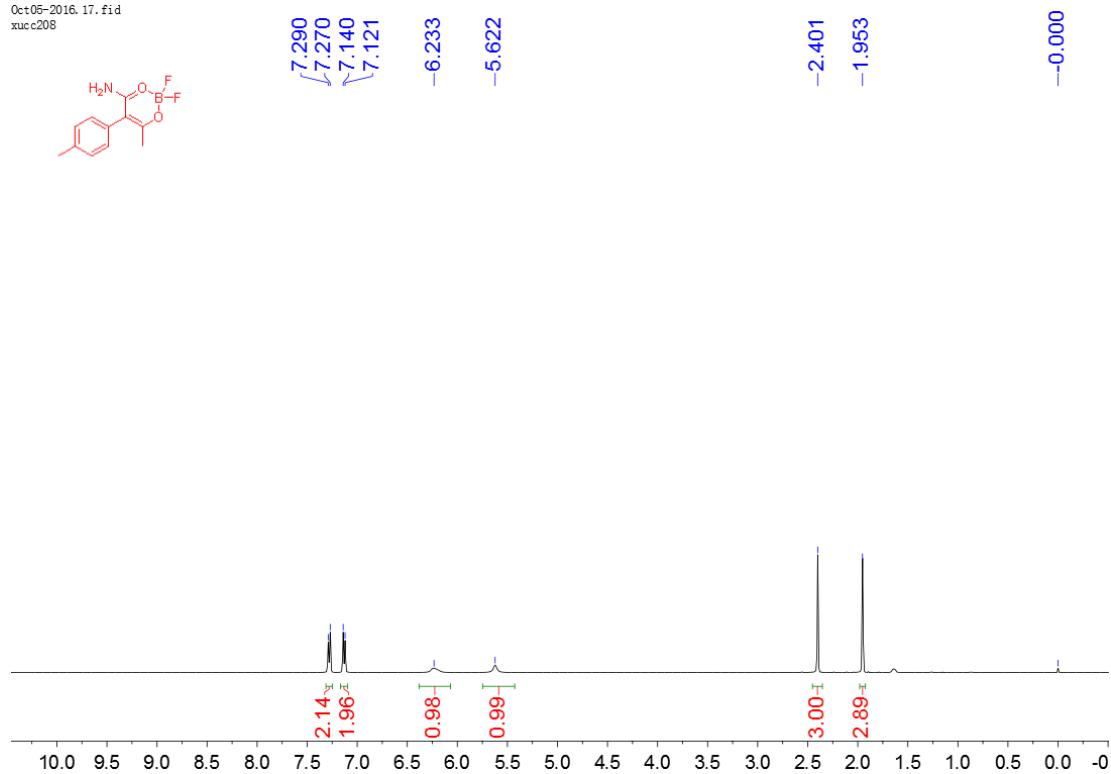
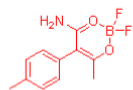


2g and 2h 172 (0.677)

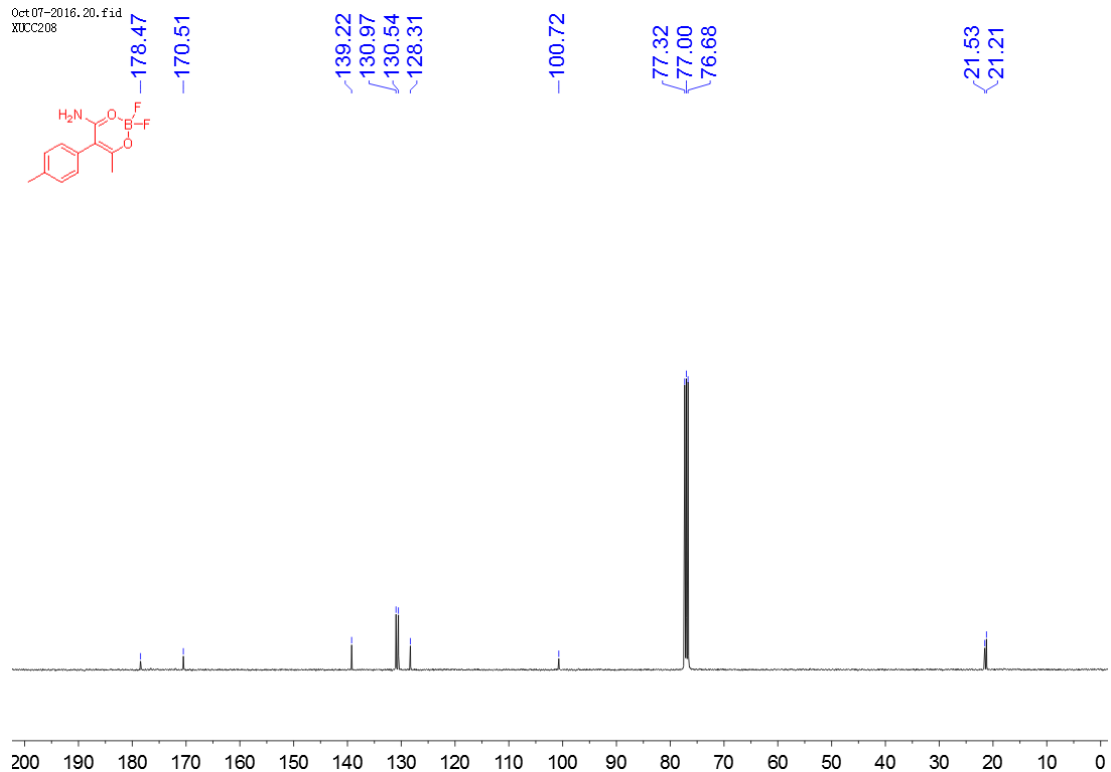
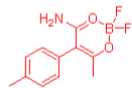


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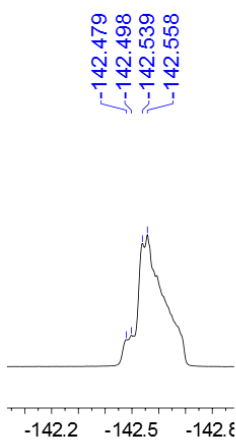
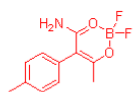
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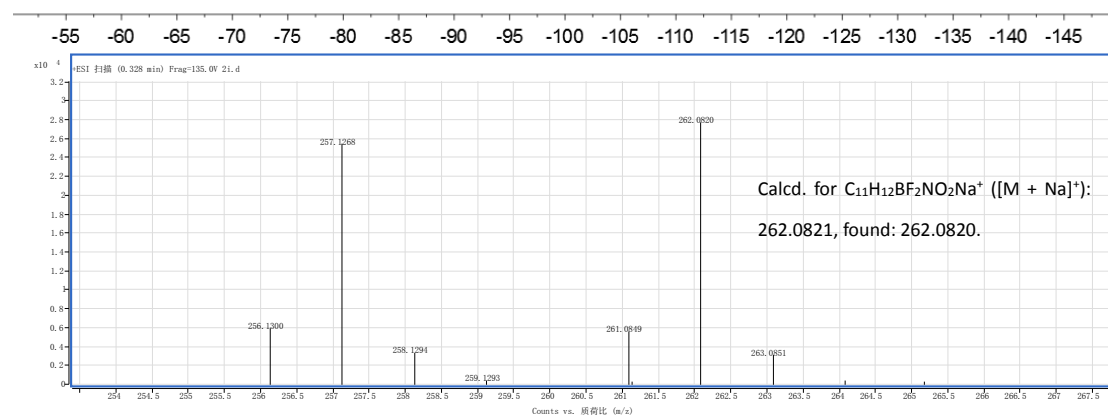
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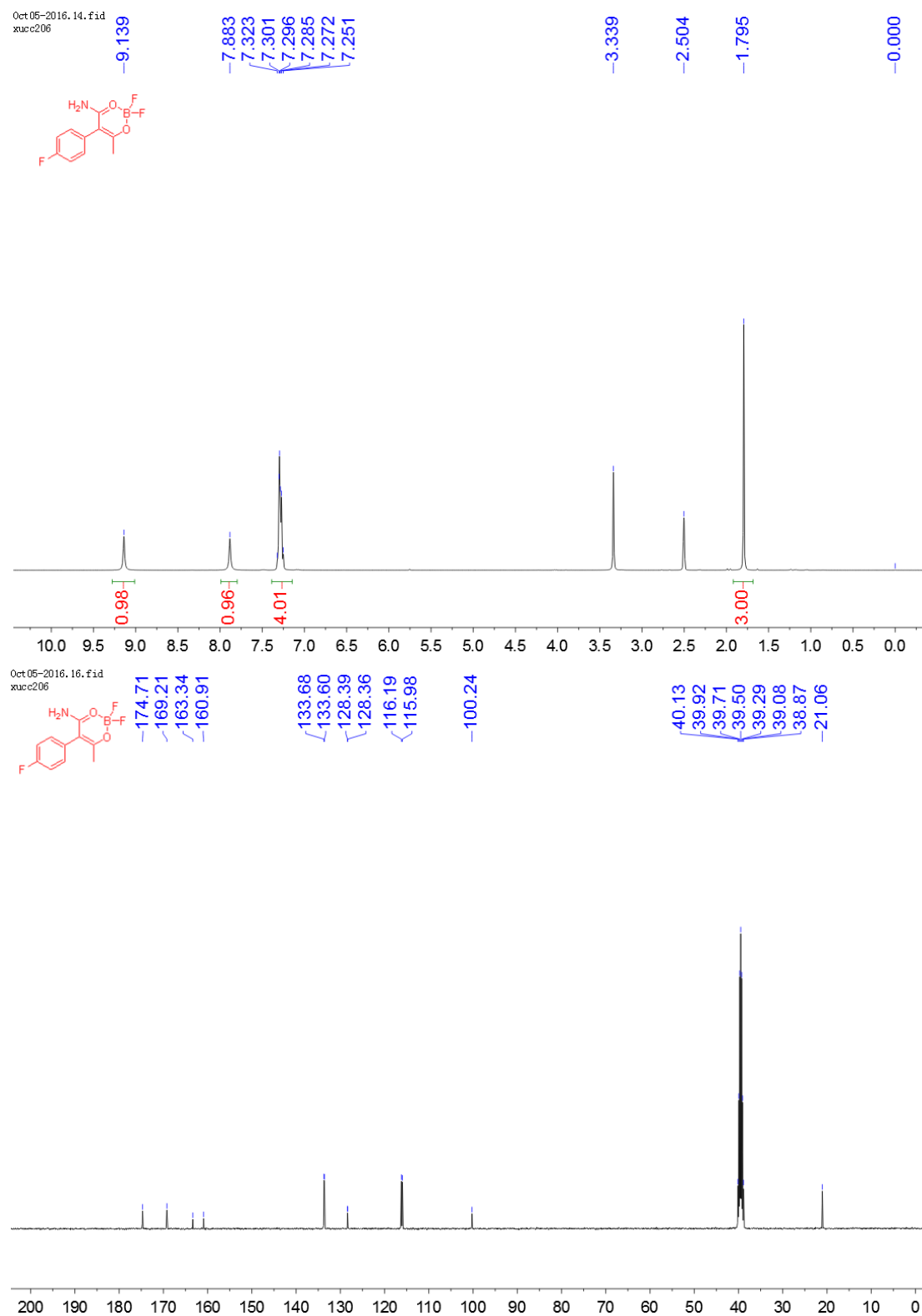
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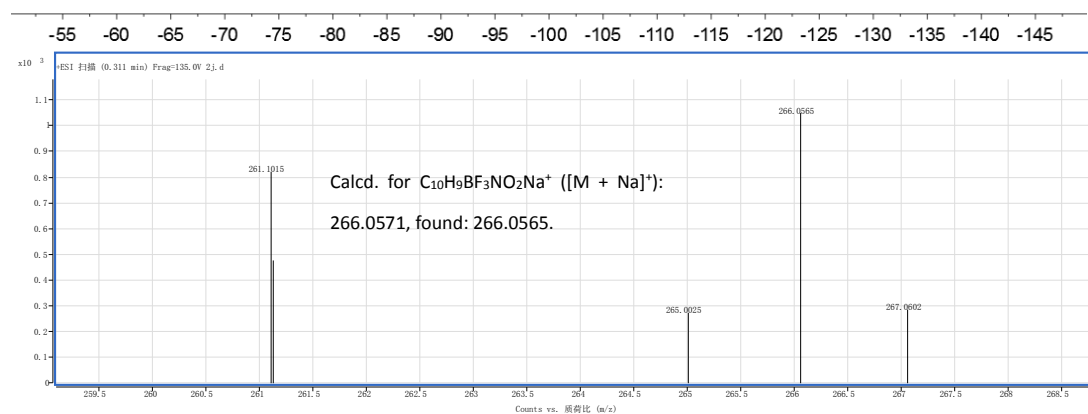
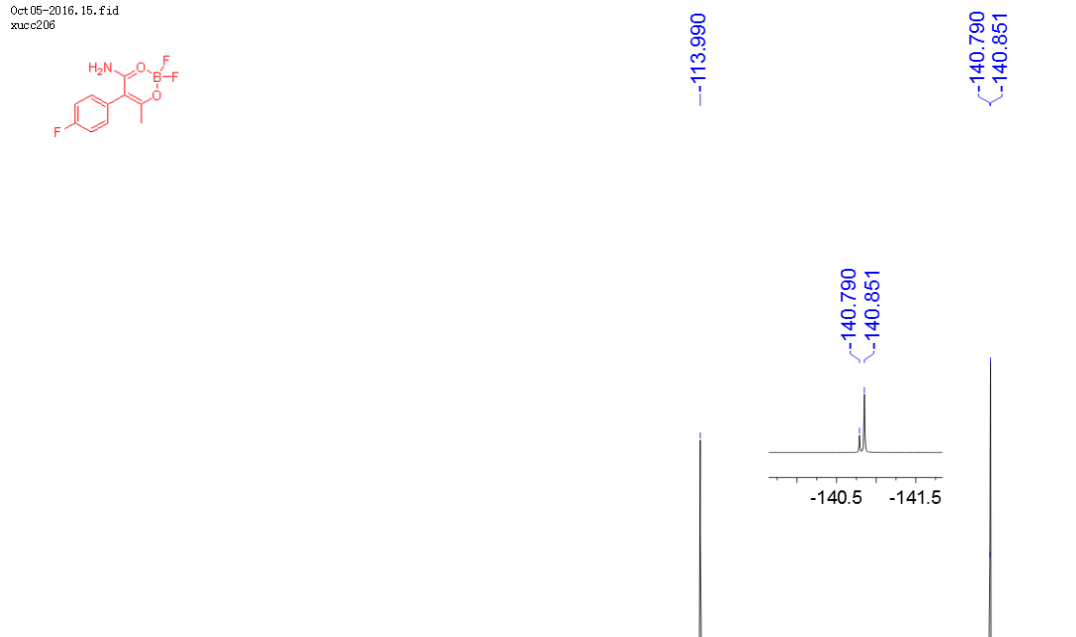
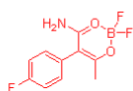
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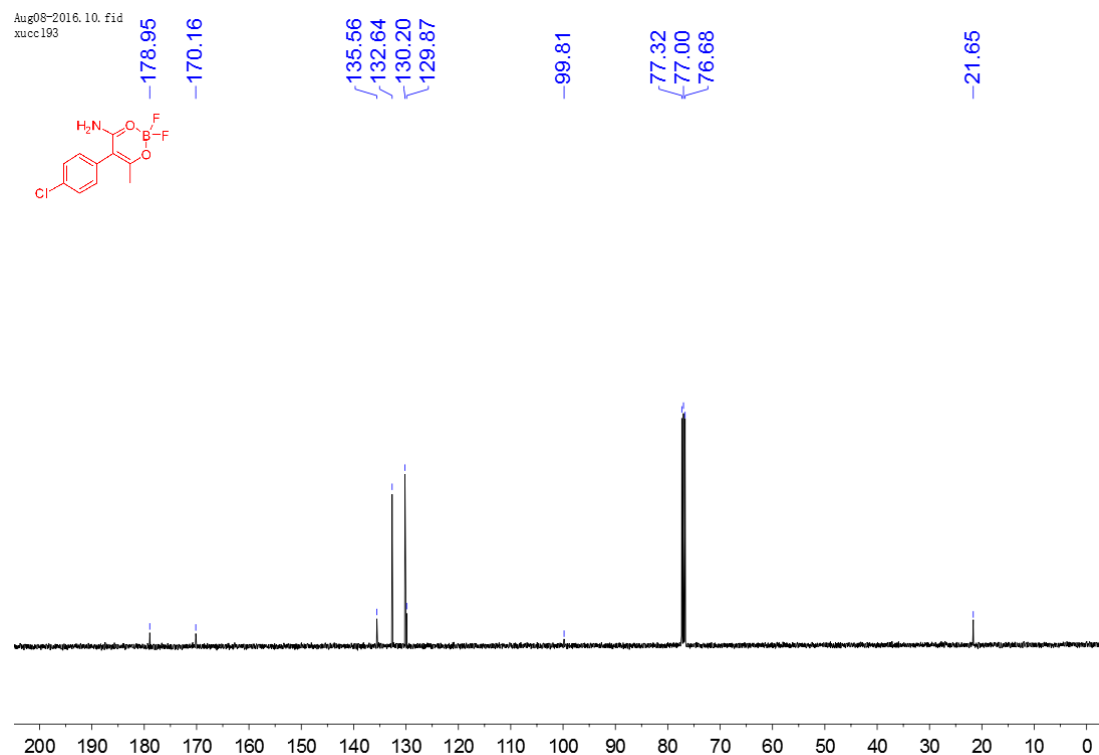
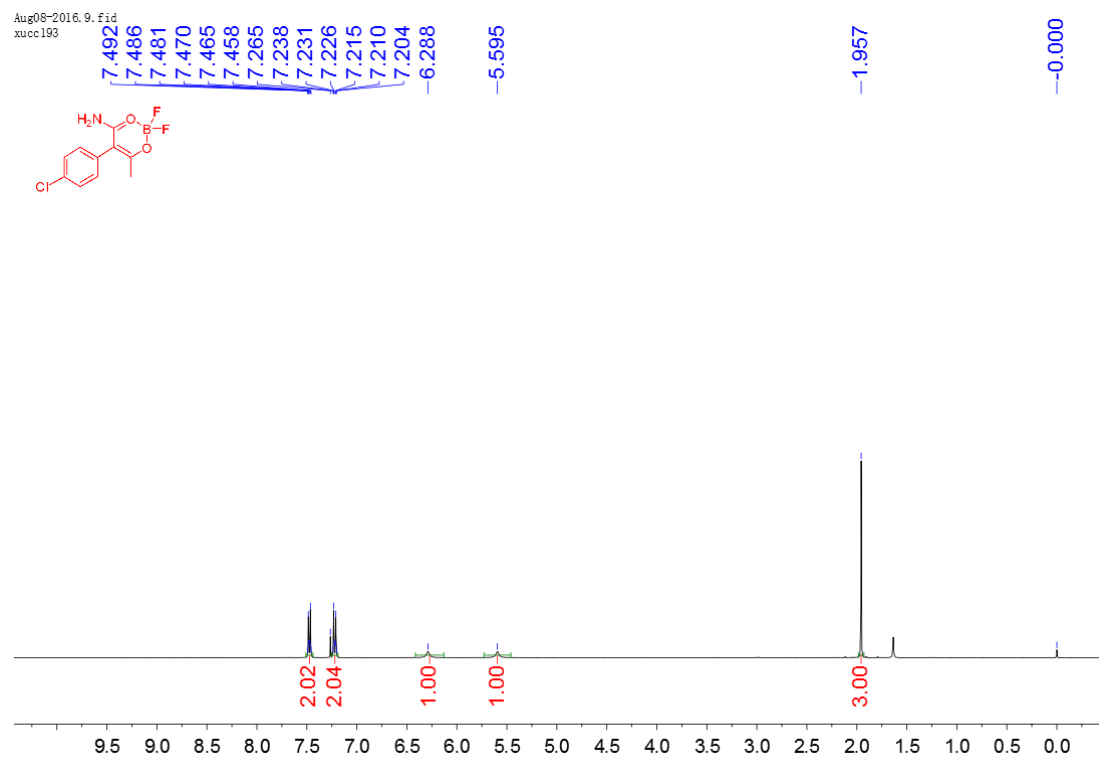
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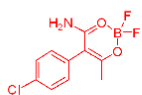
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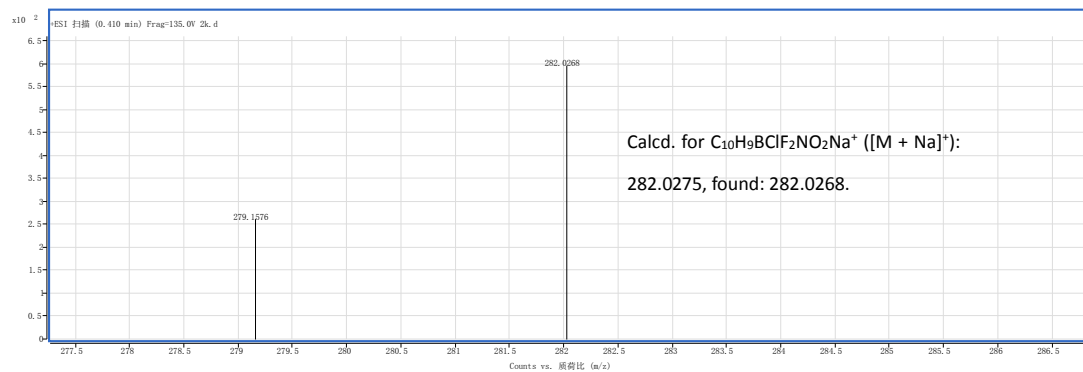
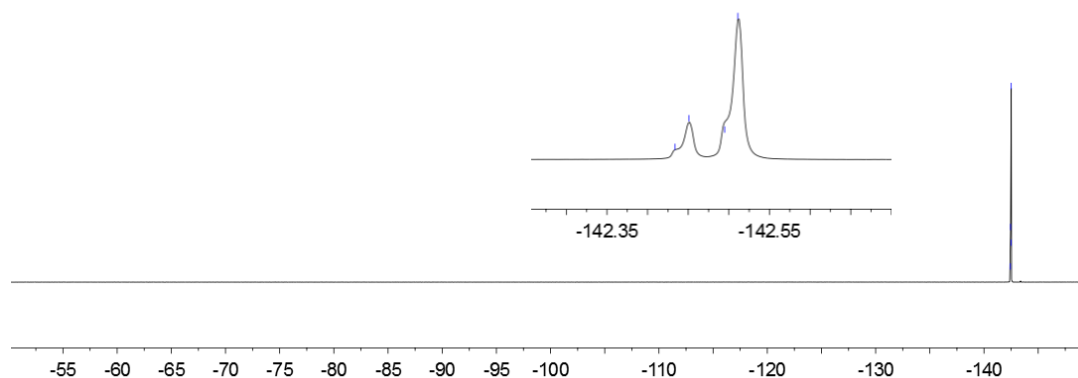


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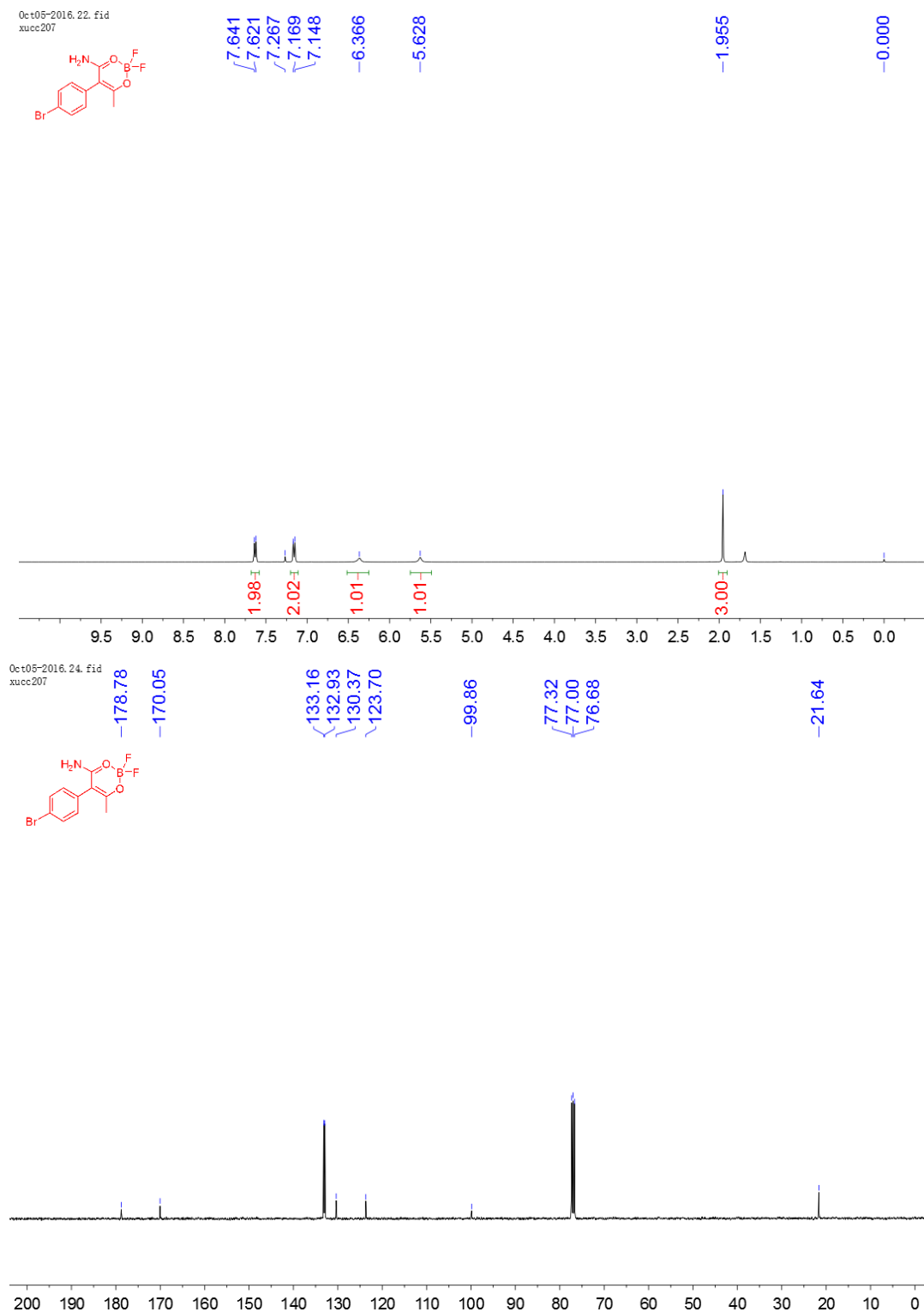


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~142.451  
~142.495  
~142.511

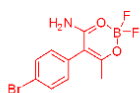
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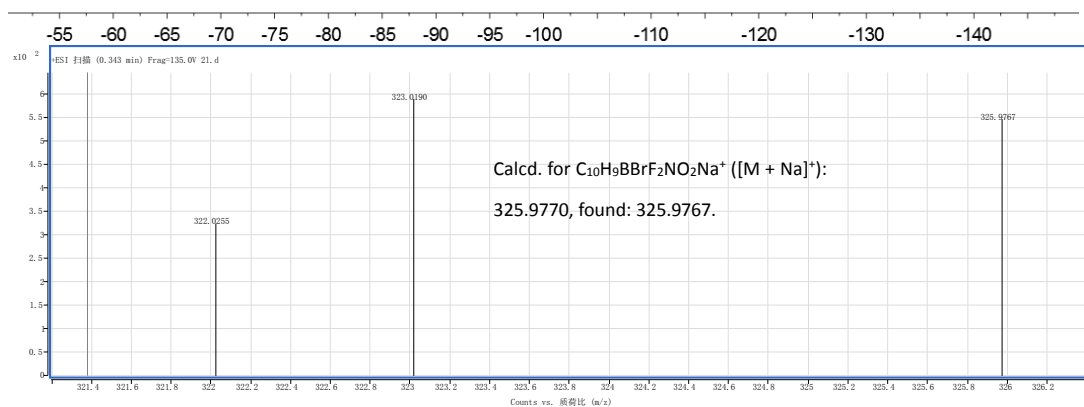
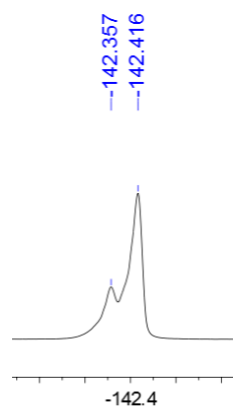
# <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR and HRMS spectra of 2l



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xuoc207

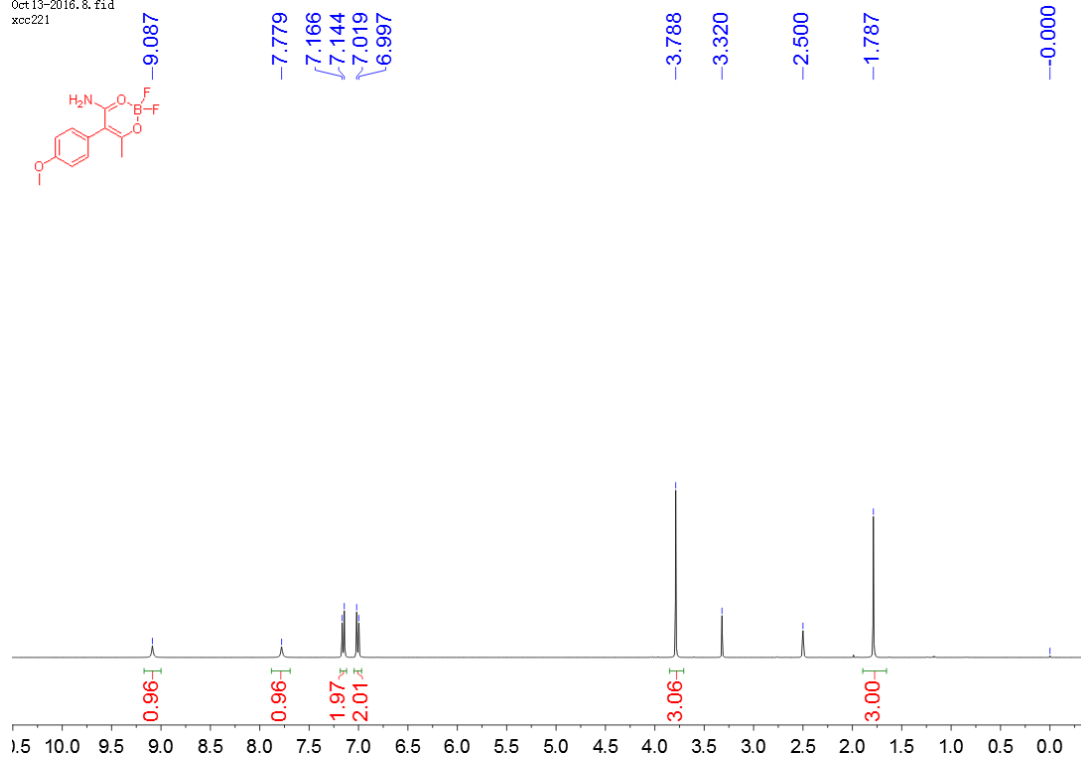


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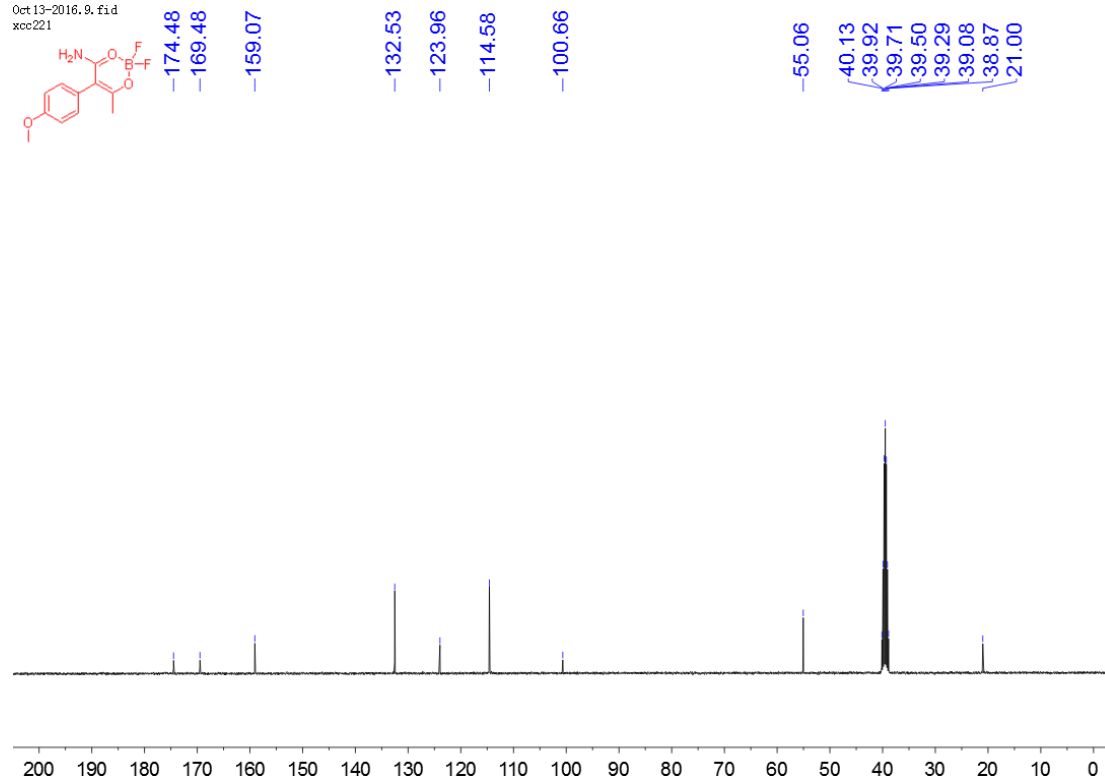


# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2m**

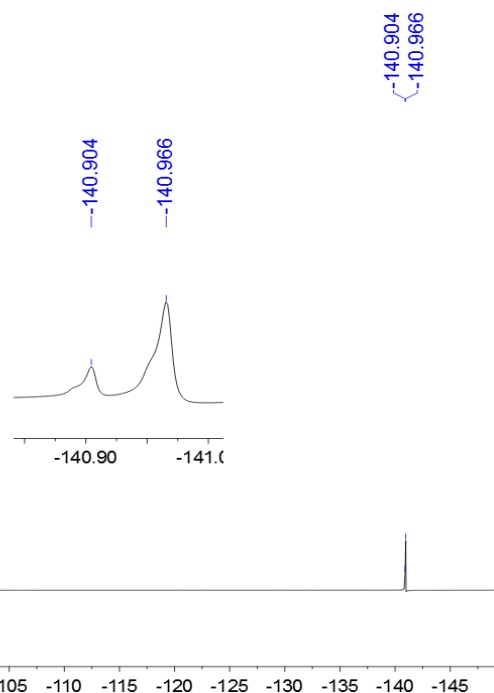
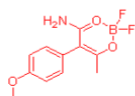
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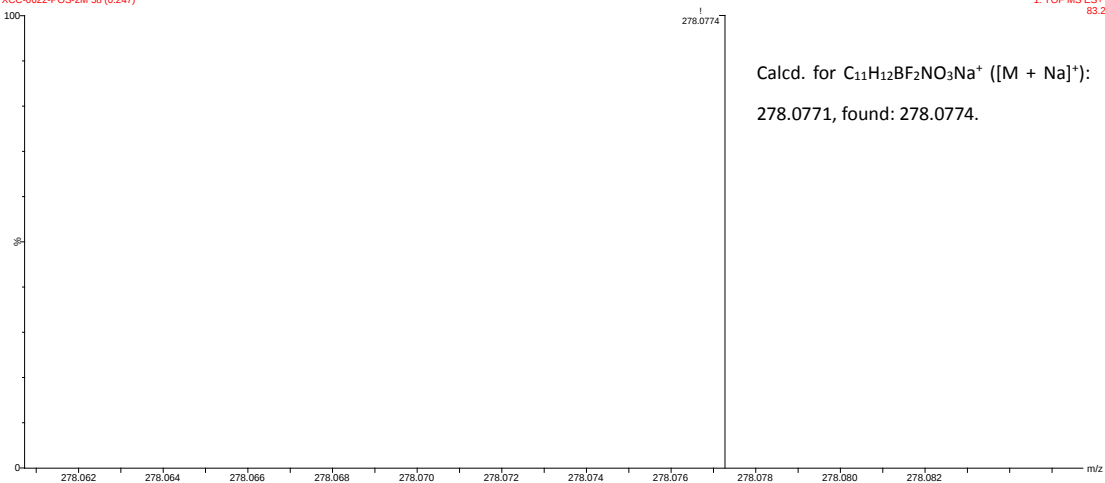
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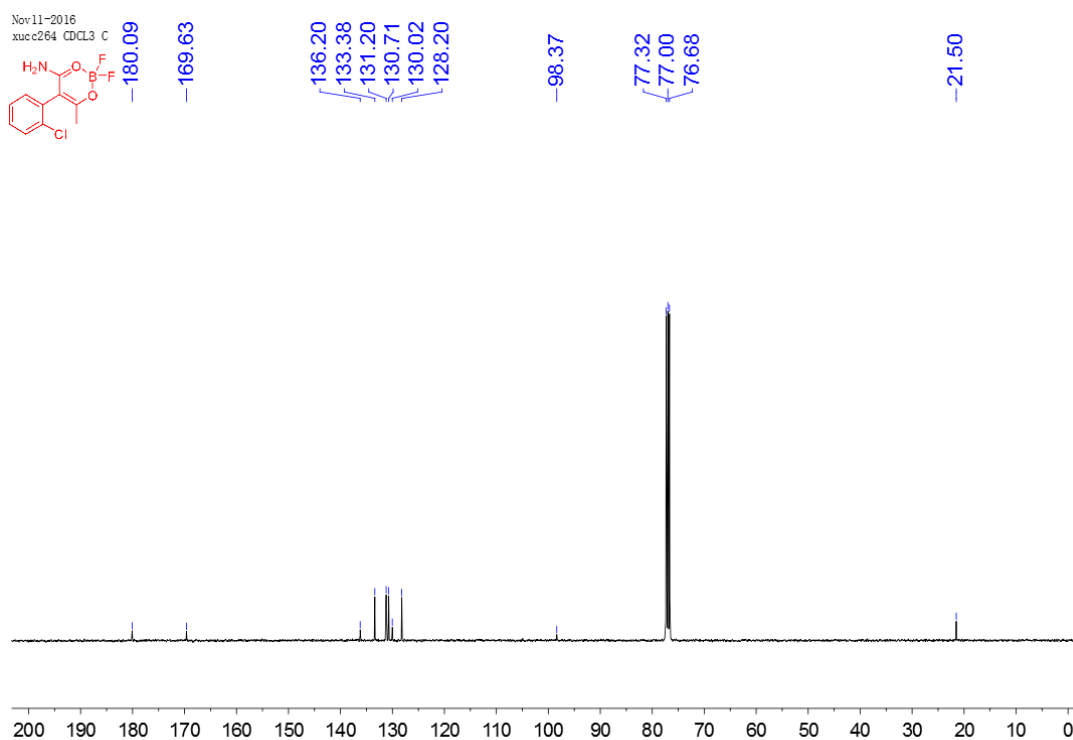
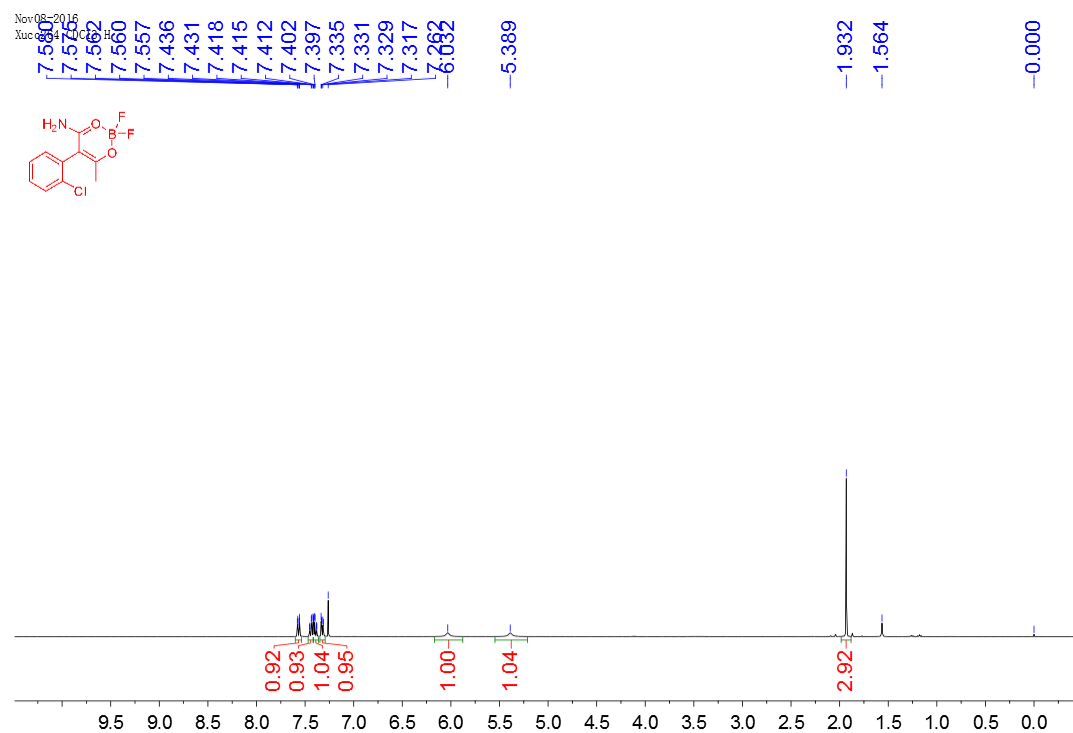
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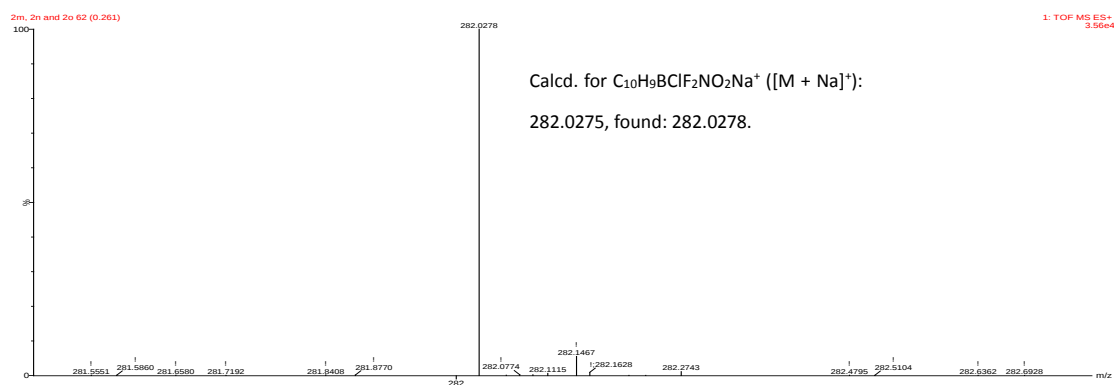
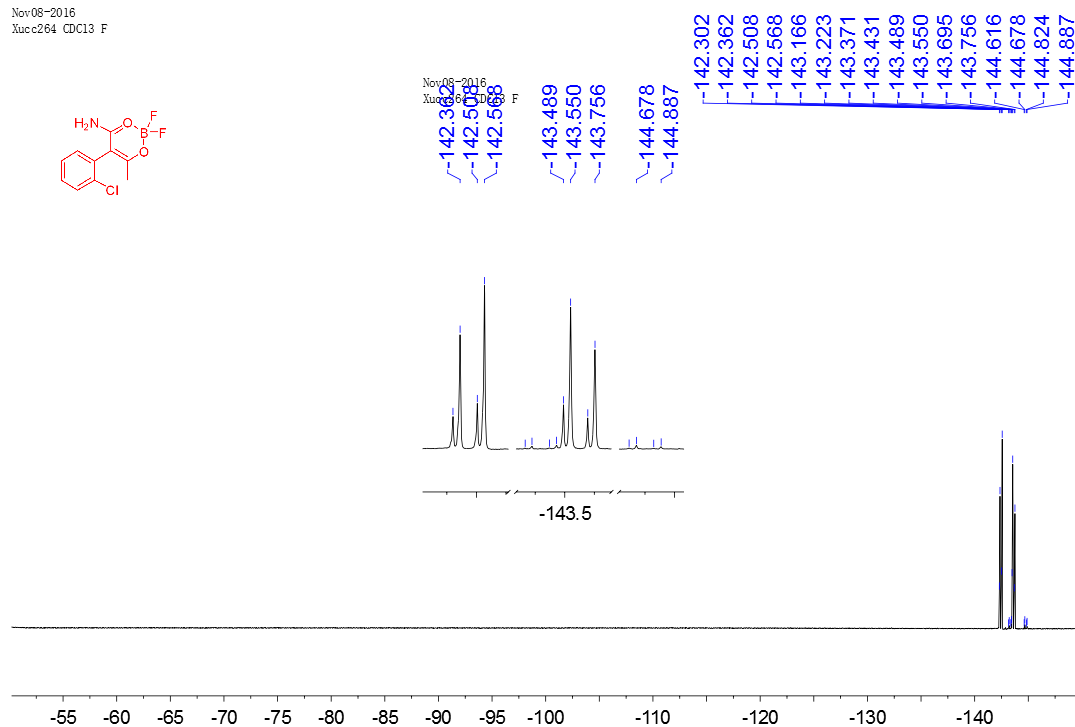
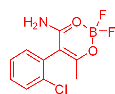
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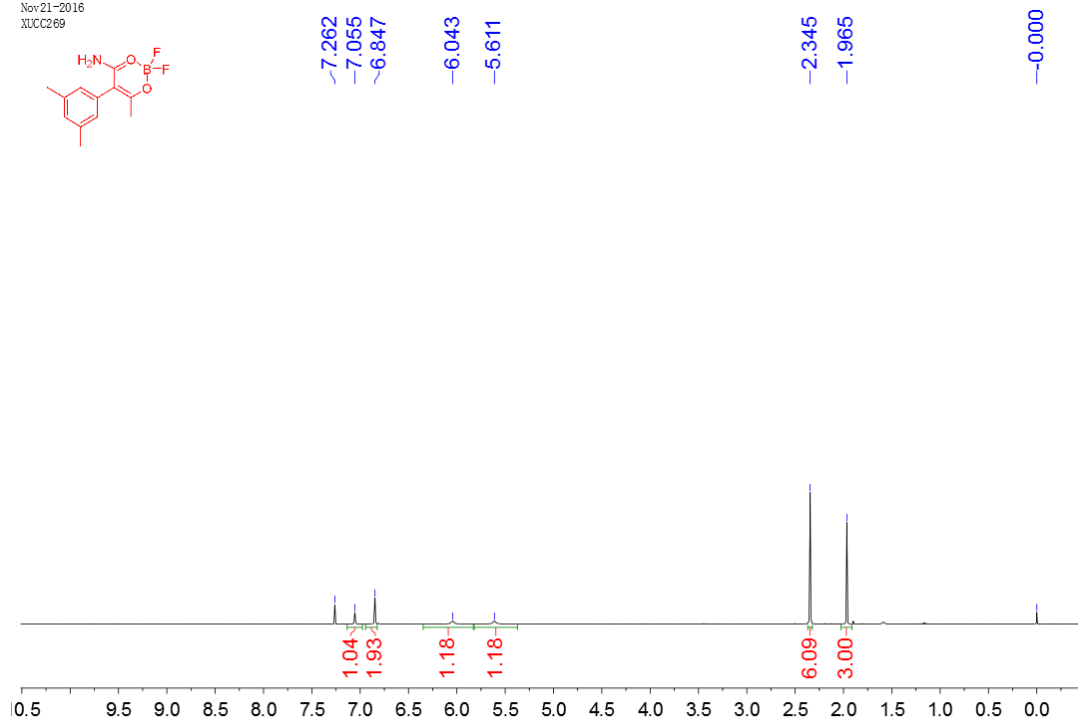
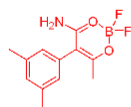


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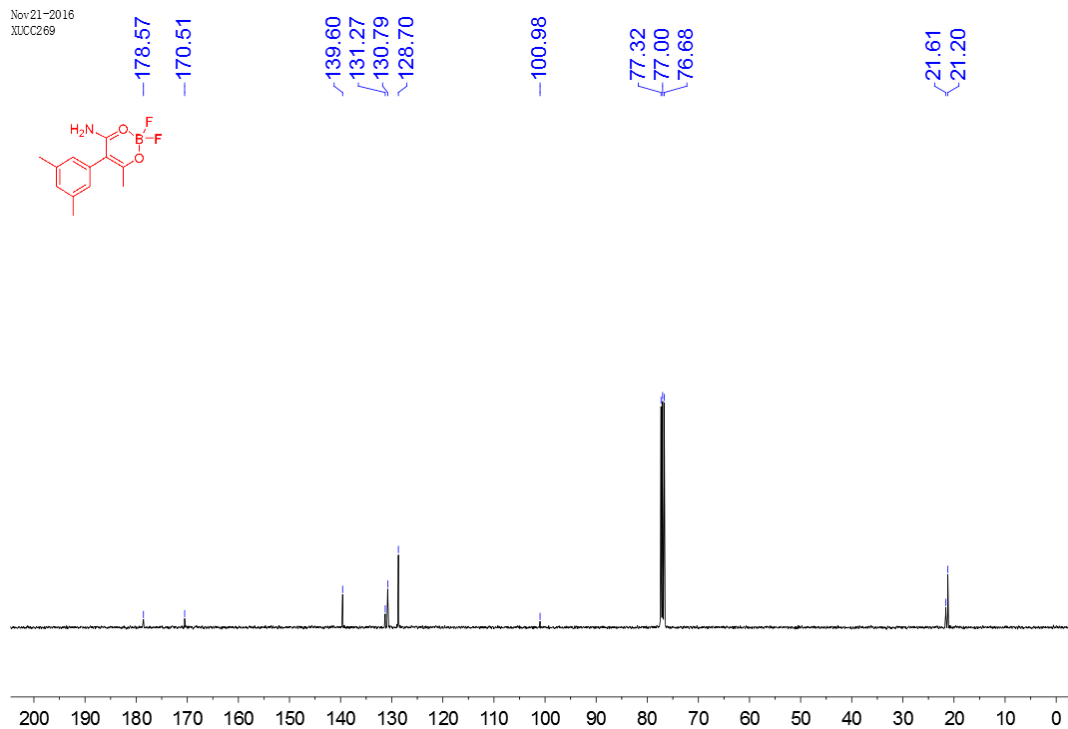
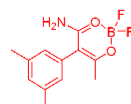


# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2o**

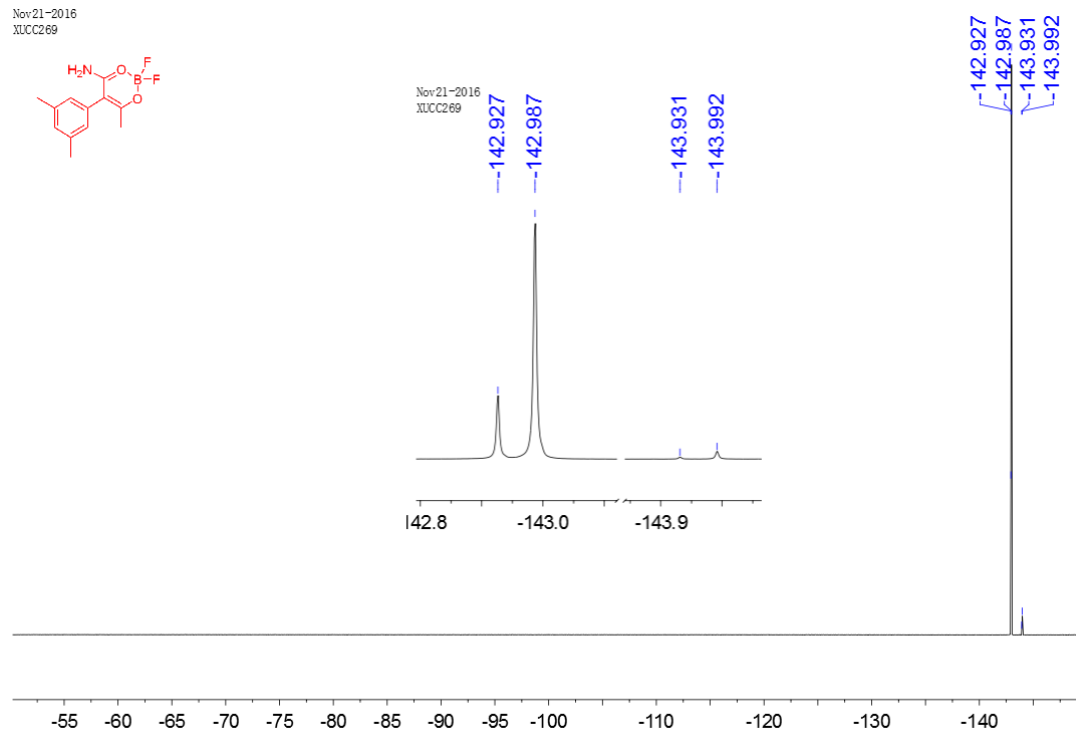
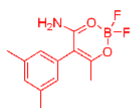
Nov21-2016  
XUCC269



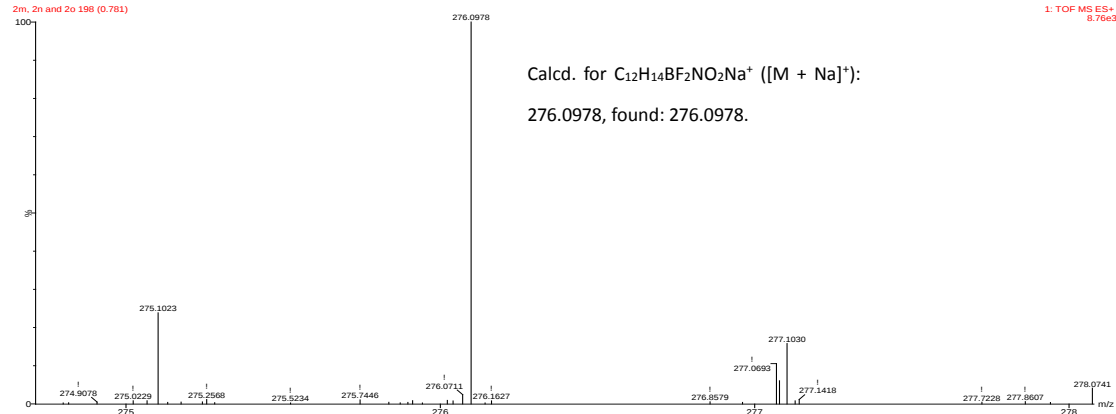
Nov21-2016  
XUCC269



Nov21-2016  
XUCC269



2m, 2n and 2o 198 (0.781)

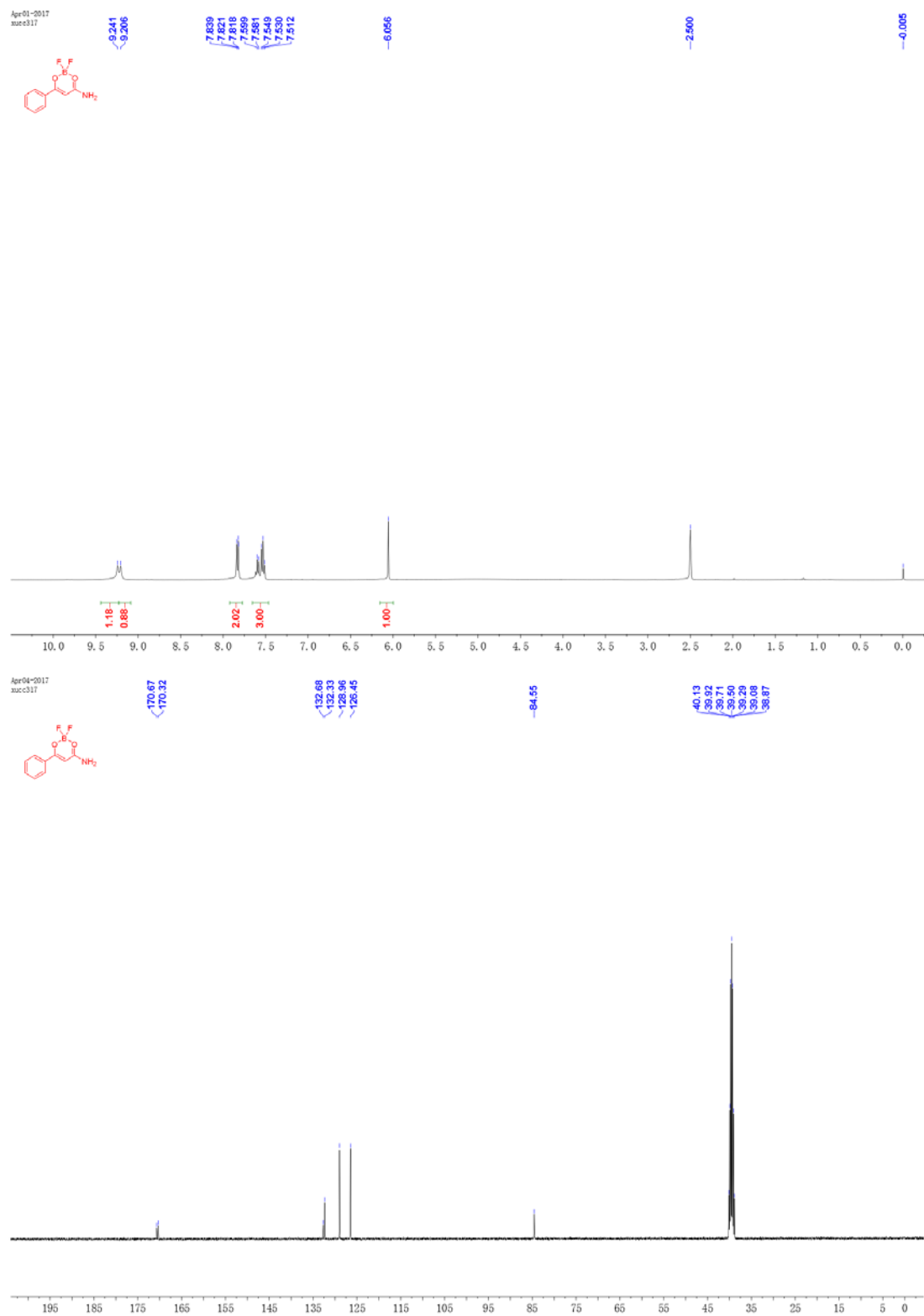


Calcd. for  $\text{C}_{12}\text{H}_{14}\text{BF}_2\text{NO}_2\text{Na}^+$  ( $[\text{M} + \text{Na}]^+$ ):

276.0978, found: 276.0978.

1: TOF MS ES+  
8.7663

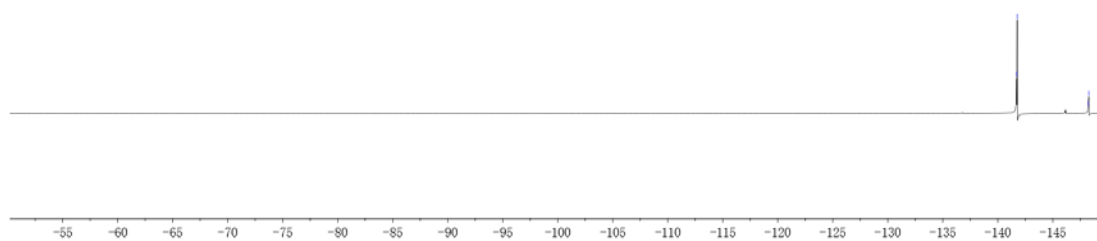
# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2p**



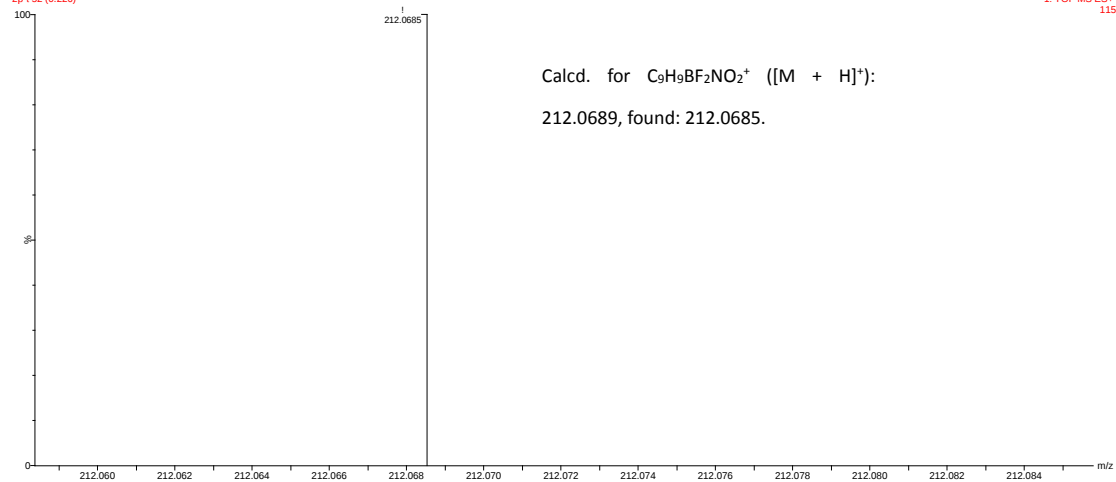
Apr-01-2017  
ms0317



-141.701  
-141.763  
-148.210  
-148.263



2p-152 (0.226)



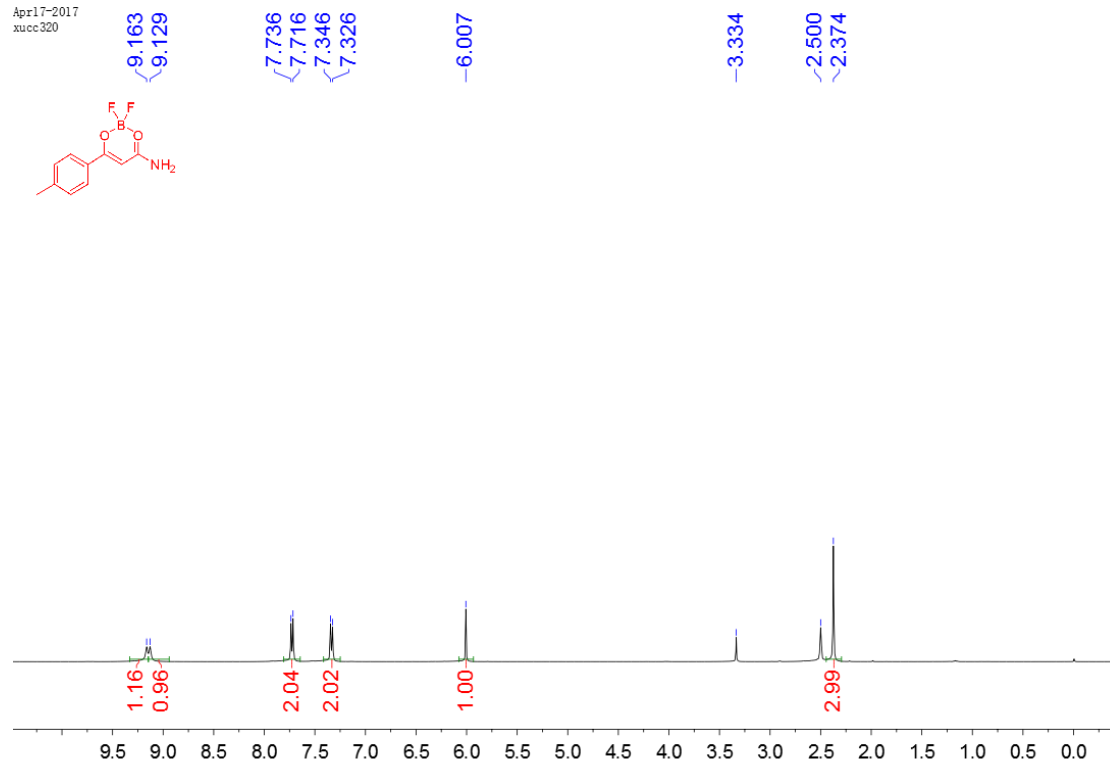
1: TOP MS ES+  
115

Calcd. for  $C_9H_9BF_2NO_2^+$  ( $[M + H]^+$ ):

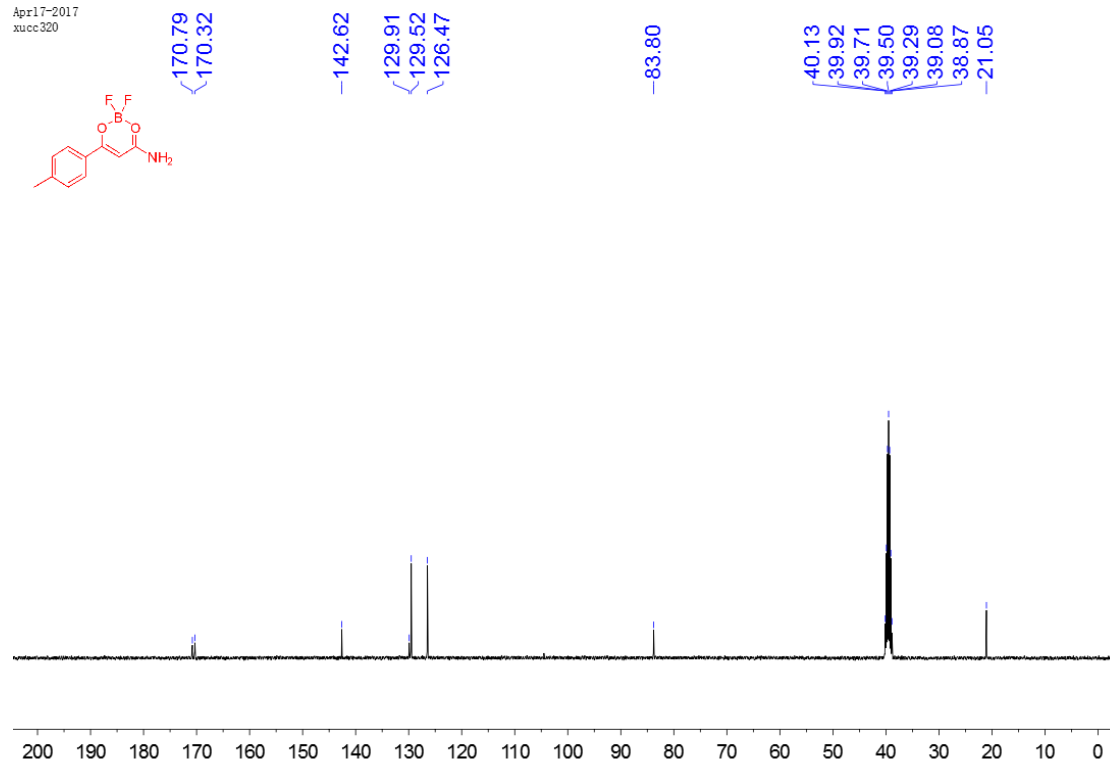
212.0689, found: 212.0685.

# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2q**

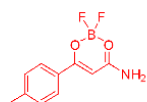
April7-2017  
xuoc320



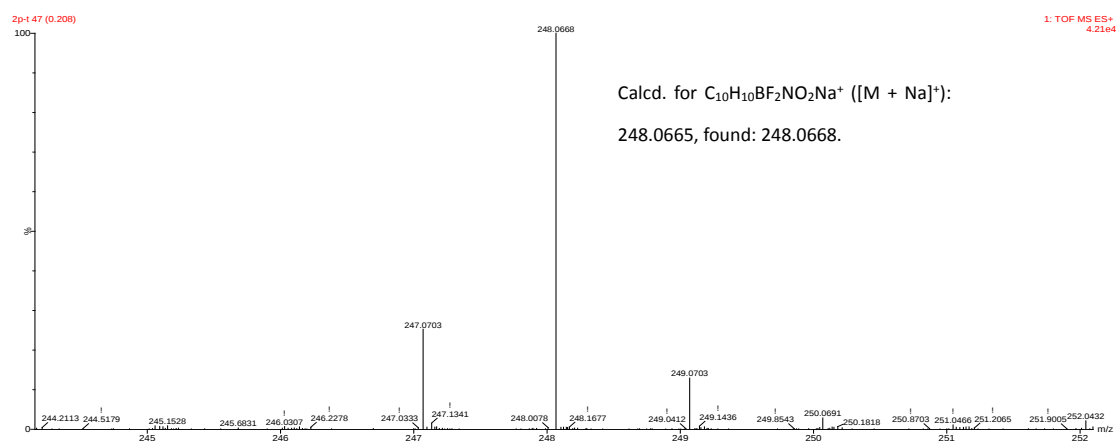
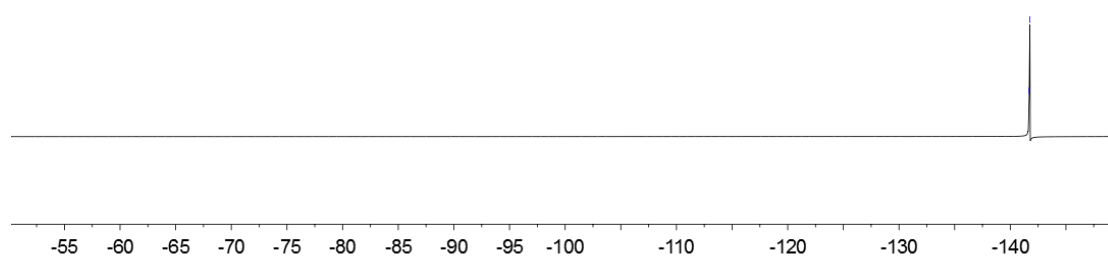
April7-2017  
xuoc320



April-2017  
xuoc320

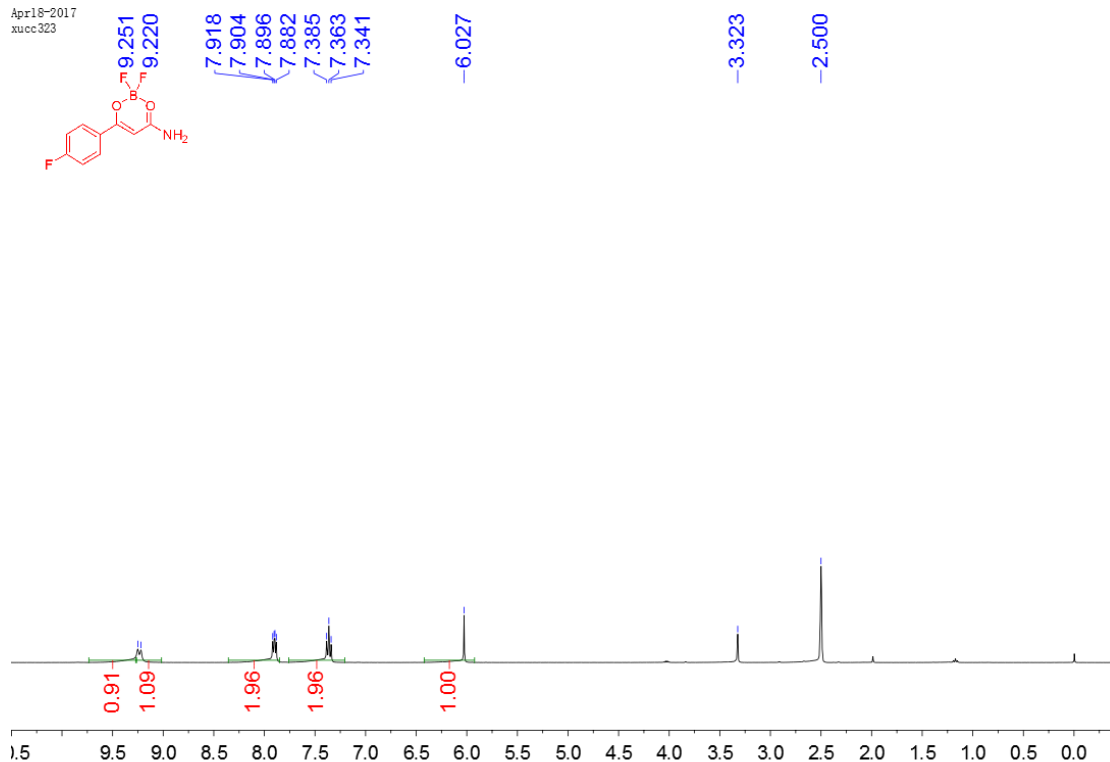


141.698  
141.760

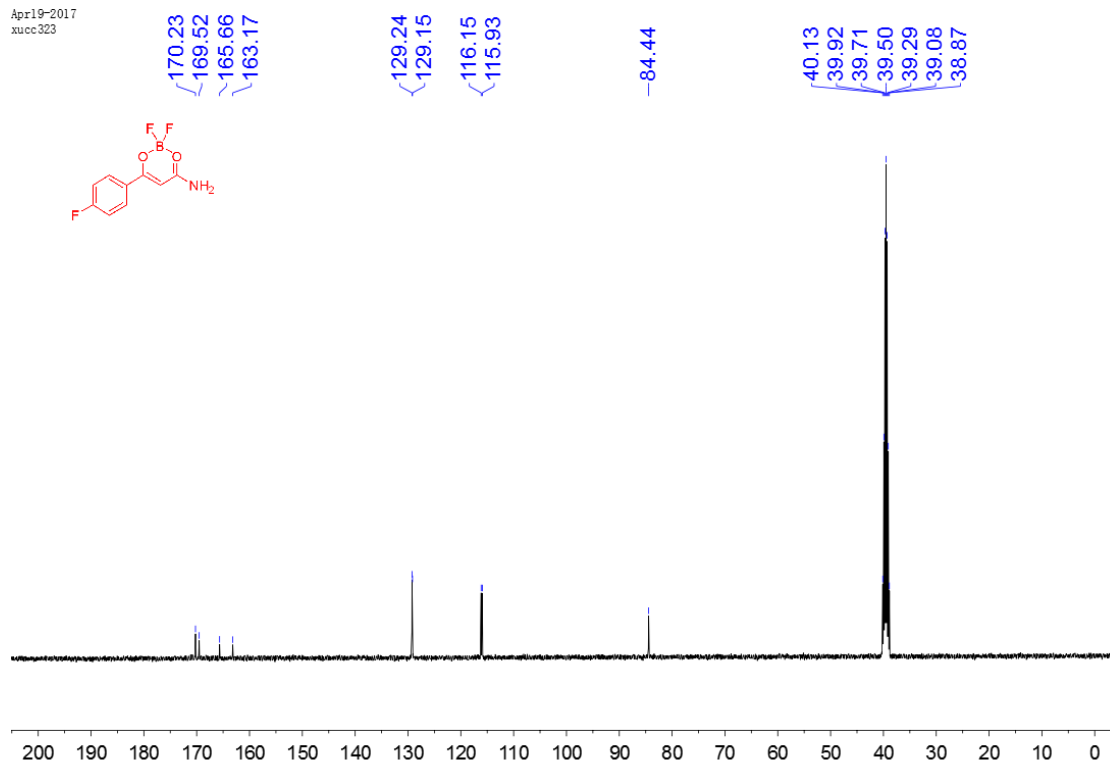


# <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR and HRMS spectra of **2r**

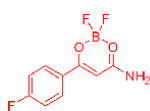
Apr18-2017  
xucc323



Apr19-2017  
xucc323

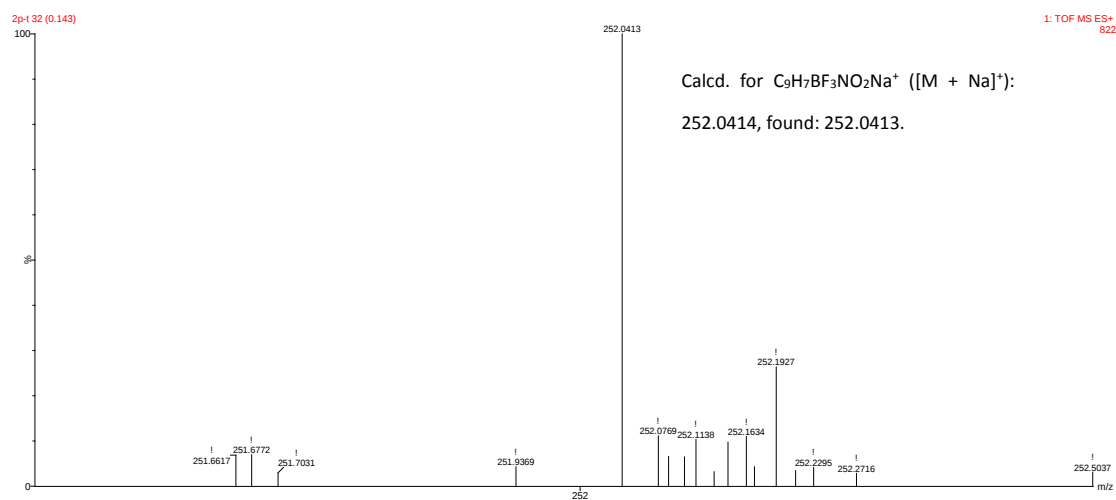
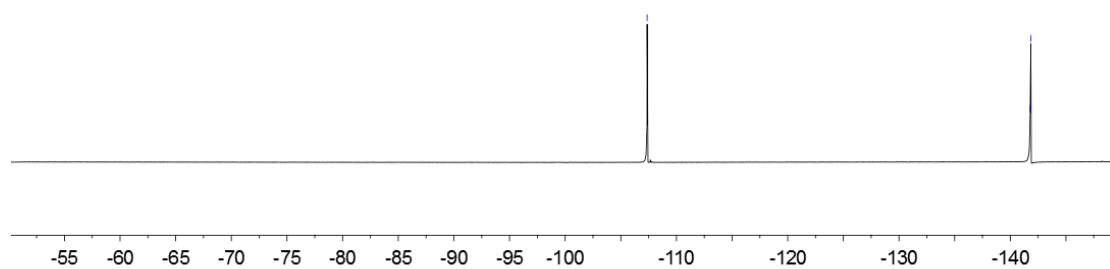


Apr18-2017  
xuoc323



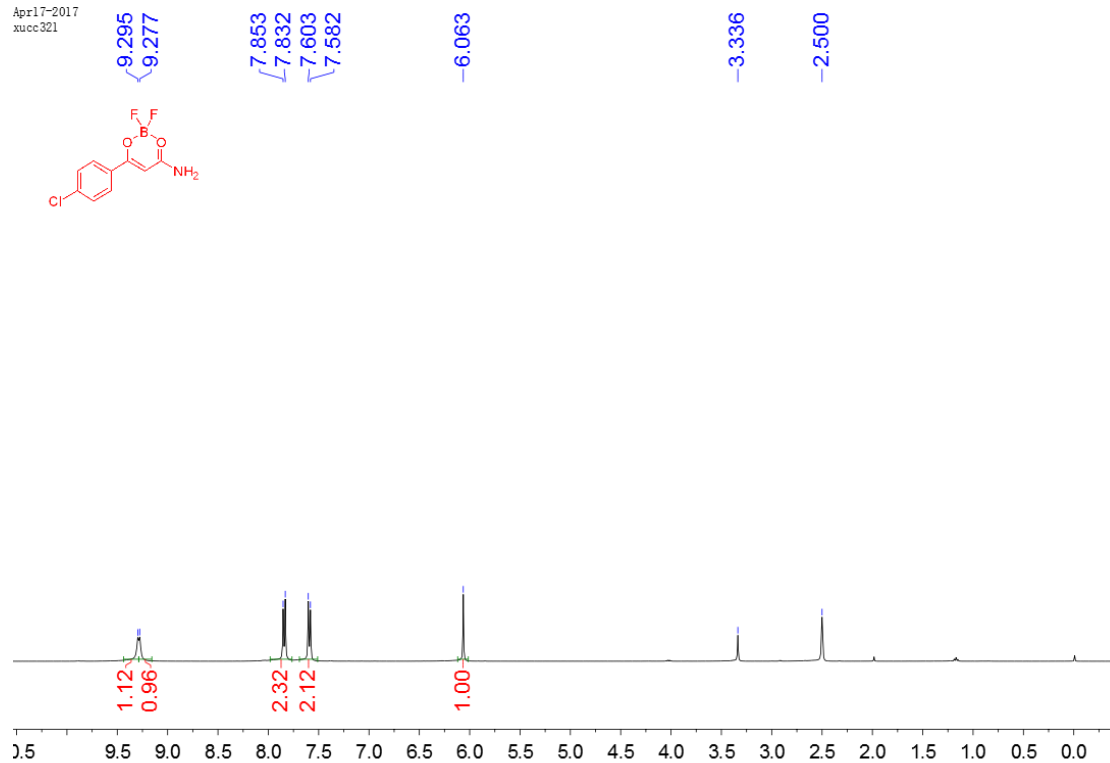
-107.366

-141.785  
-141.847

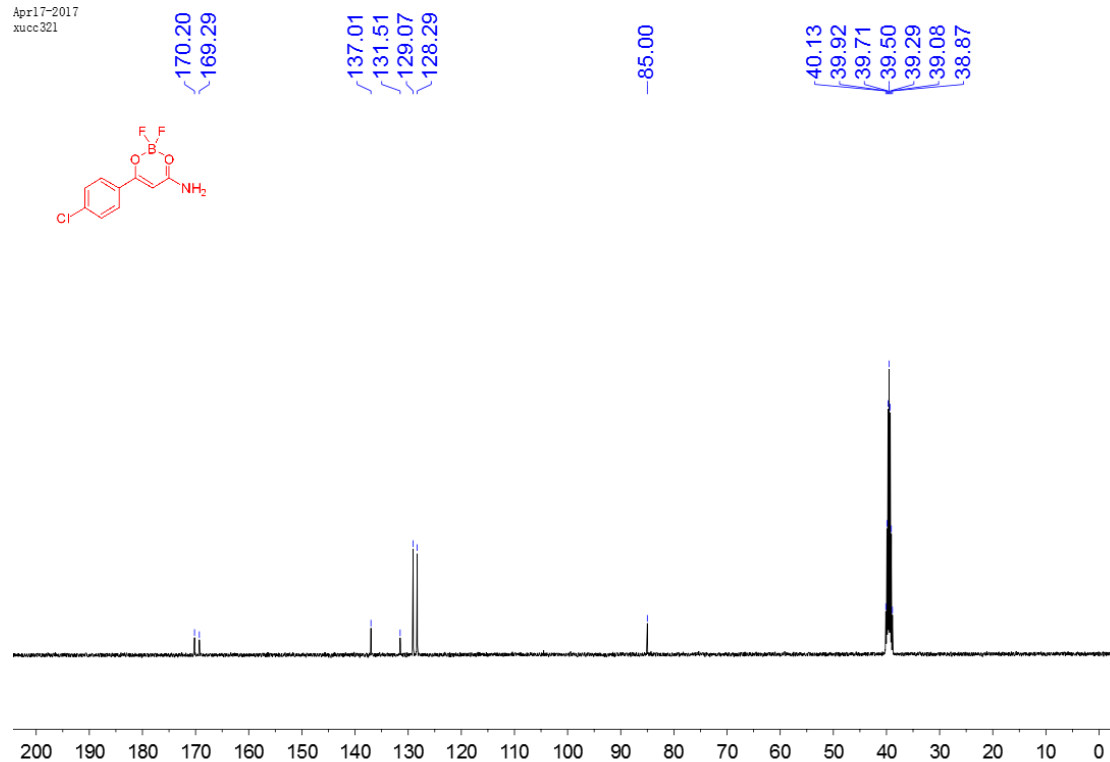


# <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR and HRMS spectra of 2s

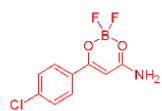
April-2017  
xuoc321



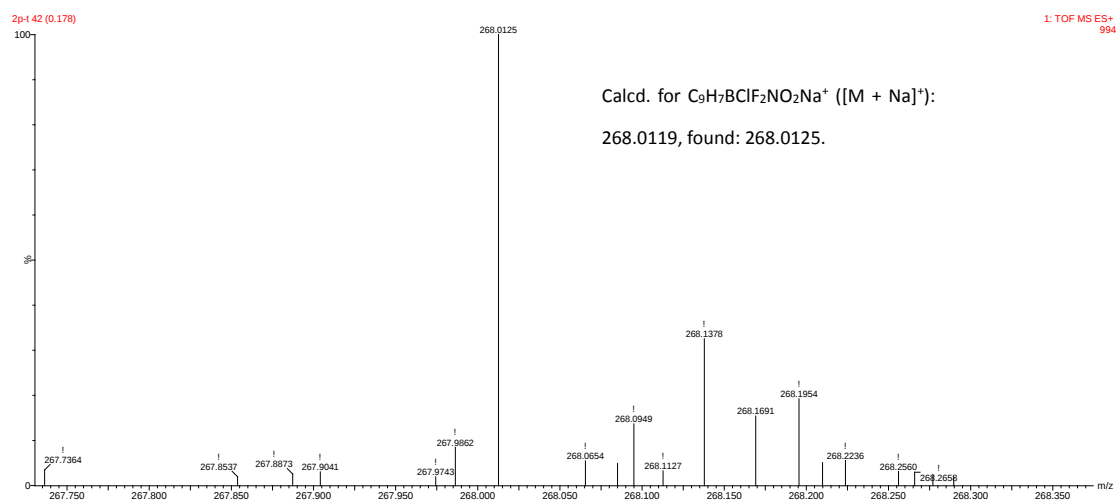
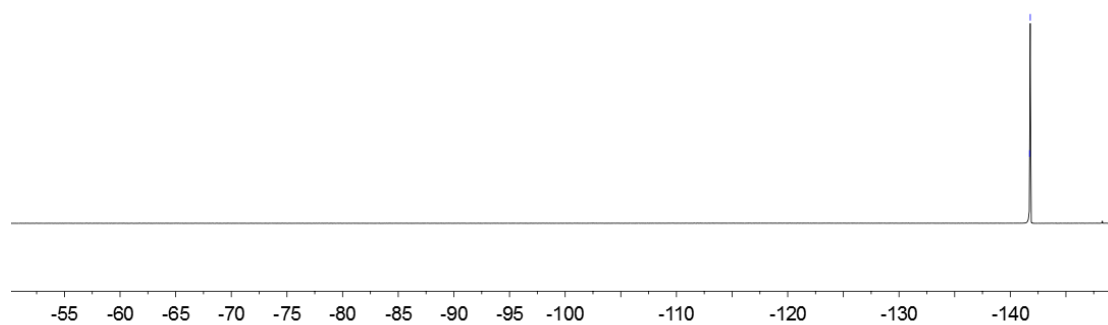
April-2017  
xuoc321



April-2017  
xuoc321

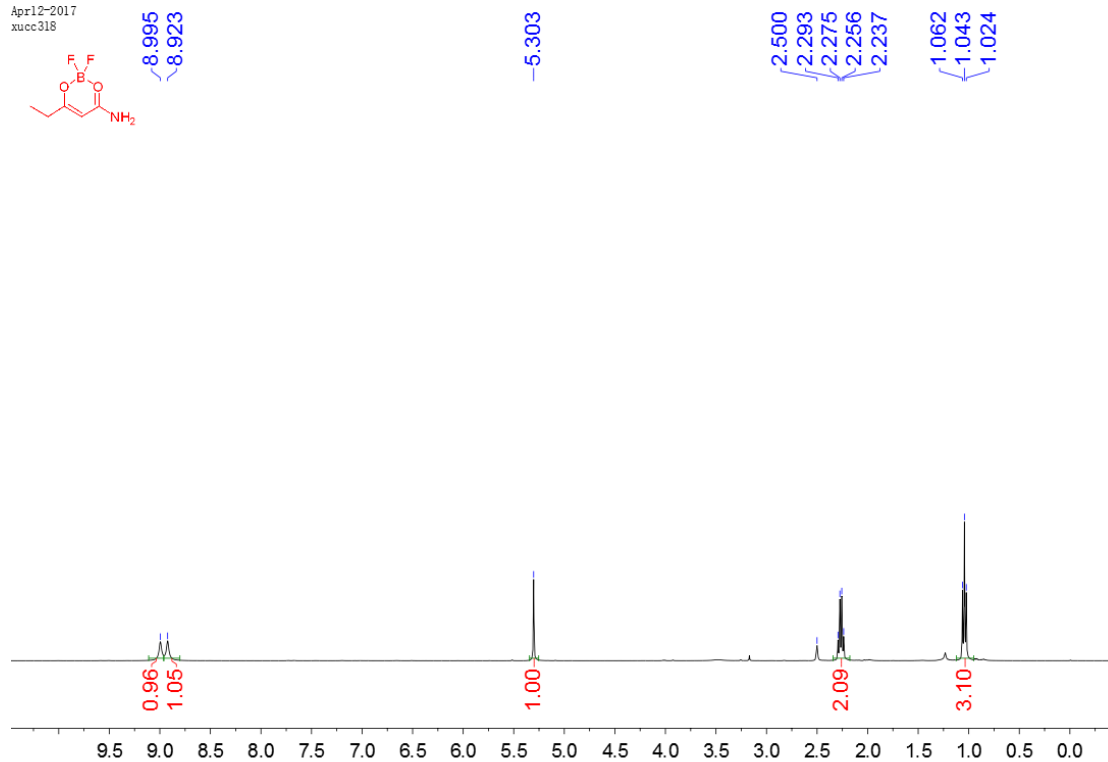
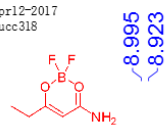


141.732  
141.794

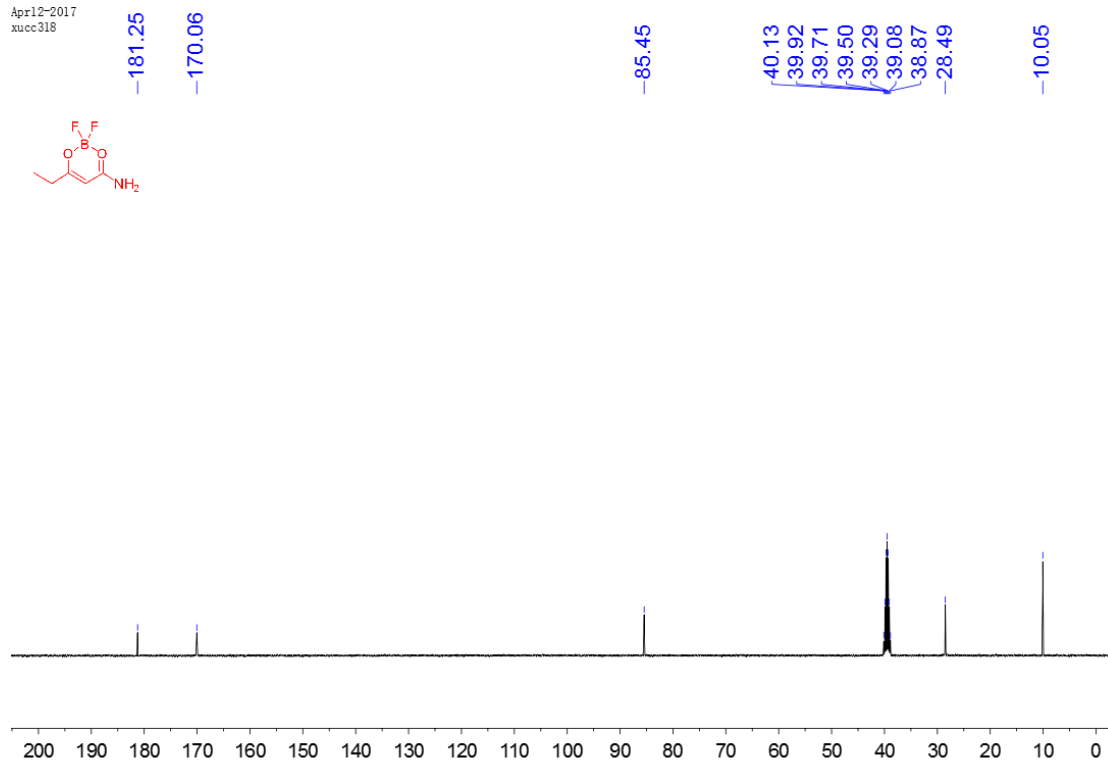
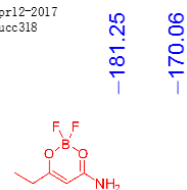


# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HMRS spectra of **2t**

Apr12-2017  
xucc318



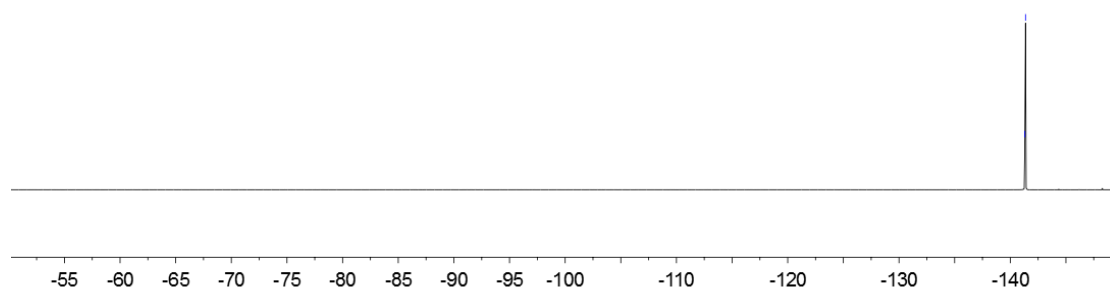
Apr12-2017  
xucc318



April 2-2017  
xucc318

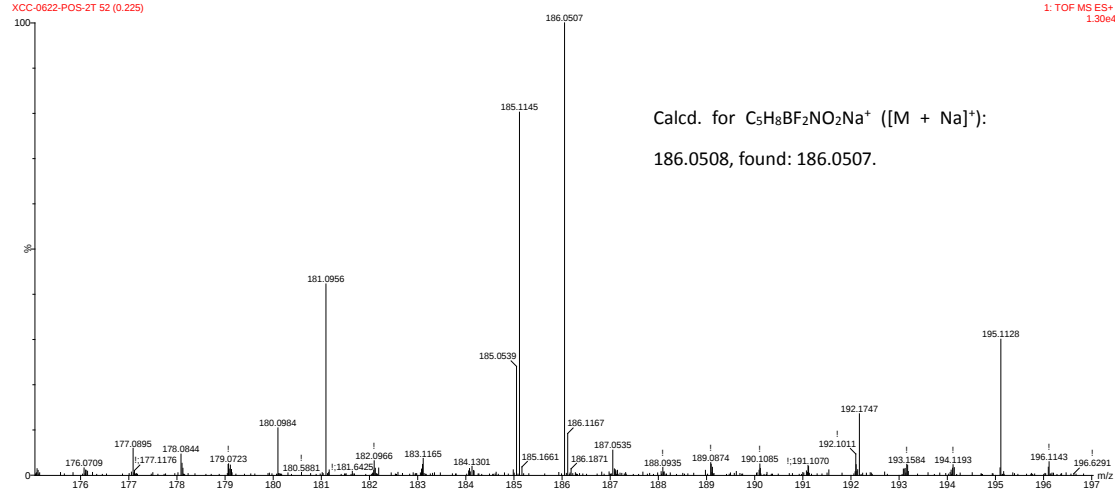


141.309  
141.370

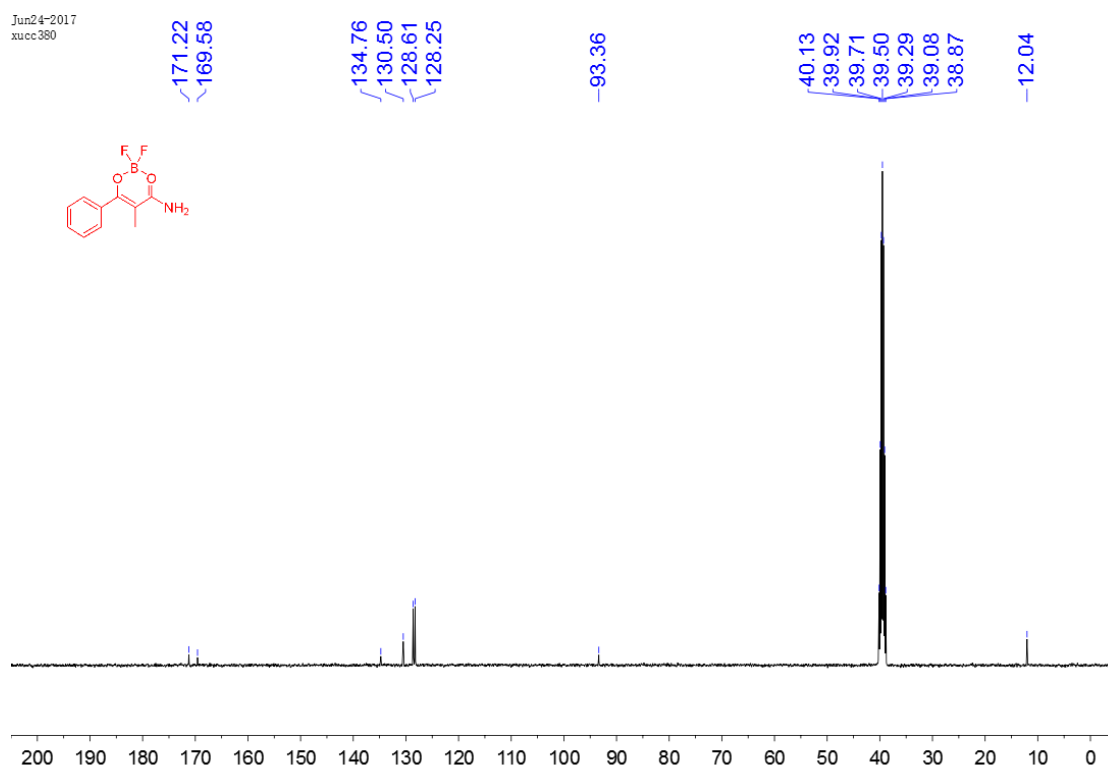
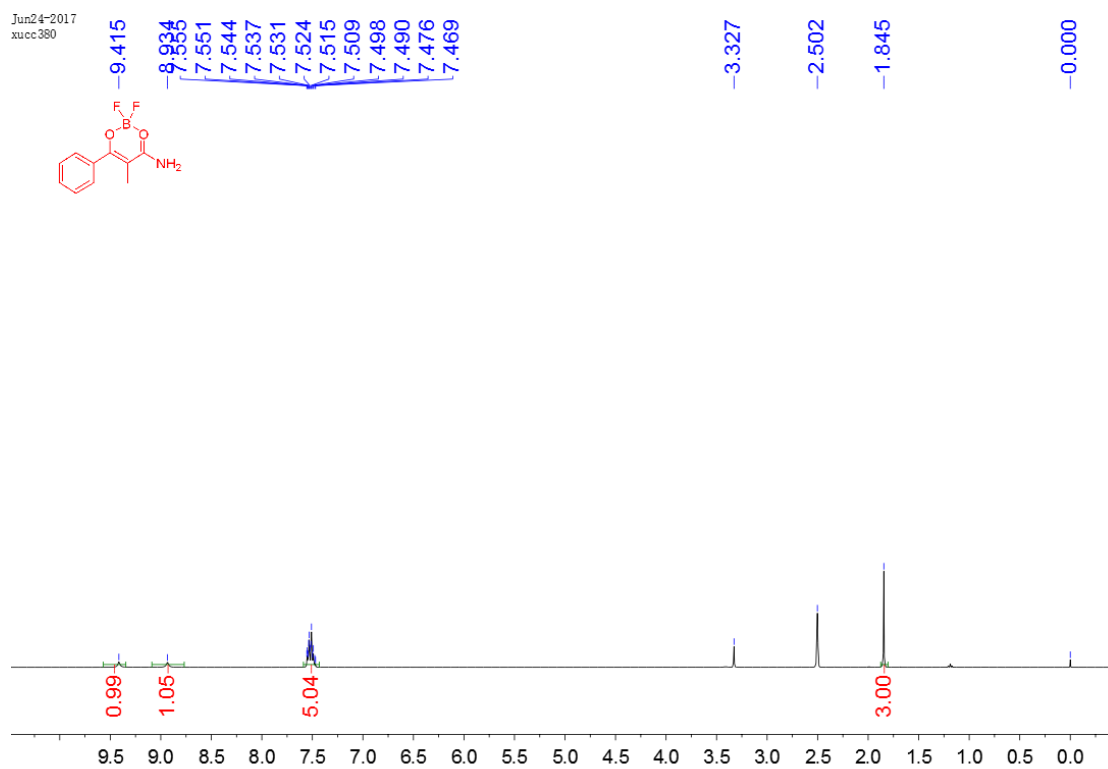


XCC-0622-POS-2T 52 (0.225)

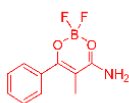
1: TOF MS ES+  
1.30e4



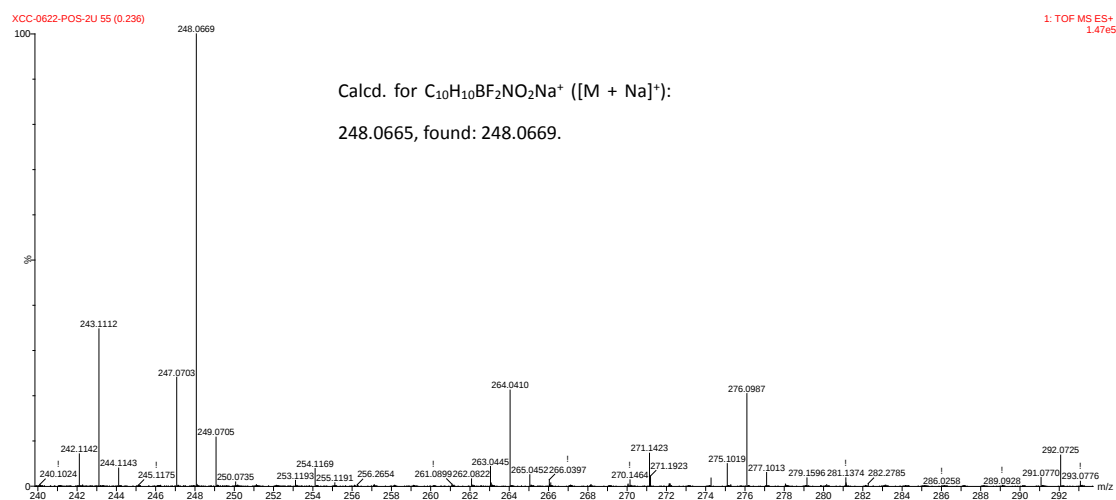
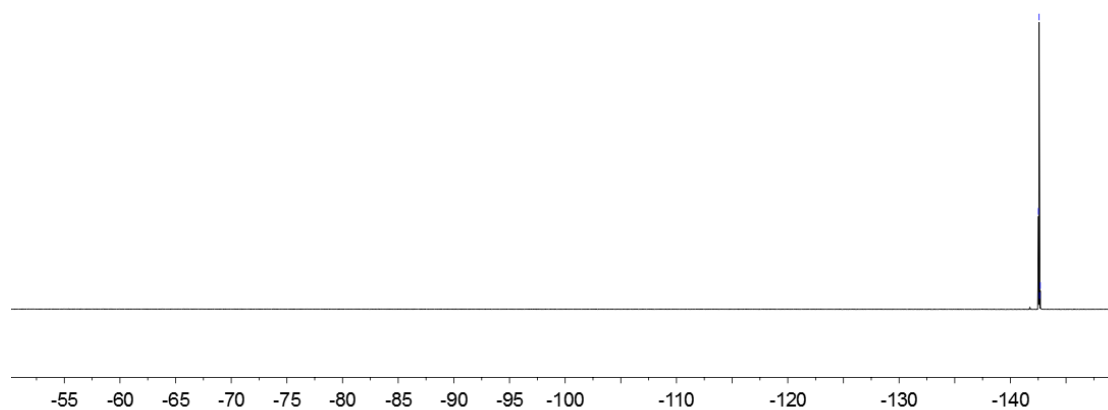
$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2u**



Jun24-2017  
xucc380

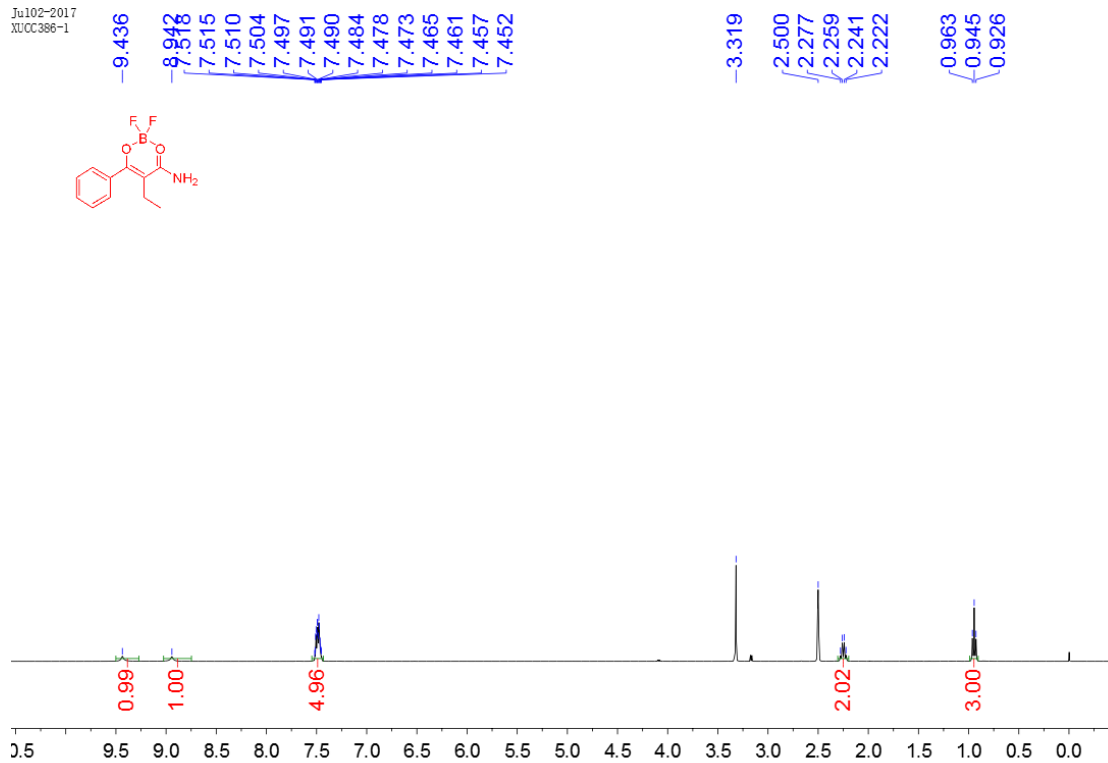


142.518  
142.581  
142.623  
142.686

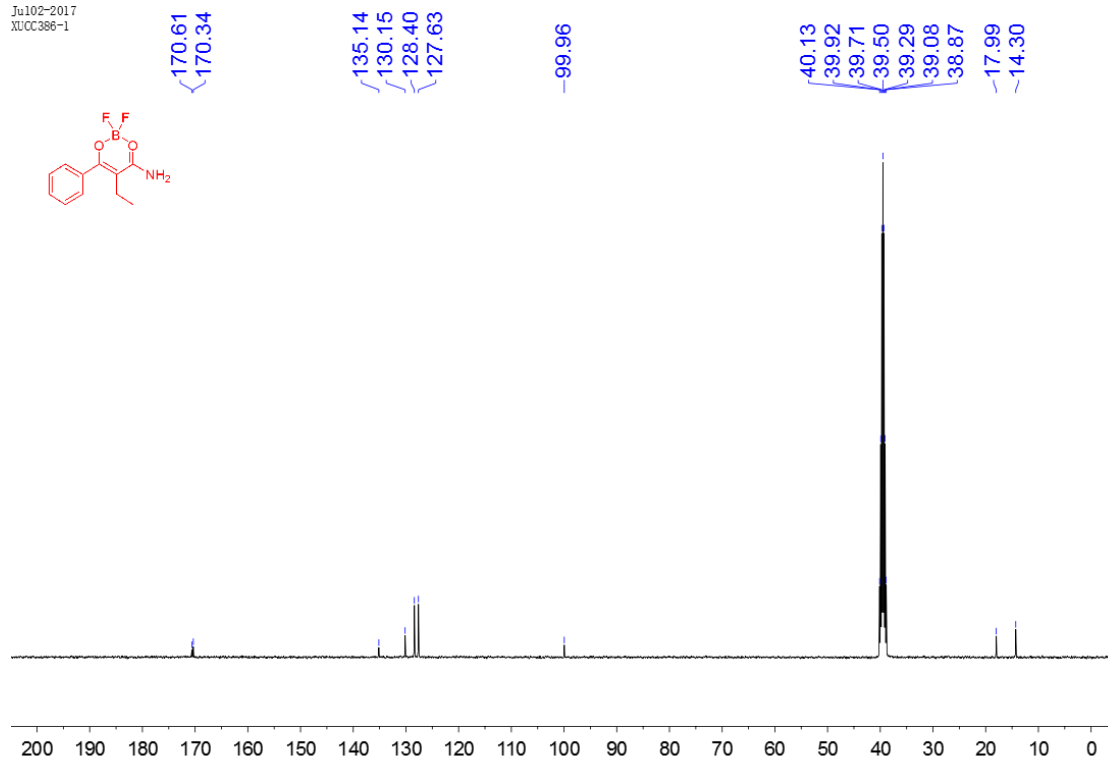


$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$  NMR and HRMS spectra of **2v**

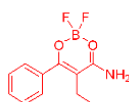
Ju102-2017  
XUCC386-1



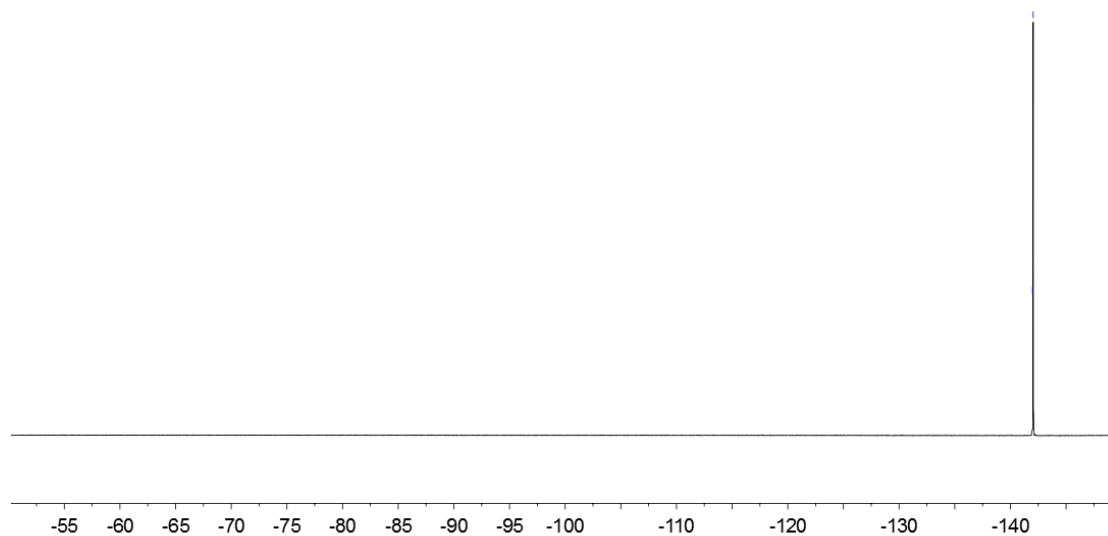
Ju102-2017  
XUCC386-1



Ju102-2017  
XUCC386-1

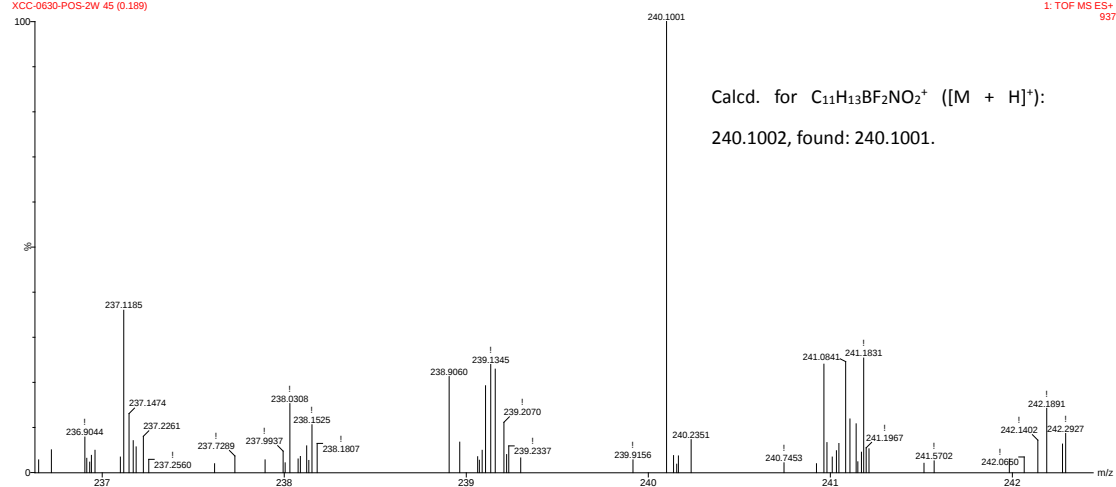


141.984  
142.046



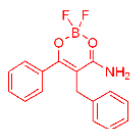
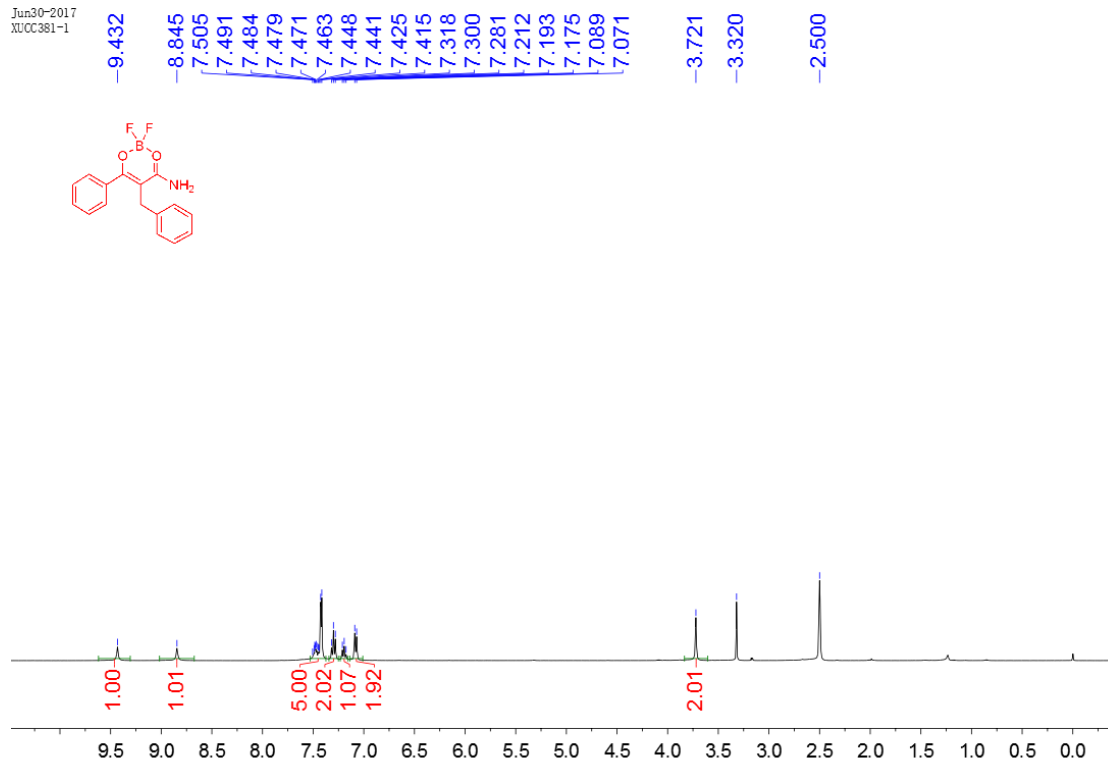
XCC-0630-POS-2W 45 (0.189)

1: TOF MS ES+  
937

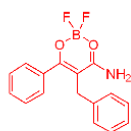
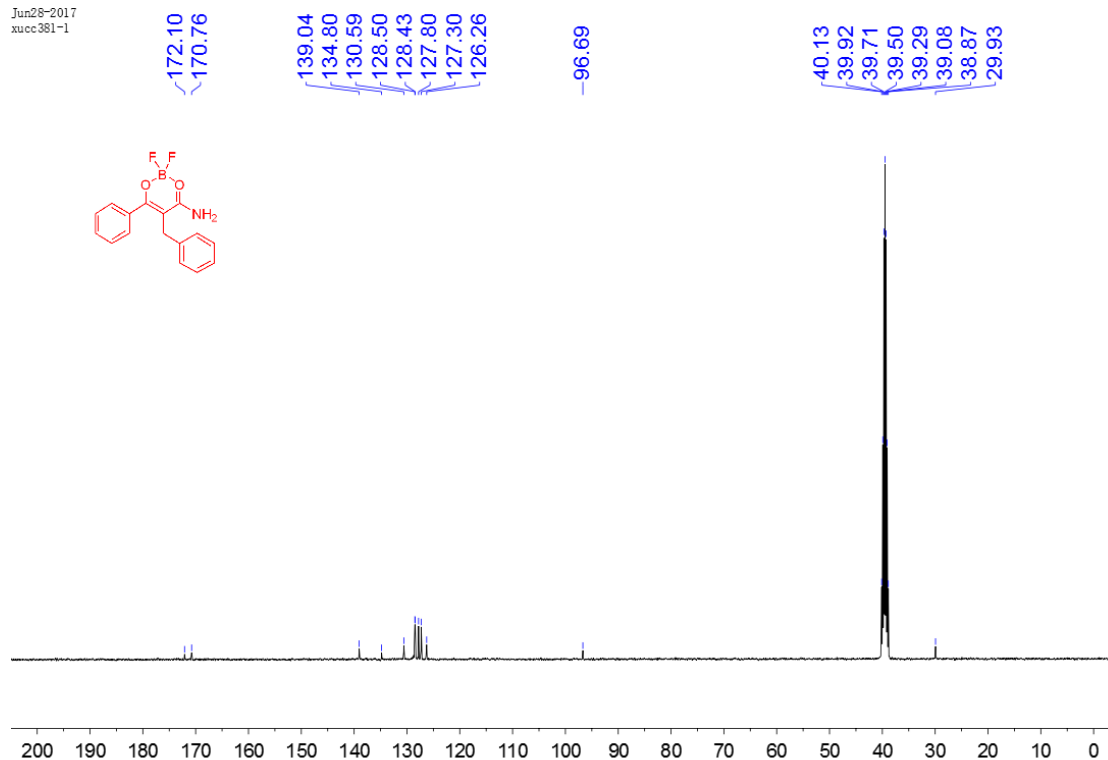


# $^1\text{H}$ , $^{13}\text{C}$ , $^{19}\text{F}$ NMR and HRMS spectra of **2w**

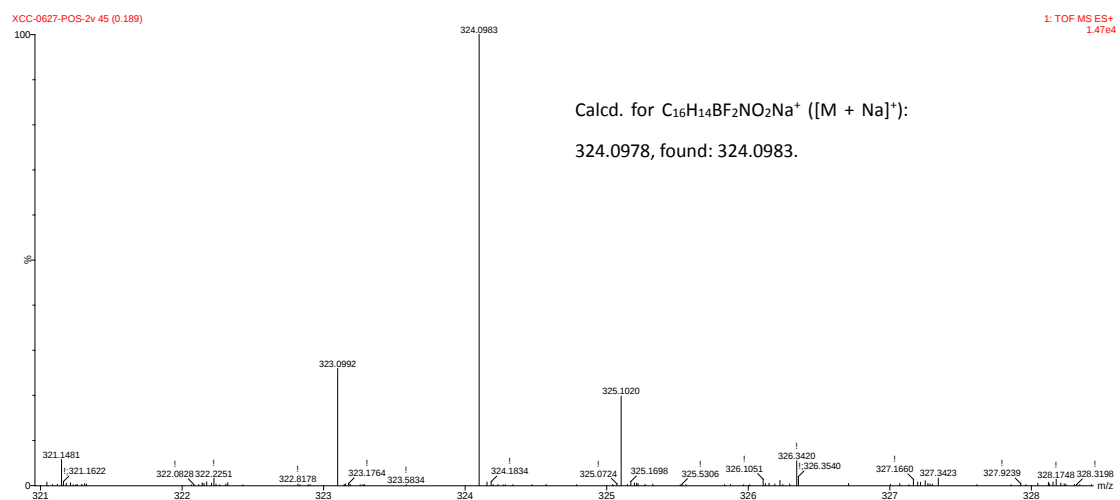
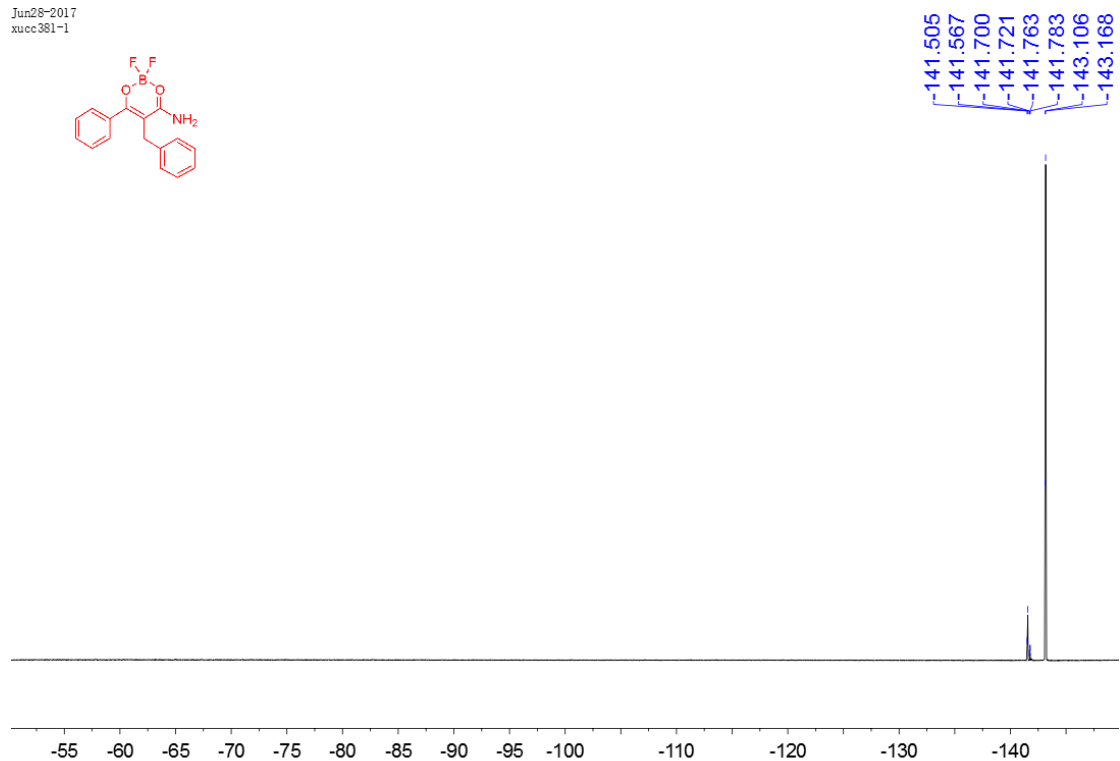
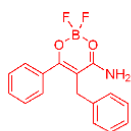
Jun30-2017  
XUCC381-1



Jun28-2017  
xuucc381-1



Jun28-2017  
xucc381-1



# Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of 2-phenyl-3-oxobutanamide (3a)

## $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of 3a

