

## Supplementary

# Design, Synthesis, and Bioactivity Evaluation of New Thiochromanone Derivatives Containing a Carboxamide Moiety

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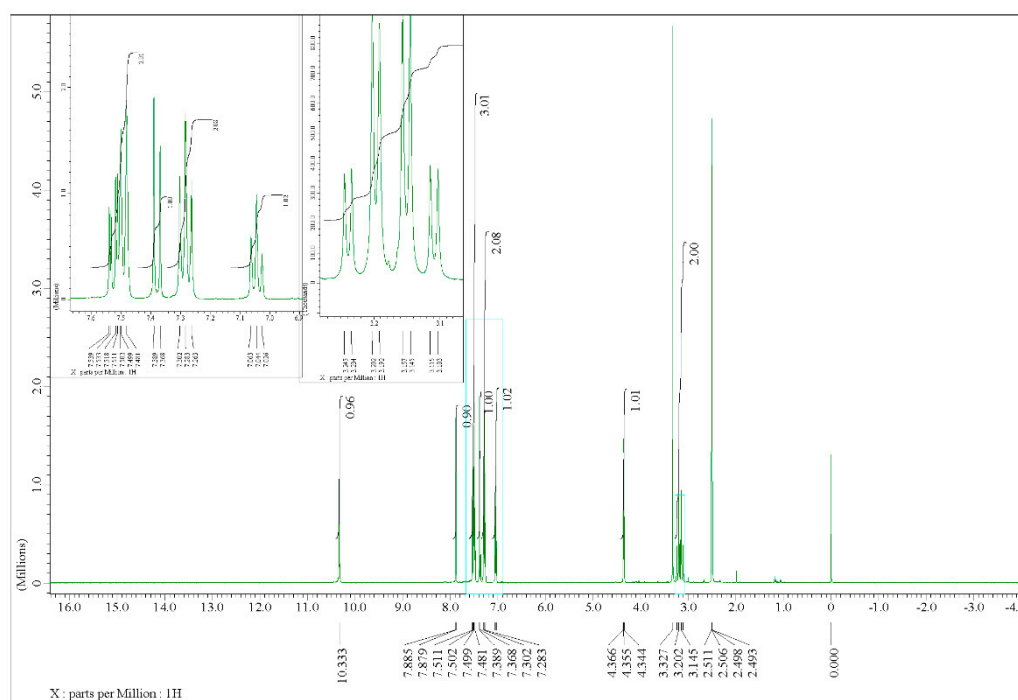
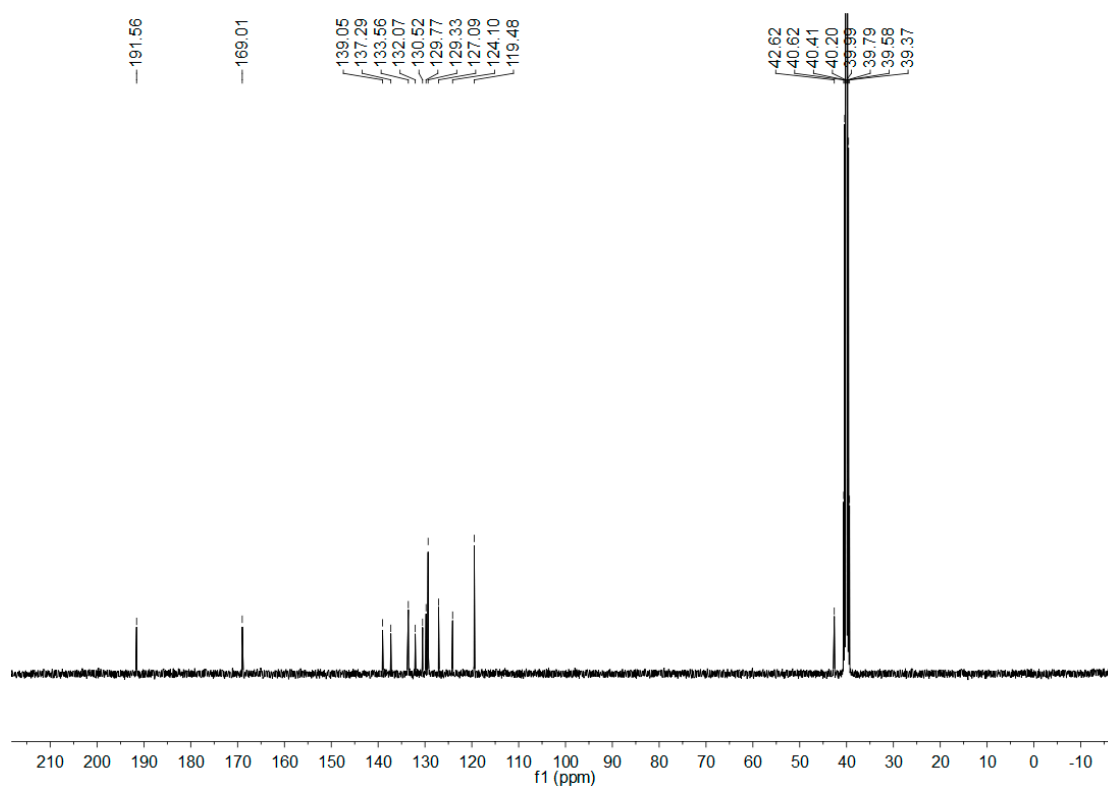
<sup>1</sup> School of Liquor and Food Engineering, Guizhou University, Guiyang 550025, China; an1378386891@163.com (L.X.), lyu1@gzu.edu.cn (L.Y.), qq1401064120@126.com (J.C.), tzf18885247153@163.com (Z.T.), sushilee0120@163.com (J.L.), wangxiaodan0516@126.com (X.W.)

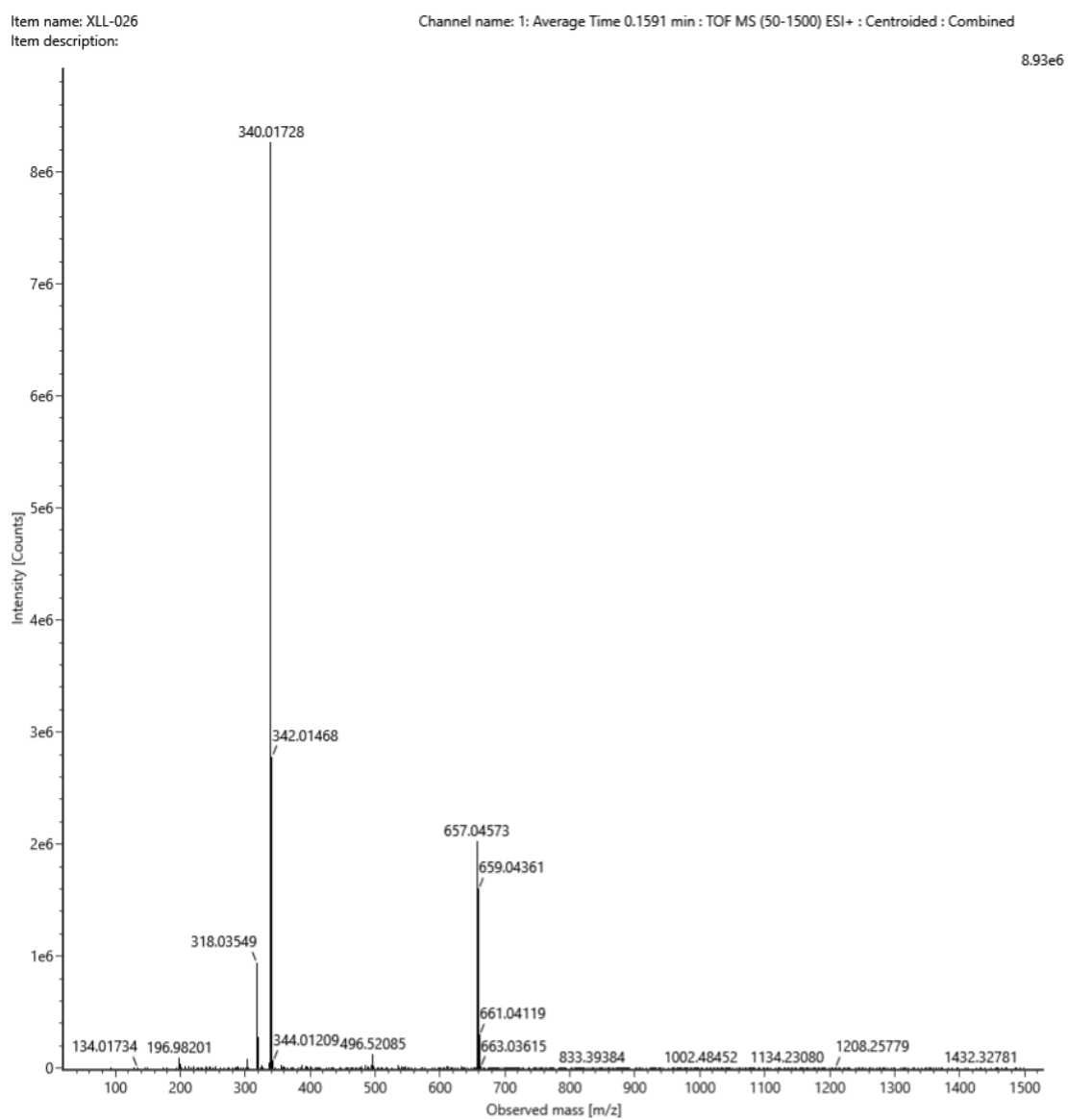
<sup>2</sup> Qiandongnan Engineering and Technology Research Center for Comprehensive Utilization of National Medicine/Key Laboratory for Modernization of Qiandongnan Miao & Dong Medicine, Kaili University, Kaili 556011, China

<sup>3</sup> Guizhou Provincial Key Laboratory of Fermentation Engineering and Biological Pharmacy, Guizhou University, Guiyang 550025, China

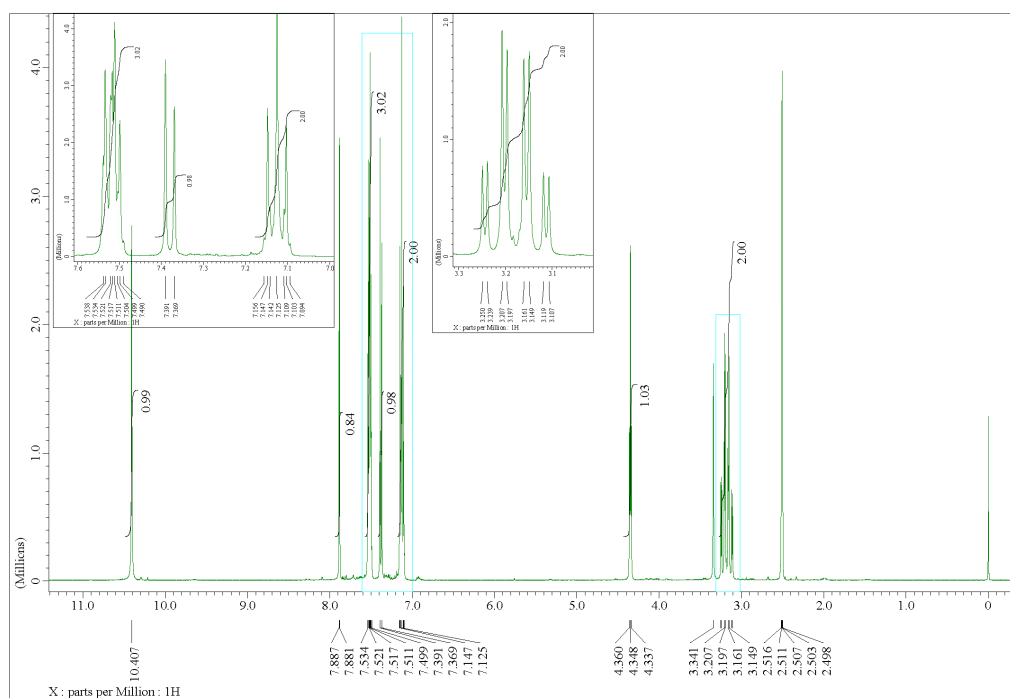
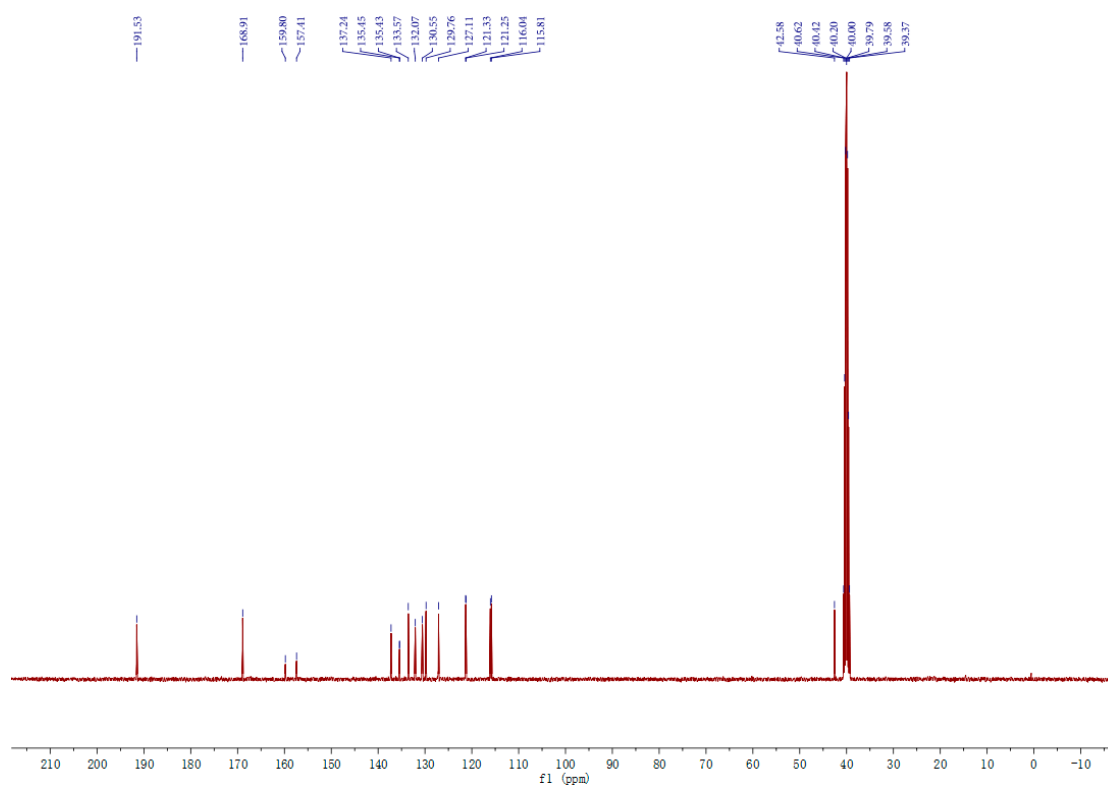
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† Lingling Xiao and Lu Yu contributed equally to this work.

 $^1\text{H}$  NMR of compound 3a $^{13}\text{C}$  NMR of compound 3a



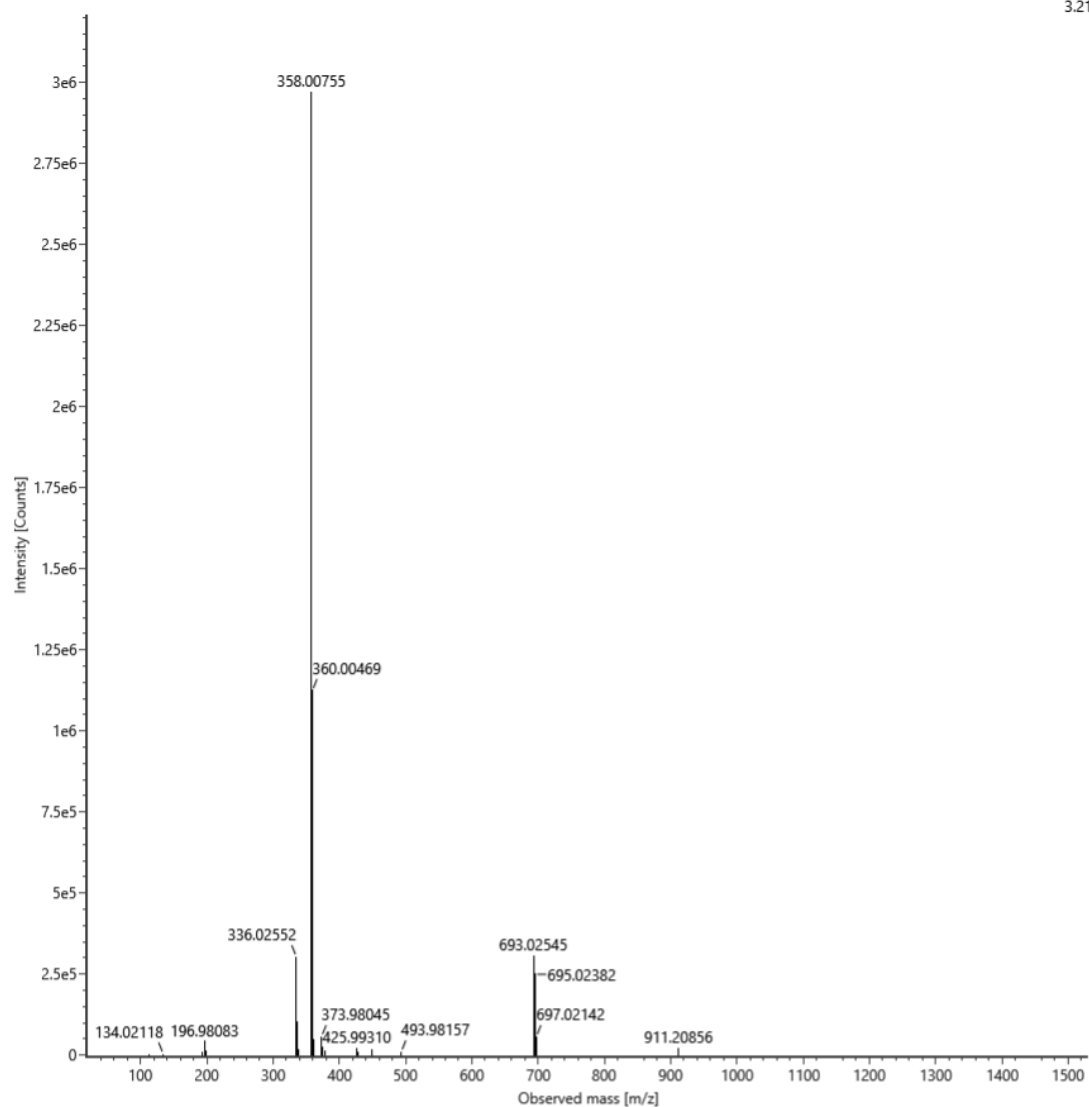
HRMS of compound 3a

 $^1\text{H}$  NMR of compound 3b $^{13}\text{C}$  NMR of compound 3b

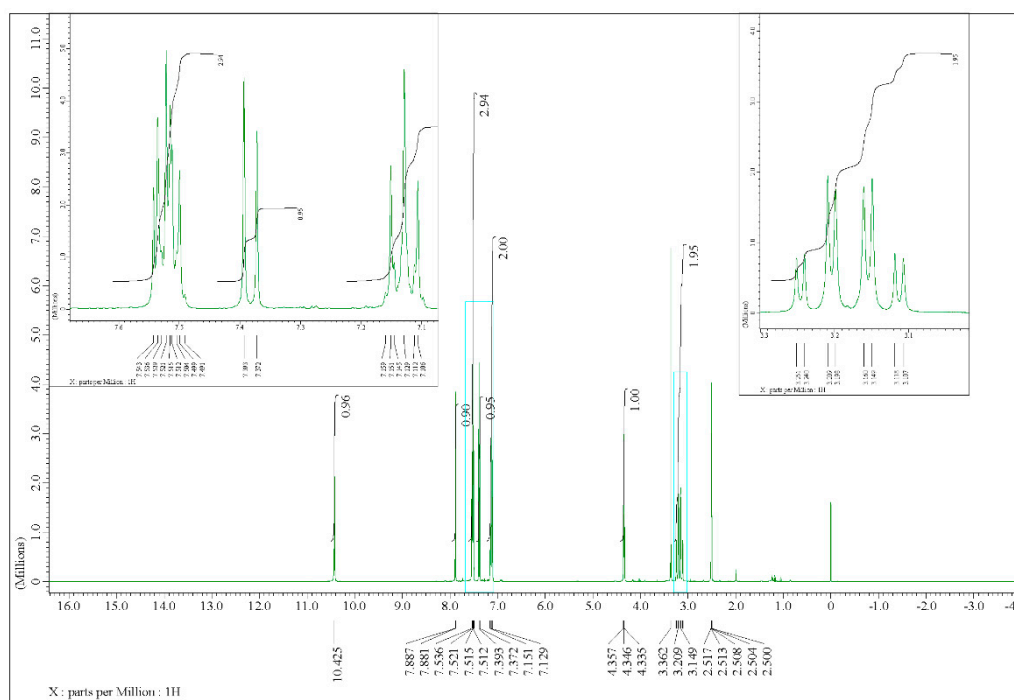
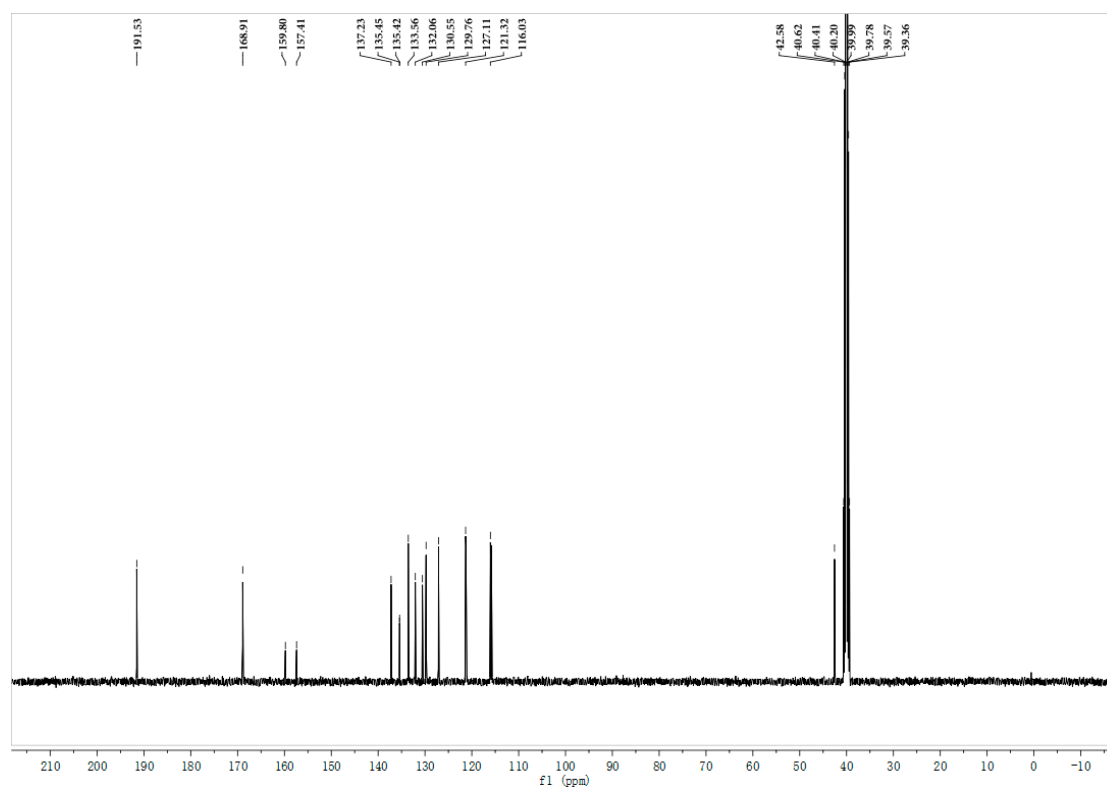
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3.21e6



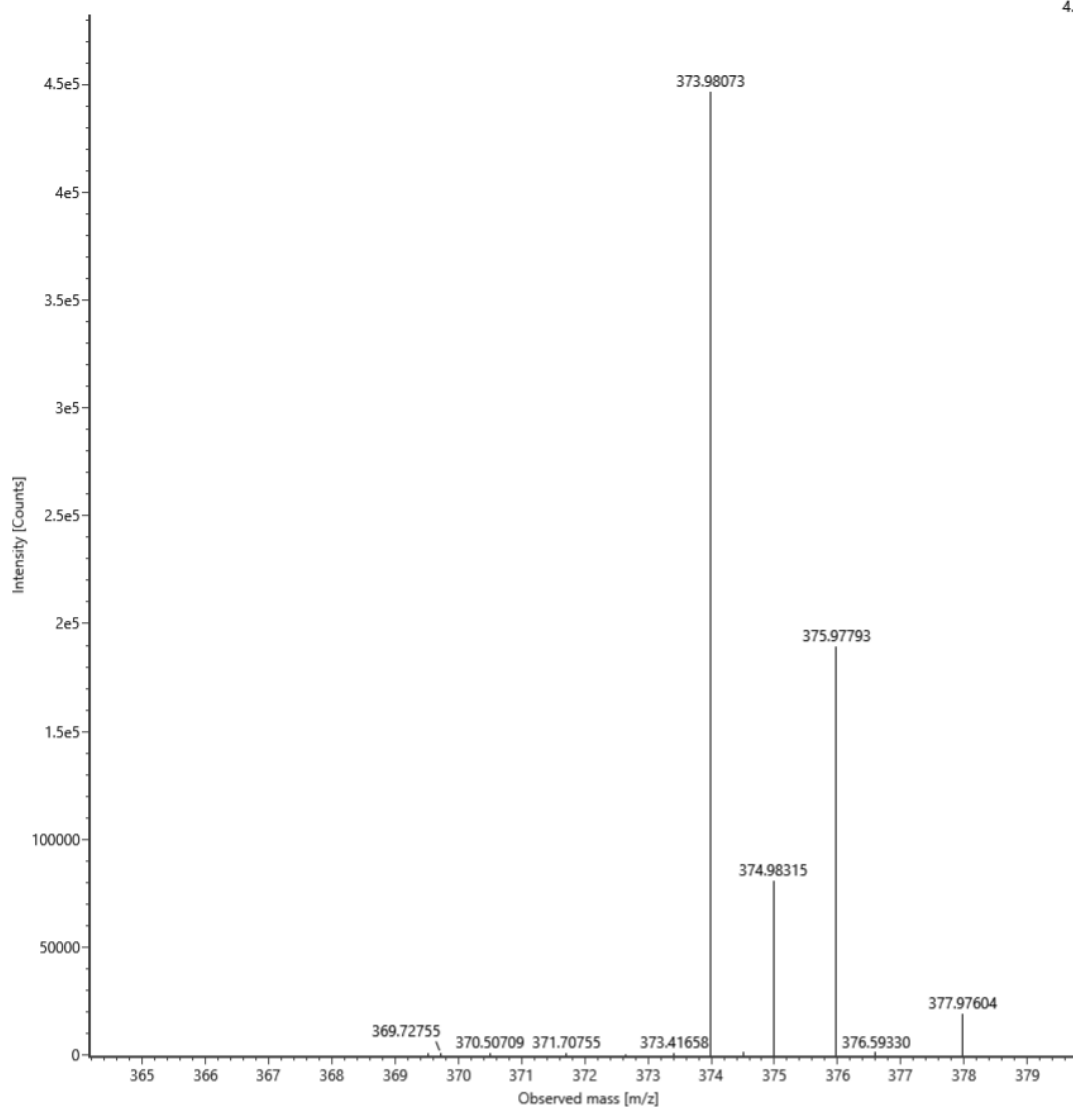
HRMS of compound 3b

<sup>1</sup>H NMR of compound 3c<sup>13</sup>C NMR of compound 3c

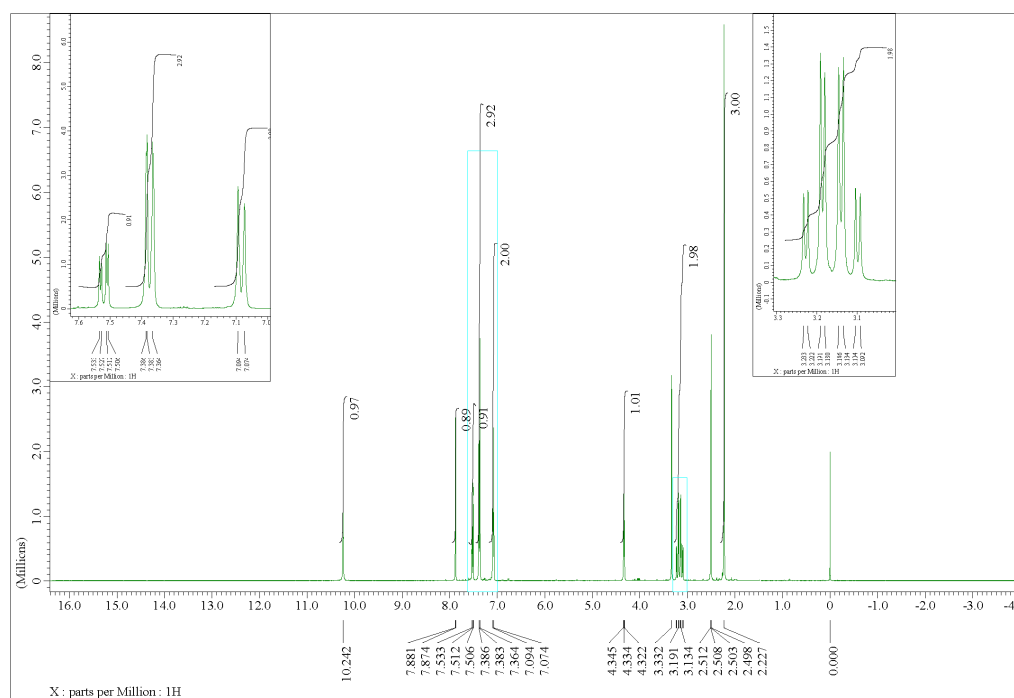
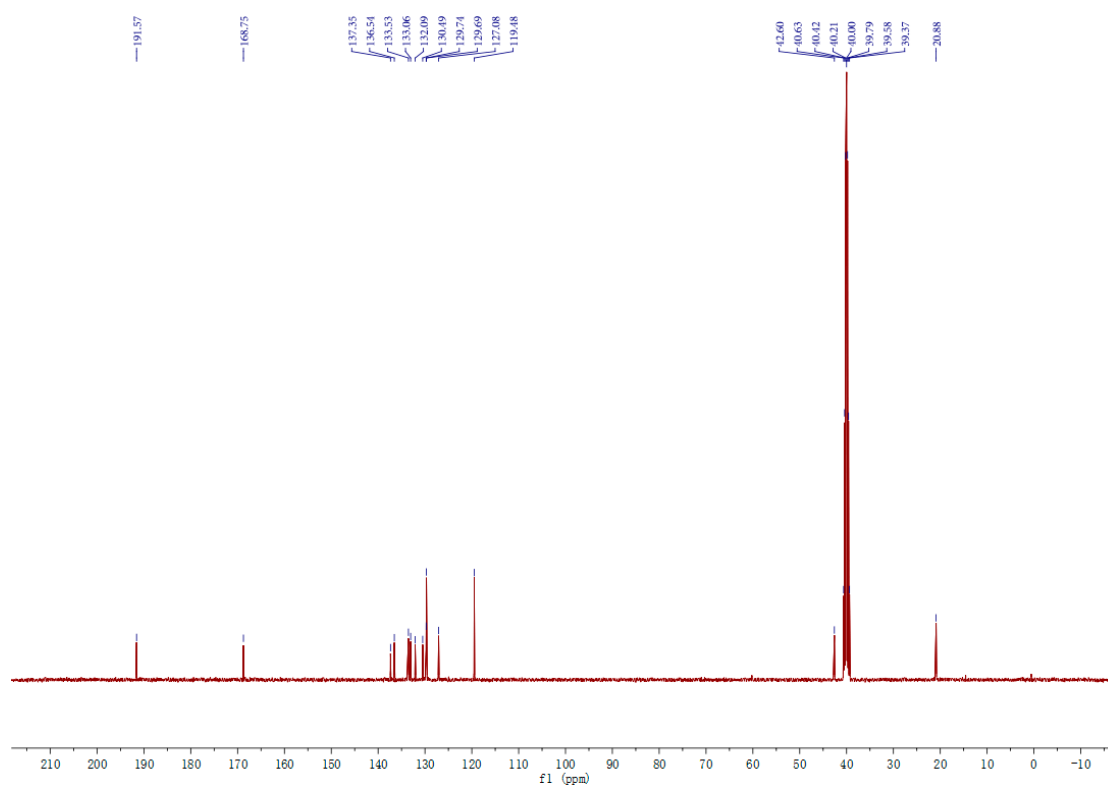
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4.82e5



HRMS of compound 3c

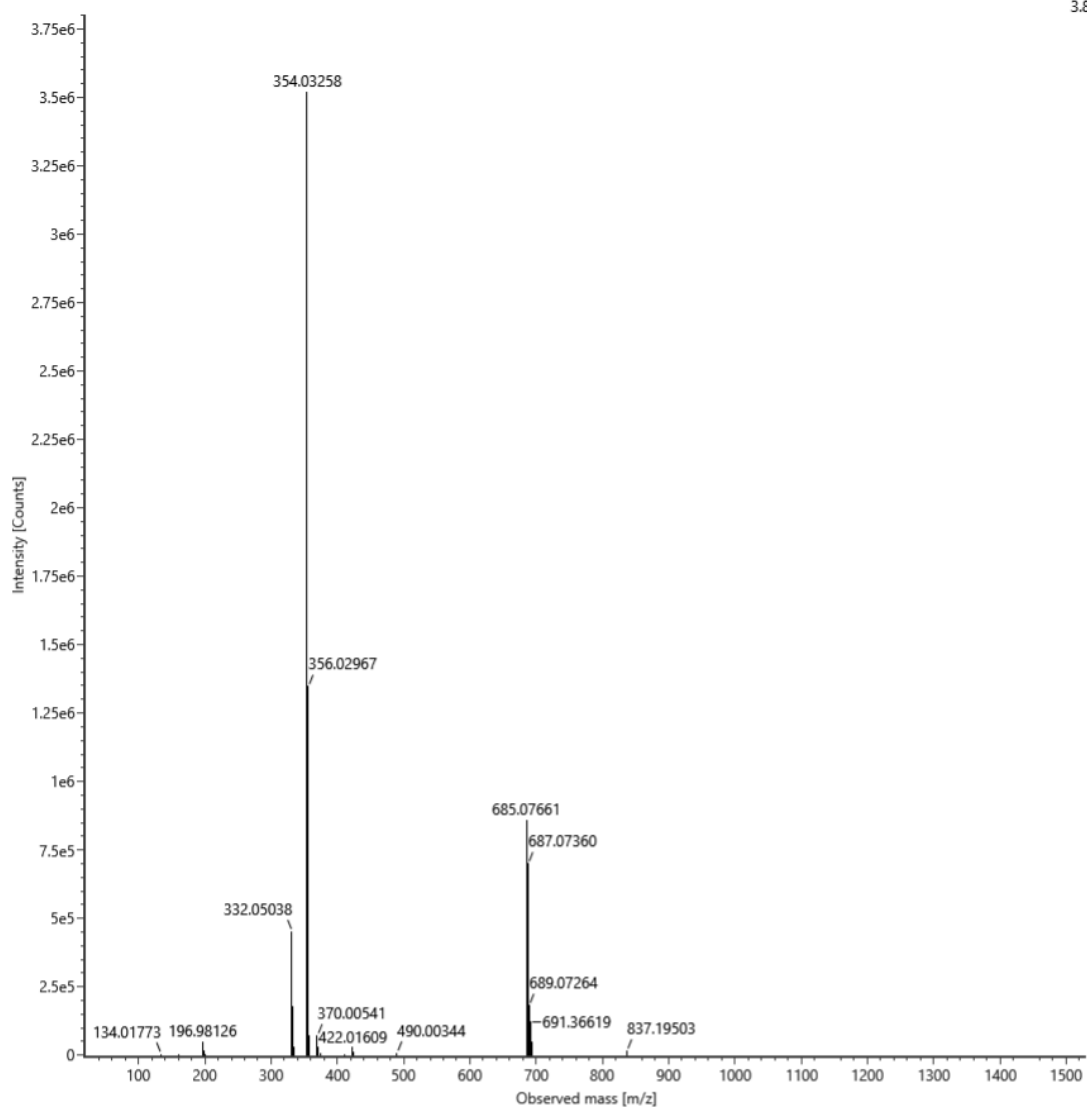
<sup>1</sup>H NMR of compound 3d<sup>13</sup>C NMR of compound 3d



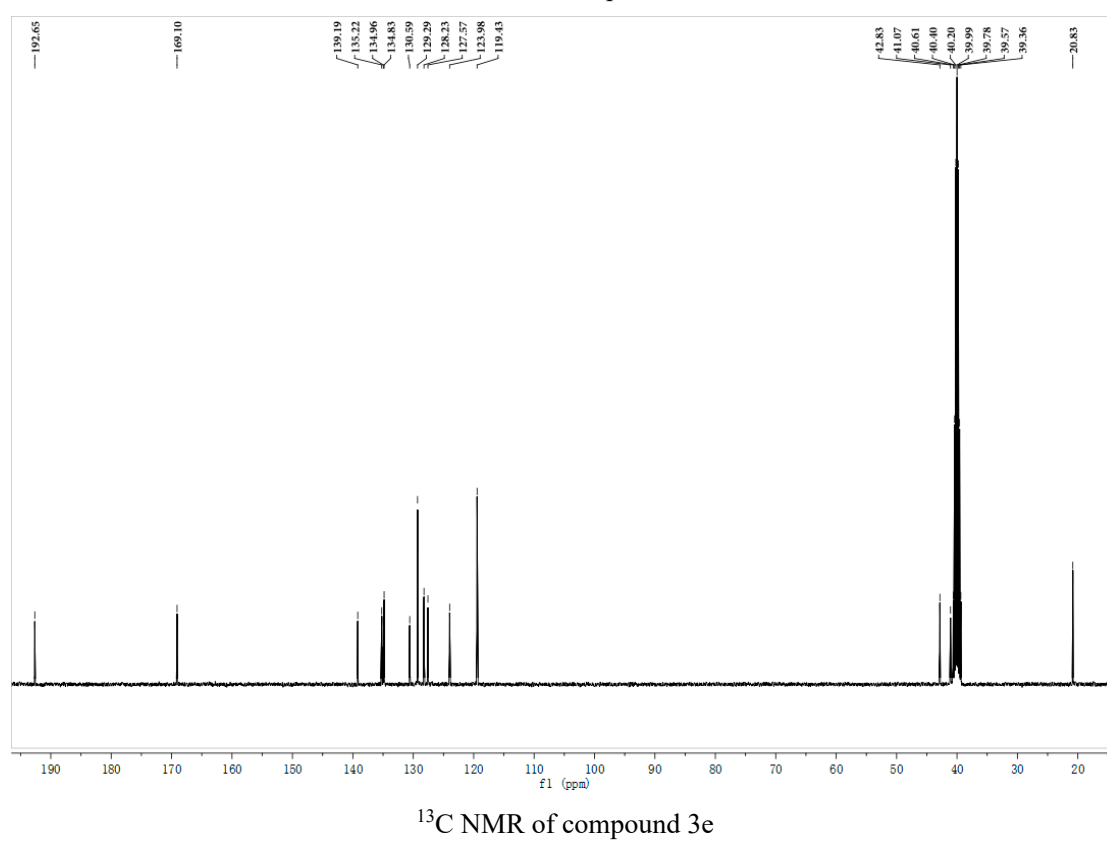
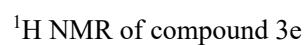
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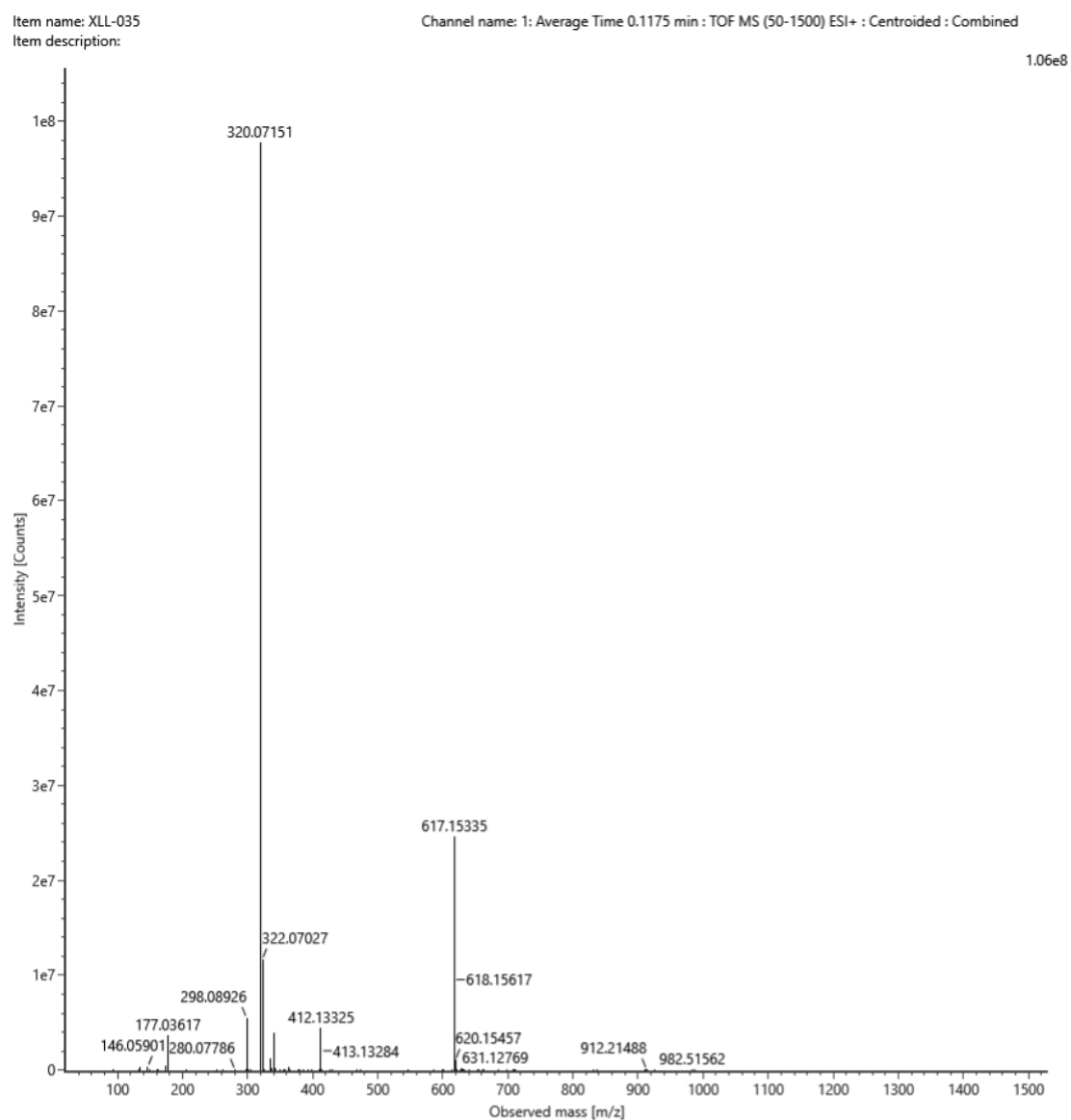
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3.8e6

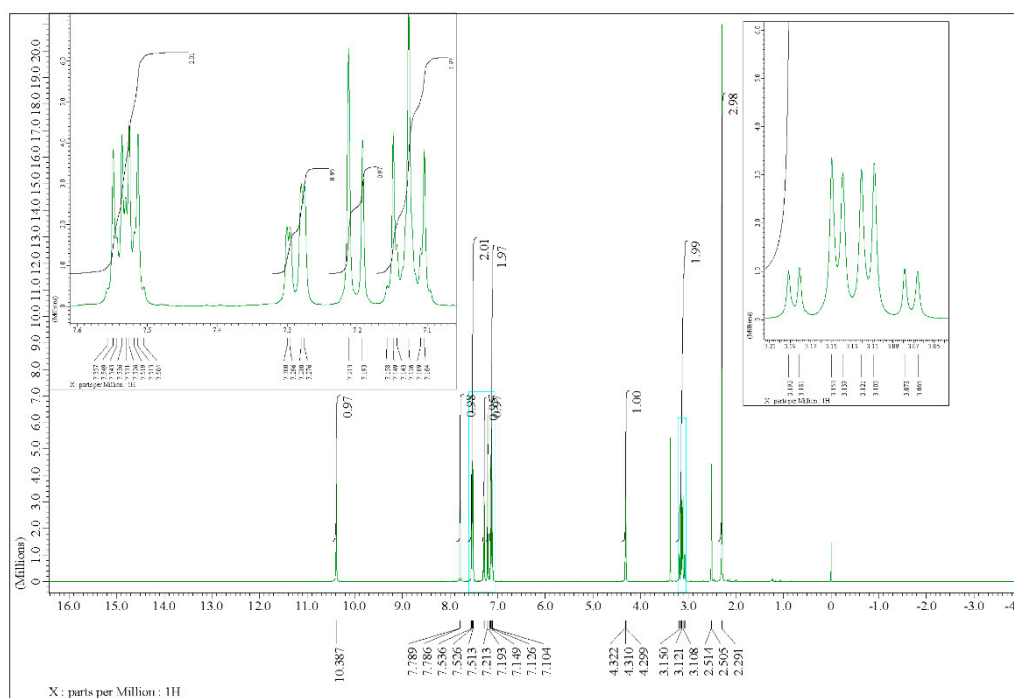
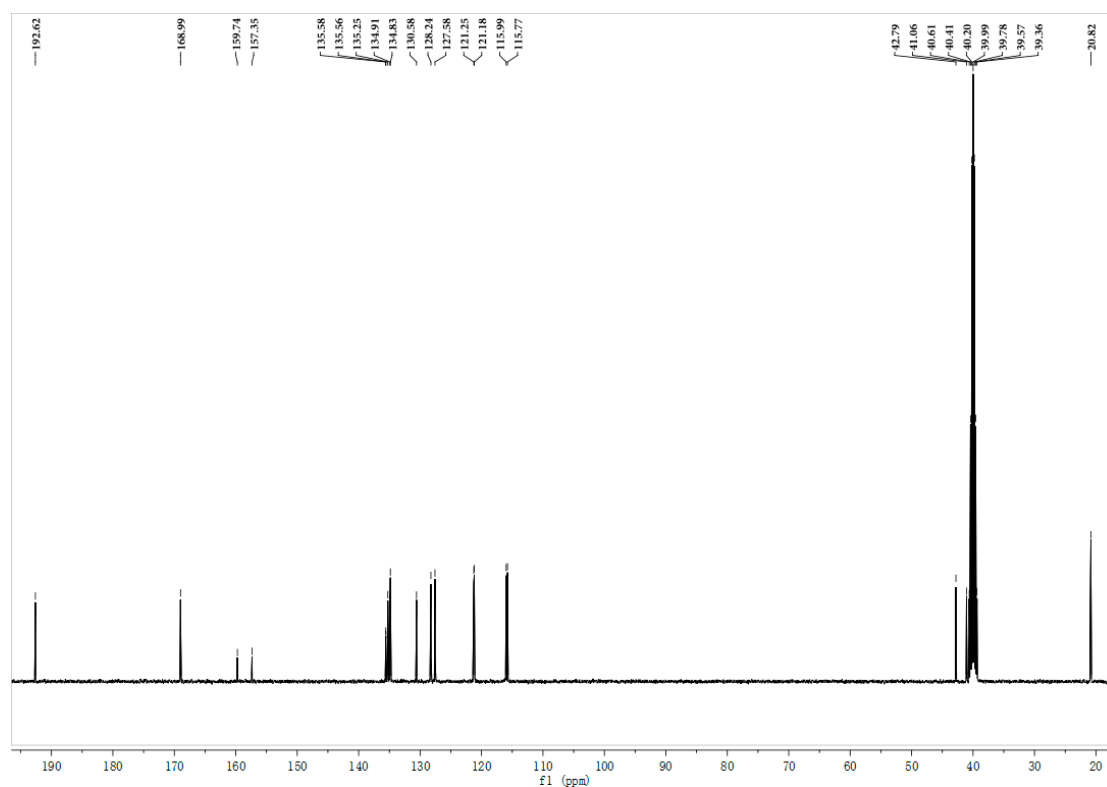


HRMS of compound 3d





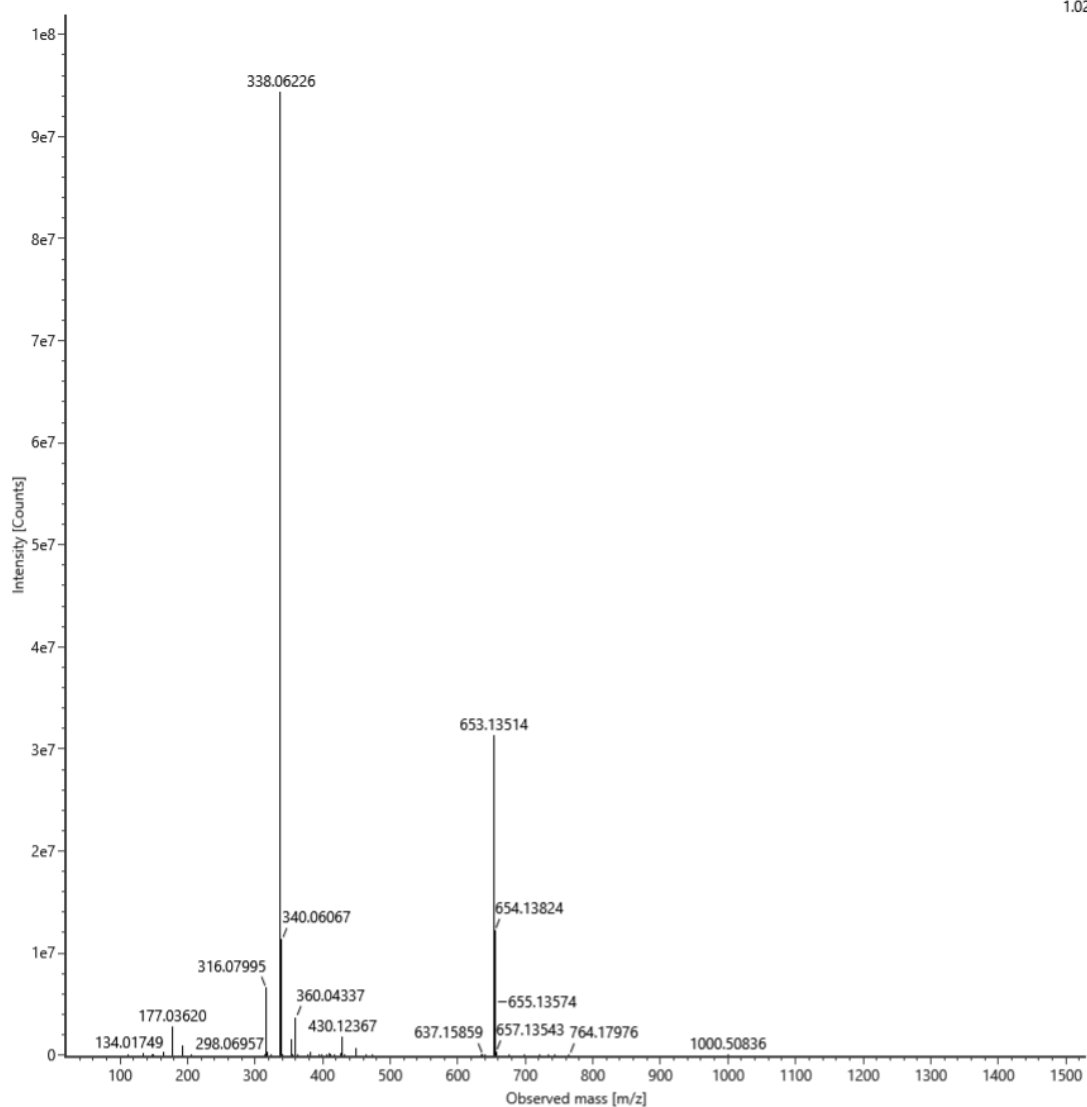
HRMS of compound 3e

<sup>1</sup>H NMR of compound 3f<sup>13</sup>C NMR of compound 3f

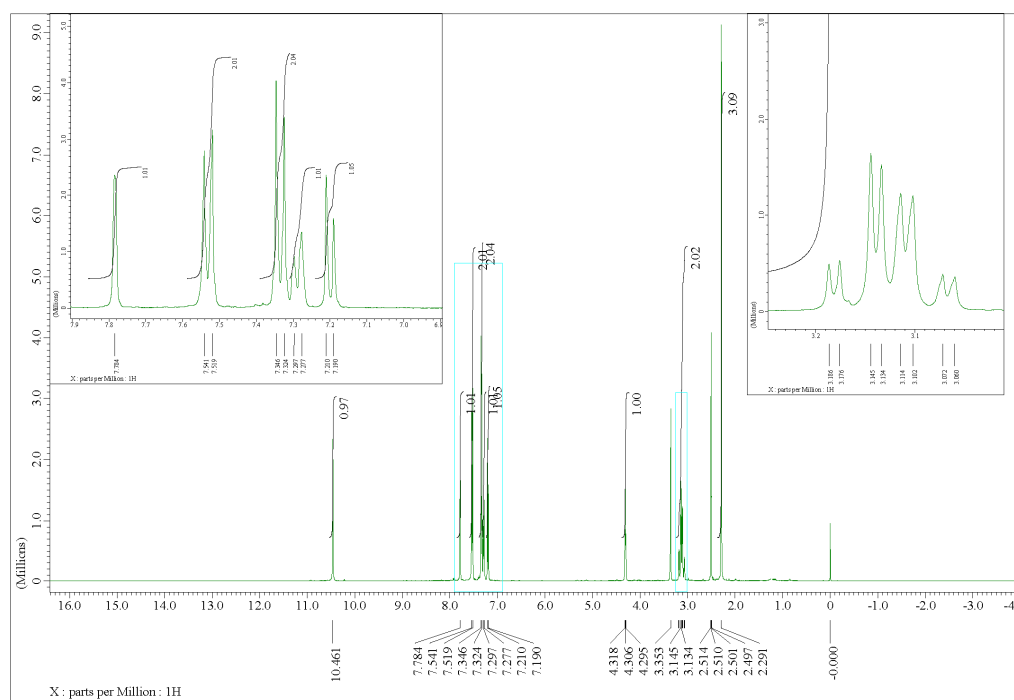
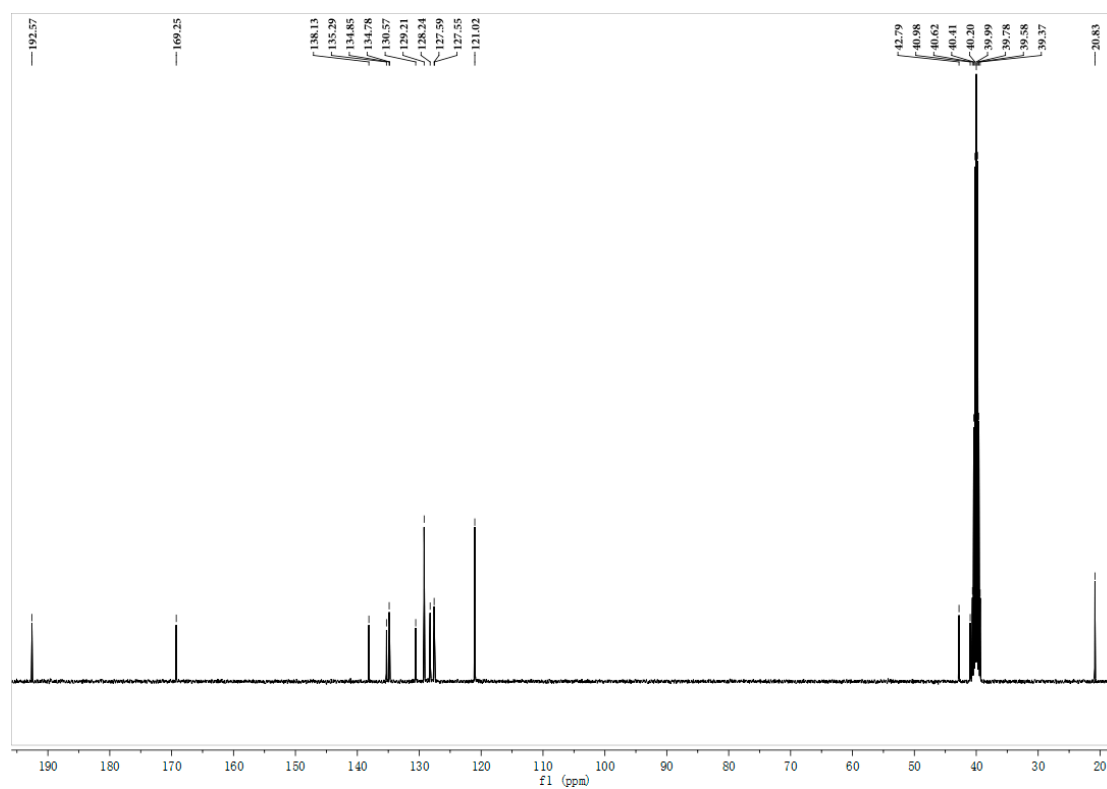
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1.02e8



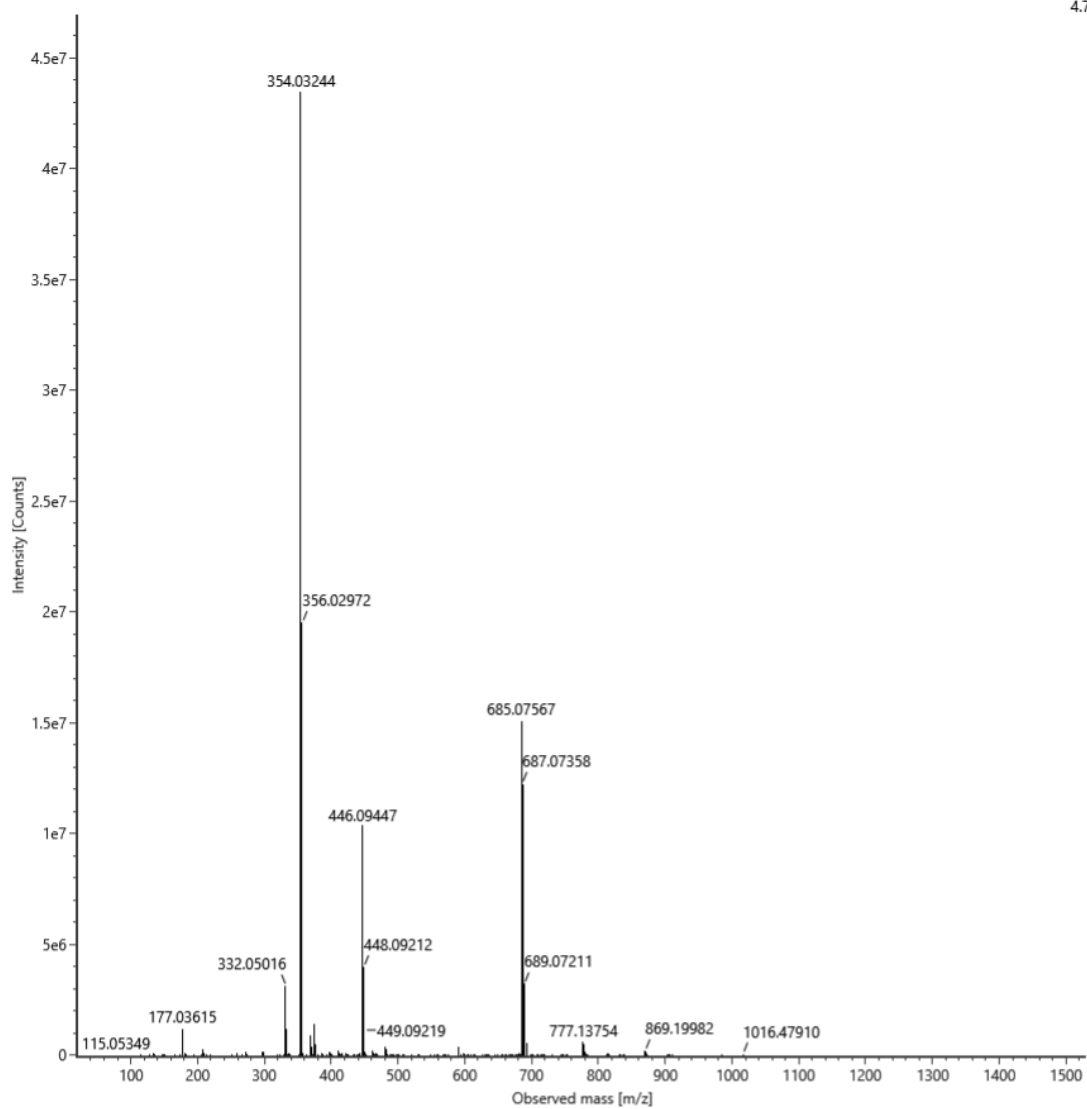
HRMS of compound 3f

<sup>1</sup>H NMR of compound 3g<sup>13</sup>C NMR of compound 3g

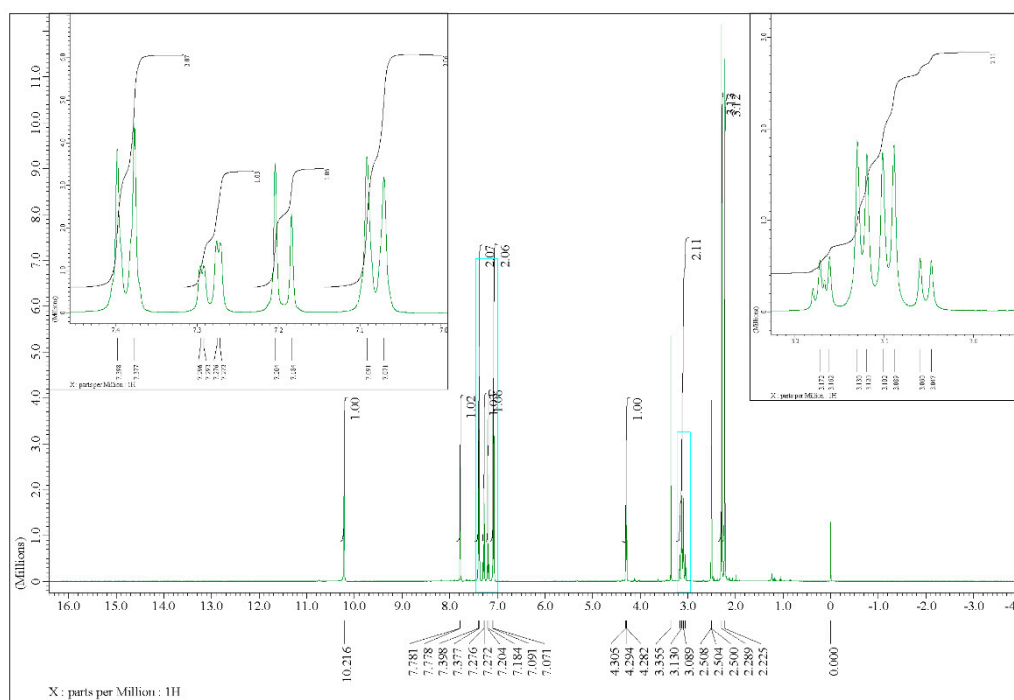
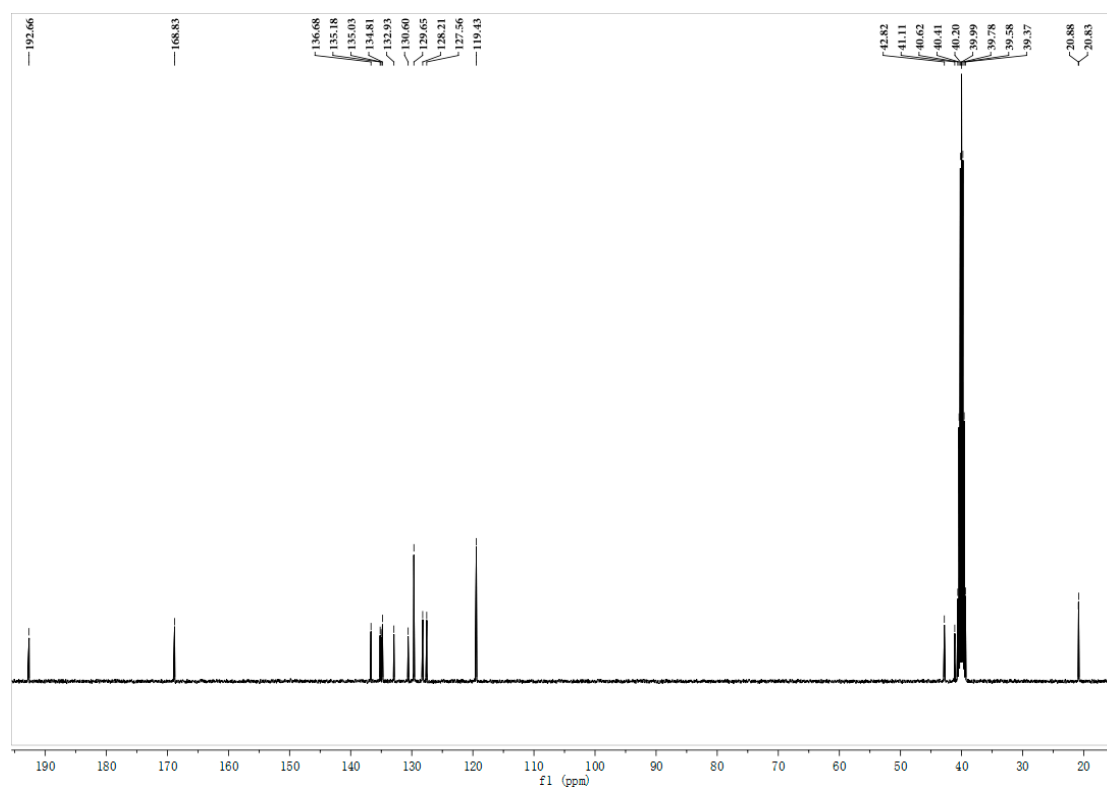
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4.7e7



HRMS of compound 3g

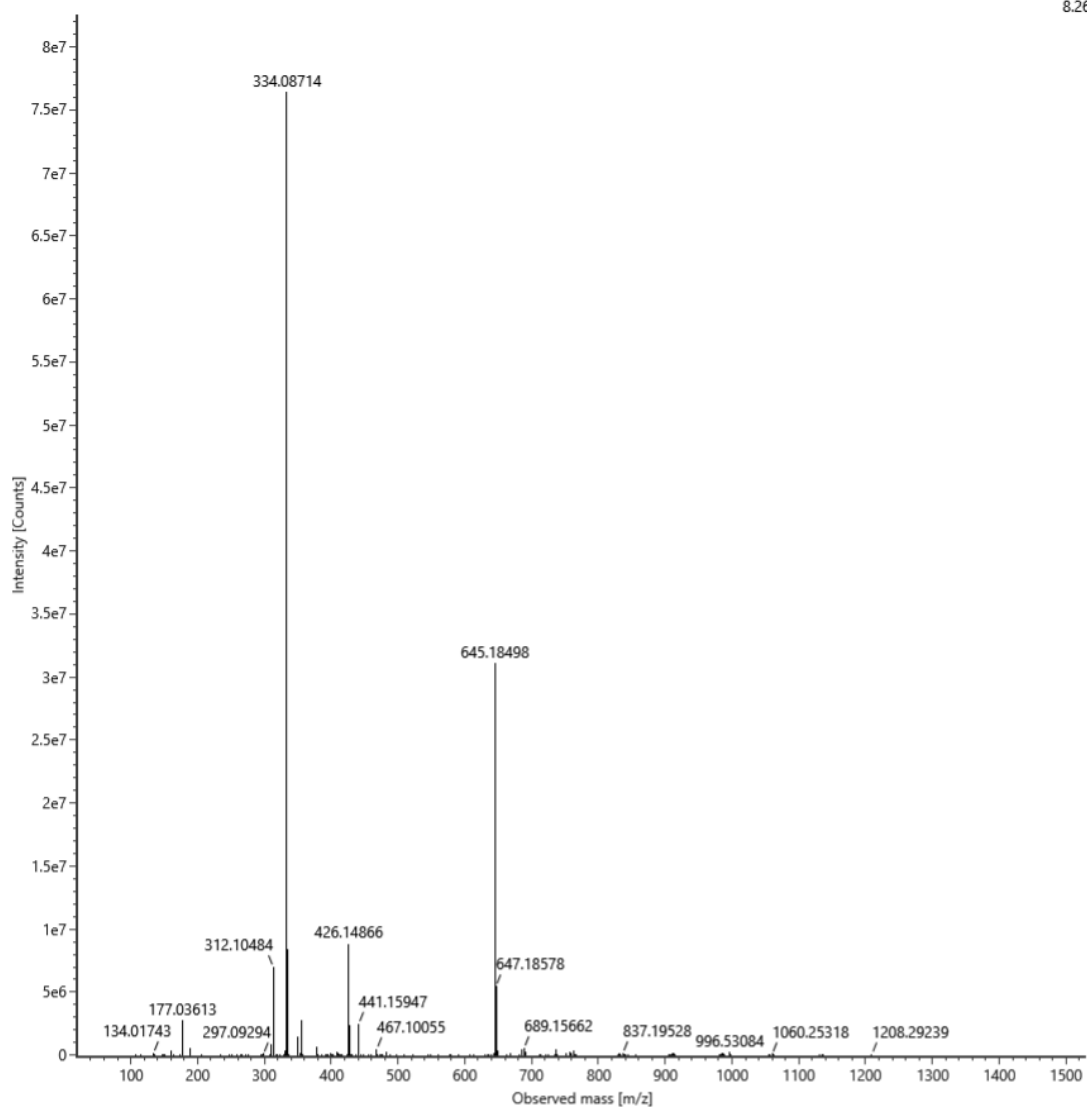
<sup>1</sup>H NMR of compound 3h<sup>13</sup>C NMR of compound 3h



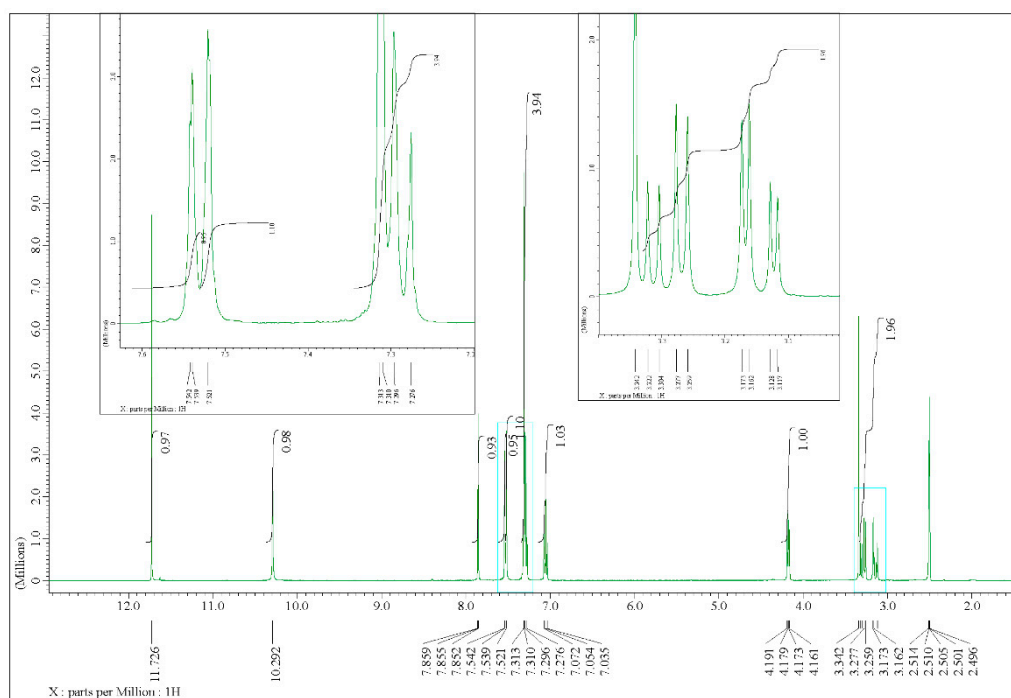
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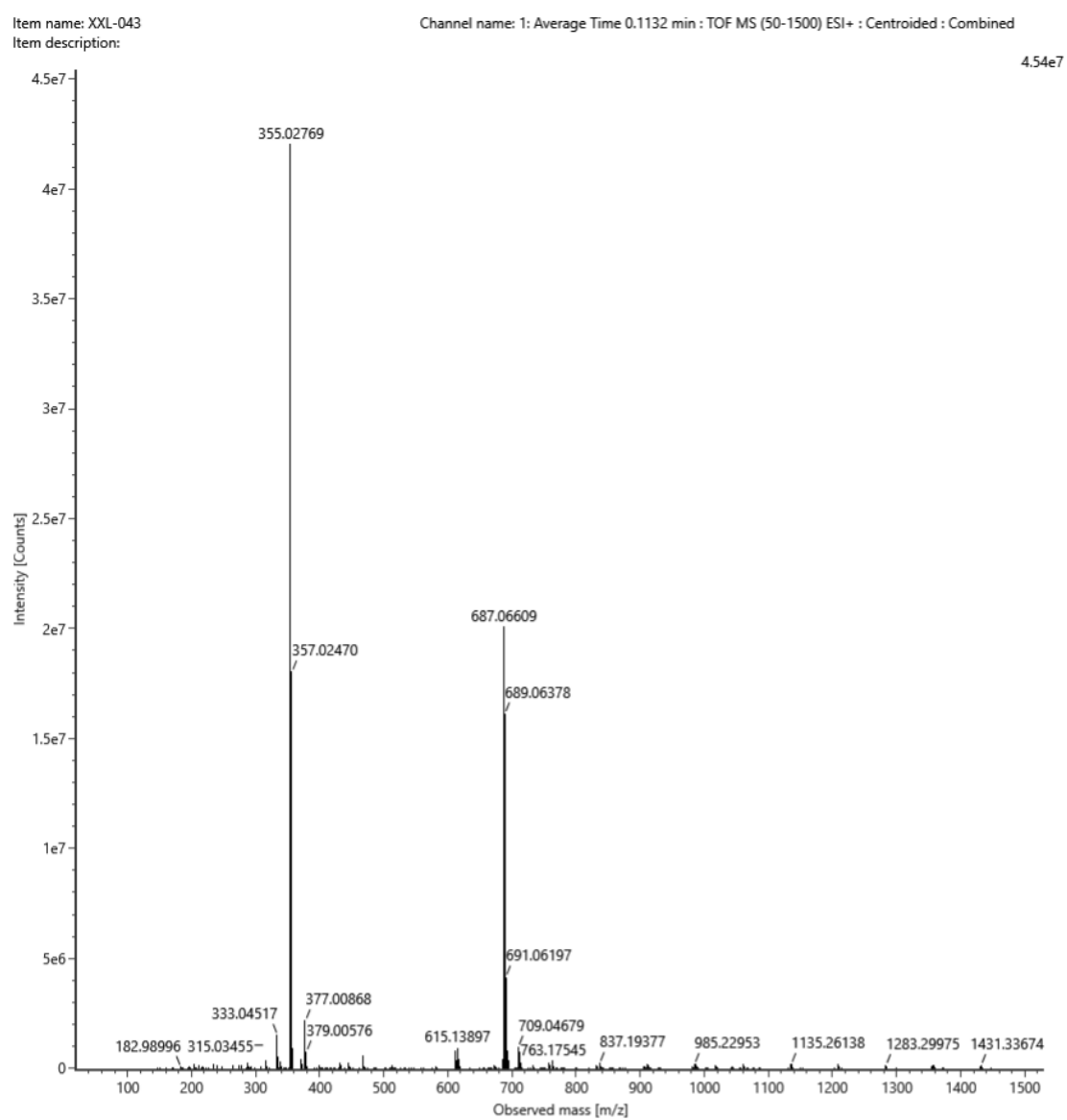
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8.26e7

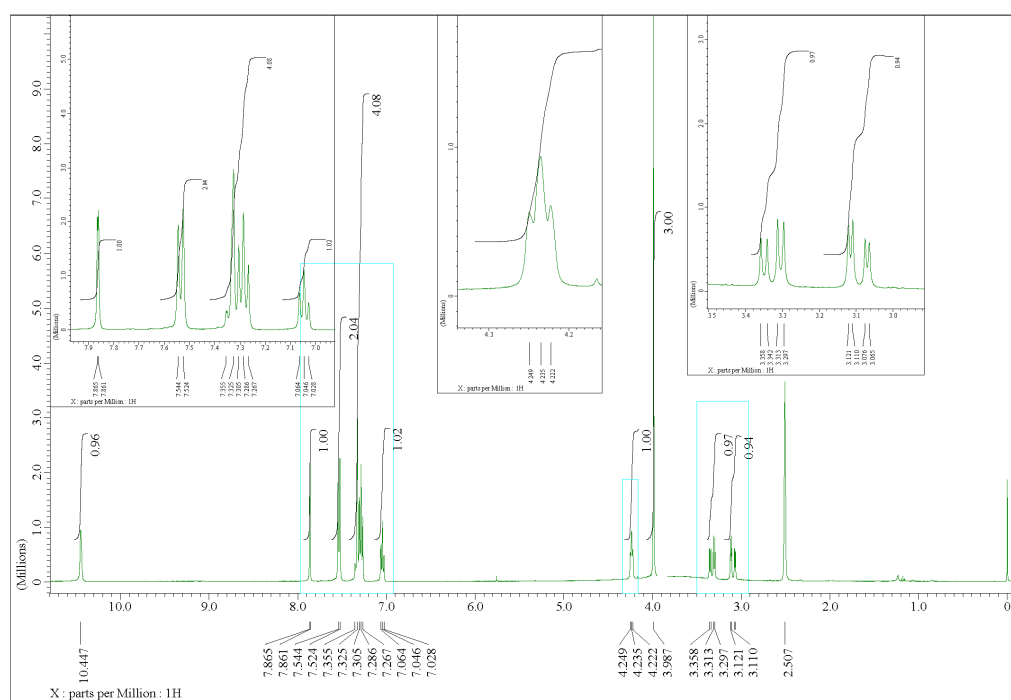
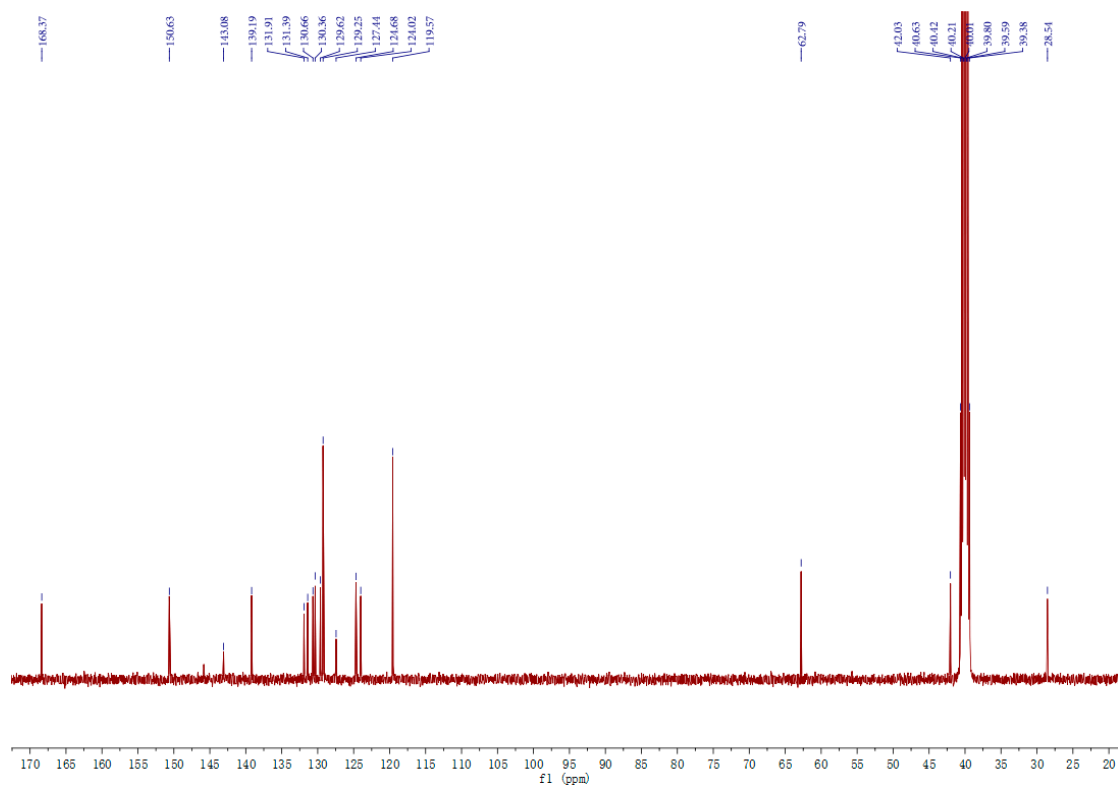


HRMS of compound 3h





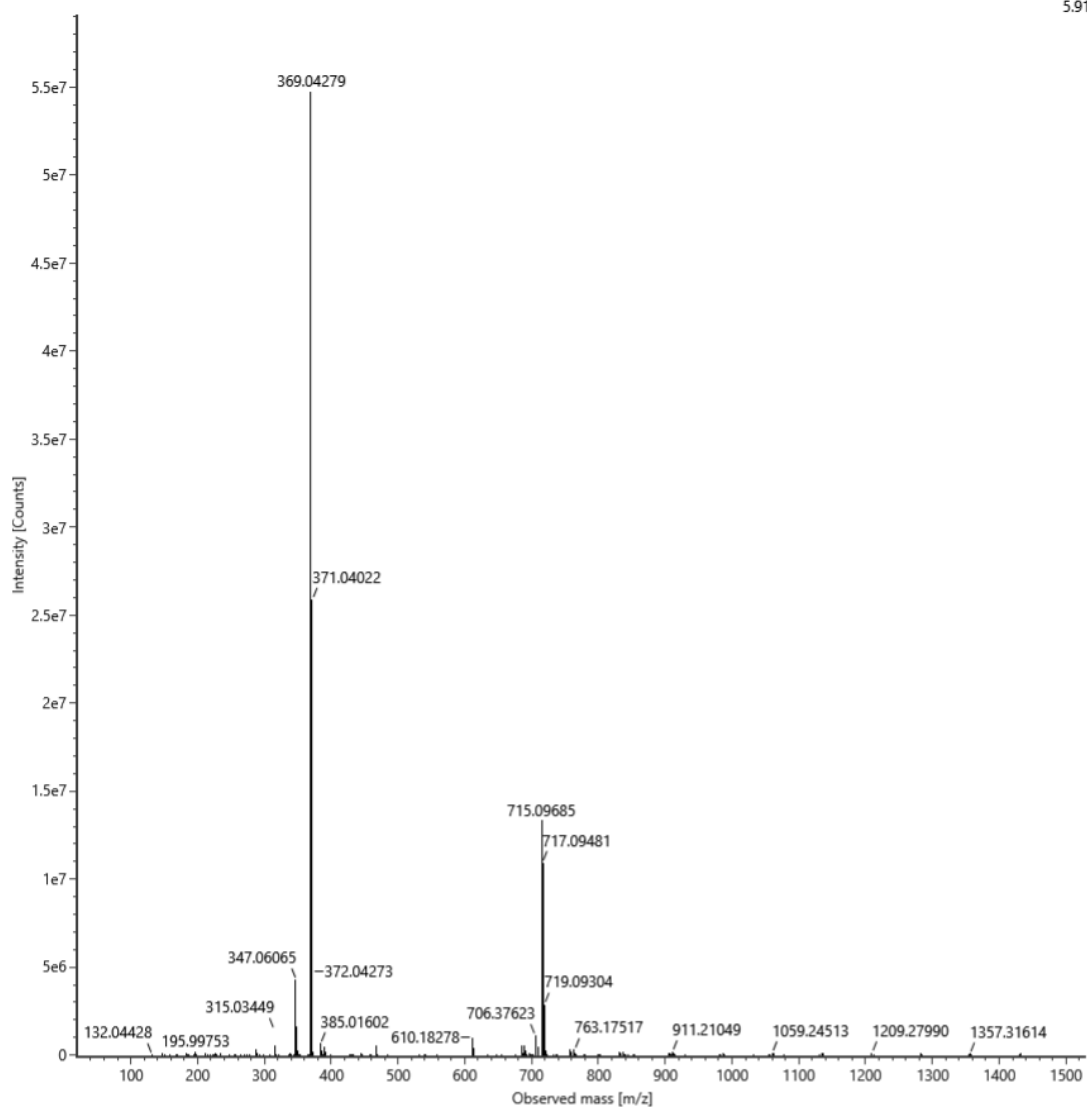
HRMS of compound 4a

 $^1\text{H}$  NMR of compound 4b $^{13}\text{C}$  NMR of compound 4b

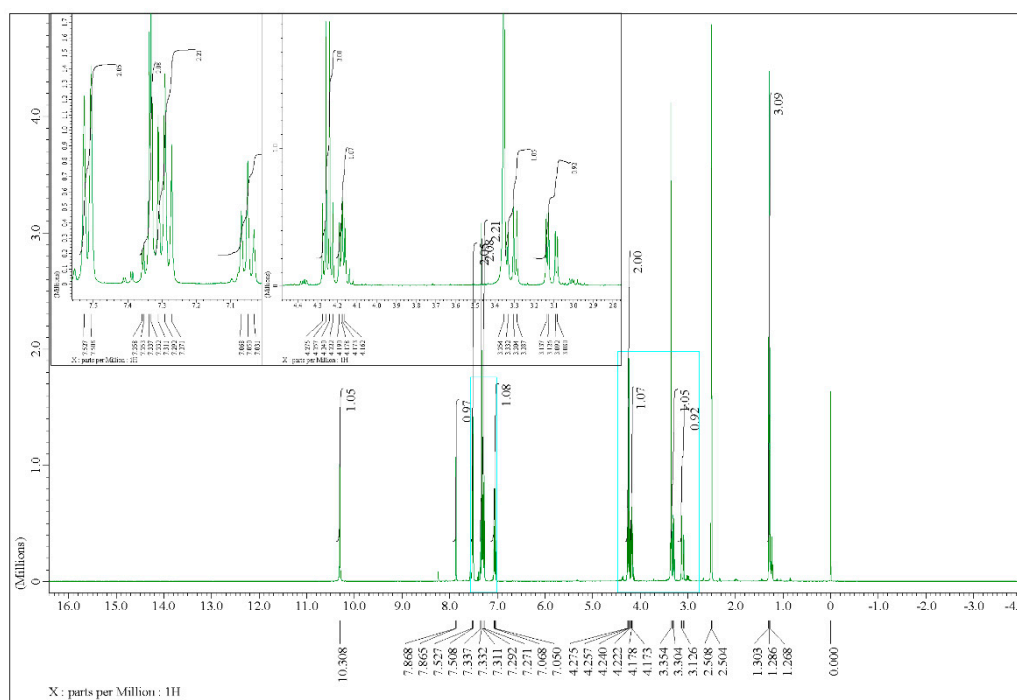
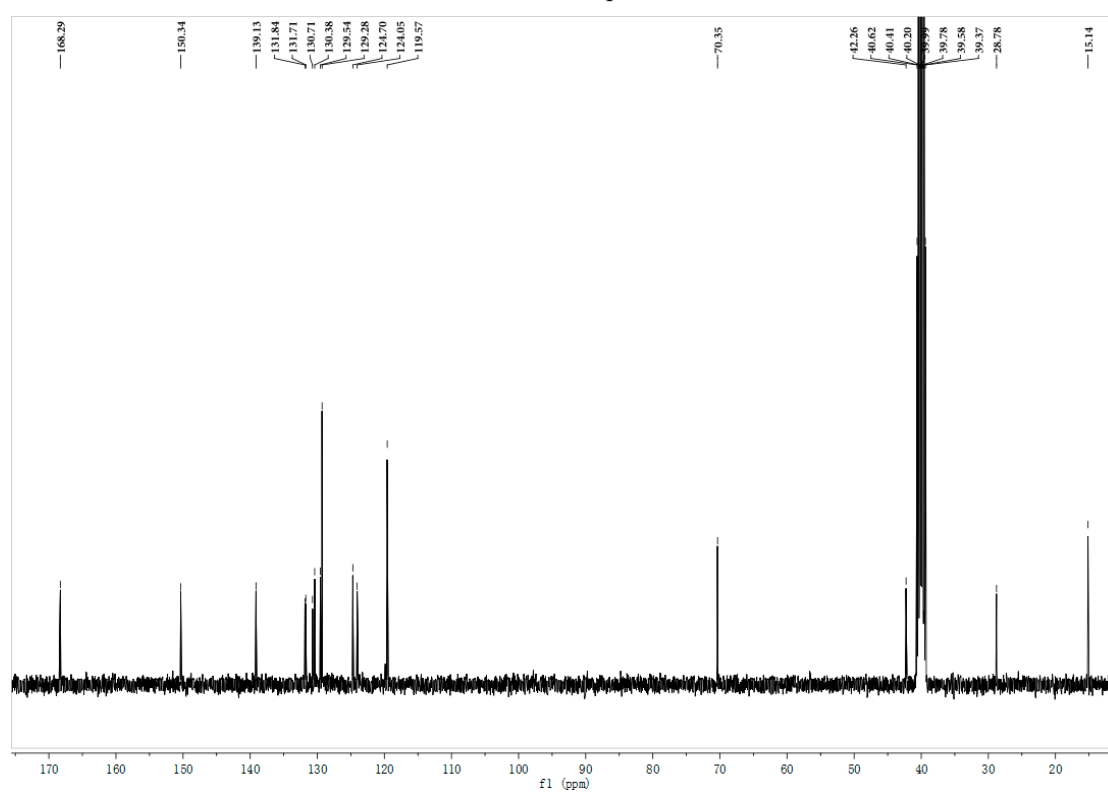
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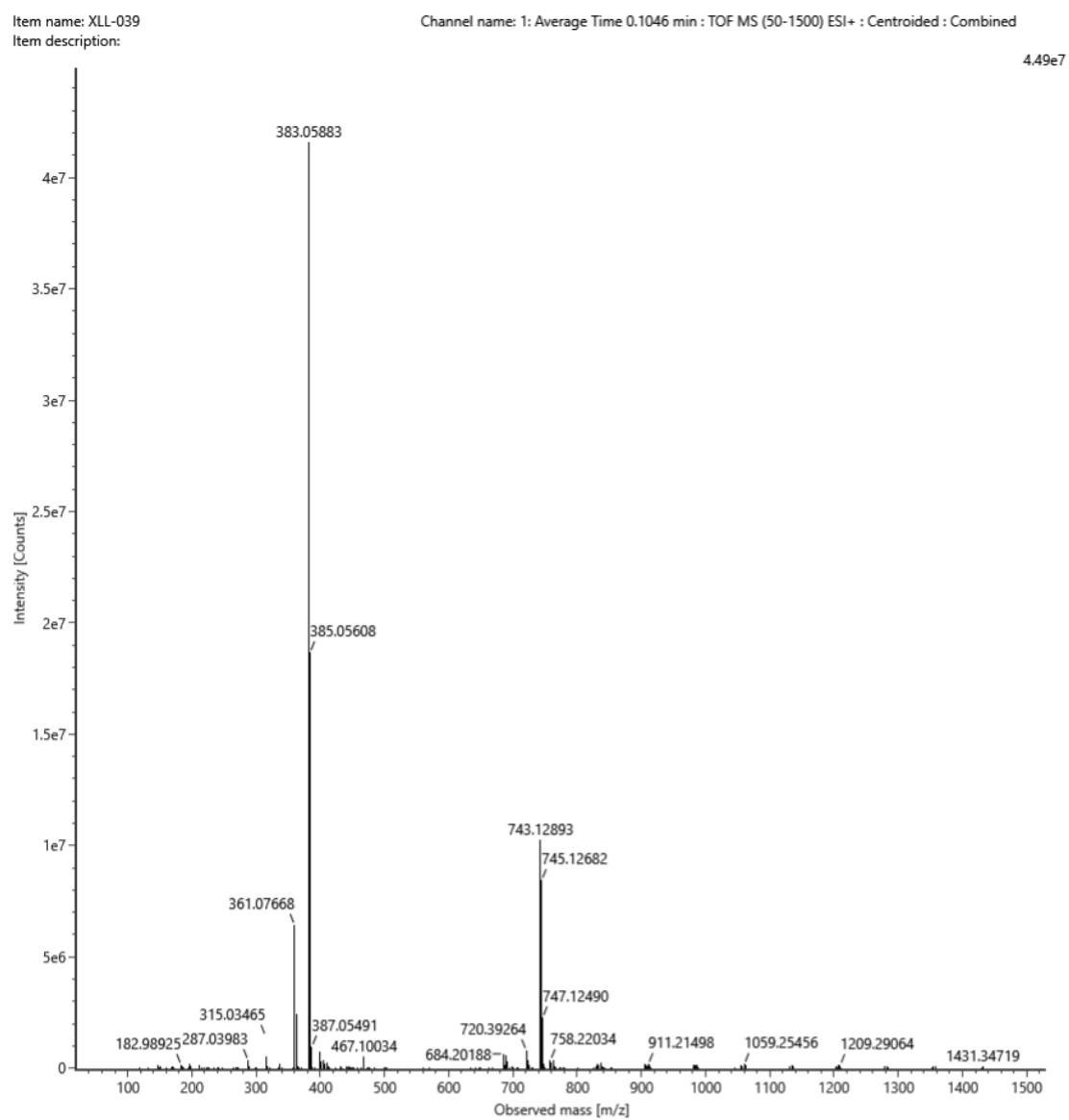
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5.91e7

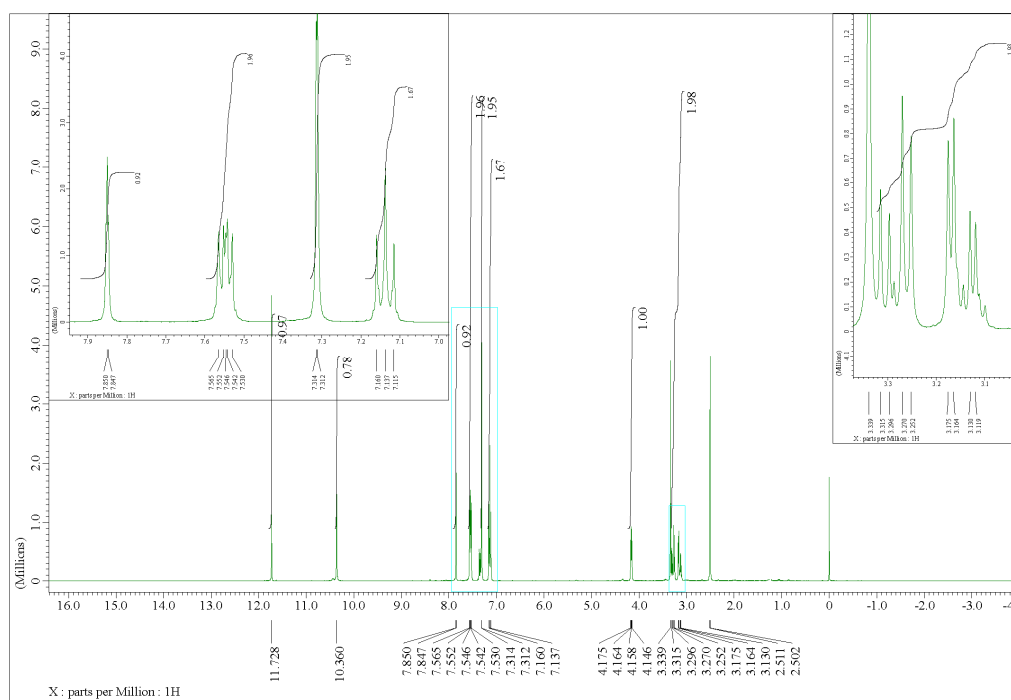
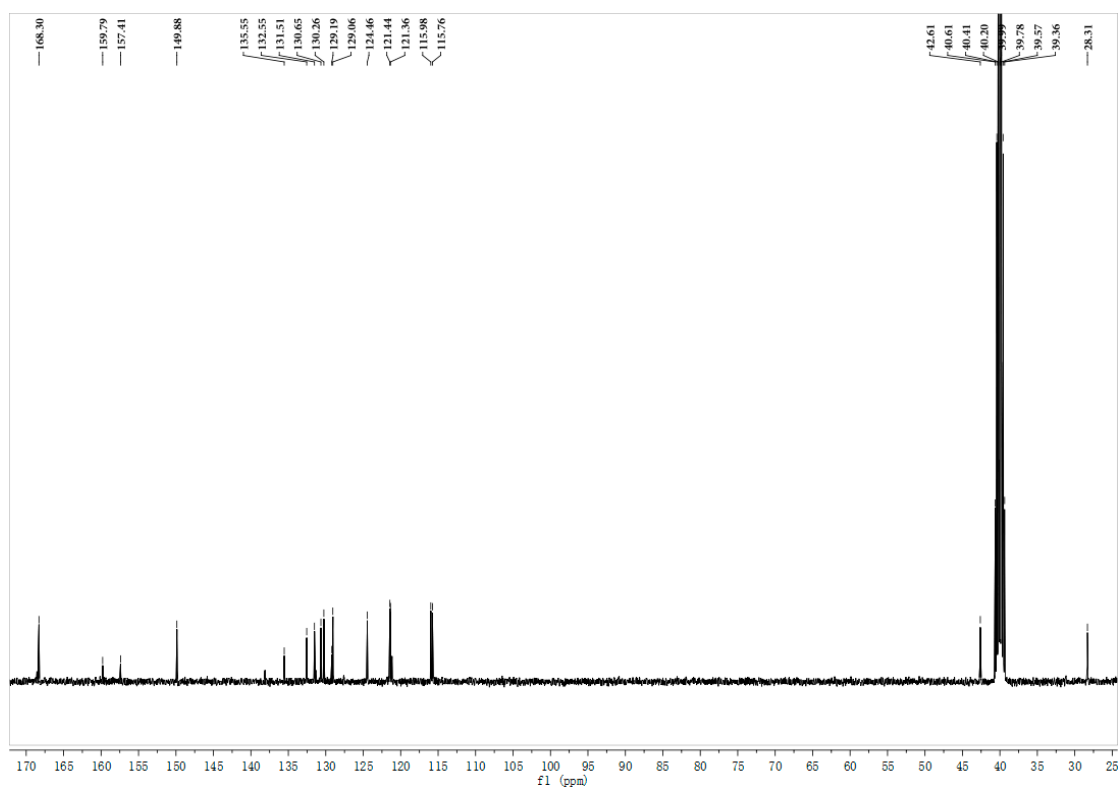


HRMS of compound 4b

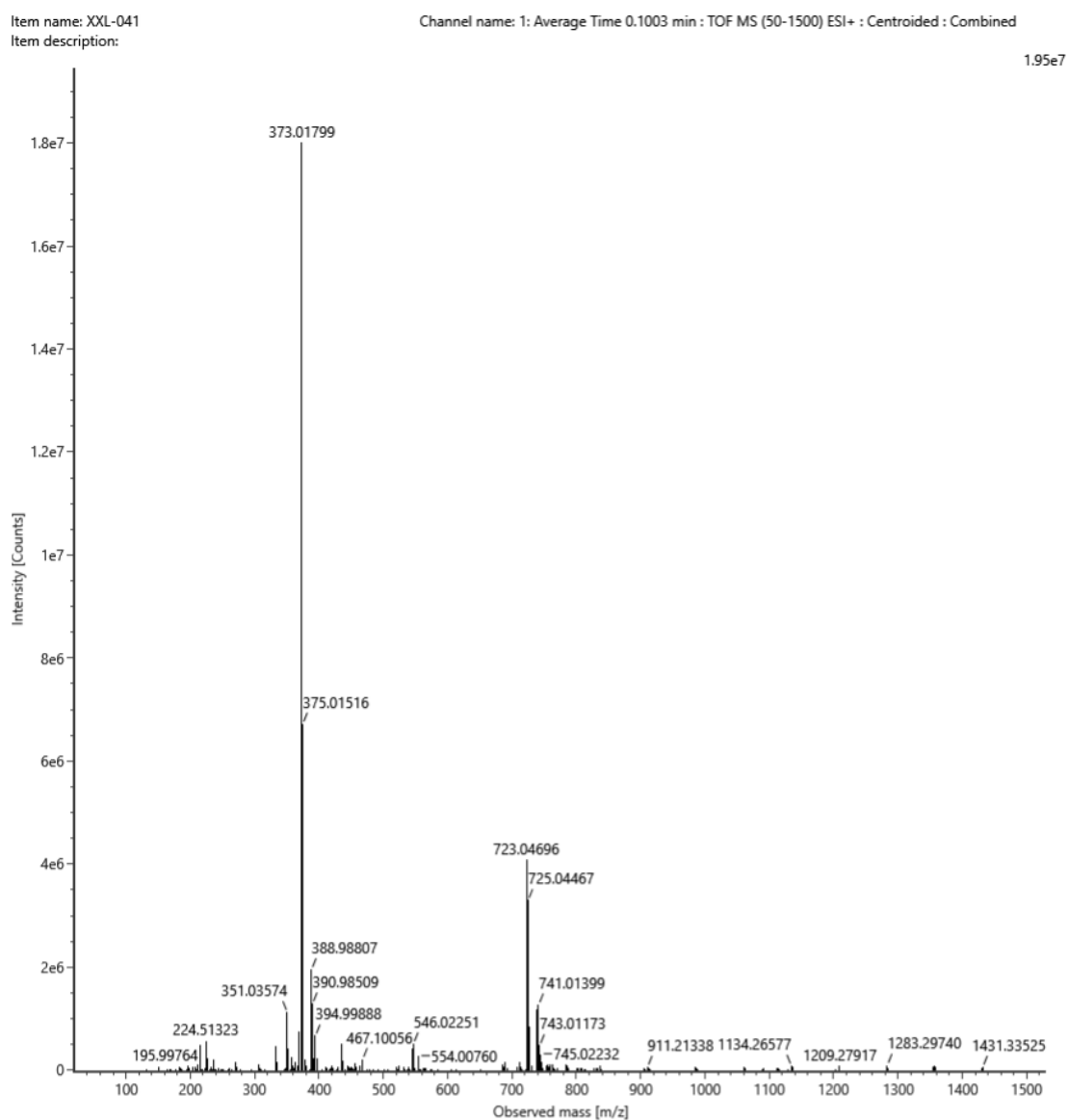
 $^1\text{H}$  NMR of compound 4c $^{13}\text{C}$  NMR of compound 4c



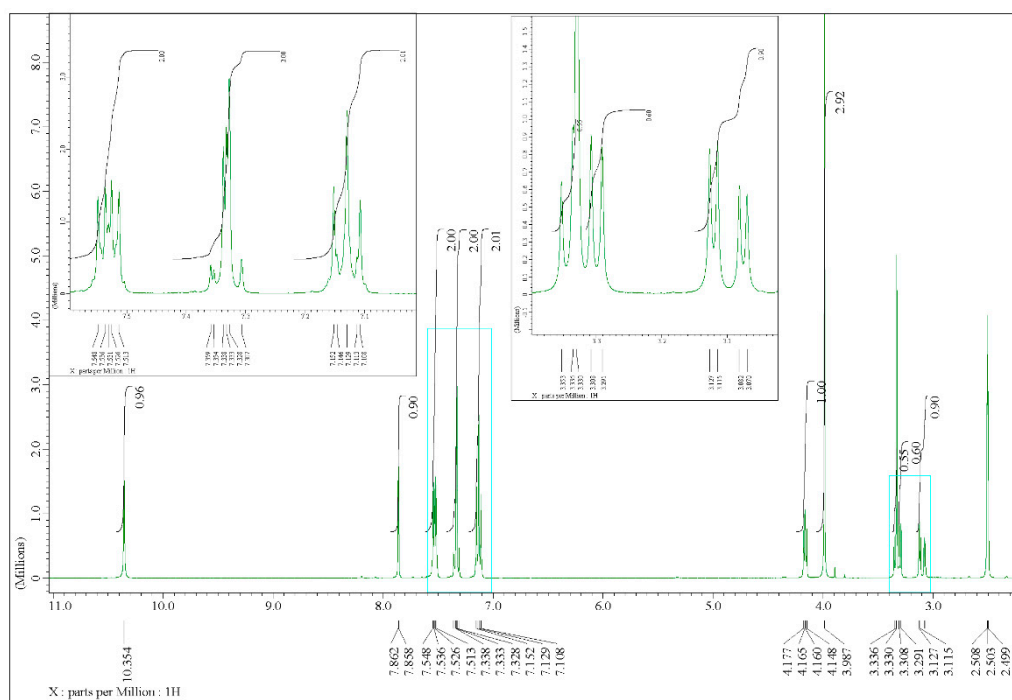
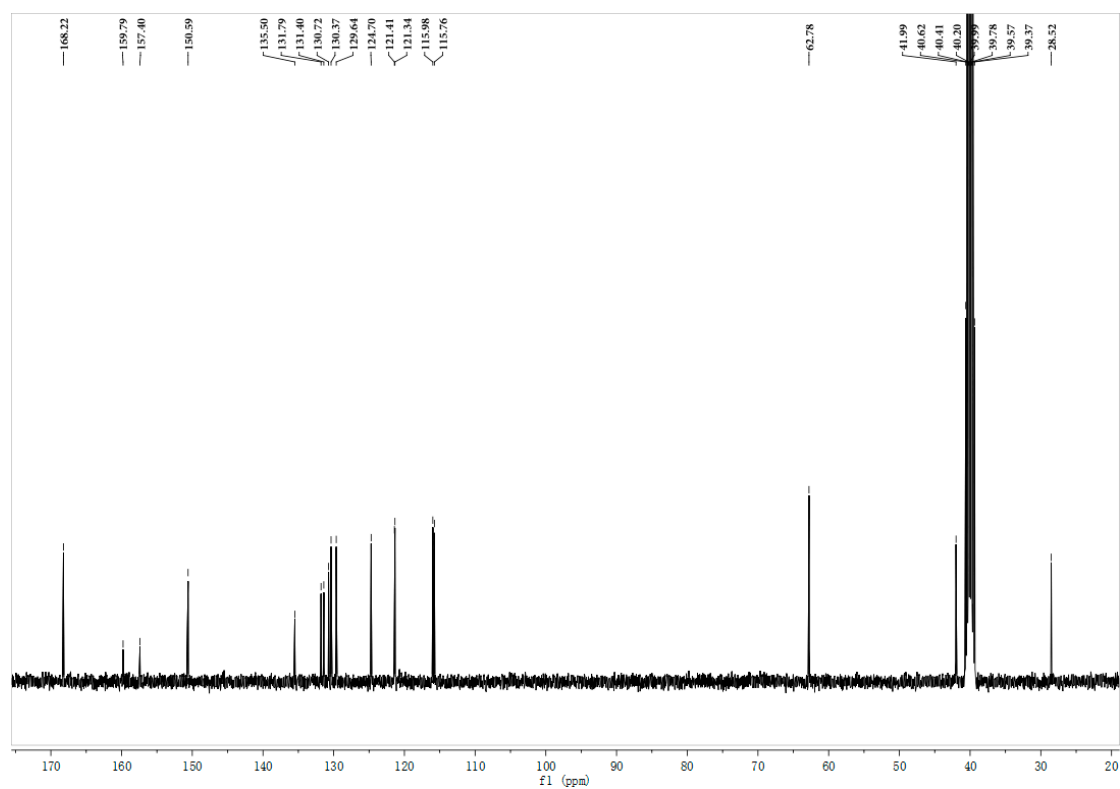
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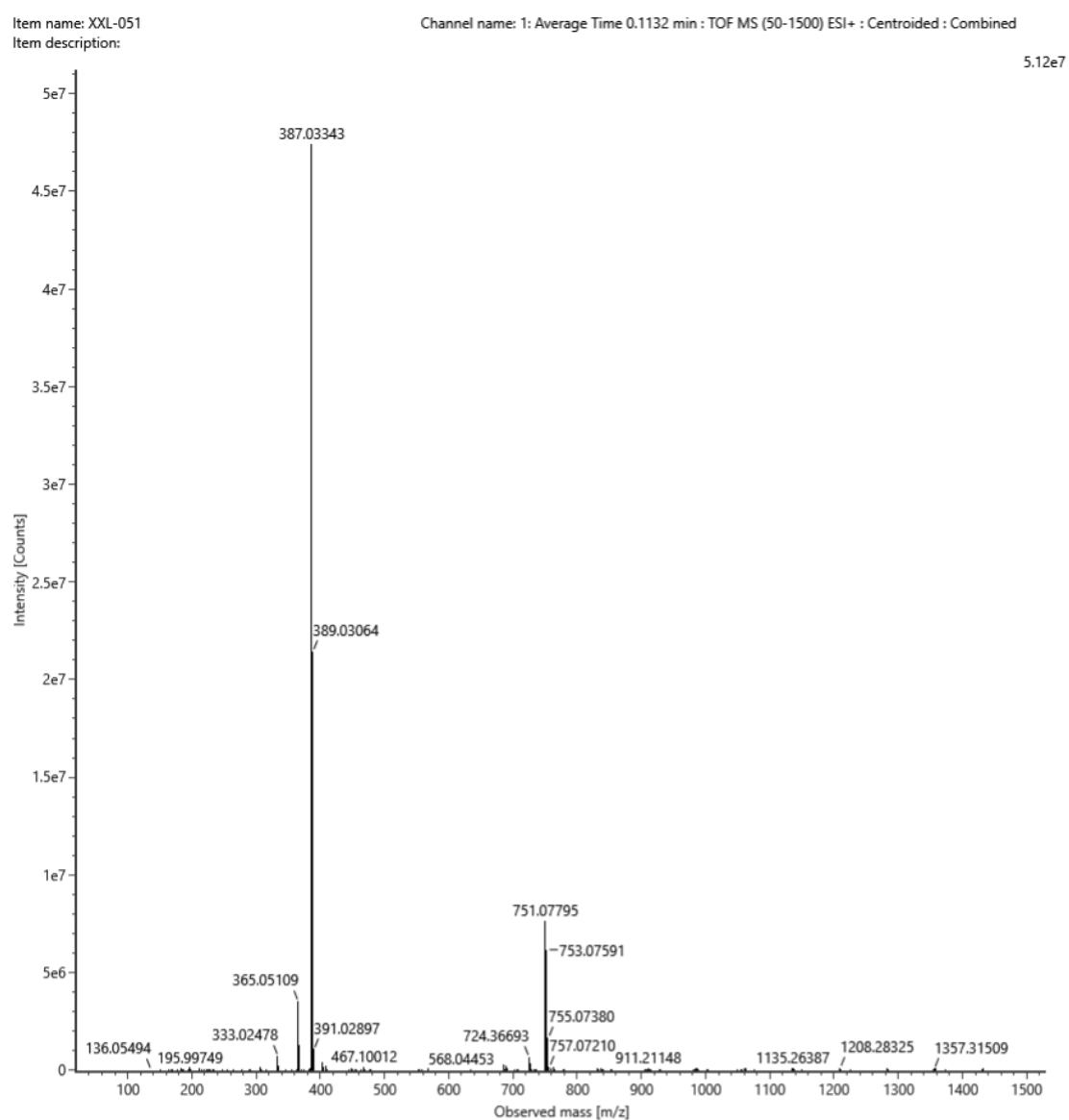
<sup>1</sup>H NMR of compound 4d<sup>13</sup>C NMR of compound 4d



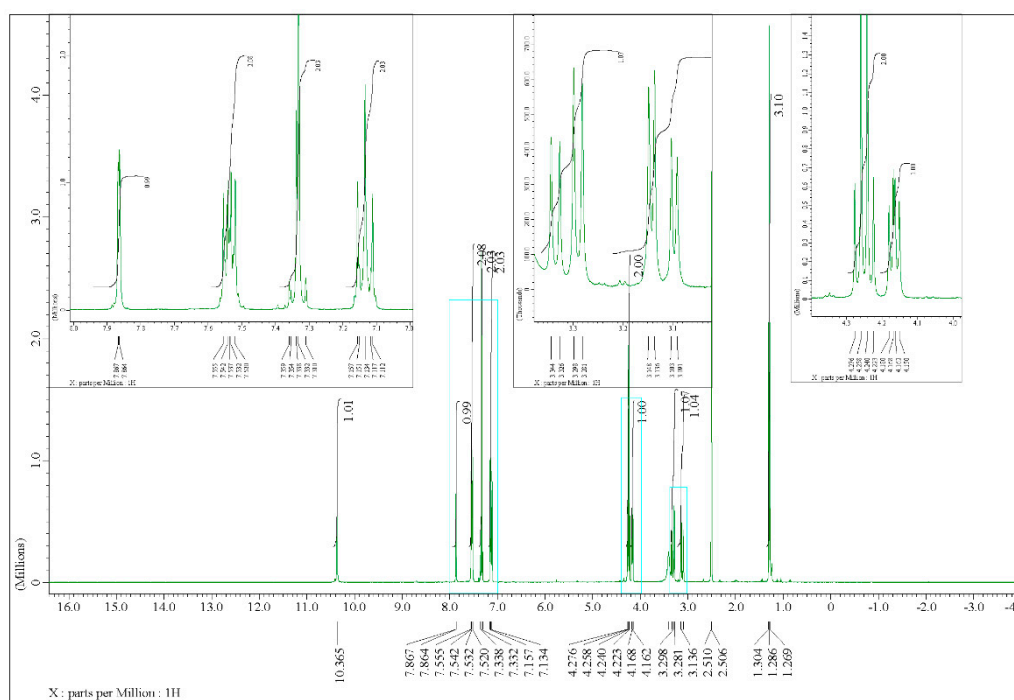
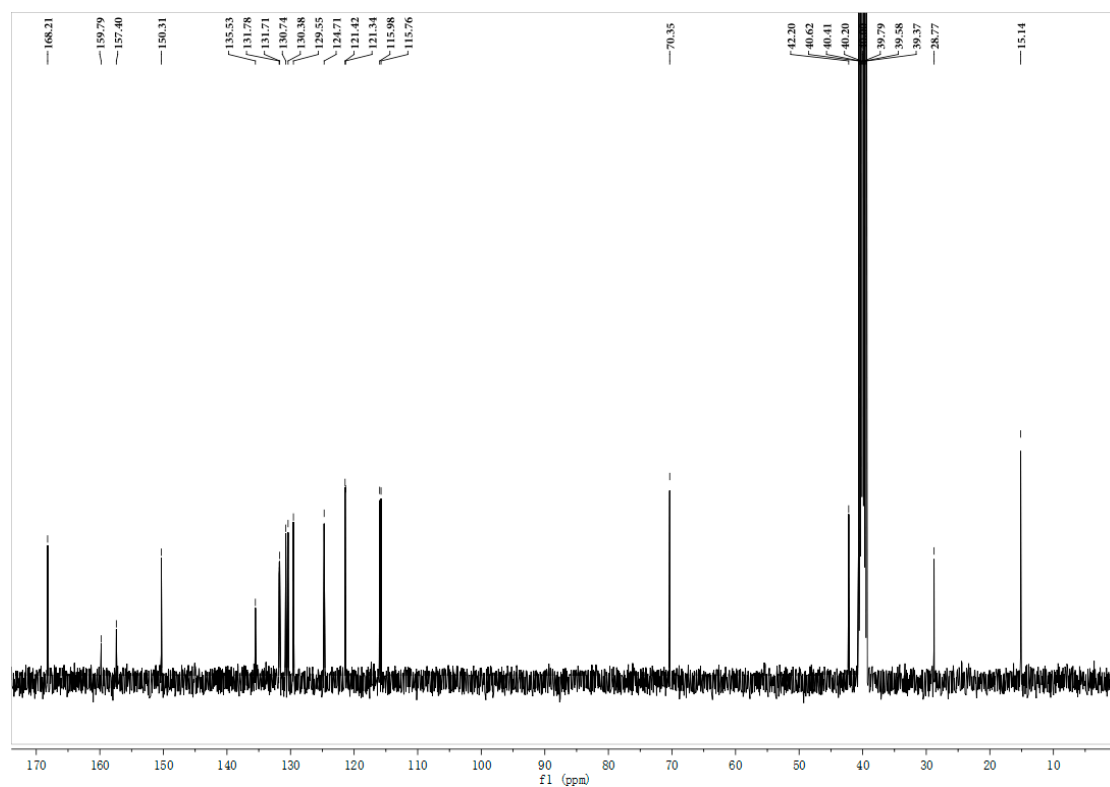


HRMS of compound 4d

 $^1\text{H}$  NMR of compound 4e $^{13}\text{C}$  NMR of compound 4e



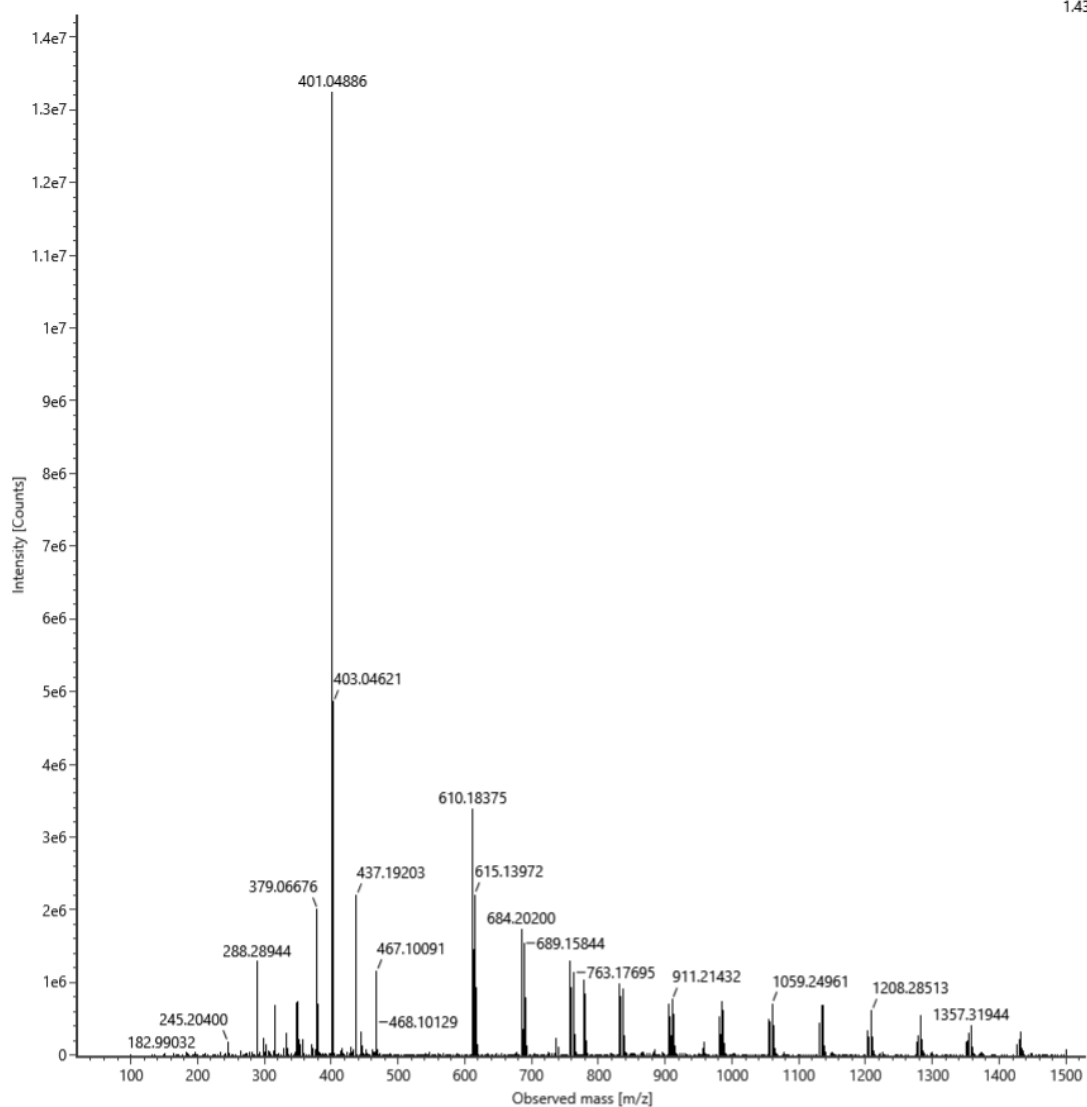
HRMS of compound 4e

 $^1\text{H}$  NMR of compound 4f $^{13}\text{C}$  NMR of compound 4f

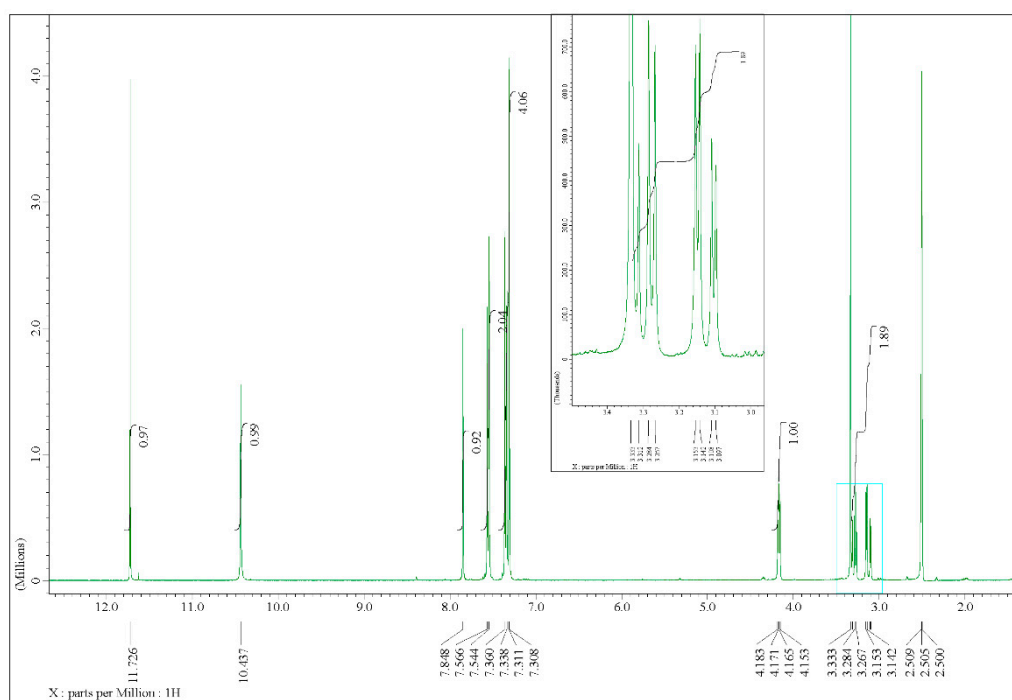
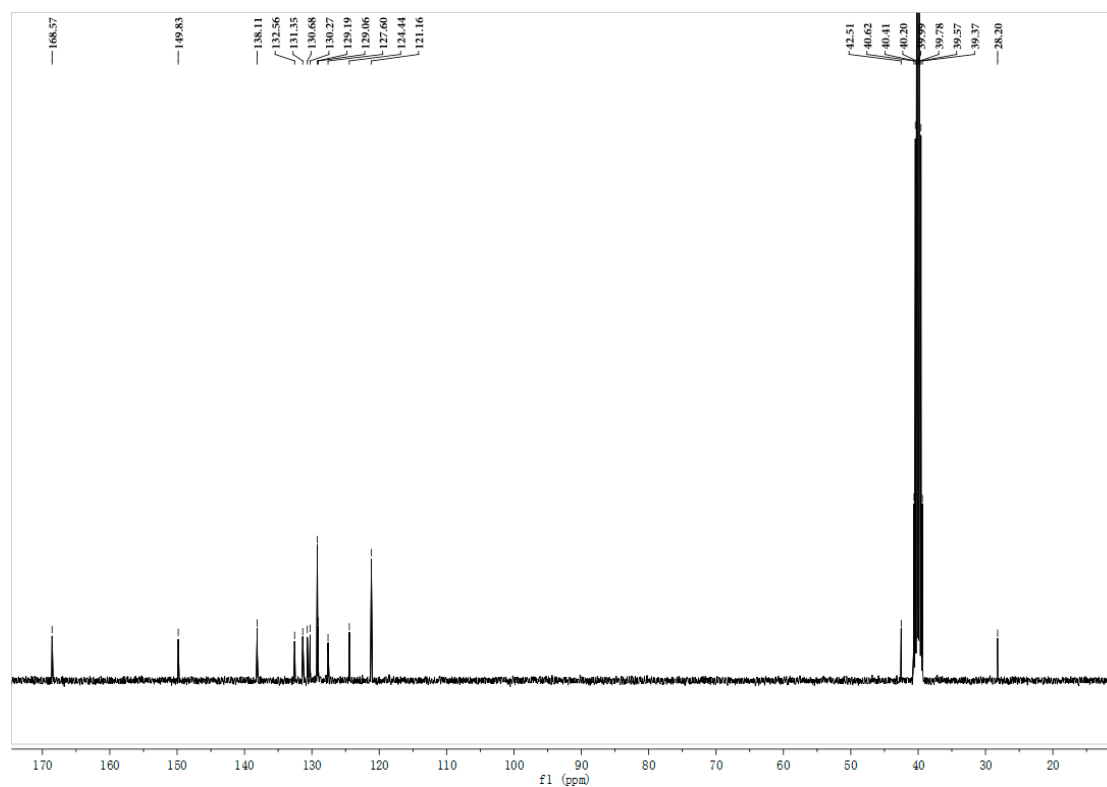
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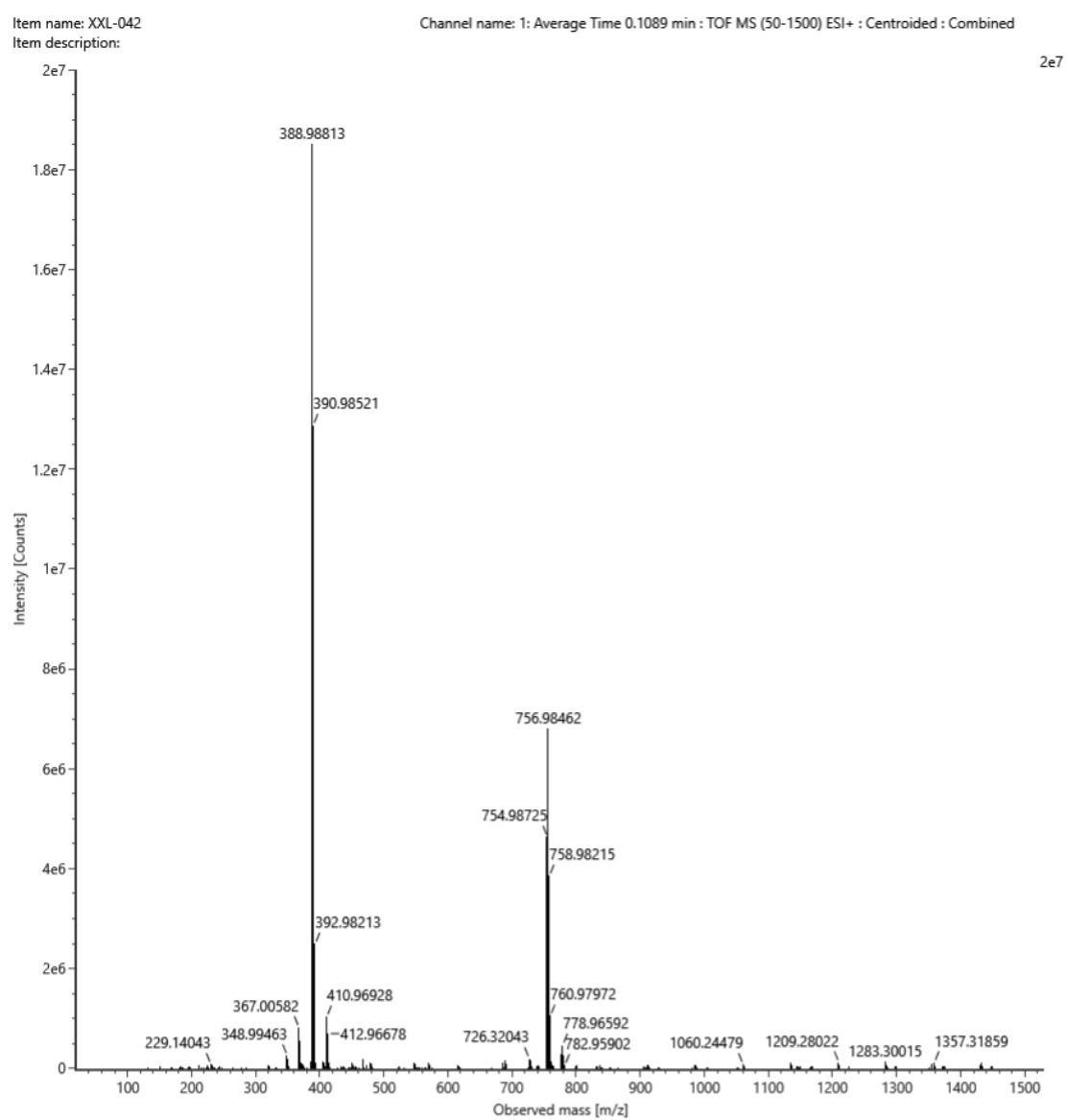
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1.43e7

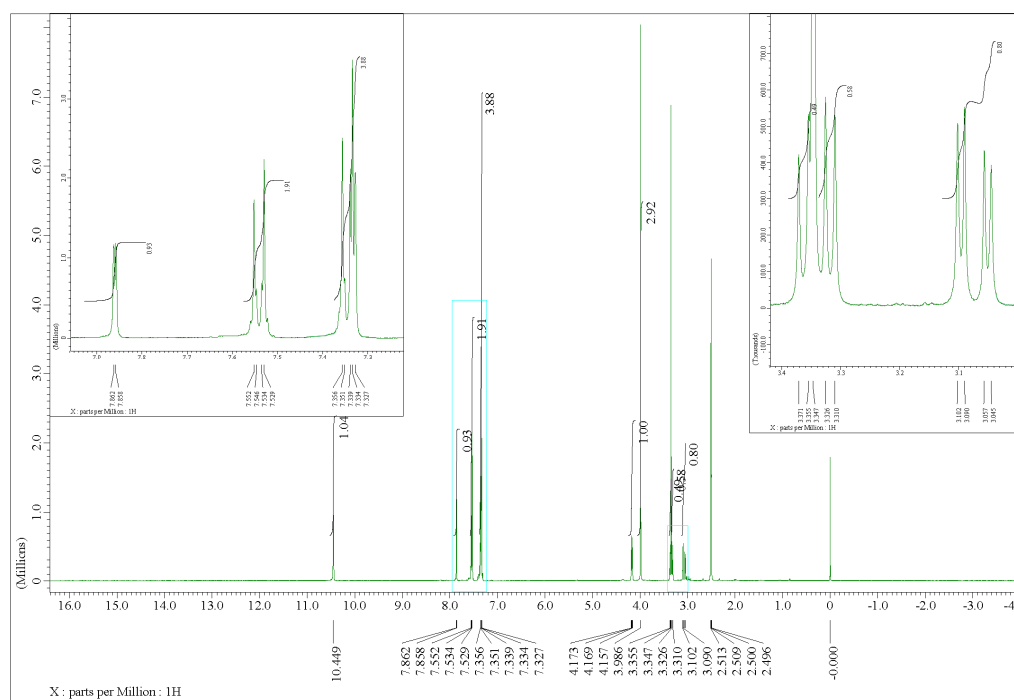
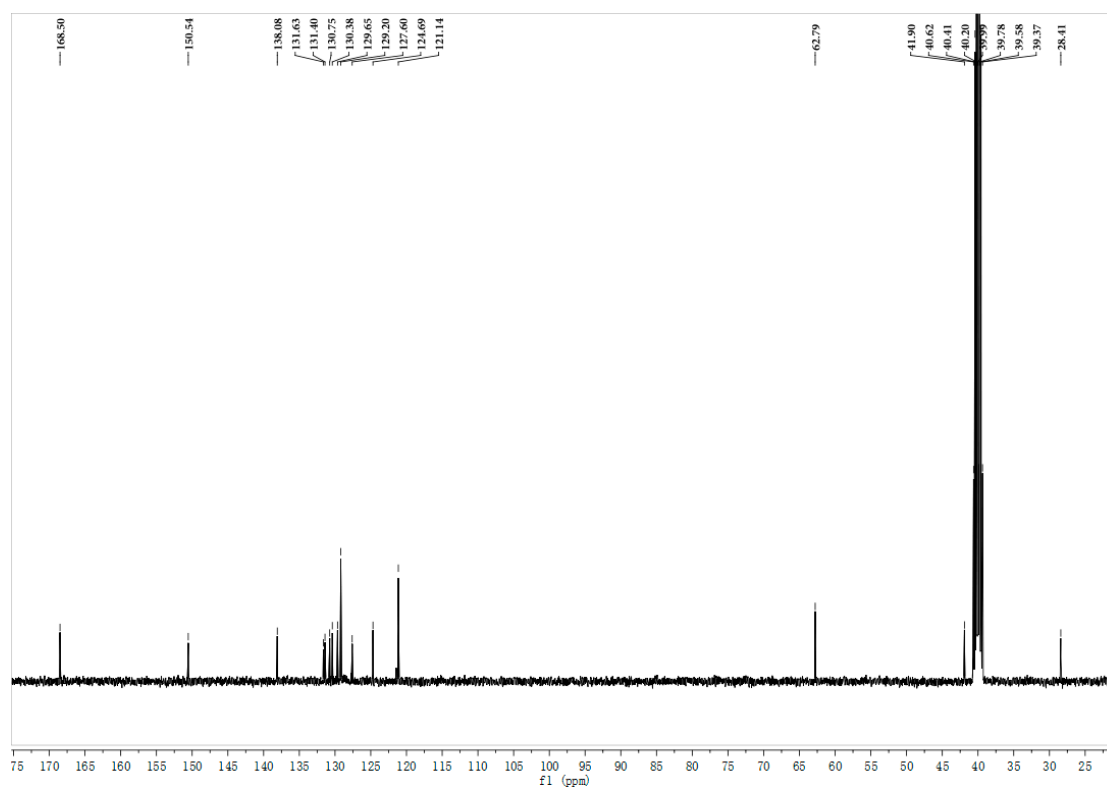


HRMS of compound 4f

 $^1\text{H}$  NMR of compound 4g $^{13}\text{C}$  NMR of compound 4g



HRMS of compound 4g

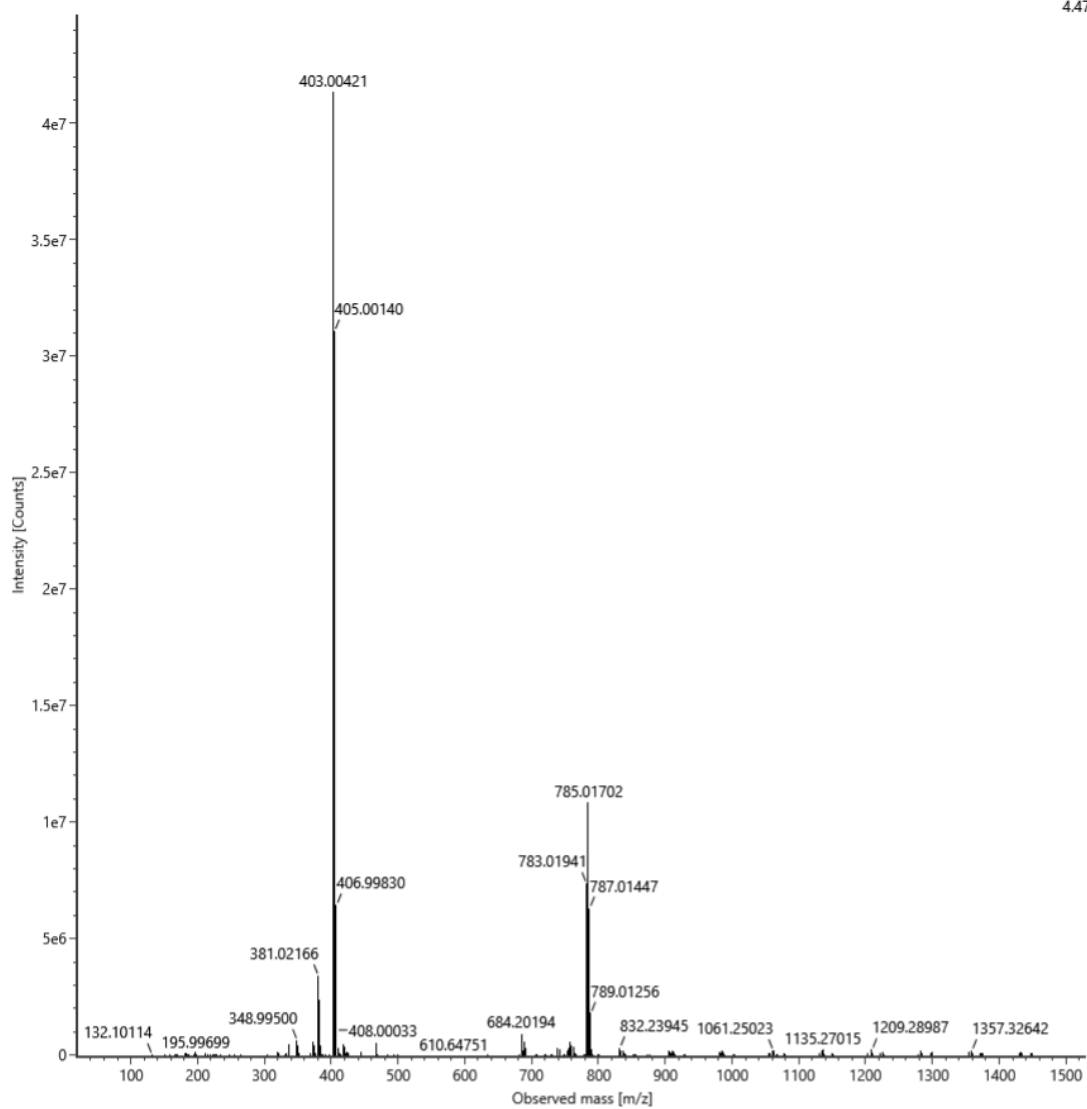
<sup>1</sup>H NMR of compound 4h<sup>13</sup>C NMR of compound 4h



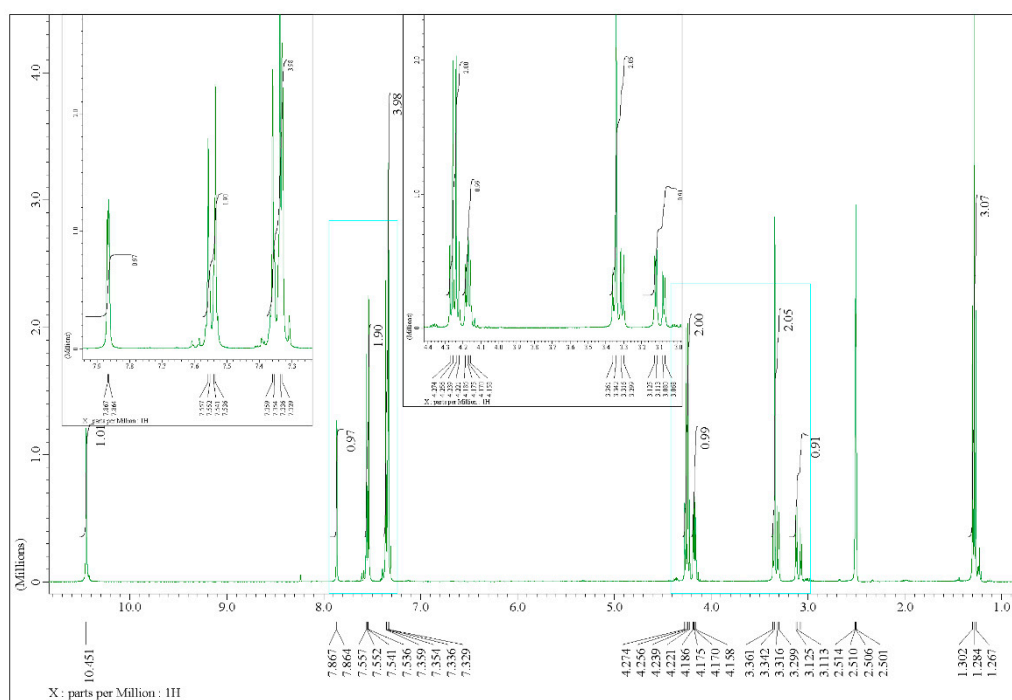
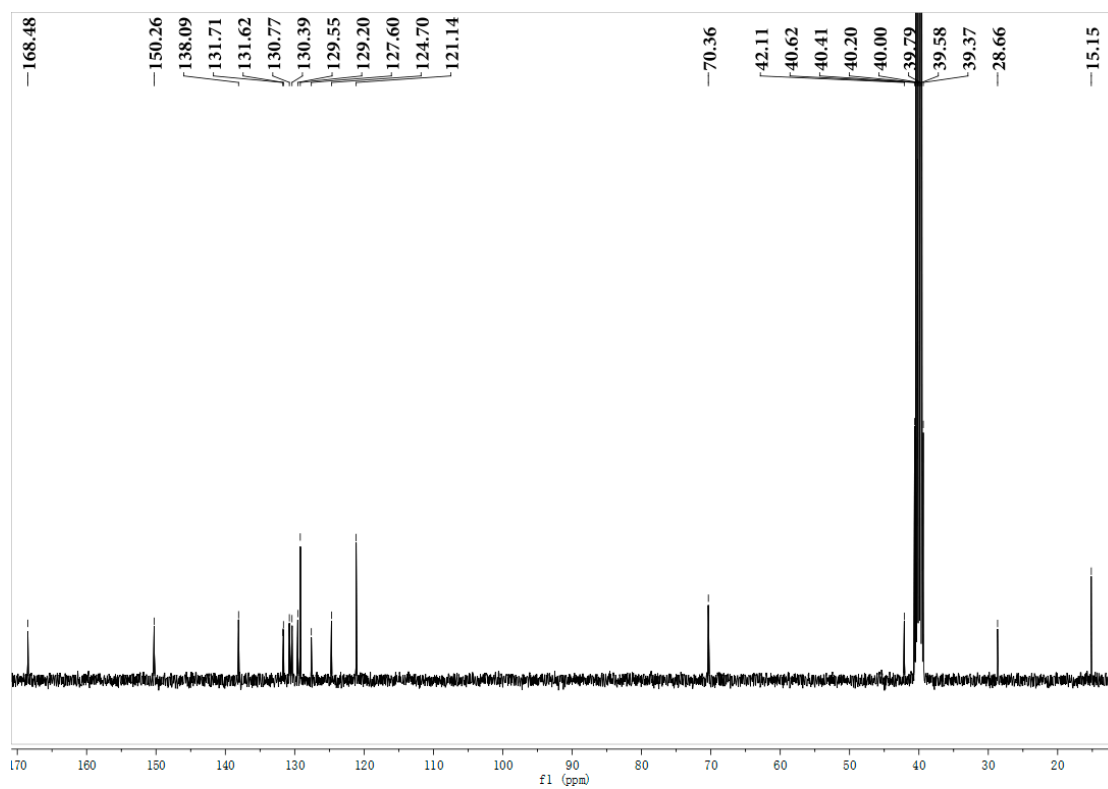
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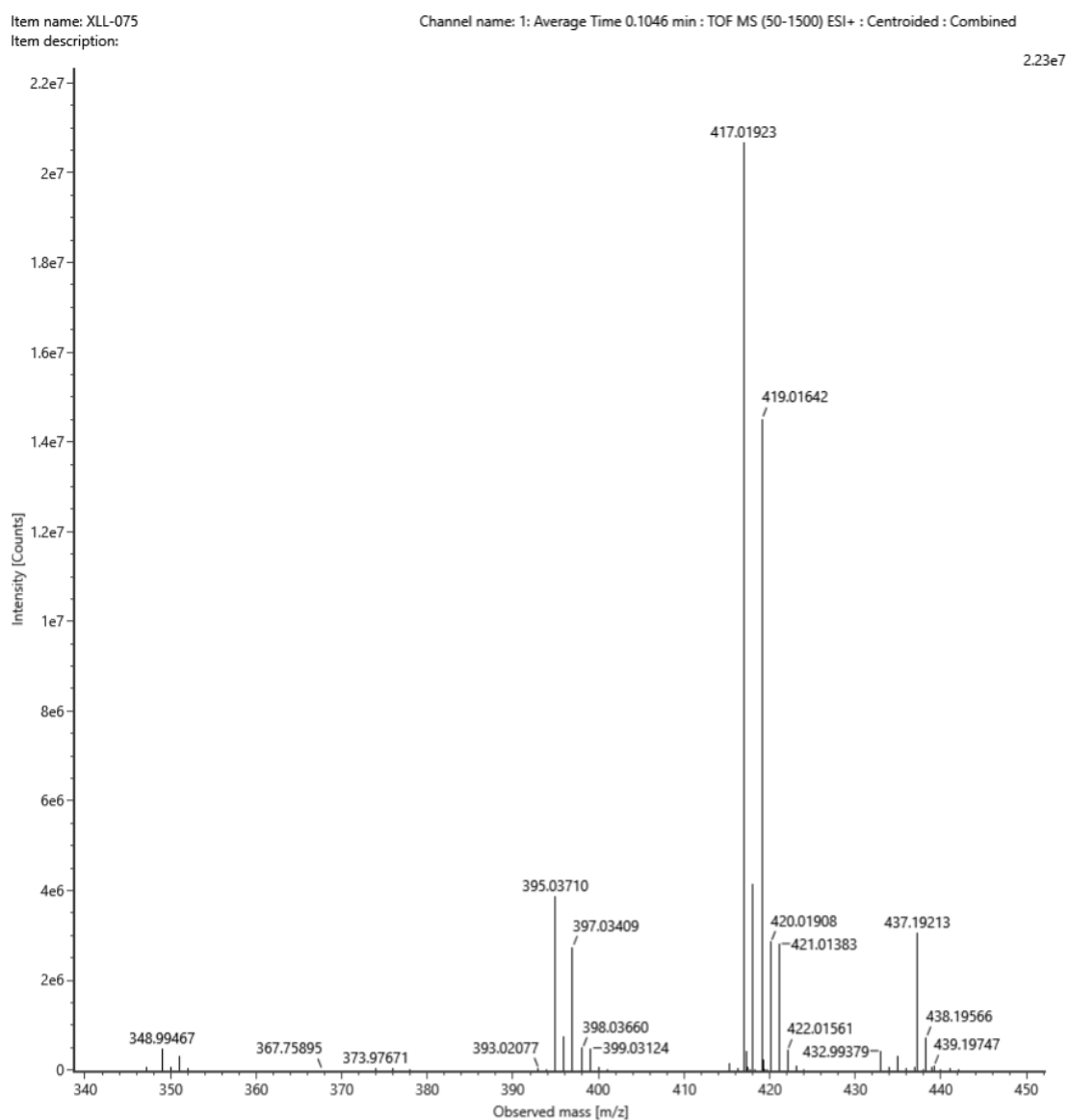
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4.47e7

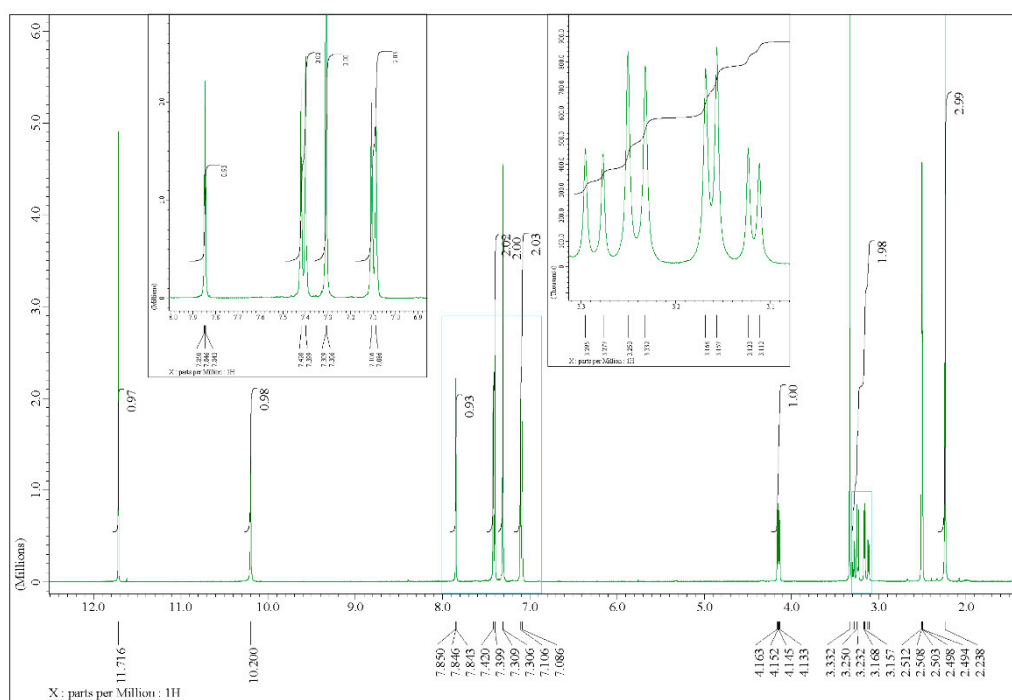
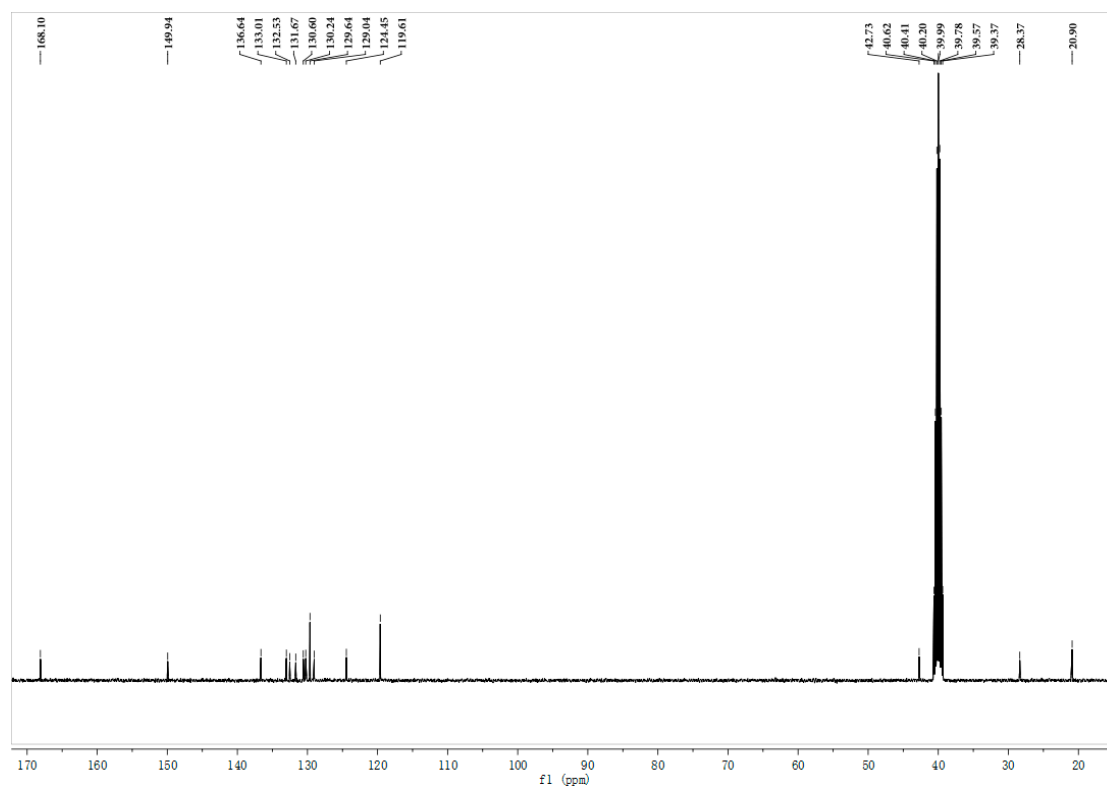


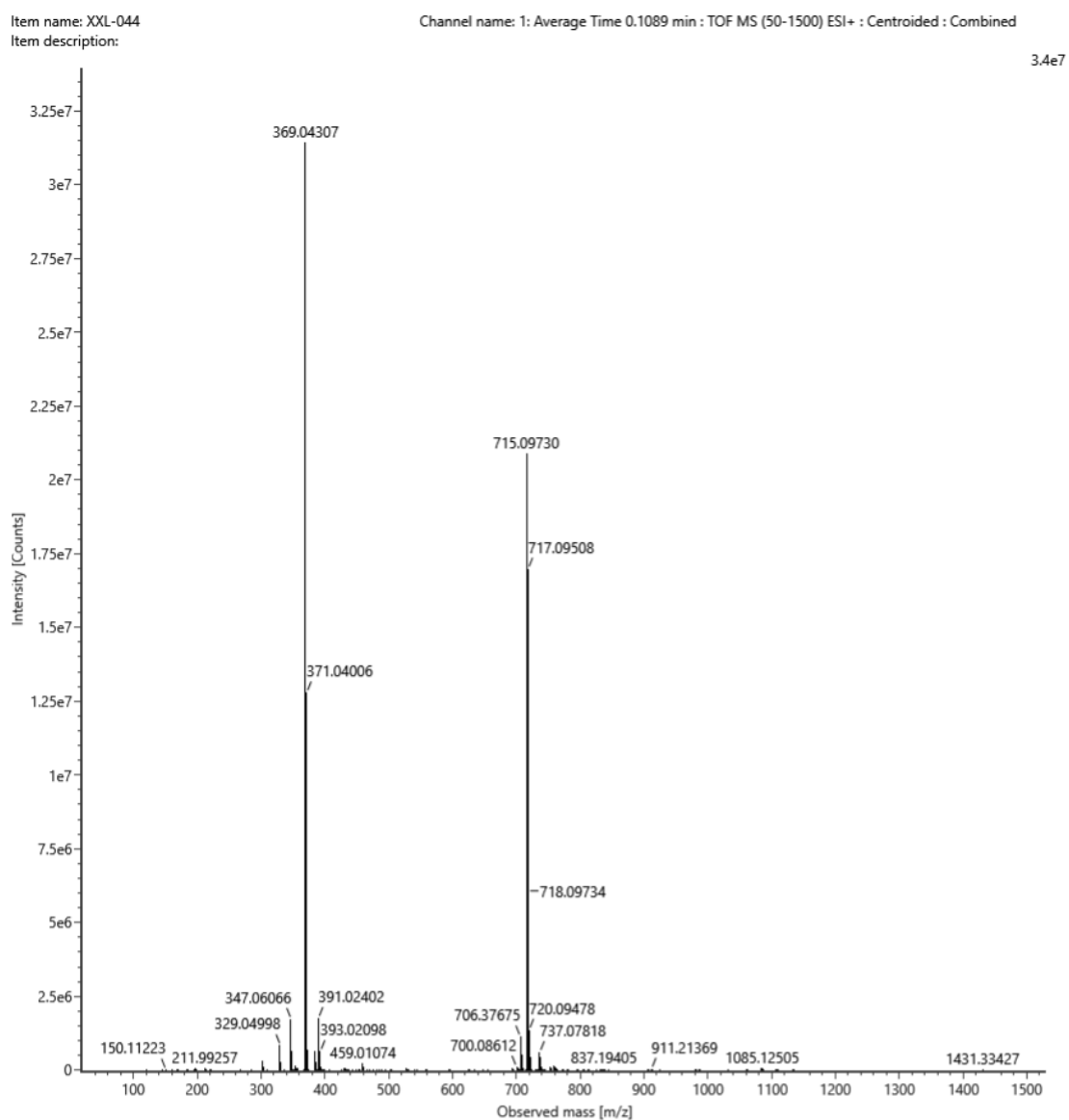
HRMS of compound 4h

<sup>1</sup>H NMR of compound 4i<sup>13</sup>C NMR of compound 4i

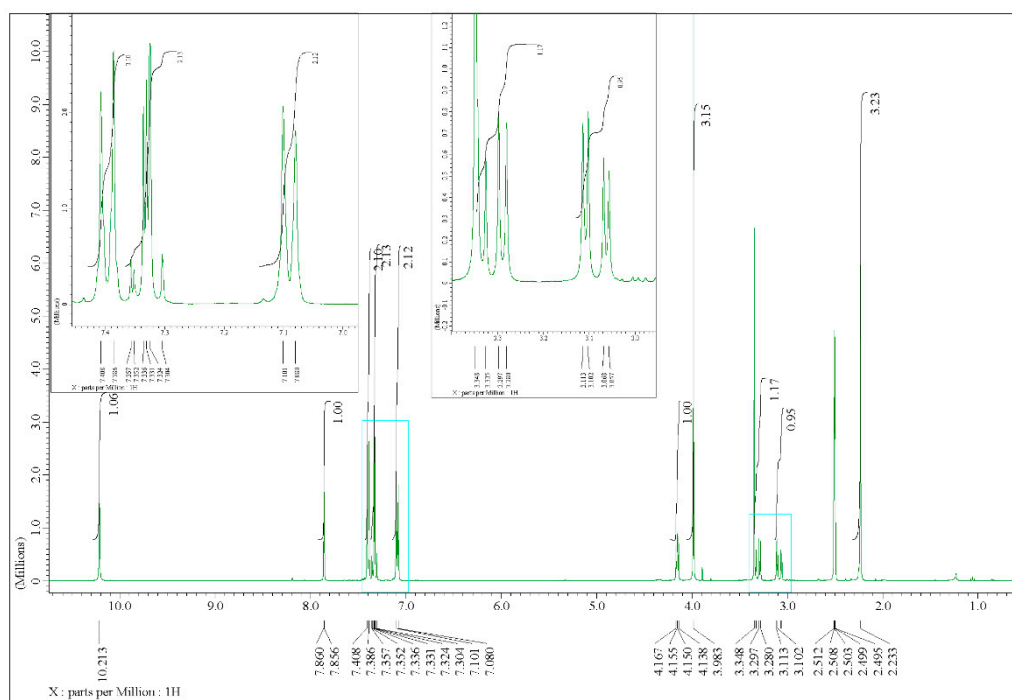
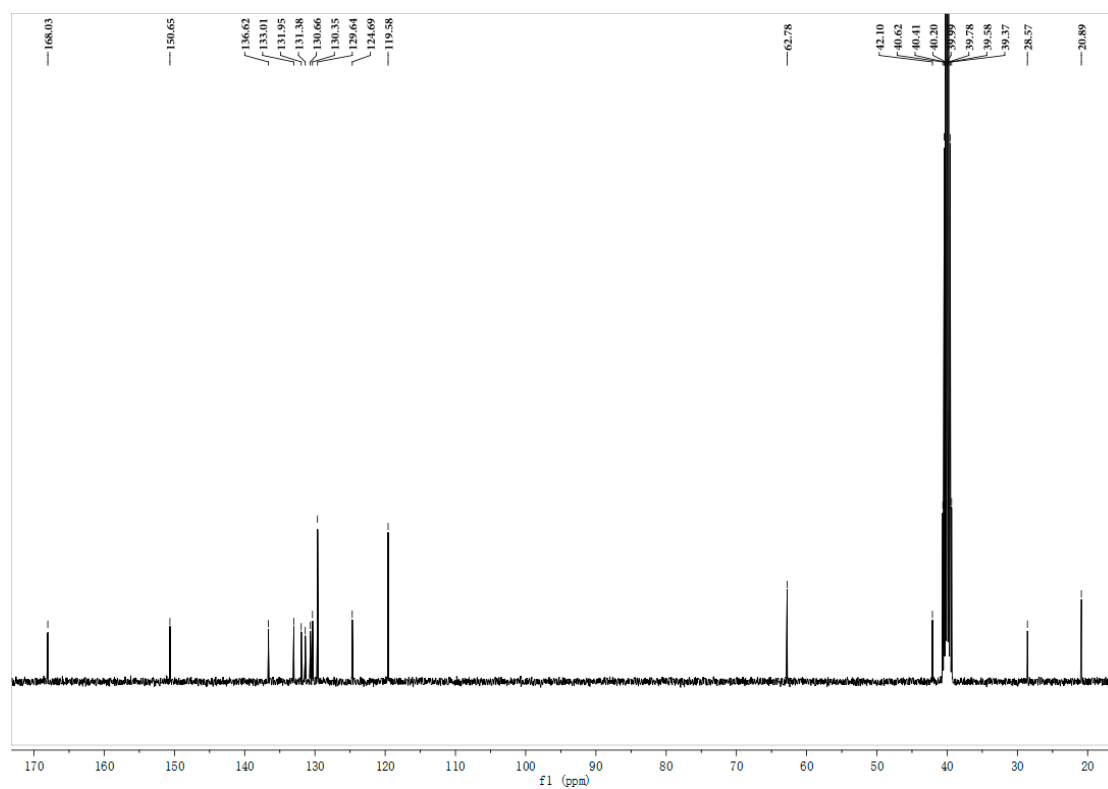


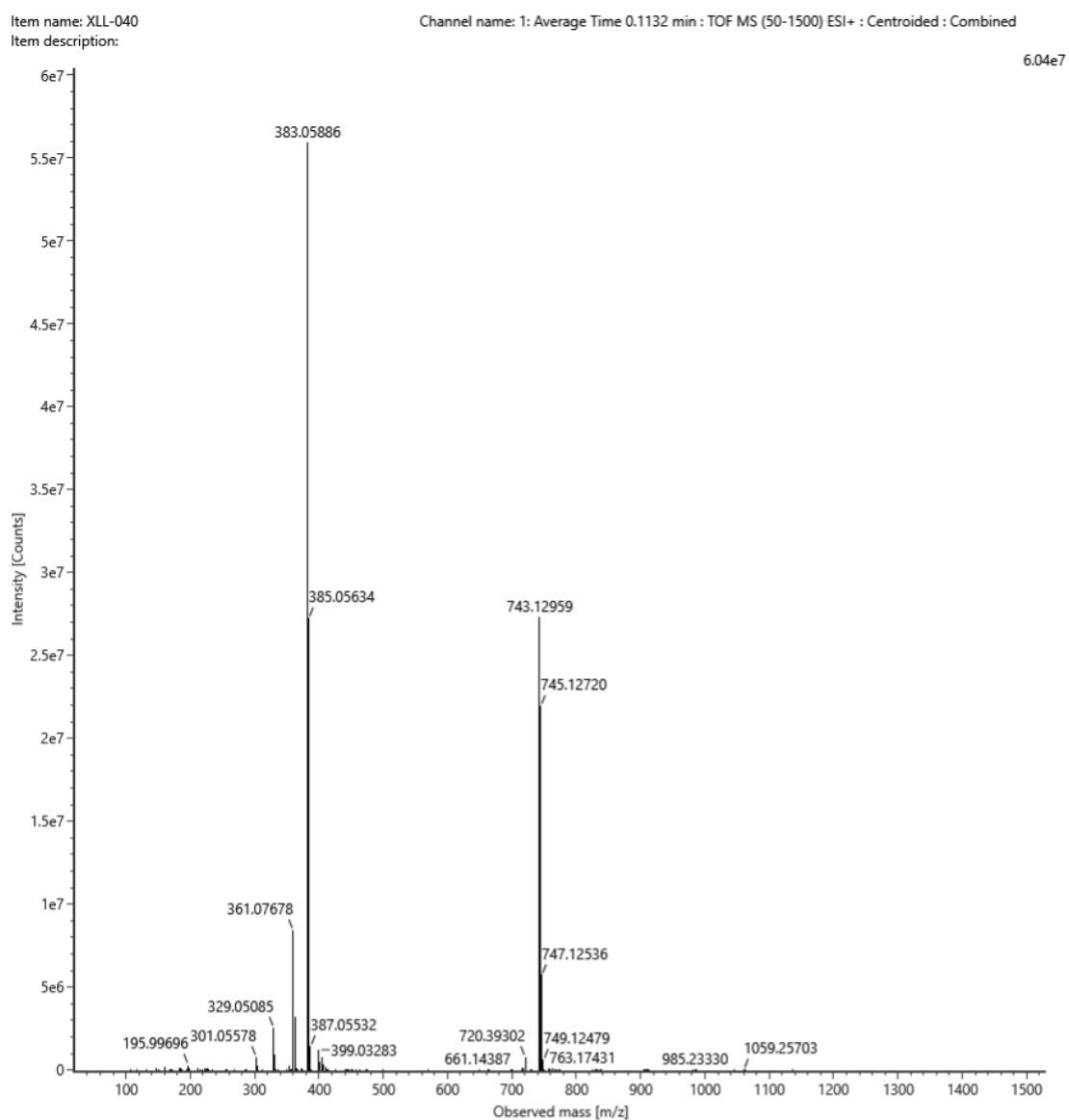
HRMS of compound 4i

<sup>1</sup>H NMR of compound 4j<sup>13</sup>C NMR of compound 4j

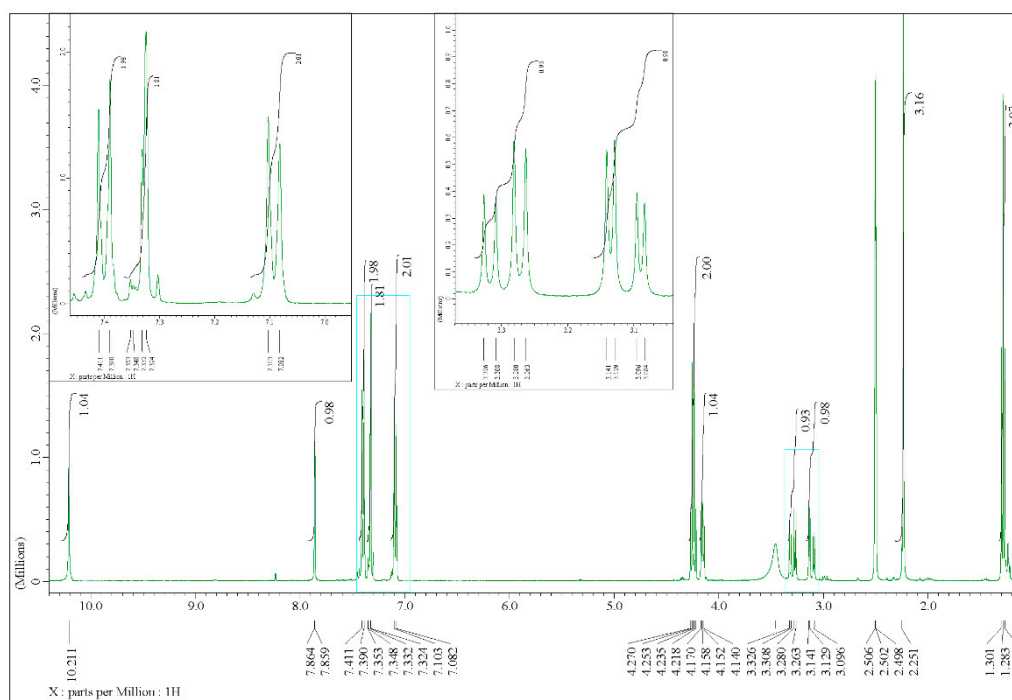
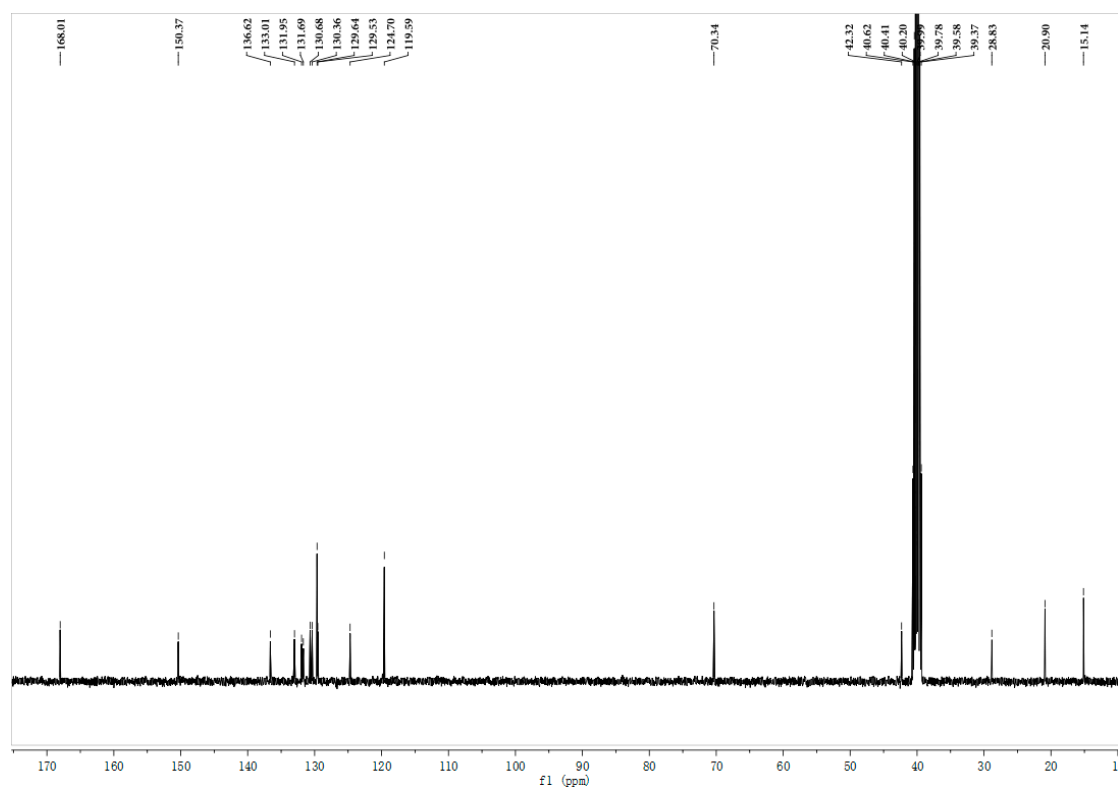


HRMS of compound 4j

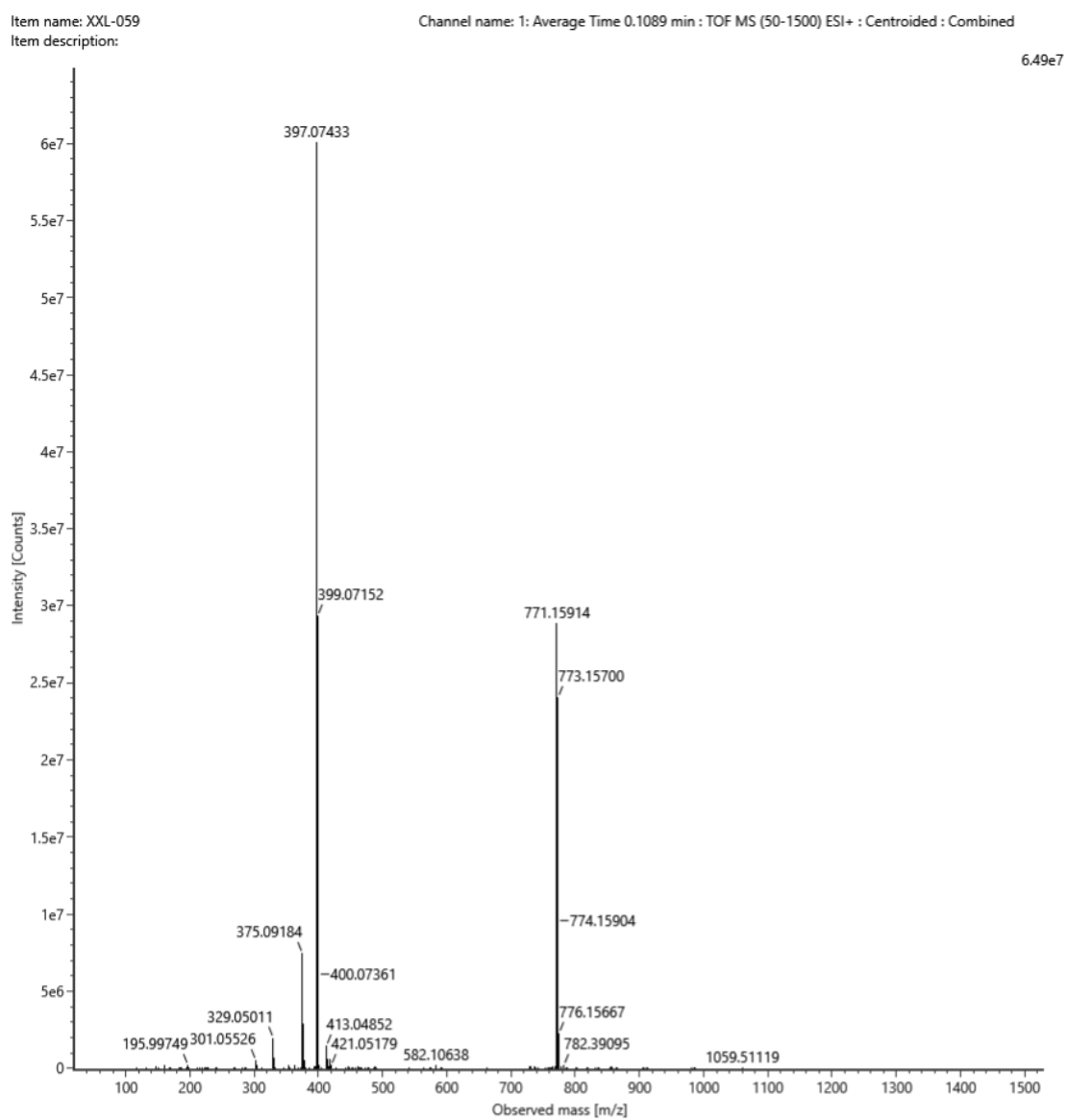
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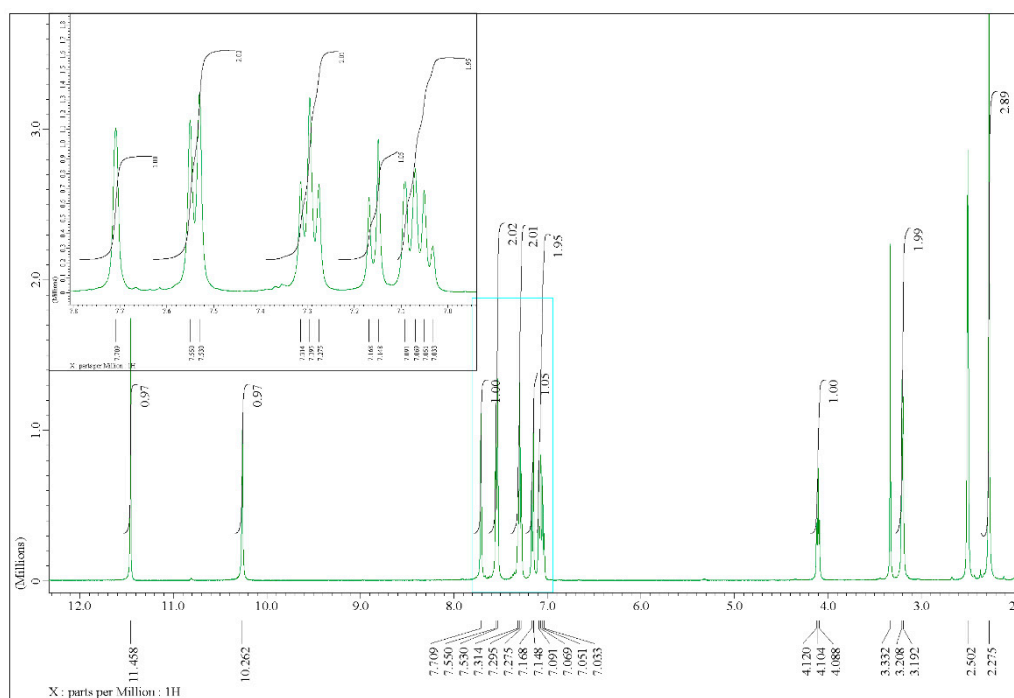
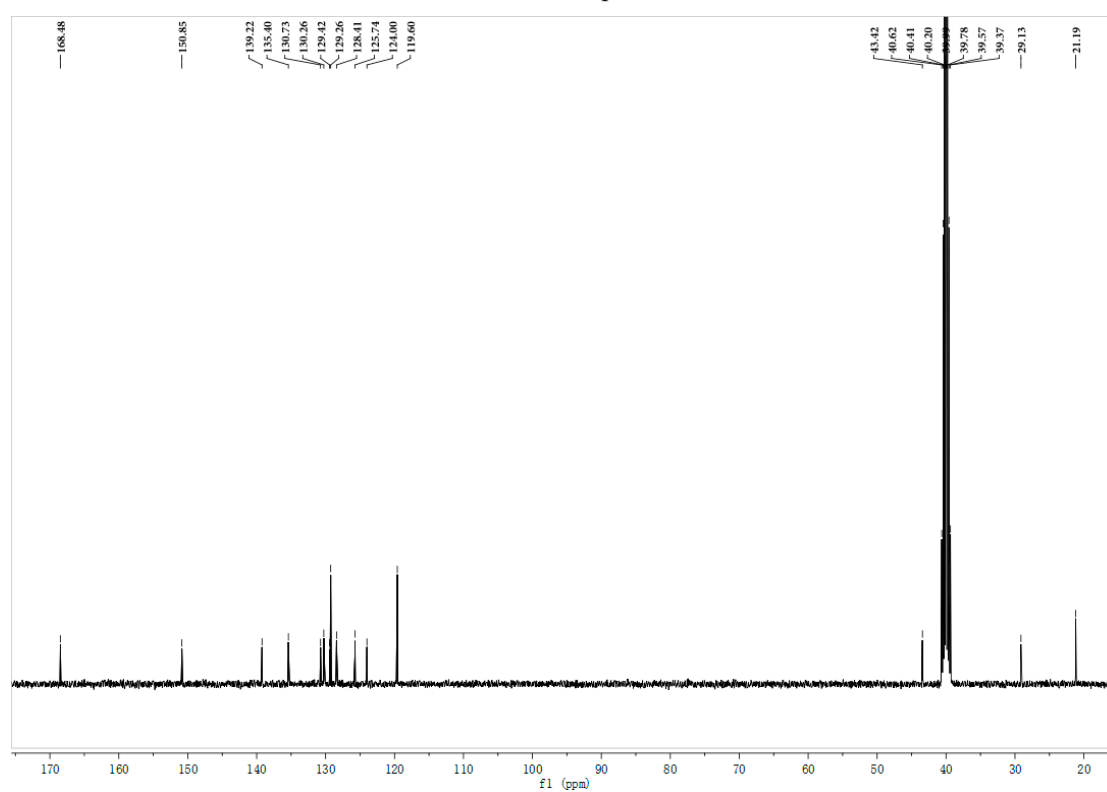
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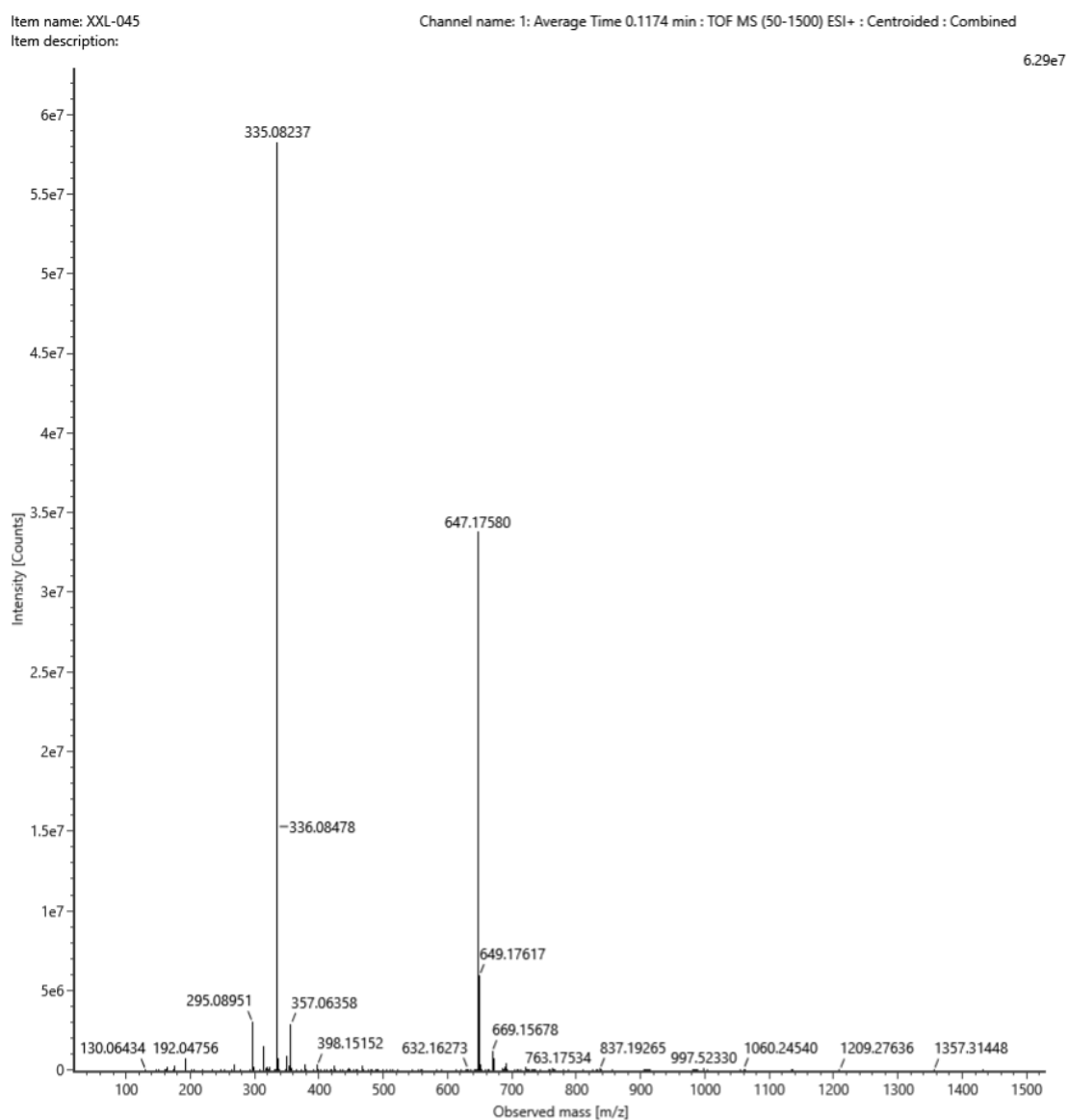
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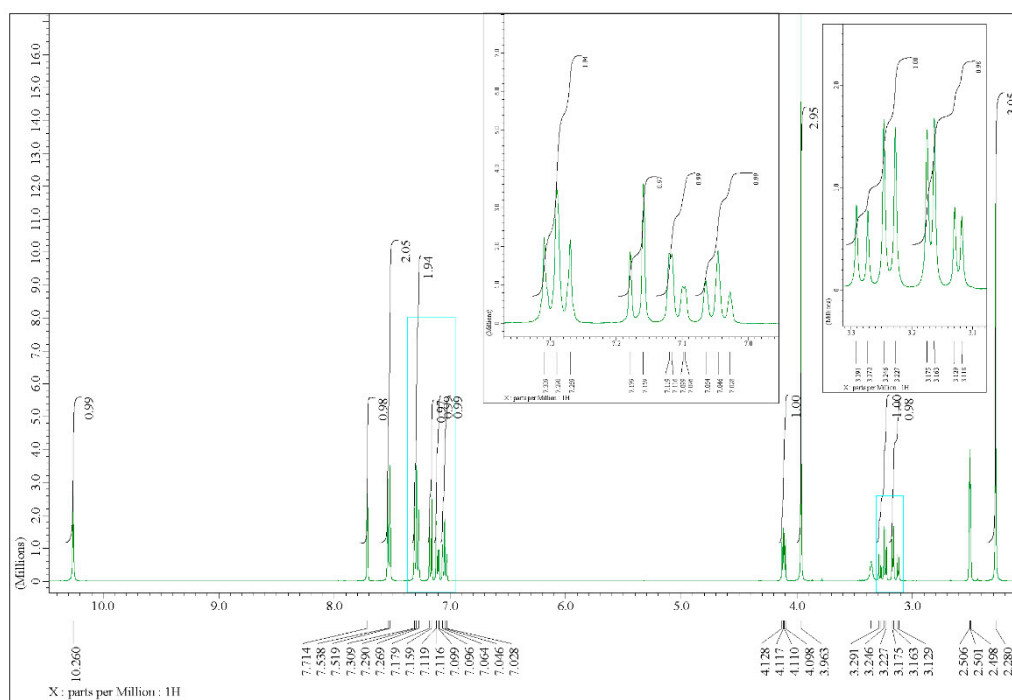
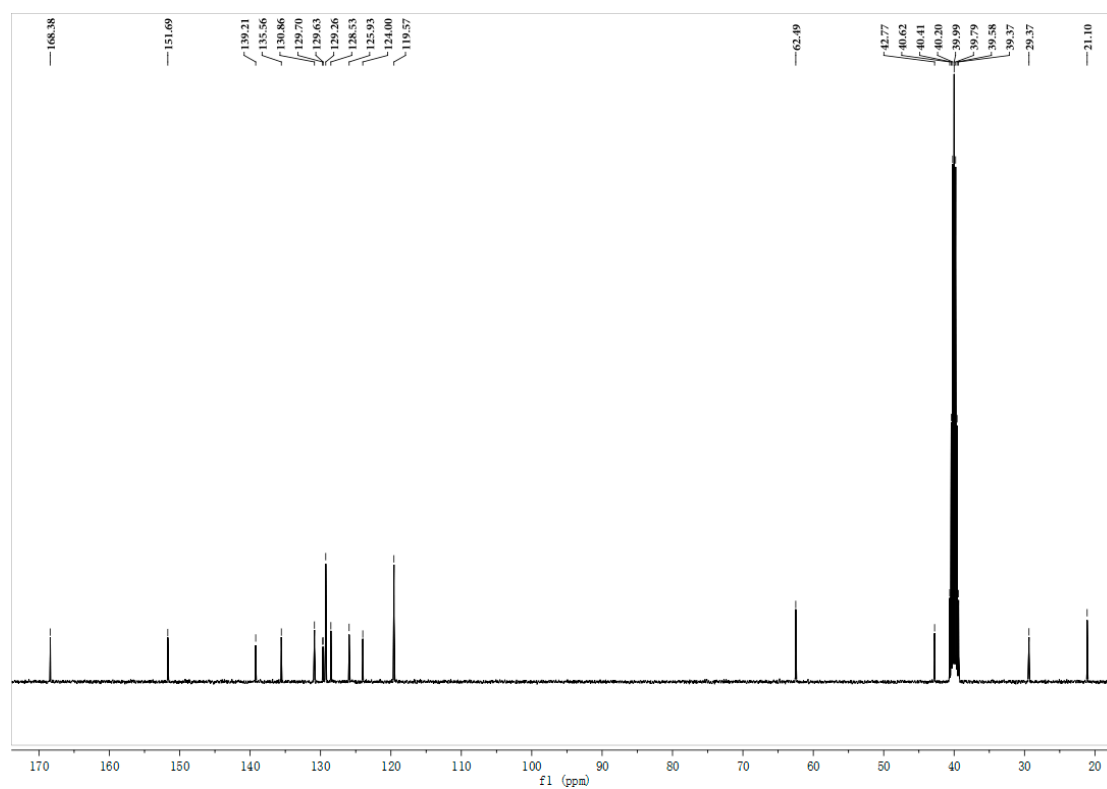


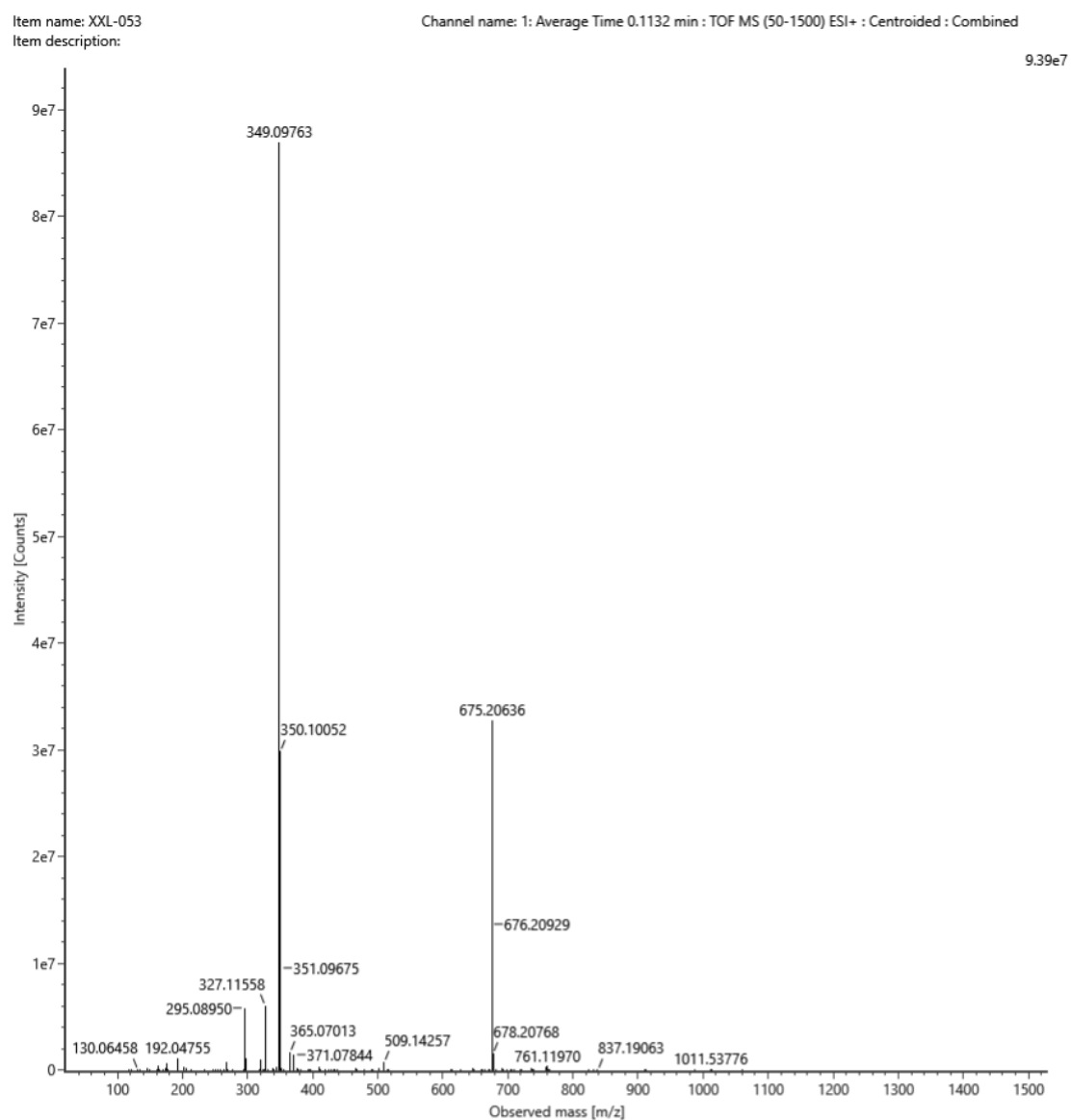
HRMS of compound 4l

<sup>1</sup>H NMR of compound 4m<sup>13</sup>C NMR of compound 4m

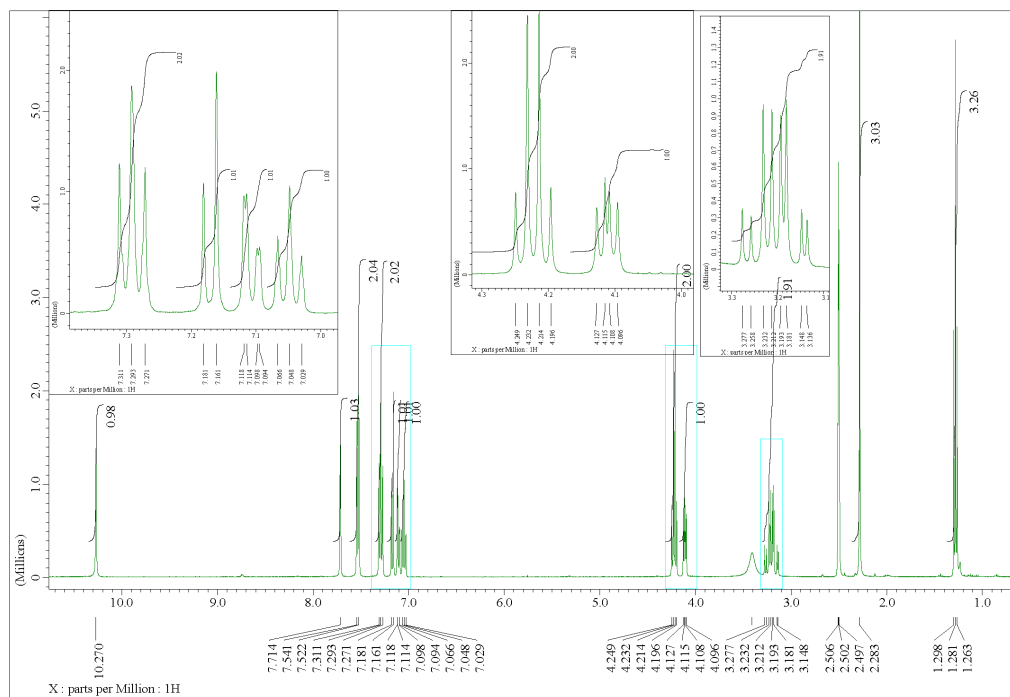
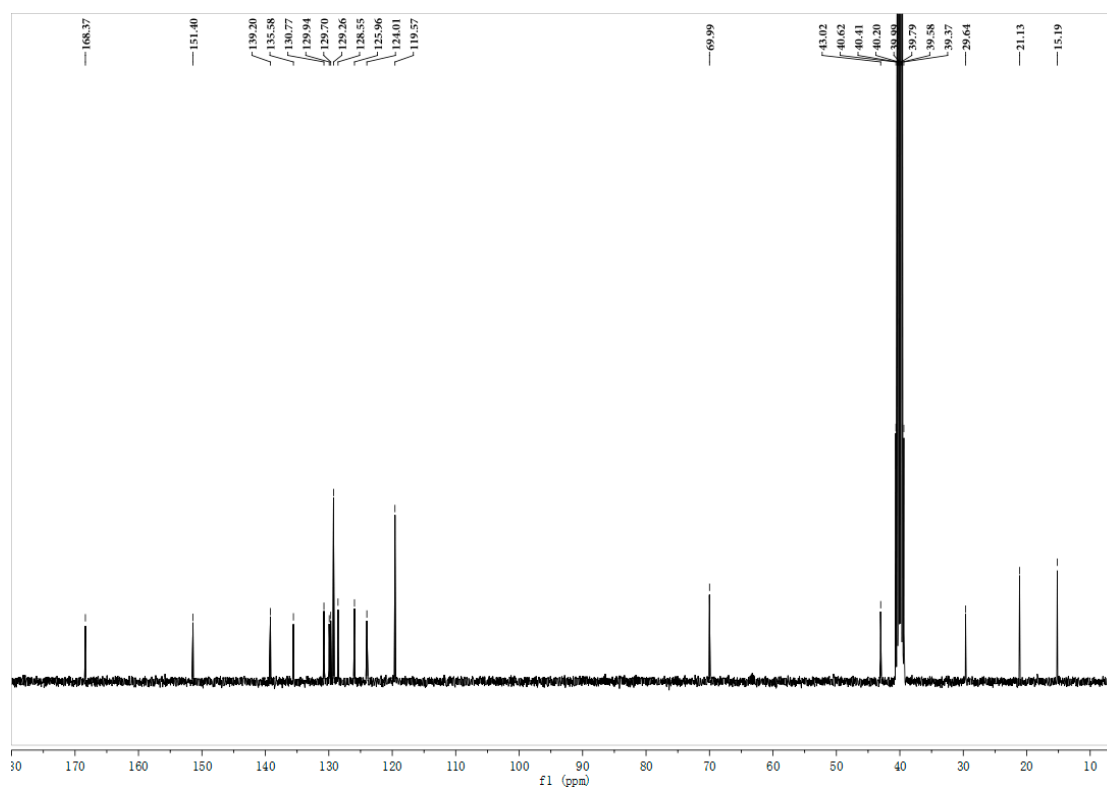


HRMS of compound 4m

<sup>1</sup>H NMR of compound 4n<sup>13</sup>C NMR of compound 4n



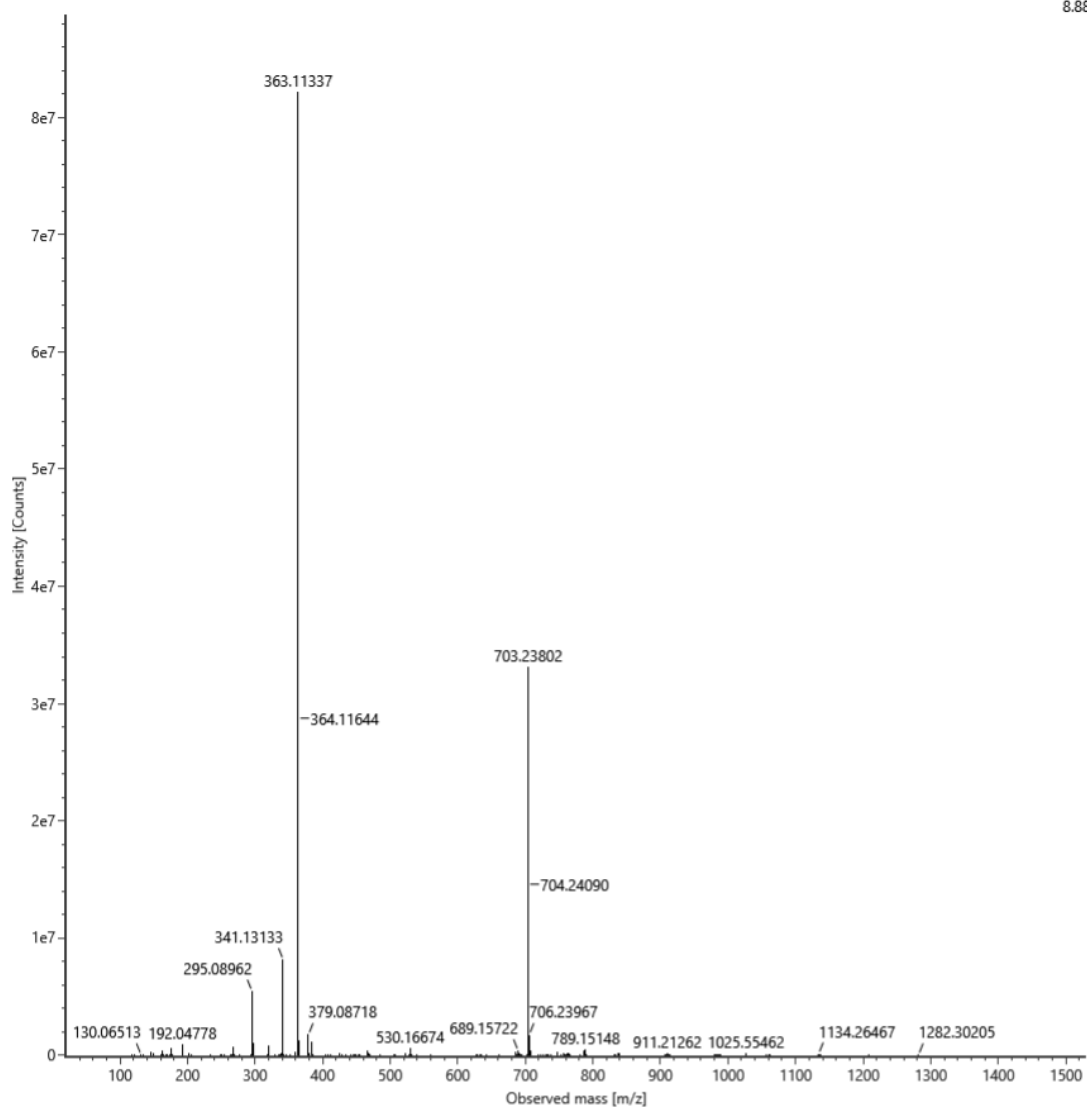
HRMS of compound 4n

<sup>1</sup>H NMR of compound 4o<sup>13</sup>C NMR of compound 4o

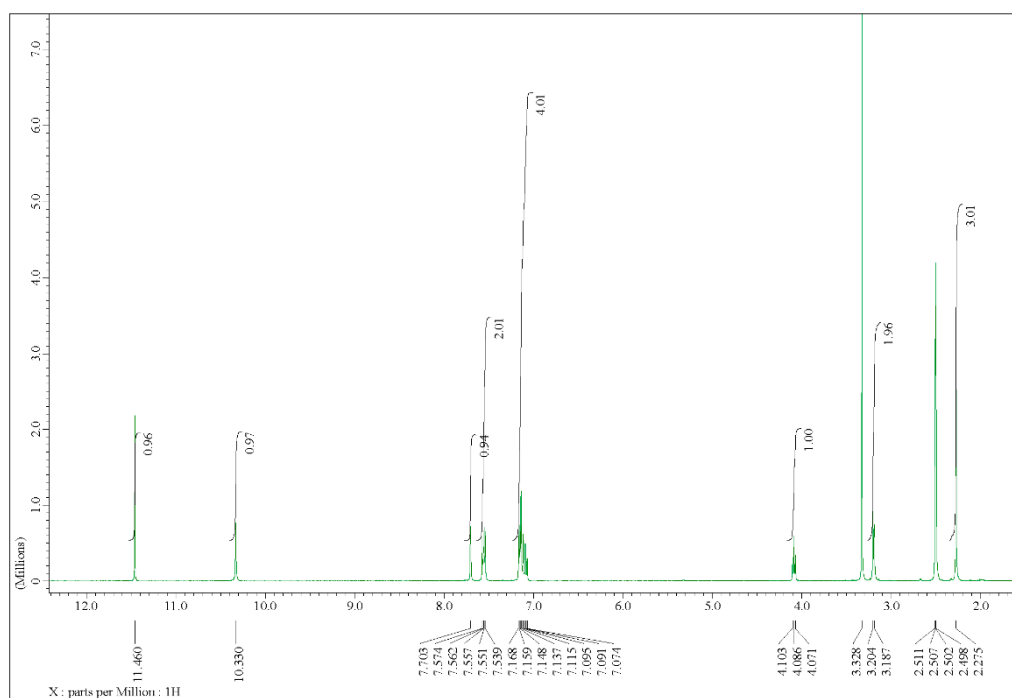
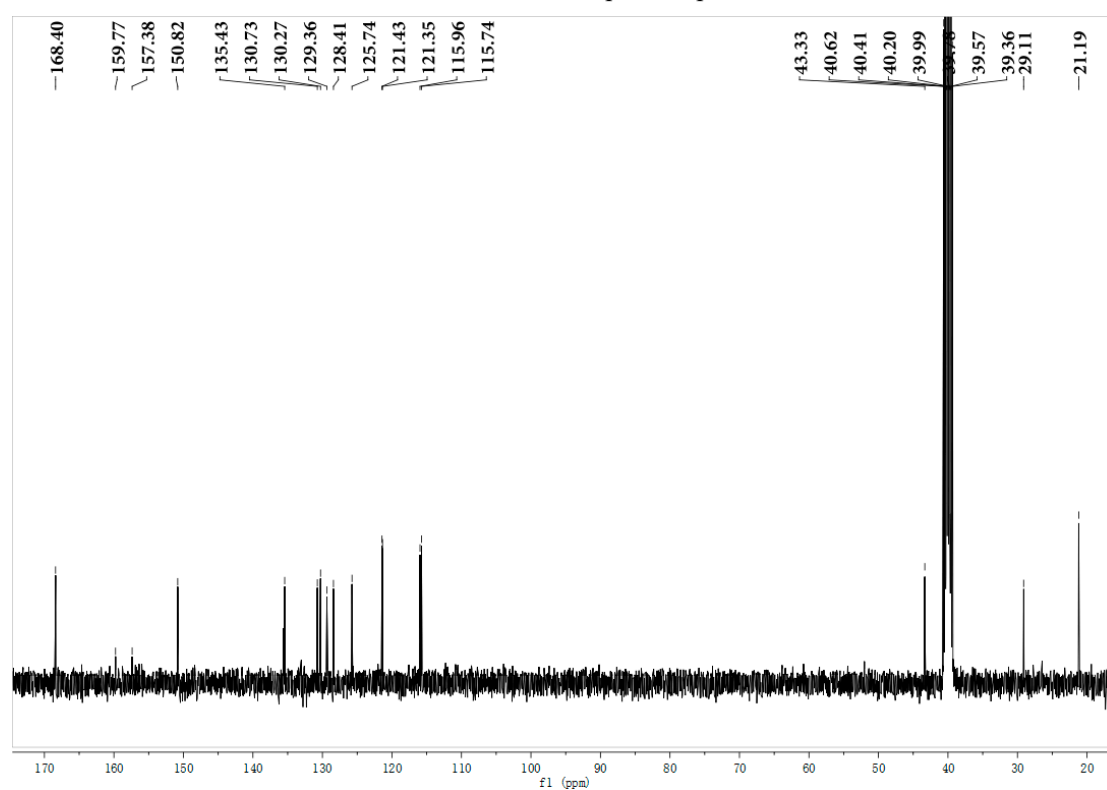
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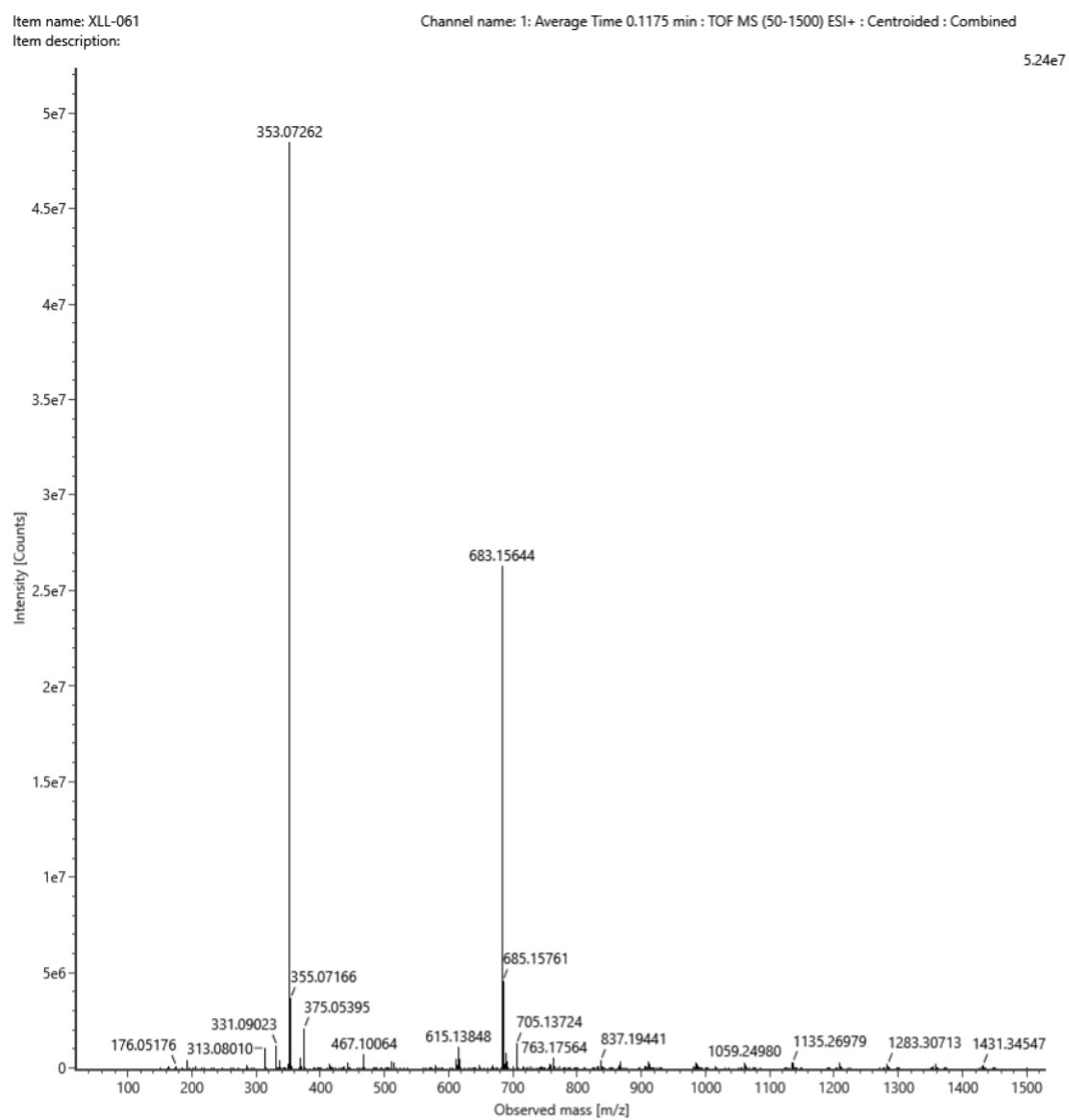
8.88e7



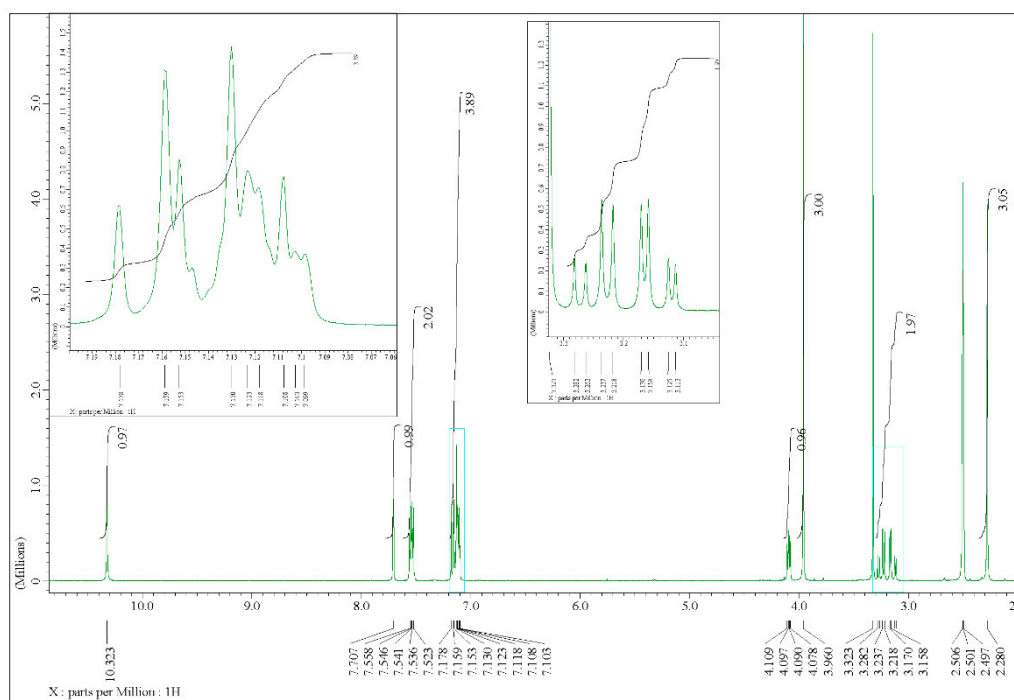
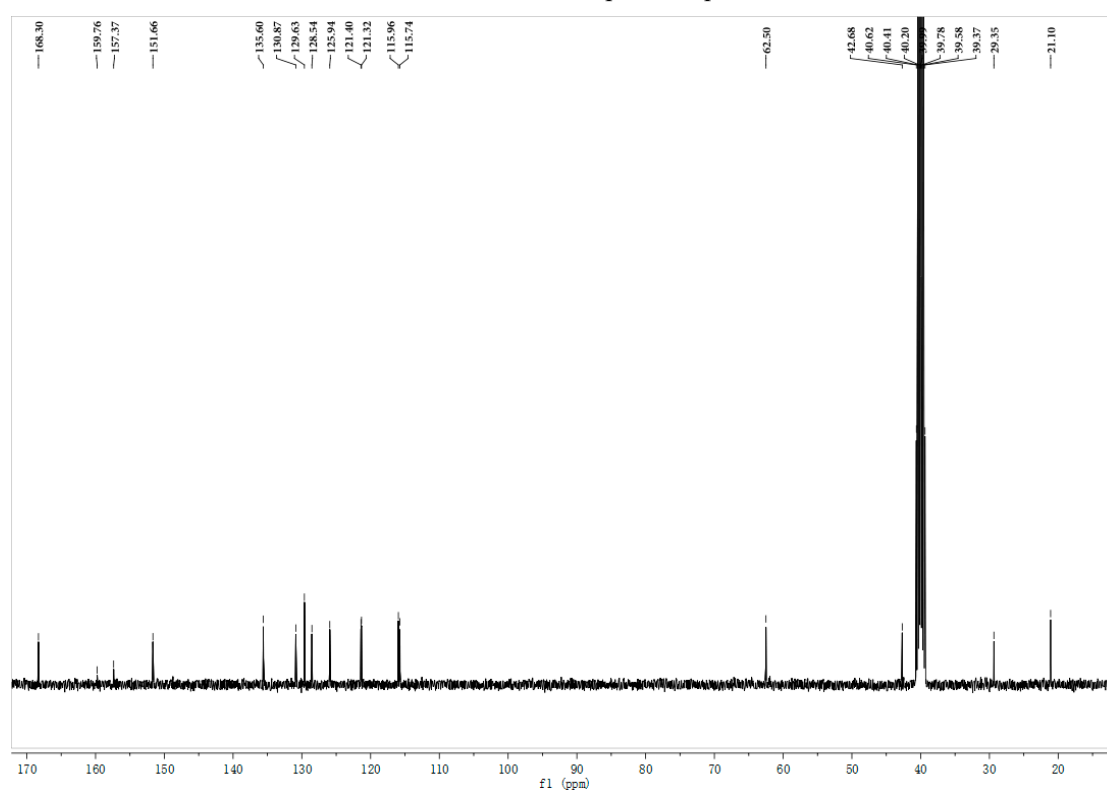
HRMS of compound 4o

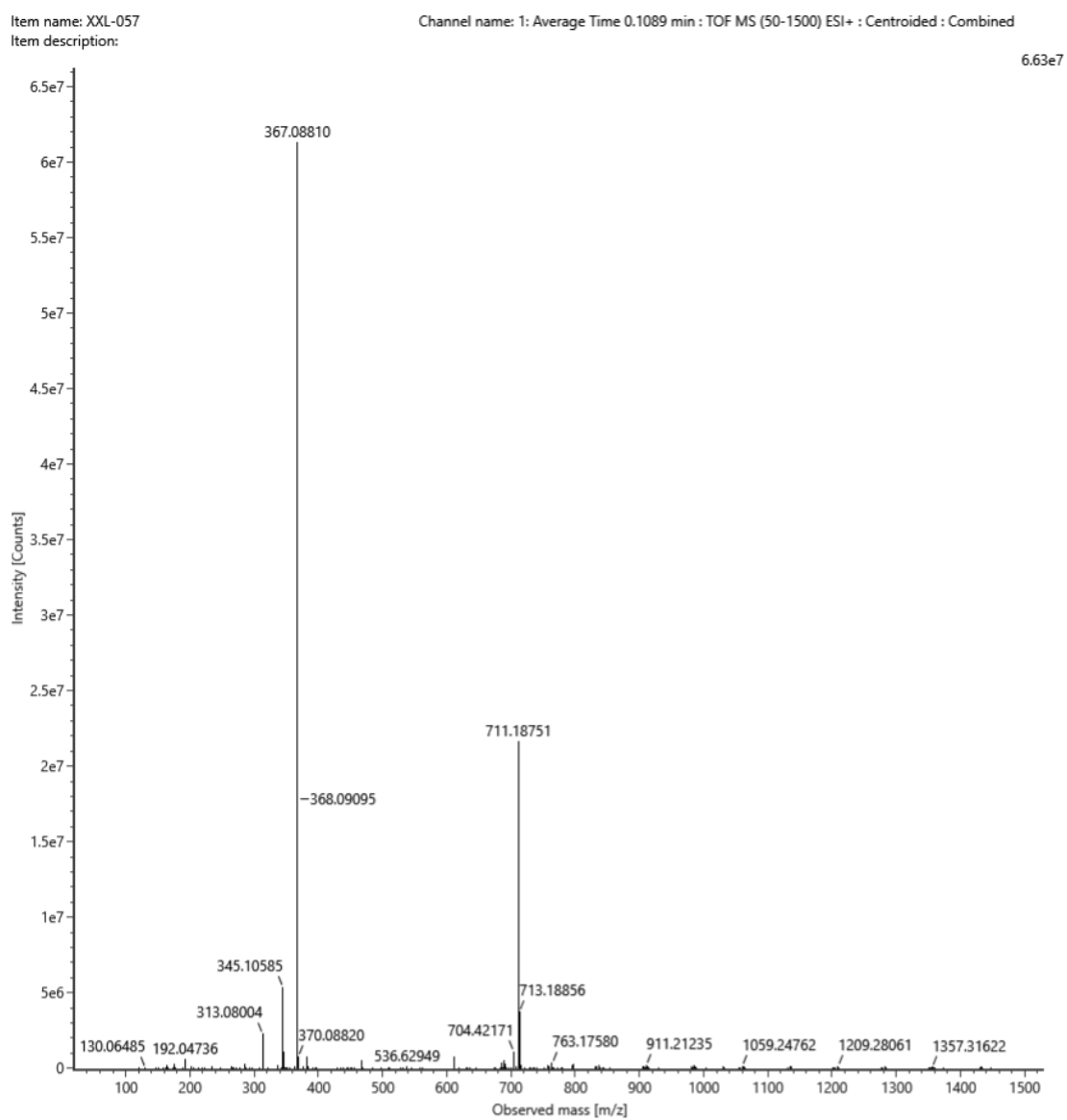
<sup>1</sup>H NMR of compound 4p<sup>13</sup>C NMR of compound 4p



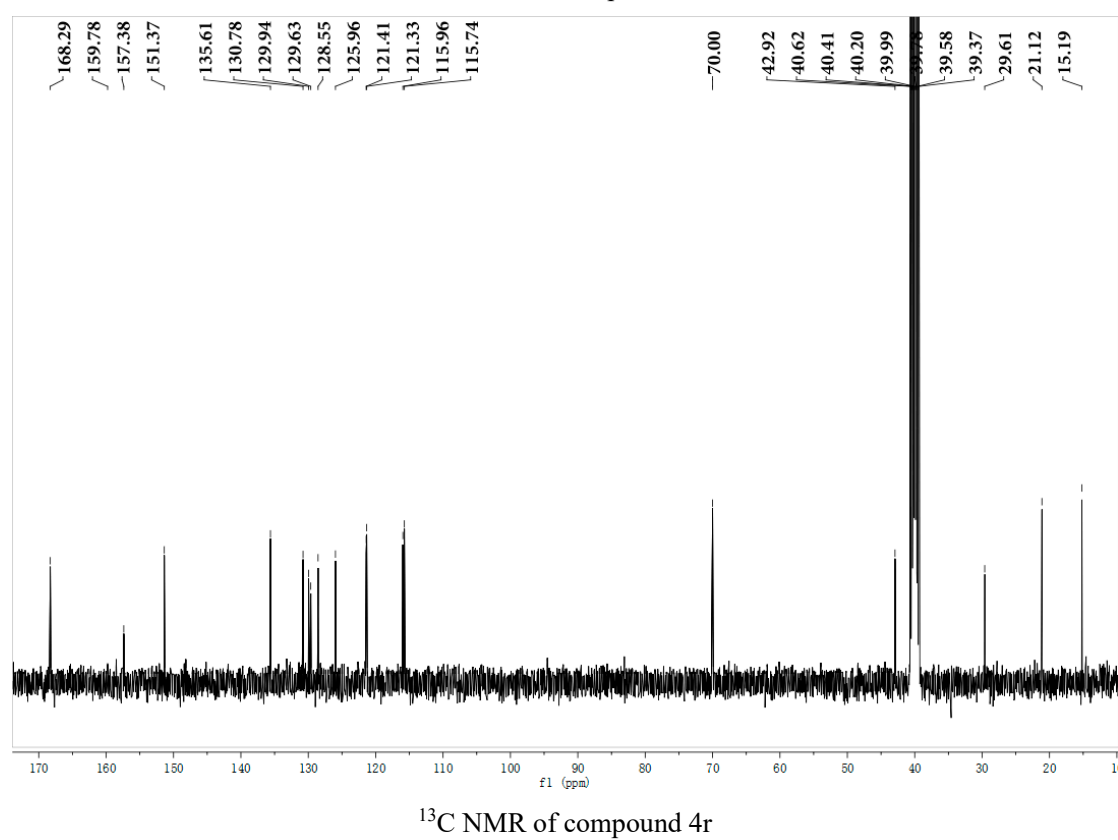
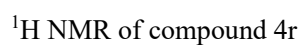


HRMS of compound 4p

 $^1\text{H}$  NMR of compound 4q $^{13}\text{C}$  NMR of compound 4q



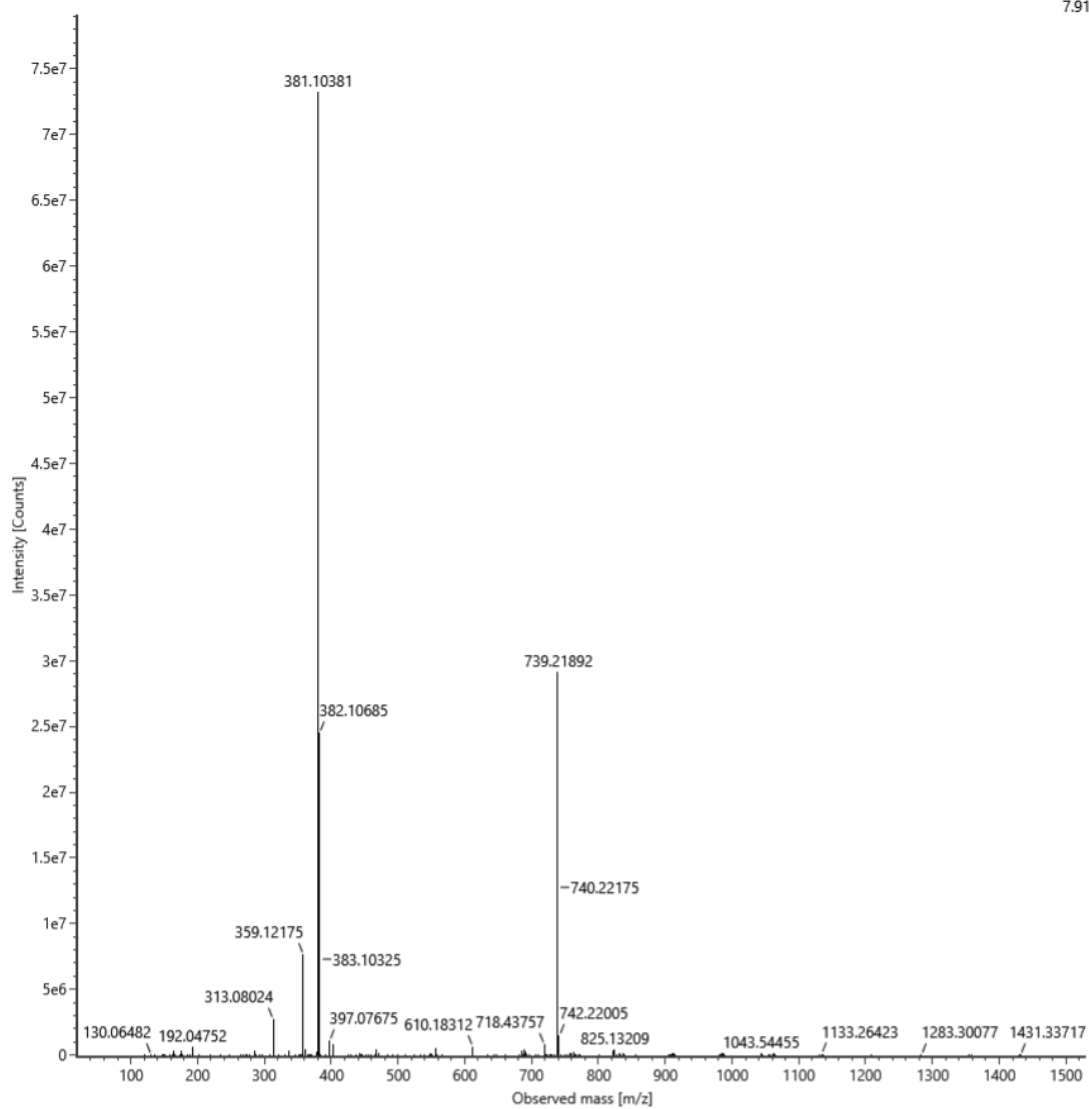
HRMS of compound 4q



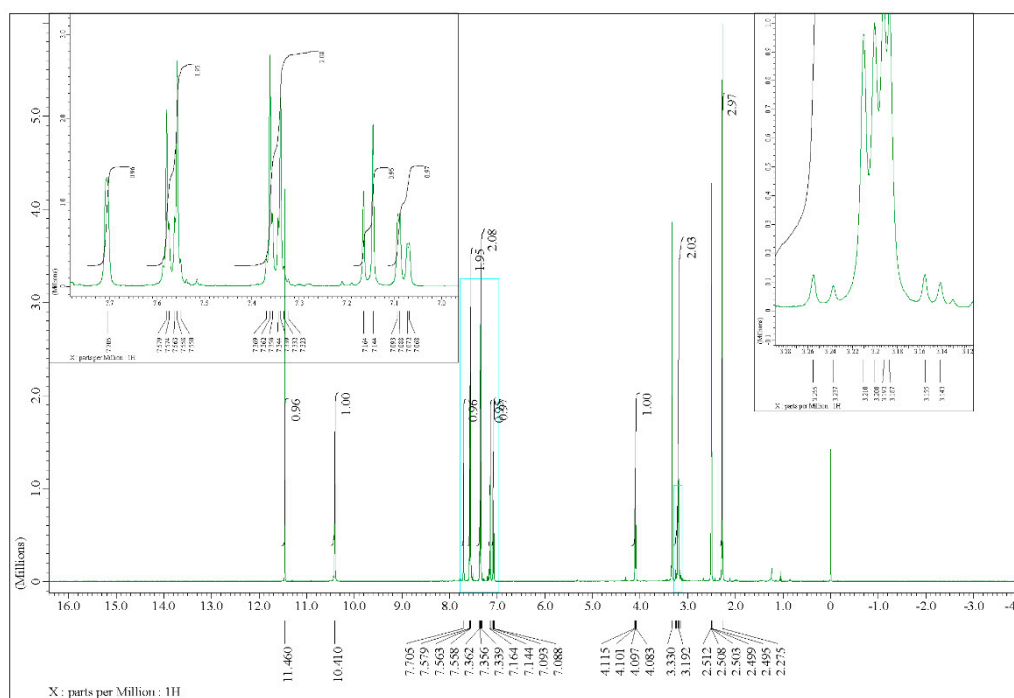
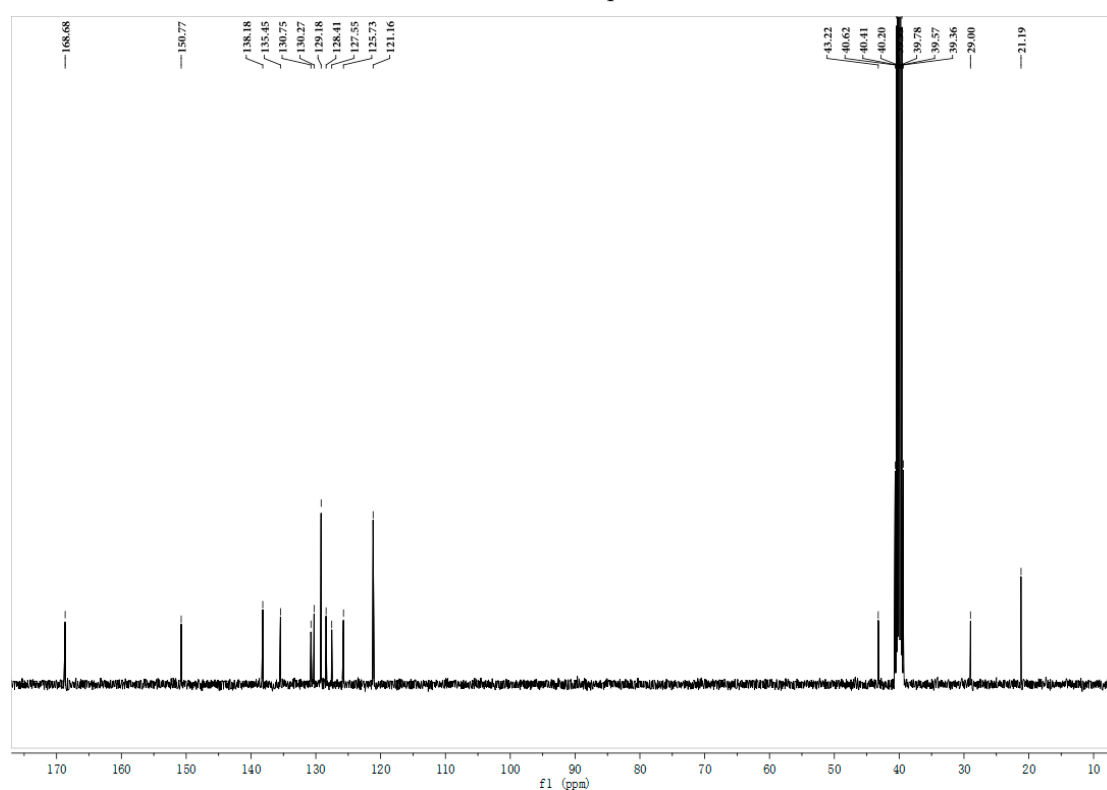
Item name: XXL-060  
Item description:

Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined

7.91e7



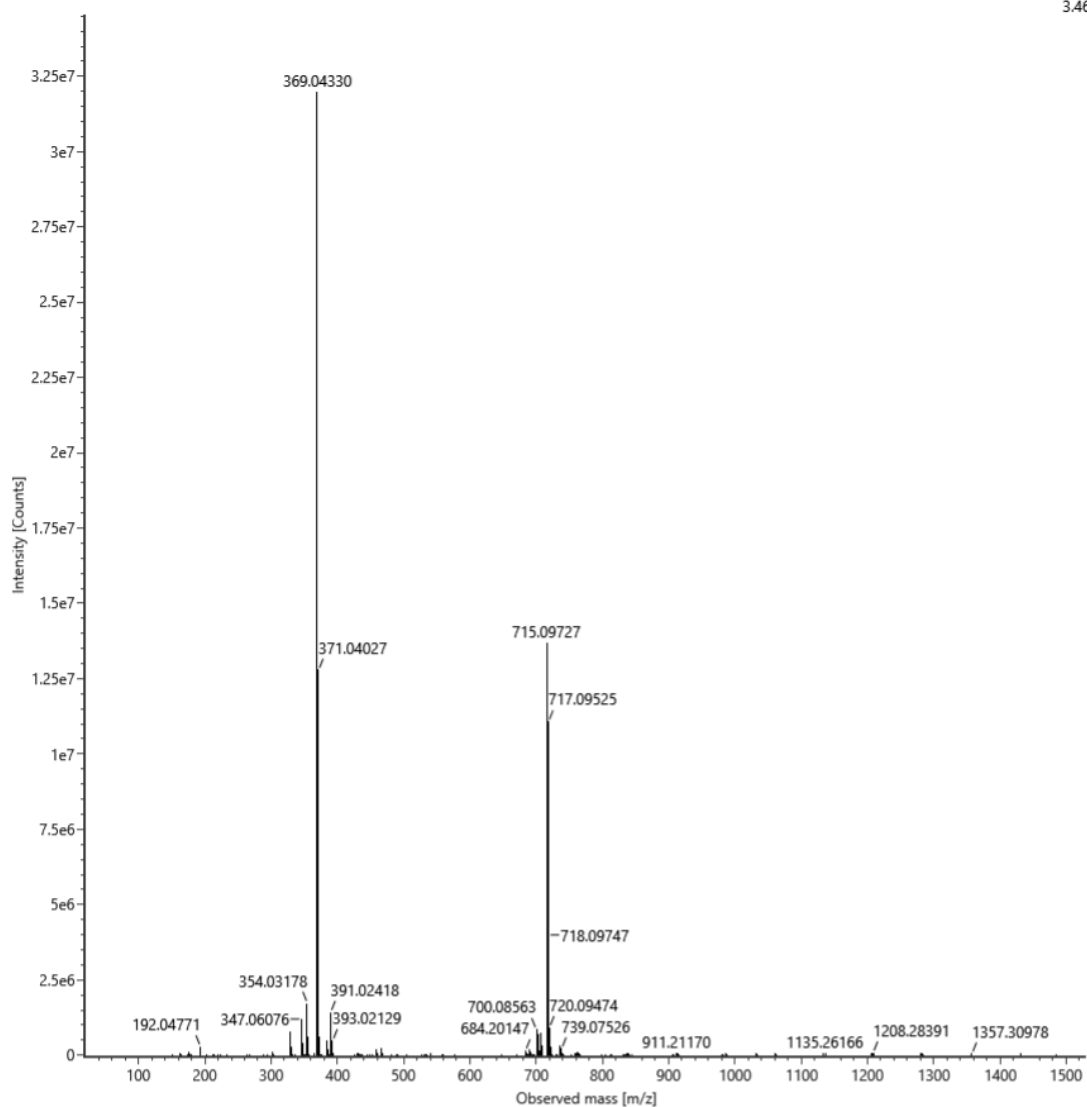
HRMS of compound 4r

<sup>1</sup>H NMR of compound 4s<sup>13</sup>C NMR of compound 4s

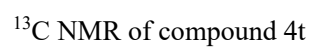
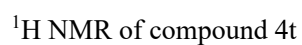
Item name: XXL-050  
Item description:

Channel name: 1: Average Time 0.1046 min : TOF MS (50-1500) ESI+ : Centroided : Combined

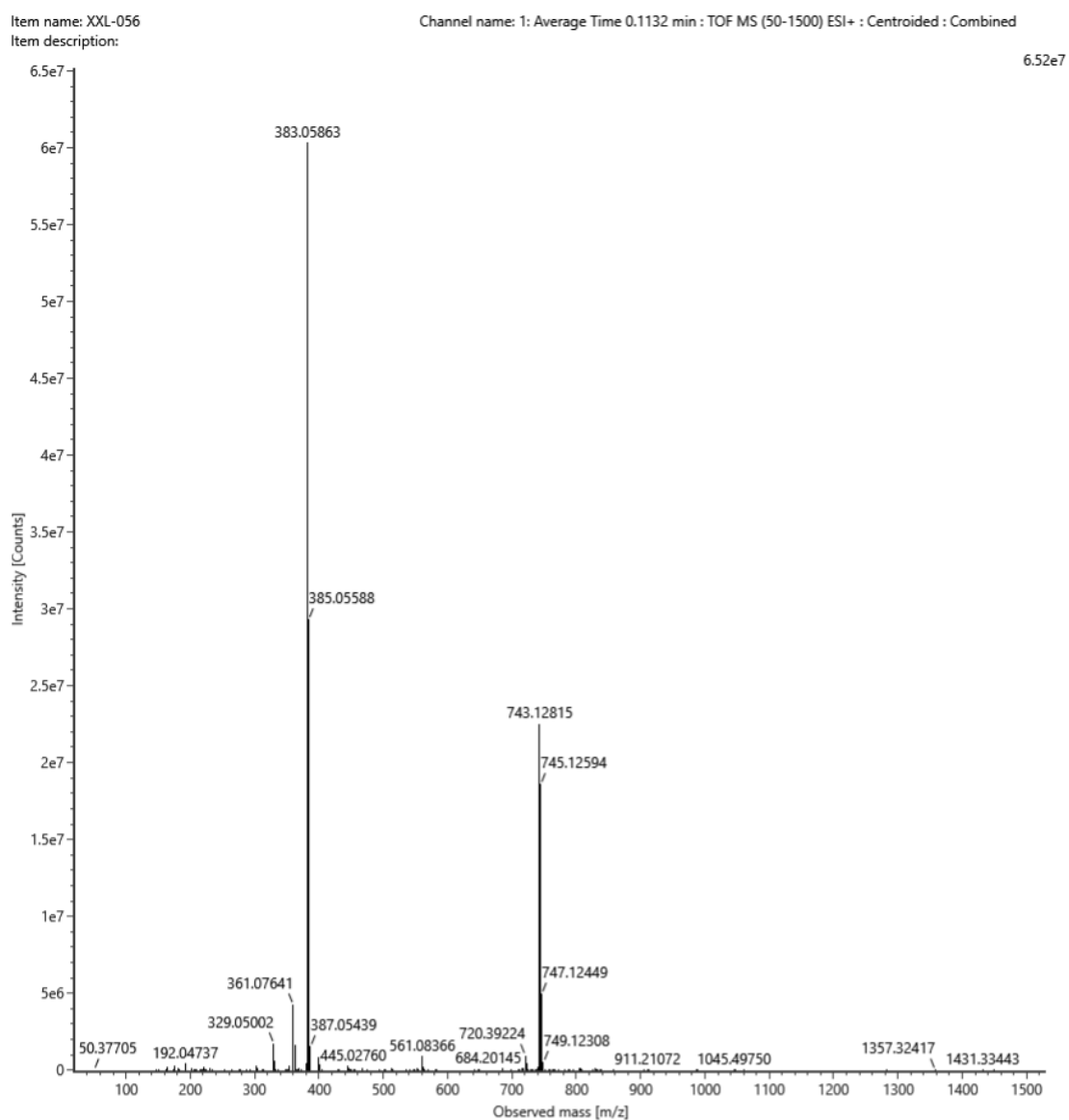
3.46e7



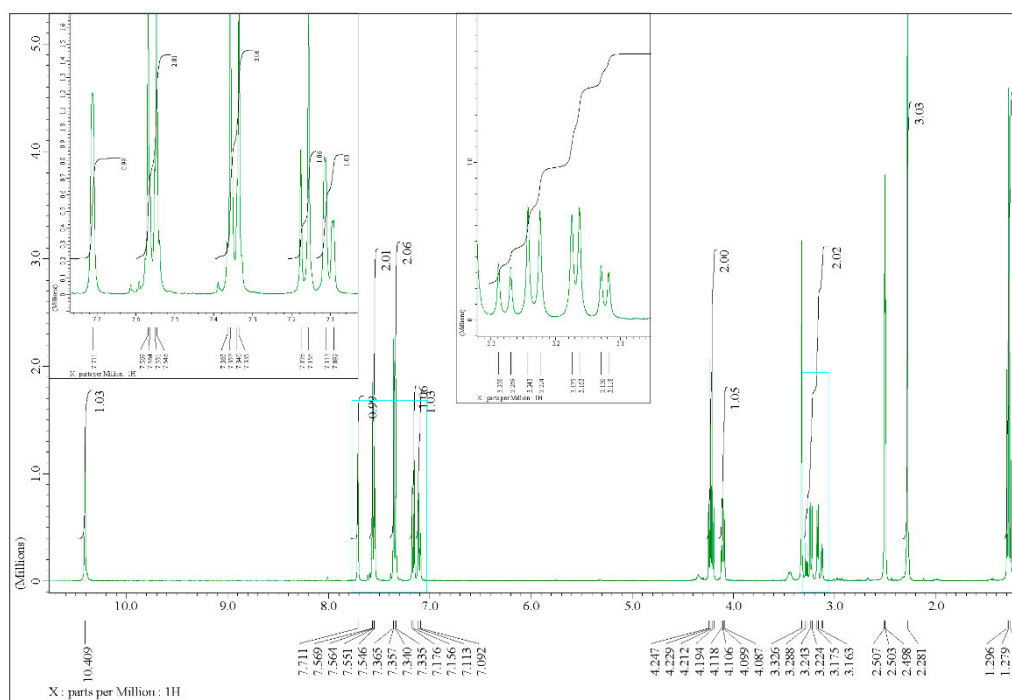
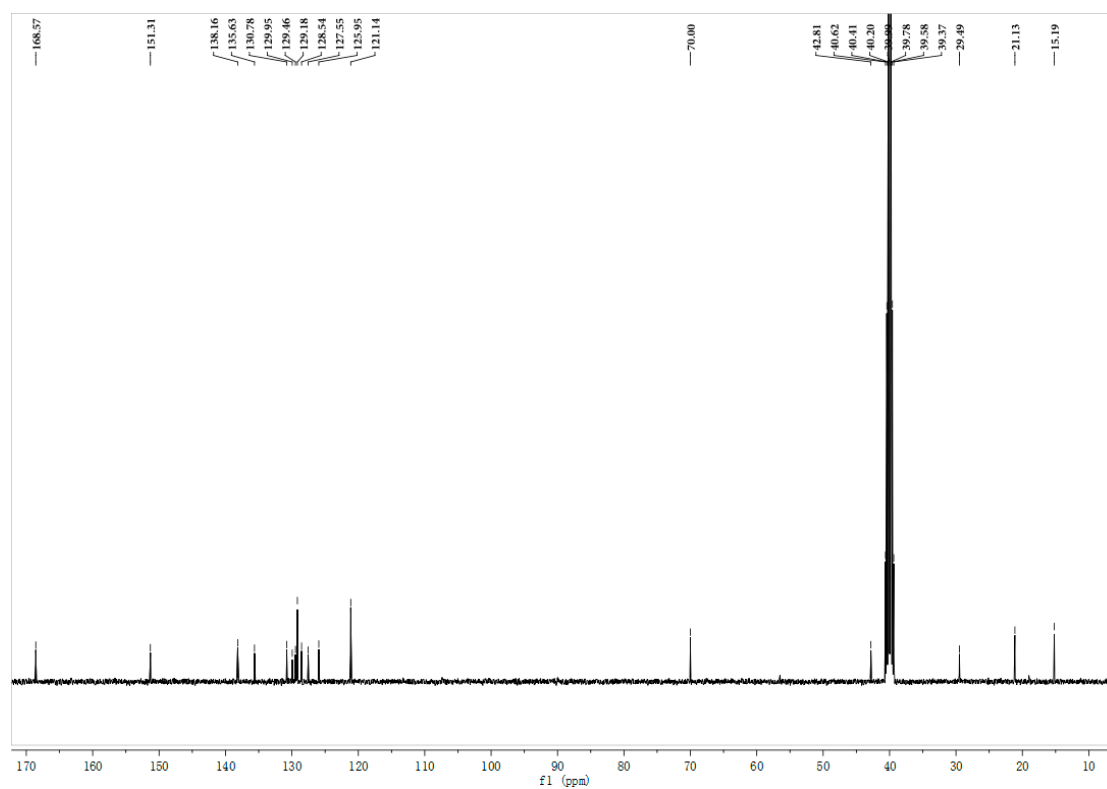
HRMS of compound 4s







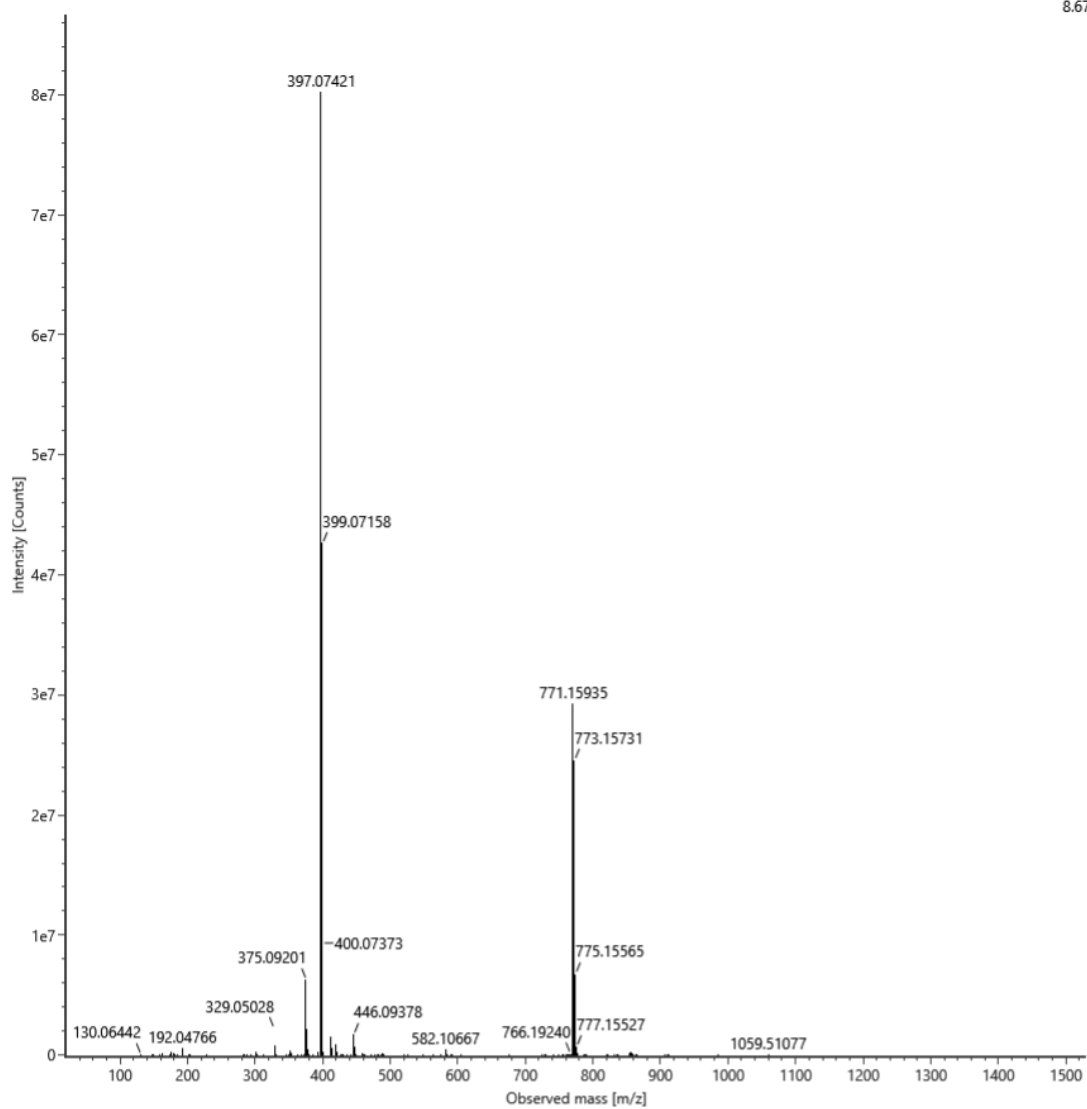
HRMS of compound 4t

<sup>1</sup>H NMR of compound 4u<sup>13</sup>C NMR of compound 4u

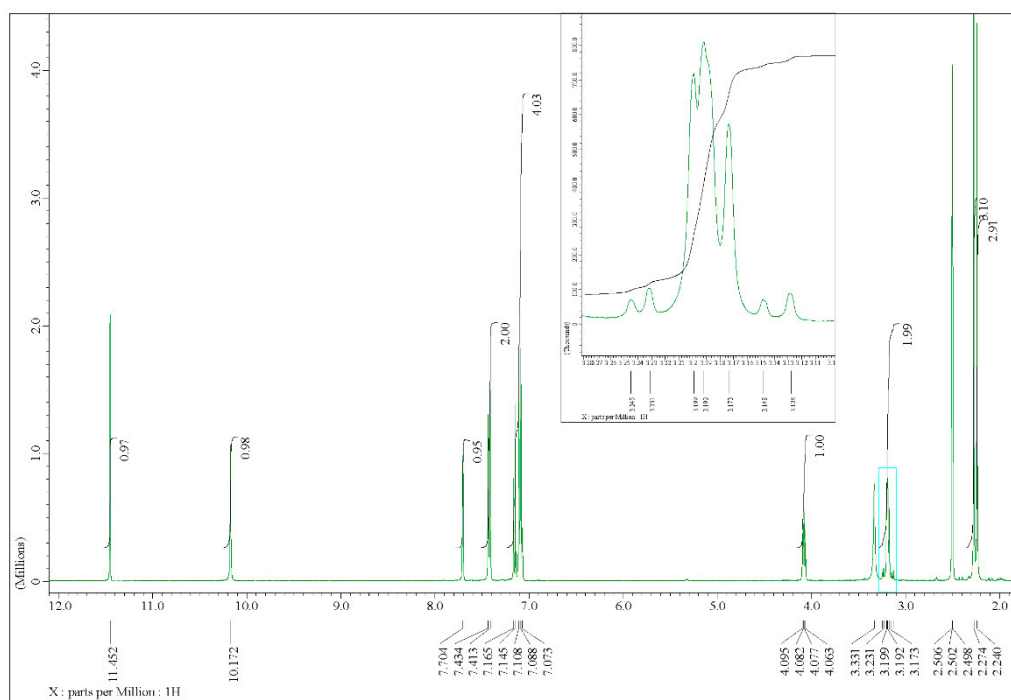
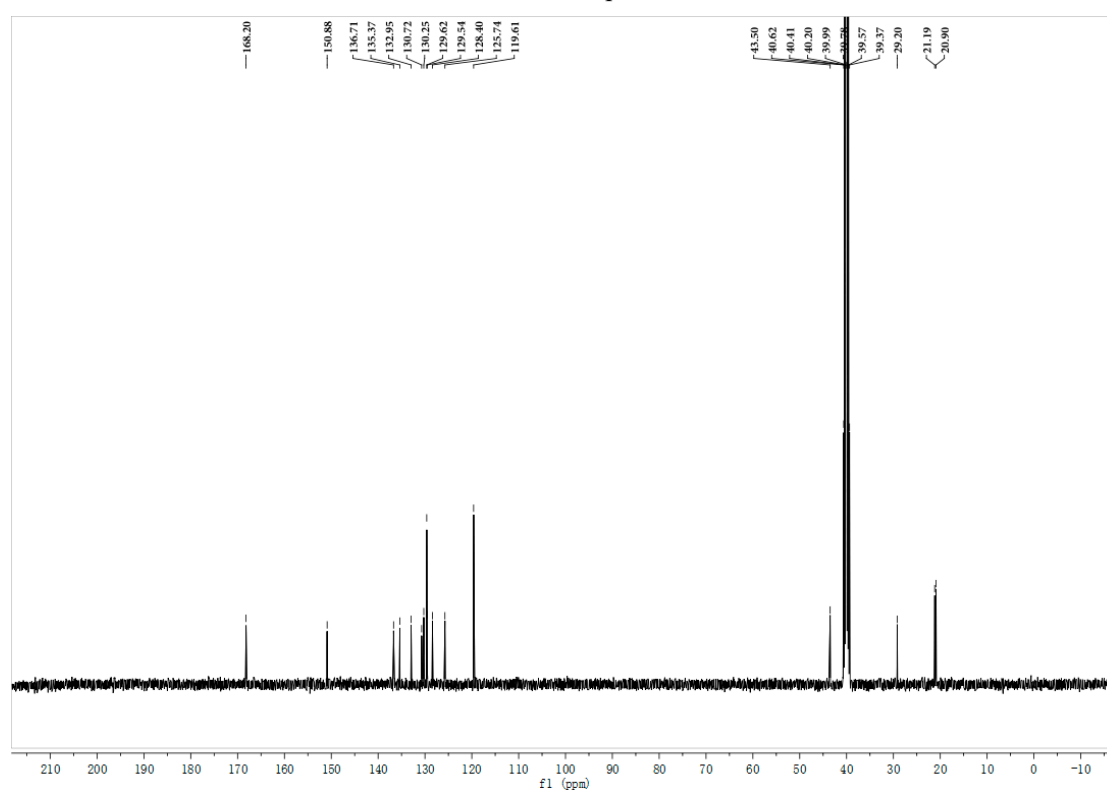
Item name: XXL-054  
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

8.67e7



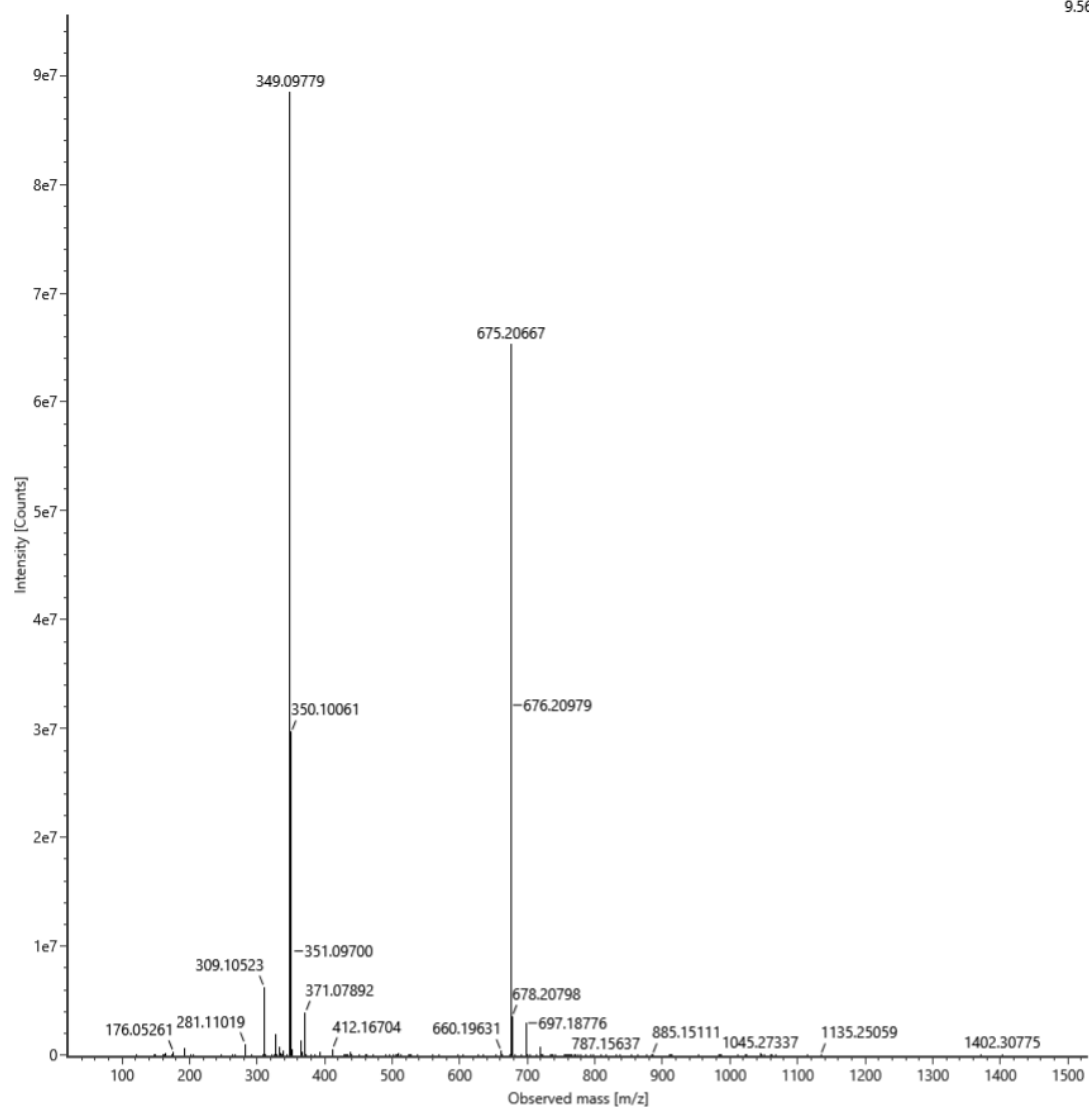
HRMS of compound 4u

 $^1\text{H}$  NMR of compound 4v $^{13}\text{C}$  NMR of compound 4v

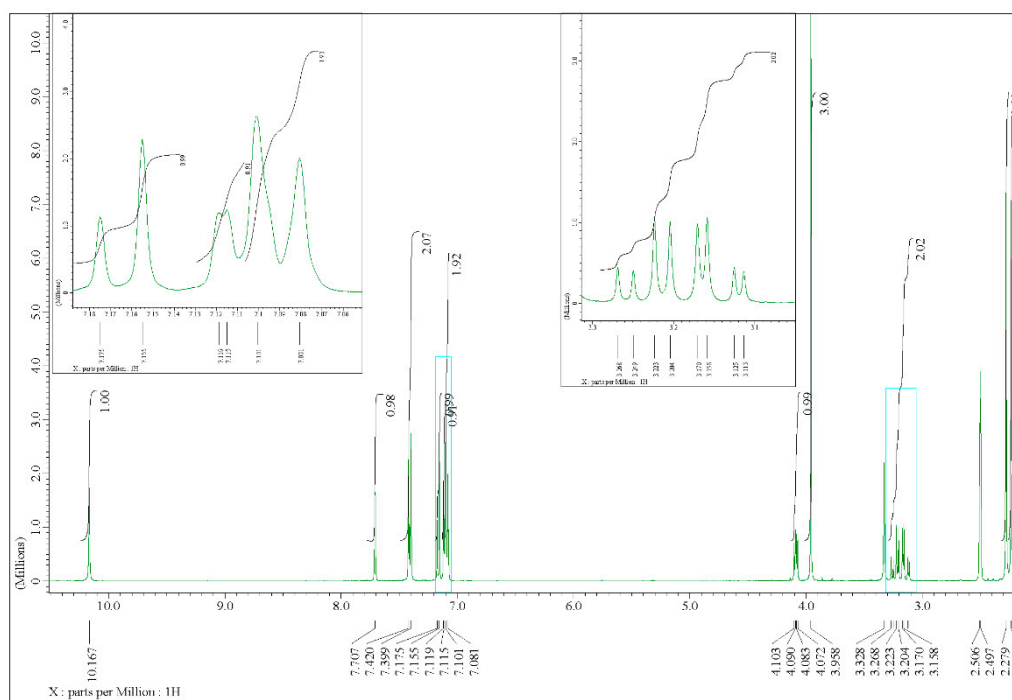
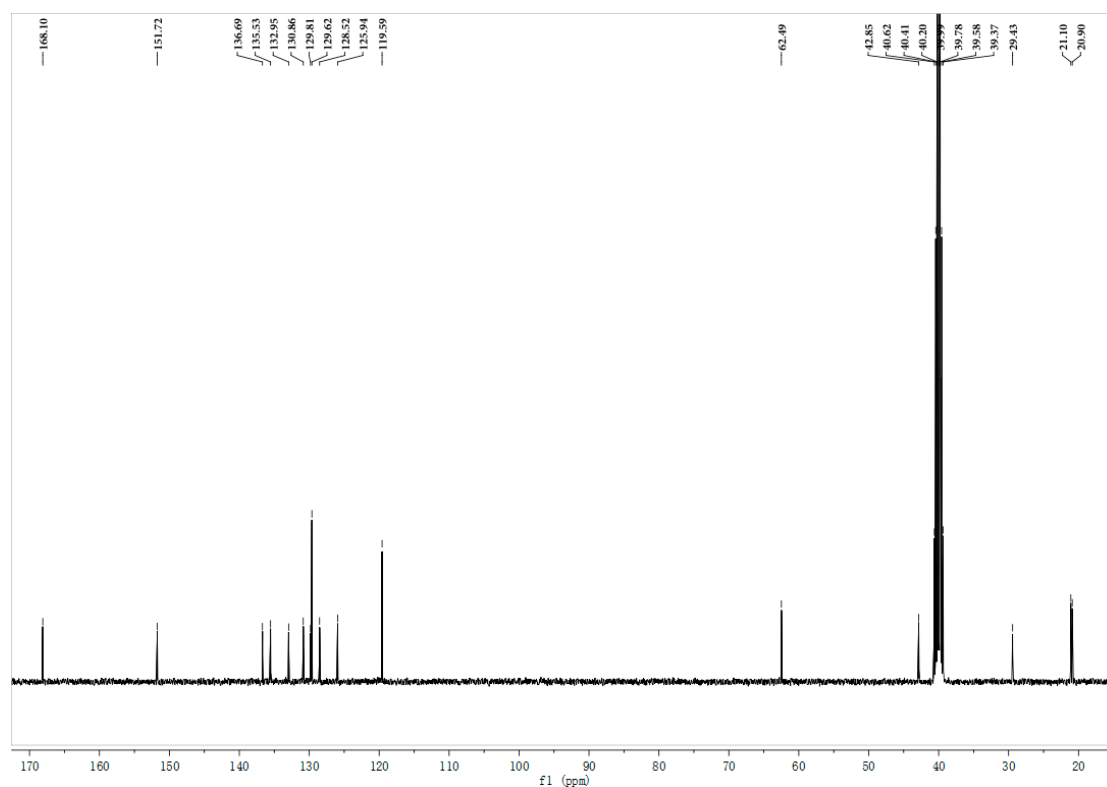
Item name: XXL-046  
Item description:

Channel name: 1: Average Time 0.1175 min : TOF MS (50-1500) ESI+ : Centroided : Combined

9.56e7



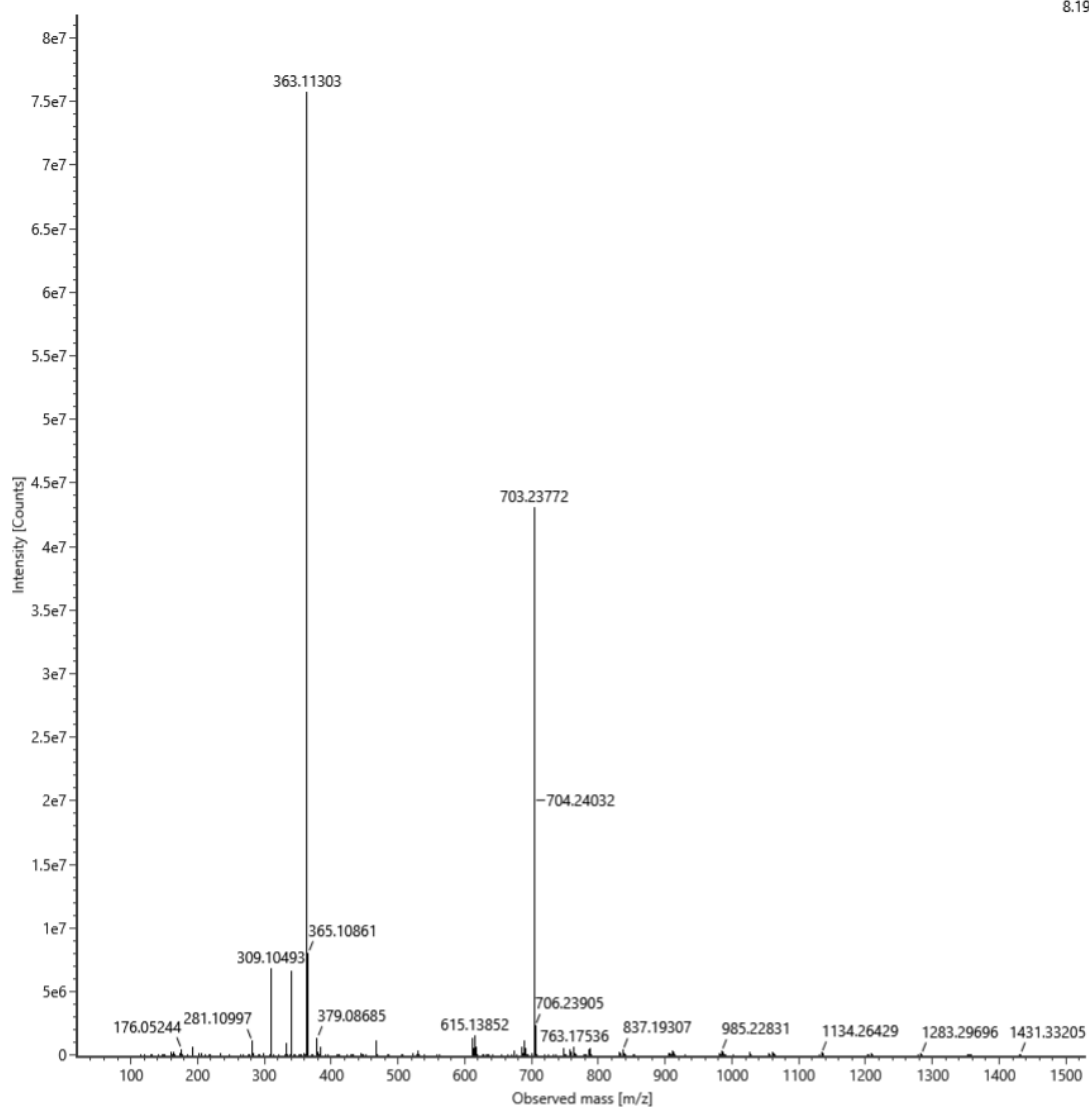
HRMS of compound 4v

<sup>1</sup>H NMR of compound 4w<sup>13</sup>C NMR of compound 4w

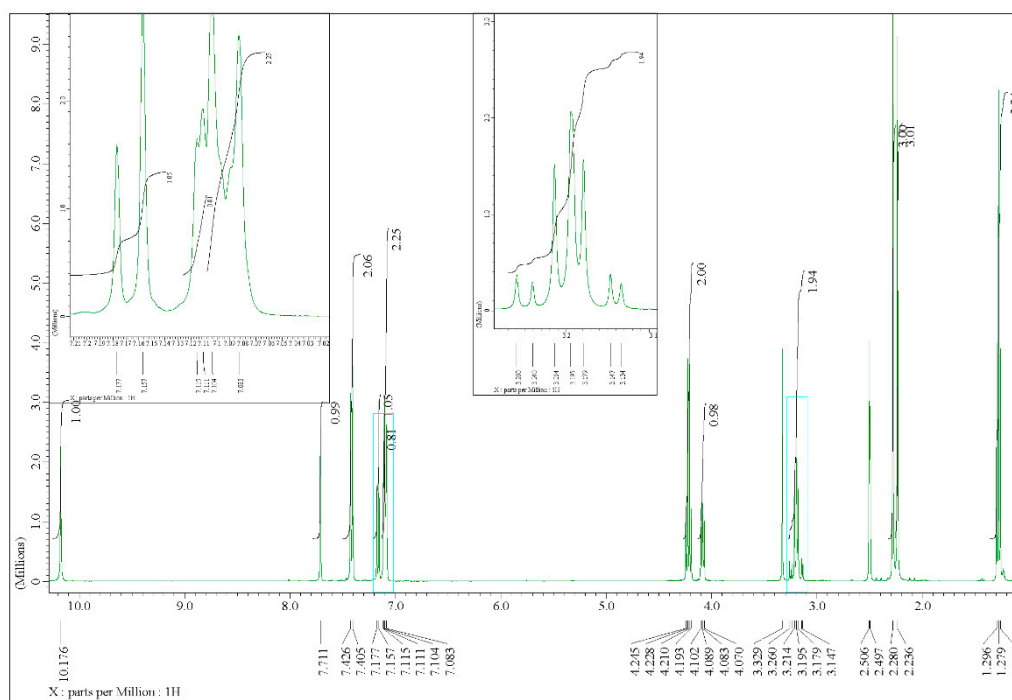
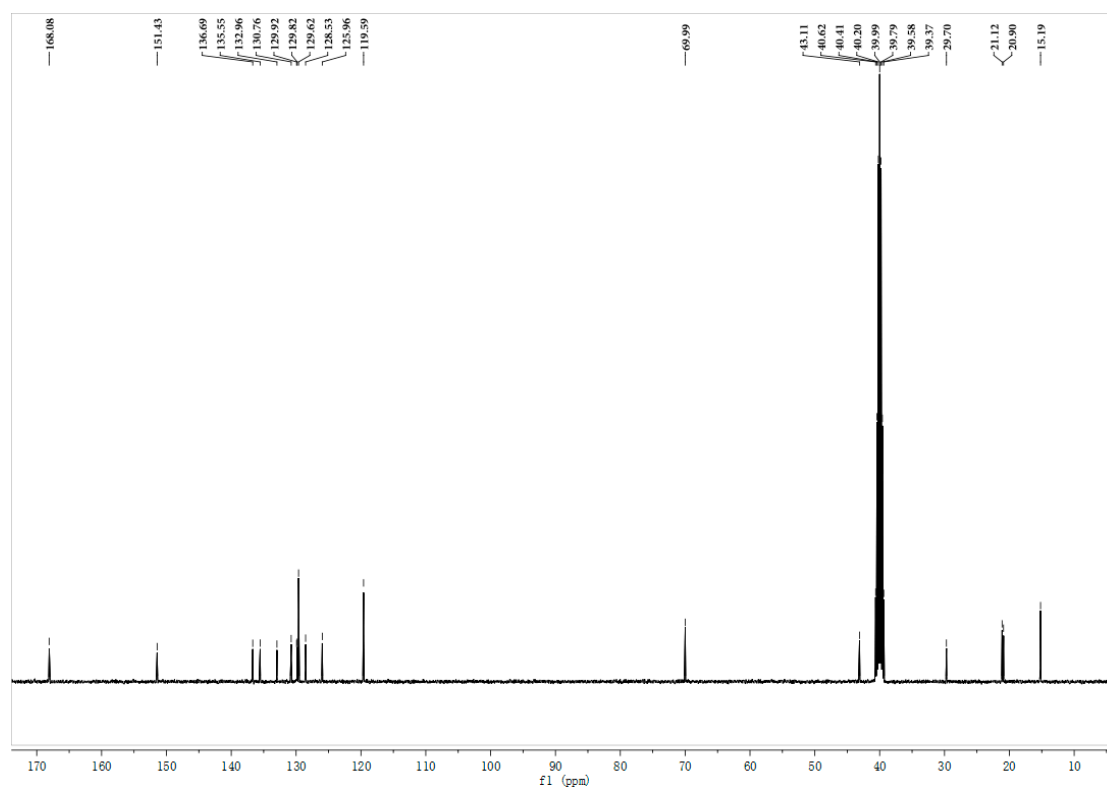
Item name: XXL-058  
Item description:

Channel name: 1: Average Time 0.1175 min : TOF MS (50-1500) ESI+ : Centroided : Combined

8.19e7



HRMS of compound 4w

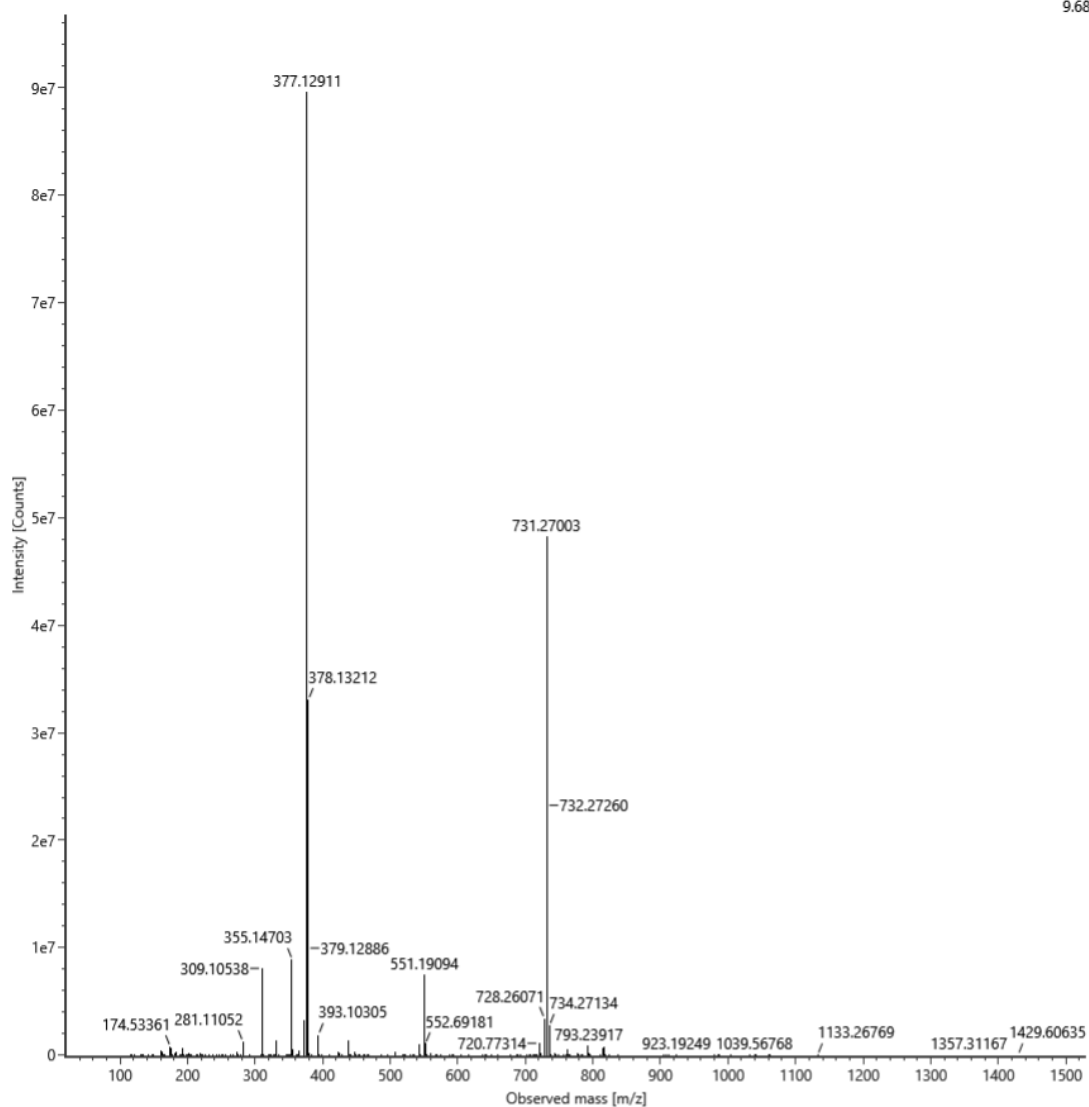
<sup>1</sup>H NMR of compound 4x<sup>13</sup>C NMR of compound 4x



Item name: XXL-055  
Item description:

Channel name: 1: Average Time 0.1217 min : TOF MS (50-1500) ESI+ : Centroided : Combined

9.68e7



HRMS of compound 4x