

## *Supplementary Material*

# **Herbicidal Activity and Molecular Docking Study of Novel ACCase Inhibitors**

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**Correspondence author:**

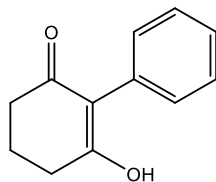
**Professor Ying Fu, Department of Applied Chemistry, College of Science,  
Northeast Agricultural University, Harbin 150030, China**

**Tel: 86-451-55190070**

**Email address: [fuying@neau.edu.cn](mailto:fuying@neau.edu.cn)**

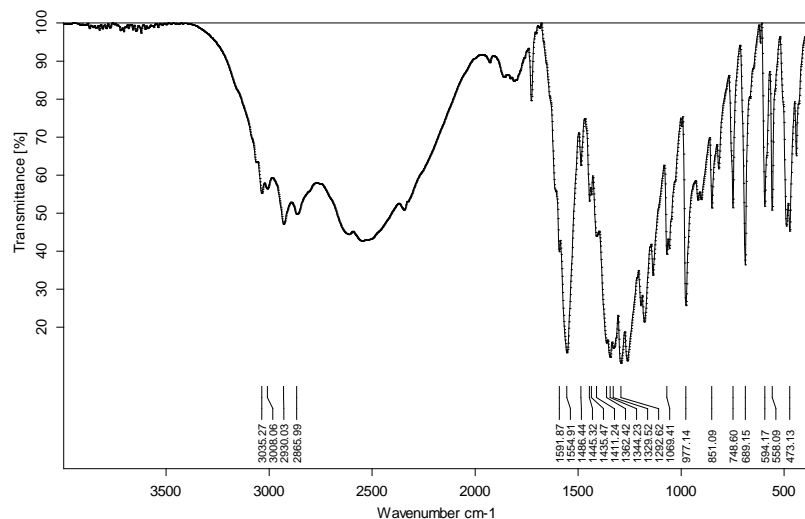
**Supplementary Information**

## Compound 2a



$C_{12}H_{12}O_2$

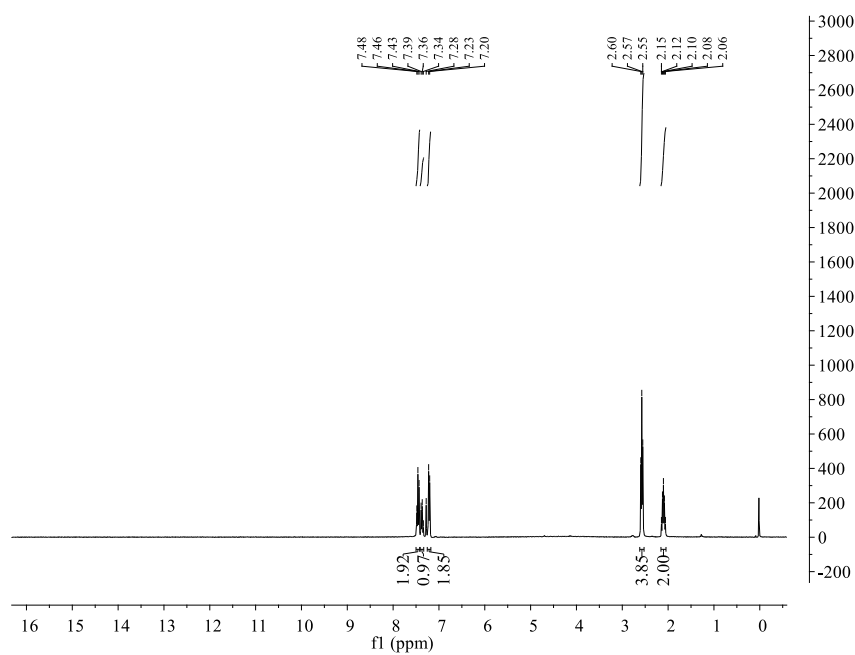
IR



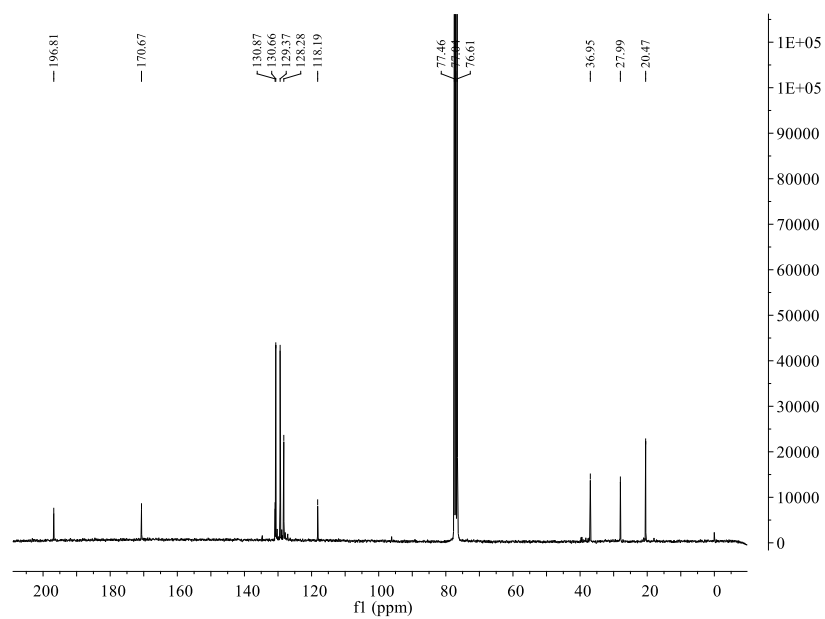
F:\Sample description.153 Sample description Instrument type and / or accessory 21/04/2018

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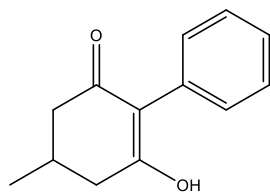
$^1H$  NMR



# <sup>13</sup>C NMR

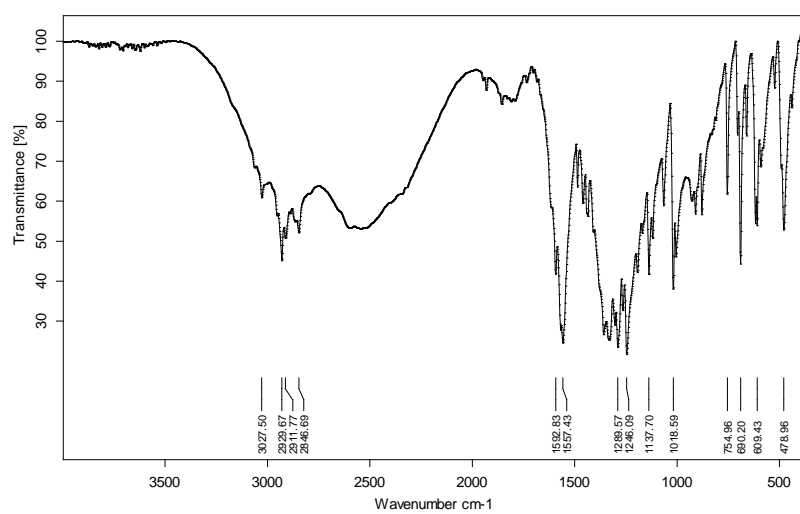


## Compound 2b

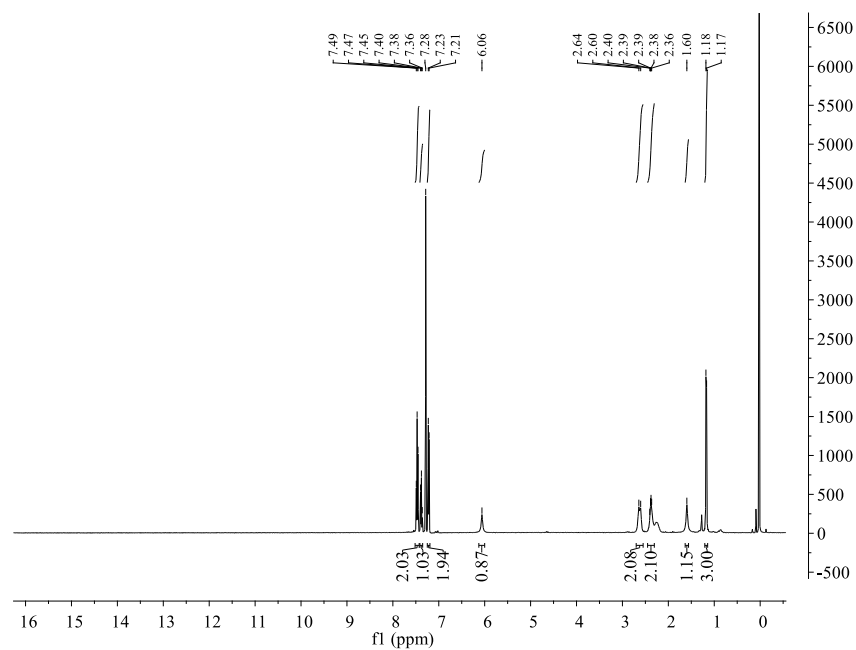


$C_{13}H_{14}O_2$

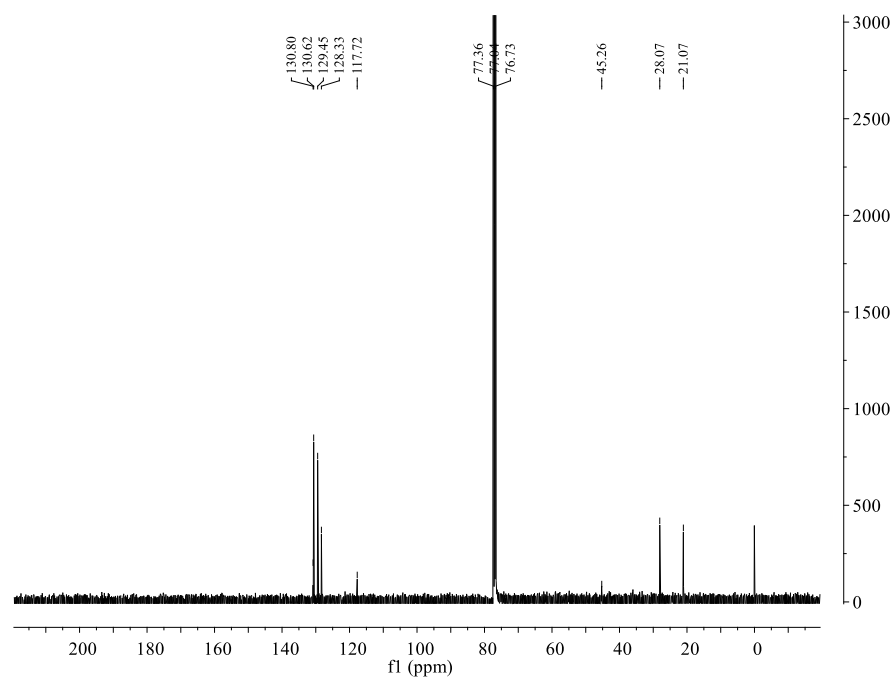
IR



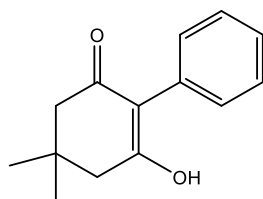
$^1H$  NMR



# <sup>13</sup>C NMR

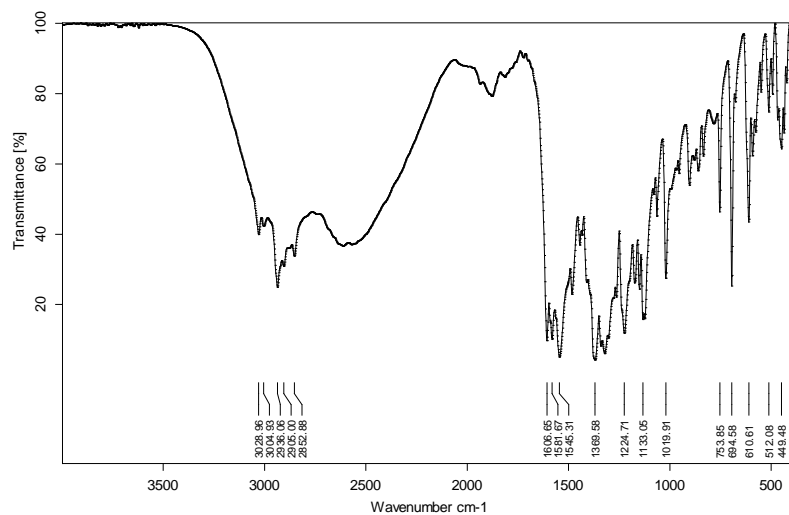


## Compound 2c

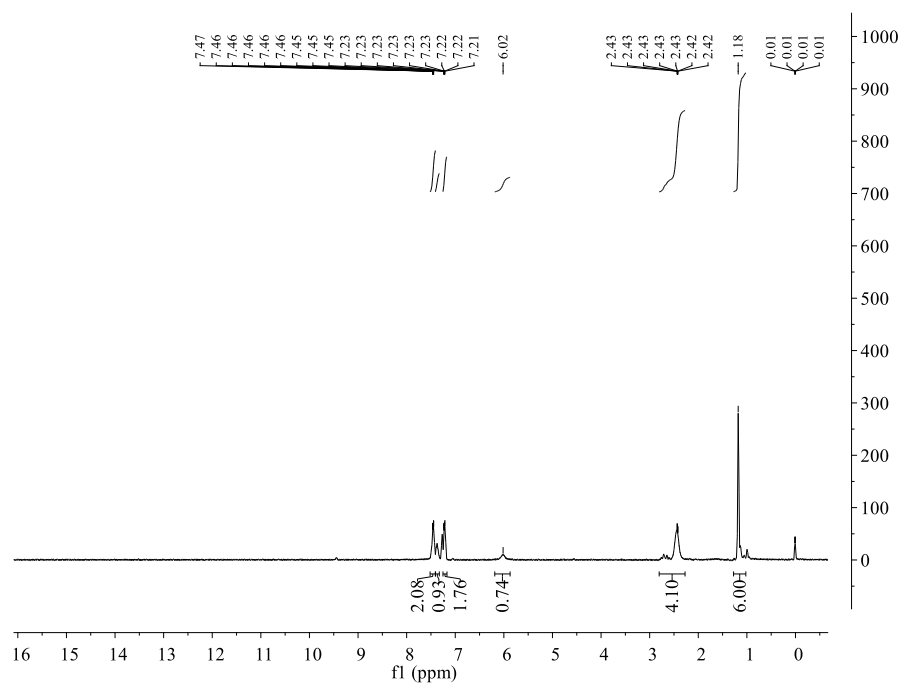


$C_{14}H_{16}O_2$

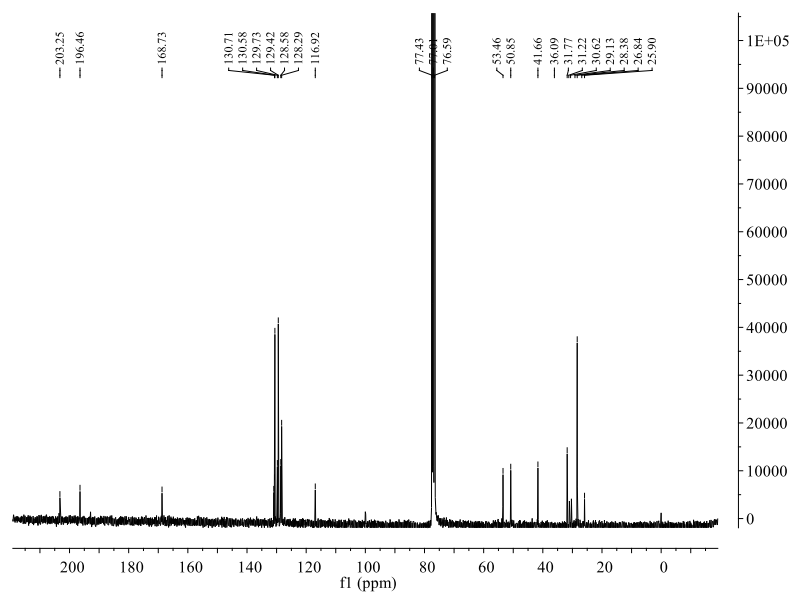
IR



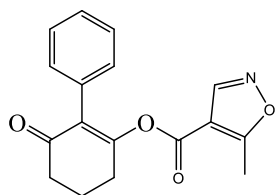
$^1H$  NMR



# <sup>13</sup>C NMR

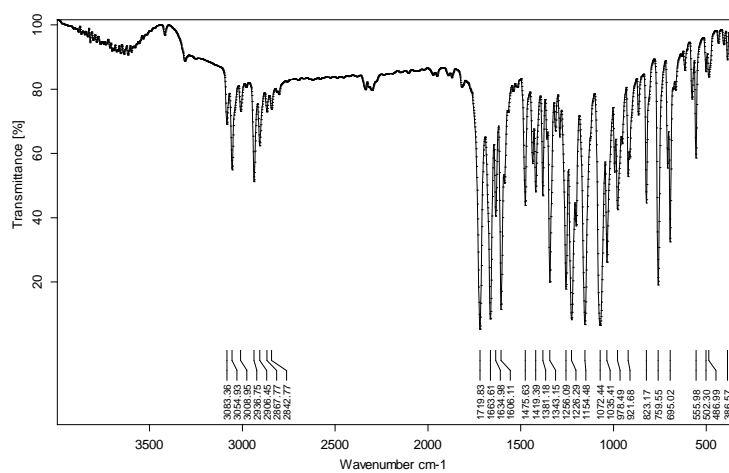


## Compound 3a

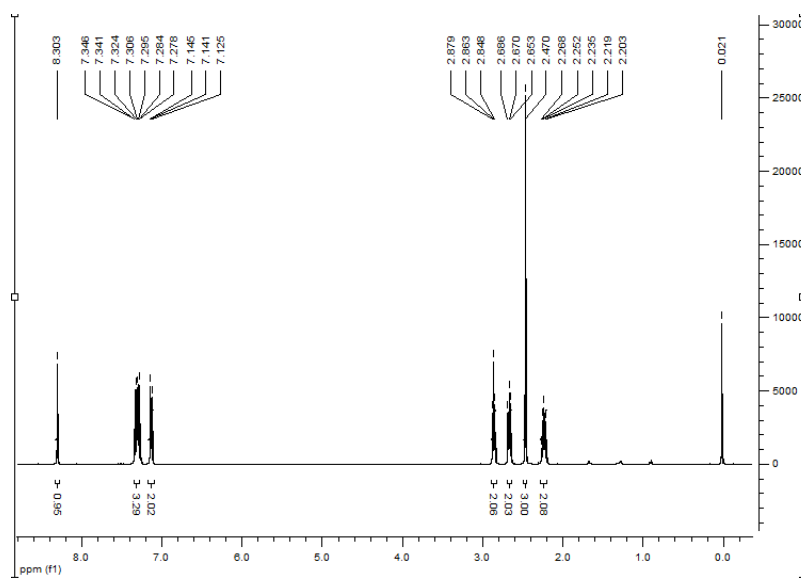


$C_{17}H_{15}NO_4$

## IR

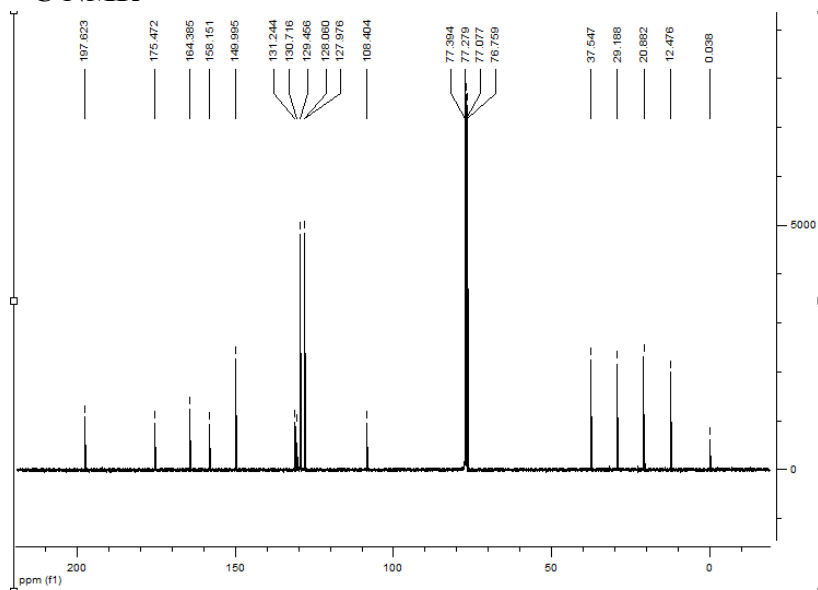


## $^1H$ NMR





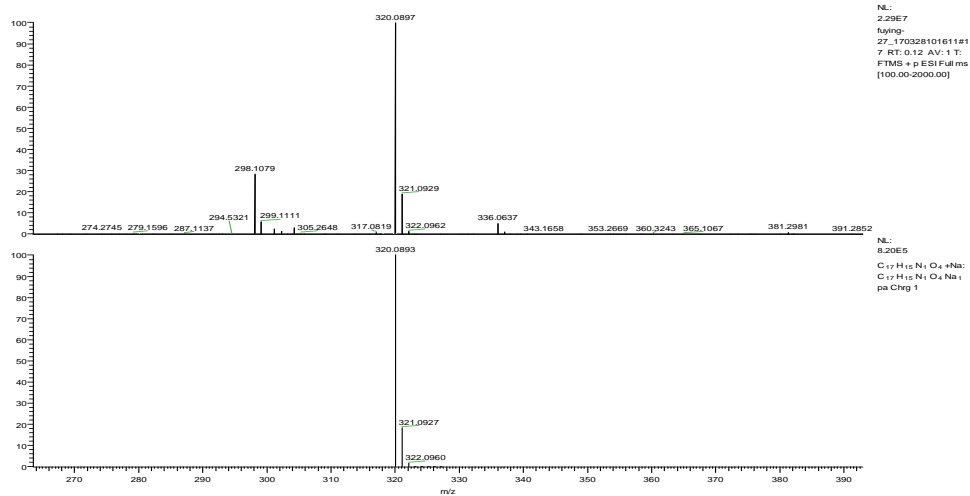
## <sup>13</sup>C NMR



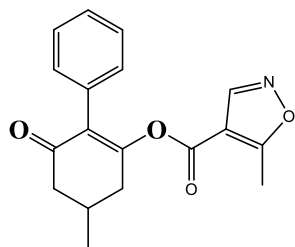
## HRMS

F:\Users\...\_27\_170328101611

2020/01/17 11:04:13 AM 27e  
3 ppm

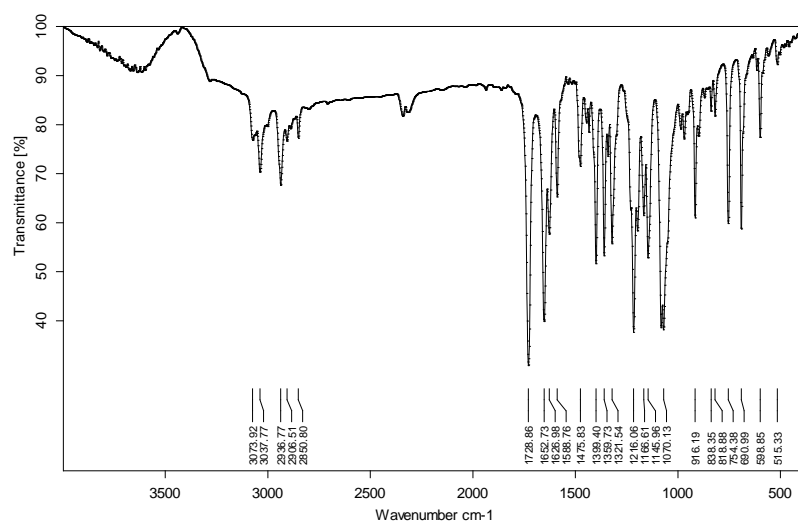


## Compound 3b

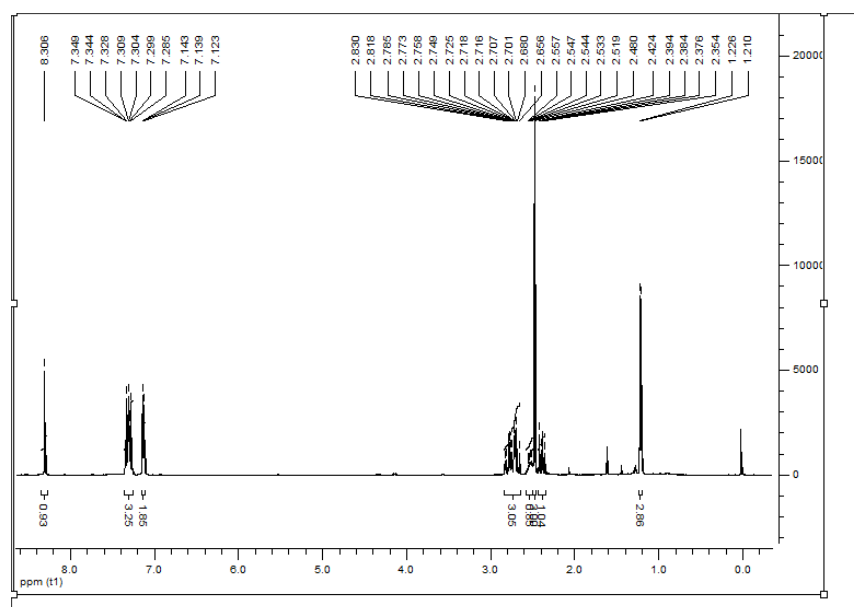


$C_{18}H_{17}NO_4$

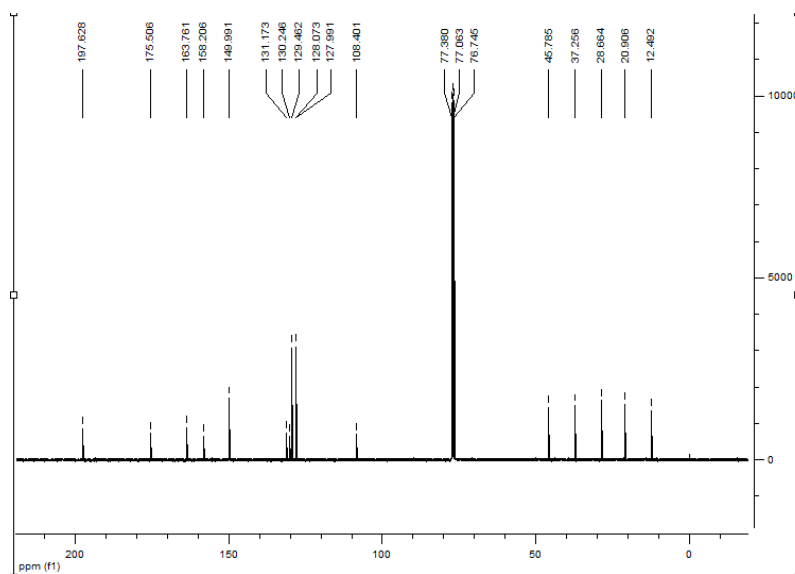
IR



$^1H$  NMR



## <sup>13</sup>C NMR

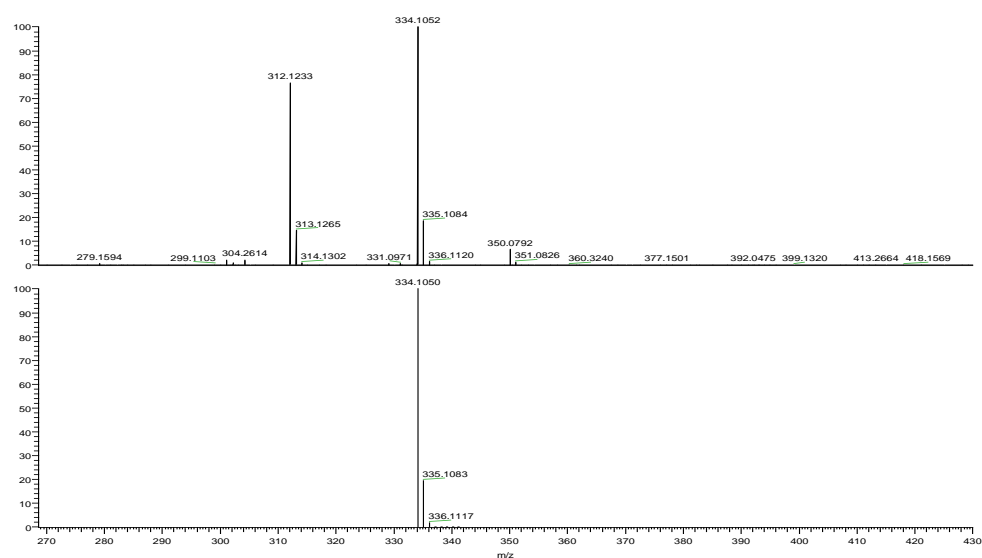


## HRMS

F:\Users\...Vuying-28\_170328145034

3/28/2017 3:03:38 PM  
.6 ppm

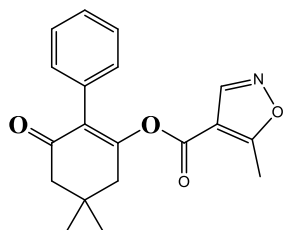
28#



NL:  
1.60E7  
Vuying-  
28\_170328145034#1  
2 RT: 0.08 AV: 1 T:  
FTMS + p ESI Full ms  
[100.00-2000.00]

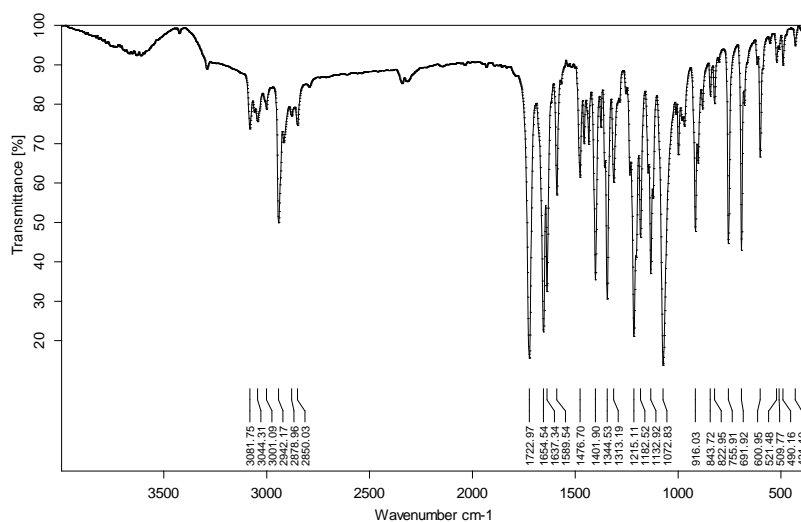
NL:  
8.11E5  
C<sub>18</sub>H<sub>17</sub>N<sub>1</sub>O<sub>4</sub>+Na:  
C<sub>18</sub>H<sub>17</sub>N<sub>1</sub>O<sub>4</sub>Na:  
pa Chrg 1

## Compound 3c

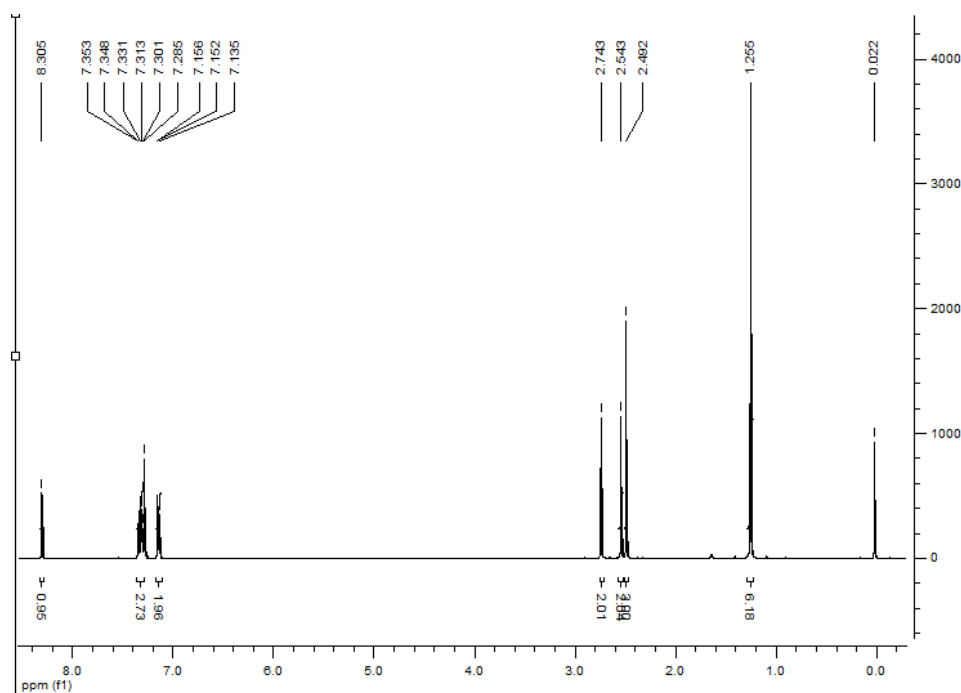


$C_{19}H_{19}NO_4$

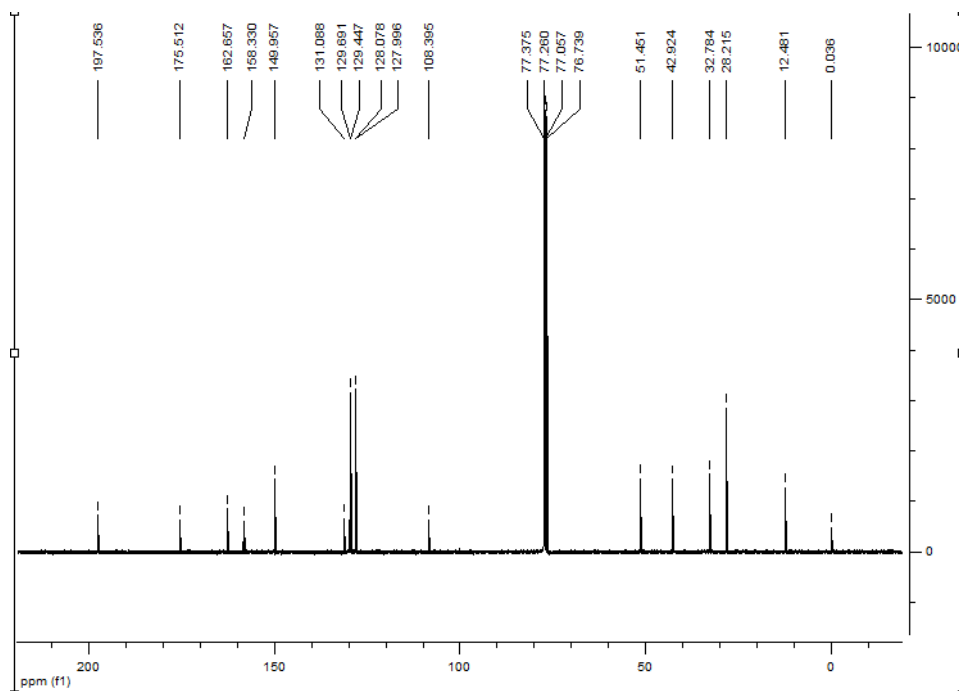
IR



$^1H$  NMR



# <sup>13</sup>C NMR

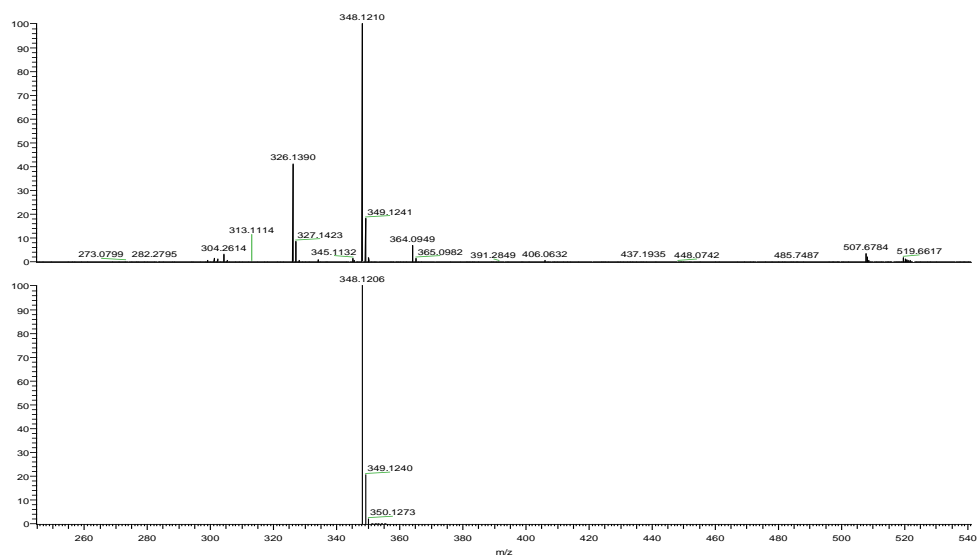


# HRMS

F:\Users\...uying-29\_170328145034

2020/07/30 08:33 PM

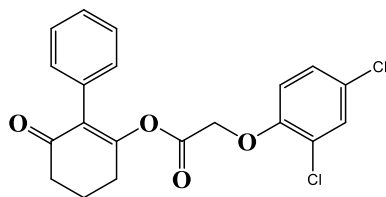
29#



NL:  
1.96E7  
fuying-  
29\_170328145034#5  
RT: 0.03 AV: 1 T:  
FTMS + p ESI Full ms  
[100.00-2000.00]

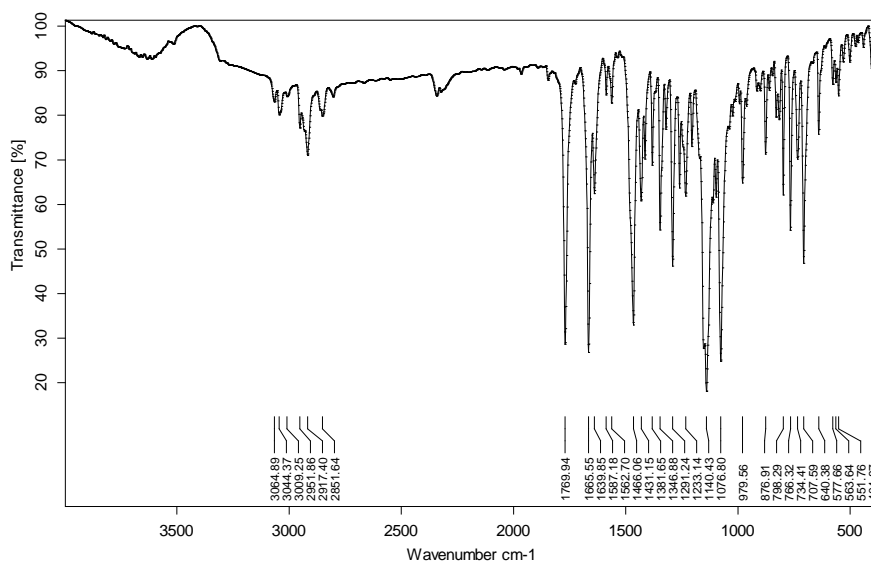
NL:  
8.03E5  
C<sub>19</sub>H<sub>19</sub>N<sub>1</sub>O<sub>4</sub>+Na:  
C<sub>19</sub>H<sub>19</sub>N<sub>1</sub>O<sub>4</sub>Na:  
pa Chg 1

## Compound 3d

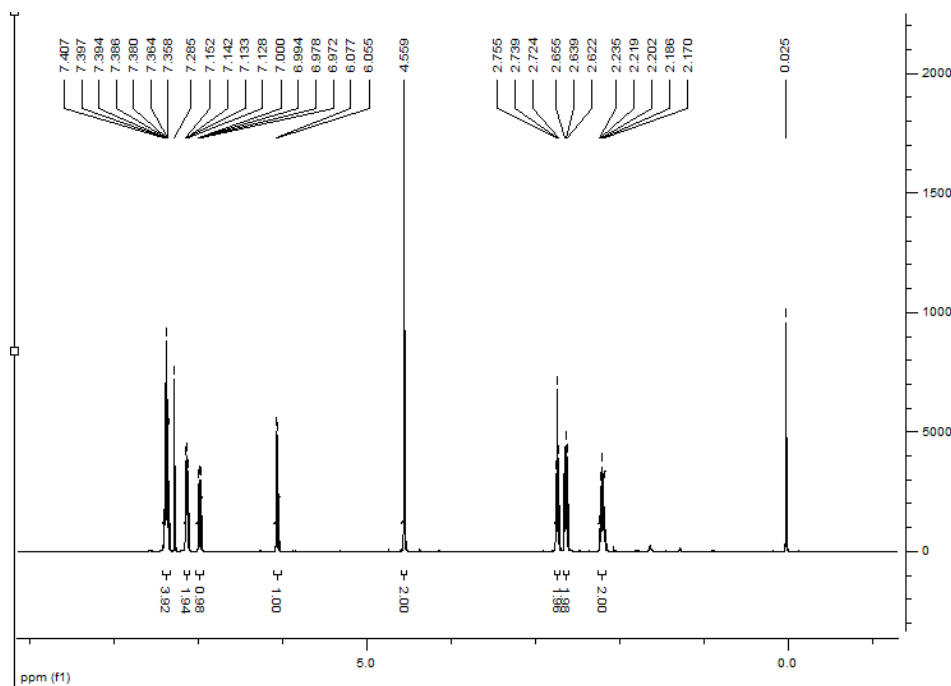


$C_{20}H_{16}Cl_2O_4$

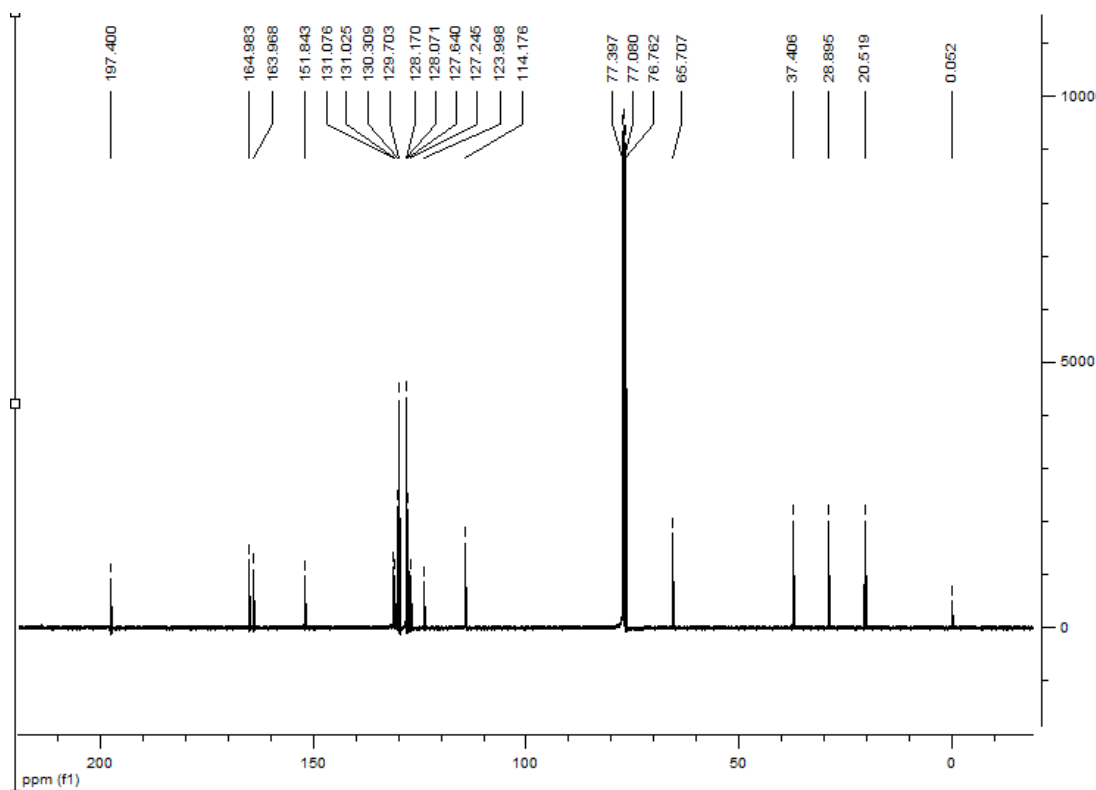
IR



$^1H$  NMR



# <sup>13</sup>C NMR

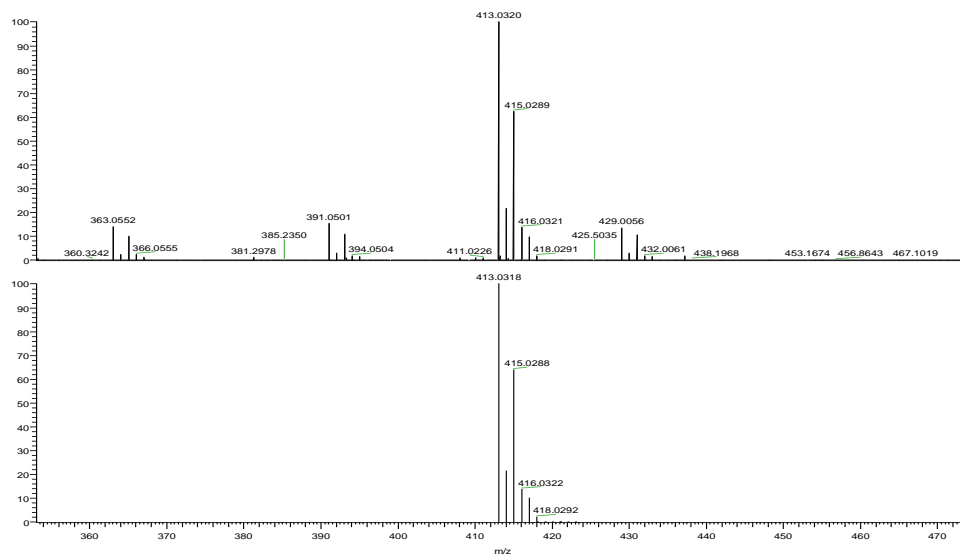


# HRMS

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3/28/2017 3:12:39 PM  
.5 ppm

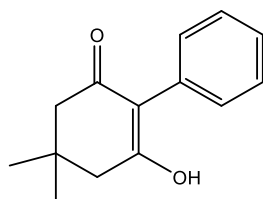
30#



NL:  
3.82E6  
Vuying-  
30\_170328145034#1  
9 RT: 0.14 AV: 1 T:  
FTMS + p ESI Full ms  
[100.00-2000.00]

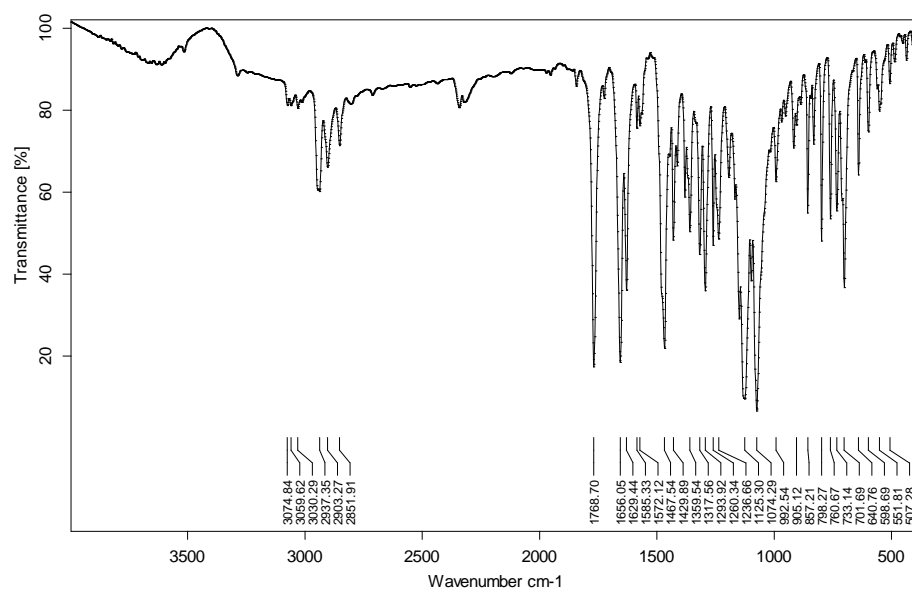
NL:  
4.58E5  
C<sub>20</sub>H<sub>18</sub>Cl<sub>2</sub>O<sub>4</sub>+Na:  
C<sub>20</sub>H<sub>18</sub>Cl<sub>2</sub>O<sub>4</sub>Na:  
pa Chrg 1

## Compound 3e

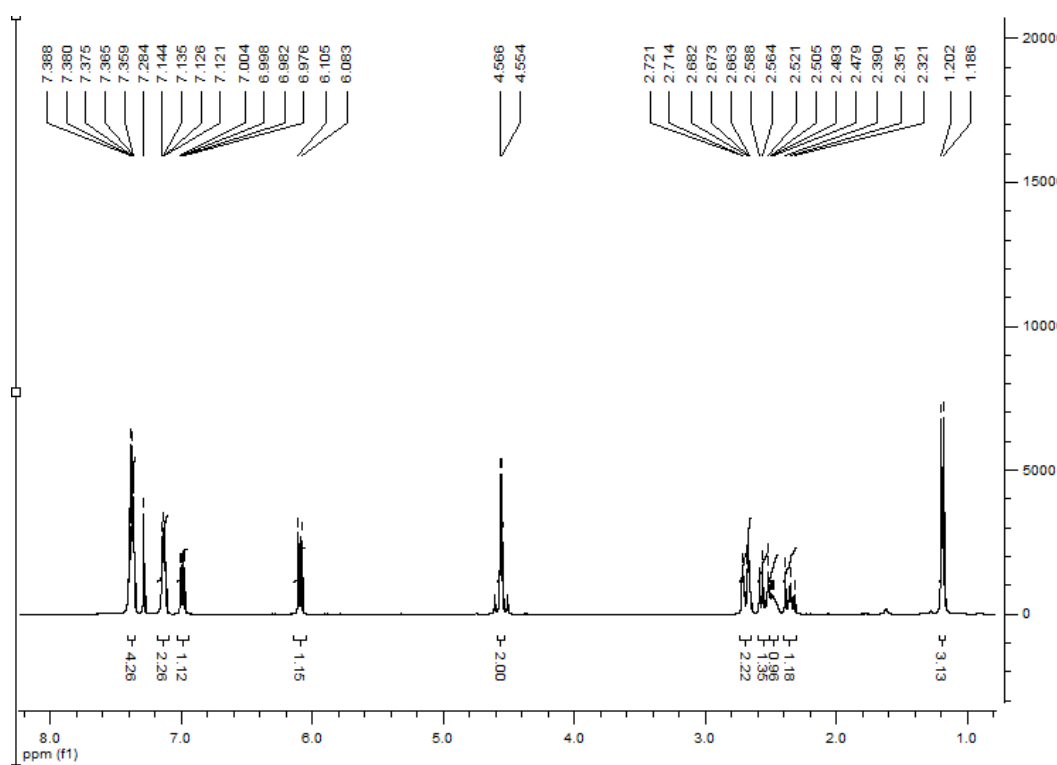


$C_{14}H_{16}O_2$

IR

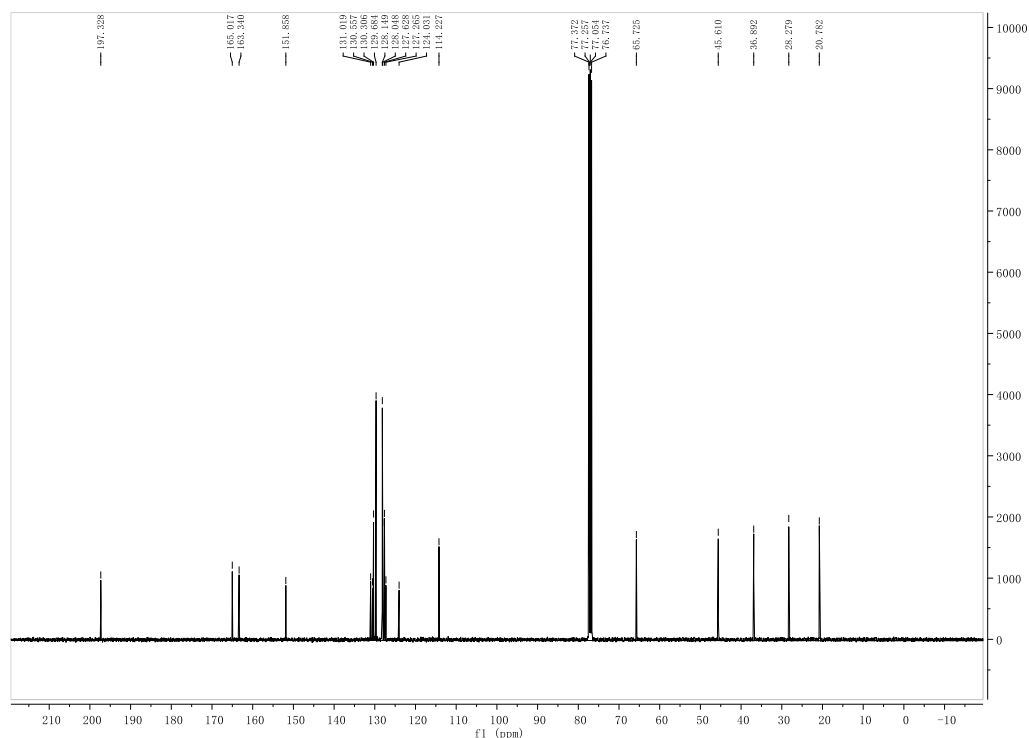


$^1H$  NMR





# <sup>13</sup>C NMR

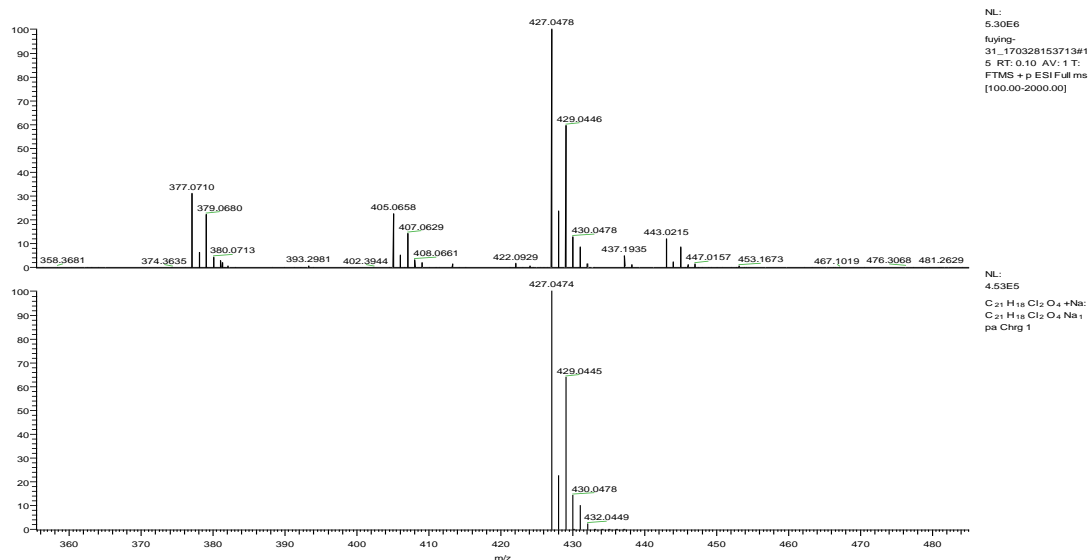


# HRMS

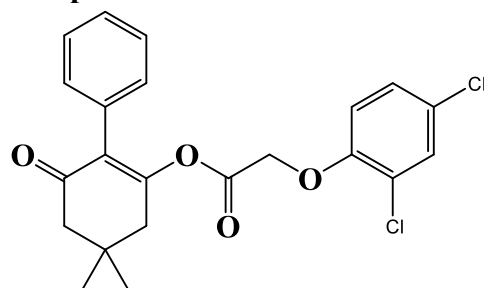
F:\Users\... \uying-31\_170328153713

3/28/2017 4:16:47 PM  
9 ppm

31#

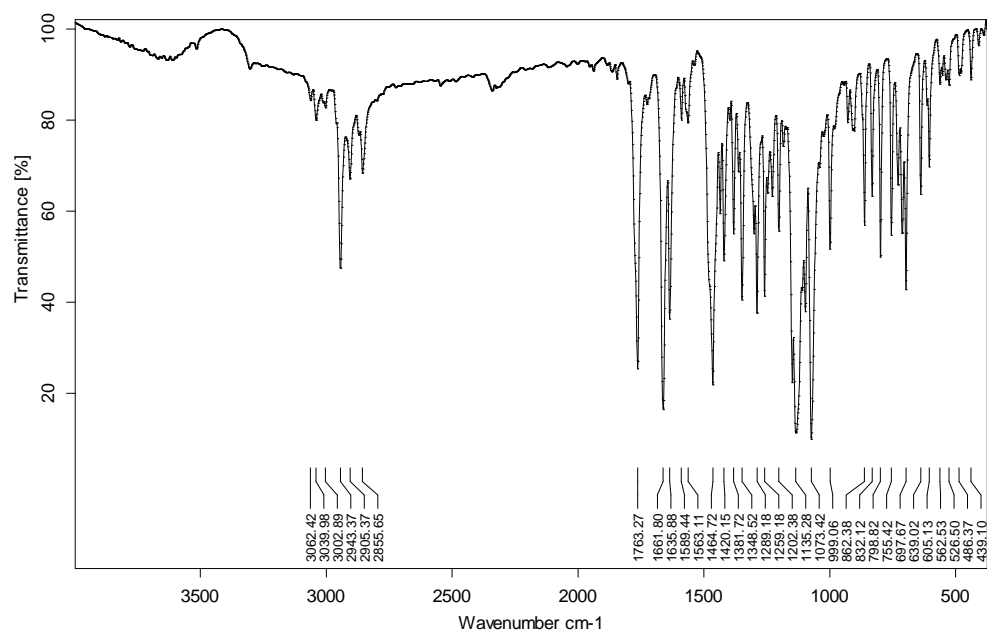


# Compound 3f

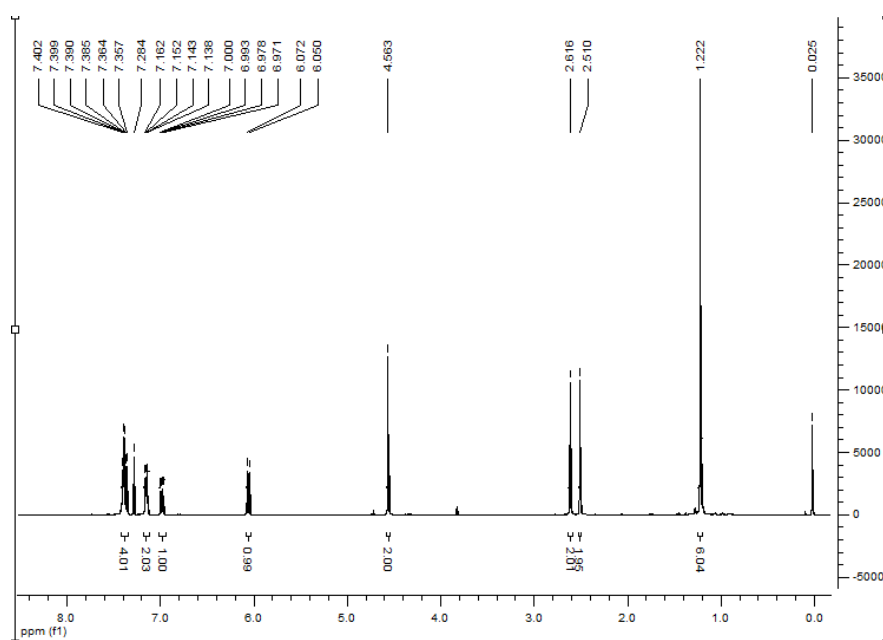


$C_{22}H_{20}Cl_2O_4$

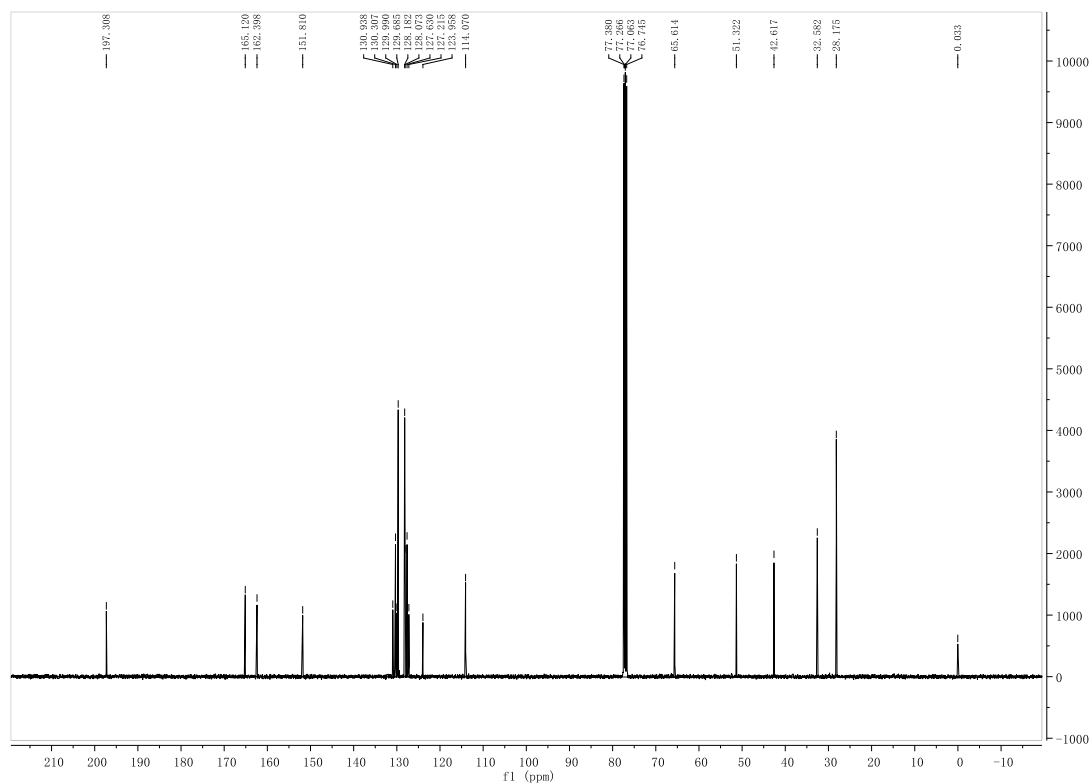
## IR



## <sup>1</sup>H NMR



## $^{13}\text{C}$ NMR

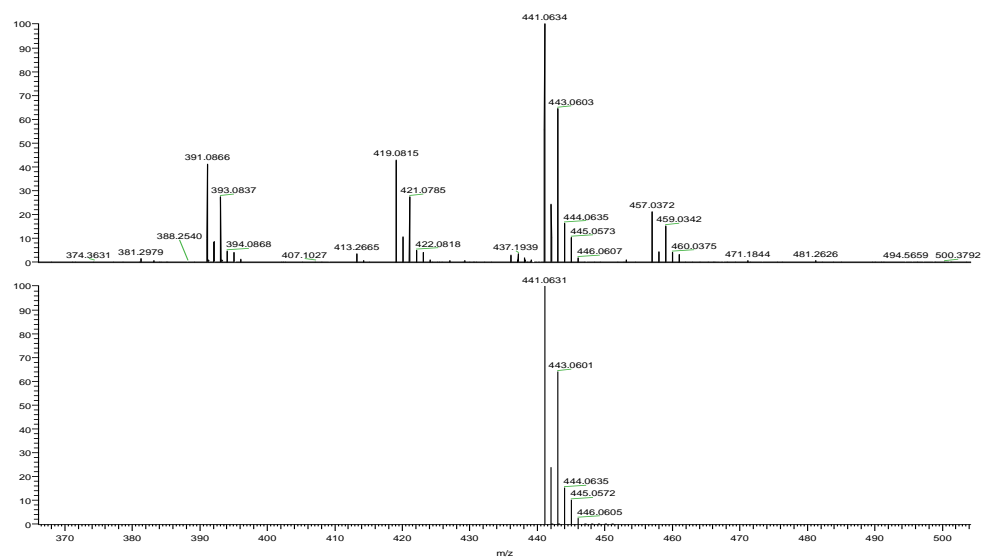


## HRMS

F:\Users\...uying-32\_170328153713

3/28/2017 4:21:51 PM  
7 ppm

32#



NL:  
3.69E6  
fuying-  
32\_170328153713#1  
1 RT: 0.08 AV: 1 T:  
FTMS + p ESI Full ms  
[100.00-2000.00]

NL:  
4.48E5  
C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>O<sub>4</sub>+Na:  
C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>O<sub>4</sub>Na:  
pa Chrg 1