

*Nine new cytochalasan alkaloids from Chaetomium globosum TW1-1 (Ascomycota, Sordariales)*

Chunmei Chen<sup>1</sup>, Qingyi Tong<sup>1</sup>, Hucheng Zhu<sup>1</sup>, Dongdong Tan<sup>1</sup>, Jinwen Zhang<sup>3</sup>, Yongbo Xue<sup>1</sup>, Guangmin Yao<sup>1</sup>, Zengwei Luo<sup>1</sup>, Jianping Wang<sup>1,\*</sup>, Yanyan Wang<sup>2,\*</sup> & Yonghui Zhang<sup>1,\*</sup>

<sup>1</sup> Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China

<sup>2</sup> First College of Clinical Medical Science, China Three Gorges University & Yichang Central People's Hospital, Yichang 443003, China

<sup>3</sup> Tongji Hospital Affiliated to Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China

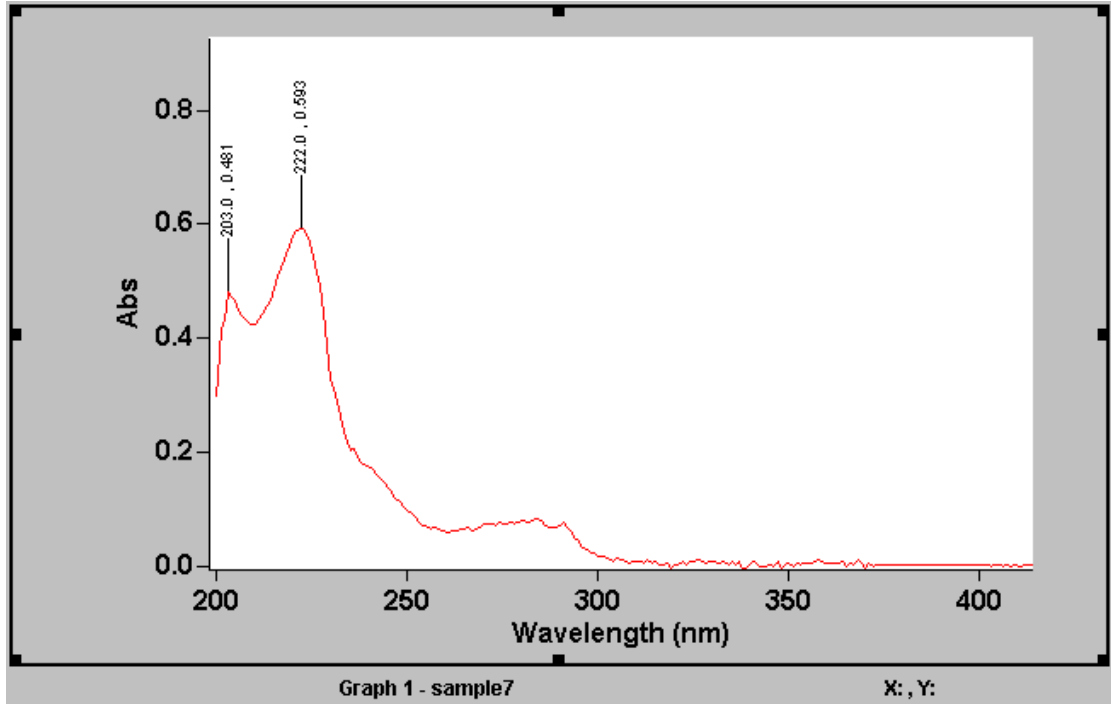
# Content

Cytotoxic activities of compounds <b>1–9</b> .....	1
UV, IR, MS, and NMR spectrum of compound <b>1</b> .....	2
UV, IR, MS, and NMR spectrum of compound <b>2</b> .....	5
UV, IR, MS, and NMR spectrum of compound <b>3</b> .....	10
UV, IR, MS, and NMR spectrum of compound <b>4</b> .....	14
UV, IR, MS, and NMR spectrum of compound <b>5</b> .....	19
UV, IR, MS, and NMR spectrum of compound <b>6</b> .....	23
UV, IR, MS, and NMR spectrum of compound <b>7</b> .....	28
UV, IR, MS, and NMR spectrum of compound <b>8</b> .....	32
UV, IR, MS, and NMR spectrum of compound <b>9</b> .....	37

**Table S1. Cytotoxic activities of compounds 1–9 ( $\mu\text{M}$ )**

Compound	HL-60	SMMC-7721	A-549	MCF-7	SW480	BEAS-2B
<b>1</b>	>40	>40	>40	>40	>40	>40
<b>2</b>	>40	>40	>40	>40	>40	>40
<b>3</b>	>40	>40	>40	>40	>40	>40
<b>4</b>	>40	>40	>40	>40	>40	>40
<b>5</b>	>40	>40	>40	>40	>40	>40
<b>6</b>	>40	>40	>40	>40	>40	>40
<b>7</b>	>40	>40	>40	>40	>40	>40
<b>8</b>	23.12	14.13	17.08	>40	30.42	23.87
<b>9</b>	10.45	>40	23.11	>40	>40	10.45
DDP	1.93	10.21	6.59	8.20	12.16	9.07

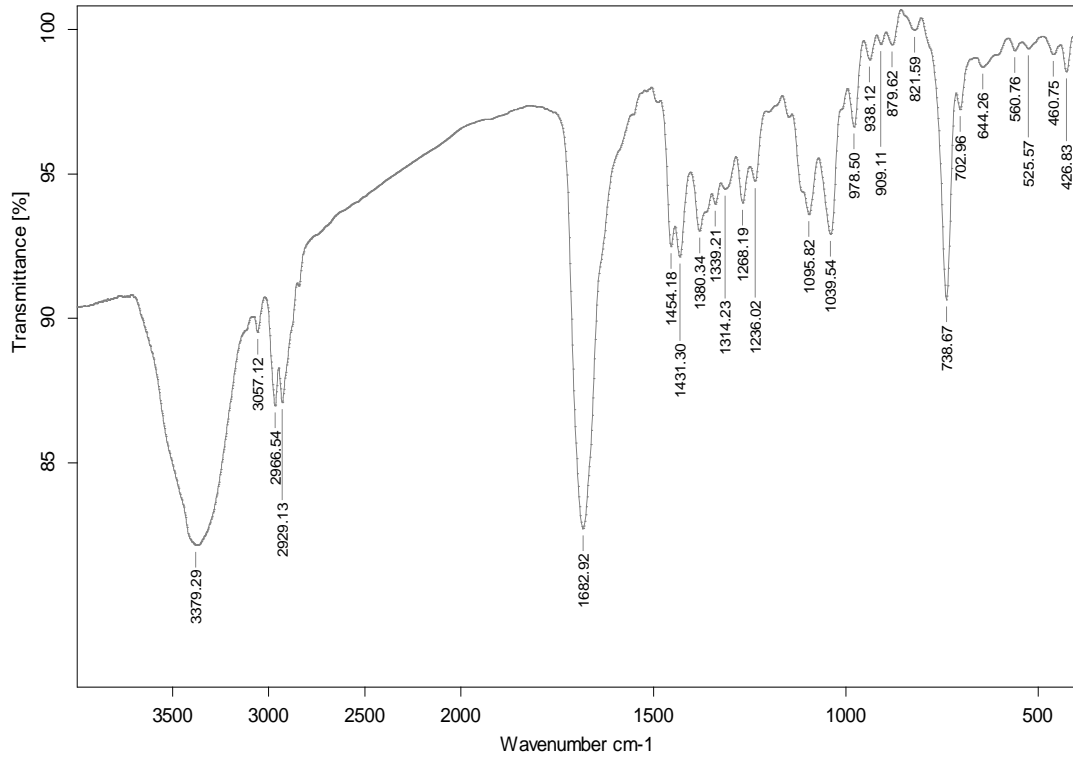
# UV spectrum of compound 1



# IR spectrum of compound 1

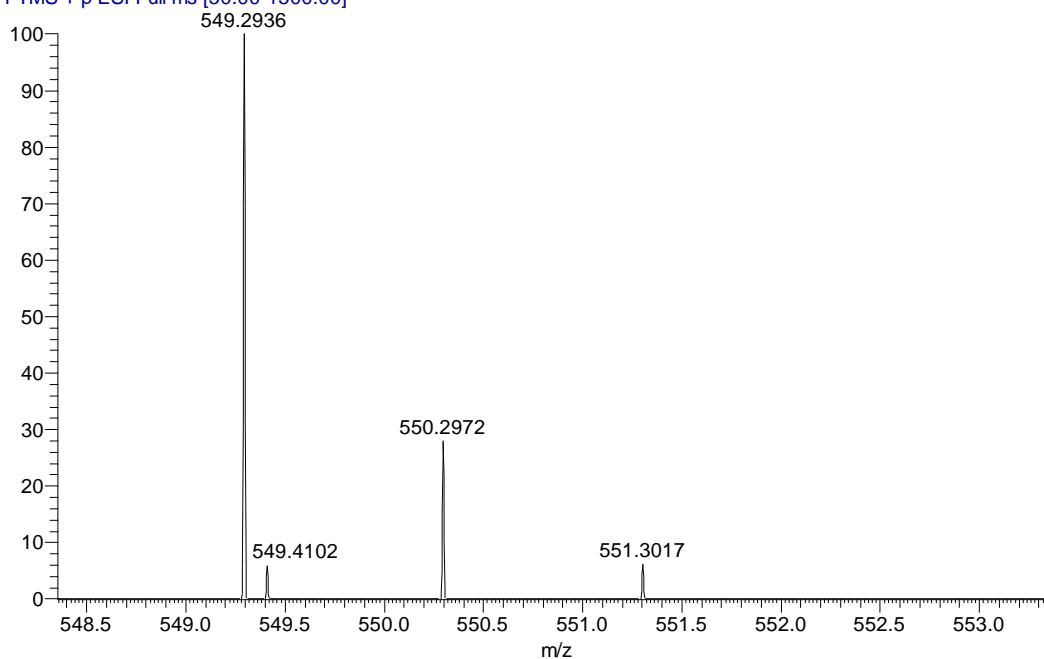
E:\同济医学院\张勇慧\20140325\CG2-7-11.0

仪器型号: Bruker Vertex 70

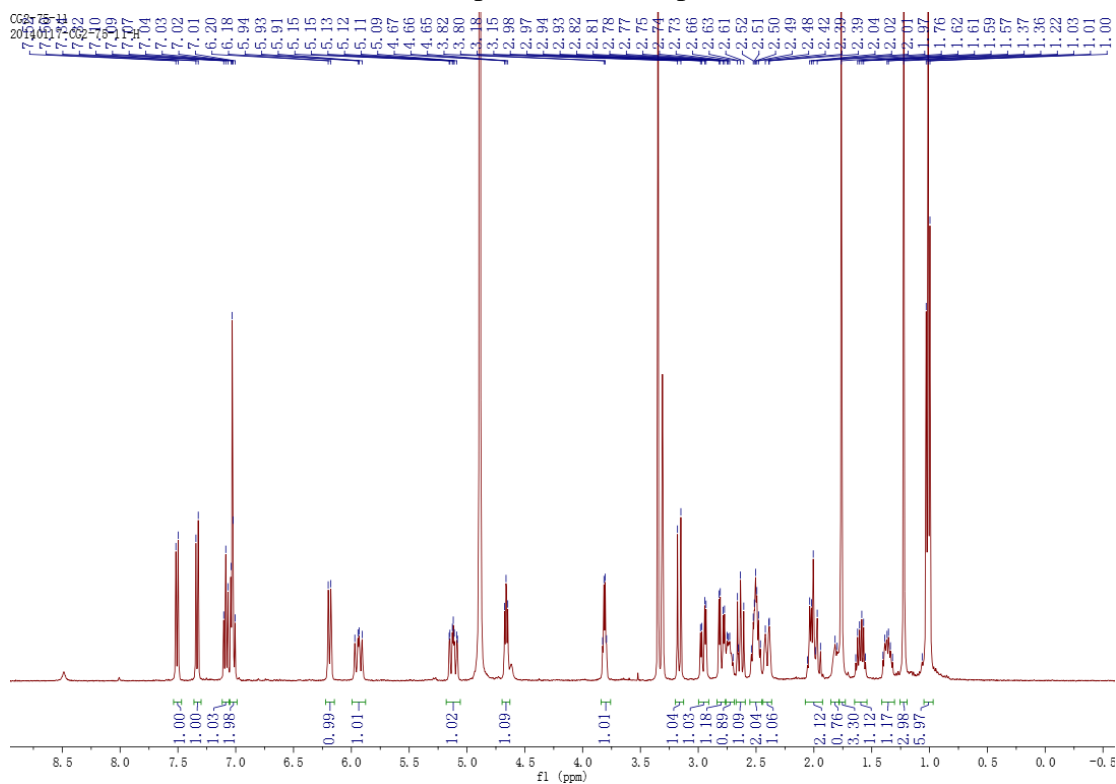


# HRESIMS spectrum of compound 1

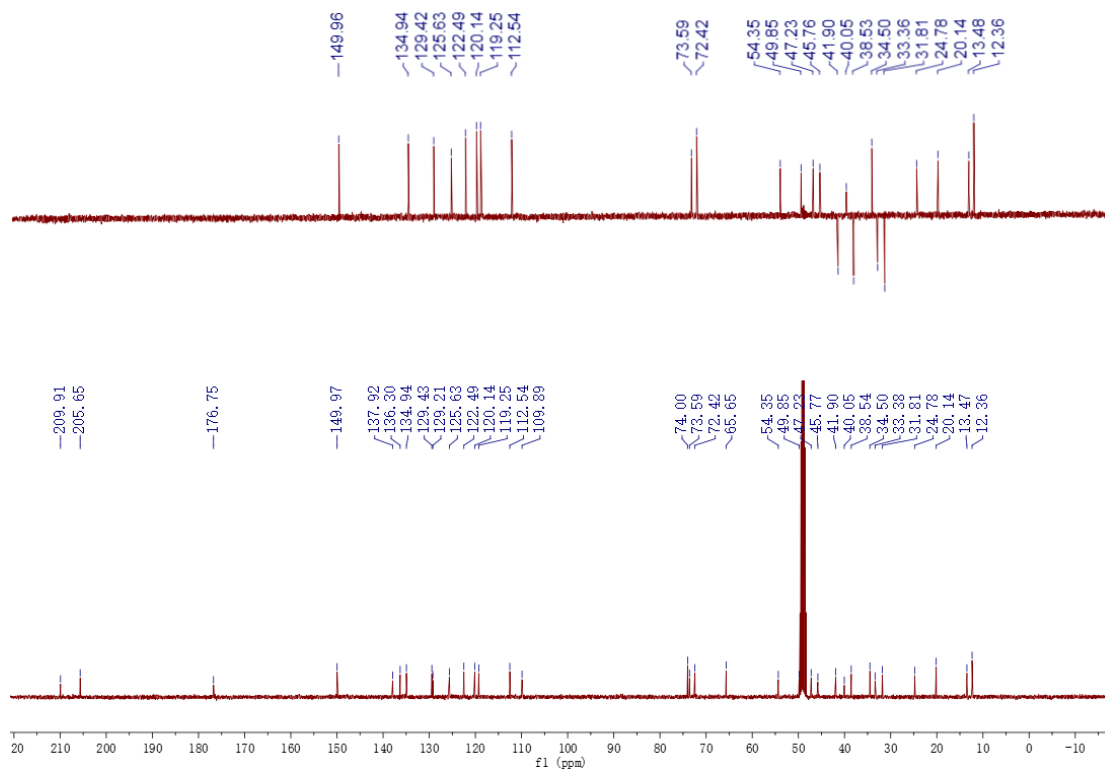
CCM2-77-11 #43 RT: 0.61 AV: 1 NL: 6.62E5  
T: FTMS + p ESI Full ms [50.00-1500.00]



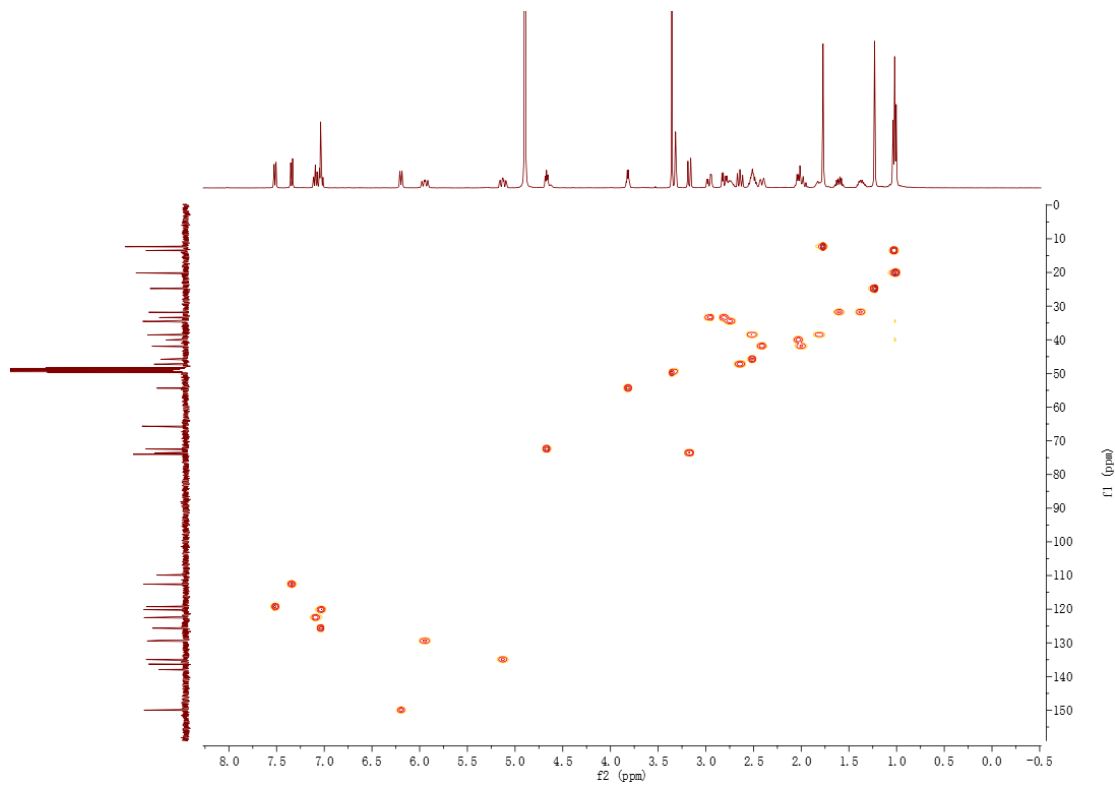
# <sup>1</sup>H NMR spectrum of compound 1



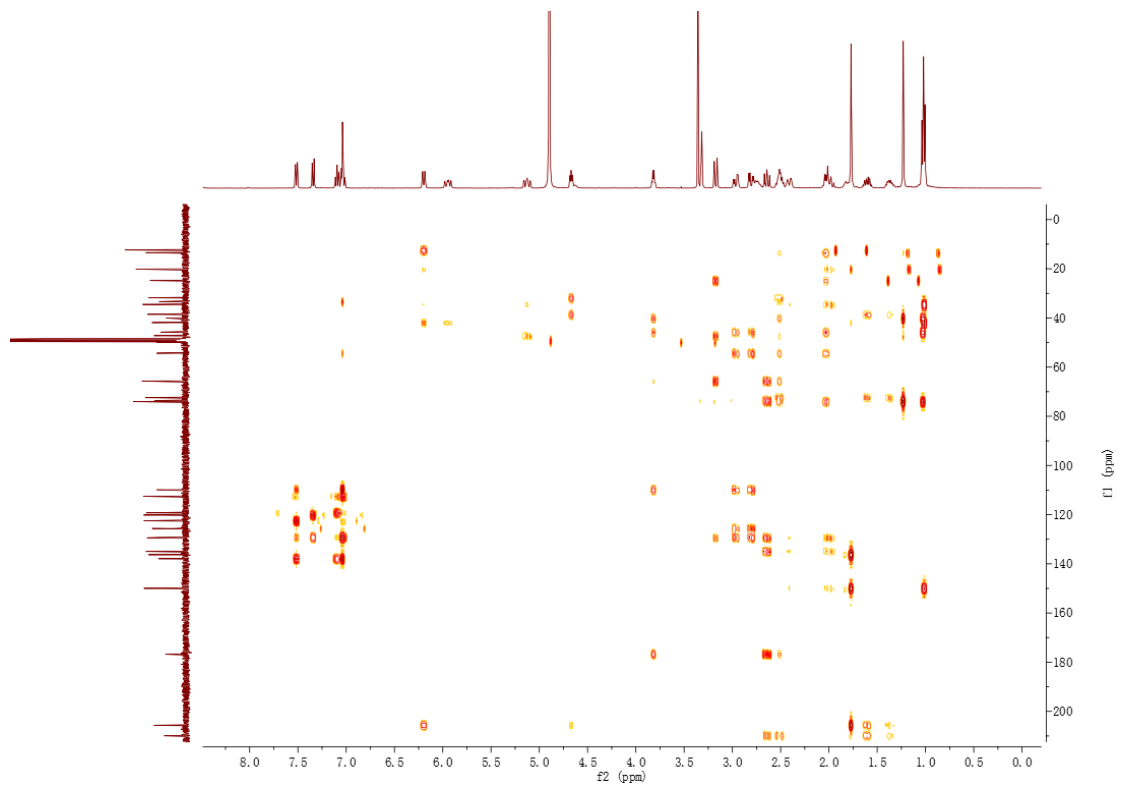
### <sup>13</sup>C NMR and DEPT spectra of compound 1



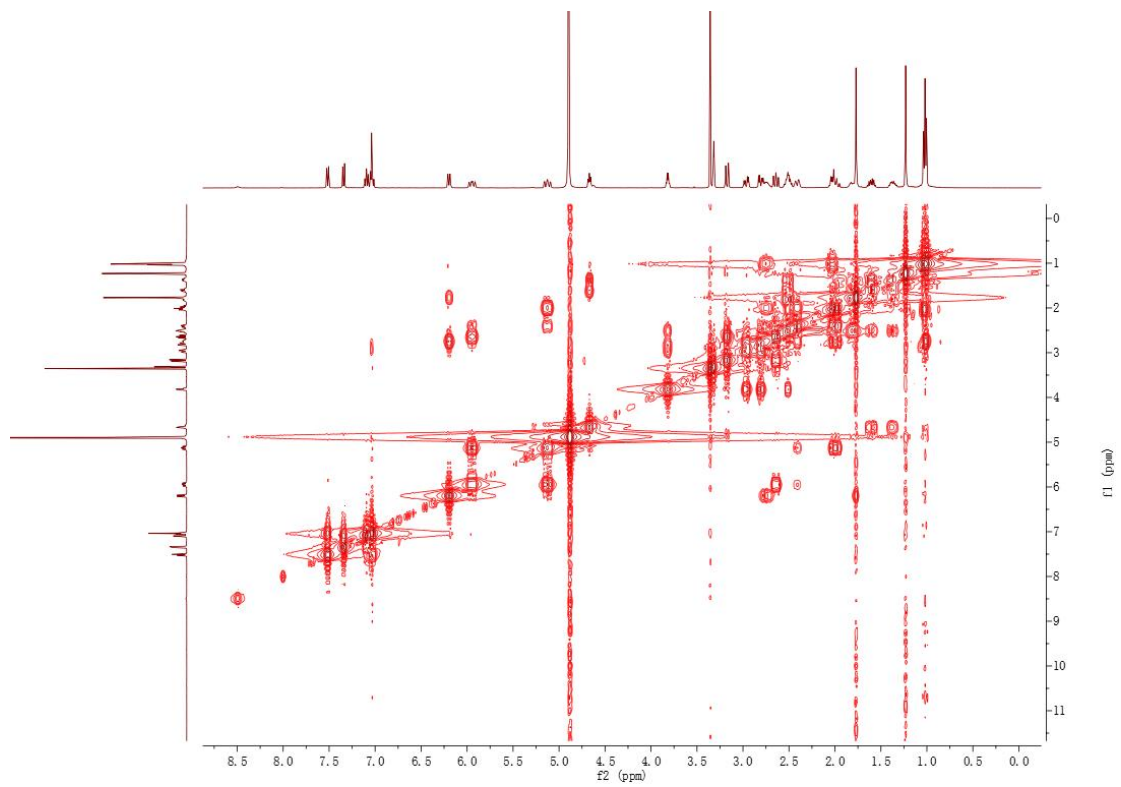
### HSQC spectrum of compound 1



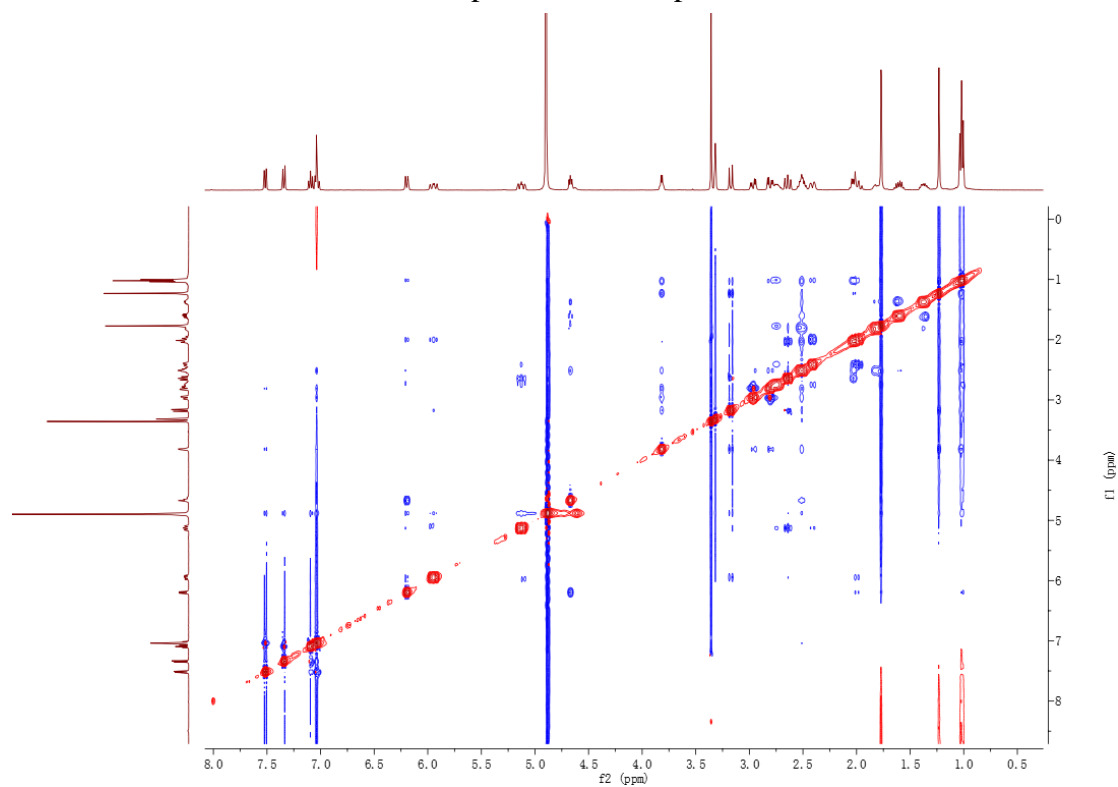
HMBC spectrum of compound 1



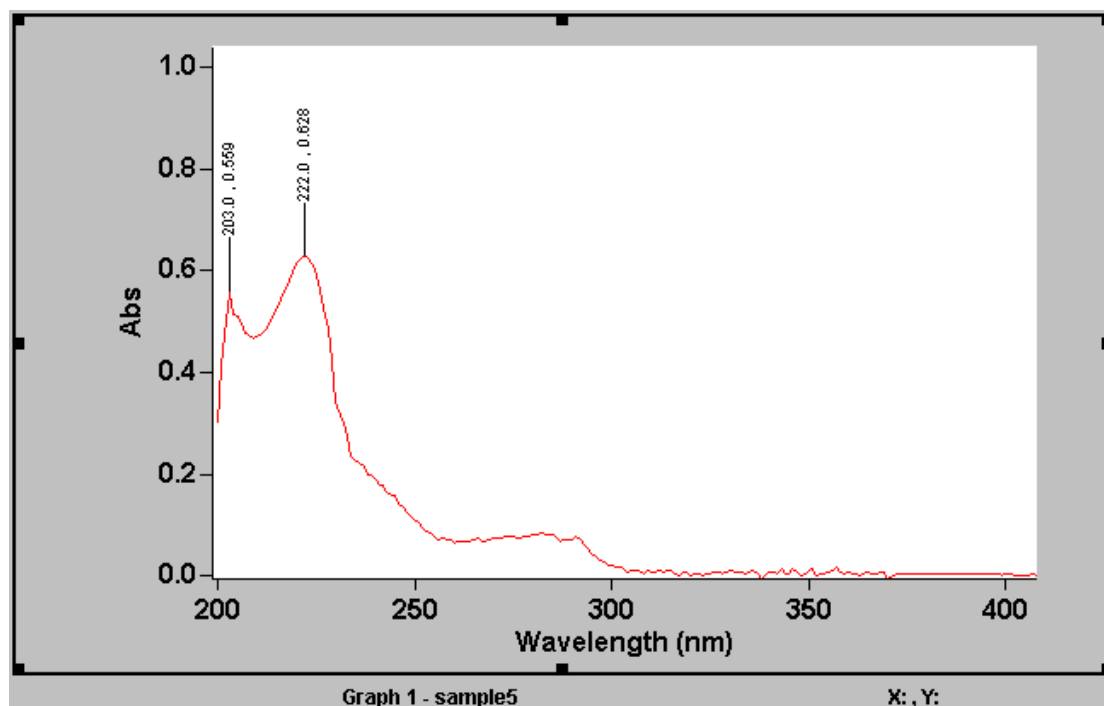
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 1



NOESY spectrum of compound 1



UV spectrum of compound 2

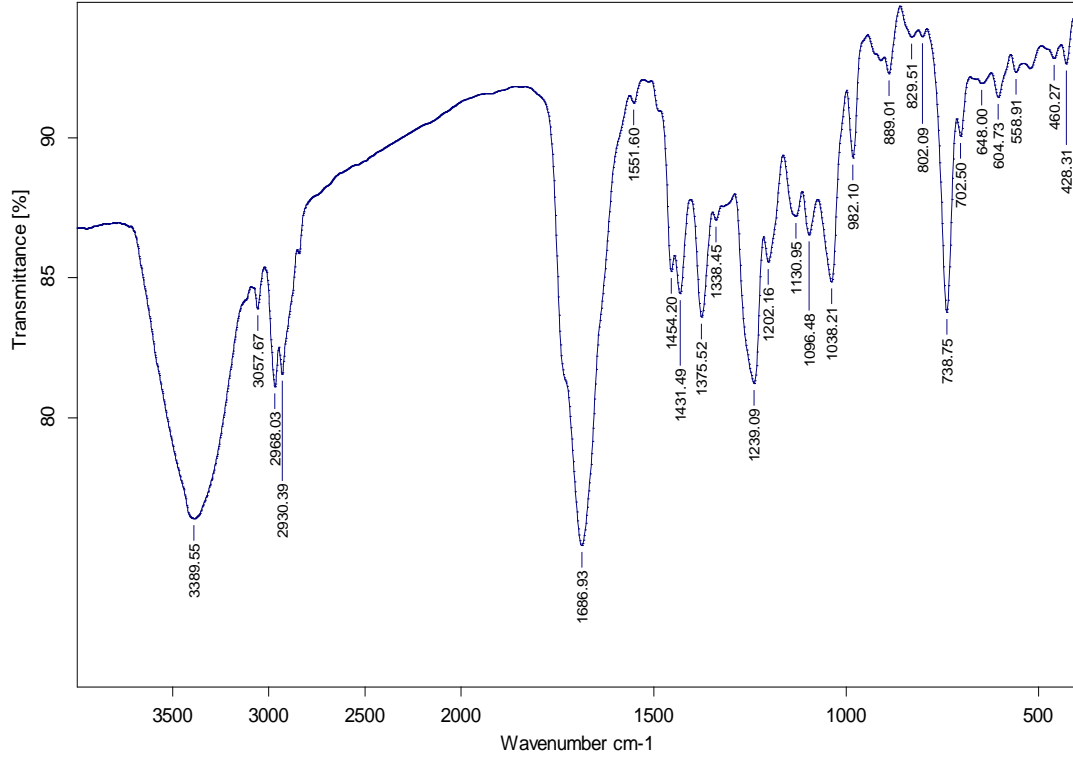




## IR spectrum of compound 2

E:\同济医学院\张勇慧\20140325\CG2-79-2.0

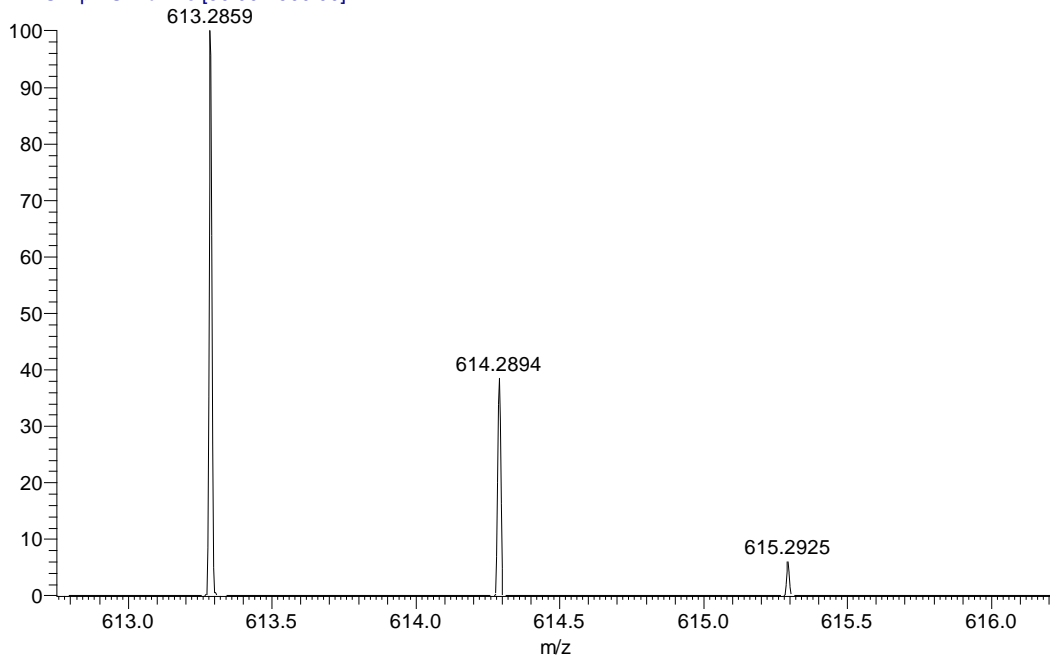
仪器型号: Bruker Vertex 70



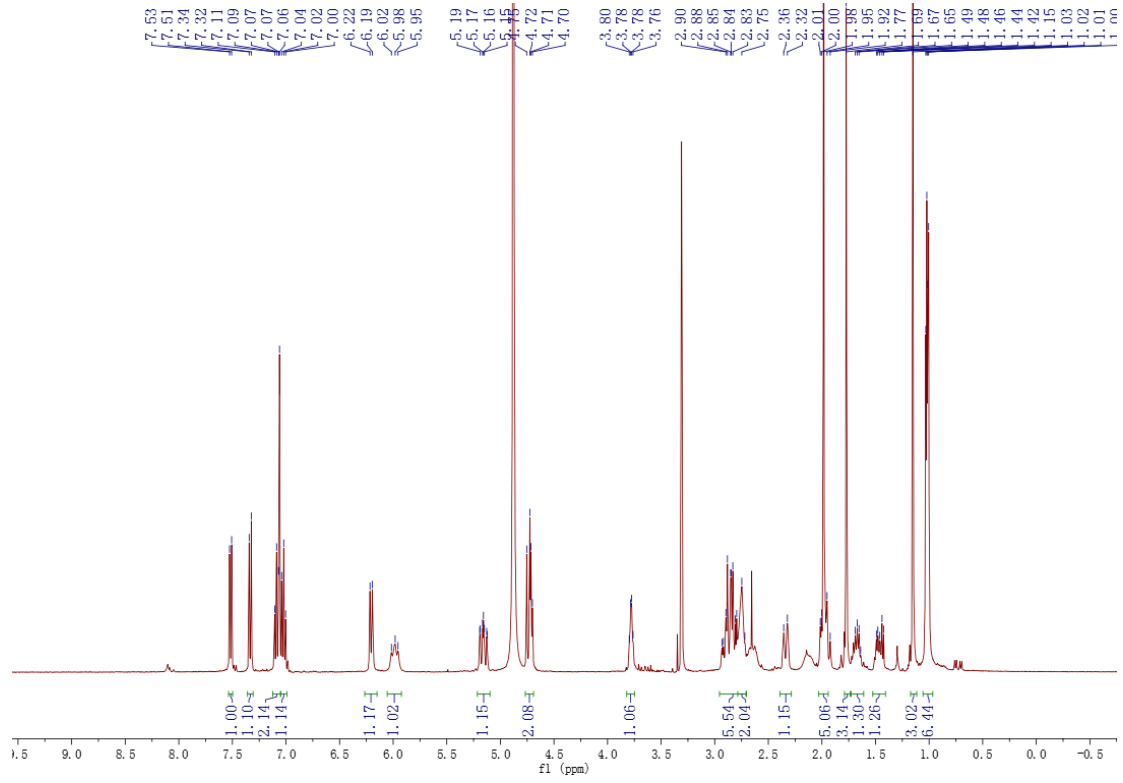
## HRESIMS spectrum of compound 2

CCM2-79-2 #22 RT: 0.31 AV: 1 NL: 1.65E7

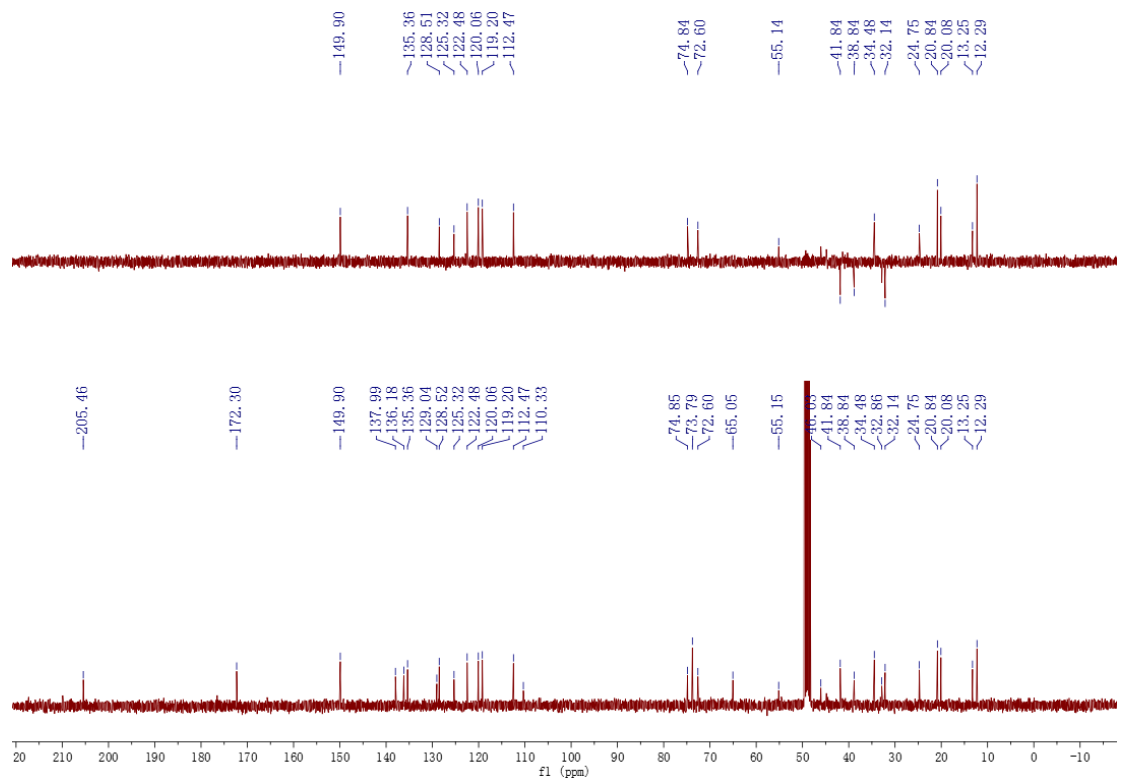
T: FTMS + p ESI Full ms [50.00-1500.00]



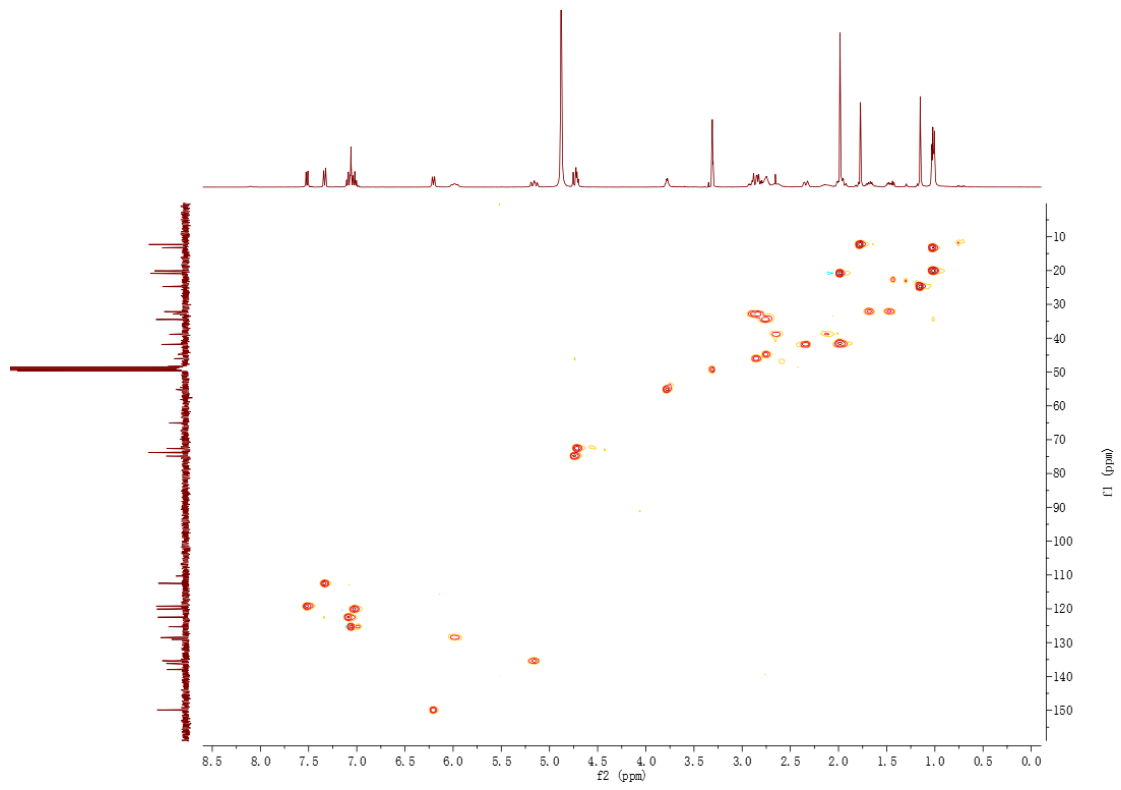
### <sup>1</sup>H NMR spectrum of compound 2



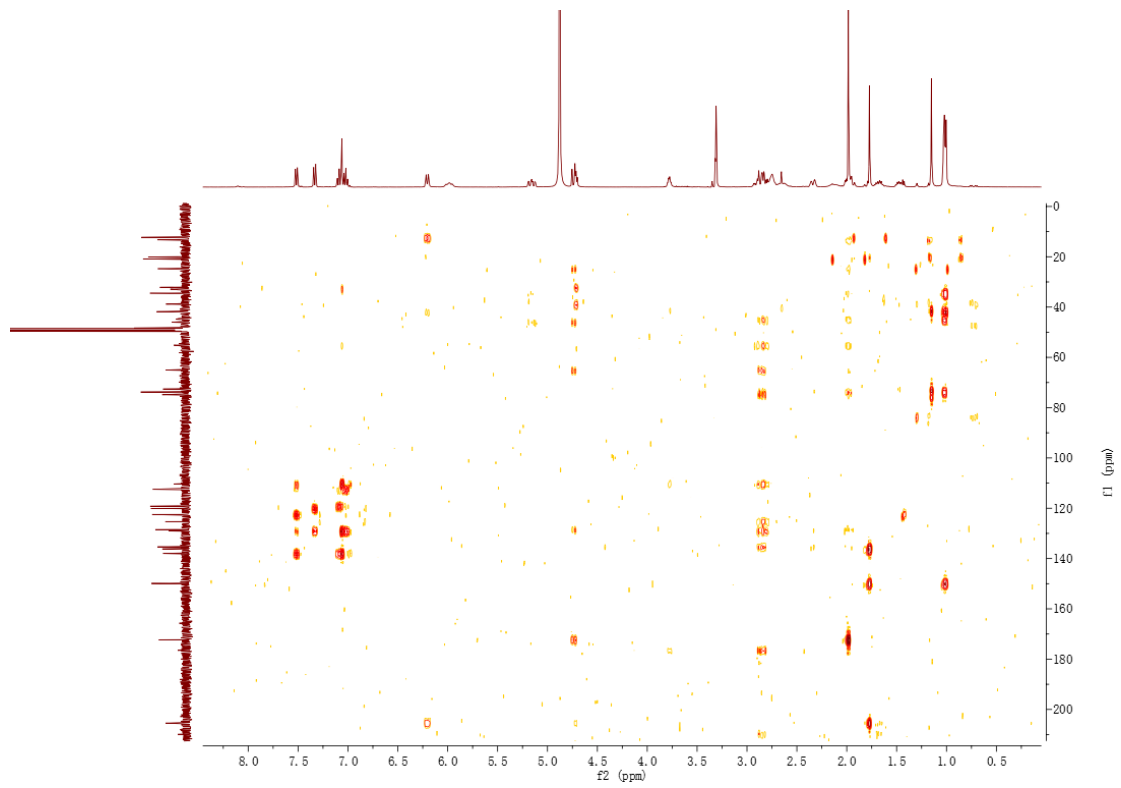
### <sup>13</sup>C NMR and DEPT spectra of compound 2



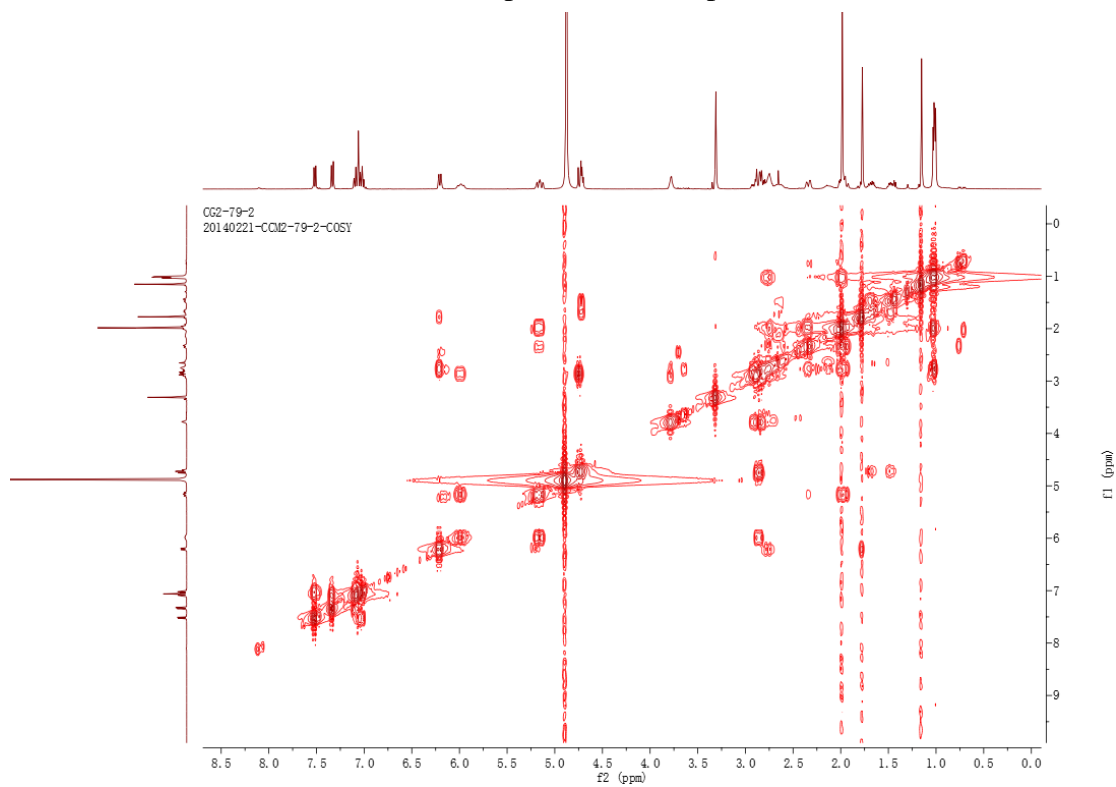
HSQC spectrum of compound 2



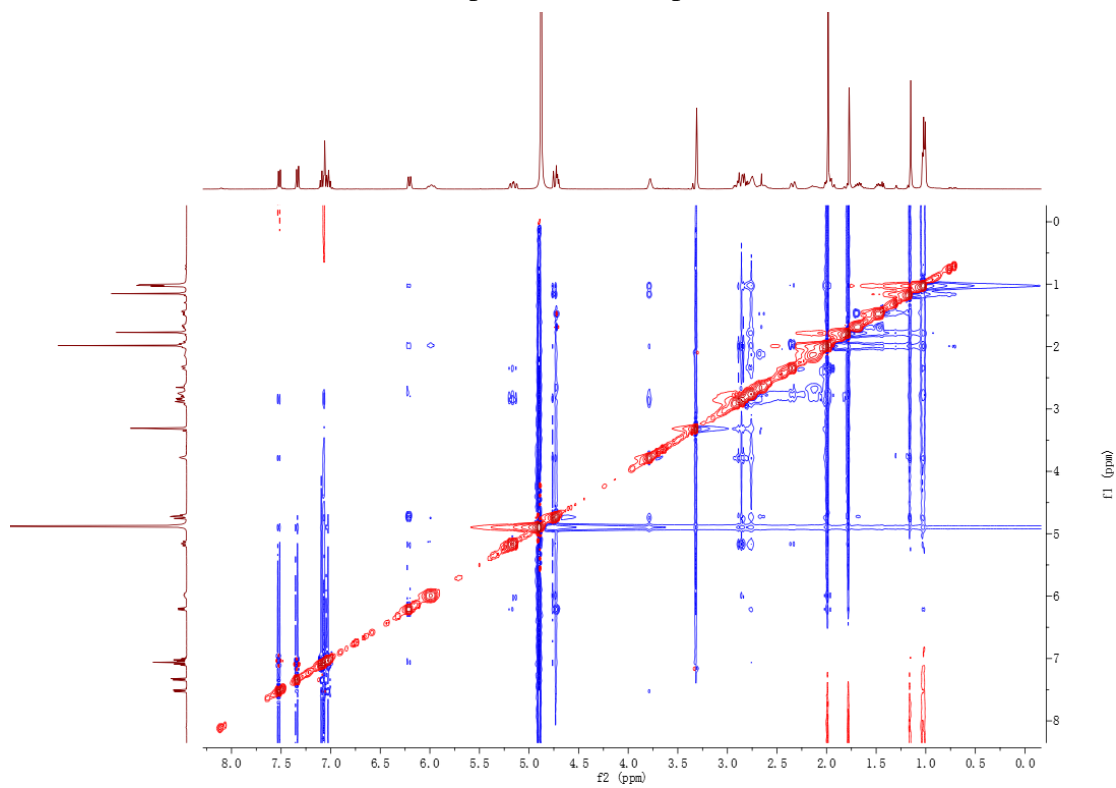
HMBC spectrum of compound 2



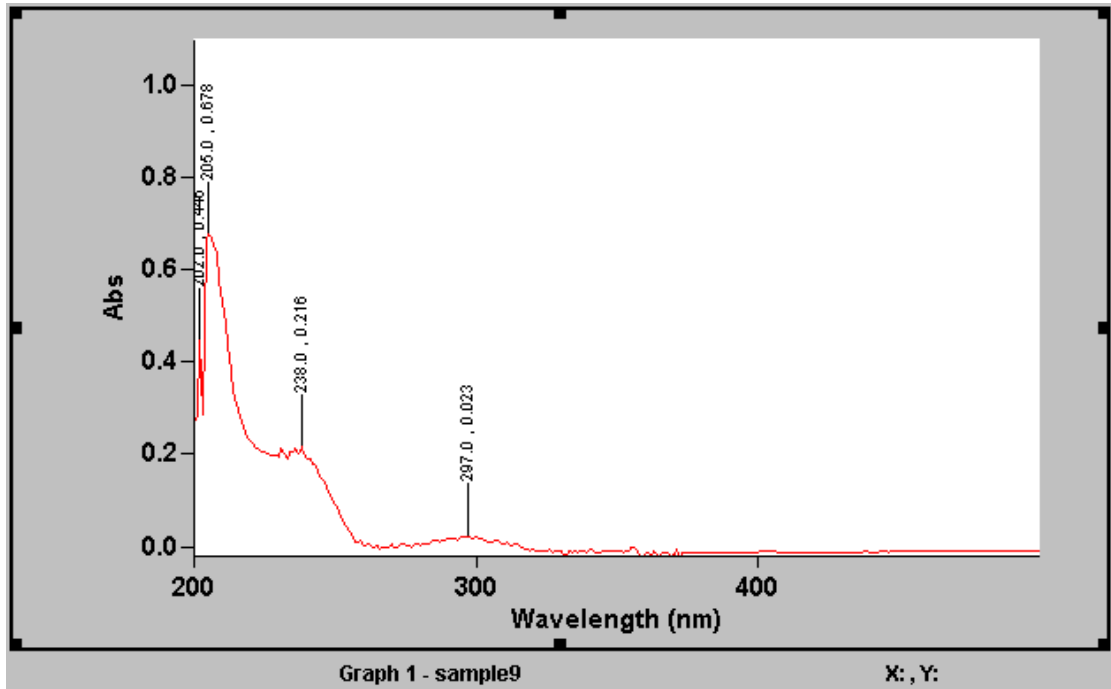
### $^1\text{H}$ - $^1\text{H}$ COSY spectrum of compound 2



### NOESY spectrum of compound 2

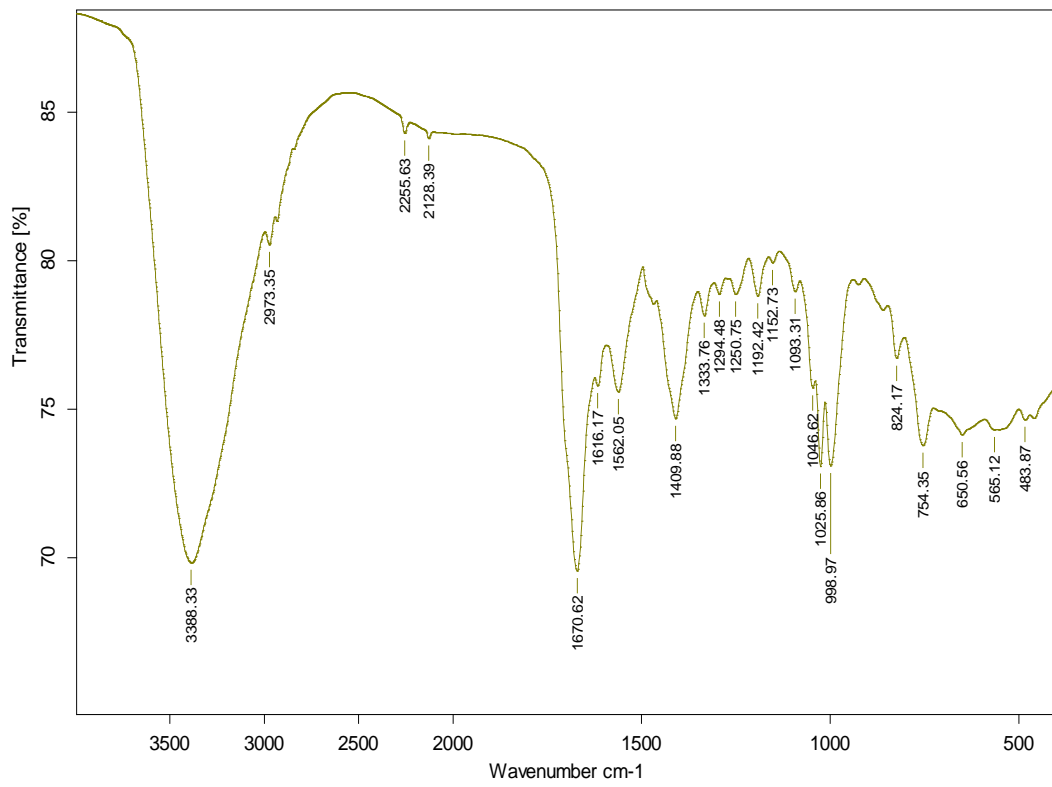


### UV spectrum of compound 3



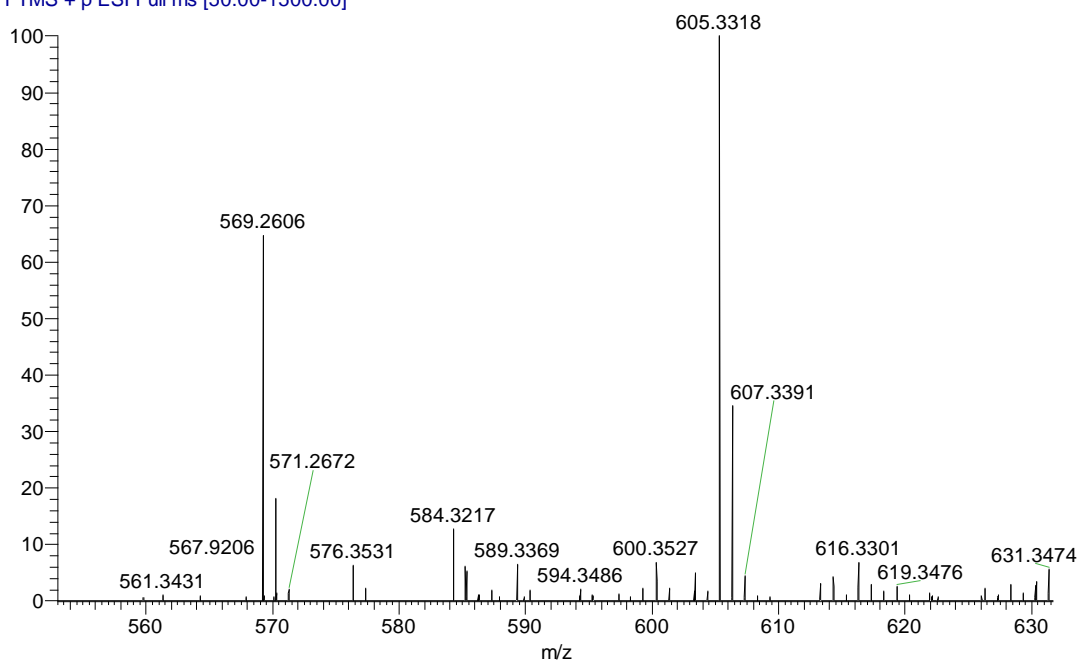
### IR spectrum of compound 3

E:\同济医学院\张勇慧\20140617\001.6

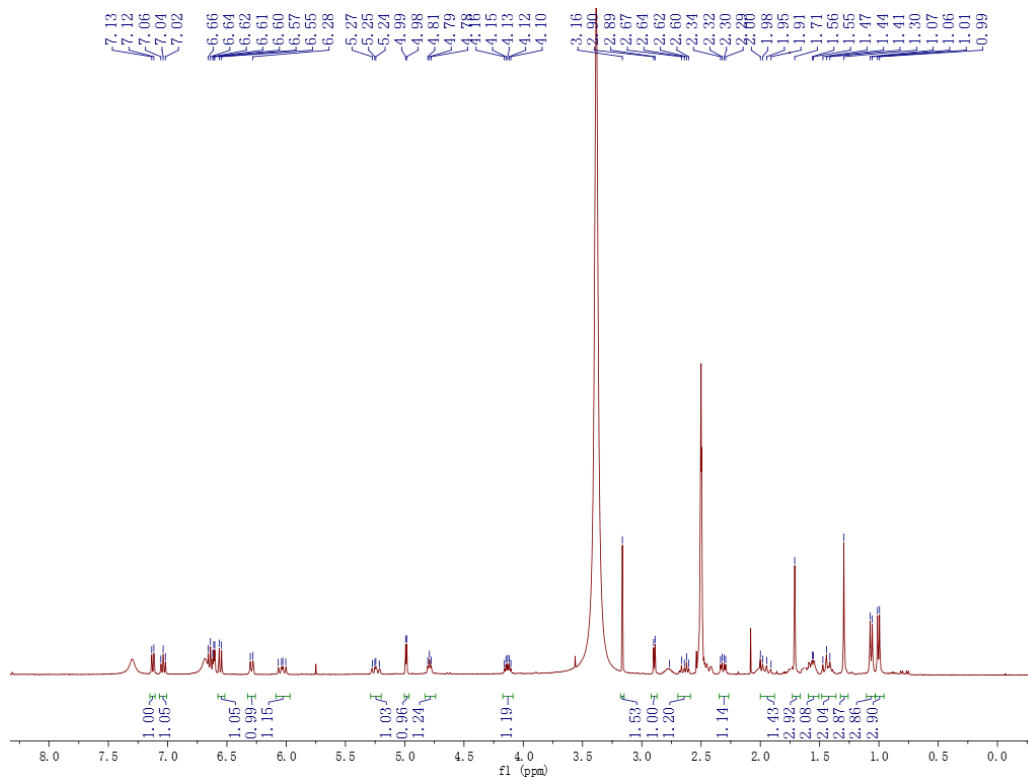


### HRESIMS spectrum of compound **3**

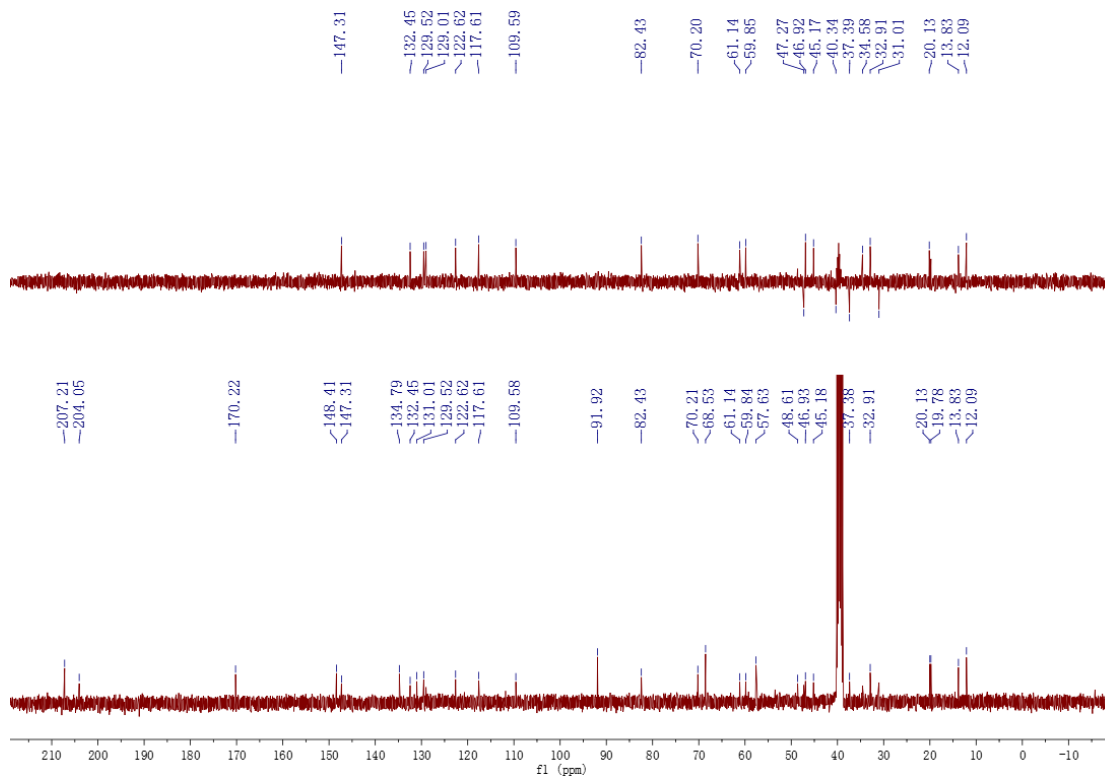
CCM2-87-22 #13 RT: 0.19 AV: 1 NL: 2.31E6  
T: FTMS + p ESI Full ms [50.00-1500.00]



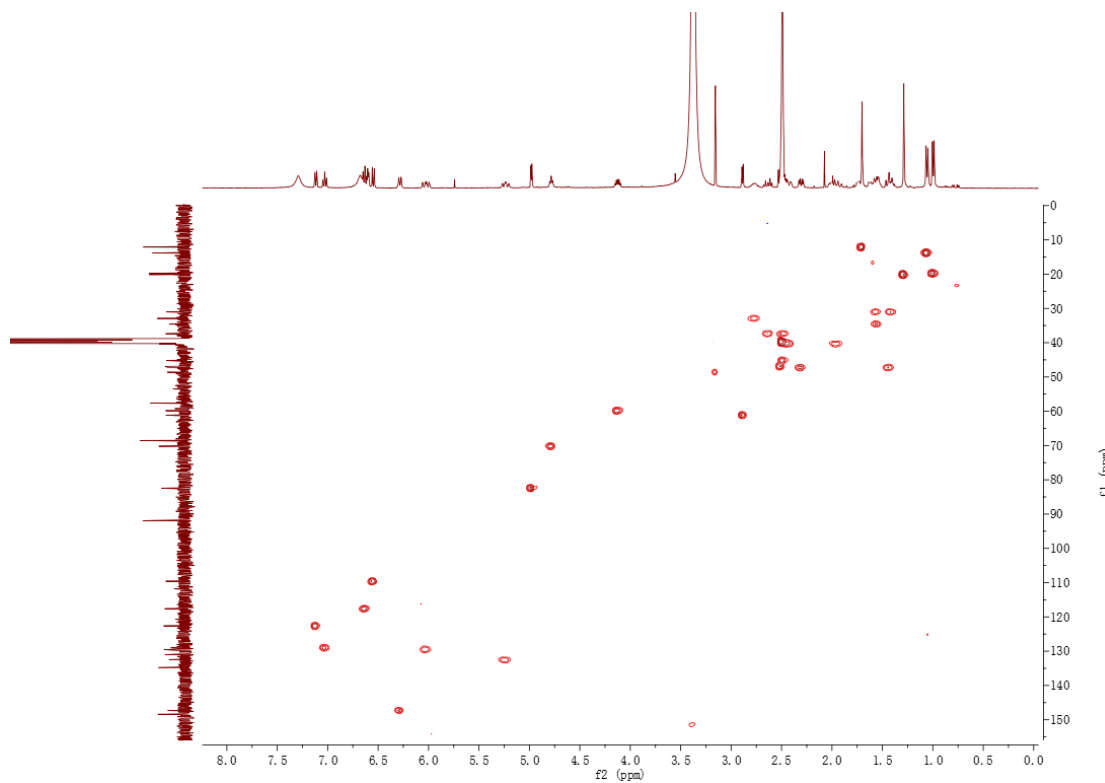
### <sup>1</sup>H NMR spectrum of compound **3**



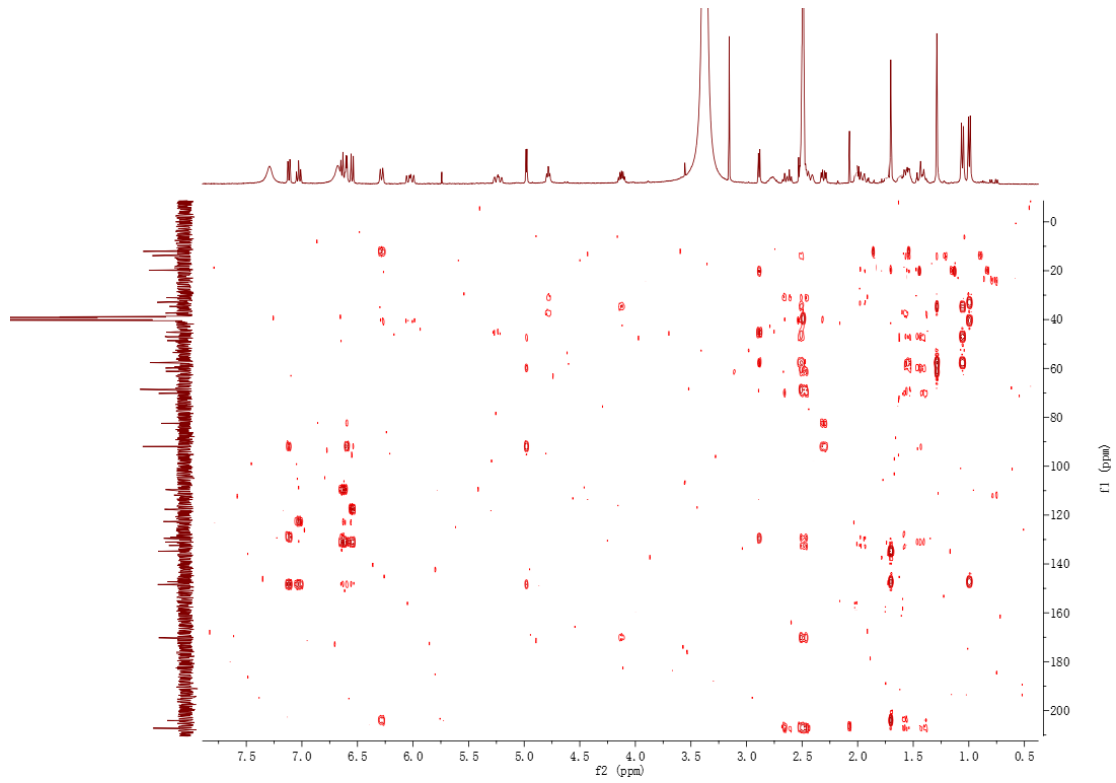
### $^{13}\text{C}$ NMR and DEPT spectra of compound 3



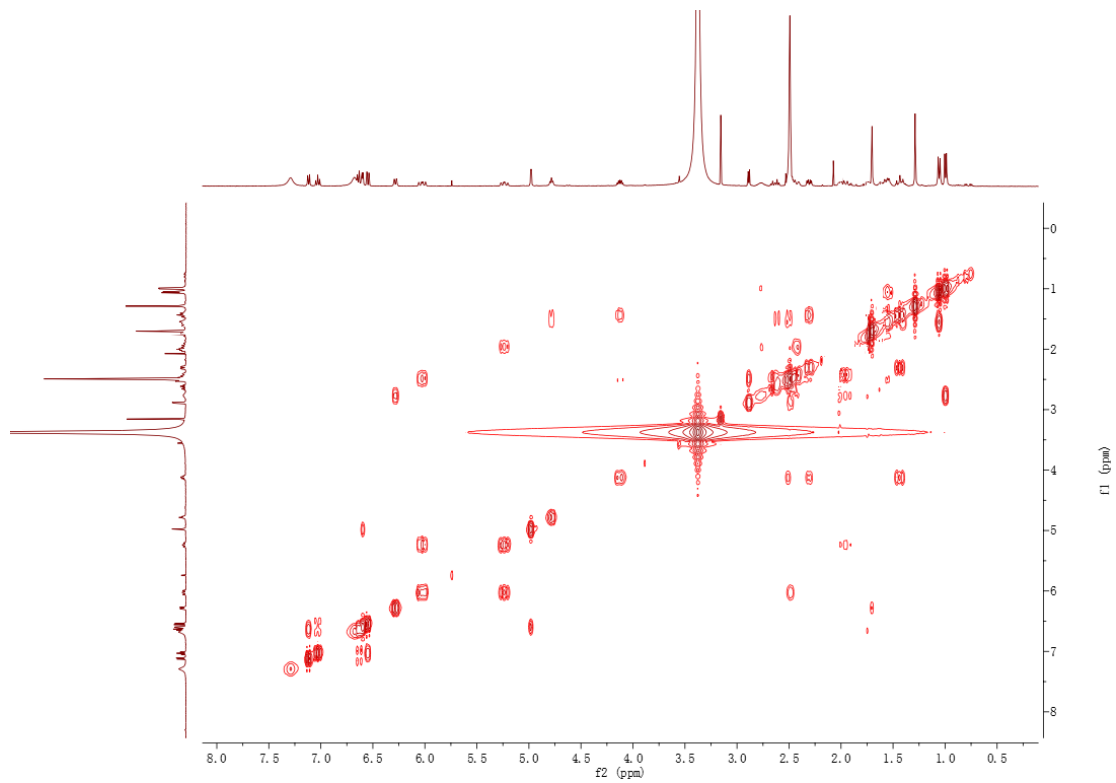
### HSQC spectrum of compound 3



HMBC spectrum of compound **3**

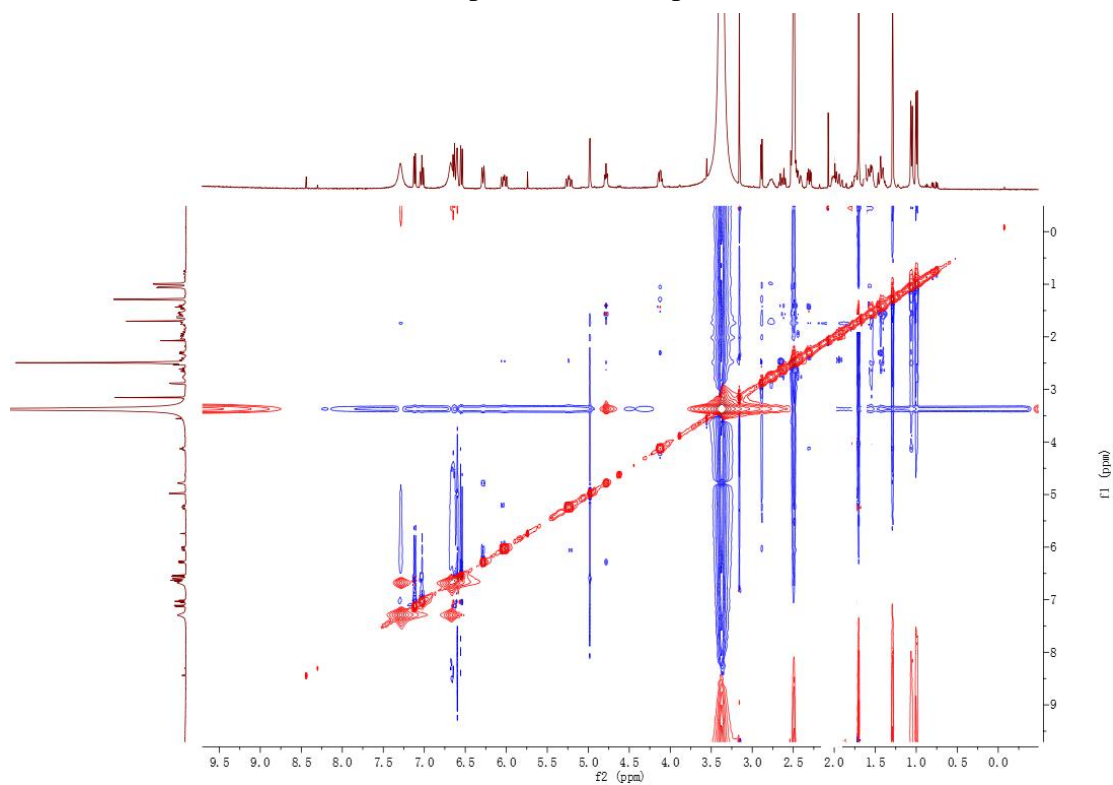


$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3**

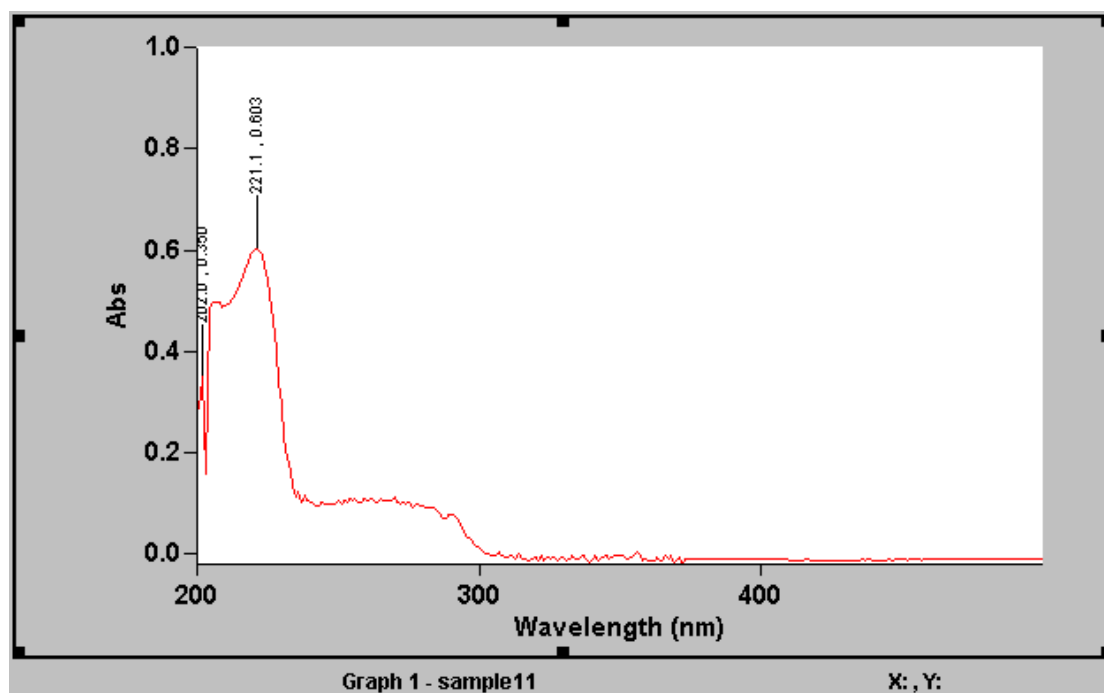




NOESY spectrum of compound 3

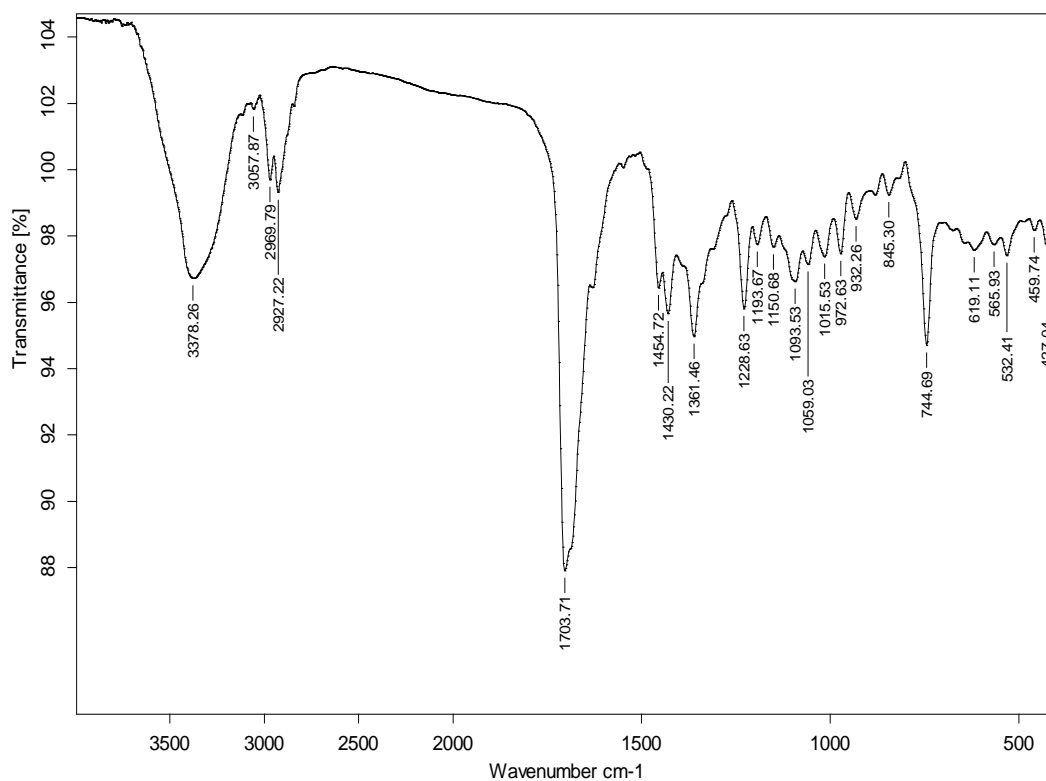


UV spectrum of compound 4



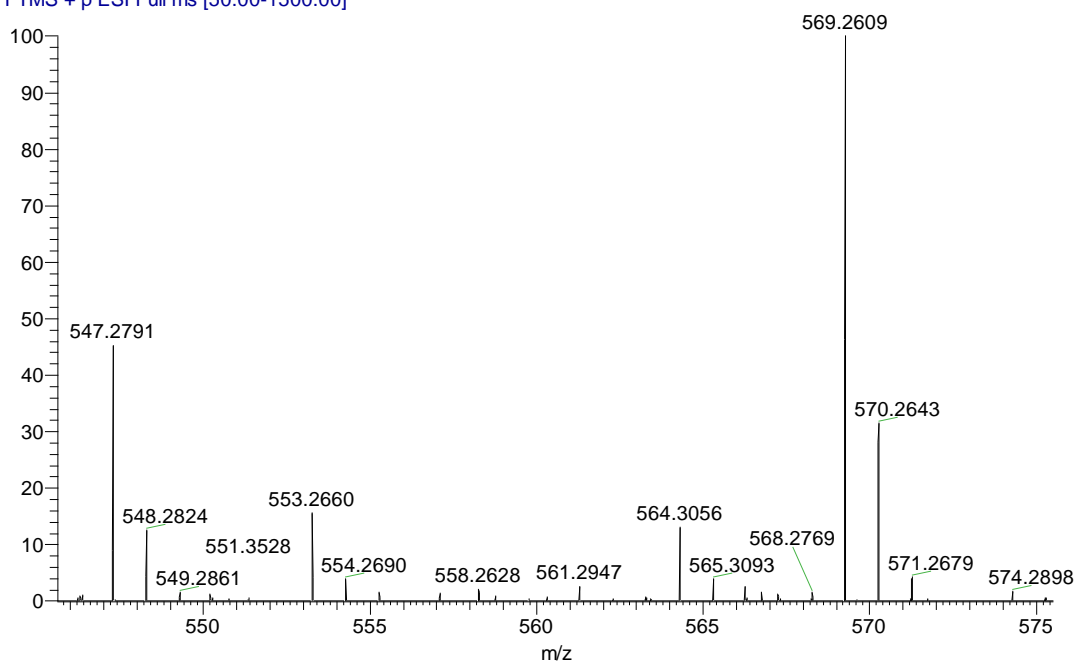
### IR spectrum of compound 4

E:\同济医学院\张勇慧\20140617\001.8

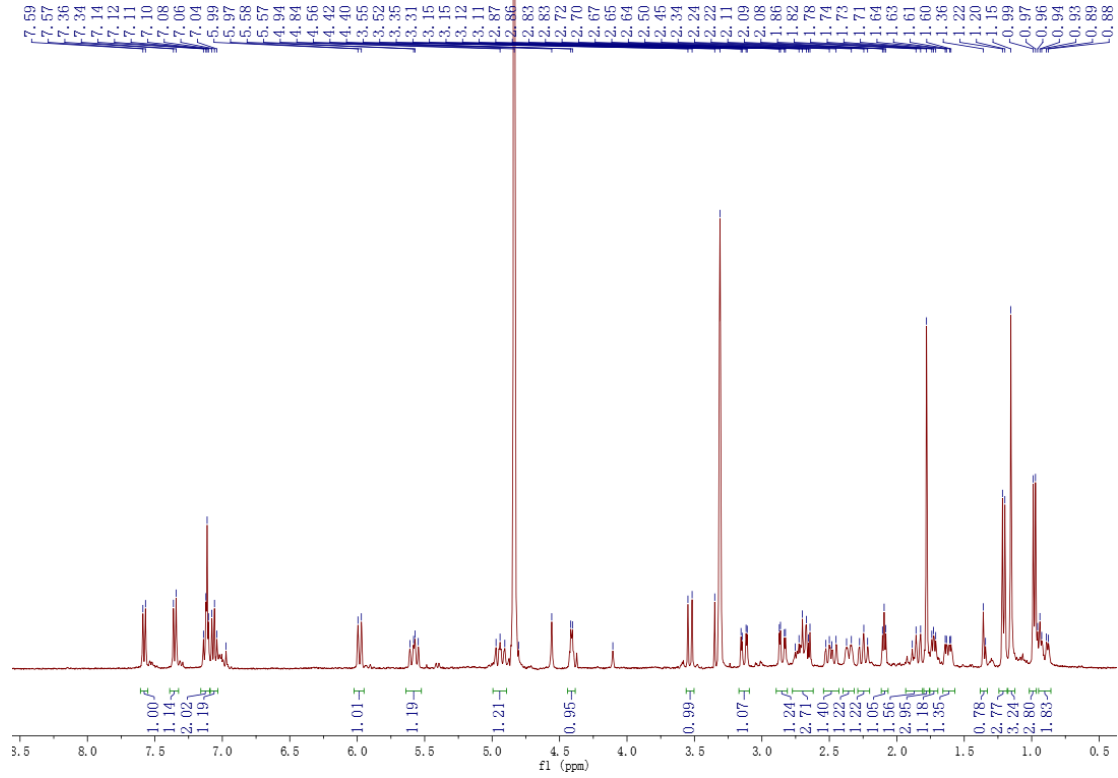


### HRESIMS spectrum of compound 4

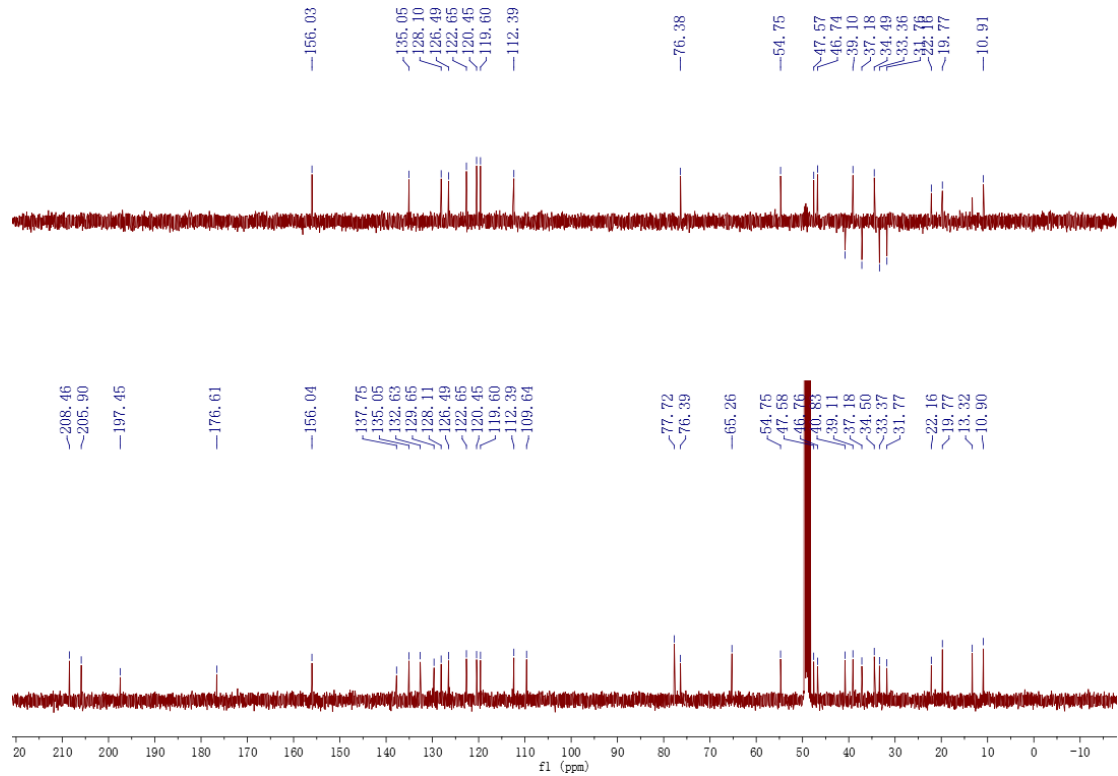
CCM2-98-5 #20 RT: 0.29 AV: 1 NL: 4.35E5  
T: FTMS + p ESI Full ms [50.00-1500.00]



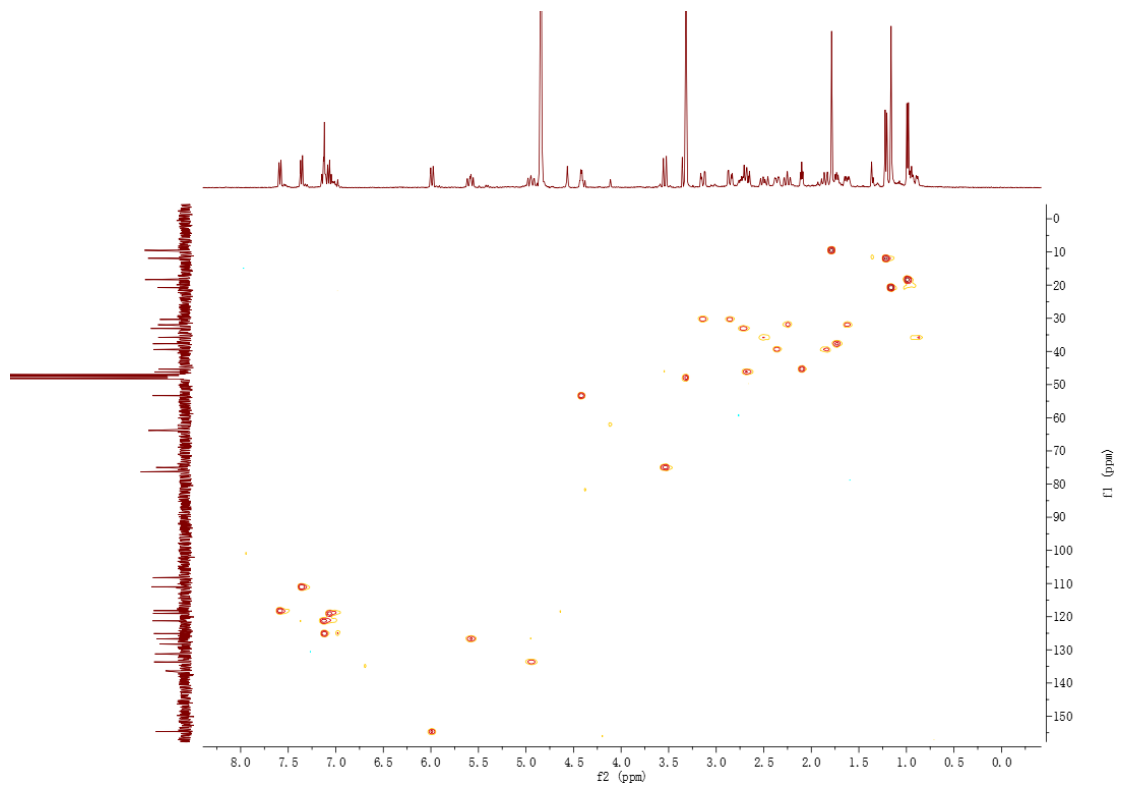
### <sup>1</sup>H NMR spectrum of compound 4



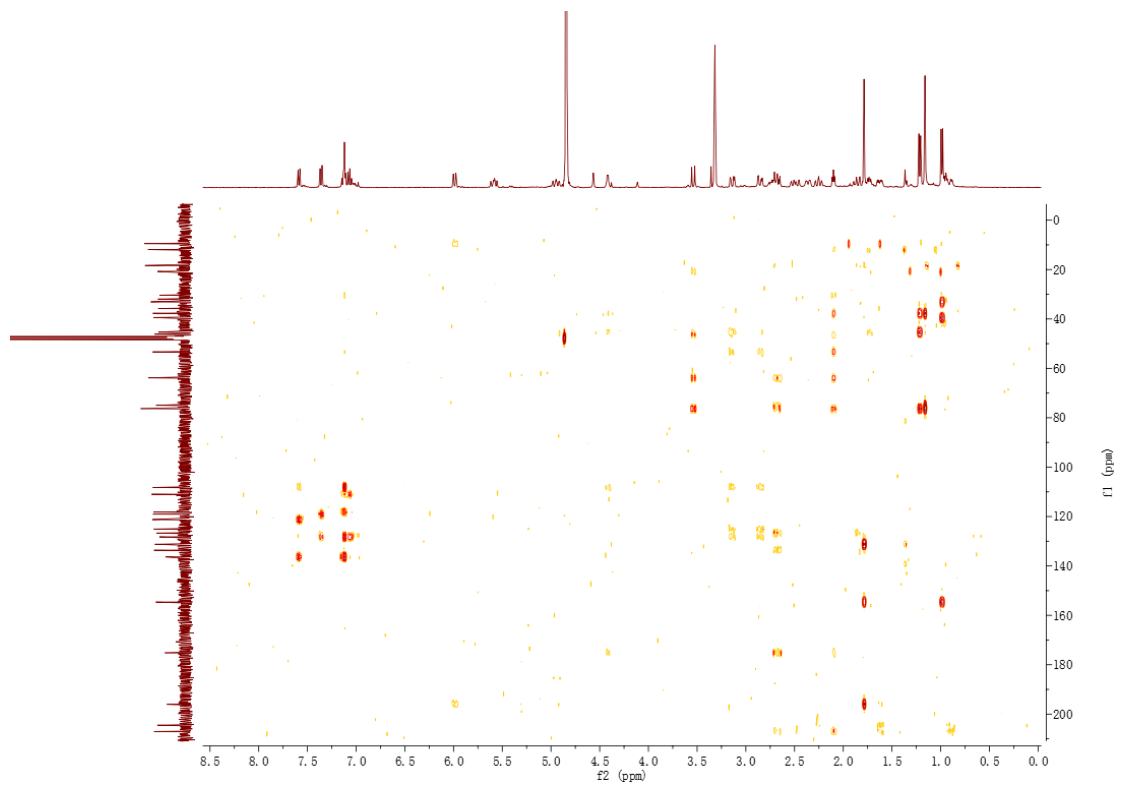
### <sup>13</sup>C NMR and DEPT spectra of compound 4



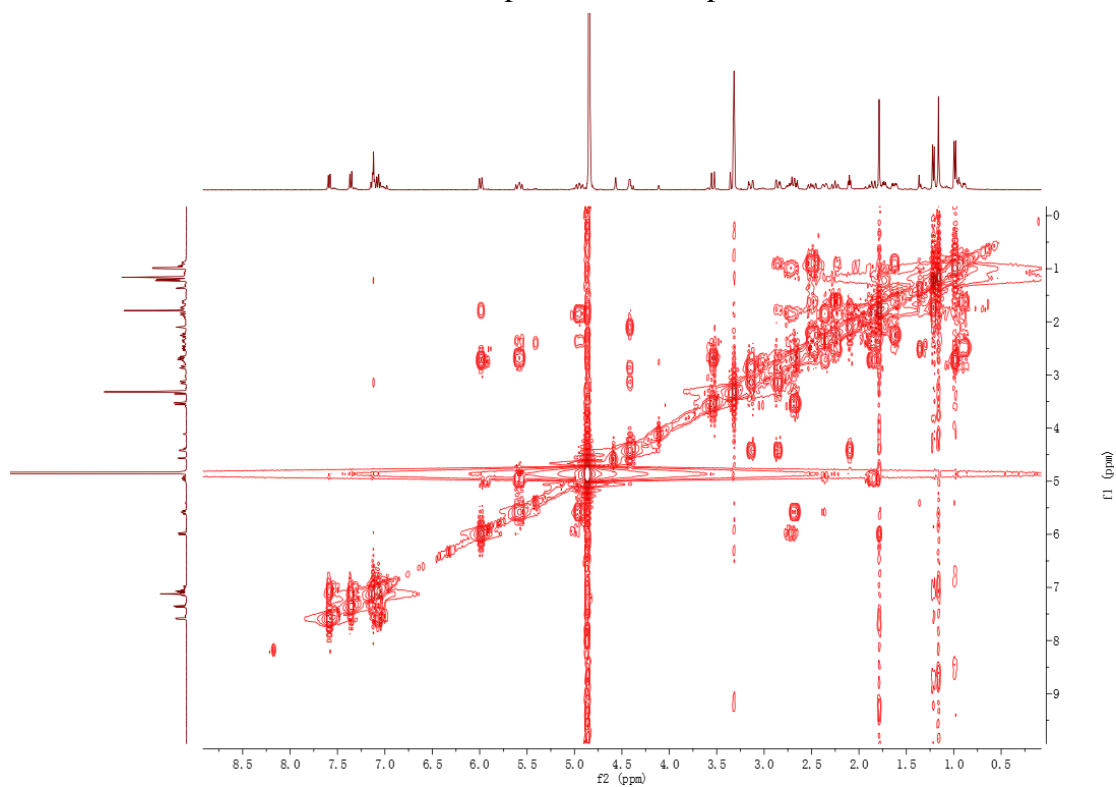
HSQC spectrum of compound **4**



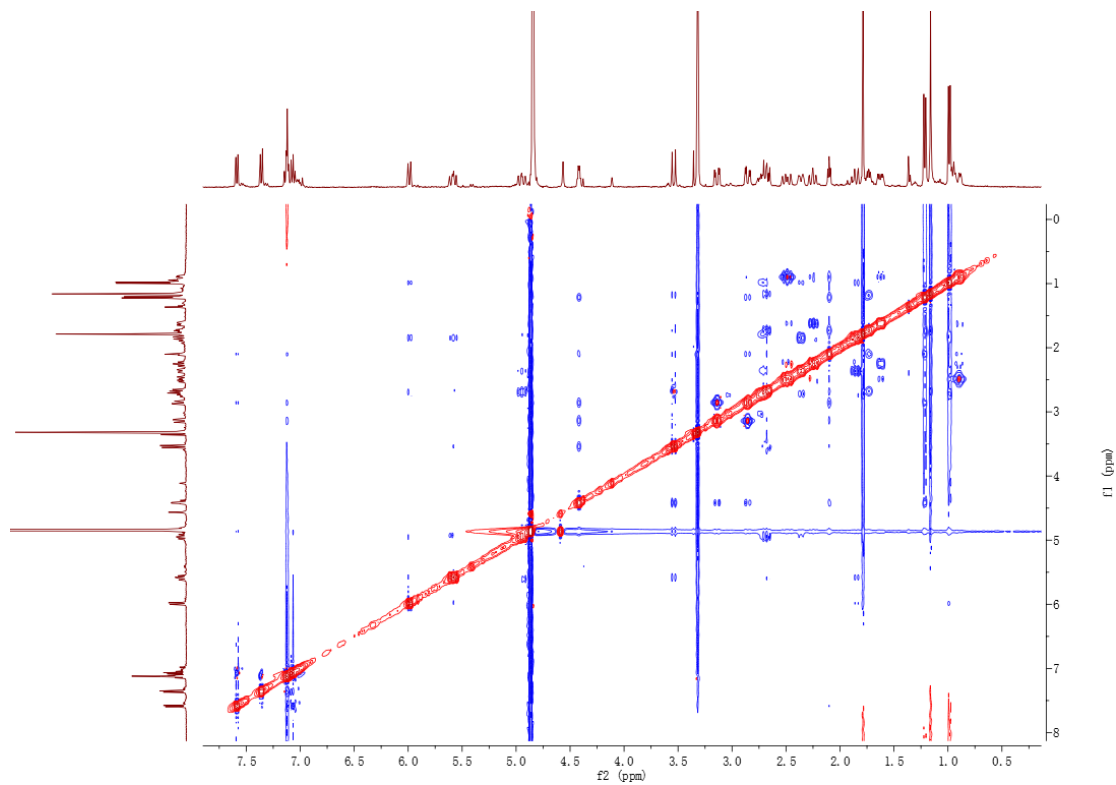
HMBC spectrum of compound **4**



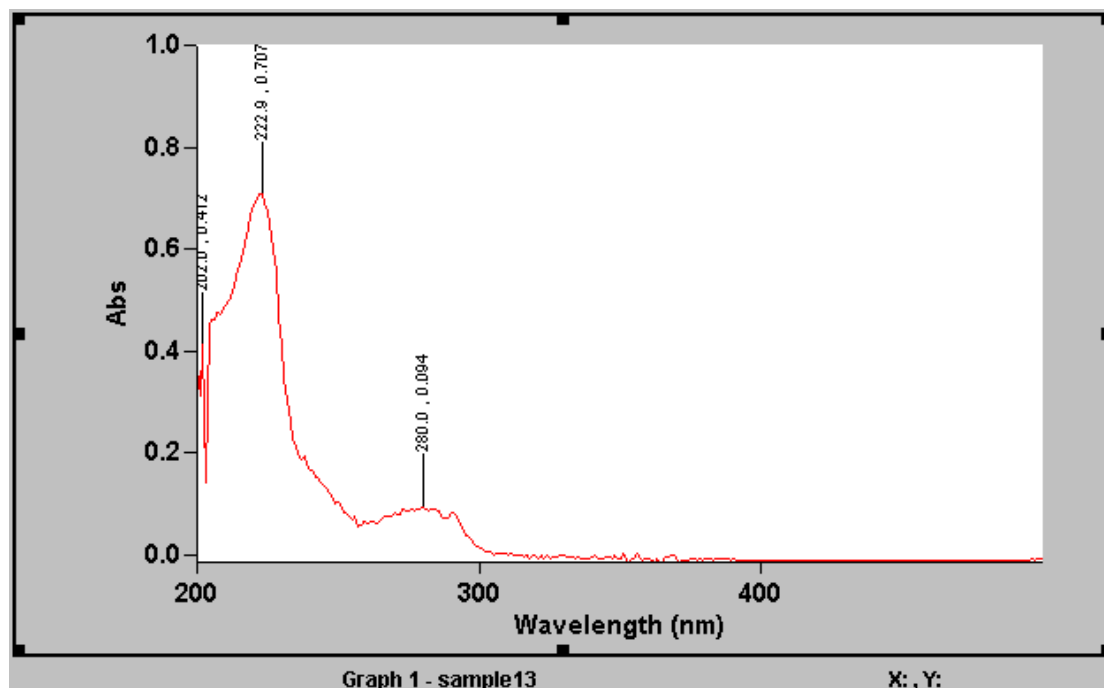
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4**



NOESY spectrum of compound **4**

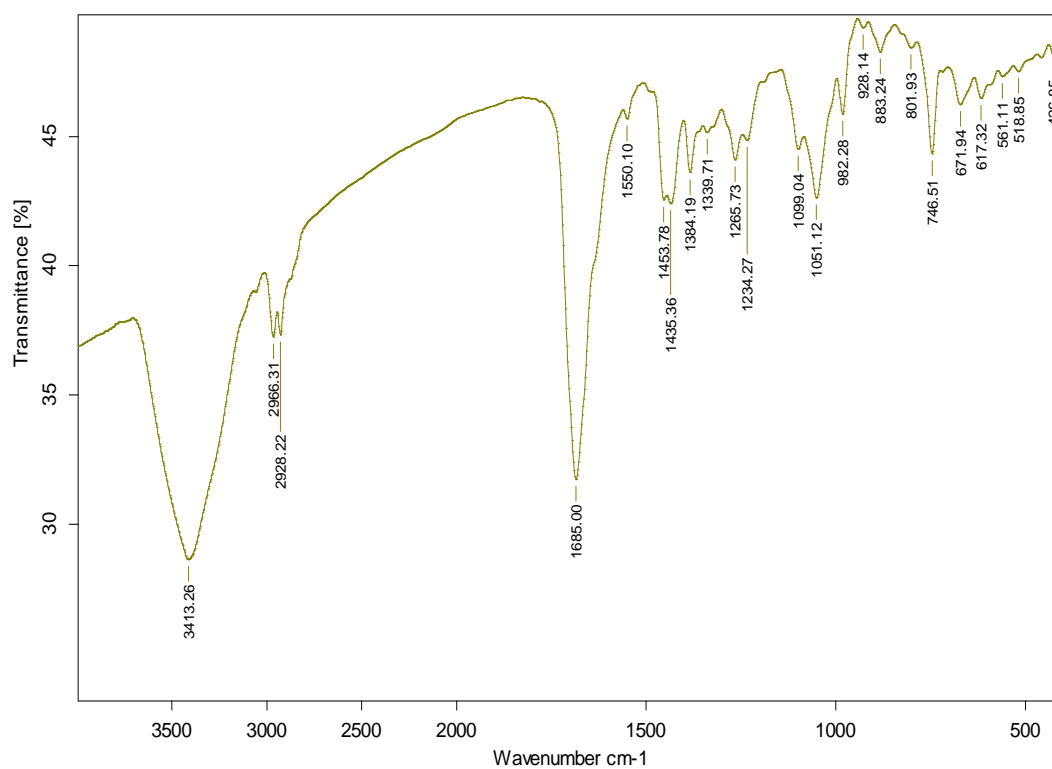


## UV spectrum of compound 5



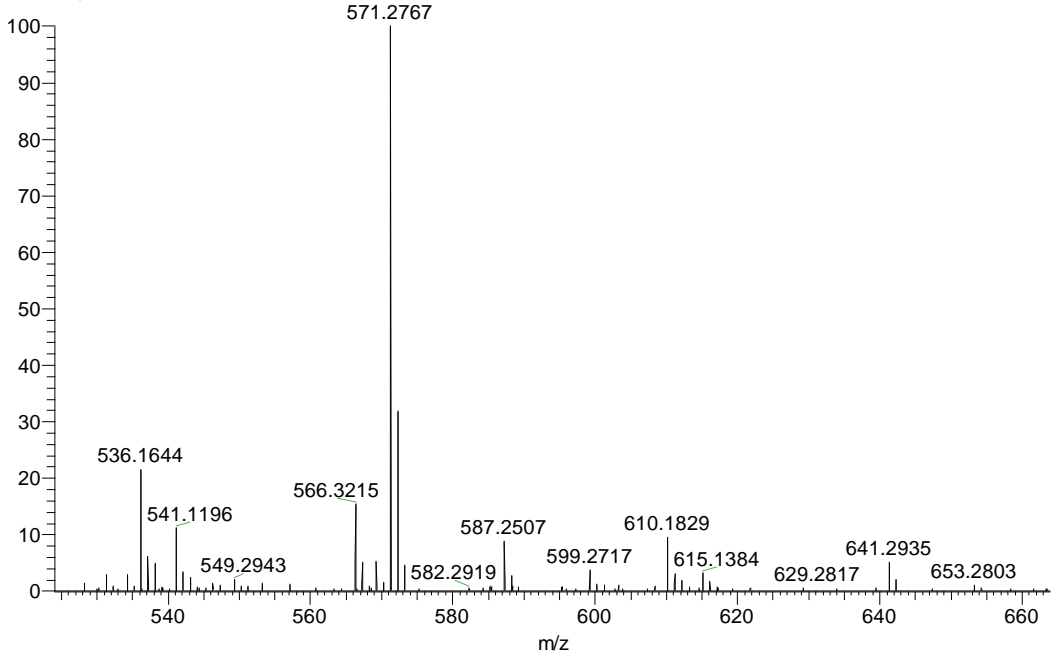
## IR spectrum of compound 5

E:\同济医学院\张勇慧\20131217\2-55-12.0

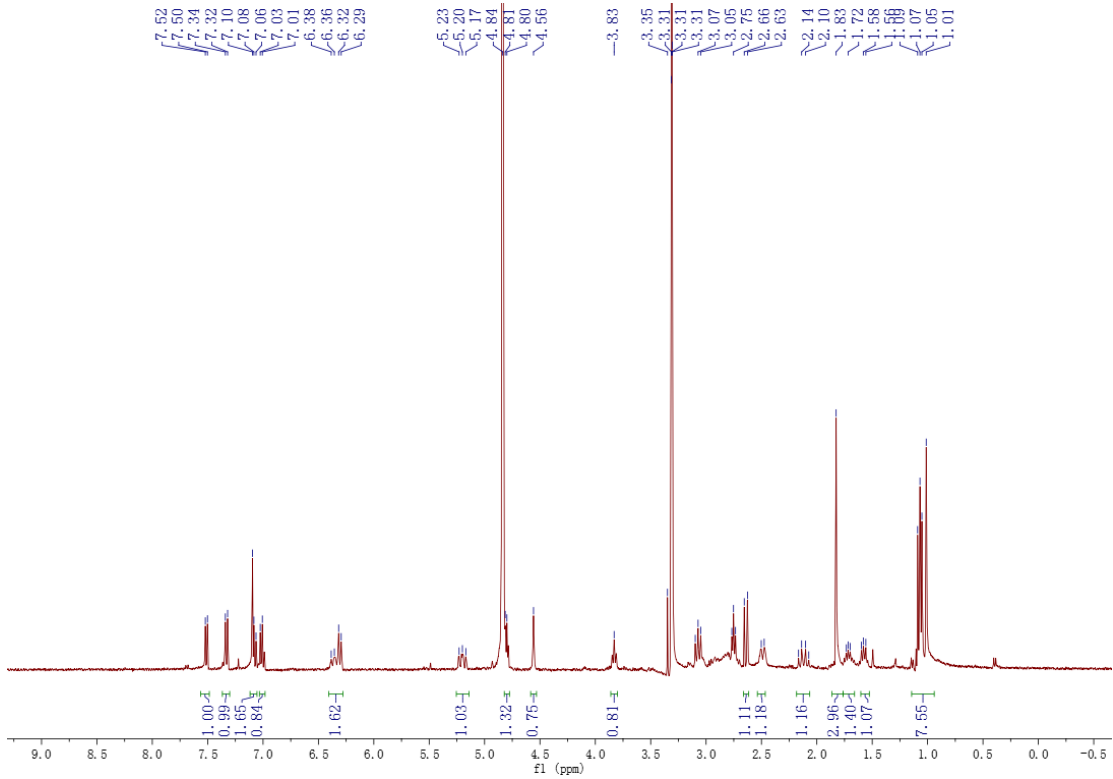


# HRESIMS spectrum of compound 5

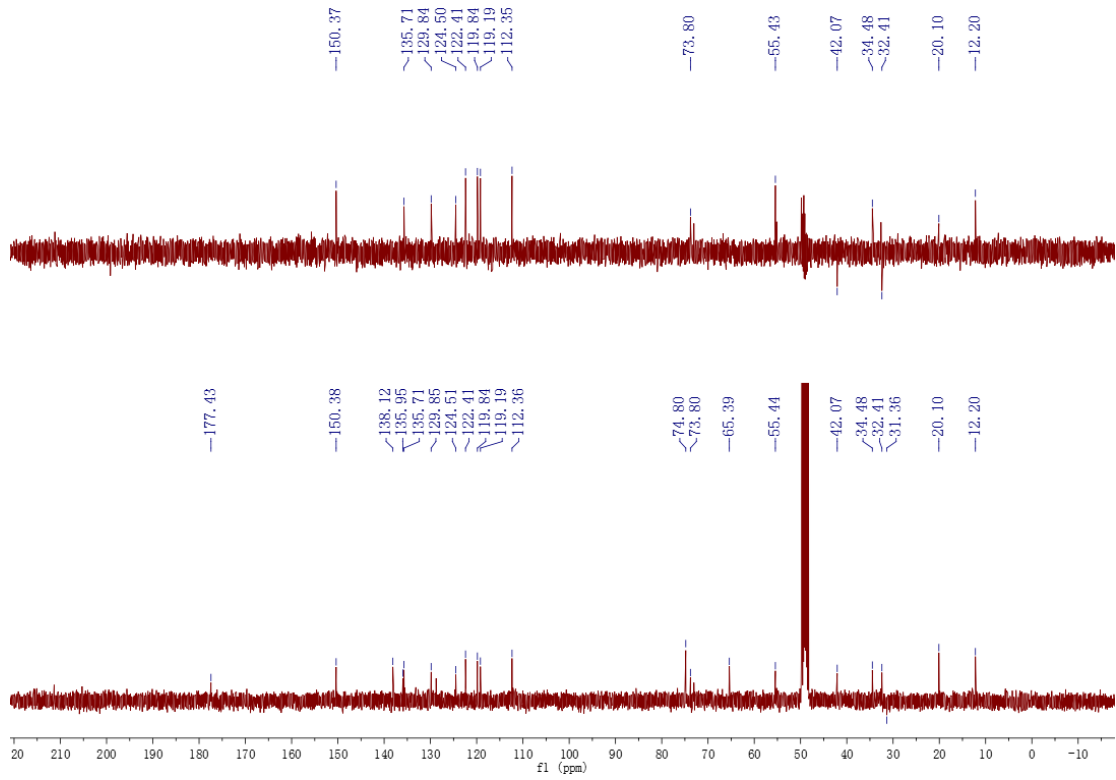
CCM2-98-7 #17 RT: 0.25 AV: 1 NL: 1.03E6  
T: FTMS + p ESI Full ms [50.00-1500.00]



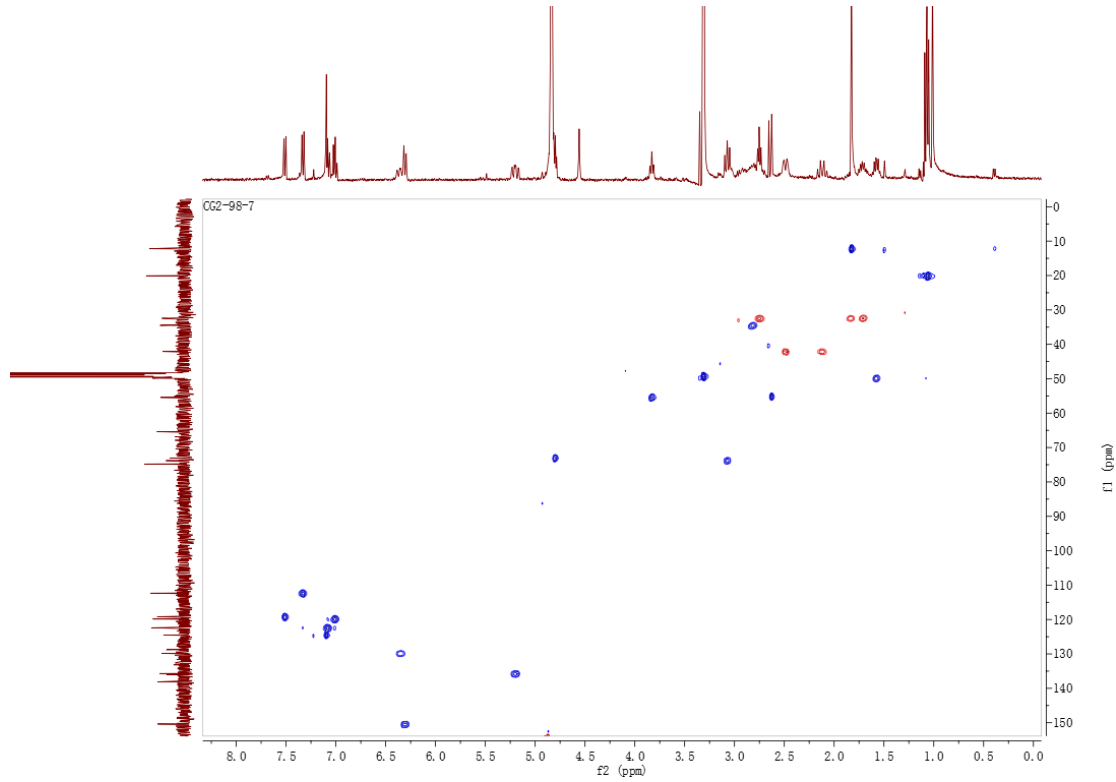
# <sup>1</sup>H NMR spectrum of compound 5



### <sup>13</sup>C NMR and DEPT spectra of compound 5

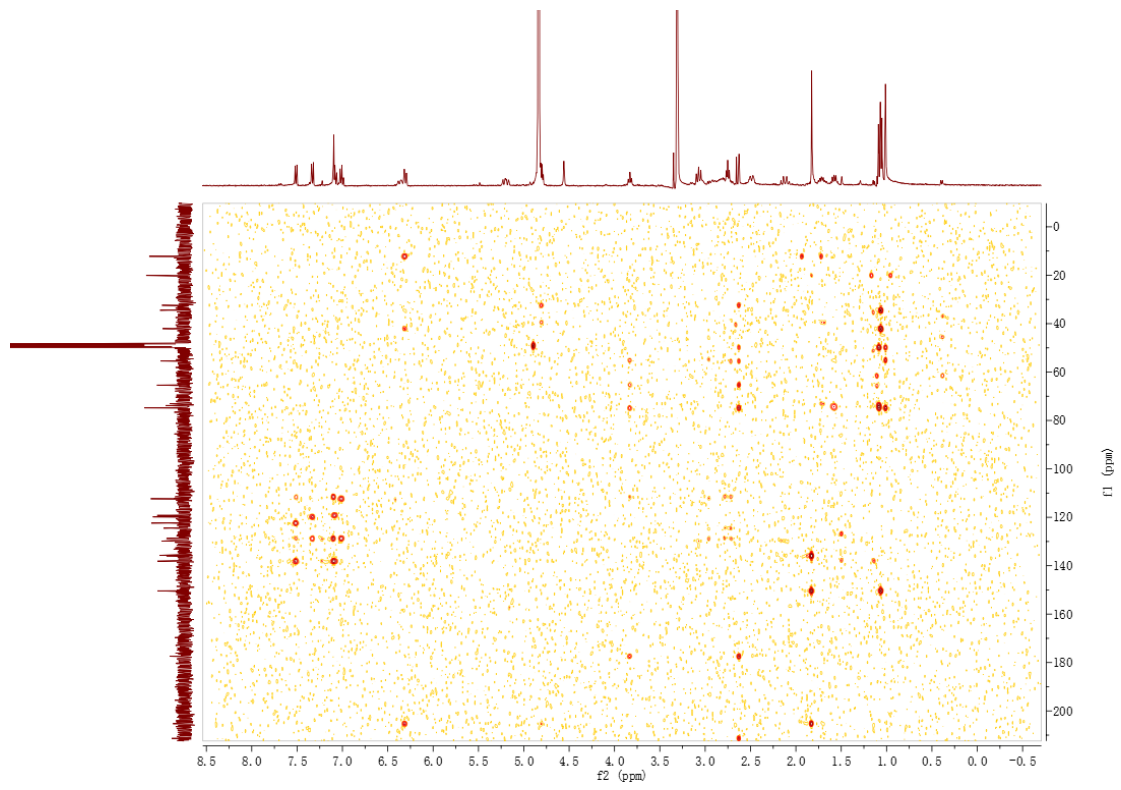


### HSQC spectrum of compound 5

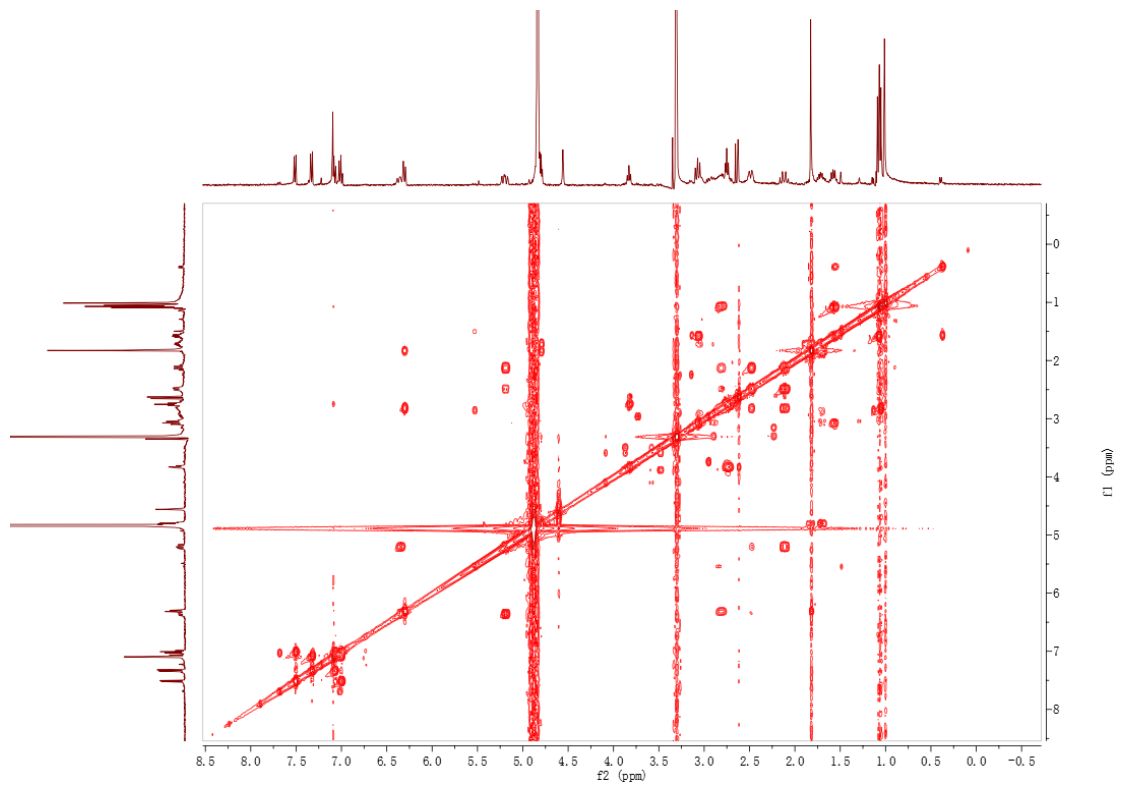




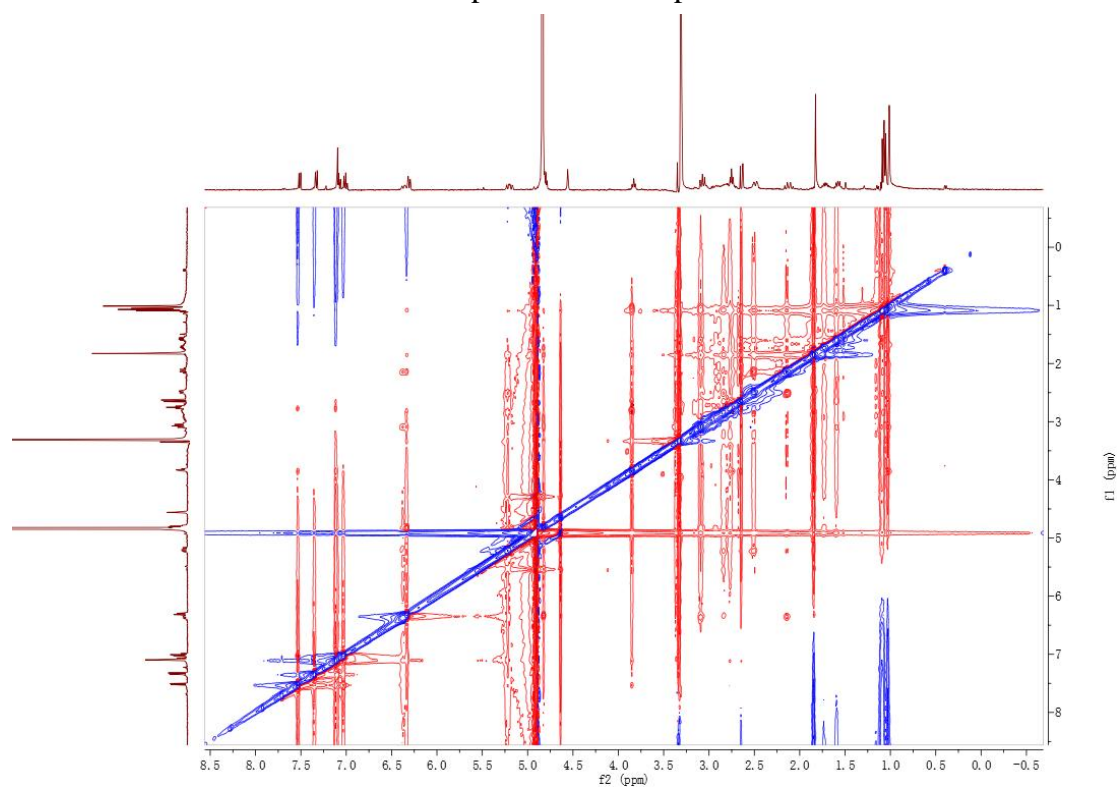
HMBC spectrum of compound 5



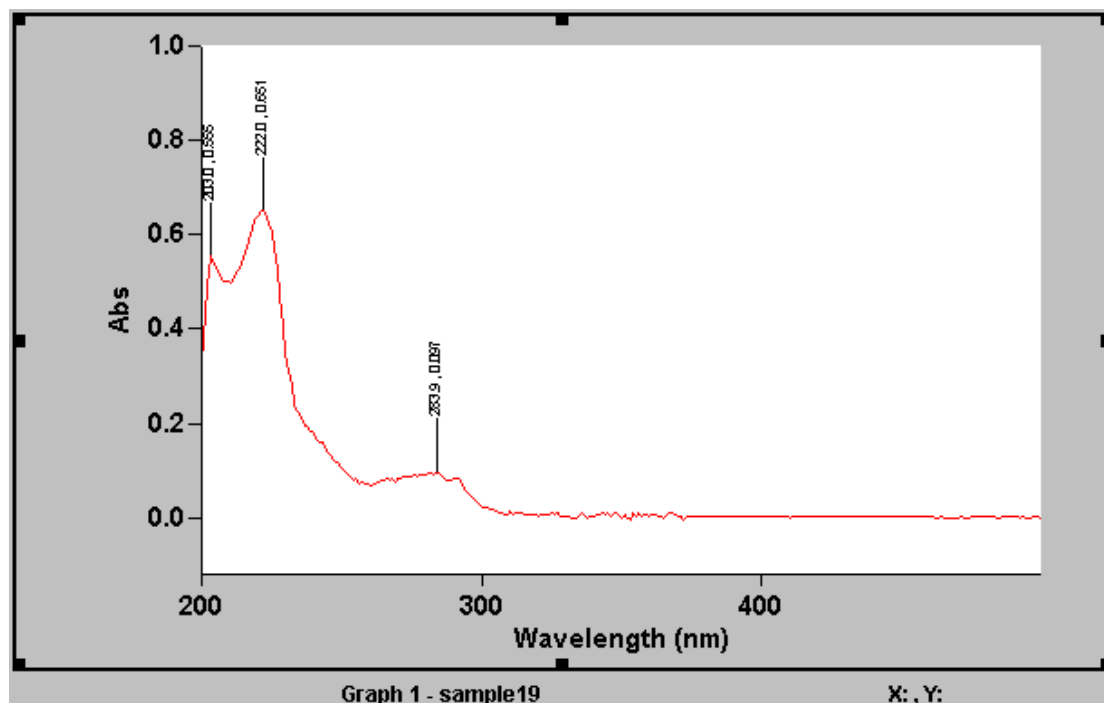
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 5



NOESY spectrum of compound 5

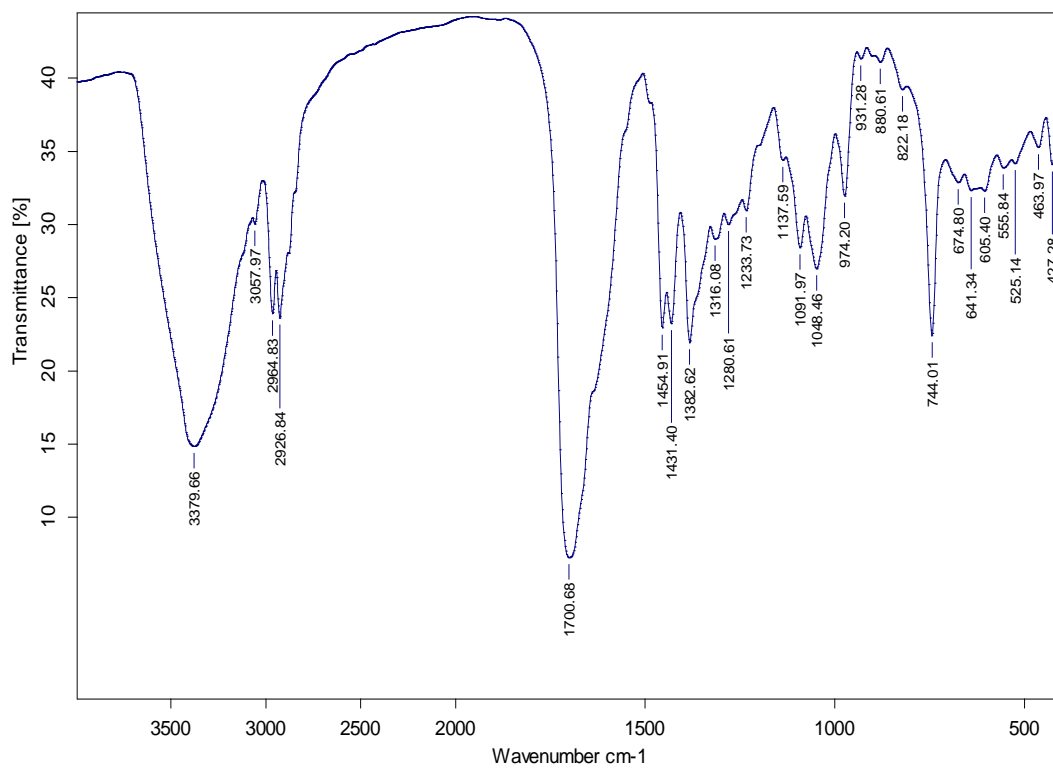


UV spectrum of compound 6



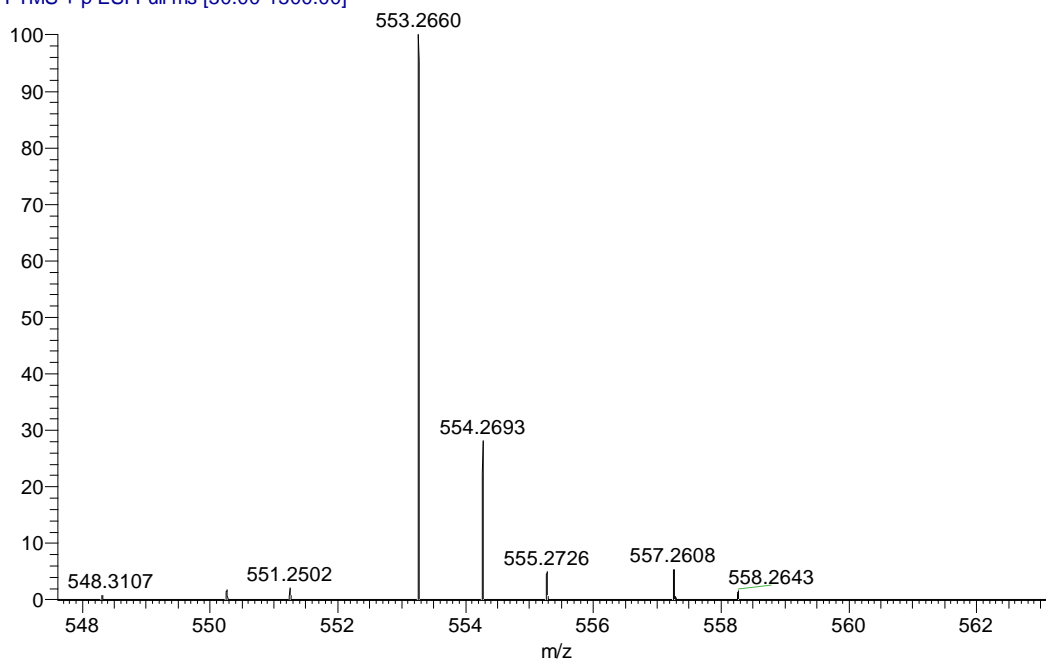
## IR spectrum of compound 6

E:\河济医学院\张勇慧\20131217\2-65-2.0

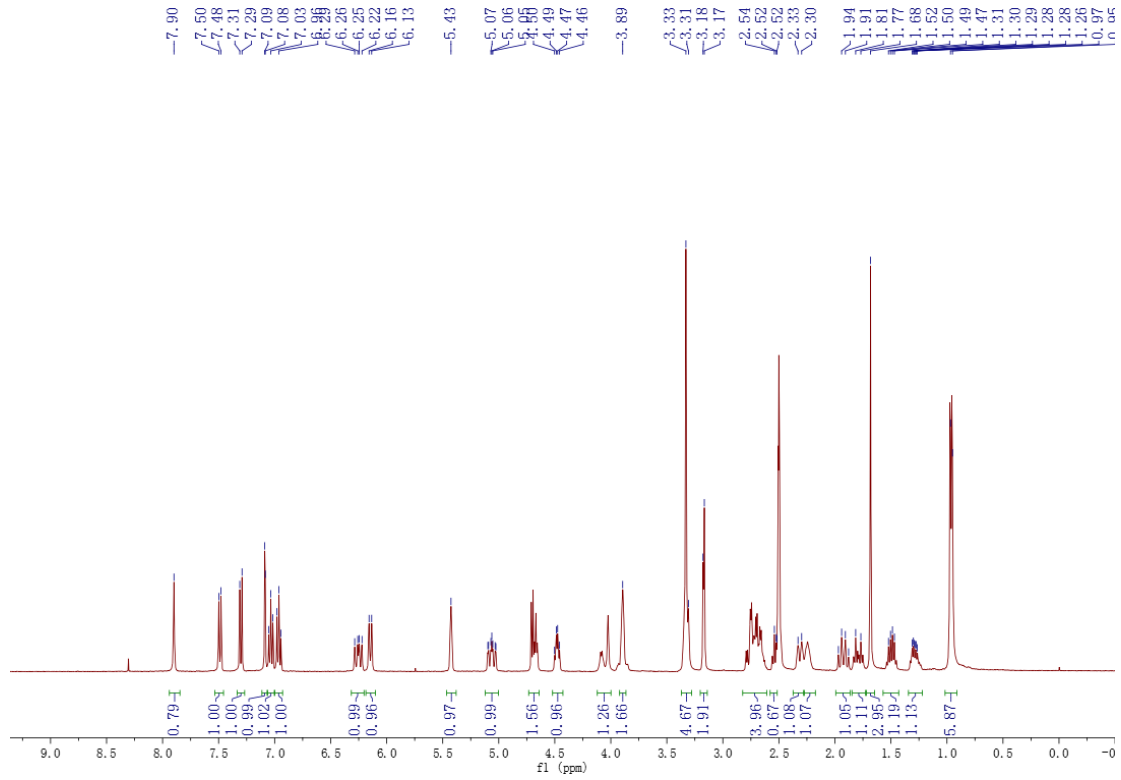


## HRESIMS spectrum of compound 6

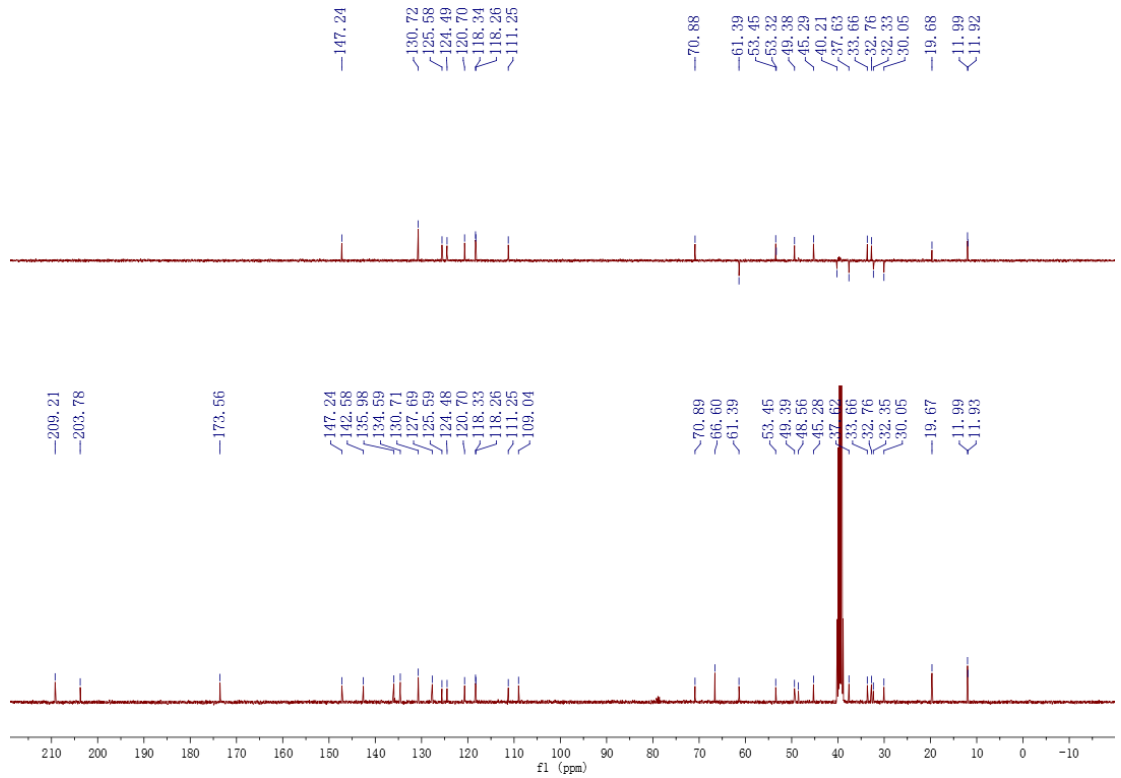
CCM2-98-4 #16 RT: 0.24 AV: 1 NL: 1.76E5  
T: FTMS + p ESI Full ms [50.00-1500.00]



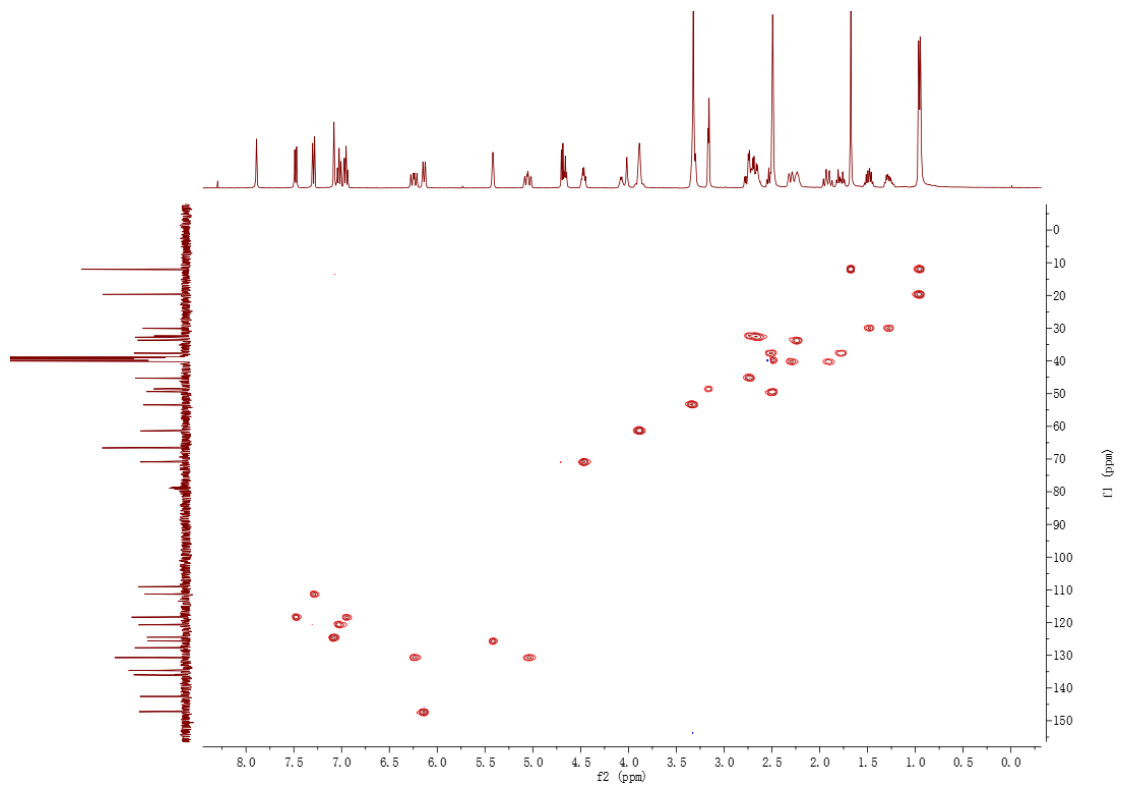
### <sup>1</sup>H NMR spectrum of compound 6



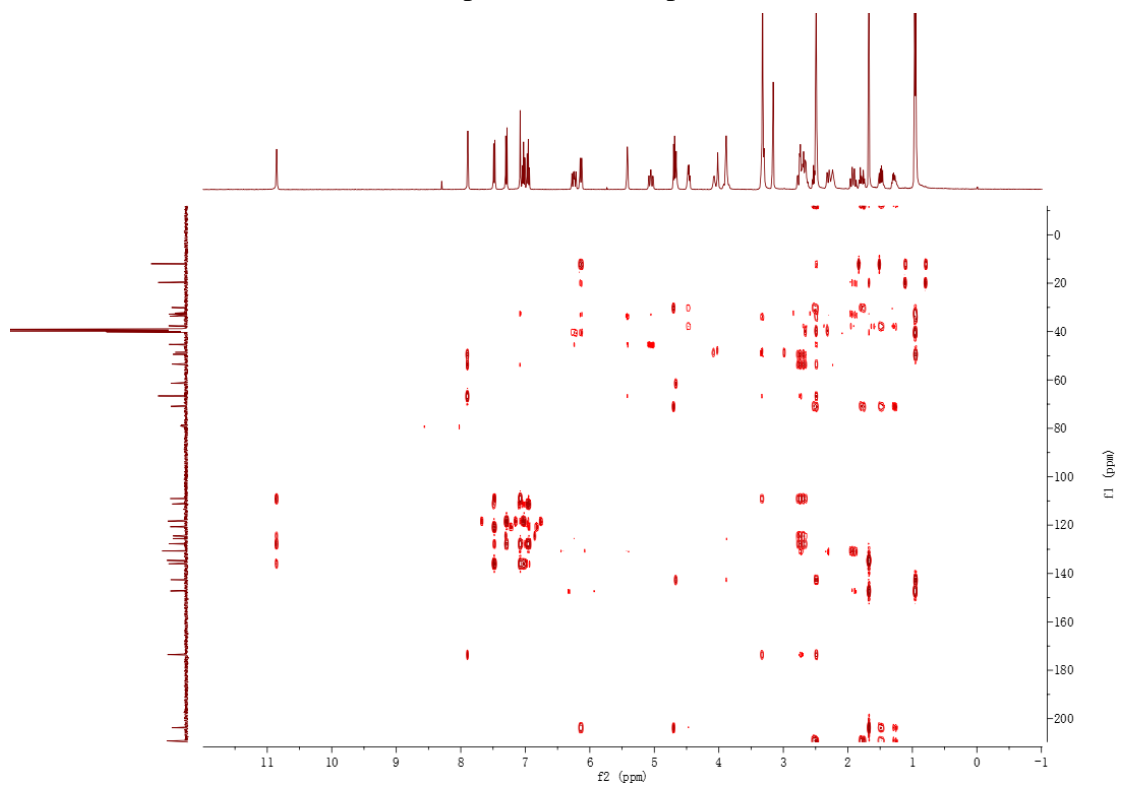
### <sup>13</sup>C NMR and DEPT spectra of compound 6



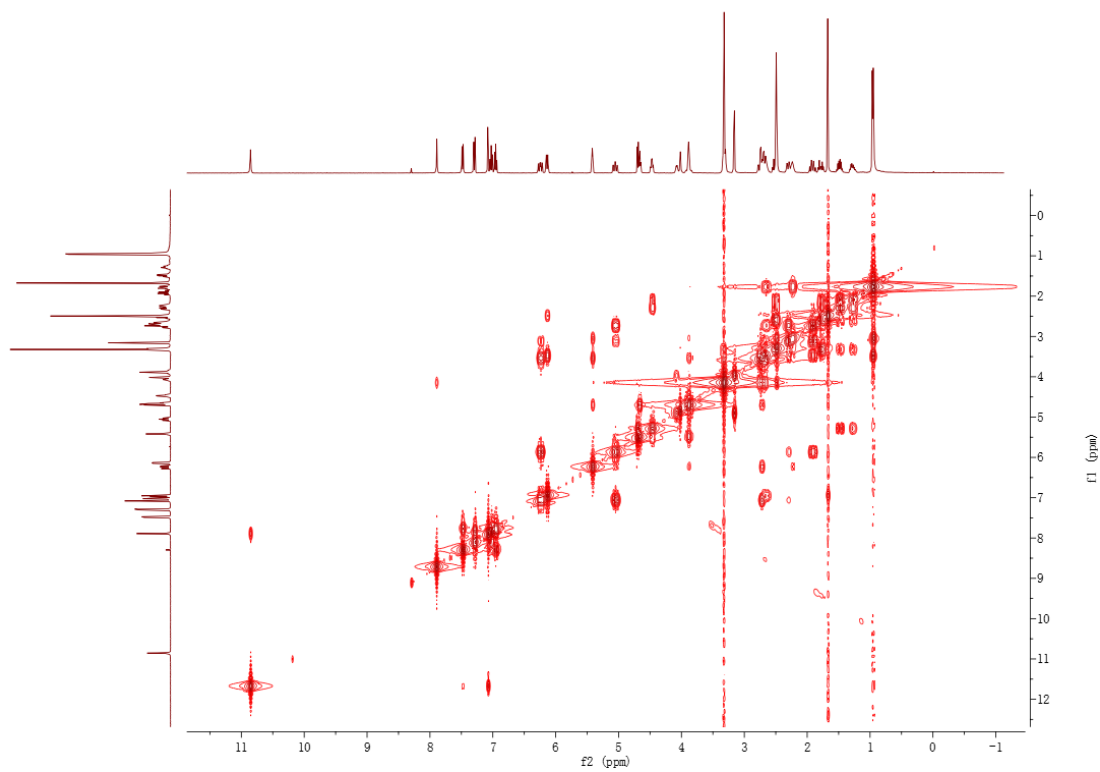
HSQC spectrum of compound **6**



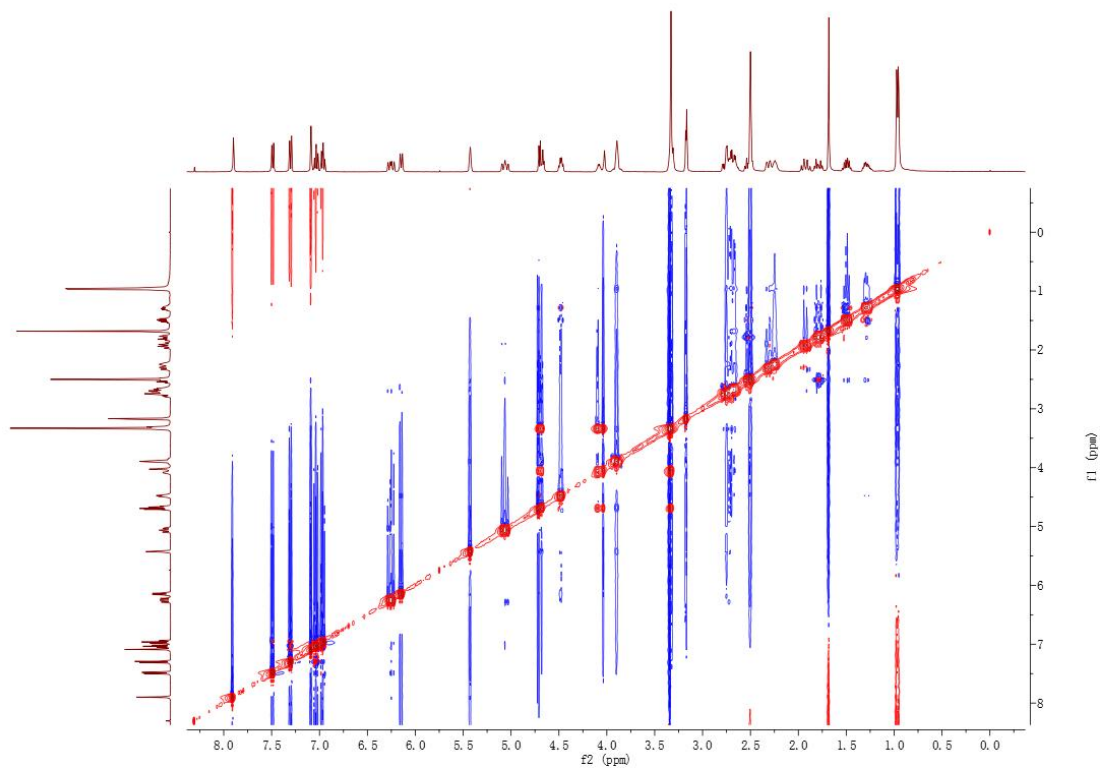
HMBC spectrum of compound **6**



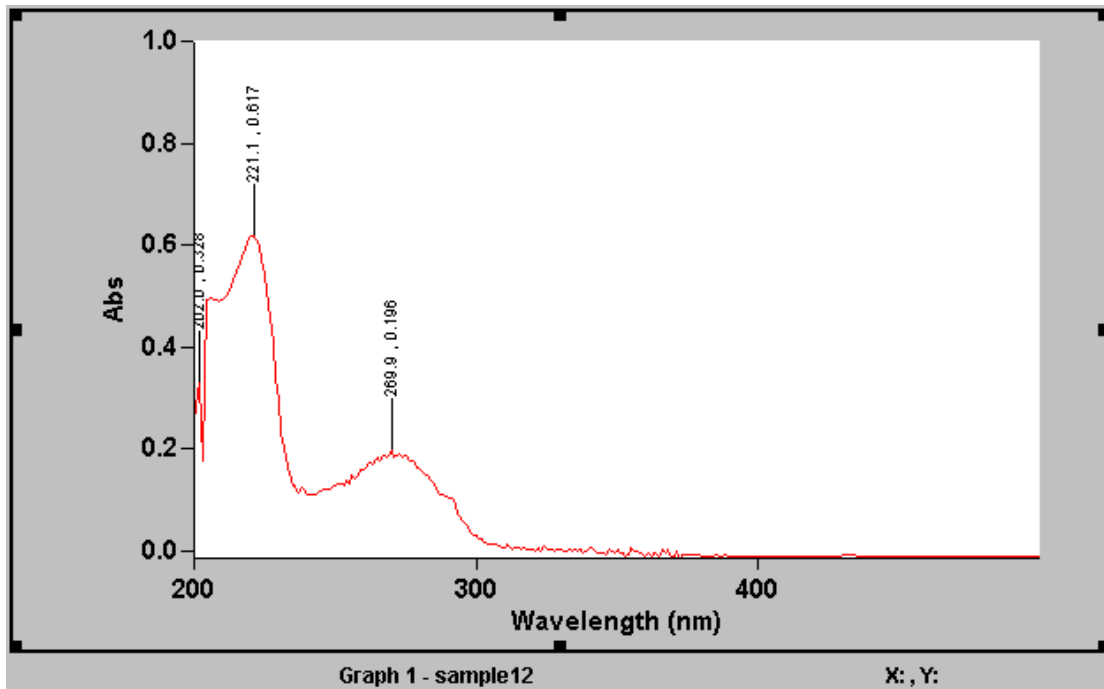
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **6**



NOESY spectrum of compound **6**

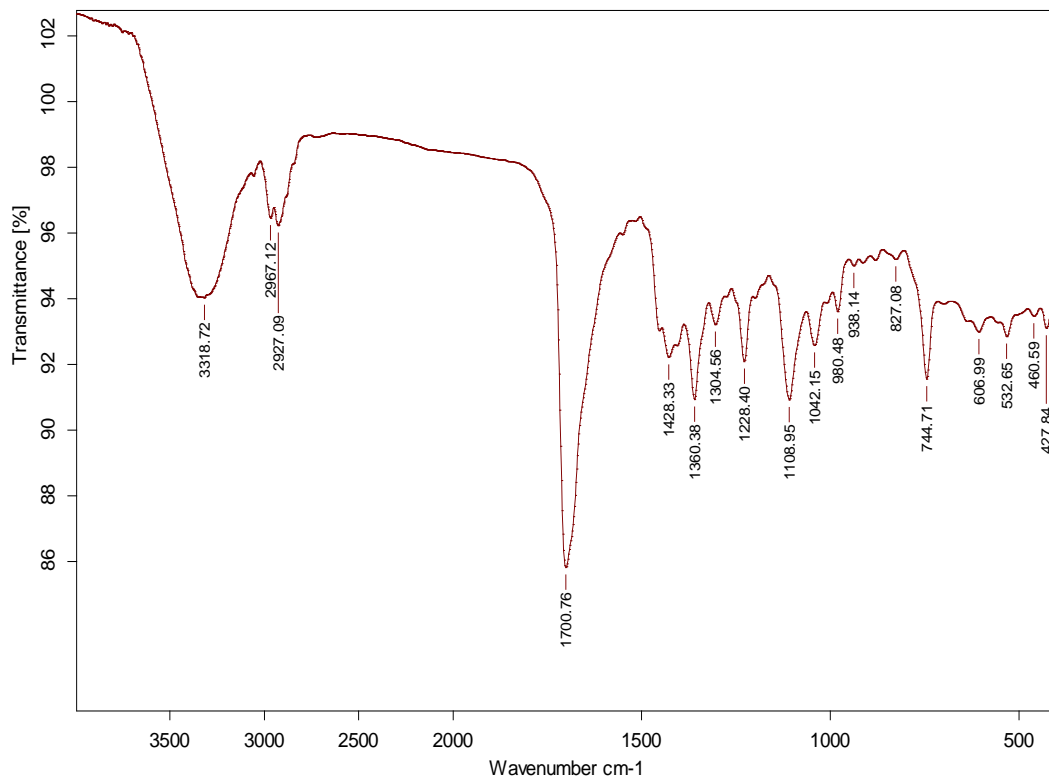


### UV spectrum of compound 7



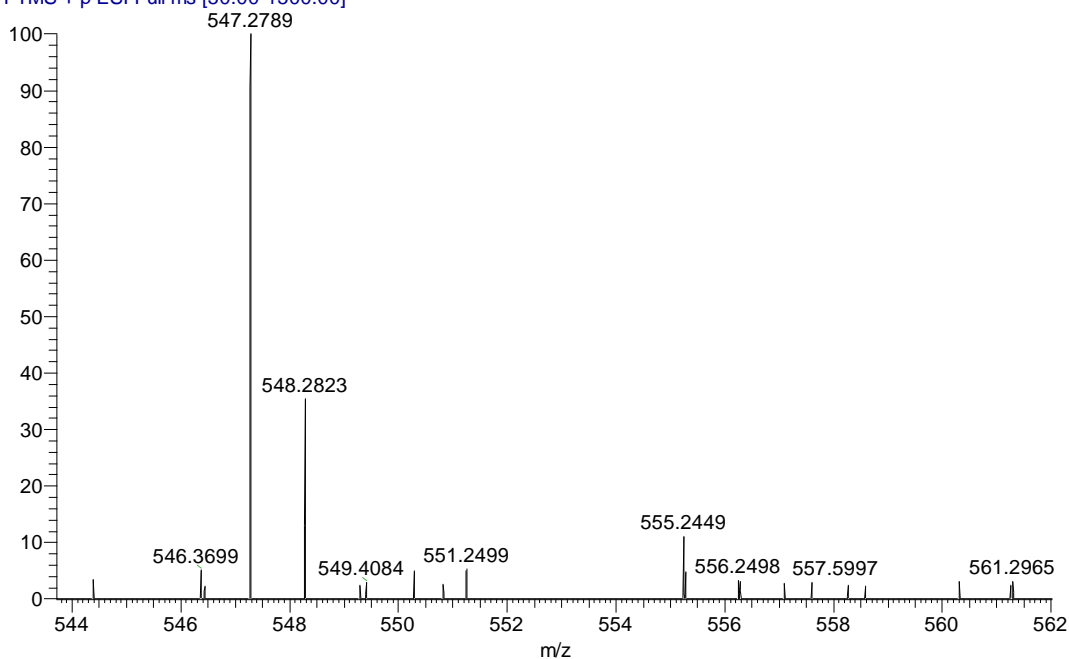
### IR spectrum of compound 7

E:\同济医学院\张勇慧\20140617\001.9

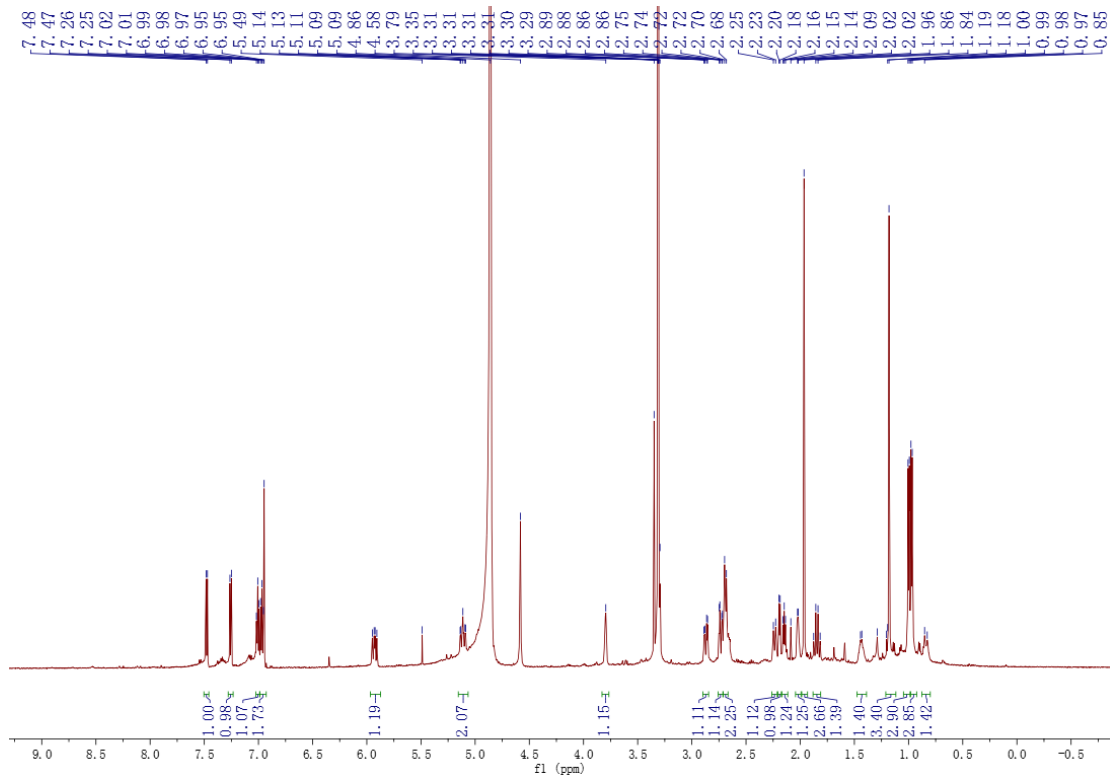


# HRESIMS spectrum of compound 7

CCM2-98-6 #21 RT: 0.31 AV: 1 NL: 1.39E5  
T: FTMS + p ESI Full ms [50.00-1500.00]

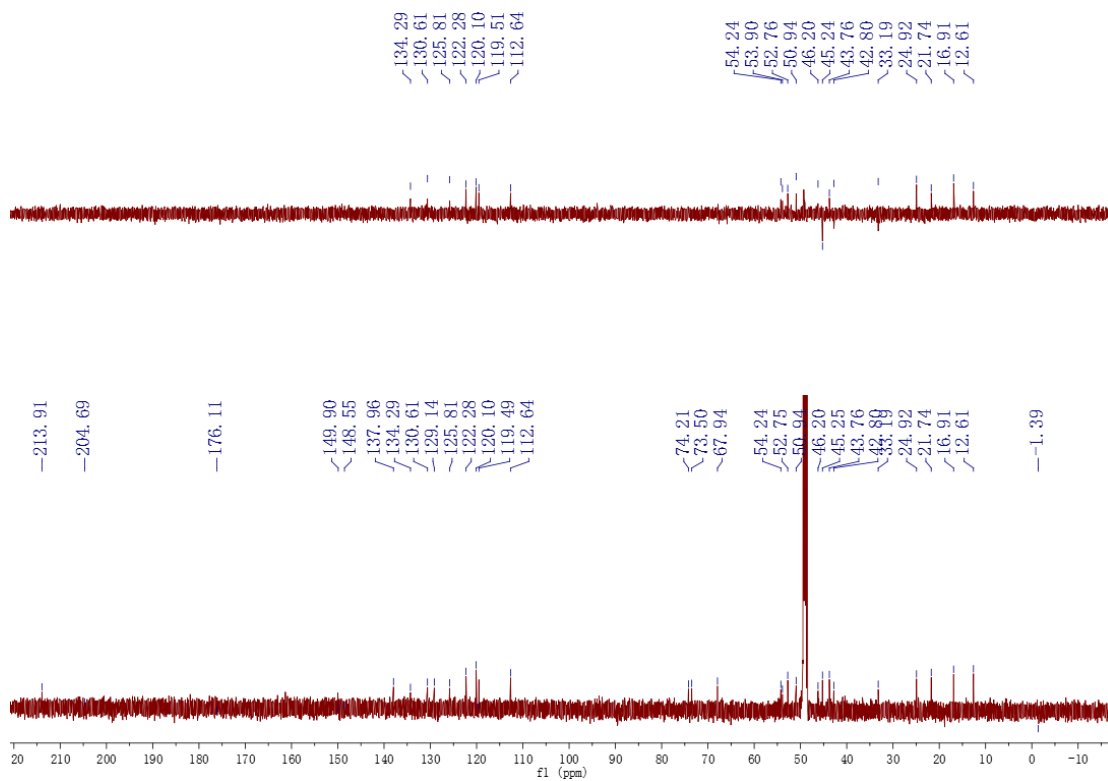


# <sup>1</sup>H NMR spectrum of compound 7

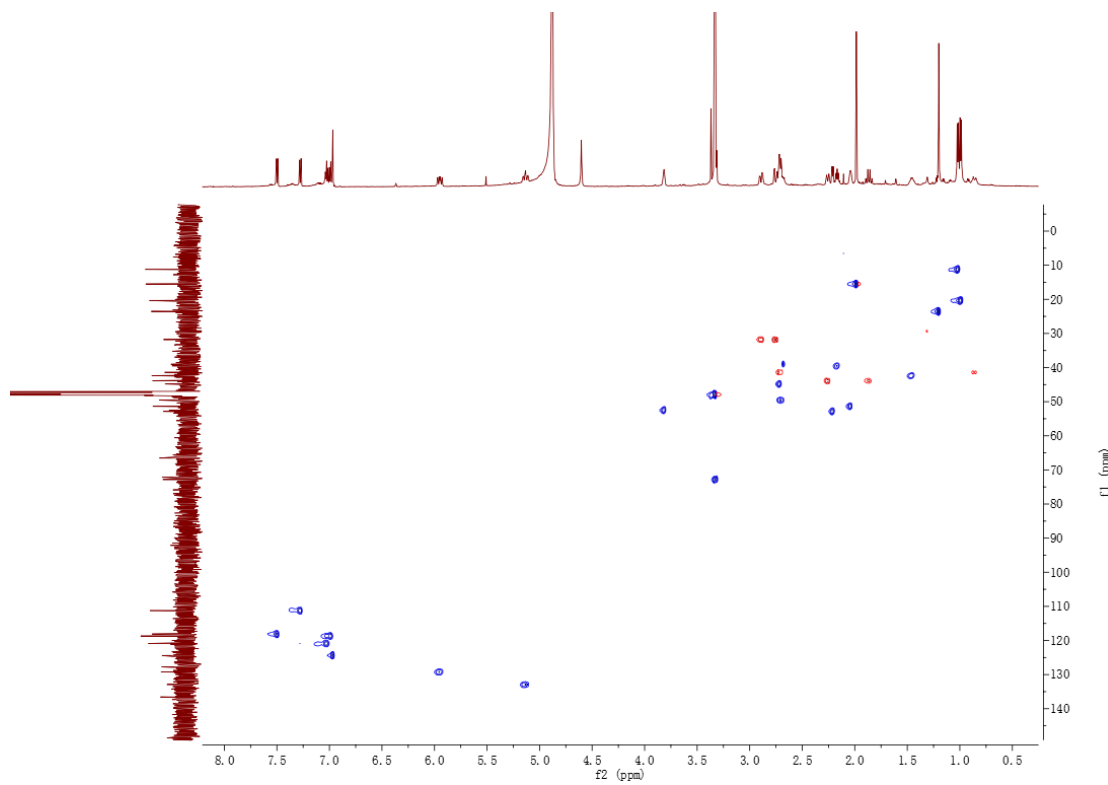




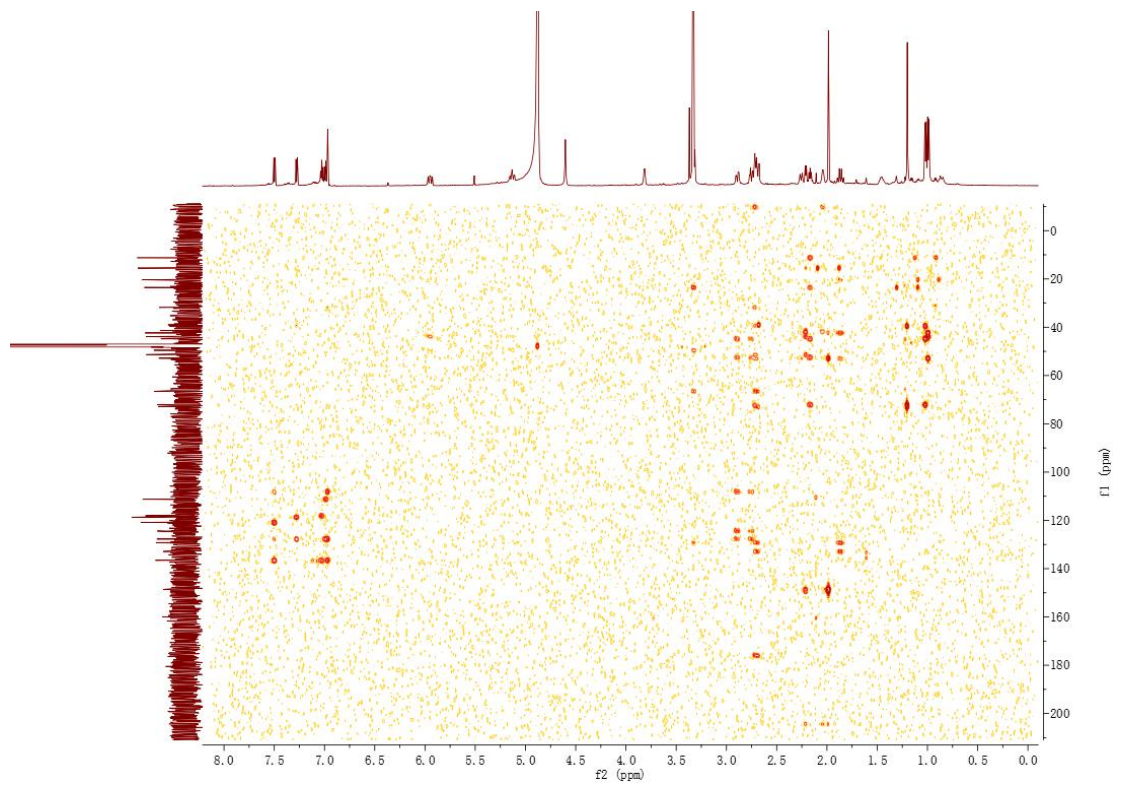
### <sup>13</sup>C NMR and DEPT spectra of compound 7



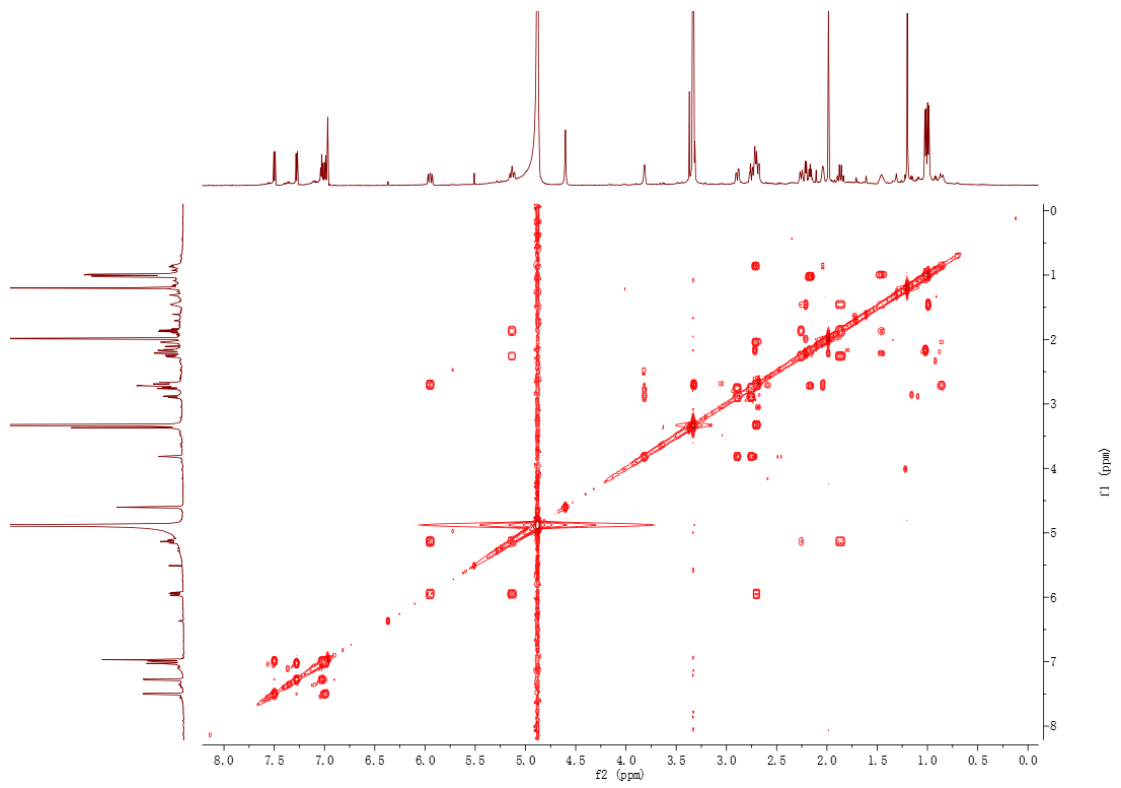
### HSQC spectrum of compound 7



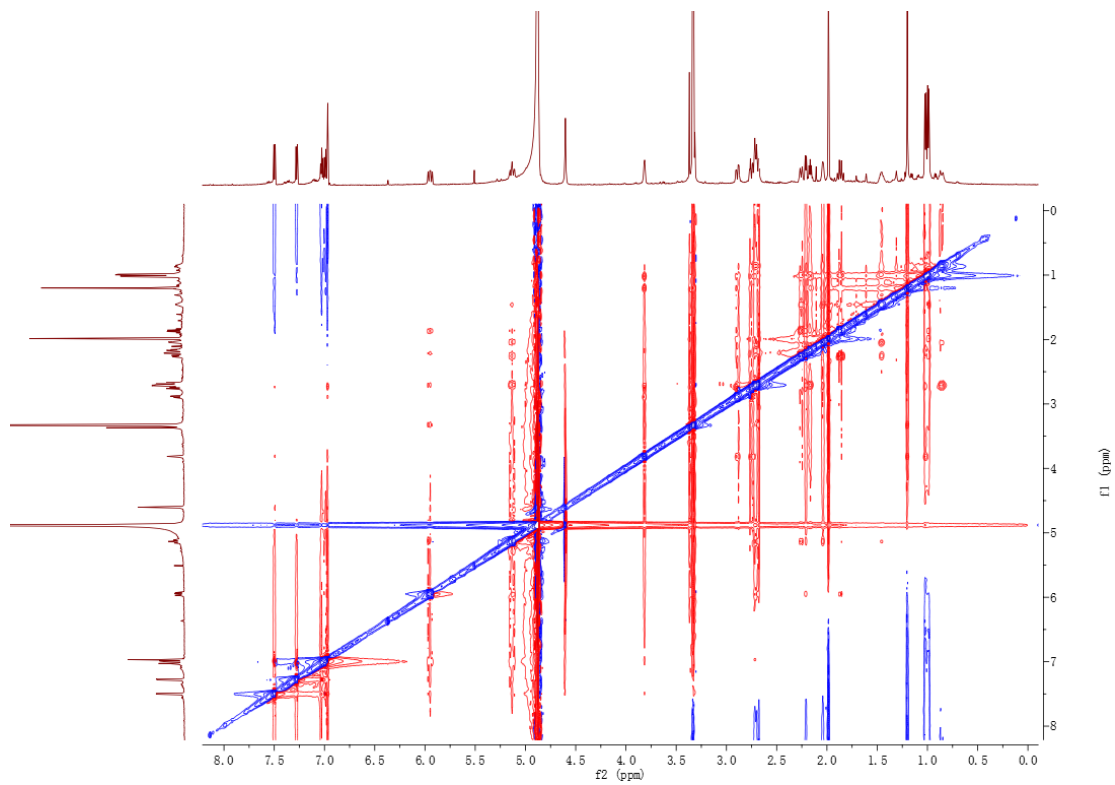
HMBC spectrum of compound 7



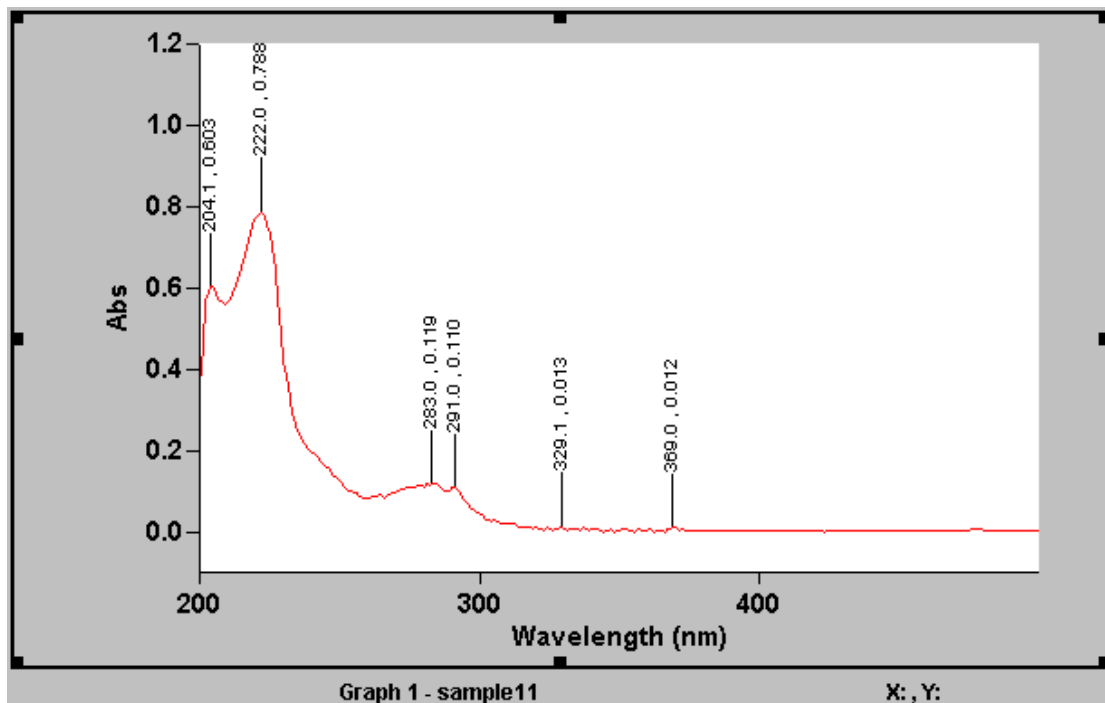
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 7



Y spectrum of compound 7

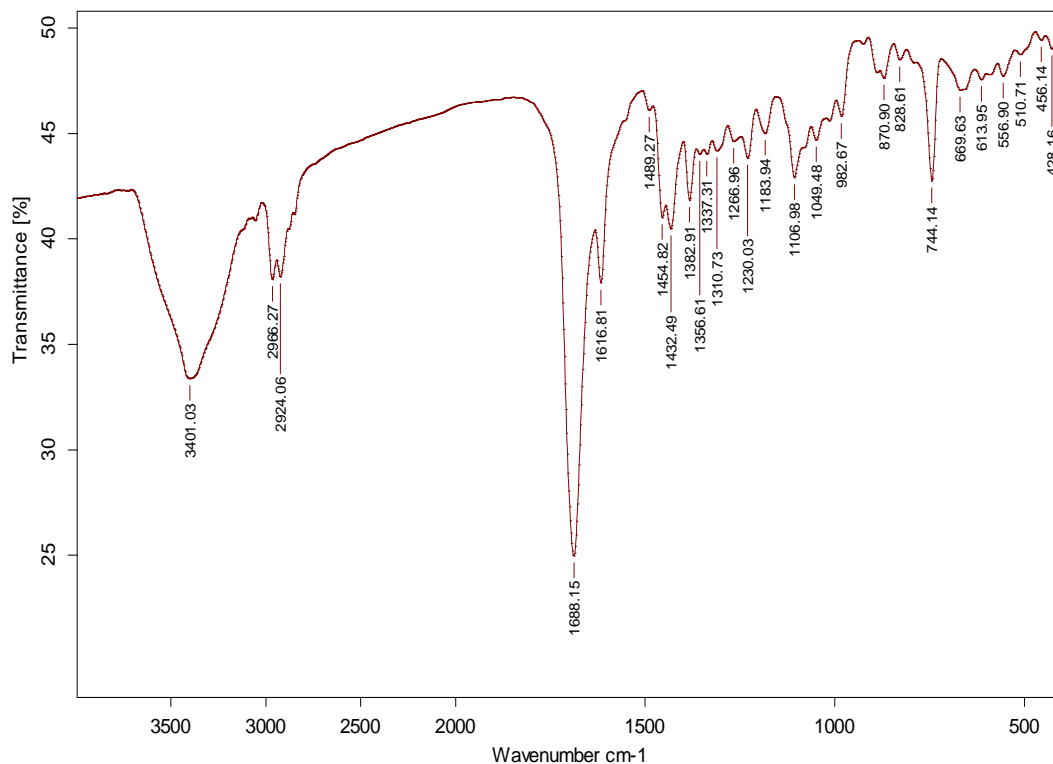


UV spectrum of compound 8



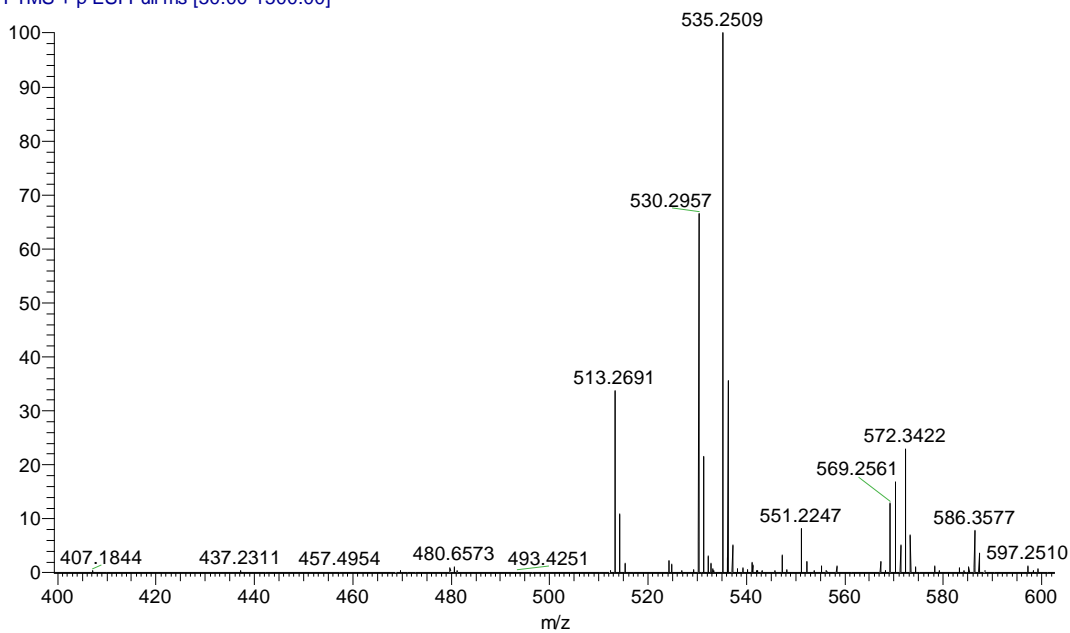
## IR spectrum of compound **8**

E:\同济医学院\张勇慧\20131217\2-64-1.0

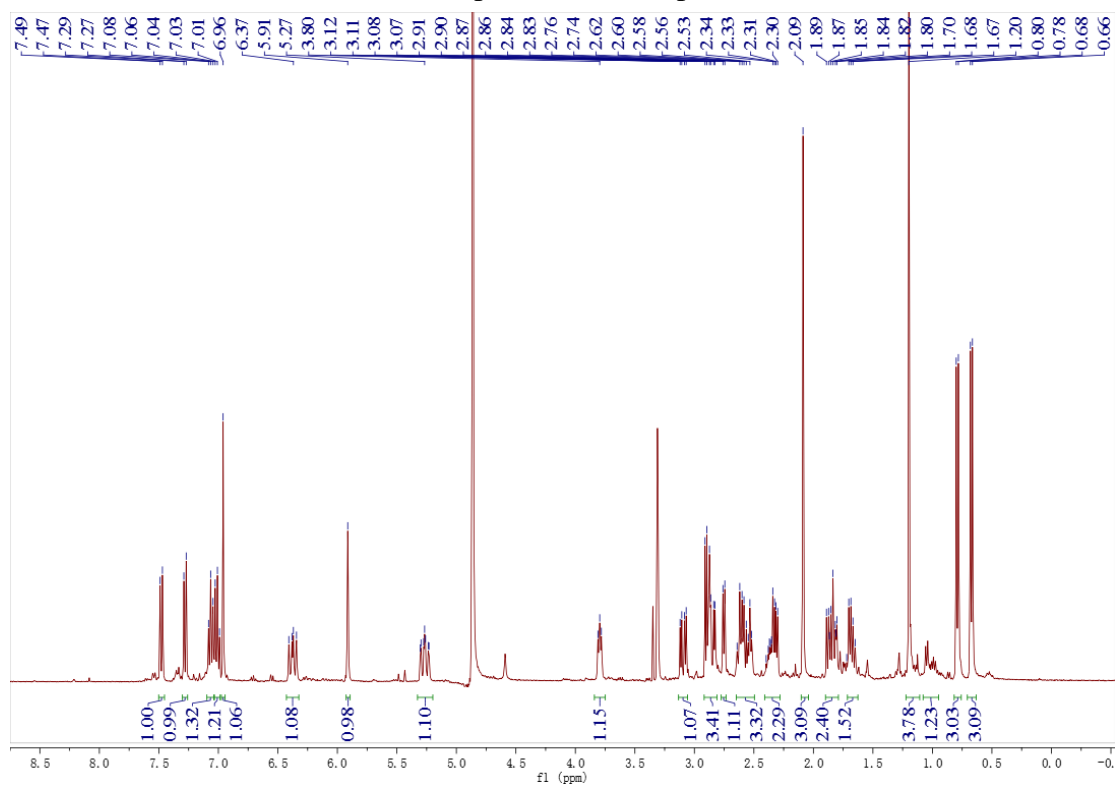


## HRESIMS spectrum of compound **8**

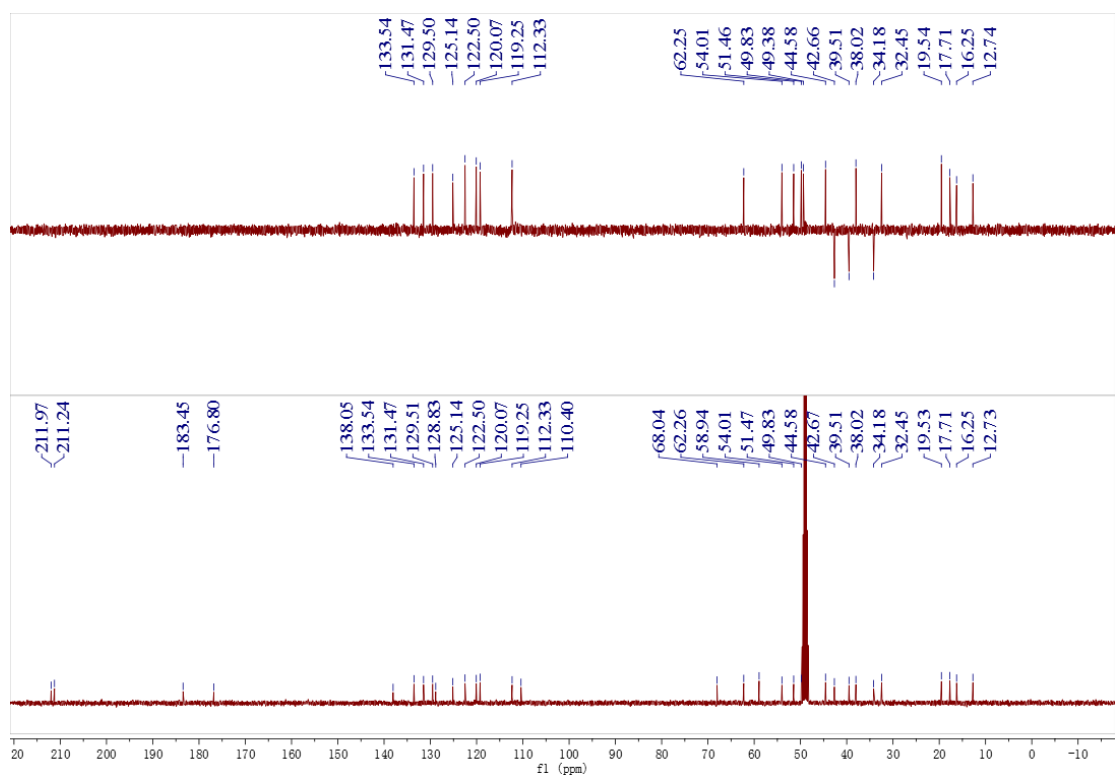
csm2-64-1 #27 RT: 0.38 AV: 1 NL: 1.15E7  
T: FTMS + p ESI Full ms [50.00-1500.00]



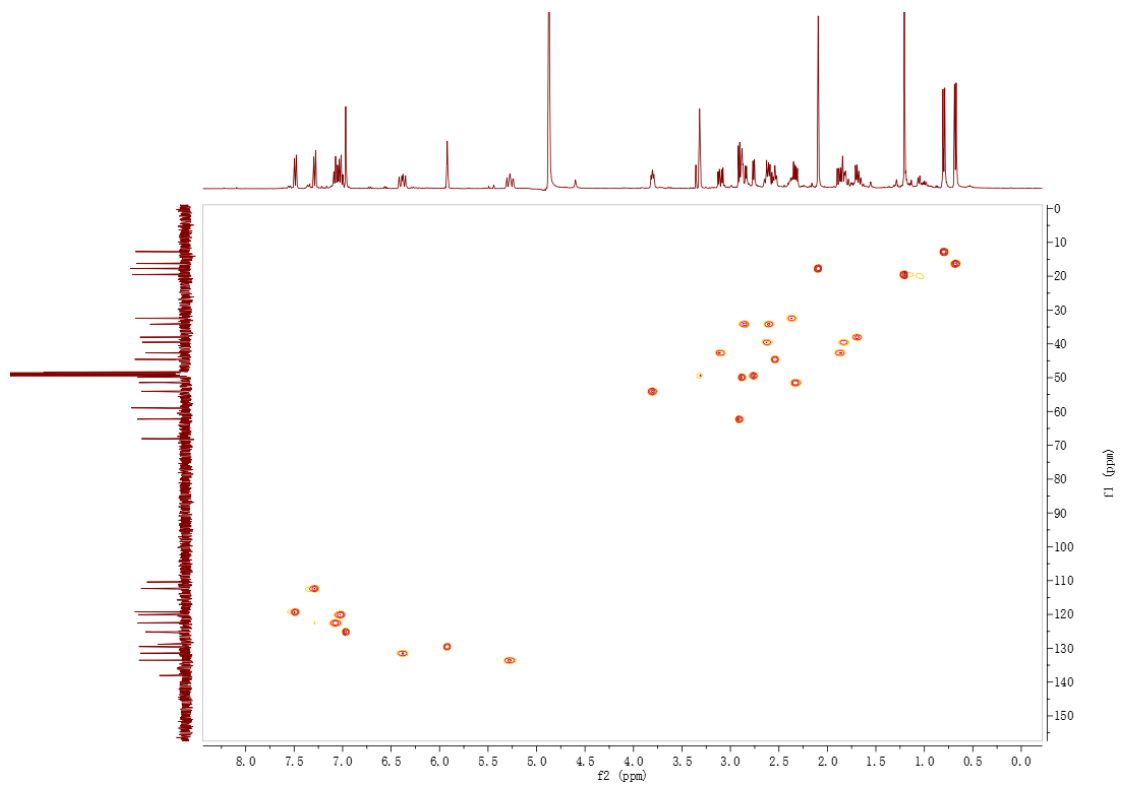
### <sup>1</sup>H NMR spectrum of compound **8**



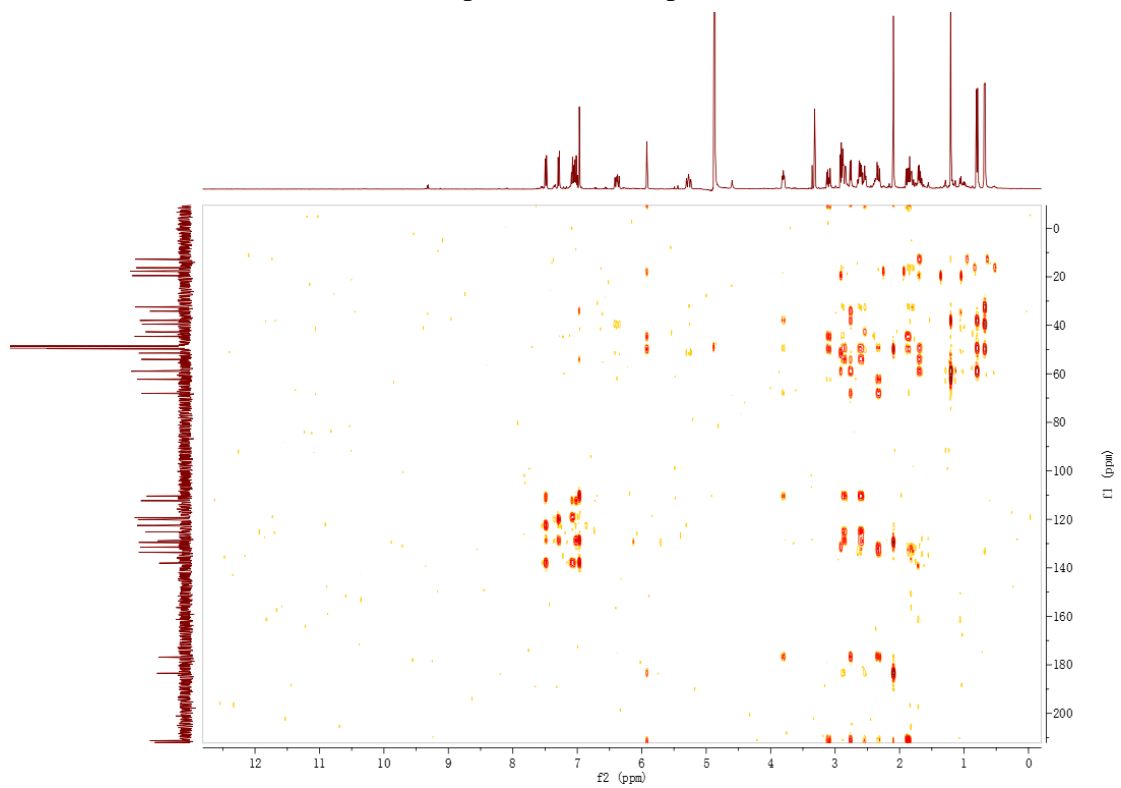
### <sup>13</sup>C NMR and DEPT spectra of compound **8**



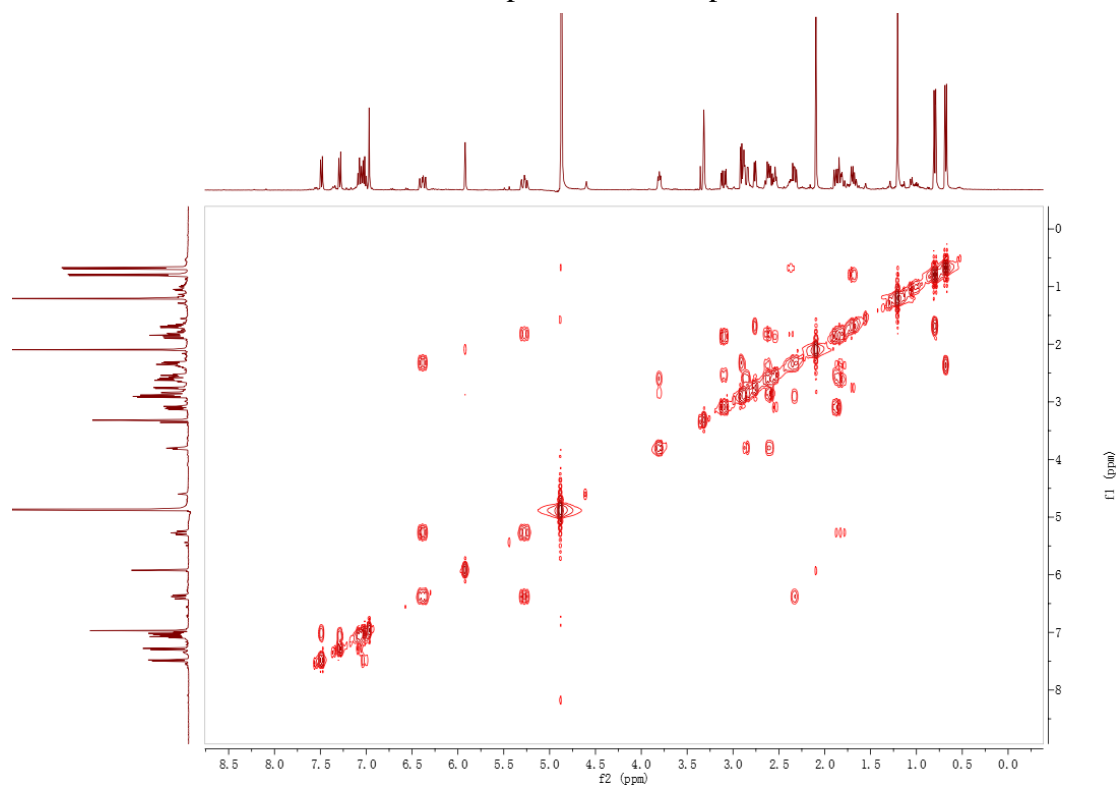
HSQC spectrum of compound **8**



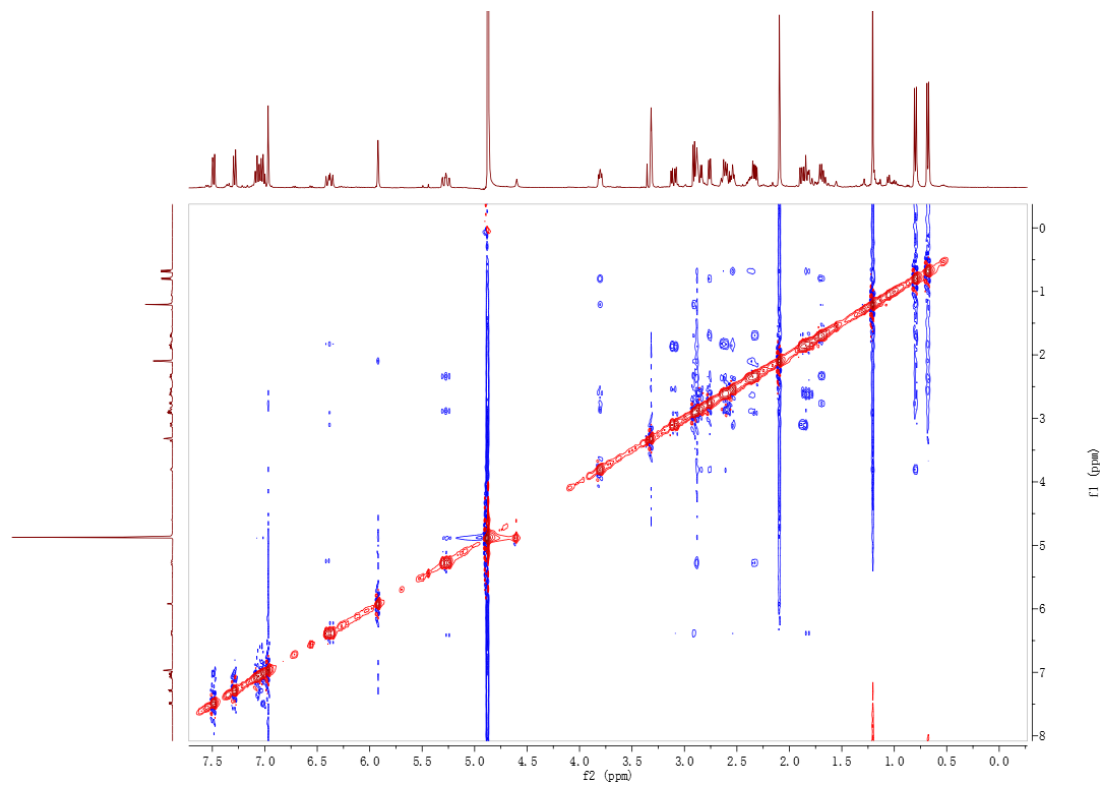
HMBC spectrum of compound **8**



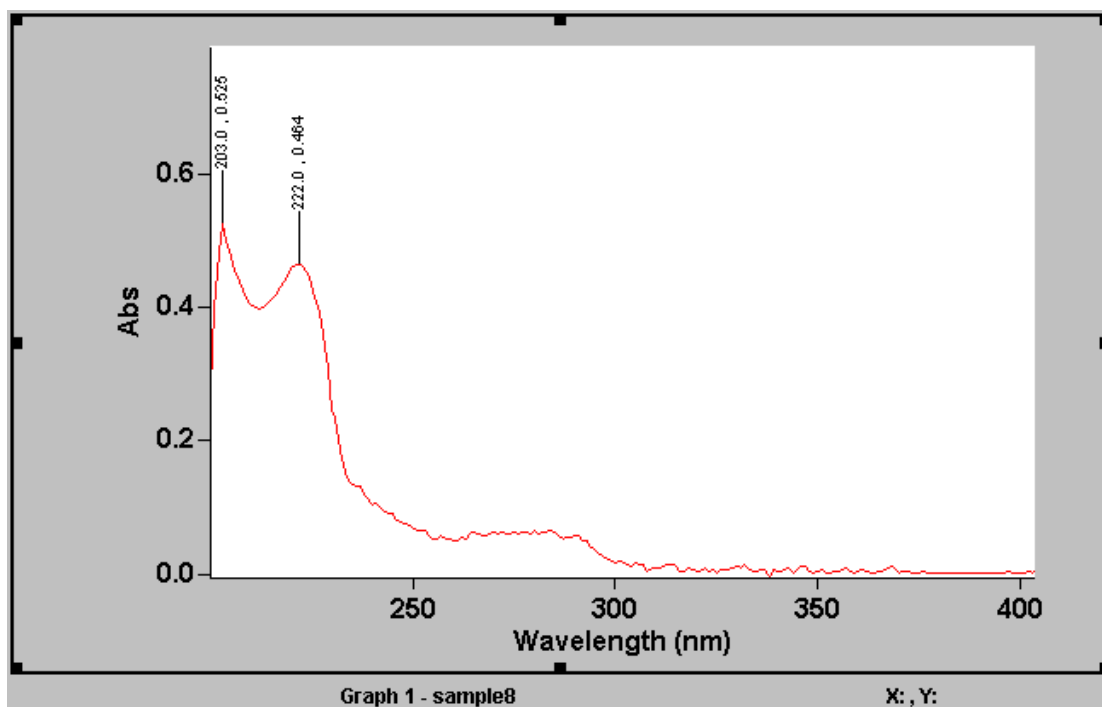
$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **8**



NOESY spectrum of compound **8**



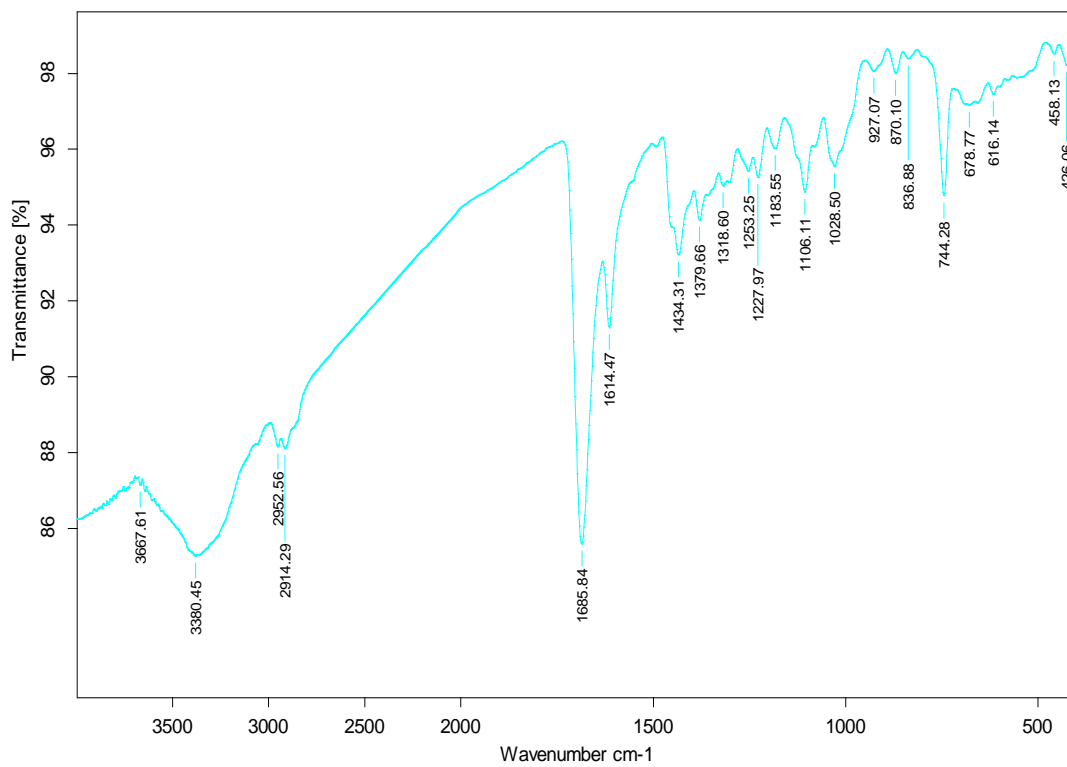
# UV spectrum of compound 9



# IR spectrum of compound 9

E:\同济医学院\张勇慧\20140325\CG2-73-1.0

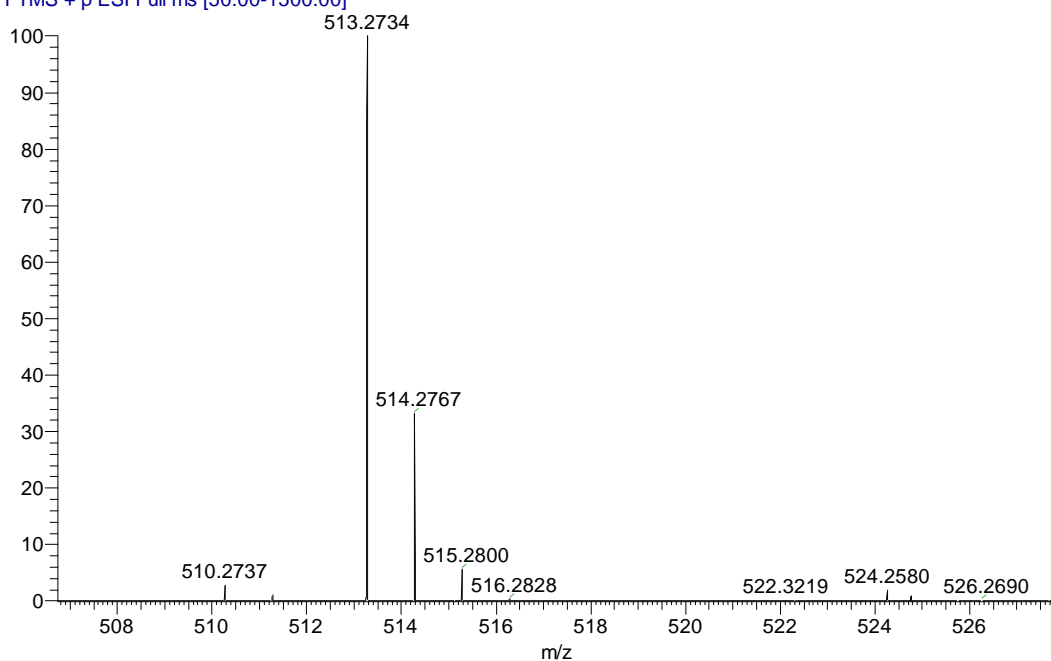
仪器型号: Bruker Vertex 70



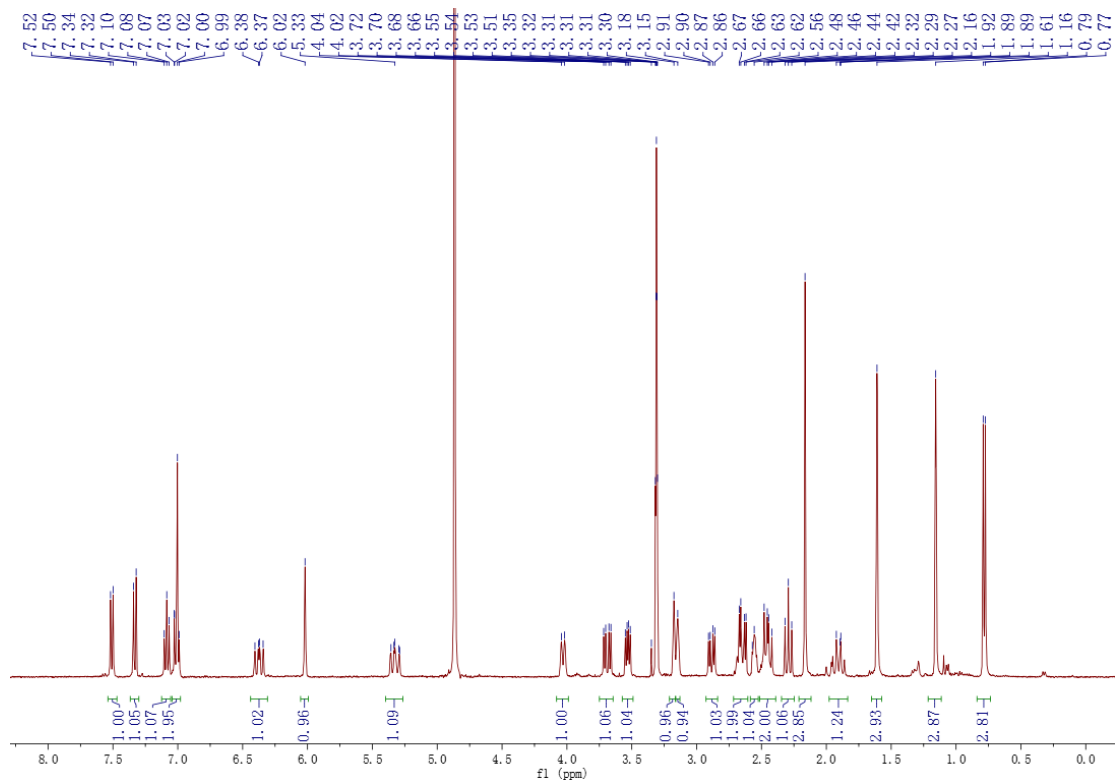


# HRESIMS spectrum of compound 9

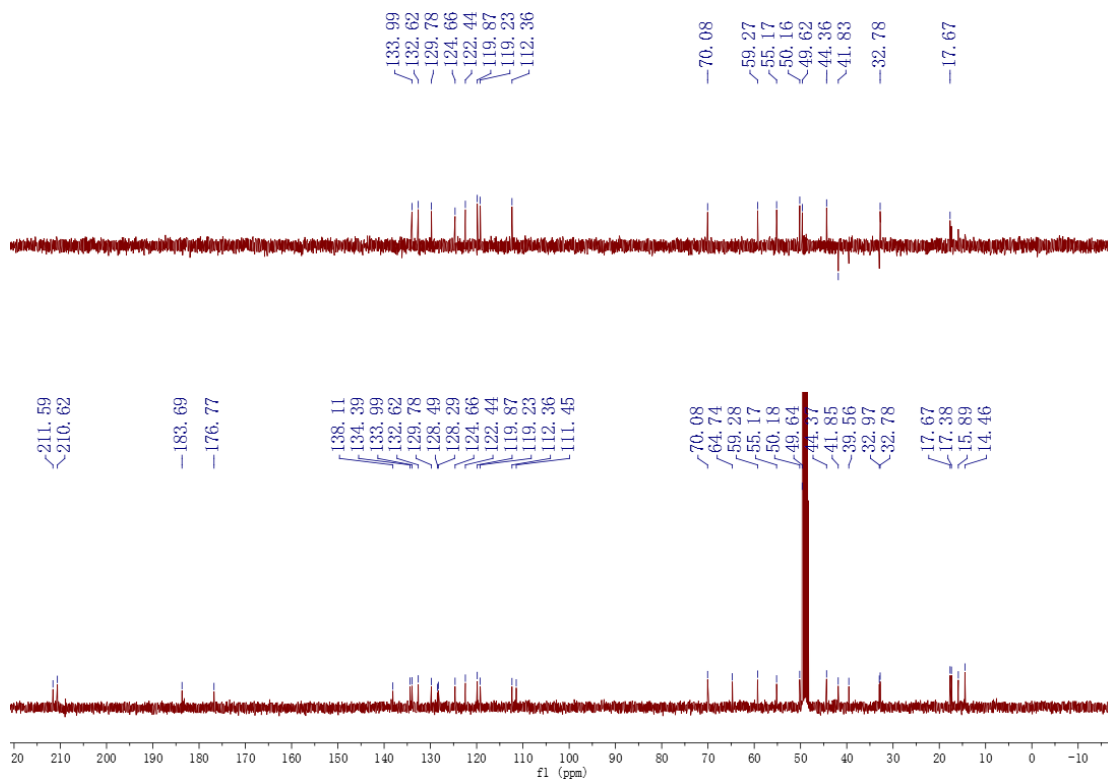
CG2-73-1 #26 RT: 0.37 AV: 1 NL: 1.19E7  
T: FTMS + p ESI Full ms [50.00-1500.00]



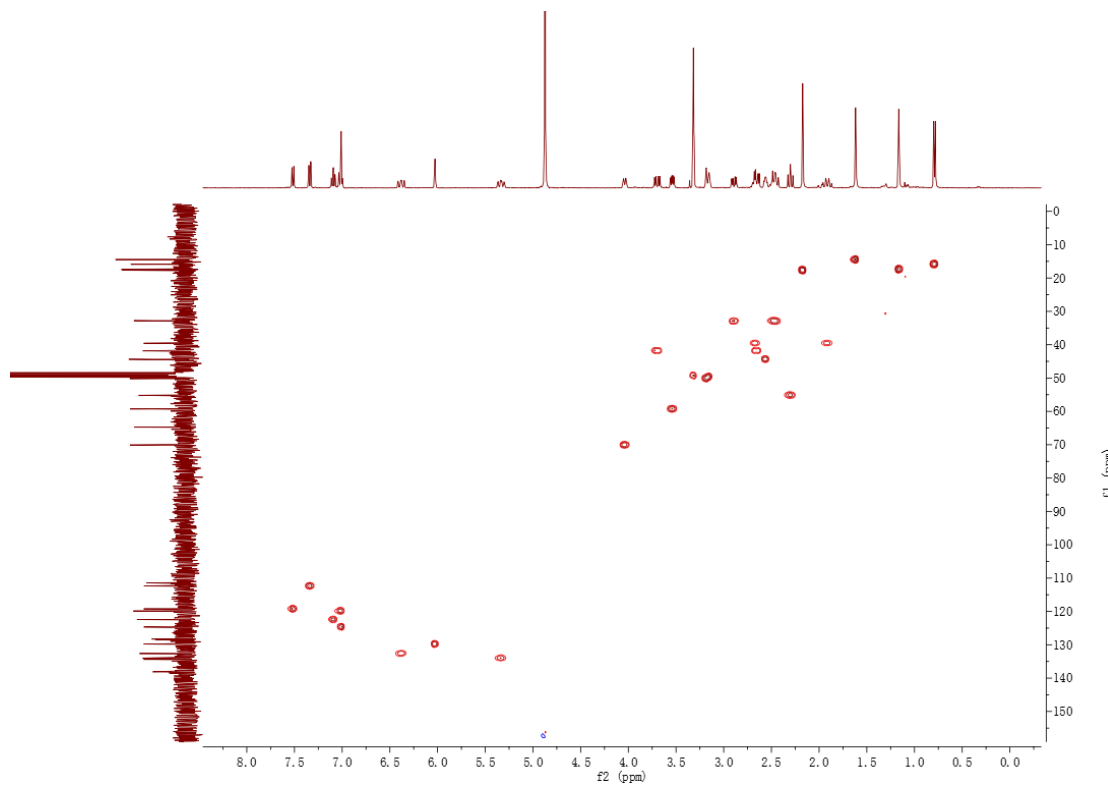
# <sup>1</sup>H NMR spectrum of compound 9



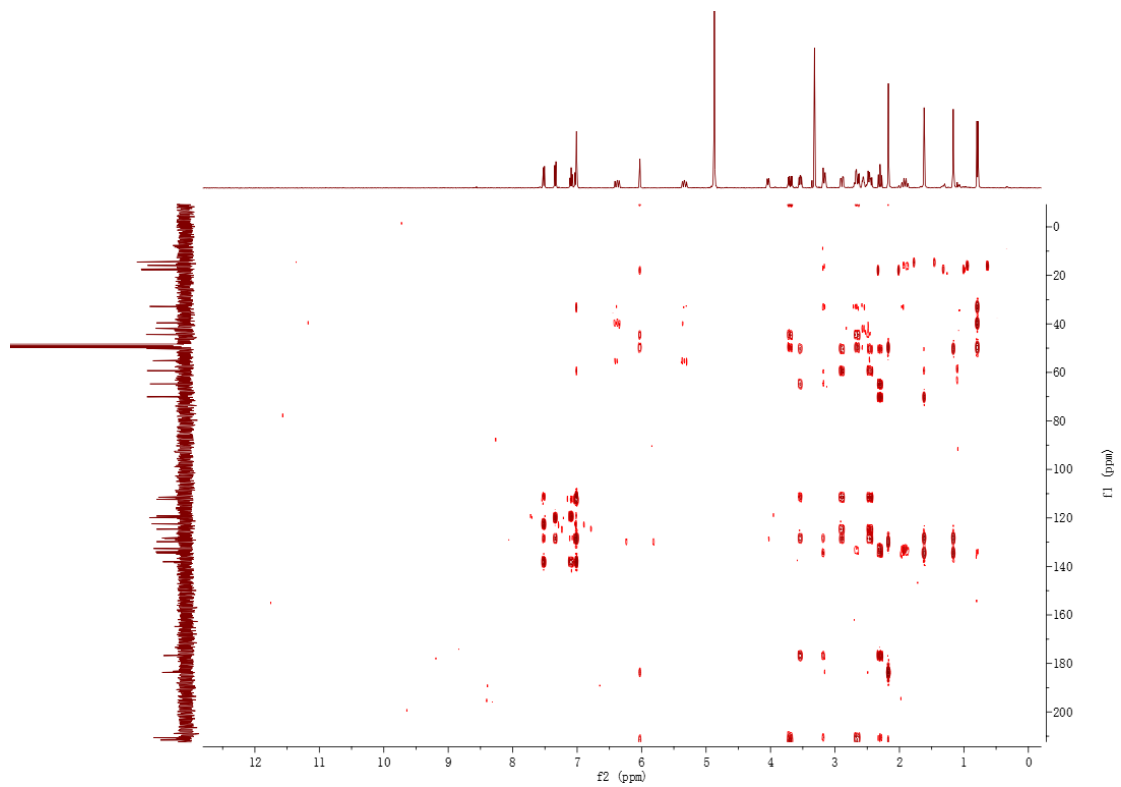
### <sup>13</sup>C NMR and DEPT spectra of compound 9



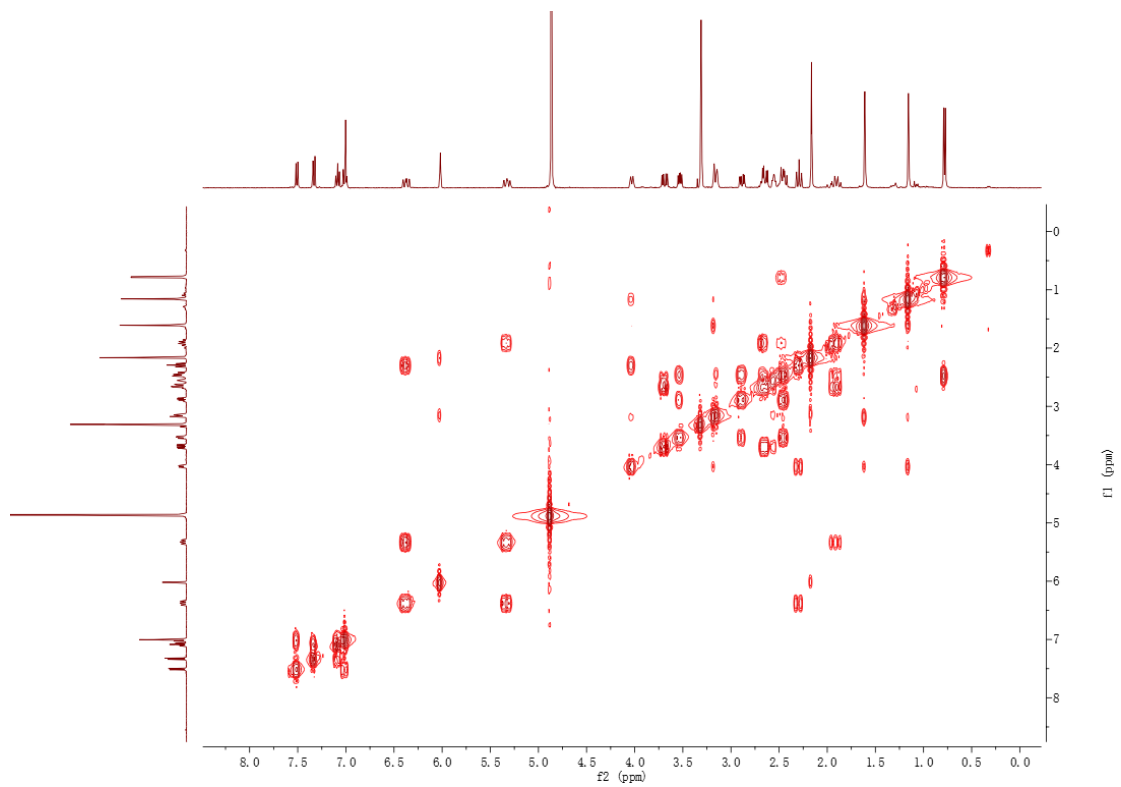
### HSQC spectrum of compound 9



HMBC spectrum of compound **9**



$^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **9**



# NOESY spectrum of compound 9

