

## **Isolation and characterization of related impurities in andrographolide sodium bisulphite injection**

### Index

#### Compound 1:

**S1.** <sup>1</sup>H NMR spectrum of compound 1 (300 MHz, CD<sub>3</sub>OD)

**S2.** <sup>13</sup>C NMR spectrum of compound 1 (75 MHz, CD<sub>3</sub>OD)

**S3.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 1

**S4.** HSQC spectrum of compound 1

**S5.** HMBC spectrum of compound 1

**S6.** ROESY spectrum of compound 1

**S7.** HRESIMS spectrum of compound 1

**S8.** IR spectrum of compound 1

**S9.** UV spectrum of compound 1 (MeOH)

#### Compound 2:

**S10.** <sup>1</sup>H NMR spectrum of compound 2 (300 MHz, DMSO-*d*<sub>6</sub>)

**S11.** <sup>13</sup>C NMR spectrum of compound 2 (75 MHz, DMSO-*d*<sub>6</sub>)

**S12.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 2

**S13.** HSQC spectrum of compound 2

**S14.** HMBC spectrum of compound 2

**S15.** ROESY spectrum of compound 2

**S16.** HRESIMS spectrum of compound 2

**S17.** IR spectrum of compound 2

**S18.** Mo<sub>2</sub>(OAc)<sub>4</sub>-induced circular dichroism (ICD) spectrum of compound 2

#### Compound 3:

**S19.** <sup>1</sup>H NMR spectrum of compound 3 (300 MHz, CD<sub>3</sub>OD)

**S20.** <sup>13</sup>C NMR spectrum of compound 3 (75 MHz, CD<sub>3</sub>OD)

**S21.** <sup>1</sup>H-<sup>1</sup>H COSY spectrum of compound 3

**S22.** HSQC spectrum of compound 3

**S23.** HMBC spectrum of compound 3

**S24.** ROESY spectrum of compound 3

**S25.** HRESIMS spectrum of compound 3

**S26.** IR spectrum of compound 3

**S27.** UV spectrum of compound 3 (MeOH)

**S28.** CD spectrum of compound 3 (MeOH)

#### Compound 4:

**S29.** <sup>1</sup>H NMR spectrum of compound 4 (300 MHz, CD<sub>3</sub>OD)

**S30.** <sup>13</sup>C NMR spectrum of compound 4 (75 MHz, CD<sub>3</sub>OD)

**S31.** HRESIMS spectrum of compound 4

**S32.** IR spectrum of compound 4

**S33.** UV spectrum of compound 4 (MeOH)

#### Compound 5:

**S34.**  $^1\text{H}$  NMR spectrum of compound **5** (300 MHz,  $\text{CD}_3\text{OD}$ )

**S35.**  $^{13}\text{C}$  NMR spectrum of compound **5** (75 MHz,  $\text{CD}_3\text{OD}$ )

**S36.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **5**

**S37.** HSQC spectrum of compound **5**

**S38.** HMBC spectrum of compound **5**

**S39.** ROESY spectrum of compound **5**

**S40.** HRESIMS spectrum of compound **5**

**S41.** IR spectrum of compound **5**

**S42.** UV spectrum of compound **5** (MeOH)

**S43.** CD spectrum of compound **5** (MeOH)

Compound **6**:

**S44.**  $^1\text{H}$  NMR spectrum of compound **6** (300 MHz,  $\text{CD}_3\text{OD}$ )

**S45.**  $^{13}\text{C}$  NMR spectrum of compound **6** (75 MHz,  $\text{CD}_3\text{OD}$ )

**S46.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **6**

**S47.** HSQC spectrum of compound **6**

**S48.** HMBC spectrum of compound **6**

**S49.** ROESY spectrum of compound **6**

**S50.** HRESIMS spectrum of compound **6**

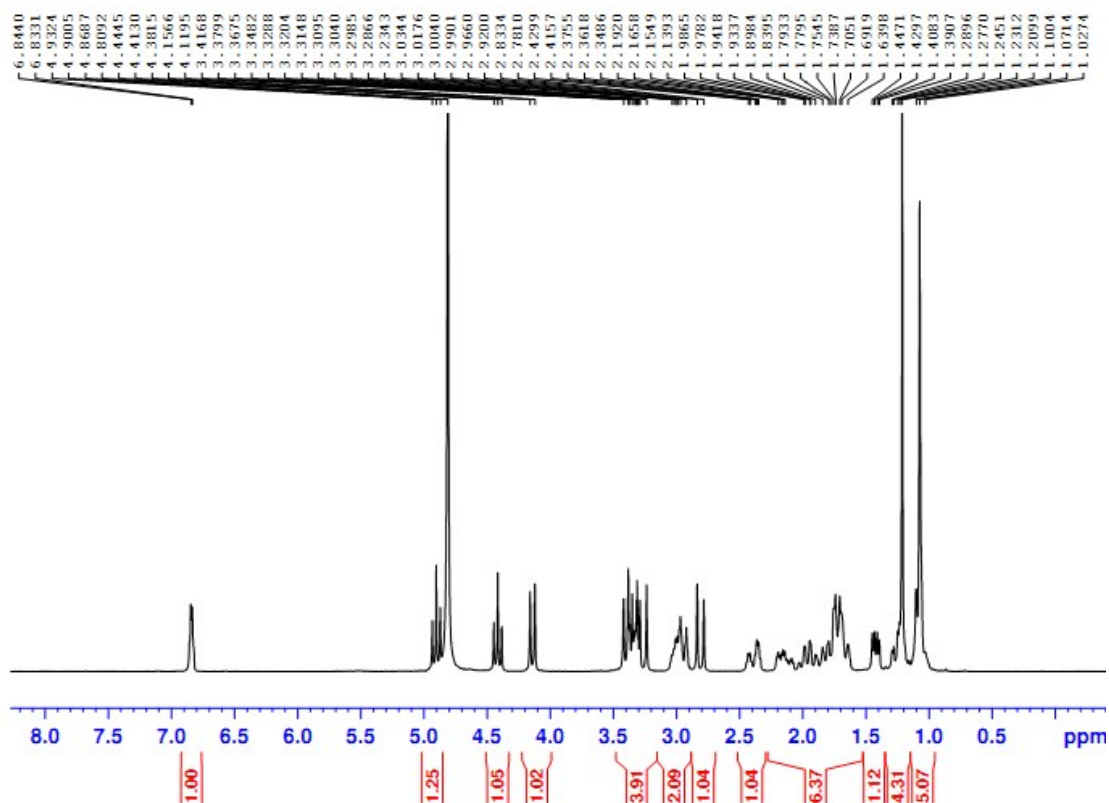
**S51.** IR spectrum of compound **6**

**S52.** UV spectrum of compound **6** (MeOH)

**S53.** CD spectrum of compound **6** (MeOH)

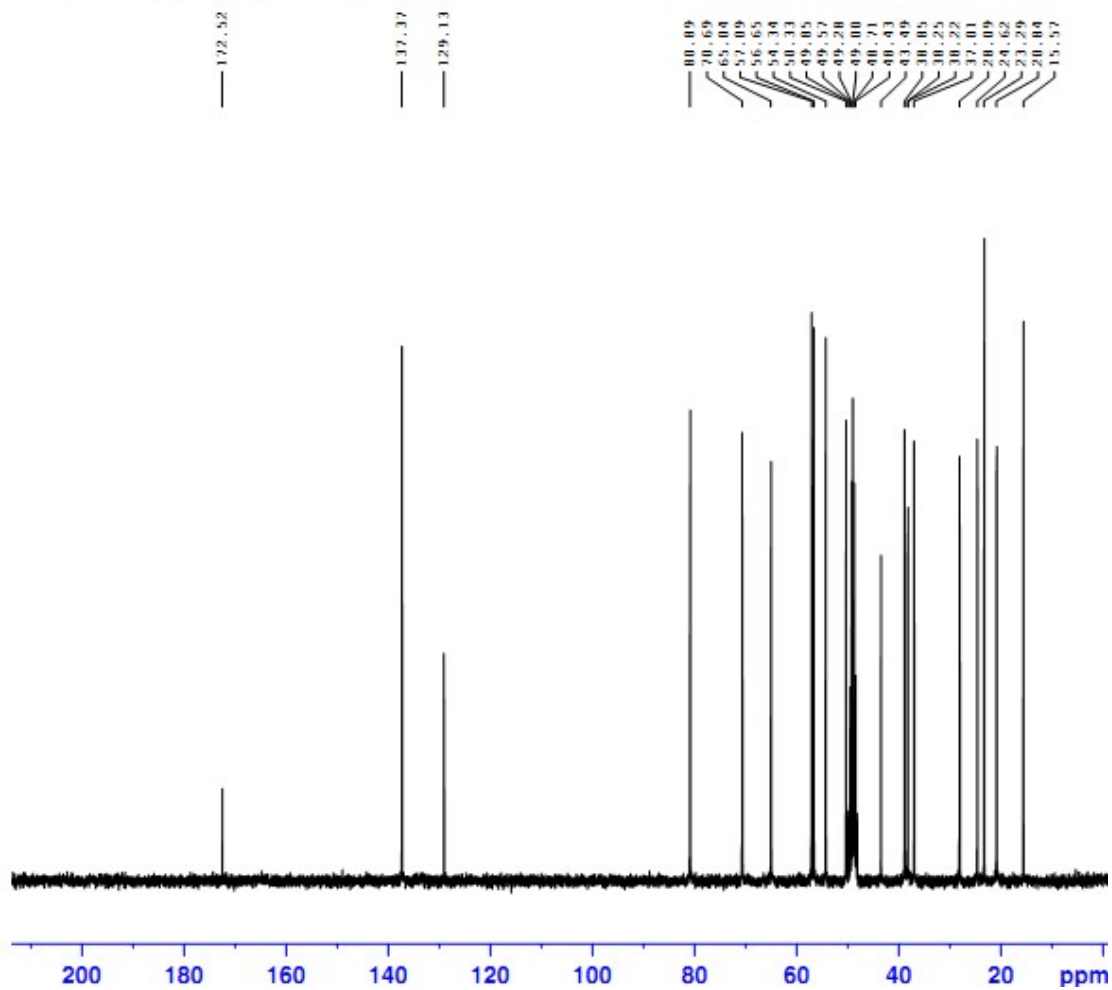
S1. <sup>1</sup>H NMR spectrum of compound 1 (300 MHz, CD<sub>3</sub>OD)

AP-B H1-NMR CD3OD 300K AV-300

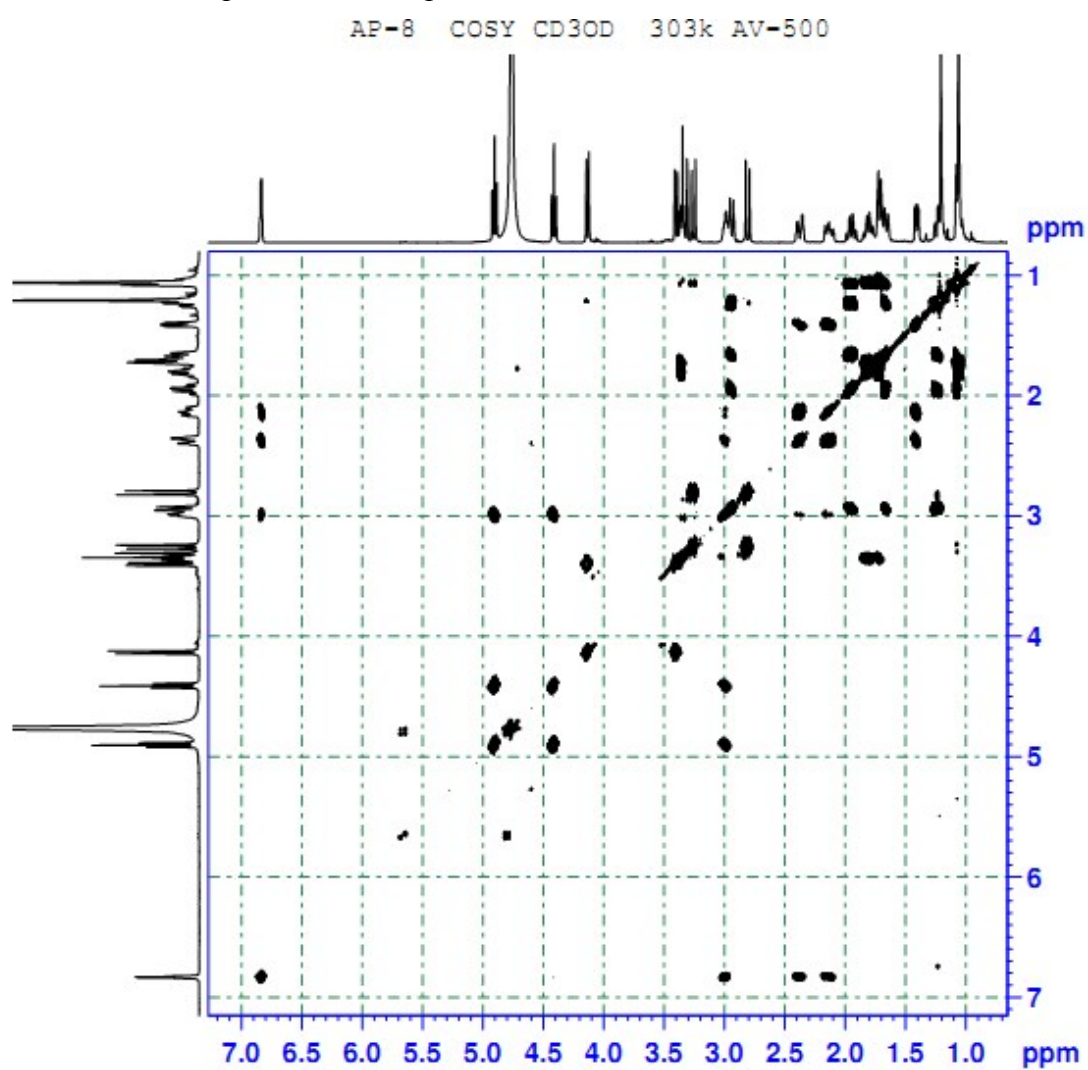


S2. <sup>13</sup>C NMR spectrum of compound 1 (75 MHz, CD<sub>3</sub>OD)

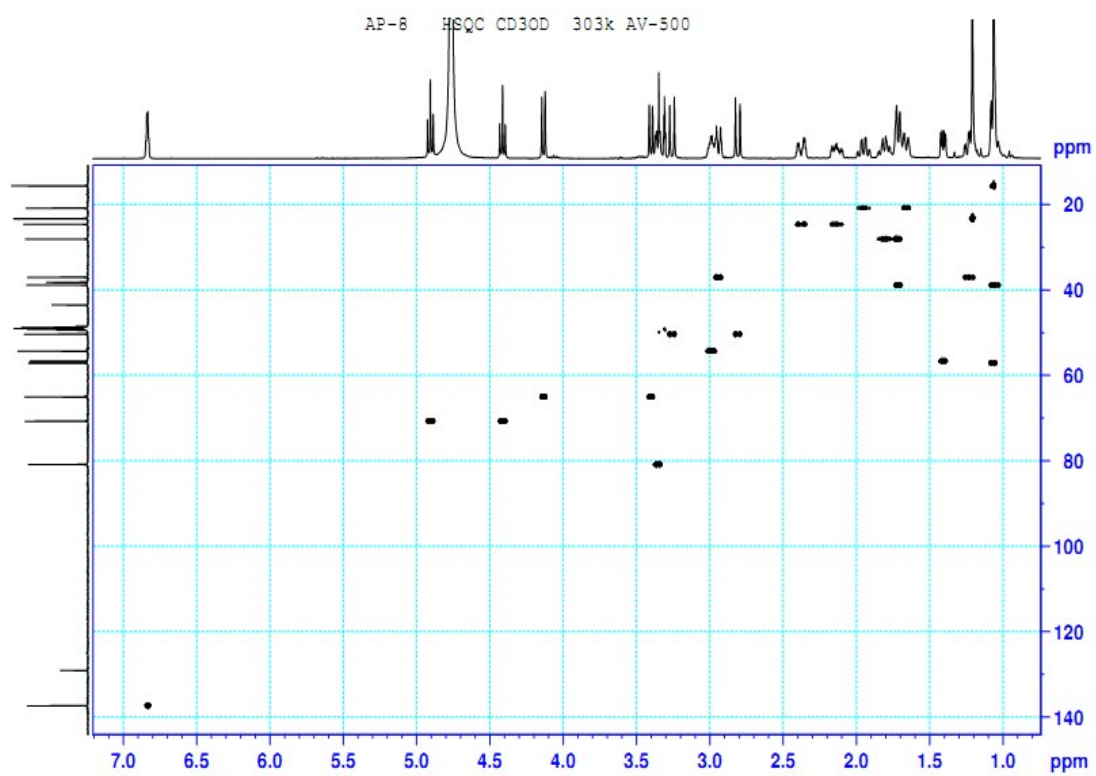
AP-8 <sup>13</sup>C-NMR CD3OD 300K AV-300



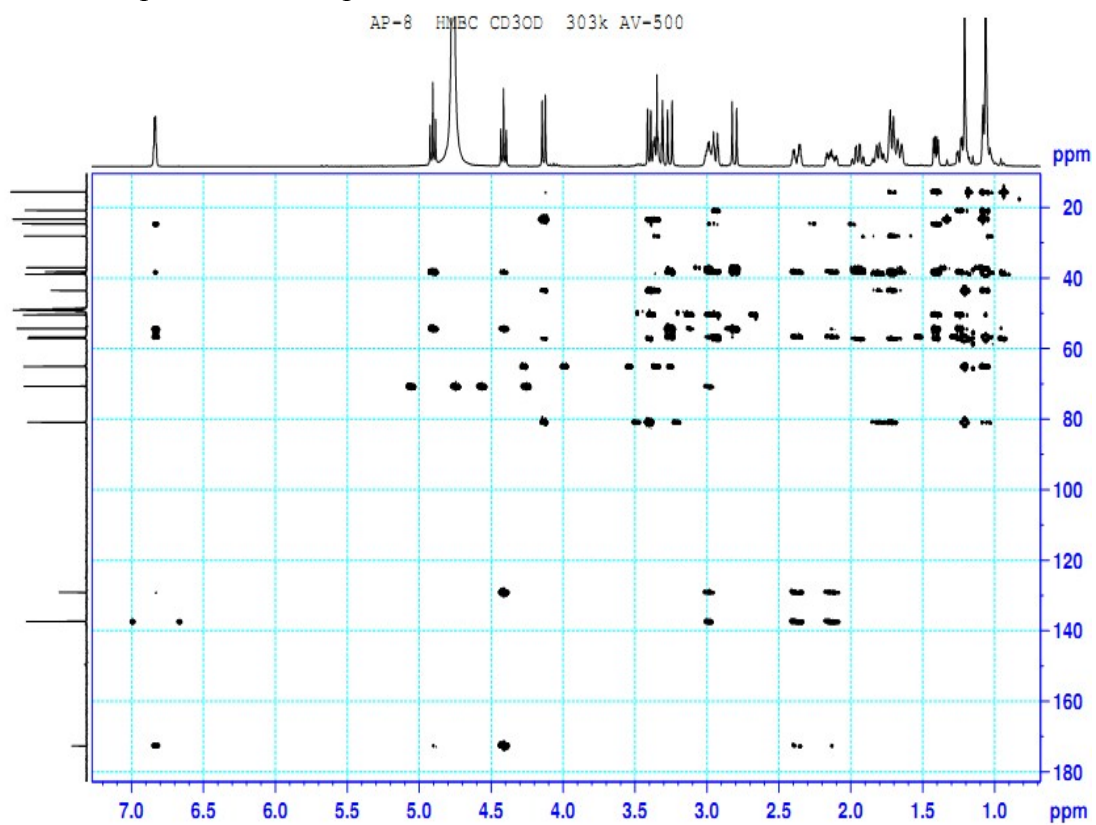
S3.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 1



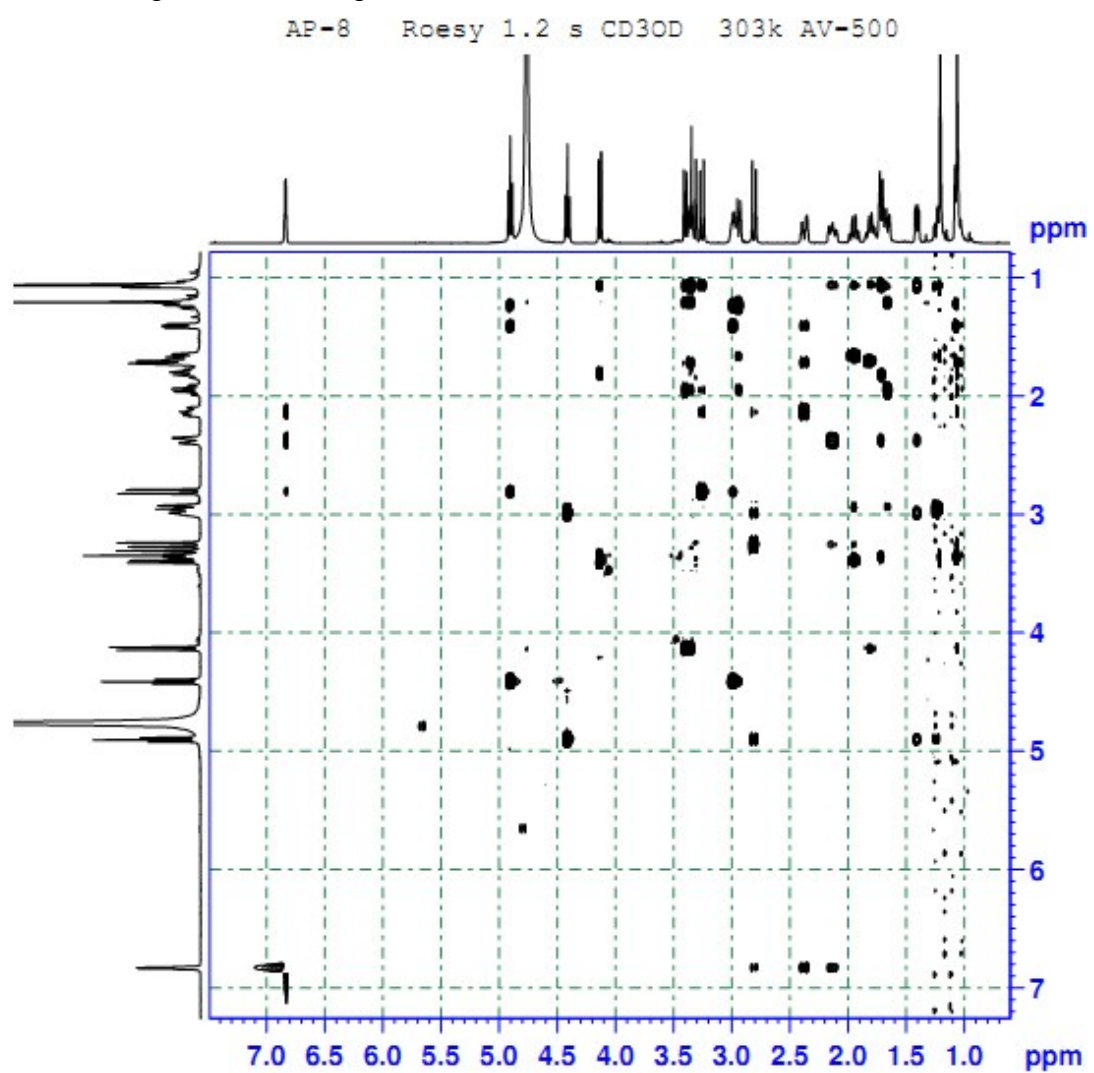
#### S4. HSQC spectrum of compound 1



# S5.HMBC spectrum of compound 1

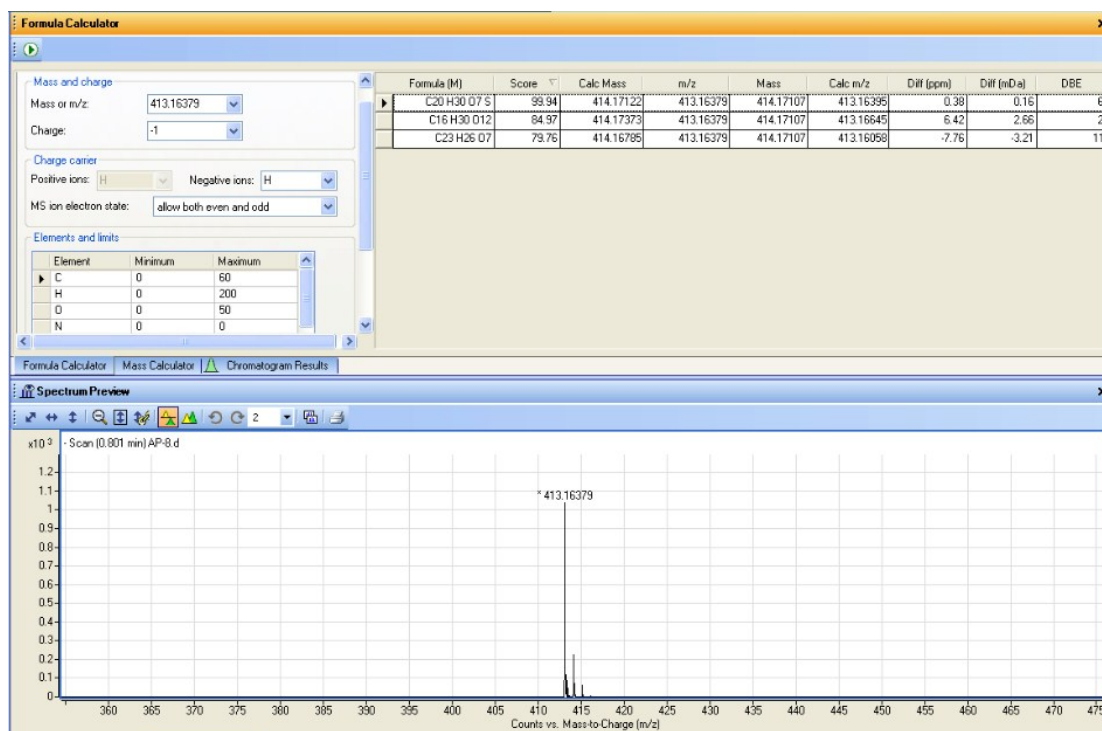


S6. ROESY spectrum of compound 1

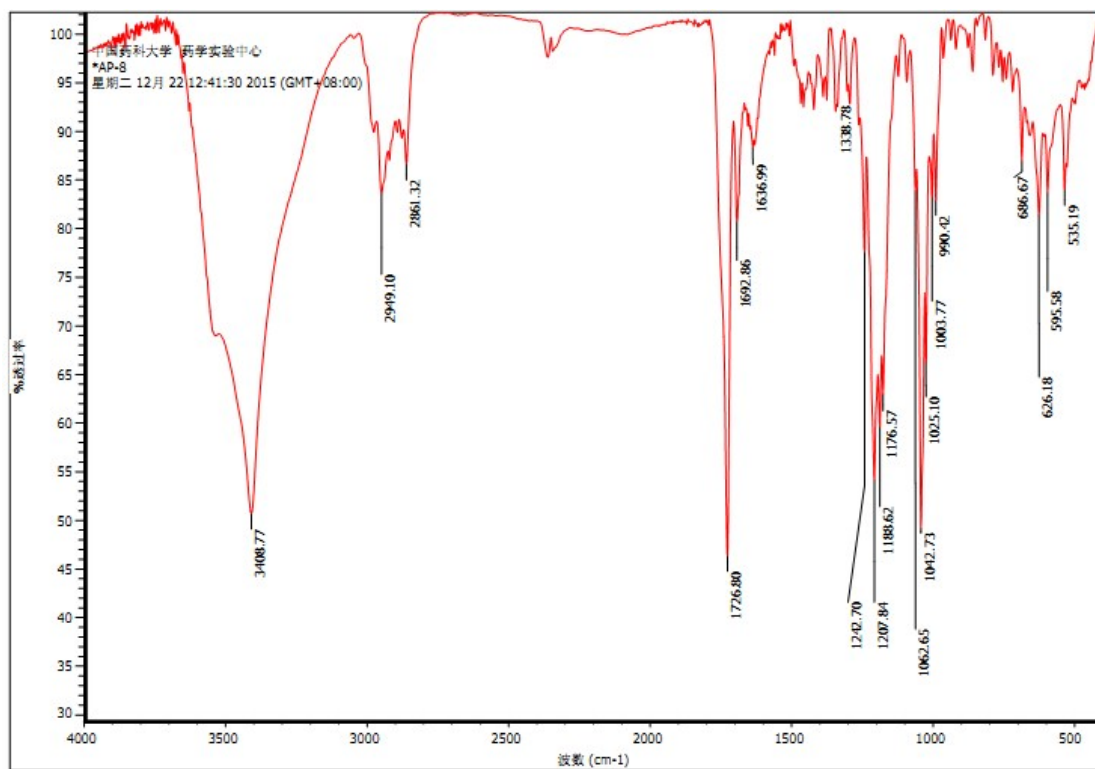




## S7. HRESIMS spectrum of compound 1

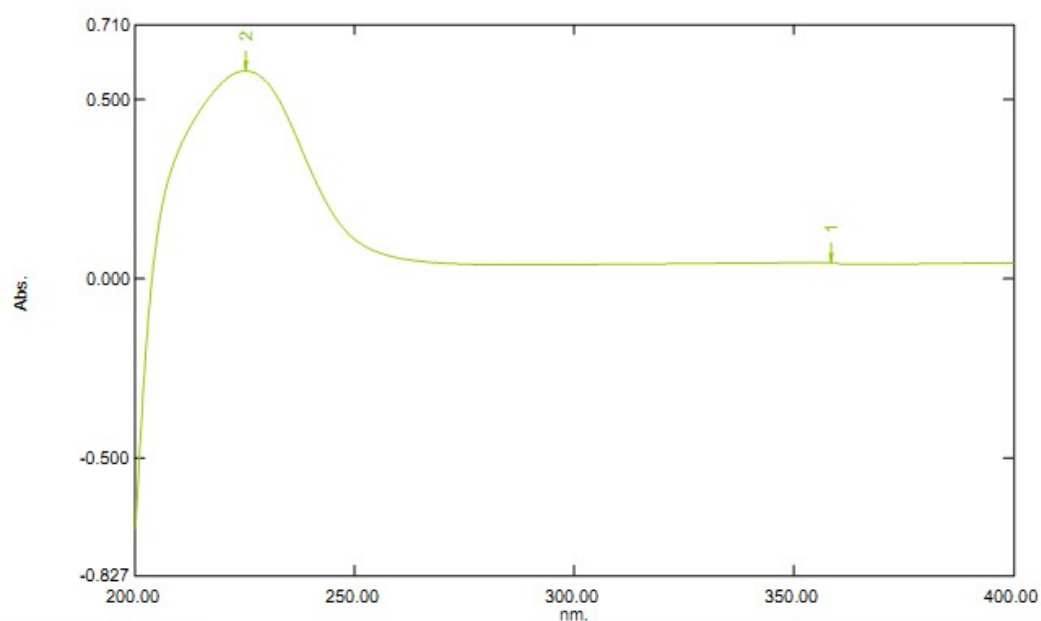


## S8. IR spectrum of compound 1



## S9. UV spectrum of compound 1 (MeOH)

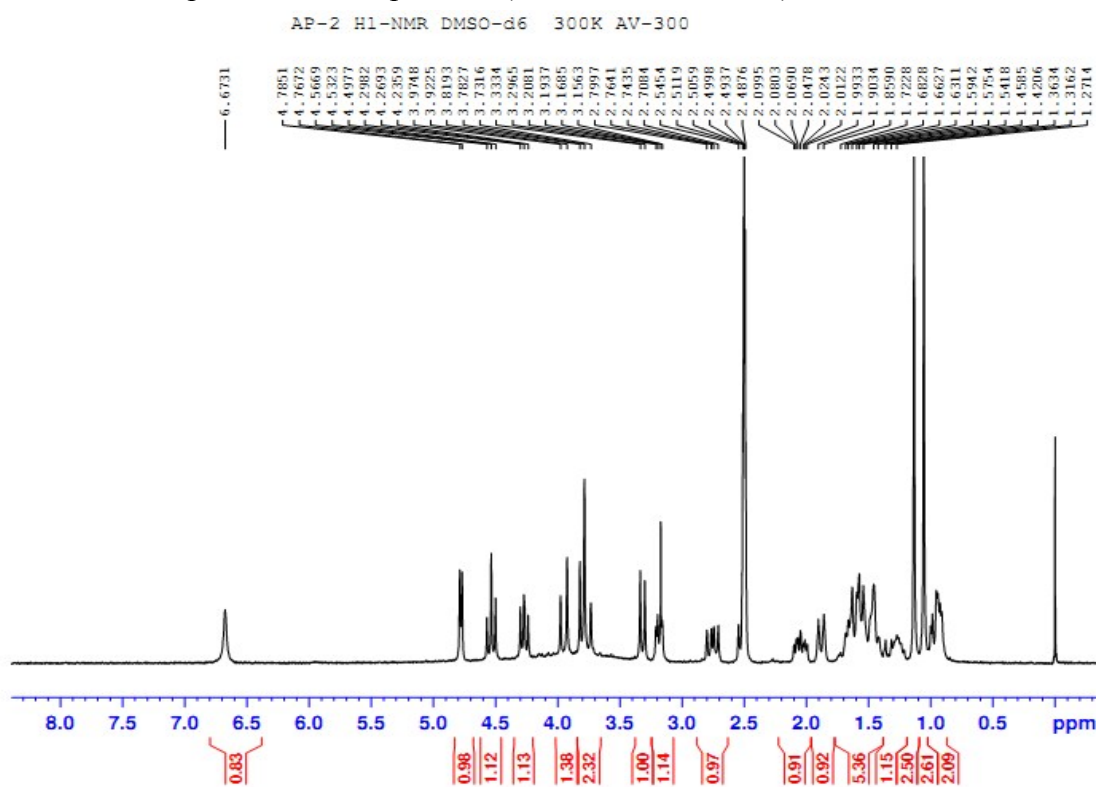
Data Set: ap-8 - RawData



Measurement Properties  
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Scan Speed: Fast  
Sampling Interval: 0.2

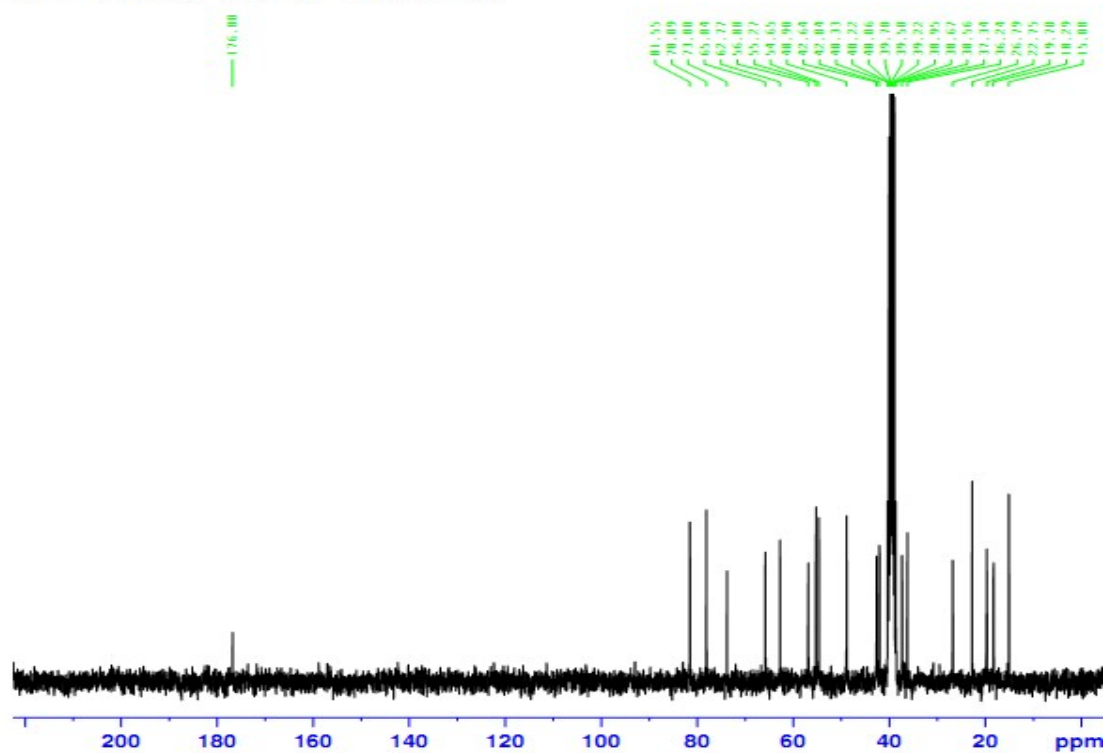
No.	P/V	Wavelength	Abs.	Description
1	Ⓢ	358.60	0.046	
2	Ⓢ	225.20	0.582	

S10. <sup>1</sup>H NMR spectrum of compound 2 (300 MHz, DMSO-d<sub>6</sub>)



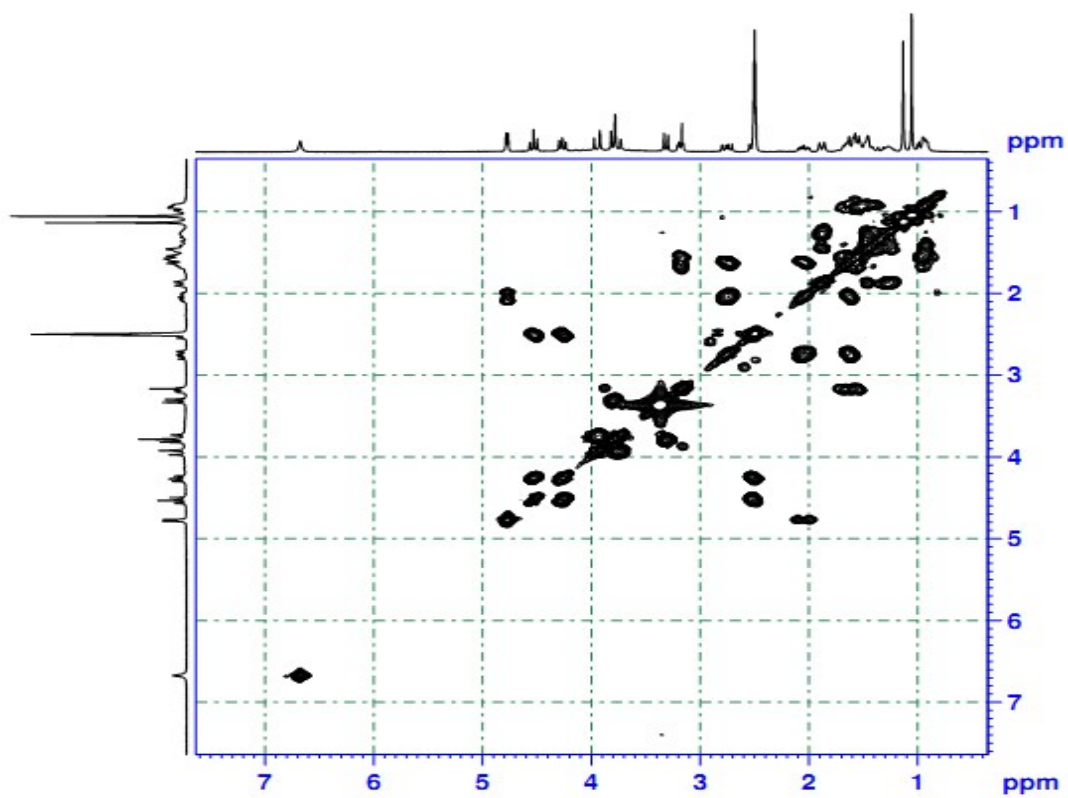
S11. <sup>13</sup>C NMR spectrum of compound 2 (75 MHz, DMSO-d<sub>6</sub>)

AP-2 13C-NMR DMSO-d6 300K AV-300

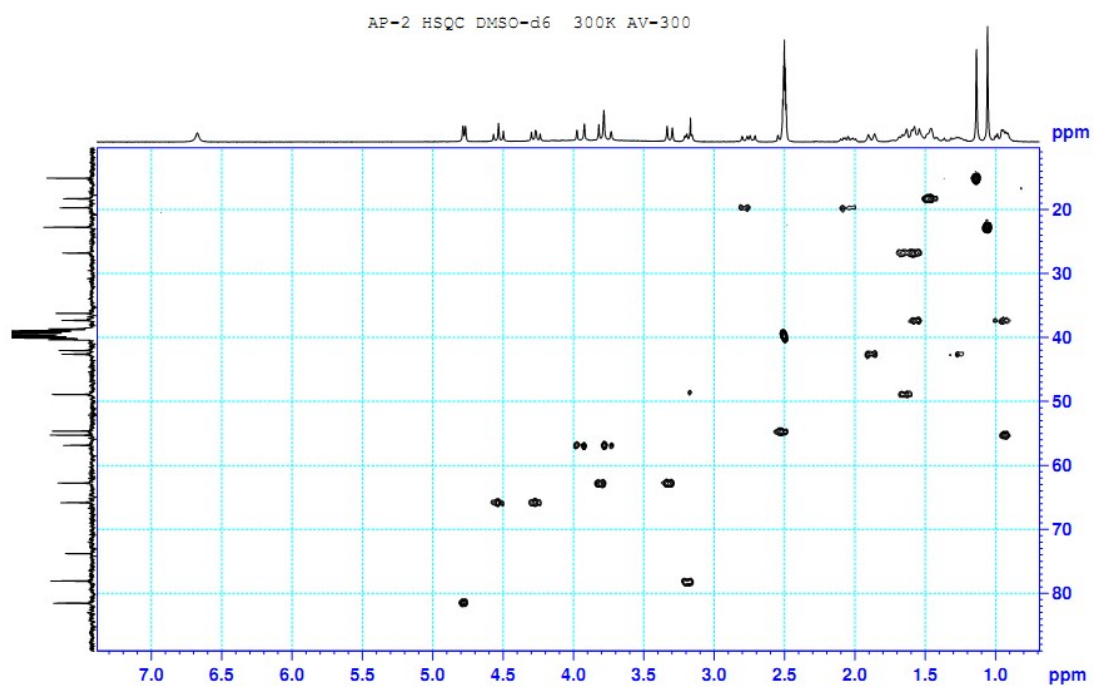


S12.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 2

AP-2 COSY DMSO-d6 300K AV-300

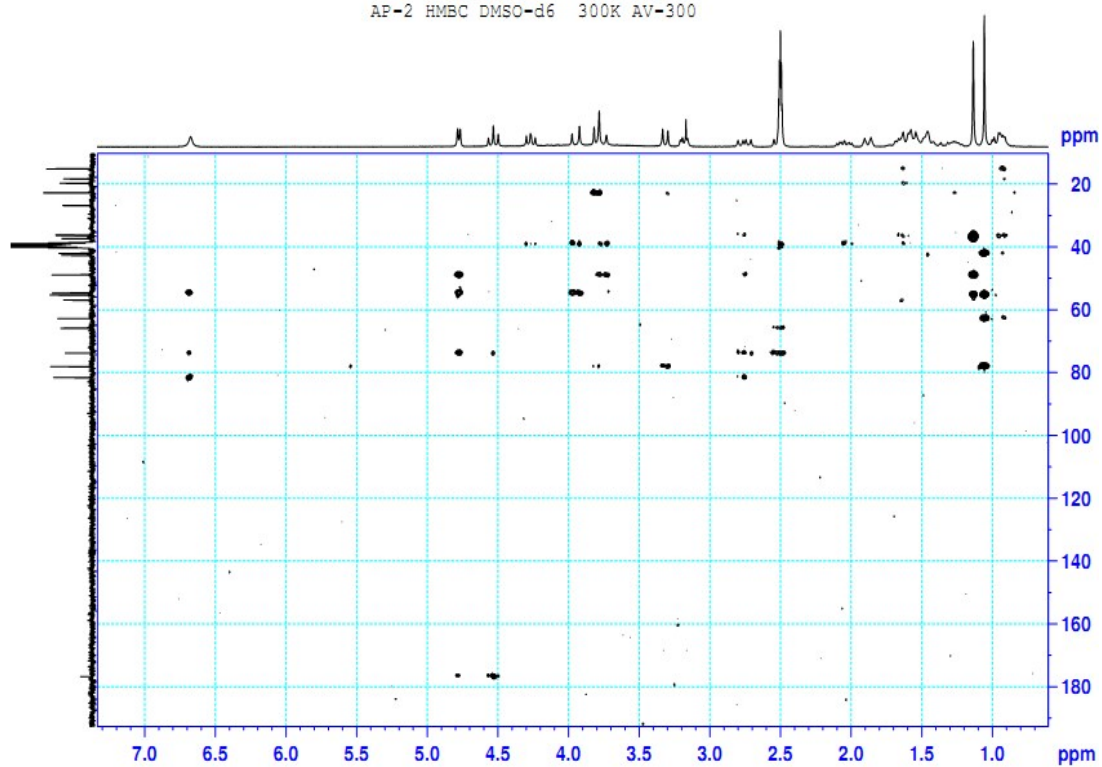


### S13. HSQC spectrum of compound 2



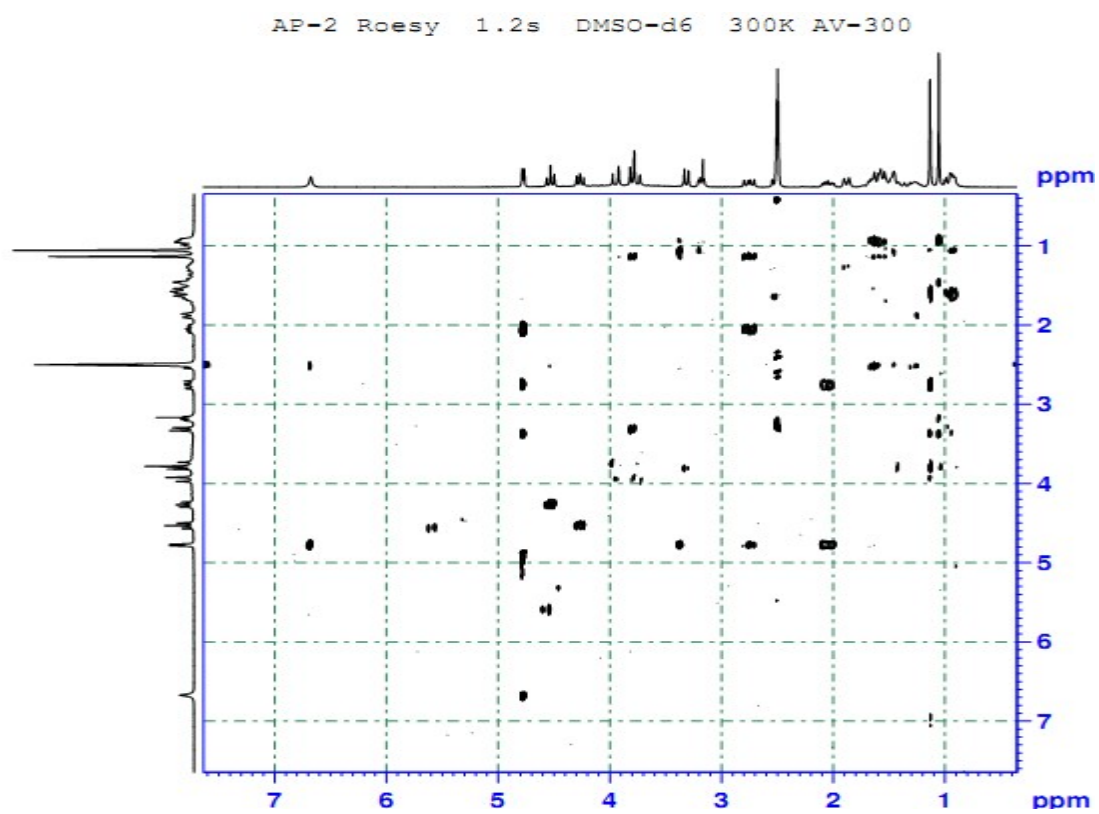
# S14.HMBC spectrum of compound 2

AP-2 HMBC DMSO-d6 300K AV-300

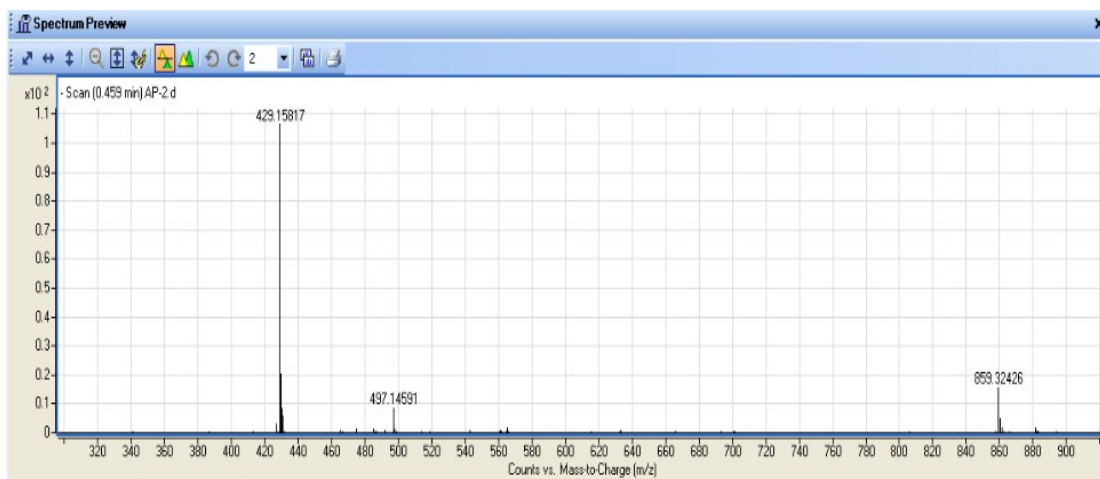




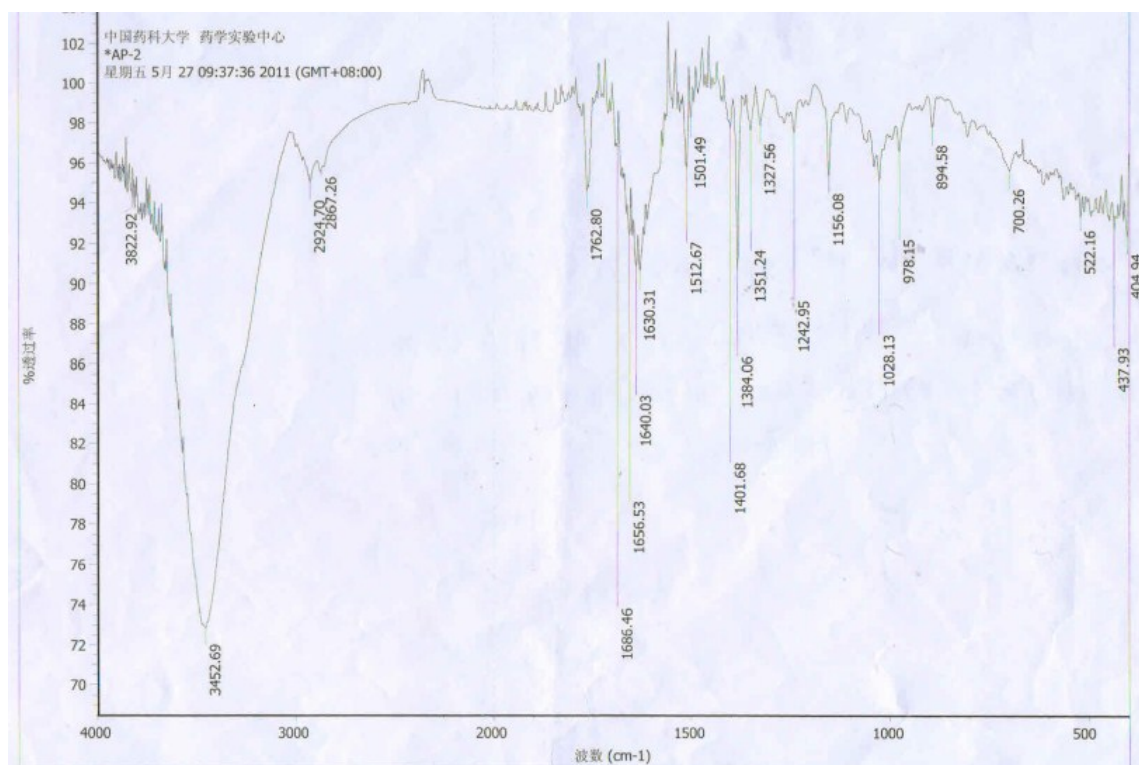
S15. ROESY spectrum of compound 2



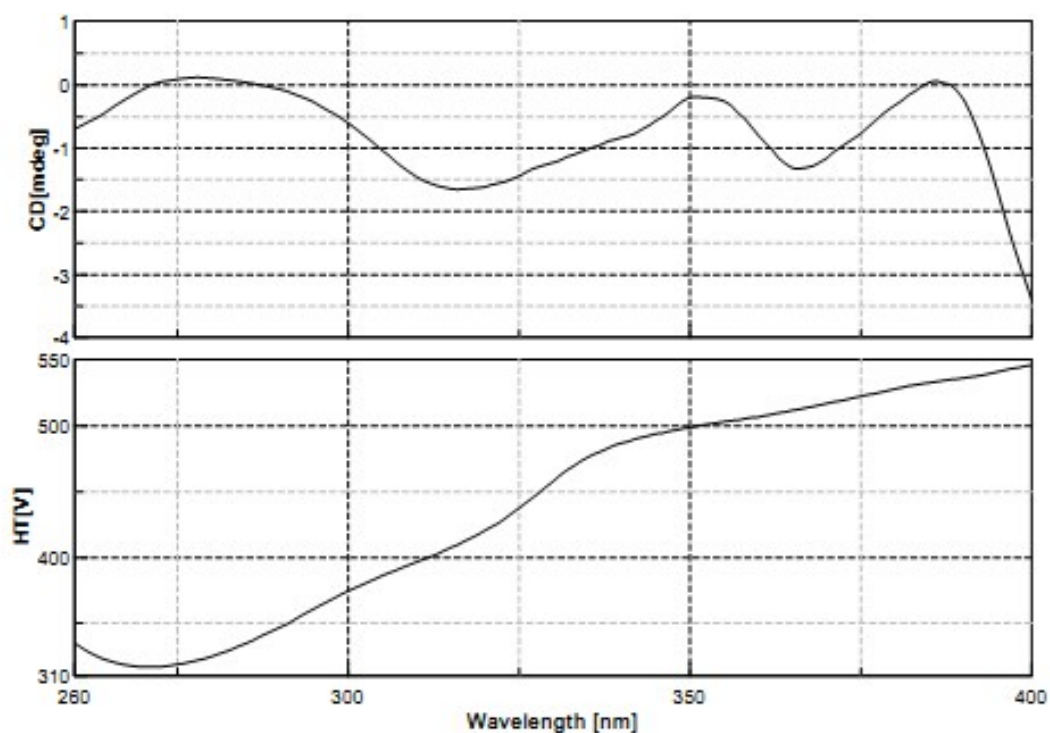
## S16. HRESIMS spectrum of compound 2



## S17. IR spectrum of compound 2

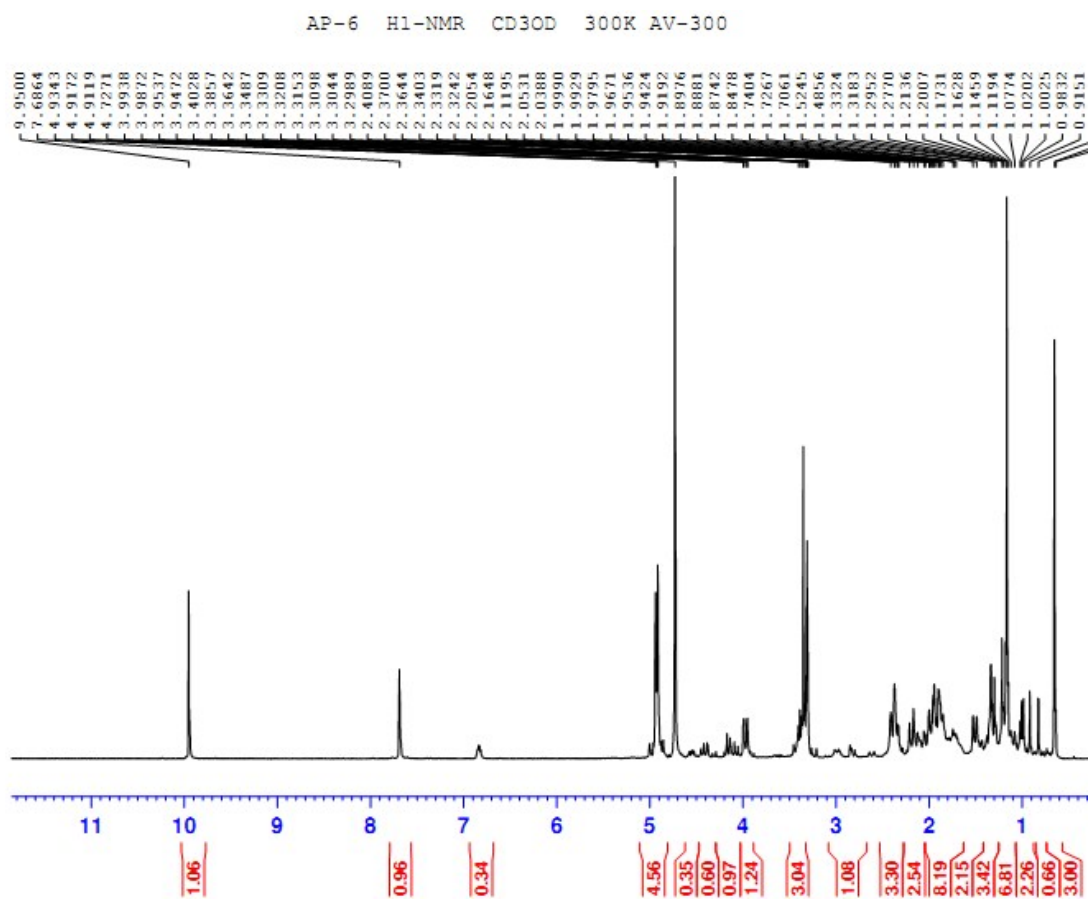


S18. Mo<sub>2</sub>(OAc)<sub>4</sub>-induced circular dichroism (ICD) spectrum of compound 2

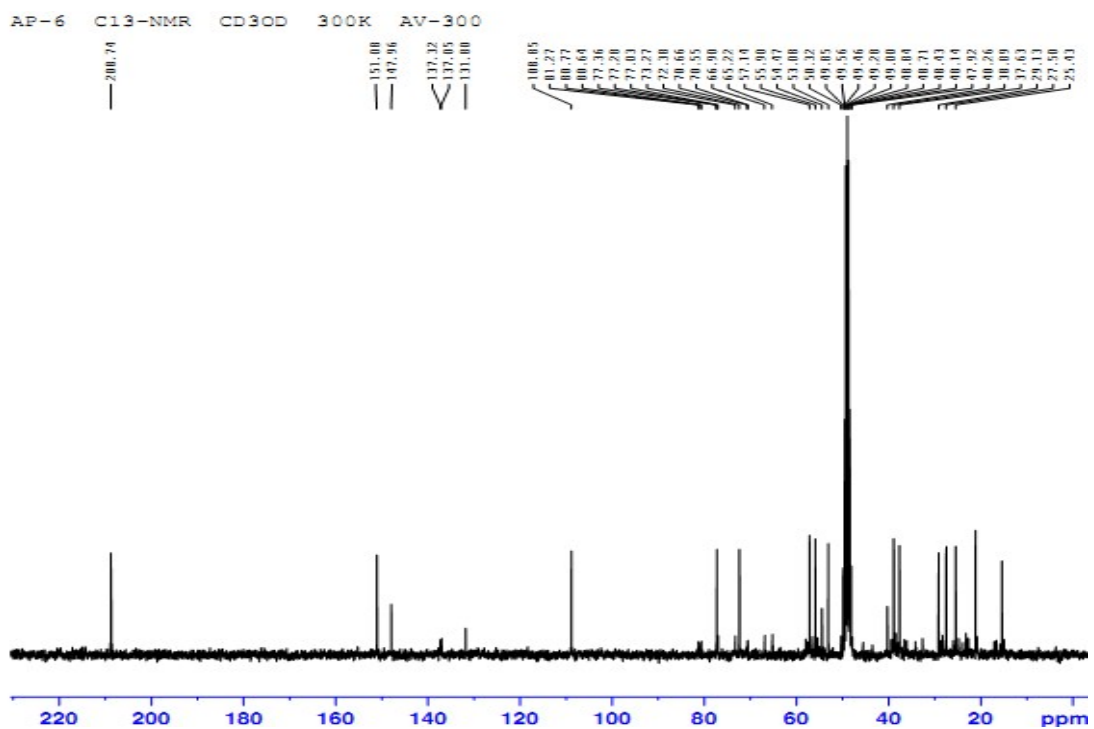


Date	2015/3/11 14:47
File name	AP-2+Mo.jws
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Response	1 sec
Sensitivity	Standard
Measurement range	400 - 260 nm
Data pitch	1nm
Scanning speed	50 nm/min
Accumulation	1
Cell Length	0.1 cm
Solvent	DMSO
Temperature	Room Temperature
Sample name	AP-2+Mo
Operator	DEMO

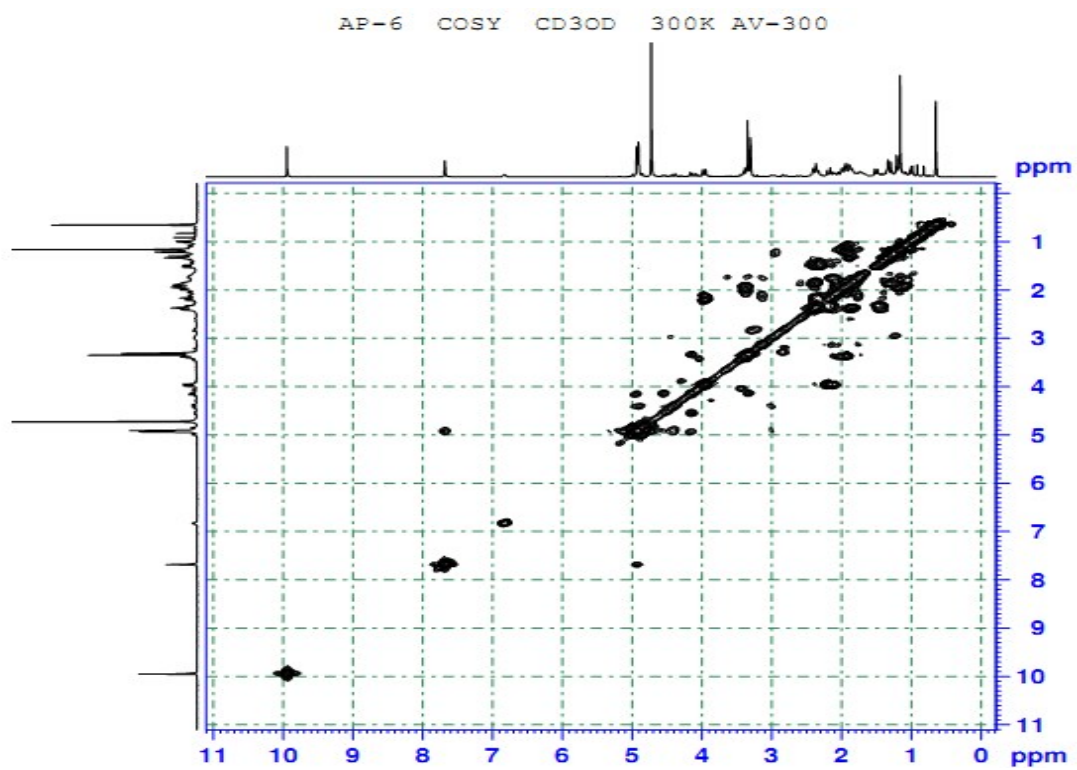
S19. <sup>1</sup>H NMR spectrum of compound 3 (300 MHz, CD<sub>3</sub>OD)



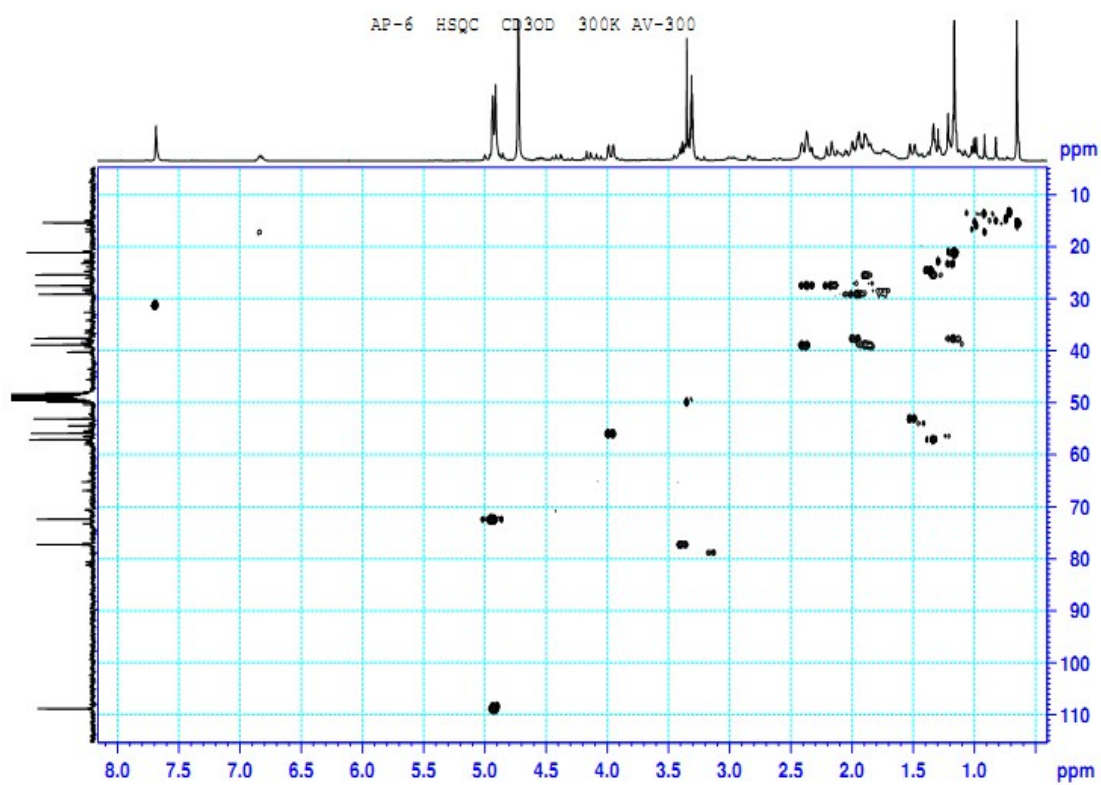
S20.  $^{13}\text{C}$  NMR spectrum of compound **3** (75 MHz,  $\text{CD}_3\text{OD}$ )



S21.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 3

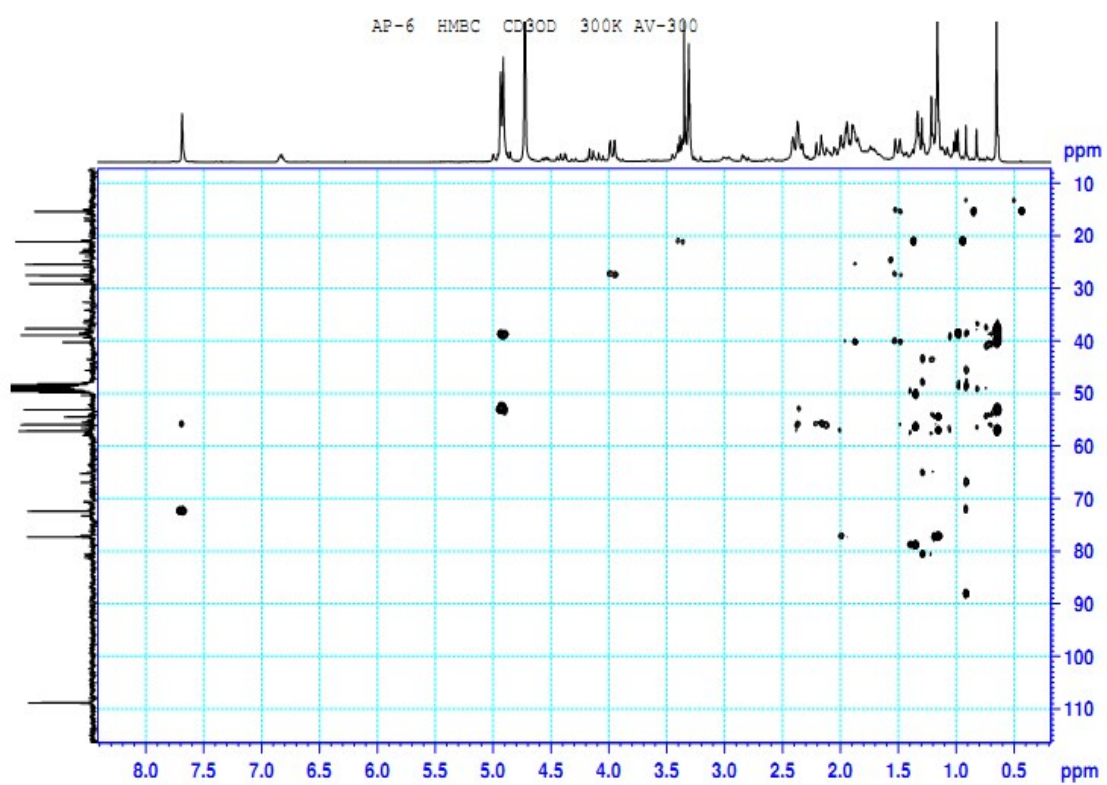


S22. HSQC spectrum of compound 3

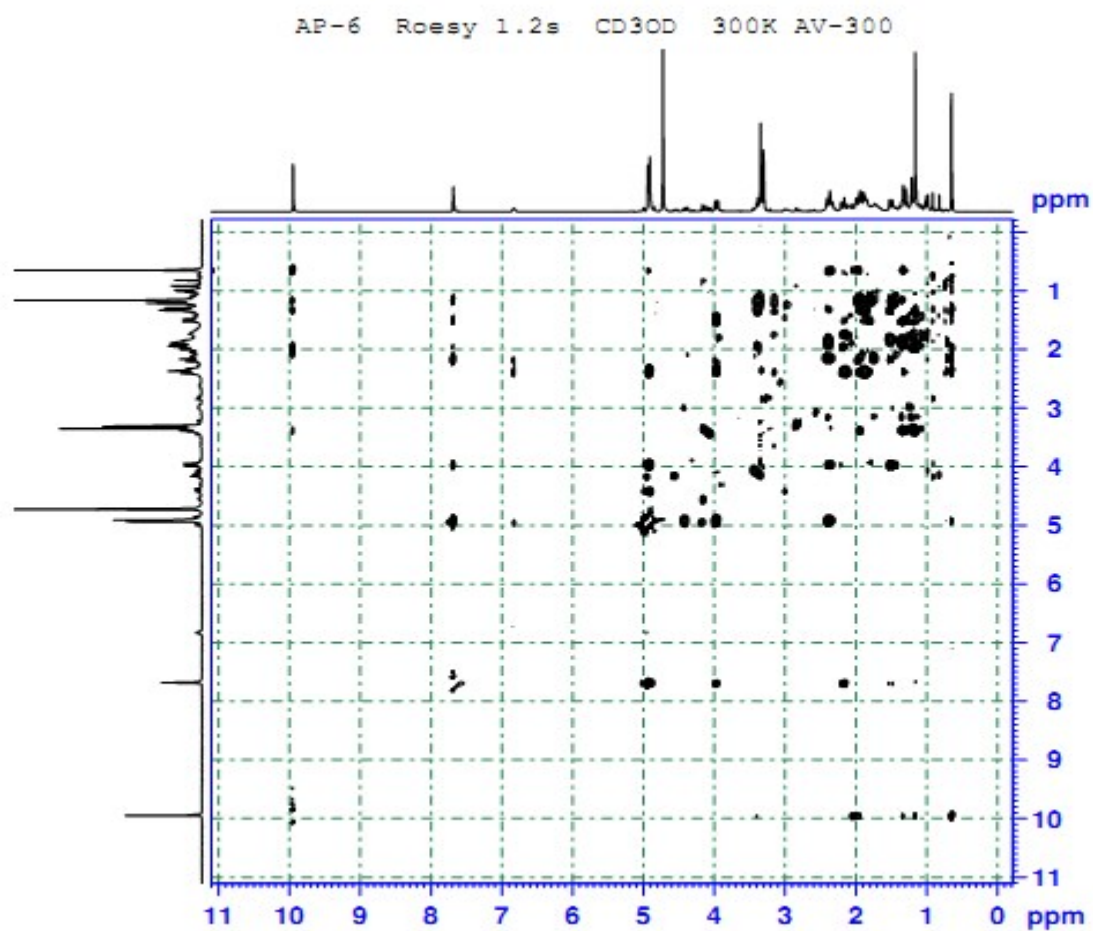




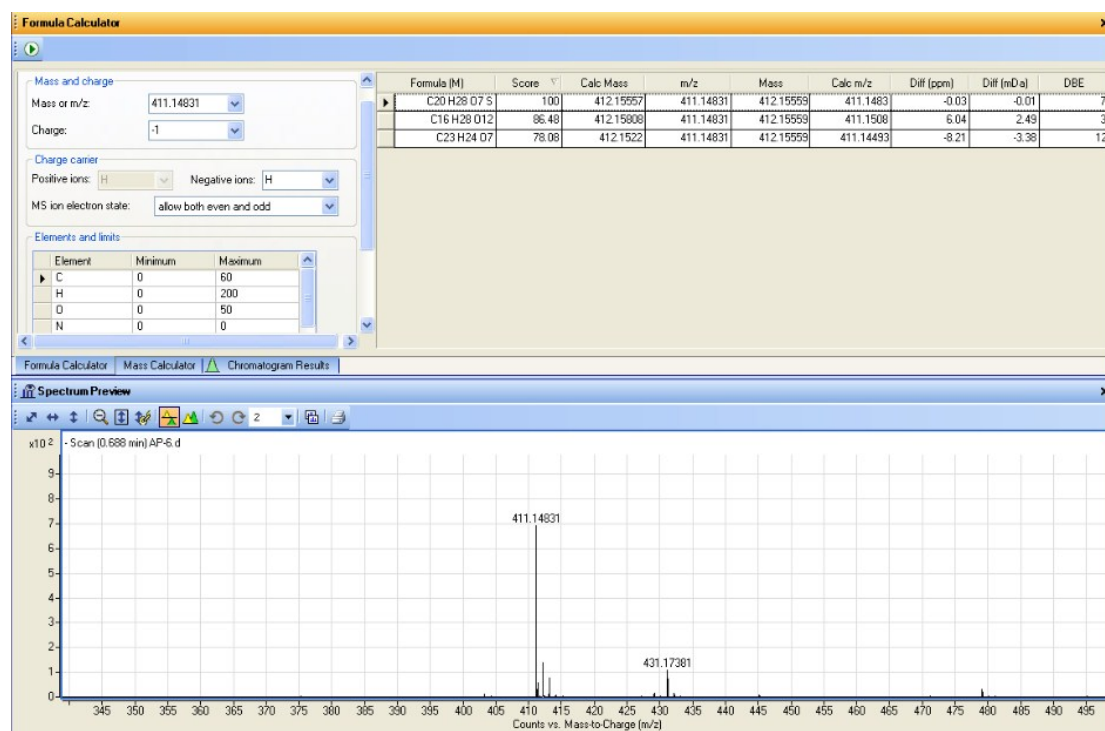
S23.HMBC spectrum of compound 3



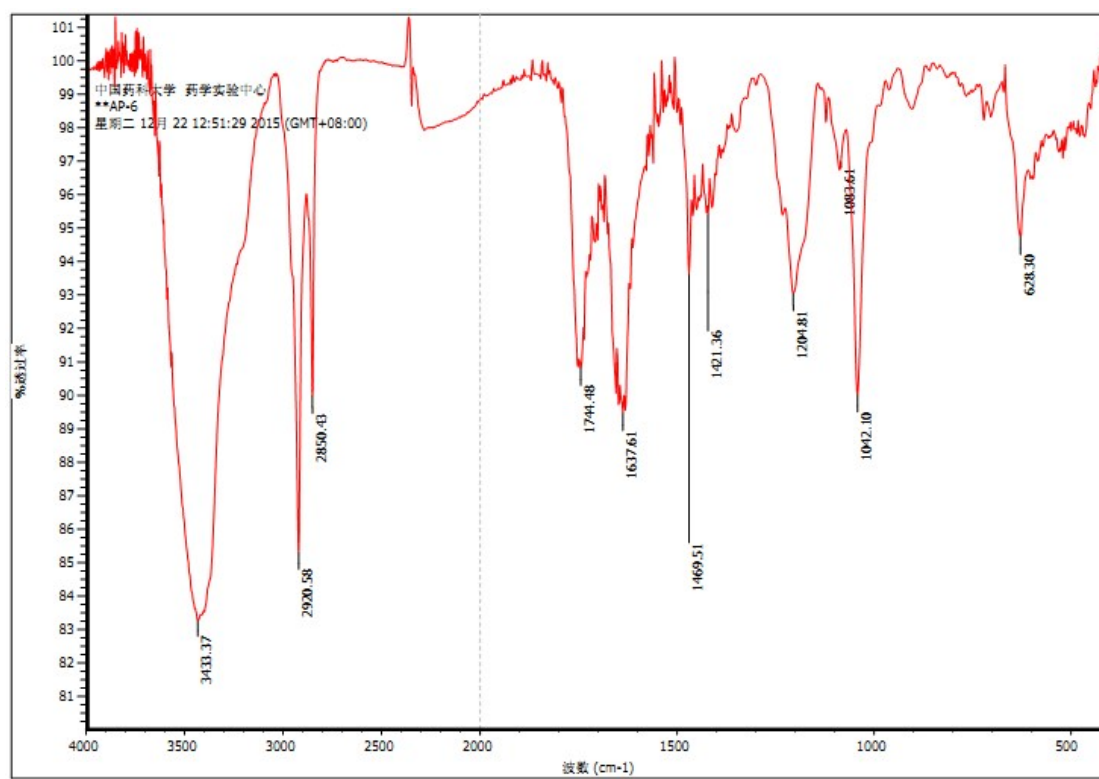
S24. ROESY spectrum of compound 3



## S25. HRESIMS spectrum of compound 3

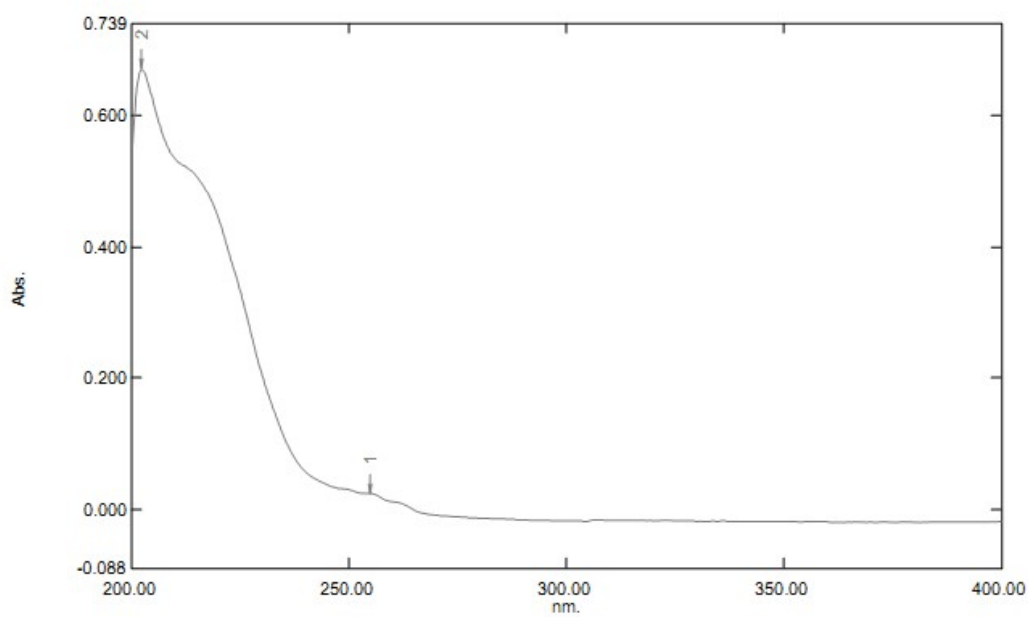


### S26. IR spectrum of compound 3



## S27. UV spectrum of compound 3 (MeOH)

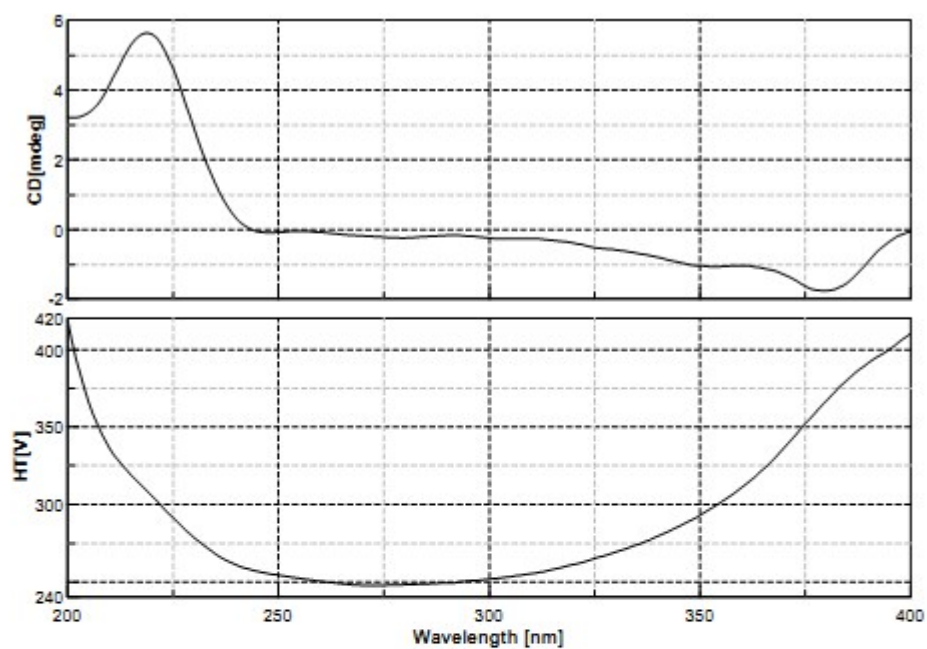
Data Set: ap-6 - RawData



Measurement Properties  
Wavelength Range (nm.): 200.00 to 400.00  
Scan Speed: Fast  
Sampling Interval: 0.2  
Auto Sampling Interval: Disabled  
Scan Mode: Auto

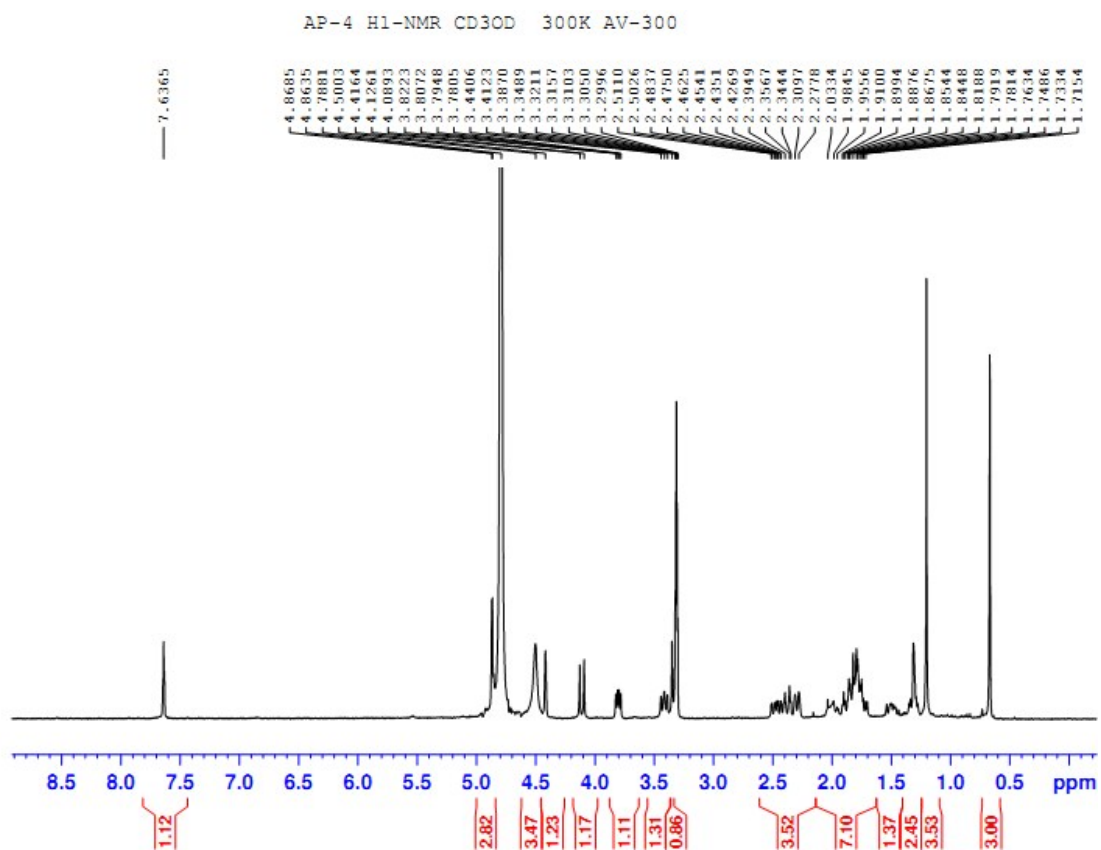
No.	P/V	Wavelength	Abs.	Description
1	⊕	254.80	0.025	
2	⊕	202.40	0.670	
3	⊖	304.40	-0.017	
4	⊖	253.60	0.025	

### S28. CD spectrum of compound 3 (MeOH)



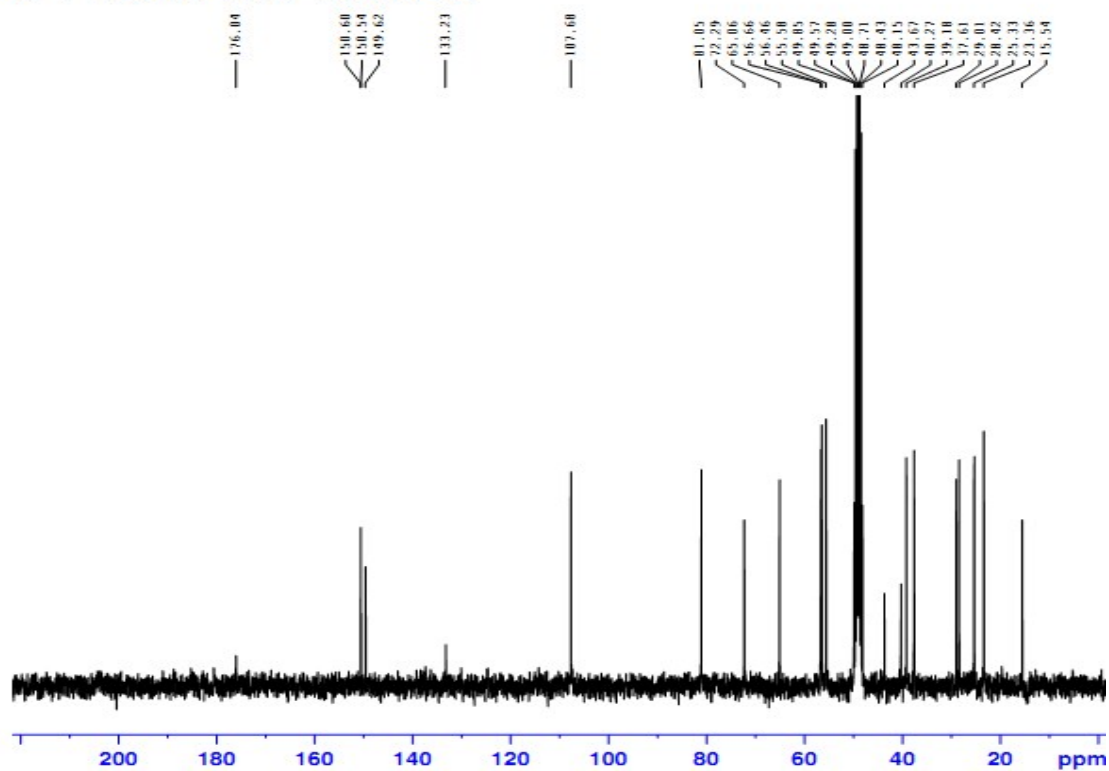
Date	2013/11/19 10:03
File name	AP-6.jws
Model	J-810
Serial No.	B050560750
Band width	1 nm
Response	1 sec
Sensitivity	Standard
Measurement range	400 - 200 nm
Data pitch	1nm
Scanning speed	100 nm/min
Accumulation	1
Cell Length	0.1 cm
Solvent	MeOH
Temperature	Room Temperature
Sample name	AP-6
Operator	DEMO

S29. <sup>1</sup>H NMR spectrum of compound 4 (300 MHz, CD<sub>3</sub>OD)



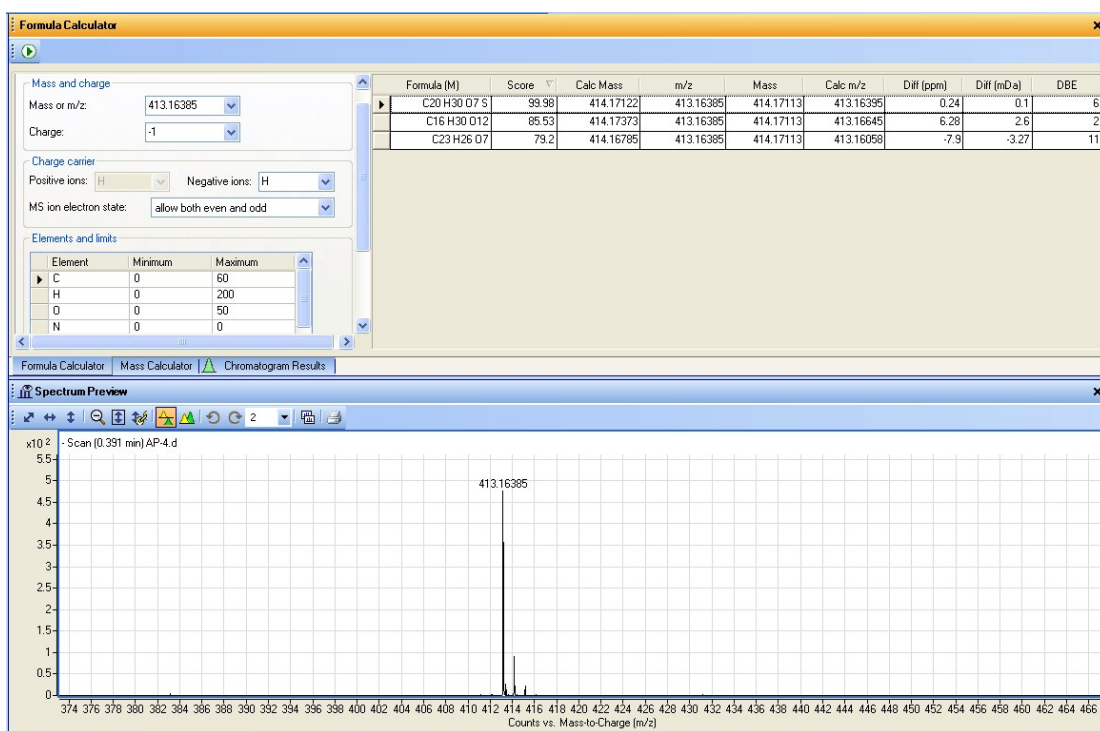
S30. <sup>13</sup>C NMR spectrum of compound 4 (75 MHz, CD<sub>3</sub>OD)

AP-4 <sup>13</sup>C-NMR CD3OD 300K AV-300

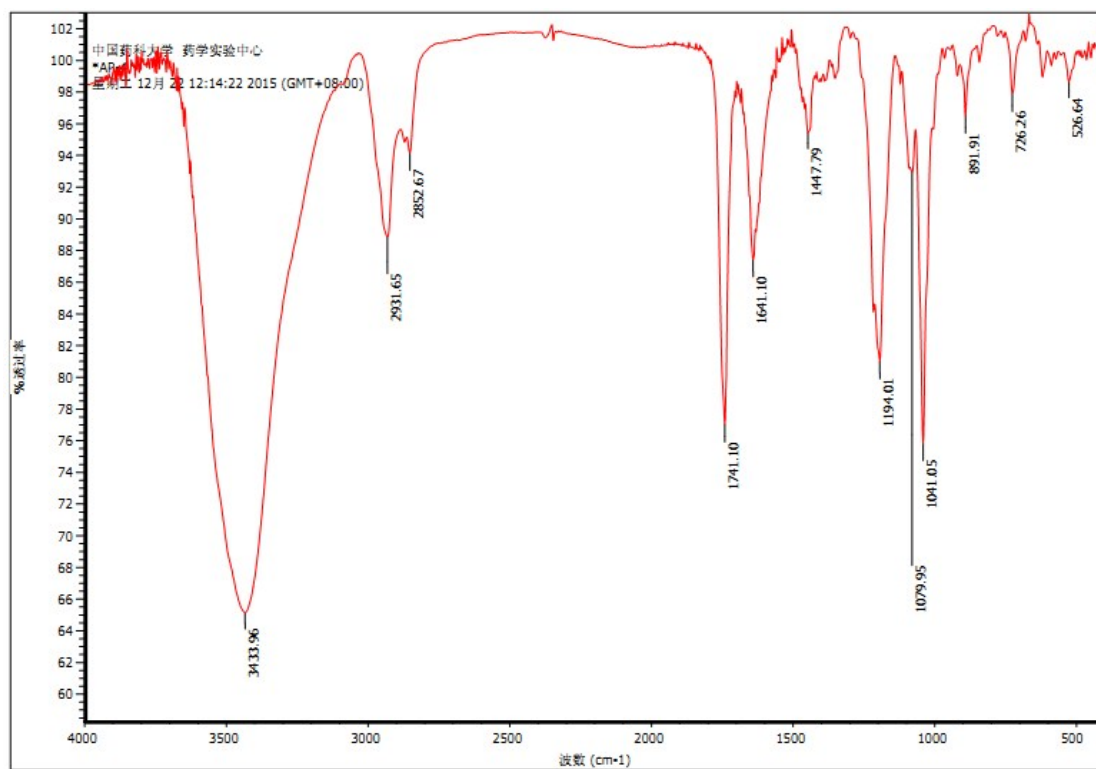




### S31. HRESIMS spectrum of compound 4

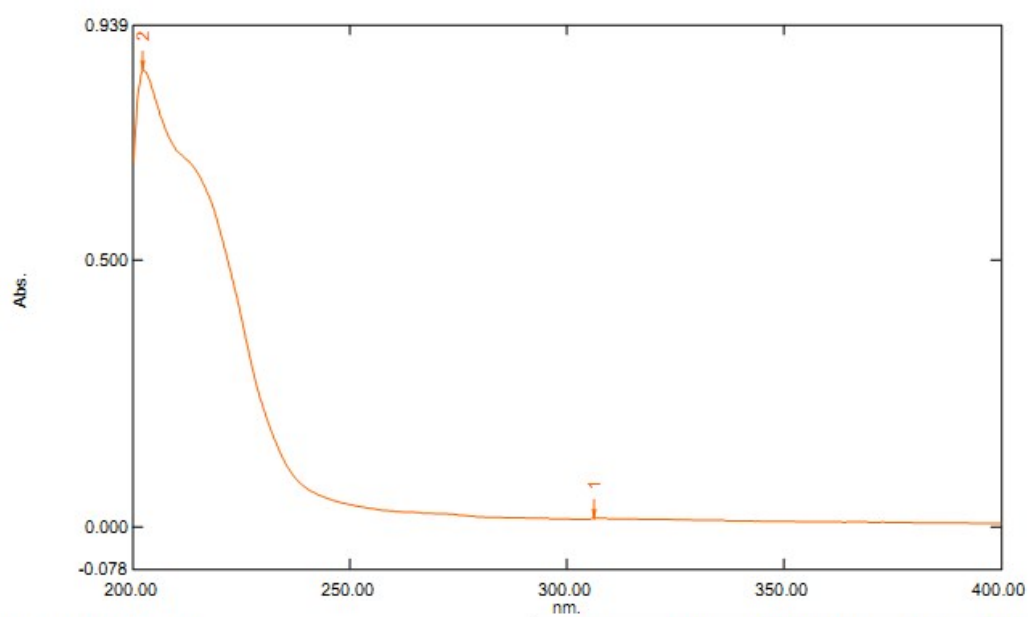


### S32. IR spectrum of compound 4



### S33. UV spectrum of compound 4 (MeOH)

Data Set: ap\_4 - RawData

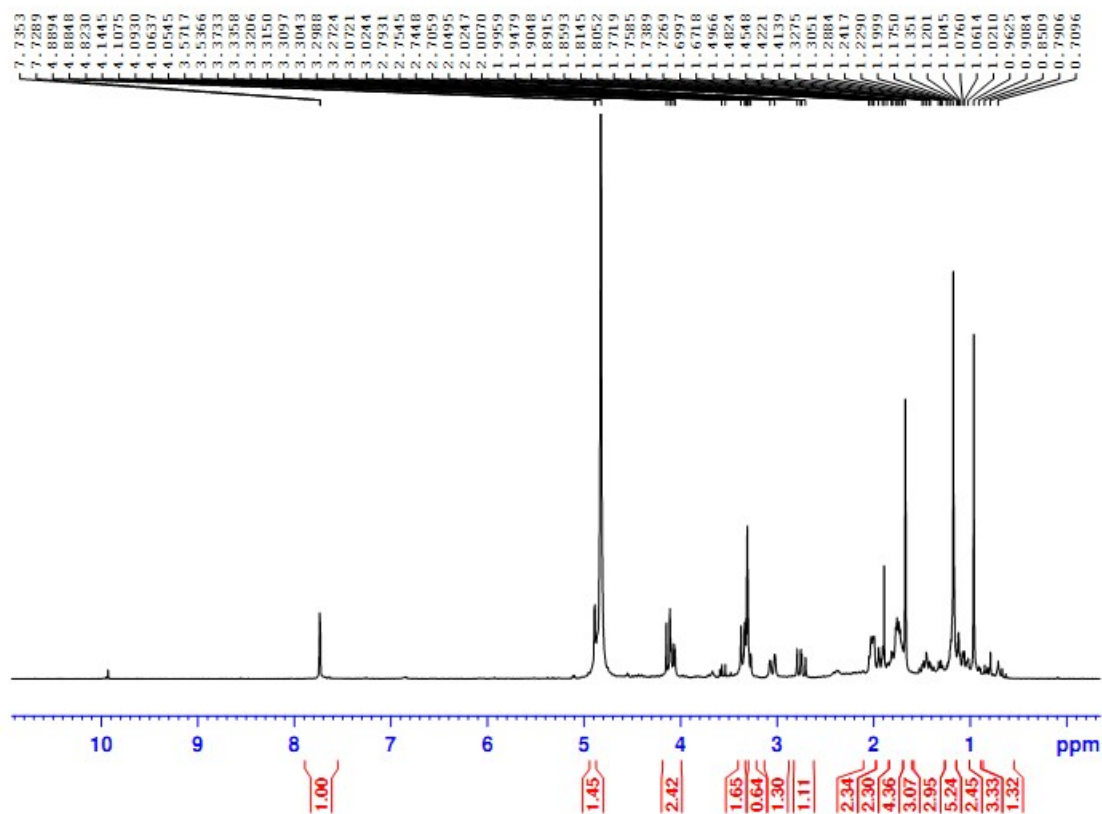


Measurement Properties  
Wavelength Range (nm.): 200.00 to 400.00  
Scan Speed: Fast  
Sampling Interval: 0.2  
Auto Sampling Interval: Disabled

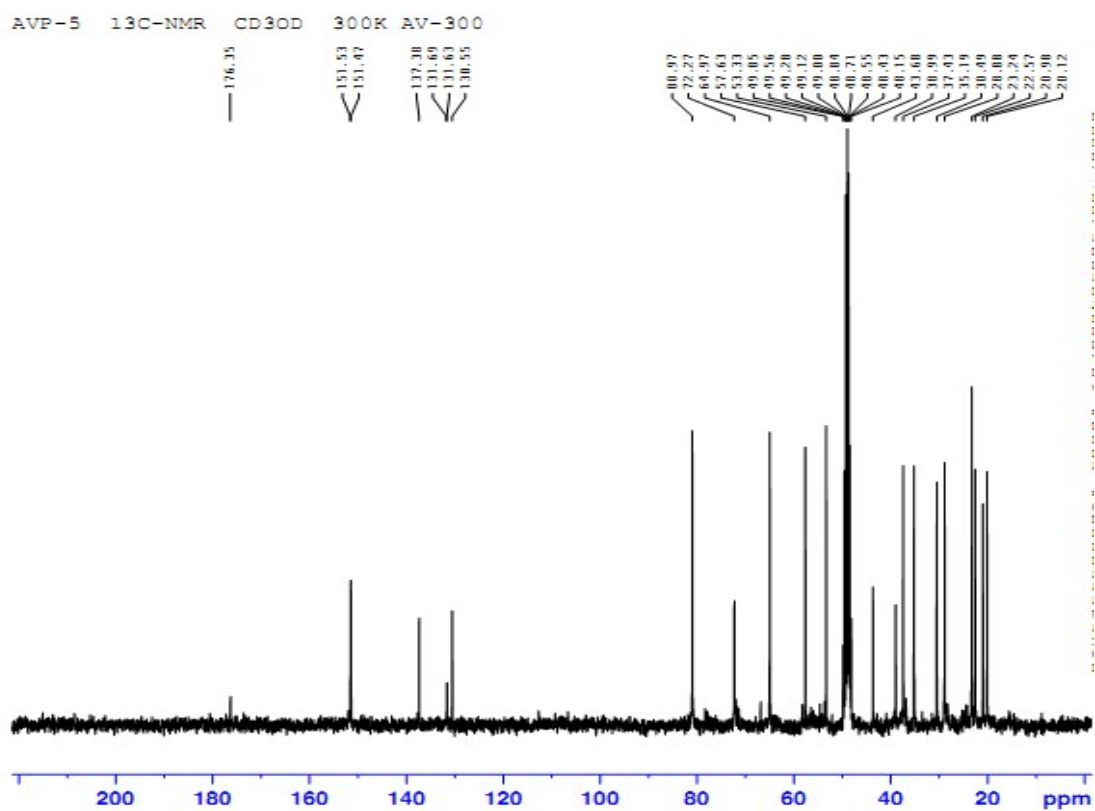
No.	P/V	Wavelength	Abs.	Description
1	⊕	306.20	0.017	
2	⊕	202.20	0.854	
3	⊕	304.40	0.014	

S34. <sup>1</sup>H NMR spectrum of compound 5 (300 MHz, CD<sub>3</sub>OD)

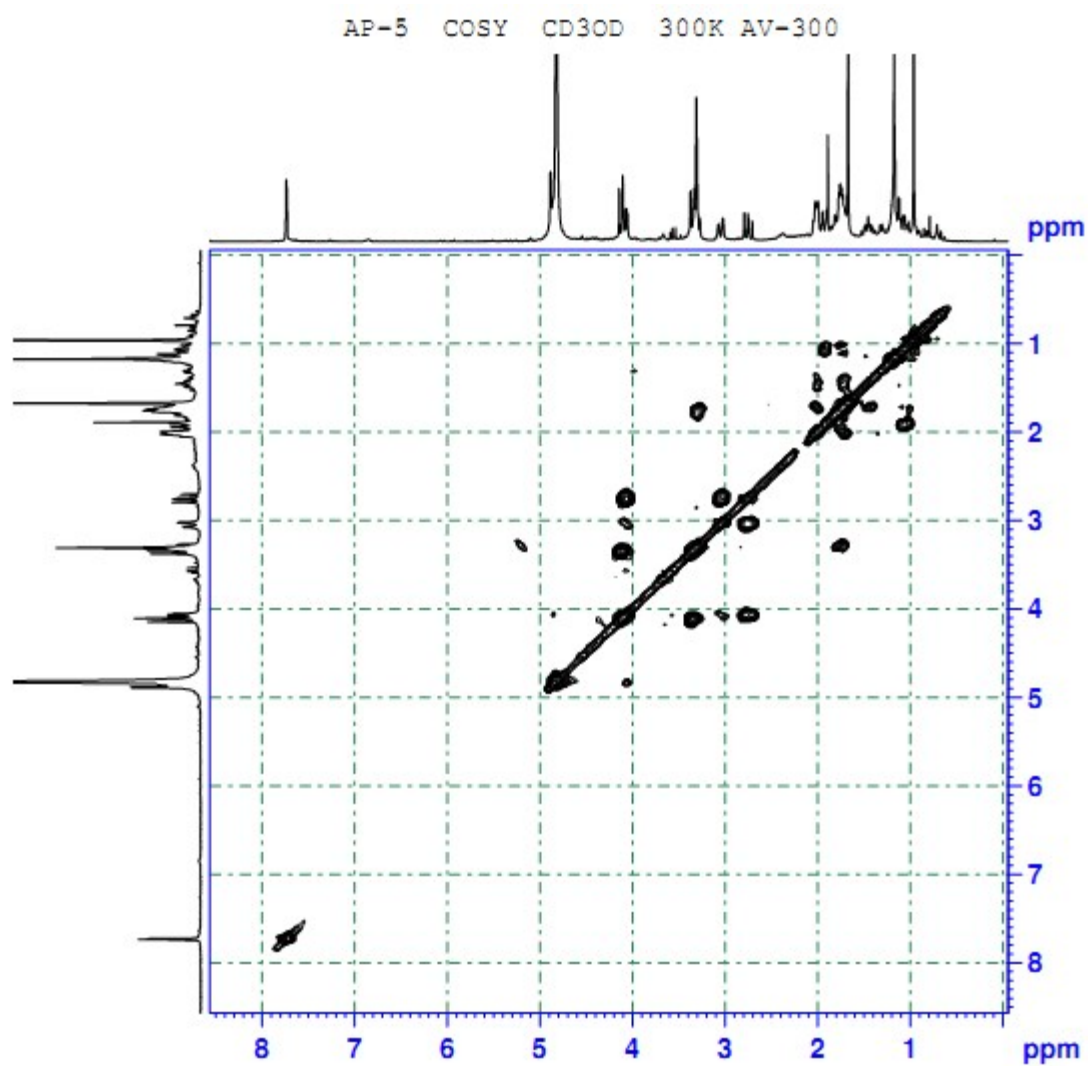
AP-5 H1-NMR CD3OD 300K AV-300



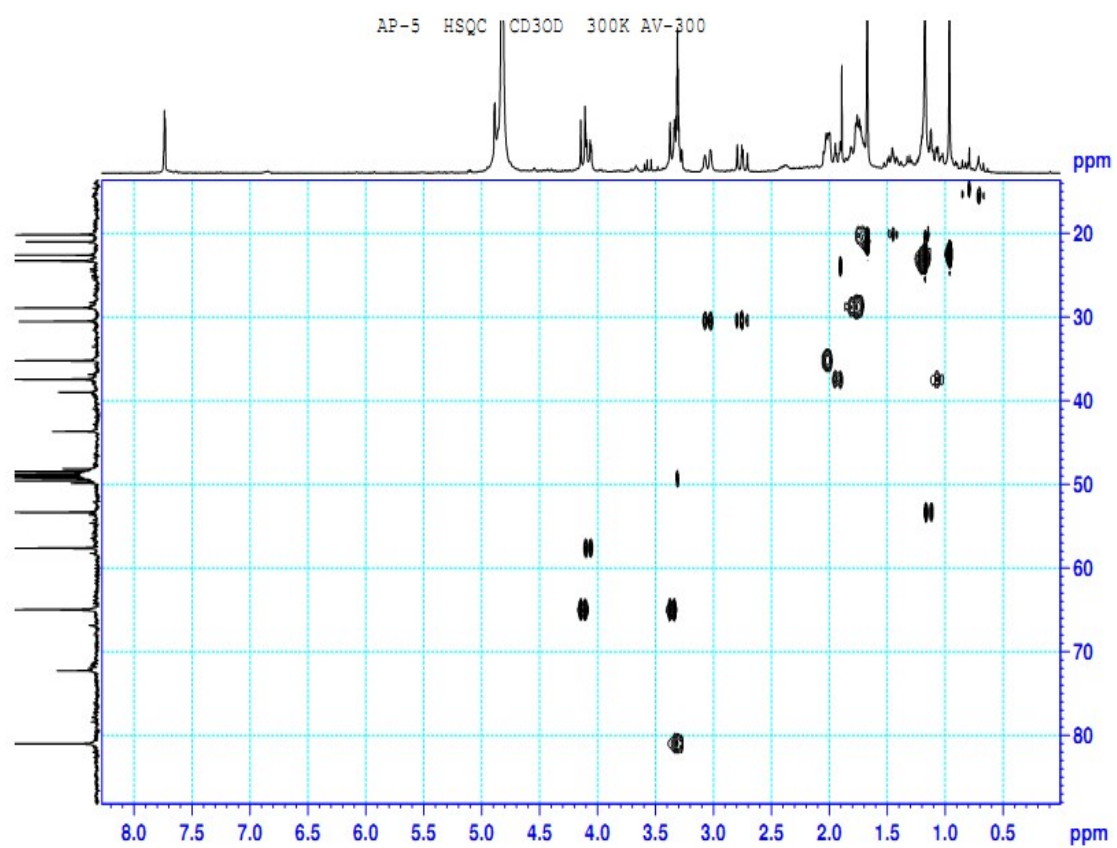
S35.  $^{13}\text{C}$  NMR spectrum of compound **5** (75 MHz,  $\text{CD}_3\text{OD}$ )



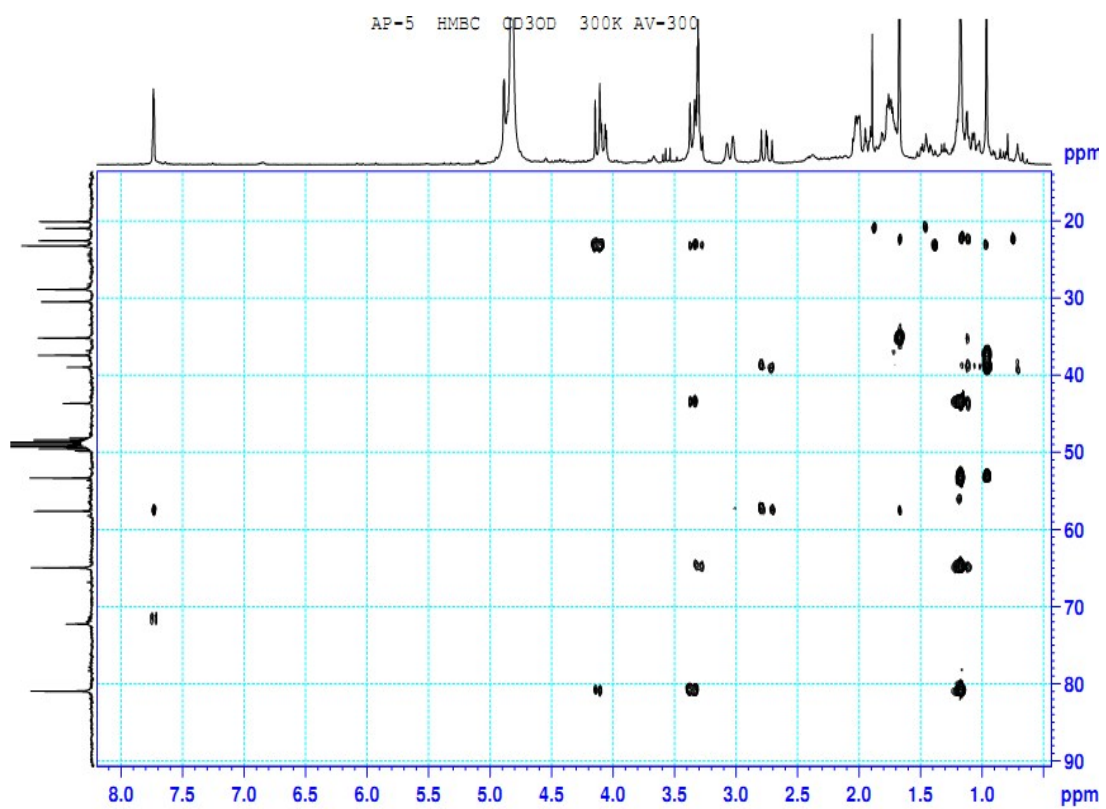
S36.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 5



S37. HSQC spectrum of compound 5

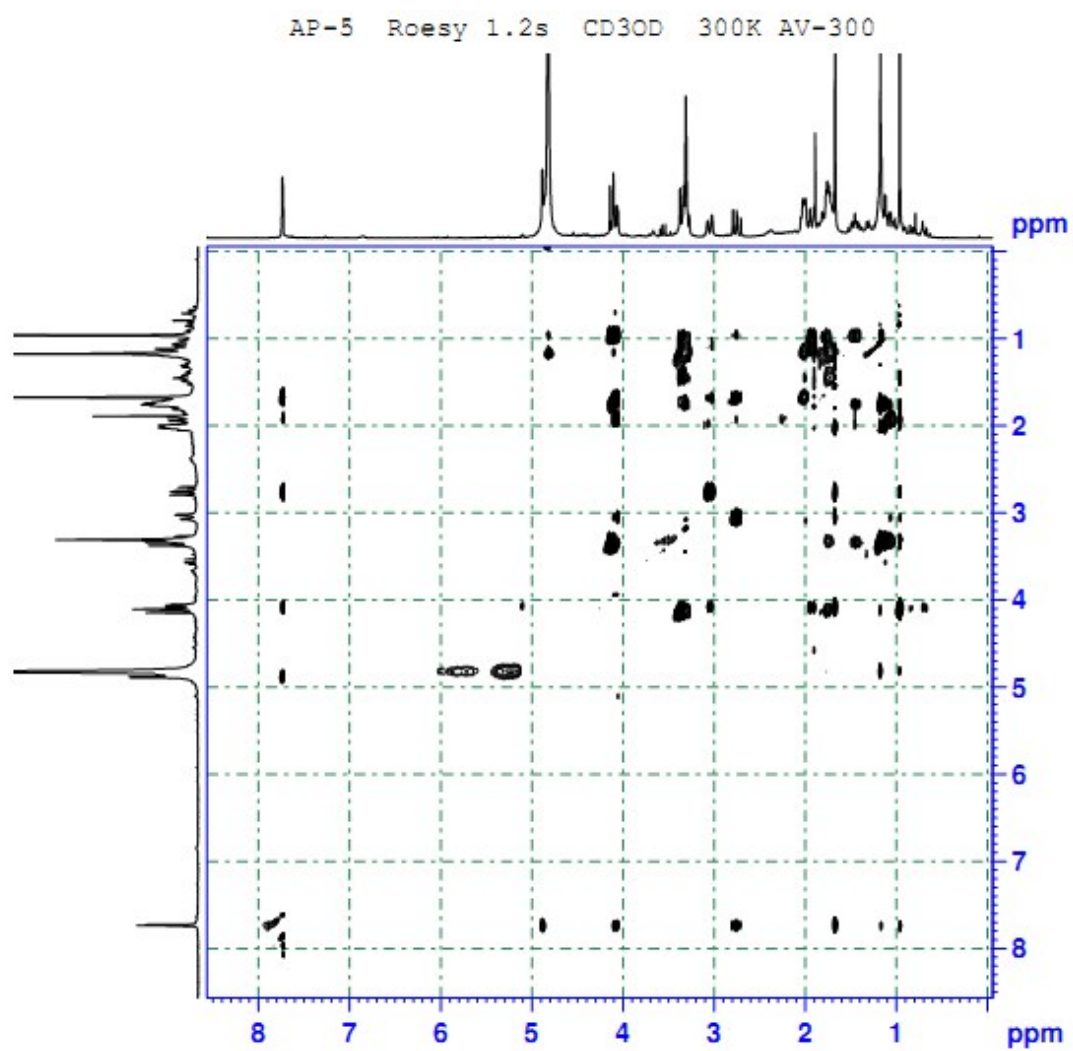


S38.HMBC spectrum of compound 5

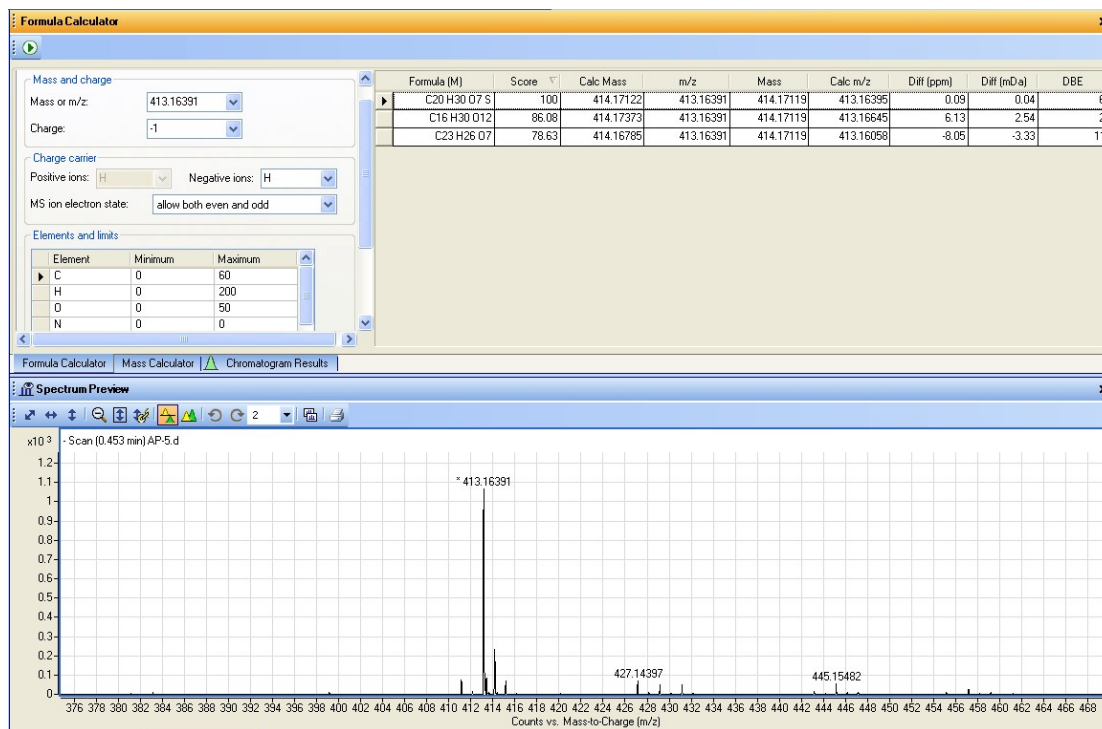




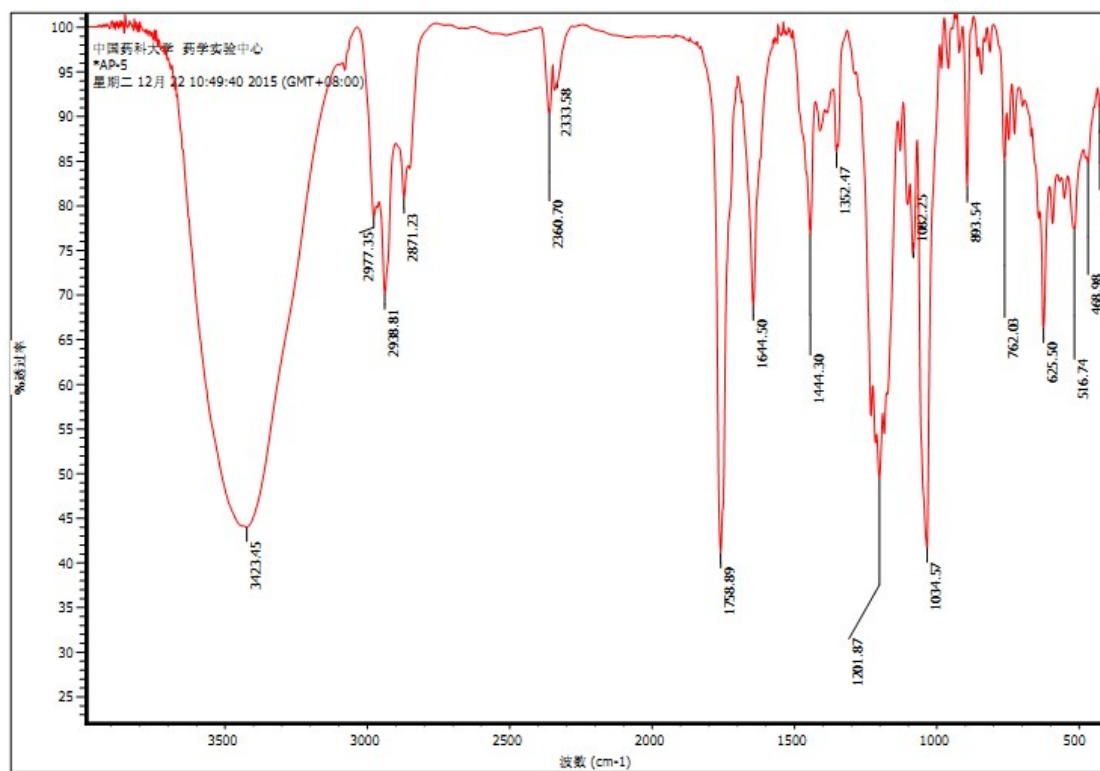
S39. ROESY spectrum of compound 5



## S40. HRESIMS spectrum of compound 5

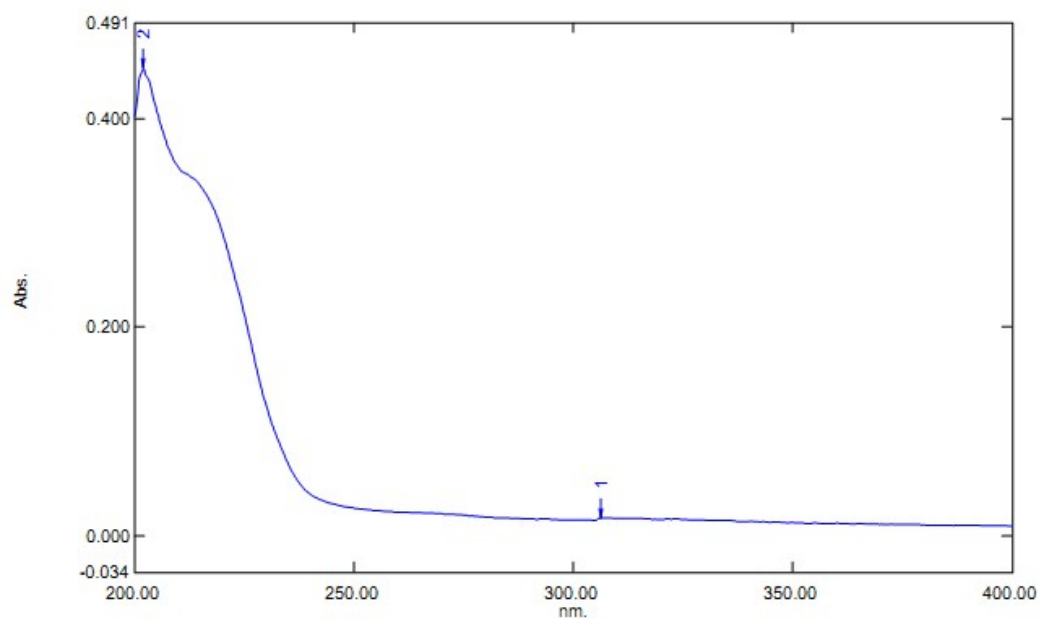


### S41. IR spectrum of compound 5



## S42. UV spectrum of compound 5 (MeOH)

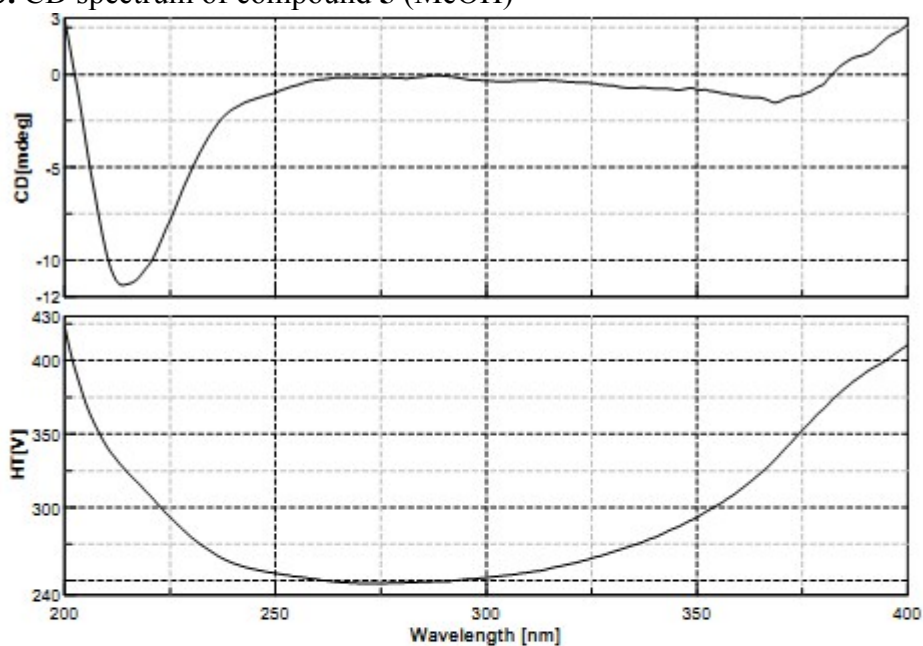
Data Set: ap\_5 - RawData



Measurement Properties  
Wavelength Range (nm.): 200.00 to 400.00  
Scan Speed: Fast  
Sampling Interval: 0.2  
Auto Sampling Interval: Disabled

No.	P/V	Wavelength	Abs.	Description
1	⊕	306.20	0.018	
2	⊕	202.00	0.447	
3	⊕	304.60	0.015	

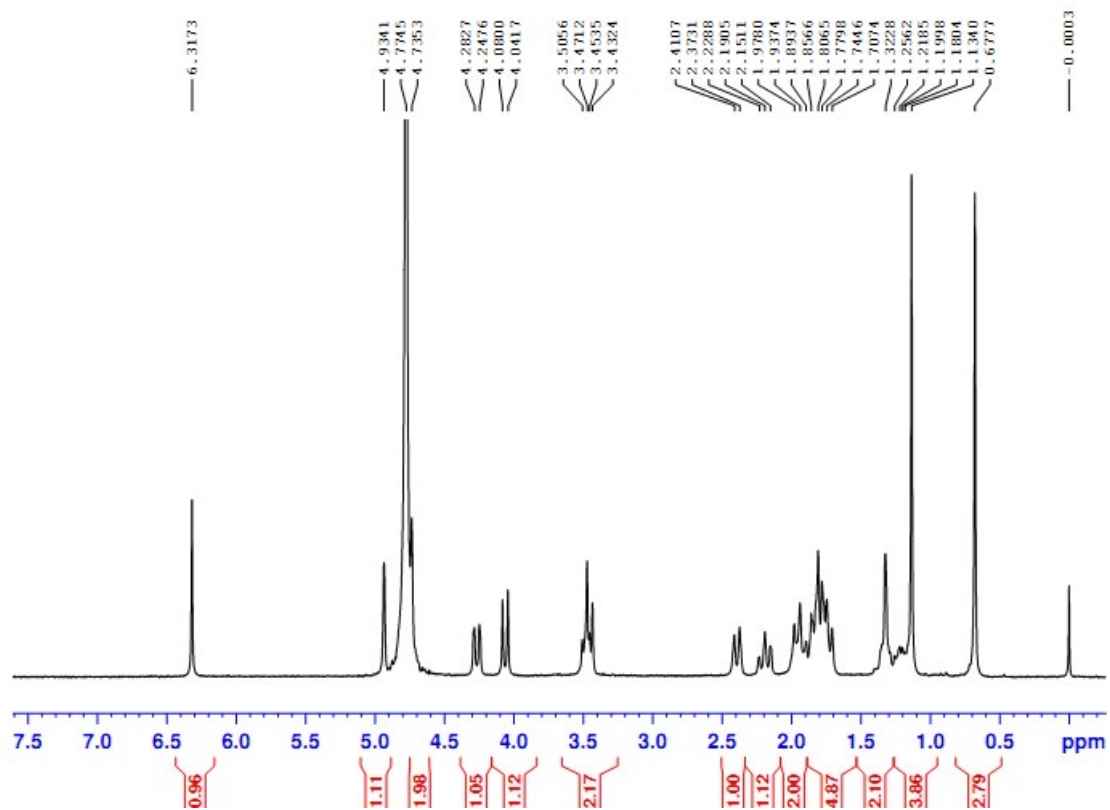
### S43. CD spectrum of compound 5 (MeOH)



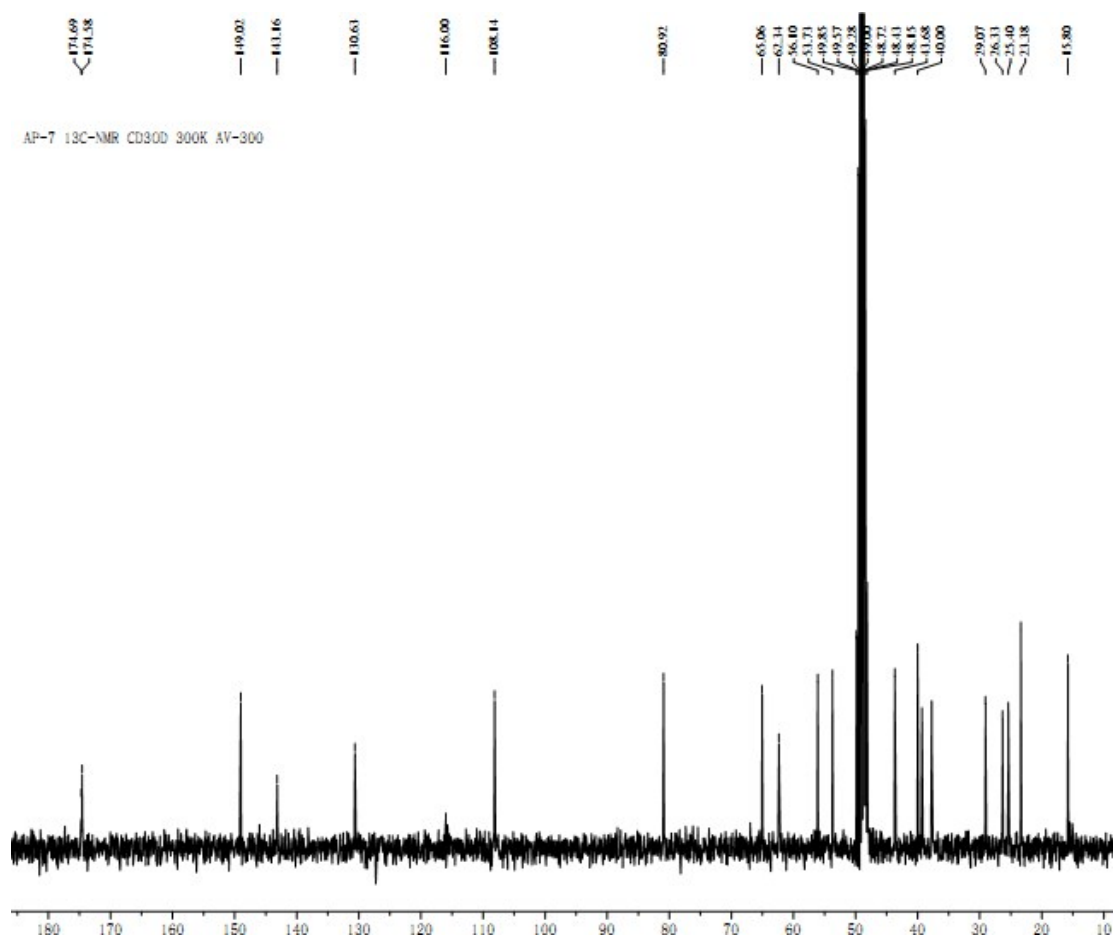
Date	2013/11/19 10:08
File name	AP-5.jws
Model	J-810
Serial No.	B050560750
Band width	1 nm
Response	1 sec
Sensitivity	Standard
Measurement range	400 - 200 nm
Data pitch	1nm
Scanning speed	100 nm/min
Accumulation	1
Cell Length	0.1 cm
Solvent	MeOH
Temperature	Room Temperature
Sample name	AP-5
Operator	DEMO

S44. <sup>1</sup>H NMR spectrum of compound 6 (300 MHz, CD<sub>3</sub>OD)

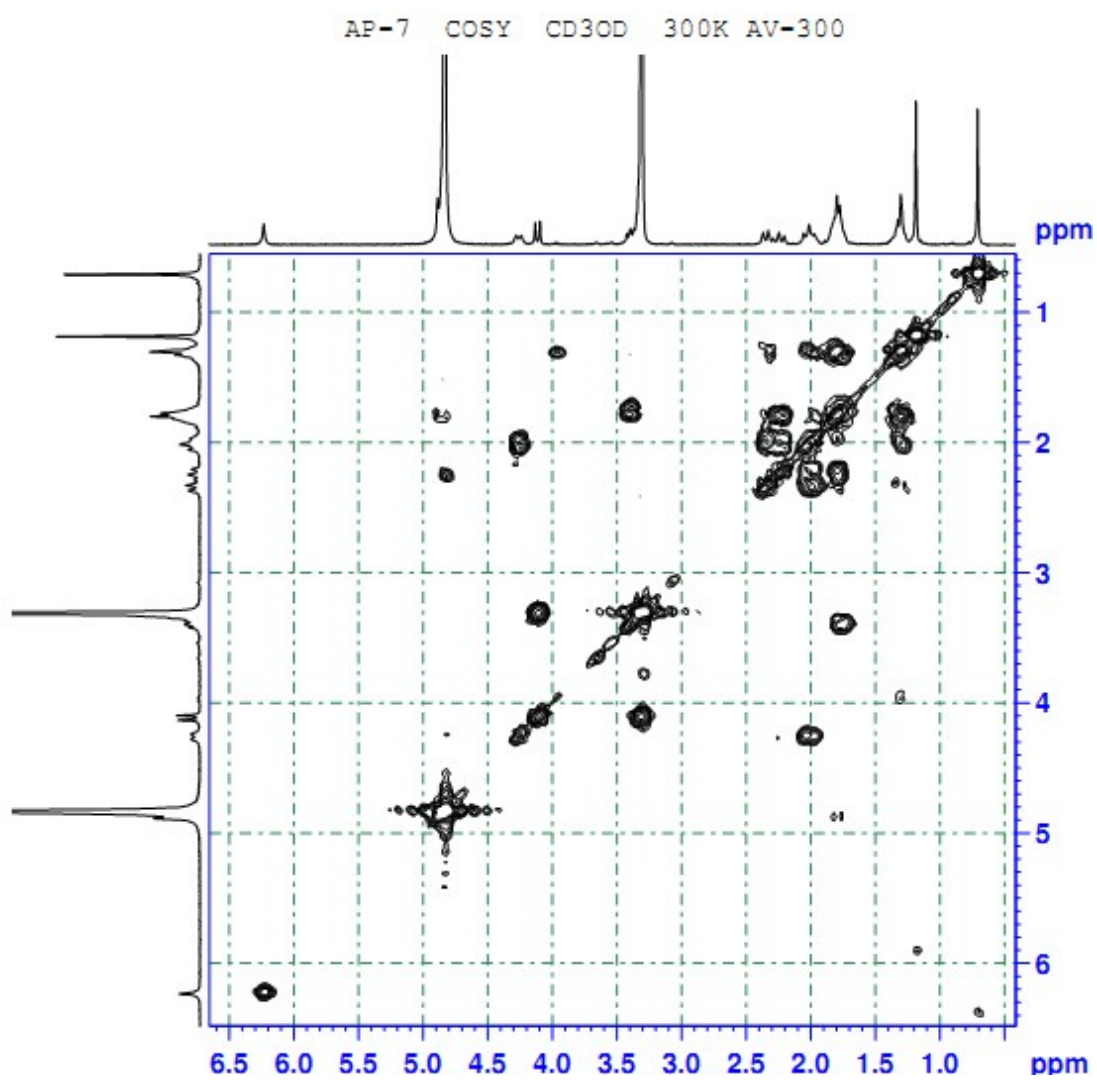
AP-7 H1 NMR CD3OD 300K AV-300



S45.  $^{13}\text{C}$  NMR spectrum of compound **6** (75 MHz,  $\text{CD}_3\text{OD}$ )

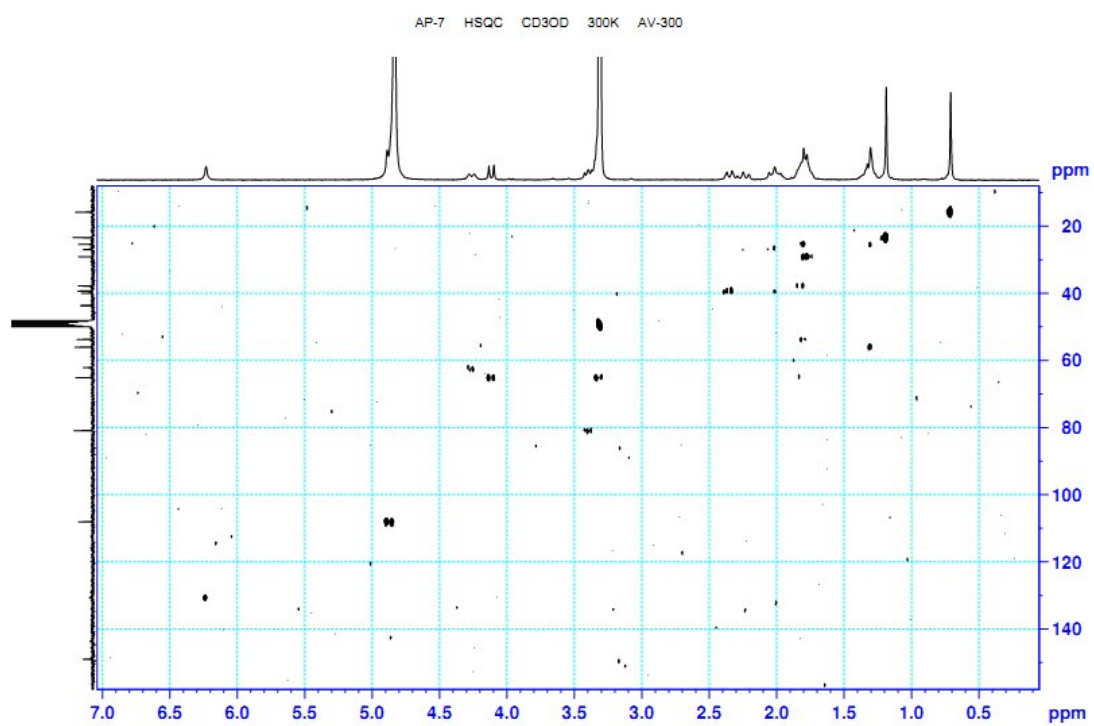


S46.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 6



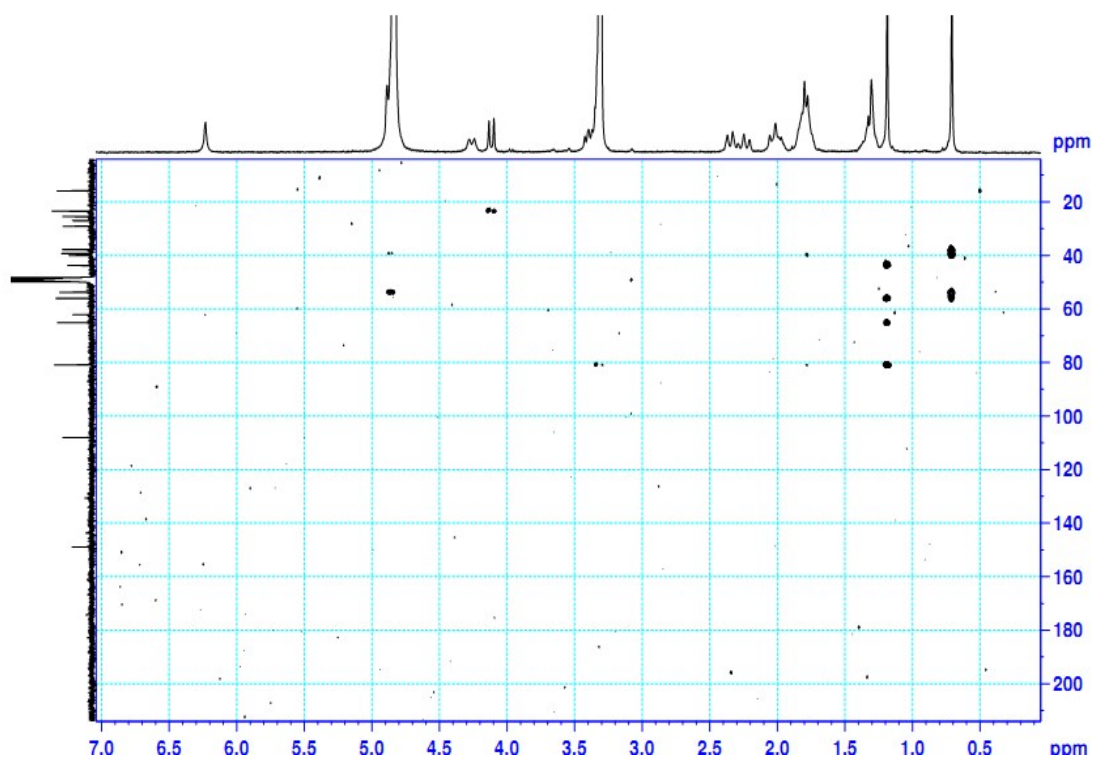


### S47. HSQC spectrum of compound 6



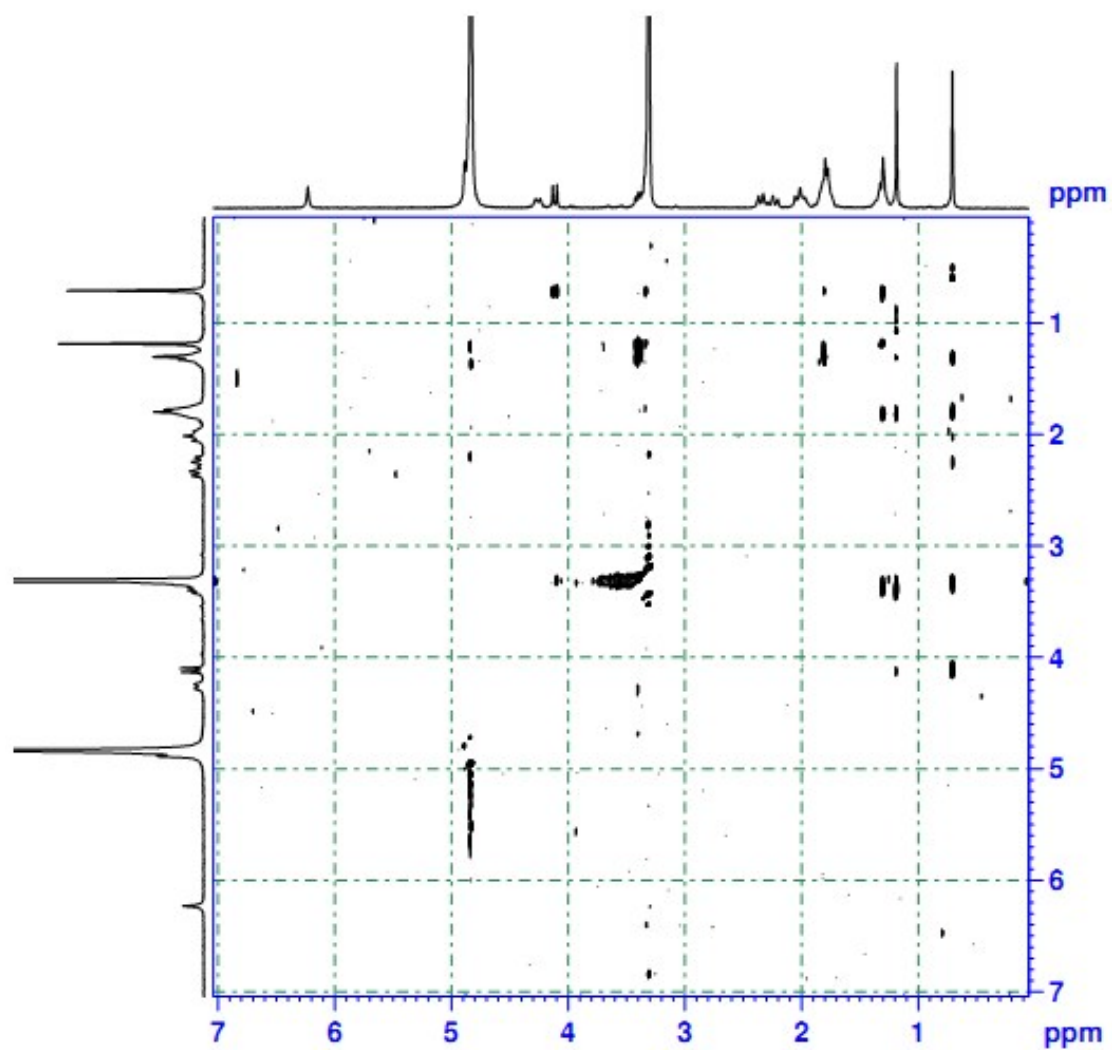
# S48.HMBC spectrum of compound 6

AP-7 HMBC CD3OD 300K AV-300

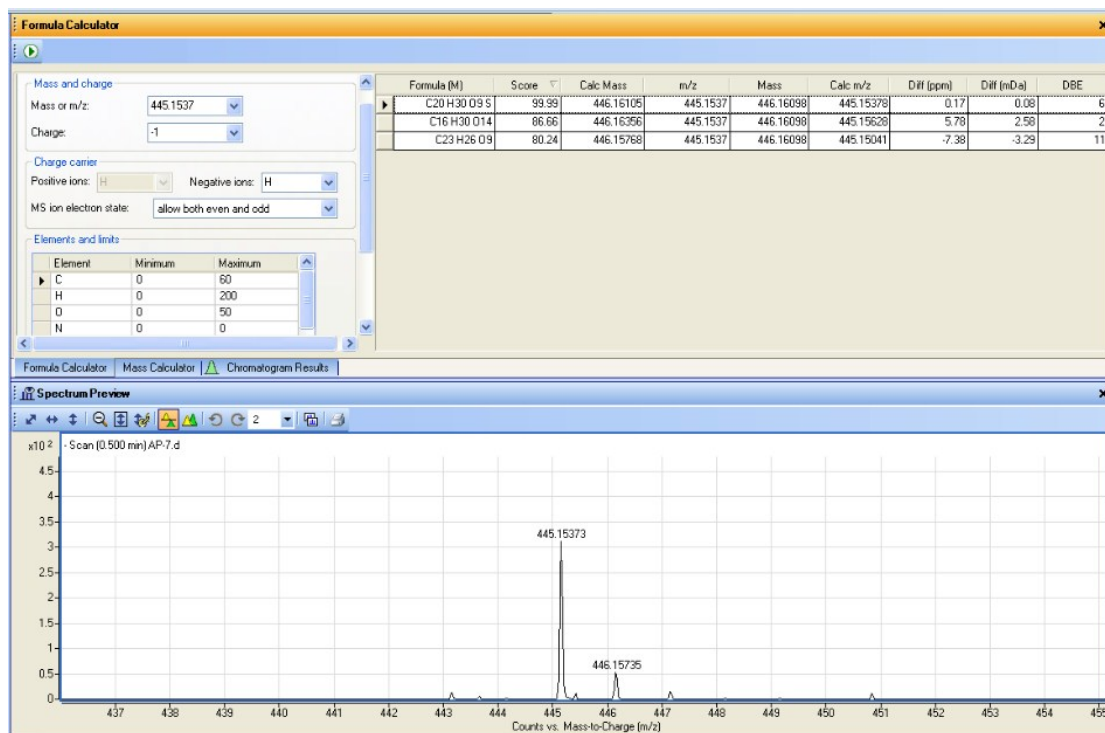


S49. ROESY spectrum of compound 6

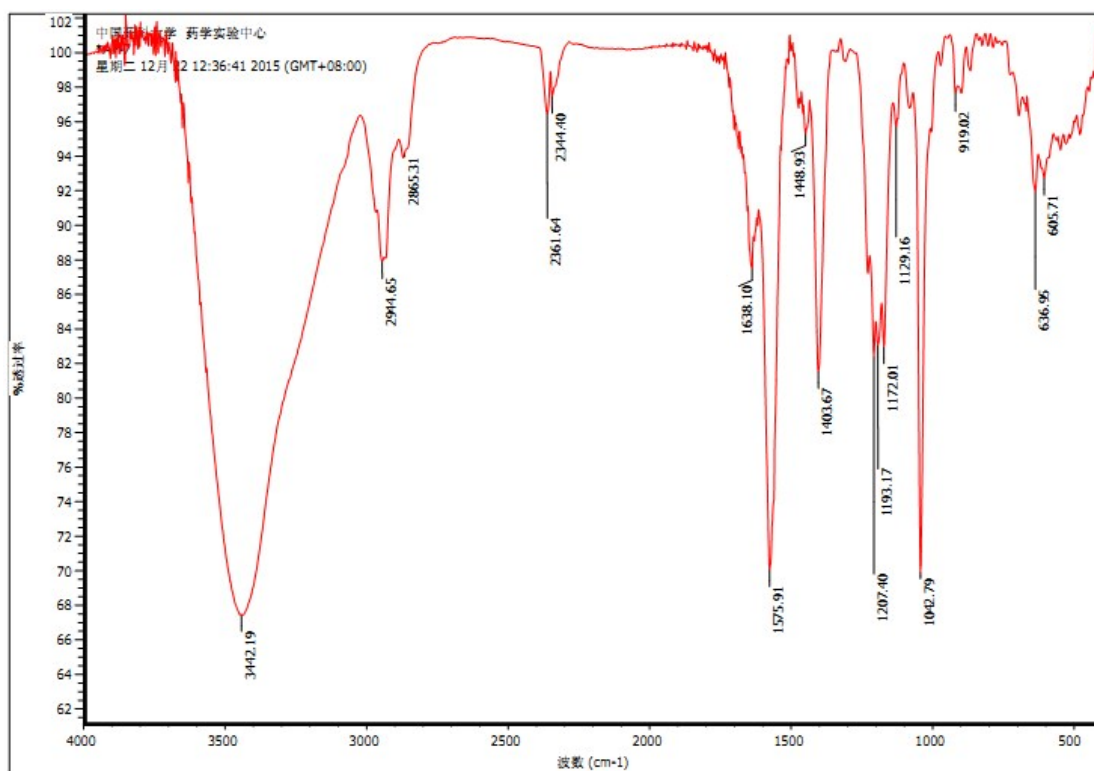
AP-7 Roesy 1,2s CD3OD 300K AV-300



## S50. HRESIMS spectrum of compound 6

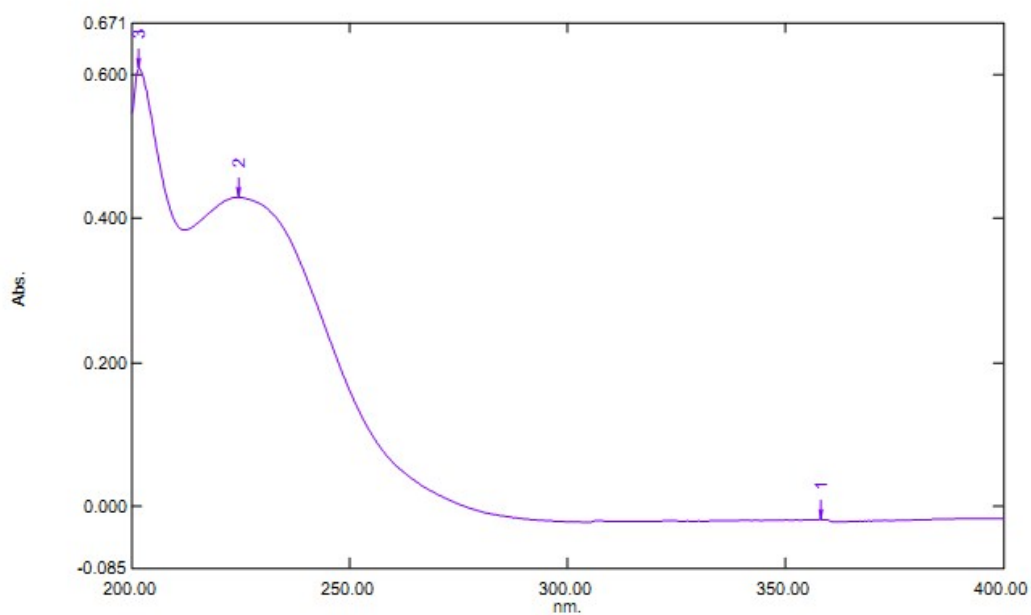


### S51. IR spectrum of compound 6



## S52. UV spectrum of compound 6 (MeOH)

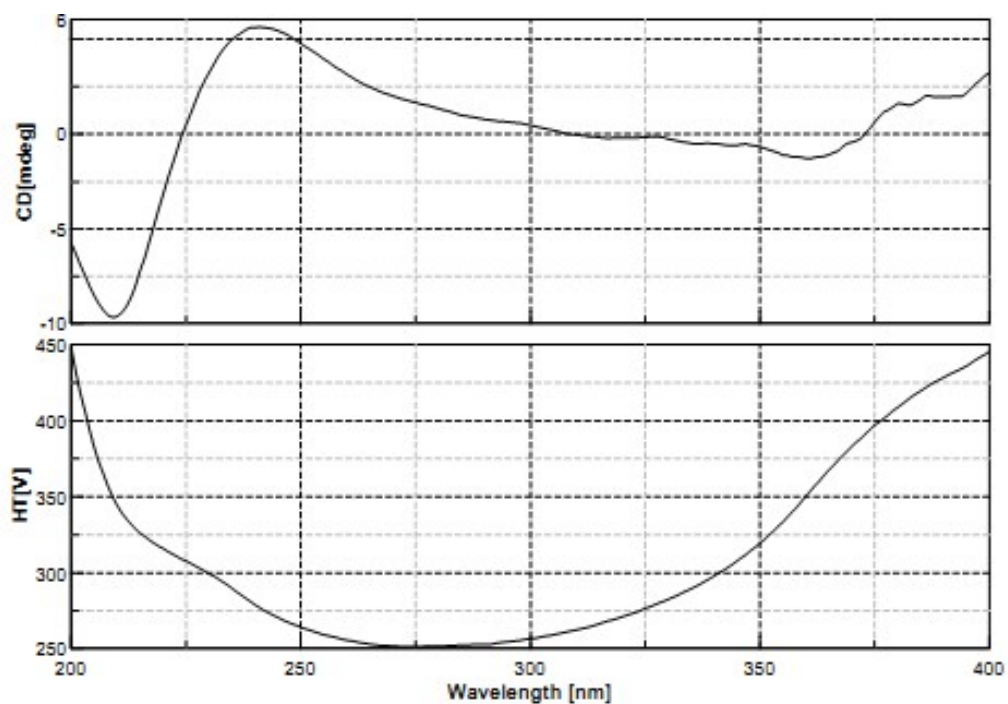
Data Set: ap-7 - RawData



Measurement Properties  
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Scan Speed: Fast  
Sampling Interval: 0.2  
Auto Sampling Interval: Disabled  
Scan Mode: Auto

No.	P/V	Wavelength	Abs.	Description
1	ⓘ	358.00	-0.018	
2	ⓘ	224.40	0.430	
3	ⓘ	201.60	0.608	
4	Ⓜ	304.20	-0.022	
5	Ⓜ	212.00	0.384	

### S53. CD spectrum of compound 6 (MeOH)



Date	2013/12/16 10:29
File name	AP-7.jws
Model	J-810
Serial No.	B050560750
Band width	1 nm
Response	1 sec
Sensitivity	Standard
Measurement range	400 - 200 nm
Data pitch	1nm
Scanning speed	100 nm/min
Accumulation	1
Cell Length	0.1 cm
Solvent	MeOH
Temperature	Room Temperature
Sample name	AP-7
Operator	DEMO