

## Supplementary data

### **Phytosteroids and triterpenoids with potent cytotoxicities from the leaves of *Chisocheton cumingianus***

**Shan-Shan Huang, Kai-Li Jian, Rui-Jun Li, Ling-Yi Kong\* and Ming-Hua Yang\***

*State Key Laboratory of Natural Medicines, Department of Natural Medicinal Chemistry, China  
Pharmaceutical University, 24 Tong Jia Xiang, Nanjing 210009, People's Republic of China*

#### **Corresponding authors**

\* Ming-Hua Yang:

*E-mail:* skeepjack@163.com

Tel/Fax: +86-25-8618-5039

\* Ling-Yi Kong:

*E-mail:* cpu\_lykong@126.com

Tel/Fax: +86-25-8327-1405

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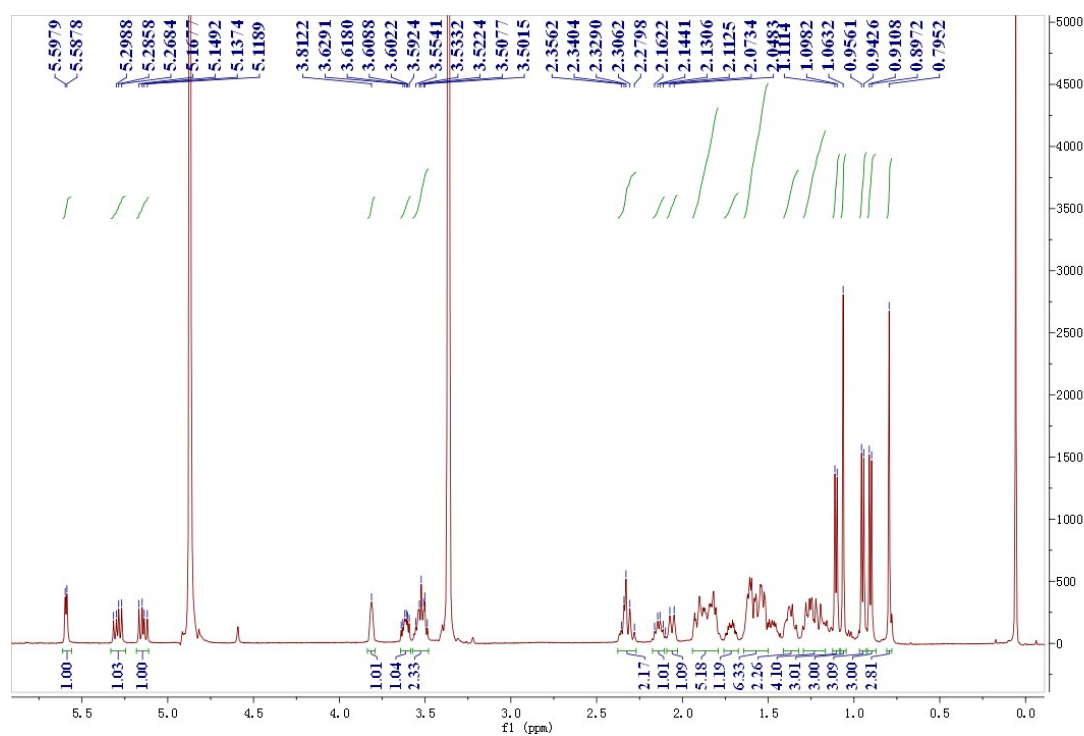


Figure S1.  $^1\text{H}$  NMR (500 MHz, methanol- $d_4$ ) spectrum of chisopanoid A (**1**)

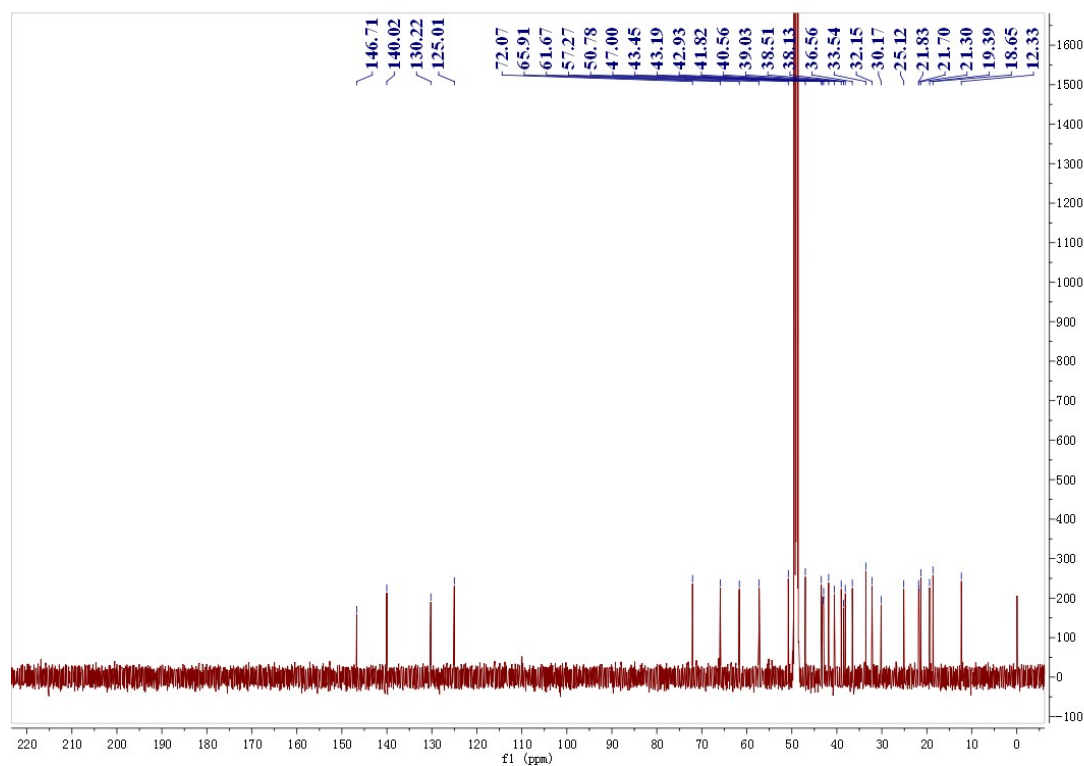


Figure S2.  $^{13}\text{C}$  NMR (125 MHz, methanol- $d_4$ ) spectrum of chisopanoid A (**1**)

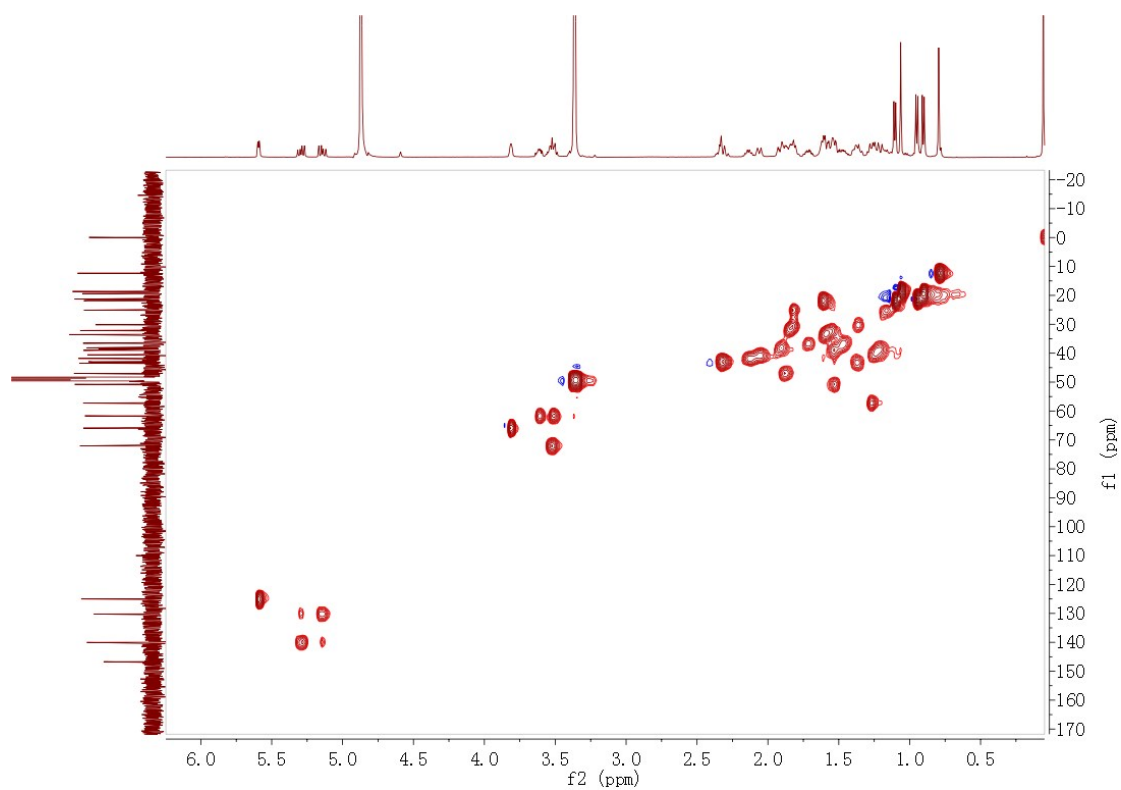


Figure S3. HSQC spectrum of chisopanoid A (1)

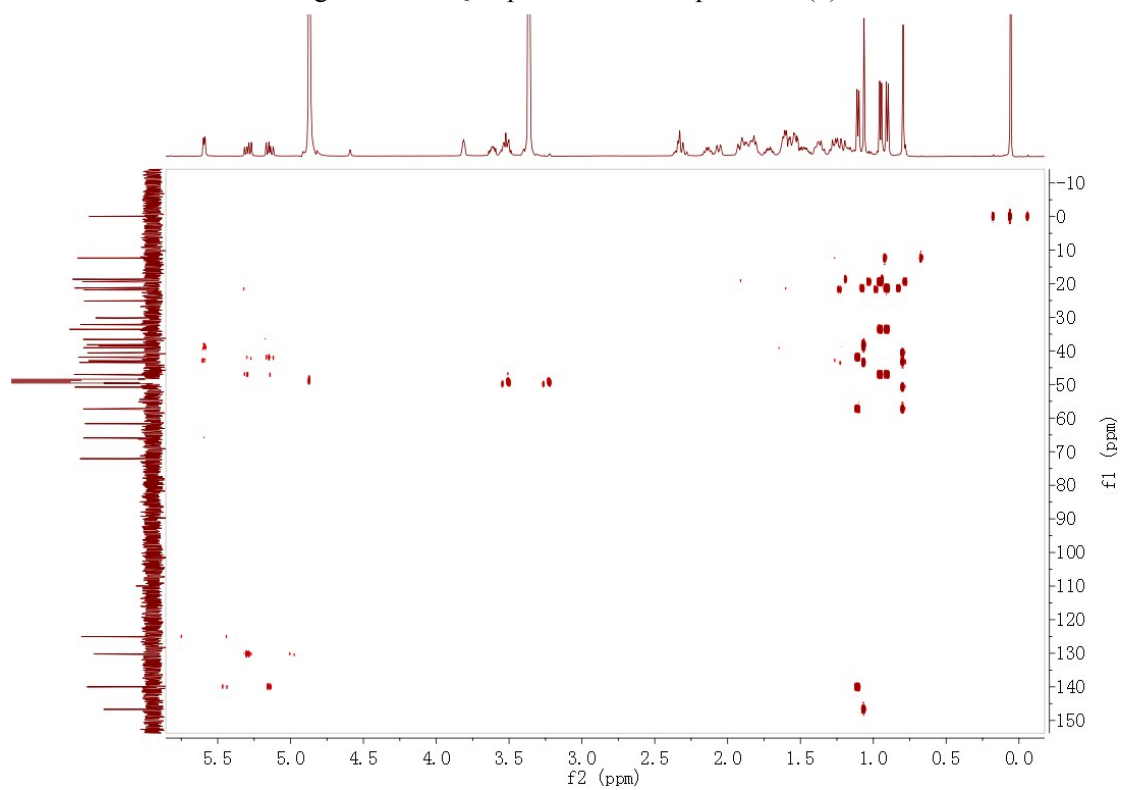


Figure S4. HMBC spectrum of chisopanoid A (1)

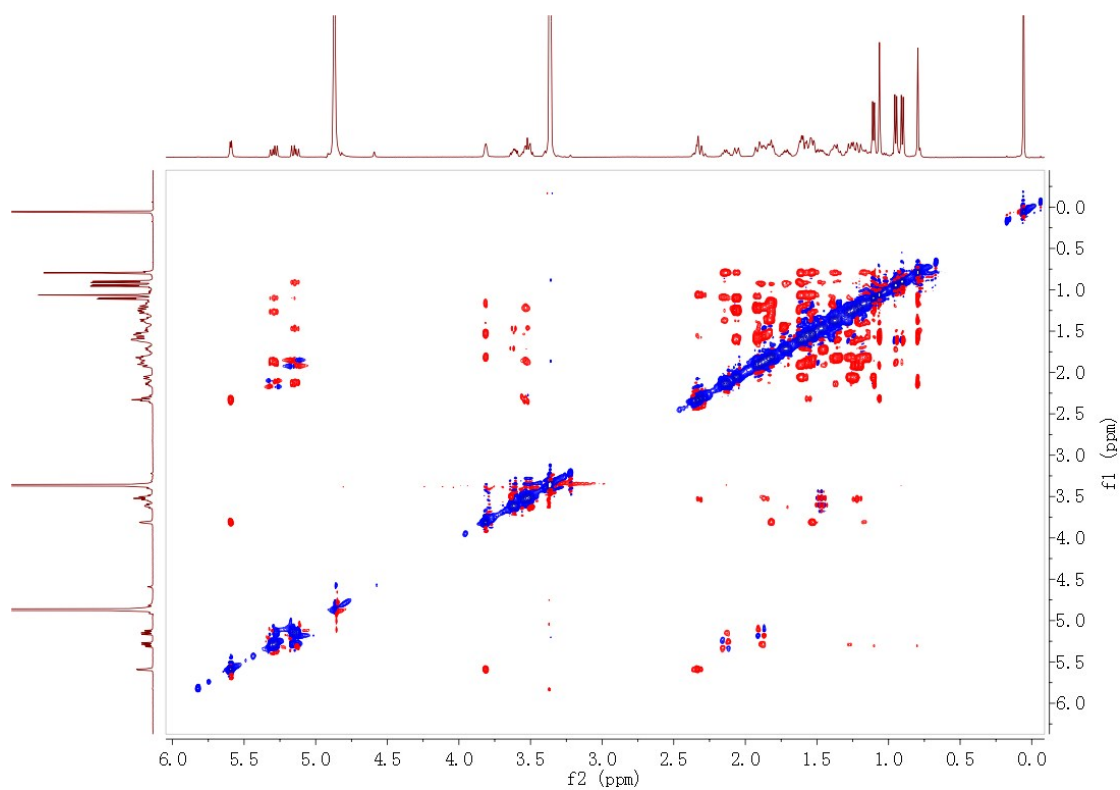
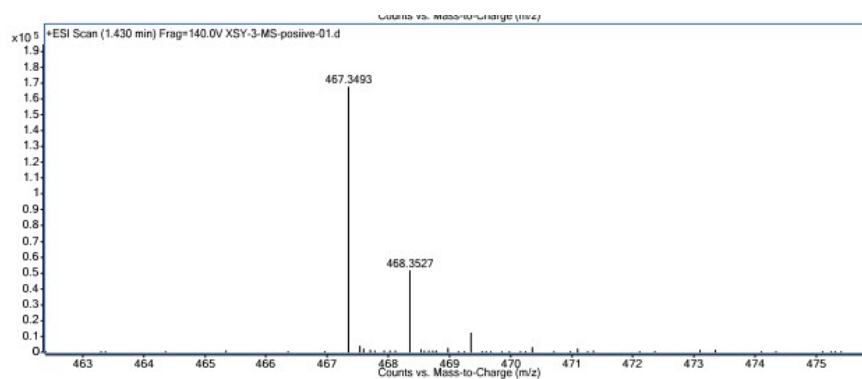


Figure S5. ROESY spectrum of chisopanoid A (**1**)



#### Elemental Composition Calculator

| Target m/z:                                      | 467.3493                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>48</sub> NaO <sub>3</sub> | 467.3496                                         |              | 0.51          |          |                     |

Figure S6. HRESIMS spectrum of chisopanoid A (**1**)

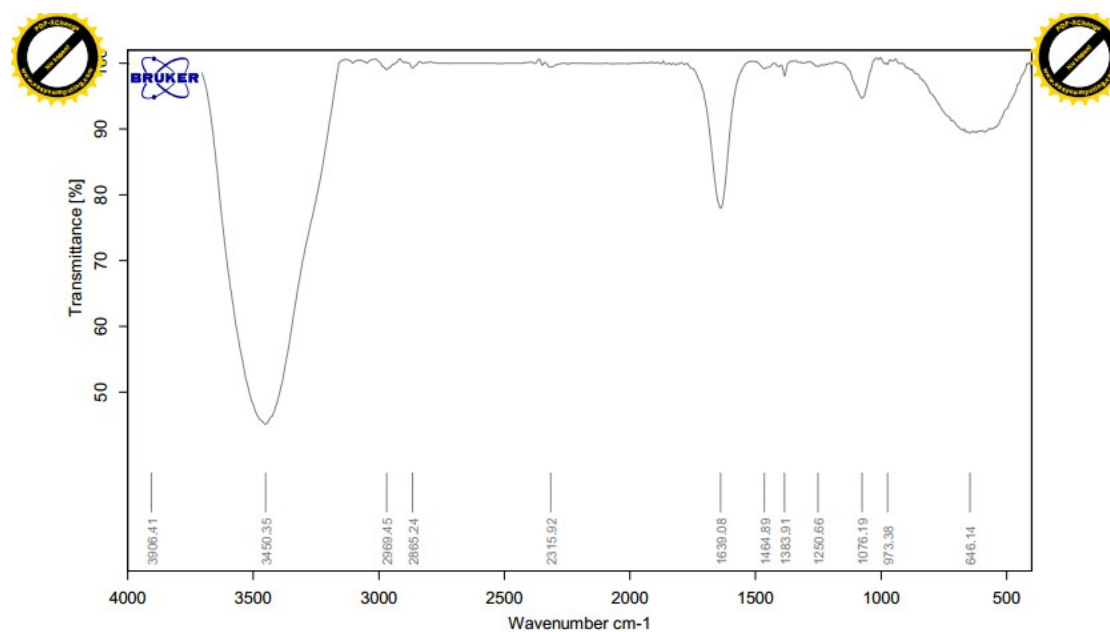


Figure S7. IR (KBr disc) spectrum of chisopanoid A (**1**)

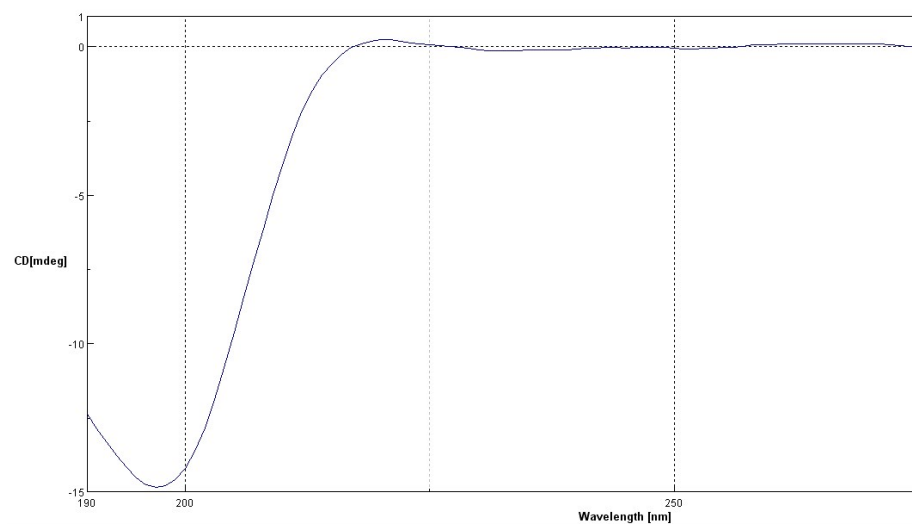


Figure S8. ECD spectra of chisopanoid A (**1**) (in MeCN).

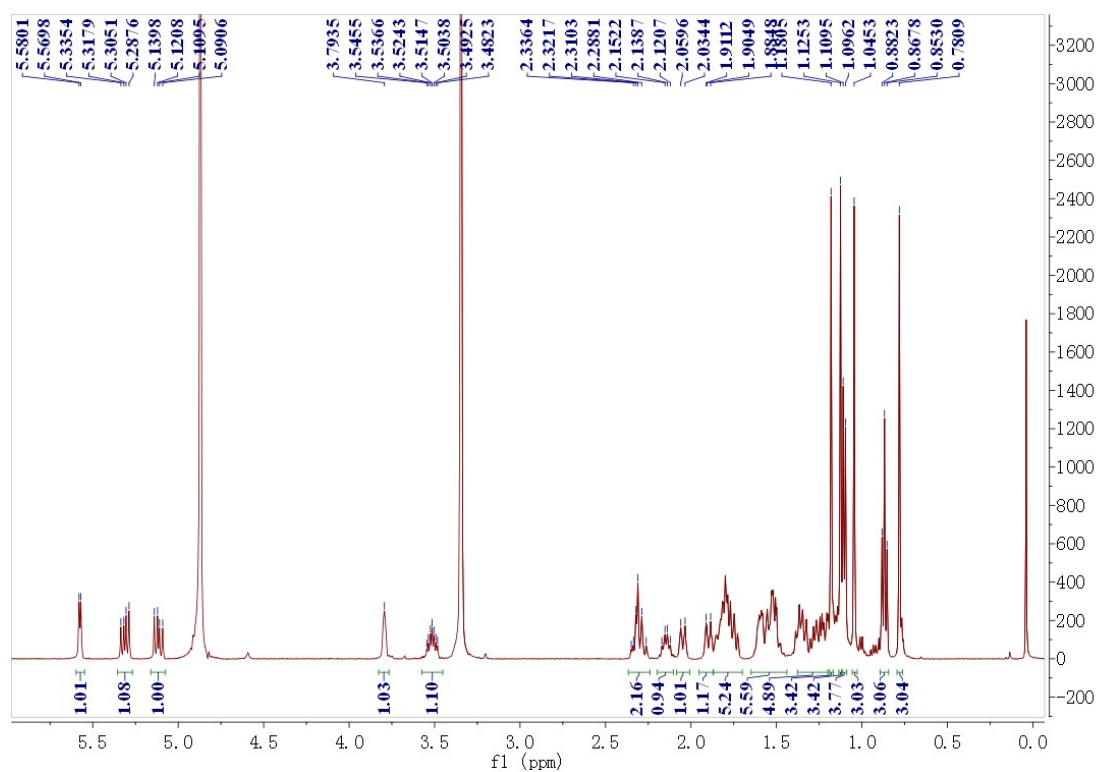


Figure S9. <sup>1</sup>H NMR (500 MHz, methanol-*d*<sub>4</sub>) spectrum of chisopanoid B (2)

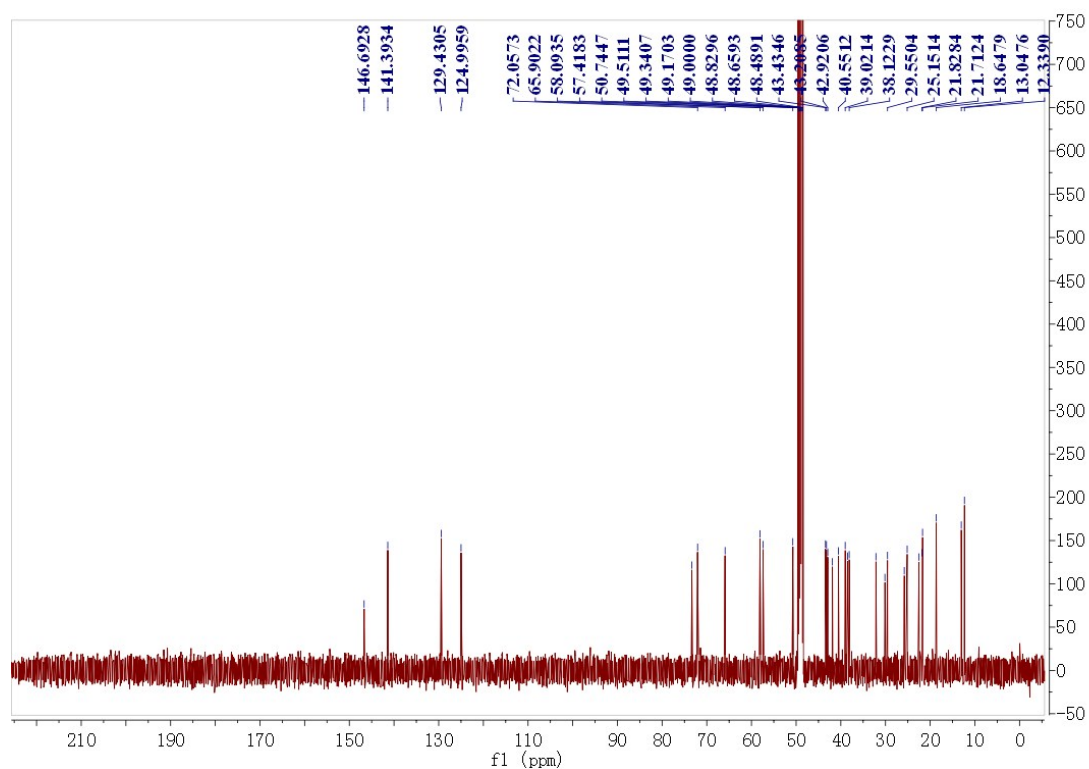


Figure S10. <sup>13</sup>C NMR (125 MHz, methanol-*d*<sub>4</sub>) spectrum of chisopanoid B (2)



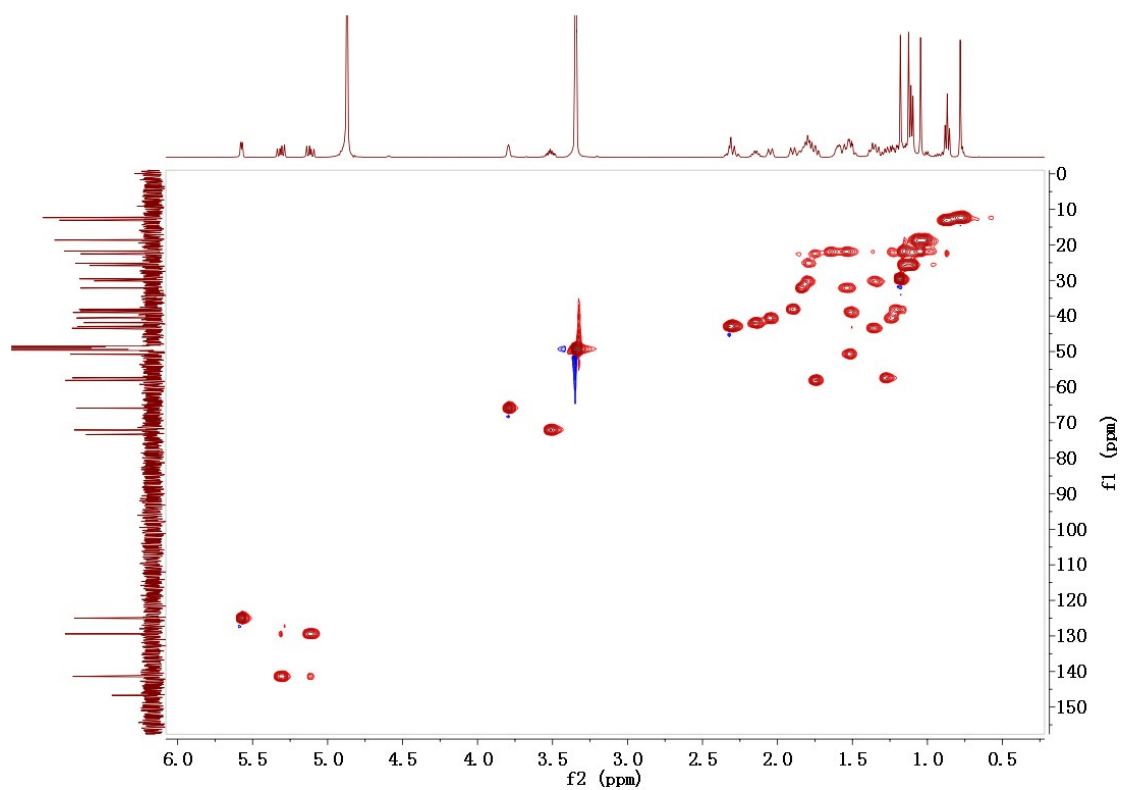


Figure S11. HSQC spectrum of chisopanoid B (2)

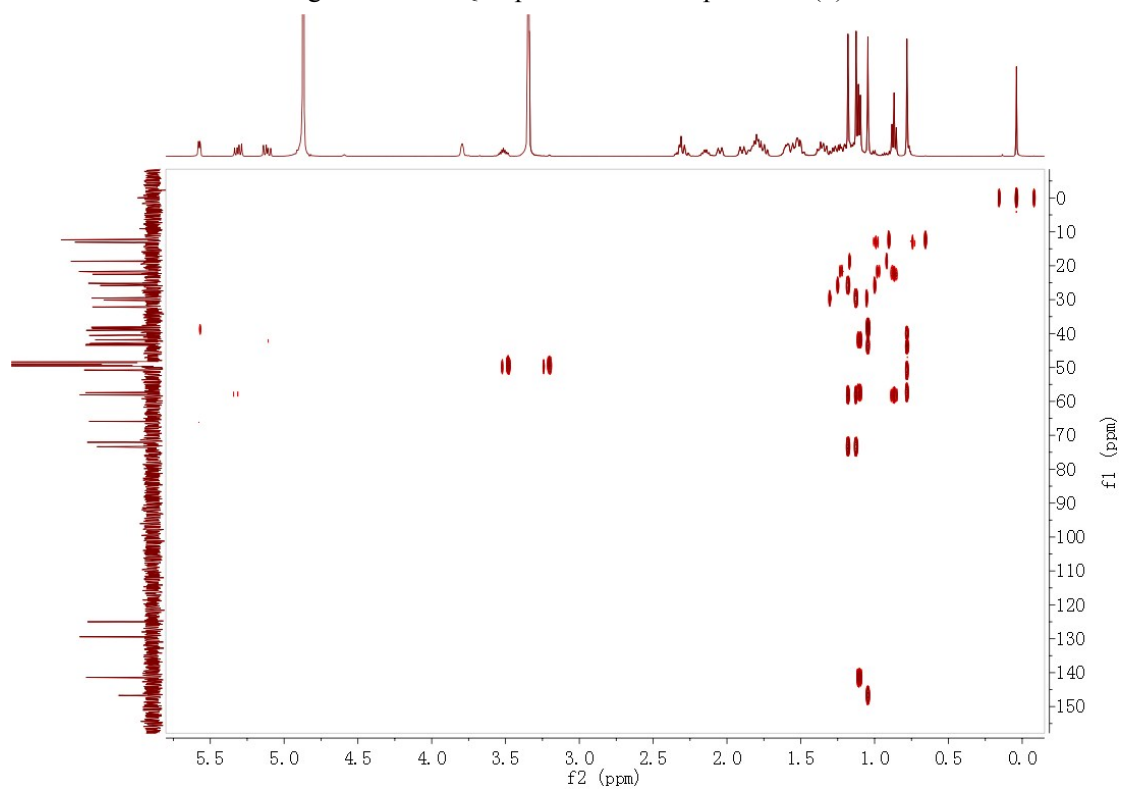


Figure S12. HMBC spectrum of chisopanoid B (2)

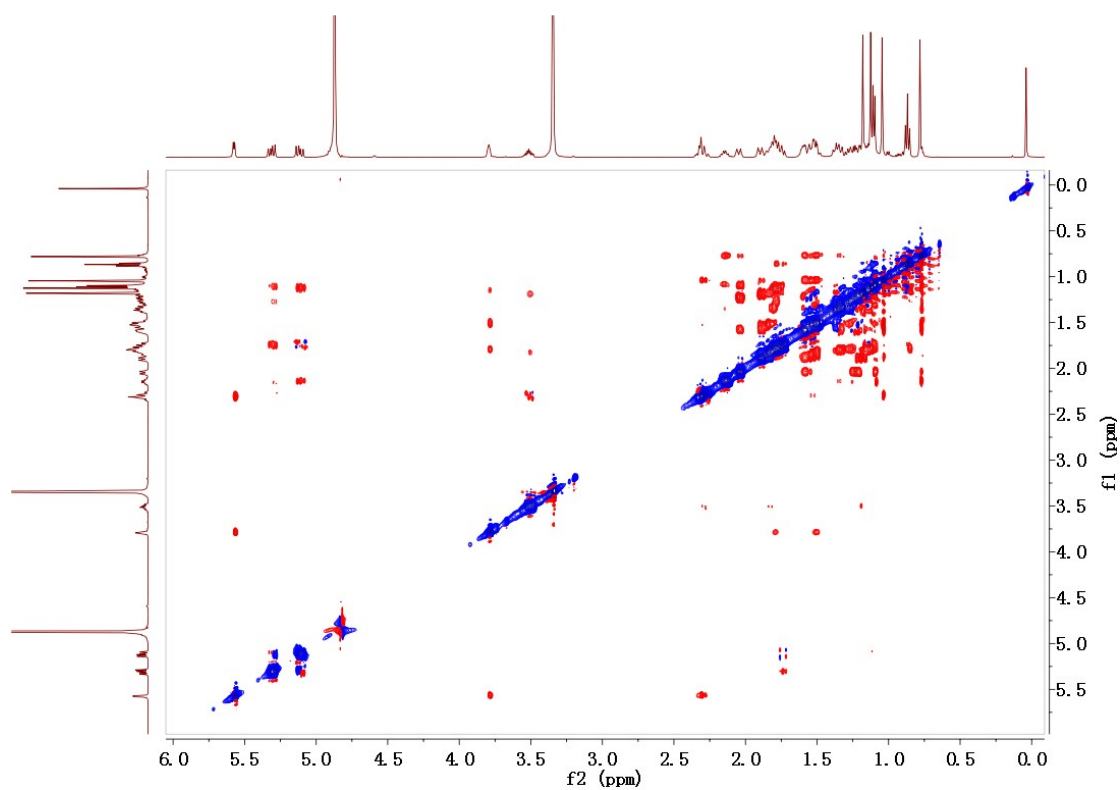
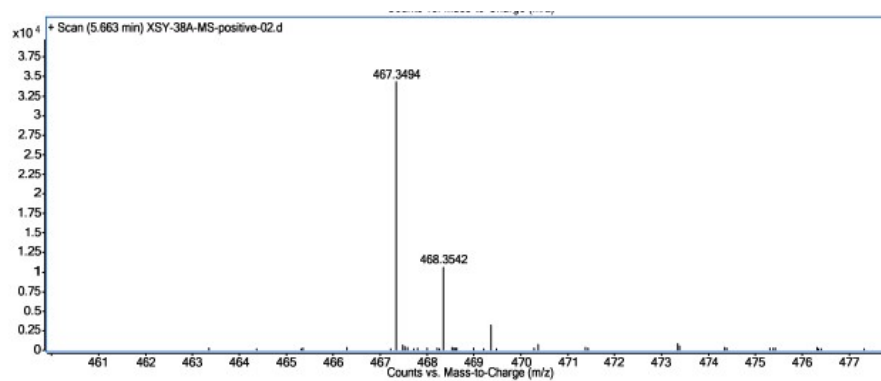


Figure S13. ROESY spectrum of chisopanoid B (2)



#### Elemental Composition Calculator

| Target m/z:                                      | 467.3494                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>28</sub> NaO <sub>3</sub> | 467.3496                                         |              | 0.32          |          |                     |

Figure S14. HRESIMS spectrum of chisopanoid B (2)

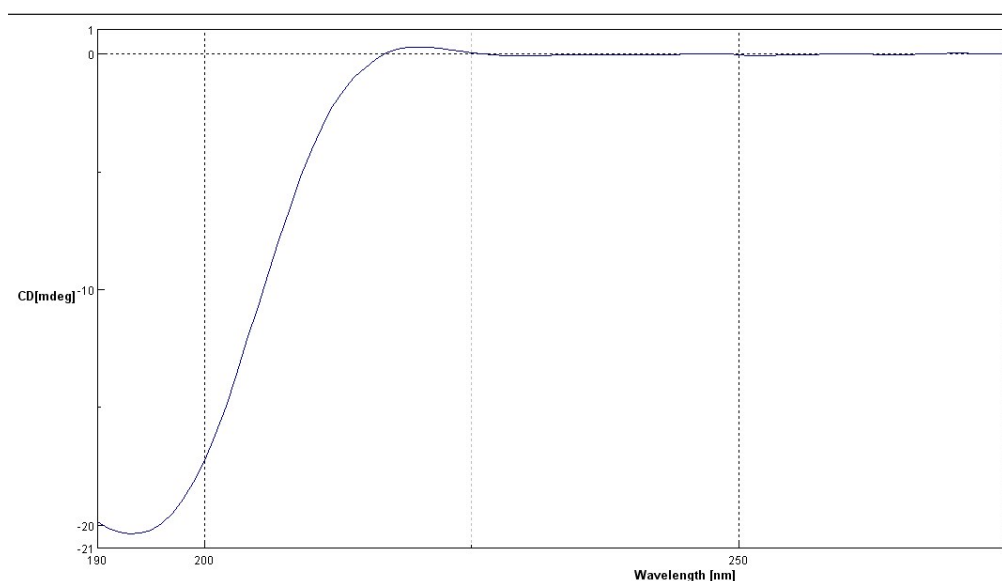


Figure S15. ECD spectra of chisopanoid B (**2**) (in MeCN).

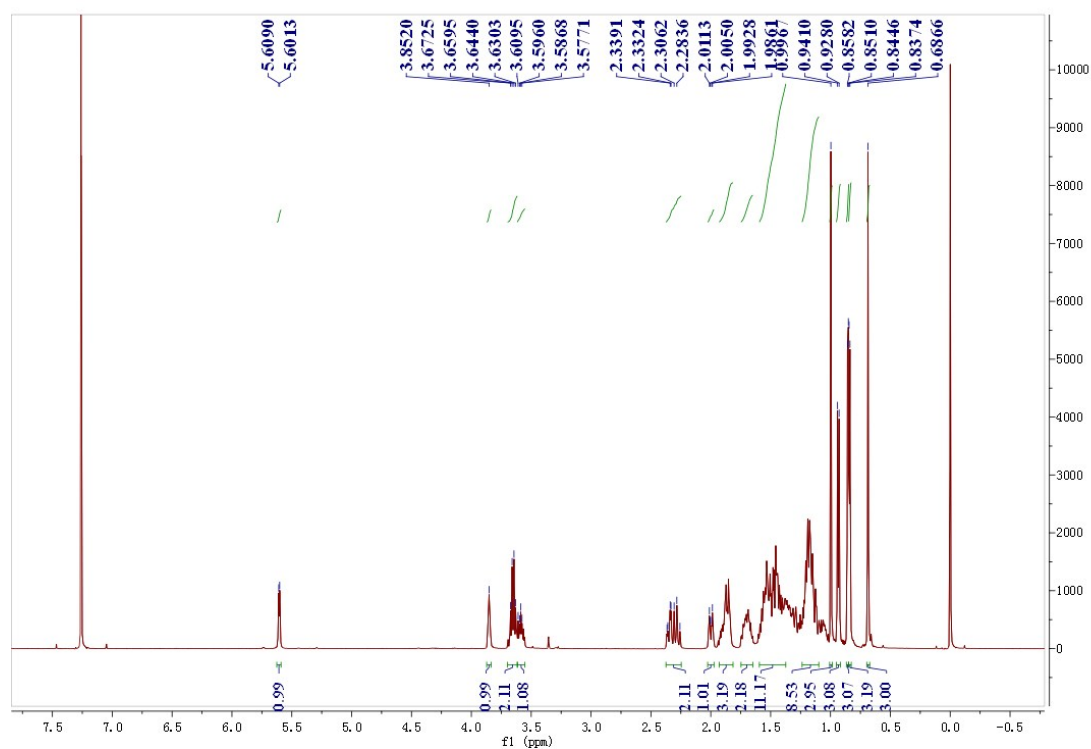


Figure S16.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of chisopanoid C (**3**)

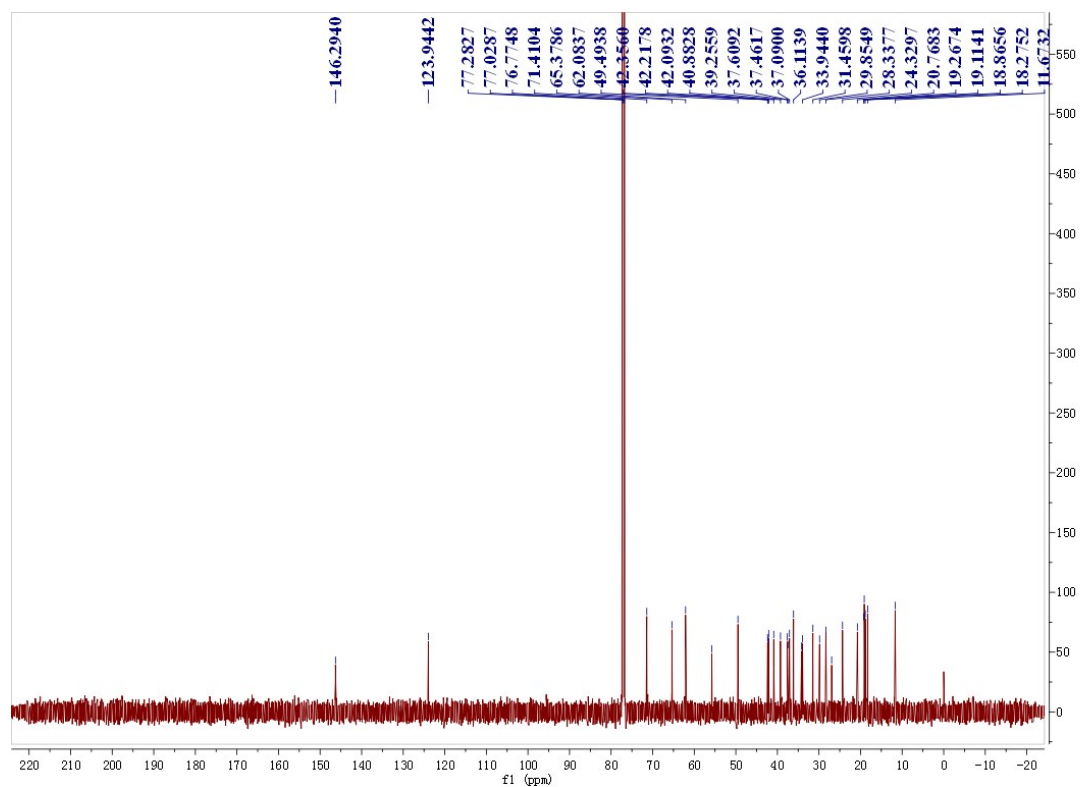


Figure S17.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of chisopanoid C (**3**)

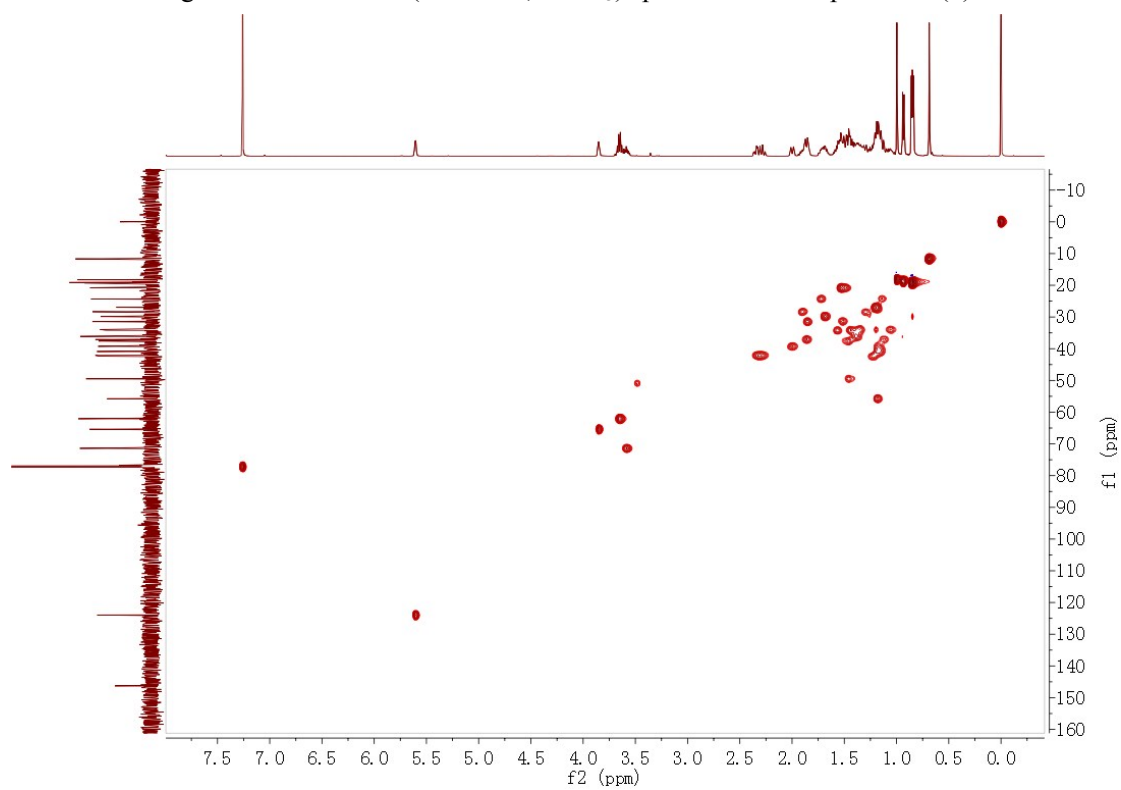


Figure S18. HSQC spectrum of chisopanoid C (**3**)

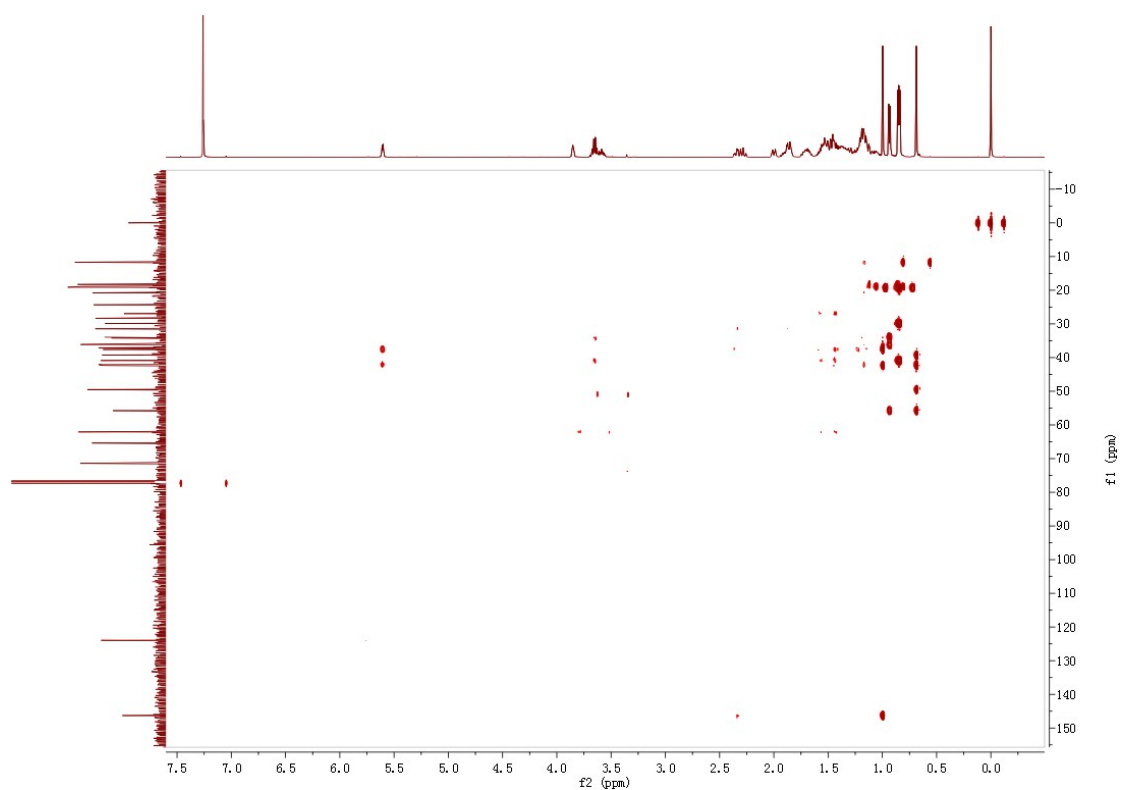


Figure S19. HMBC spectrum of chisopanoid C (**3**)

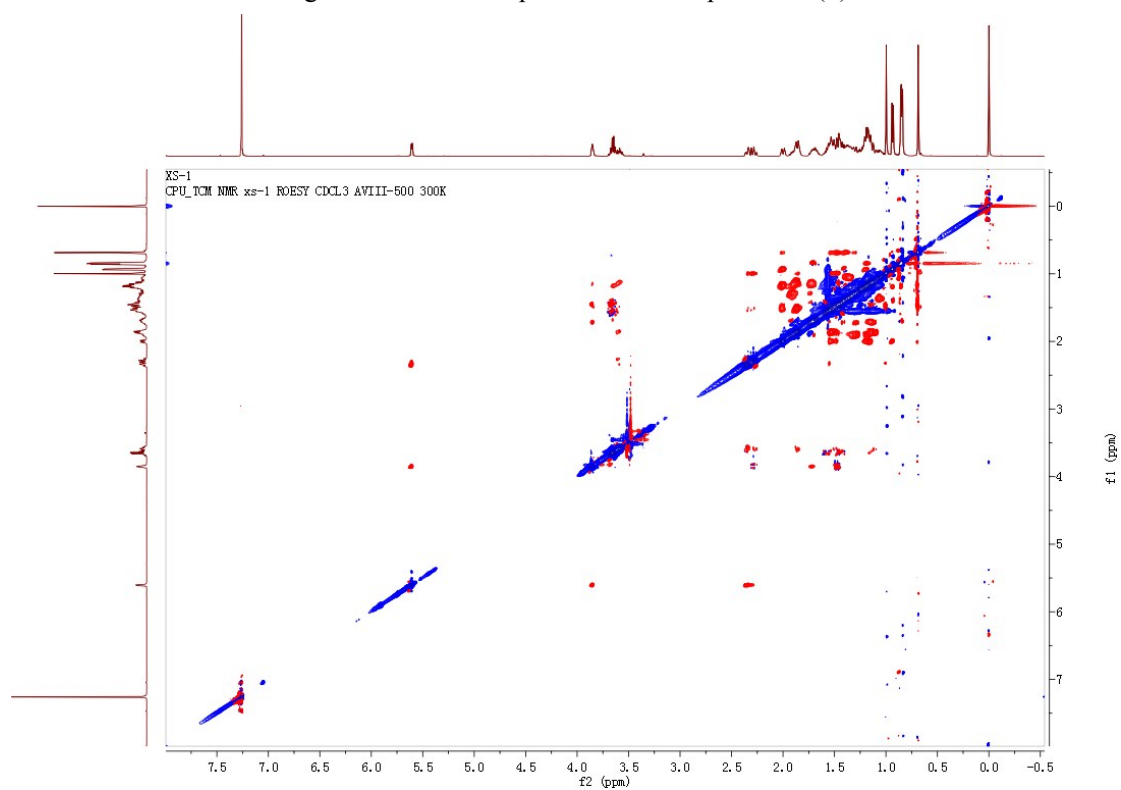
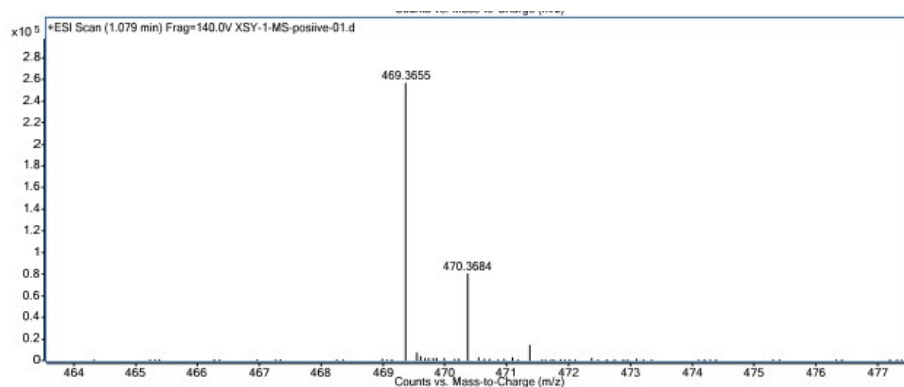


Figure S20. ROESY spectrum of chisopanoid C (**3**)



#### Elemental Composition Calculator

| Target m/z:                                      | 469.3655                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>50</sub> NaO <sub>3</sub> | 469.3652                                         |              | -0.64         |          |                     |

Figure S21. HRESIMS spectrum of chisopanoid C (**3**)

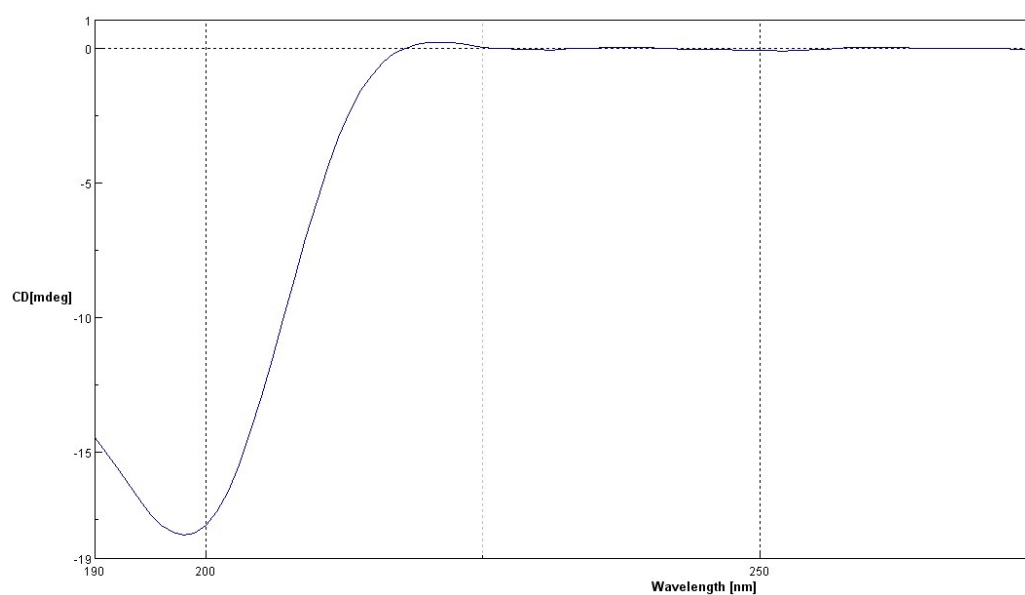


Figure S22. ECD spectra of chisopanoid C (**3**) (in MeCN).

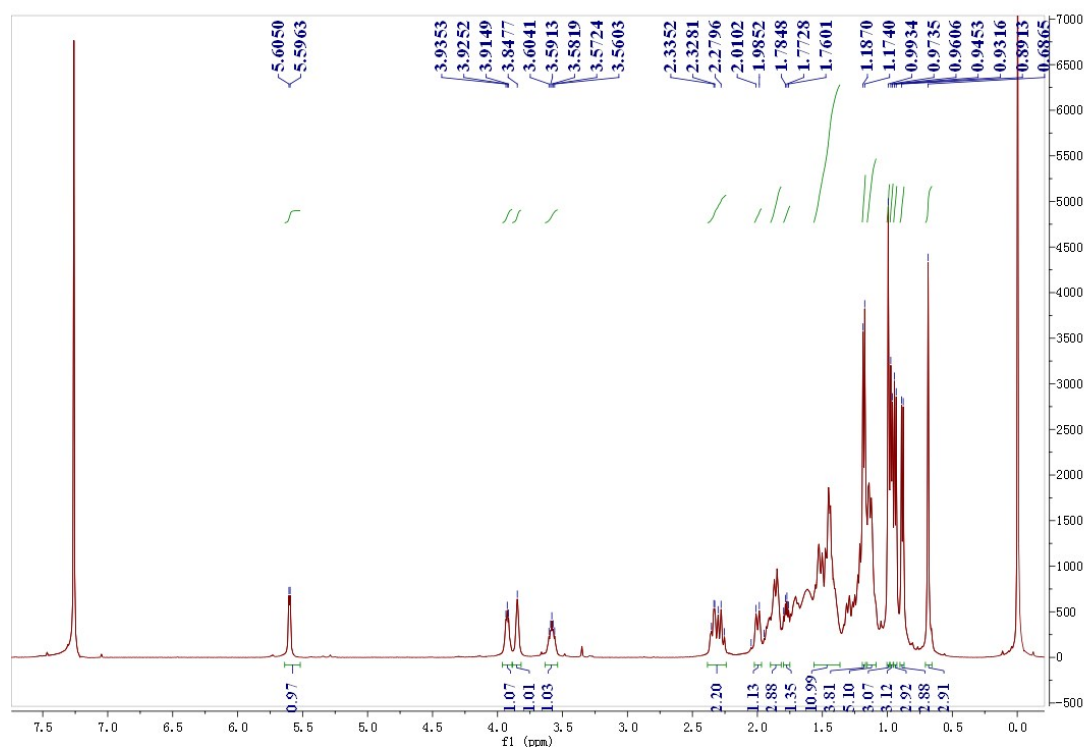


Figure S23.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of chisopanoid D (4)

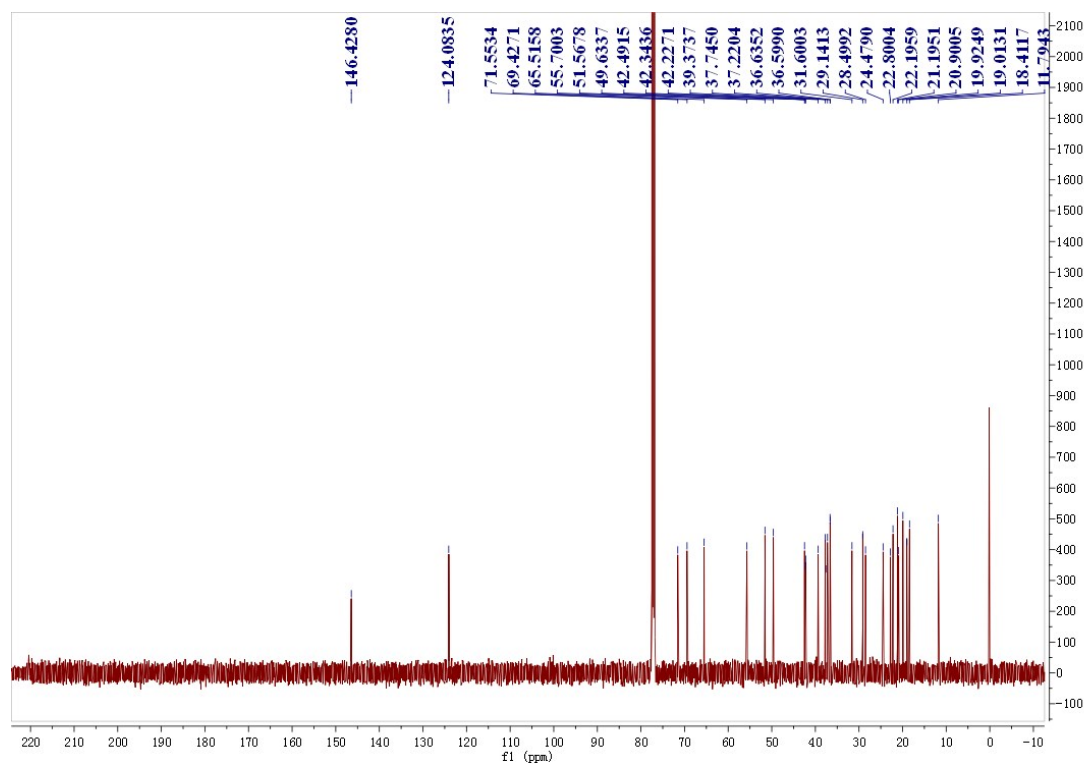


Figure S24.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of chisopanoid D (4)

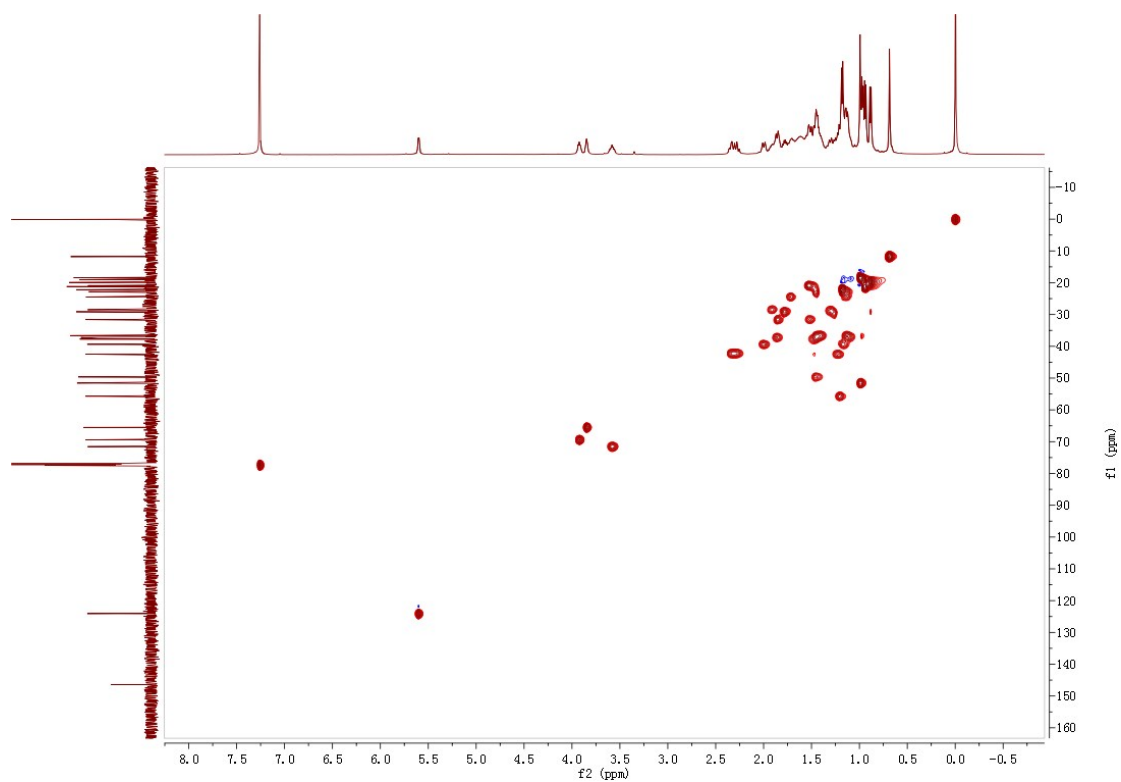


Figure S25. HSQC spectrum of chisopanoid D (4)

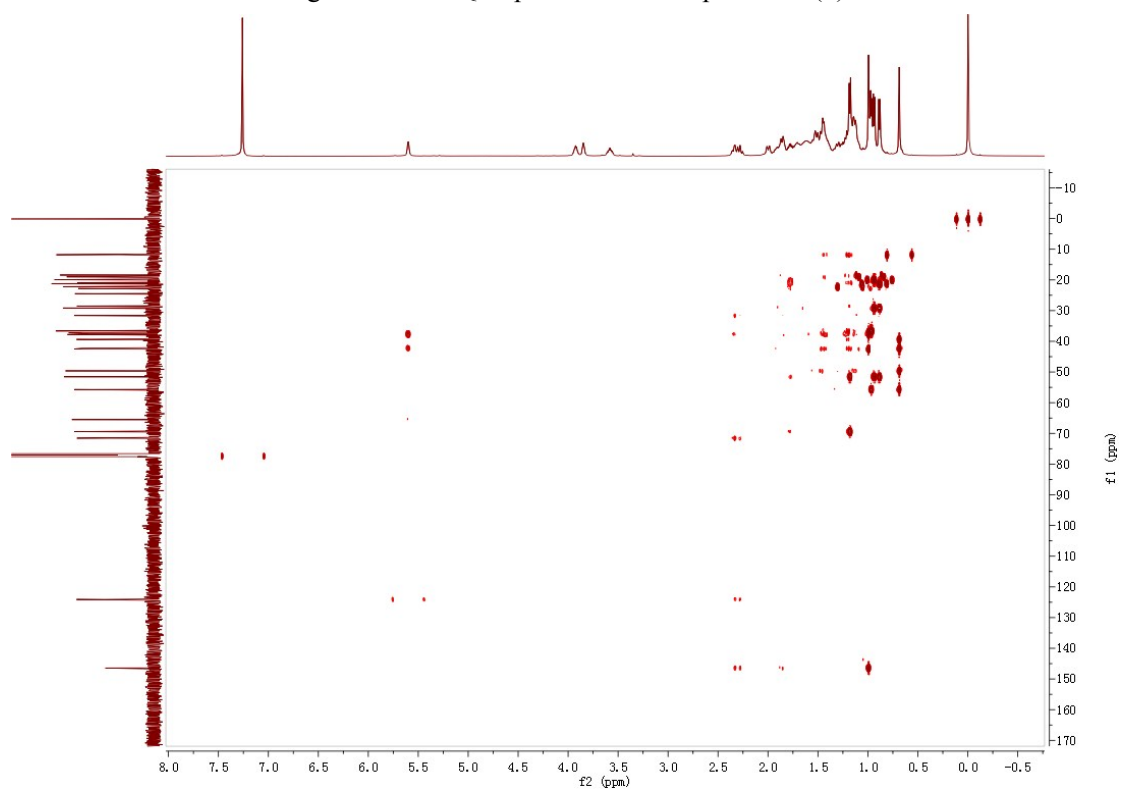


Figure S26. HMBC spectrum of chisopanoid D (4)



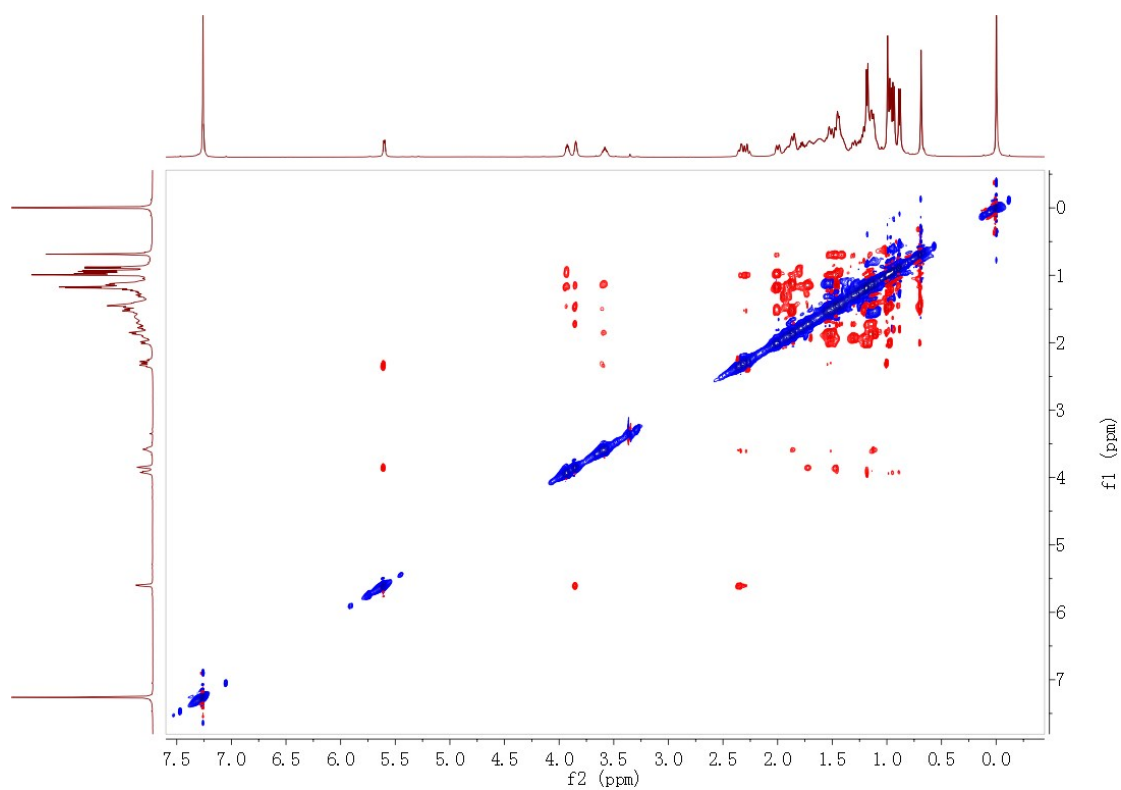
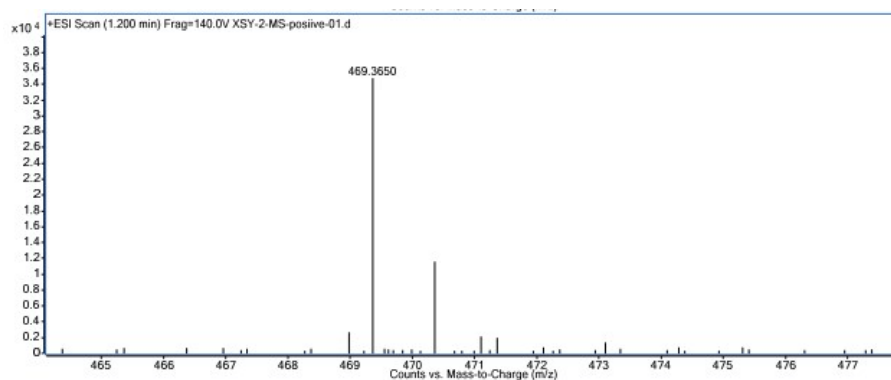


Figure S27. ROESY spectrum of chisopanoid D (4)



#### Elemental Composition Calculator

| Target m/z:                                      | 469.365                                          | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>50</sub> NaO <sub>3</sub> | 469.3652                                         |              | 0.49          |          |                     |

Figure S28. HRESIMS spectrum of chisopanoid D (4)

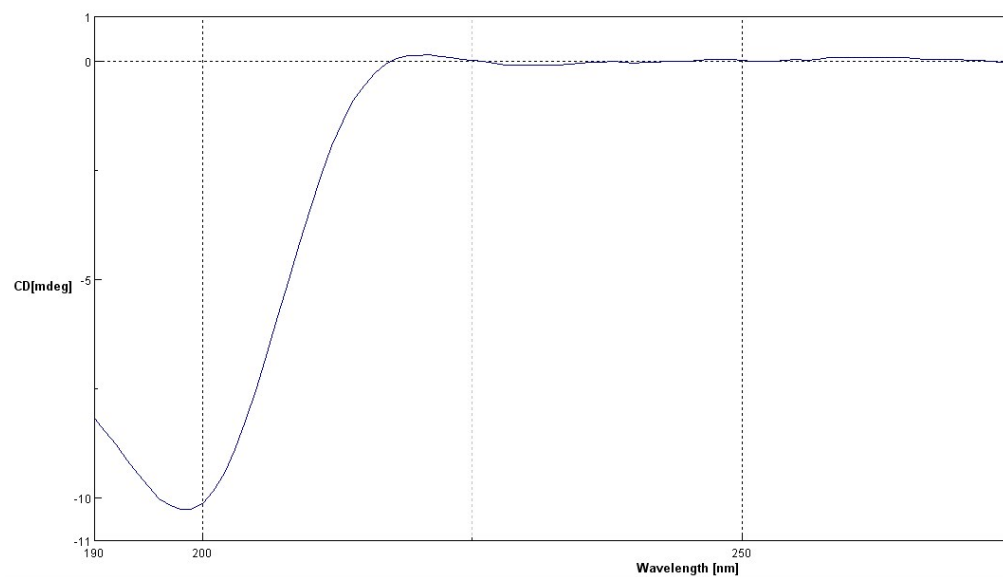


Figure S29. ECD spectra of chisopanoid D (4) (in MeCN).

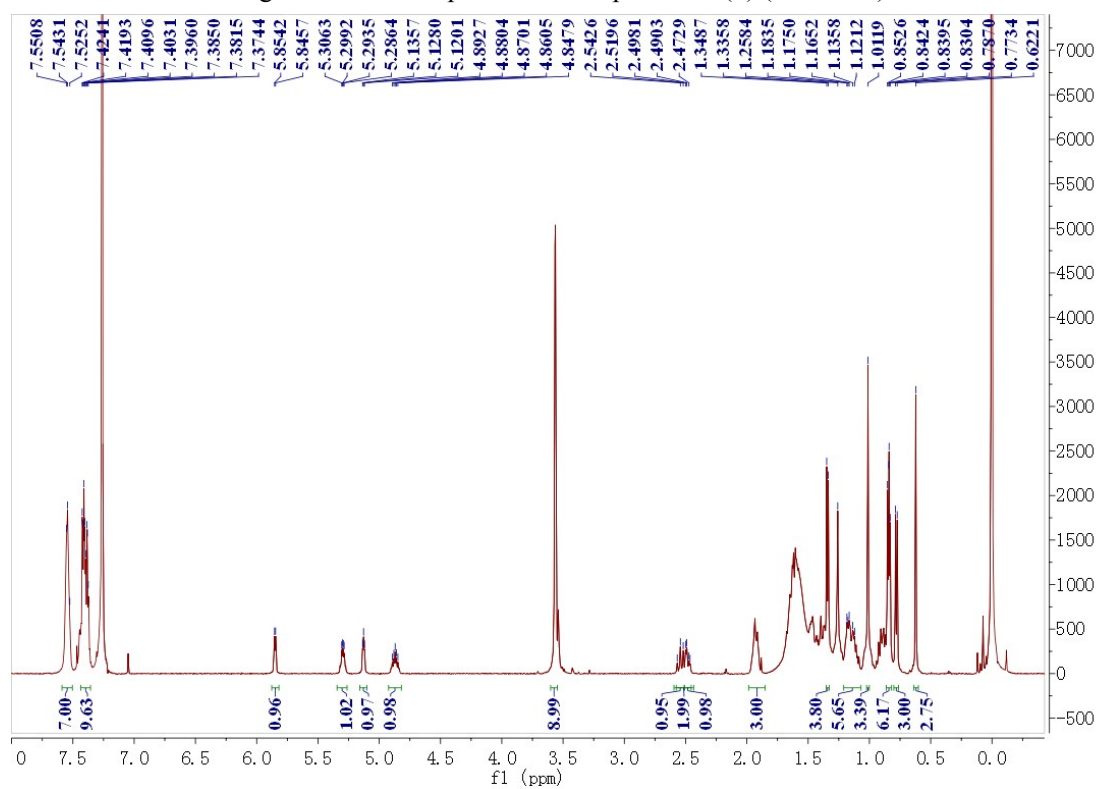


Figure S30.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of 4a

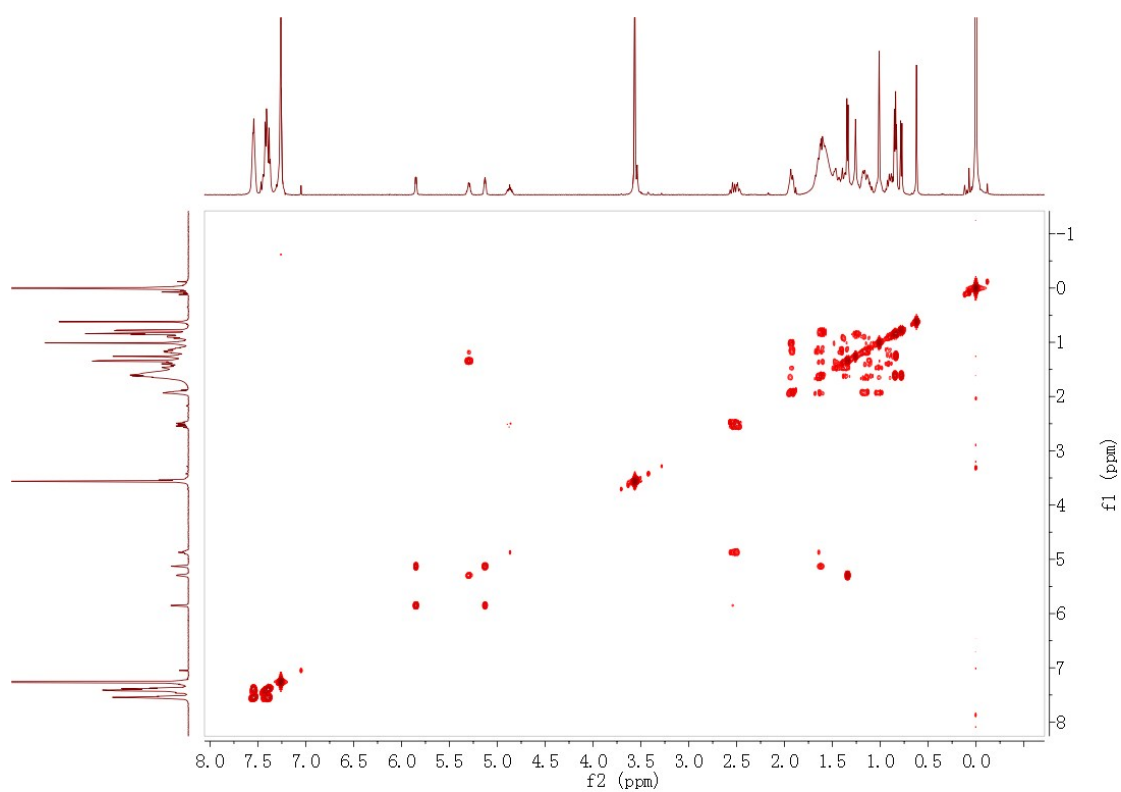


Figure S31.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4a**

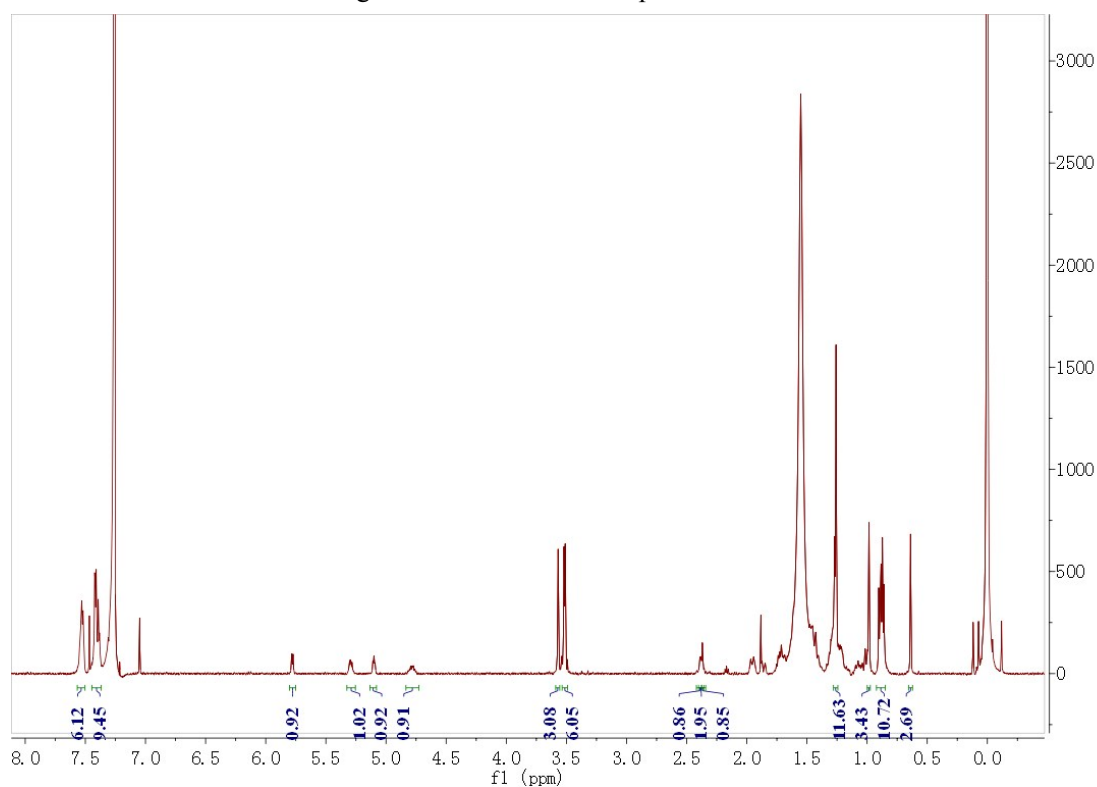


Figure S32.  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of **4b**

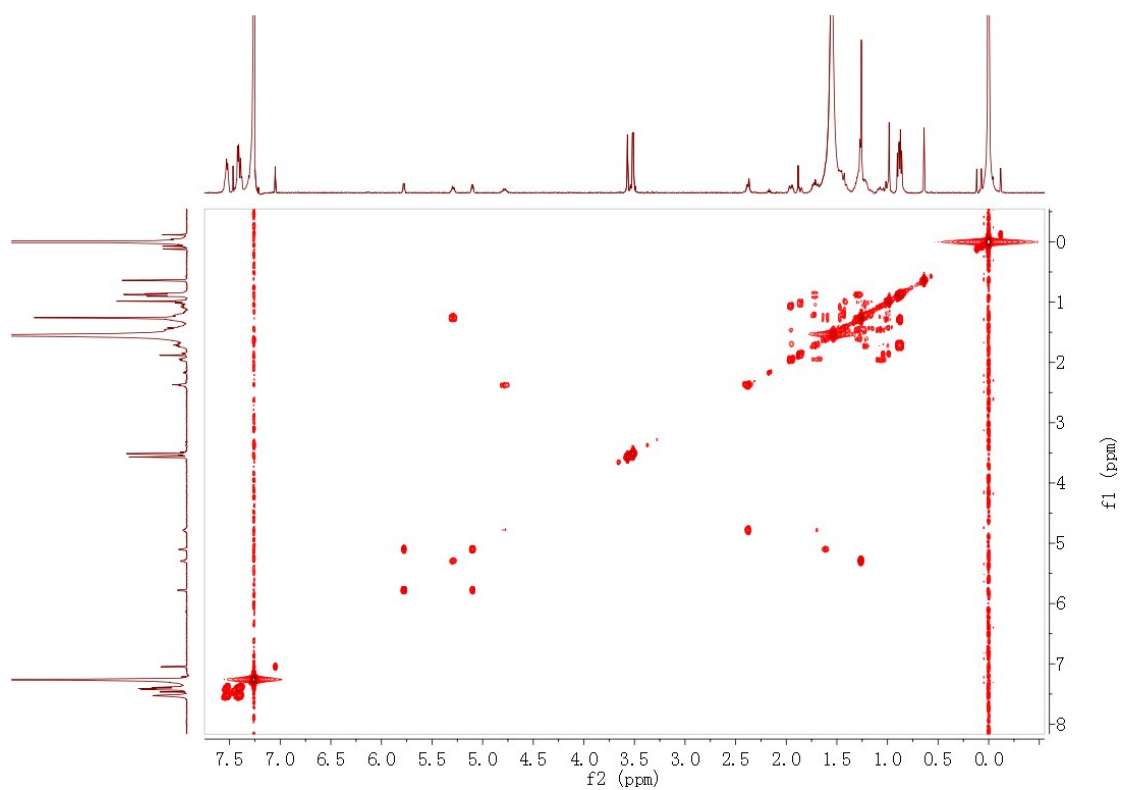


Figure S33.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4b**

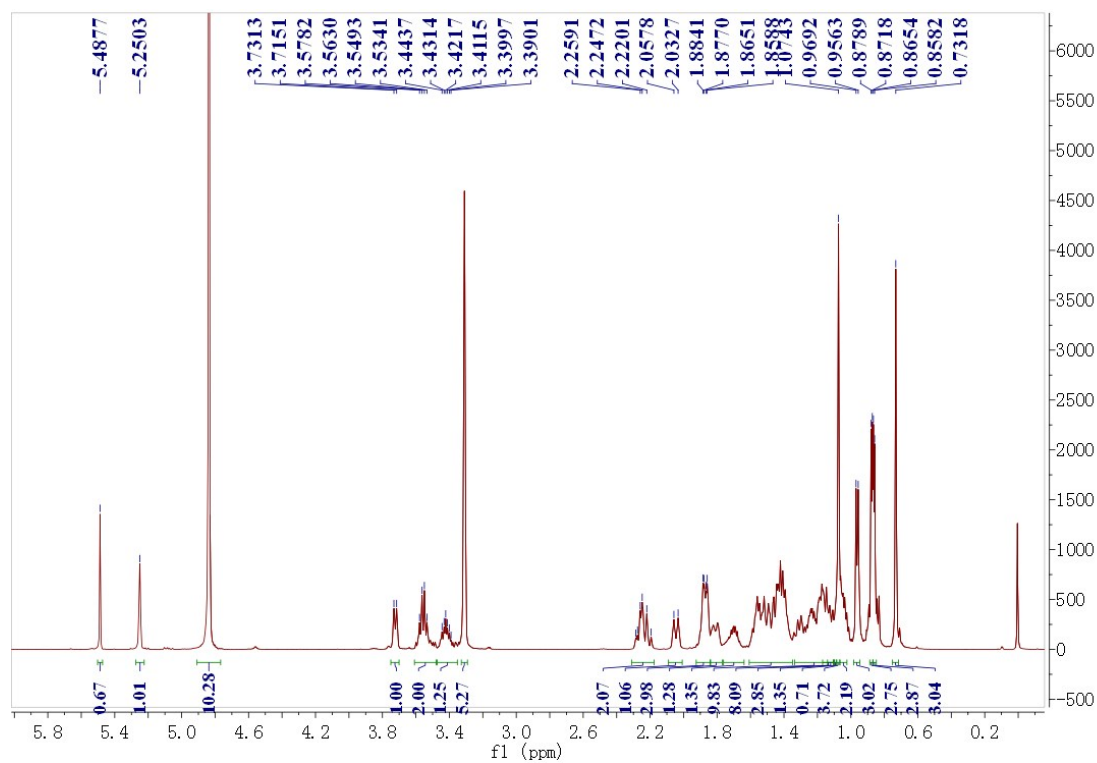


Figure S34.  $^1\text{H}$  NMR (500 MHz, methanol- $d_4$ ) spectrum of chisopanoid E (**5**)

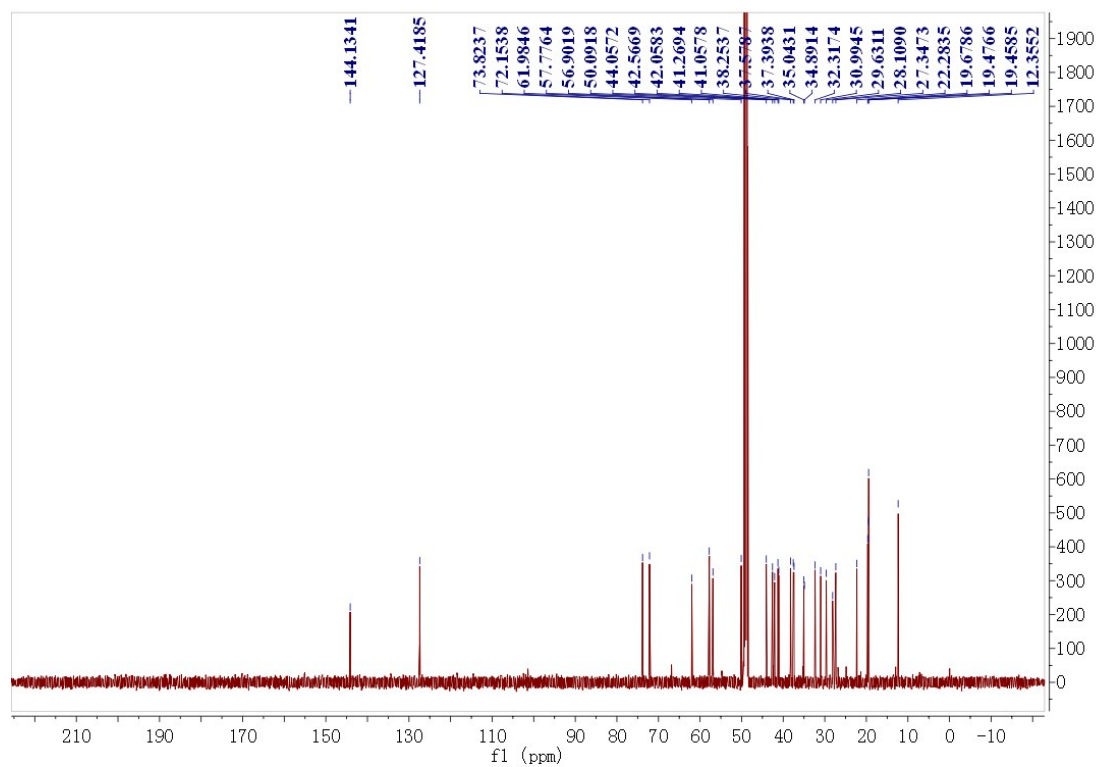


Figure S35.  $^{13}\text{C}$  NMR (125 MHz, methanol- $d_4$ ) spectrum of chisopanoid E (5)

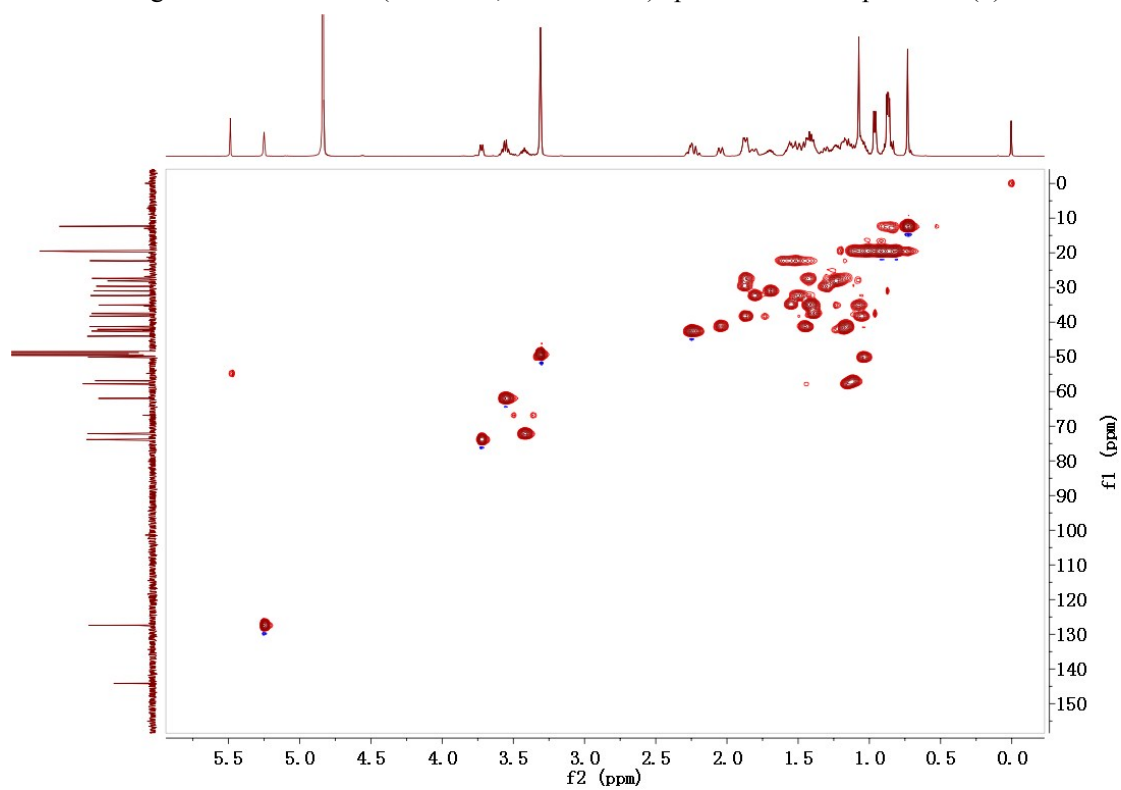


Figure S36. HSQC spectrum of chisopanoid E (5)

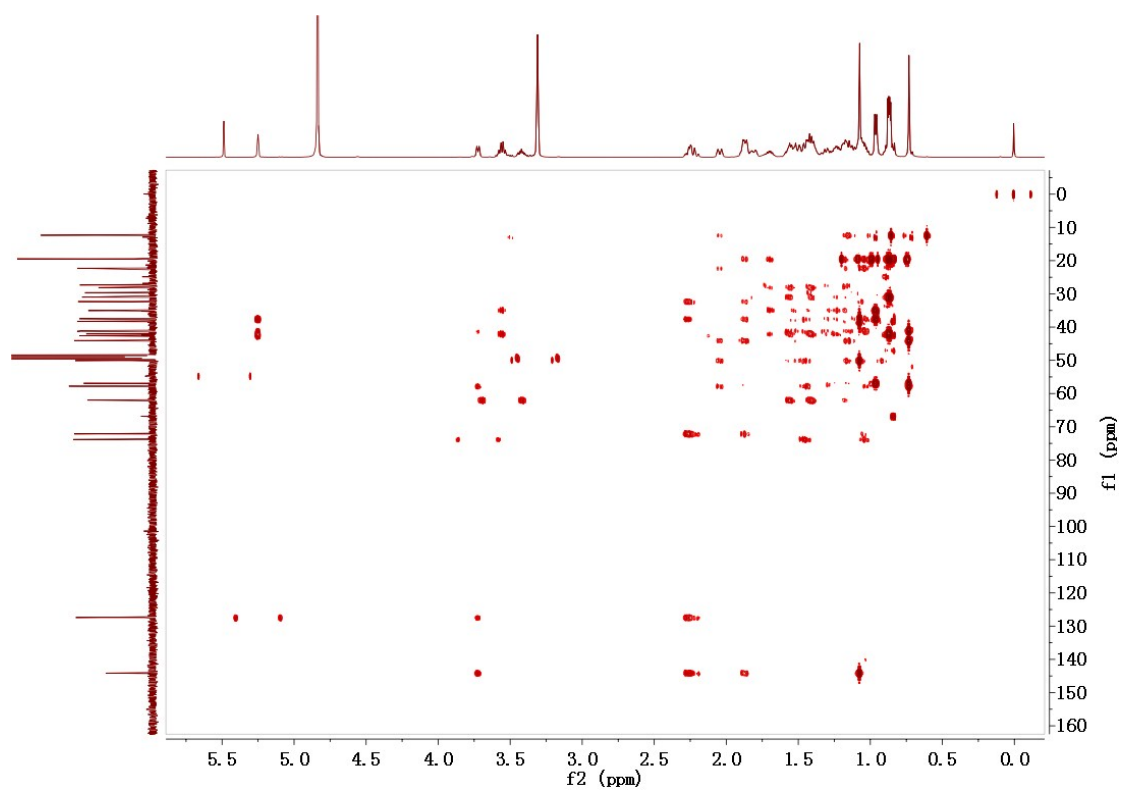


Figure S37. HMBC spectrum of chisopanoid E (**5**)

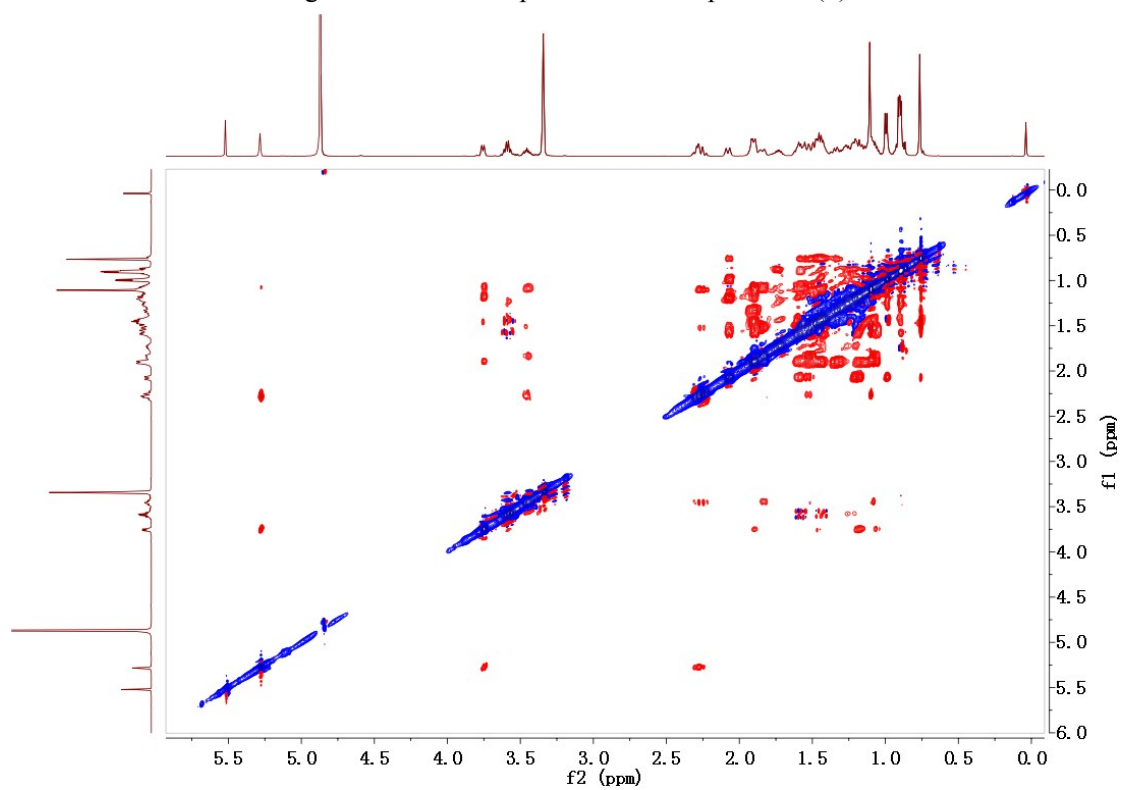
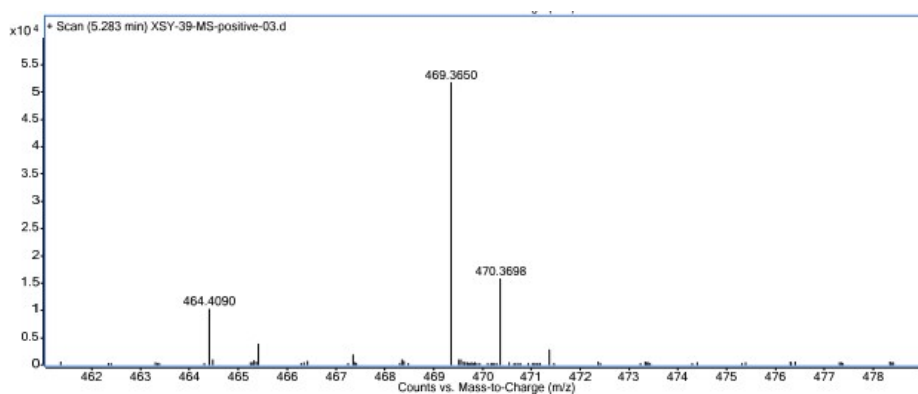


Figure S38. ROESY spectrum of chisopanoid E (**5**)



### Elemental Composition Calculator

| Target m/z:                                      | 469.365                                          | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>30</sub> NaO <sub>3</sub> | 469.3652                                         |              | 0.38          |          |                     |

Figure S39. HRESIMS spectrum of chisopanoid E (5)

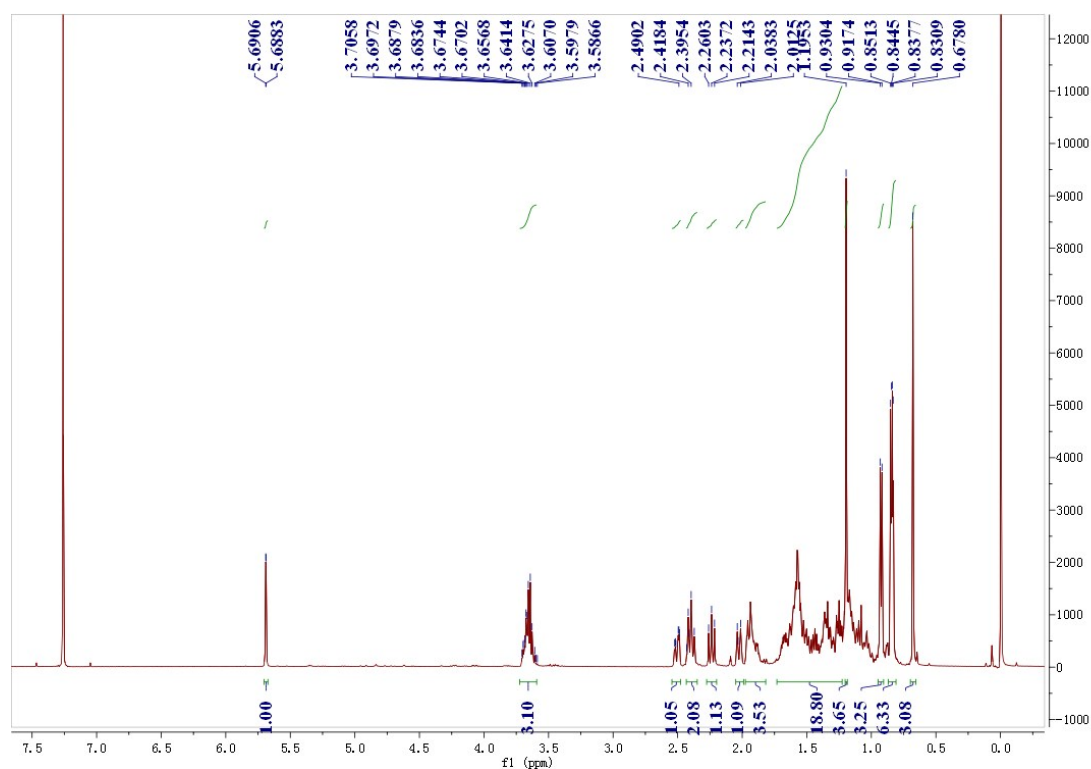


Figure S40. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of chisopanoid F (6)

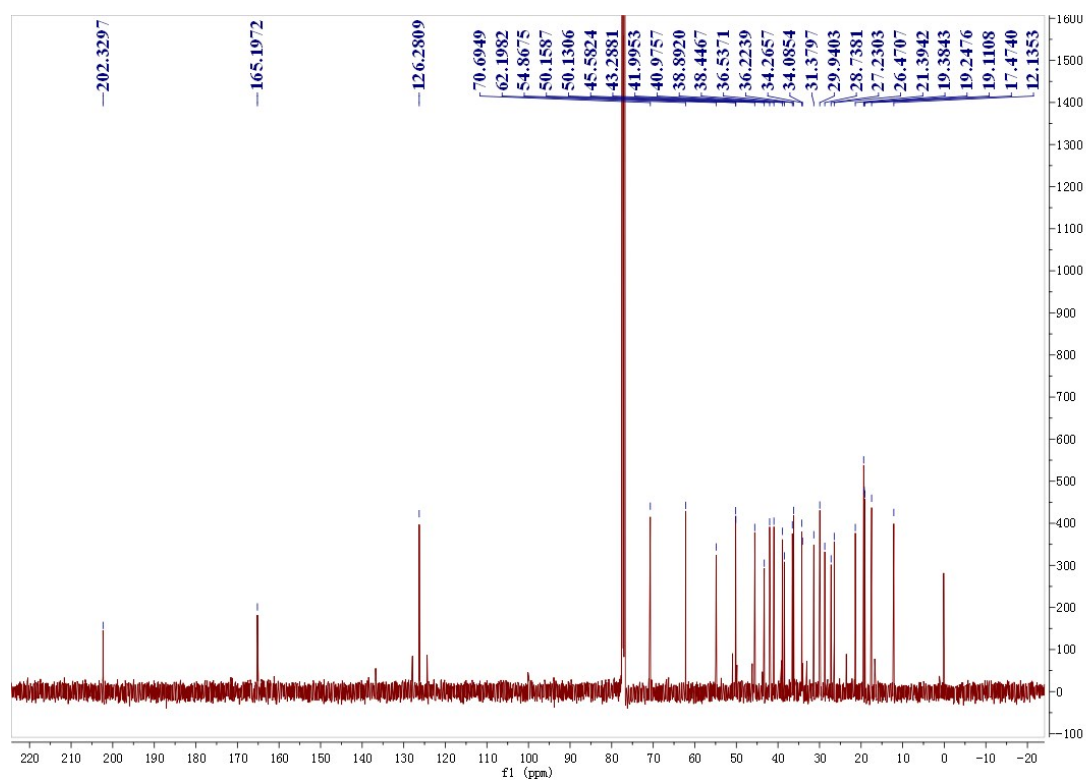


Figure S41.  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of chisopanoid F (6)

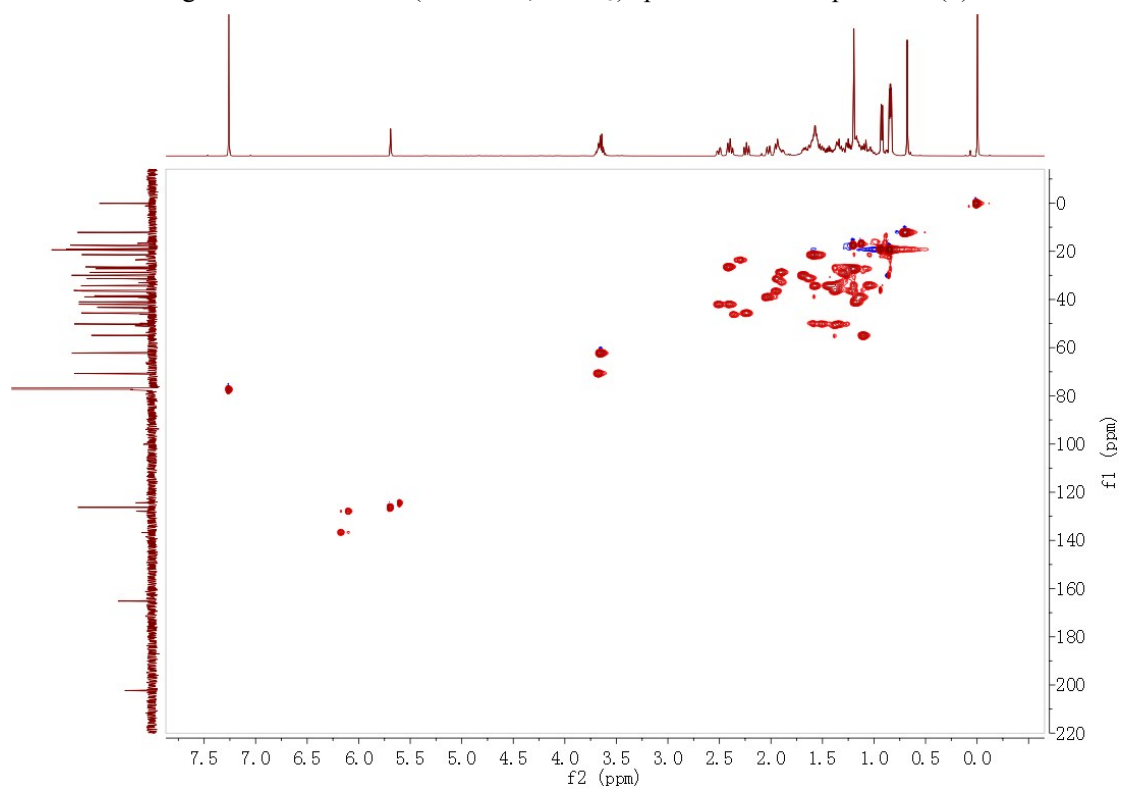


Figure S42. HSQC spectrum of chisopanoid F (6)



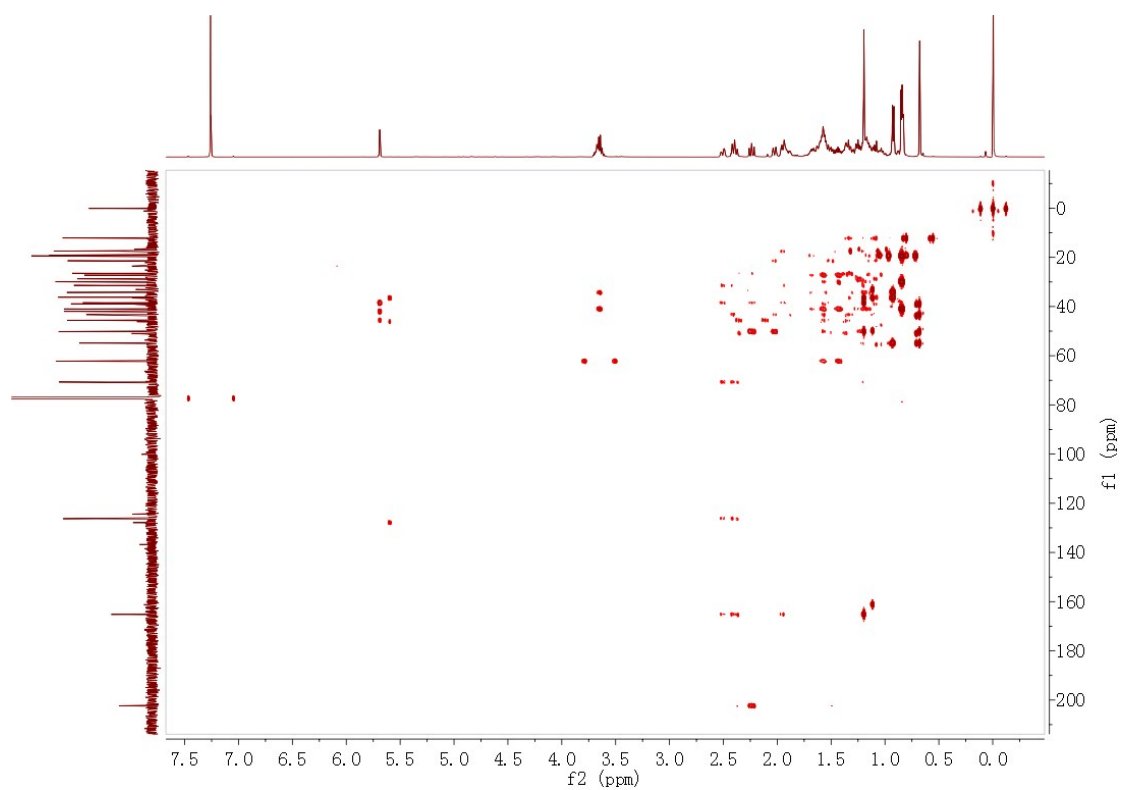


Figure S43. HMBC spectrum of chisopanoid F (6)

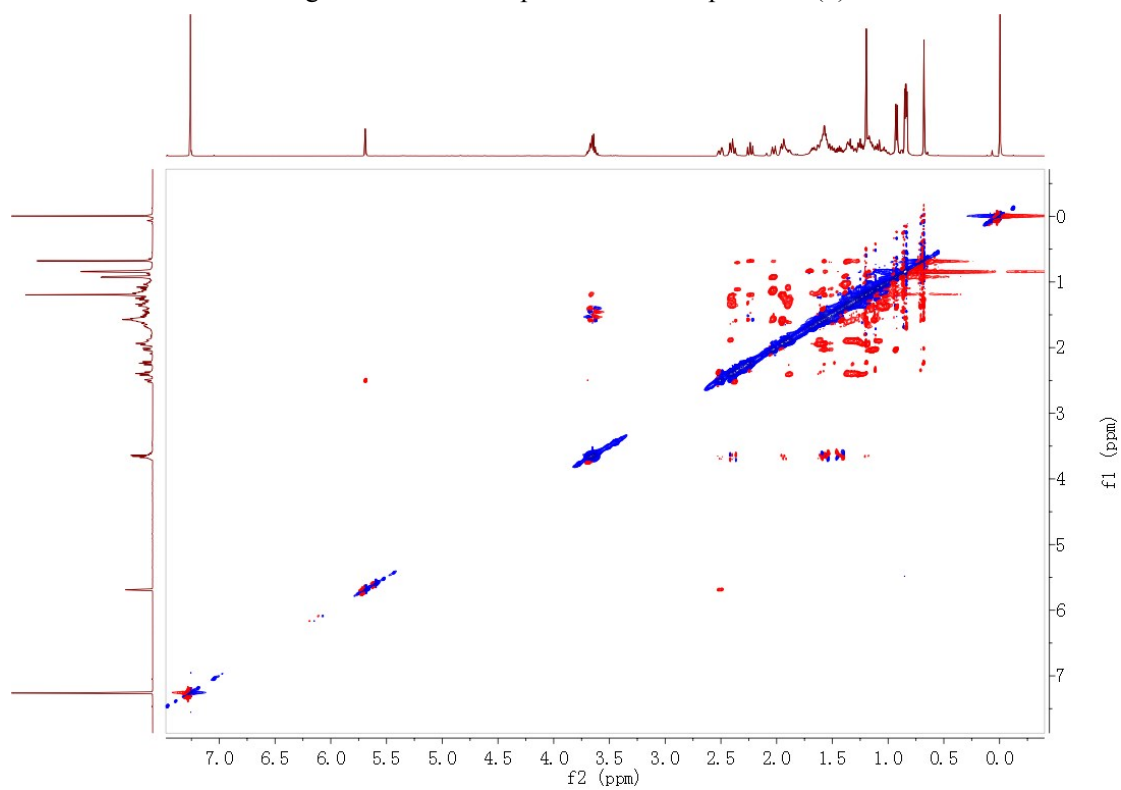
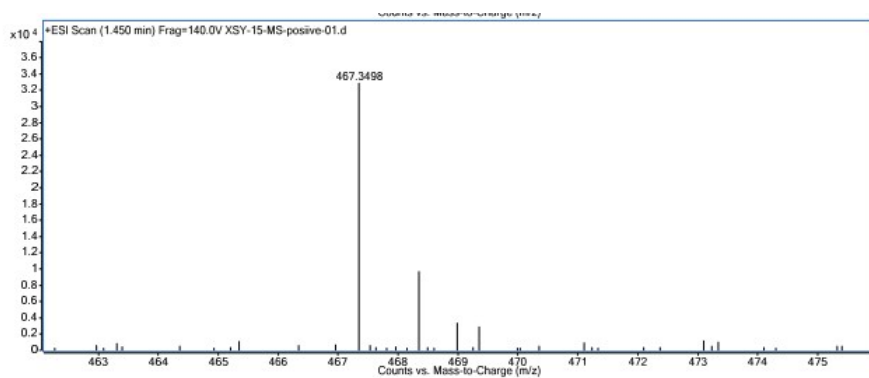


Figure S44. ROESY spectrum of chisopanoid F (6)



#### Elemental Composition Calculator

| Target m/z:                                      | 467.3498                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>48</sub> NaO <sub>3</sub> | 467.3496                                         |              | -0.54         |          |                     |

Figure S45. HRESIMS spectrum of Chisopanoid F (6)

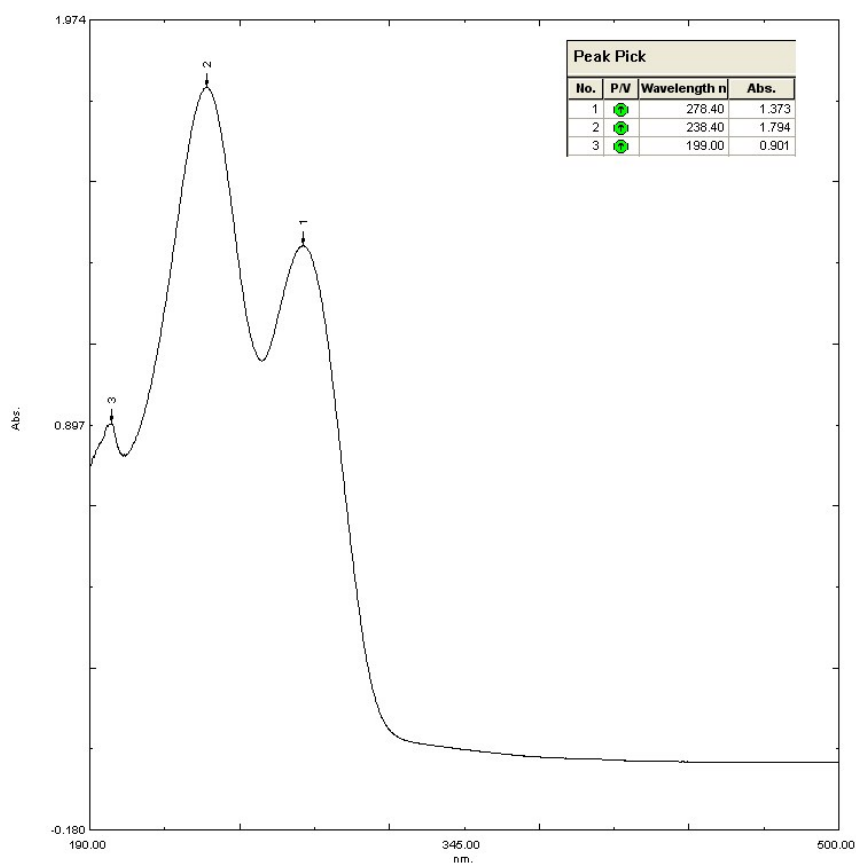


Figure S46. UV spectrum of chisopanoid F (6) in CH<sub>3</sub>OH

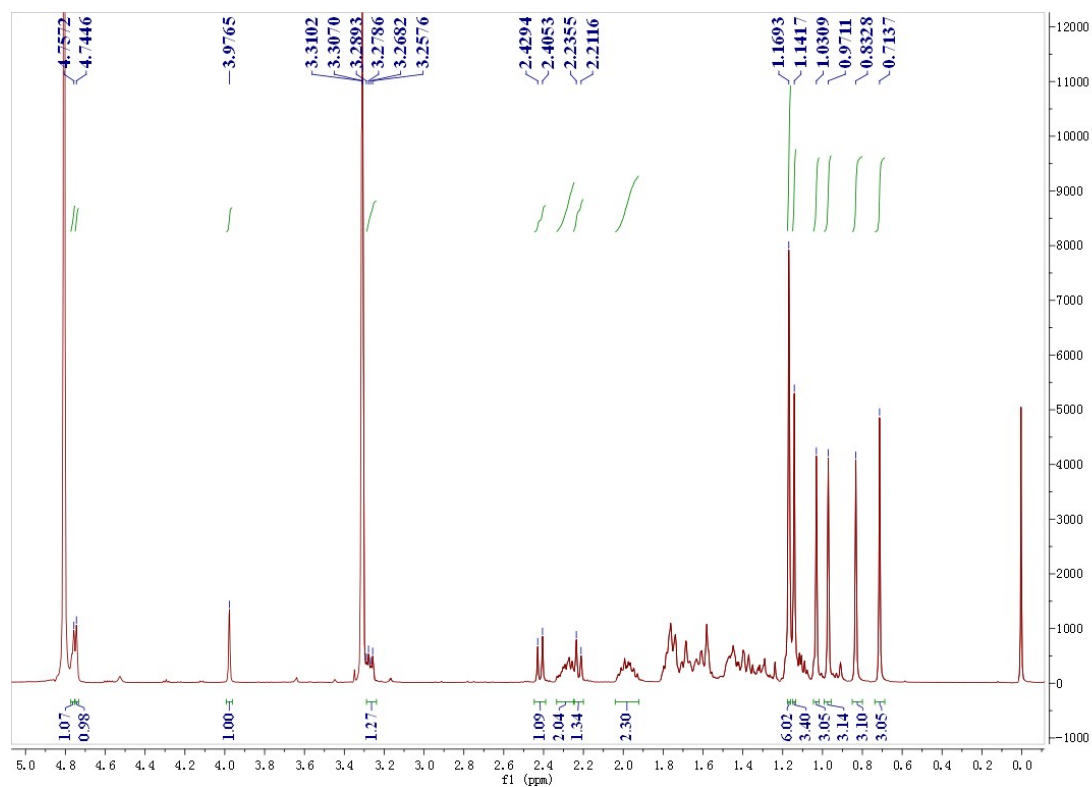


Figure S47. <sup>1</sup>H NMR (500 MHz, methanol-*d*<sub>4</sub>) spectrum of chisopanone G (7)

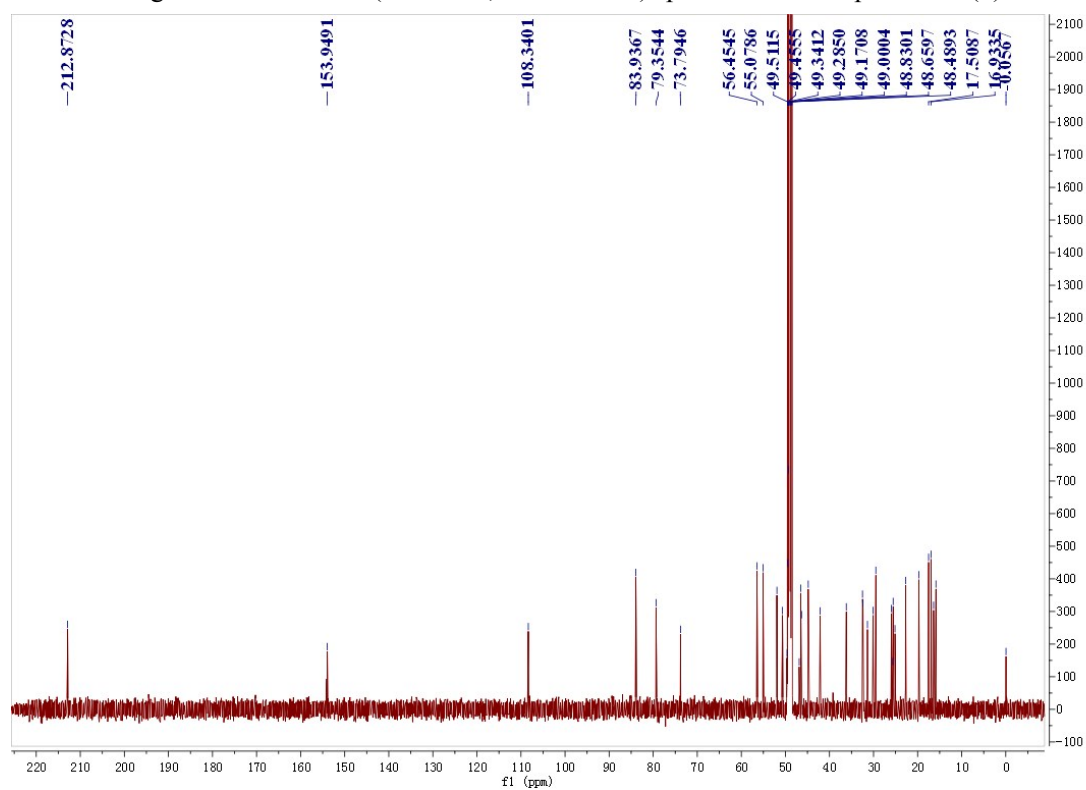


Figure S48. <sup>13</sup>C NMR (125 MHz, methanol-*d*<sub>4</sub>) spectrum of chisopanone G (7)

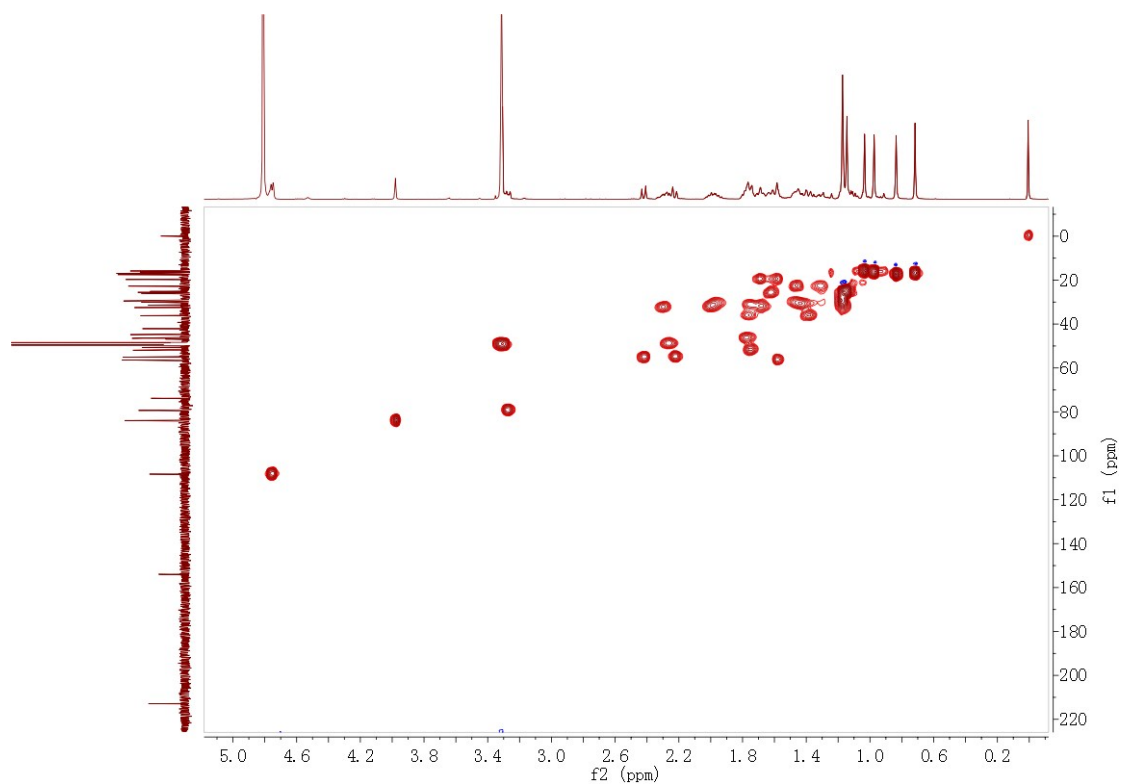


Figure S49. HSQC spectrum of chisopanone G (7)

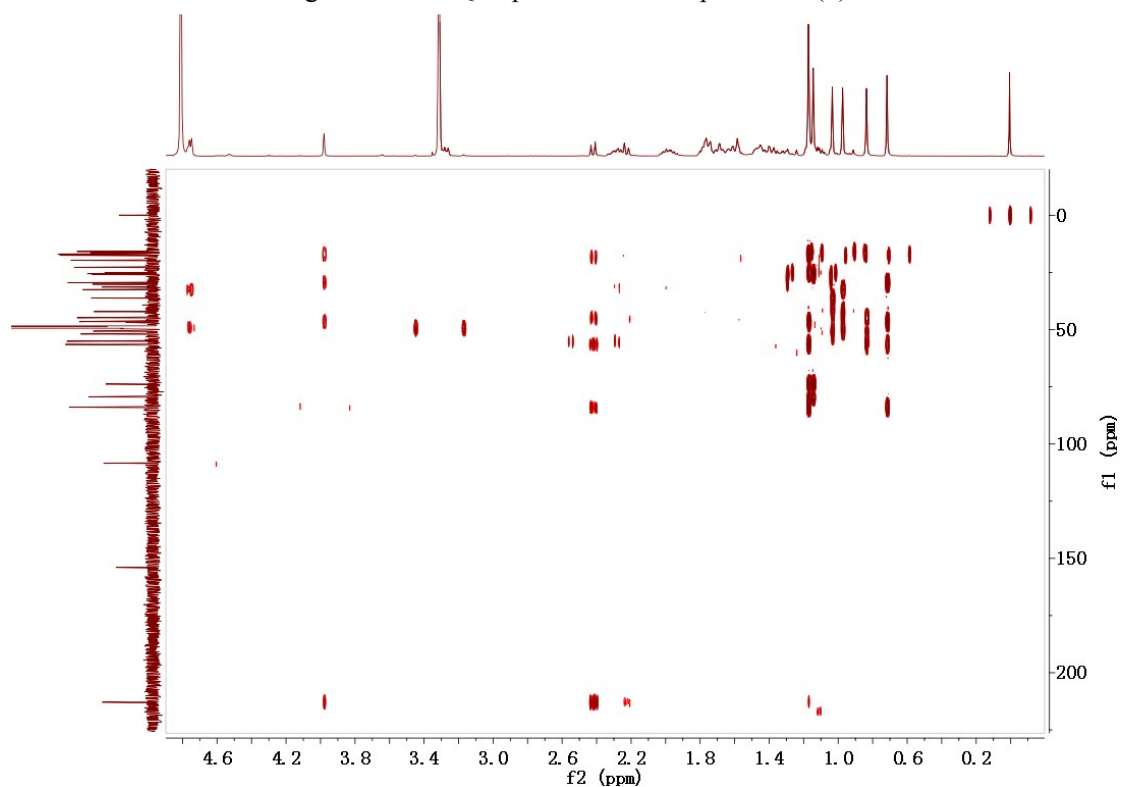


Figure S50. HMBC spectrum of chisopanone G (7)

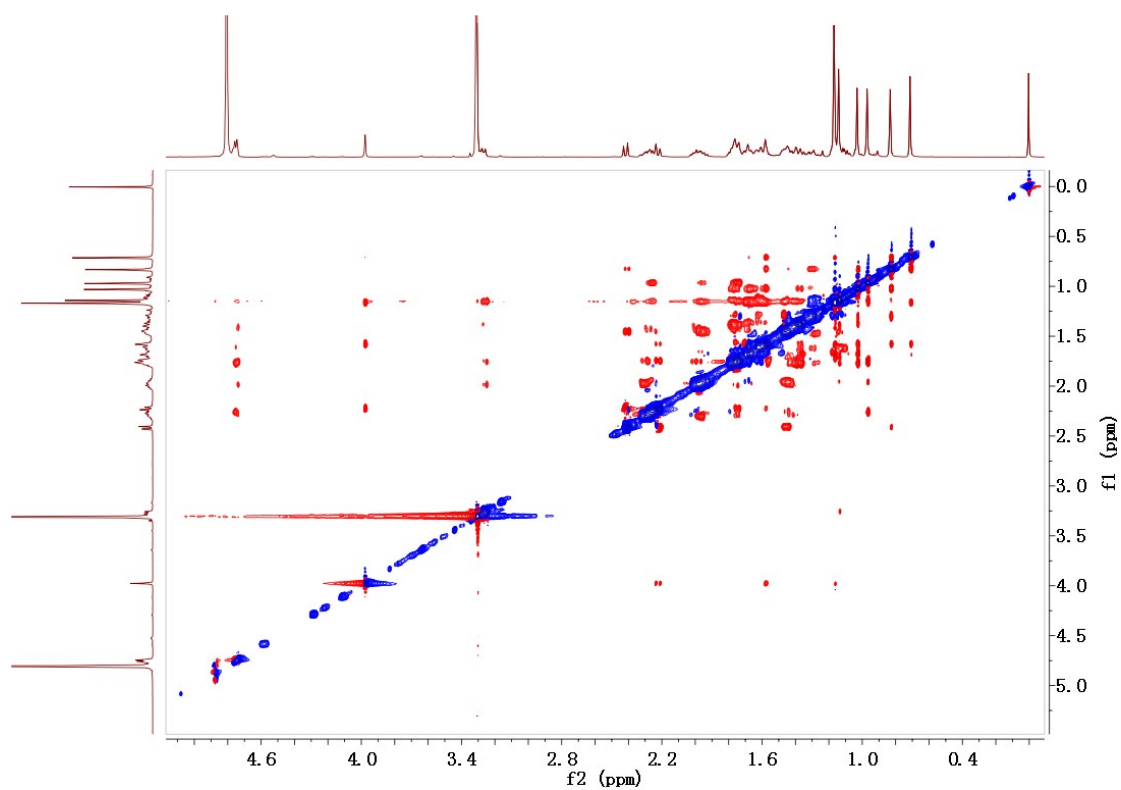
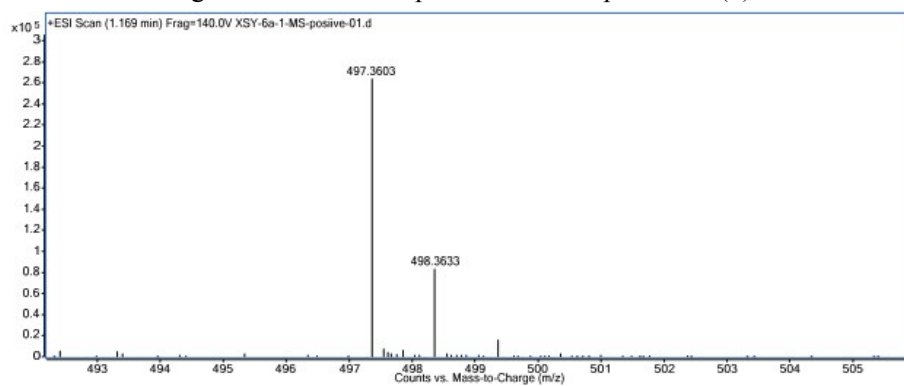


Figure S51. ROESY spectrum of chisopanone G (7)



#### Elemental Composition Calculator

| Target m/z: | 497.3603                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|-------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:   | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula | Calculated m/z                                   |              | PPM Error     |          |                     |
| C30H50NaO4  | 497.3601                                         |              | -0.43         |          |                     |

Figure S52. HRESIMS spectrum of chisopanone G (7)

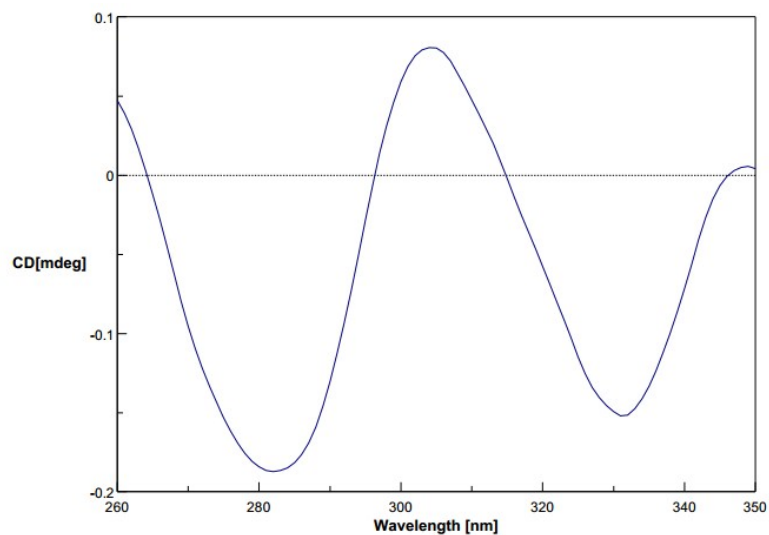


Figure S53. ECD spectrum of chisopanone G (7) in DMSO containing Mo<sub>2</sub>(OAc)<sub>4</sub> with the inherent ECD spectrum subtracted.

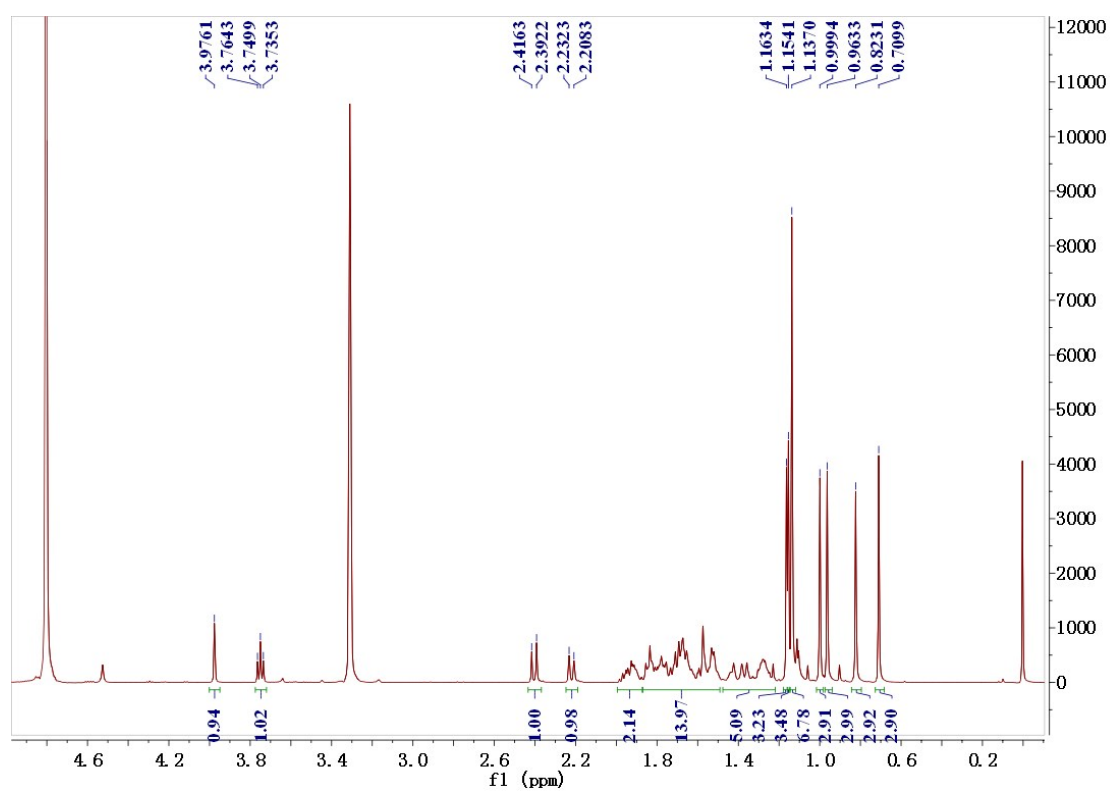


Figure S54. <sup>1</sup>H NMR (500 MHz, methanol-*d*<sub>4</sub>) spectrum of chisopanone H (8)

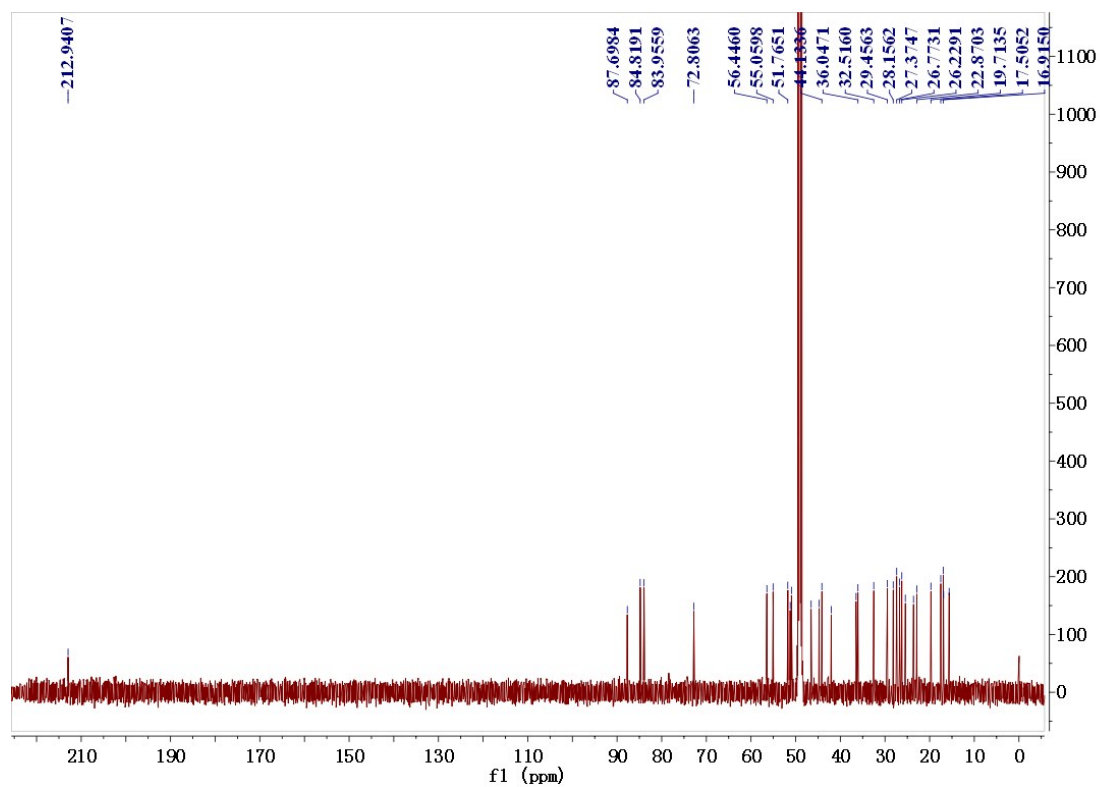


Figure S55.  $^{13}\text{C}$  NMR (125 MHz, methanol- $d_4$ ) spectrum of chisopanone H (**8**)

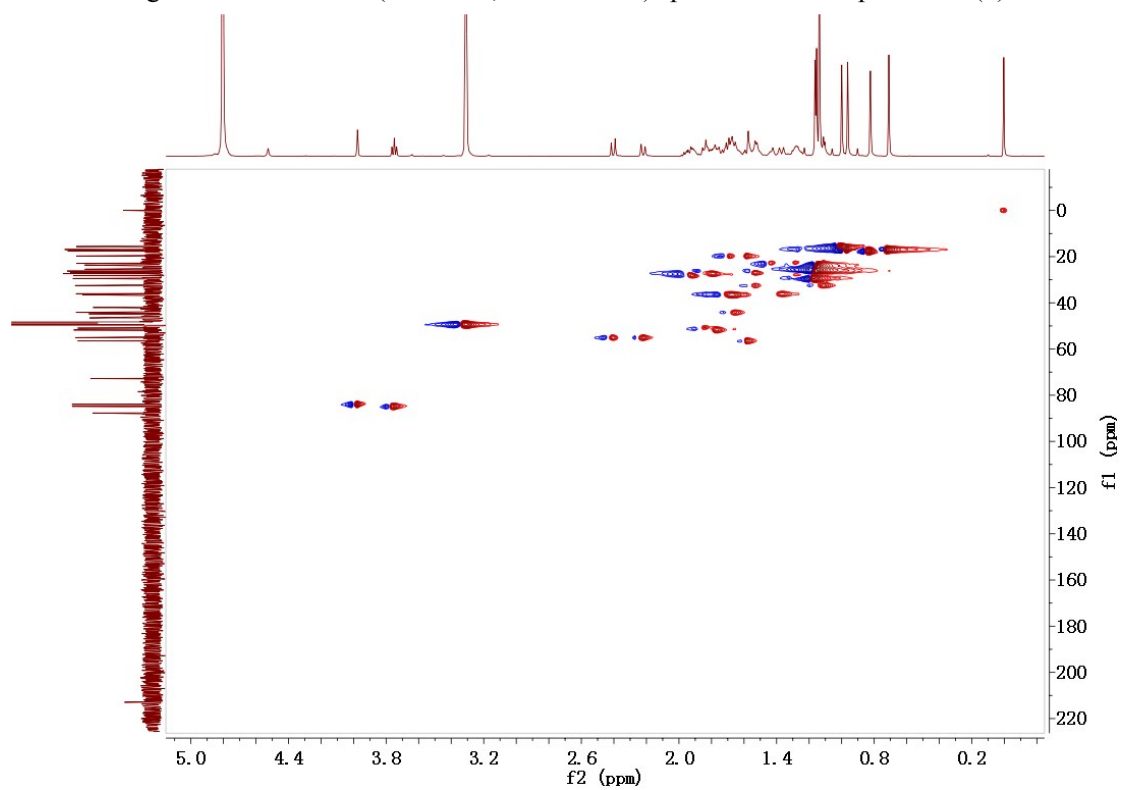


Figure S56. HSQC spectrum of chisopanone H (**8**)

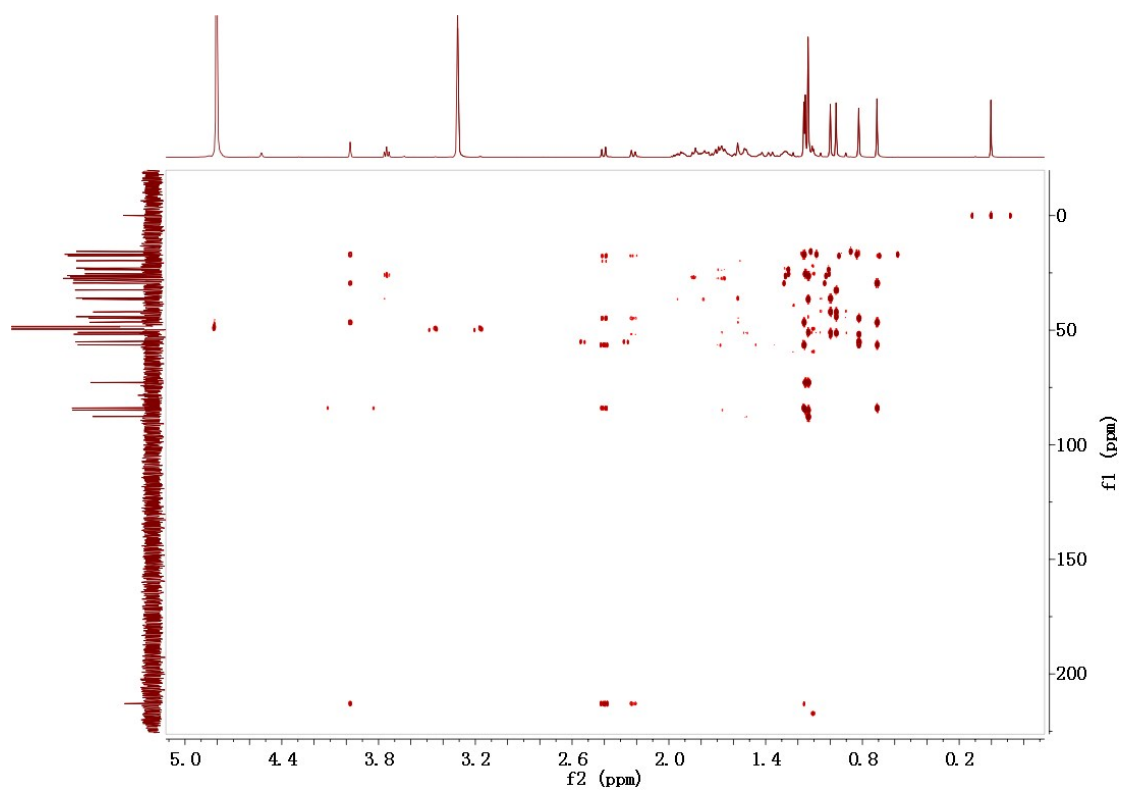


Figure S57. HMBC spectrum of chisopanone H (8)

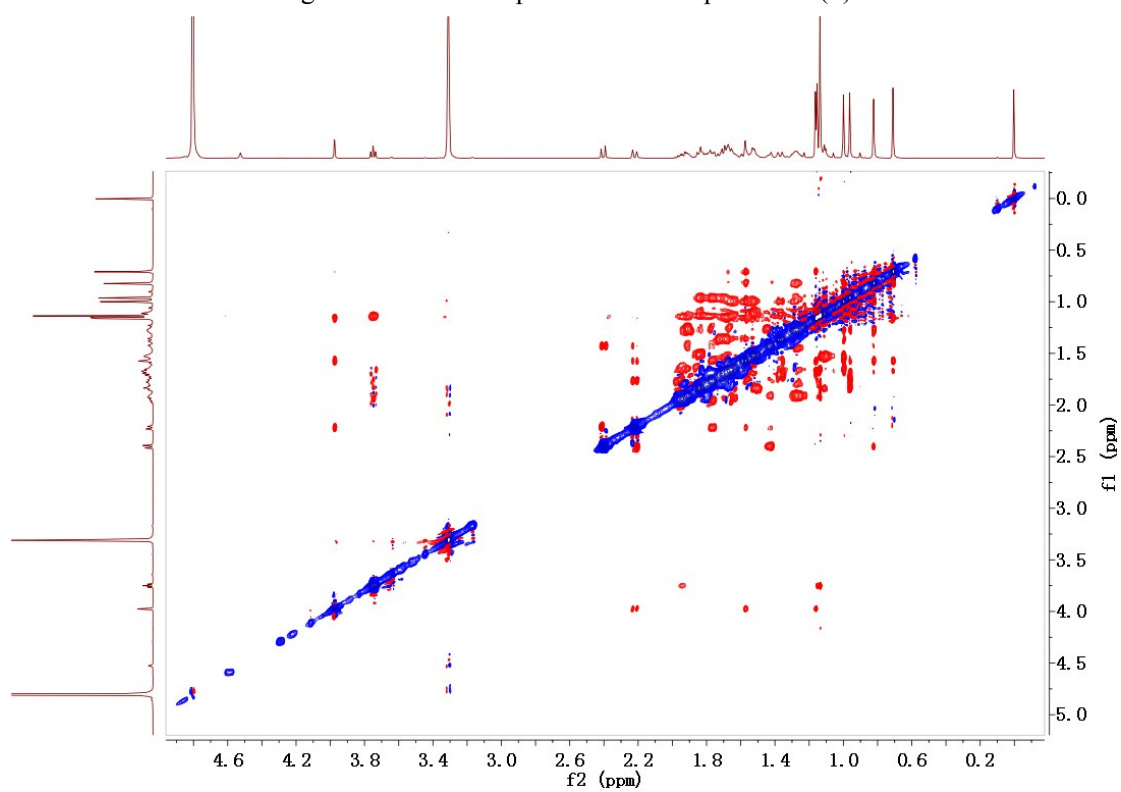
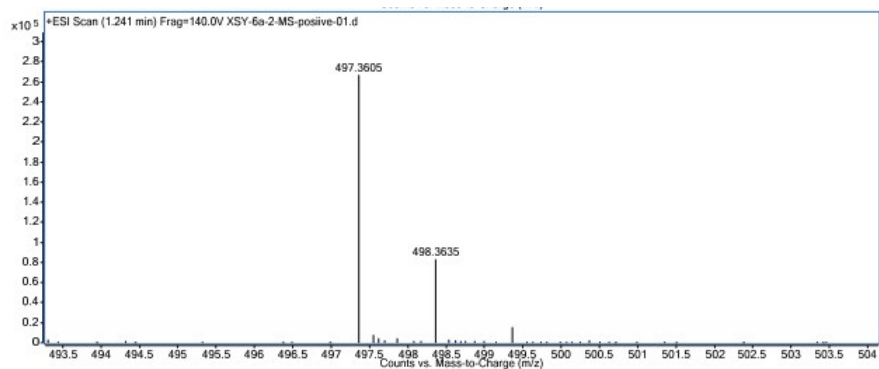


Figure S58. ROESY spectrum of chisopanone H (8)





#### Elemental Composition Calculator

| Target m/z: | 497.3605                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|-------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:   | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula | Calculated m/z                                   |              | PPM Error     |          |                     |
| C30H50NaO4  | 497.3601                                         |              | -0.83         |          |                     |

Figure S59. HRESIMS spectrum of chisopanone H (8)

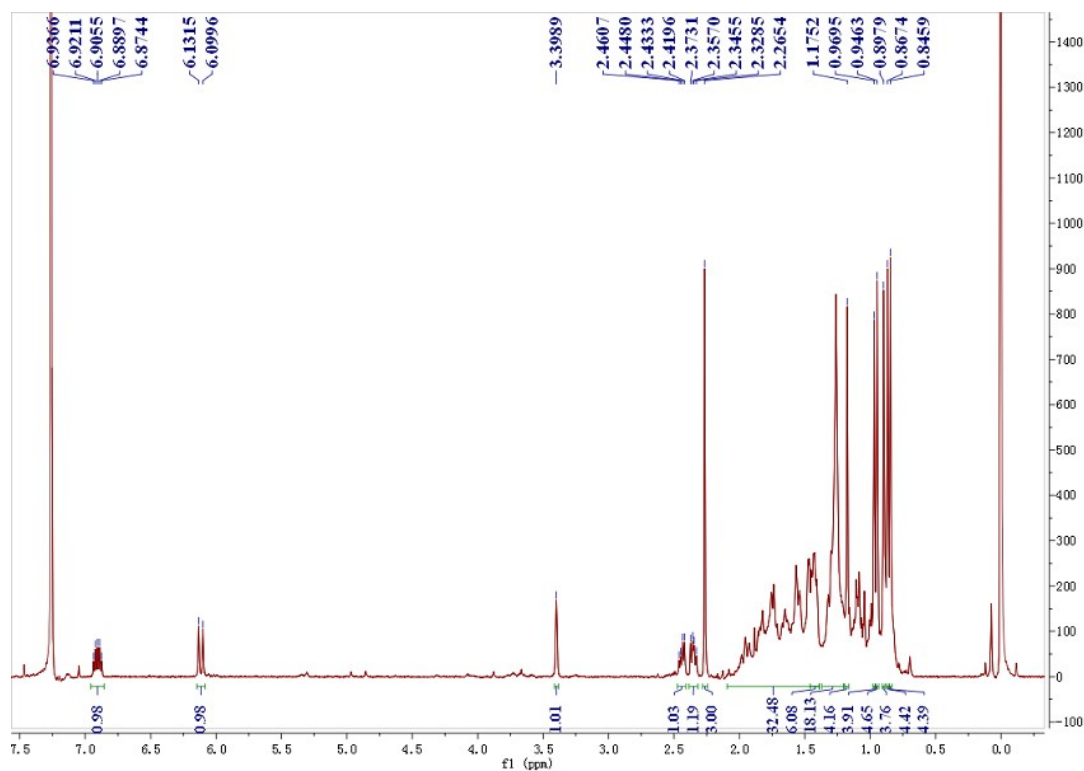


Figure S60. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of chisopanone I (9)

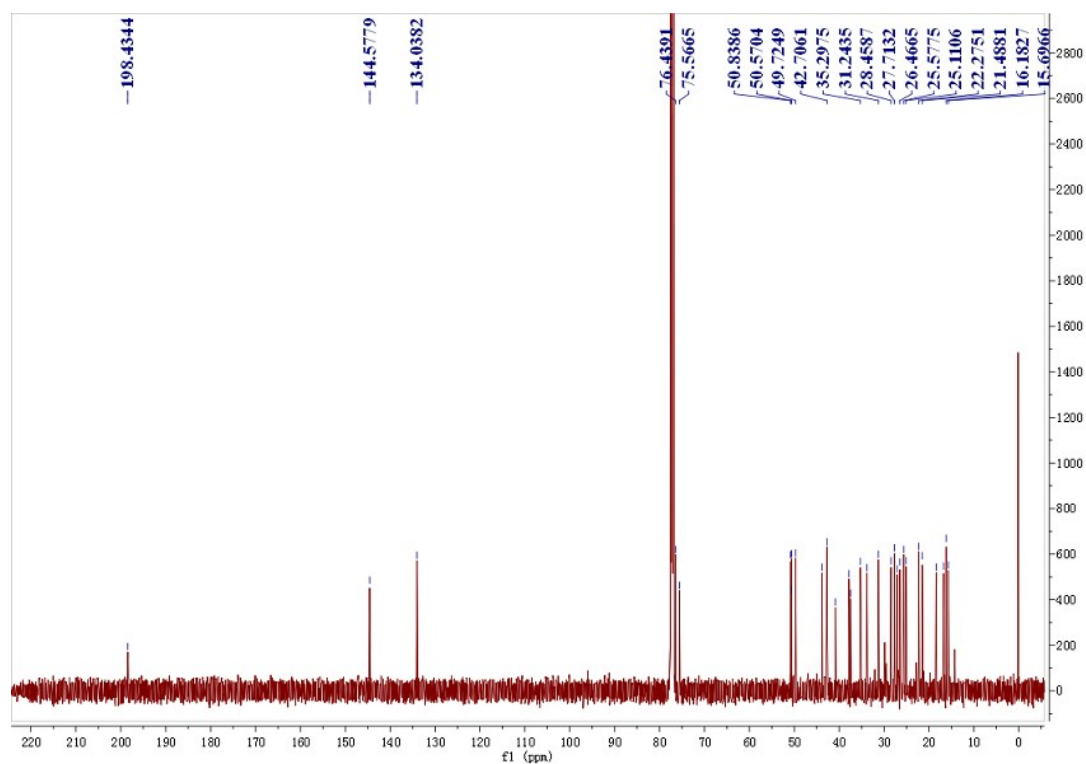


Figure S61. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) spectrum of chisopanone I (9)

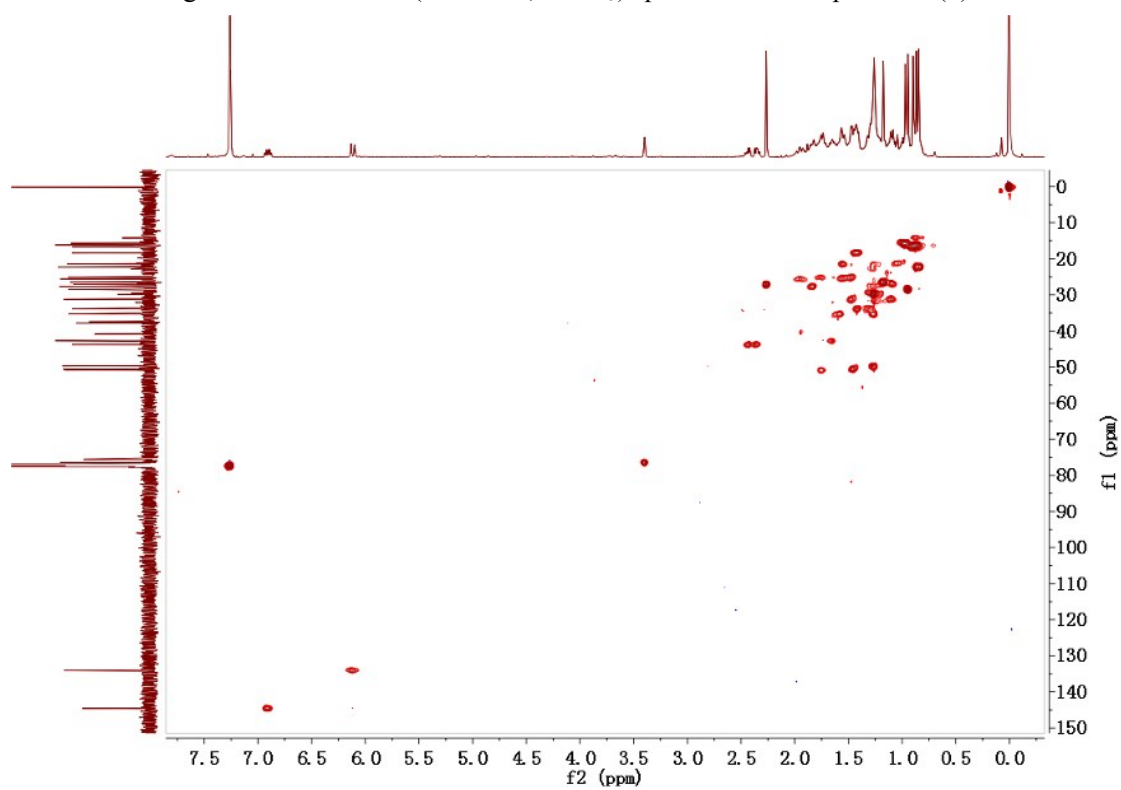


Figure S62. HSQC spectrum of chisopanone I (9)

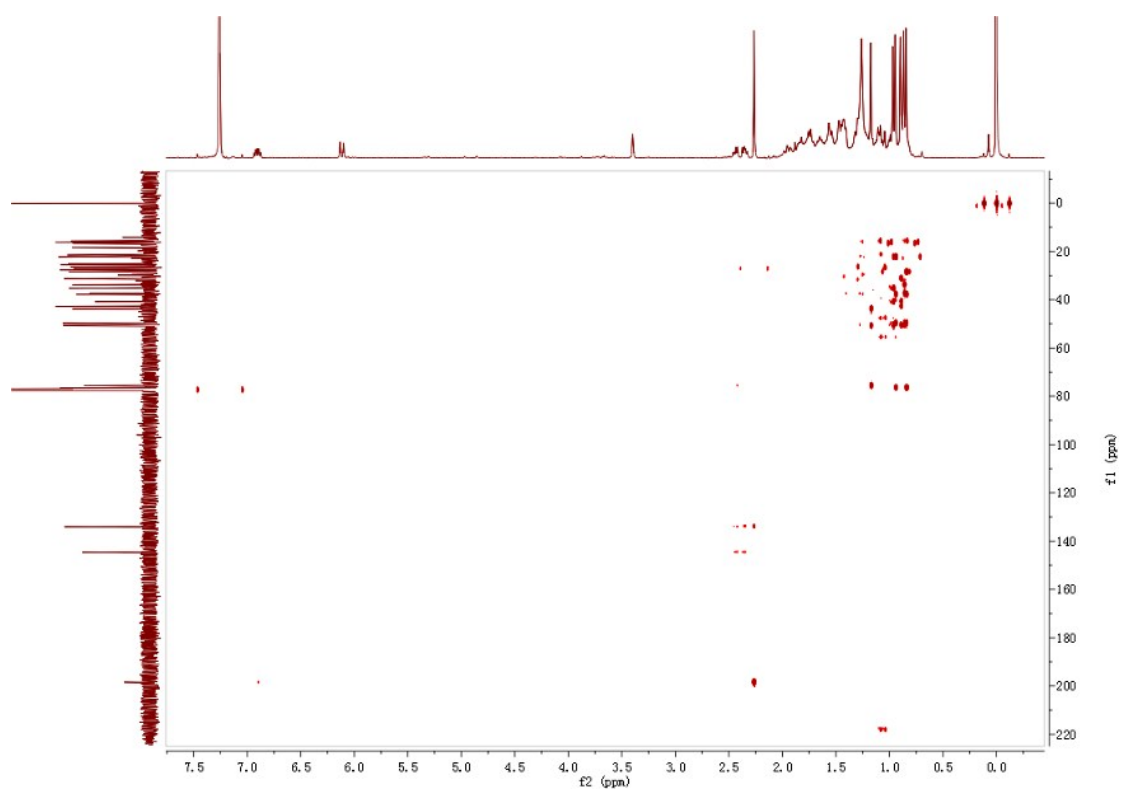


Figure S63. HMBC spectrum of chisopanone I (9)

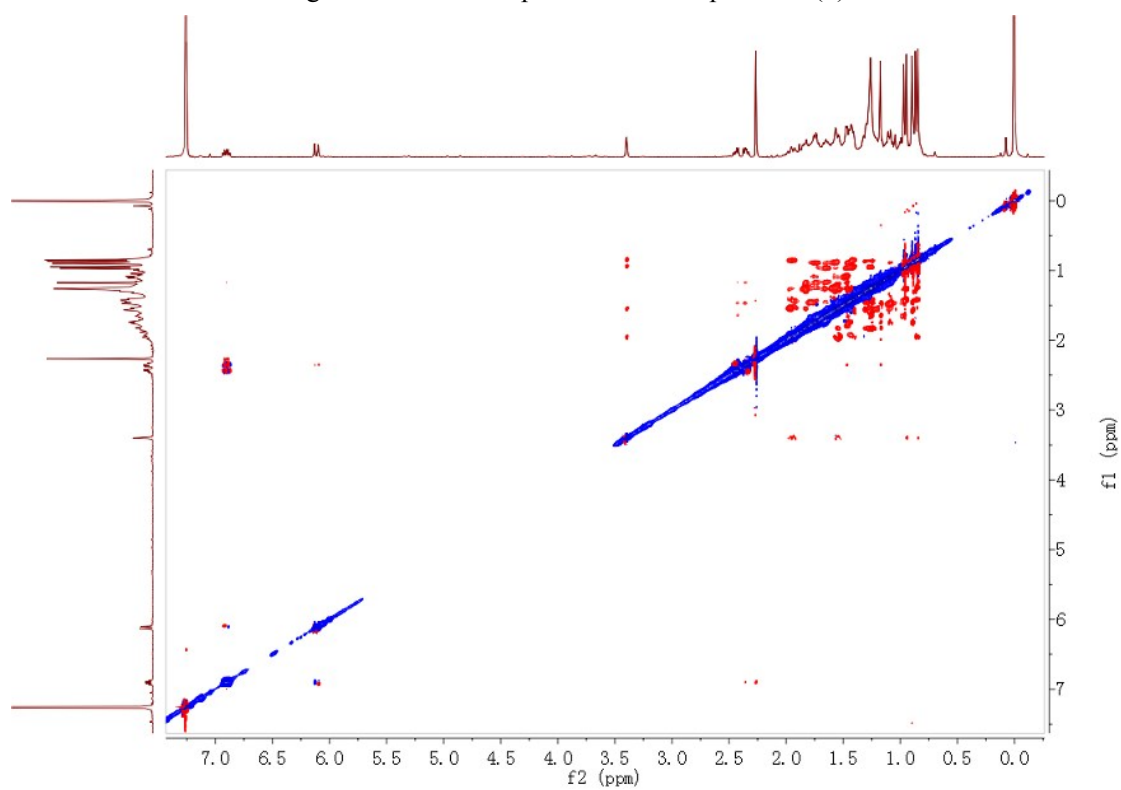
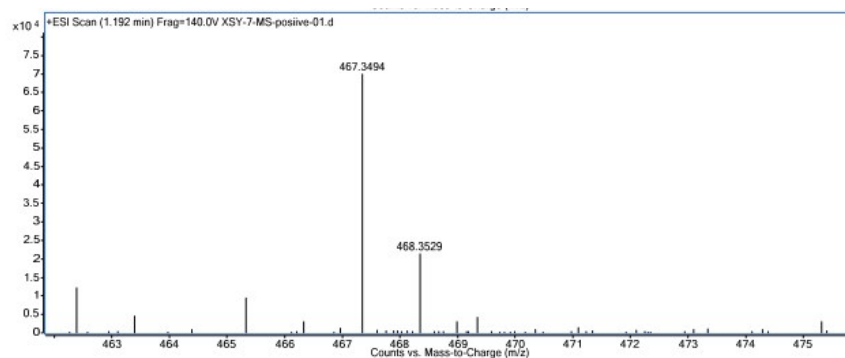


Figure S64. ROESY spectrum of chisopanone I (9)



#### Elemental Composition Calculator

| Target m/z:                                      | 467.3494                                         | Result type: | Positive ions | Species: | [M+Na] <sup>+</sup> |
|--------------------------------------------------|--------------------------------------------------|--------------|---------------|----------|---------------------|
| Elements:                                        | C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5) |              |               |          |                     |
| Ion Formula                                      | Calculated m/z                                   |              | PPM Error     |          |                     |
| C <sub>29</sub> H <sub>48</sub> NaO <sub>3</sub> | 467.3496                                         |              | 0.4           |          |                     |

Figure S65. HRESIMS spectrum of chisopanone I (9)