

Supplementary Information

Sarcosenones A–C, highly oxygenated pimarane diterpenoids from an endolichenic fungus *Sarcosomataceae* sp.

Xintong Hou,^{ab} Yang Xu,^b Shuaiming Zhu,^c Yang Zhang,^{*c} Liangdong Guo,^d Feng

Qiu^a and Yongsheng Che^{*ab}

Affiliation

^a Tianjin University of Traditional Chinese Medicine, Tianjin 300193, People's Republic of China

^b Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing 100730, People's Republic of China

^c State Key Laboratory of Toxicology & Medical Countermeasures, Beijing Institute of Pharmacology & Toxicology, Beijing 100850, People's Republic of China

^d State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, People's Republic of China

Correspondence

* To whom correspondence should be addressed.

Yongsheng Che. E-mail: cheys@im.ac.cn; Yang Zhang. E-mail: zhangyang@bmi.ac.cn.

Contents	Page
1) Figure S1. ¹ H NMR spectrum of Sarcosenone A (1 ; 600 MHz, Acetone- <i>d</i> ₆)	4
2) Figure S2. ¹³ C NMR spectrum of Sarcosenone A (1 ; 150 MHz, Acetone- <i>d</i> ₆)	5
3) Figure S3. HSQC spectrum of Sarcosenone A (1 ; 600 MHz, Acetone- <i>d</i> ₆)	6
4) Figure S4. ¹ H– ¹ H COSY spectrum of Sarcosenone A (1 ; 600 MHz, Acetone- <i>d</i> ₆)	7
5) Figure S5. HMBC spectrum of Sarcosenone A (1 ; 600 MHz, Acetone- <i>d</i> ₆)	8
6) Figure S6. NOESY spectrum of Sarcosenone A (1 ; 600 MHz, Acetone- <i>d</i> ₆)	9
7) Figure S7. HRESIMS spectrum of Sarcosenone A (1)	10
8) Figure S8. IR spectrum of Sarcosenone A (1)	11
9) Figure S9. UV spectrum of Sarcosenone A (1) in MeOH	12
10) Figure S10. Experimental CD spectrum of Sarcosenone A (1) in MeOH	12
11) Figure S11. Relative configurations and the optimized conformers for 1	13
12) Figure S12. ¹ H NMR spectrum of Sarcosenone B (2 ; 600 MHz, Acetone- <i>d</i> ₆)	14
13) Figure S13. ¹³ C NMR spectrum of Sarcosenone B (2 ; 150 MHz, Acetone- <i>d</i> ₆)	15
14) Figure S14. HSQC spectrum of Sarcosenone B (2 ; 600 MHz, Acetone- <i>d</i> ₆)	16
15) Figure S15. ¹ H– ¹ H COSY spectrum of Sarcosenone B (2 ; 600 MHz, Acetone- <i>d</i> ₆)	17
16) Figure S16. HMBC spectrum of Sarcosenone B (2 ; 600 MHz, Acetone- <i>d</i> ₆)	18
17) Figure S17. NOESY spectrum of Sarcosenone B (2 ; 600 MHz, Acetone- <i>d</i> ₆)	19
18) Figure S18. HRESIMS spectrum of Sarcosenone B (2)	20
19) Figure S19. IR spectrum of Sarcosenone B (2)	21
20) Figure S20. UV spectrum of Sarcosenone B (2) in MeOH	22
21) Figure S21. Experimental CD spectrum of Sarcosenone B (2) in MeOH	22

22) Figure S22. Relative configurations and the optimized conformers for 2	23
23) Figure S23. ¹ H NMR spectrum of Sarcosenone C (3 ; 600 MHz, CDCl ₃)	24
24) Figure S24. ¹³ C NMR spectrum of Sarcosenone C (3 ; 150 MHz, CDCl ₃)	25
25) Figure S25. HSQC spectrum of Sarcosenone C (3 ; 600 MHz, CDCl ₃)	26
26) Figure S26. ¹ H– ¹ H COSY spectrum of Sarcosenone C (3 ; 600 MHz, CDCl ₃)	27
27) Figure S27. HMBC spectrum of Sarcosenone C (3 ; 600 MHz, CDCl ₃)	28
28) Figure S28. NOESY spectrum of Sarcosenone C (3 ; 600 MHz, CDCl ₃)	29
29) Figure S29. HRESIMS spectrum of Sarcosenone C (3)	30
30) Figure S30. IR spectrum of Sarcosenone C (3)	31
31) Figure S31. UV spectrum of Sarcosenone C (3) in MeOH	32
32) Figure S32. Experimental CD spectrum of Sarcosenone C (3) in MeOH	32
33) Figure S33. Relative configurations and the optimized conformers for 3	33
34) Figure S34. NOESY spectrum of 9 α -Hydroxy-1,8(14),15-isopimaratrien -3,7,11-trione (4 ; 600 MHz, Acetone- <i>d</i> ₆)	34
35) Figure S35. Experimental CD spectrum of 9 α -Hydroxy -1,8(14),15-isopimaratrien -3,7,11-trione (4) in MeOH	35
36) Figure S36. Relative configurations and the optimized conformers for 4	36,37
37) Scheme S1. Hypothetical biosynthetic pathways for 1–4	38

Figure S1. ^1H NMR Spectrum of Sarcosenone A (**1**; 600 MHz, Acetone- d_6)

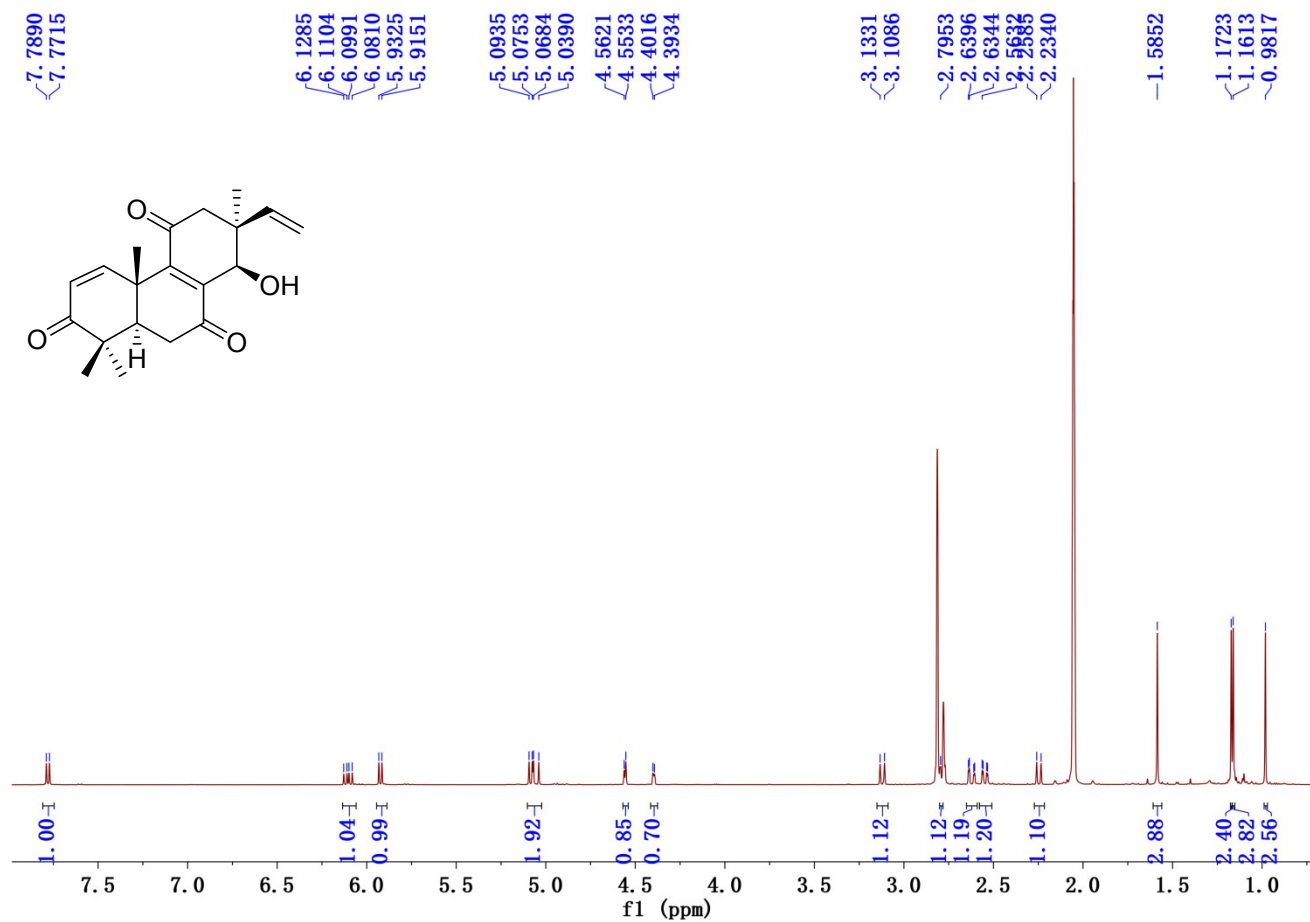


Figure S2. ^{13}C NMR Spectrum of Sarcosenone A (**1**; 150 MHz, Acetone- d_6)

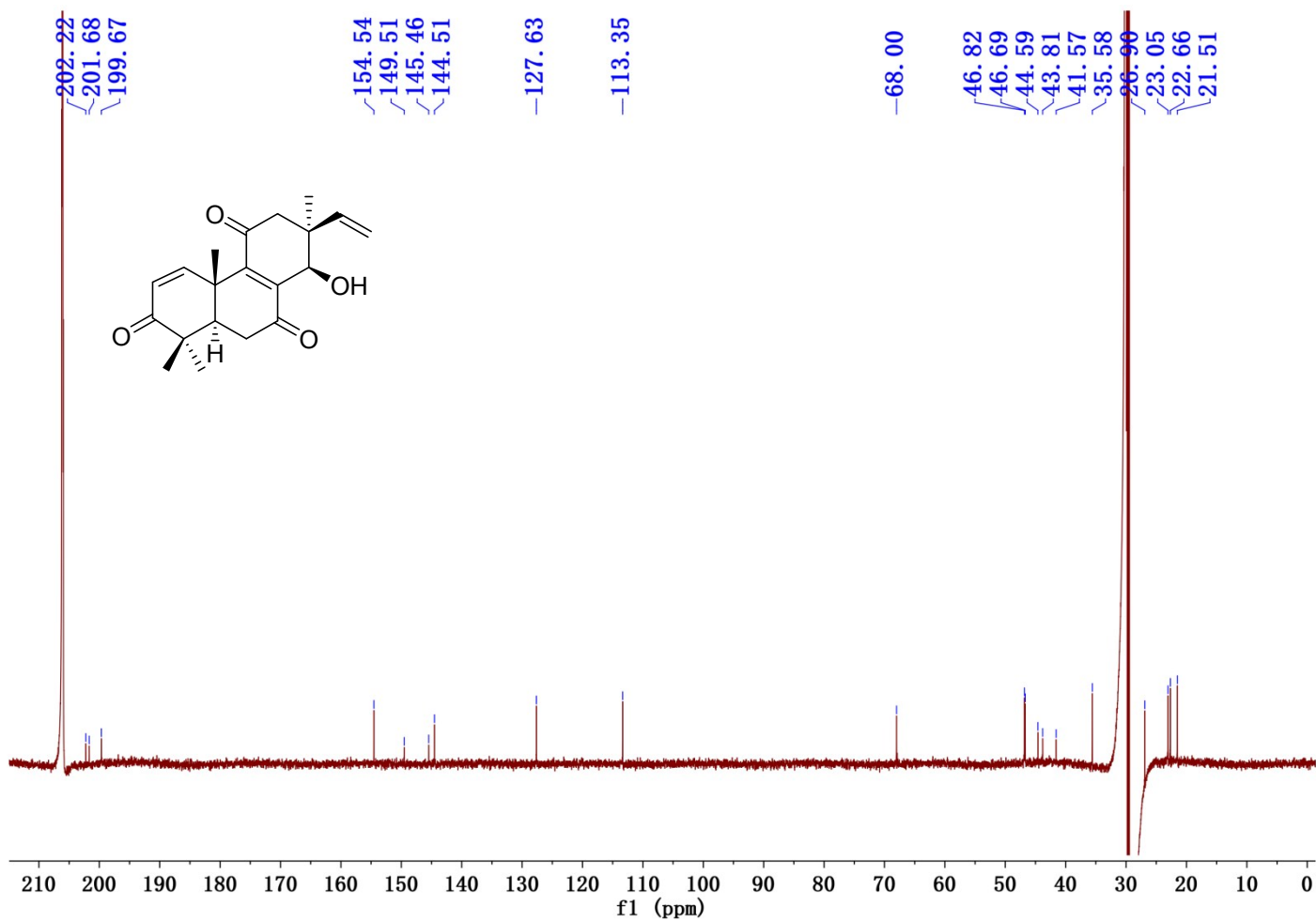


Figure S3. HSQC Spectrum of Sarcosenone A (1; 600 MHz, Acetone- d_6)

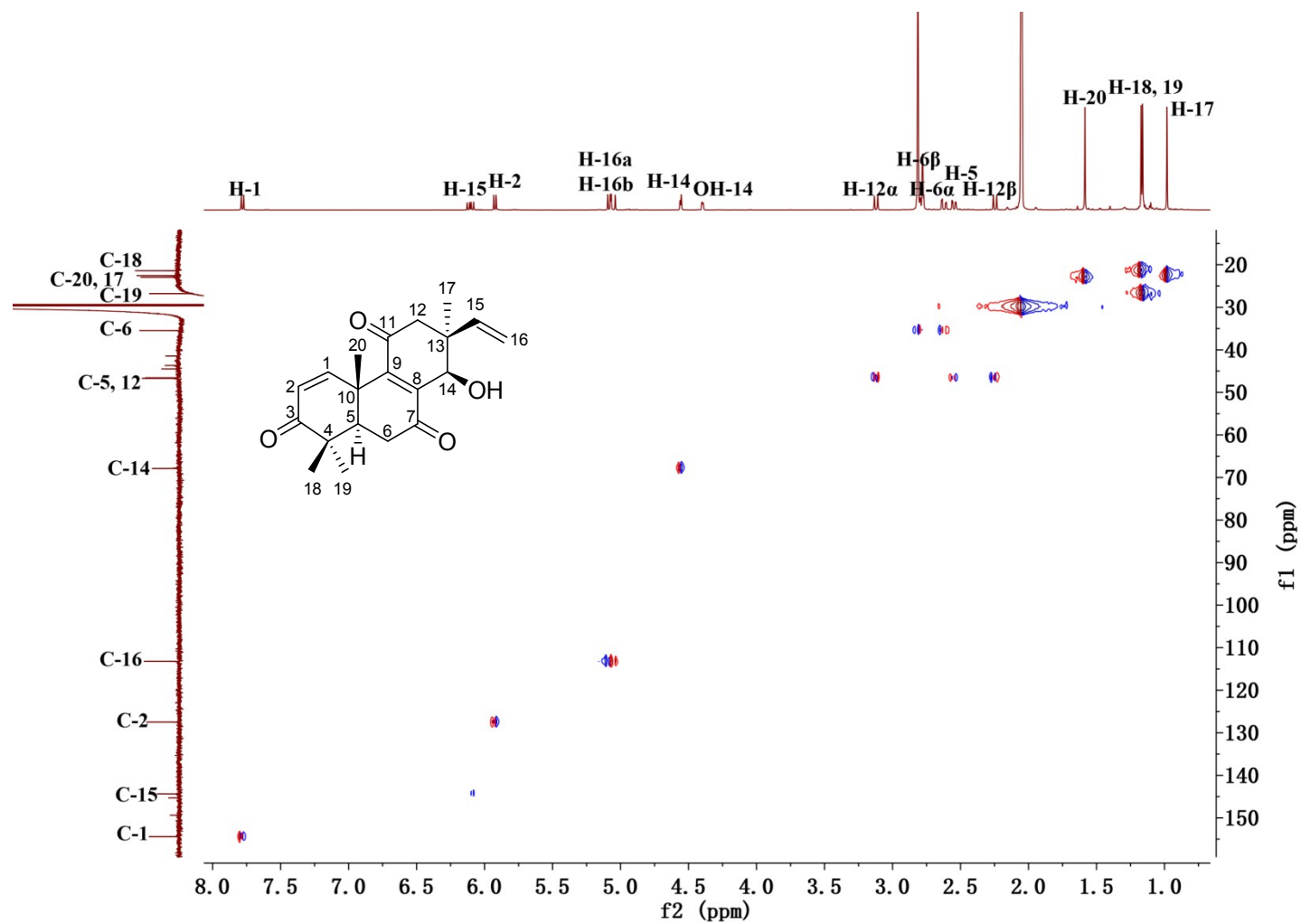


Figure S4. ^1H - ^1H COSY Spectrum of Sarcosenone A (**1**; 600 MHz, Acetone- d_6)

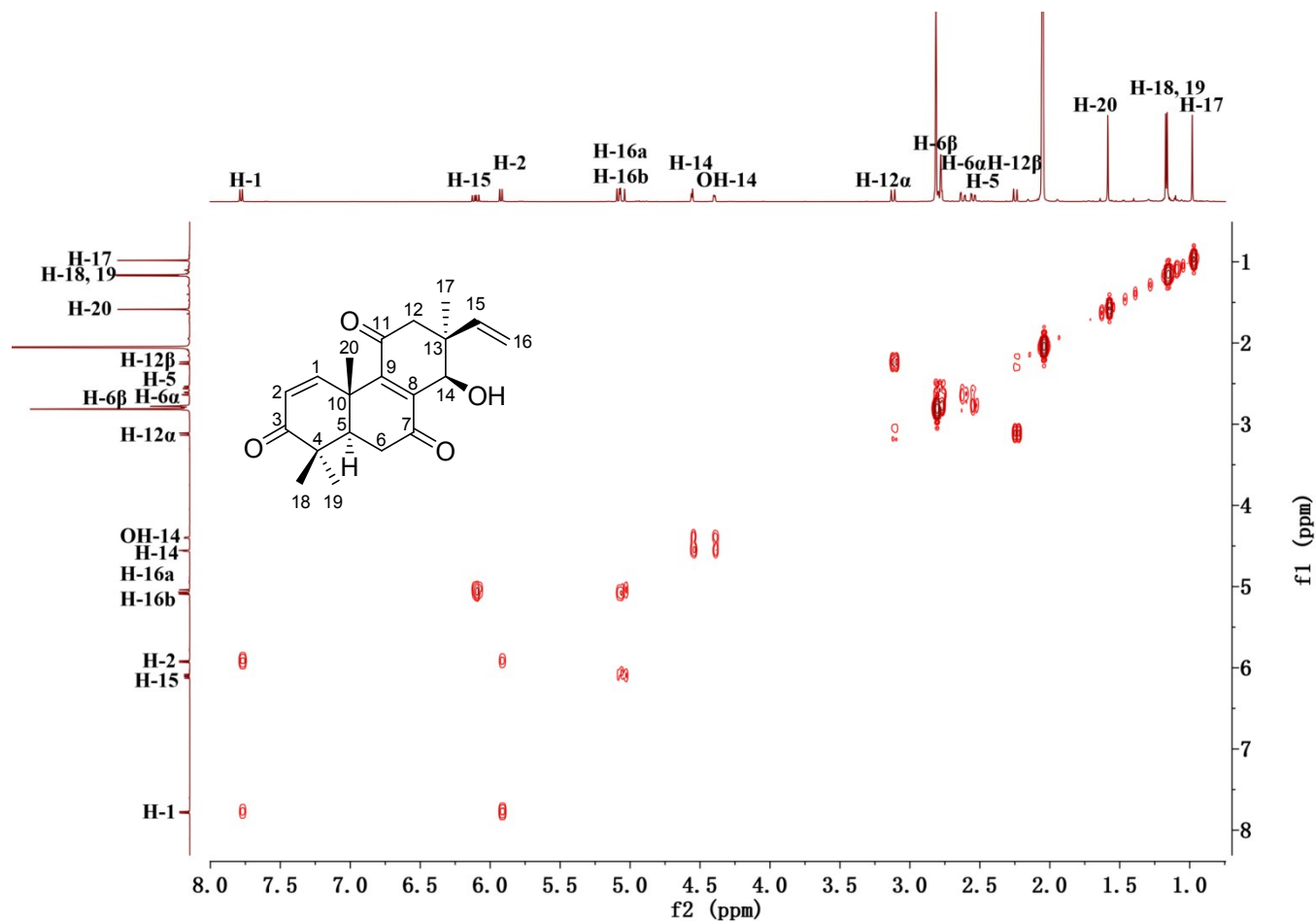


Figure S5. HMBC Spectrum of Sarcosenone A (**1**; 600 MHz, Acetone- d_6)

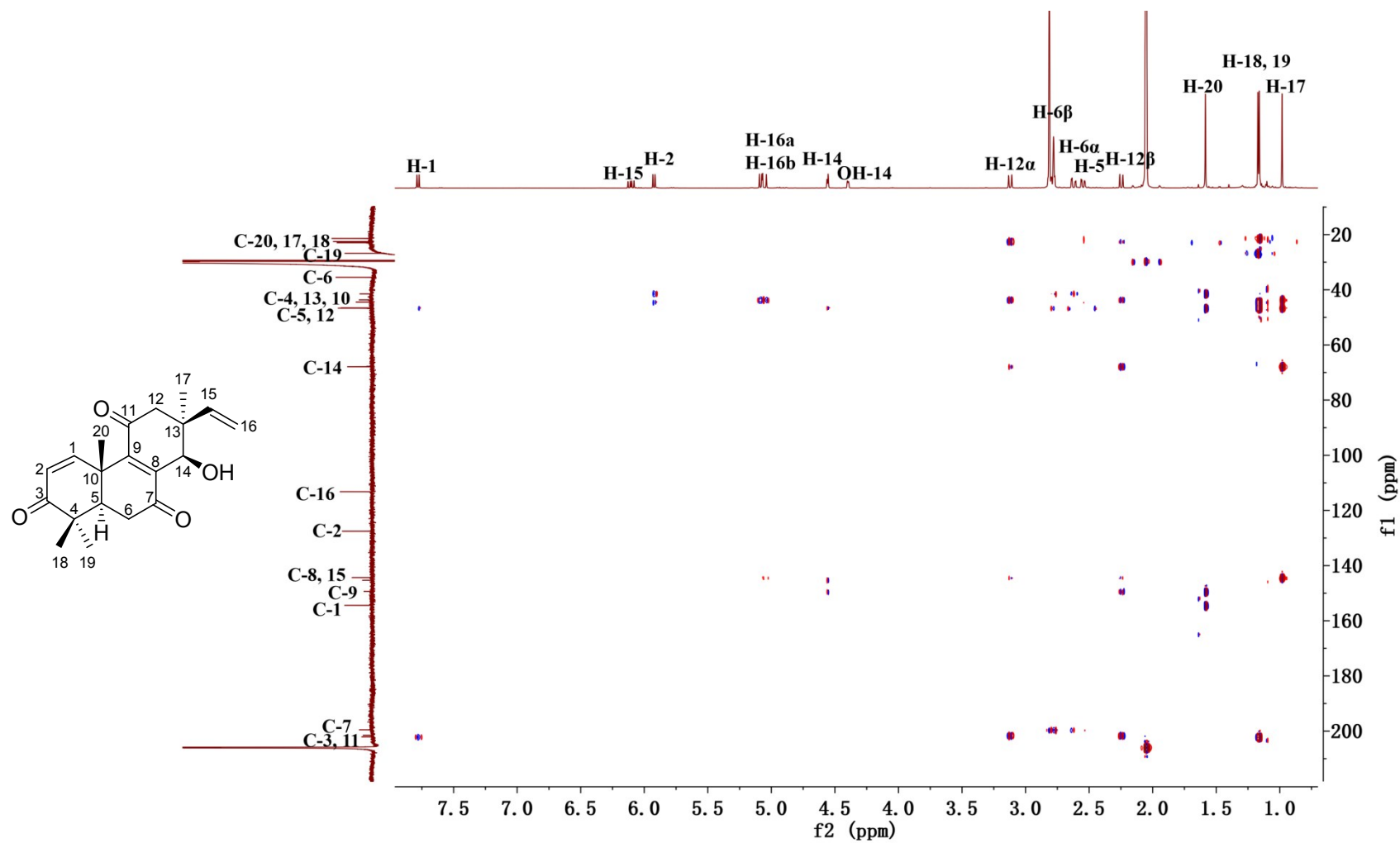


Figure S6. NOESY Spectrum of Sarcosenone A (**1**; 600 MHz, Acetone-*d*₆)

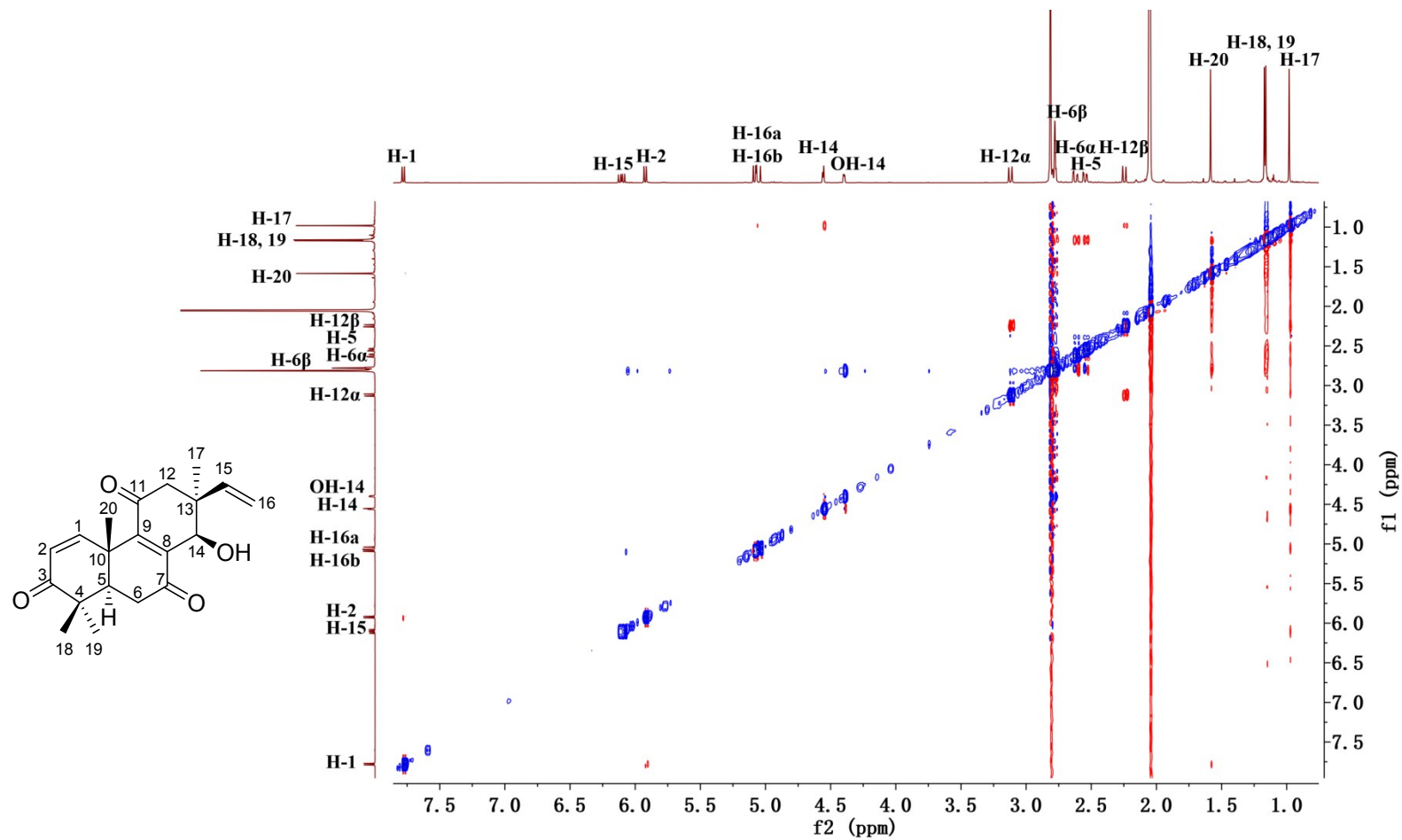


Figure S7. HRESIMS Spectrum of Sarcosenone A (1)

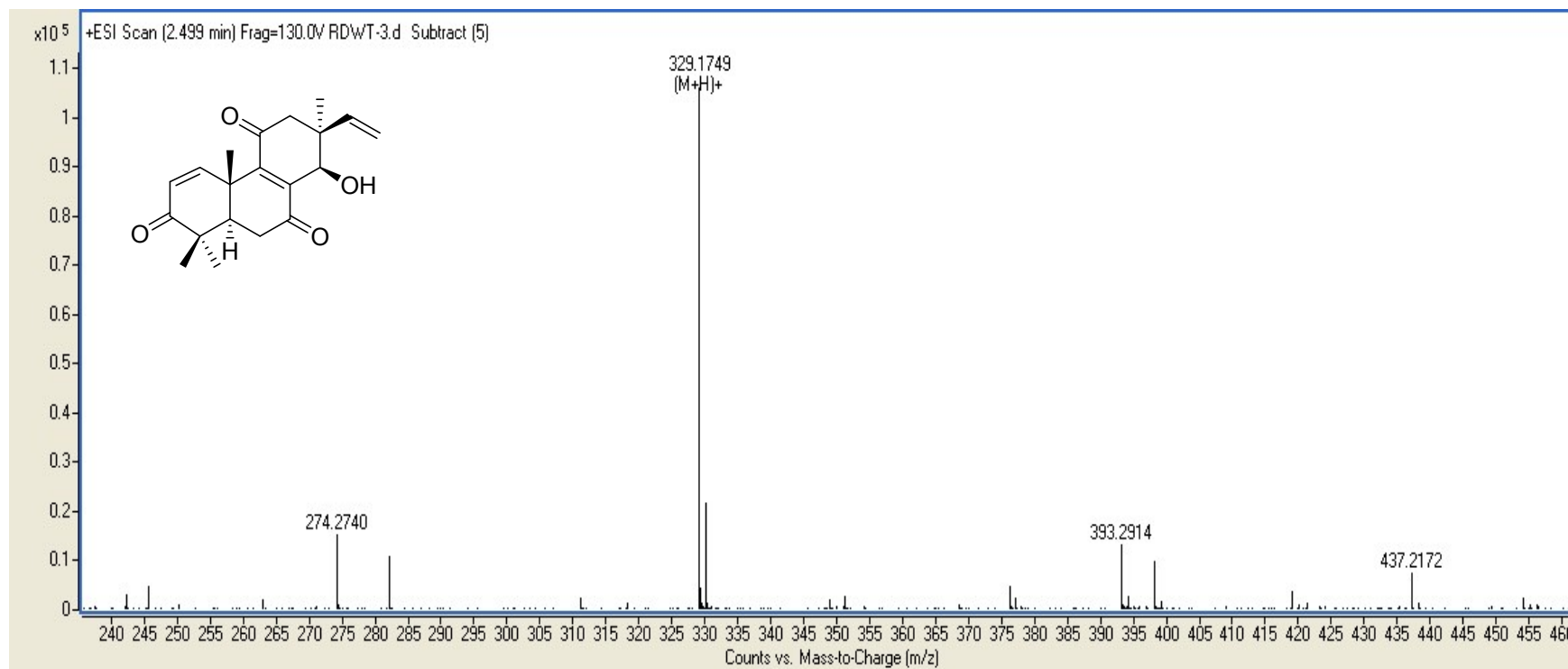


Figure S8. IR Spectrum of Sarcosenone A (1)

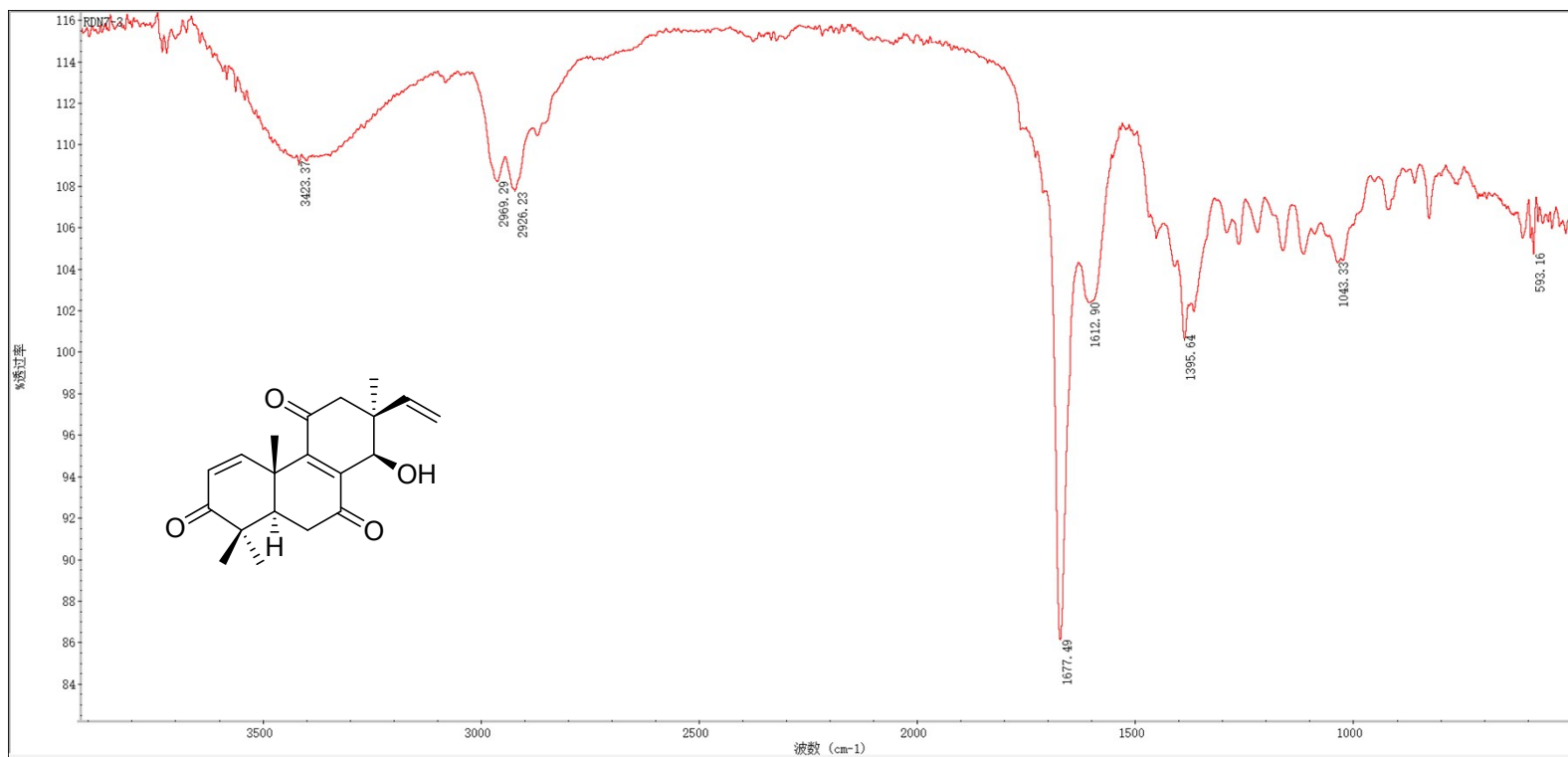


Figure S9. UV Spectrum of Sarcosenone A (1) in MeOH

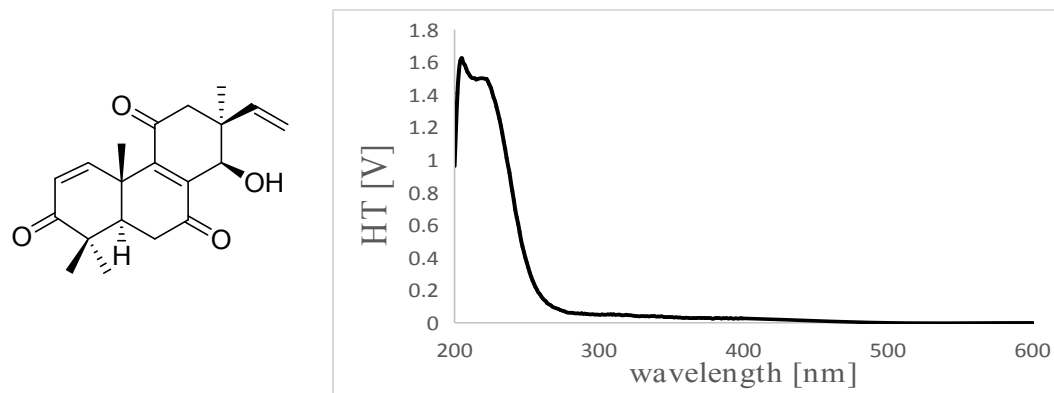


Figure S10. CD Spectrum of Sarcosenone A (1) in MeOH

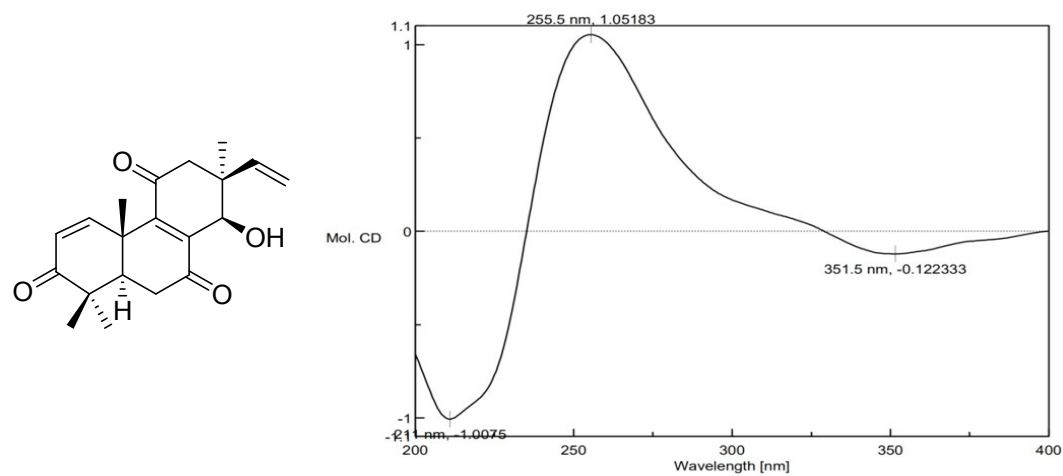
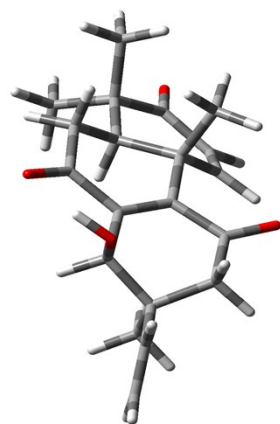
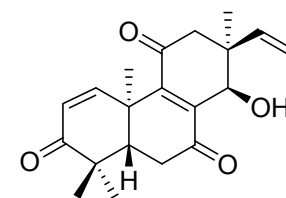
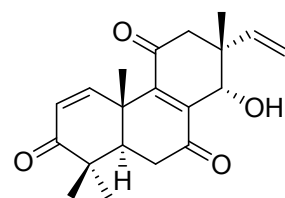
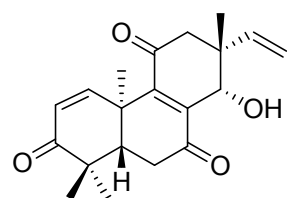
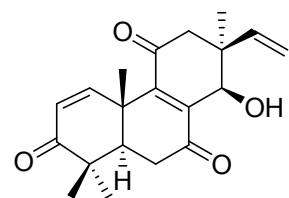
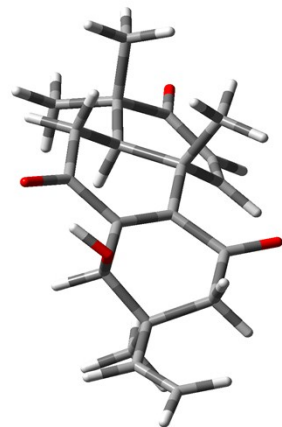


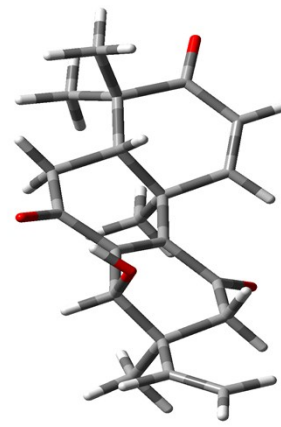
Figure S11. Relative Configurations and the Optimized Conformers for **1**



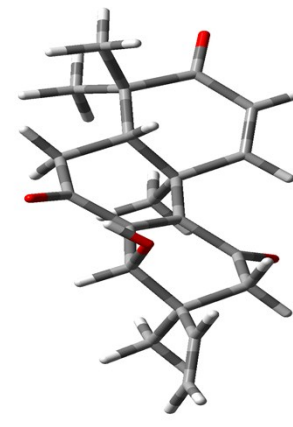
1a



1b



1c



1d

Figure S12. ^1H NMR Spectrum of Sarcosenone B (**2**; 600 MHz, Acetone- d_6)

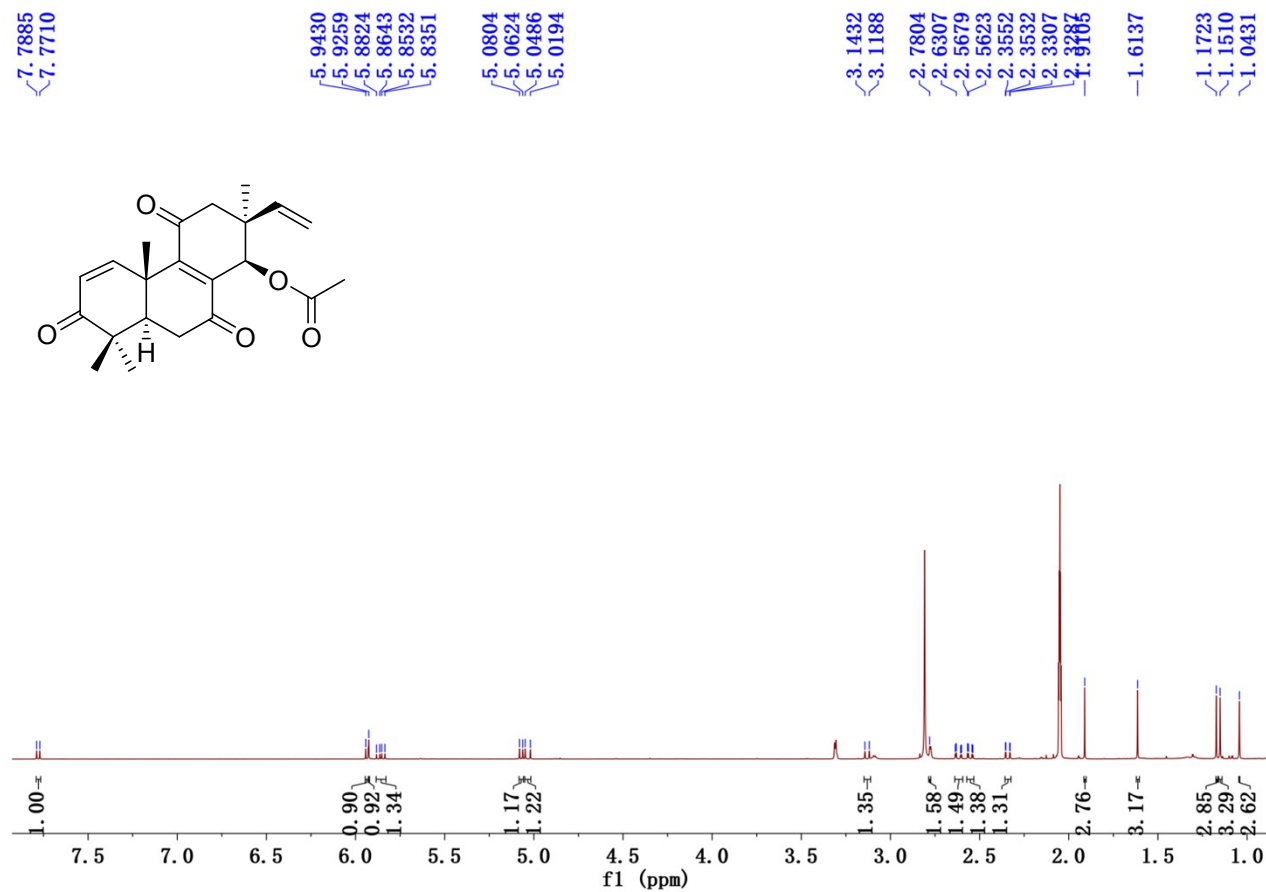


Figure S13. ^{13}C NMR Spectrum of Sarcosenone B (**2**; 150 MHz, Acetone- d_6)

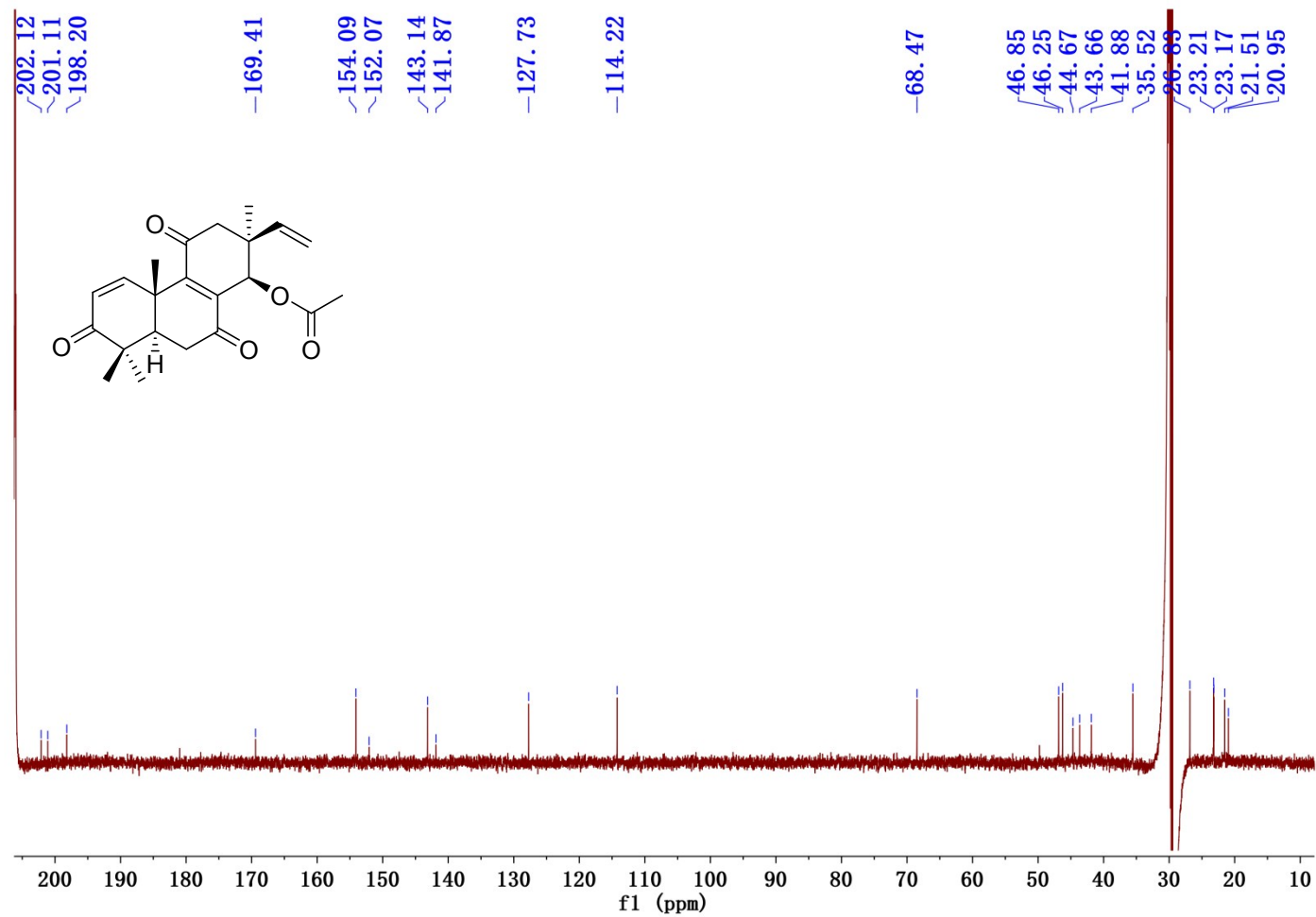


Figure S14. HSQC Spectrum of Sarcosenone B (**2**; 600 MHz, Acetone- d_6)

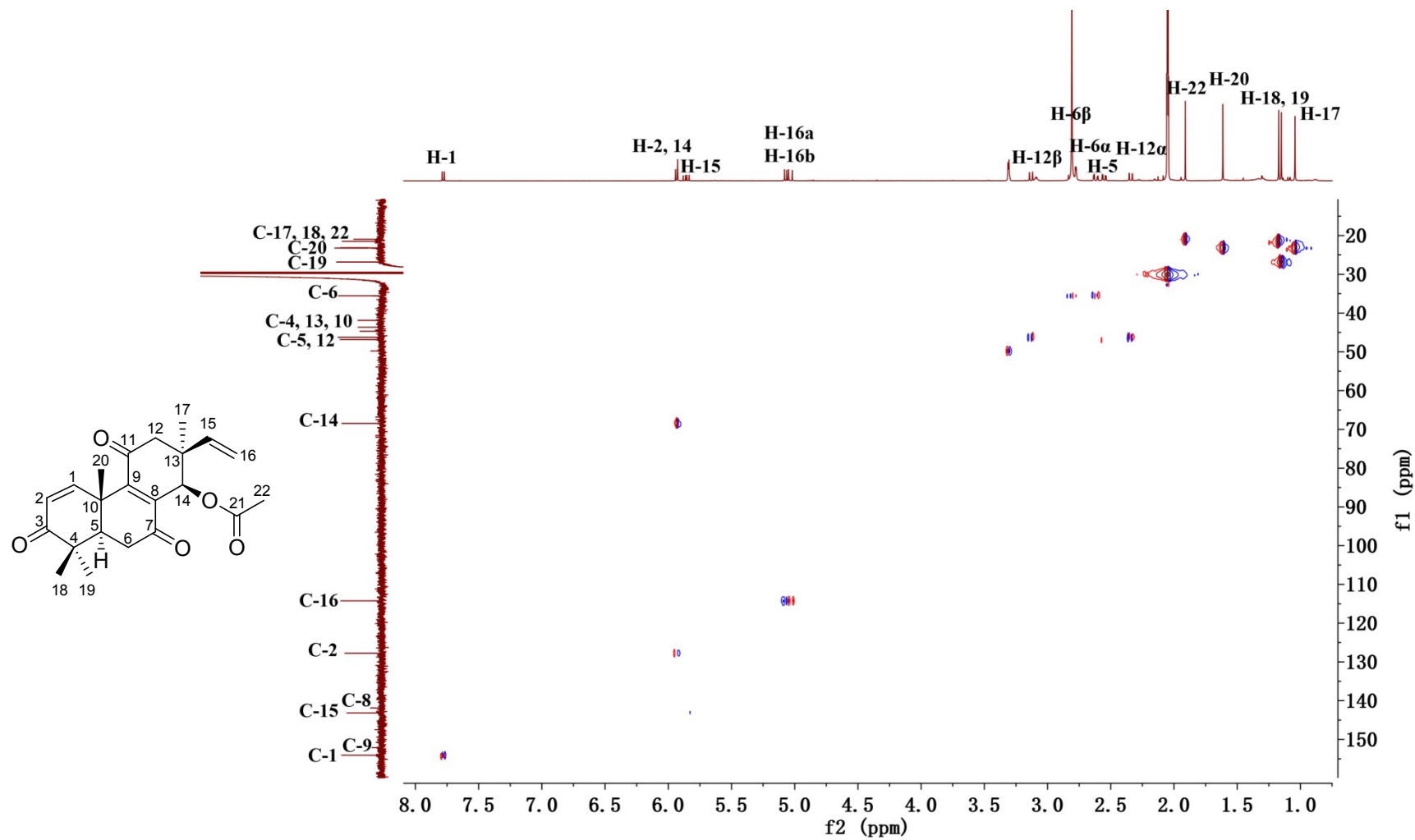


Figure S15. ^1H - ^1H COSY Spectrum of Sarcosenone B (**2**; 600 MHz, Acetone- d_6)

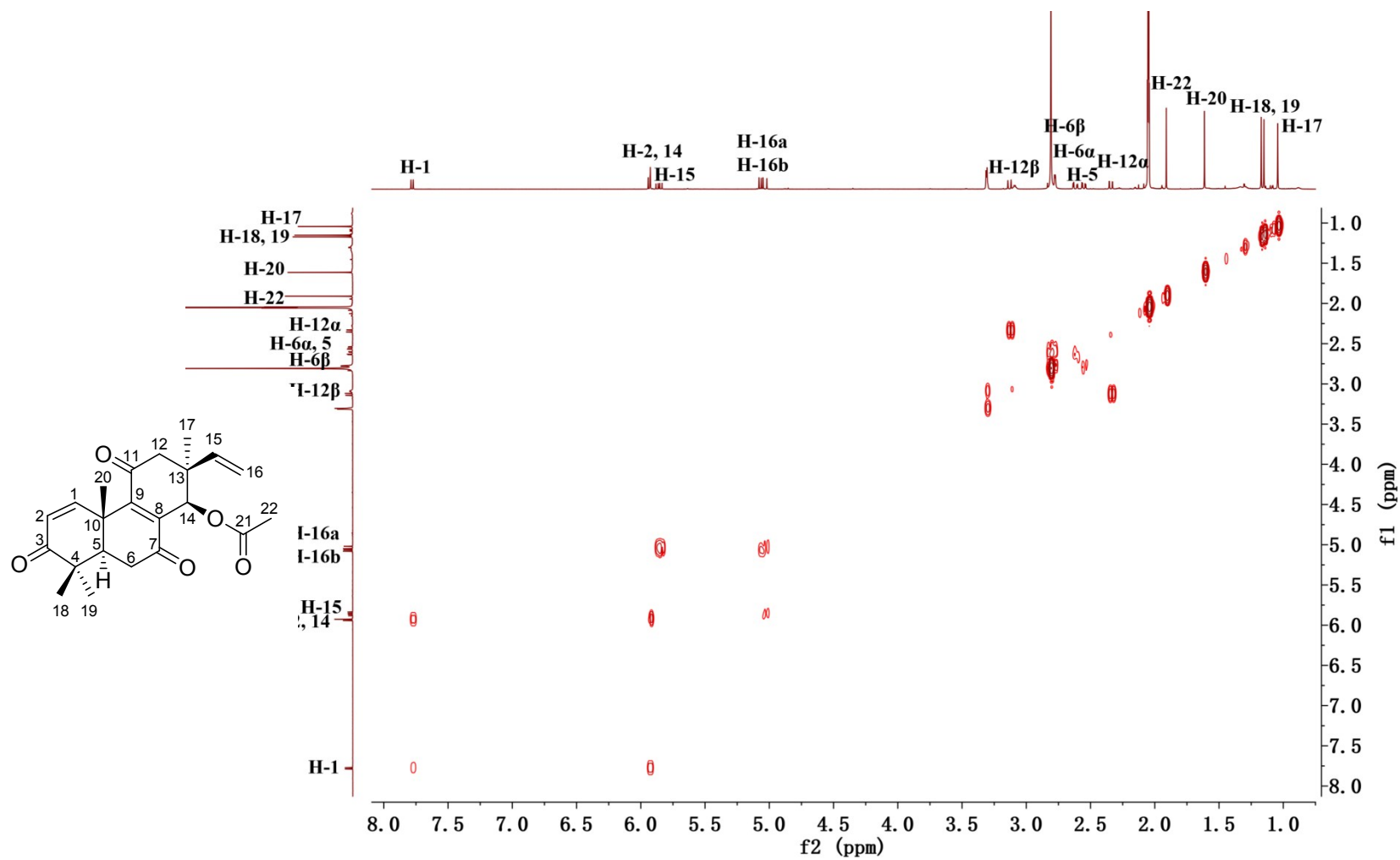


Figure S16. HMBC Spectrum of Sarcosenone B (**2**; 600 MHz, Acetone-*d*₆)

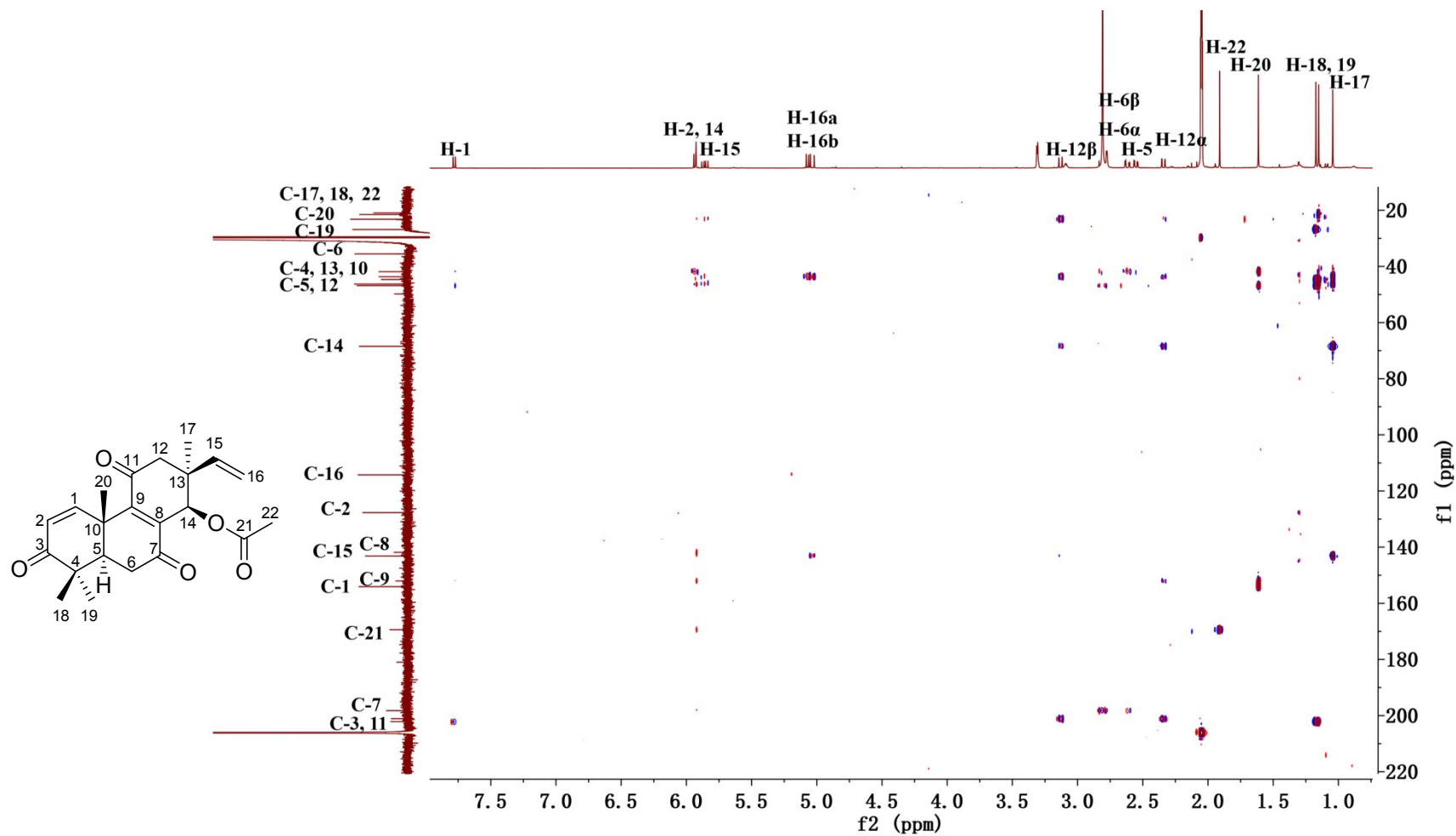


Figure S17. NOESY Spectrum of Sarcosenone B (**2**; 600 MHz, Acetone- d_6)

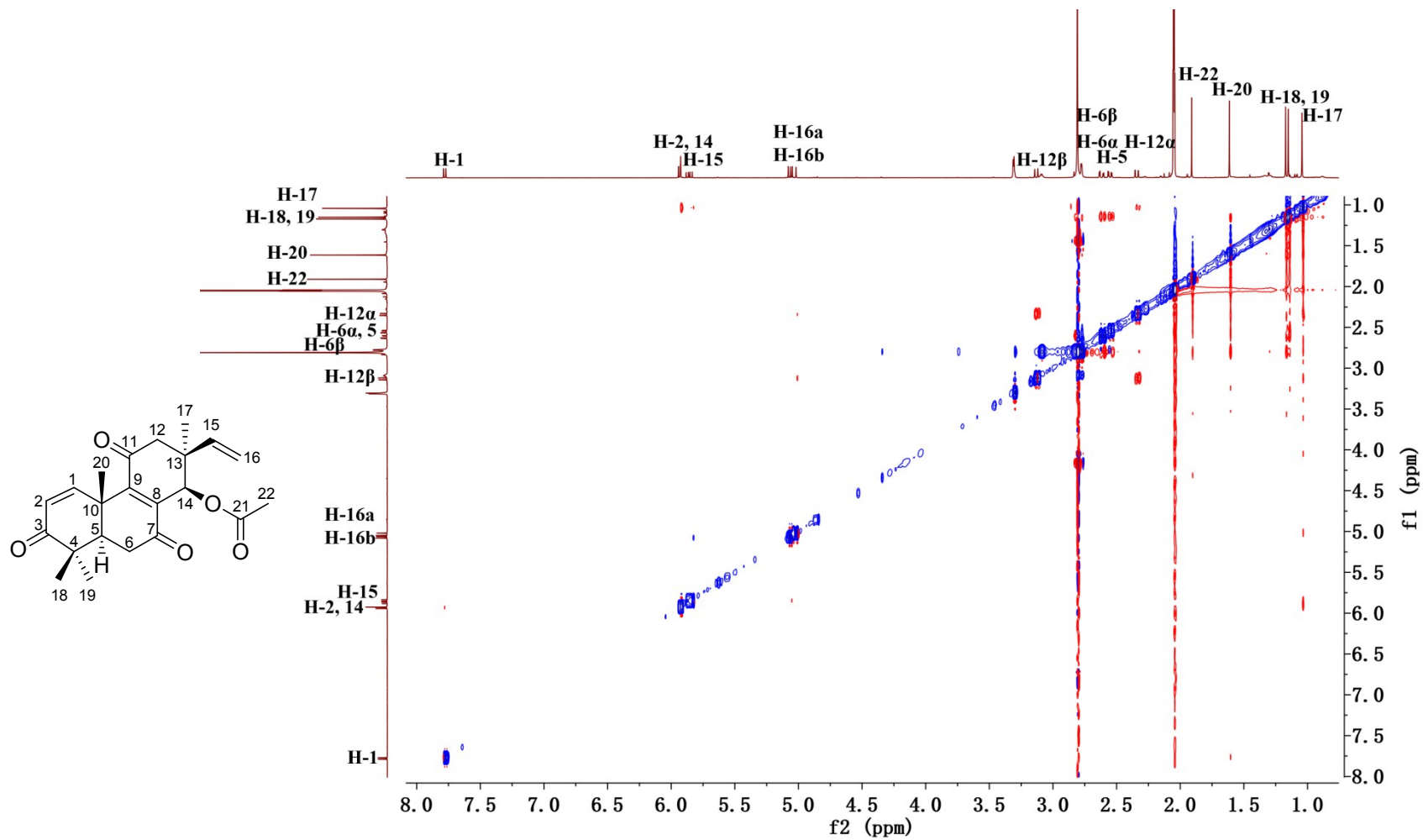


Figure S18. HRESIMS Spectrum of Sarcosenone B (2)

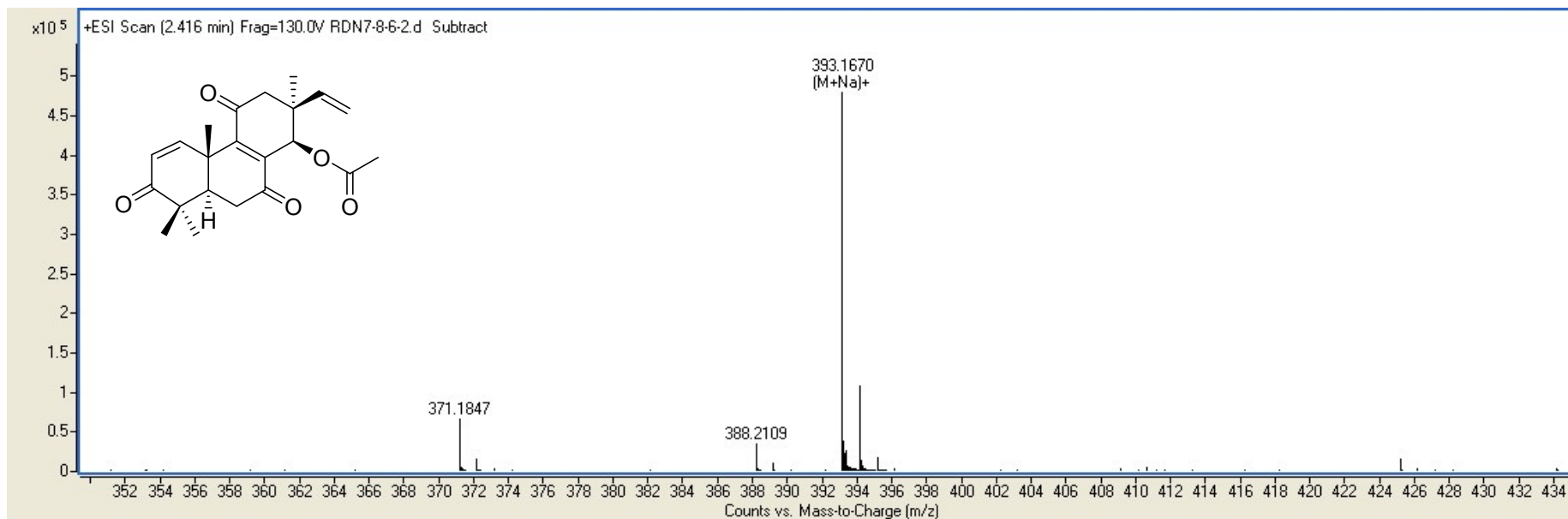


Figure S19. IR Spectrum of Sarcosenone B (2)

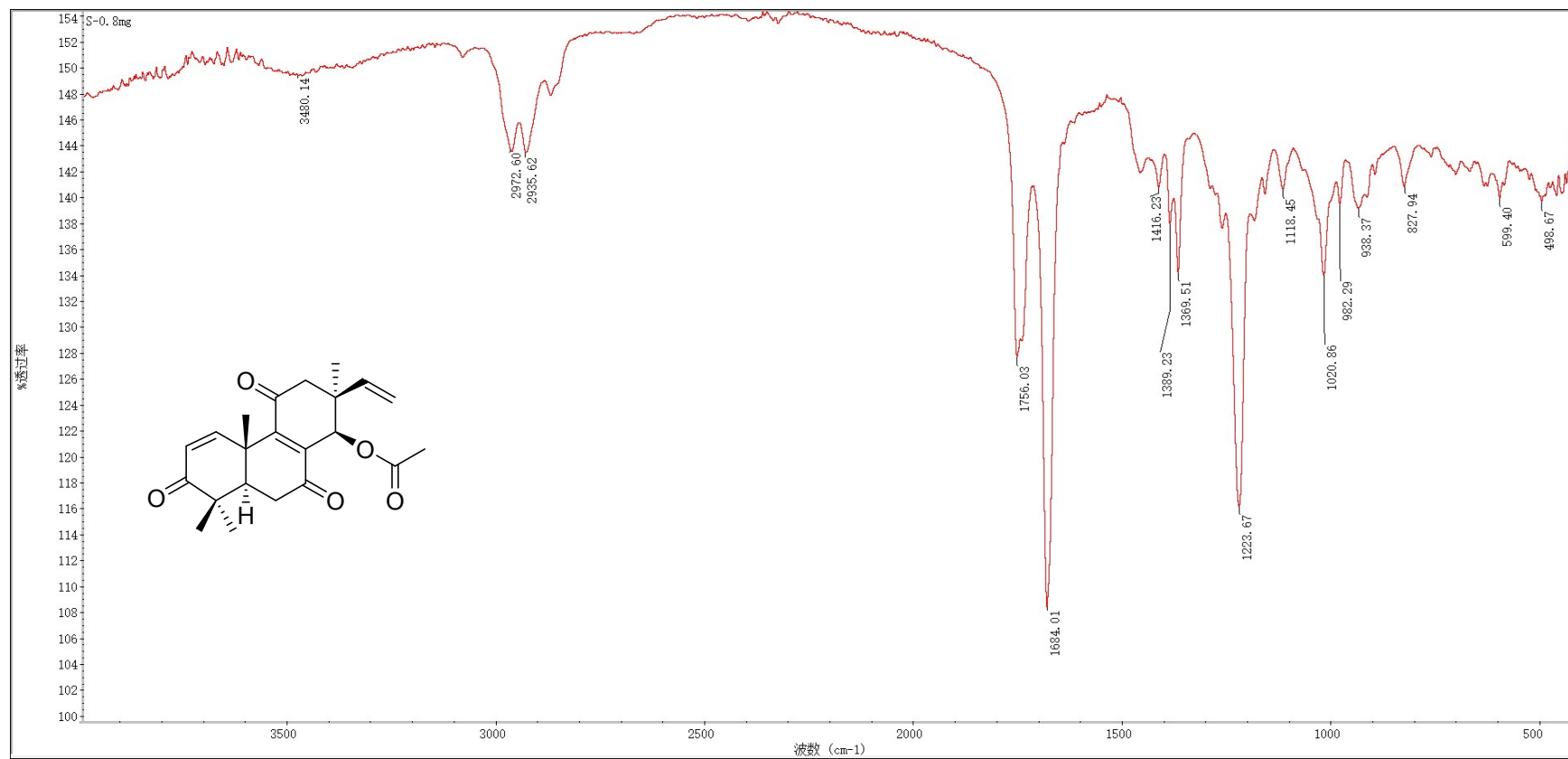


Figure S20. UV Spectrum of Sarcosenone B (2) in MeOH

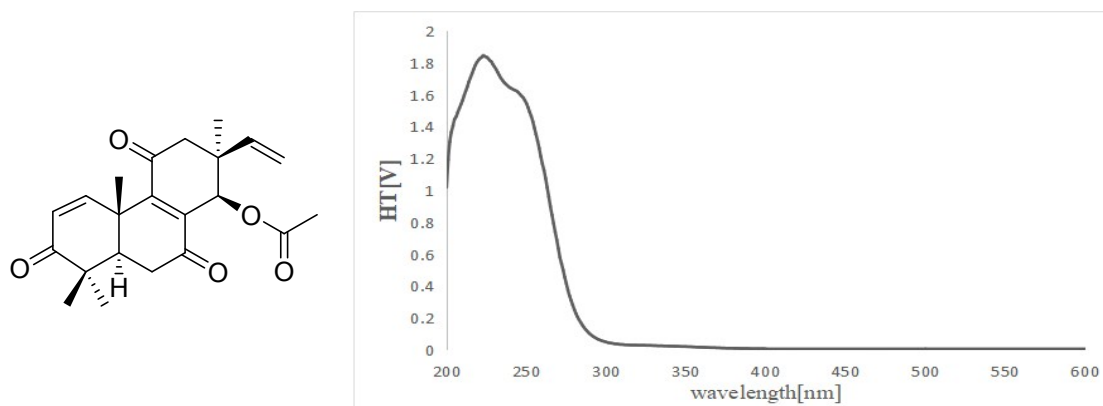


Figure S21. CD Spectrum of Sarcosenone B (2) in MeOH

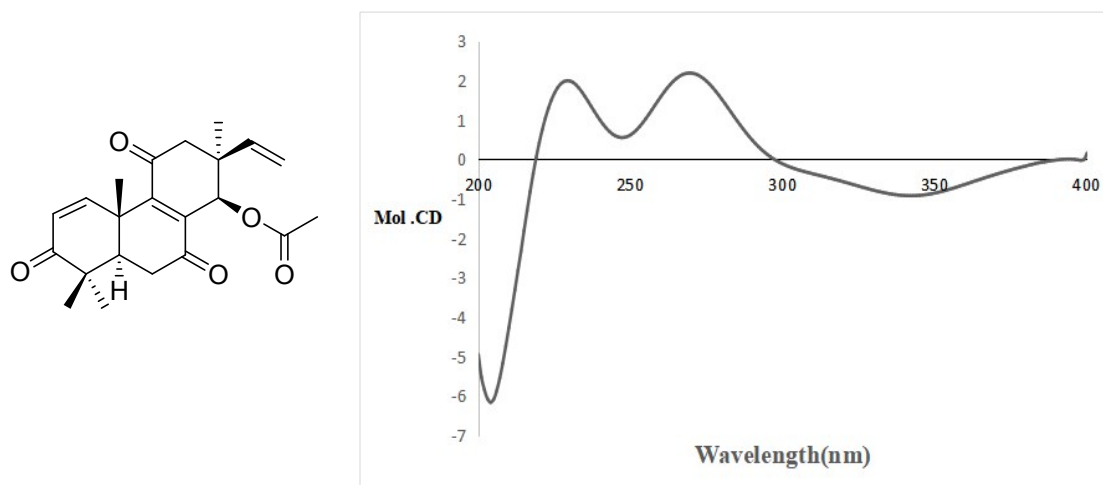
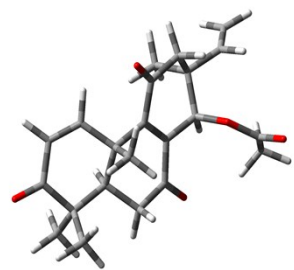
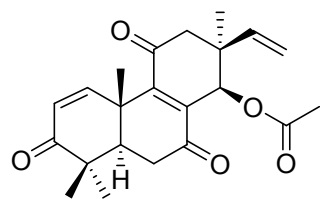
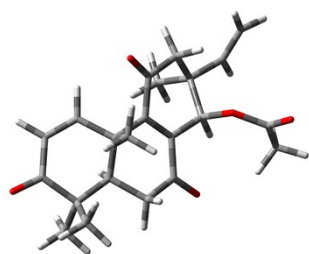
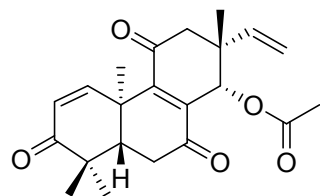


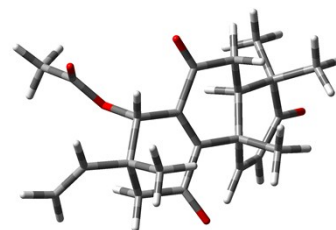
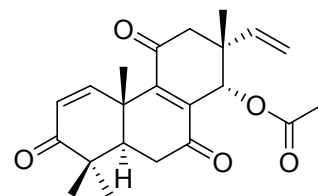
Figure S22. Relative Configurations and the Optimized Conformers for **2**



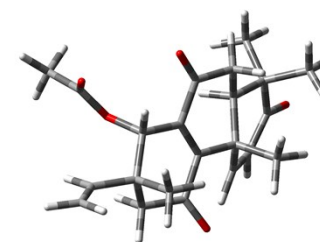
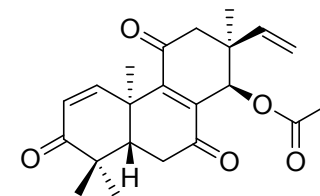
2a



2b



2c



2d

Figure S23. ^1H NMR Spectrum of Sarcosenone C (**3**; 600 MHz, CDCl_3)

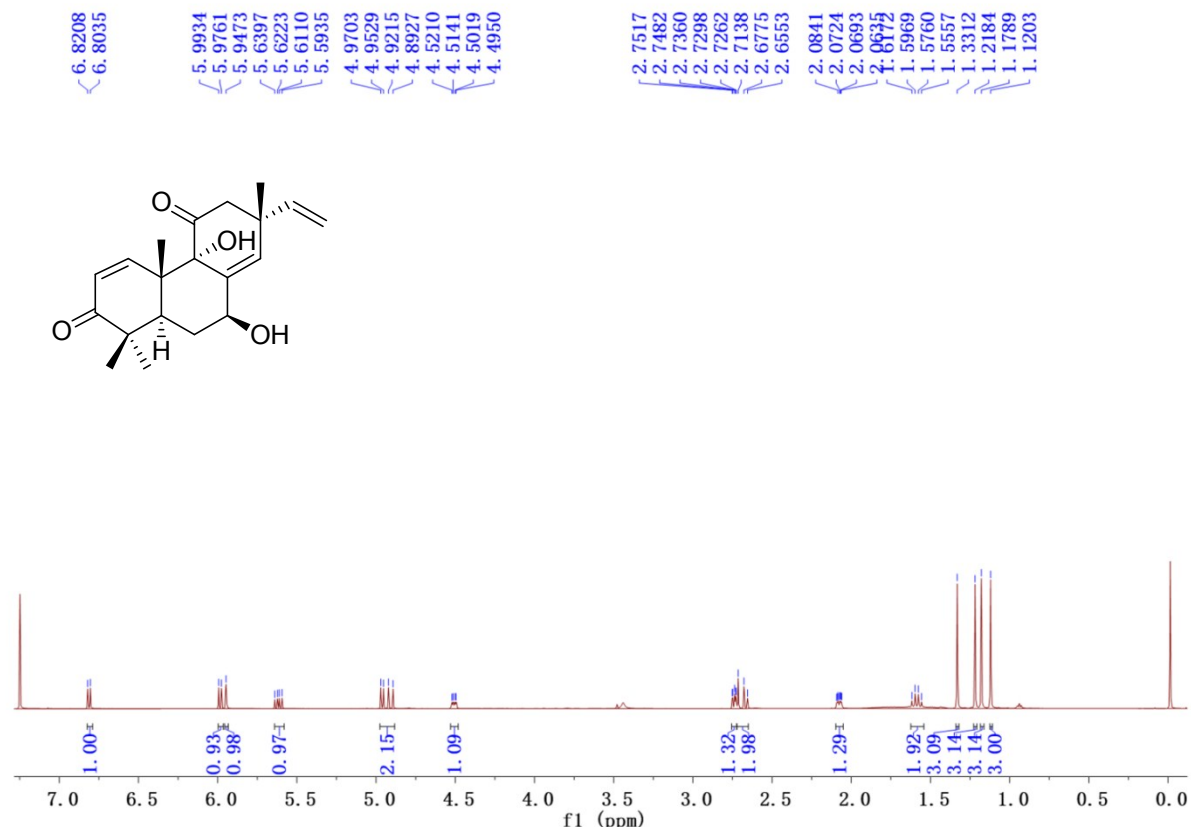


Figure S24. ^{13}C NMR Spectrum of Sarcosenone C (**3**; 150 MHz, CDCl_3)

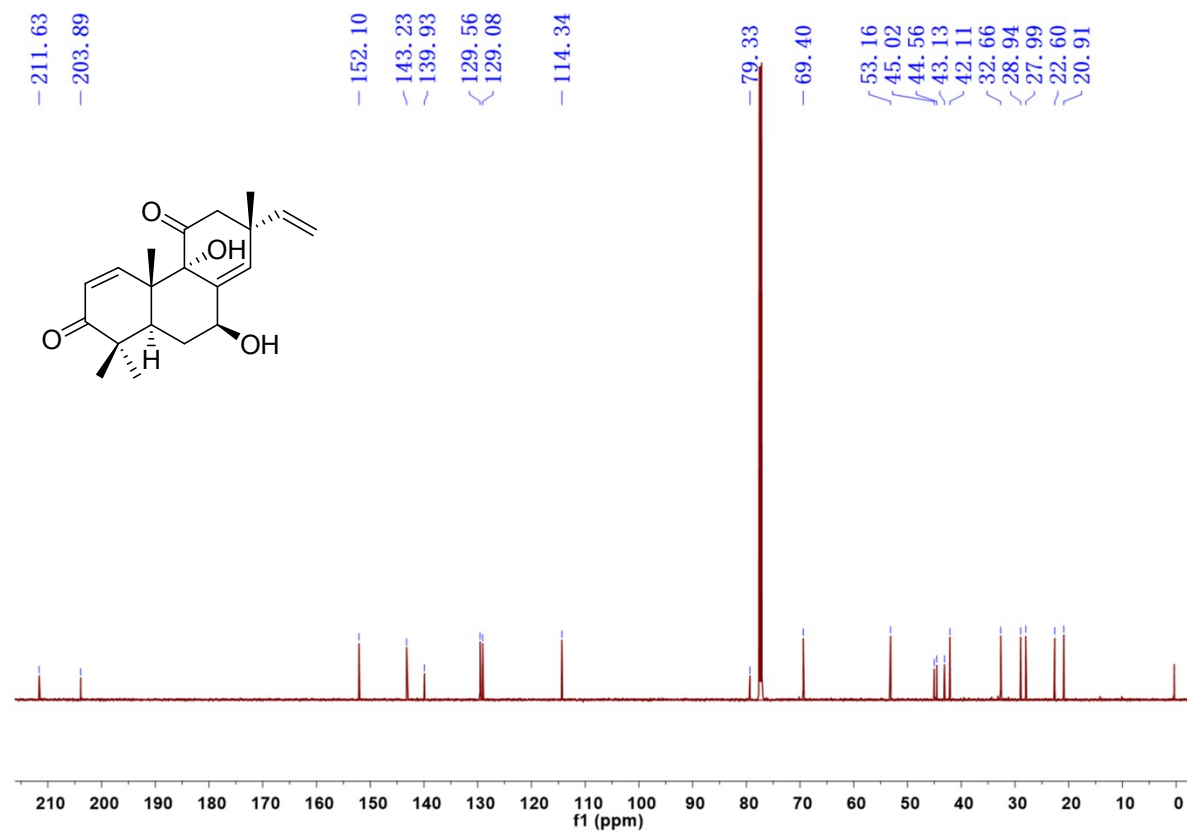


Figure S25. HSQC Spectrum of Sarcosenone C (**3**; 600 MHz, CDCl₃)

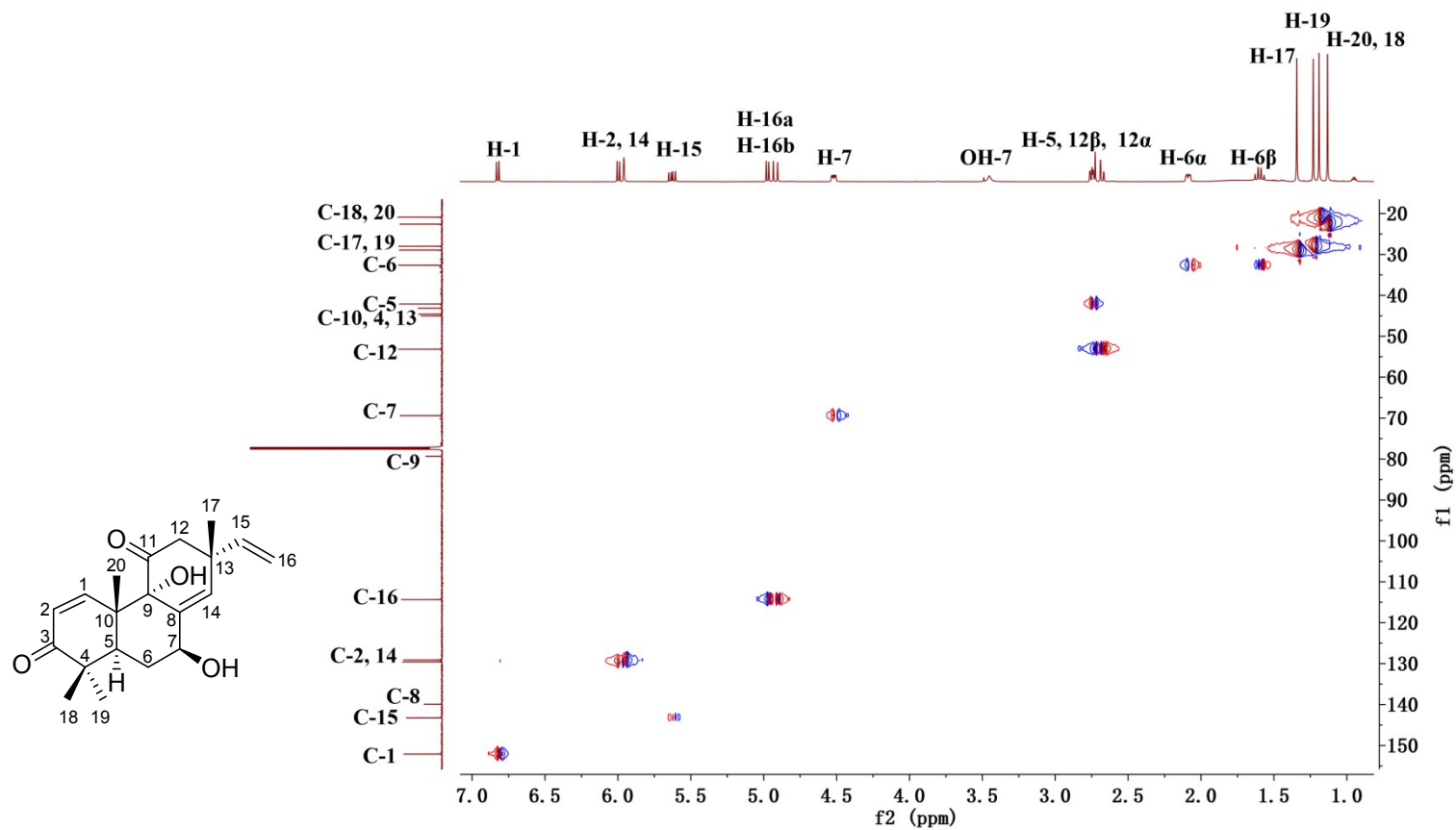


Figure S26. ^1H - ^1H COSY Spectrum of Sarcosone C (**3**; 600 MHz, CDCl_3)

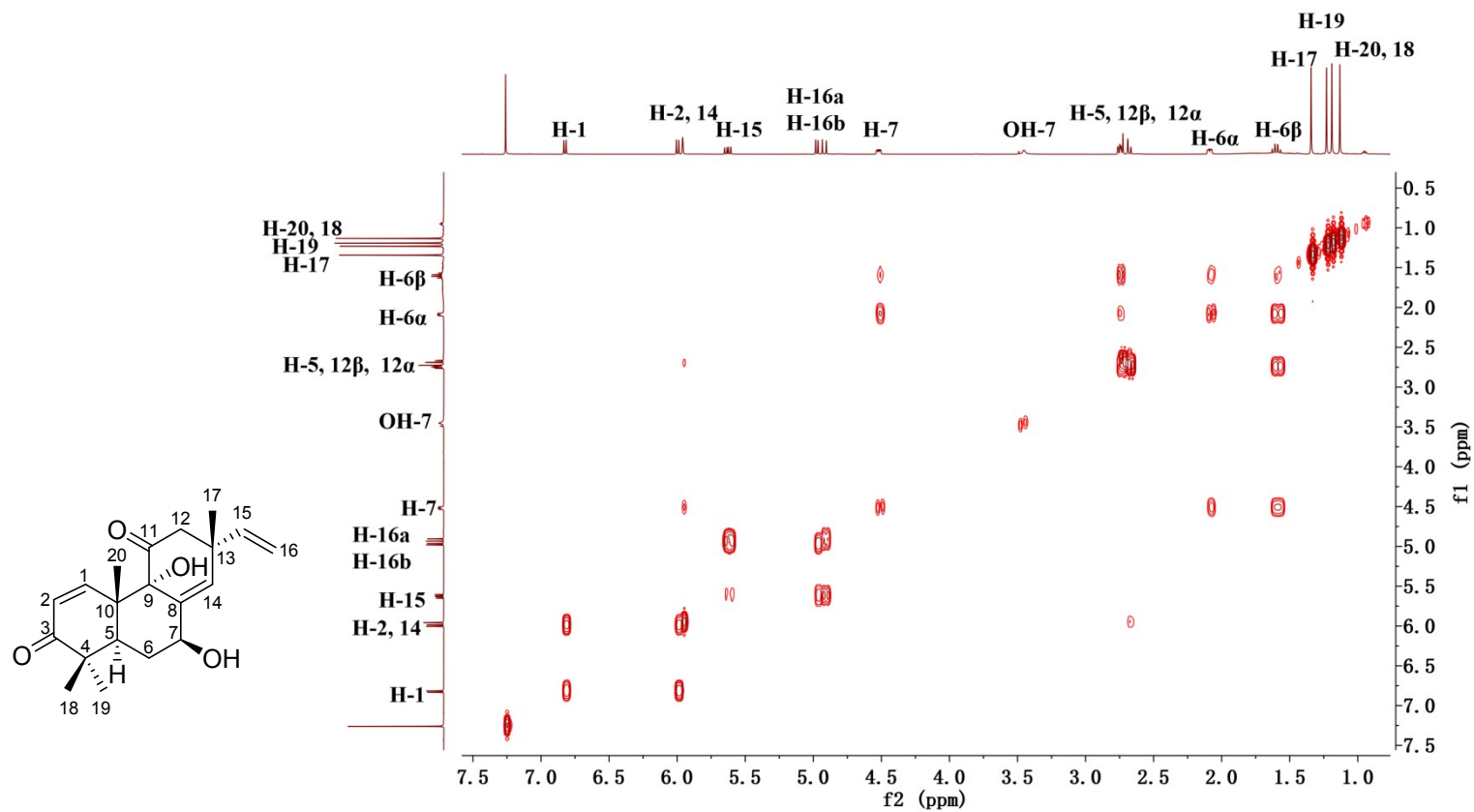


Figure S27. HMBC Spectrum of Sarcosenone C (**3**; 600 MHz, CDCl₃)

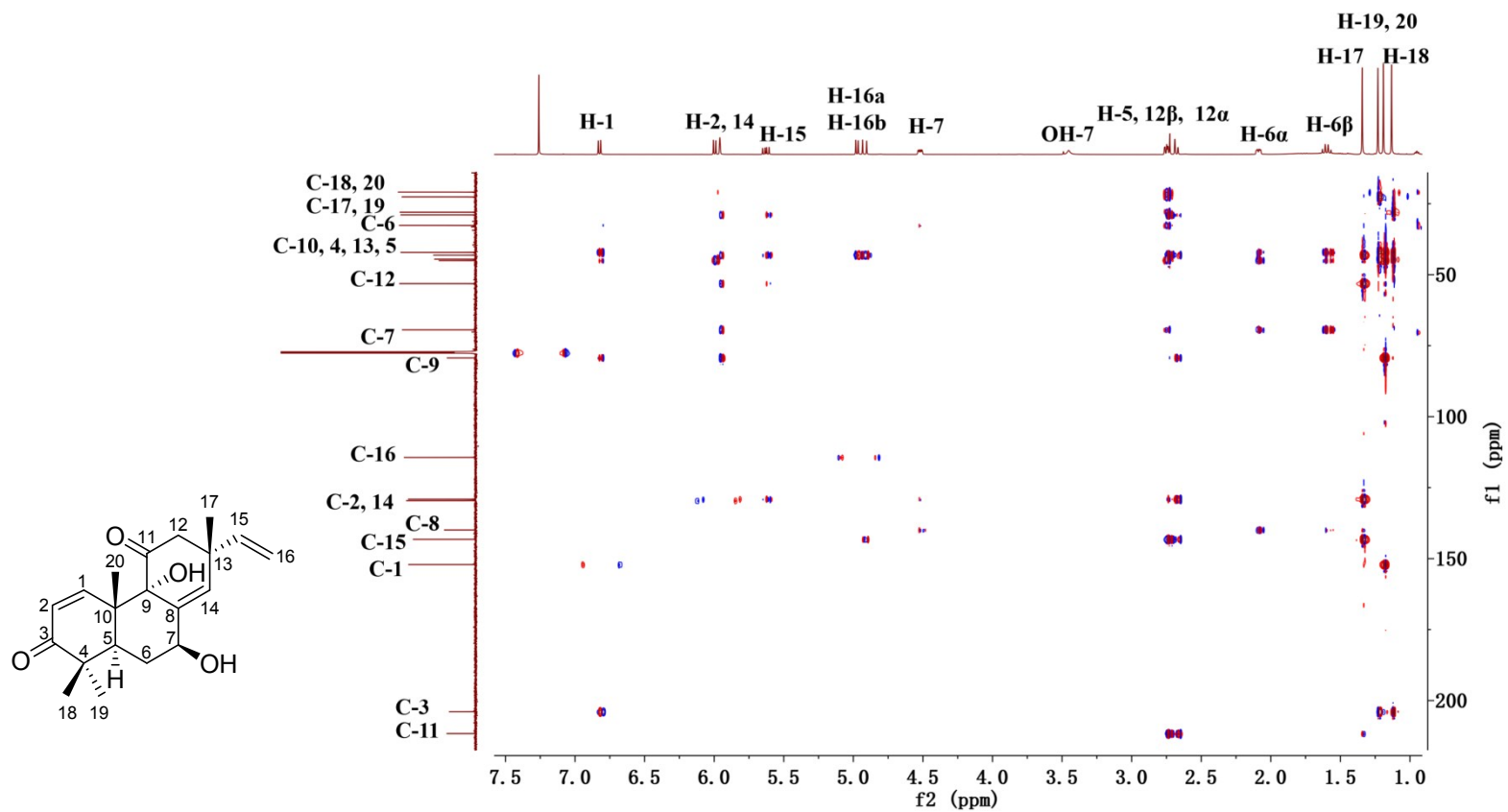


Figure S28. NOESY Spectrum of Sarcosenone C (**3**; 600 MHz, CDCl₃)

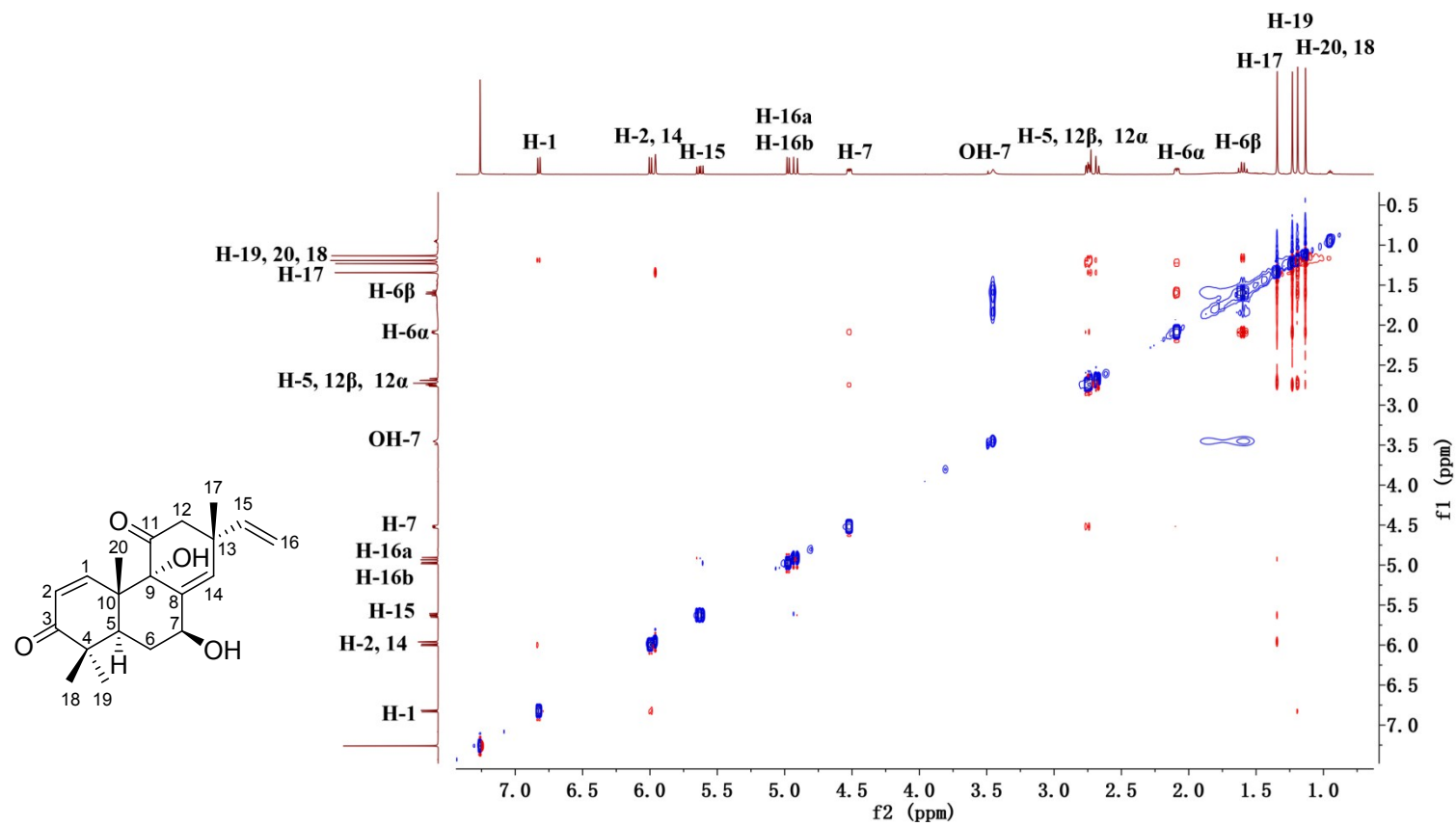


Figure S29. HRESIMS Spectrum of Sarcosenone C (3)

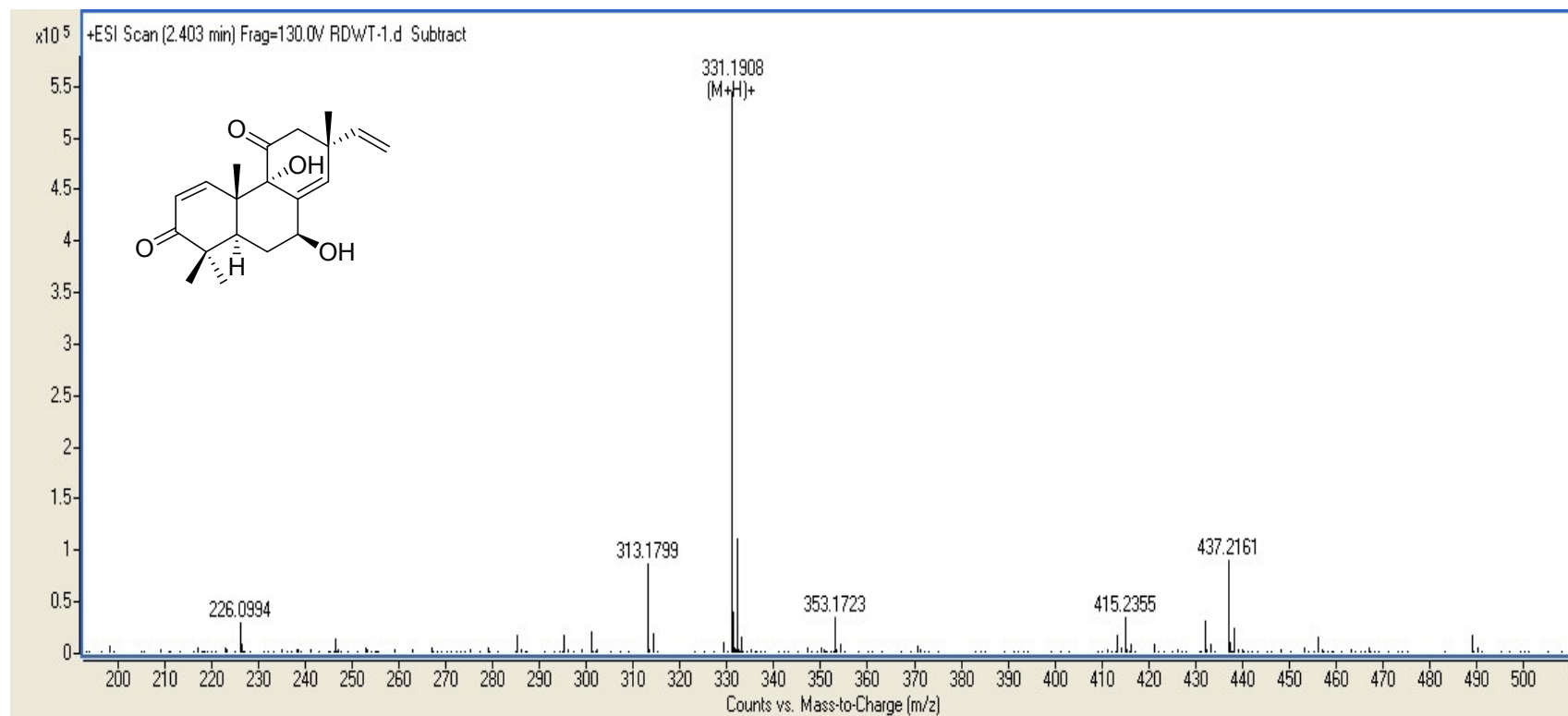


Figure S30. IR Spectrum of Sarcosenone C (3)

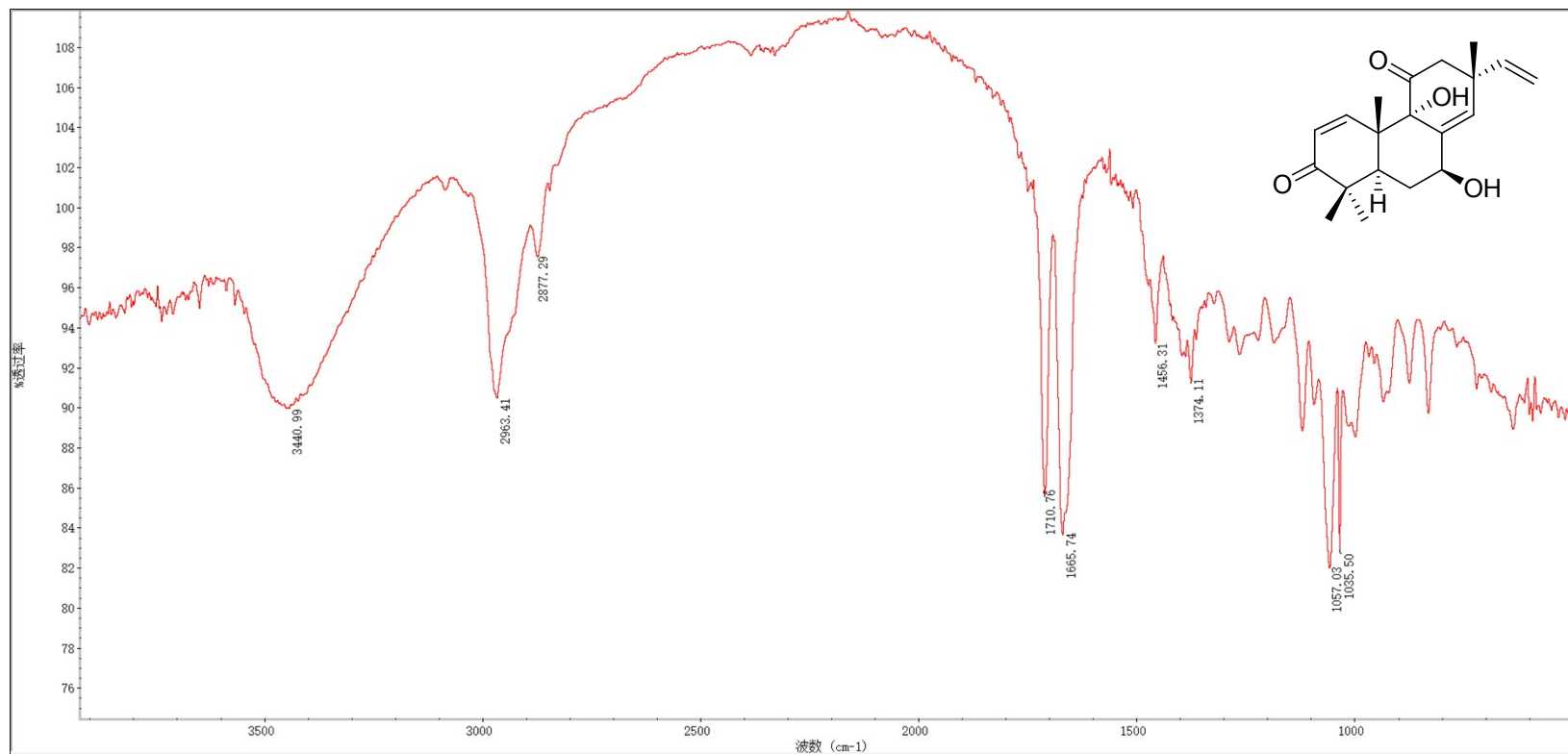


Figure S31. UV Spectrum of Sarcosenone C (**3**) in MeOH

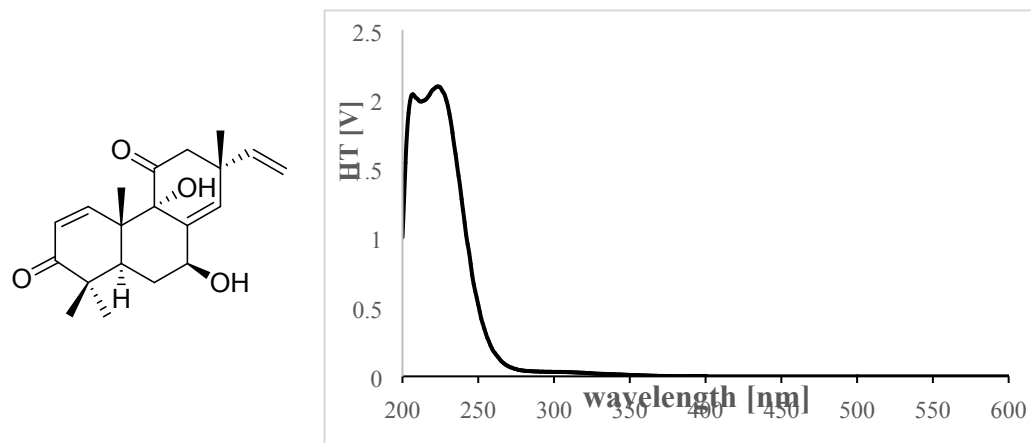


Figure S32. CD Spectrum of Sarcosenone C (**3**) in MeOH

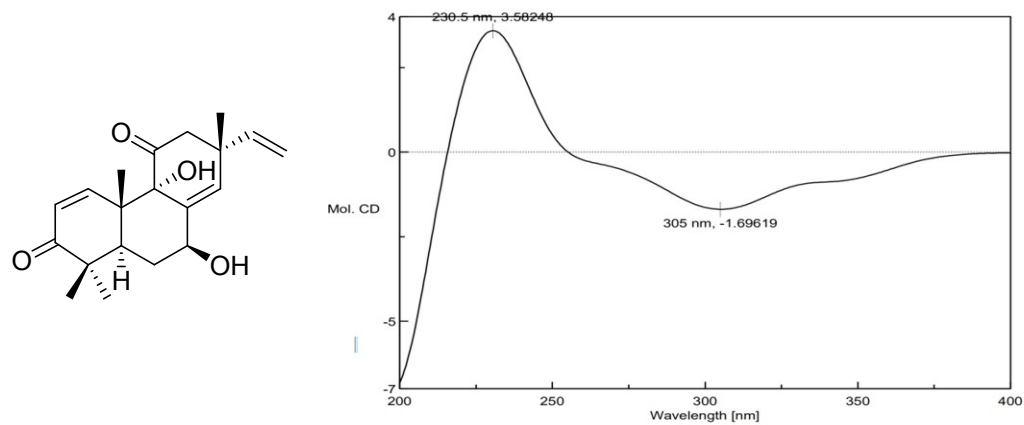
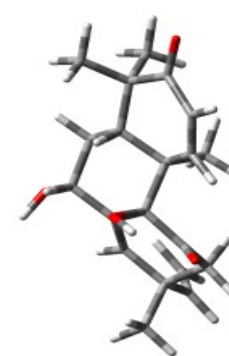
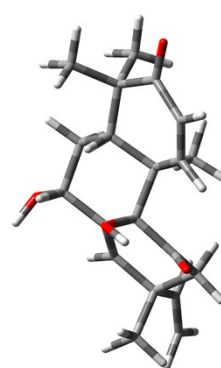
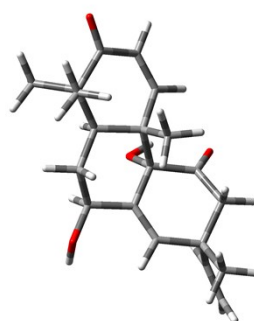
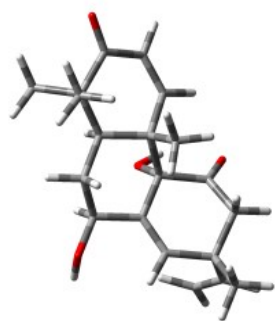
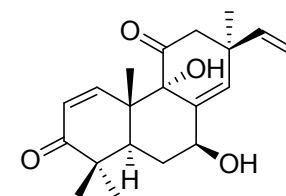
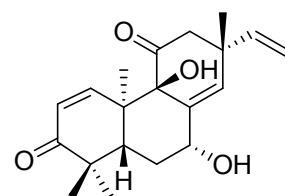
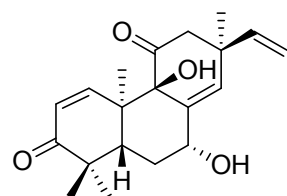
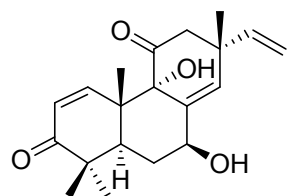


Figure S33. Relative Configurations and the Optimized Conformers for **3**



3a

3b

3c

3d

Figure S34. NOESY Spectrum of 9 α -Hydroxy-1,8(14),15-isopimaratrien-3,7,11-trione (**4**; 600 MHz, Acetone- d_6)

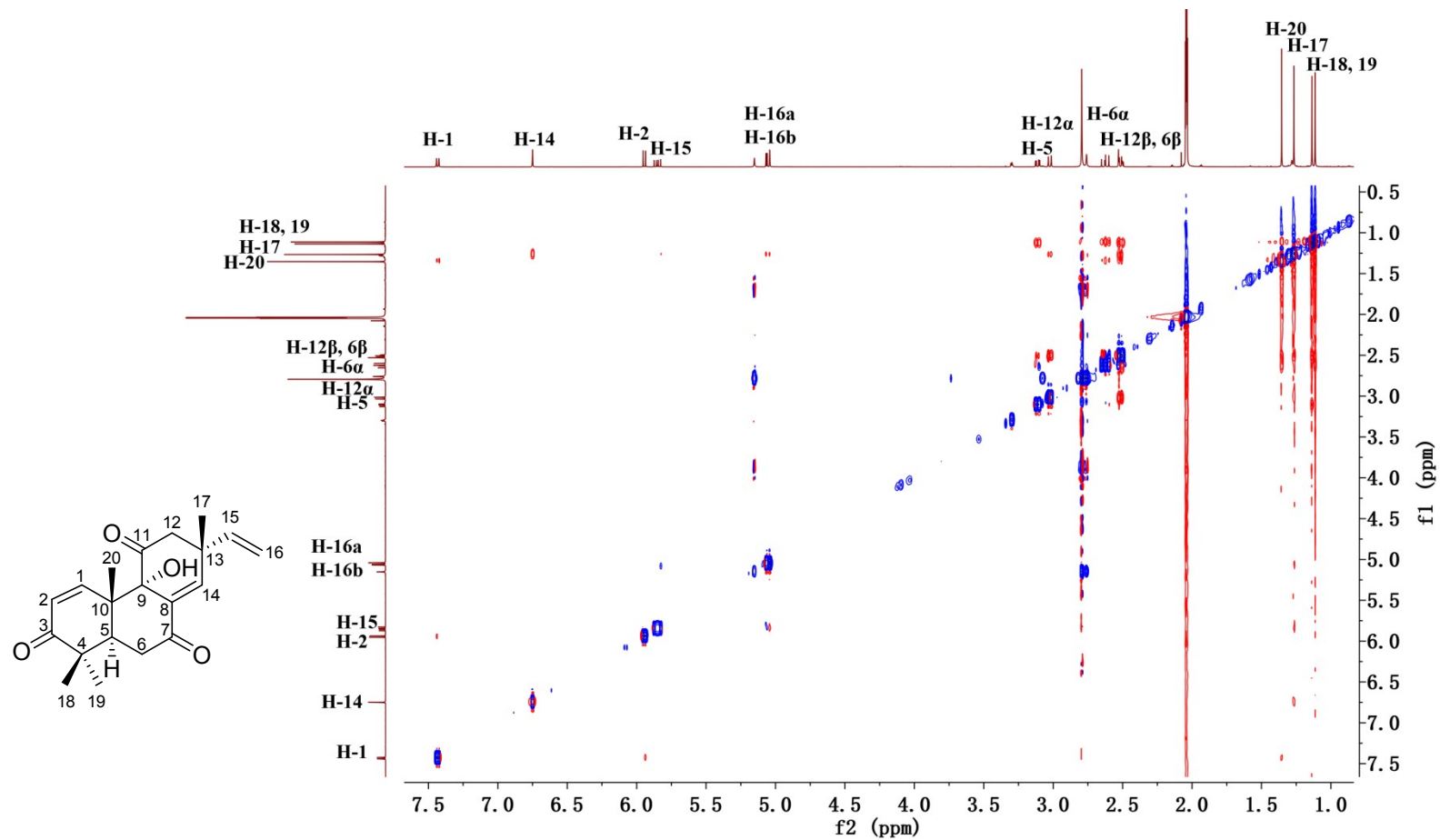


Figure S35. CD Spectrum of 9 α -Hydroxy-1,8(14),15-isopimaratrien-3,7,11-trione (**4**) in MeOH

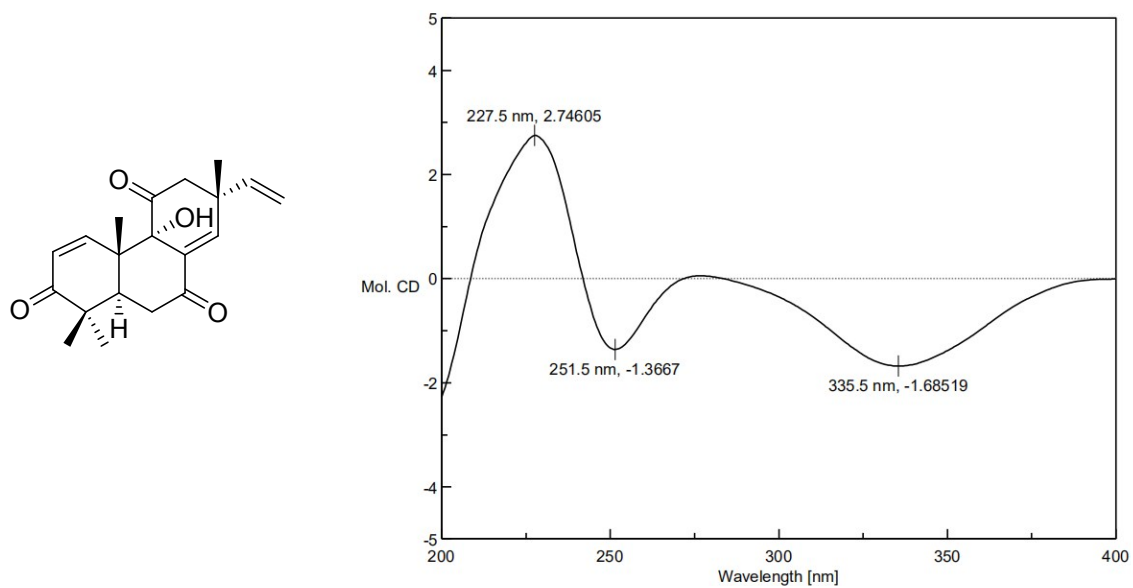
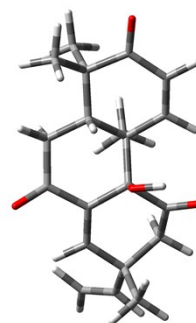
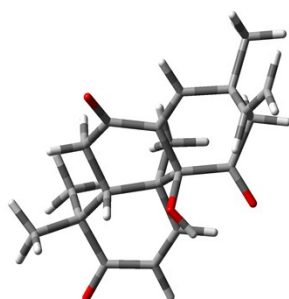
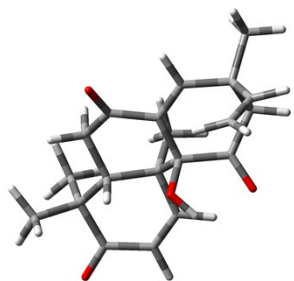
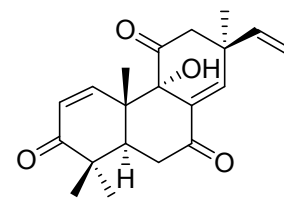
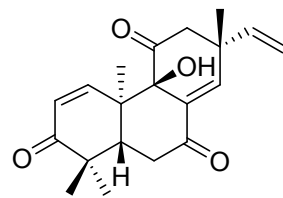
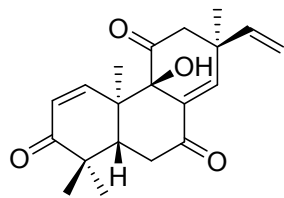
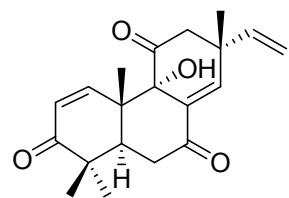


Figure S36. Relative Configurations and the Optimized Conformers for **4**

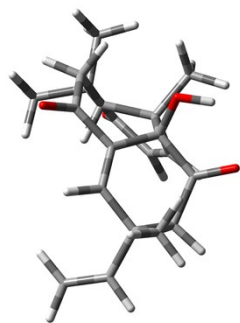
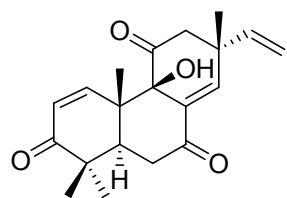


4a

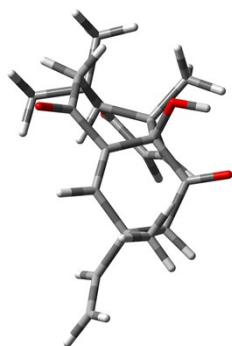
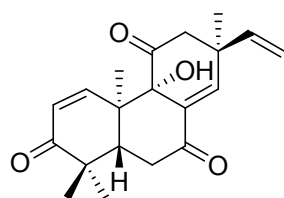
4b

4c

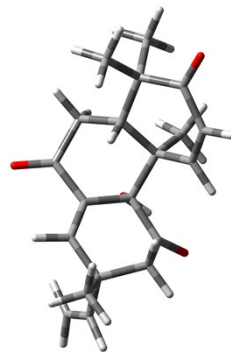
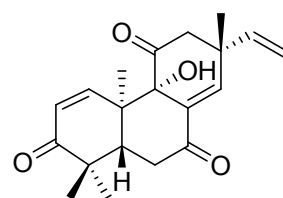
4d



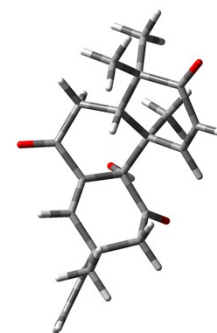
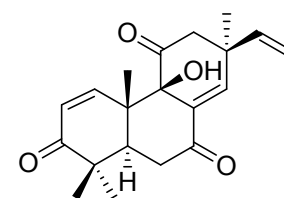
4e



4f



4g



4h

Scheme S1. Hypothetical Biosynthetic Pathways for 1–4

