

Supporting information

Alismanoid A, an unprecedented 1,2-*seco* bisabolene from *Alisma orientale* and the protective activity on H₂O₂-induced damage in SH-SY5Y cells

Zhen-Long Yu,^{a†} Yu-Lin Peng,^{a†} Chao Wang,^a Fei Cao,^b Xiao-Kui Huo,^a Xiang-Ge Tian,^c Lei Feng,^a
Jing Ning,^a Bao-Jing Zhang^a, Cheng-Peng Sun,^{*a} Xiao-Chi Ma^{*a,d}

Content

Figure S1. ^1H NMR spectrum of 1 (600 MHz, CD_3OD)	3
Figure S2. ^{13}C NMR spectrum of 1 (150 MHz, CD_3OD)	3
Figure S3. HSQC spectrum of 1 (600 MHz, CD_3OD)	4
Figure S4. HMBC spectrum of 1 (600 MHz, CD_3OD)	4
Figure S5. HRESIMS spectrum of 1	5
Figure S6. ECD spectrum of 1a	6
Figure S7. ECD spectrum of 1b	7
Figure S8. ^1H NMR spectrum of 2 (600 MHz, CD_3OD)	8
Figure S9. ^{13}C NMR spectrum of 2 (150 MHz, CD_3OD)	8
Figure S10. HSQC spectrum of 2 (600 MHz, CD_3OD)	9
Figure S11. HMBC spectrum of 2 (600 MHz, CD_3OD)	9
Figure S12. NOESY spectrum of 2 (600 MHz, CD_3OD)	10
Figure S13. HRESIMS spectrum of 2	11
Figure S14. ^1H NMR spectrum of 3 (600 MHz, CD_3OD)	11
Figure S15. ^{13}C NMR spectrum of 3 (150 MHz, CD_3OD)	12
Figure S16. HSQC spectrum of 3 (600 MHz, CD_3OD)	12
Figure S17. HMBC spectrum of 3 (600 MHz, MeOH-d_4)	13
Figure S18. COSY spectrum of 3 (600 MHz, CD_3OD)	13
Figure S19. NOESY spectrum of 3 (600 MHz, CD_3OD)	14
Figure S20. HRESIMS spectrum of 3	14
Figure S21. Lowest energy conformers for (4R,6R,7R)-2	15
Figure S22. Lowest energy conformers for (4S,6S,7S)-2	16
Table S1 Energy analysis for (4R,6R,7R)-2	16
Table S2 Energy analysis for (4S,6S,7S)-2	16

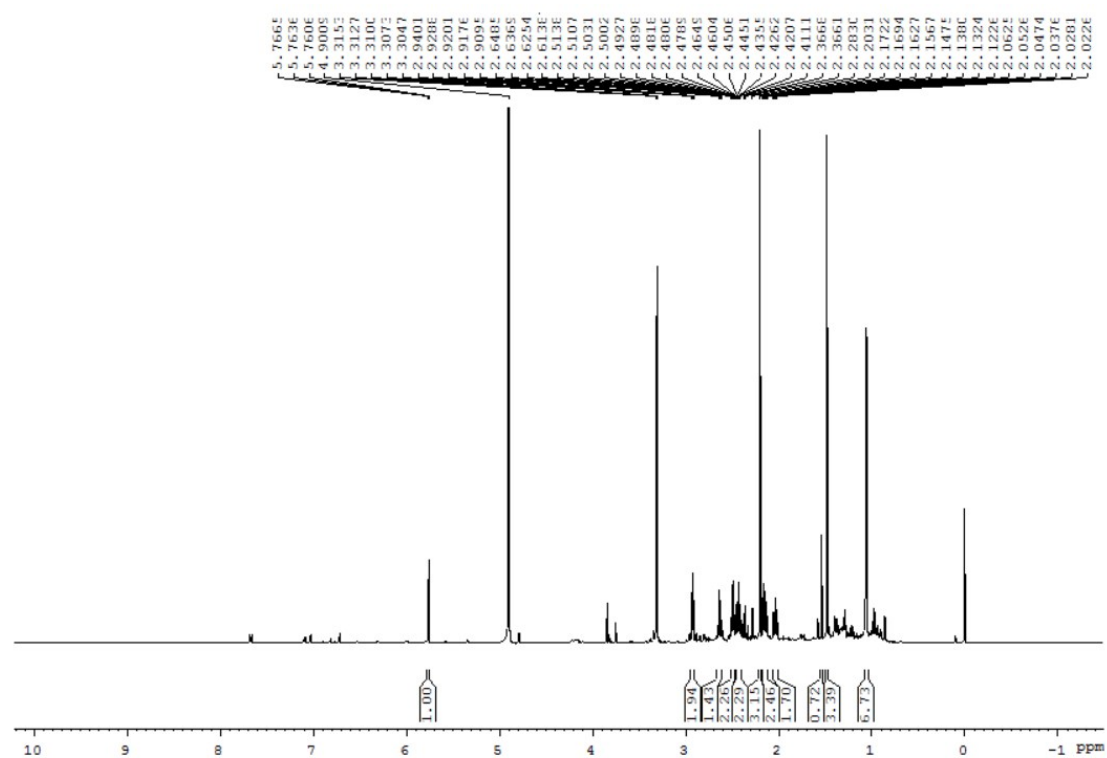


Figure S1. ^1H NMR spectrum of **1** (600 MHz, CD_3OD)

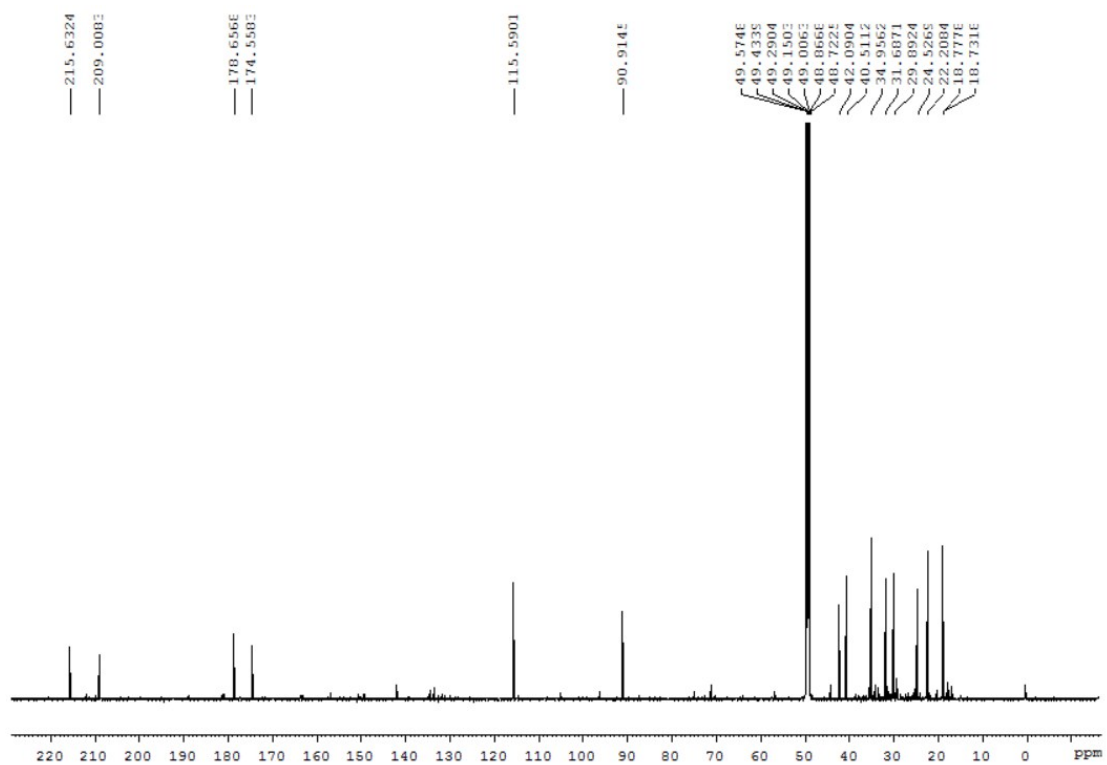


Figure S2. ^{13}C NMR spectrum of **1** (150 MHz, CD_3OD)

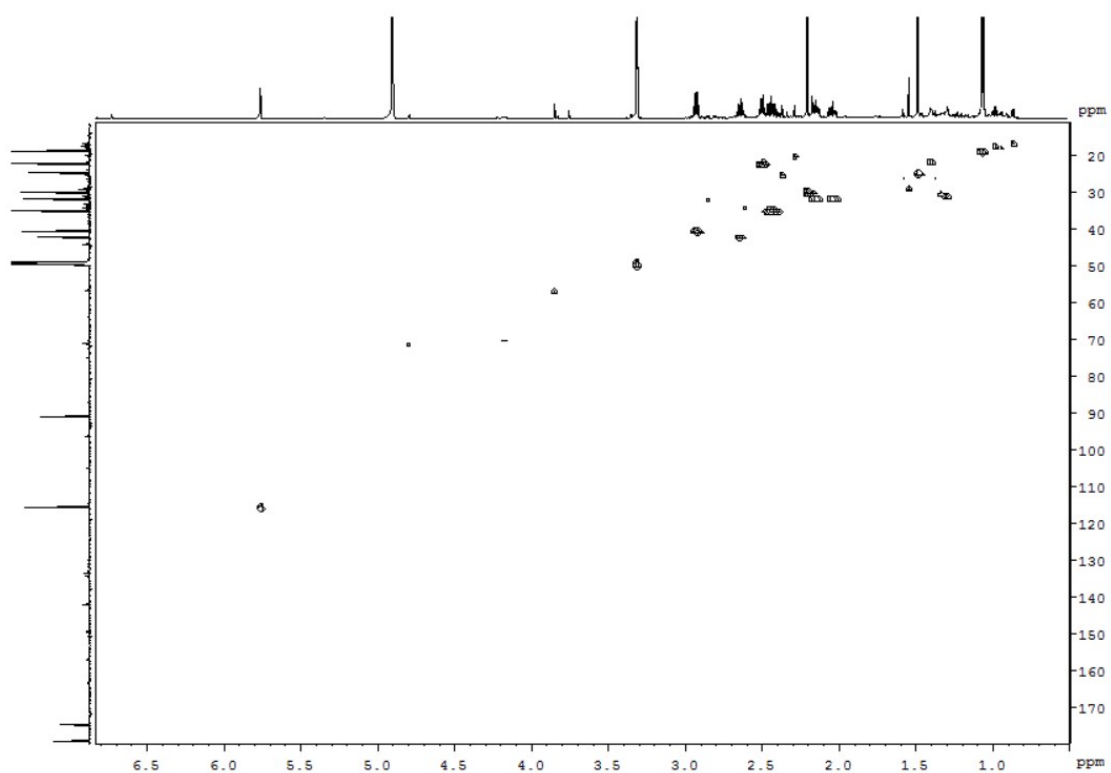


Figure S3. HSQC spectrum of 1 (600 MHz, CD₃OD)

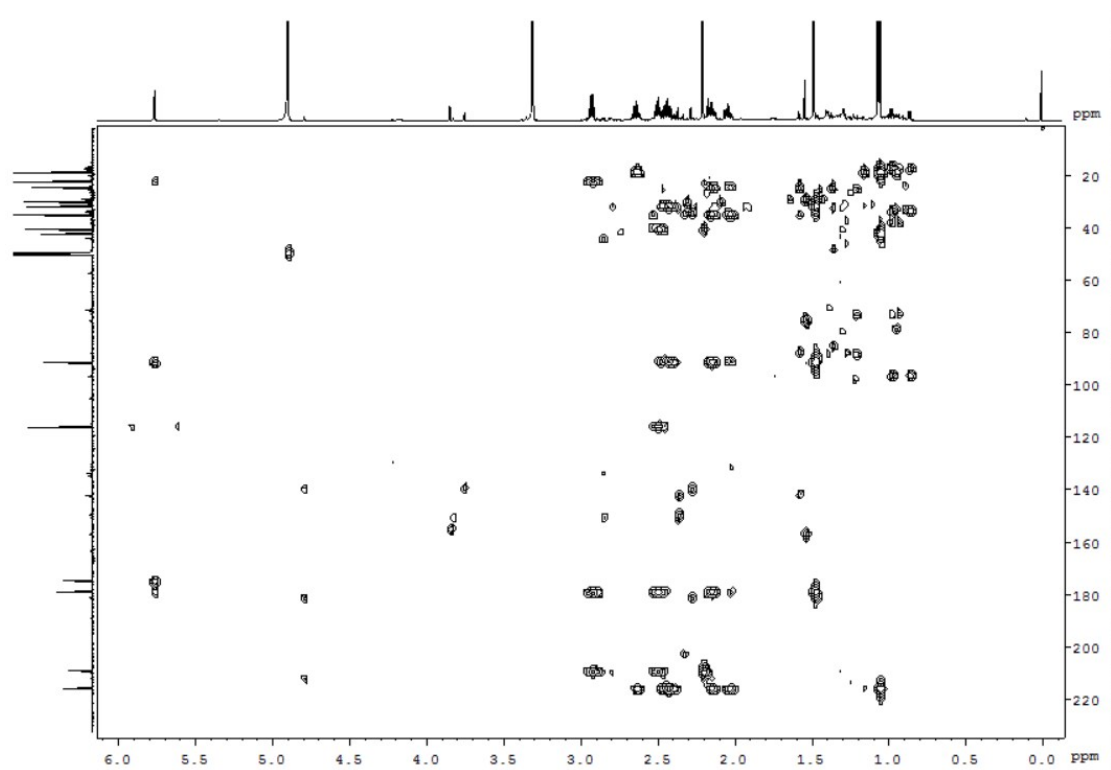


Figure S4. HMBC spectrum of 1 (600 MHz, CD₃OD)

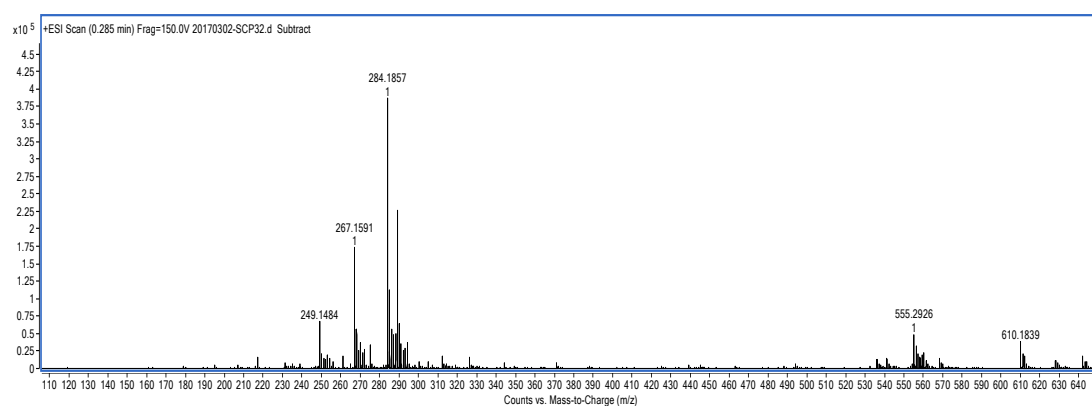


Figure S5. HRESIMS spectrum of **1**

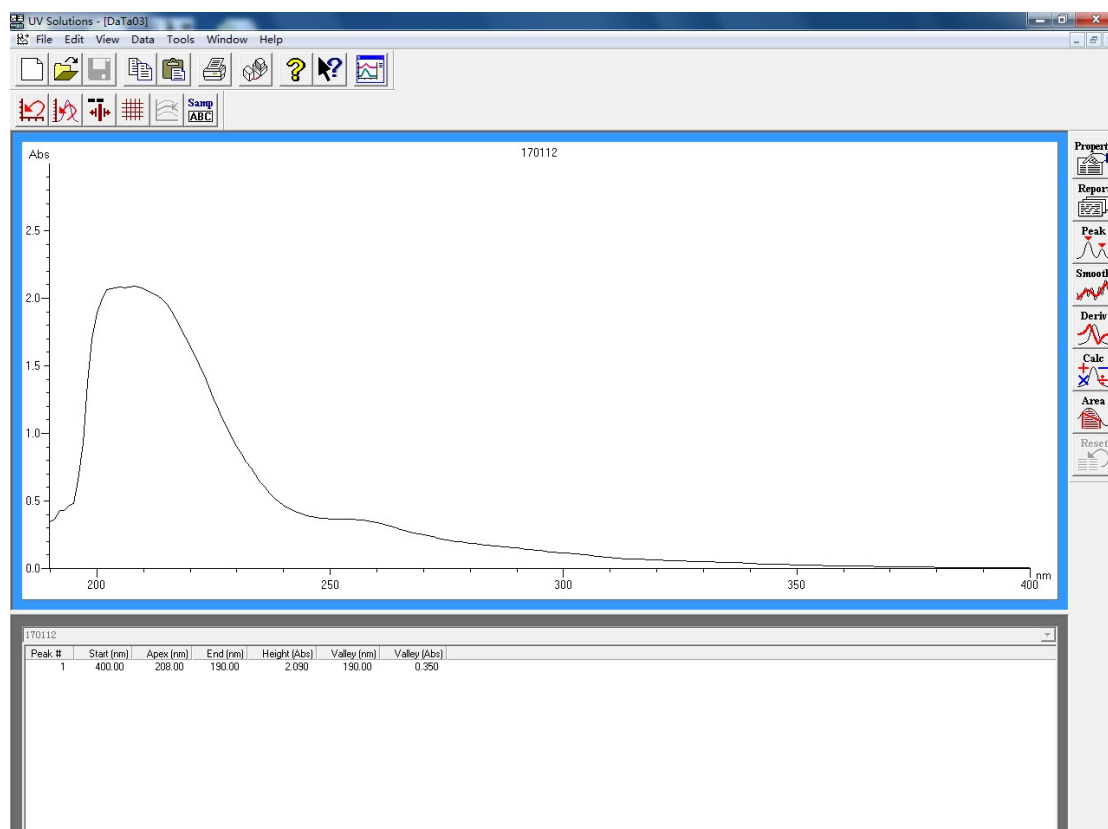


Figure S6. UV spectrum of **1**

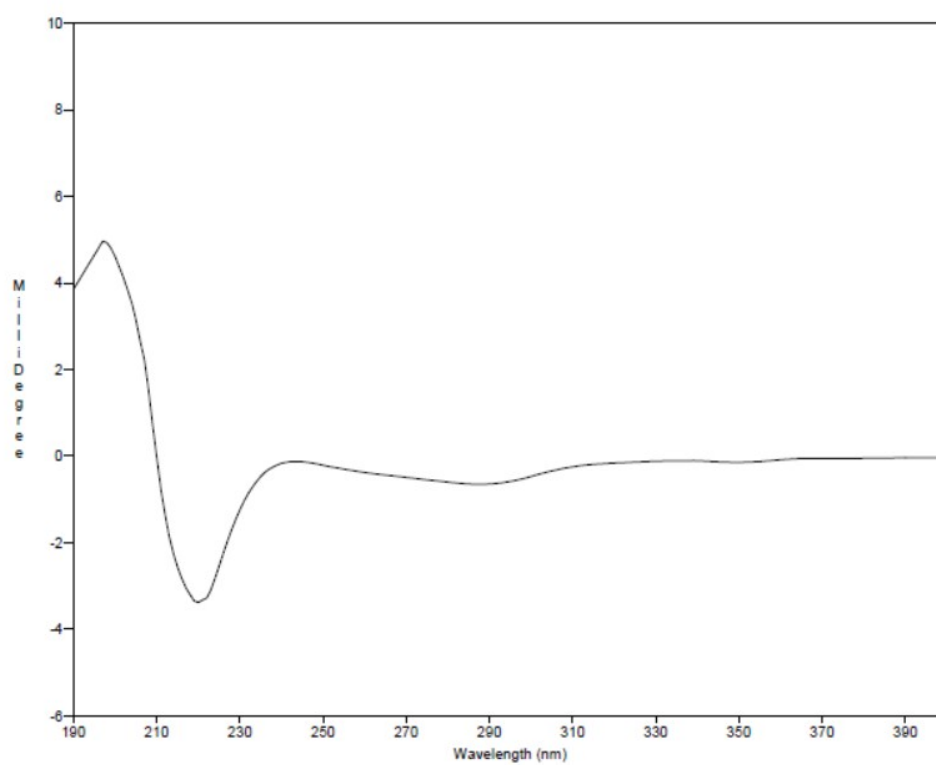


Figure S7. ECD spectrum of 1a

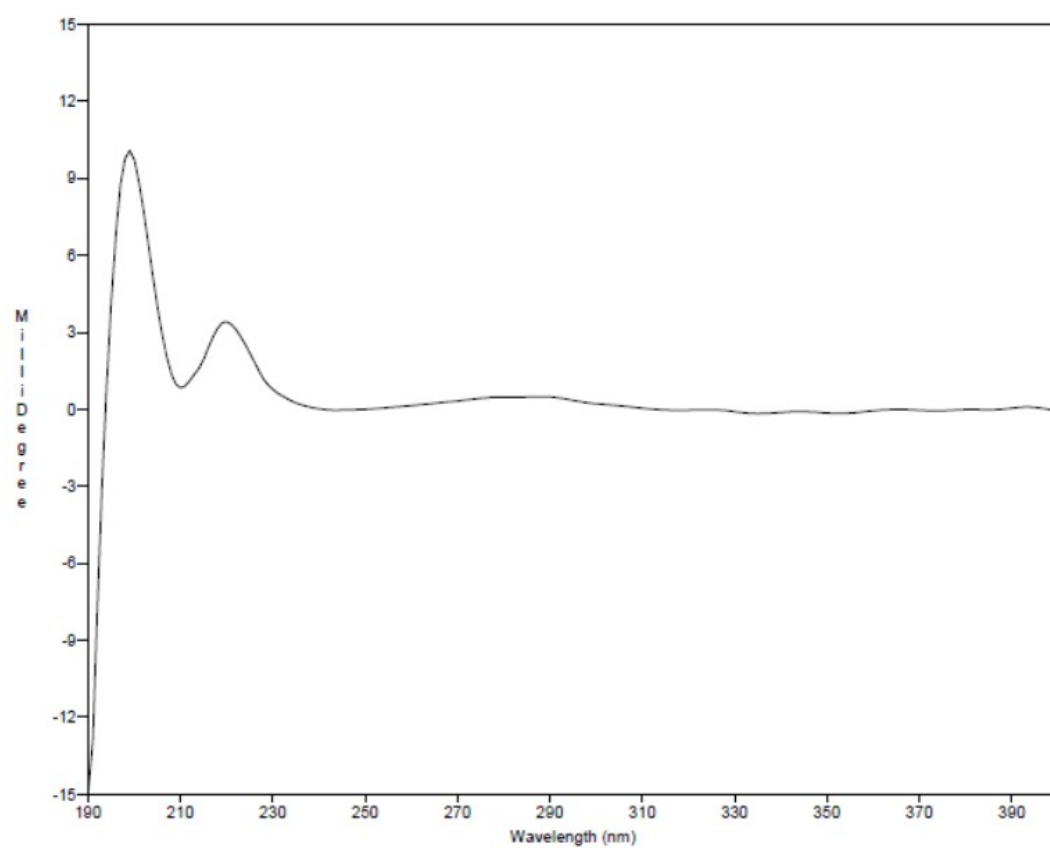


Figure S8. ECD spectrum of 1b

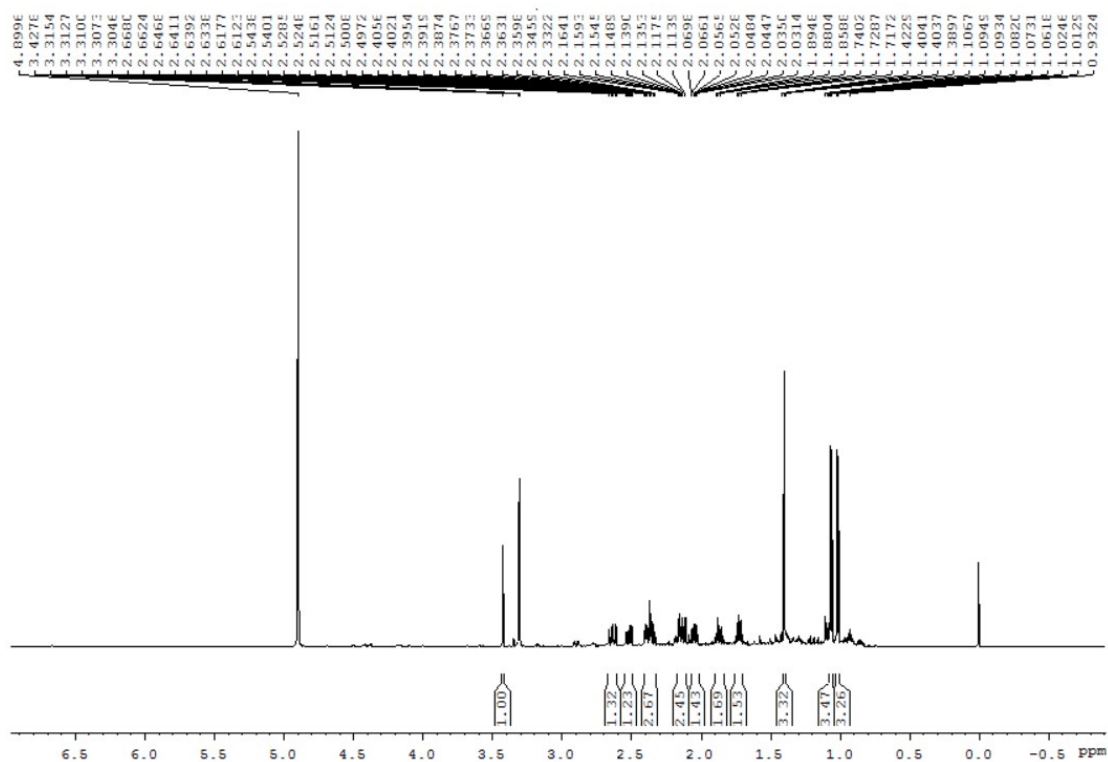


Figure S9. ¹H NMR spectrum of 2 (600 MHz, CD₃OD)

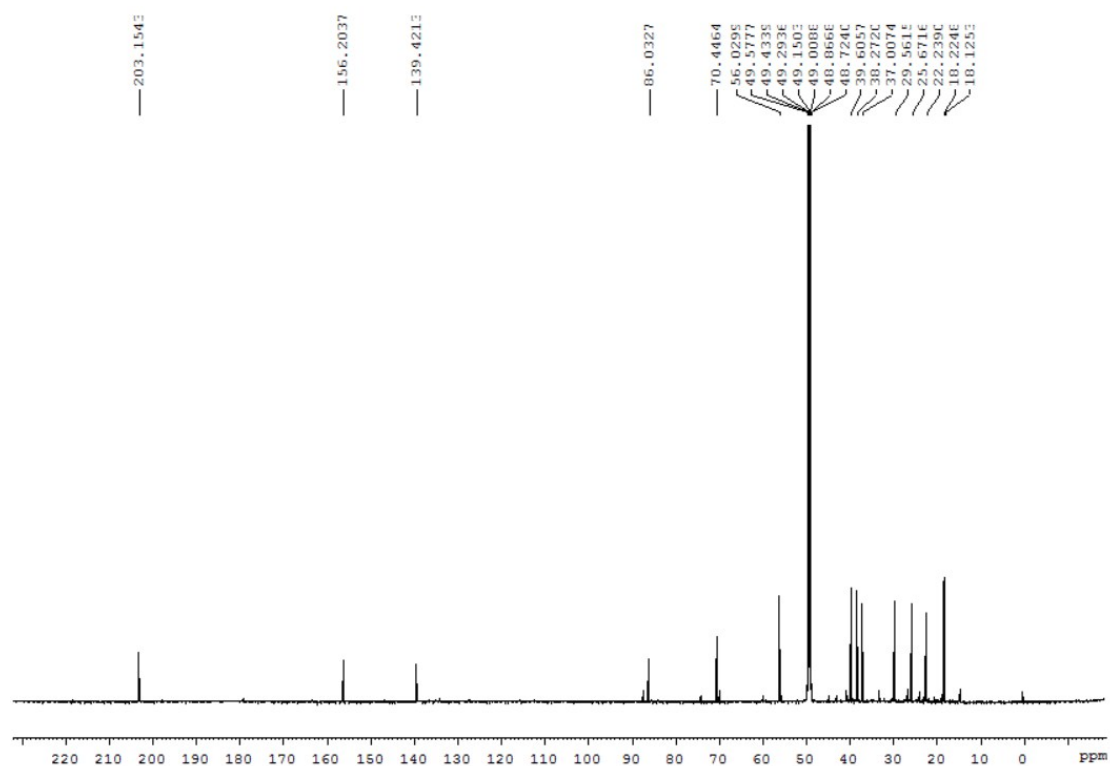


Figure S10. ¹³C NMR spectrum of 2 (150 MHz, CD₃OD)

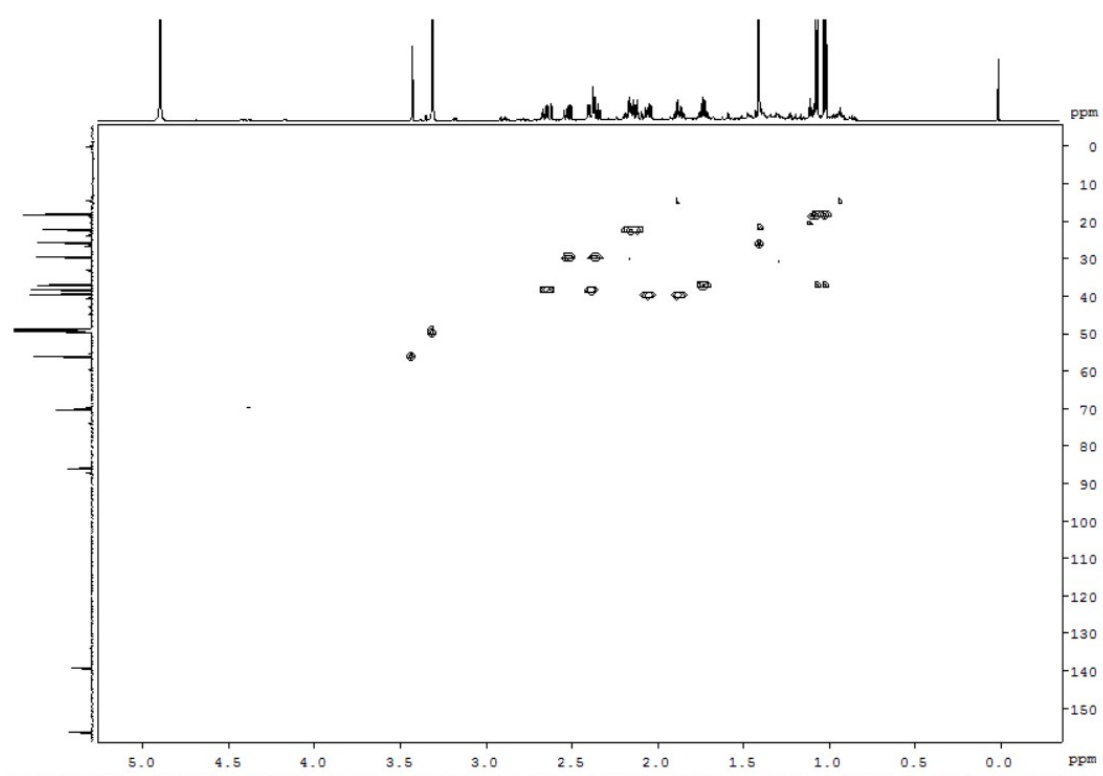


Figure S11. HSQC spectrum of 2 (600 MHz, CD_3OD)

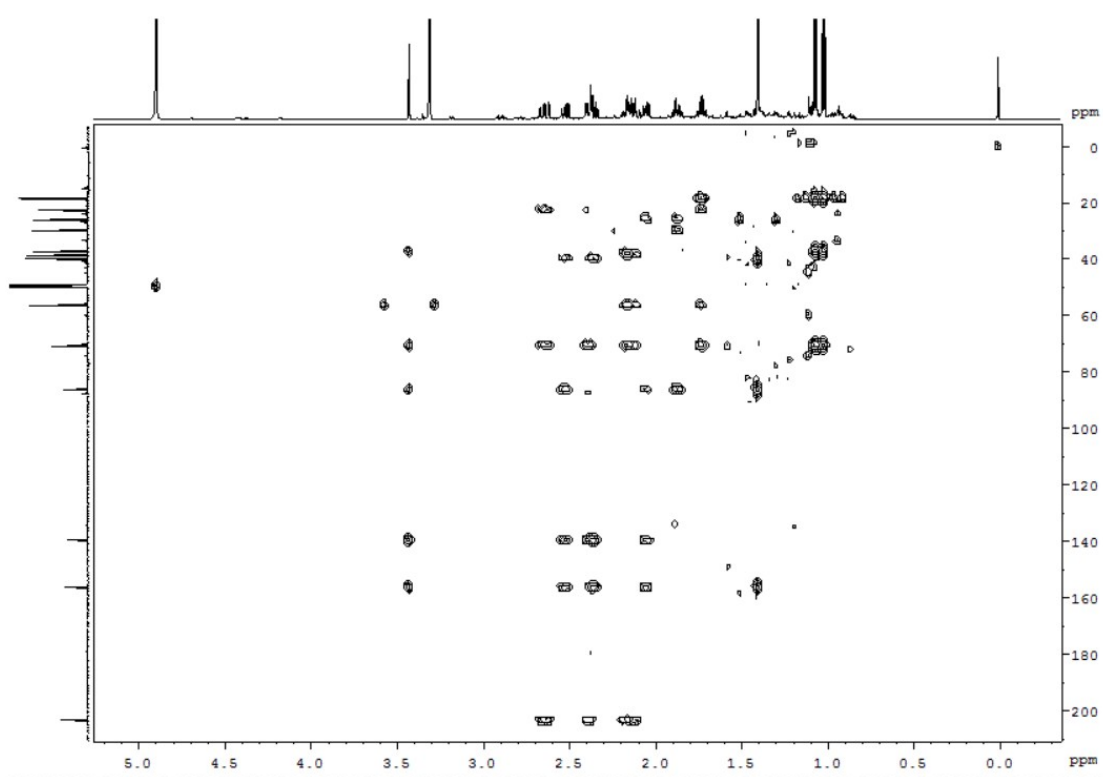


Figure S12. HMBC spectrum of 2 (600 MHz, CD_3OD)

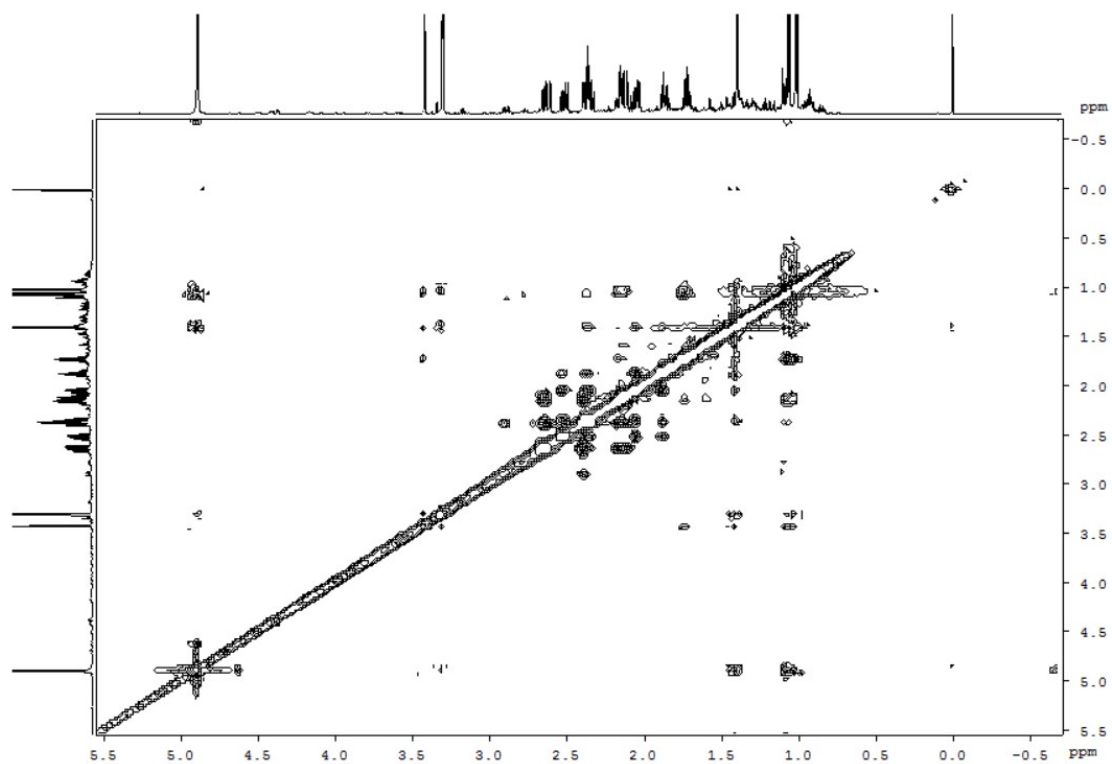


Figure S13. NOESY spectrum of **2** (600 MHz, CD₃OD)

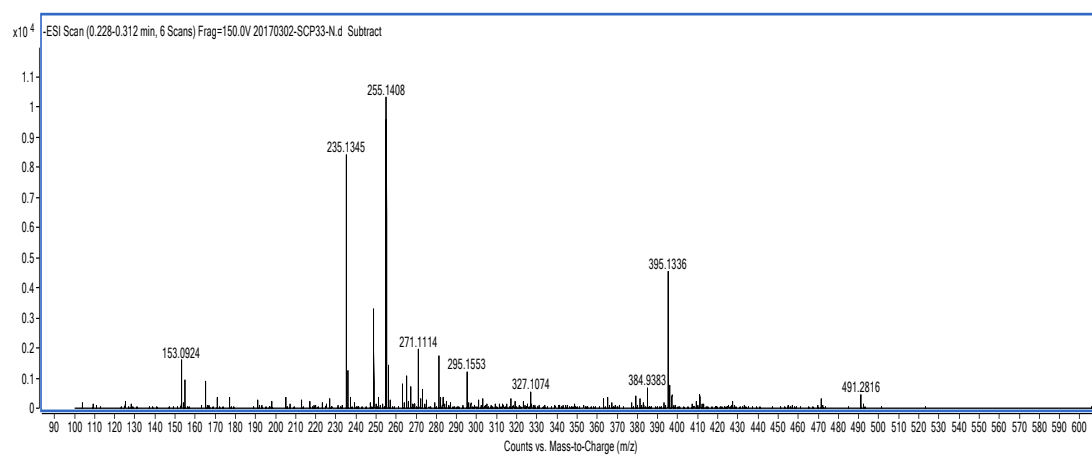


Figure S14. HRESIMS spectrum of 2

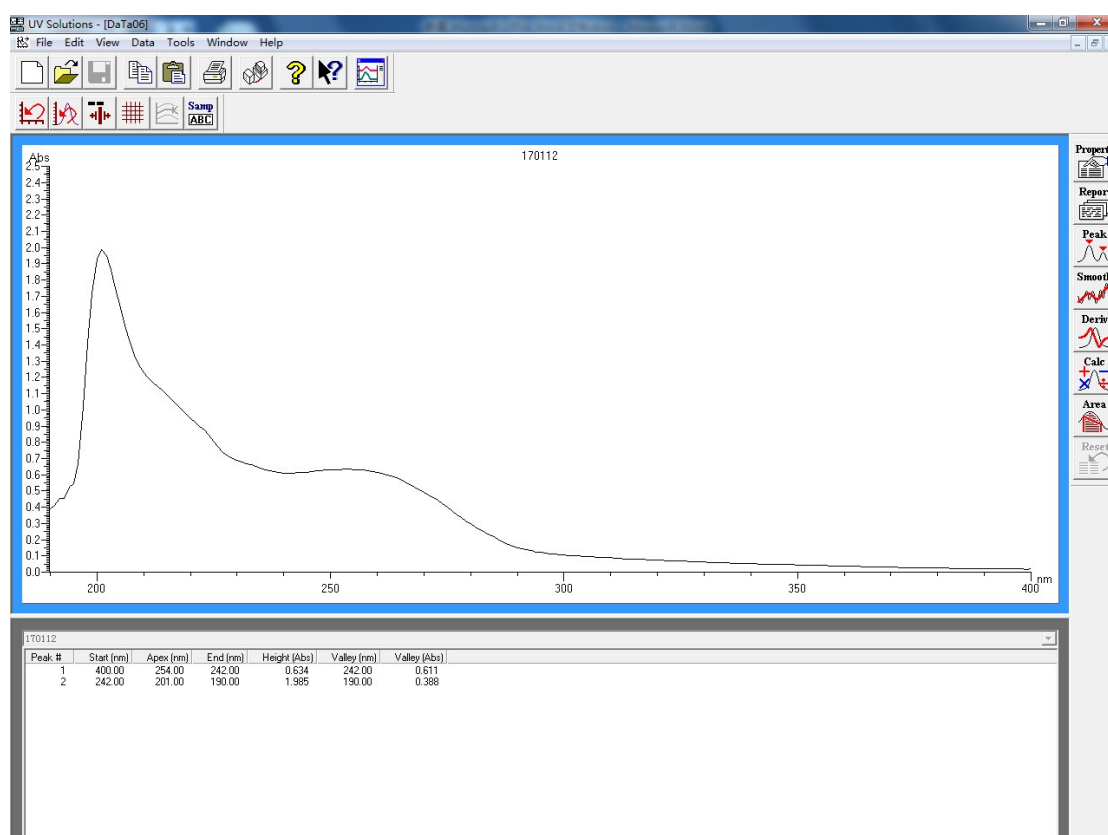


Figure S15. UV spectrum of 2

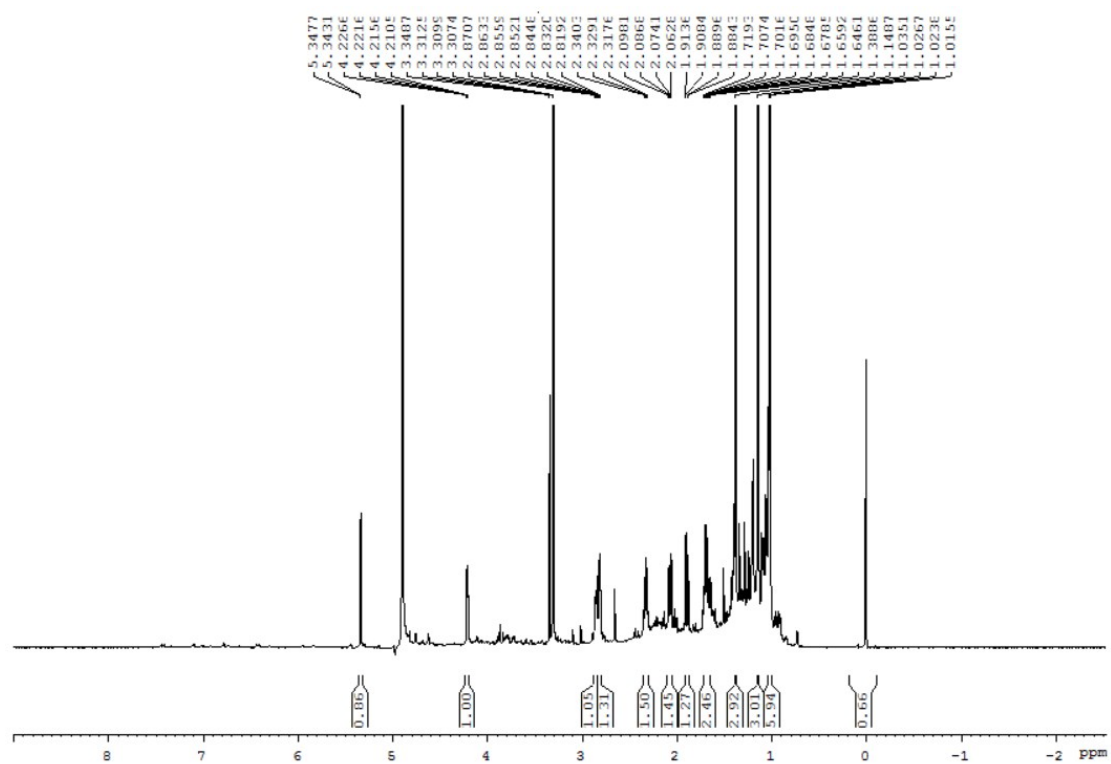


Figure S16. ^1H NMR spectrum of 3 (600 MHz, CD_3OD)

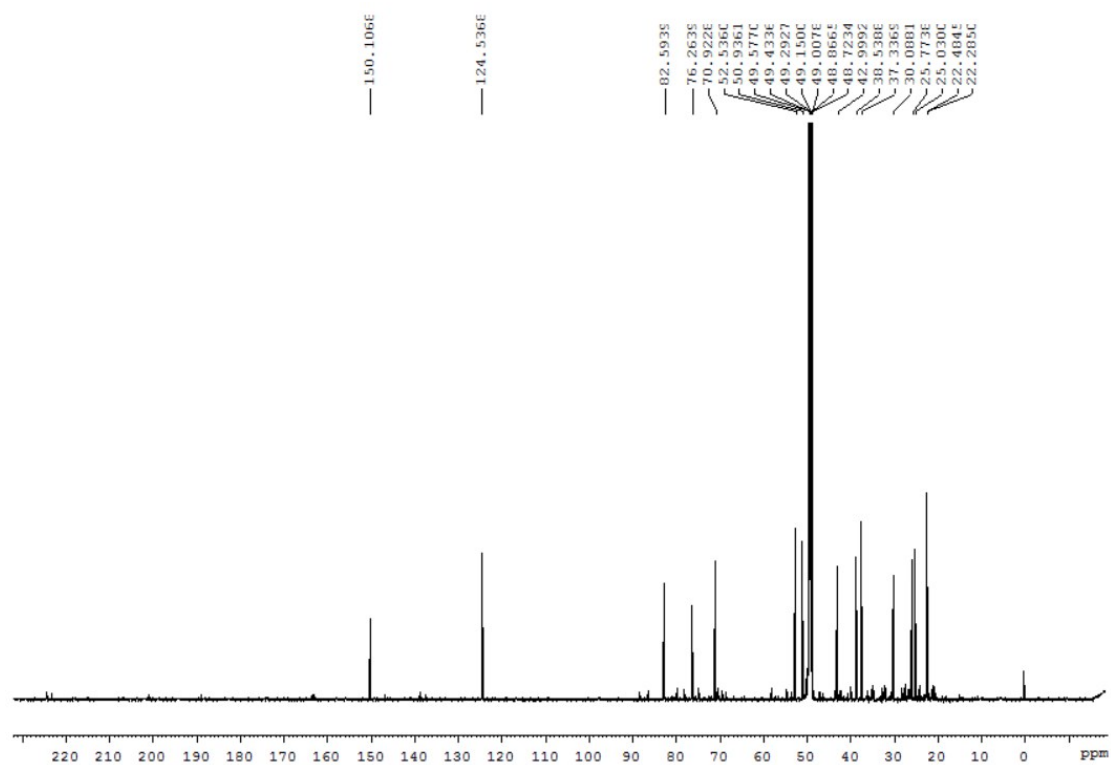


Figure S17. ^{13}C NMR spectrum of 3 (150 MHz, CD_3OD)

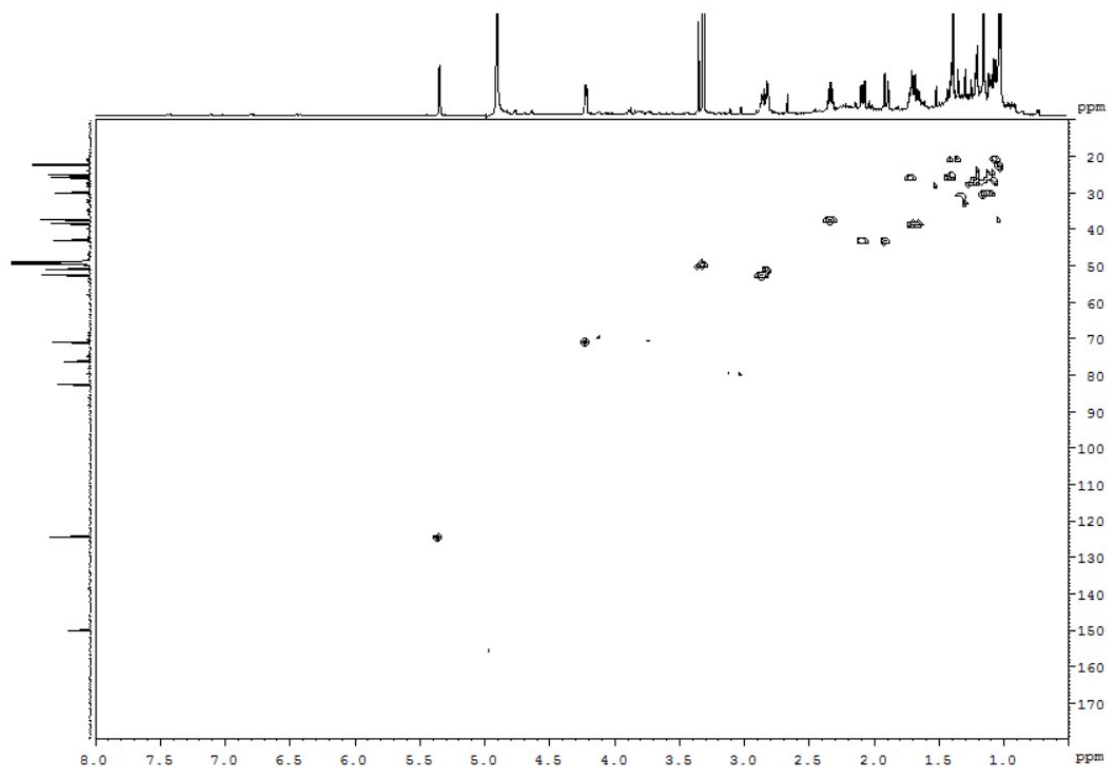


Figure S18. HSQC spectrum of 3 (600 MHz, CD_3OD)

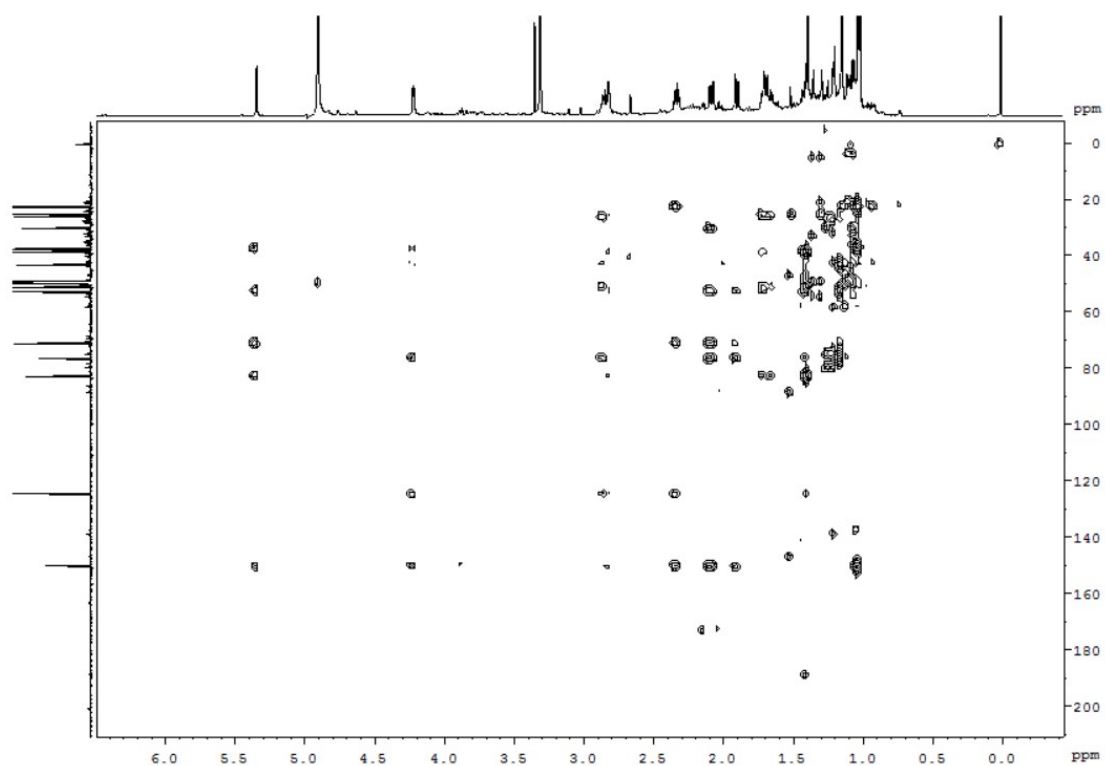


Figure S19. HMBC spectrum of 3 (600 MHz, MeOH- d_4)

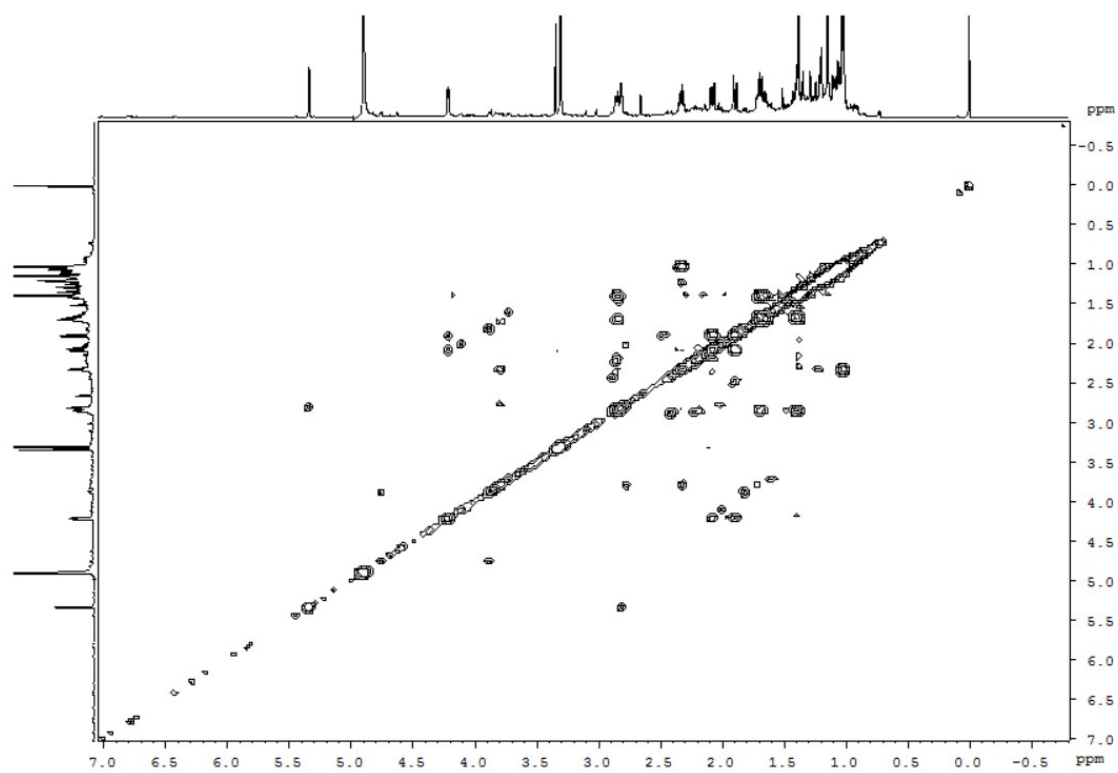


Figure S20. COSY spectrum of 3 (600 MHz, CD₃OD)

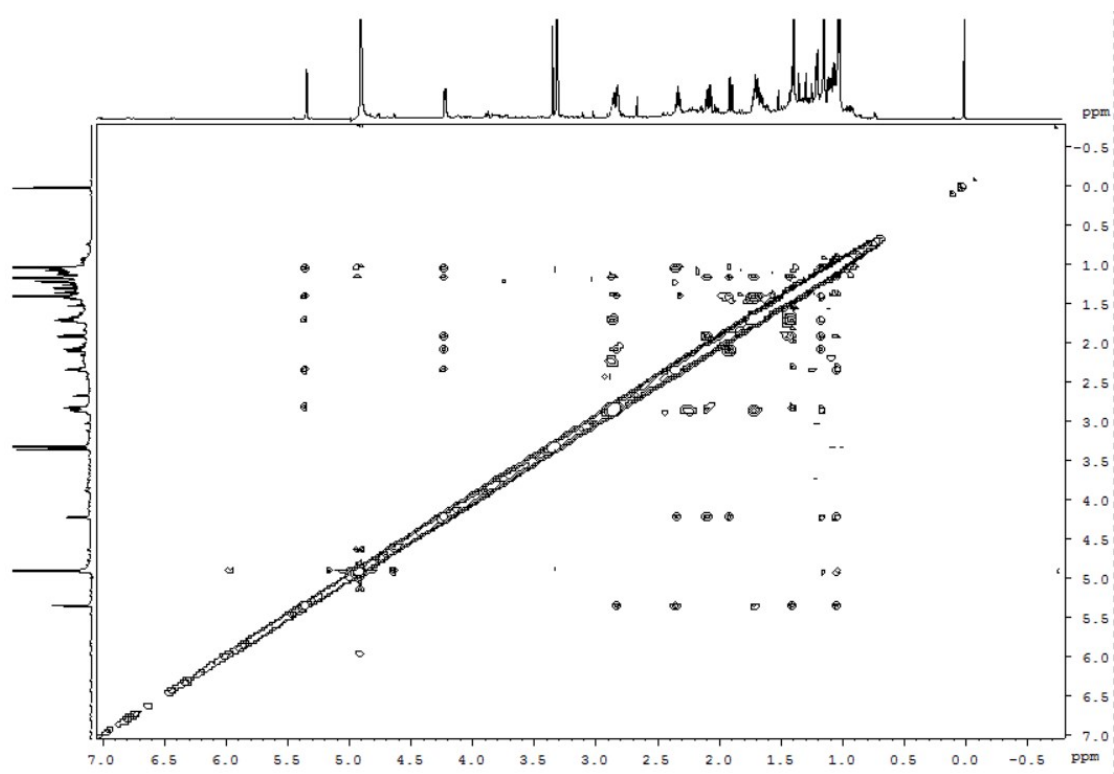


Figure S21. NOESY spectrum of 3 (600 MHz, CD₃OD)

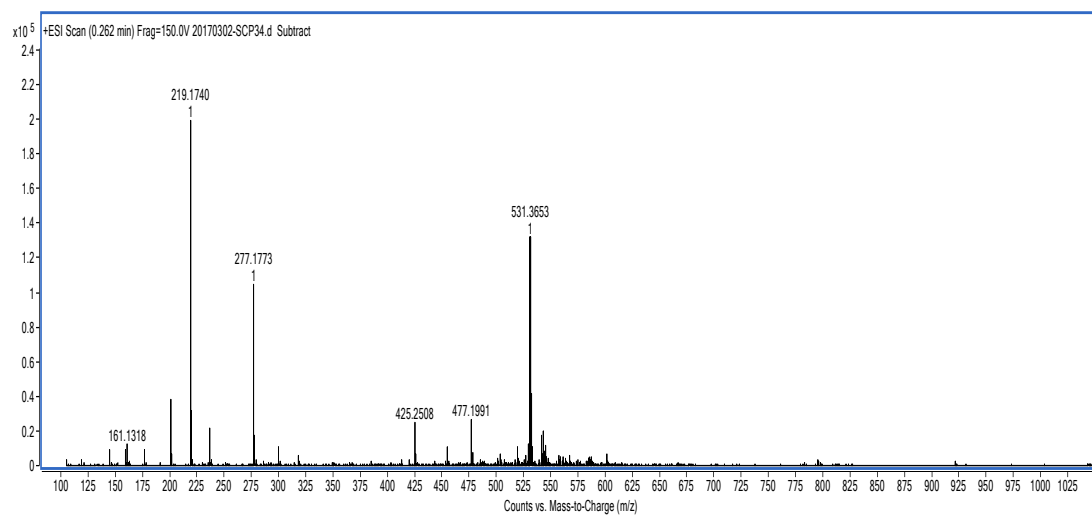


Figure S22. HRESIMS spectrum of 3

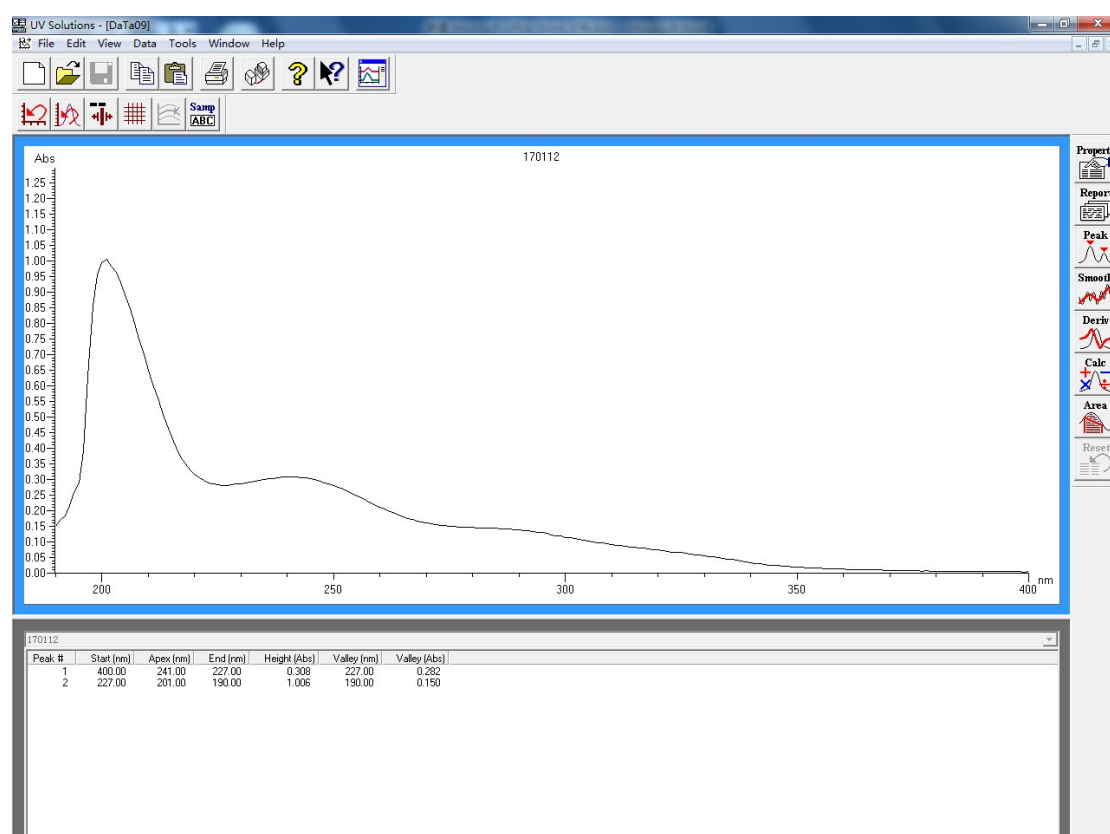
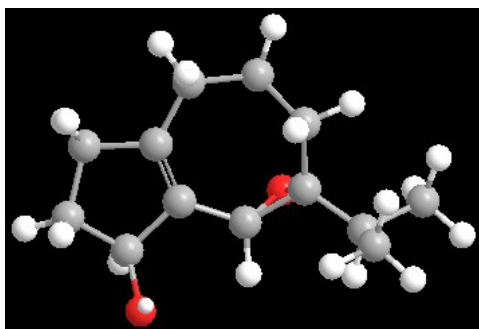
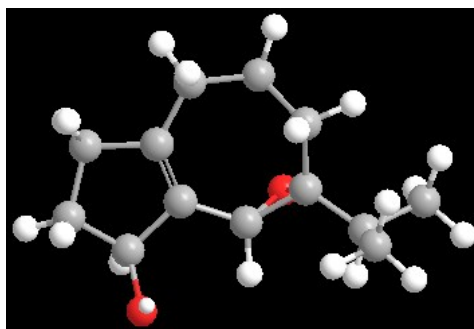


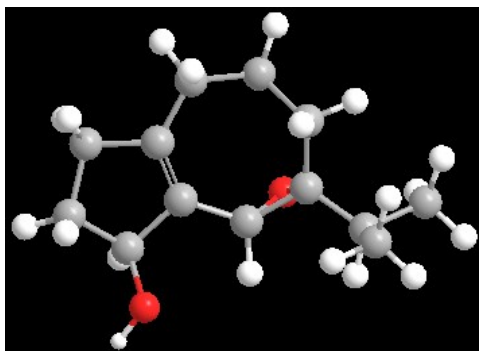
Figure S23. UV spectrum of 3



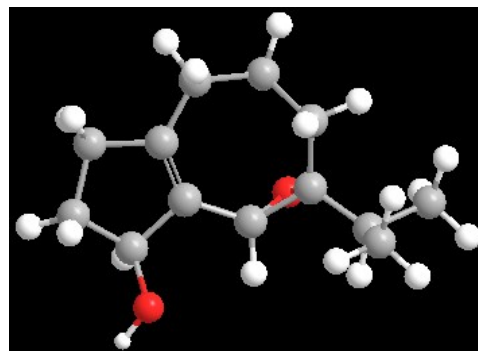
C1



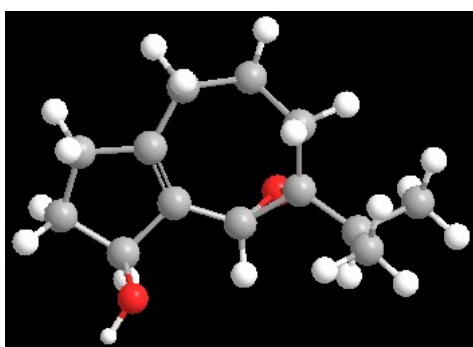
C2



C3

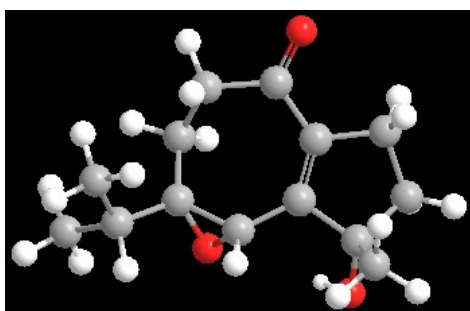


C4

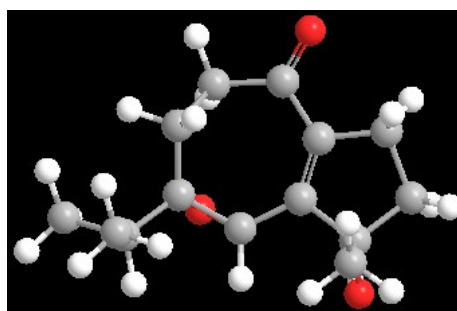


C5

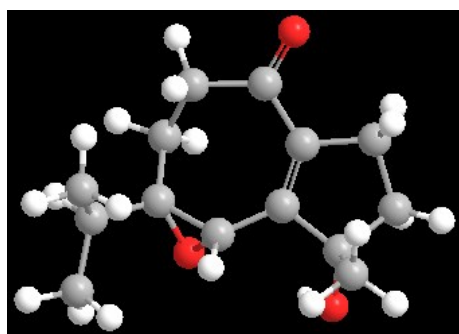
Figure S24. Lowest energy conformers for (4*R*,6*R*,7*R*)-2



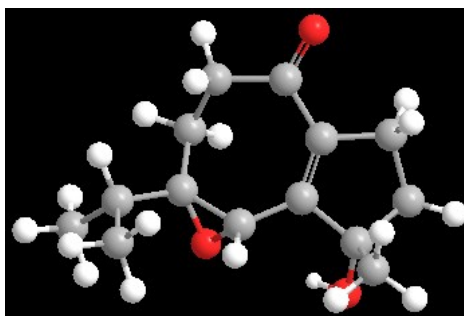
C1



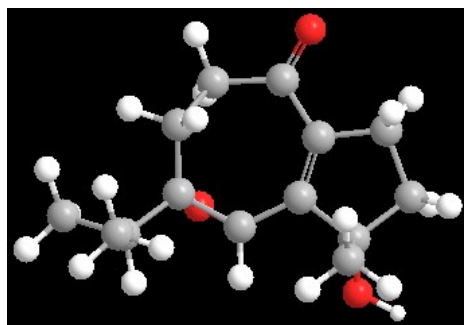
C2



C3



C4



C5

Figure S25. Lowest energy conformers for (4*S*,6*S*,7*S*)-2

Table S1 Energy analysis for (4*R*,6*R*,7*R*)-2

Conformers	HF	E	E*1060.475	exp	%
C1	-658.029327	0	0	1	0.251651
C2	-658.029265	0.000062	0.065855	0.936266	0.235613
C3	-658.02861	0.000717	0.760255	0.467547	0.117659
C4	-658.028609	0.000717	0.760679	0.467349	0.117609
C5	-658.028465	0.000862	0.913705	0.401036	0.100921

Table S2 Energy analysis for (4*S*,6*S*,7*S*)-2

Conformers	HF	E	E*1060.475	exp	%
C1	-658.029327	0	0	1	0.251651
C2	-658.029265	0.000062	0.065855	0.936266	0.235613
C3	-658.02861	0.000717	0.760255	0.467547	0.117659
C4	-658.028609	0.000717	0.760679	0.467349	0.117609
C5	-658.028465	0.000862	0.913705	0.401036	0.100921