Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Alismanoid A, an unprecedented 1,2-*seco* bisabolene from *Alisma orientale* and the protective activity on H_2O_2-induced damage in SH-SY5Y cells

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Content

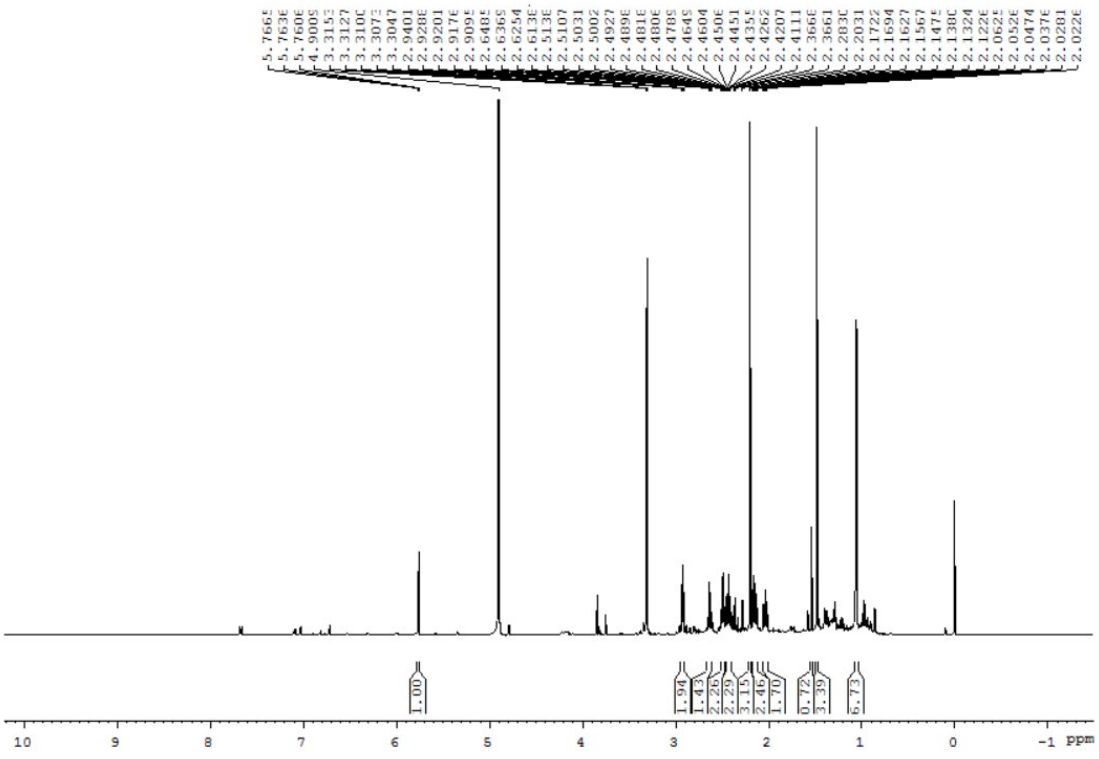


Figure S1. ^{1}H NMR spectrum of 1 (600 MHz, CD_3OD)

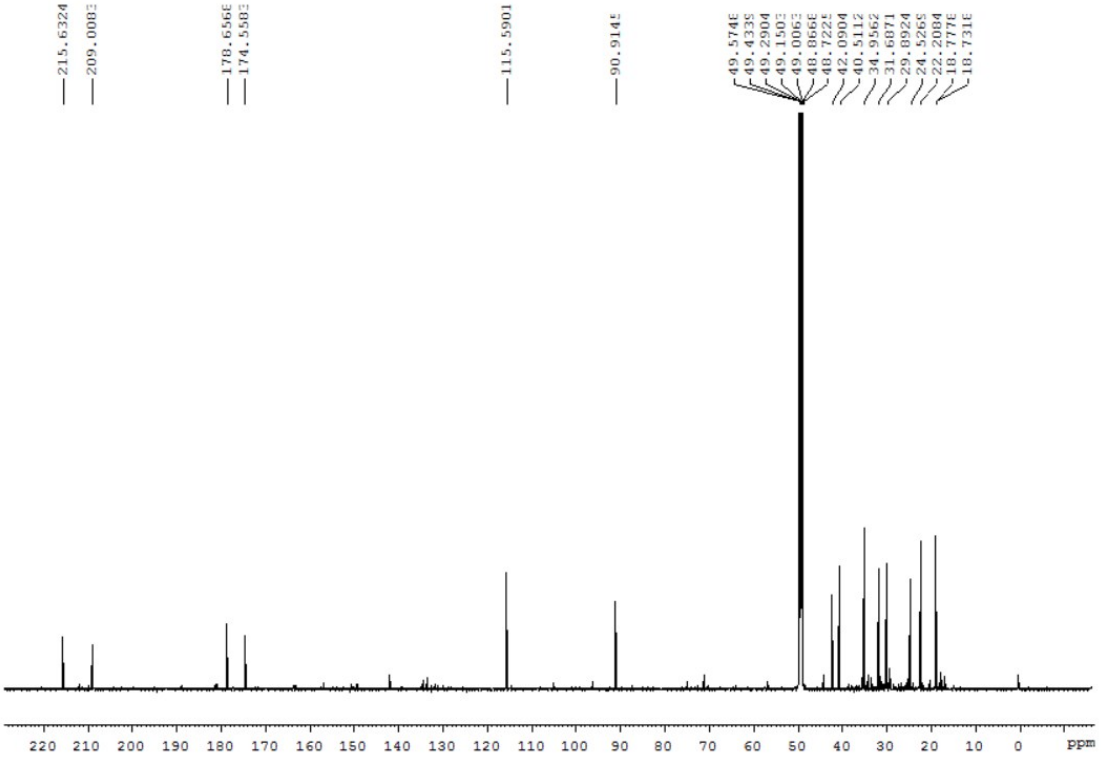


Figure S2. ^{13}C NMR spectrum of 1 (150 MHz, CD_3OD)

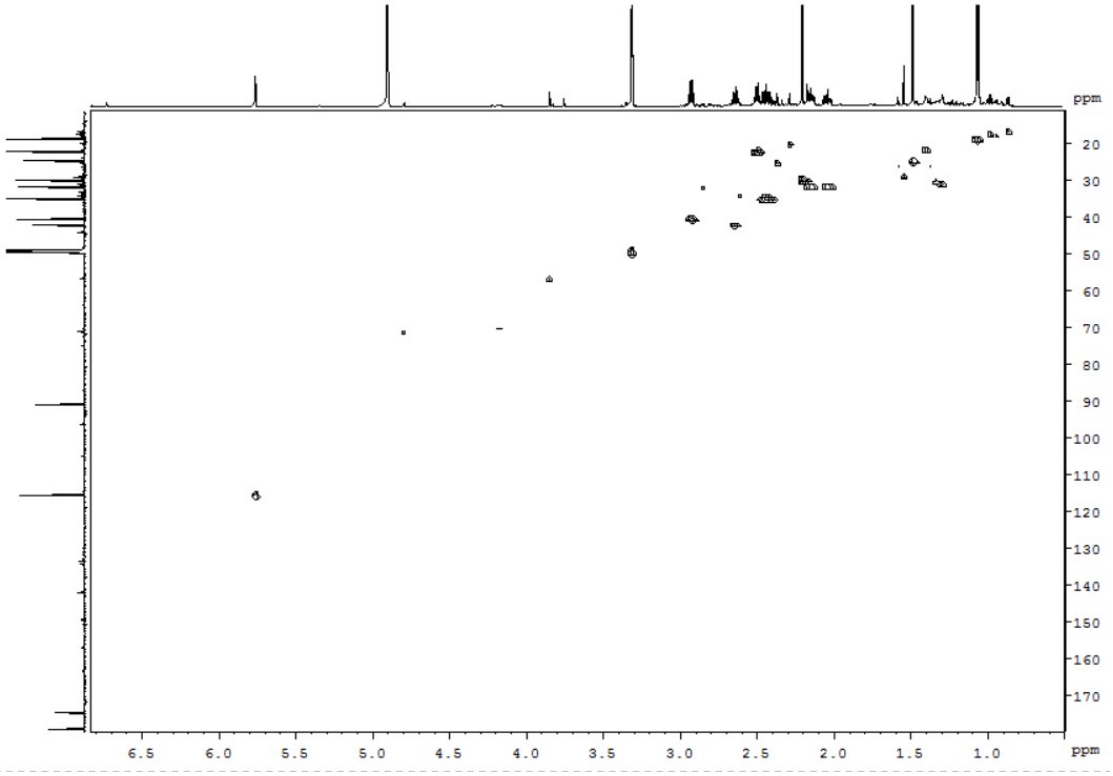


Figure S3. HSQC spectrum of 1(600 MHz, CD_3OD)

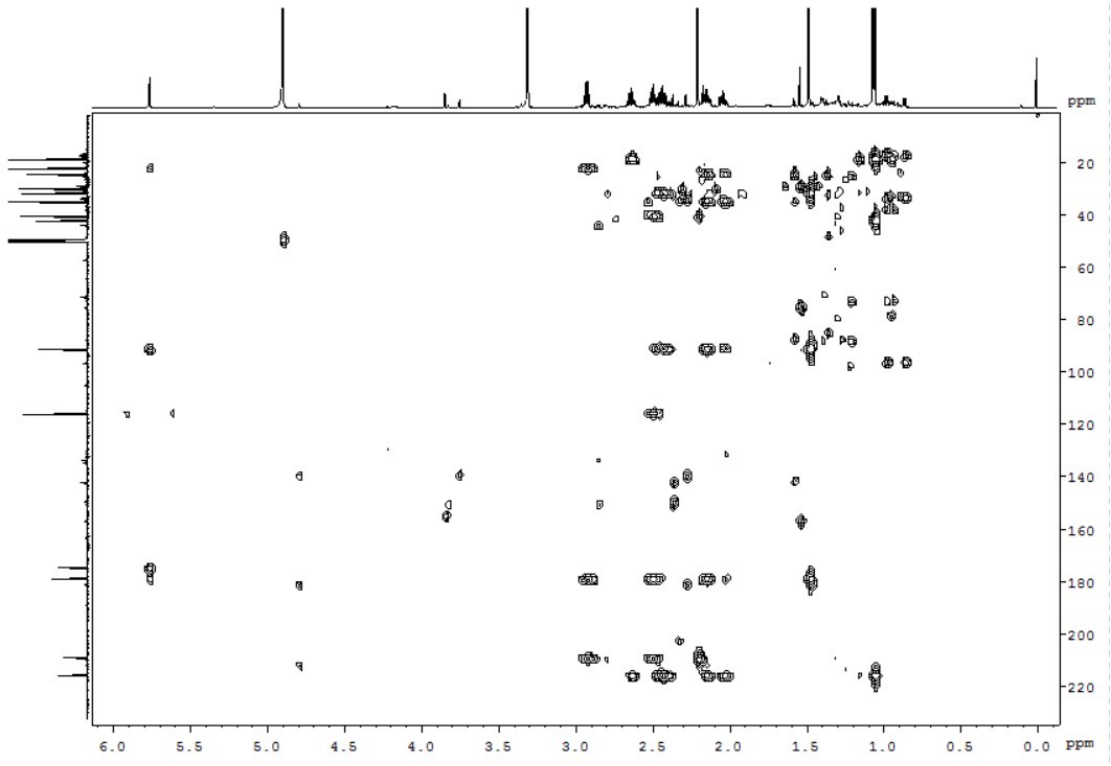


Figure S4. HMBC spectrum of 1 (600 MHz, CD_3OD)

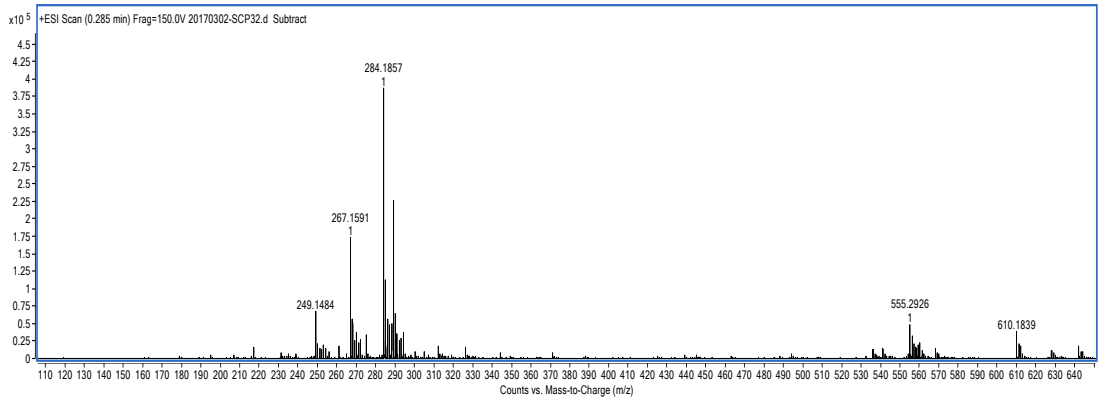


Figure S5. HRESIMS spectrum of 1

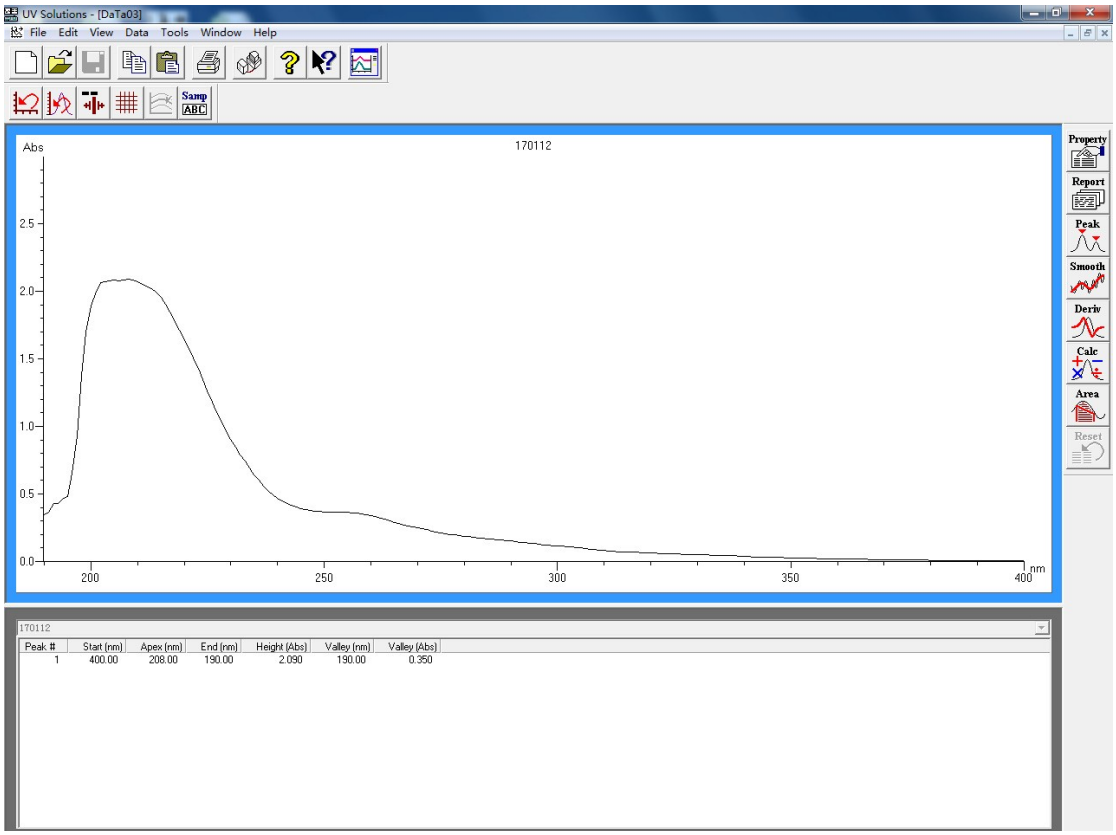


Figure S6. UV spectrum of 1

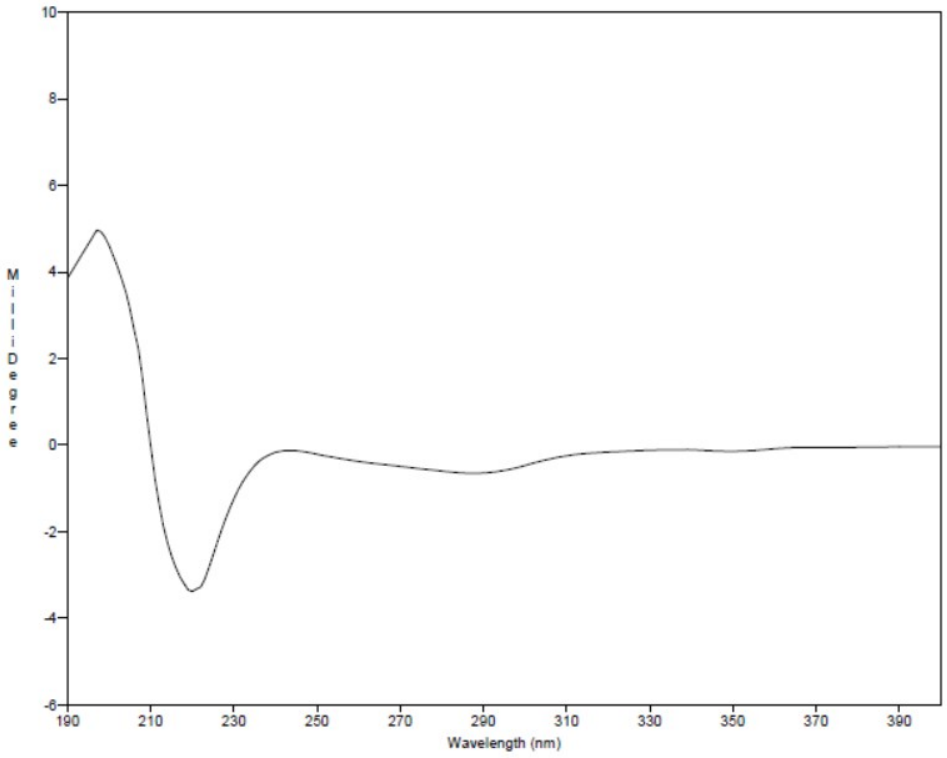


Figure S7. ECD spectrum of 1a

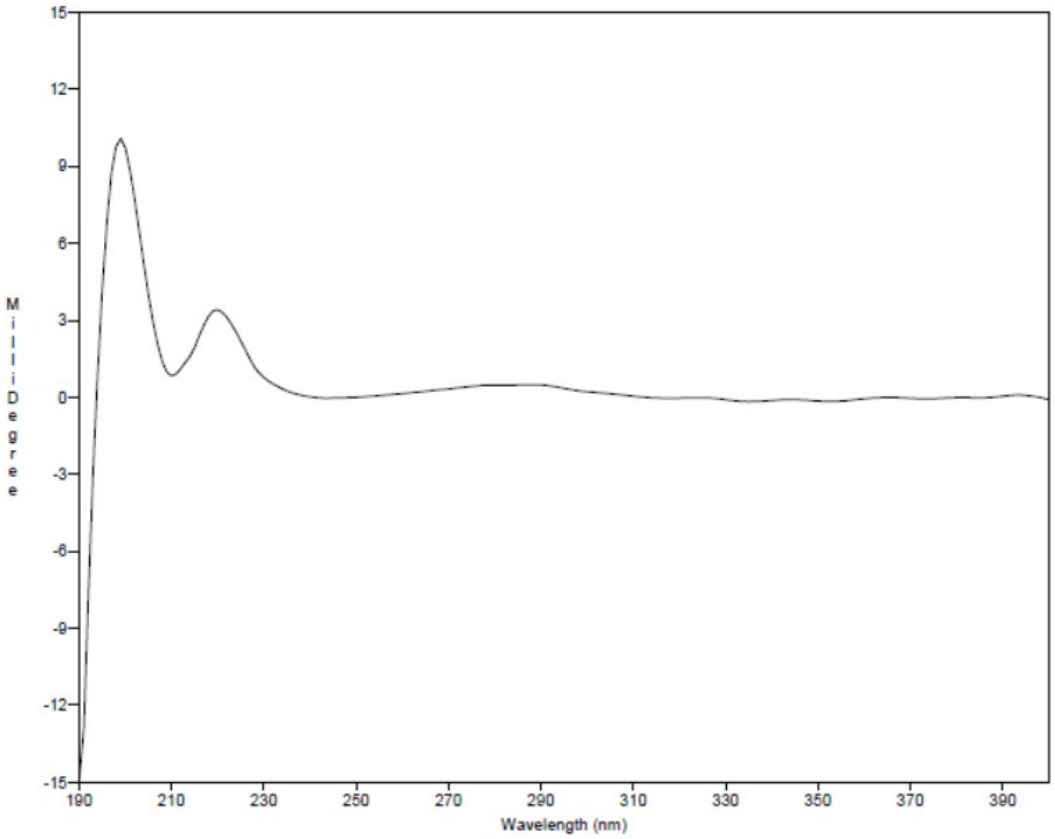


Figure S8. ECD spectrum of 1b

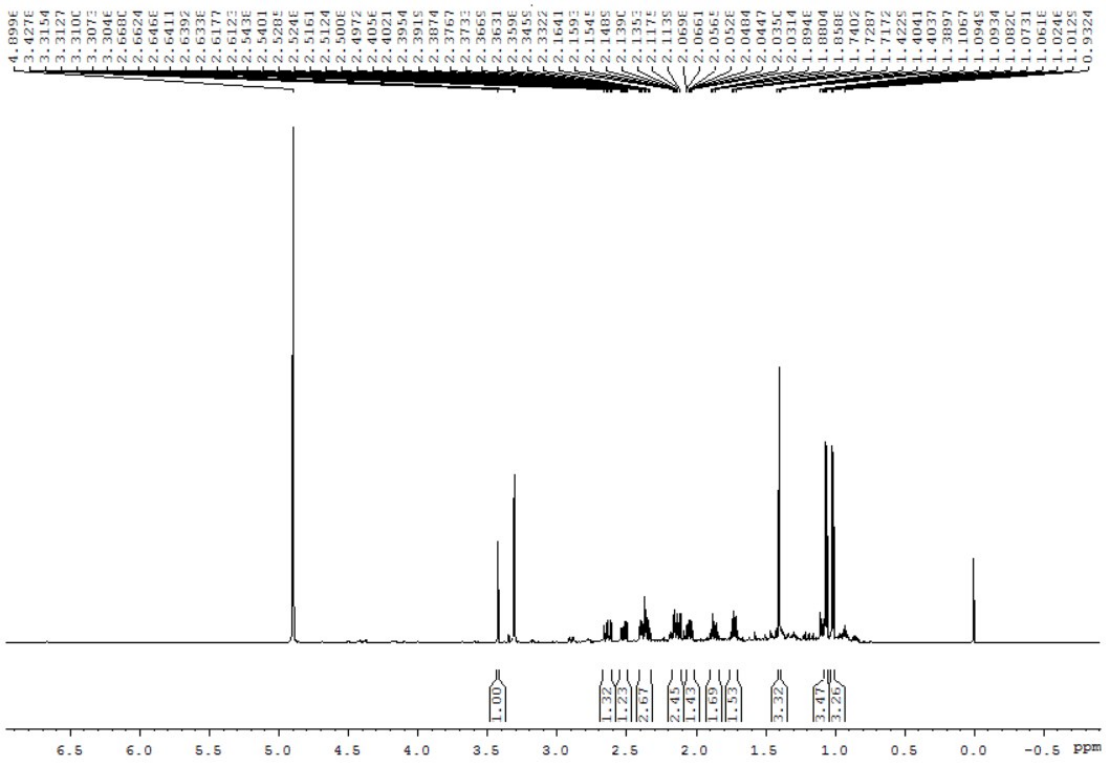


Figure S9. ^{1}H NMR spectrum of 2 (600 MHz, CD_3OD)

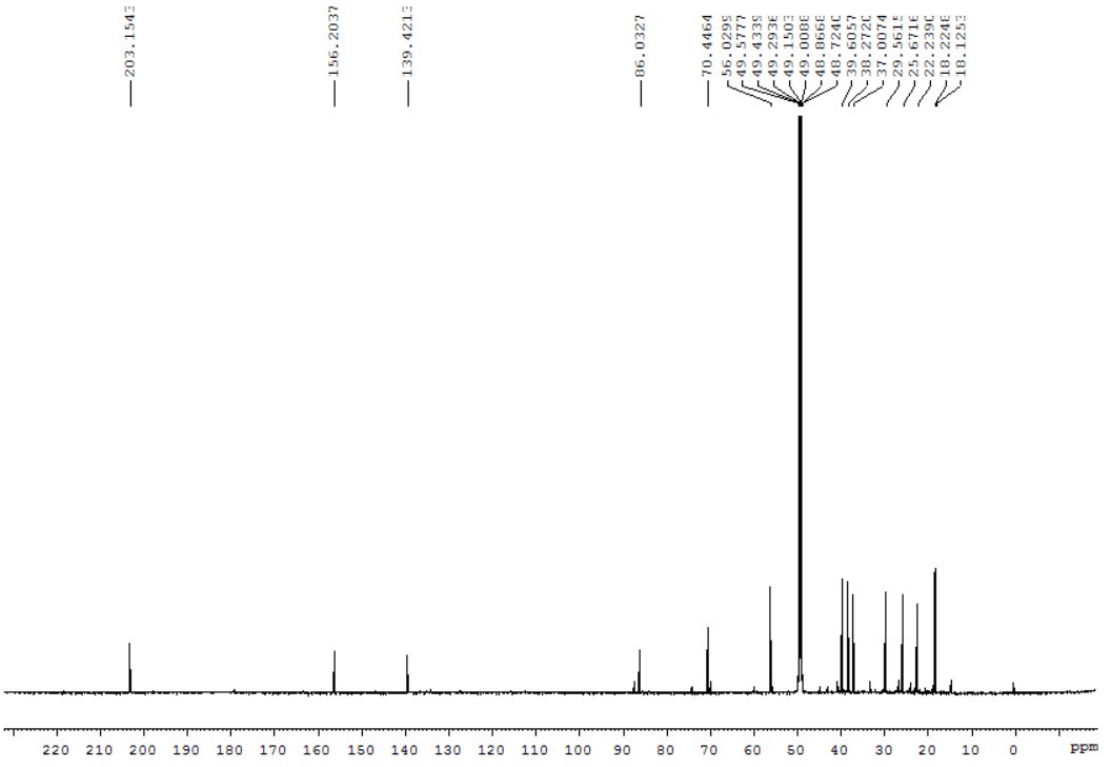


Figure S10. ^{13}C NMR spectrum of 2 (150 MHz, CD_3OD)

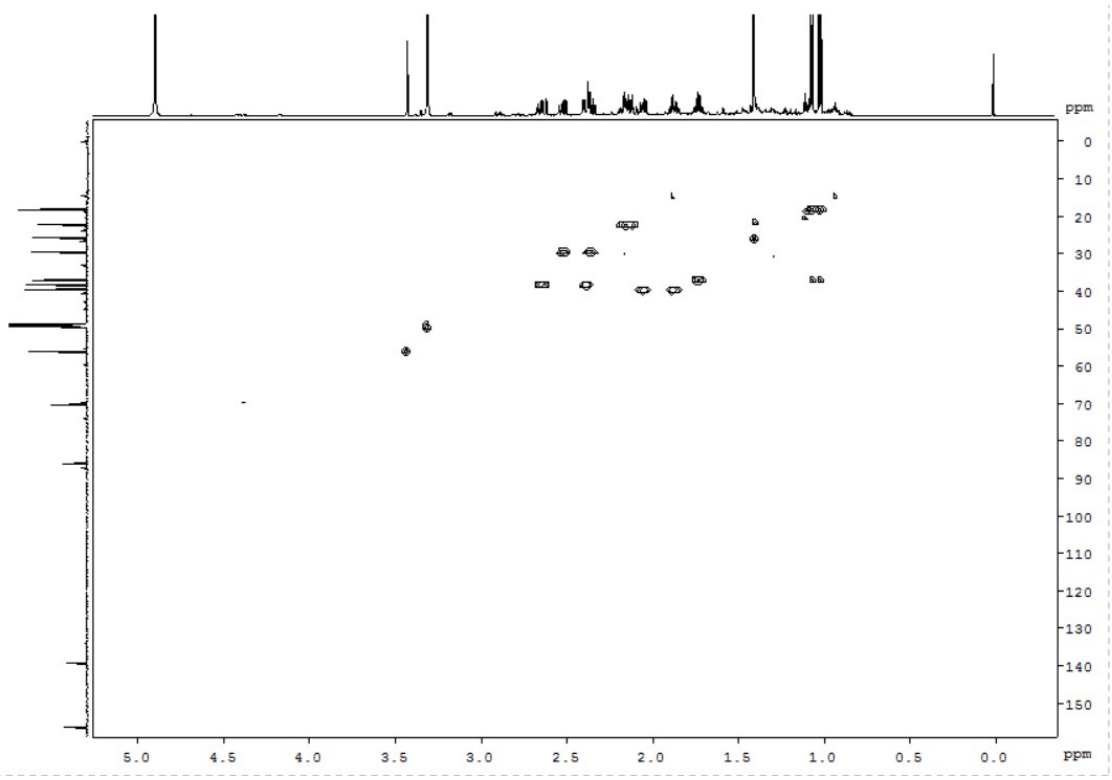


Figure S11. HSQC spectrum of 2 (600 MHz, CD_3OD)

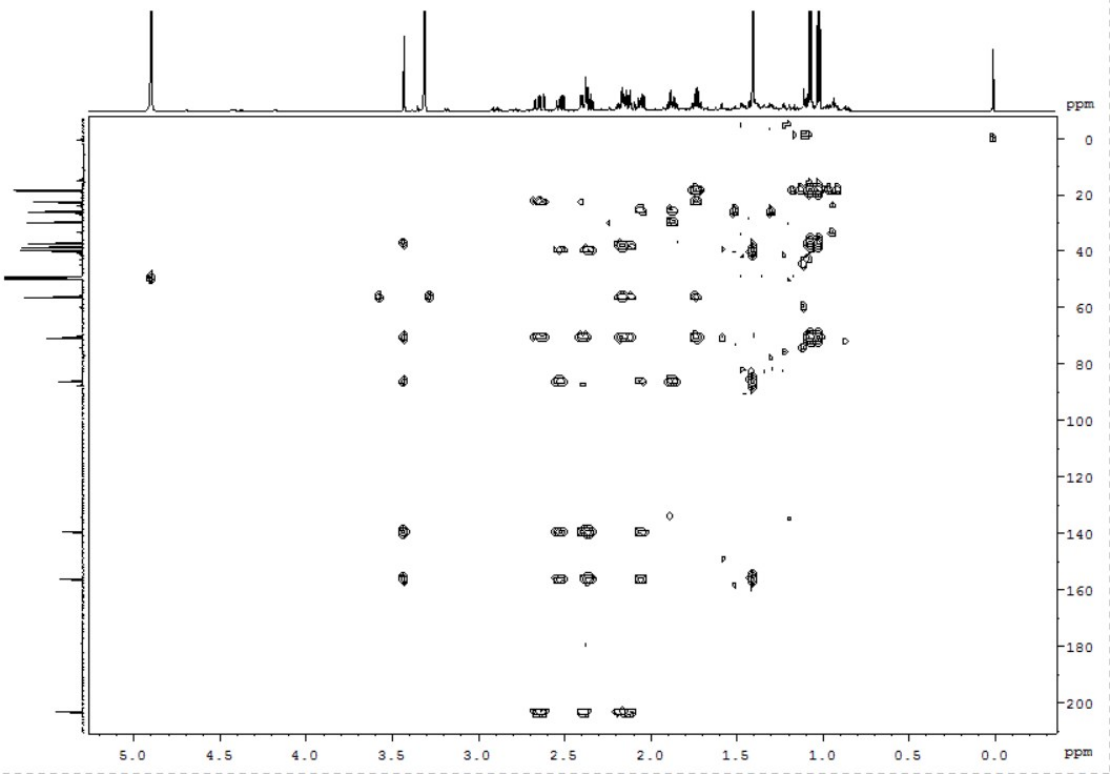


Figure S12. HMBC spectrum of 2 (600 MHz, CD_3OD)

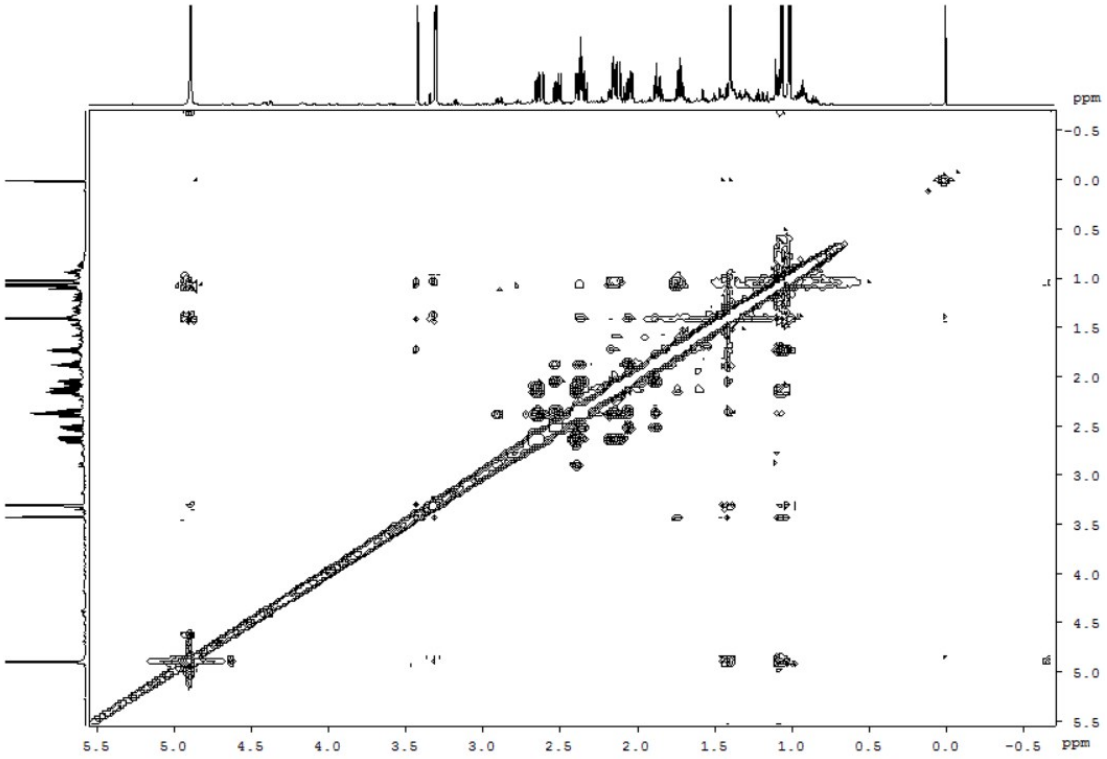


Figure S13. NOESY spectrum of 2 (600 MHz, CD_3OD)

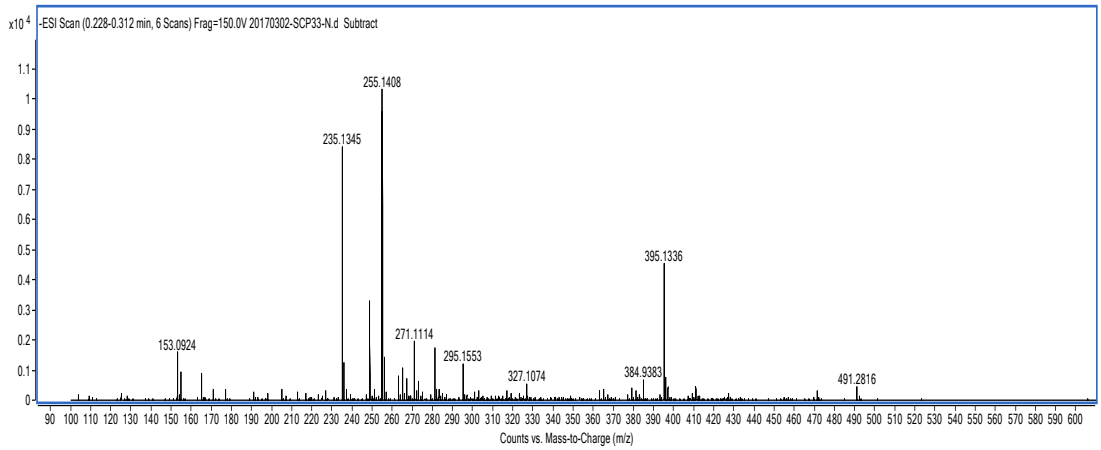


Figure S14. HRESIMS spectrum of 2

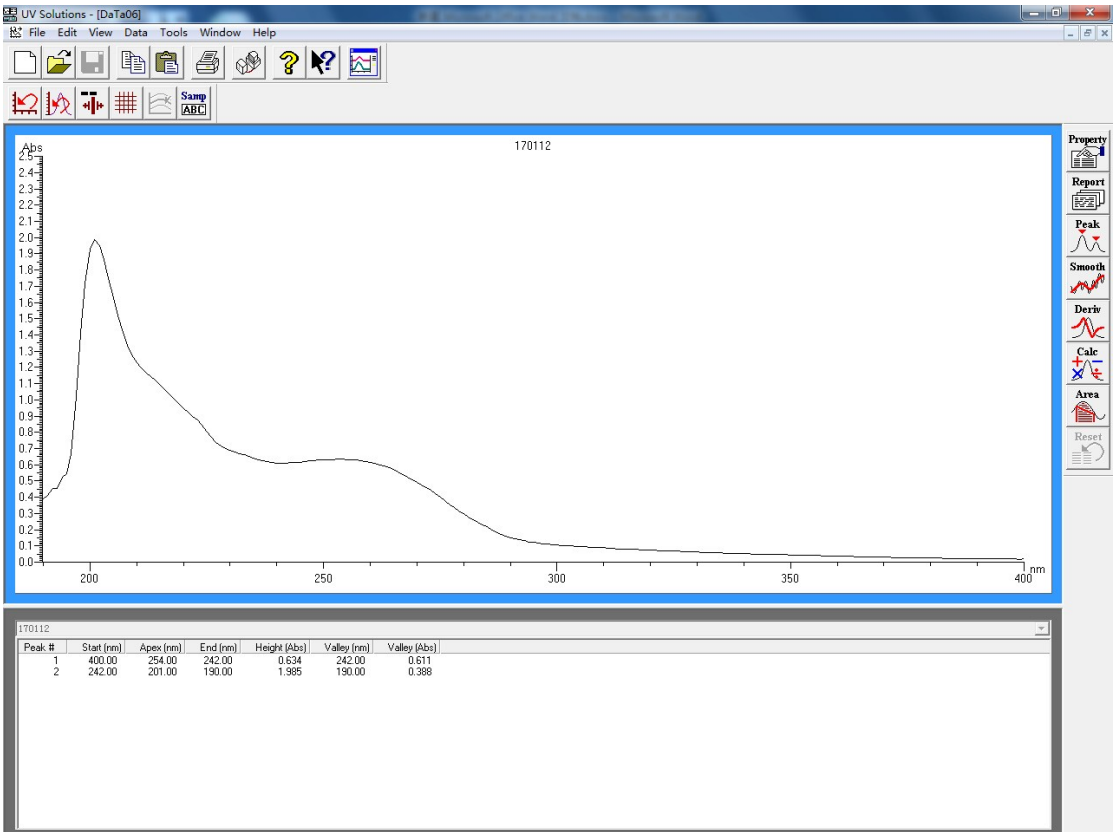


Figure S15. UV spectrum of 2

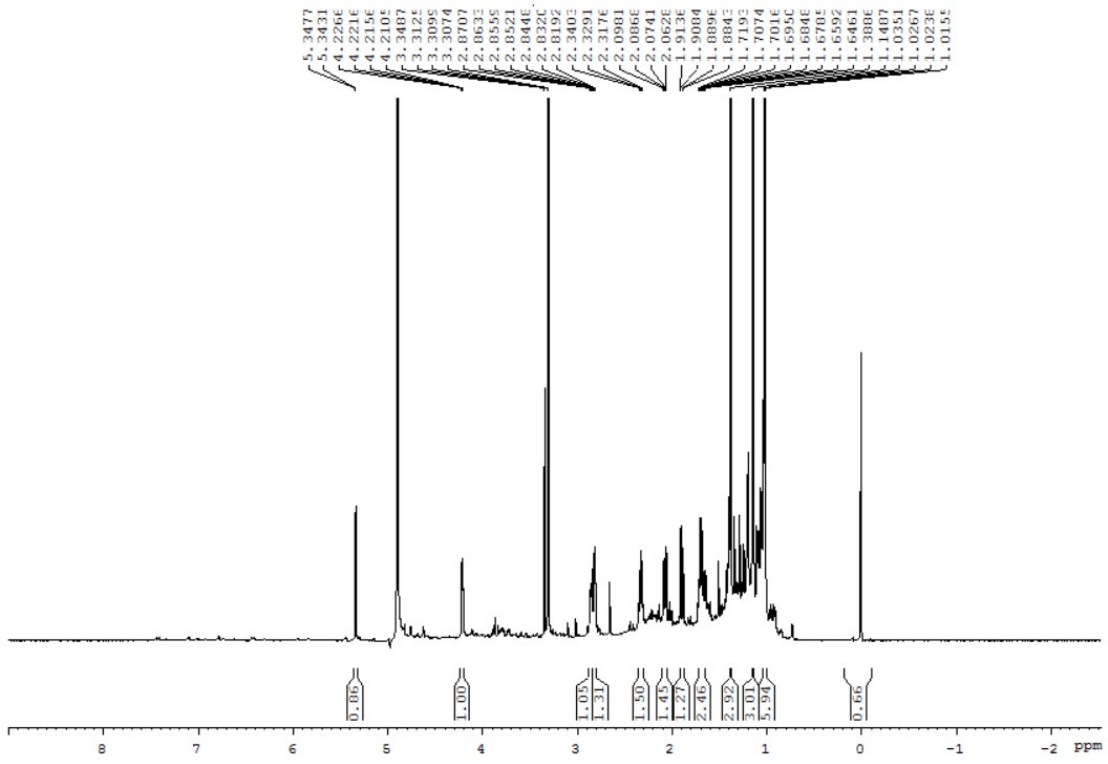


Figure S16. ^{1}H NMR spectrum of 3 (600 MHz, CD_3OD)

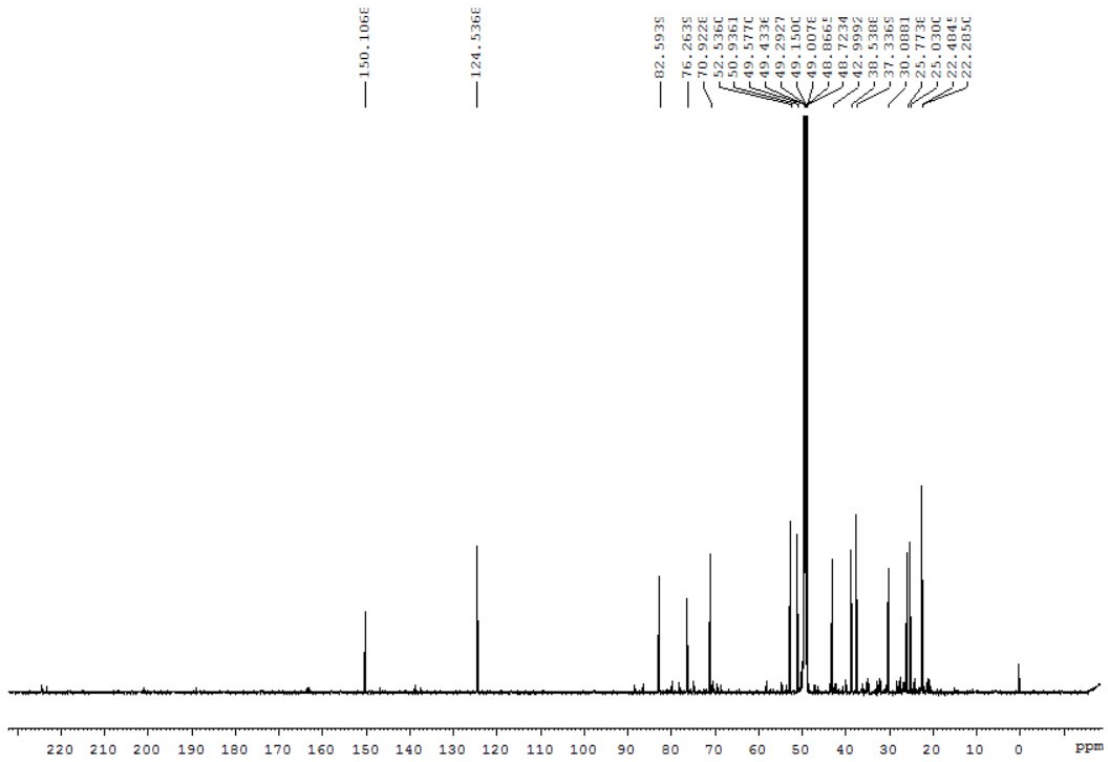


Figure S17. ^{13}C NMR spectrum of 3 (150 MHz, CD_3OD)

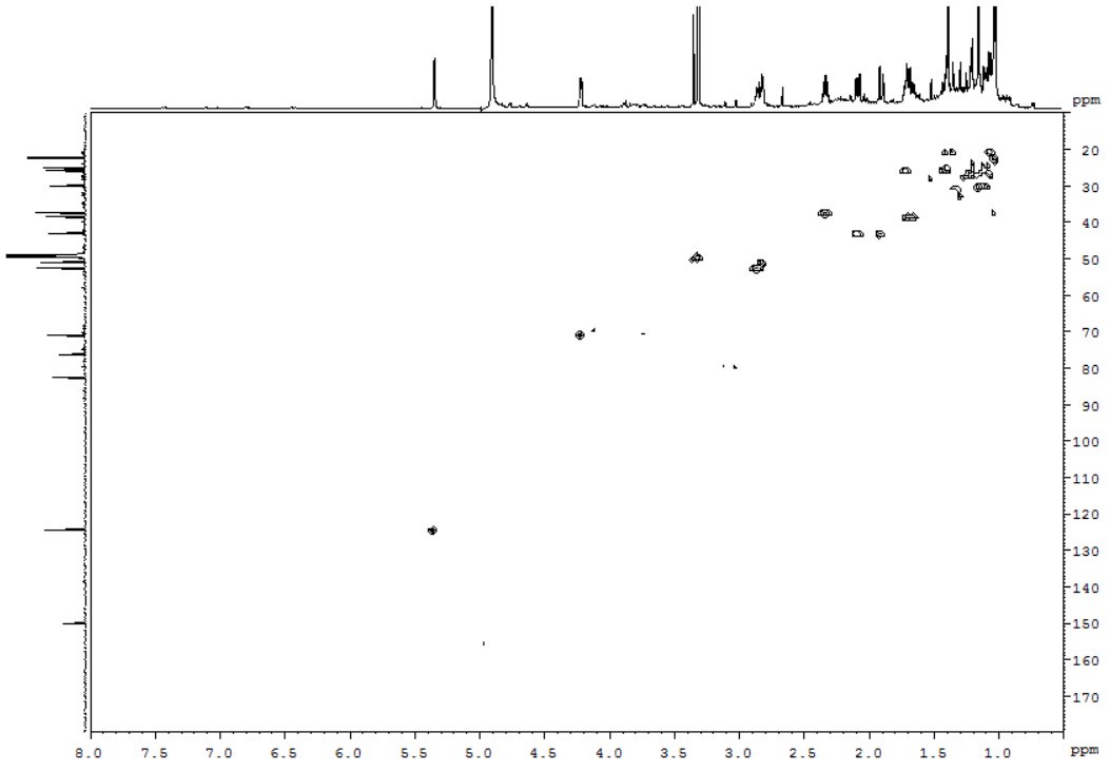


Figure S18. HSQC spectrum of 3 (600 MHz, CD_3OD)

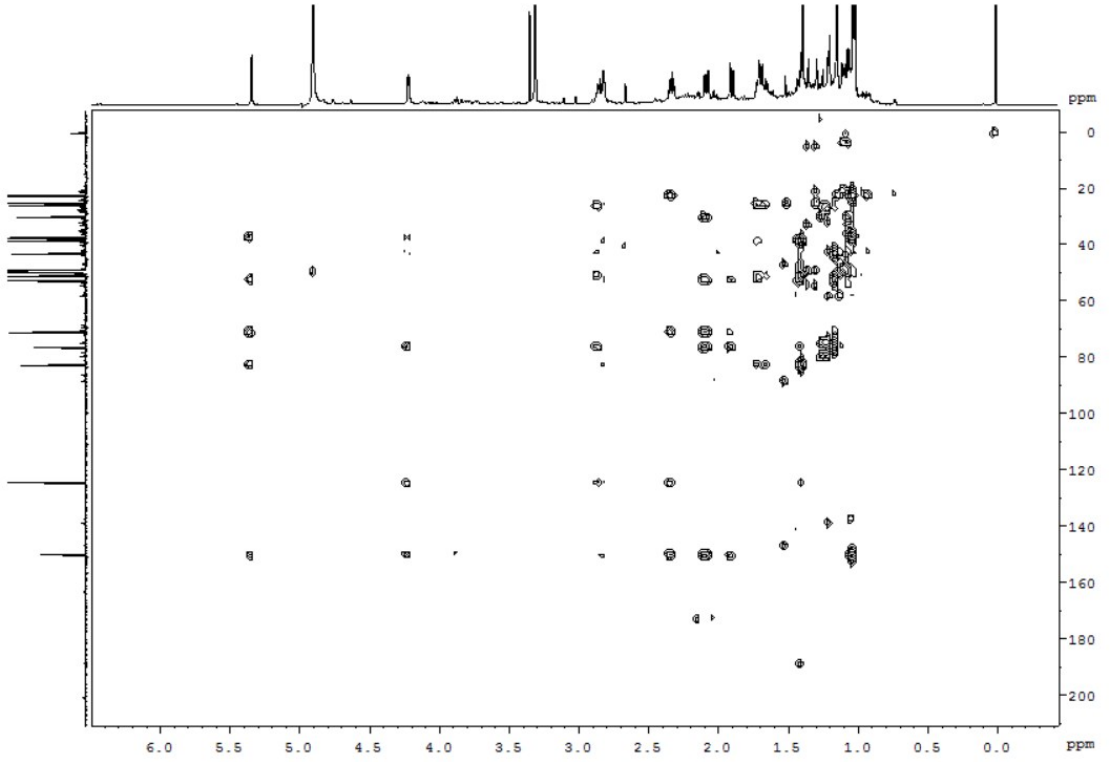


Figure S19. HMBC spectrum of 3 (600 MHz, MeOH-d_4)

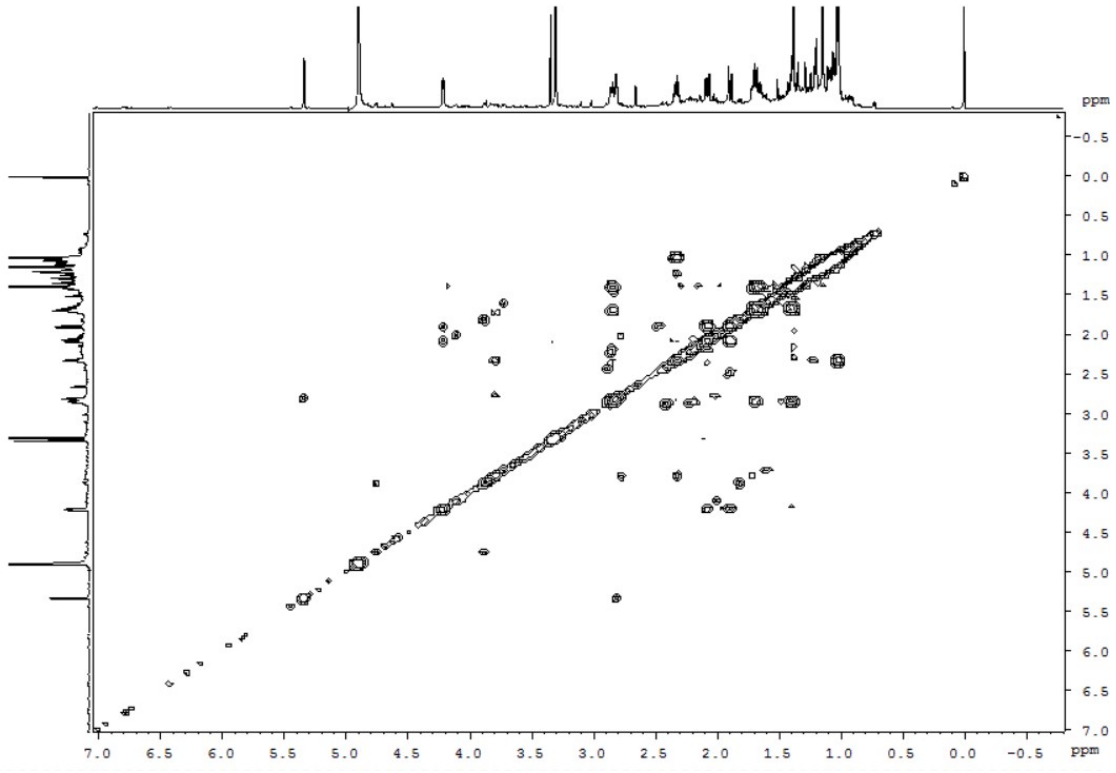


Figure S20. COSY spectrum of 3 (600 MHz, CD_3OD)

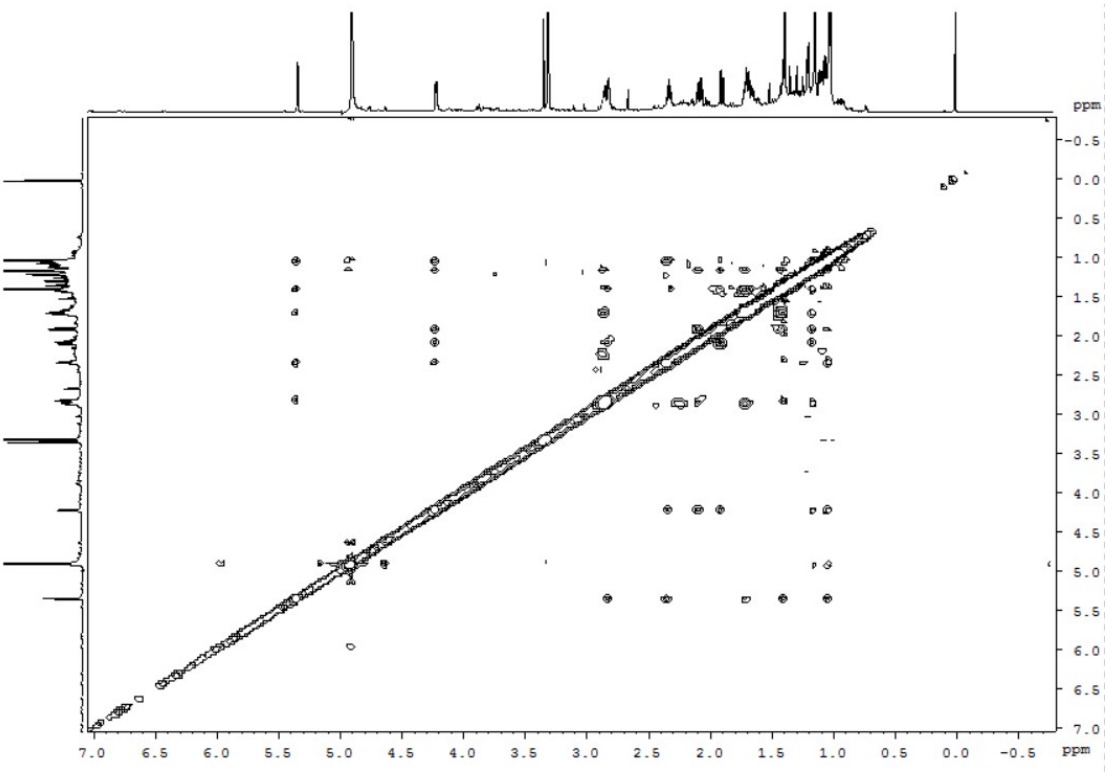


Figure S21. NOESY spectrum of 3 (600 MHz, CD_3OD)

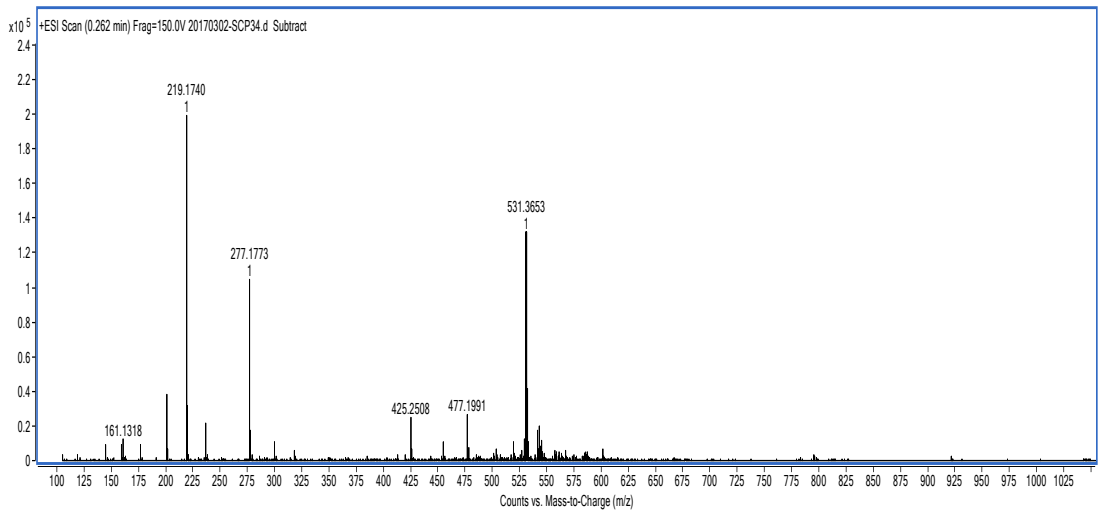


Figure S22. HRESIMS spectrum of 3

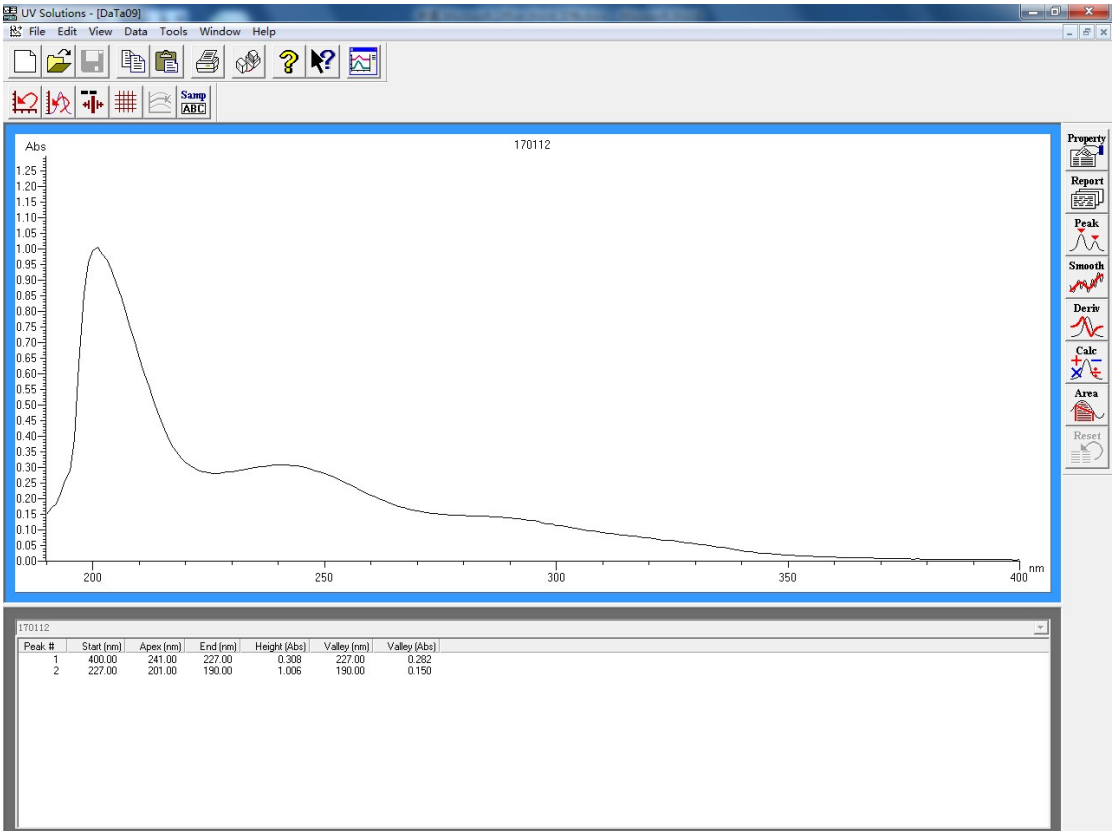
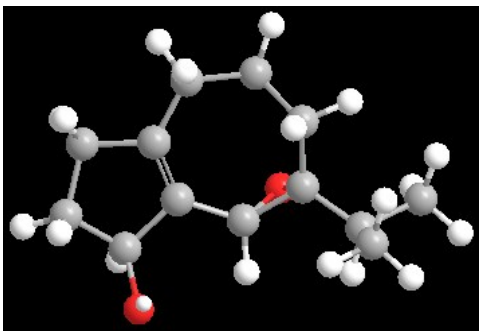
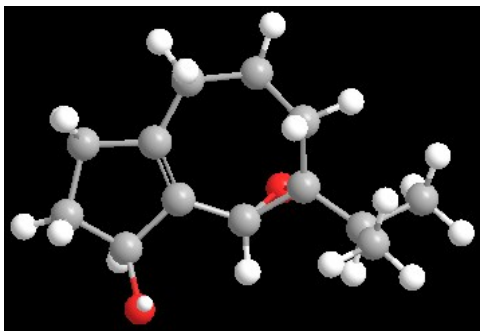


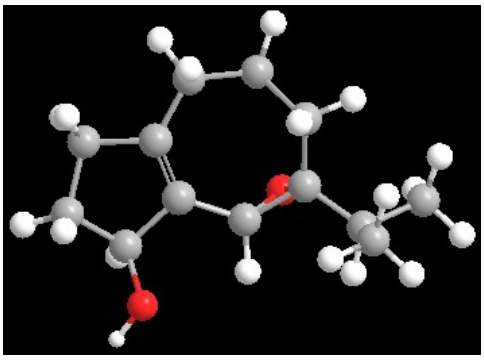
Figure S23. UV spectrum of 3



C1



C2



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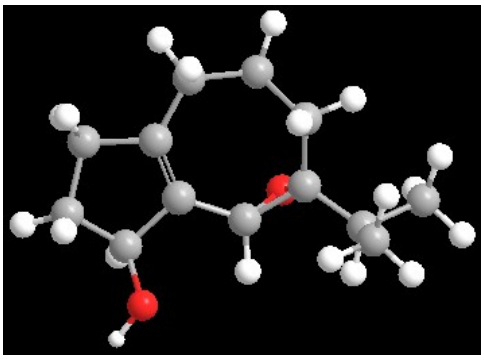

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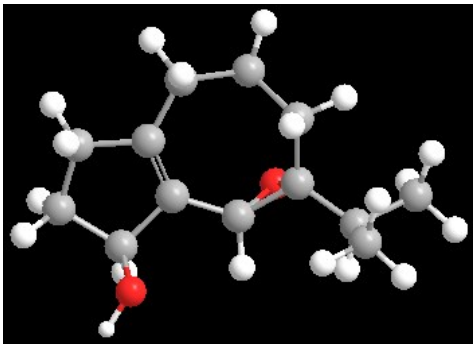
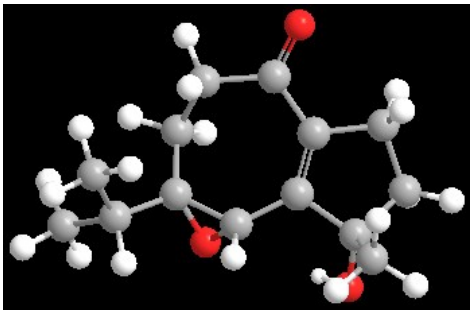
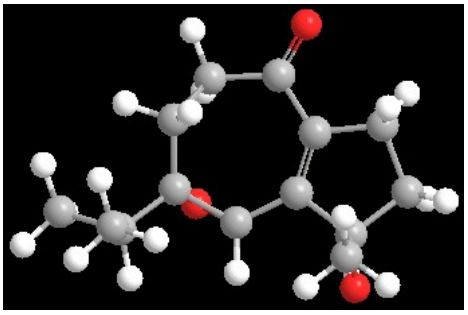


C5

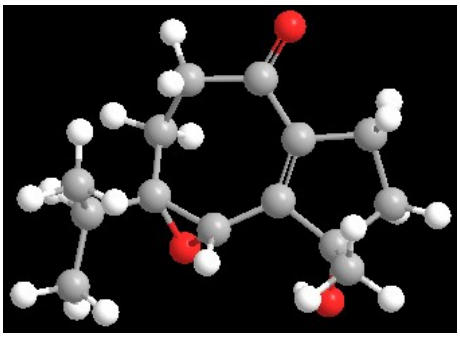
Figure S24. Lowest energy conformers for (4*R*,6*R*,7*R*)-2



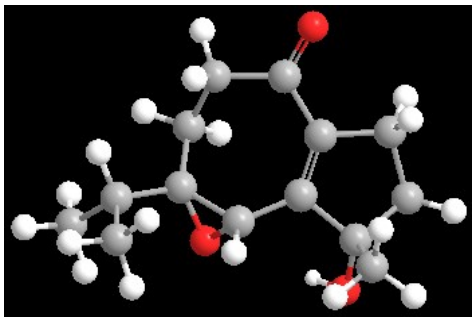
C1



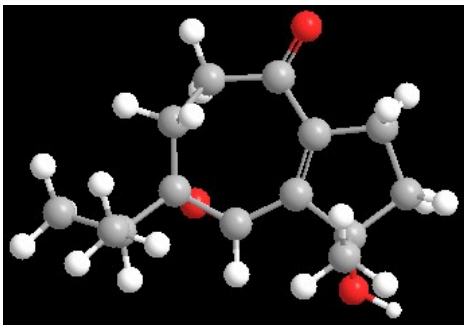
C2



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