

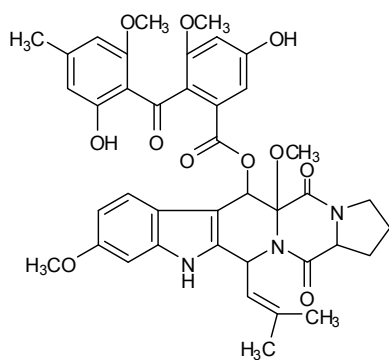
Supplementary Materials

16S rRNA Gene Sequence

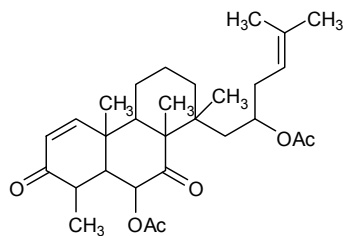
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LOCUS KJ175457 550 bp DNA linear PLN 03-FEB-2014
DEFINITION *Aspergillus fumigatus* isolate M1103.2732 18S ribosomal RNA gene, partial sequence; internal transcribed spacer 1, 5.8S ribosomal RNA gene, and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence.
ACCESSION KJ175457
VERSION KJ175457.1 GI:576867471
KEYWORDS
SOURCE *Aspergillus fumigatus*
ORGANISM [Aspergillus fumigatus](#)
Eukaryota; Fungi; Dikarya; Ascomycota; Pezizomycotina; Eurotiomycetes; Eurotiomycetidae; Eurotiales; Aspergillaceae; *Aspergillus*.
REFERENCE 1 (bases 1 to 550)
AUTHORS De Respinis,S., Weissenhorn,S., Bosshard,P.P., Petrini,L.E., Tonolla,M. and Petrini,O.
TITLE Identification of *Aspergillus* species in the Flavi and Fumigati Sections by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry
JOURNAL Unpublished
REFERENCE 2 (bases 1 to 550)
AUTHORS De Respinis,S., Weissenhorn,S., Bosshard,P.P., Petrini,L.E., Tonolla,M. and Petrini,O.
TITLE Direct Submission
JOURNAL Submitted (23-JAN-2014) Laboratory of Applied Microbiology, University of Applied Sciences of Southern Switzerland (SUPSI), Via Mirasole 22A, Bellinzona, Ticino 6501, Switzerland

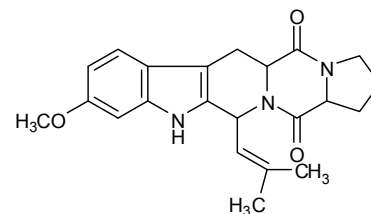
All Compounds Structures



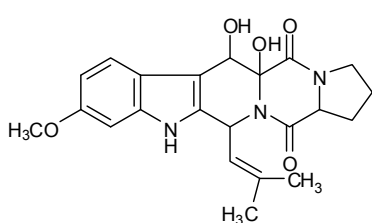
Compound 1



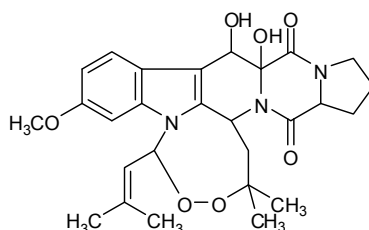
Compound 2



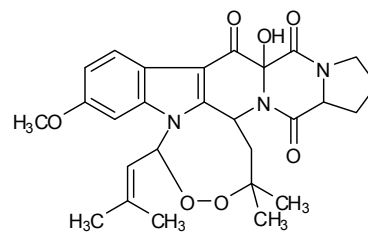
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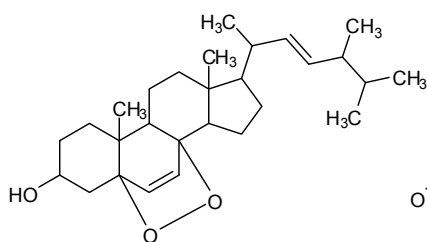
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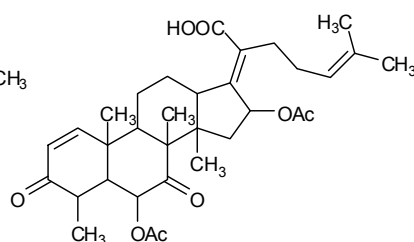
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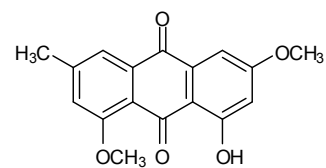
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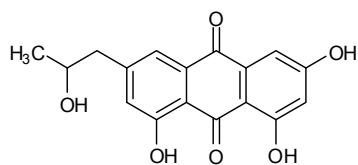
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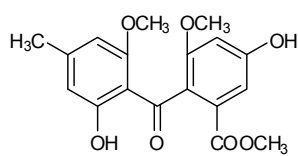
Compound 8



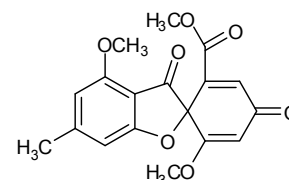
Compound 9



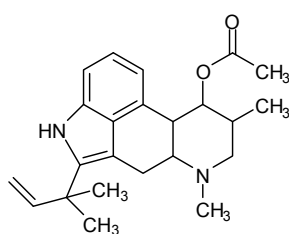
Compound 10



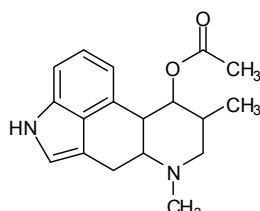
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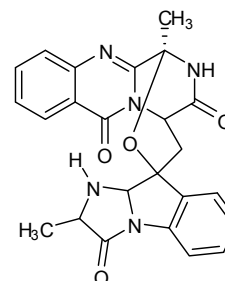
Compound 12



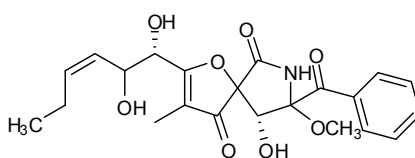
Compound 13



Compound 14



Compound 15



Compound 16

Chart 1. Structure of Compounds 1–16.

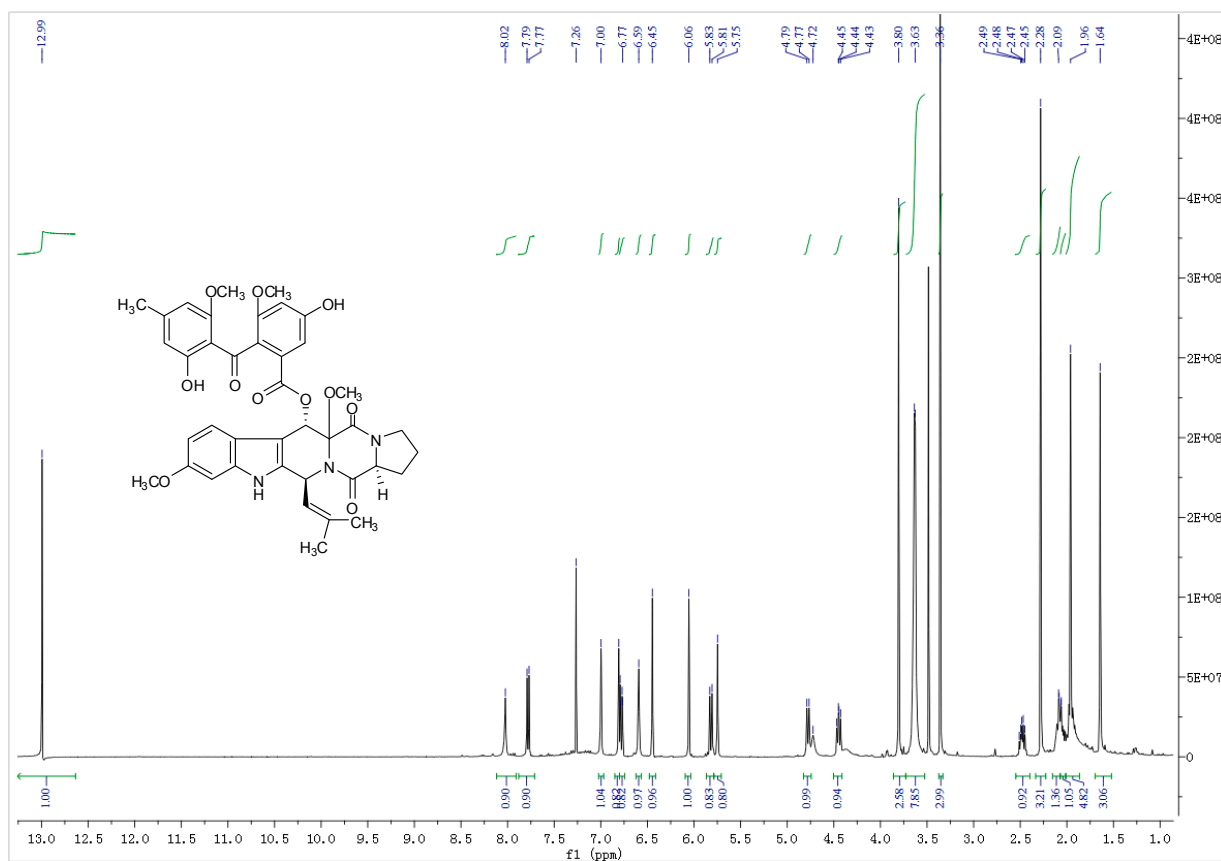


Figure S1. $^1\text{H-NMR}$ (400 MHz, CDCl_3) spectrum of compound 1.

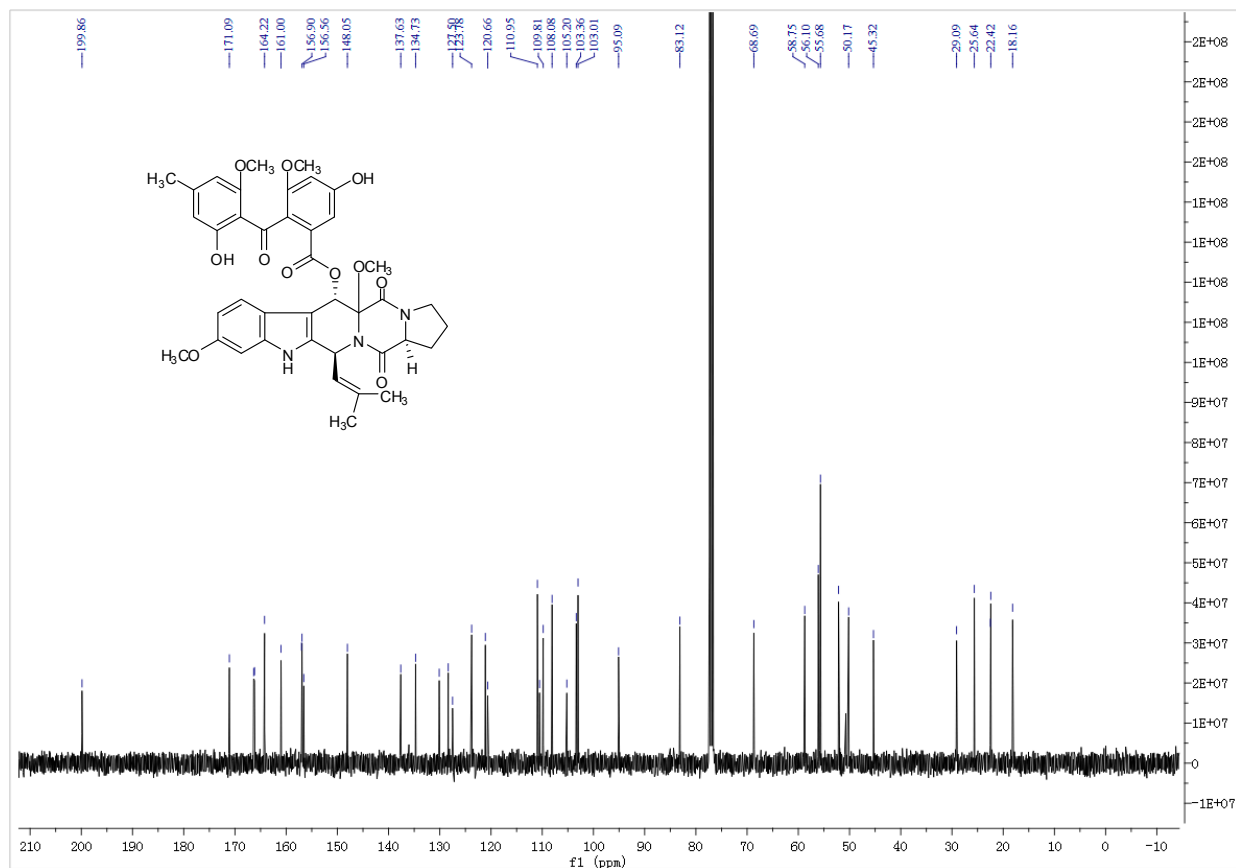


Figure S2. $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) spectrum of compound 1.

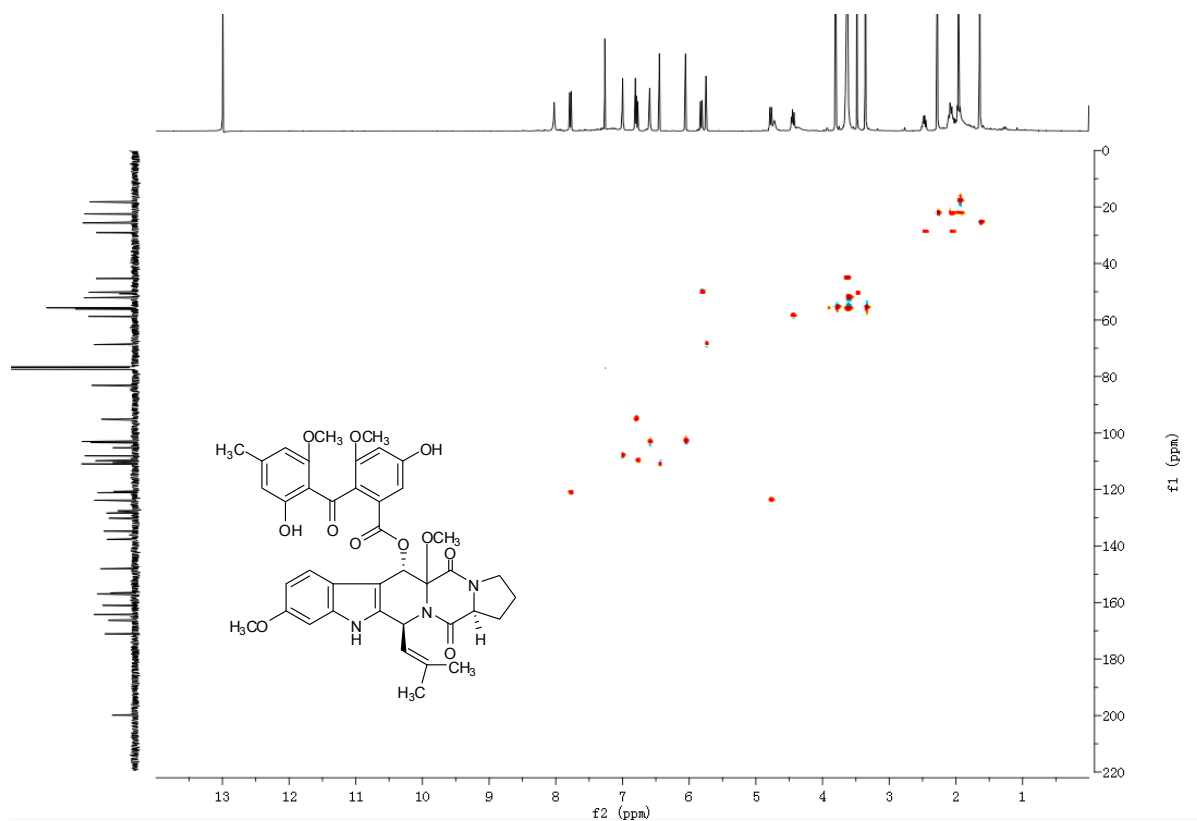


Figure S3. HSQC spectrum of compound 1.

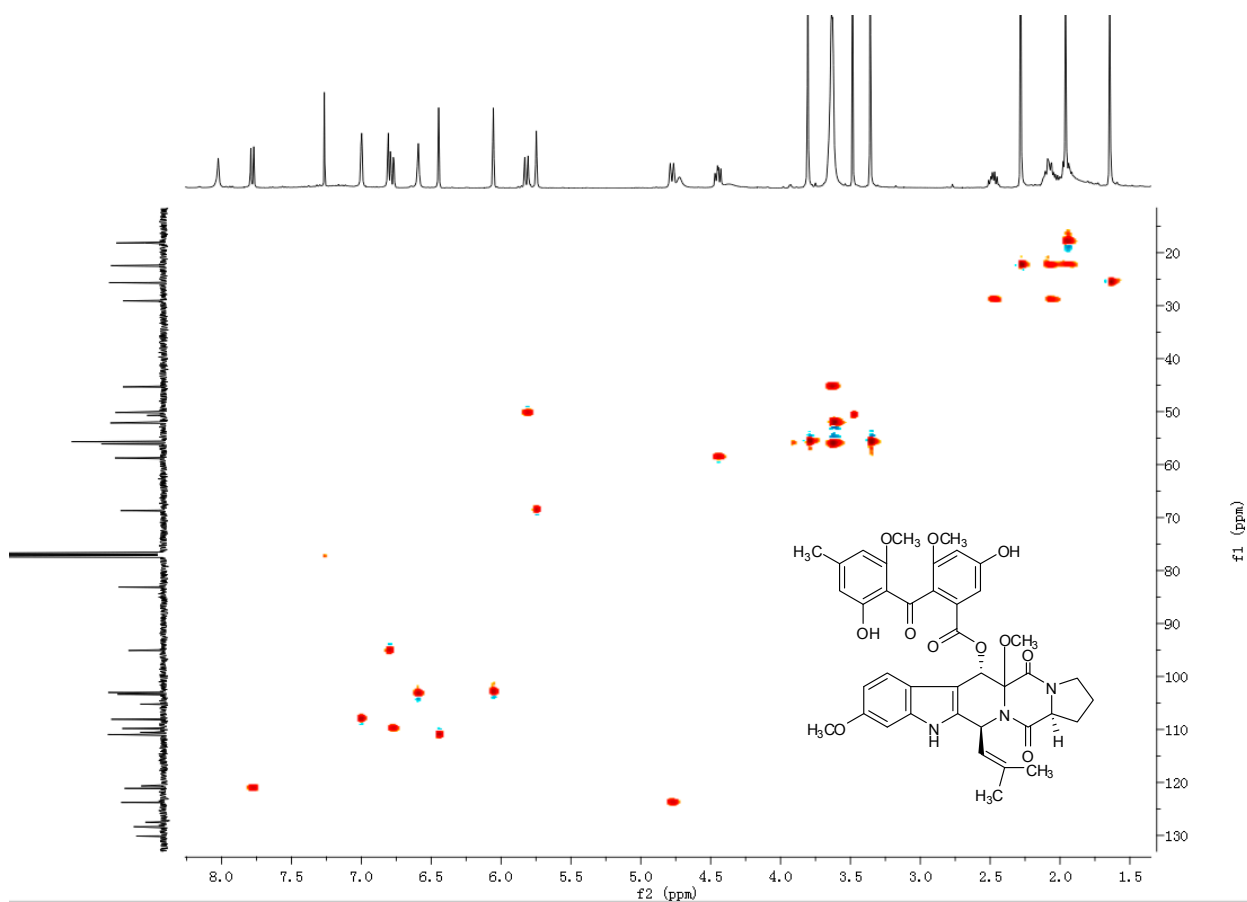


Figure S4. Expanded HSQC spectrum of compound 1.

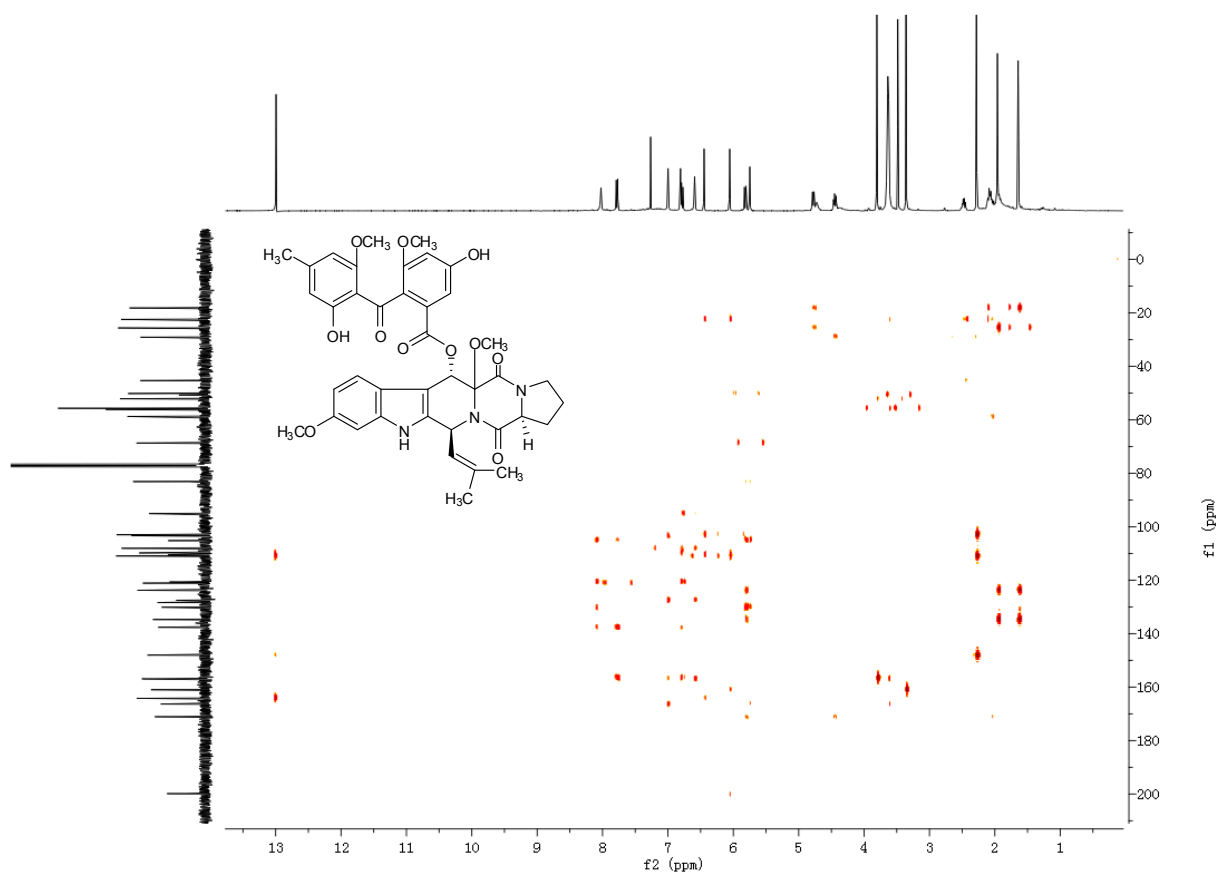


Figure S5. HMBC spectrum of compound 1.

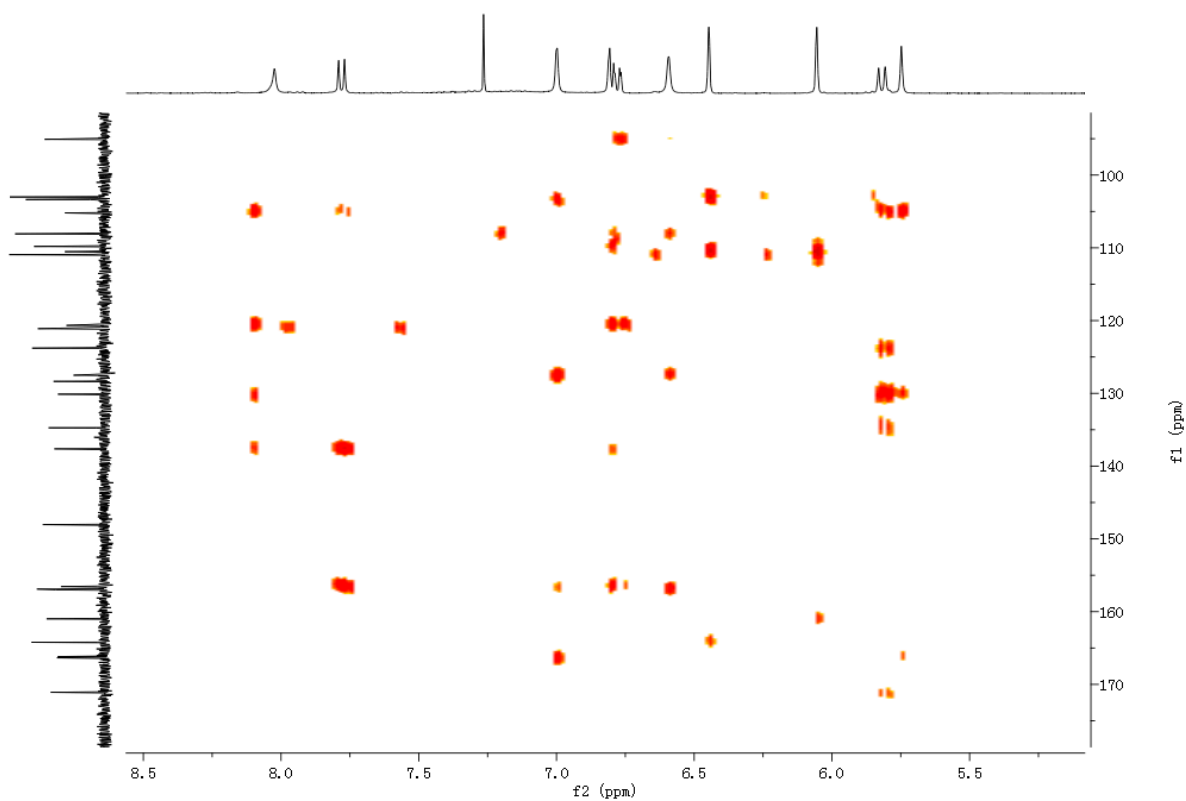


Figure S6. Expanded HMBC spectrum of compound 1.

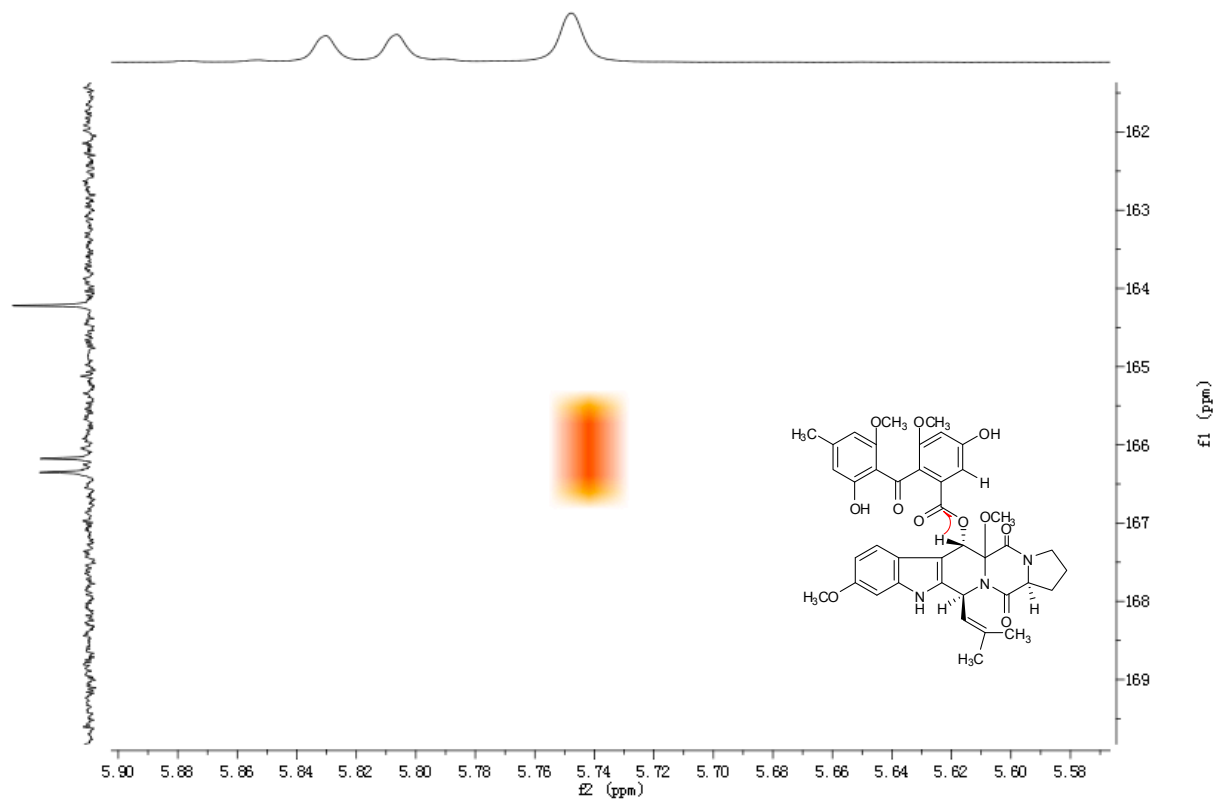


Figure S7. Key correlation signal of HMBC Spectrum of compound 1.

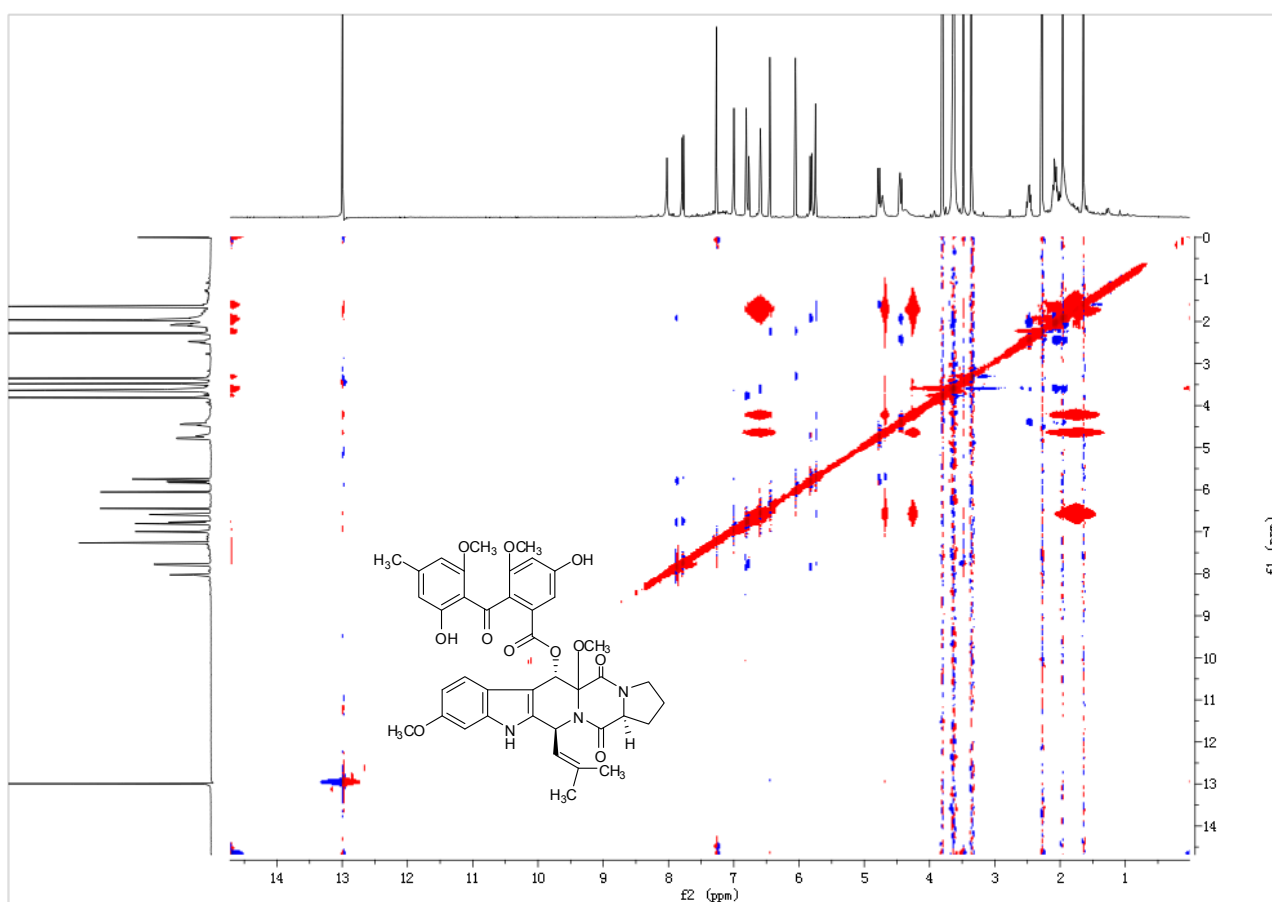


Figure S8. NOESY spectrum of compound 1.

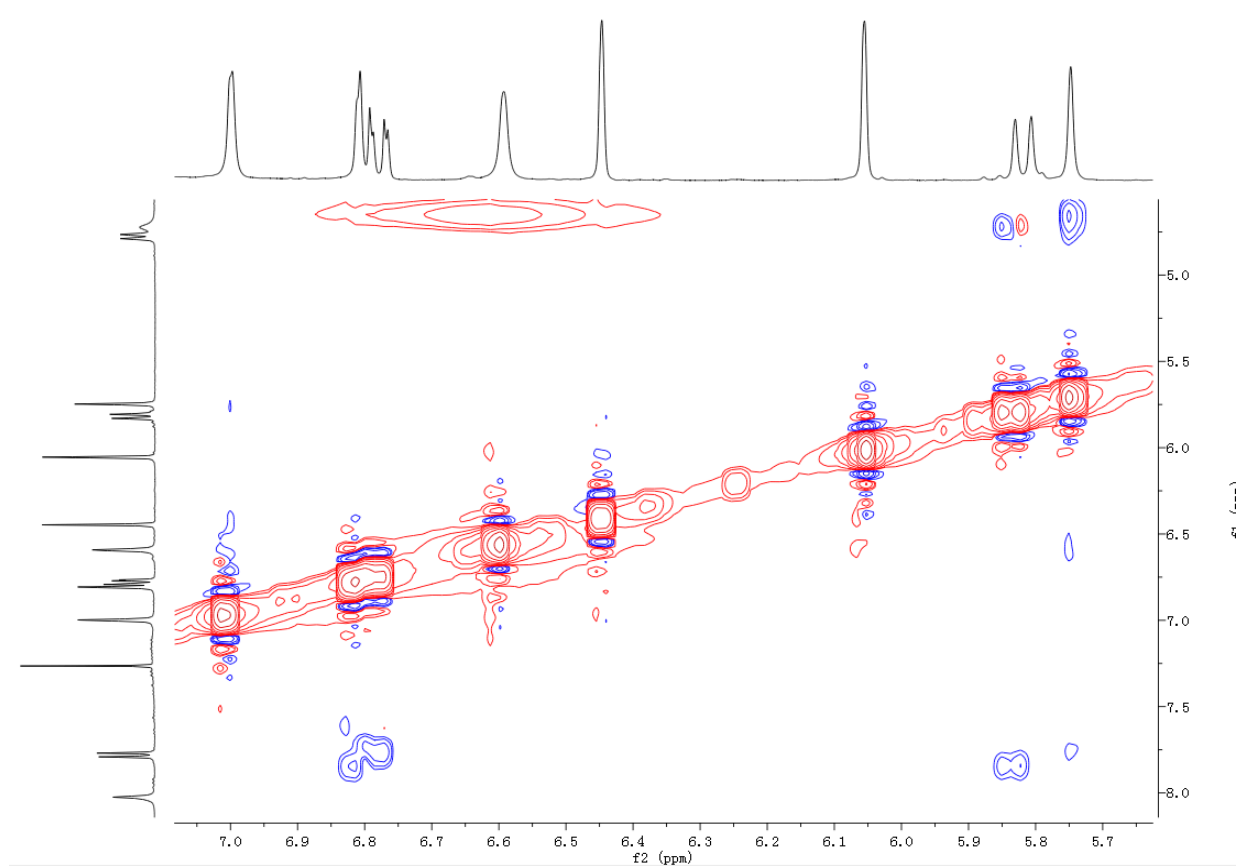


Figure S9. Expanded NOESY spectrum of compound **1**.

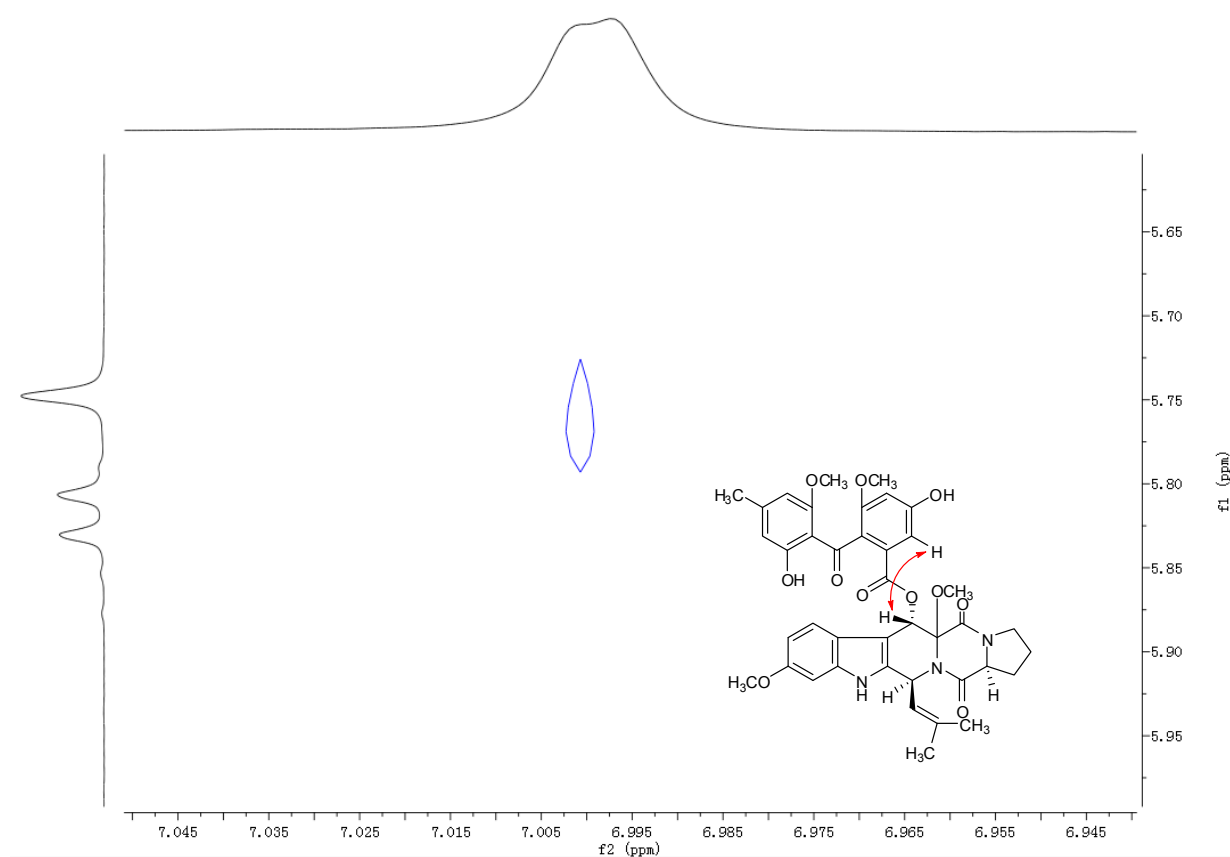


Figure S10. Key NOESY spectrum of compound **1**.

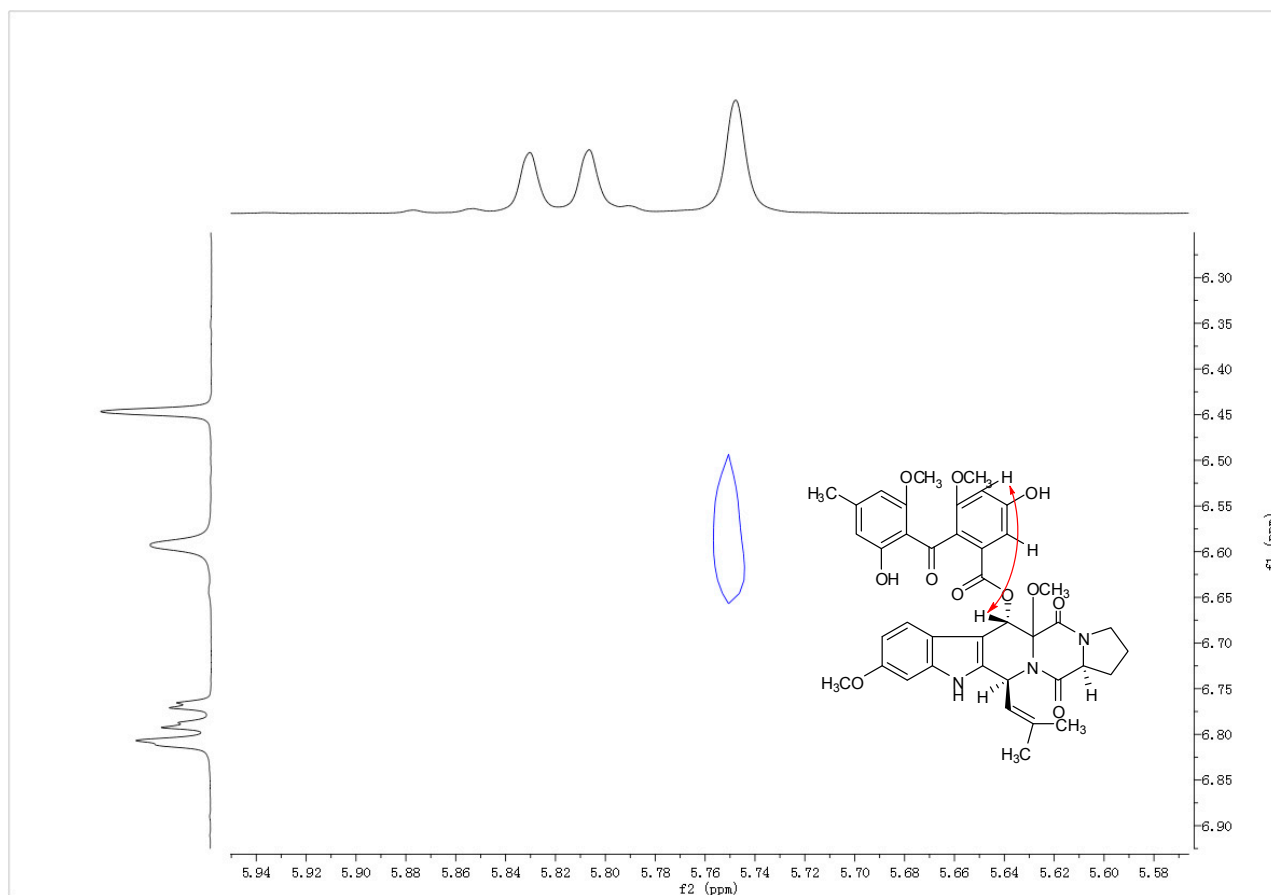
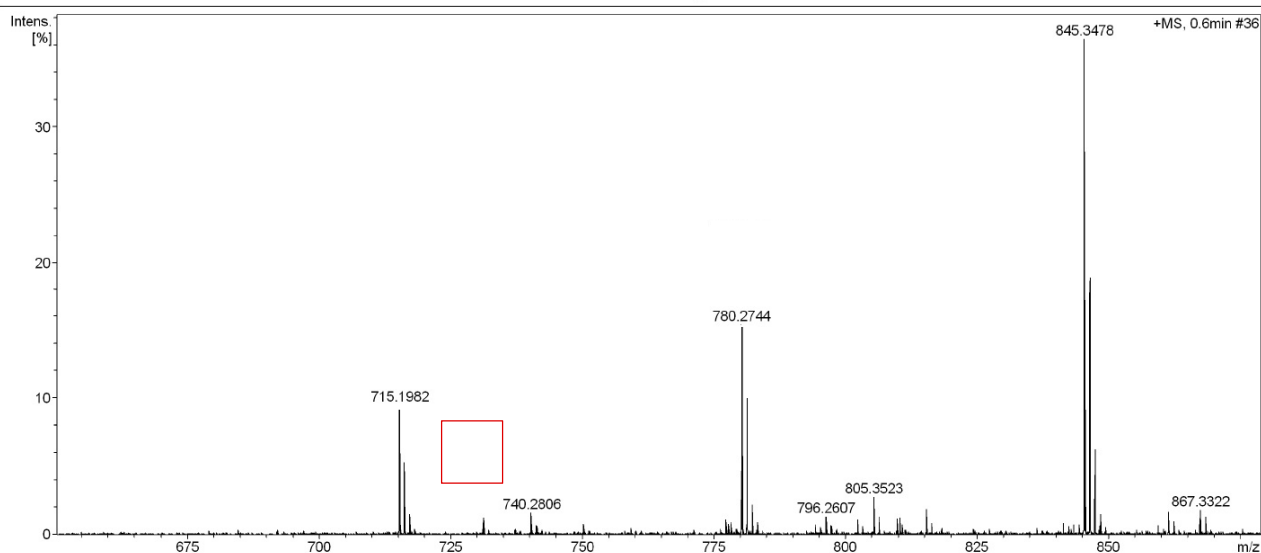


Figure S11. Key NOESY spectrum of compound 1.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
740.2806	1	C ₄₀ H ₄₂ N ₃ O ₁₁	100.00	740.2814	0.8	1.1	68.7	21.5	even	ok

Figure S12. HR-ESIMS of compound 1.

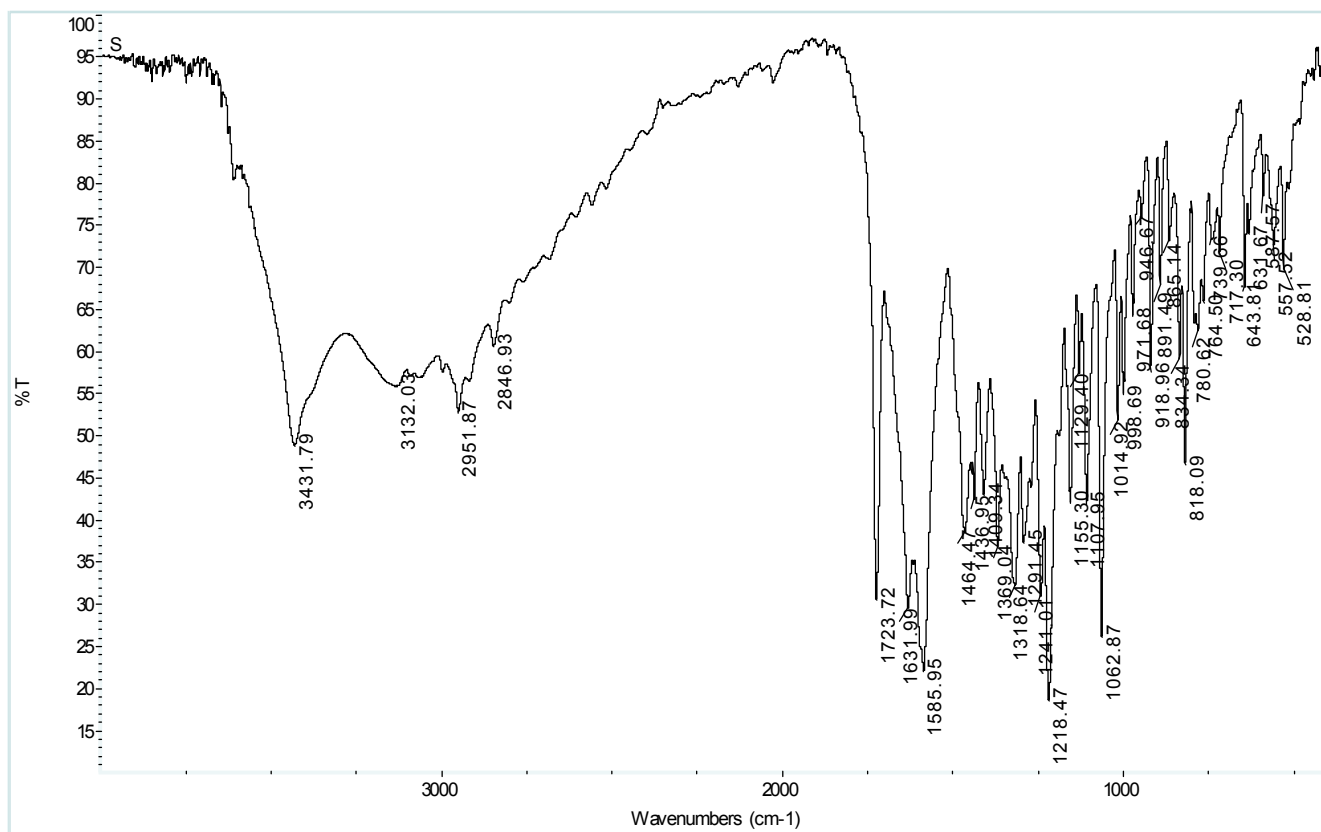


Figure S13. IR spectrum of compound 1.

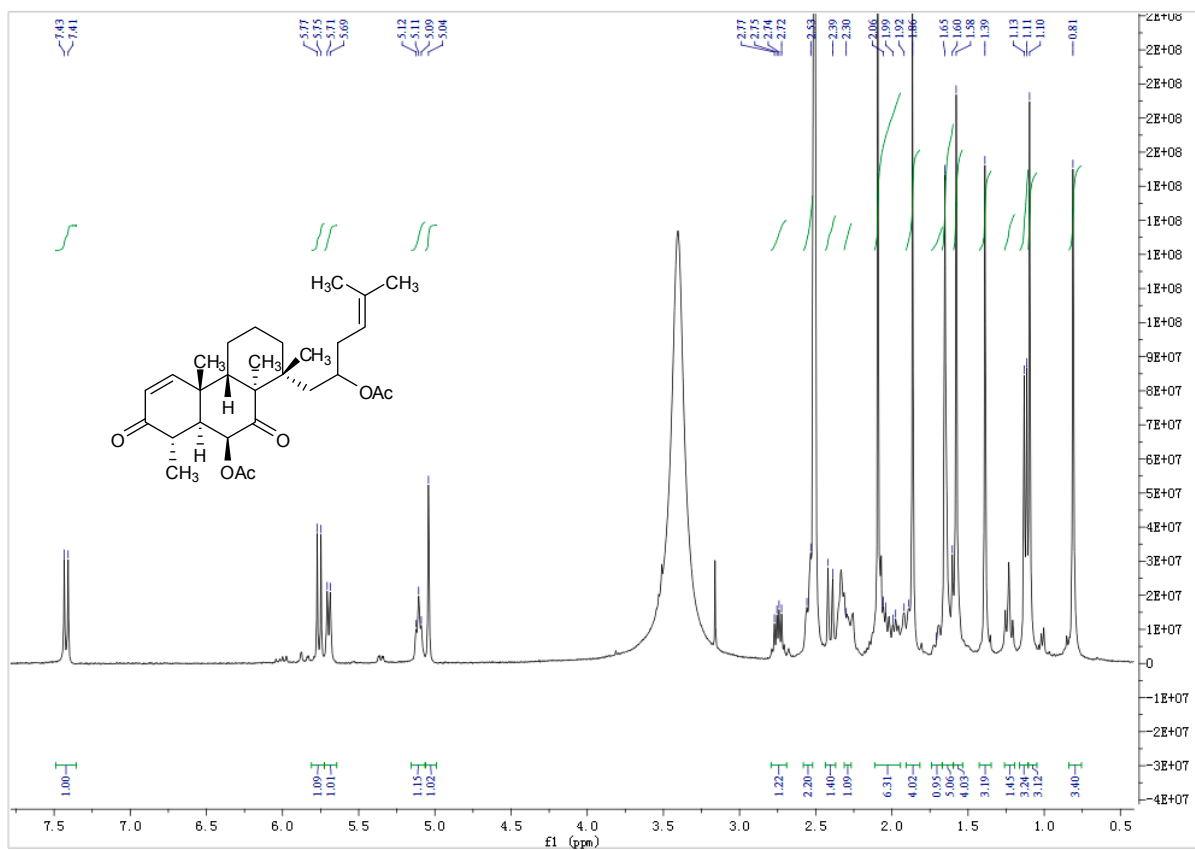


Figure S14. ¹H-NMR (400 MHz, DMSO-*d*₆) spectrum of compound 2.

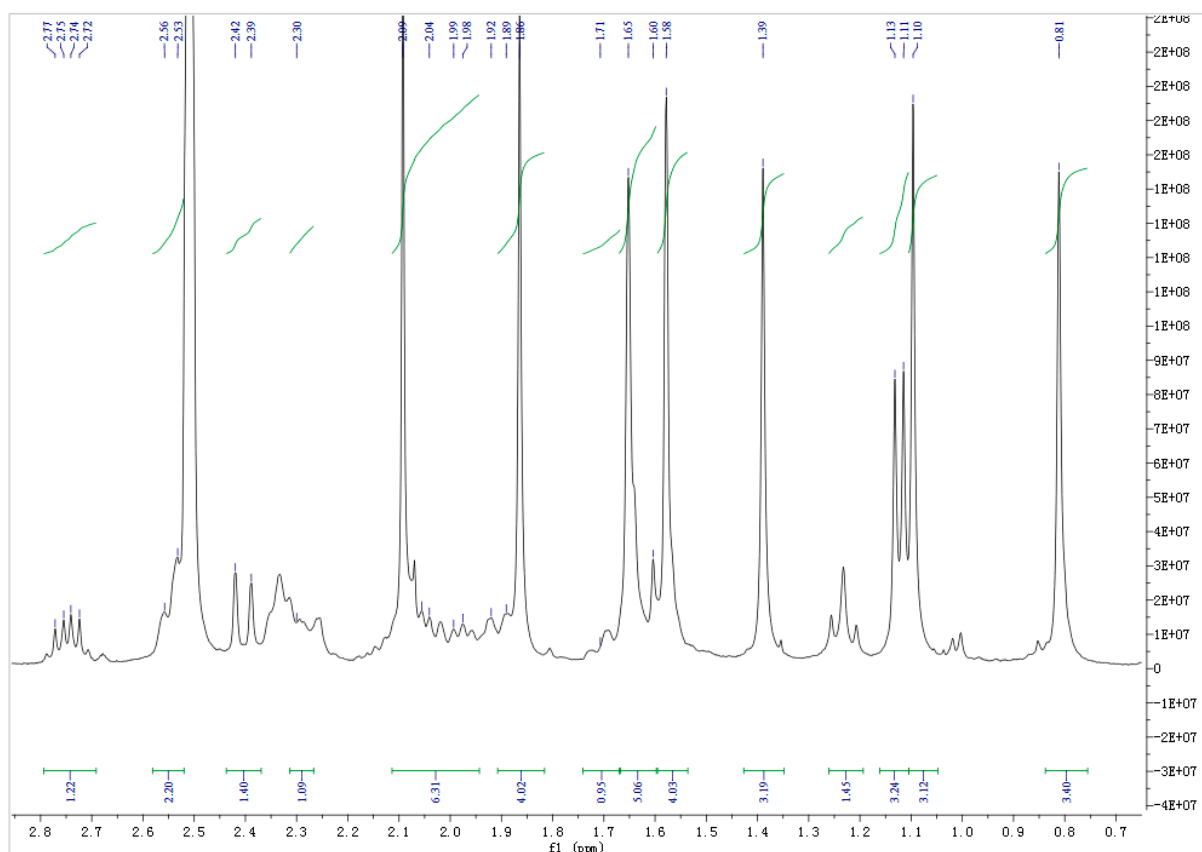


Figure S15. Expanded ^1H -NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **2**.

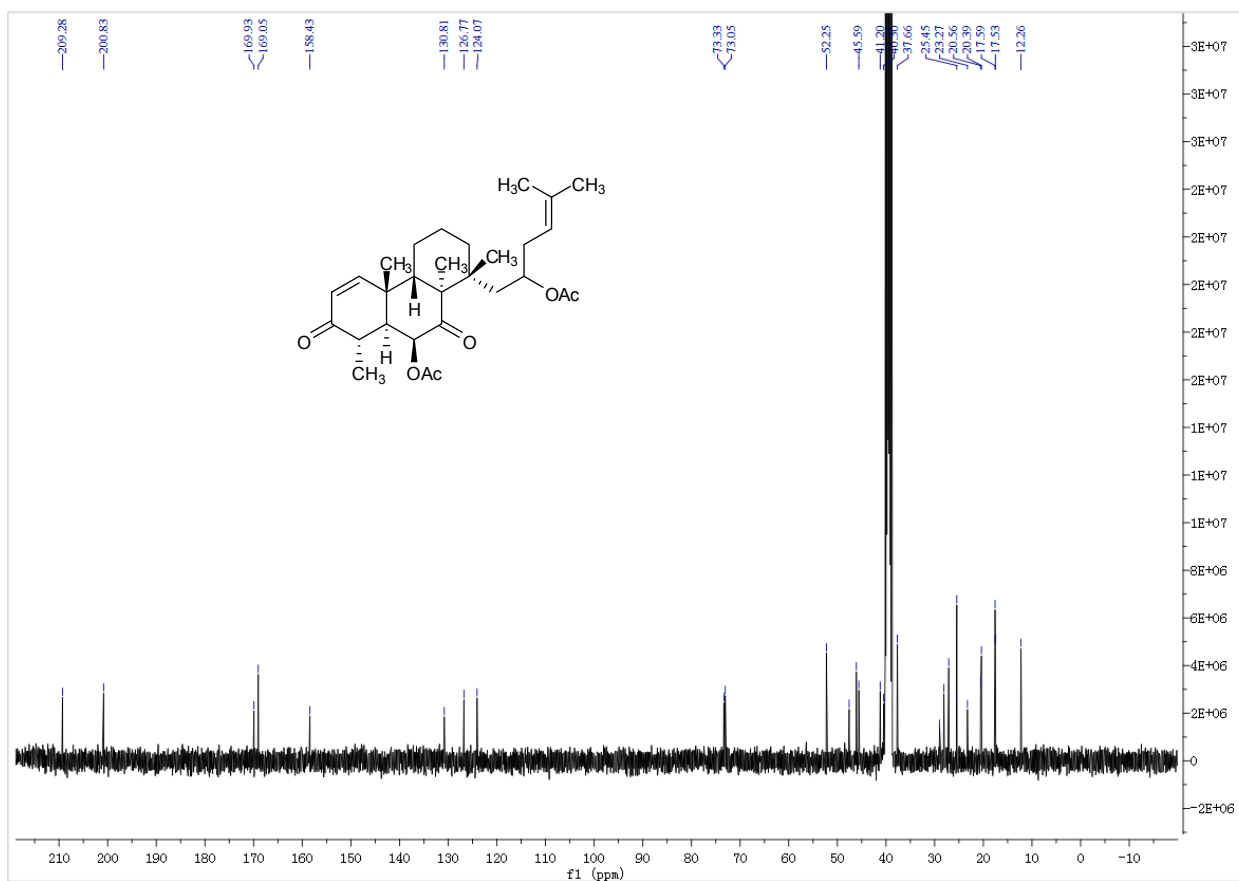


Figure S16. ^{13}C -NMR (100 MHz, $\text{DMSO-}d_6$) Spectrum of compound **2**.

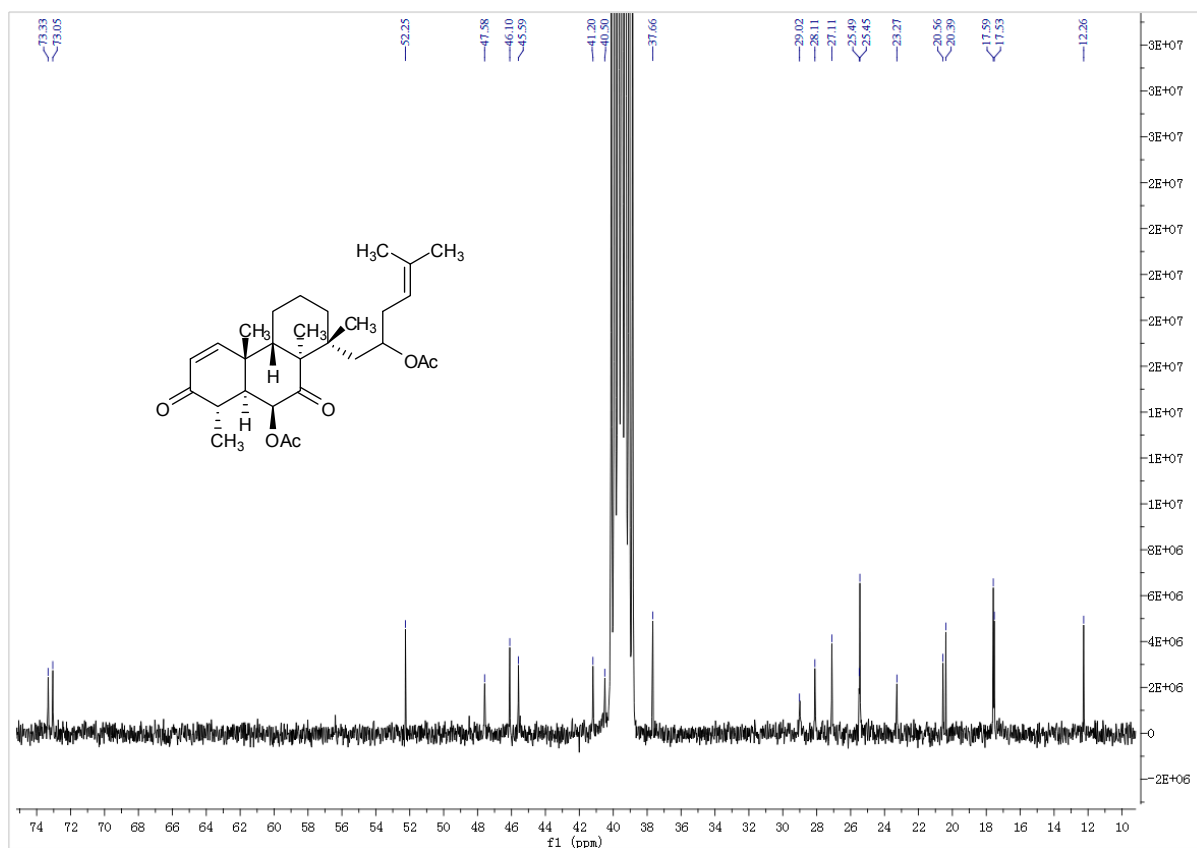


Figure S17. Expanded ^{13}C -NMR (100 MHz, $\text{DMSO-}d_6$) Spectrum of compound 2.

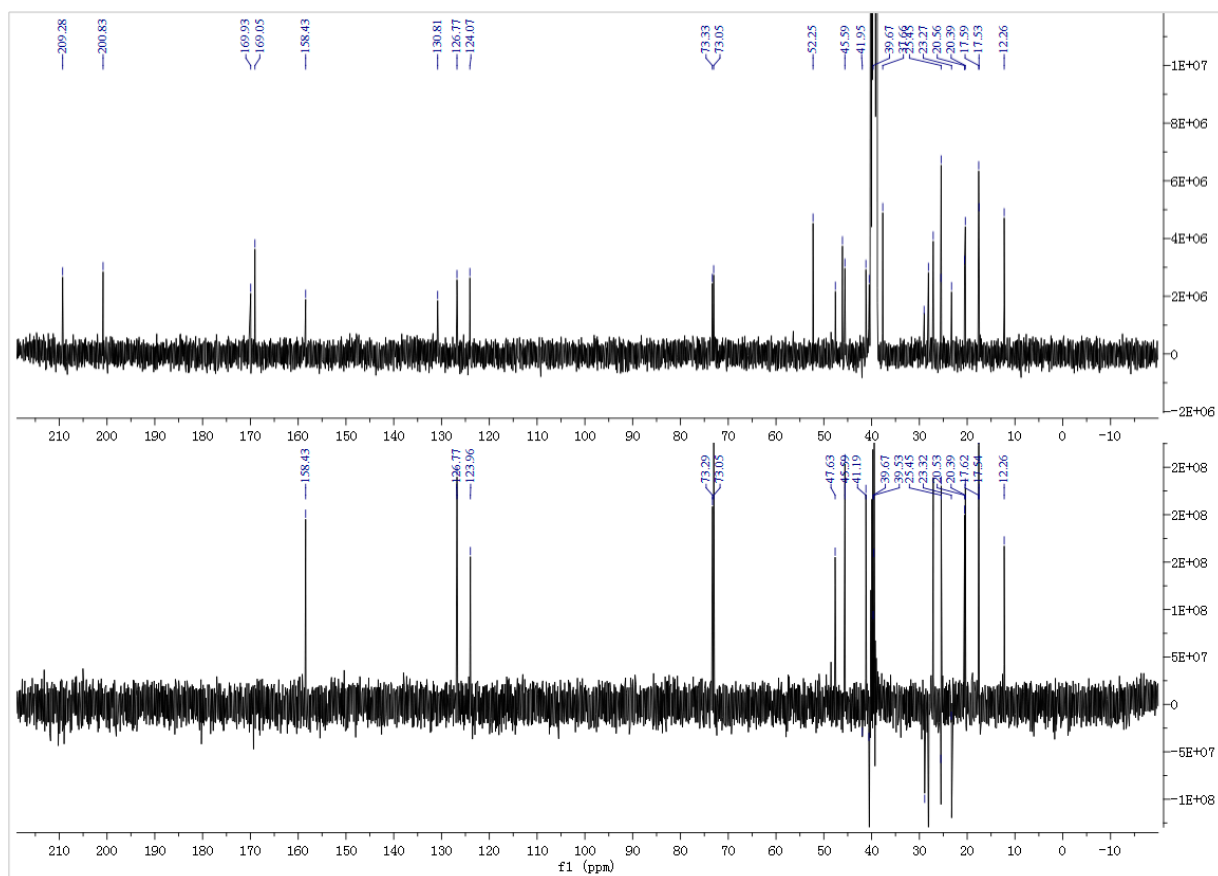


Figure S18. DEPT135 Spectrum (100 MHz, $\text{DMSO-}d_6$) of compound 2.

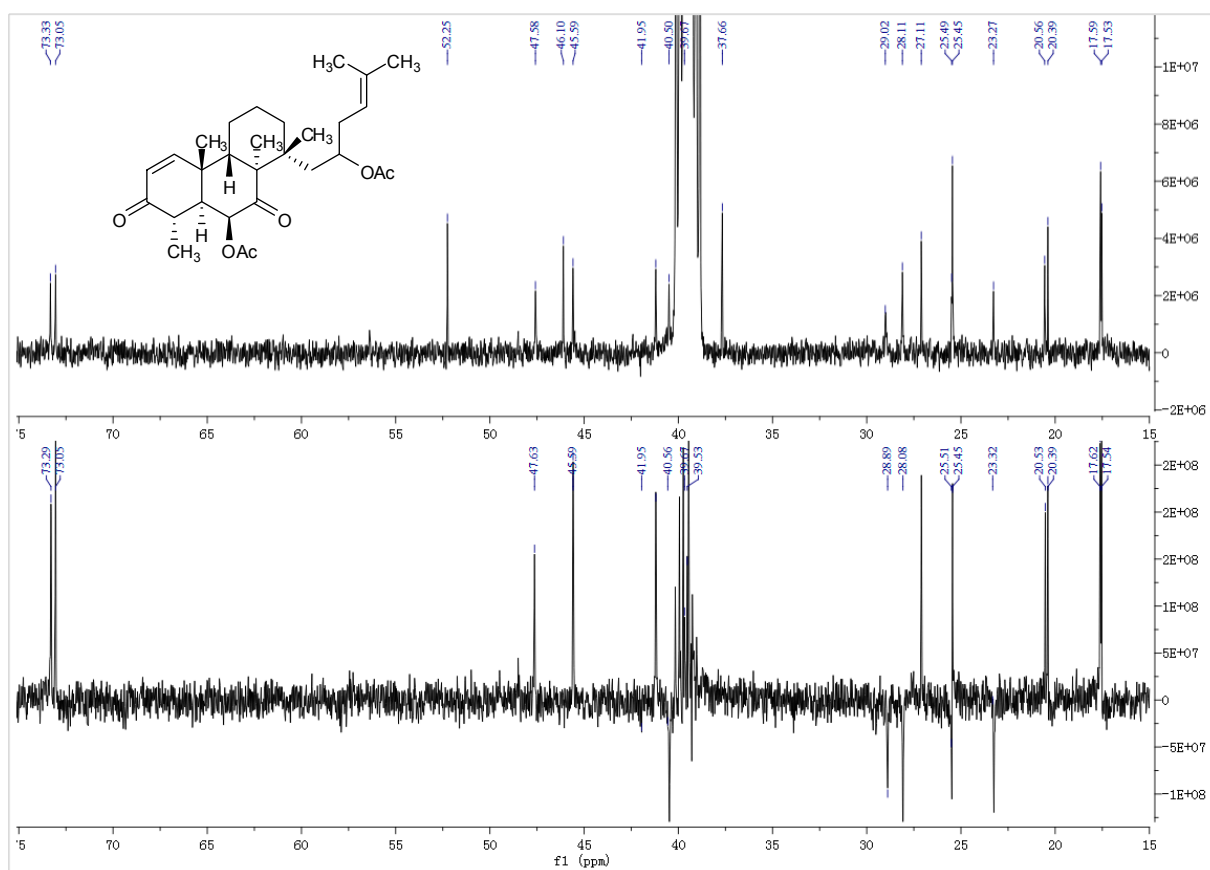


Figure S19. Expanded DEPT135 Spectrum (100 MHz, DMSO- d_6) of compound 2.

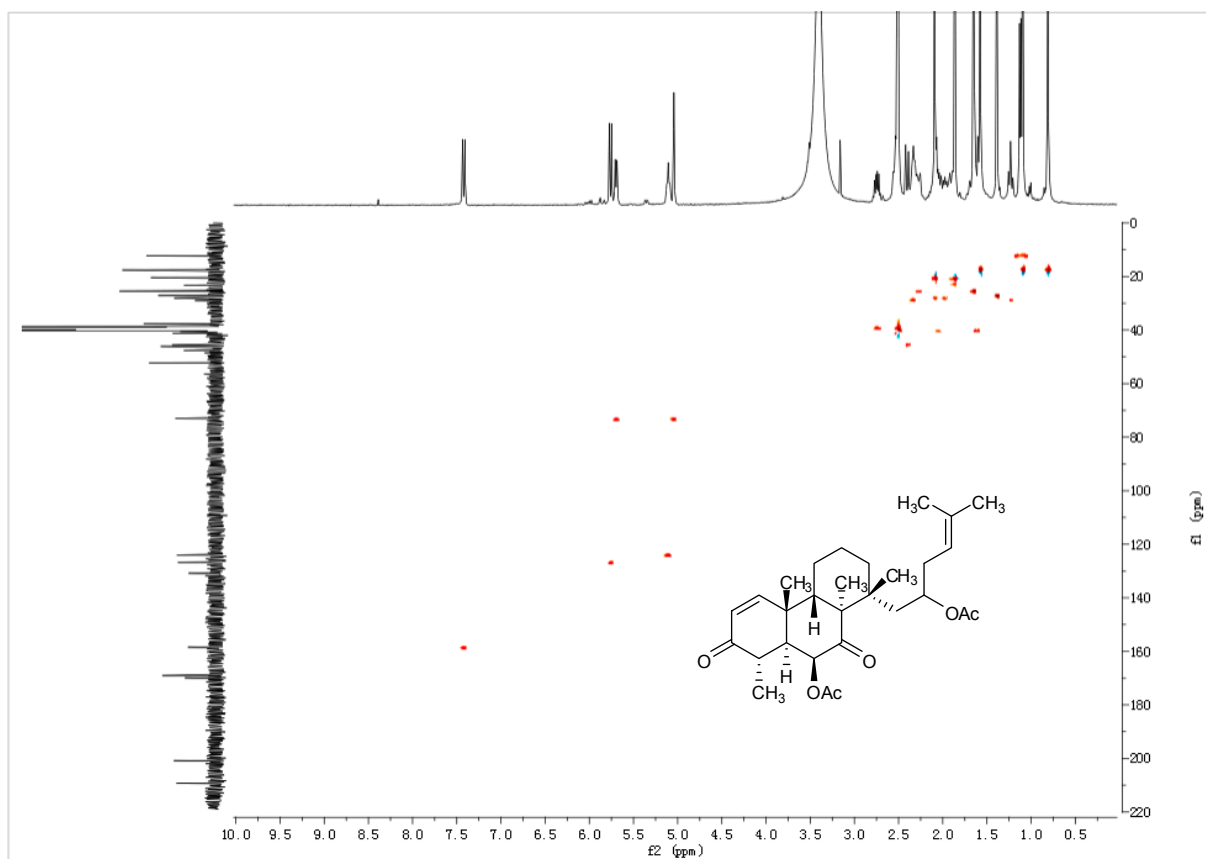


Figure S20. HSQC Spectrum of compound 2.

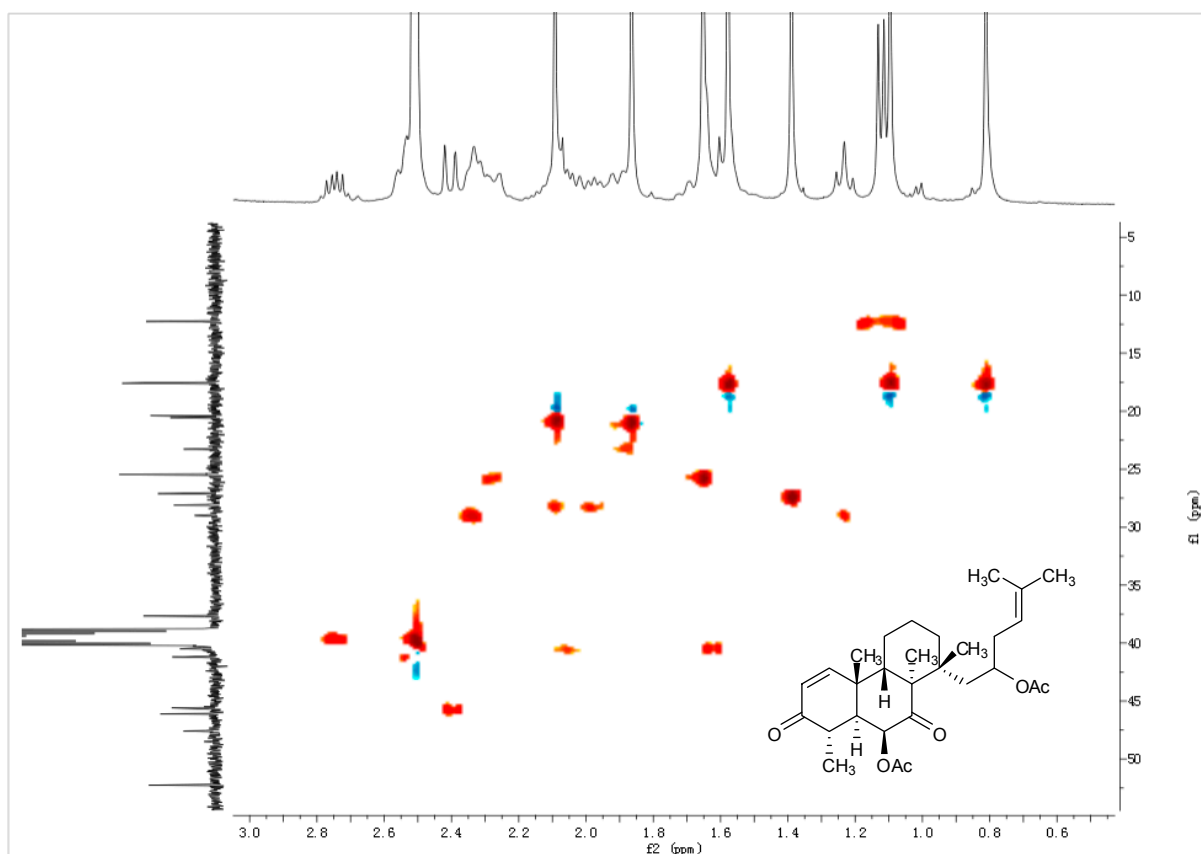


Figure S21. Expanded HSQC Spectrum of compound 2.

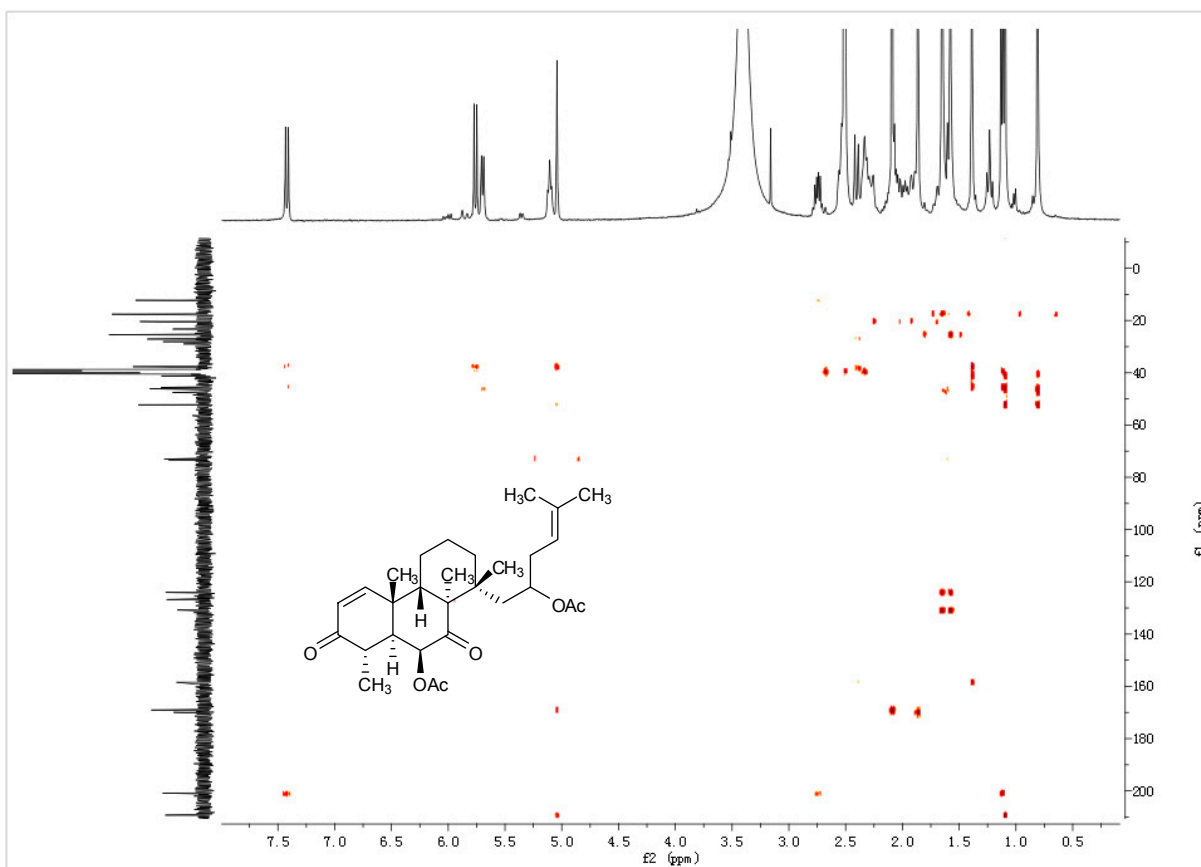


Figure S22. HMBC Spectrum of compound 2.

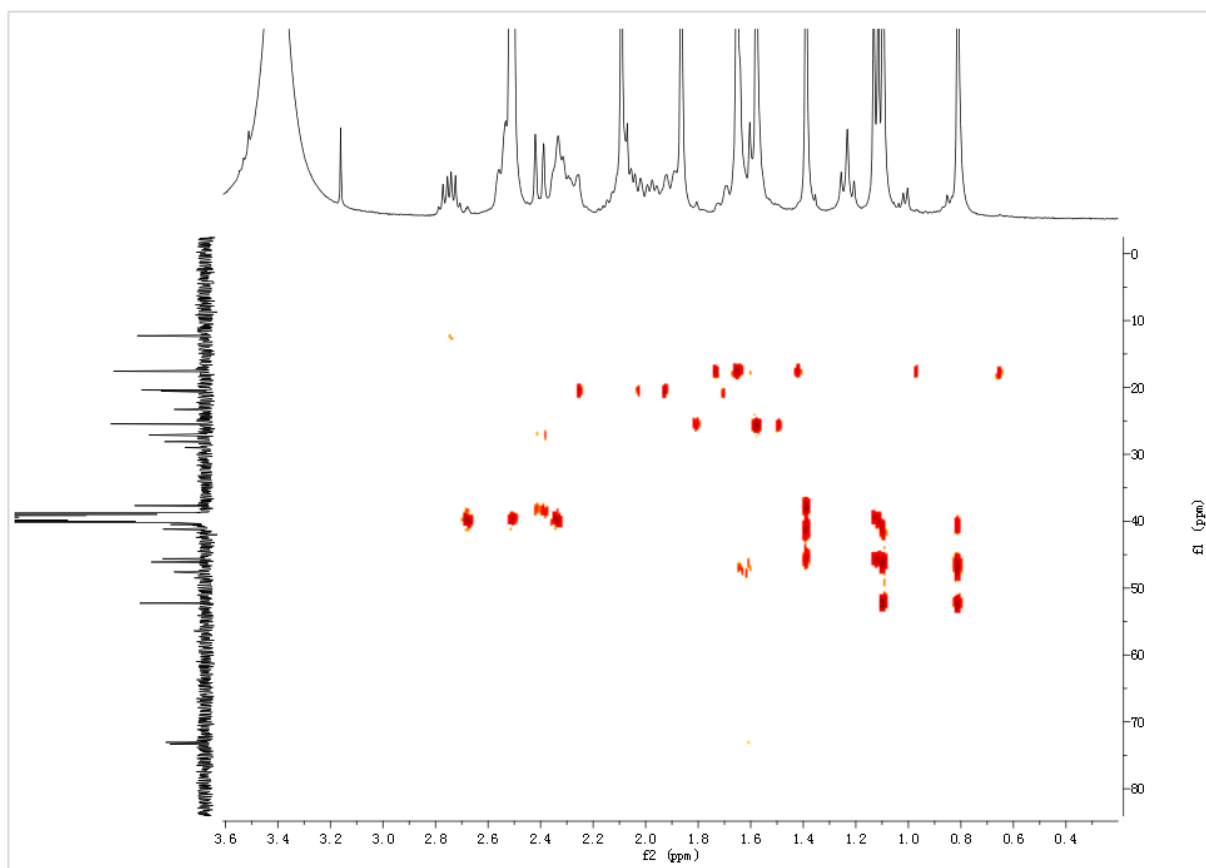


Figure S23. Expanded HMBC Spectrum of compound 2.

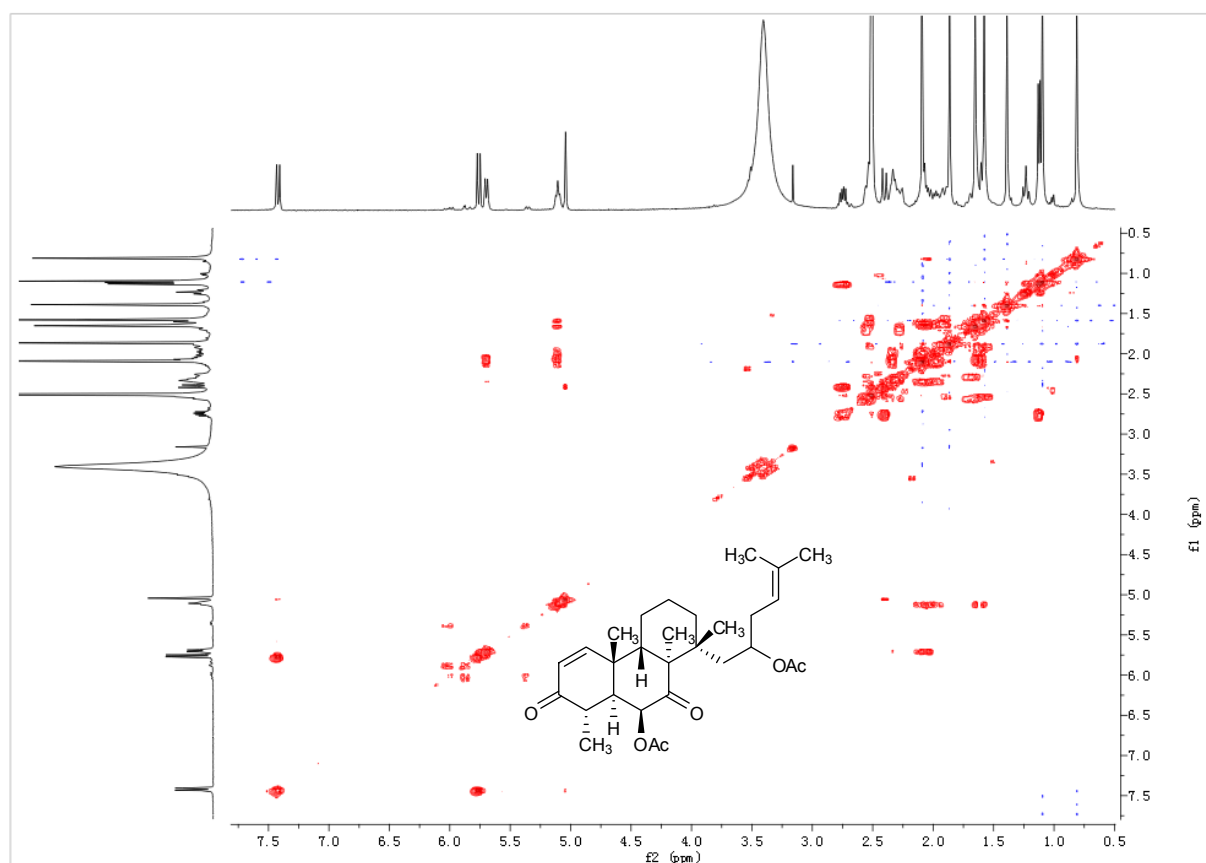


Figure S24. COSY Spectrum of compound 2.

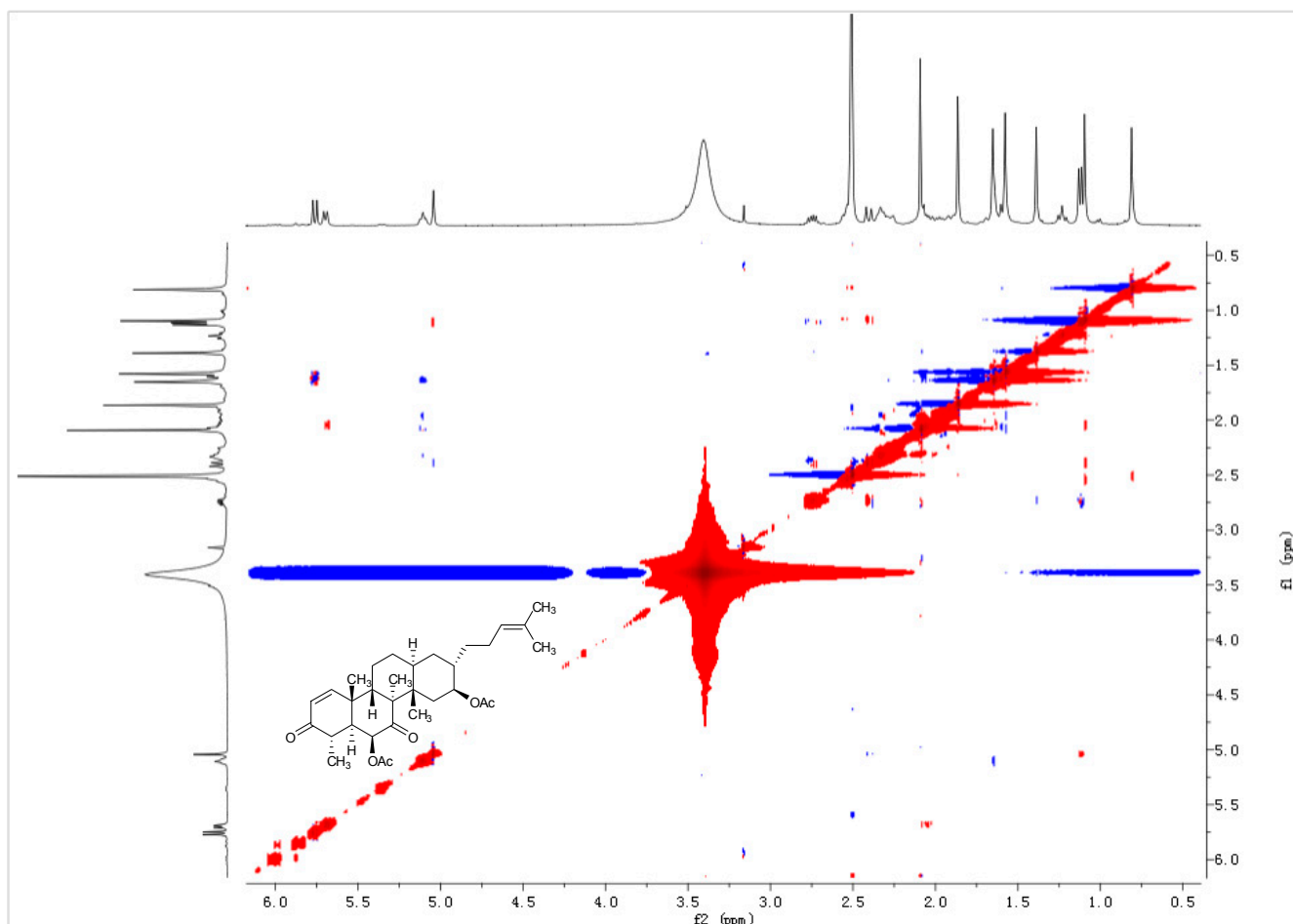
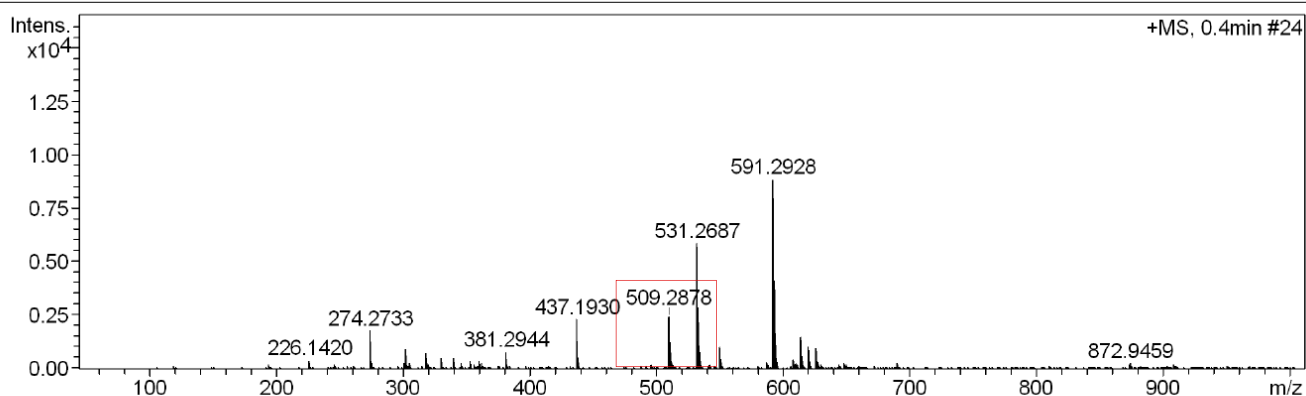


Figure S25. NOESY Spectrum of compound 2.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
509.2878	1	C ₂₉ H ₄₂ NaO ₆	100.00	509.2874	-0.4	-0.8	33.6	8.5	even	ok

Figure S26. HR-ESIMS of compound 2.