

Supplementary Information

Secopaxilline A, an Indole-Diterpenoid Alkaloid from an Aciduric

Penicillium fungus, its Identification and Semisynthesis

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Figure S1. ECD spectrum of secopaxilline A (1)

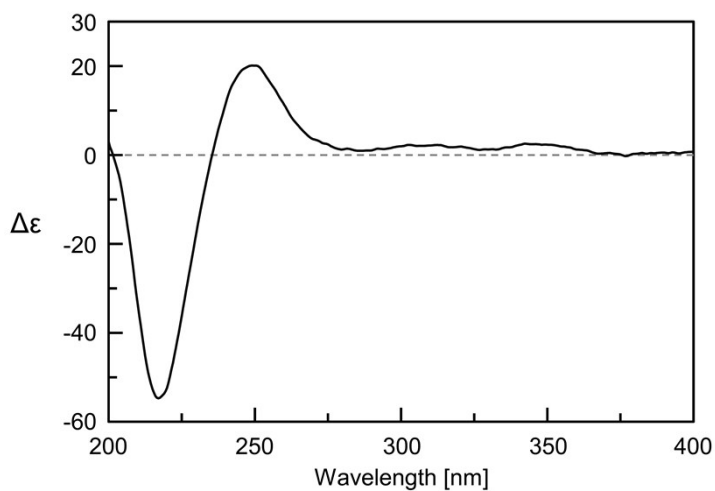


Figure S2. HPLC traces for reaction mixtures of paxilline
paxilline

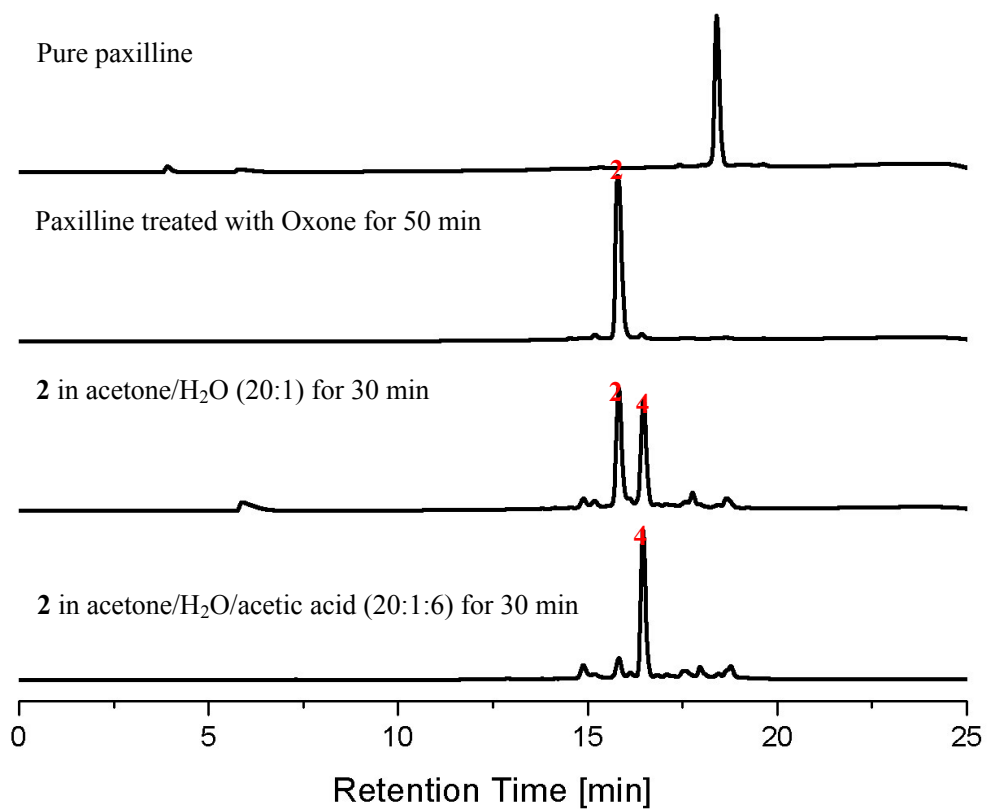


Figure S3. ESIMS spectrum of compound **2**

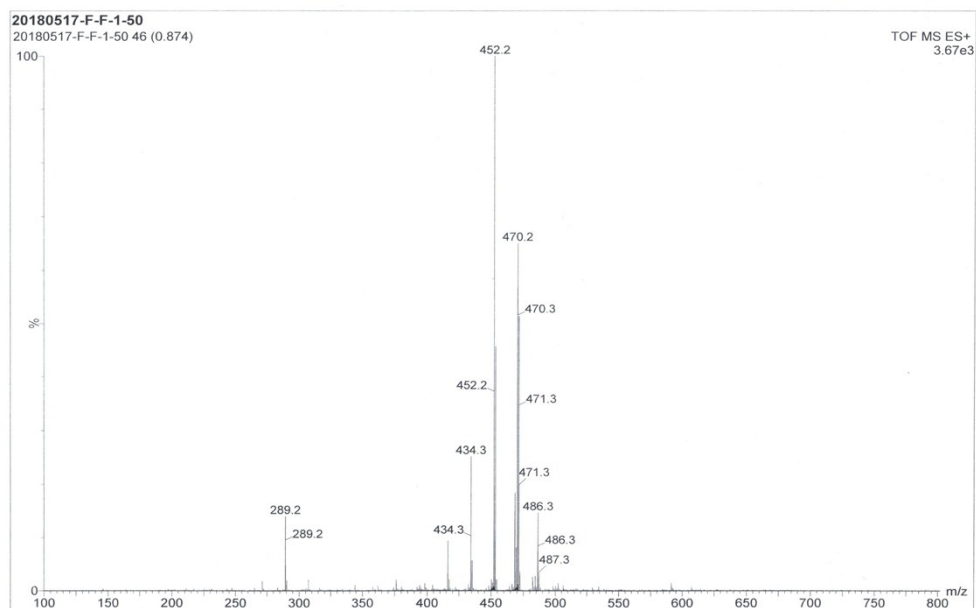


Figure S4. HPLC traces for one-pot synthesis of deacetylsecopaxilline A (**4**) from paxilline

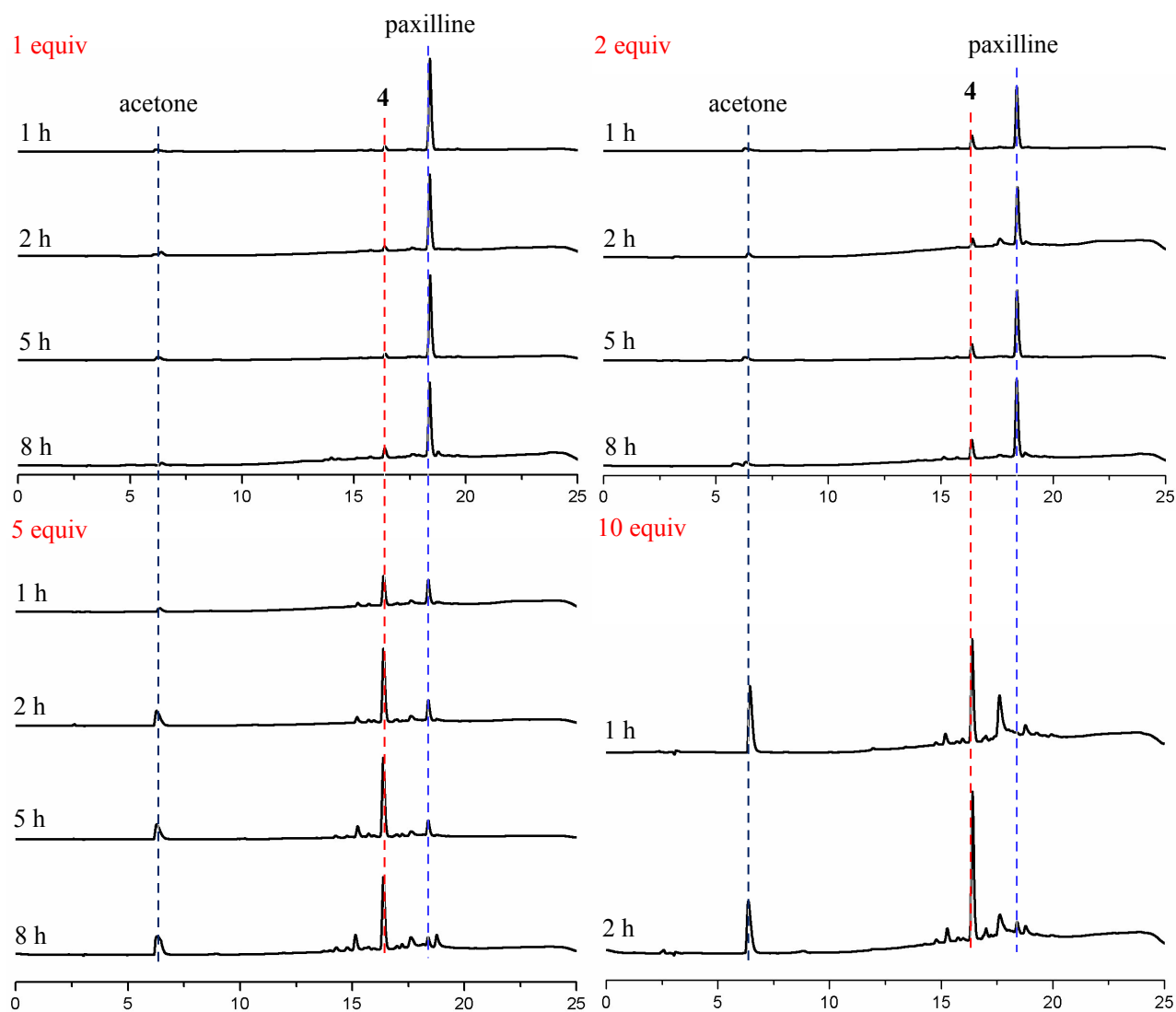


Figure S5. HRESIMS spectrum of secopaxilline A (**1**)

20180326-fyq-7-115_180326152834

3/26/2018 4:26:32 PM

fyq-7-115

20180326-fyq-7-115_180326152834 #55-56 RT: 0.44-0.44 AV: 2 NL: 7.38E7

T: FTMS + p ESI Full ms [100.00-2000.00]

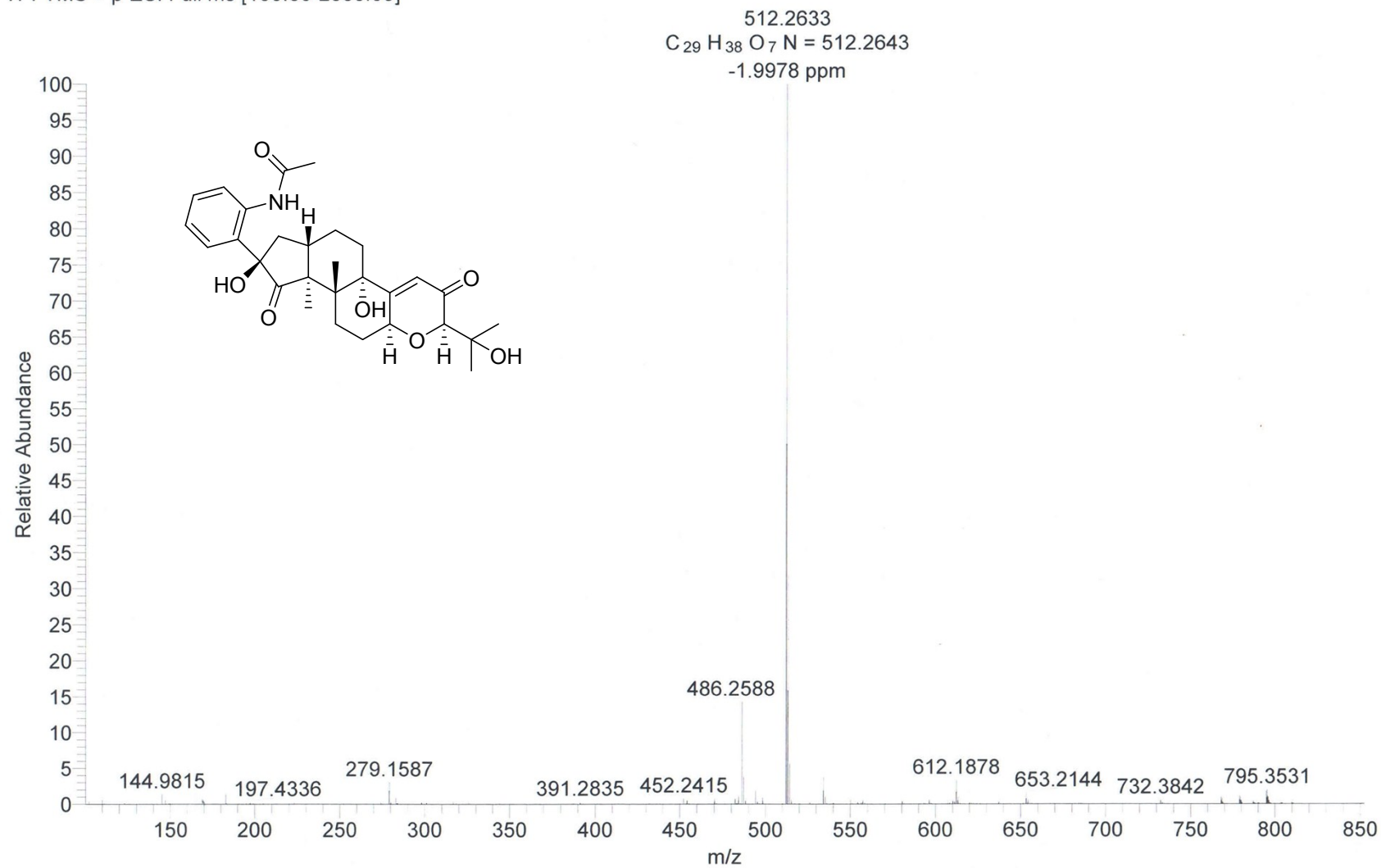


Figure S6. ¹H-NMR spectrum of secopaxilline A (**1**) in DMSO-*d*₆

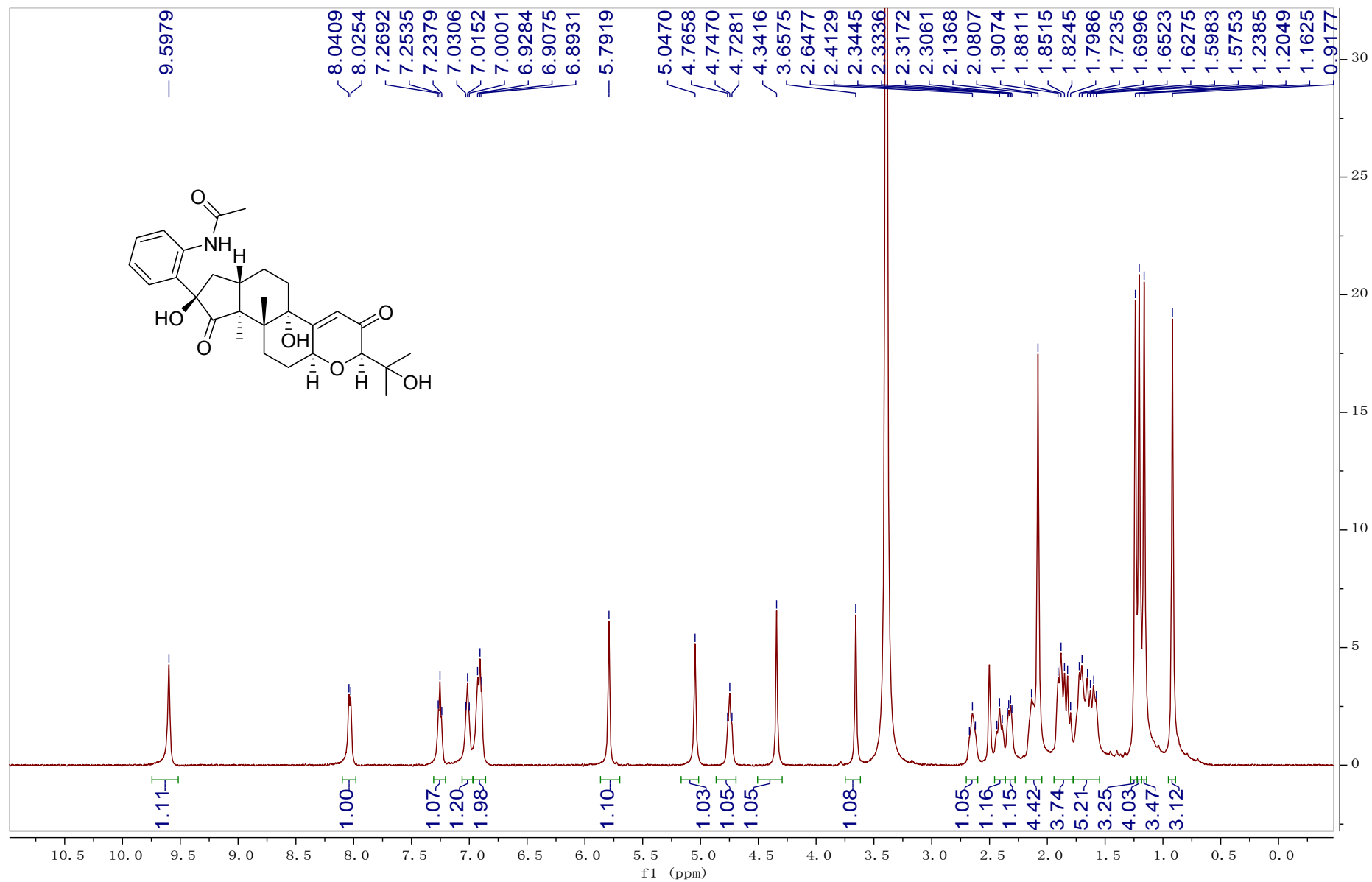


Figure S7. ^{13}C -NMR spectrum of secopaxilline A (**1**) in $\text{DMSO-}d_6$

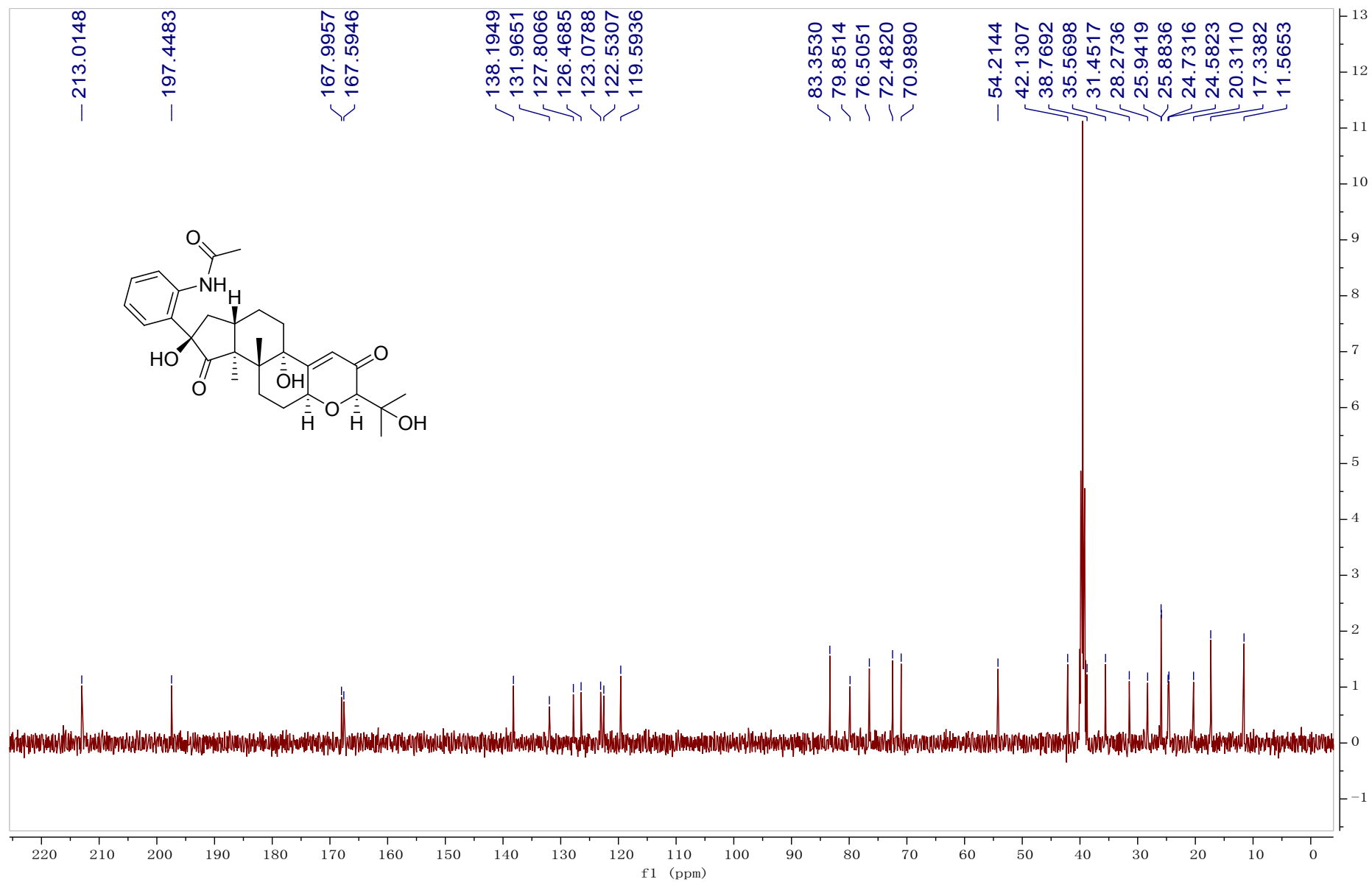


Figure S8. DEPT spectrum of secopaxilline A (**1**) in DMSO- d_6

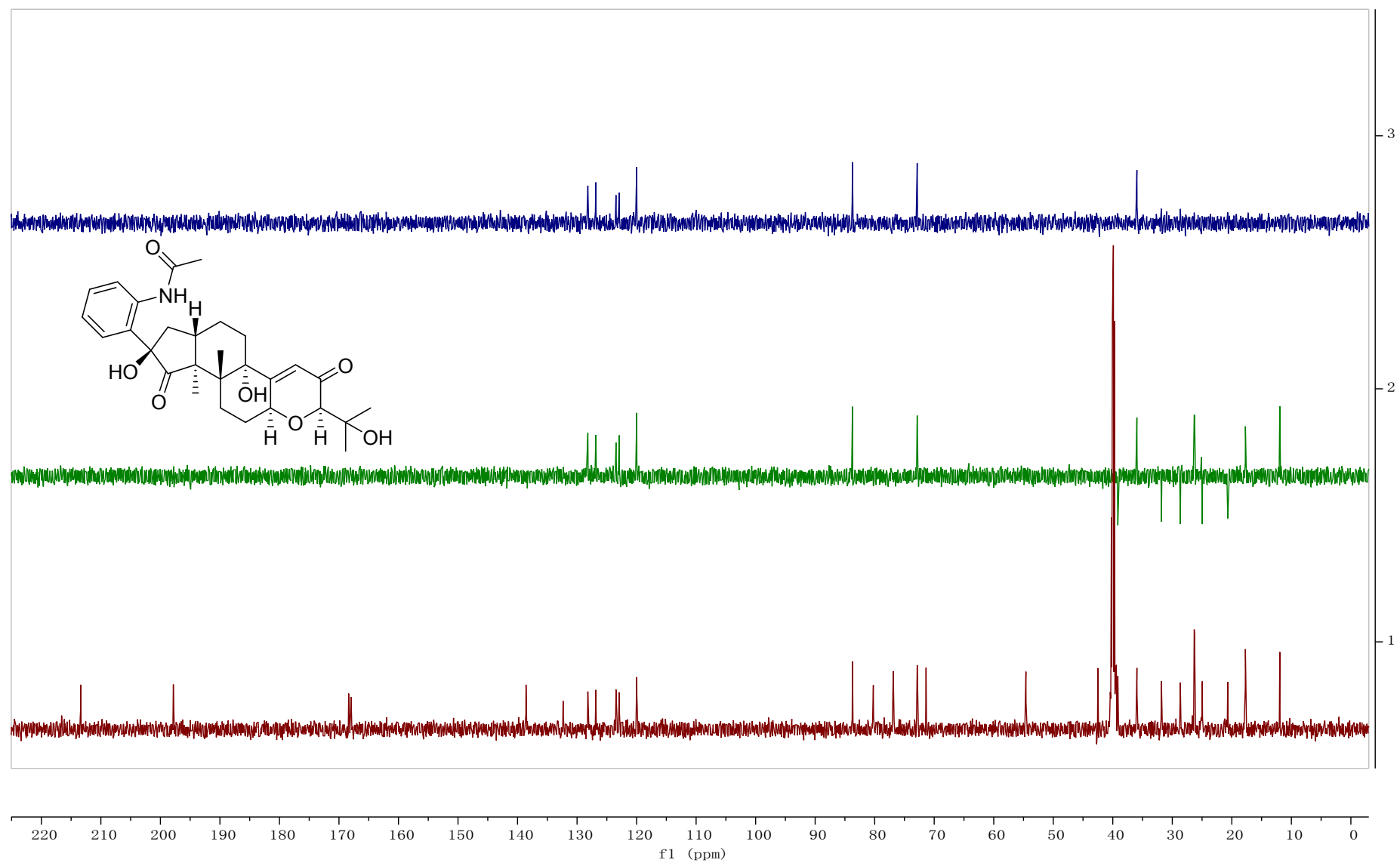


Figure S9. HSQC spectrum of secopaxilline A (**1**) in DMSO- d_6

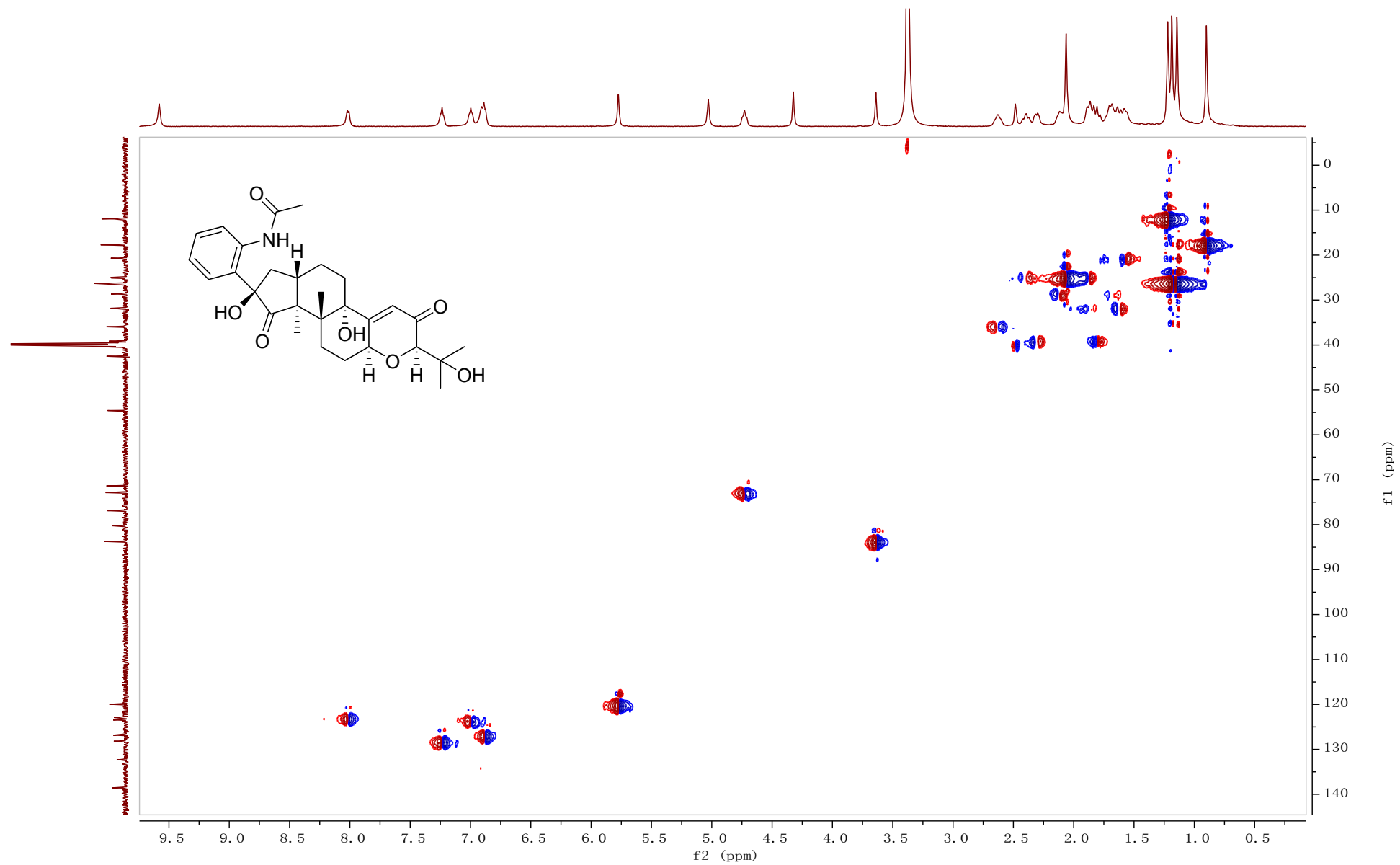


Figure S10. ^1H - ^1H COSY spectrum of secopaxilline A (**1**) in $\text{DMSO-}d_6$

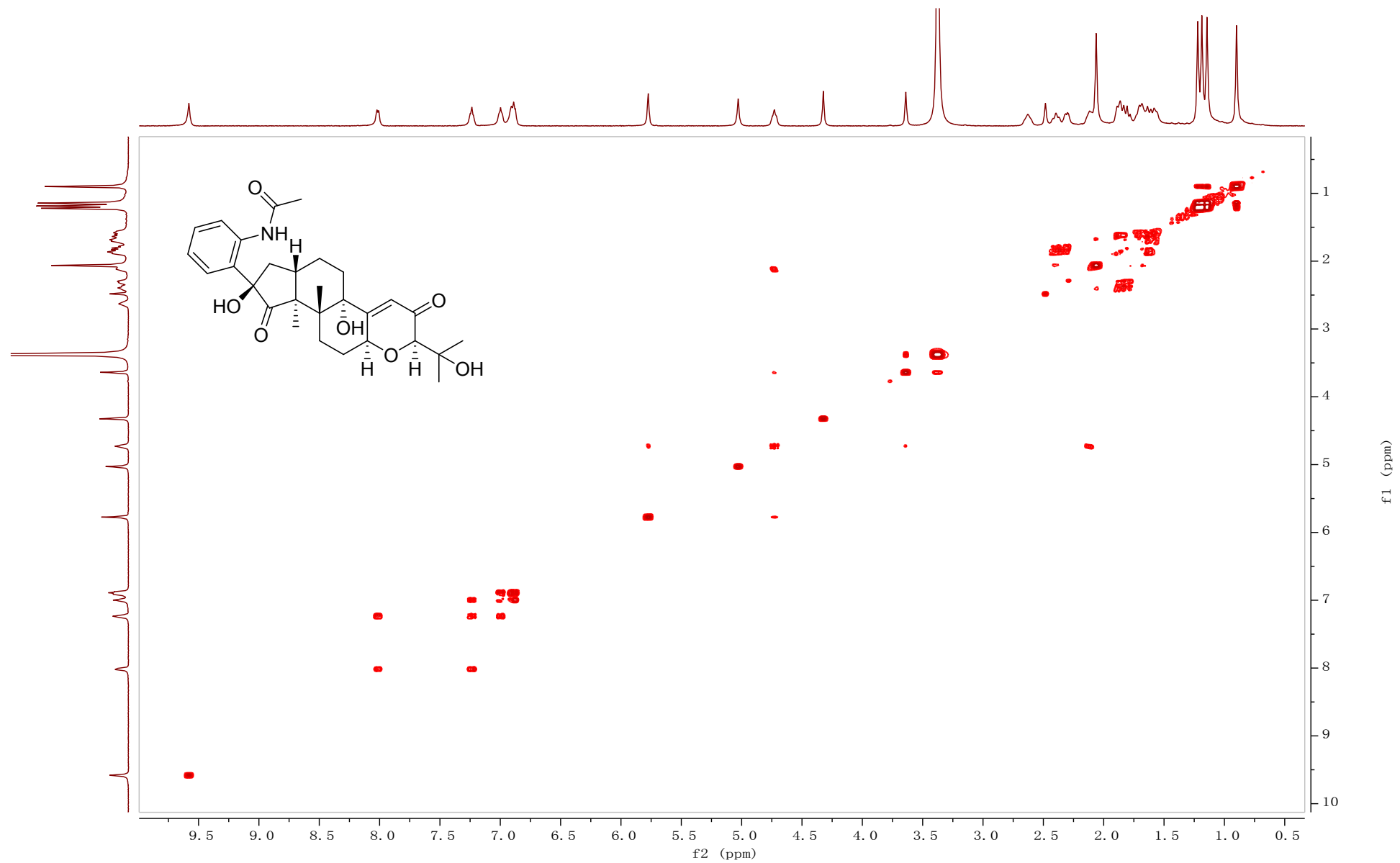


Figure S11. HMBC spectrum of secopaxilline A (1) in DMSO- d_6

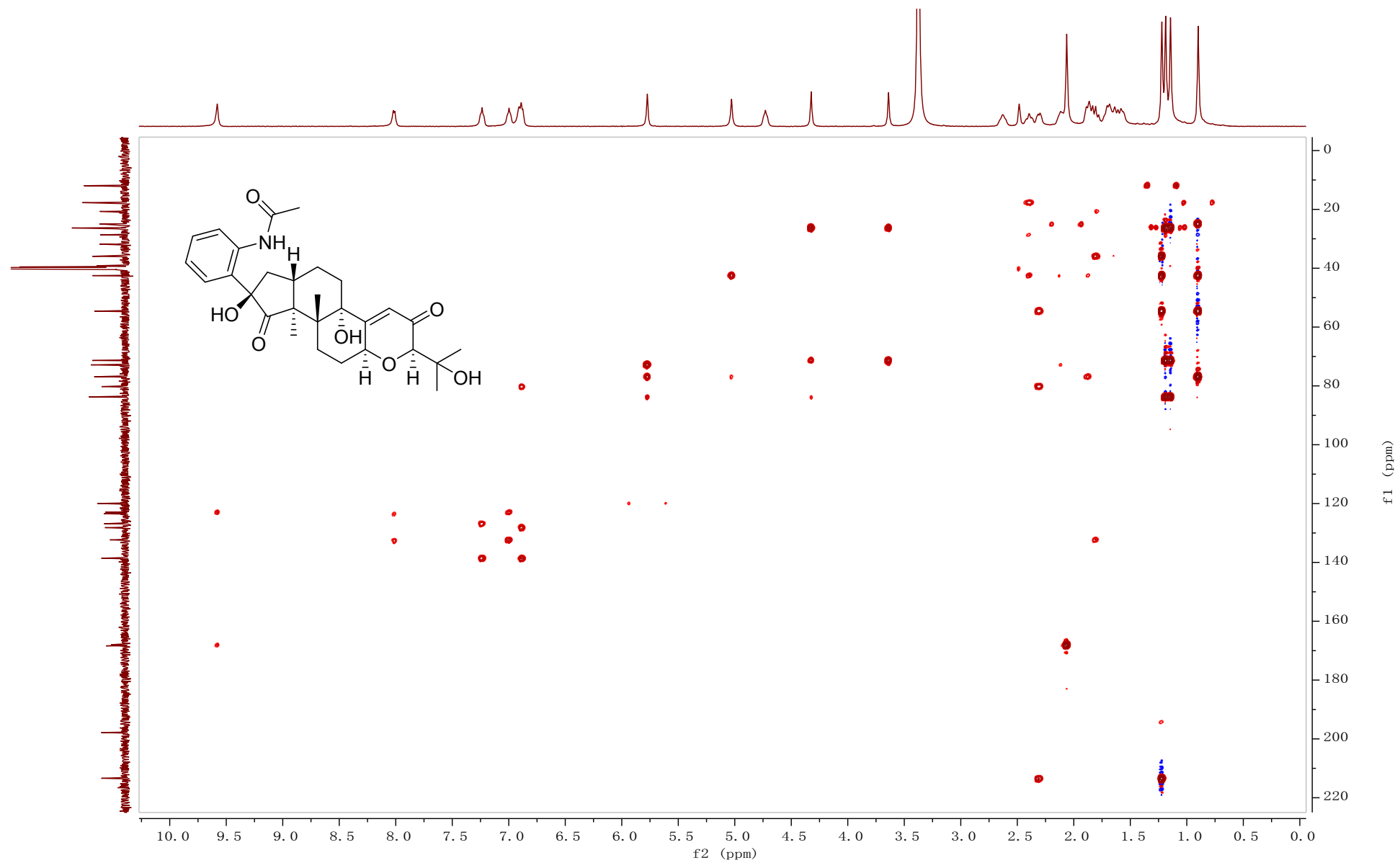


Figure S12. NOESY spectrum of secopaxilline A (1) in DMSO- d_6

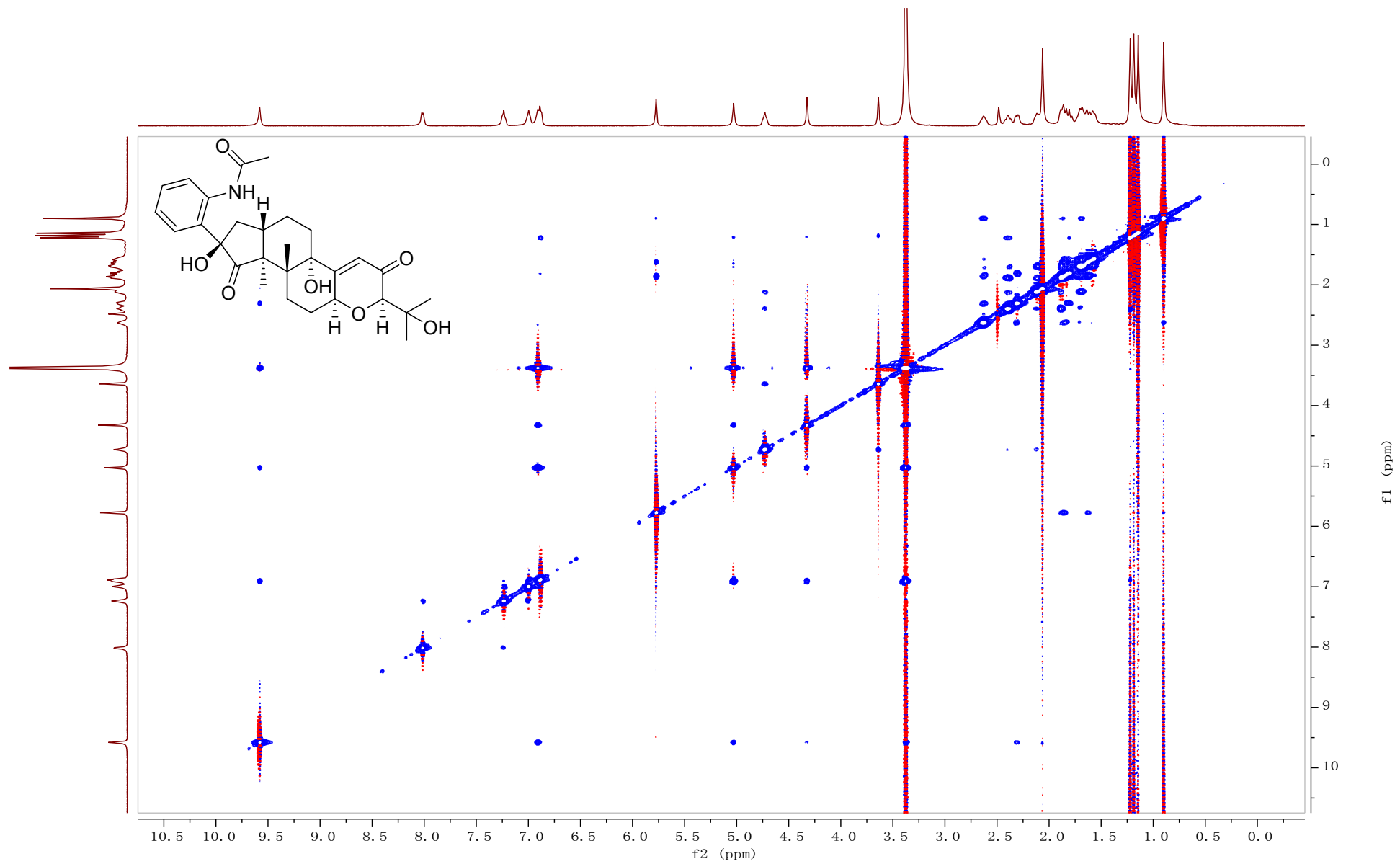


Figure S13. HRESIMS spectrum of deacetylsecopaxilline A (4)

20180521-FYQ-10-2-2_180521110353 #10 RT: 0.08 AV: 1 NL: 4.29E8
T: FTMS + p ESI Full ms [170.00-2000.00]

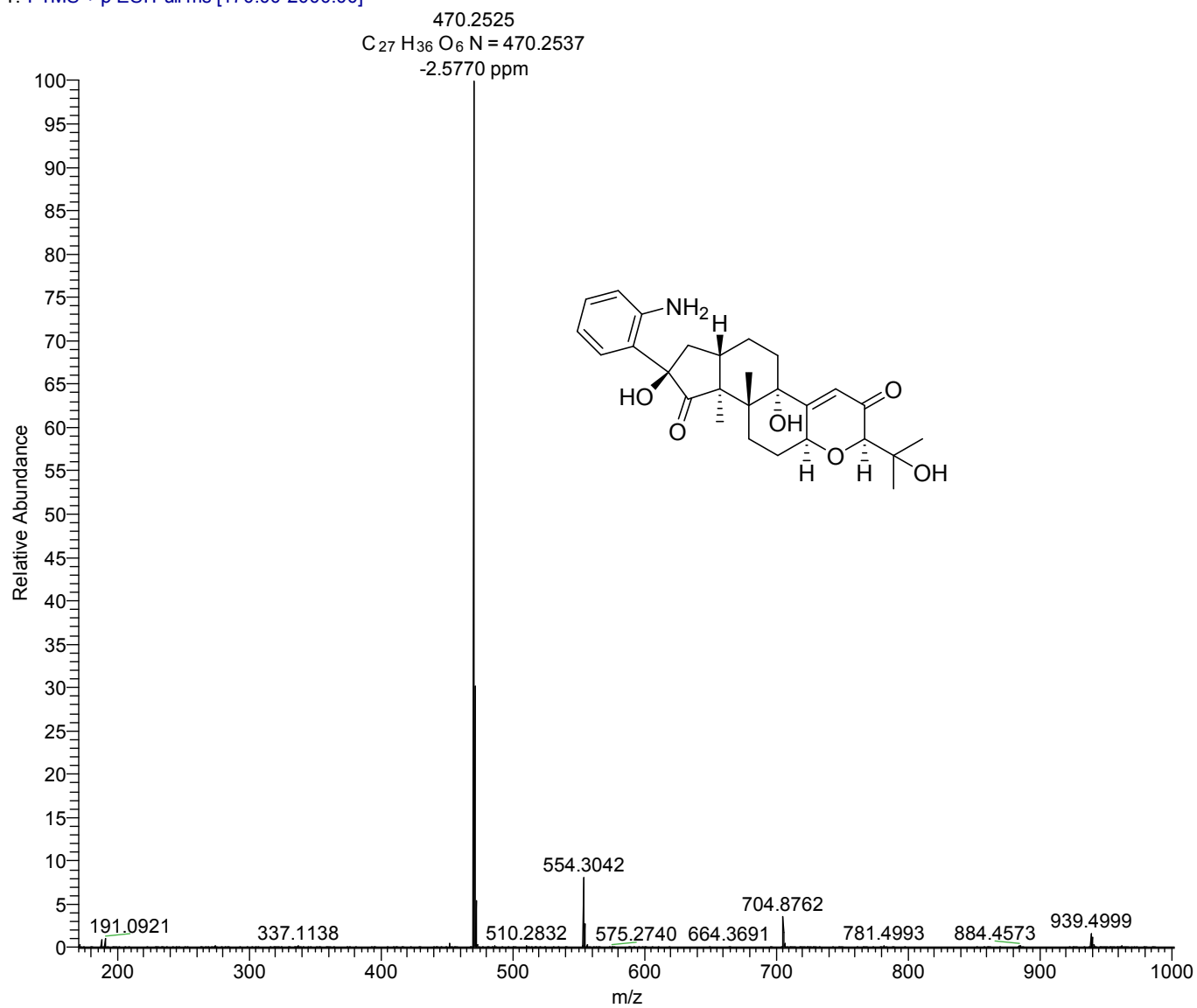


Figure S14. ¹H-NMR spectrum of deacetylsecopaxilline A (4) in DMSO-*d*₆

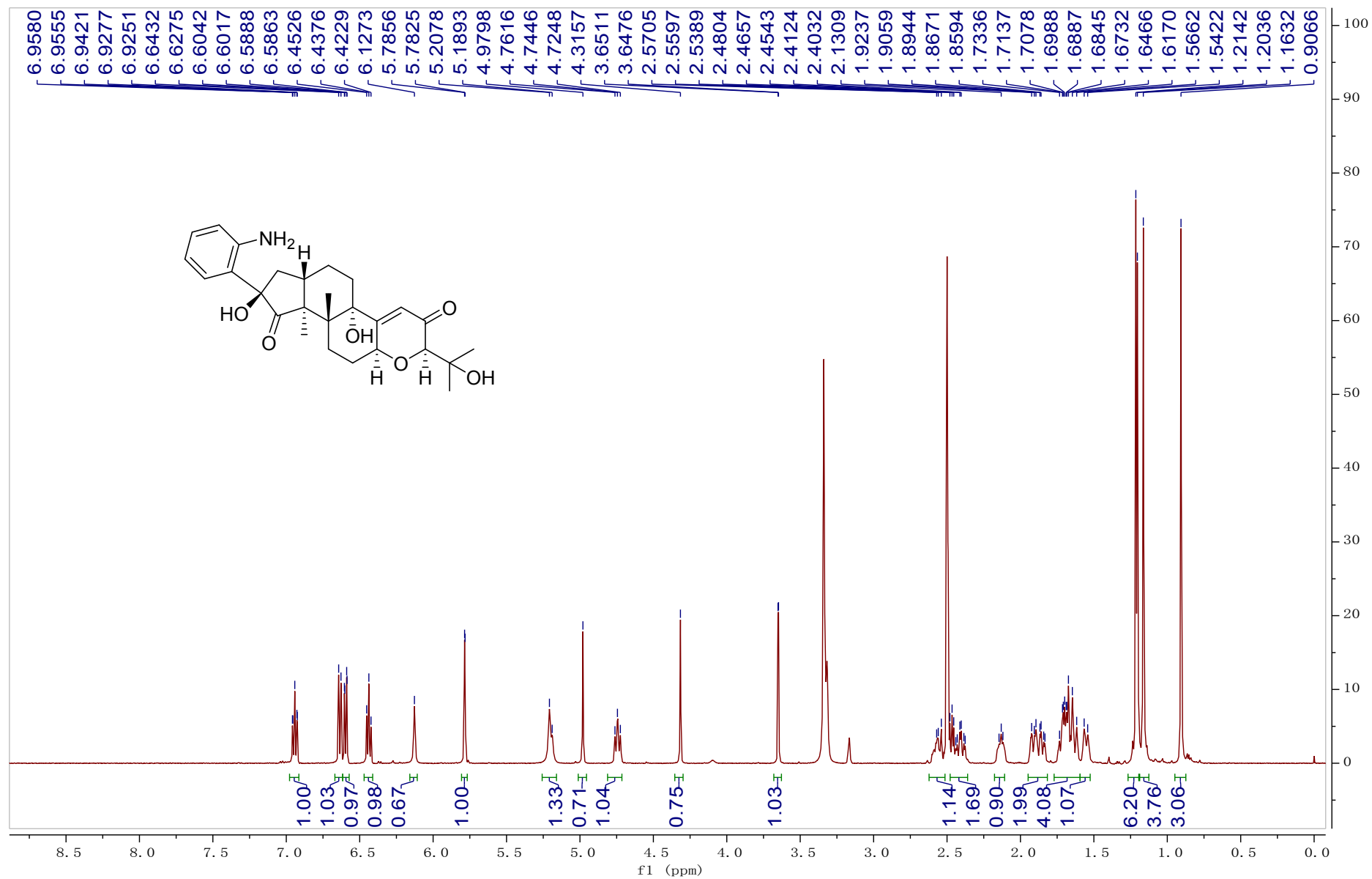


Figure S15. ^{13}C -NMR spectrum of deacetylsecopaxilline A (**4**) in $\text{DMSO-}d_6$

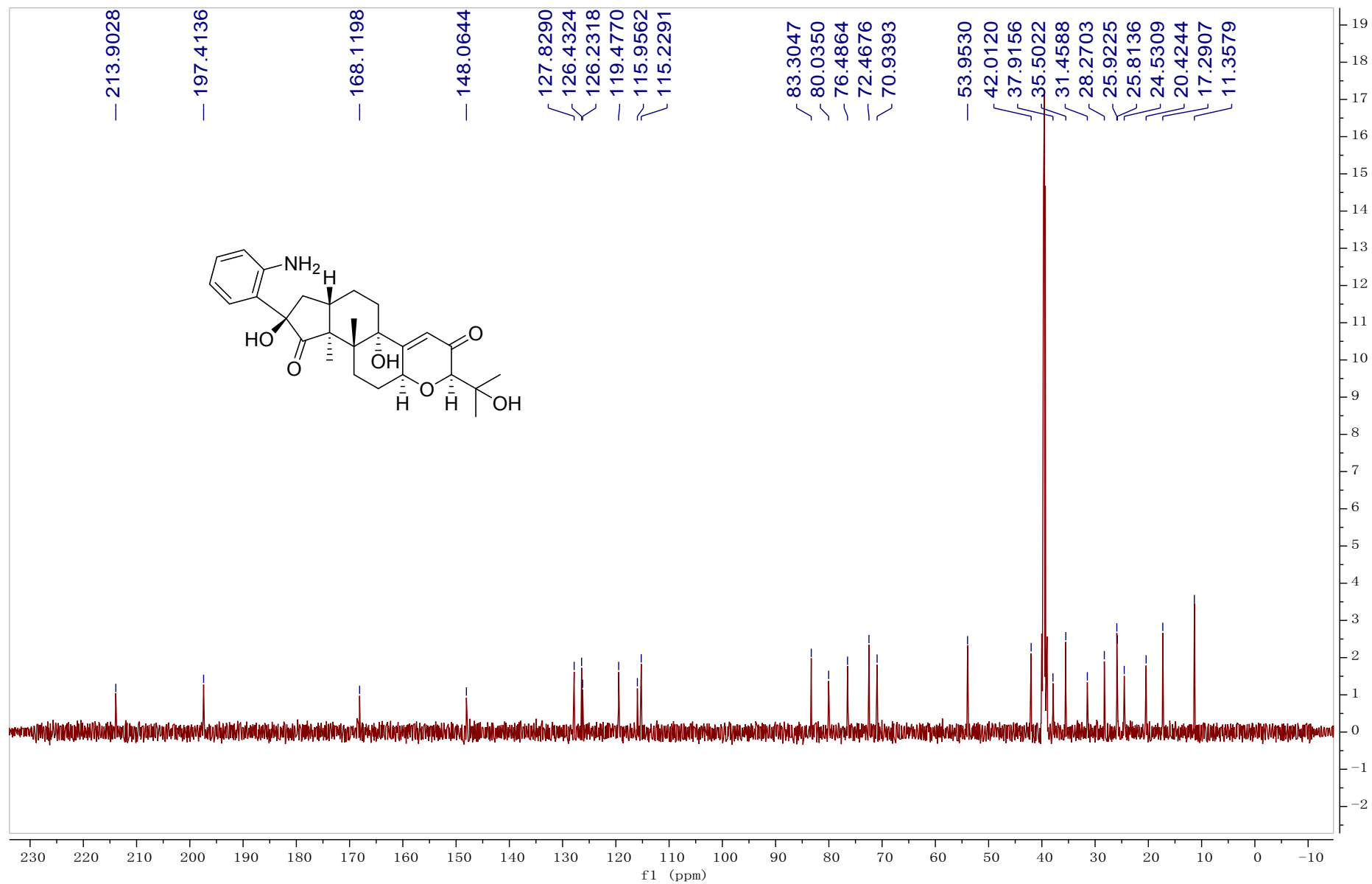


Figure S16. HSQC spectrum of deacetylsecopaxilline A (4) in DMSO- d_6

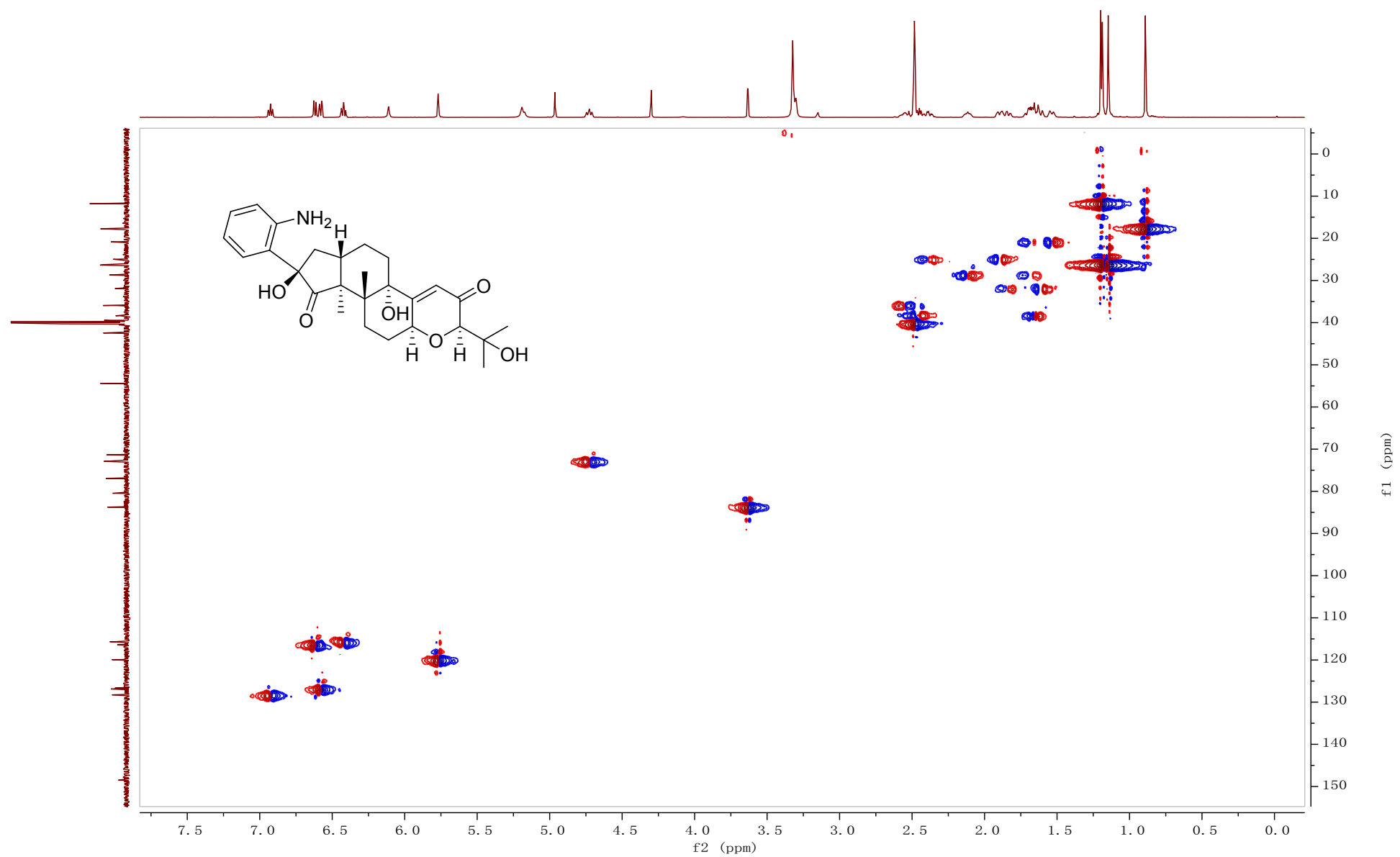


Figure S17. ^1H - ^1H COSY spectrum of deacetylsecopaxilline A (**4**) in $\text{DMSO-}d_6$

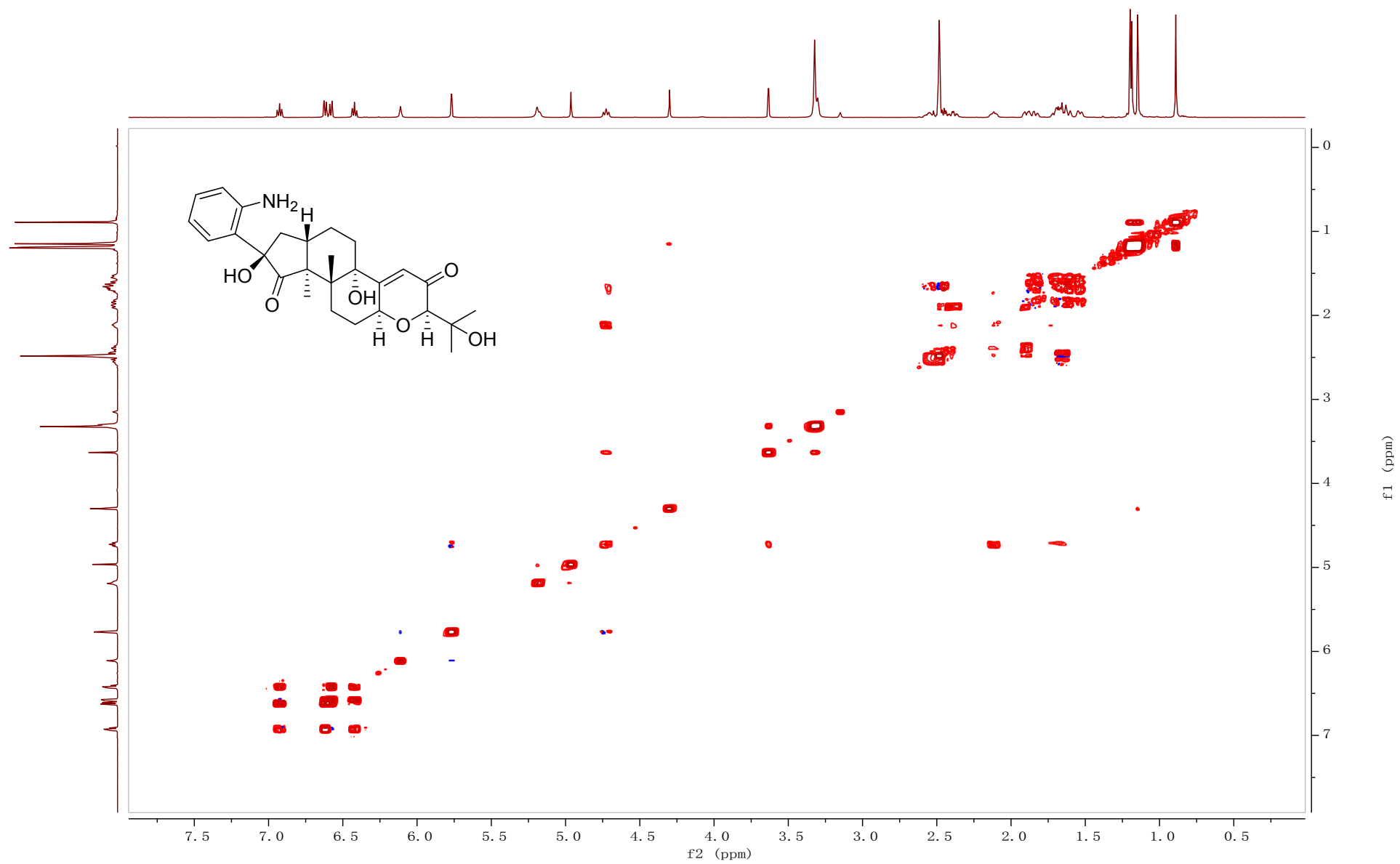


Figure S18. HMBC spectrum of deacetylsecopaxilline A (4) in DMSO- d_6

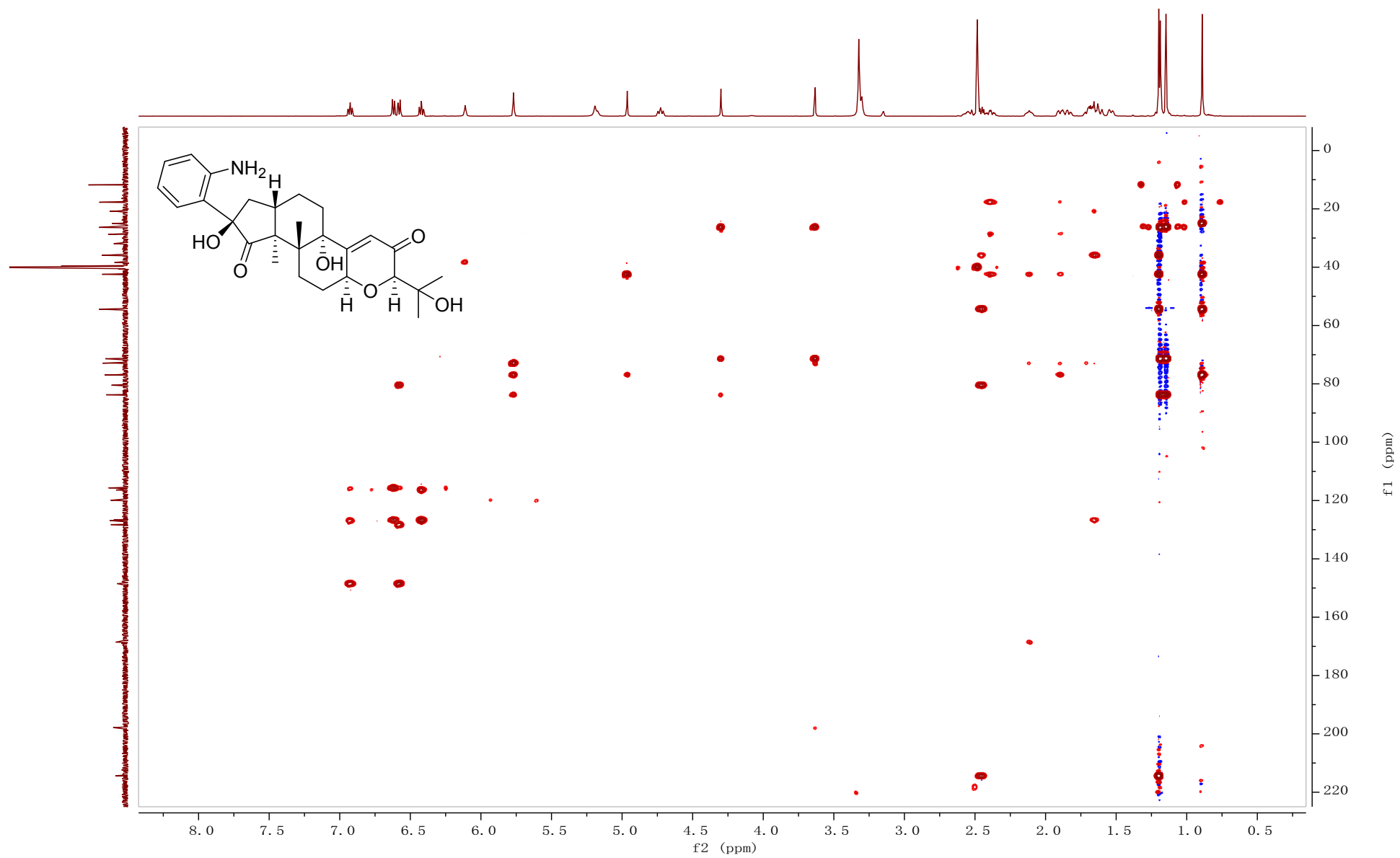


Figure S19. NOESY spectrum of deacetylsecopaxilline A (4) in DMSO- d_6

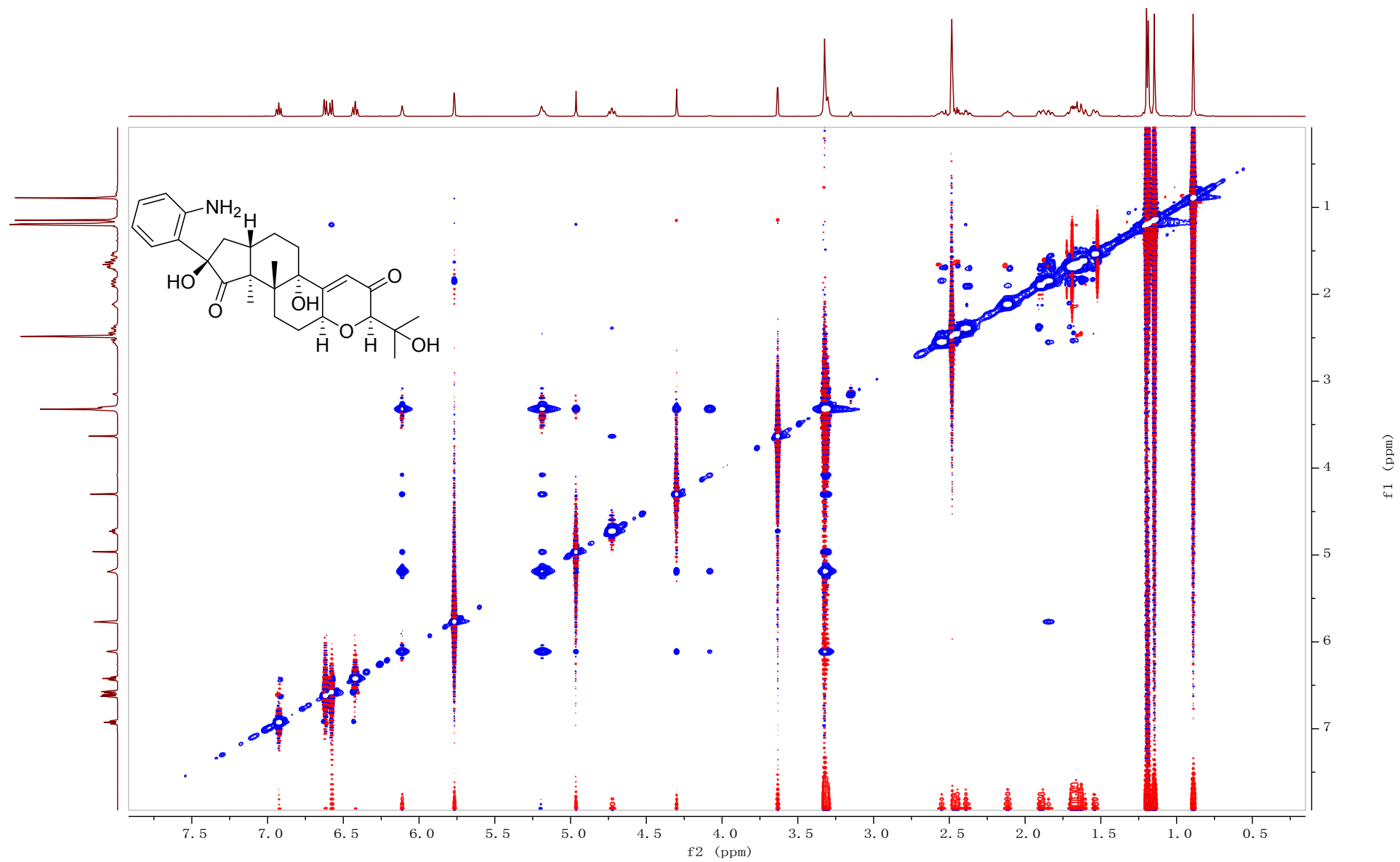


Figure S20. Comparison of the ^1H -NMR of the isolated and synthetic secopaxilline A (**1**)

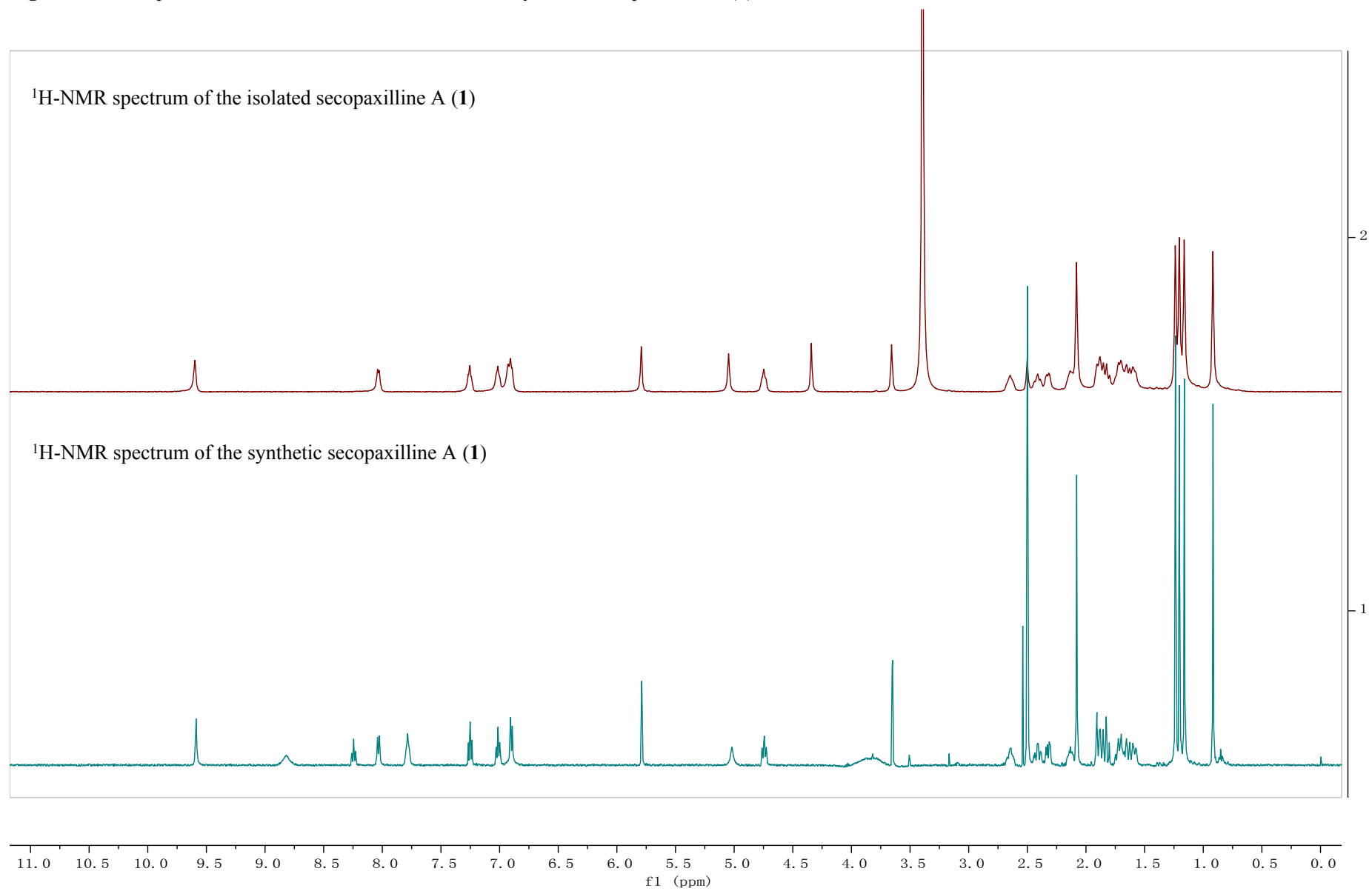


Figure S21. UV spectrum of secopaxilline A (1) and deacetylsecopaxilline A (4)

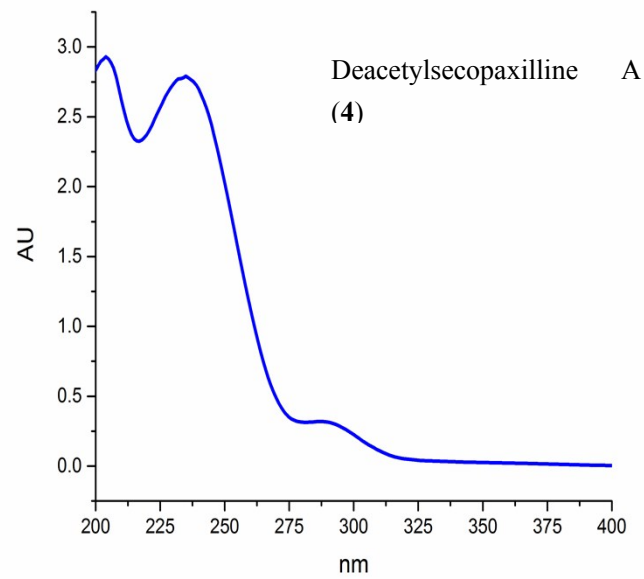
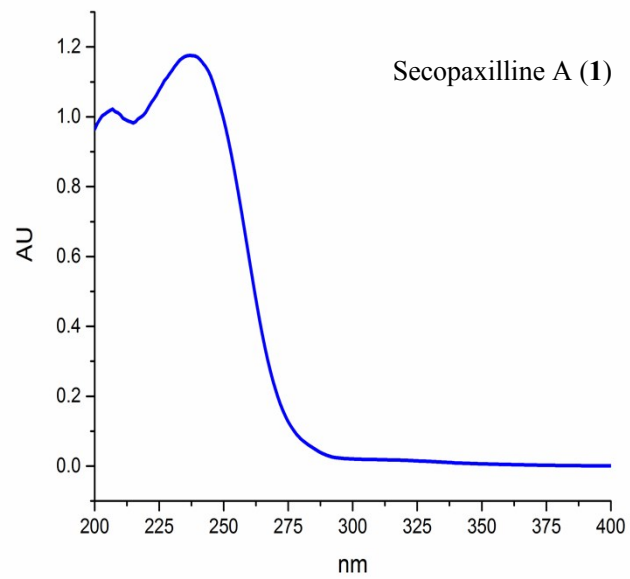


Figure S22. IR spectrum of secopaxilline A (1)

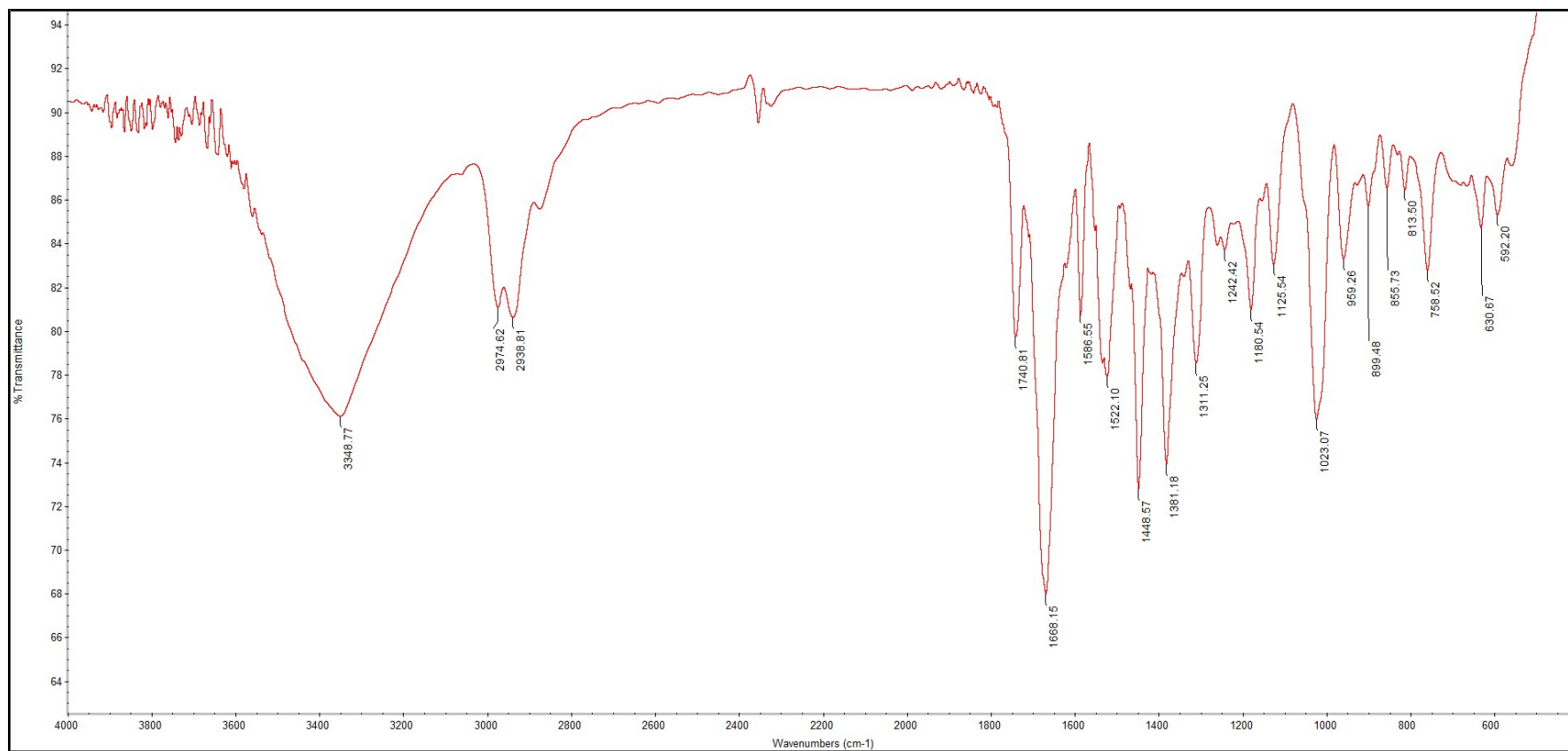


Figure S23. IR spectrum of deacetylsecopaxilline A (4)

