

**First Diamino *Daphniphyllum* Alkaloid, Daphnipaxinin, with An
Unprecedented Heterohexacyclic Skeleton from *Daphniphyllum*
*paxianum***

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Experimental Section

General Procedures: Melting point was recorded on Fisher-Johns melting point apparatus. Optical rotation was determined on a Perkin-Elmer 341 polarimeter. UV and CD spectra were measured on a JASCO J-810 instrument. IR spectra were recorded on a Perkin-Elmer 577 spectrometer. NMR spectra were measured on a Bruker AM-400 spectrometer with TMS as internal standard. EIMS (70 eV) and ESI MS were carried out on a Finnigan MAT 95 mass spectrometer, and a Finnigan LCQ^{DECA} and a Q-TOF Ultima (for HRESIMS) instruments, respectively. All solvents used were of analytical grade (Shanghai Chemical Plant). Silica gel (200-300 mesh) was used for column chromatography, and pre-coated silica gel GF₂₅₄ plates (Qingdao Haiyang Chemical Plant) were used for TLC. Sephadex LH-20 (Pharmacia Biotech, Sweden) was also used for column chromatography.

Plant Material: *Daphniphyllum paxianum* Rosenth was collected from Island Hainan of P. R. China and authenticated by Prof. Su-Hua Shi of Institute of Botany, School of Life science, Zhongshan University of P. R. China. A voucher specimen has been deposited in the Herbarium of Institute of *Materia Medica*, Shanghai Institute for Biological Sciences, Chinese Academy of Sciences (accession number: DS-2003-4Y-HN).

Figure S3. ^1H NMR spectrum of daphnipaxinin (1) in CD_3OD

Hz

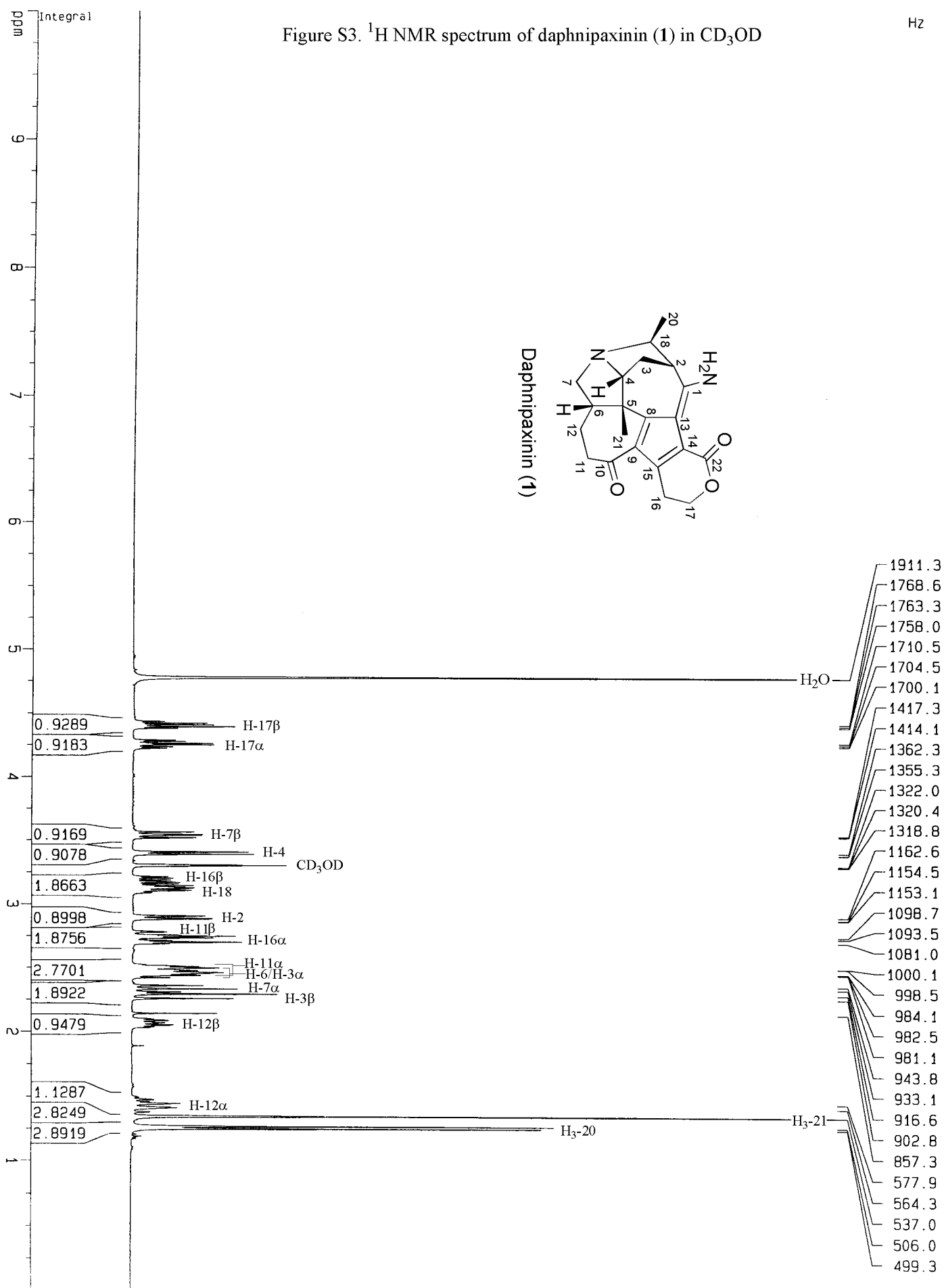


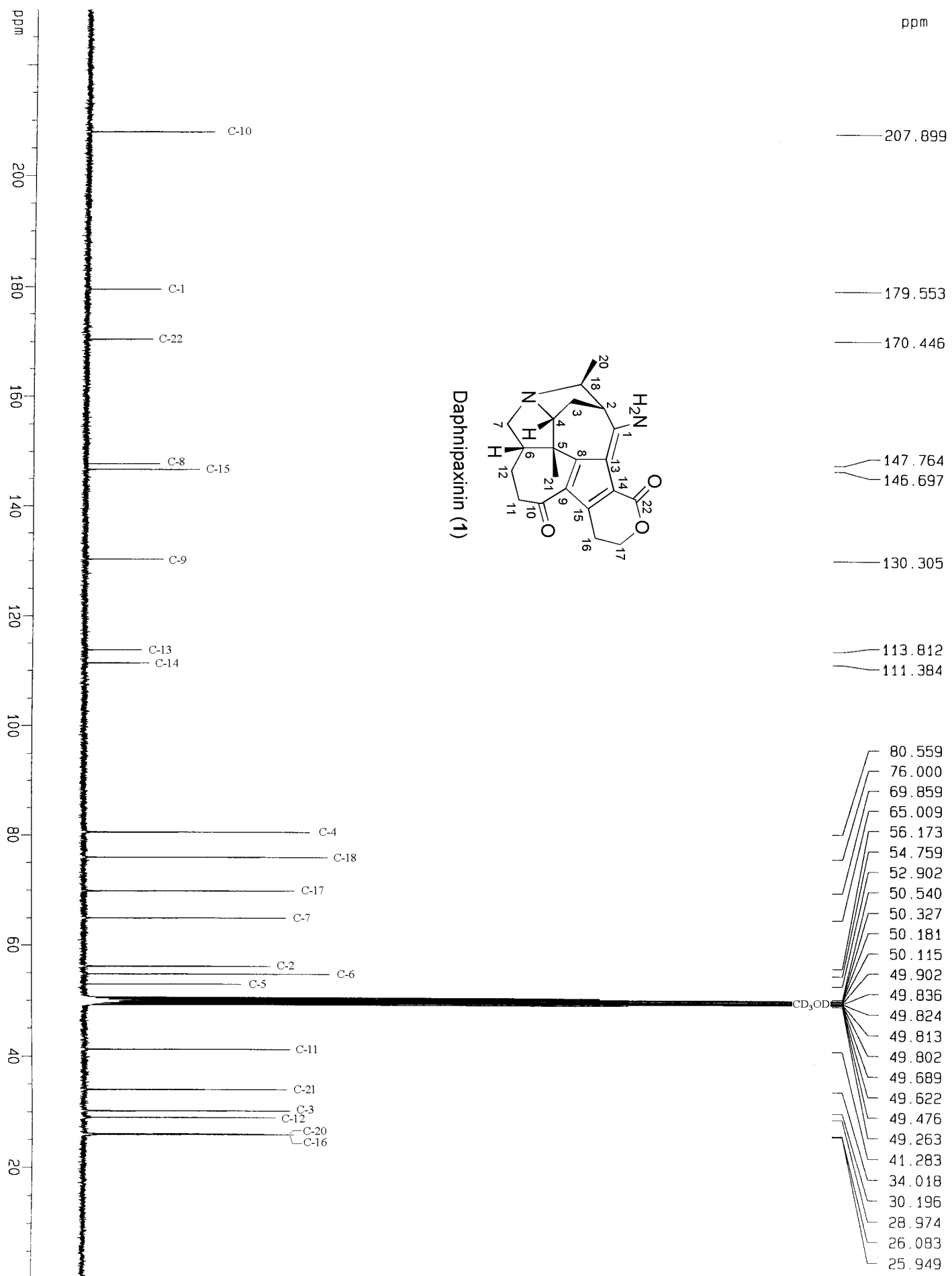
Figure S4. ^{13}C NMR spectrum of daphnipaxinin (1) in CD_3OD 

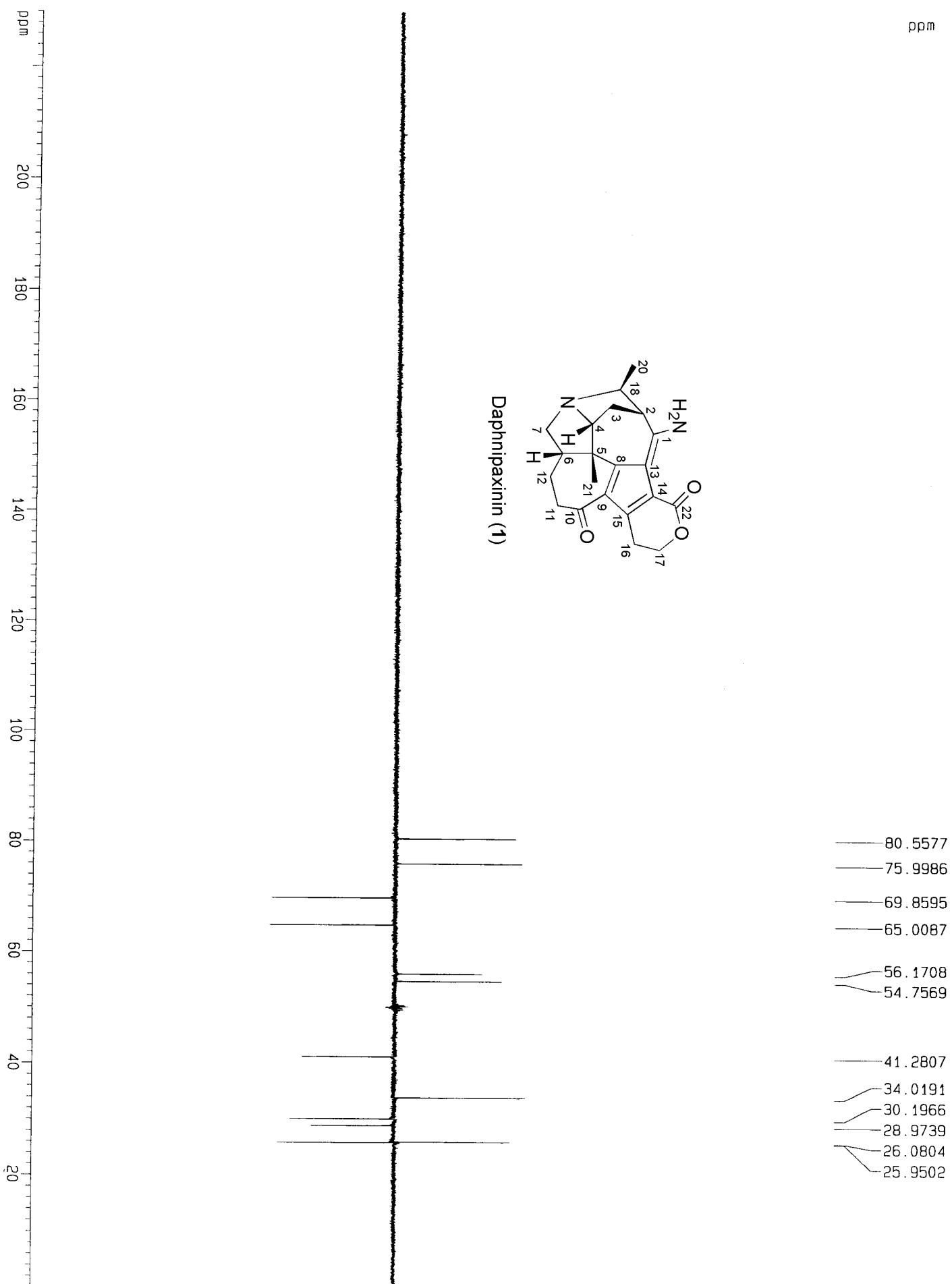
Figure S5. DEPT spectrum of daphnipaxinin (1) in CD₃OD

Figure S6. EIMS spectrum of daphnipaxinin (1)

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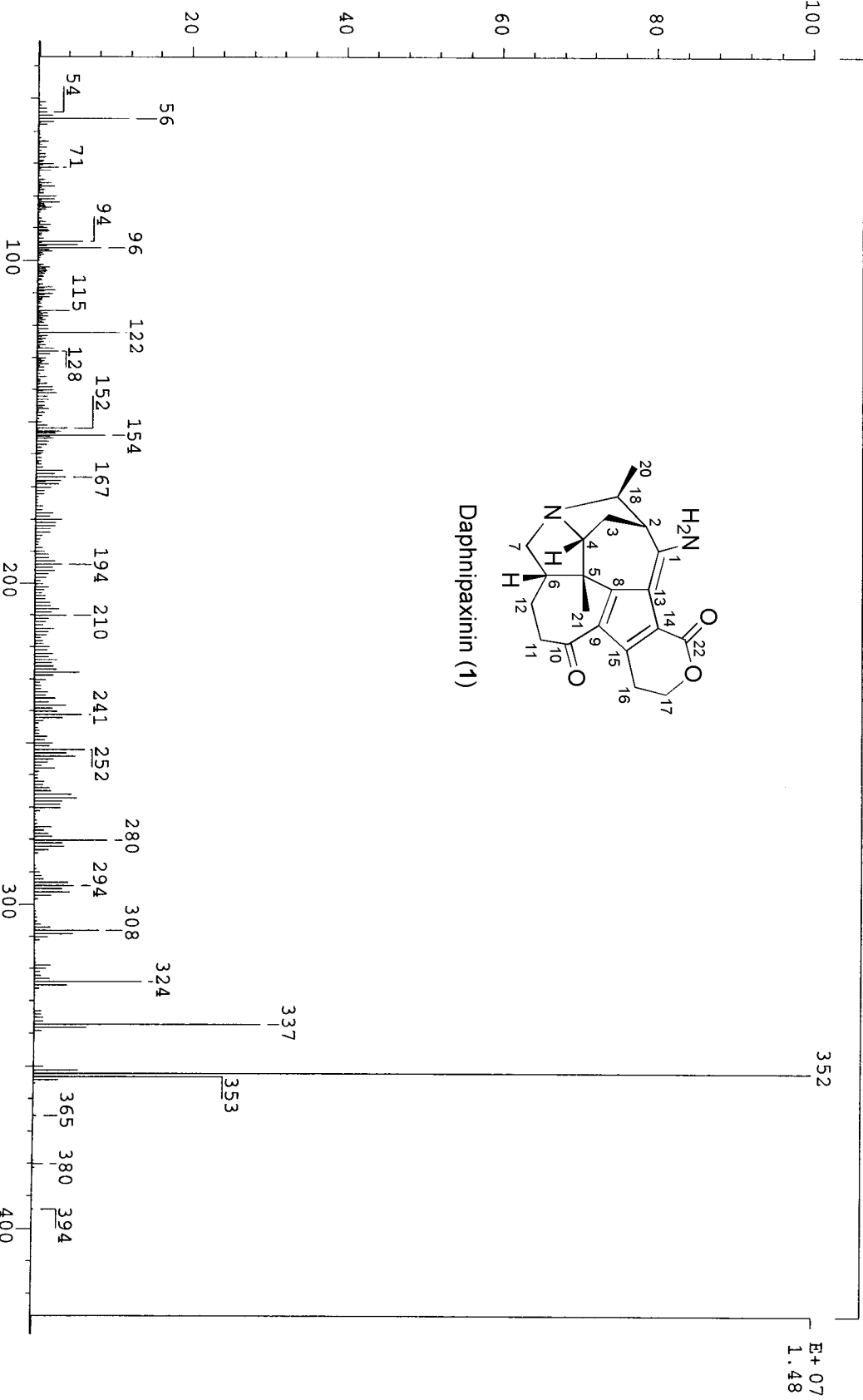
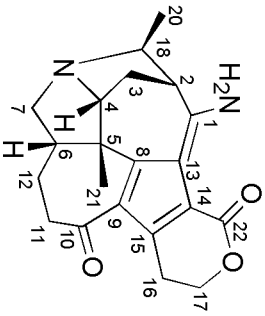
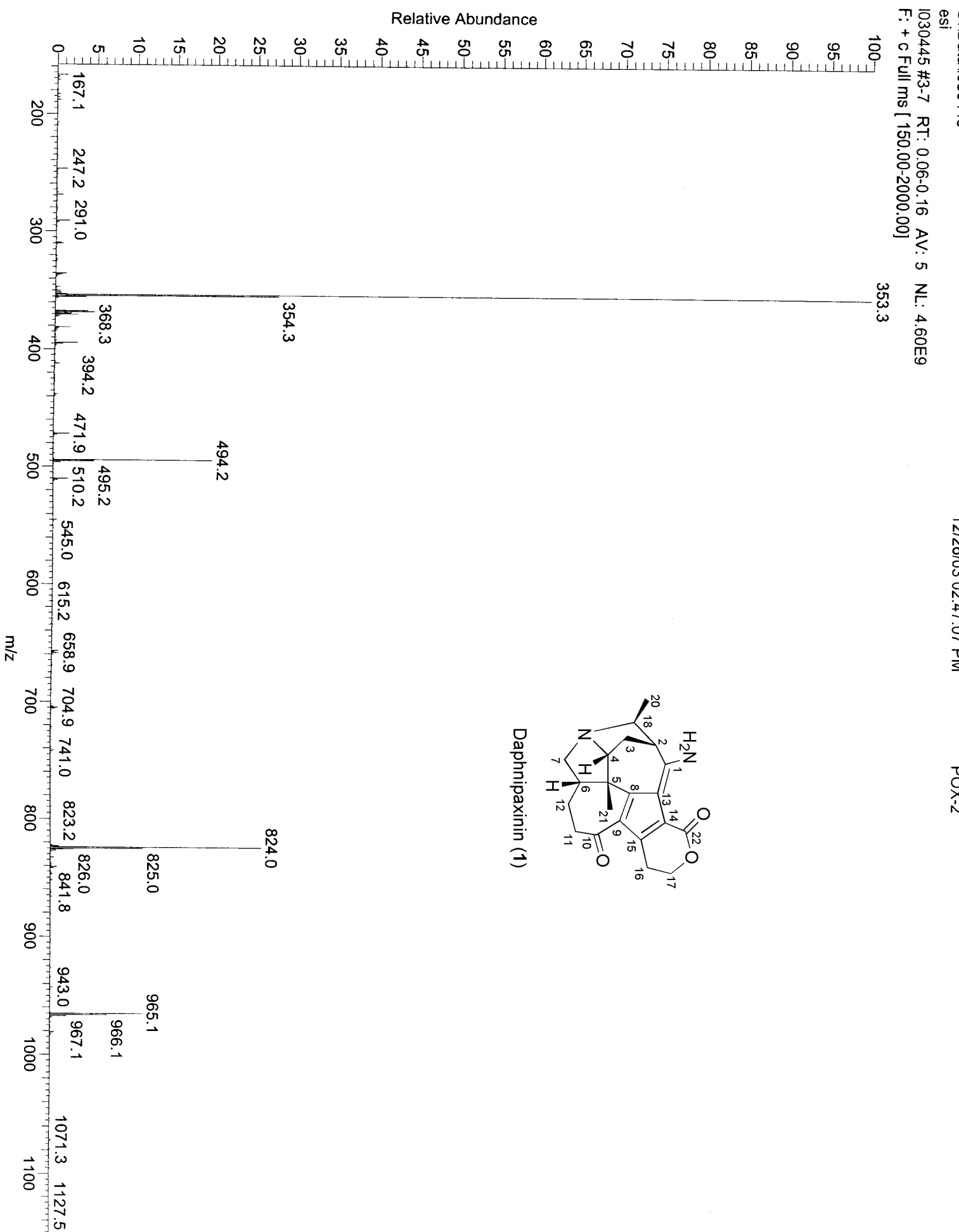


Figure S7. ESI-MS (positive) spectrum of daphnipaxinin (1)

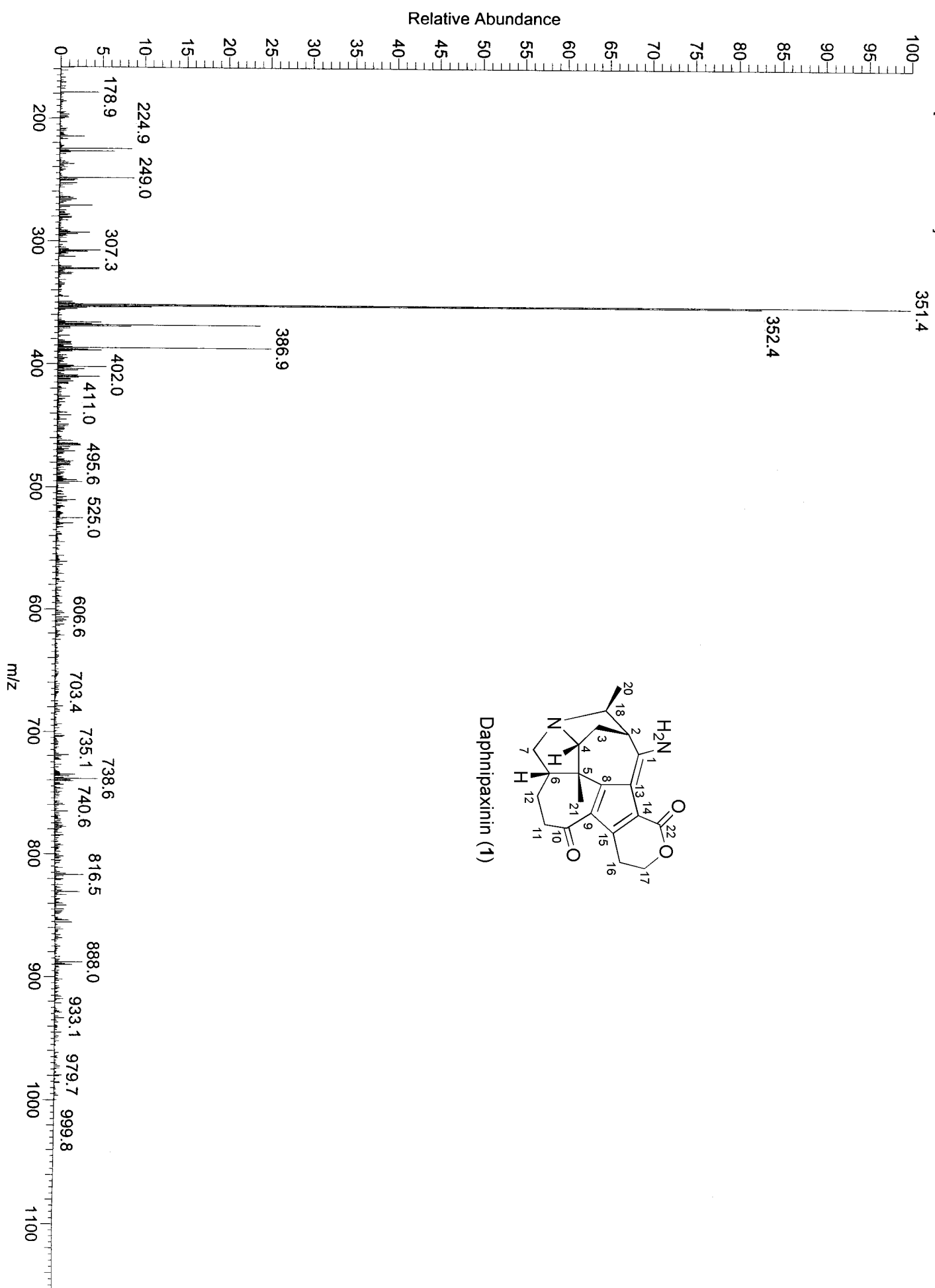


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POX-2

Figure S8. ESI-MS (negative) spectrum of daphnipaxinin (1)



Daphnipaxinin (1)

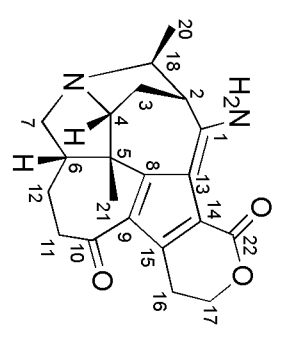


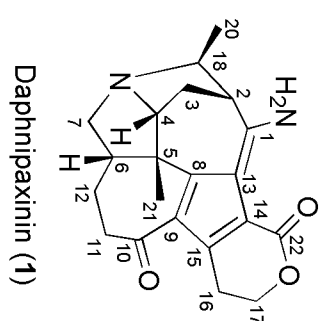
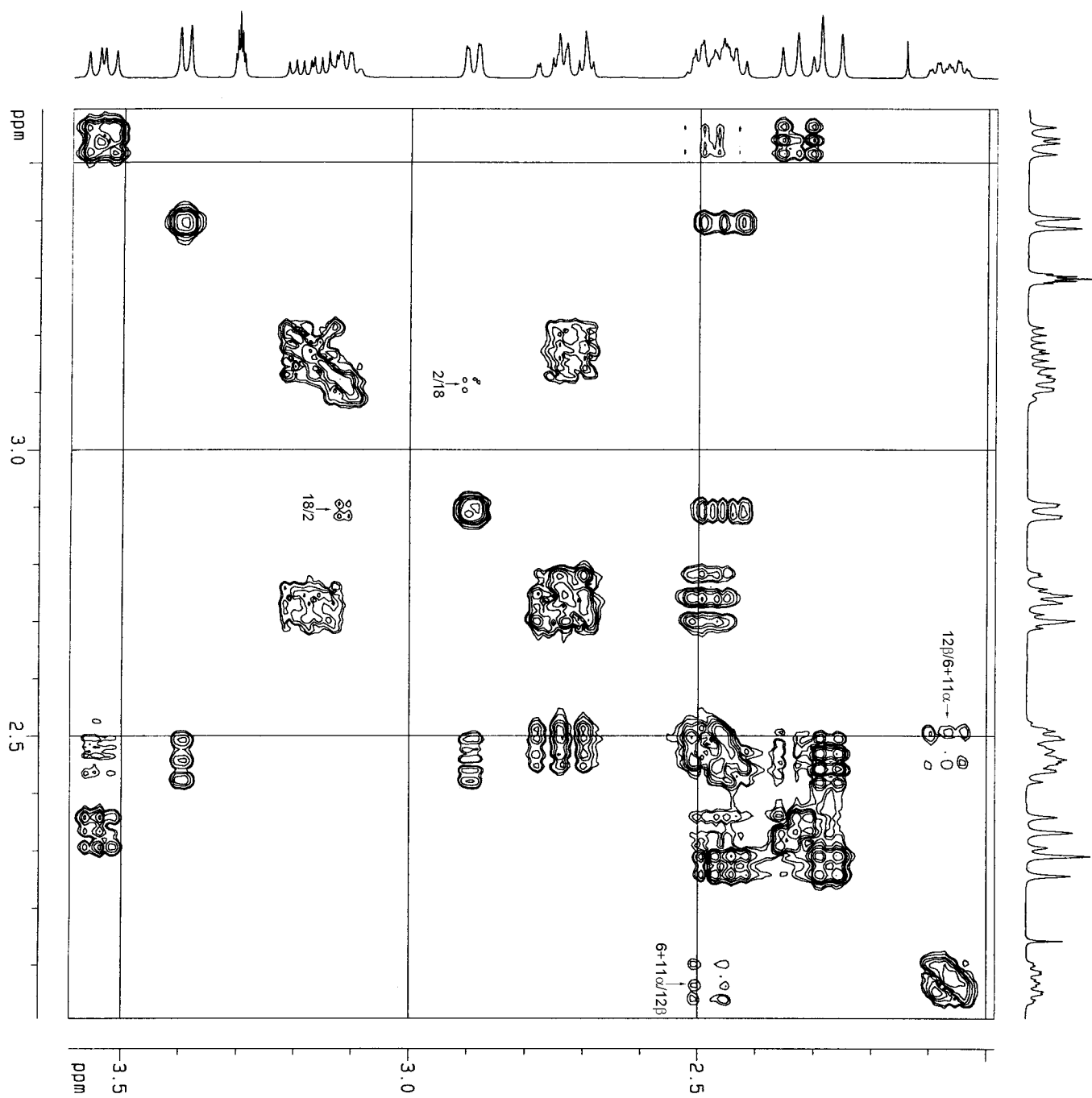
Figure S10. Expanded ^1H - ^1H COSY spectrum of daphnipaxinin (1) in CD_3OD (δ 2.0-3.6).

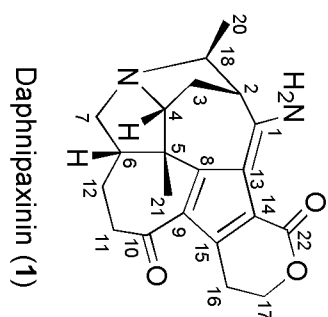
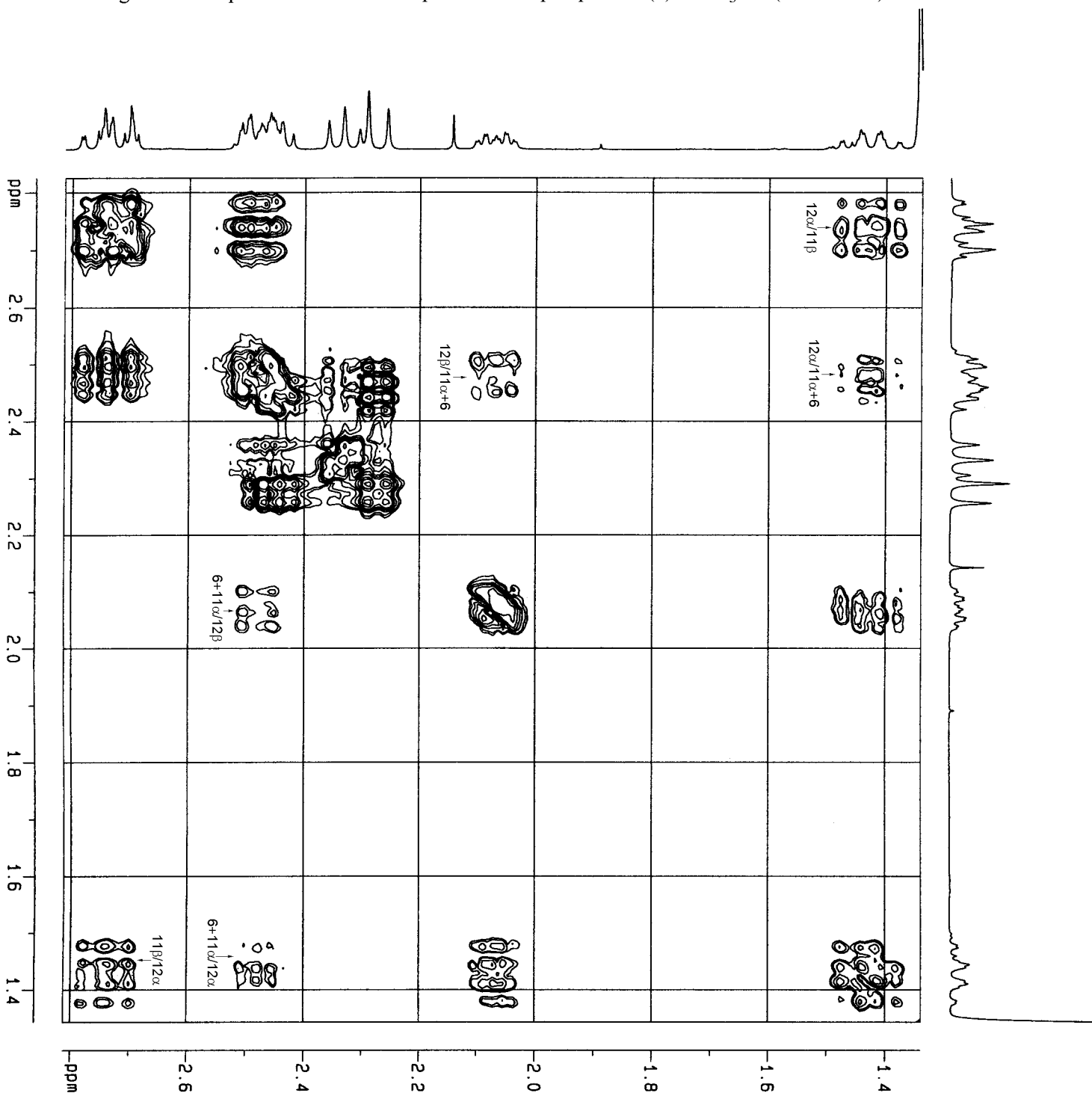
Figure S11. Expanded ^1H - ^1H COSY spectrum of daphnipaxinin (1) in CD_3OD (δ 1.35-2.73).

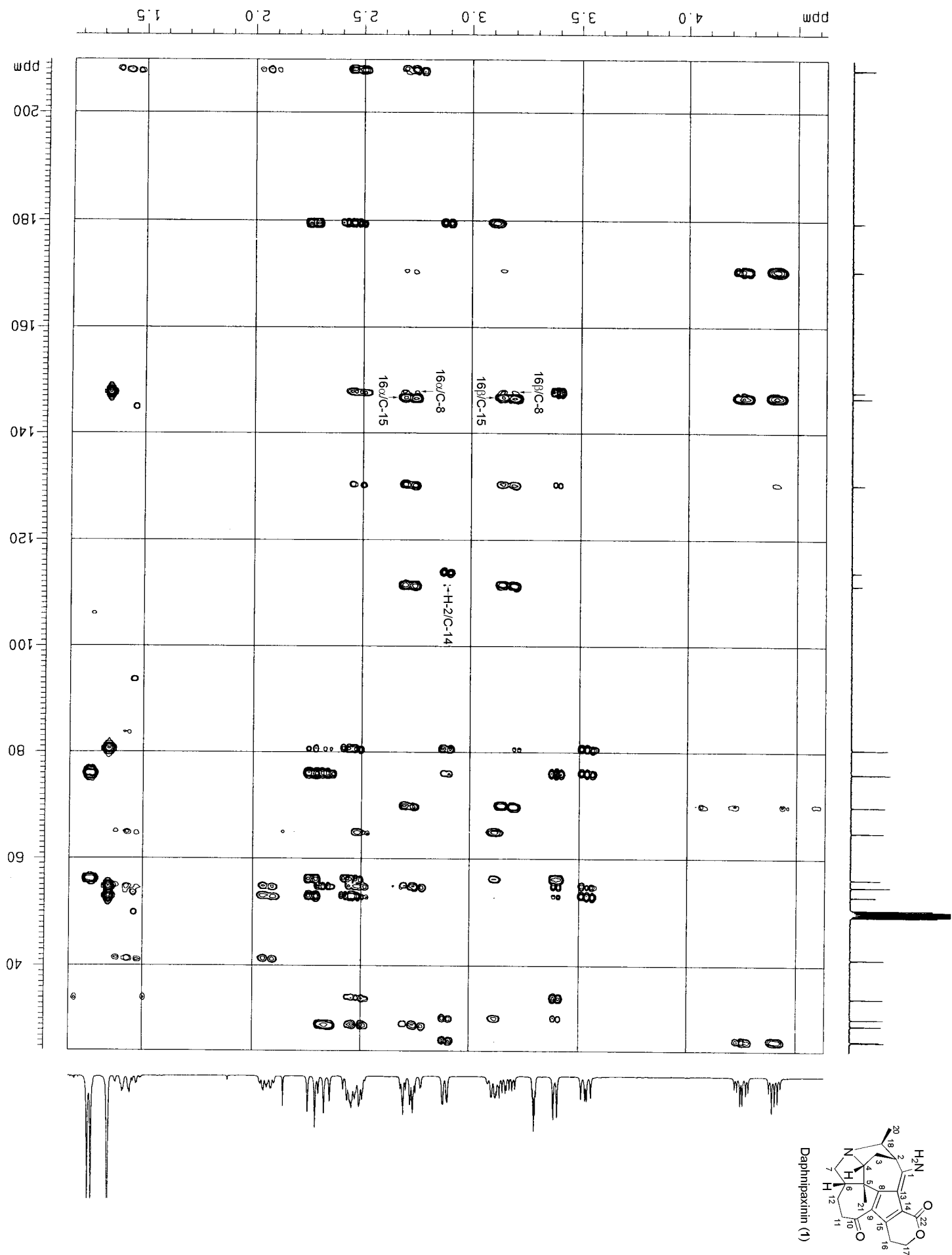
Figure S13. HMBC spectrum of daphnipaxinin (1) in CD₃OD

Figure S14. Expanded HMBC spectrum of daphnipaxinin (1) in CD₃OD.
(δ_{H} 1.2-2.95 vs δ_{C} 109.5-210)

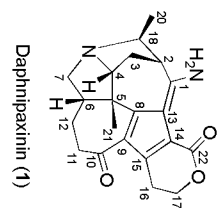
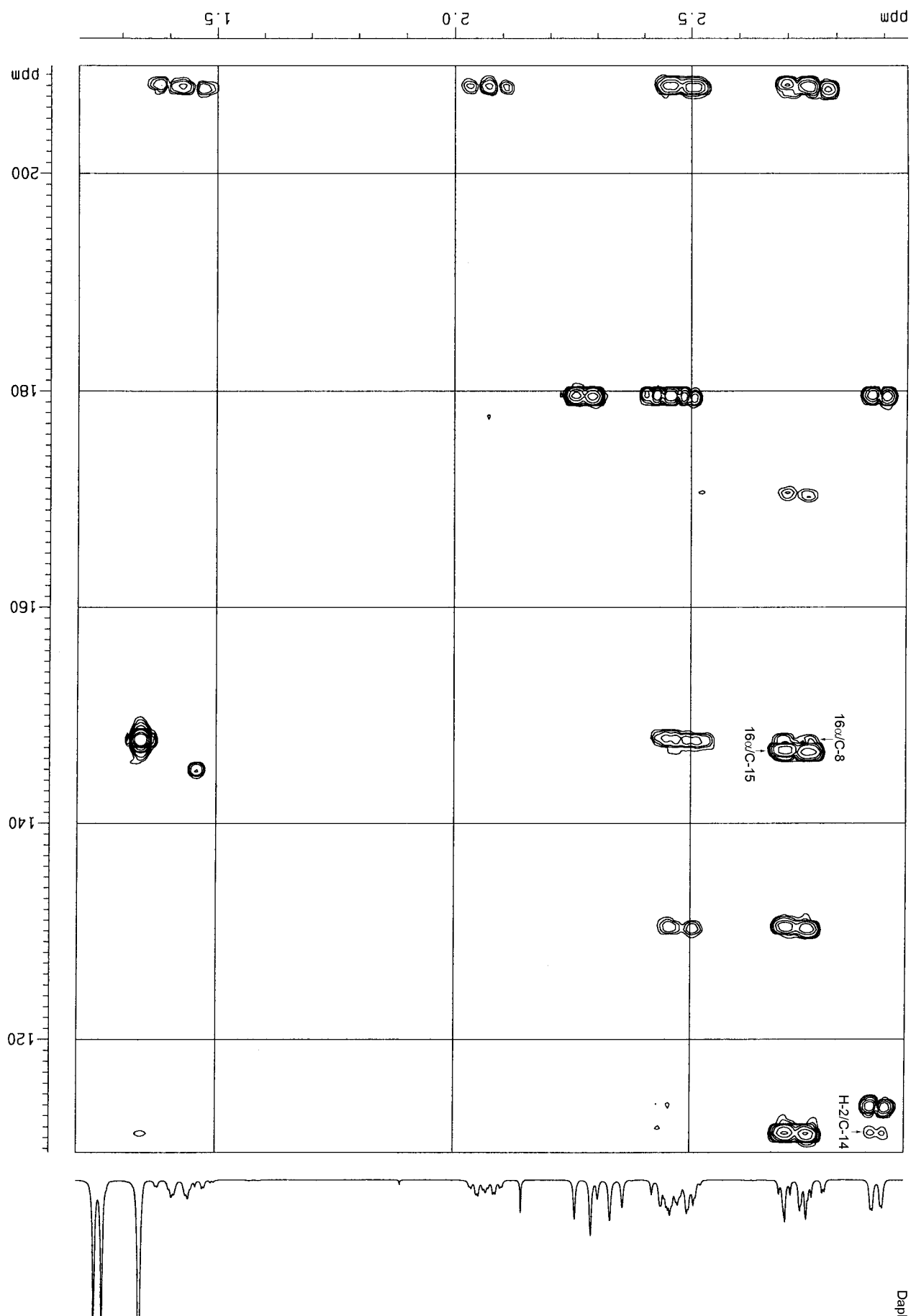


Figure S15. Expanded HMBC spectrum of daphnipaxinin (1) in CD₃OD.
(δ_{H} 3.05-4.46 vs δ_{C} 109.5-210)

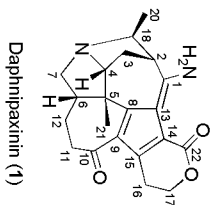
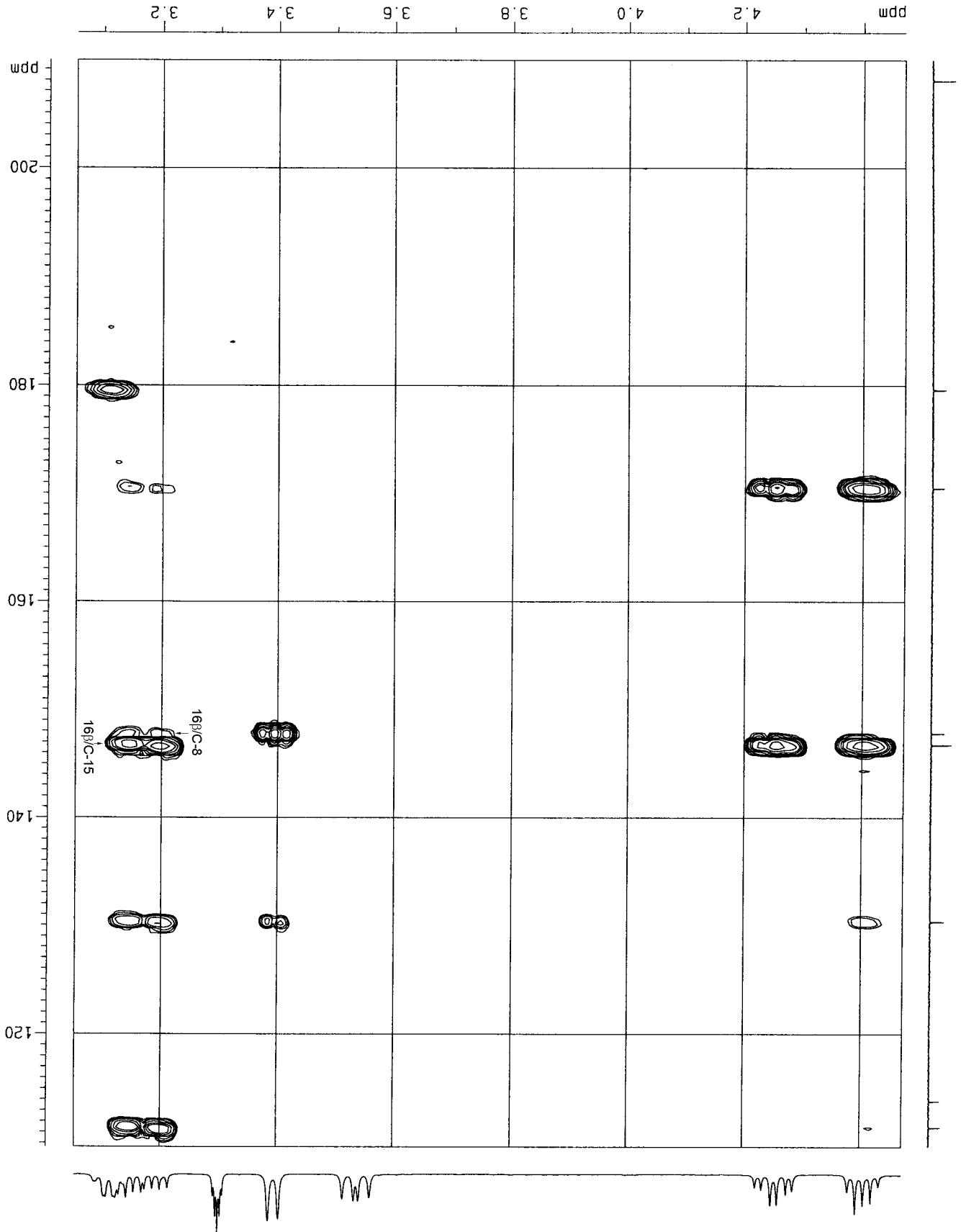


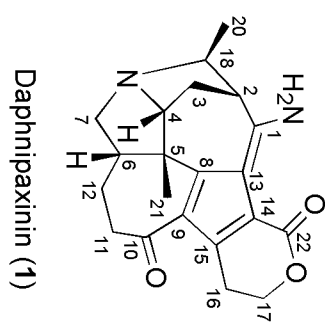
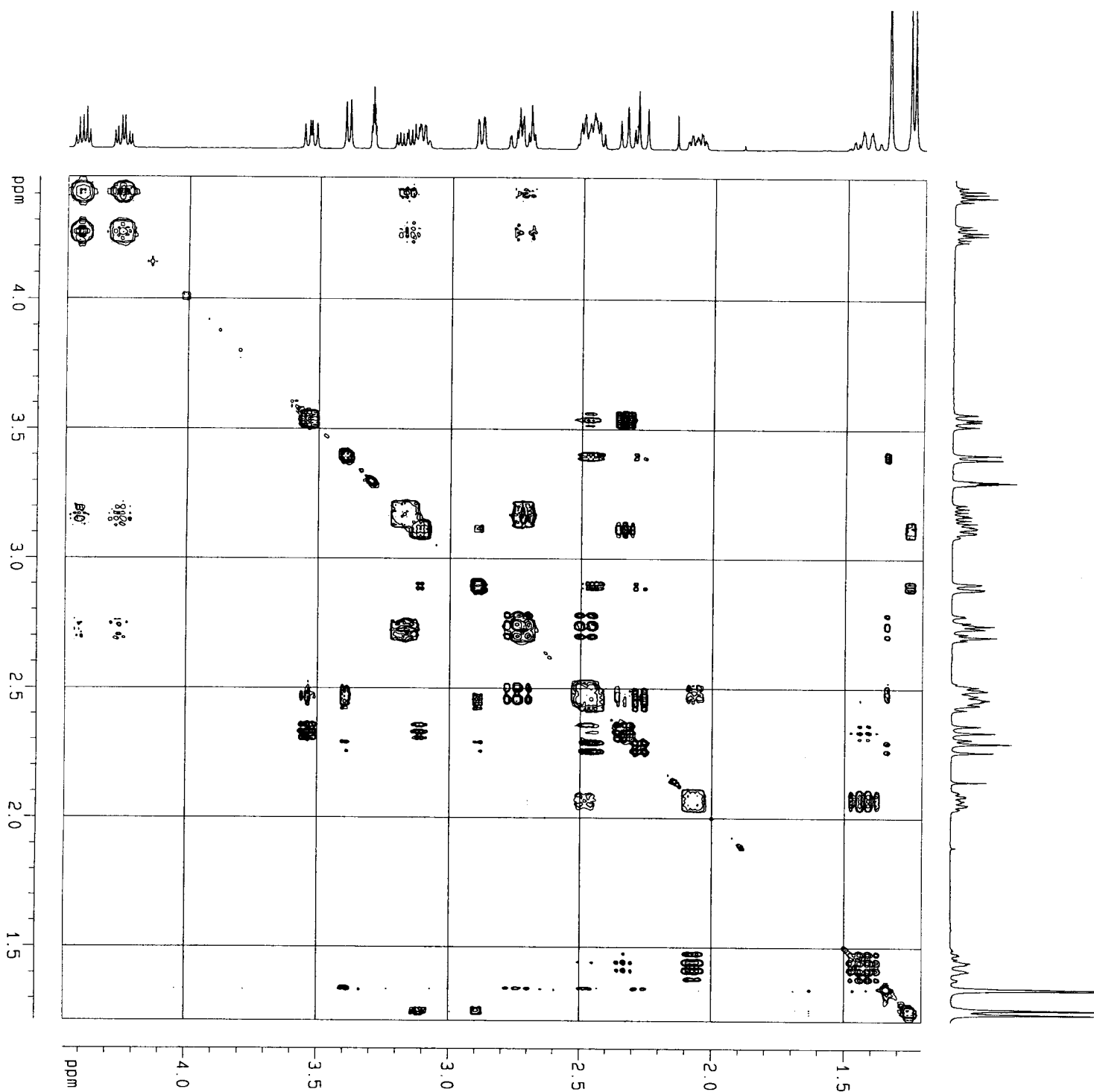
Figure S16. NOESY spectrum of daphnipaxinin (1) in CD₃OD

Figure S17. IR (KBr) spectrum of daphnipaxinin (1)

