

Supporting Information

6-Bromoindole Derivatives from the Icelandic Marine Sponge *Geodia barretti*: Isolation and Anti-Inflammatory Activity

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

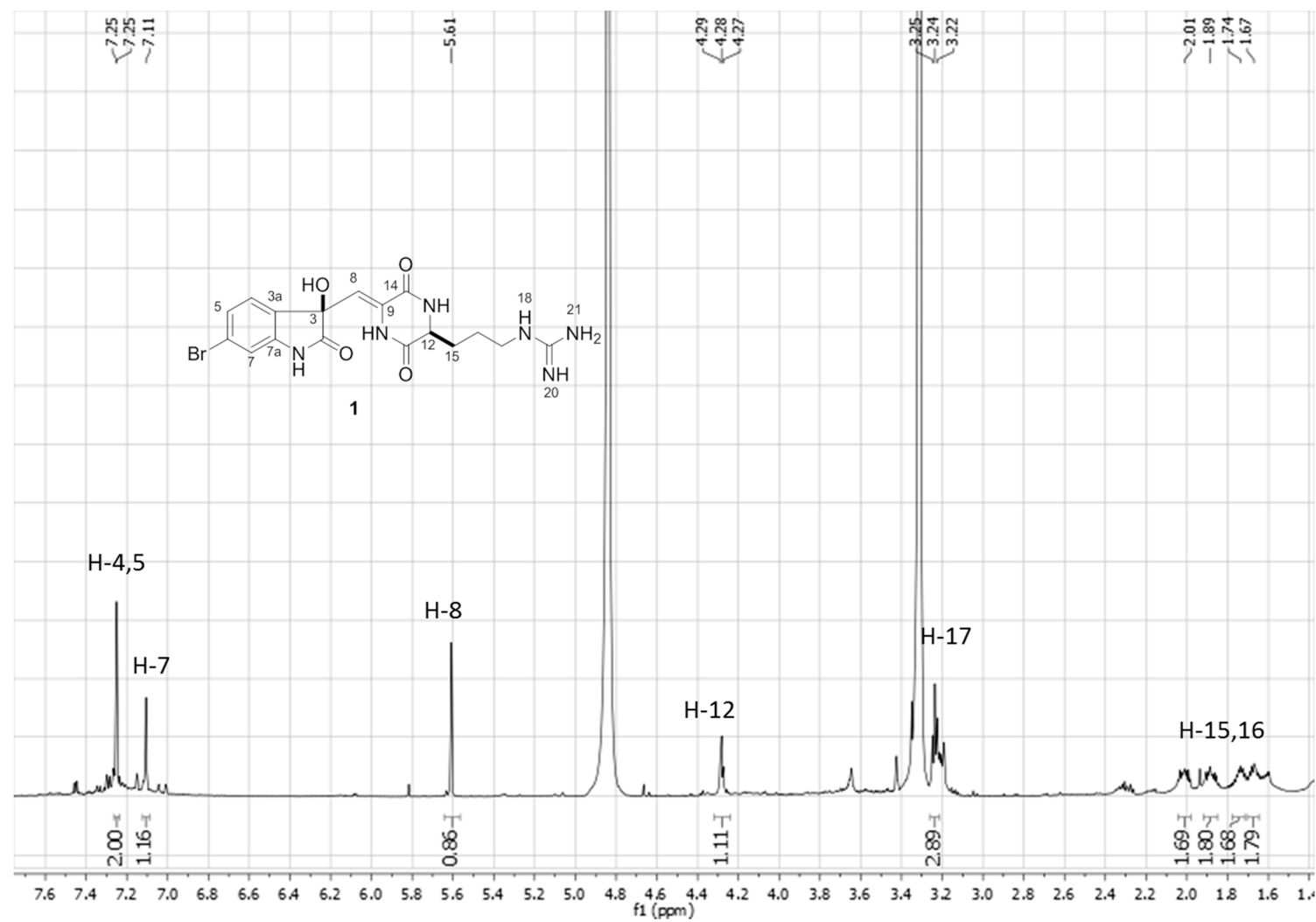


Figure S2. ^{13}C NMR spectrum of geobarrettin A (1) (150 MHz, CD_3OD)

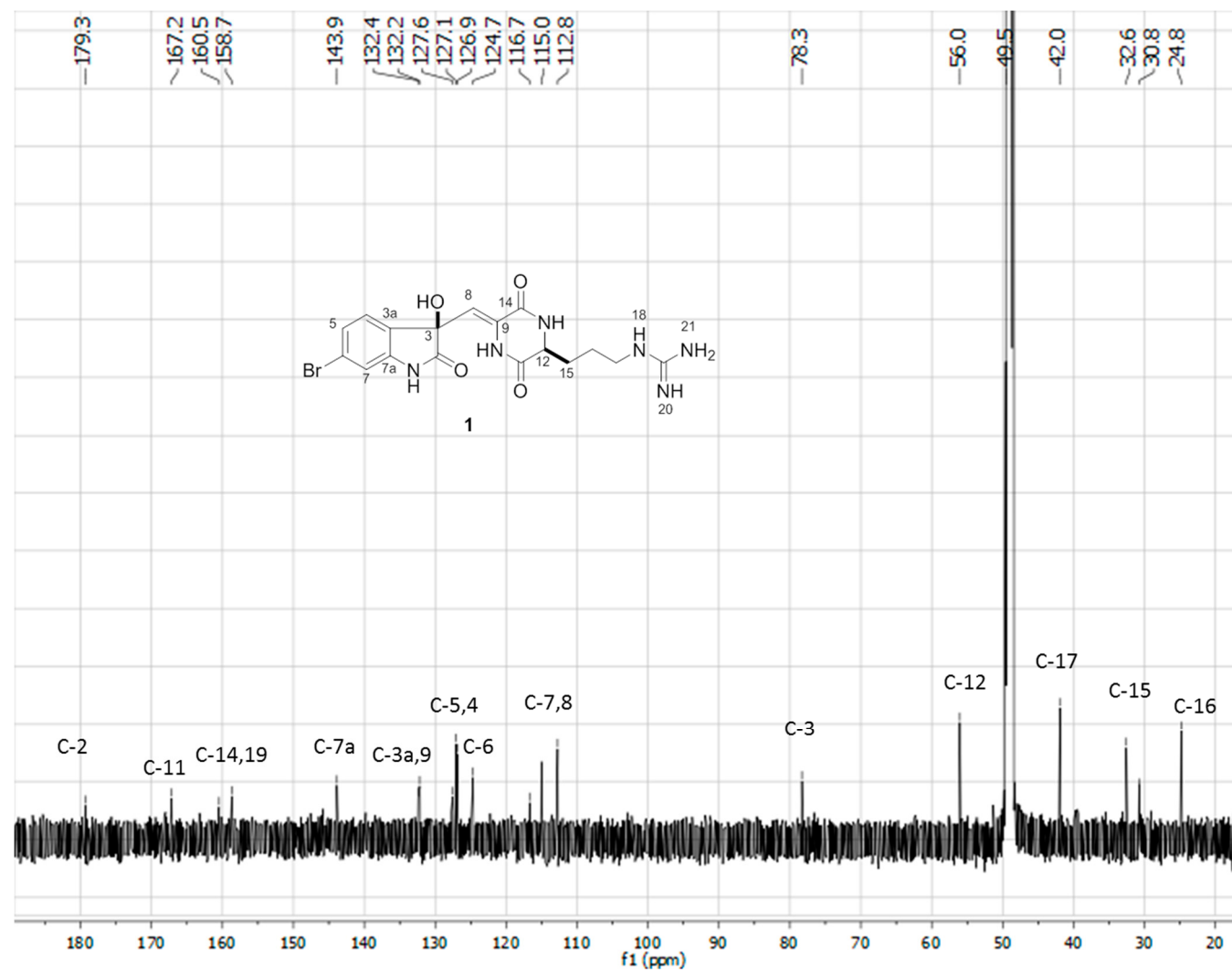


Figure S3. HSQC spectrum of geobarrettin A (**1**) (600 MHz, CD₃OD)

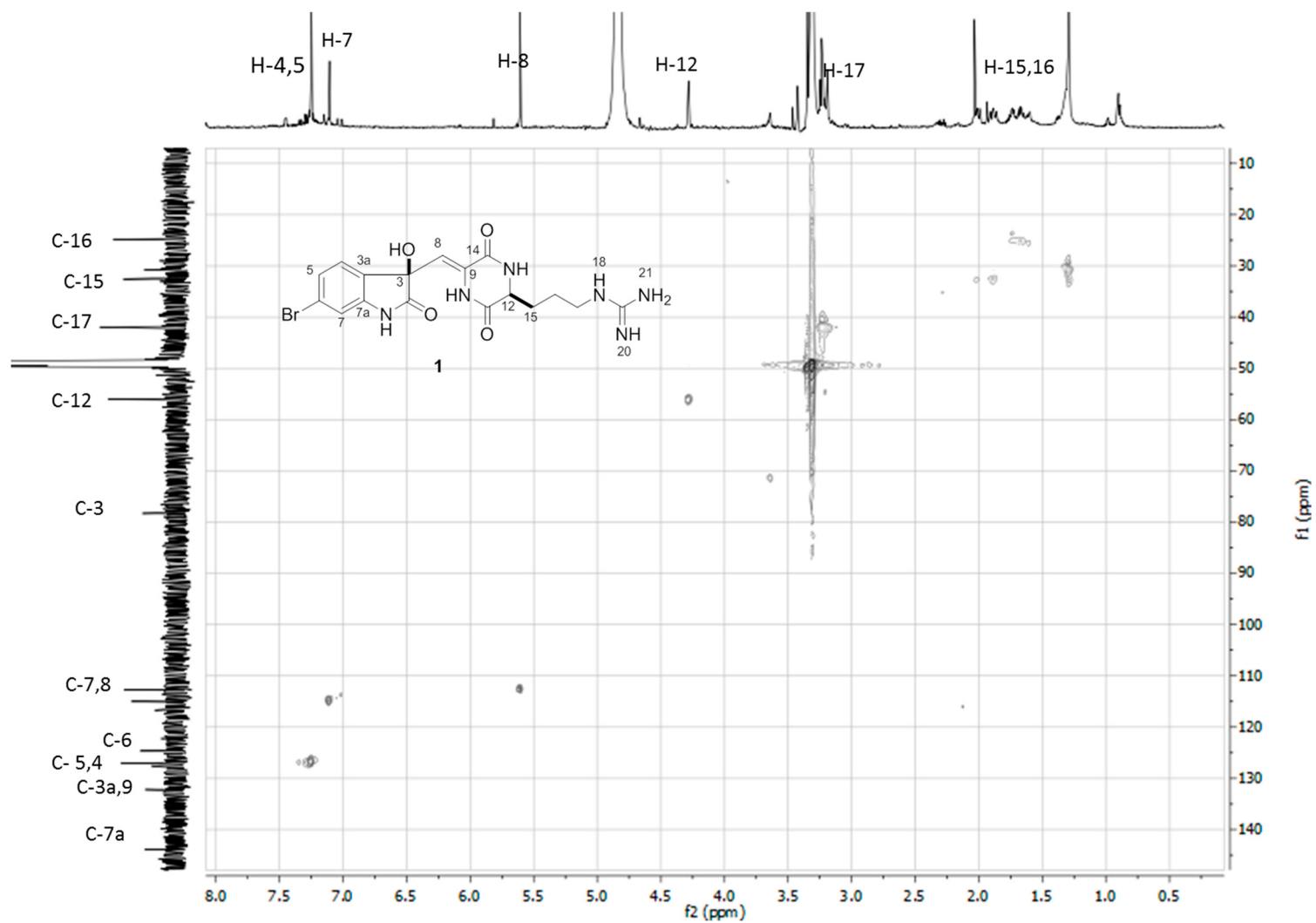


Figure S4. HMBC spectrum of geobarrettin A (**1**) (600 MHz, CD₃OD)

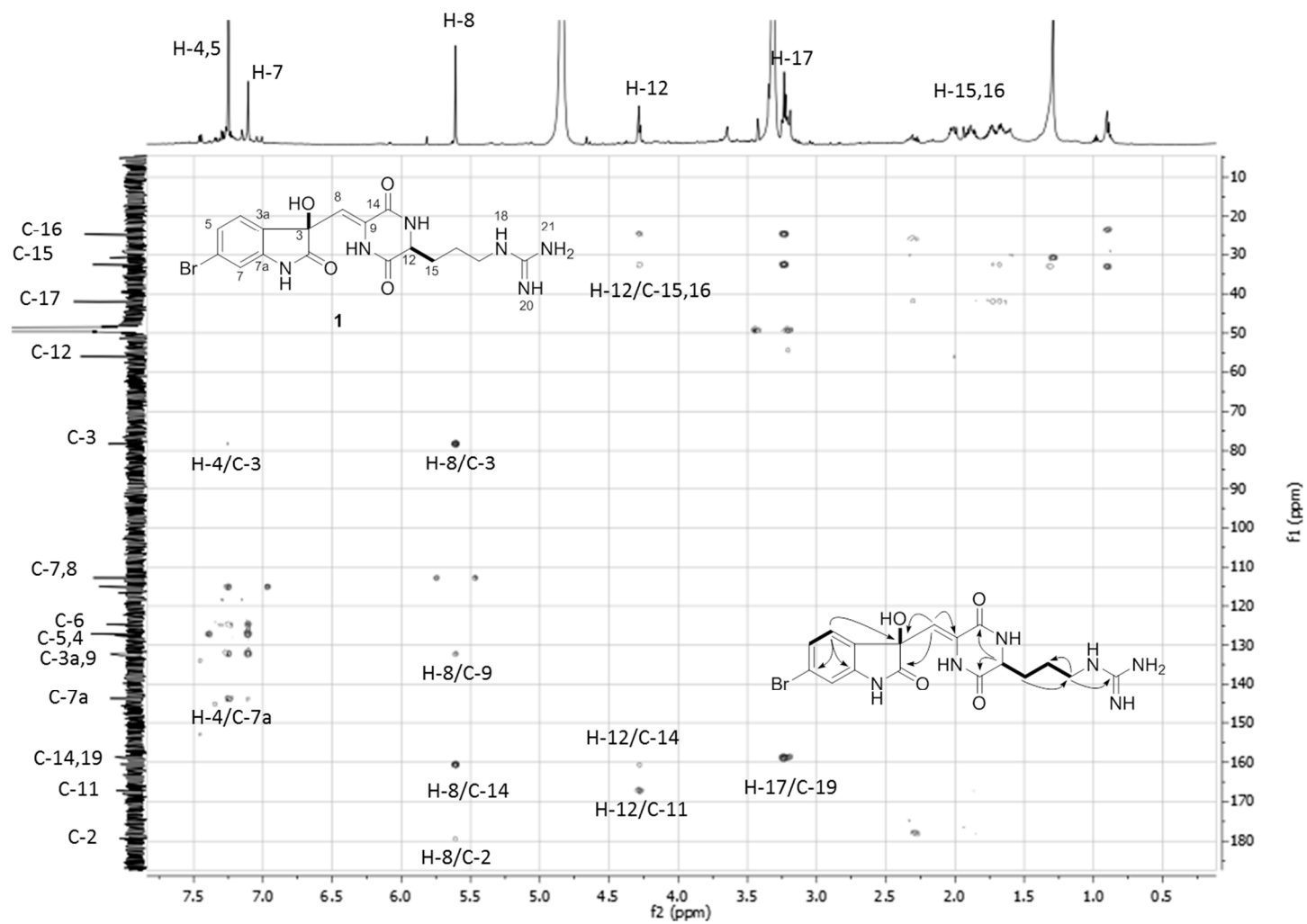


Figure S5. ^1H - ^1H COSY spectrum of geobarrettin A (**1**) (600 MHz, CD_3OD)

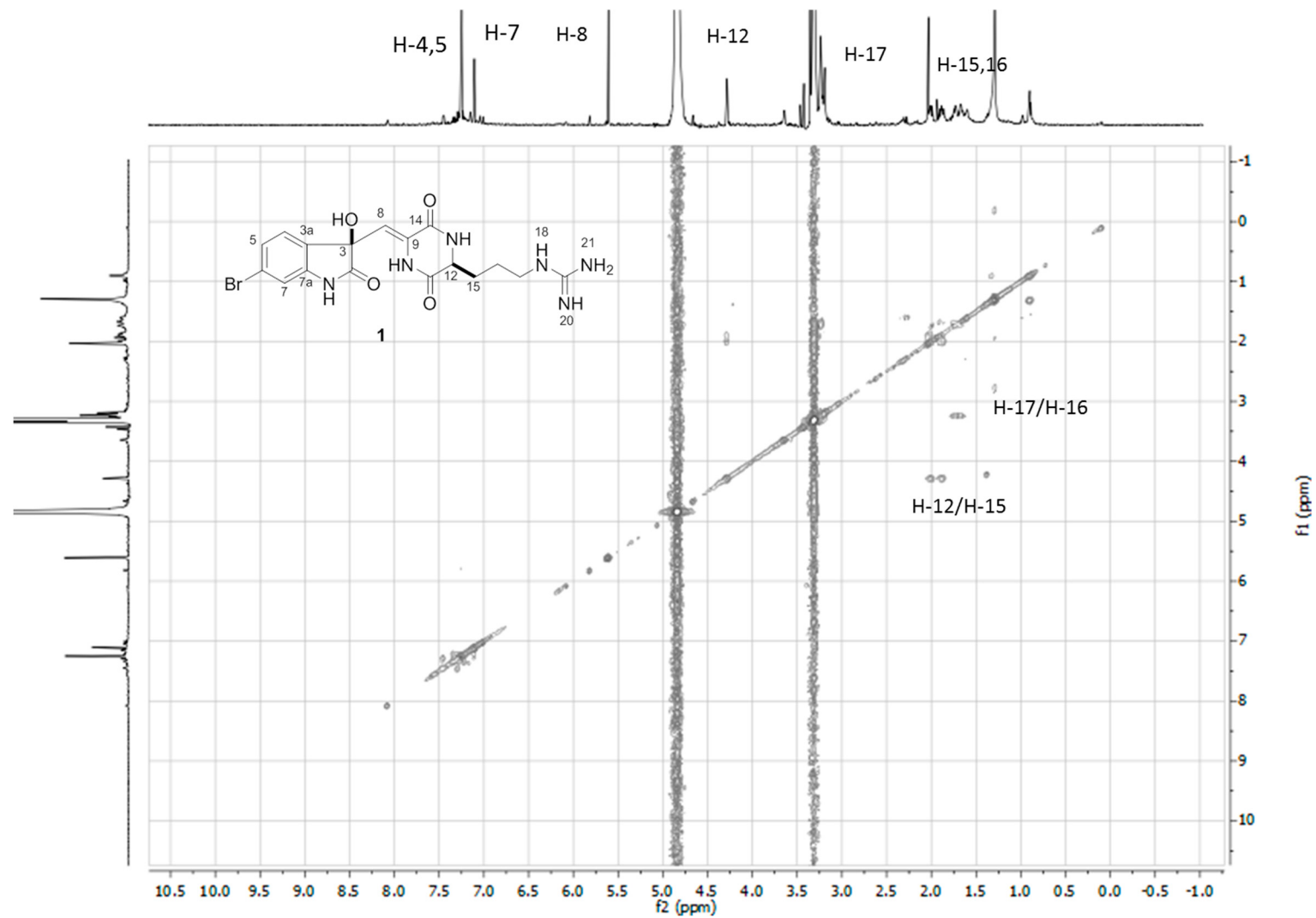


Figure S6. NOESY spectrum of geobarrettin A (**1**) (600 MHz, CD₃OD)

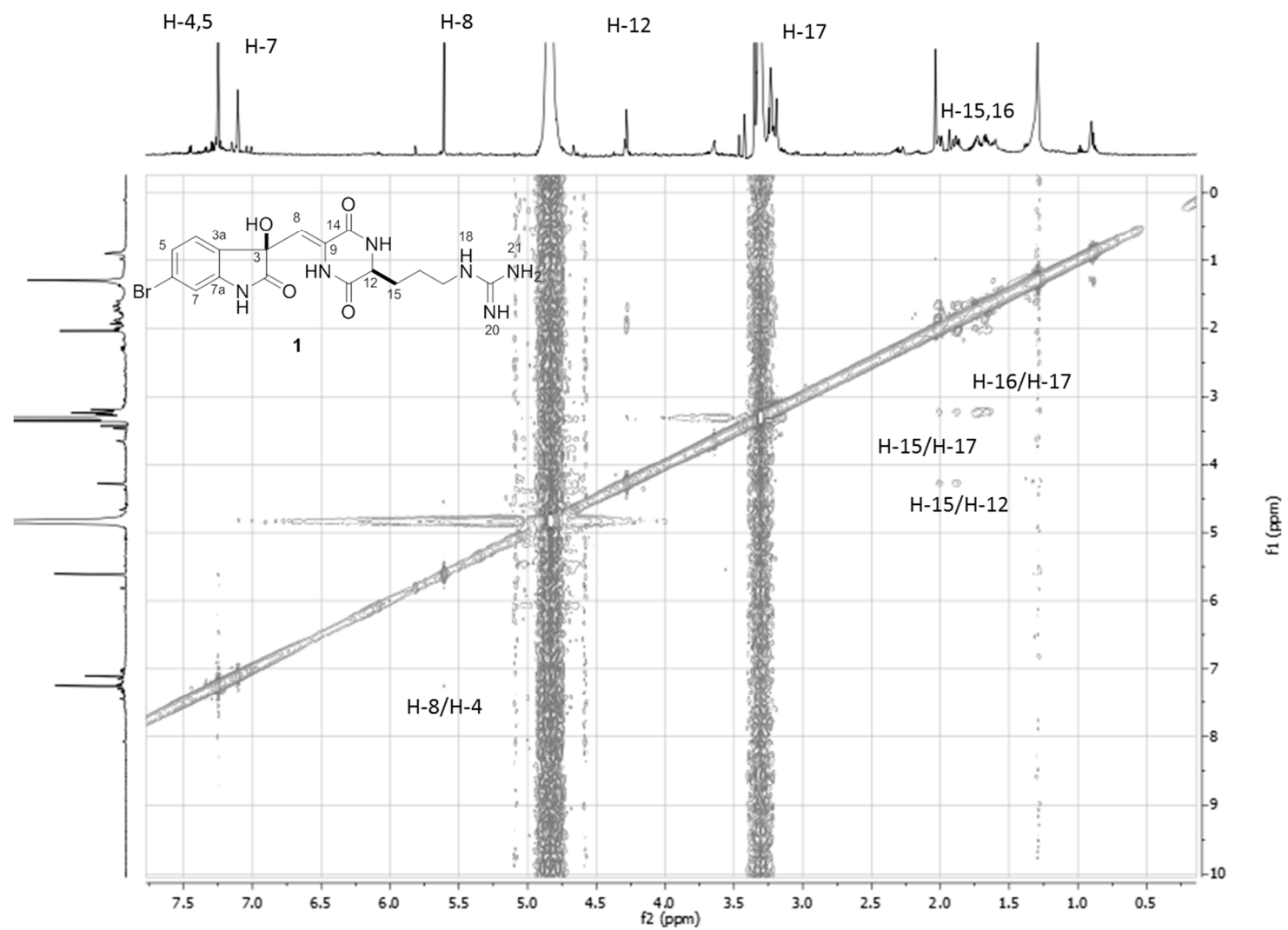


Figure S7. ^1H NMR spectrum of geobarrettin A (**1**) (600 MHz, $\text{DMSO}-d_6$)

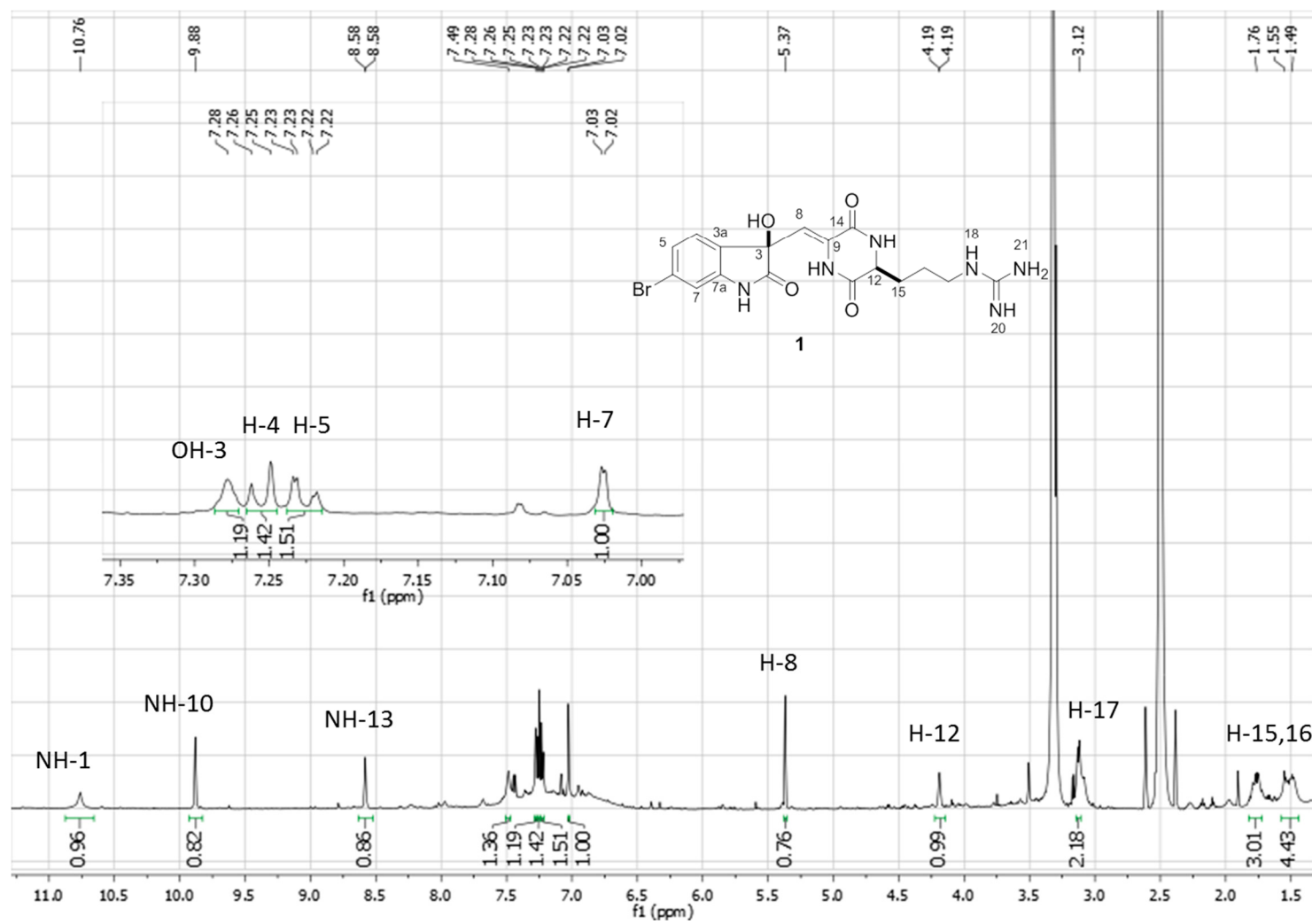


Figure S8. NOESY spectrum of geobarrettin A (1) (600 MHz, DMSO-*d*₆)

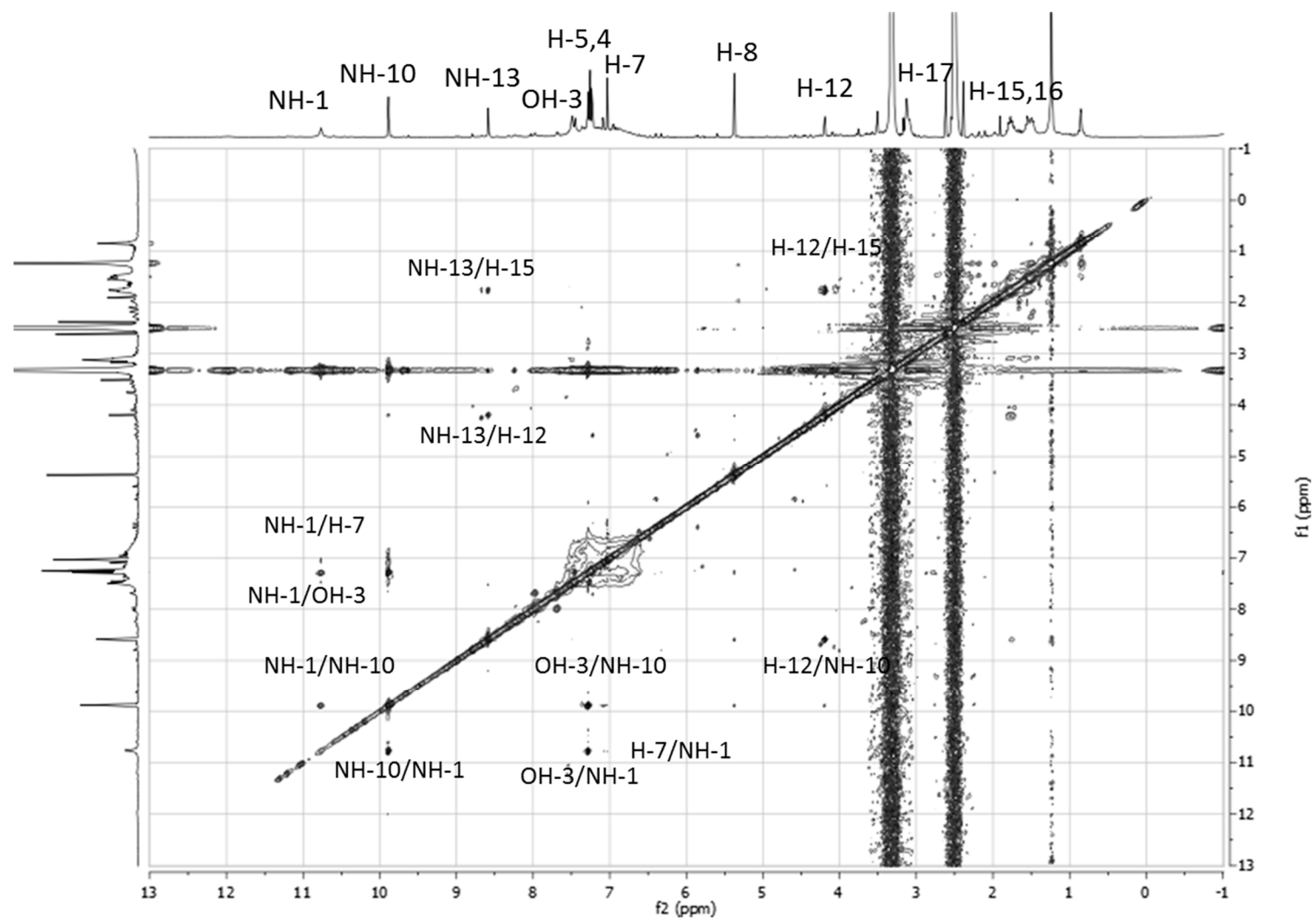


Figure S9. HRESIMS spectrum of geobarrettin A (1)

XD138B2-3

20161022_022 763 (3.113)

1: TOF MS ES+
4.30e4

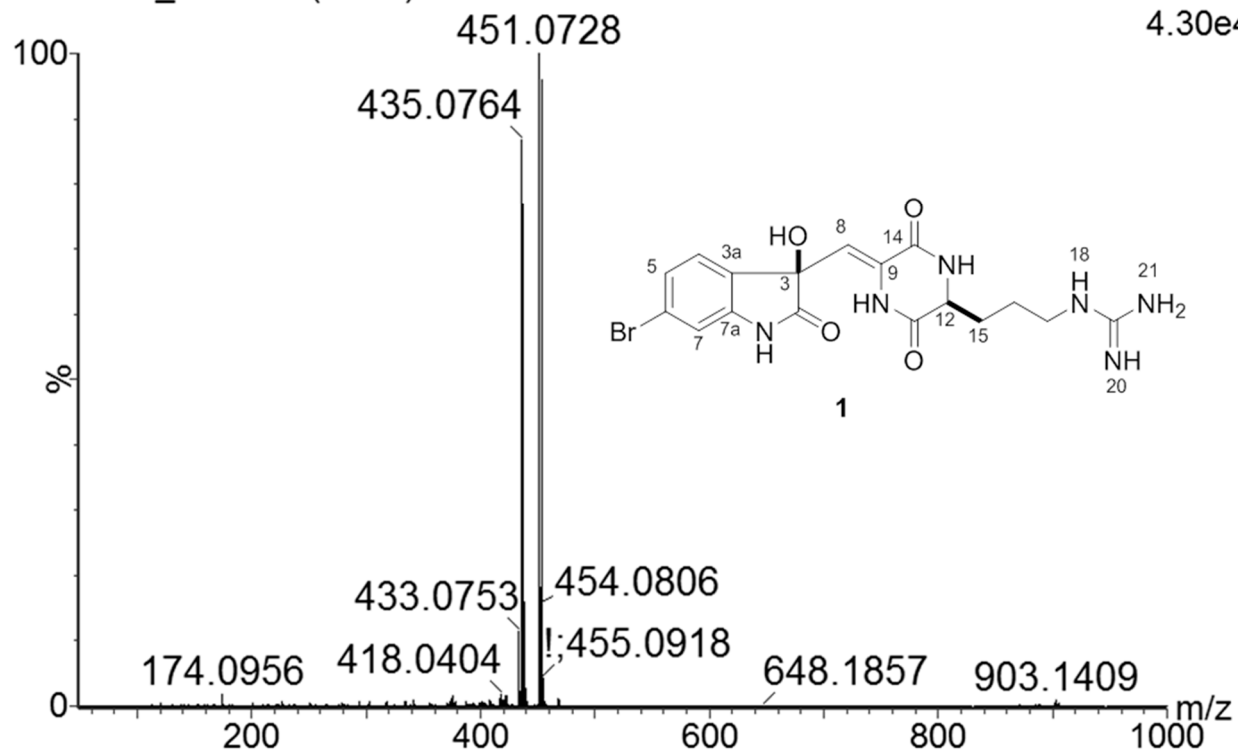


Figure S10. IR spectrum of geobarrettin A (**1**)

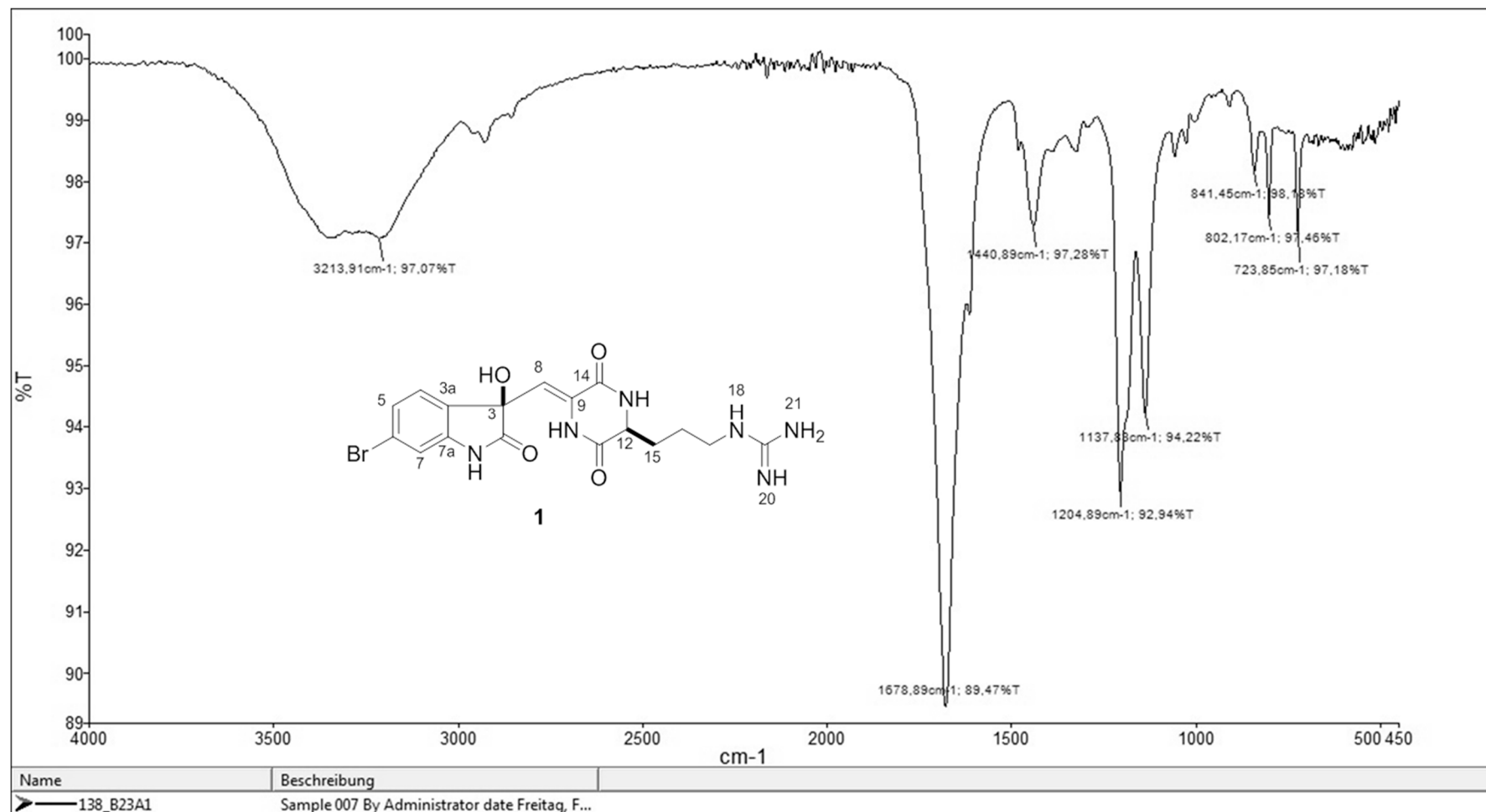


Figure S11. ^1H NMR spectrum of geobarrettin B (2) (600 MHz, CD_3OD)

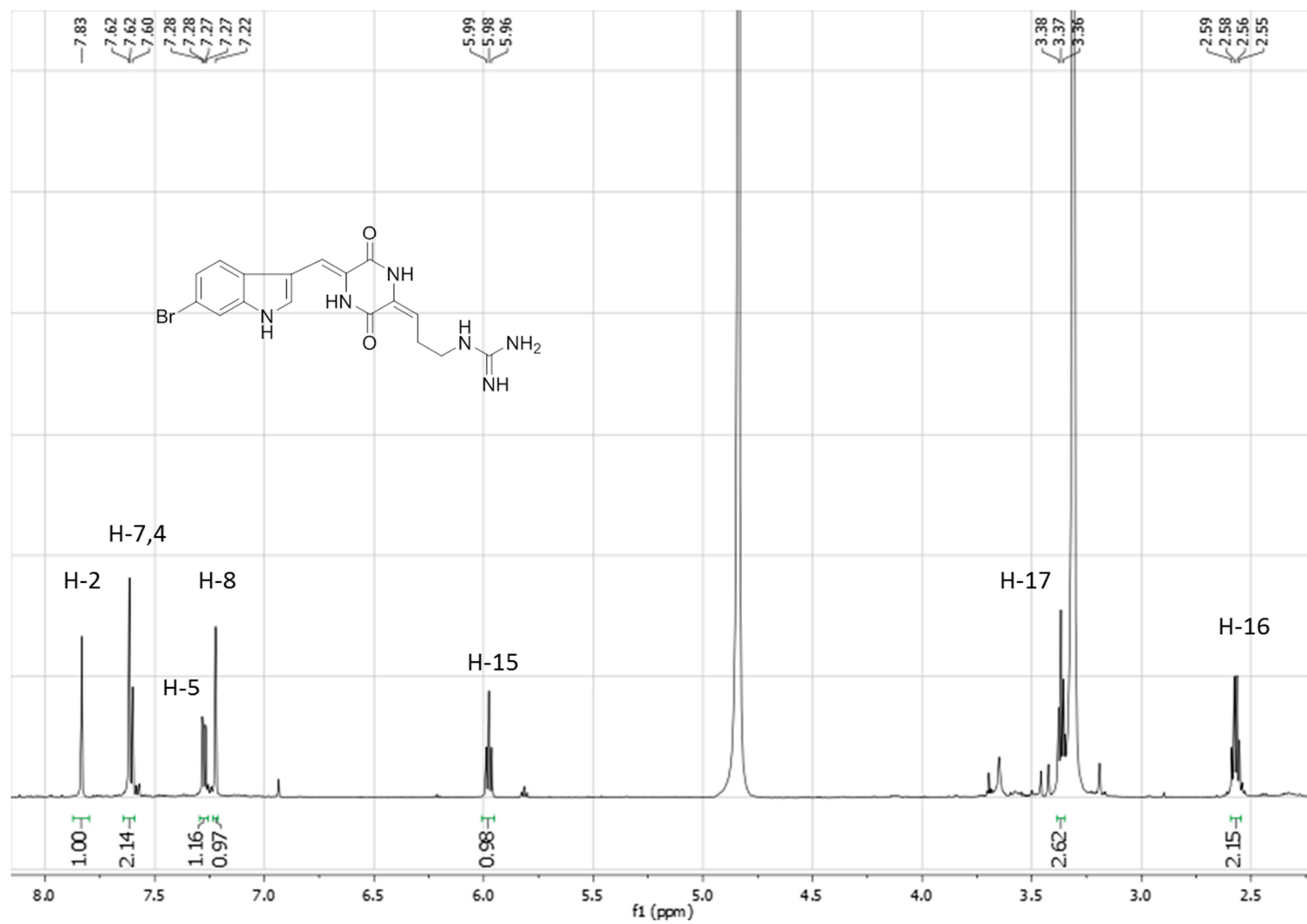


Figure S12. ^{13}C NMR spectrum of geobarrettin B (2) (150 MHz, CD_3OD)

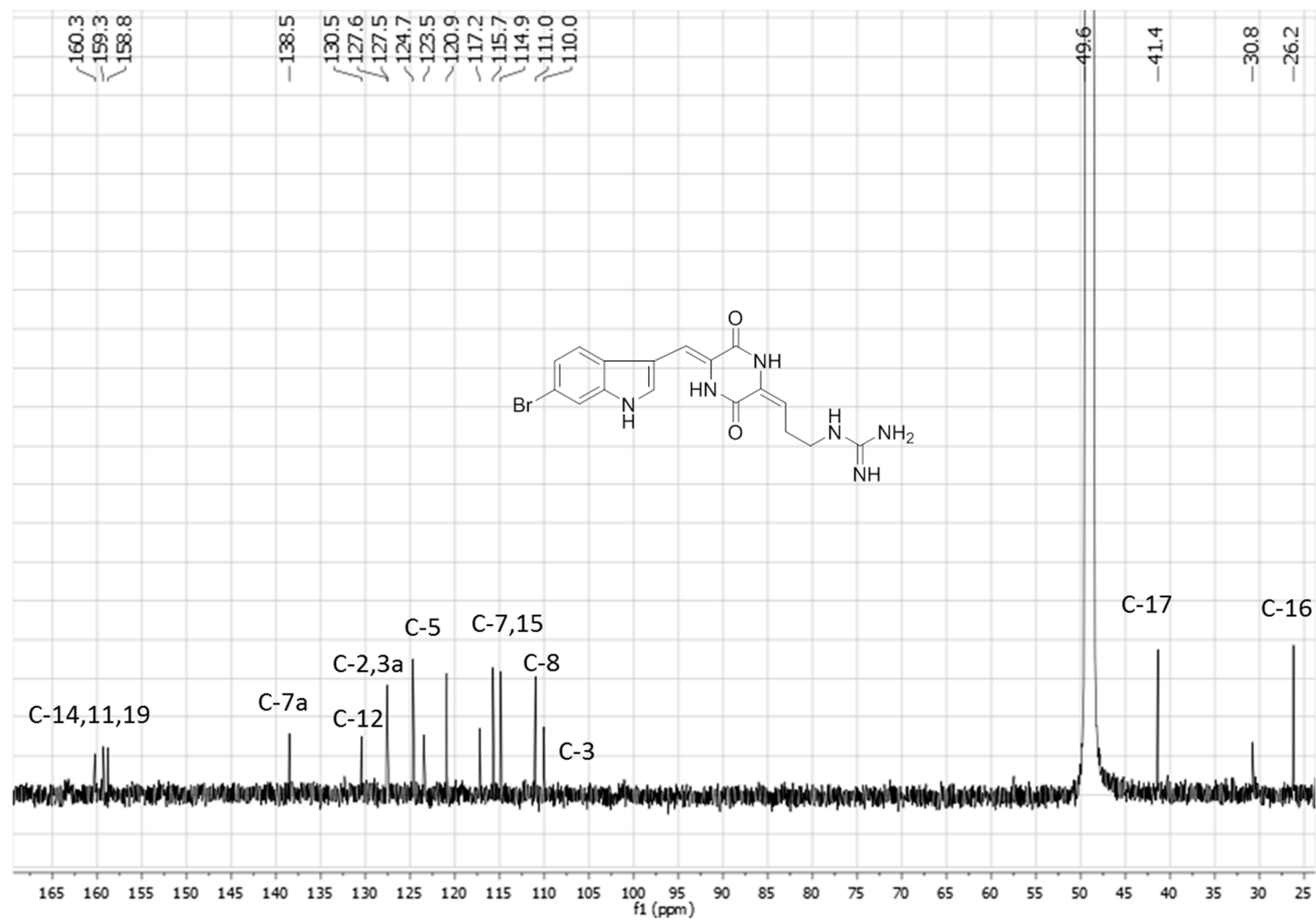


Figure S13. HSQC spectrum of geobarrettin B (2) (600 MHz, CD₃OD)

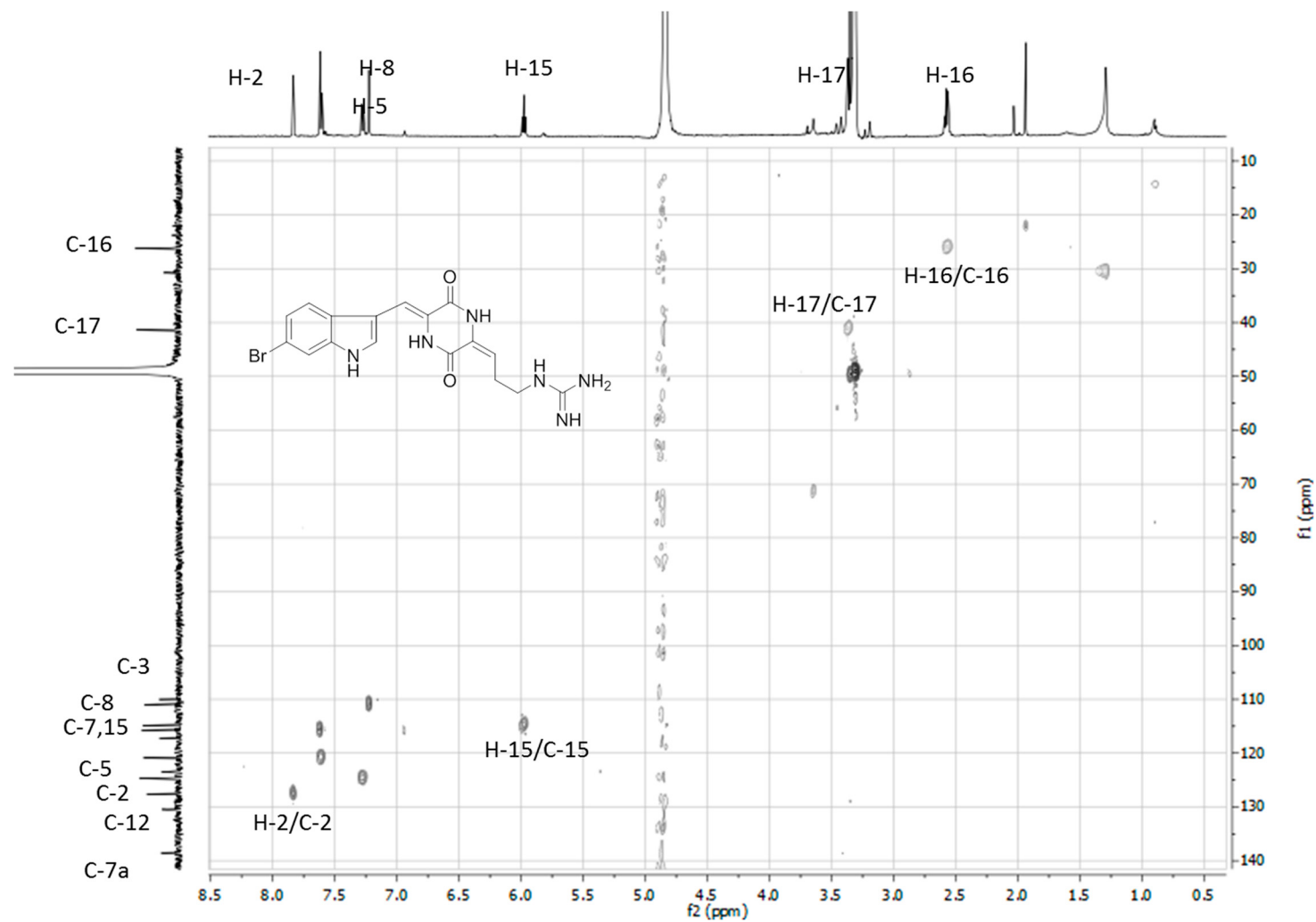


Figure S14. HMBC spectrum of geobarrettin B (**2**) (600 MHz, CD₃OD)

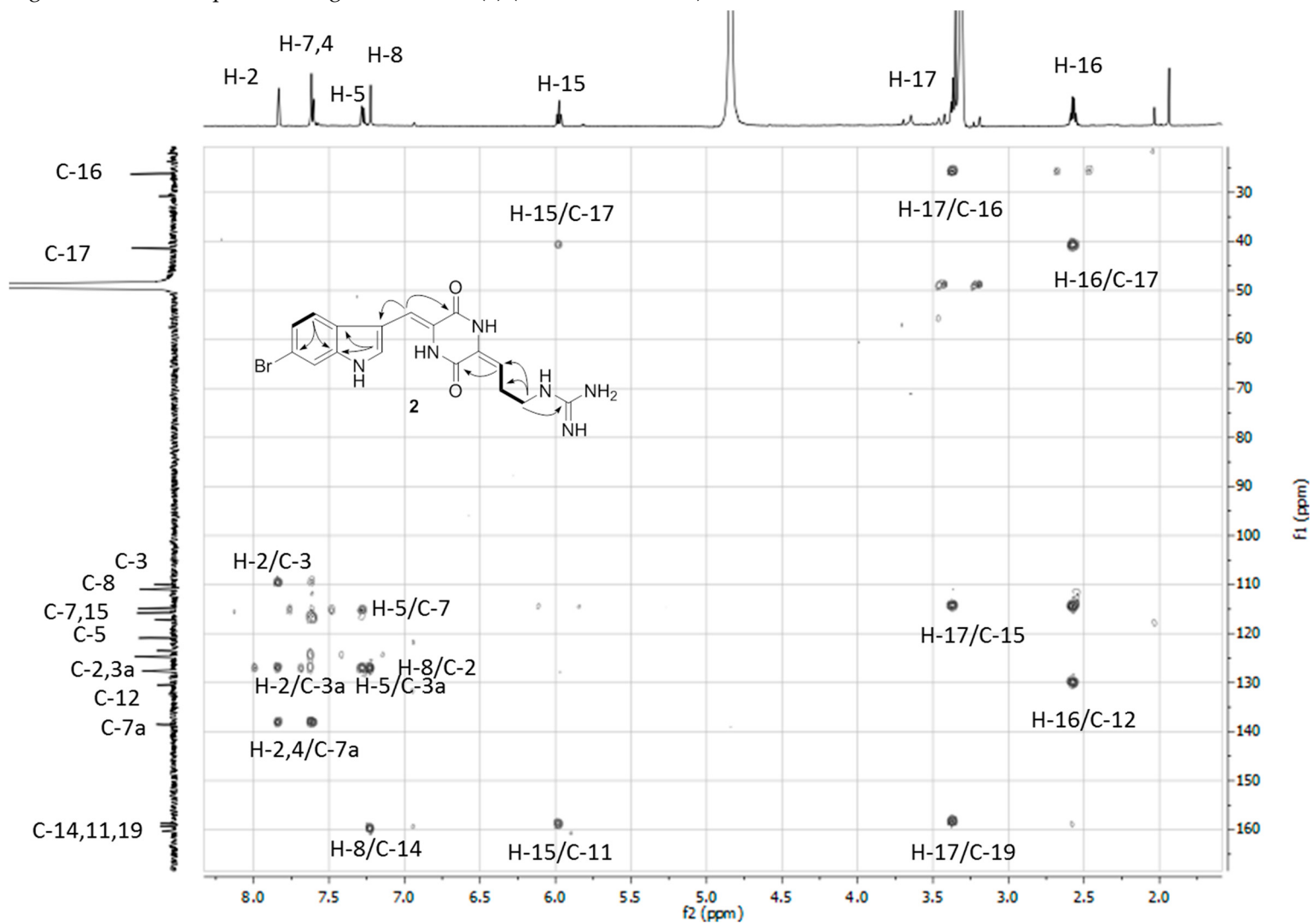


Figure S15. ^1H - ^1H COSY spectrum of geobarrettin B (**2**) (600 MHz, CD_3OD)

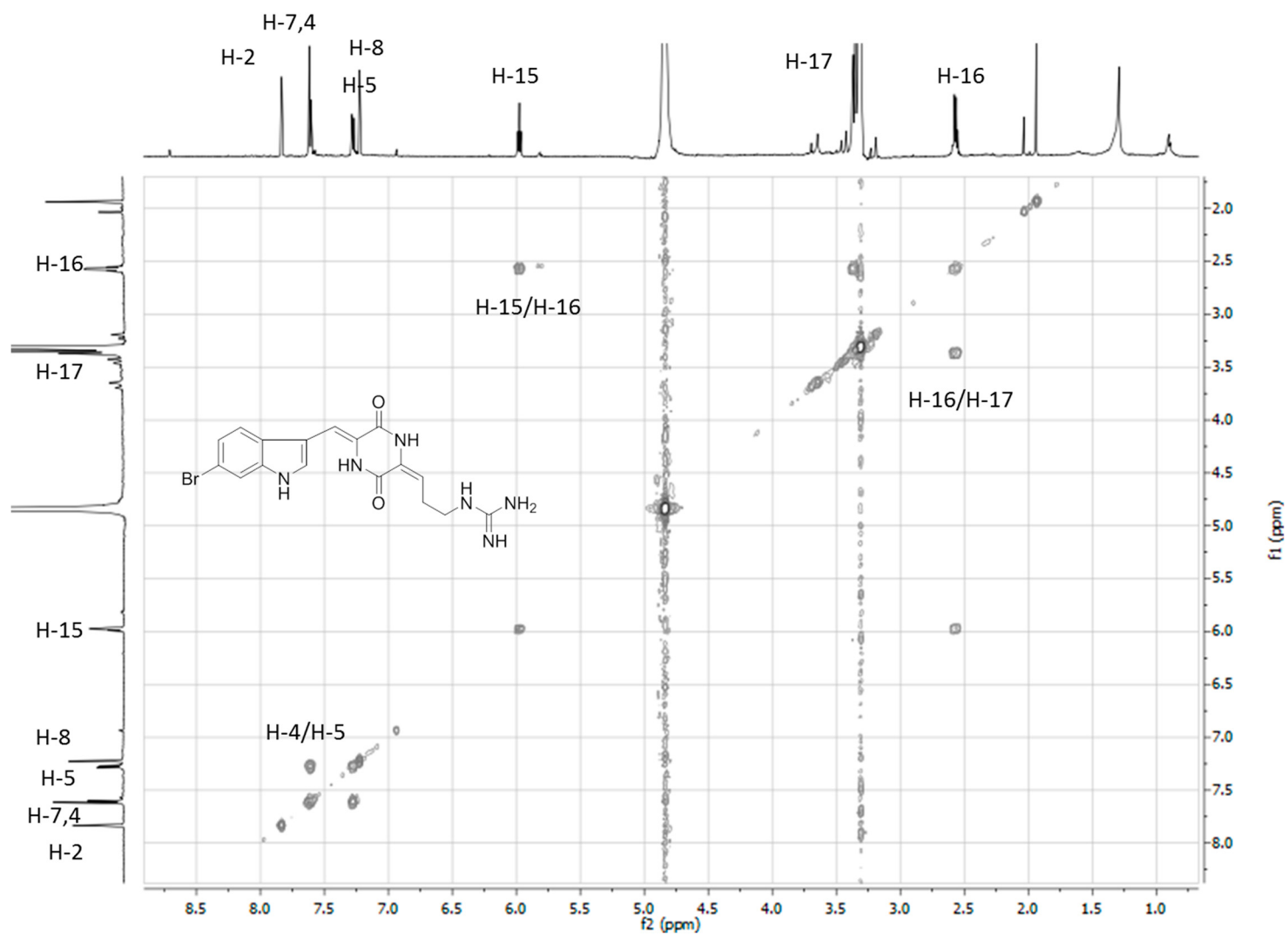


Figure S16. NOESY spectrum of geobarrettin B (2) (600 MHz, CD₃OD)

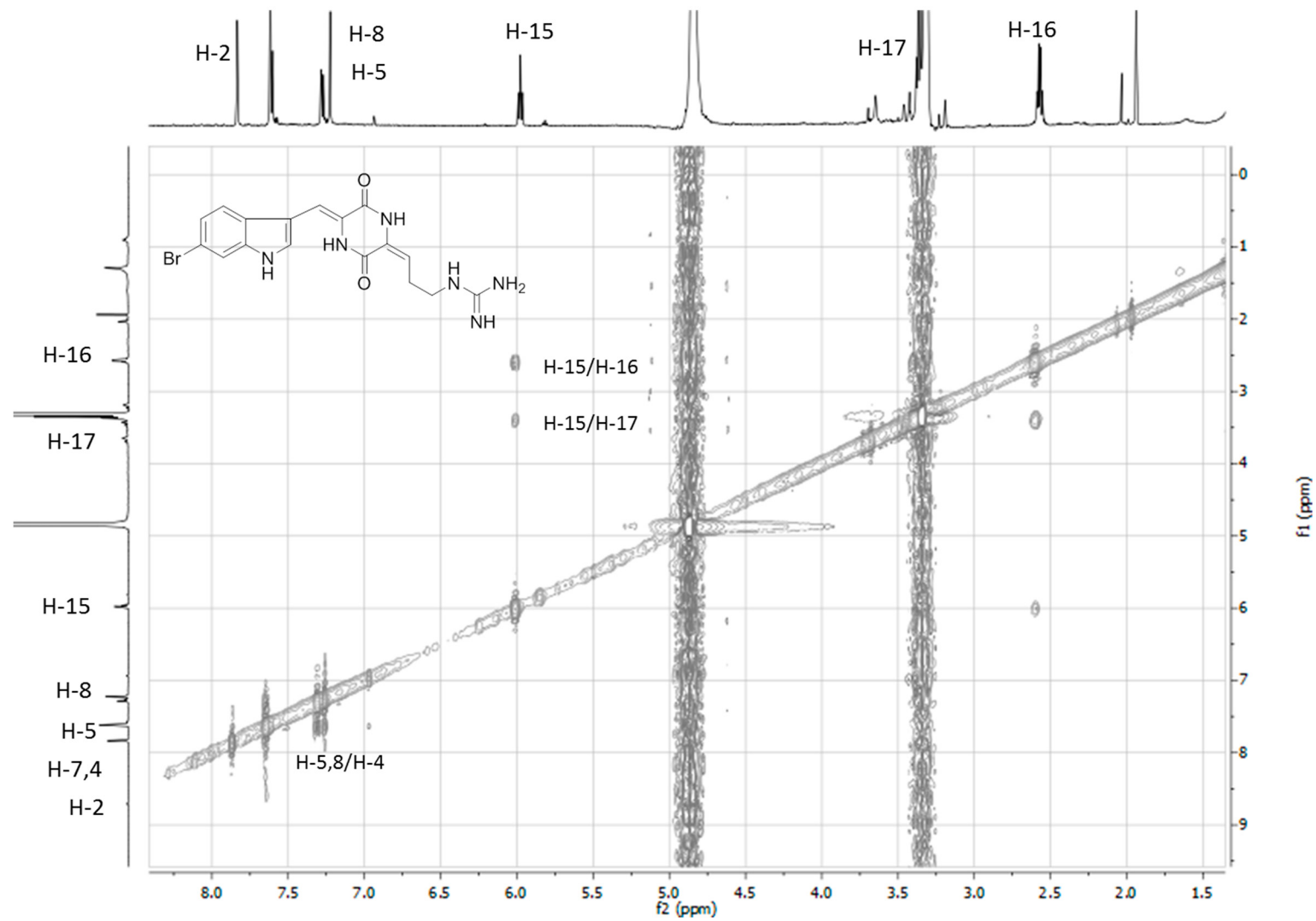


Figure S17. HRESIMS spectrum of geobarrettin B (2)

XD138B4-3

20161022_031 989 (4.023) Cm (989:991)

1: TOF MS ES+

1.01e5

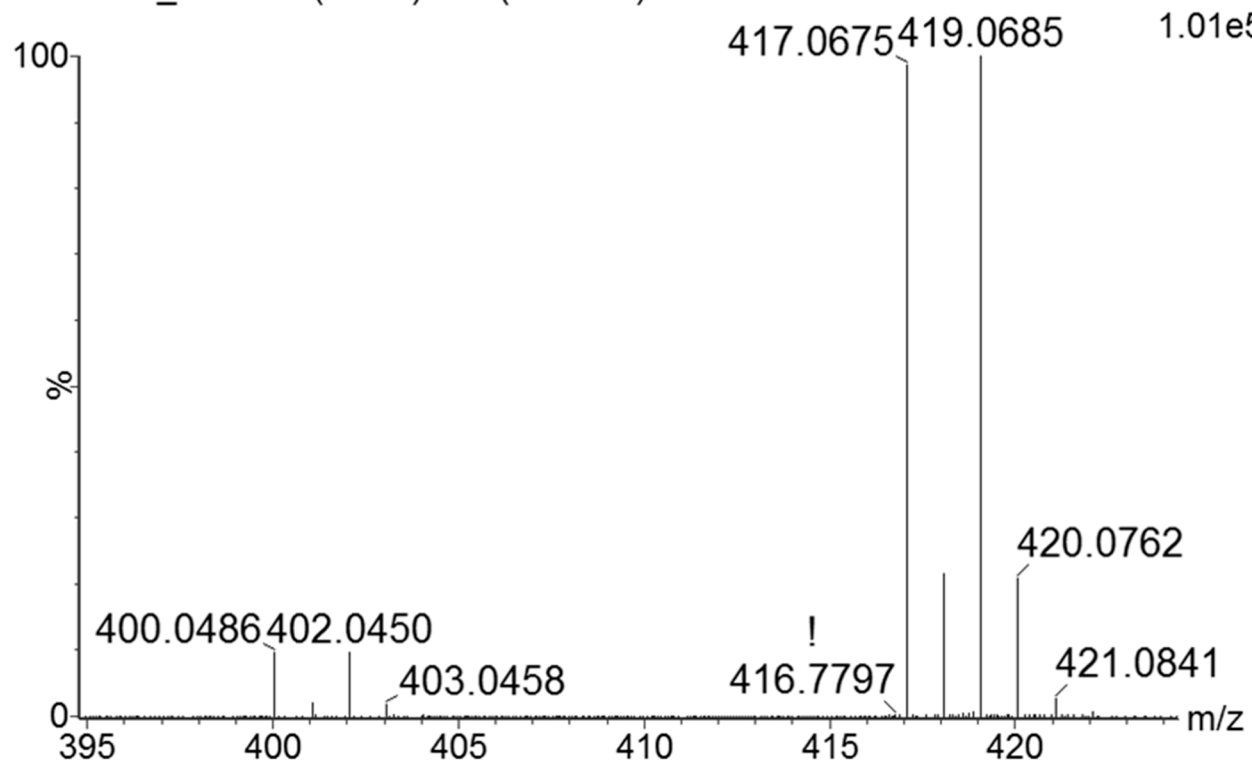


Figure S18. IR spectrum of geobarrettin B (2)

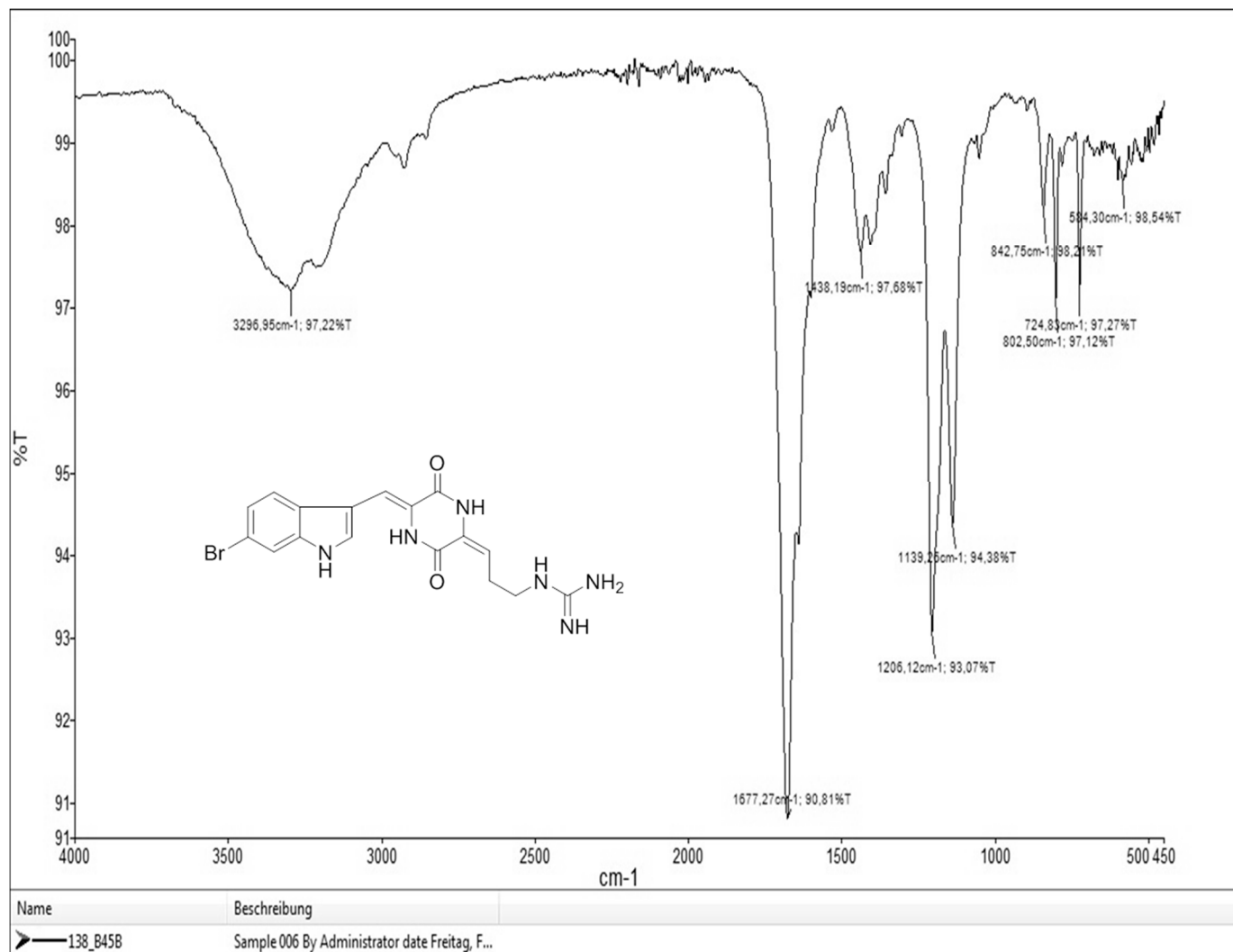


Figure S19. ^1H NMR spectrum of geobarrettin C (**3**) (600 MHz, CD_3OD)

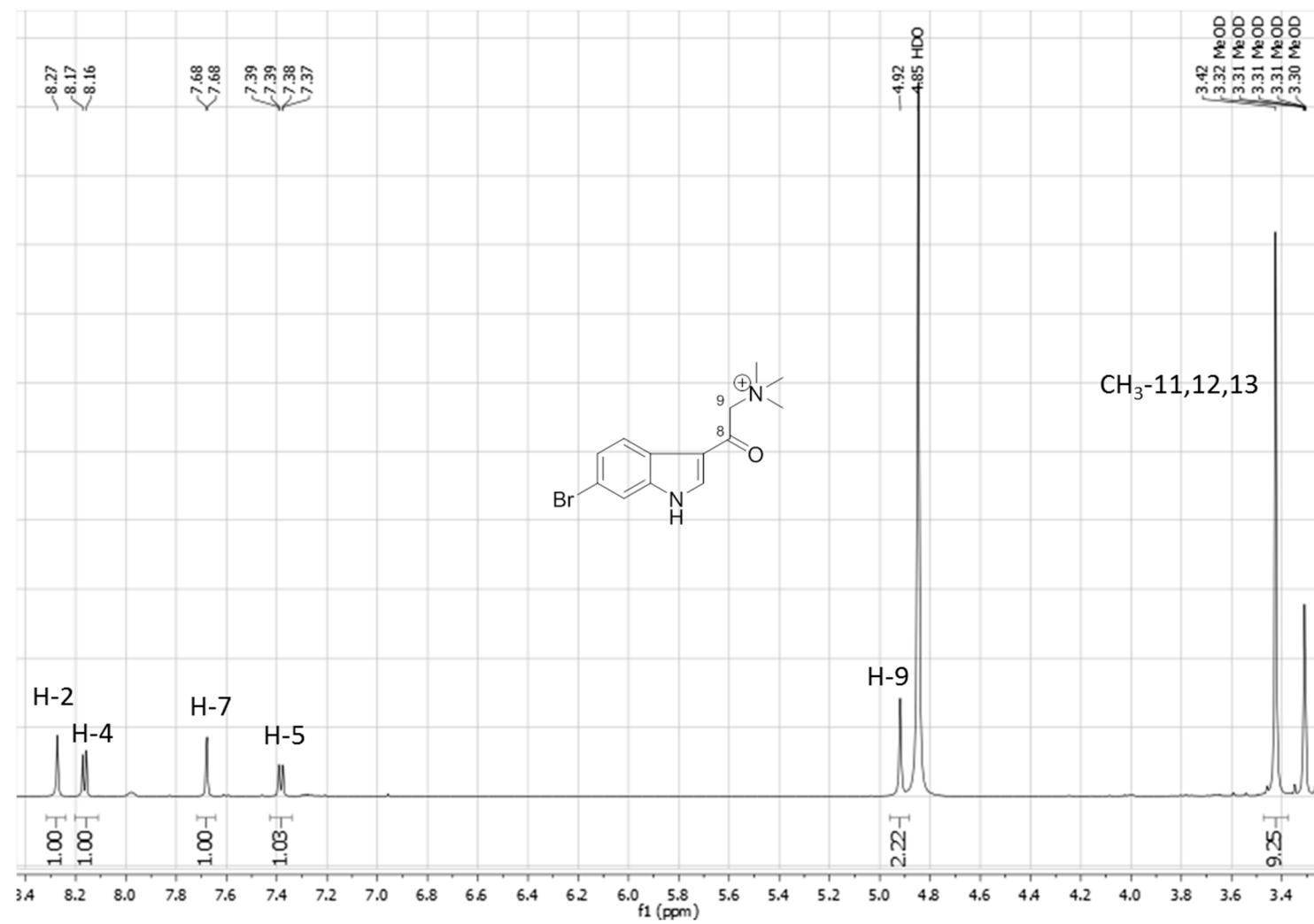


Figure S20. ^{13}C NMR spectrum of geobarrettin C (3) (150 MHz, CD_3OD)

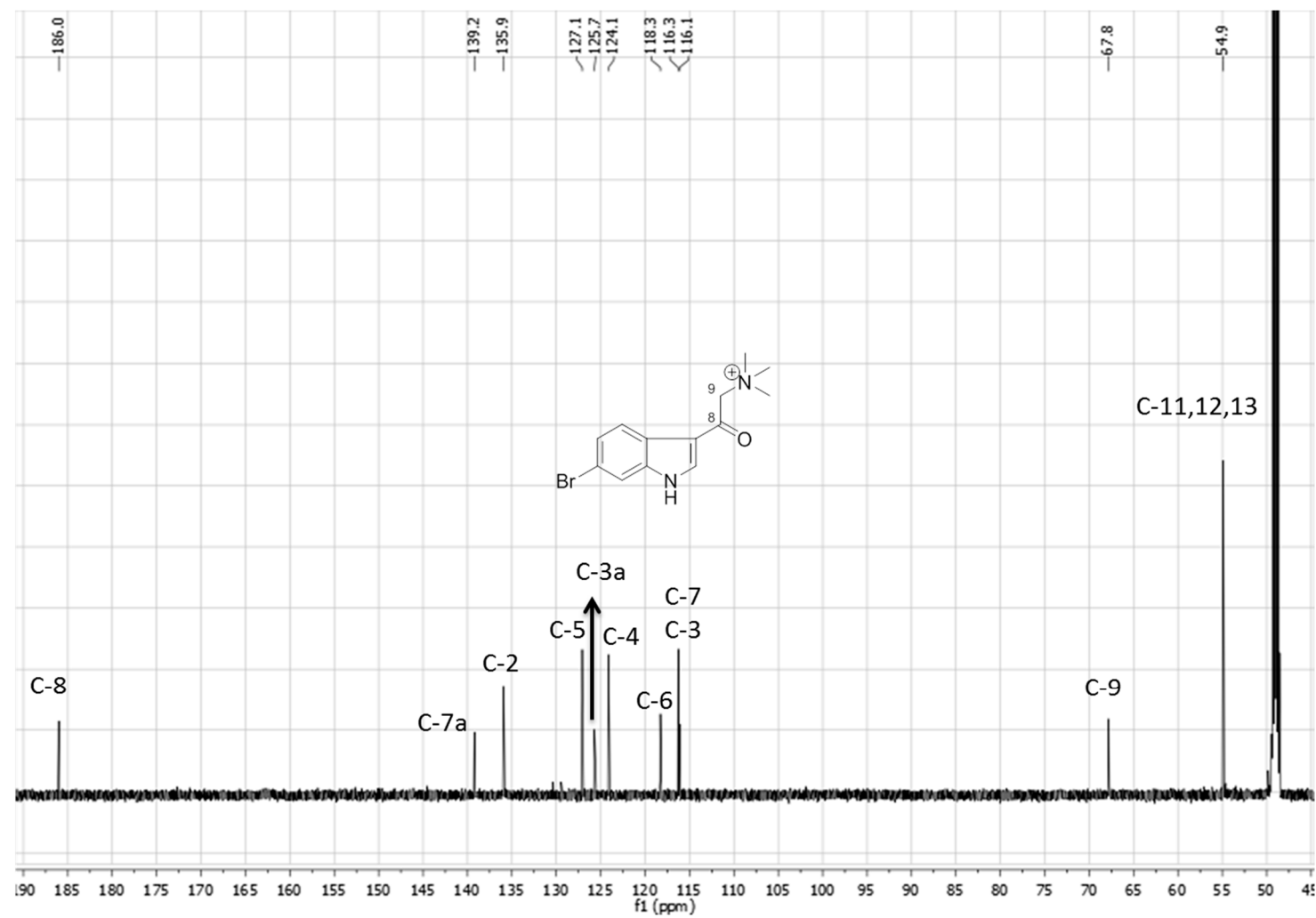


Figure S21. HSQC spectrum of geobarrettin C (3) in (400 MHz, CD₃OD)

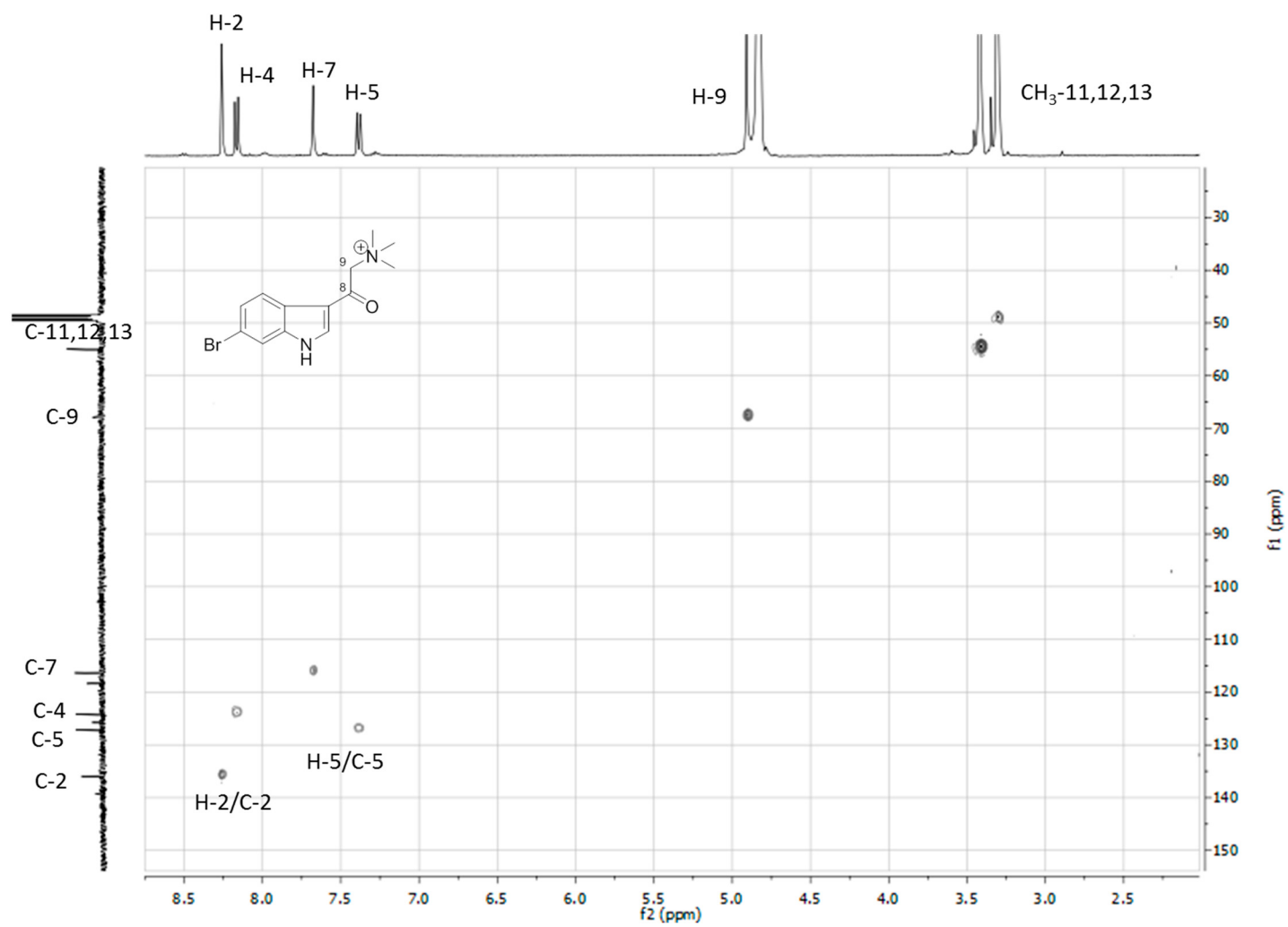


Figure S22. HMBC spectrum of geobarrettin C (**3**) (600 MHz, CD₃OD)

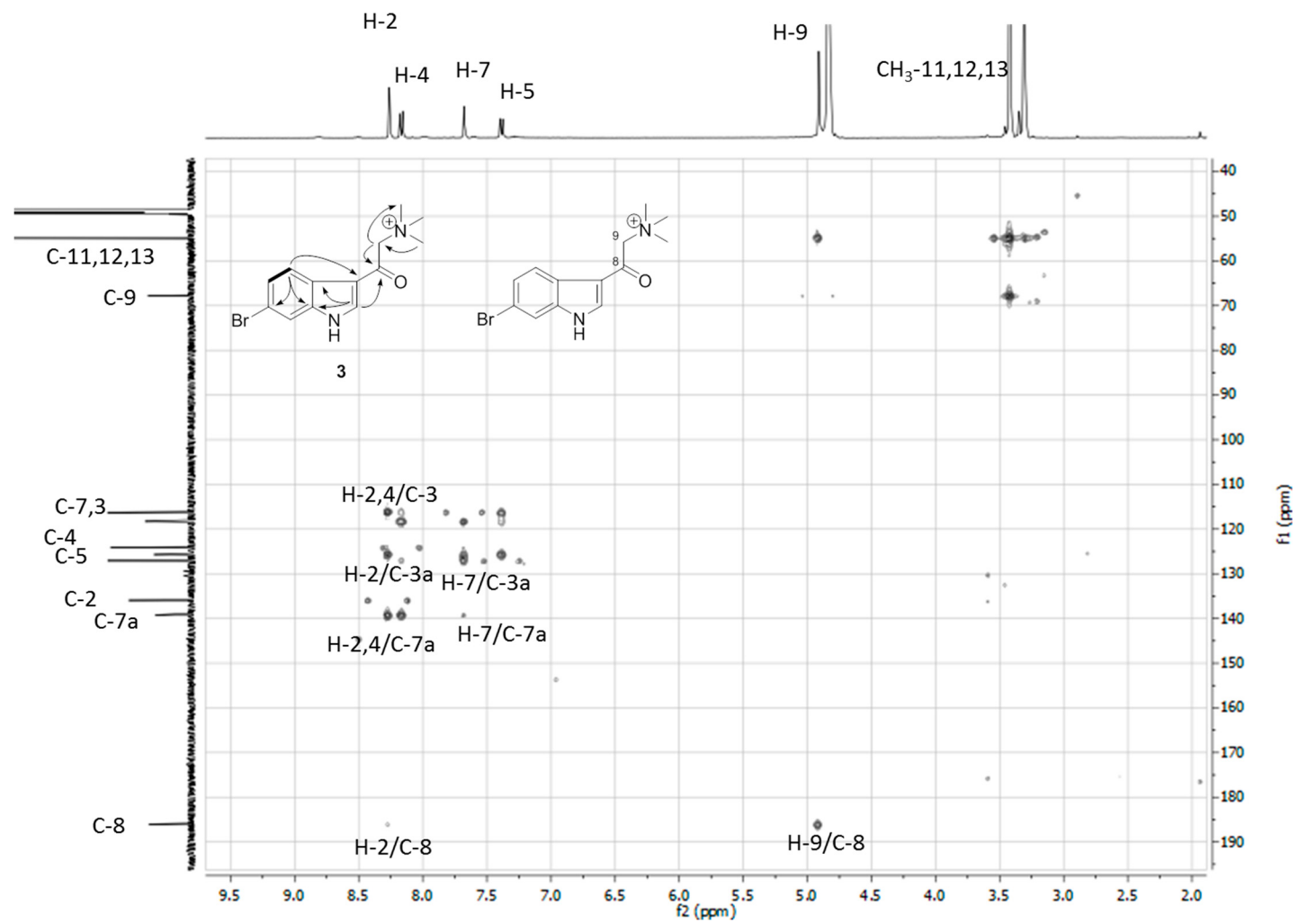


Figure S23. ^1H - ^1H COSY spectrum of geobarrettin C (3) (400 MHz, CD_3OD)

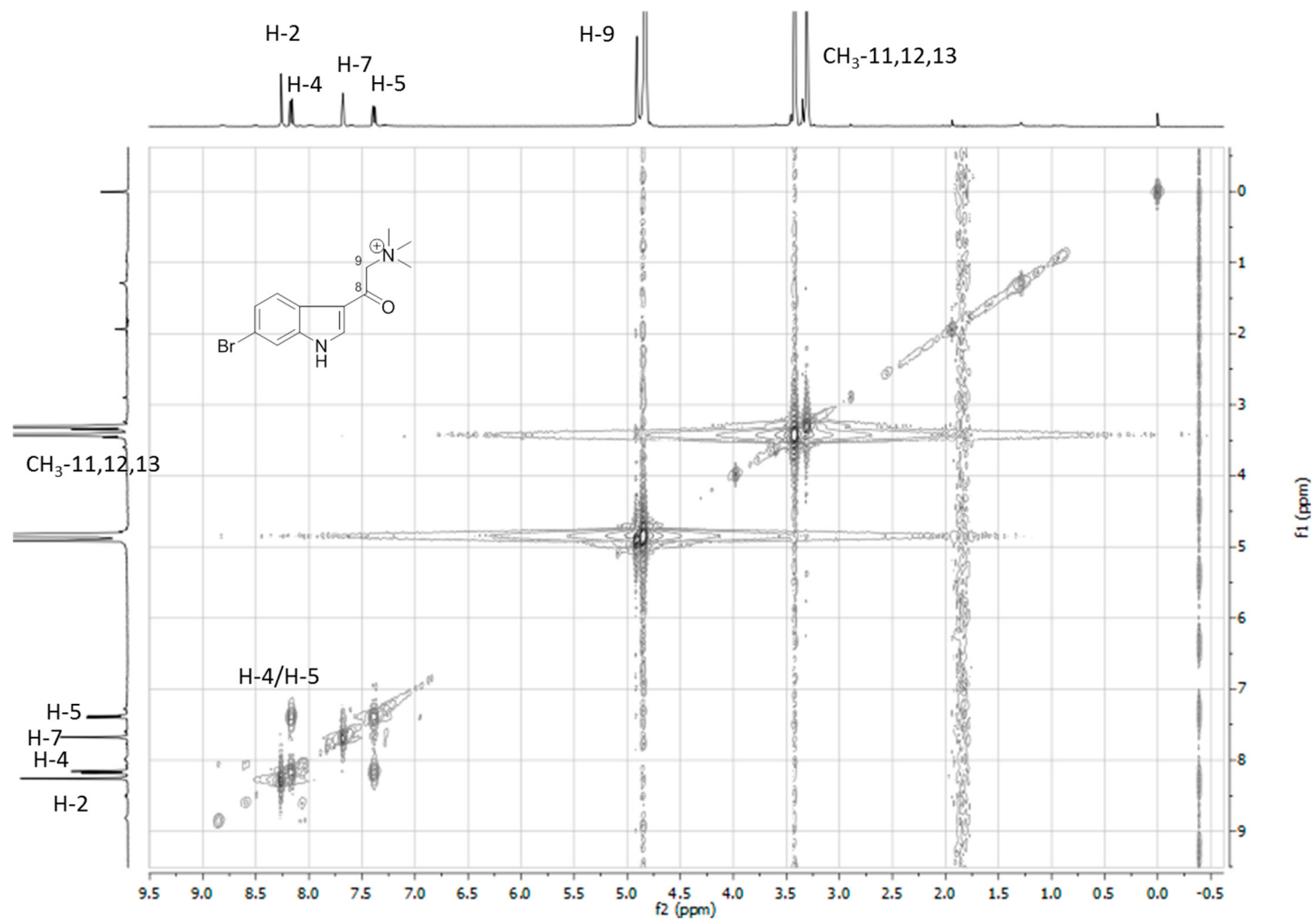


Figure S24. HRESIMS spectrum of geobarrettin C (3)

XD138B2-9

20161022_029 957 (3.895) Cm (956:959)

1: TOF MS ES+
3.74e5

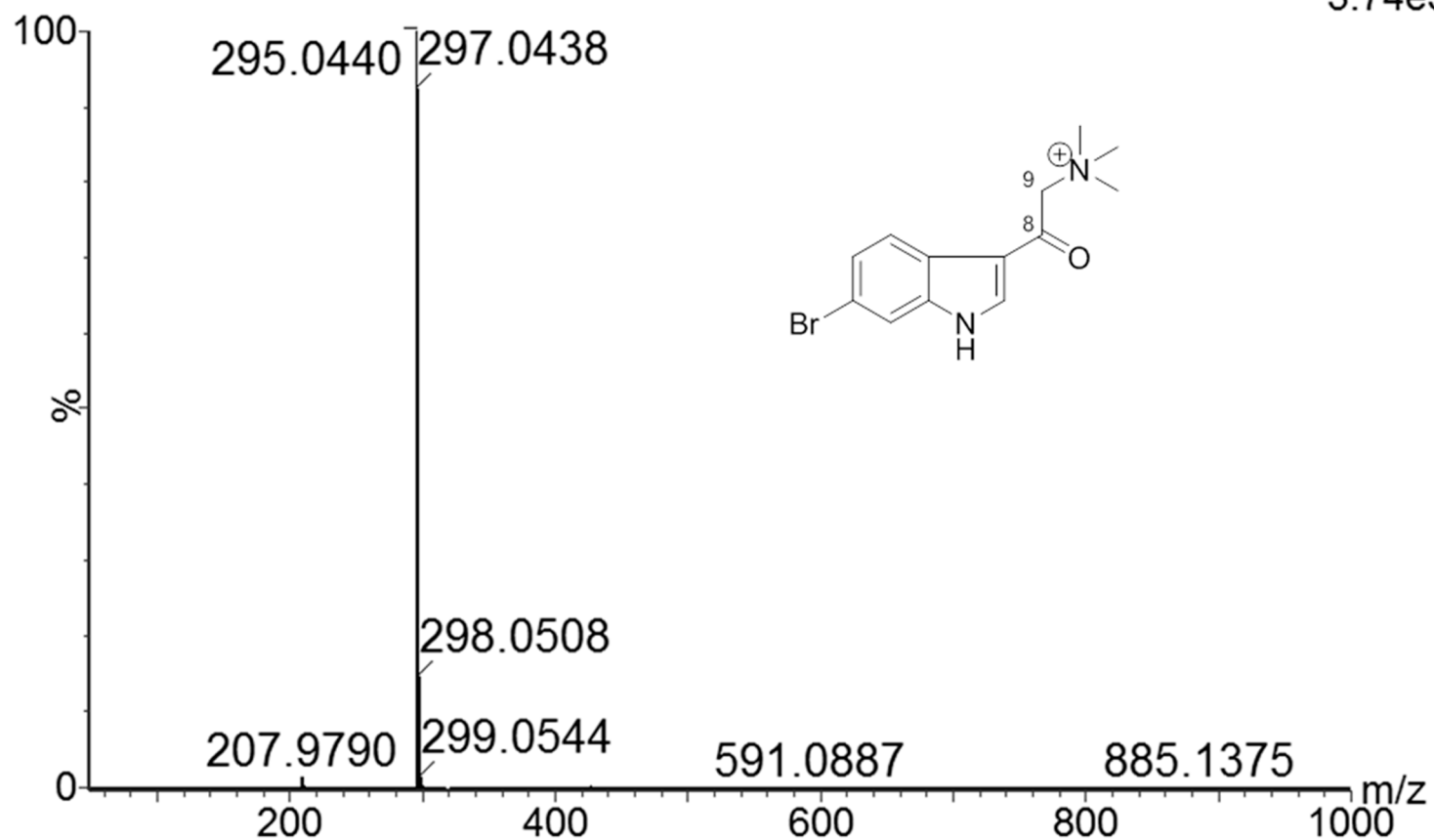


Figure S25. IR spectrum of geobarrettin C (3)

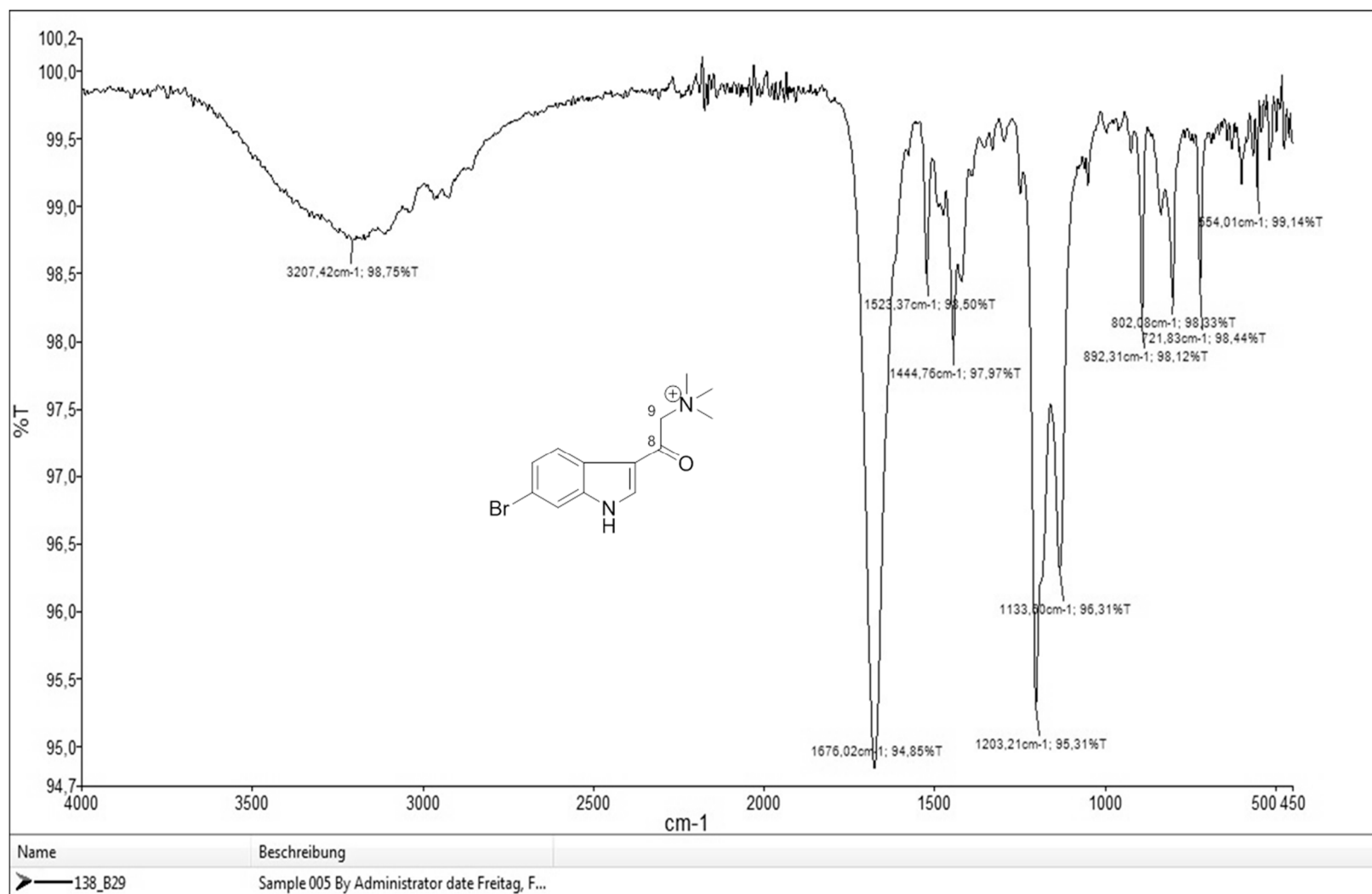


Figure S26. ^1H NMR spectrum of (*R*)-3-propyldioxindole (**8**) (400 MHz, CDCl_3)

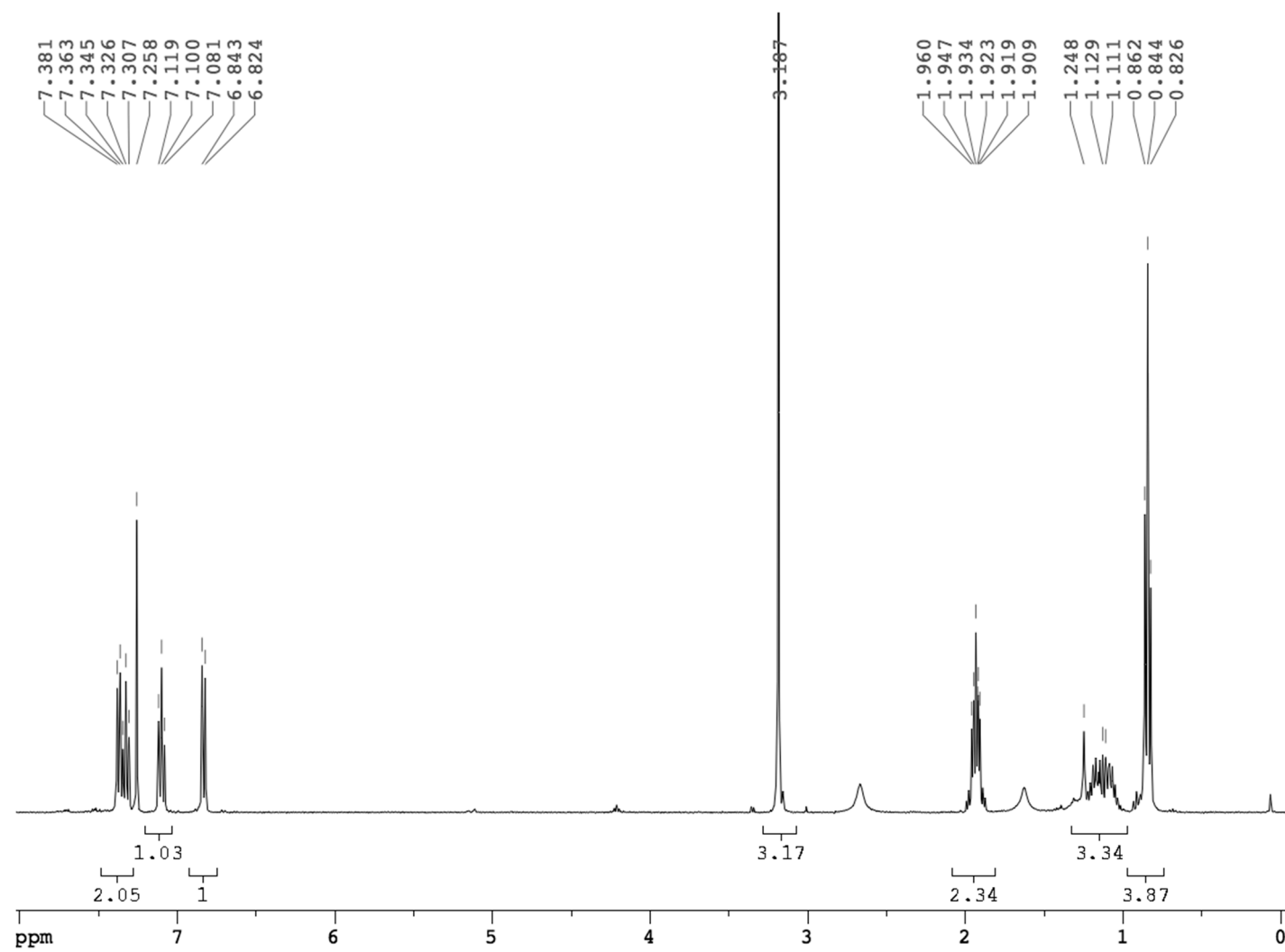


Figure S27. ^{13}C NMR spectrum of (*R*)-3-propyldioxindole (**8**) (125 MHz, CDCl_3)

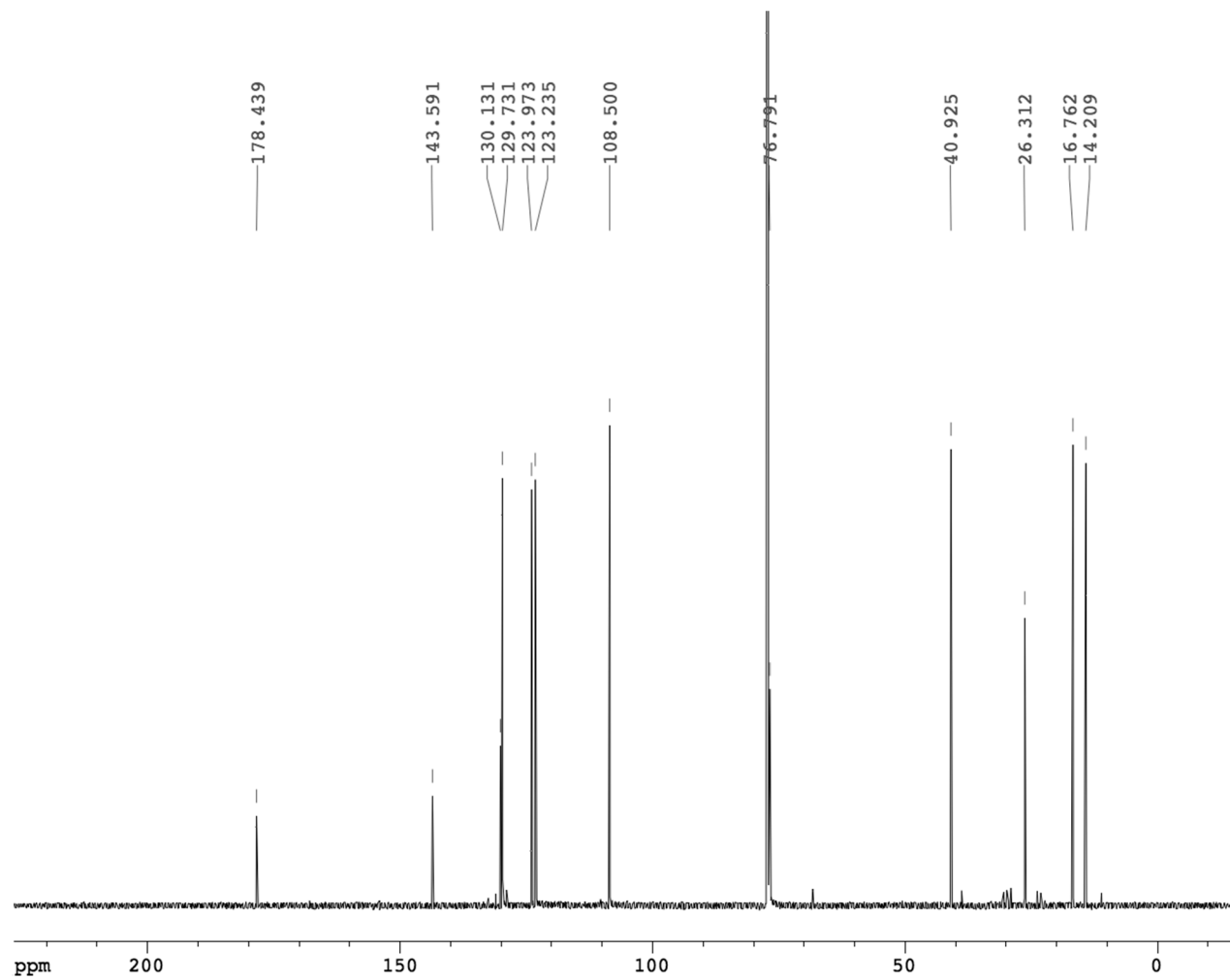


Figure S28. UV spectrum of (*R*)-3-propyldioxindole (8)

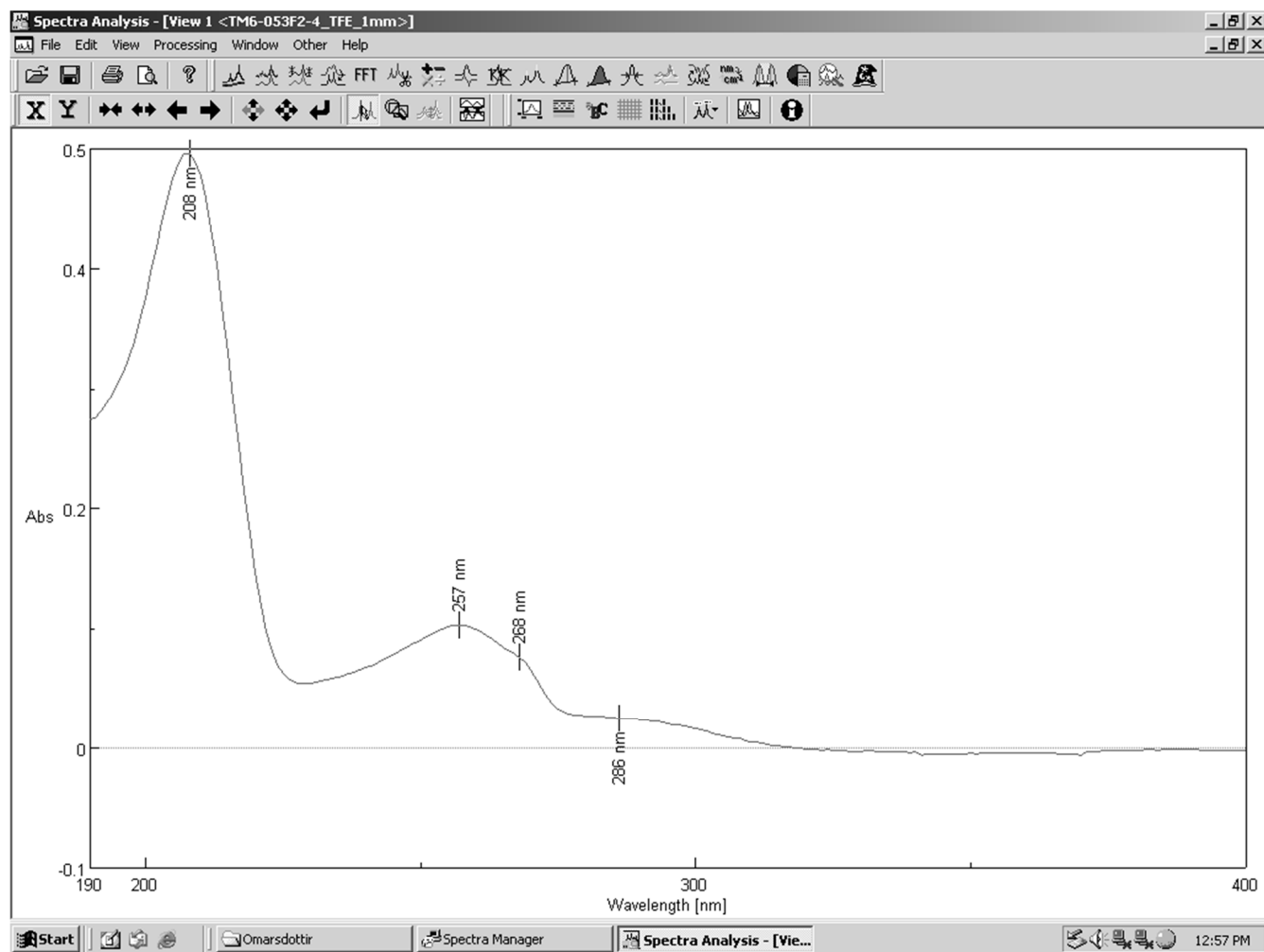


Figure S29. IR spectrum of (*R*)-3-propyldioxindole (8)

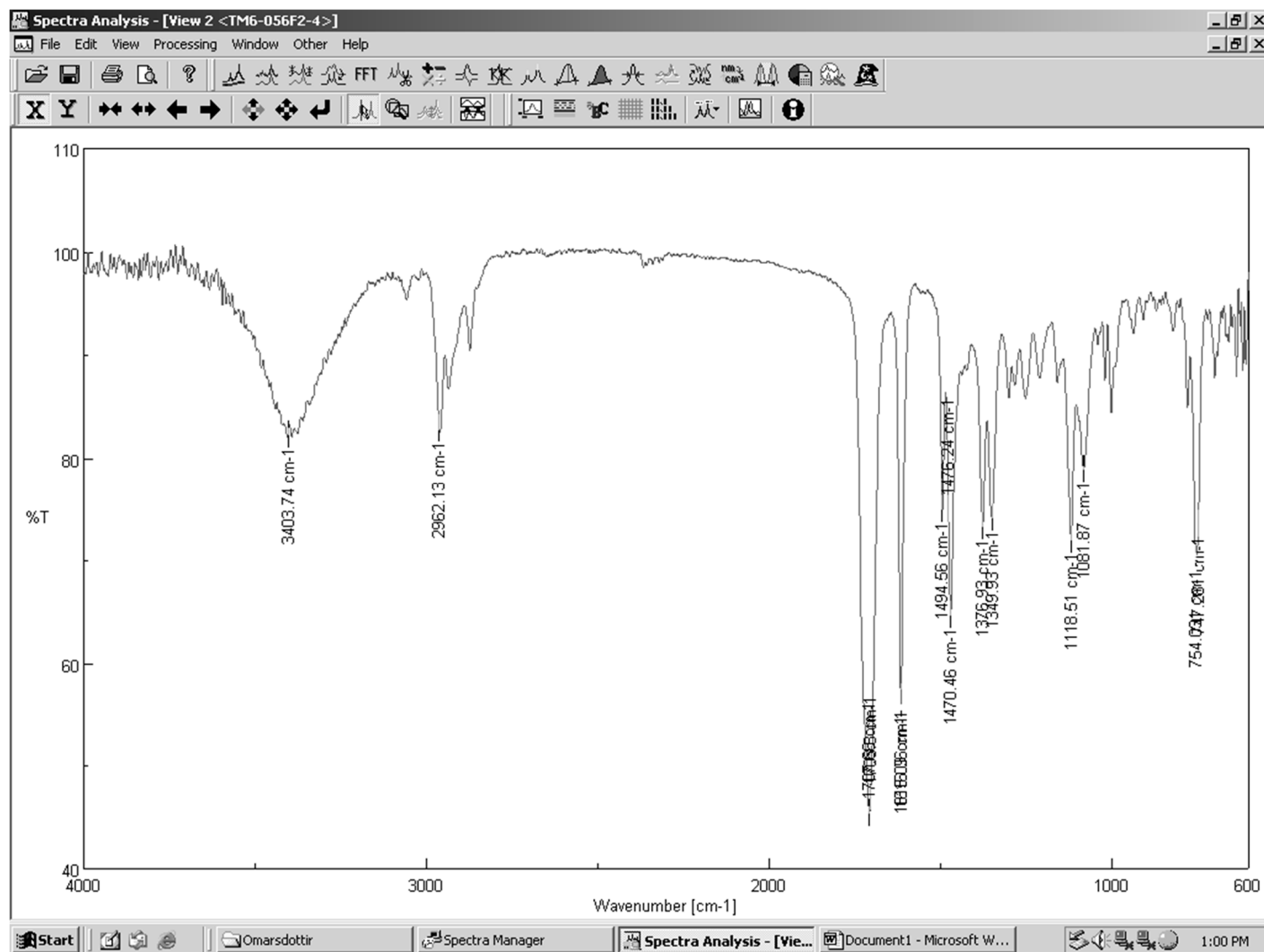
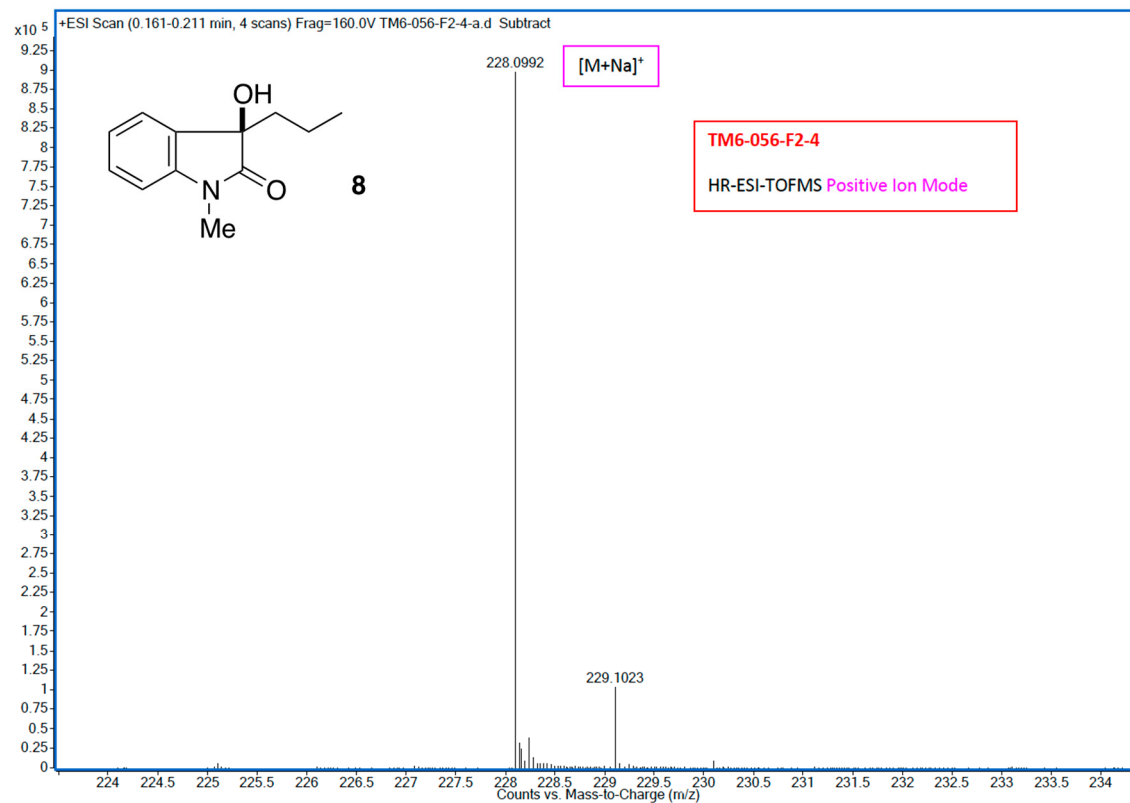


Figure S30. HRESIMS spectrum of (*R*)-3-propyldioxindole (**8**)



Search Results: Sample TM6-056-F2-4

Mass Measured	Theo. Mass	Delta (ppm)	Composition
228.0992	228.0995	-1.3	[C ₁₂ H ₁₅ N O ₂ Na] ⁺

Figure S31. UV spectrum of debromodihydrogeobarrettin A (**1a**)

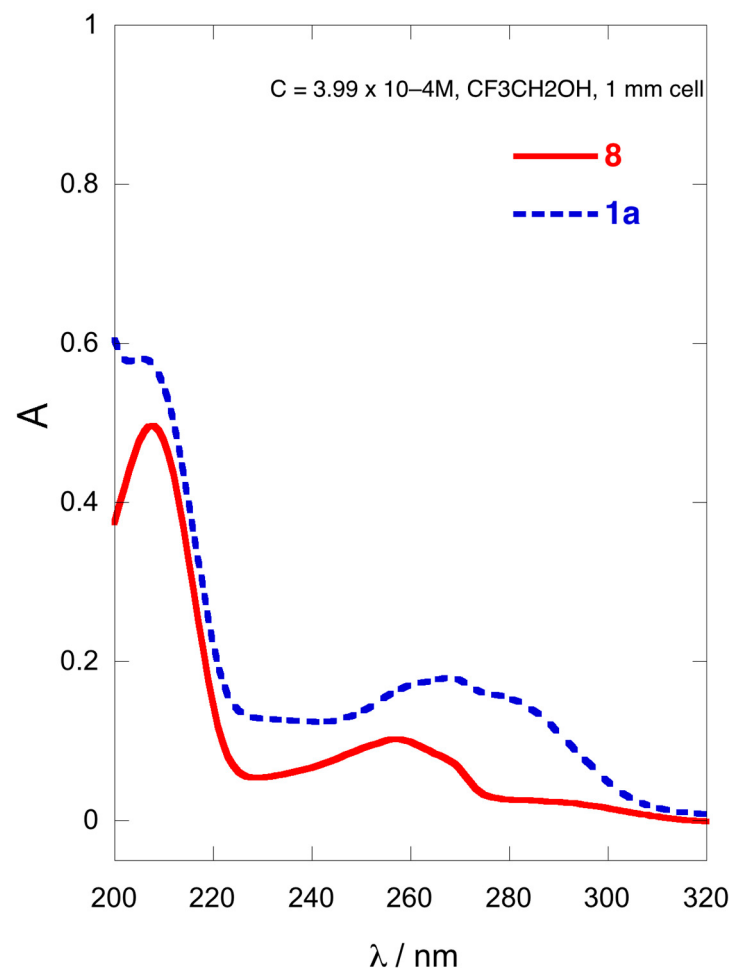


Figure S32. RP HPLC (C18) Chromatogram of L-DPT derivative of hydrolysate of debromodihydrogeobarrettin A (1a)

