

Supporting Information

Ammonificins A and B, Hydroxyethylamine chroman derivatives from a Cultured Marine Hydrothermal Vent Bacterium, *Thermovibrio ammonificans*.

Eric H. Andrianasolo,[†] Liti Haramaty,[†] Richard Rosario-Passapera,[†] Kelly Bidle,[‡]
Eileen White,^{§,⊥,∇} Costantino Vetriani,[†] Paul Falkowski[†] and Richard Lutz^{†,*}

*Center for Marine Biotechnology, Institute of Marine and Coastal Sciences, Rutgers, The
State University of New Jersey NJ 08901-8521*

Department of Biology, Rider University, 2083 Lawrenceville Rd, Lawrenceville, New Jersey 08648

*Center for Advanced Biotechnology and Medicine, Department of Molecular Biology and Biochemistry,
Rutgers, The State University of New Jersey, 679 Hoes Lane, Piscataway, New Jersey 08854*

*University of Medicine and Dentistry of New Jersey, Robert Wood Johnson Medical School,
675 Hoes Lane, Piscataway, New Jersey 08854*

The Cancer Institute of New Jersey, 195 Little Albany Street, New Brunswick, New Jersey 08903

*To whom correspondence should be addressed. Tel.: (732) 932-8959 ext. 242

Fax : (732) 932-6557 E-mail: rlutz@imcs.marine.rutgers.edu

[†] IMCS, Rutgers, The State University of New Jersey.

[‡] Department of Biology, Rider University

[§] CABM, Rutgers, The State University of New Jersey.

[⊥] University of Medicine and Dentistry of New Jersey.

[∇] The Cancer Institute of New Jersey.

Spectral Data for Ammonificin A (1) in DMSO-*d*₆

Figure S1 400 MHz ¹H NMR spectrum of Ammonificin A (1) in DMSO-*d*₆

Figure S2 400 MHz ¹H-¹H COSY spectrum of Ammonificin A (1) in DMSO-*d*₆

Figure S3 400 MHz ¹H-¹H COSY spectrum of Ammonificin A (1) in DMSO-*d*₆
(partial view of the aromatic ring region)

Figure S4 400 MHz ¹H-¹H COSY spectrum of Ammonificin A (1) in DMSO-*d*₆ (partial view
of the dihydropyran moiety and hydroxyethylamine moiety)

Figure S5 500 MHz HSQC spectrum of Ammonificin A (1) in DMSO-*d*₆ (partial
view of the aromatic ring region)

- Figure S6** 400 MHz HMBC spectrum (optimized for $J = 8\text{Hz}$) of Ammonificin A (1) in DMSO- d_6 (partial view of the aromatic ring region)
- Figure S7** 400 MHz HMBC spectrum (optimized for $J = 8\text{Hz}$) of Ammonificin A (1) in DMSO- d_6 (partial view of the dihydropyran moiety and hydroxyethylamine moiety)
- Figure S8** LR-ESI spectrum of Ammonificin A (1)
- Figure S9** 500 MHz ^1H NMR spectrum of Ammonificin B (2) in DMSO- d_6
- Figure S10** LR-ESI spectrum of Ammonificin B (2)
- Figure S11** HPLC trace Ammonificin A (1)
- Figure S12** HPLC trace Ammonificin B (2)
- Figure S13** Experimental and calculated CD spectra of Ammonificin A (1)
- Figure S14** Experimental and calculated CD spectra of Ammonificin A (1) 3*R*, 4*S*, 9*R* and Ammonificin A (2) 3*R*, 4*R*, 9*S*
- Figure S15** Phylogenetic position of *T. ammonificans* (strain HB-1^T).

Figure S1 400 MHz ^1H NMR spectrum of Ammonificin A (**1**) in $\text{DMSO-}d_6$

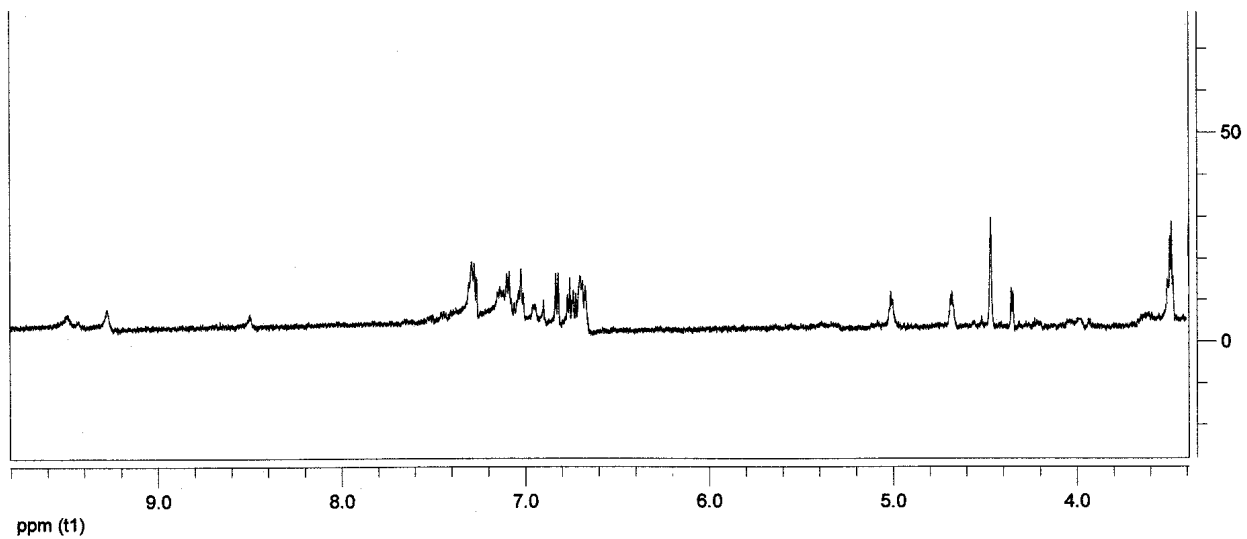


Figure S2 400 MHz ^1H - ^1H COSY spectrum of Ammonificin A (**1**) in $\text{DMSO-}d_6$

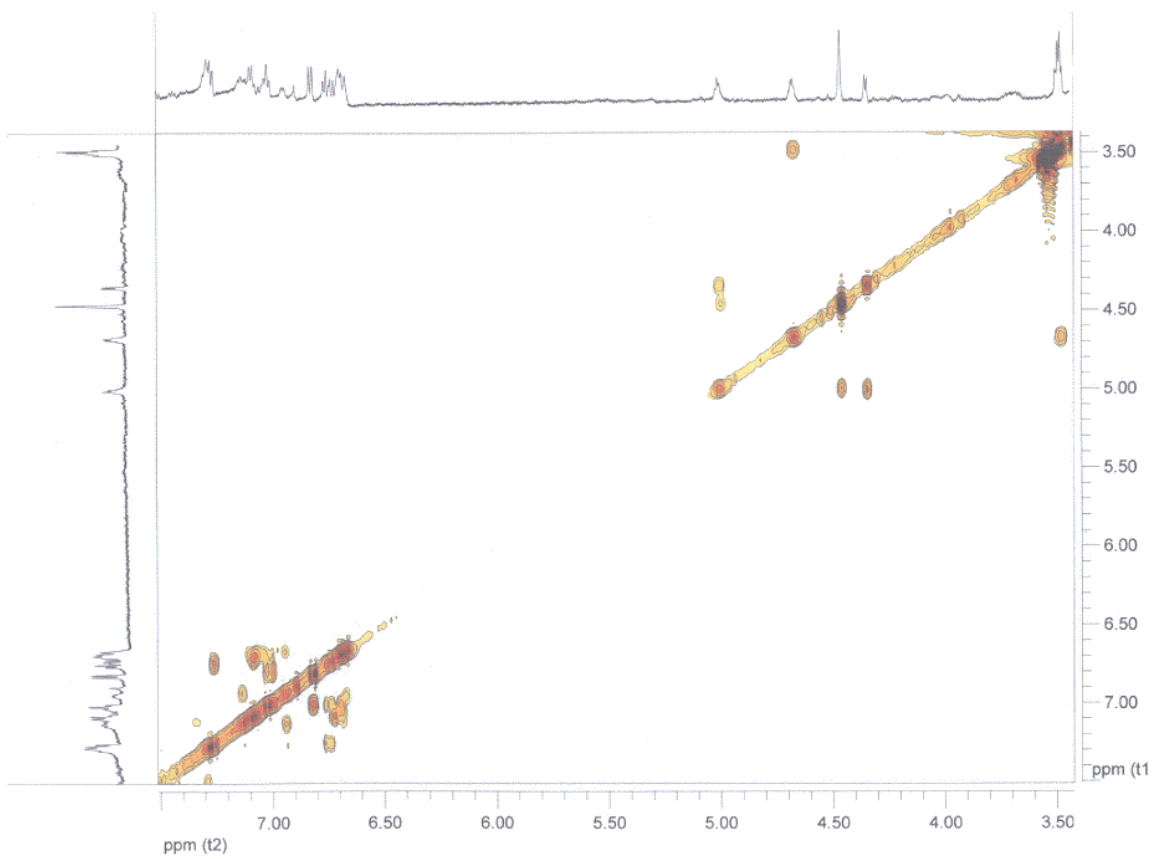


Figure S3 400 MHz ^1H - ^1H COSY spectrum of Ammonificin A (**1**) in $\text{DMSO-}d_6$ (partial view of the aromatic ring region)

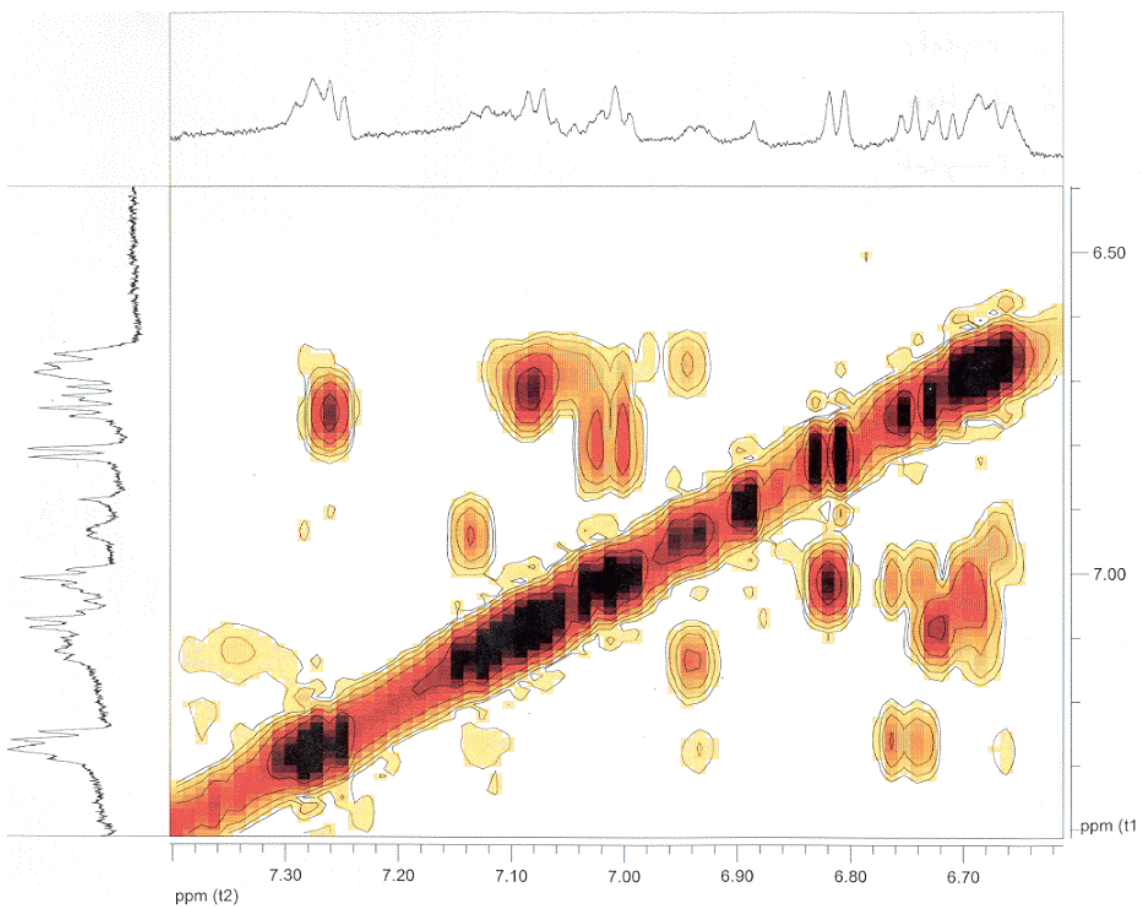


Figure S4 400 MHz ^1H - ^1H COSY spectrum of Ammonificin A (**1**) in $\text{DMSO-}d_6$ (partial view of the dihydropyran moiety and hydroxyethylamine moiety)

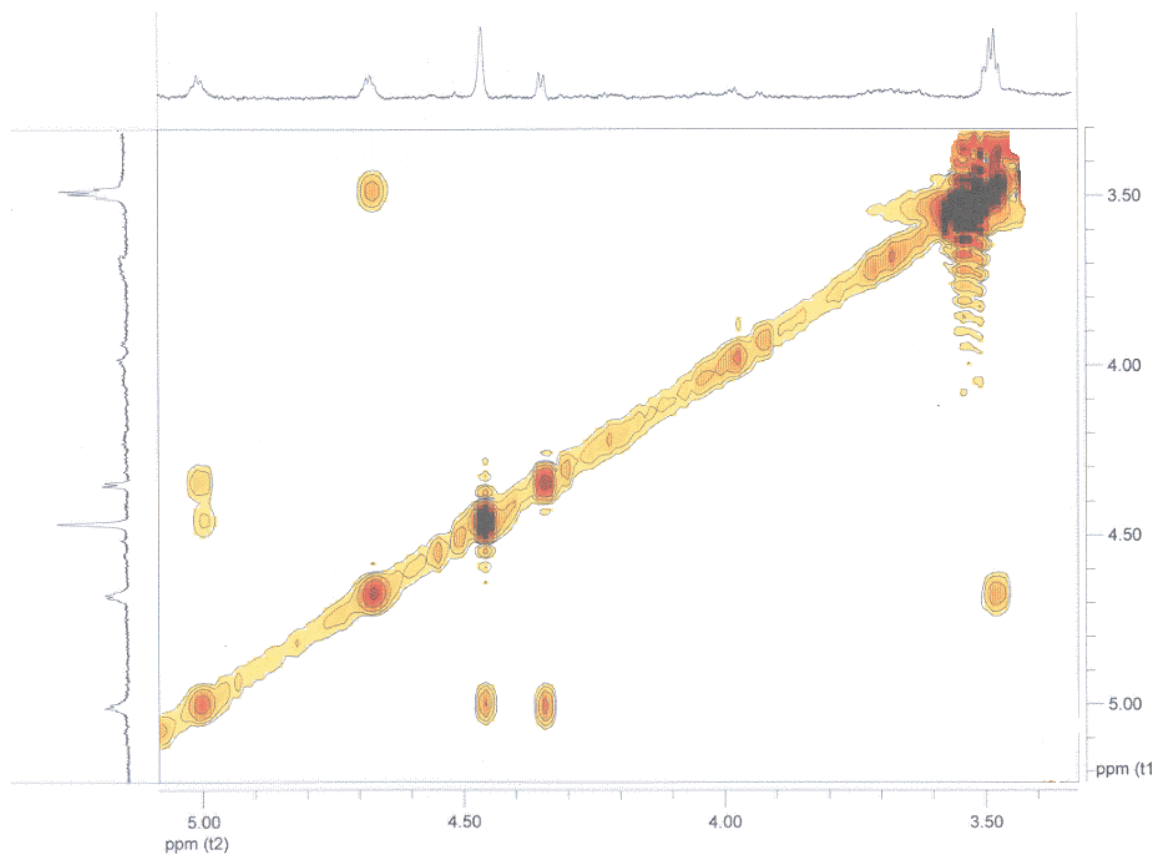


Figure S5 500 MHz HSQC spectrum of Ammonificin A (**1**) in DMSO- d_6 (partial view of the aromatic ring region)

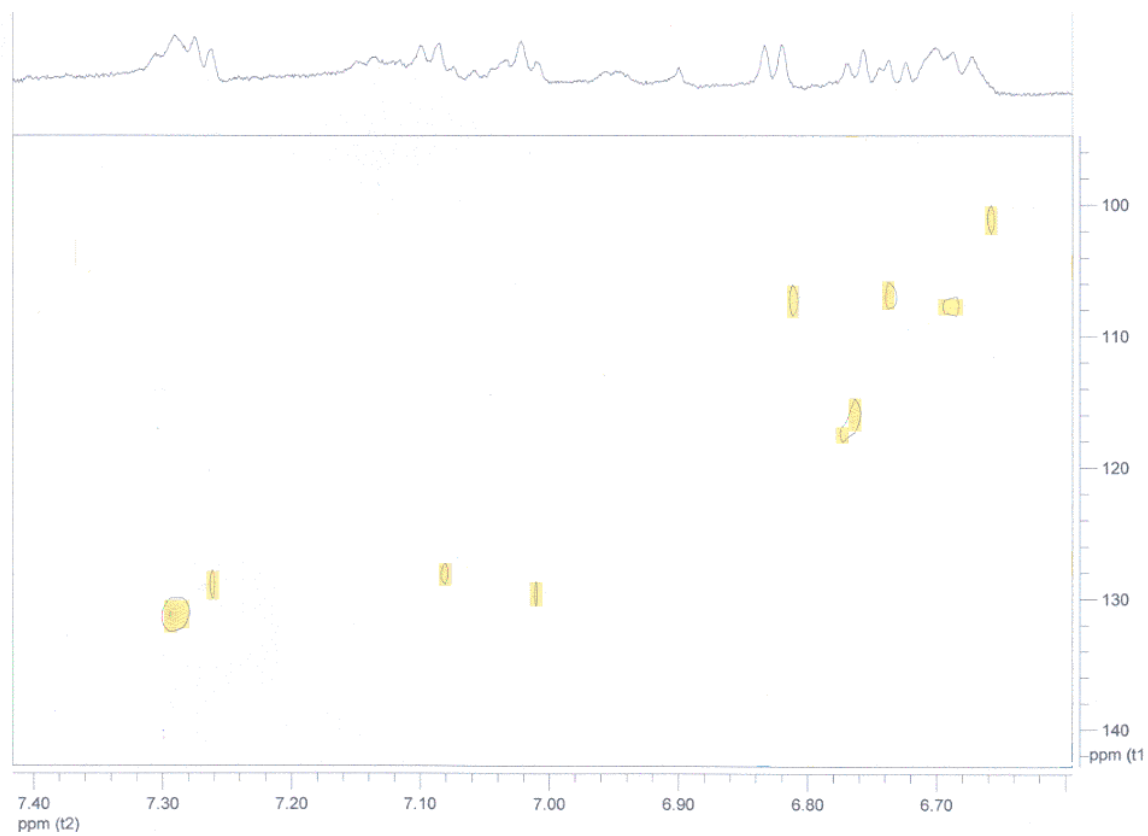


Figure S6 400 MHz HMBC spectrum (optimized for $J = 8\text{Hz}$) of Ammonificin A (1) in $\text{DMSO-}d_6$ (partial view of the aromatic ring region)

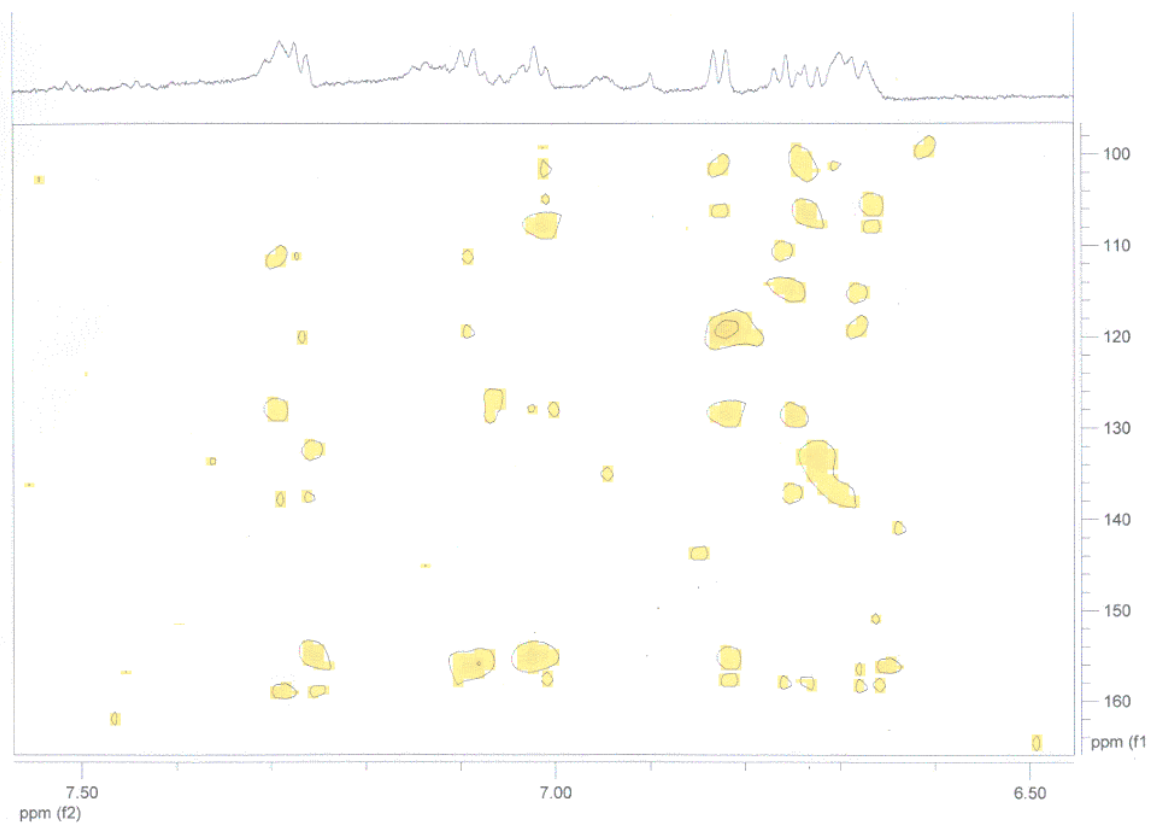


Figure S7 400 MHz HMBC spectrum (optimized for $J = 8\text{Hz}$) of Ammonificin A (**1**) in $\text{DMSO-}d_6$ (partial view of the dihydropyran moiety and hydroxyethylamine moiety)

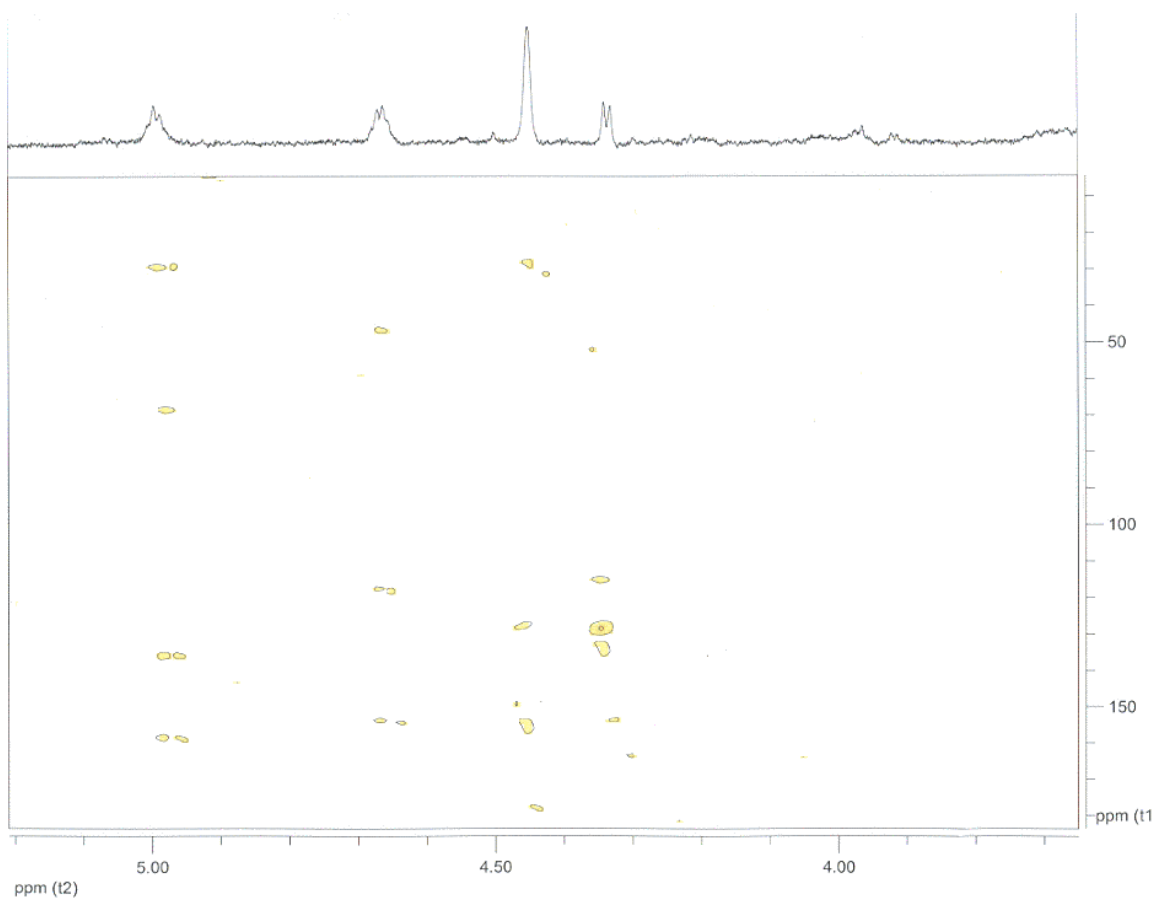


Figure S8 LR-ESI spectrum of Ammonificin A (1)

P1-ACN-positive_080403120024 #321 RT: 1.01 AV: 1 NL: 2.43E4
T: ПMS + c ESI Full ms [150.00-2000.00]

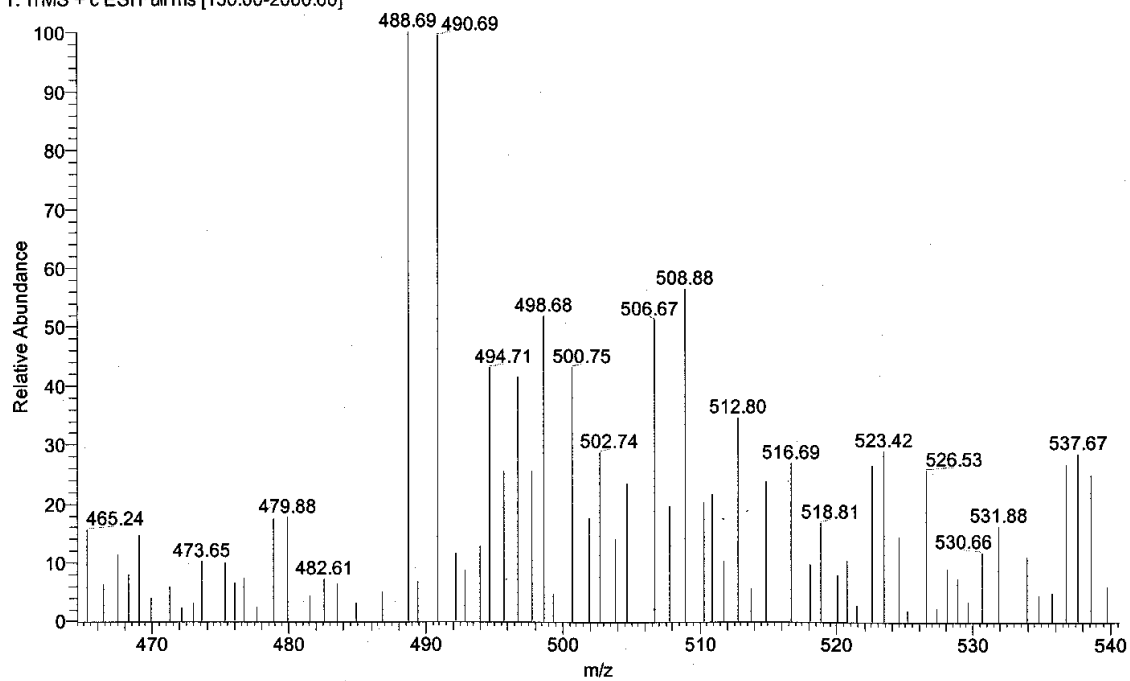


Figure S9 500 MHz ^1H NMR spectrum of Ammonificin B (**2**) in $\text{DMSO-}d_6$

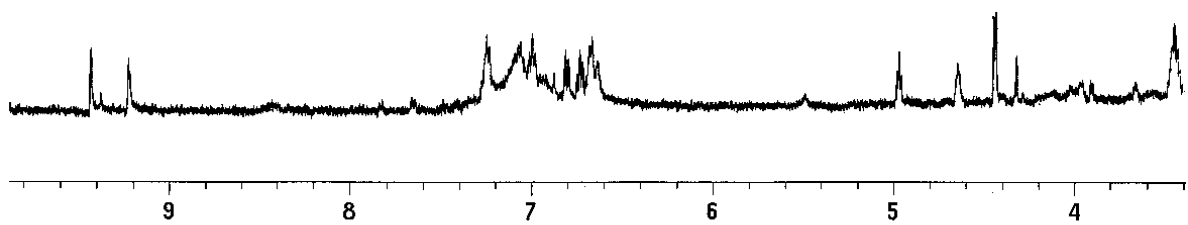


Figure S10 LR-ESI spectrum of Ammonificin B (2)

P1-ACN-positive_080403120024 #321 RT: 1.01 .AV: 1 NL: 4.45E4
T: ITMS + c ESI Full ms [150.00-2000.00]

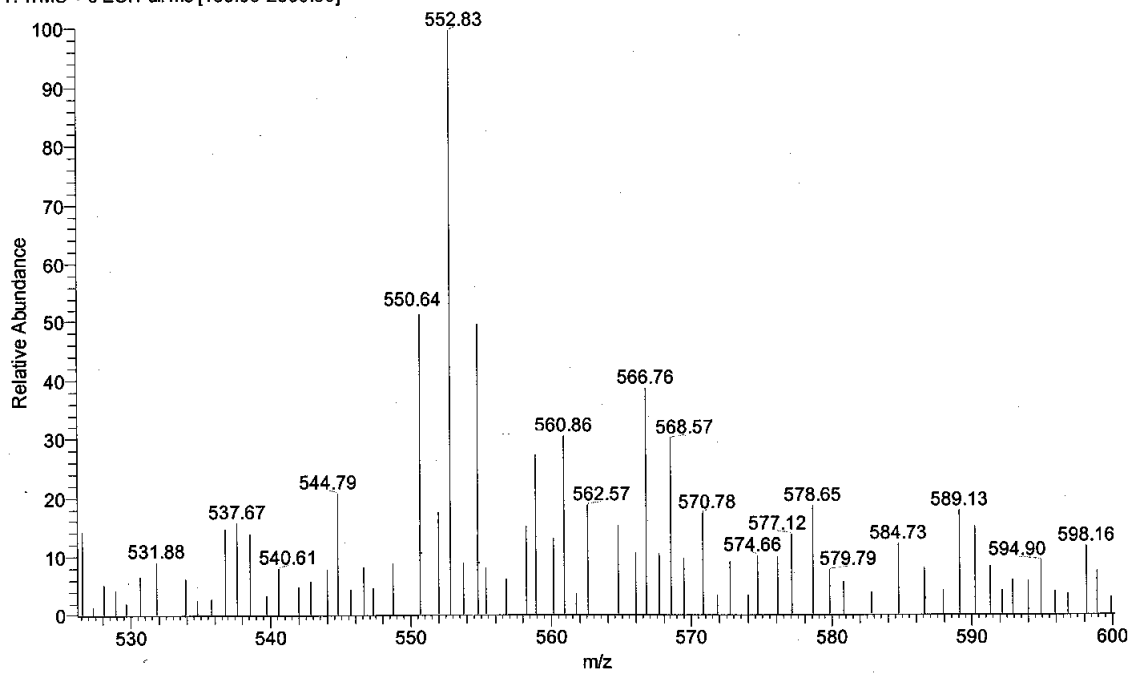


Figure S11 HPLC trace Ammonificin A (1)

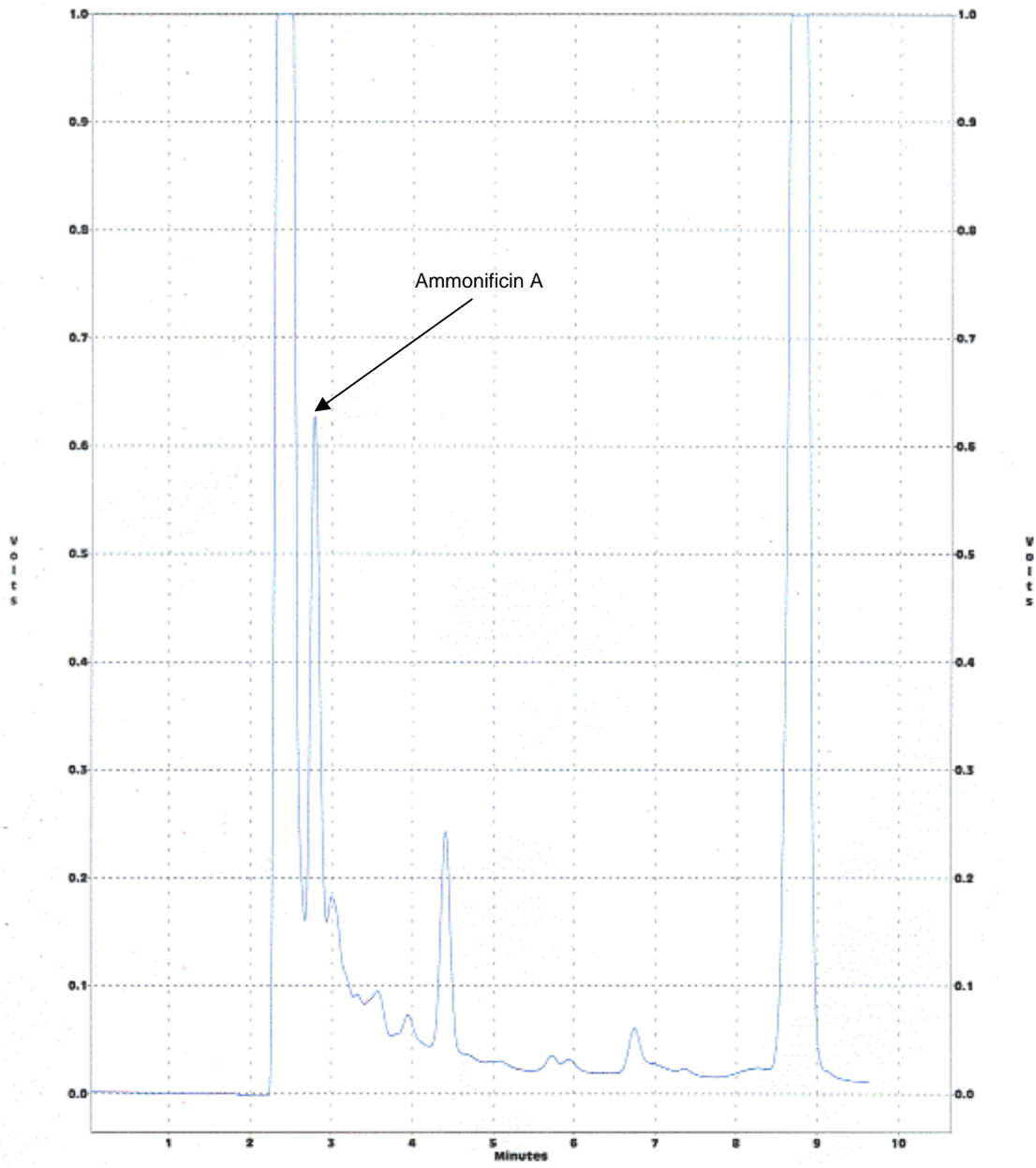


Figure S12 HPLC trace Ammonificin B (2)

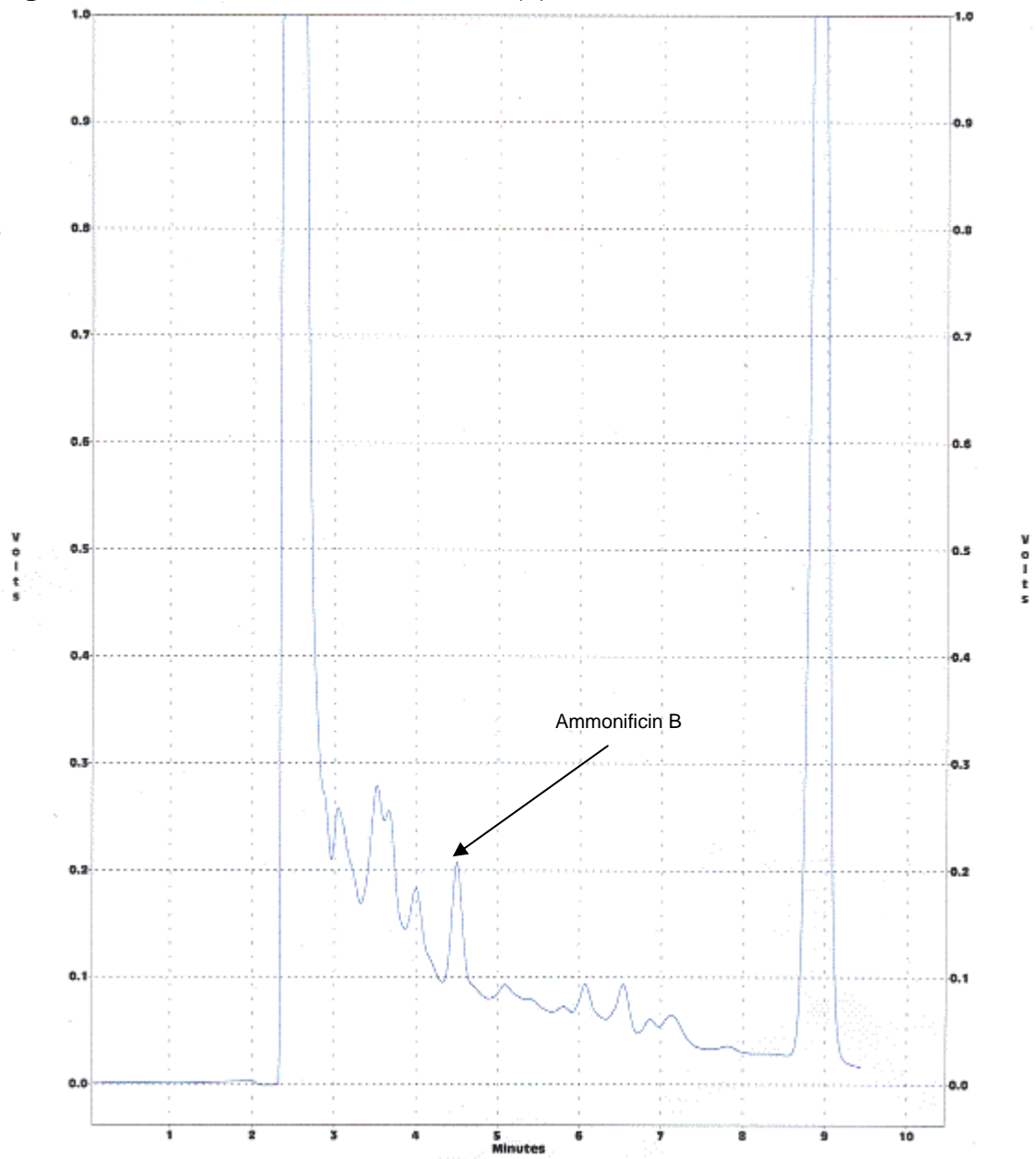
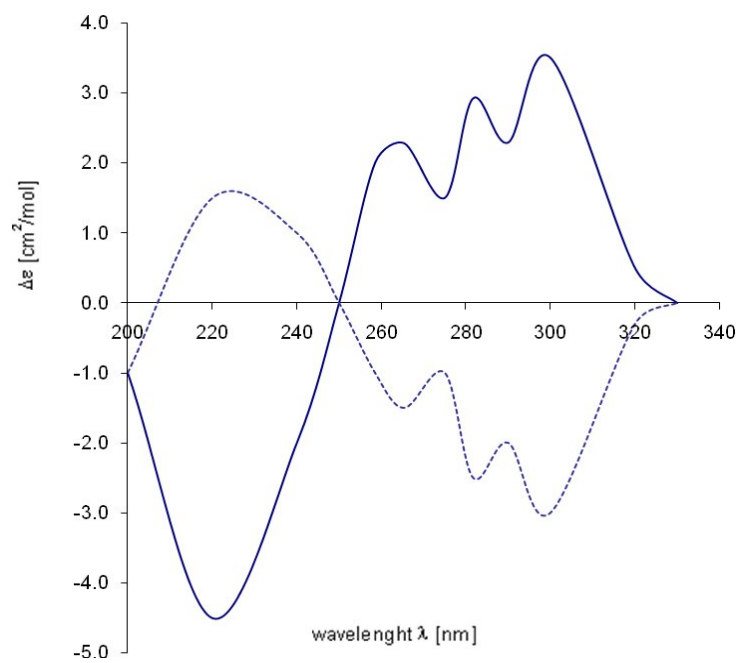
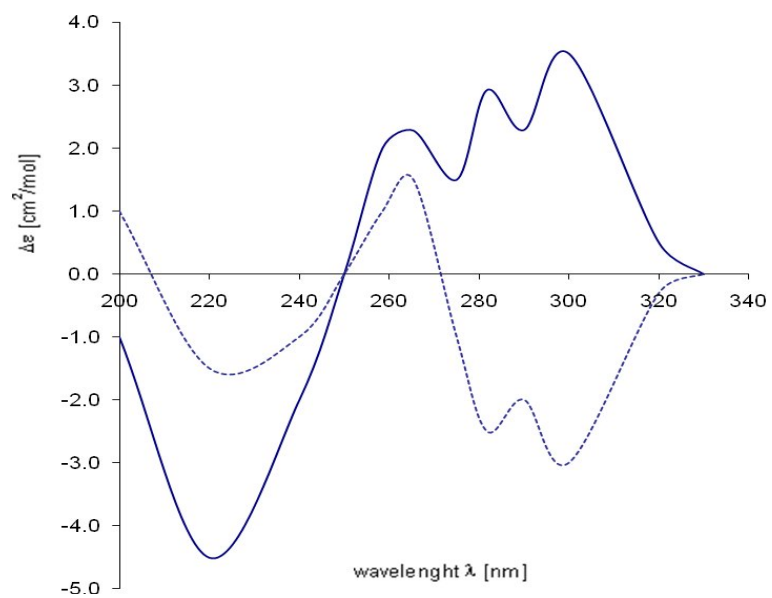


Figure S13 Experimental and calculated CD spectra of Ammonificin A (1)

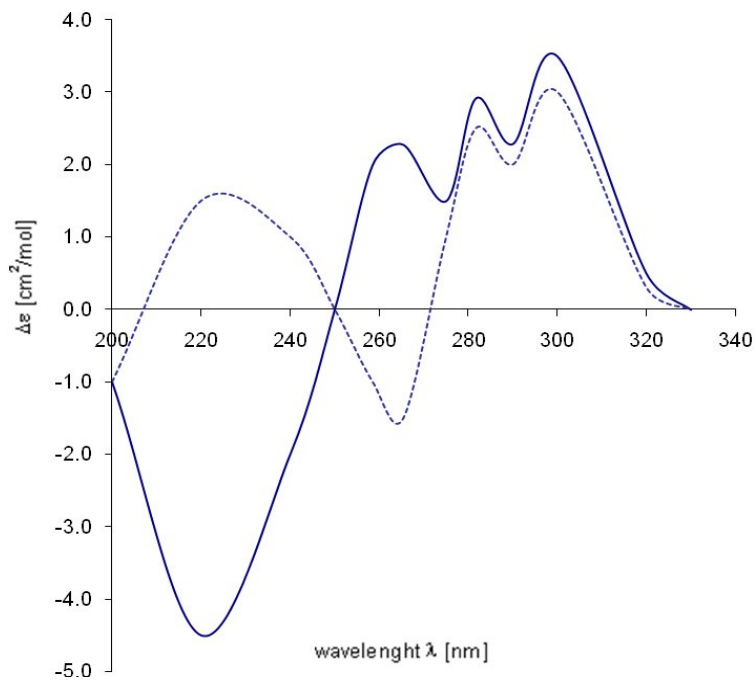


3R, 4R, 9S

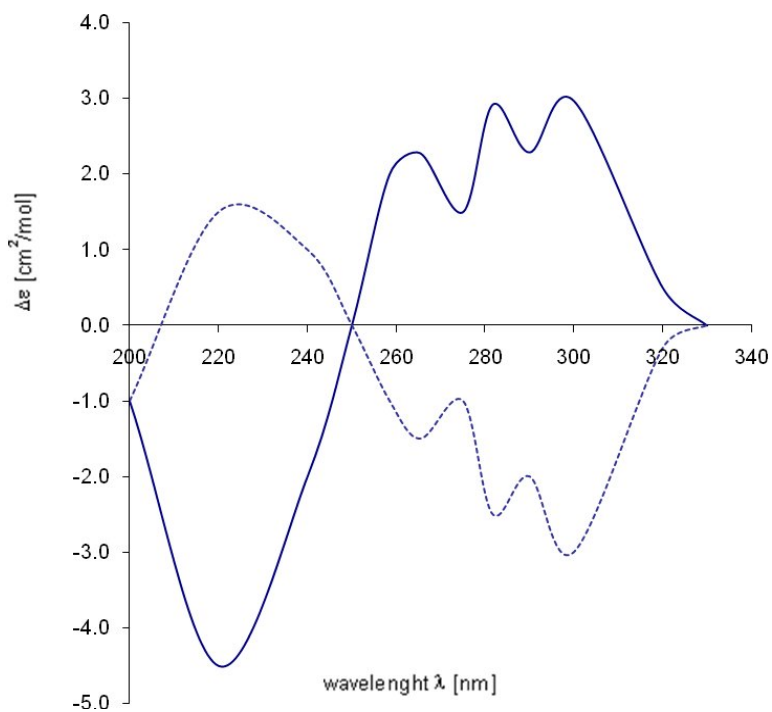


3S, 4R, 9S

Figure S14 Experimental and calculated CD spectra of Ammonificin A (**1**) 3*R*, 4*S*, 9*R* and Ammonificin A (**2**) 3*R*, 4*R*, 9*S*



3*R*, 4*S*, 9*R* for (**1**)



3*R*, 4*R*, 9*S* for (**2**)

Figure S15 Phylogenetic position of *T. ammonificans* (strain HB-1^T).

