

Supplementary Materials

Marine organisms from the Yucatan Peninsula (Mexico) as a potential natural source of antibacterial compounds

Dawrin Pech-Puch ¹, Mar Pérez-Povedano ¹, Patricia Gómez ², Marta Martínez-Guitián ³, Cristina Lasarte-Monterrubio ³, Juan Carlos Vázquez-Ucha ³, María Lourdes Novoa-Olmedo ³, Sergio Guillén-Hernández⁴, Harold Villegas-Hernández⁴, Germán Bou ³, Jaime Rodríguez ^{1,*}, Alejandro Beceiro ³ and Carlos Jiménez ^{1,*}

¹ Centro de Investigaciones Científicas Avanzadas (CICA) e Departamento de Química, Facultad de Ciencias, AE CICA-INIBIC, Universidade da Coruña, 15071 A Coruña, Spain. dawrin.j.pech@udc.es (D.P.-P.); perezpovedanomaranabel@gmail.com (M.P.-P.)

² Unidad Académica de Ecología y Biodiversidad Acuática, Instituto de Ciencias del Mar y Limnología, Universidad Nacional Autónoma de México, 04510, CDMX, México. patricia@cmarl.unam.mx (P.G.)

³ Servicio de Microbiología. Instituto de Investigación Biomédica AE CICA-INIBIC, Complejo Hospitalario Universitario A Coruña, 15006, A Coruña, Spain. m.martinez.guitian@gmail.com (M.M.-G.); crlasarm@gmail.com (C.L.-M.); juan.vazquez@udc.es (J.C.V.-U.) marianovoa@usb.ve (M.L.N.-O.); German.Bou.Arevalo@sergas.es (G.B.); Alejandro.Beceiro.Casas@sergas.es (A.B.)

⁴ Departamento de Biología Marina. Campus de Ciencias Biológicas y Agropecuarias. Universidad Autónoma de Yucatán. Carretera Mérida-Xmatkuil Km. 15.5, C.P. 97000, Mérida, Yucatán, México. ghernand@correo.uady.mx (M.G.-H.); harold.villegas@correo.uady.mx (H.V.-H.)

* Correspondence: jaime.rodriguez@udc.es (J.R.); carlos.jimenez@udc.es, (C.J.)

INDEX

Figure S1. Chromatogram of fraction R4 of <i>Amphimedon compressa</i>	S3
Figure S2-S3. NMR spectra data of subfraction R4H2 in CD ₃ OD.....	S4
Figure S4. Chromatogram of fraction R2 of <i>Agelas citrina</i>	S5
Figure S5 (+)-HRESIMS of (-)-agelasine B	S6
Figure S6-S7. NMR spectra data of (-)-agelasine B in DMSO-d ₆	S7
Table S1. Description of bacterial type strains used.....	S8
Table S2. MICs of antibiotics against bacterial pathogens.....	S9

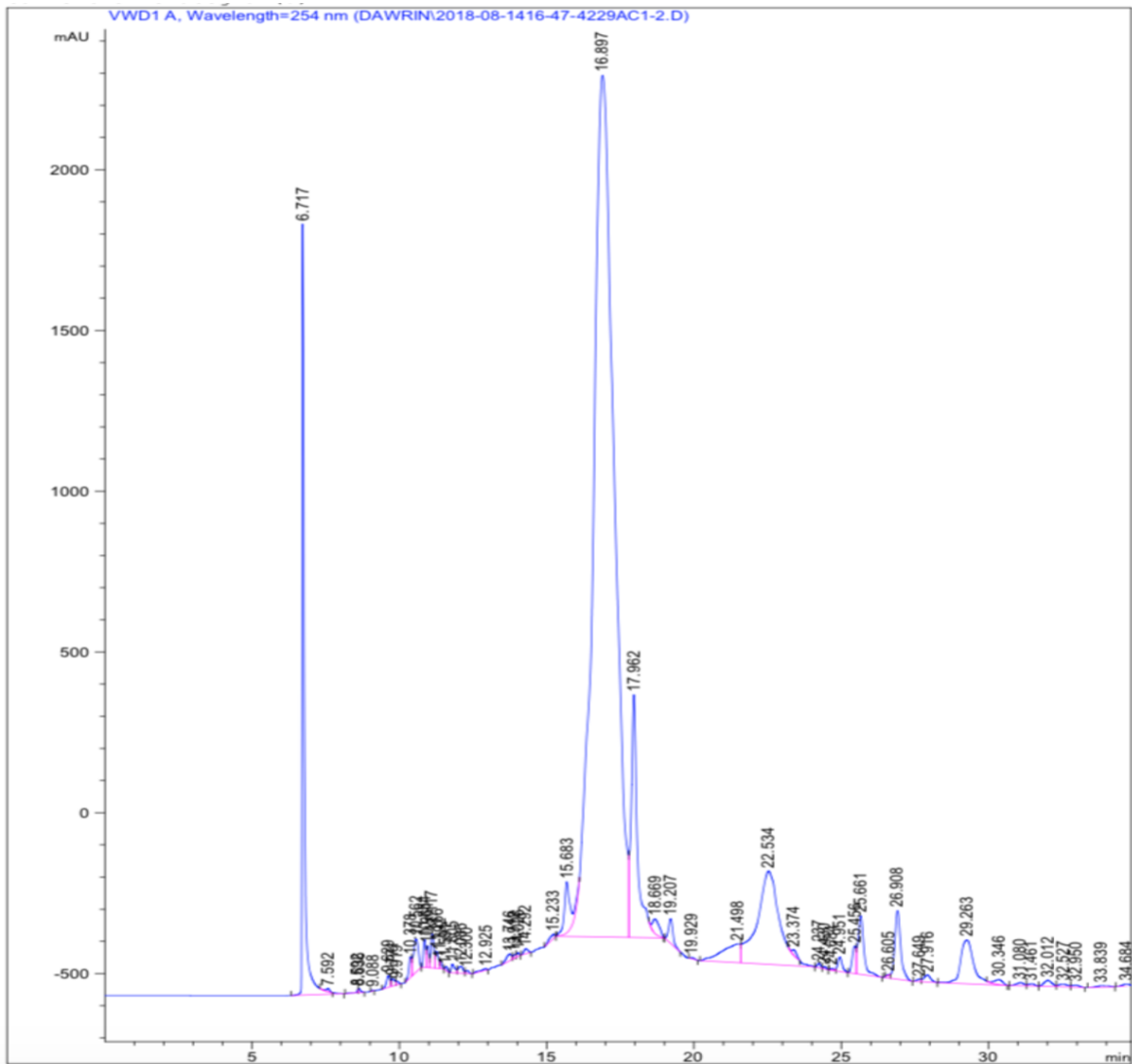


Figure S1. RP-HPLC chromatogram of the SPE fraction R4 from the sponge *Amphimedon compressa*.

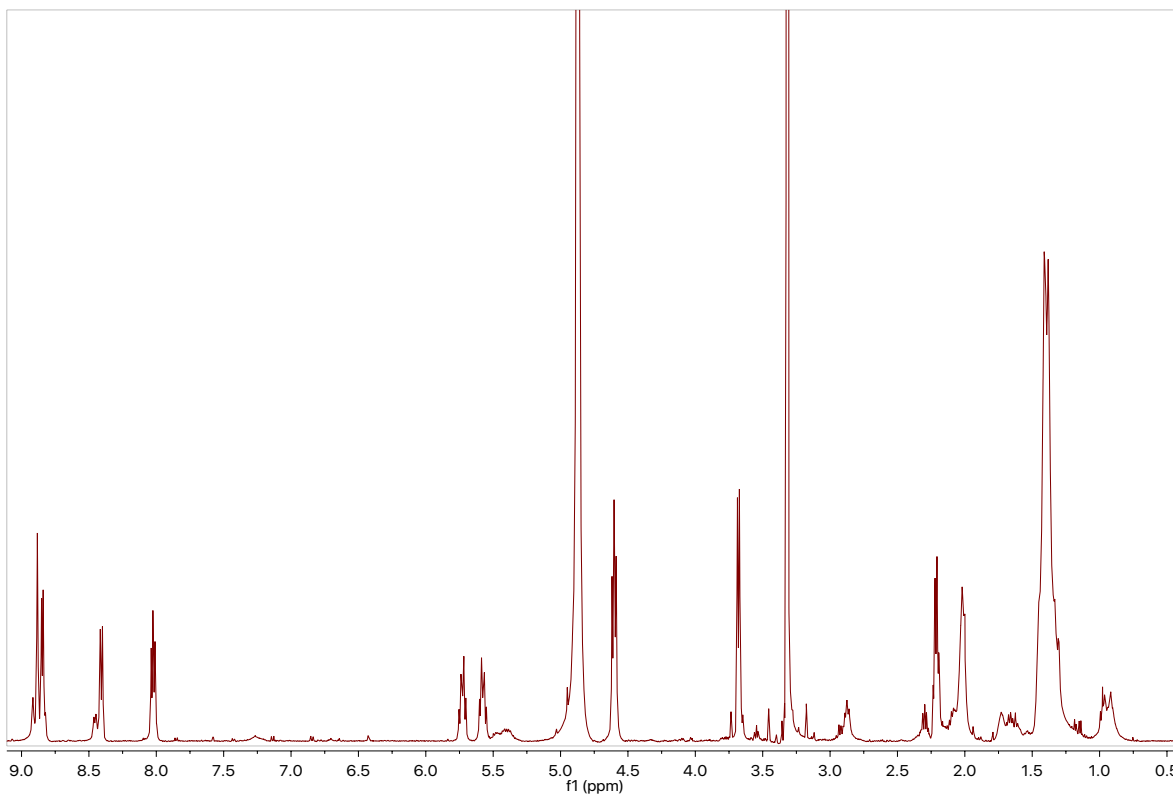


Figure S2. ^1H NMR spectrum of the R4H2 subfraction (500 MHz, CD_3OD).

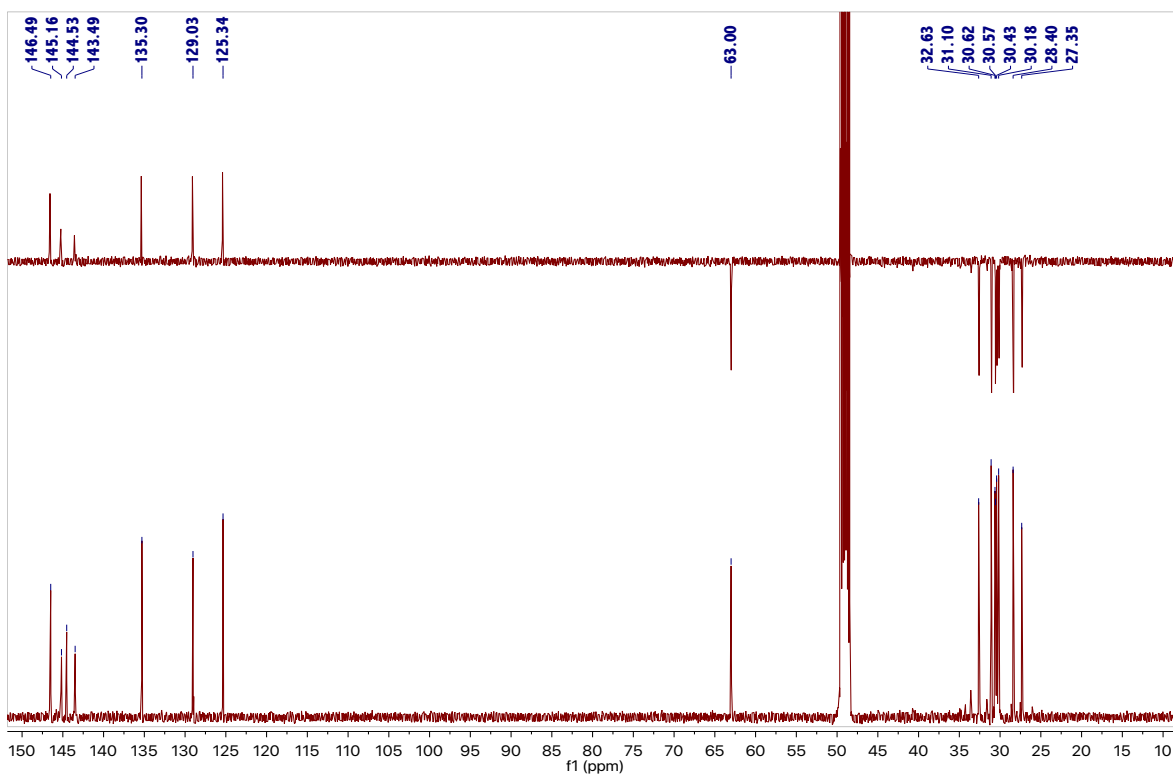


Figure S3. ^{13}C NMR and DEPT-135 spectra of the R4H2 subfraction (125 MHz, CD_3OD).

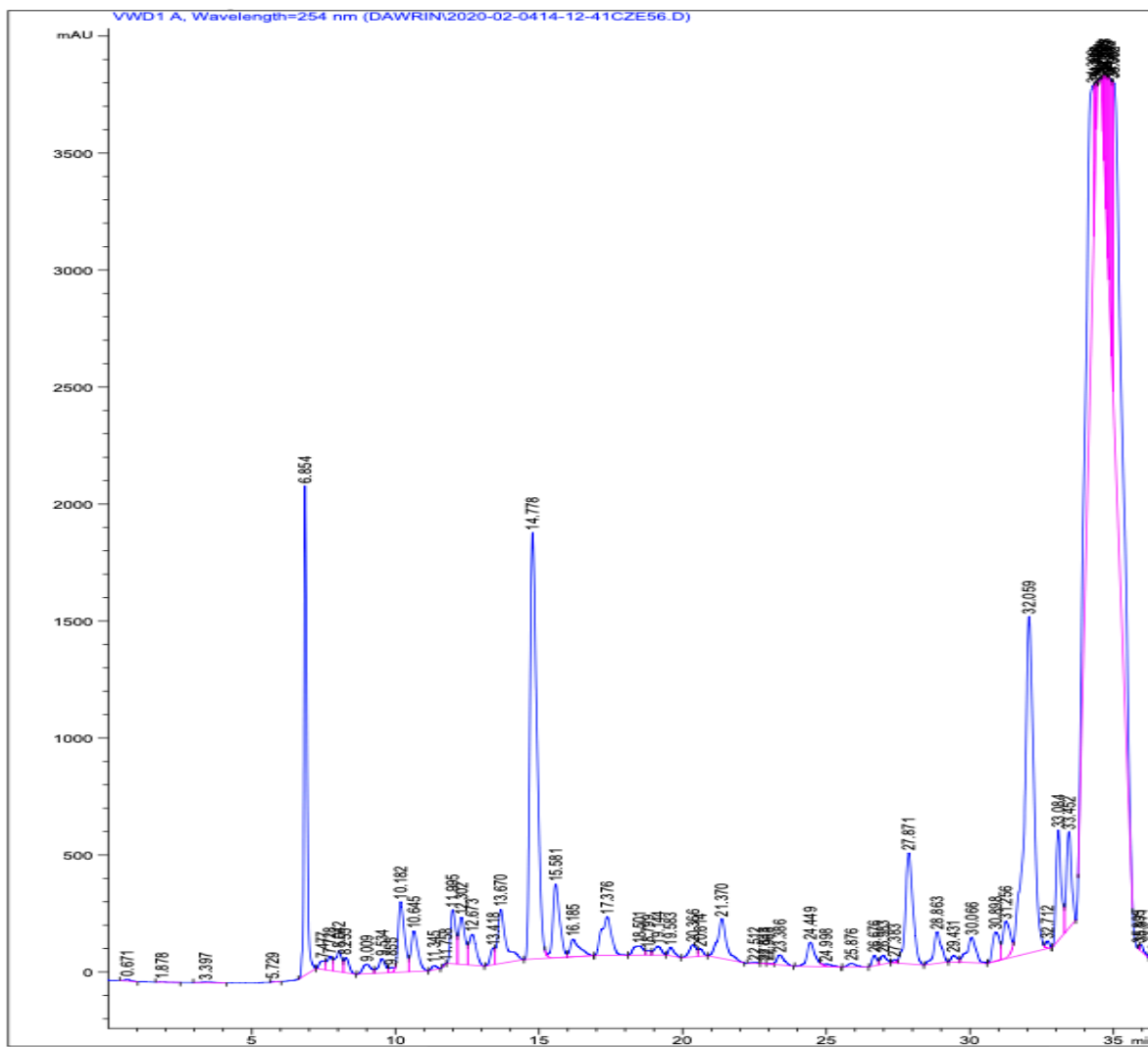


Figure S4. RP-HPLC chromatogram of the SPE subfraction R2 from the sponge *Agelas citrina*.

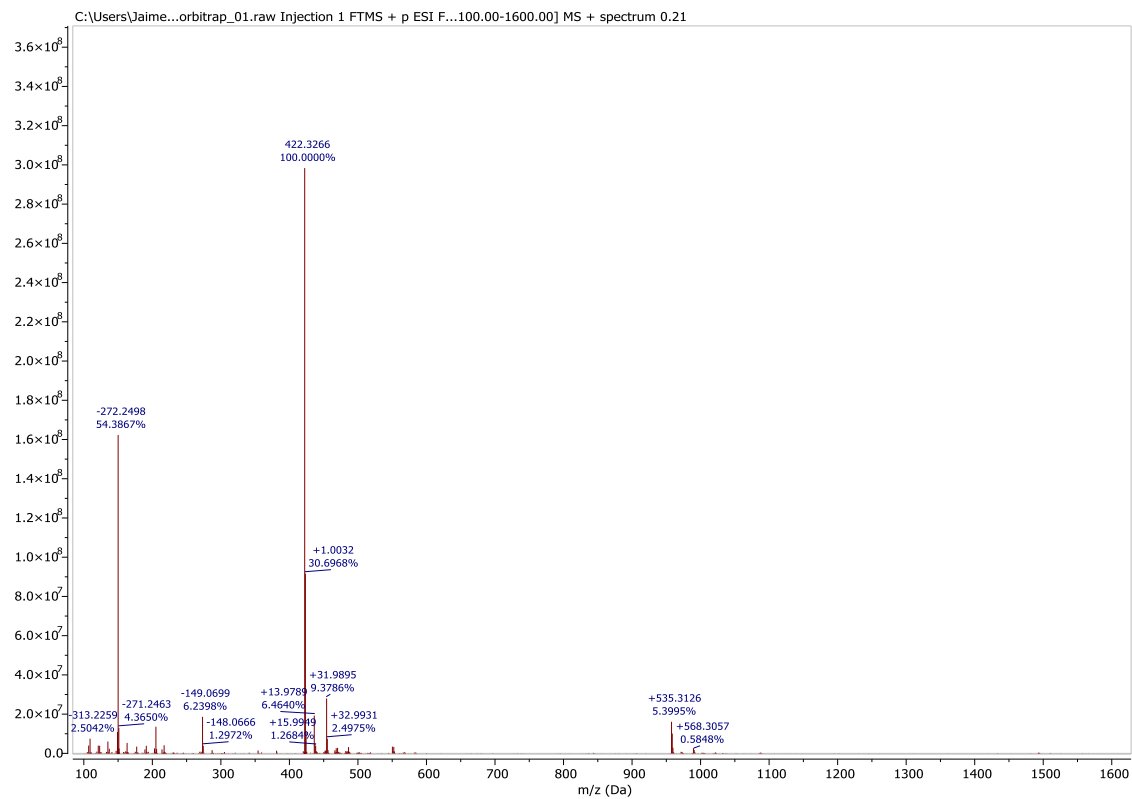


Figure S5. (+)-HRESIMS of agelasine B.

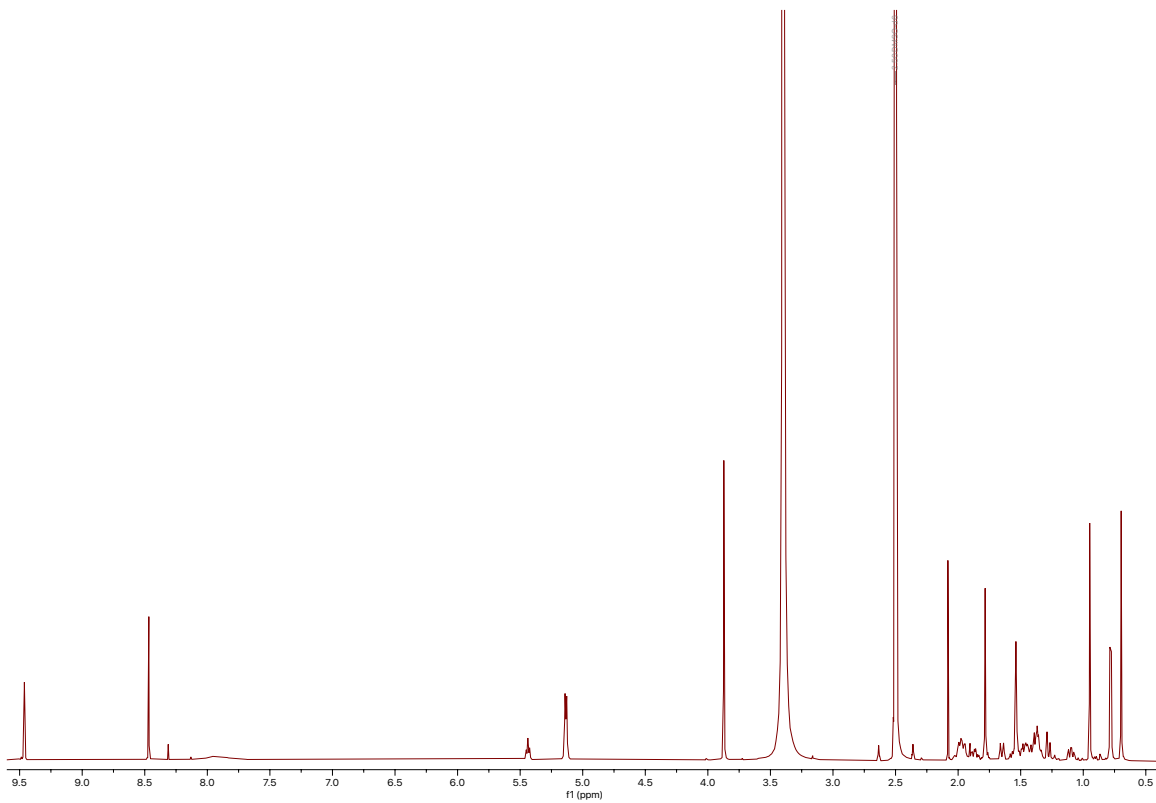


Figure S6. ^1H NMR spectrum of agelasine B (500 MHz, DMSO- d_6).

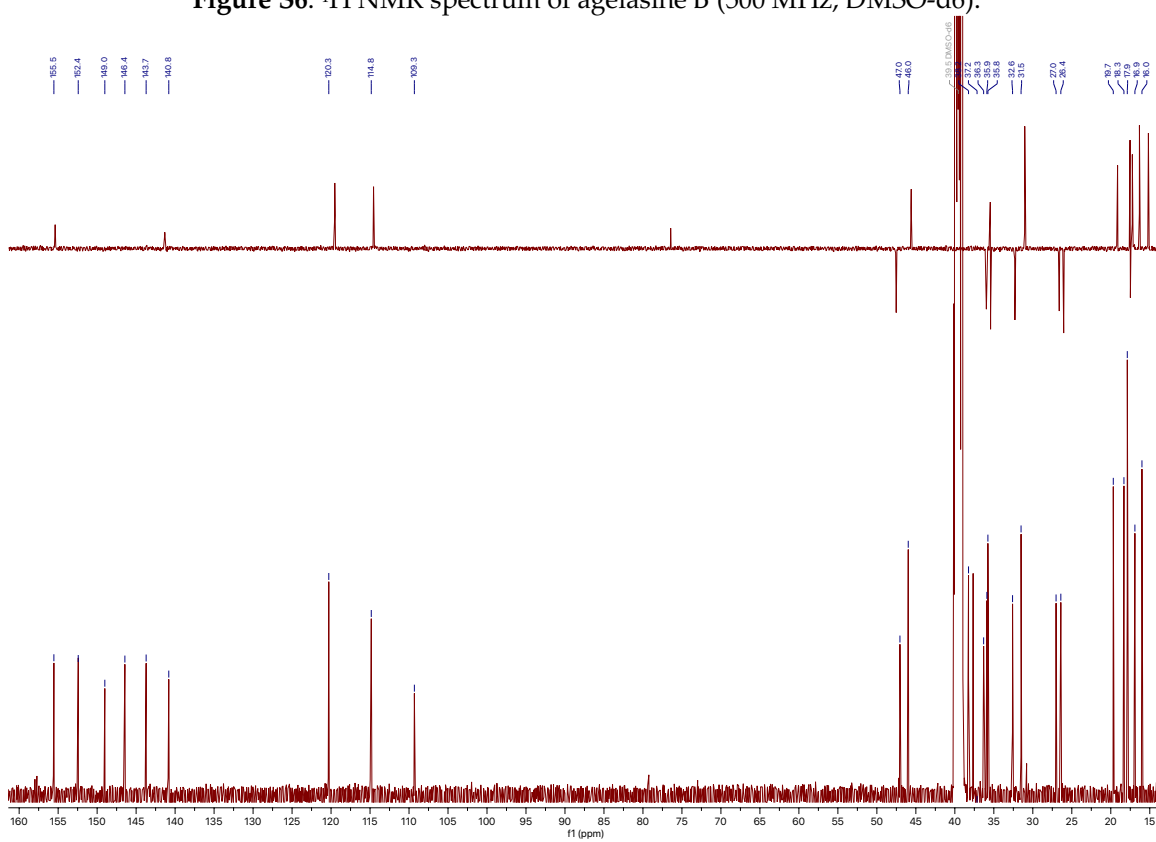


Figure S7. ^{13}C NMR and DEPT-135 spectra of agelasine B (125 MHz, DMSO- d_6).

Table S1. Description of bacterial type strains used.

Bacterial sp.	Strains	Description
<i>A. baumannii</i>	ATCC ^a 17978 ABRIM (clinical isolate)	Gram-negative rod-shaped bacterium, can produce pneumonia, blood infections, wound and surgical site infections and urinary tract infections. ¹
<i>K. pneumoniae</i>	ATCC 700603 Kp3380 (clinical isolate)	Gram-negative rod-shaped encapsulate bacterium, produces pneumonia, urinary tract infections, sepsis, meningitis, diarrhea, and soft tissue infections ²
<i>P. aeruginosa</i>	ATCC 27853 PAO1 (reference strain)	Gram-negative, encapsulated, rod-shaped bacterium. Infects the airway, urinary tract, burns and wounds, and also causes other blood infections. ³
<i>S. aureus</i>	ATCC 29213 USA LAC 300 (clinical isolate)	Gram-positive, round-shaped bacterium, one of the most common causes of bacteraemia and infective endocarditis and can also cause various skin and soft-tissue infections. ⁴

^a American Type Culture Collection

¹ Antunes, L.C.S.; Visca, P.; Towner, K.J. *Acinetobacter baumannii*: evolution of a global pathogen. *Pathog. Dis.* **2014**, *71*, 292-301

² Podschun, R.; Ullmann, U. *Klebsiella* spp. as Nosocomial Pathogens: Epidemiology, Taxonomy, Typing Methods, and Pathogenicity Factors. *Clin. Microbiol. Rev.* **1998**, *11*, 589–603.

³ Bassetti, M.; Vena, A.; Croxatto, A.; Righi, E.; Guery, B. How to manage *Pseudomonas aeruginosa* infections. *Drugs in Context* **2018**, *7*, 1–18.

⁴ Tong, S.Y.C.; Davis, J.S.; Eichenberger, E.; Holland, T.L.; Fowler, V.G. *Staphylococcus aureus* Infections: Epidemiology, Pathophysiology, Clinical Manifestations, and Management. *Clin. Microbiol. Rev.* **2015**, *28*, 603–661.