

Supporting information

Catenulobactins A and B, Heterocyclic Peptides from Culturing *Catenuloplanes* sp. with Mycolic Acid-containing Bacterium

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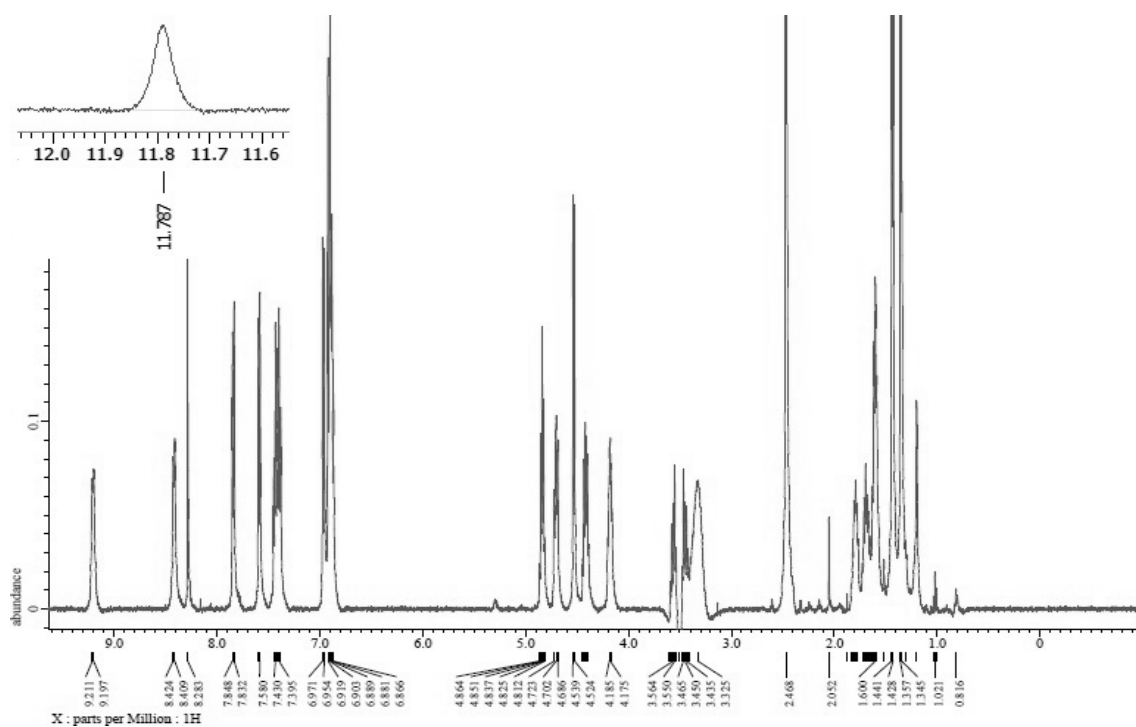


Figure S1. ¹H NMR spectrum of **1** (500 MHz, *d*₆-DMSO)

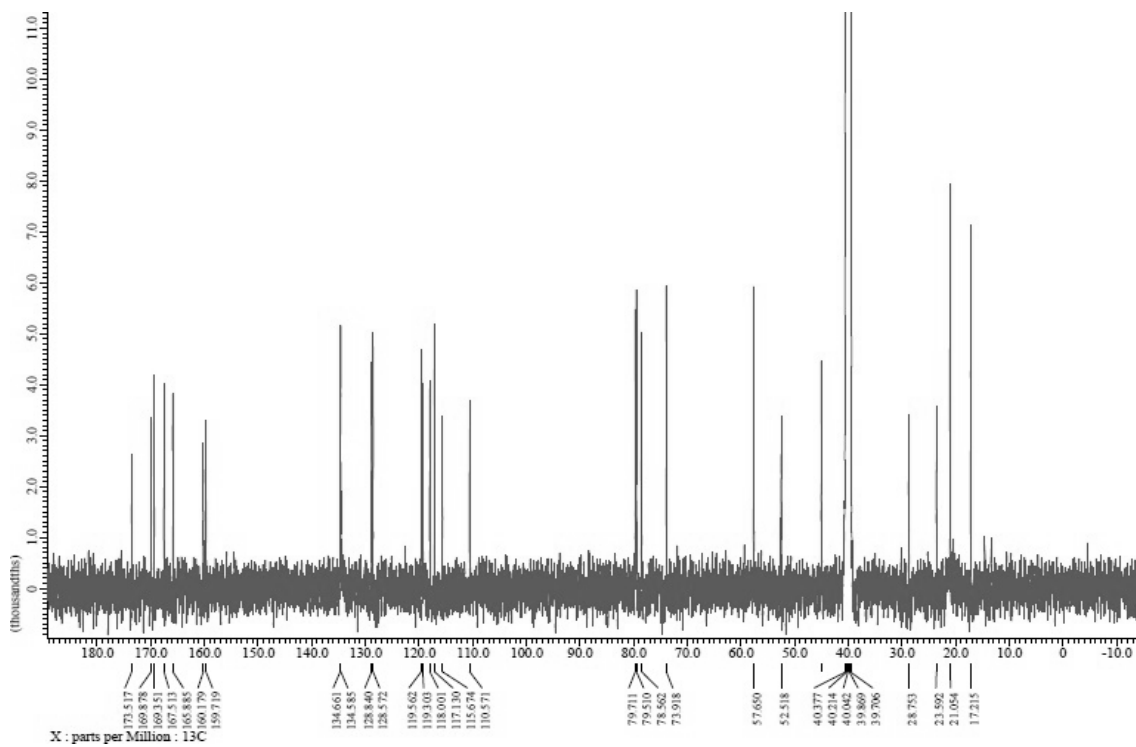


Figure S2. ¹³C NMR spectrum of **1** (500 MHz, *d*₆-DMSO)

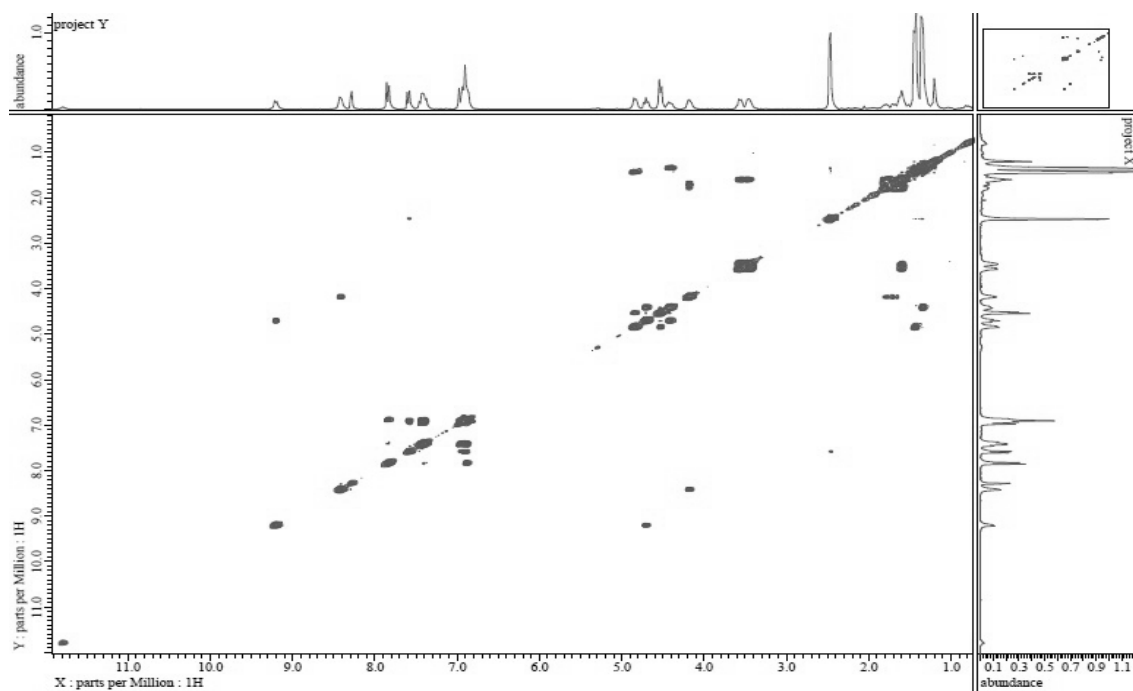


Figure S3. COSY spectrum of **1** (500 MHz, d_6 -DMSO)

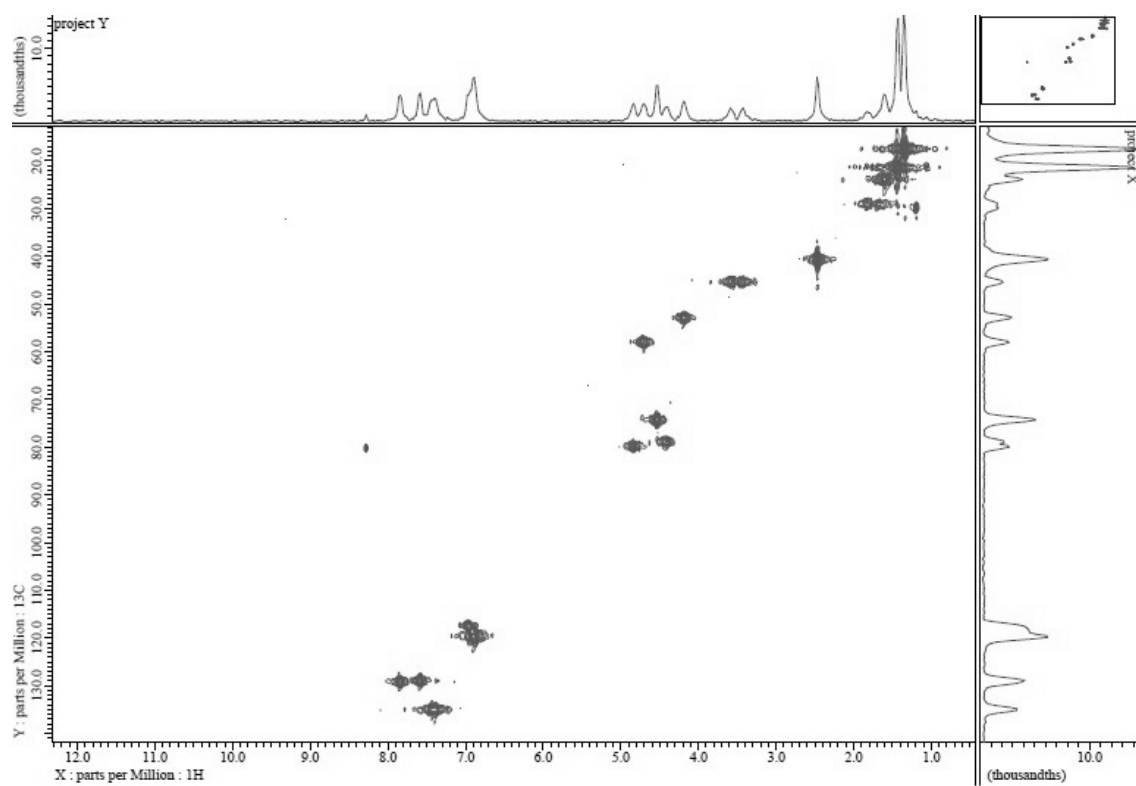


Figure S4. HMQC spectrum of **1** (500 MHz, d_6 -DMSO)

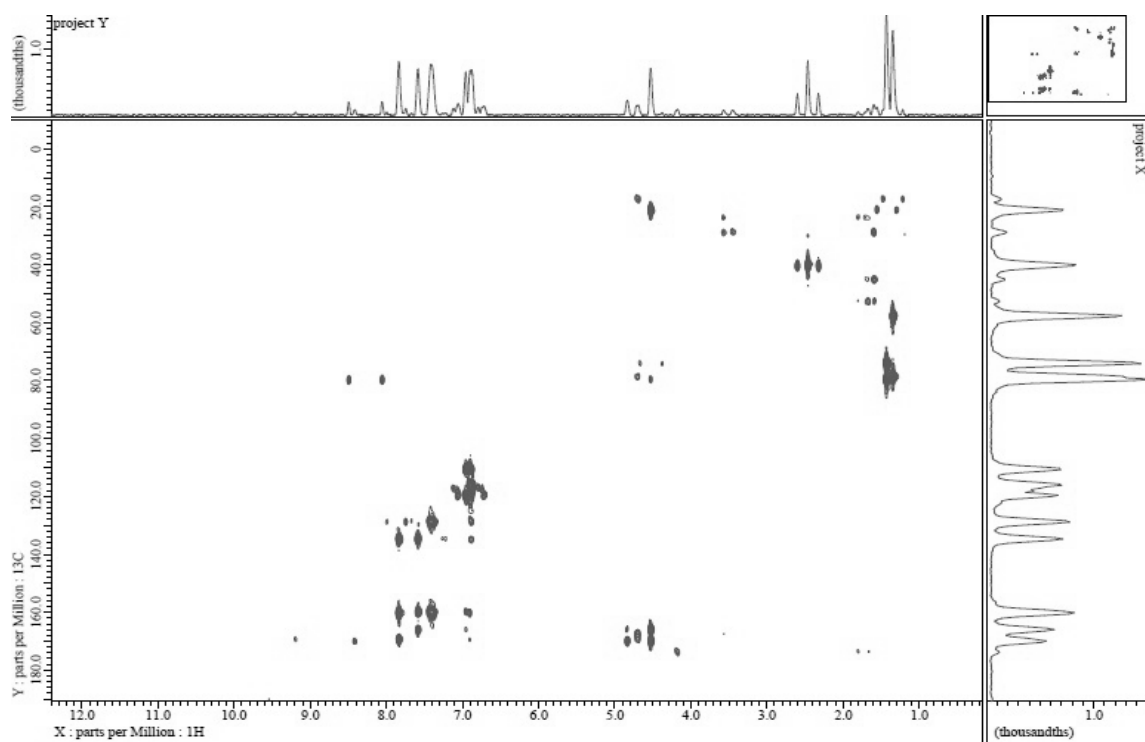


Figure S5. HMBC NMR spectrum of **1** (500 MHz, d_6 -DMSO)

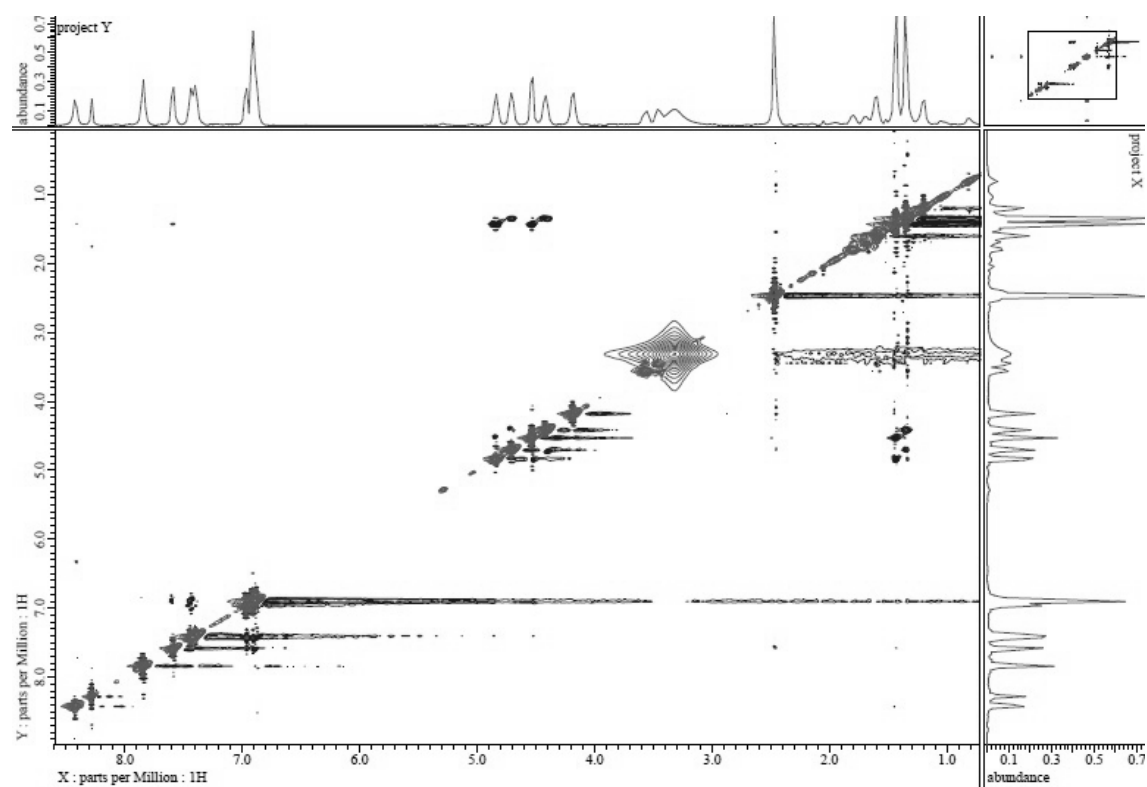


Figure S6. NOESY spectrum of **1** (500 MHz, d_6 -DMSO)

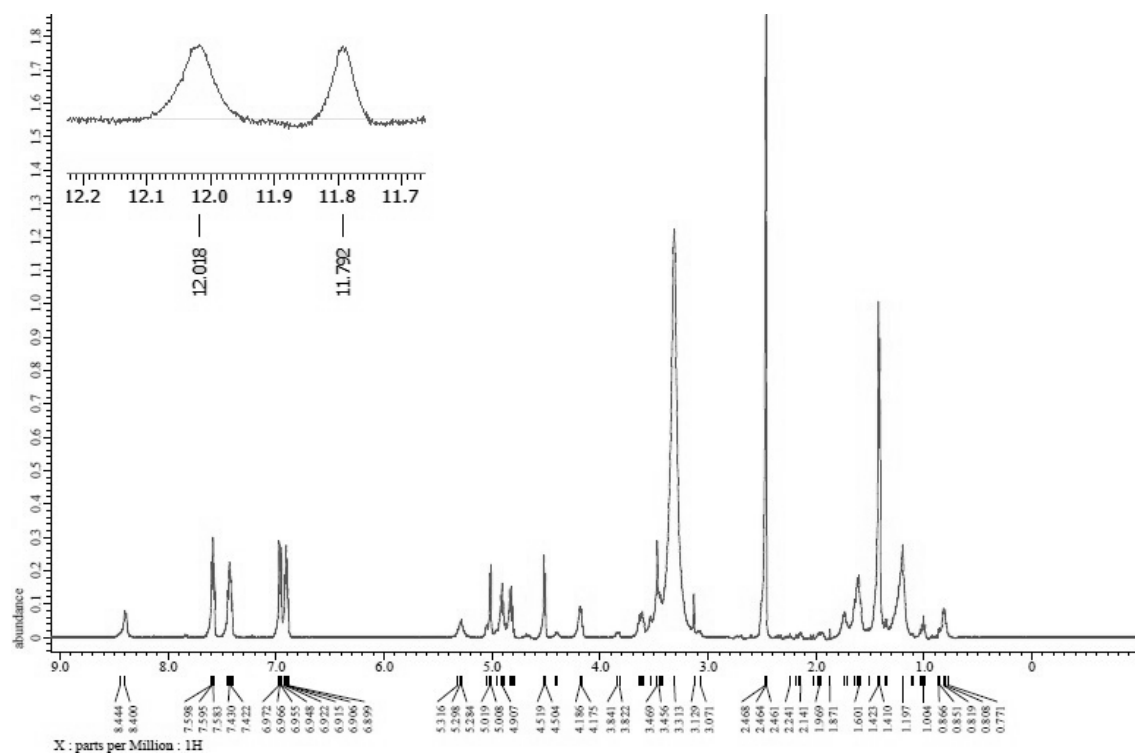


Figure S7. ¹H NMR spectrum of **2** (500 MHz, *d*₆-DMSO)

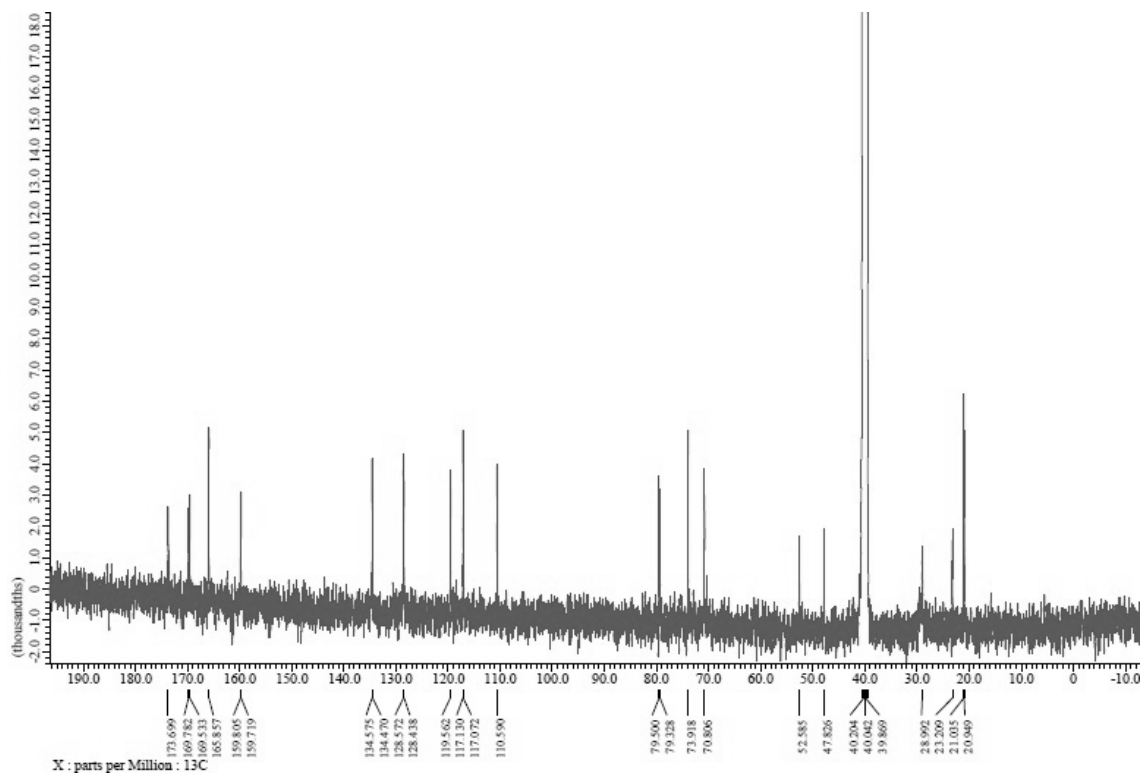


Figure S8. ¹³C NMR spectrum of **1** (500 MHz, *d*₆-DMSO)

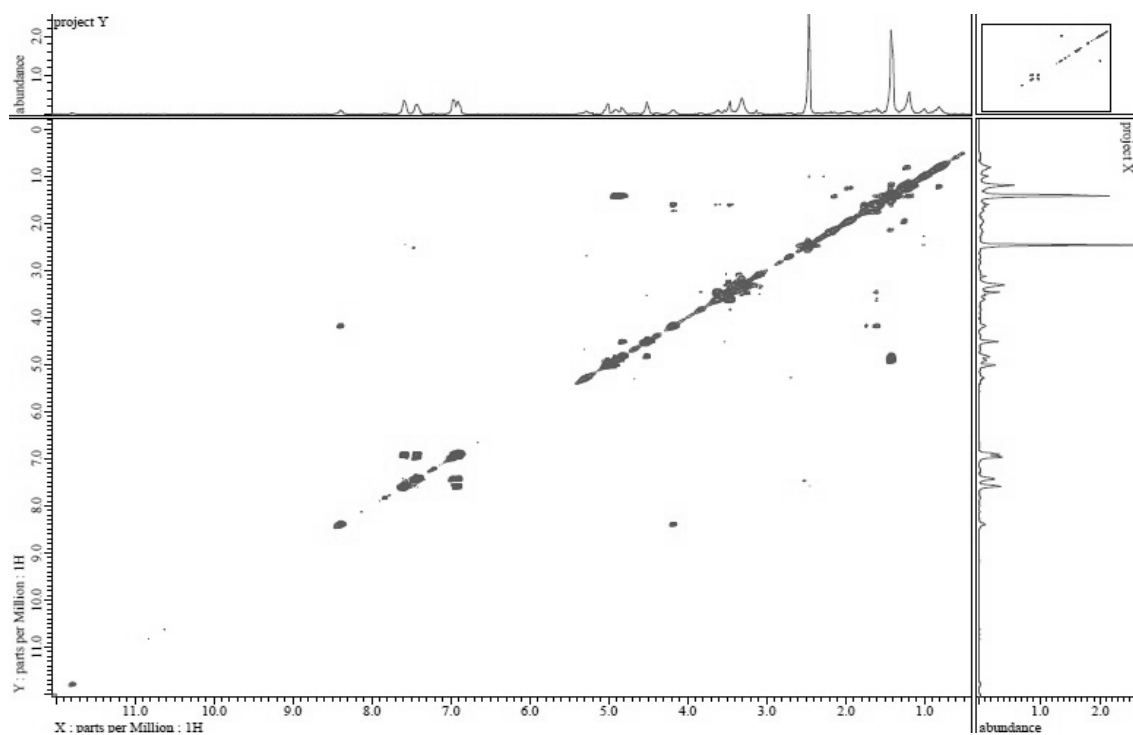


Figure S9. COSY spectrum of **2** (500 MHz, d_6 -DMSO)

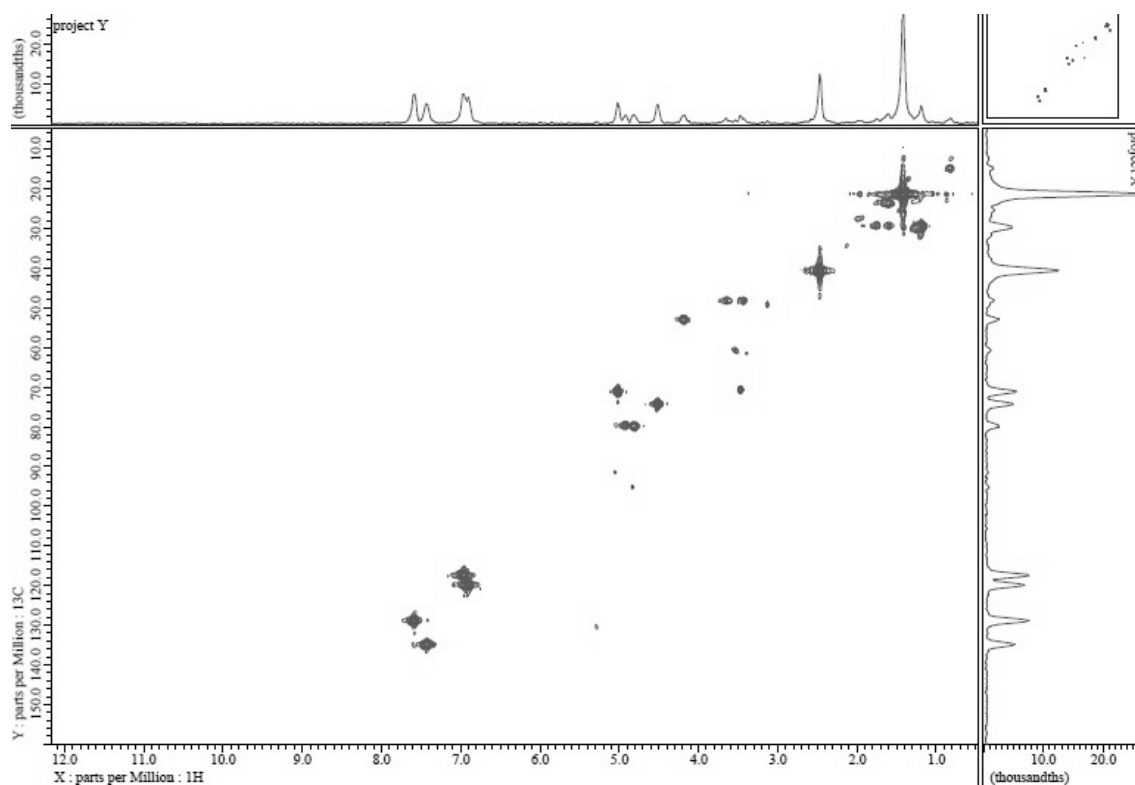


Figure S10. HMQC spectrum of **2** (500 MHz, d_6 -DMSO)

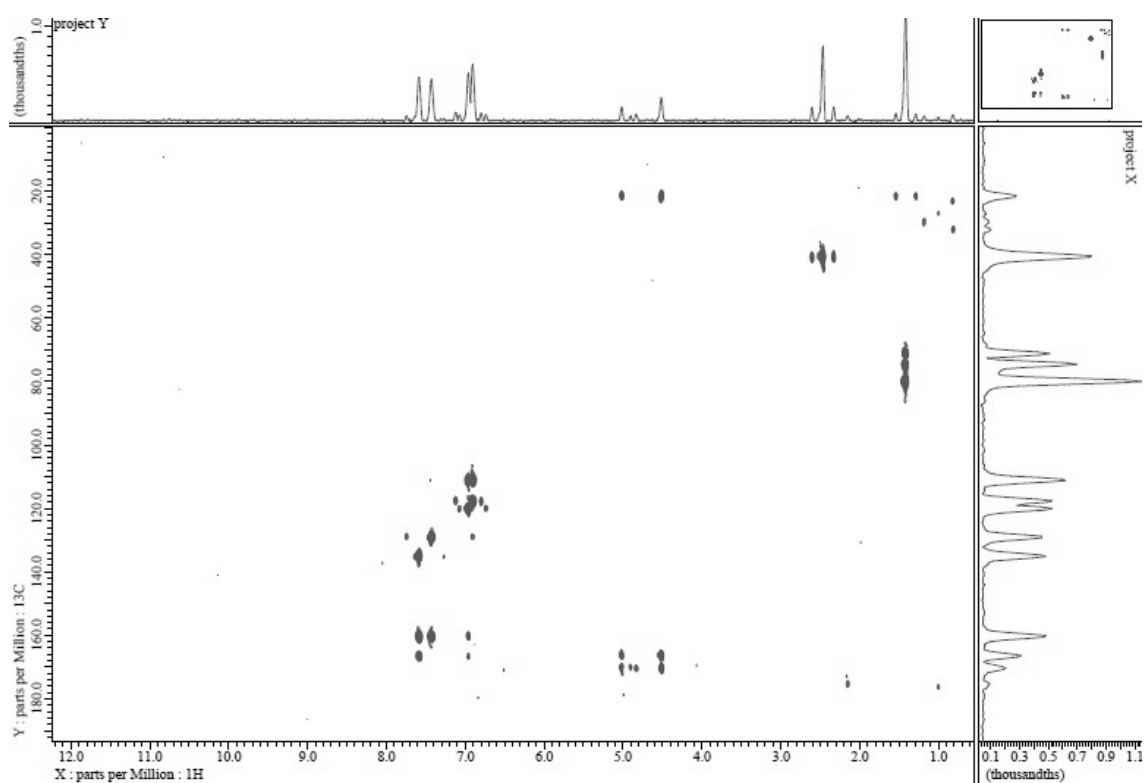


Figure S11. HMBC spectrum of **2** (500 MHz, d_6 -DMSO)

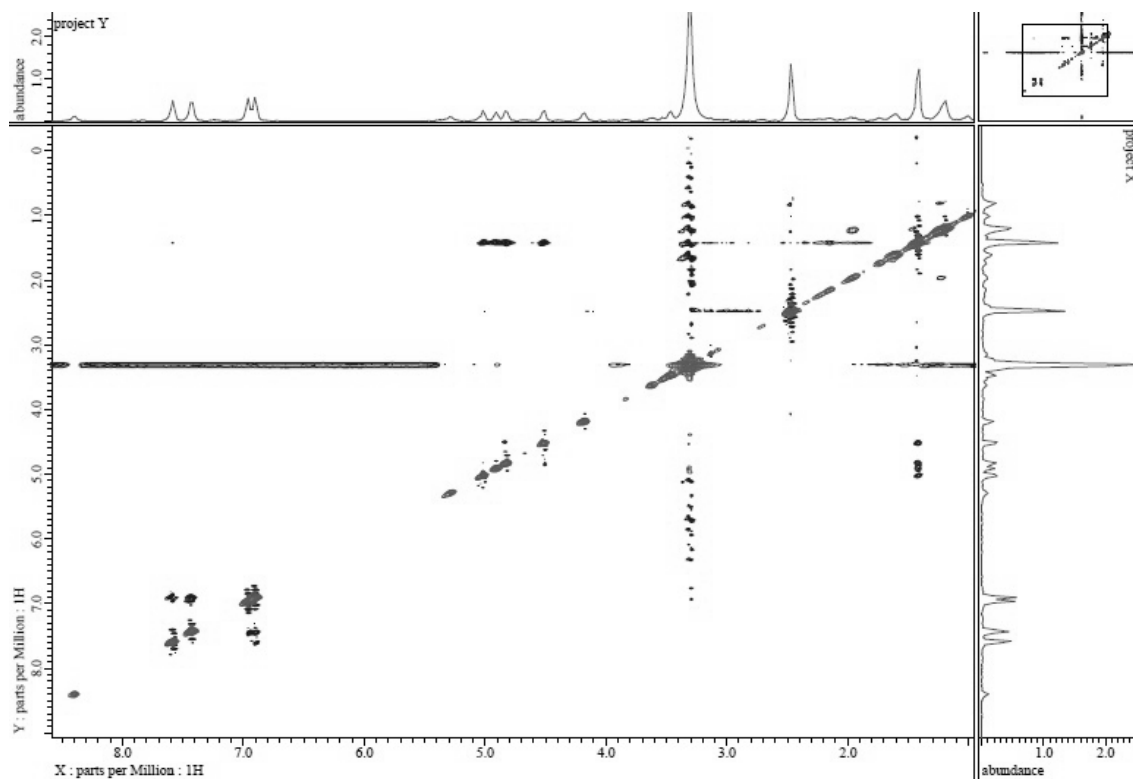


Figure S12. NOESY spectrum of **2** (500 MHz, d_6 -DMSO)

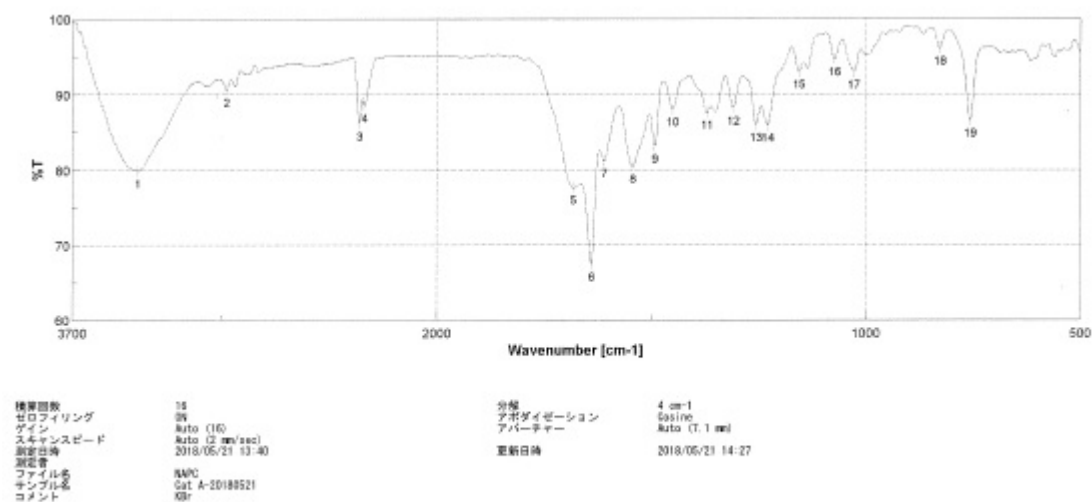


Figure S13. IR spectrum of 1

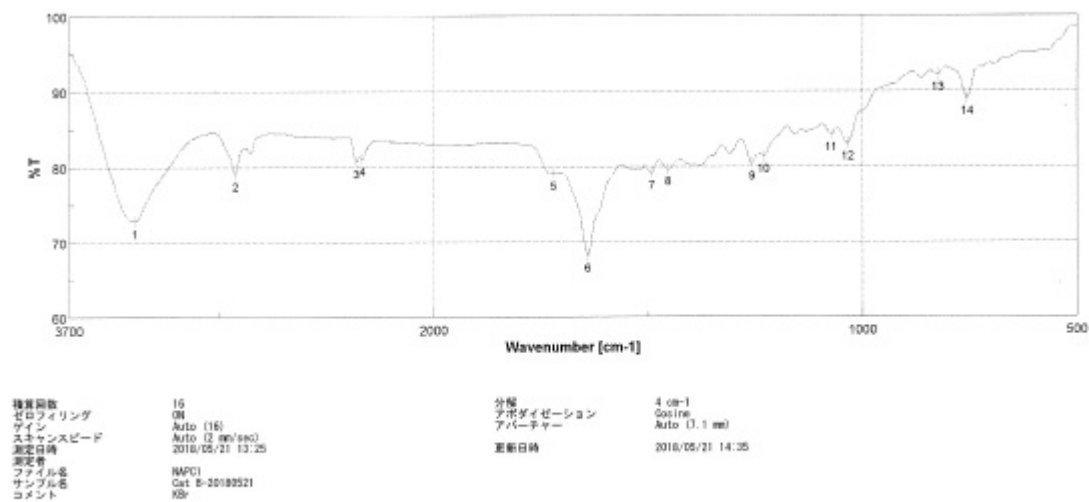
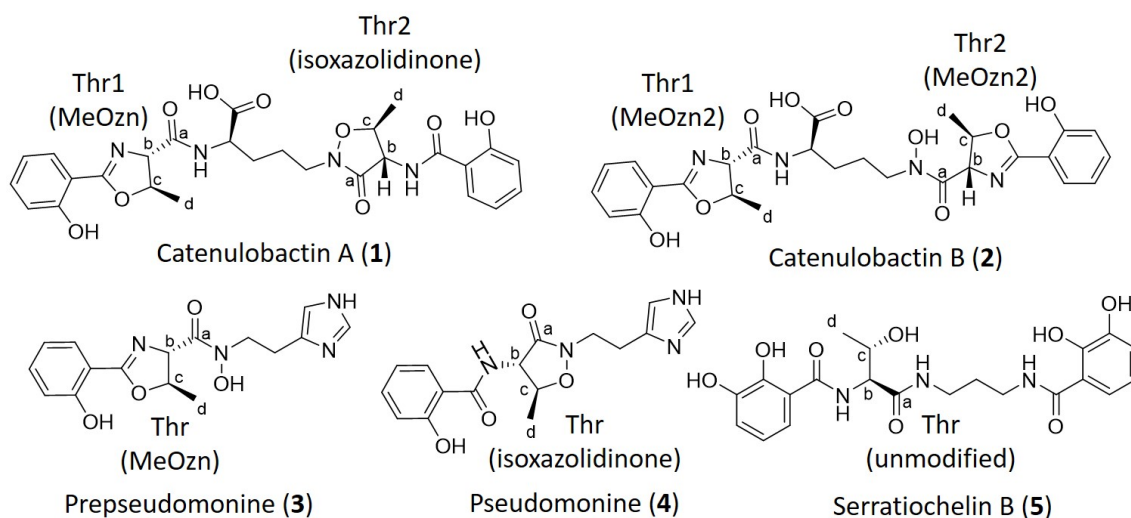


Figure S14. IR spectrum of 2



	1		2		3	4	5
position	Thr1	Thr2	Thr1	Thr2			
a	169.9	167.6	169.8	169.5	165.2	167.3	173.2
b	73.9	57.7	73.9	70.8	70.3	57.0	60.6
c	79.5	78.6	79.5	79.3	78.7	77.8	68.1
d	21.1	17.2	21.0	20.9	20.6	16.6	20.1

Figure S15. ^{13}C NMR resonances of Thr residues in catenulobactins (**1** and **2**), pre-pseudomnine (**3**)¹, pseudomnine (**4**)¹, and serratiochelin B (**5**)². The ^{13}C NMR spectra of were all recorded in d_6 -DMSO, except for the ^{13}C NMR spectrum of **5** recorded in d_4 -methanol.

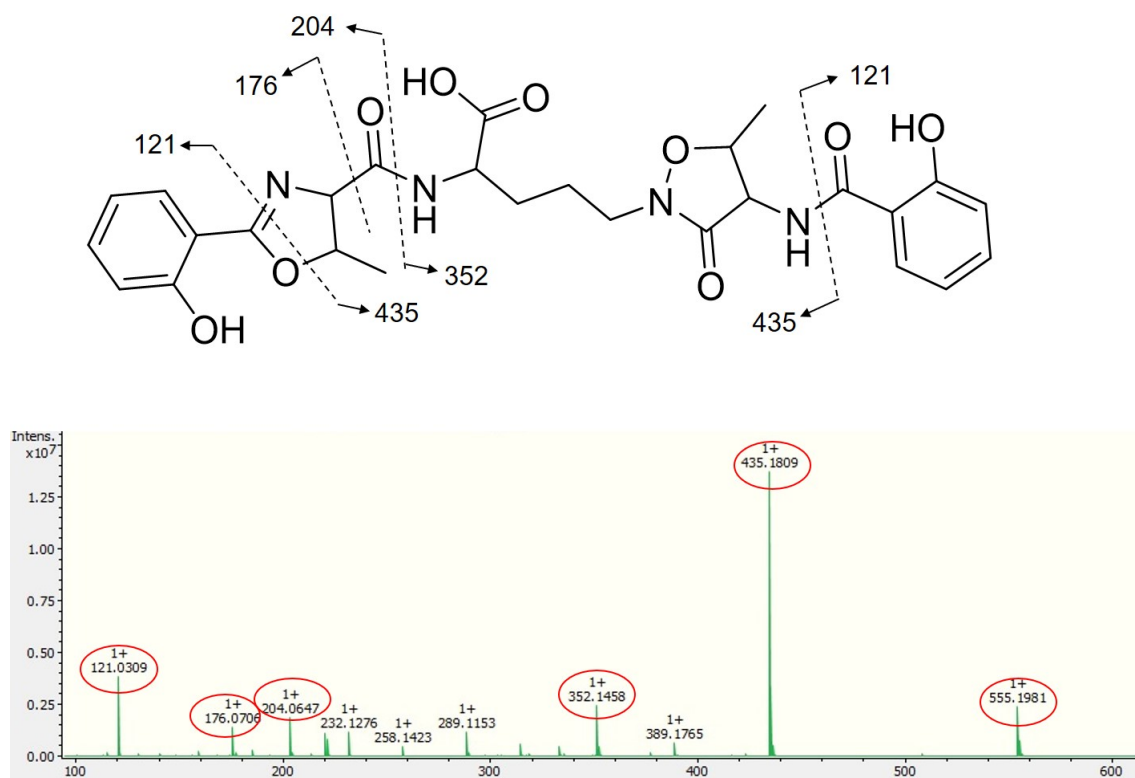


Figure S16. ESI-MS/MS analysis of **1**.

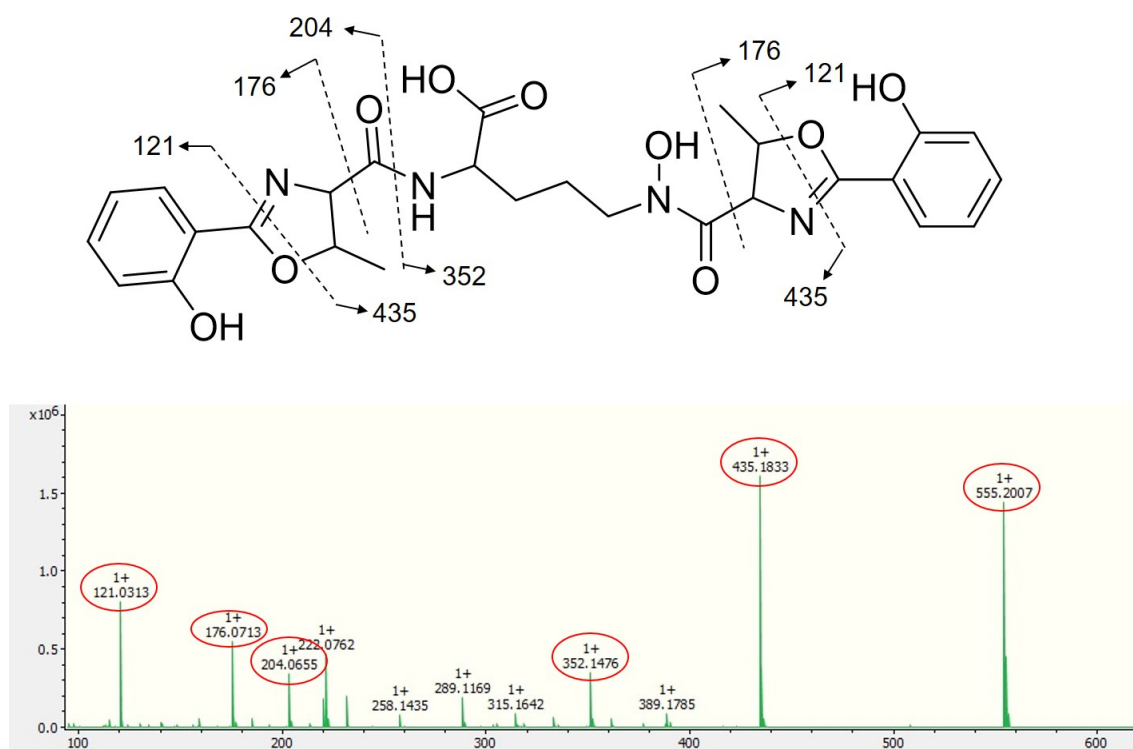


Figure S17. ESI-MS/MS analysis of **2**.

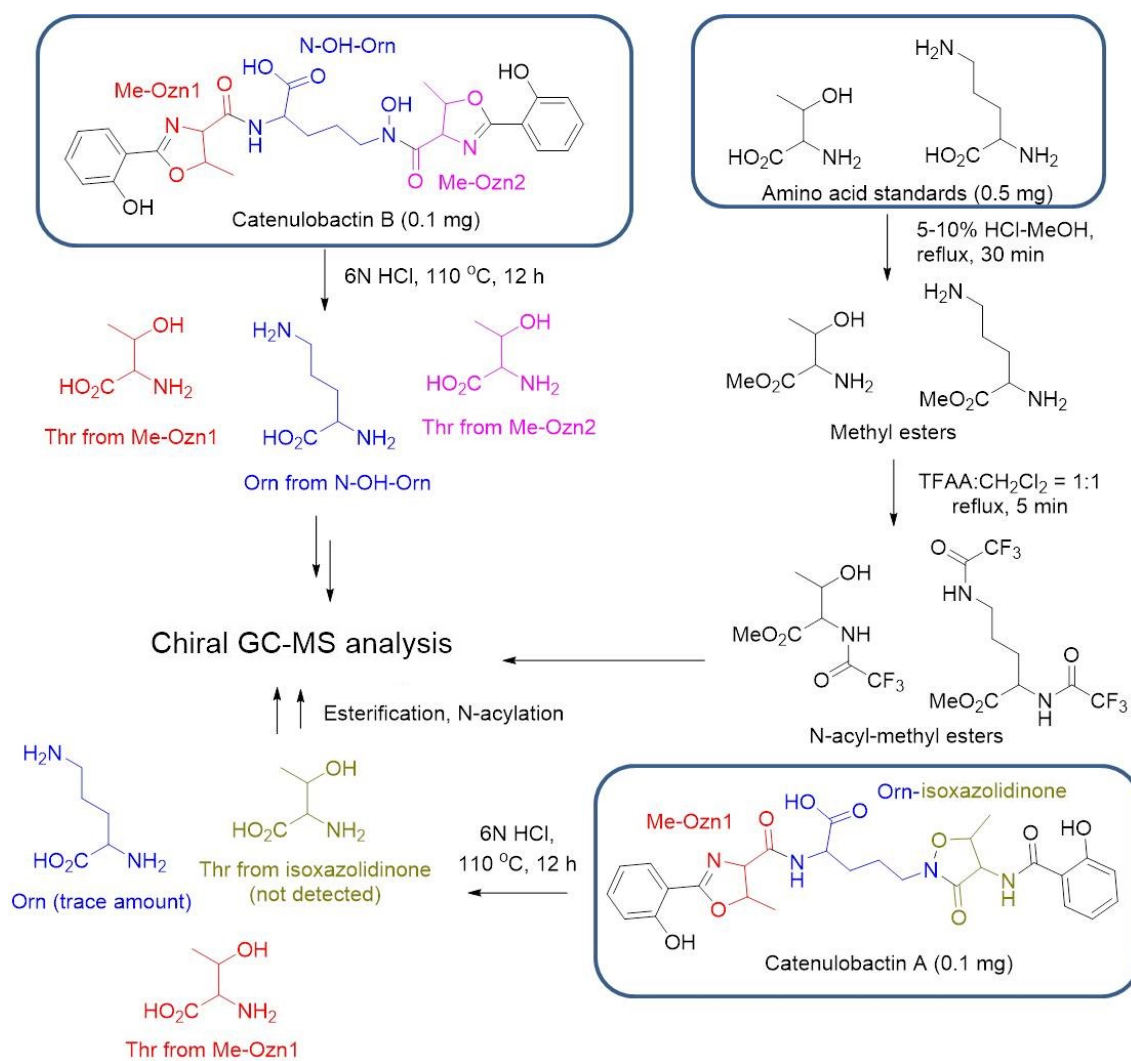


Figure S18. Outline for hydrolysis and chemical derivatization for GC-MS analysis.

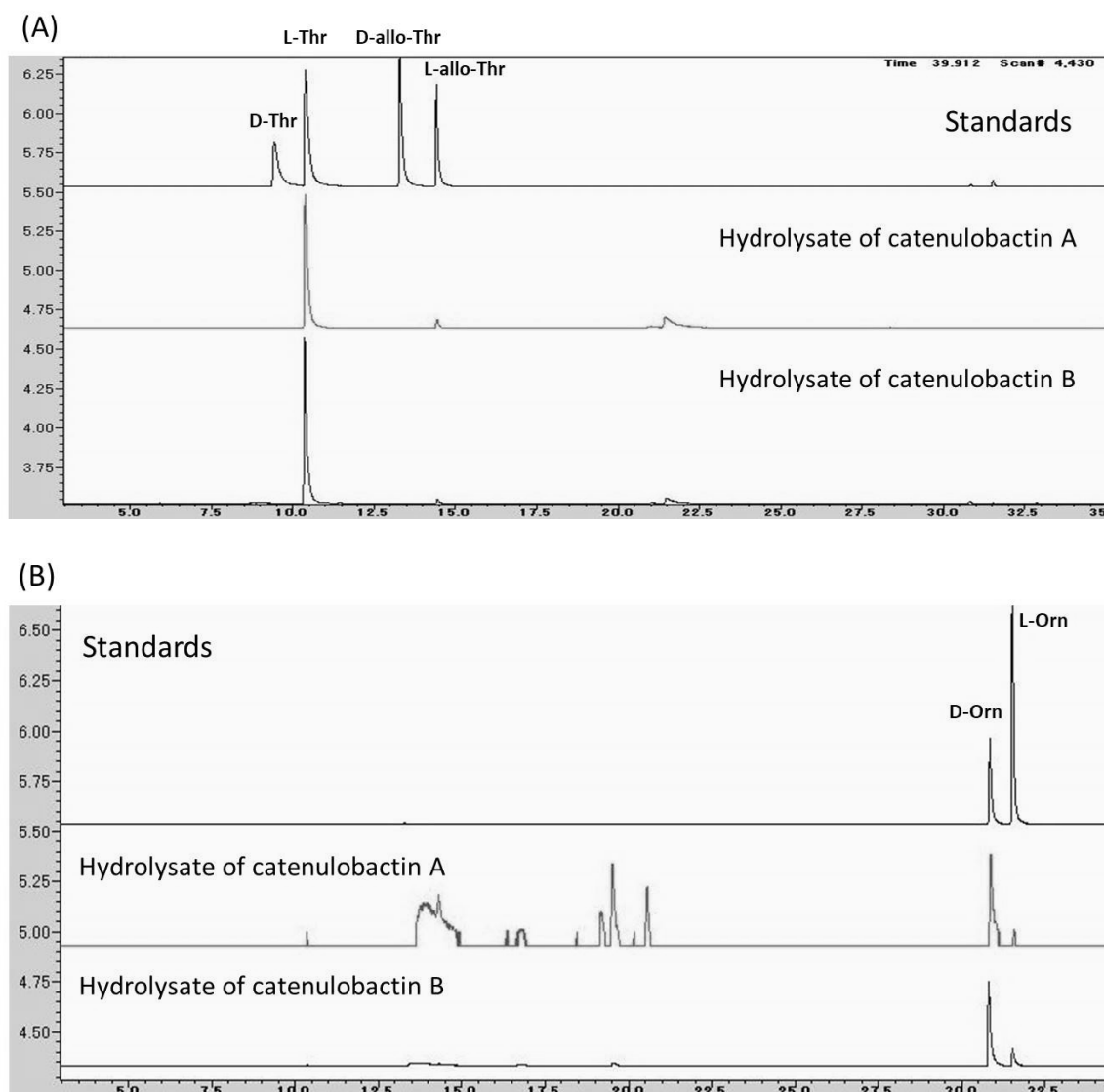


Figure S19. Chiral phase GC-MS chromatograms of amino acid standards and hydrolysates of catenulobactins derivatized with methyl ester and N-TFA. (A) m/z 152 for detection of the threonine derivatives. (B) m/z 166 for detection of the ornithine derivatives.

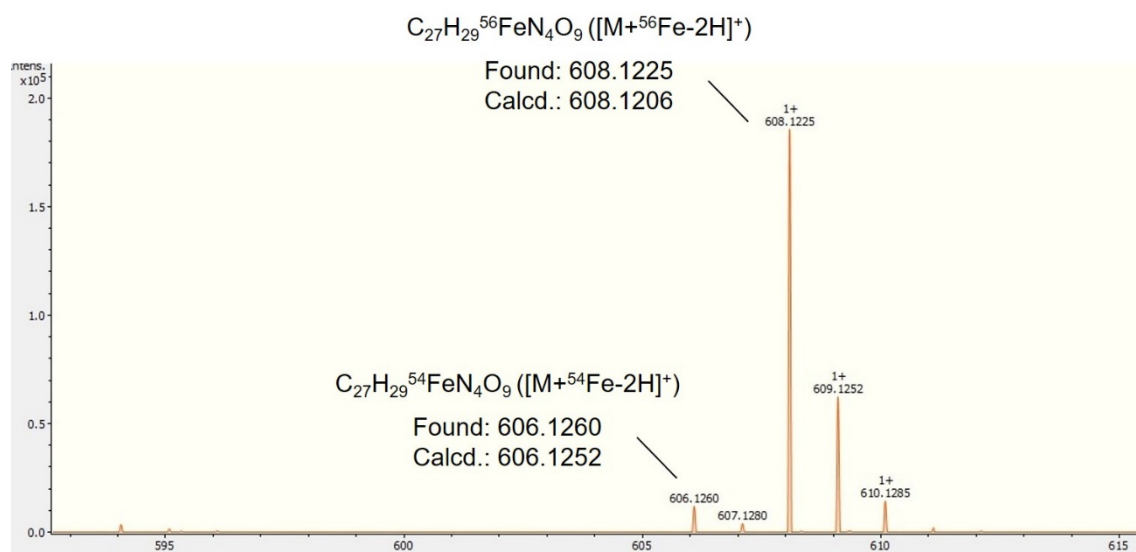


Figure S20. HR-ESI-MS spectrum of **2**-Fe(III) complex.

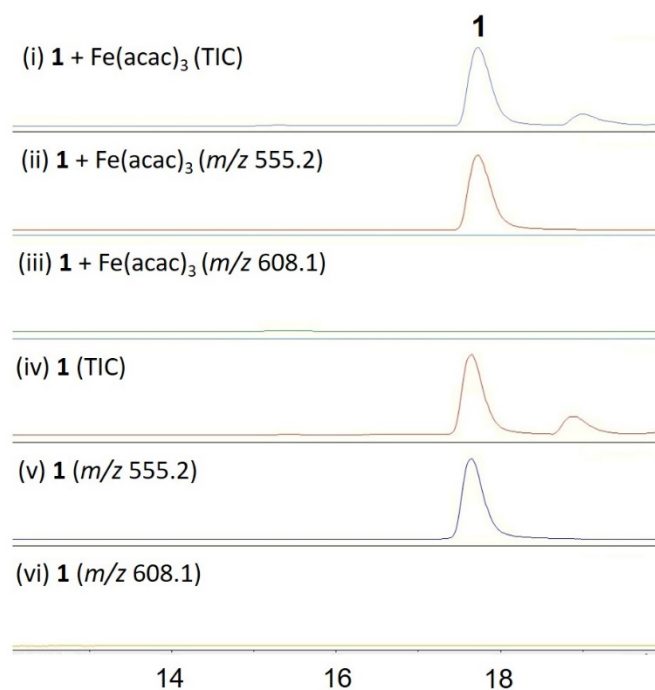


Figure S21. LC-MS charts of (i) total ion chromatogram (TIC) of **1** treated with $\text{Fe}(\text{acac})_3$, (ii) extracted ion chromatogram (EIC) of **1** treated with $\text{Fe}(\text{acac})_3$ at m/z 555.2 ($[\text{M}+\text{H}]^+$), (iii) EIC of **1** treated with $\text{Fe}(\text{acac})_3$ at m/z 608.1 ($[\text{M}+^{56}\text{Fe}-2\text{H}]^+$), (iv) TIC of **1** (untreated), (v) EIC of **1** (untreated) at m/z 555.2, and (vi) EIC of **1** (untreated) at m/z 608.1.

References

- (1) Shapiro, J. A.; Wencewicz T. A. *Metallomics*. **2017**, *9*, 463-470.
- (2) Seyedsayamdost M. R.; Cleto, S.; Carr, G.; Vlamakis, H.; João Vieira, M.; Kolter, R.; Clardy, J. *J. Am Chem. Soc.* **2012**, *134*, 13550-13553.