

Supplementary Materials: Cysteines and Disulfide-Bridged Macrocyclic Mimics of Teixobactin Analogues and Their Antibacterial Activity Evaluation against Methicillin-Resistant *Staphylococcus Aureus* (MRSA)

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Table S1. Compound number, name, chemical formula, exact mass and mass found for compounds 2–9.

Compound Number	Name	Chemical Formula	Mass Calcd (Da)	Mass Obsd (Da)
2	L-Phe1-L-Gln4-L-Ile5-linear(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₉₀ N ₁₆ O ₁₄ S ₂	1239.63	1239.62
3	L-Phe1-L-Gln4-L-Ile5-cyclo(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₈₈ N ₁₆ O ₁₄ S ₂	1237.61	1237.72
4	D-Phe1-linear(D-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₉₀ N ₁₆ O ₁₄ S ₂	1239.63	1239.62
5	D-Phe1-cyclo(D-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₈₈ N ₁₆ O ₁₄ S ₂	1237.61	1237.53
6	D-Phe1-linear(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₉₀ N ₁₆ O ₁₄ S ₂	1239.63	1239.57
7	D-Phe1-cyclo(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₃ H ₈₈ N ₁₆ O ₁₄ S ₂	1237.61	1237.56
8	N-Me-D-Phe1-linear(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₄ H ₉₂ N ₁₆ O ₁₄ S ₂	1253.64	1253.64
9	N-Me-D-Phe1-cyclo(L-Cys8-L-Arg10-L-Cys11)-teixobactin	C ₅₄ H ₉₀ N ₁₆ O ₁₄ S ₂	1251.63	1251.63

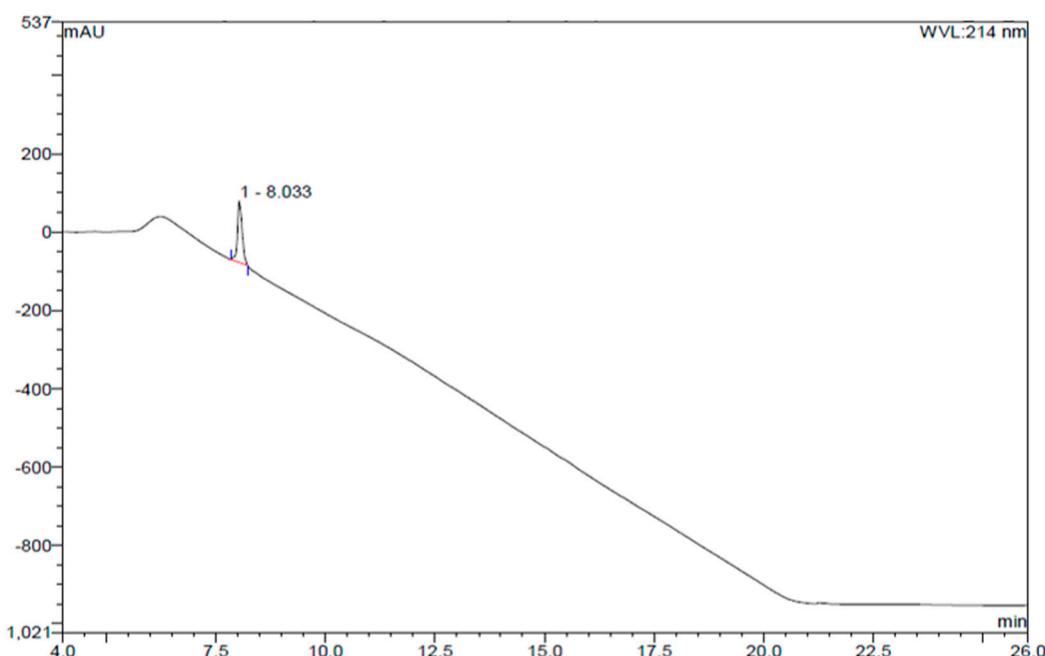


Figure S1. HPLC trace of purified teixobactin analogue 2 (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

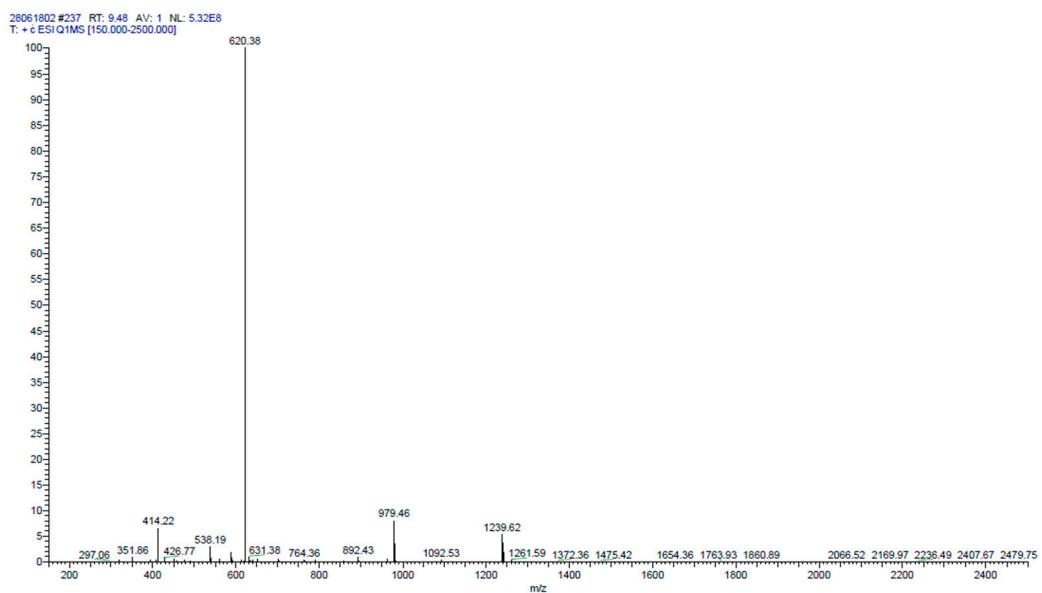


Figure S2. ESI-MS of purified teixobactin analogue **2**. Exact mass calcd. For $C_{53}H_{90}N_{16}O_{14}S_2 = 1238.63$, found $M + H^+ = 1239.62$, $M/2 + H^+ = 620.38$.

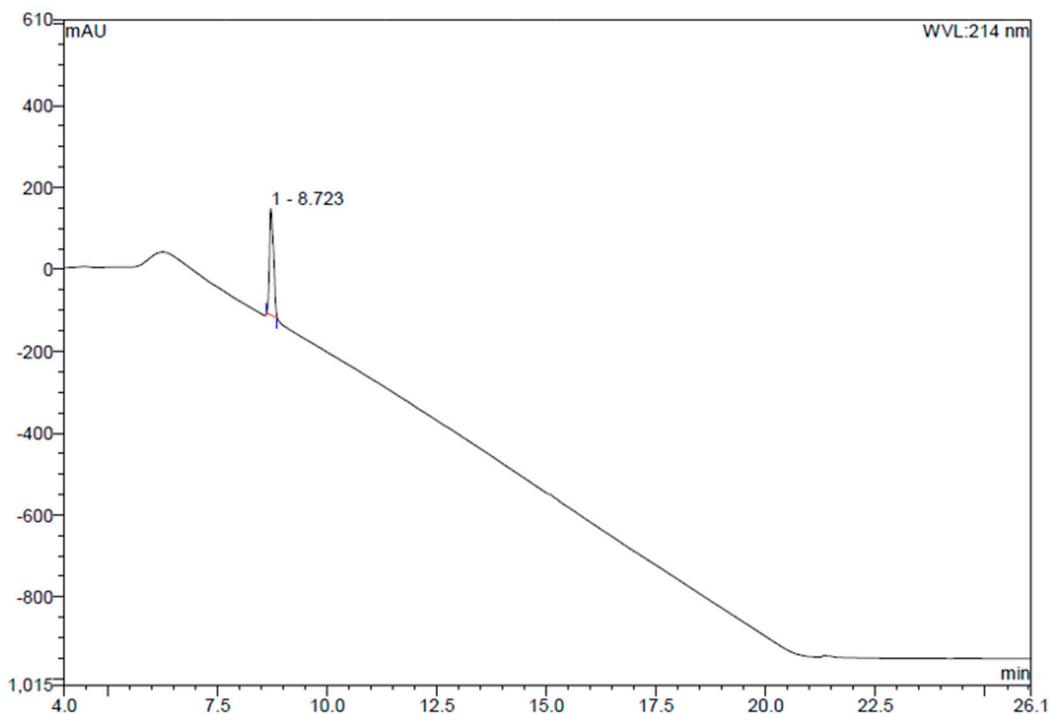


Figure S3. HPLC trace of purified teixobactin analogue **3** (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

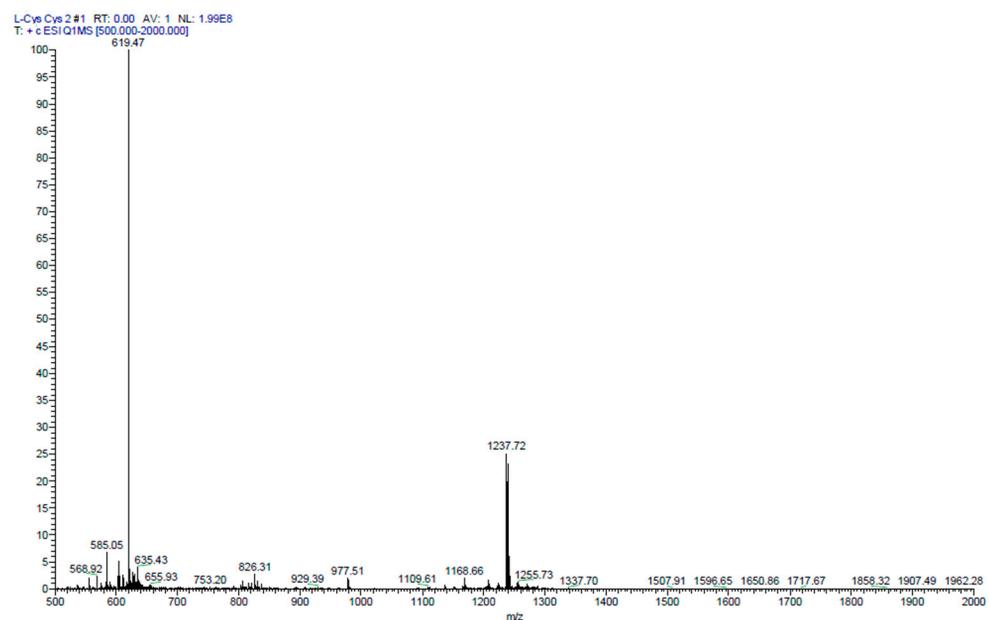


Figure S4. ESI-MS of purified teixobactin analogue **3**. Exact mass calcd. For $C_{53}H_{88}N_{16}O_{14}S_2 = 1236.61$, found $M + H^+ = 1237.72$, $M/2 + H^+ = 619.47$.

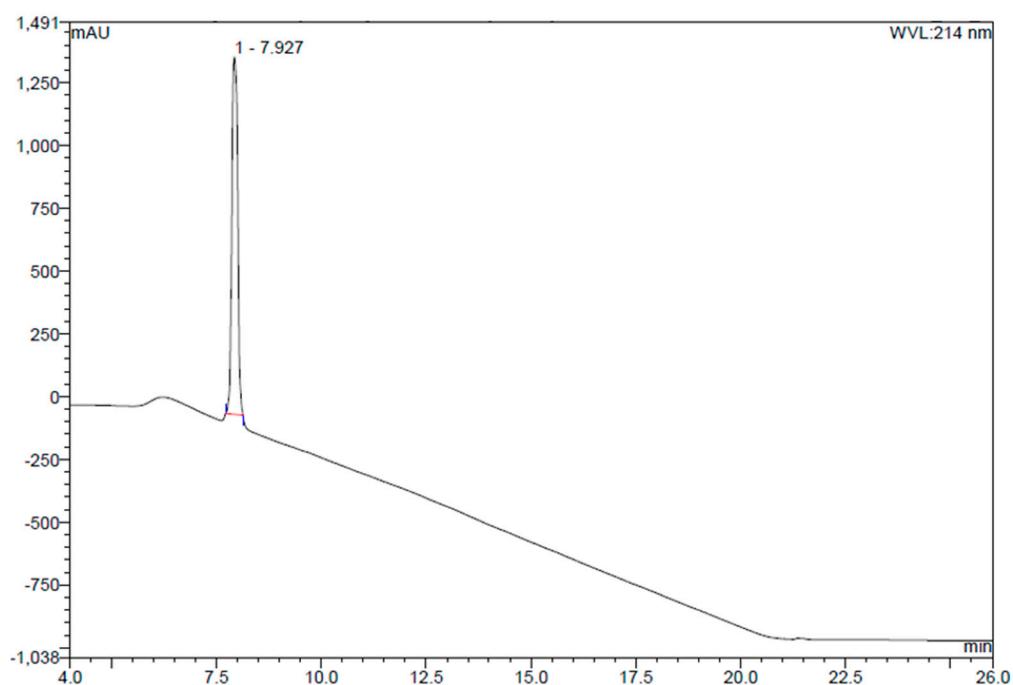


Figure S5. HPLC trace of purified teixobactin analogue **4** (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

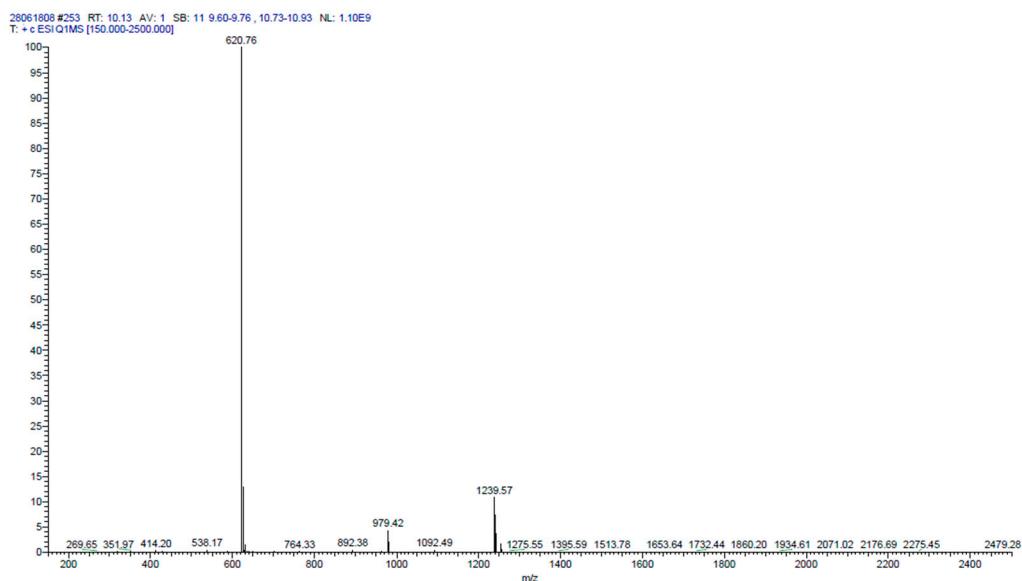


Figure S6. ESI-MS of purified Teixobactin analogue 4. Exact mass calcd. For $C_{53}H_{90}N_{16}O_{14}S_2 = 1238.63$, found $M + H^+ = 1239.57$, $M/2 + H^+ = 620.76$.

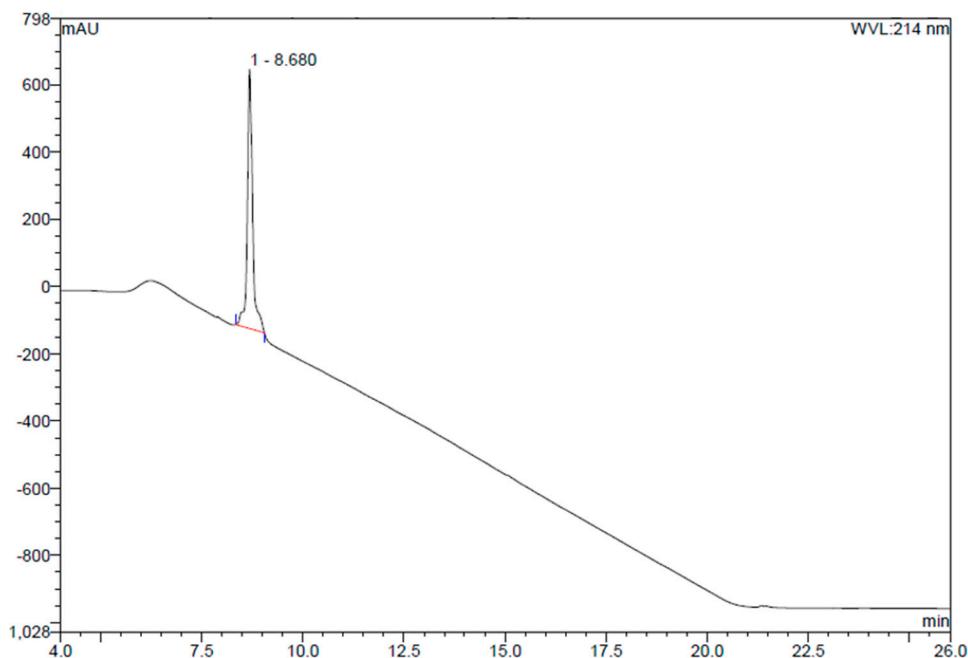


Figure S7. HPLC trace of purified teixobactin analogue 5 (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

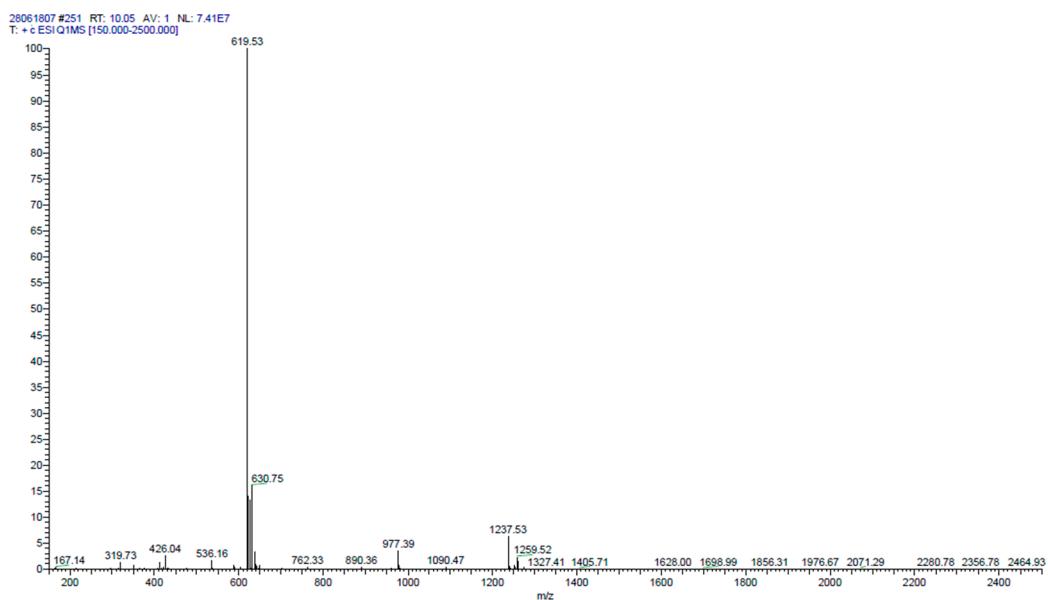


Figure S8. ESI-MS of purified teixobactin analogue **5**. Exact mass calcd. For $C_{53}H_{88}N_{16}O_{14}S_2 = 1236.61$, found $M + H^+ = 1237.53$, $M/2 + H^+ = 619.53$.

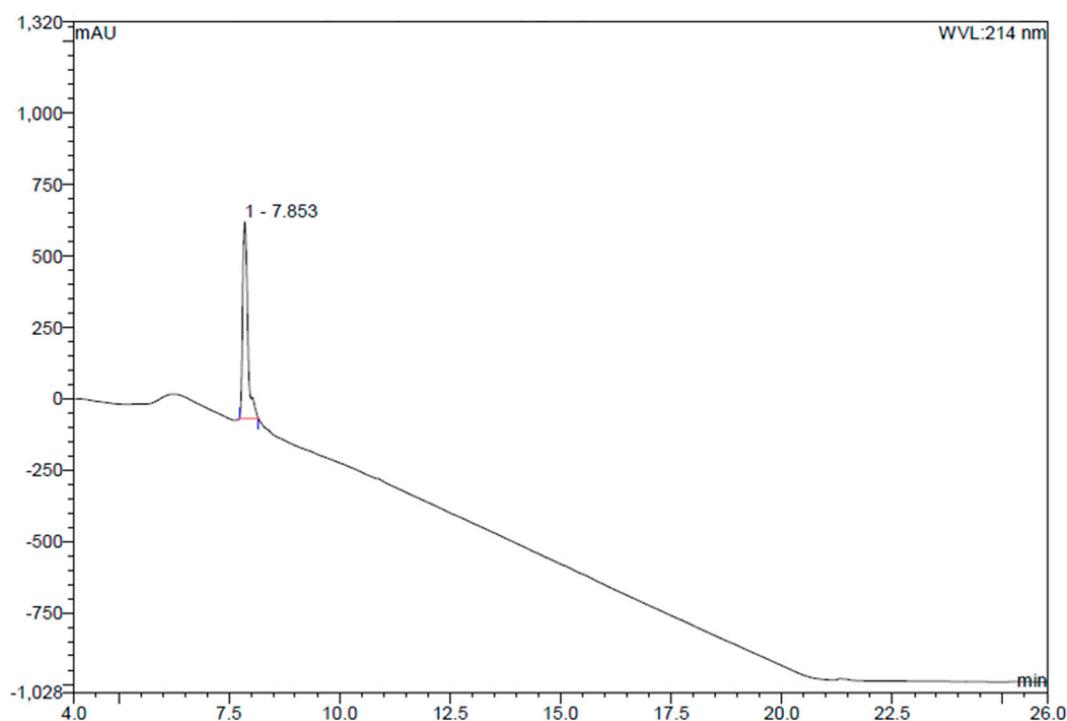


Figure S9. HPLC trace of purified teixobactin analogue **6** (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

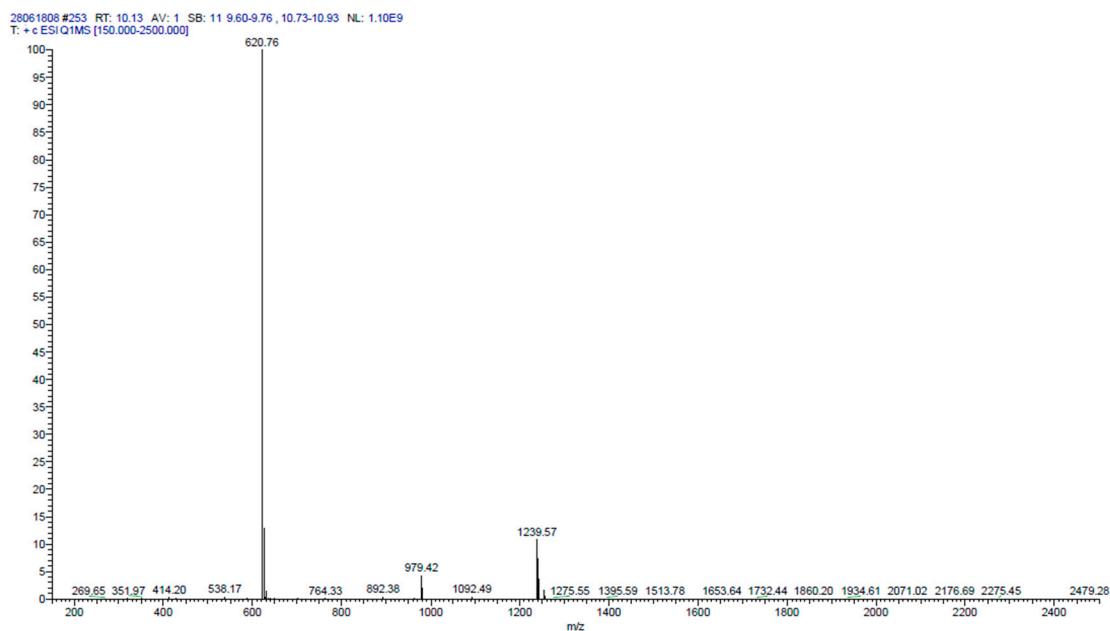


Figure S10. ESI-MS of purified teixobactin analogue **6**. Exact mass calcd. For $C_{53}H_{90}N_{16}O_{14}S_2 = 1238.63$, found $M + H^+ = 1239.57$, $M/2 + H^+ = 620.76$.

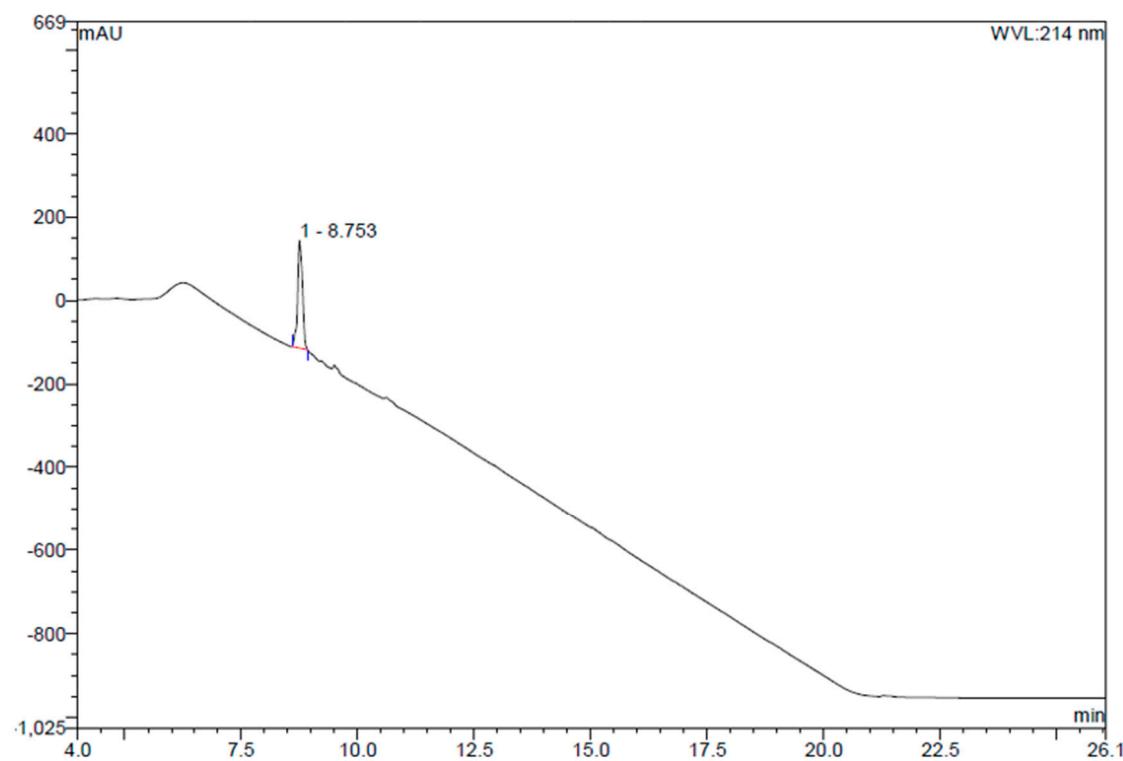


Figure S11. HPLC trace of purified teixobactin analogue **7** (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

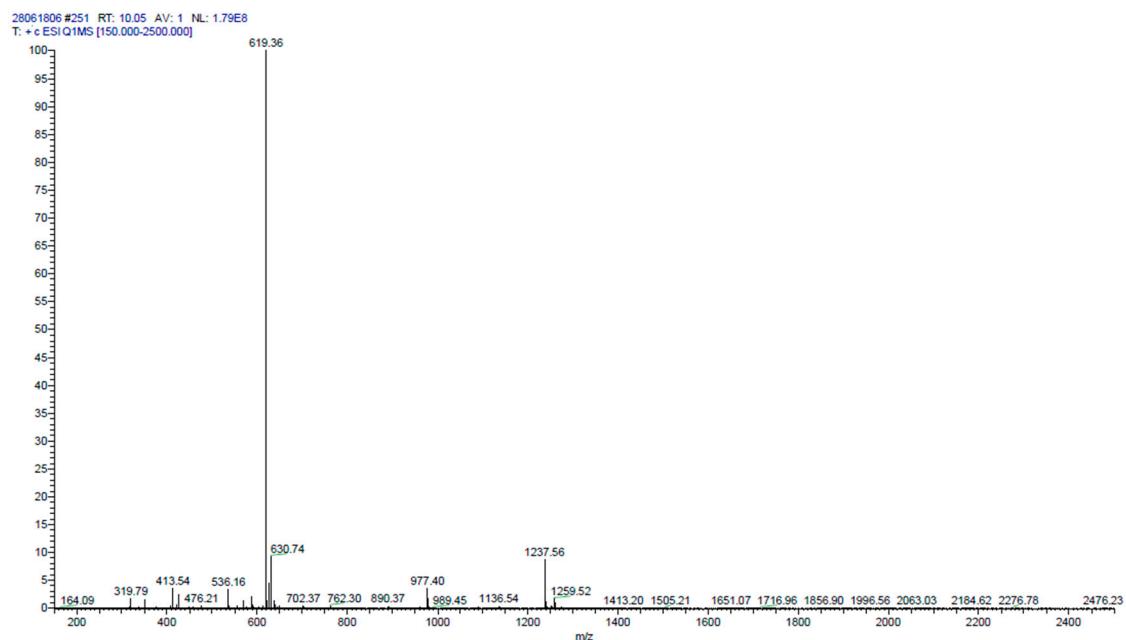


Figure S12. ESI-MS of purified teixobactin analogue 7. Exact mass calcd. For $C_{53}H_{88}N_{16}O_{14}S_2 = 1236.61$, found $M + H^+ = 1237.56$, $M/2 + H^+ = 619.36$.

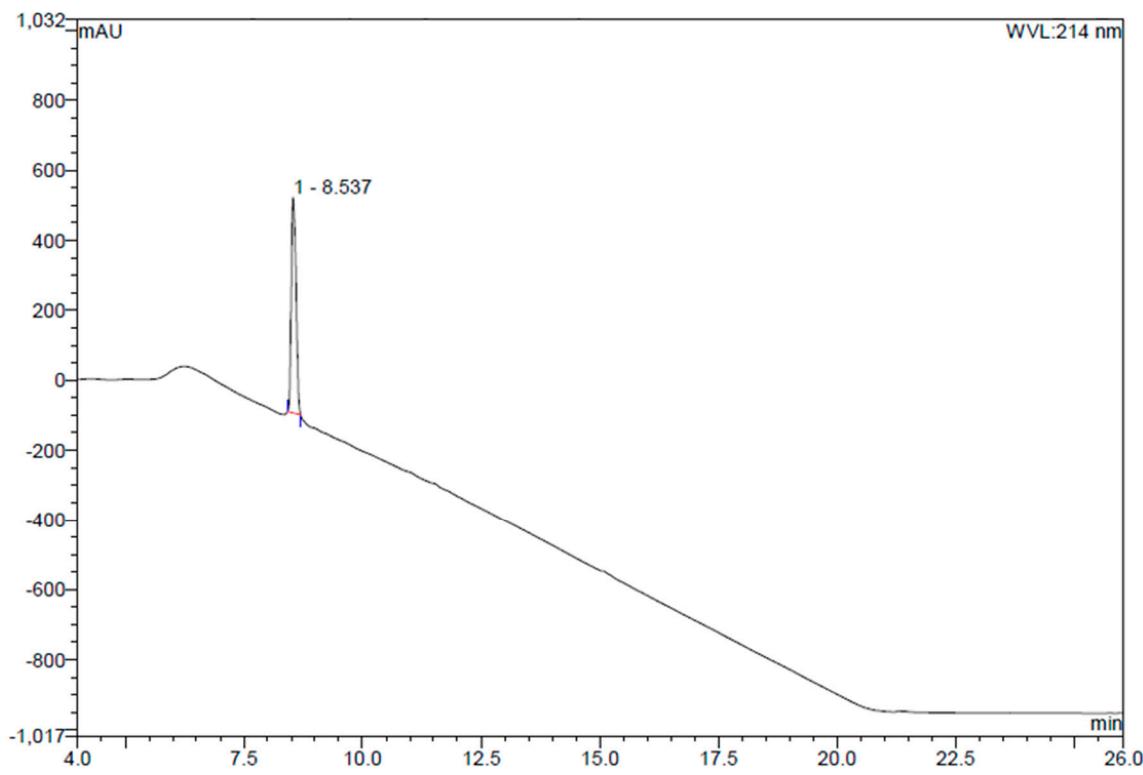


Figure S13. HPLC trace of purified teixobactin analogue 8 (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

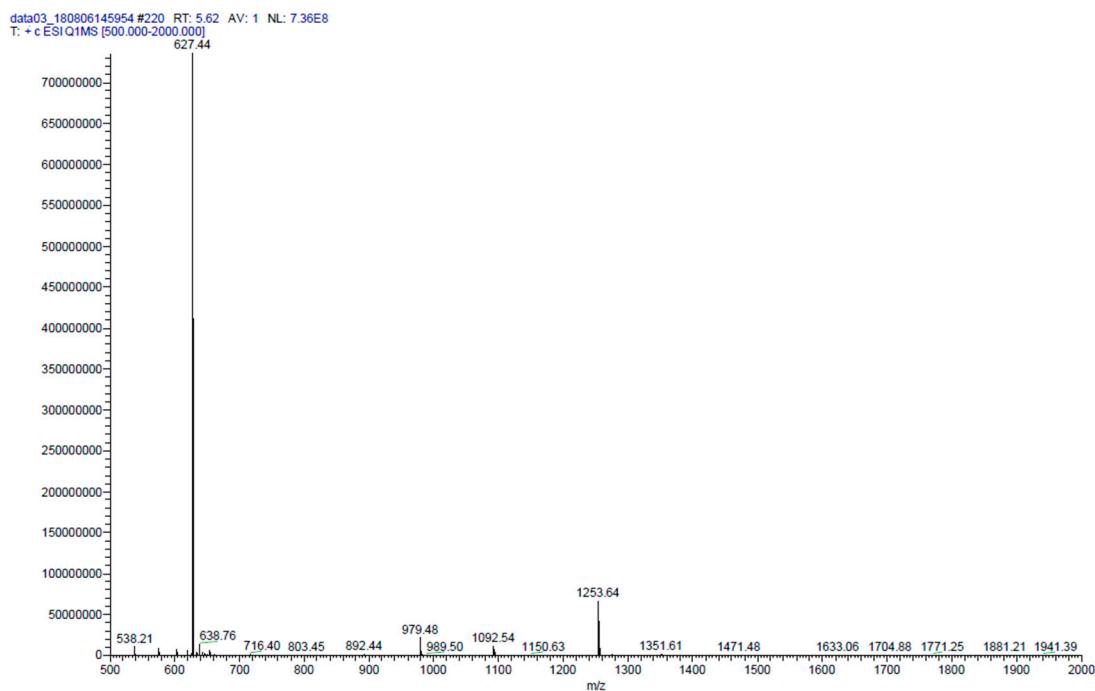


Figure S14. ESI-MS of purified teixobactin analogue **8**. Exact mass calcd. For $C_{54}H_{92}N_{16}O_{14}S_2 = 1252.64$, found $M + H^+ = 1253.64$, $M/2 + H^+ = 627.44$.

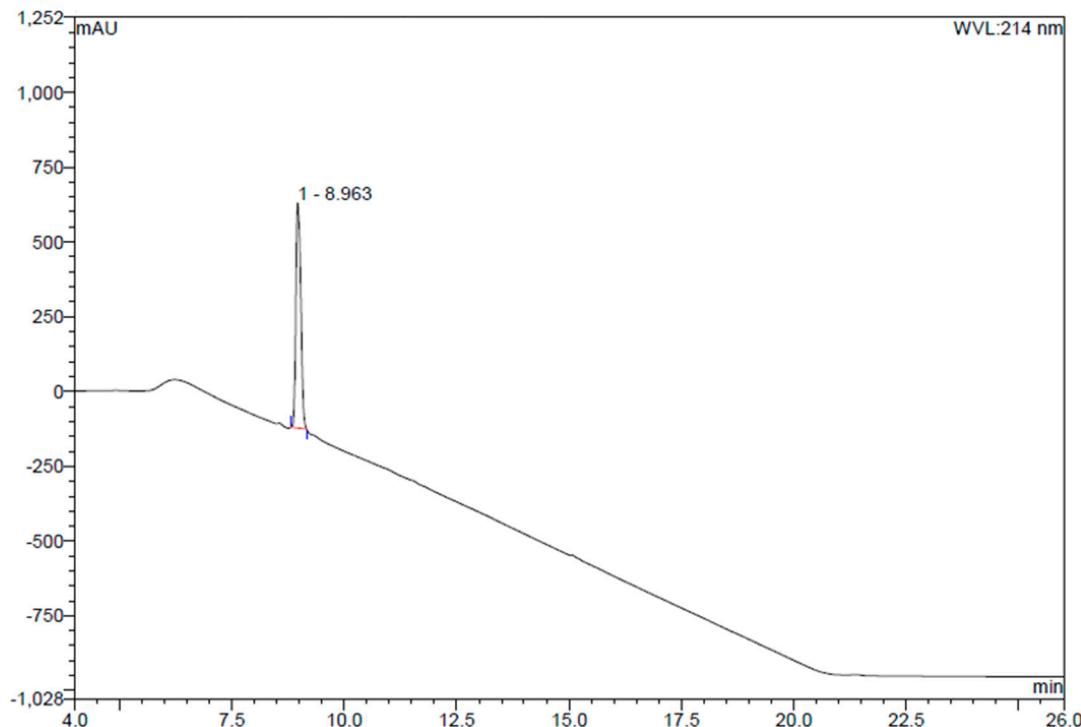


Figure S15. HPLC trace of purified teixobactin analogue **9** (gradient: 5–95% ACN in 25 min using A: 0.1% HCOOH in water, B: ACN).

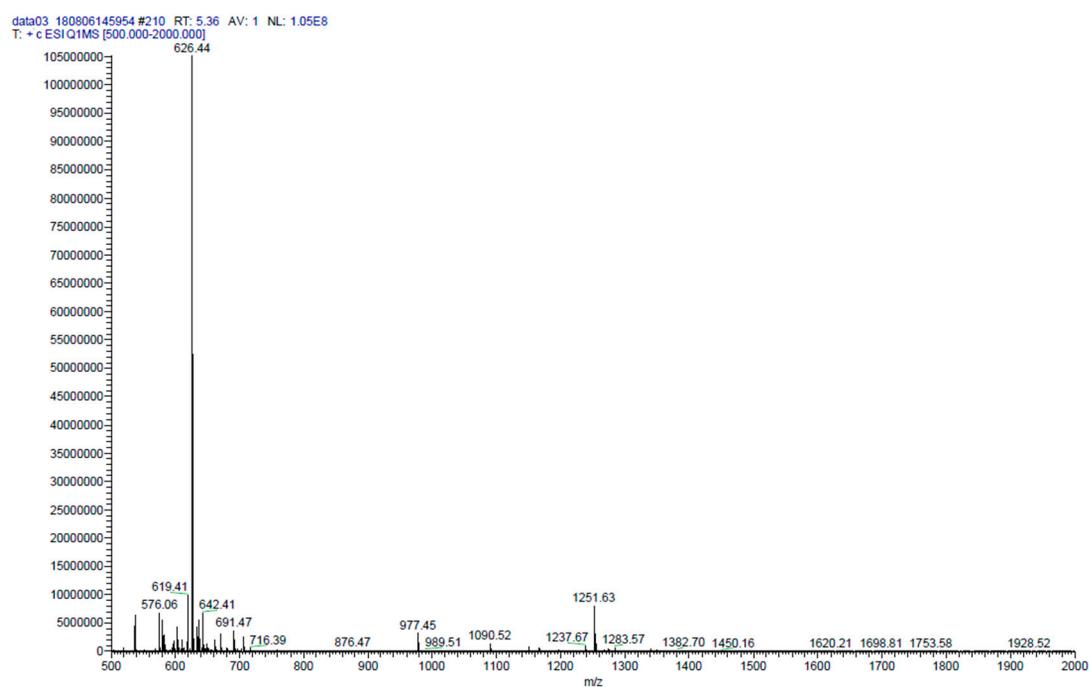


Figure S16. ESI-MS of purified teixobactin analogue 9. Exact mass calcd. For $C_{54}H_{90}N_{16}O_{14}S_2 = 1250.63$, found $M + H^+ = 1251.63$, $M/2 + H^+ = 626.24$.