Electronic Supplementary Information (ESI)

Fungal biofilm inhibitors from a human oral microbiome-derived bacterium†

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Table S1. Revised ^{1}H-NMR and ^{13}C-NMR NMR data for mutanobactin A (**1**) (500 and 100 MHz, DMSO-d_6) – Shifts shown in red have been revised.

position	Mutanobactin A (1) (original)		Mutanobactin A (1) (revised)	
	δ_C	δ_H mult. (*J* in Hz)	δ_C	δ_H mult. (*J* in Hz)
1	50.4, CH	4.43 ddd (3.7, 9.0, 11.0)	50.4, CH	4.43 ddd (3.7, 9.0, 11.0)
2a	40.4, CH_2	1.44, m	40.4, CH_2	1.44, m
2b		1.81, ddd (3.9, 10.5, 13.8)		1.81, ddd (3.9, 10.5, 13.8)
3	24.2, CH	1.59, m	24.2, CH	1.59, m
4	20.9, CH_3	0.82, d (6.6)	20.9, CH_3	0.82, d (6.6)
5	23.5, CH_3	0.92, d (6.7)	23.5, CH_3	0.92, d (6.7)
6	170.5, C		170.5, C	
7	48.0, CH	4.52, q (6.8)	48.0, CH	4.52, q (6.8)
8	17.7, CH_3	1.17, d (6.7)	17.7, CH_3	1.17, d (6.7)
9	169.7, C		169.7, C	
10	61.0, CH	4.12, dd (3.7, 8.9)	61.0, CH	4.12, dd (3.7, 8.9)
11a	29.6, CH_2	1.72, m	29.6, CH_2	1.72, m
11b		2.13, m		2.13, m
12	24.5, CH_2	1.90, m	24.5, CH_2	1.90, m
13a	46.8, CH_2	3.43, m	46.8, CH_2	3.43, m
13b		3.65, ddd (4.5, 7.5, 9.8)		3.65, ddd (4.5, 7.5, 9.8)
14	171.6, C		171.6, C	
15	58.8, CH	3.57, dd (8.3, 10.0)	58.8, CH	3.57, dd (8.3, 10.0)
16	26.2, CH	2.33, m	26.2, CH	2.33, m
17	20.4, CH_3	0.84, d (6.6)	20.4, CH_3	0.84, d (6.6)
18	18.8, CH_3	0.77, d (6.8)	18.8, CH_3	0.77, d (6.8)
19	168.8, C		168.8, C	
20	52.2, CH	4.87 ddd (2.6, 8.0, 9.0)	52.2, CH	4.87 ddd (2.6, 8.0, 9.0)
21a	28.5, CH_2	2.23, dd (2.6, 16.0)	28.4, CH_2	2.23, dd (2.6, 16.0)
21b		3.19, dd (9.0, 16.0)		3.19, dd (9.0, 16.0)
22	170.4, C		170.4, C	
23a	43.7, CH_2	2.79, m	43.7, CH_2	2.79, m
23b		3.28, m		3.28, m
24	41.0, CH	3.25, m	41.0, CH	3.25, m
25	61.7, CH	3.87, d (9.8)	61.7, CH	3.87, d (9.8)
26	167.7, C		167.7, C	
27	203.8, C		203.8, C	
28a	41.4, CH_2	2.33, m	41.4, CH_2	2.33, m
28b		2.44, dd (6.0, 16.6)		2.44, dd (6.0, 16.6)
29	23.1, CH_2	1.44, m	23.1, CH_2	1.44, m
30	28.7, CH_2	1.20, m	28.5, CH_2	1.20, m
31	22.1, CH_2	1.25, m	28.7, CH_2	1.25, m
32	28.8, CH_2	1.23, m	28.9, CH_2	1.27, m
33	22.1, CH_2	1.25, m	28.8, CH_2	1.23, m
34	31.3, CH_2	1.23, m	31.3, CH_2	1.23, m
35	28.9, CH_2	1.27, m	22.1, CH_2	1.25, m
36	14.0, CH_3	0.85, t (6.8)	14.0, CH_3	0.85, t (6.8)
C1-NH		8.59, d (9.0)		8.59, d (9.0)
C7-NH		7.77, d (6.5)		7.77, d (6.5)
C15-NH		8.05, d (8.5)		8.05, d (8.5)
C20-NH		7.23, d (8.0)		7.23, d (8.0)
C23-NH		7.90, dd (5.3, 9.0)		7.90, dd (5.3, 9.0)

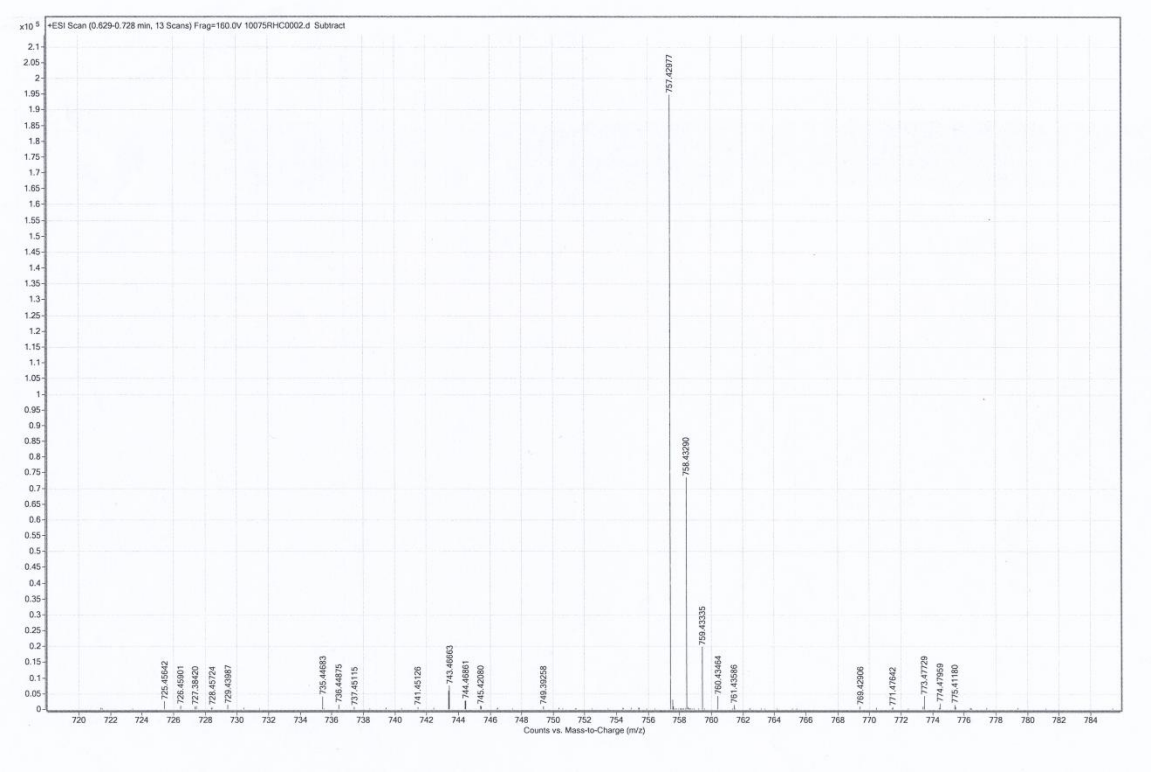

Fig. S1. HRESIMS of mutanobactin B **(2).**

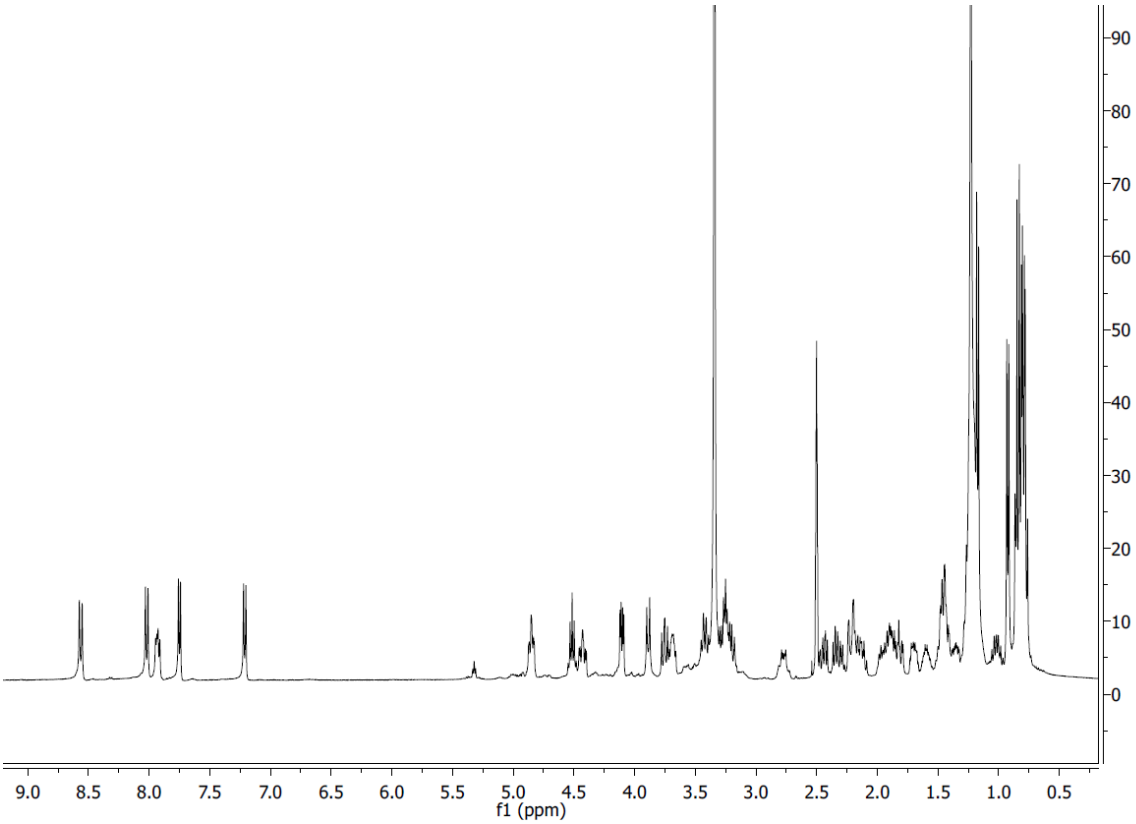

Fig. S2. ^{1}H-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B (**2**).

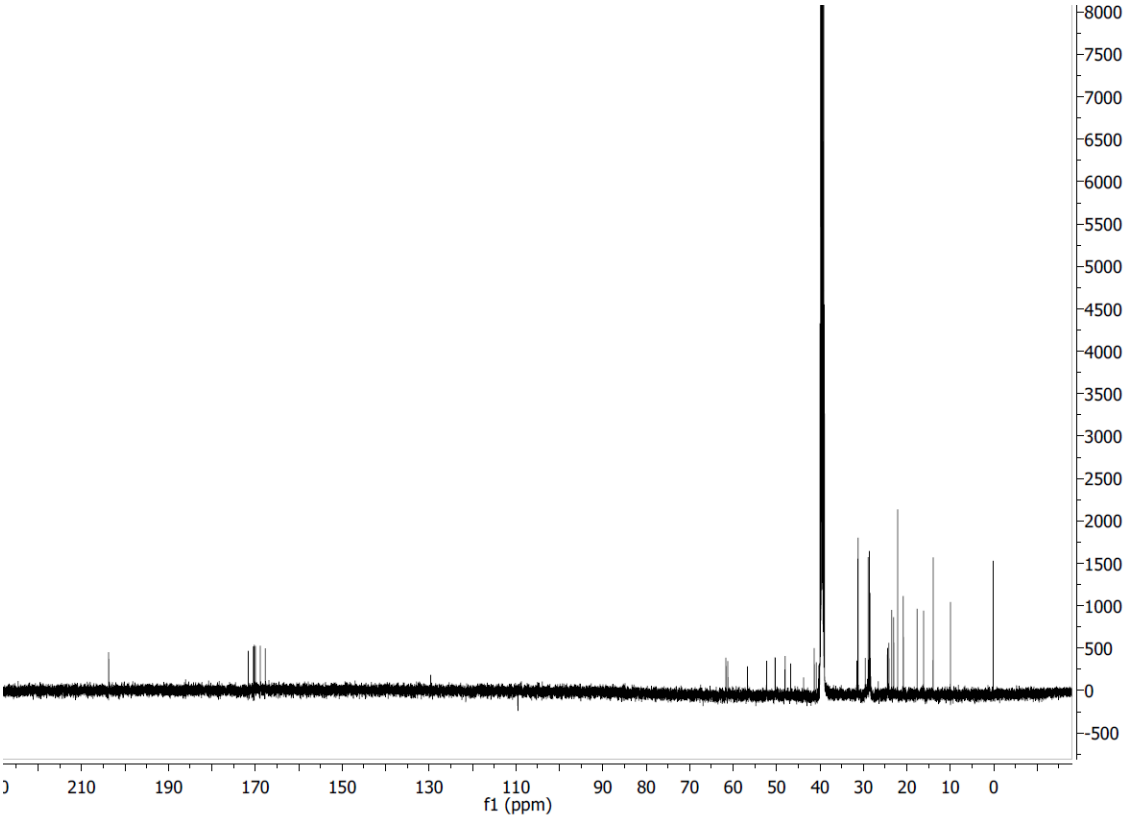

Fig. S3. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of mutanobactin B **(2).**

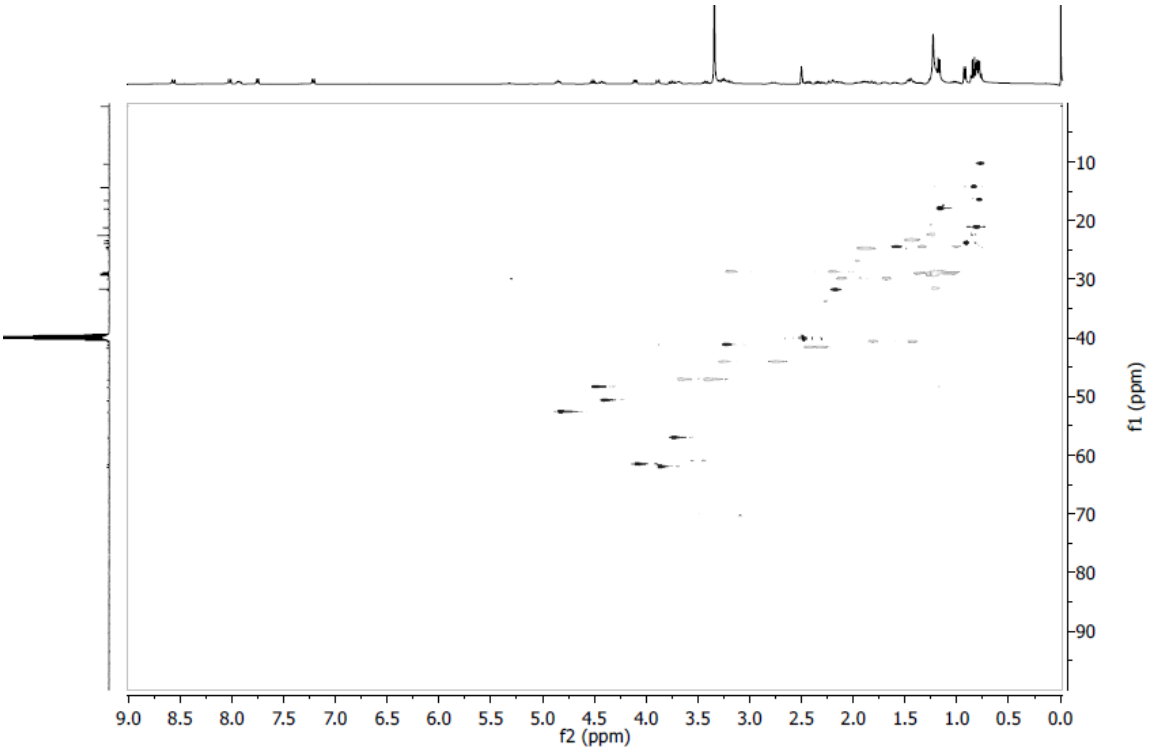

Fig. S4. ^{1}H-^{13}C HSQC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B **(2).**

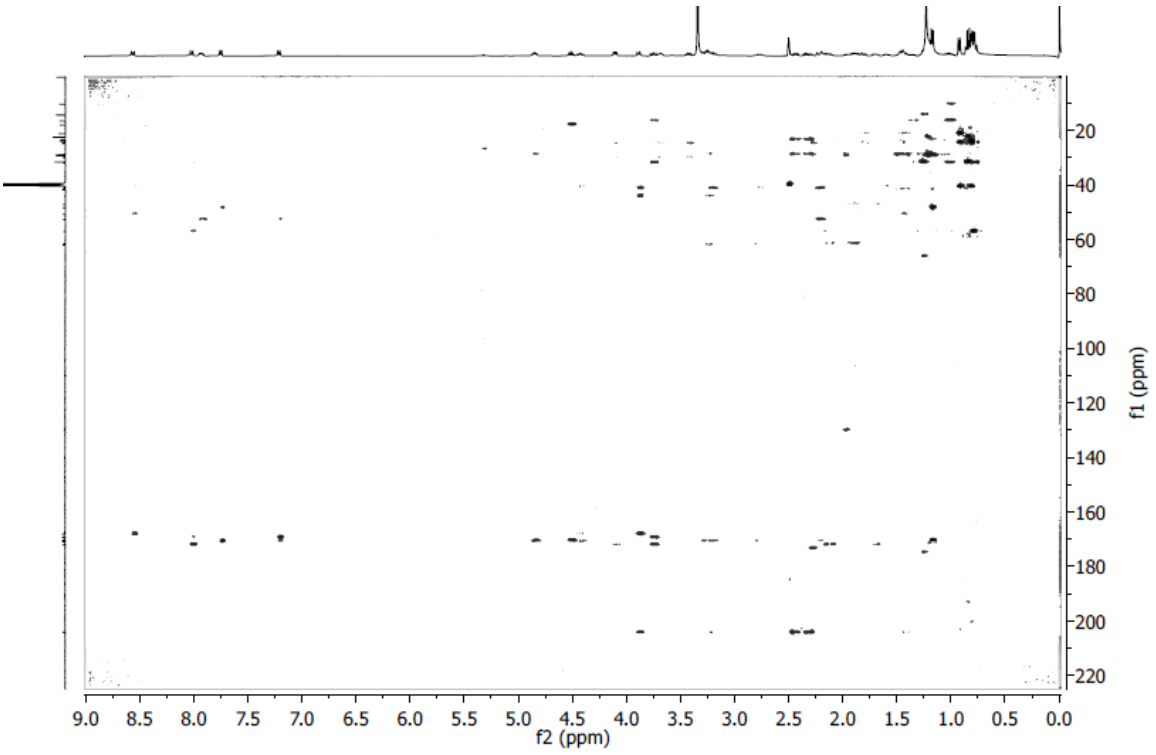

Fig. S5. ^{1}H-^{13}C HMBC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B **(2).**

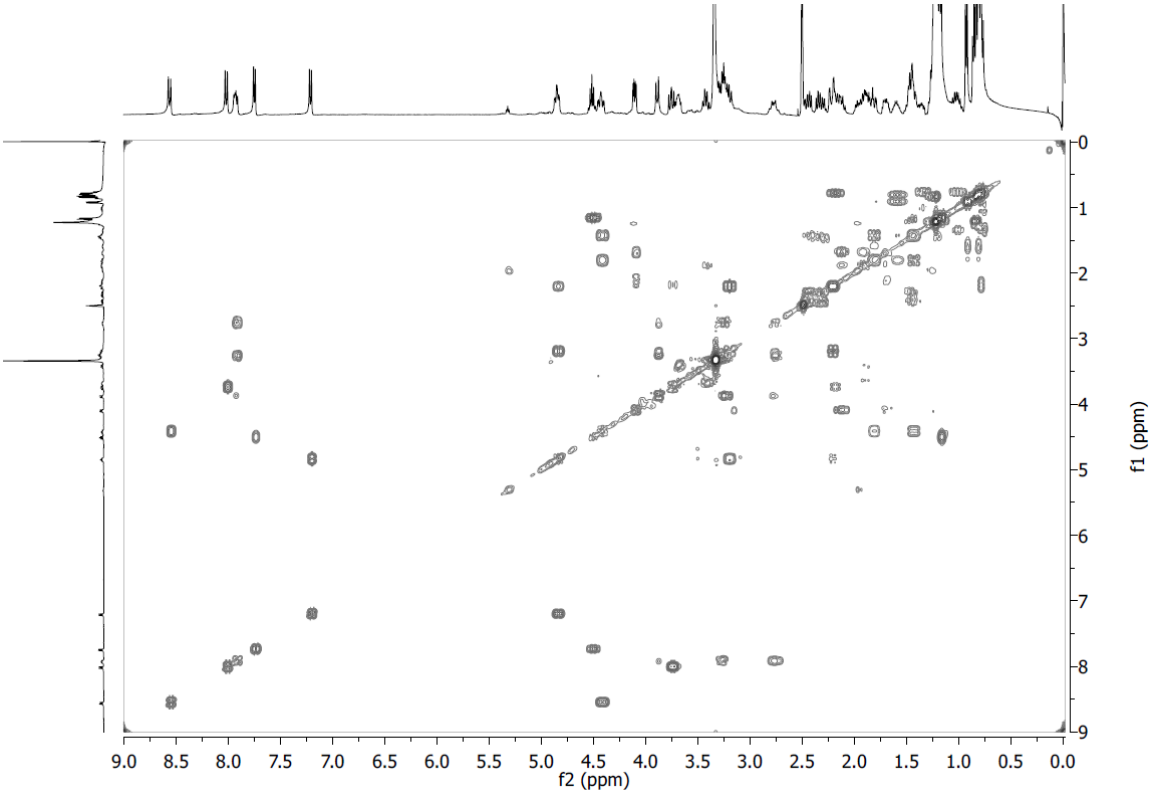

Fig. S6. ^{1}H-^{1}H COSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B **(2).**

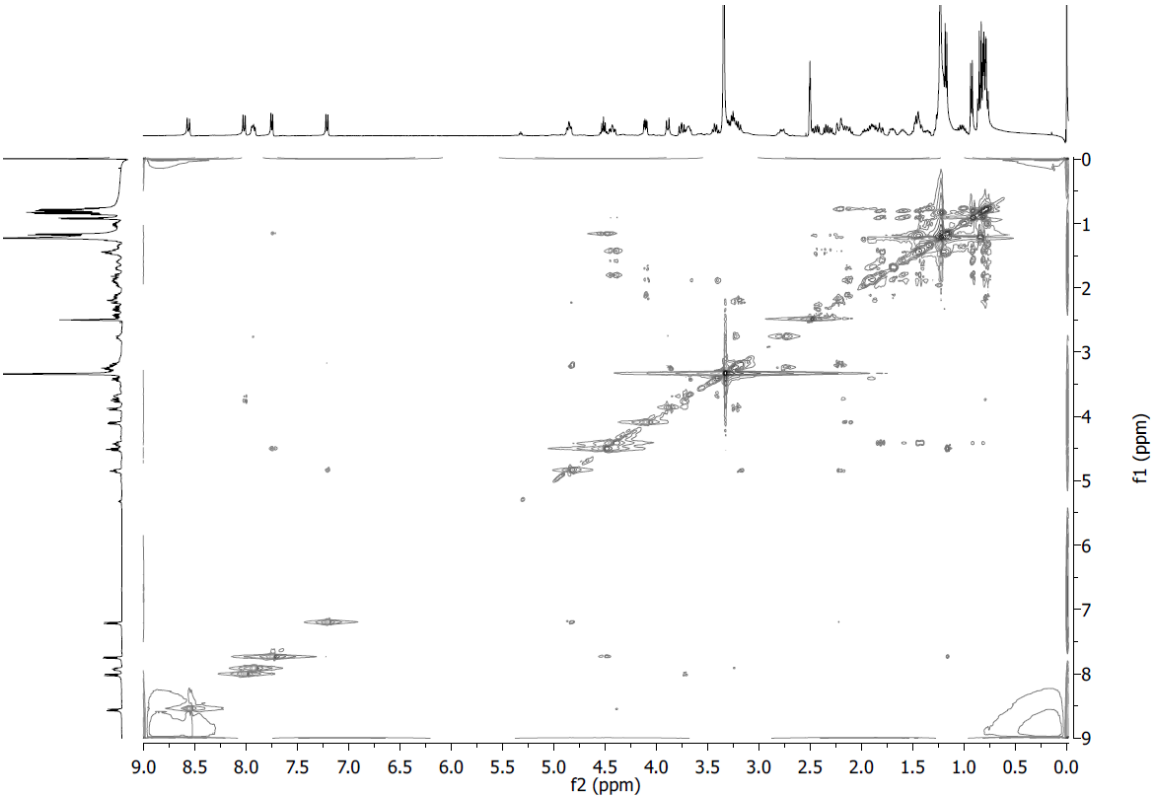

Fig. S7. ^{1}H-^{1}H TOCSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B **(2).**

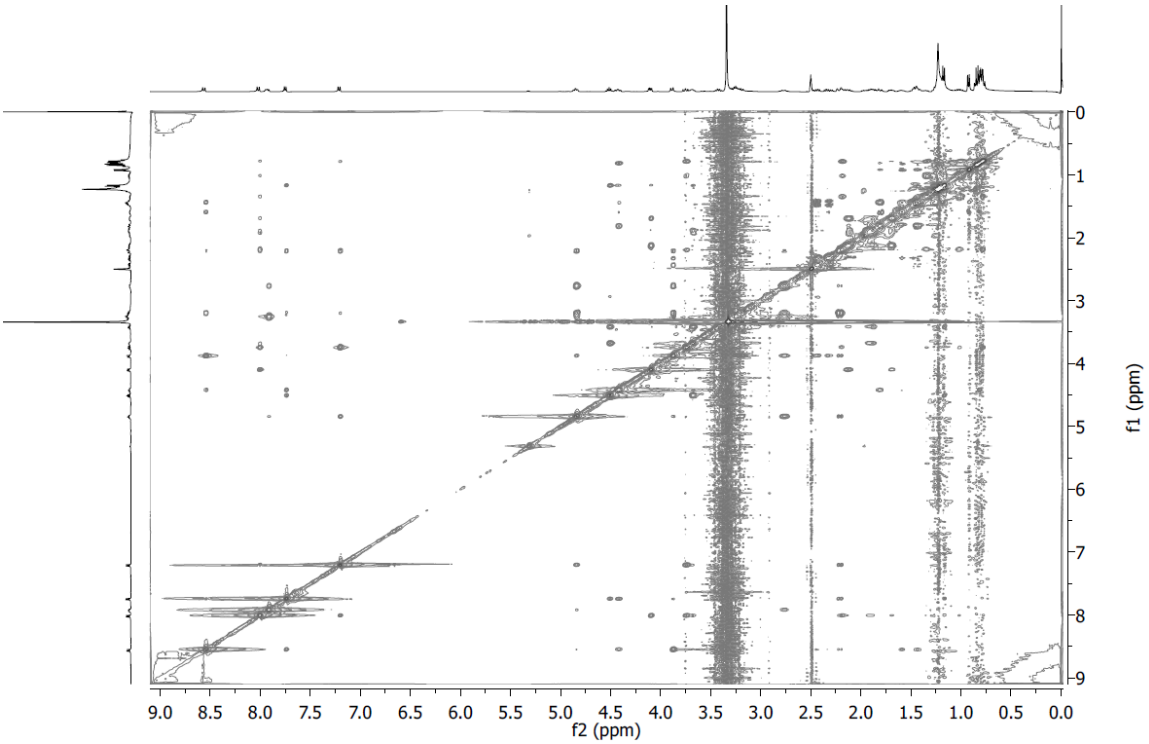

Fig. S8. ^{1}H-^{1}H NOESY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin B **(2).**

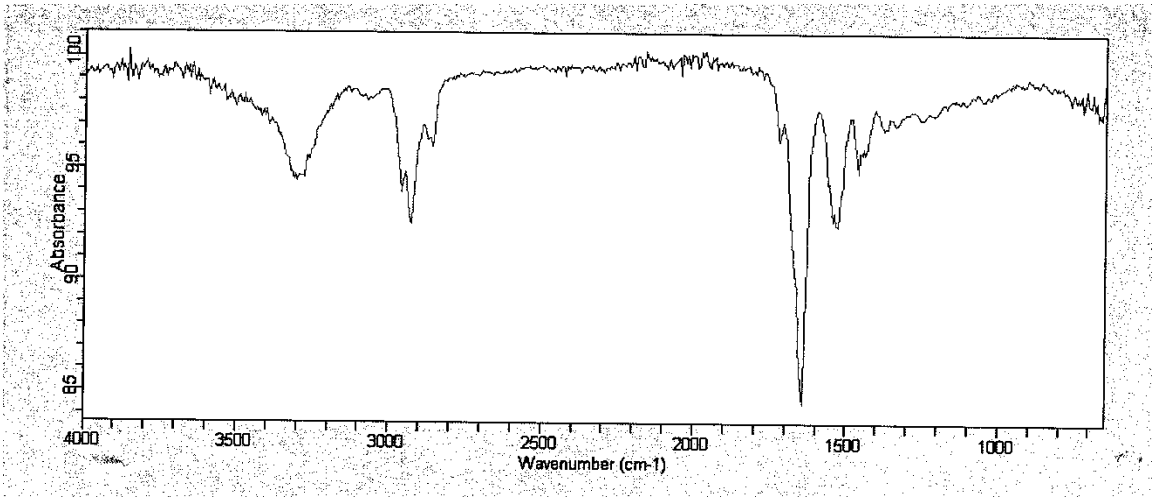

Fig. S9. FTIR spectrum of mutanobactin B **(2).**

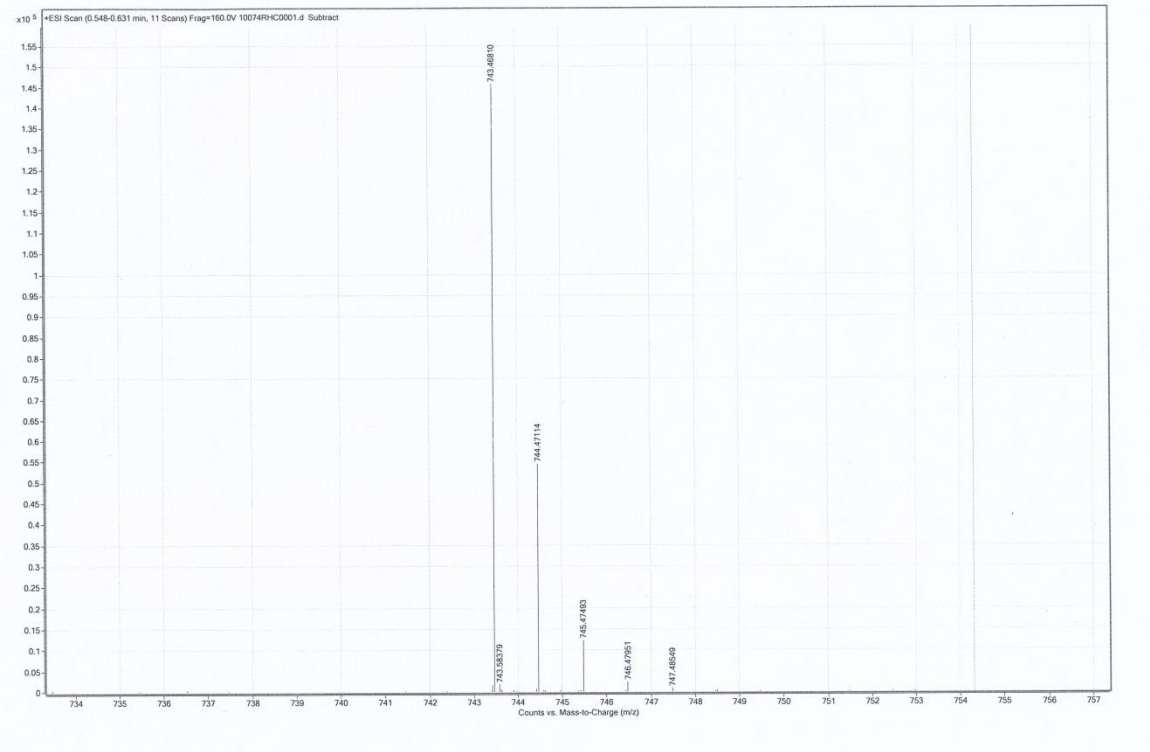

Fig. S10. HRESIMS of mutanobactin C (**3**).

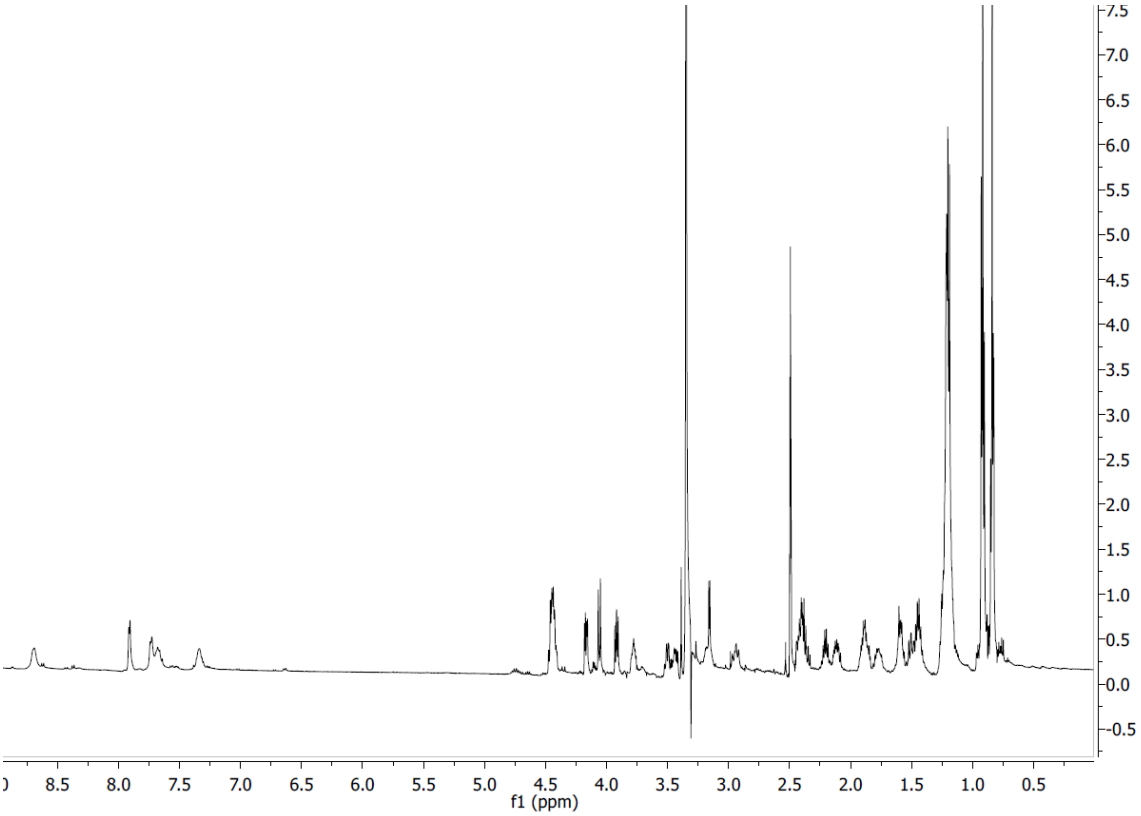

Fig. S11. ^{1}H-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C (**3**).

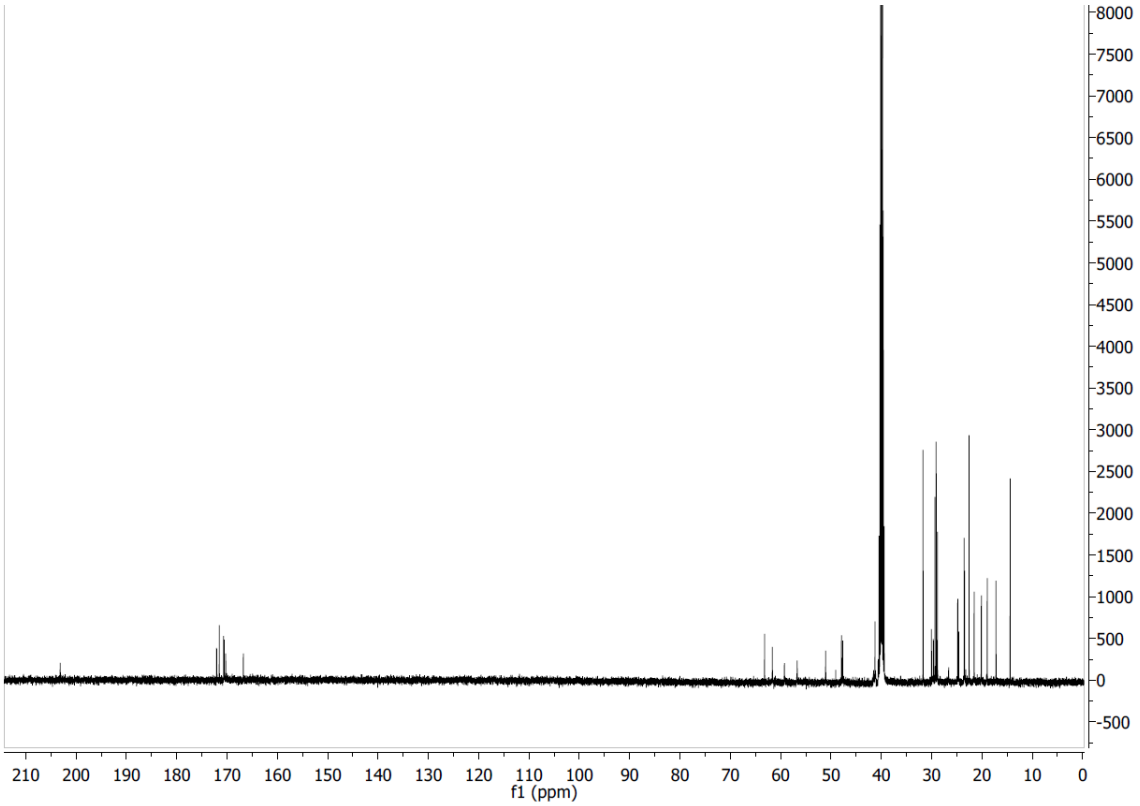

Fig. S12. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of mutanobactin C **(3).**

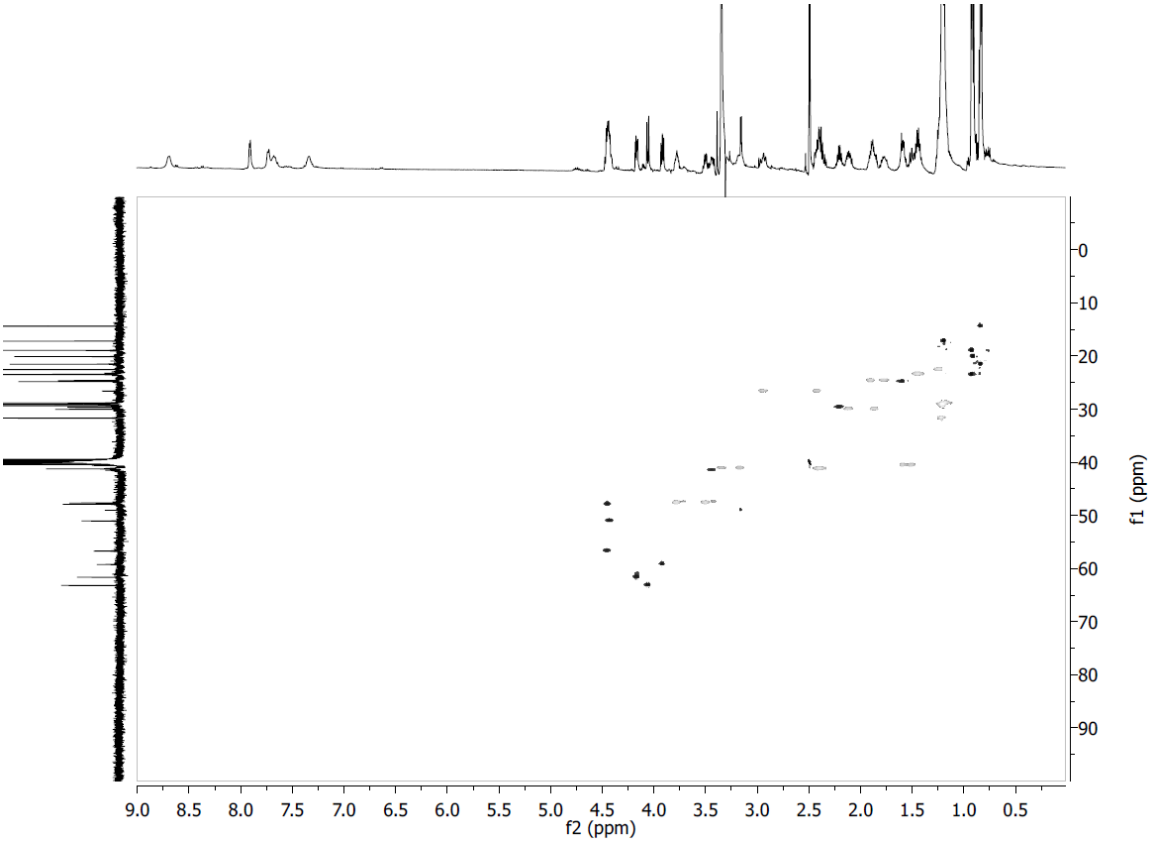

Fig. S13. ^{1}H-^{13}C HSQC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C **(3).**

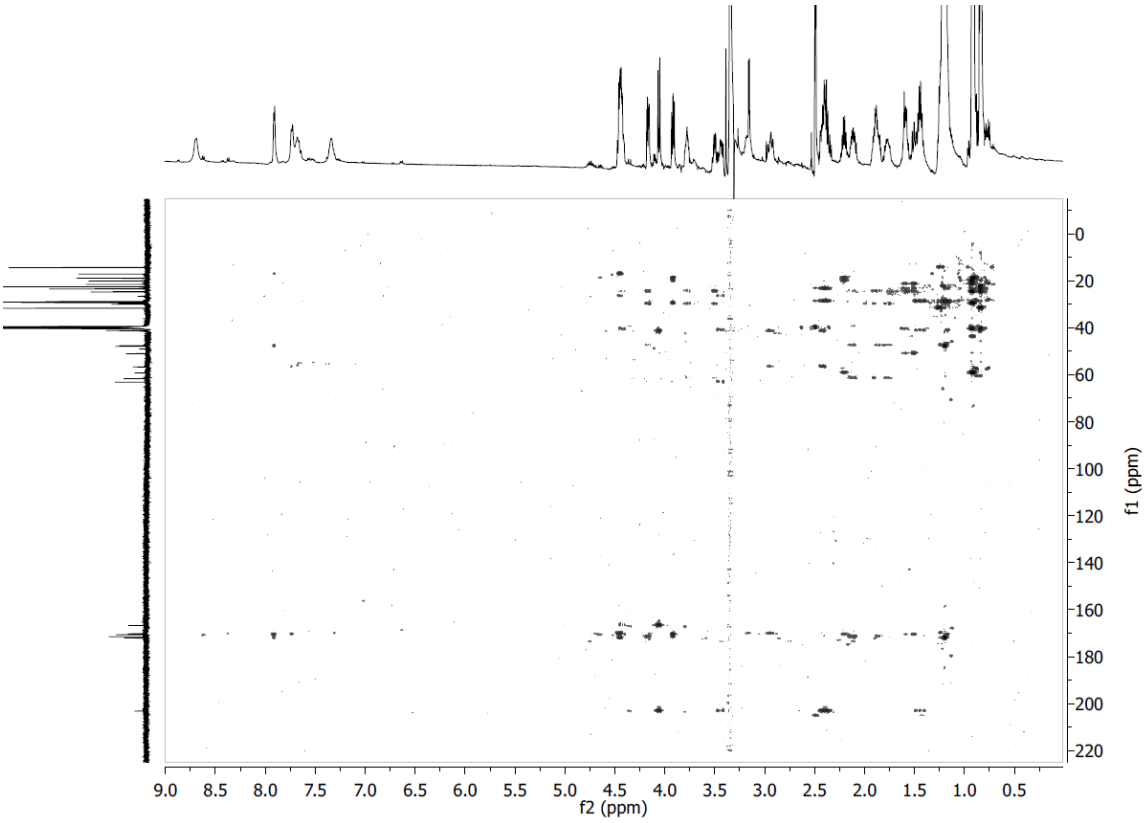

Fig. S14. ^{1}H-^{13}C HMBC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C **(3).**

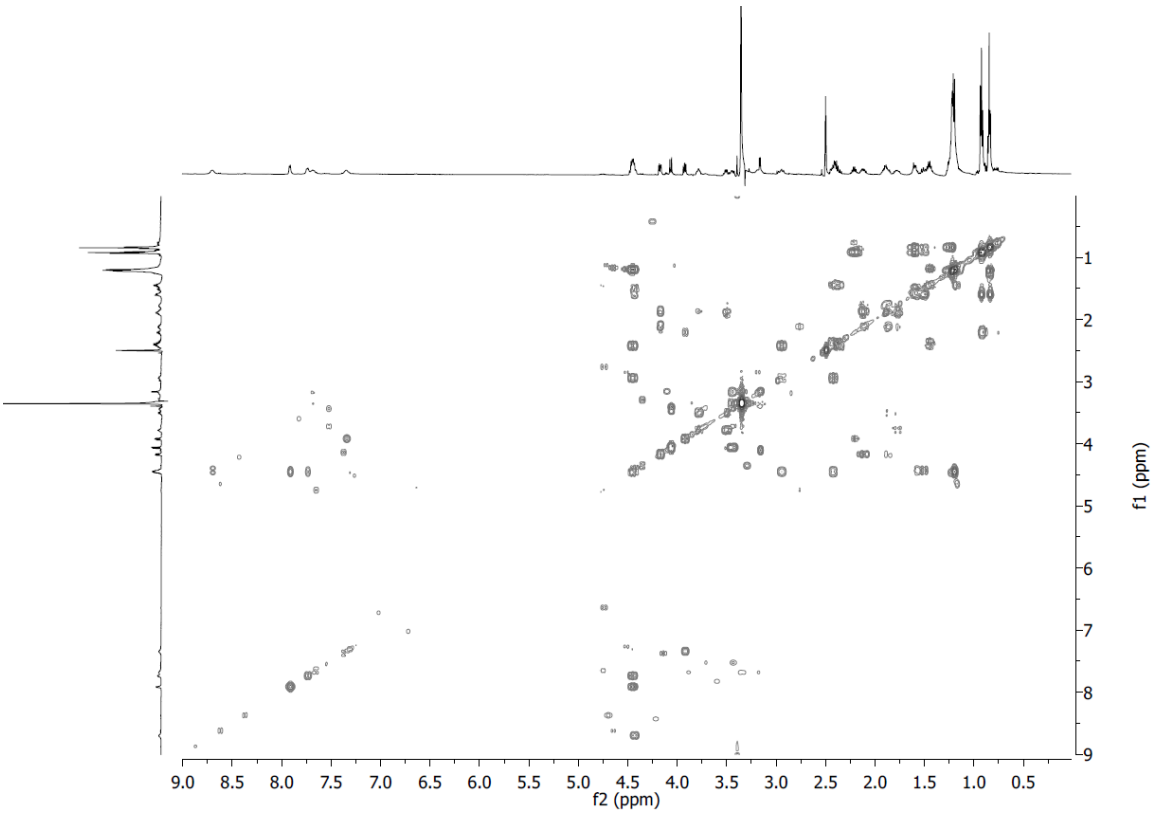

Fig. S15. ^{1}H-^{1}H COSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C **(3).**

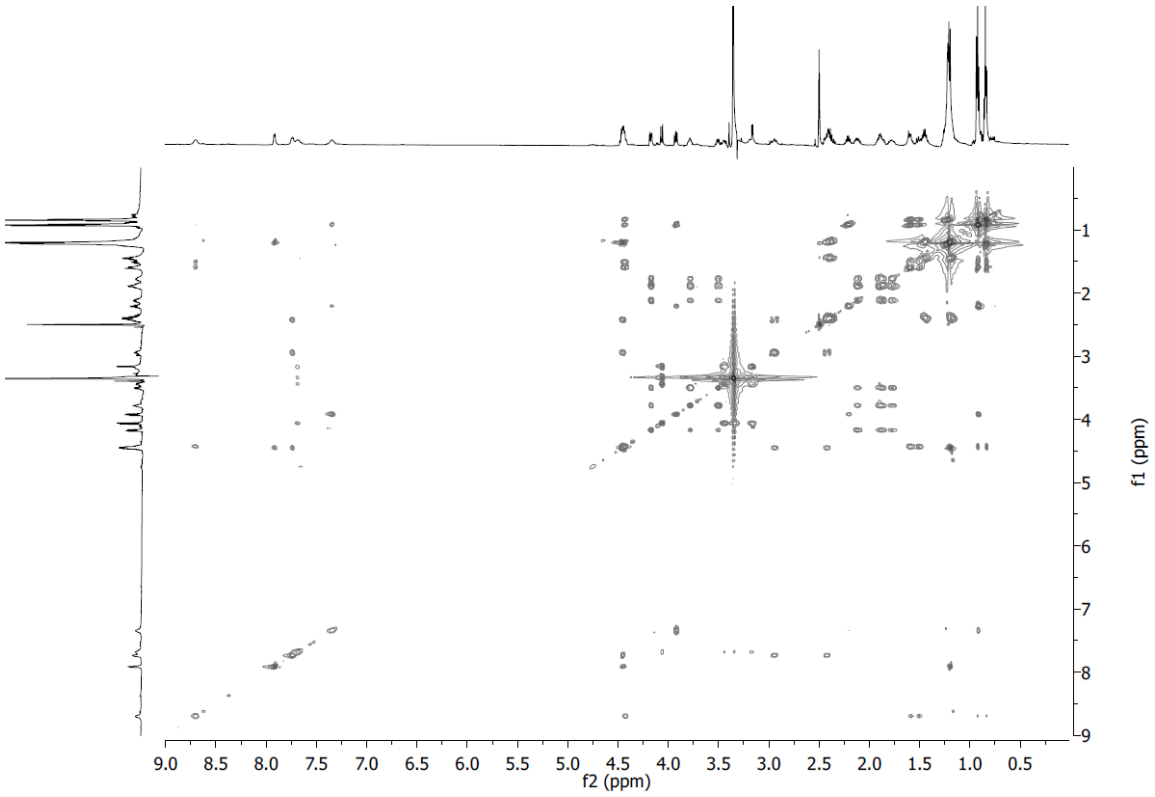

Fig. S16. ^{1}H-^{1}H TOCSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C **(3).**

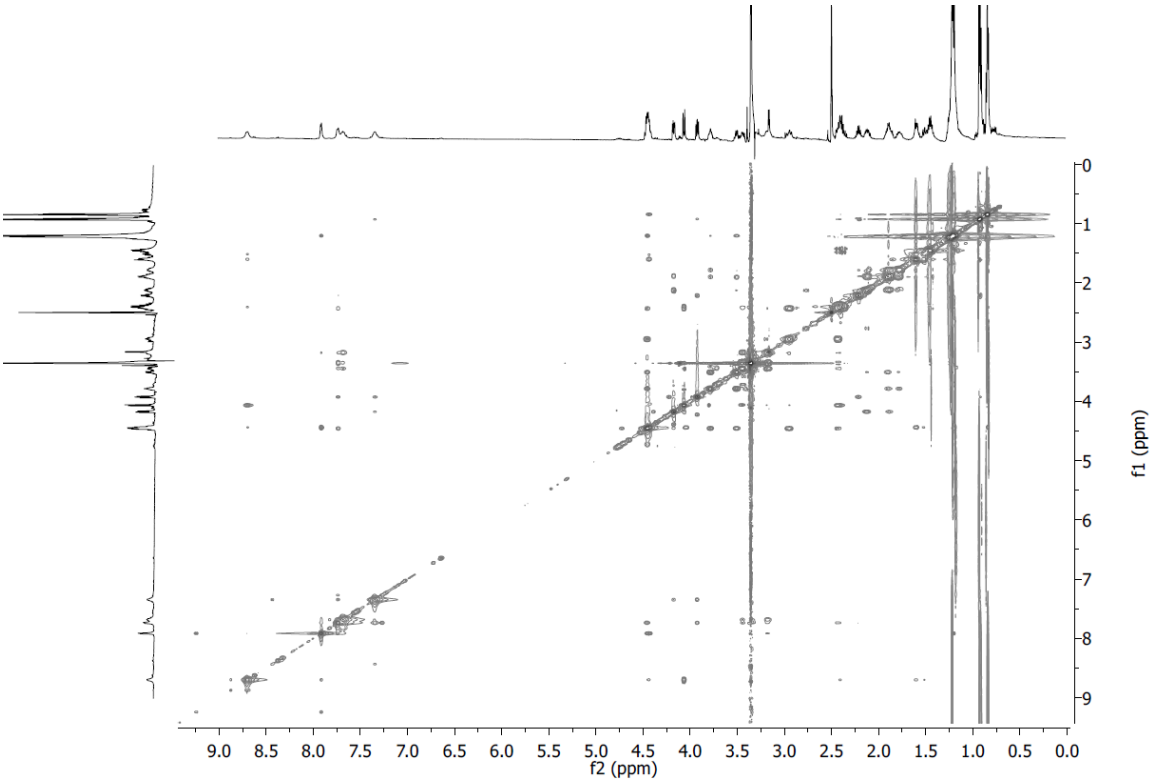

Fig. S17. ^{1}H-^{1}H NOESY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin C **(3).**

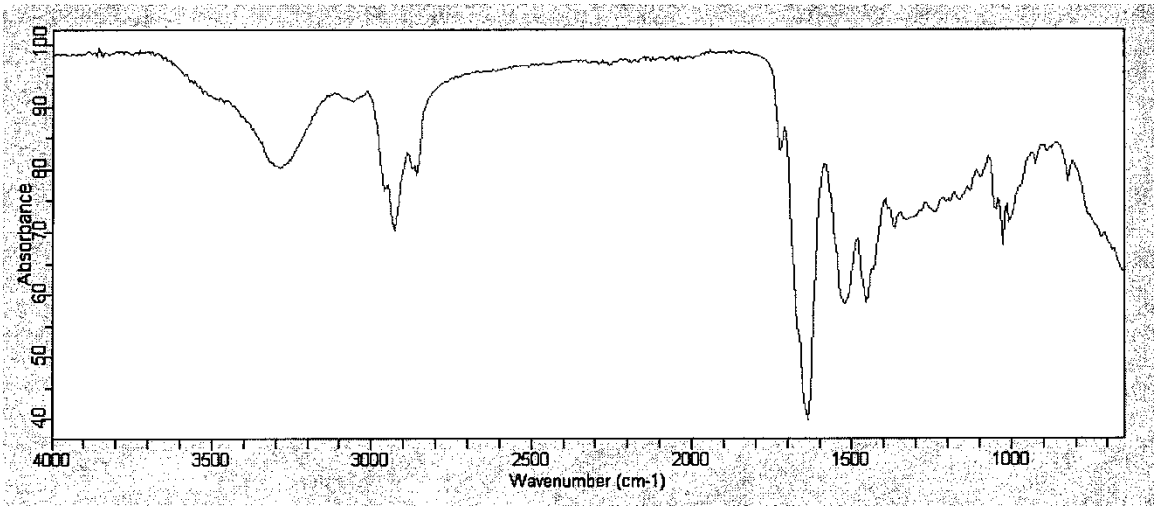

Fig. S18. FTIR spectrum of mutanobactin C **(3).**

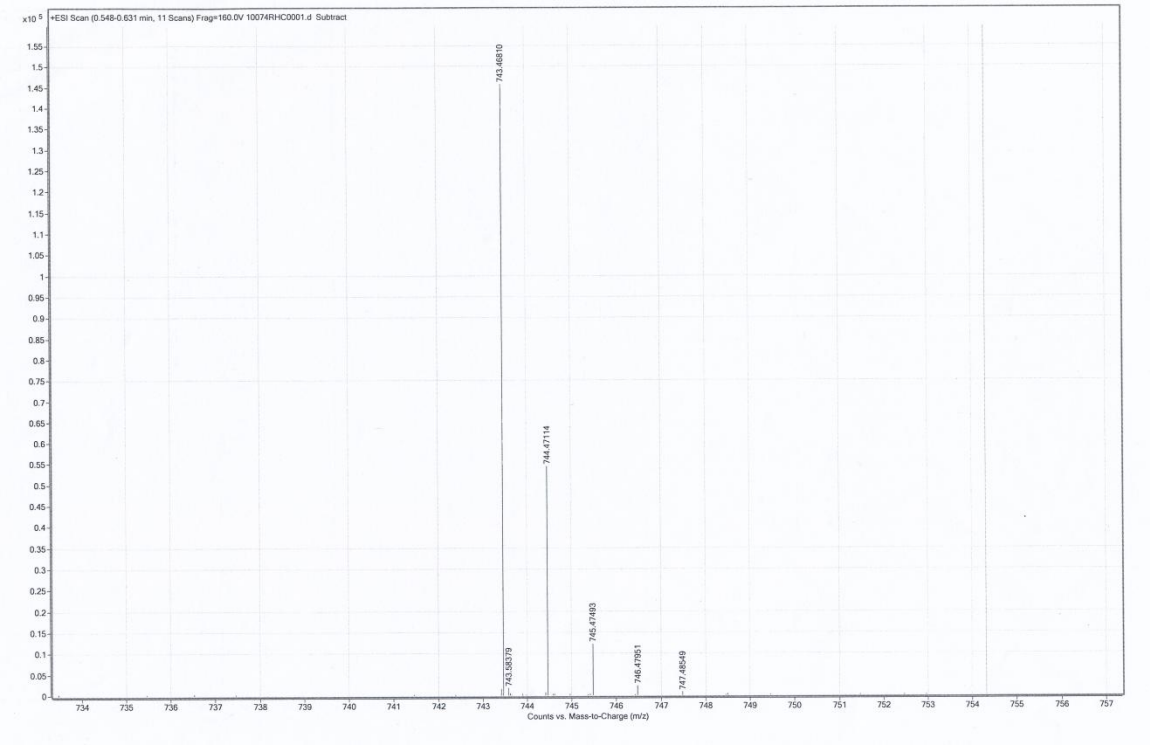

Fig. S19. HRESIMS of mutanobactin D (**4**).

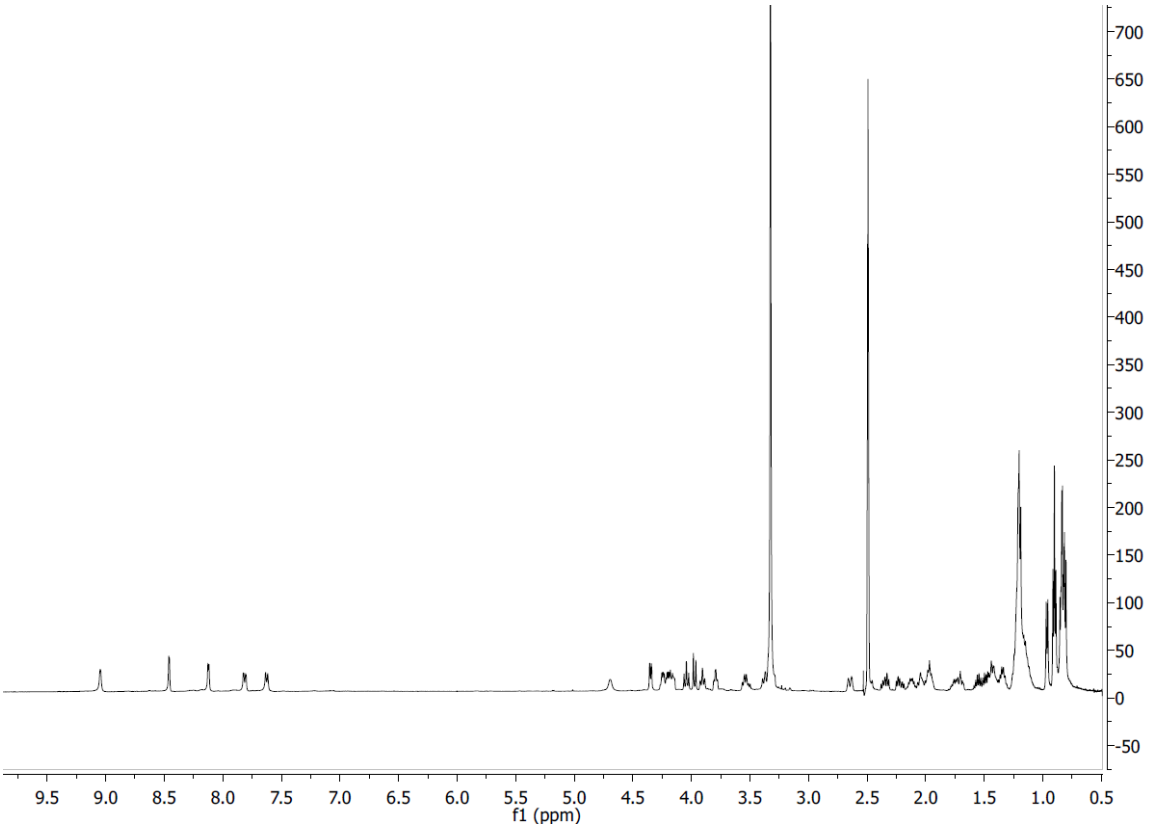

Fig. S20. ^{1}H-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

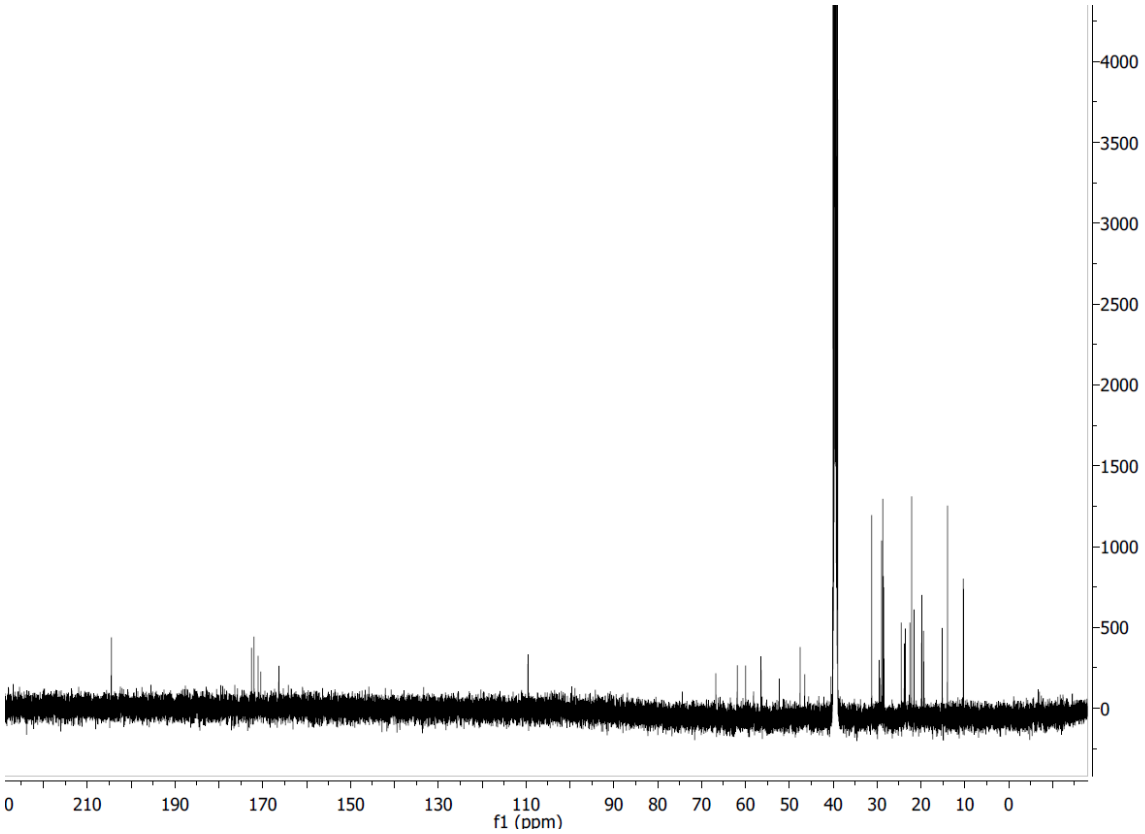

Fig. S21. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of mutanobactin D **(4).**

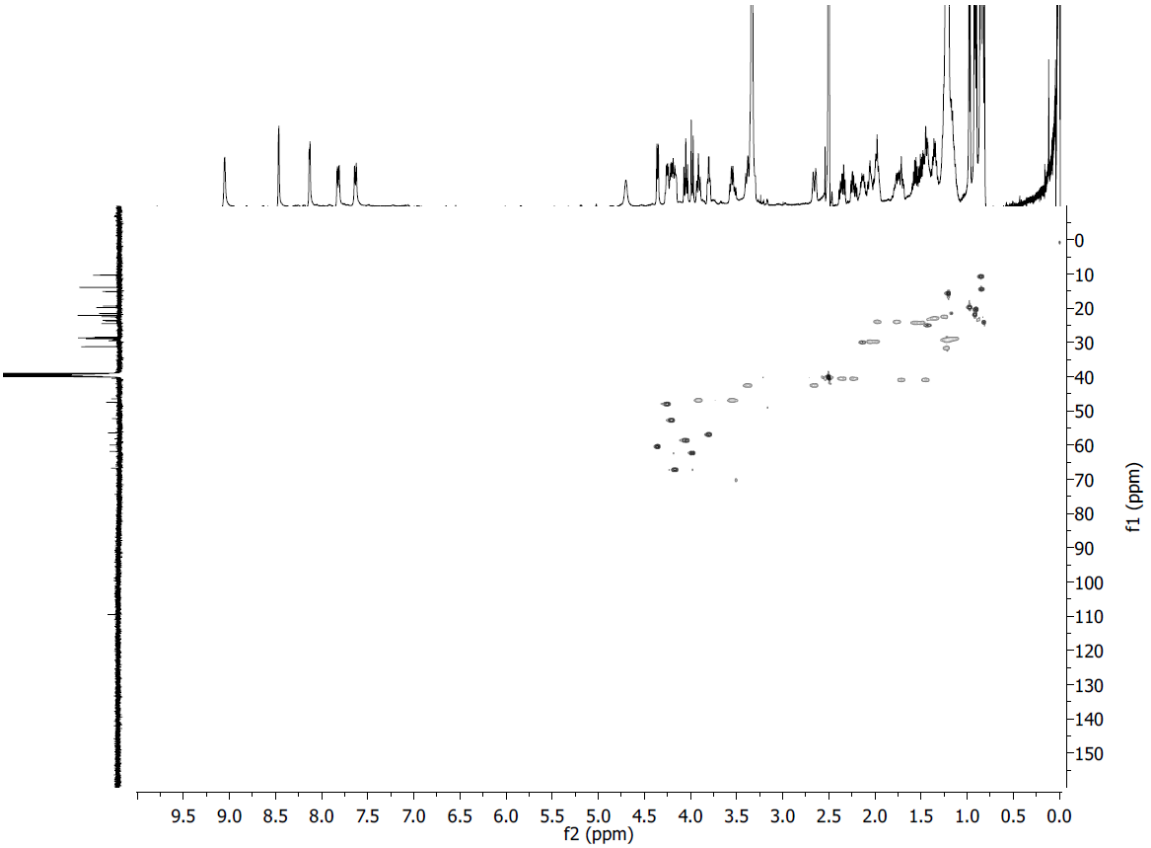

Fig. S22. ^{1}H-^{13}C HSQC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

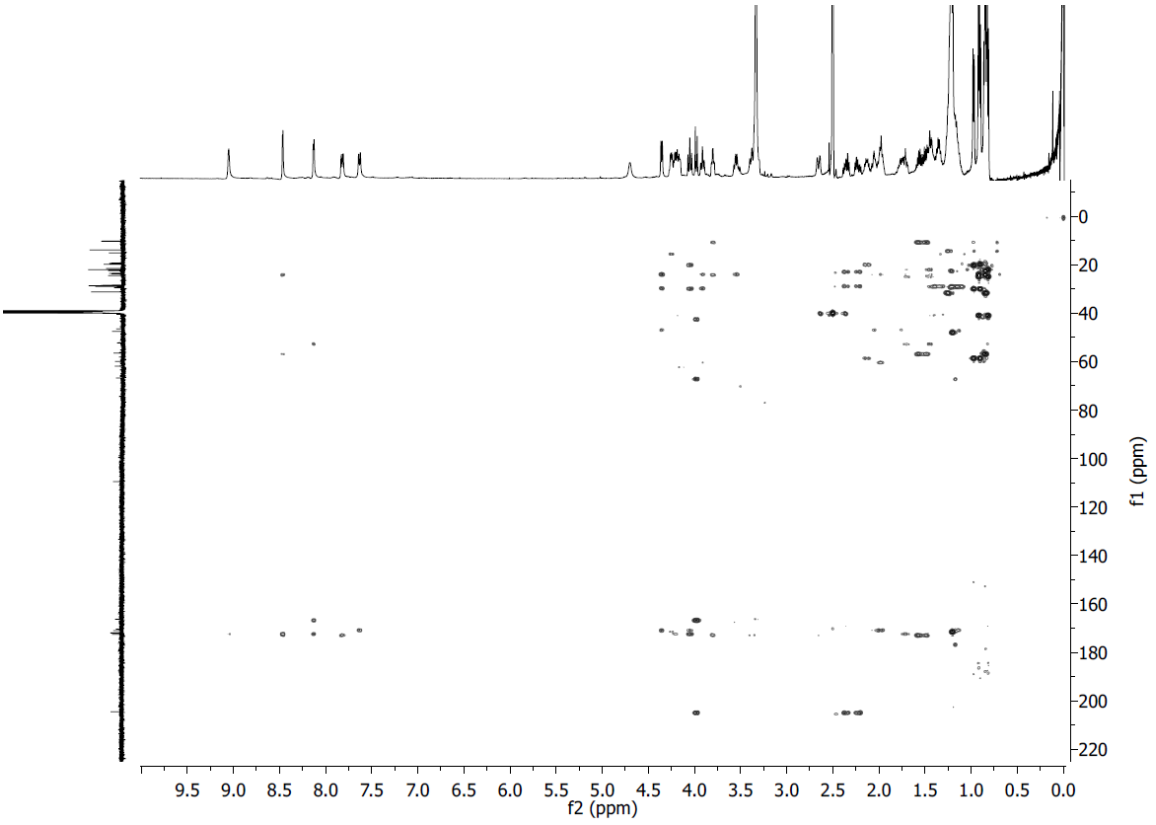

Fig. S23. ^{1}H-^{13}C HMBC-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

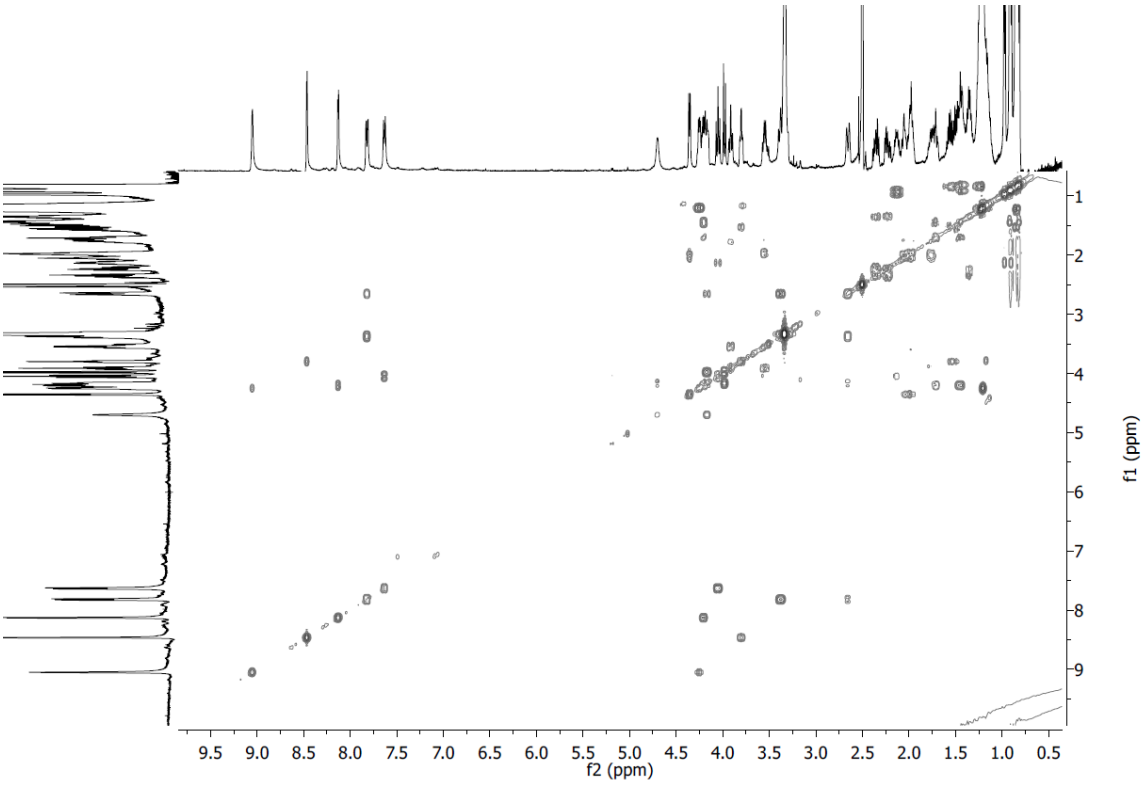

Fig. S24. ^{1}H-^{1}H COSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

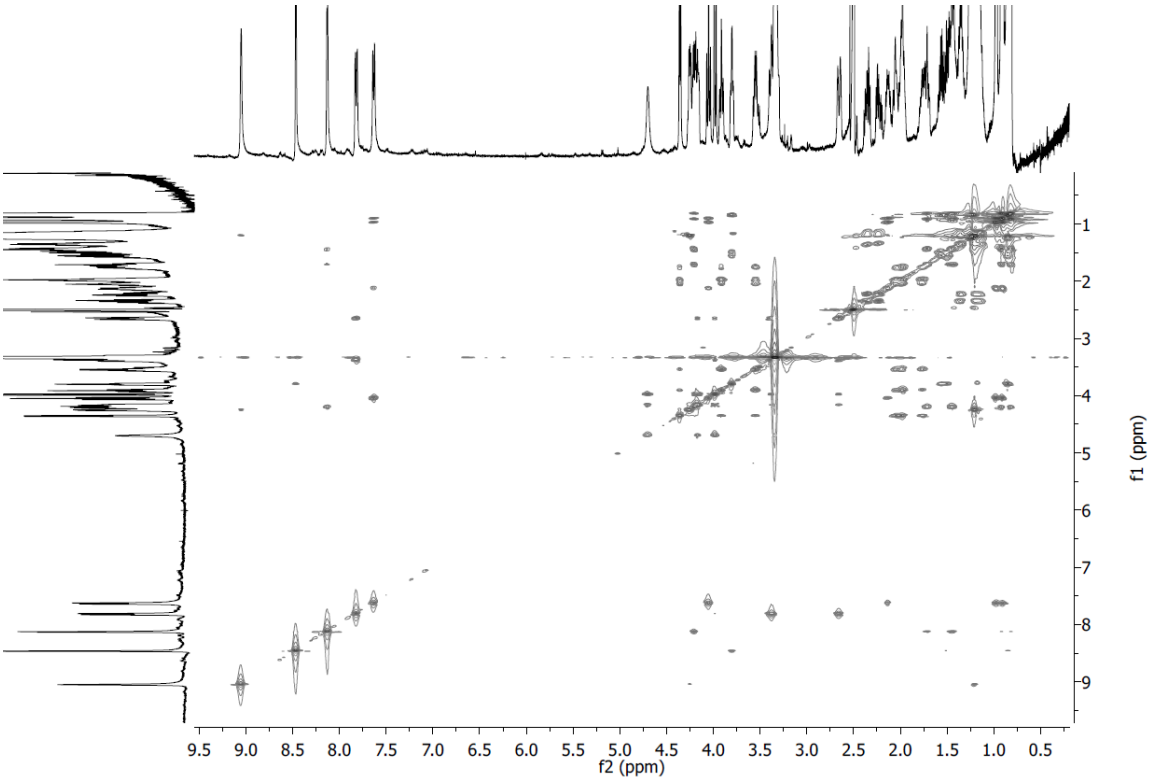

Fig. S25. ^{1}H-^{1}H TOCSY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

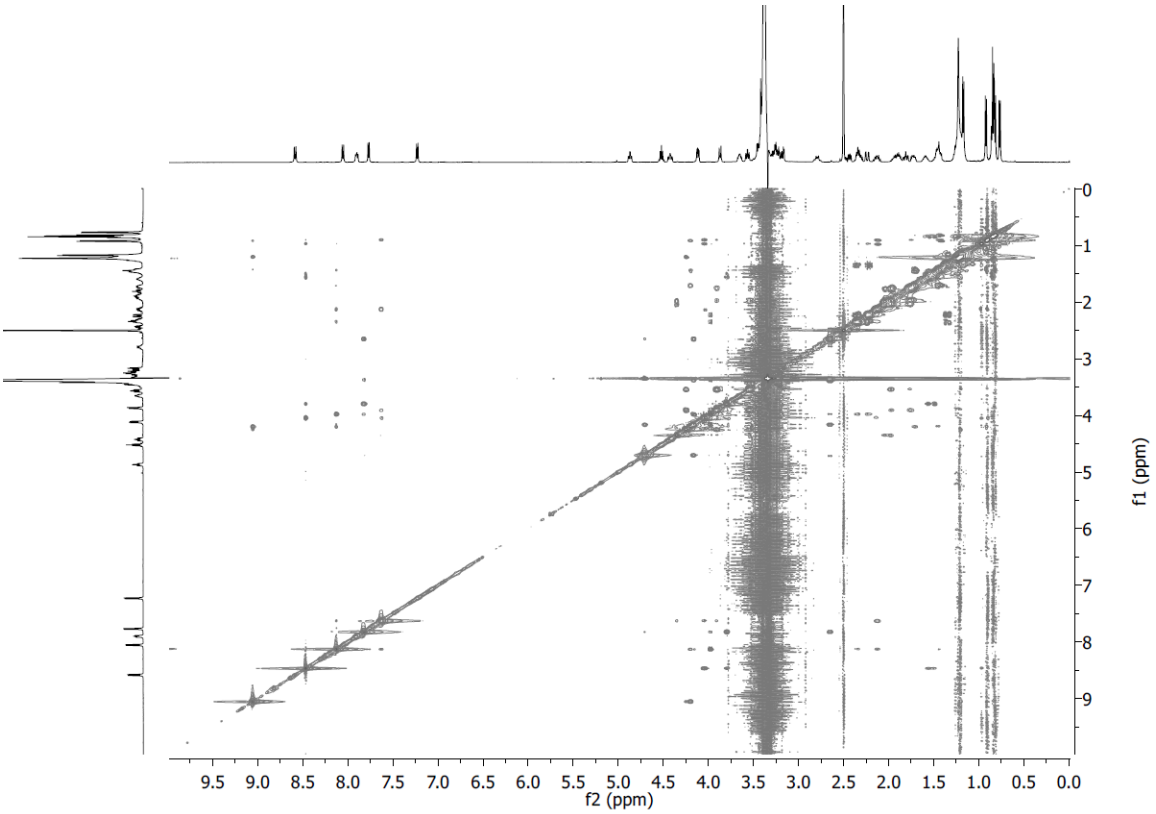

Fig. S26. ^{1}H-^{1}H NOESY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin D **(4).**

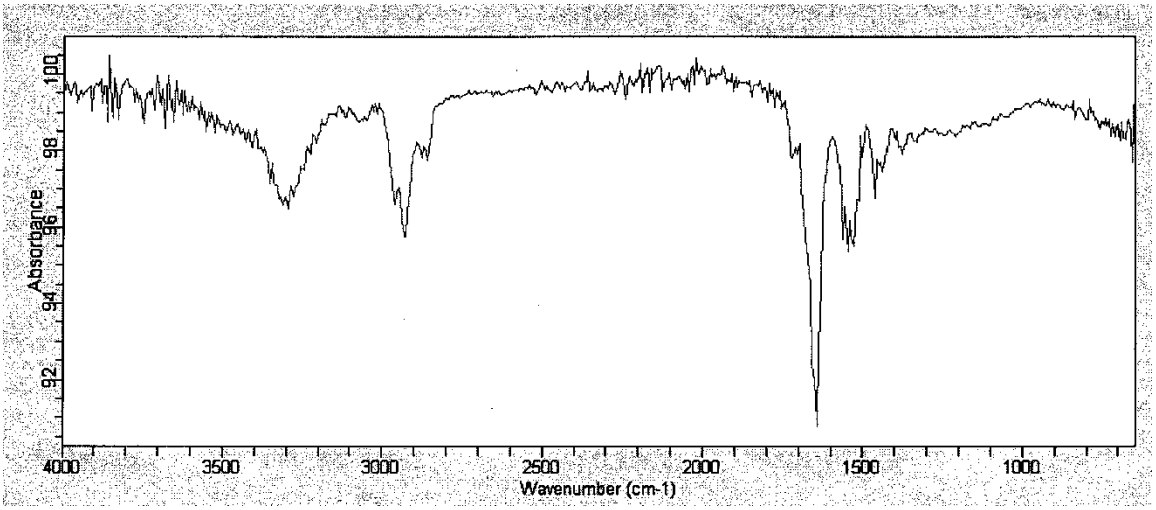

Fig. S27. FTIR spectrum of mutanobactin D **(4).**

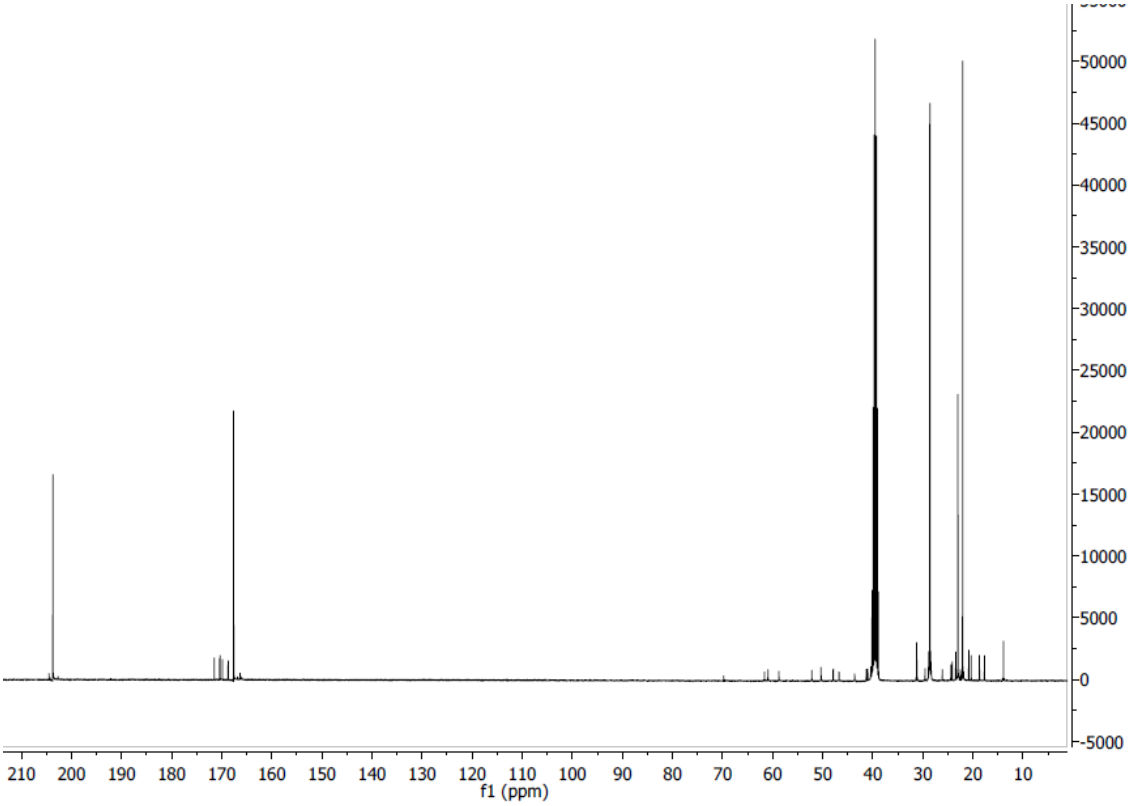

Fig. S28. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of [1-^{13}C]acetate labeled mutanobactin A.

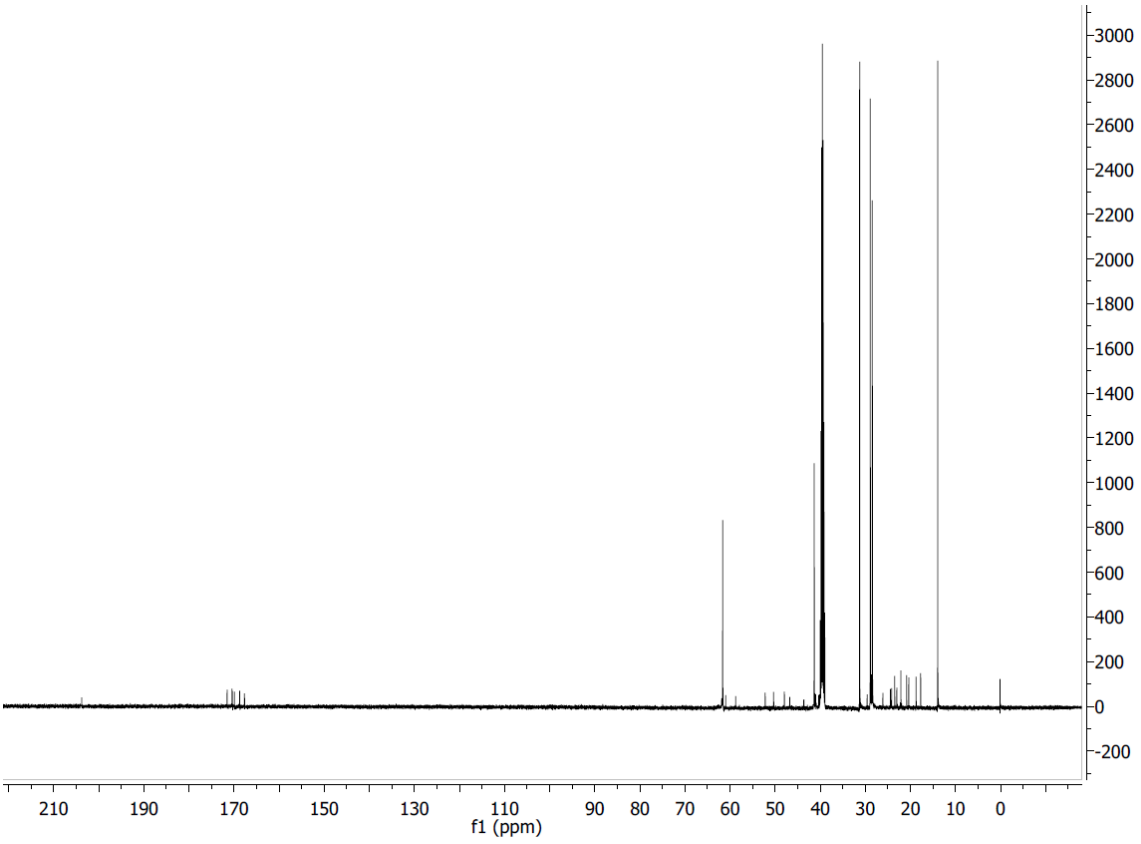

Fig. S29. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of [2-^{13}C]acetate labeled mutanobactin A.

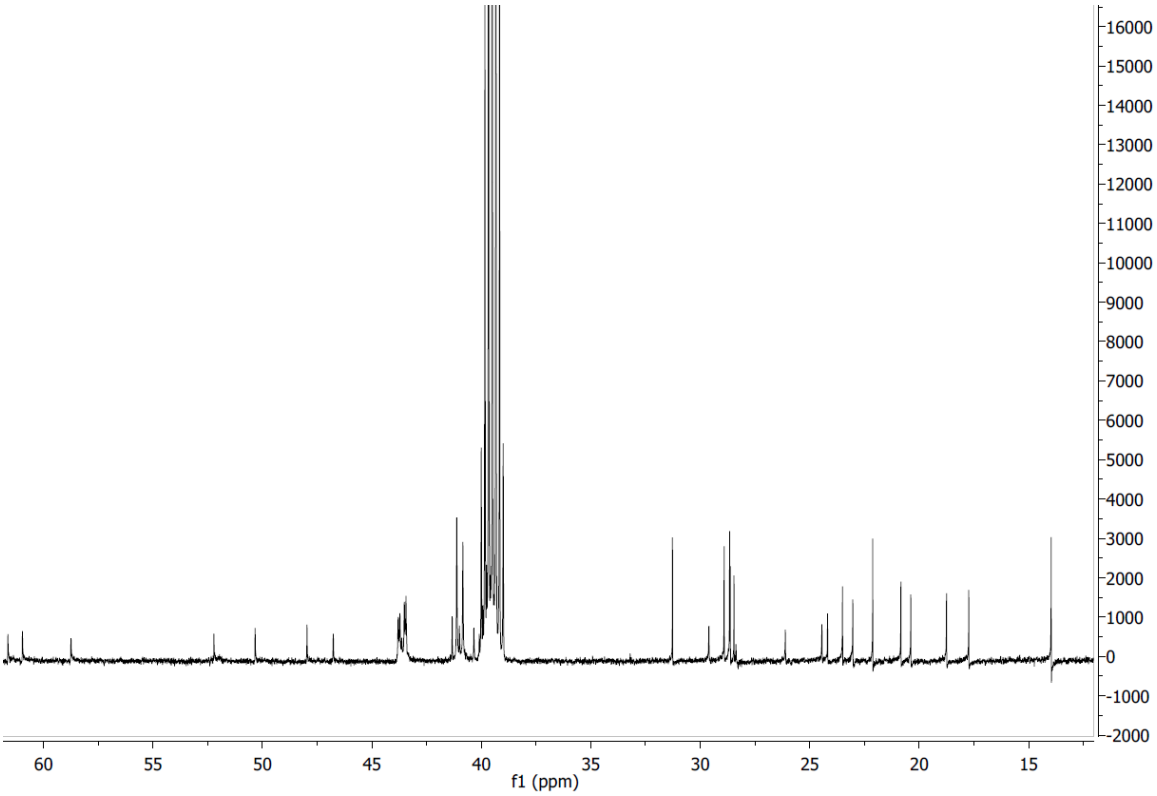

Fig. S30. ^{13}C-NMR spectrum (100 MHz, DMSO-d_6) of [^{15}N,$^{13}C_2$]glycine labeled mutanobactin A.

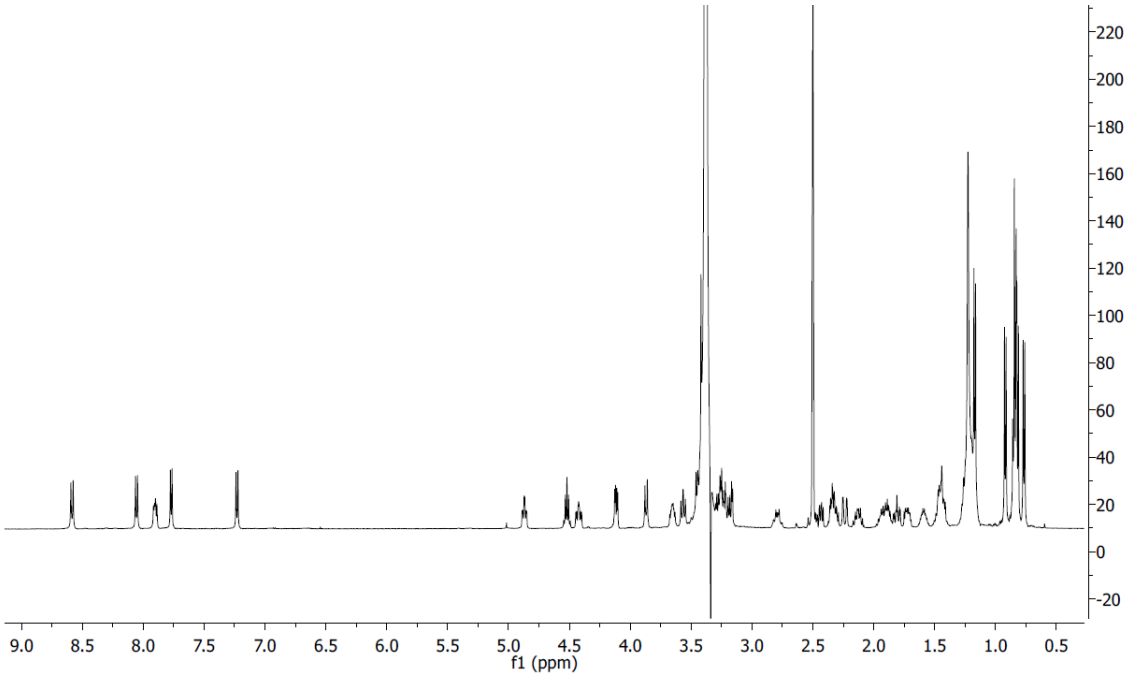

Fig. S31. ^{1}H-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin A **(1).**

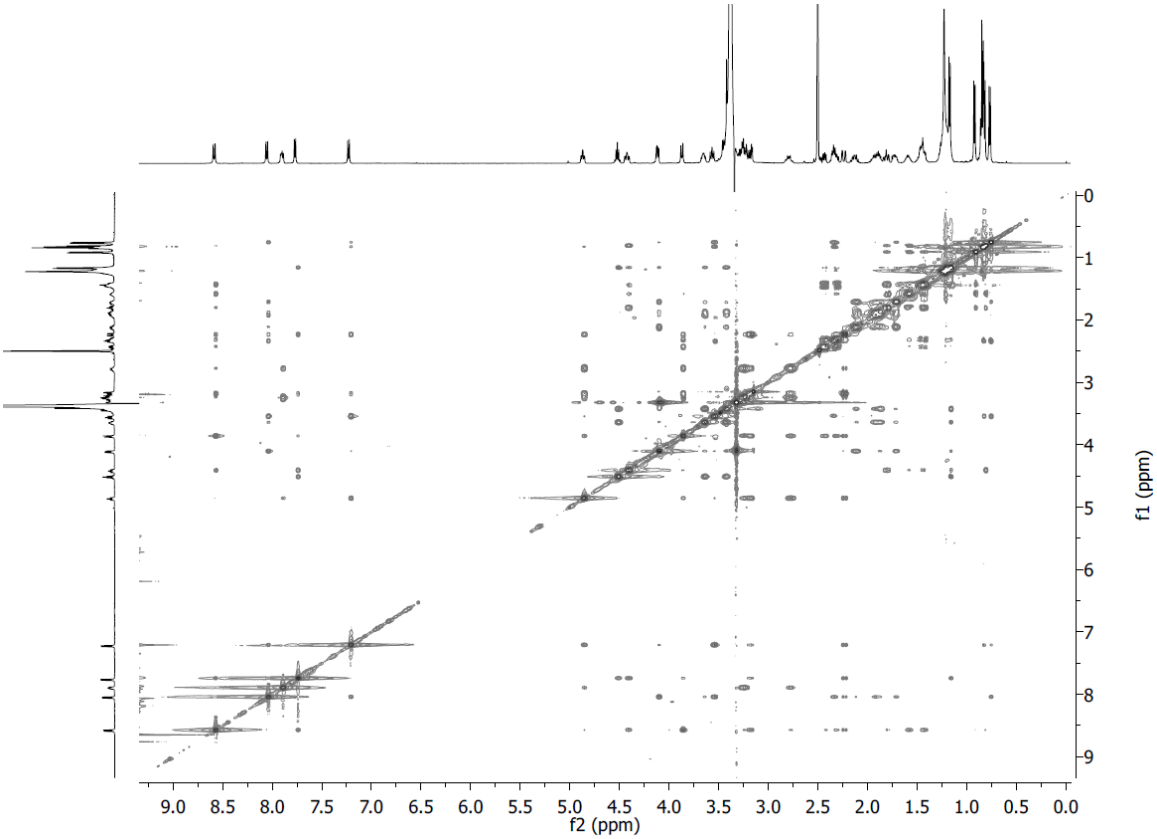

Fig. S32. ^{1}H-^{1}H NOESY-NMR spectrum (500 MHz, DMSO-d_6) of mutanobactin A **(1).**

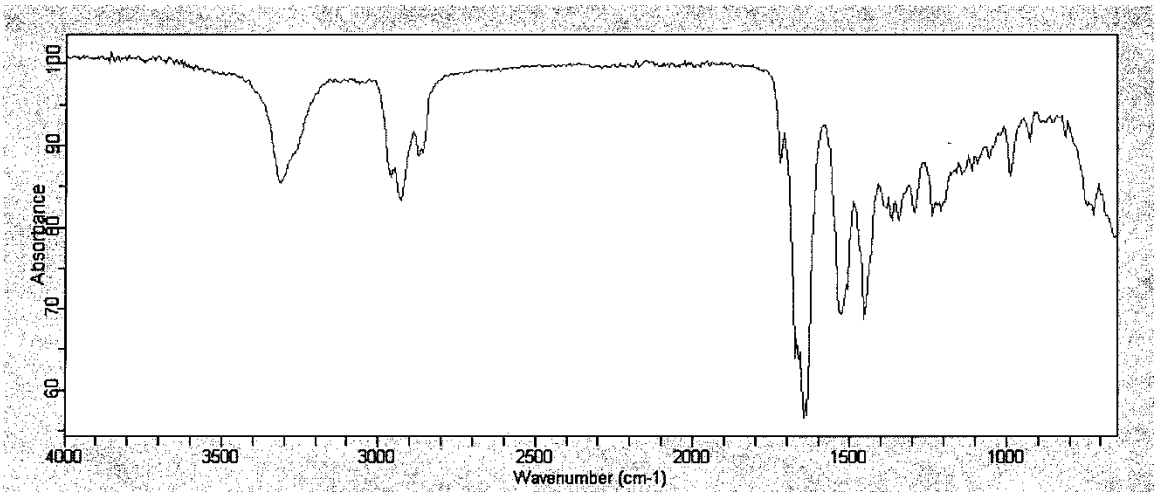

Fig. S33. FTIR spectrum of mutanobactin A (**1**).

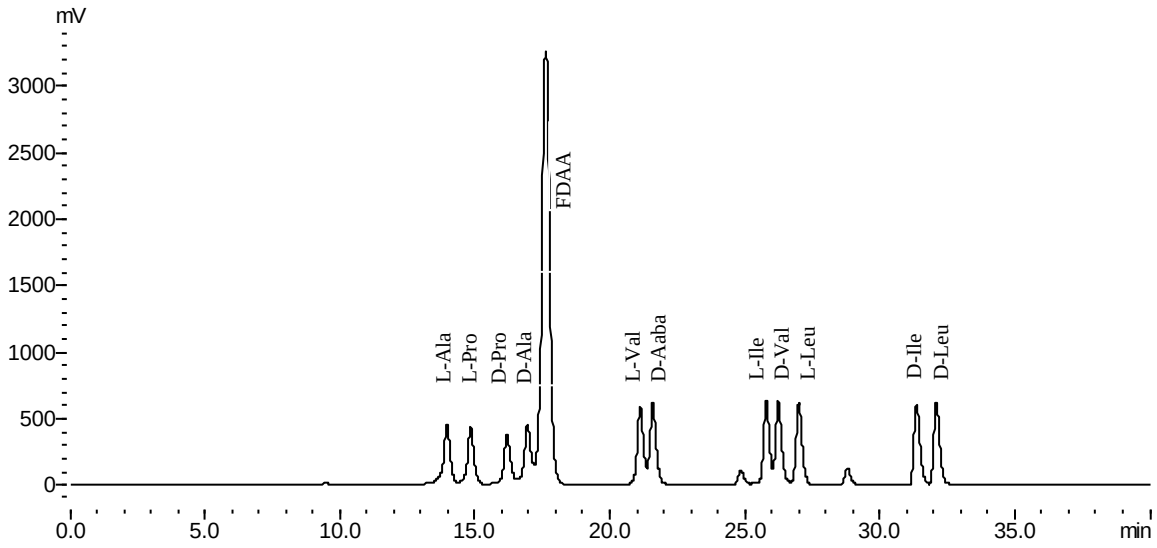

Fig. S34. Marfey's analysis of FDAA derivatized amino acid standards for the D and L forms of Aaba, Ala, Ile, Leu, Pro, and Val (note that L-Aaba elutes under the FDAA peak under this elution condition).

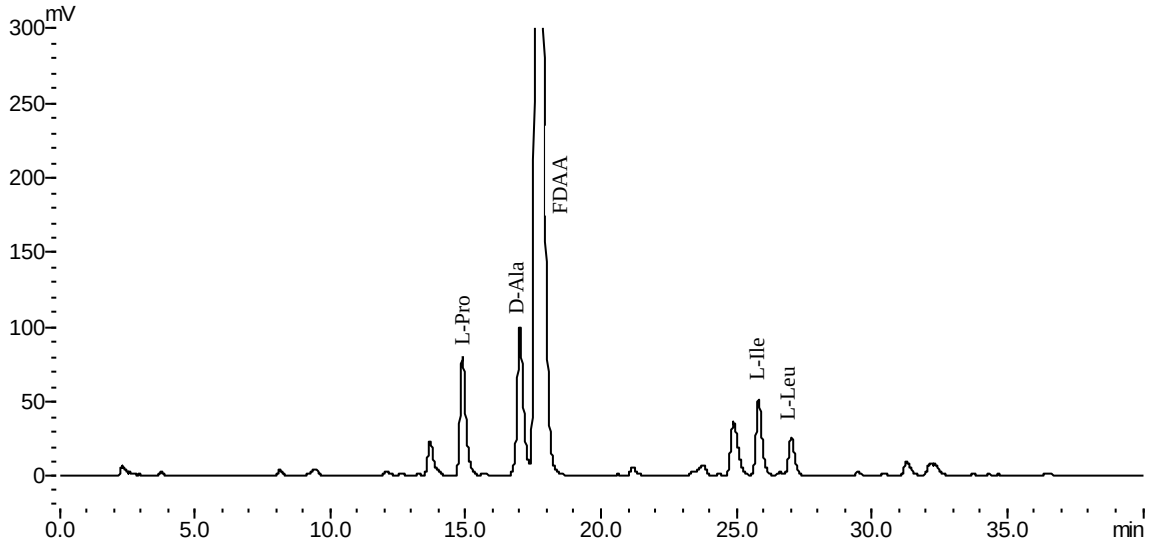

Fig. S35. Marfey's analysis of FDAA derivatized hydrolysates of **2**.

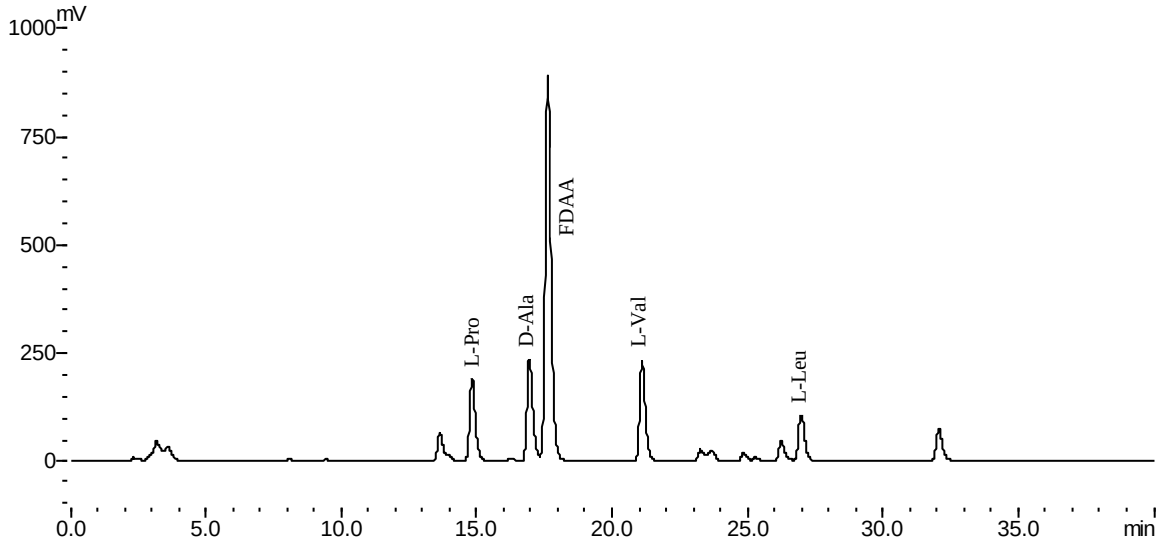

Fig. S36. Marfey's analysis of FDAA derivatized hydrolysates of **3**.

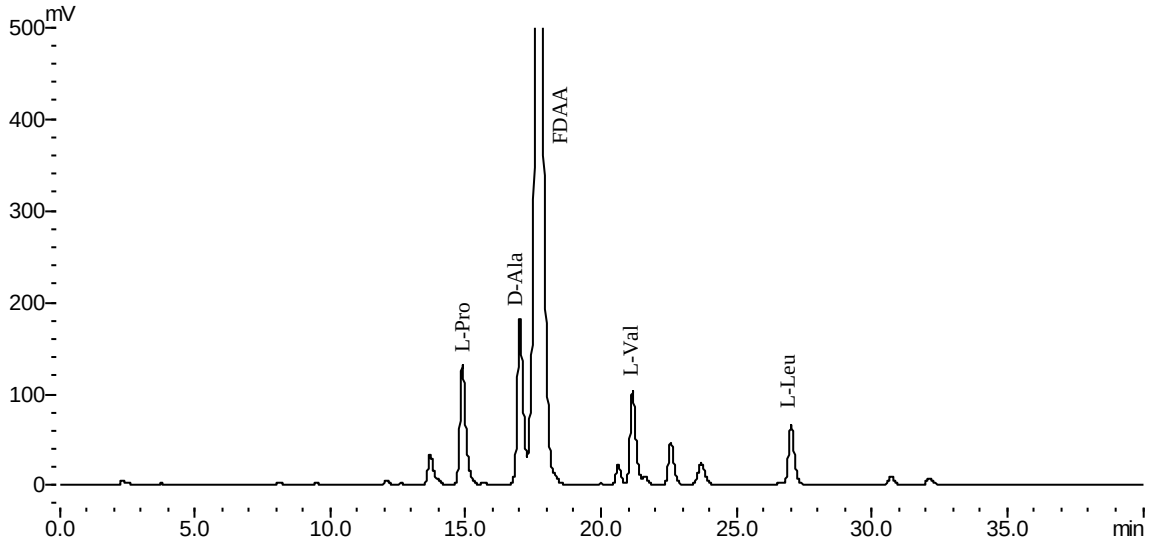

Fig. S37. Marfey's analysis (gradient elution) of FDAA derivatized hydrolysates of **4** (note that L-Aaba elutes under the FDAA peak under this elution condition).

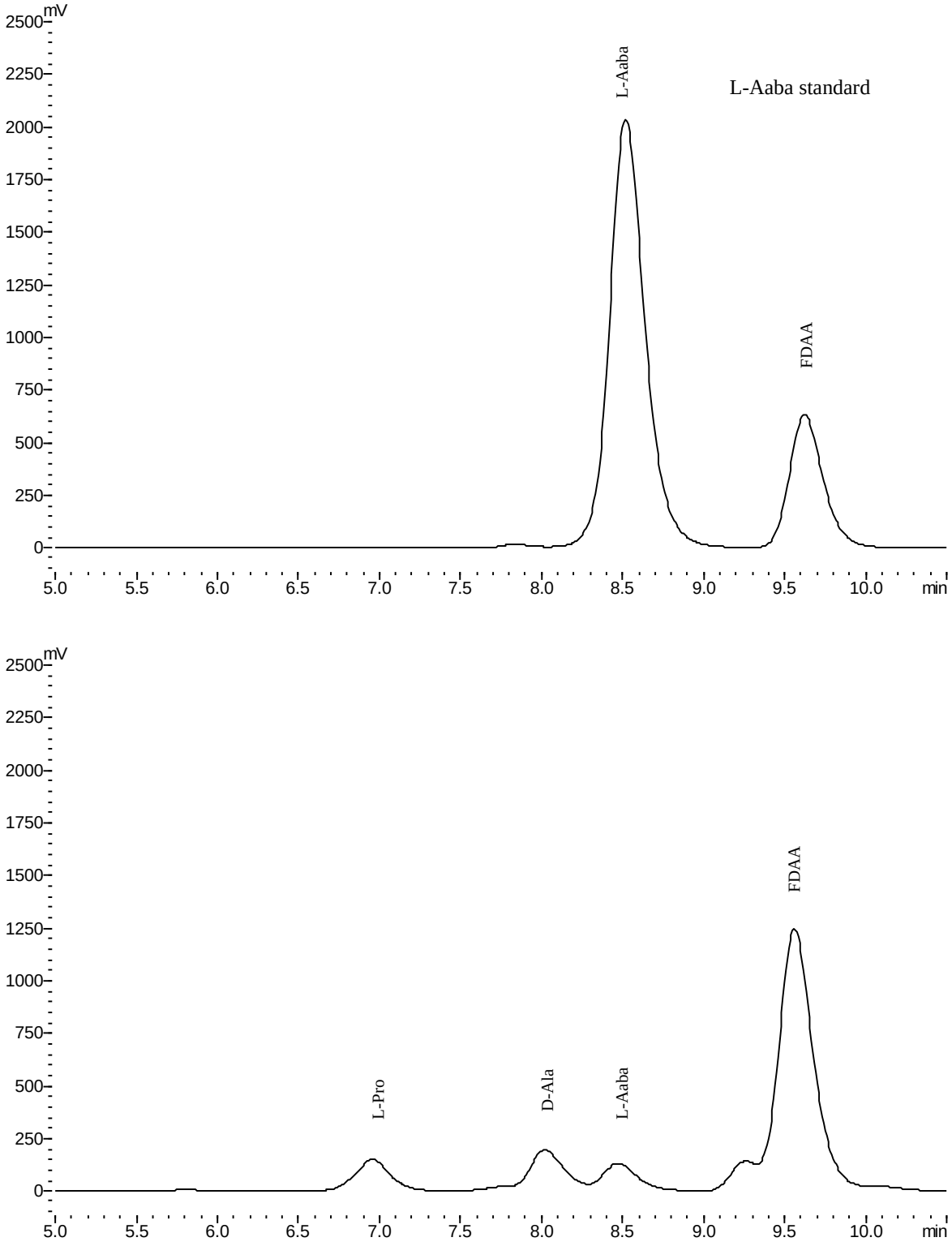

Fig. S38. Marfey's analysis (isocratic elution) of FDAA derivatized hydrolysates of **4**.

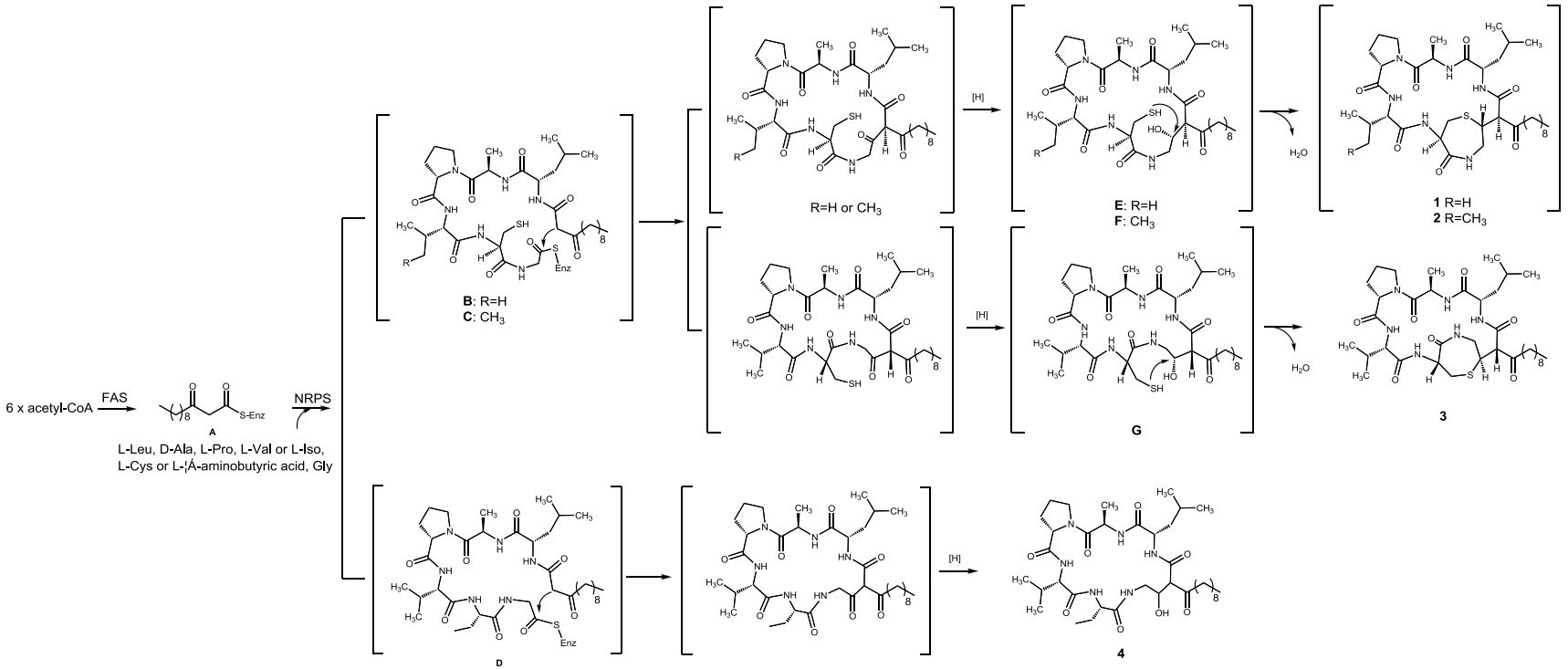

Fig. S39. Proposed biosynthetic pathways for the mutanobactins.