

Supplementary Materials

Cyclopeptide Derivatives from the Sponge-Derived Fungus

***Acremonium persicinum* F10**

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Table S1. Antifungal activities of acremonpeptide E, acremonpeptides F and their chelates (1–8)

Strains	Compounds/MIC (μM)								Amphotericin B
	1	2	3	4	5	6	7	8	
<i>A. fumigatus</i> ATCC204305	1.0	10.0	>30.0	10.0	1.0	>30.0	1.0	1.0	1.0
<i>A. niger</i> ATCC16404	3.0	30.0	>30.0	30.0	3.0	>30.0	1.0	3.0	1.0

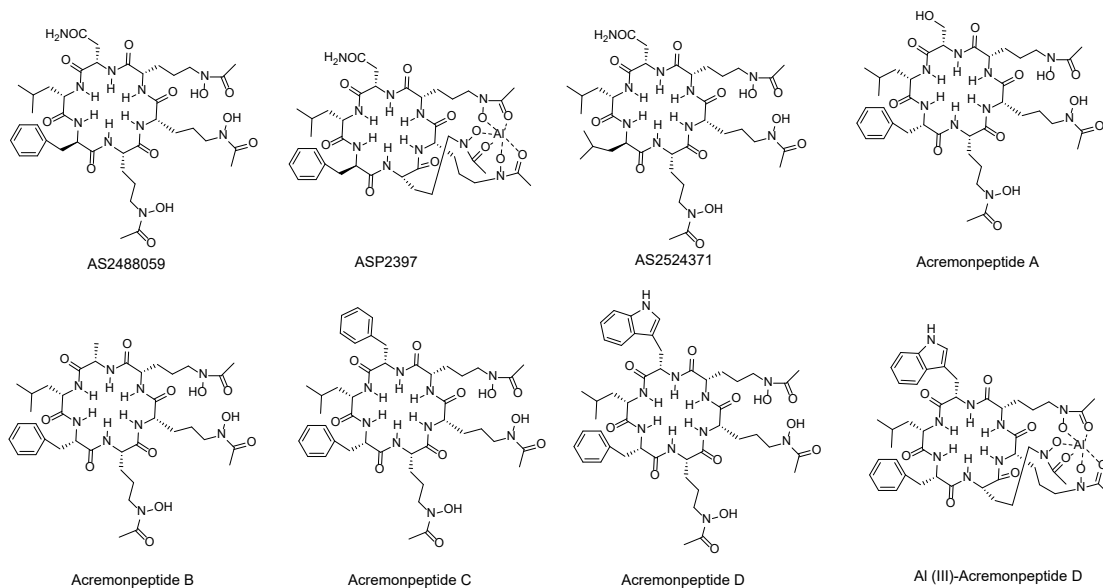


Figure S1. Chemical structures of the previously reported derivatives of ASP2397 isolated from *Acremonium persicinum*

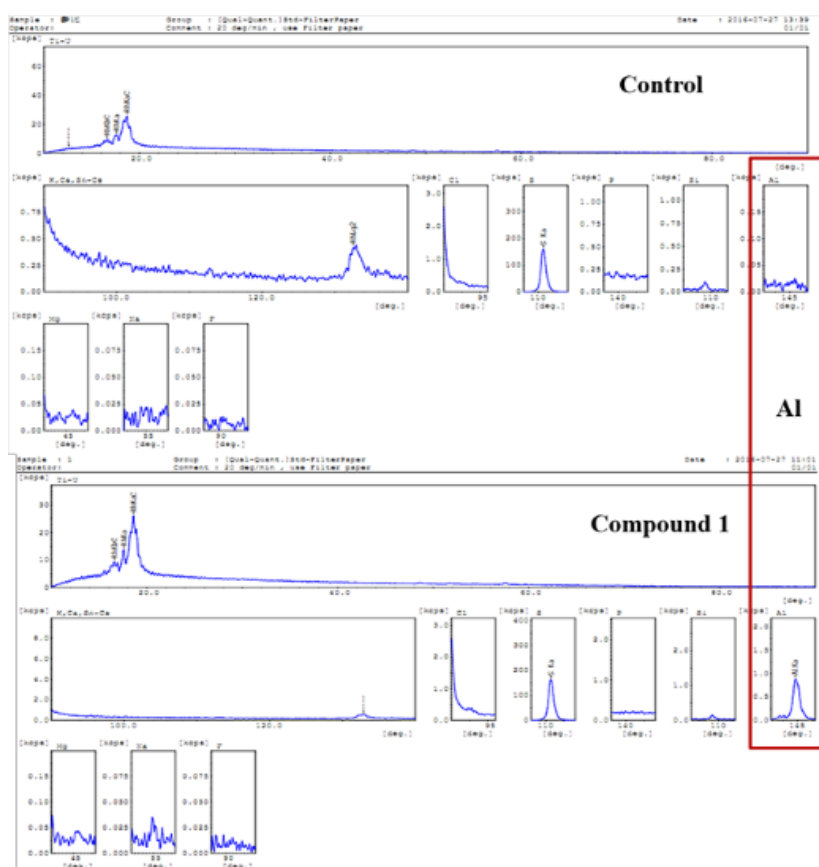


Figure S2. Elemental analysis of compound 1 by X-ray fluorescence (XRF).

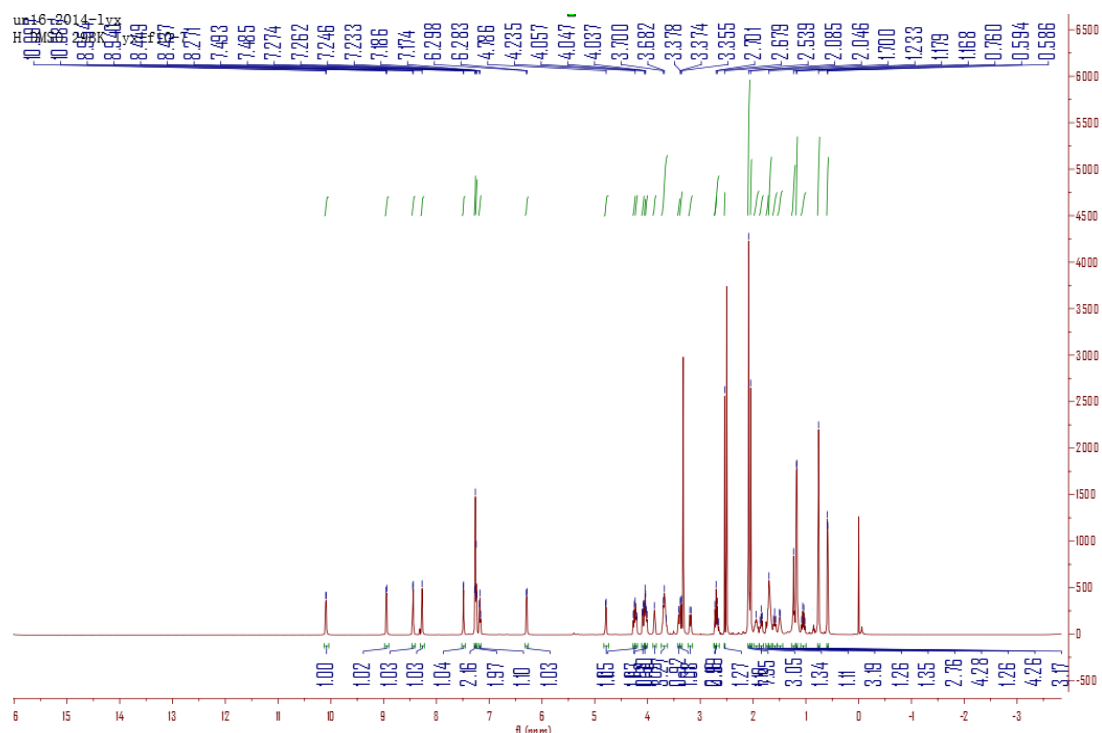


Figure S3. ^1H spectrum of Al (III)-acremoneptide E (**1**) in $\text{DMSO-}d_6$ (600 MHz).

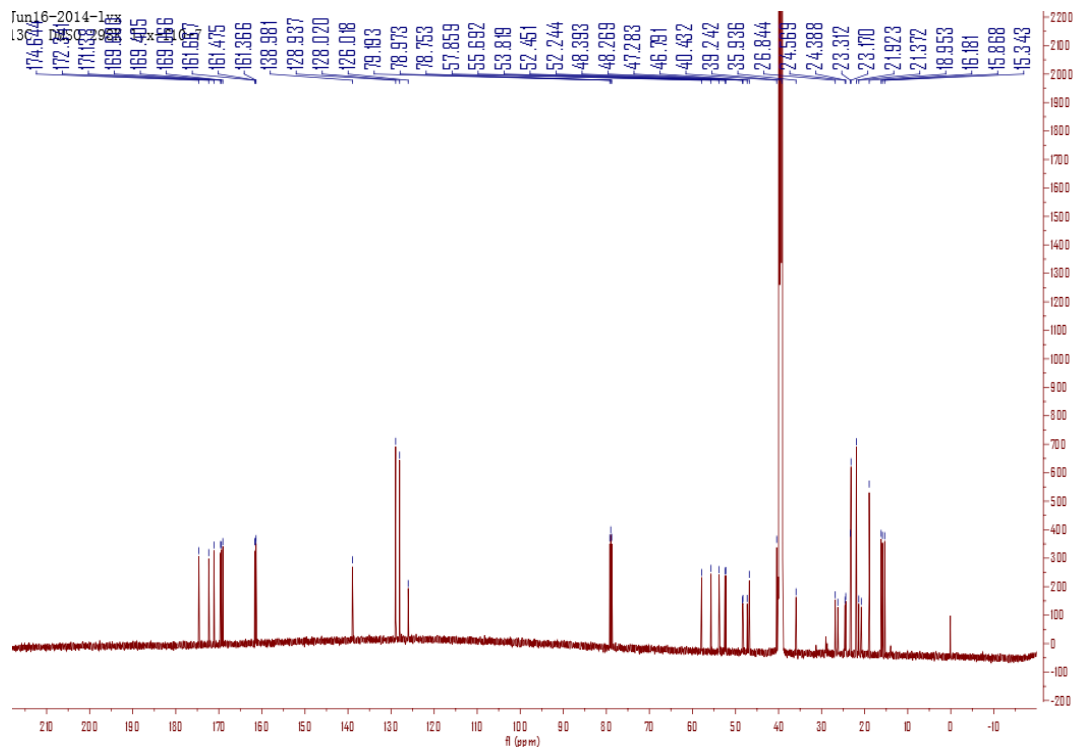


Figure S4. ^{13}C spectrum of Al (III)-acremoneptide E (**1**) in $\text{DMSO-}d_6$ (150 MHz).

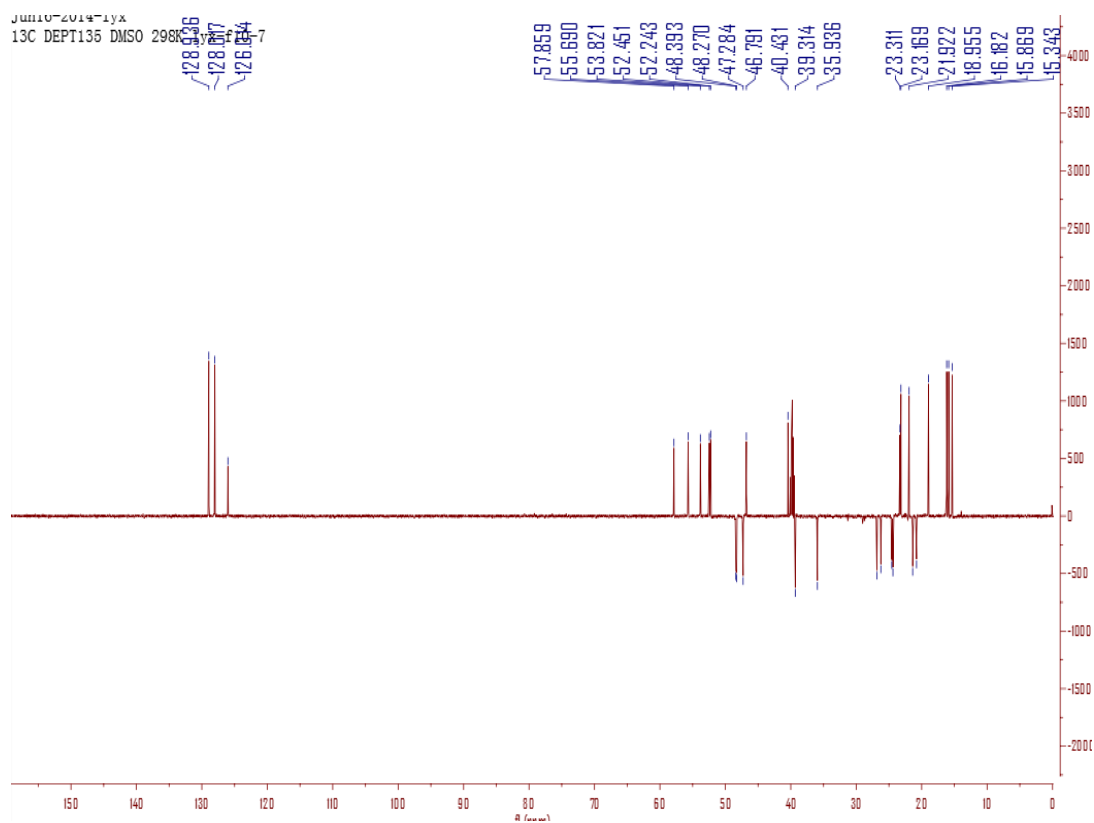


Figure S5. DEPT135 spectrum of Al (III)-acremoneptide E (**1**) in DMSO- d_6 (150 MHz).

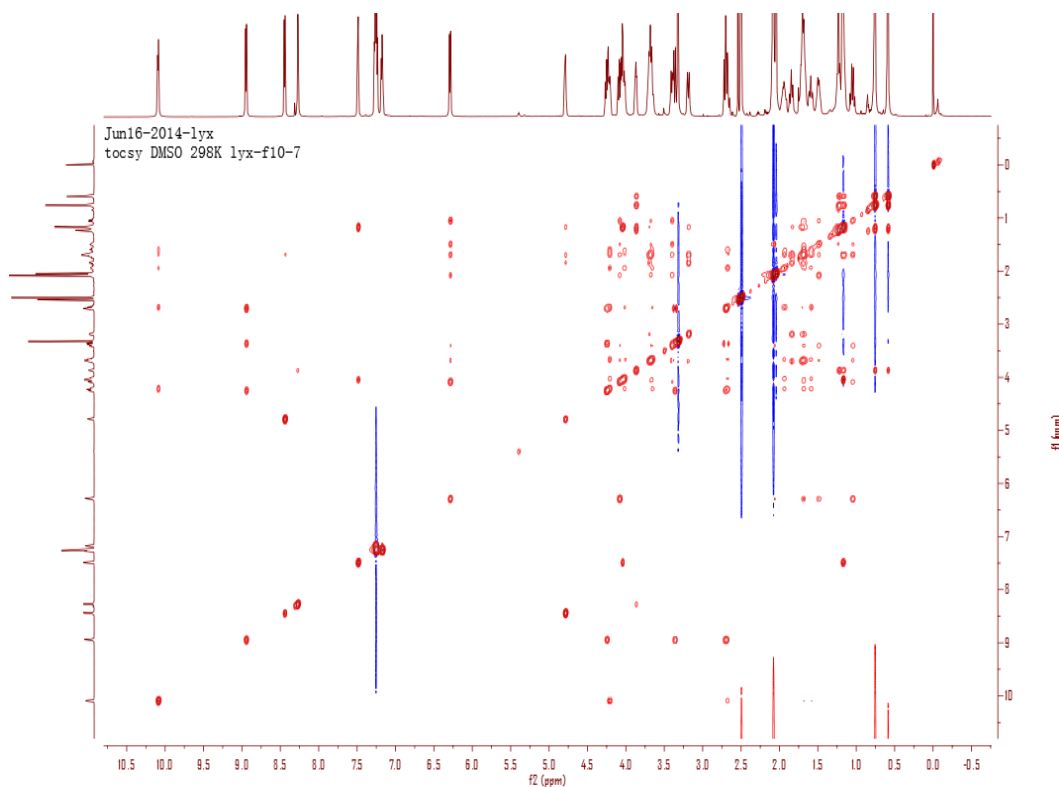


Figure S6. TOCSY spectrum of Al (III)-acremoneptide E (**1**) in DMSO- d_6

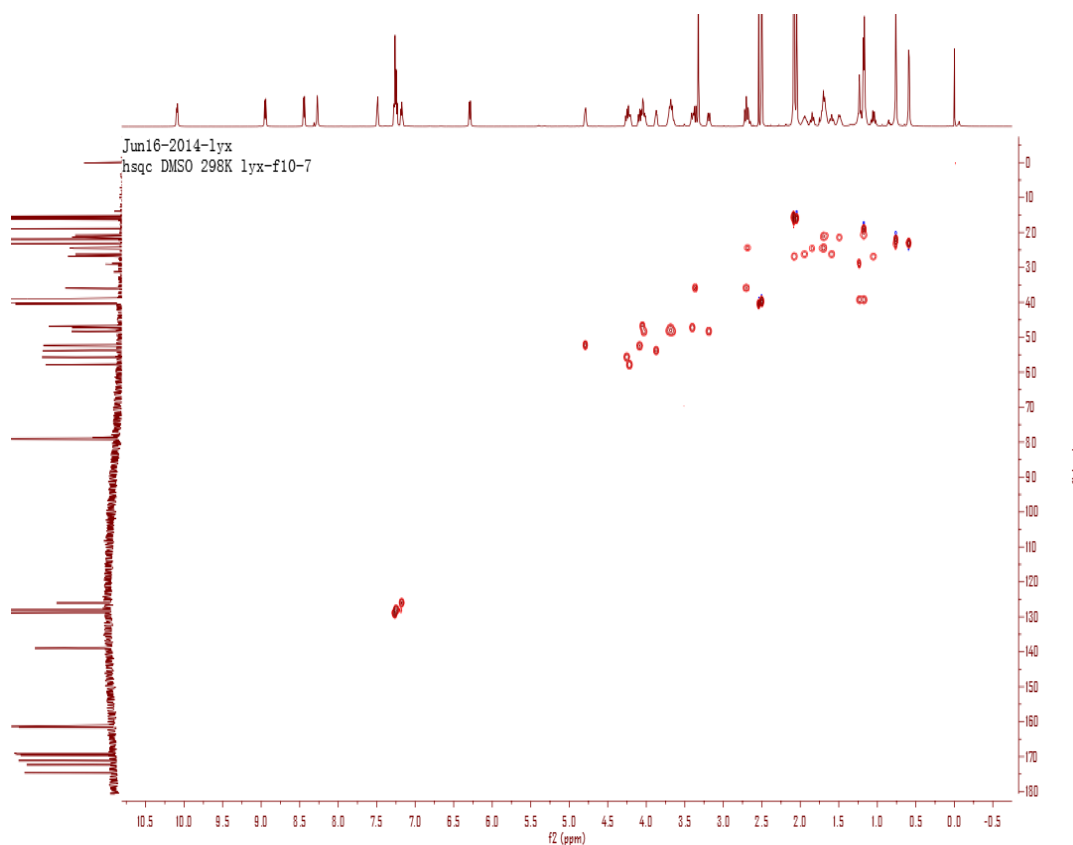


Figure S7. HSQC spectrum of Al (III)-acremoneptide E (**1**) in DMSO-*d*₆

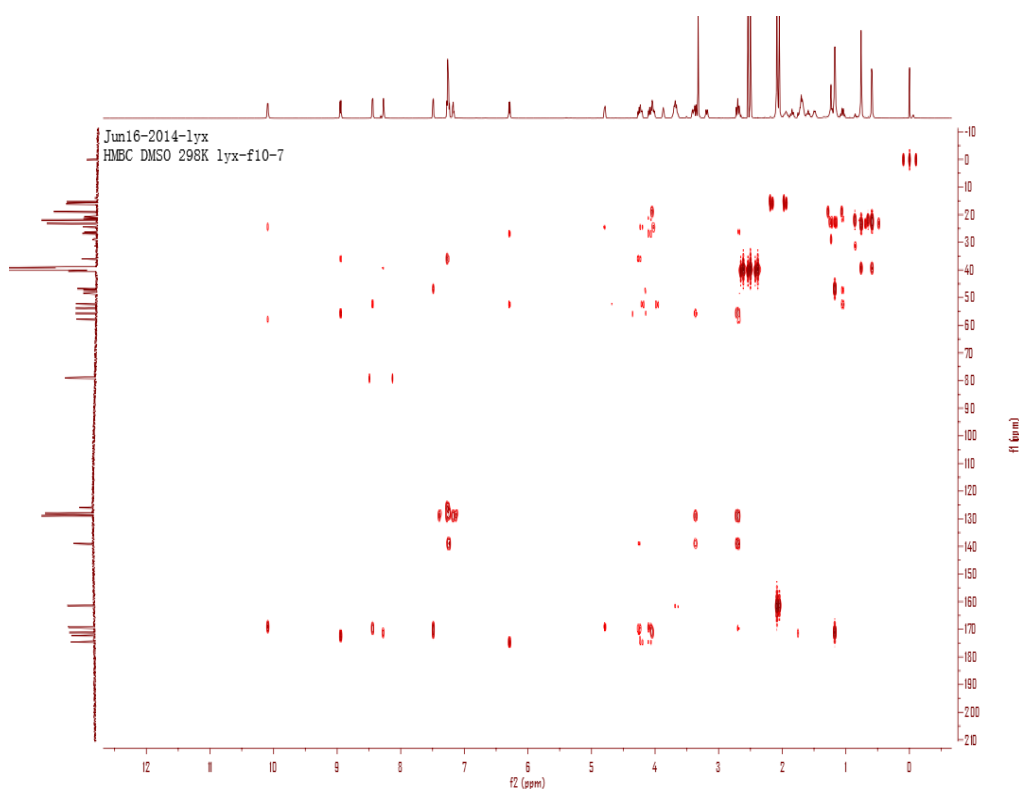


Figure S8. HMBC spectrum of Al (III)-acremoneptide E (**1**) in DMSO-*d*₆

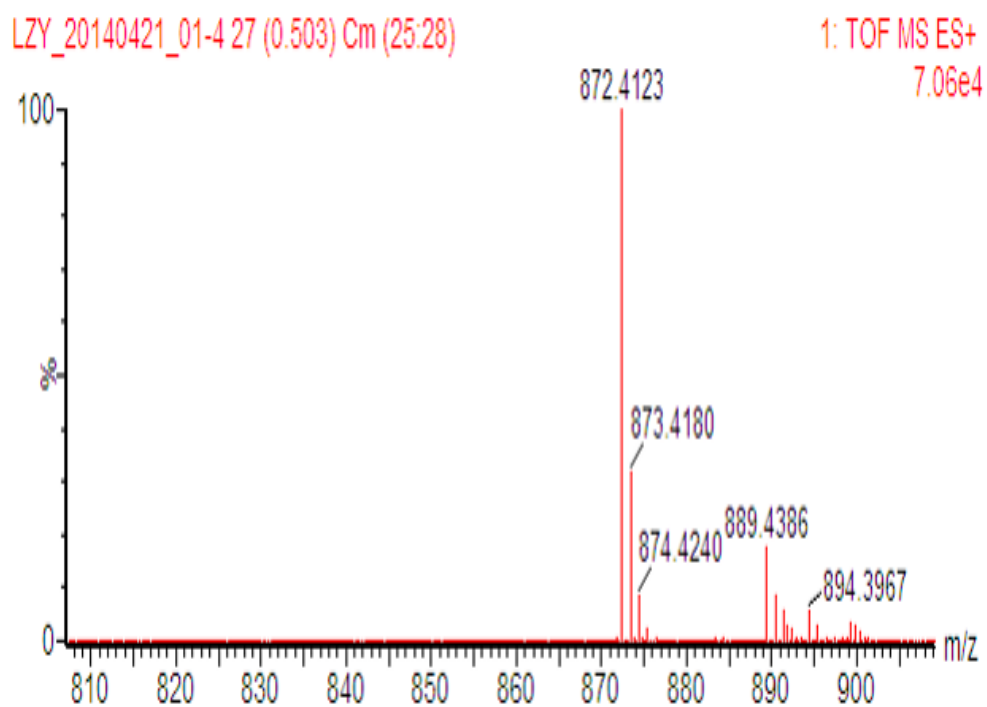


Figure S9. HRESIMS data of Al (III)-acremoneptide E (**1**)

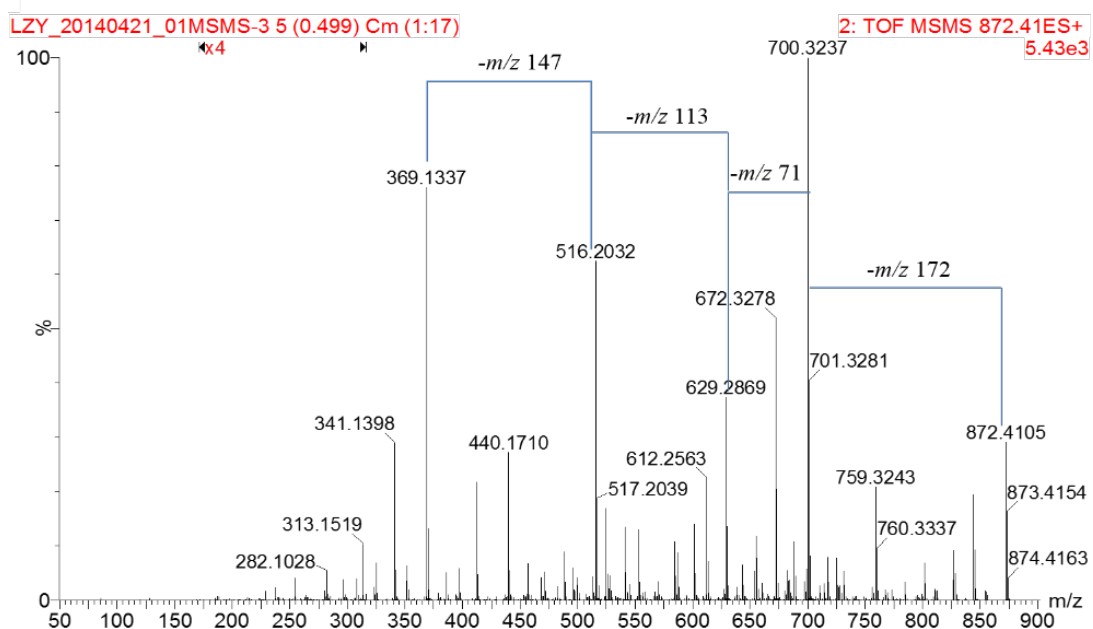


Figure S10. HRESIMS/MS fragmentation ions of Al (III)-acremoneptide E (**1**)

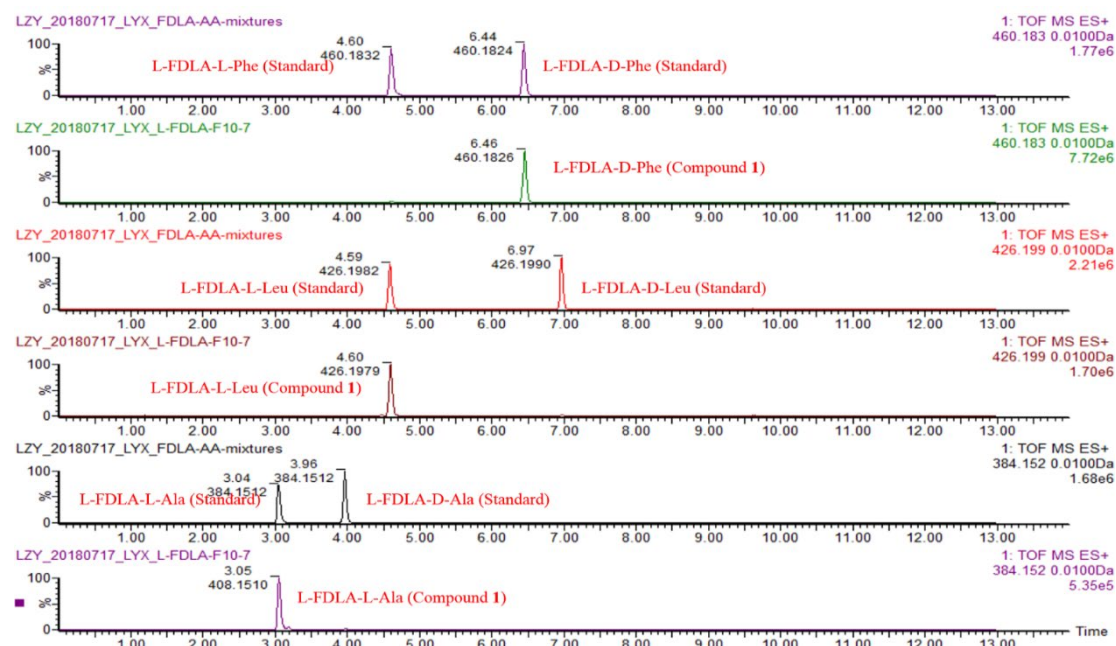


Figure S11. Mass chromatograms of the L-FDLA derivatives of standard amino acids and amino acids from Al (III)-acremoneptide E (1)

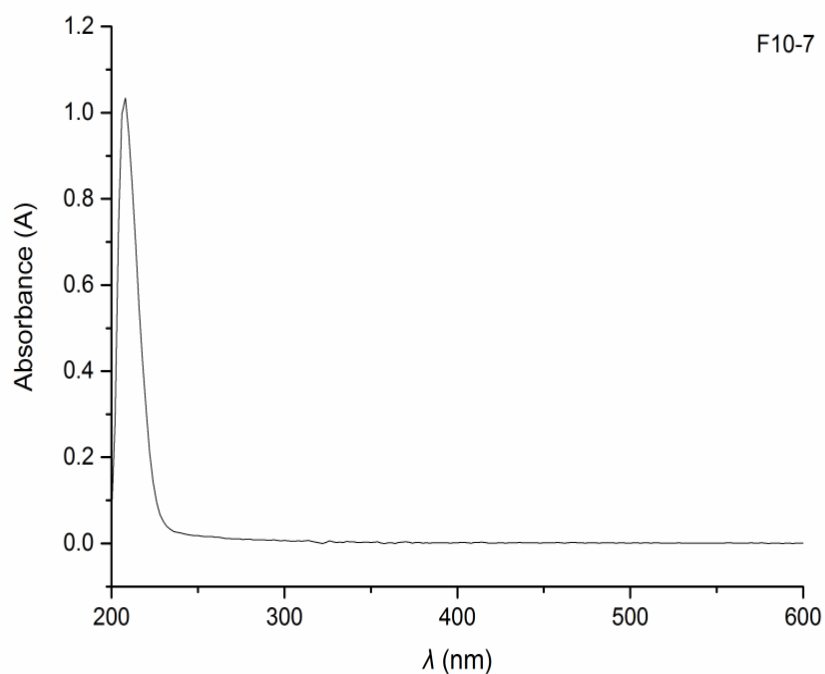


Figure S12. UV spectrum of Al (III)-acremoneptide E (1) in MeOH.

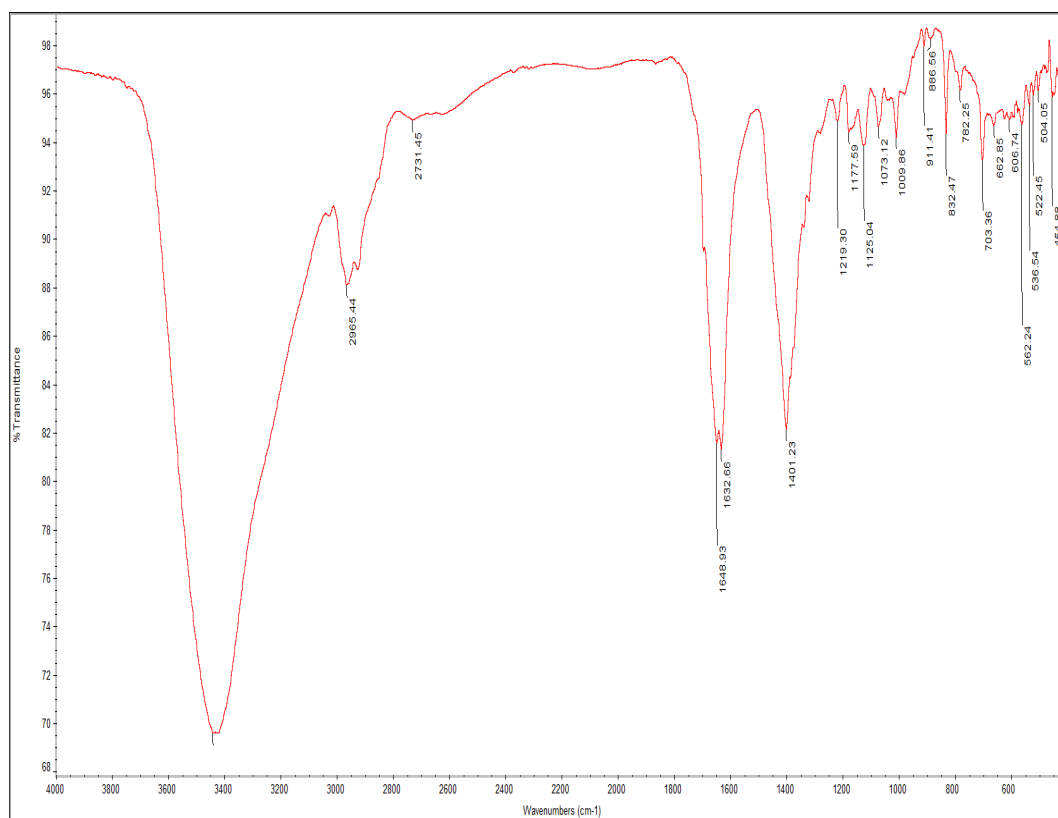
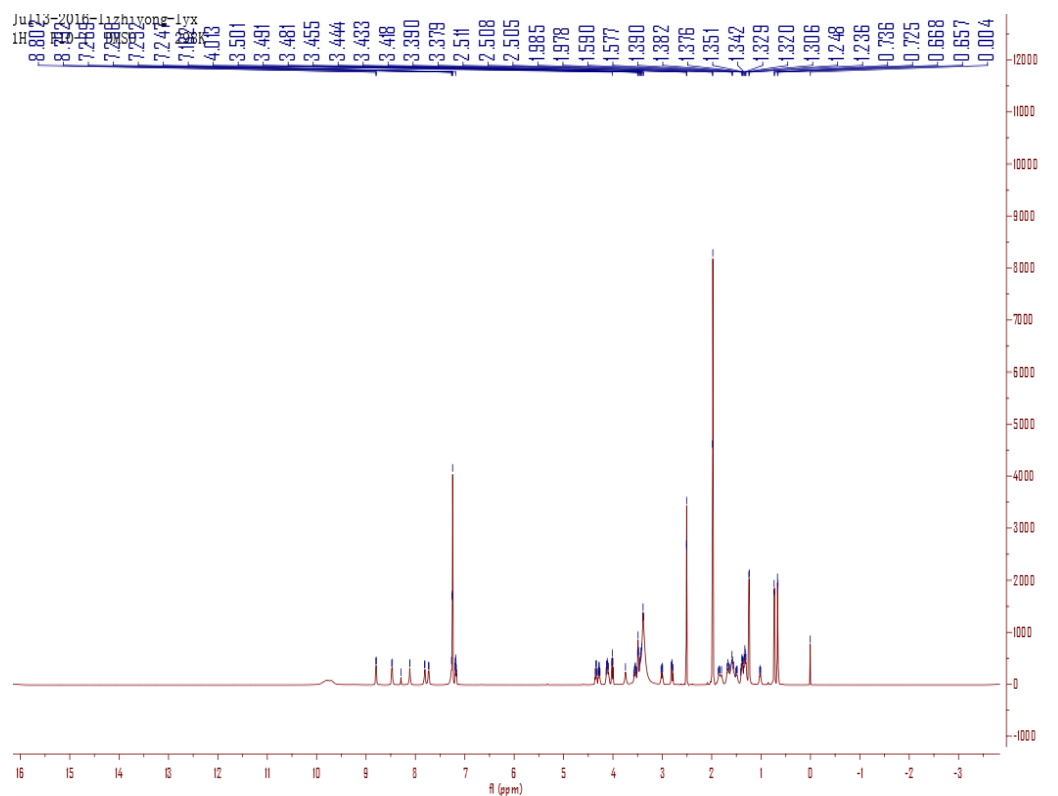


Figure S13. IR spectrum of Al (III)-acremoneptide E (1).



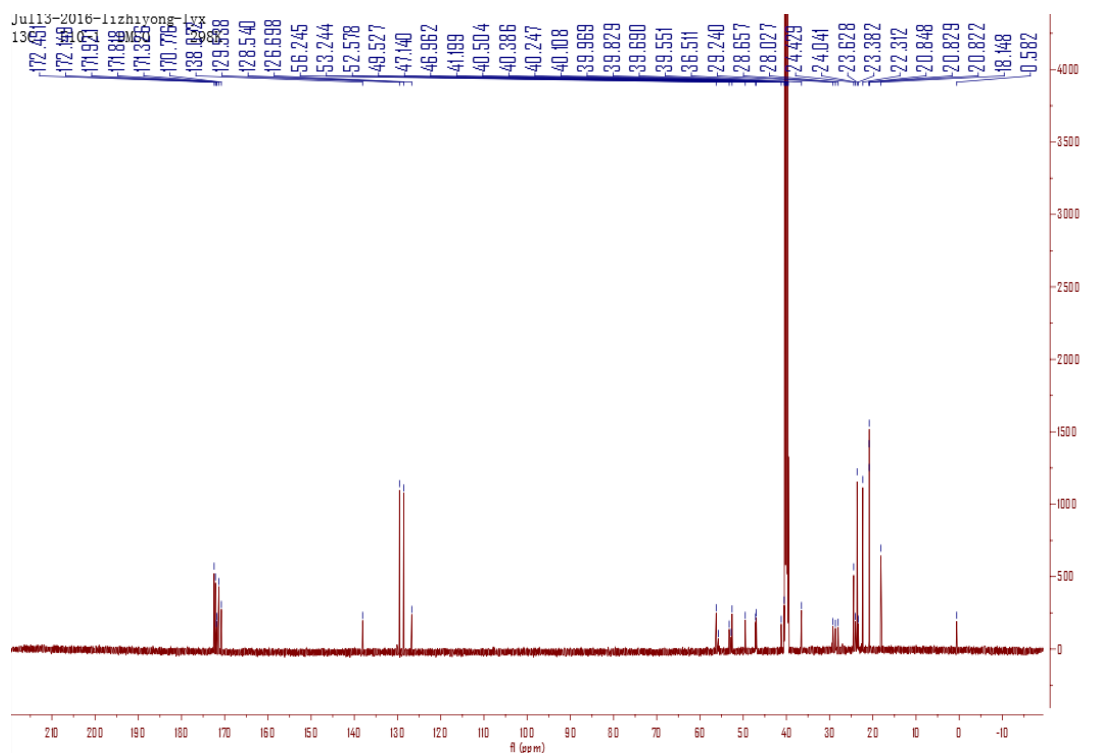


Figure S15. ^{13}C spectrum of acremoneptide E (**2**) in $\text{DMSO-}d_6$ (150 MHz).

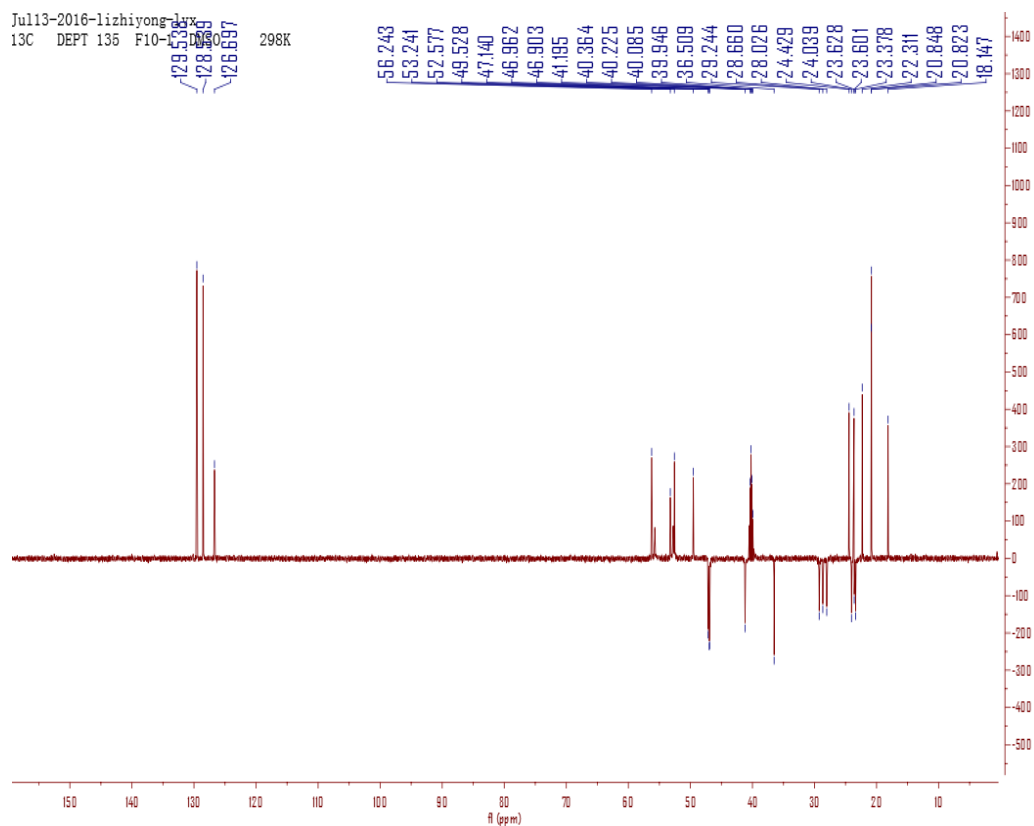


Figure S16. DEPT135 spectrum of acremoneptide E (**2**) in $\text{DMSO-}d_6$ (150 MHz).

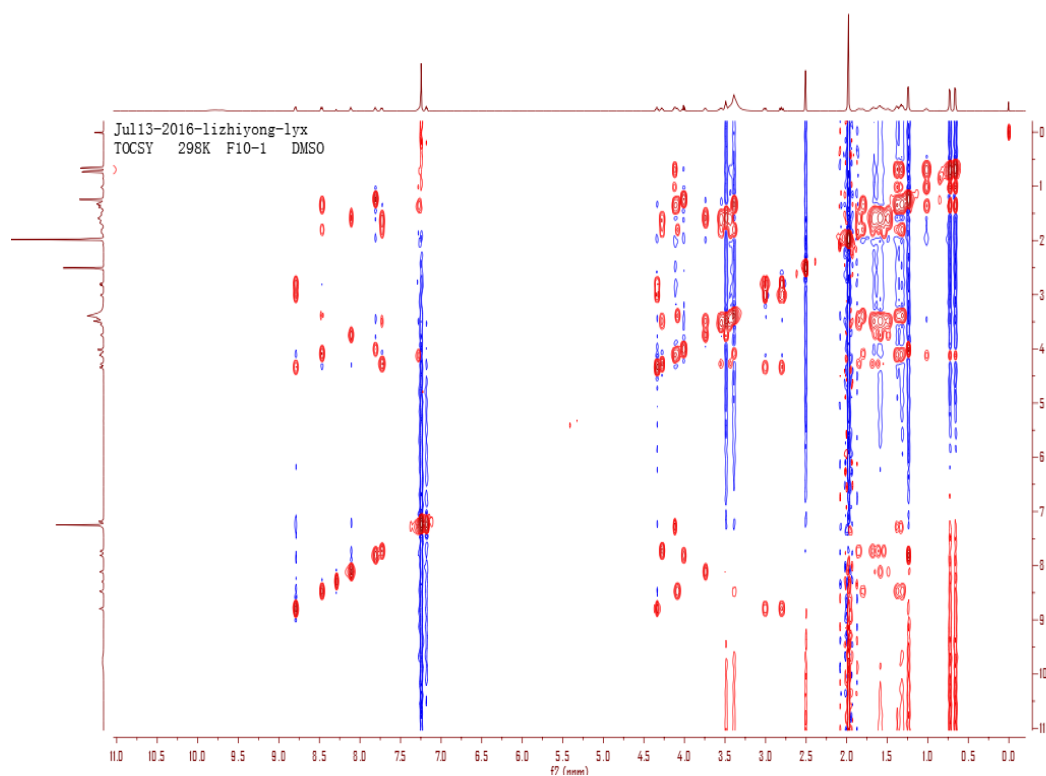


Figure S17. TOCSY spectrum of acremonpeptide E (**2**) in DMSO-*d*₆.

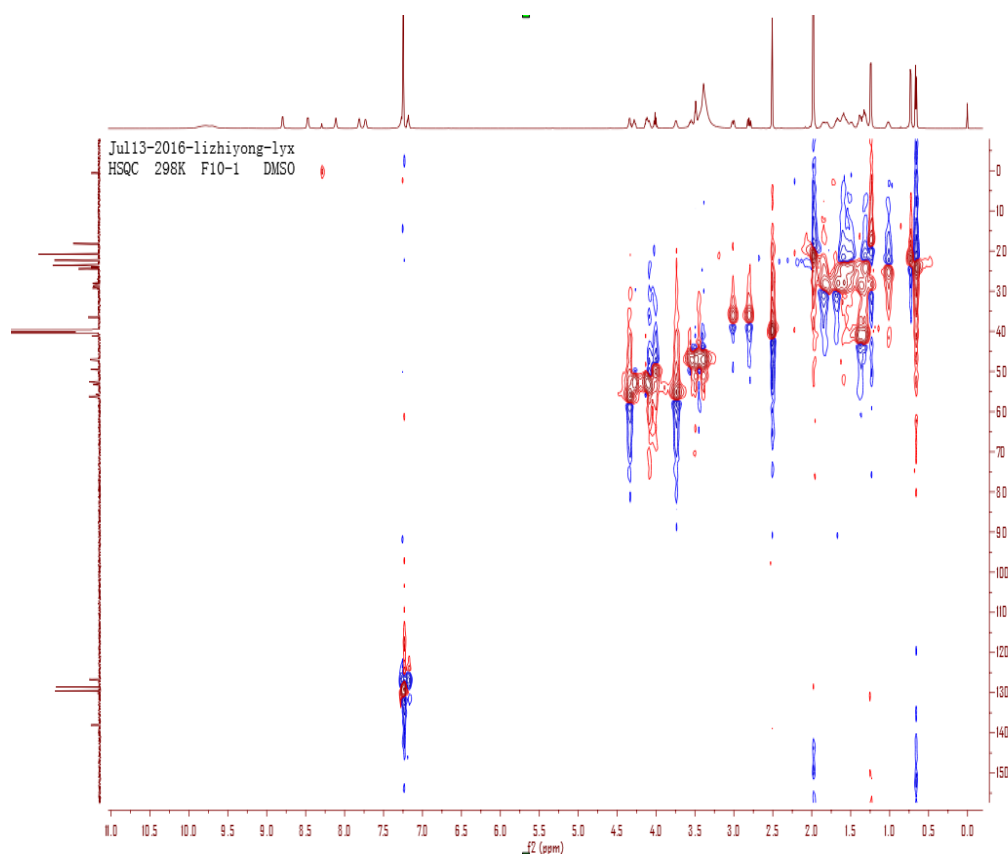


Figure S18. HSQC spectrum of acremonpeptide E (**2**) in DMSO-*d*₆.

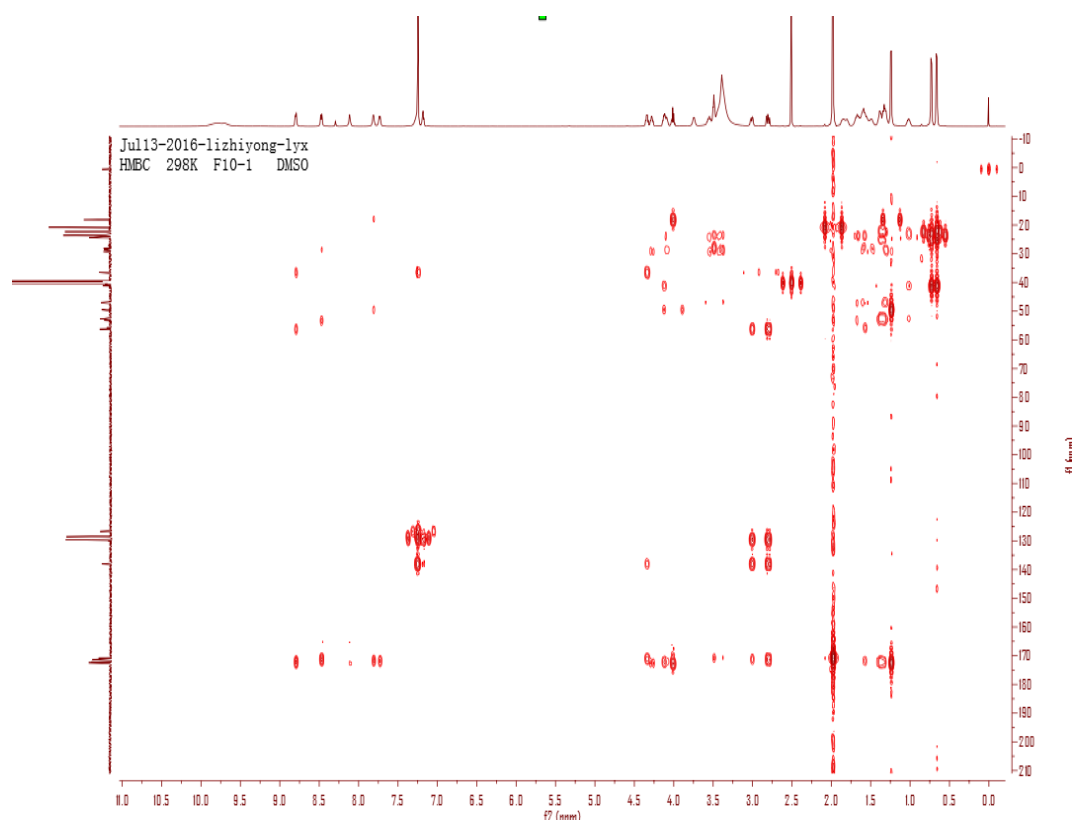


Figure S19. HMBC spectrum of acremoneptide E (**2**) in DMSO- d_6 .

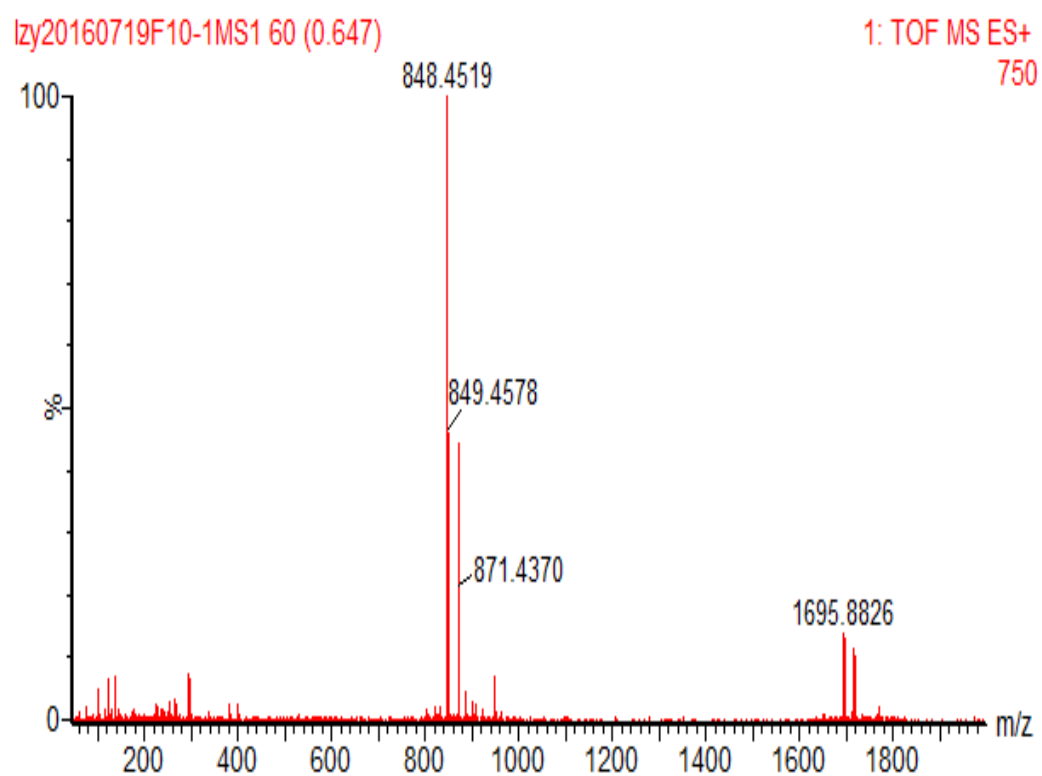


Figure S20. HRESIMS data of acremoneptide E (**2**).

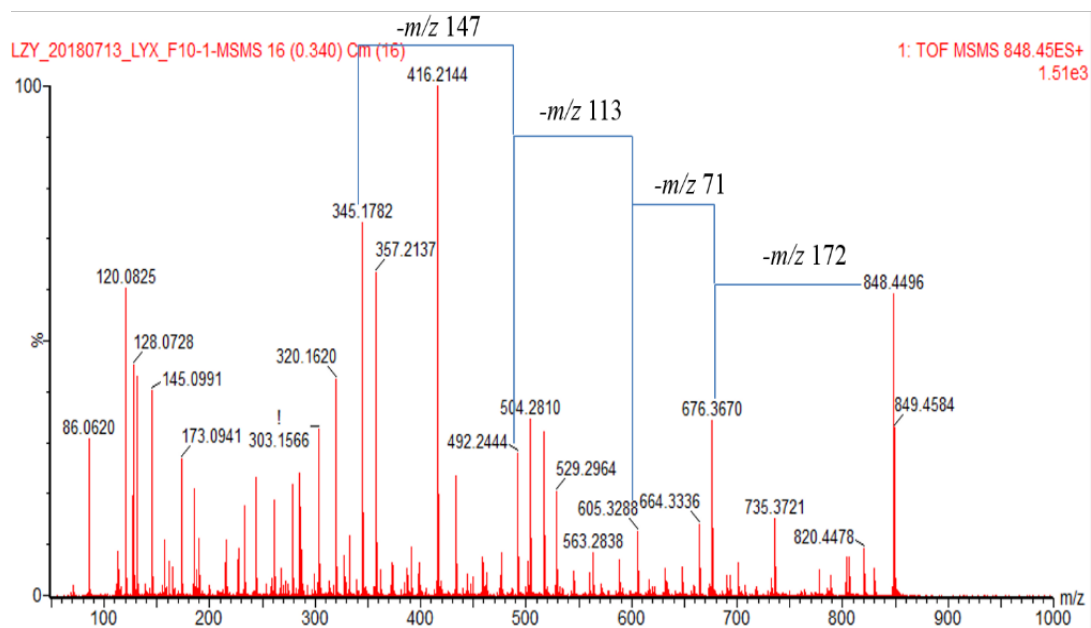


Figure S21. HRESIMS/MS fragmentation ions of acromonpeptide E (2)

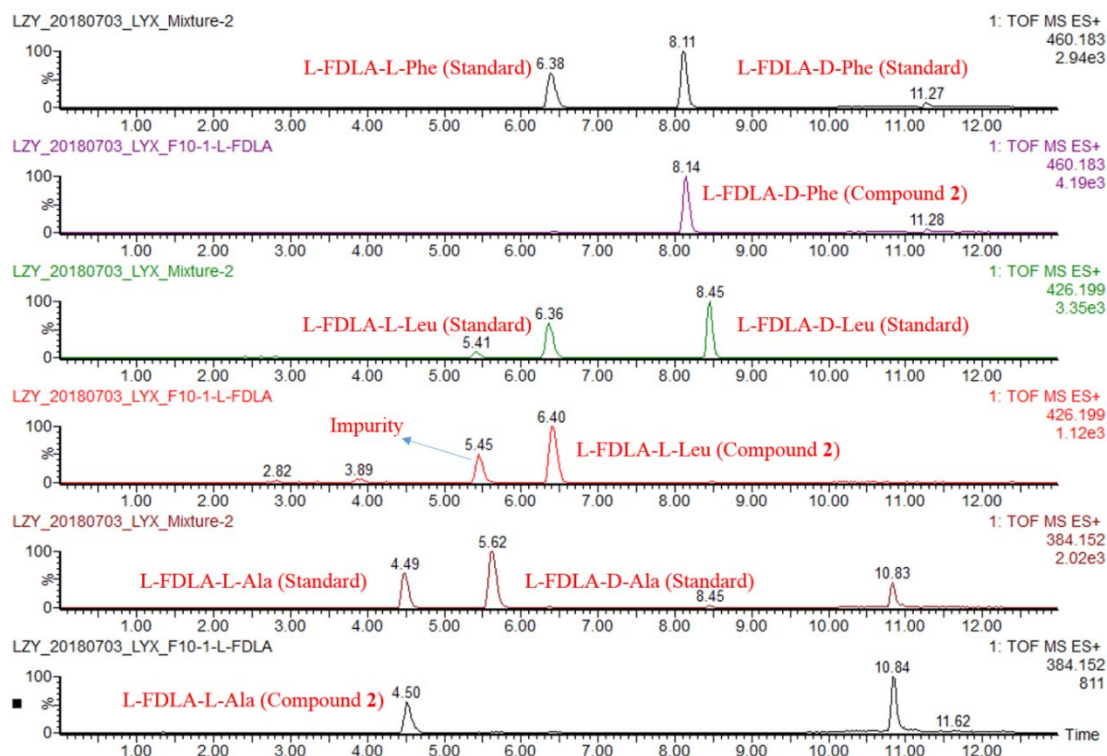


Figure S22. Mass chromatograms of the L-FDLA derivatives of standard amino acids and amino acids from acromonpeptide E (2)

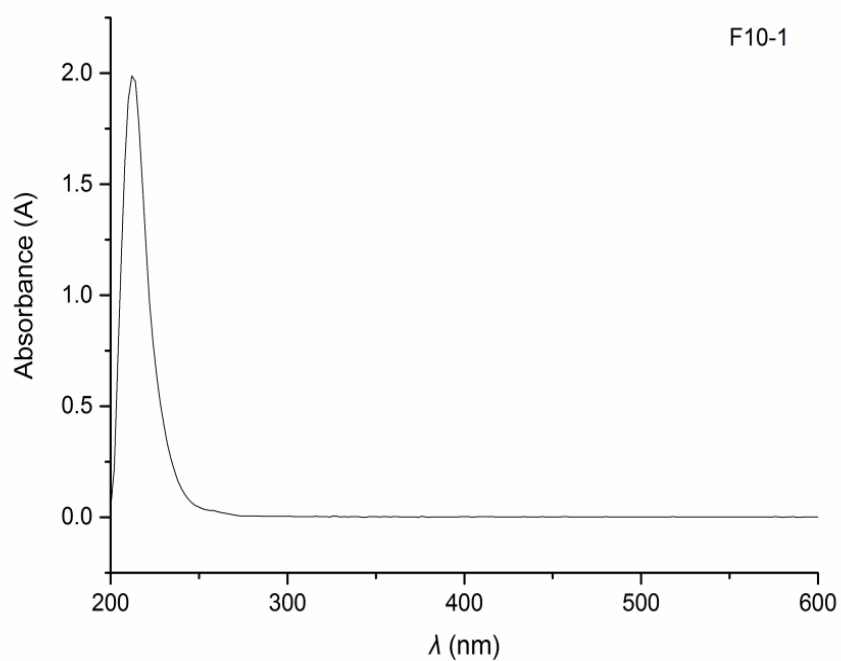


Figure S23. UV spectrum of acremoneptide E (2) in MeOH.

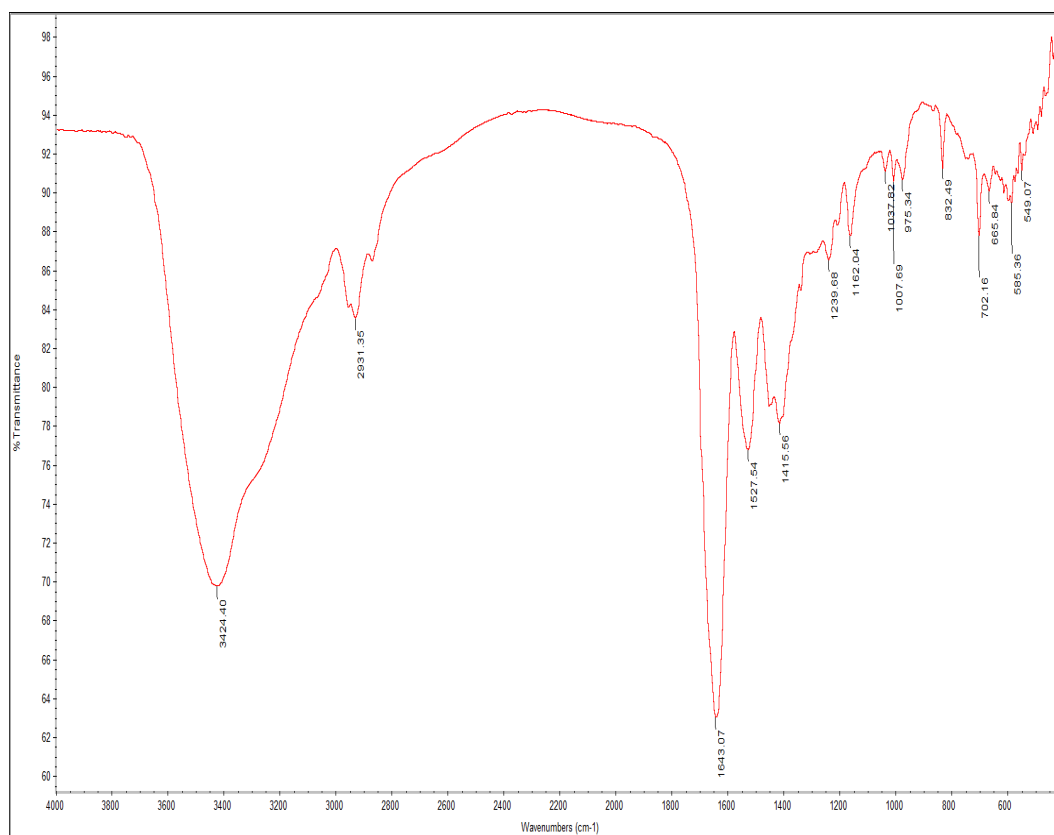


Figure S24. IR spectrum of acremoneptide E (2).

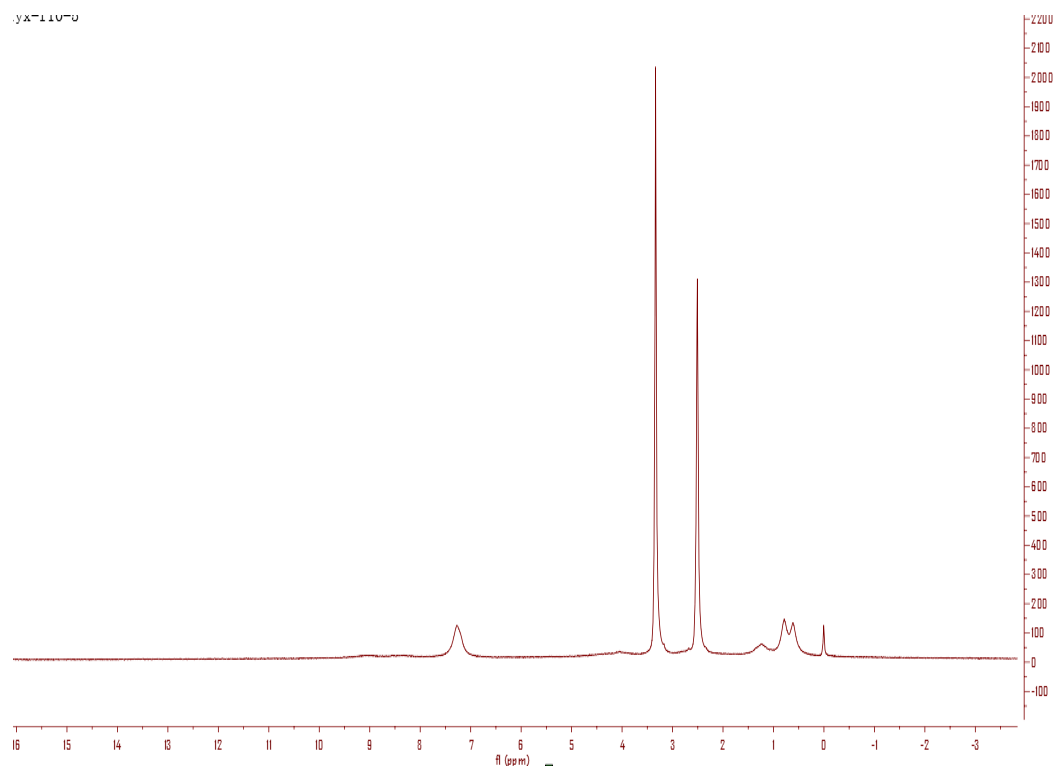


Figure S25. ¹H spectrum of Fe (III)-acremnonpeptide E (**3**) in DMSO-*d*₆ (600 MHz).

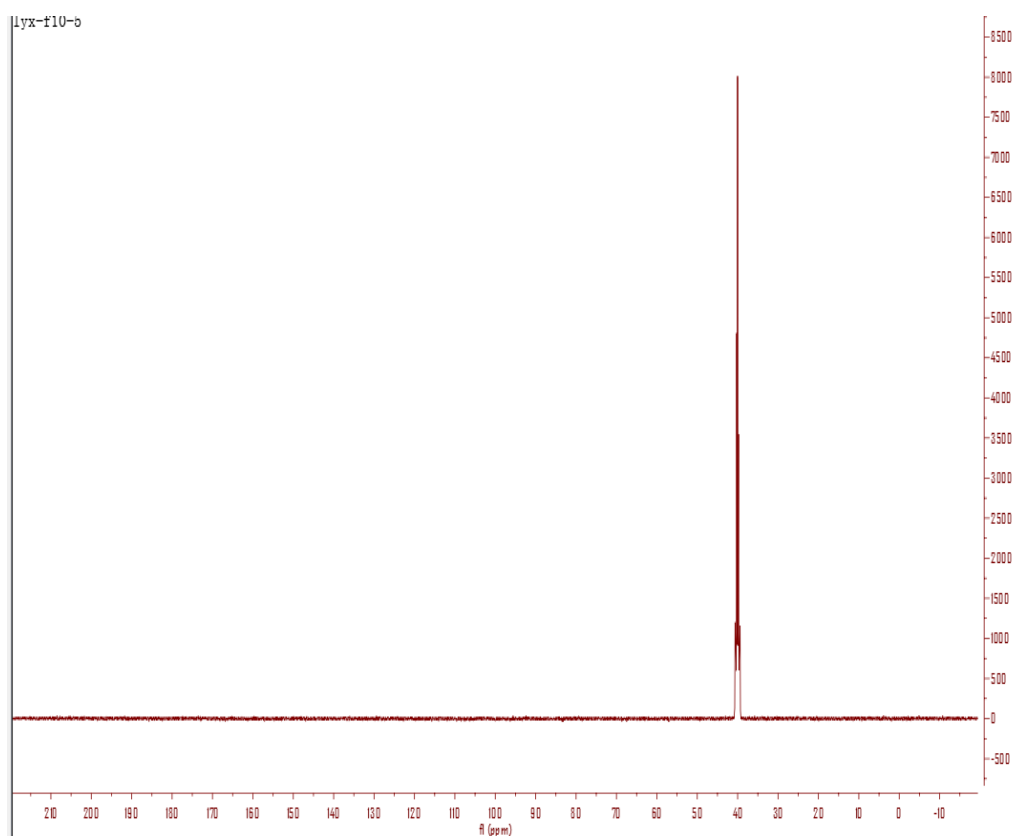


Figure S26. ¹³C spectrum of Fe (III)-acremnonpeptide E (**3**) in DMSO-*d*₆ (150 MHz).

F10-2

LZY_20160810_LYX_F10-2 47 (0.630)

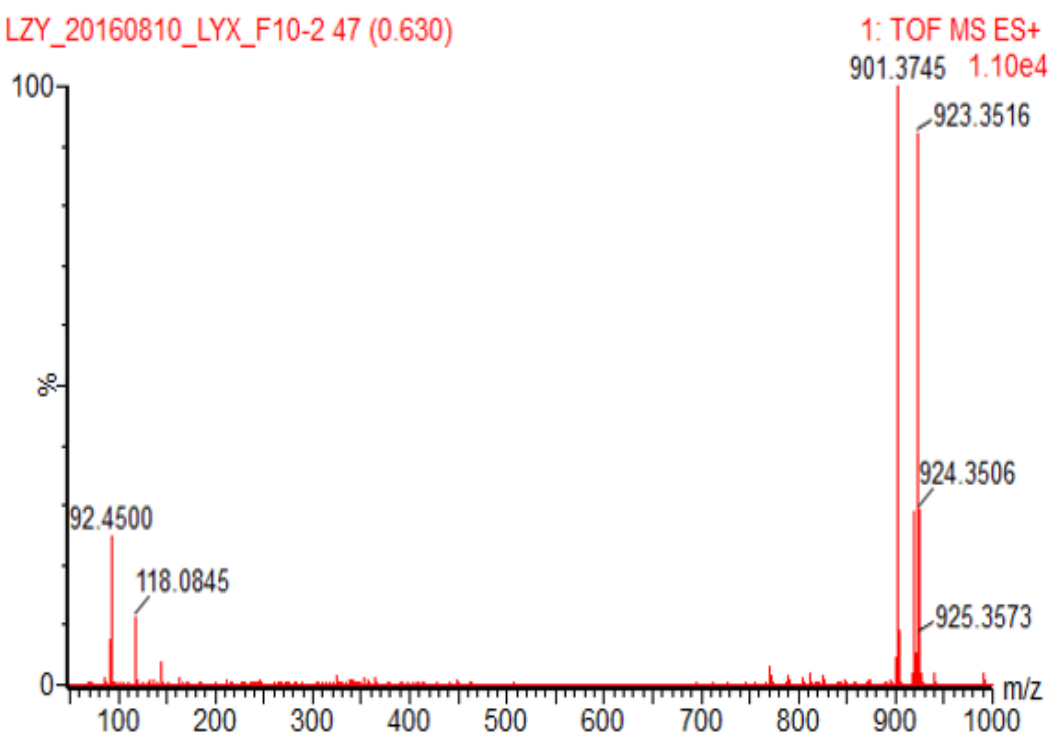


Figure S27. HRESIMS data of Fe (III)-acremonpeptide E (3).

LZY_20180713_LYX_F10-2-MSMS 16 (0.341) Cm (16:17)

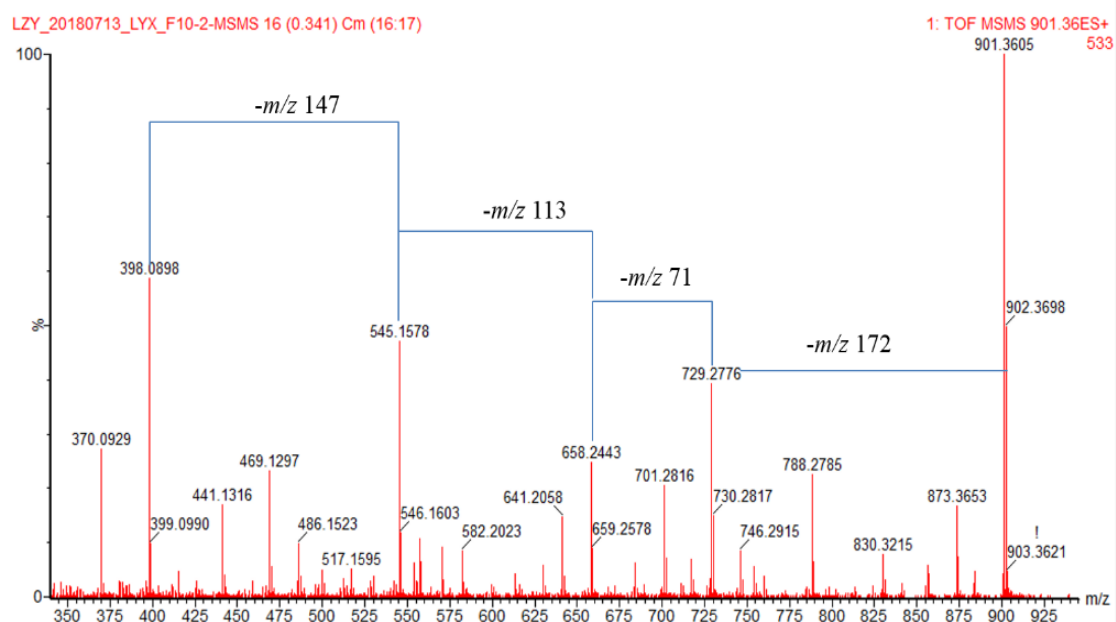


Figure S28. HRESIMS/MS fragmentation ions of Fe (III)-acremonpeptide E (3).

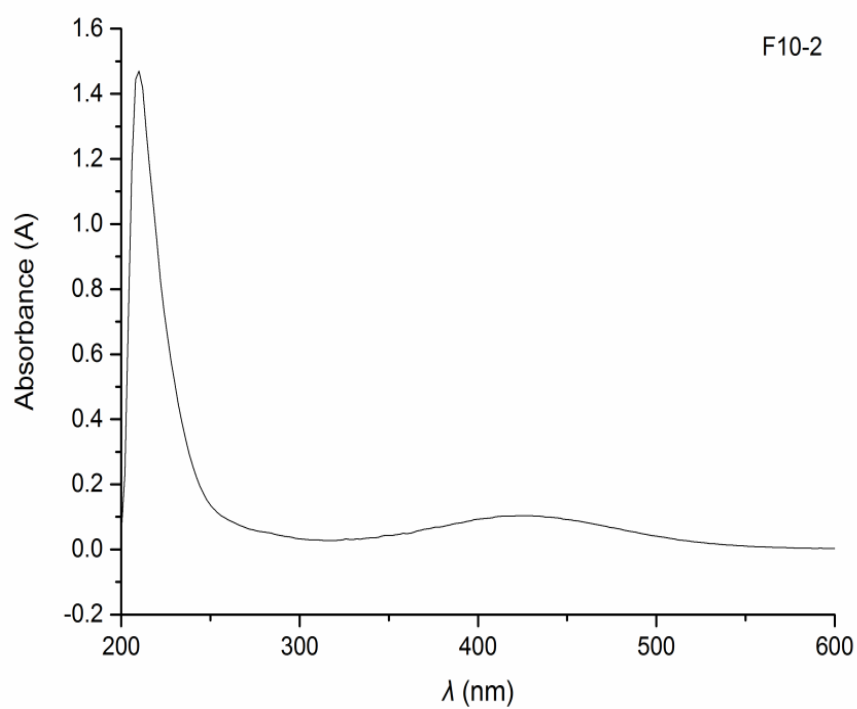


Figure S29. UV spectrum of Fe (III)-acremonpeptide E (**3**) in MeOH.

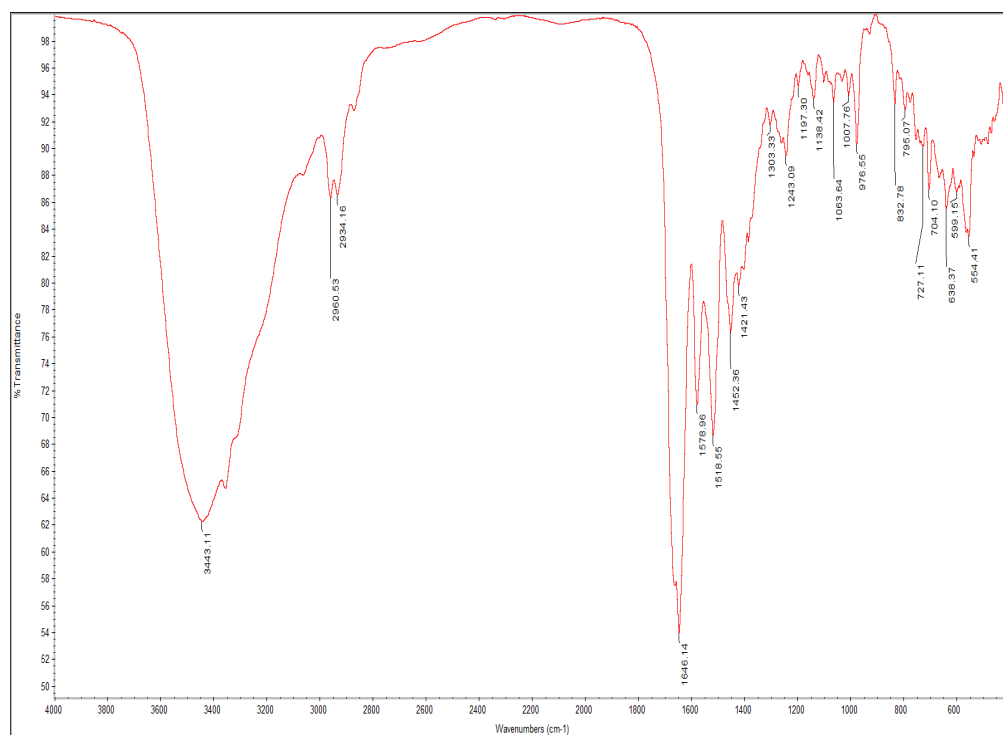


Figure S30. IR spectrum of Fe (III)-acremonpeptide E (**3**).

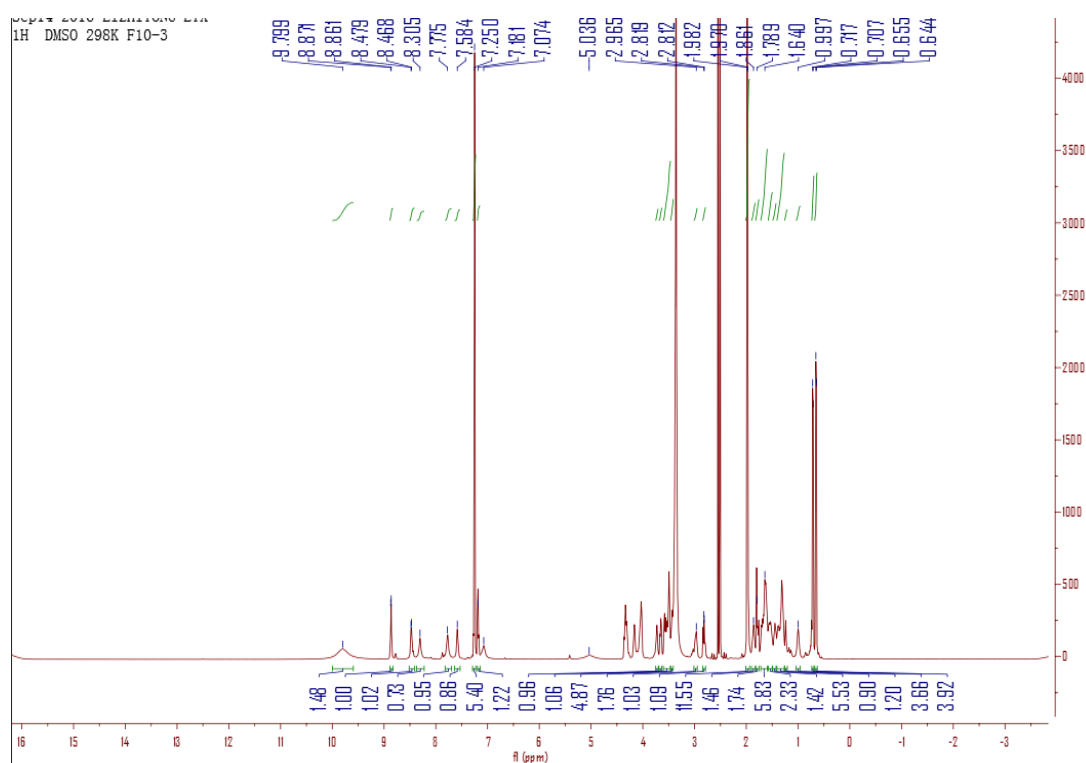


Figure S31. ^1H spectrum of acremonpeptide F (**4**) in $\text{DMSO-}d_6$ (600 MHz).

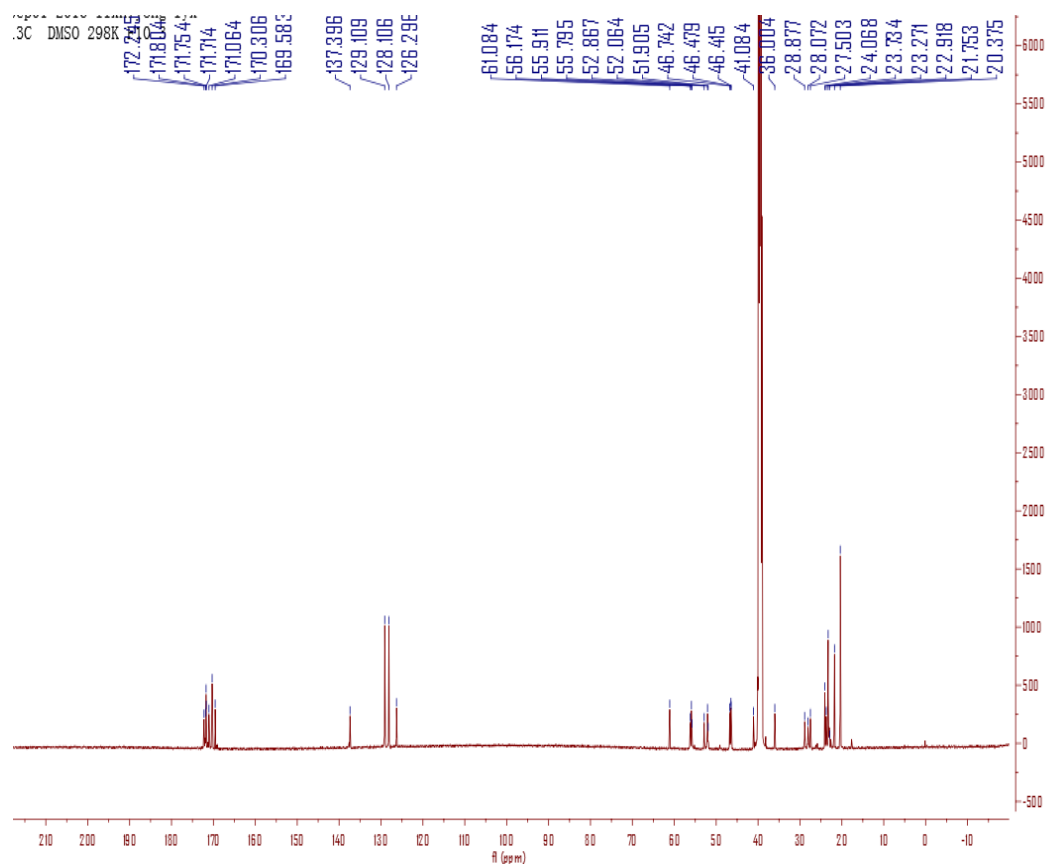


Figure S32. ^{13}C spectrum of acremonpeptide F (**4**) in $\text{DMSO-}d_6$ (150 MHz).

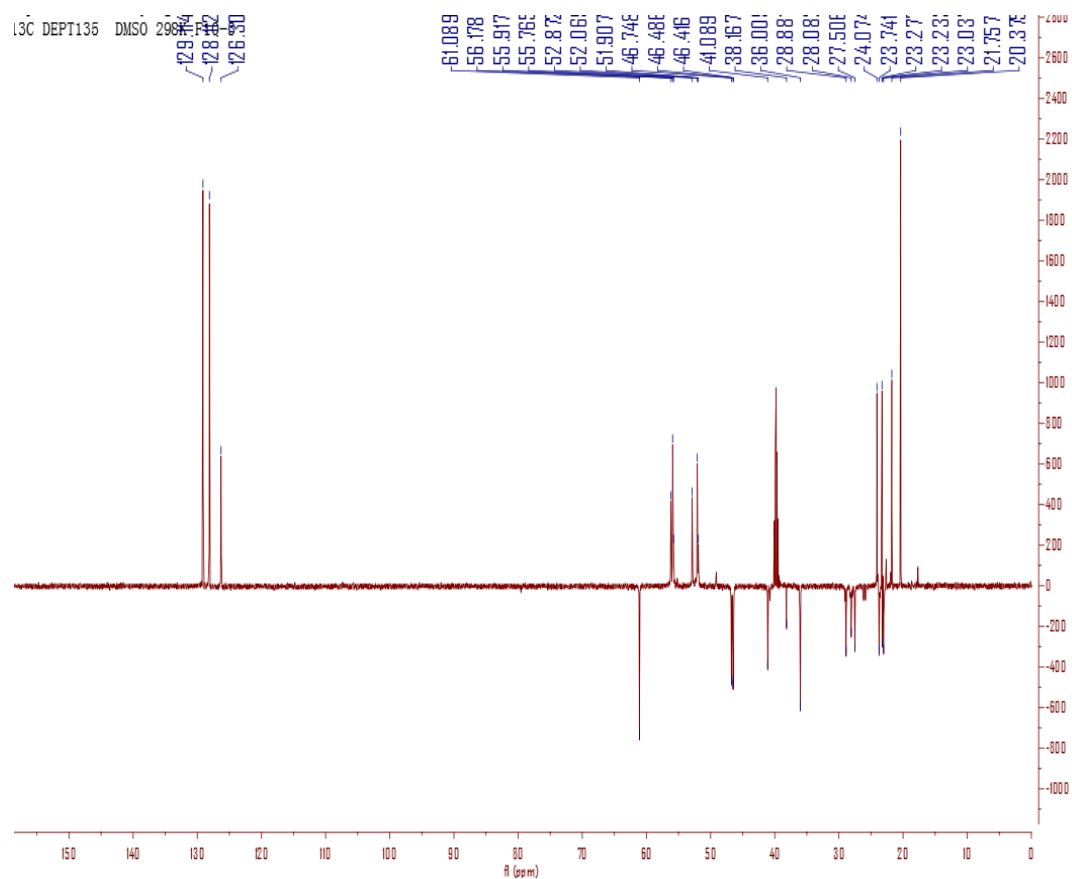


Figure S33. DEPT135 spectrum of acrimonpeptide F (**4**) in DMSO- d_6 (150 MHz).

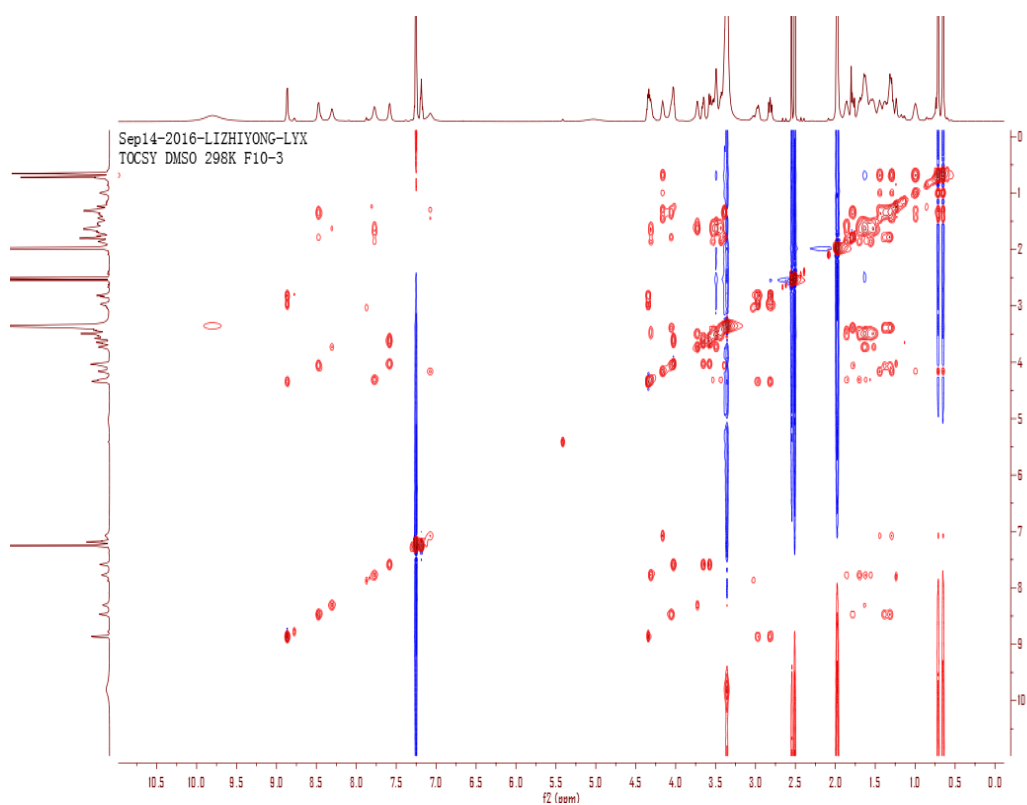


Figure S34. TOCSY spectrum of acrimonpeptide F (**4**) in DMSO- d_6 .

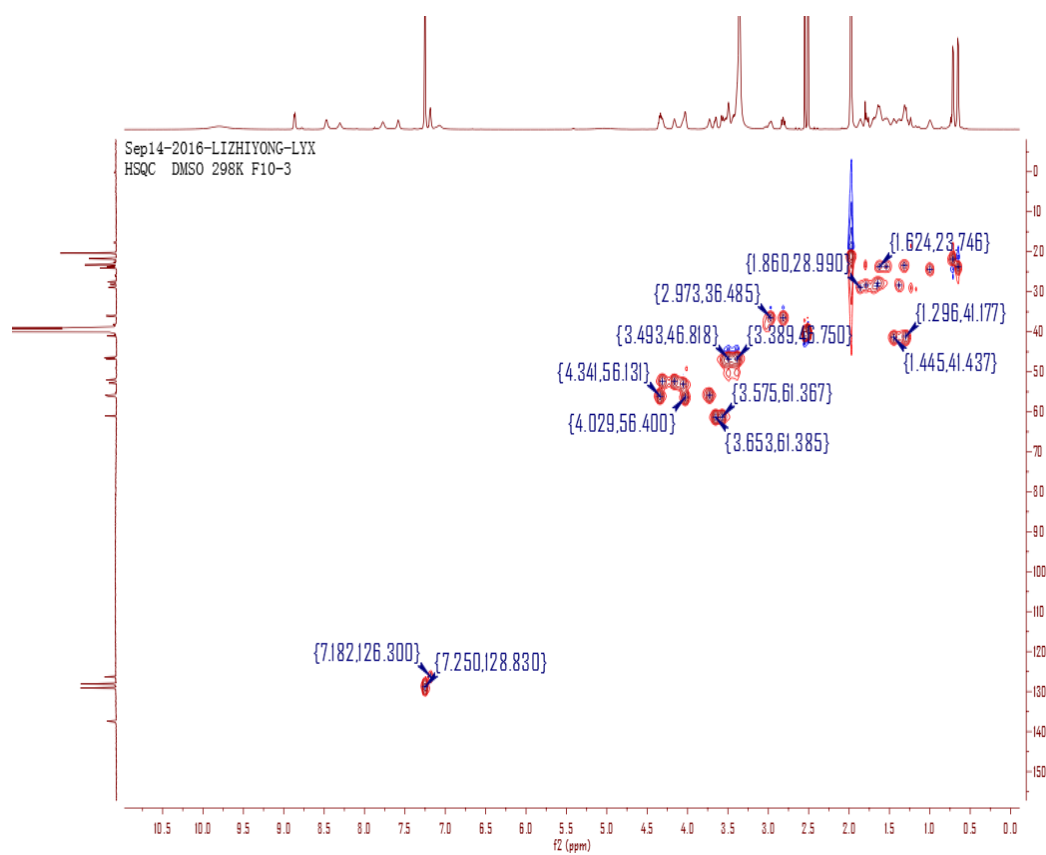


Figure S35. HSQC spectrum of acremoneptide F (**4**) in DMSO-*d*₆.

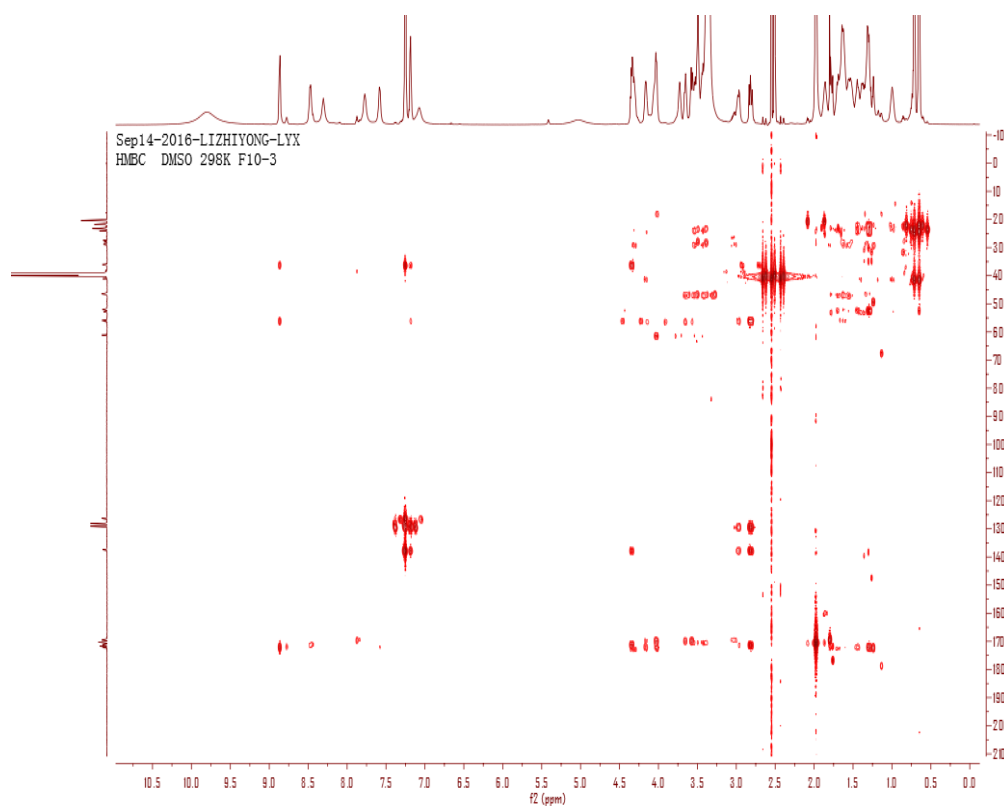


Figure S36. HMBC spectrum of acremoneptide F (**4**) in DMSO-*d*₆.

F10-3

LZY_20160913_LYX_F10-3_LCMS 427 (4.915) Cm (427:428)

1: TOF MS ES+
1.14e5

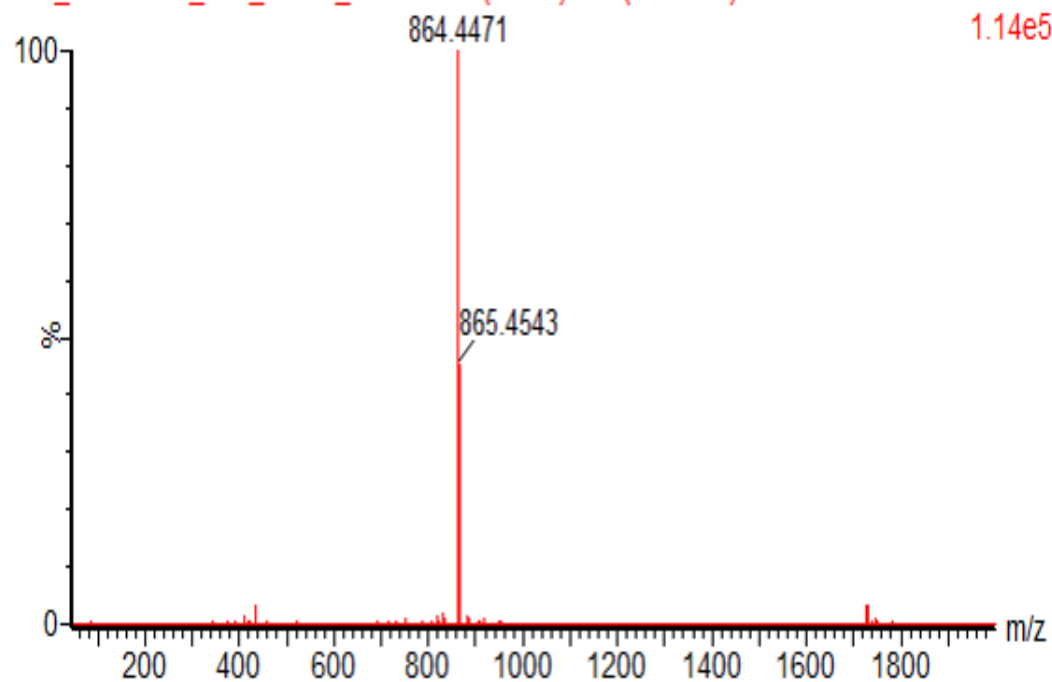


Figure S37. HRESIMS data of acremoneptide F (4).

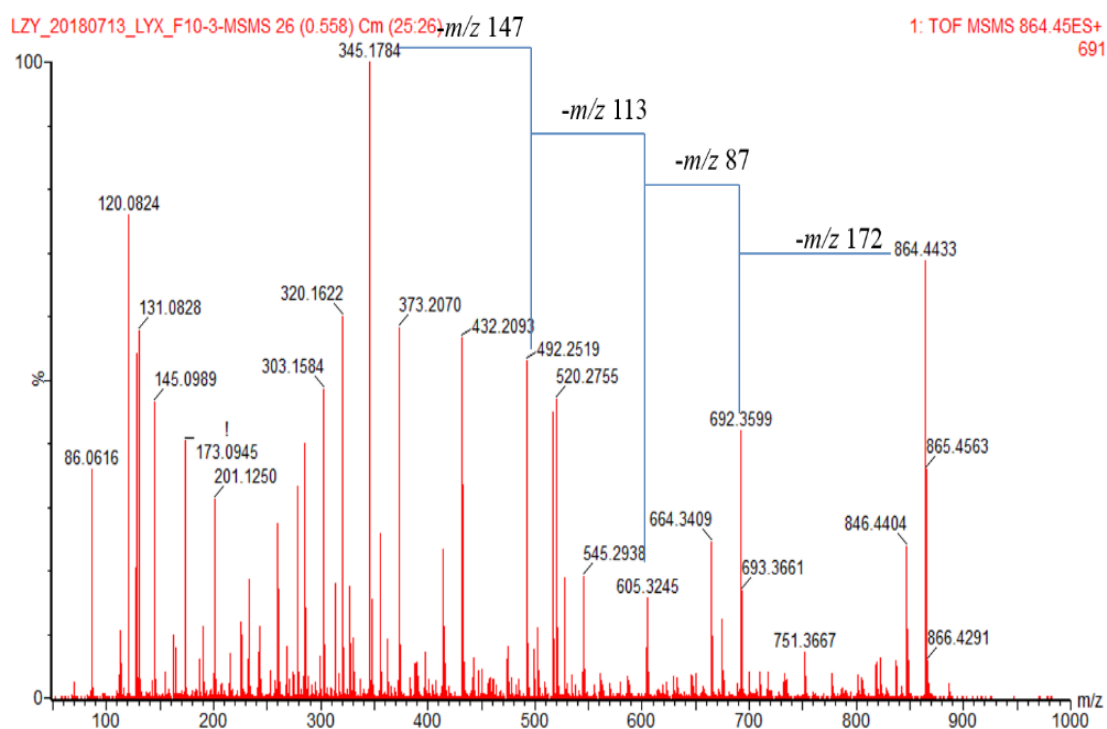


Figure S38. HRESIMS/MS fragmentation ions of acremoneptide F (4).

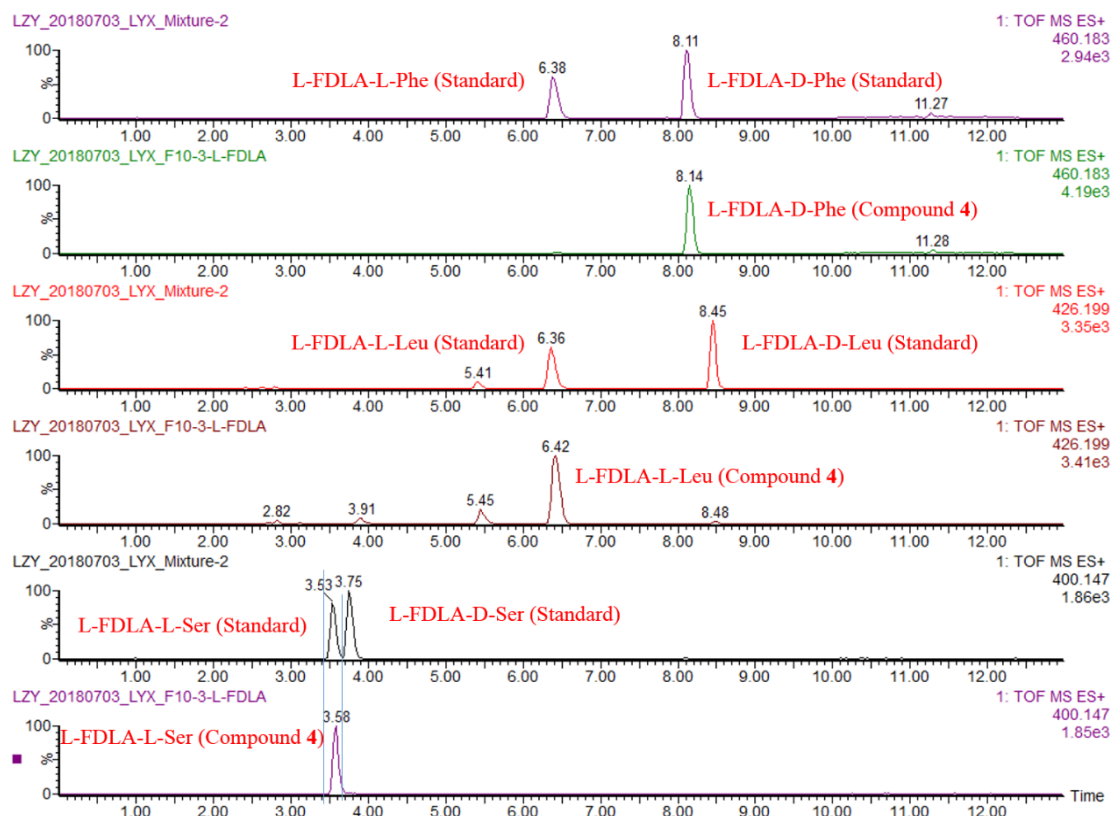


Figure S39. Mass chromatograms of the L-FDLA derivatives of standard amino acids and amino acids from acremonpeptide F (4).

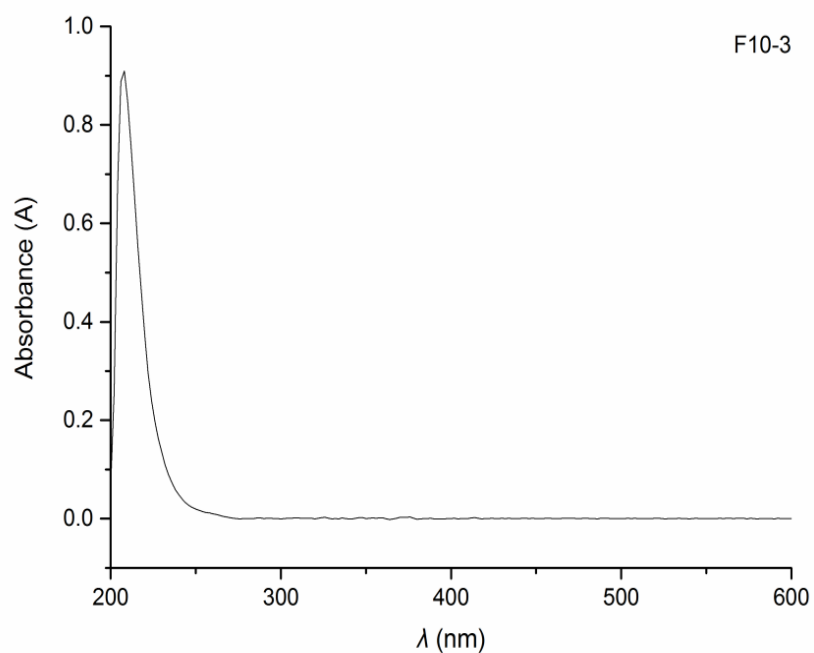


Figure S40. UV spectrum of acremonpeptide F (4) in MeOH.

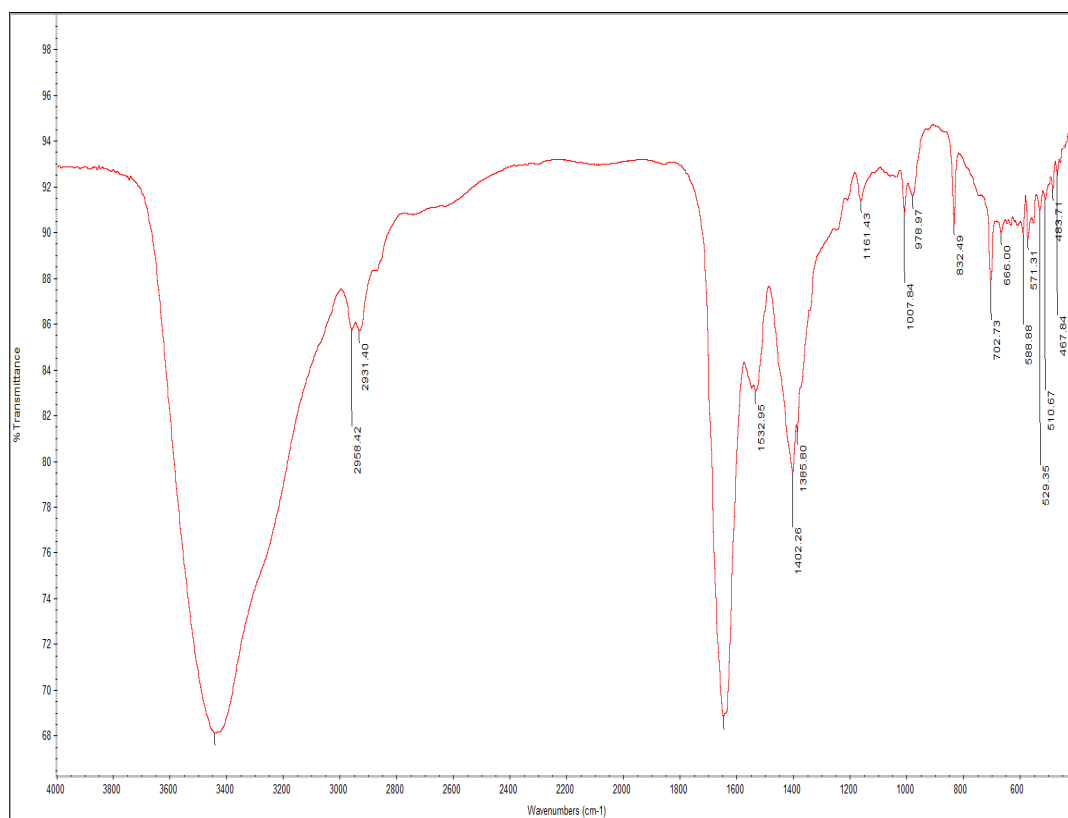


Figure S41. IR spectrum of acremonpeptide F (4).

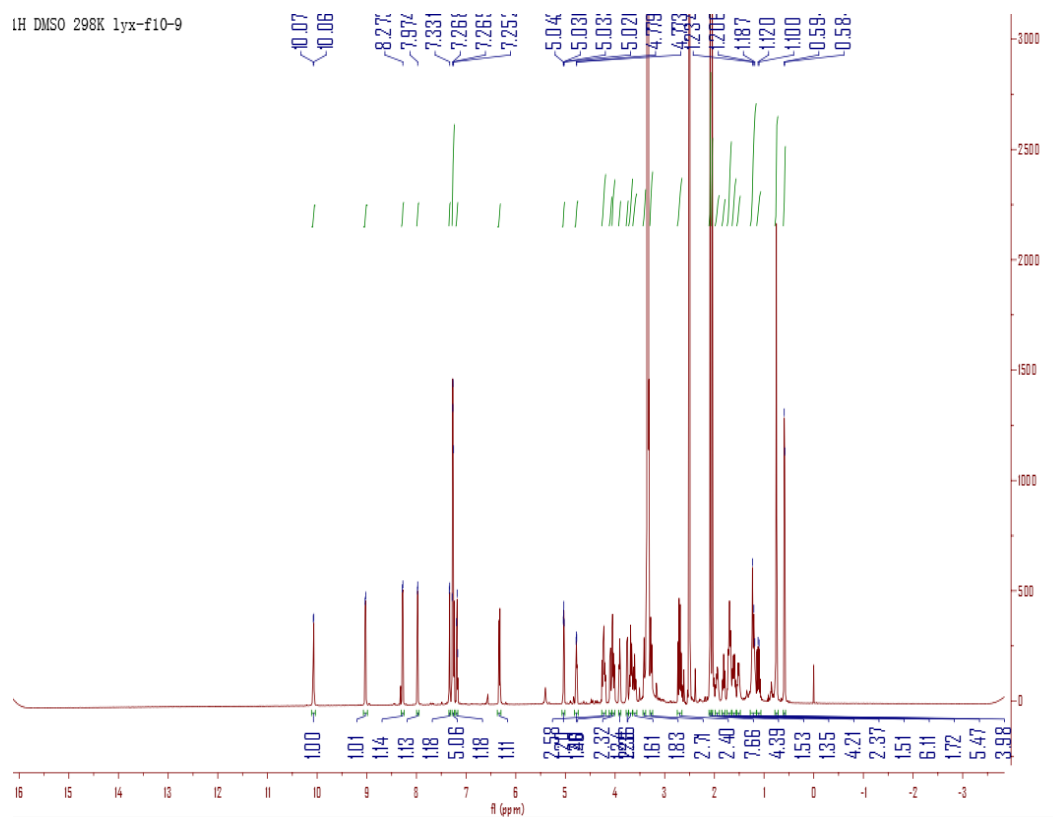


Figure S42. ¹H spectrum of Al (III)-acremonpeptide F (5) in DMSO-*d*₆ (600 MHz).

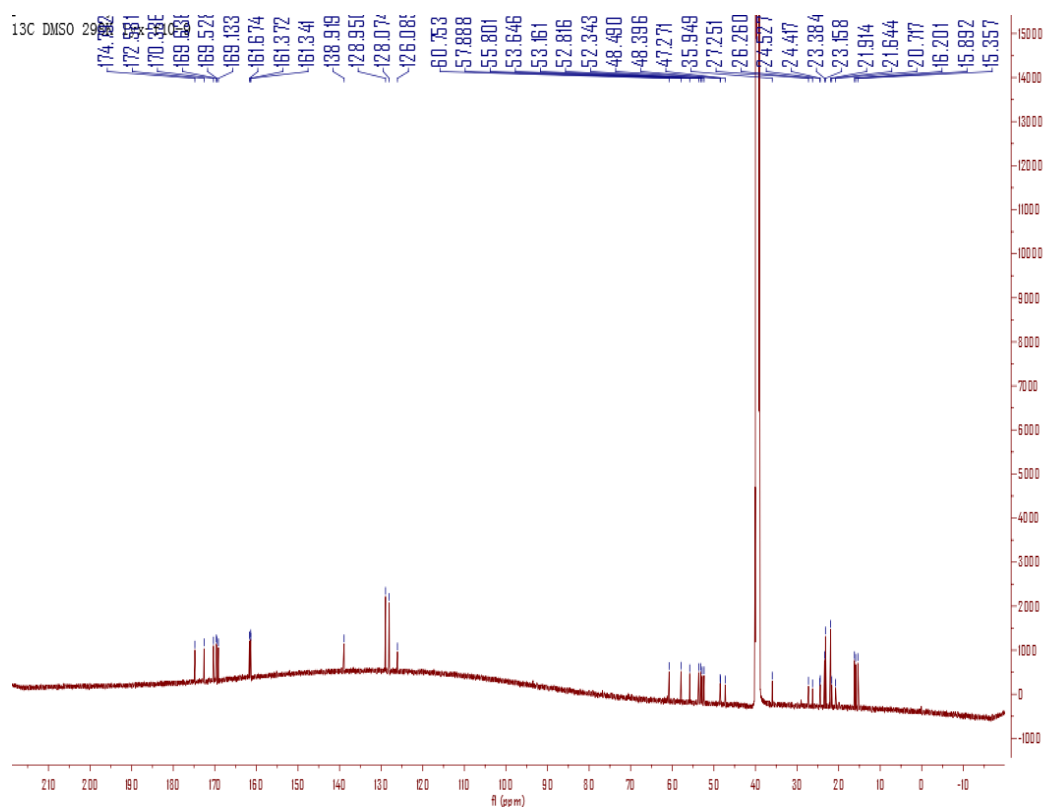


Figure S43. ¹³C spectrum of Al (III)-acremonpeptide F (5) in DMSO-*d*₆ (150 MHz).

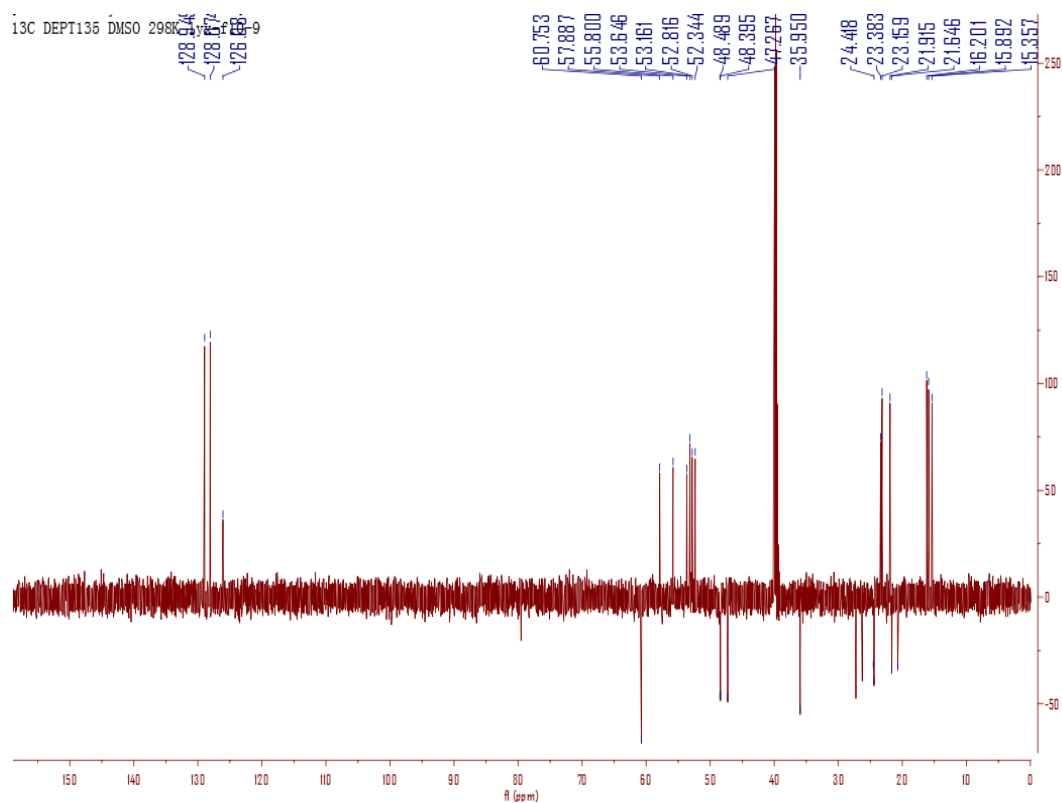


Figure S44. DEPT135 spectrum of Al (III)-acremonpeptide F (5) in DMSO-*d*₆ (150 MHz).

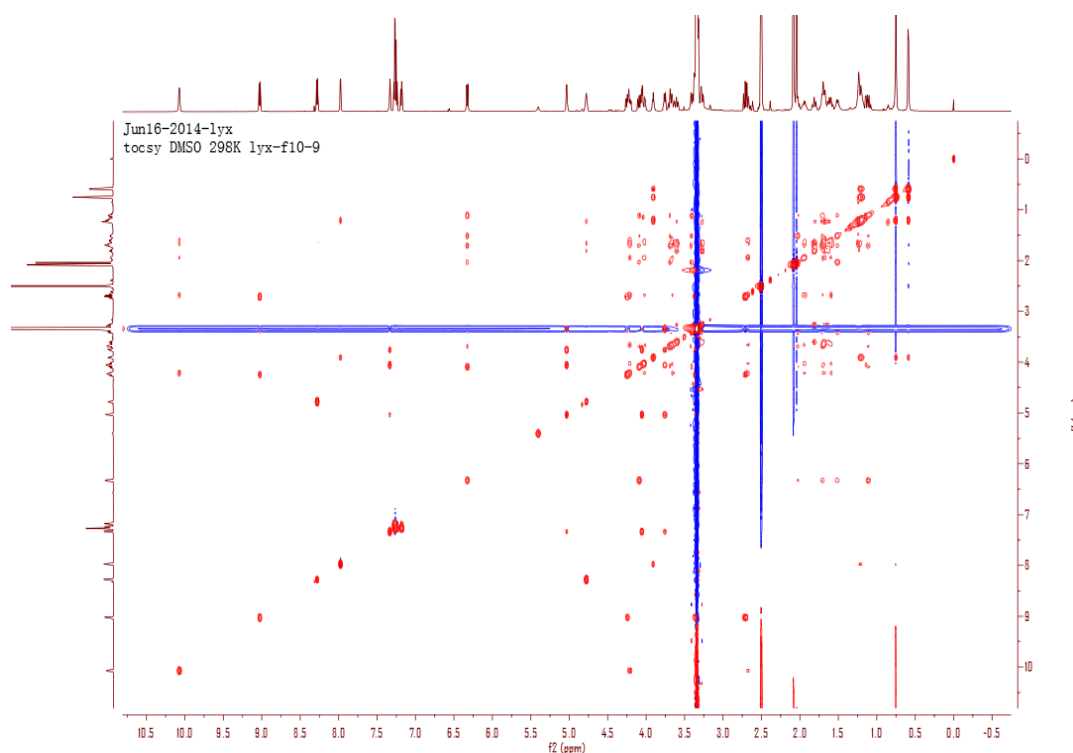


Figure S45. TOCSY spectrum of Al (III)-acremoneptide F (**5**) in DMSO- d_6 .

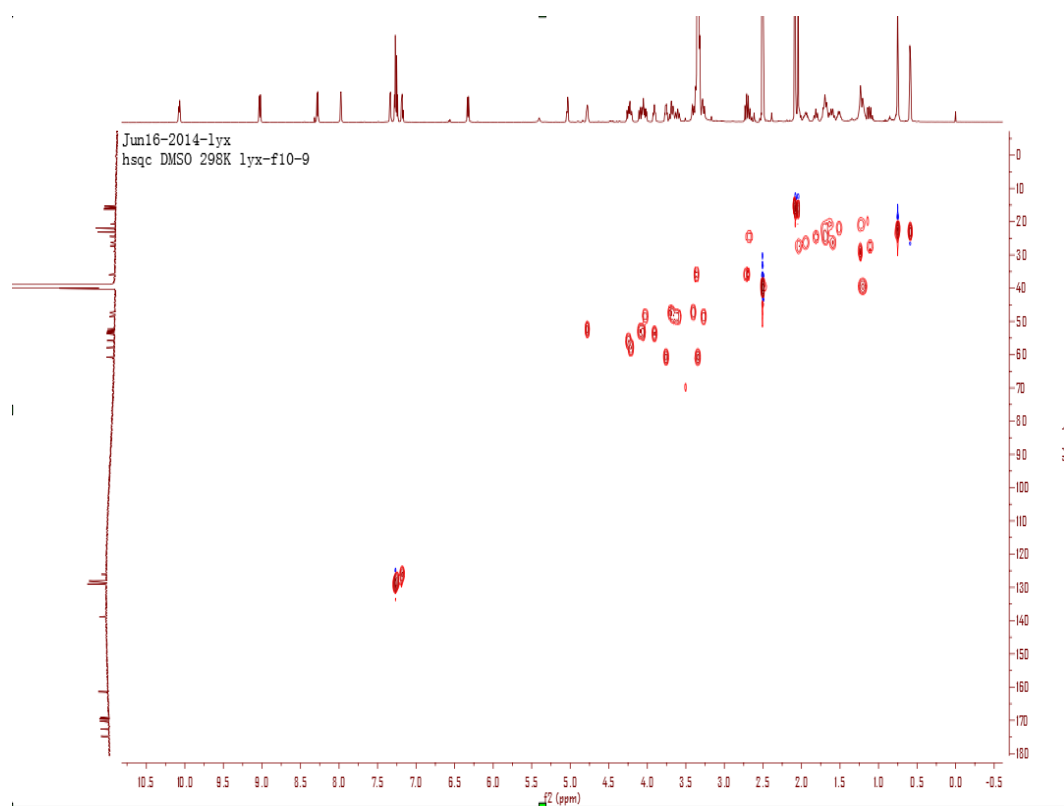


Figure S46. HSQC spectrum of Al (III)-acremoneptide F (**5**) in DMSO- d_6 .

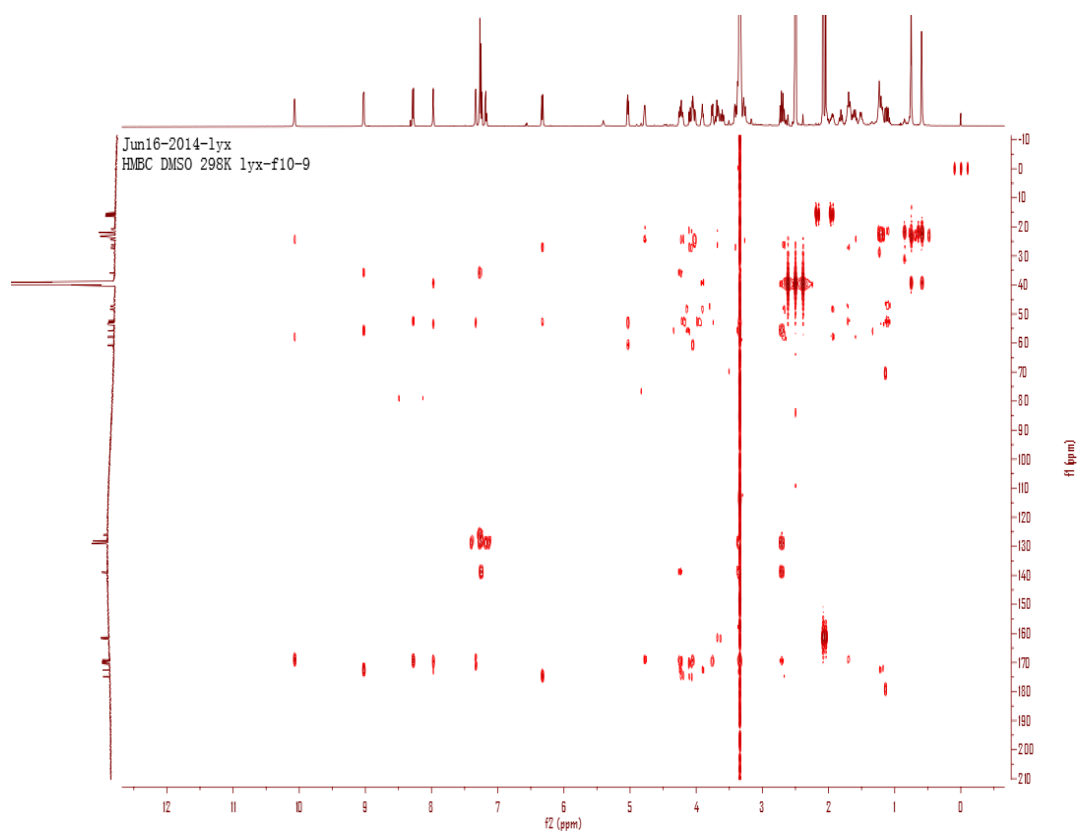


Figure S47. HMBC spectrum of Al (III)-acremoneptide F (**5**) in DMSO- d_6 .

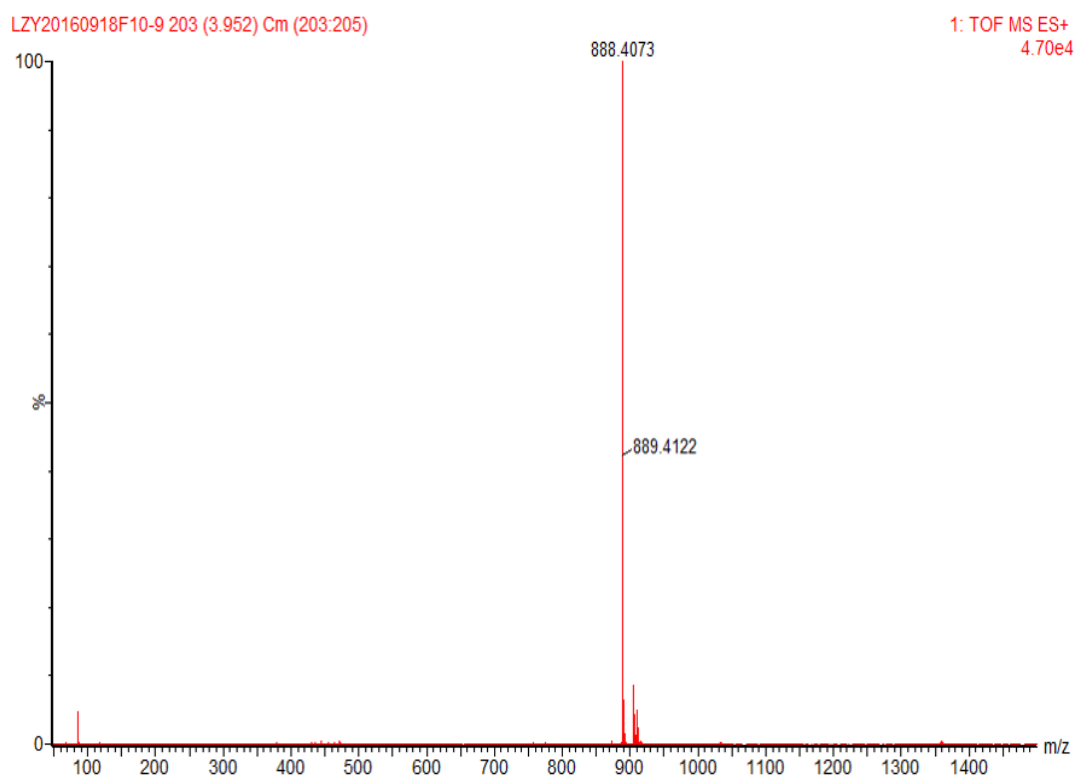


Figure S48. HRESIMS data of Al (III)-acremoneptide F (**5**).

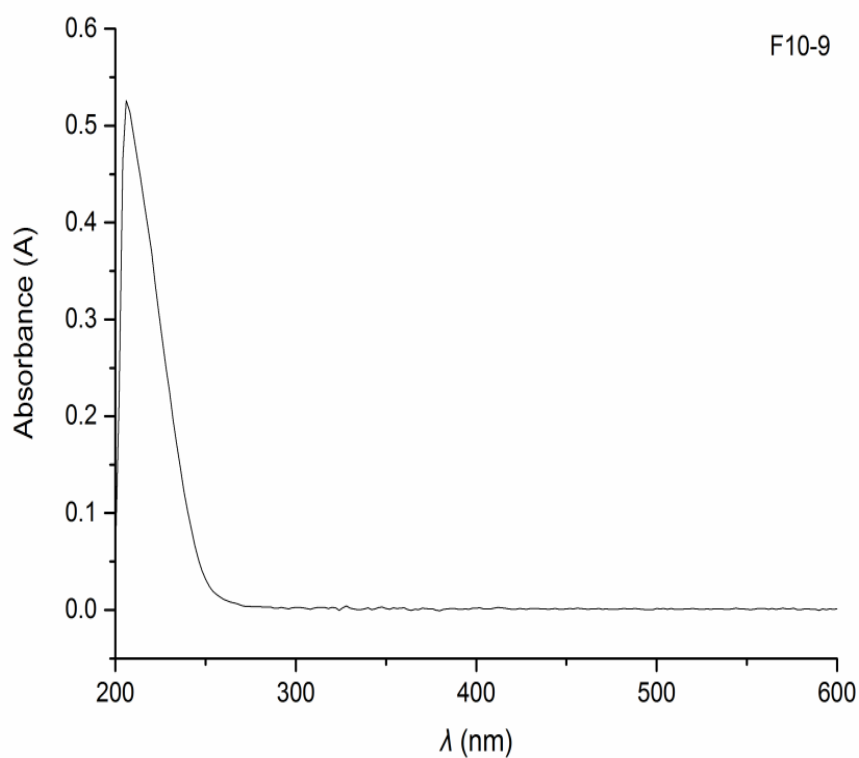


Figure S49. UV spectrum of Al (III)-acremoneptide F (5) in MeOH.

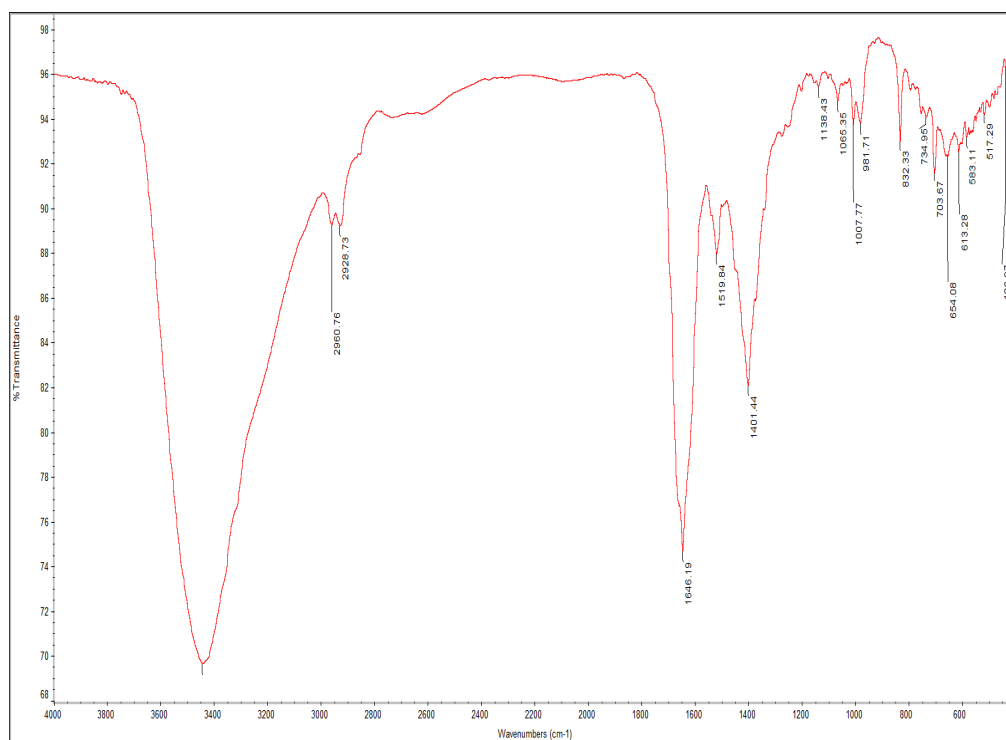


Figure S50. IR spectrum of Al (III)-acremoneptide F (5).

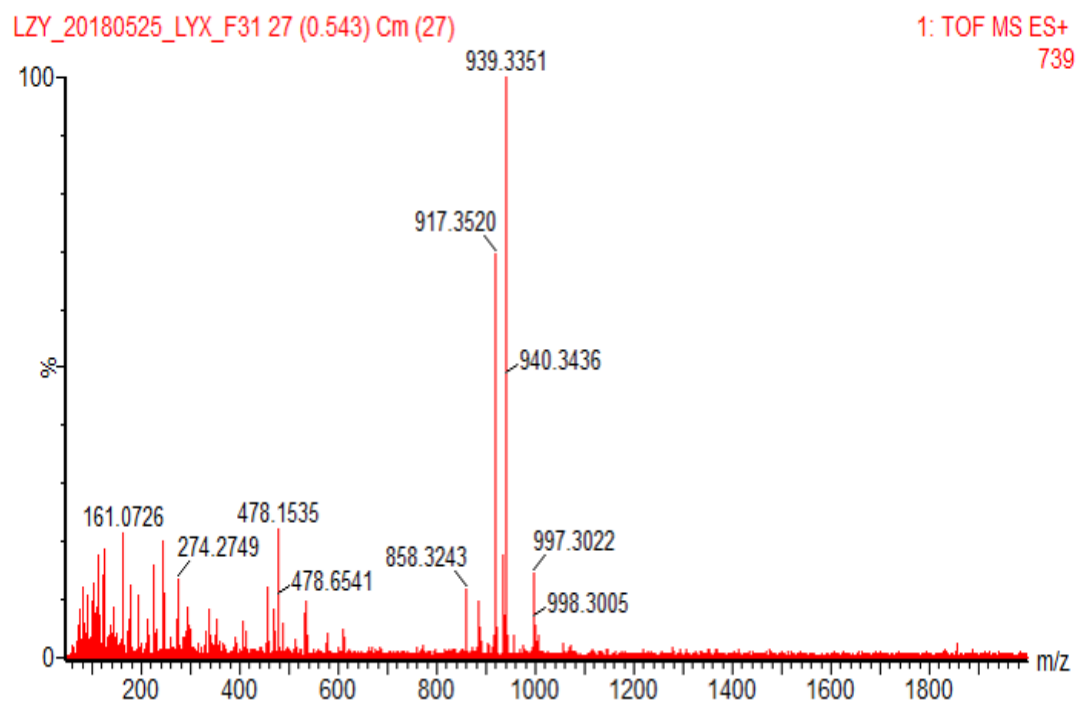


Figure S51. HRESIMS data of Fe (III)-acremoneptide F (**6**).

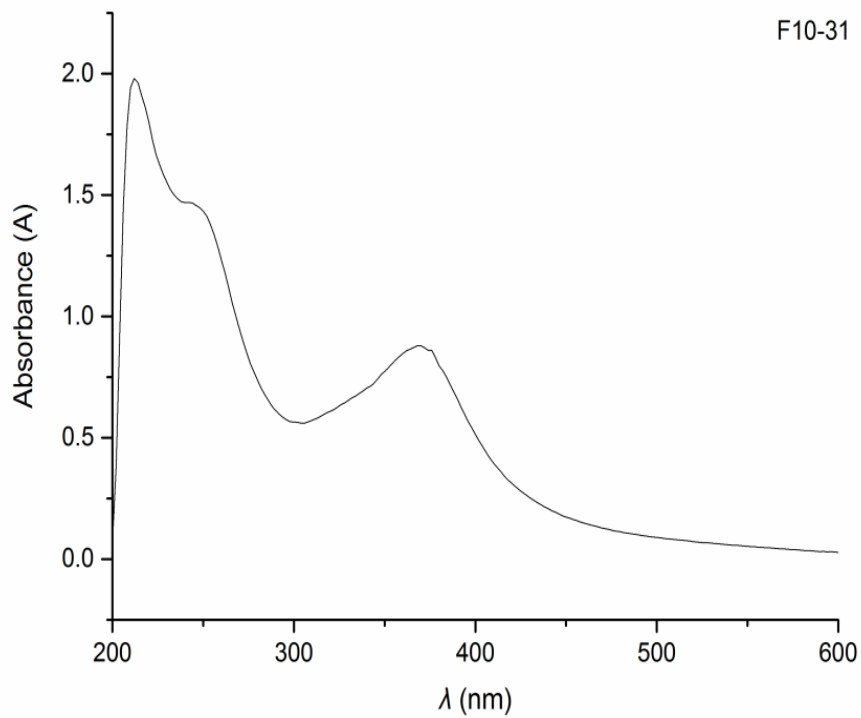


Figure S52. UV spectrum of Fe (III)-acremoneptide F (**6**) in MeOH.

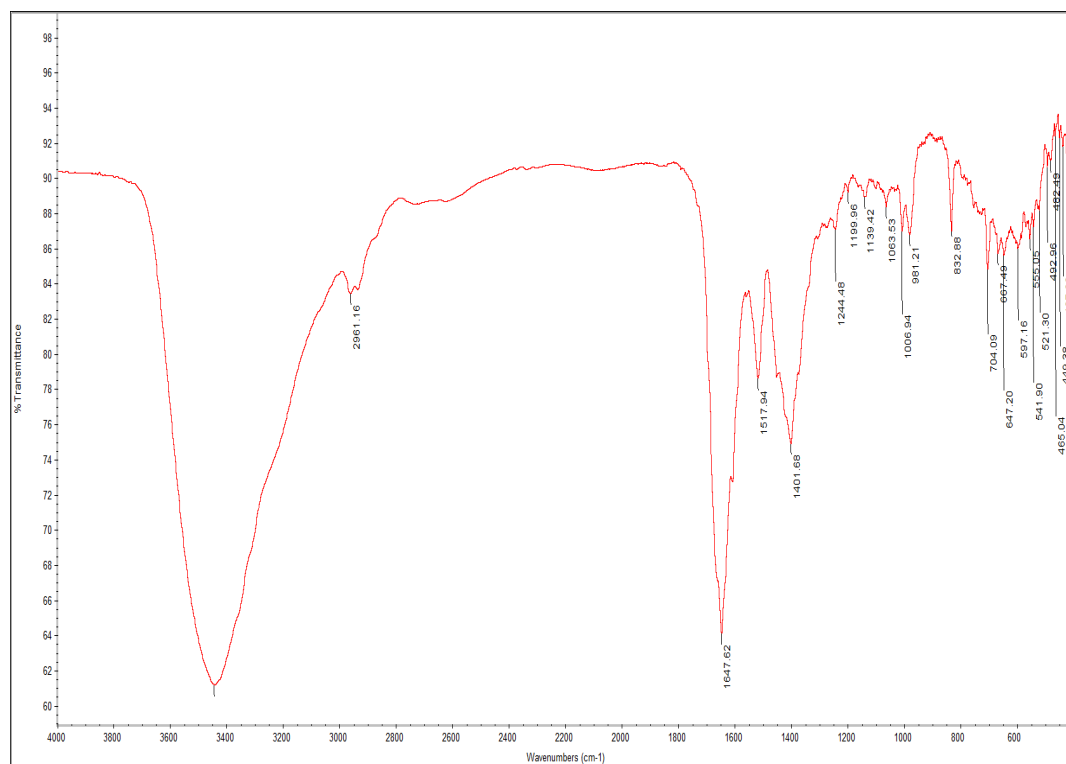


Figure S53. IR spectrum of Fe (III)-acremnonpeptide F (6).

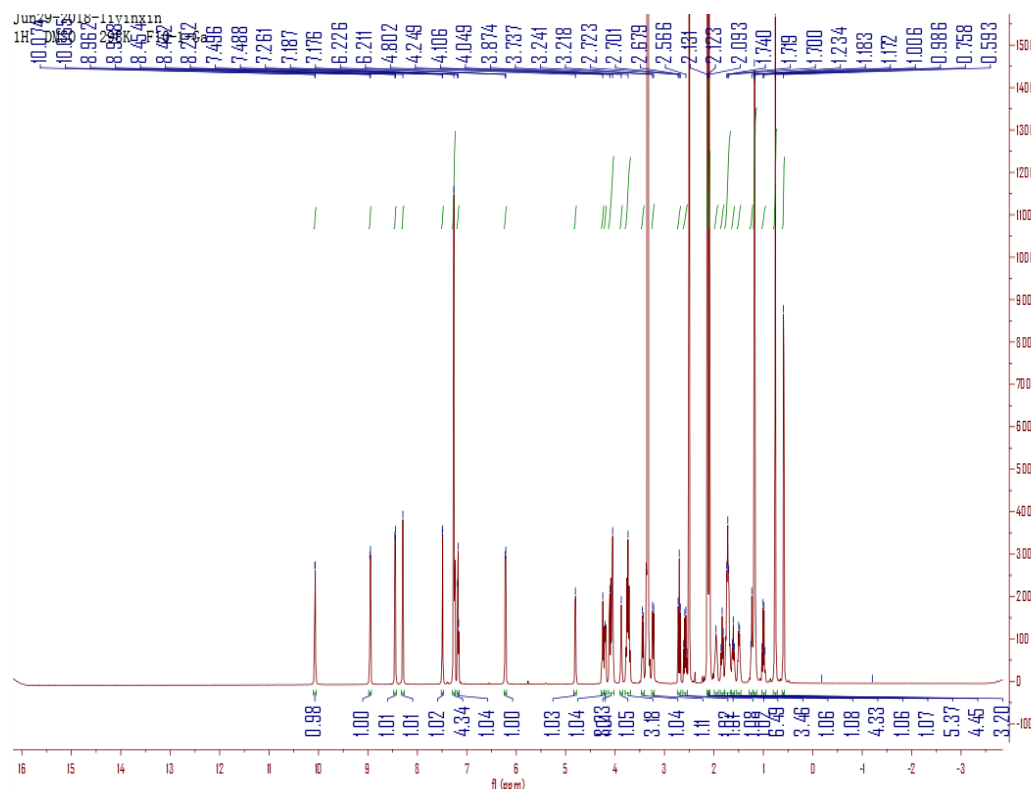


Figure S54. ¹H spectrum of Ga (III)-acremnonpeptide E (7) in DMSO-d₆ (600 MHz).

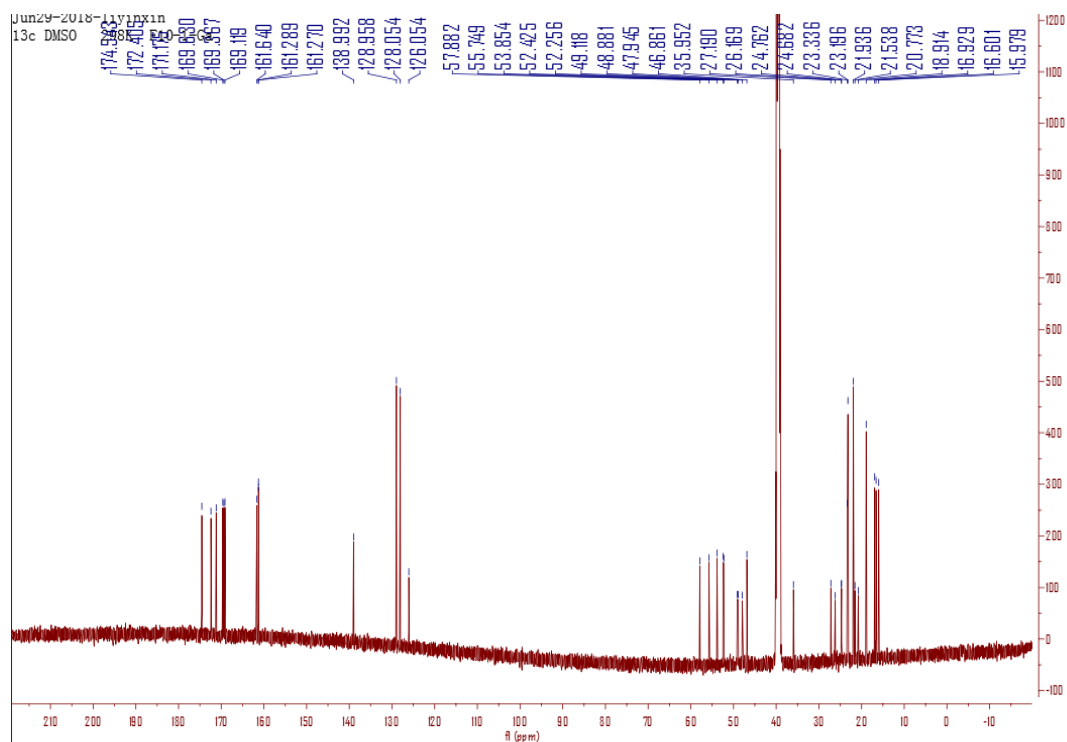


Figure S55. ^{13}C spectrum of Ga (III)-acremontepeptide E (7) in $\text{DMSO}-d_6$ (150 MHz).

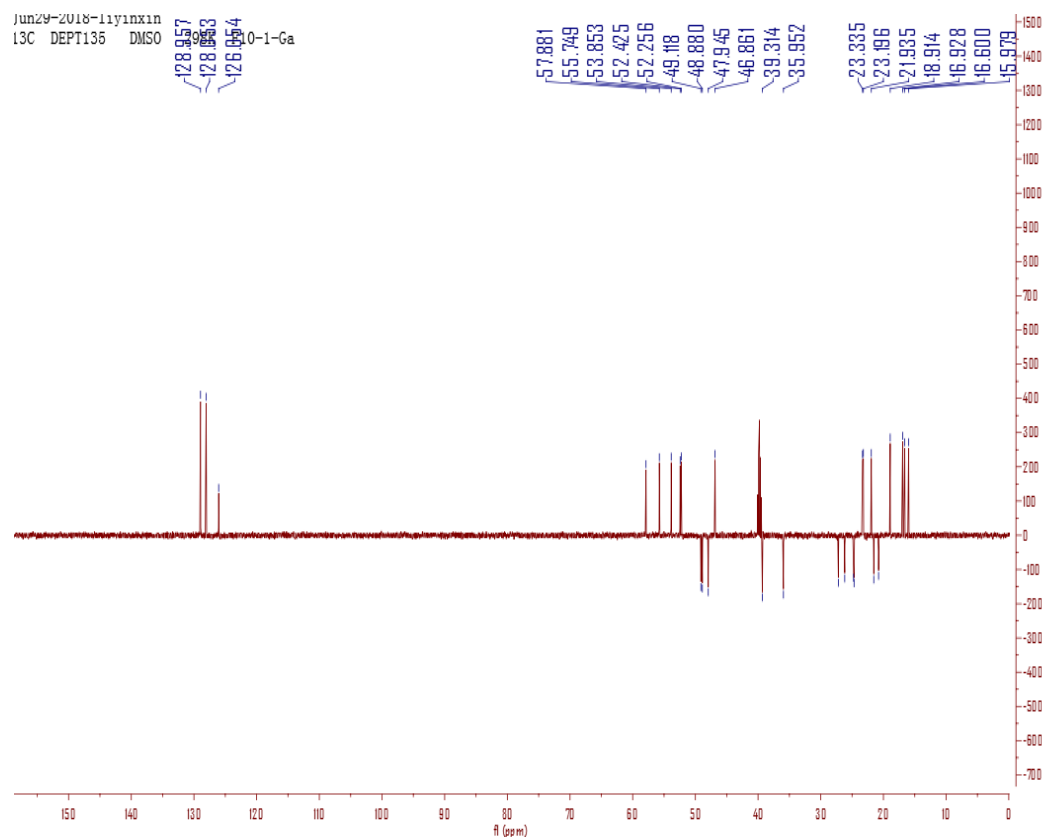


Figure S56. DEPT135 spectrum of Ga (III)-acremontepeptide E (7) in $\text{DMSO}-d_6$ (150 MHz).

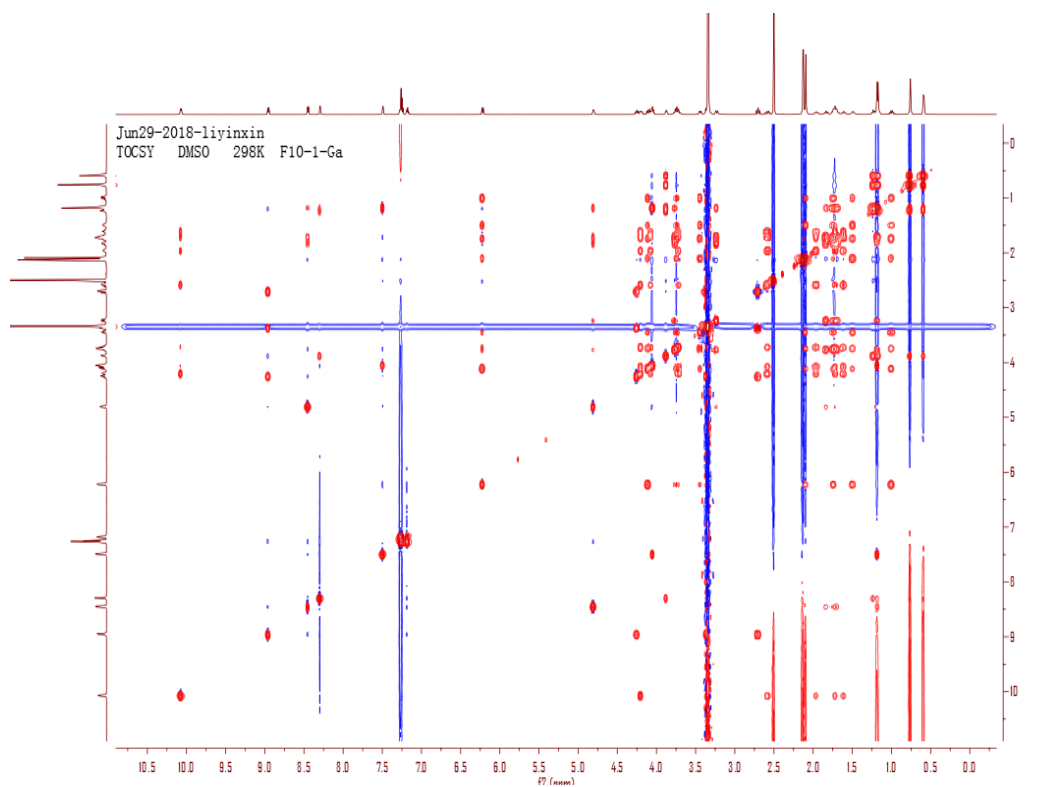


Figure S57. TOCSY spectrum of Ga (III)-acremoneptide E (7) in DMSO- d_6

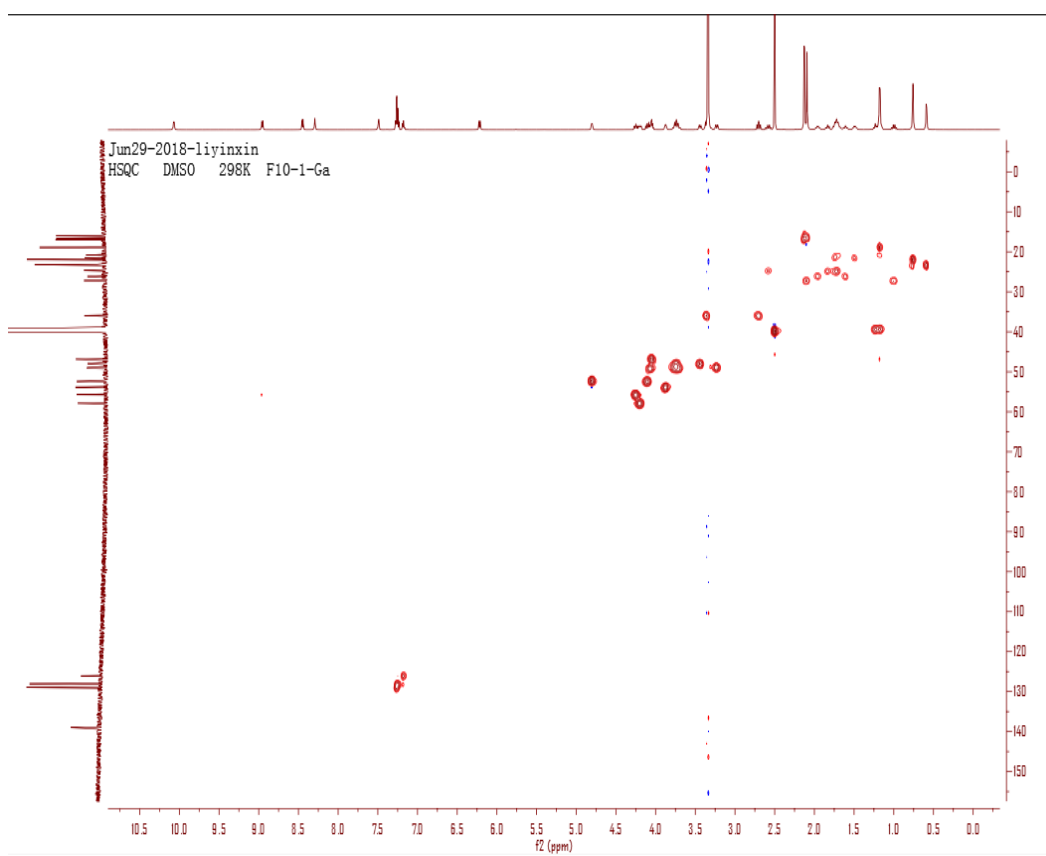


Figure S58. HSQC spectrum of Ga (III)-acremoneptide E (7) in DMSO- d_6 .

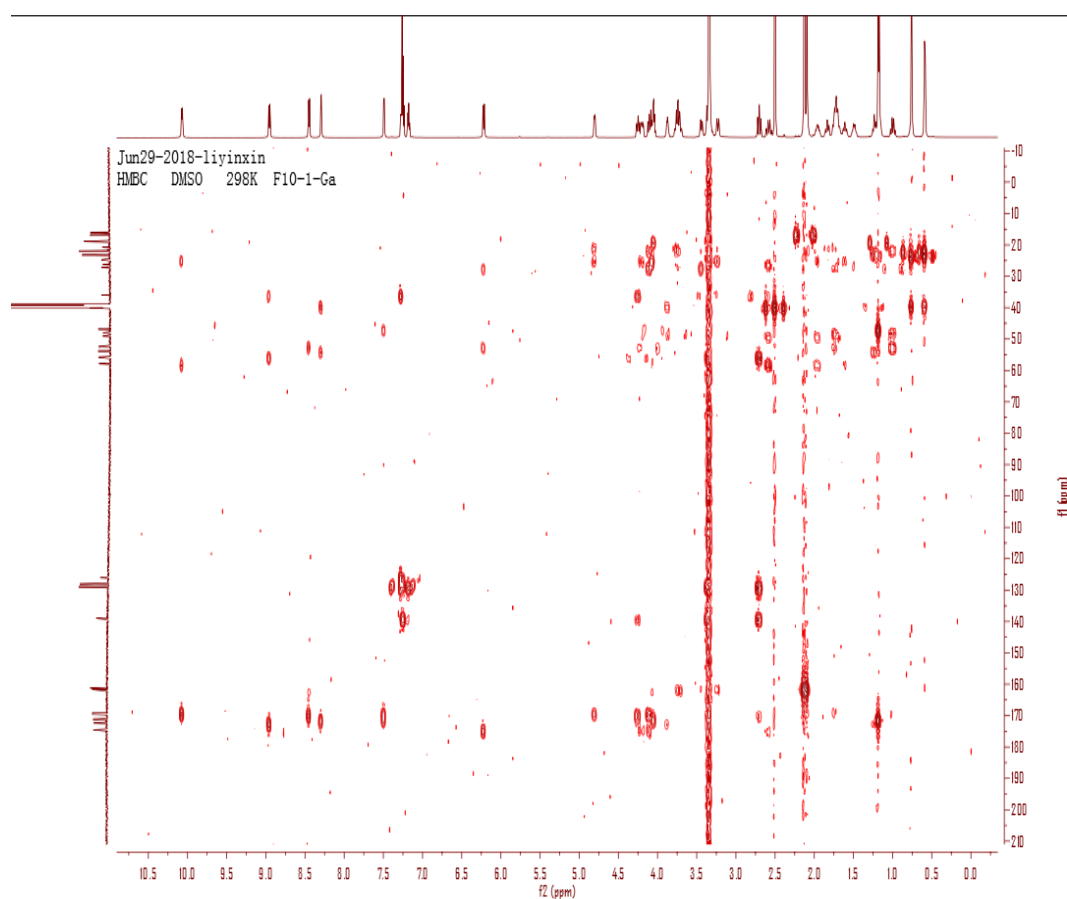


Figure S59. HMBC spectrum of Ga (III)-acremonpeptide E (7) in DMSO- d_6 .

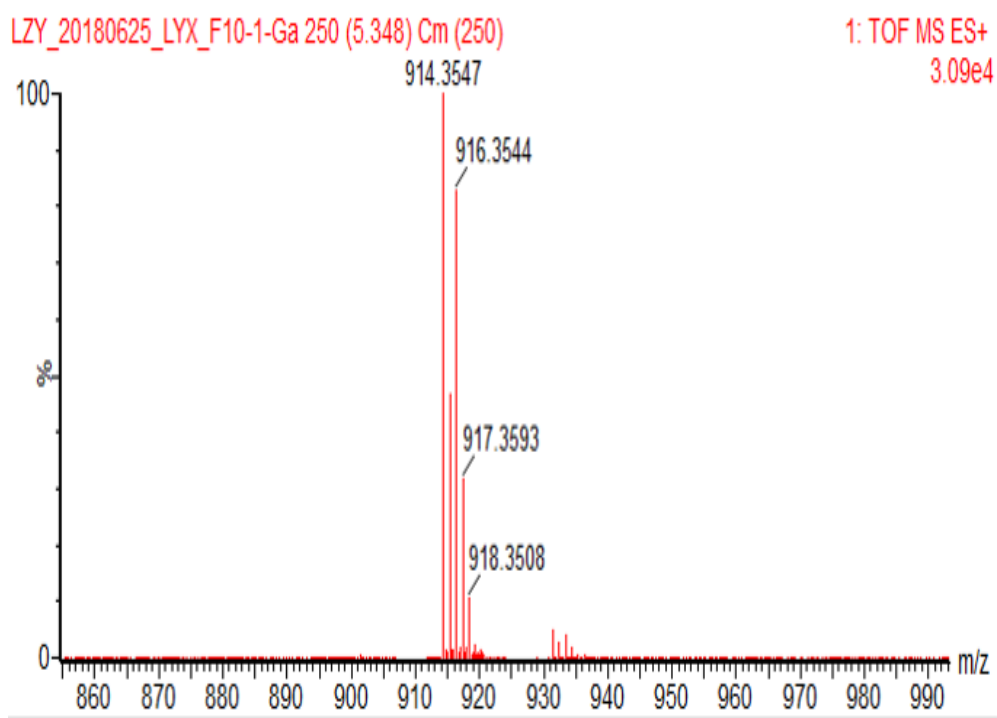


Figure S60. HRESIMS data of Ga (III)-acremonpeptide E (7).

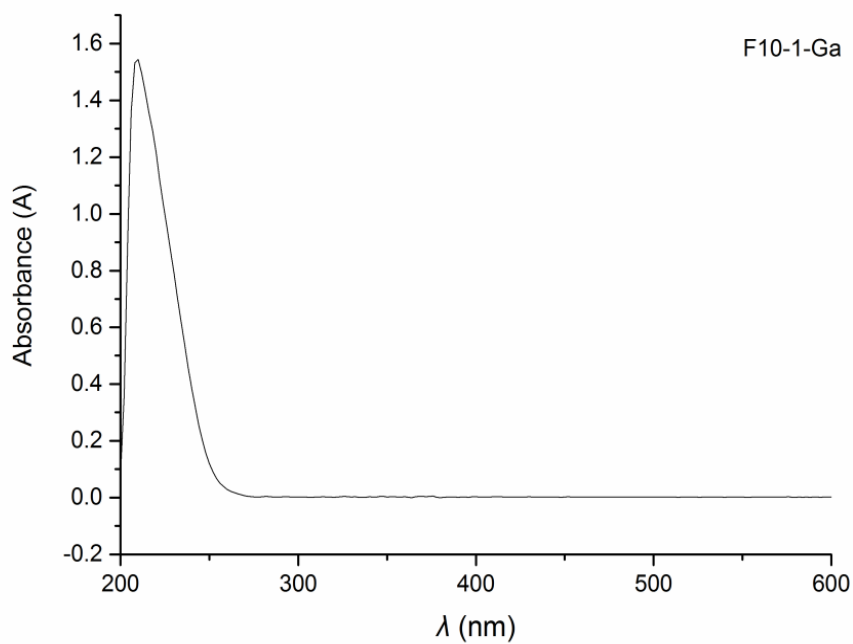


Figure S61. UV spectrum of Ga (III)-acremoneptide E (7) in MeOH.

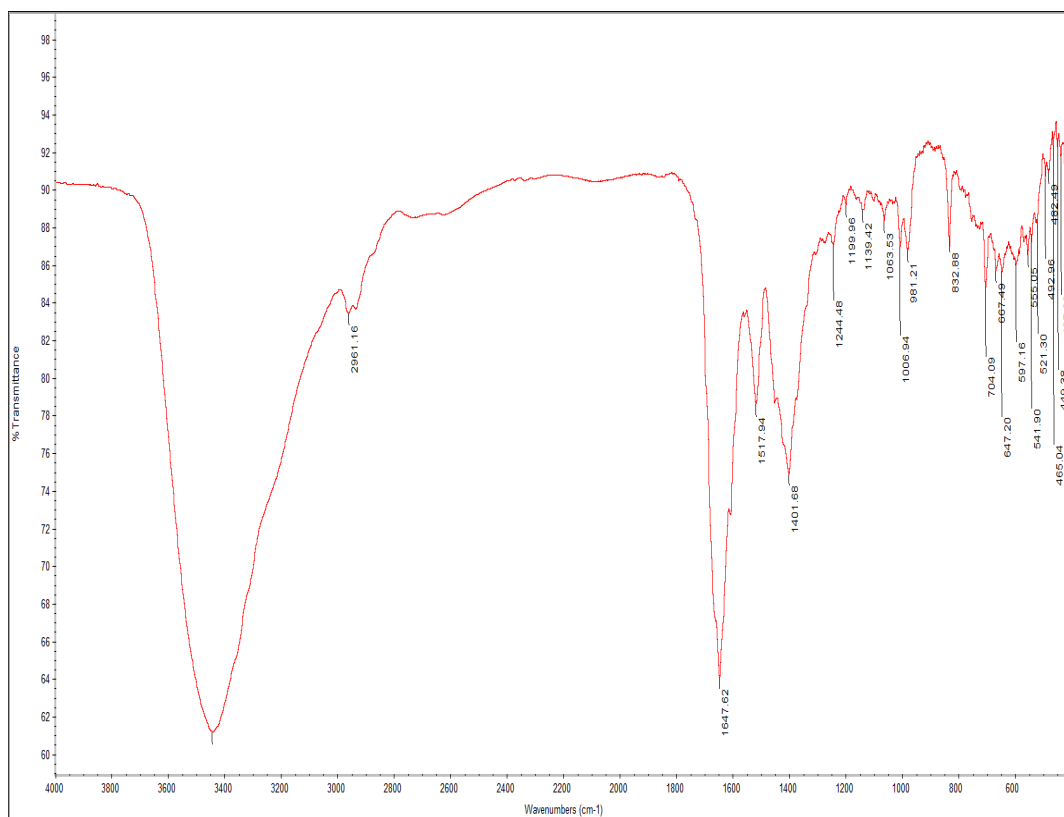


Figure S62. IR spectrum of Ga (III)-acremoneptide E (7).

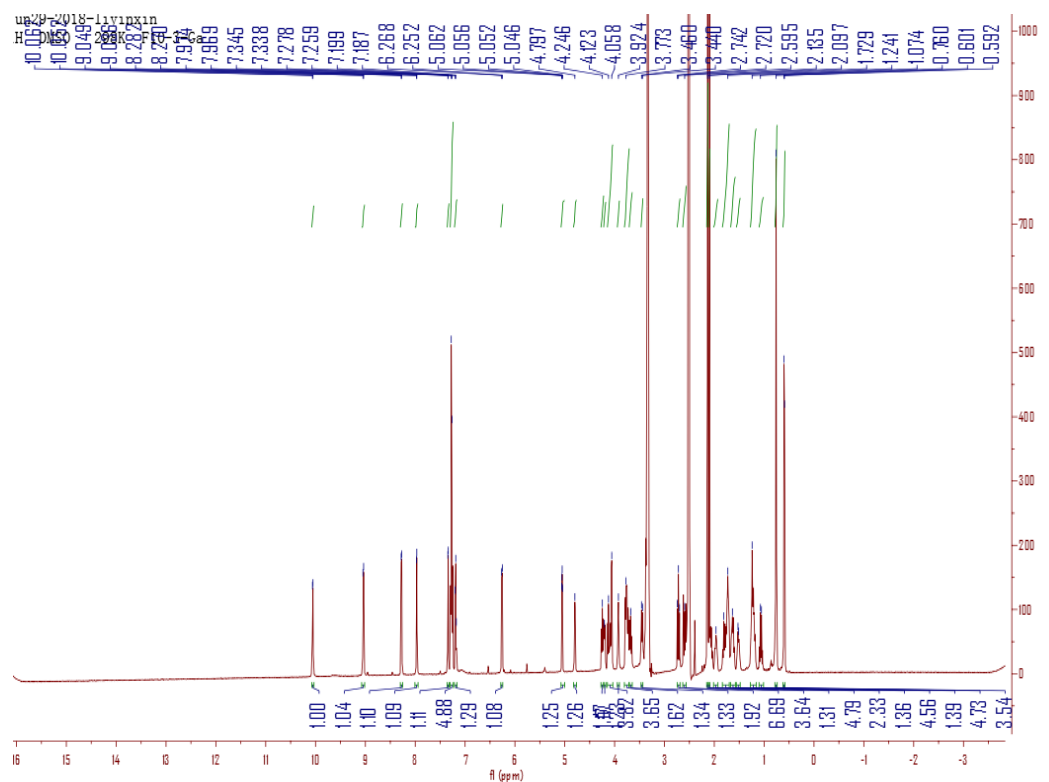


Figure S63. ^1H spectrum of Ga (III)-acremoneptide F (**8**) in $\text{DMSO}-d_6$ (600 MHz).

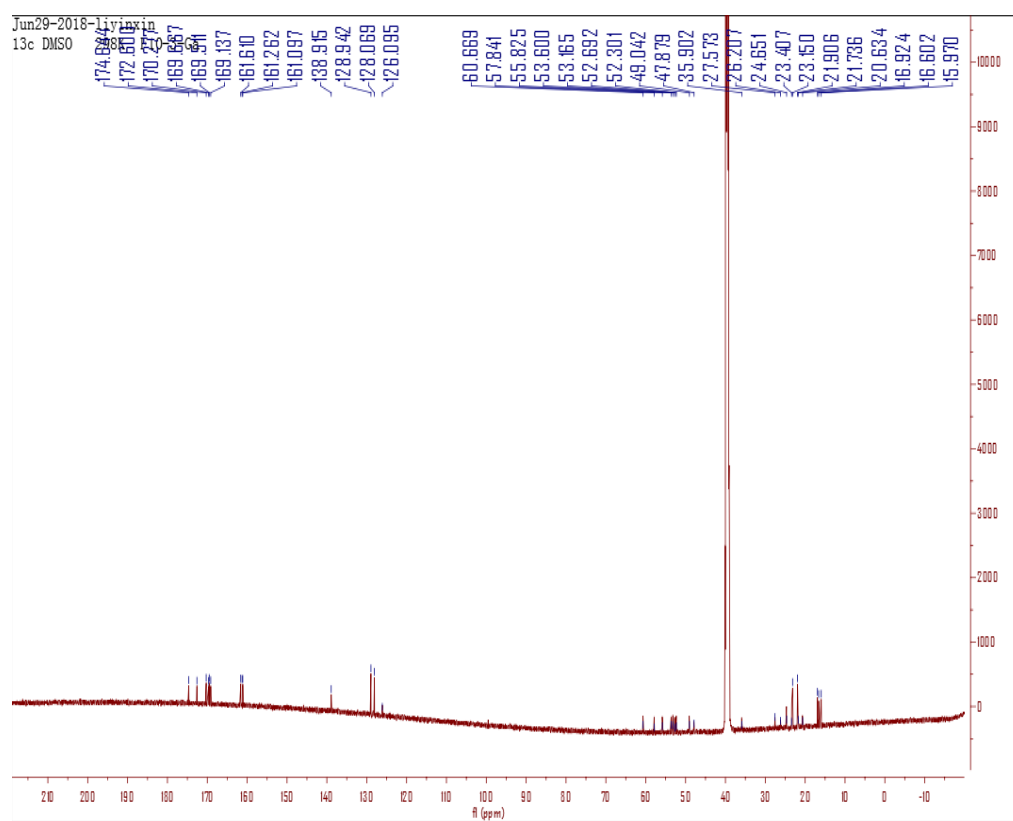


Figure S64. ^{13}C spectrum of Ga (III)-acremoneptide F (**8**) in $\text{DMSO}-d_6$ (150 MHz).

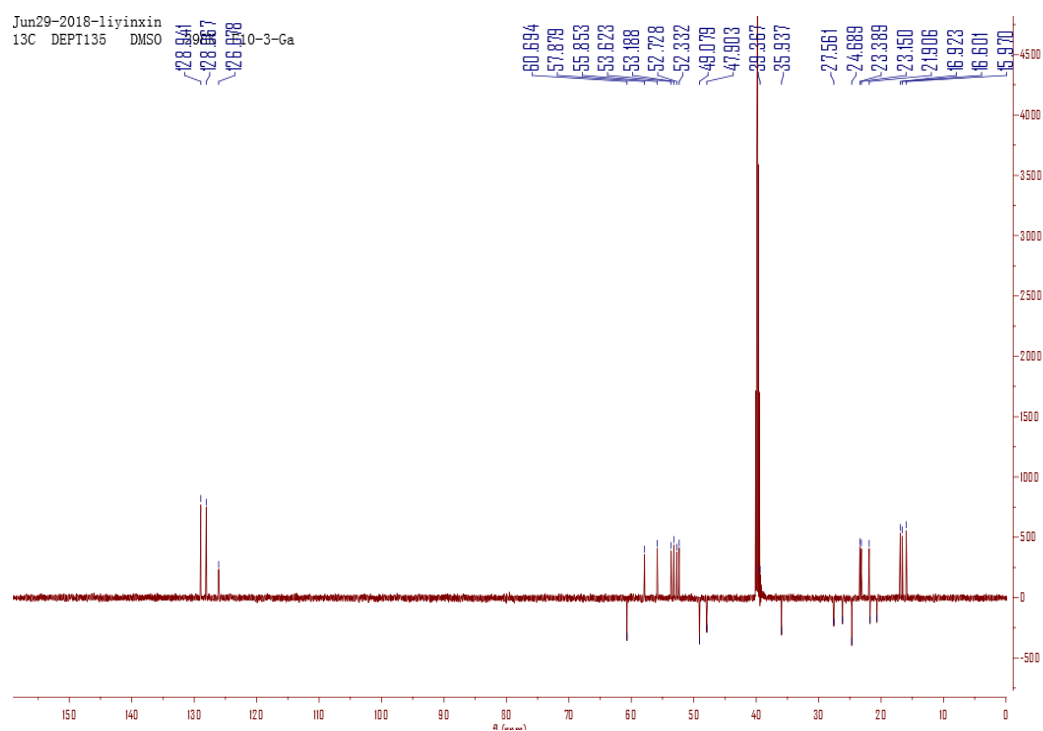


Figure S65. DEPT135 spectrum of Ga (III)-acremoneptide F (**8**) in DMSO- d_6 (150 MHz).

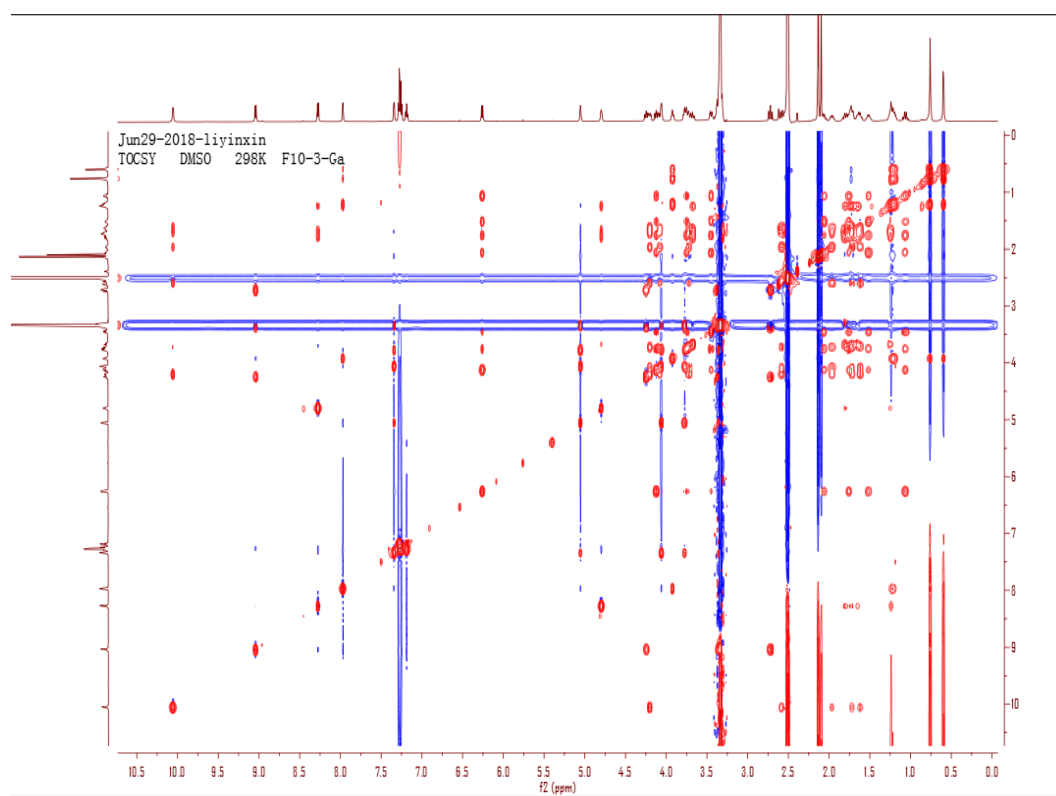


Figure S66. TOCSY spectrum of Ga (III)-acremoneptide F (**8**) in DMSO- d_6 .

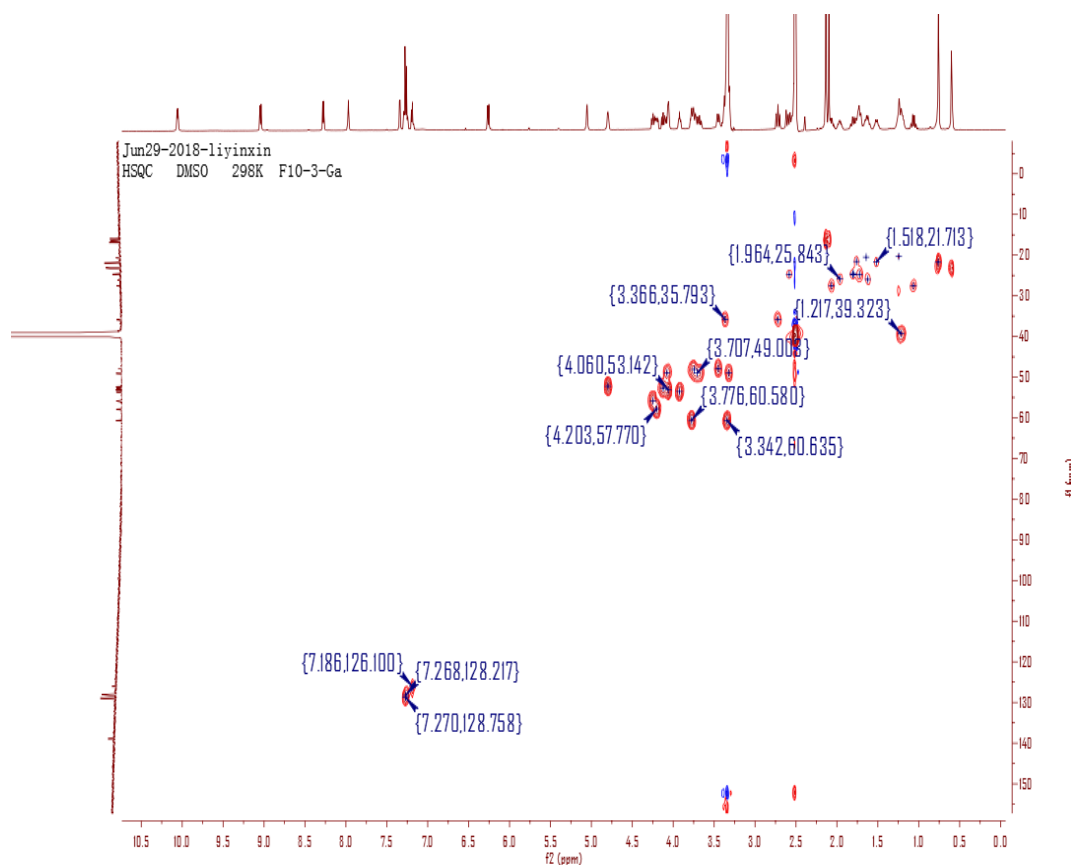


Figure S67. HSQC spectrum of Ga (III)-acremoneptide F (**8**) in DMSO- d_6 .

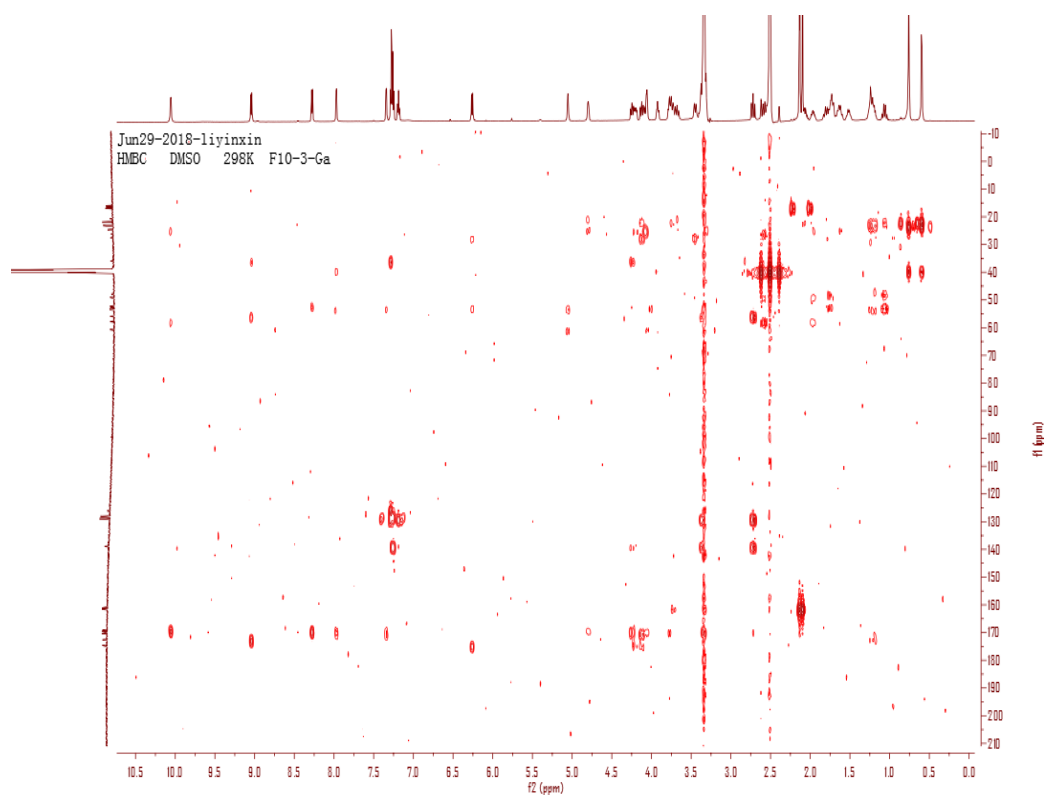


Figure S68. HMBC spectrum of Ga (III)-acremoneptide F (**8**) in DMSO- d_6 .

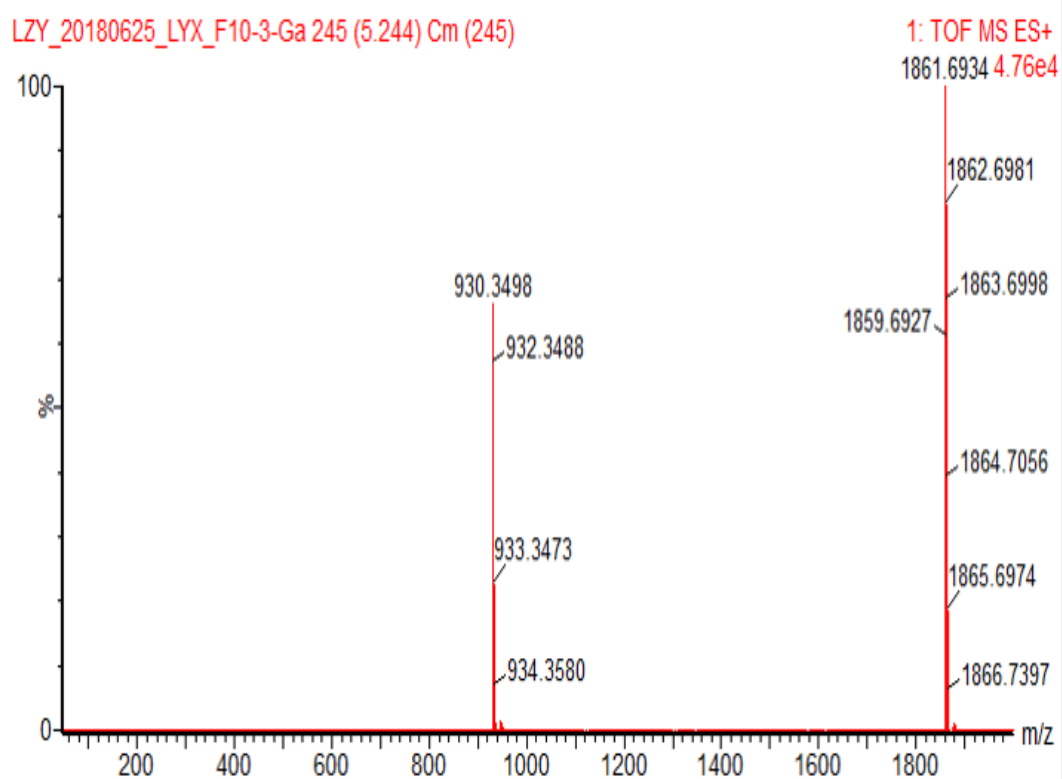


Figure S69. HRESIMS data of Ga (III)-acremoneptide F (**8**).

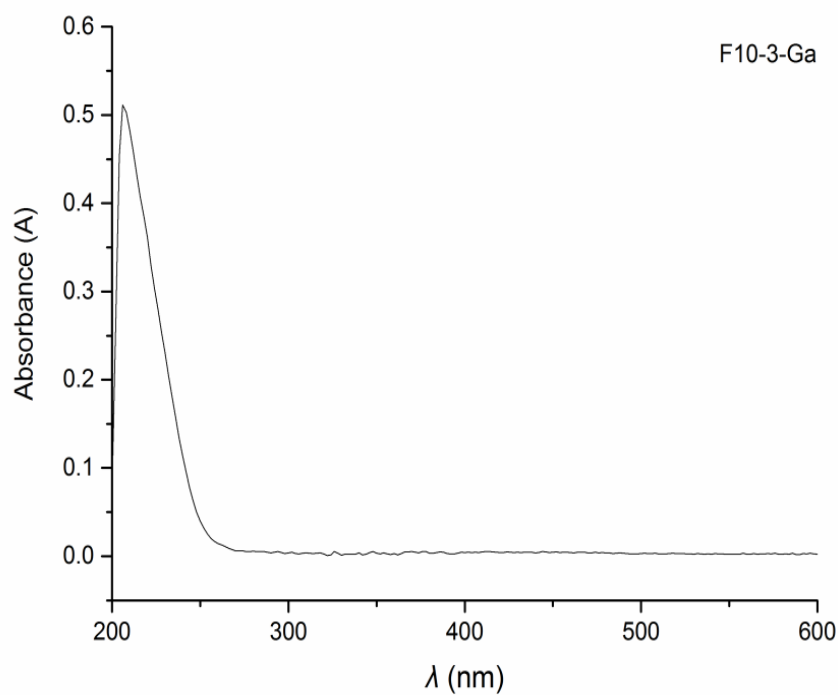


Figure S70. UV spectrum of Ga (III)-acremoneptide F (**8**) in MeOH.

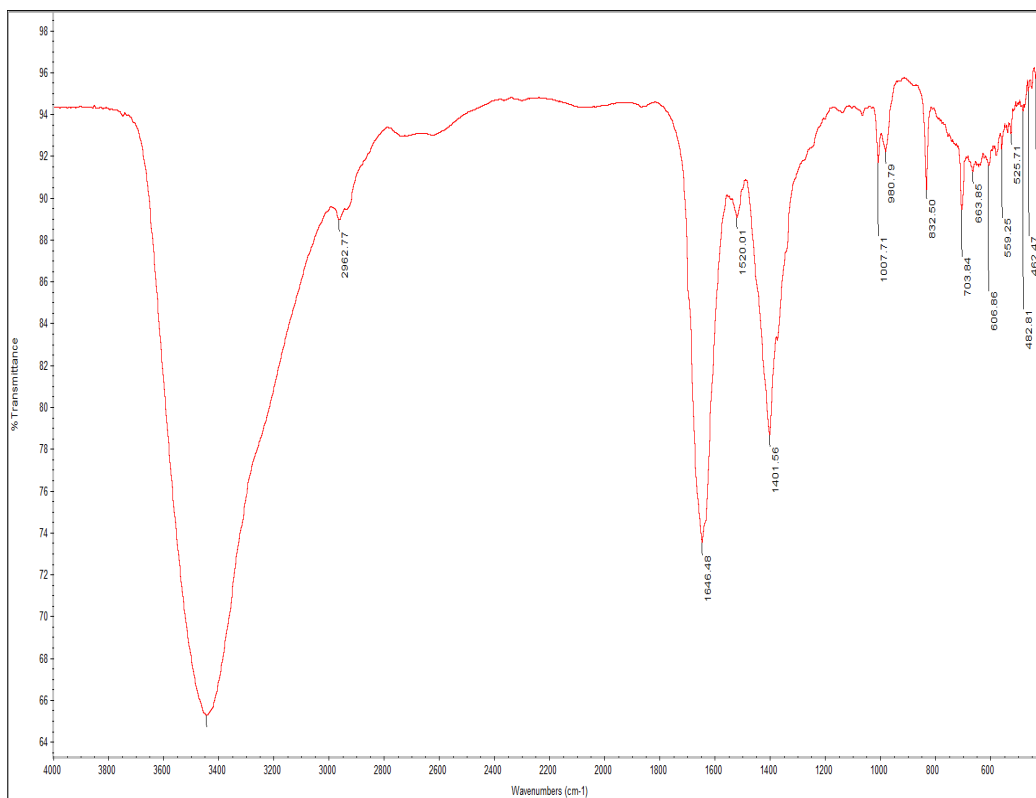


Figure S71. IR spectrum of Ga (III)-acremoneptide F (**8**).

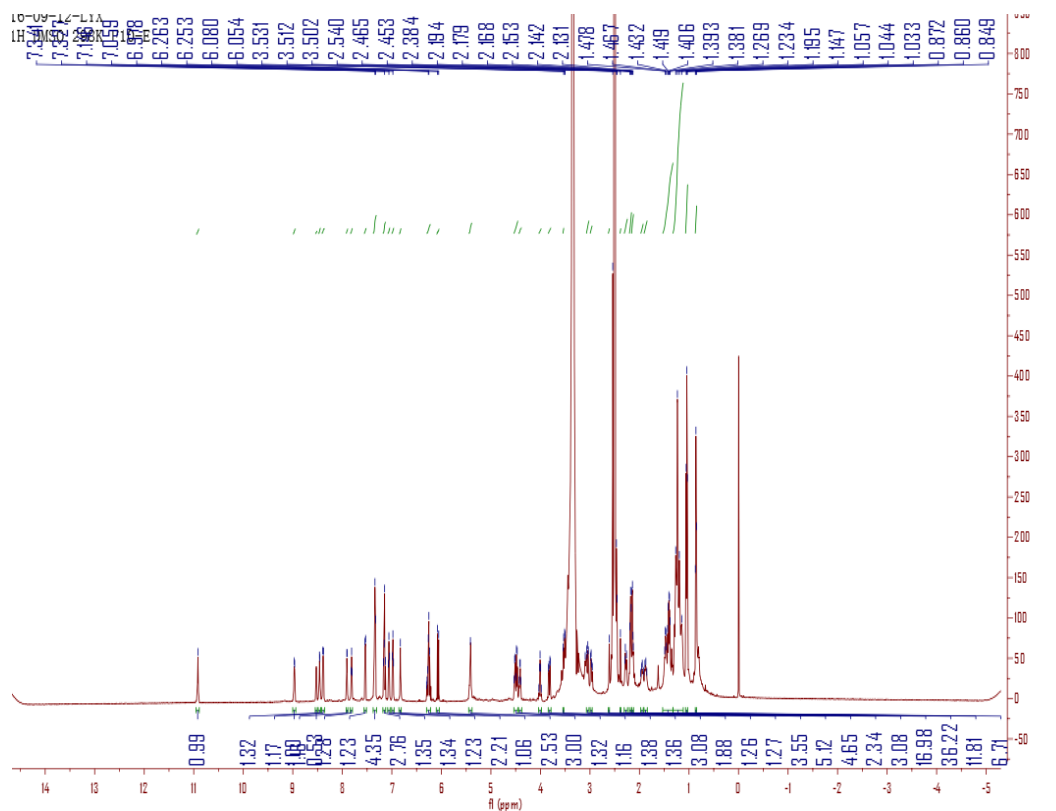


Figure S72. ^1H spectrum of aselacin D (**9**) in $\text{DMSO}-d_6$ (600 MHz).

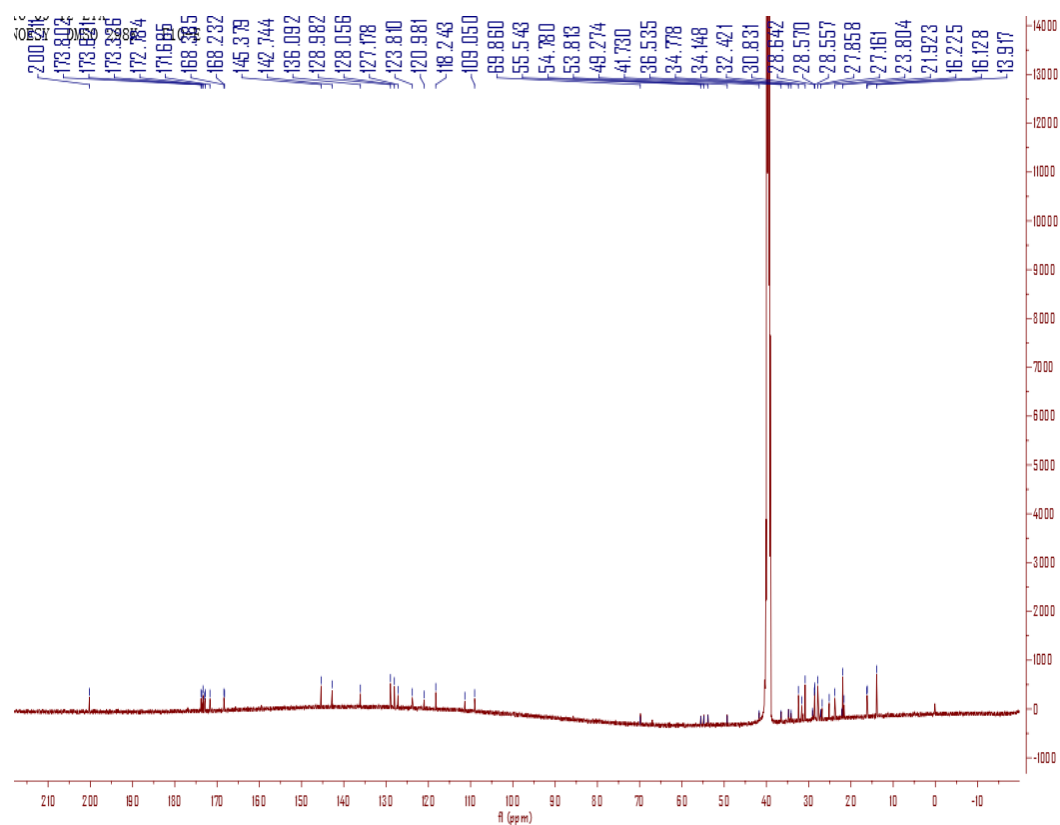


Figure S73. ¹³C spectrum of aselacin D (9) in DMSO-*d*₆ (150 MHz).

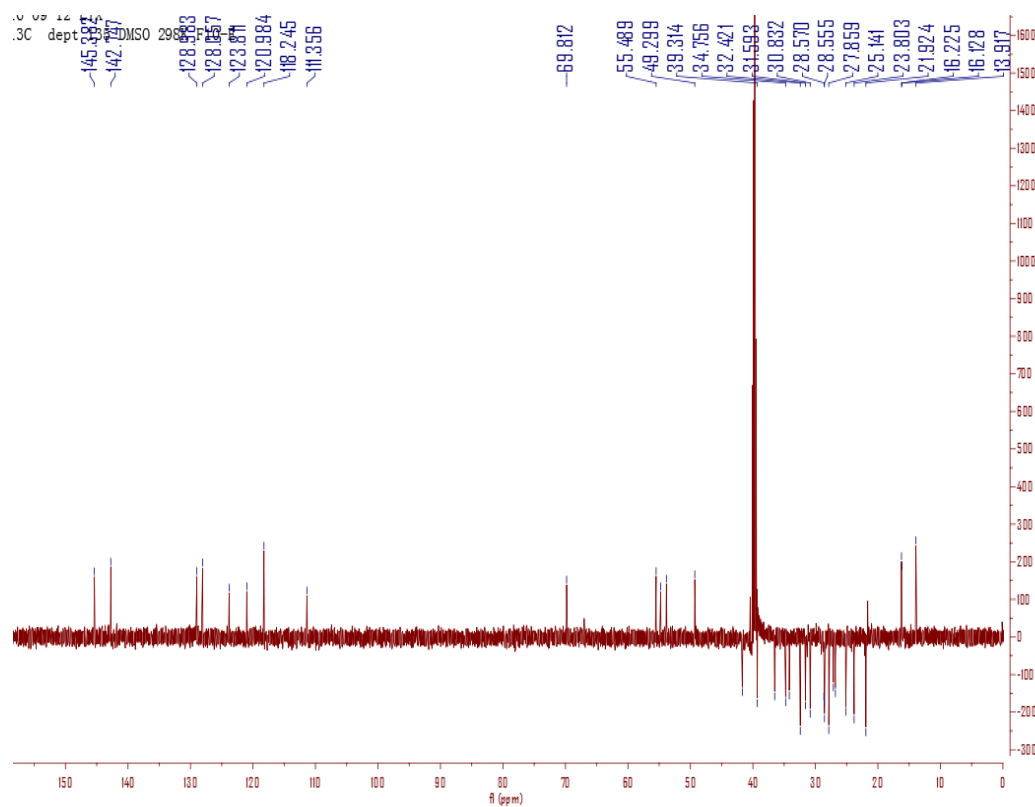


Figure S74. DEPT135 spectrum of aselacin D (9) in DMSO-*d*₆ (150 MHz).

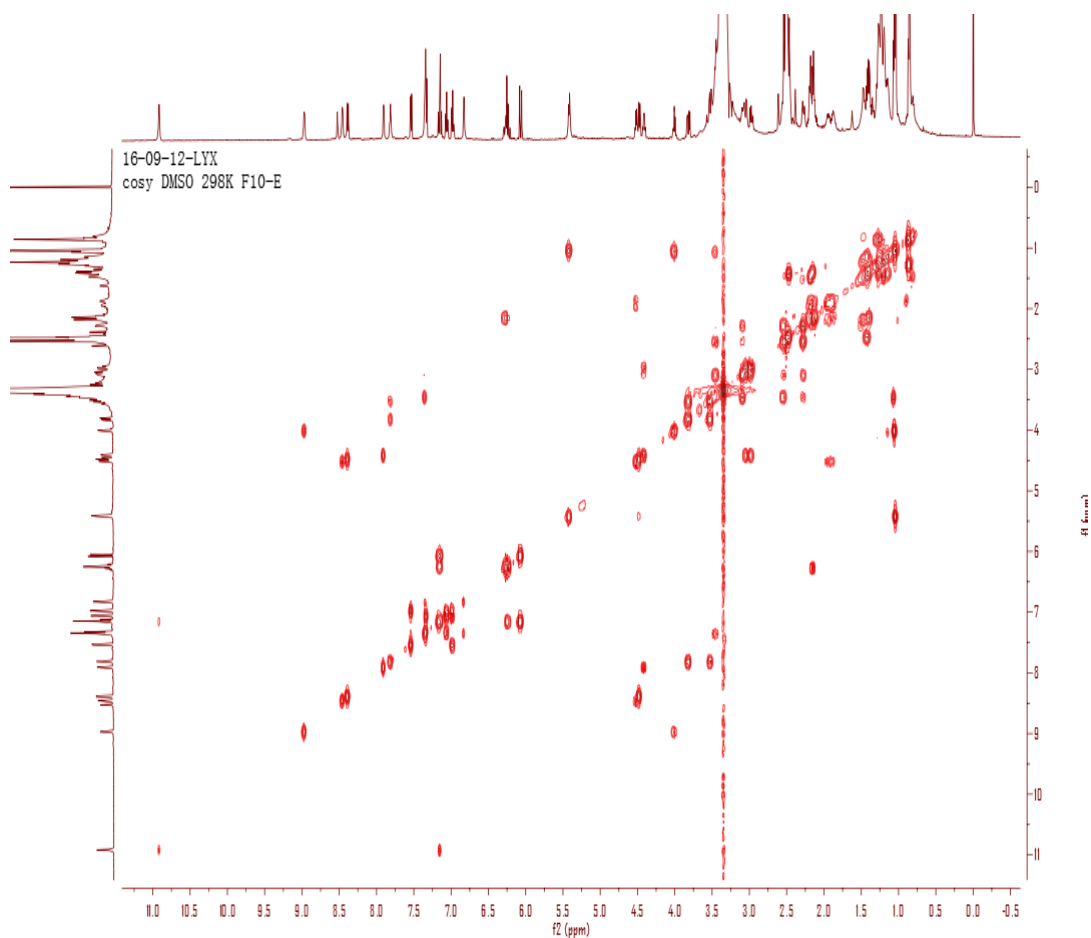


Figure S75. TOCSY spectrum of aselacin D (**9**) in DMSO- d_6

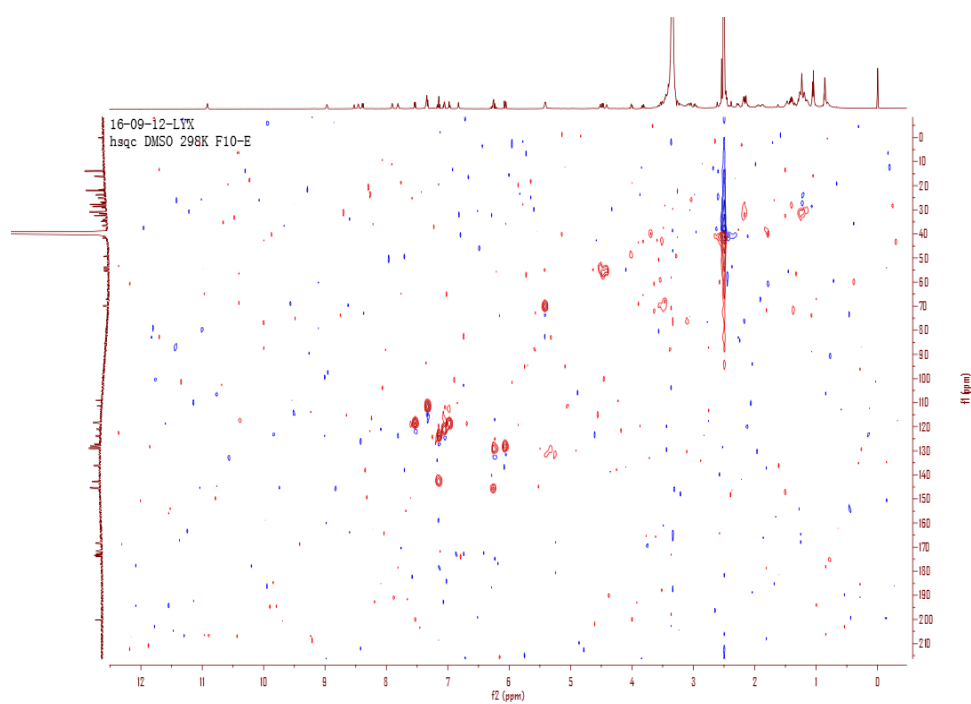


Figure S76. HSQC spectrum of aselacin D (**9**) in DMSO- d_6

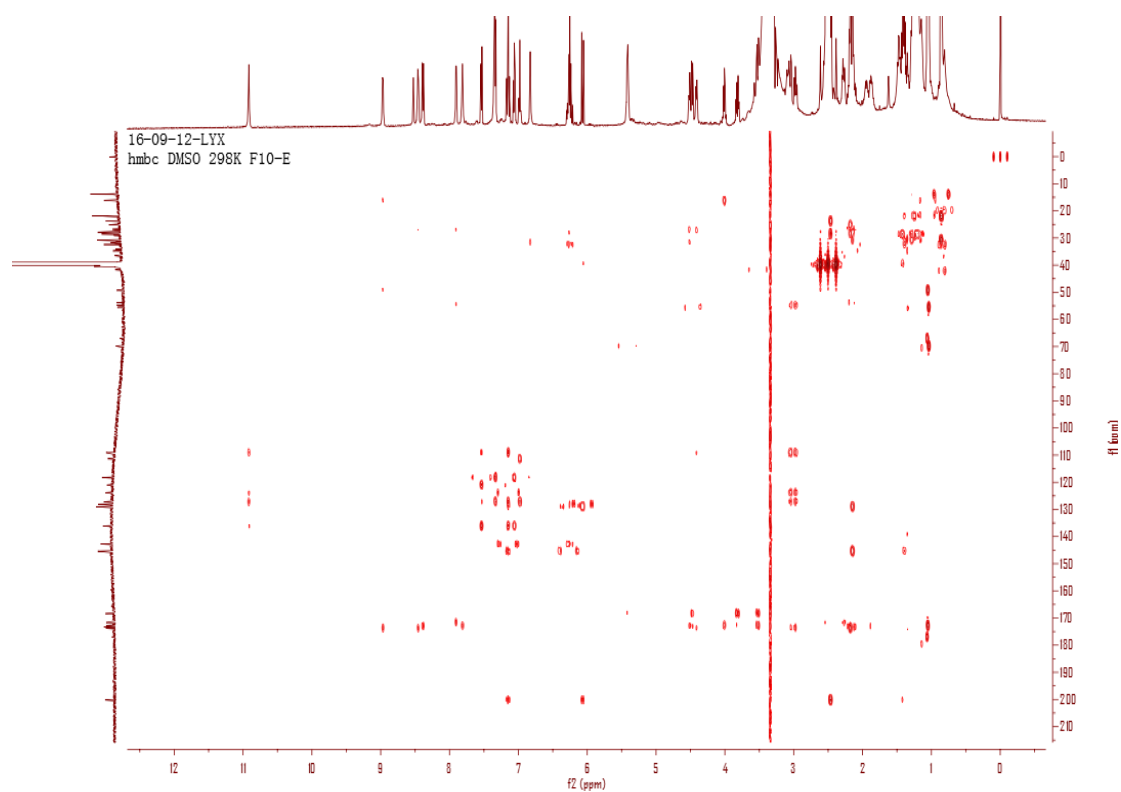


Figure S77. HMBC spectrum of aselacin D (**9**) in DMSO-*d*₆

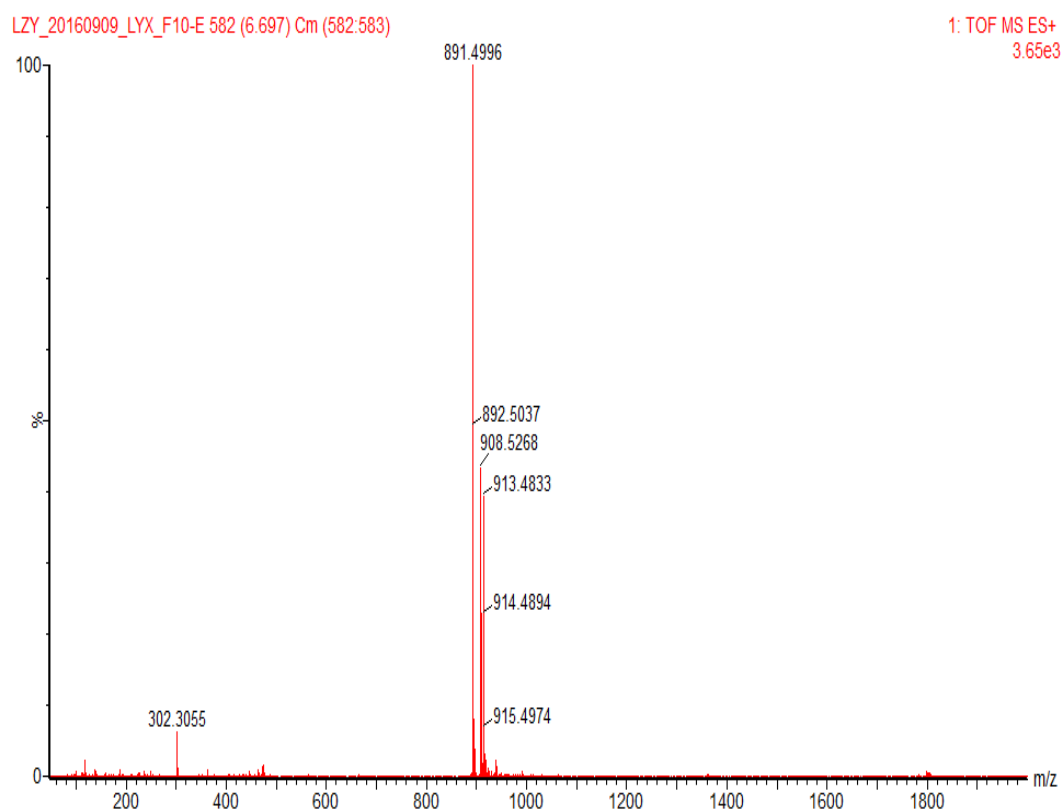


Figure S78. HRESIMS data of aselacin D (**9**)

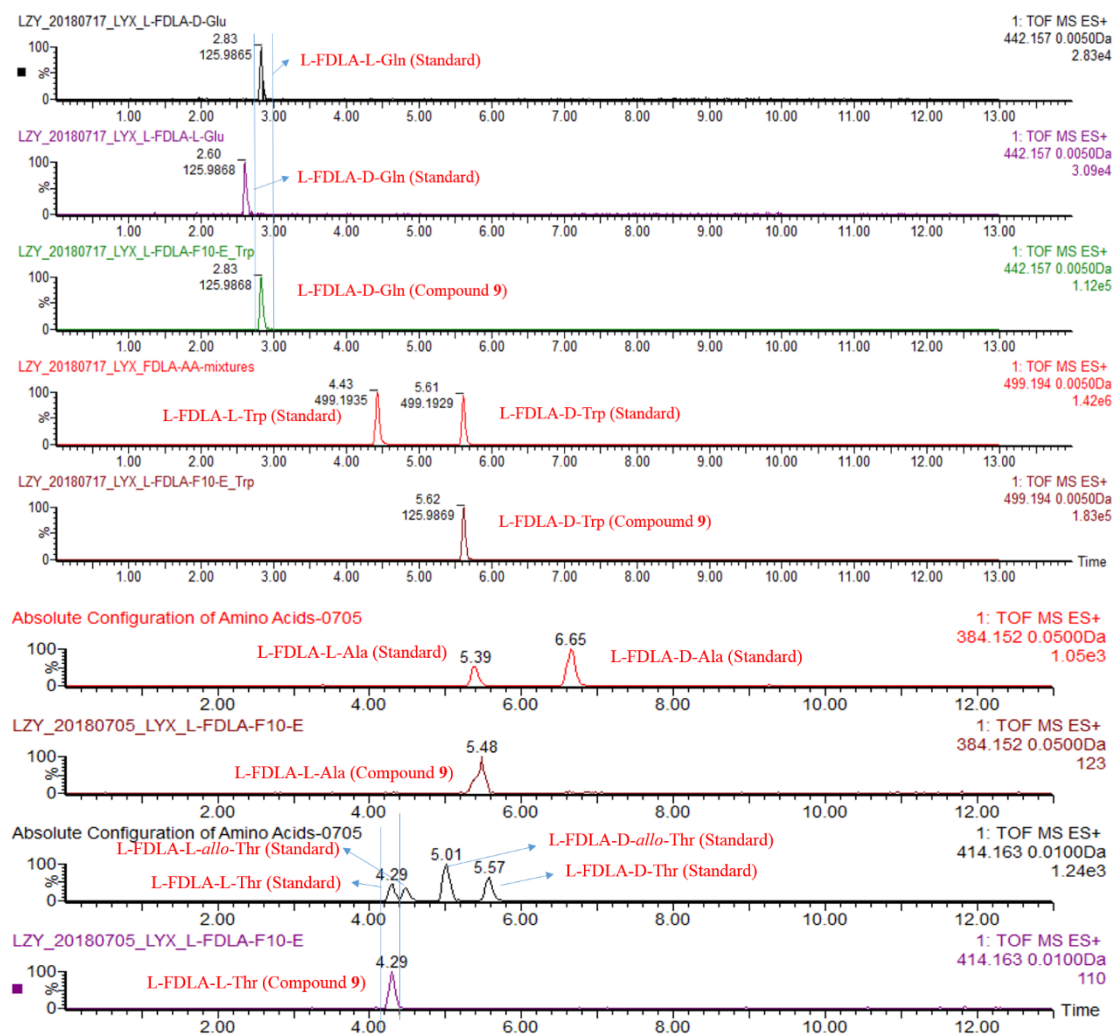


Figure S79. Mass chromatograms of the L-FDLA derivatives of standard amino acids and amino acids from aselacin D (9).

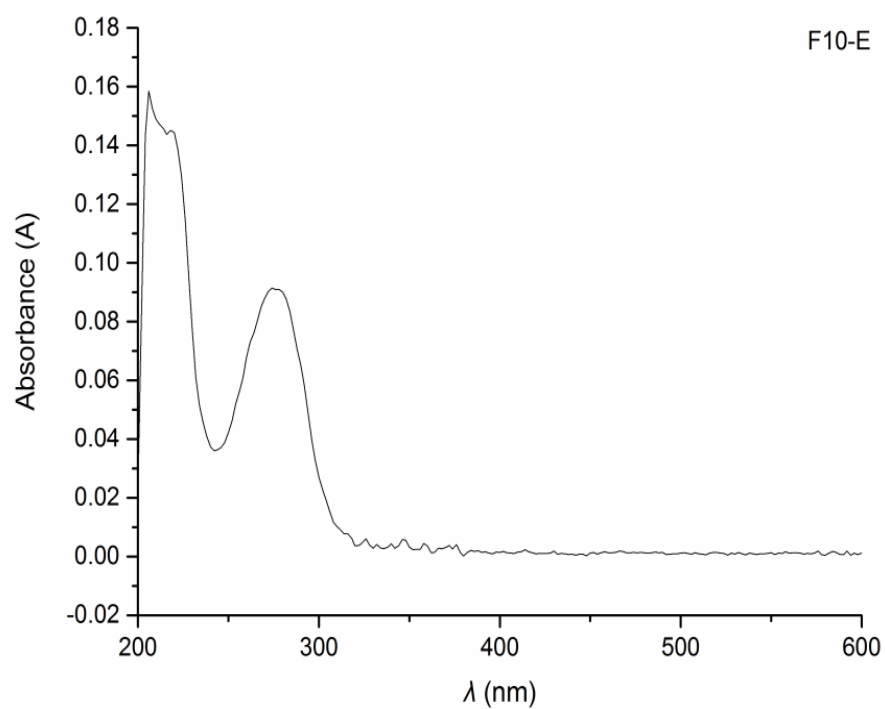


Figure S80. UV spectrum of aselacin D (**9**) in MeOH.

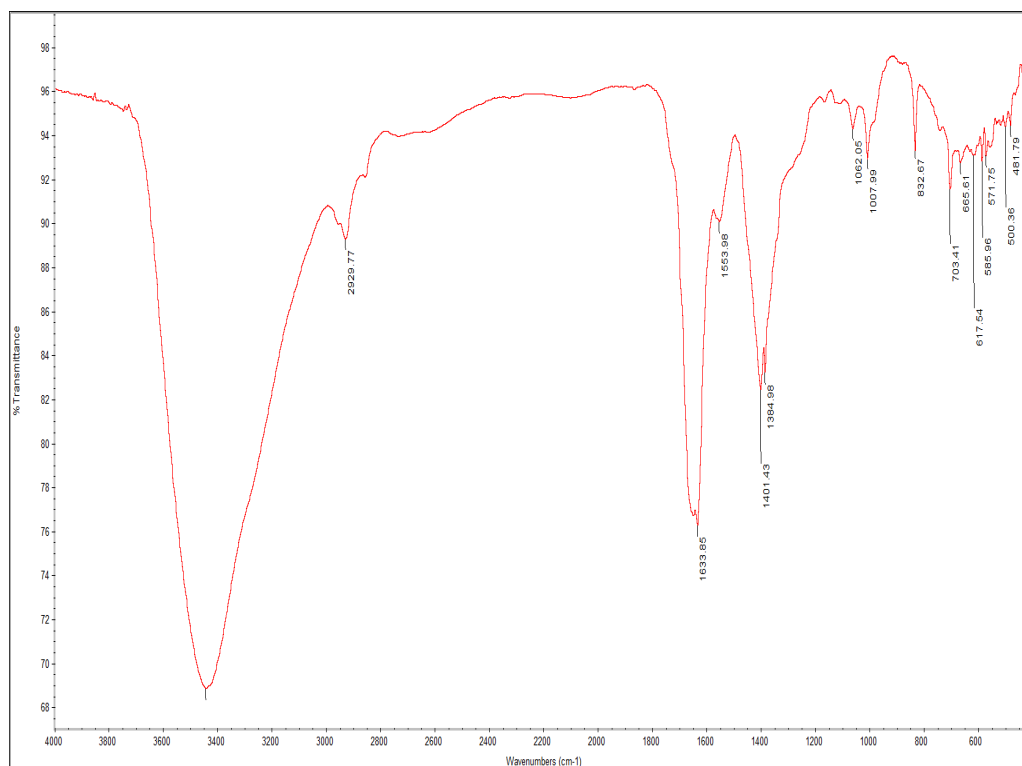


Figure S81. IR spectrum of aselacin D (**9**).