Supporting information

Revision of the Structure of Isochaetoglobosin D_b Based on NMR Analysis and Biosynthetic Consideration

Yan-duo Wang,[a] Yuan-yuan Li,[a] Xiang-mei Tan,[a] Lin Chen,[b] Zhong-qi Wei,[c] Li Shen,*[d] and Gang Ding*[a]

[a] Key Laboratory of Bioactive Substances and Resources Utilization of Chinese Herbal Medicine, Ministry of Education, Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100193, People's Republic of China.

[b] Zhengzhou Key Laboratory of Synthetic Biology of Natural Products, Henan Joint International Research Laboratory of Drug Discovery of Small Molecules, Huanghe Science and Technology College, Zhengzhou, Henan 450063, People's Republic of China.

[c] Nanjing Vocational Health College, Nanjing, Jiangsu, 210038, People's Republic of China.

[d] Institute of Translational Medicine, Medical College, Yangzhou University, Yangzhou, Jiangsu 225001, People's Republic of China.

* Correspondence should be addressed to gding@implad.ac.cn or shenli@yzu.edu.cn.

Fig. S1 HRESIMS spectrum of penochalasin C

Fig. S2 HRESIMS spectrum of isochaetoglobosin D_b[1]

Fig. S3 ^{1}H NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

Fig. S4 ^{1}H NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz)[1]

Fig. S5 ^{13}C NMR spectrum of penochalasin C in DMSO-d_6 (150 MHz)

Fig. S6 ^{13}C NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (150 MHz) [1]

Fig. S7 HSQC NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

Fig. S8 HSQC NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz) [1]

Fig. S9 COSY NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

Fig. S10 COSY NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz) [1]

Fig. S11 HMBC NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

Fig. S12 HMBC NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz) [1]

Fig. S13 NOESY NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

Fig. S14. Possible biosynthetic relationship of analogues isolated by Ding *et al*.

Fig. S15. Possible biosynthetic relationship of analogues isolated by Zhang *et al*.

Fig. S16. Possible biosynthetic relationship of analogues isolated by Qiu *et al*.

Reference

1. X. Y. Wang, X. Yan, M. J. Fang, Z. Wu, D. Wang, Y. K. Qiu, *Nat. Prod. Res*., 2017, 31, 1669-1675.

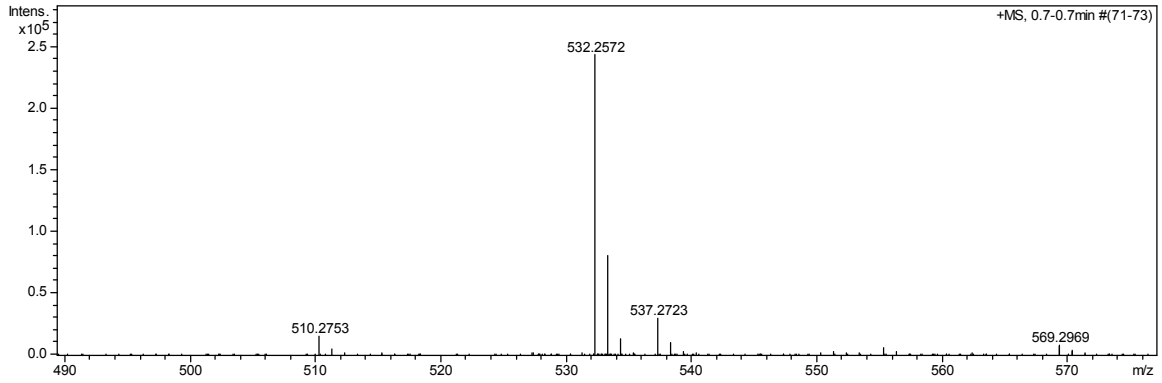

Fig. S1 HRESIMS spectrum of penochalasin C

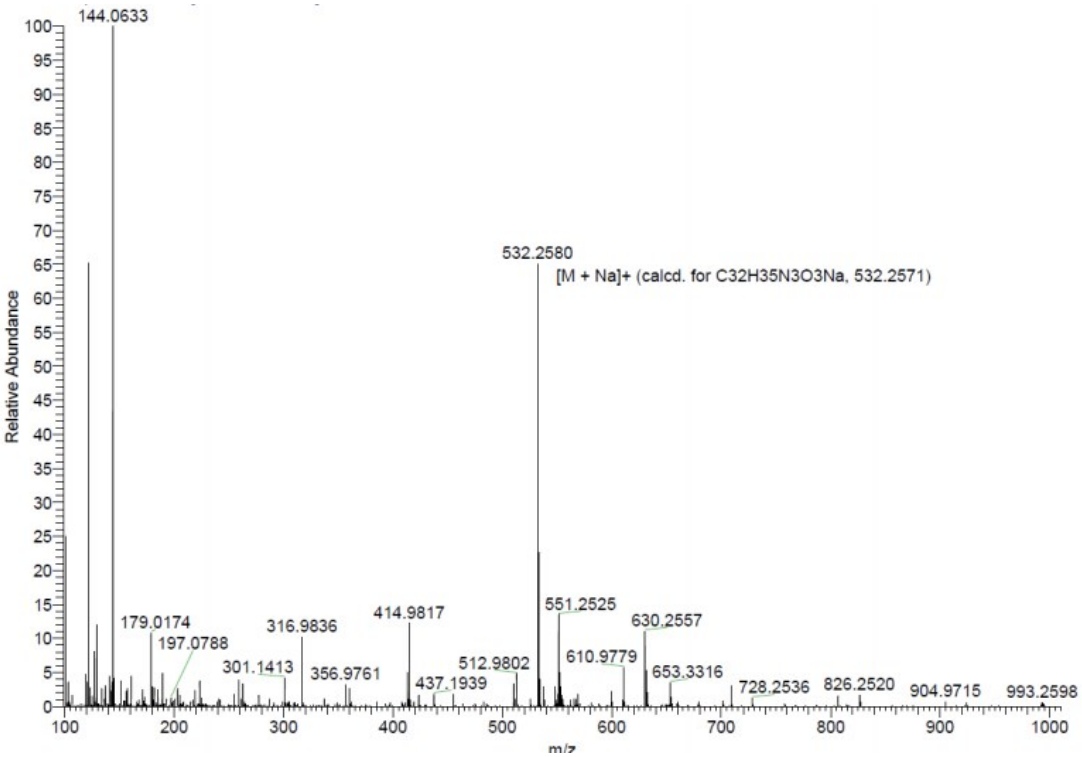

Fig. S2 HRESIMS spectrum of isochaetoglobosin D_b

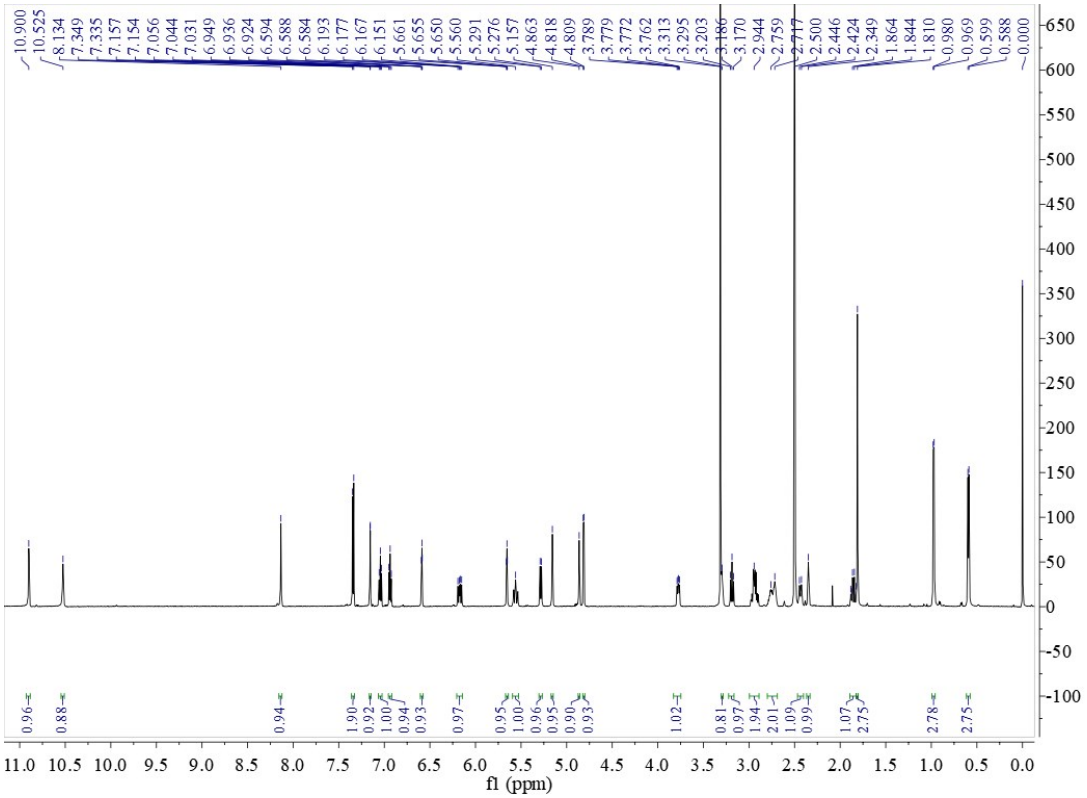

Fig. S3 ^{1}H NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

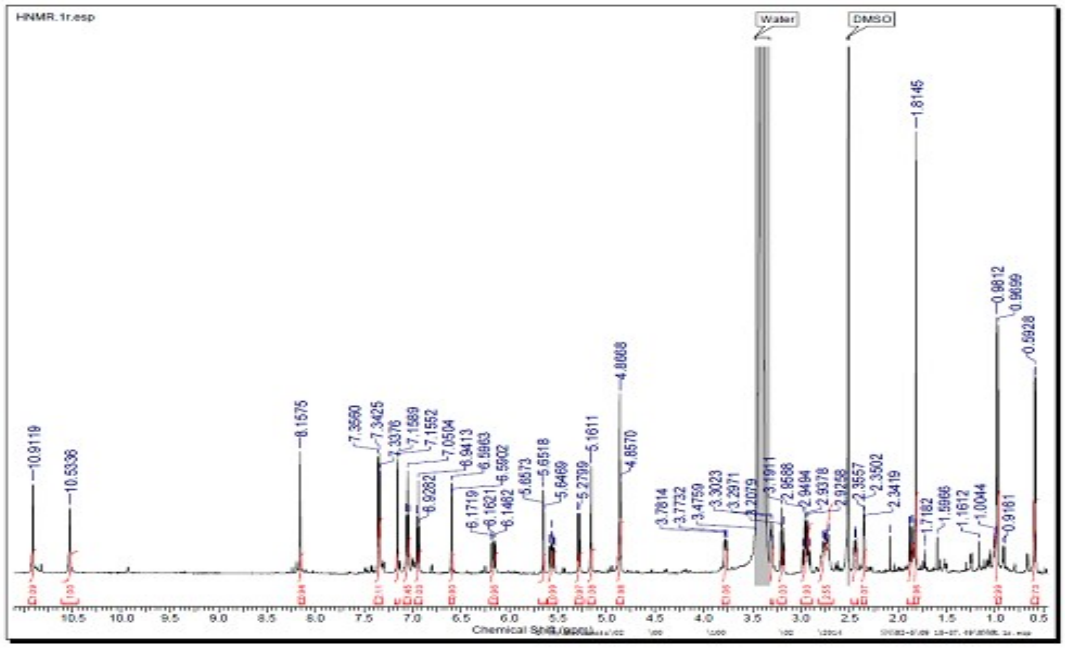

Fig. S4 ^{1}H NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz)

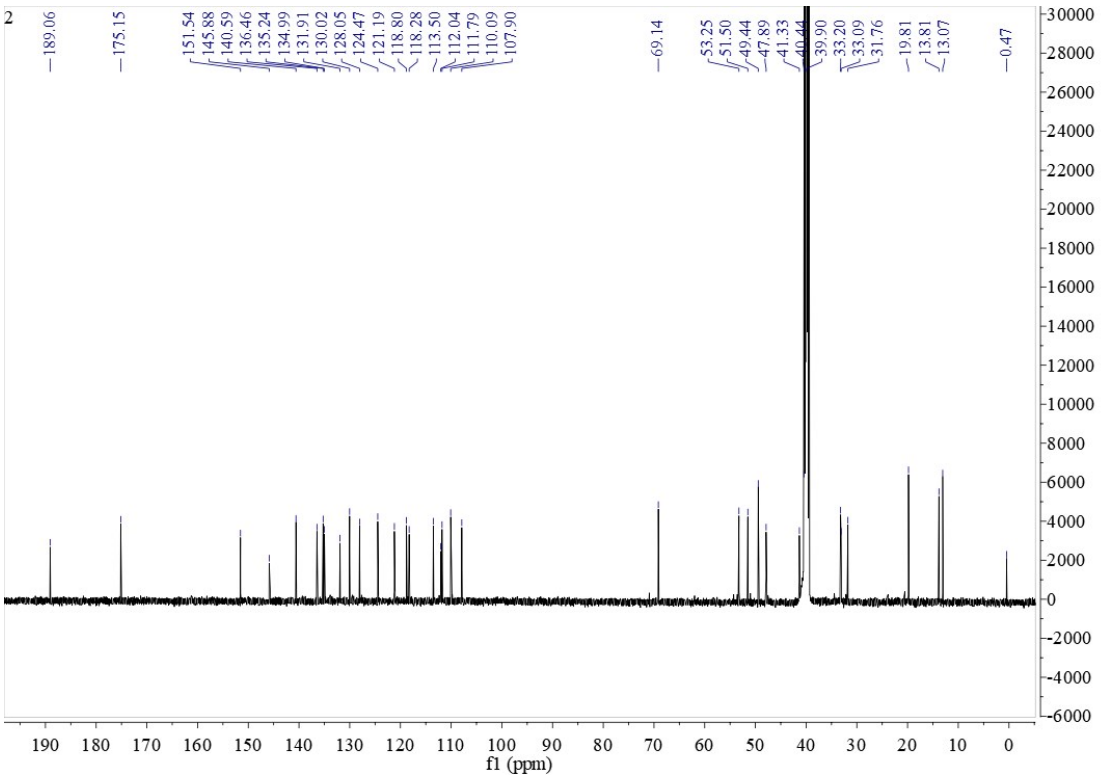

Fig. S5 ^{13}C NMR spectrum of penochalasin C in DMSO-d_6 (150 MHz)

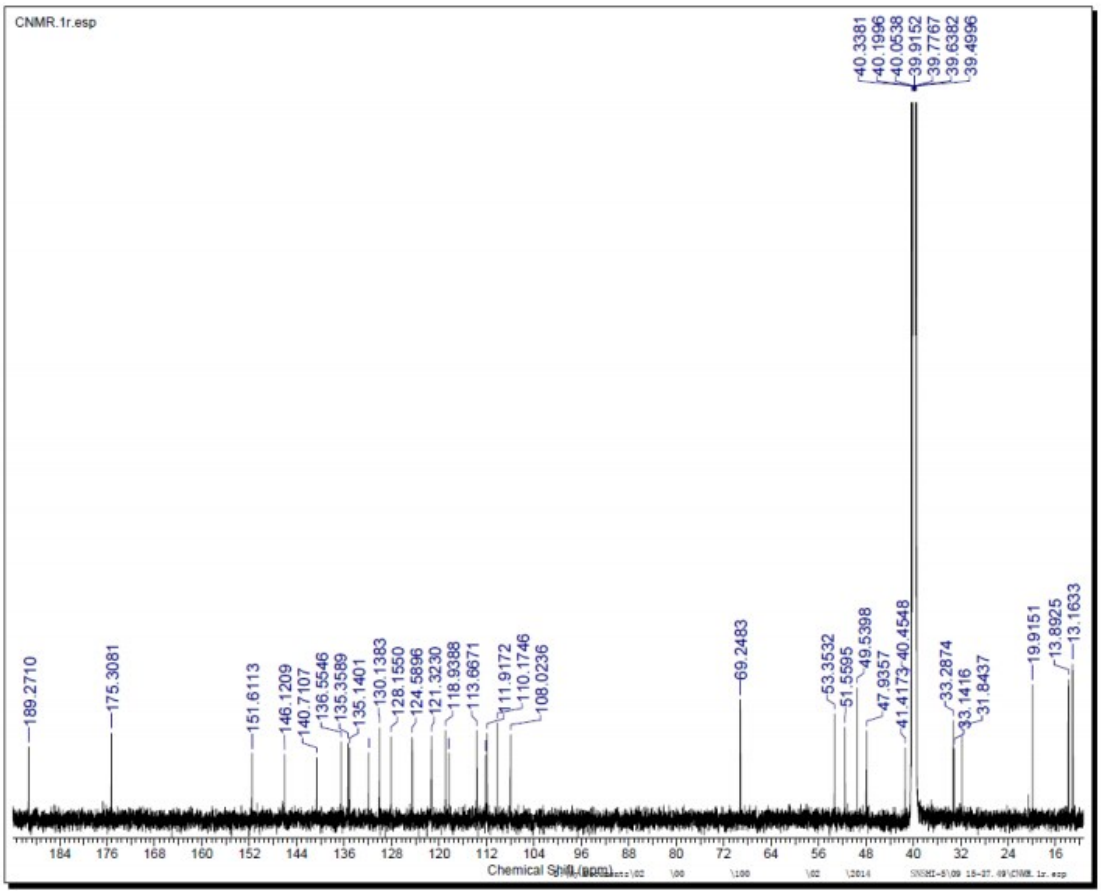

Fig. S6 ^{13}C NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (150 MHz)

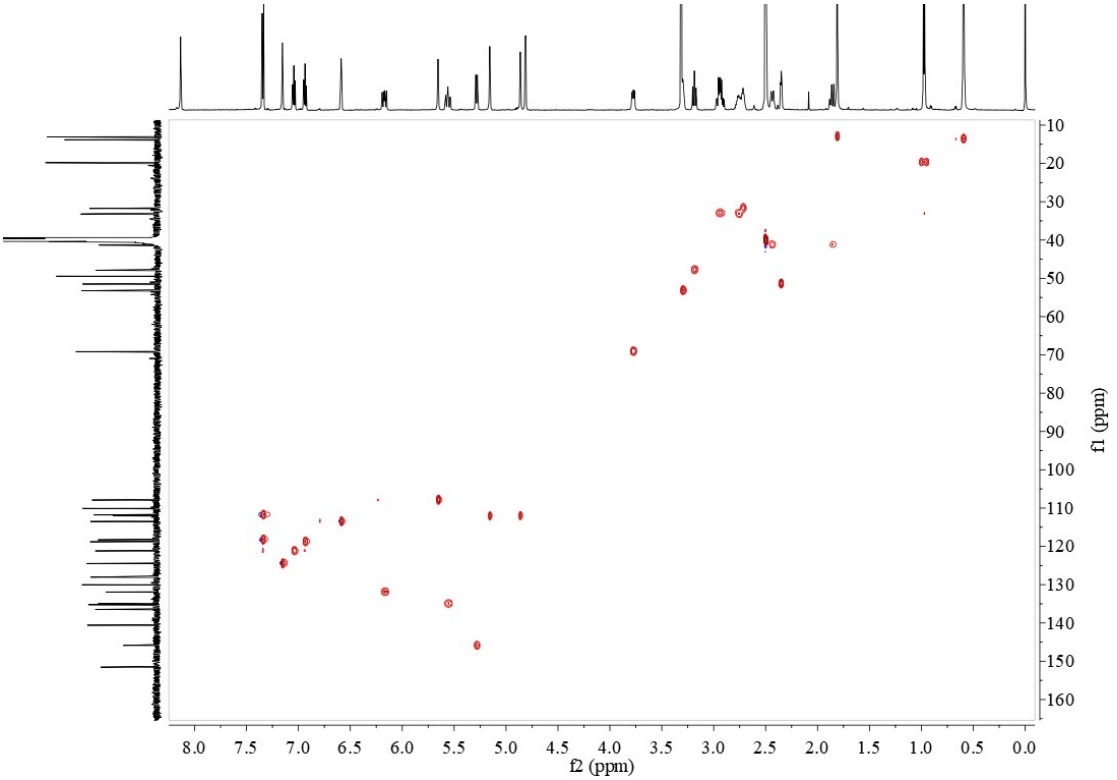

Fig. S7 HSQC NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

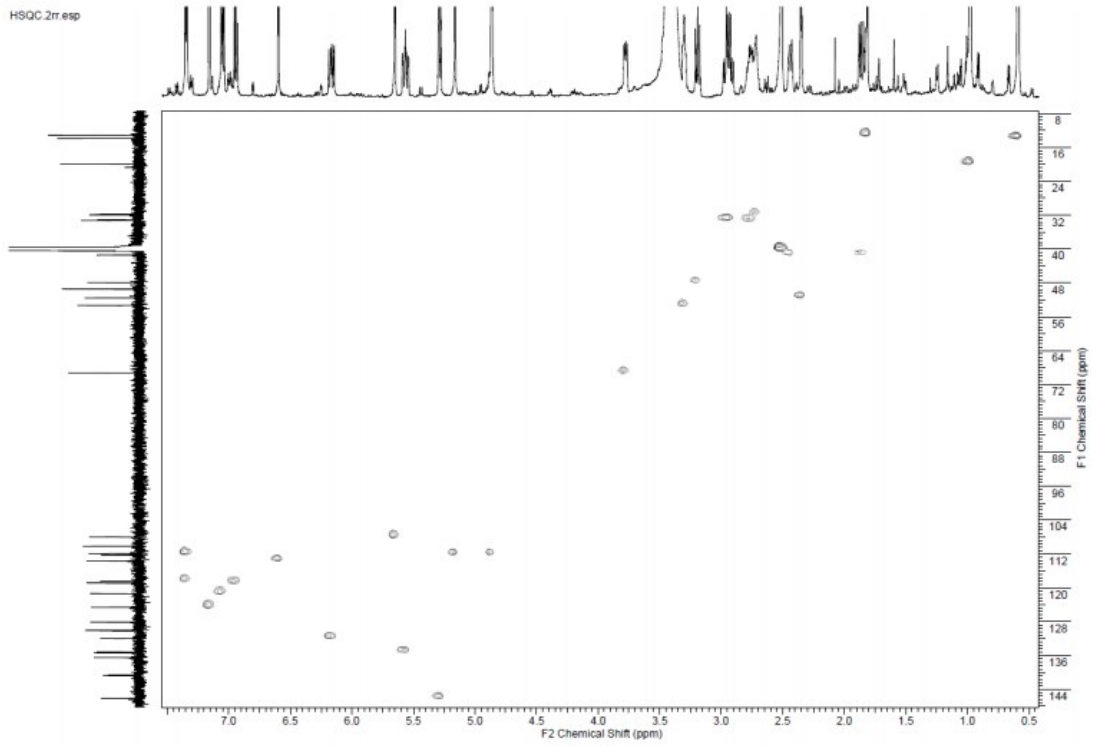

Fig. S8 HSQC NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz)

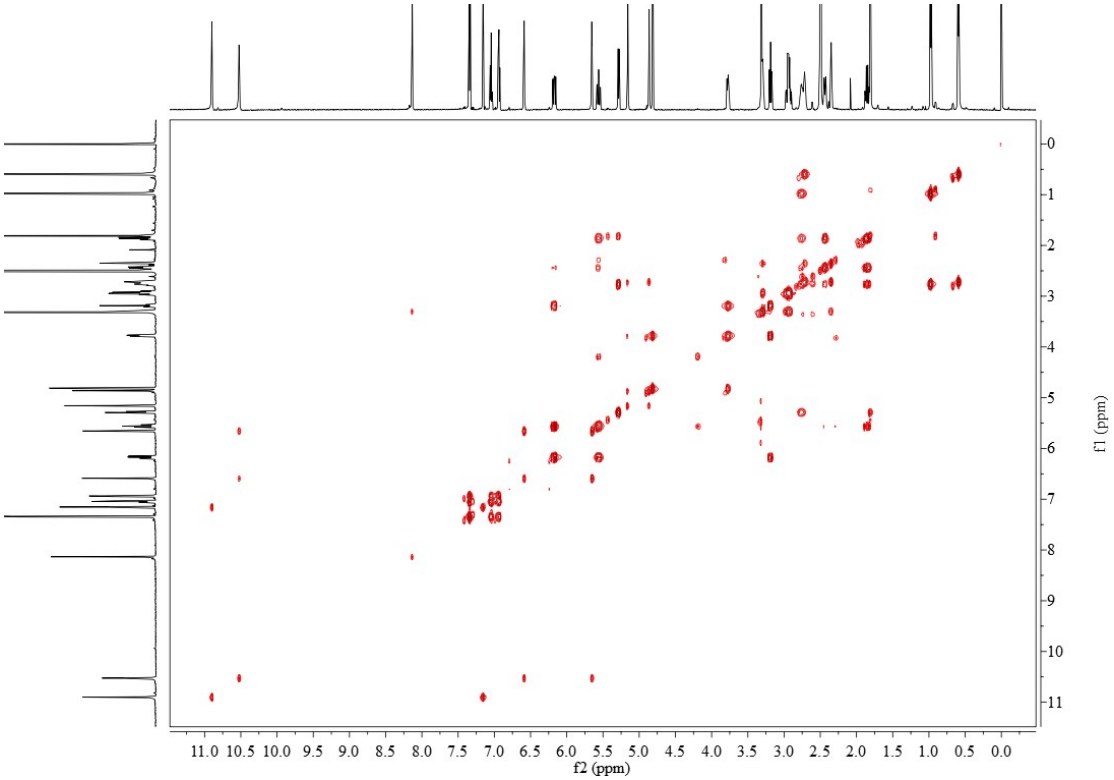

Fig. S9 COSY NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

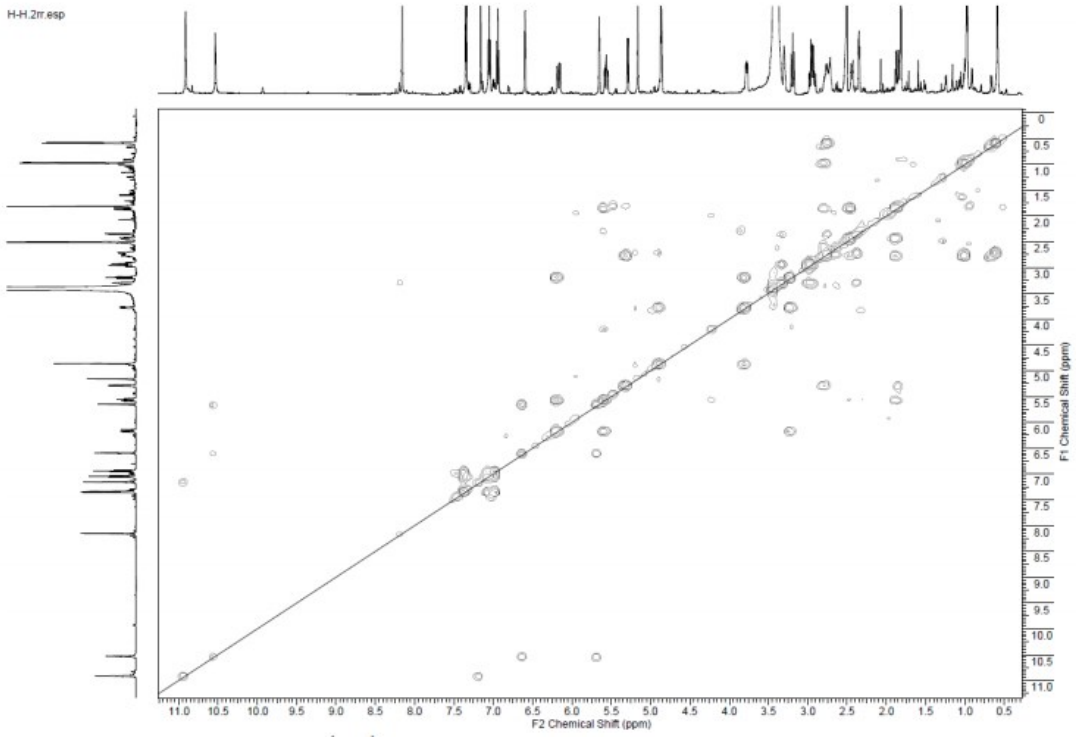

Fig. S10 COSY NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz)

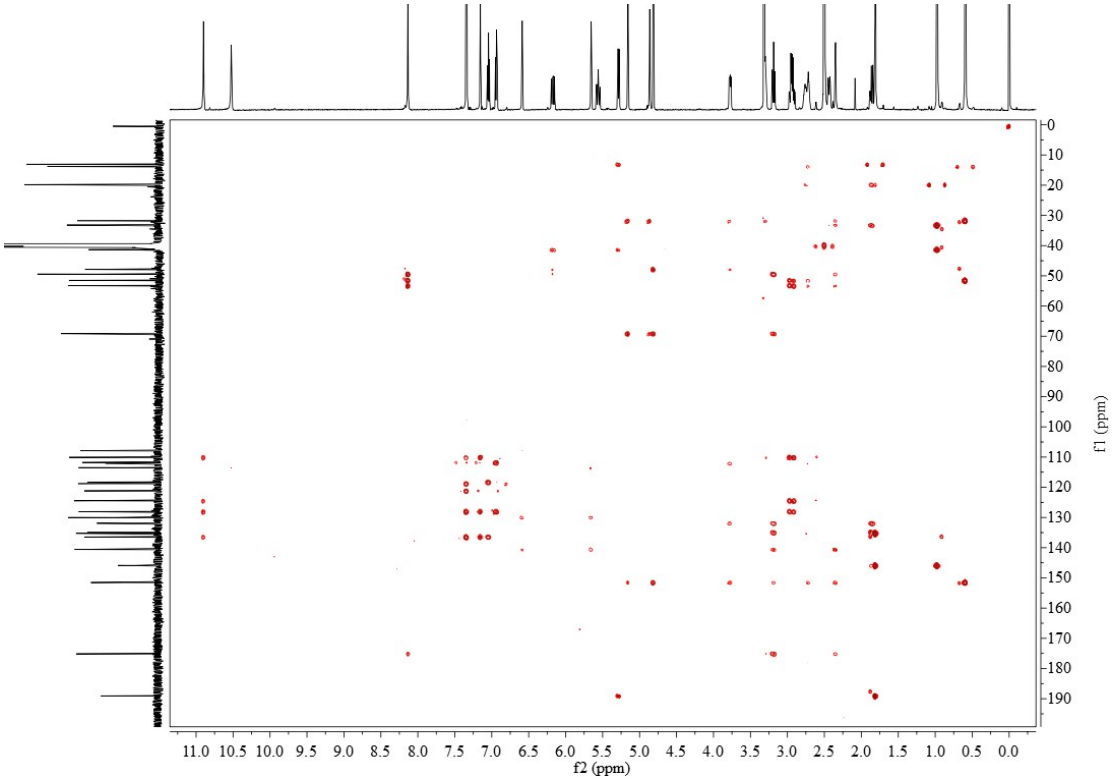

Fig. S11 HMBC NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

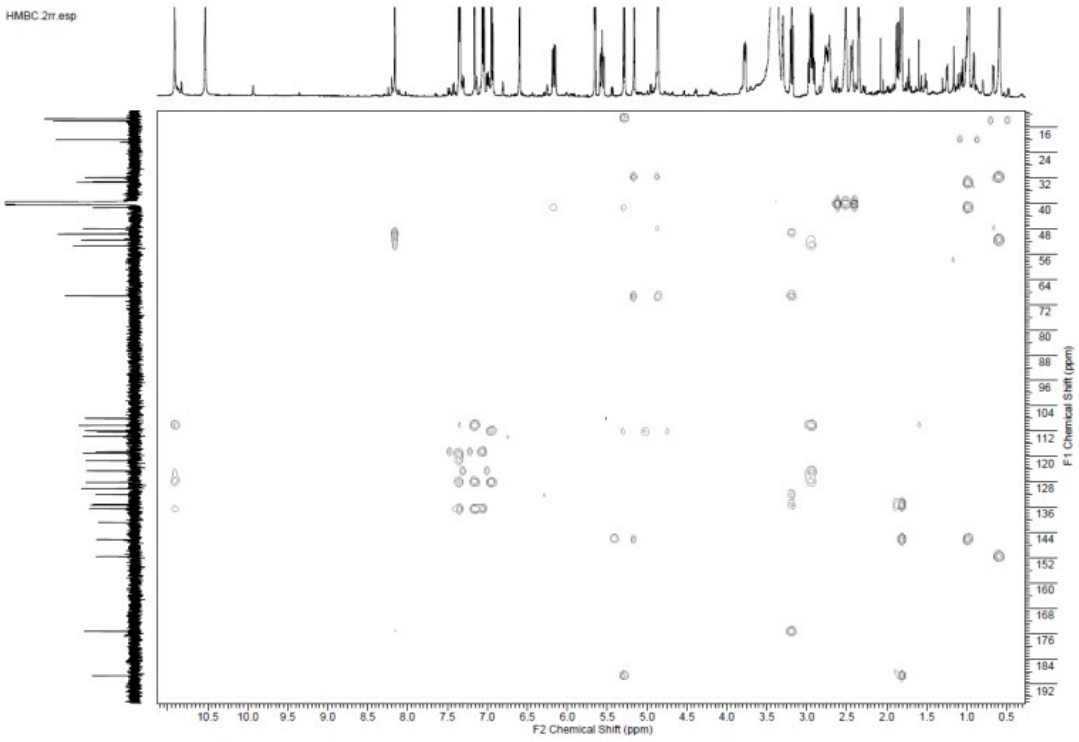

Fig. S12 HMBC NMR spectrum of isochaetoglobosin D_b in DMSO-d_6 (600 MHz)

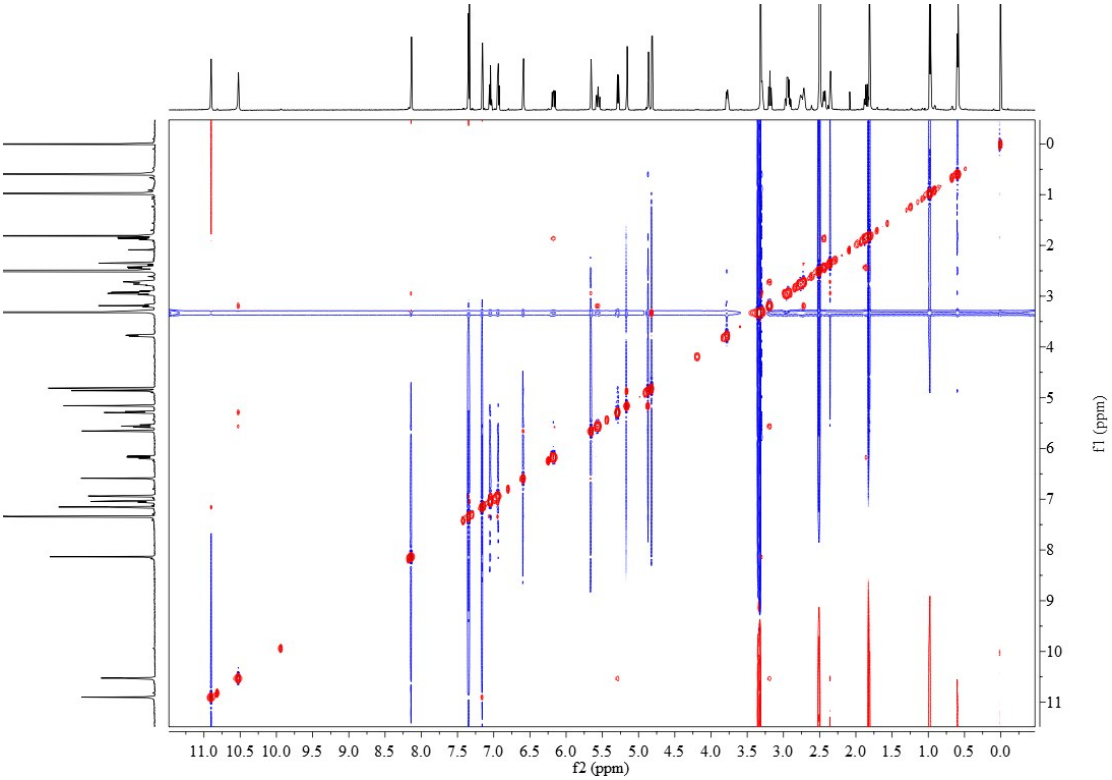

Fig. S13 NOESY NMR spectrum of penochalasin C in DMSO-d_6 (600 MHz)

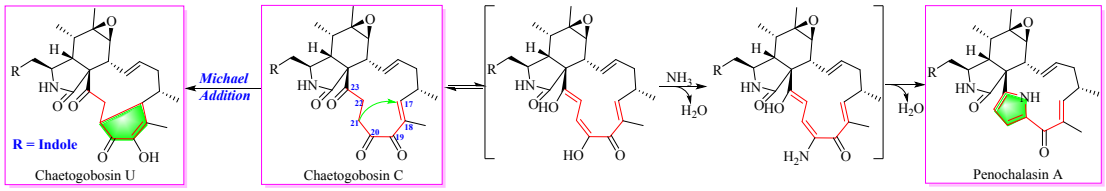

Fig. S14. Possible biosynthetic relationship of analogues isolated by Ding *et al*.

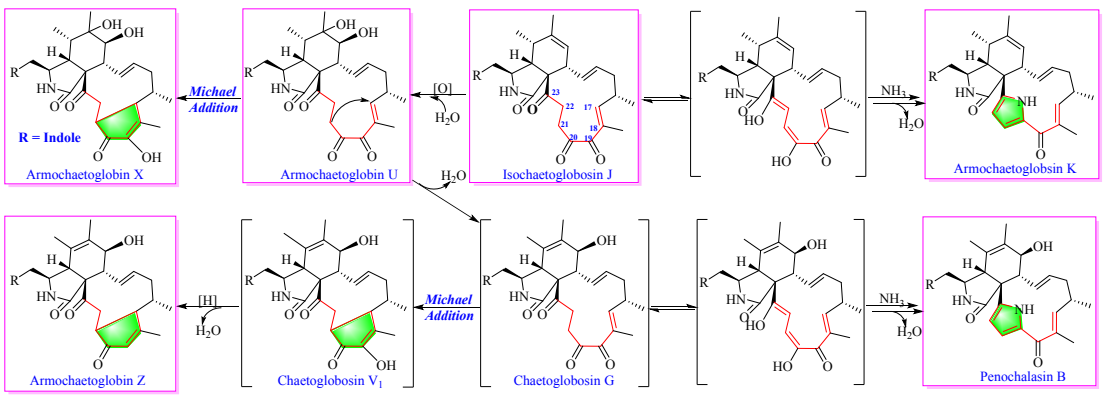

Fig. S15. Possible biosynthetic relationship of analogues isolated by Zhang *et al*.

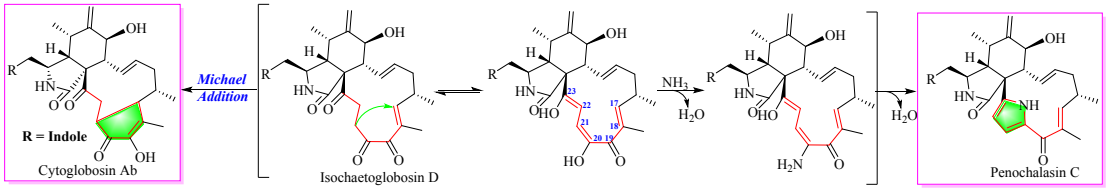

Fig. S16. Possible biosynthetic relationship of analogues isolated by Qiu *et al*.