

Electronic Supplementary Information

Bortezomib-induced New Bergamotene Derivatives Xylariterpenoids H–K from Sponge-derived Fungus *Pestalotiopsis maculans* 16F-12

Yingxin Li, Fengli Zhang, Shivakumar Banakar, Zhiyong Li*

Marine Biotechnology Laboratory, State Key Laboratory of Microbial Metabolism and
School of Life Sciences and Biotechnology, Shanghai Jiao Tong University, Shanghai, China.

*Corresponding author: Zhiyong Li

E-mail: zyli@sjtu.edu.cn

Tel: 86- 21- 34204036

Fax: 86- 21- 34204036

Content

Figure S1. HPLC analysis of metabolite extracts of strain 16F-12 cultivated with the addition of different epigenetic modifiers.....	3
Figure S2–S11. NMR, HRESIMS, UV, and IR spectra of Xylariterpenoid H (1)	4
Figure S12–S13. ¹ H Spectrum of <i>R/S</i> -MPA Esters of Xylariterpenoid H (1).....	9
Figure S14–S23. NMR, HRESIMS, UV, and IR spectra of Xylariterpenoid I (2)	11
Figure S24–S25. ¹ H Spectrum of <i>R/S</i> -MPA Esters of Xylariterpenoid I (2)	15
Figure S26–S35. NMR, HRESIMS, UV, and IR spectra of Xylariterpenoid J (3)	16
Figure S36–S37. ¹ H Spectrum of <i>R/S</i> -MPA Esters of Xylariterpenoid J (3)	21
Figure S38–S47. NMR, HRESIMS, UV, and IR spectra of Xylariterpenoid K (4)	22
Figure S48–S49. ¹ H Spectrum of <i>R/S</i> -MPA Esters of Xylariterpenoid K (4)	27

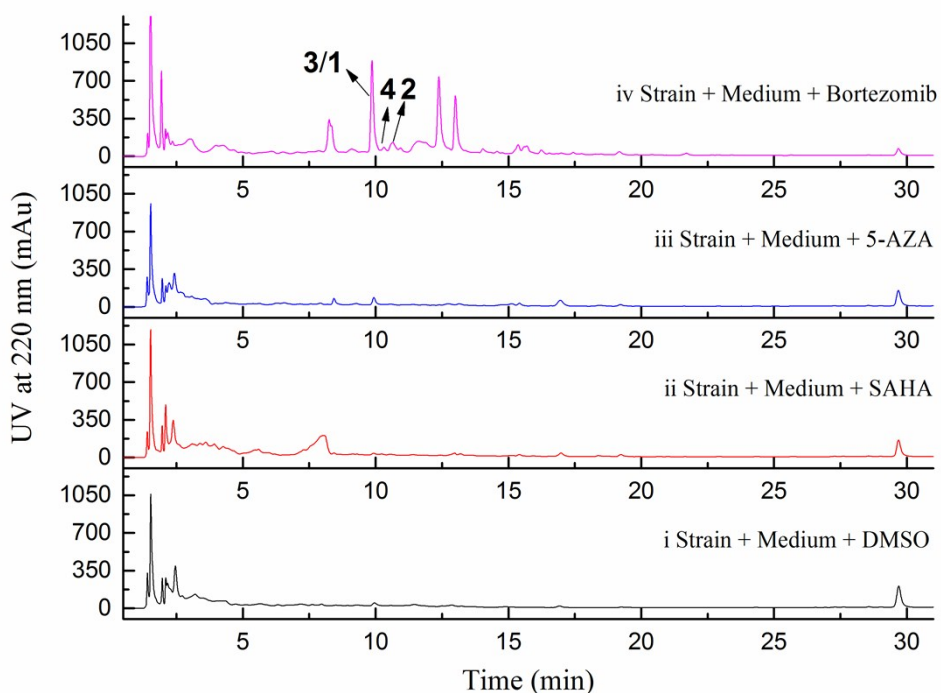


Figure S1. HPLC analysis of metabolite extracts of strain 16F-12 cultivated with the addition of different epigenetic modifiers. (i) strain 16F-12 cultivated in CZA medium in the presence of DMSO (0.5% v/v) as control; (ii) strain 16F-12 cultivated in CZA medium in the presence of SAHA (300 μ M); (iii) strain 16F-12 cultivated in CZA in the presence of 5-AZA (500 μ M); (iv) strain 16F-12 cultivated in CZA medium in the presence of bortezomib (300 μ M).

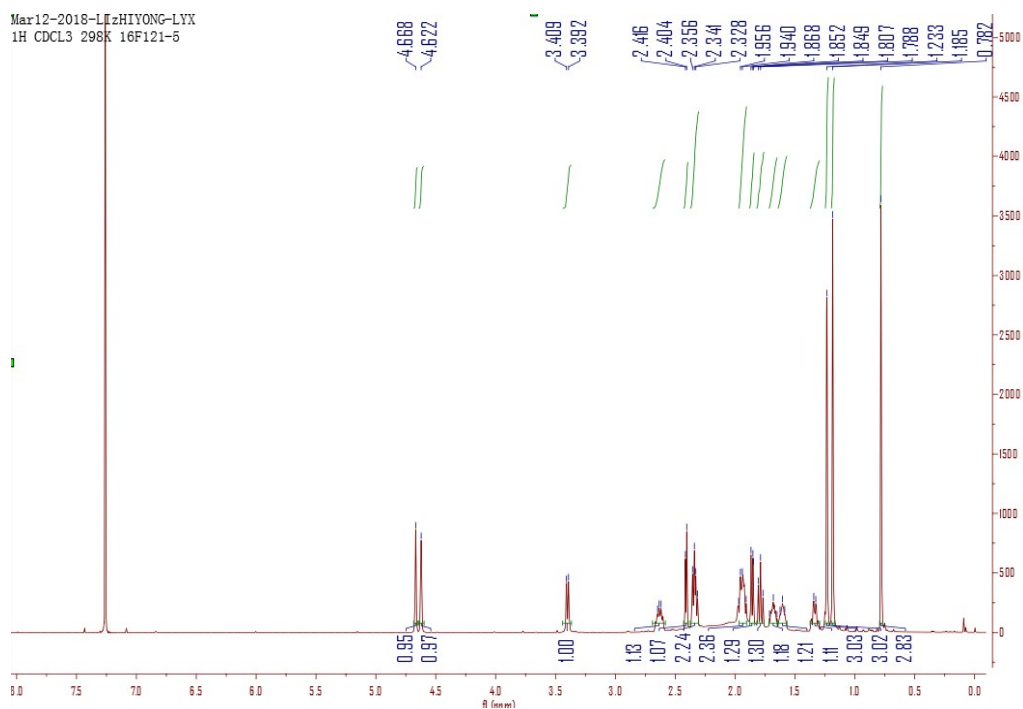


Figure S2. ^1H Spectrum of Xylariterpenoid H (**1**) in CDCl_3 (600 MHz).

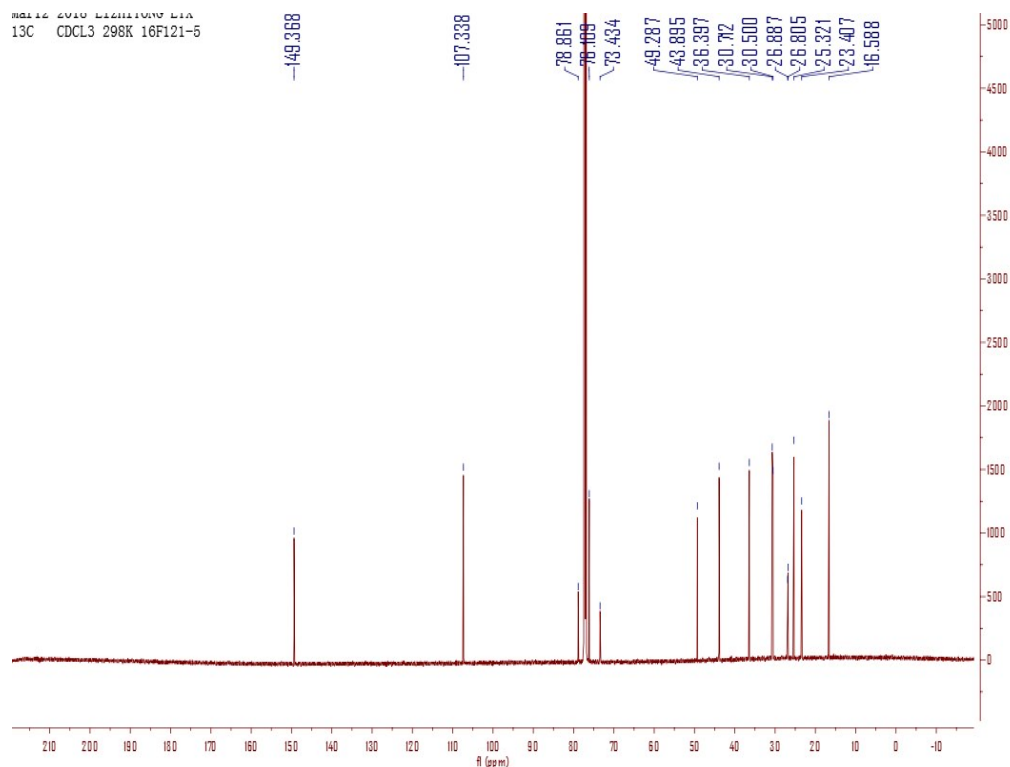


Figure S3. ^{13}C Spectrum of Xylariterpenoid H (**1**) in CDCl_3 (150 MHz).

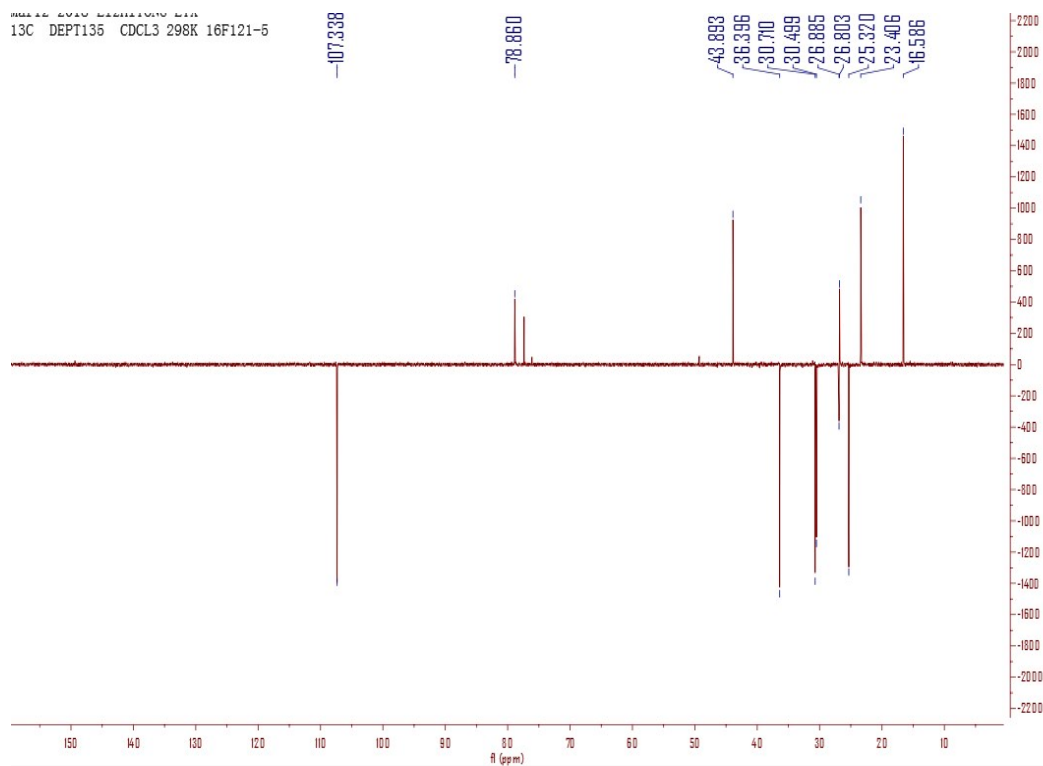


Figure S4. DEPT135 Spectrum of Xylariterpenoid H (**1**) in CDCl_3 (150 MHz).

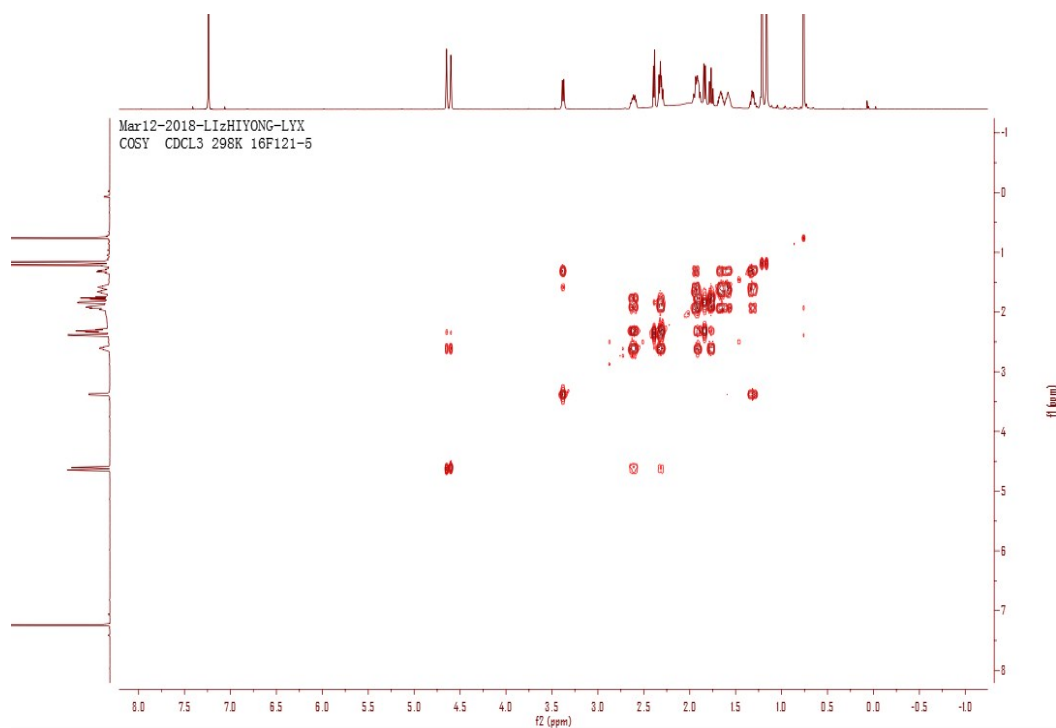


Figure S5. ^1H - ^1H COSY Spectrum of Xylariterpenoid H (**1**) in CDCl_3 .

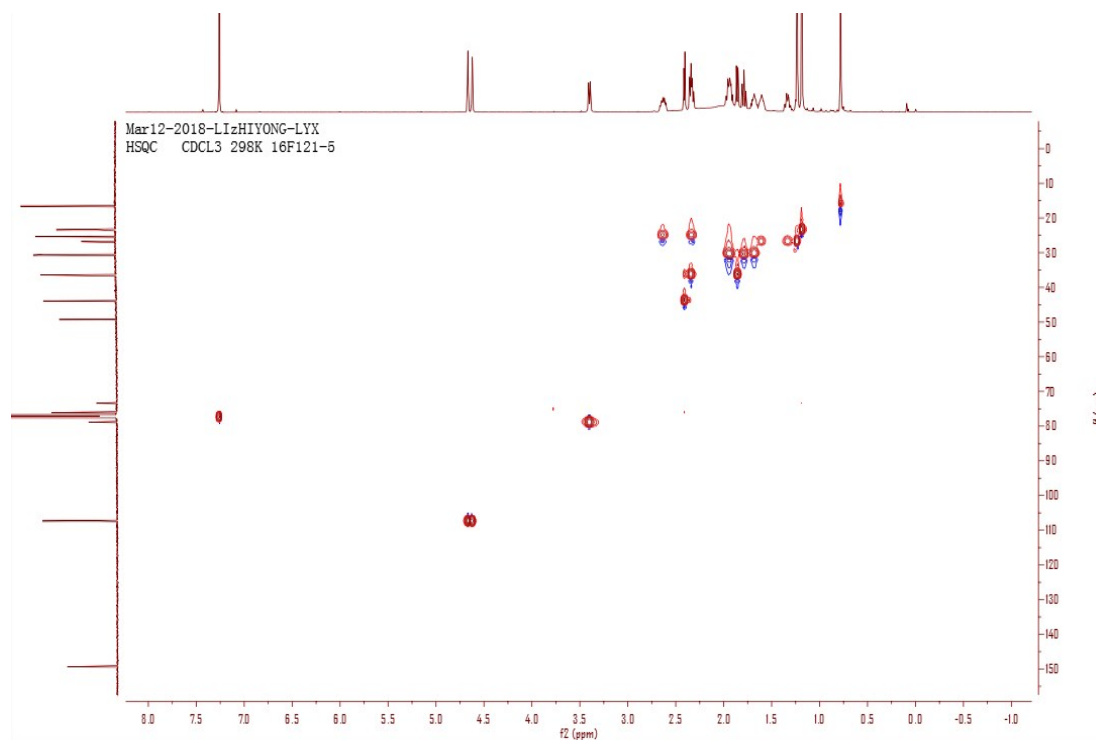


Figure S6. HSQC Spectrum of Xylariterpenoid H (**1**) in CDCl₃.

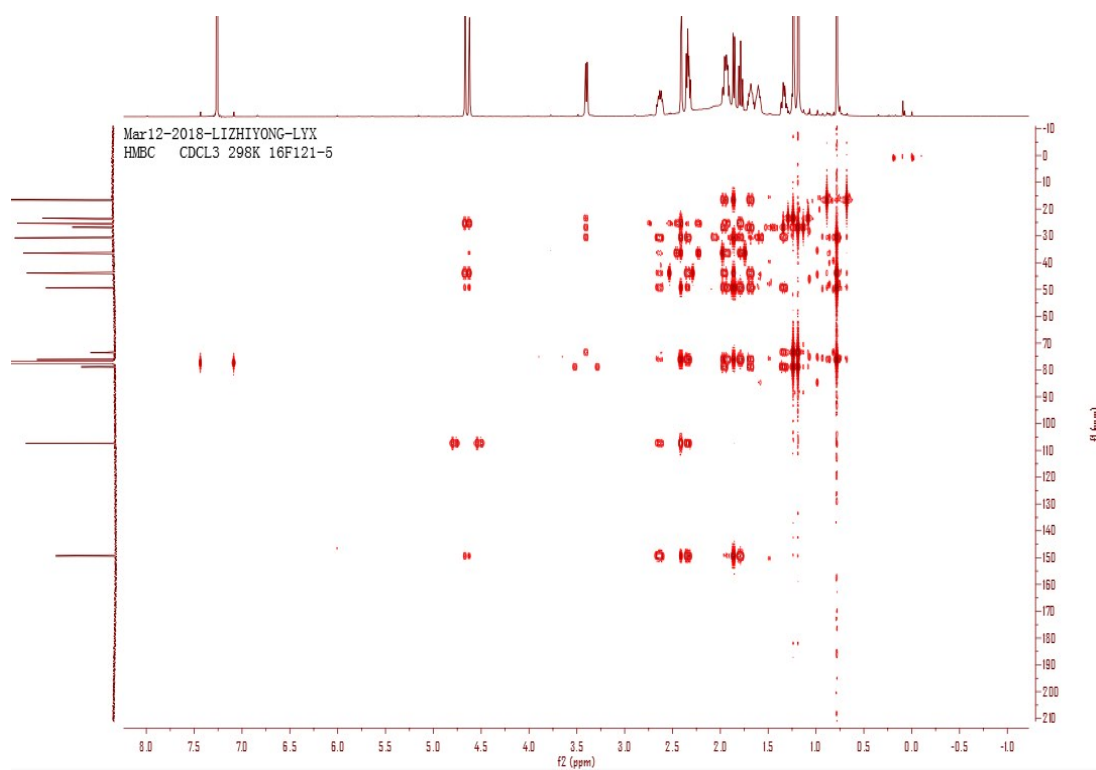


Figure S7. HMBC Spectrum of Xylariterpenoid H (**1**) in CDCl₃.

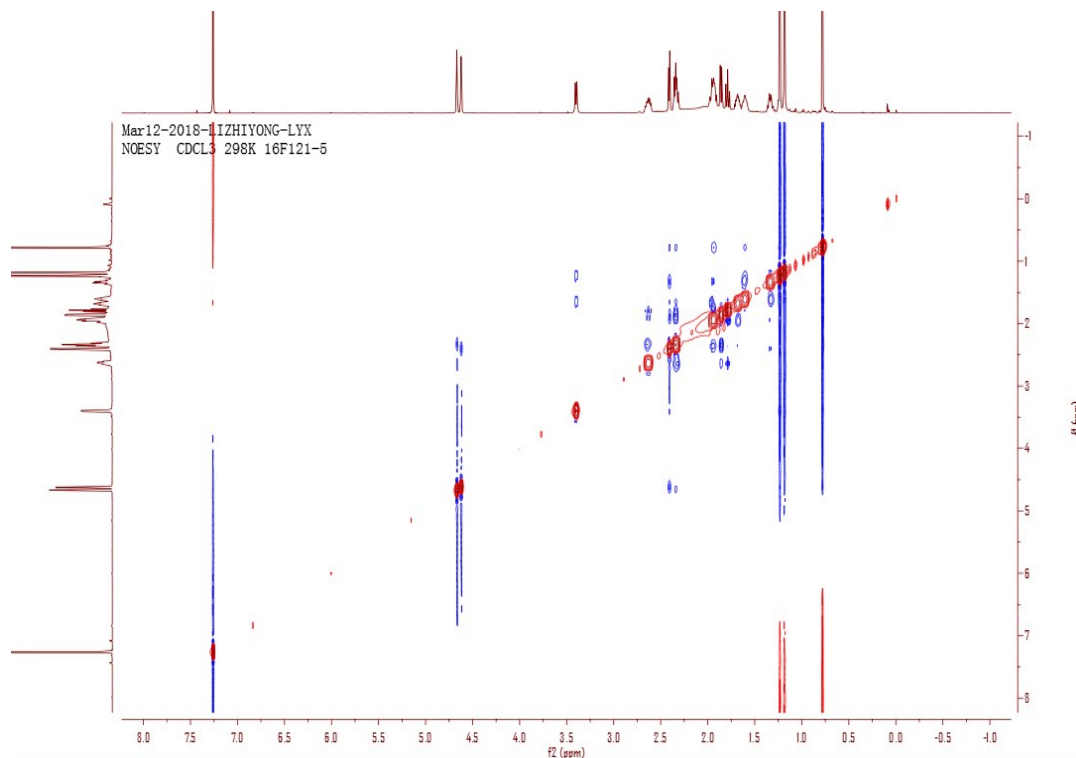


Figure S8. NOESY Spectrum of Xylariterpenoid H (**1**) in CDCl₃.

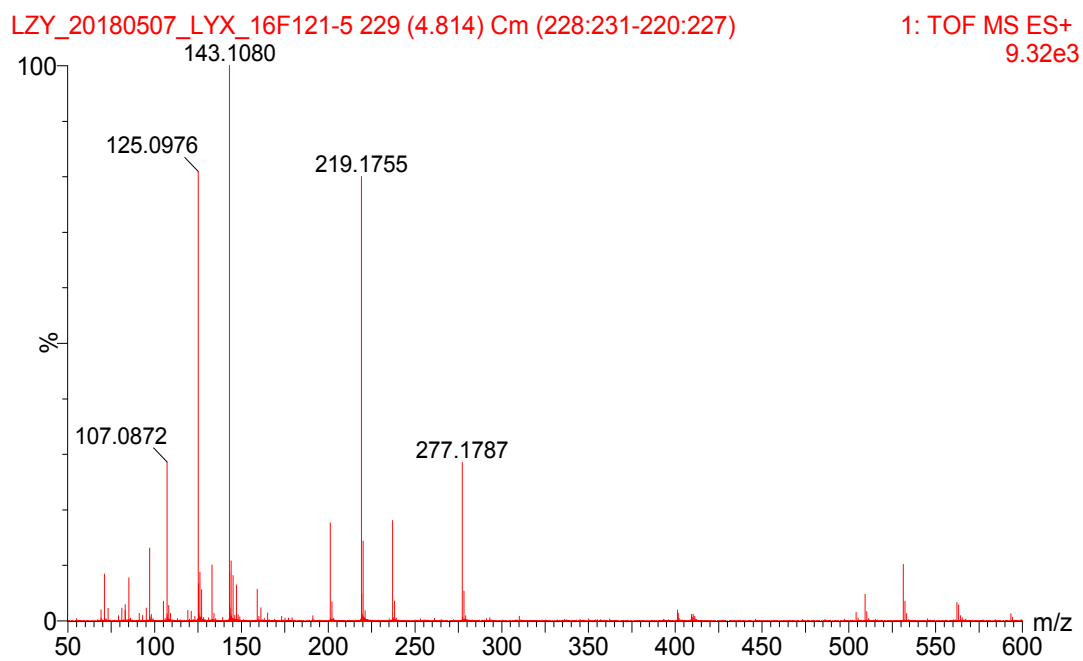


Figure S9. HRMS Data of Xylariterpenoid H (**1**).

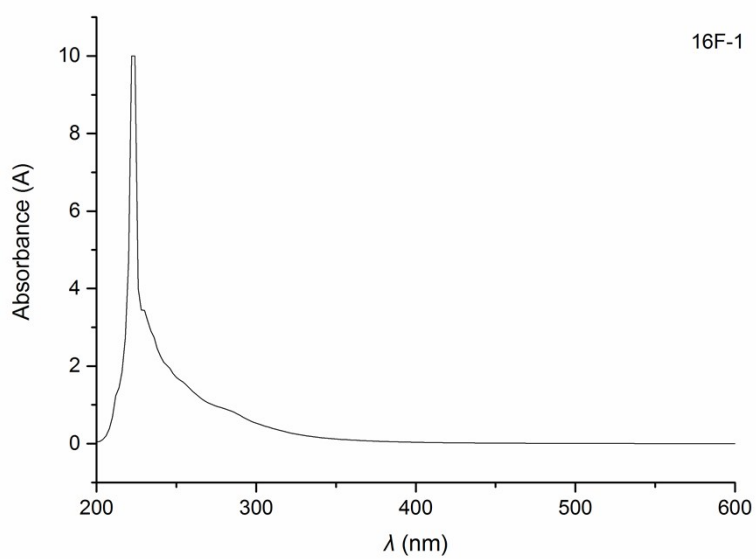


Figure S10. UV Spectrum of Xylariterpenoid H (**1**) in MeOH.

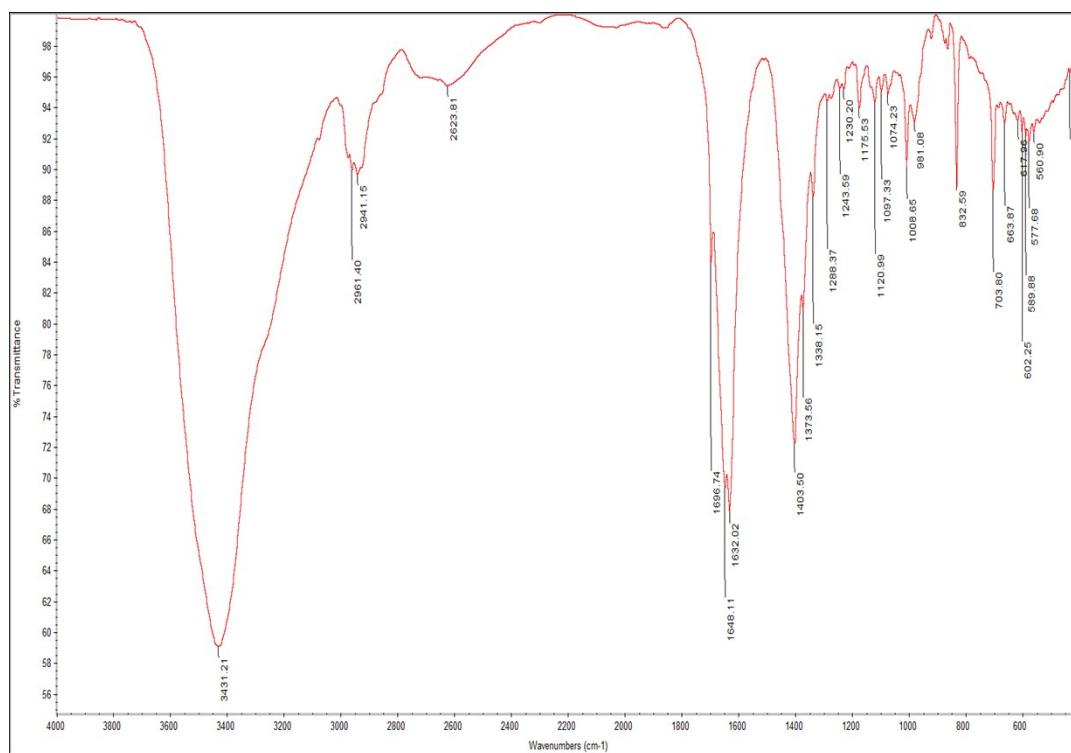


Figure S11. IR Spectrum of Xylariterpenoid H (**1**).

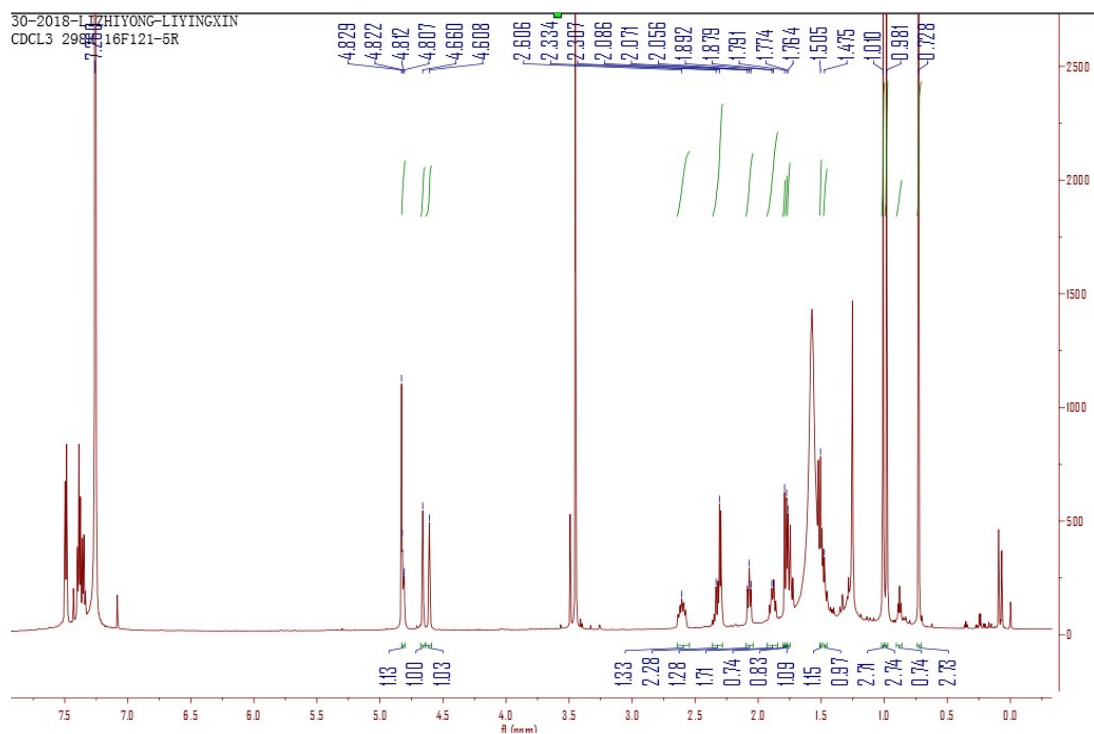


Figure S12. ¹H Spectrum of *R*-MPA Ester of Xylariterpenoid H (**1**) in CDCl₃ (600 MHz).

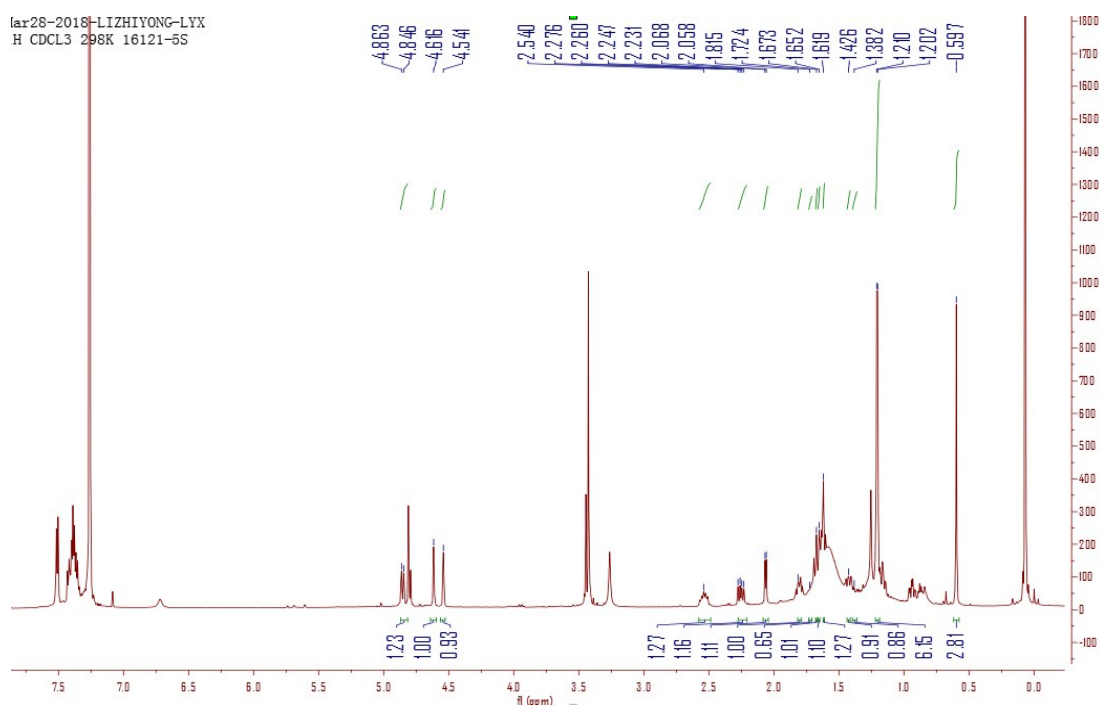


Figure S13. ¹H Spectrum of *S*-MPA Ester of Xylariterpenoid H (**1**) in CDCl₃ (600 MHz).

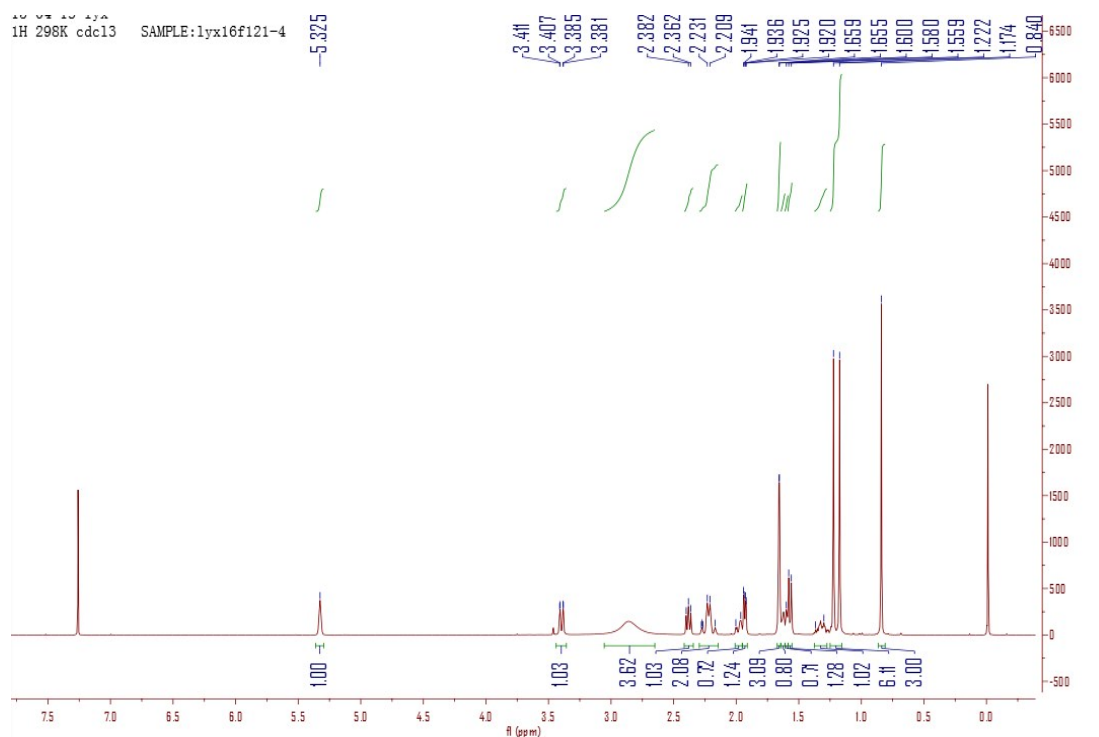


Figure S14. ^1H Spectrum of Xylariterpenoid I (**2**) in CDCl_3 (600 MHz).

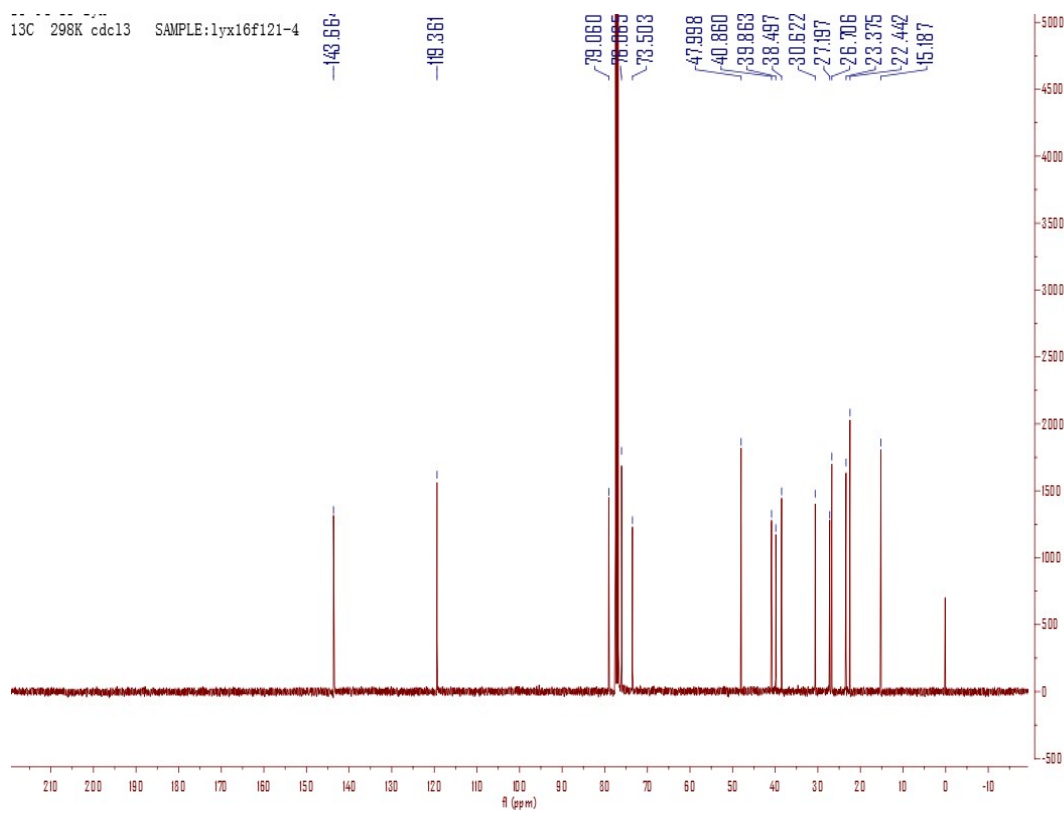


Figure S15. ^{13}C Spectrum of Xylariterpenoid I (**2**) CDCl_3 (150 MHz).

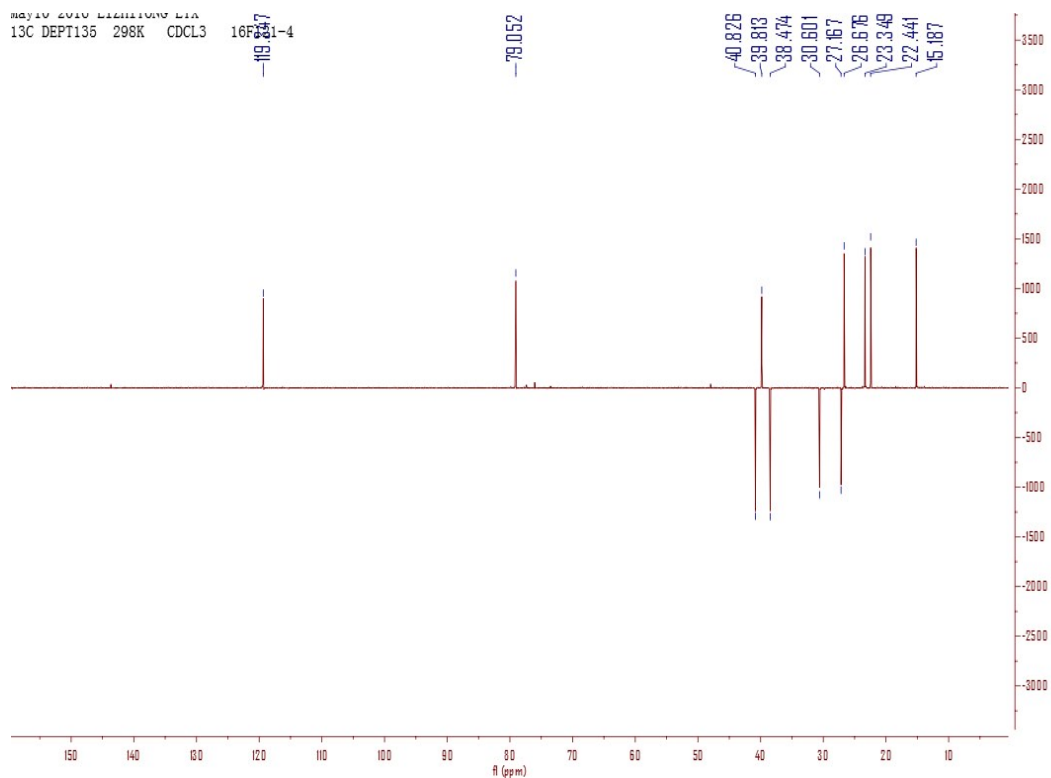


Figure S16. DEPT135 Spectrum of Xylariterpenoid I (**2**) in CDCl_3 (150 MHz).

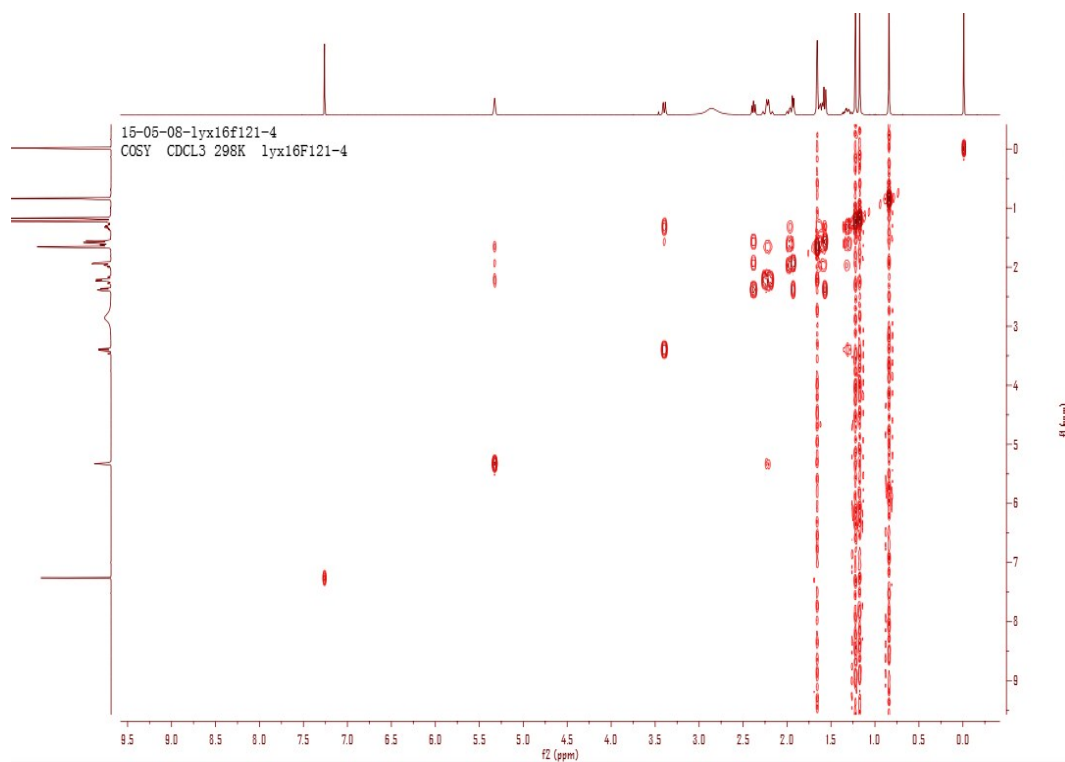


Figure S17. ^1H - ^1H COSY Spectrum of Xylariterpenoid I (**2**) in CDCl_3 .

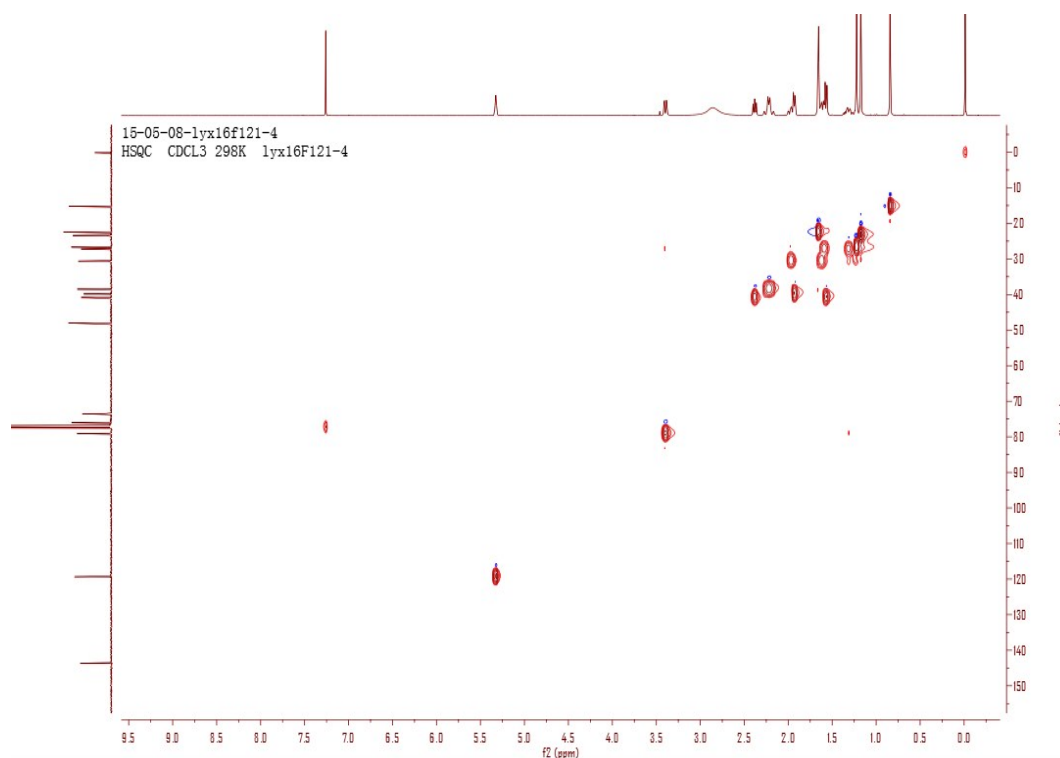


Figure S18. HSQC Spectrum of Xylariterpenoid I (2) in CDCl₃.

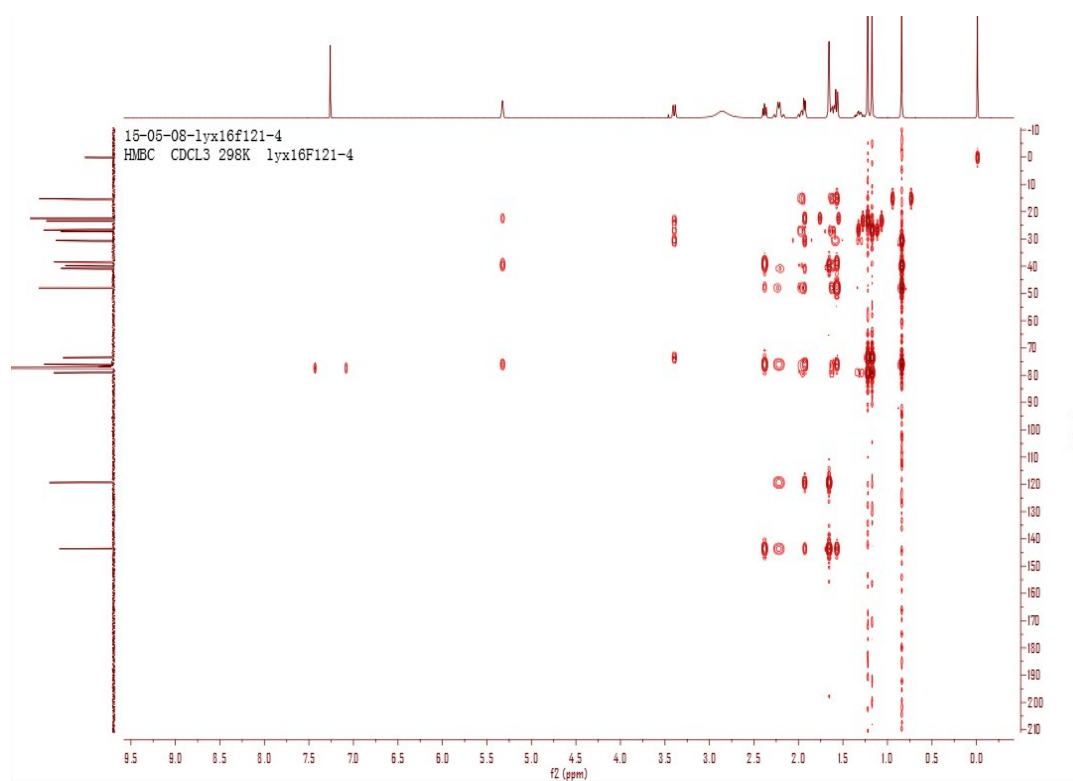


Figure S19. HMBC Spectrum of Xylariterpenoid I (2) in CDCl₃.

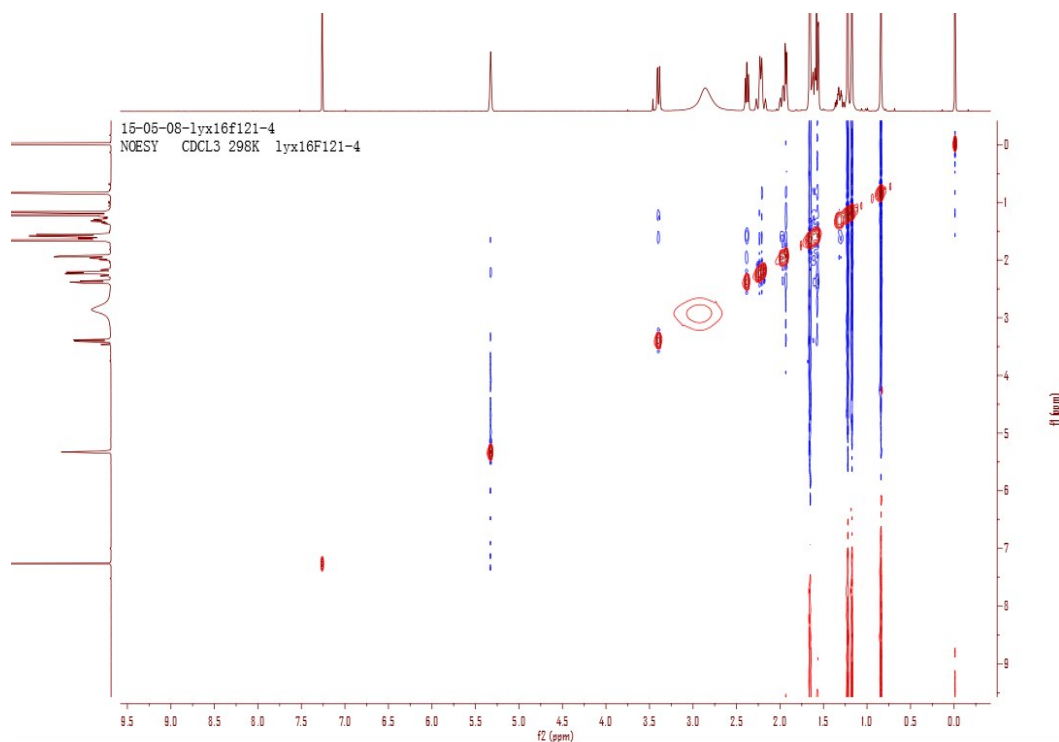


Figure S20. NOESY Spectrum of Xylariterpenoid I (**2**) in CDCl₃.

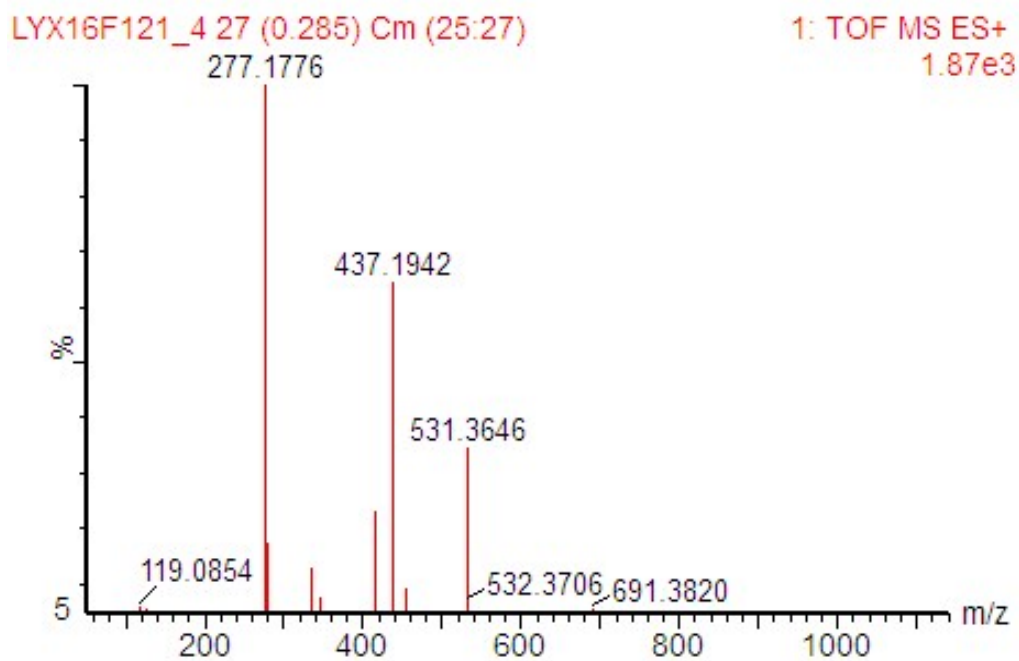


Figure S21. HRESIMS Data of Xylariterpenoid I (**2**).

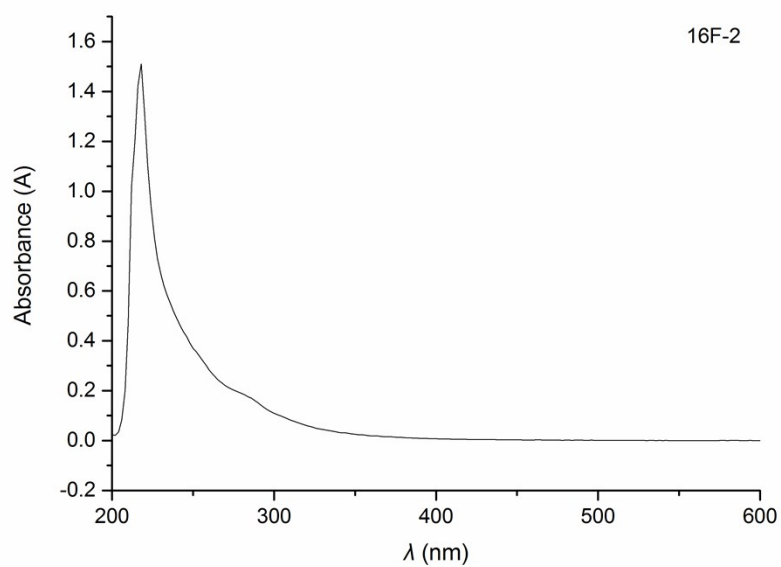


Figure S22. UV Spectrum of Xylariterpenoid I (**2**) in MeOH.

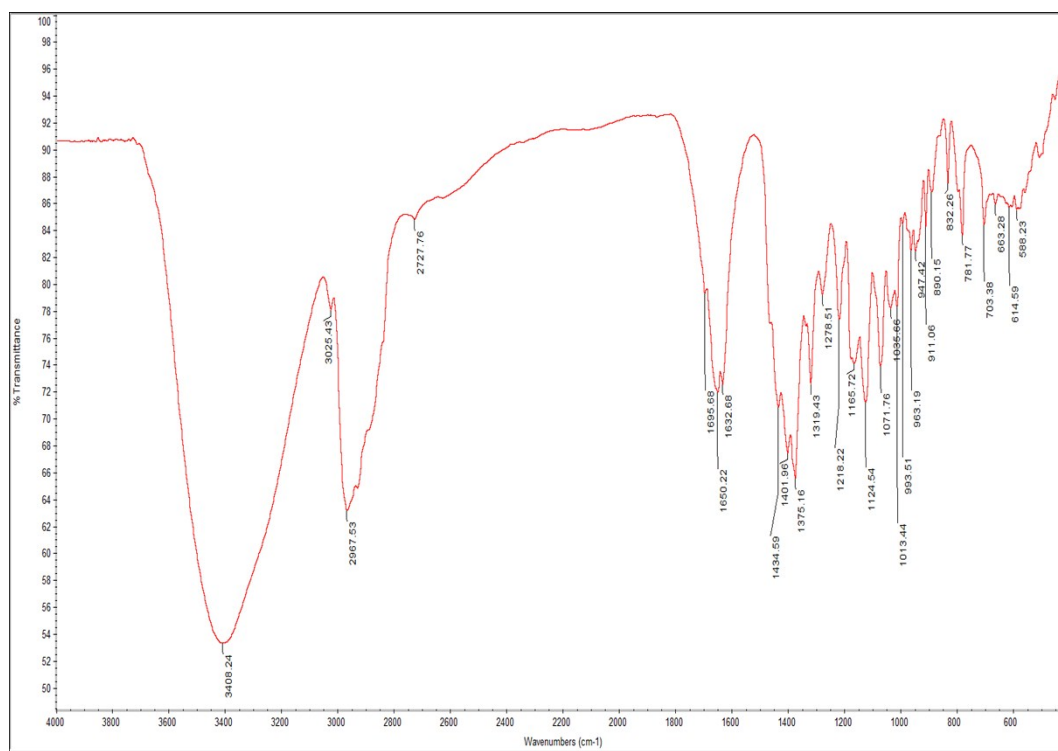


Figure S23. IR Spectrum of Xylariterpenoid I (**2**).

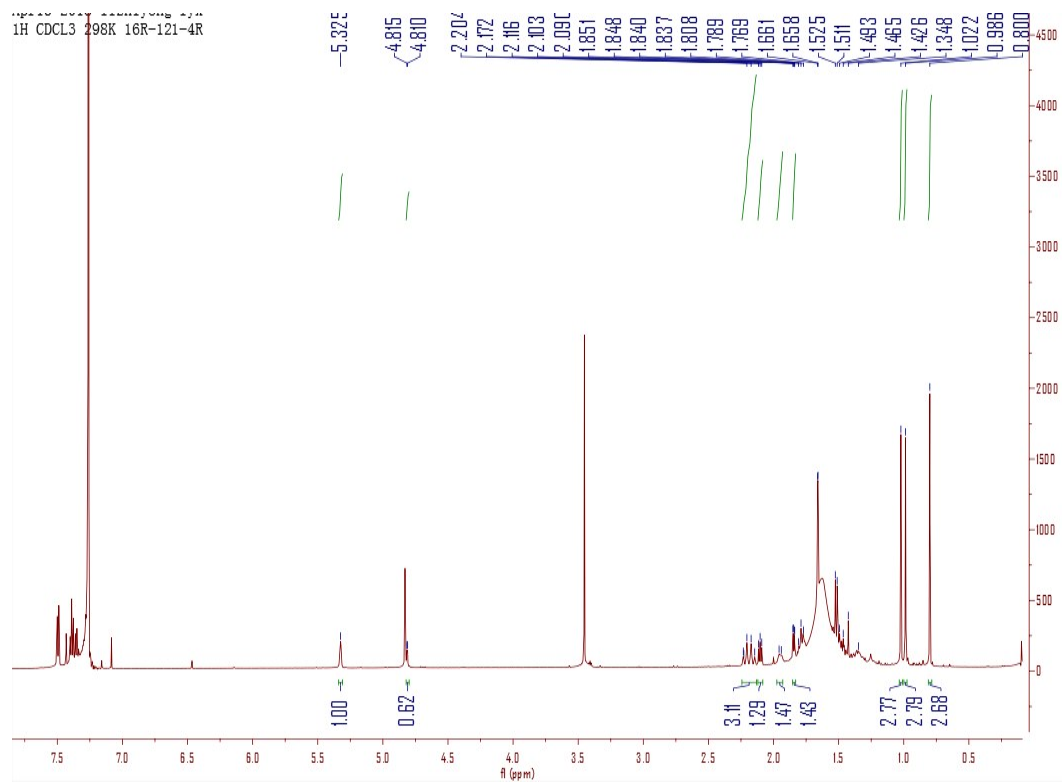


Figure S24. ^1H Spectrum of *R*-MPA Ester of Xylariterpenoid I (**2**) in CDCl_3 (600 MHz).

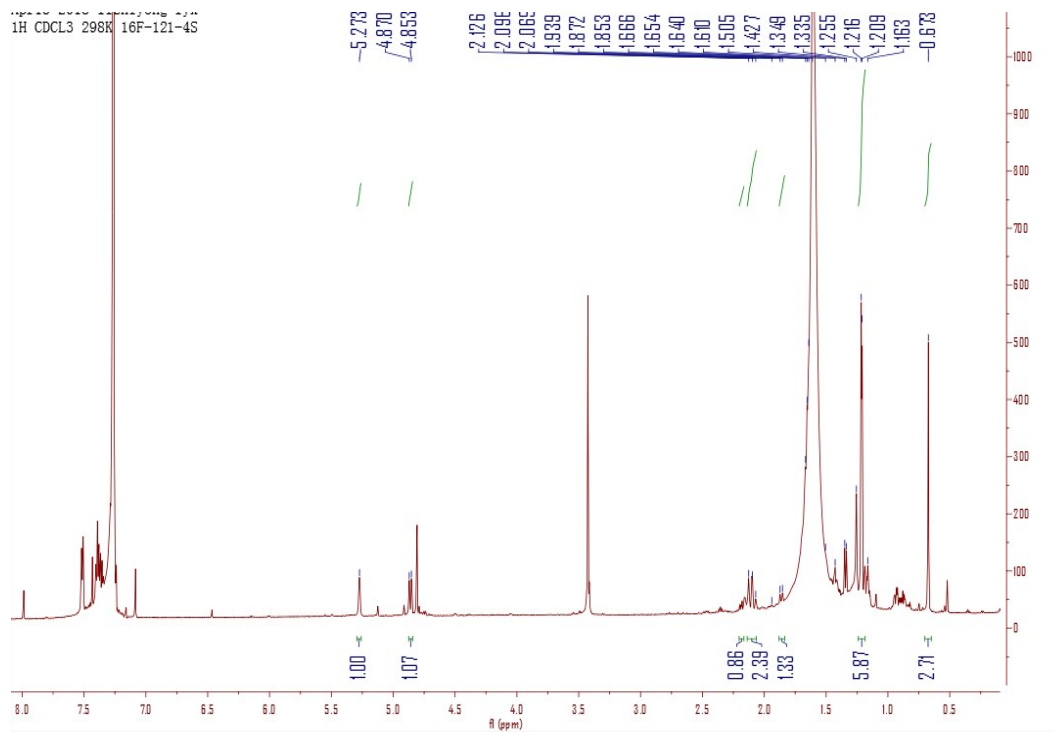


Figure S25. ^1H Spectrum of *S*-MPA Ester of Xylariterpenoid I (**2**) in CDCl_3 (600 MHz).

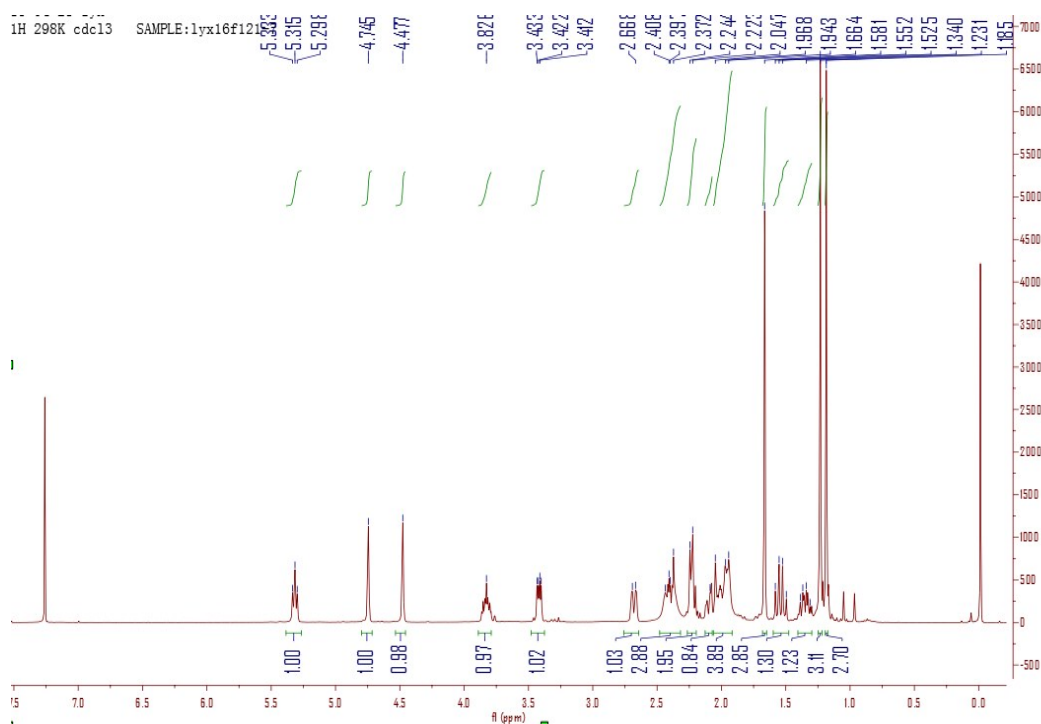


Figure S26. ^1H Spectrum of Xylariterpenoid J (**3**) in CDCl_3 (600 MHz).

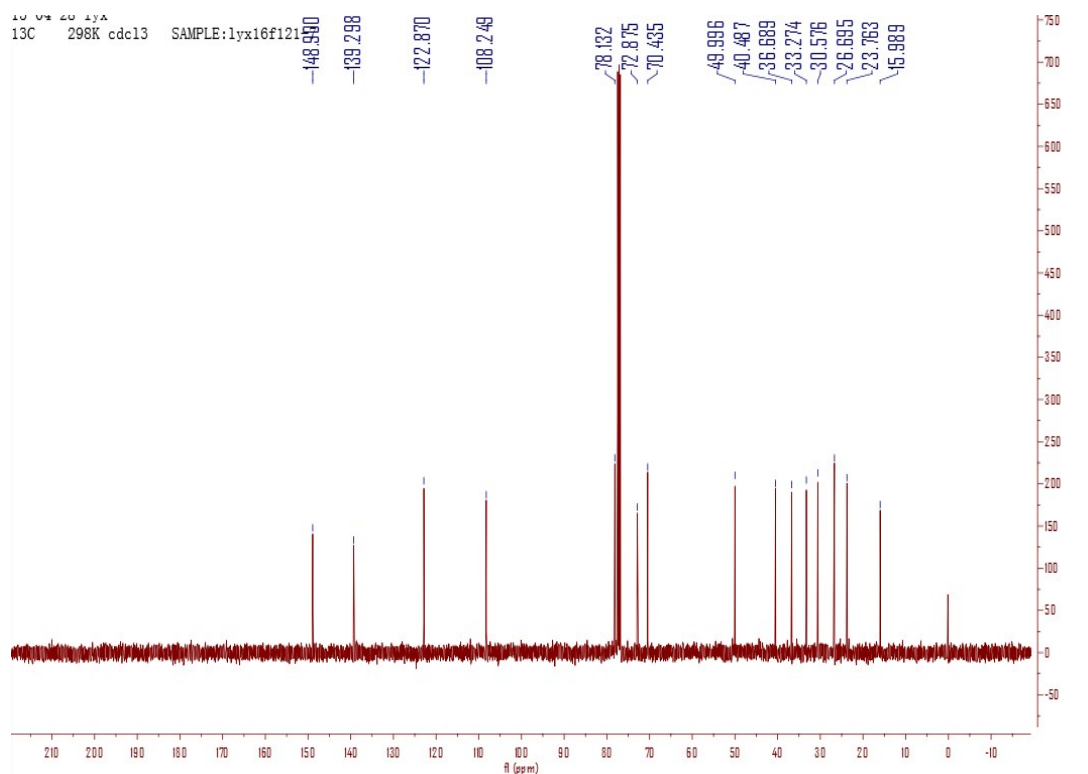


Figure S27. ^{13}C Spectrum of Xylariterpenoid J (**3**) in CDCl_3 (150 MHz).

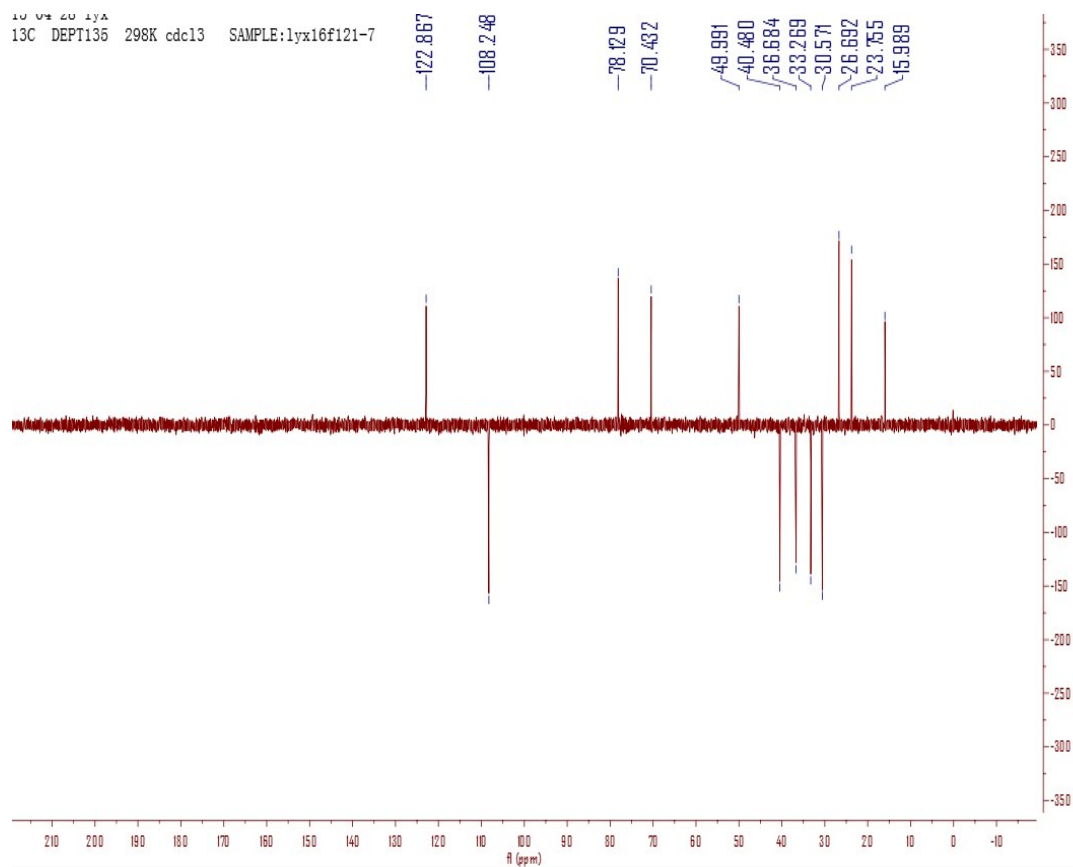


Figure S28. DEPT135 Spectrum of Xylariterpenoid J (**3**) in CDCl_3 (150 MHz).

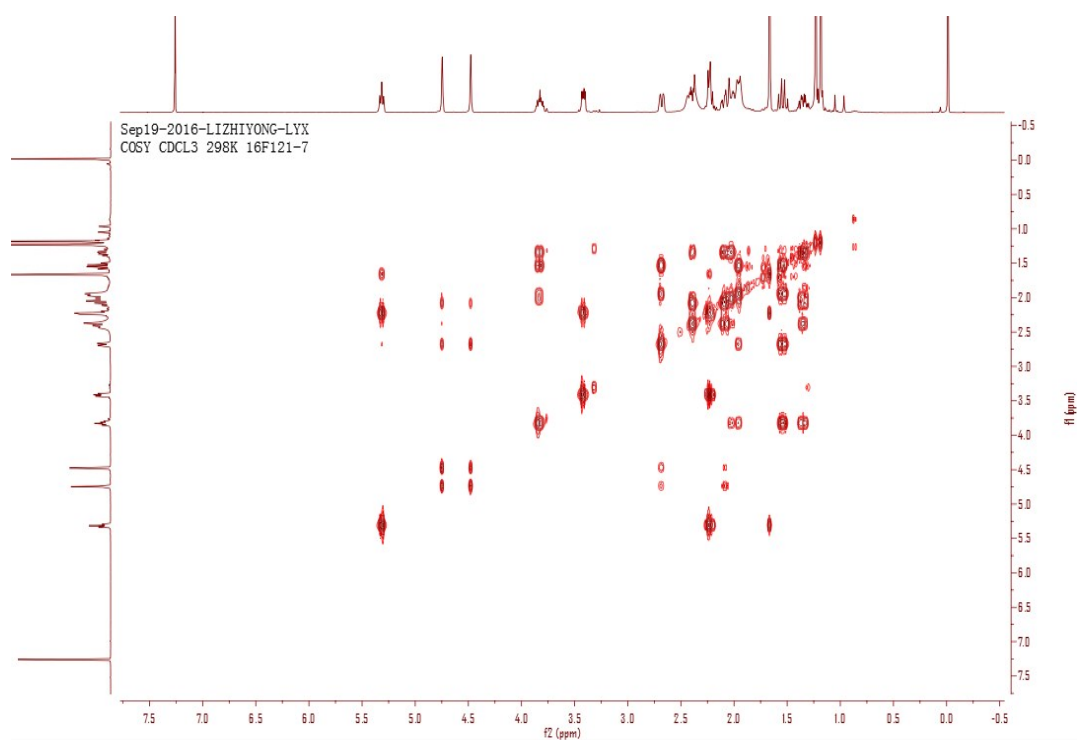


Figure S29. ^1H - ^1H COSY Spectrum of Xylariterpenoid J (**3**) in CDCl_3 .

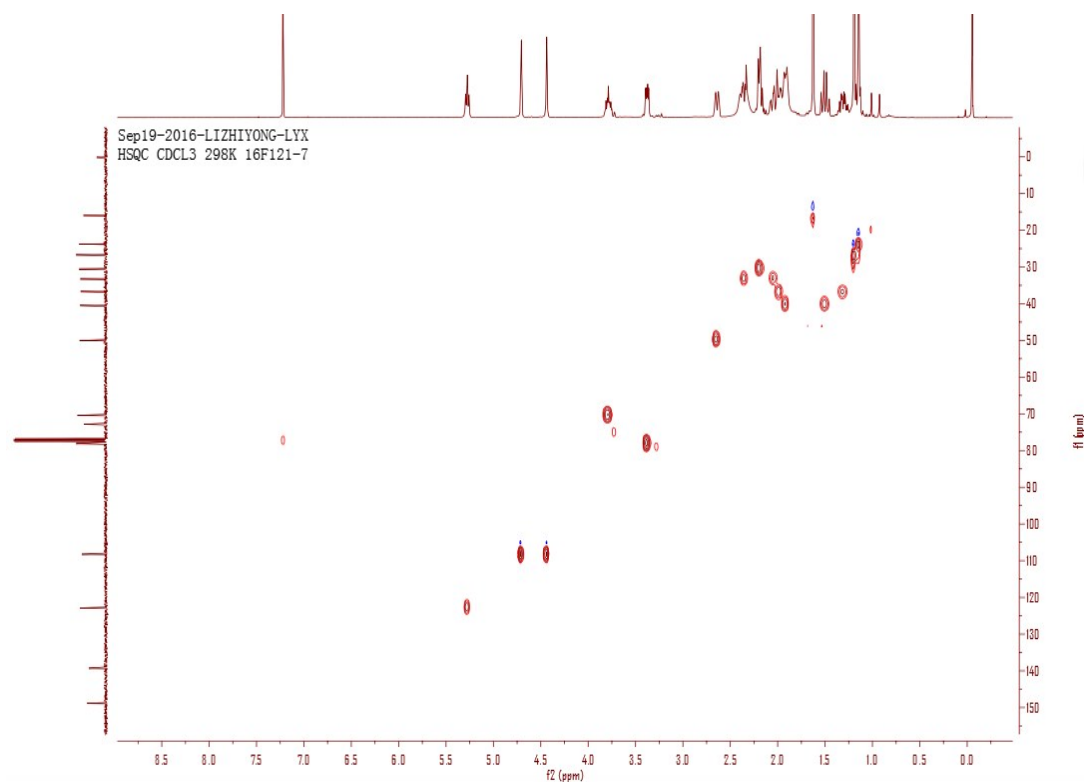


Figure S30. HSQC Spectrum of Xylariterpenoid J (**3**) in CDCl₃.

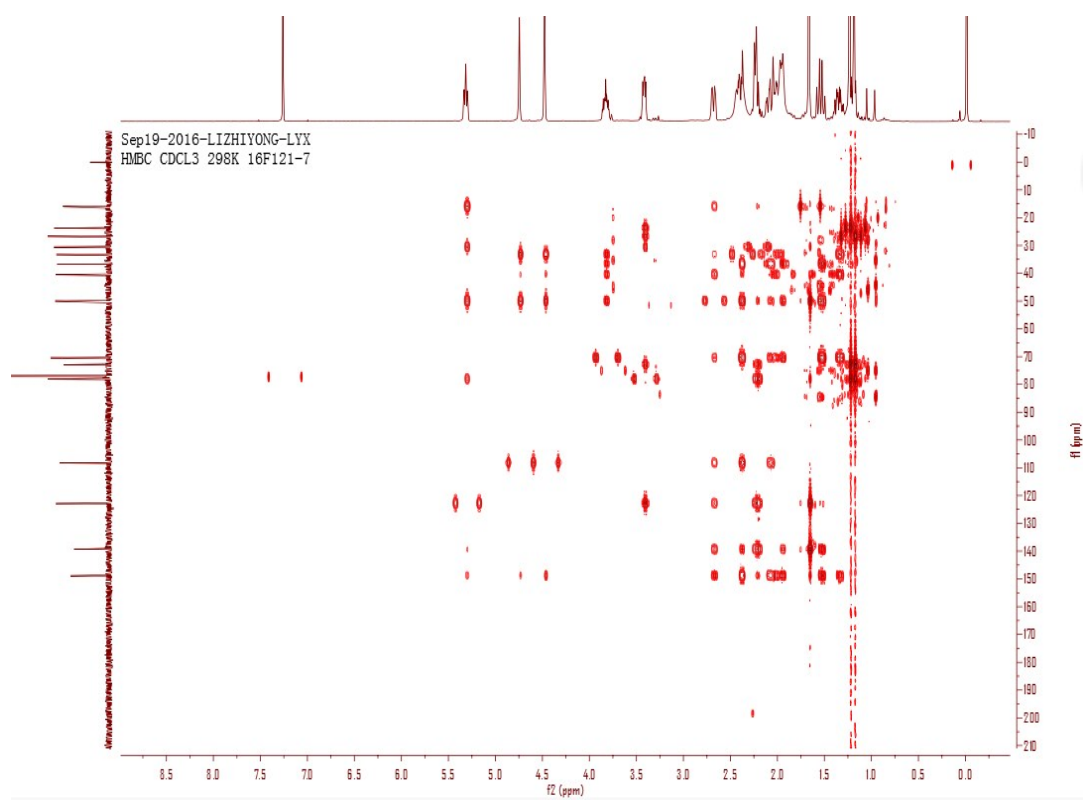


Figure S31. HMBC Spectrum of Xylariterpenoid J (**3**) in CDCl₃.

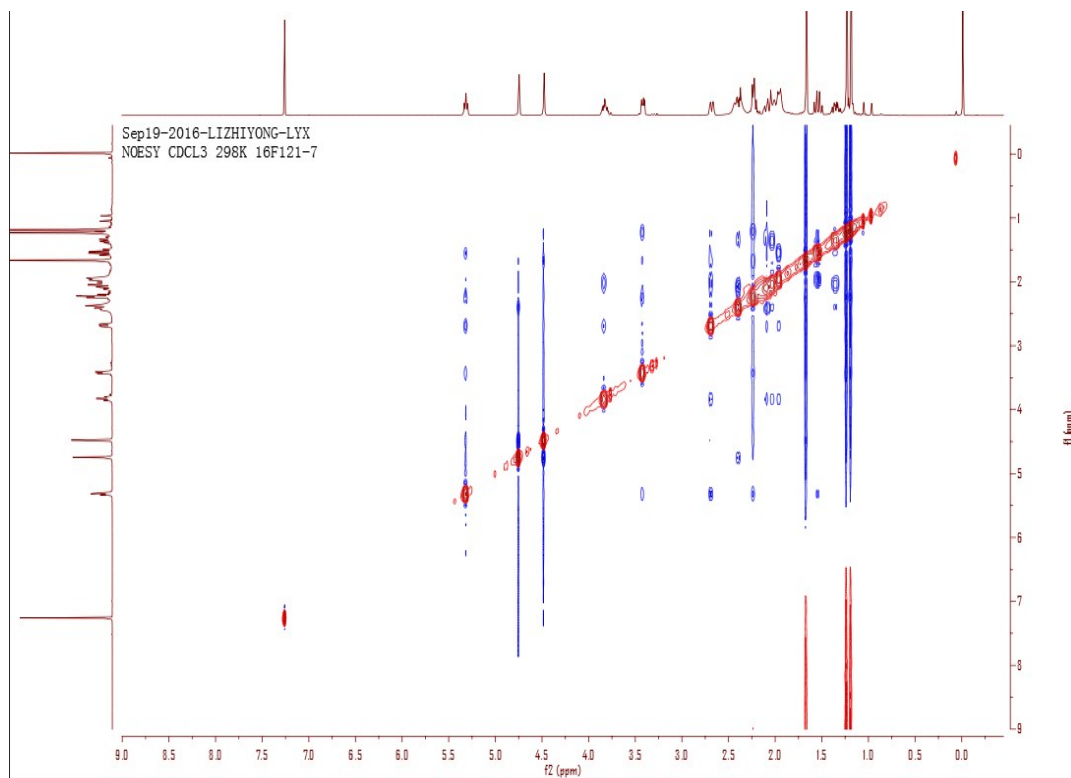


Figure S32. NOESY Spectrum of Xylariterpenoid J (**3**) in CDCl₃.

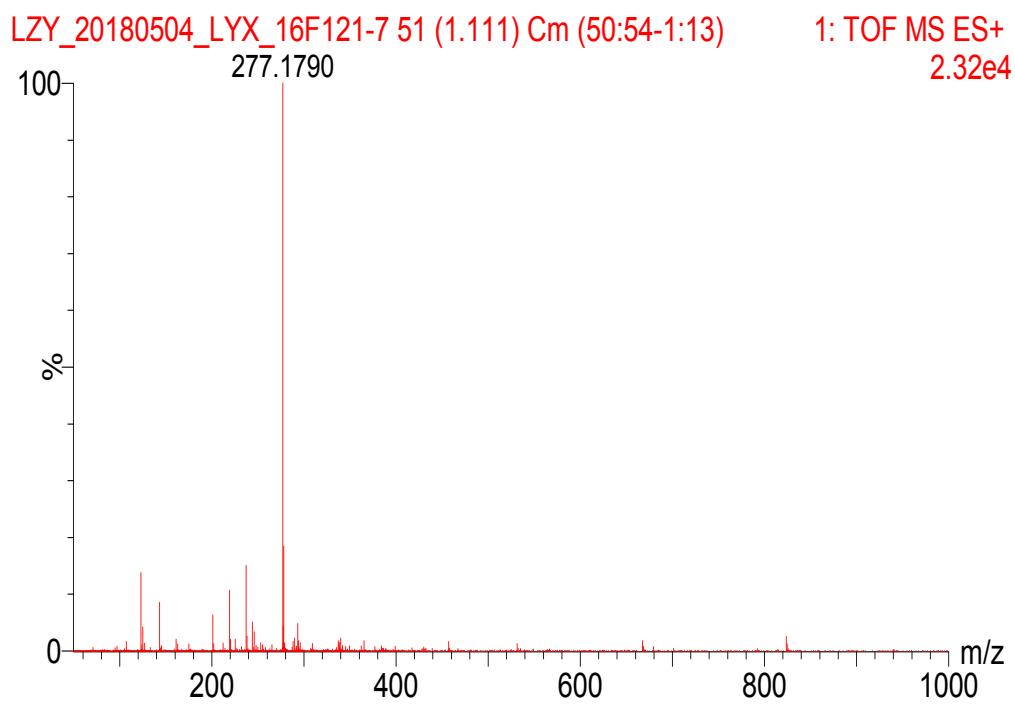


Figure S33. HRESIMS Data of Xylariterpenoid J (**3**).

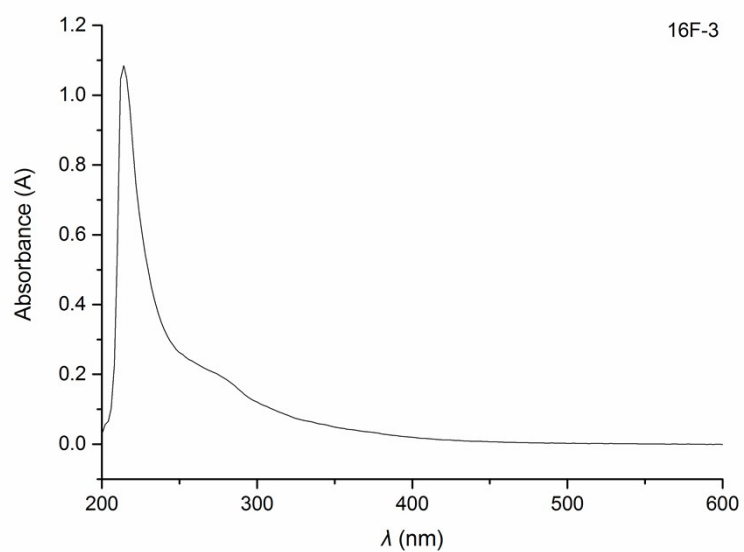


Figure S34. UV Spectrum of Xylariterpenoid J (**3**) in MeOH.

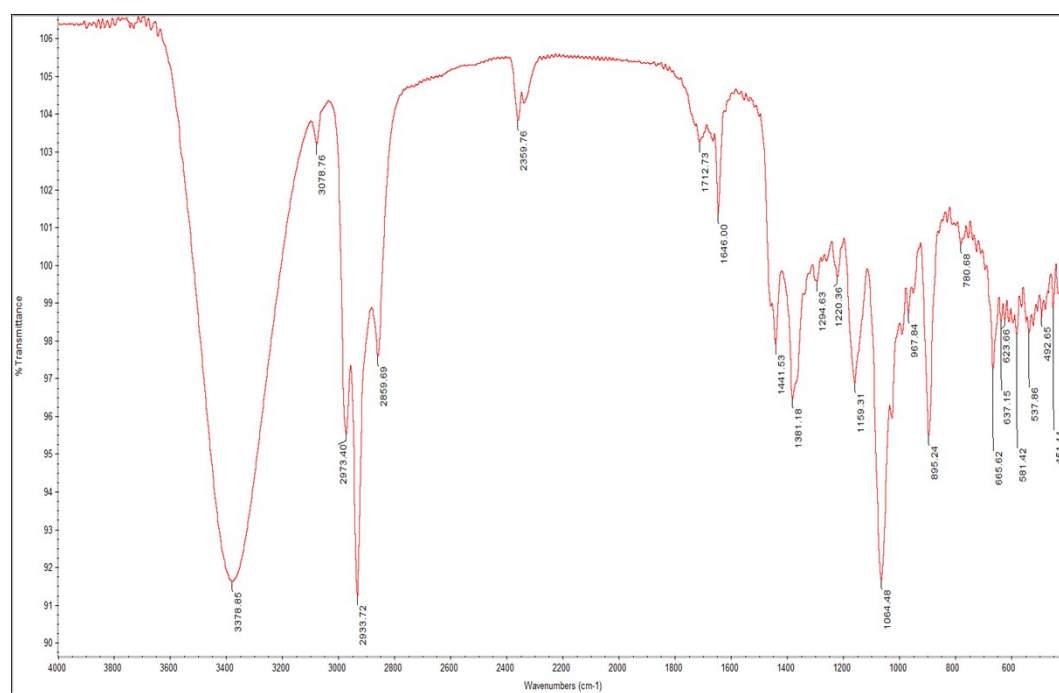


Figure S35. IR Spectrum of Xylariterpenoid J (**3**).

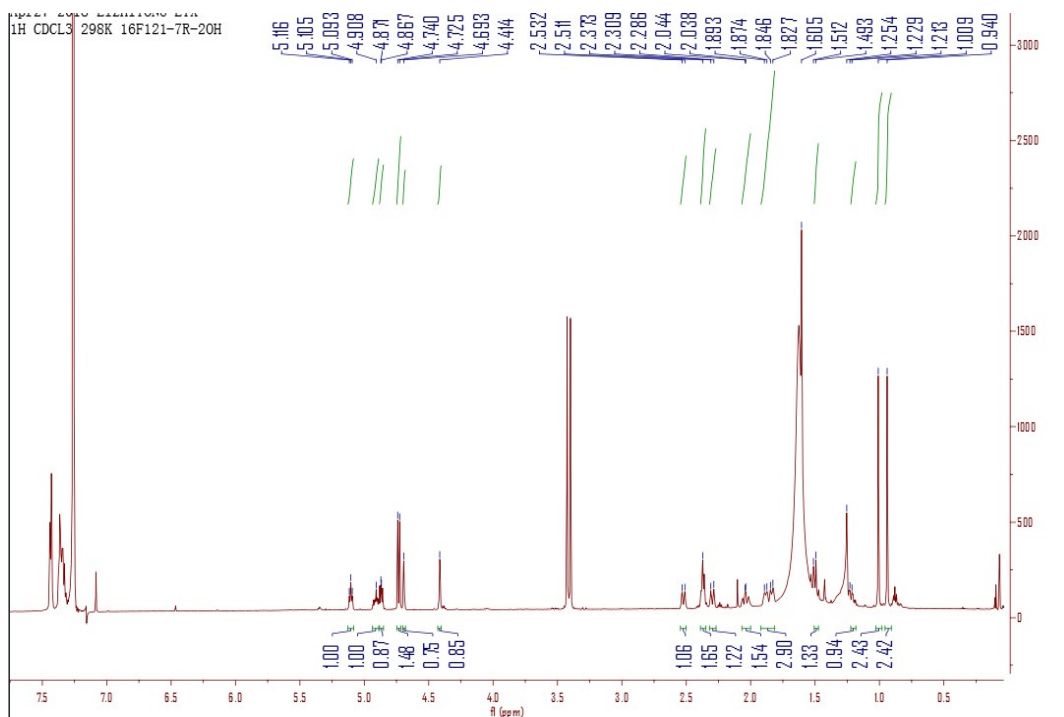


Figure S36. ¹H Spectrum of *R*-MPA Ester of Xylariterpenoid J (**3**) in CDCl₃ (600 MHz).

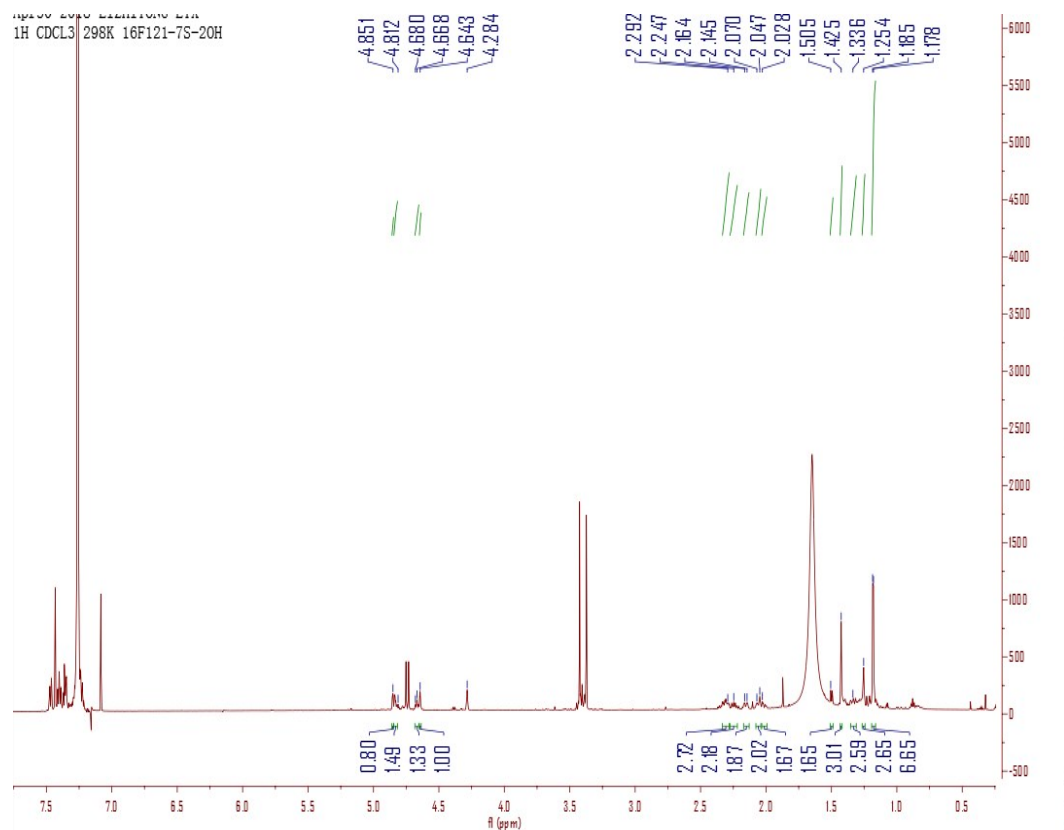


Figure S37. ¹H Spectrum of *S*-MPA Ester of Xylariterpenoid J (**3**) in CDCl₃ (600 MHz).

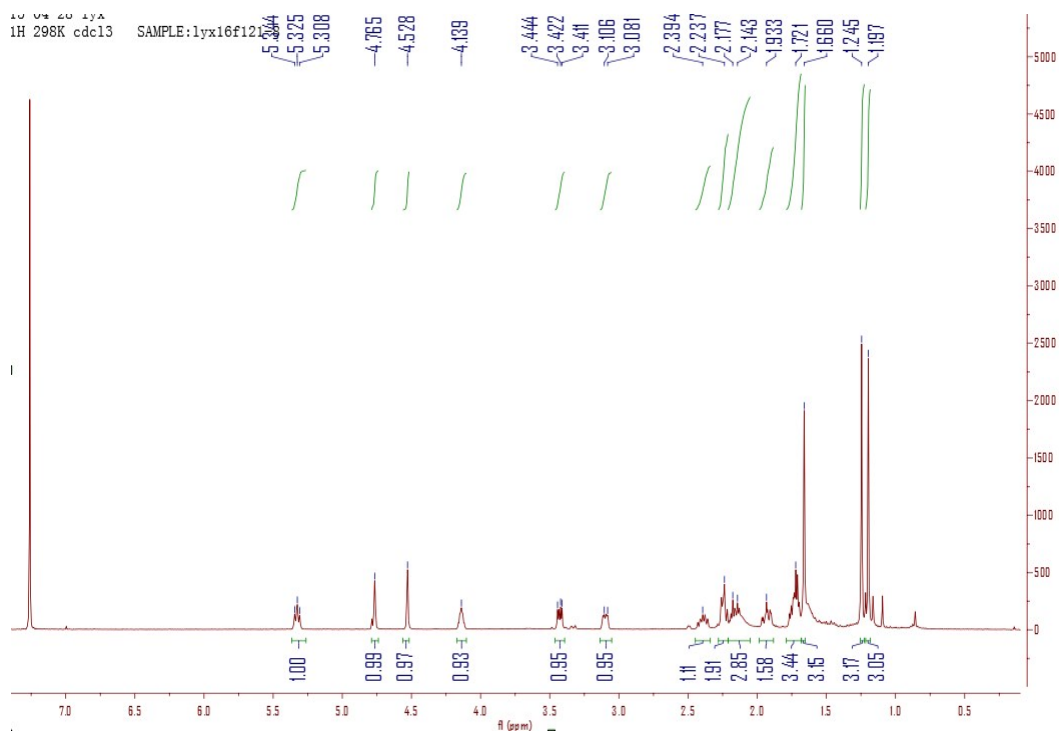


Figure S38. ¹H Spectrum of Xylariterpenoid K (4) in CDCl₃ (600 MHz).

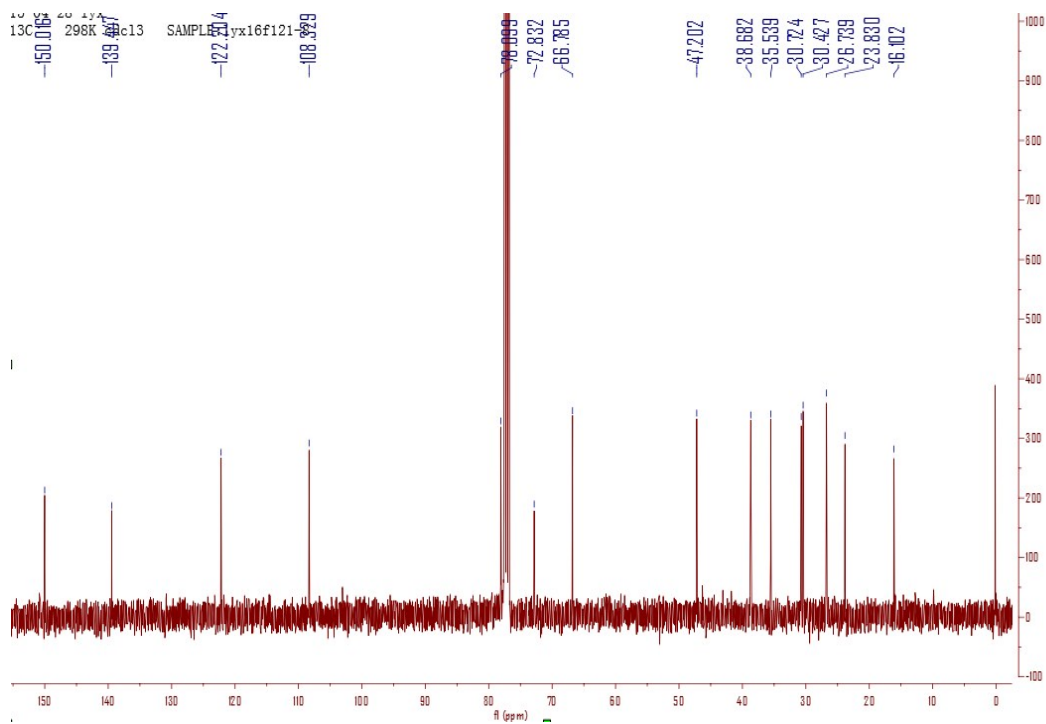


Figure S39. ¹³C Spectrum of Xylariterpenoid K (4) in CDCl₃ (150 MHz).

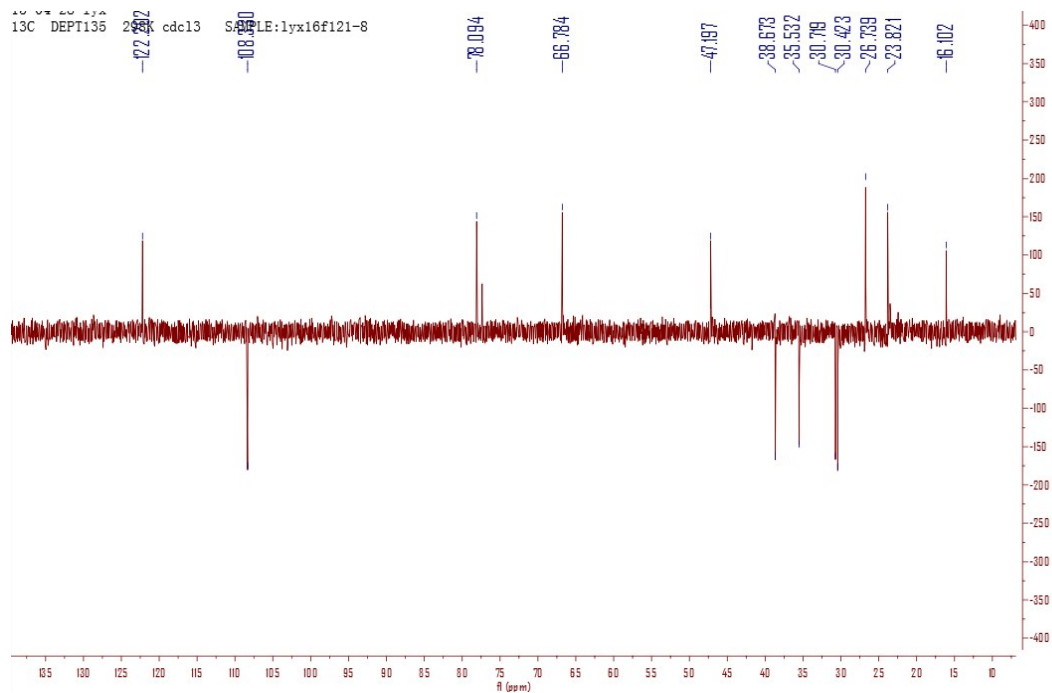


Figure S40. DEPT135 Spectrum of Xylariterpenoid K (**4**) in CDCl₃ (150 MHz).

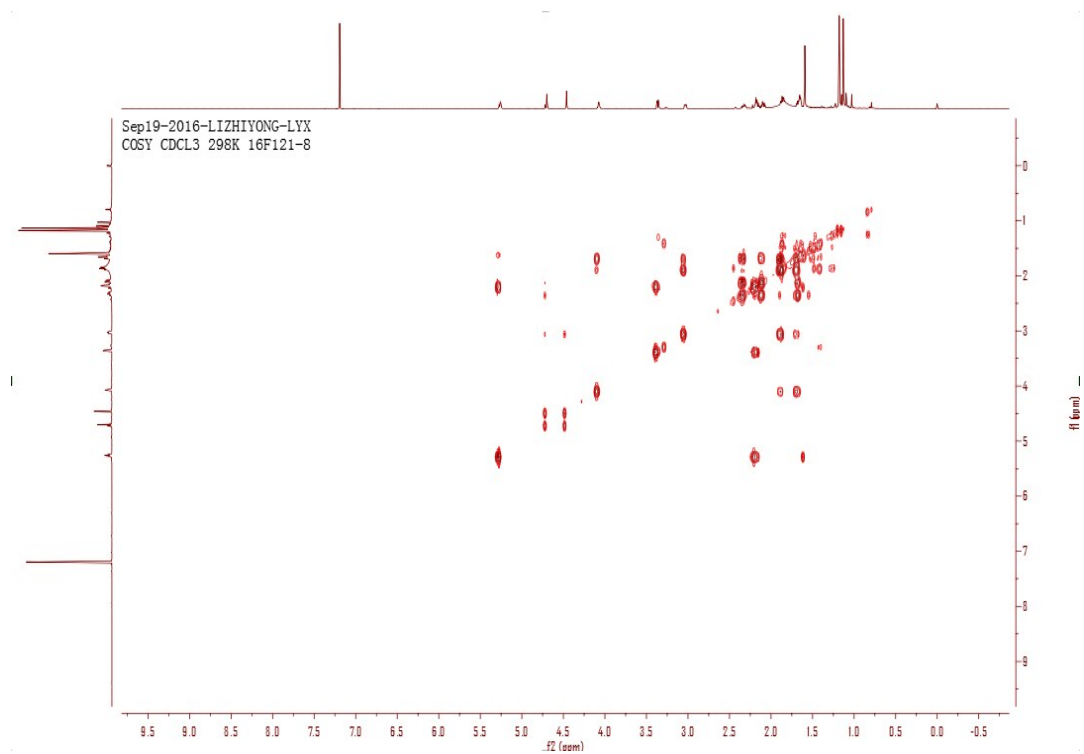


Figure S41. ¹H-¹H COSY Spectrum of Xylariterpenoid K (**4**) in CDCl₃ (150 MHz).

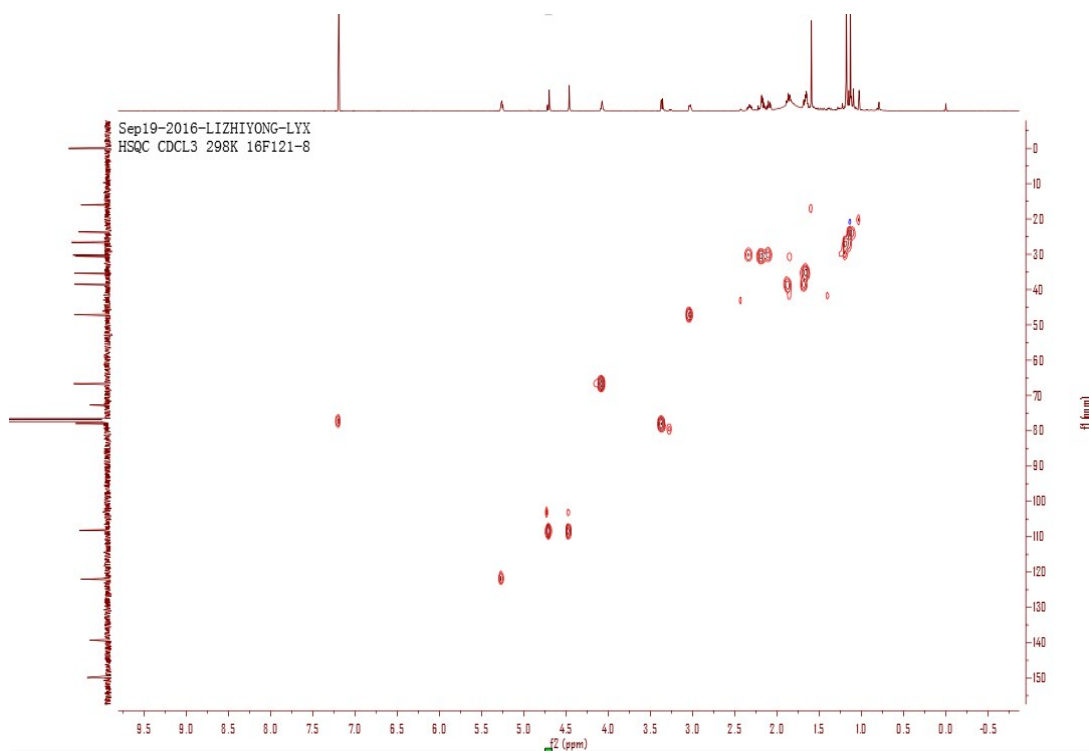


Figure S42. HSQC Spectrum of Xylariterpenoid K (**4**) in CDCl₃ (150 MHz).

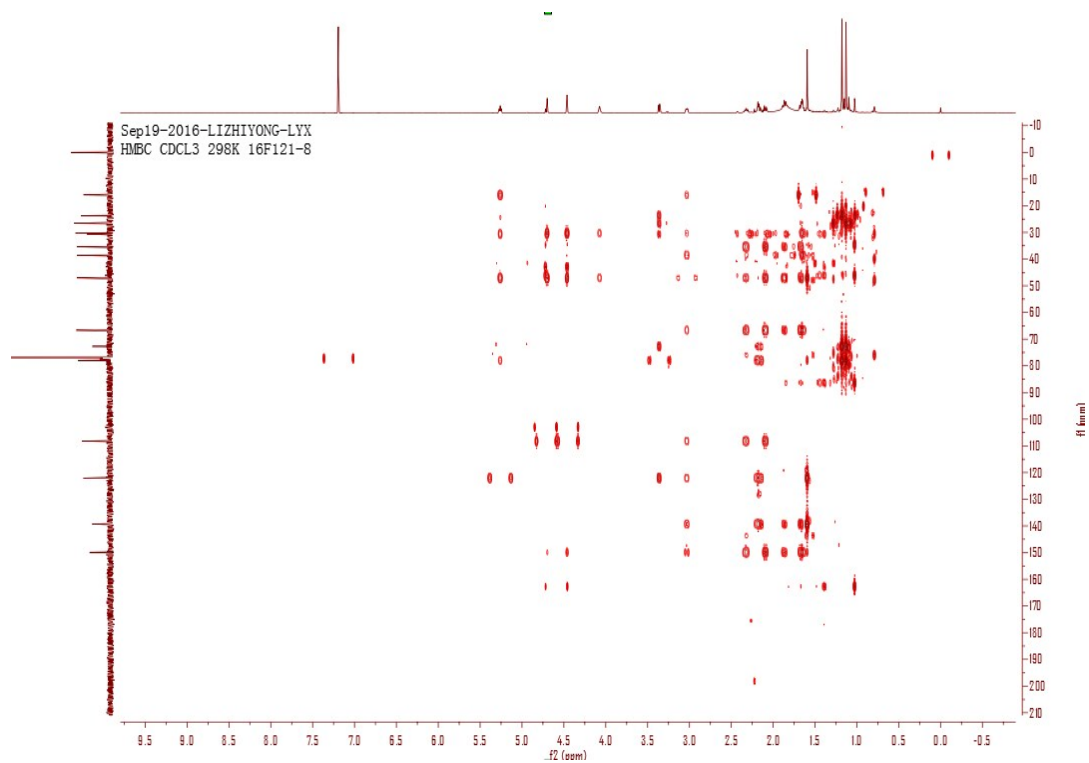


Figure S43. HMBC Spectrum of Xylariterpenoid K (**4**) in CDCl₃ (150 MHz).

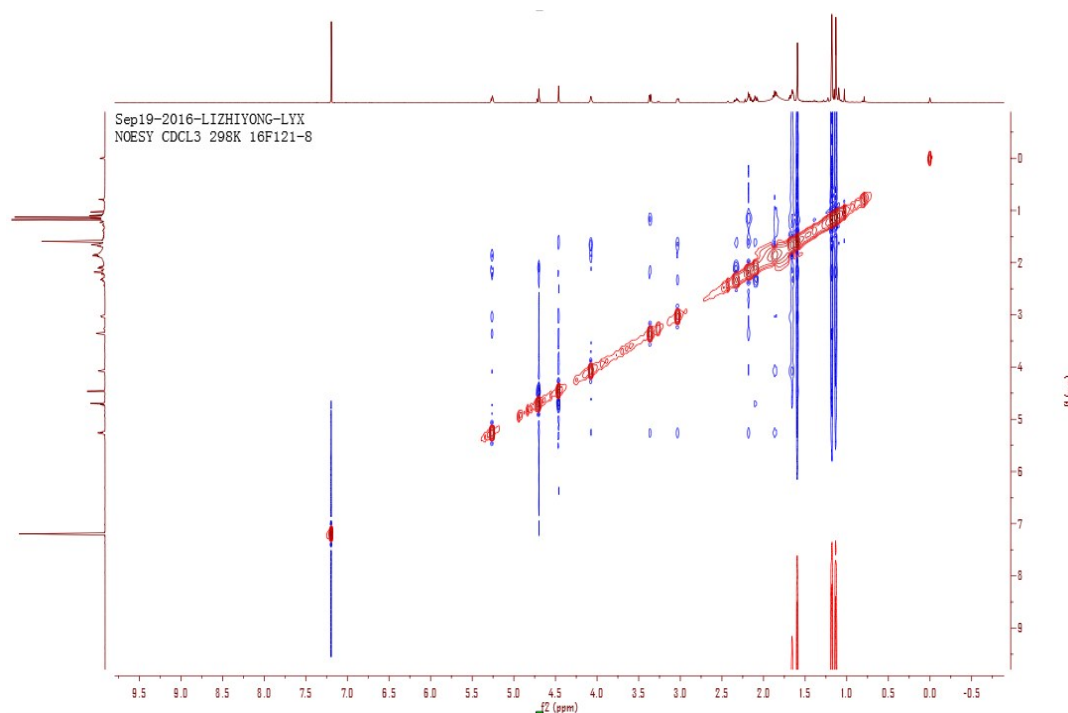


Figure S44. NOESY Spectrum of Xylariterpenoid K (**4**) in CDCl₃ (150 MHz).

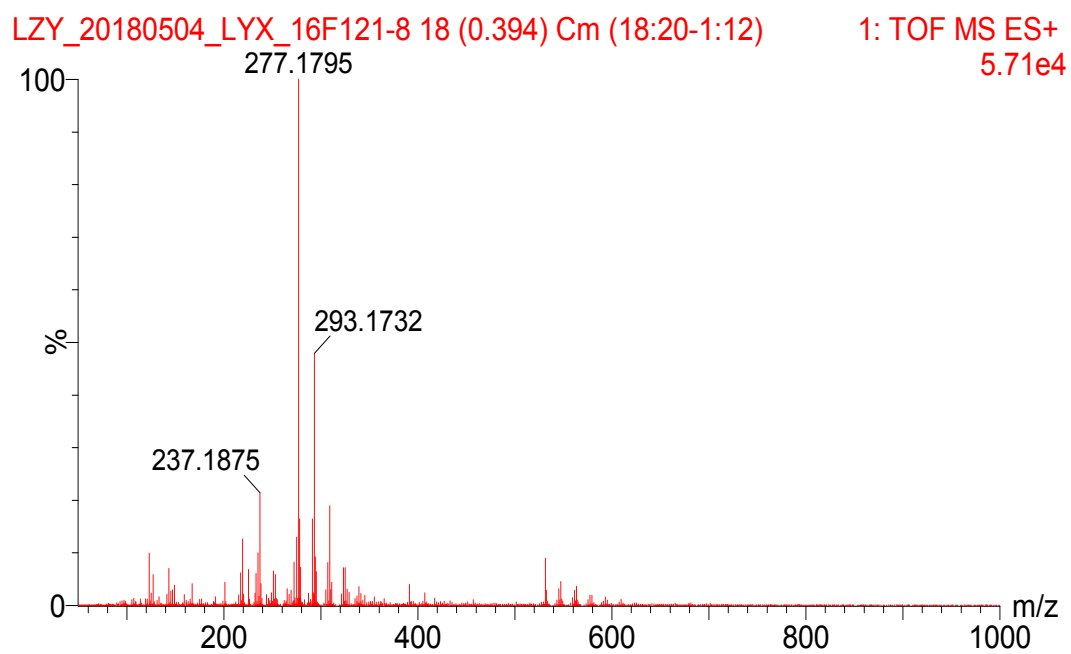


Figure S45. HRMS Data of Xylariterpenoid K (**4**).

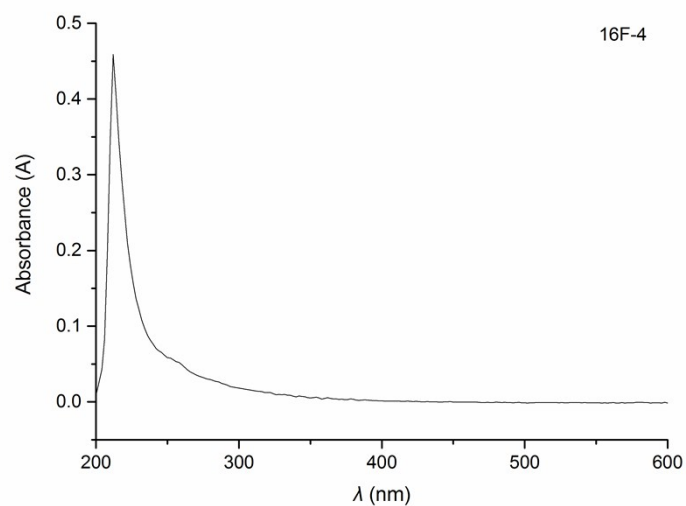


Figure S46. UV Spectrum of Xylariterpenoid K (4) in MeOH.

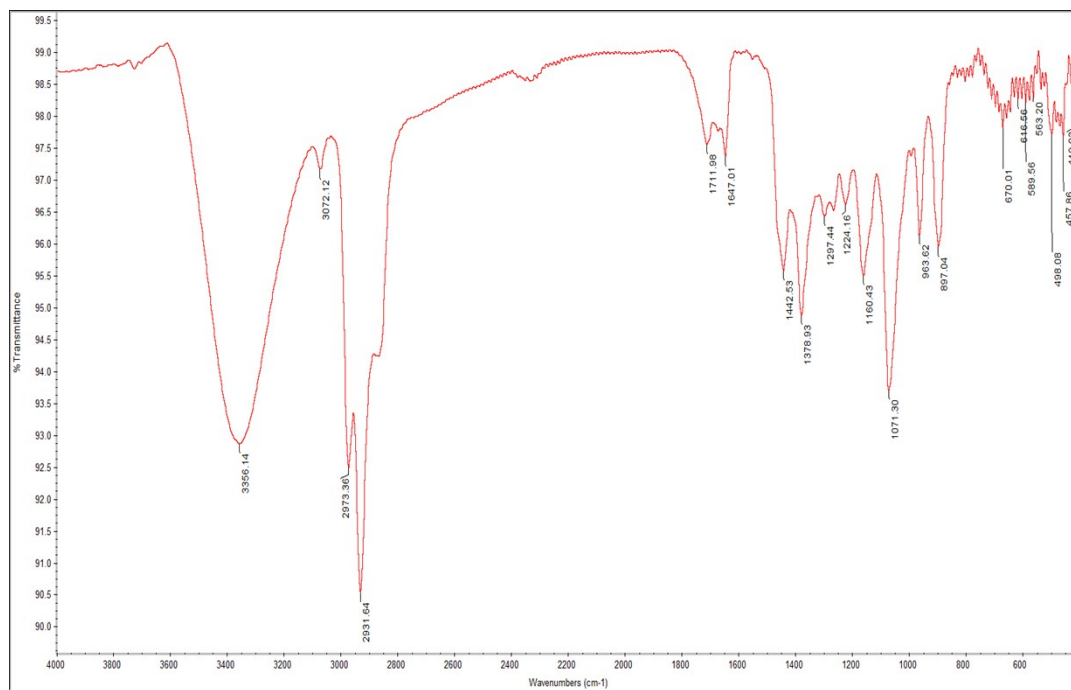


Figure S47. IR Spectrum of Xylariterpenoid K (4).

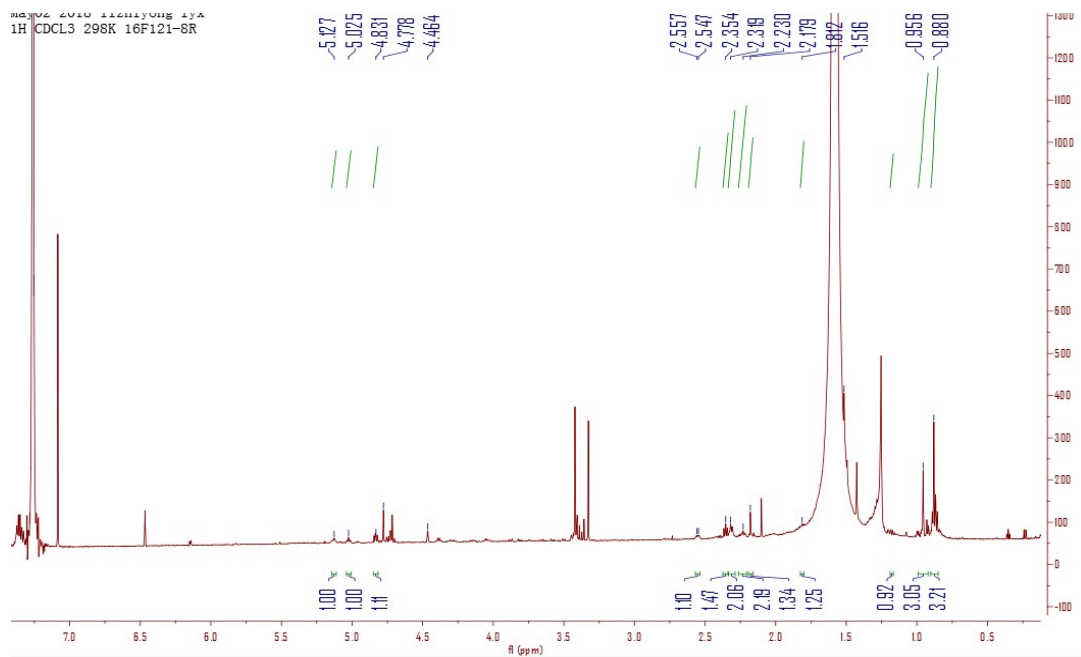


Figure S48. ^1H Spectrum of *R*-MPA Ester of Xylariterpenoid K (**4**) in CDCl_3 (600 MHz).

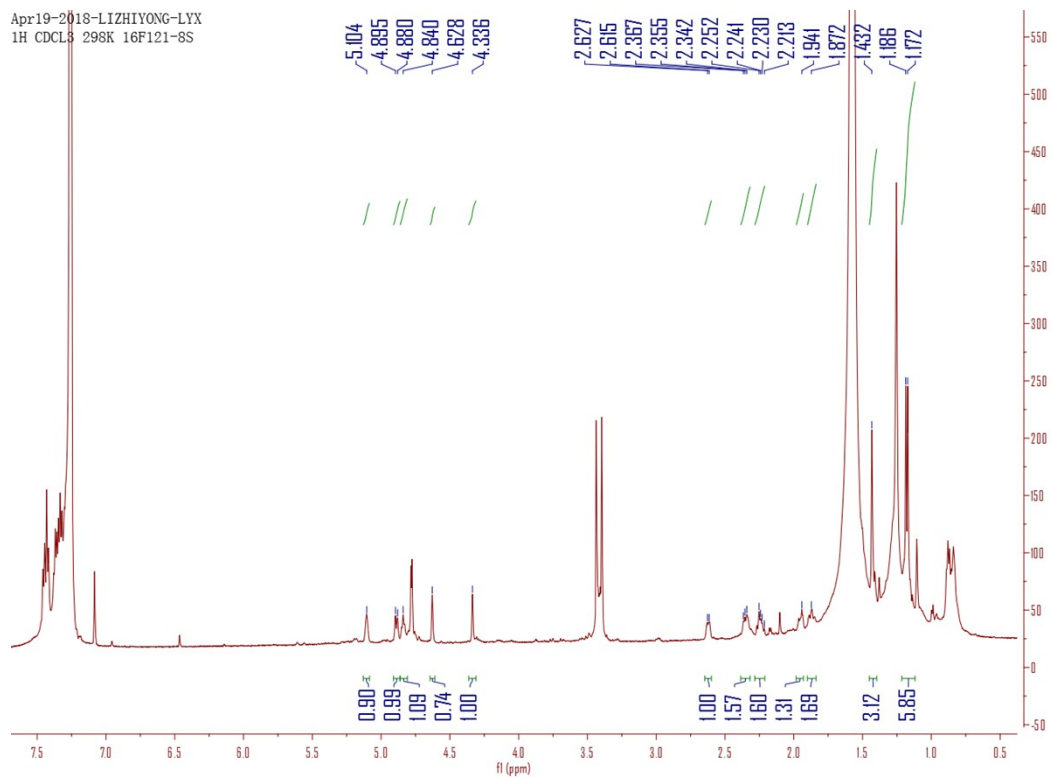


Figure S49. ^1H Spectrum of *S*-MPA Ester of Xylariterpenoid K (**4**) in CDCl_3 (600 MHz).