Electronic Supplementary Information (ESI)

Heptaketides from the Endophytic Fungus Pleosporales sp. F46 and

Their Antifungal and Cytotoxic Activities

Gang Li,^a Ke Xu,^b Wen-Qi Chen,^a Zhi-Hao Guo,^a Yu-Tong Liu,^a Ya-Nan Qiao,^b Yong Sun,^b Gang Sun,^a Xiao-Ping Peng^a and Hong-Xiang Lou*^{ab}

^a Department of Natural Medicinal Chemistry and Pharmacognosy, School of Pharmacy, Qingdao University, Qingdao 266021, People's Republic of China.
^b Department of Natural Product Chemistry, Key Laboratory of Chemical Biology of Ministry of Education, School of Pharmaceutical Sciences, Shandong University, Jinan 250012, People's Republic of China.

*Corresponding Author: Tel: +86-531-8838-2012. Fax: +86-531-8838-2019. E-mail: louhongxiang@sdu.edu.cn (H.-X. Lou).

TABLE OF CONTENTS

Figure S1. ¹H NMR spectrum (400 MHz) of 1 in CDCl₃.

Figure S2. ¹³C NMR spectrum (100 MHz) of 1 in CDCl₃.

Figure S3. HSQC spectrum (400 MHz) of 1 in CDCl₃.

Figure S4. HMBC spectrum (400 MHz) of 1 in CDCl₃.

Figure S5. ¹H-¹H COSY spectrum (400 MHz) of 1 in CDCl₃.

Figure S6. NOESY spectrum (400 MHz) of 1 in CDCl₃.

Figure S7. ESIHRMS spectrum of 1.

Figure S8. IR spectrum of 1.

Figure S9. ¹H NMR spectrum (400 MHz) of 2 in CD₃OD.

Figure S10. 13 C NMR spectrum (100 MHz) of 2 in CD₃OD.

Figure S11. HSQC spectrum (400 MHz) of 2 in CD₃OD.

Figure S12. HMBC spectrum (400 MHz) of 2 in CD₃OD.

Figure S13. ^{1}H - ^{1}H COSY spectrum (400 MHz) of 2 in CD₃OD.

Figure S14. NOESY spectrum (400 MHz) of 2 in CD₃OD.

Figure S15. ESIHRMS spectrum of 2.

Figure S16. IR spectrum of 2.

Figure S17. ¹H NMR spectrum (600 MHz) of **3** in CD₃OD.

Figure S18. ¹³C NMR spectrum (150 MHz) of 3 in CD₃OD.

Figure S19. HSQC spectrum (600 MHz) of 3 in CD₃OD.

Figure S20. HMBC spectrum (600 MHz) of 3 in CD₃OD.

Figure S21. 1 H- 1 H COSY spectrum (600 MHz) of 3 in CD₃OD.

Figure S22. NOESY spectrum (600 MHz) of 3 in CD₃OD.

Figure S23. ESIHRMS spectrum of 3.

Figure S24. IR spectrum of 3.

Figure S25. ¹H NMR spectrum (400 MHz) of 4 in CD₃OD.

Figure S26. ¹³C NMR spectrum (150 MHz) of 4 in CD₃OD.

Figure S27. HSQC spectrum (600 MHz) of 4 in CD₃OD.

Figure S28. HMBC spectrum (600 MHz) of 4 in CD₃OD.

Figure S29. ¹H-¹H COSY spectrum (600 MHz) of 4 in CD₃OD.

Figure S30. NOESY spectrum (600 MHz) of 4 in CD₃OD.

Figure S31. ESIHRMS spectrum of 4.

Figure S32. IR spectrum of 4.

Figure S33. ¹H NMR spectrum (400 MHz) of 5 in CD₃OD.

Figure S34. ¹³C NMR spectrum (100 MHz) of 5 in CD₃OD.

Figure S35. HSQC spectrum (400 MHz) of 5 in CD₃OD.

Figure S36. HMBC spectrum (400 MHz) of 5 in CD₃OD.

Figure S37. ¹H-¹H COSY spectrum (400 MHz) of 5 in CD₃OD.

Figure S38. NOESY spectrum (400 MHz) of 5 in CD₃OD.

Figure S39. ESIHRMS spectrum of 5.

Figure S40. IR spectrum of 5.

Figure S41. ¹H NMR spectrum (400 MHz) of 6 in DMSO- d_6 .

Figure S42. ¹³C NMR spectrum (100 MHz) of 6 in DMSO- d_6 .

Figure S43. HSQC spectrum (400 MHz) of 6 in DMSO- d_6 .

Figure S44. HMBC spectrum (400 MHz) of 6 in DMSO- d_6 .

Figure S45. ¹H-¹H COSY spectrum (400 MHz) of 6 in DMSO- d_6 .

Figure S46. NOESY spectrum (400 MHz) of 6 in DMSO- d_6 .

Figure S47. ESIHRMS spectrum of 6.

Figure S48. IR spectrum of 6.

Figure S49. ¹H NMR spectrum (400 MHz) of 7 in DMSO- d_6 .

Figure S50. ¹³C NMR spectrum (100 MHz) of 7 in DMSO- d_6 .

Figure S51. HSQC spectrum (400 MHz) of 7 in DMSO- d_6 .

Figure S52. HMBC spectrum (400 MHz) of 7 in DMSO- d_6 .

Figure S53. ¹H-¹H COSY spectrum (400 MHz) of 7 in DMSO- d_6 .

Figure S54. NOESY spectrum (400 MHz) of 7 in DMSO- d_6 .

Figure S55. ESIHRMS spectrum of 7.

Figure S56. IR spectrum of 7.

Figure S57. ¹H NMR spectrum (400 MHz) of 8 in CD₃OD.

Figure S58. ¹³C NMR spectrum (100 MHz) of 8 in CD₃OD.

Figure S59. HSQC spectrum (400 MHz) of 8 in CD₃OD.

Figure S60. HMBC spectrum (400 MHz) of 8 in CD₃OD.

Figure S61. ^{1}H - ^{1}H COSY spectrum (400 MHz) of 8 in CD₃OD.

Figure S62. NOESY spectrum (400 MHz) of 8 in CD₃OD.

Figure S63. ESIHRMS spectrum of 8.

Figure S64. IR spectrum of 8.

Figure S65. ¹H NMR spectrum (400 MHz) of 9 in DMSO- d_6 .

Figure S66. ¹³C NMR spectrum (100 MHz) of 9 in DMSO- d_6 .

Figure S67. HSQC spectrum (400 MHz) of 9 in DMSO- d_6 .

Figure S68. HMBC spectrum (400 MHz) of 9 in DMSO- d_6 .

Figure S69. ¹H-¹H COSY spectrum (400 MHz) of 9 in DMSO- d_6 .

Figure S70. NOESY spectrum (400 MHz) of 9 in DMSO- d_6 .

Figure S71. ESIHRMS spectrum of 9.

Figure S72. IR spectrum of 9.

Figure S73. ¹H NMR spectrum (400 MHz) of 10 in CD₃OD.

Figure S74. ¹³C NMR spectrum (150 MHz) of **10** in CD₃OD.

Figure S75. ESIHRMS spectrum of 10.

Figure S76. IR spectrum of 10.

Figure S77. ¹H NMR spectrum (400 MHz) of 11 in CD₃OD.

Figure S78. ¹³C NMR spectrum (100 MHz) of 11 in CD₃OD.

Figure S79. NOESY spectrum (400 MHz) of 11 in CD₃OD.

Figure S80. ESIHRMS spectrum of 11.

Figure S81. IR spectrum of 11.

Figure S82. Experimental (black, solid) and calculated (red, dash) ECD curves of compound 10.

Figure S83. Experimental (black, solid) and calculated (red, dash) ECD curves of compound 11.

Figure S84. LC-ESI-HRMS analysis of the crude extract of endophytic fungus *Pleosporales* sp. F46.

 Table S1. The antifungal and cytotoxic activities of compounds 1-11.



Figure S1. ¹H NMR spectrum (400 MHz) of 1 in CDCl₃.



Figure S2. ¹³C NMR spectrum (100 MHz) of 1 in CDCl₃.



Figure S3. HSQC spectrum (400 MHz) of 1 in CDCl₃.



Figure S4. HMBC spectrum (400 MHz) of 1 in CDCl₃.



Figure S5. ¹H-¹H COSY spectrum (400 MHz) of 1 in CDCl₃.



Figure S6. NOESY spectrum (400 MHz) of 1 in CDCl₃.



Figure S7. ESIHRMS spectrum of 1.



Figure S8. IR spectrum of 1.



Figure S9. ¹H NMR spectrum (400 MHz) of 2 in CD₃OD.



Figure S10. ¹³C NMR spectrum (100 MHz) of 2 in CD₃OD.



Figure S11. HSQC spectrum (400 MHz) of 2 in CD₃OD.



Figure S12. HMBC spectrum (400 MHz) of 2 in CD₃OD.



Figure S13. ¹H-¹H COSY spectrum (400 MHz) of 2 in CD₃OD.



Figure S14. NOESY spectrum (400 MHz) of 2 in CD₃OD.



Figure S15. ESIHRMS spectrum of 2.



Figure S16. IR spectrum of 2.



Figure S17. ¹H NMR spectrum (600 MHz) of **3** in CD₃OD.



Figure S18. ¹³C NMR spectrum (150 MHz) of 3 in CD₃OD.



Figure S19. HSQC spectrum (600 MHz) of 3 in CD₃OD.



Figure S20. HMBC spectrum (600 MHz) of 3 in CD₃OD.



Figure S21. ¹H-¹H COSY spectrum (600 MHz) of 3 in CD₃OD.



Figure S22. NOESY spectrum (600 MHz) of 3 in CD₃OD.



Figure S23. ESIHRMS spectrum of 3.



Figure S24. IR spectrum of 3.



Figure S25. ¹H NMR spectrum (400 MHz) of 4 in CD₃OD.



Figure S26. ¹³C NMR spectrum (150 MHz) of 4 in CD₃OD.



Figure S27. HSQC spectrum (600 MHz) of 4 in CD₃OD.



Figure S28. HMBC spectrum (600 MHz) of 4 in CD₃OD.



Figure S29. ¹H-¹H COSY spectrum (600 MHz) of 4 in CD₃OD.



Figure S30. NOESY spectrum (600 MHz) of 4 in CD₃OD.



Figure S31. ESIHRMS spectrum of 4.


Figure S32. IR spectrum of 4.



Figure S33. ¹H NMR spectrum (400 MHz) of 5 in CD₃OD.



Figure S34. ¹³C NMR spectrum (100 MHz) of 5 in CD₃OD.



Figure S35. HSQC spectrum (400 MHz) of 5 in CD₃OD.



Figure S36. HMBC spectrum (400 MHz) of 5 in CD₃OD.



Figure S37. ¹H-¹H COSY spectrum (400 MHz) of 5 in CD₃OD.



Figure S38. NOESY spectrum (400 MHz) of 5 in CD₃OD.



Figure S39. ESIHRMS spectrum of 5.



Figure S40. IR spectrum of 5.



Figure S41. ¹H NMR spectrum (400 MHz) of 6 in DMSO-*d*₆.



Figure S42. ¹³C NMR spectrum (100 MHz) of 6 in DMSO- d_6 .



Figure S43. HSQC spectrum (400 MHz) of 6 in DMSO- d_6 .



Figure S44. HMBC spectrum (400 MHz) of 6 in DMSO- d_6 .



Figure S45. ¹H-¹H COSY spectrum (400 MHz) of 6 in DMSO-*d*₆.



Figure S46. NOESY spectrum (400 MHz) of 6 in DMSO- d_6 .



Figure S47. ESIHRMS spectrum of 6.



Figure S48. IR spectrum of 6.



Figure S49. ¹H NMR spectrum (400 MHz) of 7 in DMSO-*d*₆.



Figure S50. ¹³C NMR spectrum (100 MHz) of 7 in DMSO- d_6 .



Figure S51. HSQC spectrum (400 MHz) of 7 in DMSO- d_6 .



Figure S52. HMBC spectrum (400 MHz) of 7 in DMSO- d_6 .



Figure S53. $^{1}H^{-1}H$ COSY spectrum (400 MHz) of 7 in DMSO- d_{6} .



Figure S54. NOESY spectrum (400 MHz) of 7 in DMSO- d_6 .



Figure S55. ESIHRMS spectrum of 7.



Figure S56. IR spectrum of 7.



Figure S57. ¹H NMR spectrum (400 MHz) of 8 in CD₃OD.



Figure S58. ¹³C NMR spectrum (100 MHz) of 8 in CD₃OD.



Figure S59. HSQC spectrum (400 MHz) of 8 in CD₃OD.



Figure S60. HMBC spectrum (400 MHz) of 8 in CD₃OD.



Figure S61. ¹H-¹H COSY spectrum (400 MHz) of 8 in CD₃OD.



Figure S62. NOESY spectrum (400 MHz) of 8 in CD₃OD.



Figure S63. ESIHRMS spectrum of 8.



Figure S64. IR spectrum of 8.



Figure S65. ¹H NMR spectrum (400 MHz) of 9 in DMSO-*d*₆.



Figure S66. ¹³C NMR spectrum (100 MHz) of 9 in DMSO- d_6 .



Figure S67. HSQC spectrum (400 MHz) of 9 in DMSO- d_6 .


Figure S68. HMBC spectrum (400 MHz) of 9 in DMSO- d_6 .



Figure S69. ¹H-¹H COSY spectrum (400 MHz) of 9 in DMSO- d_6 .



Figure S70. NOESY spectrum (400 MHz) of 9 in DMSO- d_6 .



Figure S71. ESIHRMS spectrum of 9.



Figure S72. IR spectrum of 9.



Figure S73. ¹H NMR spectrum (400 MHz) of 10 in CD₃OD.



Figure S74. ¹³C NMR spectrum (150 MHz) of 10 in CD₃OD.



Figure S75. ESIHRMS spectrum of 10.



Figure S76. IR spectrum of 10.



Figure S77. ¹H NMR spectrum (400 MHz) of 11 in CD₃OD.



Figure S78. ¹³C NMR spectrum (100 MHz) of 11 in CD₃OD.



Figure S79. NOESY spectrum (400 MHz) of 11 in CD₃OD.



Figure S80. ESIHRMS spectrum of 11.



Figure S81. IR spectrum of 11.



Figure S82. Experimental (black, solid) and calculated (red, dash) ECD curves of compound 10.



Figure S83. Experimental (black, solid) and calculated (red, dash) ECD curves of compound 11.



Figure S84. LC-ESI-HRMS analysis of the crude extract of endophytic fungus *Pleosporales* sp. F46.

Table S1.	The	antifungal	and	cyte	otoxic	activitie	s of	com	pounds	1-1	11.
		4 /									

No.	1	2	3	4	5	6	7	8	9	10	11	Fluconazole	Adriamycin
Candida albicans SC5314	128	>128	>128	>128	>128	>128	>128	>128	>128	>128	>128	2.0	
(µg mL ⁻¹)													
Α549 (μΜ)	>80	>80	>80	>80	>80	>80	>80	>80	>80	>80	>80		1.5±0.1
SMMC-721 (µM)	>80	>80	>80	>80	>80	>80	>80	>80	>80	>80	>80		1.3±0.2
MDA-MB-231 (µM)	>80	>80	>80	>80	>80	>80	22.4±1.1	>80	>80	>80	>80		0.45±0.1