## **Supporting information**

Title: New Compounds from a Hydrothermal Vent Crab-Associated Fungus Aspergillus

versicolor. XZ-4

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Fig. S73. Chiral HPLC Analysis of Acid Hydrolysate of 1 and 4.



**Fig. S1.** <sup>1</sup>H NMR spectrum in  $CD_3OD-d_4$  for compound **1**.

**Fig. S2.** <sup>13</sup>C NMR spectrum in CD<sub>3</sub>OD- $d_4$  for compound 1.





**Fig. S3.** DEPT spectrum in  $CD_3OD$ - $d_4$  for compound 1.

**Fig. S4.** COSY spectrum in  $CD_3OD-d_4$  for compound 1.





**Fig. S5.** HMQC spectrum in  $CD_3OD$ - $d_4$  for compound 1.

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**Fig. S16.** <sup>13</sup>C NMR spectrum in CD<sub>3</sub>OD- $d_4$  for compound **3**.



Fig. S17. DEPT spectrum in  $CD_3OD-d_4$  for compound 3.



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**Fig. S22.** <sup>13</sup>C NMR spectrum in CD<sub>3</sub>OD- $d_4$  for compound 4.



Fig. S23. DEPT spectrum in  $CD_3OD-d_4$  for compound 4.



**Fig. S24.** COSY spectrum in  $CD_3OD$ - $d_4$  for compound 4.



Fig. S25. HMQC spectrum in  $CD_3OD-d_4$  for compound 4.



Fig. S26. HMBC spectrum in  $CD_3OD-d_4$  for compound 4.



**Fig. S27.** <sup>1</sup>H NMR spectrum in CD<sub>3</sub>OD-*d*<sub>4</sub> for compound **5**.



Fig. S28. <sup>13</sup>C NMR spectrum in  $CD_3OD-d_4$  for compound 5.



Fig. S29. DEPT spectrum in  $CD_3OD$ - $d_4$  for compound 5.



Fig. S30. COSY spectrum in  $CD_3OD-d_4$  for compound 5.



Fig. S31. HMQC spectrum in  $CD_3OD-d_4$  for compound 5.



**Fig. S32.** HMBC spectrum in  $CD_3OD-d_4$  for compound **5**.



**Fig. S33.** NOESY spectrum in  $CD_3OD$ - $d_4$  for compound **5**.







**Fig. S35.** <sup>1</sup>H NMR spectrum in CD<sub>3</sub>OD- $d_4$  for compound 6.



**Fig. S36.** <sup>13</sup>C NMR spectrum in  $CD_3OD-d_4$  for compound 6.



Fig. S37. DEPT spectrum in  $CD_3OD-d_4$  for compound 6.



Fig. S38. COSY spectrum in  $CD_3OD$ - $d_4$  for compound 6.



Fig. S39. HMQC spectrum in  $CD_3OD-d_4$  for compound 6.



Fig. S40. HMBC spectrum in  $CD_3OD-d_4$  for compound 6.



Fig. S41. NOESY spectrum in  $CD_3OD-d_4$  for compound 6.



**Fig. S42.** <sup>1</sup>H NMR spectrum in CD<sub>3</sub>OD-*d*<sub>4</sub> for compound **7**.



**Fig. S43.** <sup>13</sup>C NMR spectrum in  $CD_3OD-d_4$  for compound 7.



Fig. S44. DEPT spectrum in  $CD_3OD-d_4$  for compound 7.



**Fig. S45.** COSY spectrum in  $CD_3OD$ - $d_4$  for compound 7.



Fig. S46. HMQC spectrum in  $CD_3OD-d_4$  for compound 7.



**Fig. S47.** HMBC spectrum in  $CD_3OD-d_4$  for compound 7.



**Fig. S48.** NOESY spectrum in  $CD_3OD-d_4$  for compound 7.



Fig. S49. <sup>1</sup>H NMR spectrum in CD<sub>3</sub>OD-*d*<sub>4</sub> for compound 8.



Fig. S50. <sup>13</sup>C NMR spectrum in  $CD_3OD-d_4$  for compound 8.



Fig. S51. DEPT spectrum in CD<sub>3</sub>OD-*d*<sub>4</sub> for compound 8.



Fig. S52. COSY spectrum in  $CD_3OD-d_4$  for compound 8.



Fig. S53. HMQC spectrum in  $CD_3OD-d_4$  for compound 8.



Fig. S54. HMBC spectrum in  $CD_3OD-d_4$  for compound 8.



**Fig. S55.** <sup>1</sup>H NMR spectrum in  $CD_3OD$ - $d_4$  for compound 9.



Fig. S56. <sup>13</sup>C NMR spectrum in  $CD_3OD-d_4$  for compound 9.



Fig. S57. DEPT spectrum in CD<sub>3</sub>OD-*d*<sub>4</sub> for compound 9.



Fig. S58. COSY spectrum in  $CD_3OD-d_4$  for compound 9.



**Fig. S59.** HMQC spectrum in  $CD_3OD-d_4$  for compound **9**.



Fig. S60. HMBC spectrum in  $CD_3OD-d_4$  for compound 9.



Fig. S61. HRMS for compound 1.

Spectrum from pos-9 wiff (sample 1) - Sample009, Experiment 1, +TOF MS (100 - 1000) from 0.219 to 0.350 min





Spectrum from pos-8 wiff (sample 1) - Sample008, Experiment 1, +TOF MS (100 - 1000) from 0.181 to 0.350 min





Spectrum from pos-10.wiff (sample 1) - Sample010, Experiment 1, +TOF MS (100 - 1000) from 0.198 to 0.388 min



Fig. S64. HRMS for compound 4.

Spectrum from pos-7.wiff (sample 1) - Sample007, Experiment 1, +TOF MS (100 - 1000) from 0.222 to 0.374 min





Spectrum from pos-2 wiff (sample 1) - Sample002, Experiment 1, +TOF MS (100 - 1000) from 0.221 to 0.356 min



## Fig. S66. HRMS for compound 6.

Spectrum from pos-3.wiff (sample 1) - Sample003, Experiment 1, +TOF MS (100 - 1000) from 0.199 to 0.372 min



Fig. S67. HRMS for compound 7.

Spectrum from pos-1.wiff (sample 1) - Sample001, Experiment 1, +TOF MS (100 - 1000) from 0.227 to 0.285 min



## Fig. S68. HRMS for compound 8.

Spectrum from pos-5.wiff (sample 1) - Sample005, Experiment 1, +TOF MS (100 - 1000) from 0.218 to 0.352 min





Spectrum from pos-4.wiff (sample 1) - Sample004, Experiment 1, +TOF MS (100 - 1000) from 0.220 to 0.355 min



Fig. S70. B3LYP/6-31+G (d, p) optimized & calculated ECD spectra of conformations of compound 2. The theoretical ECD spectra for 14R was obtained by directly reversing the spectra of 14S.



Fig. S71. B3LYP/6-31+G (d, p) optimized & calculated ECD spectra of conformations of compound 3. The theoretical ECD spectra for 3S, 14R and 3R, 14R were obtained by directly reversing the spectra of 3R, 14S and 3S, 14S.



Fig. S72. B3LYP/6-31+G (d, p) optimized & calculated ECD spectra of conformations of compound 7. The theoretical ECD spectra for 3S, 10R was obtained by directly reversing the



Fig. S73. Chiral HPLC Analysis of Acid Hydrolysate of 1 and 4.

