

Supporting Information

Seven New Cytotoxic Phenylspirodrimane Derivatives from the Endophytic Fungus, *Stachybotrys chartarum*

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Bioactivity assay

Cytotoxic activities were evaluated by the MTT method against three human tumor cell lines, including MDA-MB-231, U2-OS, and MCF-7. Cisplatin and doxorubicin were used as the positive control medicines. The IC₅₀ values were shown in Table S1.

Table S1. Cytotoxicities of stachybochartins A-D and G in three human tumor cell lines with MTT method.

compound	cytotoxicity (IC ₅₀ , μ M)		
	MDA-MB-231	U2-OS	MCF-7
Stachybochartin A	21.7 \pm 2.1	19.8 \pm 2.5	> 50
Stachybochartin B	17.6 \pm 0.6	11.2 \pm 2.1	> 50
Stachybochartin C	11.6 \pm 1.6	14.5 \pm 3.1	> 50
Stachybochartin D	10.4 \pm 0.9	9.2 \pm 0.1	> 50
Stachybochartin G	5.6 \pm 0.1	4.5 \pm 2.2	> 50
Cisplatin	11.3 \pm 0.6	5.9 \pm 1.3	-
Doxorubicin	1.0 \pm 0.1	1.2 \pm 0.9	-

Data were expressed as means \pm SD of three independent experiments.

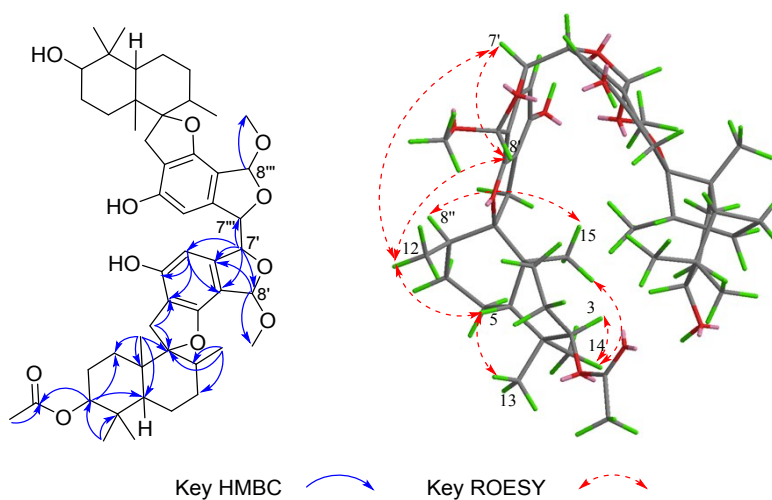


Figure S1. The key HMBC and ROESY correlations of **2**

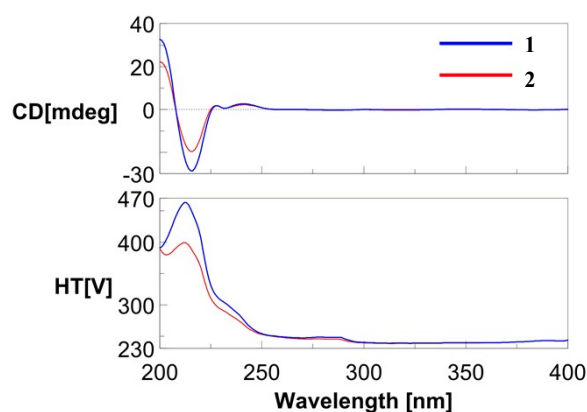


Figure S2. The comparison of the experimental ECD spectra of **1** and **2**

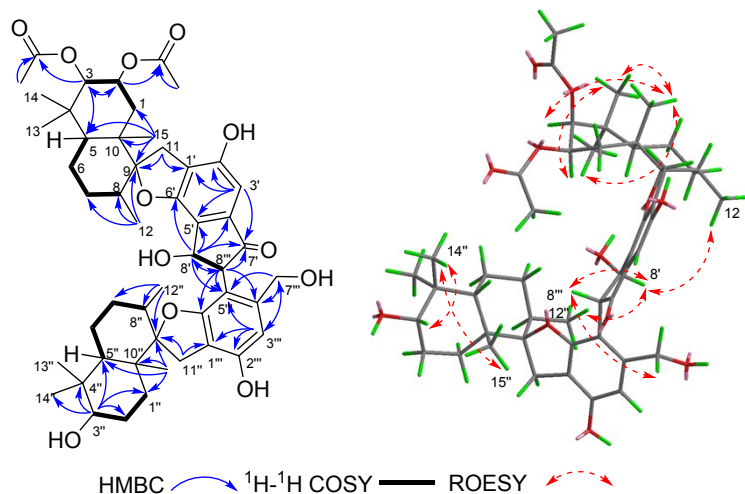


Figure S3. The key HMBC and key ROESY correlations of stachybochartin D (4).

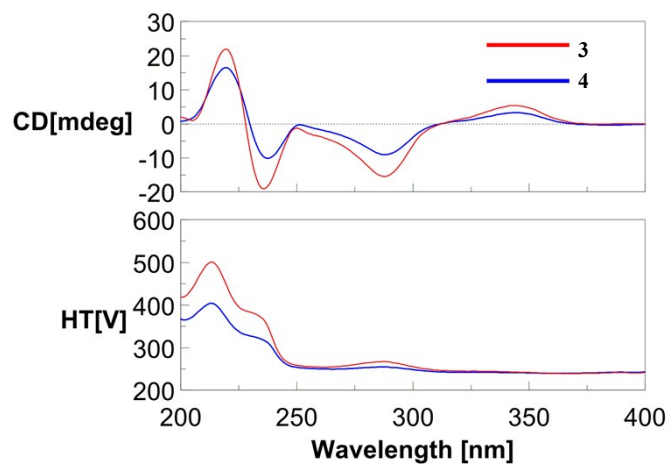


Figure S4. The ECD spectra of stachybochartin C (3) and stachybochartin D (4) in MeOH.

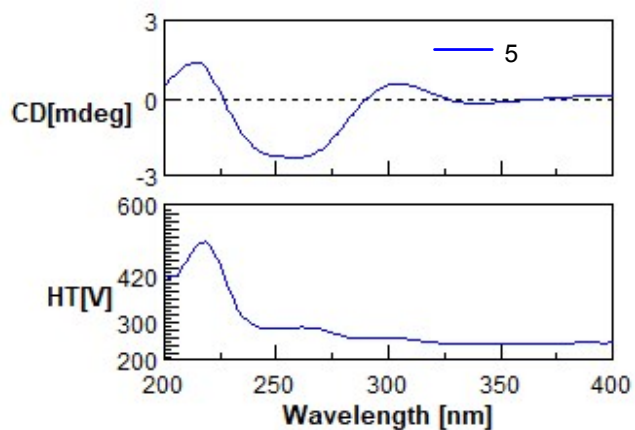


Figure S5. The experimental ECD spectra of 5.

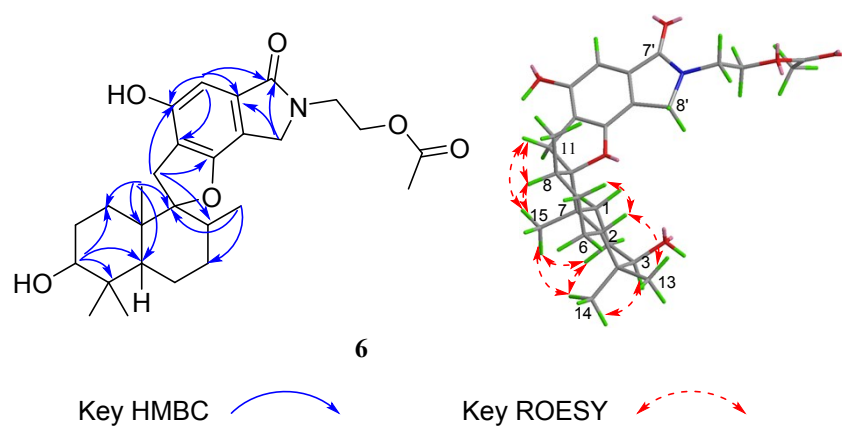


Figure S6. The key HMBC and ROESY correlations of stachybochartin F (6)

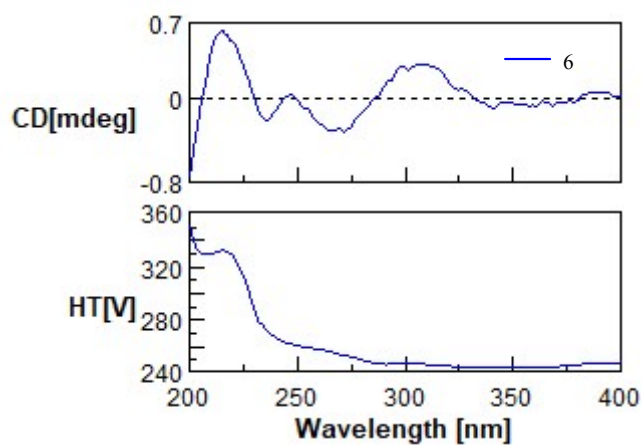


Figure S7. The experimental ECD spectra of stachybochartin F (6).

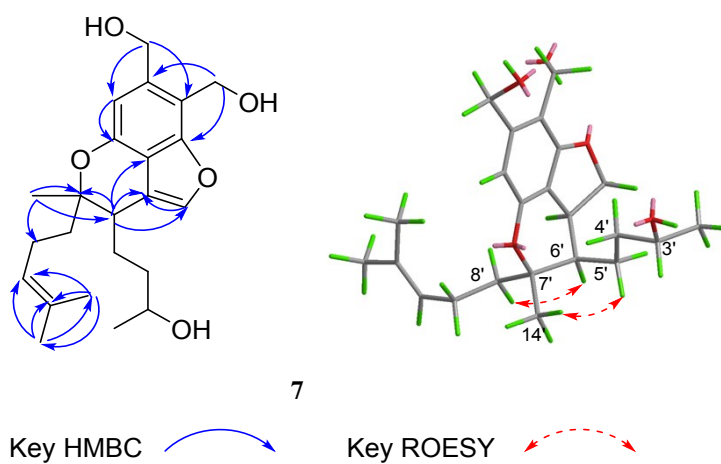


Figure S8. The key HMBC and ROESY correlations of stachybochartin G (7)

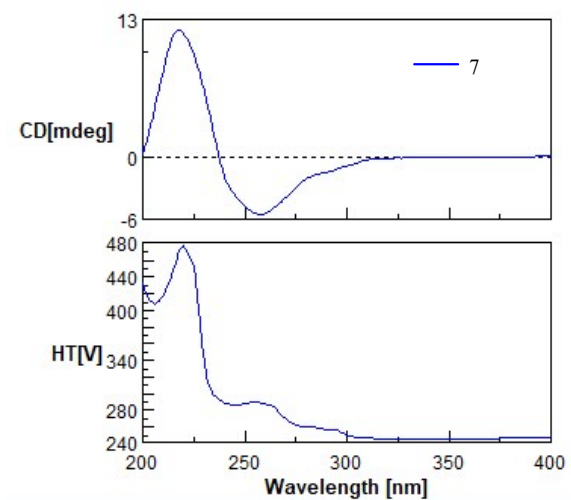


Figure S9. The experimental ECD spectra of stachybochartin G (7).

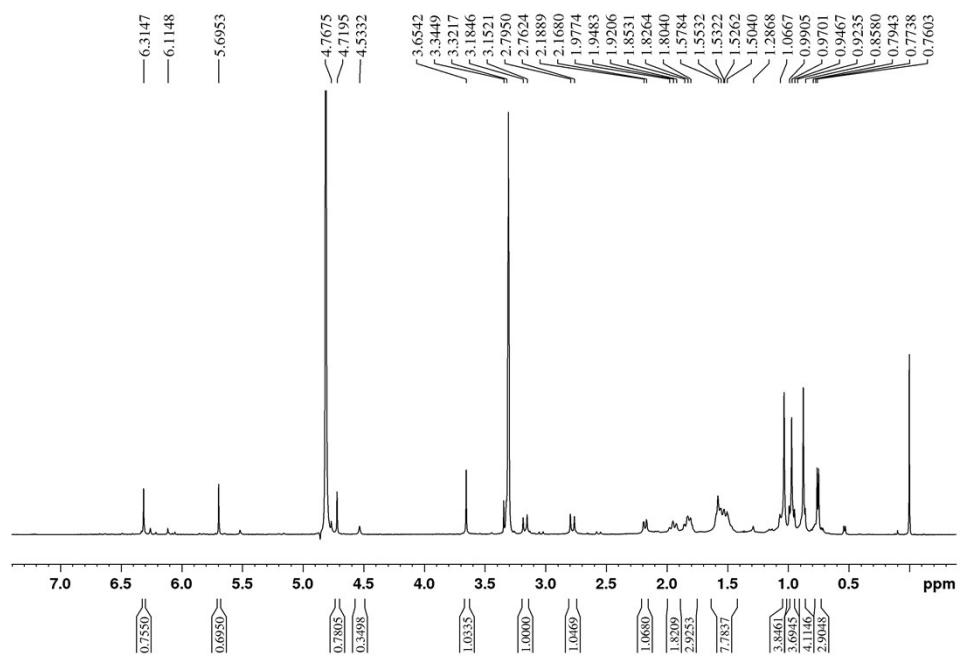


Figure S10. ^1H NMR spectrum of stachybochartin A (1) in CD_3OD .

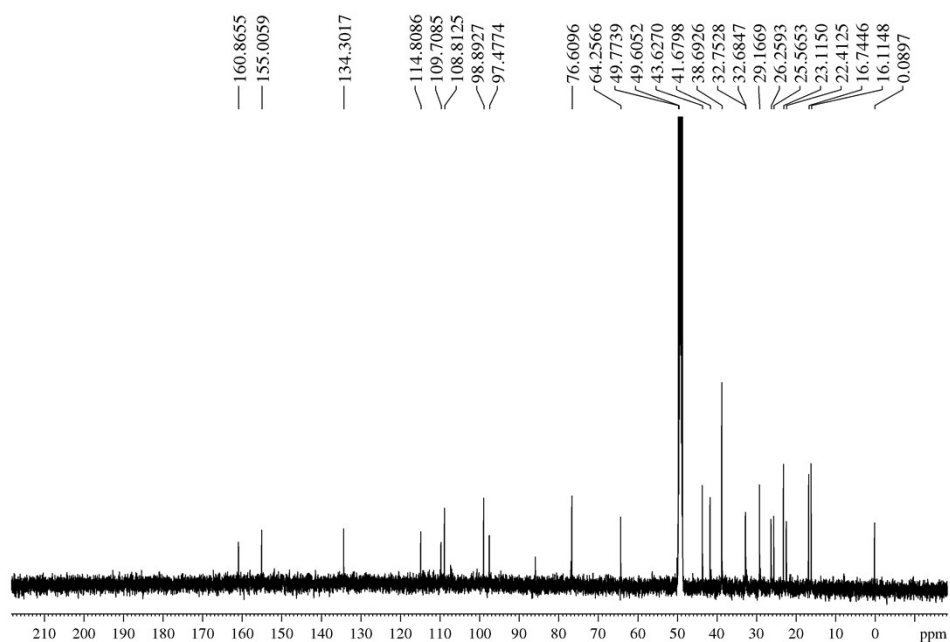


Figure S11. ^{13}C NMR spectrum of stachybochartin A (**1**) in CD_3OD .

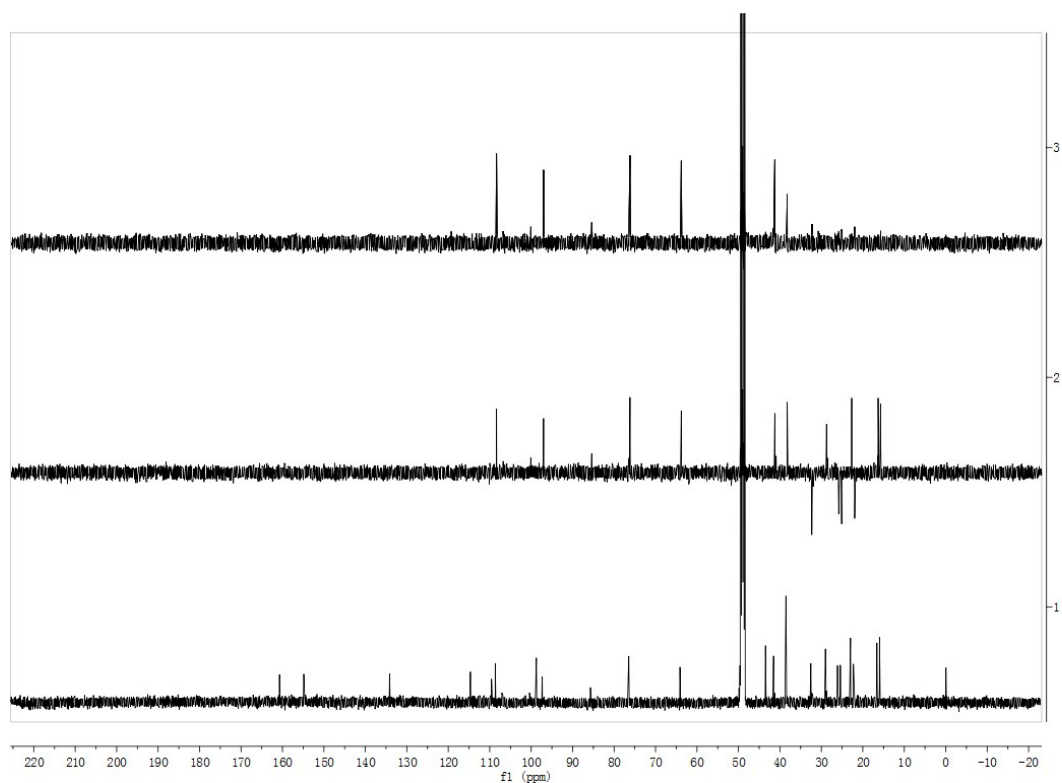


Figure S12. DEPT spectrum of stachybochartin A (**1**) in CD_3OD .

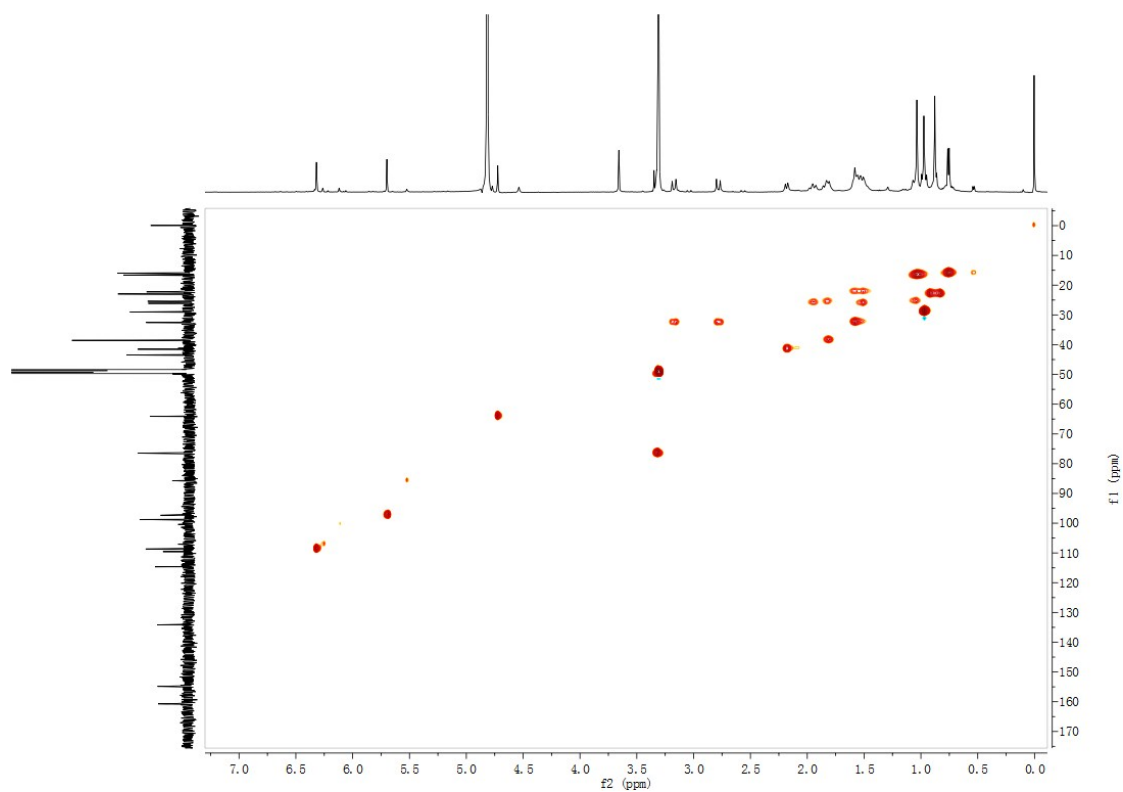


Figure S13. HSQC spectrum of stachybochartin A (**1**) in CD₃OD.

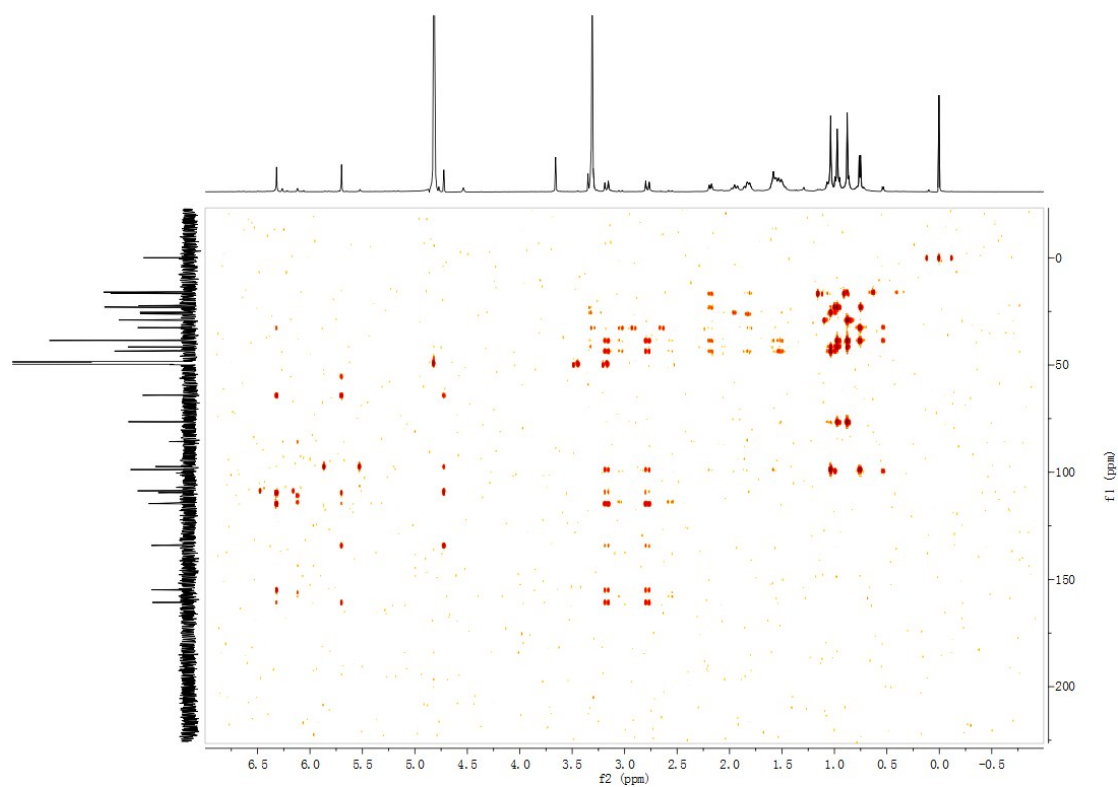


Figure S14. HMBC spectrum of stachybochartin A (**1**) in CD₃OD.

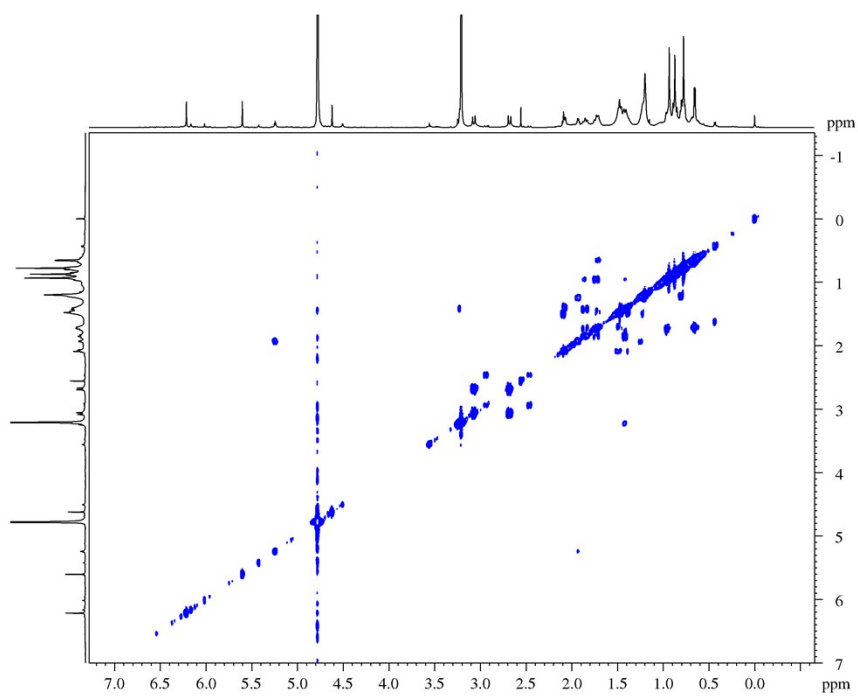


Figure S15. ^1H - ^1H COSY spectrum of stachybochartin A (**1**) in CD_3OD

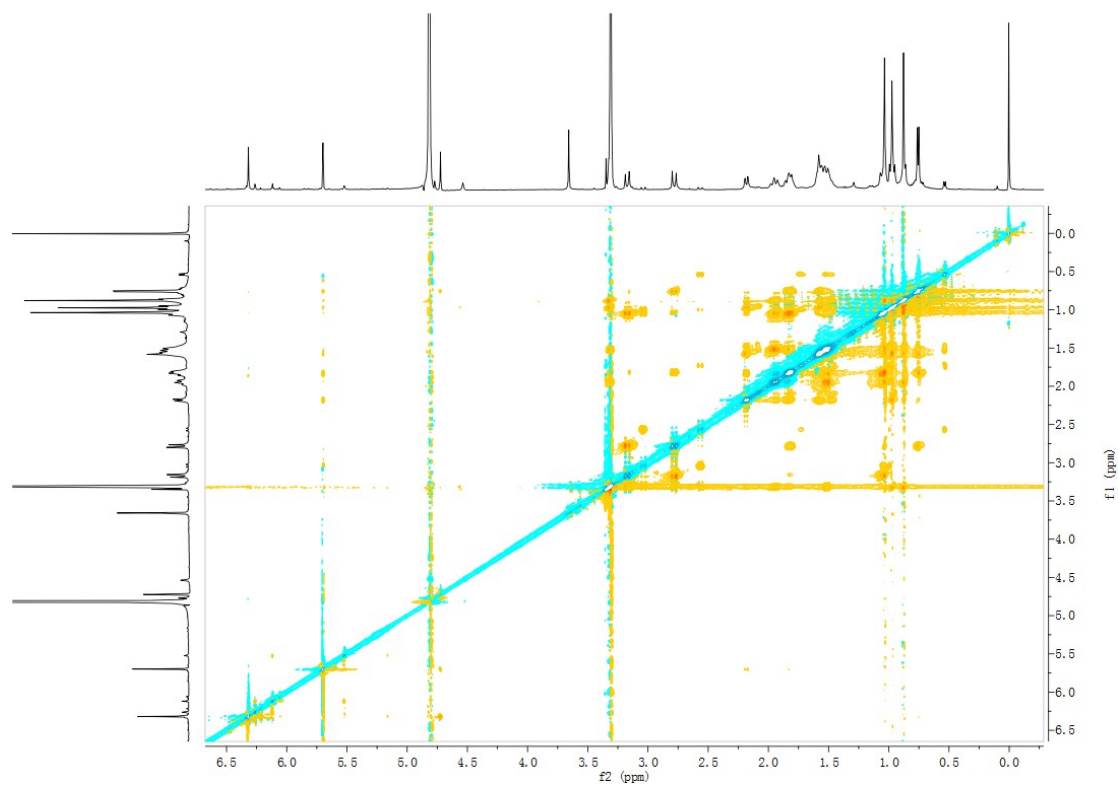
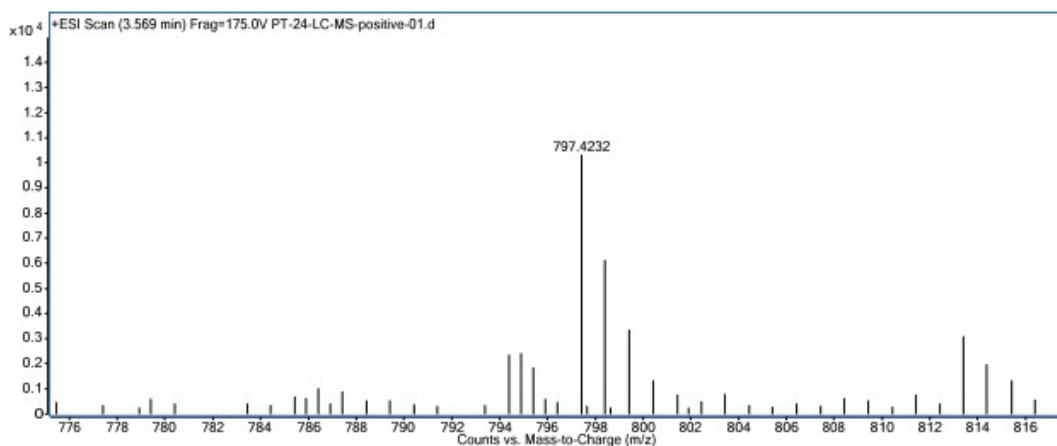


Figure S16. ROESY spectrum of stachybochartin A (**1**) in CD_3OD .



Elemental Composition Calculator

Target m/z:	797.4232	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₄₆ H ₆₂ NaO ₁₀	797.4235		0.37		



Figure S17. HRESIMS spectrum of stachybochartin A (1).

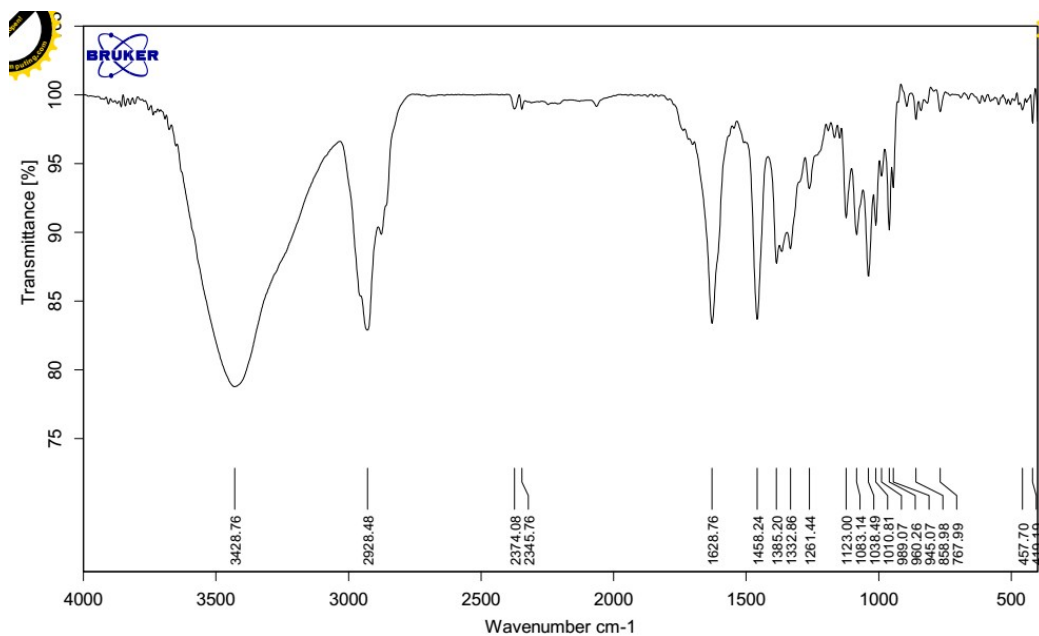


Figure S18. IR (KBr disc) spectrum of stachybochartin A (1)

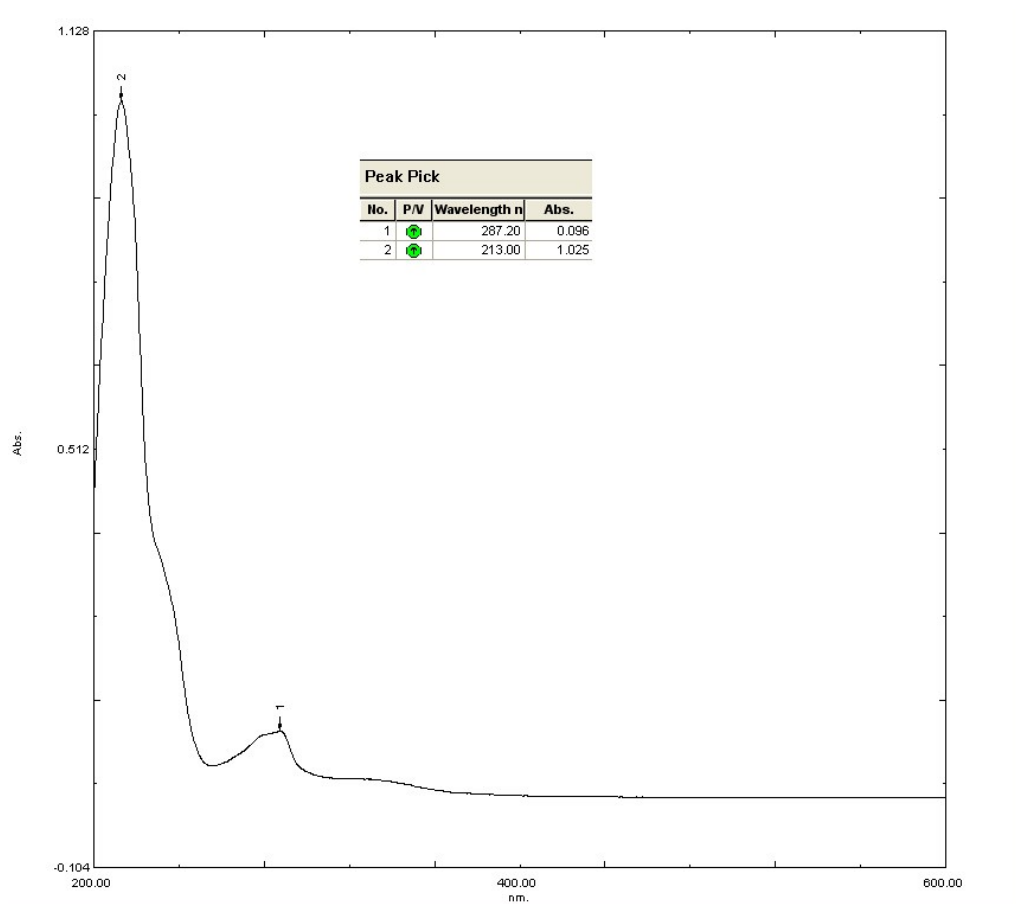


Figure S19. UV spectrum of stachybochartin A (1)

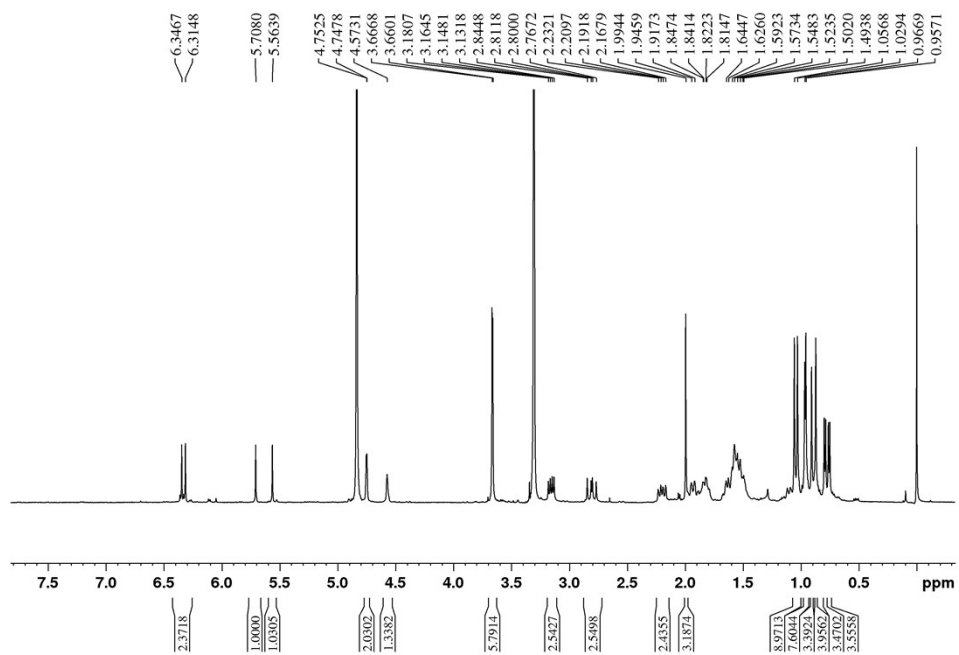


Figure S20. ^1H NMR spectrum of stachybochartin B (2) in CD_3OD .

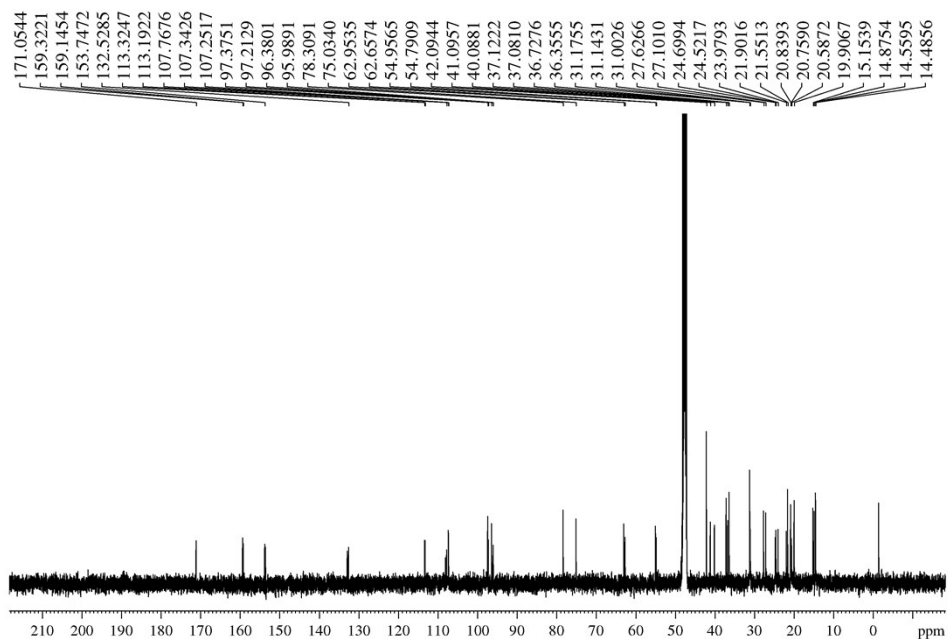


Figure S21. ^{13}C NMR spectrum of stachybochartin B (**2**) in CD_3OD .

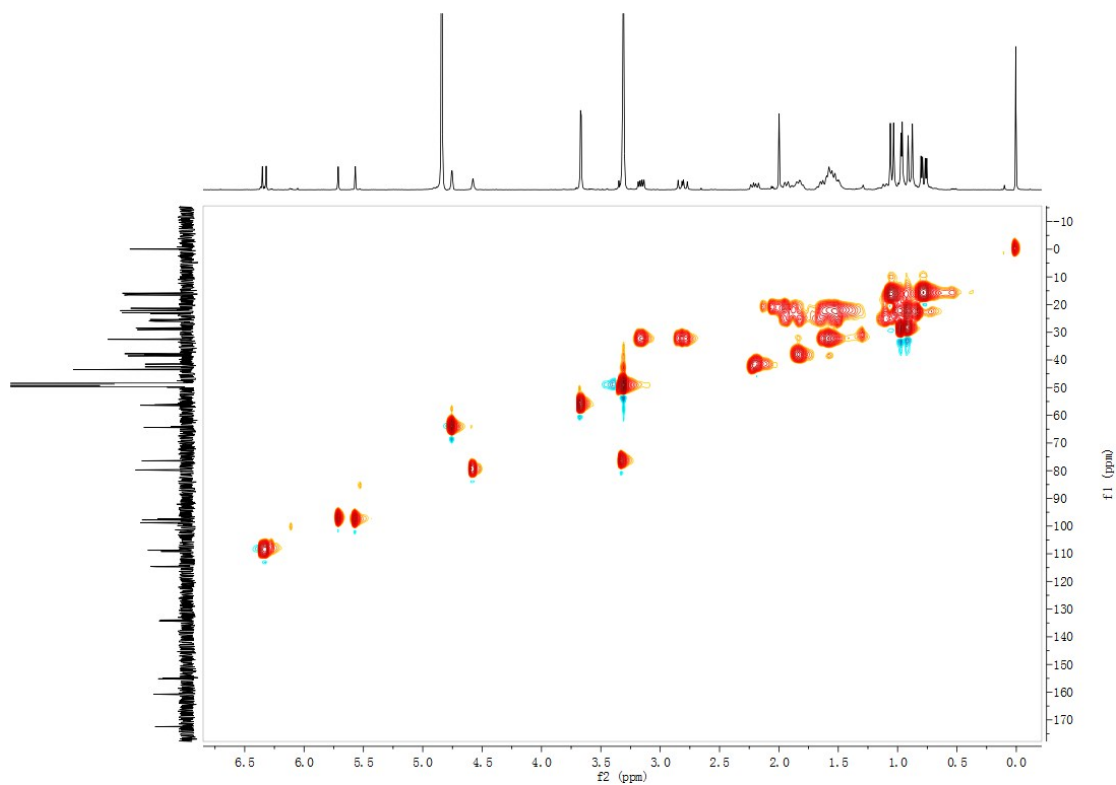


Figure S22. HSQC spectrum of stachybochartin B (**2**) in CD_3OD .

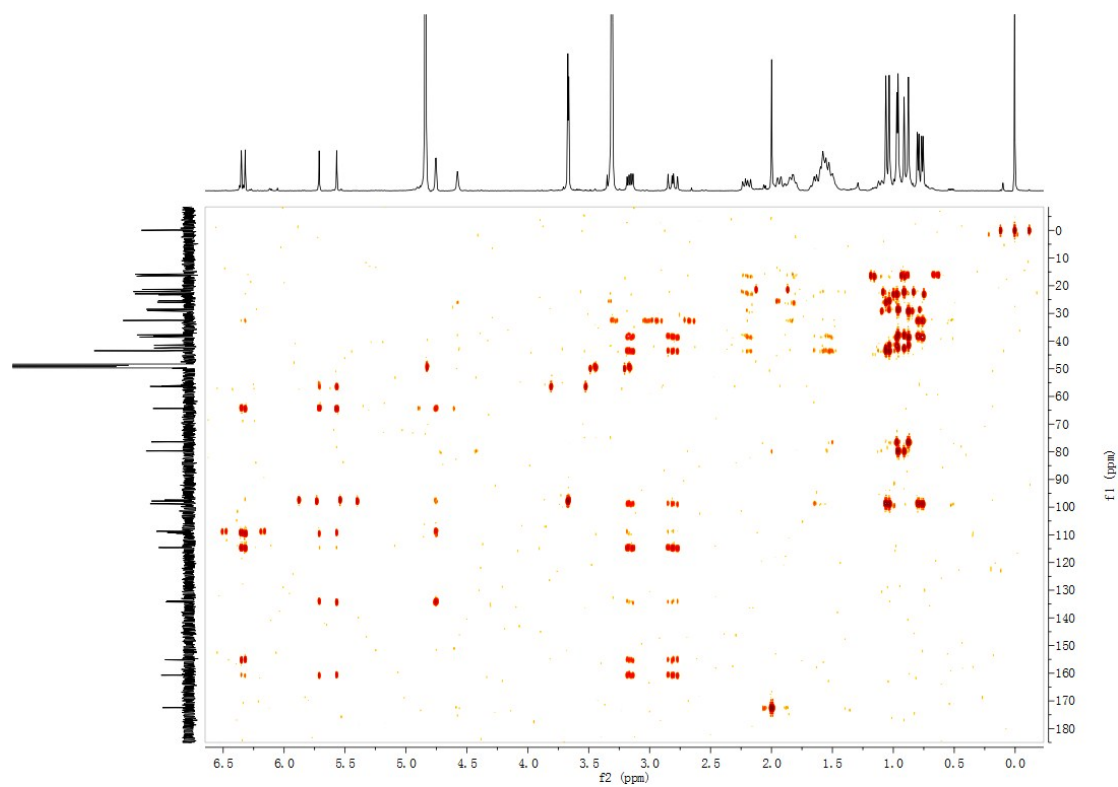


Figure S23. HMBC spectrum of stachybochartin B (**2**) in CD_3OD .

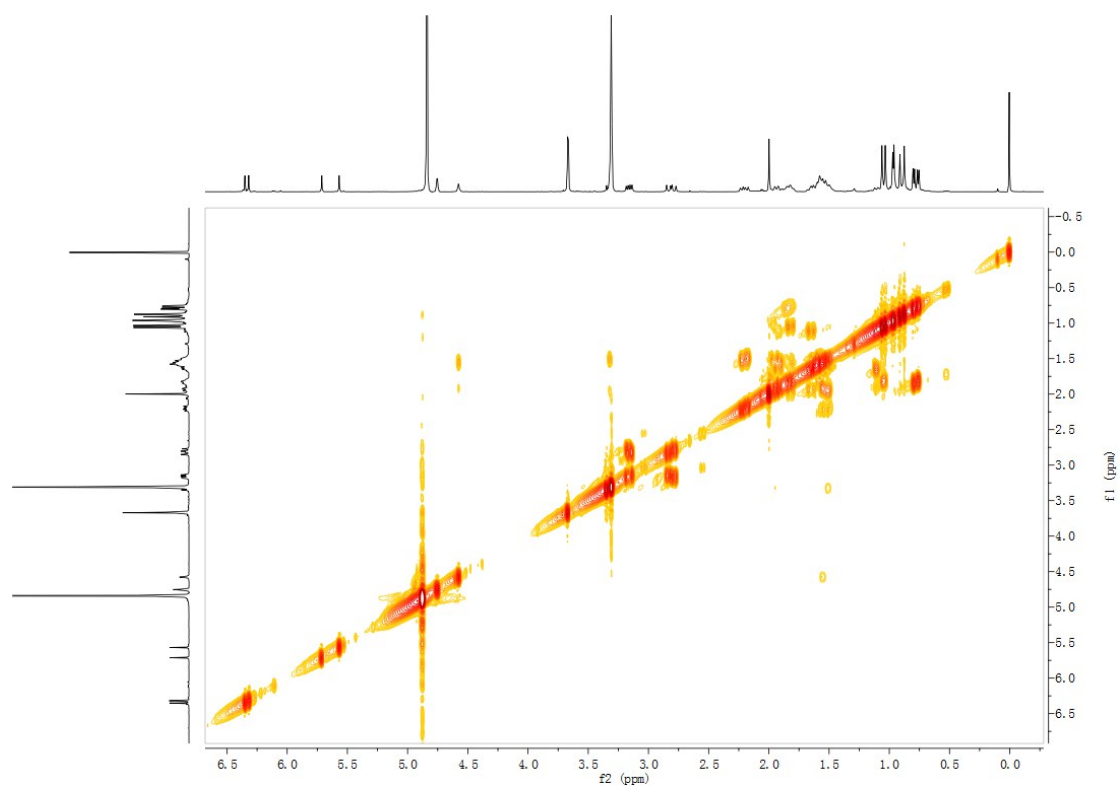


Figure S24. ^1H - ^1H COSY spectrum of stachybochartin B (**2**) in CD_3OD .

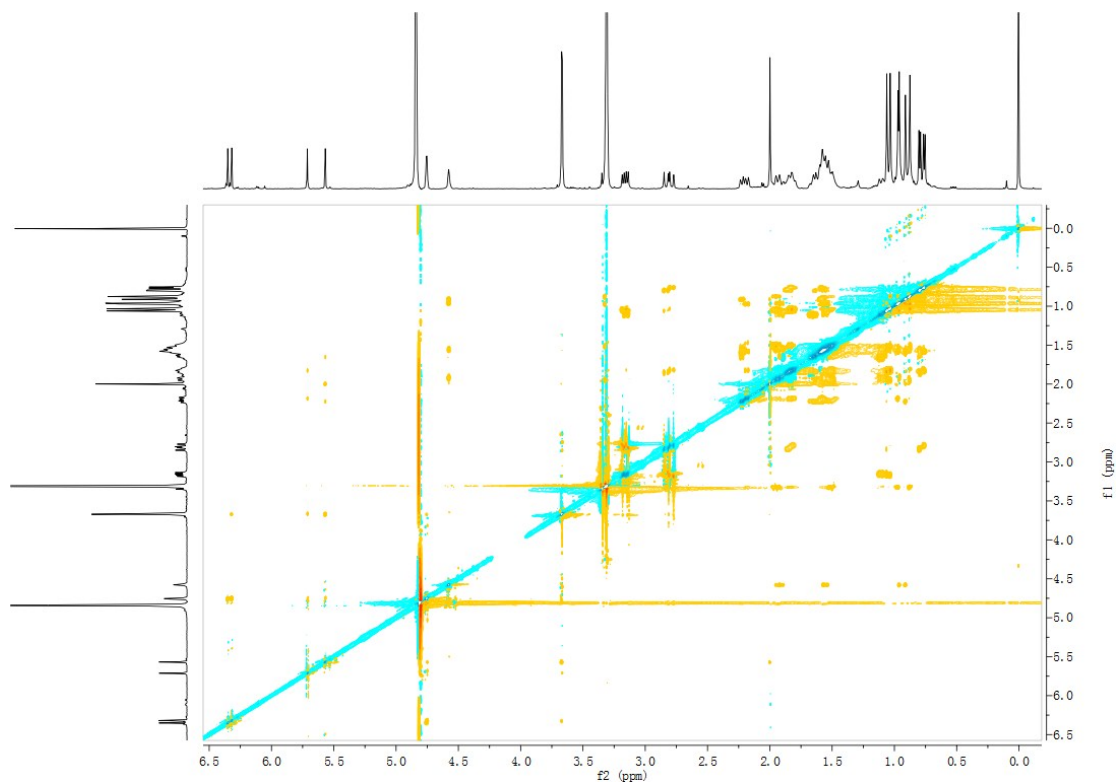
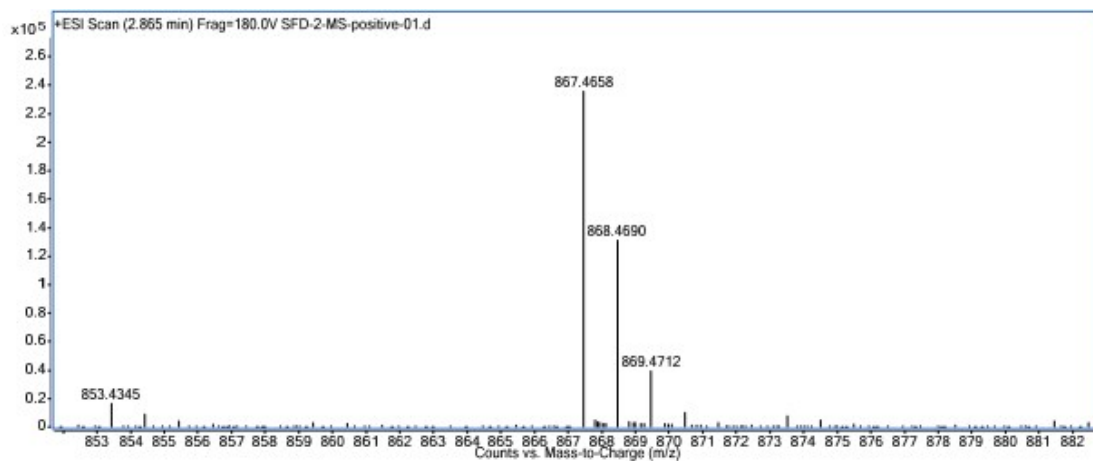


Figure S25. ROESY spectrum of stachybochartin B (**2**) in CD₃OD.



Elemental Composition Calculator

Target m/z:	867.4658	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C50H68NaO11	867.4654		-0.4		



Figure S26. HRESIMS spectrum of stachybochartin B (**2**).

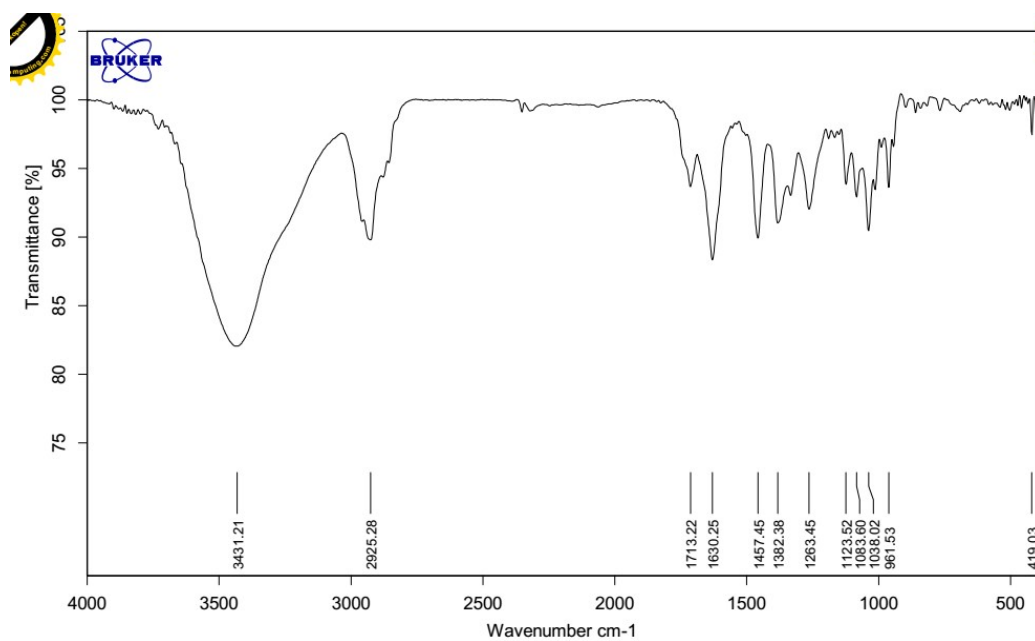


Figure S27. IR (KBr disc) spectrum of stachybochartin B (2).

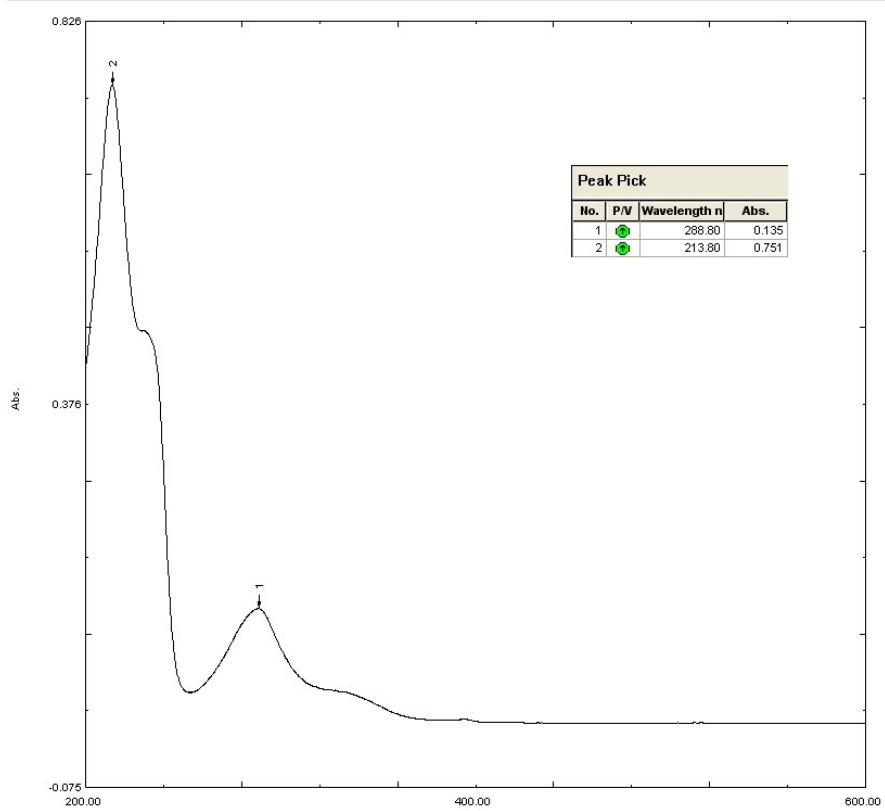


Figure S28. UV spectrum of stachybochartin B (2).

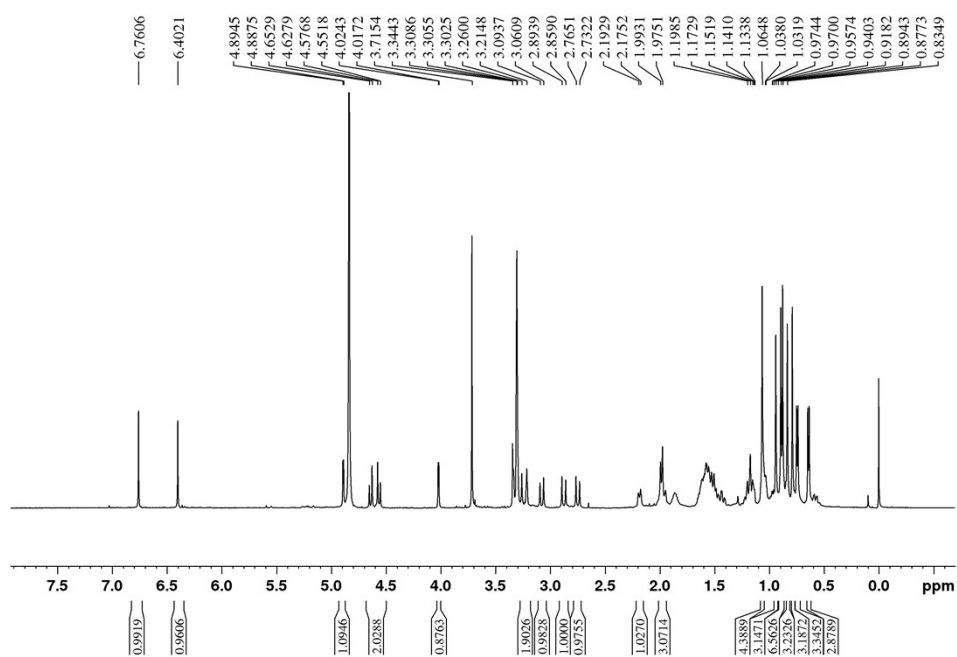


Figure S29. ^1H NMR spectrum of stachybochartin C (**3**) in CD_3OD .

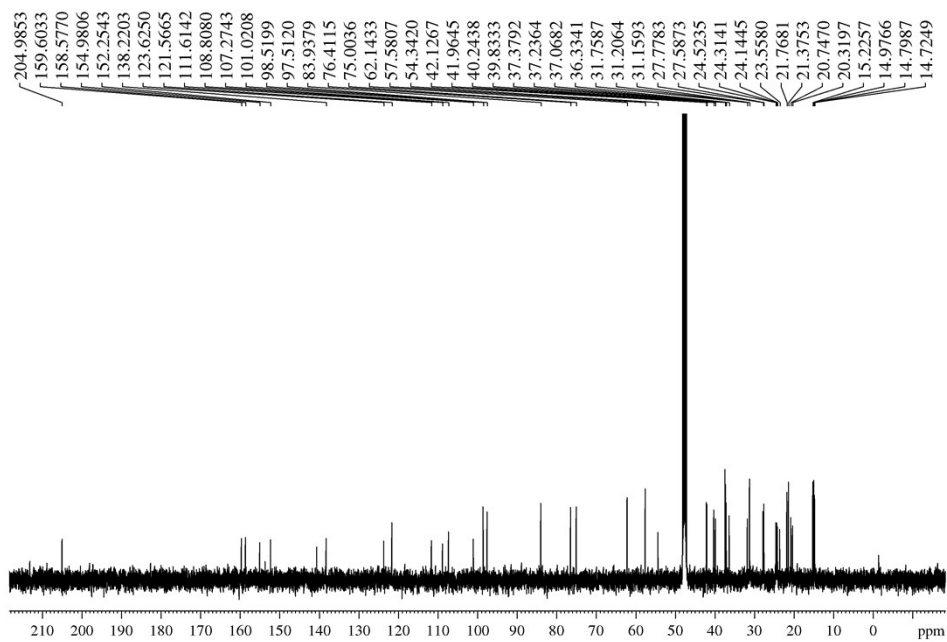


Figure S30. ^{13}C NMR spectrum of stachybochartin C (**3**) in CD_3OD .

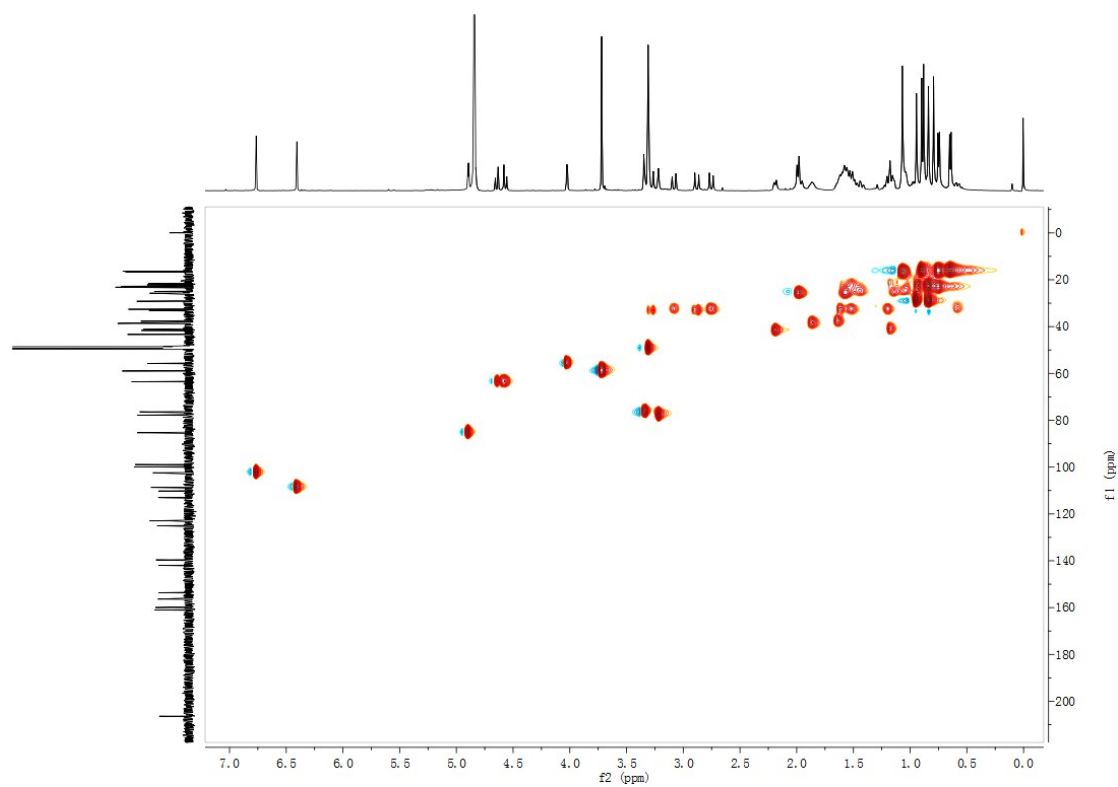


Figure S31. HSQC spectrum of stachybochartin C (**3**) in CD₃OD.

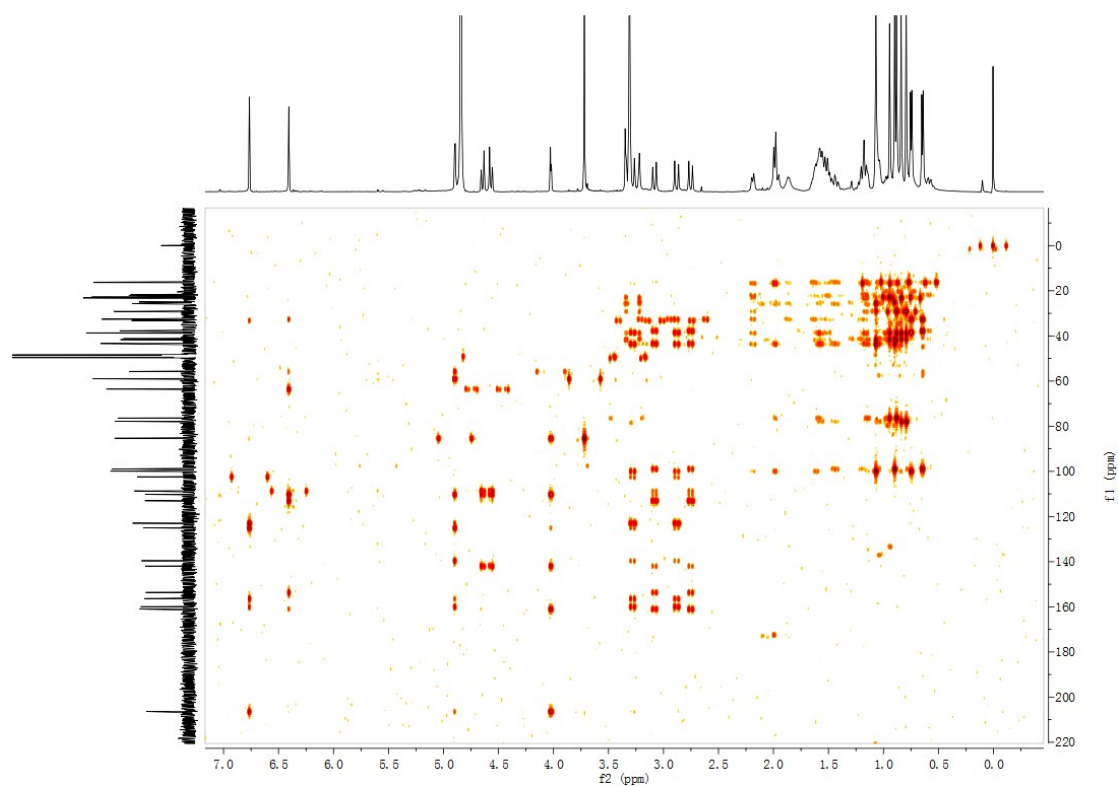


Figure S32. HMBC spectrum of stachybochartin C (**3**) in CD₃OD.

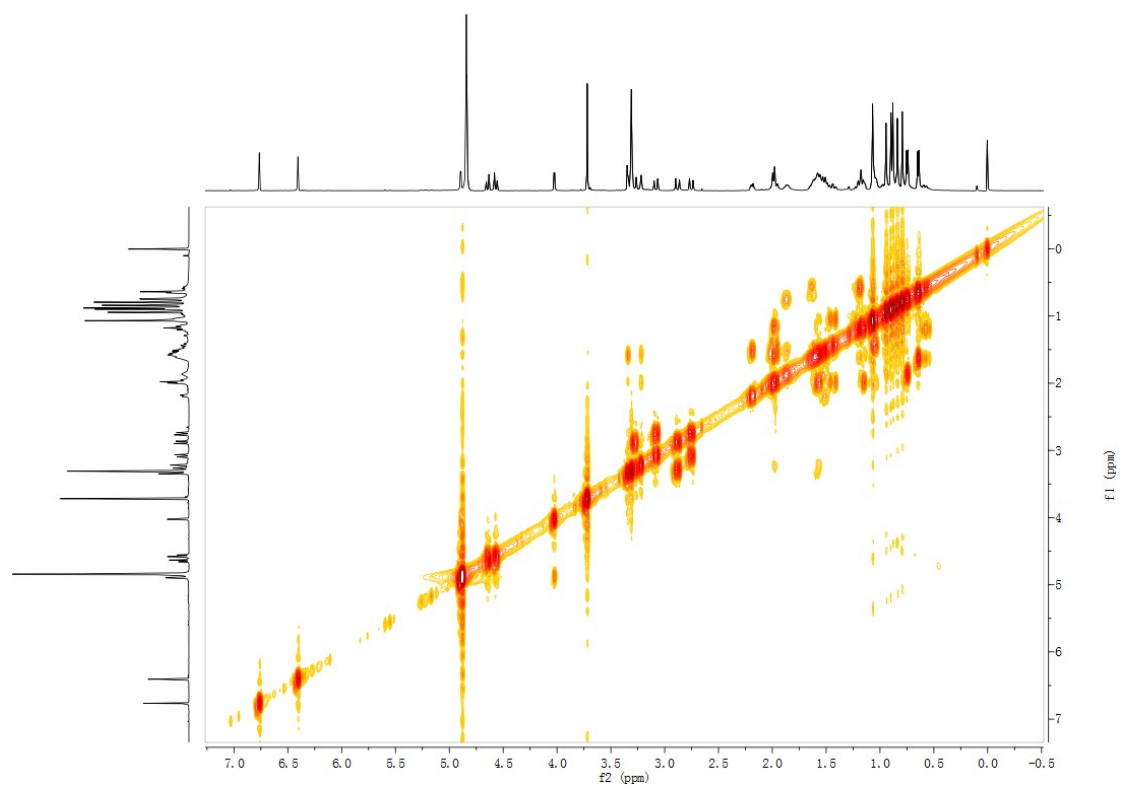


Figure S33. ^1H - ^1H COSY spectrum of stachybochartin C (**3**) in CD_3OD .

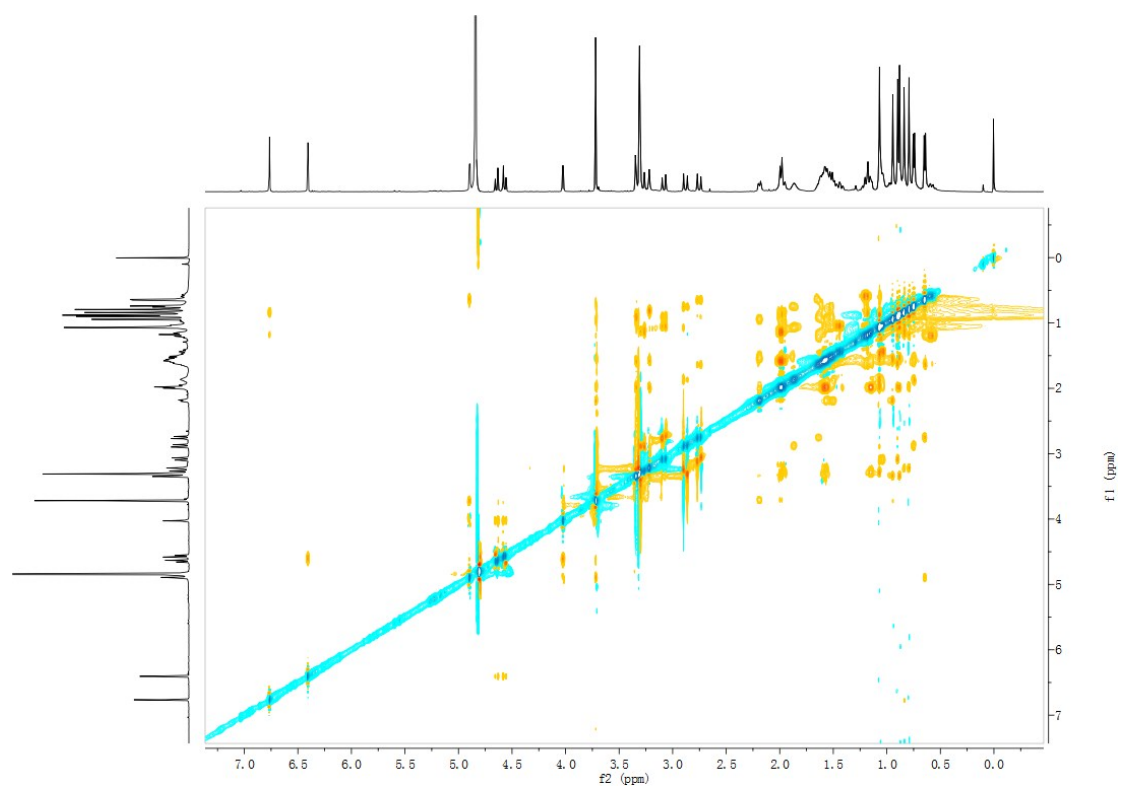
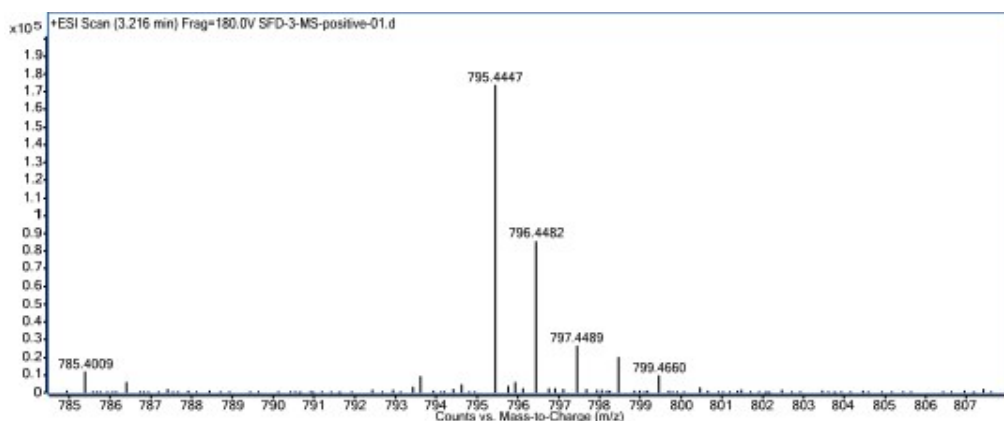


Figure S34. ROESY spectrum of stachybochartin C (**3**) in CD_3OD .



Elemental Composition Calculator

Target m/z:	795.4447	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z	PPM Error			
C ₄₇ H ₆₄ NaO ₉	795.4443	-0.4			



Figure S35. HRESIMS spectrum of stachybochartin C (3).

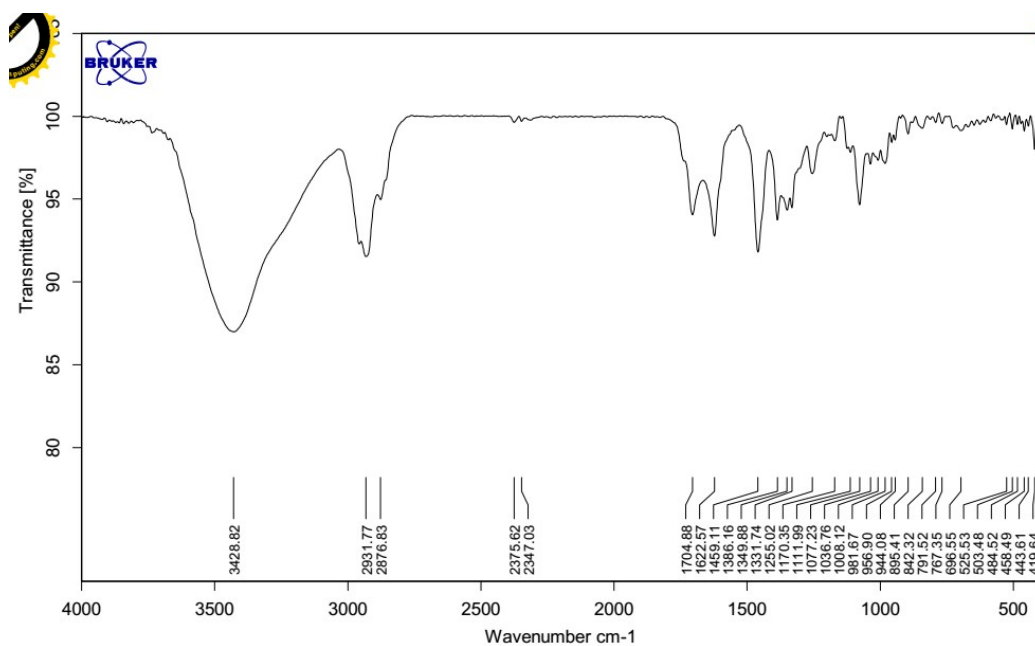


Figure S36. IR (KBr disc) spectrum of stachybochartin C (3).

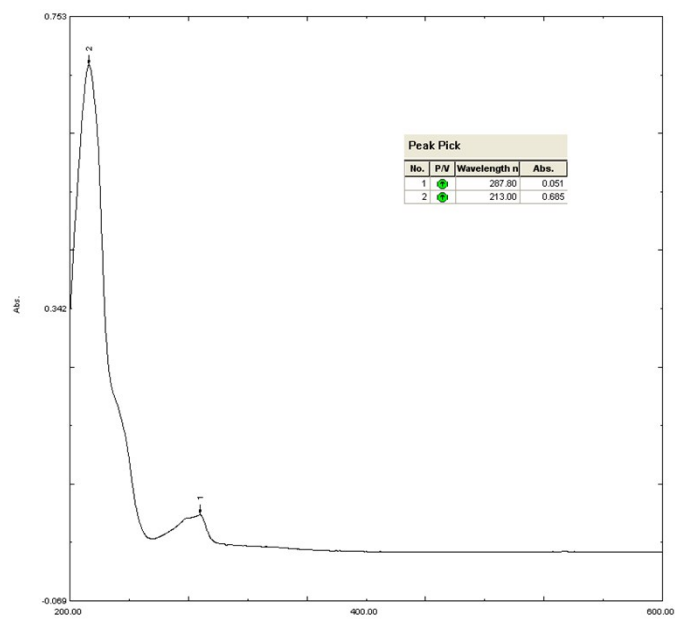


Figure S37. UV spectrum of stachybochartin C (3).

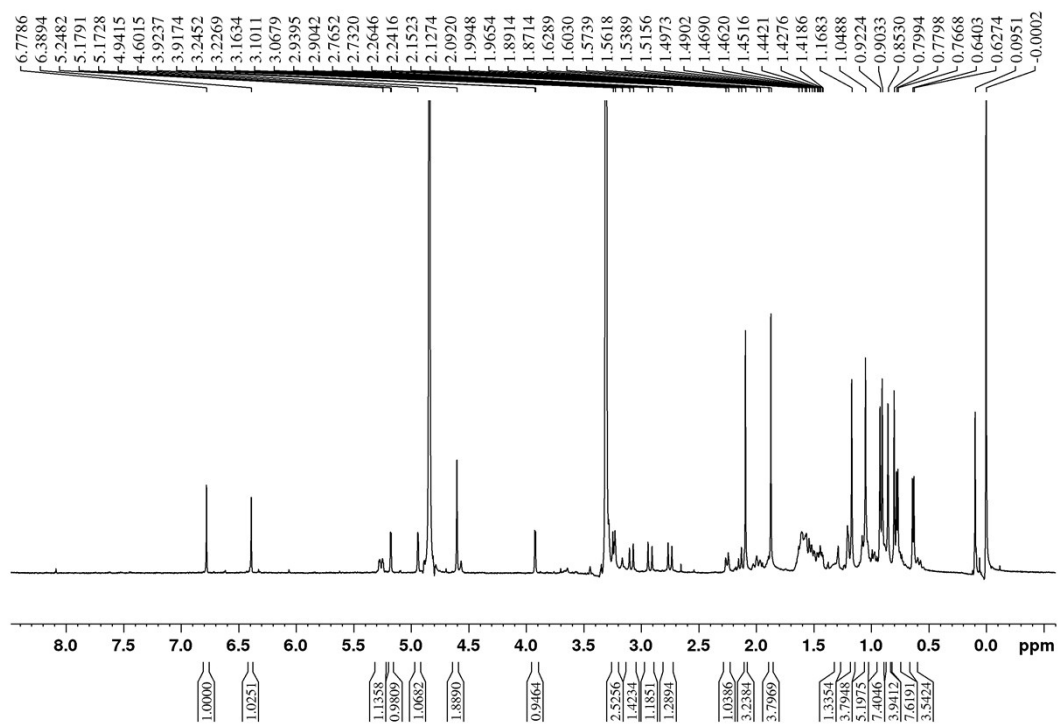


Figure S38. ¹H NMR spectrum of stachybochartin D (4) in CD₃OD.

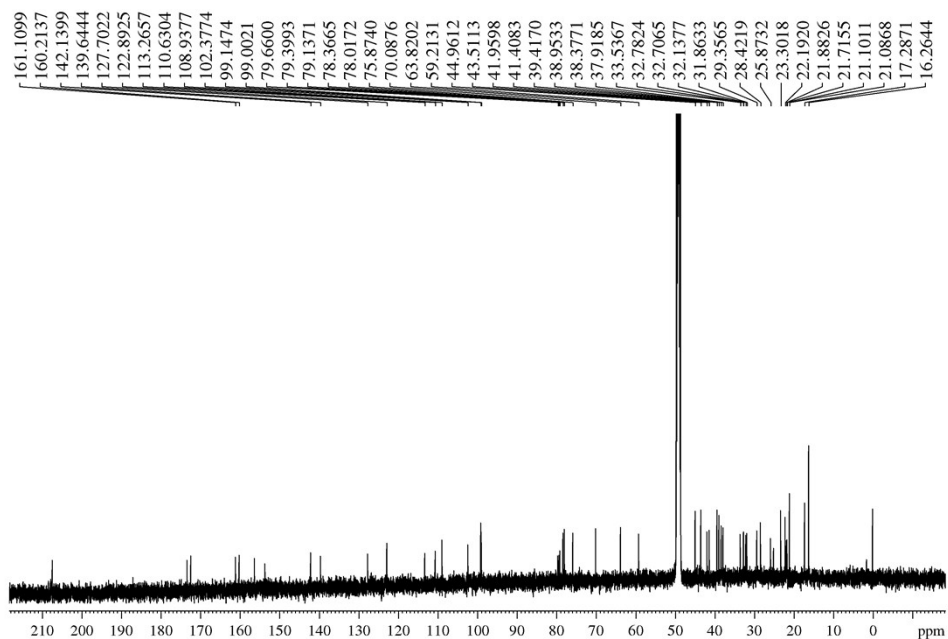


Figure S39. ^{13}C NMR spectrum of stachybochartin D (4) in CD_3OD .

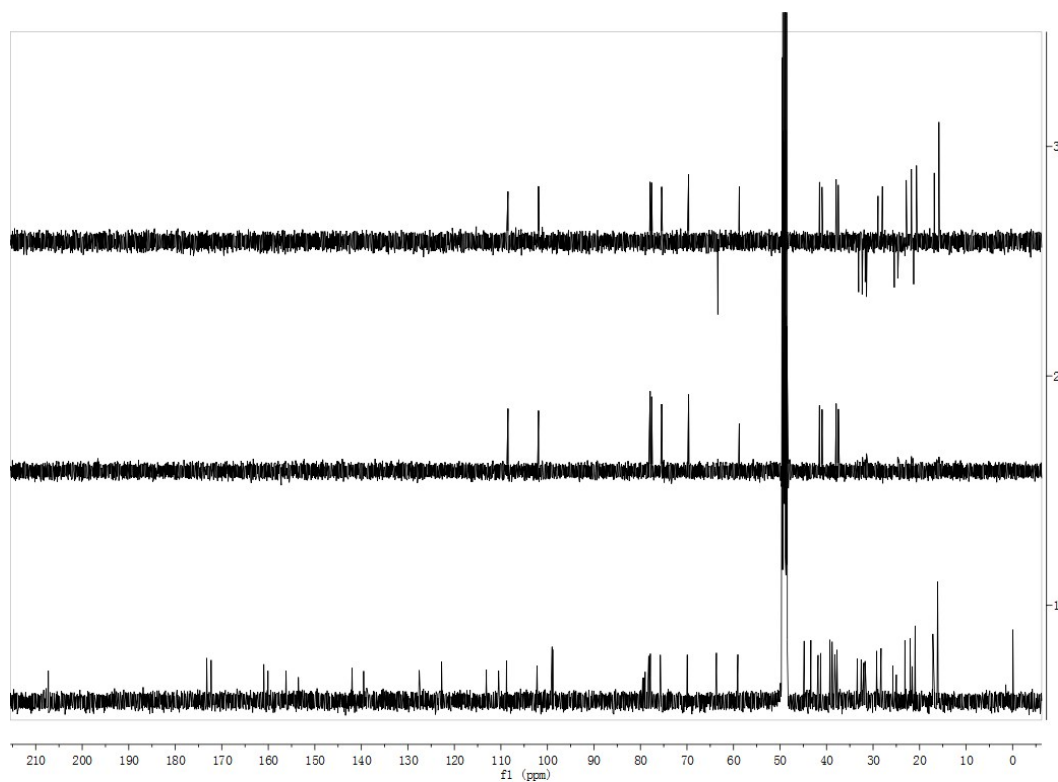


Figure S40. DEPT spectrum of stachybochartin D (4) in CD_3OD .

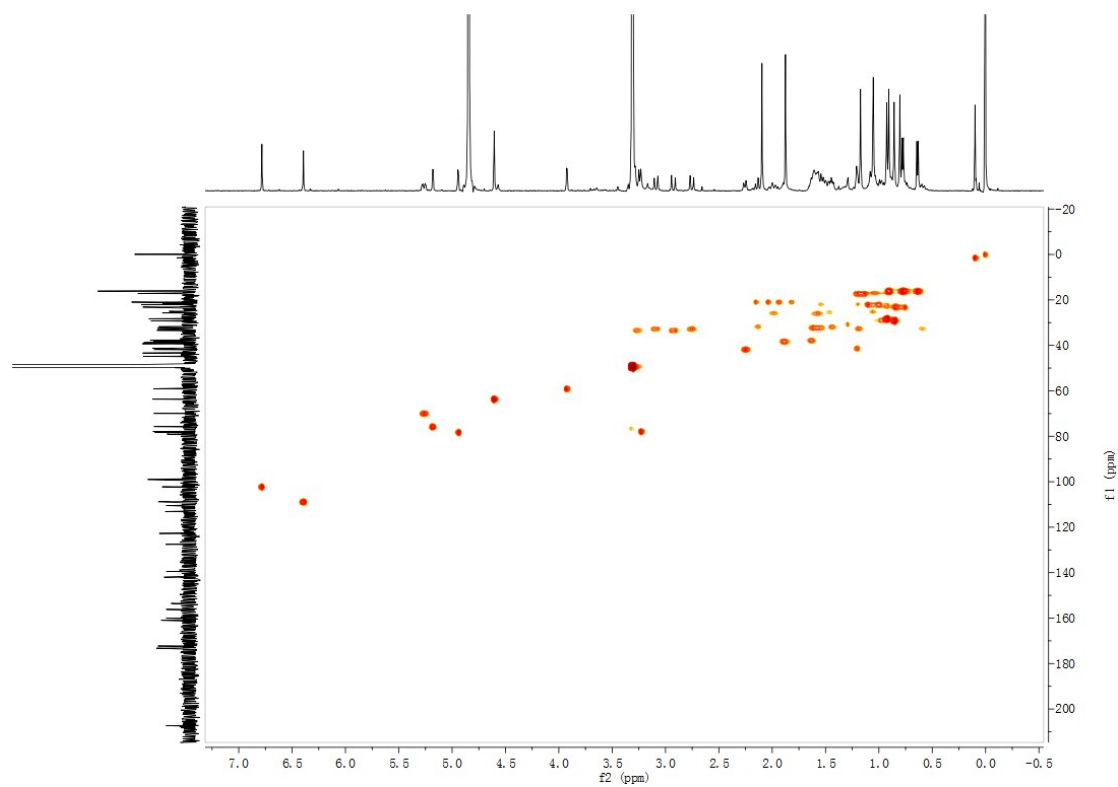


Figure S41. HSQC spectrum of stachybochartin D (4) in CD₃OD.

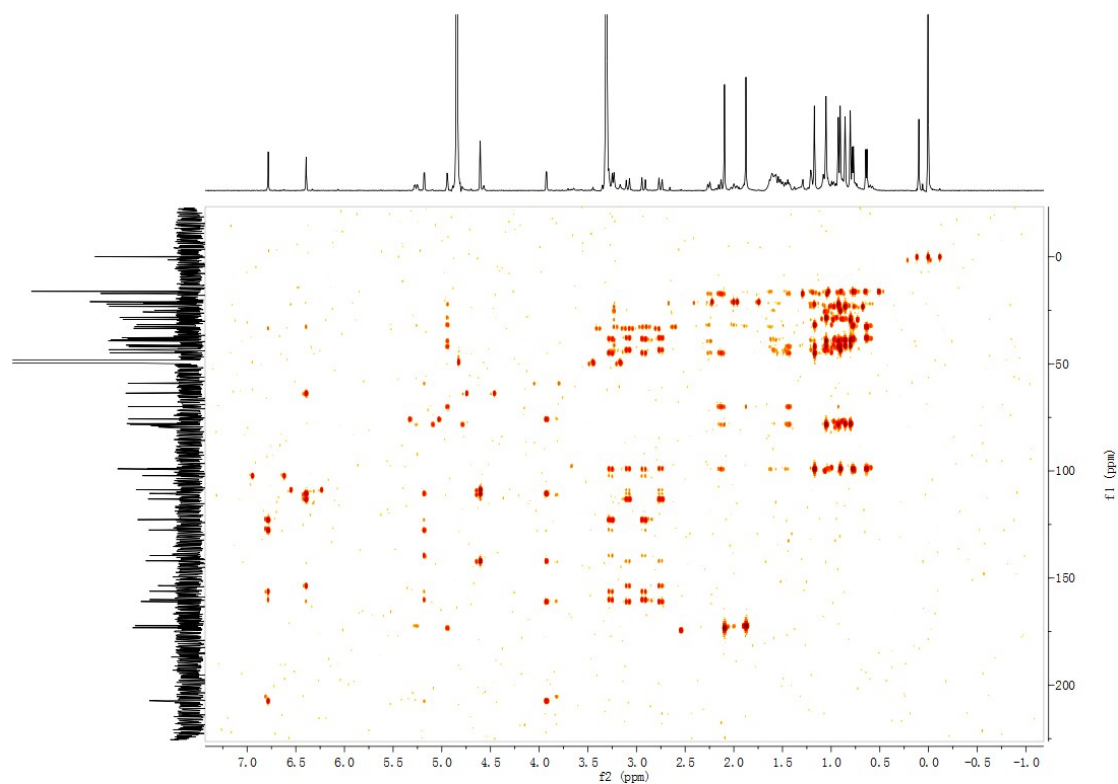


Figure S42. HMBC spectrum of stachybochartin D (4) in CD₃OD.

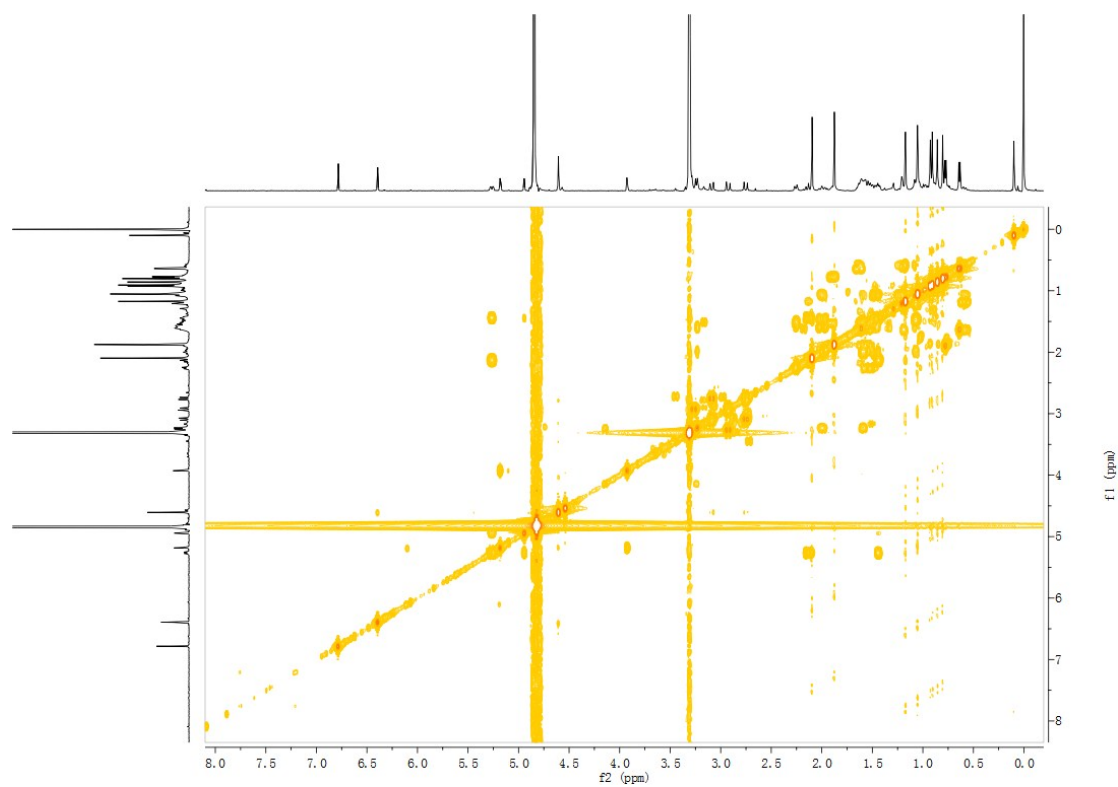


Figure S43. ^1H - ^1H COSY spectrum of stachybochartin D (**4**) in CD_3OD .

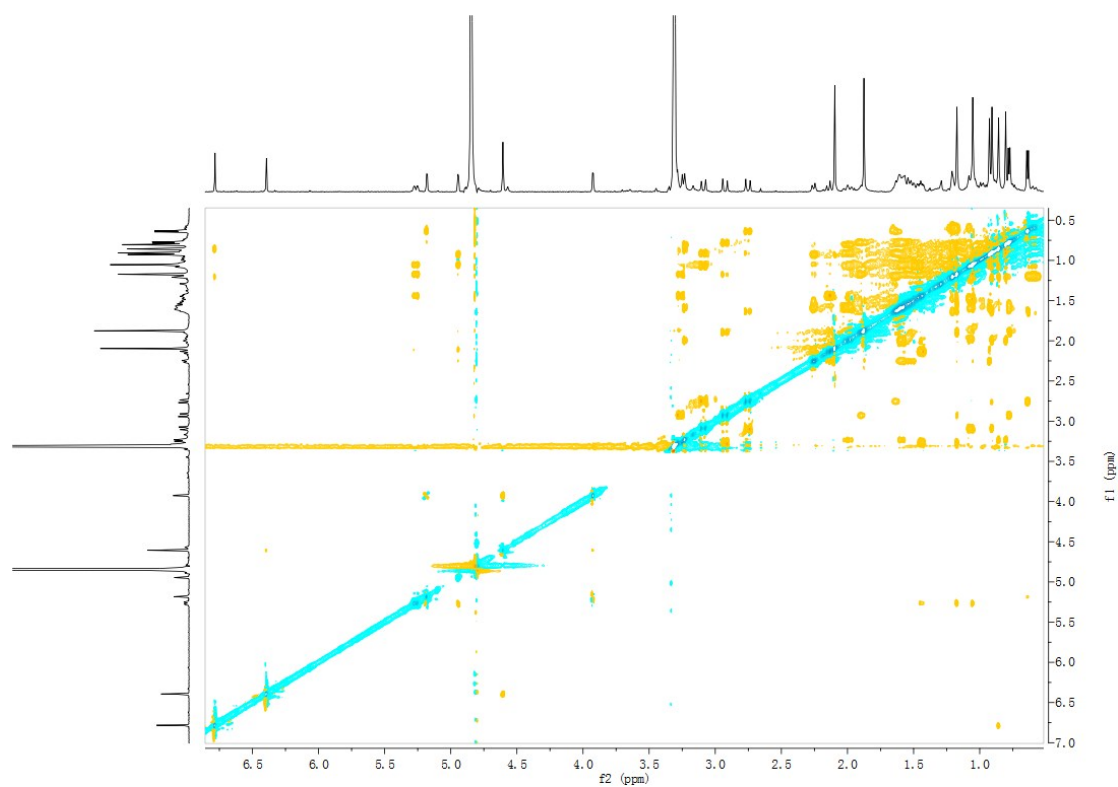
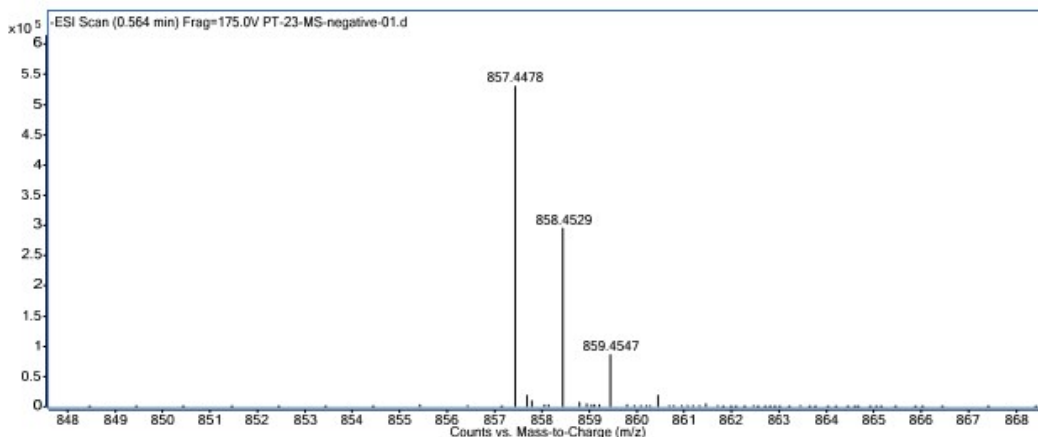


Figure S44. ROESY spectrum of stachybochartin D (**4**) in CD_3OD .



Elemental Composition Calculator

Target m/z:	857.4478	Result type:	Negative ions	Species:	[M-H] ⁻
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Cl (0-5)				
Ion Formula	Calculated m/z	PPM Error			
C ₅₀ H ₆₅ O ₁₂	857.4482	0.38			



Figure S45. HRESIMS spectrum of stachybochartin D (4).

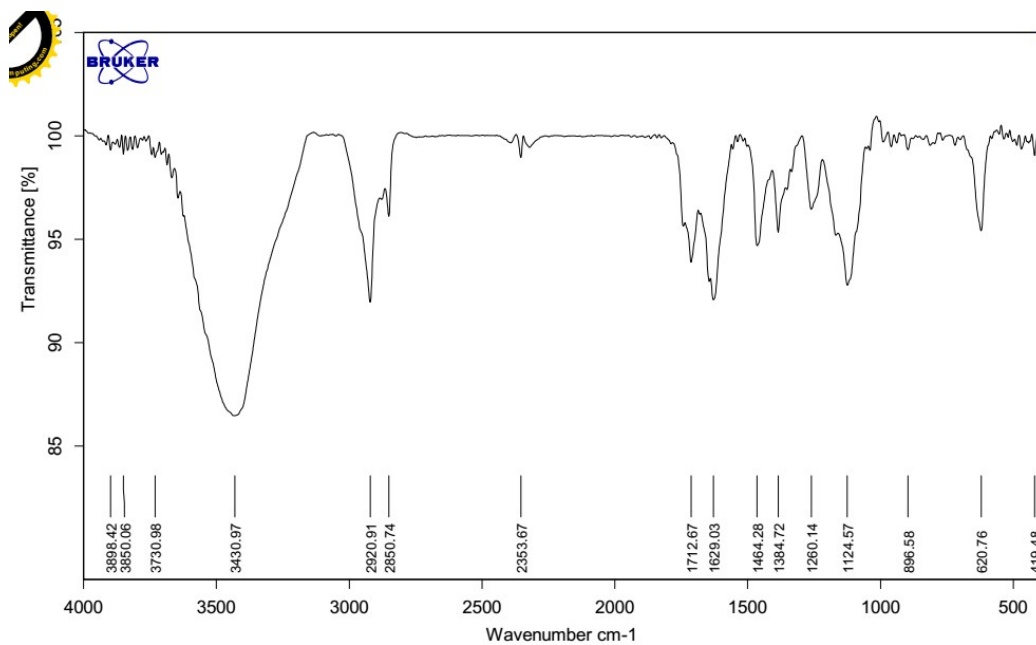


Figure S46. IR (KBr disc) spectrum of stachybochartin D (4).

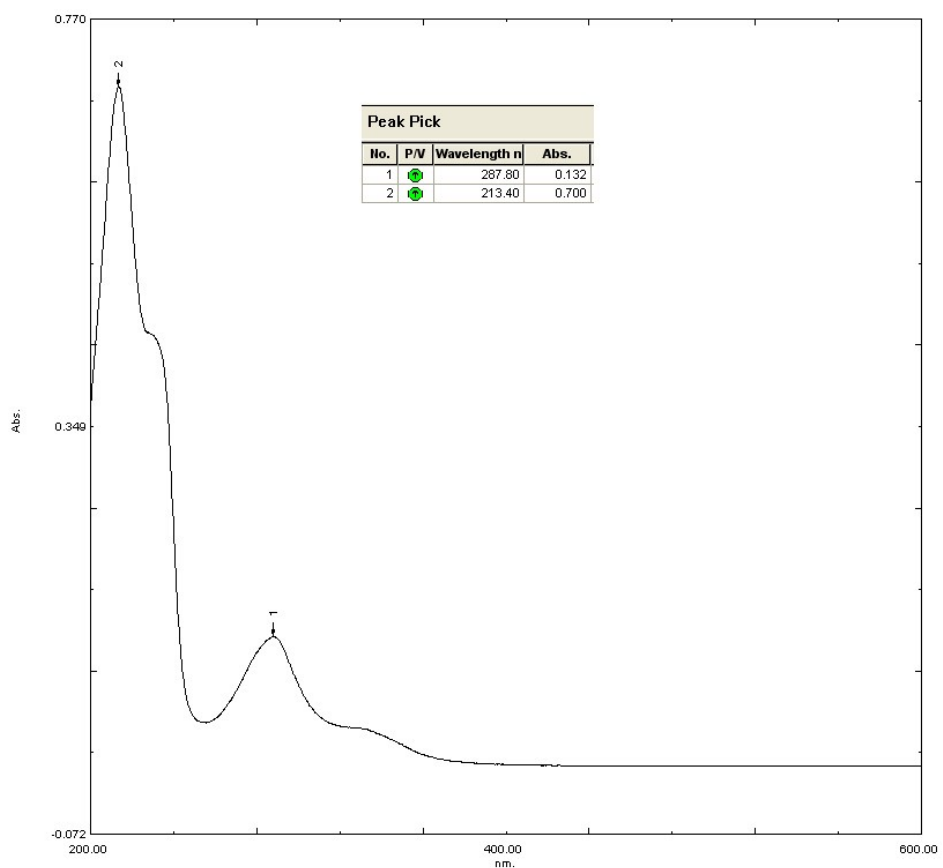


Figure S47. UV spectrum of stachybochartin D (4).

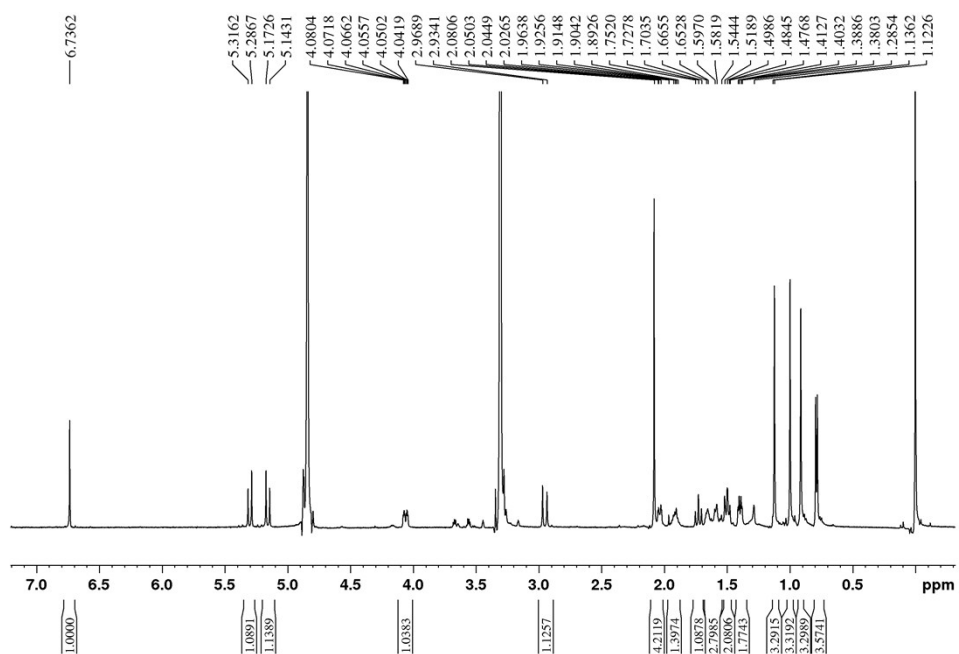


Figure S48. ¹H-NMR spectrum (500 MHz) of stachybochartin E (5) in CD₃OD.

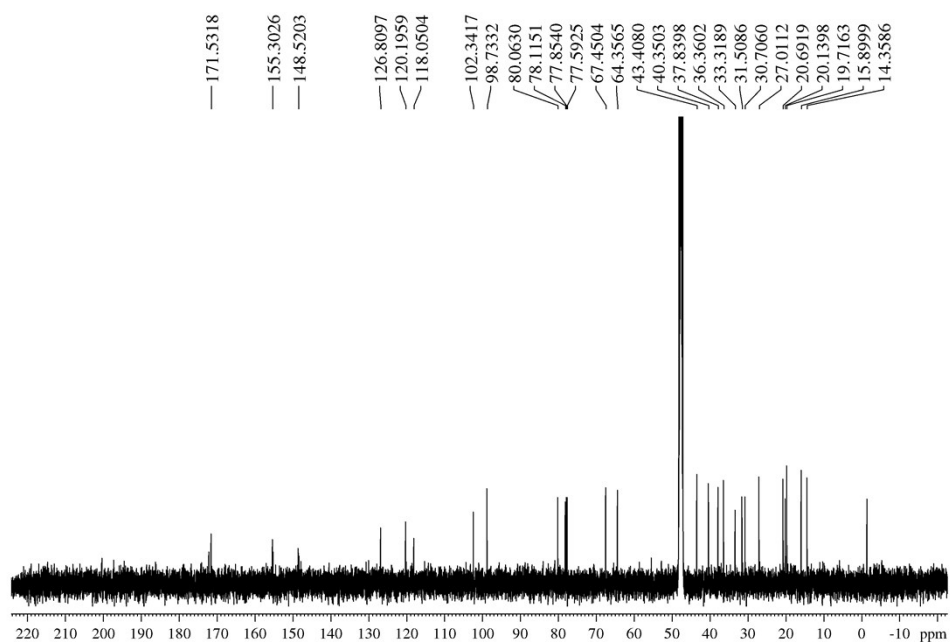


Figure S49. ^{13}C -NMR spectrum (125 MHz) of stachybochartin E (**5**) in CD_3OD .

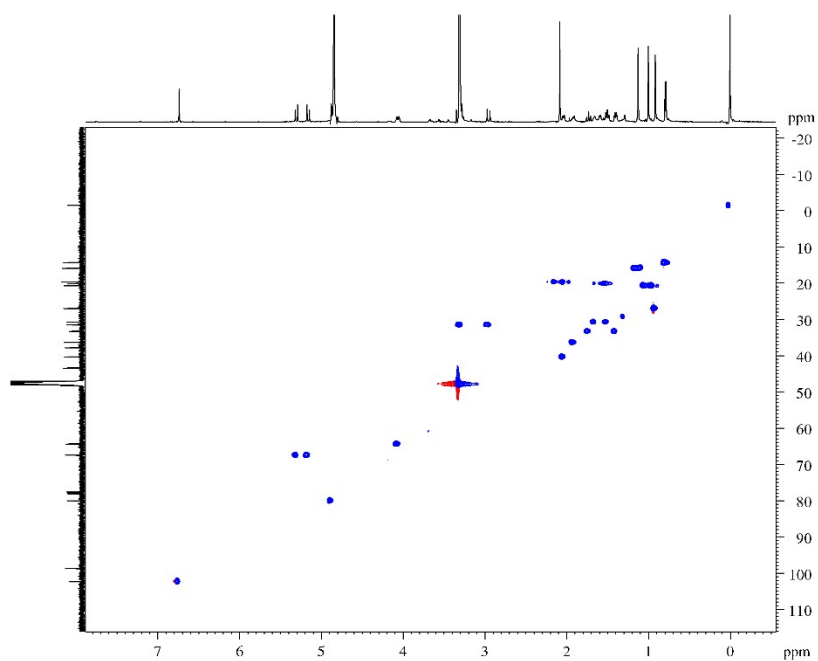


Figure S50. HSQC spectrum of stachybochartin E (**5**) in CD_3OD

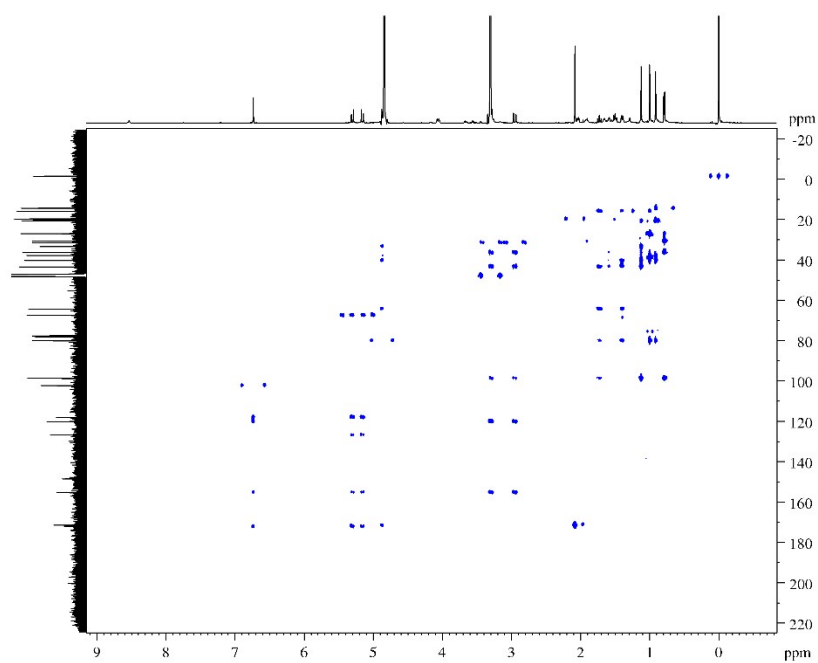


Figure S51. HMBC spectrum of stachybochartin E (**5**) in CD₃OD

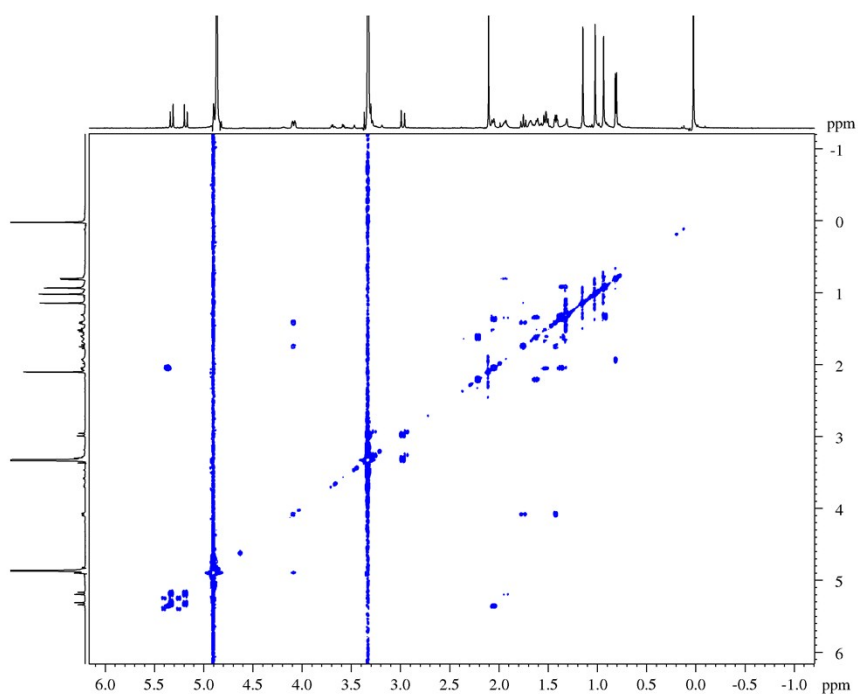


Figure S52. ¹H-¹H COSY spectrum of stachybochartin E (**5**) in CD₃OD.

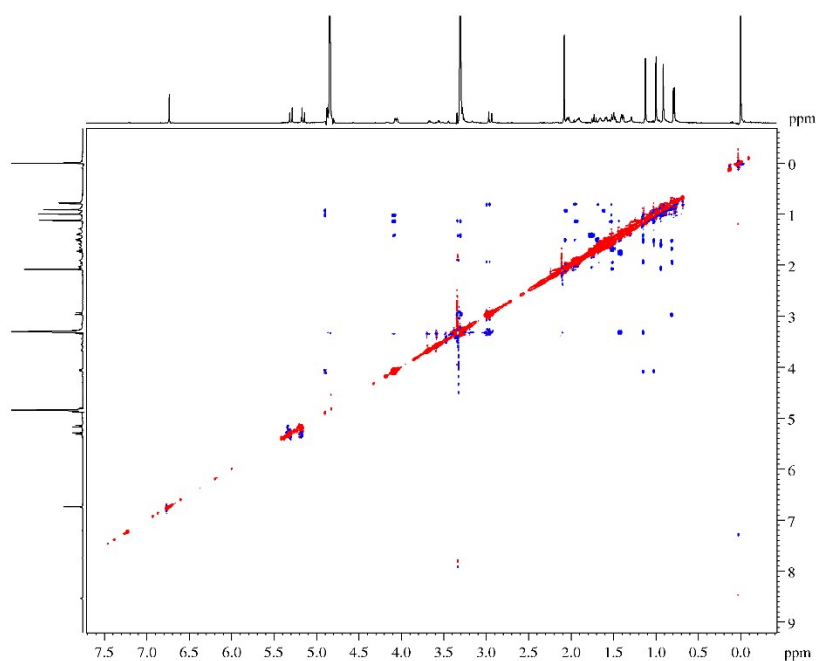
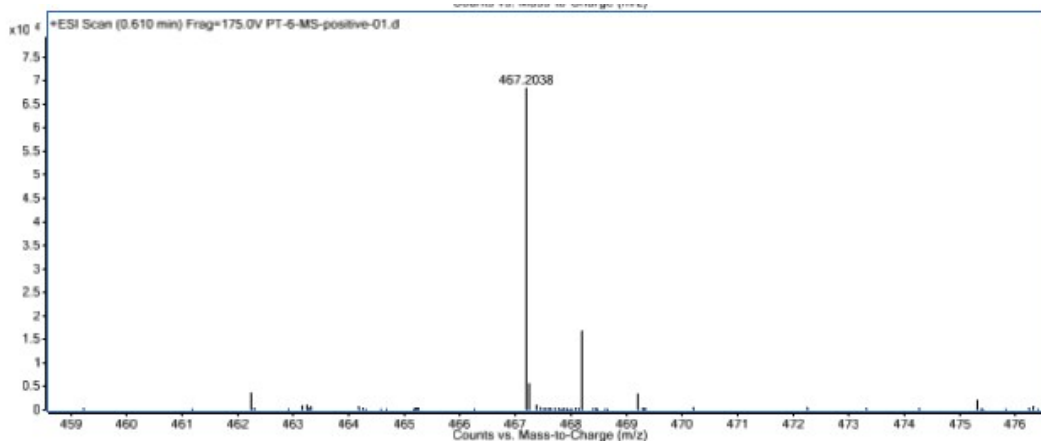


Figure S53. ROESY spectrum of stachybochartin E (5) in CD₃OD



Elemental Composition Calculator

Target m/z:	467.2038	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₅ H ₃₂ NaO ₇	467.2040		0.55		



Figure S54. HRESIMS spectrum of stachybochartin E (5).

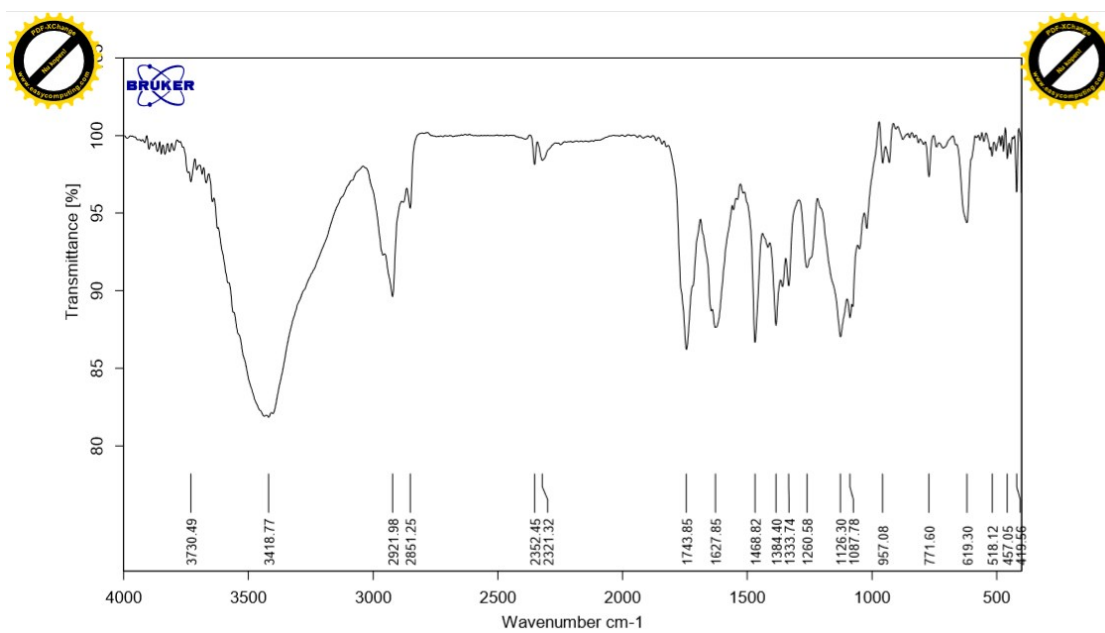


Figure S55. IR (KBr disc) spectrum of stachybochartin E (5).

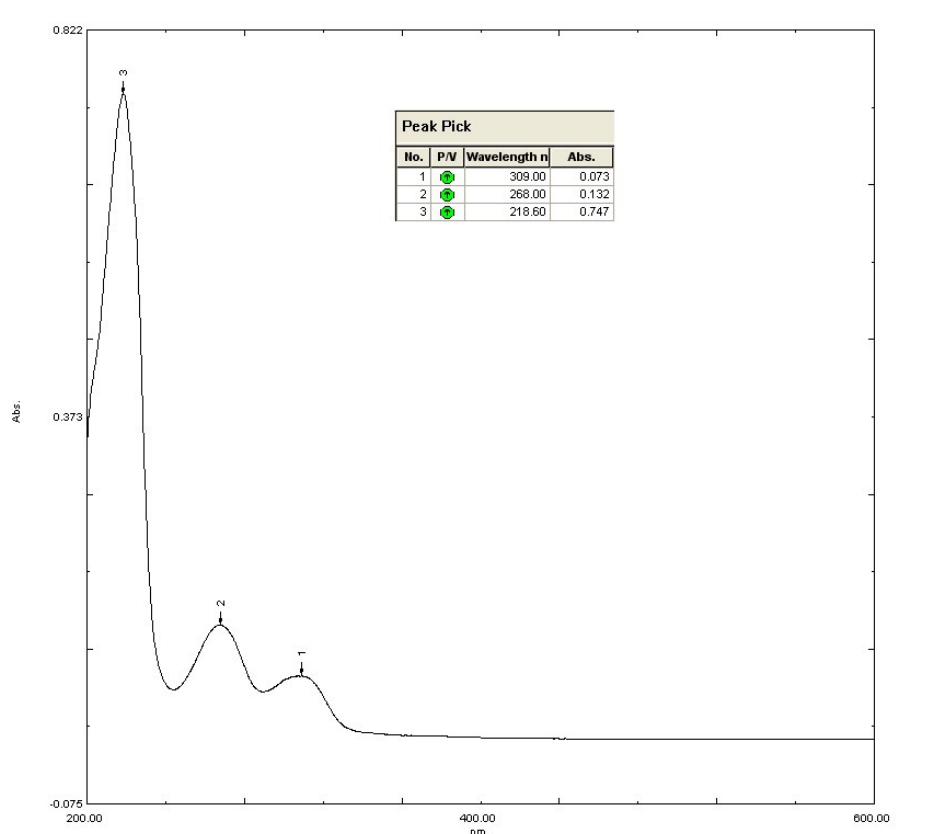


Figure S56. UV spectrum of stachybochartin E (5).

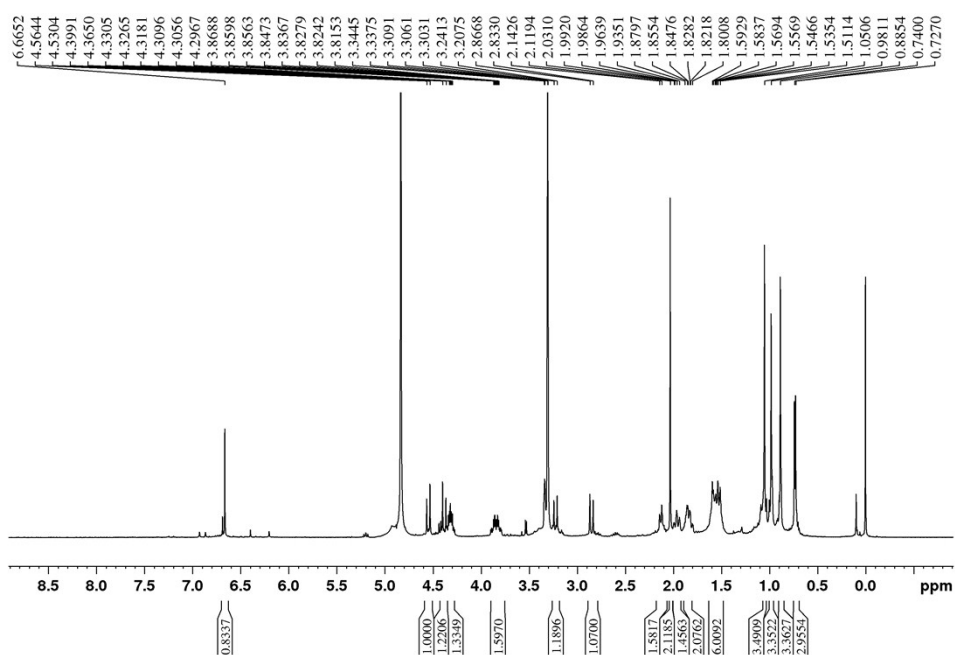


Figure S57. ^1H -NMR spectrum (500 MHz) of stachybochartin F (**6**) in CD_3OD .

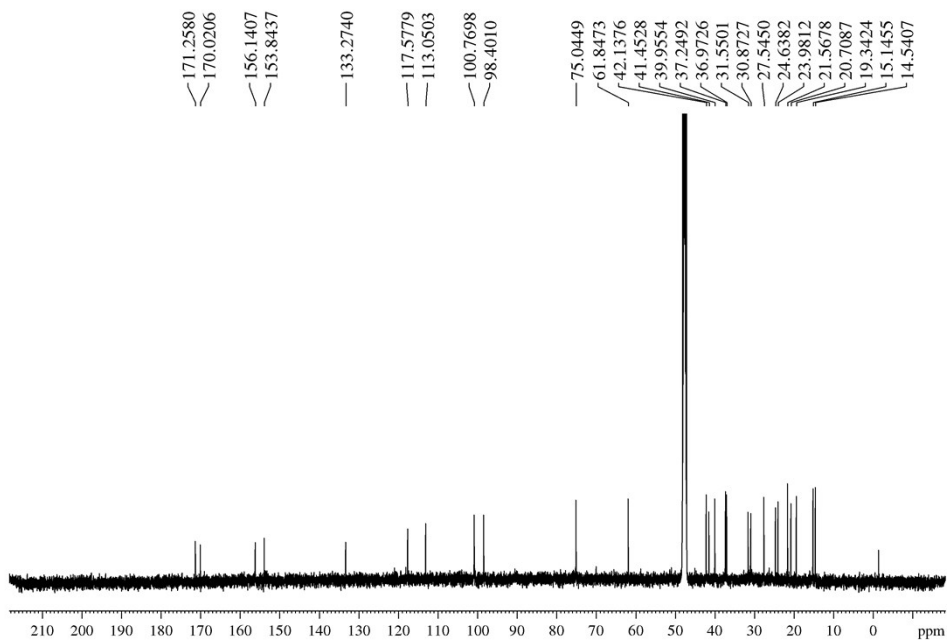


Figure S58. ^{13}C -NMR spectrum (125 MHz) of stachybochartin F (**6**) in CD_3OD .

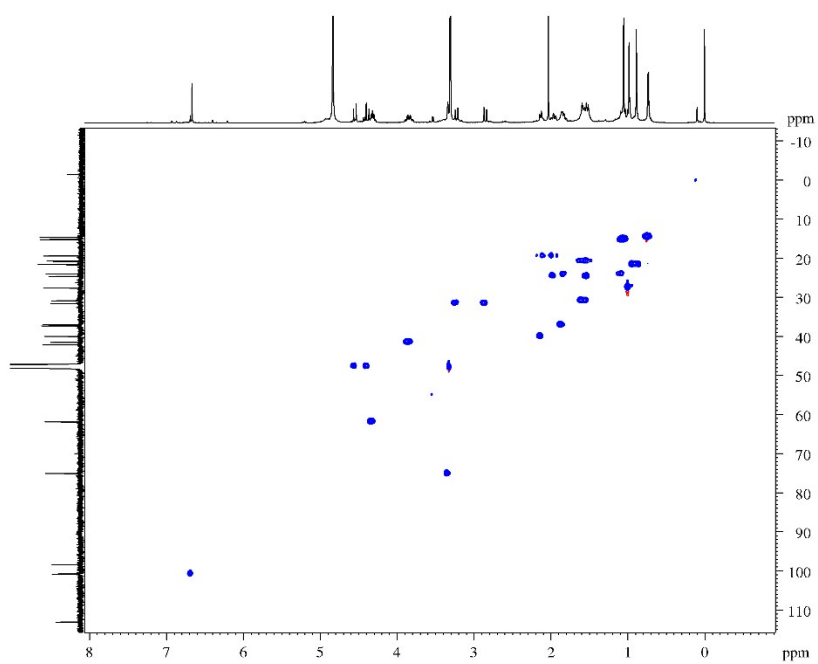


Figure S59. HSQC spectrum of stachybochartin F (6) in CD₃OD

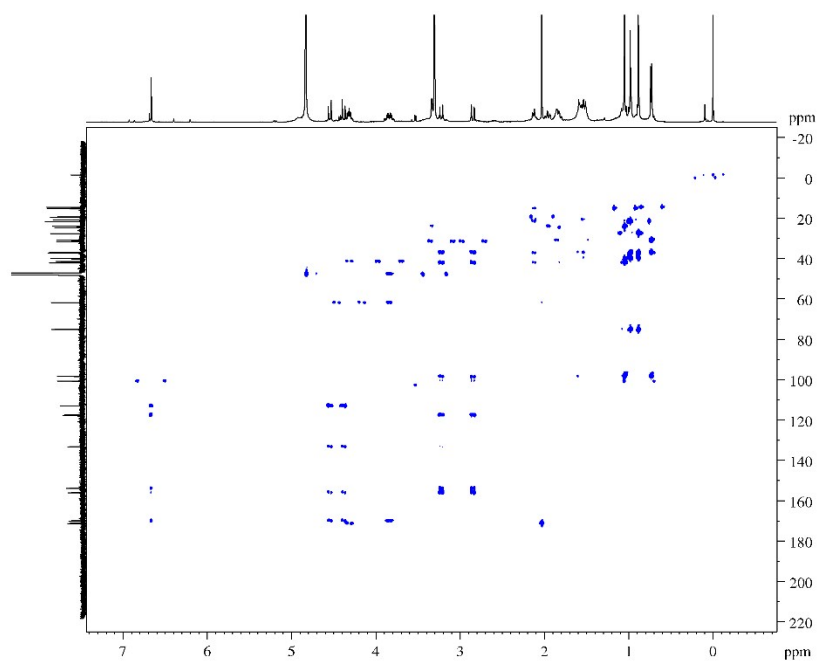


Figure S60. HMBC spectrum of stachybochartin F (6) in CD₃OD

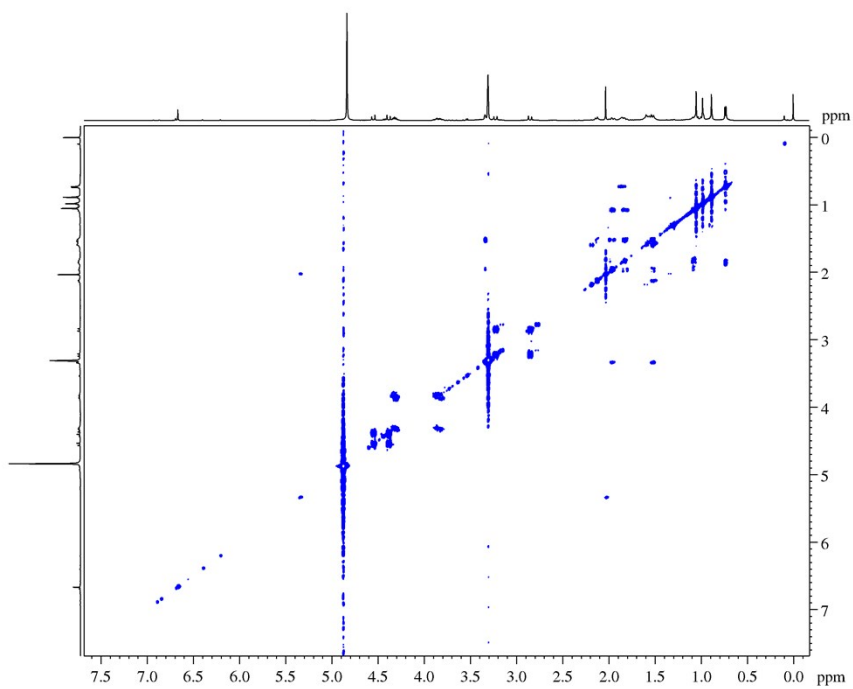


Figure S61. ¹H-¹H COSY spectrum of stachybochartin F (**6**) in CD₃OD.

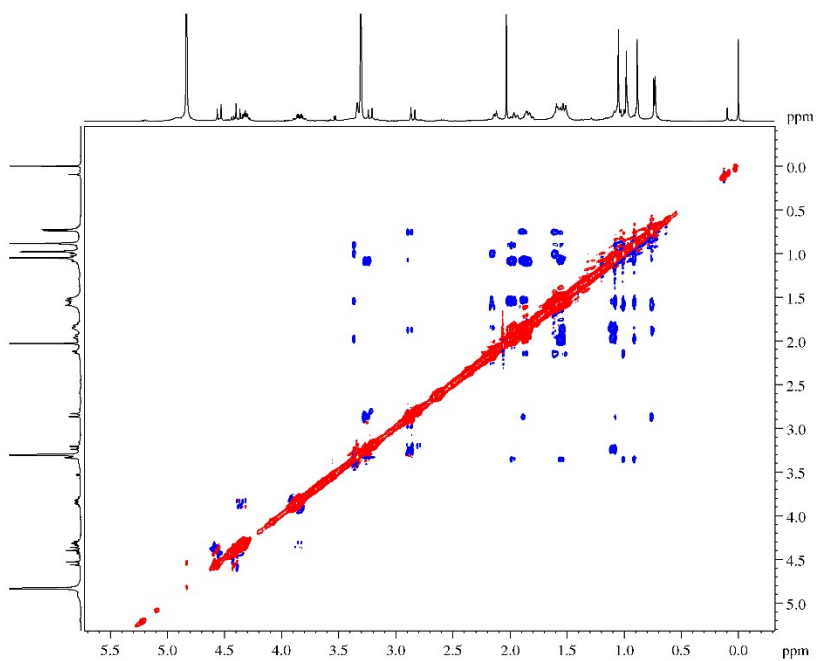
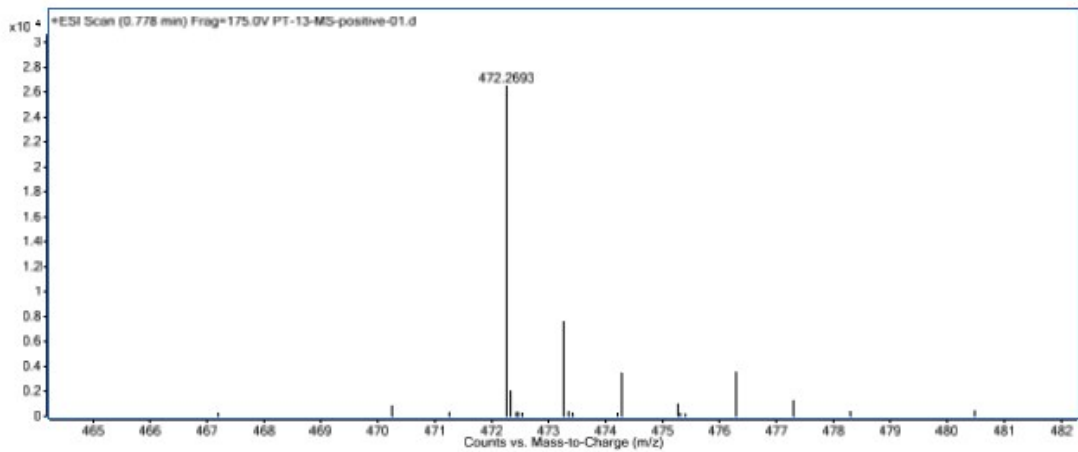


Figure S62. ROESY spectrum of stachybochartin F (**6**) in CD₃OD



Elemental Composition Calculator

Target m/z:	472.2693	Result type:	Positive ions	Species:	[M+H] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₇ H ₃₈ N ₆ O ₆	472.2694		0.21		



Figure S63. HRESIMS spectrum of stachybochartin F (6).

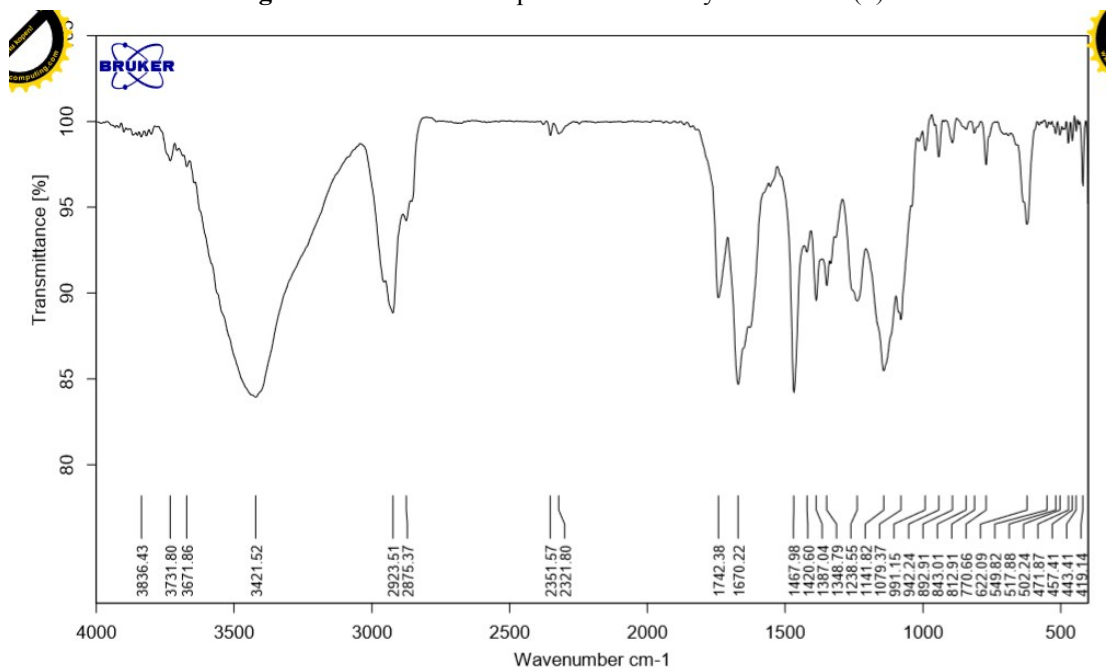


Figure S64. IR (KBr disc) spectrum of stachybochartin F (6).

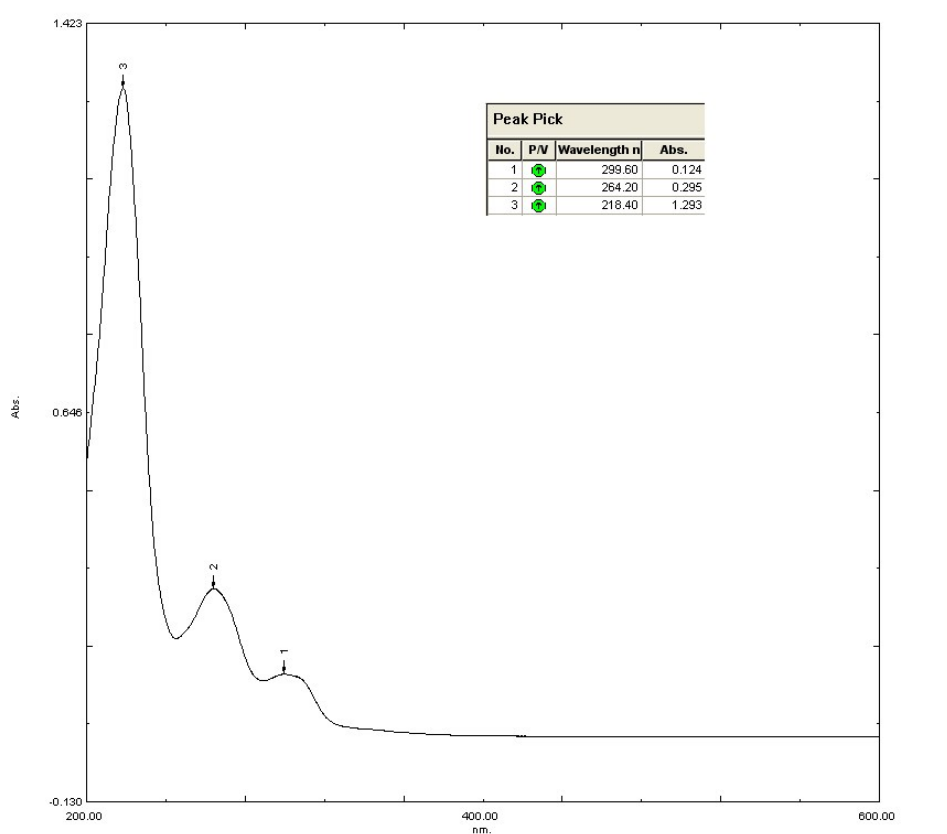


Figure S65. UV spectrum of stachybochartin F (6).

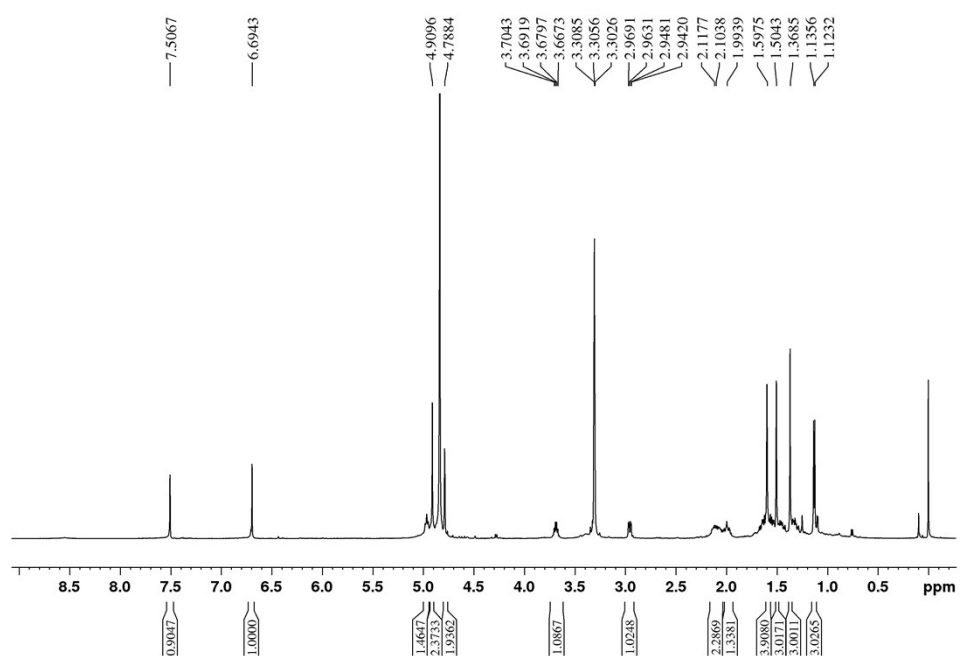


Figure S66. ¹H-NMR spectrum (500 MHz) of stachybochartin G (7) in CD₃OD.

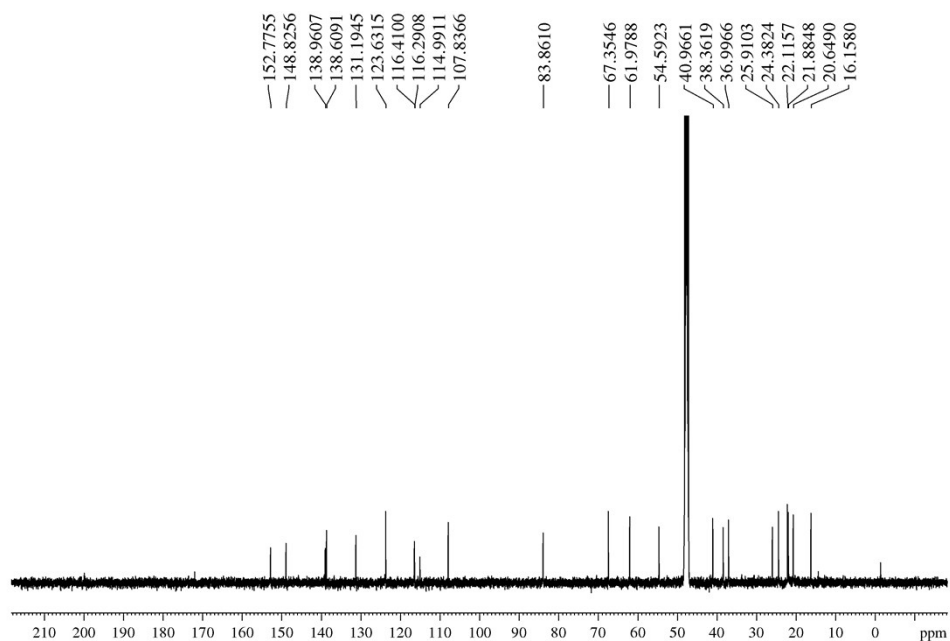


Figure S67. ^{13}C -NMR spectrum (125 MHz) of stachybochartin G (7) in CD_3OD .

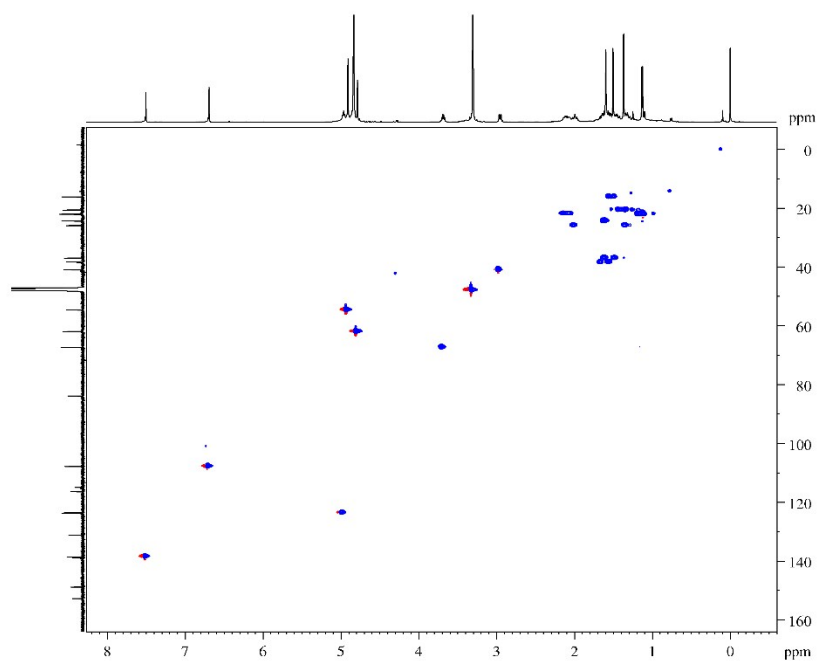


Figure S68. HSQC spectrum of stachybochartin G (7) in CD_3OD

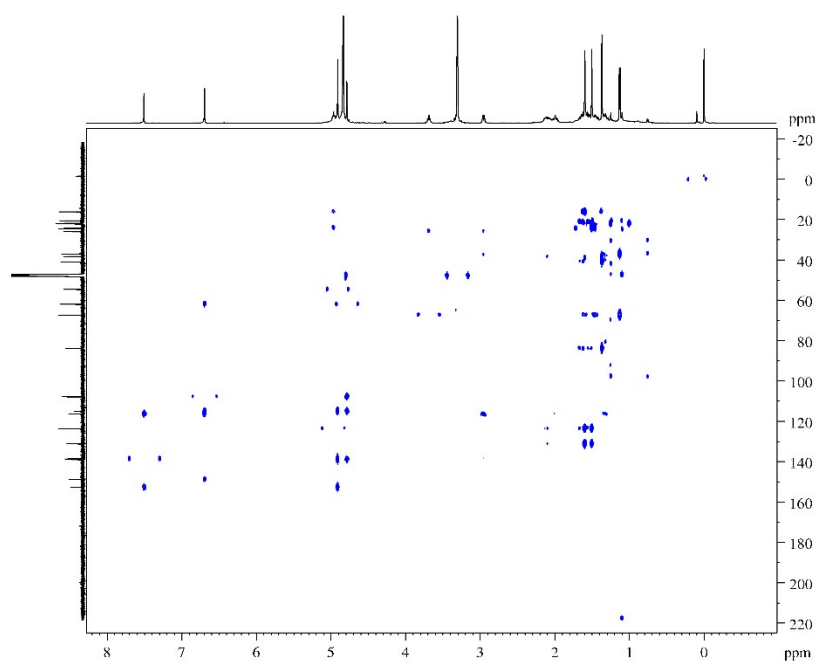


Figure S69. HMBC spectrum of stachybochartin G (7) in CD₃OD

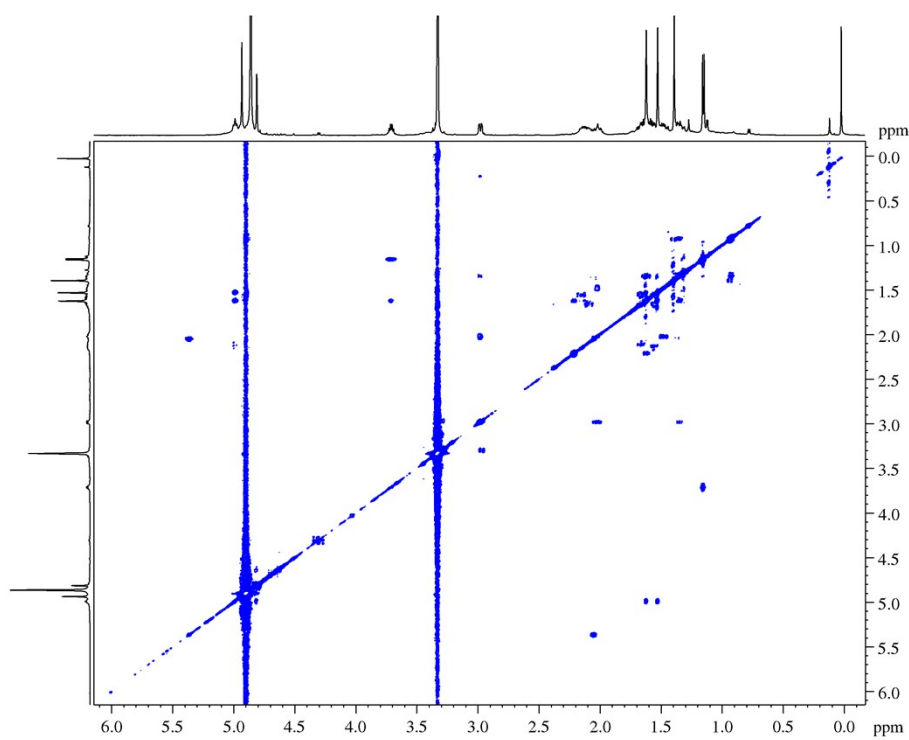


Figure S70. ¹H-¹H COSY spectrum of stachybochartin G (7) in CD₃OD.

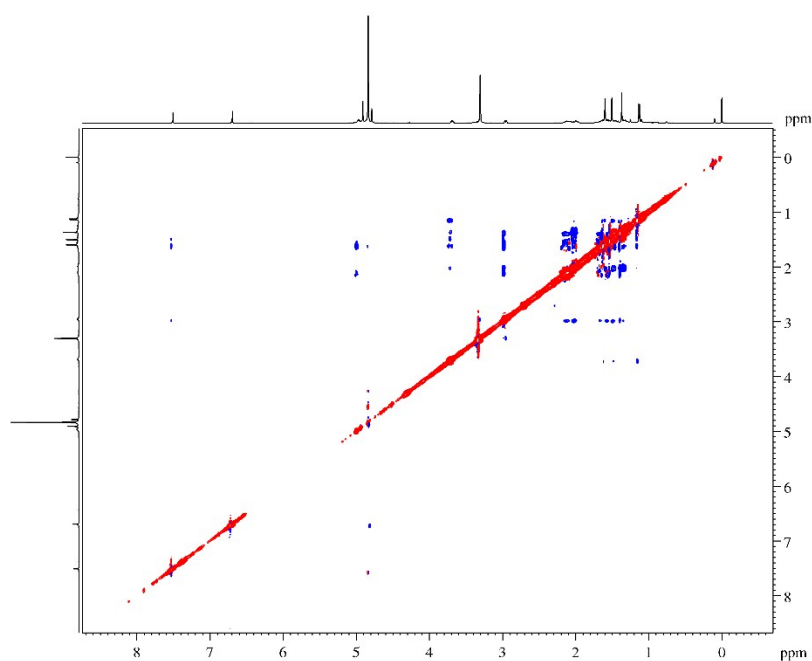
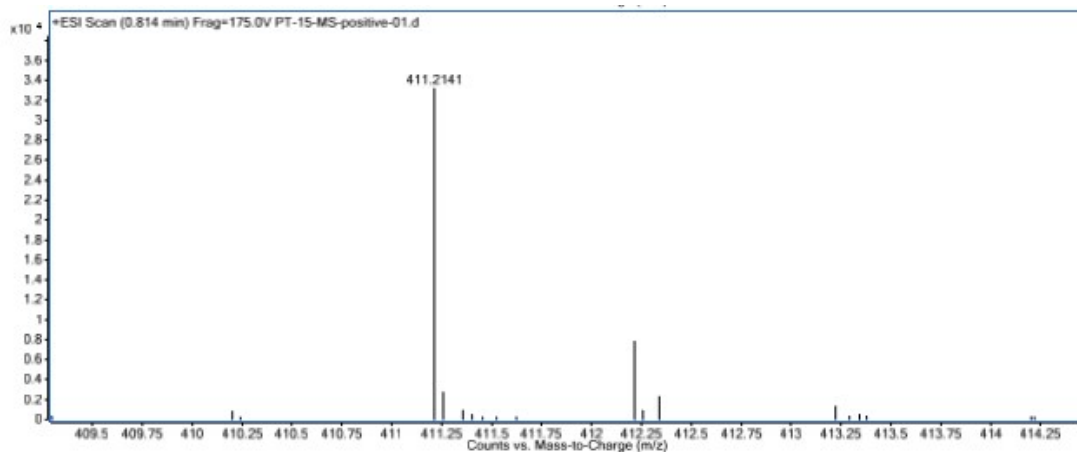


Figure S71. ROESY spectrum of stachybochartin G (7) in CD₃OD



Elemental Composition Calculator

Target m/z:	411.2141	Result type:	Positive ions	Species:	[M+Na] ⁺
Elements:	C (0-80); H (0-120); O (0-30); N(0-10); Na (0-5)				
Ion Formula	Calculated m/z		PPM Error		
C ₂₃ H ₃₂ NaO ₅	411.2142		0.30		



Figure S72. HRESIMS spectrum of stachybochartin G (7).

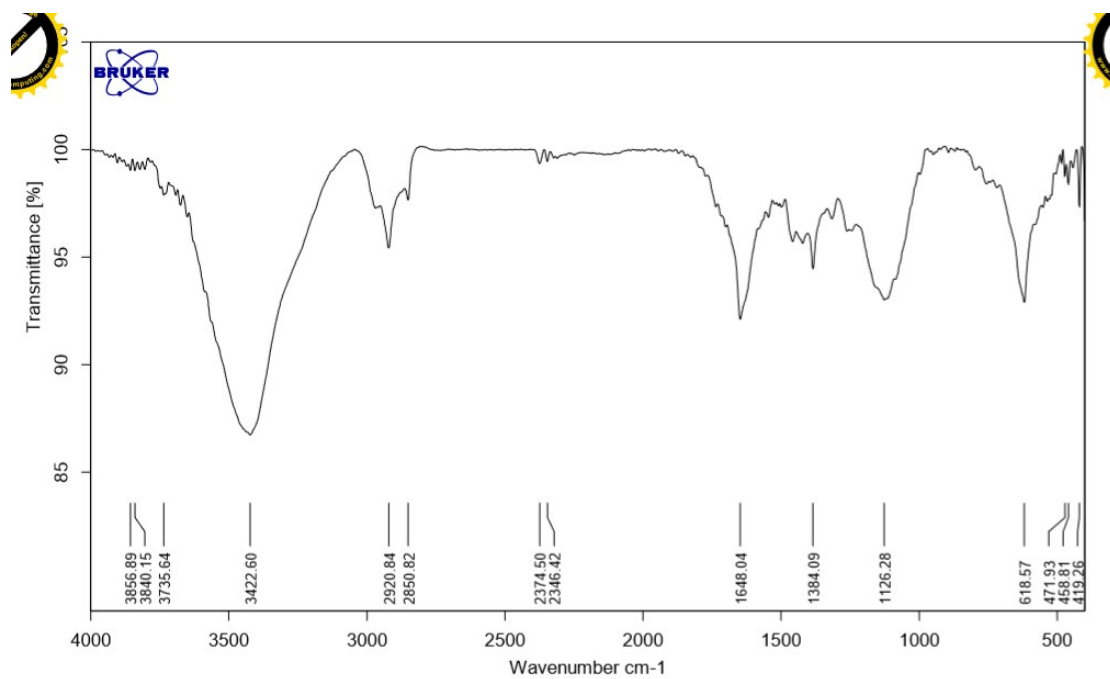


Figure S73. IR (KBr disc) spectrum of stachybochartin G (7).

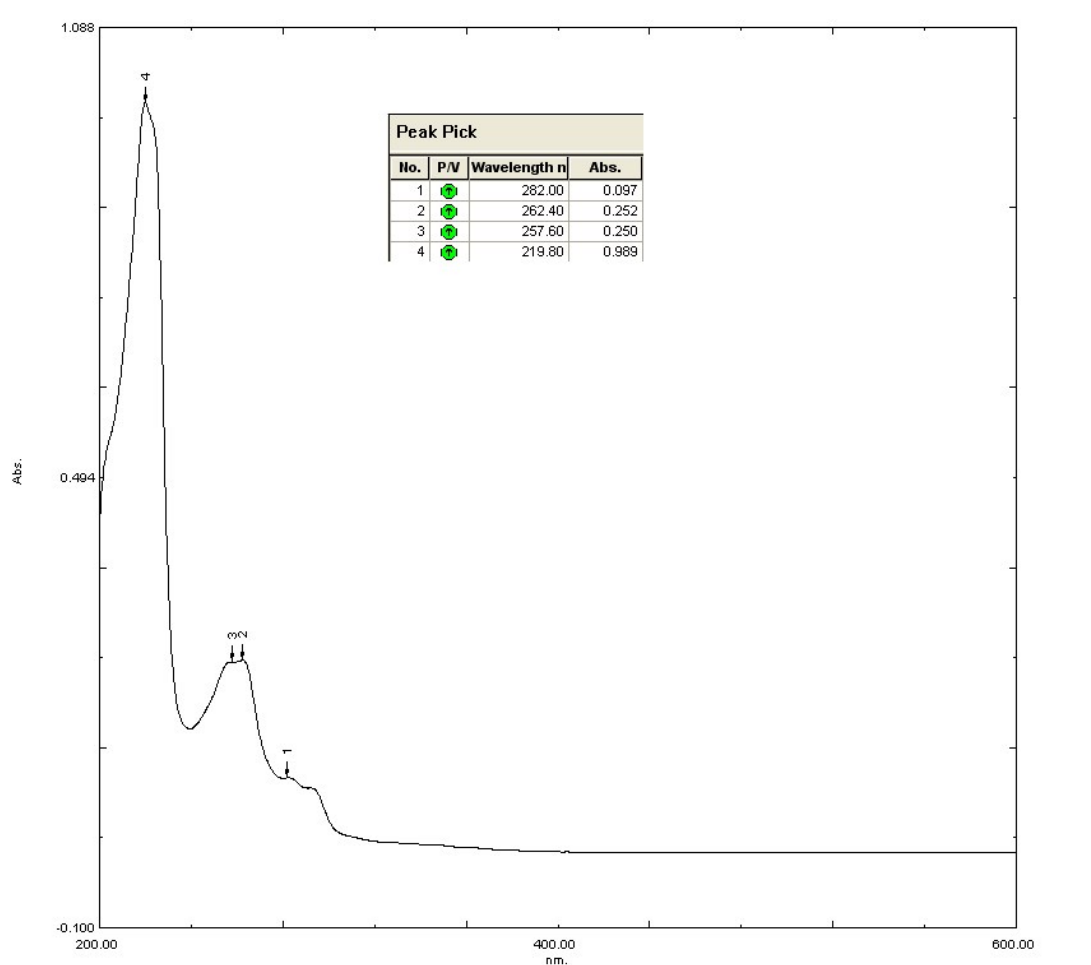


Figure S74. UV spectrum of stachybochartin G (7).

