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Antiviral and Anti-inflammatory Meroterpenoids: Stachybonoids A-F from the Crinoid-Derived Fungus *Stachybotrys chartarum* 952

Panpan Zhang,^{a1} Yongfang Li,^{a1} Chunxiu Jia,^c Jiajia Lang,^c Shah-Iram Niaz,^a Jing Li,^a Jie Yuan,^d
Jianchen Yu,^d Senhua Chen,^{ab*} and Lan Liu^{ab*}

a. School of Marine Sciences, Sun Yat-Sen University, Guangzhou 510006, China. Email:
cesllan@mail.sysu.edu.cn; Tel: 020-84725459

b. Key Laboratory of Functional Molecules from Oceanic Microorganisms, Department of Education
of Guangdong Province, Sun Yat-Sen University, Guangzhou 510006, China.

c. School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, China.

d. Zhongshan School of Medicine, Sun Yat-Sen University, Guangzhou, P.R. China.

1. These authors contributed equally to this work.

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Figure S1. ^1H (400 MHz) NMR Spectrum of Stachybonoid A (**1**) in Pyridine- d_5

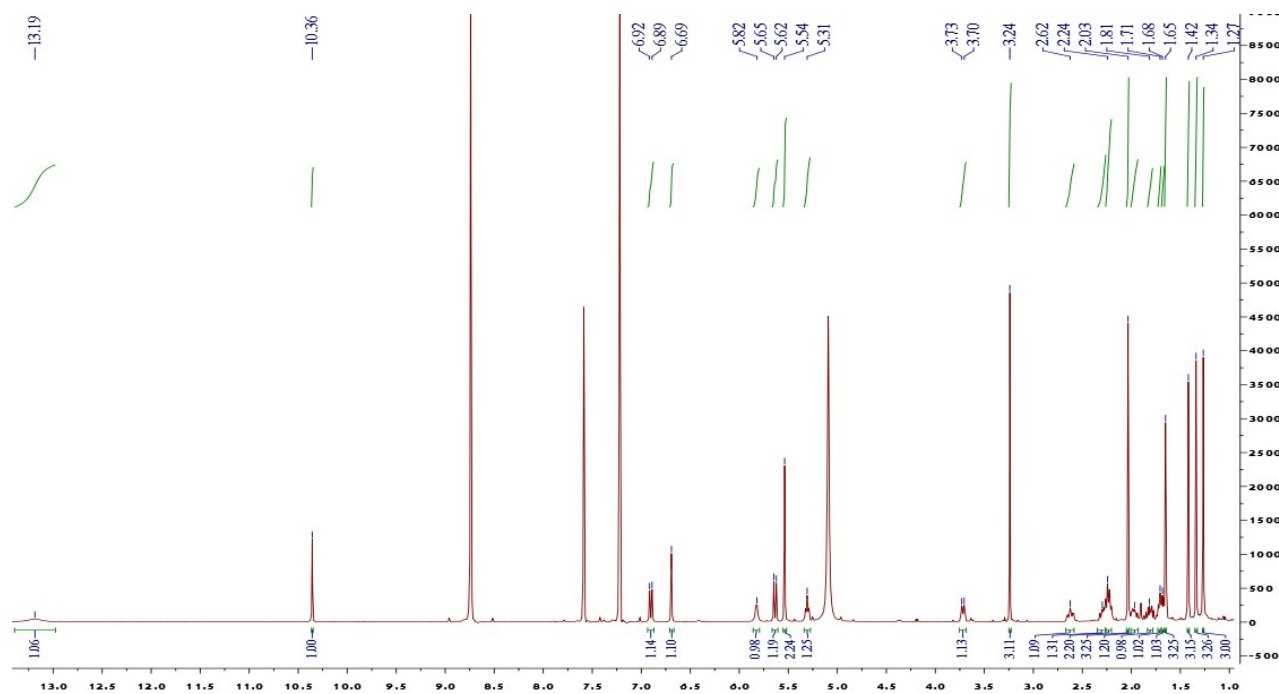


Figure S2. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid A (**1**) in Pyridine- d_5

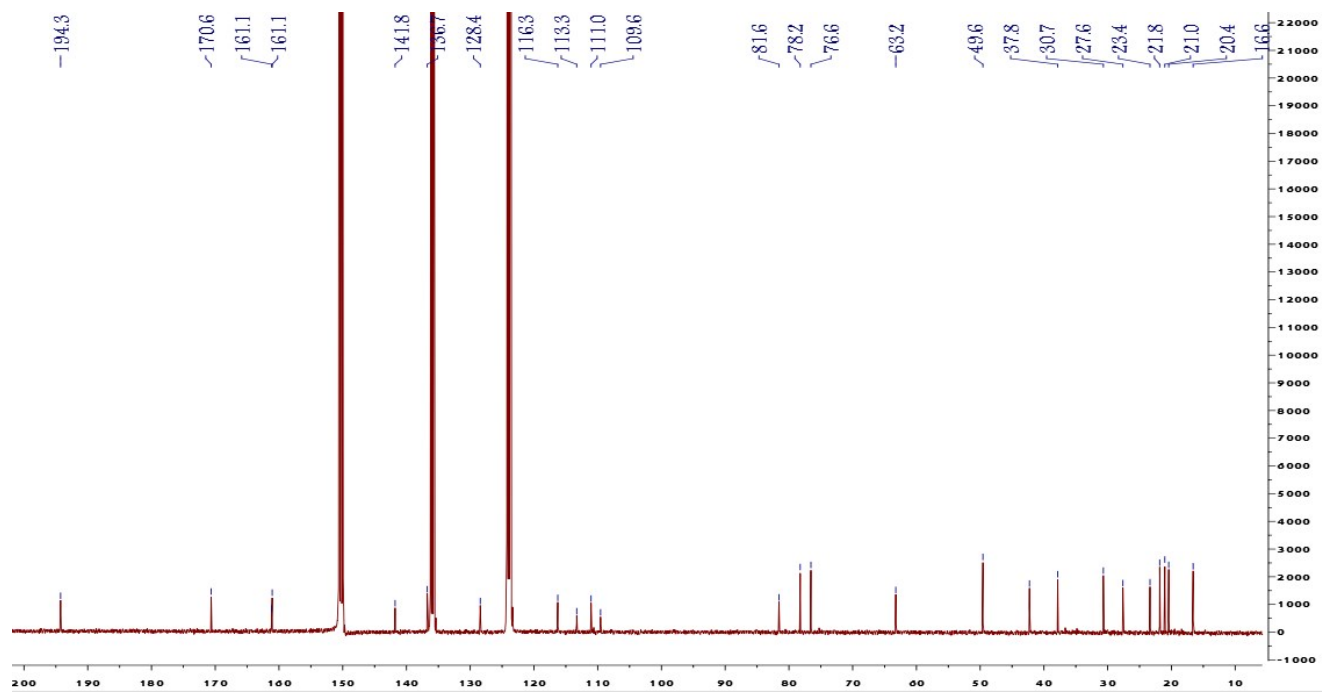


Figure S3. DEPT-90 Spectrum of Stachybonoid A (**1**) in Pyridine-*d*₅

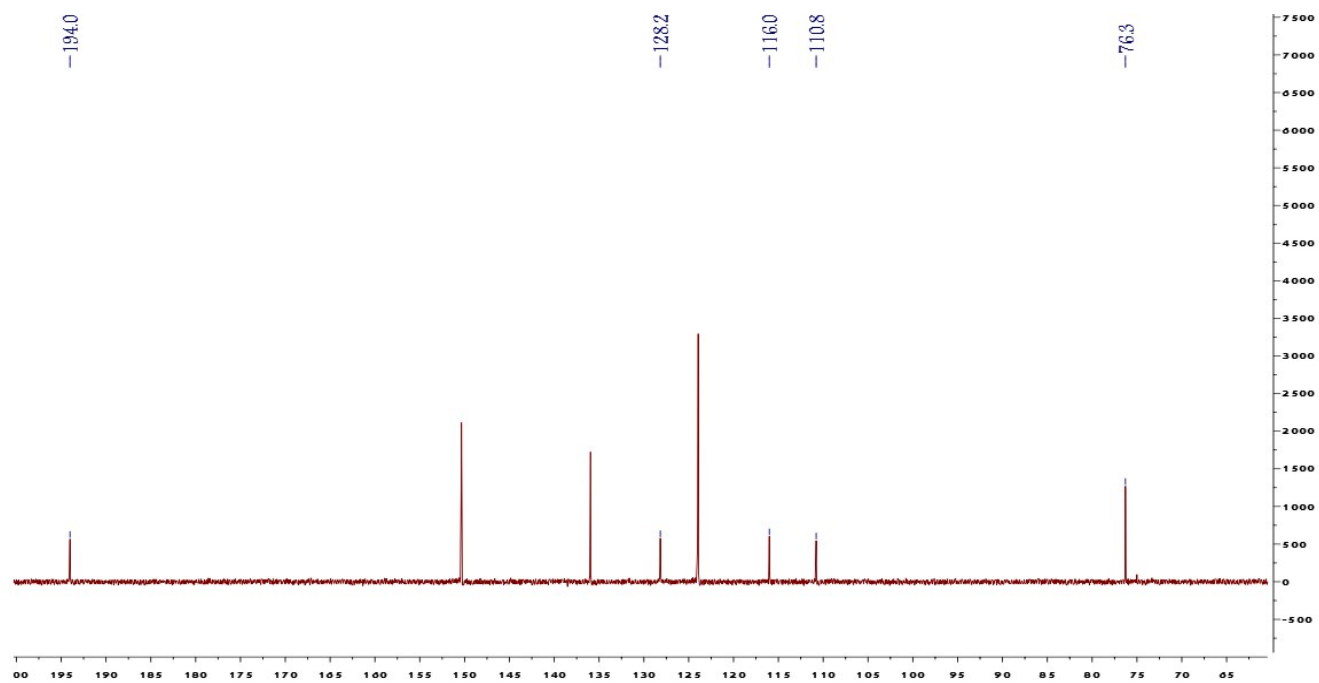


Figure S4. DEPT-135 Spectrum of Stachybonoid A (**1**) in Pyridine-*d*₅

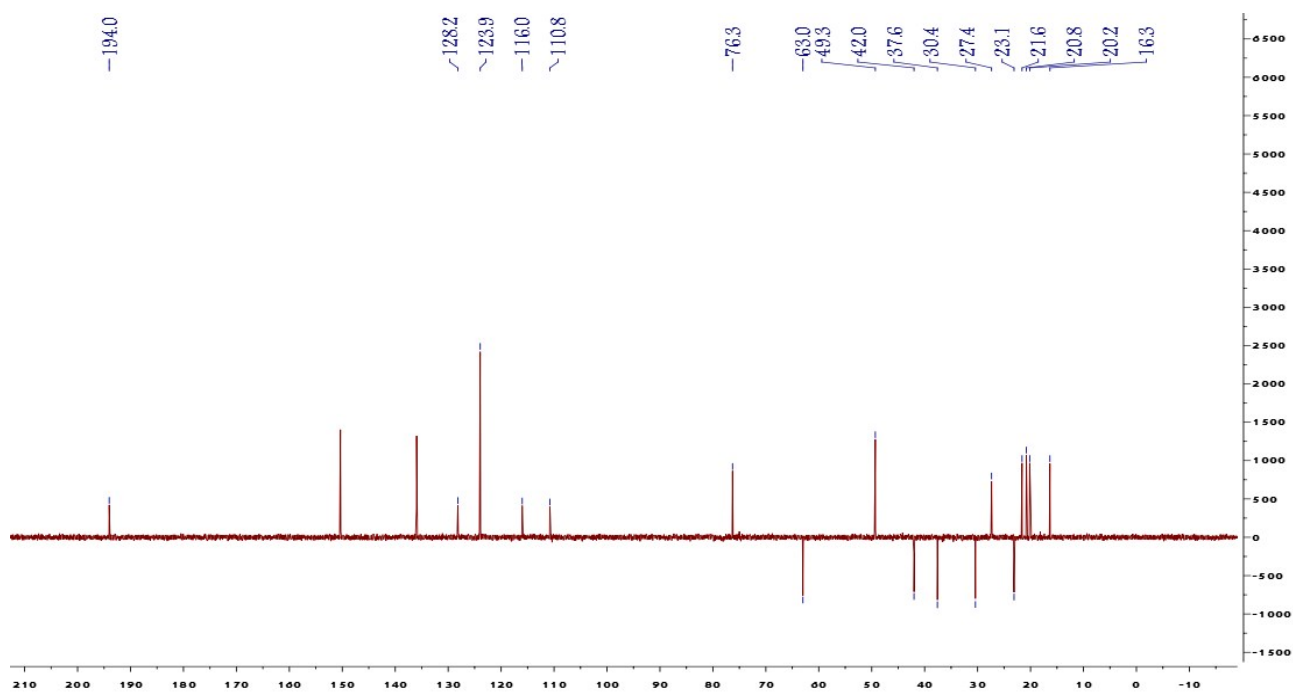


Figure S5. HSQC Spectrum of Stachybonoid A (**1**) in Pyridine-*d*₅

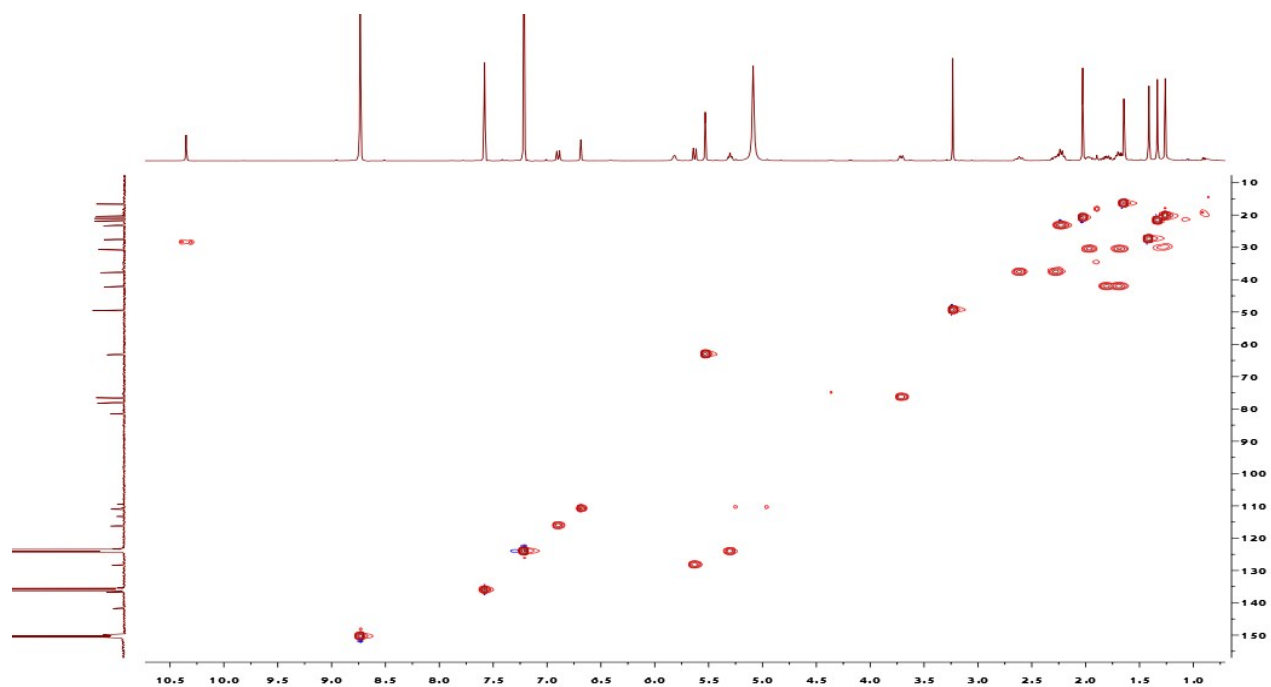


Figure S6. HMBC Spectrum of Stachybonoid A (**1**) in Pyridine-*d*₅

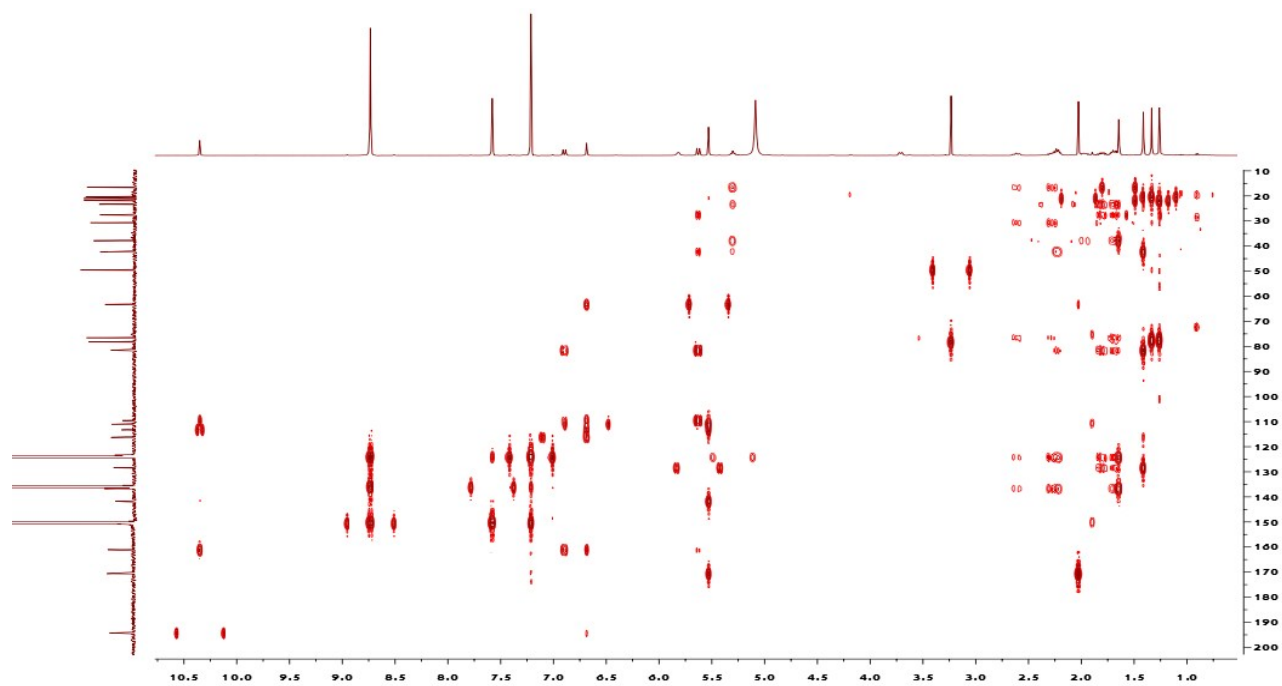


Figure S7. ^1H - ^1H COSY Spectrum of Stachybonoid A (**1**) in Pyridine- d_5

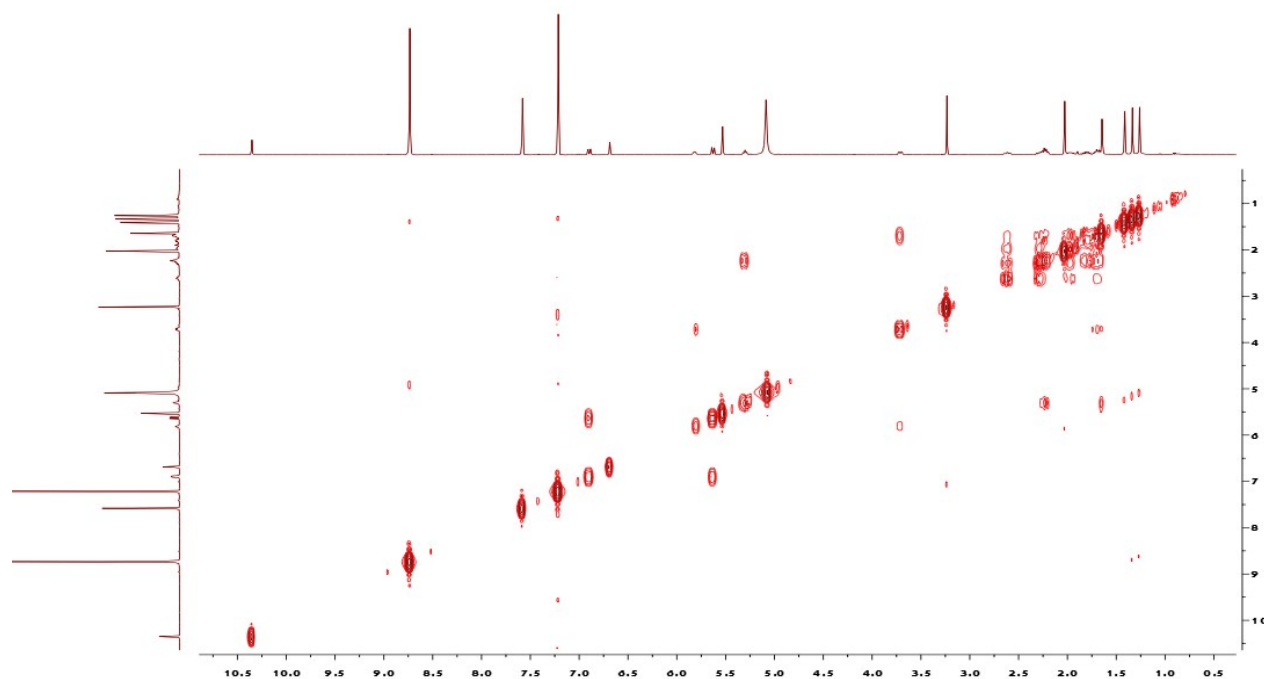


Figure S8. NOESY Spectrum of Stachybonoid A (**1**) in Pyridine- d_5

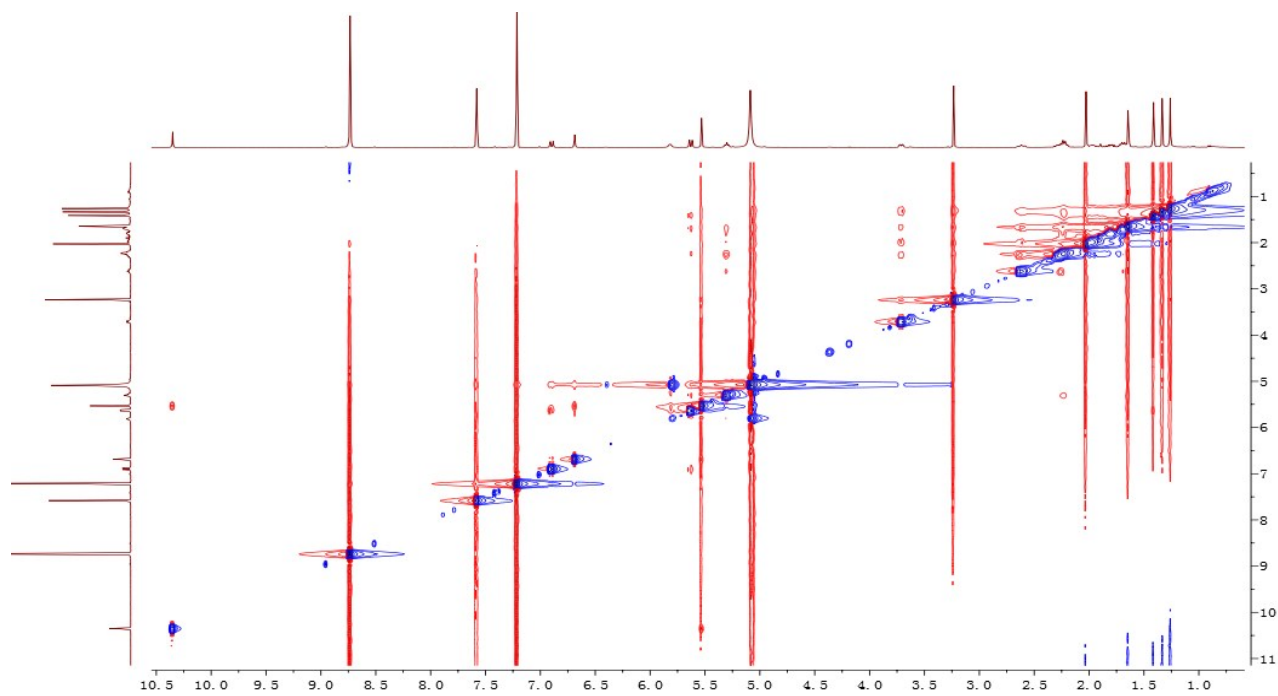


Figure S9. HR-ESIMS of Stachybonoid A (1)

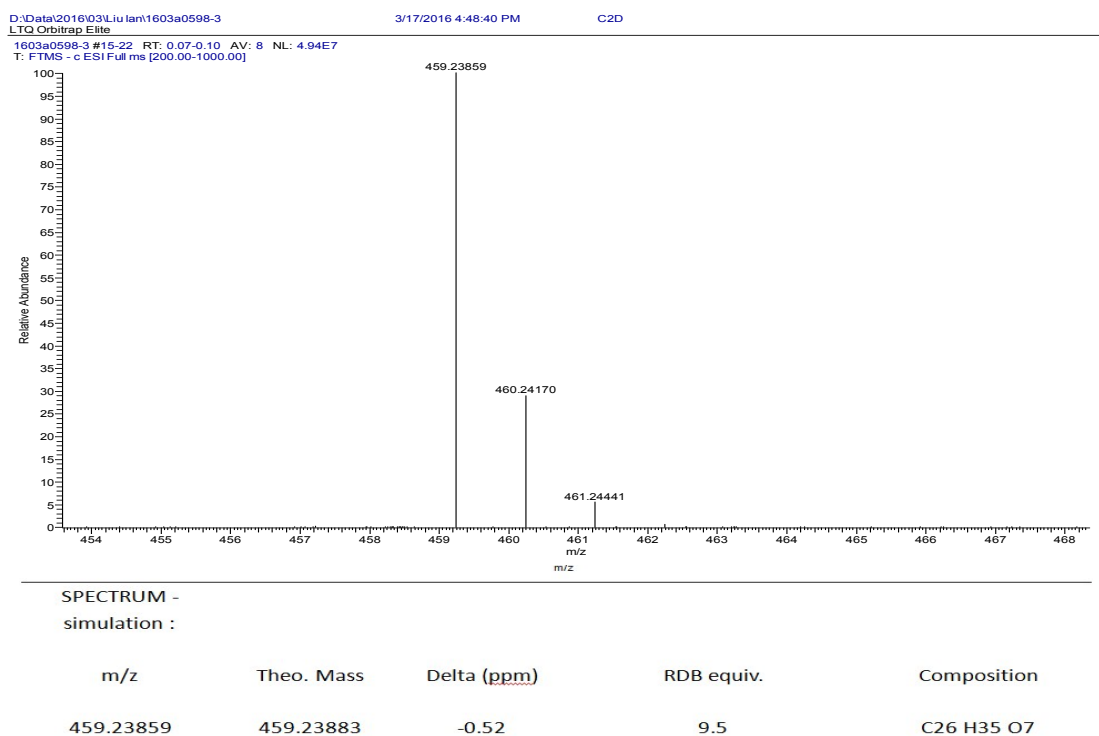


Figure S10. ^1H (400 MHz) NMR Spectrum of Stachybonoid B (2) in Pyridine- d_5

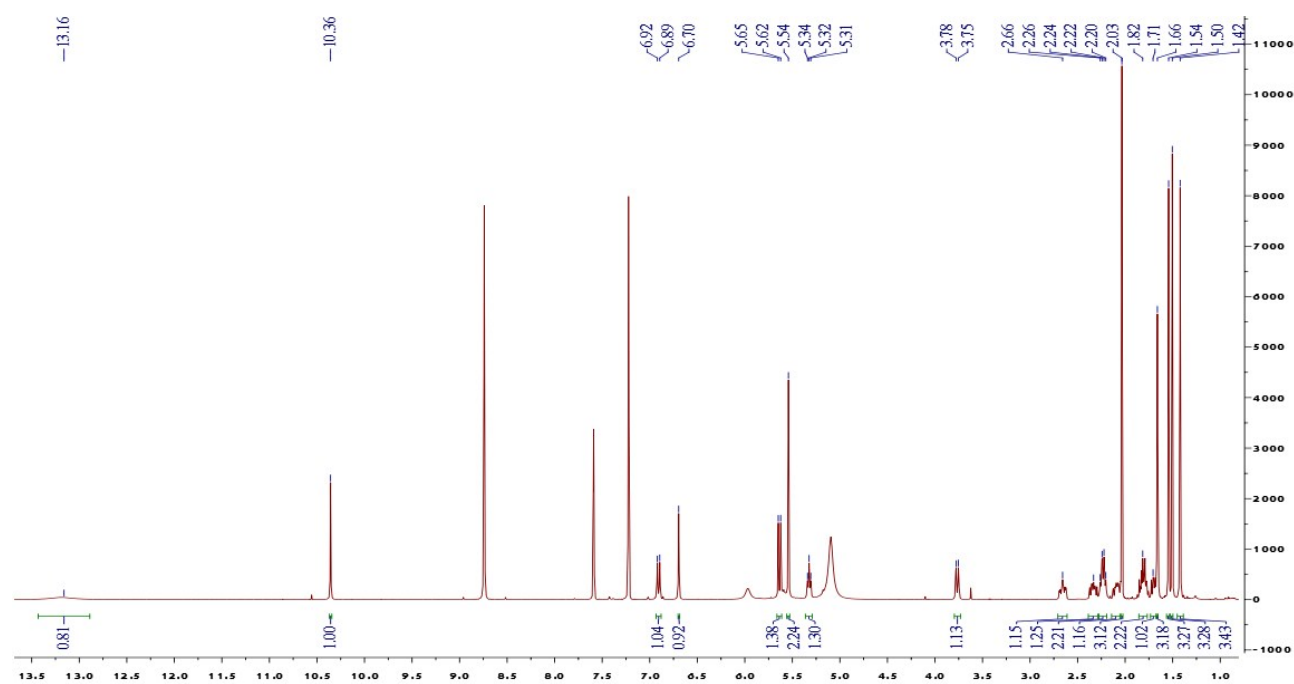


Figure S11. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid B (**2**) in Pyridine- d_5

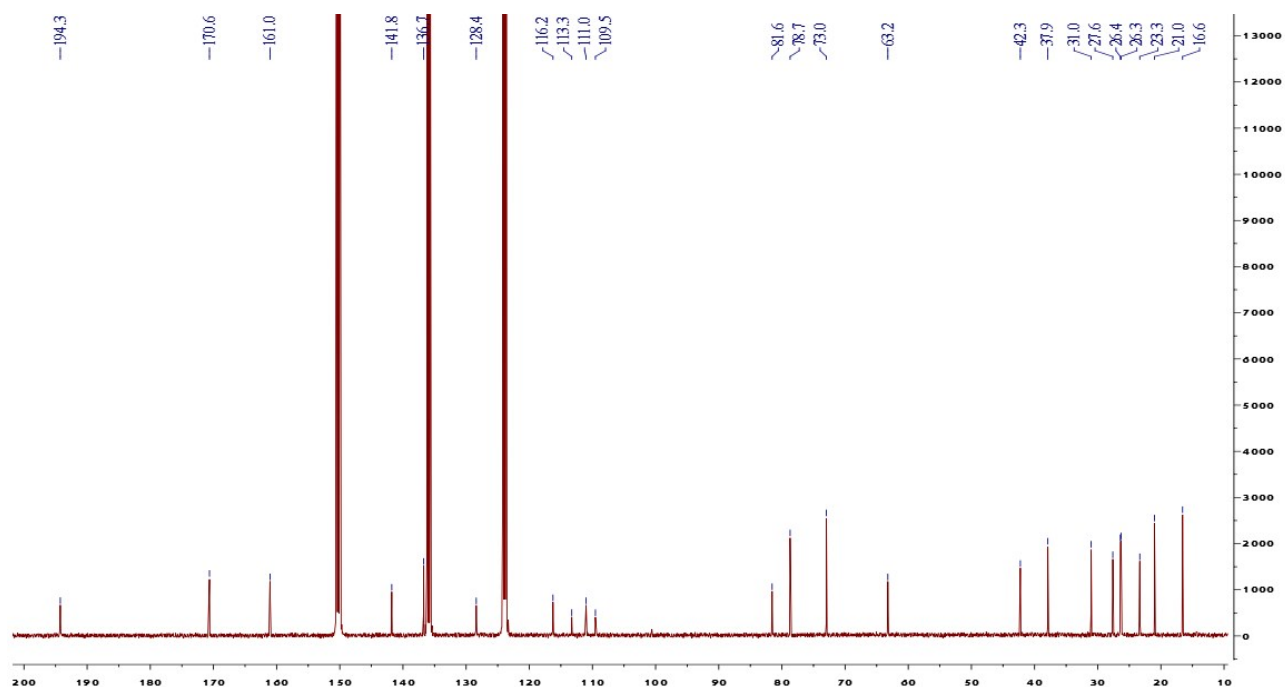


Figure S12. DEPT-90 Spectrum of Stachybonoid B (**2**) in Pyridine- d_5

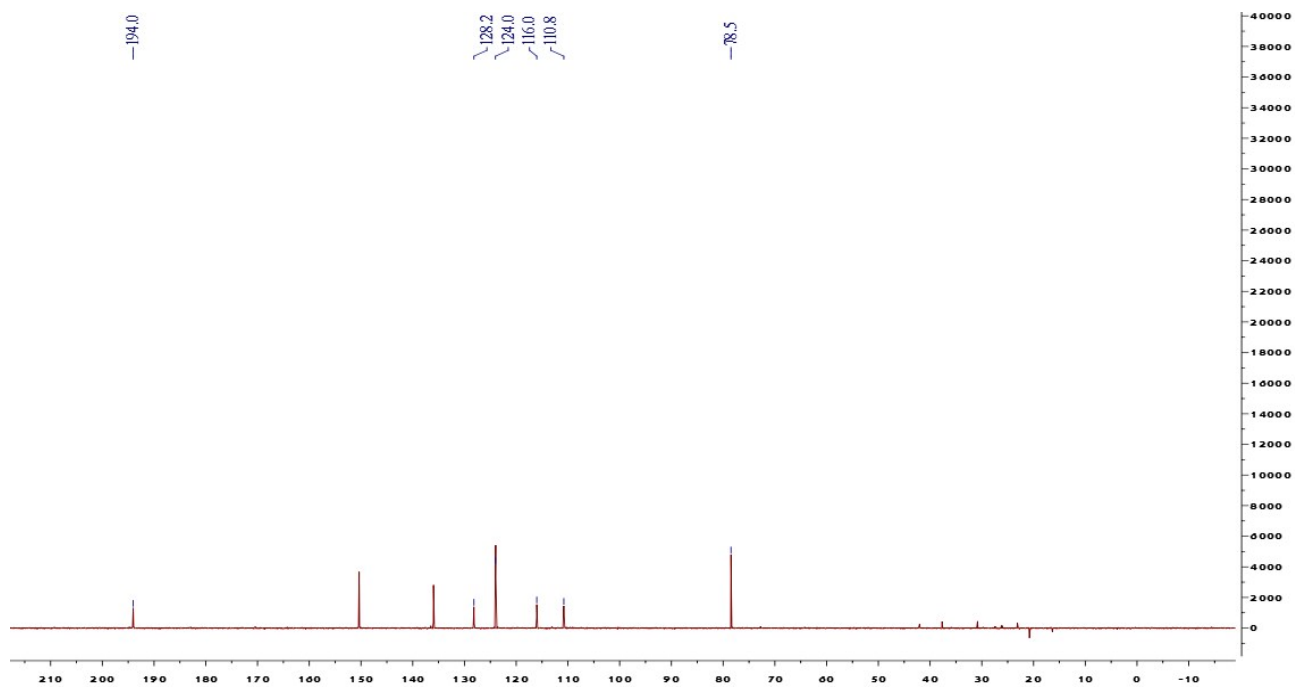


Figure S13. DEPT-135 Spectrum of Stachybonoid B (**2**) in Pyridine-*d*₅

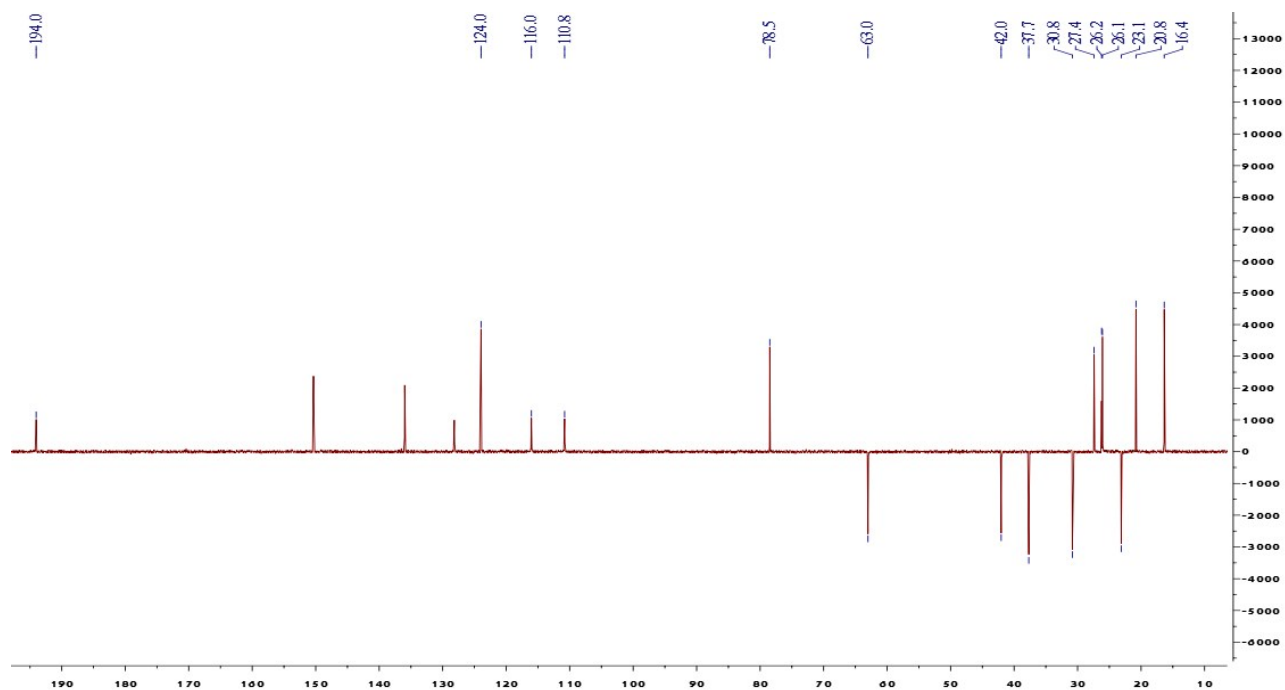


Figure S14. HSQC Spectrum of Stachybonoid B (**2**) in Pyridine-*d*₅

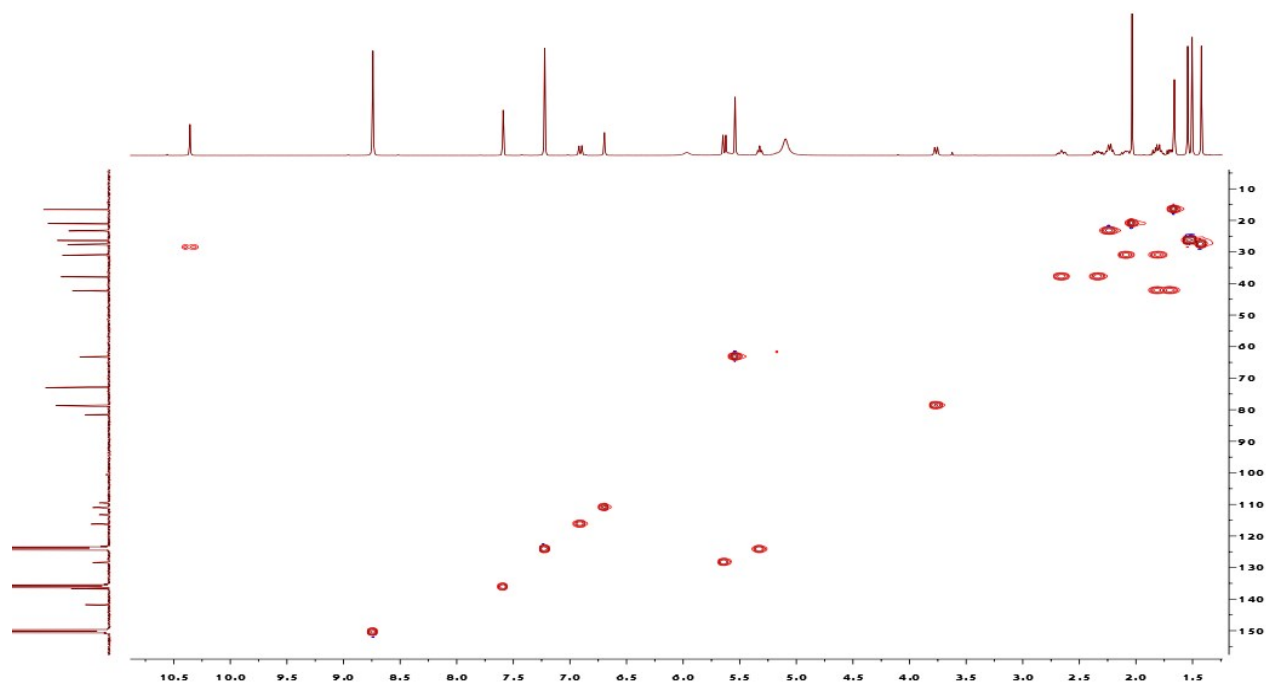


Figure S15. HMBC Spectrum of Stachybonoid B (2) in Pyridine-*d*₅

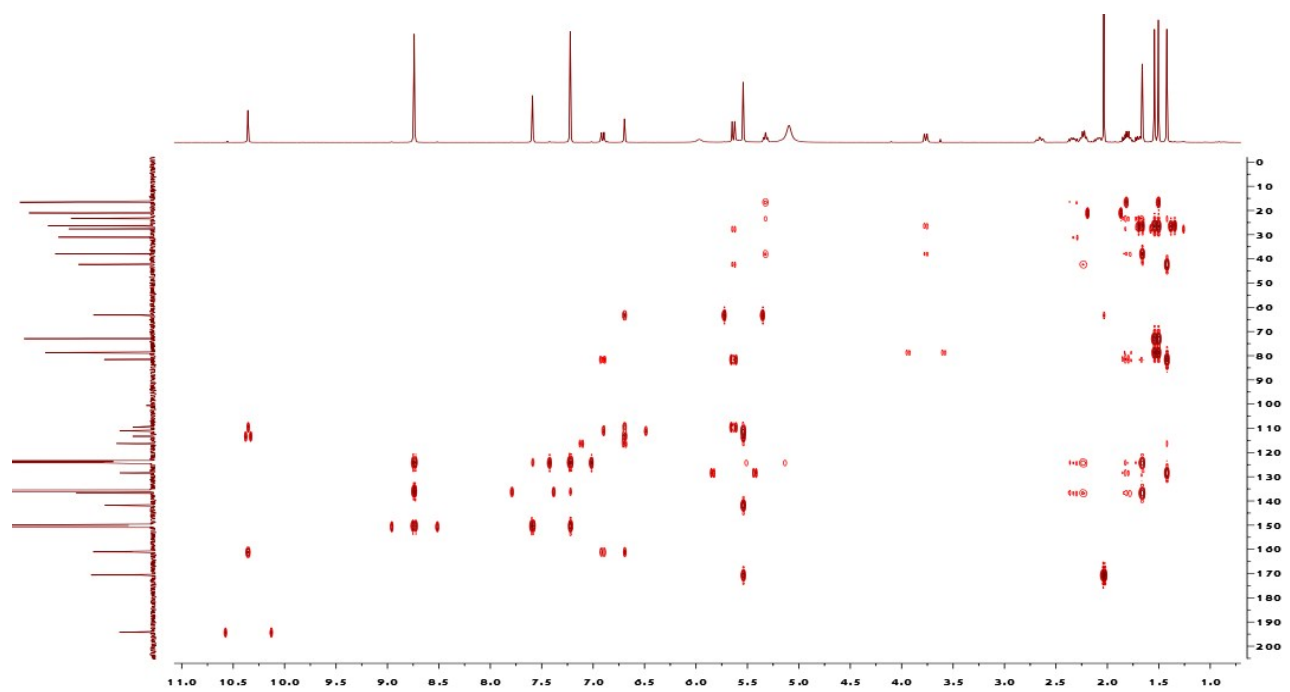


Figure S16. ¹H-¹H COSY Spectrum of Stachybonoid B (2) in Pyridine-*d*₅

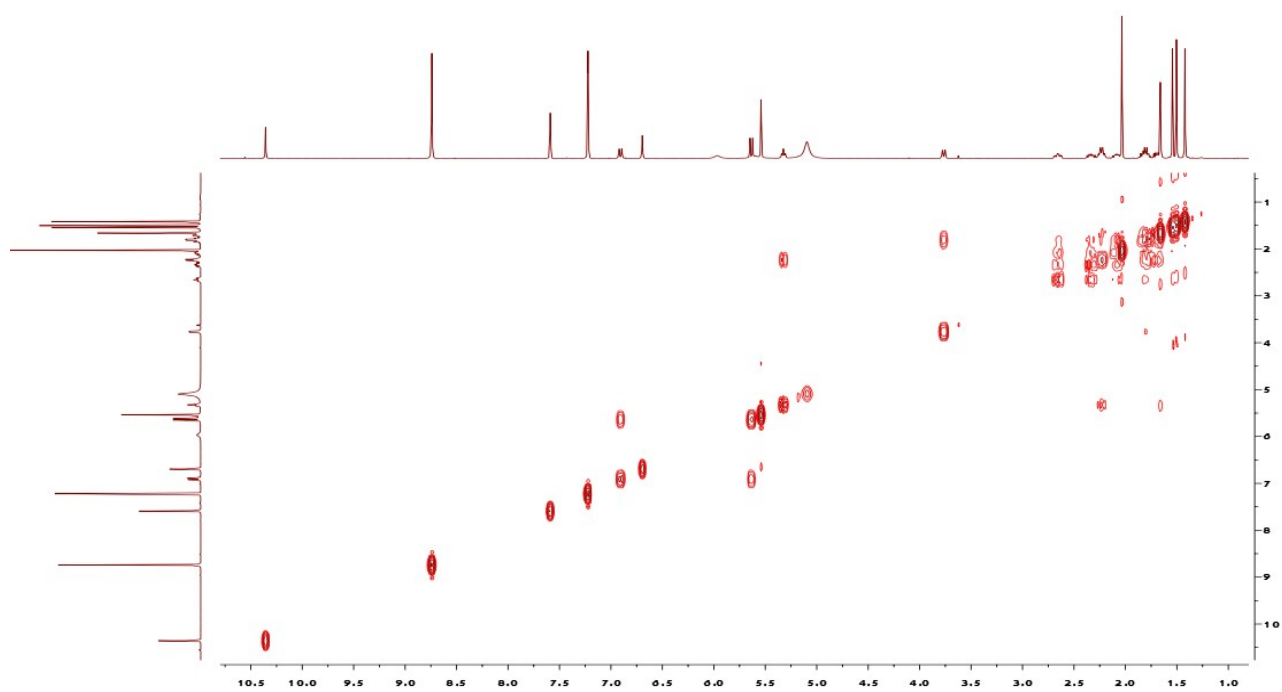


Figure S17. NOESY Spectrum of Stachybonoid B (**2**) in Pyridine-*d*₅

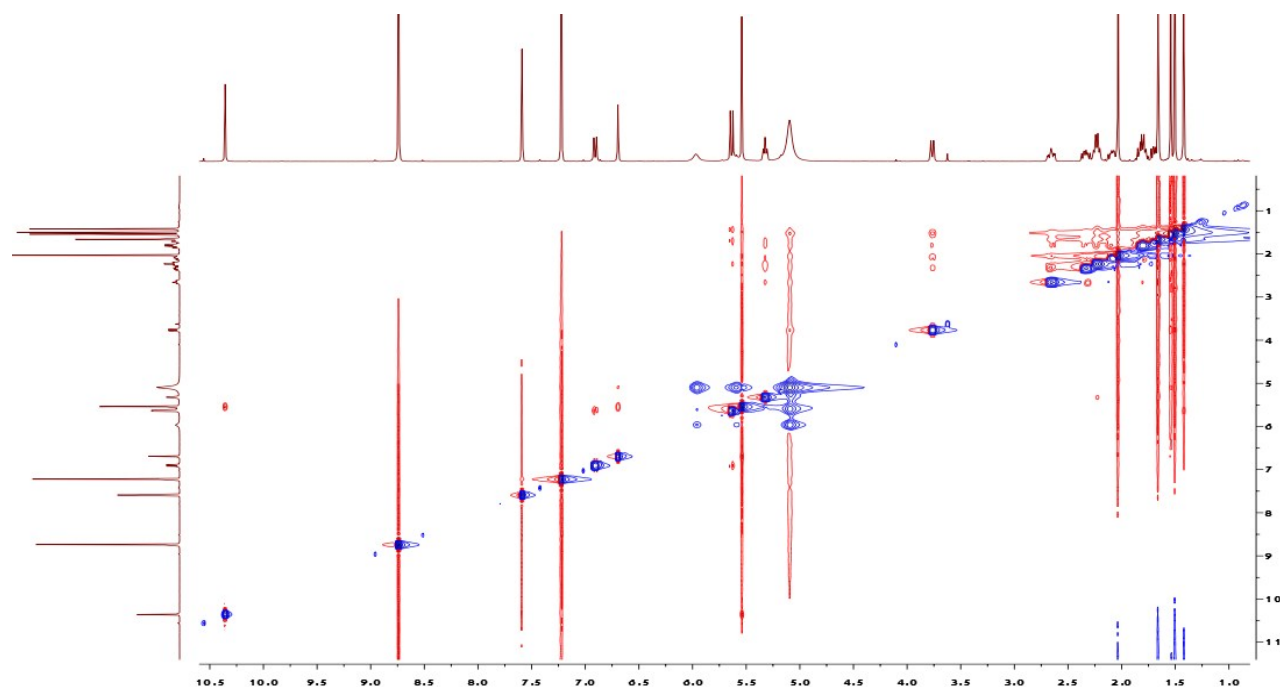
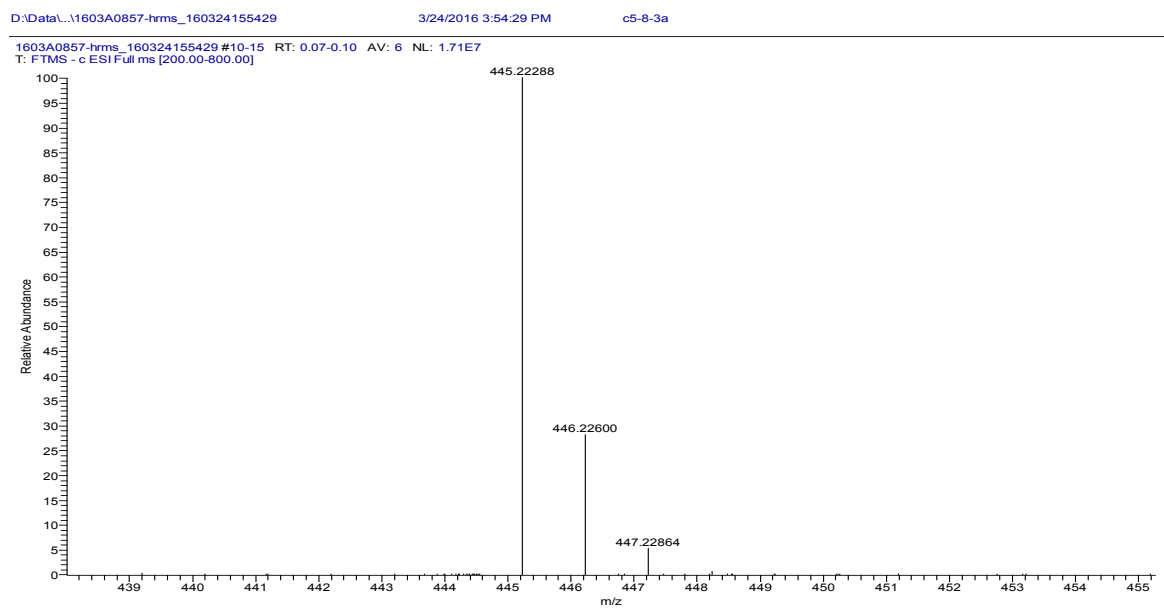


Figure S18. HR-ESIMS of Stachybonoid B (**2**)



SPECTRUM -
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
445.22288	445.22318	-0.67	9.5	C ₂₅ H ₃₃ O ₇

Figure S19. ^1H (400 MHz) NMR Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

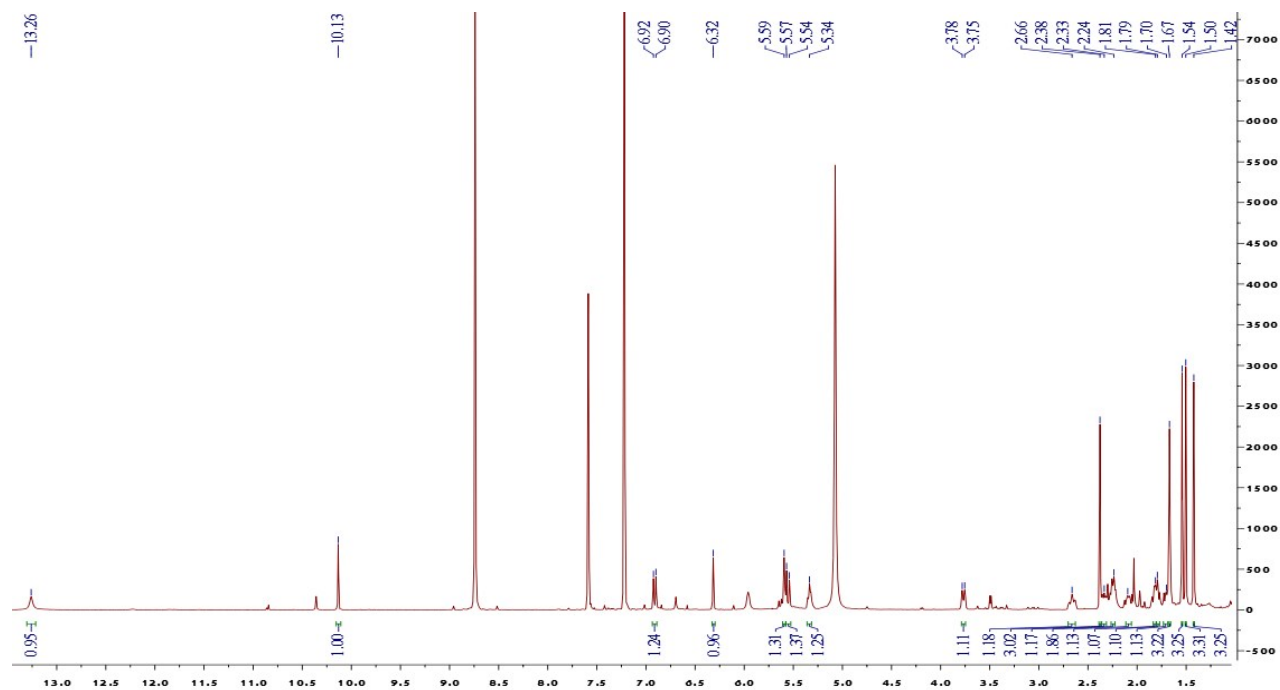


Figure S20. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

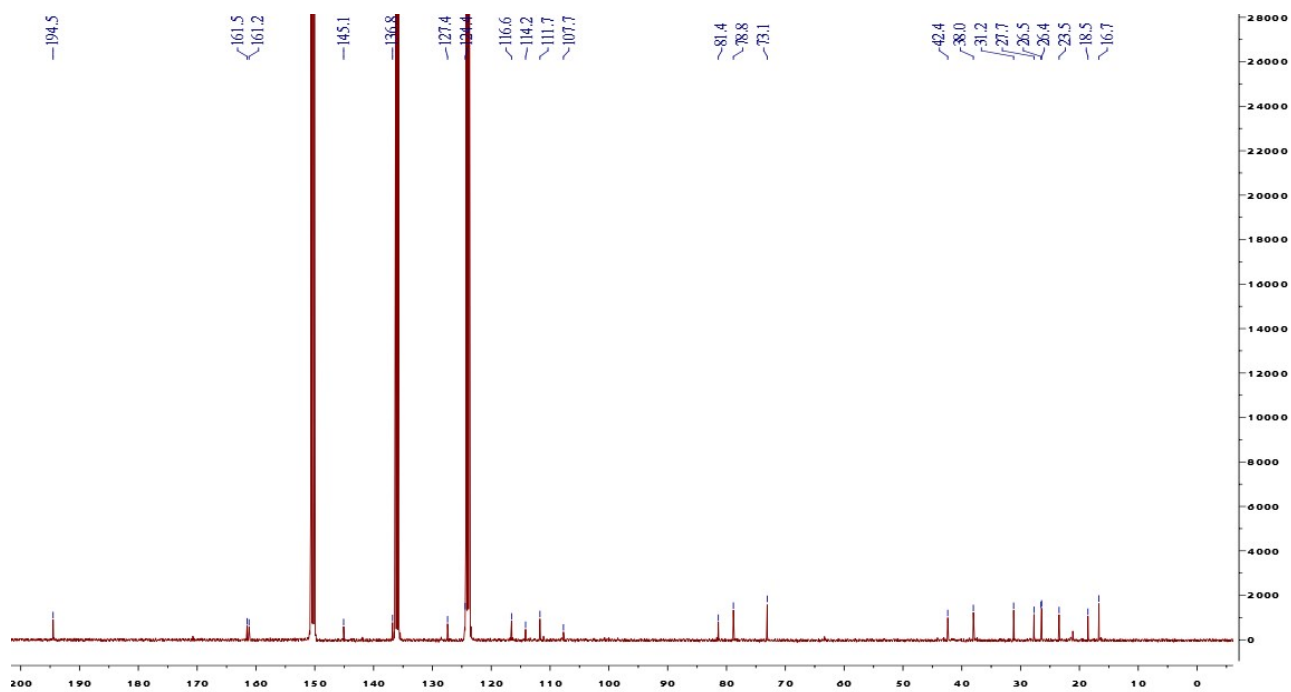


Figure S21. DEPT-90 Spectrum of Stachybonoid C (**3**) in Pyridine-*d*₅

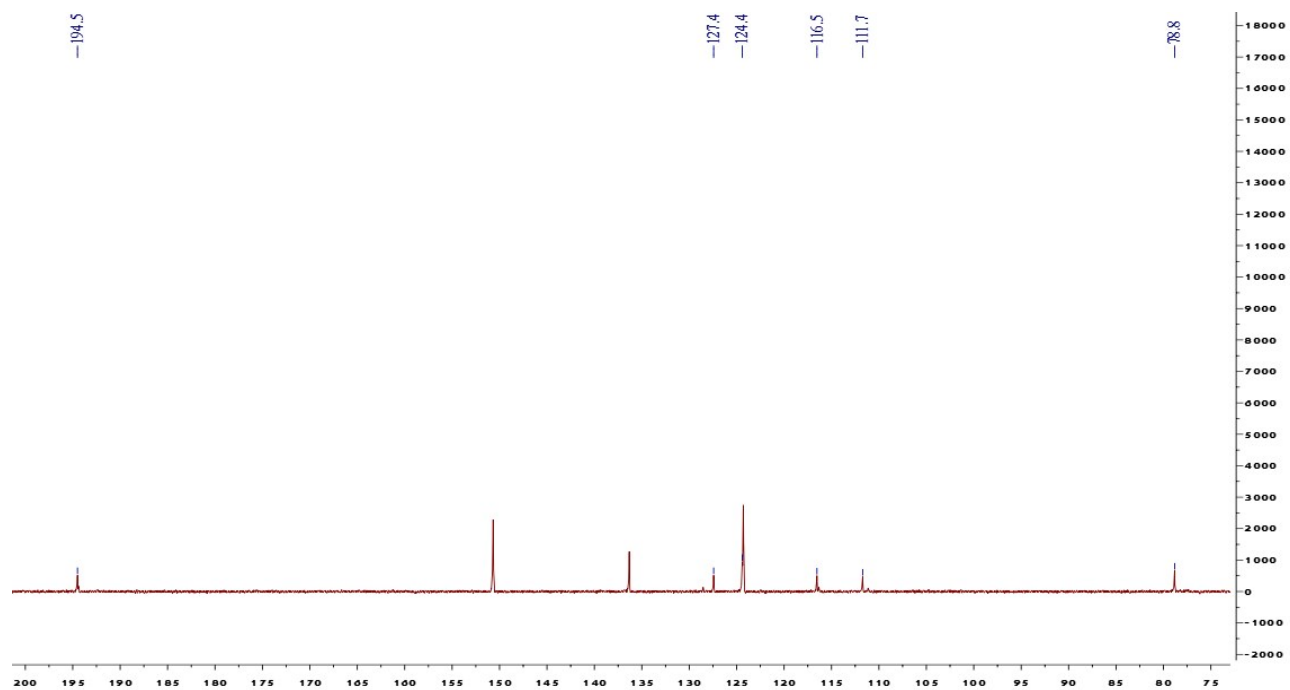


Figure S22. DEPT-135 Spectrum of Stachybonoid C (**3**) in Pyridine-*d*₅

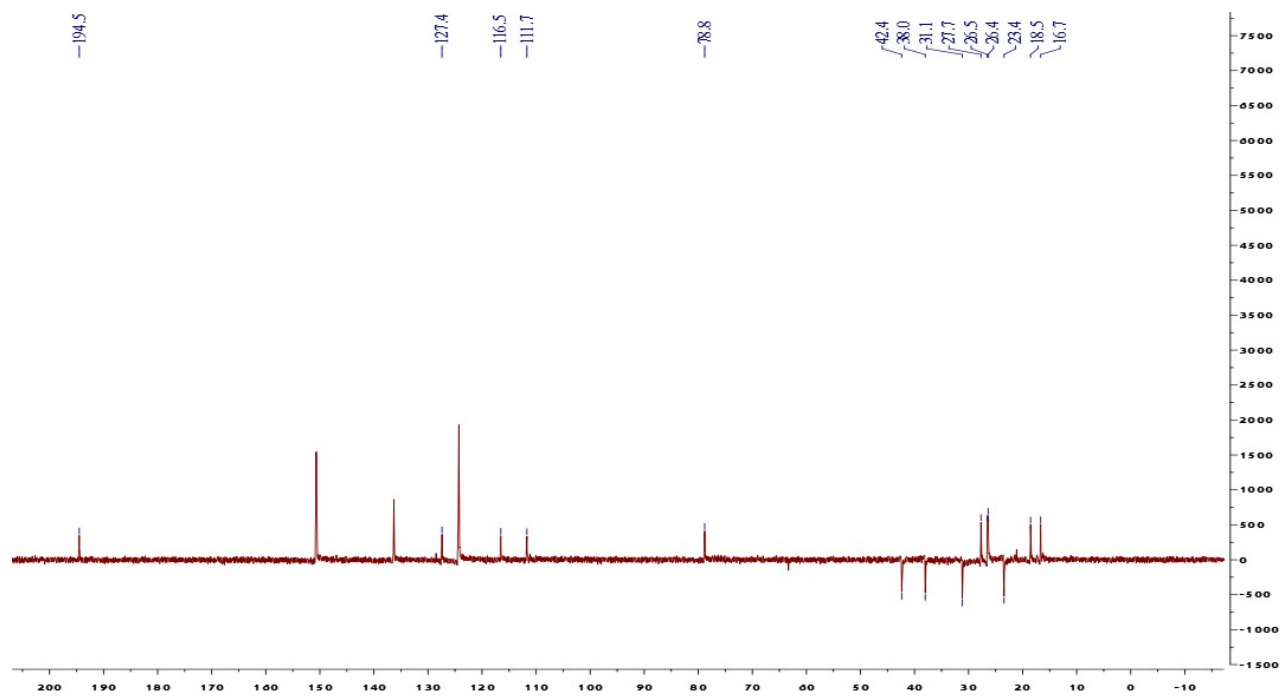


Figure S23. HSQC Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

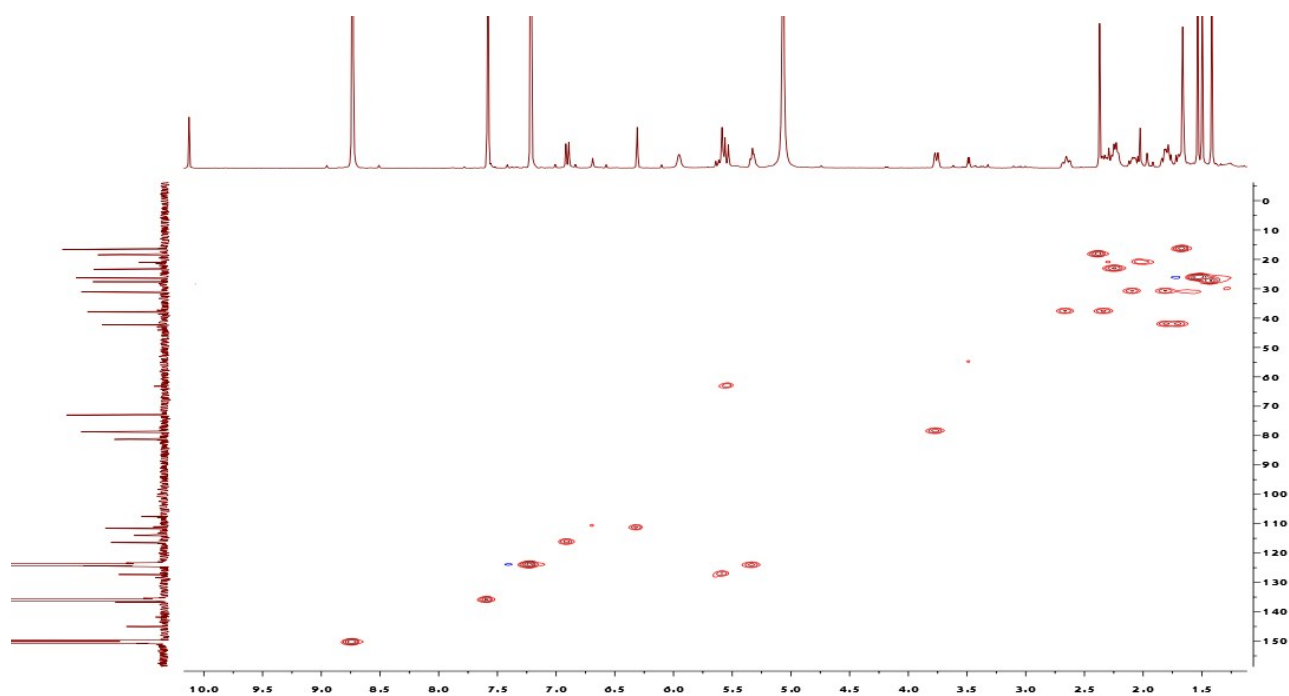


Figure S24. HMBC Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

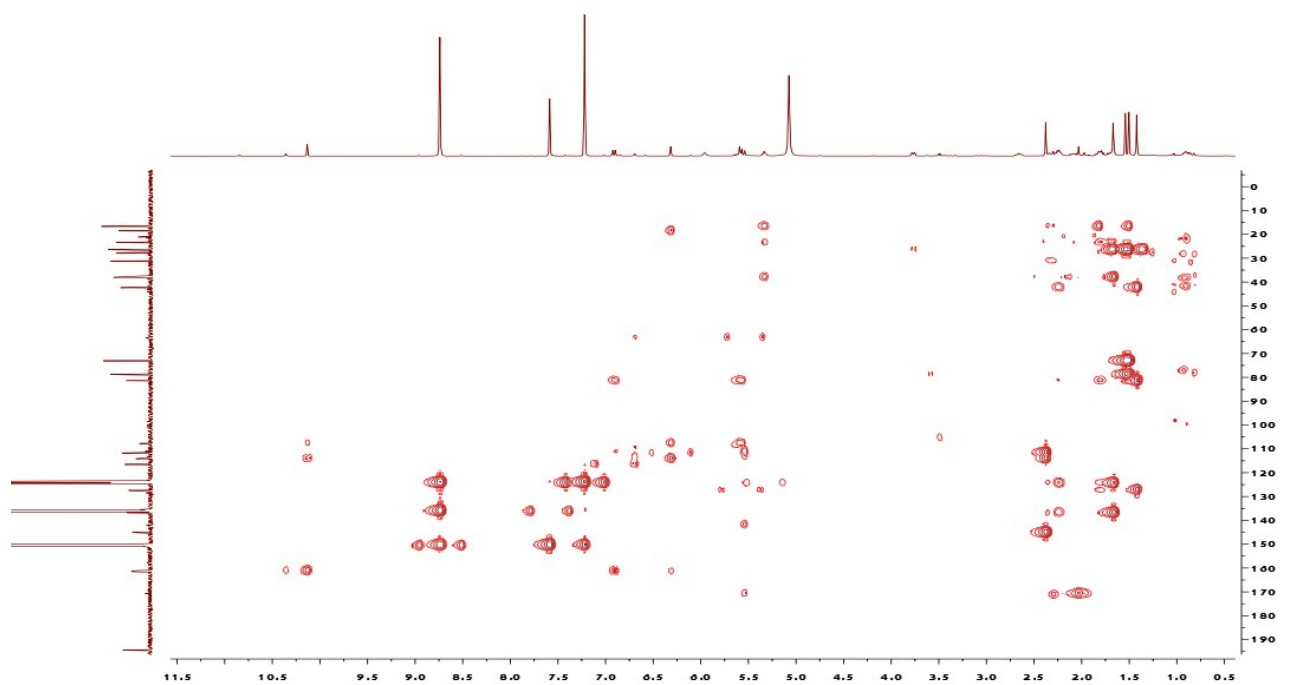


Figure S25. ^1H - ^1H COSY Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

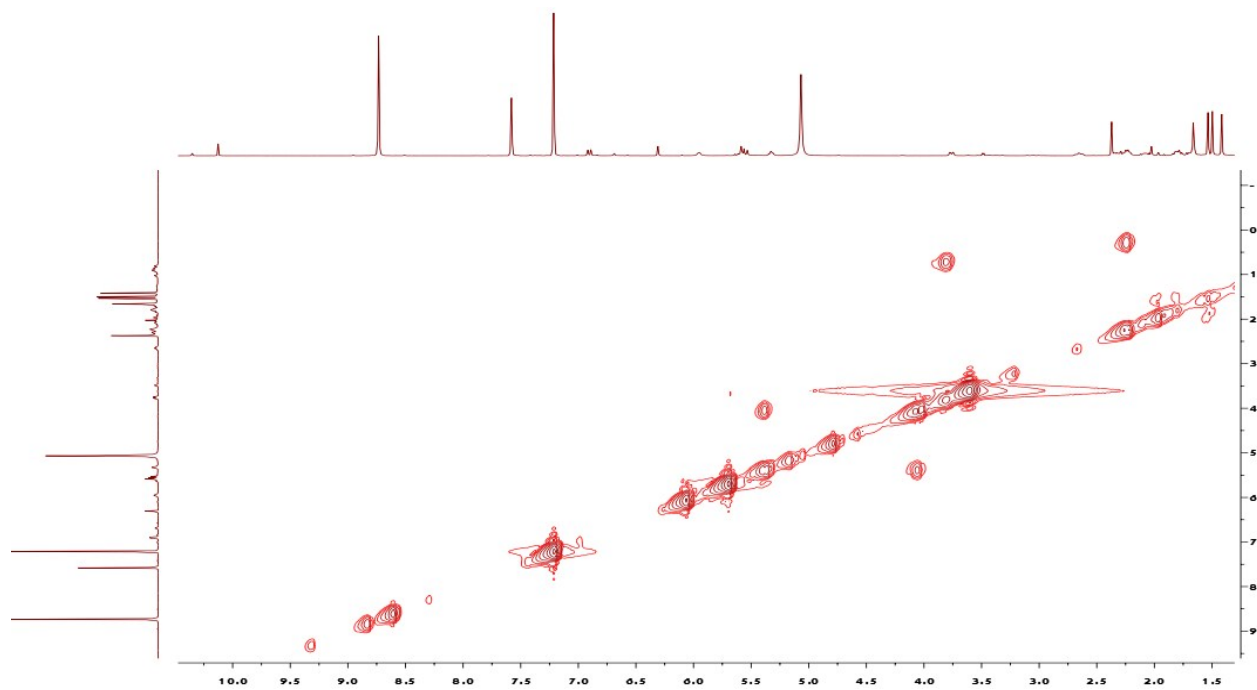


Figure S26. NOESY Spectrum of Stachybonoid C (**3**) in Pyridine- d_5

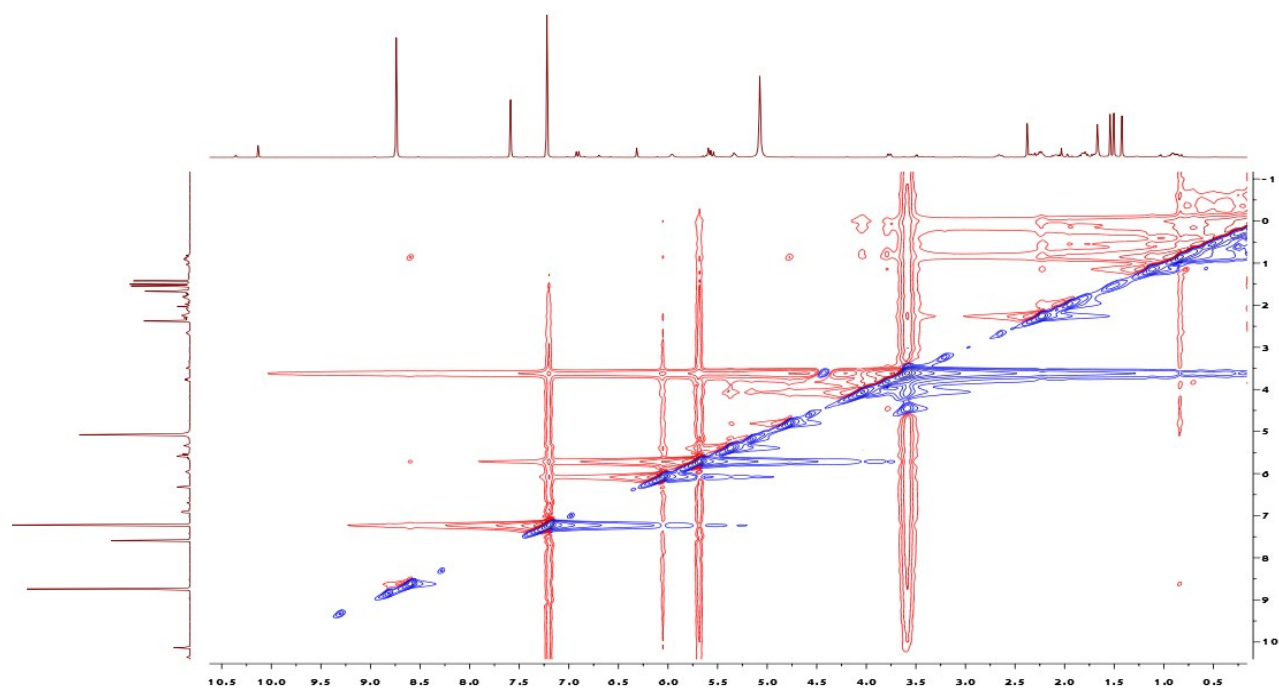


Figure S27. HR-ESIMS of Stachybonoid C (**3**)

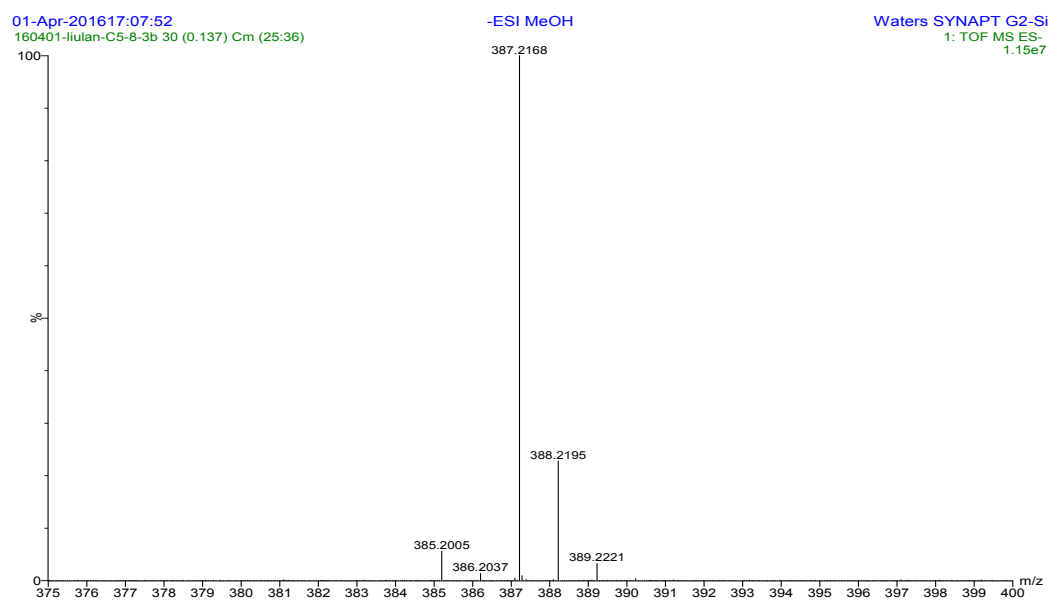


Figure S28. ^1H (400 MHz) NMR Spectrum of Stachybonoid D (**5**) in Pyridine- d_5

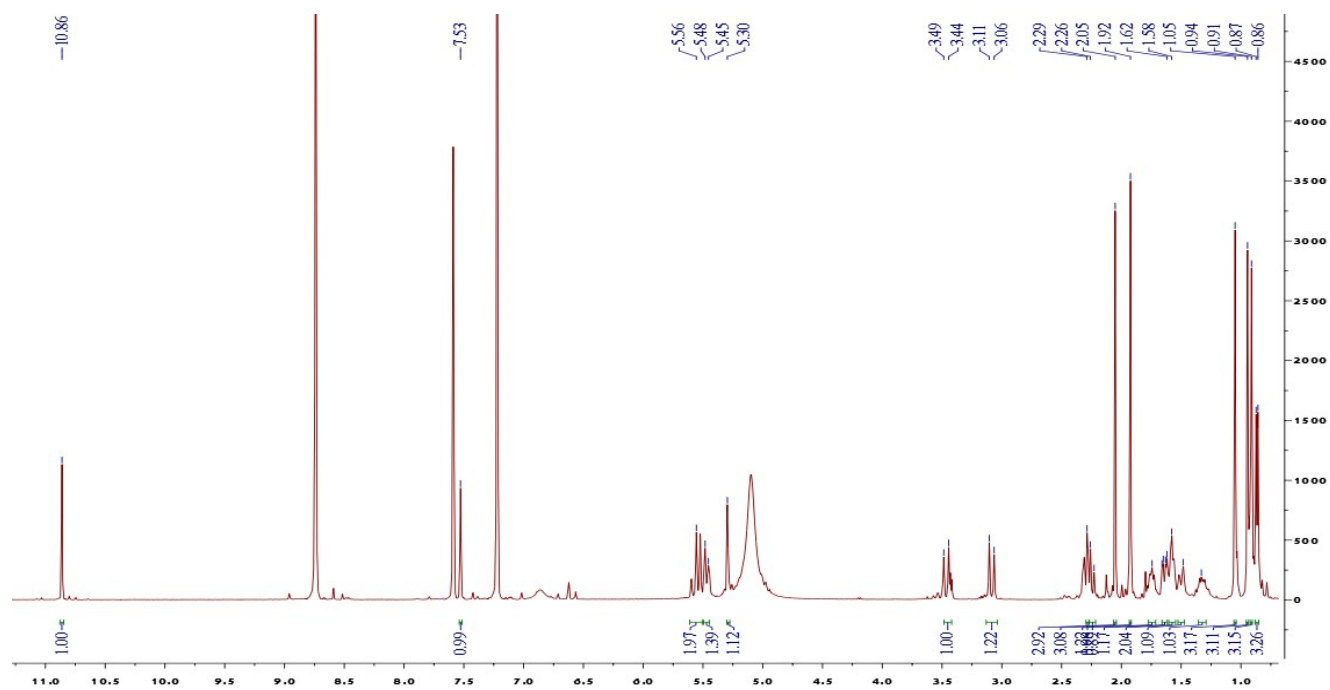


Figure S29. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid D (**5**) in Pyridine- d_5

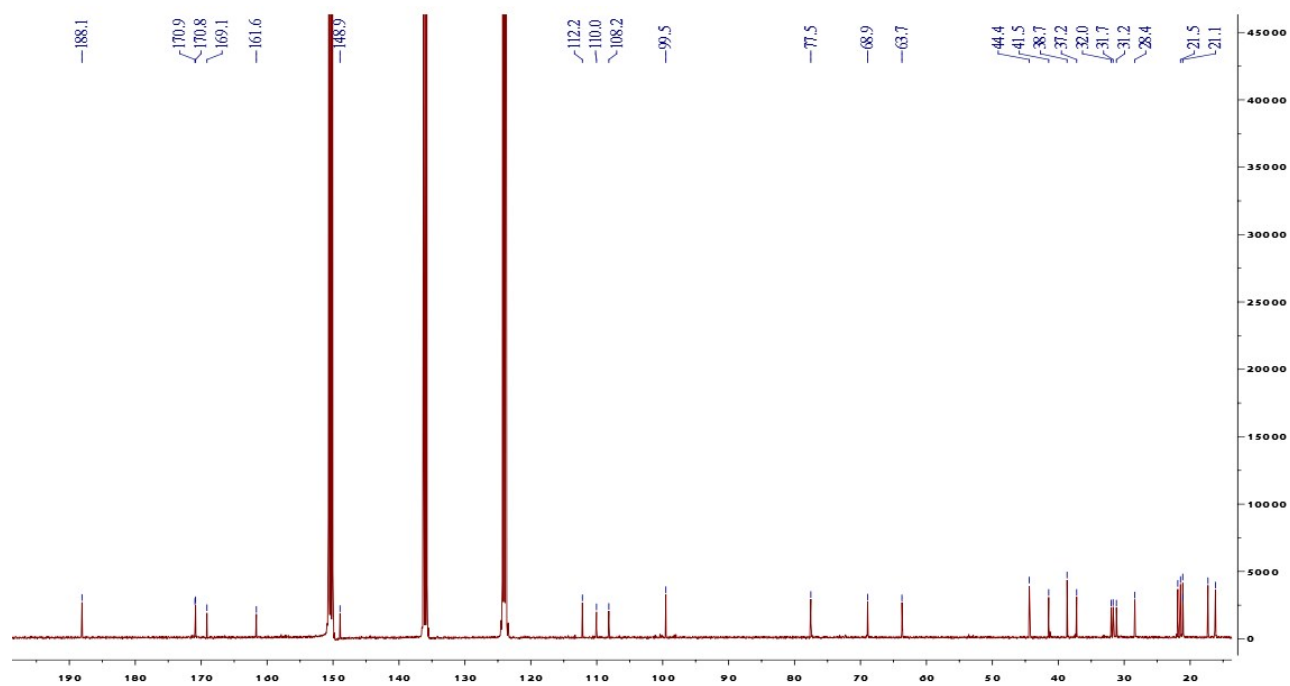


Figure S30. DEPT-90 Spectrum of Stachybonoid D (**5**) in Pyridine- d_5

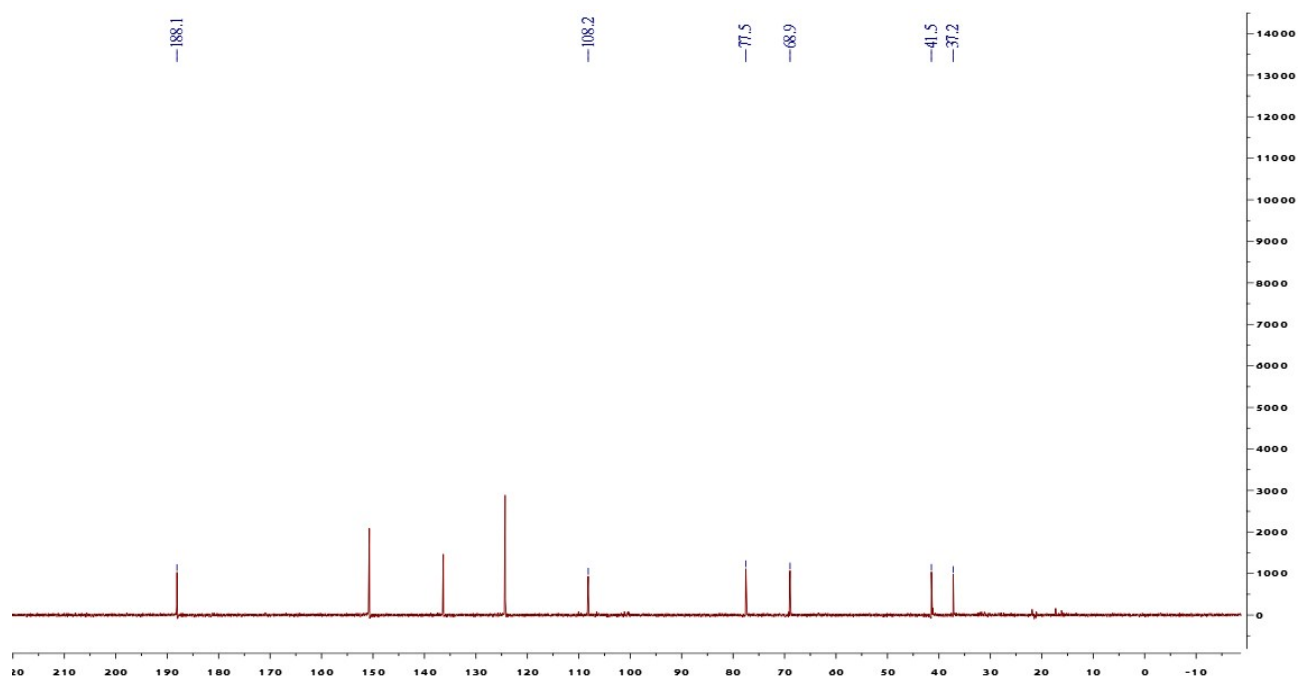


Figure S31. DEPT-135 Spectrum of Stachybonoid D (**5**) in Pyridine-*d*₅

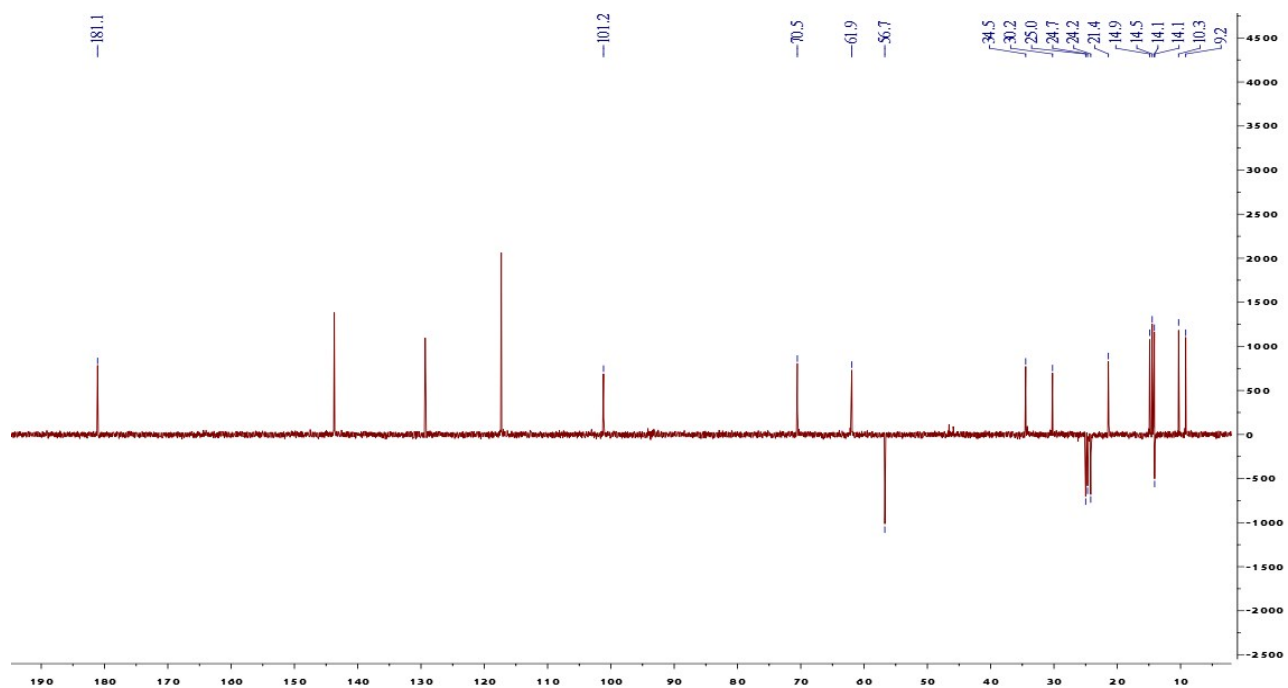


Figure S32. HSQC Spectrum of Stachybonoid D (**5**) in Pyridine-*d*₅

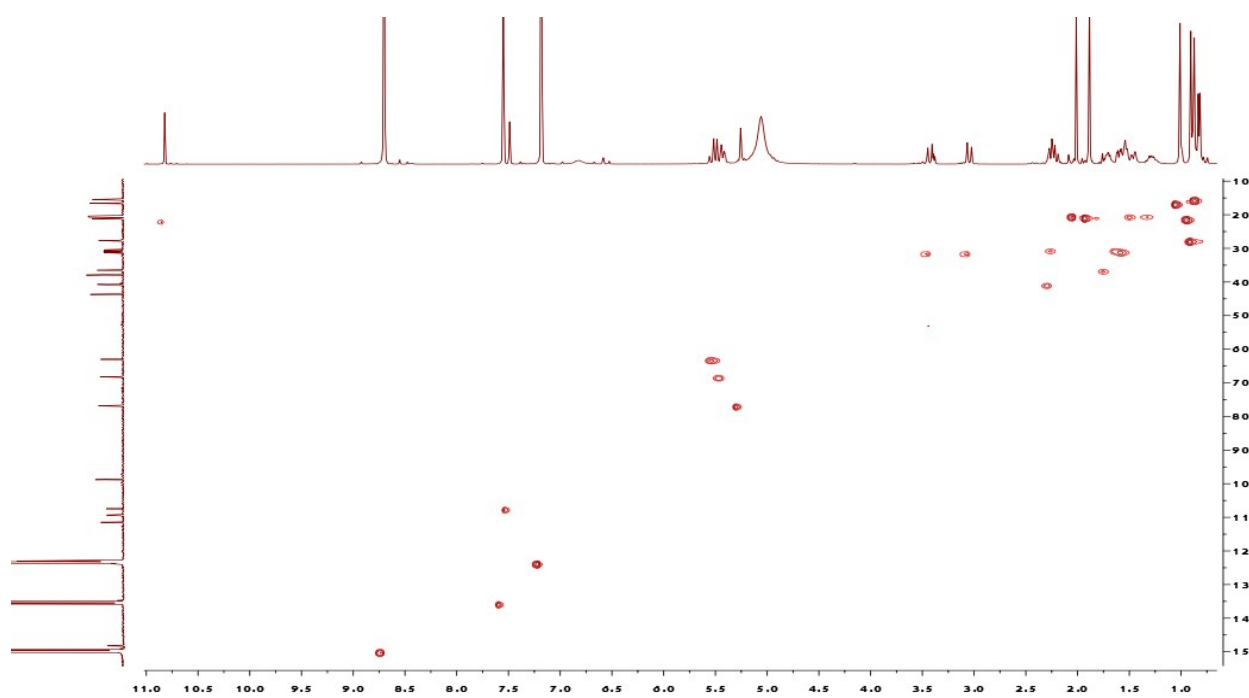


Figure S33. HMBC Spectrum of Stachybonoid D (**5**) in Pyridine-*d*₅

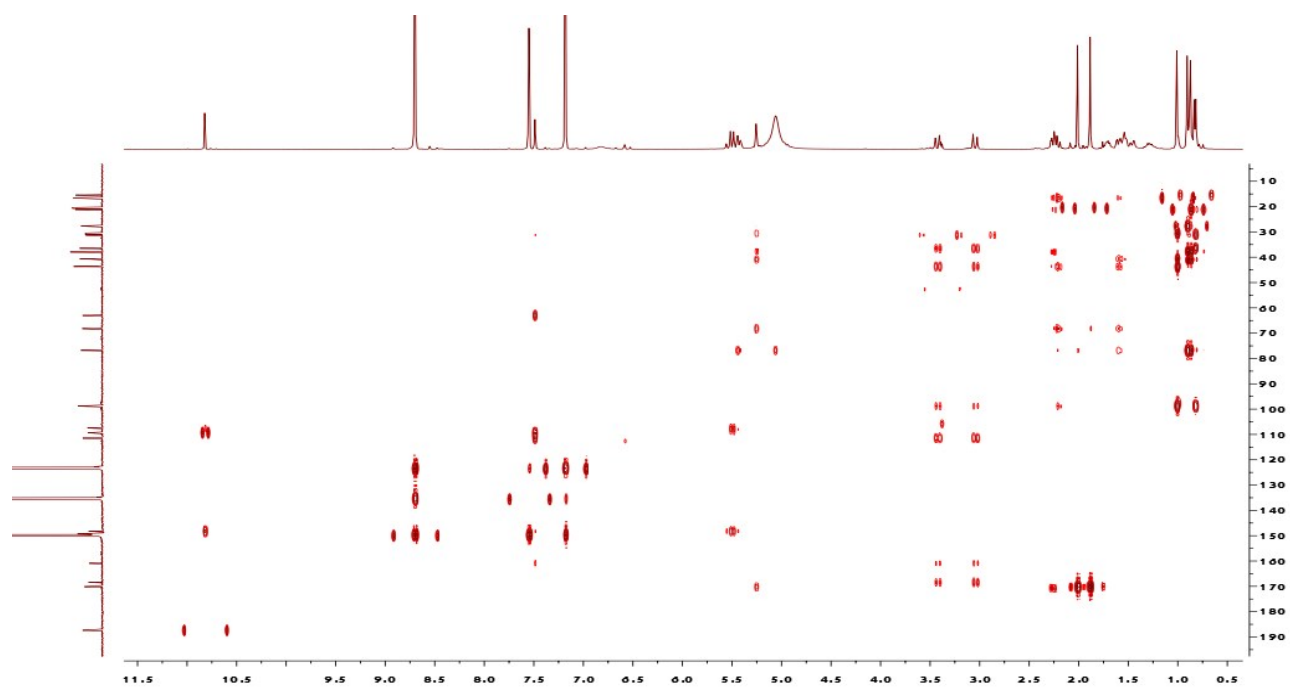


Figure S34. ¹H-¹H COSY Spectrum of Stachybonoid D (**5**) in Pyridine-*d*₅

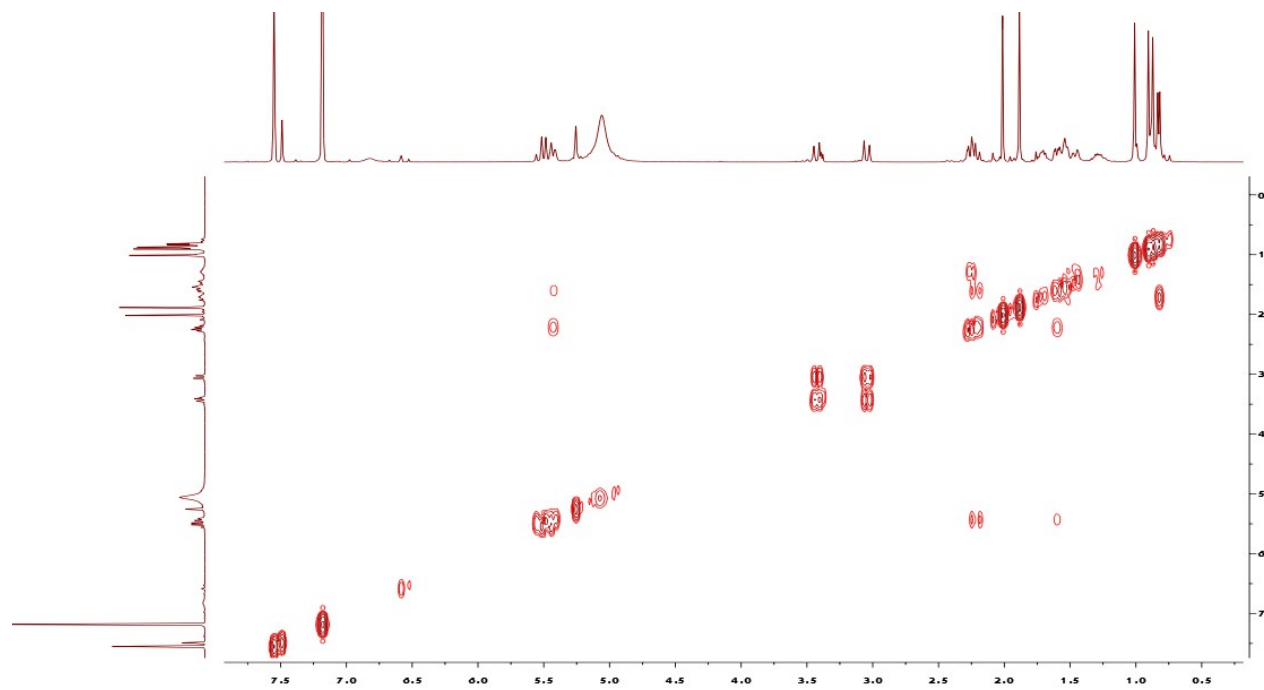


Figure S35. NOESY Spectrum of Stachybonoid D (**5**) in Pyridine-*d*₅

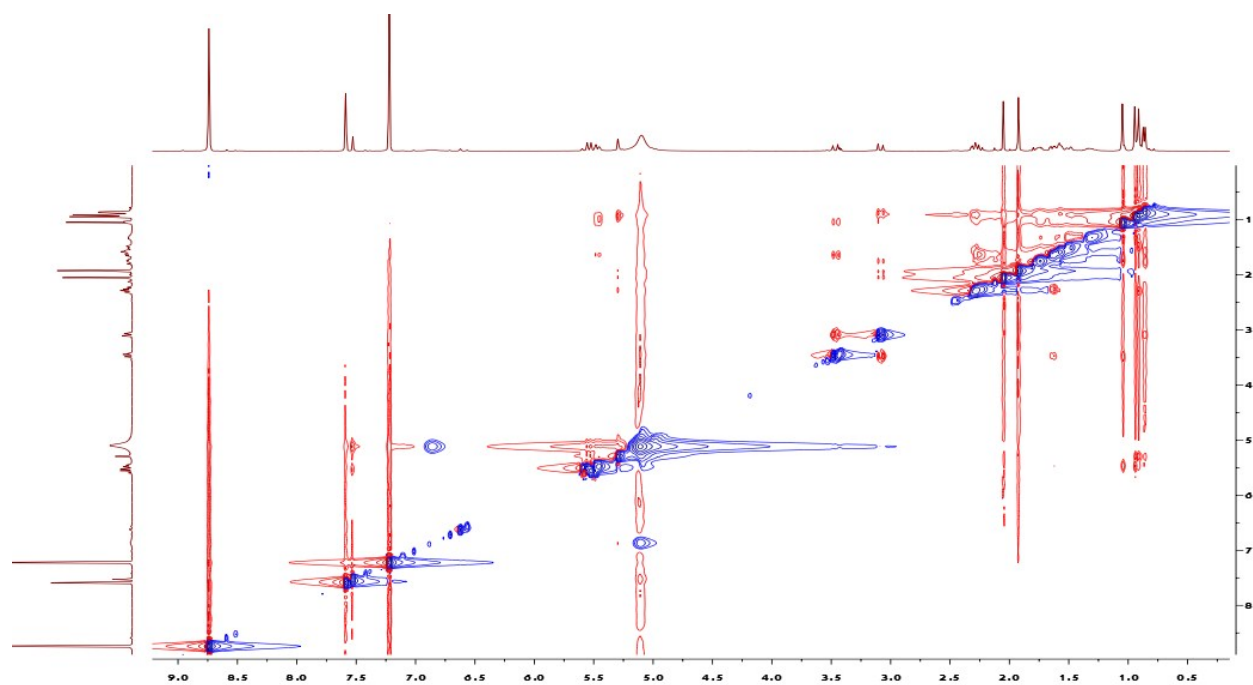


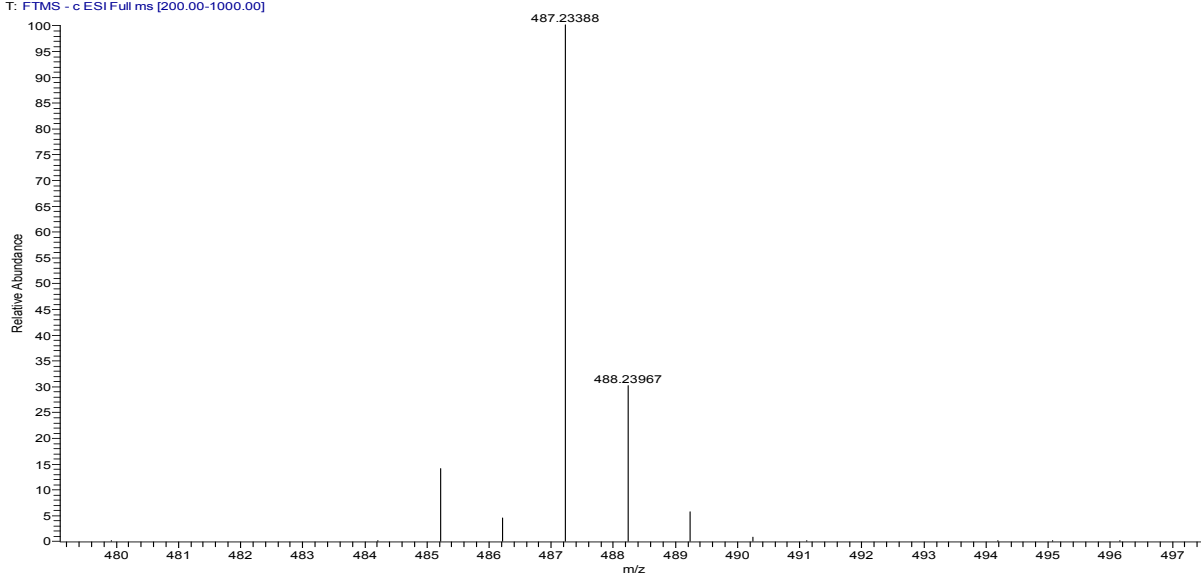
Figure S36. HR-ESIMS of stachybonoid D (**5**)

D:\Data\2016\03\Liu\lan\1603a0598-4

3/17/2016 4:51:50 PM

C-8-3A3

1603a0598-4 #15-20 RT: 0.07-0.09 AV: 6 SB: 21 0.01-0.04 , 0.21-0.28 NL: 2.12E7
T: FTMS - c ESI Full ms [200.00-1000.00]



SPECTRUM -
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
487.23388	487.23374	0.28	10.5	C27 H35 O8

Figure S37. ^1H (400 MHz) NMR Spectrum of Stachybonoid E (**6**) in Pyridine- d_5

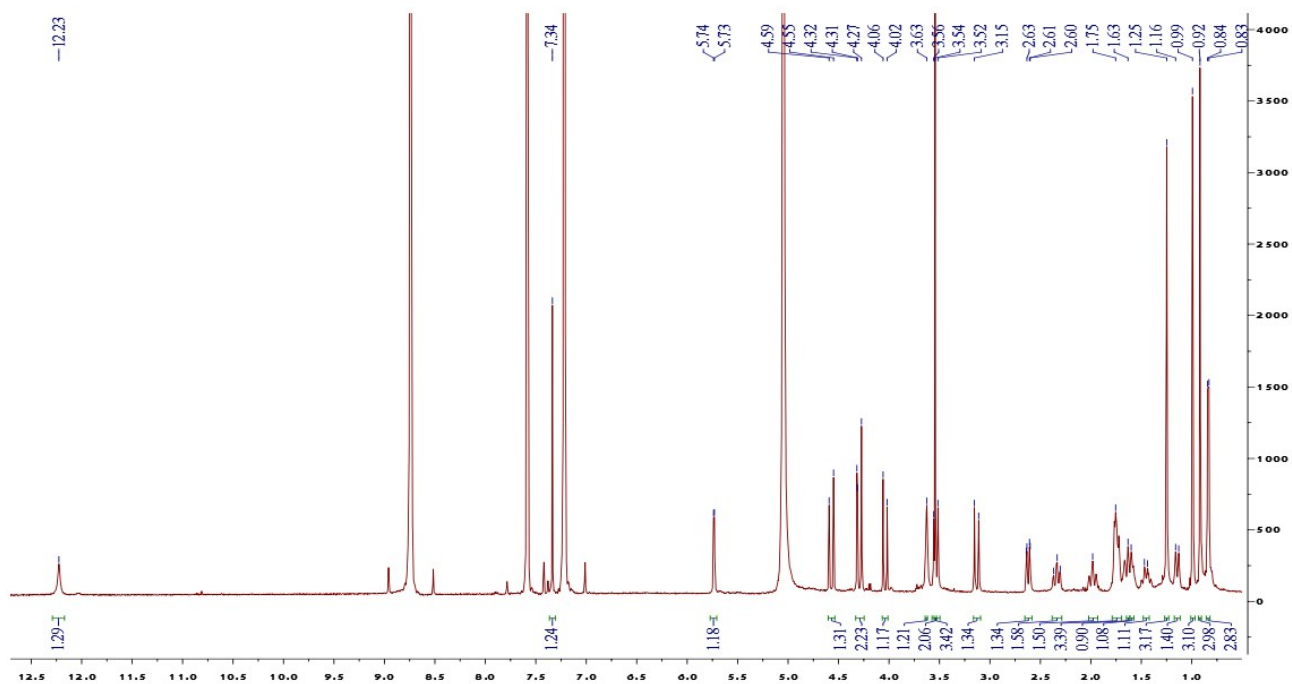


Figure S38. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid E (**6**) in Pyridine- d_5

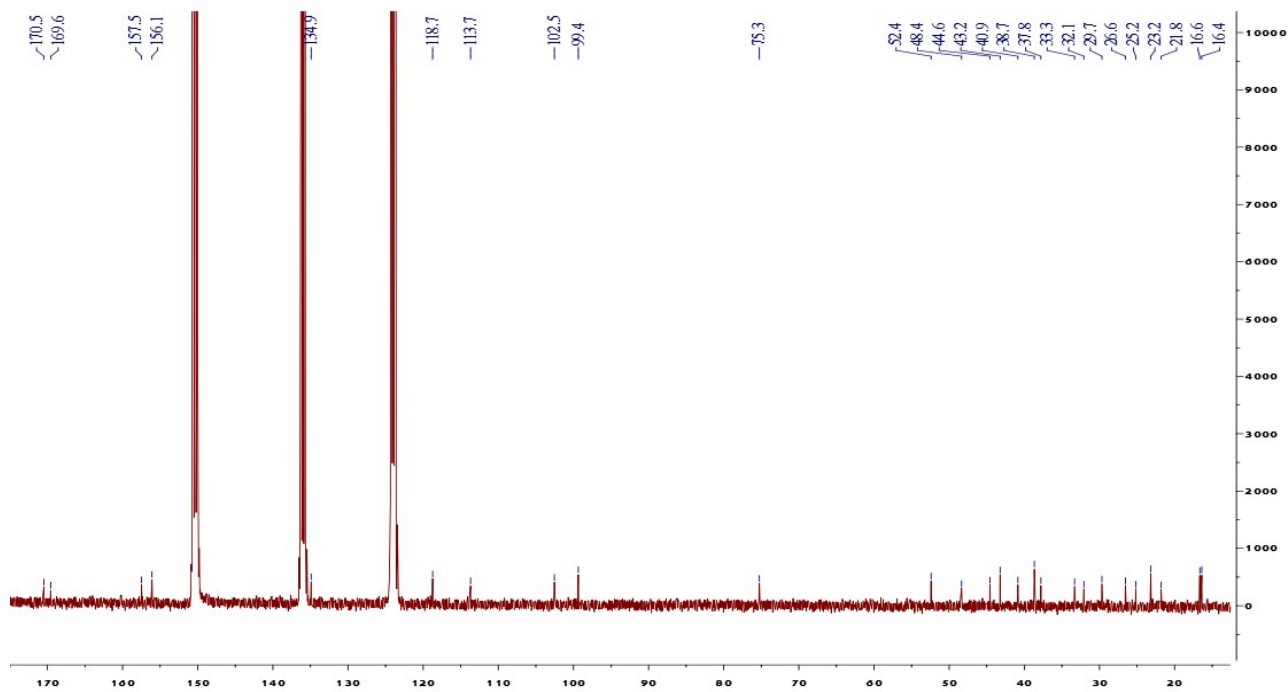


Figure S39. DEPT-90 Spectrum of Stachybonoid E (**6**) in Pyridine-*d*₅

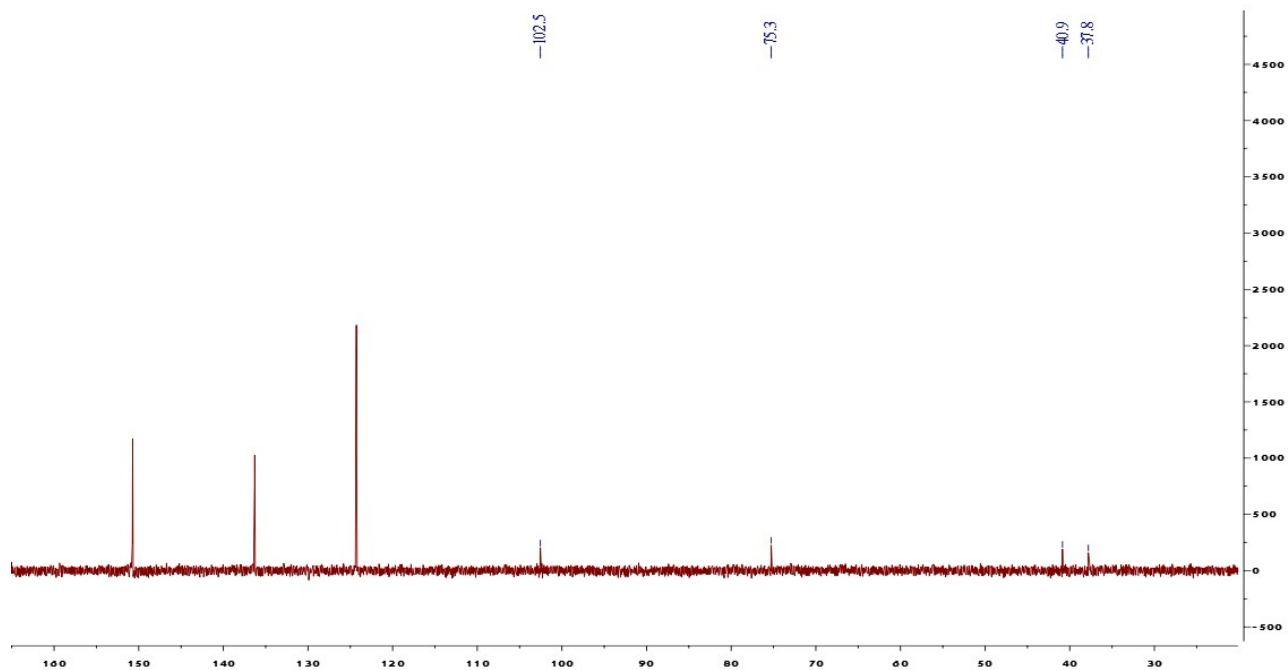


Figure S40. DEPT-135 Spectrum of Stachybonoid E (**6**) in Pyridine-*d*₅

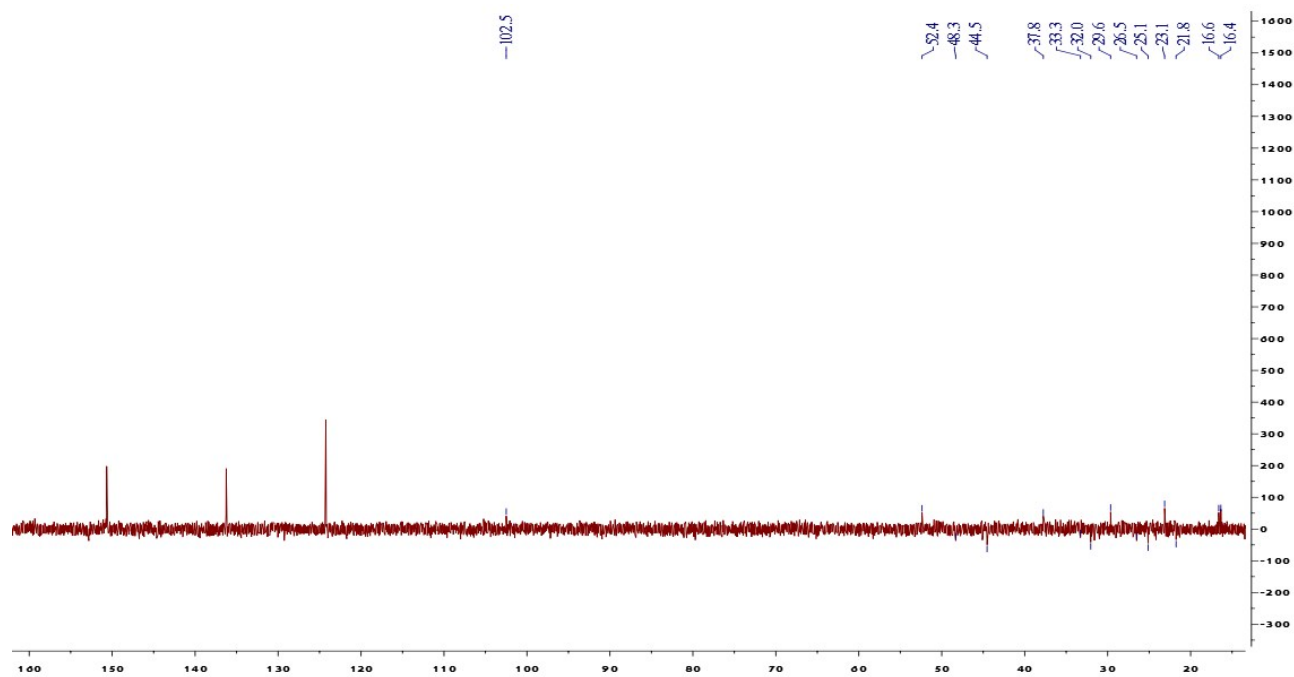


Figure S41. HSQC Spectrum of Stachybonoid E (6) in Pyridine- d_5

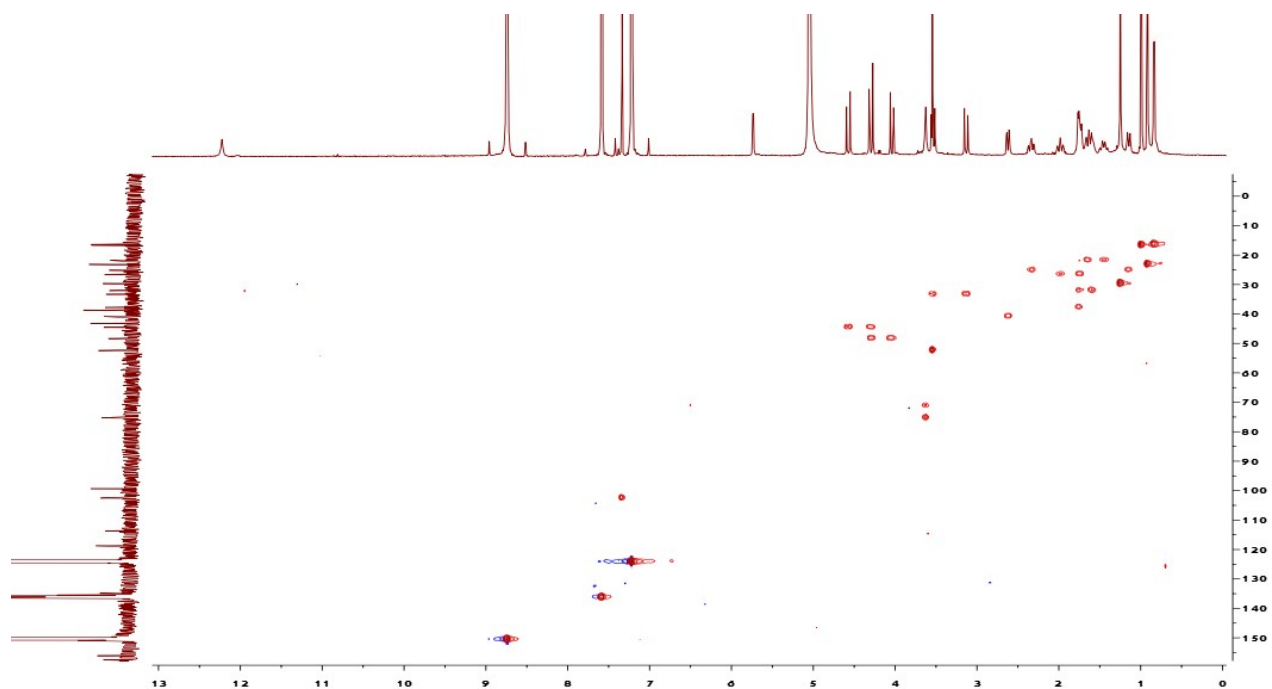


Figure S42. HMBC Spectrum of Stachybonoid E (6) in Pyridine- d_5

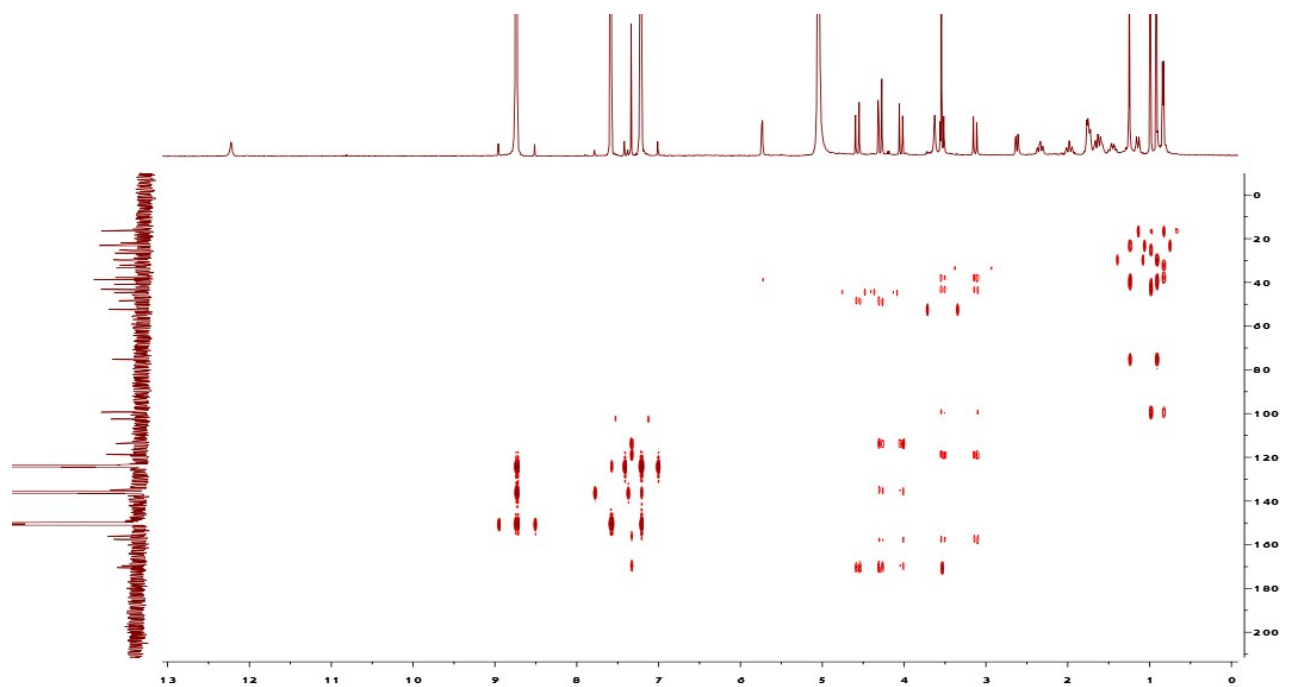


Figure S43. ^1H - ^1H COSY Spectrum of Stachybonoid E (**6**) in Pyridine- d_5

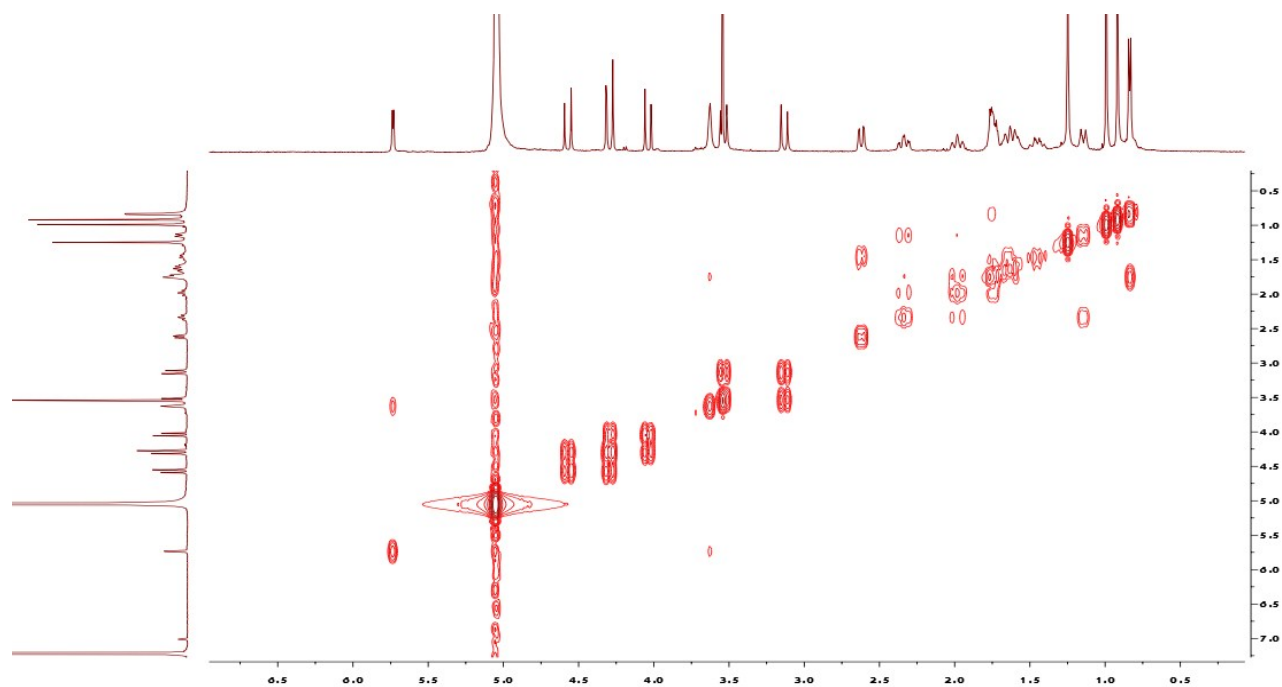


Figure S44. NOESY Spectrum of Stachybonoid E (**6**) in Pyridine- d_5

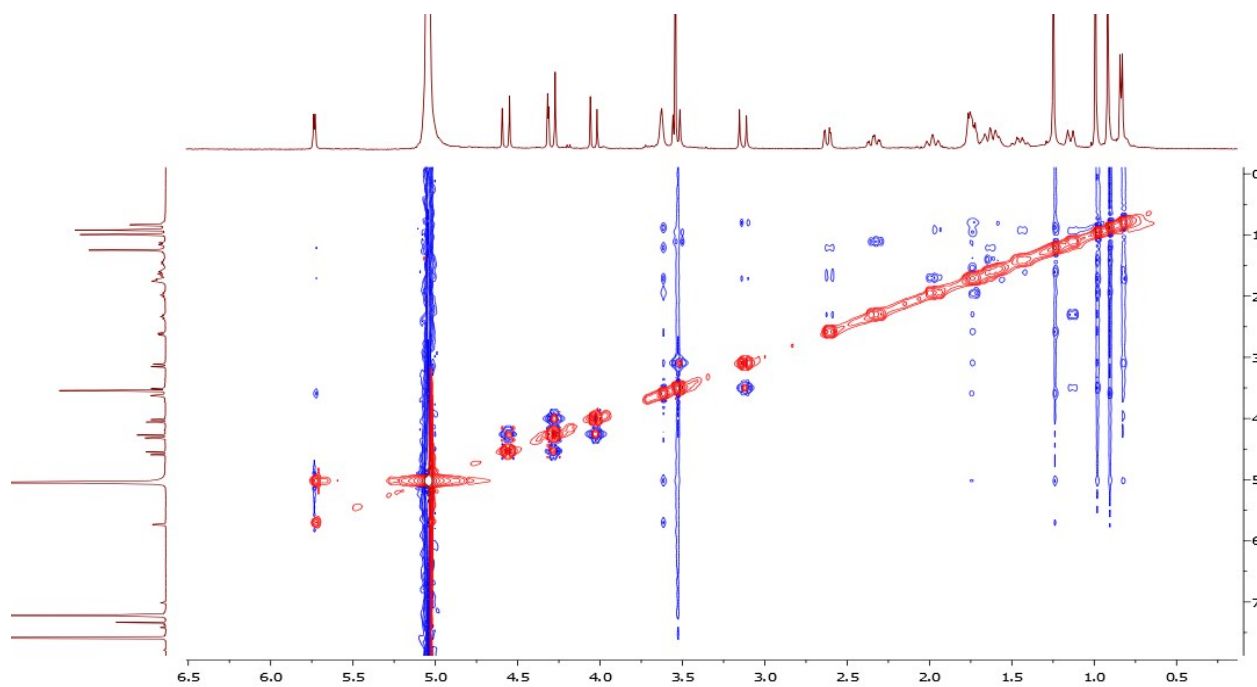
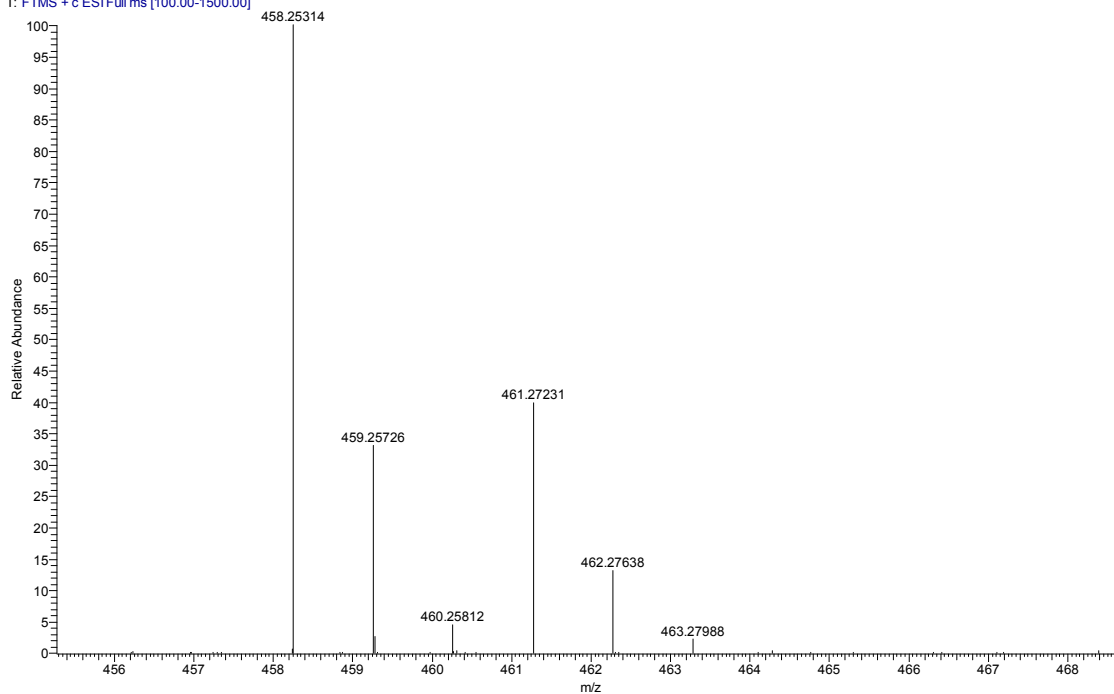


Figure S45. HR-ESIMS of Stachybonoid E (6)

1704A0194-2 #14-19 RT: 0.08-0.11 AV: 6 NL: 7.82E5
T: FTMS + c ESI Full ms [100.00-1500.00]



SPECTRUM -
simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
458.25314	458.25371	-1.25	9.5	C26 H36 O6 N

Figure S46. ^1H (400 MHz) NMR Spectrum of Stachybonoid F (7) in Pyridine- d_5

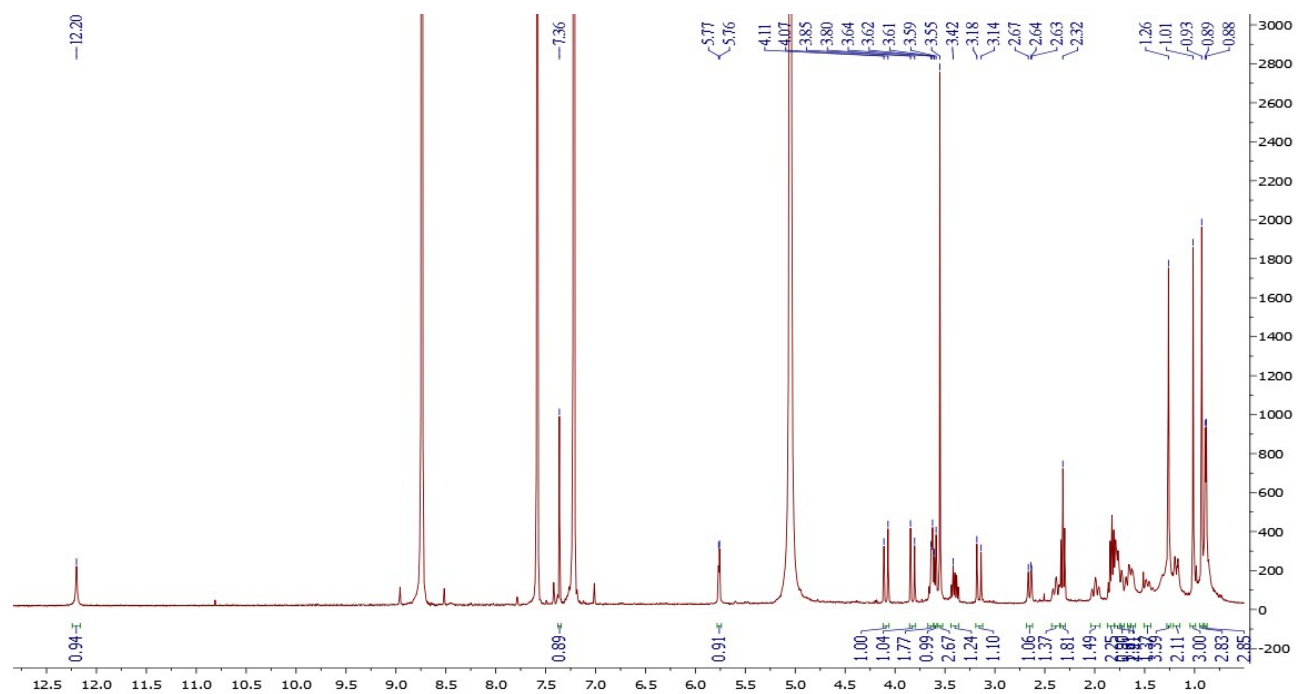


Figure S47. ^{13}C (100 MHz) NMR Spectrum of Stachybonoid F (7) in Pyridine- d_5

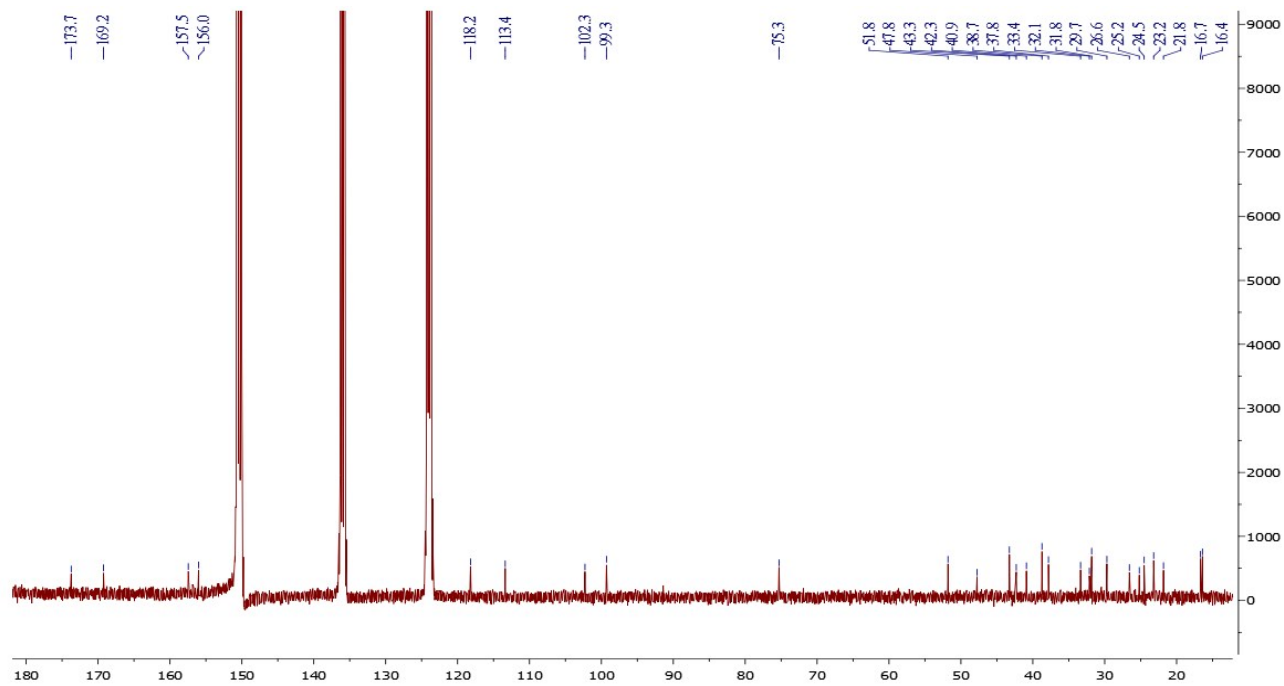


Figure S48. DEPT-90 Spectrum of Stachybonoid F (7) in Pyridine-*d*₅

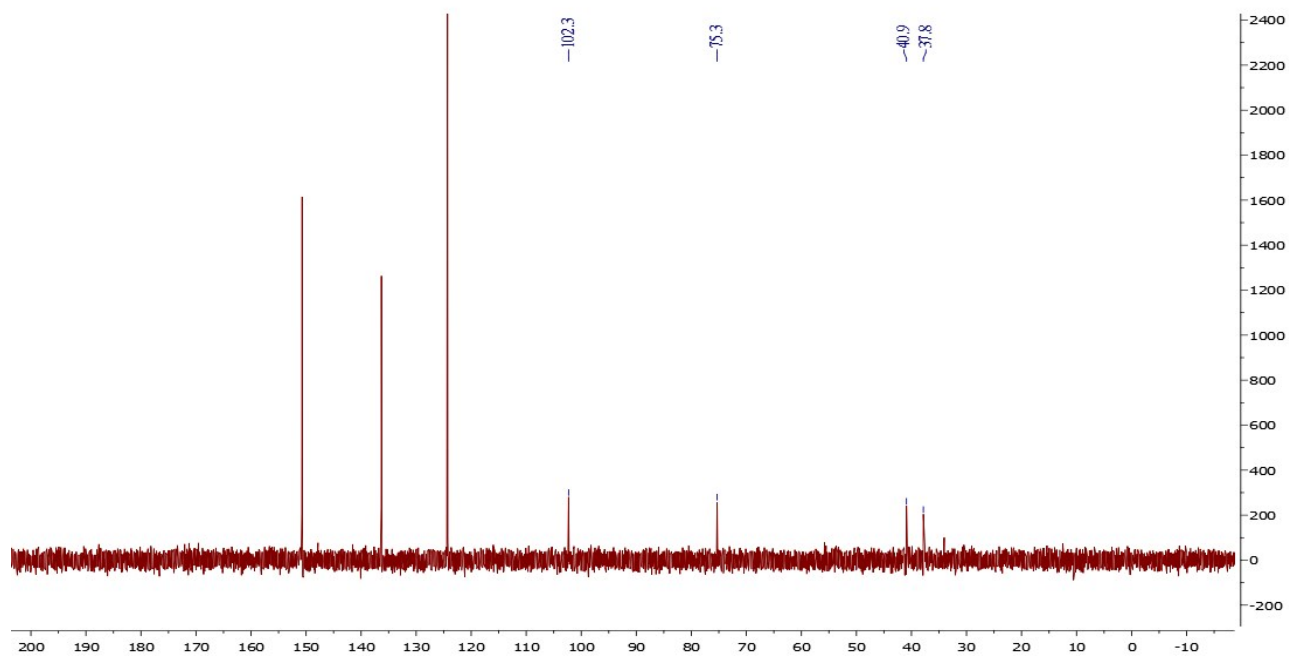


Figure S49. DEPT-135 Spectrum of Stachybonoid F (7) in Pyridine-*d*₅

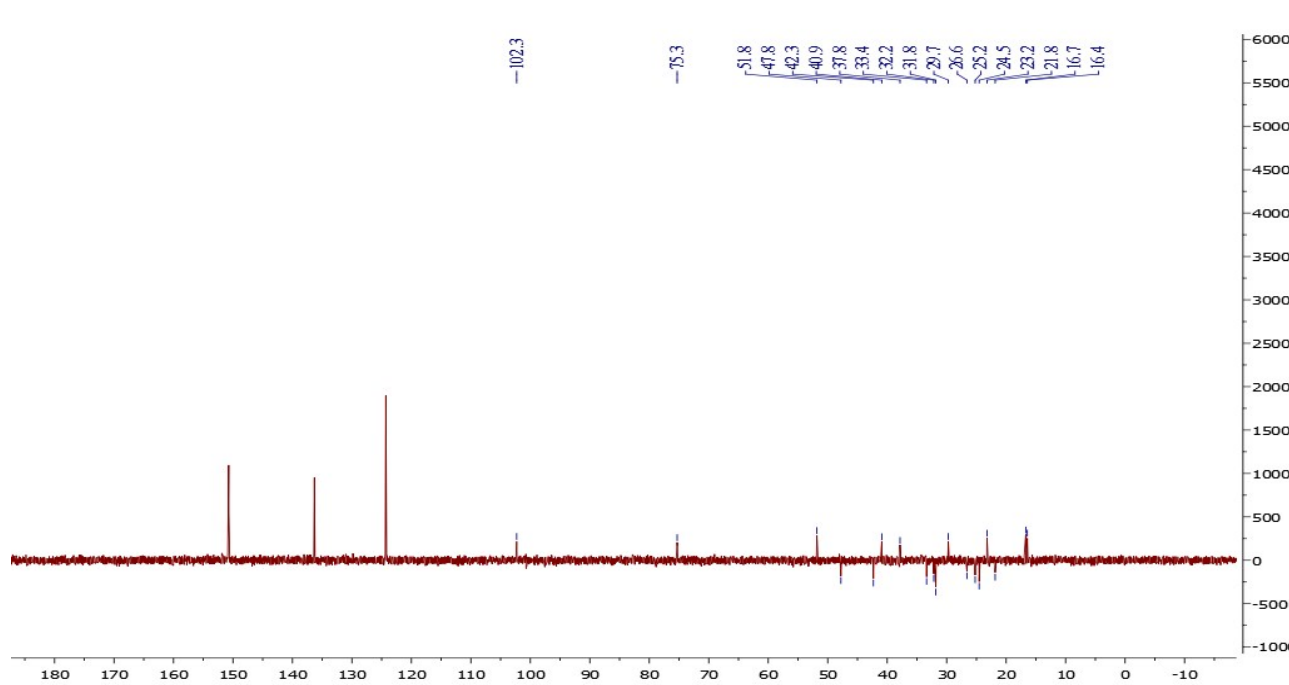


Figure S50. HSQC Spectrum of Stachybonoid F (7) in Pyridine- d_5

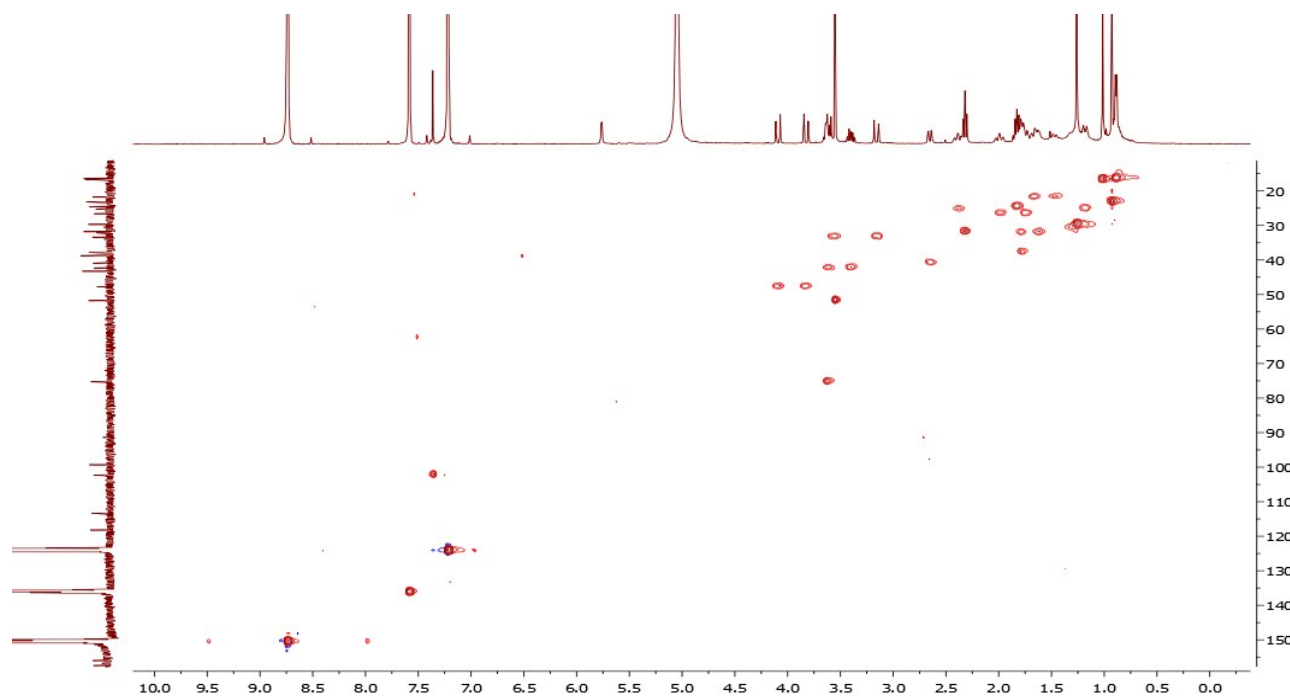


Figure S51. HMBC Spectrum of Stachybonoid F (7) in Pyridine- d_5

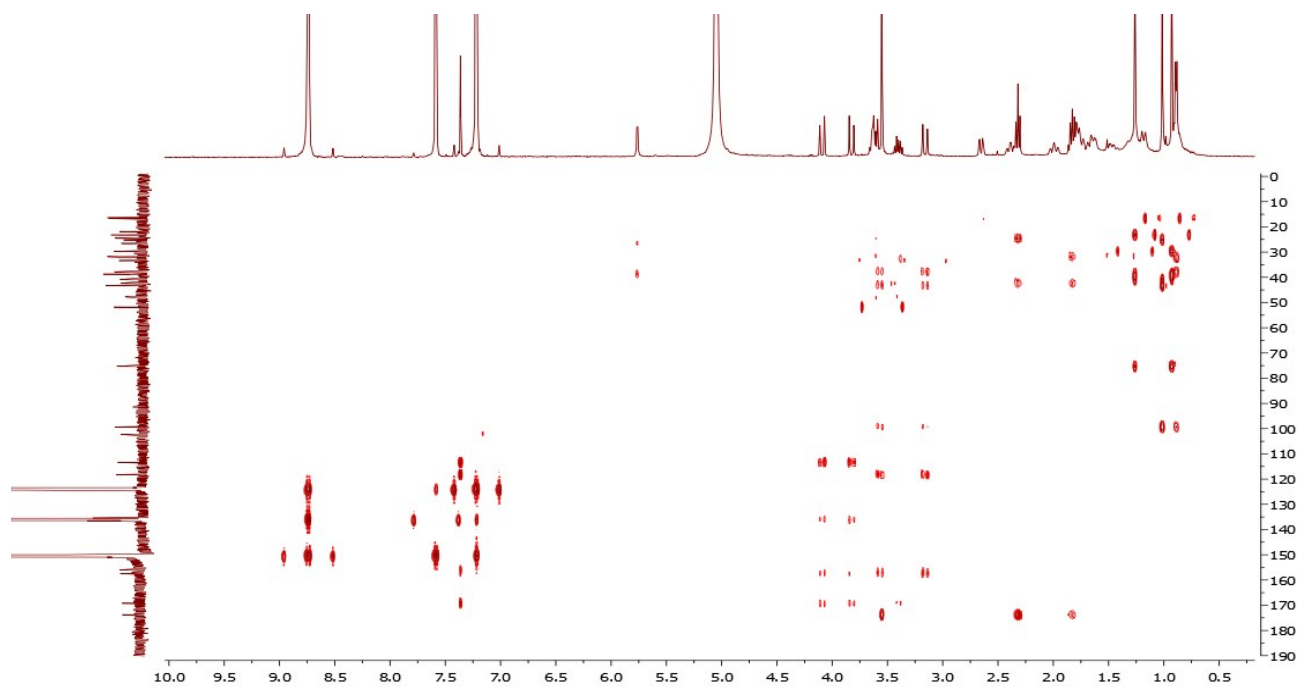


Figure S52. ^1H - ^1H COSY Spectrum of Stachybonoid F (7) in Pyridine- d_5

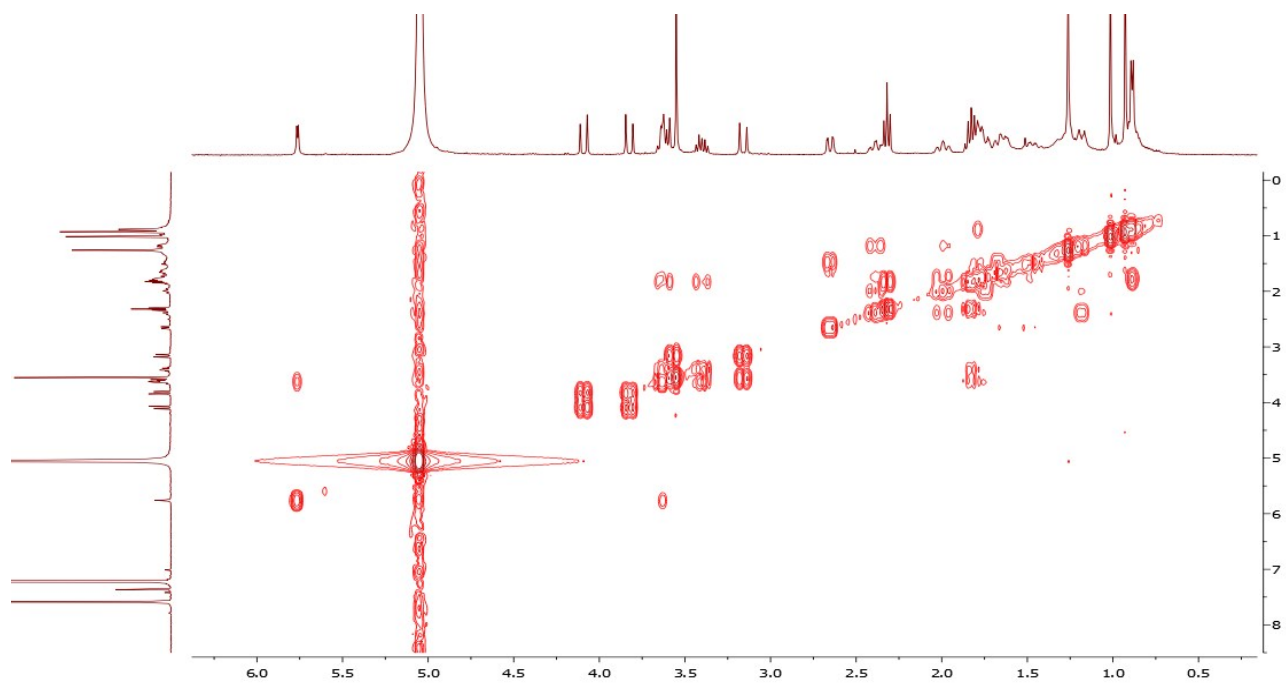


Figure S53. NOESY Spectrum of Stachybonoid F (7) in Pyridine- d_5

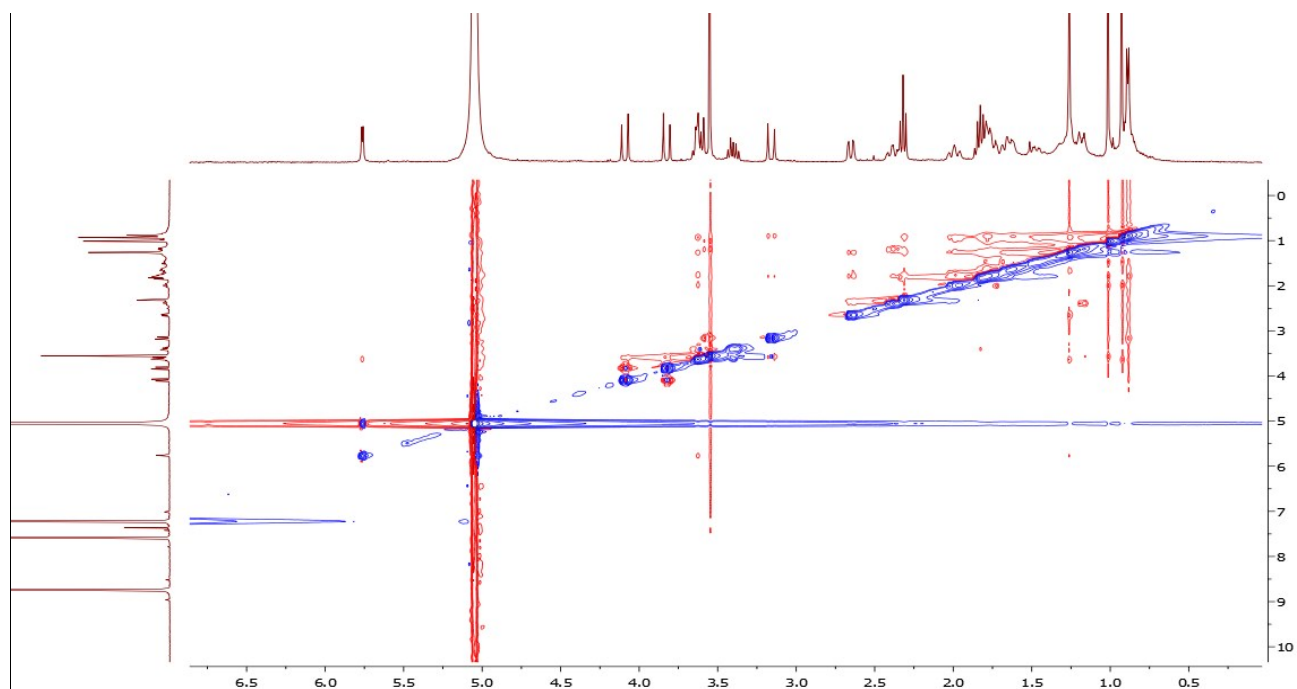
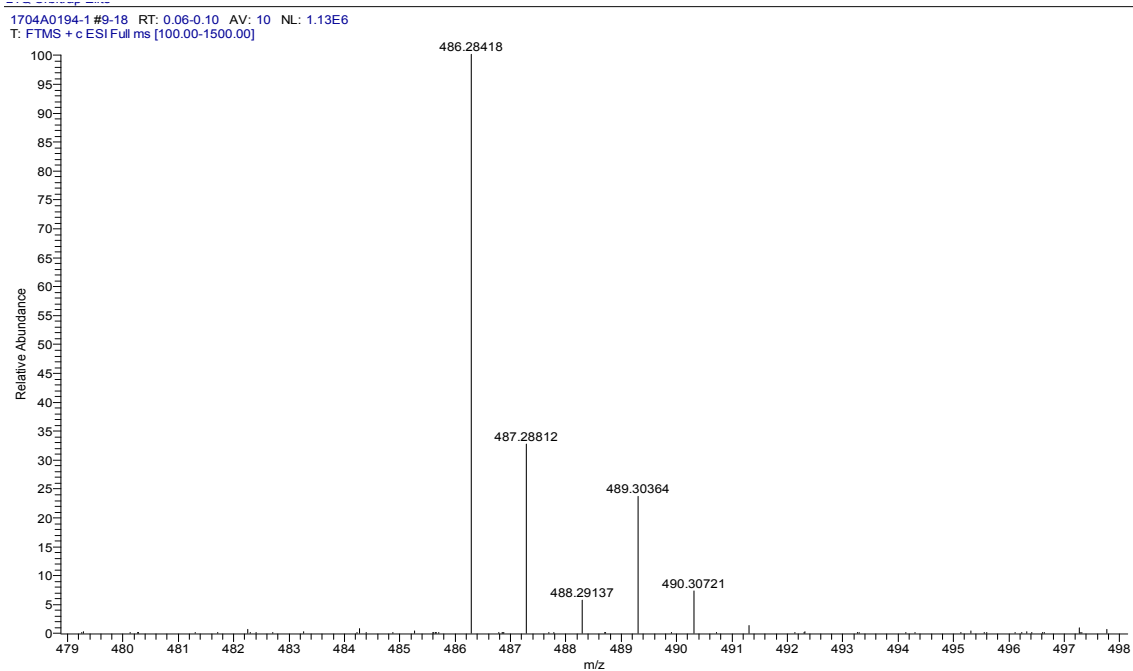


Figure S54. HR-ESIMS of Stachybonoid F (7)



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
486.28418	486.28501	-1.72	9.5	C28 H40 O6 N

Figure S55. ^1H (400 MHz) NMR Spectrum of (S)-MTPA ester derivative (1a) in Pyridine- d_5

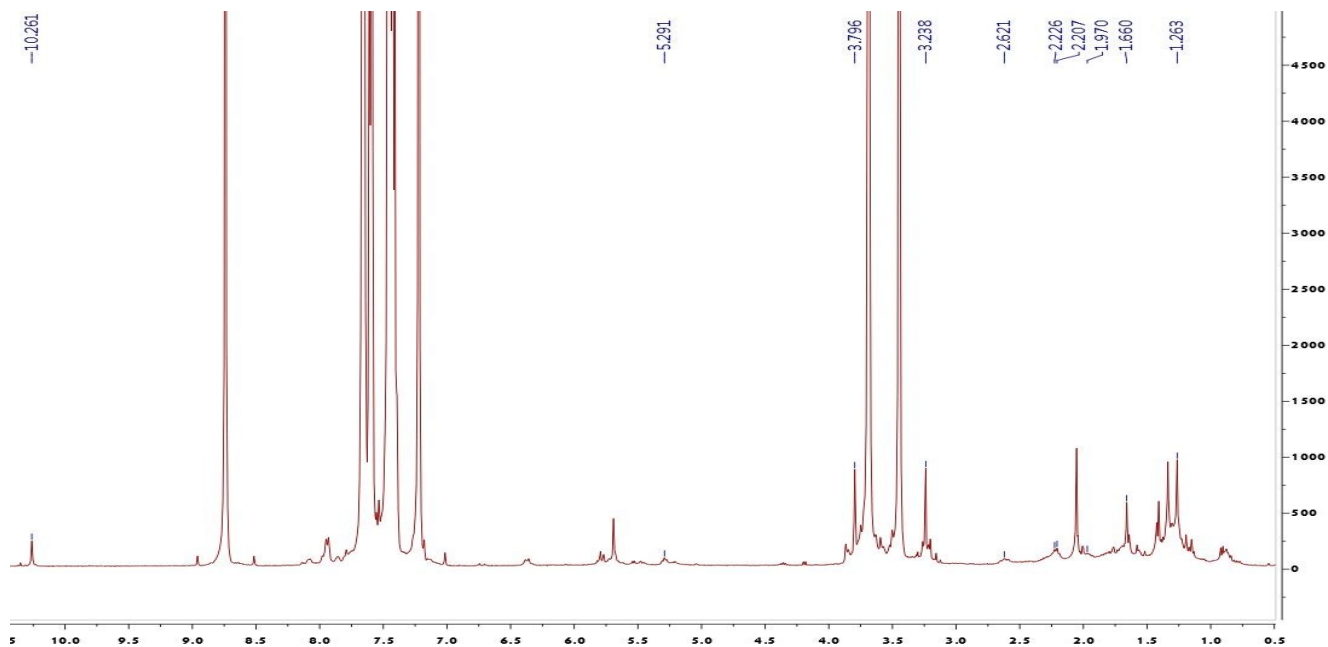


Figure S56. ^1H (400 MHz) NMR Spectrum of (R)-MTPA ester derivative (**1b**) in Pyridine- d_5

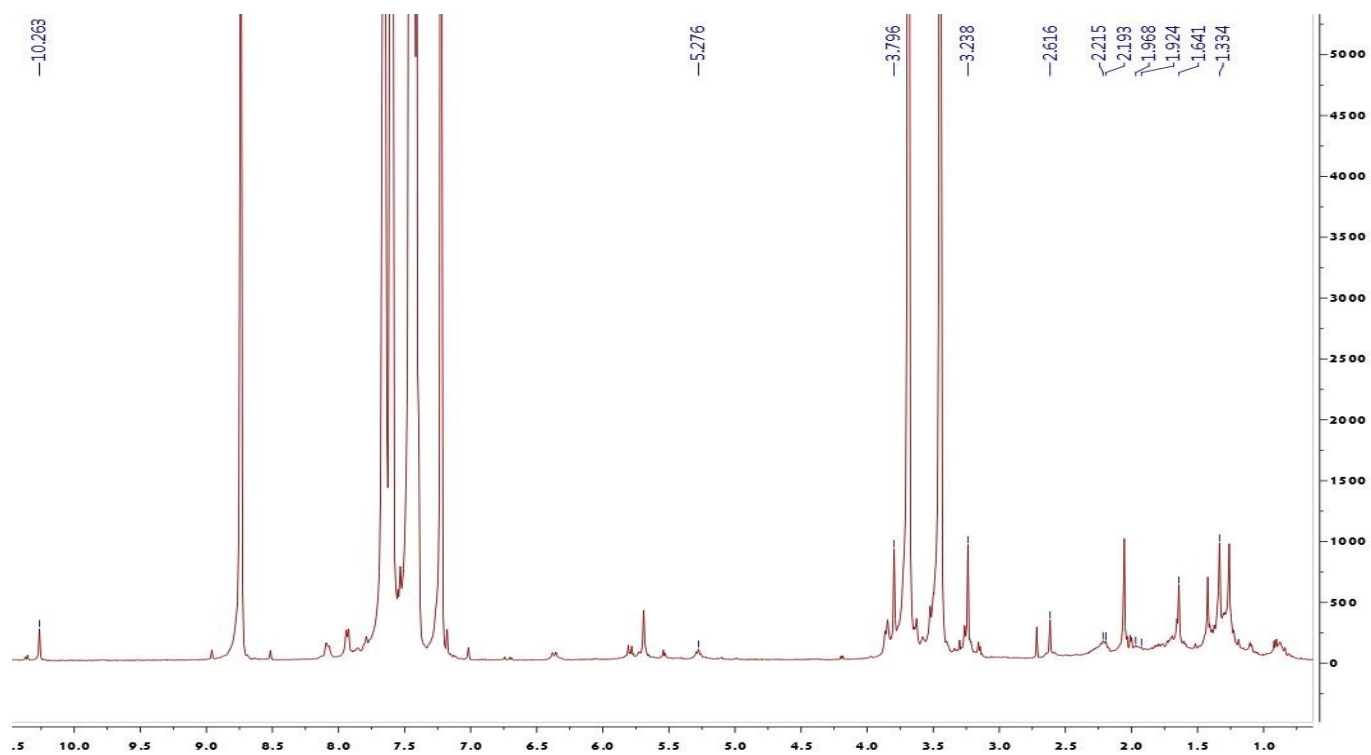


Figure S57. Structure of **8** resulting from single-crystal X-ray diffraction. Single crystal X-ray crystallographic data was obtained on a Rigaku Oxford diffractometer equipped with graphite-monochromatized Cu K α radiation ($\lambda = 1.54178 \text{ \AA}$) at 298(2) K. Structure solution and refinement were performed with SHELXS-97, and all non-hydrogen atoms were refined anisotropically using the full-matrix least-squares method. All hydrogen atoms were positioned by geometric calculations and difference Fourier overlapping calculations. C₂₃H₃₀O₅, M = 386.49, orthorhombic crystal (0.55 × 0.50 × 0.40 mm), colorless block, space group P212121; unit cell dimensions $a = 10.88250(10) \text{ \AA}$, $b = 13.45840(10) \text{ \AA}$, $c = 13.64720(10) \text{ \AA}$, $V = 1998.78(3) \text{ \AA}^3$; $Z = 40$; a total of 3657 unique reflections [$R(\text{int}) = 0.0178$] was measured, of which 3657 were observed ($|F|^2 \geq 2\sigma|F|^2$); the final refinement gave $R_1 = 0.0278$, $wR2 = 0.0709$, and $S = 1.078$; Flack parameter = 0.00(3). Crystallographic data for the structure of **8** have been submitted to the Cambridge Crystallographic Data Centre as supplementary publication CCDC 1563788.)

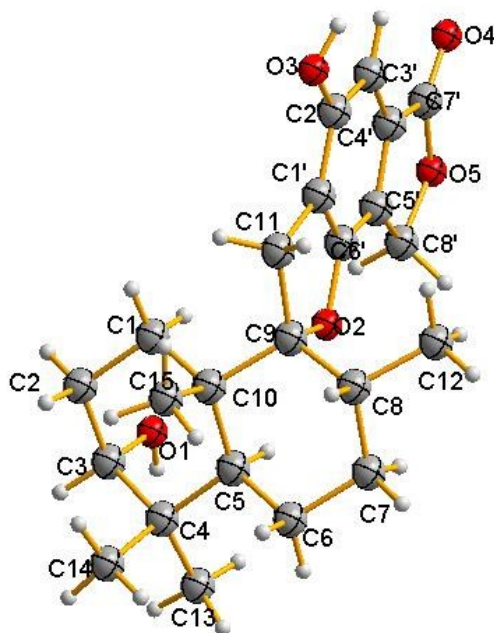


Figure S58. The dose-response curves for NO production of compounds **4**, **7** and **8**

