

Supplementary materials for

Mono- and dimeric naphthalenones from marine-derived fungus

Leptosphaerulina chartarum 3608

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Figure S1. ^1H (400 MHz) NMR spectrum of ($\pm$)-leptothalenone A (**1**) in CD_3OD .

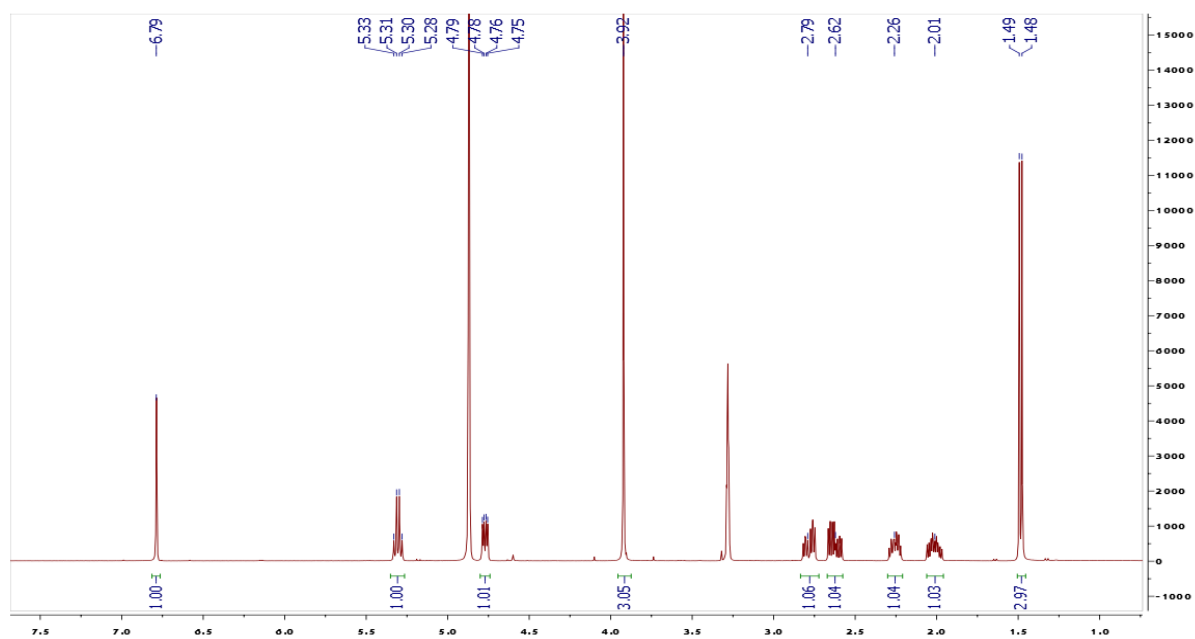


Figure S2. ^{13}C (100 MHz) NMR spectrum of ($\pm$)-leptothalenone A (**1**) in CD_3OD .

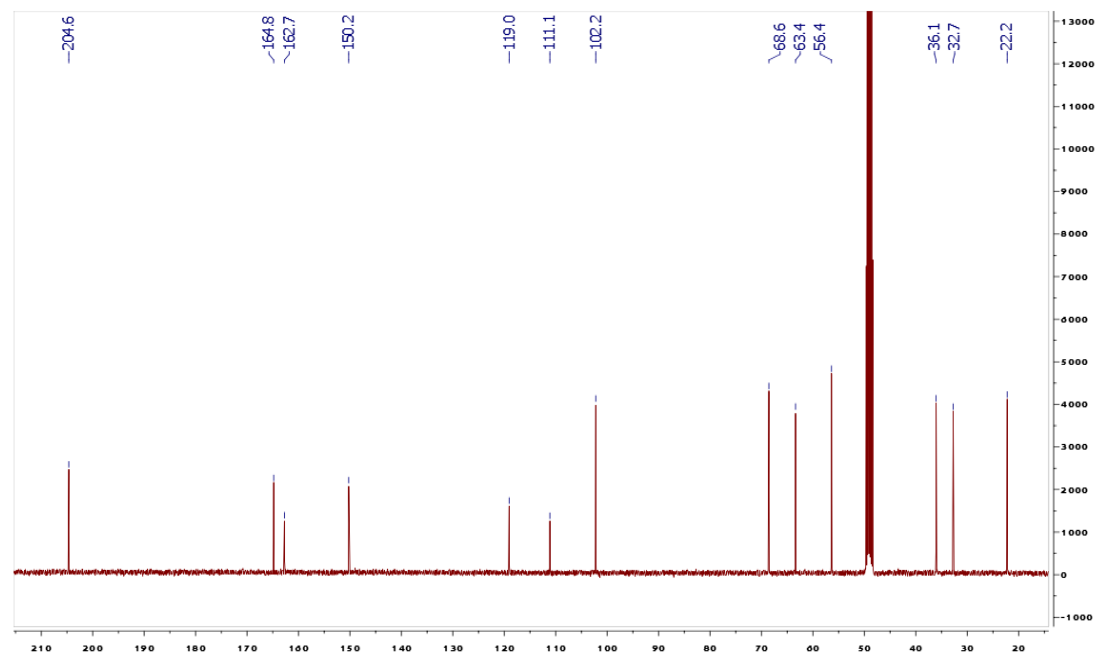


Figure S3. DEPT-90 spectrum of ($\pm$)-leptothalenone A (**1**) in CD₃OD.

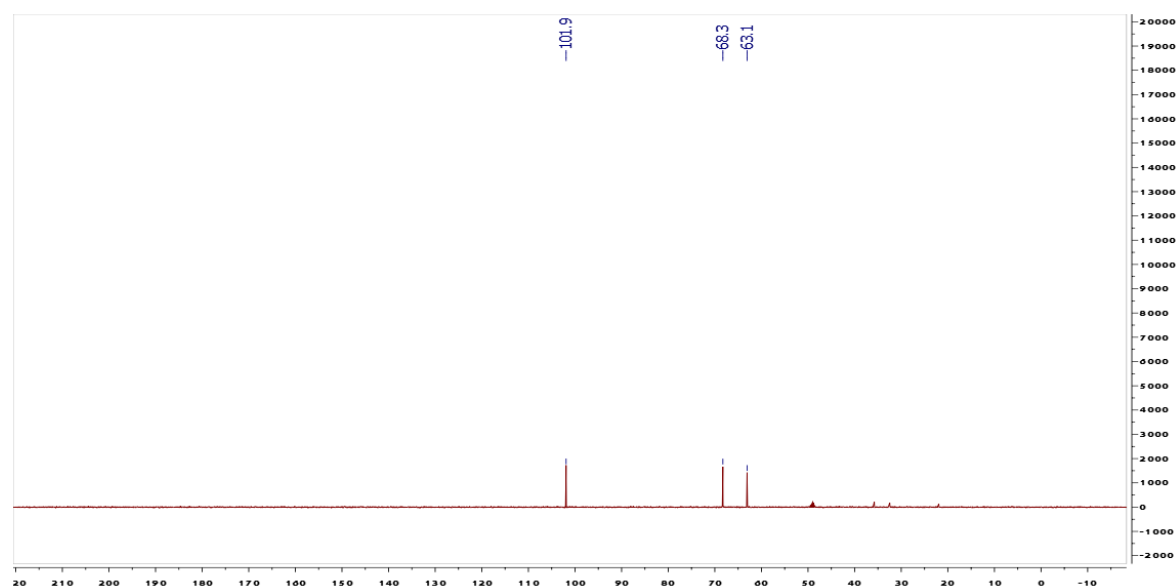


Figure S4. DEPT-135 spectrum of ($\pm$)-leptothalenone A (**1**) in CD₃OD.

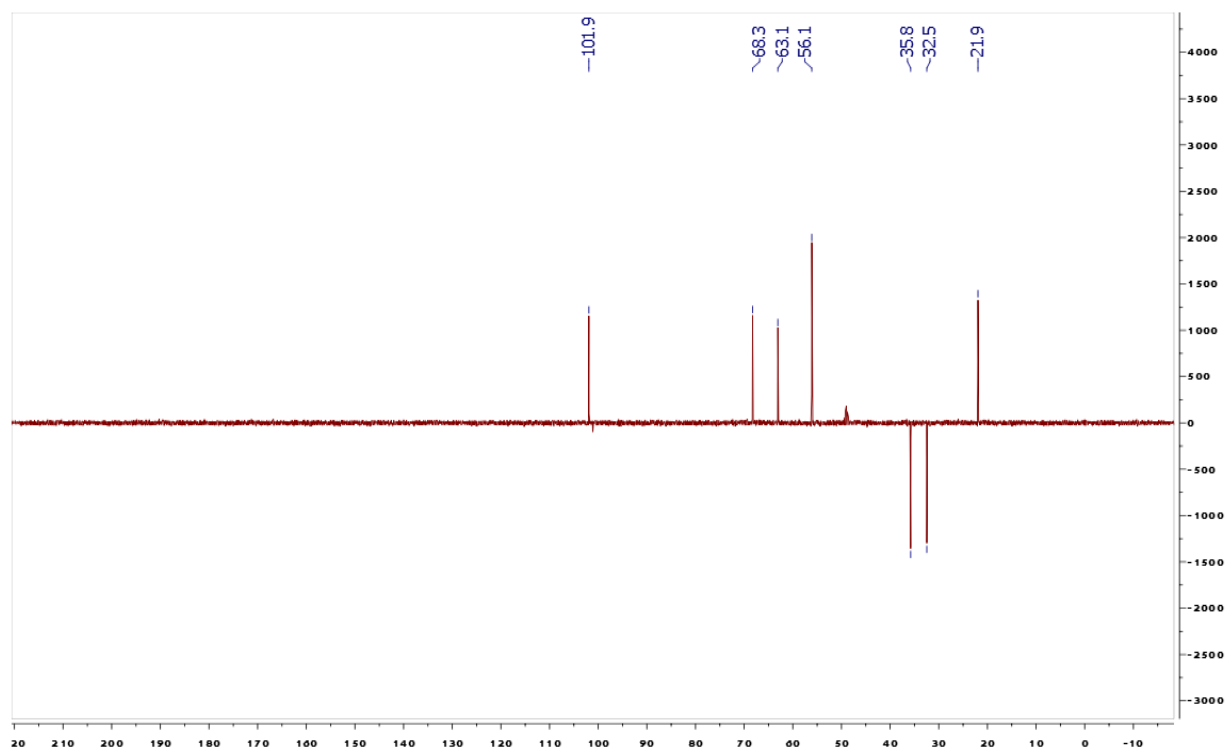


Figure S5. HSQC spectrum of ($\pm$)-leptothalenone A (**1**) in CD₃OD.

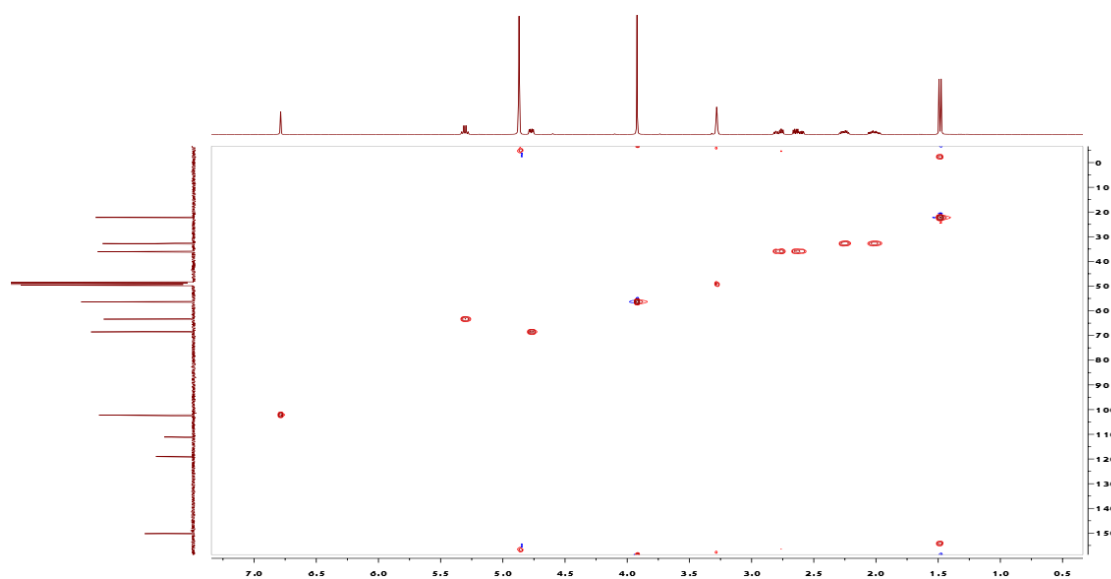


Figure S6. HMBC spectrum of ($\pm$)-leptothalenone A (**1**) in CD₃OD.

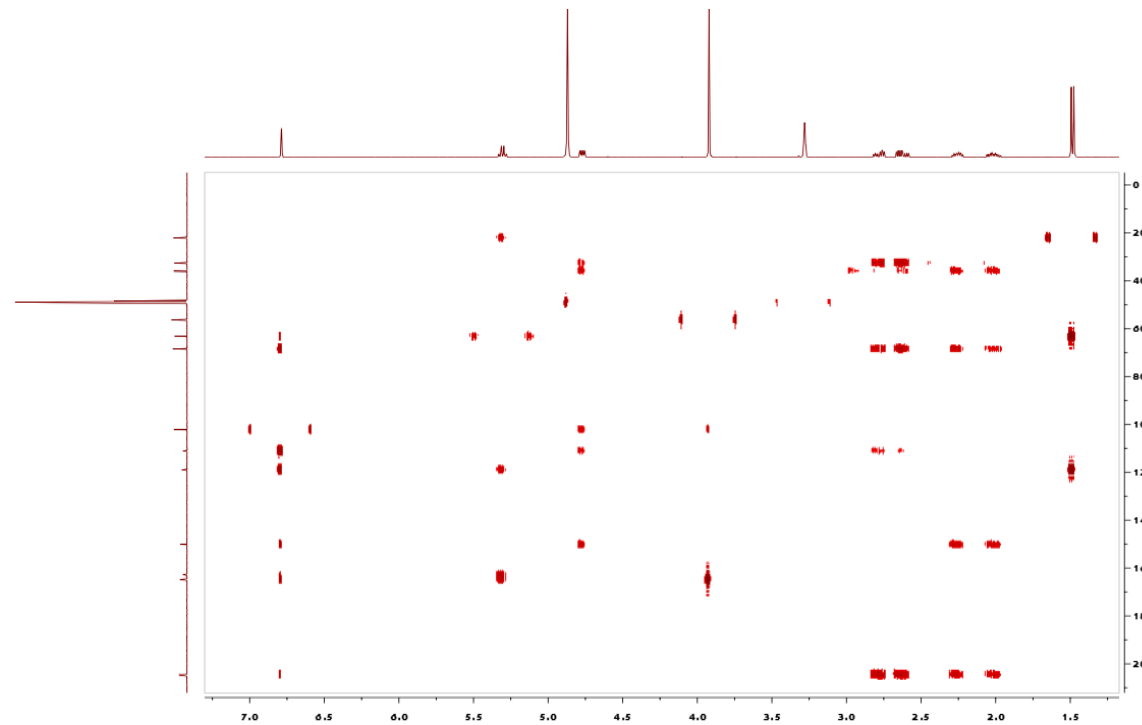


Figure S7. ^1H - ^1H COSY spectrum of ($\pm$)-leptothalenone A (**1**) in CD_3OD .

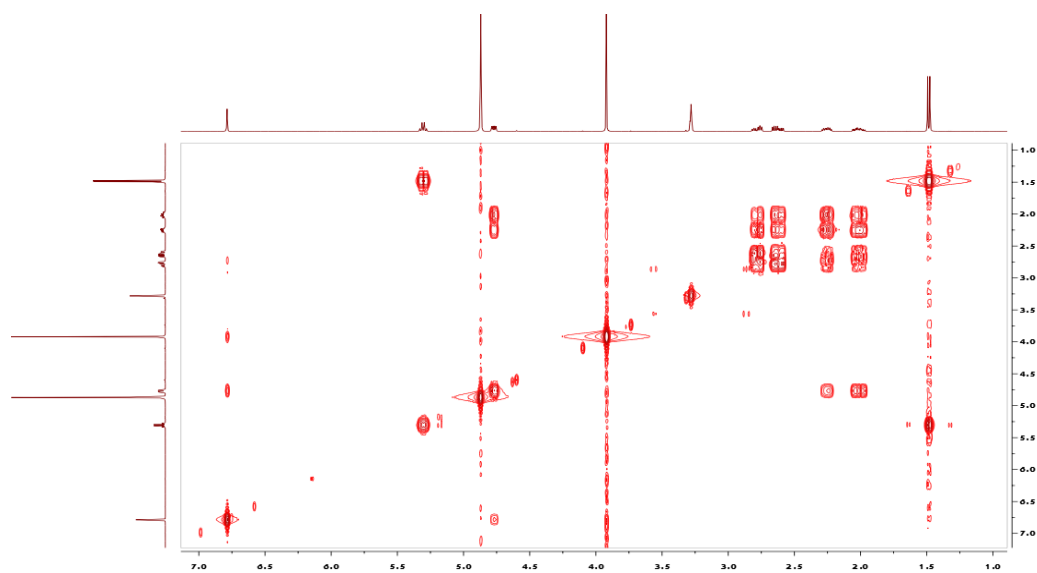


Figure S8. NOESY spectrum of ($\pm$)-leptothalenone A (**1**) in CD_3OD .

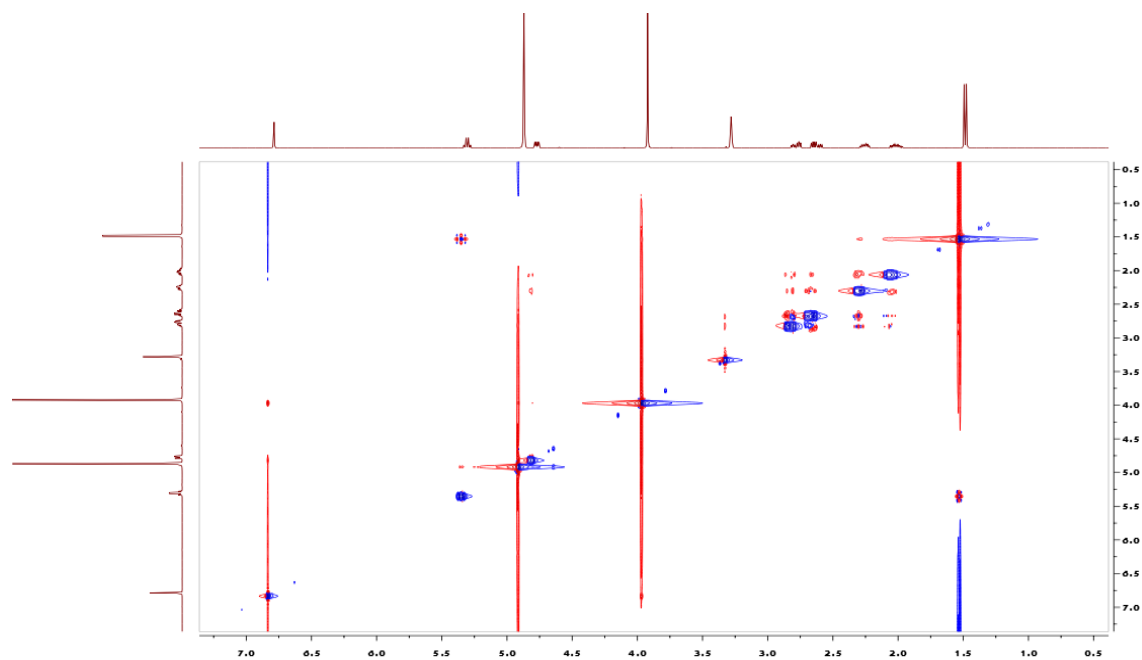


Figure S9. HR-ESIMS of ($\pm$)-leptothalenone A (**1**) in CD₃OD.

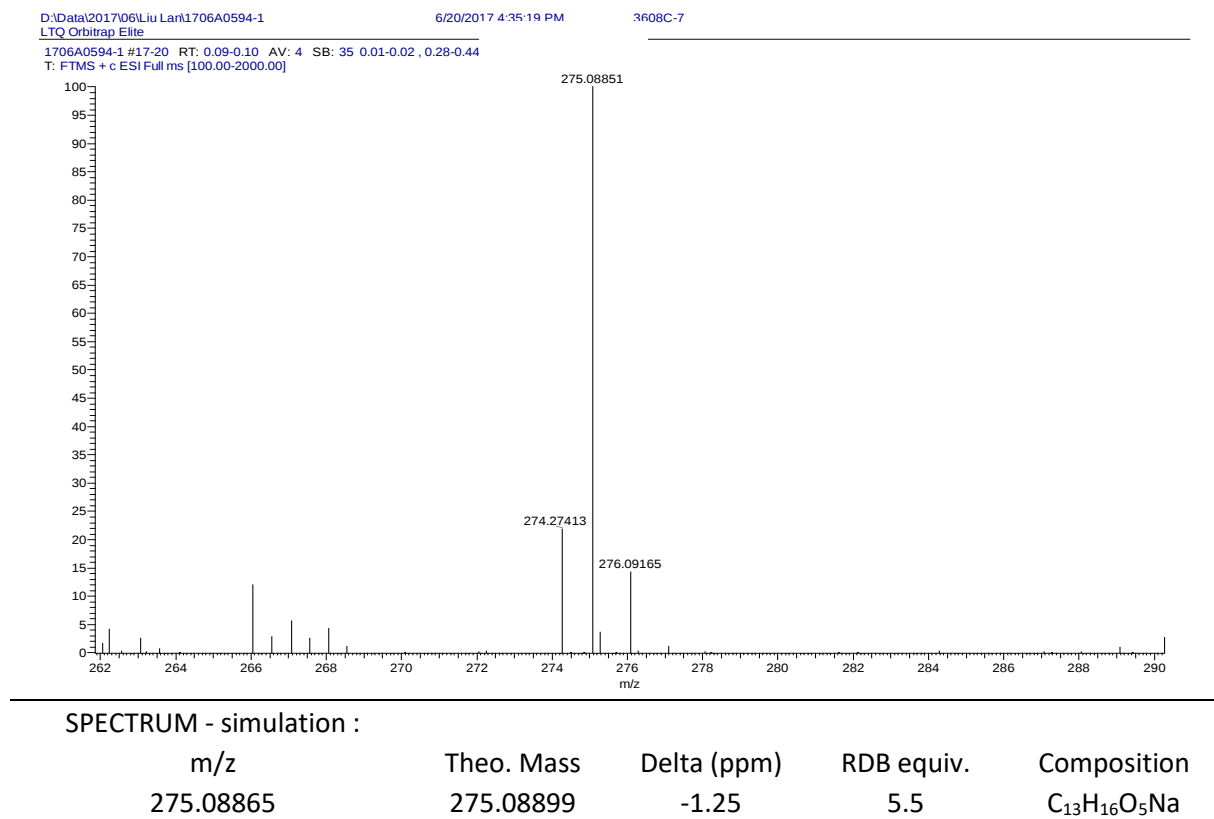


Figure S10. ¹H (400 MHz) NMR spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-**2**) in CD₃OD.

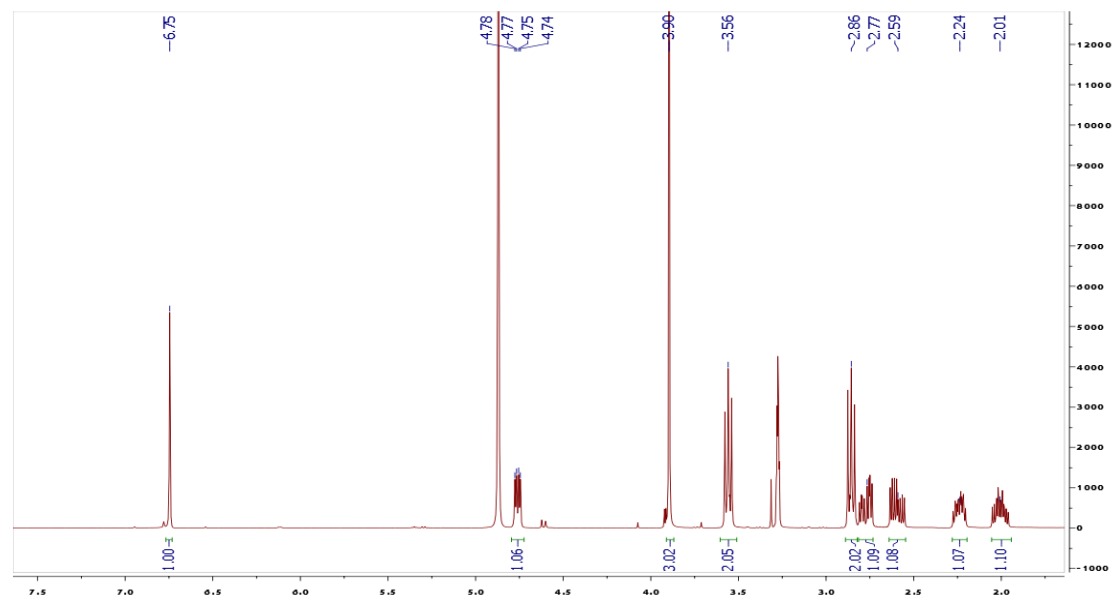


Figure S11. ^{13}C (100 MHz) NMR spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD_3OD .

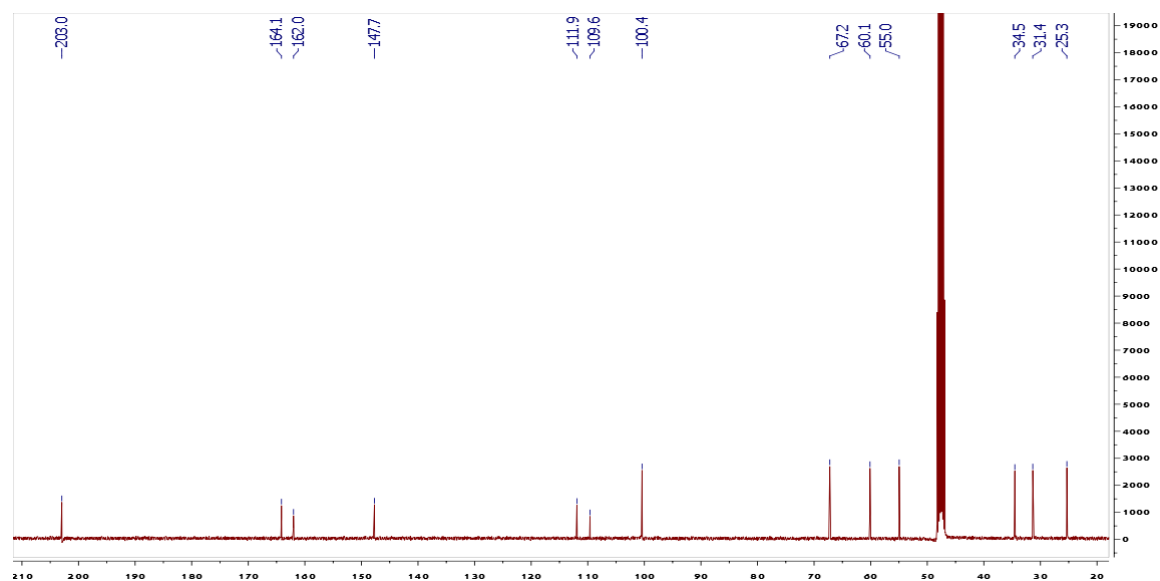


Figure S12. DEPT-90 spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD_3OD .

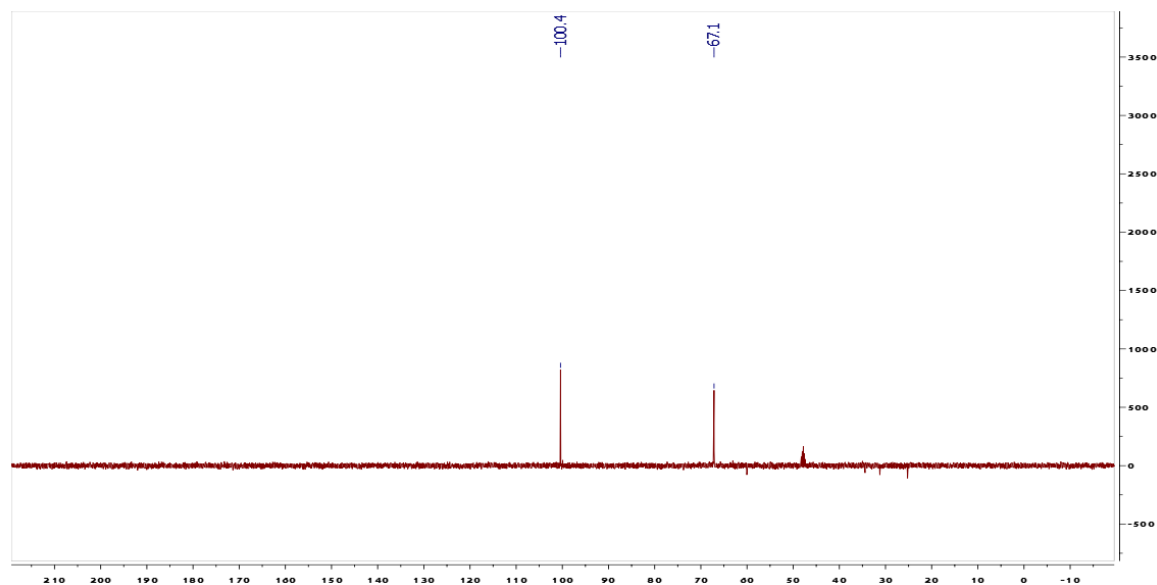


Figure S13. DEPT-135 spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.

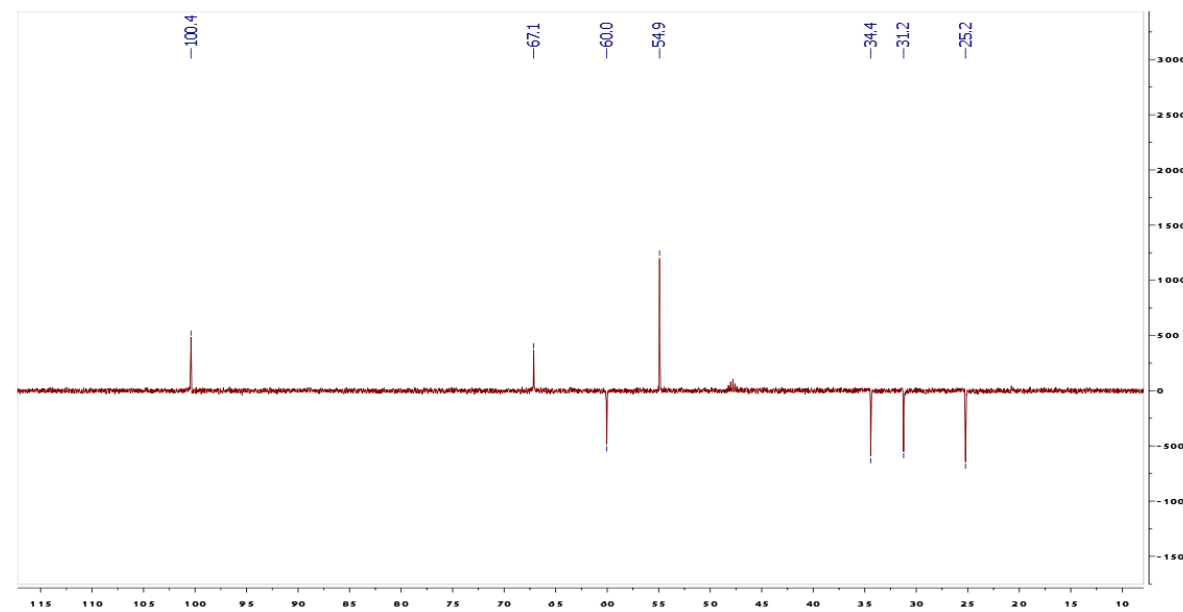


Figure S14. HSQC spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.

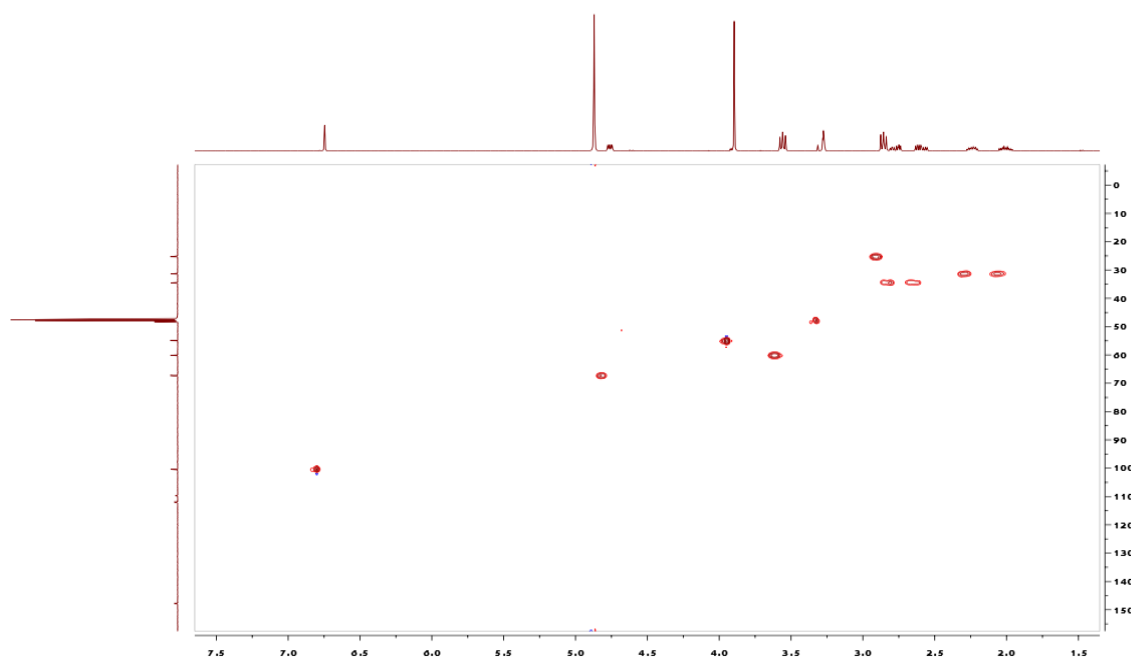


Figure S15. HMBC spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.

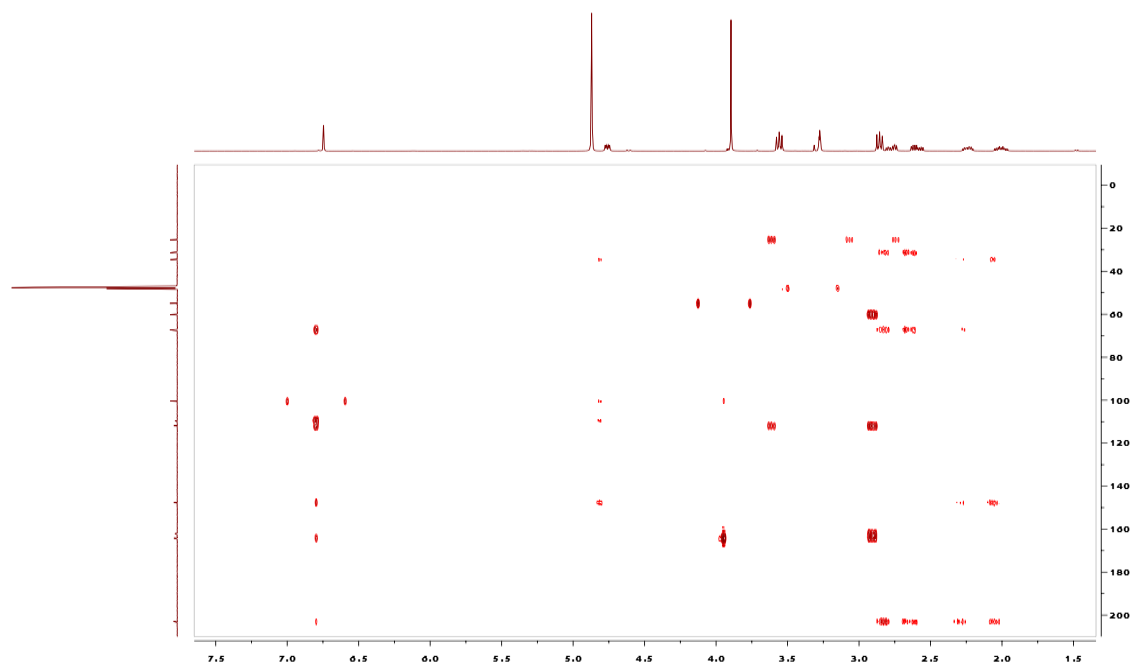


Figure S16. ¹H-¹H COSY spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.

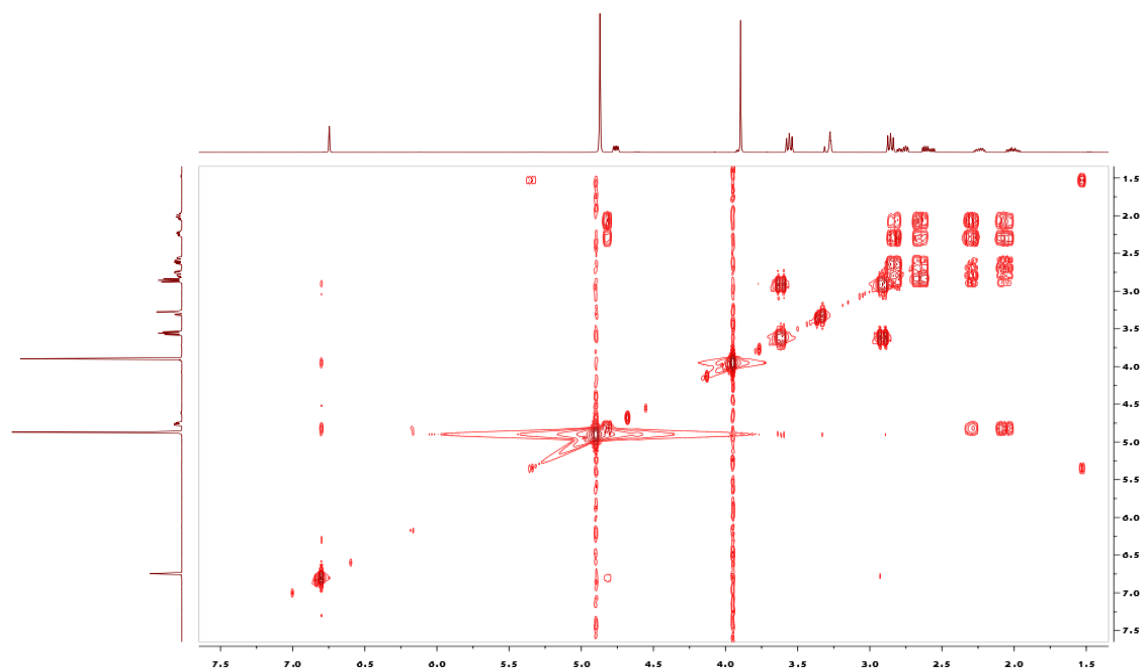


Figure S17. NOESY spectrum of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.

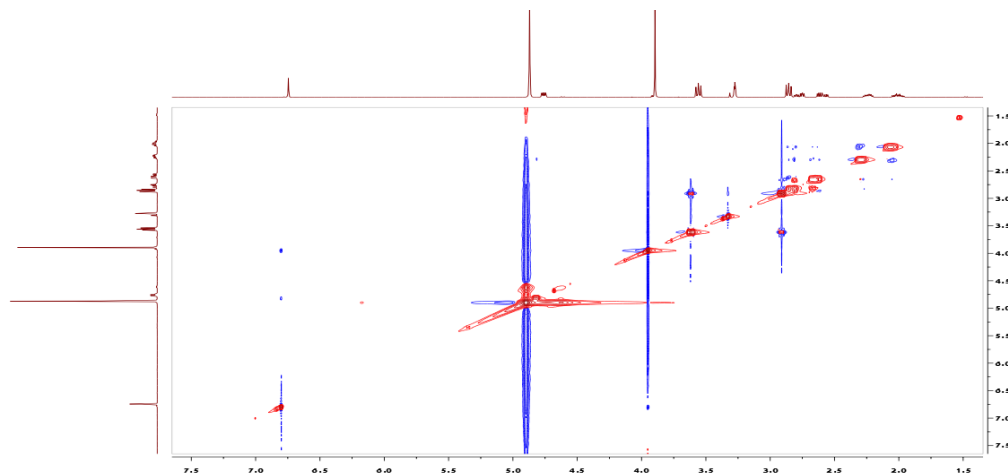
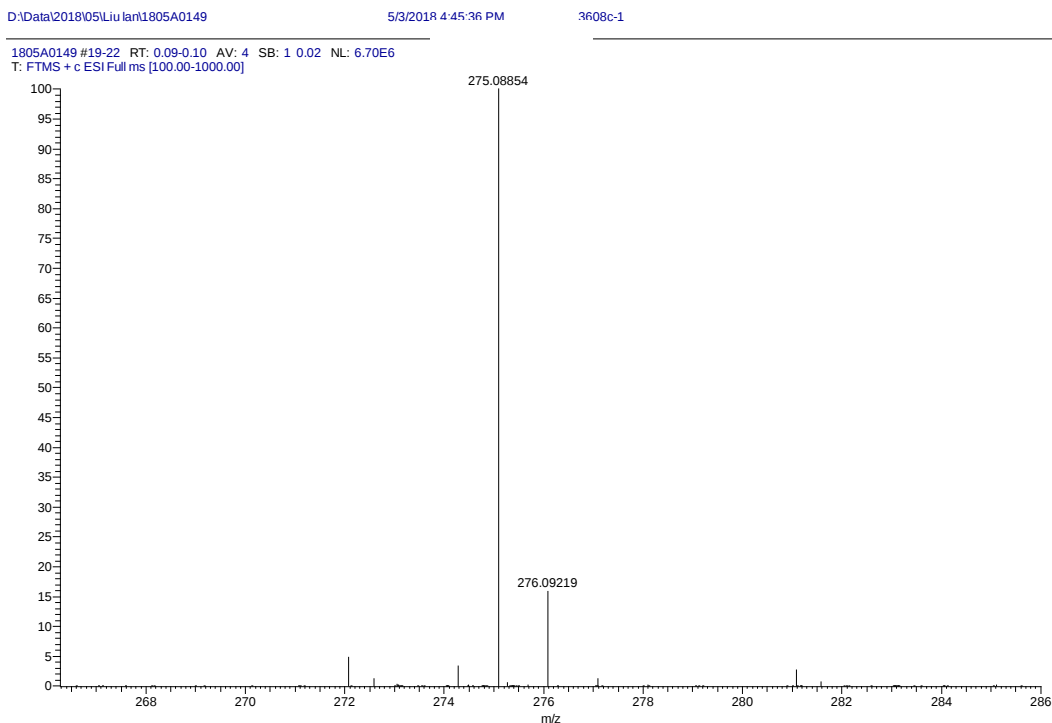


Figure S18. ESIMS of (-)-4,8-dihydroxy-7- (2-hydroxy-ethyl)-6-methoxy-3,4-dihydro-2*H*-naphthalen-1-one ((-)-2) in CD₃OD.



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
275.08854	275.08899	-1.65	5.5	C ₁₃ H ₁₆ O ₅ Na

Figure S19. ^1H (400 MHz) NMR spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD_3OD .

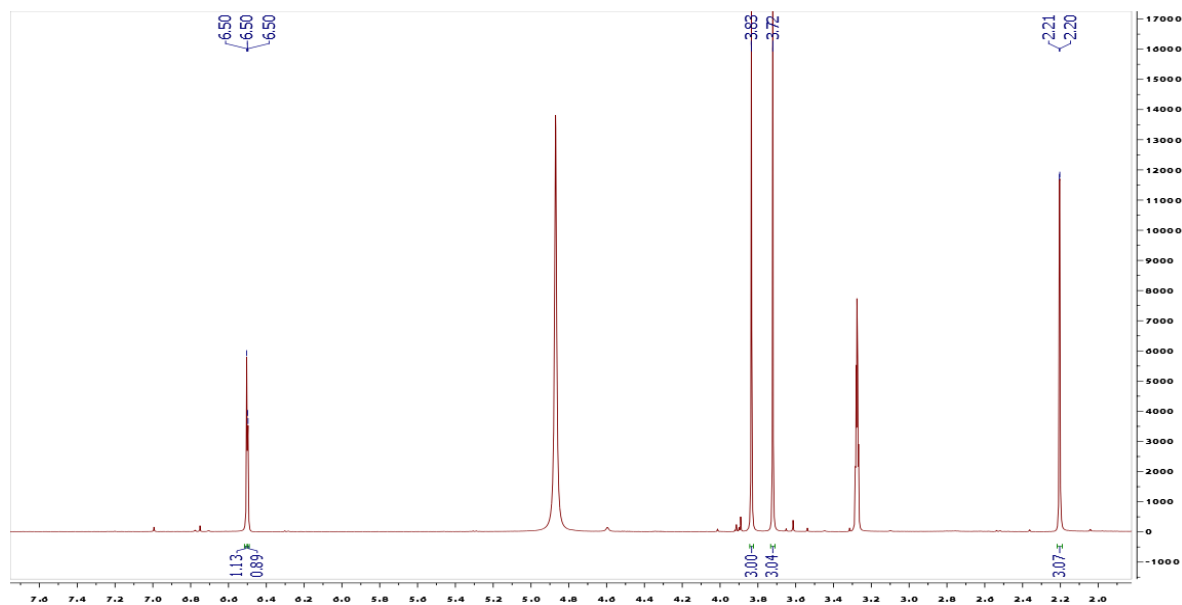


Figure S20. ^{13}C (100 MHz) NMR spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD_3OD .

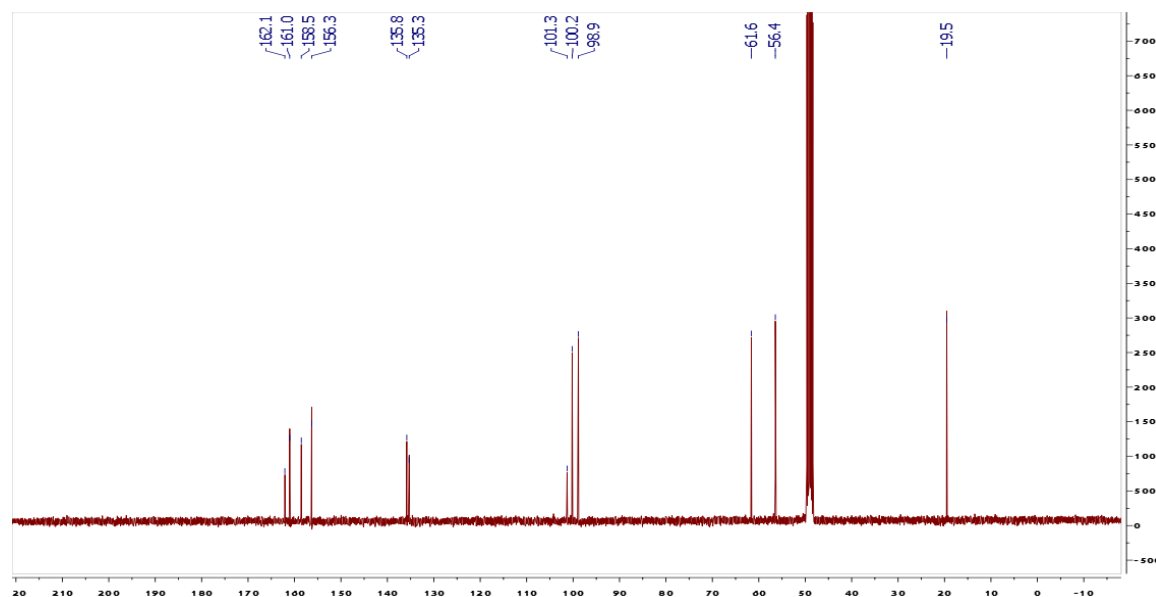


Figure S21. DEPT-90 spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD₃OD.

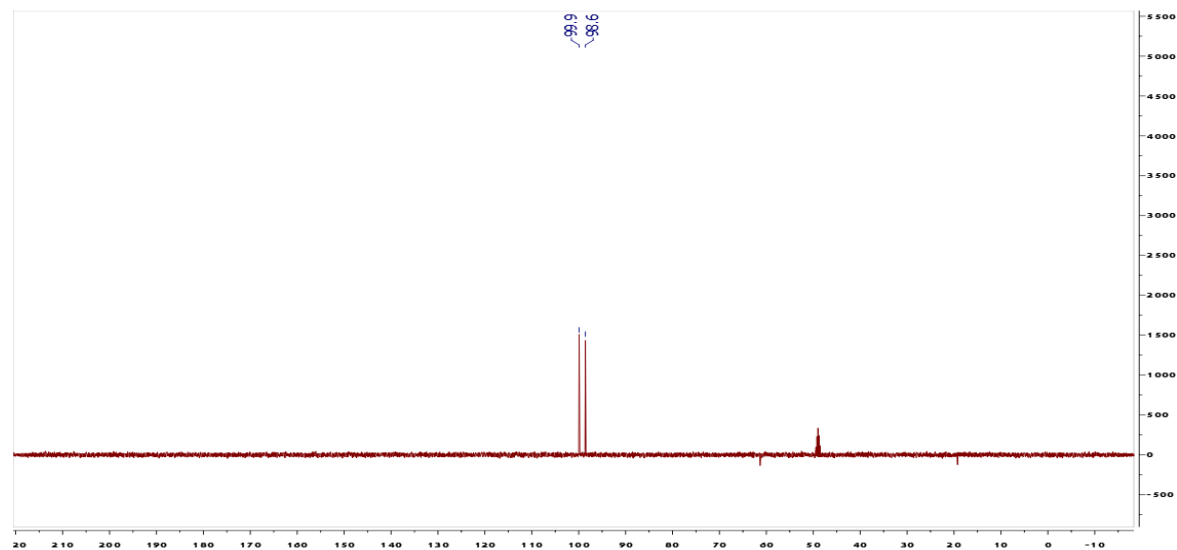


Figure S22. DEPT-135 spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD₃OD.

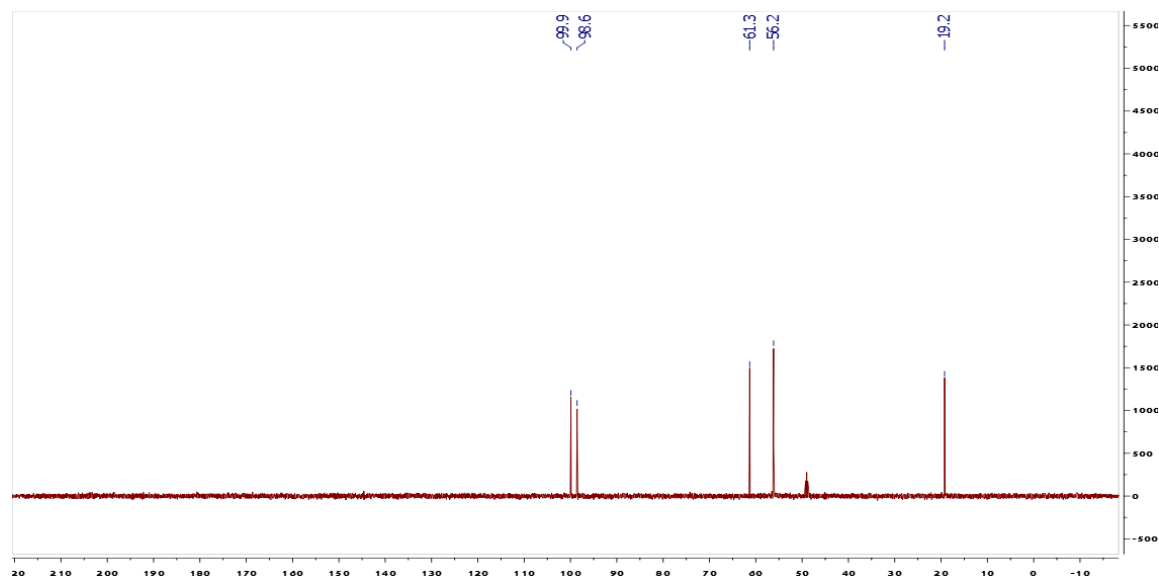


Figure S23. HSQC spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD₃OD.

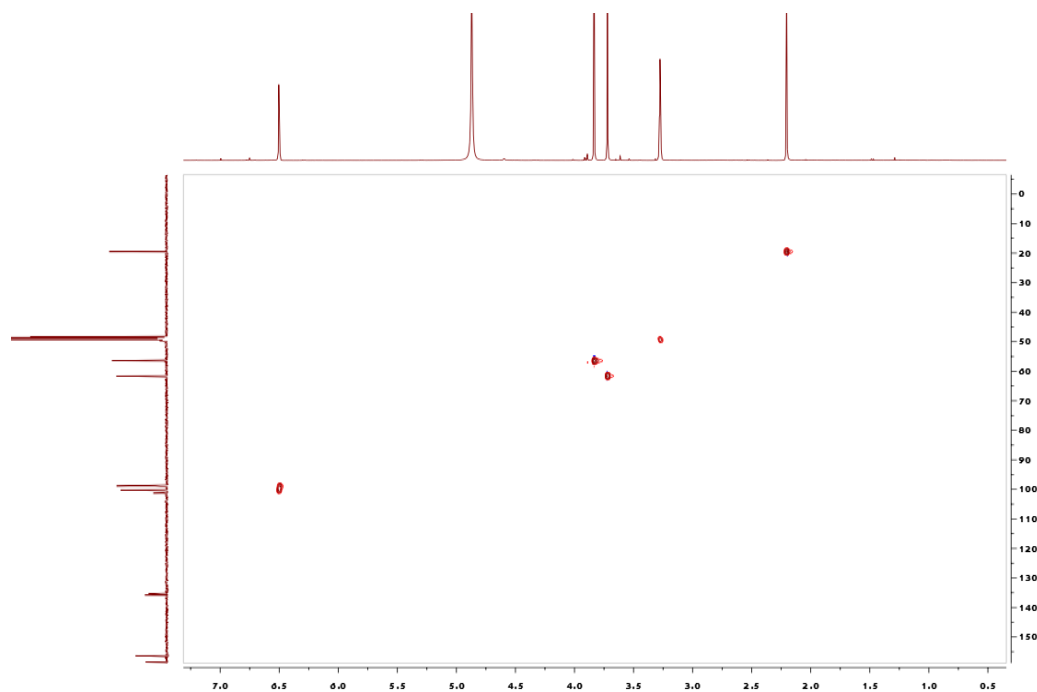


Figure S23. HMBC spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD₃OD.

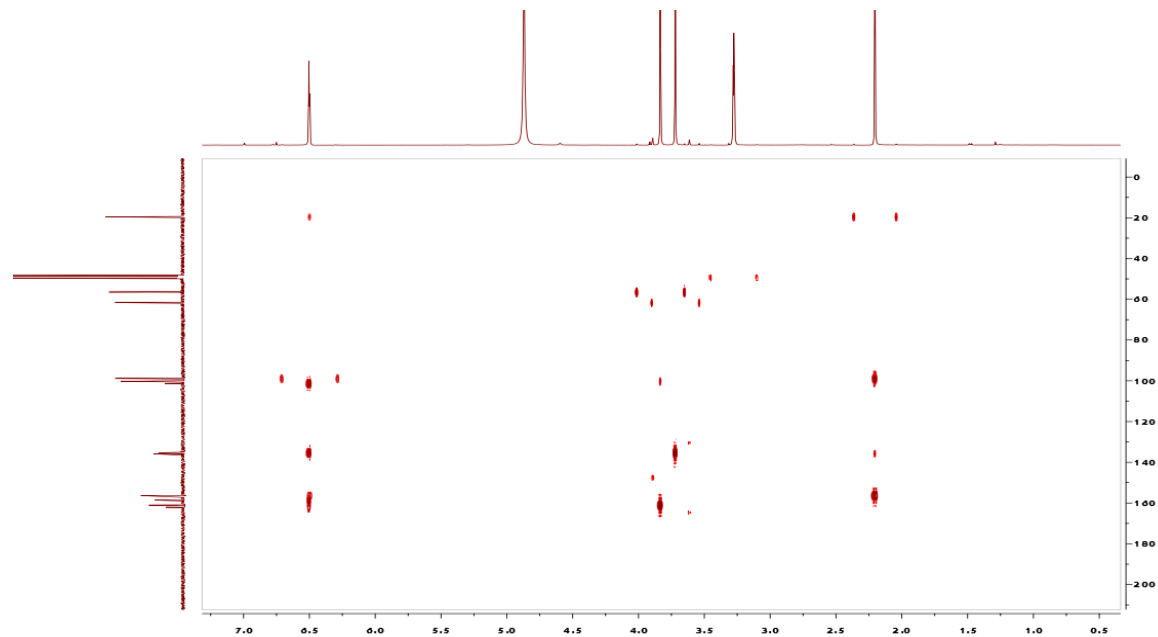


Figure S25 ^1H - ^1H COSY spectrum of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD_3OD .

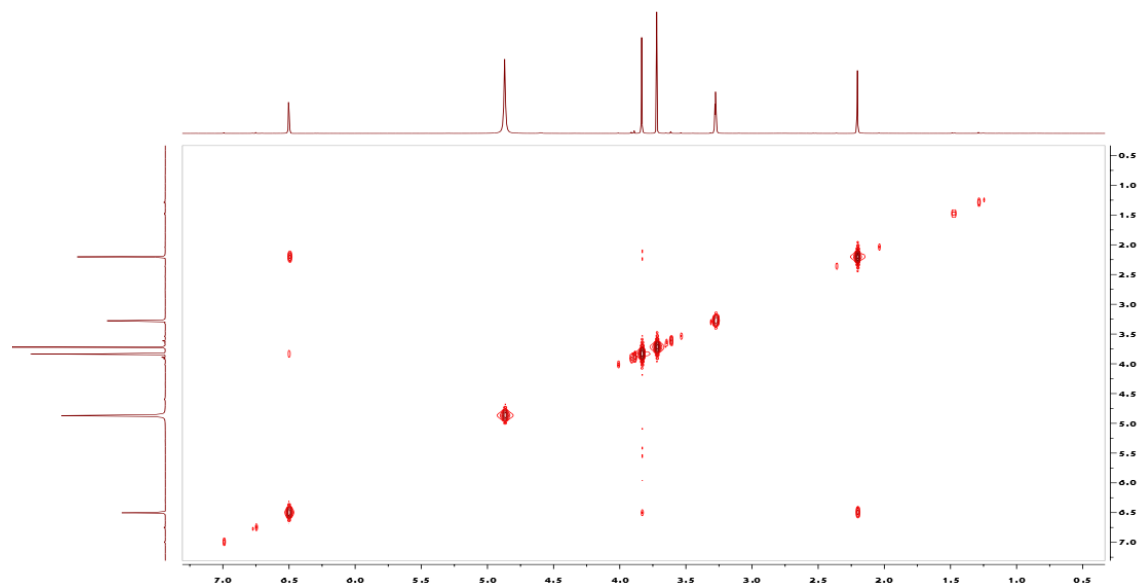
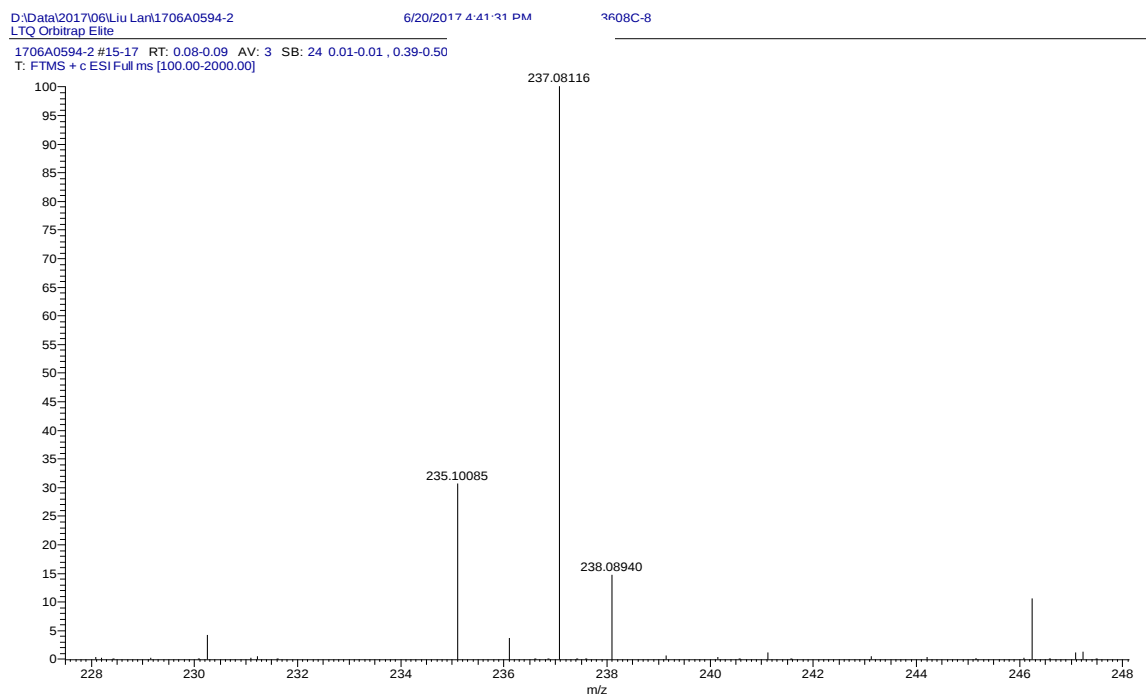


Figure S26. HR-ESIMS of 6-hydroxy-5,8-dimethoxy-3-methyl-1*H*-isochromen-1-one (**4**) in CD_3OD .



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
237.07572	237.07575	-0.13	6.5	C ₁₂ H ₁₃ O ₅

Figure S27. ^1H (400 MHz) NMR spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (5) in CD_3OD .

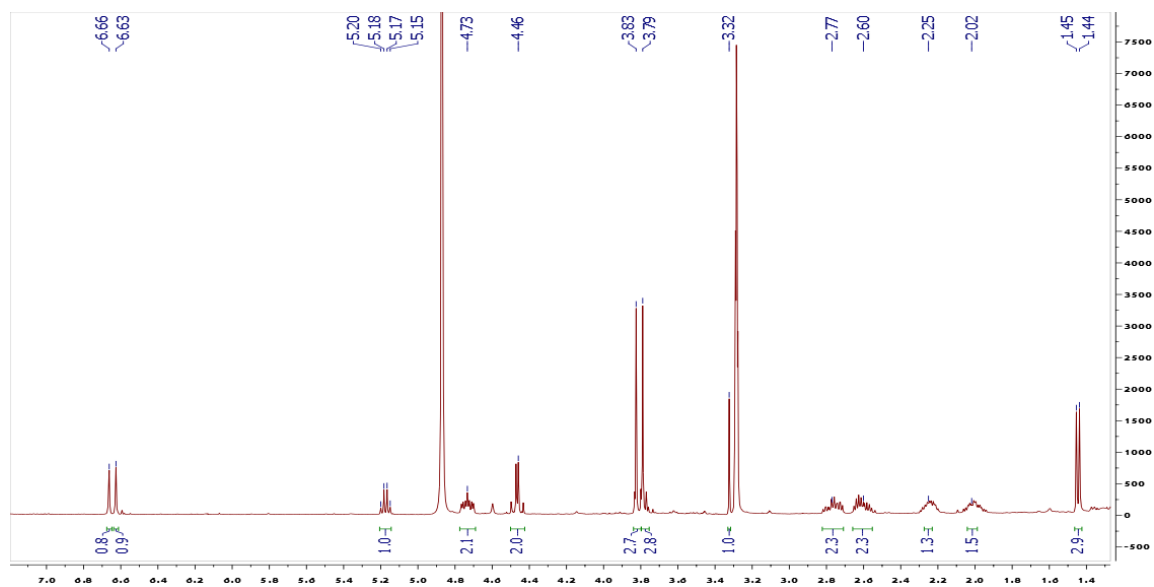


Figure S28. ^{13}C (100 MHz) NMR spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (5) in CD_3OD .

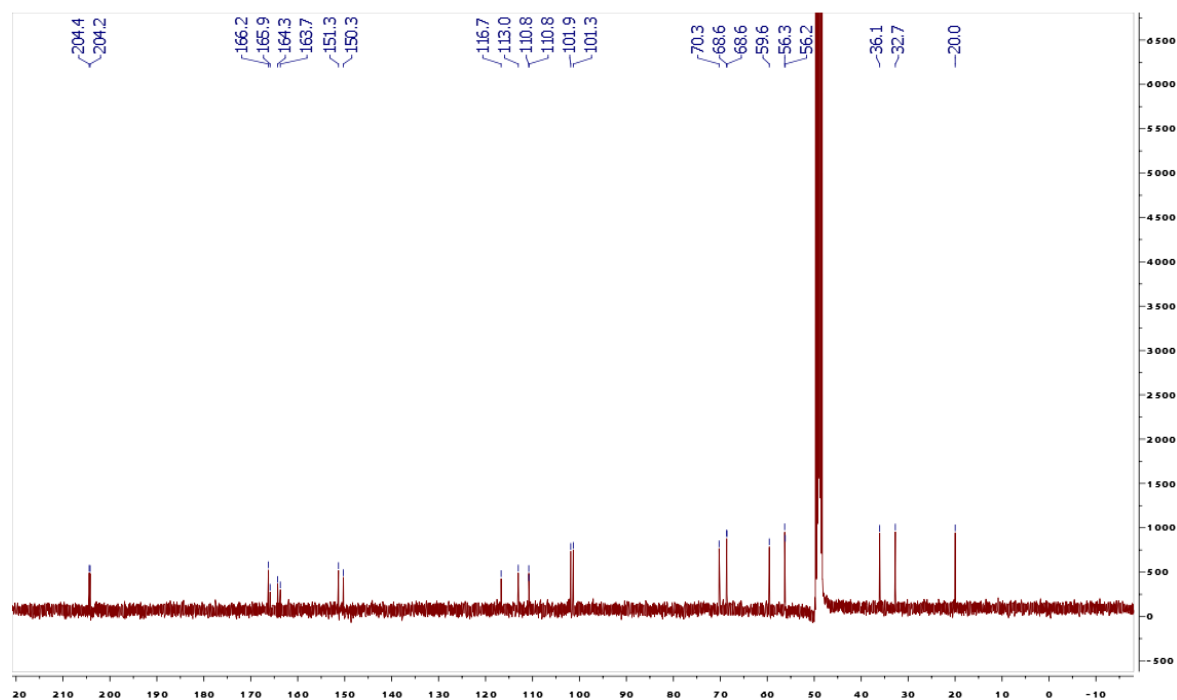


Figure S29. DEPT-90 spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (**5**) in CD₃OD.

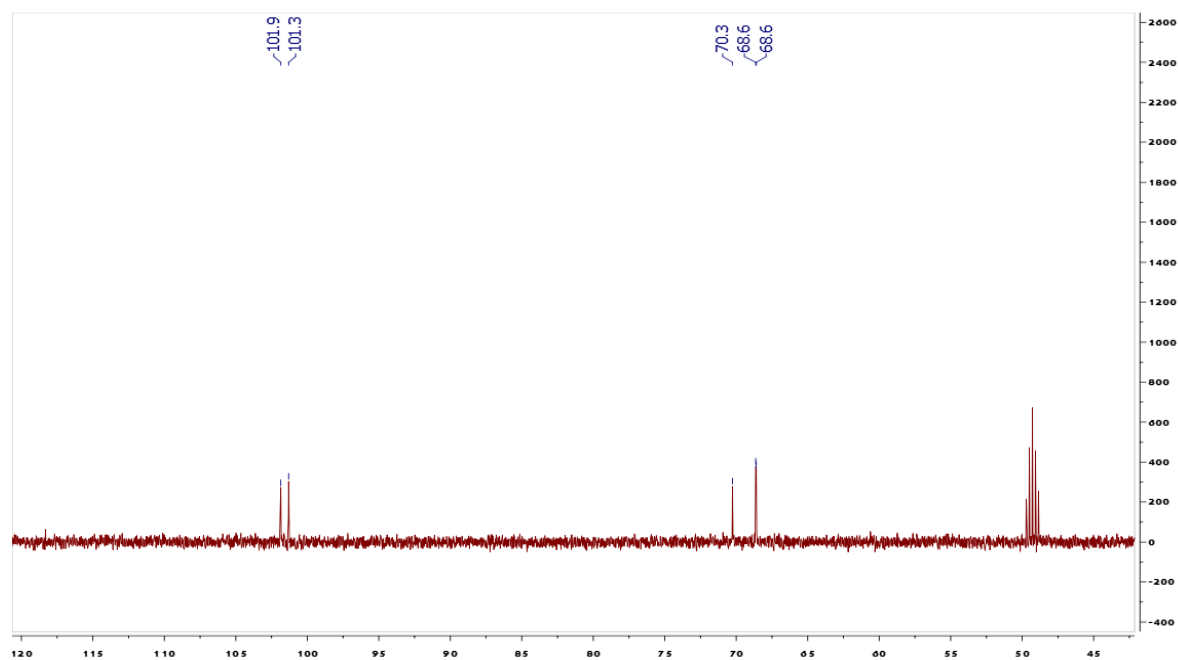


Figure S30. DEPT-135 spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (**5**) in CD₃OD.

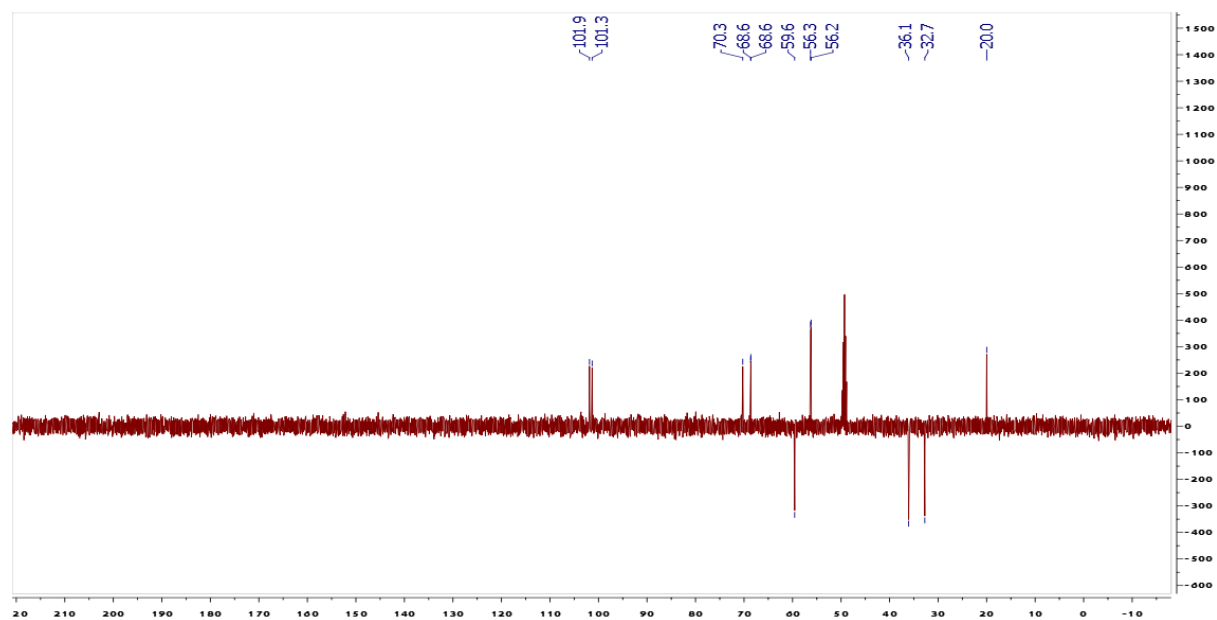


Figure S31. HSQC spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (**5**) in CD₃OD.

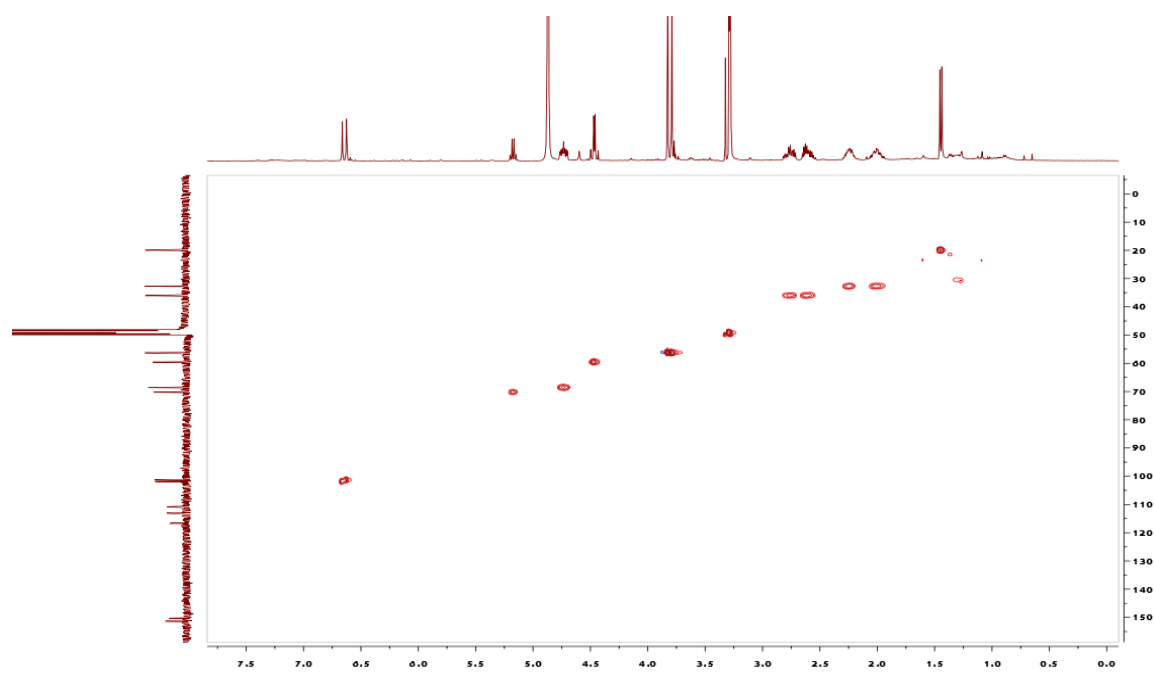


Figure S32. HMBC spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (**5**) in CD₃OD.

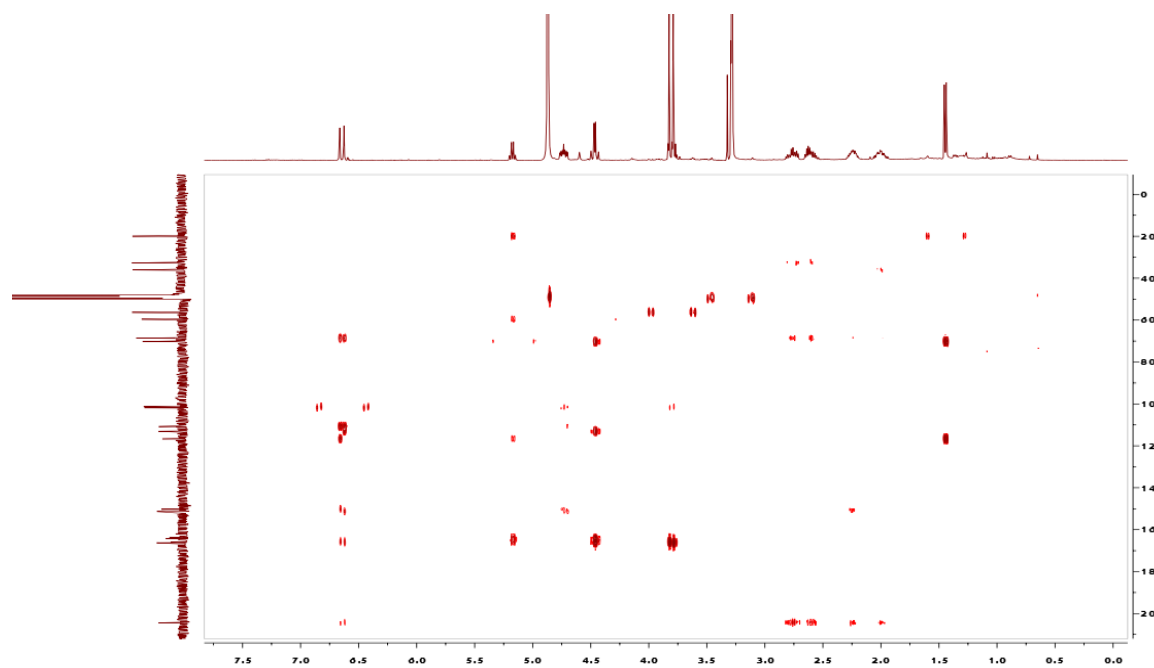


Figure S33. ^1H - ^1H COSY spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (5) in CD_3OD .

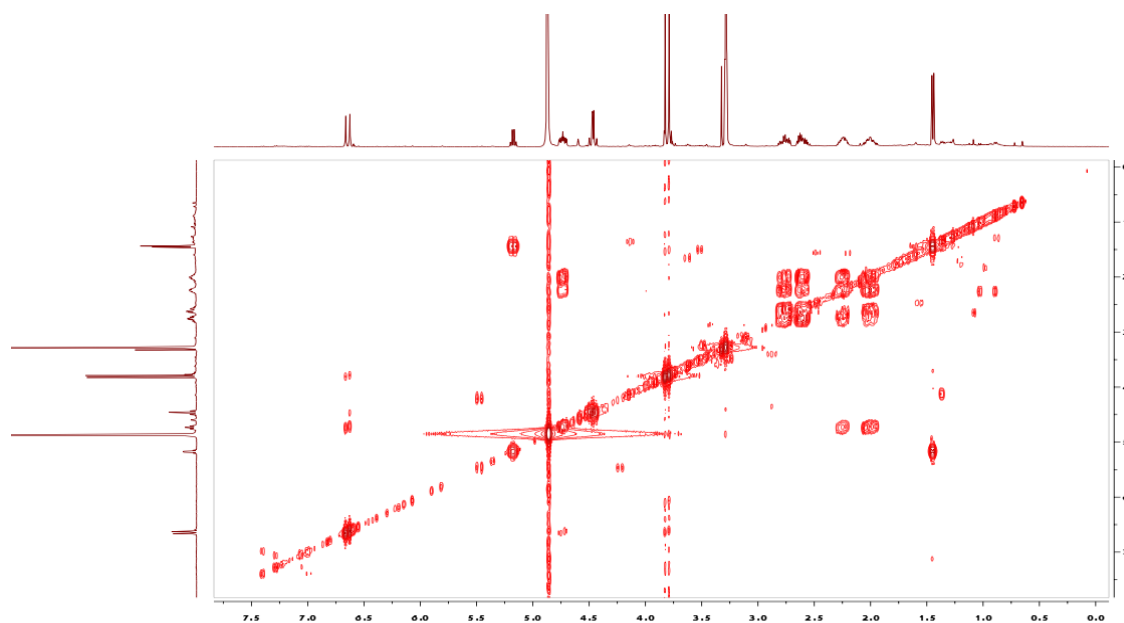


Figure S34. NOESY spectrum of (4*S*, 10*R*, 4'*S*)-leptothalenone B (5) in CD_3OD .

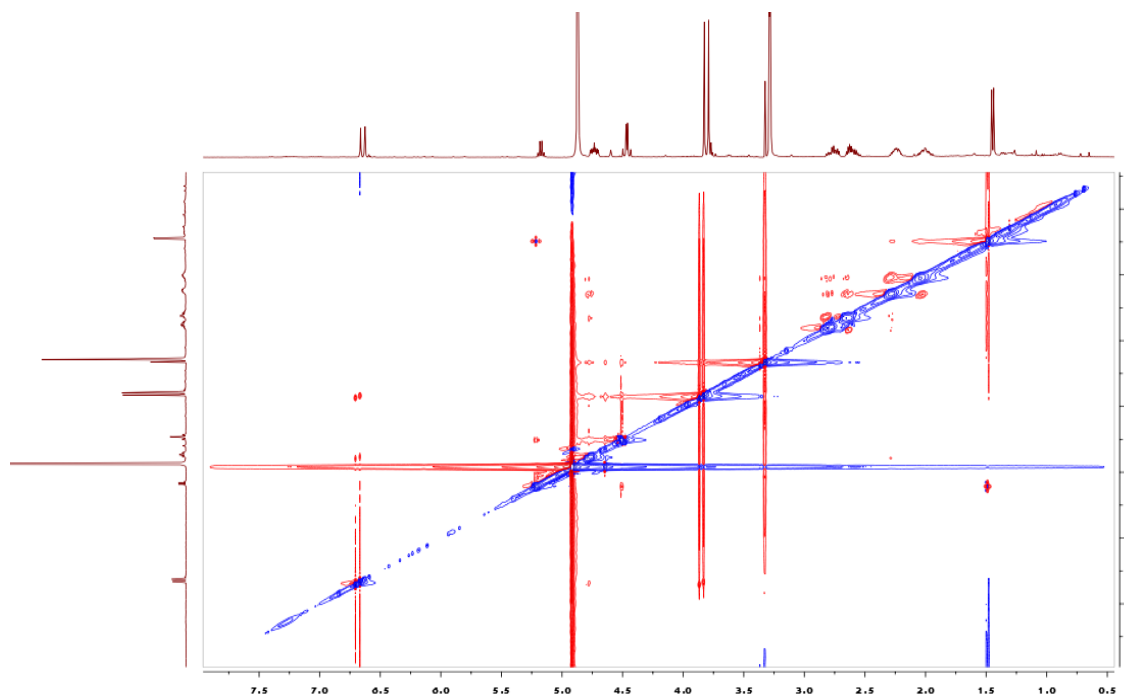
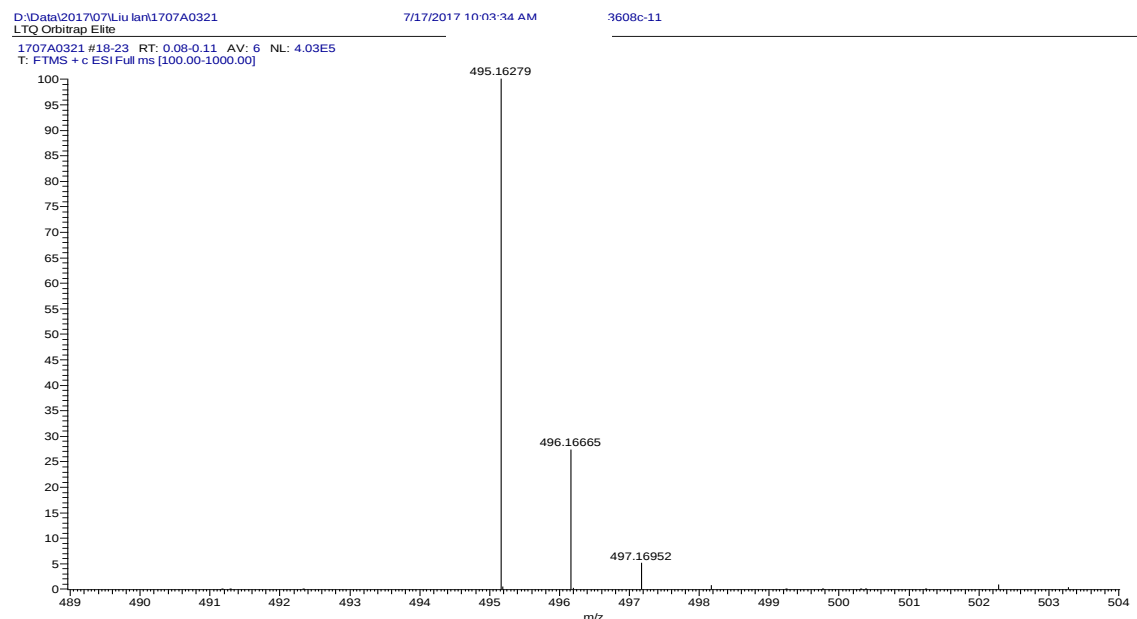


Figure S35. HR-ESIMS of (4*S*, 10*R*, 4'*S*)-leptothalenone B (**5**).



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
495.16279	495.16255	0.48	11.5	C ₂₅ H ₂₈ O ₉ Na

Figure S36. ¹H (400 MHz) NMR spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

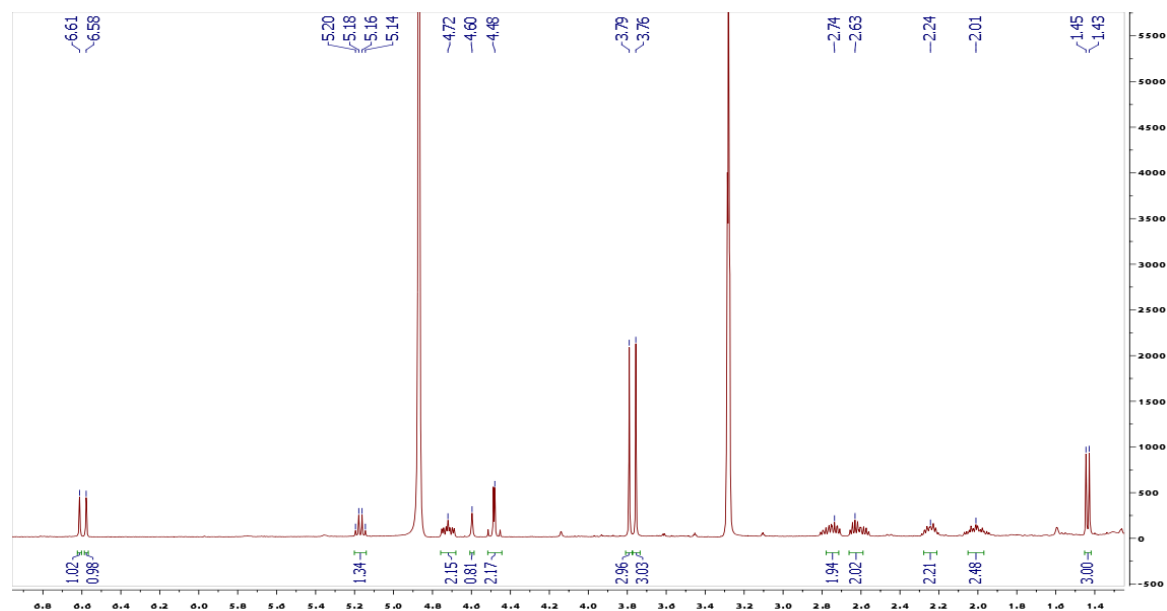


Figure S37. ^{13}C (100 MHz) NMR spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD_3OD .

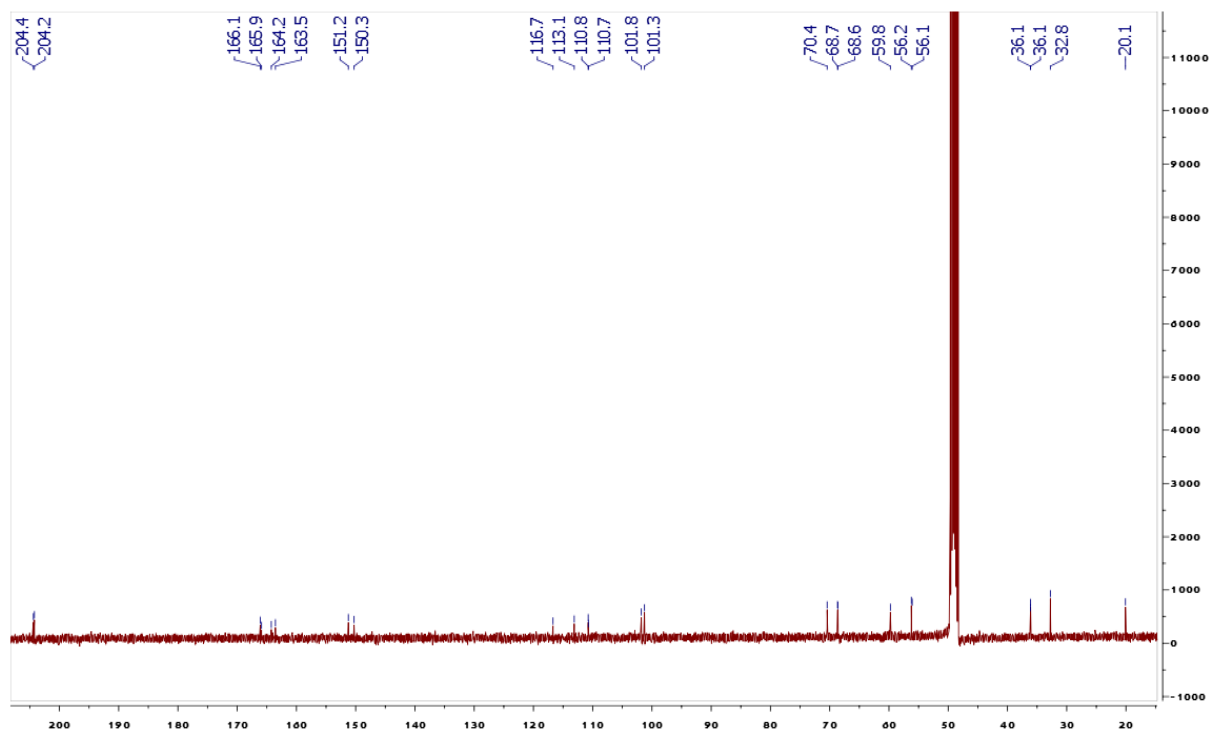


Figure S38. DEPT-90 spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD_3OD .

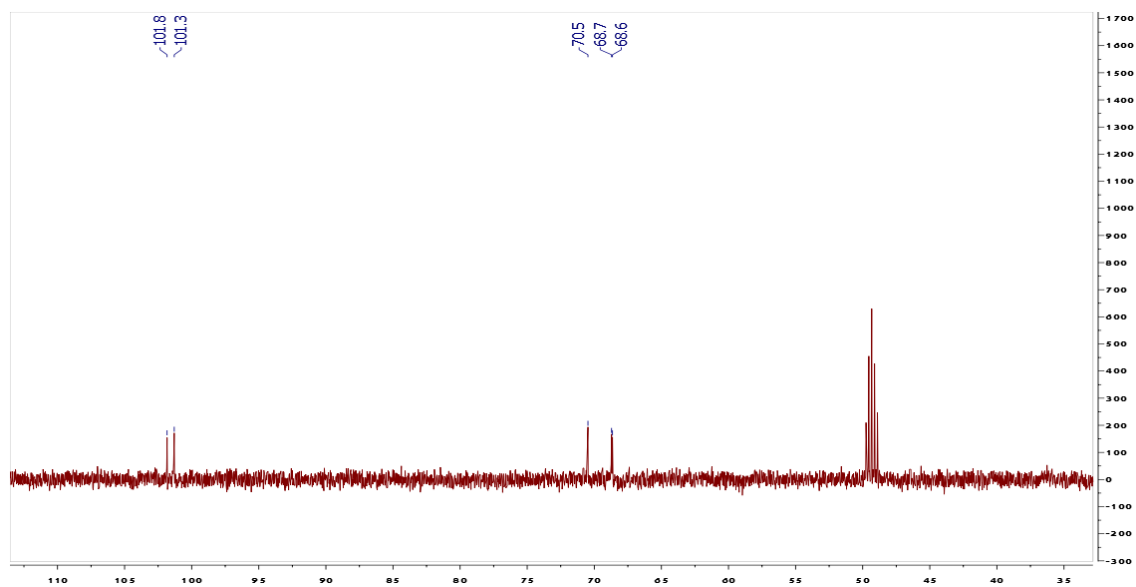


Figure S39. DEPT-135 spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

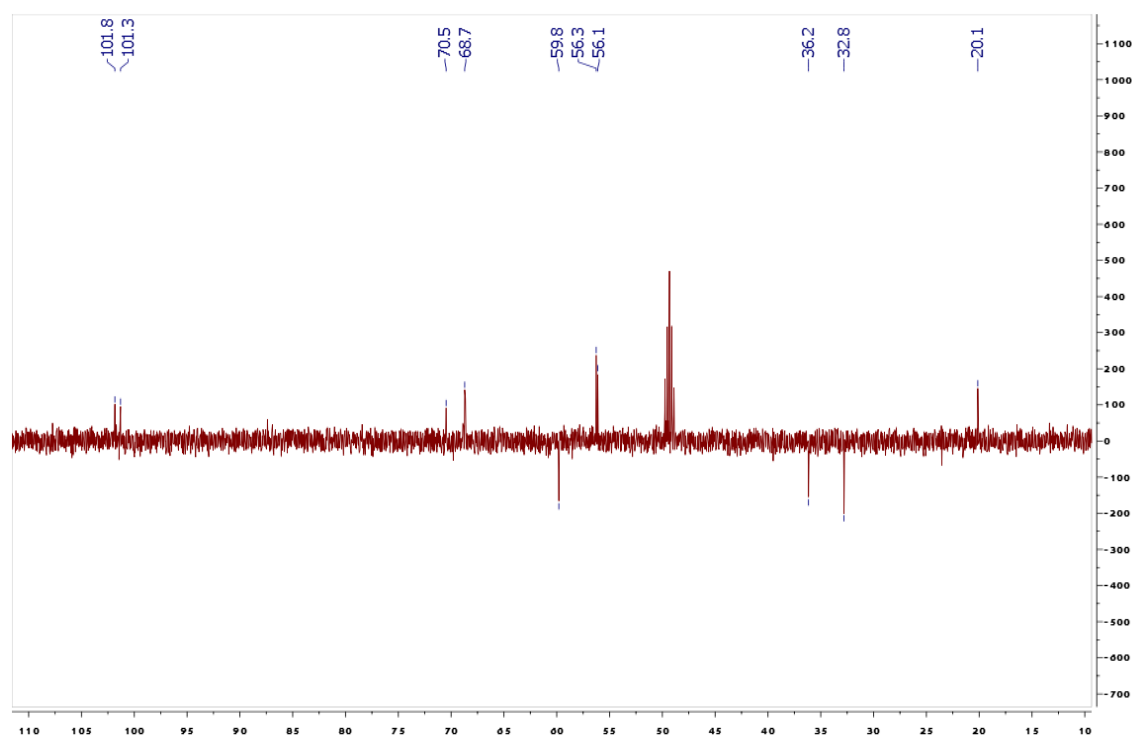


Figure S40. HSQC spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

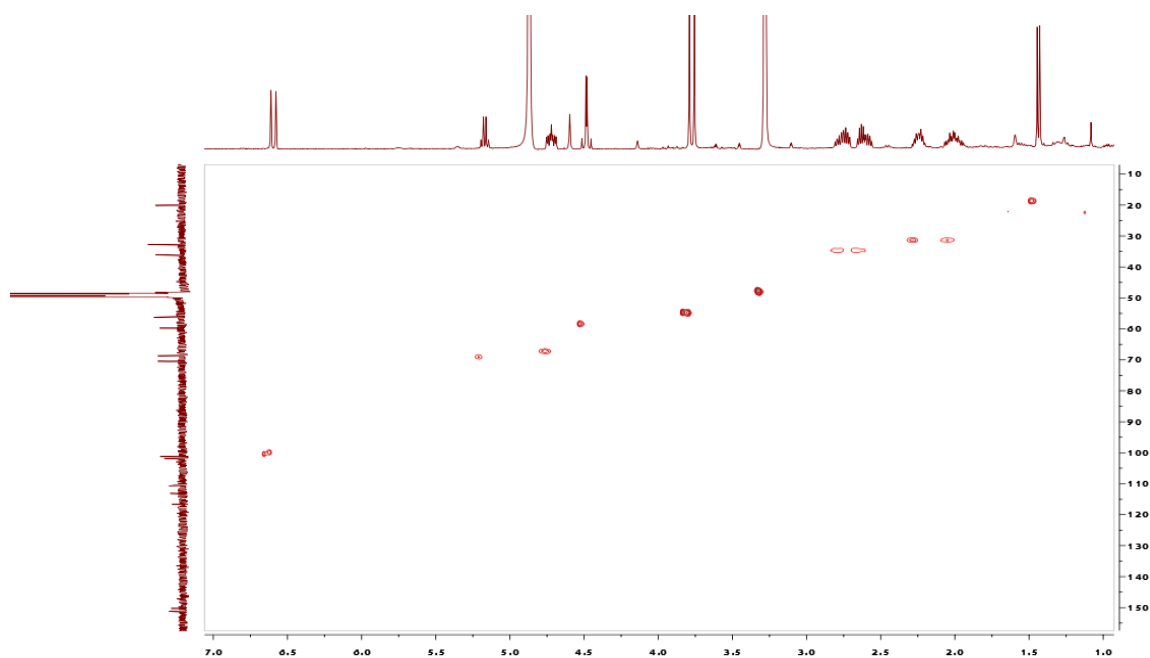


Figure S41. HMBC spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

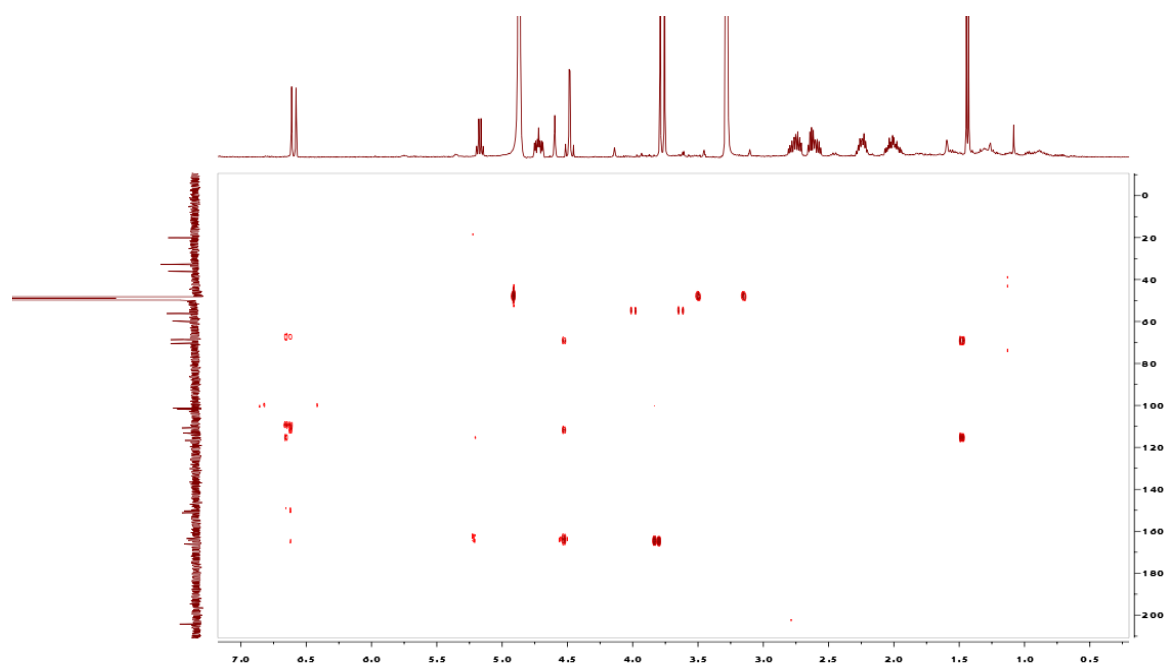


Figure S42. ¹H-¹H COSY spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

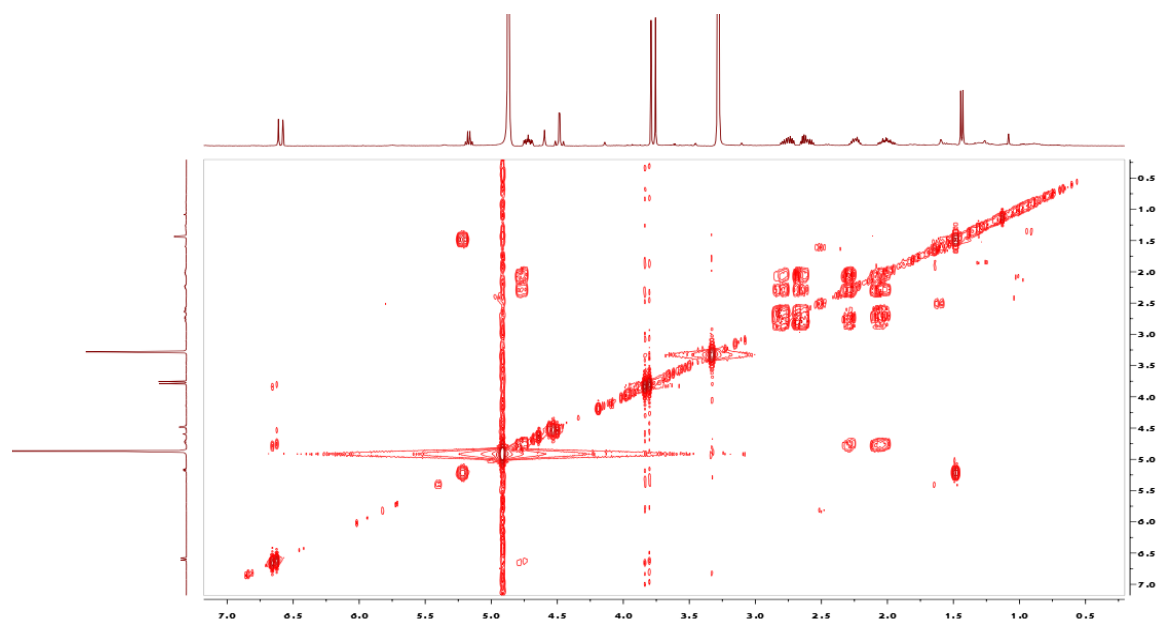


Figure S43. NOESY spectrum of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.

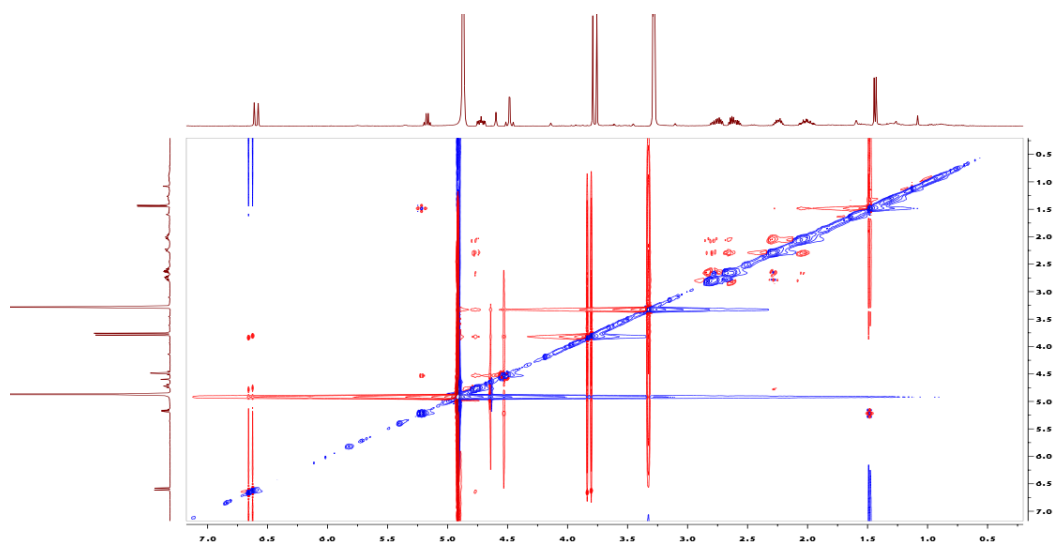
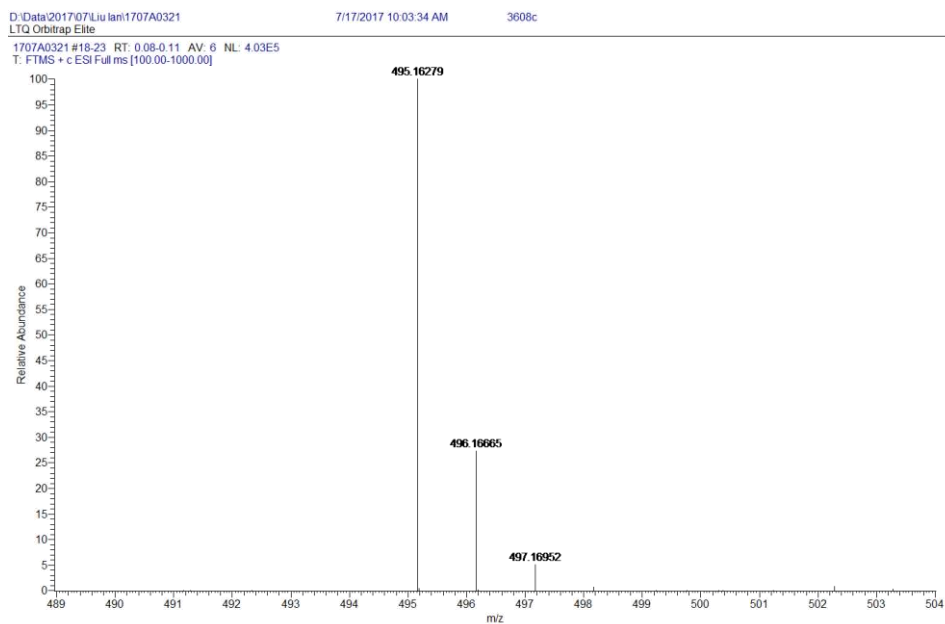


Figure S44. HR-ESIMS of (4*R*, 10*S*, 4'*S*)-leptothalenone B (**6**) in CD₃OD.



SPECTRUM - simulation :

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
495.16279	495.16255	0.48	11.5	C ₂₅ H ₂₈ O ₉ Na

Figure S45. Structure of **3** 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 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. C₁₂H₁₄O₅, M = 238.23, orthorhombic crystal (0.40 × 0.30 × 0.30 mm), bronze block, space group P212121; unit cell dimensions $a = 5.298$ Å, $b = 12.14910$ (10) Å, $c = 16.69040$ (10) Å, $V = 1074.293$ (11) Å³; $Z = 4$; a total of 2163 unique reflections [$R(\text{int}) = 0.0224$] was measured; the final refinement gave $R_1 = 0.0334$, $wR_2 = 0.0885$, and $S = 1.121$; Flack parameter = 0.00(6). Crystallographic data for the structure of **5** have been submitted to the Cambridge Crystallographic Data Centre as supplementary publication CCDC 1830777.)

