

Supporting Information

Discovery of *p*-Terphenyl Metabolites as Potential Phosphodiesterase PDE4D Inhibitors from the Coral-Associated Fungus *Aspergillus* sp. ITBBc1

Zhikai Guo ^{1,*}, Ailiman Abulaizi ⁵, Ling Huang ⁴, Zijun Xiong ¹, Shiqing Zhang ¹, Tianmi Liu ^{3,*}, Rong Wang ^{2,*}

¹ Hainan Key Laboratory of Tropical Microbe Resources, Institute of Tropical Bioscience and Biotechnology, Chinese Academy of Tropical Agricultural Sciences & Key Laboratory for Biology and Genetic Resources of Tropical Crops of Hainan Province, Hainan Institute for Tropical Agricultural Resources, Haikou 571101, China

² Hainan Provincial Key Laboratory of Tropical Maricultural Technologies, Hainan Academy of Ocean and Fisheries Sciences, Haikou 571126, China

³ Hainan Testing Center for the Quality and Safety of Aquatic Products, Hainan Aquatic Technology Extension Station, Haikou 570206, China

⁴ Key Laboratory of Tropical Biological Resources of Ministry of Education, School of Pharmaceutical Sciences, Hainan University, Haikou 570208, China

⁵ State Key Laboratory of Pharmaceutical Biotechnology, Institute of Functional Biomolecules, School of Life Sciences, Nanjing University, Nanjing 210023, China

* Correspondence: guozhikai@itbb.org.cn (Z.G.); ltm600@163.com (T.L.); wangrong1982@gmail.com (R.W.)

Figure S1. ^1H NMR (500 MHz, acetone- d_6) spectrum of compound **1**.

Figure S2. ^{13}C NMR (125 MHz, acetone- d_6) spectrum of compound **1**.

Figure S3. DEPT135 spectrum of compound **1**.

Figure S4. HSQC spectrum of compound **1**.

Figure S5. HMBC spectrum of compound **1**.

Figure S6. ^1H - ^1H COSY spectrum of compound **1**.

Figure S7. ROESY spectrum of compound **1**.

Figure S8. The HRESIMS spectrum of compound **1**.

Figure S9. UV spectrum of compound **1**.

Figure S10. IR spectrum of compound **1**.

Figure S11. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **2**.

Figure S12. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **2**.

Figure S13. DEPT135 spectrum of compound **2**.

Figure S14. HSQC spectrum of compound **2**.

Figure S15. HMBC spectrum of compound **2**.

Figure S16. ^1H - ^1H COSY spectrum of compound **2**.

Figure S17. ROESY spectrum of compound **2**.

Figure S18. The HRESIMS spectrum of compound **2**.

Figure S19. UV spectrum of compound **2**.

Figure S20. IR spectrum of compound **2**.

Figure S21. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **3**.

Figure S22. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **3**.

Figure S23. DEPT135 spectrum of compound **3**.

Figure S24. HSQC spectrum of compound **3**.

Figure S25. HMBC spectrum of compound **3**.

Figure S26. ^1H - ^1H COSY spectrum of compound **3**.

Figure S27. ROESY spectrum of compound **3**.

Figure S28. The HRESIMS spectrum of compound **3**.

Figure S29. UV spectrum of compound **3**.

Figure S30. IR spectrum of compound **3**.

Figure S31. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **4**.

Figure S32. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **4**.

Figure S33. DEPT135 spectrum of compound **4**.

Figure S34. HSQC spectrum of compound **4**.

Figure S35. HMBC spectrum of compound **4**.

Figure S36. ^1H - ^1H COSY spectrum of compound **4**.

Figure S37. ROESY spectrum of compound **4**.

Figure S38. The HRESIMS spectrum of compound **4**.

Figure S39. UV spectrum of compound **4**.

Figure S40. IR spectrum of compound **4**.

Figure S41. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **5**.

Figure S42. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **5**.

Figure S43. DEPT135 spectrum of compound **5**.

Figure S44. HSQC spectrum of compound **5**.

Figure S45. HMBC spectrum of compound **5**.

Figure S46. ^1H - ^1H COSY spectrum of compound **5**.

Figure S47. NOESY spectrum of compound **5**.

Figure S48. The HRESIMS spectrum of compound **5**.

Figure S49. UV spectrum of compound **5**.

Figure S50. IR spectrum of compound **5**.

Figure S51. Predicted biosynthetic pathway for compound **5**.

Figure S1 ^1H NMR (500 MHz, acetone- d_6) spectrum of compound **1**.

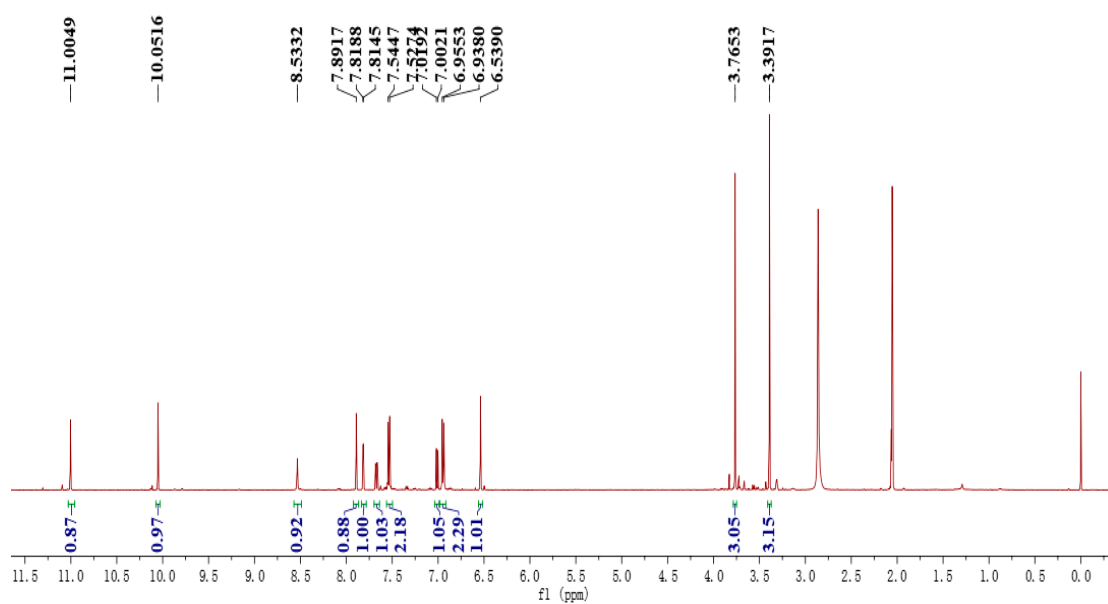


Figure S2. ^{13}C NMR (125 MHz, acetone- d_6) spectrum of compound **1**.

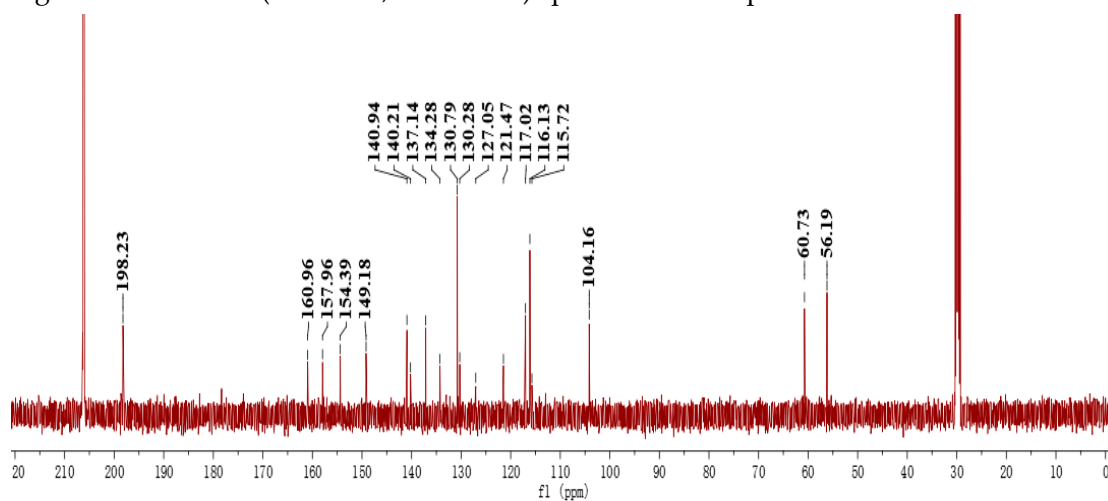


Figure S3. DEPT135 spectrum of compound **1**.

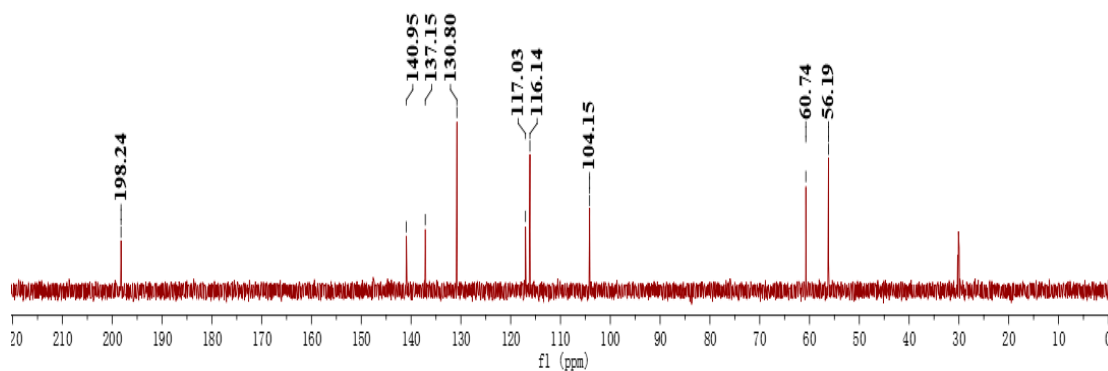


Figure S4. HSQC spectrum of compound 1.

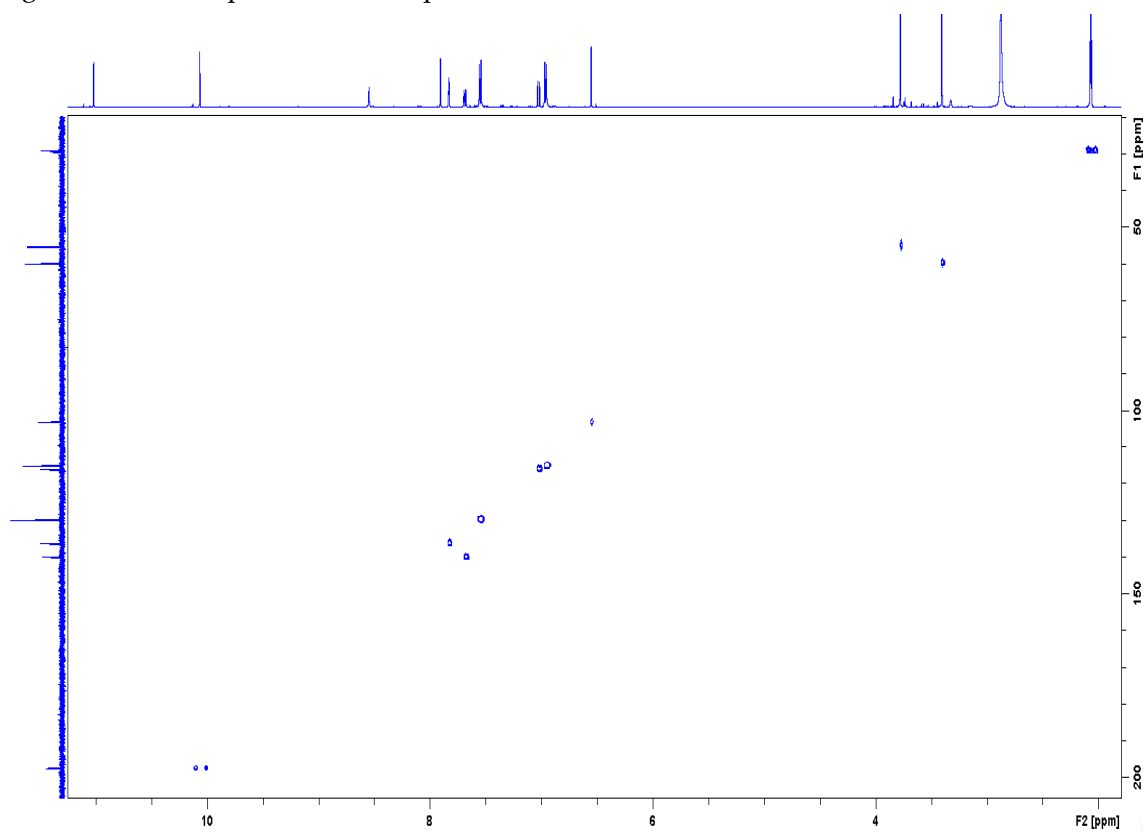


Figure S5. HMBC spectrum of compound 1.

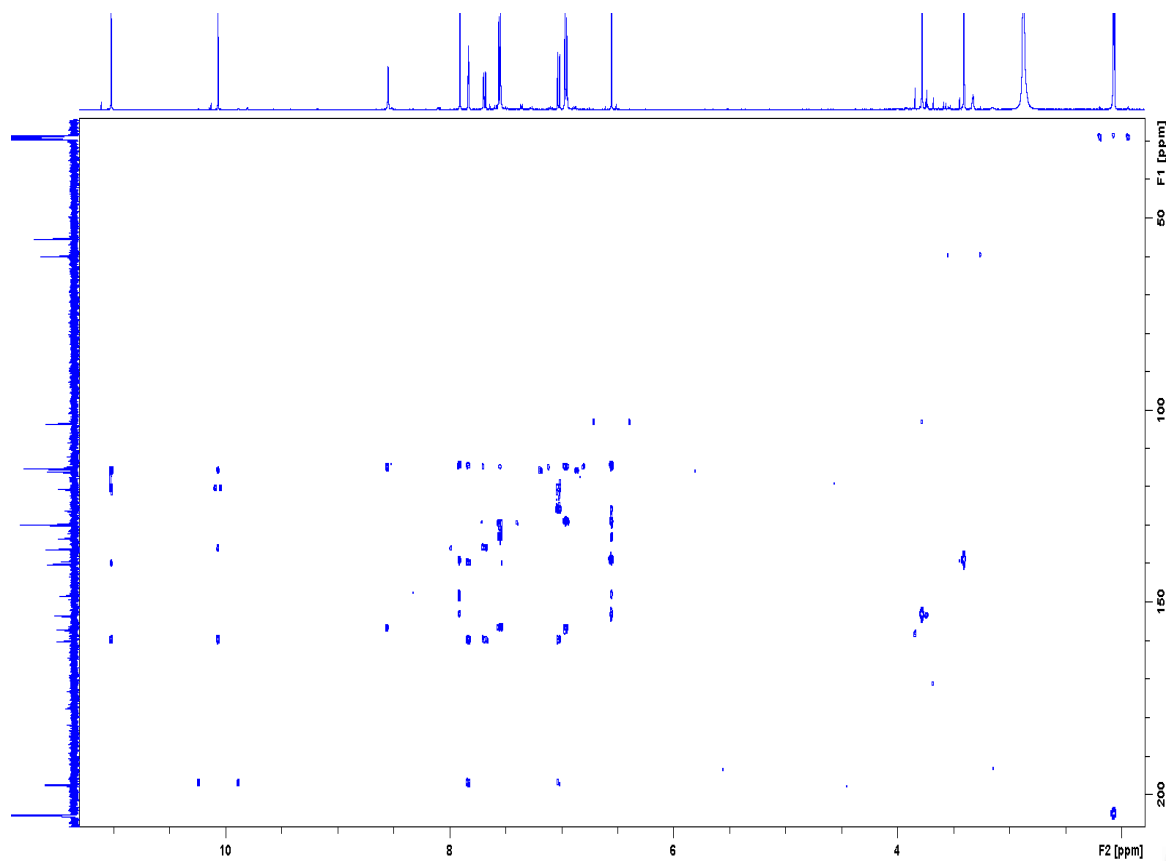


Figure S6. ^1H - ^1H COSY spectrum of compound **1**.

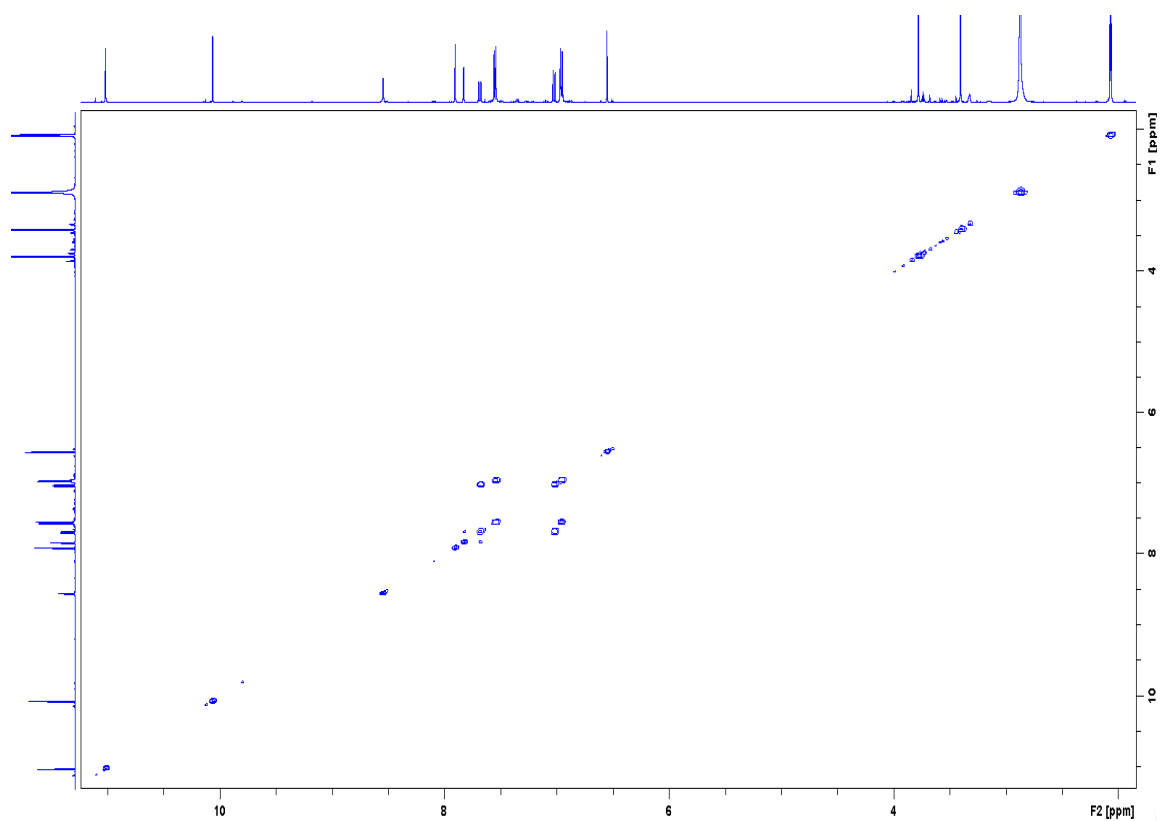


Figure S7. ROESY spectrum of compound **1**.

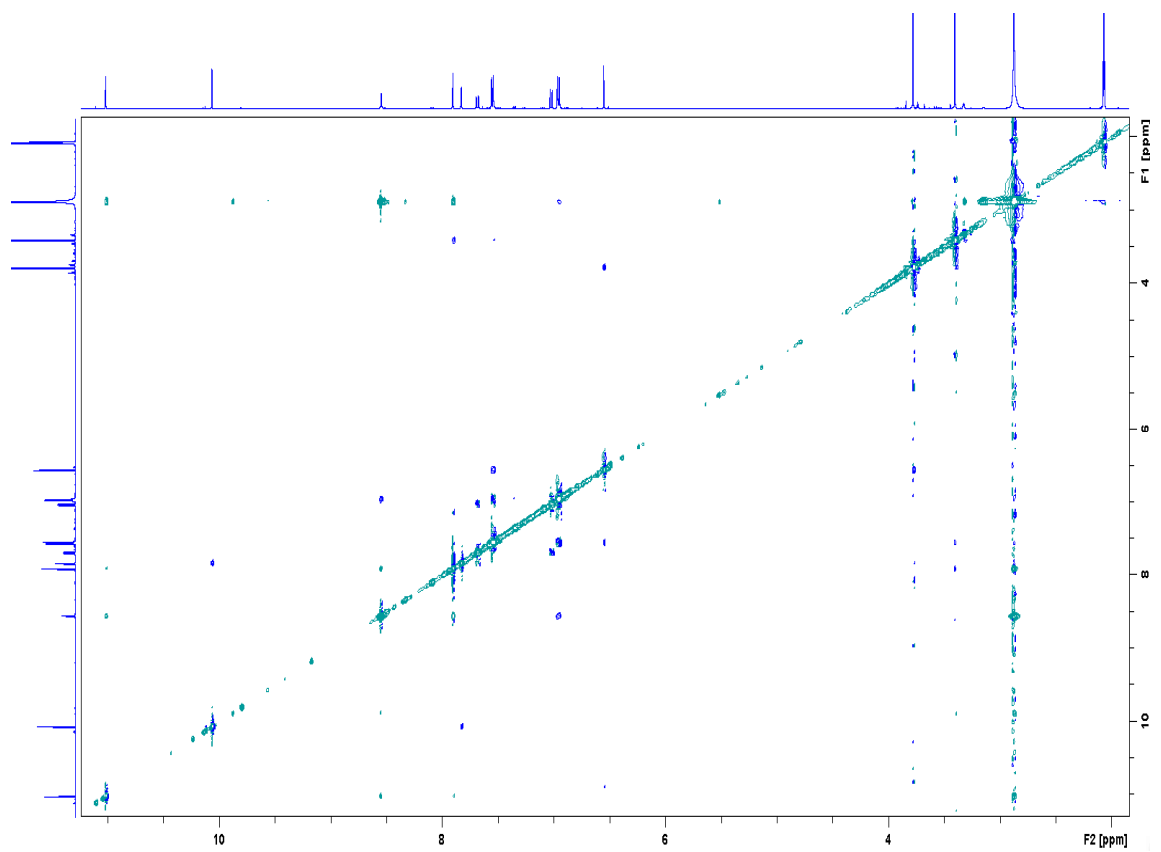


Figure S8. The HRESIMS spectrum of compound **1**.

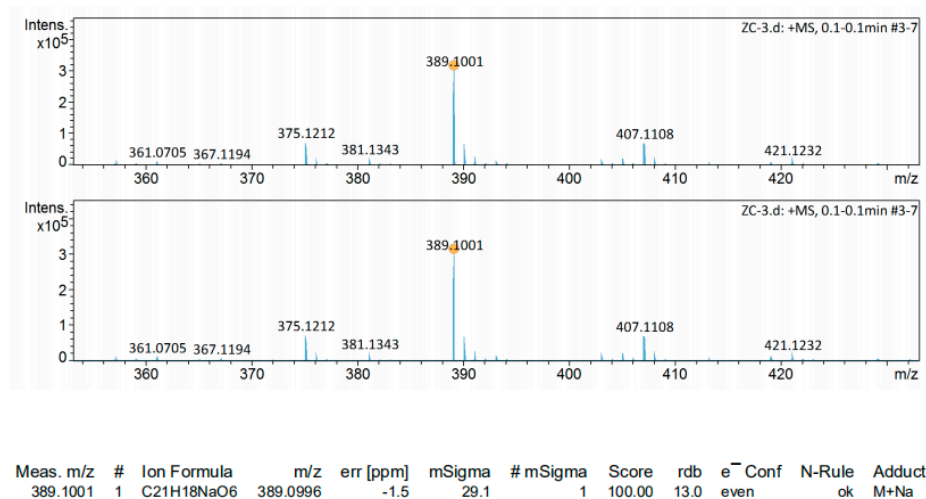
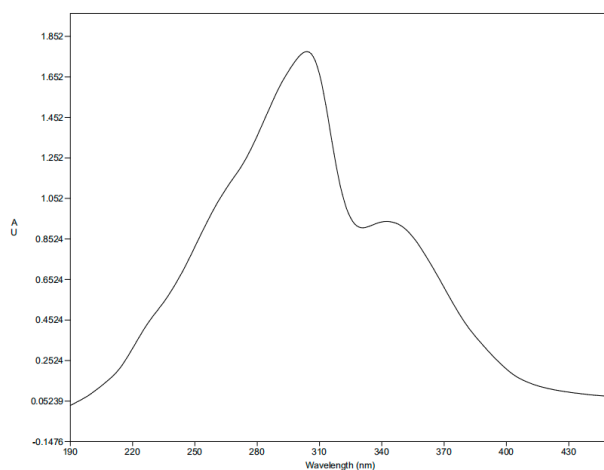


Figure S9. UV spectrum of compound **1**.



Bio-Kline Software V4.80 Date : 2022/10/22 Time : 21:29:43

COMMENTS :
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MOS-500 Spectrometer
Spectrum measurement
Acq duration = 0.2 s
Fentes bandwidth = 5 nm
HV = 126 V
BioKline V4.80

Figure S10. IR spectrum of compound **1**.

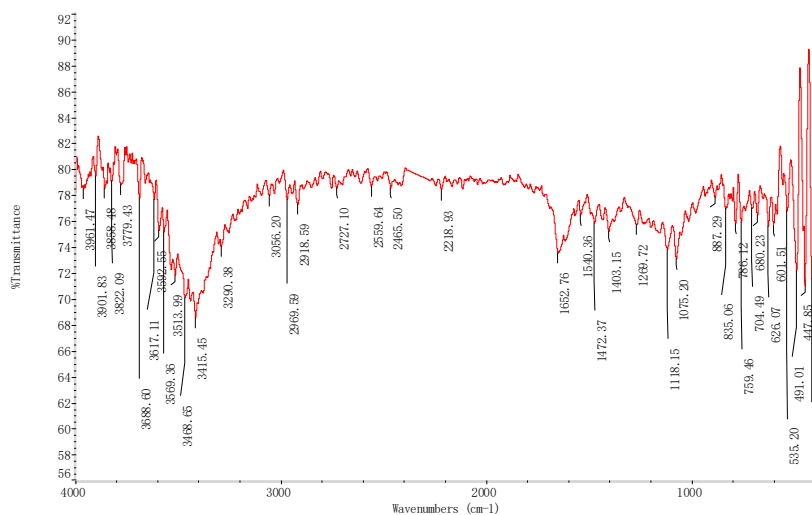


Figure S11. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 2.

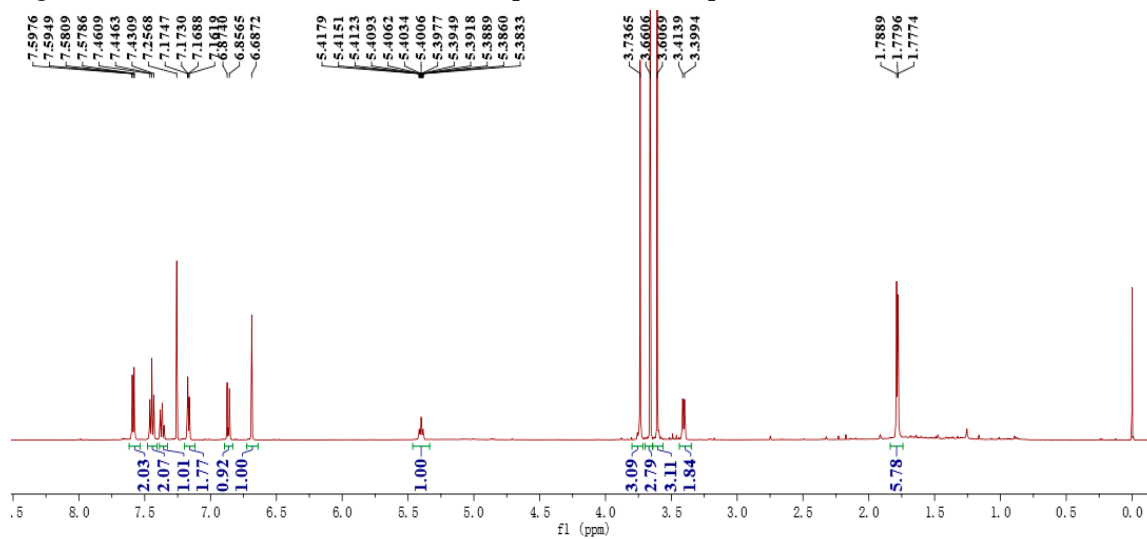


Figure S12. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 2.

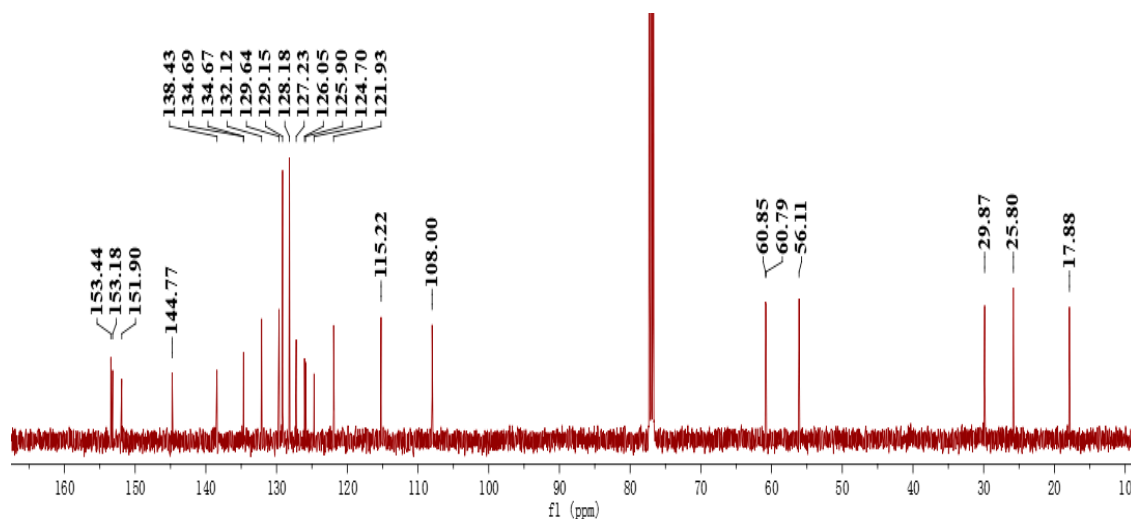


Figure S13. DEPT135 spectrum of compound 2

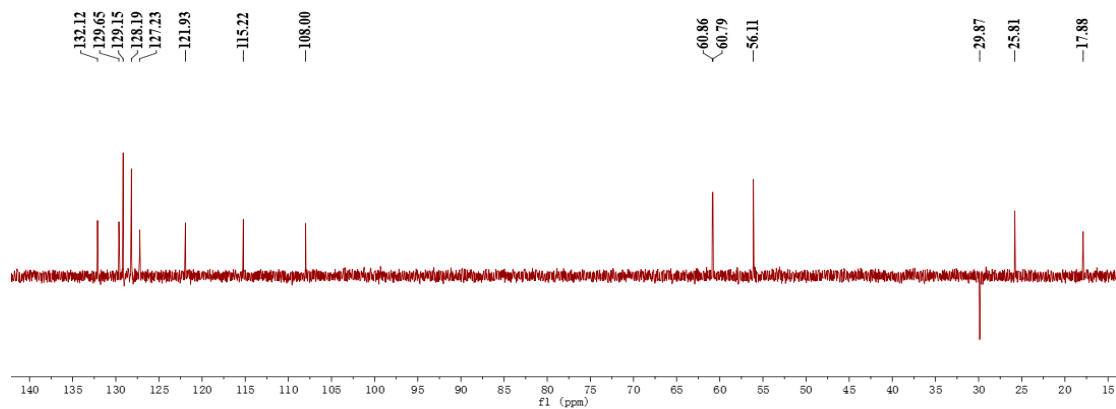


Figure S14. HSQC spectrum of compound 2.

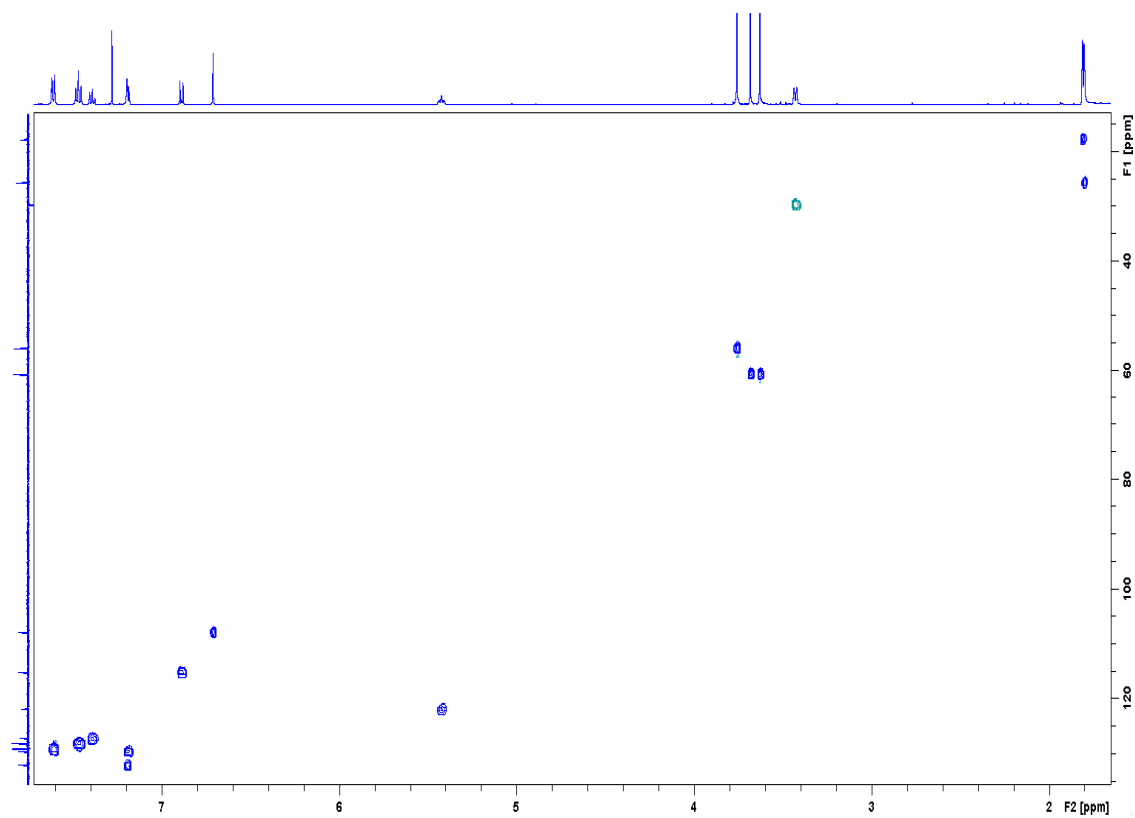


Figure S15. HMBC spectrum of compound 2.

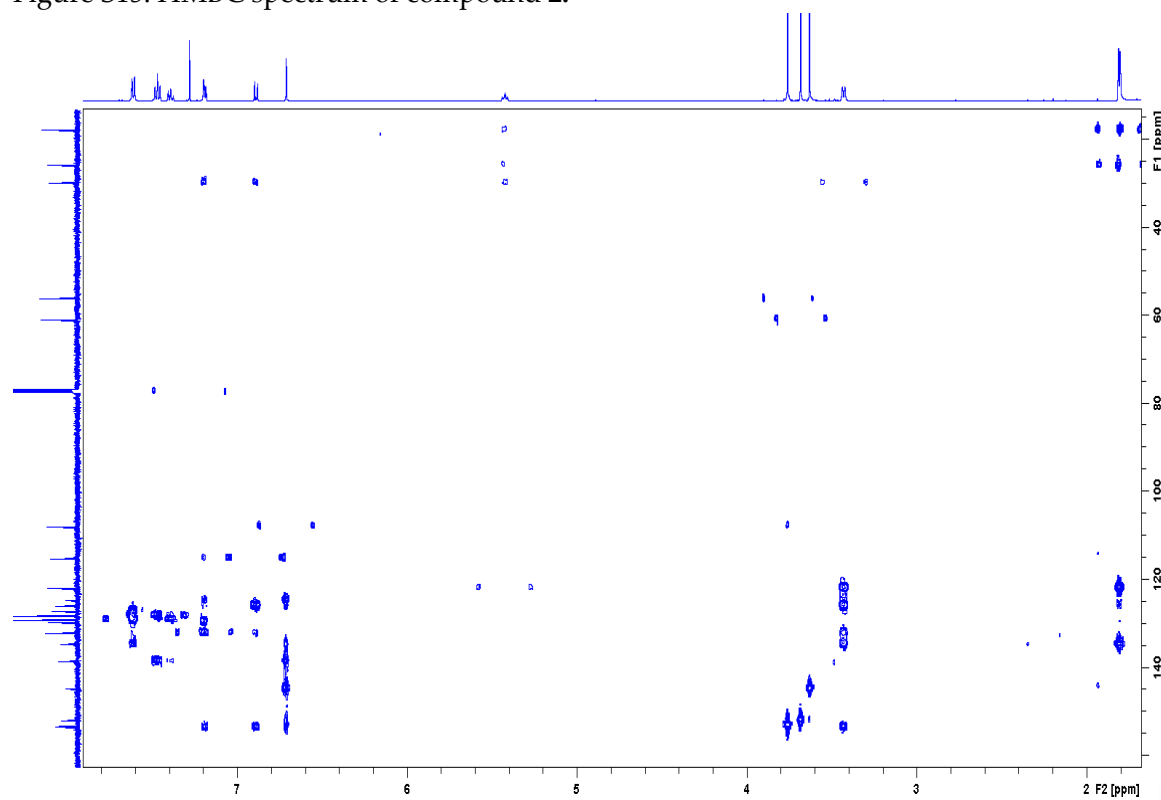
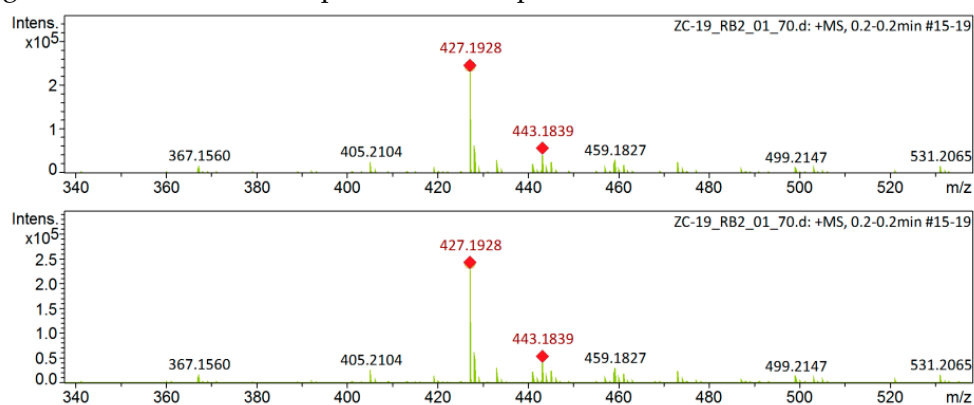
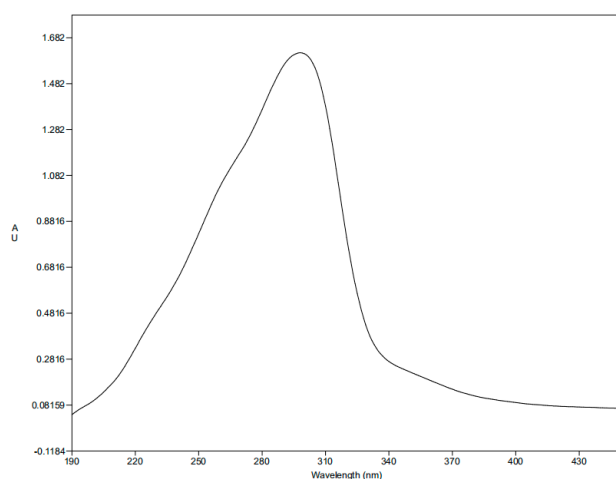


Figure S18. The HRESIMS spectrum of compound 2.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
427.1928	1	C ₂₆ H ₂₈ NaO ₄	427.1880	-11.2	7.1	1	100.00	13.0	even		ok	M+Na

Figure S19. UV spectrum of compound 2.



Bio-Kine Software V4.80 Date : 2022/10/22 Time : 21:52:49

COMMENTS :
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MOS-500 Spectrometer
Spectrum measurement
Acq duration = 0.2 s
Folies bandwidth = .5 nm
HV = 126 V
BioKine V4.80

Figure S20. IR spectrum of compound 2.

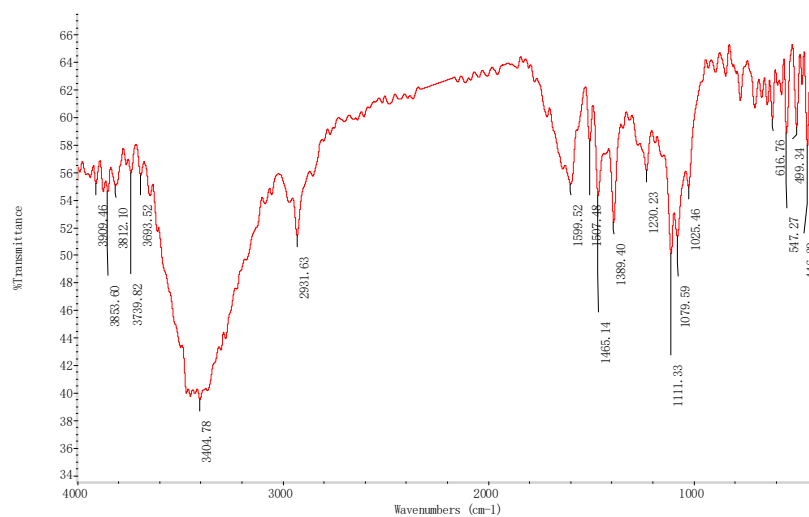


Figure S21. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **3**.

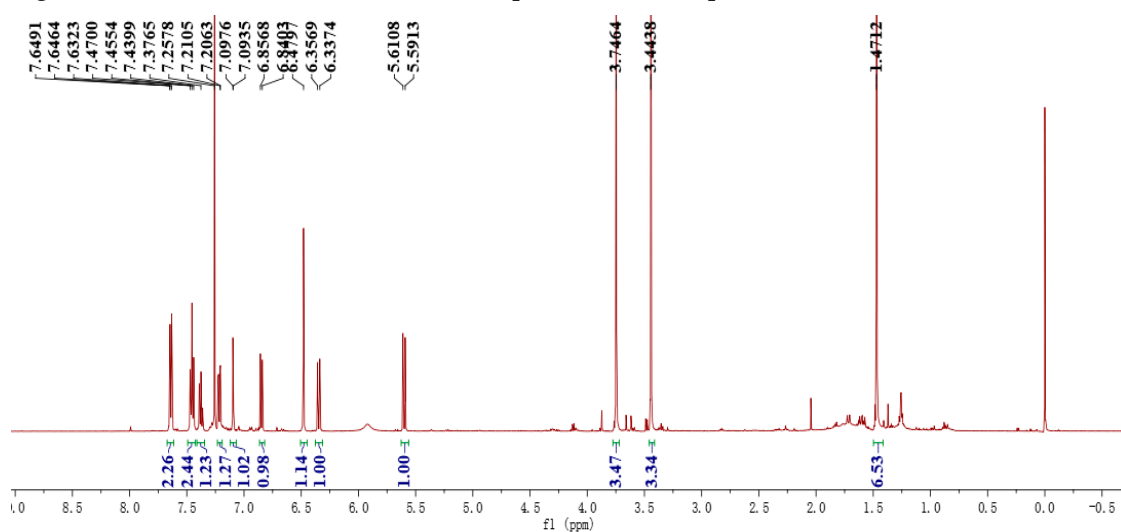


Figure S22. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **3**.

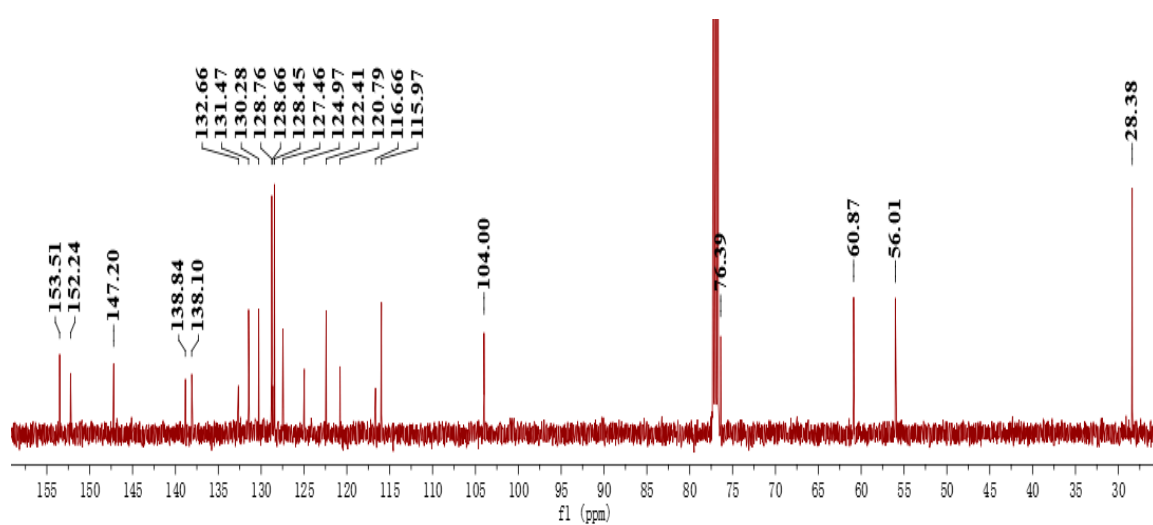


Figure S23. DEPT135 spectrum of compound **3**.

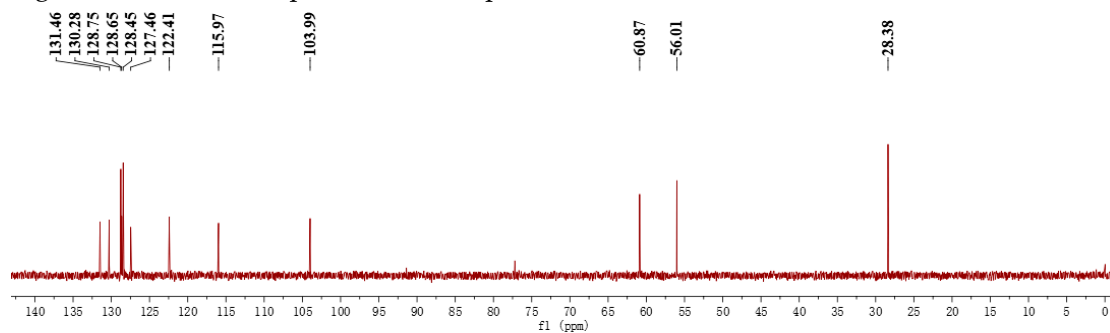


Figure S24. HSQC spectrum of compound 3.

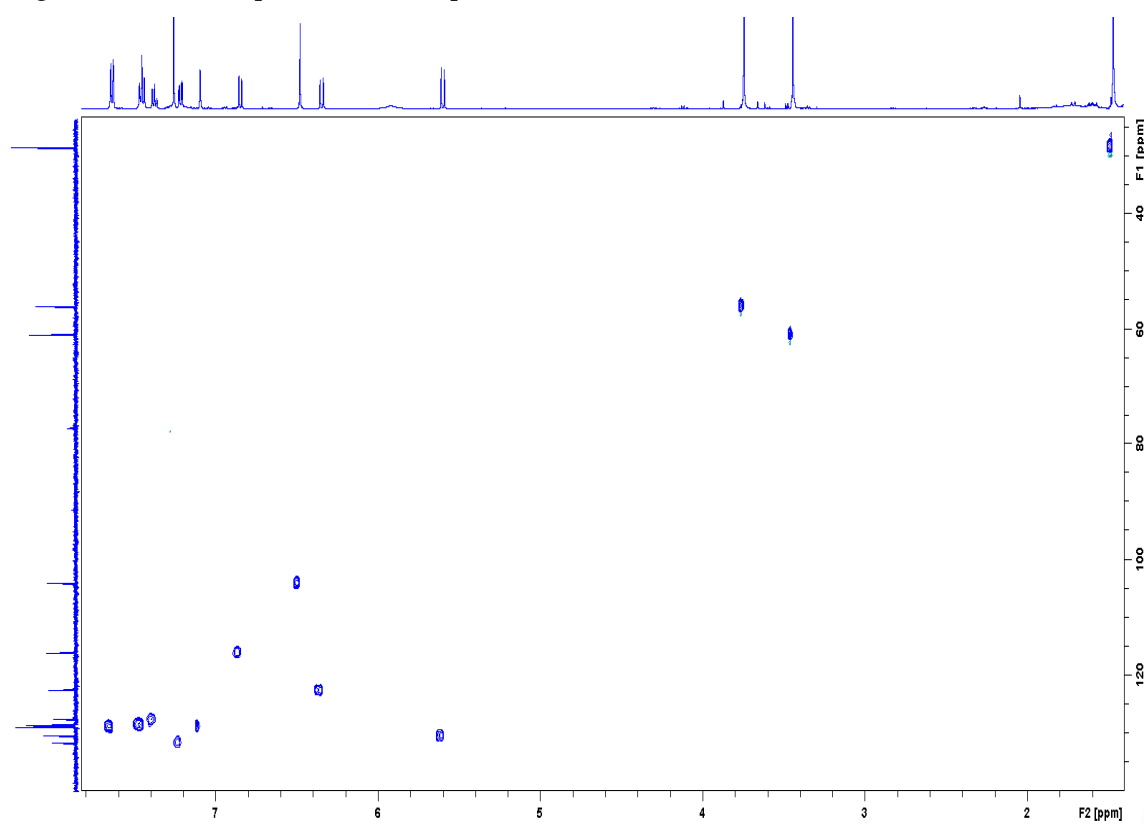


Figure S25. HMBC spectrum of compound 3.

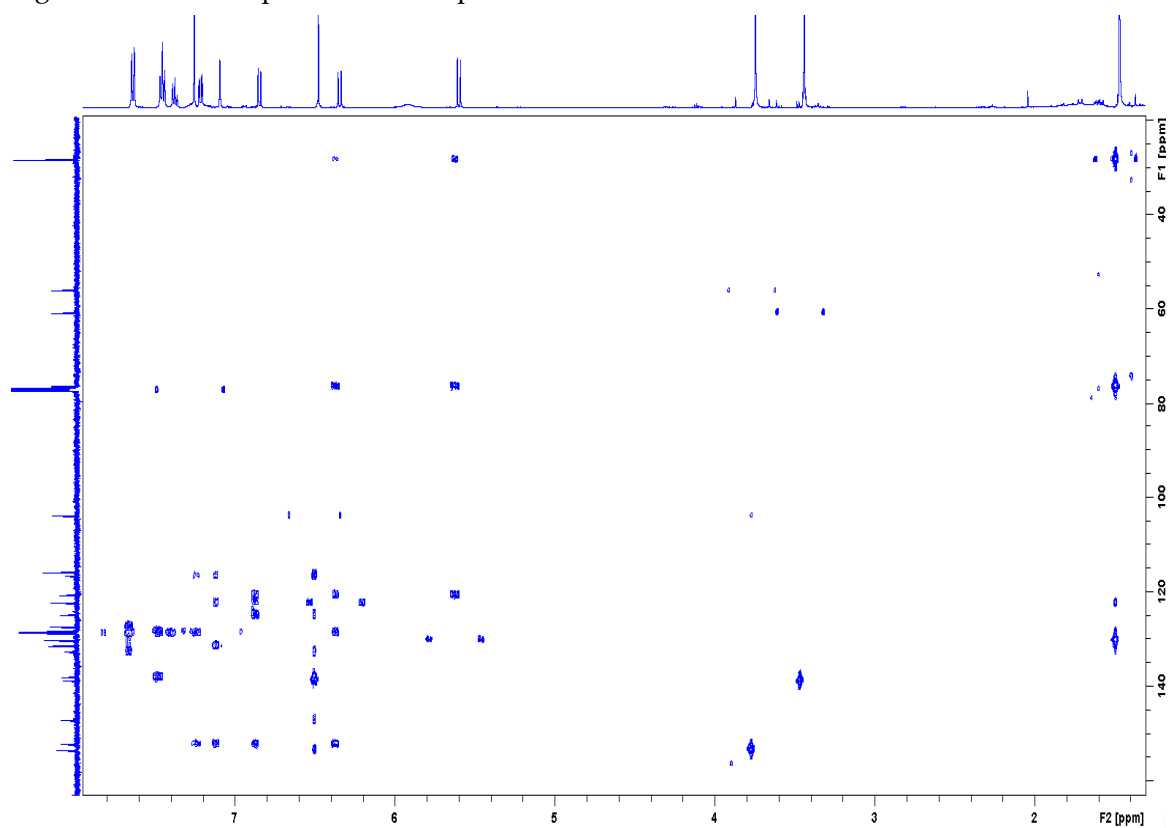


Figure S26. ^1H - ^1H COSY spectrum of compound 3.

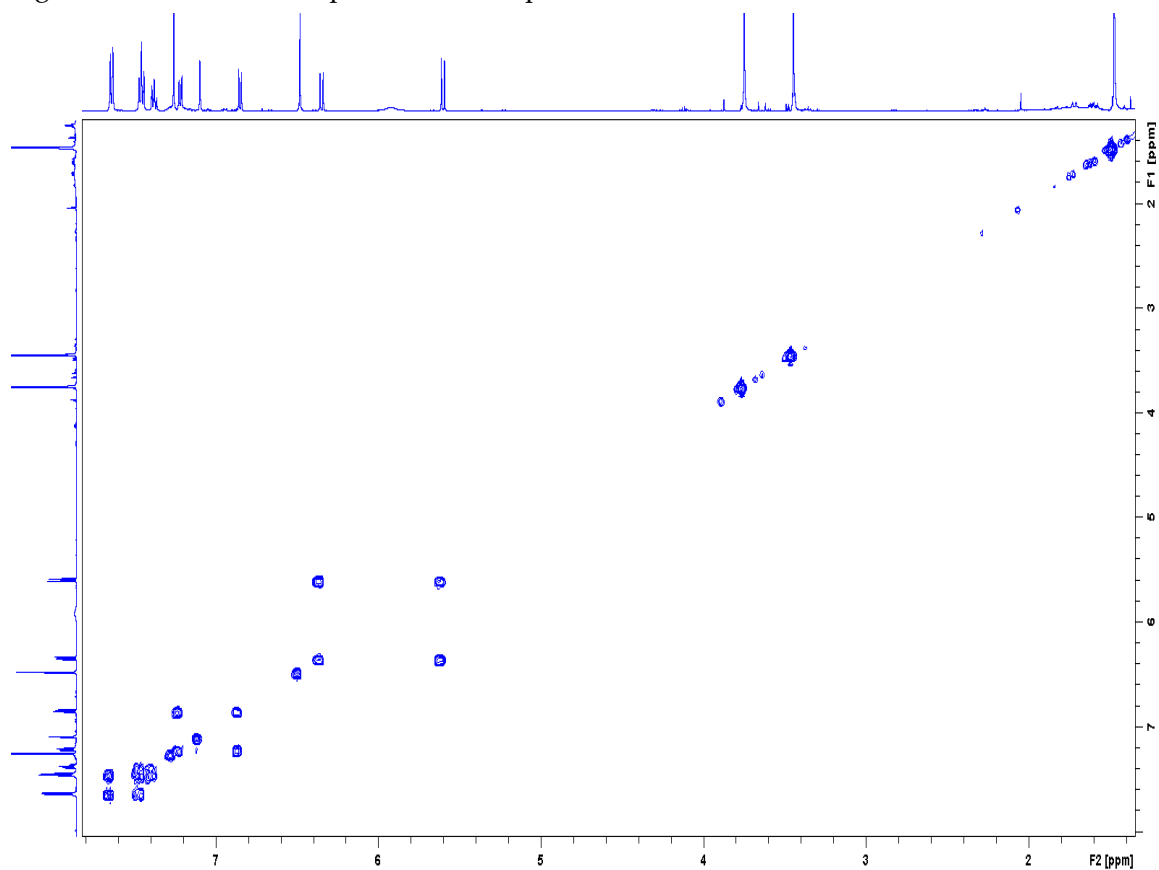


Figure S27. ROESY spectrum of compound 3.

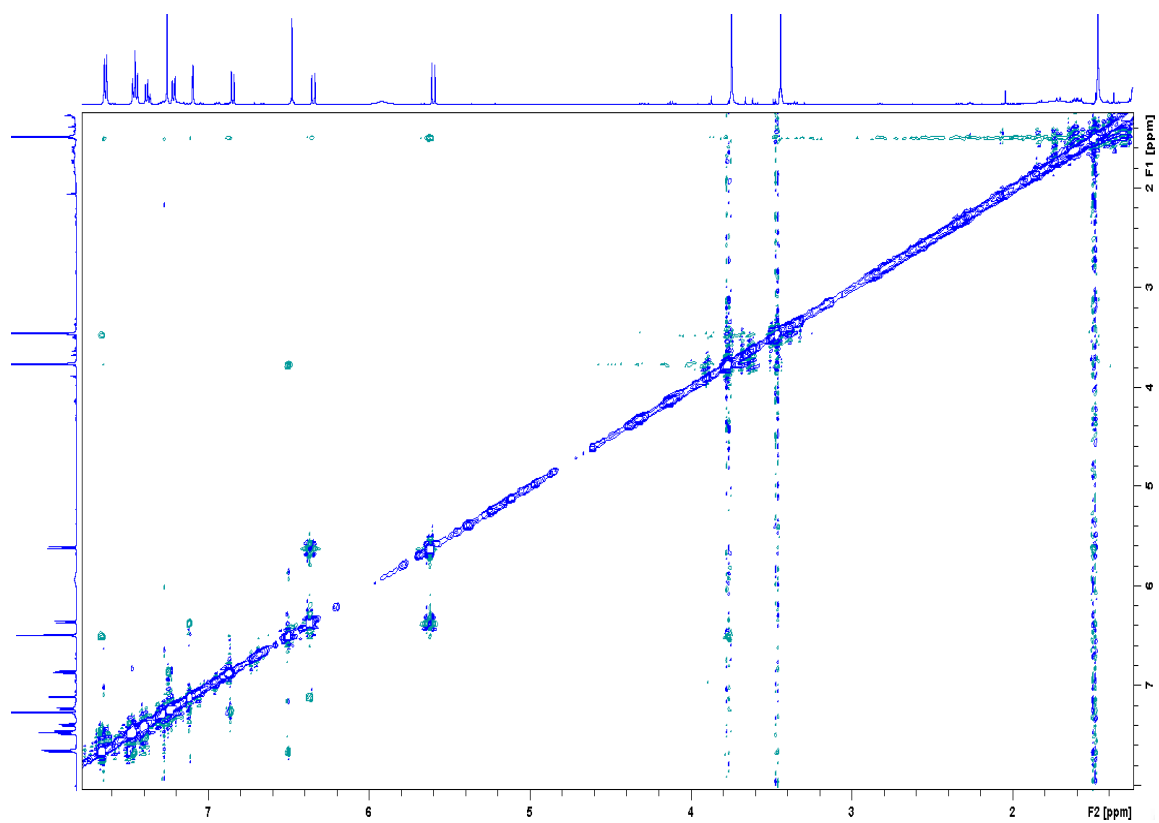


Figure S28. The HRESIMS spectrum of compound **3**.

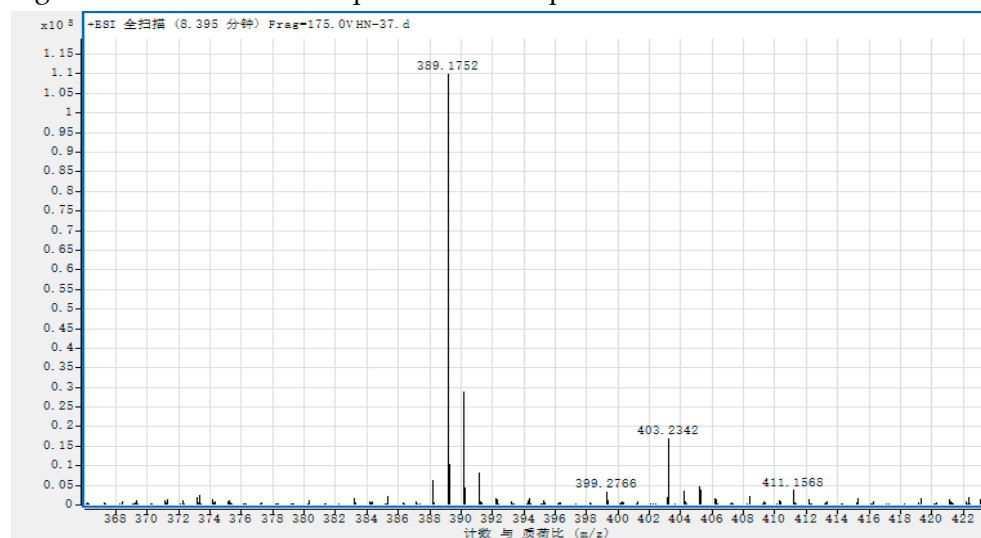


Figure S29. UV spectrum of compound **3**.

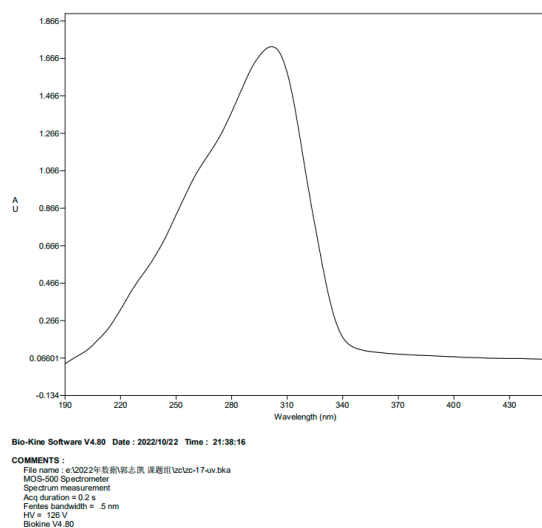


Figure S30. IR spectrum of compound **3**.

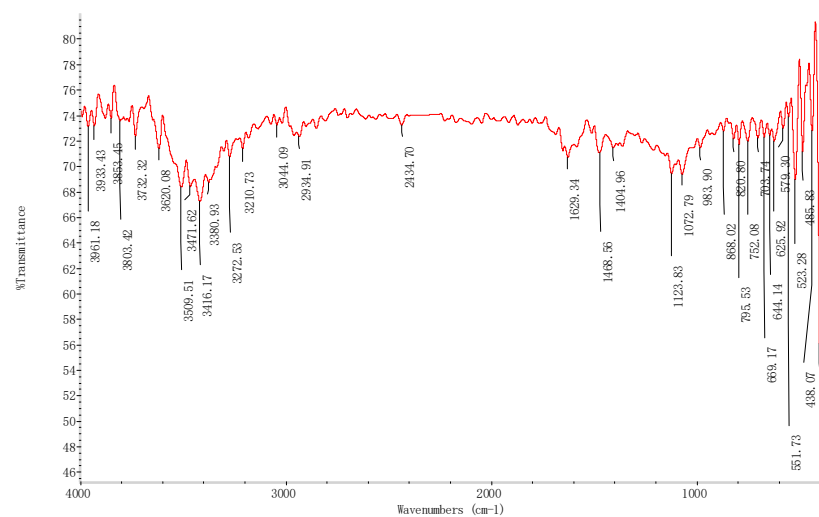


Figure S31. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **4**.

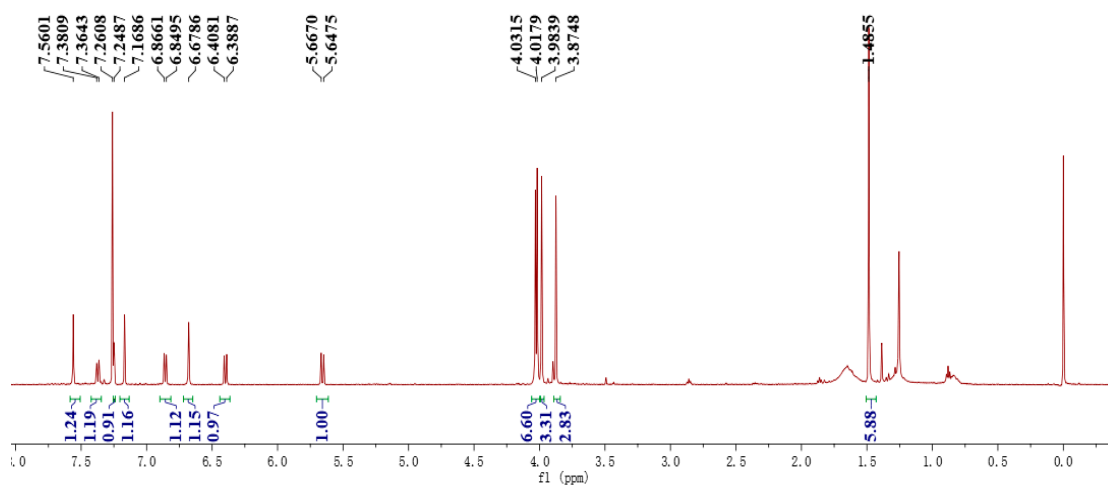


Figure S32. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **4**.

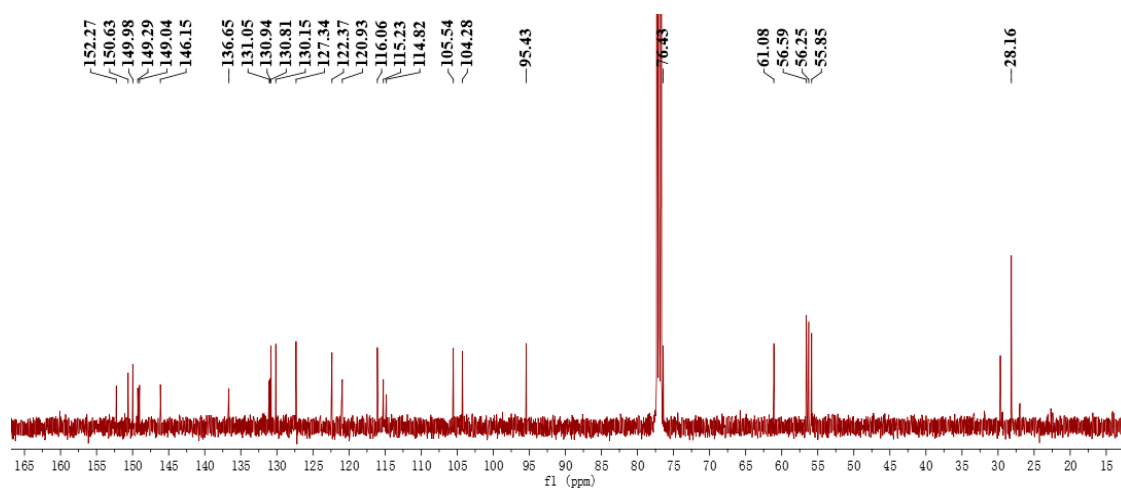


Figure S33. DEPT135 spectrum of compound **4**.

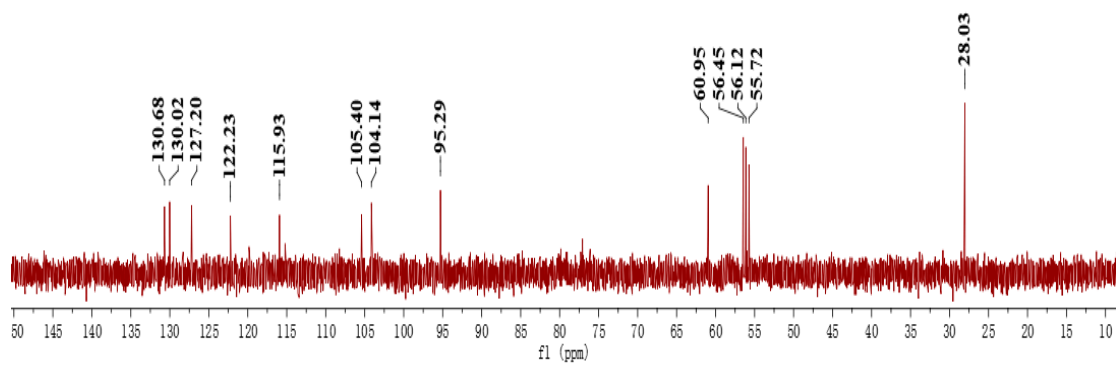


Figure S34. HSQC spectrum of compound 4.

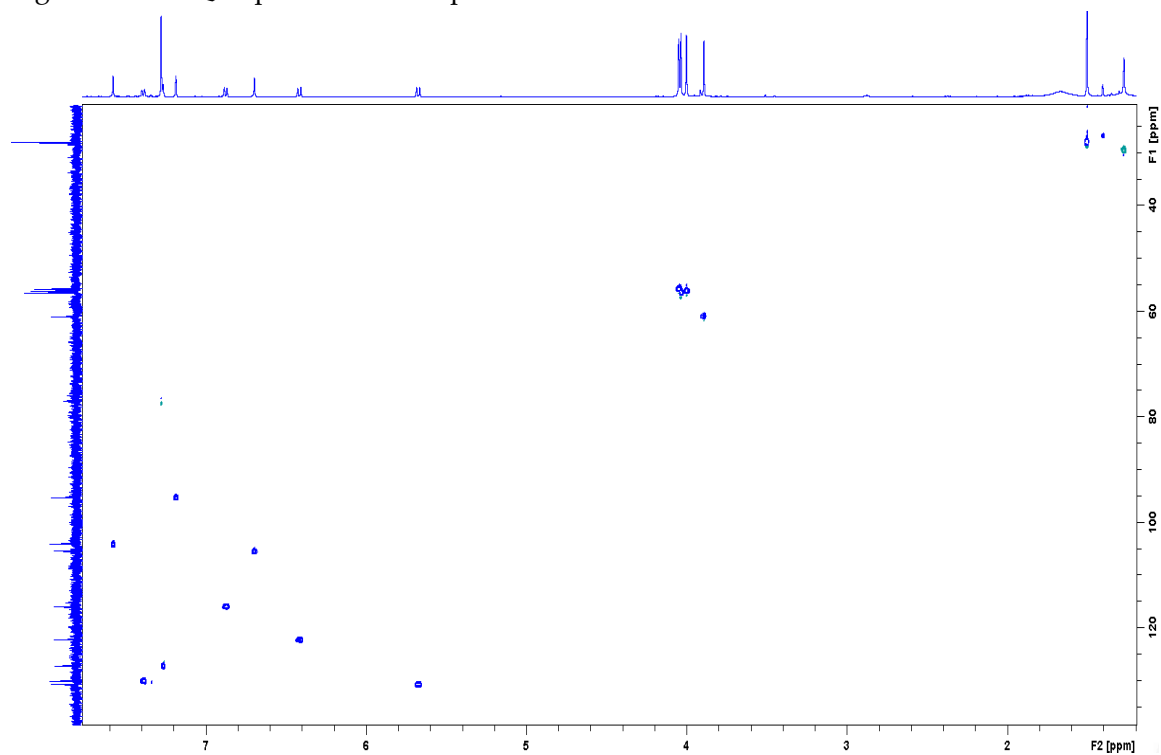


Figure S35. HMBC spectrum of compound 4.

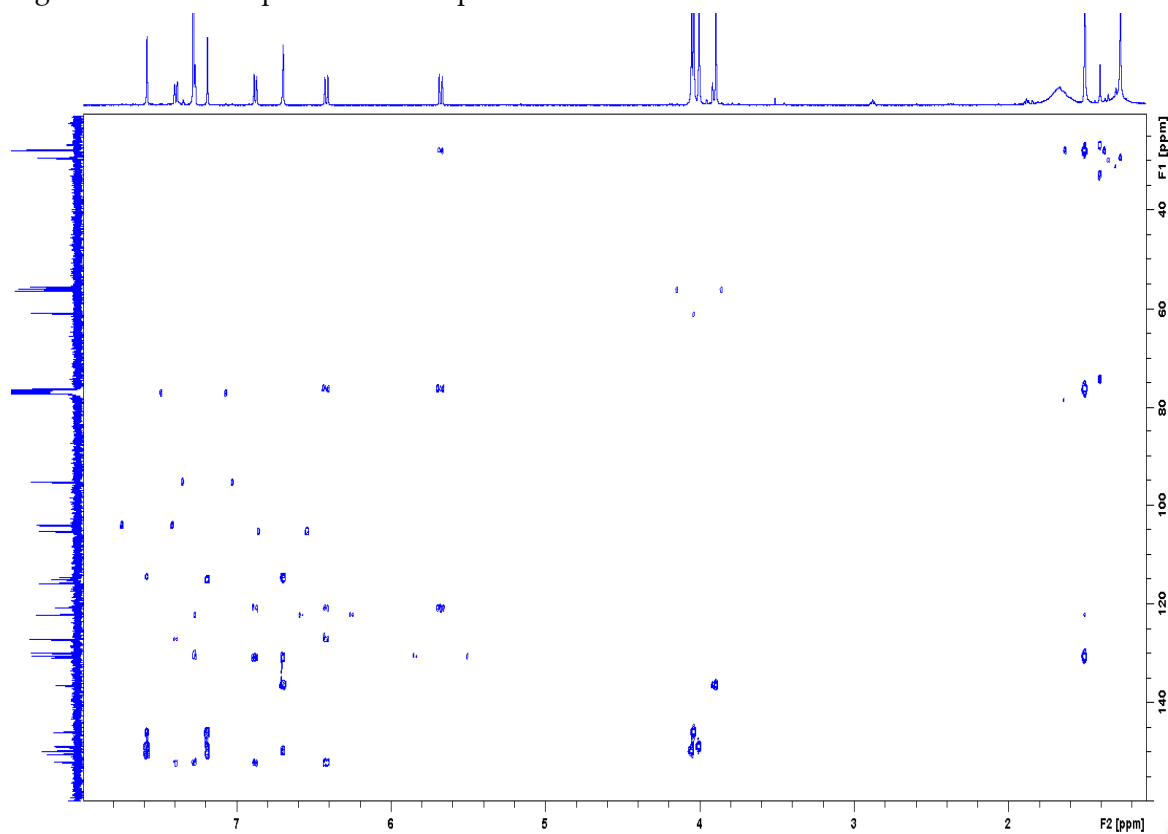


Figure S36. ^1H - ^1H COSY spectrum of compound **4**.

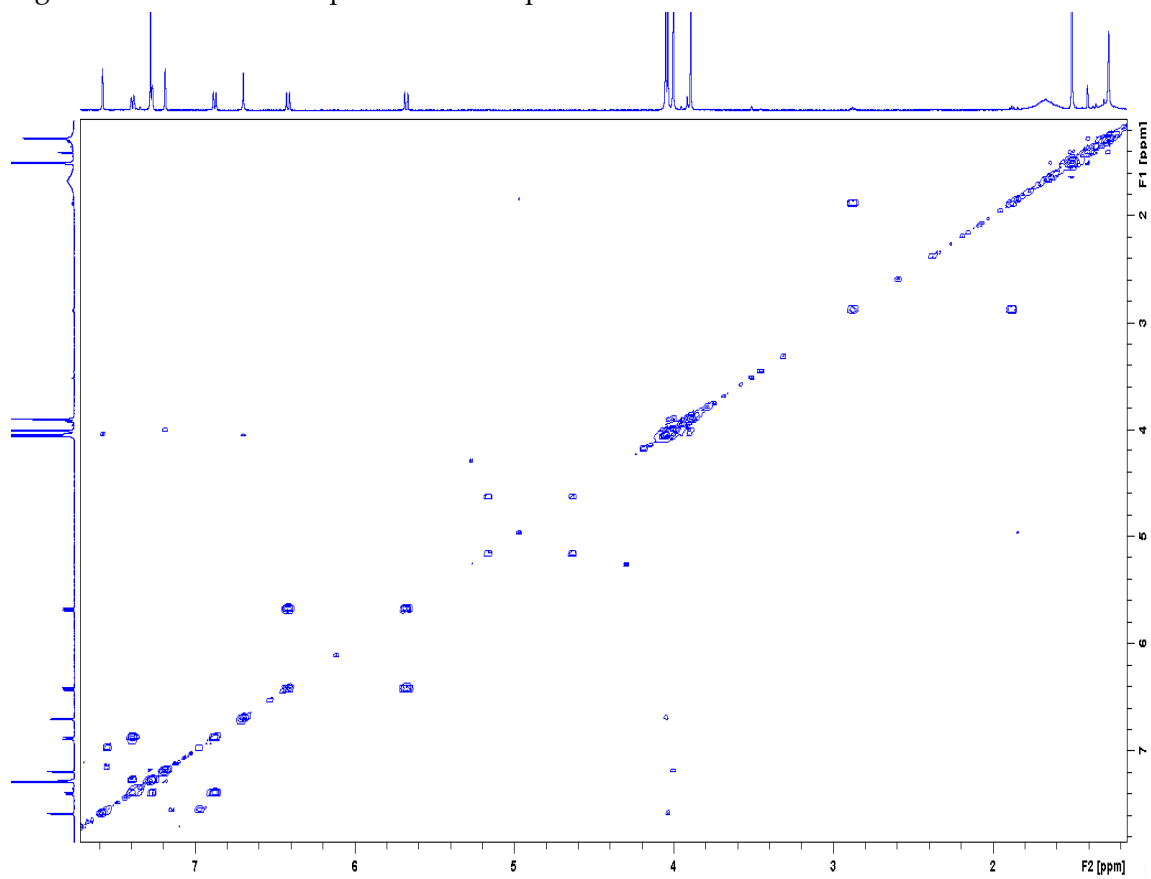


Figure S37. ROESY spectrum of compound **4**.

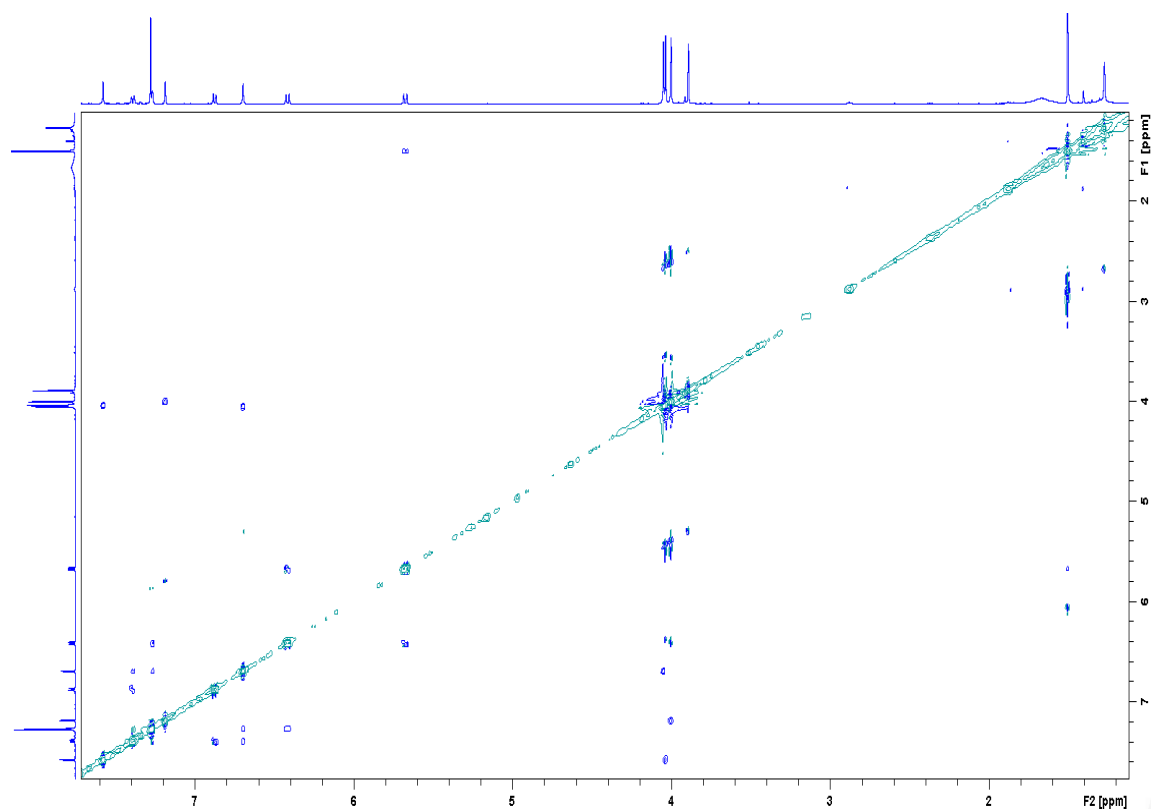


Figure S38. The HRESIMS spectrum of compound **4**.

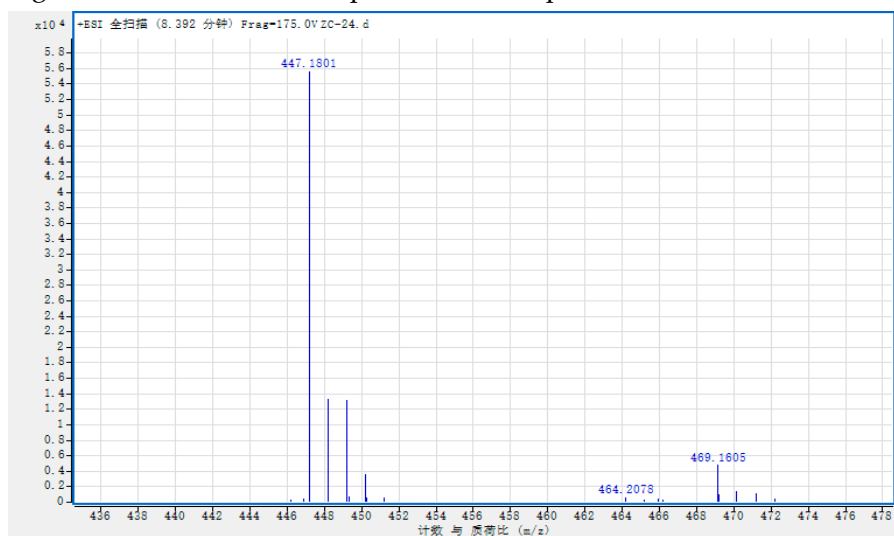
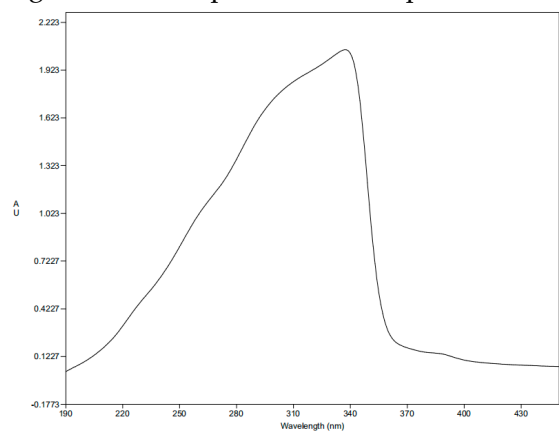


Figure S39. UV spectrum of compound **4**.



COMMENTS :
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 MOS-500 Spectrometer
 Spectrum measurement
 Acq duration = 0.2 s
 Filter bandwidth = 5 nm
 HV = 150 V
 BioKine V4.80

Figure S40. IR spectrum of compound **4**.

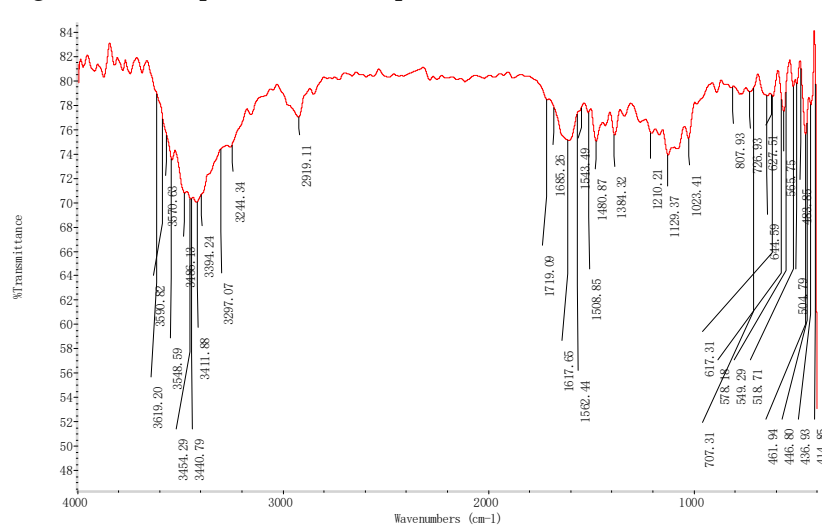


Figure S41. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **5**.

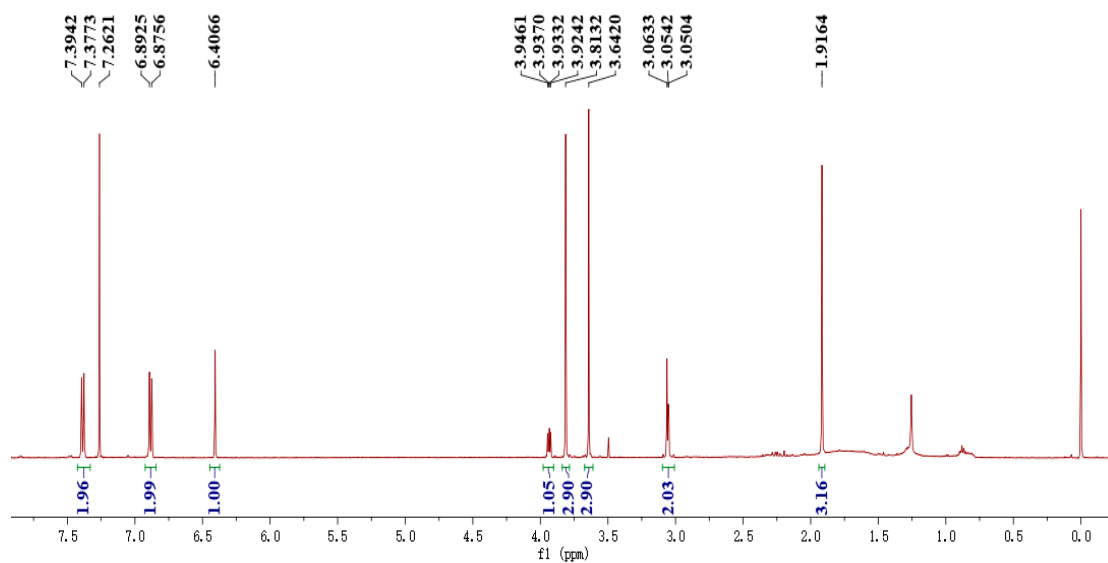


Figure S42. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **5**.

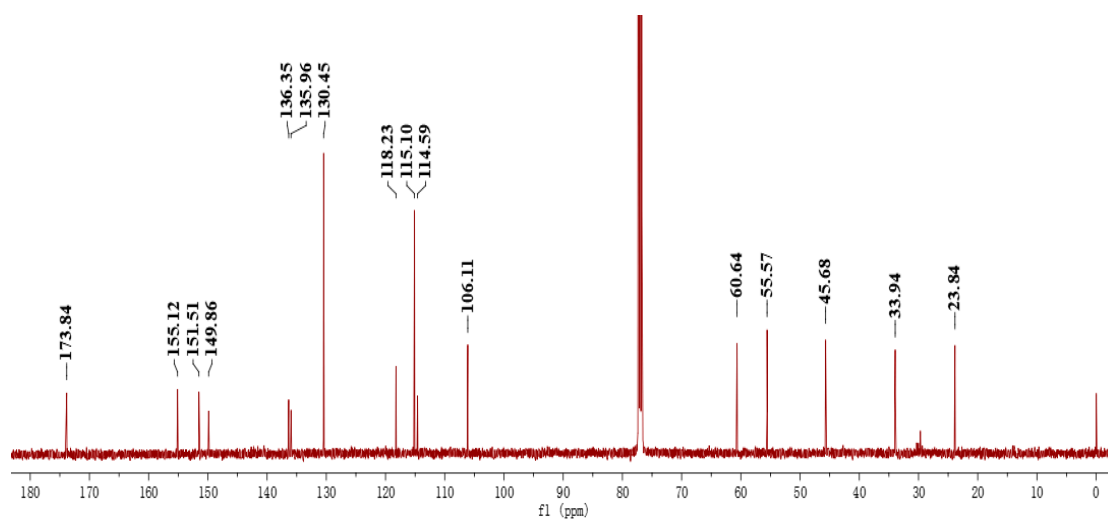


Figure S43. DEPT135 spectrum of compound **5**.

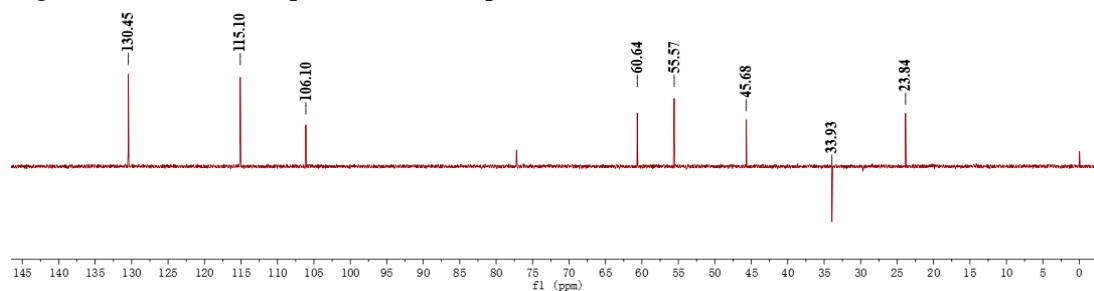


Figure S44. HSQC spectrum of compound 5.

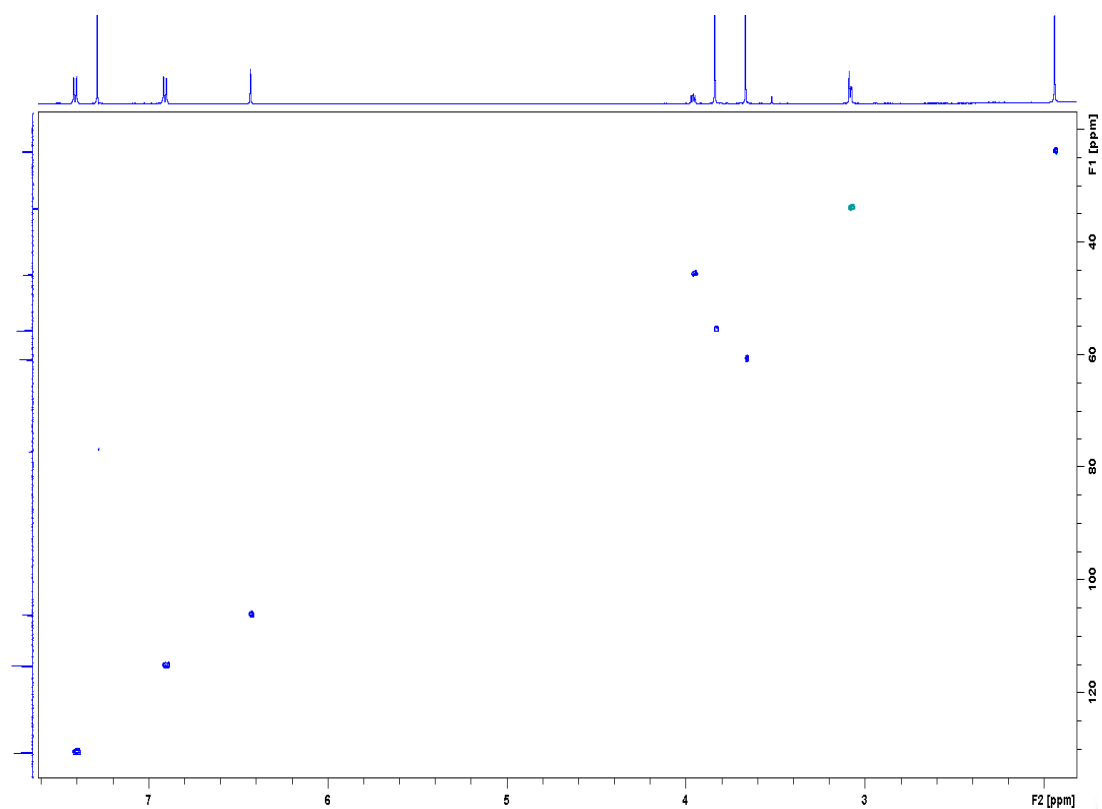


Figure S45. HMBC spectrum of compound 5.

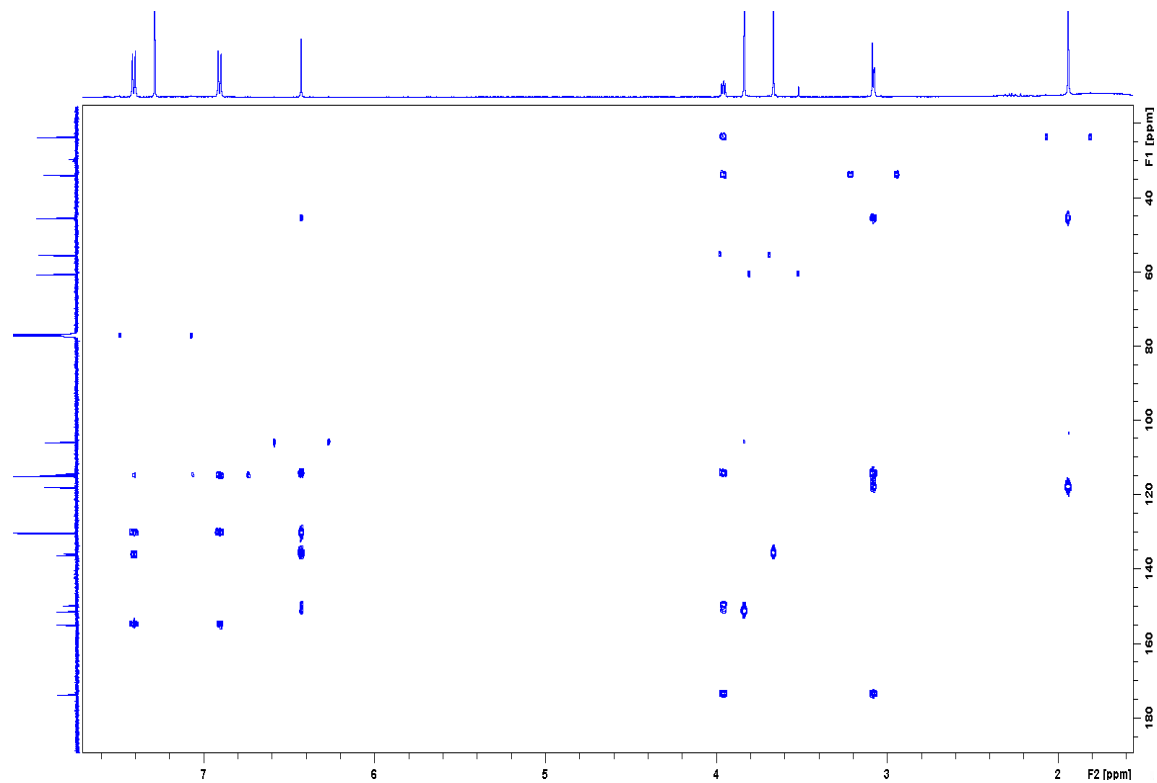


Figure S46. ^1H - ^1H COSY spectrum of compound 5.

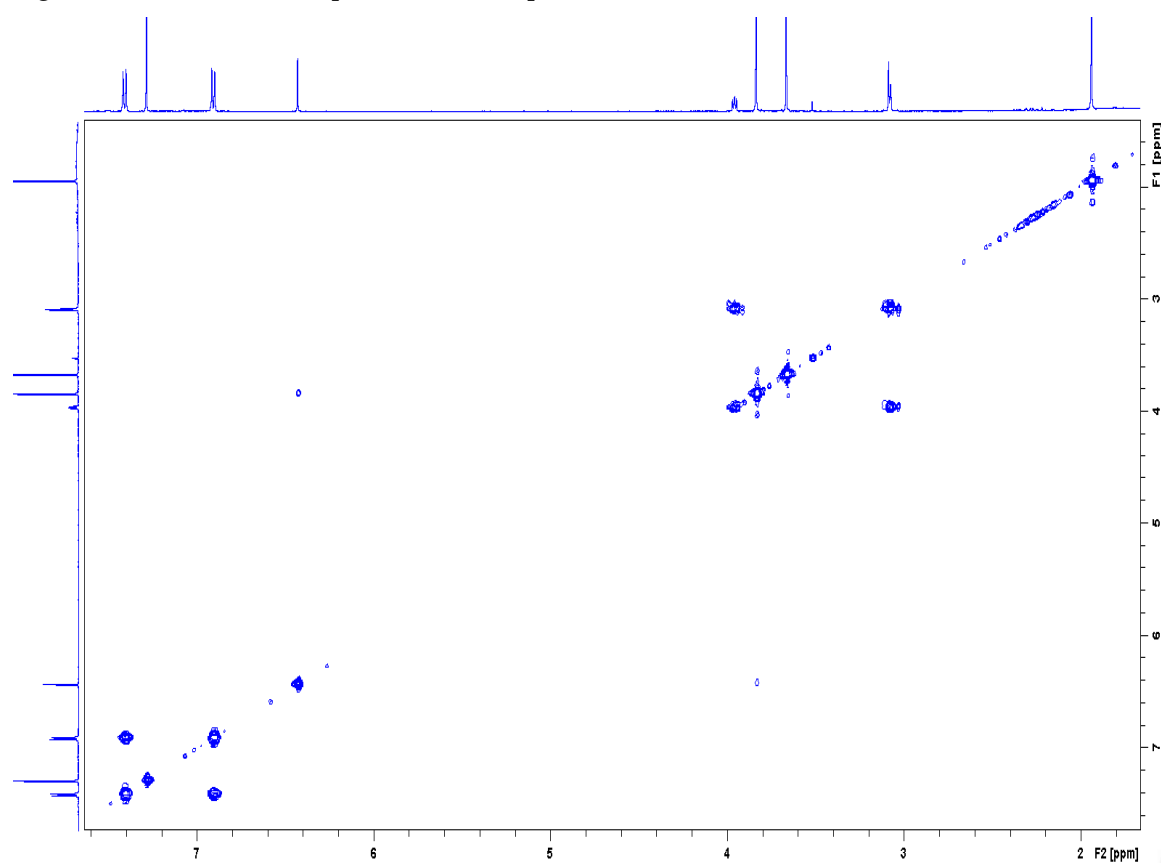


Figure S47. NOESY spectrum of compound 5.

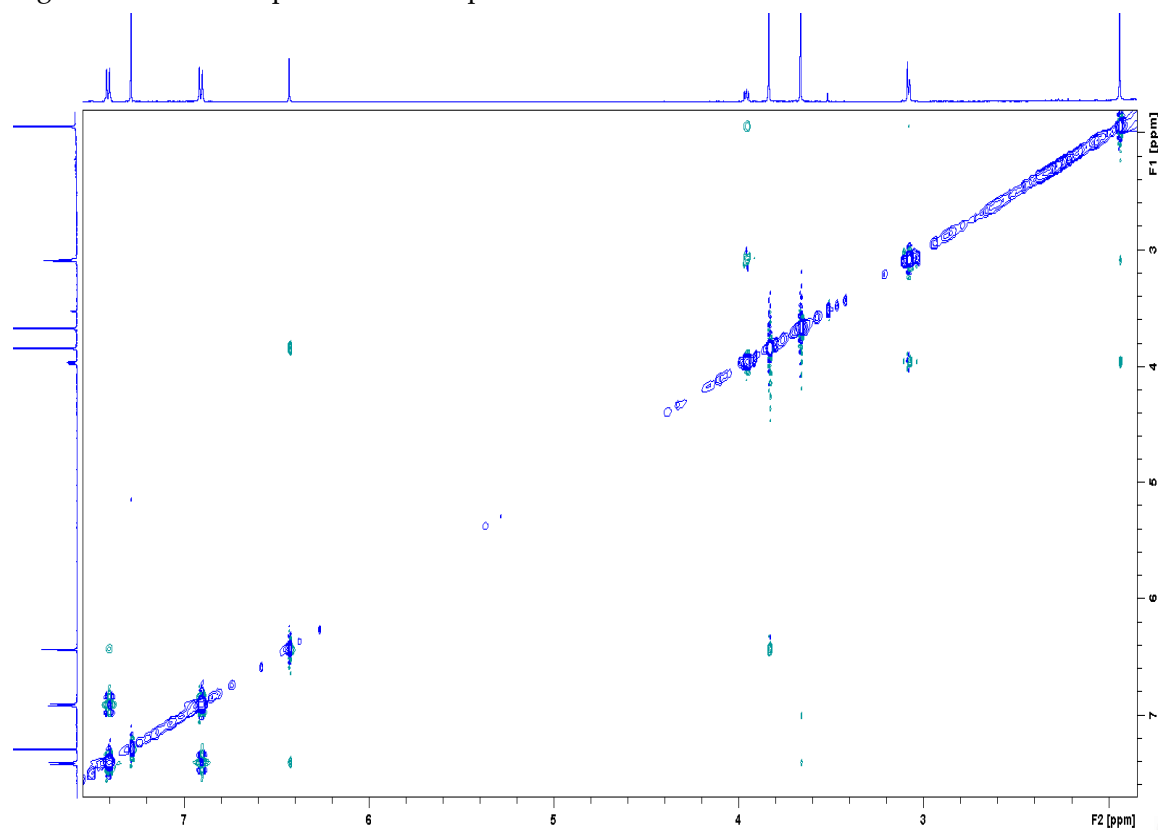
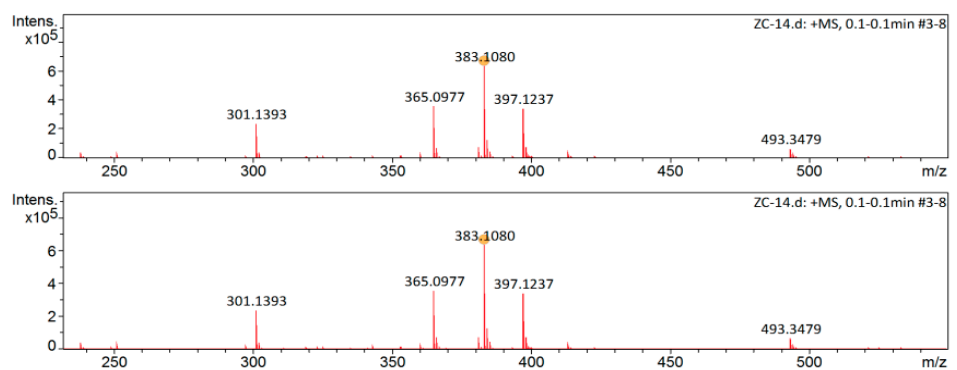
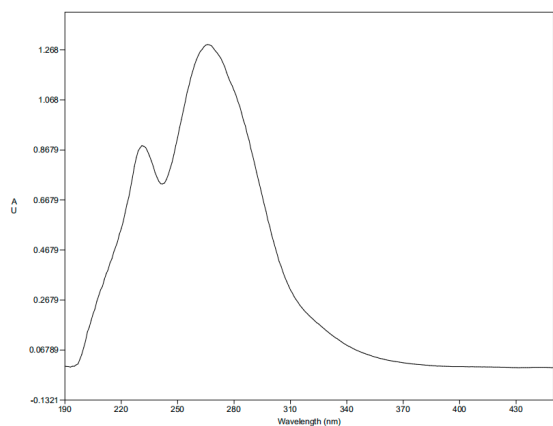


Figure S48. The HRESIMS spectrum of compound 5.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
383.1080	1	C ₁₉ H ₂₀ NaO ⁺	383.1101	5.5	23.4	1	100.00	10.0	even	ok	M+Na

Figure S49. UV spectrum of compound 5.



Bio-Kline Software V4.80 Date : 2022/10/23 Time : 1:04:25

COMMENTS :
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MOS-500 Spectrometer
Spectrum measurement
Acq duration = 0.2 s
Femto bandwidth = 5 nm
HV = 173 V
BioKline V4.80

Figure S50. IR spectrum of compound 5.

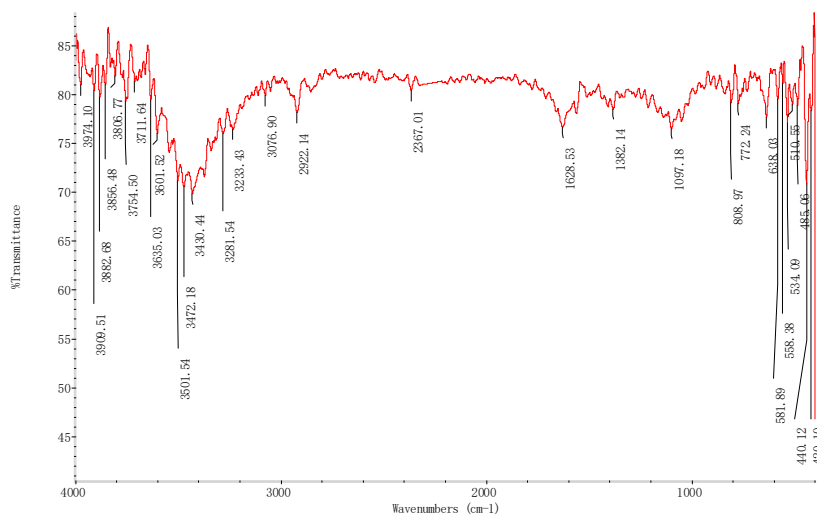


Figure S51. Predicted biosynthetic pathway for compound 5.

