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Electronic Supplementary Information (ESI)

New prenylxanthones, polyketide hemiterpenoid pigments from the endophytic fungus *Emericella* sp. XL029 and their anti-agricultural pathogenic fungal and antibacterial activities

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List of ESI

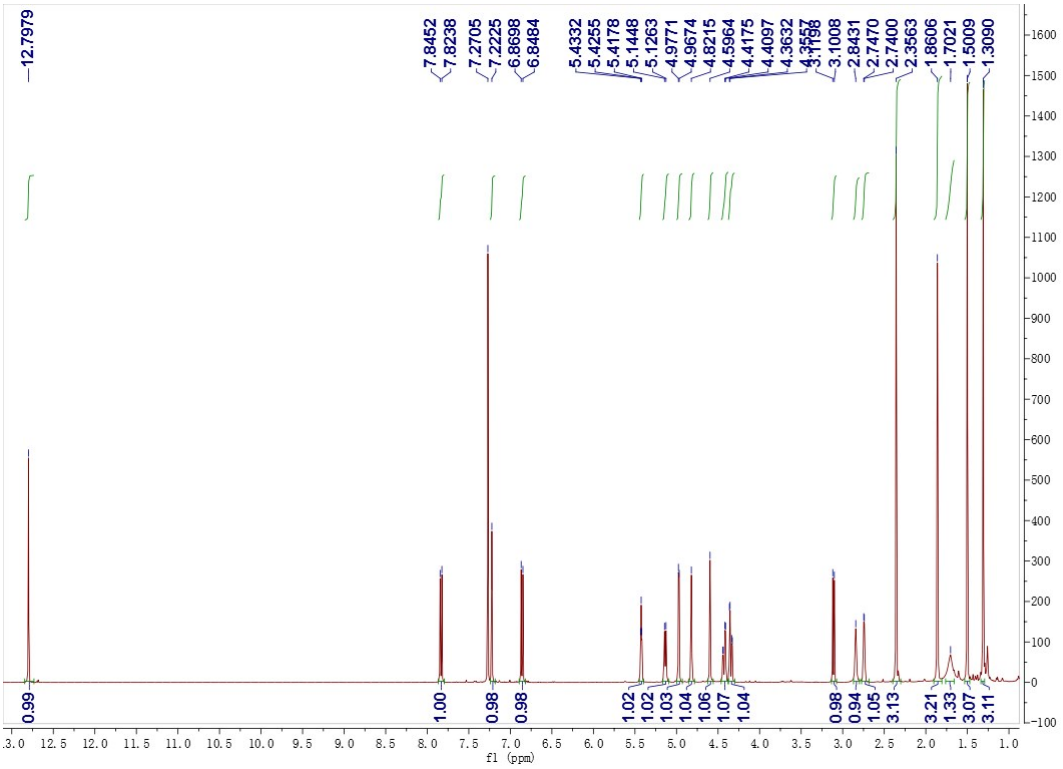


Figure S1. ^{1}H NMR spectrum of **1** ($CDCl_3$, 400 MHz)

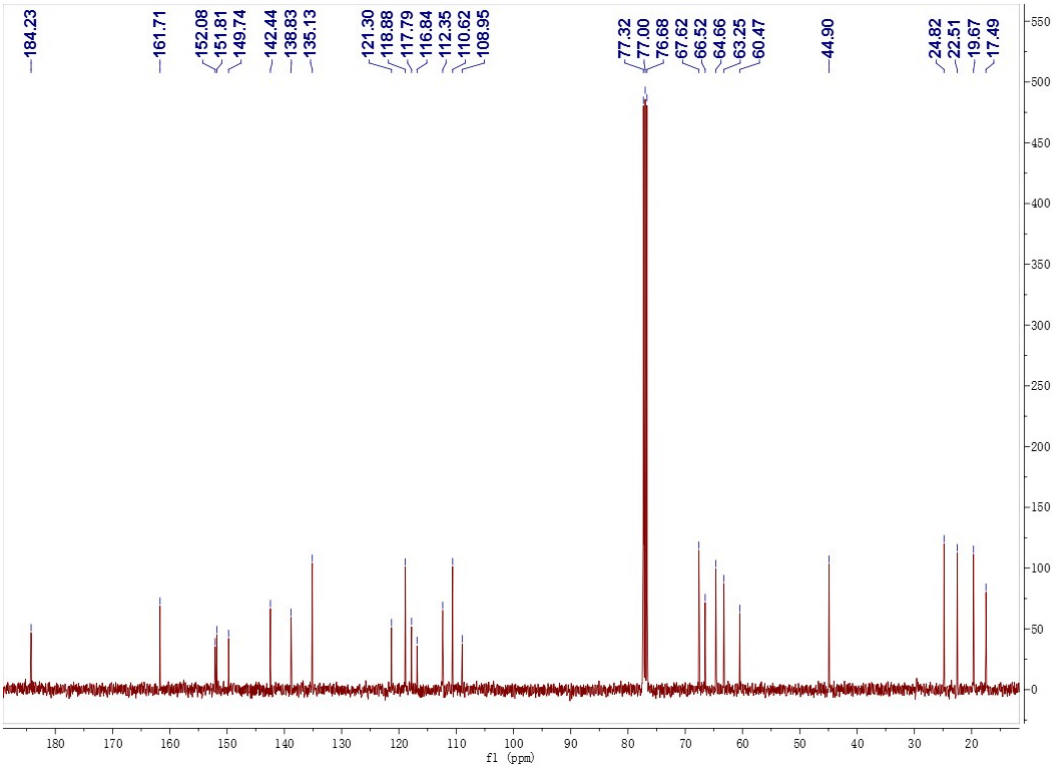


Figure S2. ^{13}C NMR spectrum of **1** ($CDCl_3$, 100 MHz)

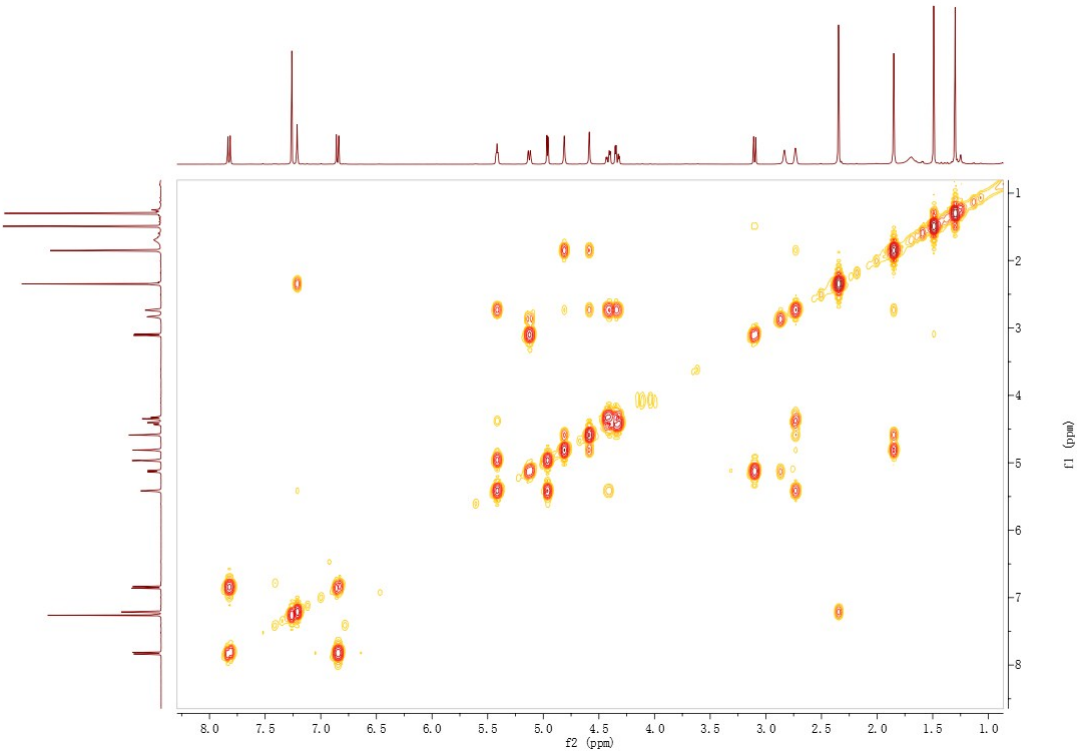


Figure S3. ^{1}H, ^{1}H COSY spectrum of **1** ($CDCl_3$)

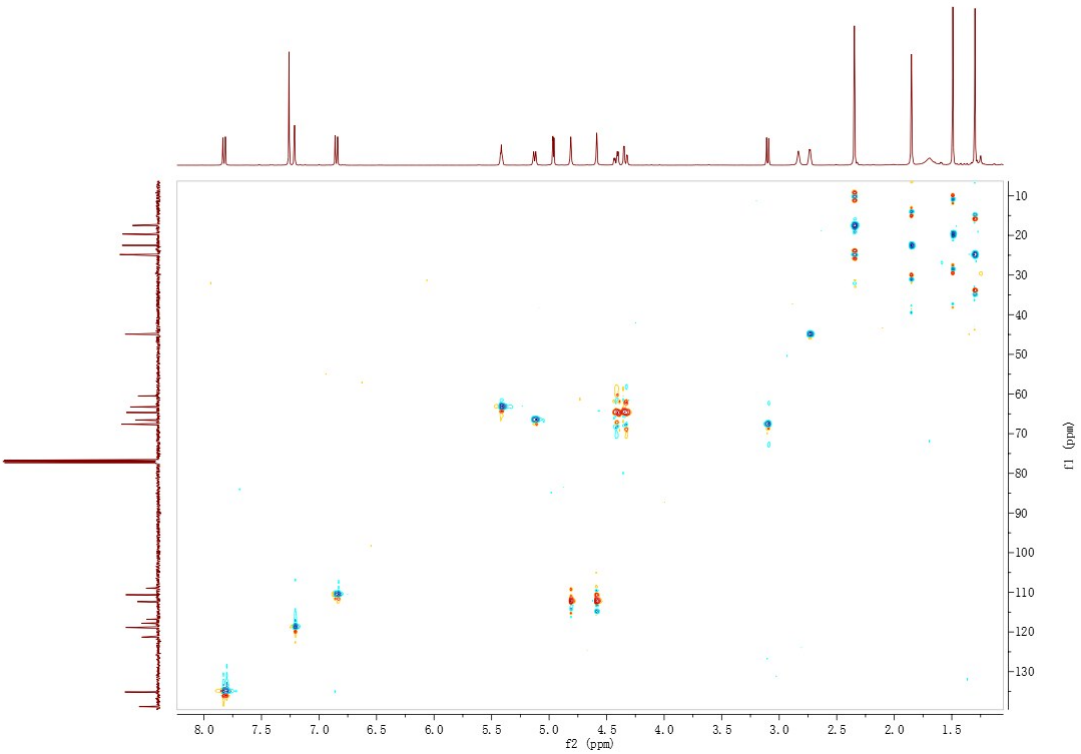


Figure S4. HMQC spectrum of **1** ($CDCl_3$)

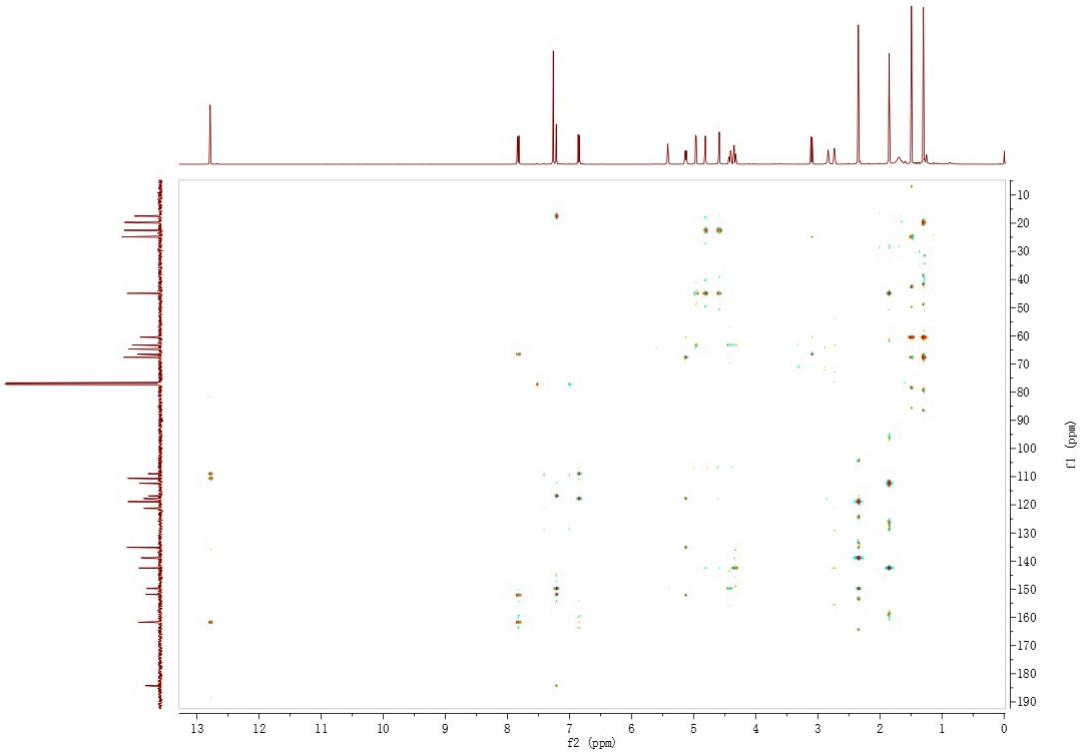


Figure S5. HMBC spectrum of **1** ($CDCl_3$)

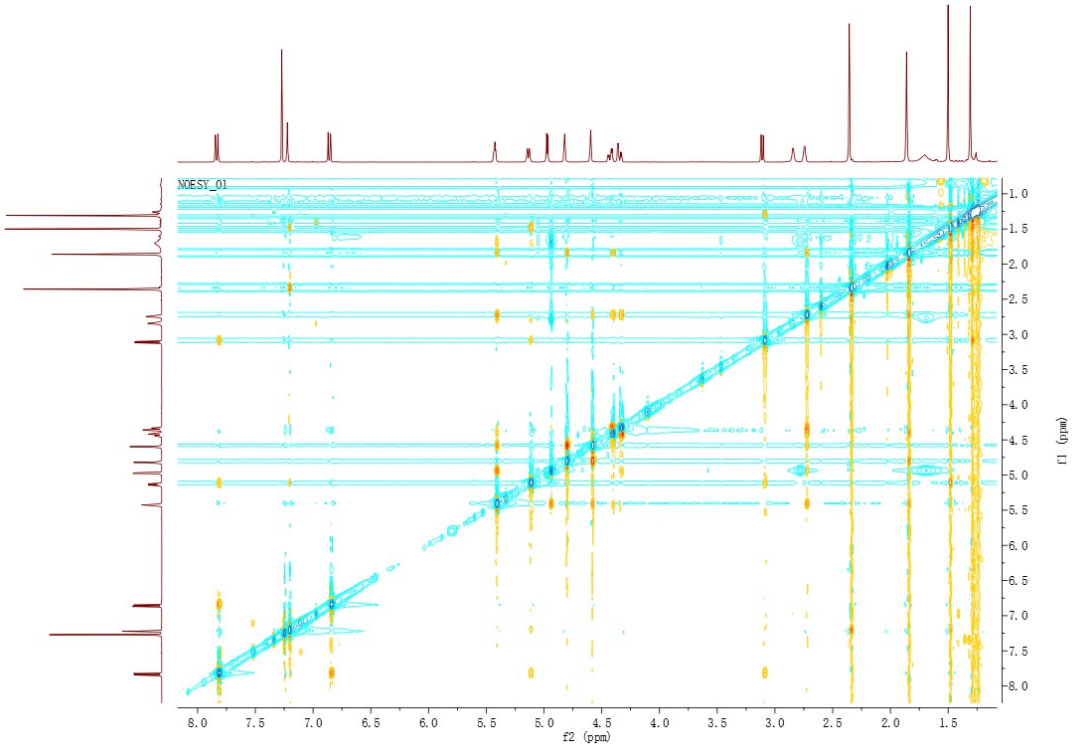


Figure S6. NOESY spectrum of **1** ($CDCl_3$)

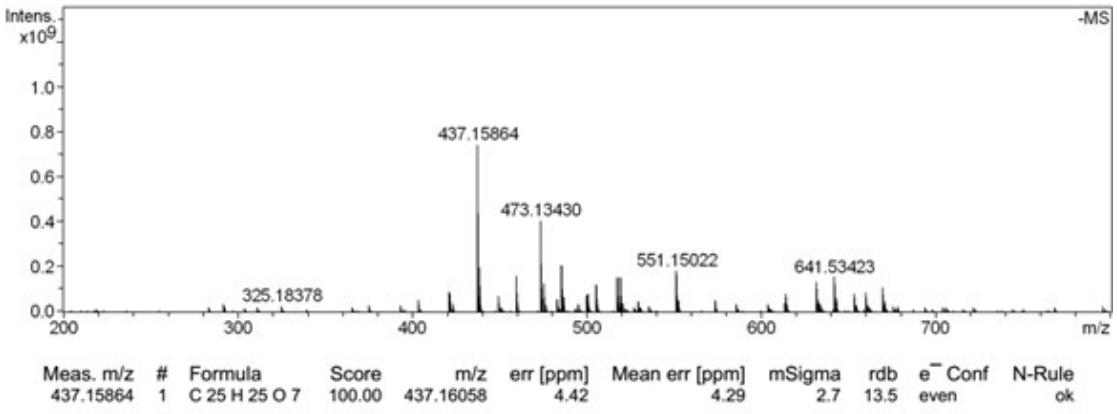


Figure S7. HRESIMS spectrum of **1**

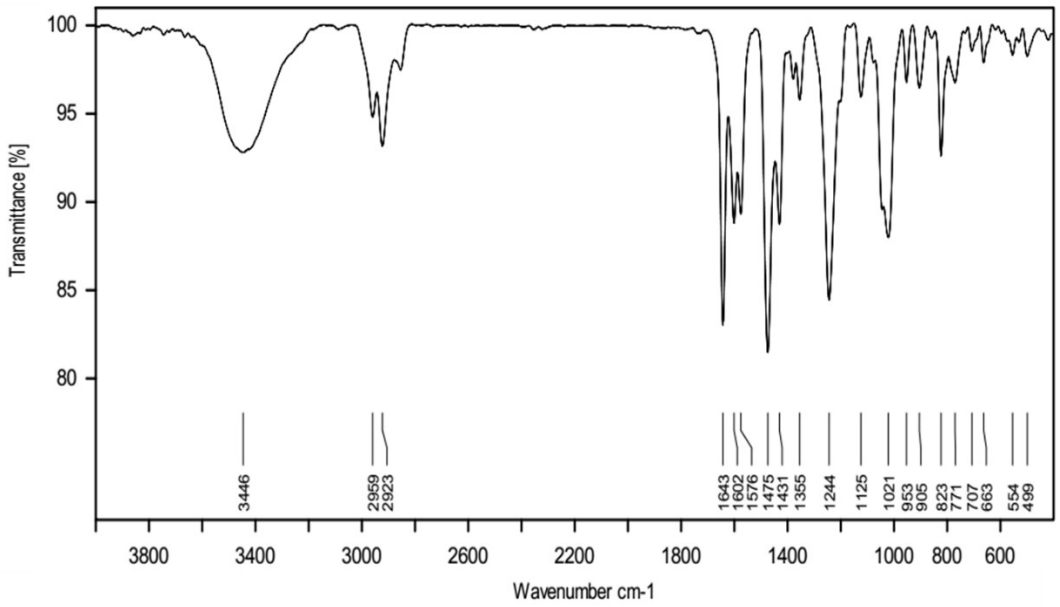


Figure S8. IR spectrum of **1**

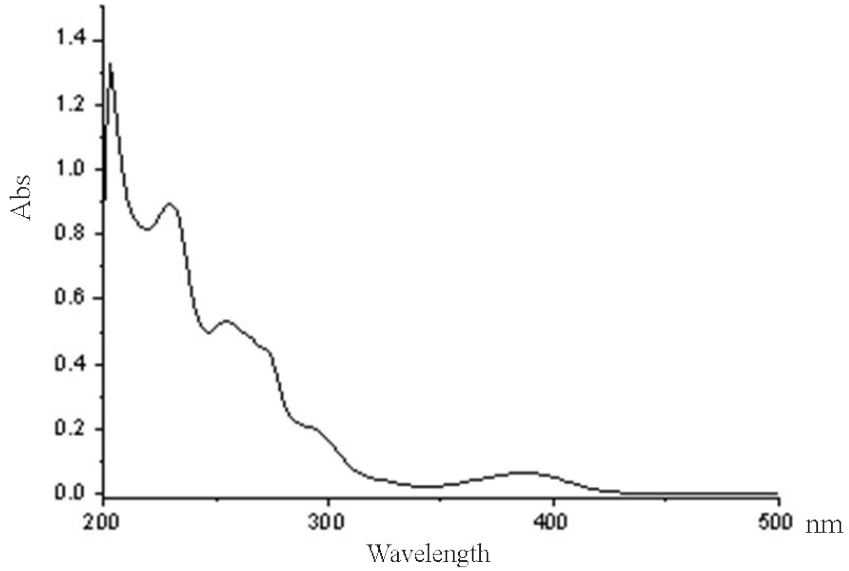


Figure S9. UV spectrum of **1**

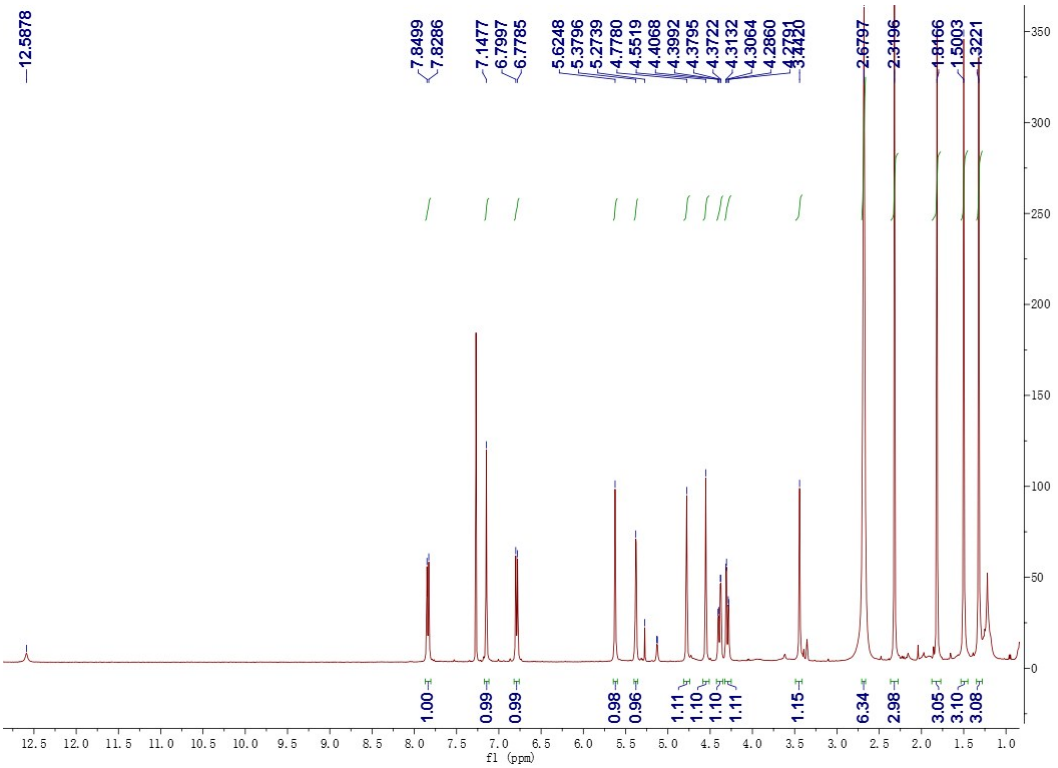


Figure S10. ^{1}H NMR spectrum of **2** ($CDCl_3$, 400 MHz)

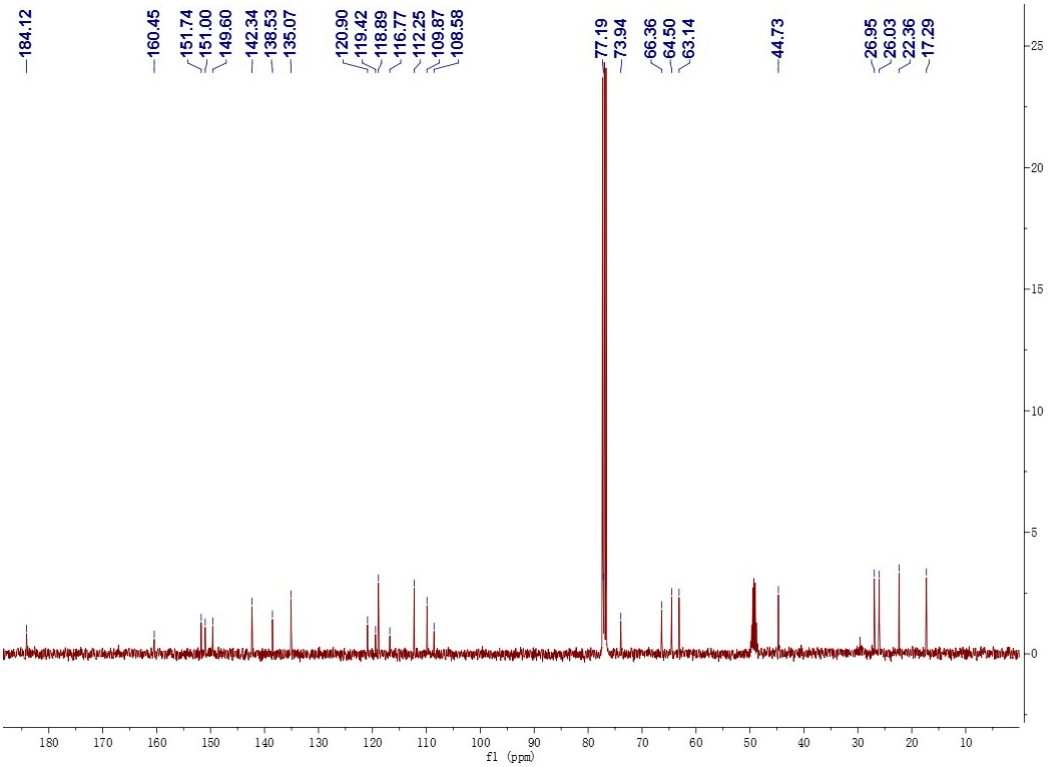


Figure S11. ^{13}C NMR spectrum of **2** ($CDCl_3$, 100 MHz)

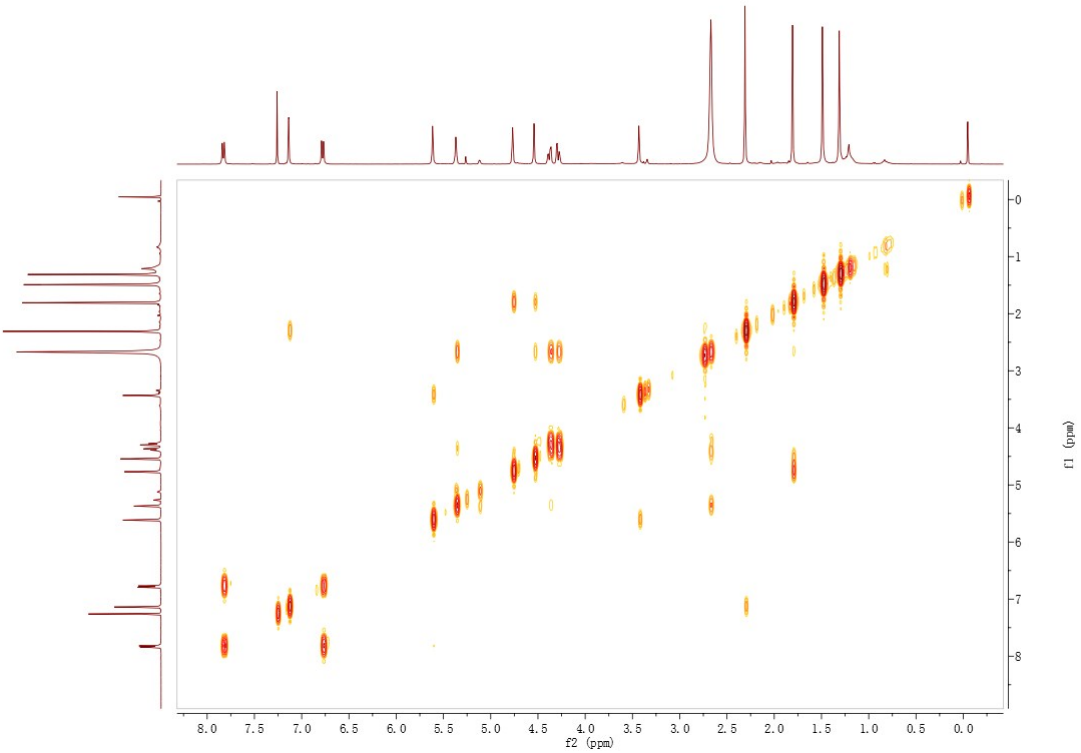


Figure S12. ^{1}H, ^{1}H COSY spectrum of **2** ($CDCl_3$)

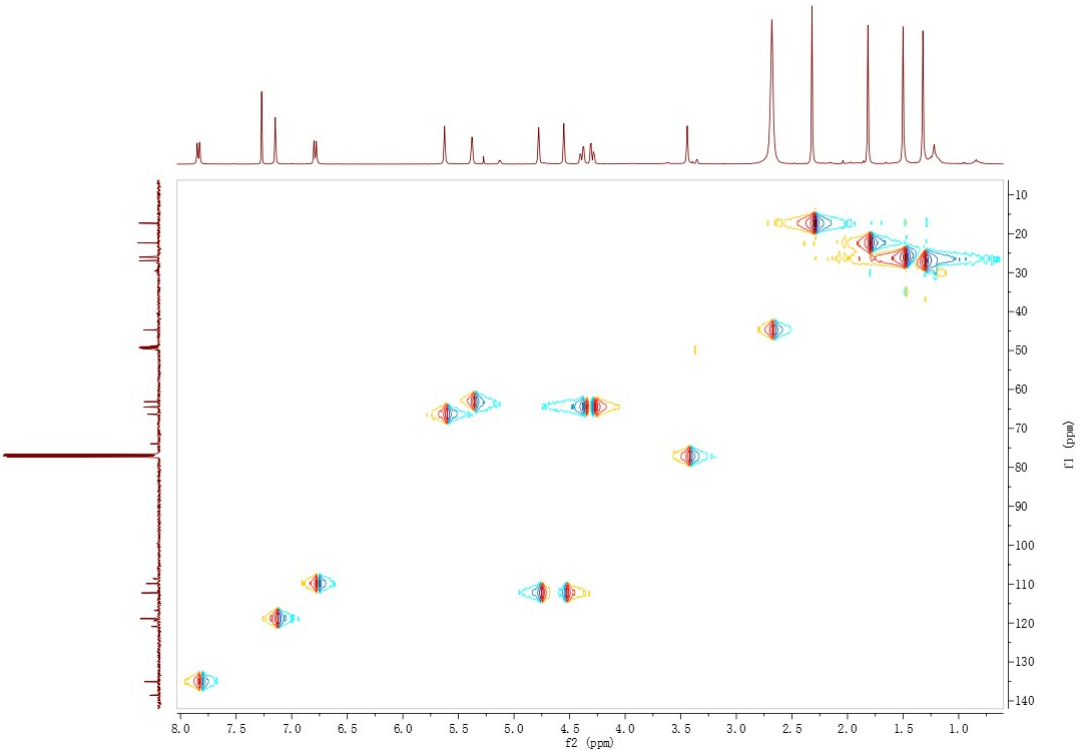


Figure S13. HMQC spectrum of **2** ($CDCl_3$)

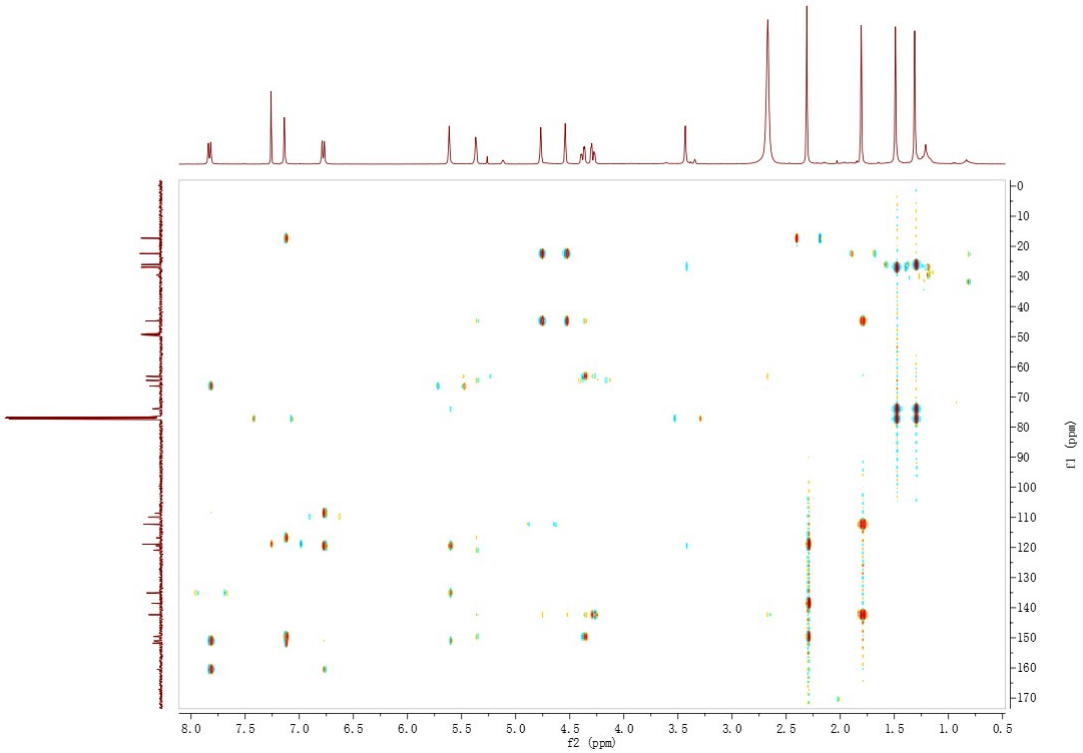


Figure S14. HMBC spectrum of **2** ($CDCl_3$)

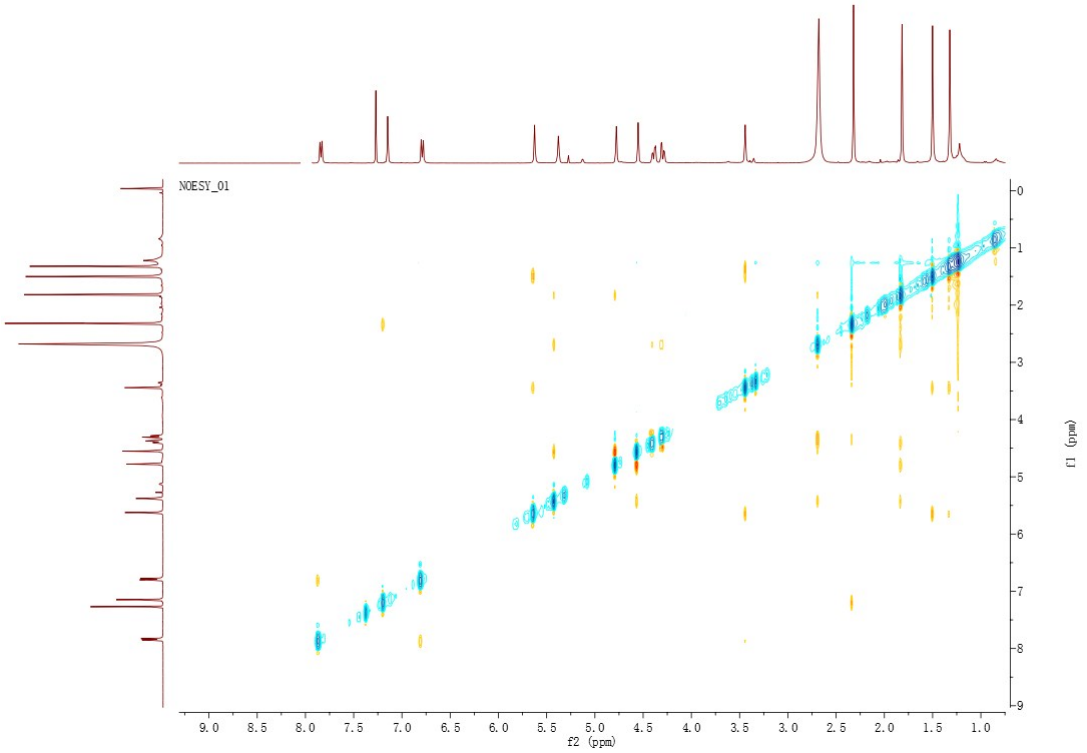
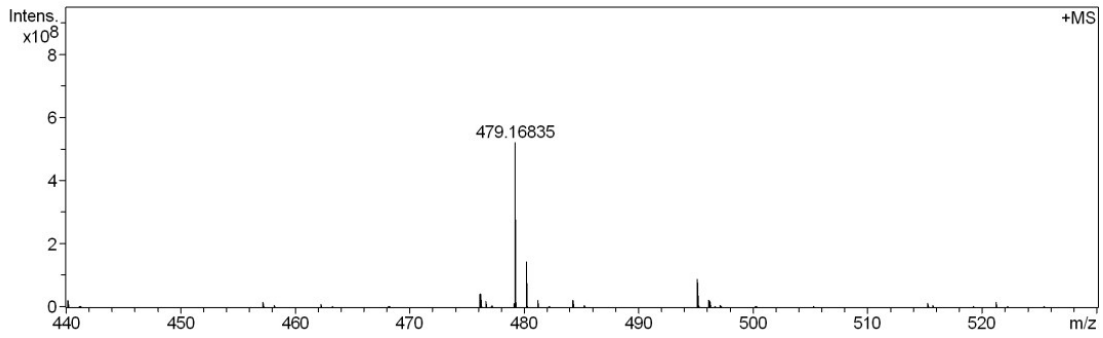


Figure S15. NOESY spectrum of **2** ($CDCl_3$)



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
479.16835	1	C 22 H 20 N 10 Na O 2	42.16	479.16629	-4.29	-4.39	5.1	17.5	even	ok
	2	C 23 H 23 N 6 O 6	86.13	479.16736	-2.06	-2.13	5.1	15.5	even	ok
	3	C 25 H 28 Na O 8	100.00	479.16764	-1.48	-1.52	5.2	11.5	even	ok

Figure S16. HRESIMS spectrum of **2**

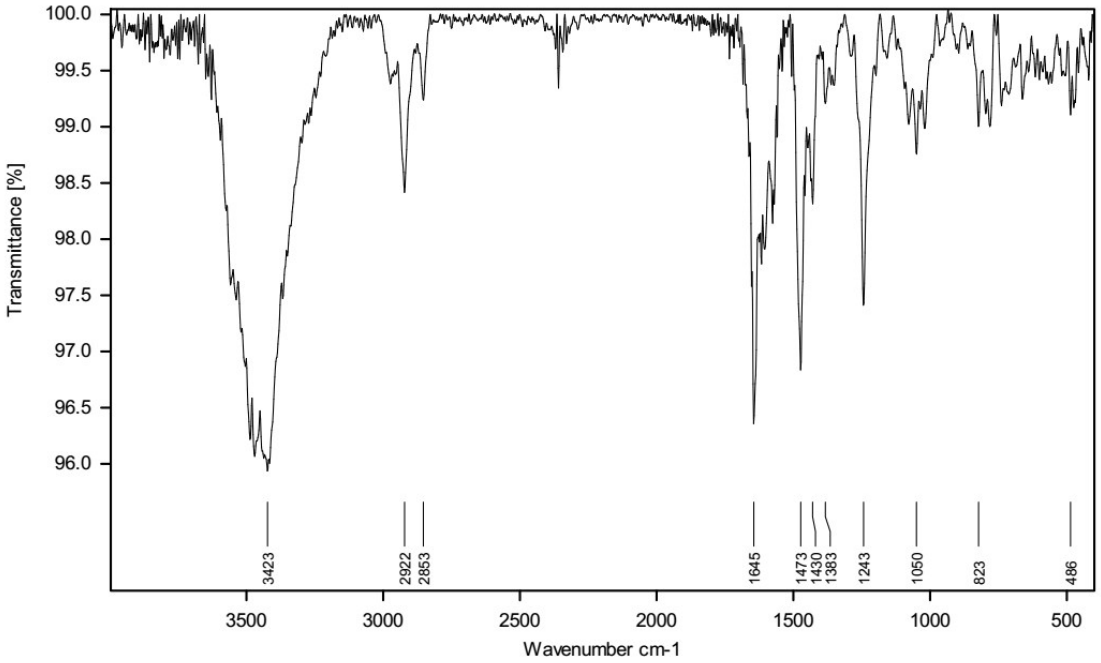


Figure S17. IR spectrum of **2**

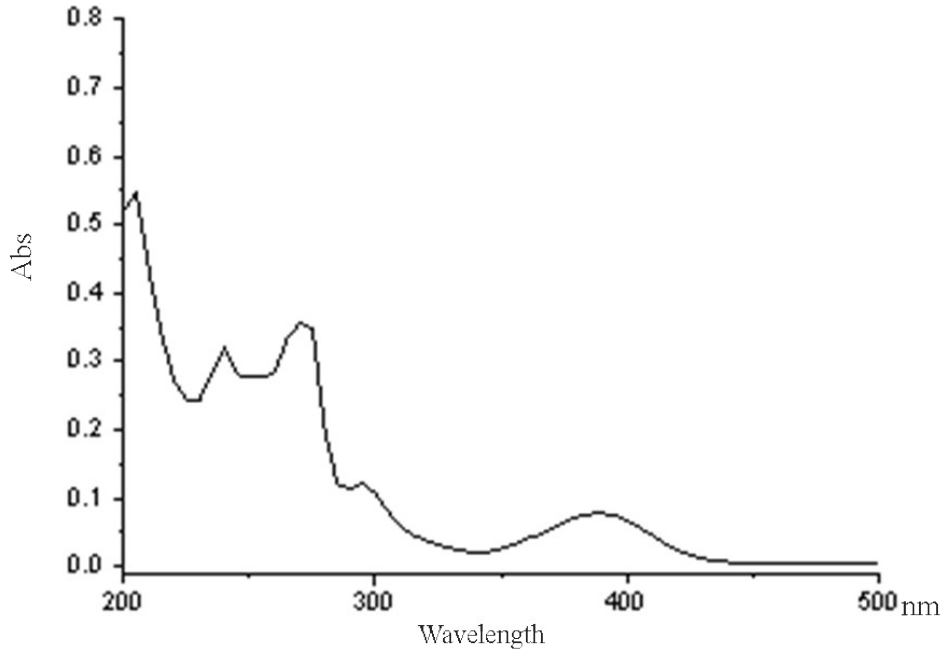


Figure S18. UV spectrum of **2**

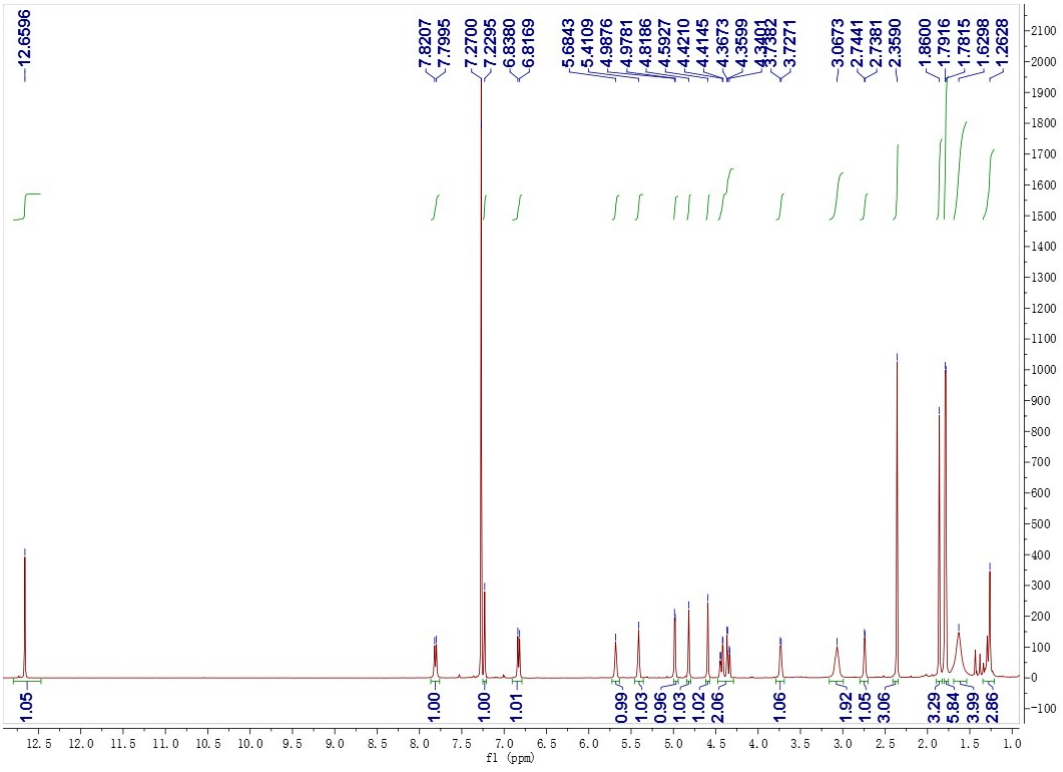


Figure S19. ^{1}H NMR spectrum of **3** ($CDCl_3$, 400 MHz)

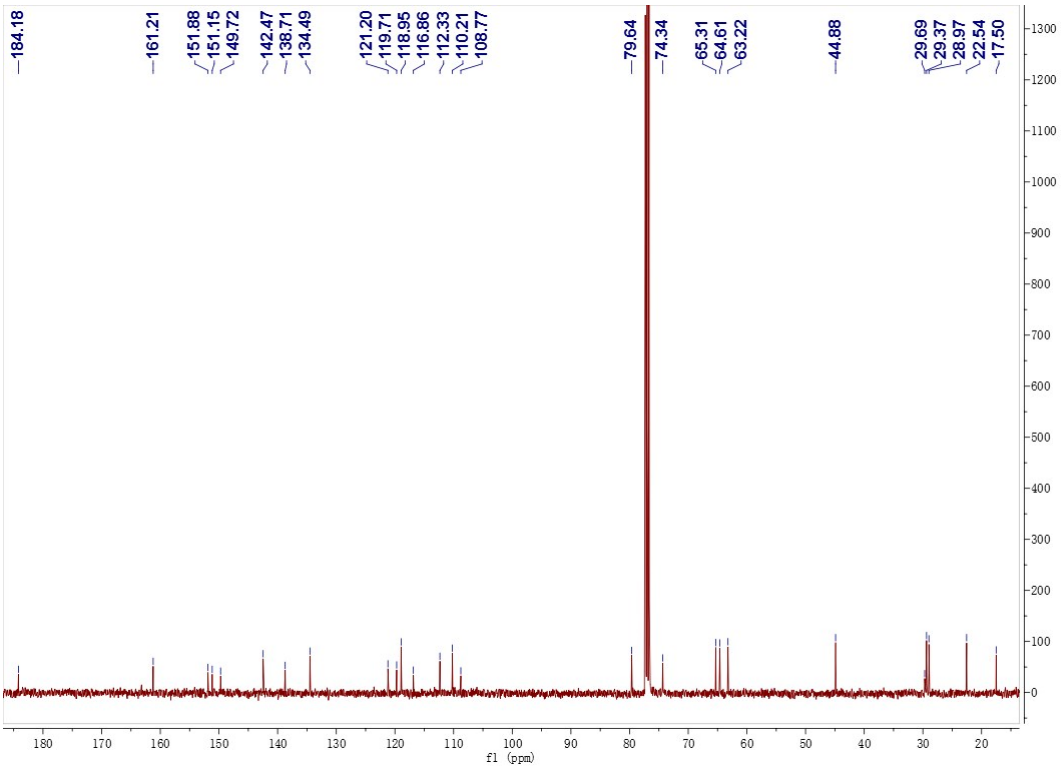


Figure S20. ^{13}C NMR spectrum of **3** ($CDCl_3$, 100 MHz)

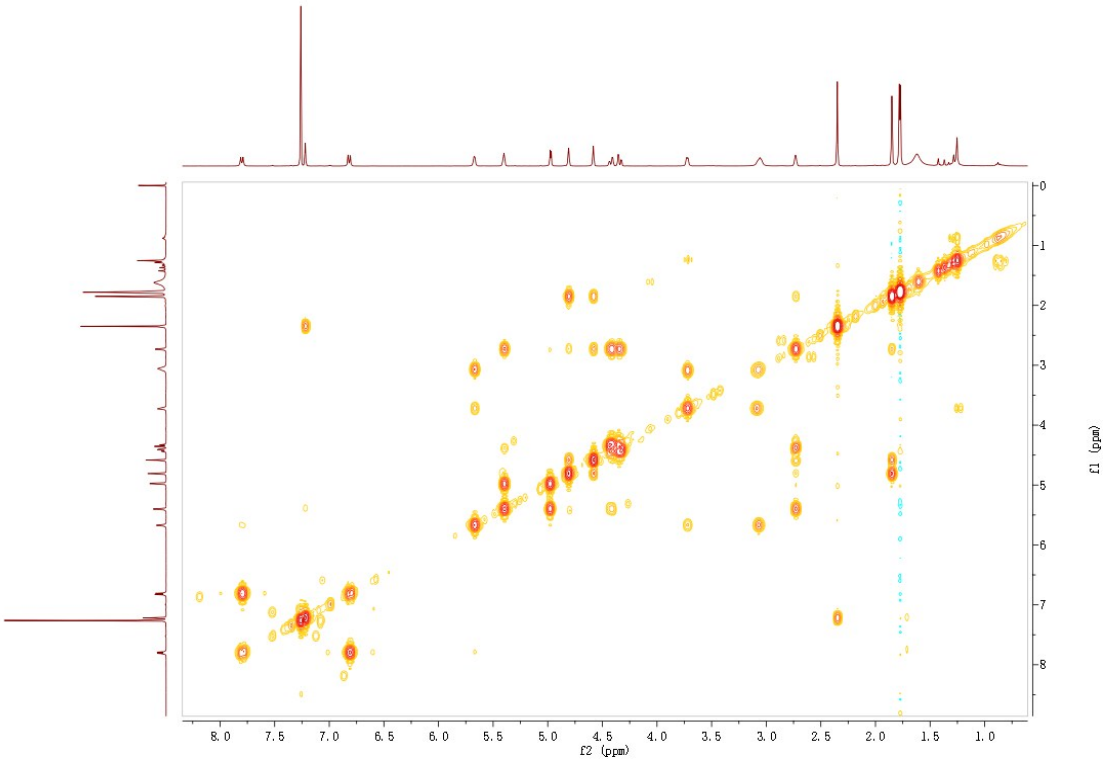


Figure S21. ^{1}H, ^{1}H COSY spectrum of **3** ($CDCl_3$)

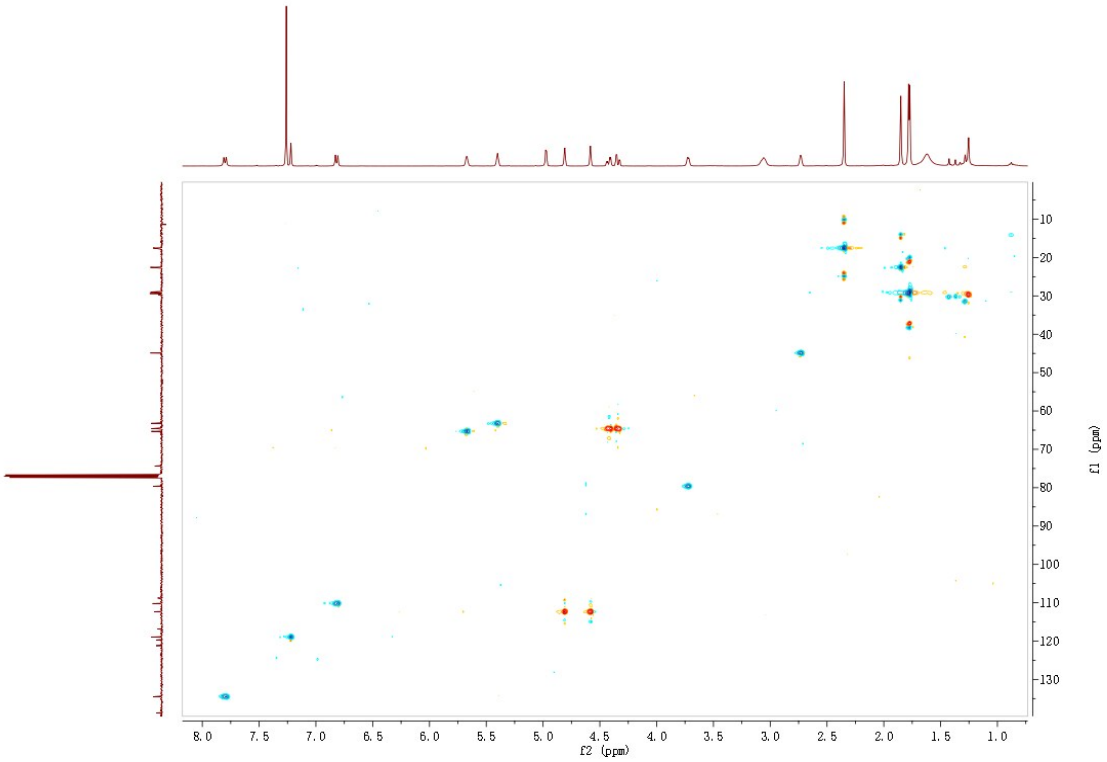


Figure S22. HMQC spectrum of **3** ($CDCl_3$)

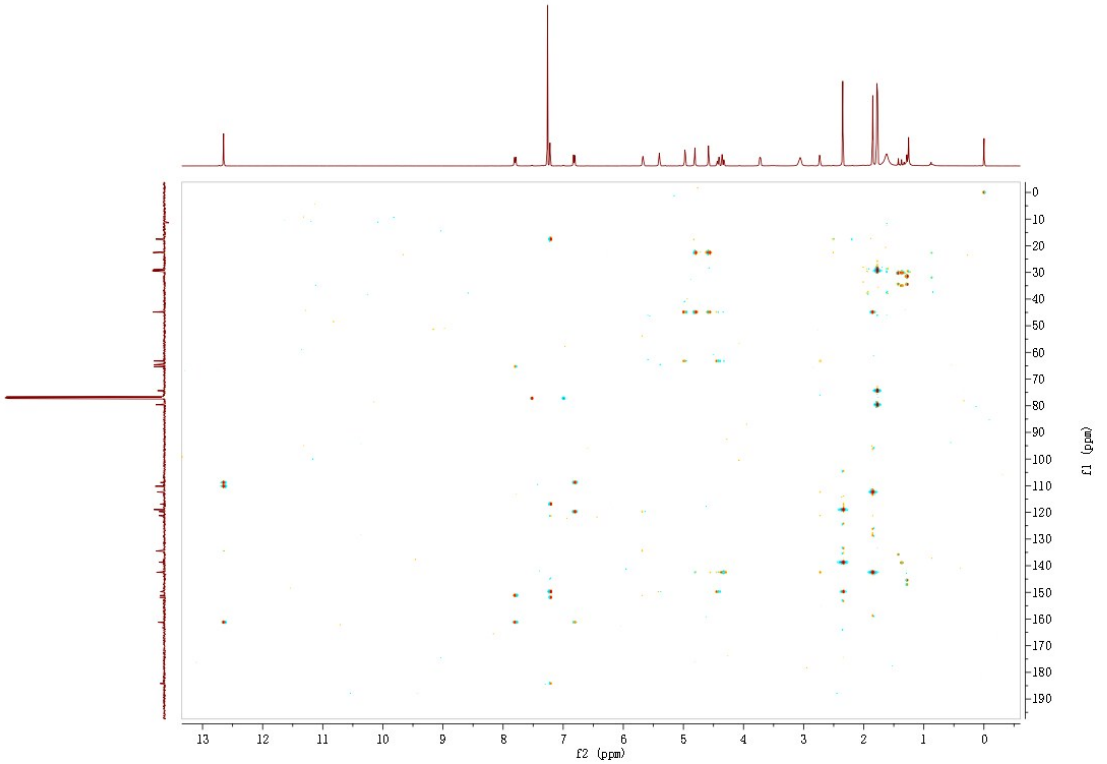


Figure S23. HMBC spectrum of **3** ($CDCl_3$)

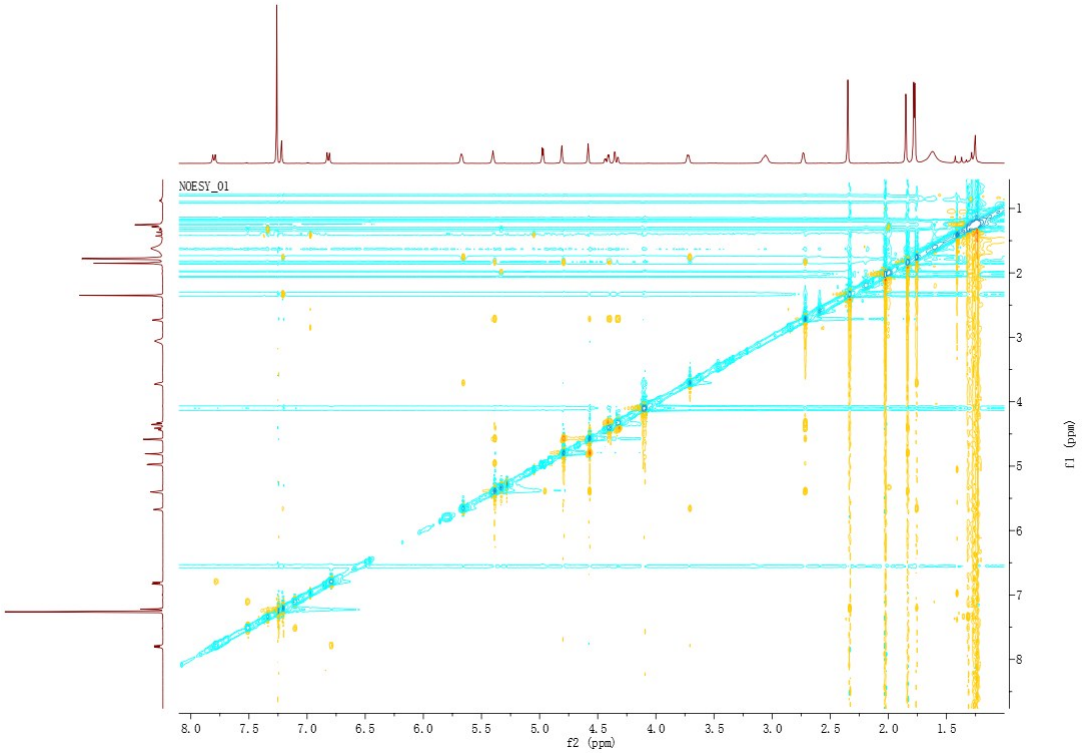
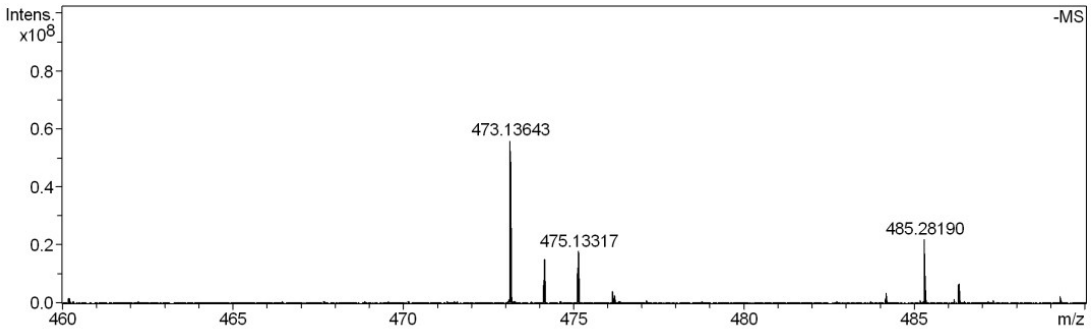


Figure S24. NOESY spectrum of **3** ($CDCl_3$)



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
473.13643	1	C 25 H 26 Cl O 7	100.00	473.13725	1.74	1.98	24.2	12.5	even	ok

Figure S25. HRESIMS spectrum of **3**

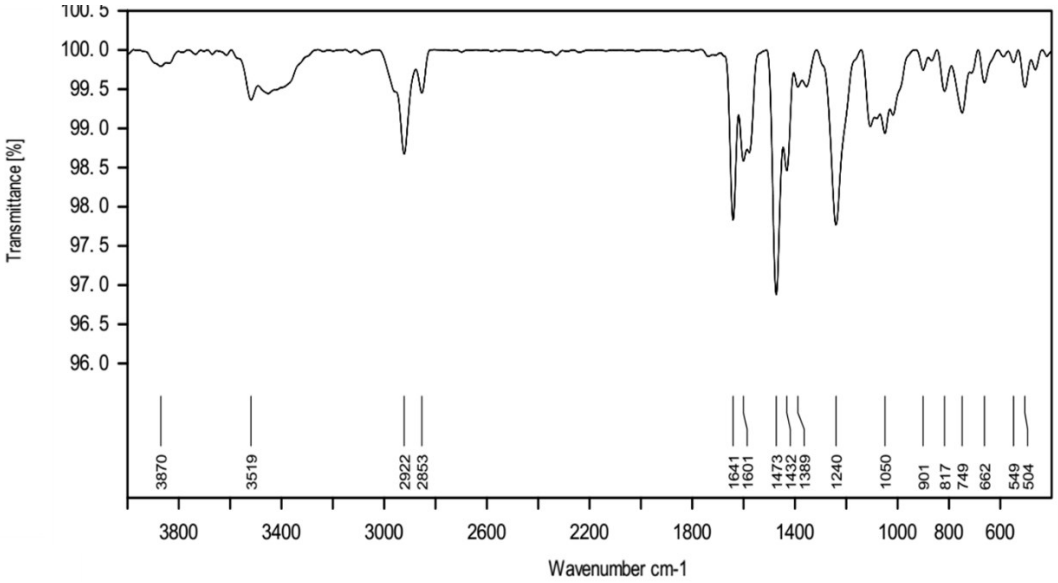


Figure S26. IR spectrum of **3**

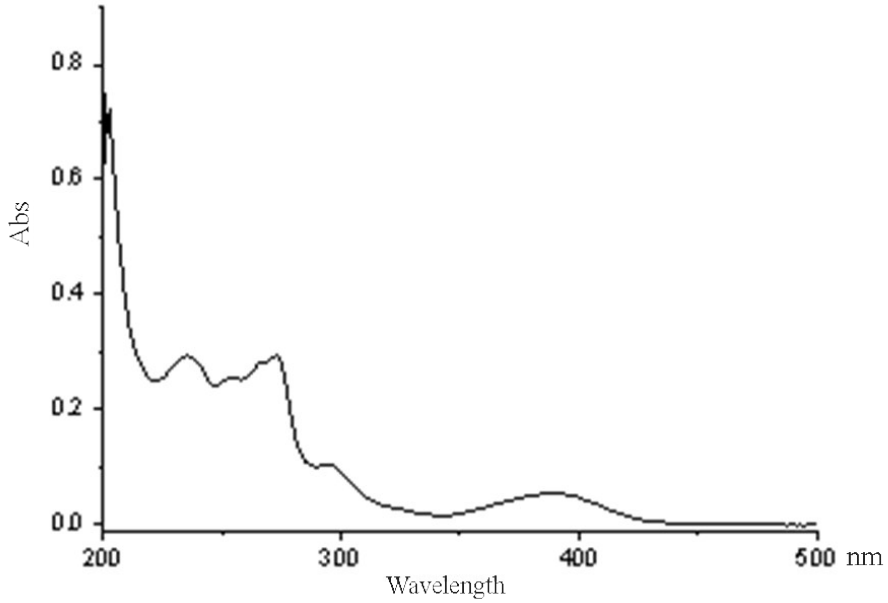


Figure S27. UV spectrum of **3**

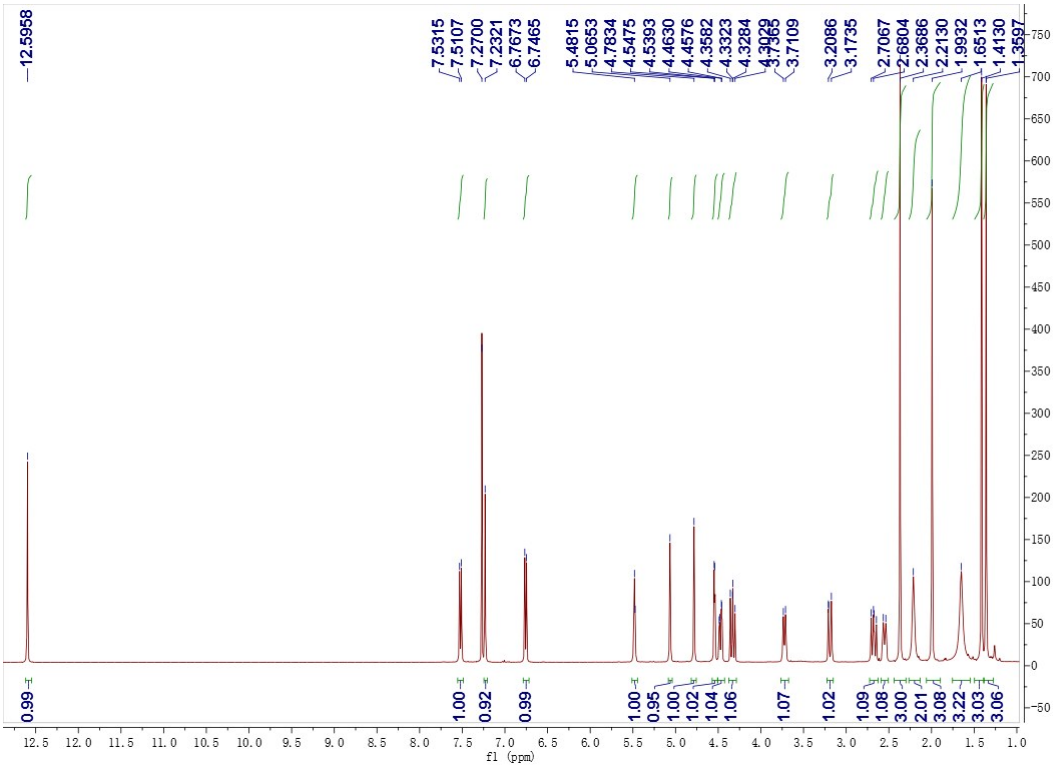


Figure S28. ^{1}H NMR spectrum of **4** ($CDCl_3$, 400 MHz)

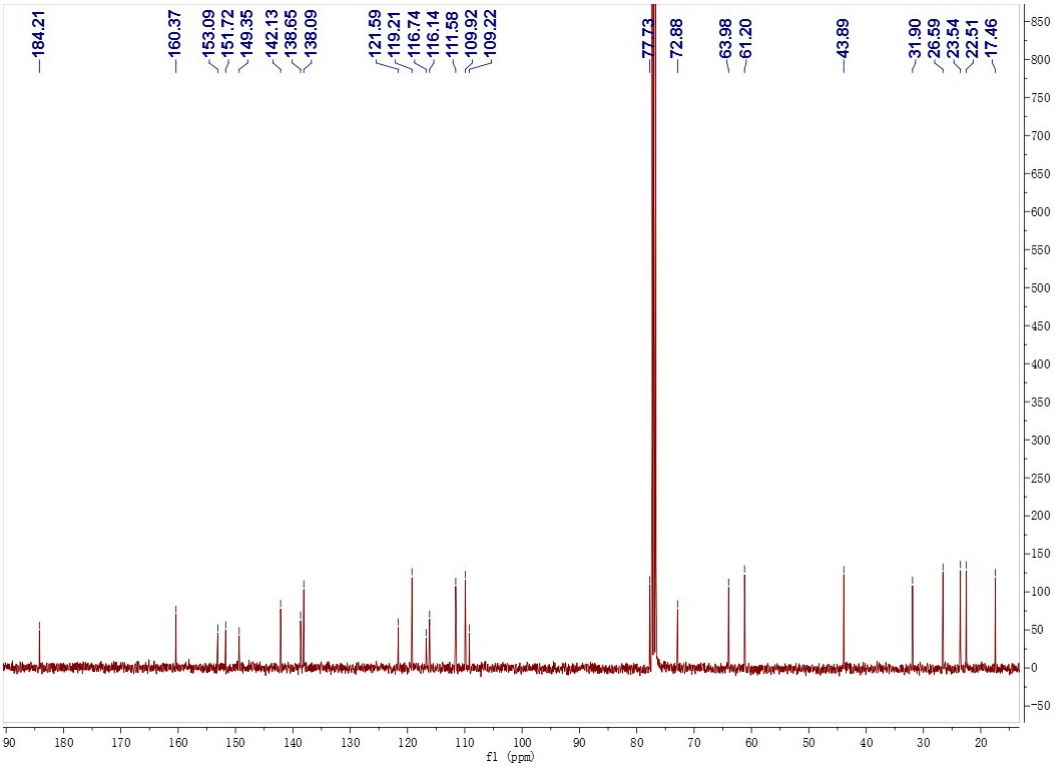


Figure S29. ^{13}C NMR spectrum of **4** ($CDCl_3$, 100 MHz)

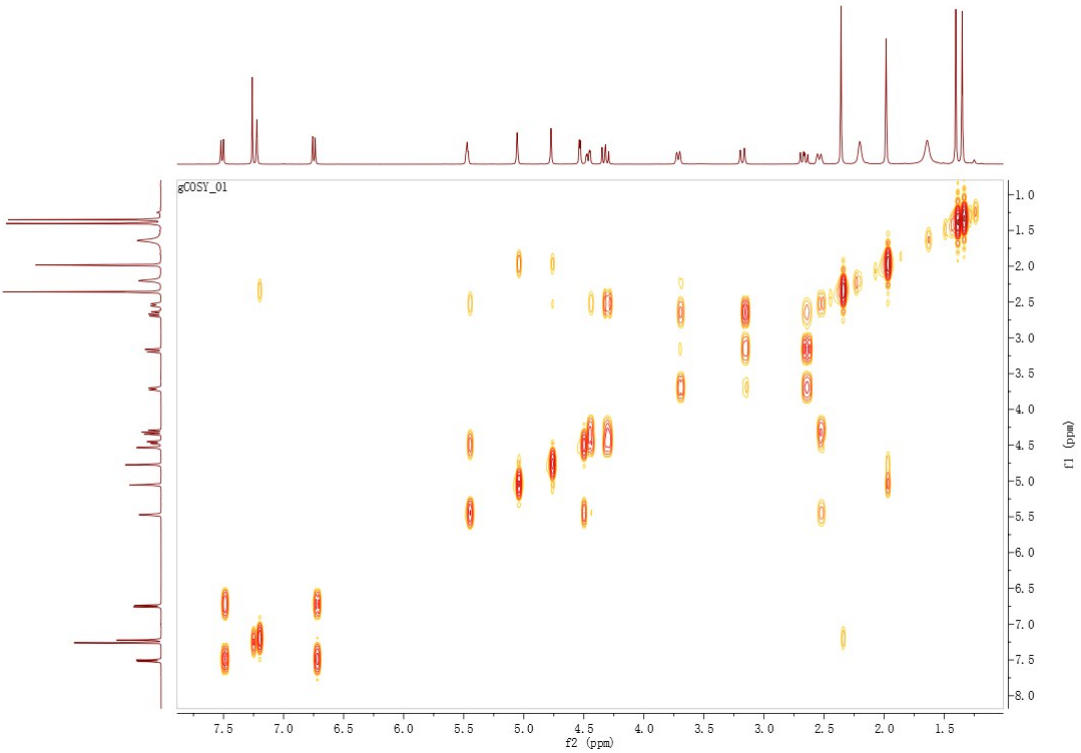


Figure S30. ^{1}H, ^{1}H COSY spectrum of **4** ($CDCl_3$)

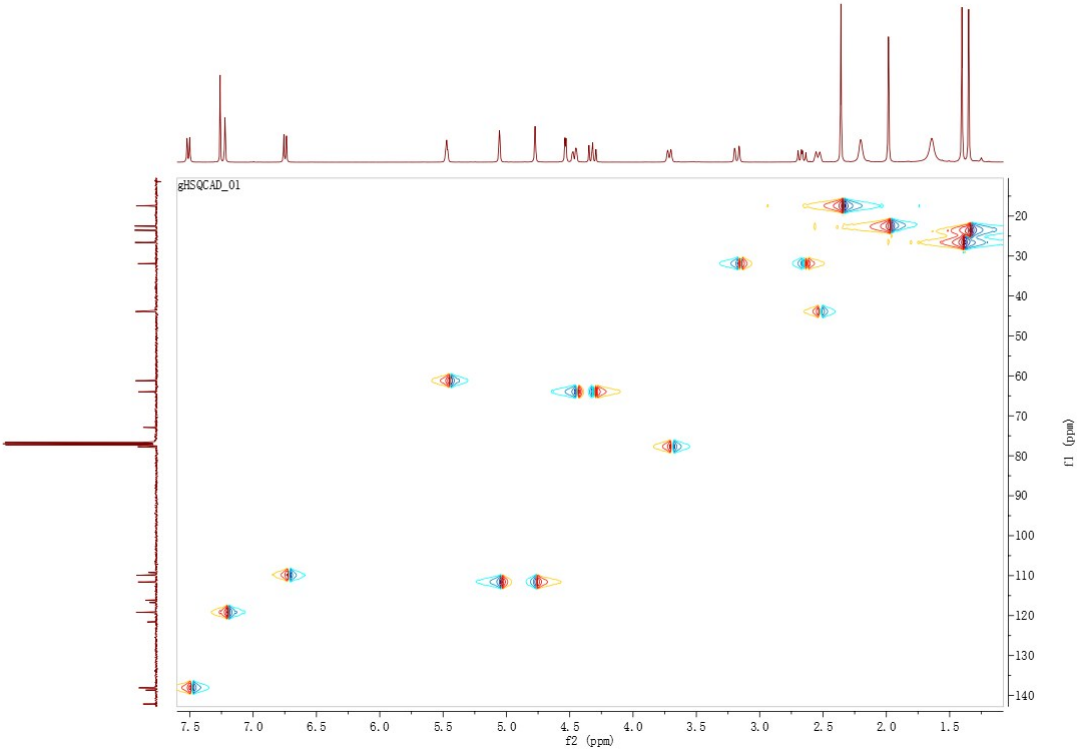


Figure S31. HMQC spectrum of **4** ($CDCl_3$)

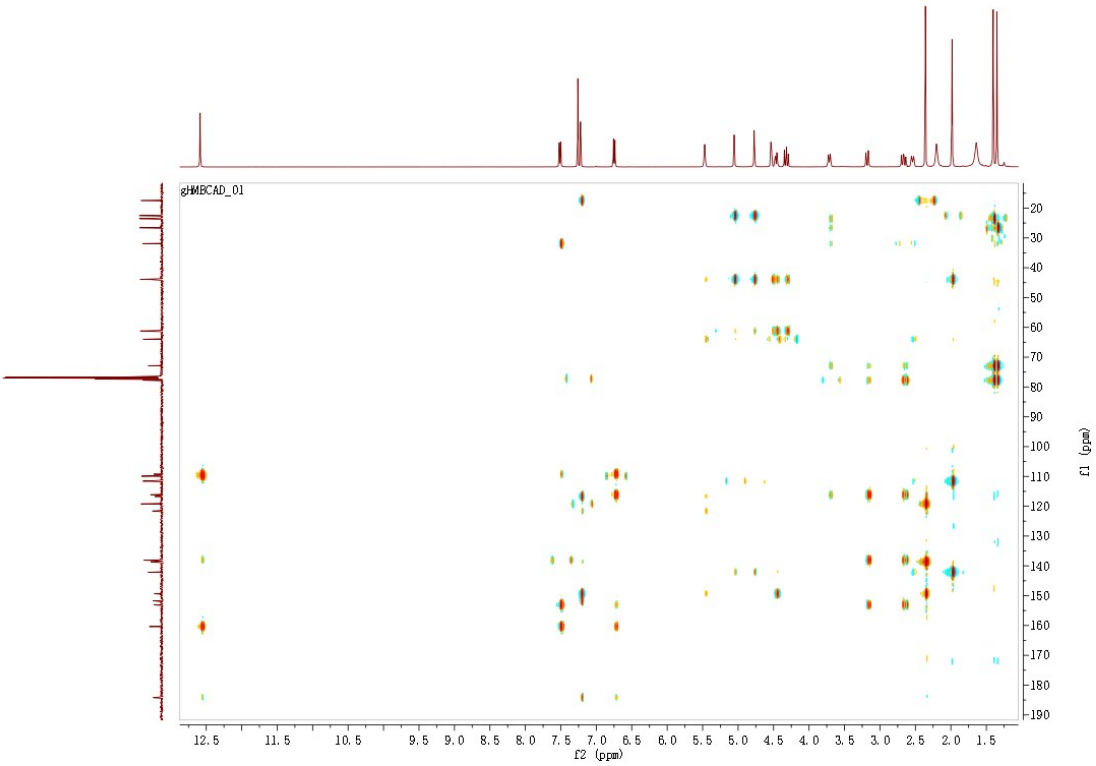


Figure S32. HMBC spectrum of **4** ($CDCl_3$)

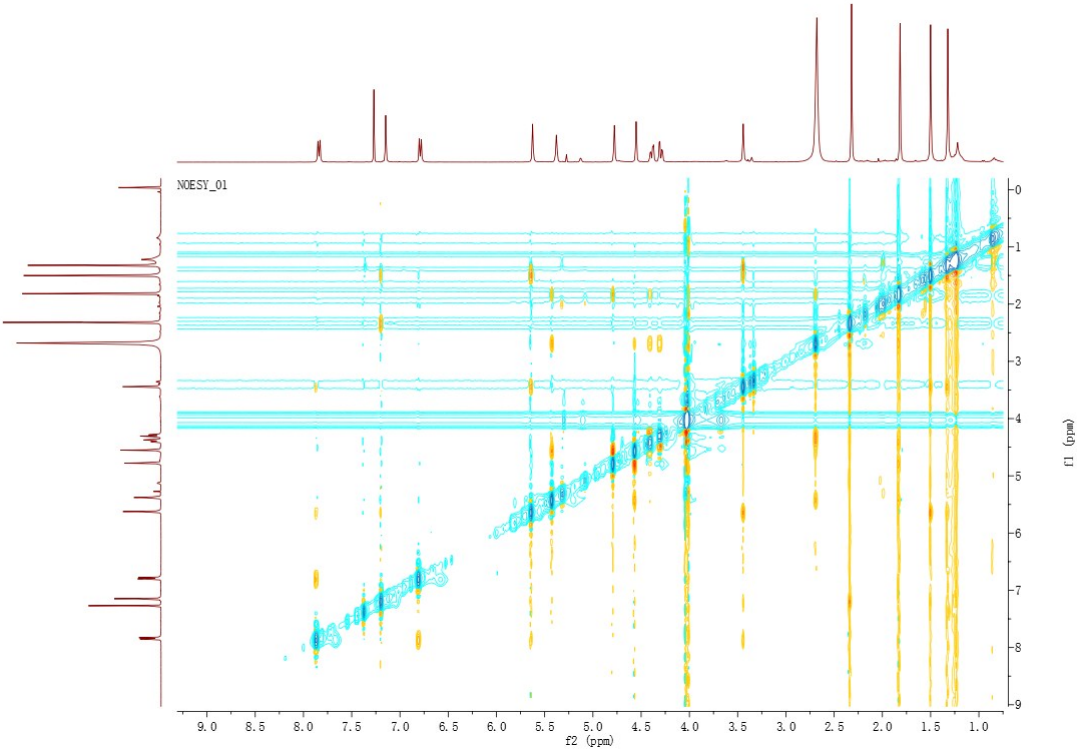
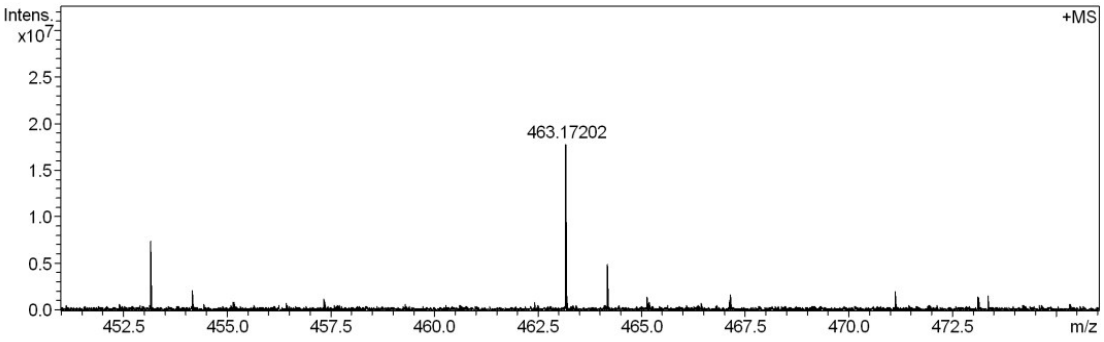


Figure S33. NOESY spectrum of **4** ($CDCl_3$)



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSig ma	rdb	e⁻ Conf	N-R ule
463.17202	1	C 25 H 28 Na O 7	100.00	463.17272	1.52	1.49	3.3	11.5	even	ok

Figure S34. HRESIMS spectrum of **4**

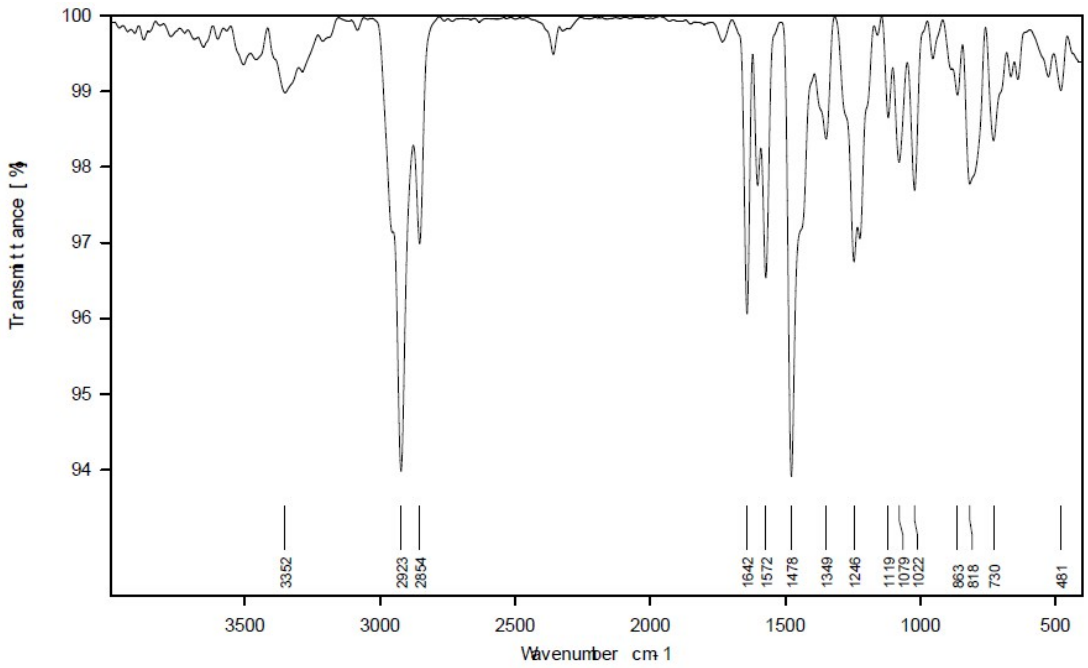


Figure S35. IR spectrum of **4**

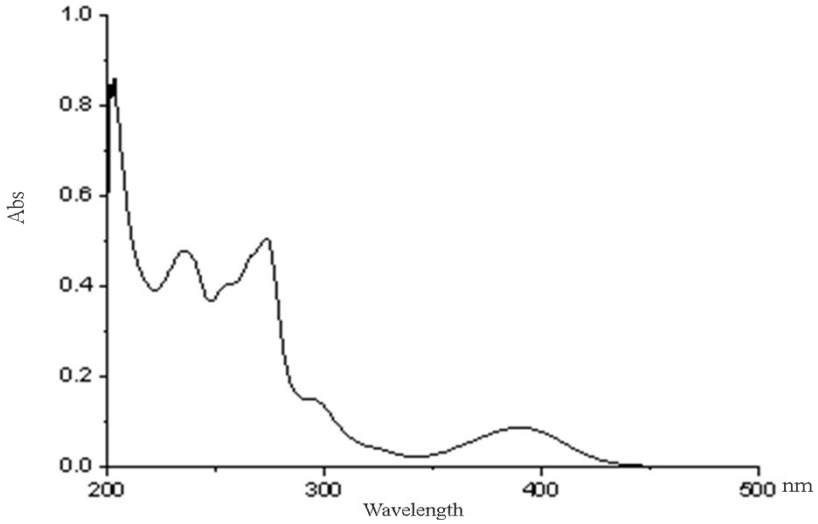


Figure S36. UV spectrum of **4**

Empirical formula	$C_{25}H_{28}O_7$
Formula weight	440.47
Temperature/K	293
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.2804(3)
b/Å	17.2710(6)
c/Å	10.3842(4)
α/°	90
β/°	101.759(4)
γ/°	90
Volume/Å^3	1102.72(8)
Z	2
ρ_{calc}g/cm^3	1.327
μ/mm^{-1}	0.097
F(000)	468.0
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	7.012 to 52.744
Index ranges	$-7 \leq h \leq 7$, $-21 \leq k \leq 21$, $-8 \leq l \leq 12$
Reflections collected	7828
Independent reflections	4482 [R_{int} =0.0246, R_{sigma} = 0.0495]
Data/restraints/parameters	4482/1/305
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1072
Final R indexes [all data]	R_1 = 0.0631, wR_2 = 0.1177
Largest diff. peak/hole / e Å^{-3}	0.15/-0.23
Flack parameter	0.5(6)

Table S1. X-ray crystallographic data of **4**

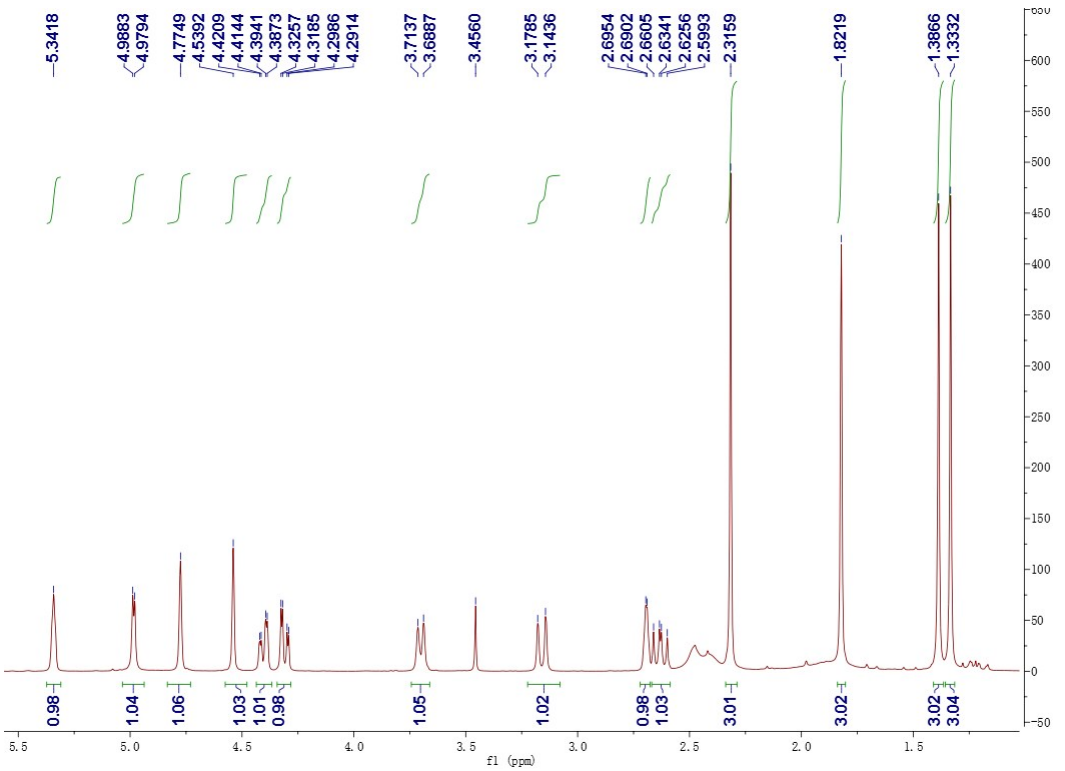


Figure S37. ^{1}H NMR spectrum of **5** ($CDCl_3$, 400 MHz)

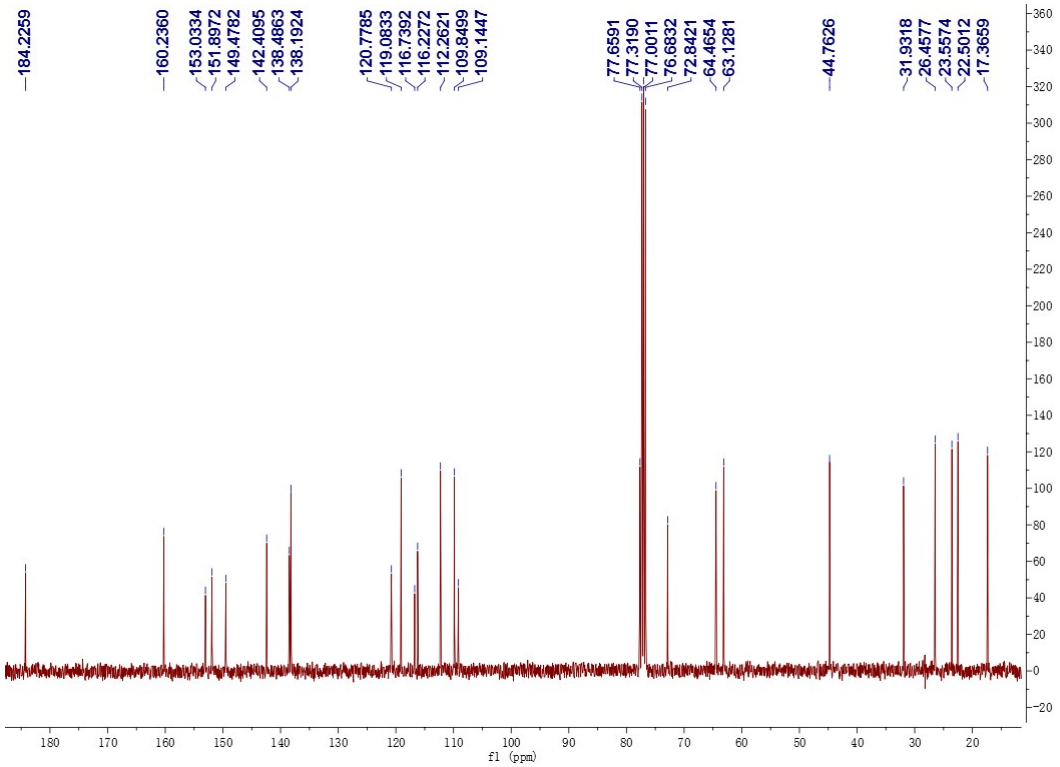


Figure S38. ^{13}C NMR spectrum of **5** ($CDCl_3$, 100 MHz)

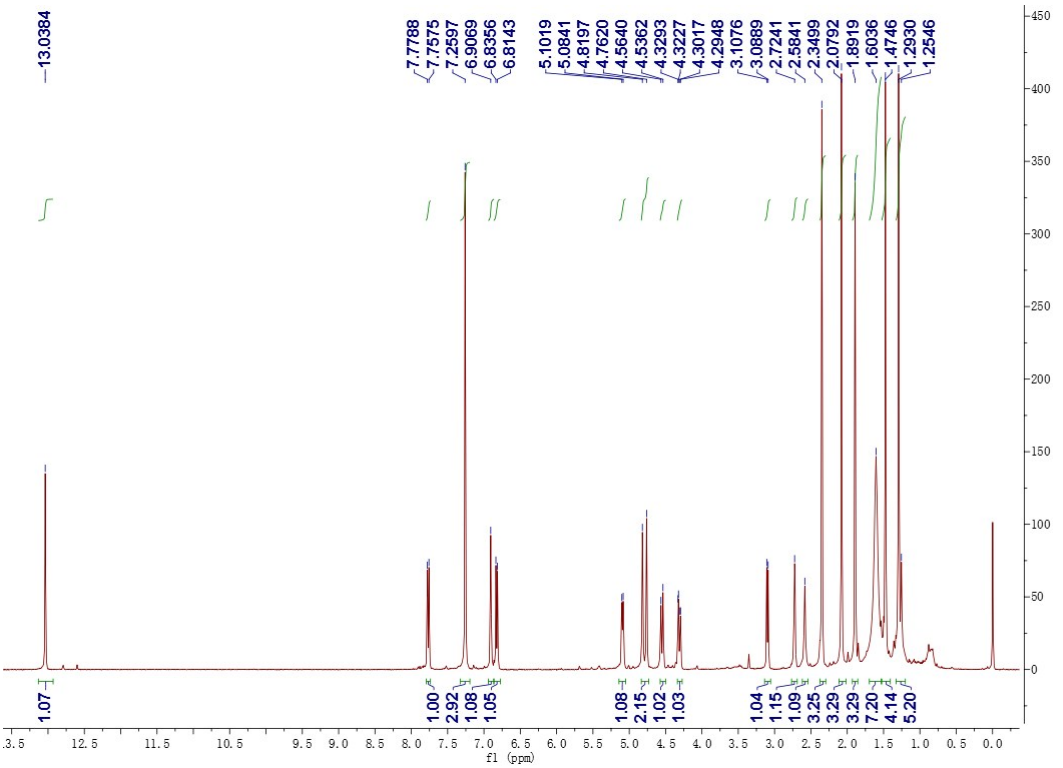


Figure S39. ^{1}H NMR spectrum of **6** ($CDCl_3$, 400 MHz)

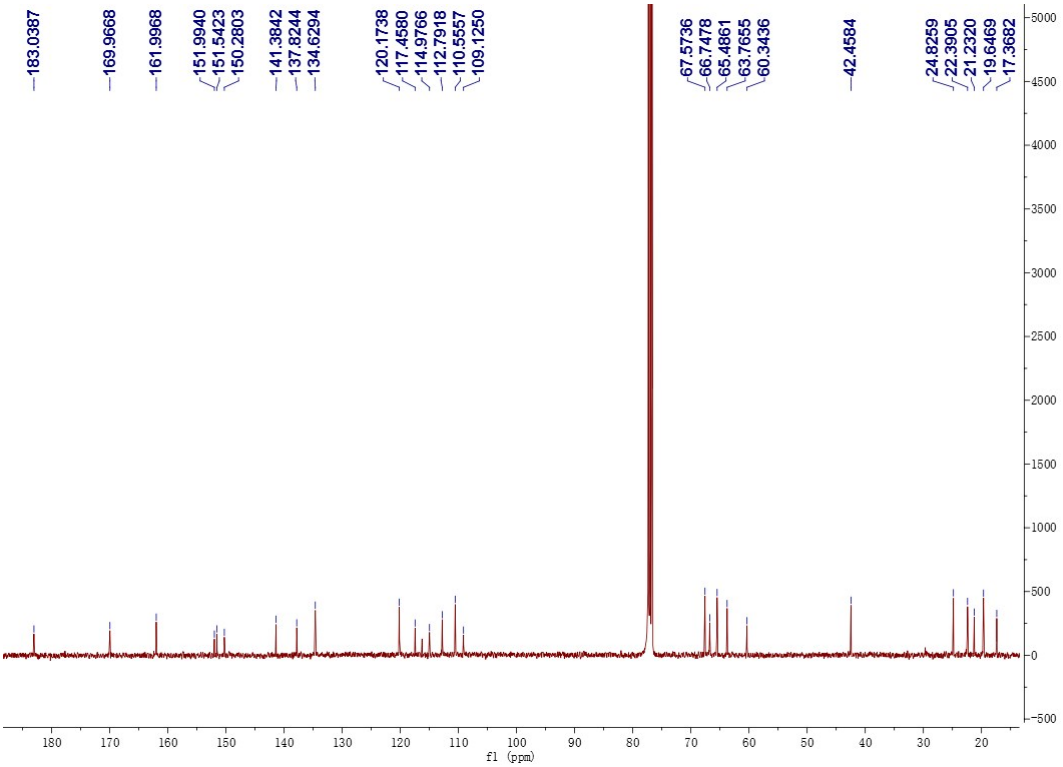


Figure S40. ^{13}C NMR spectrum of **6** ($CDCl_3$, 100 MHz)

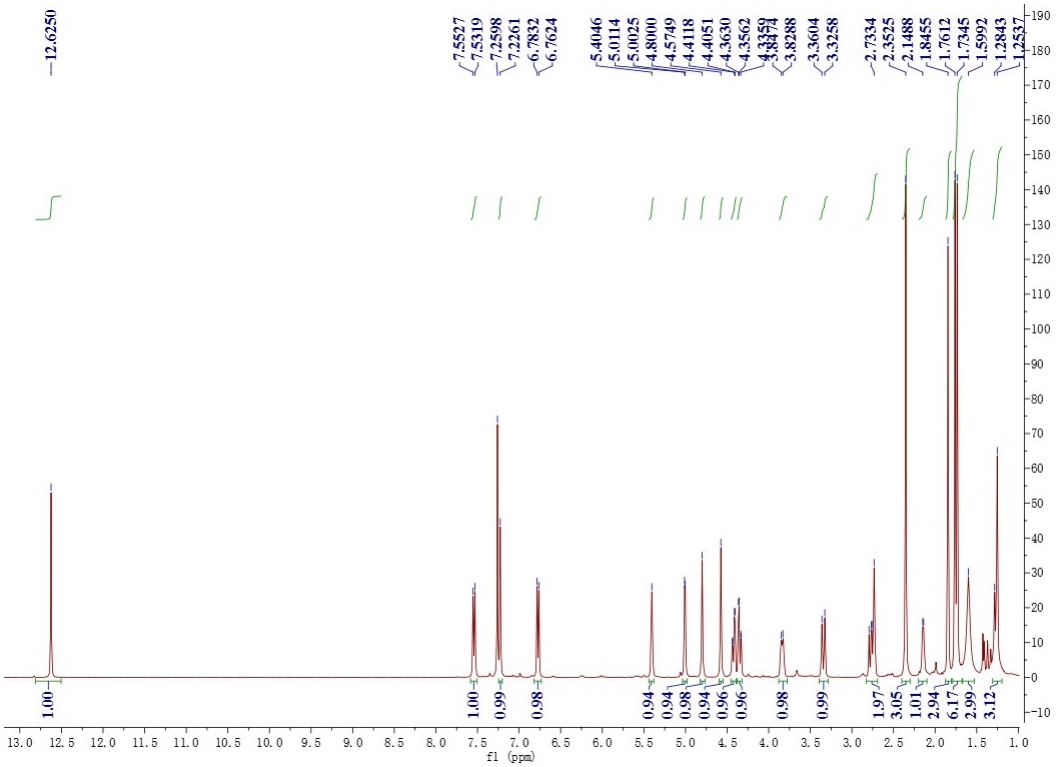


Figure S41. ^{1}H NMR spectrum of **7** ($CDCl_3$, 400 MHz)

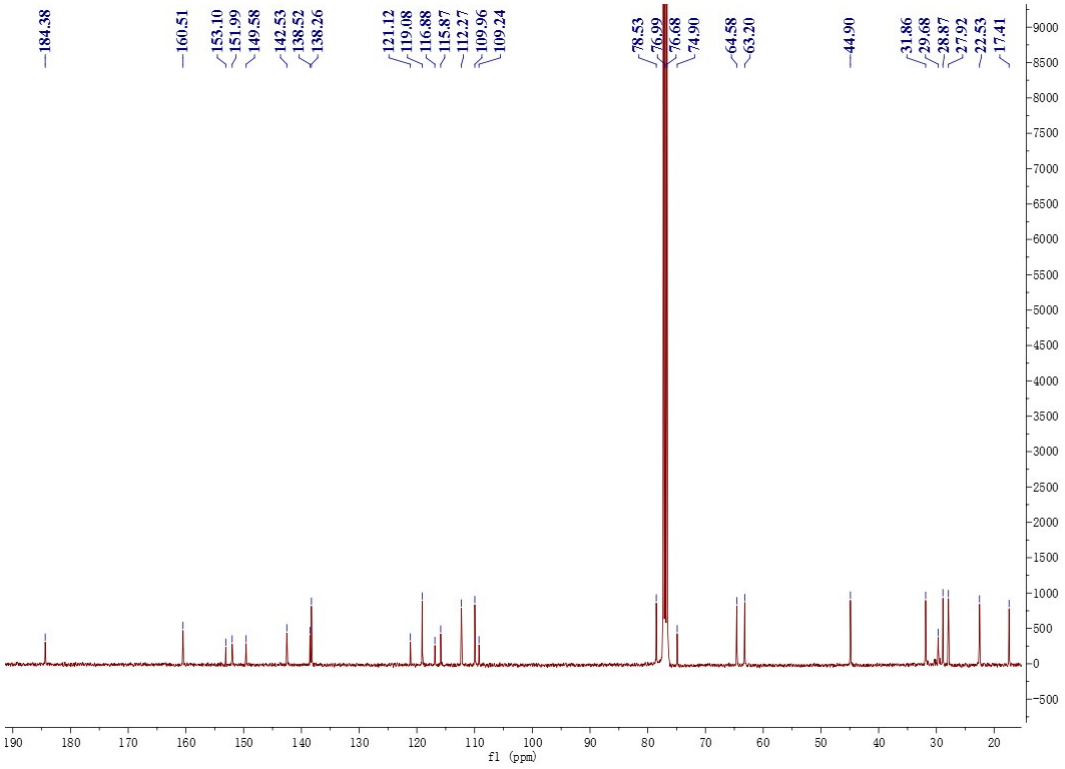


Figure S42. ^{13}C NMR spectrum of **7** ($CDCl_3$, 100 MHz)

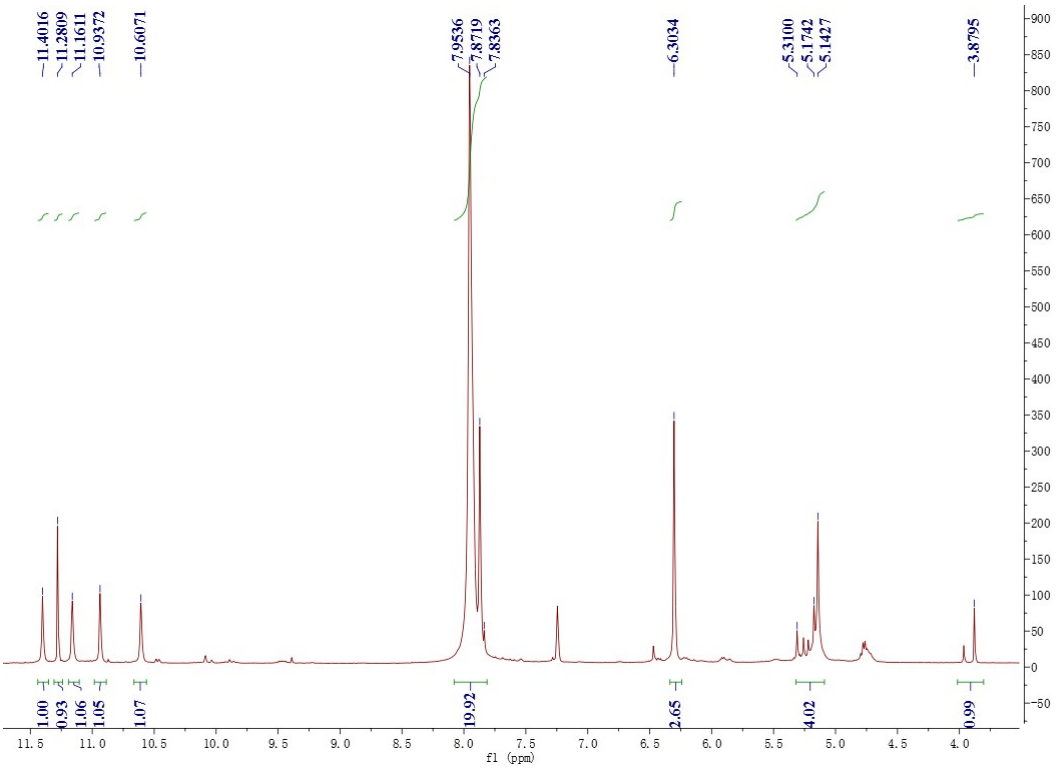


Figure S43. ^{1}H NMR spectrum of **8** ($CDCl_3$, 400 MHz)

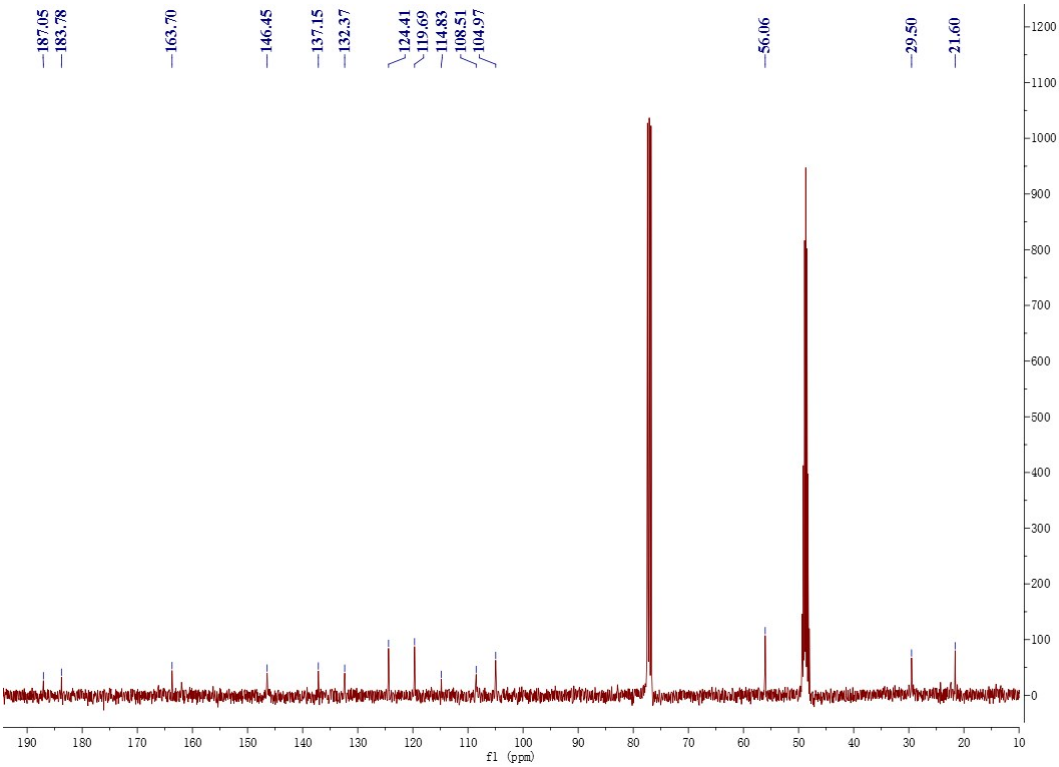


Figure S44. ^{13}C NMR spectrum of **8** ($CDCl_3$, 100 MHz)

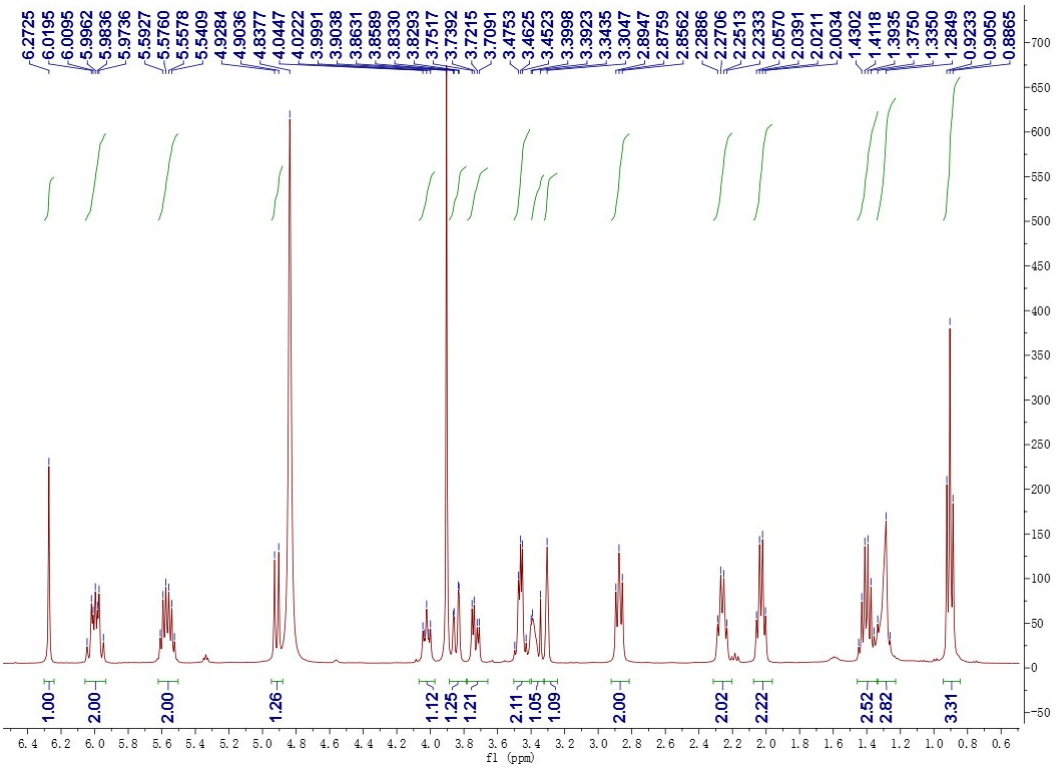


Figure S45. ^{1}H NMR spectrum of **9** (CD_3OD, 400 MHz)

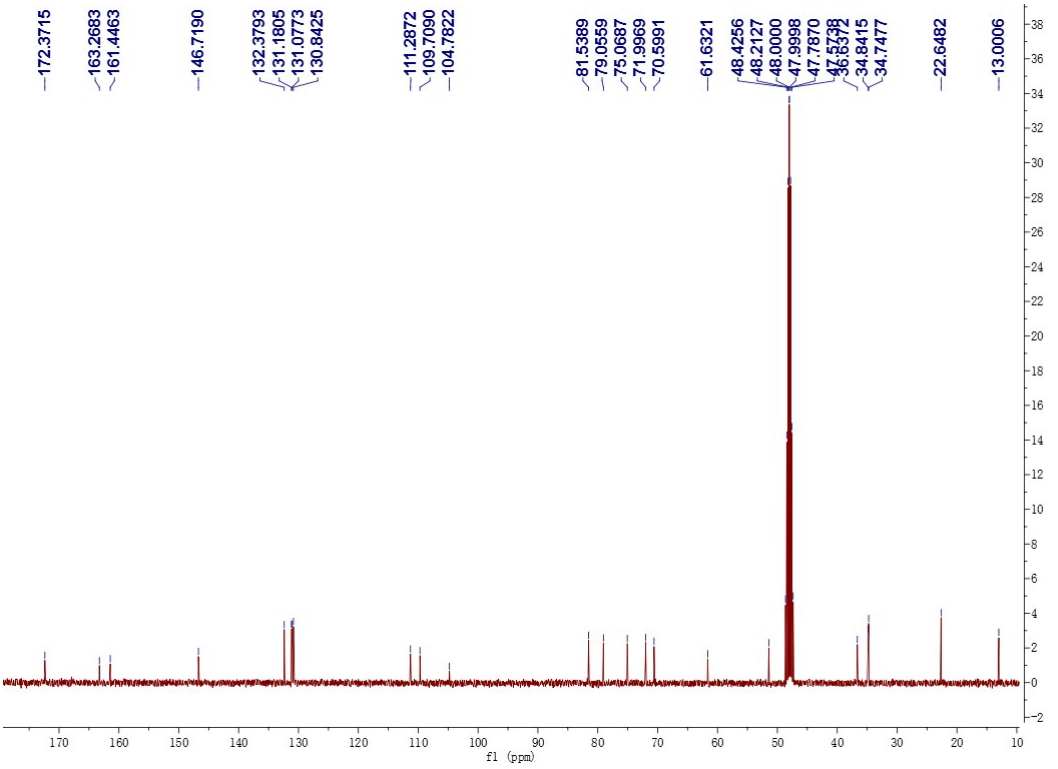


Figure S46. ^{13}C NMR spectrum of **9** (CD_3OD, 100 MHz)