

Supporting Information

Phragmalin-type limonoids from the fruits of *Chukrasia tabularis* and their anti-inflammatory activity

Shu-Jun Dai ¹, Yu-Zhen Wu ¹, Xiu-Juan Xin ¹ and Fa-Liang An ^{1,2*}

¹ State Key Laboratory of Bioreactor Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, China

² Marine Biomedical Science and Technology Innovation Platform of Lin-gang Special Area, No.4, Lane 218, Haiji Sixth Road, Shanghai 201306, China

*Correspondence: flan2016@ecust.edu.cn; Tel.: +86-21-6425-3823

Contents

Figure S1.	^1H NMR (500 MHz, CDCl_3) spectrum of compound 1
Figure S2.	^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 1
Figure S3.	HSQC spectrum of compound 1 in CDCl_3
Figure S4.	^1H - ^1H COSY spectrum of compound 1 in CDCl_3
Figure S5.	HMBC spectrum of compound 1 in CDCl_3
Figure S6.	ROESY spectrum of compound 1 in CDCl_3
Figure S7.	HRESIMS spectrum of compound 1
Figure S8.	^1H NMR (500 MHz, CDCl_3) spectrum of compound 2
Figure S9.	^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 2
Figure S10.	HSQC spectrum of compound 2 in CDCl_3
Figure S11.	^1H - ^1H COSY spectrum of compound 2 in CDCl_3
Figure S12.	HMBC spectrum of compound 2 in CDCl_3
Figure S13.	ROESY spectrum of compound 2 in CDCl_3
Figure S14.	HRESIMS spectrum of compound 2
Figure S15.	^1H NMR (500 MHz, CDCl_3) spectrum of compound 3
Figure S16.	^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 3
Figure S17.	HSQC spectrum of compound 3 in CDCl_3
Figure S18.	^1H - ^1H COSY spectrum of compound 3 in CDCl_3
Figure S19.	HMBC spectrum of compound 3 in CDCl_3
Figure S20.	ROESY spectrum of compound 3 in CDCl_3
Figure S21.	HRESIMS spectrum of compound 3
Figure S22.	^1H NMR (500 MHz, CDCl_3) spectrum of compound 4
Figure S23.	^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 4
Figure S24.	HSQC spectrum of compound 4 in CDCl_3
Figure S25.	^1H - ^1H COSY spectrum of compound 4 in CDCl_3
Figure S26.	HMBC spectrum of compound 4 in CDCl_3
Figure S27.	ROESY spectrum of compound 4 in CDCl_3
Figure S28.	HRESIMS spectrum of compound 4
Figure S29.	^1H NMR (500 MHz, CDCl_3) spectrum of compound 5
Figure S30.	^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 5
Figure S31.	HSQC spectrum of compound 5 in CDCl_3
Figure S32.	^1H - ^1H COSY spectrum of compound 5 in CDCl_3
Figure S33.	HMBC spectrum of compound 5 in CDCl_3
Figure S34.	ROESY spectrum of compound 5 in CDCl_3
Figure S35.	HRESIMS spectrum of compound 5

Figure S1. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **1**

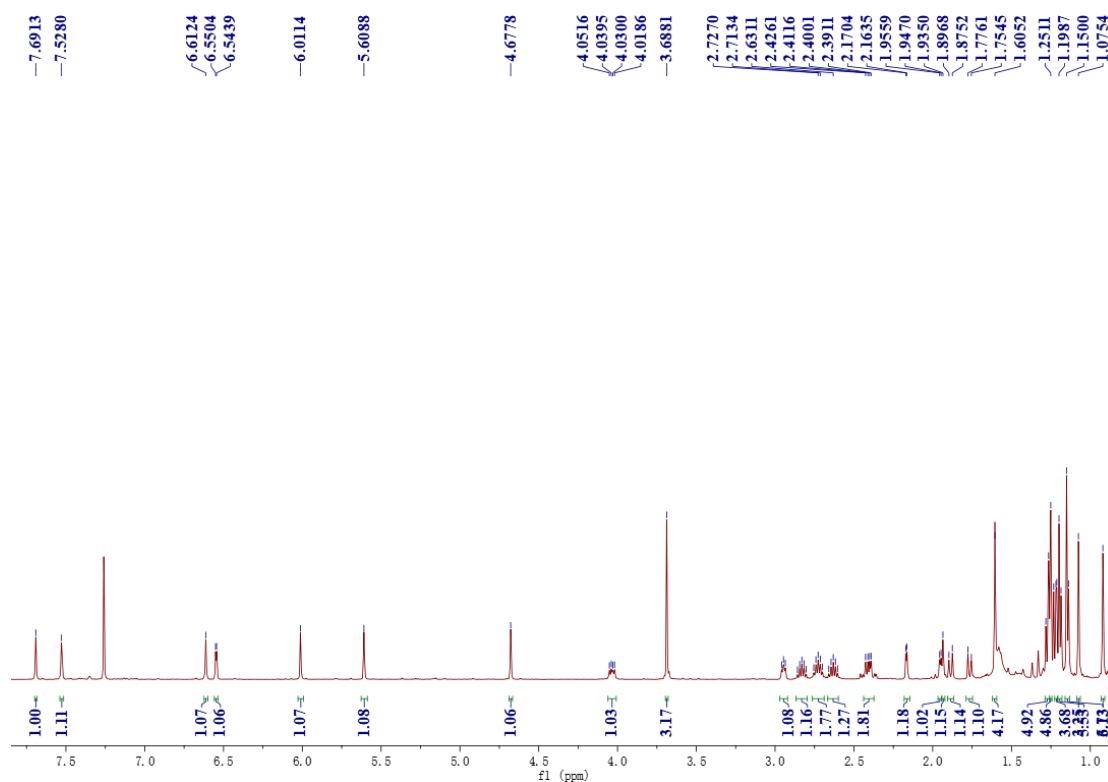


Figure S2. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **1**

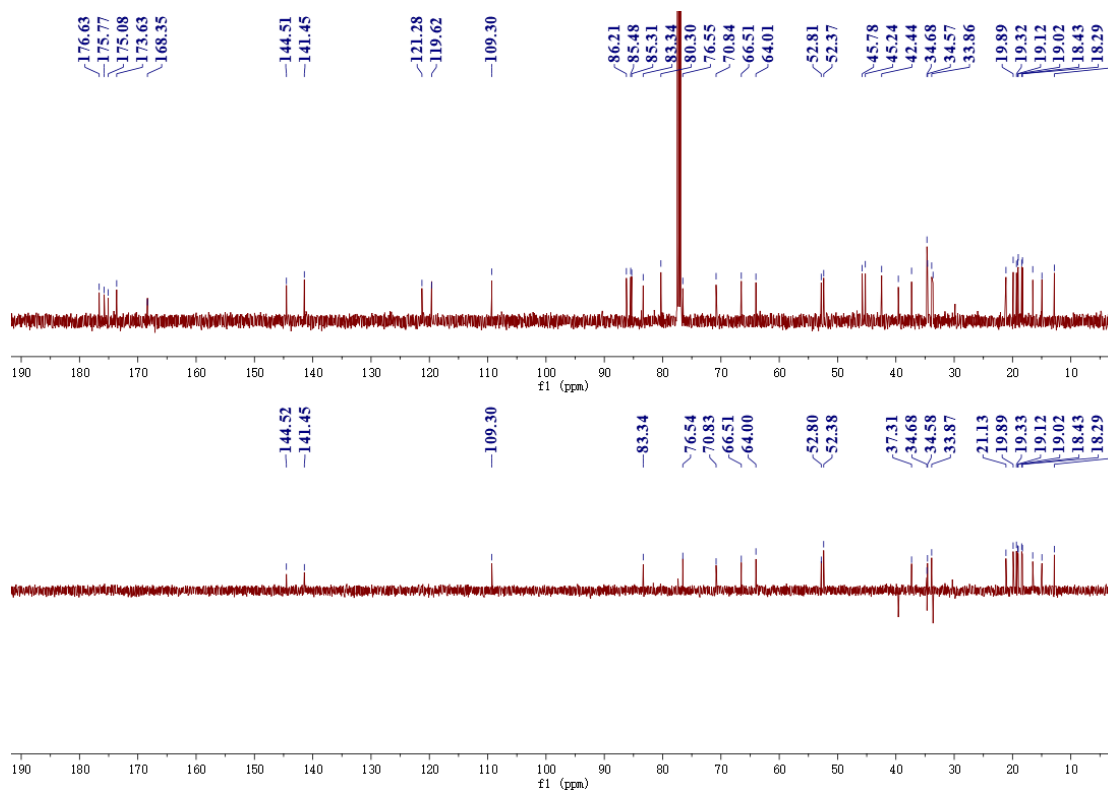


Figure S3. HSQC spectrum of compound **1** in CDCl₃

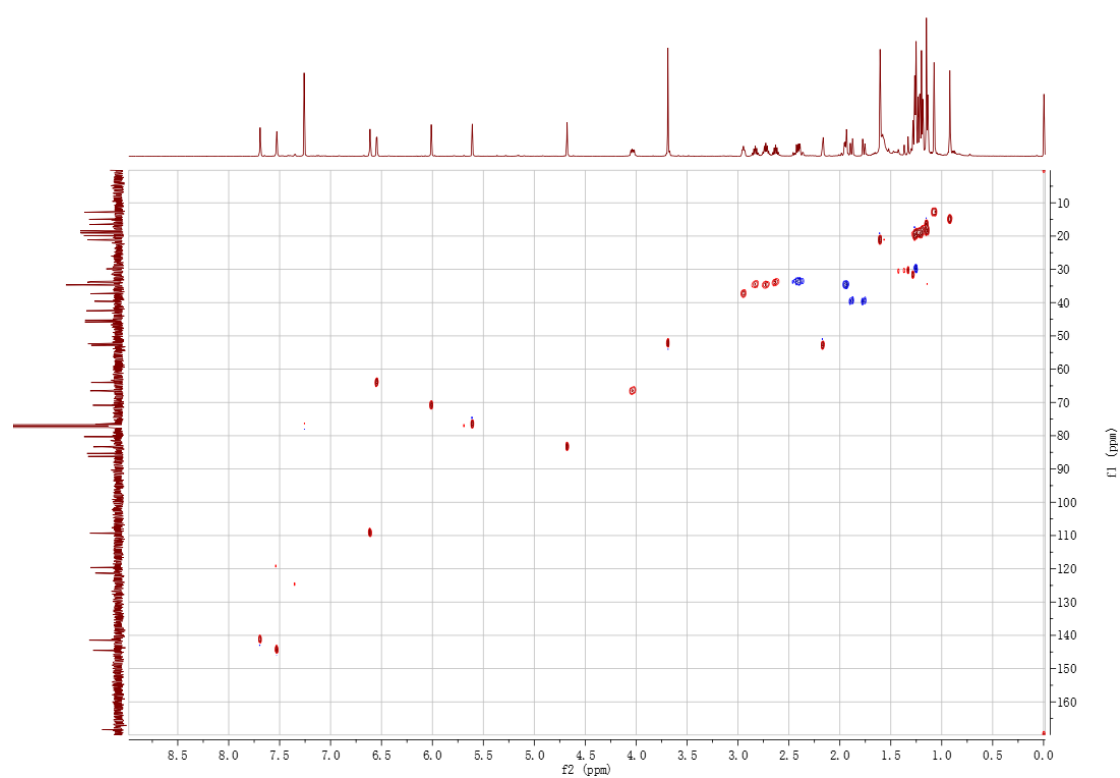


Figure S4. ¹H-¹H COSY spectrum of compound **1** in CDCl₃

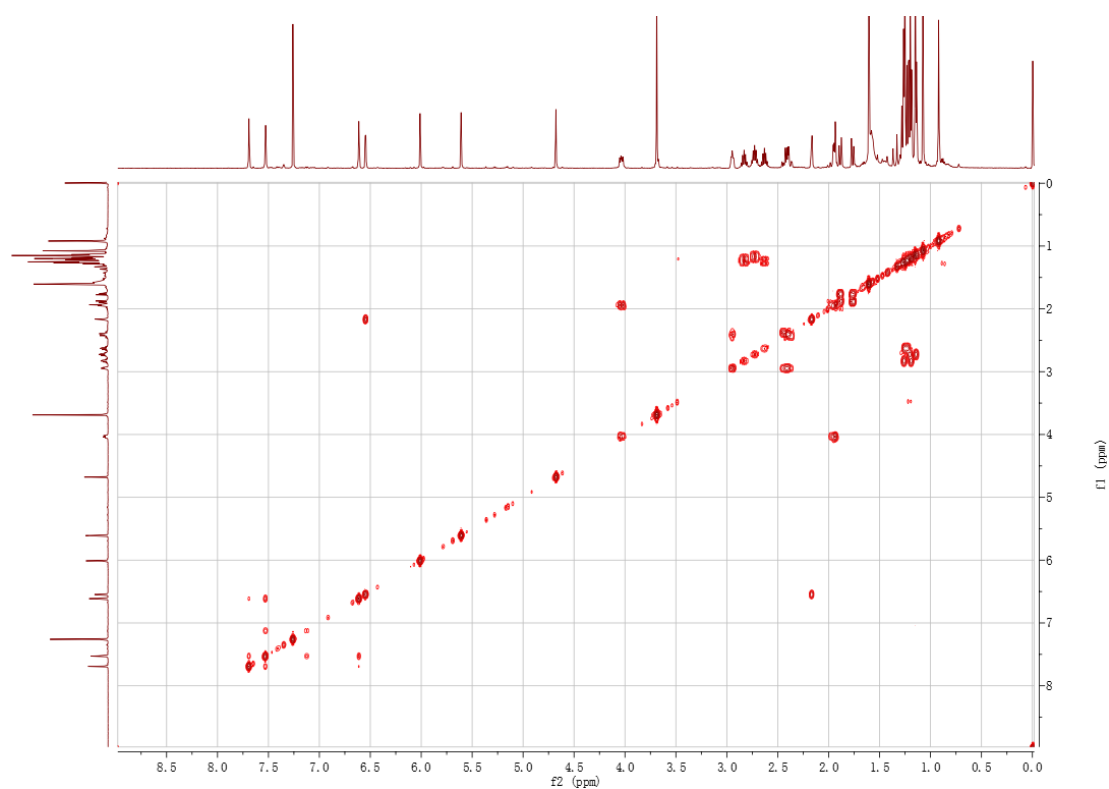


Figure S5. HMBC spectrum of compound **1** in CDCl₃

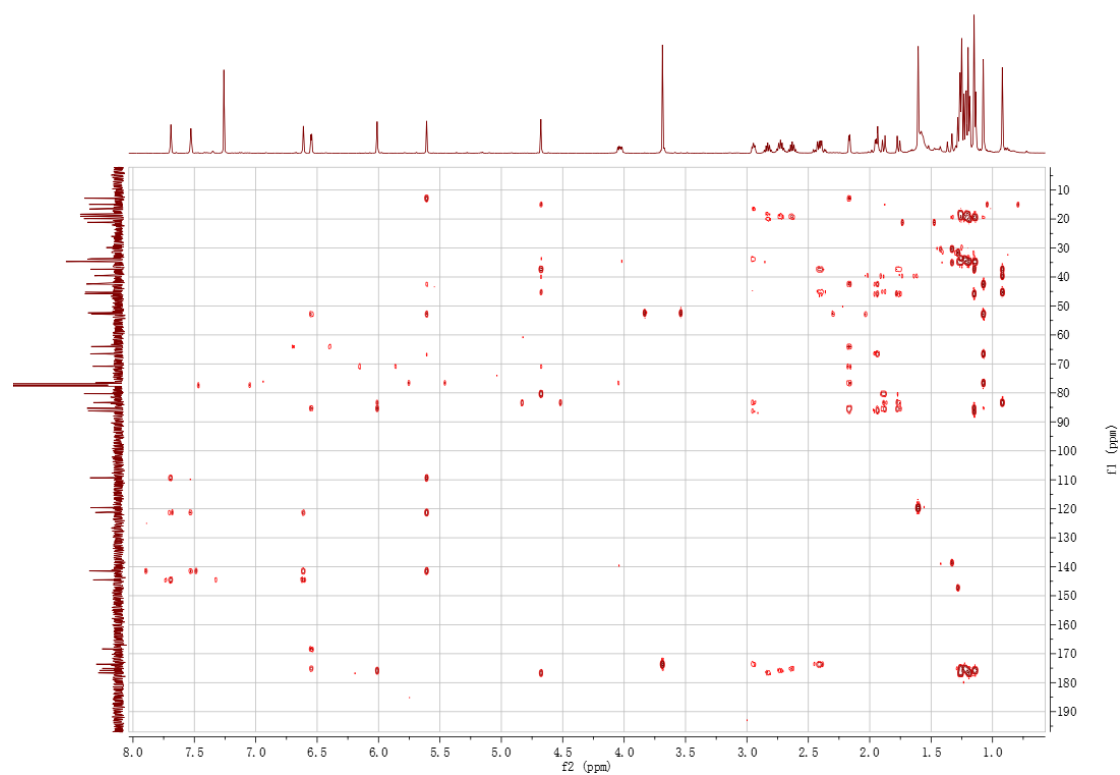


Figure S6. ROESY spectrum of compound **1** in CDCl₃

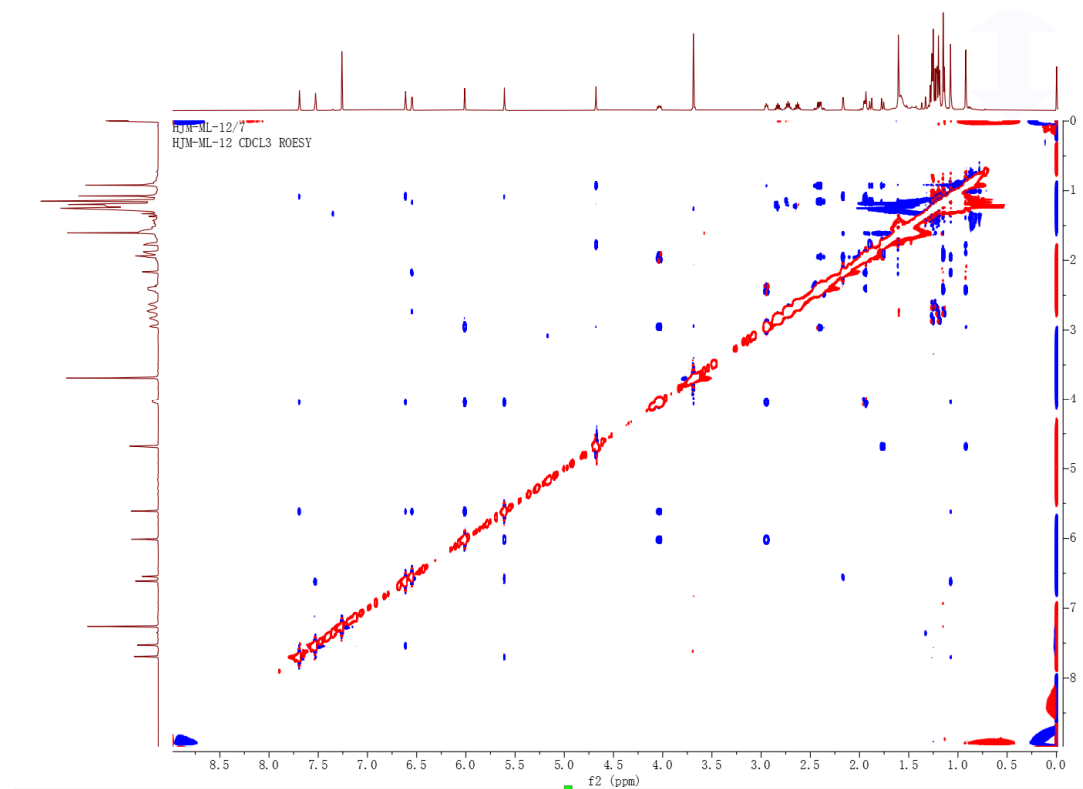


Figure S7. HRESIMS spectrum of compound 1

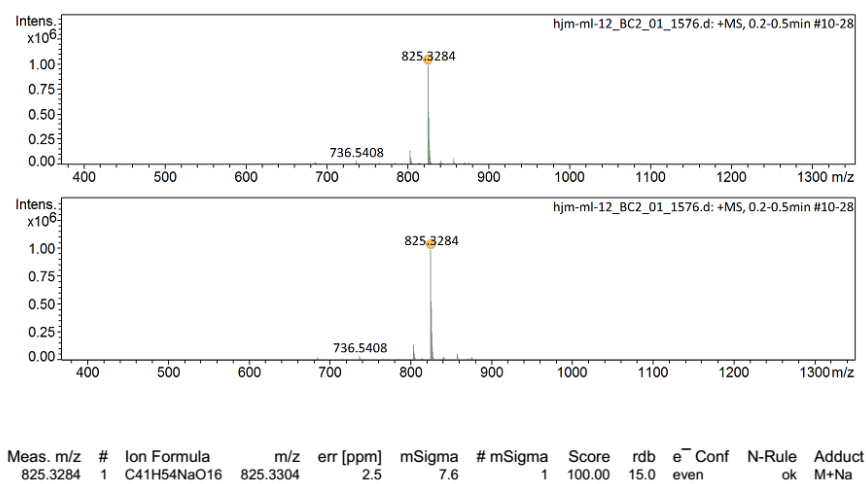


Figure S8. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 2

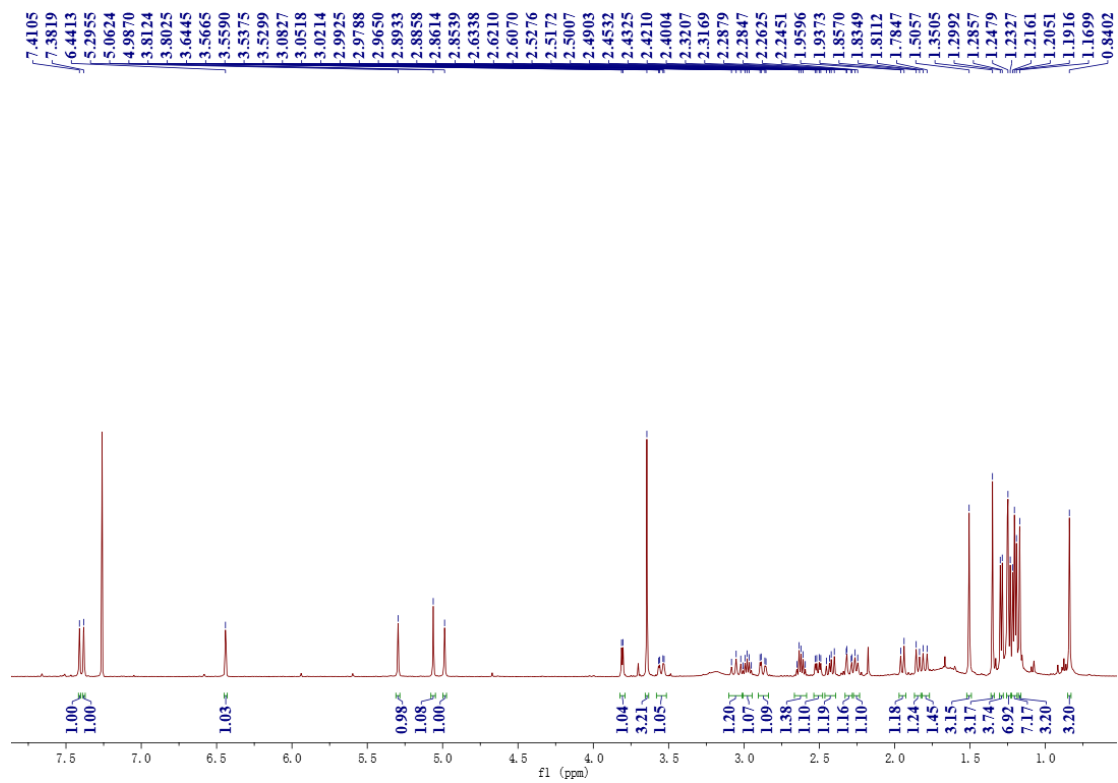


Figure S9. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **2**

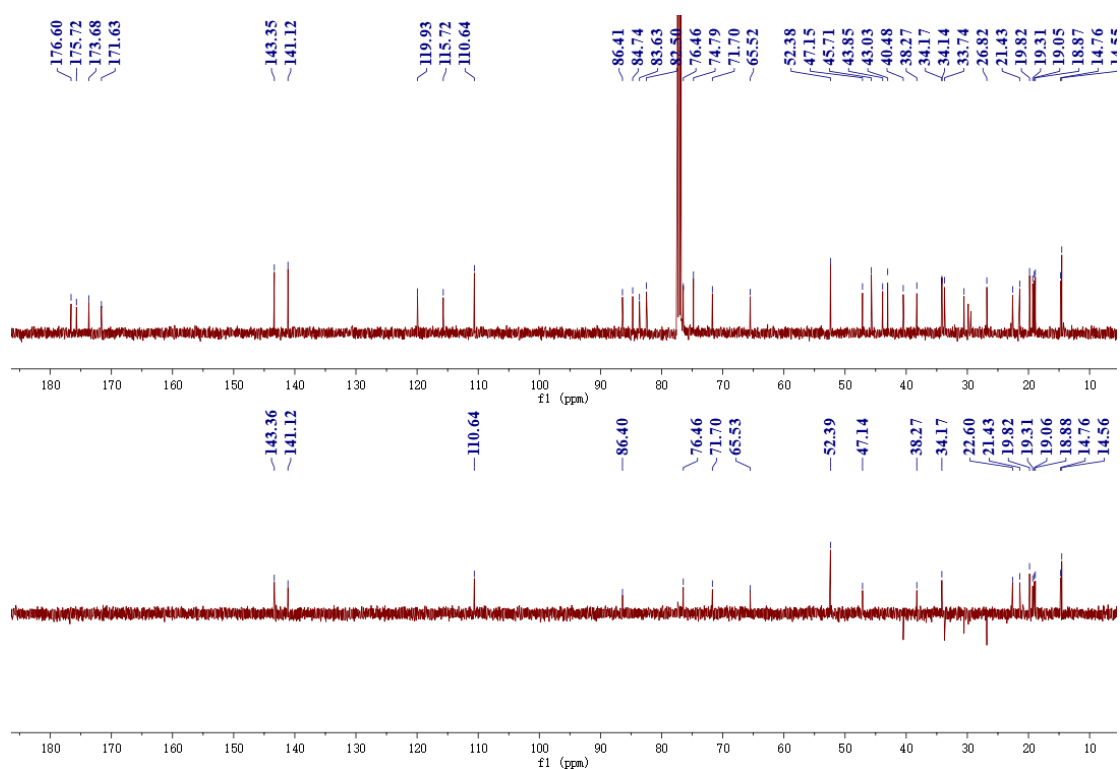


Figure S10. HSQC spectrum of compound **2** in CDCl_3

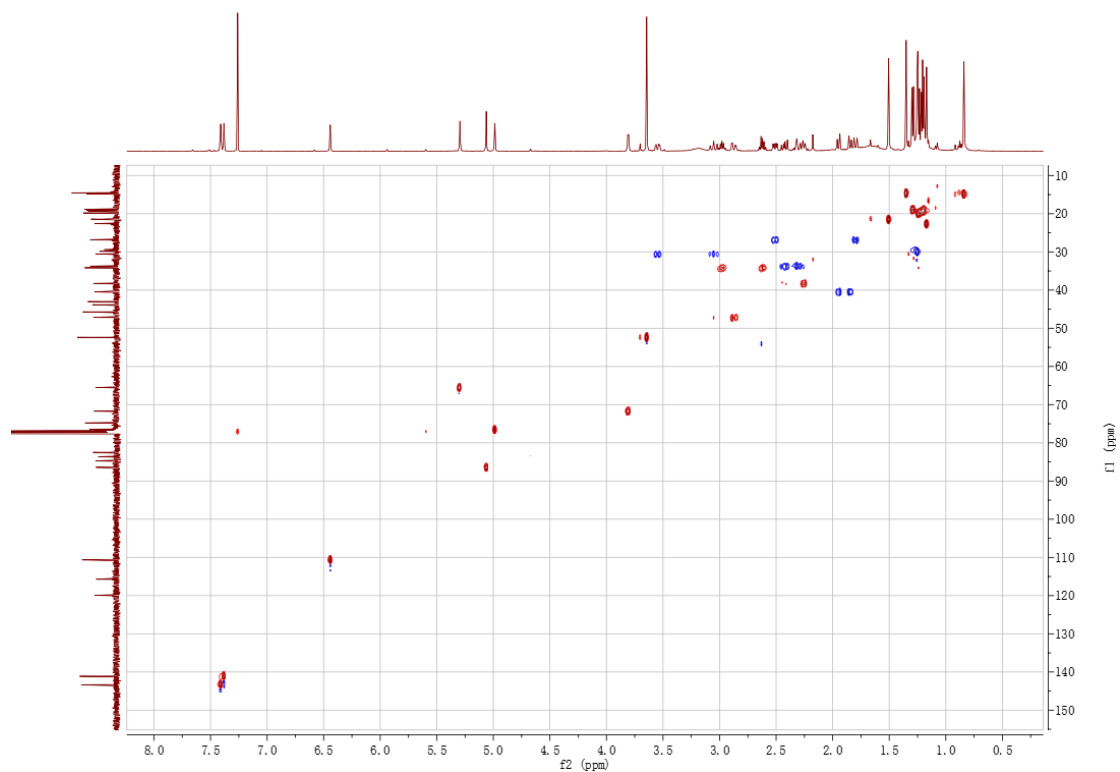


Figure S11. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3

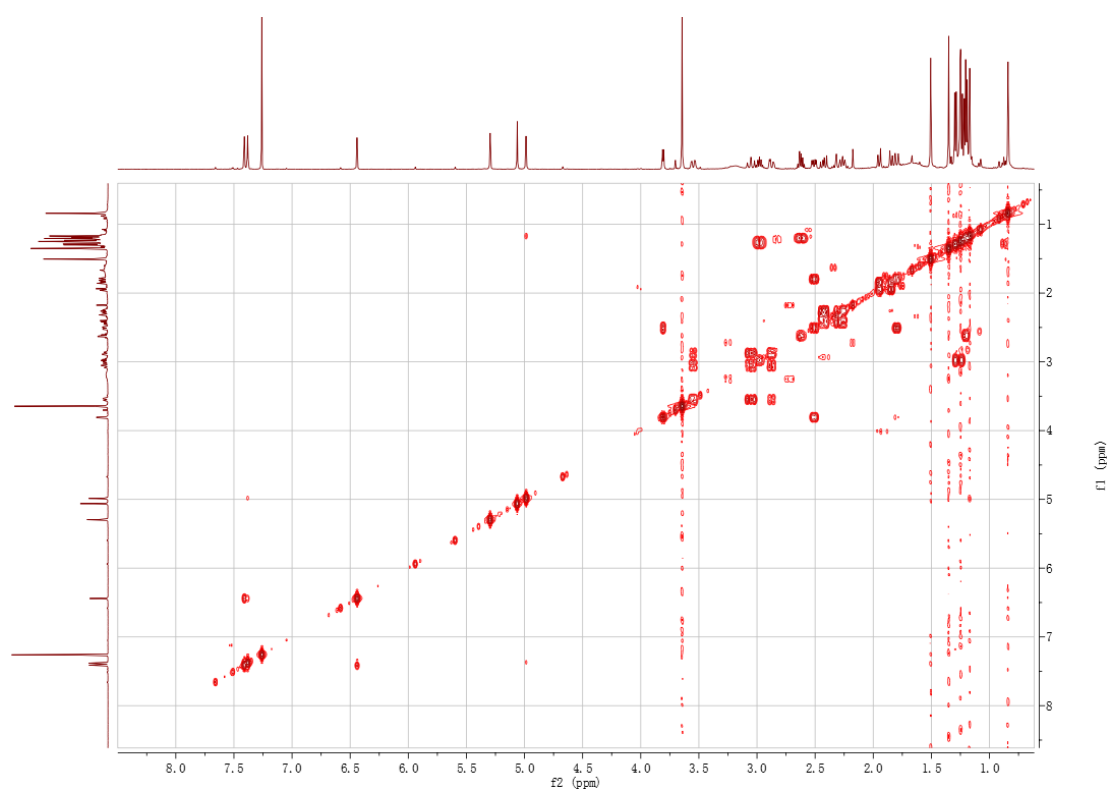


Figure S12. HMBC spectrum of compound **2** in CDCl_3

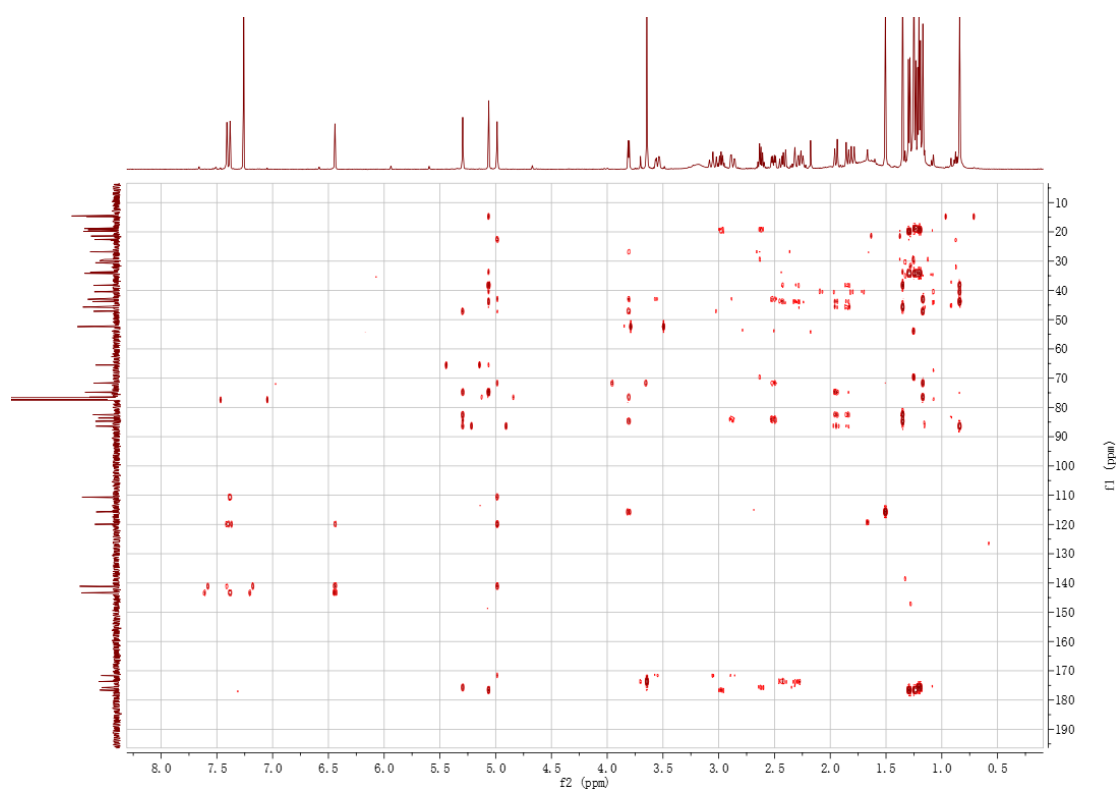


Figure S13. ROESY spectrum of compound **2** in CDCl₃

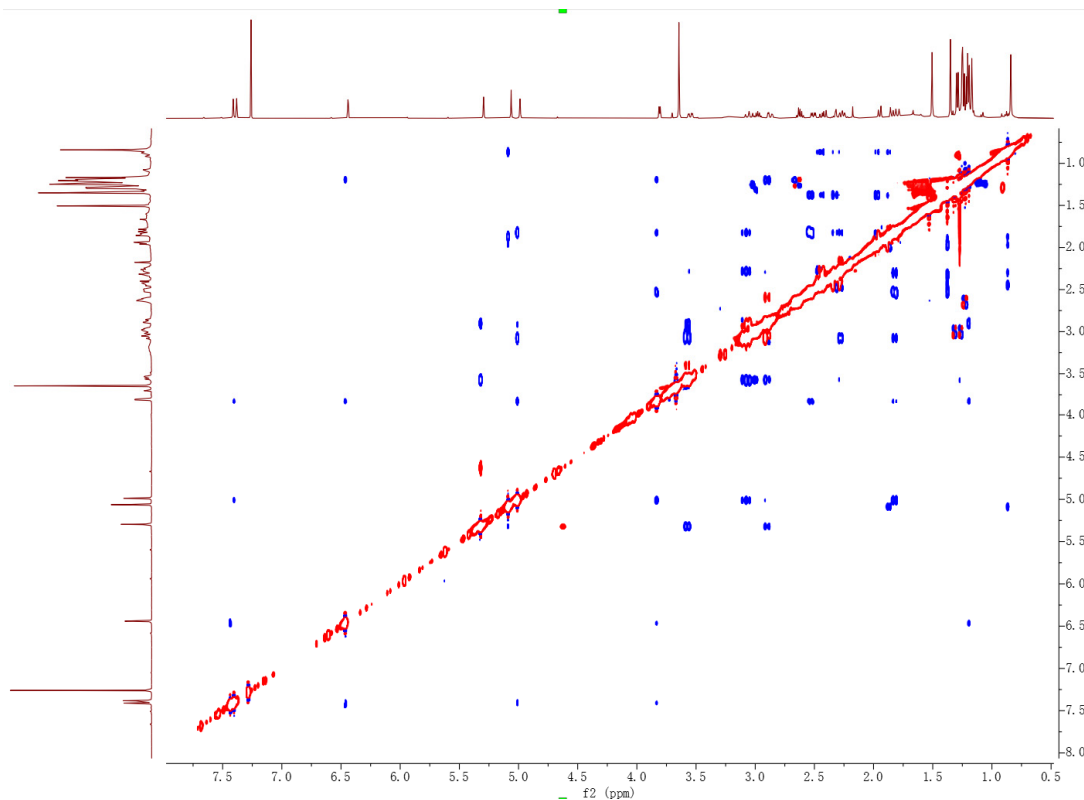
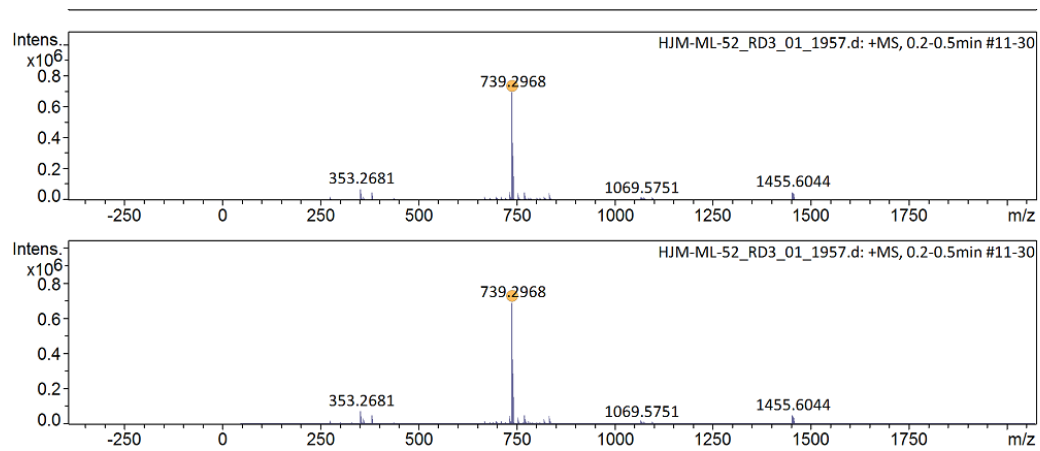


Figure S14. HRESI-MS spectrum of compound **2**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
739.2968	1	C37H48NaO14	739.2936	-4.2	3.1	1	100.00	14.0	even	ok	M+Na

Figure S15. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 3

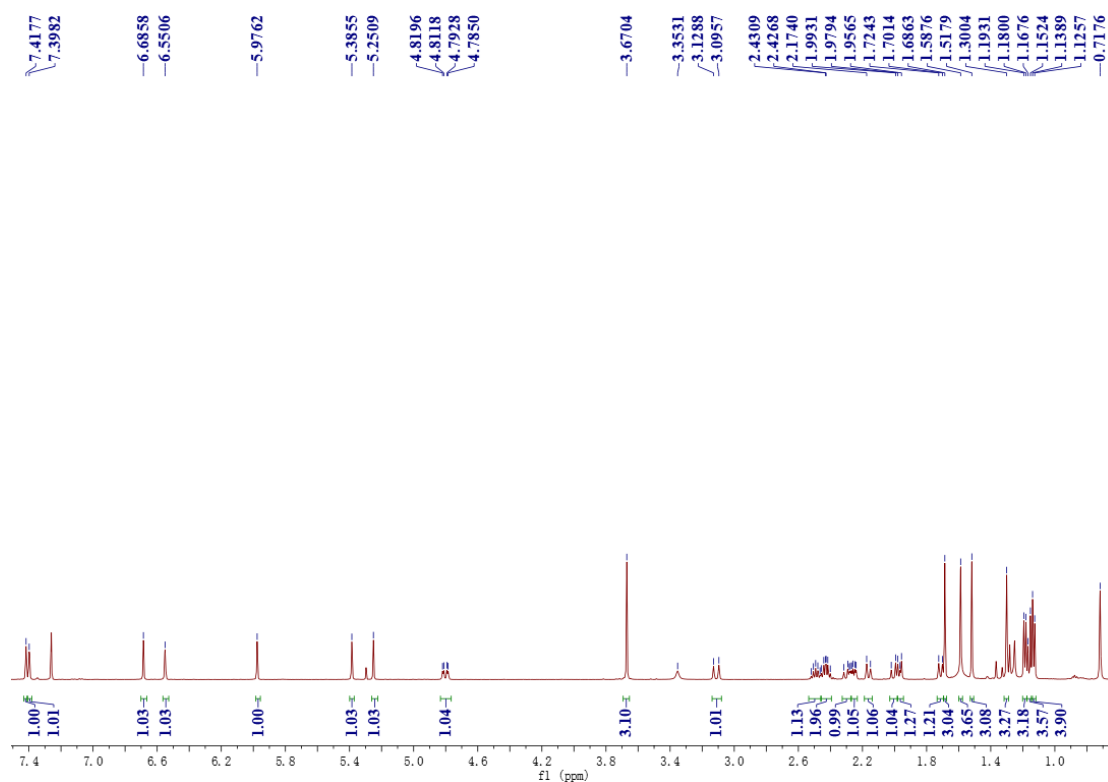


Figure S16. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 3

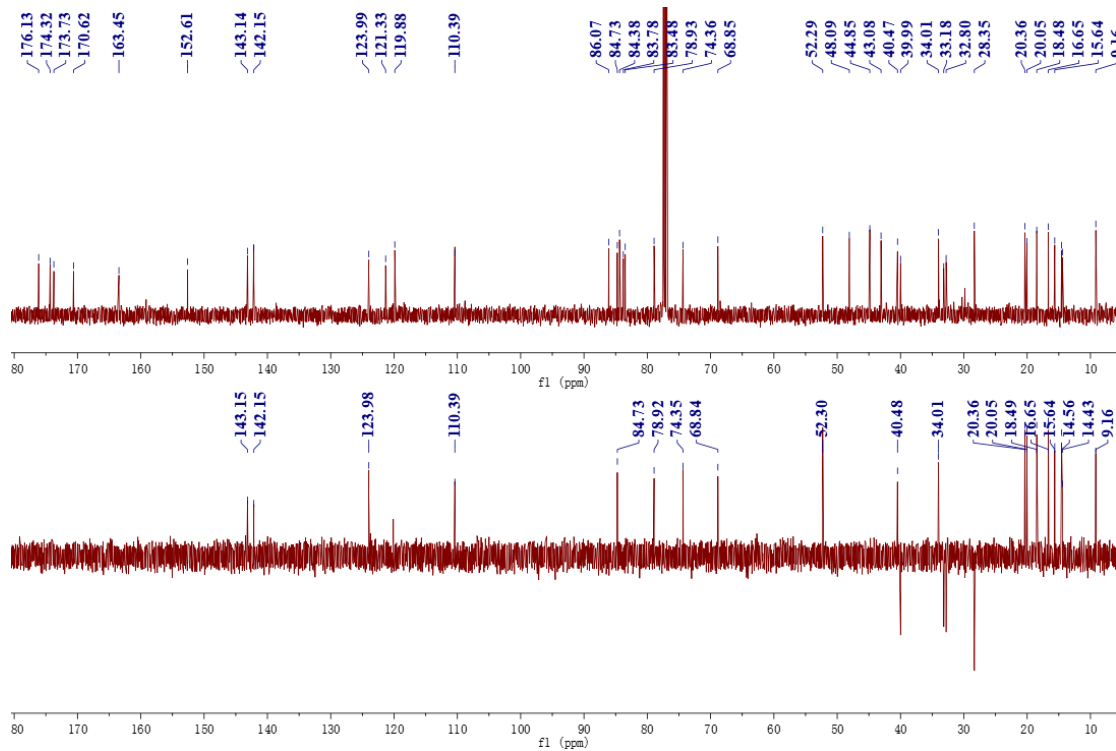


Figure S17. HSQC spectrum of compound **3** in CDCl₃

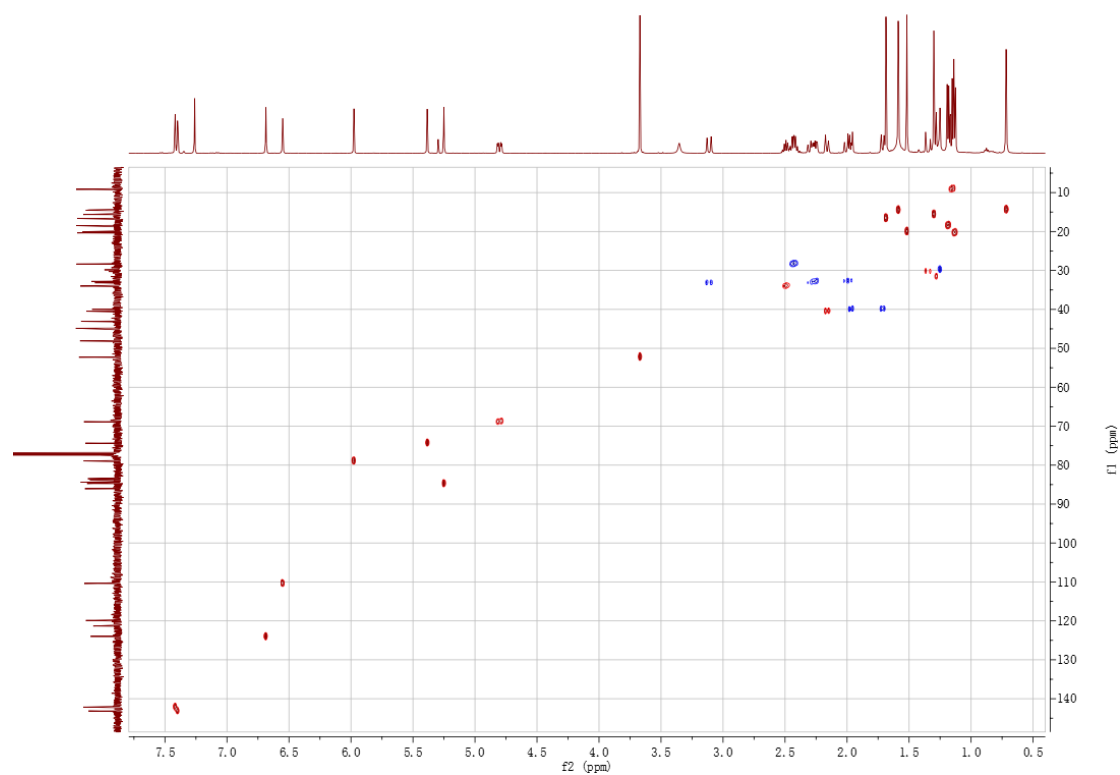


Figure S18. ¹H-¹H COSY spectrum of compound **3** in CDCl₃

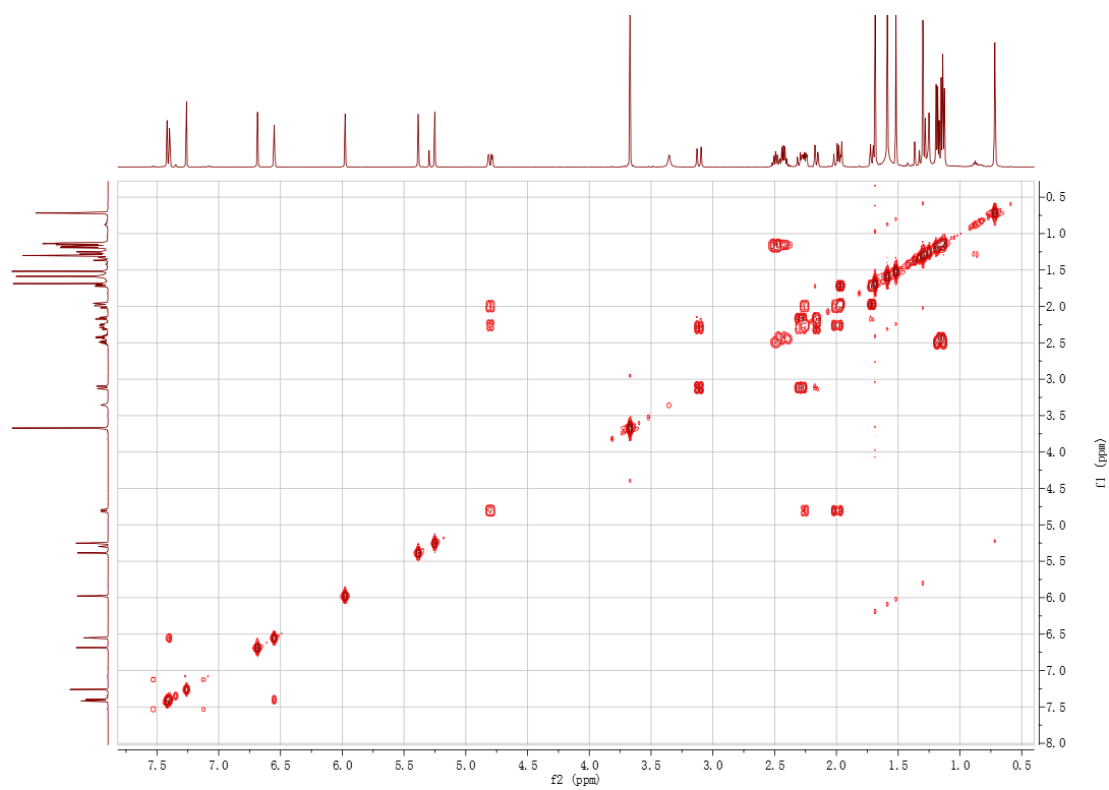


Figure S19. HMBC spectrum of compound **3** in CDCl₃

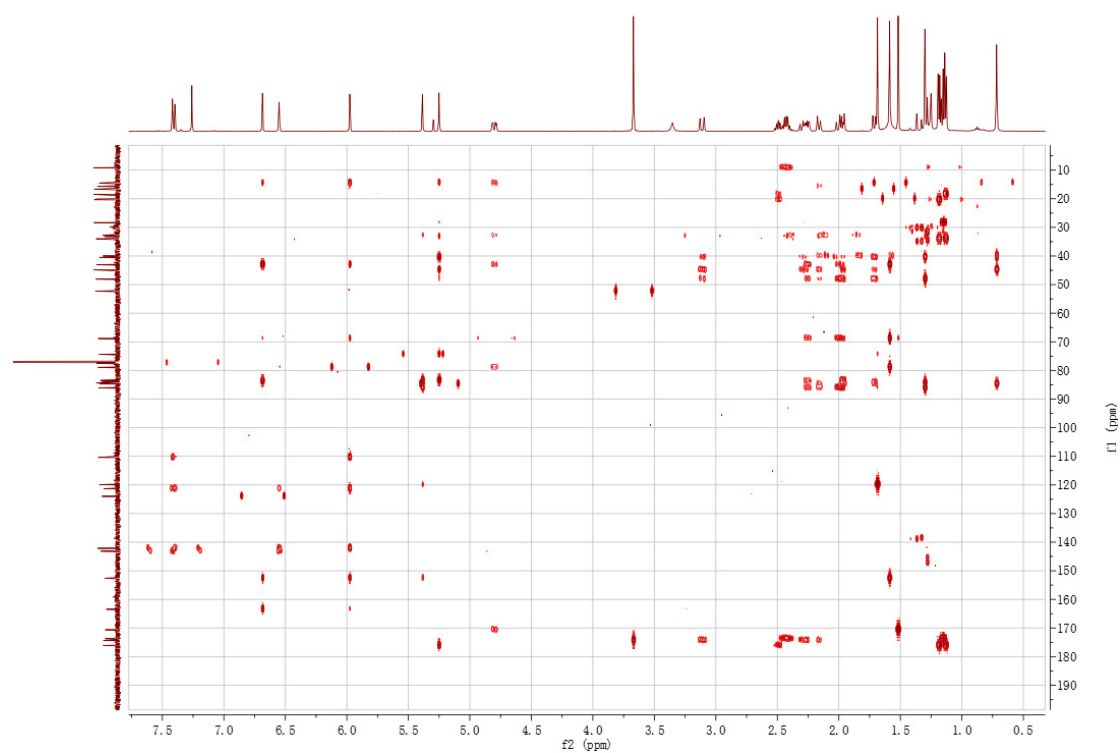


Figure S20. ROESY spectrum of compound **3** in CDCl₃

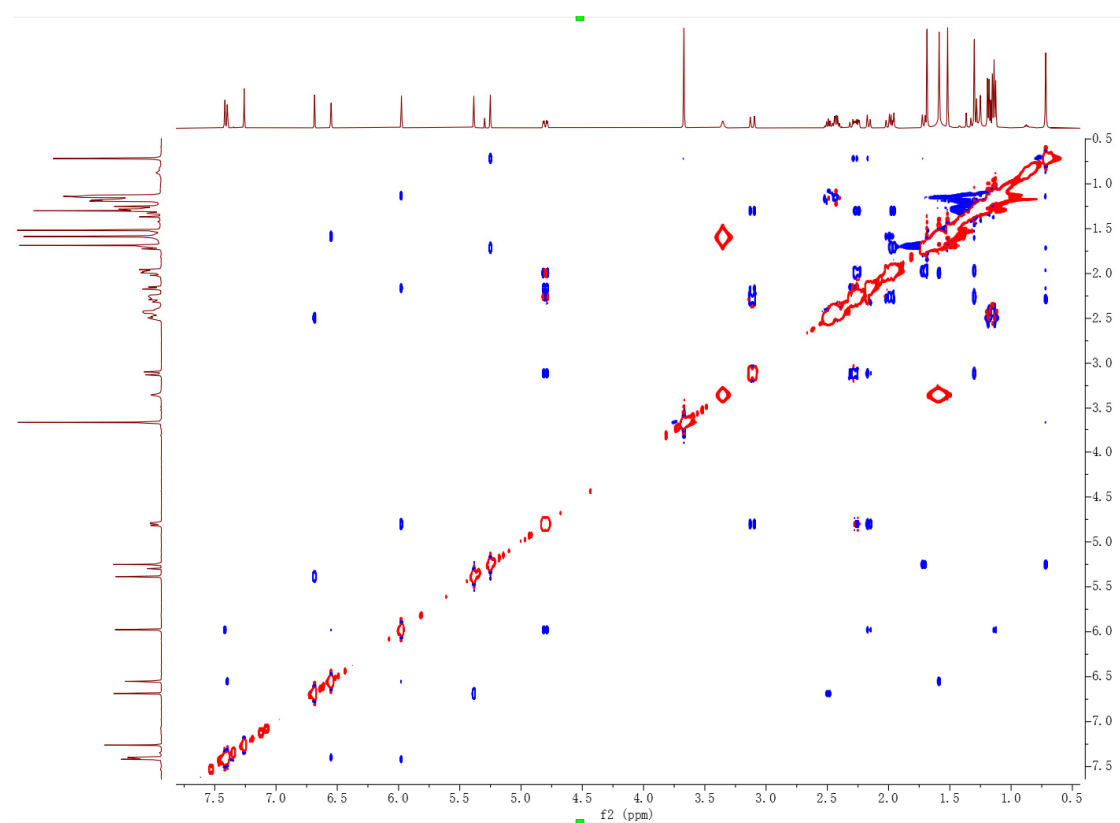
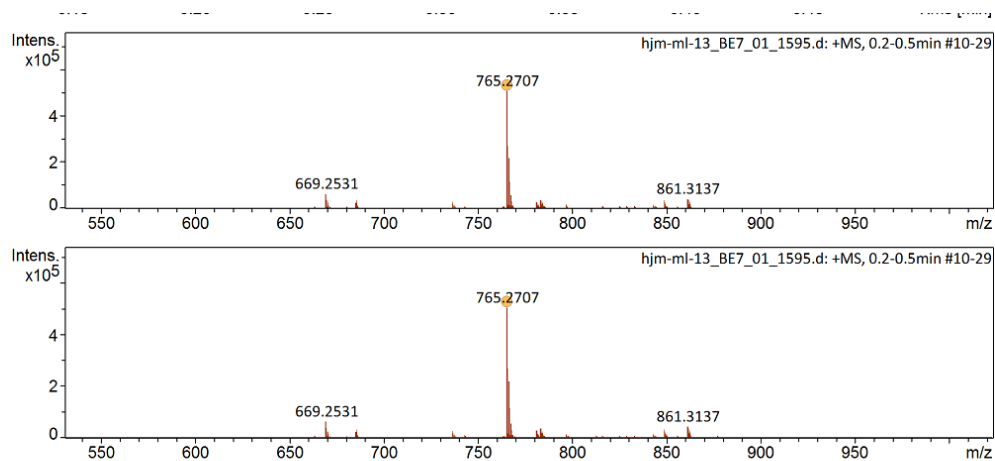


Figure S21. HRESI-MS spectrum of compound 3



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
765.2707	1	C38H46NaO15	765.2729	2.8	4.8	1	100.00	16.0	even	ok	M+Na

Figure S22. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 4

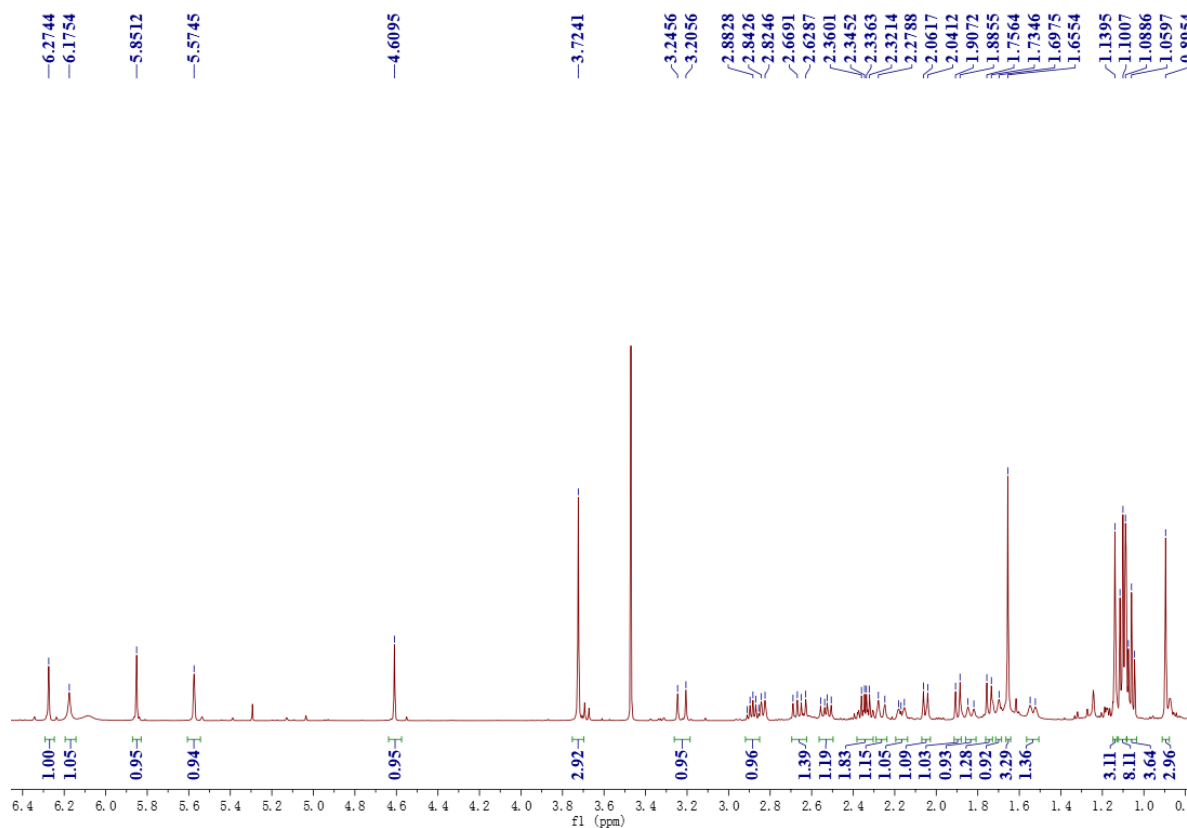


Figure S23. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **4**

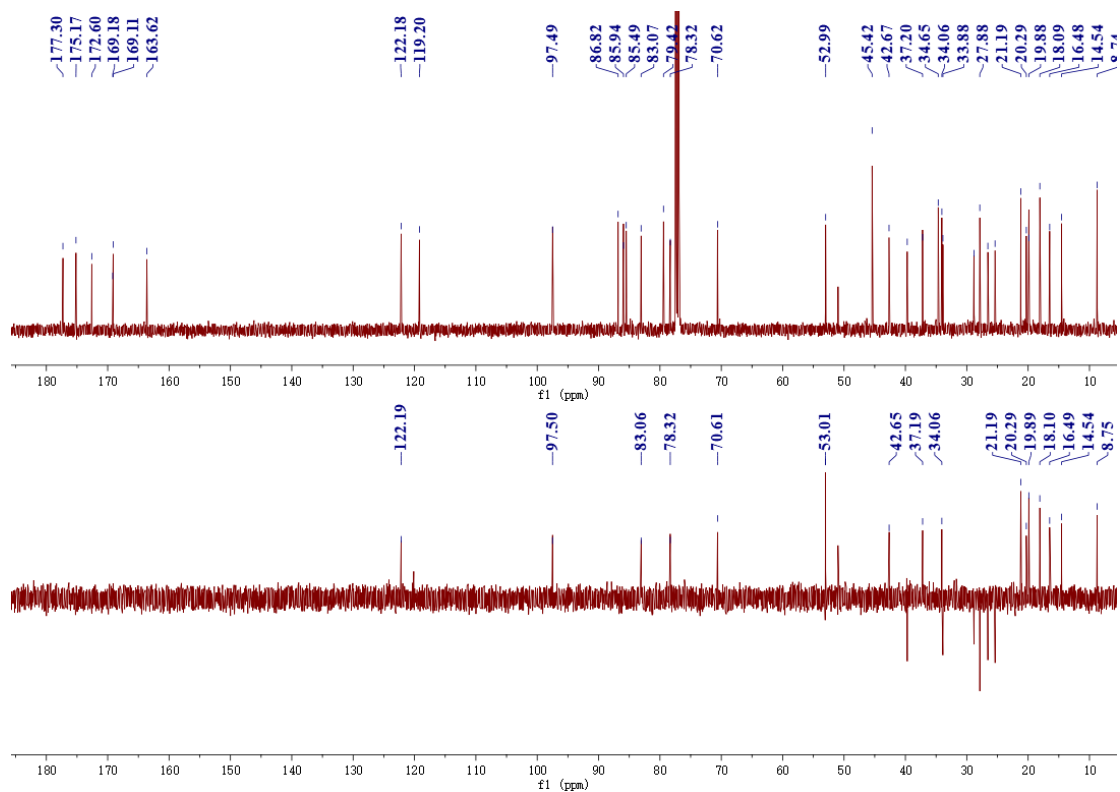


Figure S24. HSQC spectrum of compound **4** in CDCl_3

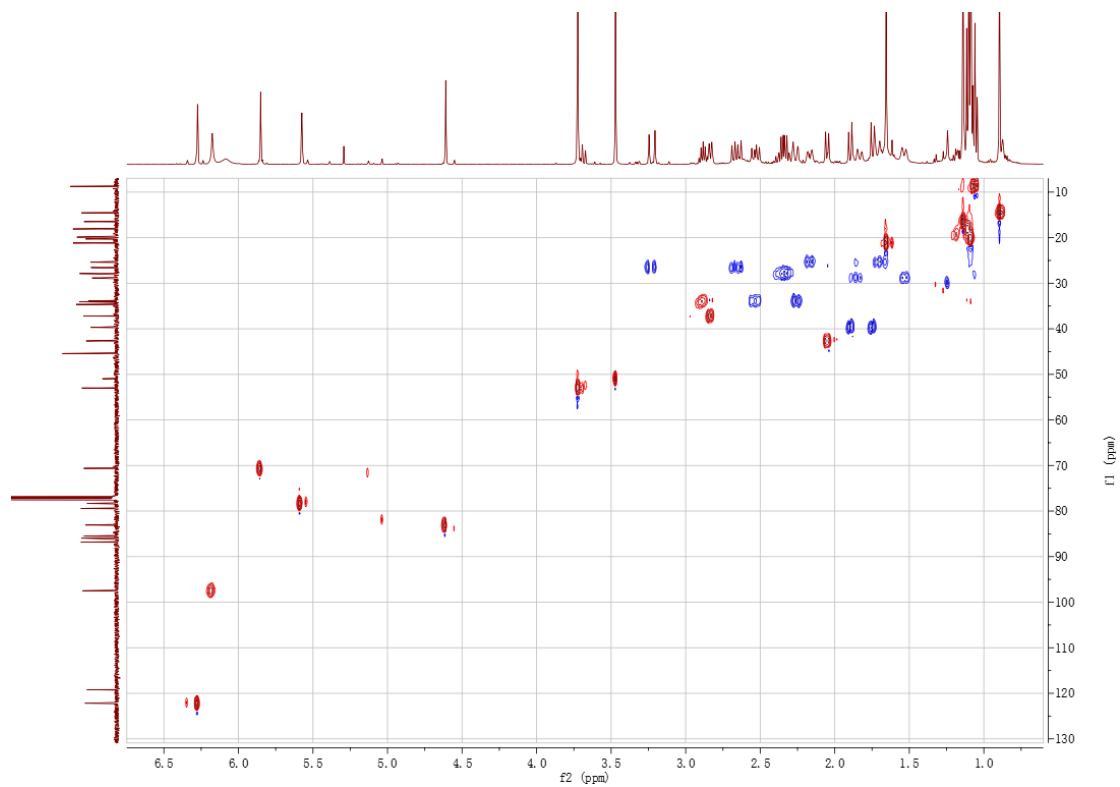


Figure S25. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3

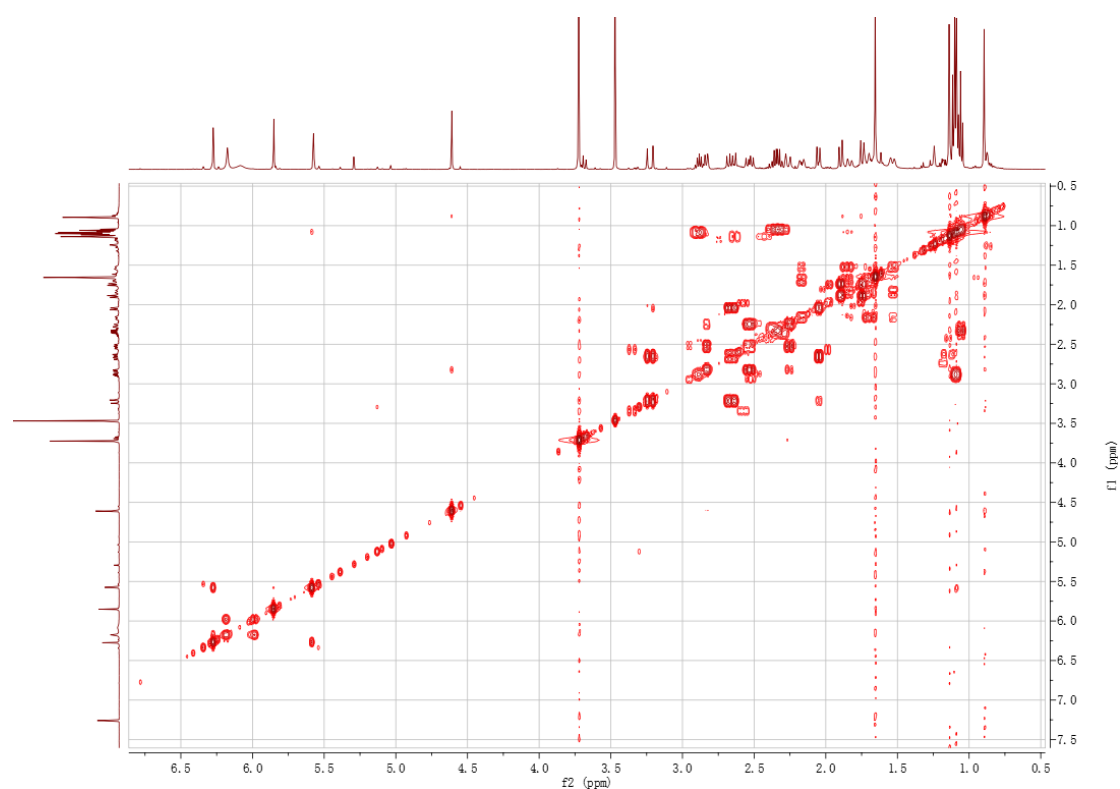


Figure S26. HMBC spectrum of compound **4** in CDCl_3



Figure S27. ROESY spectrum of compound **4** in CDCl₃

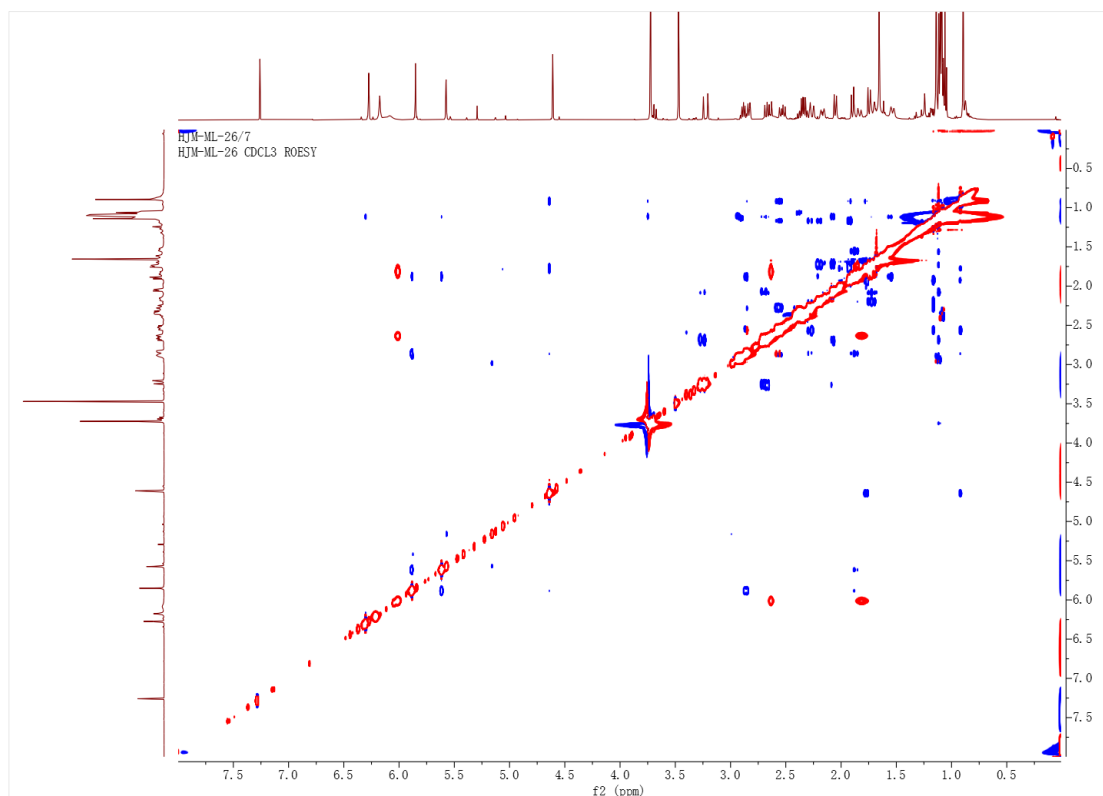
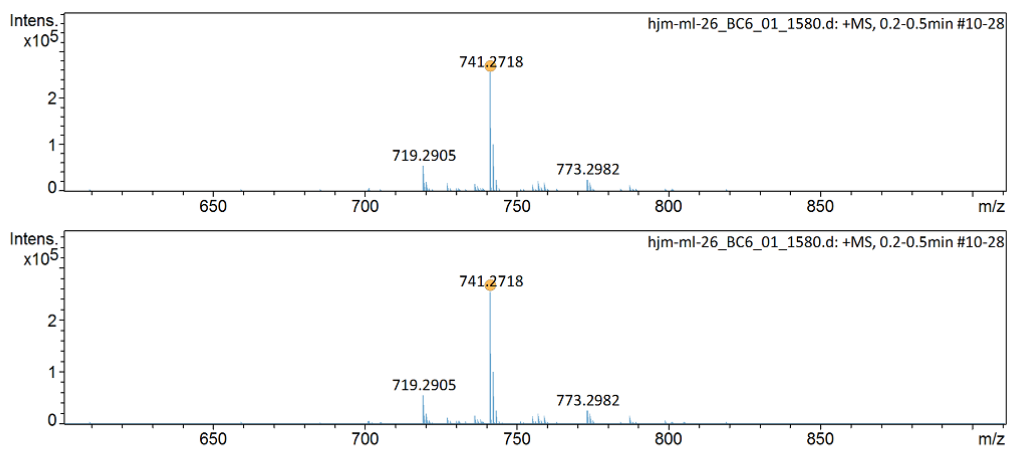


Figure S28. HRESI-MS spectrum of compound **4**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
741.2718	1	C ₃₆ H ₄₆ NaO ₁₅	741.2729	1.5	5.0	1	100.00	14.0	even	ok	M+Na

Figure S29. ^1H NMR (500 MHz, CDCl_3) spectrum of compound **5**

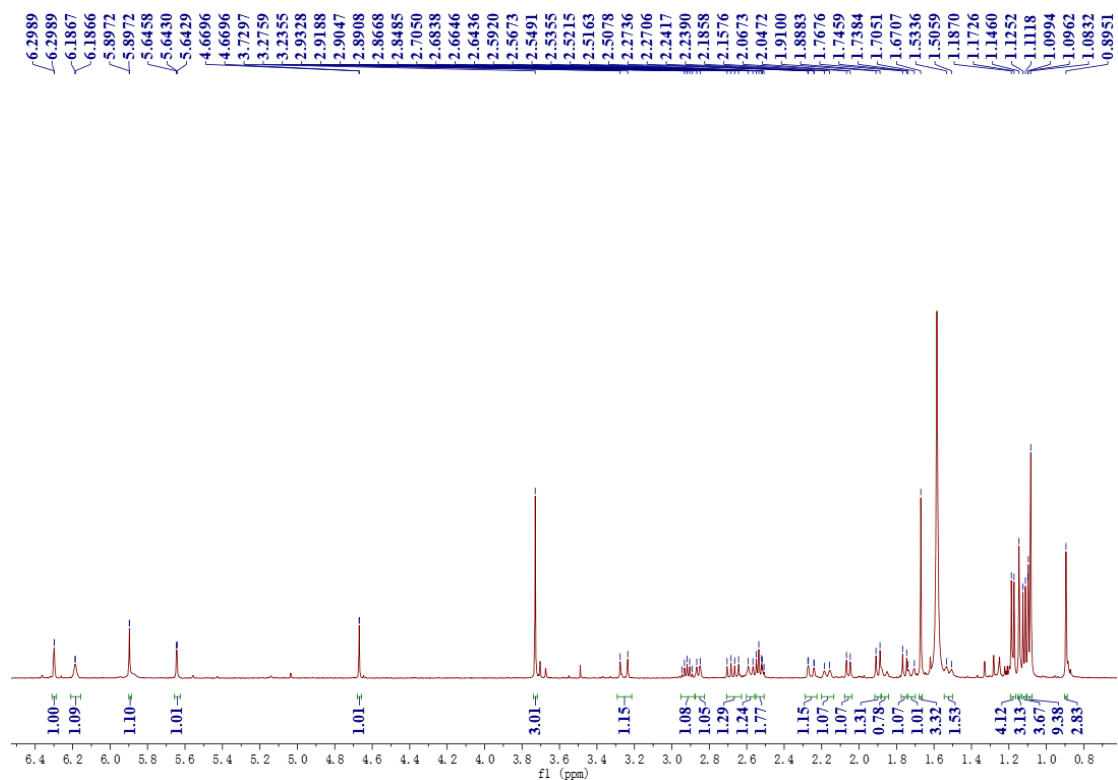


Figure S30. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound **5**

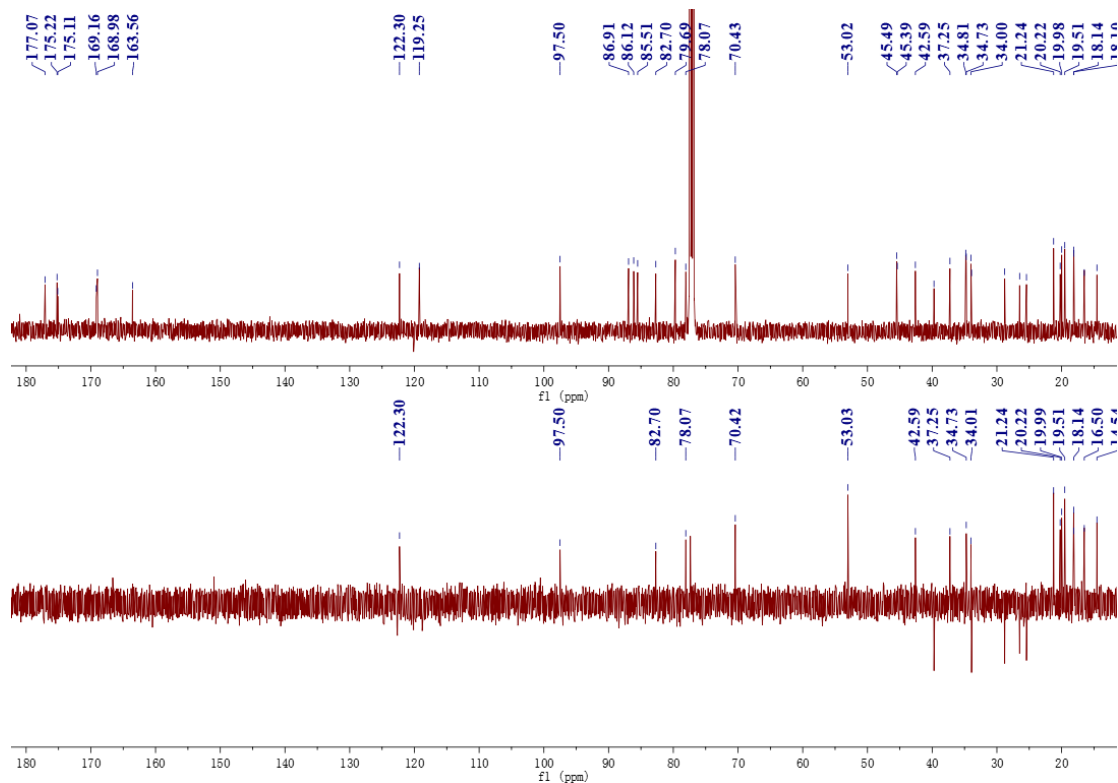


Figure S31. HSQC spectrum of compound **5** in CDCl₃

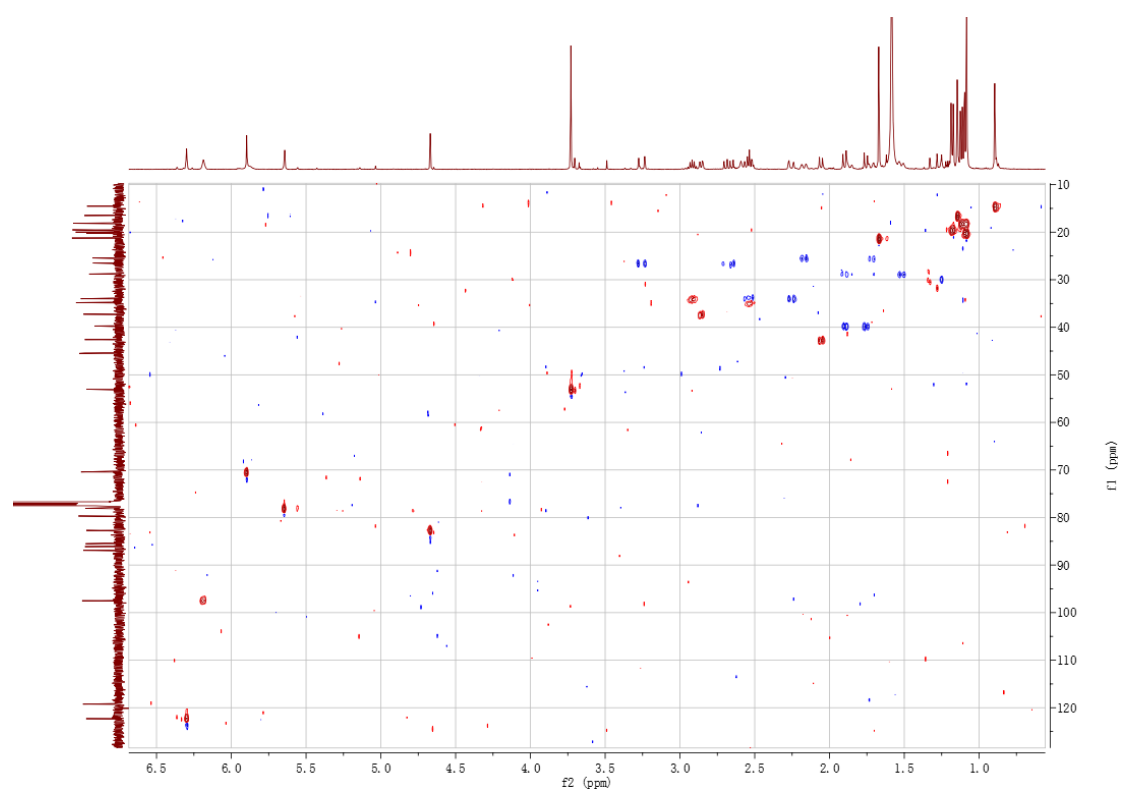


Figure S32. ¹H-¹H COSY spectrum of compound **5** in CDCl₃

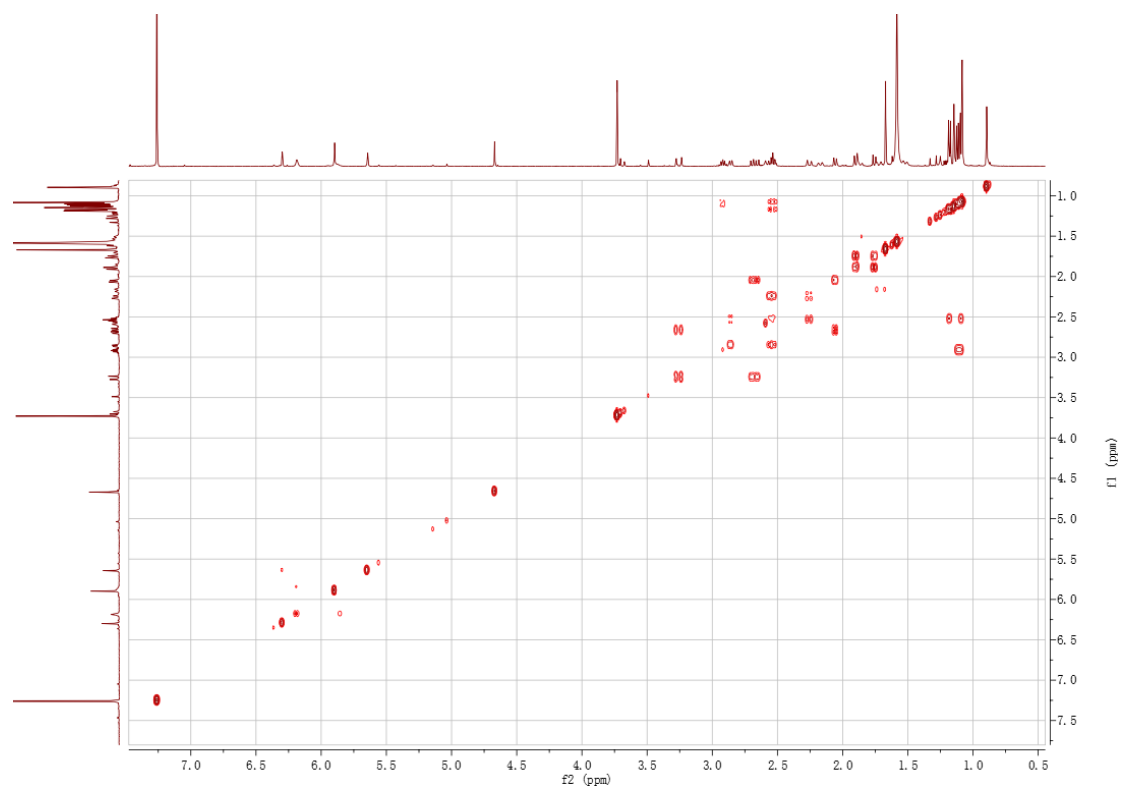


Figure S33. HMBC spectrum of compound **5** in CDCl₃

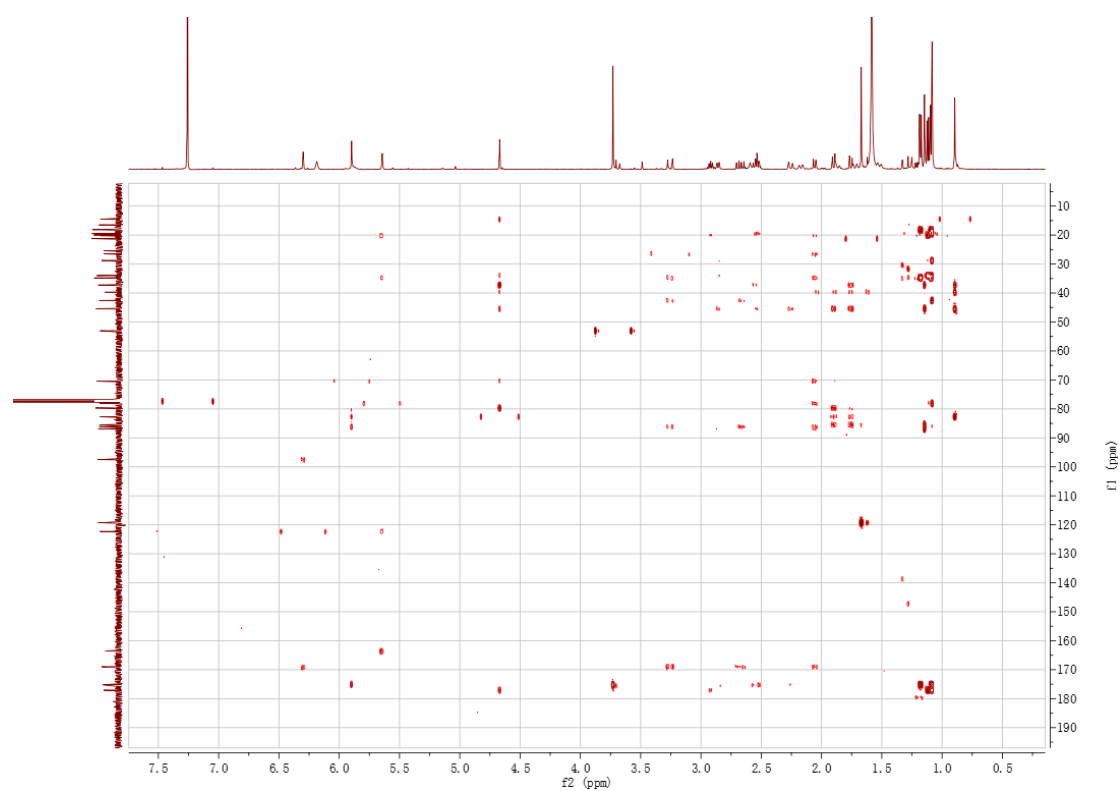


Figure S34. ROESY spectrum of compound **5** in CDCl₃

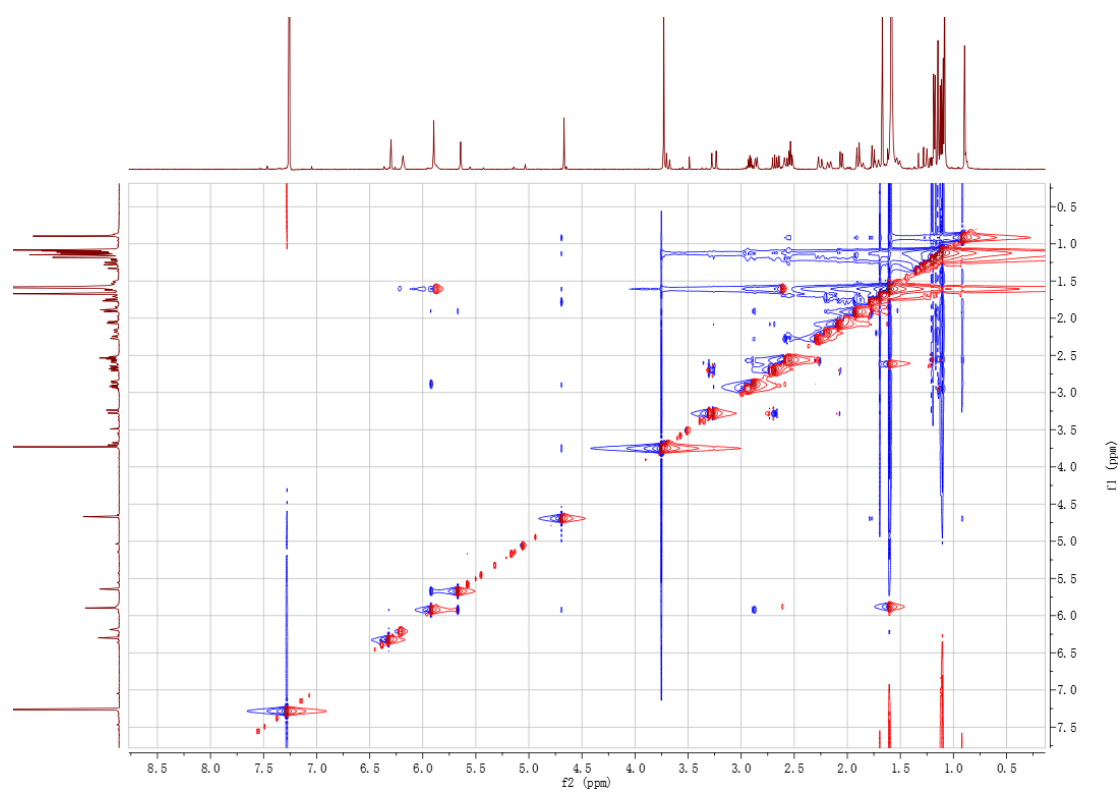
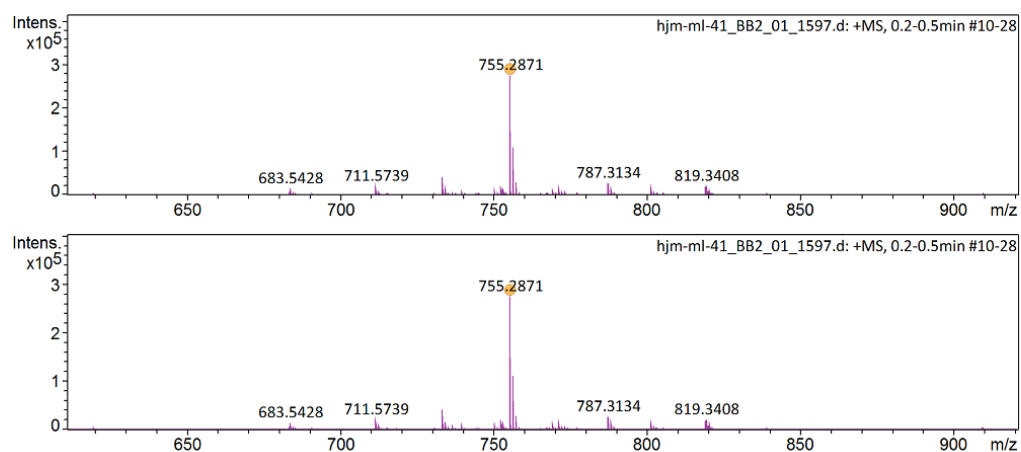


Figure S35. HRESIMS spectrum of compound 5



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
755.2871	1	C ₃₇ H ₄₈ NaO ₁₅	755.2885	2.0	7.3	1	100.00	14.0	even	ok	M+Na