Supporting Information

2-(2-Phenylethyl)chromone-Sesquiterpene Hybrids from

Agarwood of Aquilaria sinensis: Characterization and

Biological Activity Evaluation

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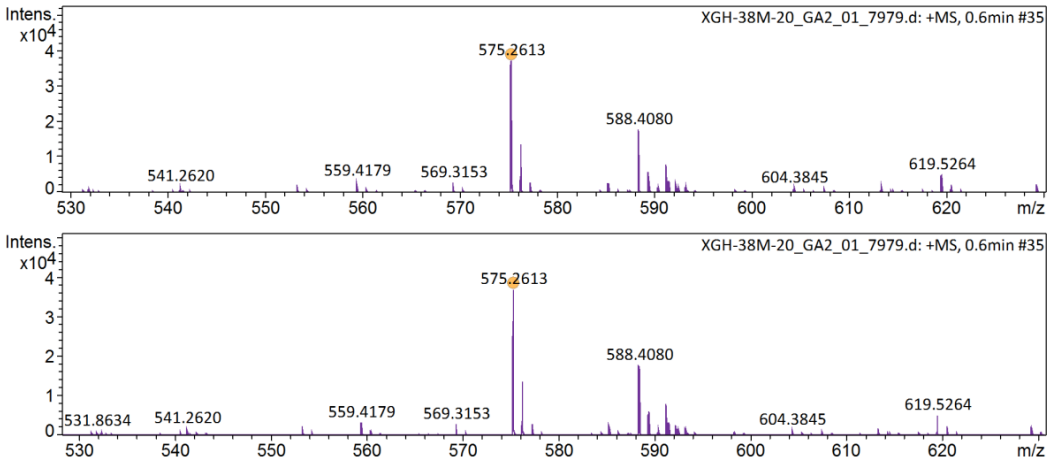
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule	Ion Formula
575.2613	1	C32H40NaO8	575.2615	0.4	6.7	1	100.00	13.0	even	ok	C32H40NaO8

Figure S1. HR-ESI-MS spectrum of compound **1**

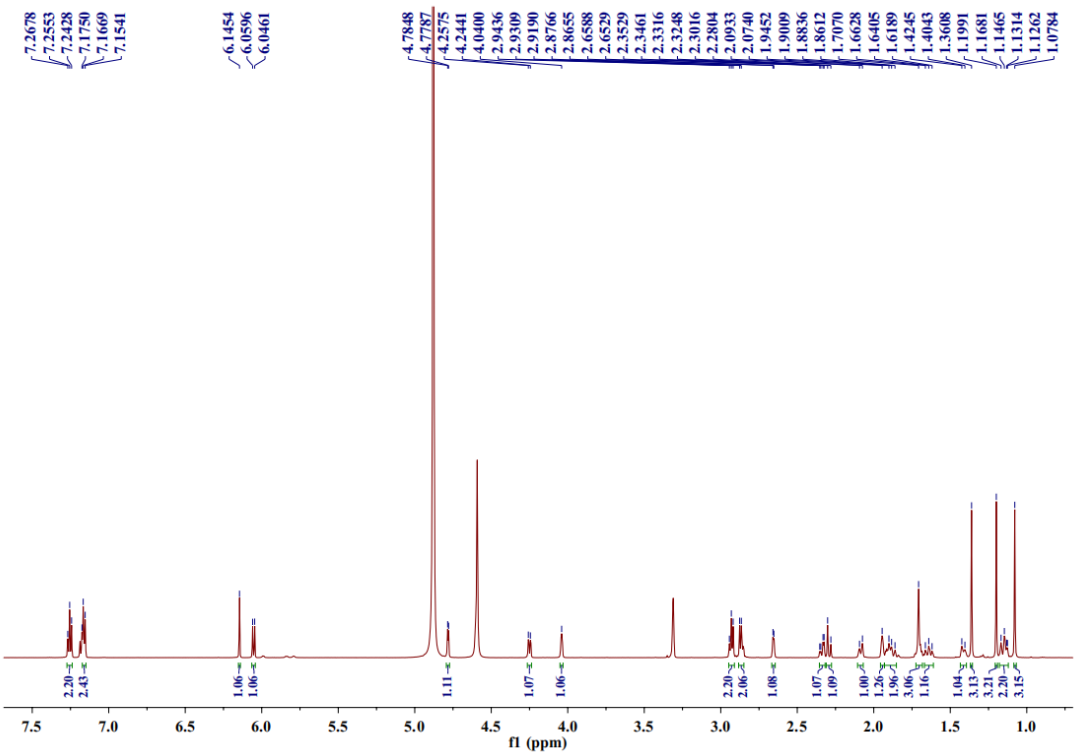


Figure S2. ^{1}H NMR spectrum of compound **1** in MeOH-d_4 (500 MHz)

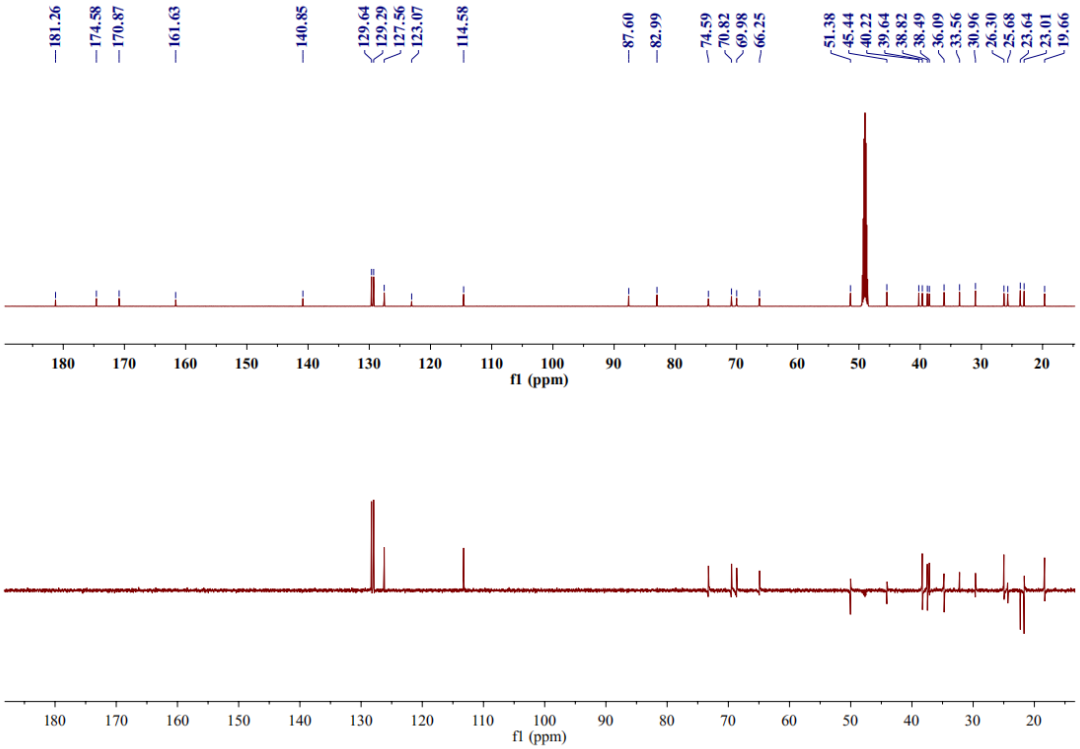


Figure S3. ^{13}C NMR and DEPT 135 spectra of compound **1** in MeOH-d_4 (125 MHz)

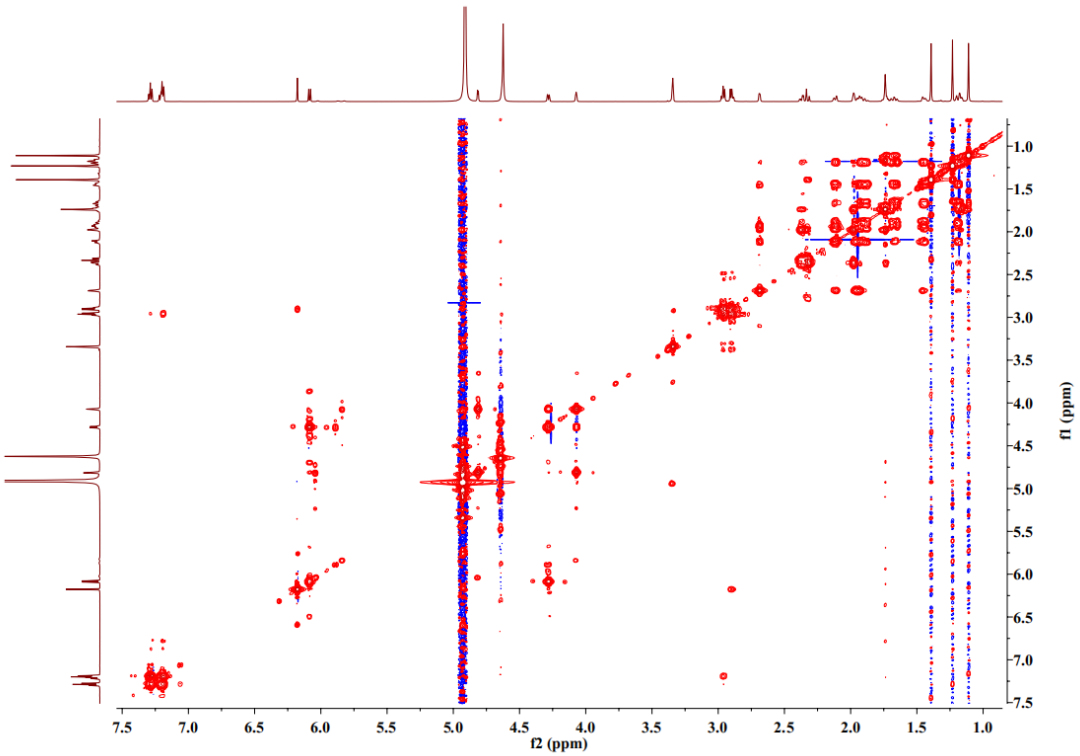


Figure S4. ^{1}H-^{1}H COSY spectrum of compound **1** in MeOH-d_4

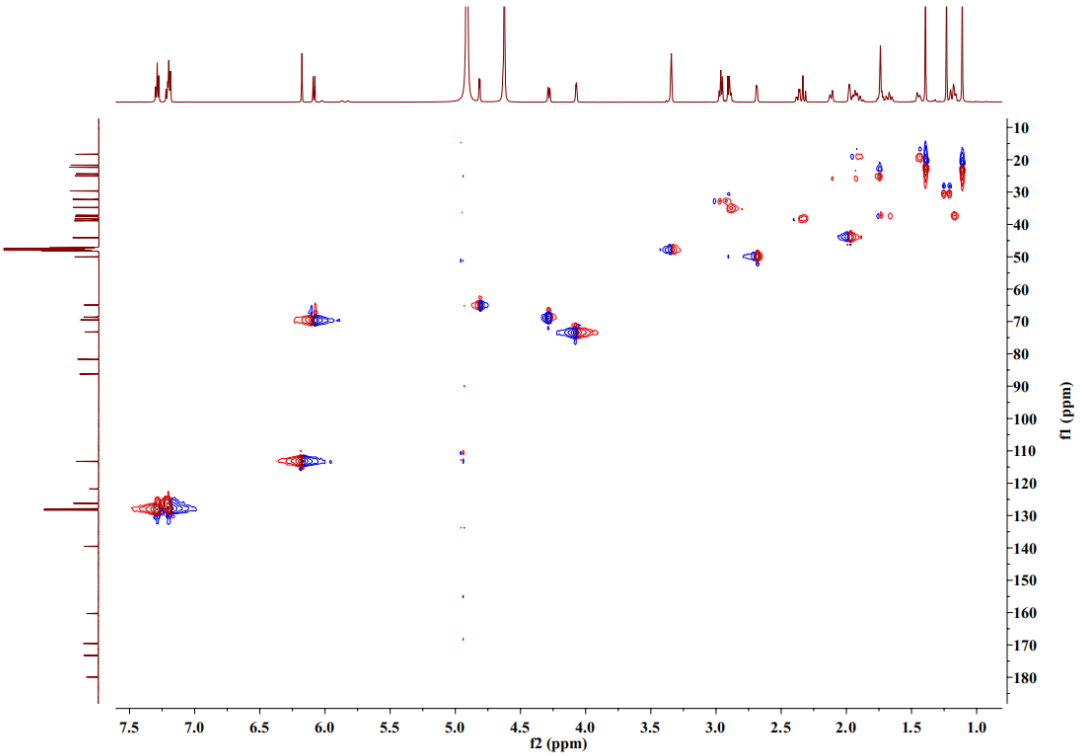


Figure S5. HSQC spectrum of compound **1** in MeOH-d_4

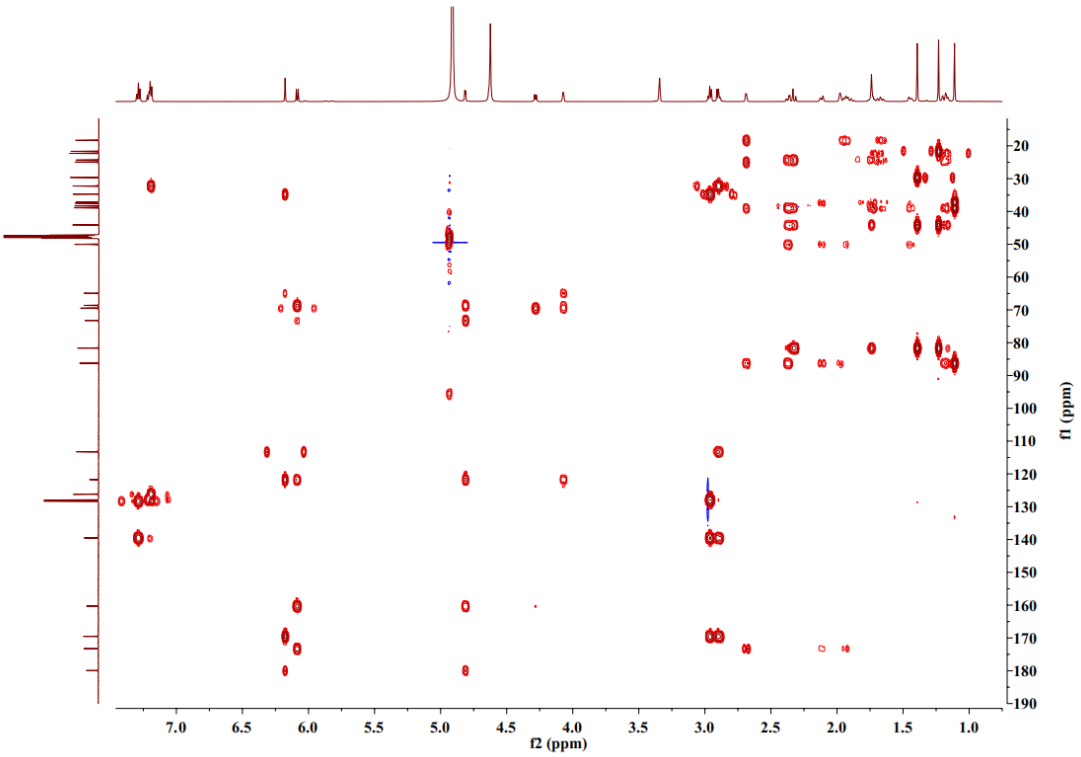


Figure S6. HMBC spectrum of compound **1** in MeOH-d_4

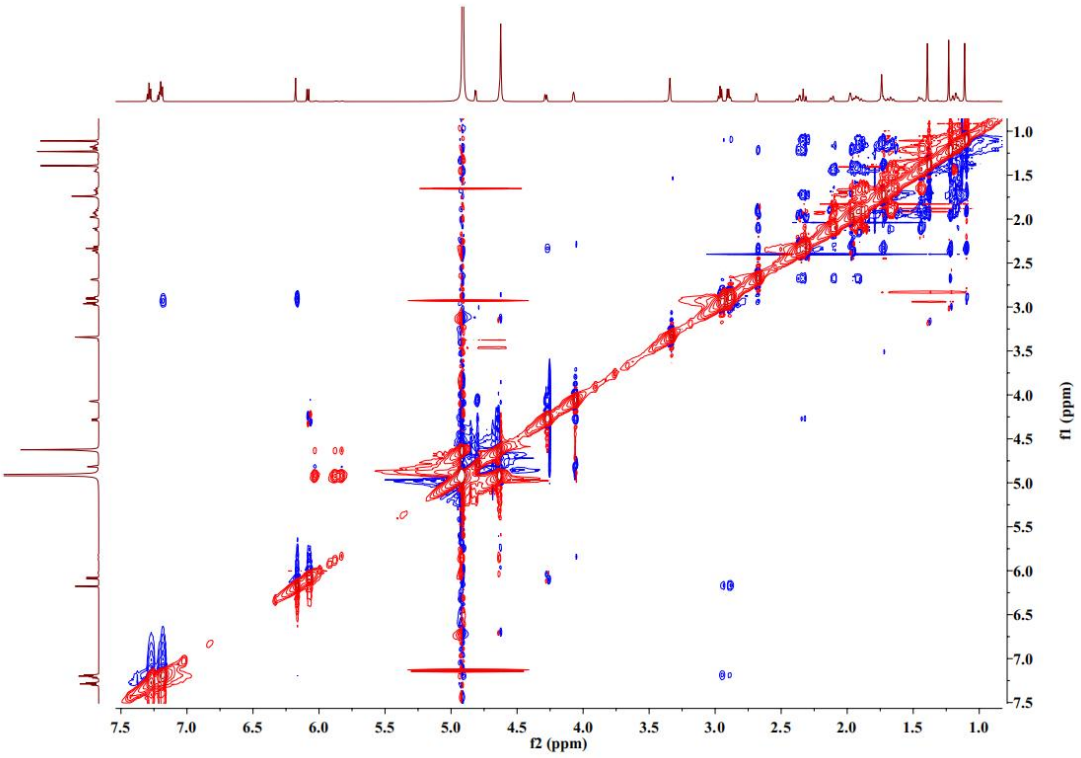
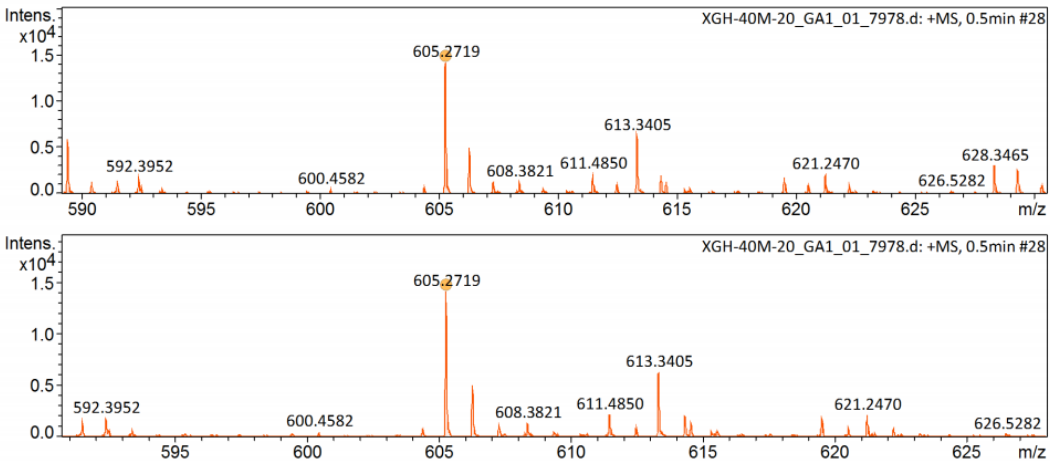


Figure S7. ROESY spectrum of compound **1** in MeOH-d_4



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule	Ion Formula
605.2719	1	C33H42NaO9	605.2721	0.3	8.5	1	100.00	13.0	even	ok	C33H42NaO9

Figure S8. HR-ESI-MS spectrum of compound **2**

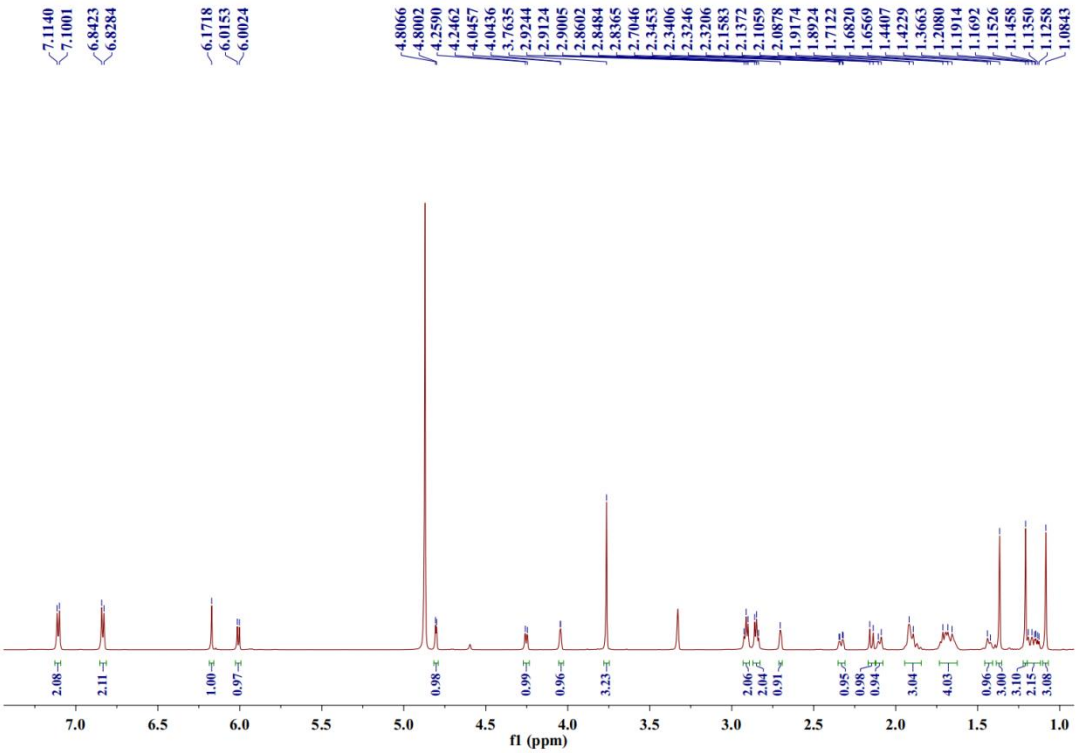


Figure S9. ^{1}H NMR spectrum of compound **2** in MeOH-d_4 (500 MHz)

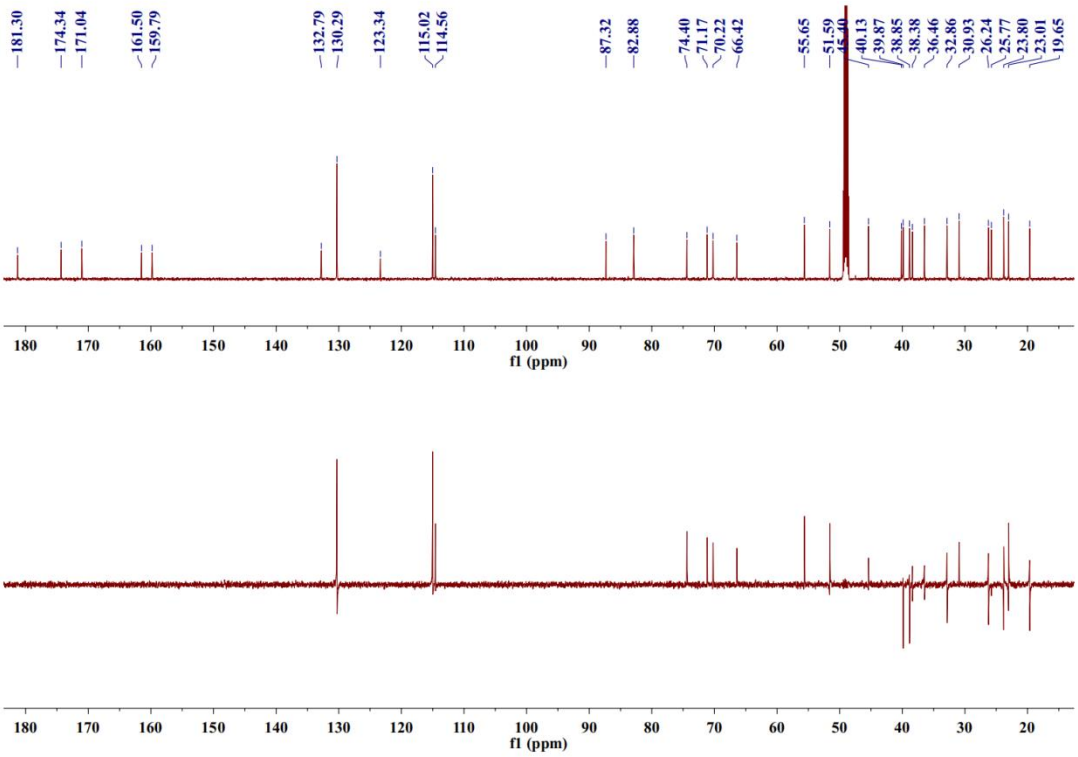


Figure S10. ^{13}C NMR and DEPT 135 spectra of compound **2** in MeOH-d_4 (125 MHz)

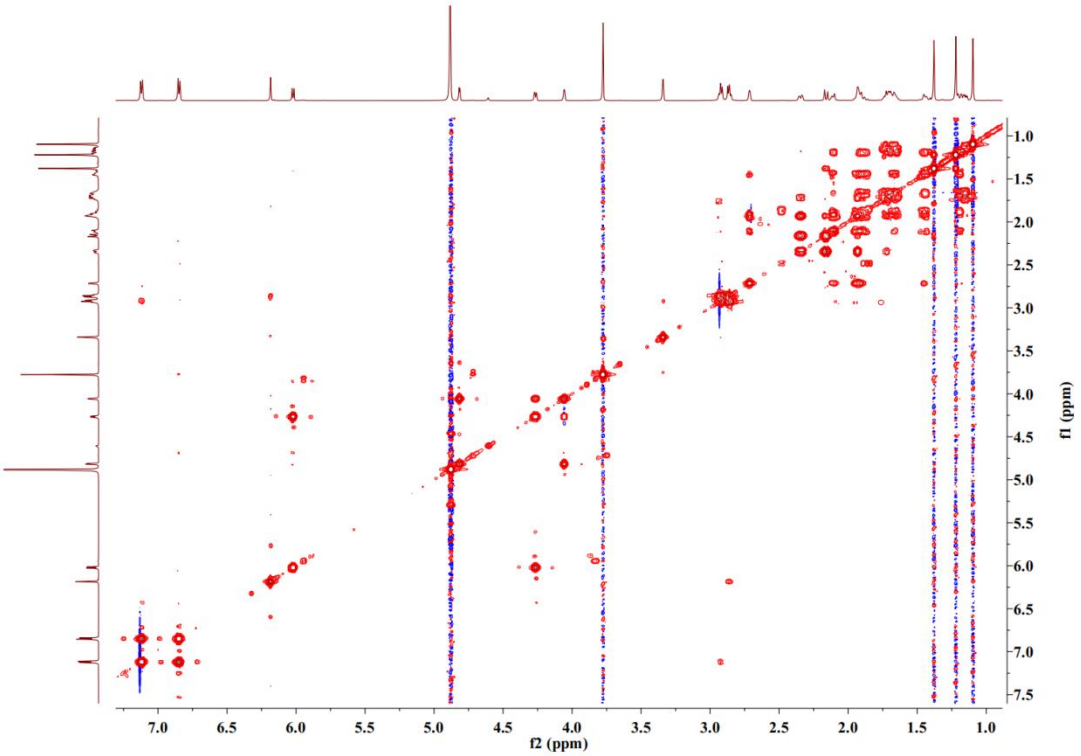


Figure S11. ^{1}H-^{1}H COSY spectrum of compound **2** in MeOH-d_4

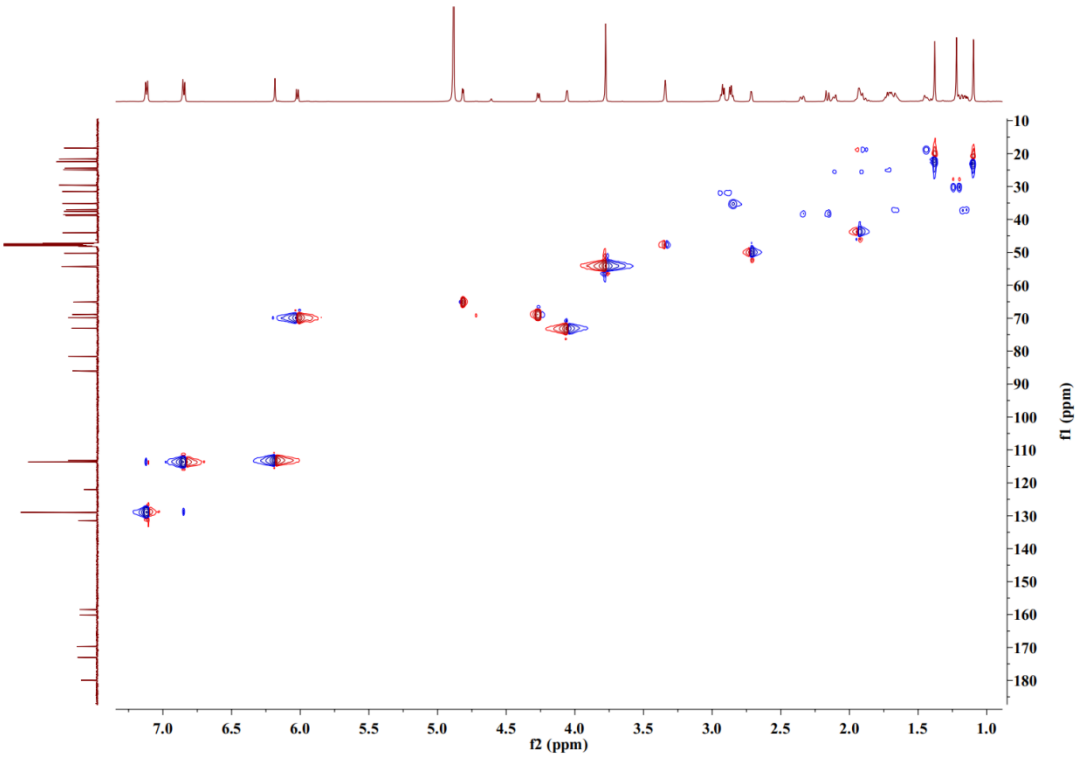


Figure S12. HSQC spectrum of compound **2** in MeOH-d_4

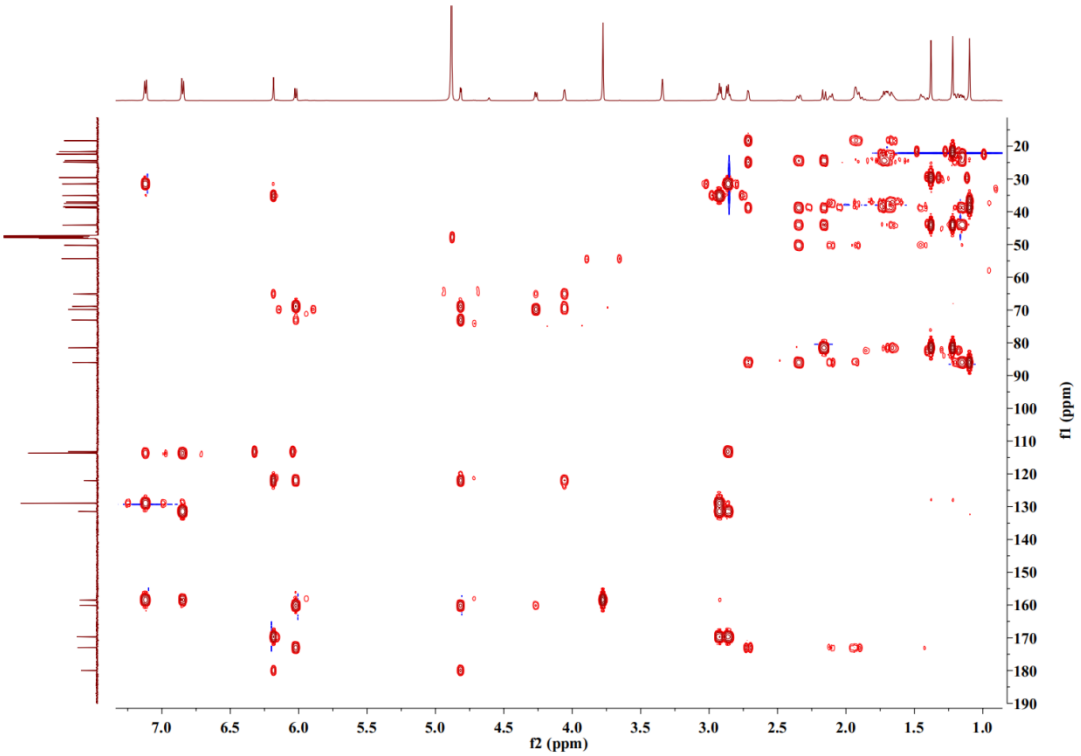


Figure S13. HMBC spectrum of compound **2** in MeOH-d_4

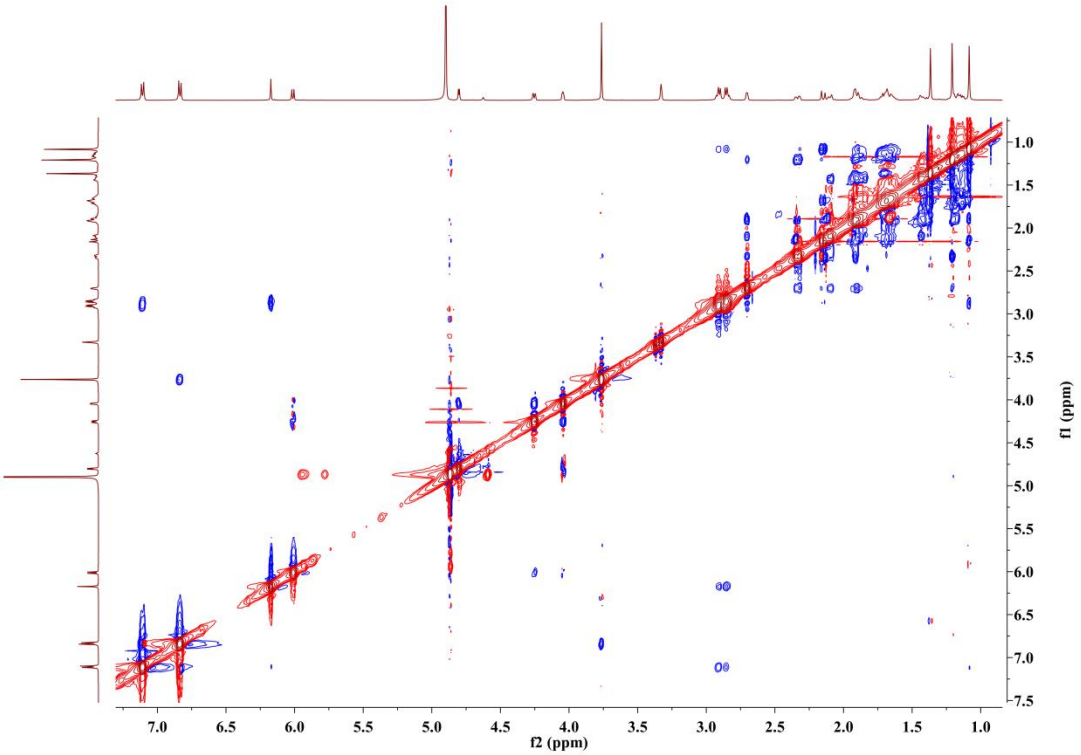
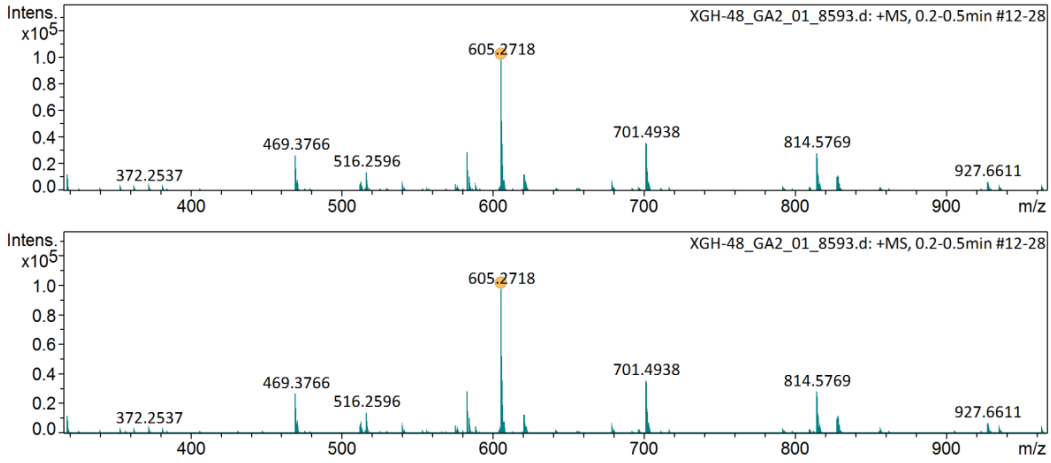


Figure S14. ROESY spectrum of compound **2** in MeOH-d_4



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule	Ion Formula
605.2718	1	C33H42NaO9	605.2721	0.4	3.2	1	100.00	13.0	even	ok	C33H42NaO9

Figure S15. HR-ESI-MS spectrum of compound 3

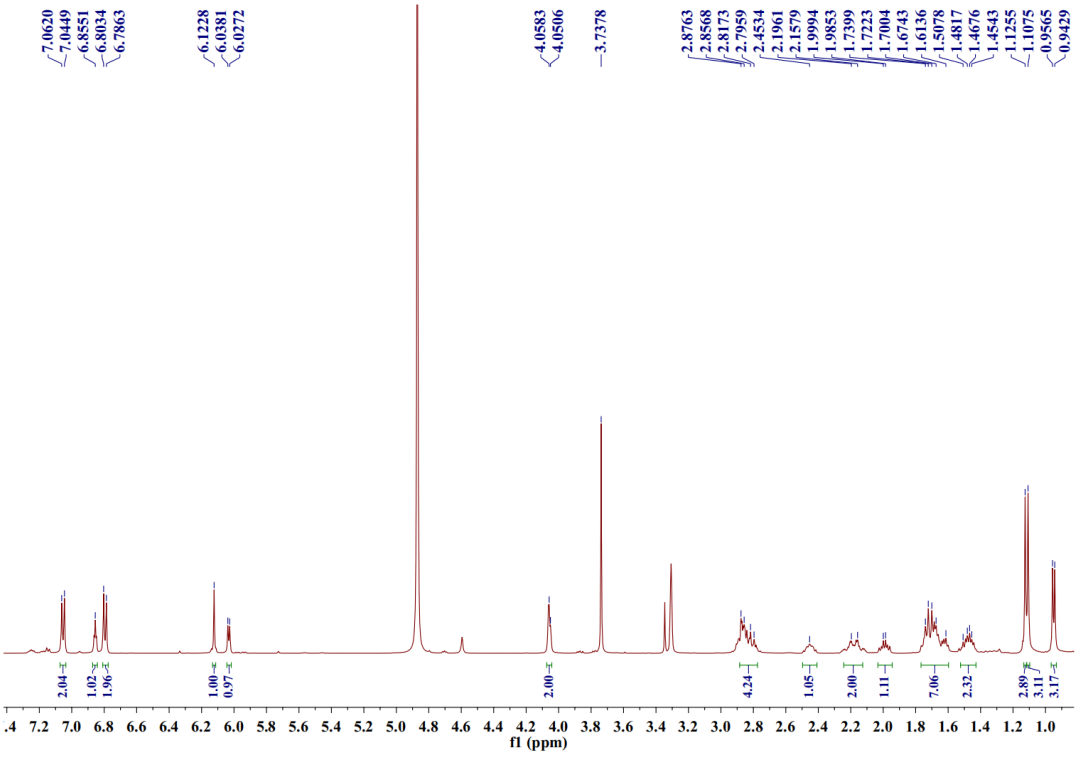


Figure S16. ^{1}H NMR spectrum of compound **3** in MeOH-d_4 (600 MHz)

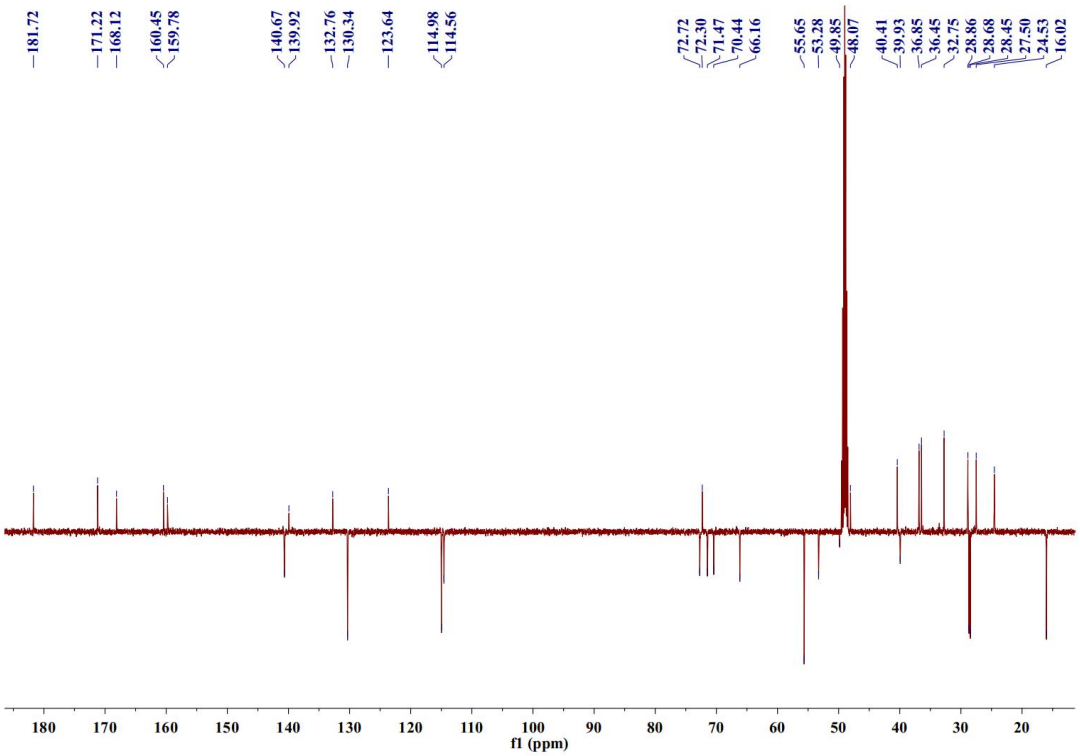


Figure S17. DEPT 135 spectra of compound **3** in MeOH-d_4 (125 MHz)

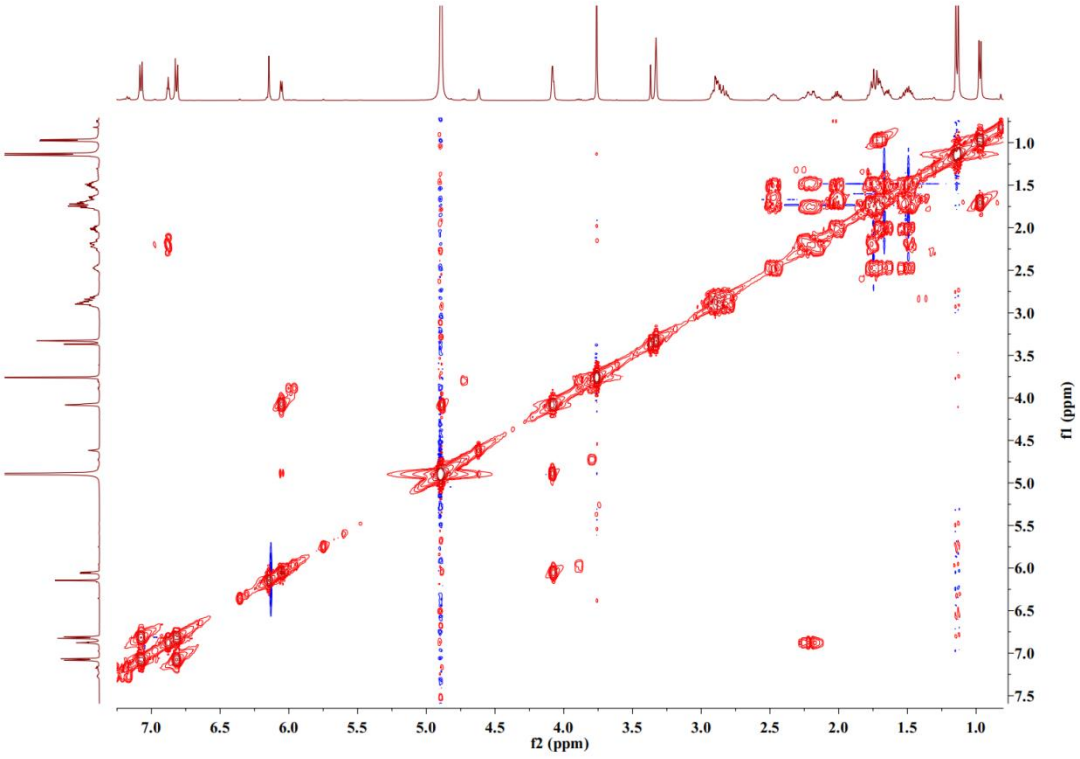


Figure S18. ^{1}H-^{1}H COSY spectrum of compound **3** in MeOH-d_4

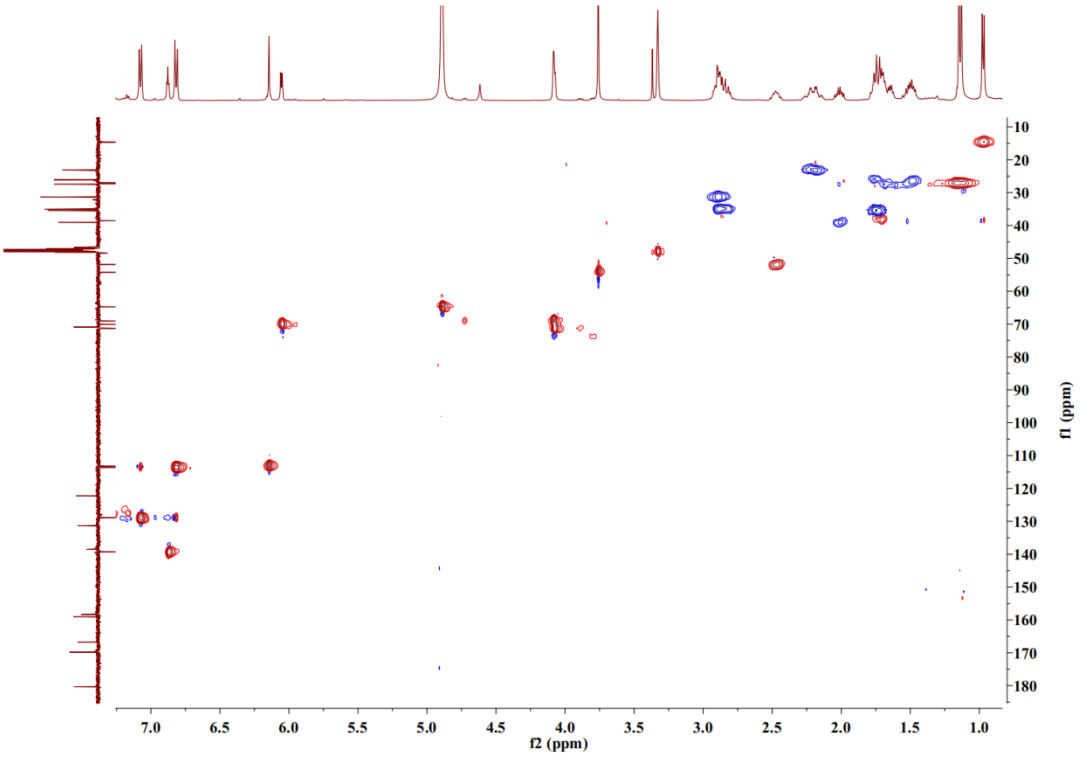


Figure S19. HSQC spectrum of compound **3** in MeOH-d_4

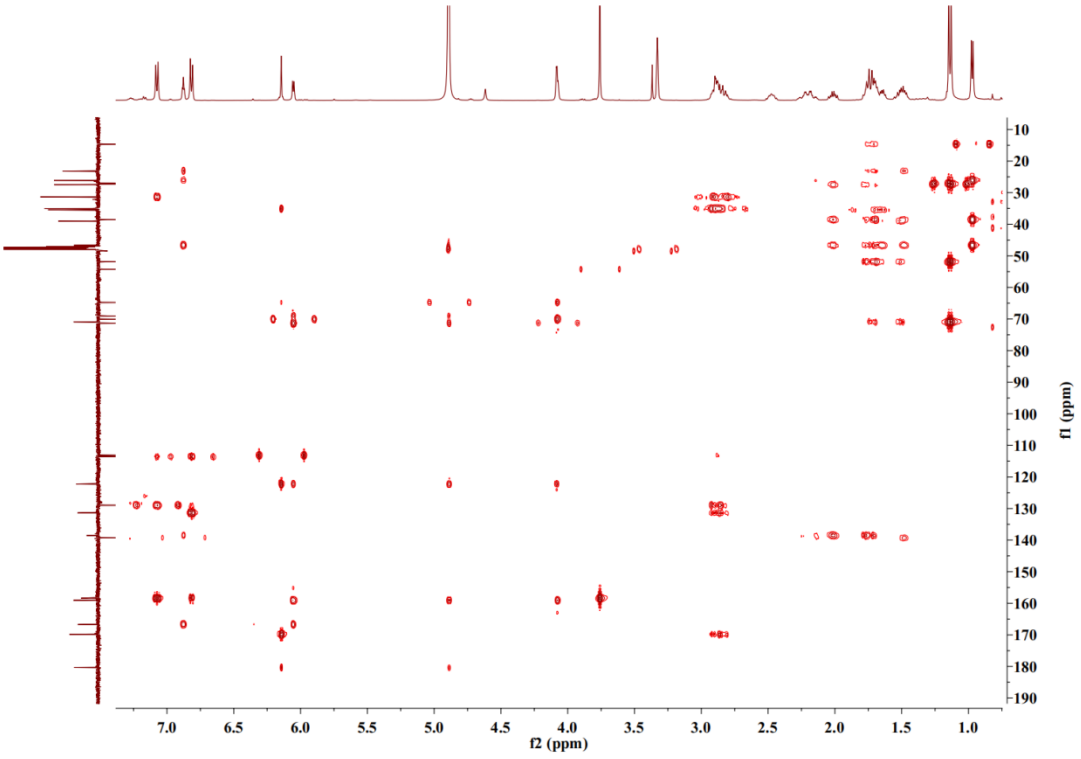


Figure S20. HMBC spectrum of compound **3** in MeOH-d_4

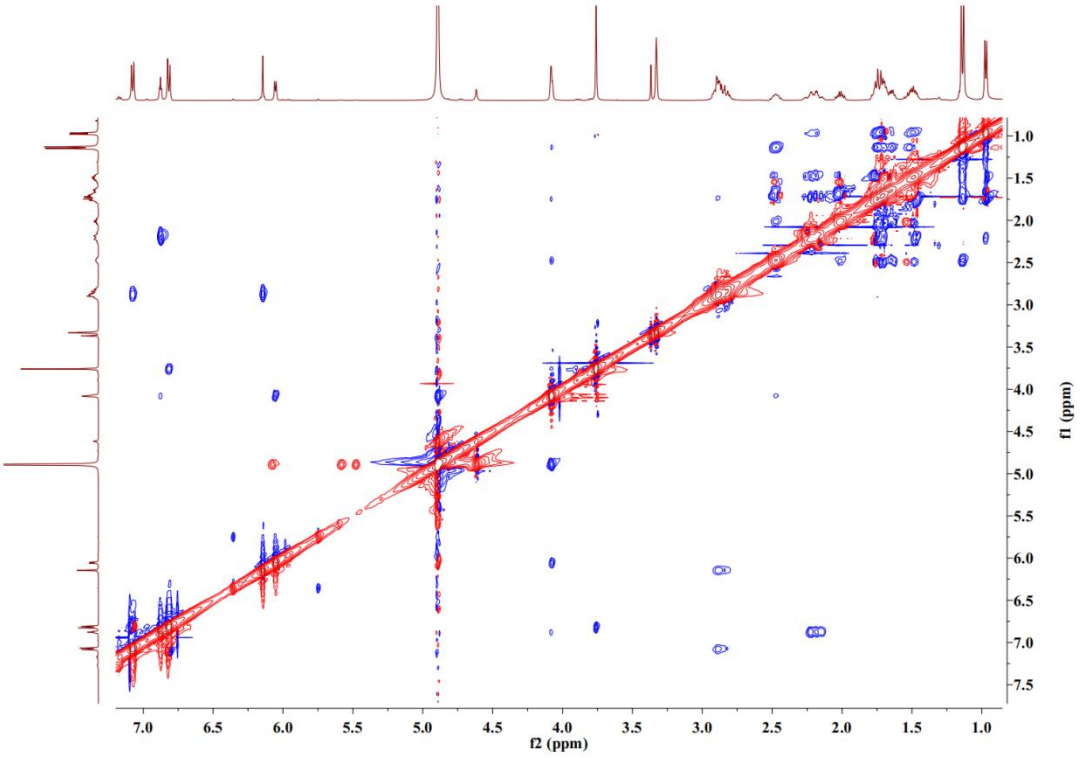


Figure S21. ROESY spectrum of compound **3** in MeOH-d_4

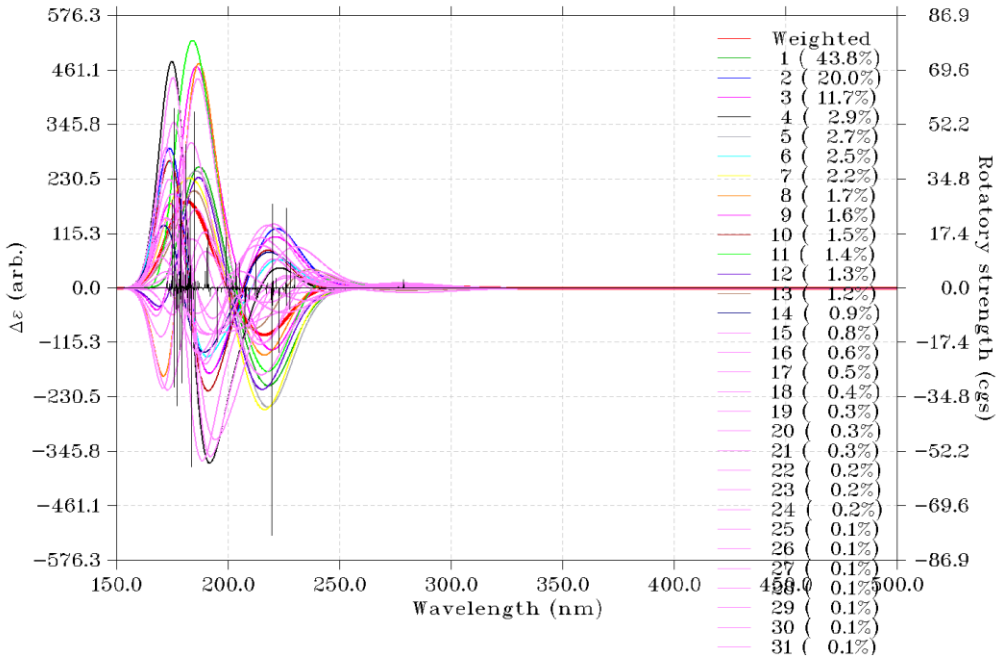


Figure S22. ECD calculation image-1 of compound **1**

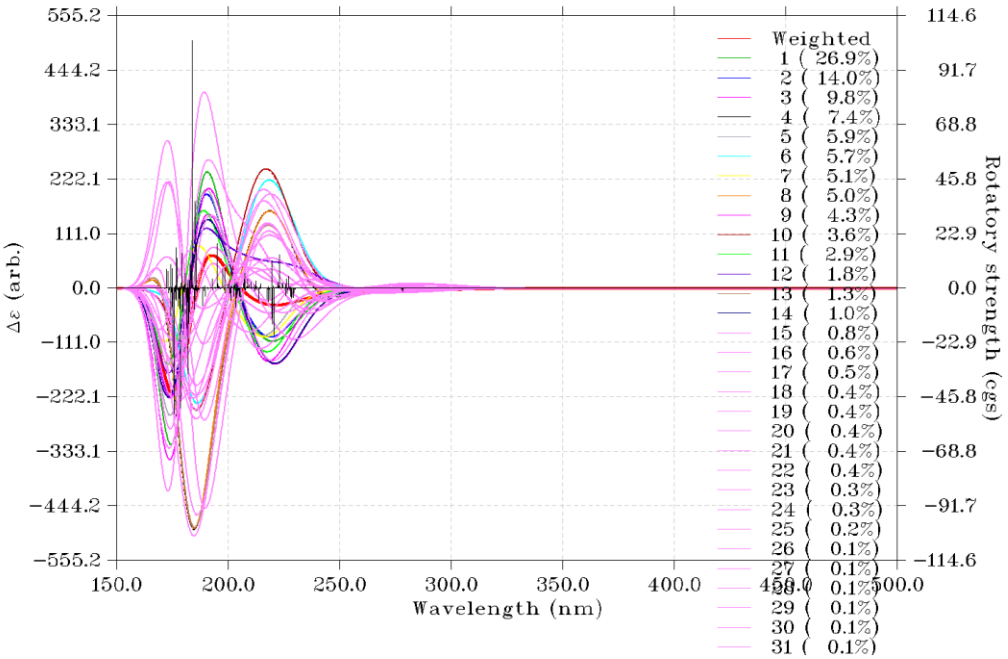


Figure S23. ECD calculation image-2 of compound **1**

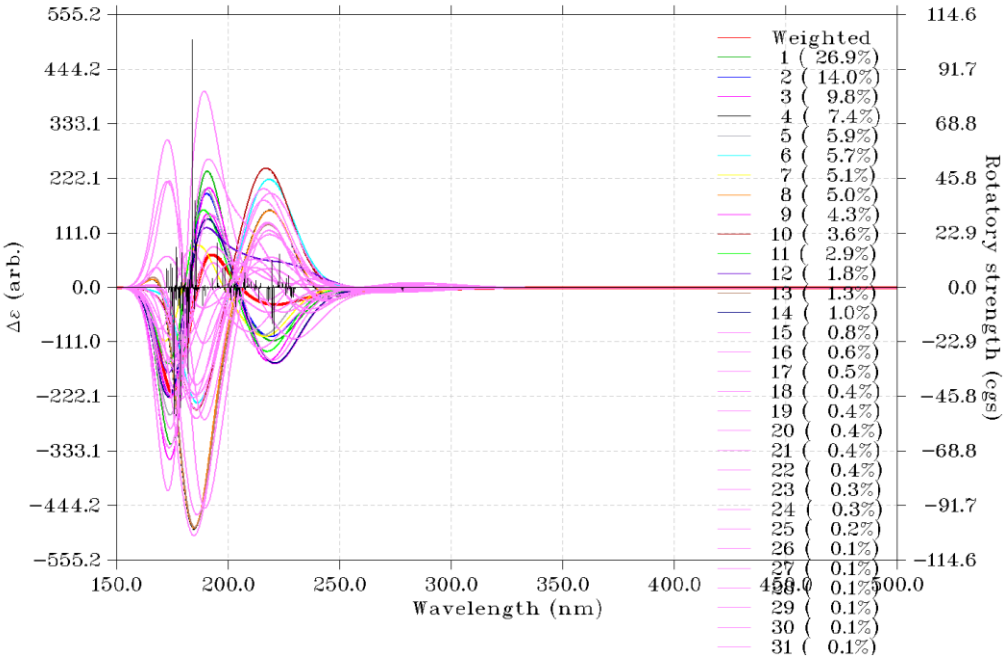


Figure S24. ECD calculation image-1 of compound **2**

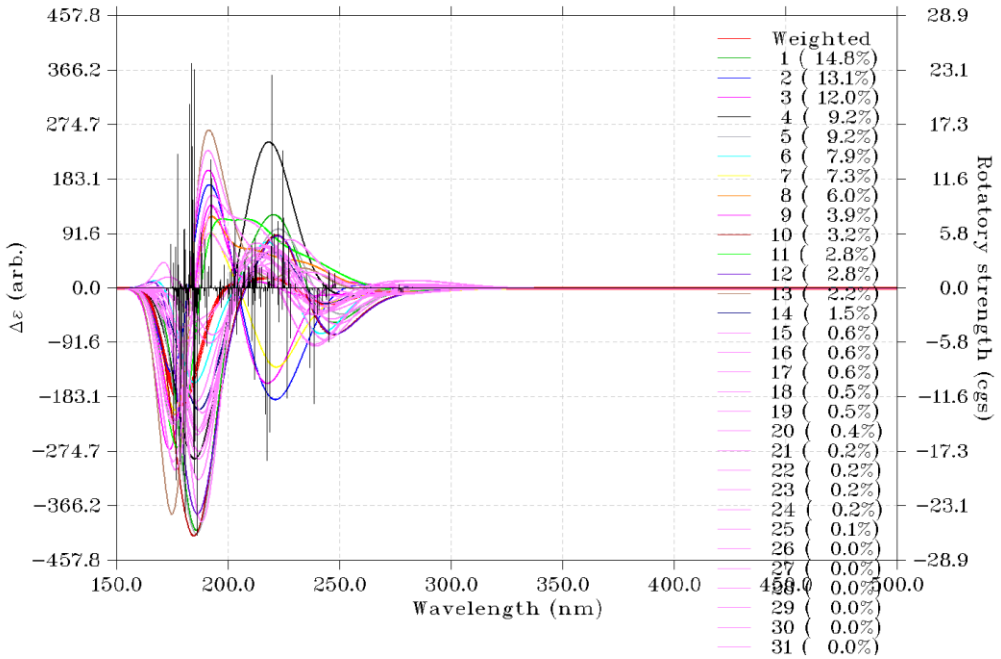


Figure S25. ECD calculation image-2 of compound **2**

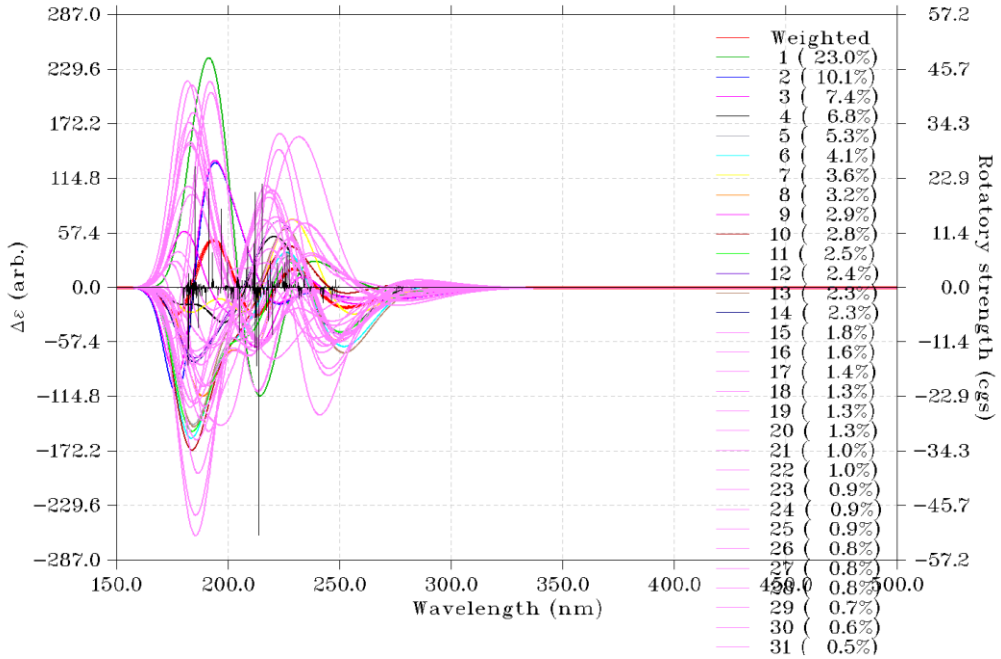


Figure S26. ECD calculation image-1 of compound **3**

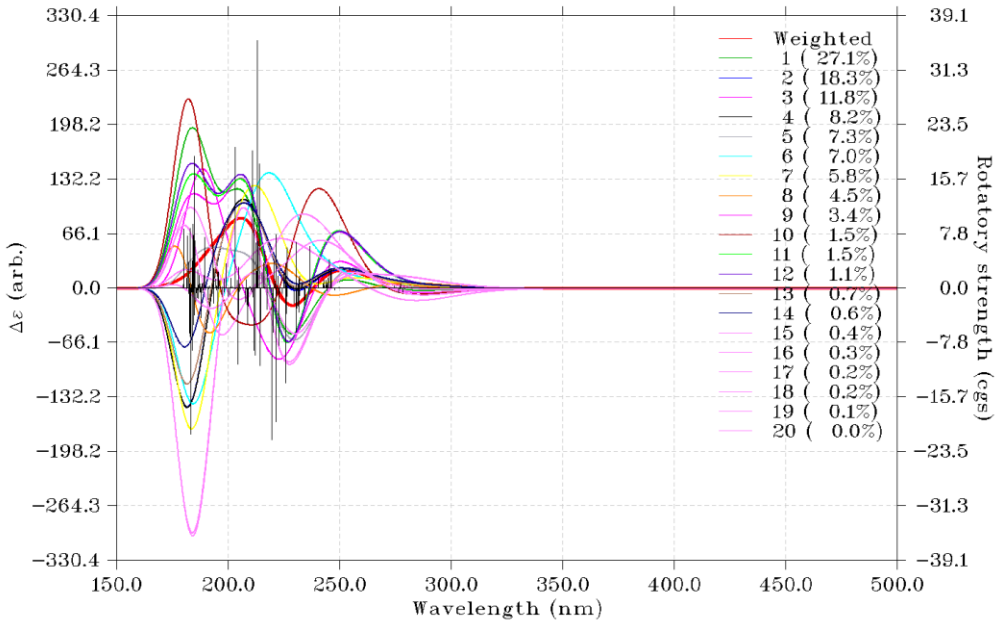


Figure S27. ECD calculation image-2 of compound **3**