

Supporting Information

Sesquiterpene lactones with anti-inflammatory activity from the Halophyte *Sonchus brachyotus* DC

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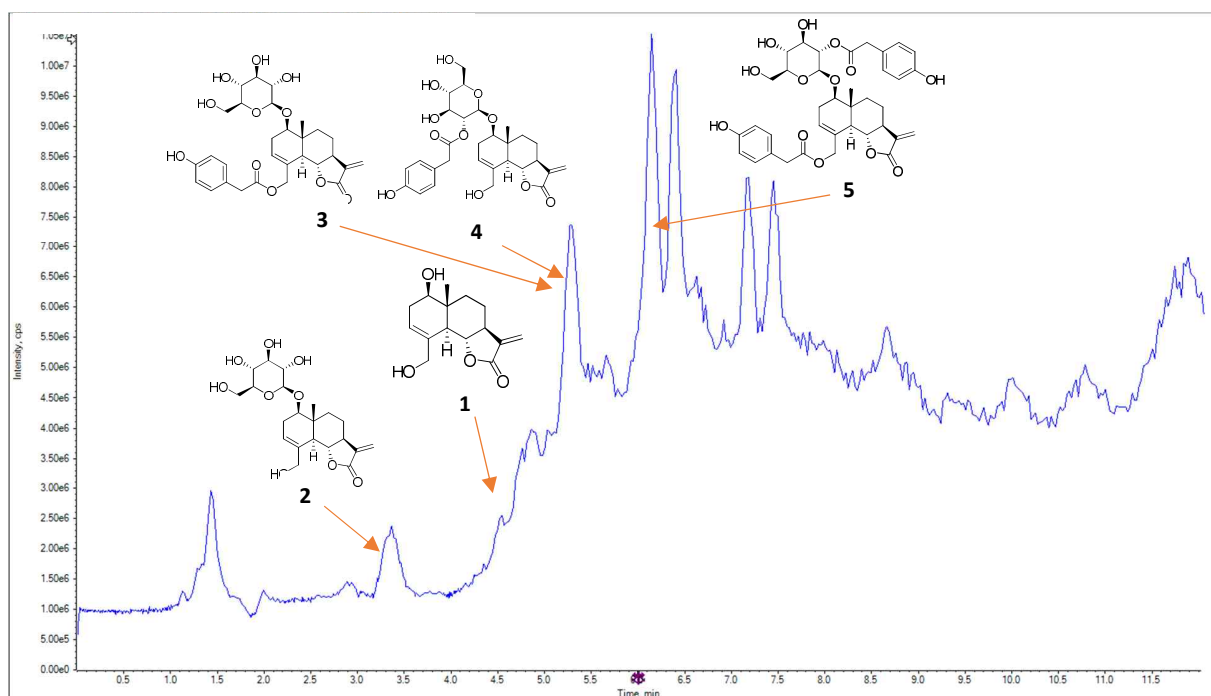
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Positive LC-MS chromatography with an AB X500R qTOF mass spectrometer

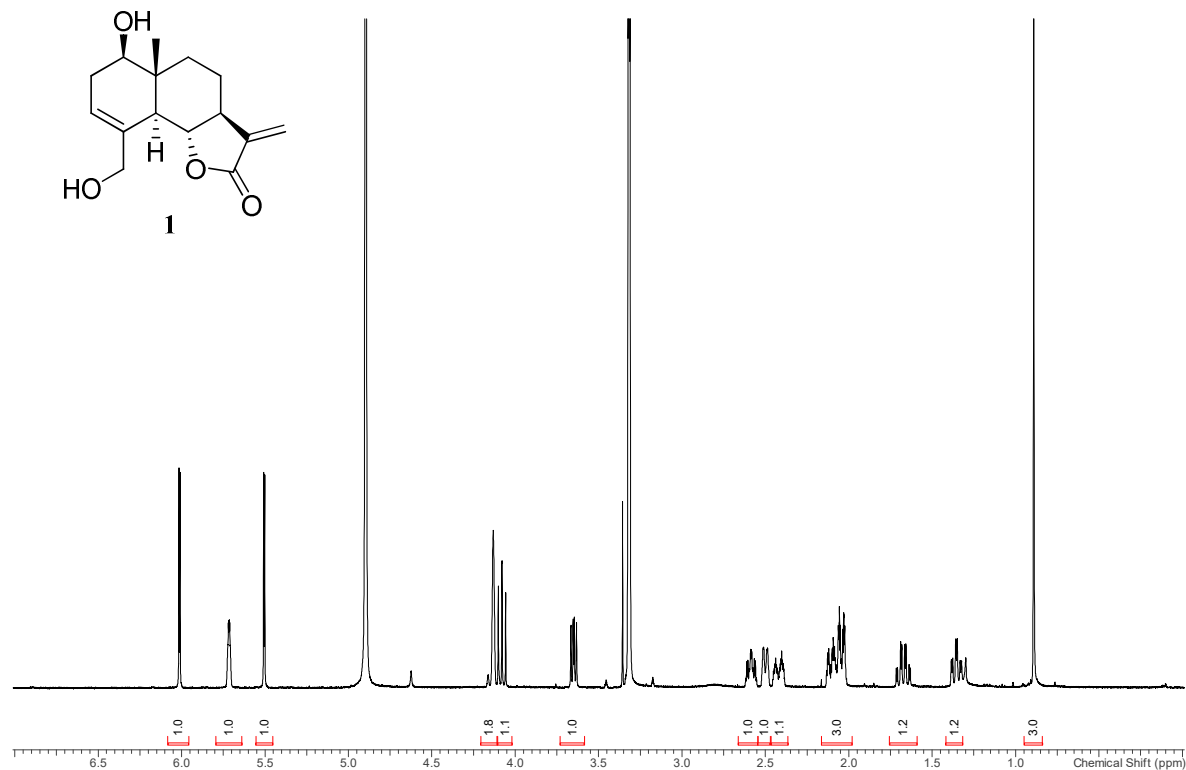
- Solvents : A - H₂O with 0.1 % formic acid, B - acetonitrile (0–12 min, 10–75% B)
- Column : Synergy Fusion-RP (50 × 2.0 mm)
- Flow rate : 0.3 mL/min

Figure S1. Fingerprint of the BuOH fraction of *S. brachyotus*.

Table S1. ^1H (500 MHz) and ^{13}C (125 MHz) data for compound **2** in CD_3OD .
(δ in ppm, J values in parenthesis)

no	δ_{C}	δ_{H} , mult(J Hz)
1	80.9, CH	3.90, dd(9.5, 6.4)
2	30.0, CH_2	α : 2.60, m β : 2.14, m
3	123.1, CH	5.75, br s
4	137.7, C	
5	50.7, CH	2.56, m
6	83.0, CH	4.08, t(11.0)
7	52.0, CH	2.58, m
8	22.2, CH_2	α : 2.09, br d(12.3) β : 1.64, qd(12.3, 3.4)
9	35.6, CH_2	α : 1.47, td(13.7, 1.5) β : 2.15, m
10	41.2, C	
11	140.9, C	
12	172.5, C	
13	117.2, CH_2	5.50, d(3.2); 6.01, d(3.2)
14	12.3, CH_3	0.95, s
15	65.3, CH_2	4.12, d(15.2); 4.16, d(15.2)
1'	101.4, CH	4.35, d(7.8)
2'	75.1, CH	3.16, dd(9.1, 7.8)
3'	78.2, CH	3.34, dd(9.1, 9.5)
4'	71.9, CH	3.26, t(9.5)
5'	78.0, CH	3.24, ddd(9.5, 5.6, 1.2)
6'	63.0, CH_2	3.66, dd(11.7, 5.6)); 3.86, dd(11.7, 1.2)

(A)



(B)

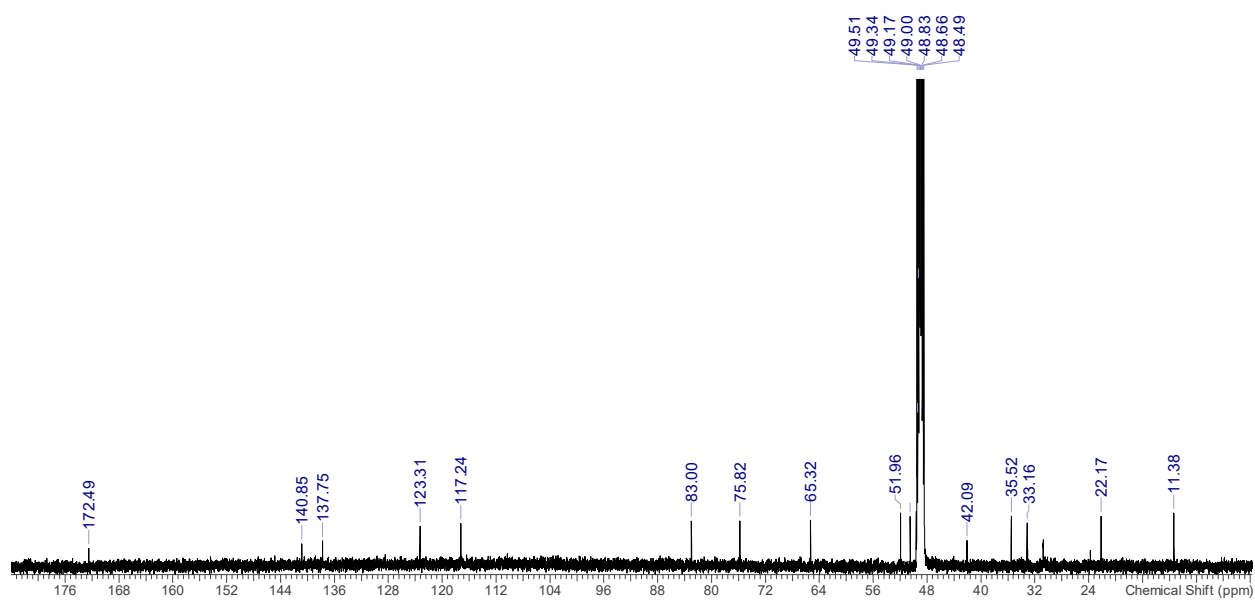


Figure S2. (A) ¹H (500 MHz) and (B) ¹³C NMR (125 MHz) spectra of compound 1 in CD₃OD.

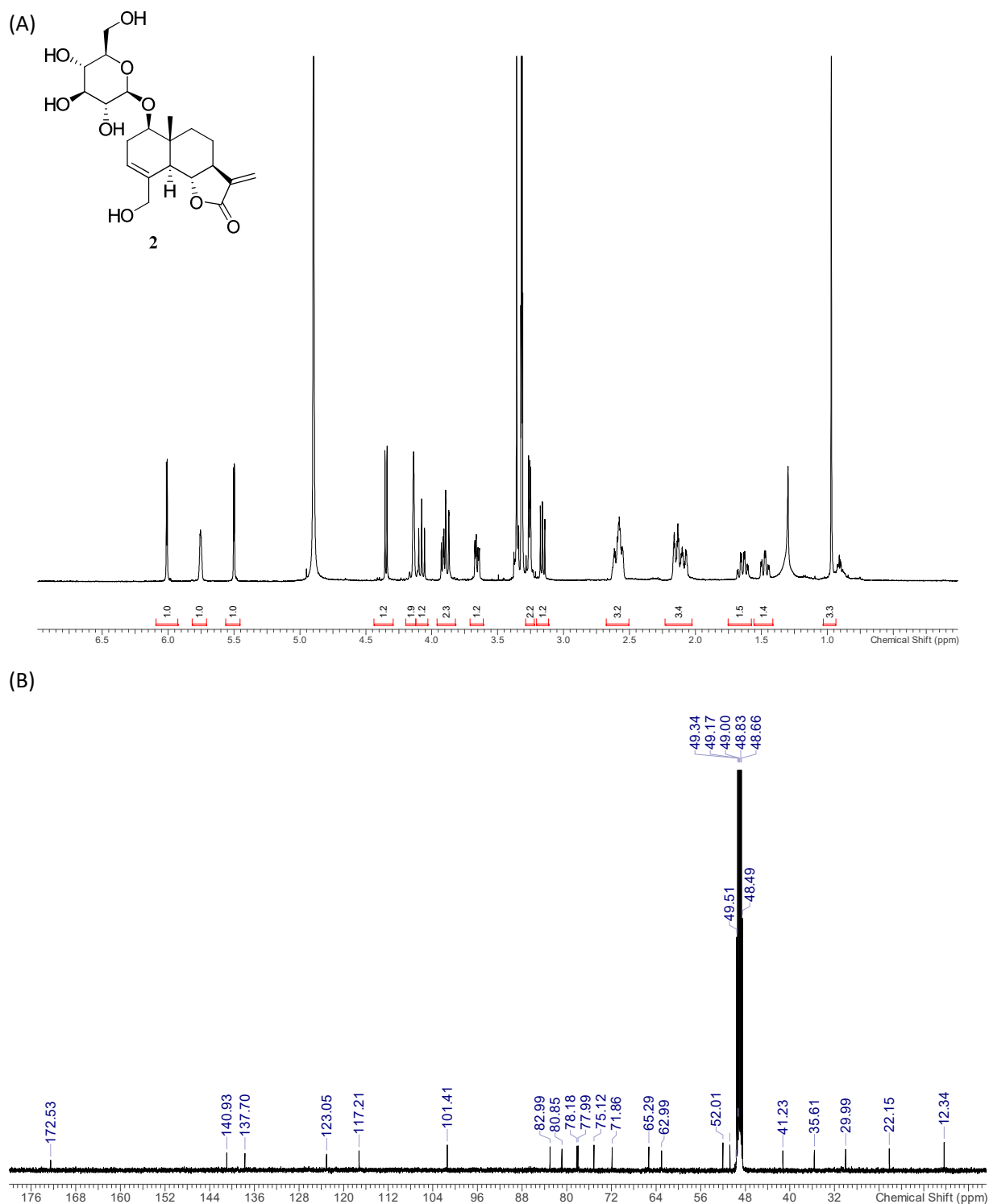


Figure S3. (A) ^1H (500 MHz) and (B) ^{13}C NMR (125 MHz) spectra of compound **2** in CD₃OD.

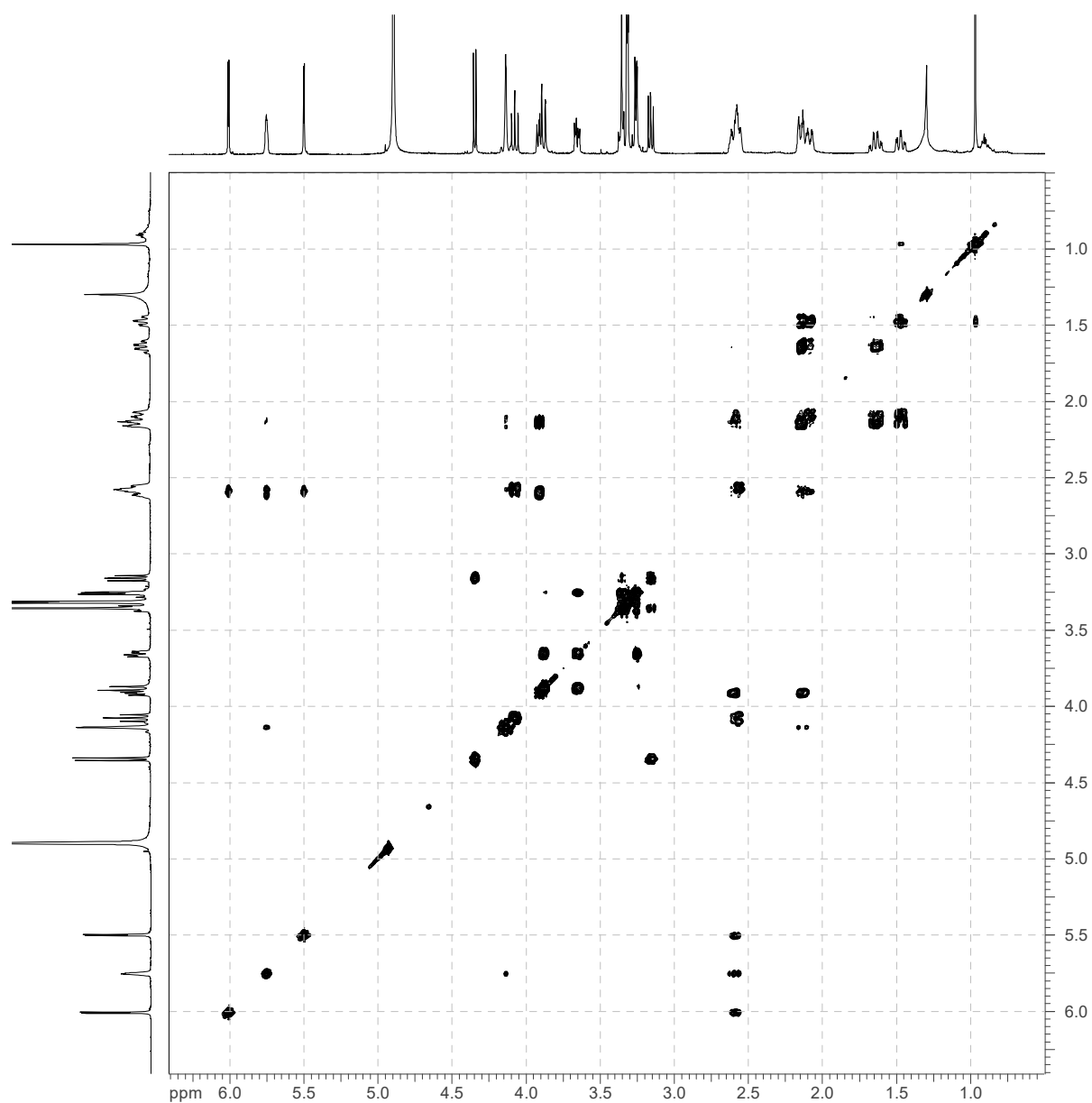


Figure S4. COSY spectrum (500 MHz) of compound **2** in CD₃OD.

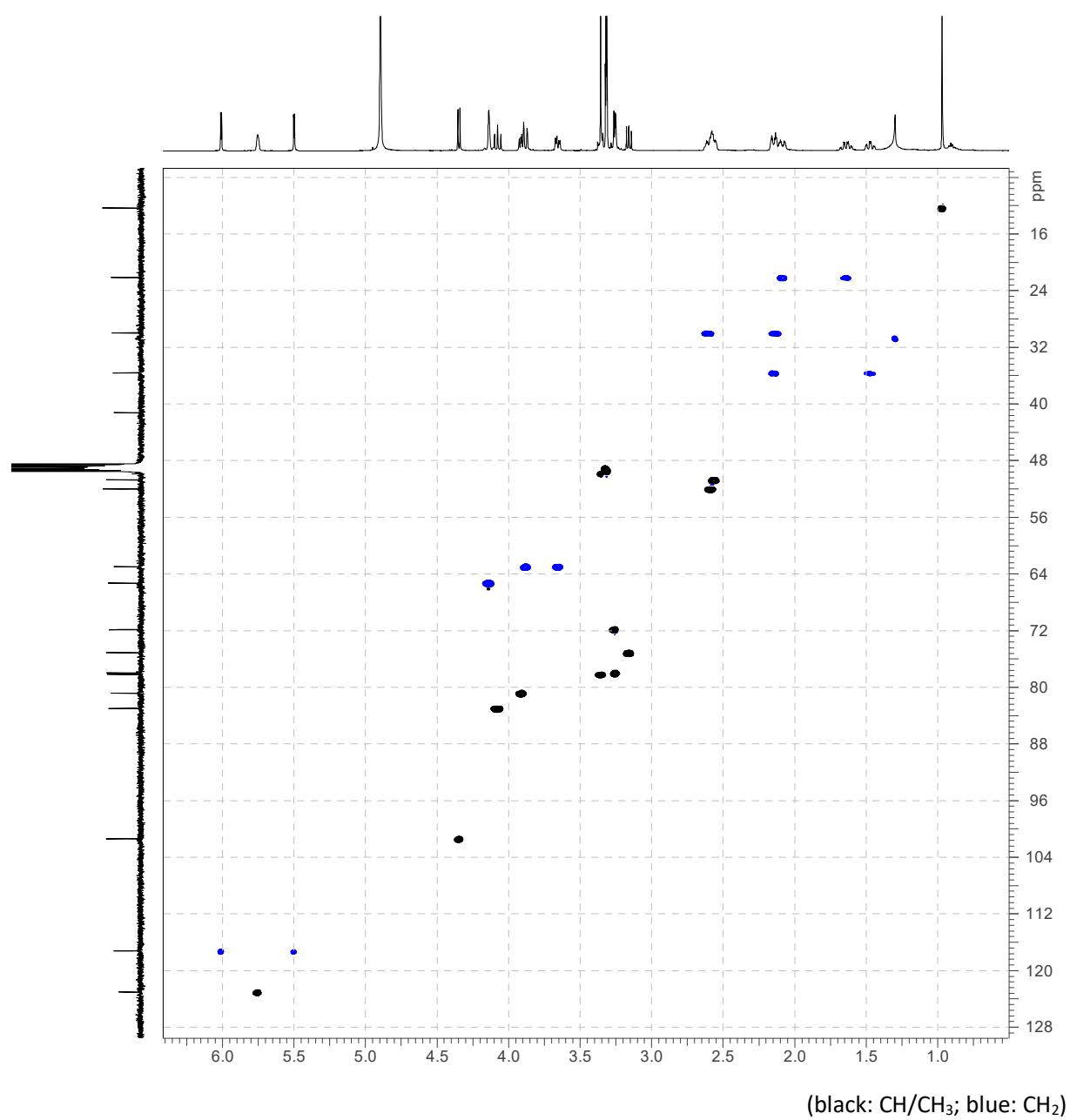


Figure S5. HSQC spectrum (500 MHz) of compound 2 in CD₃OD.

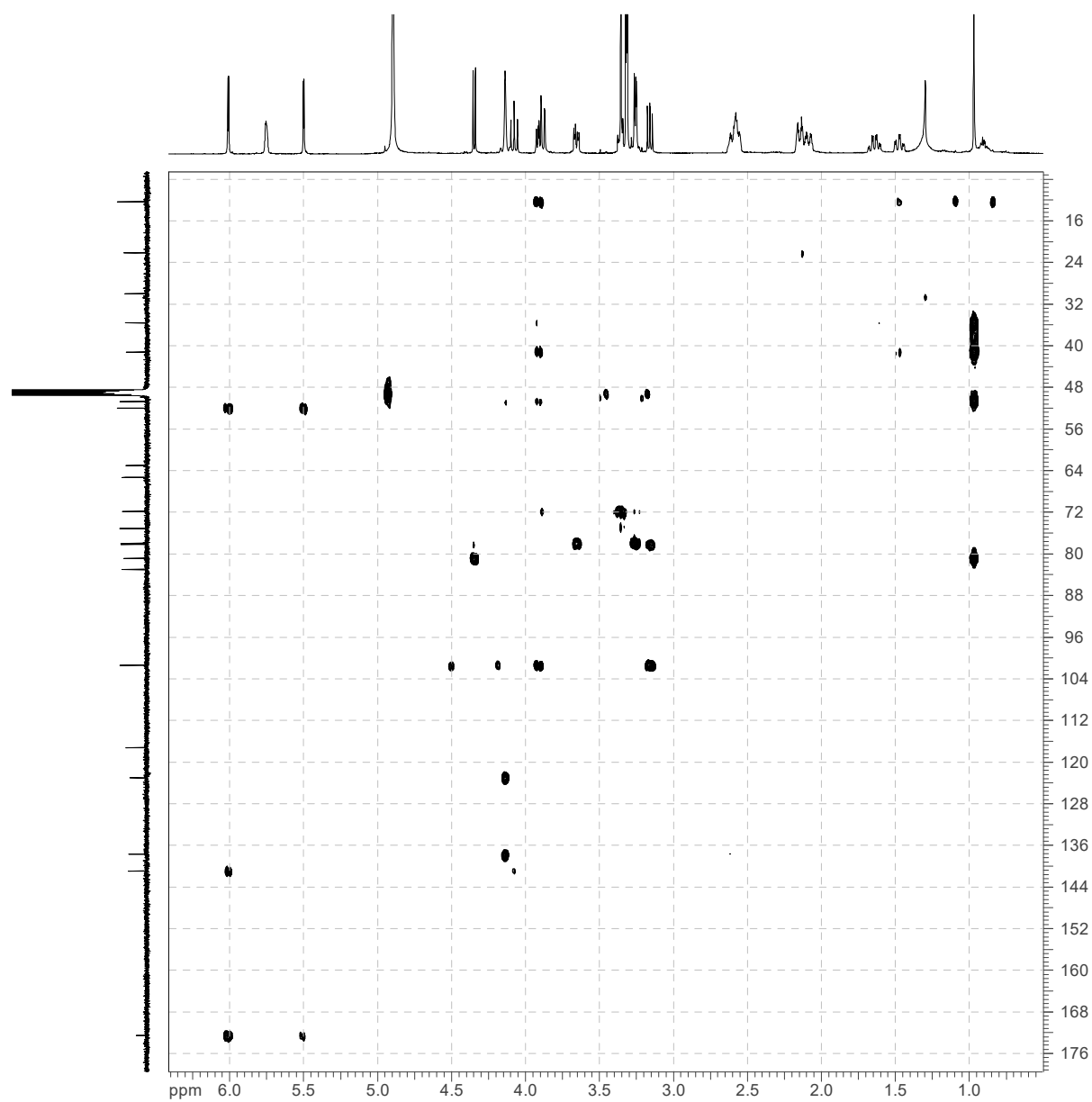


Figure S6. HMBC spectrum (500 MHz) of compound **2** in CD₃OD.

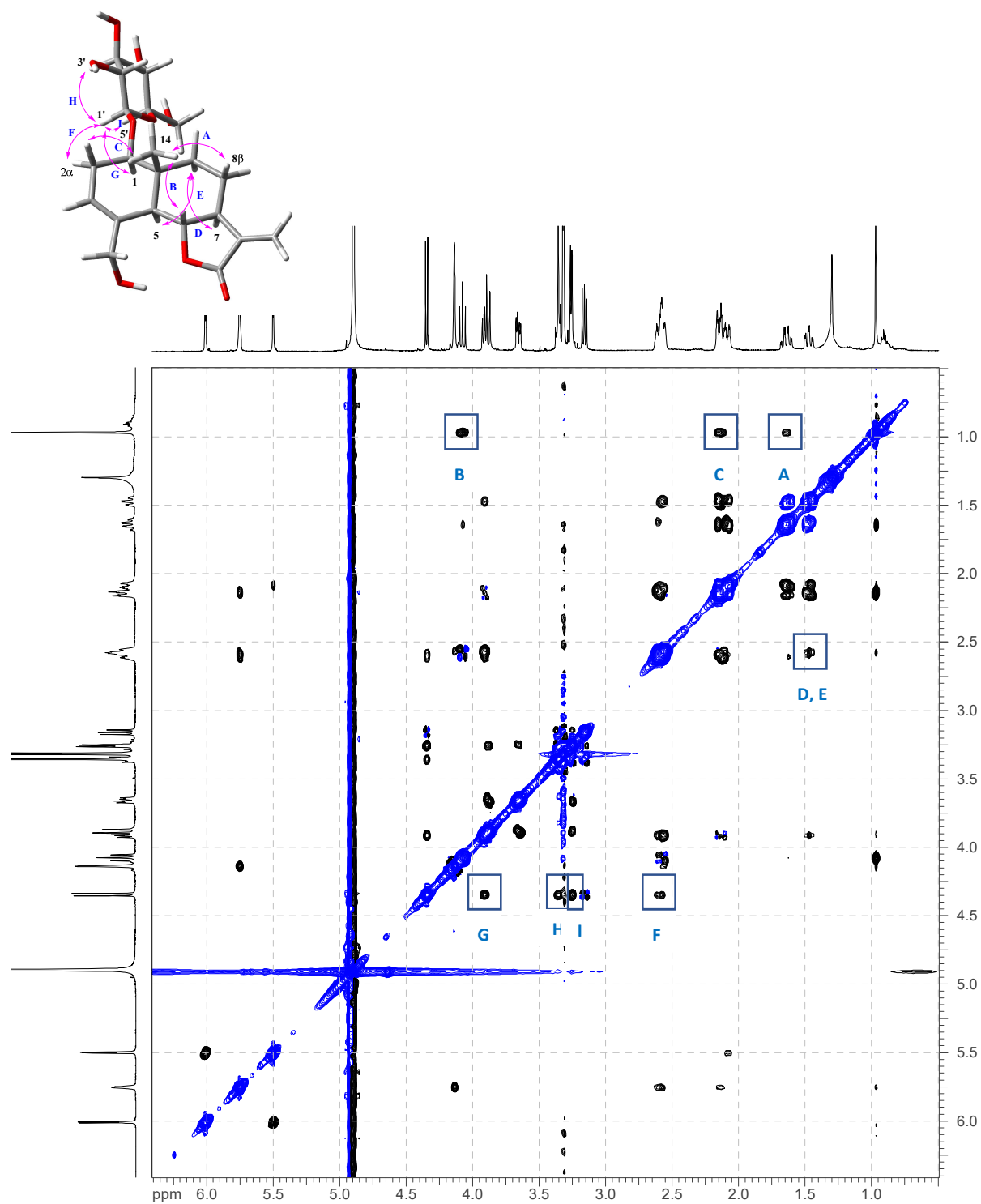
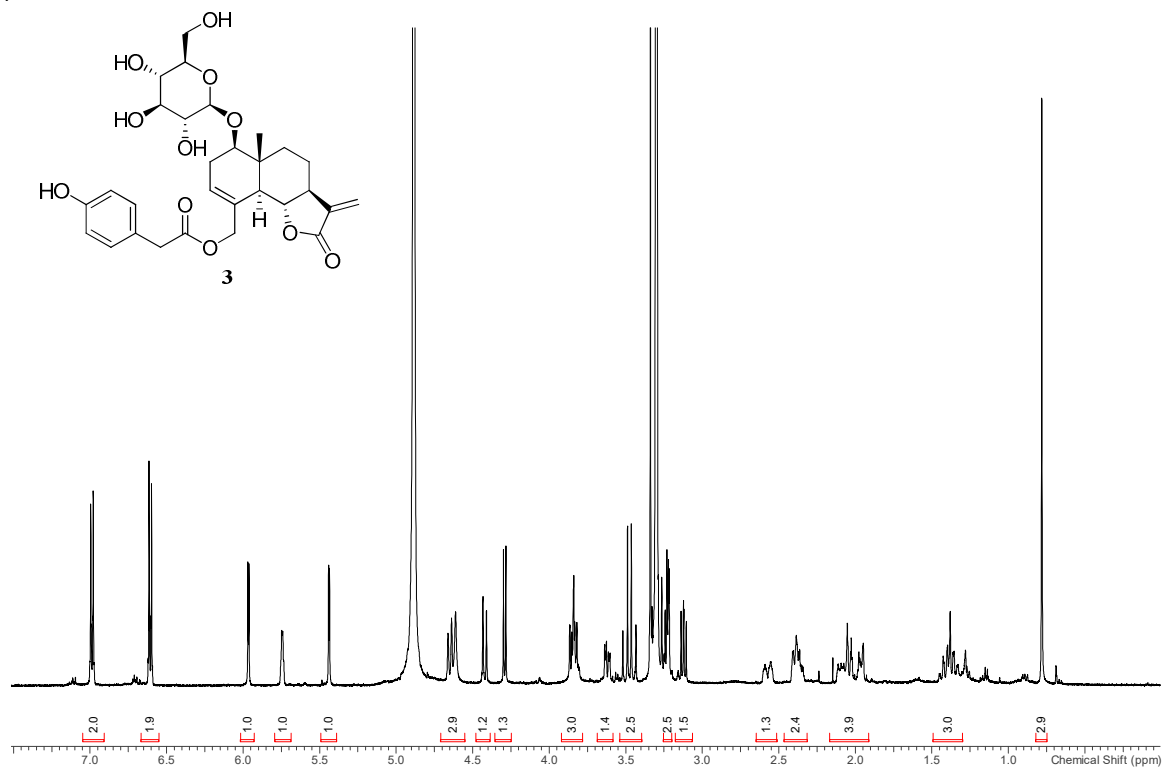


Figure S7. ROESY spectrum (500 MHz) of compound **2** in CD₃OD.

(A)



(B)

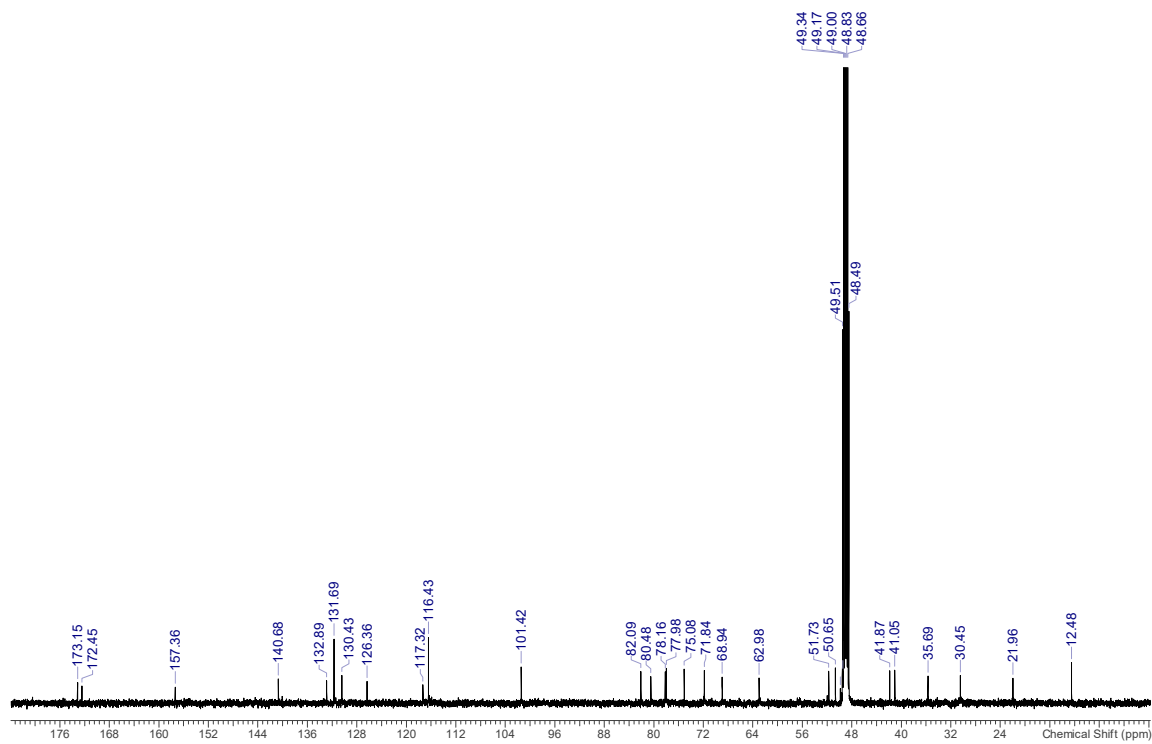
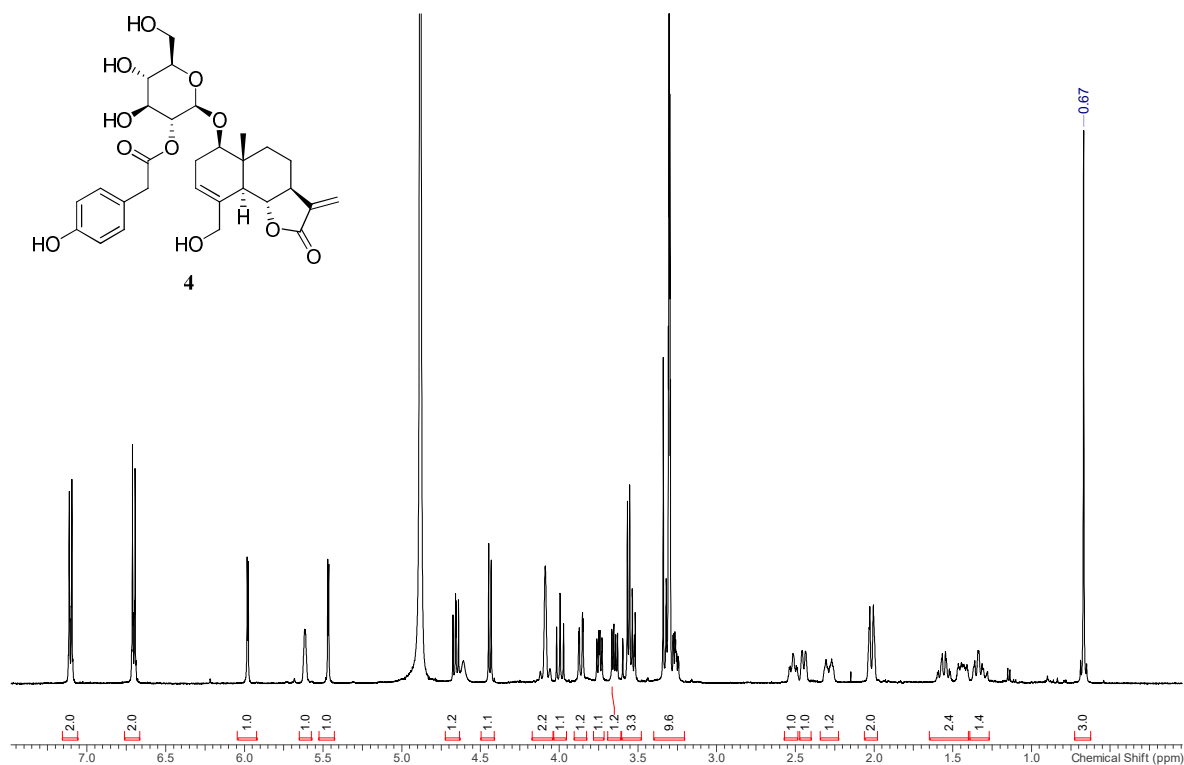


Figure S8. (A) ^1H (500 MHz) and (B) ^{13}C NMR (125 MHz) spectra of compound **3** in CD_3OD .

(A)



(B)

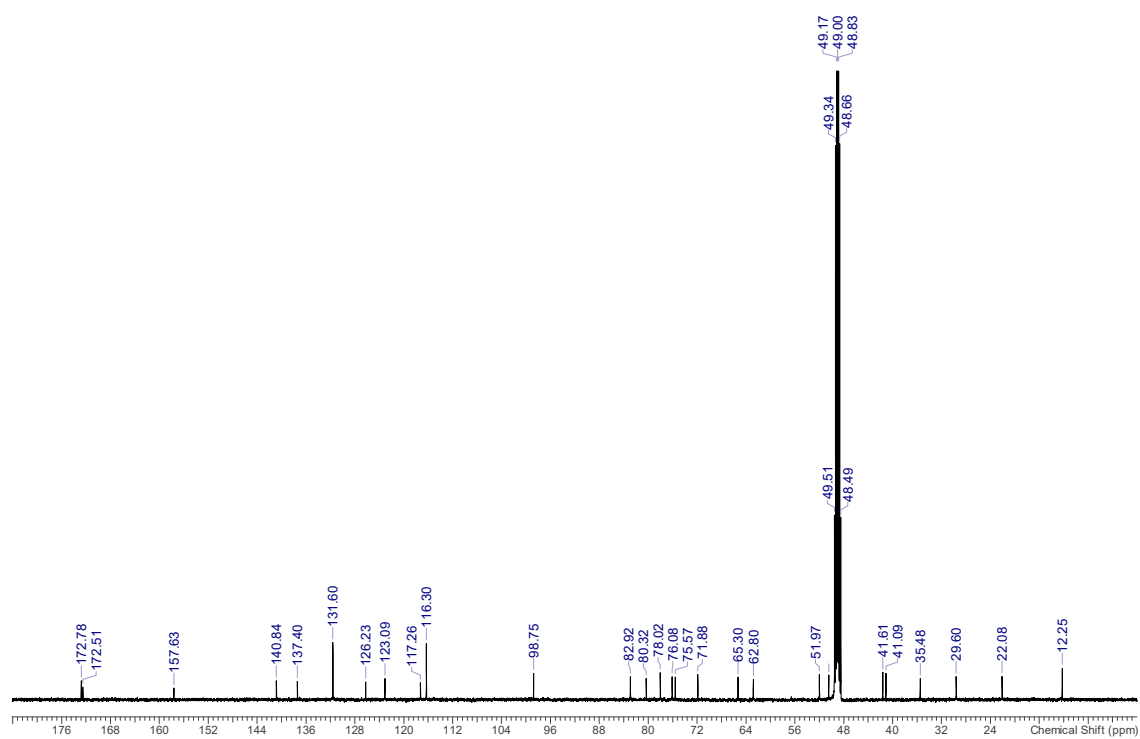


Figure S9. (A) ^1H (500 MHz) and (B) ^{13}C NMR (125 MHz) spectra of compound 4 in CD_3OD .

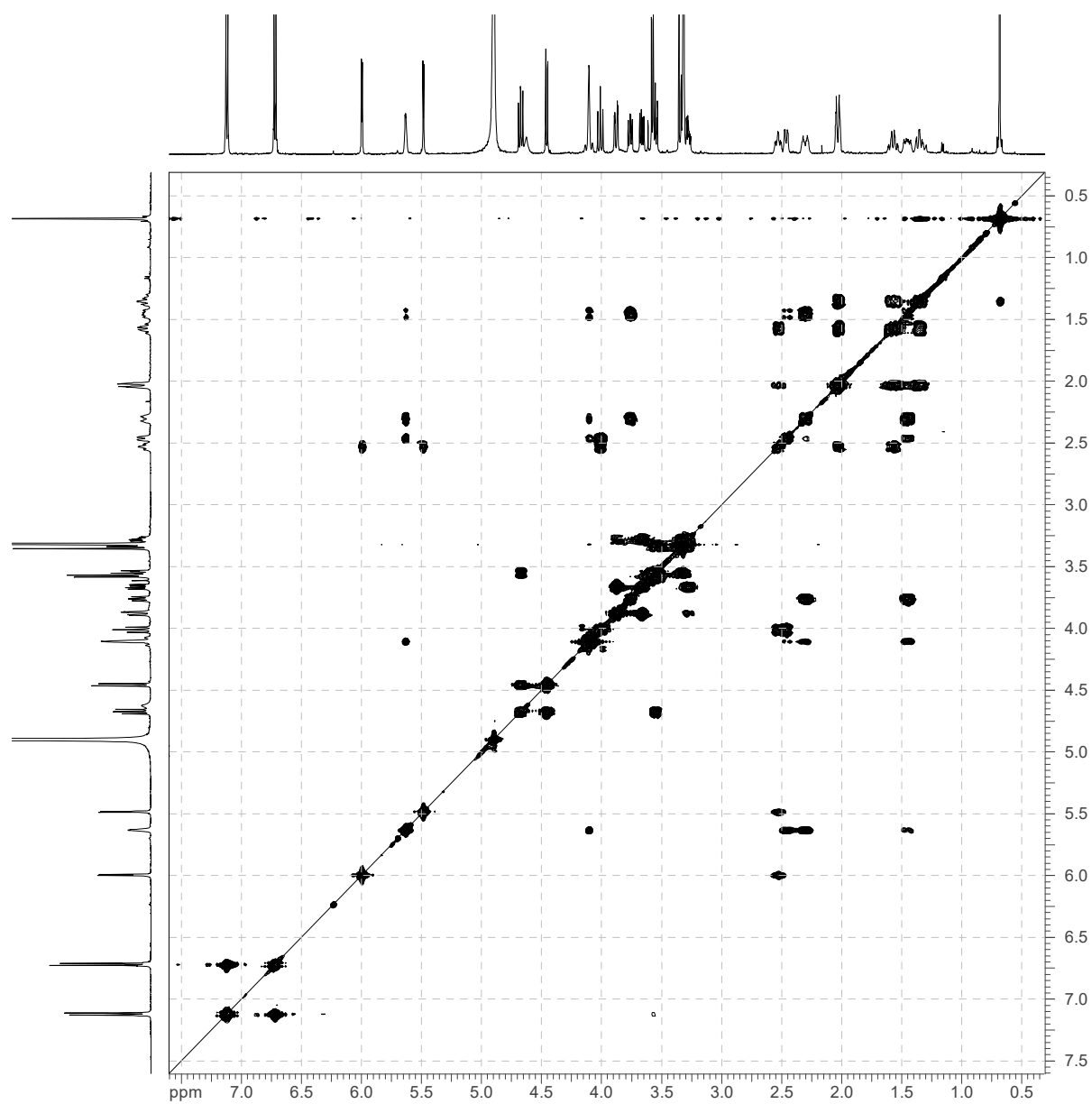


Figure S10. COSY spectrum (500 MHz) of compound **4** in CD₃OD.

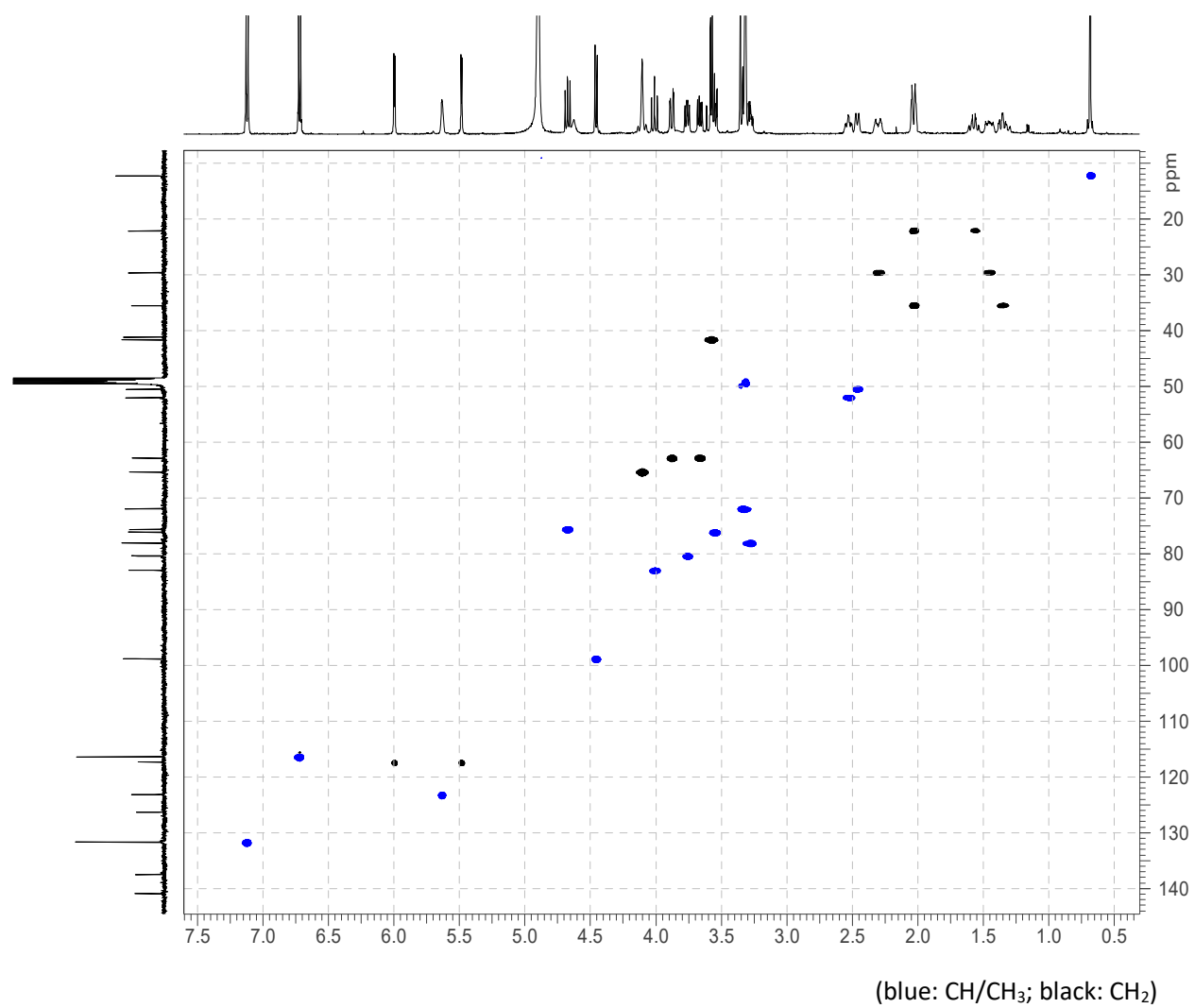


Figure S11. HSQC spectrum (500 MHz) of compound **4** in CD₃OD.

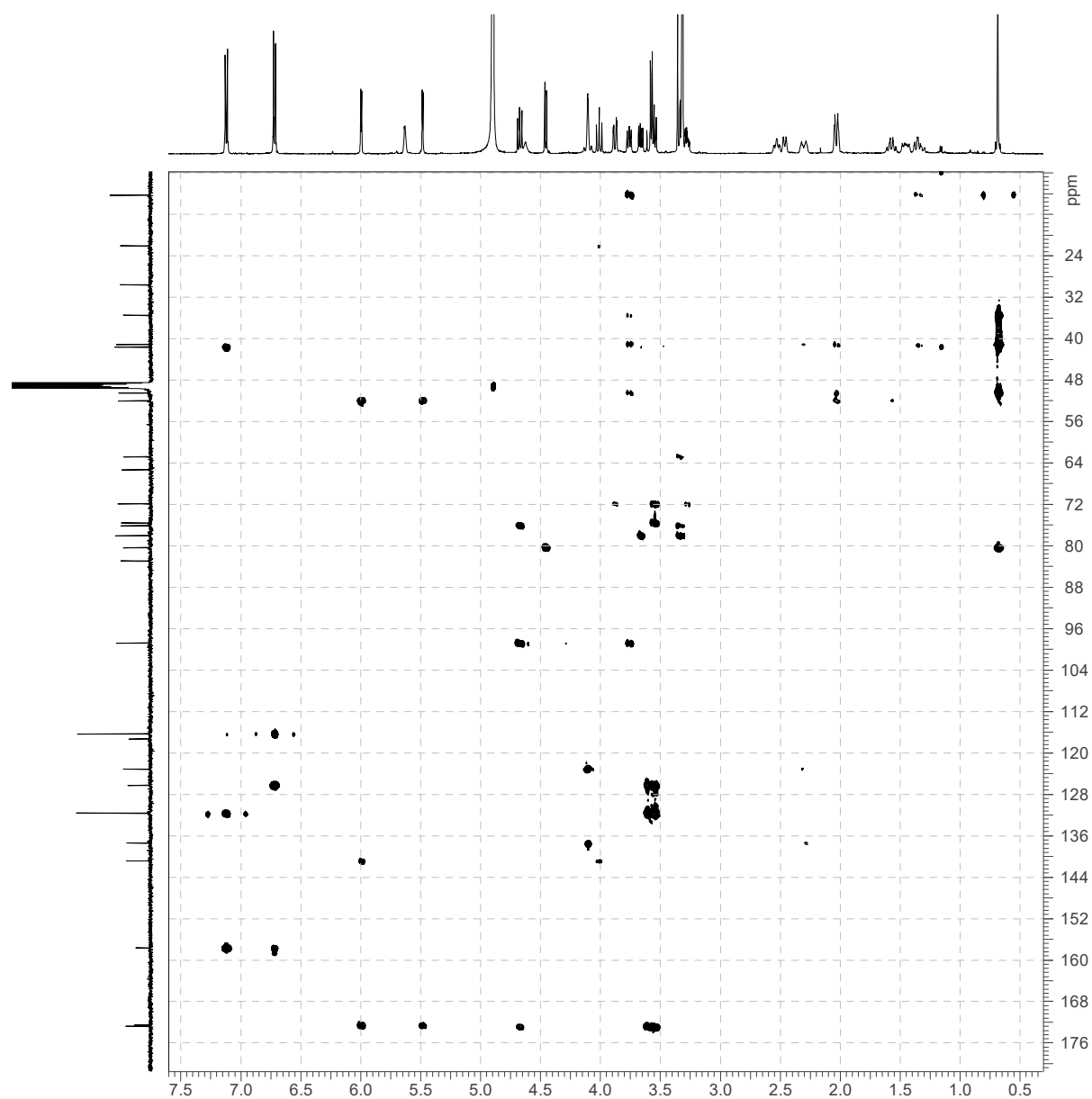


Figure S12. HMBC spectrum (500 MHz) of compound **4** in CD₃OD.

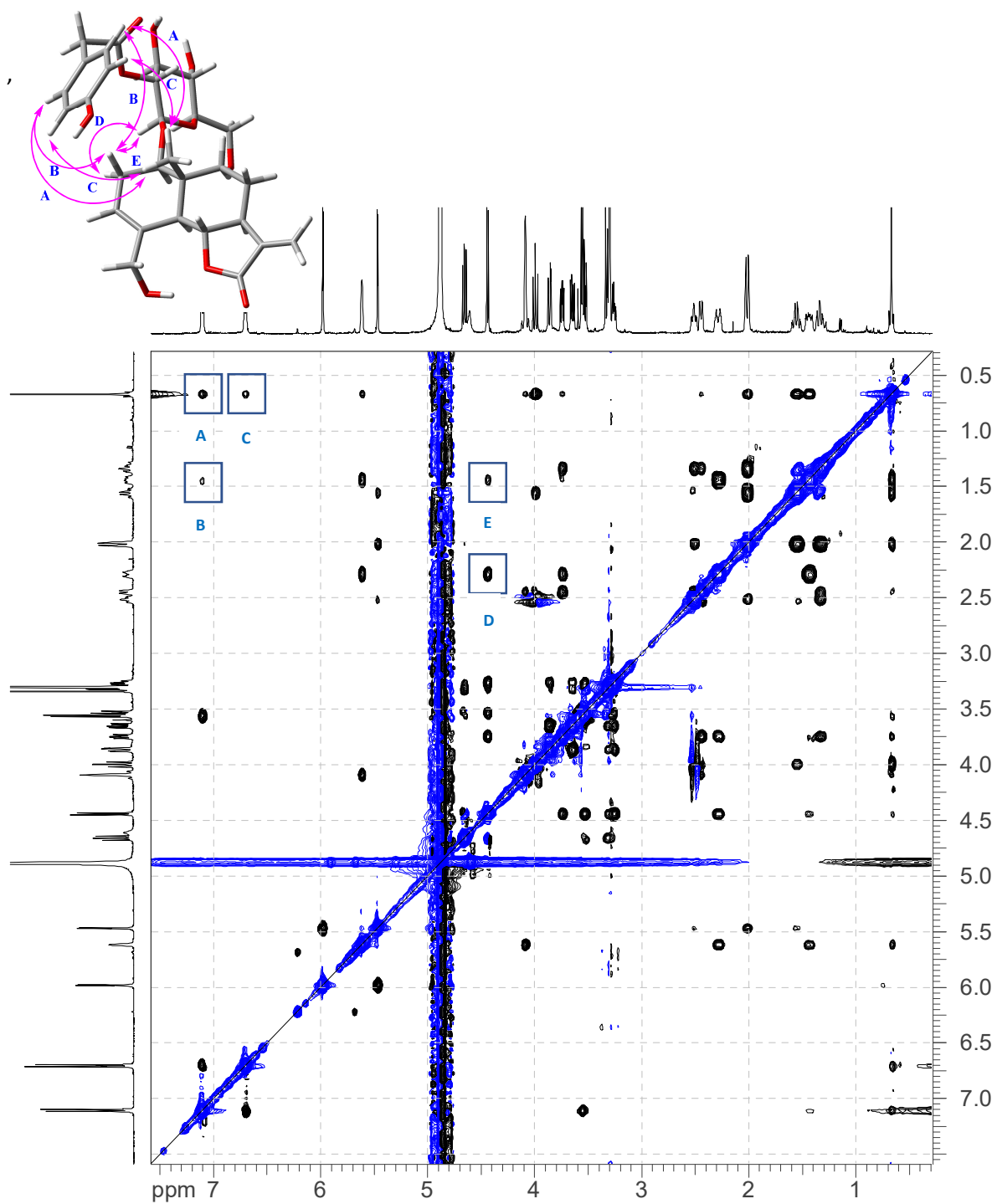


Figure S13. ROESY (500 MHz) spectrum of compound **4** in CD₃OD.

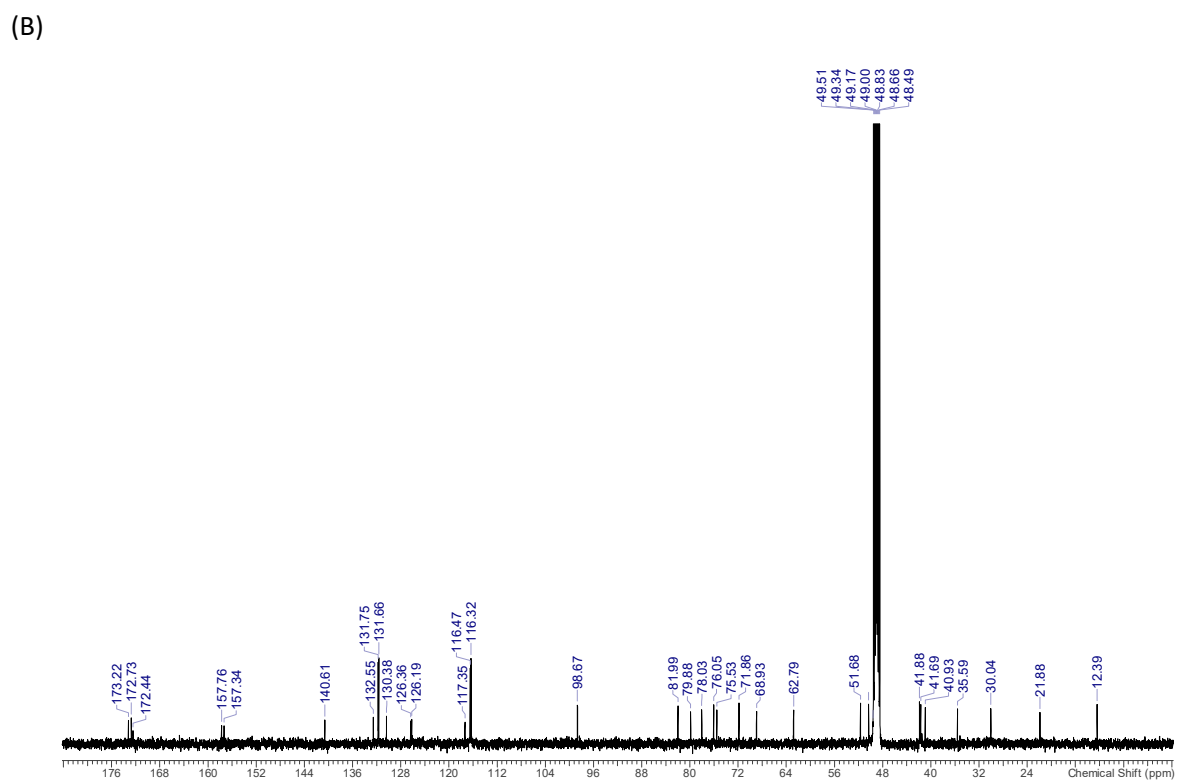
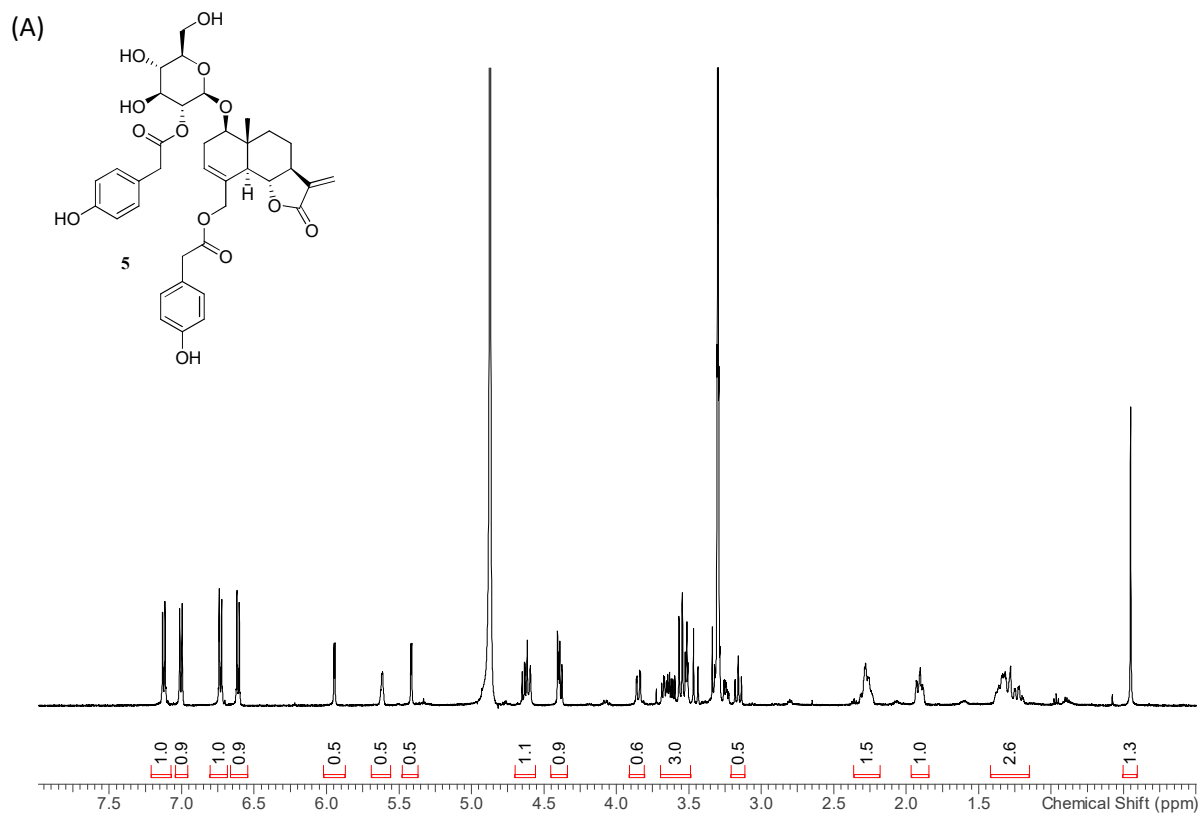


Figure S14. (A) ^1H (500 MHz) and (B) ^{13}C NMR (125 MHz) spectra of compound 5 in CD_3OD .

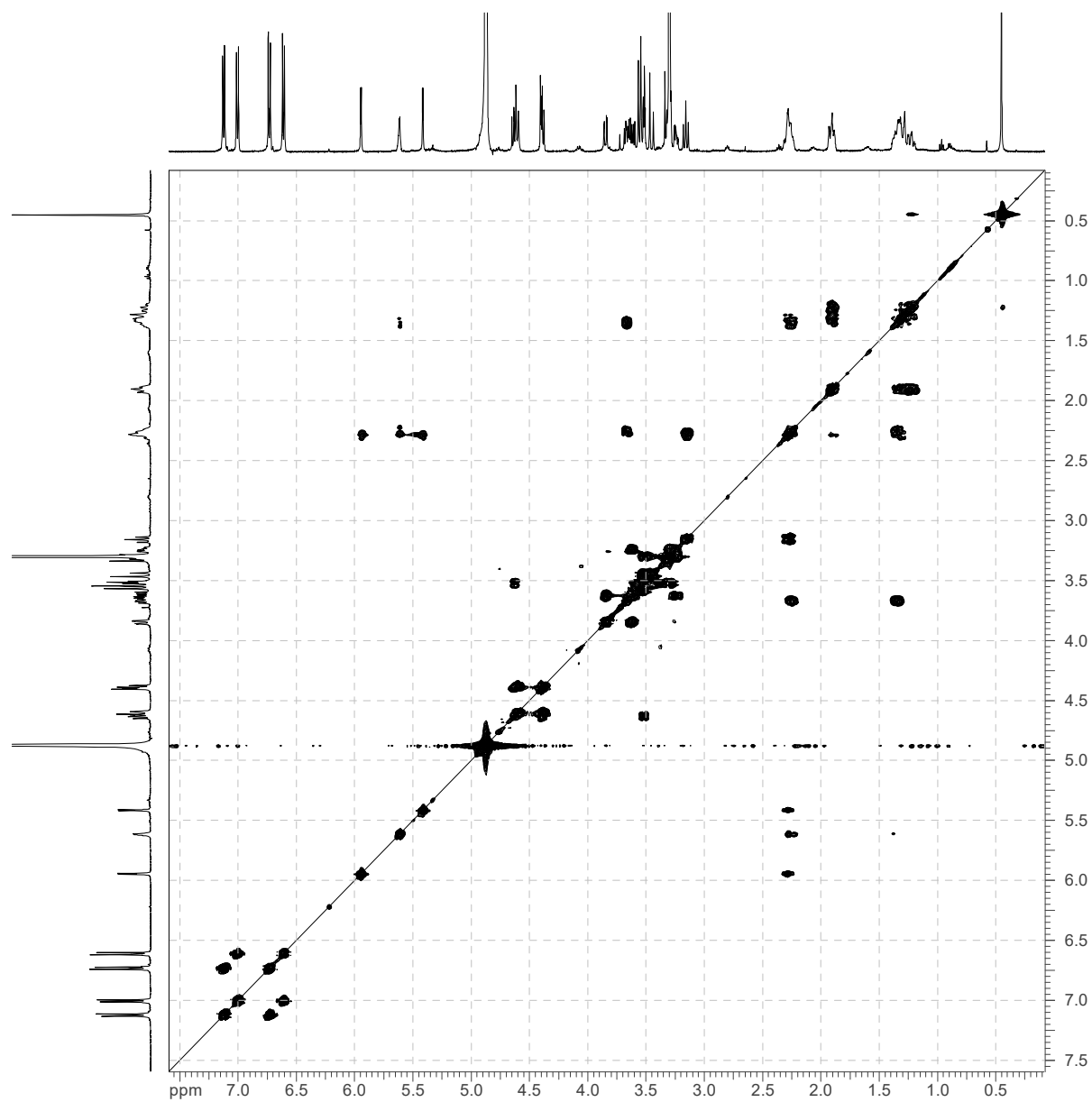


Figure S15. COSY spectrum (500 MHz) of compound **5** in CD₃OD.

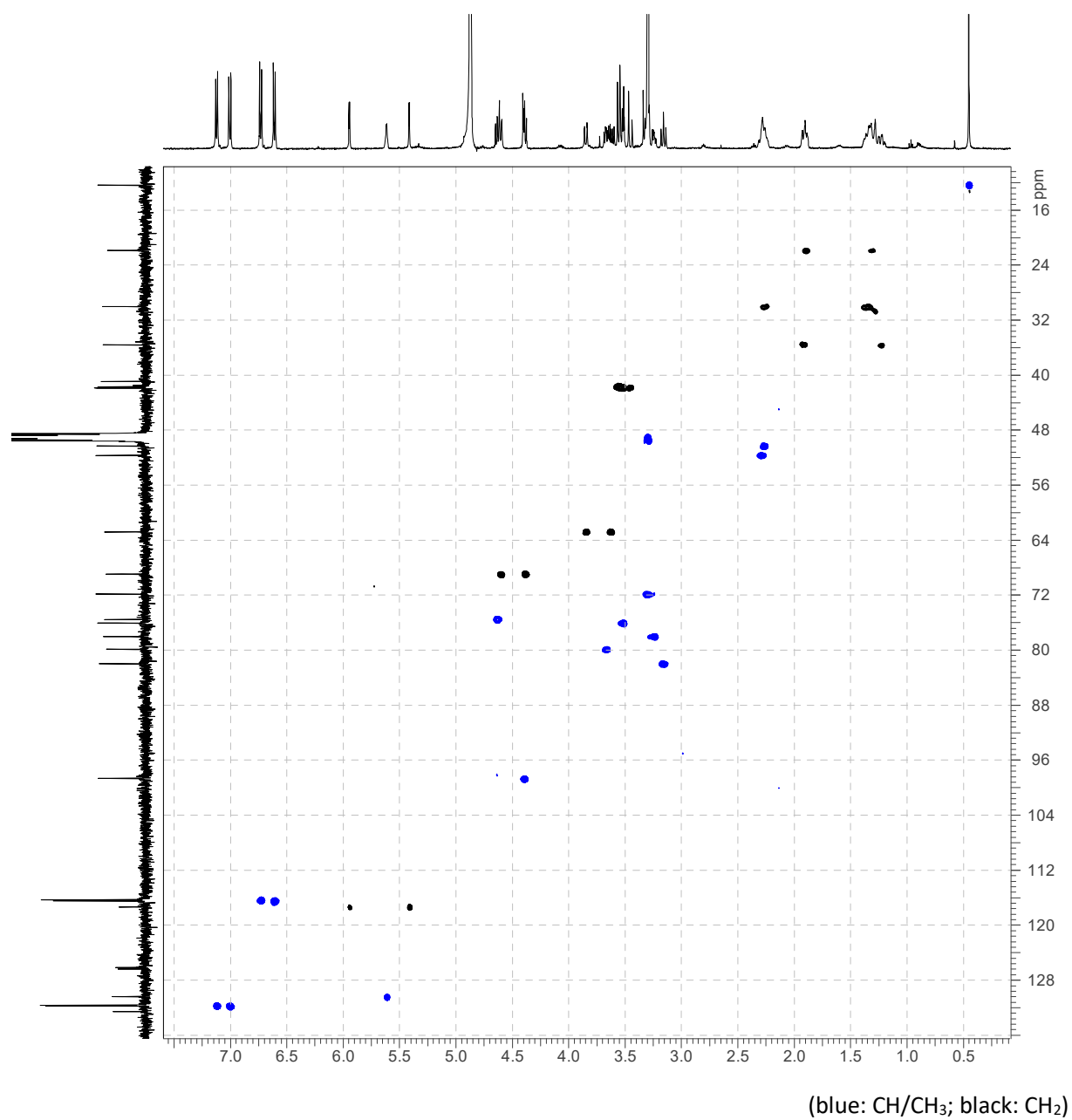


Figure S16. HSQC spectrum (500 MHz) of compound **5** in CD₃OD.

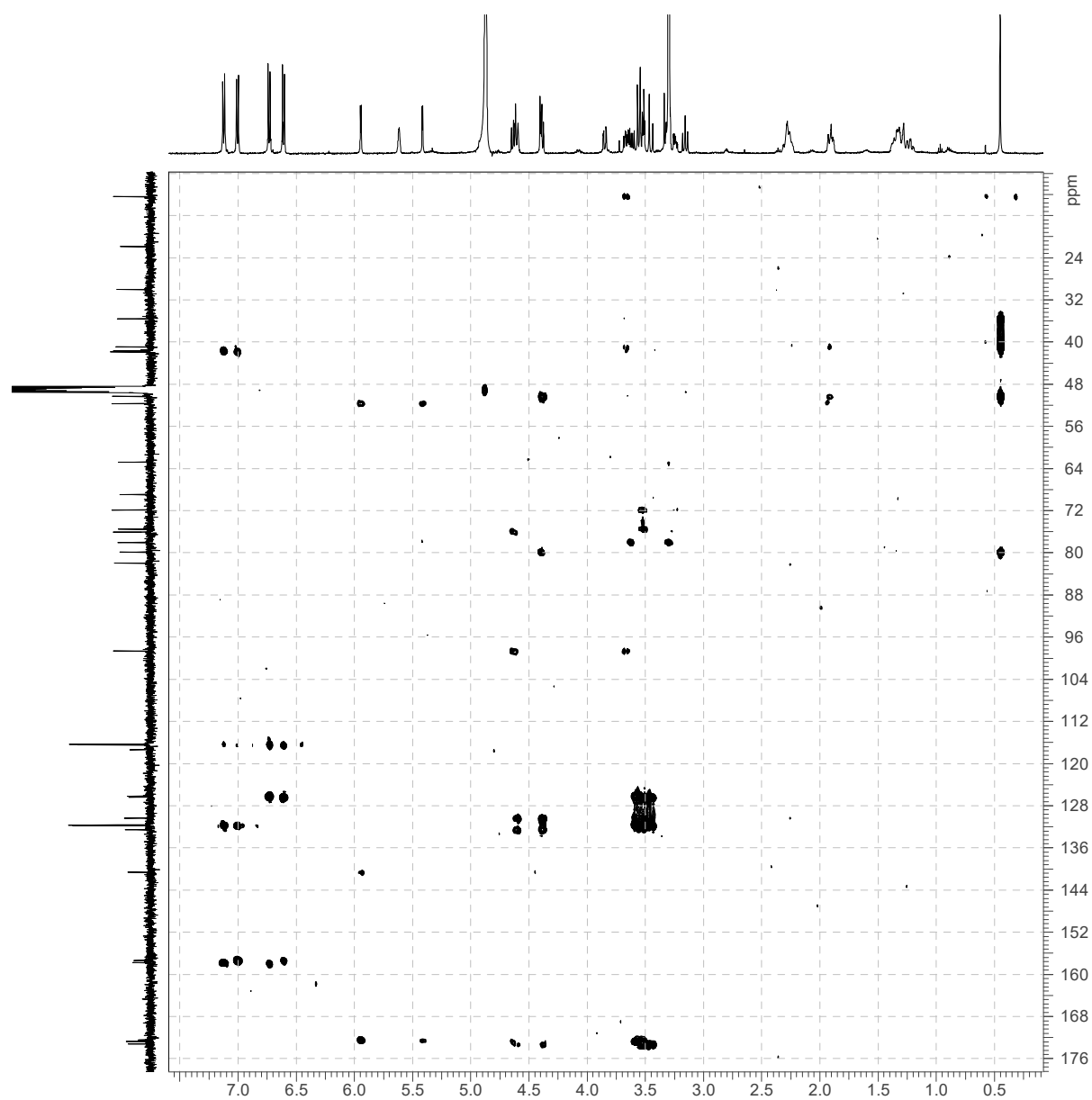


Figure S17. HMBC spectrum (500 MHz) of compound **5** in CD₃OD.

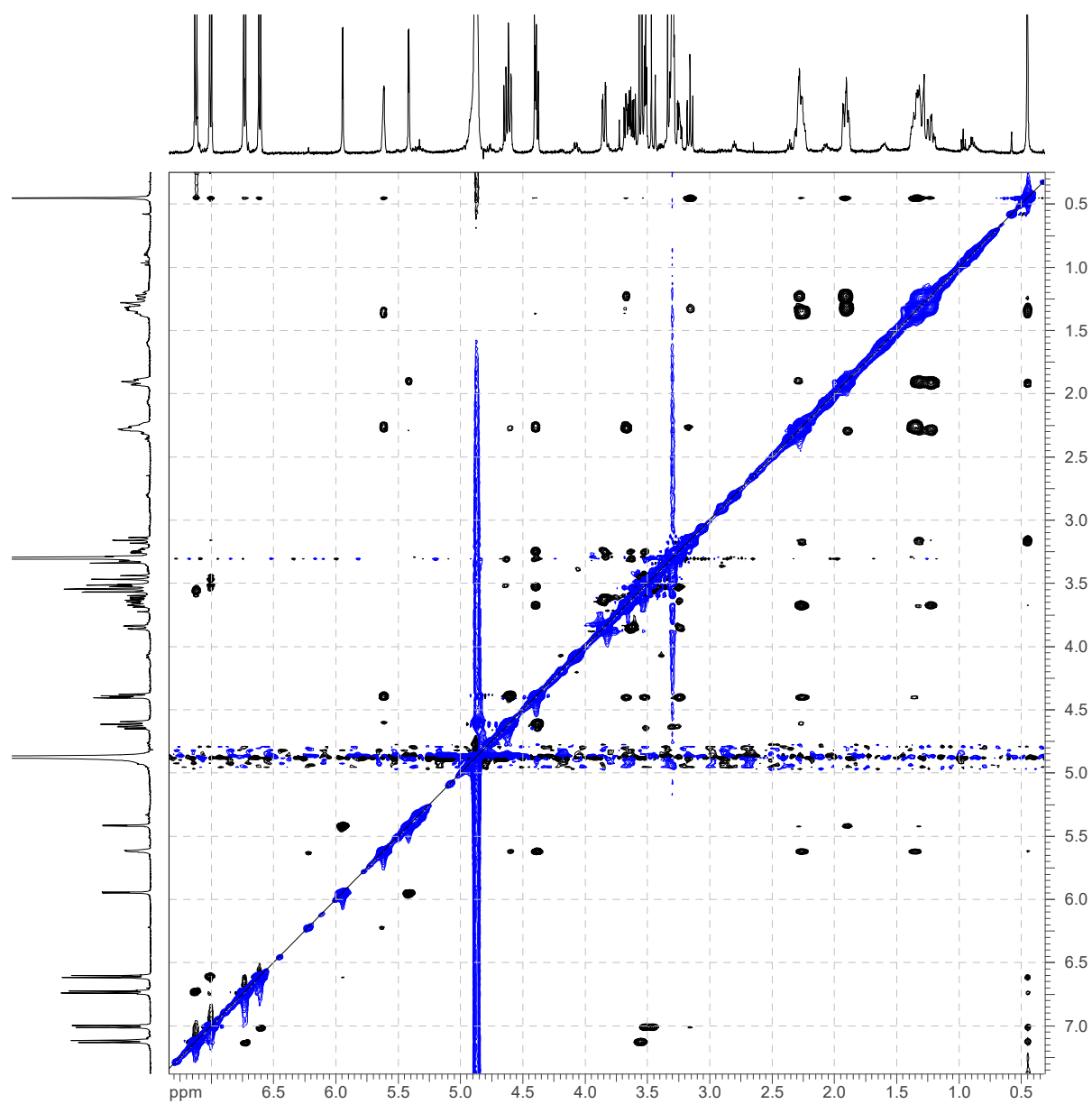


Figure S18. ROESY (500 MHz) spectrum of compound **5** in CD₃OD.