

Supplementary Information

Dibenzofuran, 4-Chromanone, Acetophenone, and Dithiecine Derivatives: Cytotoxic Constituents from *Eupatorium fortunei*

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Table S1. Calculated physicochemical properties of compound 1.

Property	Value
Number of H-bond acceptors	4
Number of H-bond donors	2
Molecular weight	346.38 g/mol
ALogP98	5.08
Molecular surface area	347.01 Å ²
Molecular polar surface area	70.67 Å ²
ADMET absorption level	Good

Table S2. Predicted targets of compound 1.

Target	Description	Max Tc	P-Value
PON1	Serum paraoxonase/arylesterase 1	0.34	2.784e-21
CELA1	Chymotrypsin-like elastase family member 1	0.41	1.144e-14
CBR1	Carbonyl reductase [NADPH] 1	0.31	3.485e-08
NQO1	NAD(P)H dehydrogenase [quinone] 1	0.31	7.109e-08

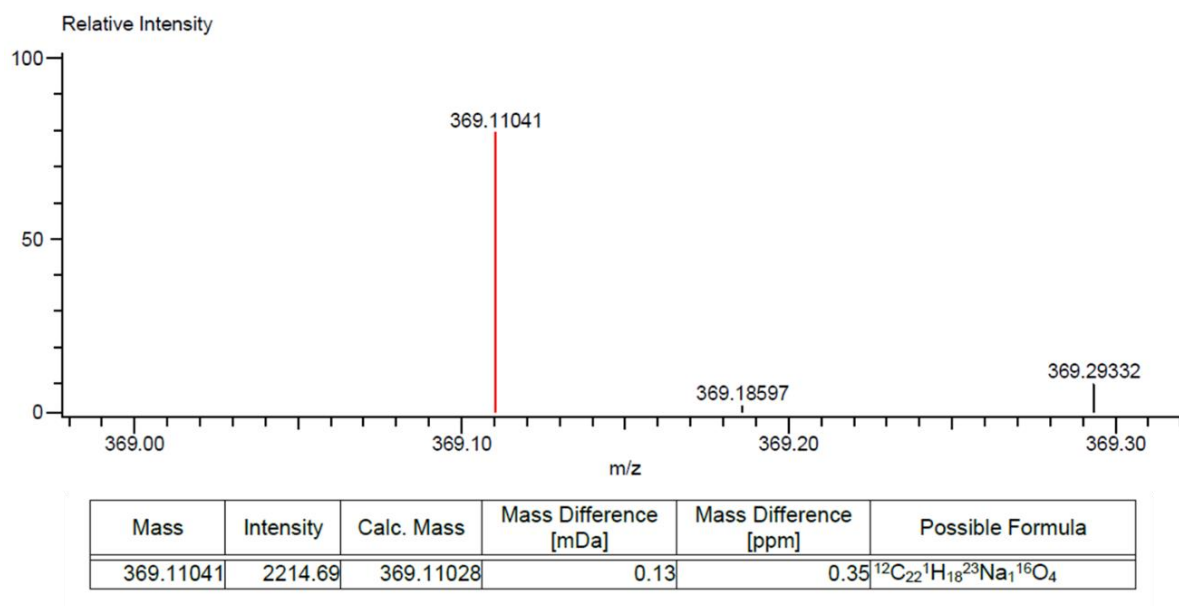


Figure S1. HR-ESI-MS spectrum of **1**.

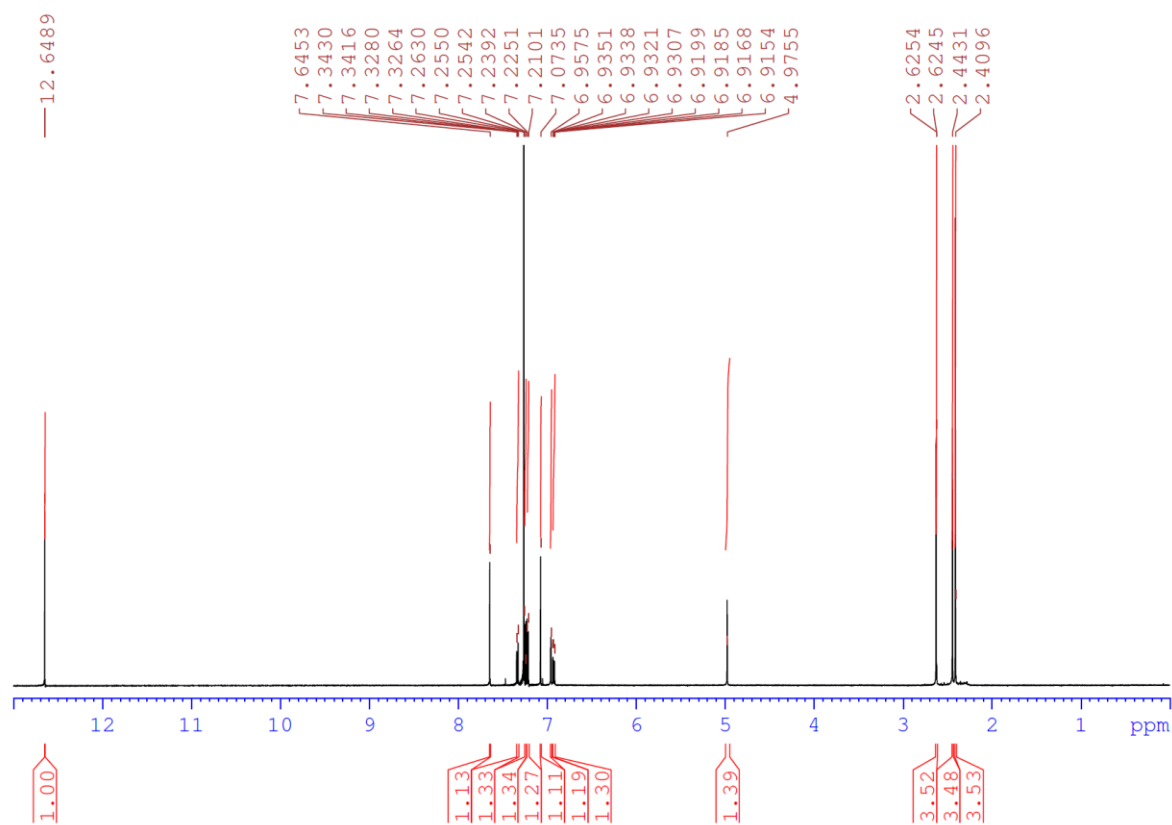


Figure S2. ^1H -NMR spectrum (CDCl_3 , 500 MHz) of **1**.

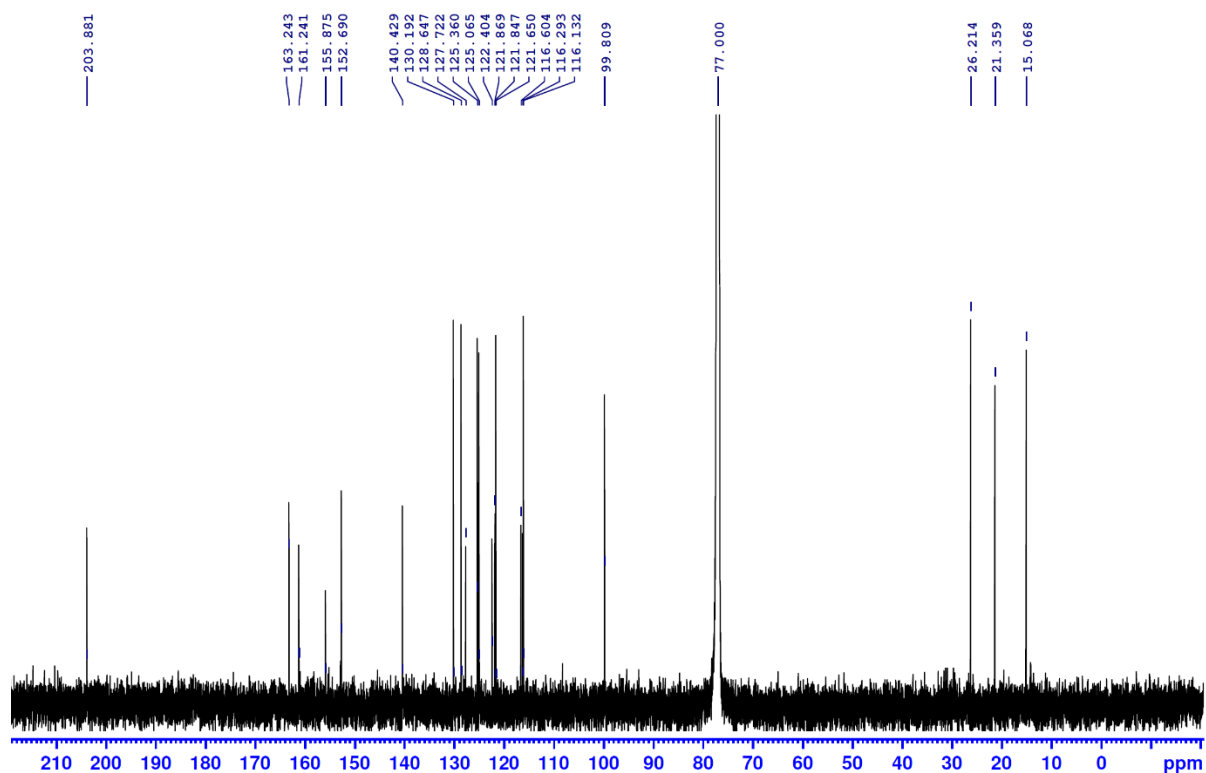


Figure S3. ^{13}C -NMR spectrum (CDCl_3 , 125 MHz) of **1**.

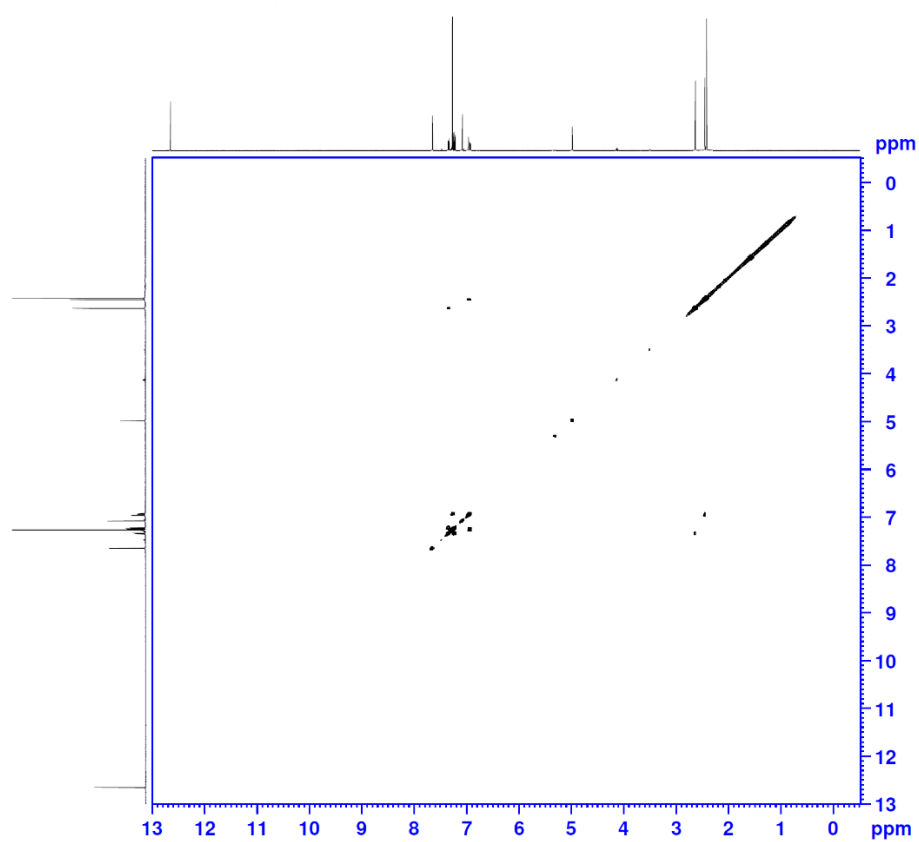


Figure S4. ^1H - ^1H COSY spectrum of **1**.

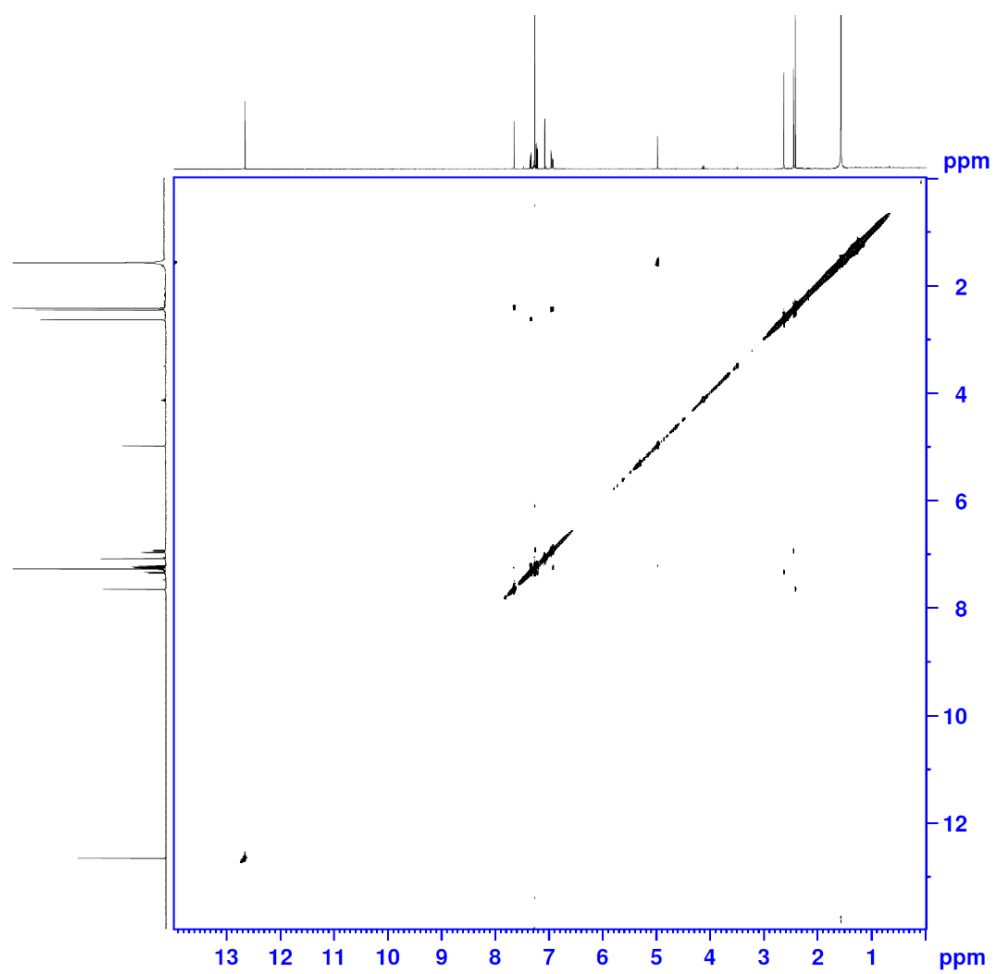


Figure S5. ROESY spectrum of 1.

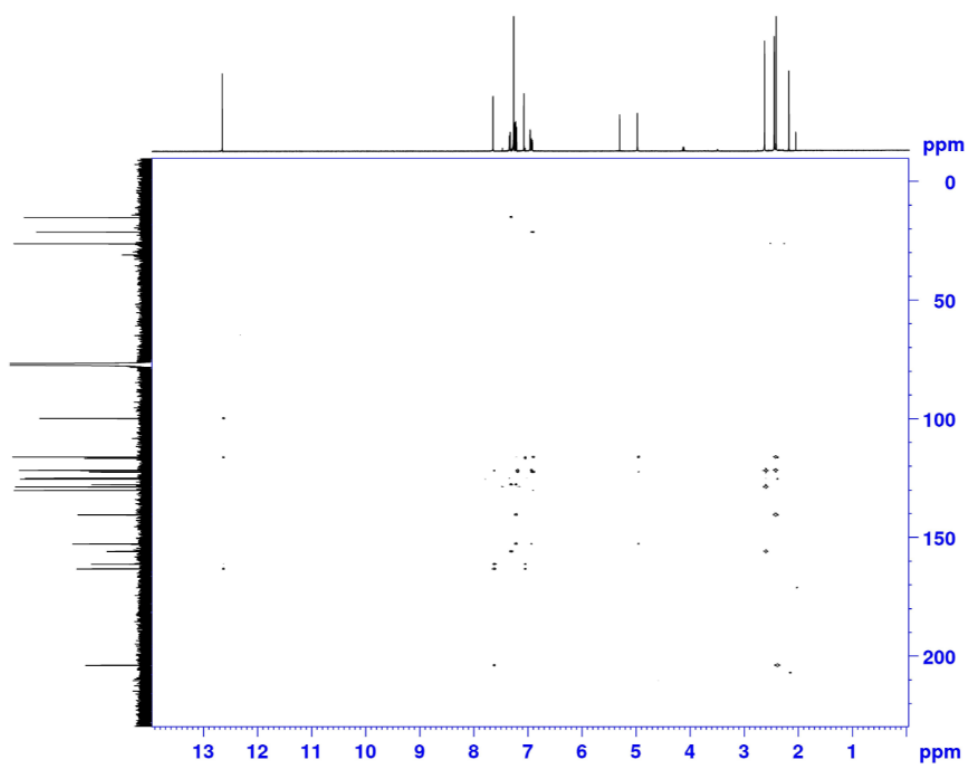


Figure S6. HMBC spectrum of 1.

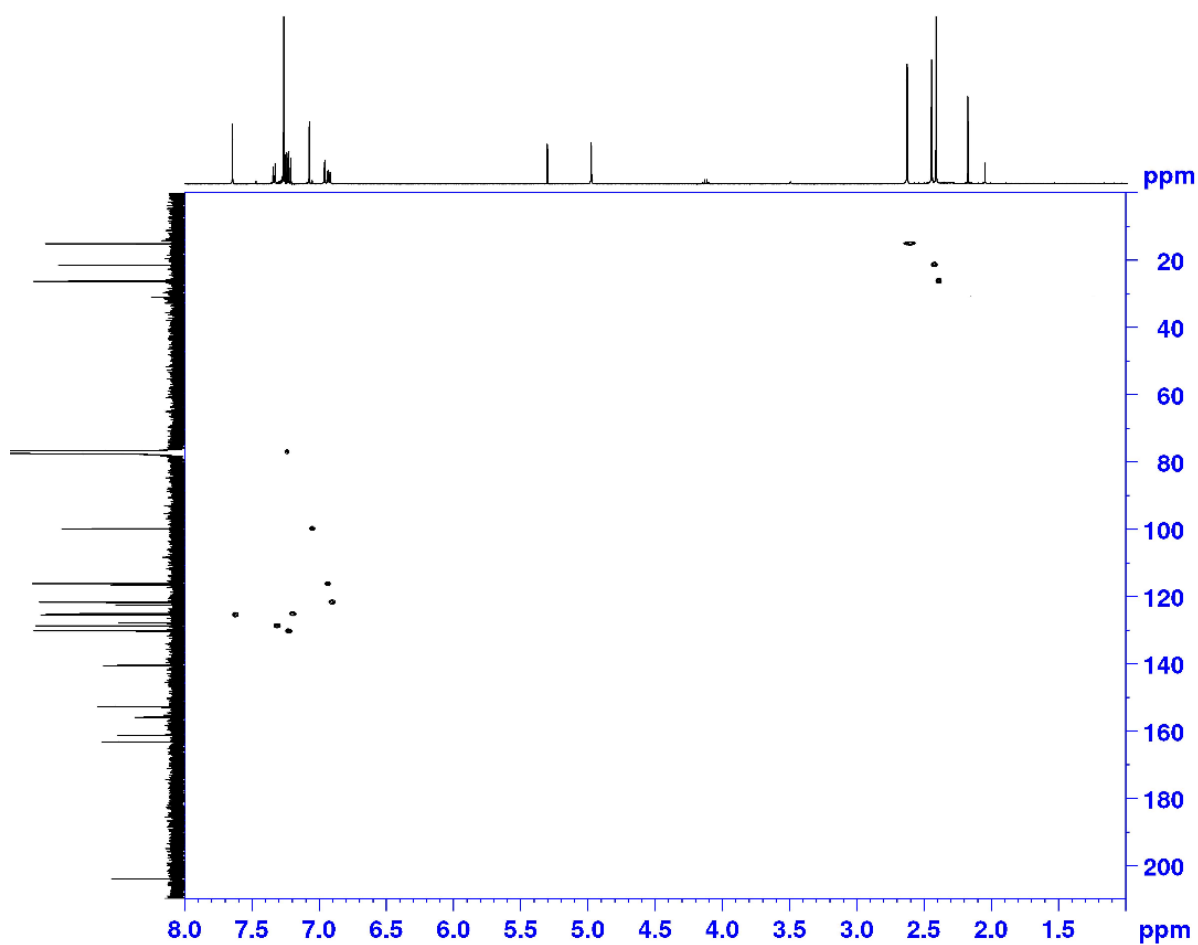
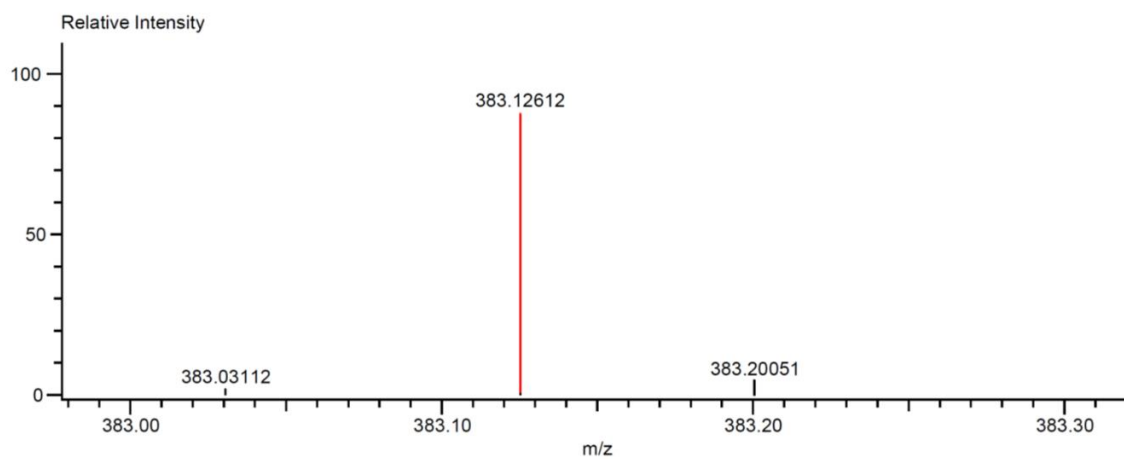


Figure S7. HSQC spectrum of 1.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
383.12612	2282.32	383.12593	0.19	0.49	$^{12}\text{C}_{23}\text{H}_{20}^{23}\text{Na}_1^{16}\text{O}_4$

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

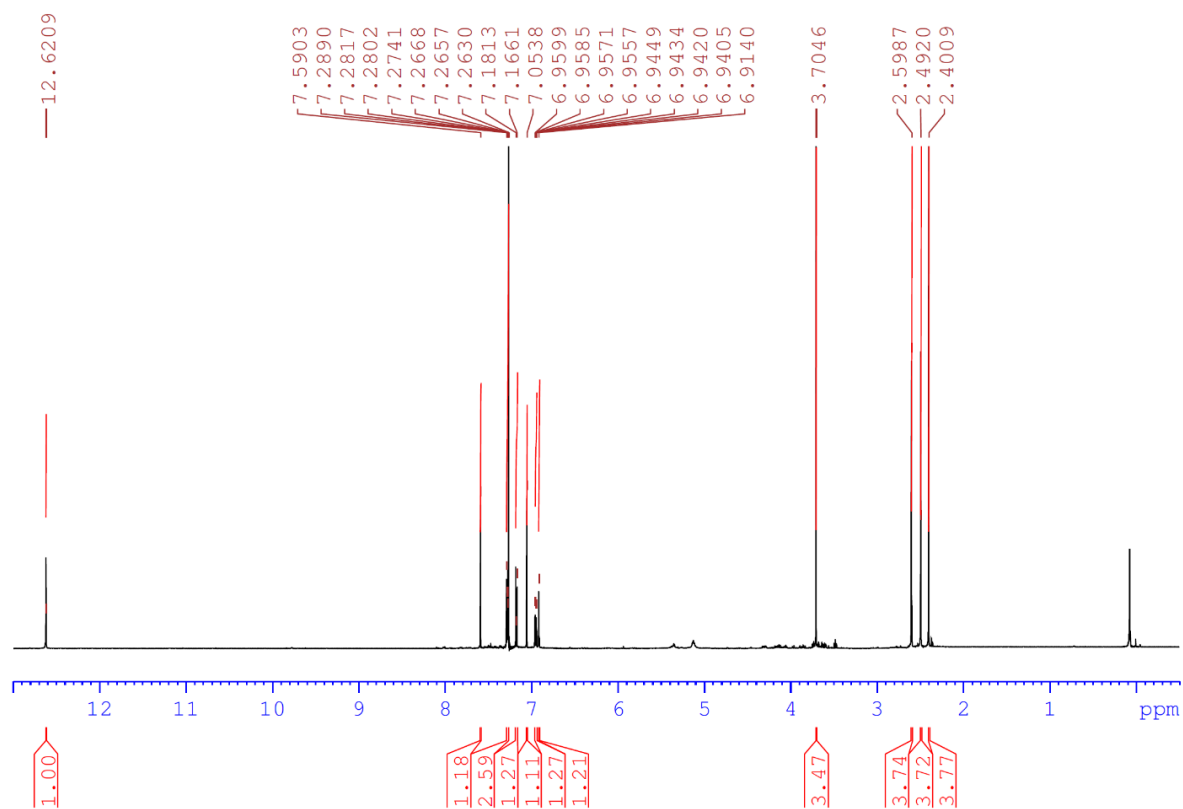


Figure S9. ¹H-NMR spectrum (CDCl₃, 500 MHz) of **2**.

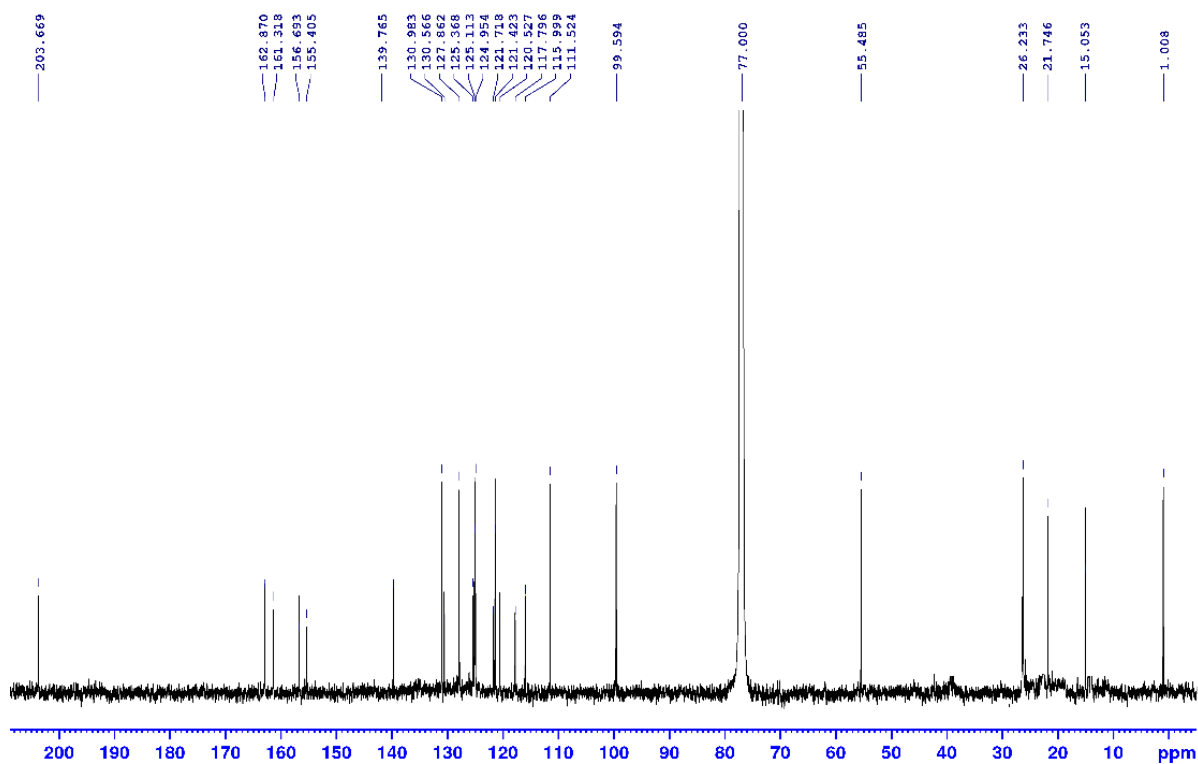


Figure S10. ¹³C-NMR spectrum (CDCl₃, 125 MHz) of **2**.

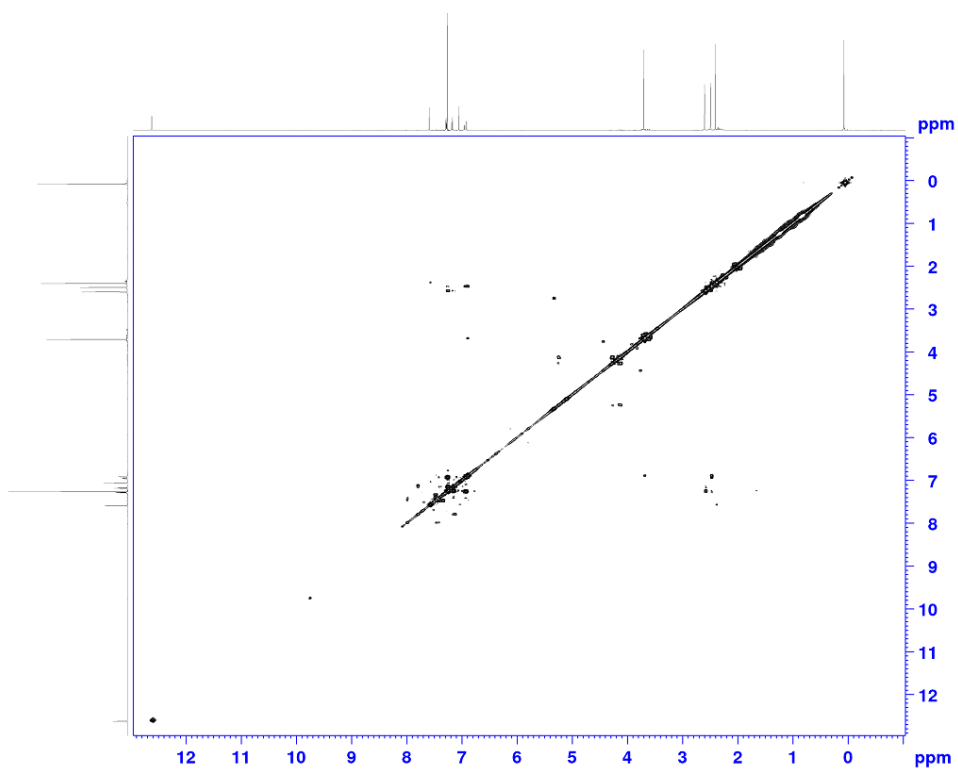


Figure S11. ^1H - ^1H COSY spectrum of **2**.

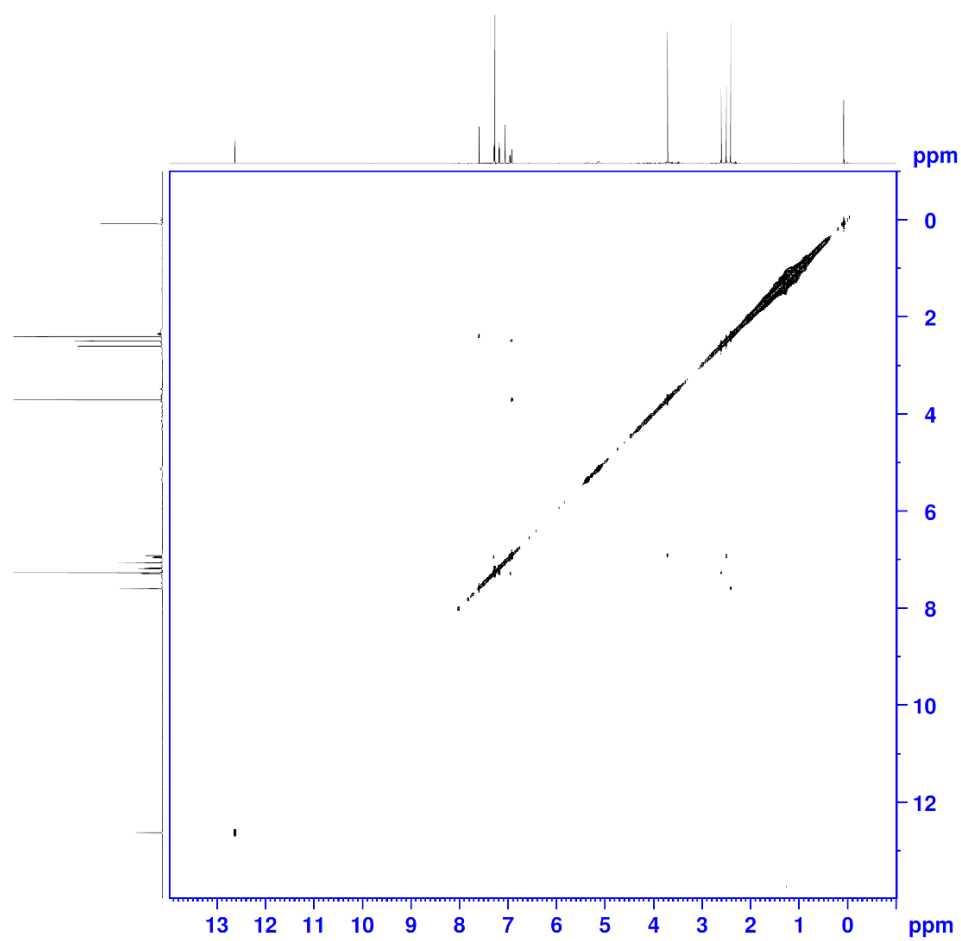


Figure S12. ROESY spectrum of **2**.

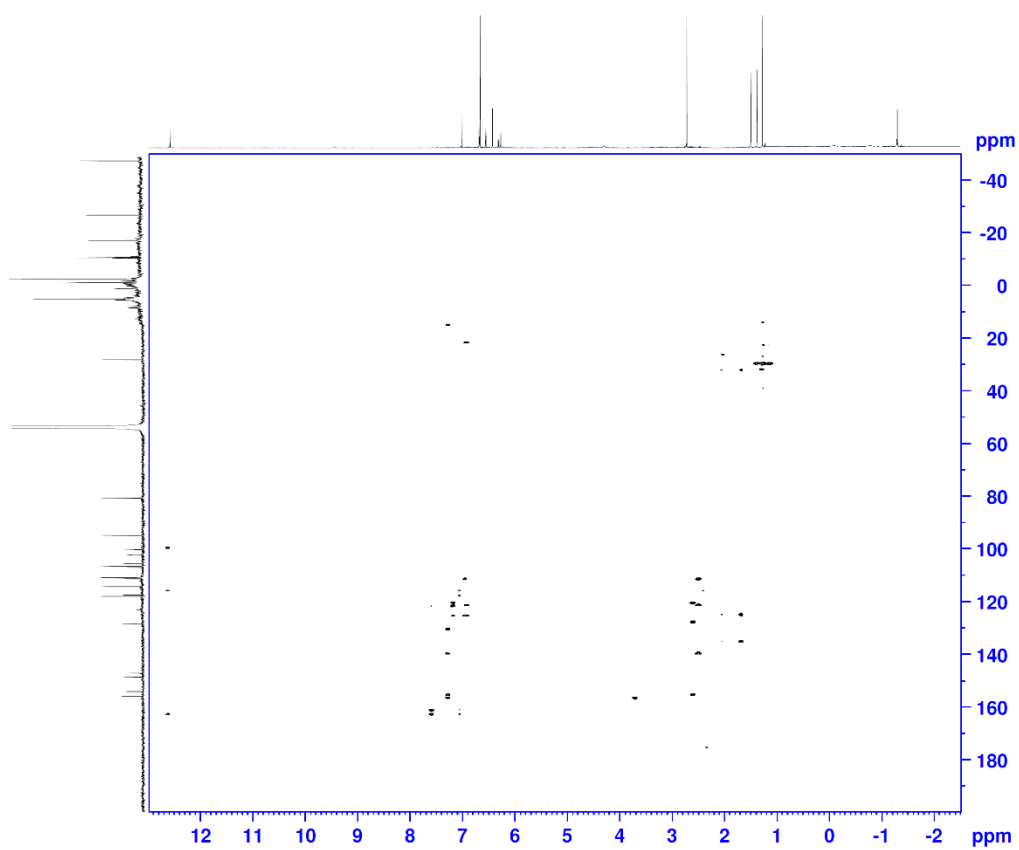


Figure S13. HMBC spectrum of 2.

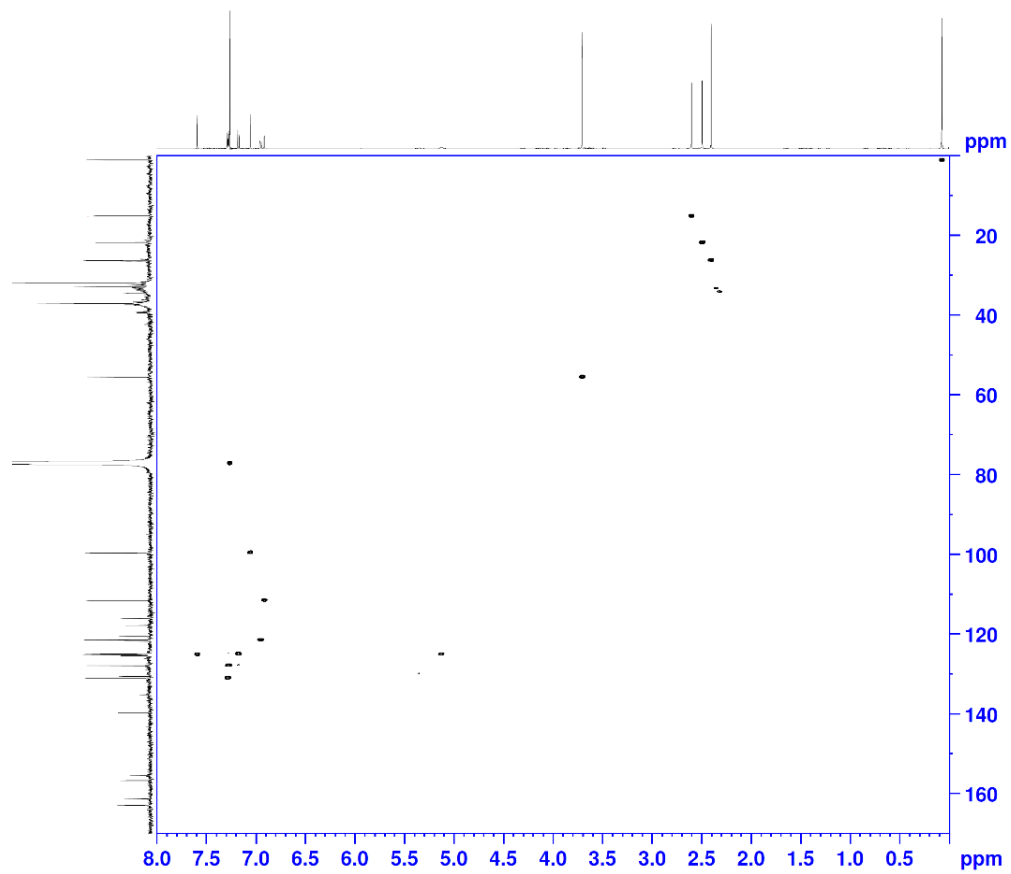


Figure S14. HSQC spectrum of 2.

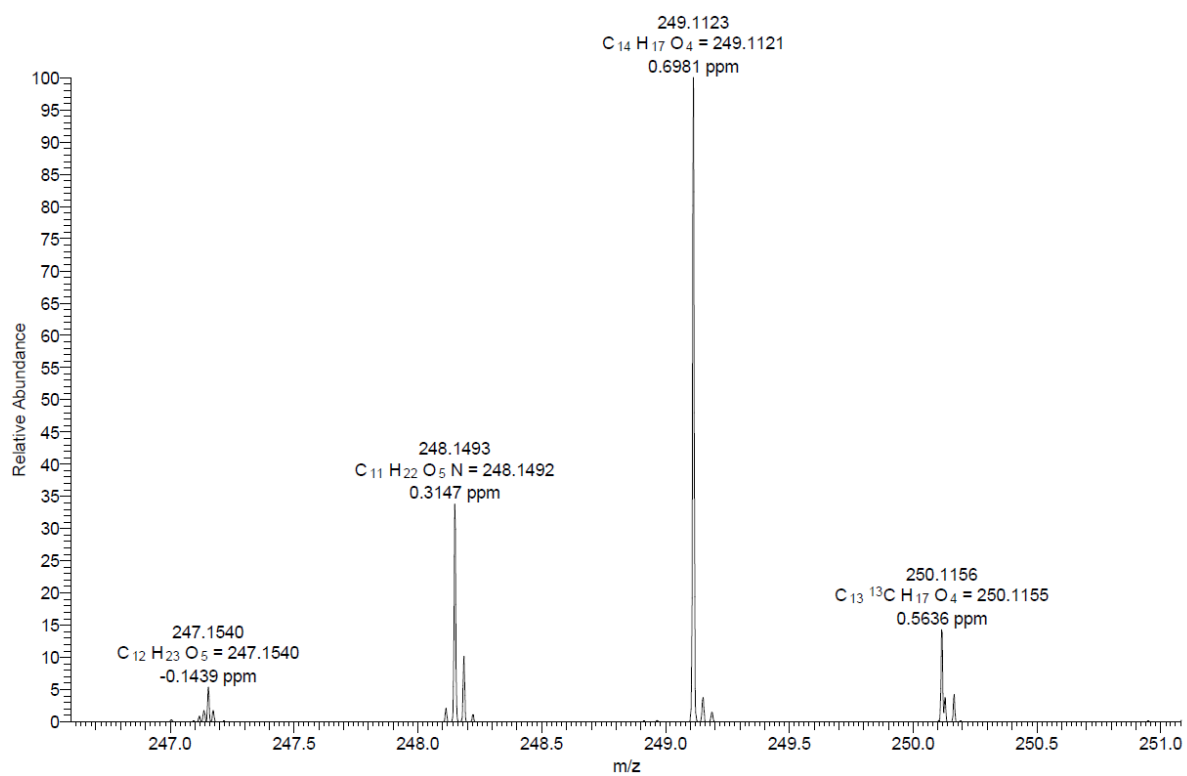


Figure S15. HR-ESI-MS spectrum of 3.

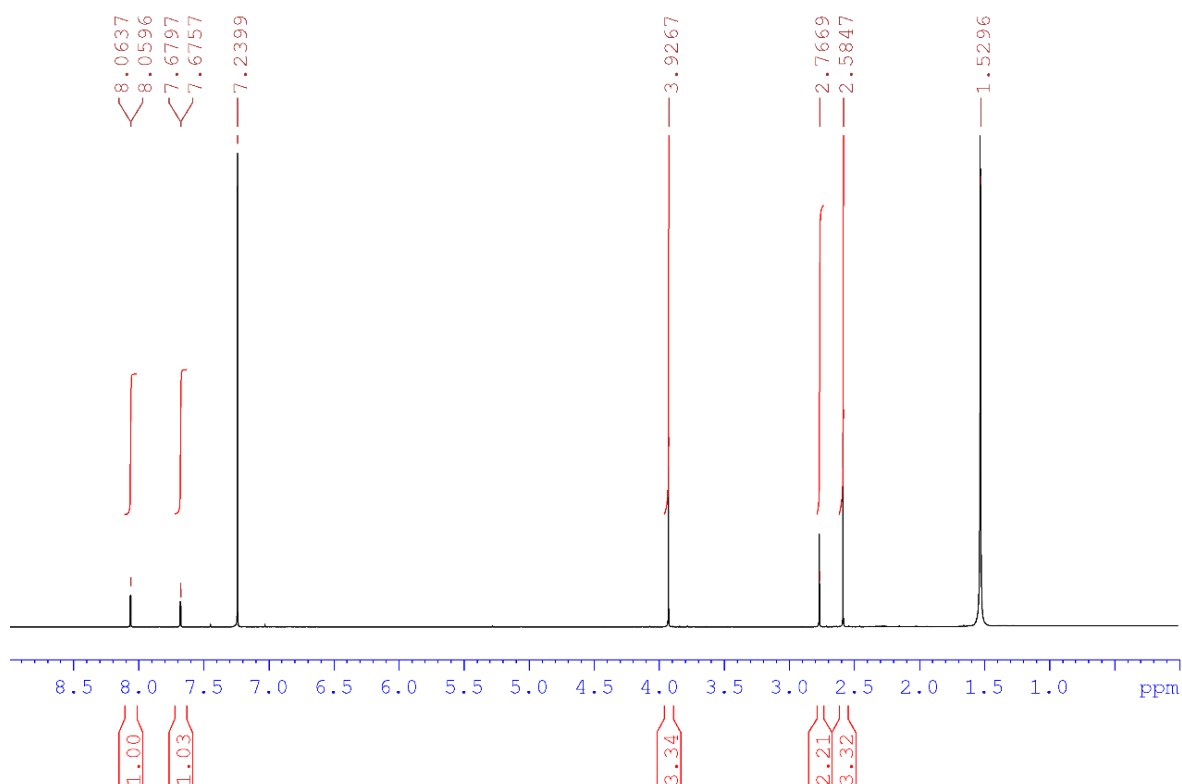


Figure S16. 1H -NMR spectrum ($CDCl_3$, 500 MHz) of 3.

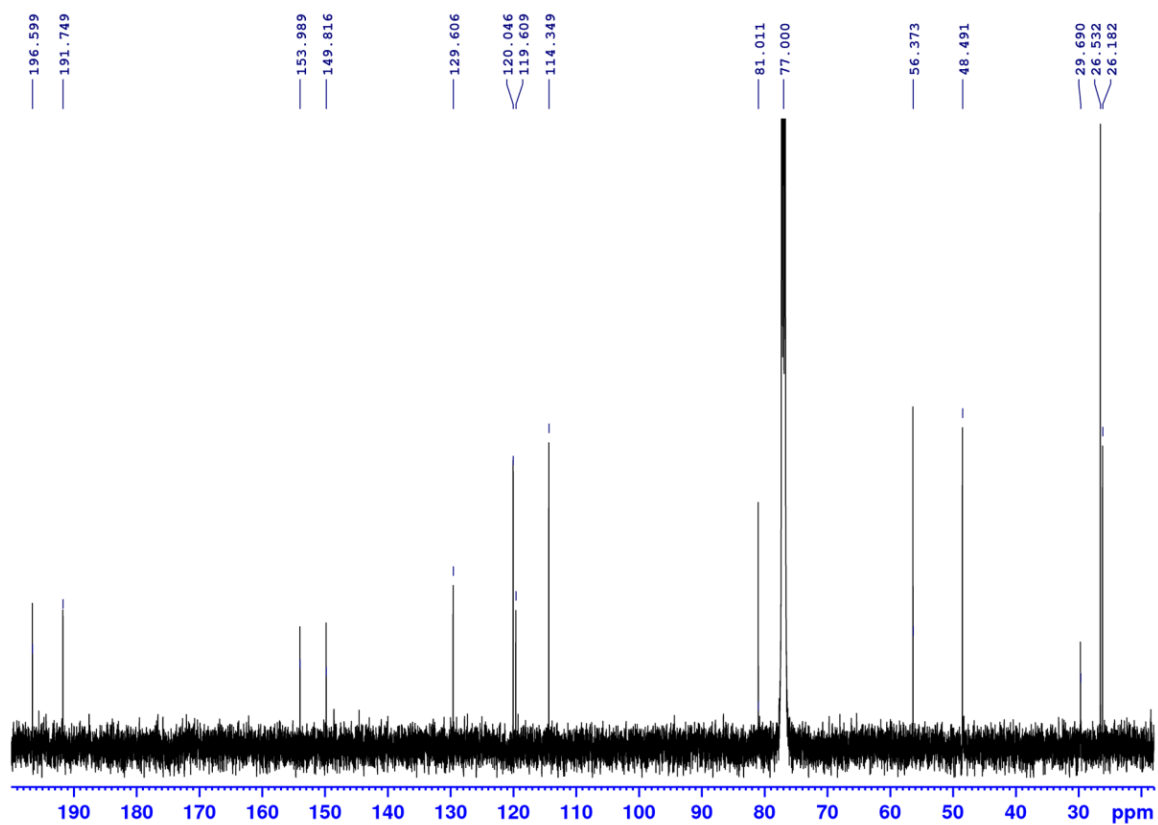


Figure S17. ^{13}C -NMR spectrum (CDCl_3 , 125 MHz) of **3**.

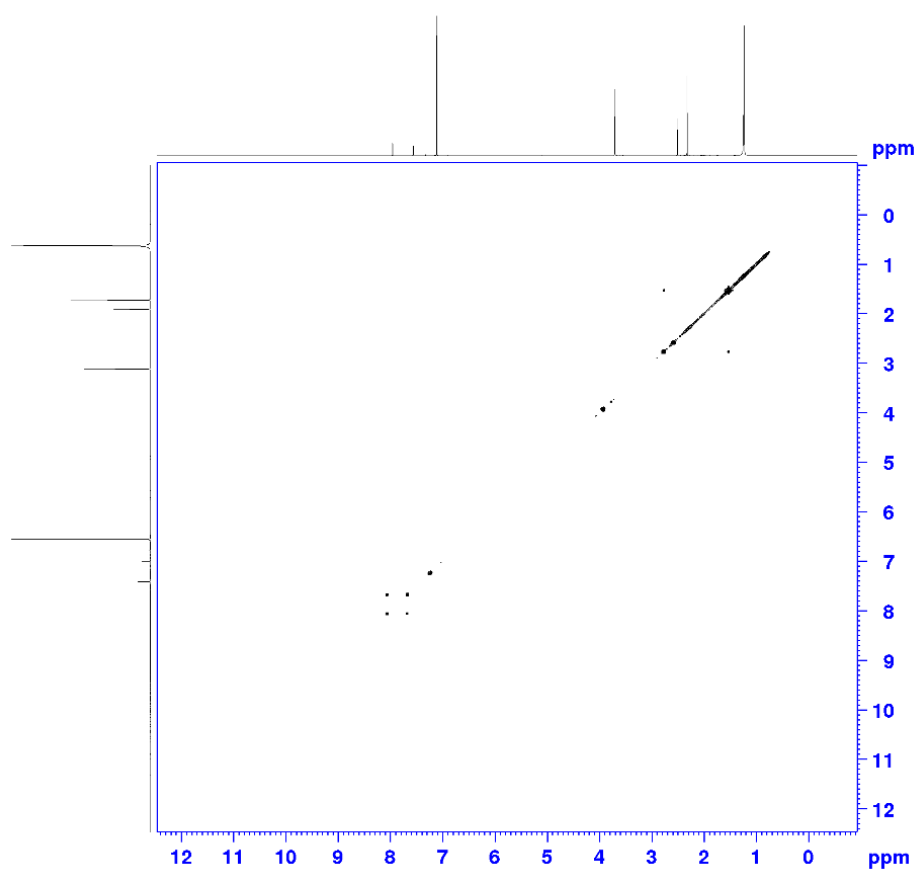


Figure S18. ^1H - ^1H COSY spectrum of **3**.

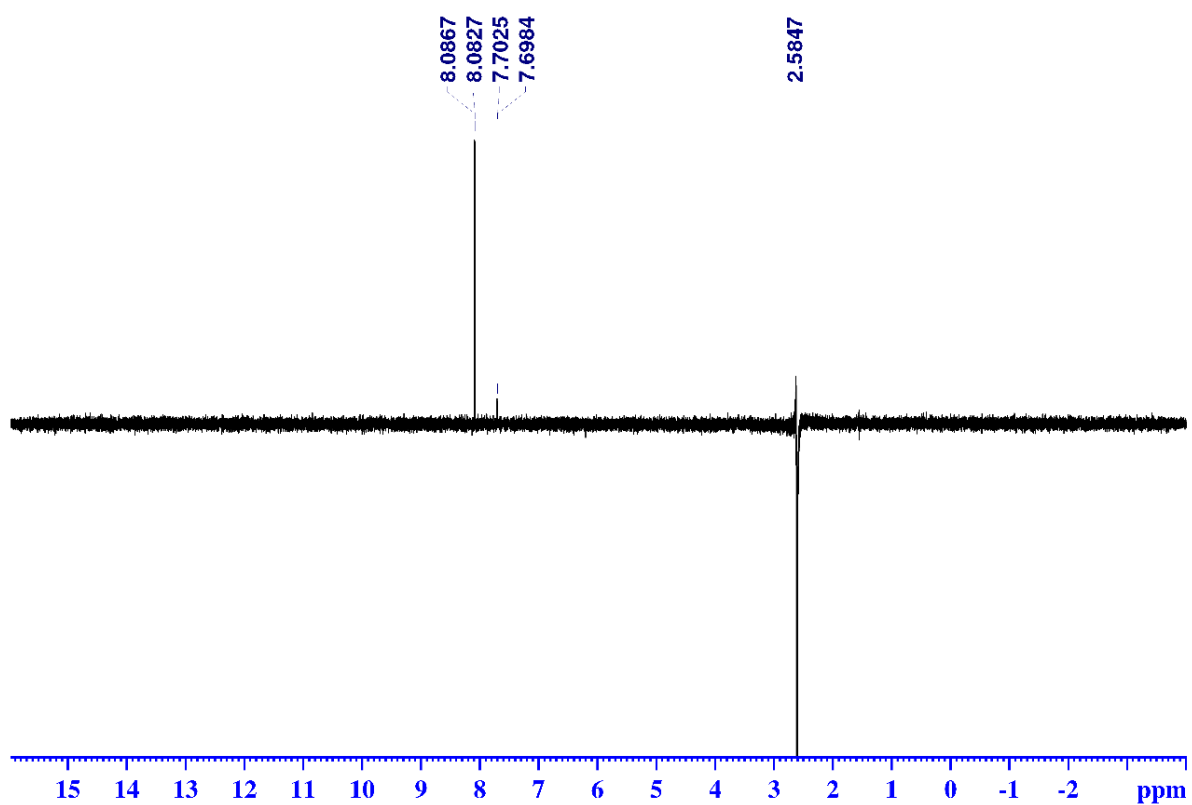


Figure S19. 1D selective NOESY (δ_H 2.58) spectrum of 3.

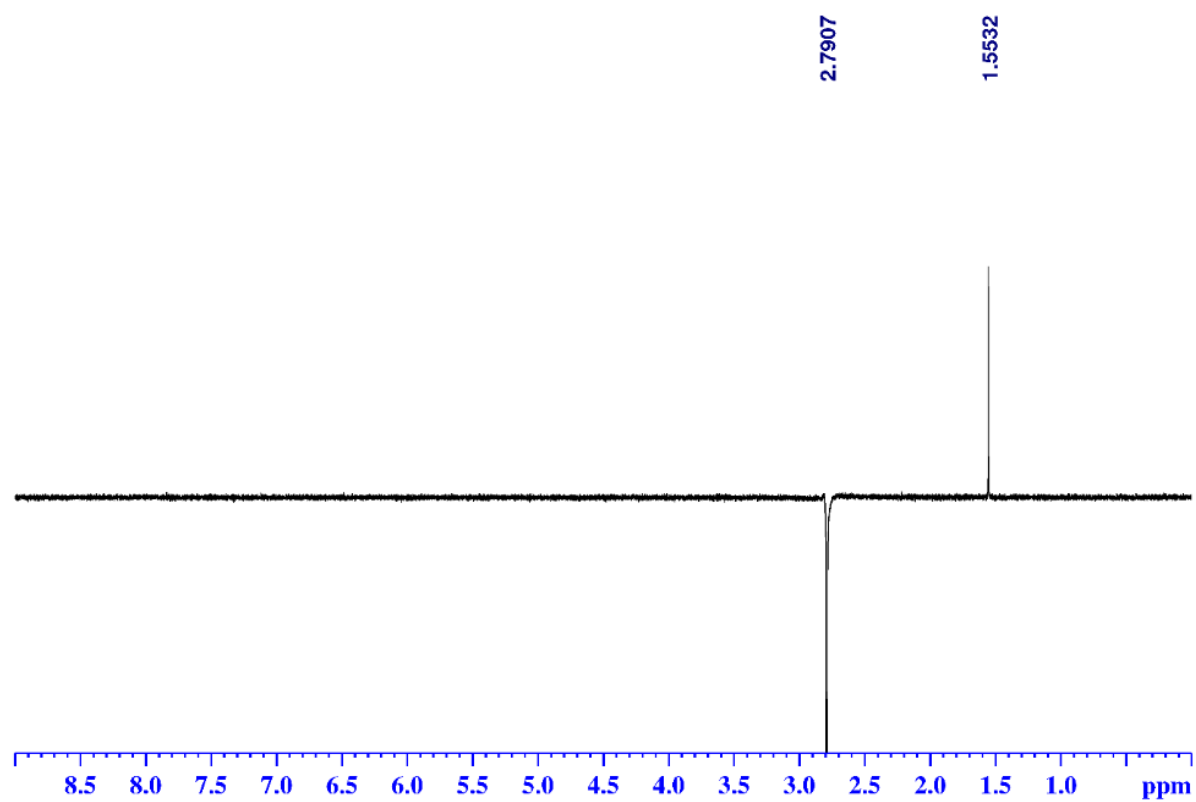


Figure S20. 1D selective NOESY (δ_H 2.79) spectrum of 3.

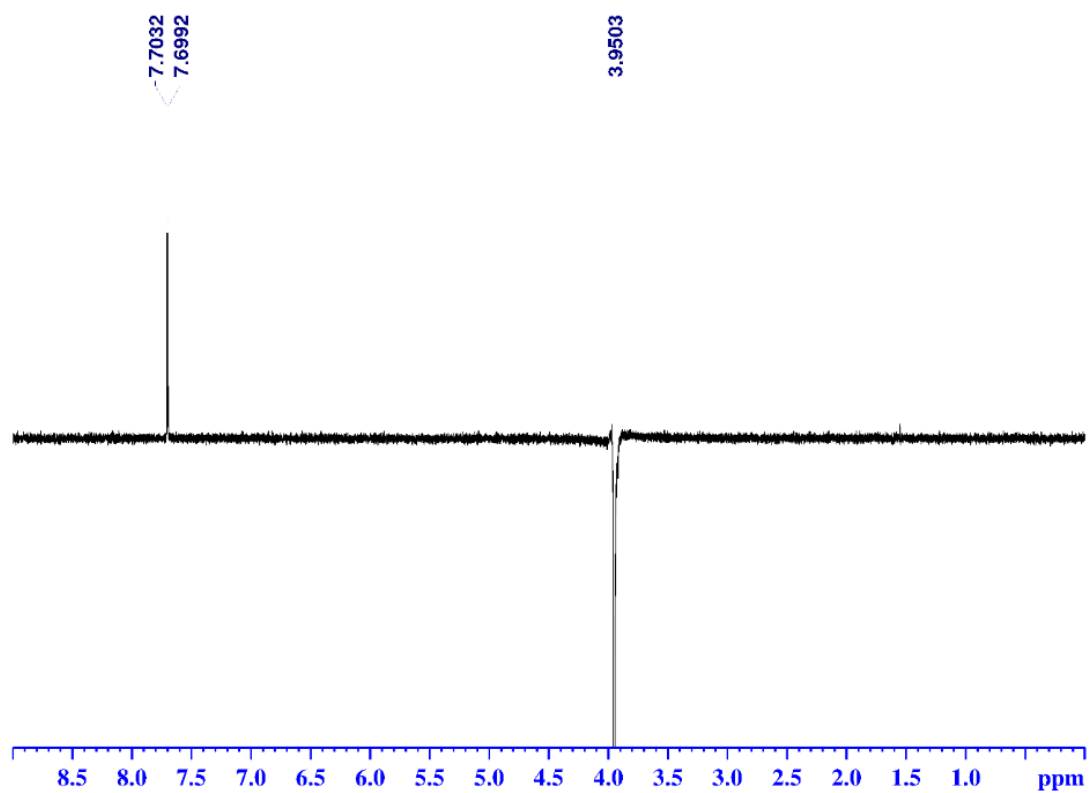


Figure S21. 1D selective NOESY (δ_{H} 3.95) spectrum of 3.

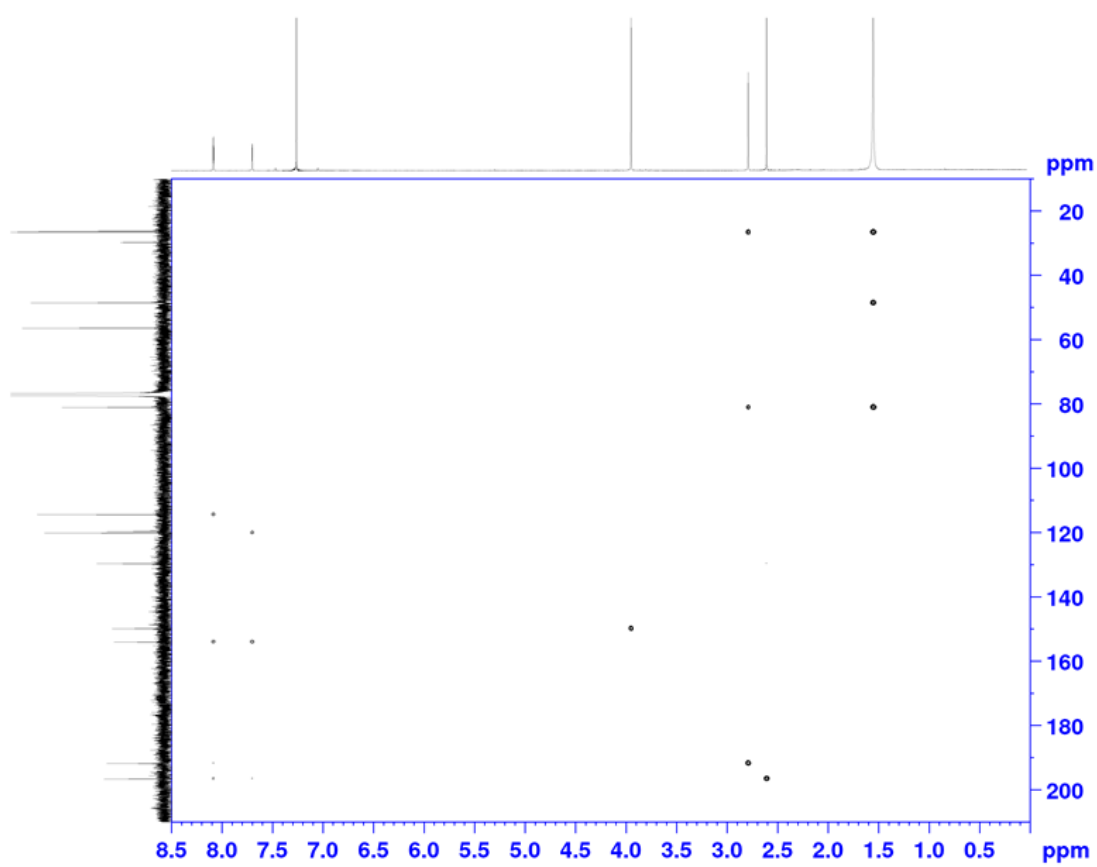


Figure S22. HMBC spectrum of 3.

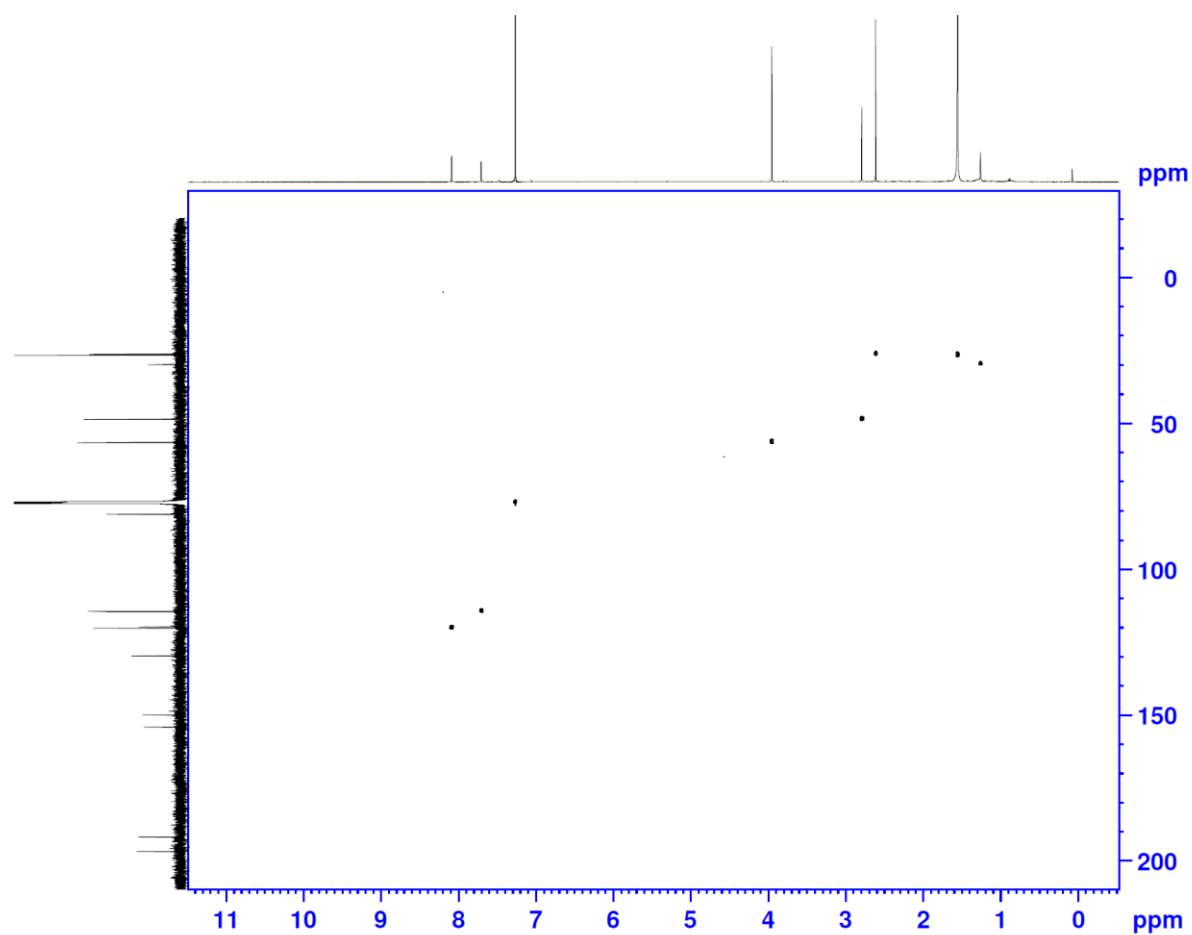
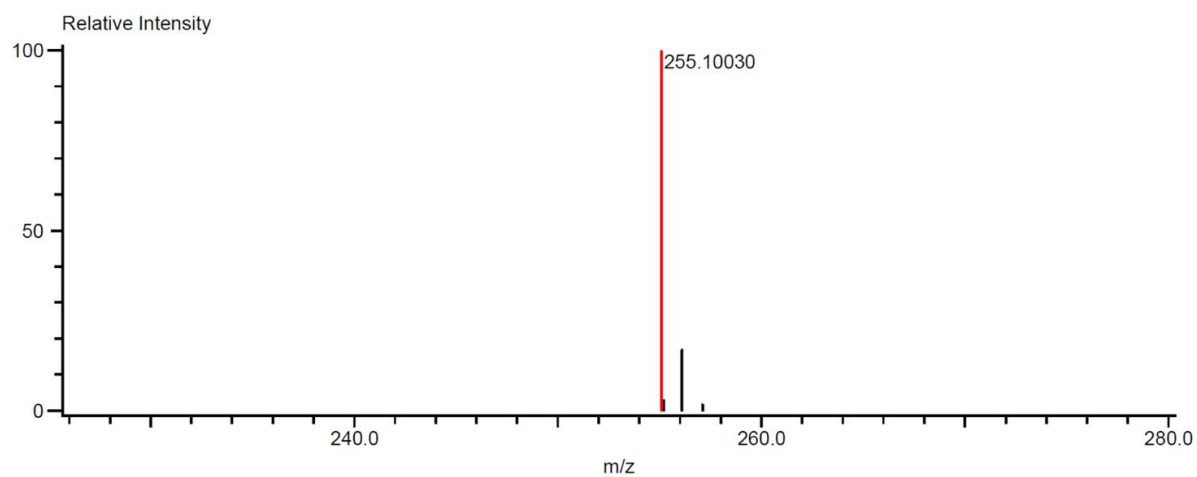


Figure S23. HSQC spectrum of 3.



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
255.10030	30162.90	255.09971	0.58	2.29	$^{12}\text{C}_{14}^{1}\text{H}_{16}^{23}\text{Na}^{16}\text{O}_3$

Figure S24. HR-ESI-MS spectrum of 4.

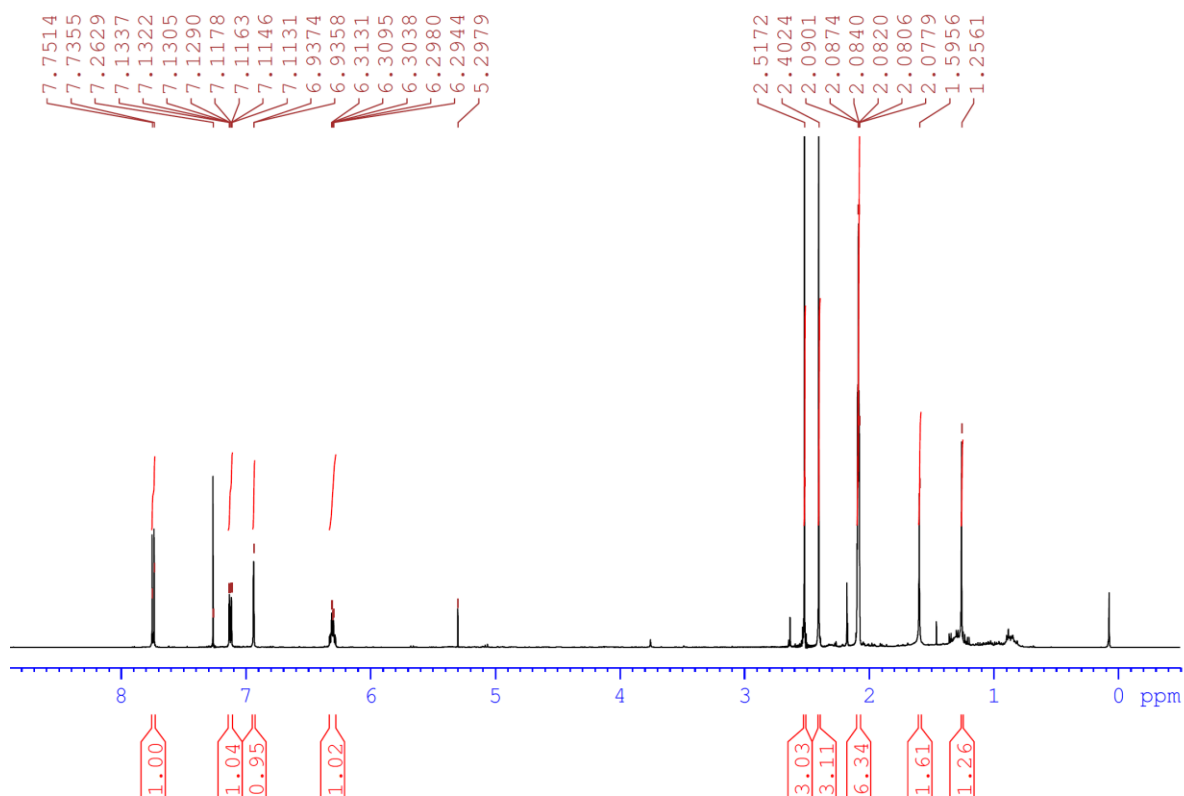


Figure S25. ¹H-NMR spectrum (CDCl₃, 500 MHz) of **4**.

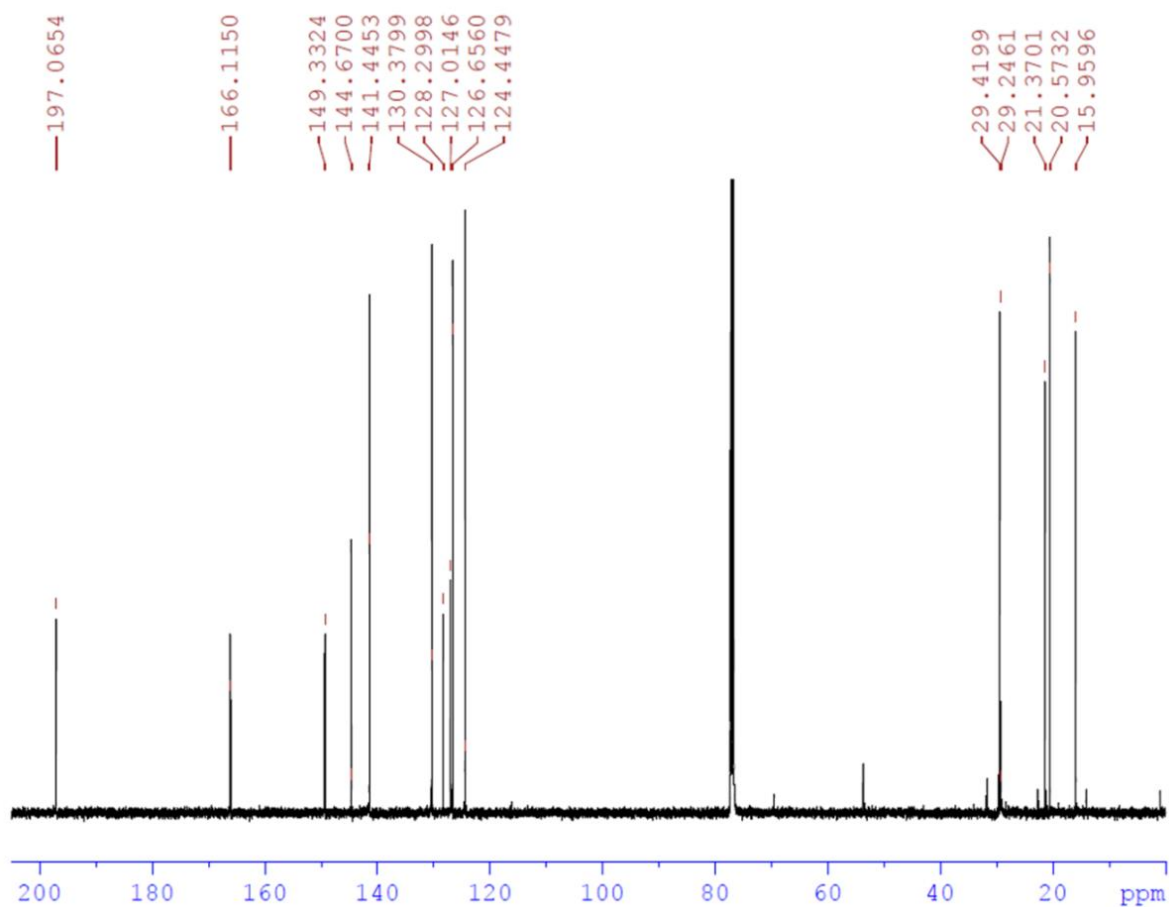


Figure S26. ¹³C-NMR (CDCl₃, 125 MHz) spectrum of **4**.

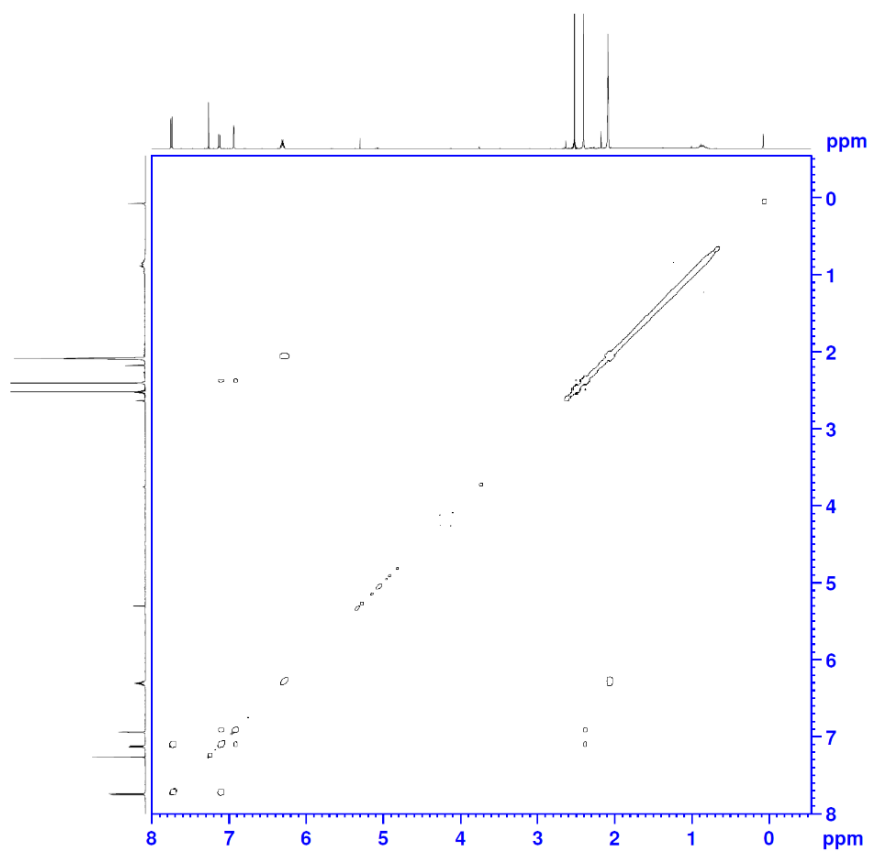


Figure S27. ^1H - ^1H COSY spectrum of **4**.

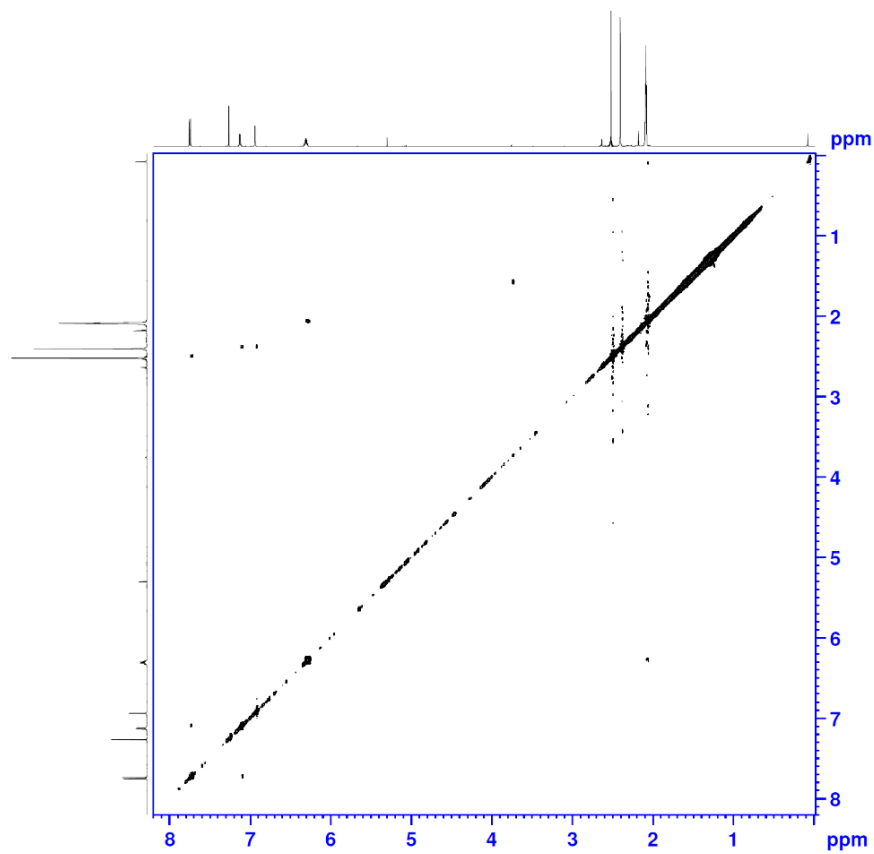


Figure S28. ROESY spectrum of **4**.

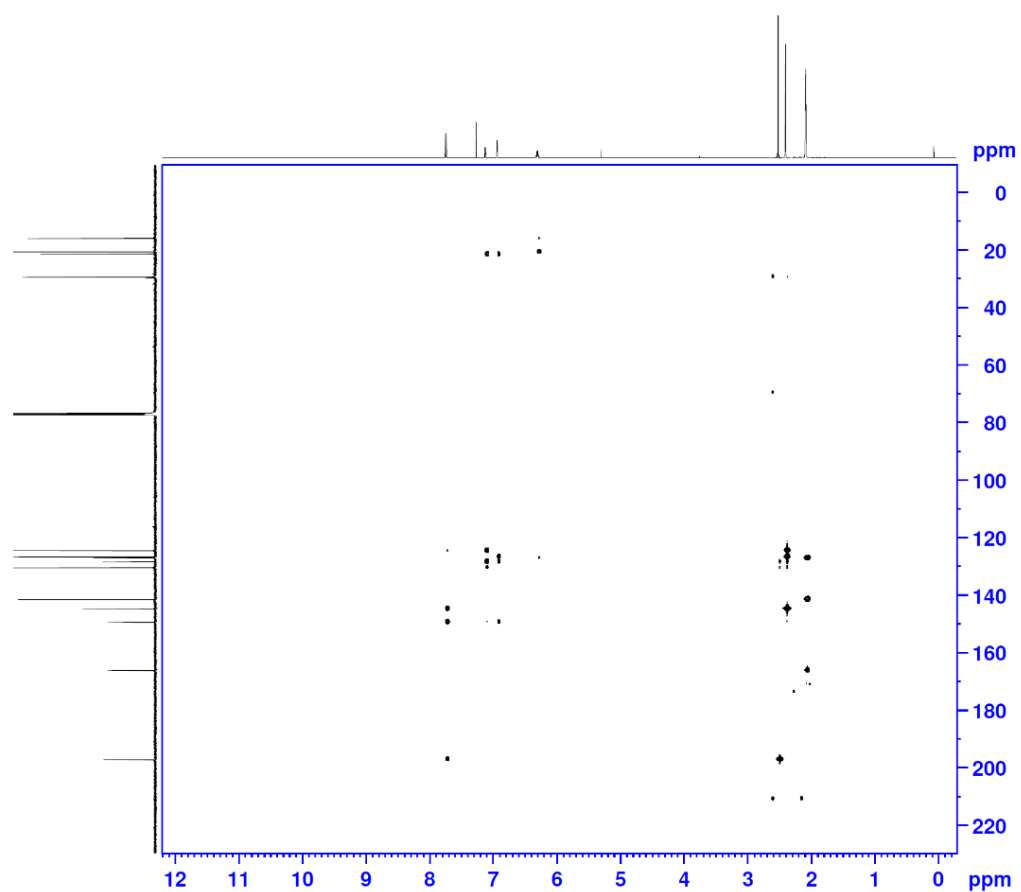


Figure S29. HMBC spectrum of 4.

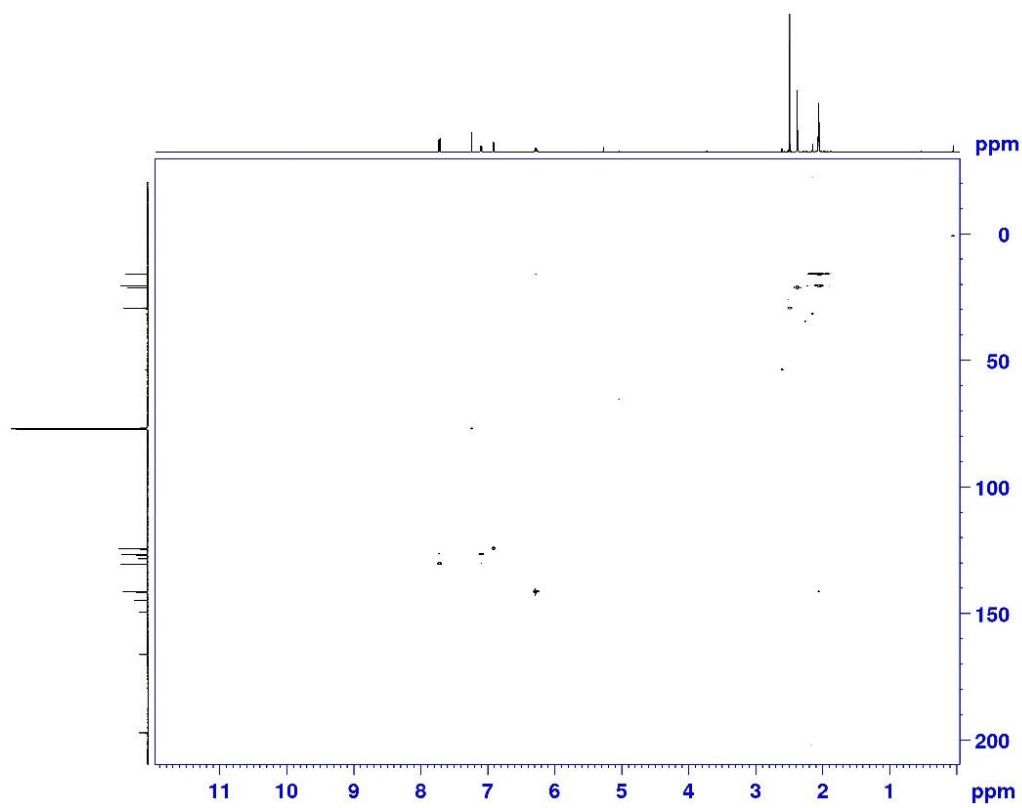


Figure S30. HSQC spectrum of 4.

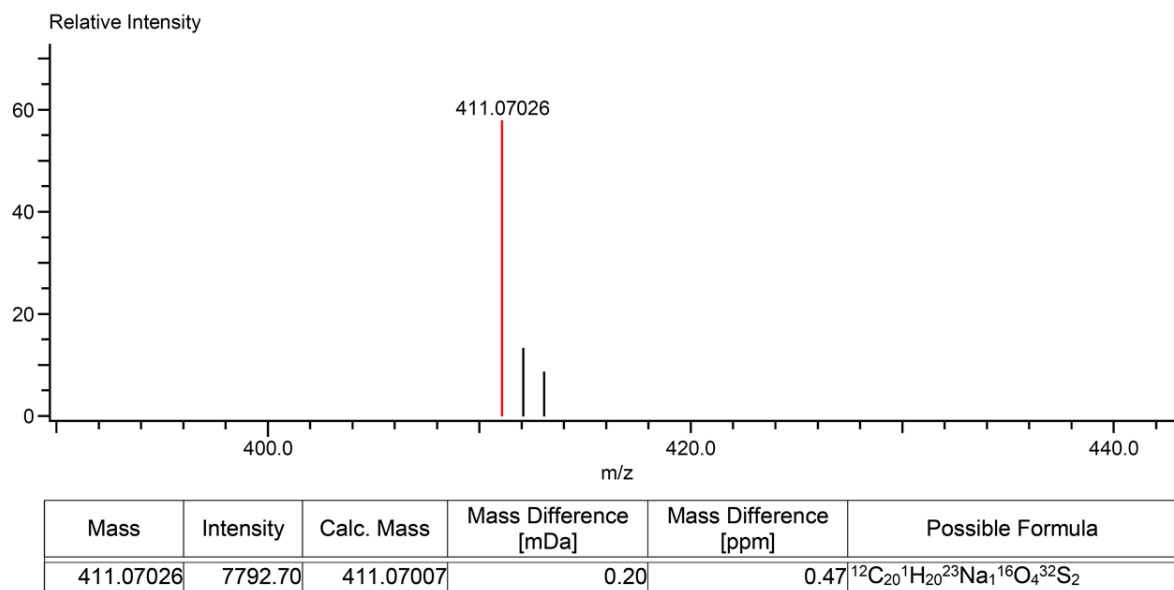


Figure S31. HR-ESI-MS spectrum of **5**.

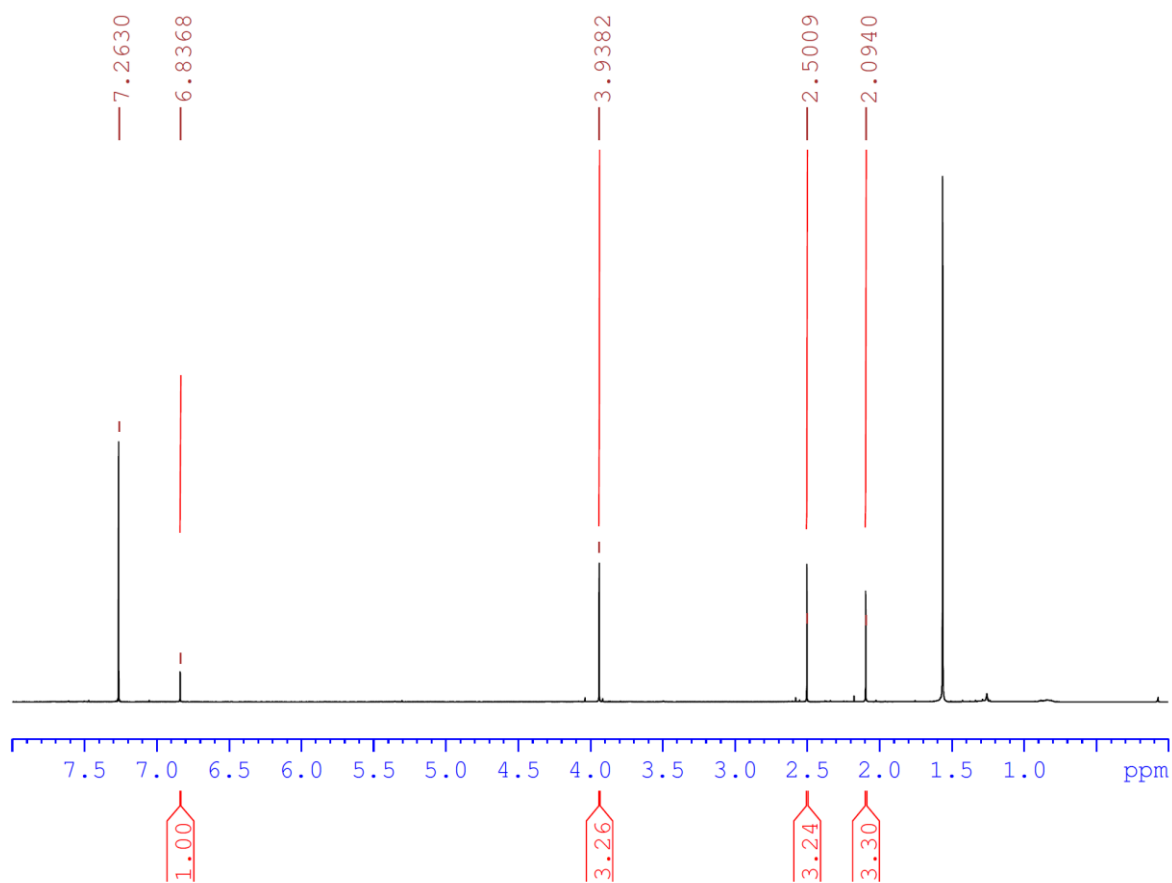


Figure S32. ^1H -NMR spectrum (CDCl_3 , 500 MHz) of **5**.

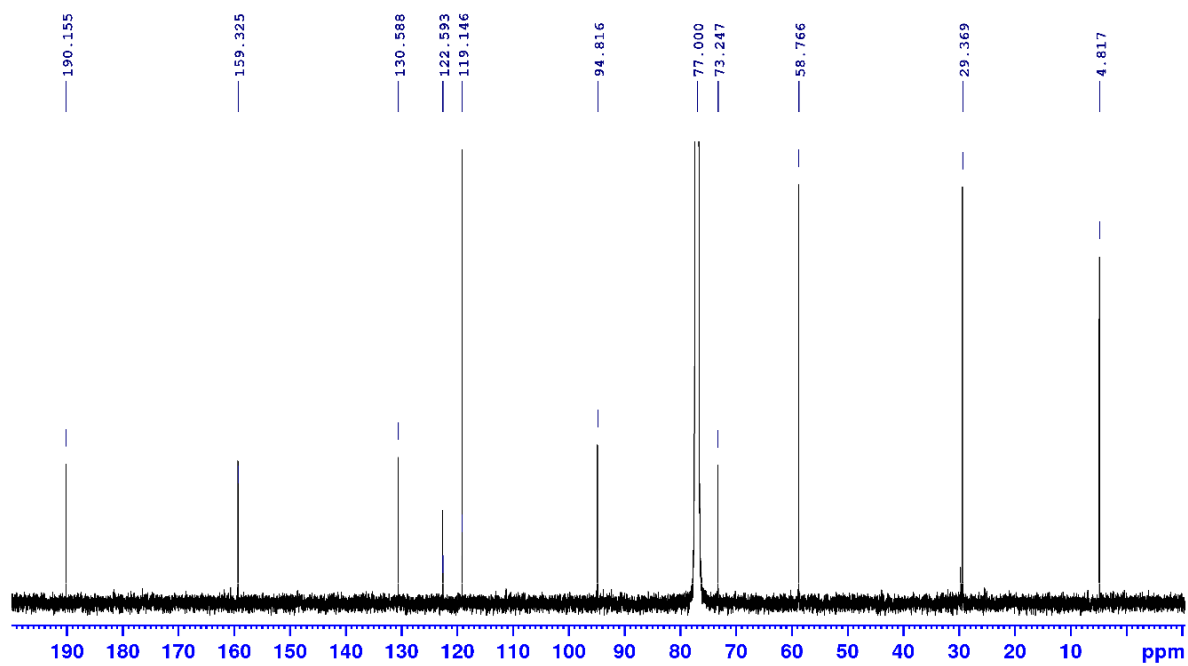


Figure S33. ^{13}C -NMR spectrum (CDCl_3 , 125 MHz) of 5.

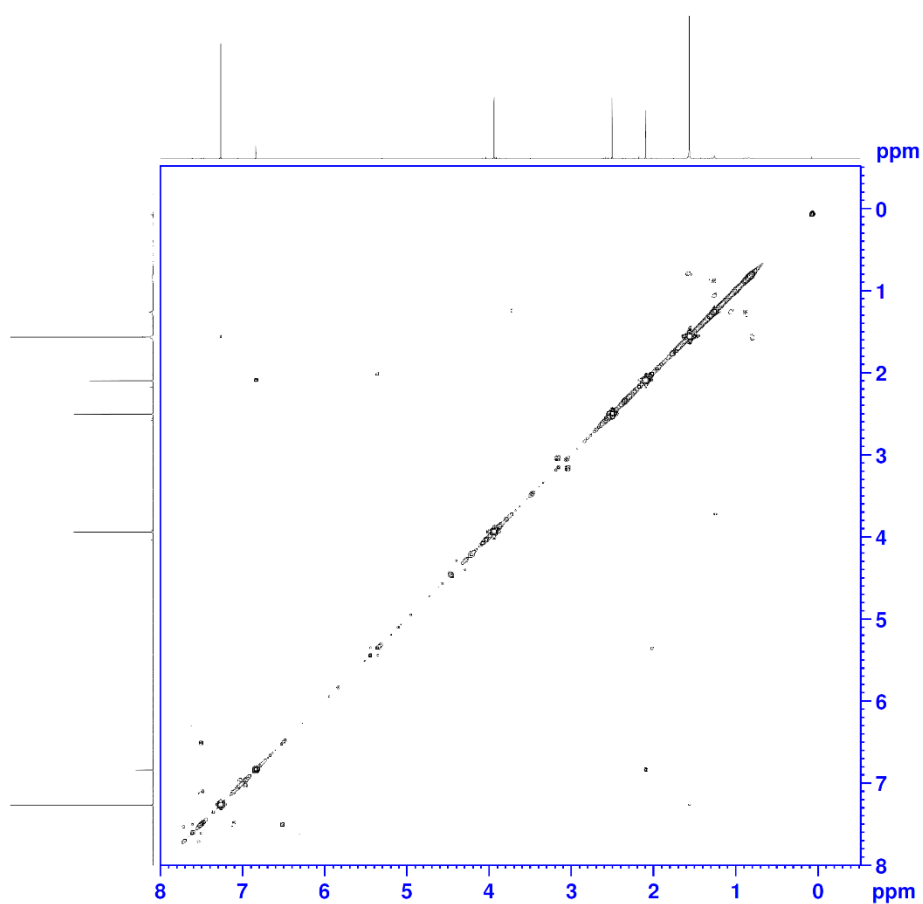


Figure S34. ^1H - ^1H COSY spectrum of 5.

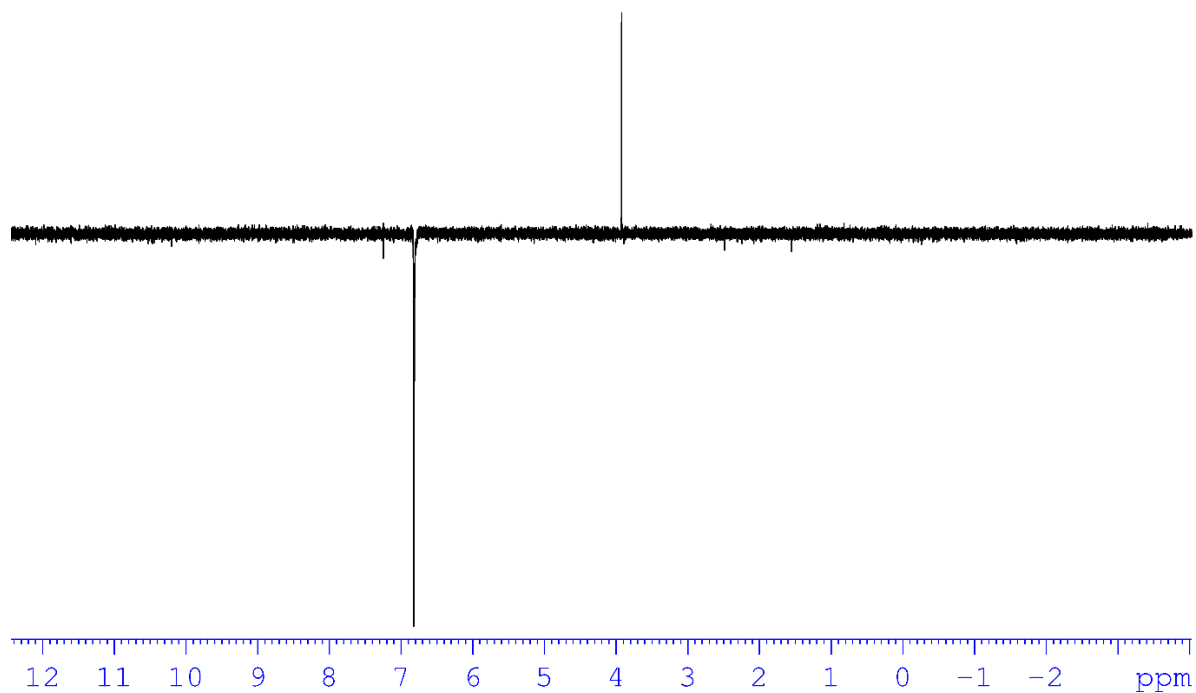


Figure S35. 1D selective NOESY (δ_{H} 6.84) spectrum of 5.

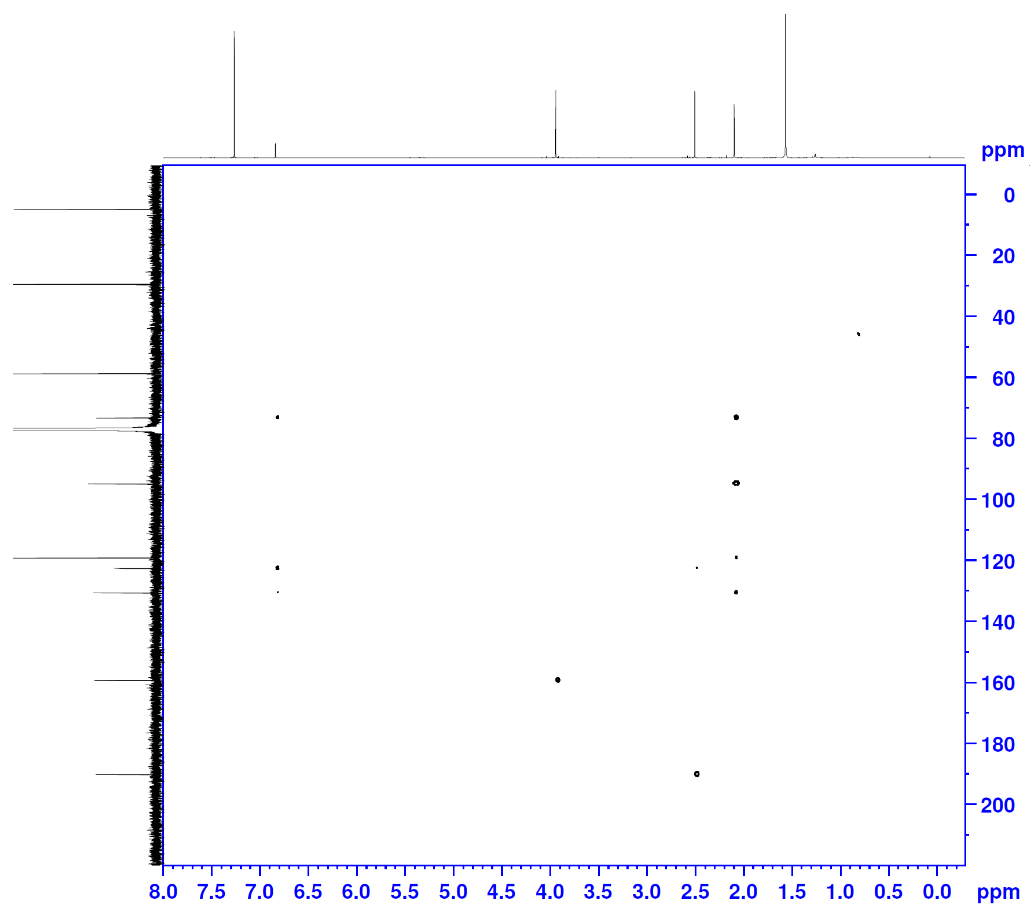


Figure S36. HMBC spectrum of 5.

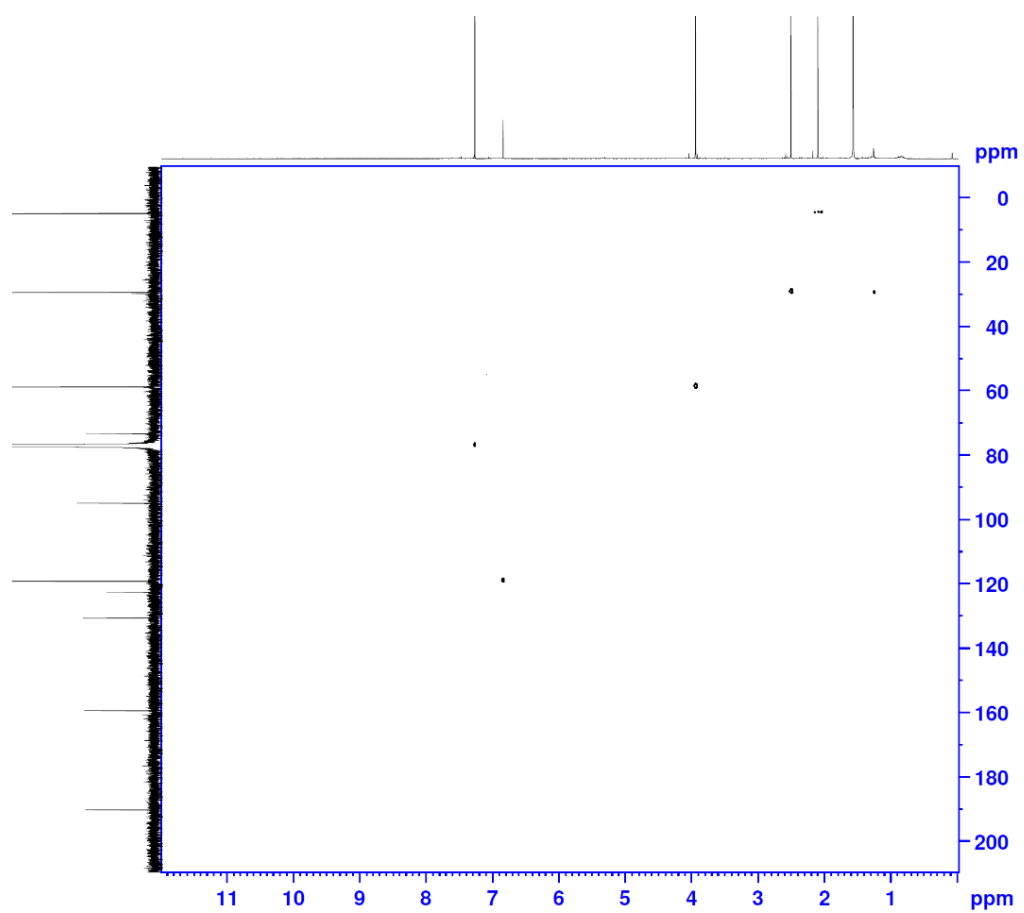


Figure S37. HSQC spectrum of 5.