

# **Constituents of *Pulicaria inuloides* and cytotoxic activities of two methoxylated flavonols**

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## **SUPPLEMENTARY MATERIAL**

**Figure S1.** LRESIMS and HRESIMS of compound **2**.

**Figure S2.**  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{CDCl}_3$ .

**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **2** in  $\text{CDCl}_3$ .

**Figure S4.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**.

**Figure S5.** COSY correlations for compound **2**.

**Figure S6.** NOESY spectrum of compound **2**.

**Figure S7.** HSQC spectrum of compound **2**.

**Figure S8.** HMBC spectrum of compound **2**.

**Figure S9.** HMBC correlations for compound **2**.

**Figure S10.**  $^1\text{H}$  NMR spectrum of compound **9** in  $\text{CDCl}_3$ .

**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound **9** in  $\text{CDCl}_3$ .

**Figure S12.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **9**.

**Figure S13.** NOESY spectrum of compound **9**.

**Figure S14.** HSQC spectrum of compound **9**.

**Figure S15.** HMBC spectrum of compound **9**.

**Figure S16.**  $^1\text{H}$  NMR spectrum of the mixture containing compound **3** in  $\text{CDCl}_3$ .

**Figure S17.**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{CDCl}_3$ .

**Figure S18.**  $^1\text{H}$  NMR spectrum of compound **8** in  $\text{CDCl}_3$ .

**Figure S19.**  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{CDCl}_3$ .

**Figure S20.**  $^1\text{H}$  NMR spectrum of compound **4** in  $\text{CDCl}_3$ .

**Figure S21.**  $^1\text{H}$  NMR spectrum of compound **5** in  $\text{CDCl}_3$ .

**Figure S22.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$ .

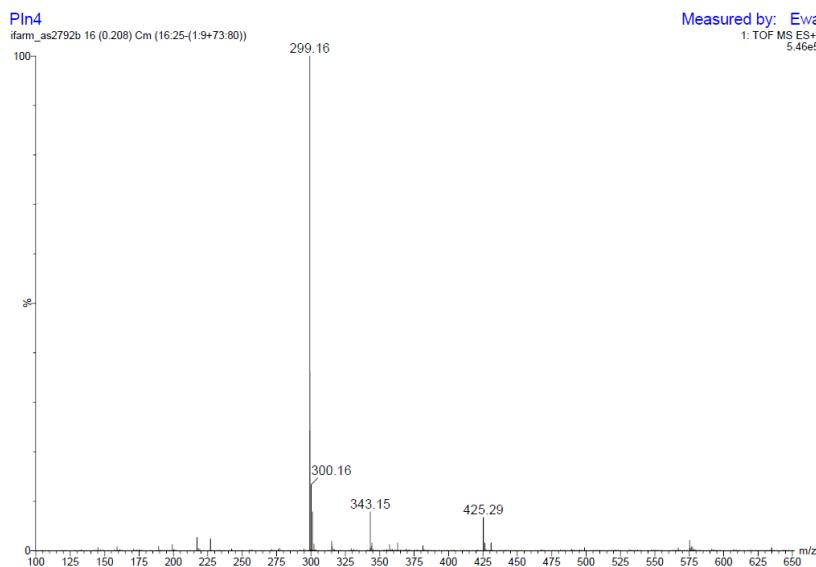
**Figure S23.**  $^1\text{H}$  NMR spectrum of compound **10** in  $\text{CDCl}_3$ .

**Figure S24.**  $^1\text{H}$  NMR spectrum of compound **11** in  $\text{CDCl}_3$ .

**Figure S25.**  $^1\text{H}$  NMR spectrum of compound **12** in  $\text{CDCl}_3$ .

**Figure S26.**  $^1\text{H}$  NMR spectrum of compound **13** in  $\text{CDCl}_3$ .

**Figure S27.**  $^1\text{H}$  NMR spectrum of compound **13** in  $\text{DMSO-d}_6$ .



### Single Mass Analysis

Tolerance = 3.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

48 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-200 H: 0-200 O: 0-5 Na: 0-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
299.1620	299.1623	-0.3	-1.0	5.5	C17 H24 O3 Na	1171.9	n/a	n/a	17	24	3	1

**Figure S1.** LRESIMS and HRESIMS of compound 2.

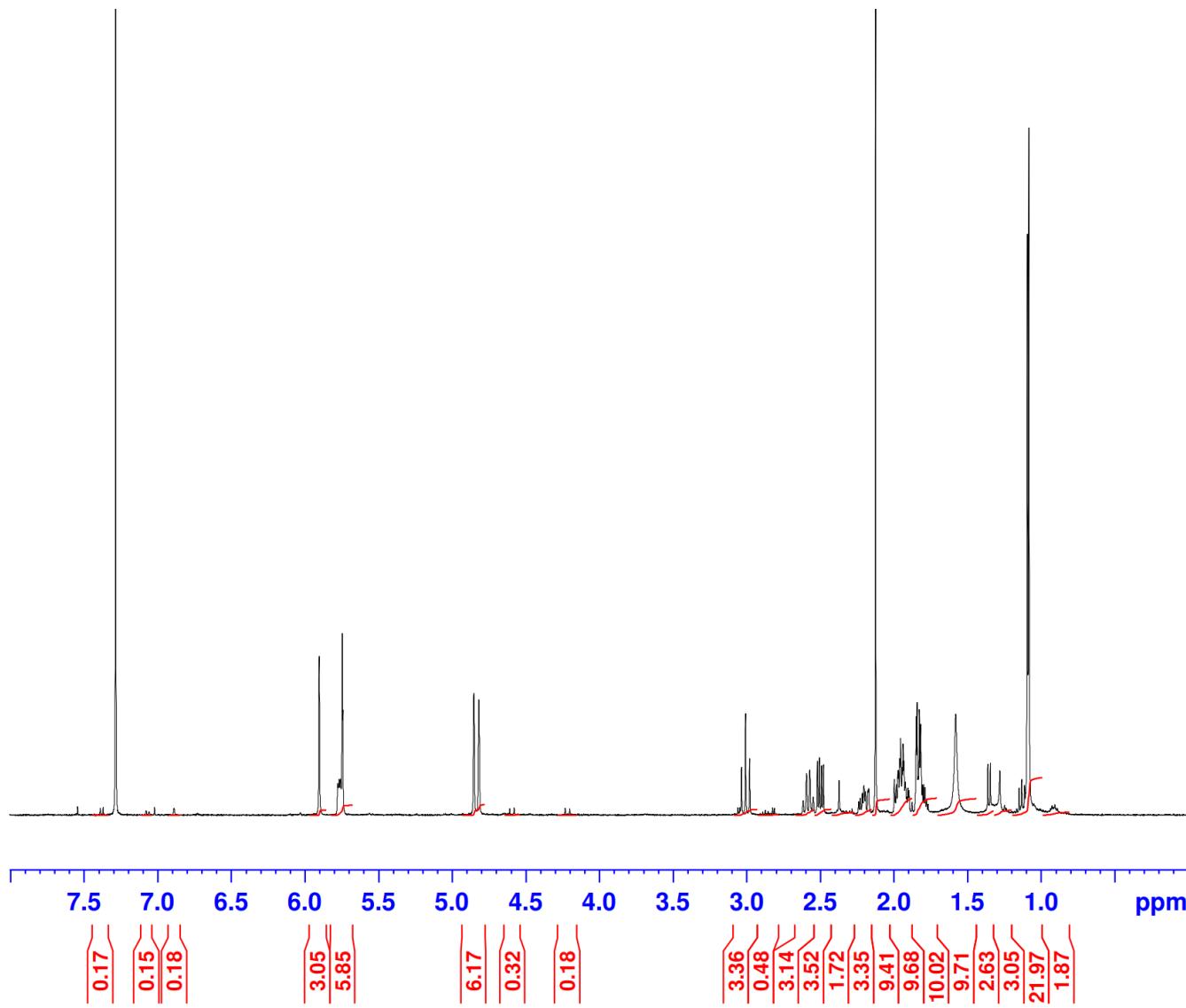
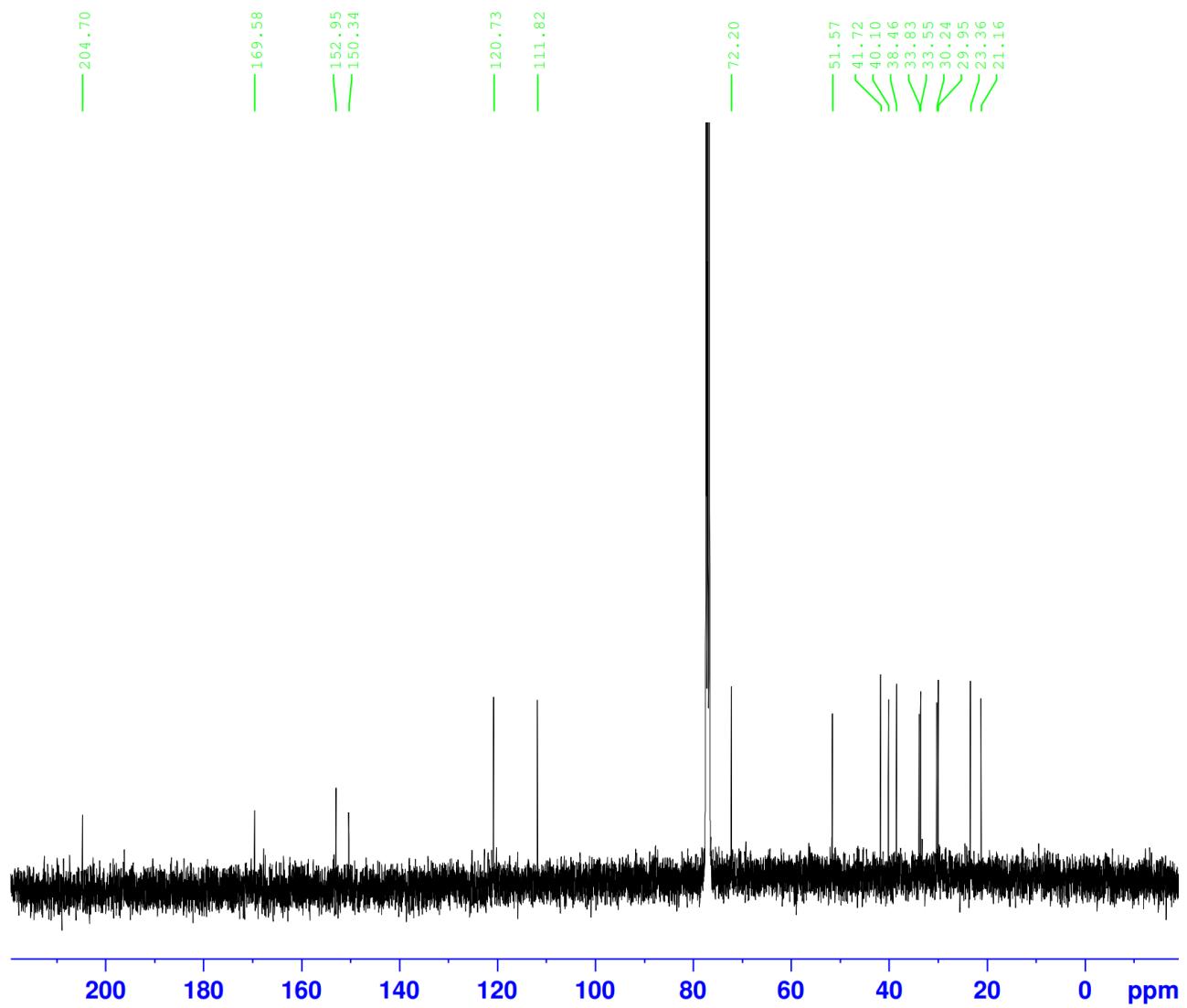
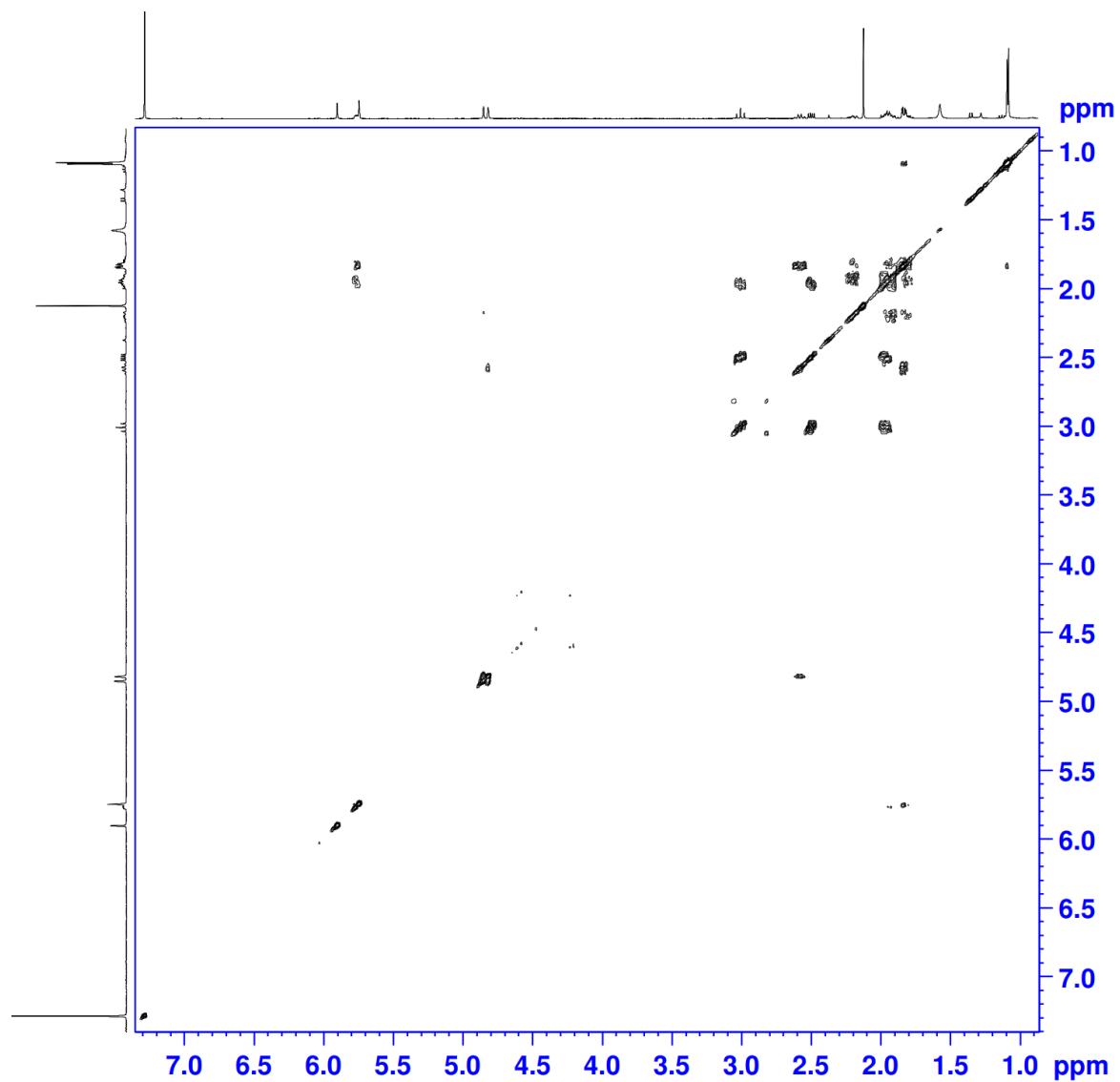


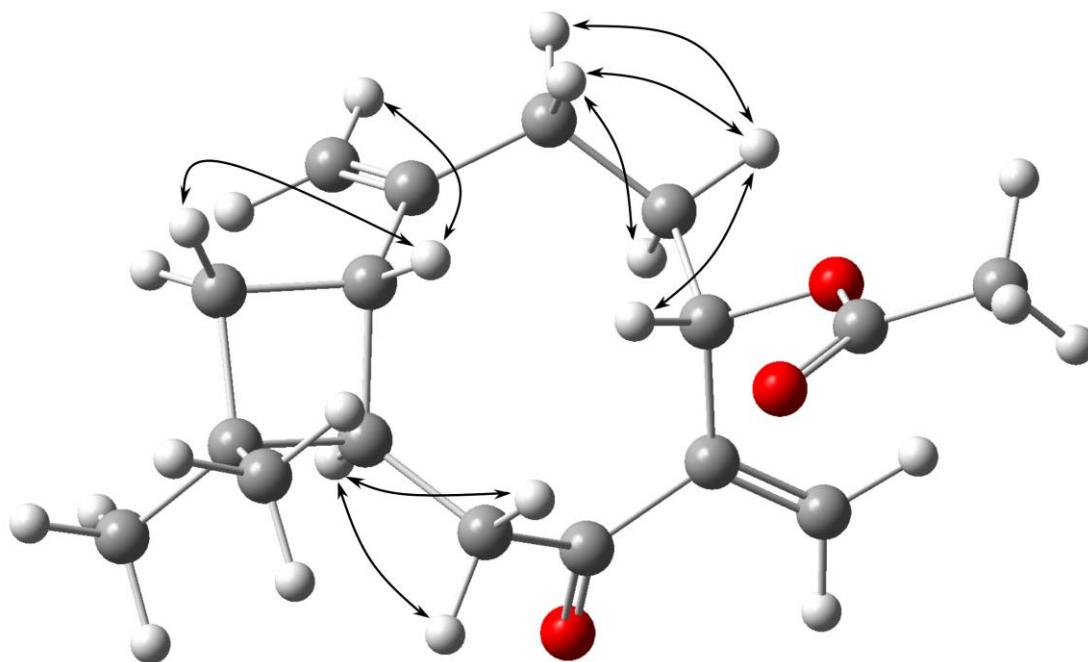
Figure S2.  $^1\text{H}$  NMR spectrum of compound 2 in  $\text{CDCl}_3$ .



**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound 2 in  $\text{CDCl}_3$ .

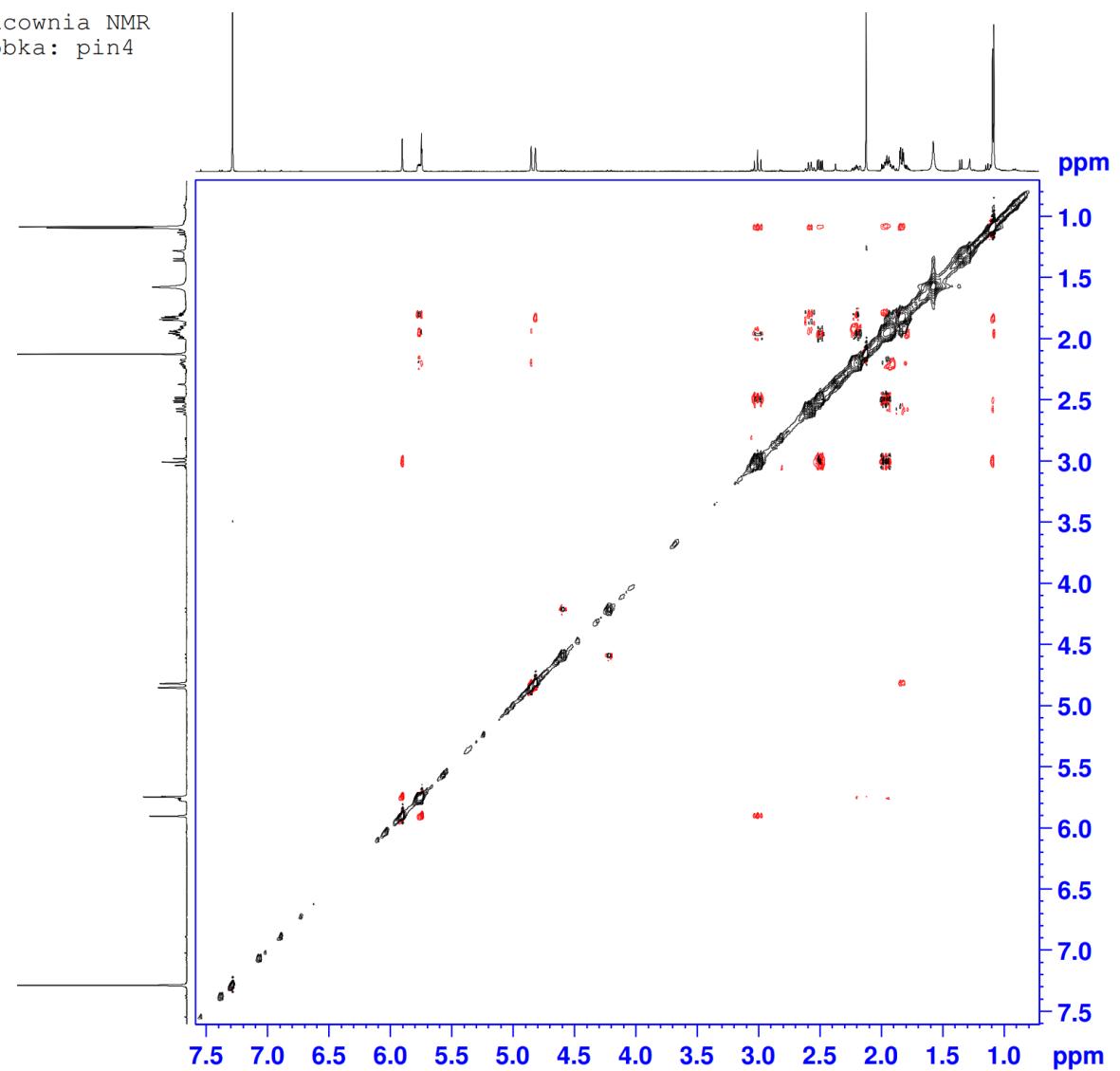


**Figure S4.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**.



**Figure S5.** COSY correlations for compound 2

Pracownia NMR  
Probka: pin4



**Figure S6.** NOESY spectrum of compound 2.

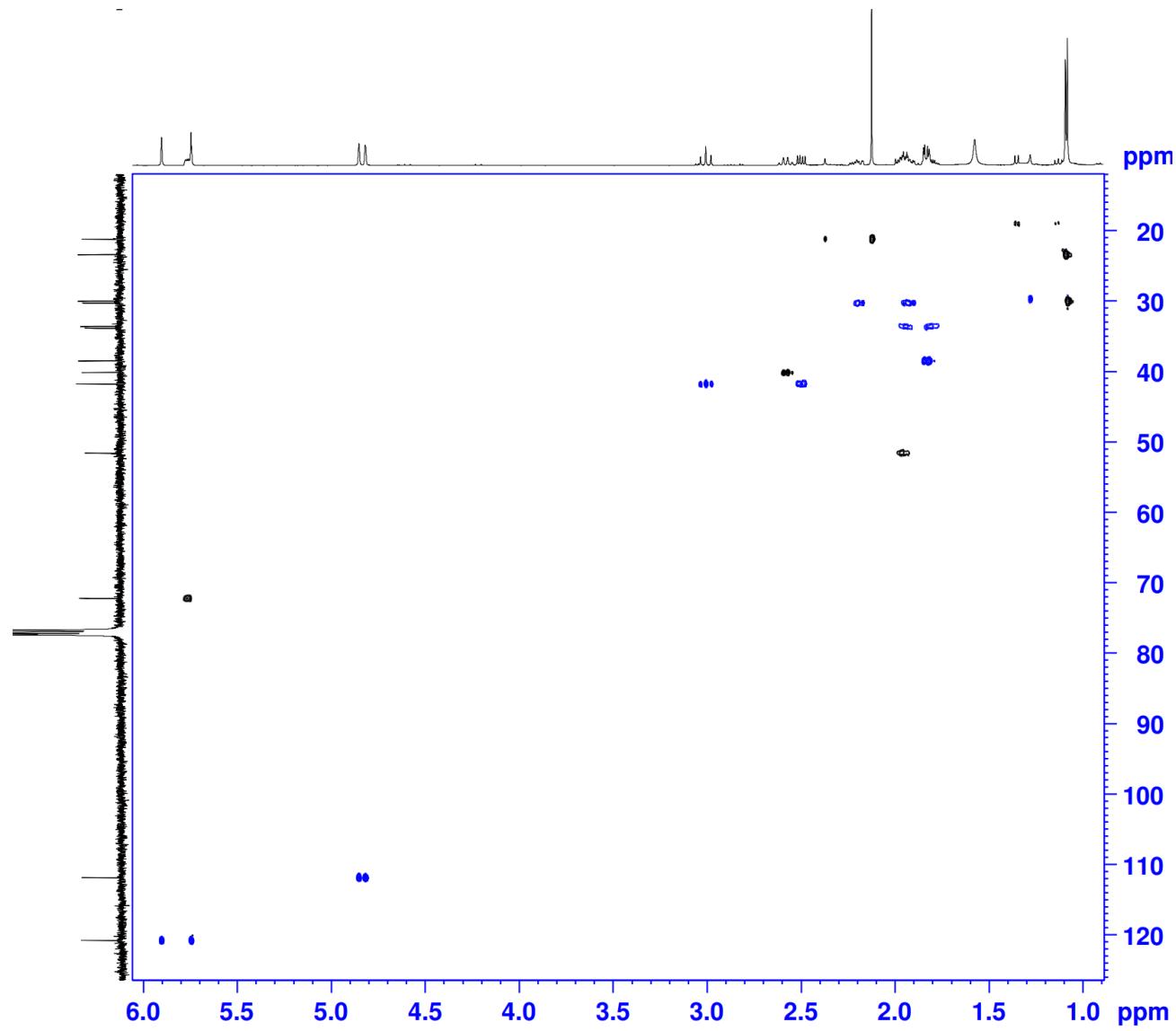


Figure S7. HSQC spectrum of compound 2.

Probka: pin4

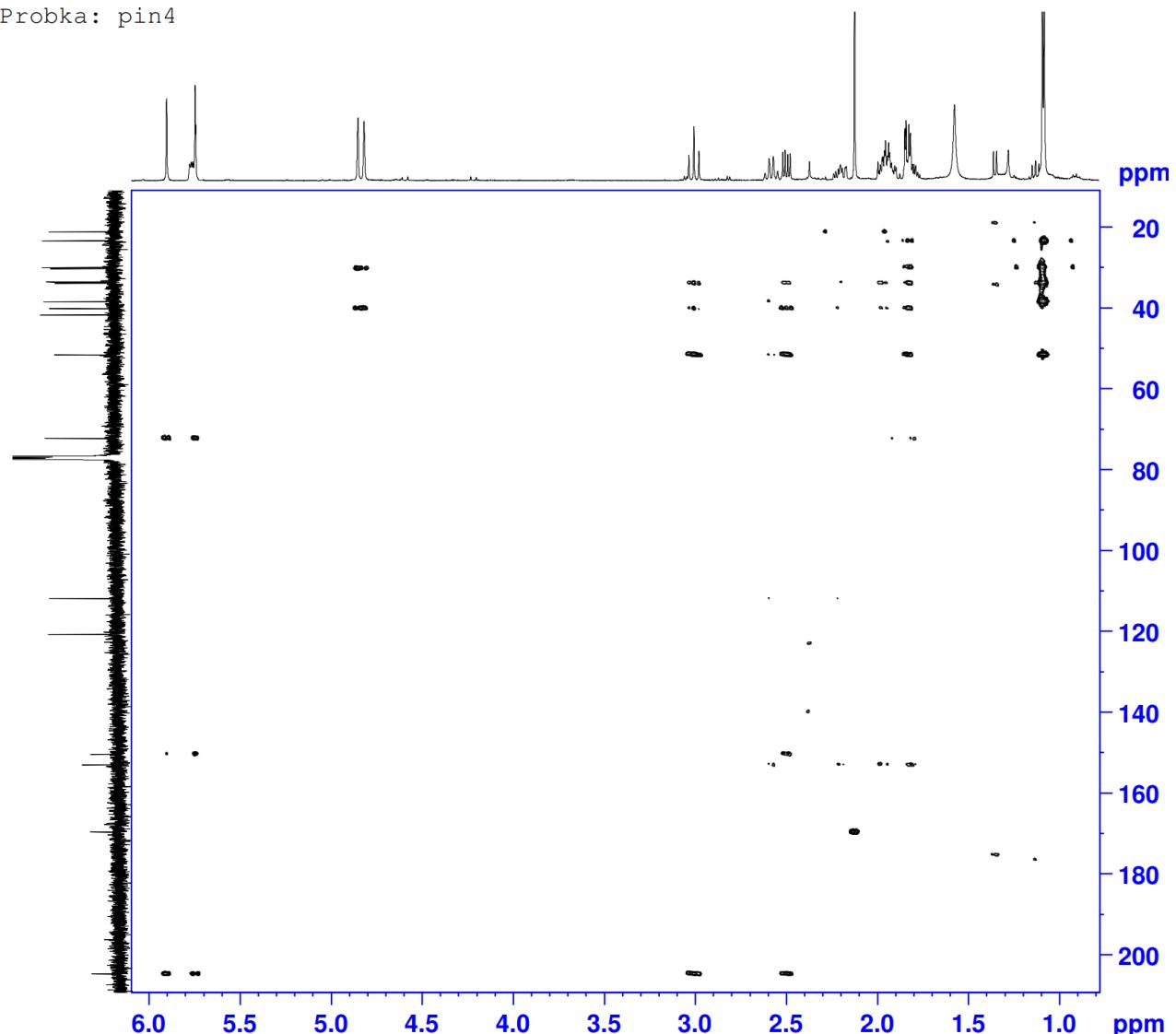
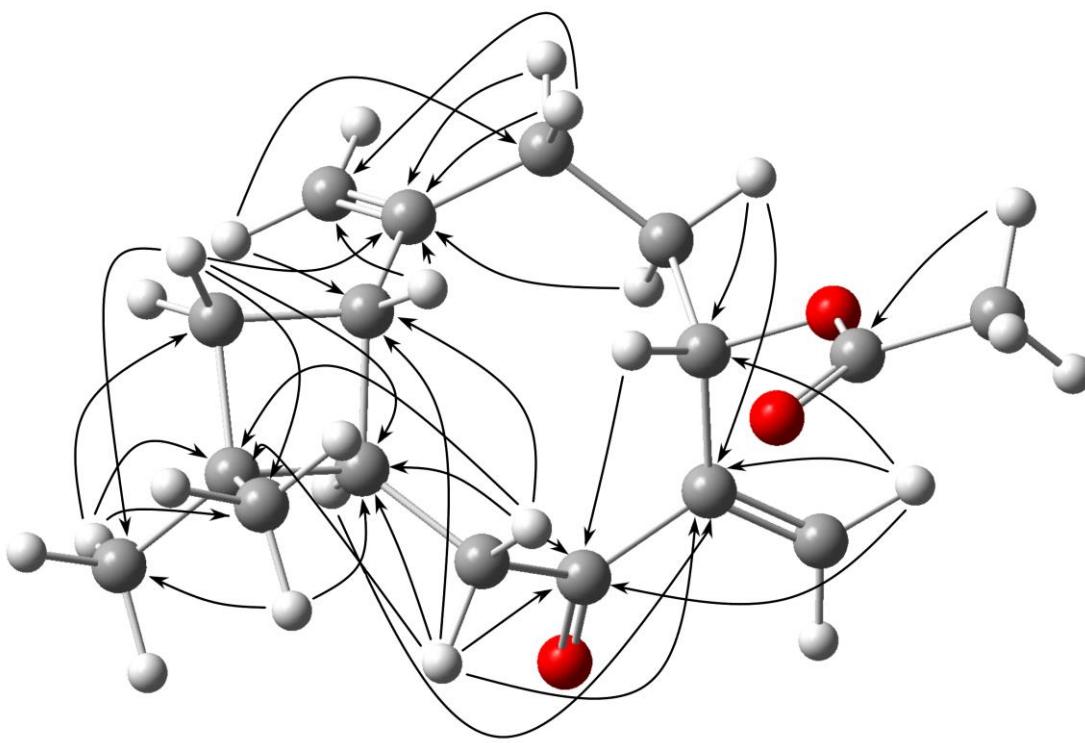
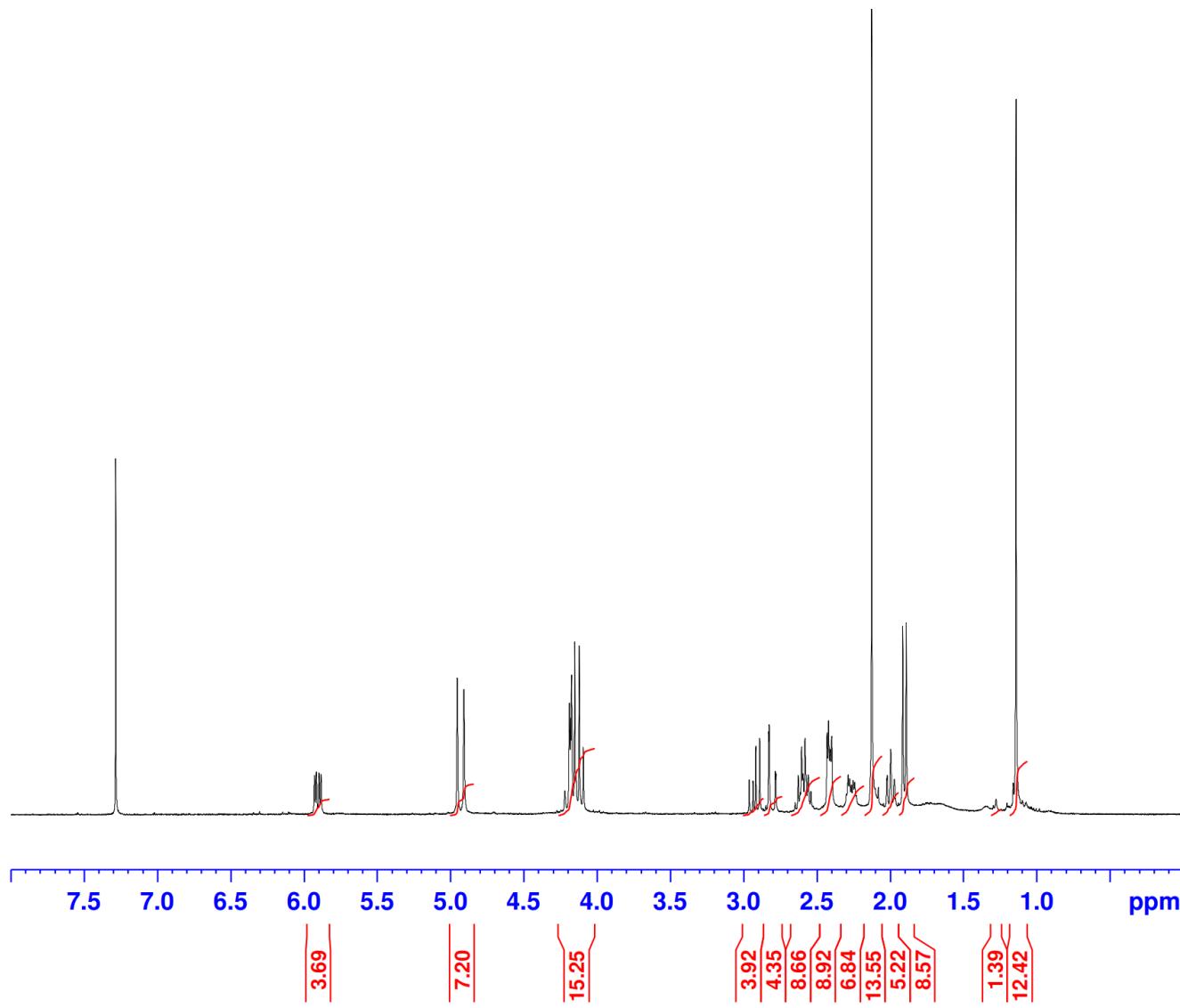


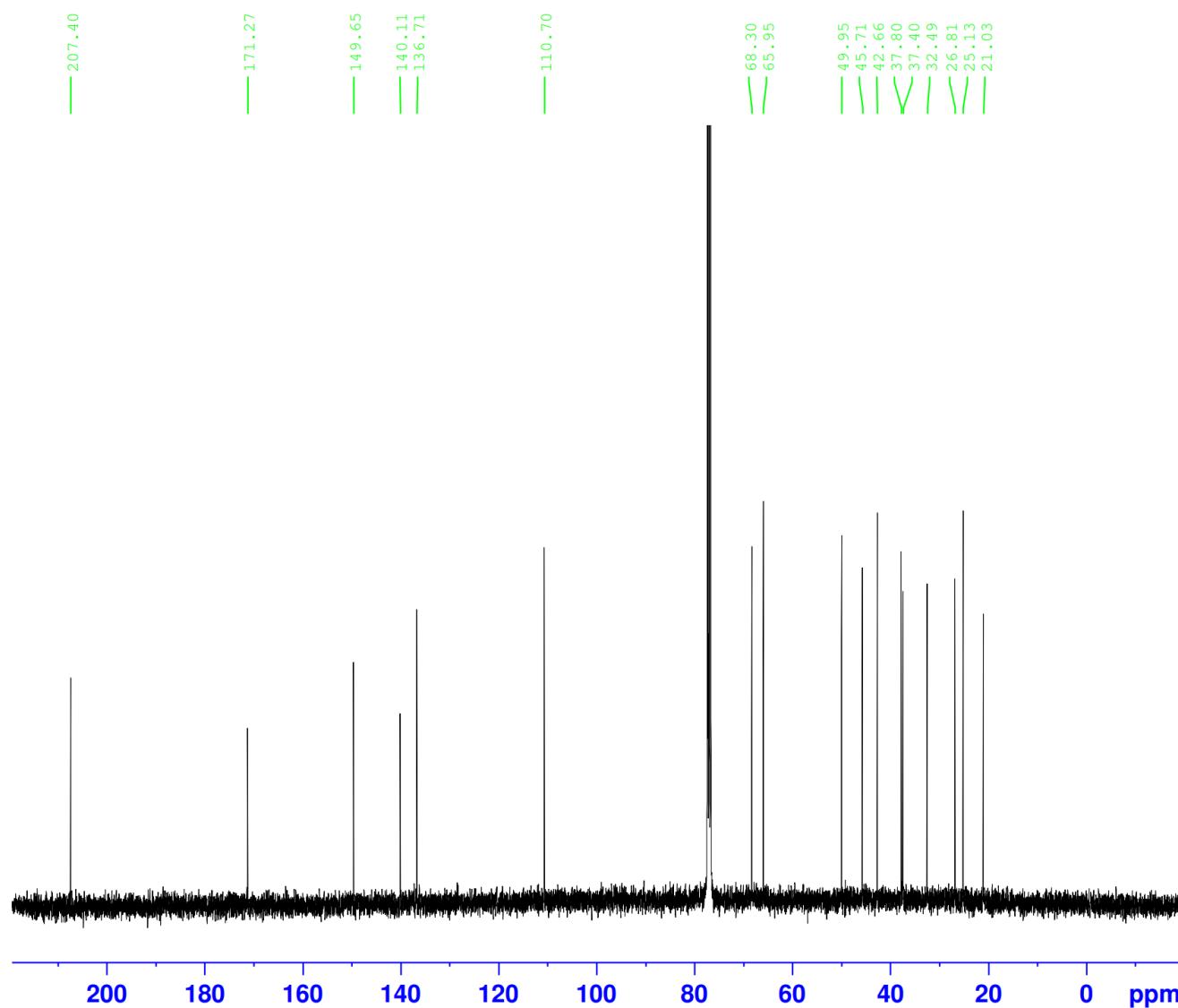
Figure S8. HMBC spectrum of compound 2.



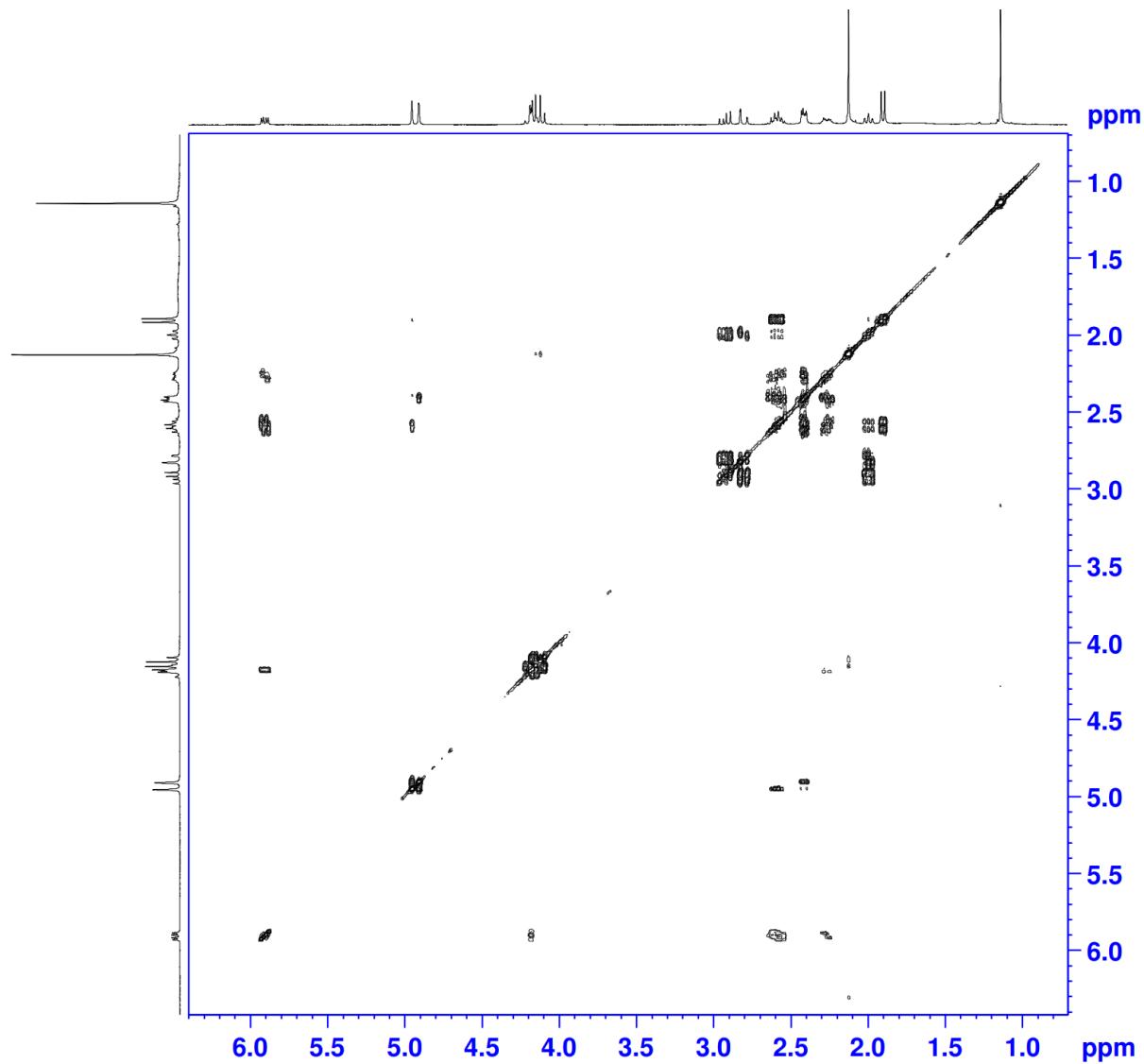
**Figure S9.** HMBC correlations for compound 2



**Figure S10.** <sup>1</sup>H NMR spectrum of compound **9** in  $\text{CDCl}_3$ .



**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound **9** in  $\text{CDCl}_3$ .



**Figure S12.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 9.

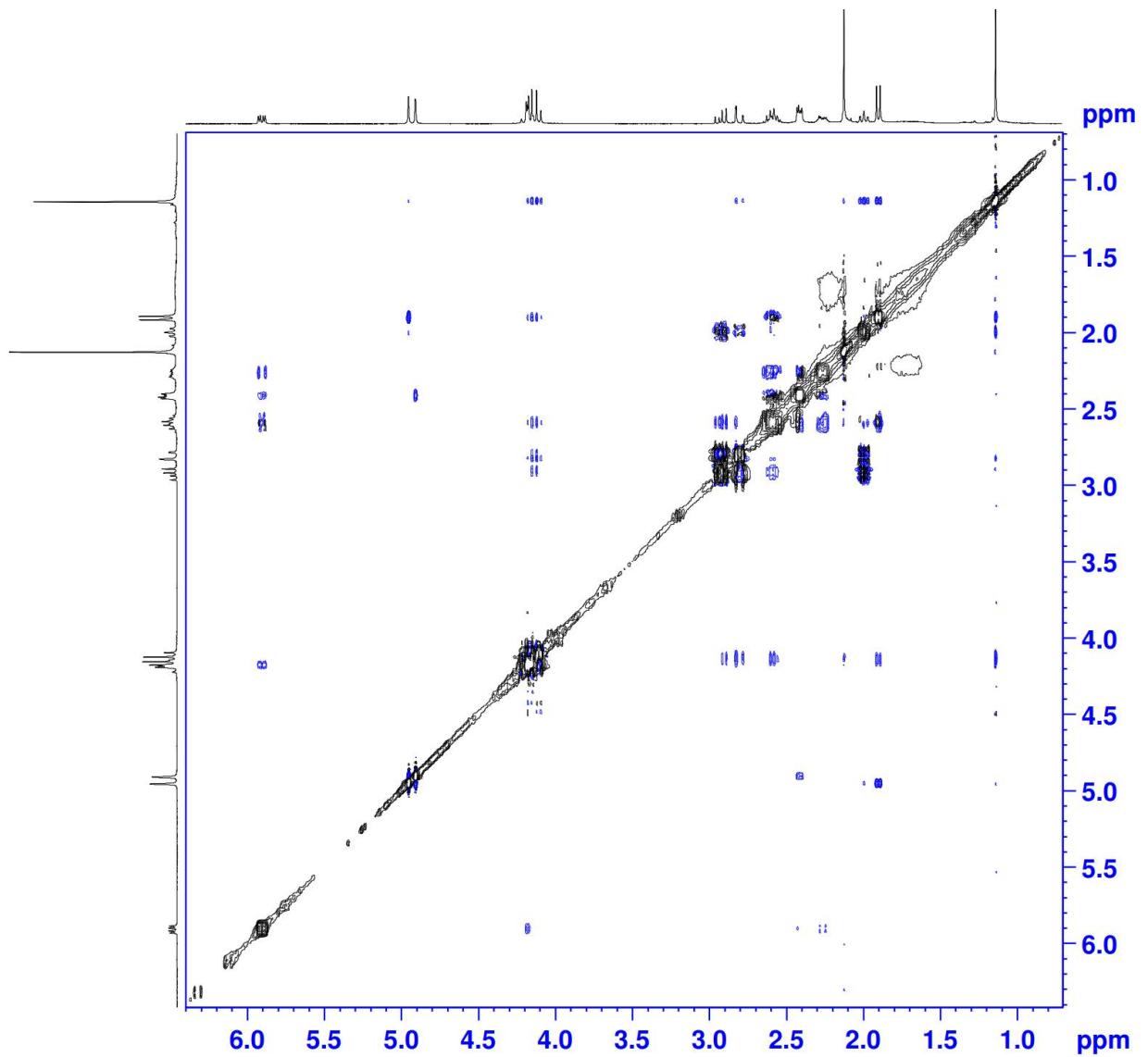
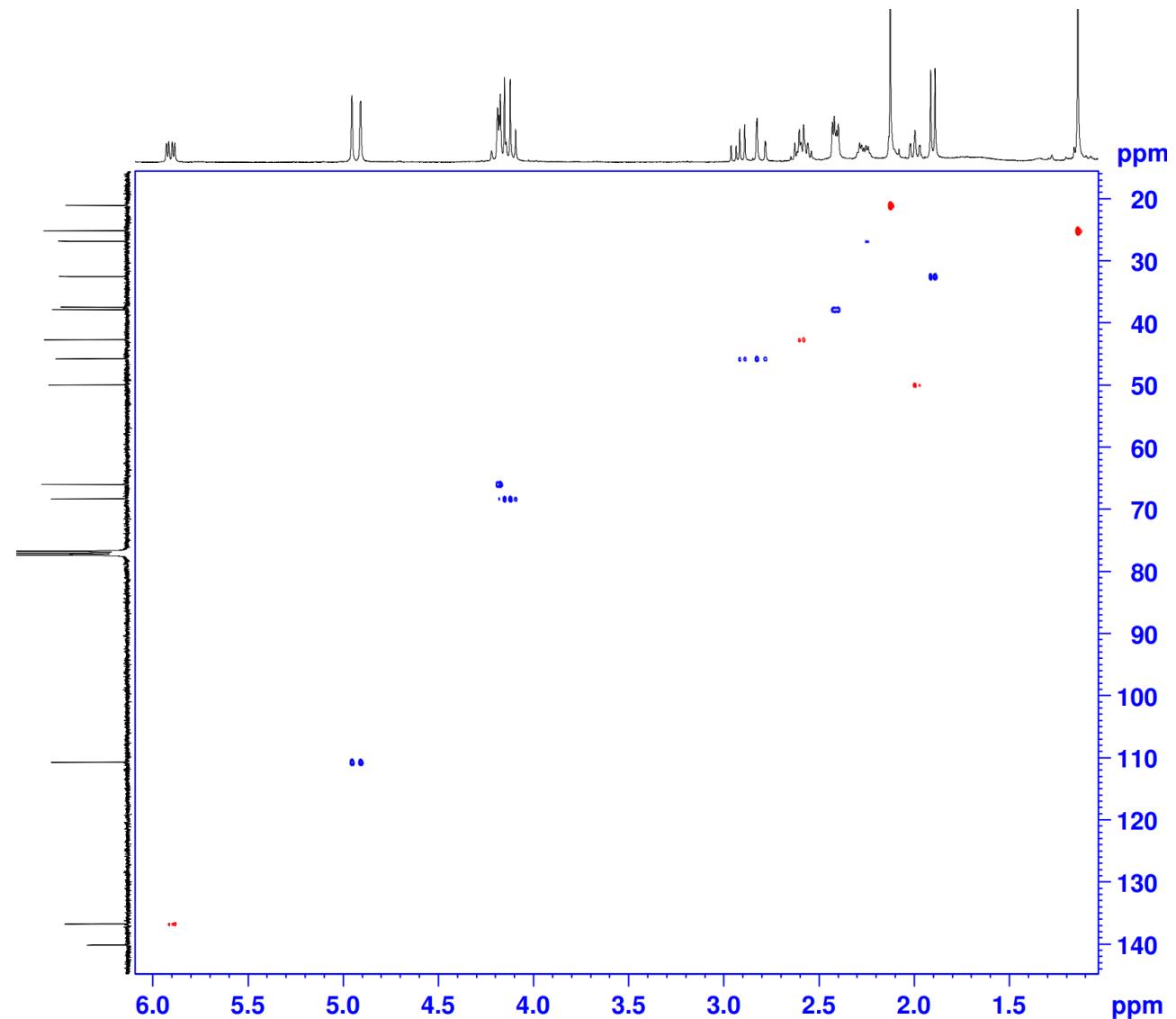


Figure S13. NOESY spectrum of compound 9.



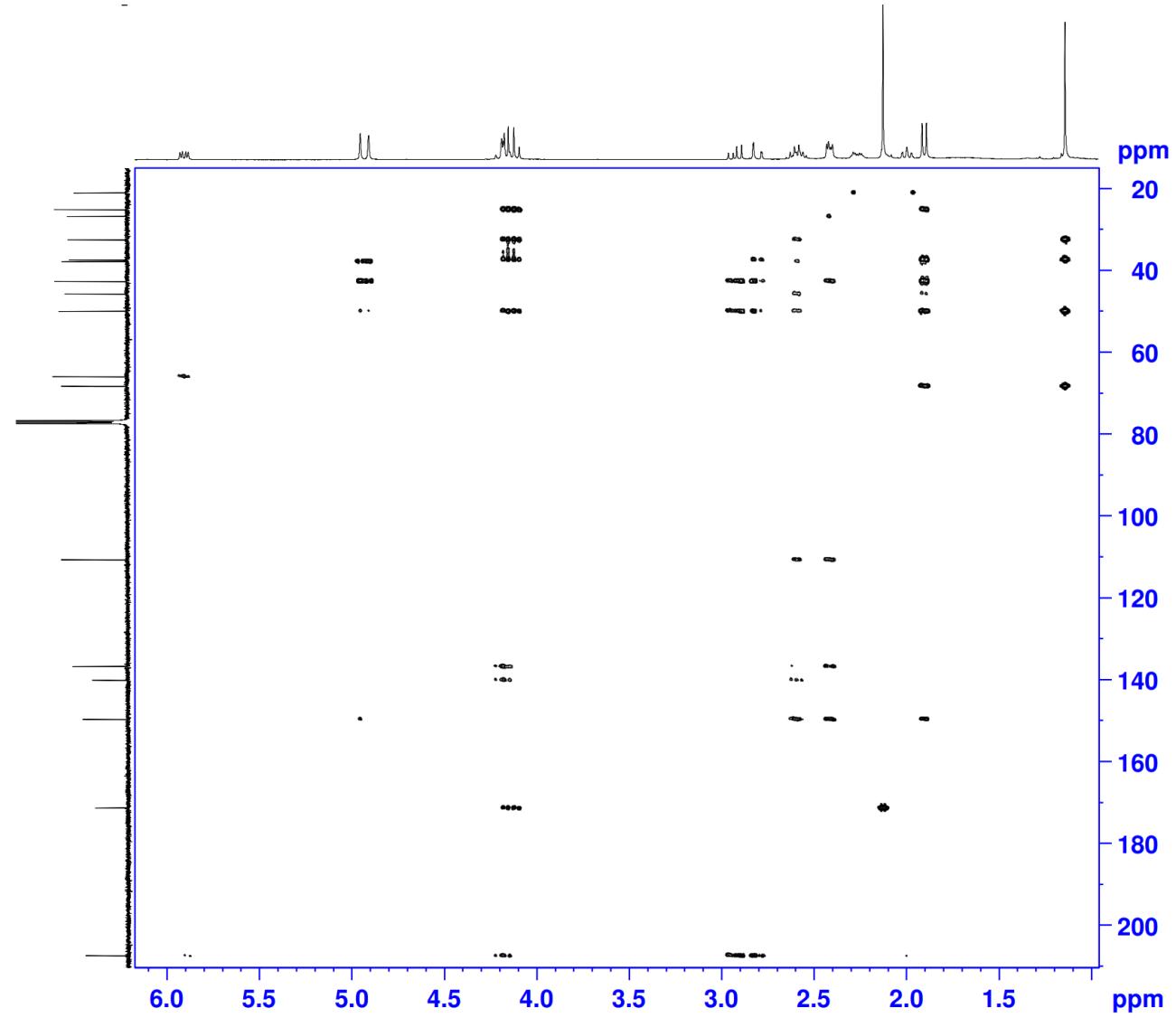
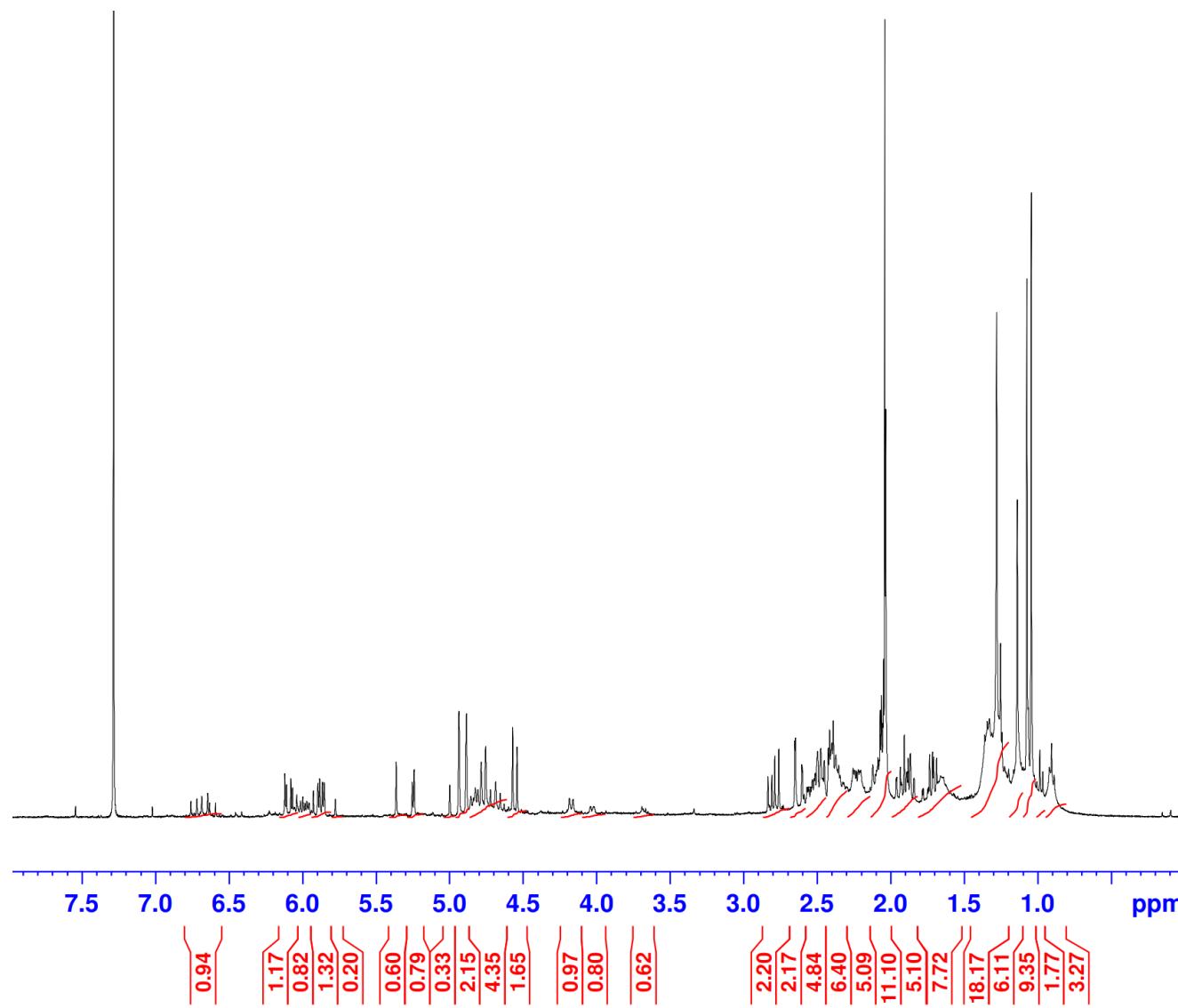
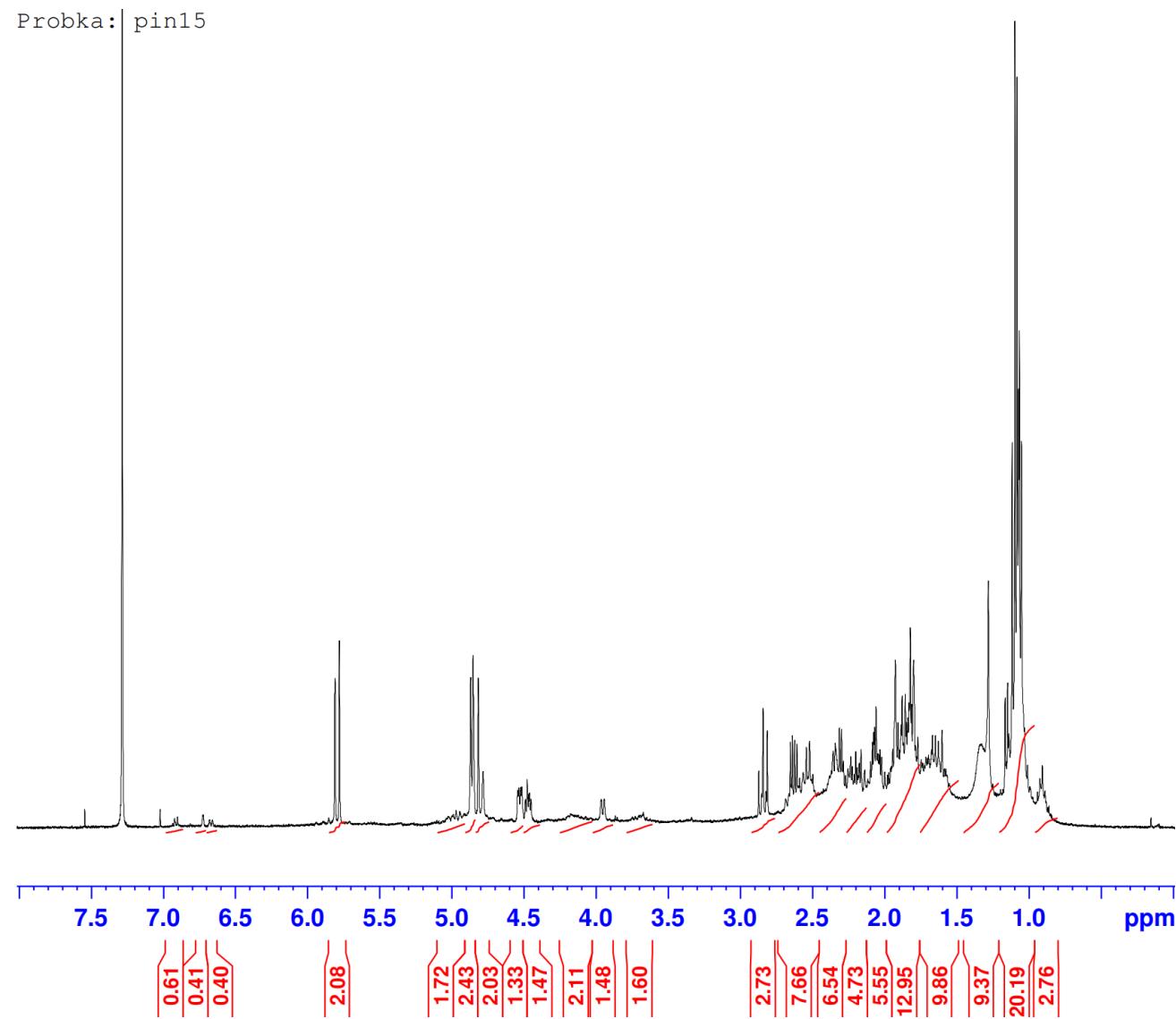


Figure S15. HMBC spectrum of compound 9.

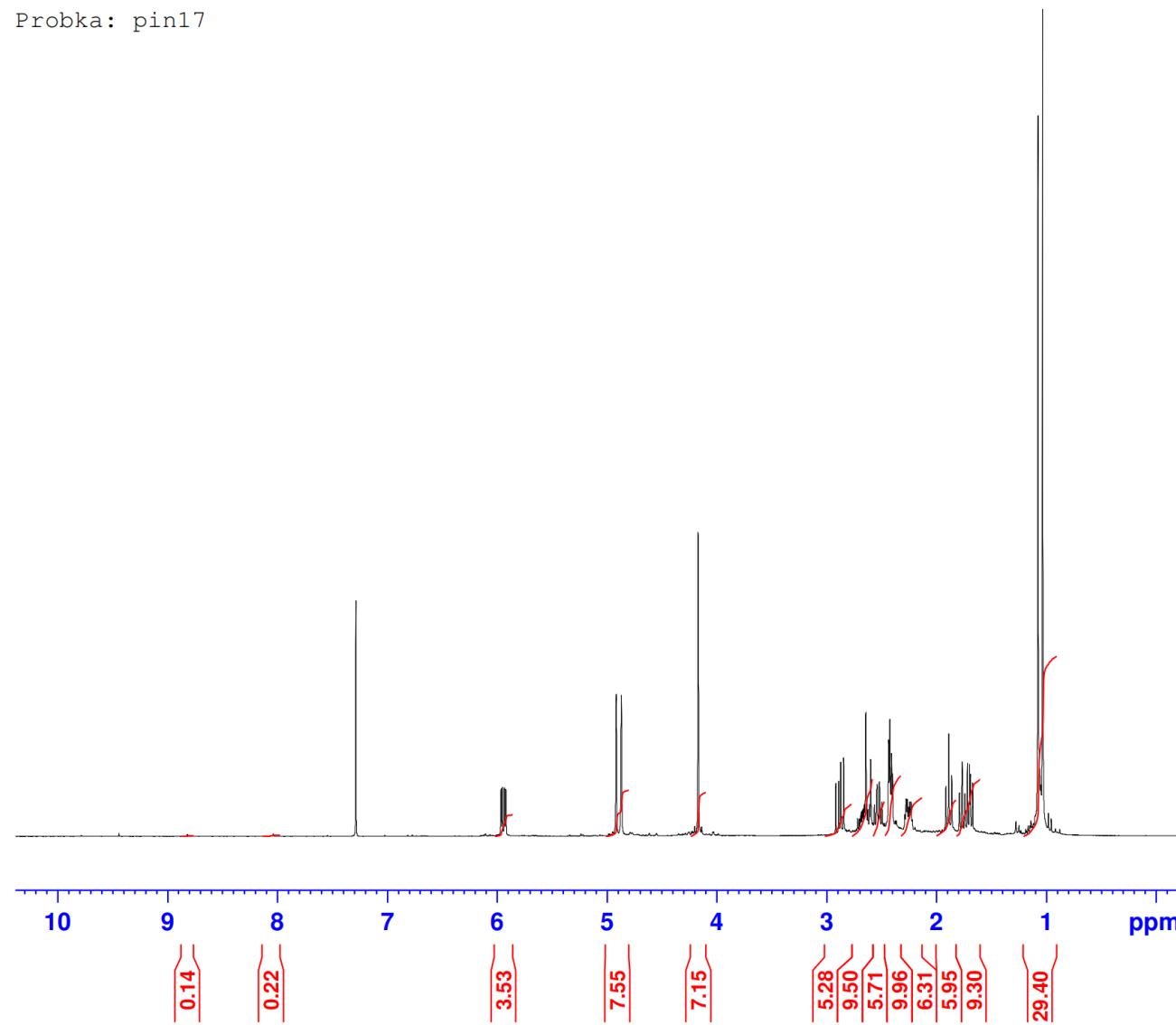


**Figure S16.**  $^1\text{H}$  NMR spectrum of the mixture containing compound 3 in  $\text{CDCl}_3$ .



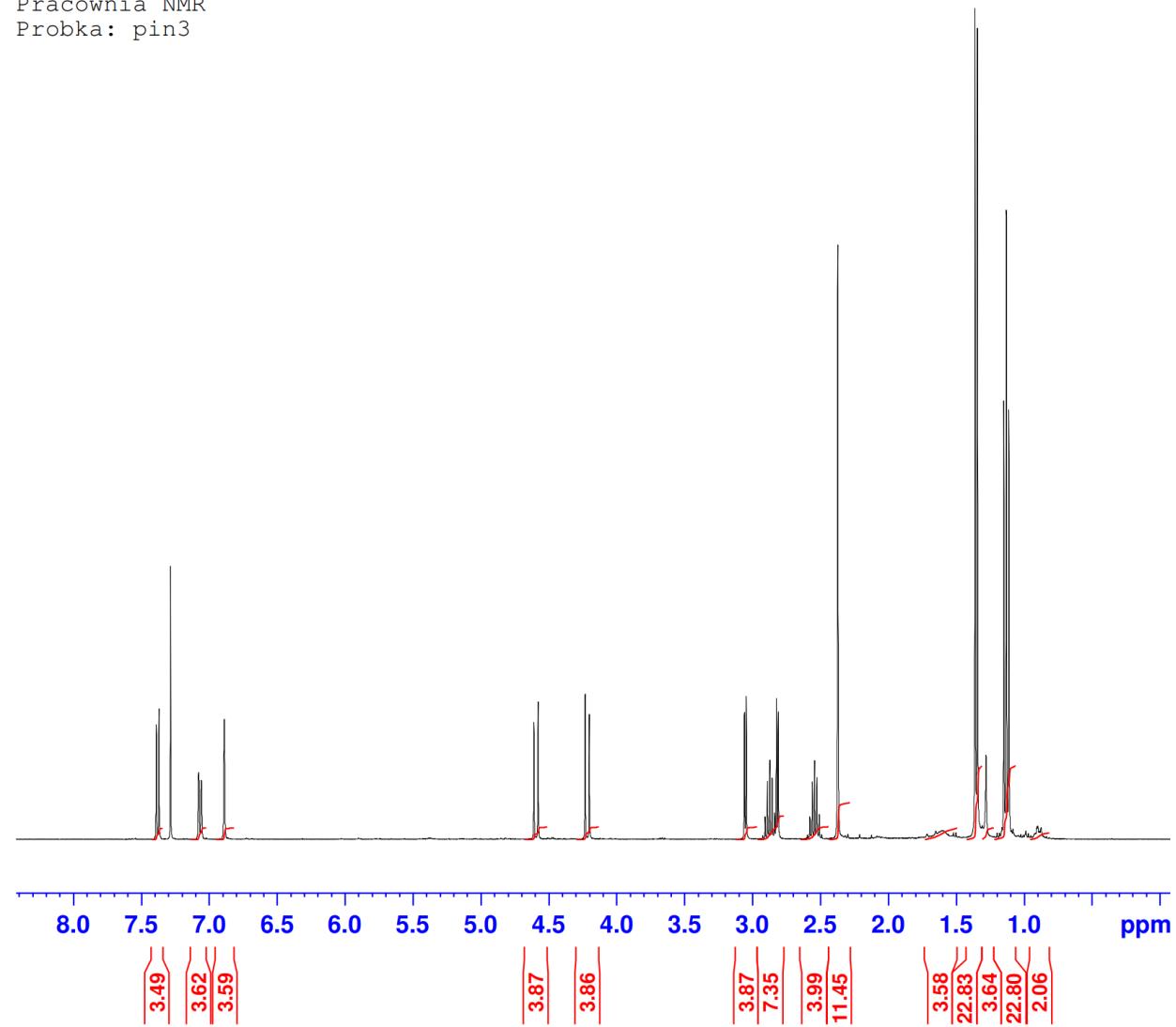
**Figure S17.**  $^1\text{H}$  NMR spectrum of compound **7** in  $\text{CDCl}_3$ .

Probka: pin17



**Figure S18.**  $^1\text{H}$  NMR spectrum of compound **8** in  $\text{CDCl}_3$ .

Pracownia NMR  
Probka: pin3



**Figure S19.**  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{CDCl}_3$ .

Pracownia NMR  
Probka: pin14

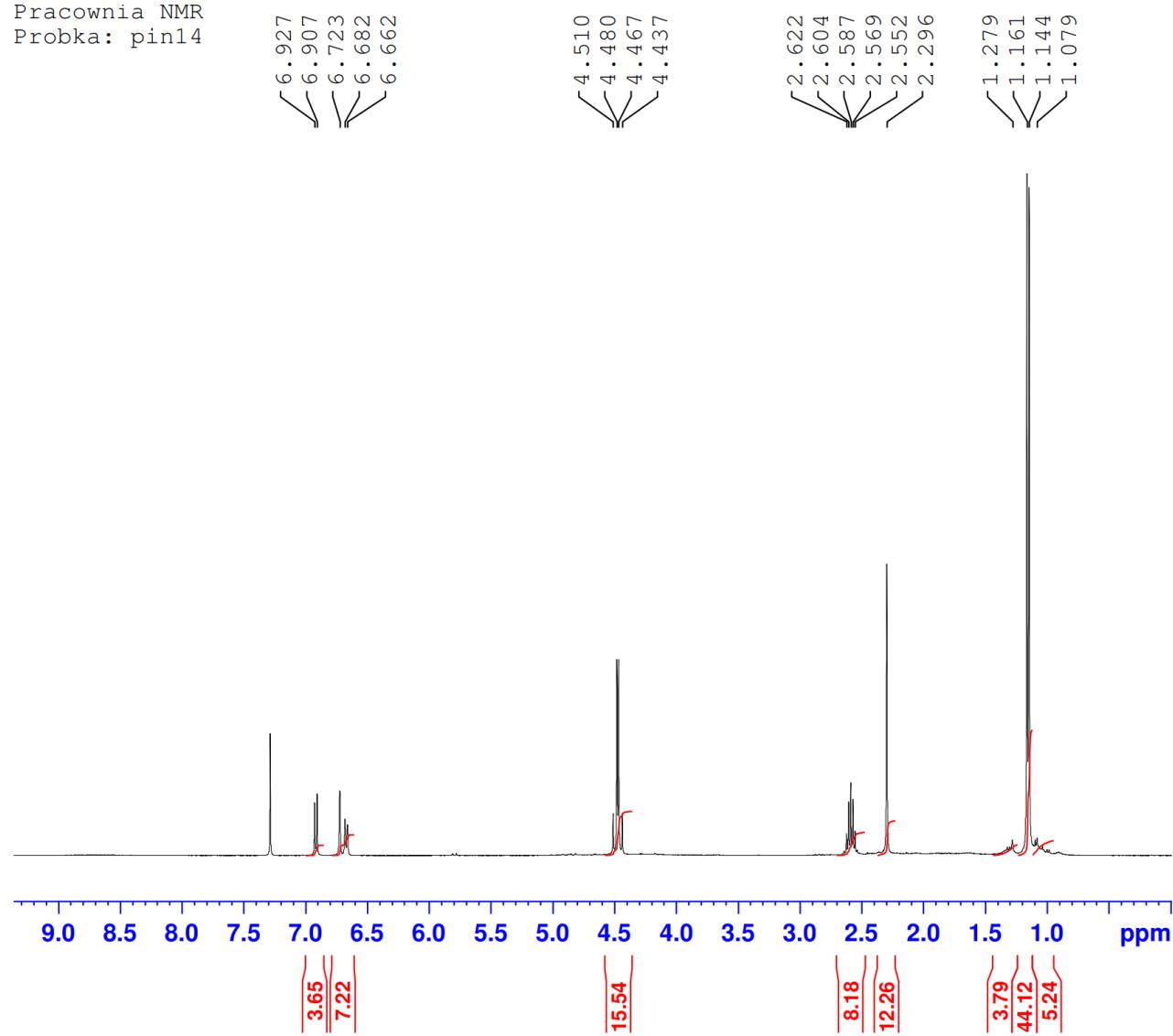
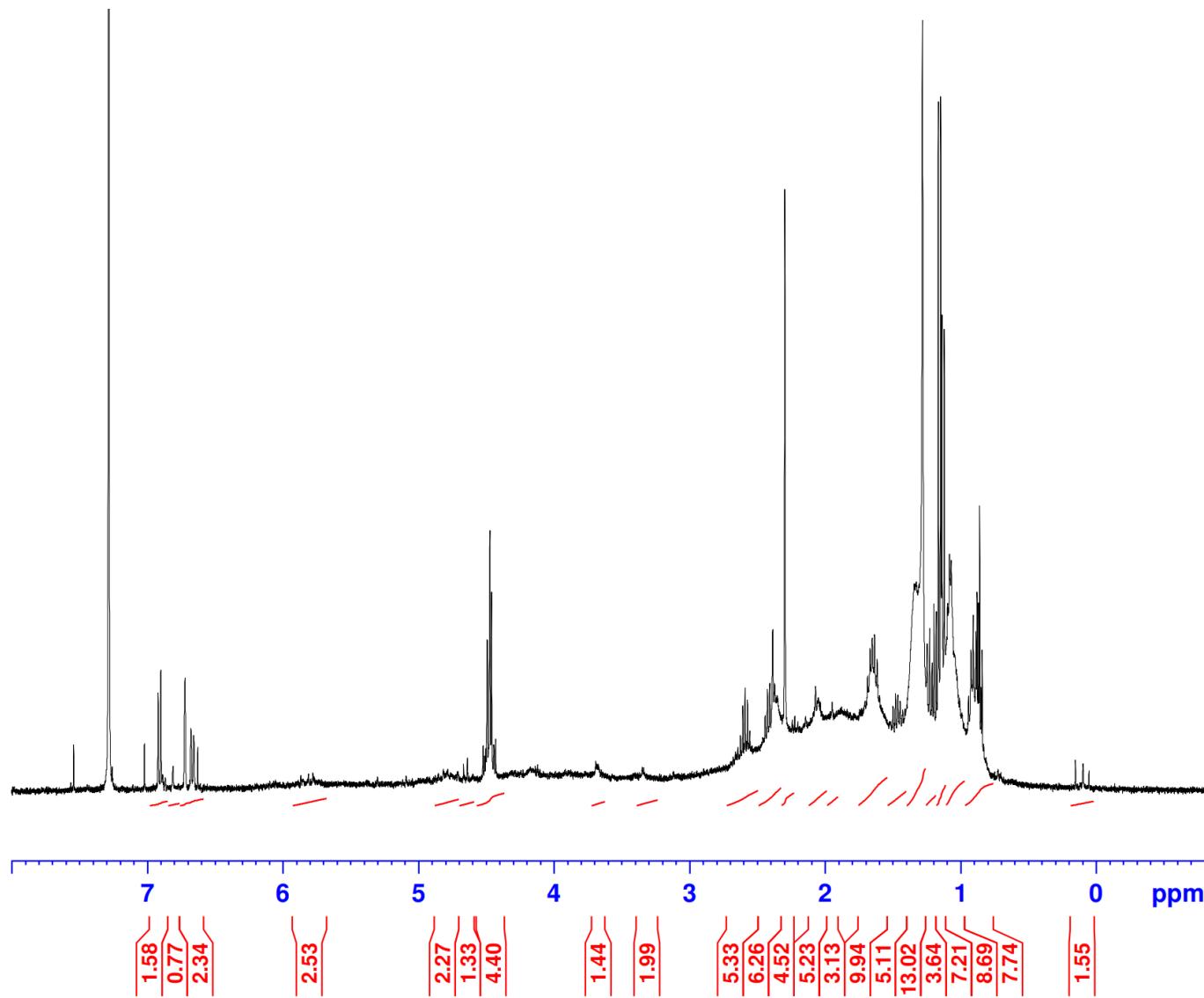
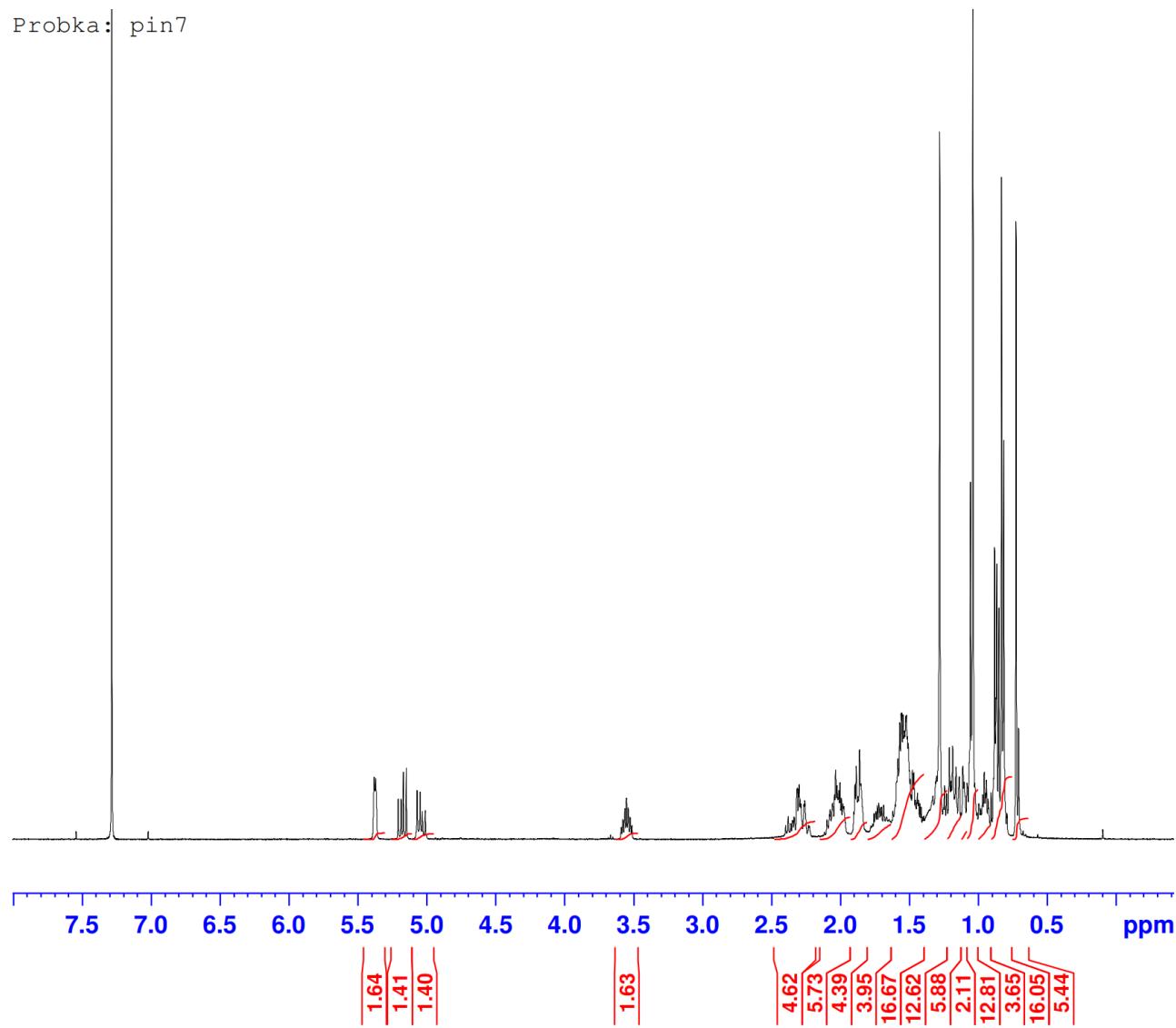


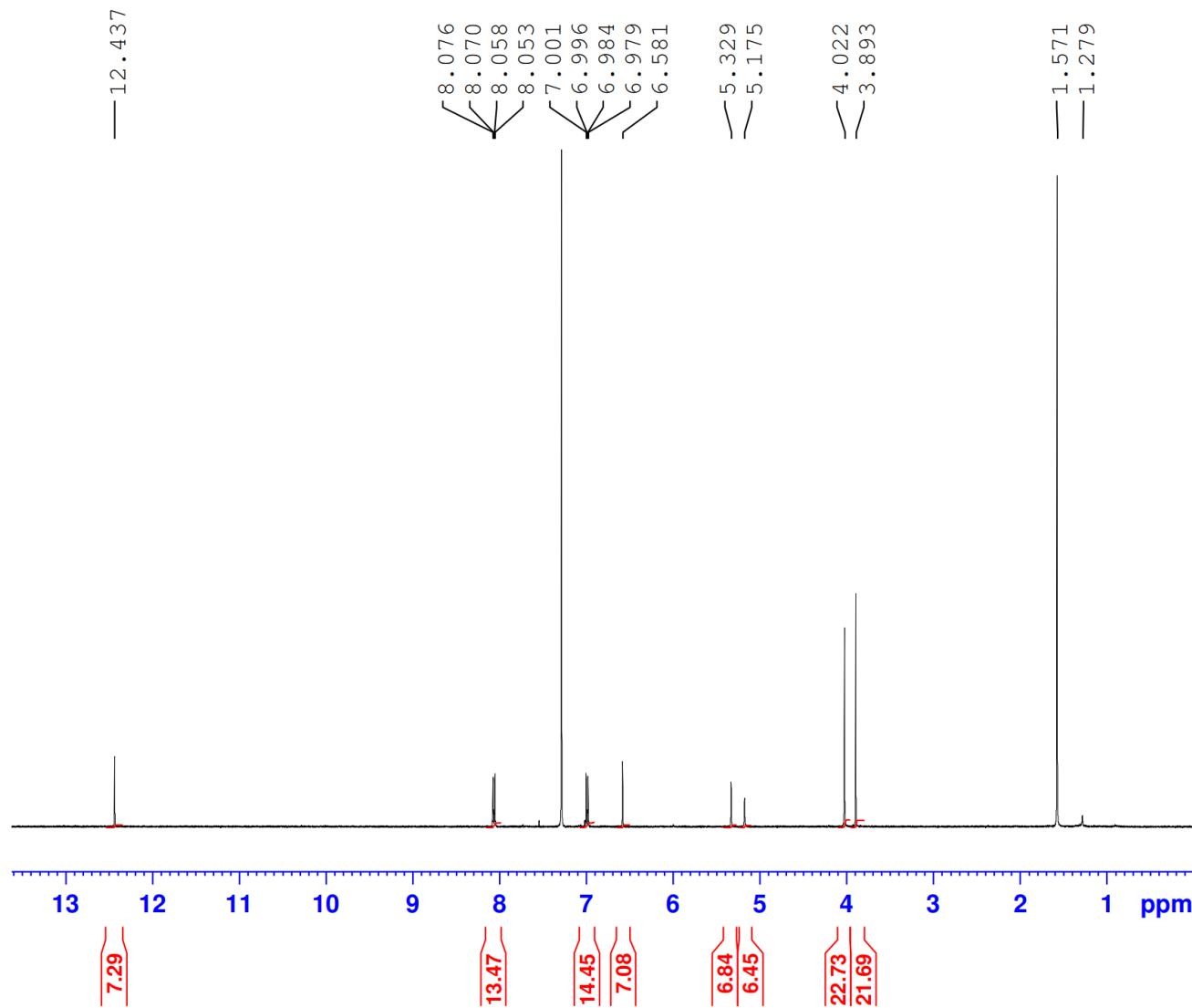
Figure S20.  $^1\text{H}$  NMR spectrum of compound 4 in  $\text{CDCl}_3$ .



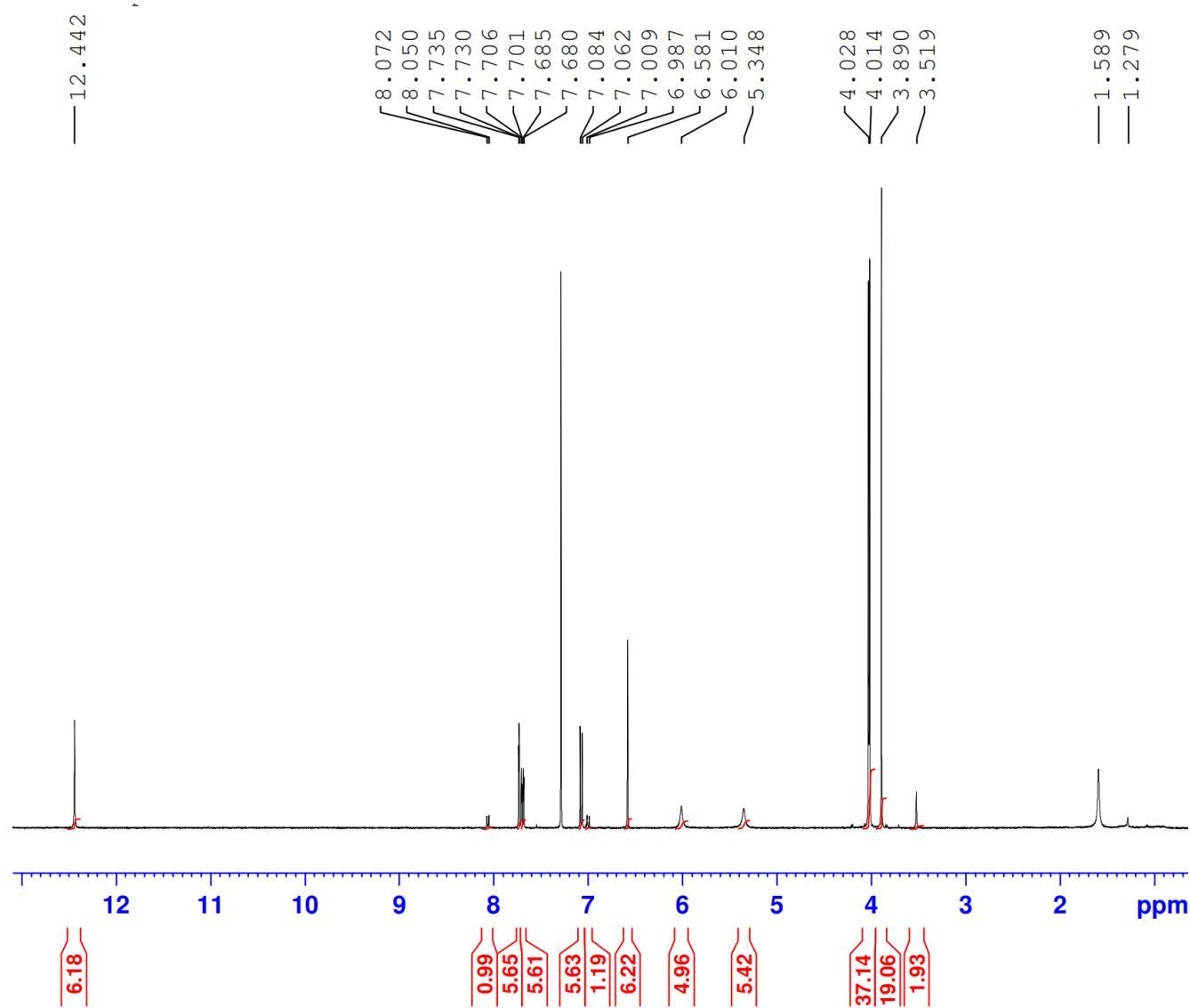
**Figure S21.** <sup>1</sup>H NMR spectrum of compound **5** in  $\text{CDCl}_3$ .



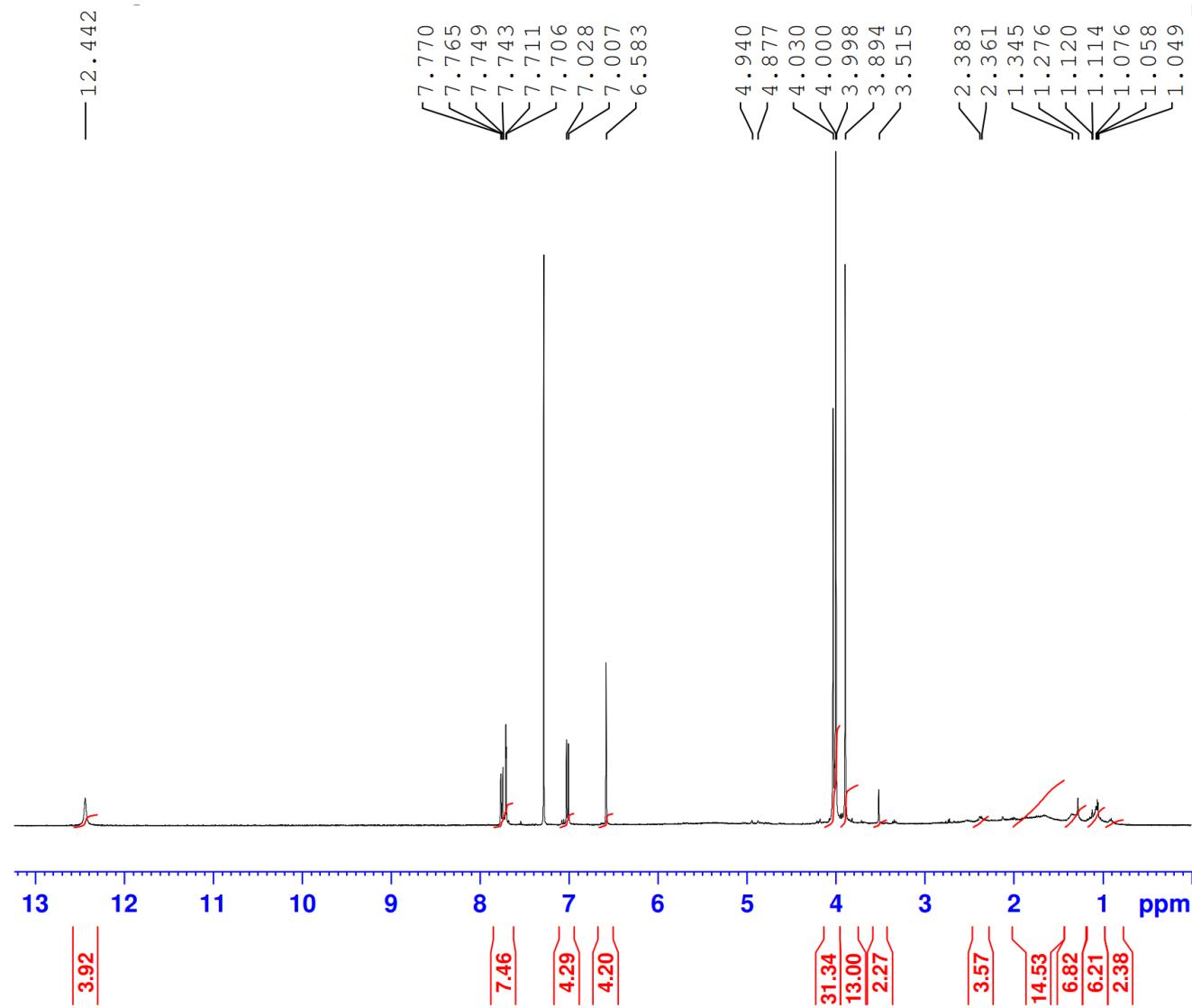
**Figure S22.**  $^1\text{H}$  NMR spectrum of compound **6** in  $\text{CDCl}_3$ .



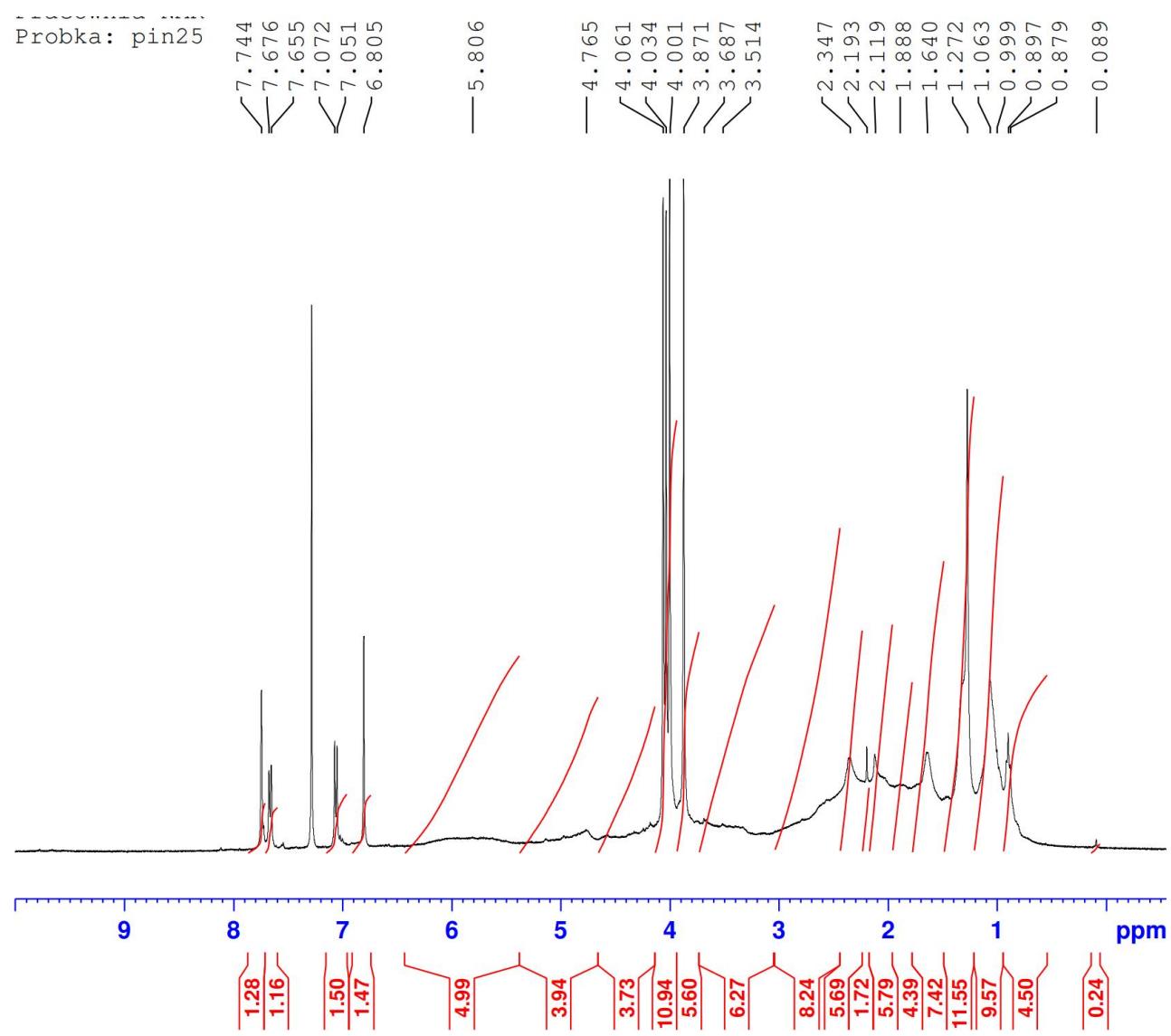
**Figure S23.**  $^1\text{H}$  NMR spectrum of compound **10** in  $\text{CDCl}_3$ .



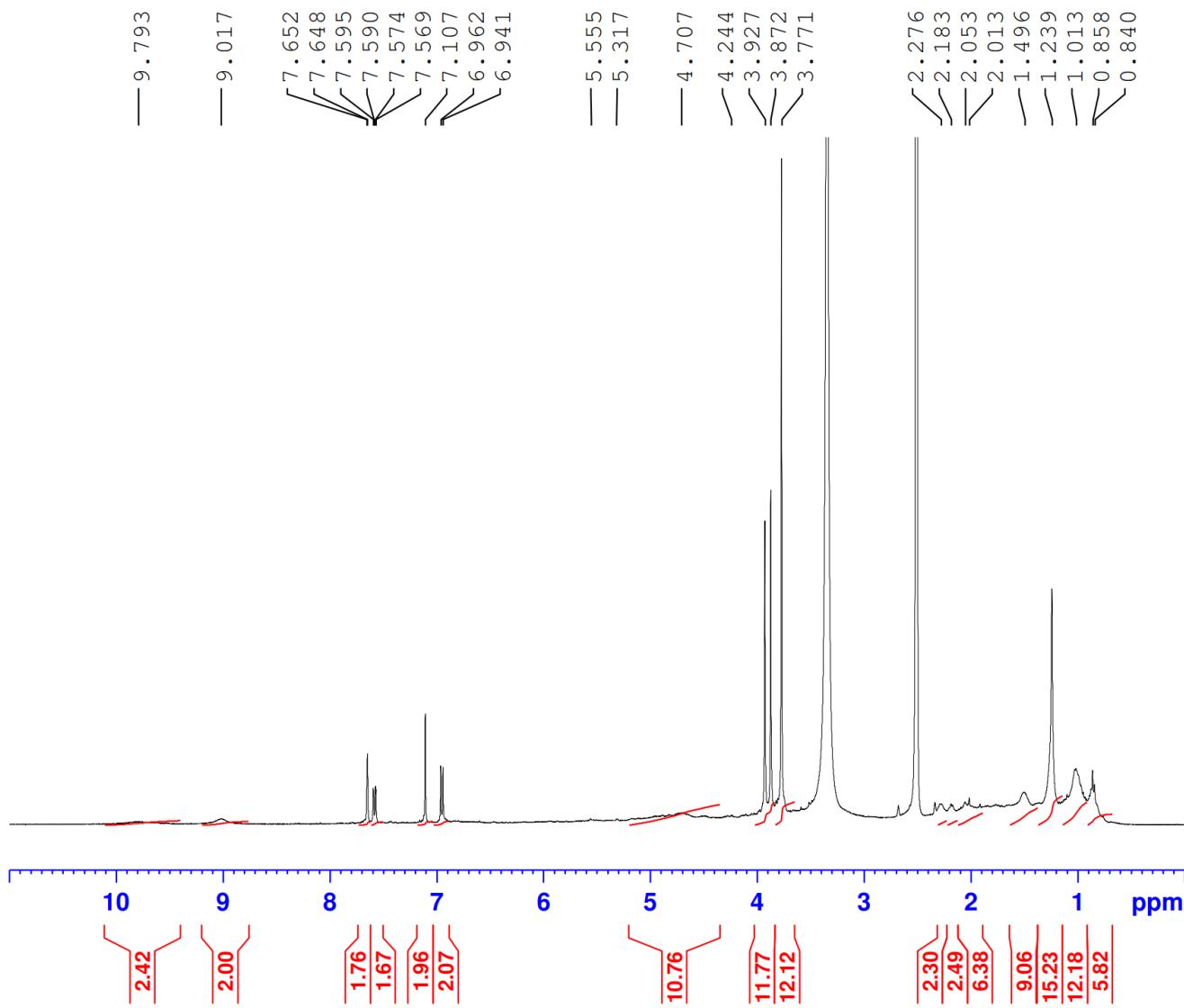
**Figure S24.**  $^1\text{H}$  NMR spectrum of compound **11** in  $\text{CDCl}_3$ .



**Figure S25.**  $^1\text{H}$  NMR spectrum of compound **12** in  $\text{CDCl}_3$ .



**Figure S26.**  $^1\text{H}$  NMR spectrum of compound **13** in  $\text{CDCl}_3$ .



**Figure S27.**  $^1\text{H}$  NMR spectrum of compound **13** in  $\text{DMSO-d}_6$ .