Supporting Information

Paratrimerin I, cytotoxic acridone alkaloid from the roots of *Paramignya trimera*

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ABSTRACT:

Bioactivity-guided fractionation of the $CHCl_3$-soluble extract of the roots of *Paramignya trimera* was carried out to obtain a new acridone alkaloid, paratrimerin I. Its structure was elucidated based on NMR spectroscopic data interpretation. Paratrimerin I showed noteworthy cytotoxicity against the HepG2 human hepatocellular and MCF-7 human breast carcinoma cell lines, with the submicromolar IC_{50} values of 0.43 and 0.26 μM, respectively. The *N*-methyl, C-4 methoxy, and C-5 hydroxy groups in the acridone skeleton can be proposed as a structural feature for good cytotoxicity.

Keywords: *Paramignya trimera*, alkaloid, acridone, cytotoxicity.

Table S1. ^{1}H (500 MHz) and ^{13}C (125 MHz) NMR Data of **1** and **2** in $CDCl_3$

position	**1**		**2**
	δ_C, type	δ_H (*J* in Hz)	δ_H (*J* in Hz)
1	160.0, C		
2	94.1, CH	6.39, s	6.39, s
3	160.4, C		
4	130.3, C		
4a	142.3, C		
5	146.6, C		
6	120.6, CH	7.15, dd (7.6, 1.9)	7.12, dd (7.6, 2.0)
7	122.8, CH	7.12, t (7.6)	7.15, t (7.6)
8	118.1, CH	7.91, dd (7.6, 1.9)	7.93, dd (7.6, 2.0)
8a	124.9, C		
9	182.4, C		
9a	106.5, C		
10a	137.6, C		
N-Me	46.5, CH_3	3.83, s	3.81, s
OH-1			14.03, s
OMe-1	56.4, CH_3	3.96, s	
OMe-3			3.96, s
OMe-4	60.6, CH_3	3.80, s	3.80, s

Table S2. Cytotoxicity of **1**–**4** against the HepG2 and MCF-7 Cell Lines

compound	IC_{50} (μM)	
	HepG2	MCF-7
1	0.43	0.26
2	0.54	0.22
3	1.19	0.40
4	> 10	3.92
doxorubicin[a]	0.28	1.31

[a]Positive control.

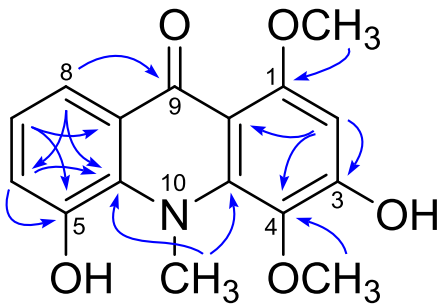

Figure S1. HMBC correlations observed for paratrimerin I.

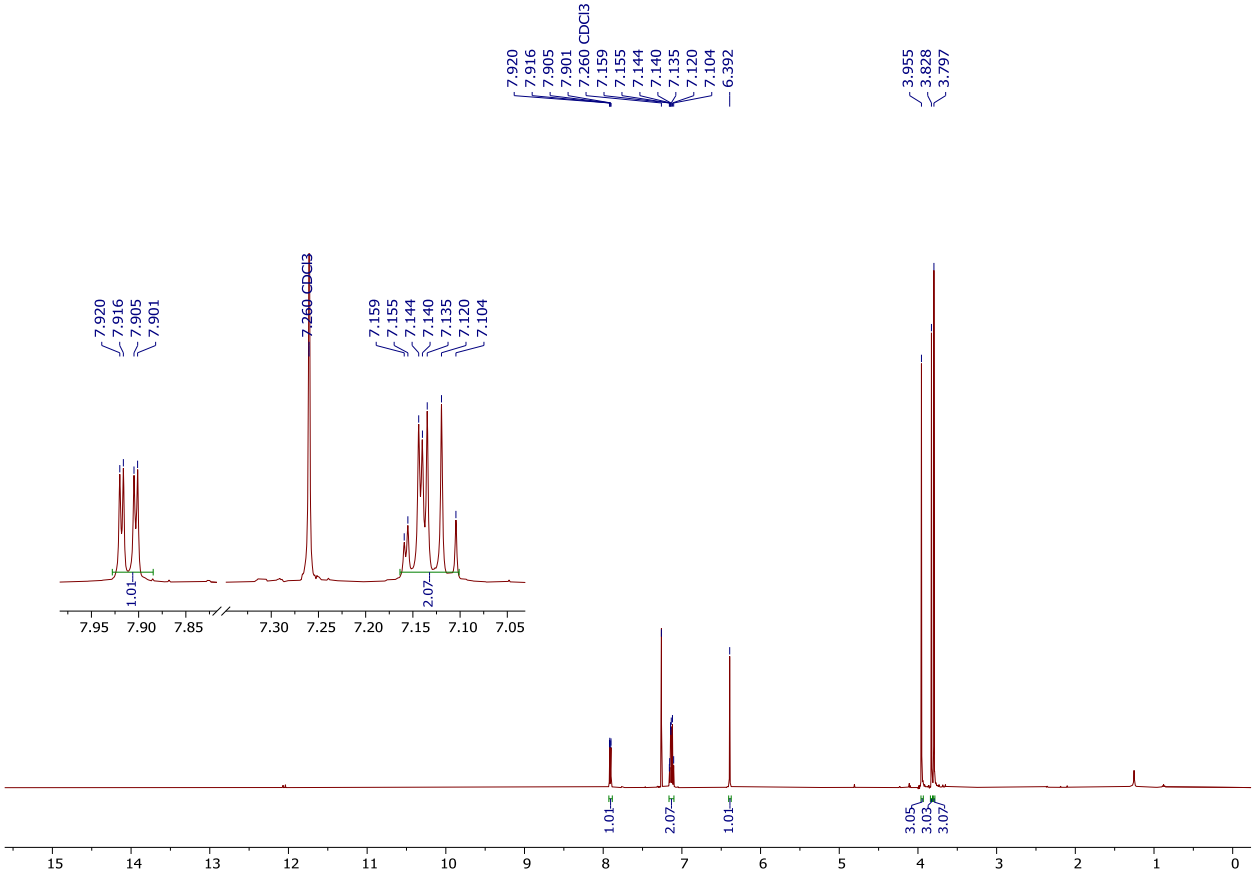

Figure S2. ^{1}H NMR spectrum of compound **1** ($CDCl_3$, 500 MHz)

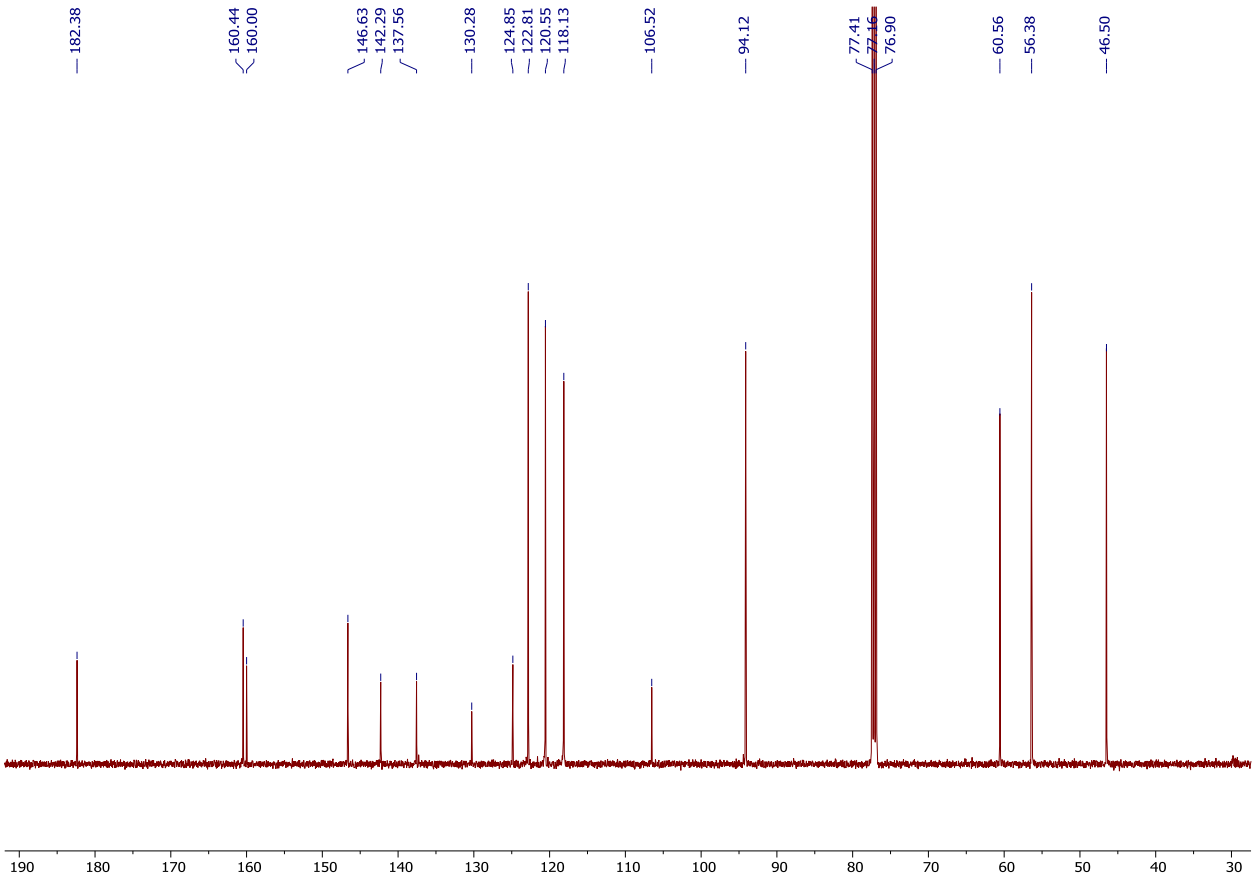

Figure S3. ^{13}C NMR spectrum of compound **1** ($CDCl_3$, 125 MHz)

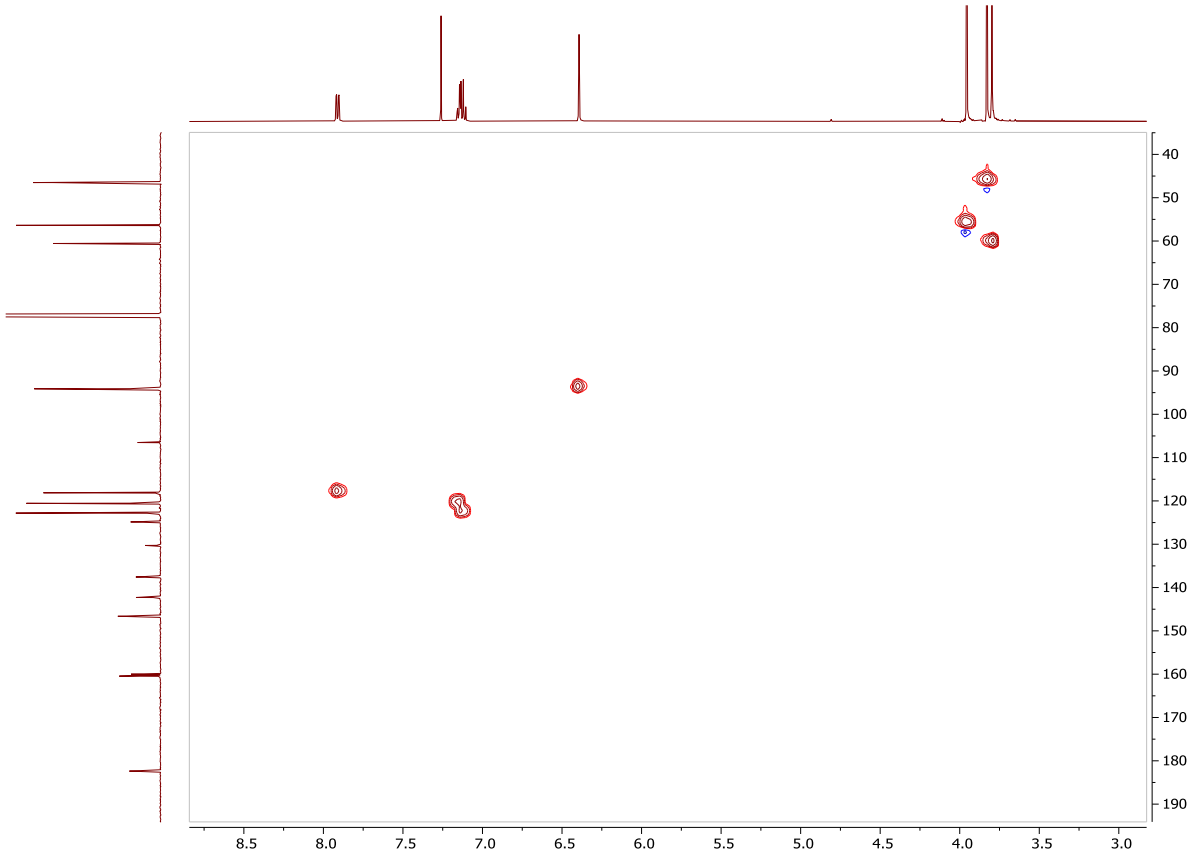

Figure S4. HSQC spectrum of compound **1**

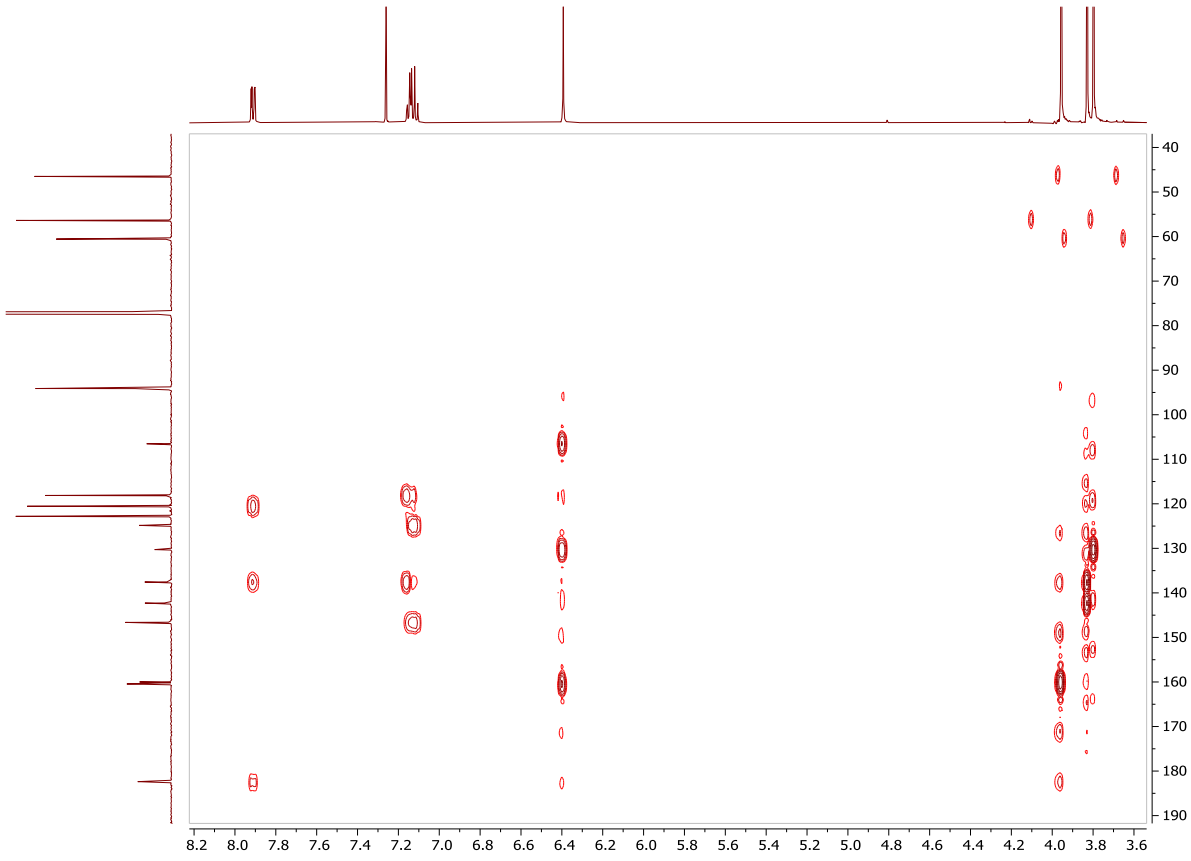

Figure S5. HMBC spectrum of compound **1**

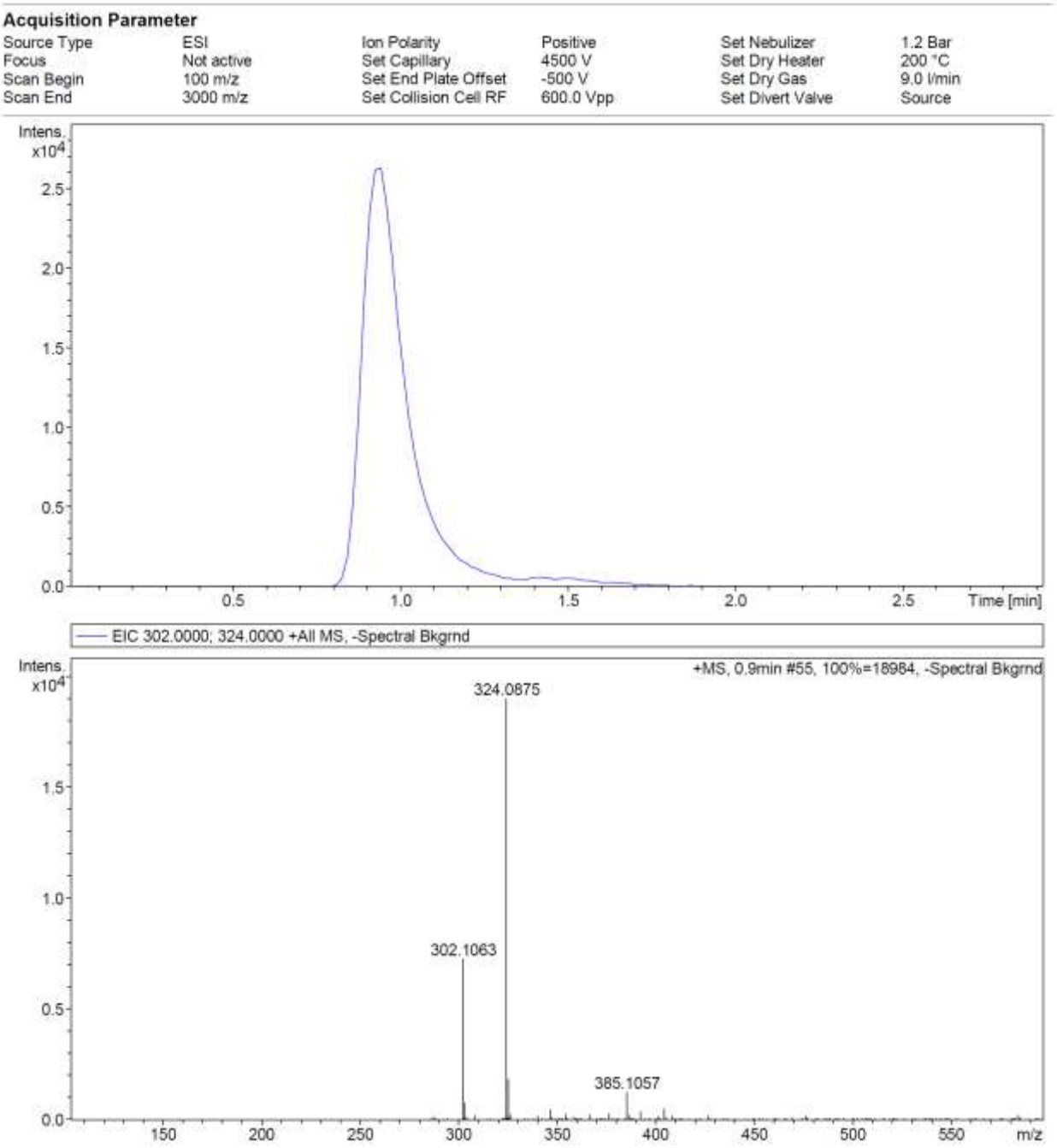

Figure S6. HRESIMS of compound **1**

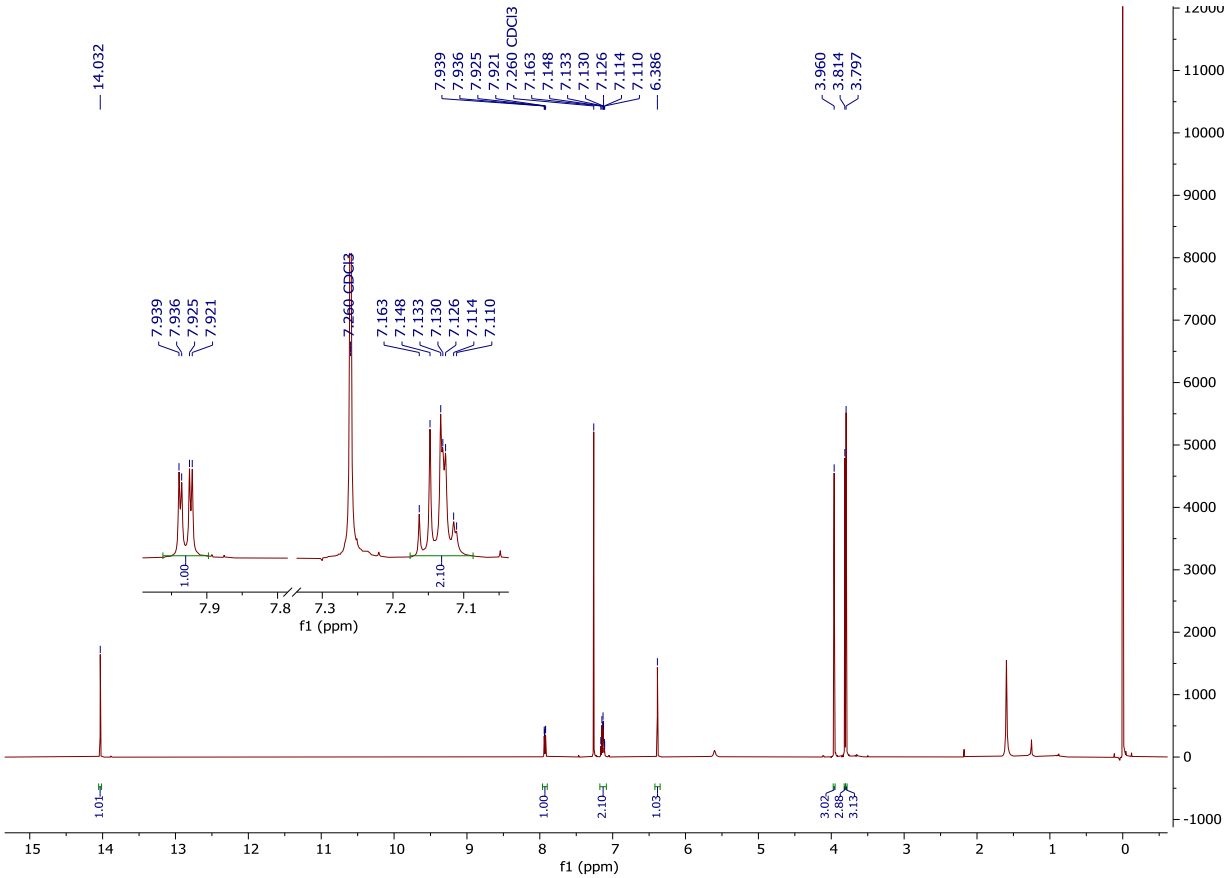

Figure S7. ^{1}H NMR spectrum of compound **2** ($CDCl_3$, 500 MHz)