

# Supporting Information

*Rec. Nat. Prod.* X:X (2022) XX-XX

## Tigliane-Type Diterpenoids from the Seeds of *Croton tiglium*

Lijuan Zhang<sup>1</sup>, Fei Li<sup>2</sup>, Jianyong Zhu<sup>3</sup> and Qian Niu<sup>1\*</sup>

<sup>1</sup>*Department of Pharmacy, Bozhou Vocational and Technical College, Bozhou 236800, P.R. China*

<sup>2</sup>*Bozhou City Food and Drug Inspection Center, Bozhou 236800, P.R. China*

<sup>3</sup>*Clinical Laboratory Medicine Center, Yueyang Hospital of Integrated Traditional Chinese and Western Medicine, Shanghai University of Traditional Chinese Medicine, Shanghai 200437, P.R. China*

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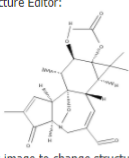
Chemical Structure similarity

REFERENCES  
 Research Topic  
 Author Name  
 Company Name  
 Document Identifier  
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Similarity Range	Substances
≥ 99 (most similar)	0
95-98	8
90-94	46
85-89	133
80-84	523
75-79	1732
70-74	7285
65-69	30283
0-64 (least similar)	85725

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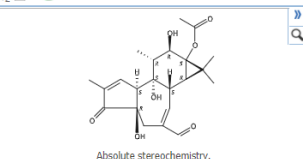
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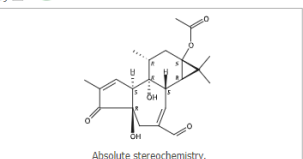
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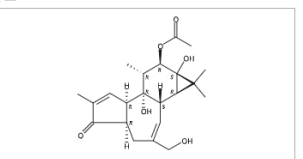
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0 of 8 Substances Selected

Analyze by:  
 Substance Role  
 Biological Study 4  
 Properties 4  
 Analytical Study 3  
 Reactant or Reagent 3  
 Uses 3  
 Preparation 2  
 Occurrence 1  
 Process 1  
 Show More

Score: 96  
 1. **30358-72-6**  
  
 Absolute stereochemistry.

Score: 96  
 2. **60857-09-2**  
  
 Absolute stereochemistry.

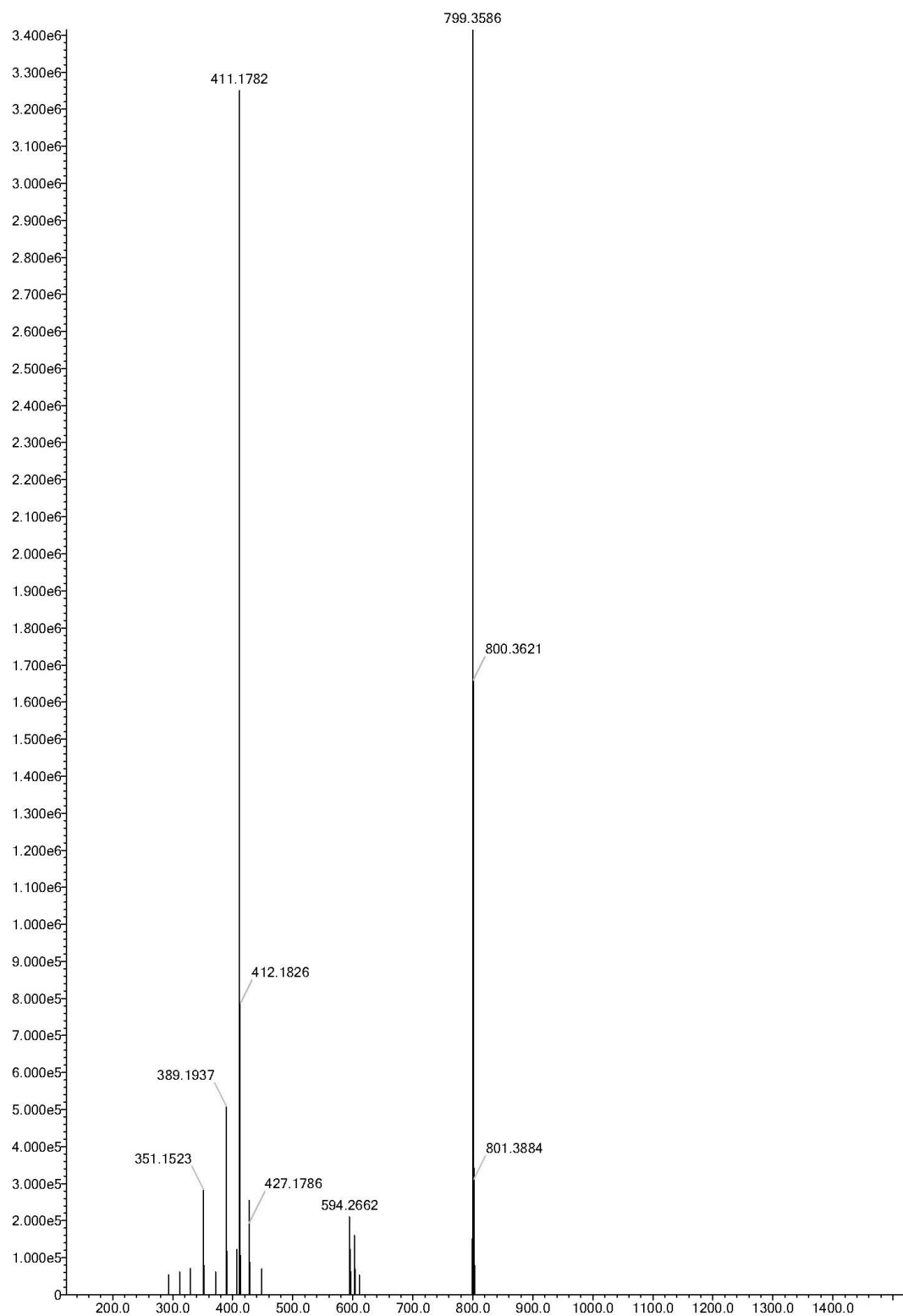
Score: 96  
 3. **64181-02-8**  
  
 Absolute stereochemistry.

**C<sub>22</sub>H<sub>28</sub>O<sub>7</sub>**  
 1#Cyclopropano[3,4]benz[1,2-*e*]azulene-3-carboxaldehyde, 9a-(acetyloxy)-1a,1b,4a,5,7a,7b,8,9,9a-decahydro-4a,7b,9-trihydroxy-1,1,6,8-tetramethyl-5-oxo-, [1a*R*-(1a*a*,1b*b*,4a*b*,7a*c*,7b*c*,8*c*,9*b*,9a*c*)]-(*9C*)  
 Key Physical Properties  
 Spectra

**C<sub>22</sub>H<sub>28</sub>O<sub>6</sub>**  
 1#Cyclopropano[3,4]benz[1,2-*e*]azulene-3-carboxaldehyde, 9a-(acetyloxy)-1a,2,4,4a,5,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-5-oxo-, (1a*R*,31b,5,4a*R*,7a,5,7b*R*,8*R*,8a*S*)-  
 Key Physical Properties  
 Spectra

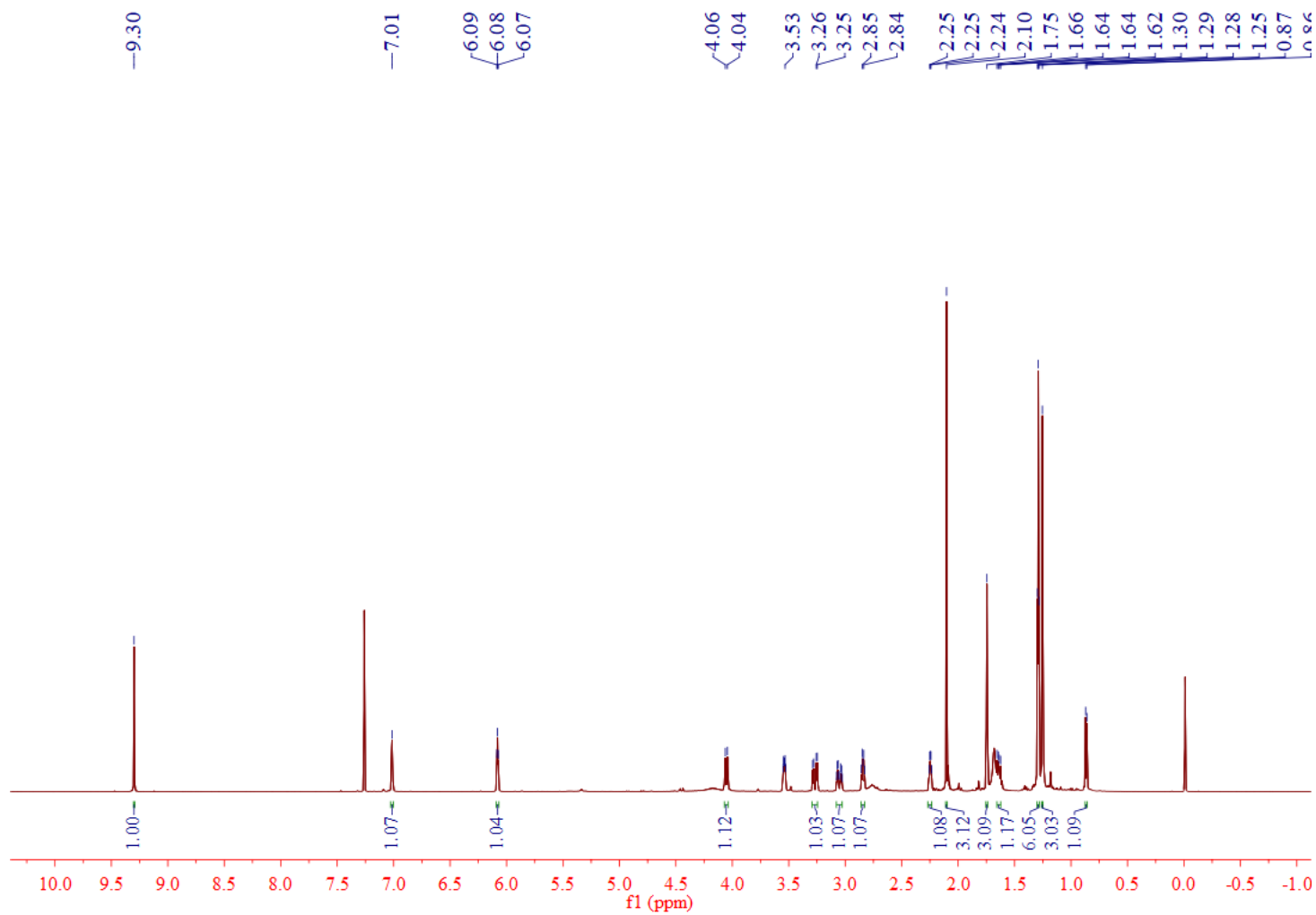
**C<sub>22</sub>H<sub>30</sub>O<sub>6</sub>**  
 5#Cyclopropano[3,4]benz[1,2-*e*]azulene-5-one, 9-(acetyloxy)-1,1a,1b,4,4a,7a,7b,8,9,9a-decahydro-7b,9a-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-, [1a*R*-(1a*a*,1b*b*,4a*c*,7a*c*,7b*c*,8*c*,9*b*,9a*c*)]-(*9C*)  
 Key Physical Properties  
 Spectra

Figure S1: Scifinder search of compound 1



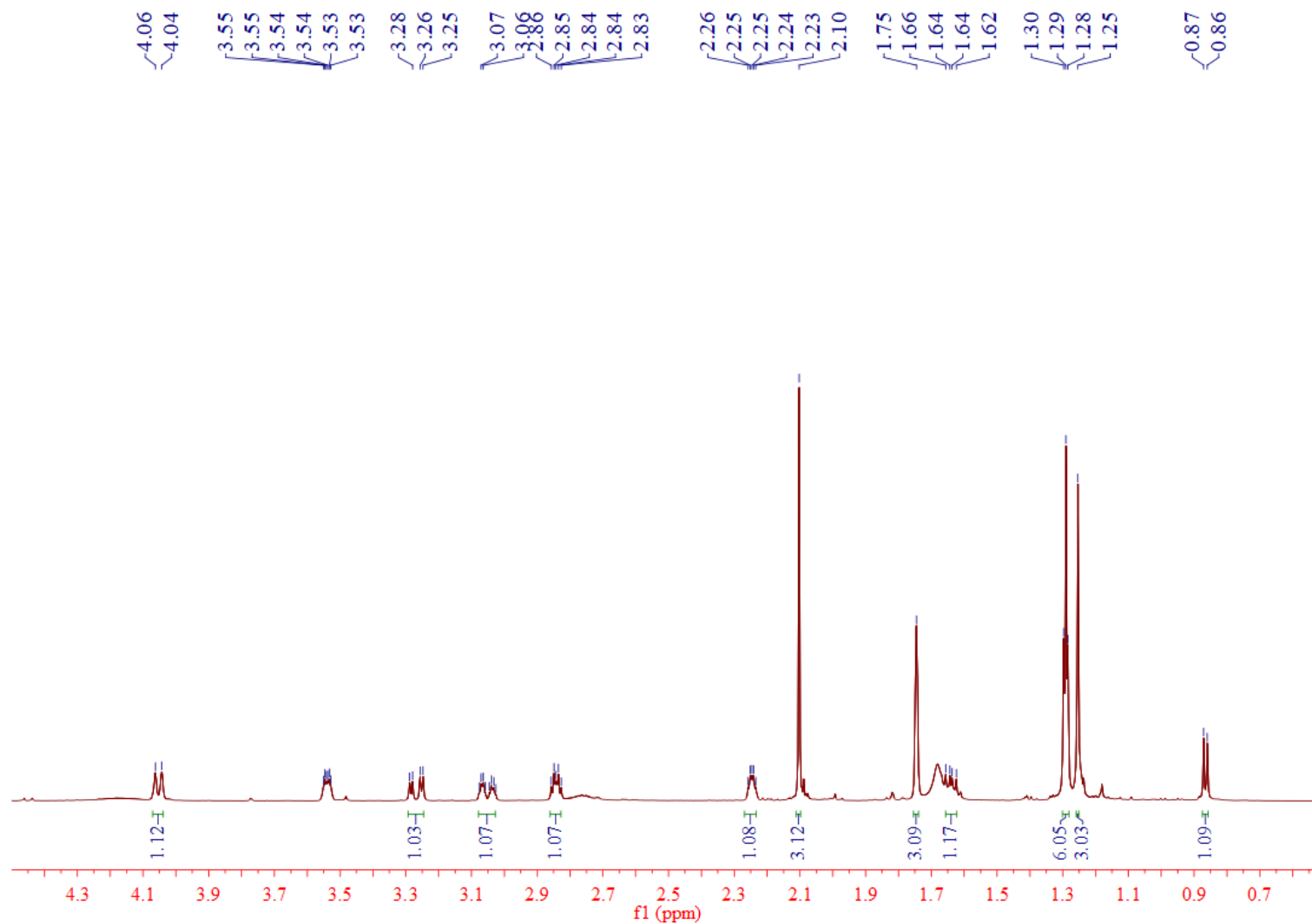
$C_{22}H_{28}O_6Na^+$ : Meas.  $m/z$  411.1782; Pred.  $m/z$  411.1778

**Figure S2:** HR-ESIMS spectrum of compound **1**



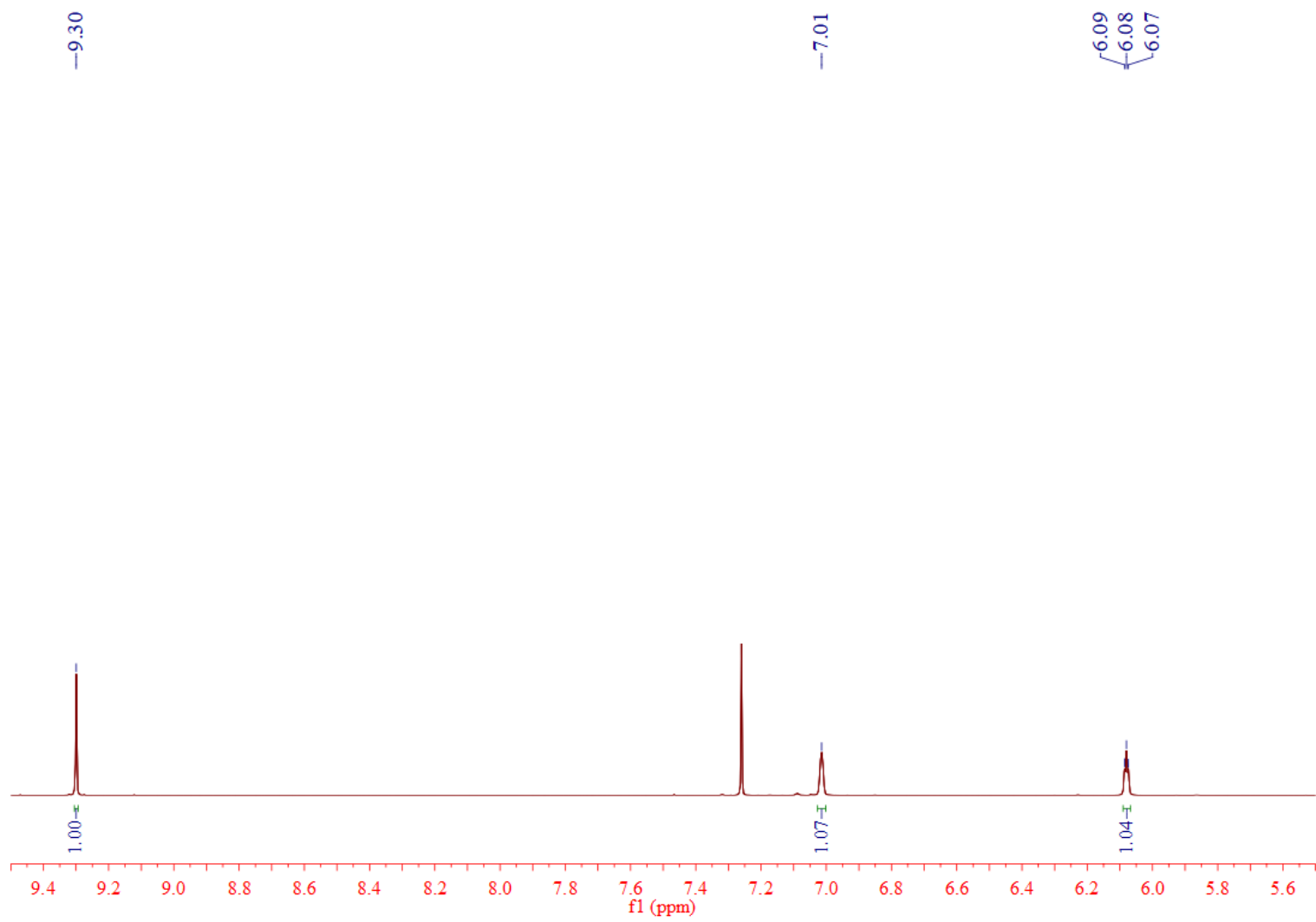
**Figure S3:** <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1**

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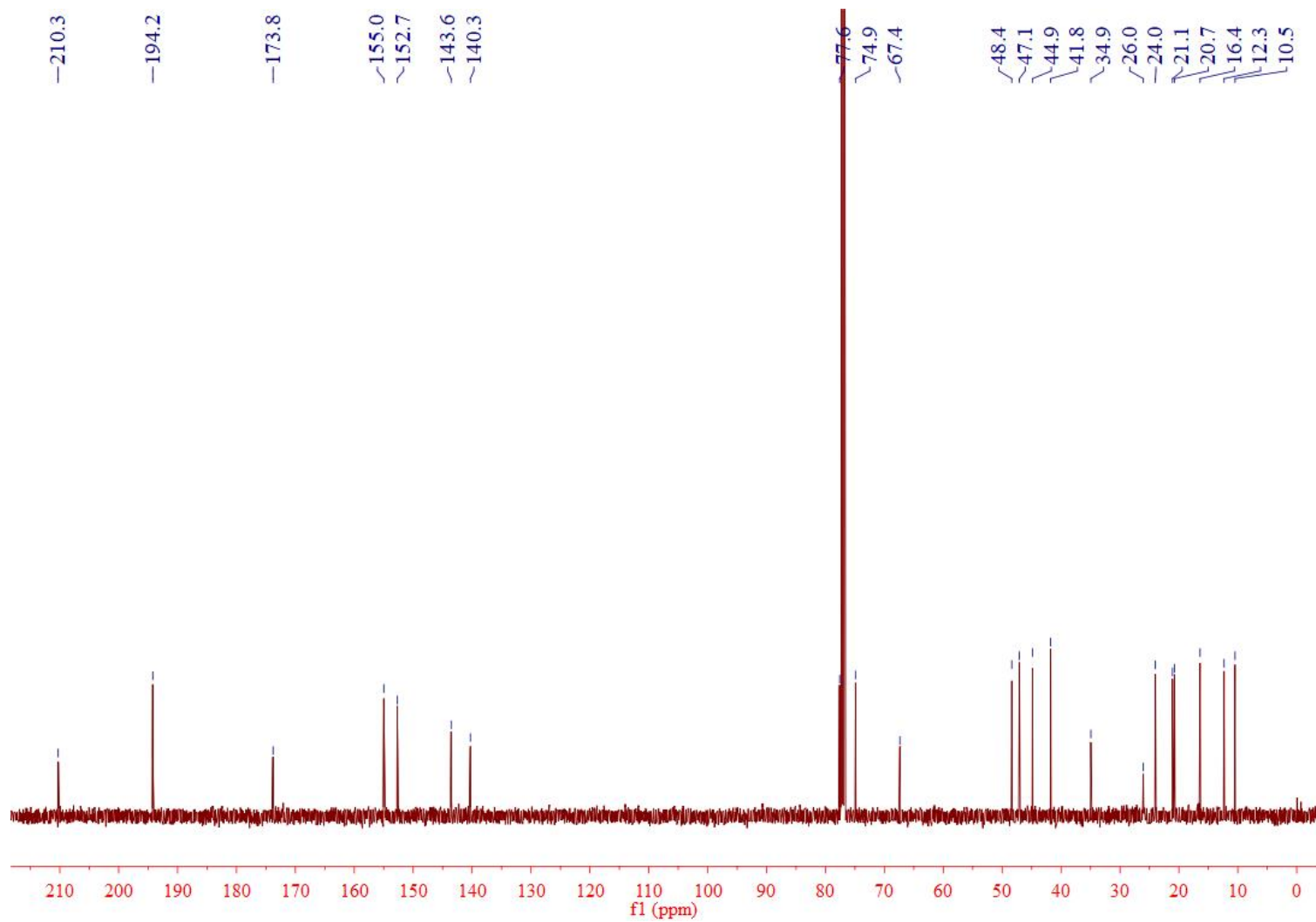
**Figure S4:** Enlarged <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1** ( $\delta_{\text{H}}$  0.5–4.5 ppm)

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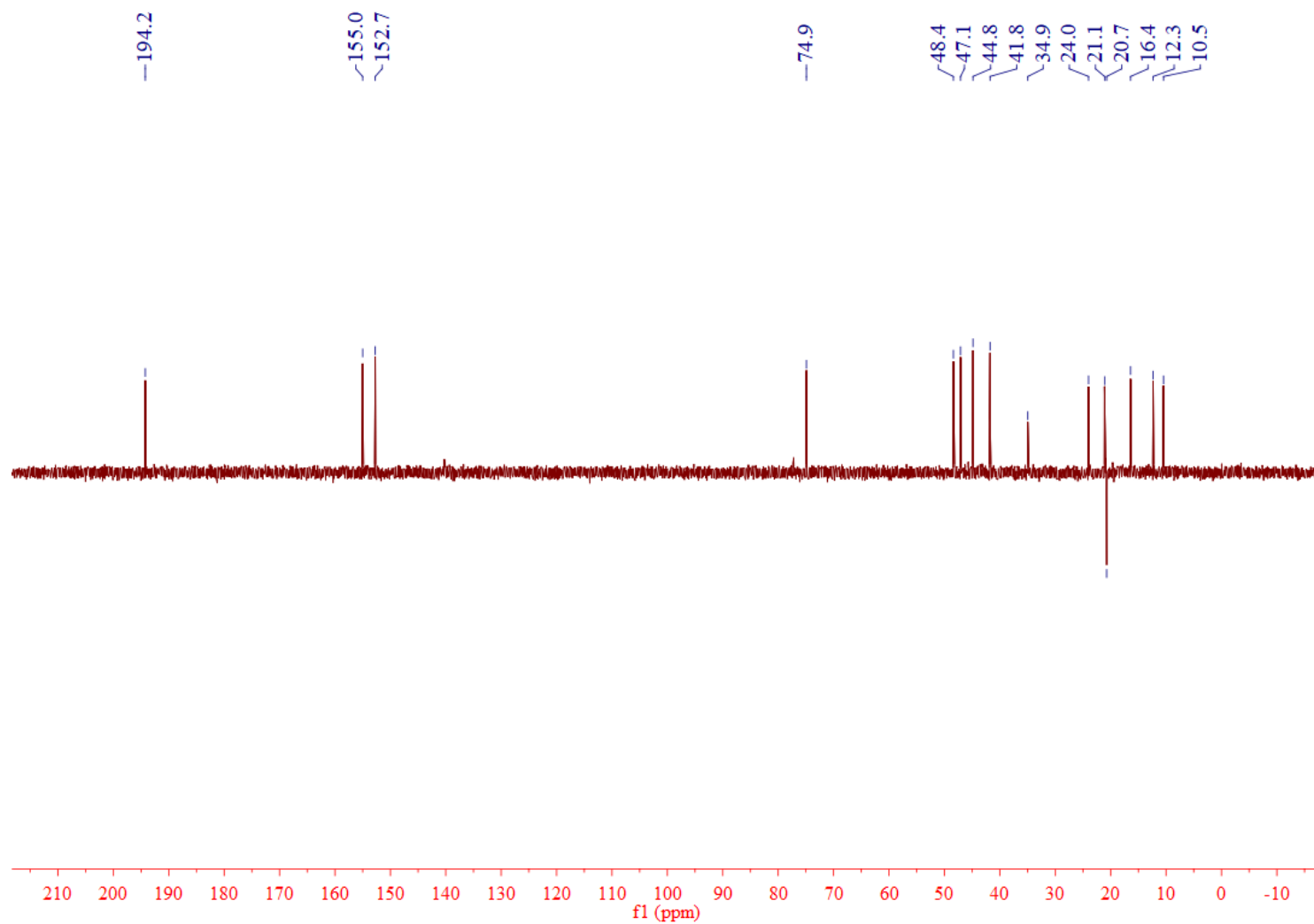
**Figure S5:** Enlarged <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound **1** ( $\delta_{\text{H}}$  5.5–9.5 ppm)

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**Figure S6:** <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound **1**

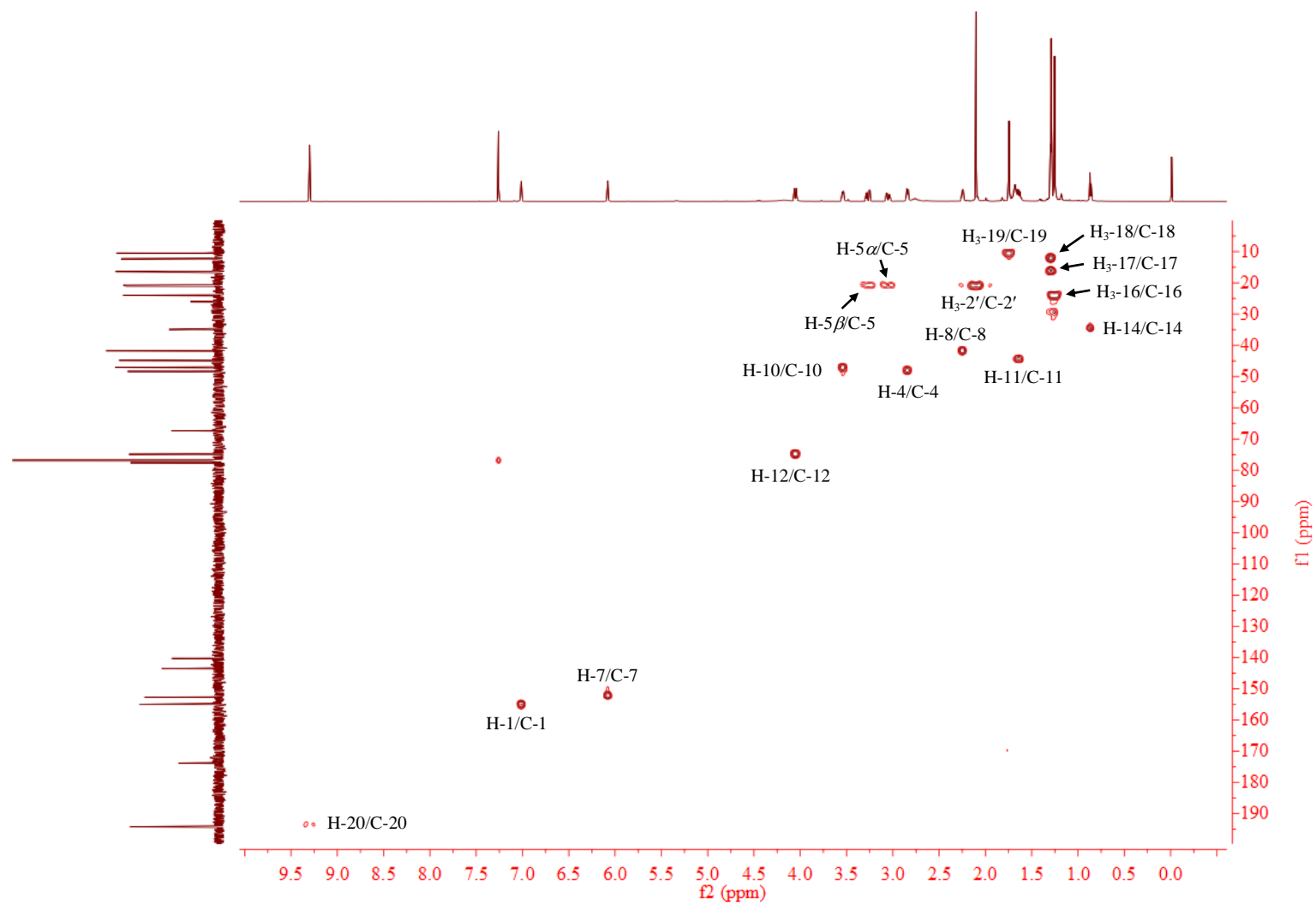
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**Figure S7:** DEPT135 (125 MHz, CDCl<sub>3</sub>) spectrum of compound **1**

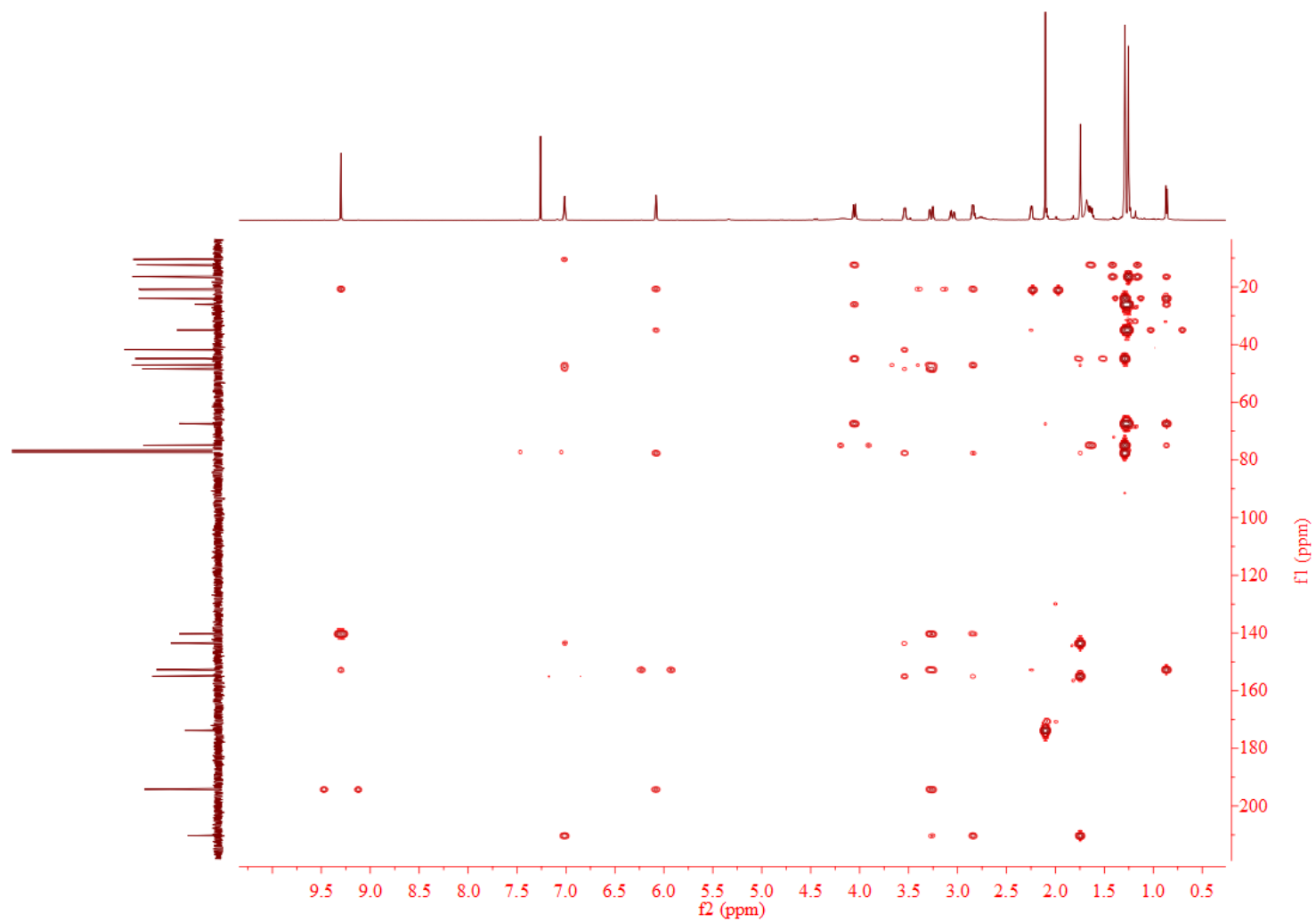
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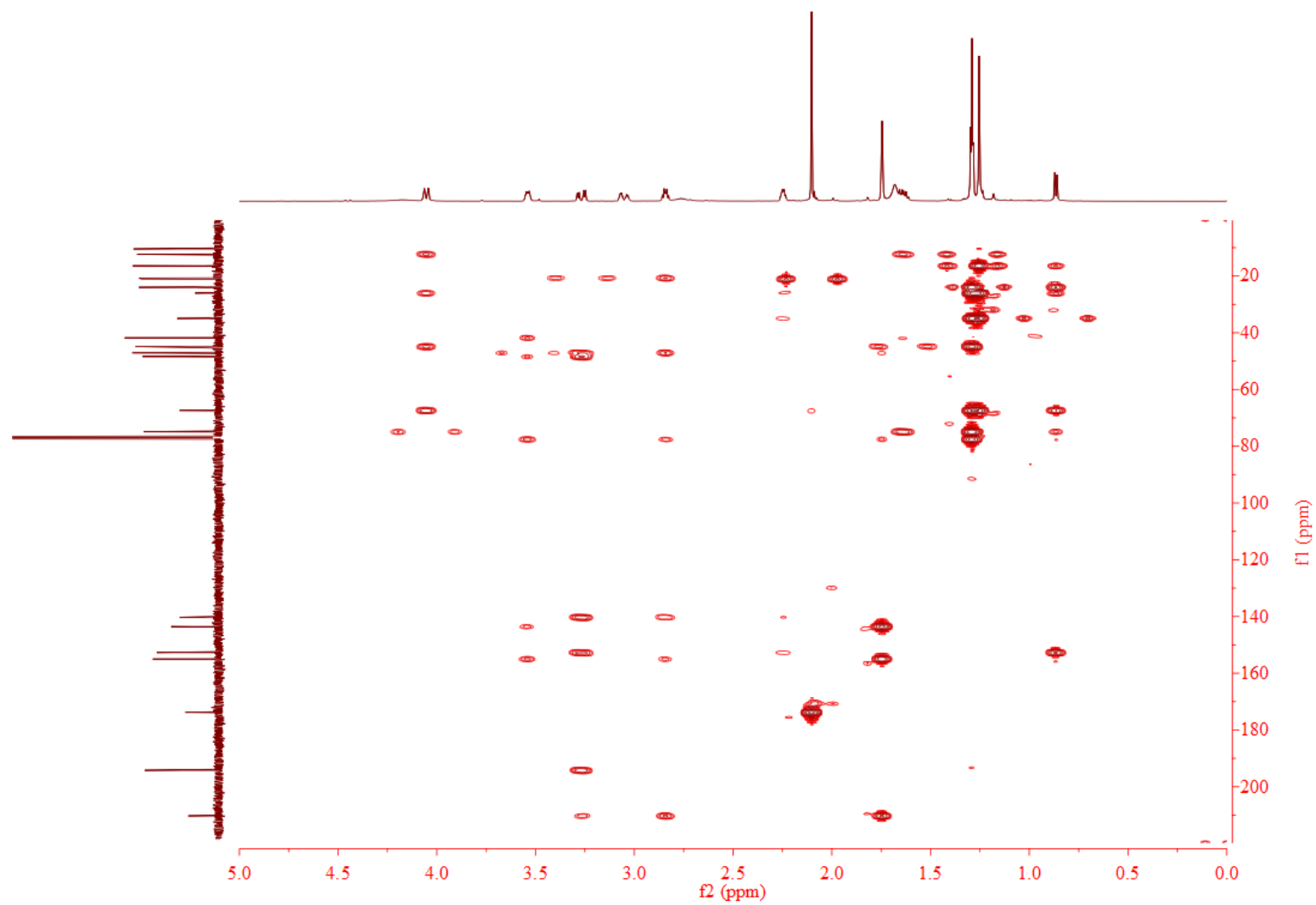
**Figure S8:** HSQC spectrum of compound **1**

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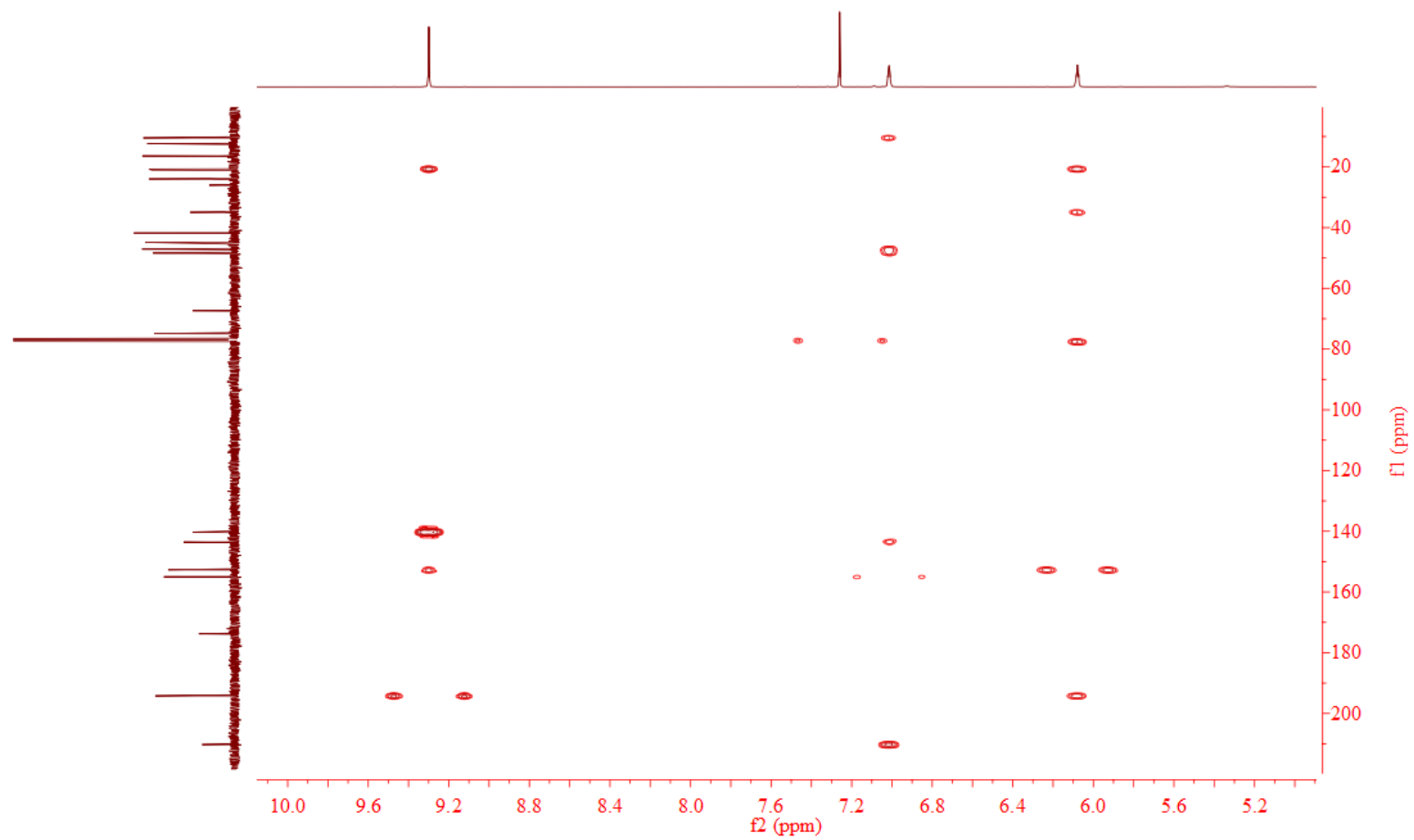
**Figure S9:** HMBC spectrum of compound **1**

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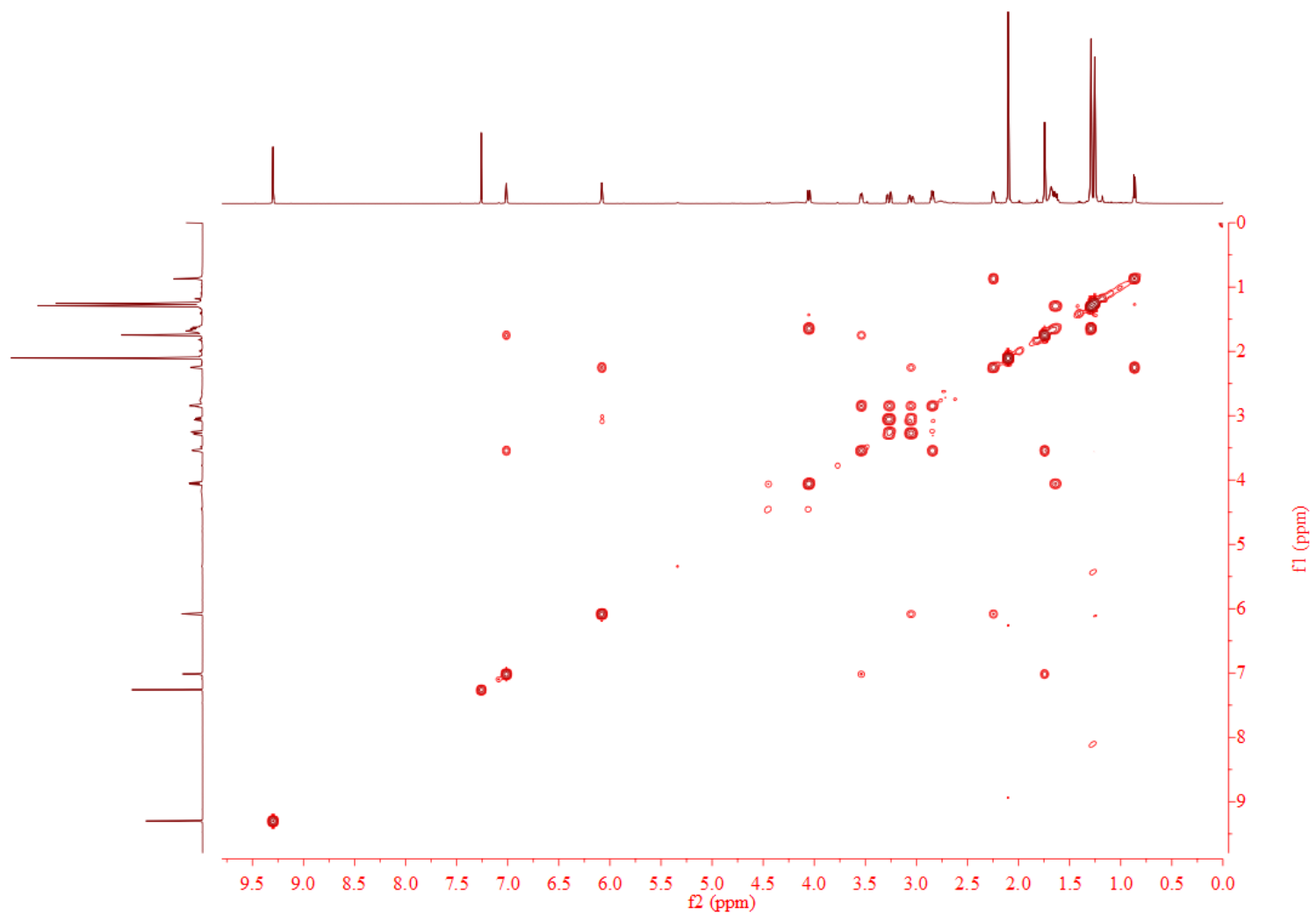
**Figure S10:** HMBC spectrum of compound **1** ( $\delta_{\text{H}}$  0–5 ppm)

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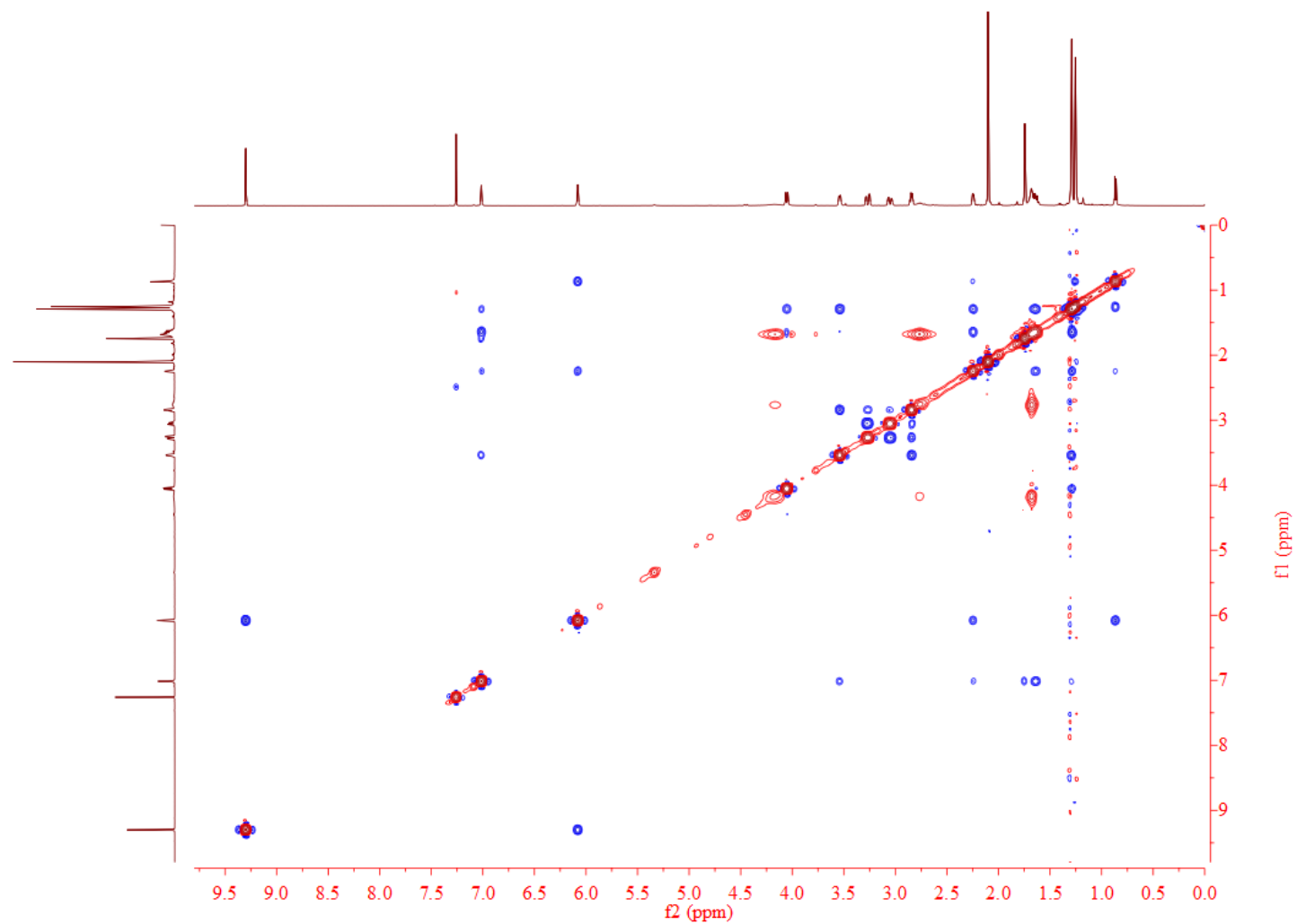
**Figure S11:** HMBC spectrum of compound **1** ( $\delta_{\text{H}}$  5–10 ppm)

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

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**Figure S13:** NOESY spectrum of compound **1**

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The complete crystallographic data of **1** were deposited at the Cambridge Crystallographic Data Centre (CCDC 2170690).

Bond precision:	C-C = 0.0027 Å	Wavelength=1.54184	
Cell:	a=8.8843(1)	b=9.4628(1)	c=24.2964(3)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2042.61(4)	2042.61(4)	
Space group	P 21 21 21	P 21 21 21	
Hall group	P 2ac 2ab	P 2ac 2ab	
Moiety formula	C22 H28 O6	C22 H28 O6	
Sum formula	C22 H28 O6	C22 H28 O6	
Mr	388.44	388.44	
Dx, g cm <sup>-3</sup>	1.263	1.263	
Z	4	4	
Mu (mm <sup>-1</sup> )	0.748	0.748	
F000	832.0	832.0	
F000'	834.68		
h,k,lmax	11,12,30	11,11,30	
Nref	4416[ 2531]	4323	
Tmin,Tmax	0.874,0.928	0.795,1.000	
Tmin'	0.799		
Correction method=	# Reported T Limits: Tmin=0.795 Tmax=1.000		
AbsCorr =	MULTI-SCAN		
Data completeness=	1.71/0.98	Theta(max)= 78.875	
R(reflections)=	0.0312( 4214)	wR2(reflections)=	
S =	1.050	0.0824( 4323)	
Npar=	261		

**Figure S14:** X-ray crystallographic data of compound **1**